Acta Crystallographica Section F
Structural Biology and Crystallization Communications
ISSN 1744-3091

Detection and analysis of unusual features in the structural model and structure-factor data of a birch pollen allergen

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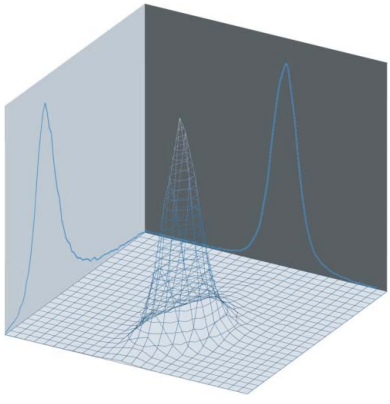
Received 12 January 2012
Accepted 24 February 2012

Physically improbable features in the model of the birch pollen structure Bet v 1d (PDB entry 3k78) are faithfully reproduced in electron density generated with the deposited structure factors, but these structure factors themselves exhibit properties that are characteristic of data calculated from a simple model and are inconsistent with the data and error model obtained through experimental measurements. The refinement of the 3k78 model against these structure factors leads to an isomorphous structure different from the deposited model with an implausibly small R value (0.019). The abnormal refinement is compared with normal refinement of an isomorphous variant structure of Bet v 1l (PDB entry 1fm4). A variety of analytical tools, including the application of Diederichs plots, $R\sigma$ plots and bulk-solvent analysis are discussed as promising aids in validation. The examination of the Bet v 1d structure also cautions against the practice of indicating poorly defined protein chain residues through zero occupancies. The recommendation to preserve diffraction images is amplified.

1. Introduction

During a routine search of the public *PDB_REDO* database (Joosten *et al.*, 2011) for a crystal structure model of birch pollen protein Bet v 1, a significant discrepancy between the originally reported R values ($R_{\rm free}$ = 0.298, $R_{\rm work}$ = 0.274) and the conservatively re-refined structure of PDB entry 3k78 (Bet v 1d) was detected (0.177, 0.126). These R values are unexpectedly low for a 2.8 Å structure. At the same time, the electron-density map provided by the Uppsala Electron Density Server, EDS (Kleywegt *et al.*, 2004), publicly accessible through the PDBe (Velankar *et al.*, 2010), shows numerous side chains that do not fit the experimental electron density. The EDS service also reported a negative bulk-solvent contribution B factor and a negligibly small bulk-solvent contribution scale factor, which is abnormal for an experimentally determined protein structure (Fokine & Urzhumtsev, 2002). Given the fact that the R values calculated by *PDB_REDO* from the data without refinement (0.265, 0.275; a new $R_{\rm free}$ set was calculated by *PDB_REDO*) agreed reasonably well with the values reported in the PDB header (0.298, 0.273), an accidental swap of experimentally observed structure factors F(obs) against the final calculated structure factors F(calc) when generating the deposited structure-factor file can be excluded (in that case also the reproduced R values without refinement would be improbably low). In view of these discrepancies it seemed sensible to re-examine the 3k78 model and the associated deposited diffraction data.

The crystal structure model of birch pollen hypoallergen Bet v 1d (Zaborsky *et al.*, 2010), PDB code 3k78, was reported as solved by molecular replacement (MR) from the nearly sequence identical model of the hypoallergenic isoform Bet v 1l (Marković-Housley *et al.*, 2003), PDB entry 1fm4. The model structures are isomorphous ($P2_1$) with cell constants identical within experimental error. 1fm4 itself was derived by MR from the $C222_1$ structure model of the clinically important inhalant major allergen, Bet v 1a (Gajhede *et al.*, 1996; PDB entry 1bv1). A sequence alignment including additional information relevant to the following discussion is provided in Fig. 1.



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BETV1A P15494 1BV1 MGVFNYETET TSVIPAARLF KAFILDGDNL FPKVAPQAIS SVENIEGNGG PGTIKKISFP  60
BETV1L P43185 1FM4 MGVFNYETEA TSVIPAARMF KAFILDGDKL VPKVAPQAIS SVENIEGNGG PGTIKKINFP  60
BETV1D P43177 3K78 MGVFNYEIET TSVIPAARLF KAFILDGDNL VPKVAPQAIS SVENIEGNGG PGTIKKINFP  60
                   ******* *: ********:* ********:* .********* ********** *******.**

BETV1A P15494 1BV1 EGFPFKYVKD RVDEVDHTNF KYNYSVIEGG PIGDTLEKIS NEIKIVATPD GGSILKISNK 120
BETV1L P43185 1FM4 EGFPFKYVKD RVDEVDHTNF KYNYSVIEGG PVGDTLEKIS NEIKIVATPD GGCVLKISNK 120
BETV1D P43177 3K78 EGFPFKYVKD RVDEVDHTNF KYNYSVIEGG PVGDTLEKIS NEIKIVATPD GGCVLKISNK 120
                   *****:**** ********** :********* :********* ***:****** **.:******

BETV1A P15494 1BV1 YHTKGDHEVK AEQVKASKEM GETLLRAVES YLLAHSDAYN  160
BETV1L P43185 1FM4 YHTKGNHEVK AEQVKASKEM GETLLRAVES YLLAHSDAYN  160
BETV1D P43177 3K78 YHTKGNHEVK AEQVKASKEM GETLLRAVES YLLAHSDAYN  160
                   *****:***: *:***:**:** ********** **********
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Figure 1
Sequence alignment of Bet v 1 allergens. The yellow codes indicate sequence differences between search model 1fm4 and 3k78, while the red highlights indicate nine residues that contain zero occupancy atoms in both models, 1fm4 and 3k78, although at different atoms as detailed in the text and summarized in Fig. 8. Alignment by *ClustalW* (Larkin *et al.*, 2007).

The 3k78 model was refined against structure factors with 2.8 Å resolution, and 1fm4 was refined at 2.0 Å. Both structures appear unremarkable (in a technical sense, no insult to biological relevance intended), and the refinement statistics and protocols reported in the PDB entries are appropriate for the resolution. However, on closer inspection, both the model and the structure-factor data of 3k78 exhibit highly unlikely, physically improbable (if not impossible) features. For reference, the results of the 3k78 analysis and re-refinement are compared with those obtained for the isomorphous 1fm4 structure of good and reproducible quality. This comparison may provide useful reference for the aspiring crystallographer and can serve as teaching material.

2. Structure models and re-refinement

The two models were originally refined using different programs, *CNS* 1.0 (Brünger *et al.*, 1998), and *REFMAC*5 (Murshudov *et al.*, 1997, 2011; Winn *et al.*, 2001), with different refinement protocols. To aid comparison, a common isotropic *B*-factor refinement protocol with *REFMAC* was used in both cases, with parameters adjusted appropriate to each refinement.

The mmCIF structure-factor files and PDB coordinate files were downloaded from the PDBe (Velankar *et al.*, 2010). Structure-factor files were converted into mtz files using the programs of the *CCP*4 suite (Winn, 2003; Winn *et al.*, 2011) through the *CCP*4*i* user interface (Potterton *et al.*, 2003). The original $R_{\rm free}$ data sets were kept (except in an additional refinement of 3k78 for graphing purposes discussed in §3). Original maximum-likelihood maps were computed *via* *REFMAC* (zero cycles) with automated weighting from original coordinates and structure factors, and in case of 3k78 also the TLS parameters were read in from the deposited coordinate file. The procedures for analysis of the structure-factor data are provided in §3.

The common *REFMAC* protocol included isotropic individual *B* factors, flat bulk-solvent model (Jiang & Brünger, 1994), and riding H atoms were used in these refinements. The *REFMAC* X-ray matrix weight (Murshudov *et al.*, 2011) and *B*-factor restraint weights were manually adjusted by monitoring the negative cross-validation log-likelihood ($-{\rm LL}_{\rm free}$) minimum at convergence (Tickle, 2007).

2.1. Coordinates and model 1fm4

The coordinate file of the Bet v 1l search model, 1fm4, reveals no unusual features. The PDB file contains residues 2–160 of the sequence, but the residue numbers in the coordinate file are decremented by 1 compared to the aligned sequences in Fig. 1. As specified in REMARK 480, occupancies for the surface exposed, terminal side-chain atoms of Lys28, Lys65, Lys80, Lys103, Lys129, Glu131, Gln132, Lys134 and Lys137 are set to zero (§4, Fig. 8). Zero side-chain occupancies usually indicate that the side chains were poorly defined in electron density owing to displacement such as disorder or multiple conformations, and instead of accepting the correspondingly high displacement parameters or *B* factors from the refinement, the occupancies of such atoms are manually set to zero. While still common practice, such is not necessarily the best way to indicate the limited knowledge of their actual position (*c.f.* discussion in §4).

2.2. Re-refinement of 1fm4

Progress in the methodology of macromolecular refinement has led to steady improvements of the programs, and major efforts to re-refine already deposited PDB models have been undertaken in the *PDB_REDO* effort (Joosten *et al.*, 2011). In this work, the purpose of re-refining the already good 1fm4 structure is not to generate a better model (which ultimately would also require some minor rebuilding) but to provide a benchmark for the applied procedure and an example of the characteristics of a well refined model in order to appreciate the abnormal refinement of 3k78.

1fm4 was already well refined with *CNS*1.0 about a decade ago. During the multiple weight adjustment runs *REFMAC* reached stable convergence after about 30 cycles, with a resolution-typical X-ray matrix weight of 0.2 and restraint weight σs for *B*-factor main-chain 1–2, 1–3 neighbors and side-chain 1–2, 1–3 neighbors adjusted to 3, 5, 7 and 9 Å^2, which is reasonable given the empirical values (Tronrud, 1996). The re-refined *REFMAC* model differs very little from the original model. The overall coordinate r.m.s.d. between models on all atoms is 0.247 Å and on Cα is 0.078 Å, which is well below the historic value for 100% sequence identity expected from the Chothia and Lesk function (Chothia & Lesk, 1986). No significant geometry improvements resulted during re-refinement, and both 1fm4 and its re-refined model are of good quality. No attempts at model rebuilding were made, which probably could close the slightly increased R–$R_{\rm free}$ gap (Tickle *et al.*, 1998*b*, 2000) compared with the original refinement. A subset of refinement statistics relevant to the structure comparison are compiled in Table 1. Considering the different programs (*CNS*1.0 *versus* *REFMAC*5.6), the differences in protocol, as well as different X-ray and restraint weight optimization, this result is quite reassuring and attests to the reproducibility of crystallographic refinement.

The *B* factors of the previously 'unoccupied' side-chain atoms with reset occupancy refined as expected to high *B* factors, and the inspection of the electron density of these residues in *COOT* (Emsley *et al.*, 2010) shows the corresponding and increasing weakening of density along the side-chain terminals (§4, Fig. 9). Apart from polishing the model '*ad tedium*' (the term originally being coined by Phil Evans), the well refined 1fm4 model remains fully valid even

Table 1
Selected refinement statistics.

Statistics for 1fm4 and its re-refinement are normal. The values highlighted in bold for the 3k78 re-refinements are unusual or highly improbable given the 2.8 Å resolution. They include too low overall *B* factor; no bulk-solvent contributions; absurdly low *R* values; near perfect correlation between observed and calculated structure factors; and atypically high *REFMAC* X-ray matrix weights. n.r. not reported.

	1fm4 deposited	1fm4 re-refined isotropic *B*	3k78 deposited, hybrid TLS	3k78 re-refined, hybrid TLS	3k78 re-refined, isotropic *B*
Space group	$P2_1$	$P2_1$	$P2_1$	$P2_1$	$P2_1$
a (Å)	33.13	33.13	32.97	32.97	32.97
b (Å)	57.23	57.23	57.01	57.01	57.01
c (Å)	38.65	38.65	38.93	38.93	38.93
β (°)	91.94	91.94	92.27	92.27	92.27
Resolution (Å)	28.66–1.97	28.66–1.99†	32.95‡–2.80	25.56–-2.80	25.56–-2.80
Last resolution shell (Å)	2.09–1.97	2.04–1.99	2.87–2.80	2.87–2.80	2.87–2.80
No. of reflections	9658	8659	3184	3184	3184
Atoms of zero occupancy	29	0	29	29	29 at 0.01
Refinement program	*CNS* 1.0	*REFMAC* 5.6.0117	*REFMAC* 5.2.0019 TLS	*REFMAC* 5.6.0117 TLS	*REFMAC* 5.6.0117
Riding H atoms	n.r.	Yes	No	Yes	No
R_{free} set	10% random	10% random	9.8% random§	4.8% random	4.8% random¶
B Wilson (Å^2)	12.2	18.9	45.2	27.6††	27.6††
B mean overall (Å^2)	16.3	18.7	26.8	**3.67**‡‡	15.2
*B*_sol (Å^2), *k*_sol	66.1, n.r.	24.0, 0.37	−10.00, 0.01§§	**−10.00, 0.03**	**No bulk solvent**
R_{free}, overall (last shell)	0.240 (0.388)	0.213 (0.400)	0.298 (0.387)	**0.132 (0.250)**	**0.040 (0.062)**
R-work, overall (last shell)	0.197(0.359)	0.159(0.234)	0.273(0.350)	**0.069 (0.105)**	**0.019(0.048)**
Coordinate e.s.u. from R_{free} (Å)	0.160	0.187	0.379	0.235	**0.072**
Correlation between F_c and F_o		0.962	0.934	0.993	**0.999**
Correlation, F_c and F_o free		0.929	0.919	0.968	**0.997**
Ramachandran regions % (*COOT*)	97.5/2.5/0	97.5/2.5/0	92.2/2.0/5.8	92.2/2.0/5.8	91.0/6.5/2.6
R.m.s.d. bonds (Å)	0.009	0.011	0.017¶¶	0.015	0.011
R.m.s.d. angles (°)	1.30	1.62	1.54¶¶	1.82	1.69
R.m.s.d. all atoms (Å)	0.247	0.247	0.705†††	0.705†††	0.640†††
R.m.s.d. main chain (Å)	0.081	0.081	0.352†††	0.352†††	0.367†††
R.m.s.d. C*α* (Å)	0.078	0.078	0.295†††	0.295†††	0.302†††
X-ray term matrix weight‡‡‡	n.r.	0.2	n.r.	Default	**0.6**
B-factor restraint weight§§§ (Å^2)	n.r.	3/5/7/9	n.r.	Default	5/7/9/11

† Deposited data extend only to 1.99 Å. ‡ This is a reporting error in the PDB header caused by *REFMAC*. Actual low resolution limit is 25.56 Å. § The deposited structure-factor file contains only a 5% cross-validation data set. ¶ A 10% *a posteriori* cross-validation set gives practically the same result. †† From *TRUNCATE*. ‡‡ Residual *B* factors, some atoms show the low *B*-factor cutoff of 2.0 Å^2. §§ From the EDS report. ¶¶ Not including the zero occupancy residues. With zero occupancy residues reset, 0.032 Å and 2.136°. ††† R.m.s.d. against the original 3k78 model. ‡‡‡ In *REFMAC*, the actual X-ray term weight (W_a in *CNS*/*X-PLOR*) is obtained as the product of the user-selectable X-ray matrix weight times the ratio of the trace of the geometry Hessian divided by the trace of the X-ray Hessian matrix. The *REFMAC* X-ray matrix weight is therefore not the same as W_a. Ian Tickle has kindly pointed me to the respective *REFMAC* source code for verification. §§§ *REFMAC B*-factor restraint weight *σ*s (Å^2), for main-chain 1–2, 1–3 neighbors, and side-chain 1–2, 1–3 neighbors.

under different refinement protocols executed nearly a decade later. As stated above, setting the occupancies of side-chain atoms of residues with weak density to zero seems to be unnecessary and could probably be avoided.

2.3. Coordinates and model 3k78

Although the 3k78 Bet v 1d model has five backbone torsion angle outliers and numerous severe geometry deviations in the residues with zero occupancy atoms, it is otherwise unremarkable. The coordinate file of 3k78 contains residues 3–159 of the sequence, with the residue numbers matching the sequence alignment in Fig. 1 (*i.e.* incremented from 1fm4 by 1). However, for the residues containing zero occupancy atoms (Asn29, Lys66, Lys81, Lys104, Lys130, Glu132, Gln133, Lys135 and Lys138) an interesting pattern emerges: the zero occupancies are systematically shifted in atom number to lower values, *i.e.* it is not the terminal side-chain atoms that are unoccupied, but the zero occupancies move towards the C*β*, and even to the (in the PDB file but not physically) adjacent backbone O atoms of the respective residue, while the terminal atoms of the residues become occupied again (§4, Fig. 8). This pattern is physically highly improbable, but no explanation for this selection of zero occupancy atoms has been reported. These physically improbable model features do, however, lead to some interesting features in the electron density of the original refinement (§4, Fig. 9). The substantial bond distance deviations of most of the residues with zero occupancy atoms are listed in §4, Fig. 10. The remaining deviations can be found in the 3k78 PDB header REMARK 500 records or may be generated with RUN500 from *CCP4i*.

2.4. Original refinement of 3k78

The model was originally refined using the *REFMAC* hybrid TLS–isotropic *B*-factor refinement (Painter & Merritt 2006; Murshudov *et al.*, 2011) with a single TLS group. Given the 2.8 Å resolution, hybrid TLS refinement would not be unusual or unreasonable, although a rationale for the choice of protocol, parameterization, and analysis of the (small) TLS contributions is absent (Zaborsky *et al.*, 2010). Original density maps were calculated from unchanged deposited data and coordinates *via* a zero cycle refinement run in *REFMAC* (including the published TLS groups and matrices). The resulting *R* values (0.304, 0.269) were in reasonable agreement with those reported in the PDB header (0.298, 0.273) and by *PDB_REDO* (0.265, 0.275).

When the original coordinate file is loaded into *COOT* (Emsley *et al.*, 2010), difference density peaks > 5*σ* clearly indicate that several residues such as Ile8, Gln37, Glu43, Gly52, Lys56, Glu61, Arg71, Asp110, Glu128, Tyr151 and His155 should be modeled with different conformations (Fig. 2), in agreement with the findings of the EDS service (Kleywegt *et al.*, 2004) which can be readily accessed *via* the PDB validation links. While such modeling errors are not unusual, they can easily be corrected. There was no support for the claim of unidentified density in the core of the molecule made in the 3k78 publication (Zaborsky *et al.*, 2010). Instead, two chemically plausible water molecules included in the model can be discerned in the

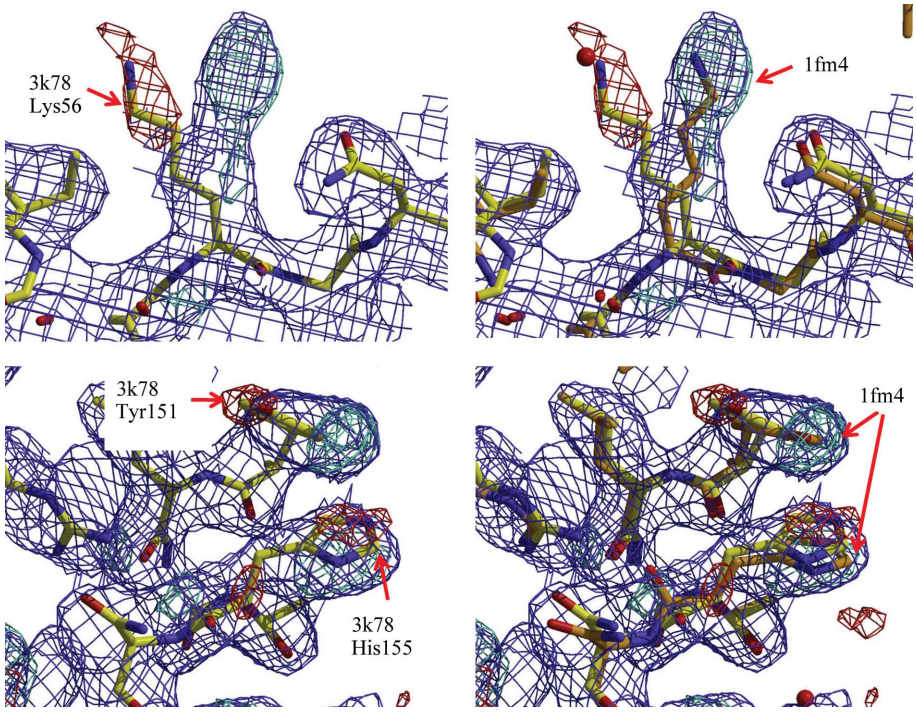


Figure 2
Electron density of original 3k78 model. $2mF_o - DF_c$ electron density contoured at 0.8σ (blue), 5σ $mF_o - DF_c$ difference density (positive light green, negative red). The left panel shows the misplaced residues in the original 3k78 model (yellow carbon stick model) and in the original electron density, reconstructed as described in the text. No refinement has been conducted, but the correct placement of the residues can be easily recognized. The right panels show the same electron density, but now additionally with the starting model 1fm4 (not a re-refined 3k78 model) loaded into *COOT*. The starting model 1fm4 (orange carbon stick model) fits the electron density better than the deposited model, which indicates that the 3k78 model has not been properly refined (or that the structure factors do not match the model).

electron density. Given the relatively high R values and poor geometry of the side chains with zero occupancy atoms in the published model, rebuilding and re-refinement of 3k78 appeared promising.

2.5. Isotropic *B*-factor refinement of 3k78

The original 3k78 coordinates were used without rebuilding (only the zero occupancies were reset to 0.01) for isotropic B-factor refinement. Initially a resolution-appropriate low X-ray matrix weight of 0.1 was used to keep the geometry tight and repair the originally distorted zero-occupancy residues. The same B-factor restraint weights as for 1fm4 (3/5/7/9 Å^2) were used for 30 cycles. The refinement did not reach convergence, but the R values already dropped unexpectedly quickly to 0.131 and 0.068. Inspection of the model geometry showed that the model overall had in fact improved, and maps showed that the misplaced residues Ile8, Gln37, Glu43, Gly52, Lys56, Glu61, Arg71, Asp110, Glu128, Tyr151 and His155 all had assumed correct positions practically identical to those in 1fm4 with good geometry in the remarkably noiseless density map. Nine water atoms from 1fm4 that also occupied density in the 3k78 map were added to the new model by a simple cut and paste.

At that point of the refinement the R values had already reached values typical for atomic resolution structures. Given the negative bulk-solvent B factor of −10 Å^2 and small bulk-solvent scale factor of 0.026 e$^-$ Å^{-3}, no sensible bulk-solvent scattering contribution seemed to be present, and the assumption of calculated structure factors was made. As a consequence, (*a*) the bulk-solvent correction was turned off, (*b*) no riding H atoms were included, (*c*) X-ray matrix weights were increased to 0.6, (*d*) B-factor restraint weights were loosened up to their physically reasonable limit (5/7/9/11 Å^2) as established by empirical values (Tronrud, 1996).

The refinement, with its atypical protocol for any experimental protein structure, reached stable convergence at R values of 0.040 and 0.019, with stable geometry and practically the same target r.m.s.d. values as 1fm4 (Table 1). The resulting density maps were practically noiseless, with the only remaining significant difference density features in the vicinity of the residues with unoccupied side-chain atoms. According to *PROCHECK* (Laskowski, 2001) or RUN500, the entire model had excellent geometry quality. Tedium was declared and no manual rebuilding of the side chains with unoccupied atoms was attempted.

At this point it was clearly established that (*a*) the deposited structure factors are calculated structure factors, (*b*) the resulting re-refined model resembles in most details the mutated search model, (*c*) that the original model has not, or not properly, been refined against these structure factors (or had been altered from a model essentially similar to the re-refined model and after the structure factors had been calculated).

3. Analysis of structure factors

Given the highly improbable refinement results inconsistent with experimental data at 2.8 Å resolution, a closer examination of the deposited structure-factor data was undertaken.

3.1. Intensity statistics and *R*-value analysis

The data for 1fm4 and for 3k78 were collected in-house on rotating anode sources and recorded on imaging plate detectors, with reported

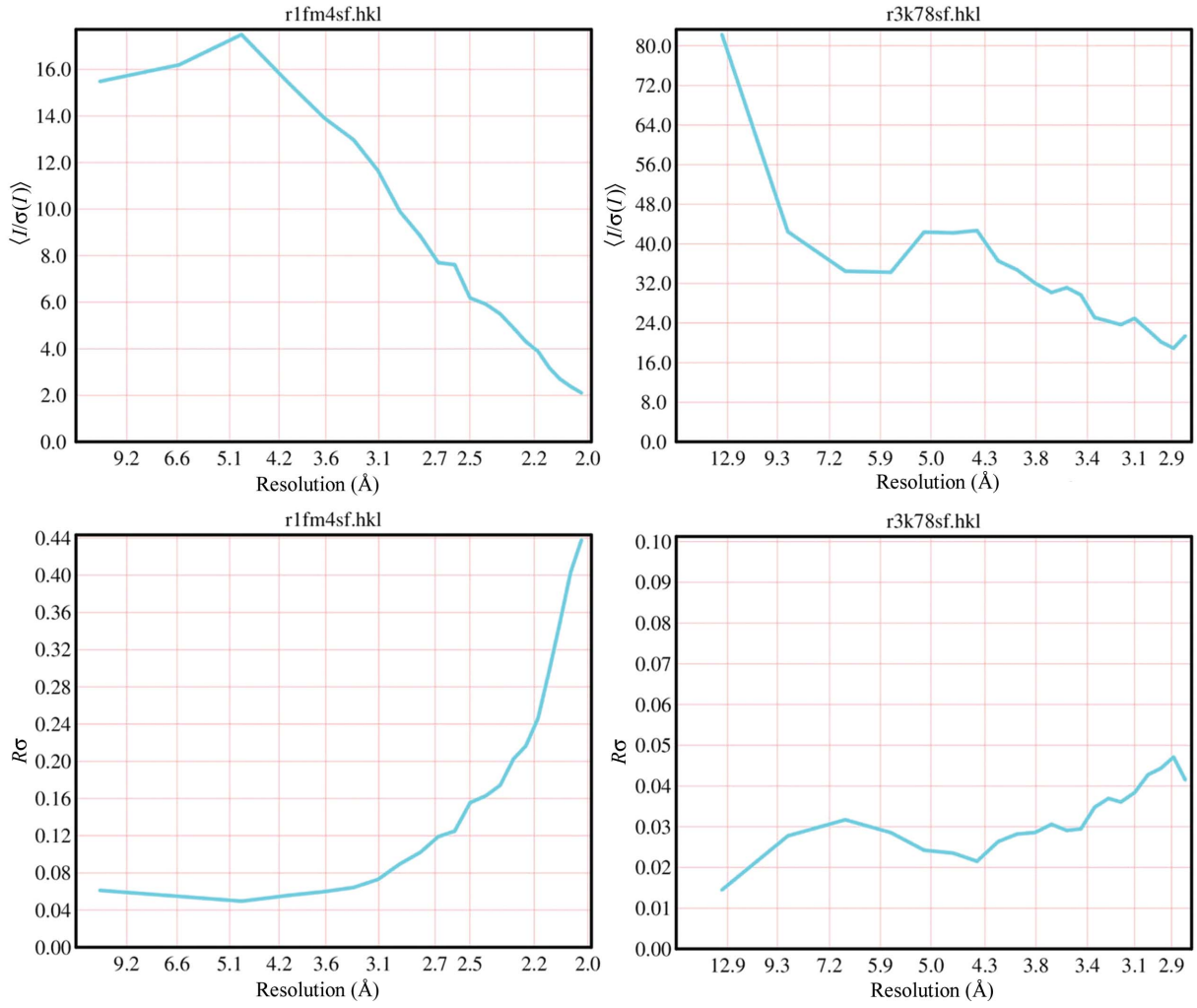


Figure 3
Mean $I/\sigma(I)$ and $R\sigma$ *versus* resolution for 1fm4 and 3k78. The left column shows what can be considered representative statistics for experimental diffraction data (1fm4). The $I/\sigma(I)$ *versus* resolution graphs generally reproduce the trend of the Wilson plots, which are readily available *via TRUNCATE* from the *CCP*4 suite. Note for 3k78 (left column) the abnormally high values of $I/\sigma(I)$ as well as the sharp increase at low resolution, normally not observed with protein structures containing bulk-solvent contributions which supress the strong high-resolution scattering contributions. In the second row, 1fm4 intensities display the normal increase of $R\sigma$ *versus* resolution, and its values are representative of what is expected for a data set that is useful to a mean $I/\sigma(I)$ level of about 2.0 in the highest resolution shell. 3k78 data in contrast show absurdly low values for $R\sigma$ corresponding to the extremely high mean $I/\sigma(I)$ values, with a mean $I/\sigma(I)$ of over 20 in the last resolution shell (*c.f.* Table 2). Figure panels are PostScript plots generated by *XPREP*.

redundancies of 3.3 and 2.1 respectively, and should be comparable. In absence of unmerged intensity data, a *SHELX* (Sheldrick, 2008) format data file was generated from the mtz structure-factor amplitudes, read into *XPREP* (George Sheldrick, Bruker AXS) with HKL3 format option, and converted to intensities following the basic, error-propagation-based F to I conversion (see *e.g.* Rupp, 2009, pp. 328), *i.e.* $I = F^2$, $\sigma(I) = 2F\sigma(F)$.

Table 2
Comparison of key intensity statistics of 1fm4 *versus* 3k78.

Unusual or improbable values are shown in bold. The overall mean $I/\sigma(I)$ of 3k78 is more representative of strong synchrotron data (not in-house data), while the mean $I/\sigma(I)$ in the last (highest) resolution shell is atypically high, indicating that the noise level in the highest resolution shell is improbably low. The maximum $I/\sigma(I)$ is unreasonably high, and the $R\sigma$ is again improbably and atypically low. See also Fig. 3 and Supplementary Table 3(*a*).

XPREP analysis	1fm4	3k78
Unique reflections	9658	3346
$\lvert E^2 - 1\rvert$	0.755	0.773
Resolution range (Å)	28.66–1.99	25.56–2.80
Last resolution shell (Å)	2.09–1.99	2.90–2.80
Redundancy from PDB (all, last)	3.3 (1.9)	2.1 (1.5)
Completeness (all, last)	96.2 (75.9)	92.5 (76.6)
Mean I (all, last)	170.9 (30.3)	59.7 (21.0)
Mean $I/\sigma(I)$ (all, last)	8.16 (2.29)	**31.29 (20.34)**
Max $I/\sigma(I)$	35.9	**615.1**
$R\sigma$ (all, last)	0.092 (0.412)	**0.026 (0.044)**

While the mean I, mean $I/\sigma(I)$, and $R\sigma$ (Schneider & Sheldrick, 2002) values for 1fm4 are typical, the 3k78 data show highly unusual features (Table 2, Supplementary Table 3*b*[1], Fig. 3). The value of $R\sigma$ for validation is based on the fact that it allows computation and assessment of an *a posteriori* $R_{\rm merge}$-like data-quality indicator when unmerged data or images for proper reprocessing are not available owing to the unfortunate absence of a formal obligation to deposit unmerged intensity data or diffraction images. $R\sigma = \sum_{\mathbf{h}} \sigma_{(\mathbf{h})i} / \sum_{\mathbf{h}} I_{(\mathbf{h})i}$ tends to be somewhat lower than the corresponding linear $R_{\rm merge}$. For a discussion of the various merging R values see Diederichs &

[1] Supplementary materials have been deposited in the IUCr electronic archive (Reference: WD5176).

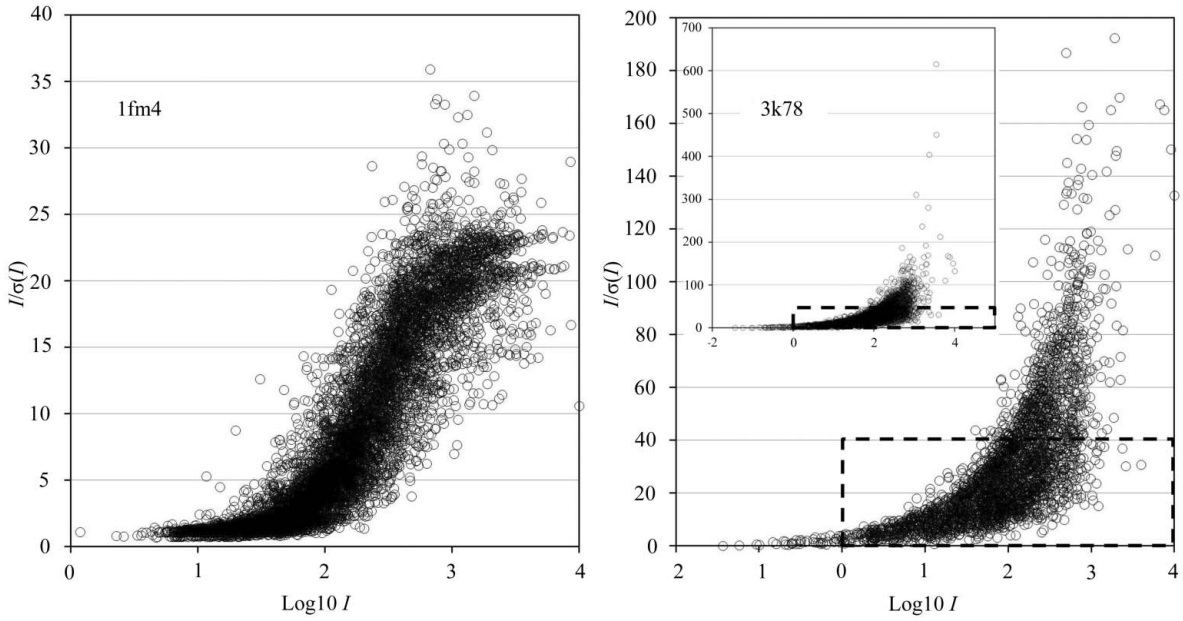


Figure 4
Diederichs plots for 1fm4 and 3k78. The left panel depicts the graph of $I/\sigma(I)$ *versus* log(I) for each unique reflection in the 1fm4 data set. It can be clearly seen that the sigmoid shape of the distribution levels off at around 20 to 30 $I/\sigma(I)$, as established and expected for normal data sets (Diederichs, 2010). In contrast, data for 3k78 show a steady increase to improbable $I/\sigma(I)$ values, indicating that they are not influenced by or do not contain any instrumentation-related measurement errors. The dashed boxes show how the 1fm4 graphs would scale into the 3k78 plots. The insert includes the extreme values for 3k78 which are omitted in the main panel. Note that the original Diederichs plots are based on unmerged intensities (which are not available, but redundancies are comparable between 1fm4 and 3k78). Merged reflections will have $I/\sigma(I)$ values higher by approximately the square root of the redundancy (K. Diederichs, personal communication).

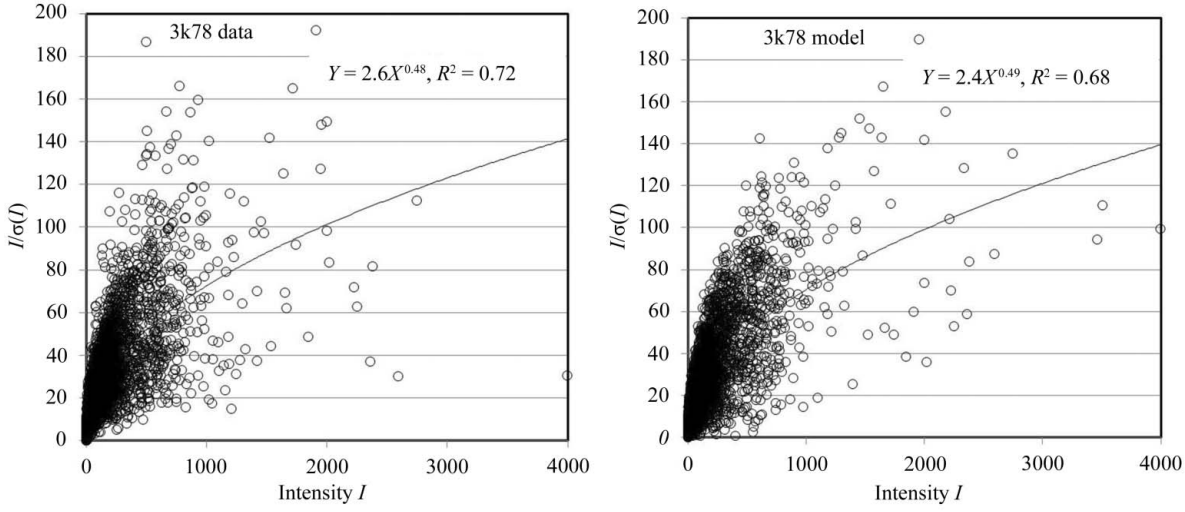


Figure 5
Model of the experimental uncertainties. The left panel depicts the graph of $I/\sigma(I)$ *versus* (I) for the 1fm4 data set (*i.e.*, a subsection of a non-log Diederichs plot). The distribution follows the $I^{1/2}$ *versus* I parabola (a.k.a. power law), indicating that the σs are derived without limiting experimental errors from I(calc) or F(calc). Adding random noise as described in the text yields an error distribution (right panel) that closely resembles that of the deposited data (left panel).

Karplus (1997); Weiss (2001); Rupp (2009); and Einspahr & Weiss (2012).

3.2. Diederichs plots

The improbably low $R\sigma$ values in 3k78 data are caused by a discrepancy between the intensities and their exceptionally low standard uncertainties. In addition to Poisson-statistics-derived counting errors, multiple other sources of instrumental errors limit the achievable signal to noise ratio, that is, $I/\sigma(I)$. This has been investigated in detail (Diederichs, 2010), and Diederichs notes that even with good crystals the $I/\sigma(I)$ ratio of the strongest (unmerged) observations is rarely above 30 even in the lowest resolution shell. It is obvious then, that 'counting statistics are not the limiting factor, as individual reflections may well have many more than 10 000 counts, which would allow $I/\sigma(I)$ ratios of more than 100 and low-resolution R factors of better than 1%' (Diederichs, 2010). The paper also provides multiple plots of $I/\sigma(I)$ *versus* log(I) which show distinct plateaux at around $I/\sigma(I)$ values of about 20 to 30.

In absence of original unmerged intensity data and to account for possible effects of redundancy, the 1fm4 data with a reported overall redundancy of 3.3 and of 3k78 with a redundancy of 2.1 were

compared with the aid of Diederichs plots (Fig. 4). 1fm4 shows the behavior expected for a normal data set, while 3k78 shows extremely high $I/\sigma(I)$ values and completely atypical behavior, and are apparently unlimited by any instrument measurement errors.

The resulting improbably high signal-to-noise ratios in turn indicate that these standard uncertainties are not based on any experimental variances. Some analysis of a possible origin can be provided by examining a non-logarithmic version of the Diederichs plot. A simple power law fit of the deposited data reveals that the signal-to-noise ratio $I/\sigma(I)$ is essentially proportional to the square root of I, which is expected if the $\sigma(I)$ is computed from $I^{1/2}$. An error model closely reproducing the deposited standard uncertainties can be obtained by generating a random error from the absolute inverse cumulative normal distribution around mean zero with a σ of 3.0 *via* the *Excel* NORMINV function, and forming the square root of the product of this random error with I. From these $I/\sigma(I)$ values (Fig. 5), F and $\sigma(F)$ follow again by basic error propagation, with an atypical $\sigma(F)$ distribution very similar to the deposited standard uncertainties. Spreadsheets including the calculations and additional graphs are included in the supplementary material.

3.3. Bulk-solvent content analysis

Proteins contain large fractions of disordered solvent, whose bulk-solvent scattering contributions supress the low-resolution intensities in an experimentally collected protein diffraction data set. The low-resolution structure factors calculated without bulk-solvent contributions should be significantly higher than the observed structure factors, while at the same time the R values for a refinement of a not bulk-solvent-corrected structure should be much higher than for a properly bulk-solvent-corrected structure. Representative graphs and a review of bulk-solvent scattering models can be found in Fokine & Urzhumtsev (2002) and in basic textbooks (*e.g.* Rupp, 2009).

The original cross-validation data set contained only 4.8% of the data (162 reflections), and in the two lowest resolution shells the

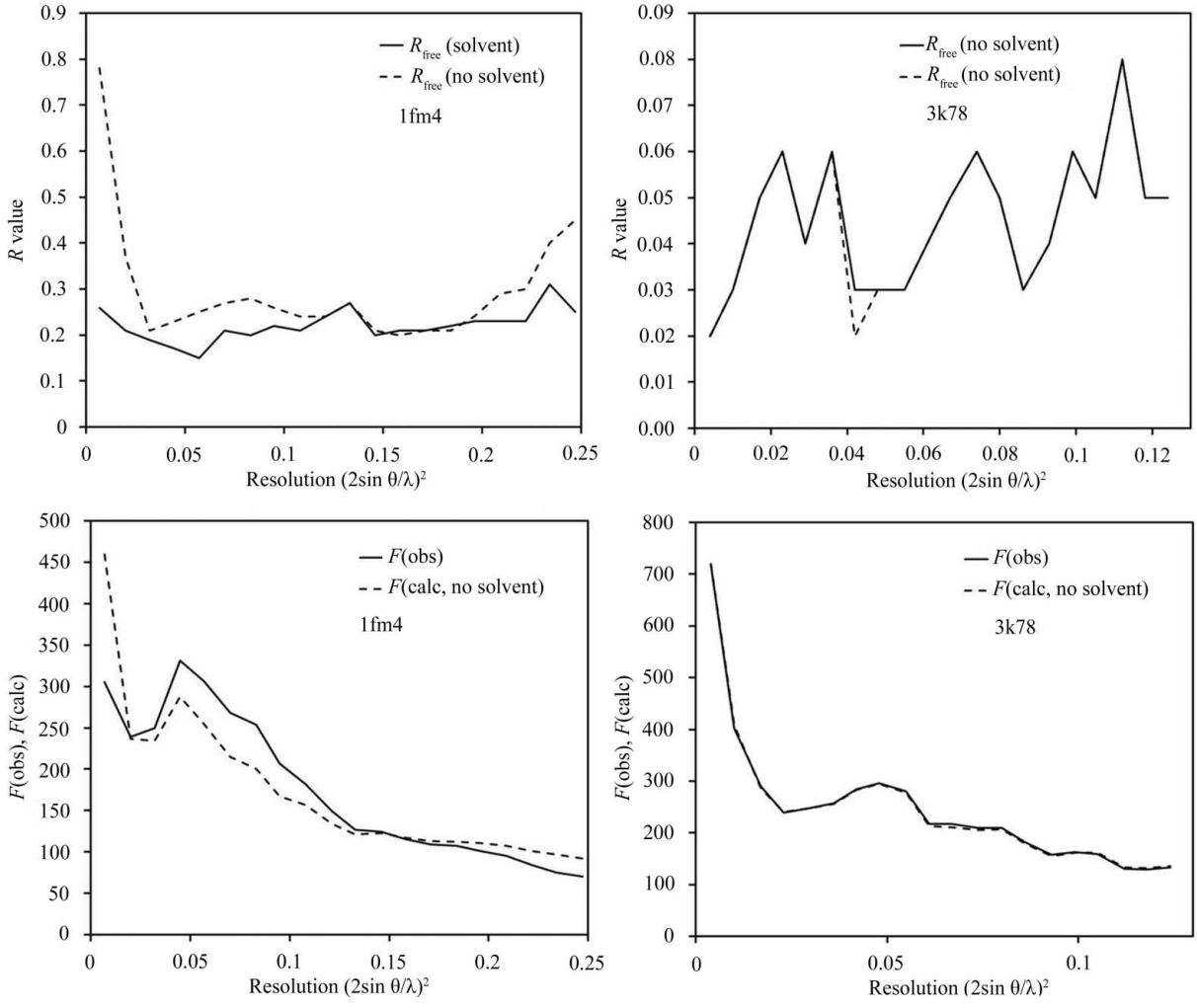


Figure 6
Bulk-solvent contribution analysis for 1fm4 and 3k78. The left panels depict the expected, nearly textbook-like behavior of a normal crystal structure like 1fm4. The top row shows the resolution-dependent behavior of R_{free} when the bulk-solvent correction is included (solid lines) and when it is not included (dashed lines) in the R-value calculation. 1fm4 shows the expected increase of low the resolution R values in the absence of bulk-solvent correction, indicating that bulk-solvent scattering contributions are present in the observed data. Such is not the case for 3k78. Bottom row: the presence of bulk-solvent contributions also causes the low-resolution calculated structure factors (dashed line) to be higher that the observed ones (solid), which are appropriately attenuated by the disordered bulk scattering contributions in 1fm4. There is no difference between F(obs) and F(calc) for 3k78, again indicating the absence of bulk-solvent scattering in the structure-factor data.

original 3k78 data contained no or only one cross-validation reflection, respectively. For the overall data range, the uncertainty in R_{free} (Kleywegt & Brünger, 1996; Tickle *et al.*, 1998*a*) is still acceptable with the low number of crossvalidation reflections, but for plotting in shells the R_{free} count is too low to be of practical value. For plotting, new *a posteriori* R_{free} data (Brünger, 1997) were obtained from new cross-validation data sets with 10% random selection against which the coordinate-perturbed starting model from the first 3k78 isotropic refinement was refined. Even with this suboptimal cross-validation procedure, the isotropic *B*-factor refinements reproduced the same *R* values of around 0.04/0.02. The R_{free} *versus* resolution plots for 3k78 were still noisy but show the same trend as plots from the original cross-validation set, and these data were used in the following analysis.

Structure factors and *R* values were calculated by *REFMAC* with and without bulk-solvent correction from the respective re-refined models of 1fm4 and 3k78. The R_{free} *versus* resolution plots as well as *F*(calc) and *F*(obs) *versus* resolution show expected behavior for 1fm4 consistent with bulk-solvent scattering contributions (Fig. 6). The same plots for 3k78 indicate absence of bulk-solvent scattering contributions in the structure factors, consistent with the negative bulk-solvent correction and trivially small bulk-solvent scale factor reported by *REFMAC* and the EDS report. The R_{free} plot for 3k78 shows the same lack of the strong increase in low resolution *R* value that would be expected for the refinement in the absence of a bulk-solvent correction and resembles the findings for the fabricated C3b structure (Janssen *et al.*, 2007). Given identical *F*(obs) and *F*(calc) without bulk-solvent contribution, logarithmic intensity ratio data plots (not shown) again replicate the situation demonstrated for the C3b structure.

For the purpose of validation, bulk-solvent parameters need to be calculated reliably from the original data. The EDS data at present suffer from some divergences, leading to a multimodal distribution probably caused by certain threshold or limit values for the bulk-solvent parameters. A consistent calculation using the flat bulk-solvent contribution (Afonine *et al.*, 2005; Afonine 2012) model using *phenix.refine* (Adams *et al.*, 2010) provides ∼40 000 valid bulk-solvent contribution *B*-factor–scale-factor pairs. The probability distribution function represented in Fig. 7 is consistent with the earlier published smaller set of data (Fokine & Urzhumtsev, 2002). Entry 3k78, the fabricated entry 2hr0 (Janssen *et al.*, 2007), and two entries that are now updated (1n0q and 1n0r) but contained erroneously deposited calculated structure factors (Mosavi *et al.*, 2002), could be clearly identified as outliers given the distribution in Fig. 7.

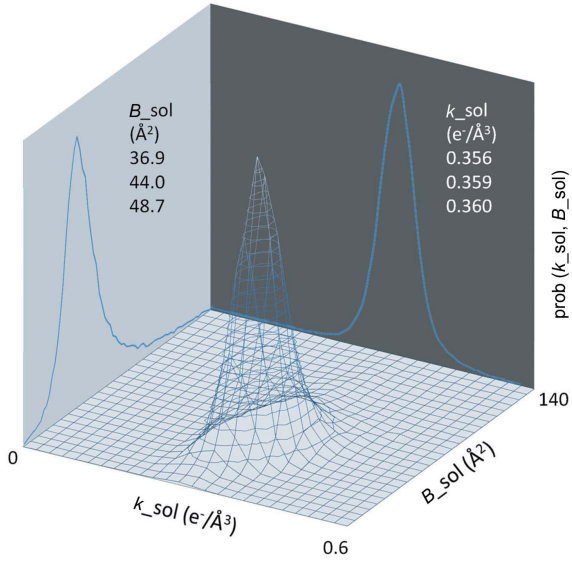


Figure 7
Probability distribution function of bulk-solvent correction parameters. The plot shows the distribution of bulk-solvent parameter pairs (scale factor and *B* factor) calculated from 40 000 PDB entries where valid parameters could be refined using *phenix.refine*. The walls of the plot show the separate distributions of *k*_sol and *B*_sol, with mode, median and mean listed next to the respective graphs. Raw data are included in the supplementary material.

4. Improbable model features caused by zero occupancies

The pattern that the zero occupancy atoms of 3k78 residues (Asn29, Lys66, Lys81, Lys104, Lys130, Glu132, Gln133, Lys135 and Lys138) display seems to be caused by a shift of zero occupancies to atoms with atom numbers decremented consistently by 2. This shift causes the backbone O atoms of the respective residue to become unoccupied, while the terminal atoms of the residues become occupied again (Fig. 8 and Supplementary Table 4*a*). Such errors could be introduced during the preparation of molecular replacement models. In case of experimental structure factors, the electron-density map will indicate the error by positive difference density peaks in place of the atoms missing in the model. In case of 3k78, however, the atom absences propagate into the electron density.

Quite unexpected is that in original 3k78 maps (§2.4) no $2mF_o - DF_c$ density for the unoccupied missing atoms down to near-noise levels below 0.5σ nor difference density the $mF_o - DF_c$ maps is visible for unoccupied atoms, including the backbone O atoms in Lys130, Glu132 and Gln133 (Fig. 9). The weak difference density for Lys135 probably results from incorrect placement. Given the reported typical main-chain *B* factors (∼30–35 Å^2) of the adjacent, covalently connected backbone atoms, this behavior is very unusual and improbable. Following the lysine side chains towards the solvent, there is again clear density for the solvent-exposed C^{ε} and N^{ζ} atoms of the lysine residues, but they are untethered by hydrogen bonds or other contacts. These observations are characteristic of data calculated from a model with zero occupancy atoms.

Setting occupancies of protein atoms that are poorly defined or absent in electron density to zero has very little effect on the overall model quality or refinement itself: zero occupancy as well as a very high *B* factor both lead to respectively zero or negligible scattering contributions, and either will have an insignificant effect on the rest of the model. Inspection of the electron density of the side-chain atoms of residues with reset occupancy in the re-refined 1fm4 model illustrate the fact that such atoms simply refine to high *B* factors and

RES C SSEQ ATOMS 1FM4	RES C SSEQ ATOMS 3K78
LYS A 28 CE NZ	ASN A 29 CB CG
LYS A 65 CE NZ	LYS A 66 CG CD
LYS A 80 CD CE NZ	LYS A 81 CB CG CD
LYS A 103 CD CE NZ	LYS A 104 CB CG CD
LYS A 129 CG CD CE NZ	LYS A 130 O CB CG CD
GLU A 131 CG CD OE1 OE2	GLU A 132 O CB CG CD
GLN A 132 CG CD OE1 NE2	GLN A 133 O CB CG CD
LYS A 134 CG CD CE NZ	LYS A 135 O CB CG CD
LYS A 137 CD CE NZ	LYS A 138 CB CG CD

Figure 8
Zero occupancy atoms in 1fm4 and 3k78. Condensed REMARK 480 from PDB headers. The atoms in 3k78 (right-hand columns) are shifted towards lower atom numbers compared to 1fm4, causing the zero occupancies to progress towards the main chain including the backbone O, and the terminal atoms of the side chain to become occupied again. This situation is physically improbable. See also Supplementary Table 4*a*.

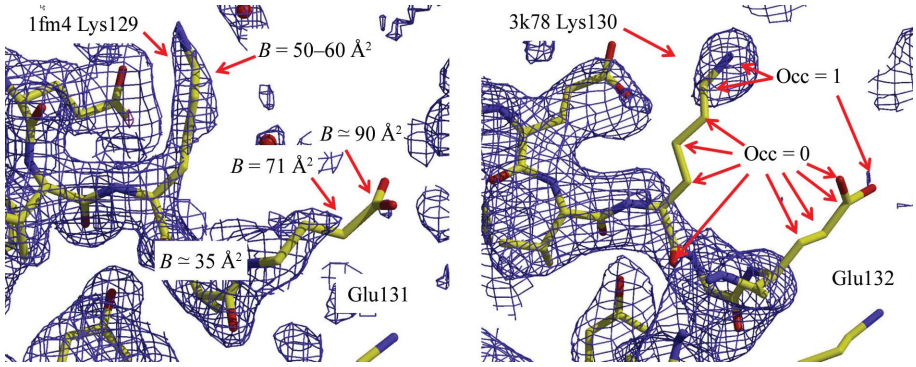


Figure 9
Normal and pathological side-chain density. 2 $mF_o - DF_c$ electron density contoured at 0.8σ. The left panel shows the progressive weakening of electron density owing to displacement of the side-chain atoms, after re-refinement with the originally zero occupancies reset to 1. The *B* factors are restrained against unreasonable increases between subsequent adjacent atoms, and in normal situations show a continuous increase along the side chain. The right panel shows an improbable scenario where atoms that had previously zero occupancies assigned refine to extreme *B* factors at the limit of what the restraints allow and the electron density abruptly disappears, and, in the case of Lys130, abruptly reappears for the terminal C^{ε} and N^{ζ} side chain atoms. This is also true but less visible owing to the stronger main-chain *B*-factor restrains for the Lys130 backbone O atom. These observations provide a first indication that the deposited structure factors do not to contain any contributions from the unoccupied atoms. Note that in some real scenarios the terminal lysine N^{ζ} for example can be tethered through non-covalent interactions with inter- or intra-molecular neighboring residues and become better defined than the remaining hydrophobic side-chain atoms. This is however not the case for Lys130 of 3k78. All density figures were prepared with *XtalView* (McRee, 1999) and rendered by *Raster3d* (Merritt & Bacon, 1997).

Original *WHAT_CHECK* report of 3k78 bond distance violations

102 LYS	(104)	A	CE	NZ	1.64	4.9
119 TYR	(121)	A	CB	CG	1.60	4.1
122 LYS	(124)	A	CB	CG	1.66	4.7
144 ARG	(146)	A	CB	CG	1.65	4.2

WHAT_CHECK report of 3k78 with occupancies reset

27 ASN	(29)	A	CA	CB	1.41	-6.2
27 ASN	(29)	A	CG	OD1	1.01	-11.0
27 ASN	(29)	A	CG	ND2	1.67	16.4
64 LYS	(66)	A	CD	CE	1.68	5.2
79 LYS	(81)	A	CA	CB	1.41	-6.0
102 LYS	(104)	A	CA	CB	1.39	-7.2
102 LYS	(104)	A	CD	CE	1.40	-4.1
102 LYS	(104)	A	CE	NZ	1.64	4.9
119 TYR	(121)	A	CB	CG	1.60	4.1
122 LYS	(124)	A	CB	CG	1.66	4.7
128 LYS	(130)	A	CD	CE	1.32	-6.8
130 GLU	(132)	A	C	O	1.31	4.1
130 GLU	(132)	A	CD	OE2	1.69	23.1
131 GLN	(133)	A	CD	OE1	1.45	11.1
131 GLN	(133)	A	CD	NE2	1.45	5.8
133 LYS	(135)	A	C	O	1.54	15.6
133 LYS	(135)	A	CA	CB	1.35	-8.9
133 LYS	(135)	A	CD	CE	1.37	-5.1
136 LYS	(138)	A	CD	CE	1.24	-9.3
144 ARG	(146)	A	CB	CG	1.65	4.2

Figure 10
WHAT_CHECK report of bond distance violations for 3k78. The last column contains the deviation from known r.m.s. values, expressed in σ levels. Setting atoms to zero occupancies can lead to missing them during model validation and correction. In the case of 3k78, even a backbone atom distance violation of 15.6σ would go undetected (but the PDB validation reports it in REMARK 500).

display correspondingly weak electron density (Fig. 9). Nevertheless, it should be kept in mind that for many cases of local disorder, large isotropic displacement (*B*) factors are not a physically correct description either (Merritt, 2012). A number of other inconsistencies and problems however can be introduced by zero occupancy atoms in the chain of a protein model.

(i) Despite the fact that these unoccupied atoms are not included in the refinement, they do remain in the model but may not be included in the calculation of the r.m.s. deviation from geometry restrain target values listed in the PDB header. Table 1 lists such a discrepancy for 3k78.

(ii) An additional problem caused by the zero occupancies is that geometry validation programs may be misled. For example, *WHAT_CHECK* (Hooft *et al.*, 1996) properly warns of zero occupancy atoms but does not compute their geometry deviations, leaving the corresponding errors unlisted. Fig. 10 demonstrates this scenario for entry 3k78. *MolProbity* (Davis *et al.*, 2007) also excludes atoms with occupancies below 0.02 and also does not report side-chain bond distance and angle violations (J. Richardson, personal communication). However, the PDB validation does include zero occupancy atoms in the preparation of geometry violation statistics for REMARK 480 and 500 (available as RUN500 from the *CCP*4*i* interface).

(iii) Not all display programs recognise zero occupancies, while at the same time the *B* factors of those atoms can be set to an arbitrary, non-representative (often low) value which again may be misinterpreted, or missed in *B*-factor analysis.

5. Conclusions

The findings surfacing during model refinement in §2 and amplified during the structure factor analysis in §3 and the feature propagation discussed in §4 provide consistent and very convincing evidence that (*a*) the structure-factor data deposited for 3k78 are calculated structure factors, (*b*) the resulting re-refined model resembles in most details the mutated search model, (*c*) that the original model has not, or not properly, been refined against these structure factors (or had been altered from a model essentially similar to the re-refined model and after the structure factors had been calculated). Being not refined against the deposited structure factors, the 3k78 model at present at least lacks experimental basis. The findings leading to the above conclusions are summarized below.

(i) The deposited structure factors do not contain any bulk-solvent contribution.

(ii) The noise level of the data is abysmally small and nearly constant over the entire resolution range, consistent with a truncated calculated data set with inappropriate error model.

(iii) The Diederichs plots show almost orders of magnitude higher signal-to-noise ratios than expected for real data, indicative of absence of instrumentation errors in calculated structure factors and in the error model.

(iv) The structure factors deposited for the PDB entry 3k78 are in fact calculated structure factors, and their standard uncertainties are not based on experimental errors.

(v) Because the original refinement against these structure factors gives the same R values as reported or calculated by *PDB_REDO* and in this work, a simple error of swapping the F(obs) and F(calc) columns during data deposition can be excluded.

(vi) The refinement statistics reported in the PDB header are inconsistent with actual refinement against the structure-factor data.

(vii) The model refines against the deposited 2.8 Å data without the need for bulk-solvent correction, no H atoms, atypical X-ray matrix weights, to near-zero R values, compatible only with calculated structure factors.

(viii) The model obtained by re-refinement does not correspond to the deposited model, but is in details closer to the molecular replacement starting model.

(ix) The non-physical zero occupancy residues in the model are faithfully reproduced in the electron density calculated from the deposited structure-factor data, which is inconsistent with experimental data obtained from a real protein structure.

(x) Numerous residues of the original model are not located in their electron density, but return to the exact position of the density when refined. This is consistent with these parts of the re-refined model being manipulated after the structure factors were generated from it.

Each of these points alone is reason for concern, and when combined and evaluated against prior expectations, they leave no doubt that model and data of 3k78 are incompatible and that the deposited structure factors are not based on actual experiments, and their standard uncertainties are not based on experimental errors.

Following basic scientific epistemology, strong and convincing evidence would have to be provided to overcome these doubts (Rupp, 2010). In case of an error during deposition, this should be trivial to achieve, and database integrity could be easily restored. At least an experimental data set which refines to the deposited structure, or unmerged intensity data reprocessed from the original images should be supplied. Most convincing and irrefutably, the presentation of actual diffraction images which produce data representing the deposited model would establish the facts.

6. A few recommendations

Considerable efforts by the PDB validation task force (Read, 2011) will make it much less likely that poorly refined models, models inconsistent with data, or implausible data will enter the public databases. Nevertheless, it remains a fact that – irrespective of the cause of the problem – in the case of 3k78 a calculated data set also incompatible with the associated coordinate entry has been successfully deposited. The example of 3k78 provides a few additional suggestions that might be useful not just for *a posteriori* validation during deposition but also particularly for the aspiring crystallographer during structure refinement.

(i) Diffraction image deposition and archival. The need for preserving diffraction images for scientific reasons has been officially suggested by the IUCr in 2008 (Baker *et al.*, 2008) and a standing IUCr committee on data deposition has been formed in 2011. Although matters of policies and technical issues remain to be resolved, there is little doubt that image deposition is a timely and beneficial practice for scientific reasons. As an additional side-effect, image deposition allowing reprocessing would immediately resolve any questions of data provenance. Successful redeposition of the correct observed structure factors of entries 1n0q and 1n0r (Mosavi *et al.*, 2002), reprocessed form original diffraction images collected a decade ago, clearly demonstrates the value of proper image data archiving.

(ii) Bulk-solvent correction. It would be useful if all refinement programs consistently report the bulk-solvent B factor and also the bulk-solvent scale factor in the REMARK 3 section of the PDB header. Implausible values could be readily detected and corrective action taken already during refinement. The bulk-solvent scale factor actually becomes a more useful measure than the bulk-solvent B factor, particularly at the spurious solvent contents refined from calculated structure factors.

(iii) Setting the occupancy of protein chain atoms to zero as an indication of positional uncertainty is physically not correct. Accepting high B factors (which are not necessarily a correct physical description of substantial disorder either) causes less problems, such as geometry validation programs not including unoccupied atoms in the validation statistics. Isolated backbone zero occupancies are physically not meaningful and should be correspondingly flagged as a serious problem. Side-chain atoms may be absent owing to radiation damage, and in such cases the use of zero occupancies as an indicator could be arguably justified.

(iv) The Diederichs plot (§3.2) seems to be a valuable tool in spotting anomalies in diffraction data, particularly as far as the signal-to-noise ratios, *i.e.* $I/\sigma(I)$ and the instrumentation error model is concerned. Potential for abuse by fitting calculated error models to the sigmoid distribution does exist.

(v) $R\sigma$ (§3.1) can serve as a useful *a posteriori* measure for the plausibility of the error model and signal-to-noise levels in the absence of any merging R values.

(vi) *A posteriori*, the *PDB_REDO* database can be examined for improbably high discrepancies between the originally reported R values and the conservatively re-refined structure of a PDB entry.

(vii) In the absence of image deposition, and as an option requiring no special effort, more refinement data could be deposited. At least the F(calc) set could be submitted in addition to F(obs) to allow easy detection of simple column swapping or other possible deposition mistakes. Even better, the Fourier coefficients for the final electron-density map should be deposited, because this map ultimately represents what the crystallographer was interpreting during model building. EDS can only reconstruct maps from what it is provided with, which presently are only the deposited structure-factor amplitudes and the model coordinates.

Finally, despite all the diagnostics and validation tools available during model building, refinement, and ultimately upon PDB deposition, one needs to recollect that not the PDB but the individual crystallographer bears the final – and sometimes far reaching (Petsko, 2007) – responsibility for the correctness of the deposited model.

I wish to anonymously acknowledge several colleagues who provided critical comments and detailed information about the refinement and data analysis programs used in this work. Ed Pozharski extracted raw data from the EDS database. P. Afonine computed bulk-solvent contributions with an improved bulk-solvent parameter implementation in *phenix.refine*. Reviewers have pointed out a number of didactical and presentational improvements to the

manuscript. The *REFMAC* command script, the input files, and the results for the isotropic *B*-factor refinement of 3k78 as well as the *XPREP* data analysis and bulk-solvent data are deposited as supplementary materials. The hyperlink to *PDB_REDO* of 3k78 is http://www.cmbi.ru.nl/pdb_redo/k7/3k78/index.html, for the EDS report http://eds.bmc.uu.se/cgi-bin/eds/uusfs?pdbCode=3k78, and the electron density can be loaded *via* the EDS link to the *ASTEX Viewer* at http://eds.bmc.uu.se/cgi-bin/eds/eds_astex.pl?infile=3k78&centre=A61.

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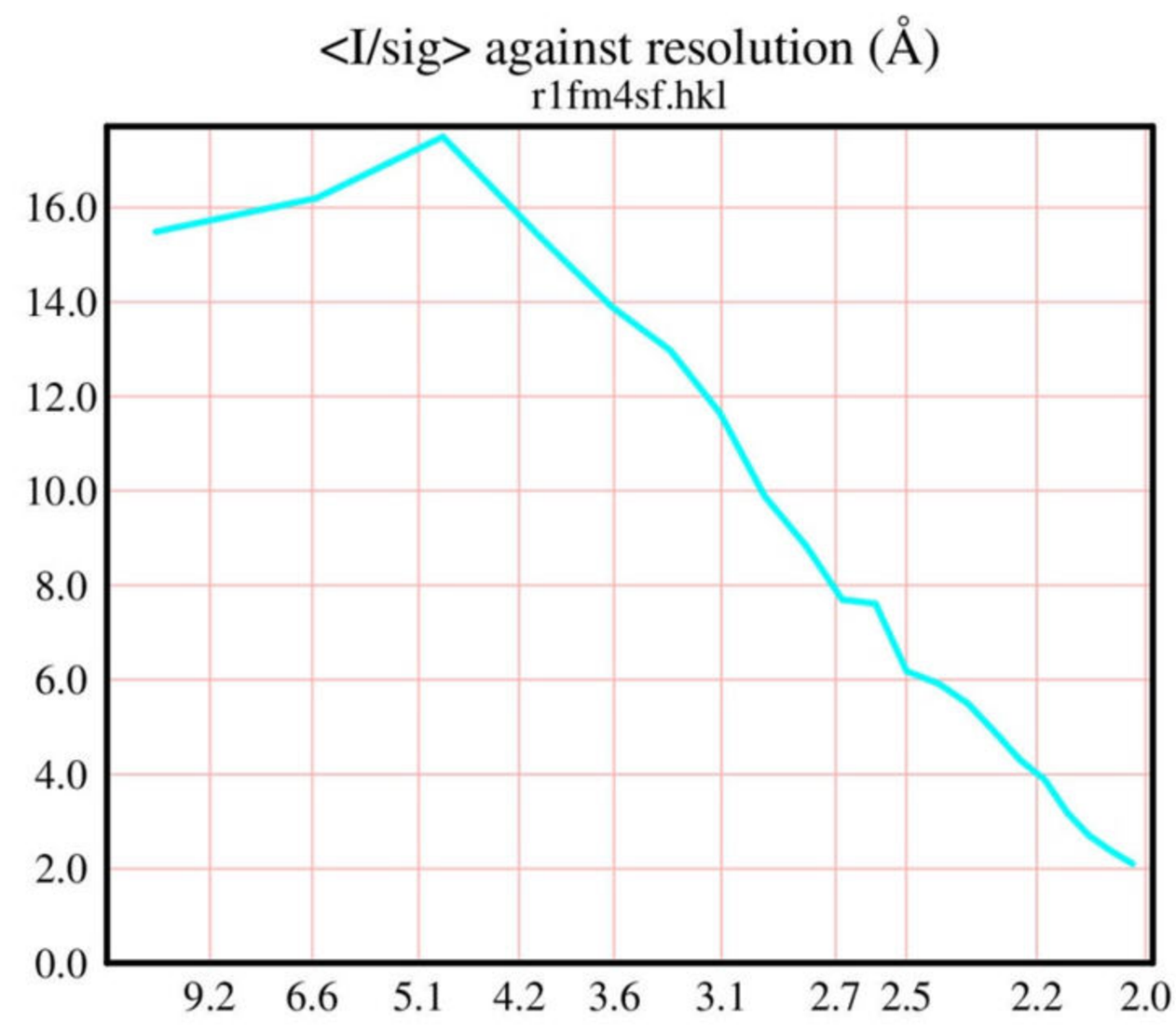
3K78
LYS56

1FM4

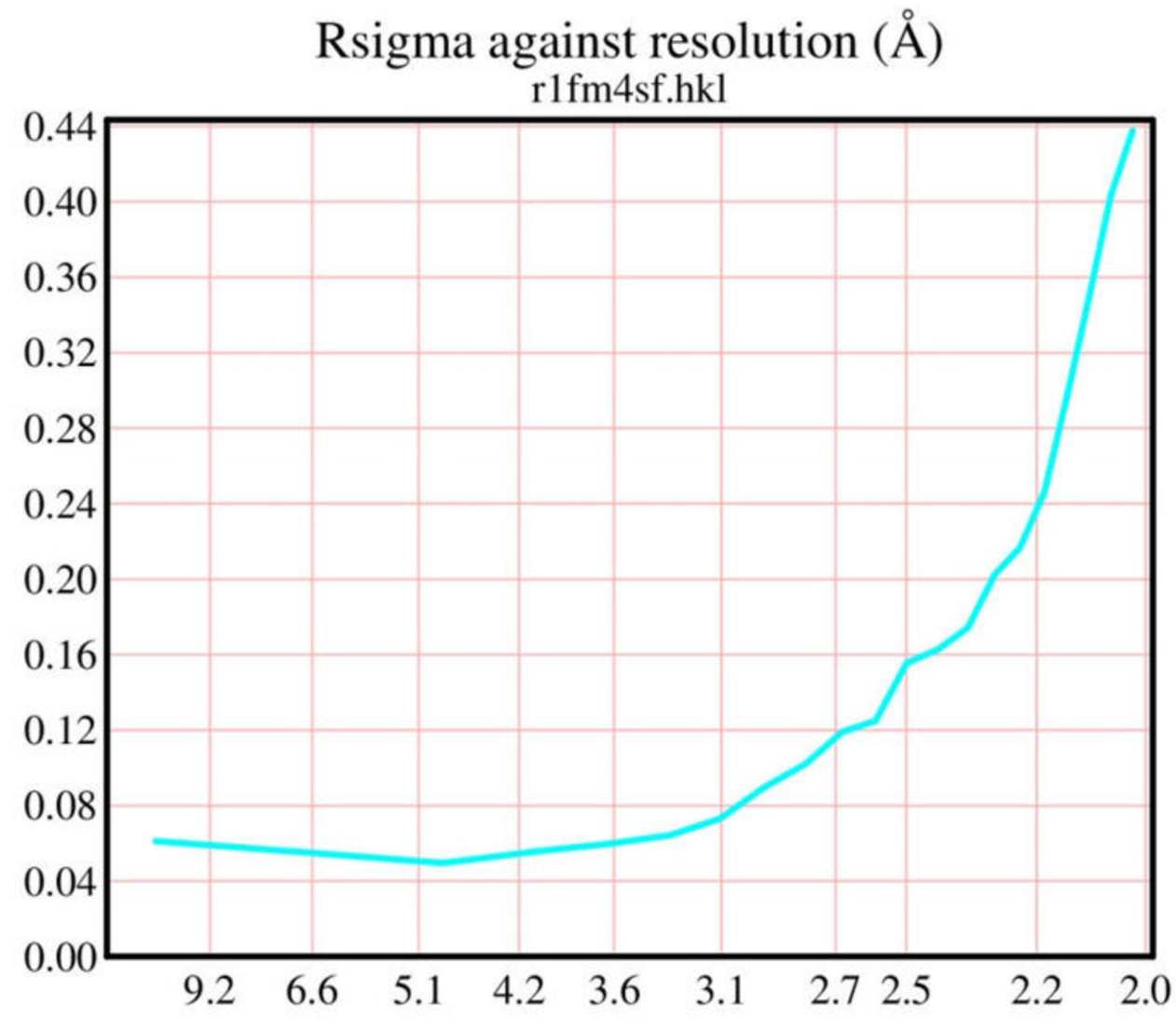
3K78
TYR151

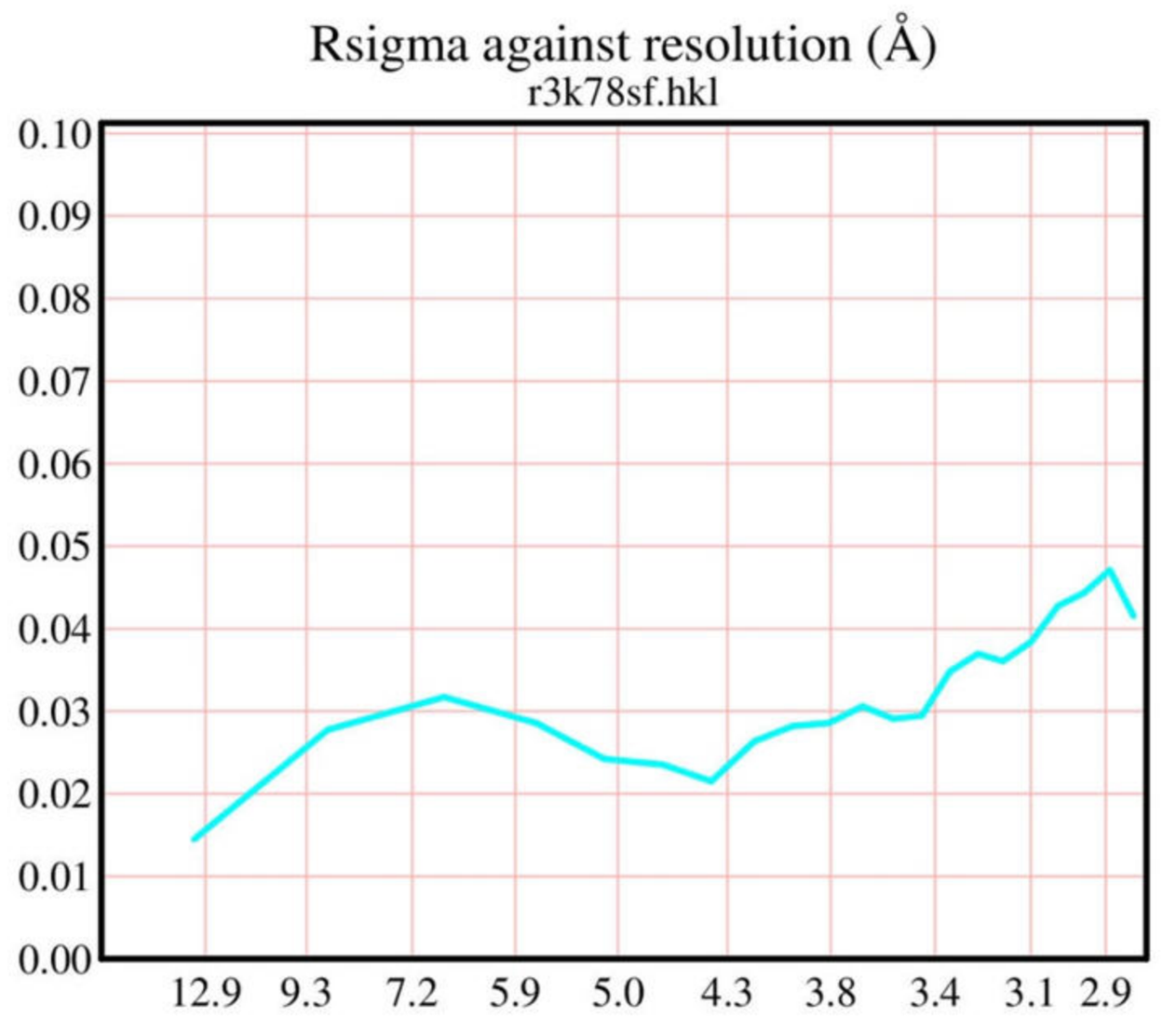
3K78
HIS155

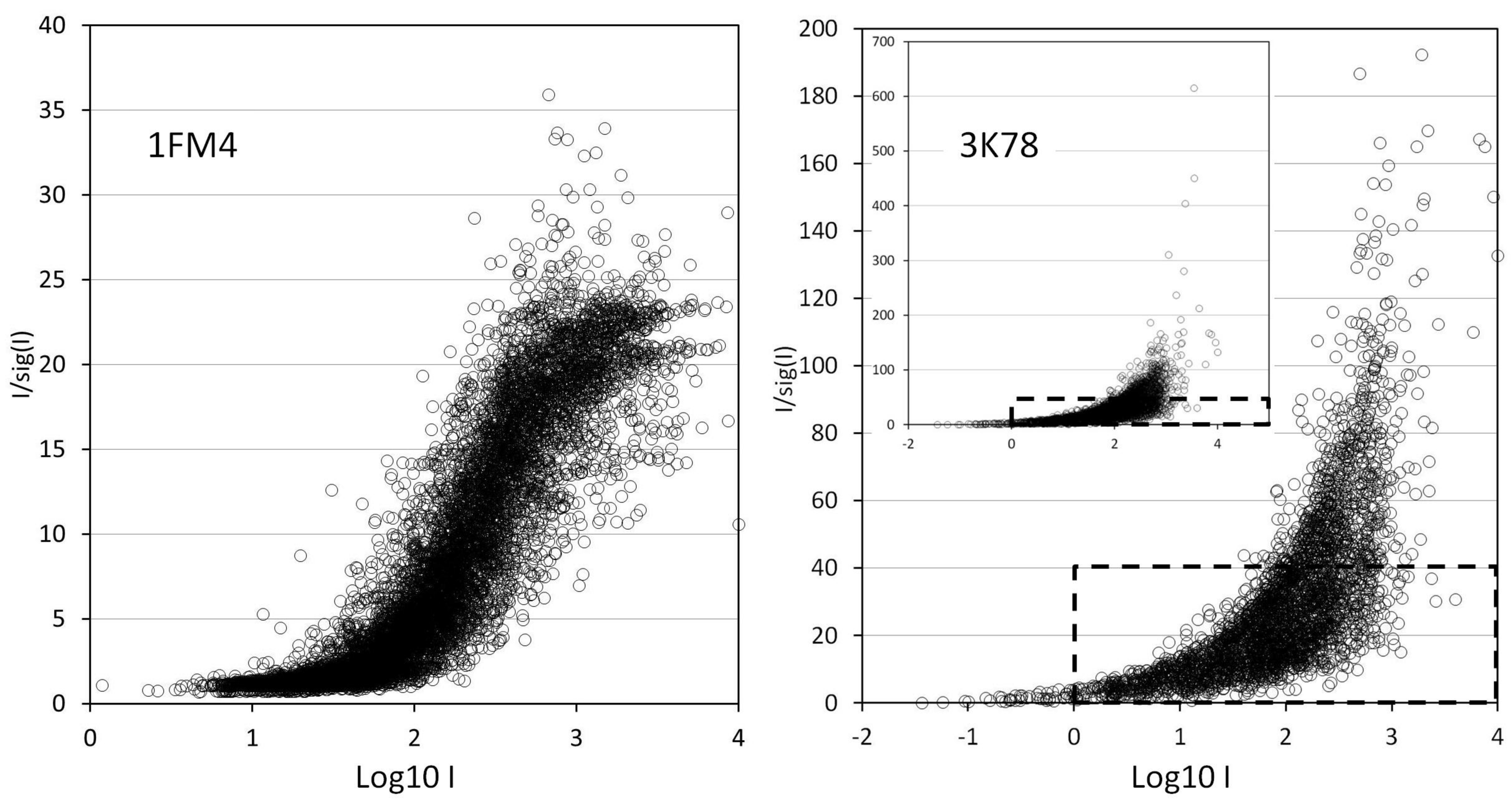
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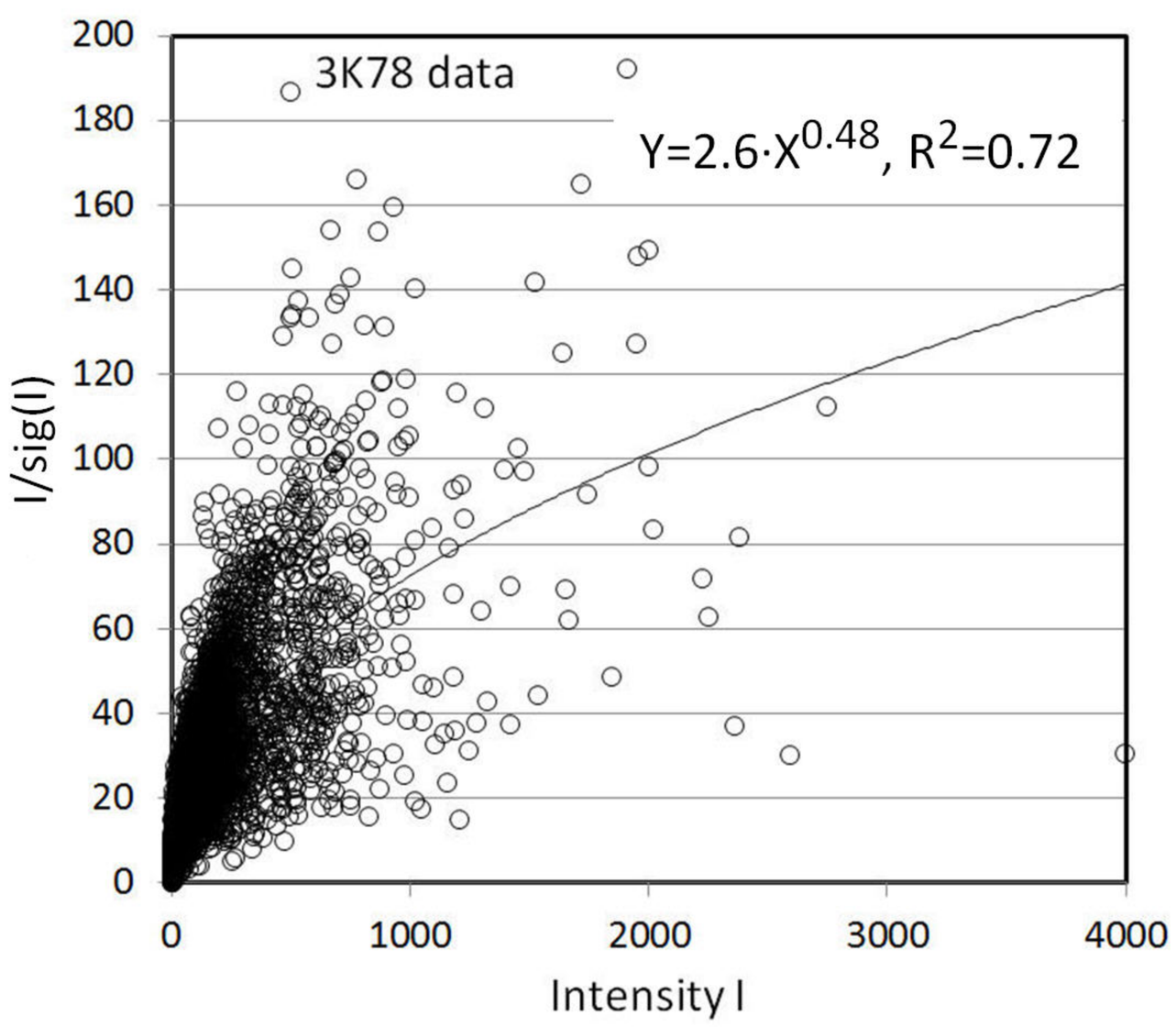

<I/sig> against resolution (Å)
r1fm4sf.hkl
16.0
14.0
12.0
10.0
8.0
6.0
4.0
2.0
0.0
9.2
6.6
5.1
4.2
3.6
3.1
2.7
2.5
2.2
2.0

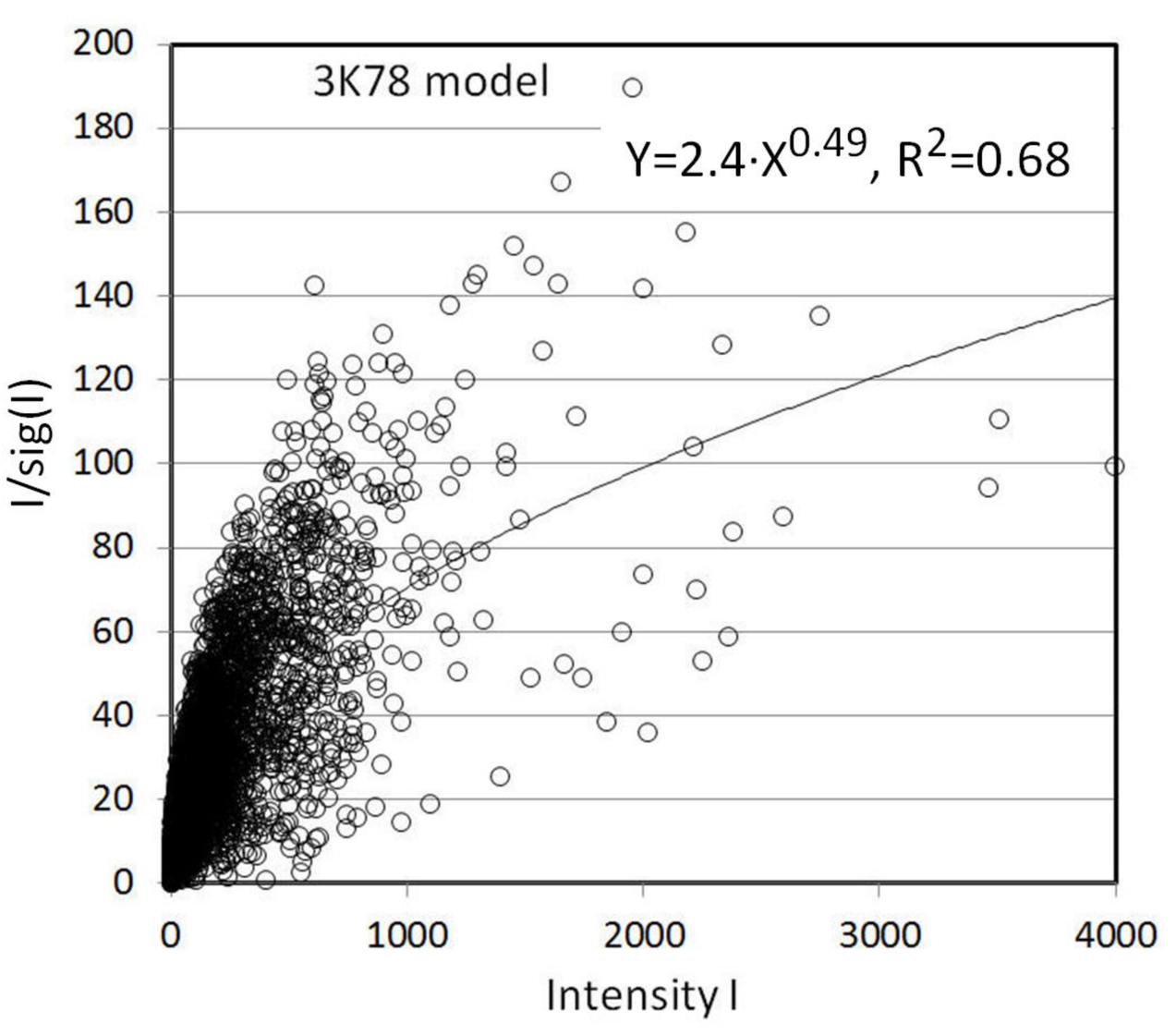

<I/sig> against resolution (Å)
r3k78sf.hkl
80.0
72.0
64.0
56.0
48.0
40.0
32.0
24.0
16.0
8.0
0.0
12.9
9.3
7.2
5.9
5.0
4.3
3.8
3.4
3.1
2.9

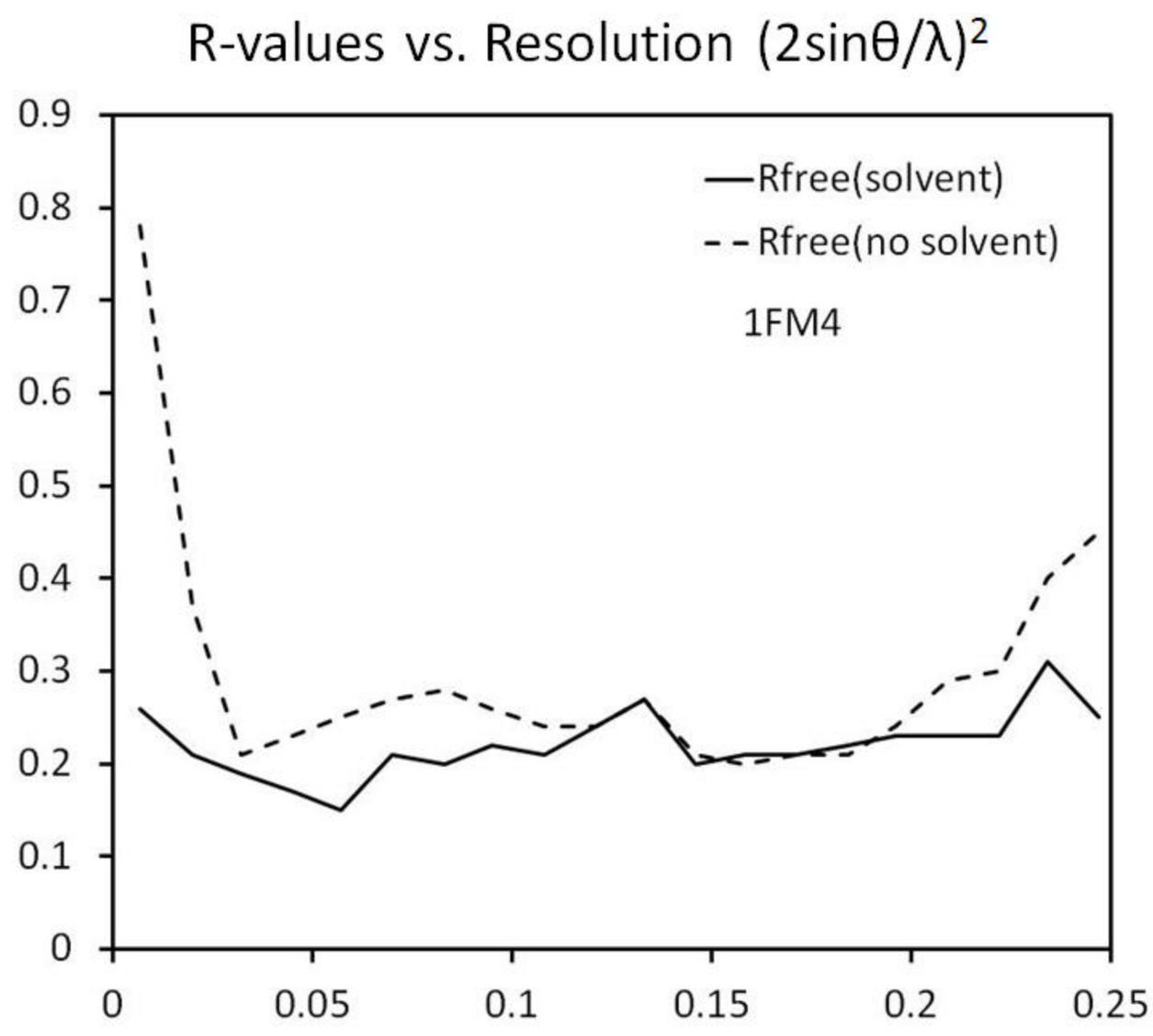

Rsigma against resolution (Å)
r1fm4sf.hkl
0.44
0.40
0.36
0.32
0.28
0.24
0.20
0.16
0.12
0.08
0.04
0.00
9.2
6.6
5.1
4.2
3.6
3.1
2.7
2.5
2.2
2.0

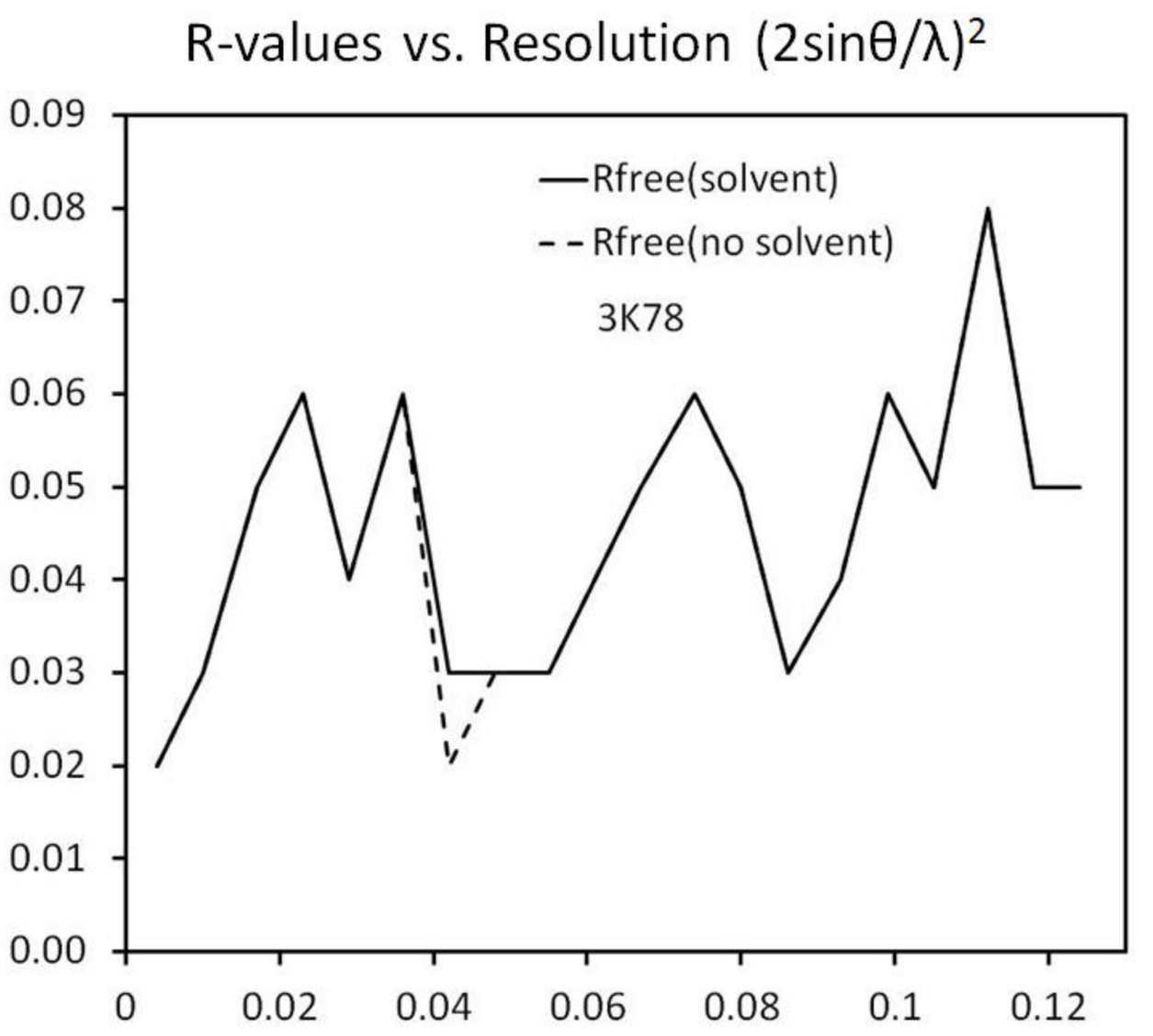

Rsigma against resolution (Å)
r3k78sf.hkl
0.10
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0.00
12.9
9.3
7.2
5.9
5.0
4.3
3.8
3.4
3.1
2.9

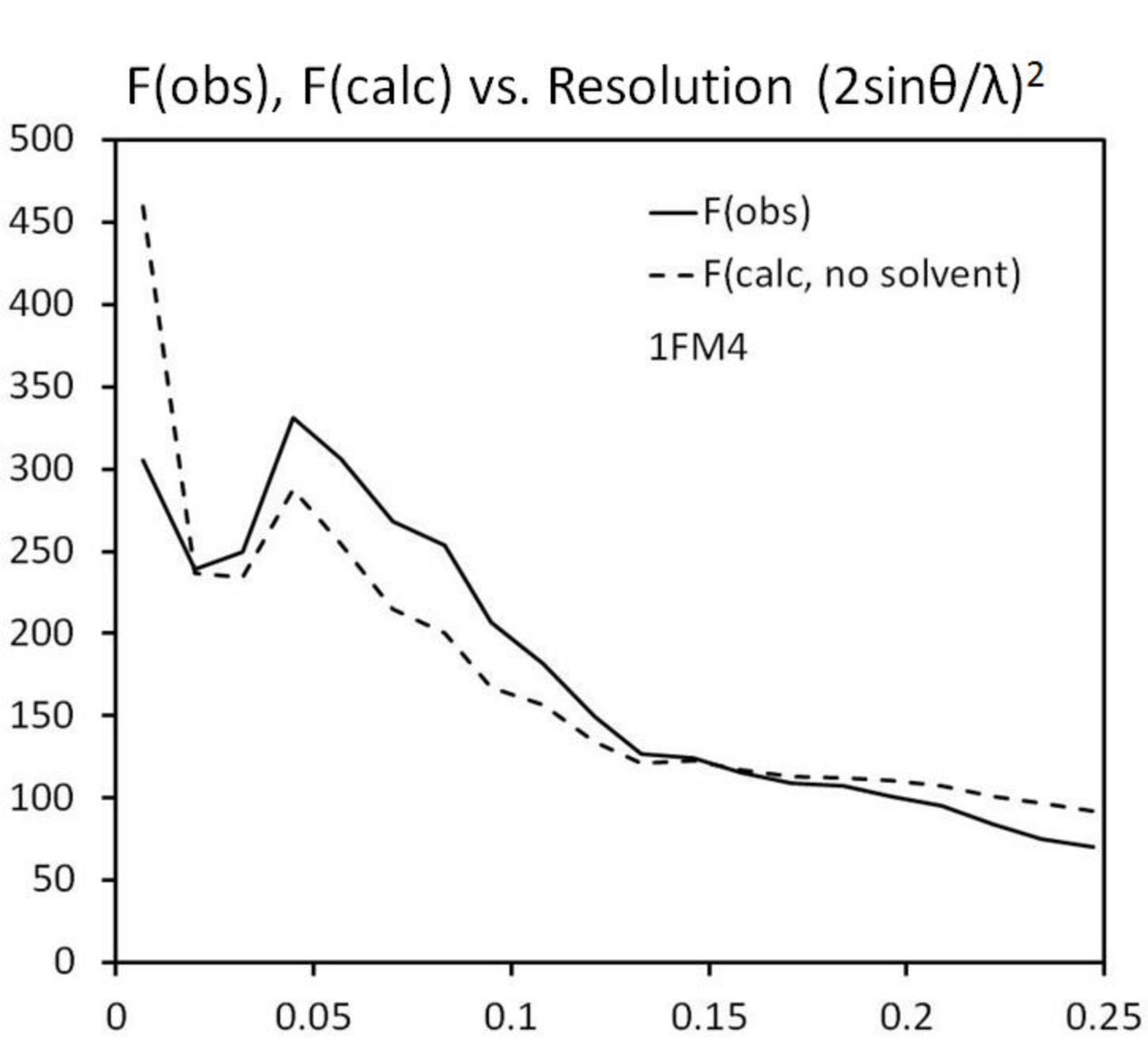

1FM4
I/sig(I)
Log10 I
0
5
10
15
20
25
30
35
40
0
1
2
3
4
3K78
I/sig(I)
Log10 I
0
20
40
60
80
100
120
140
160
180
200
-2
-1
0
1
2
3
4
0
100
200
300
400
500
600
700
-2
0
2
4

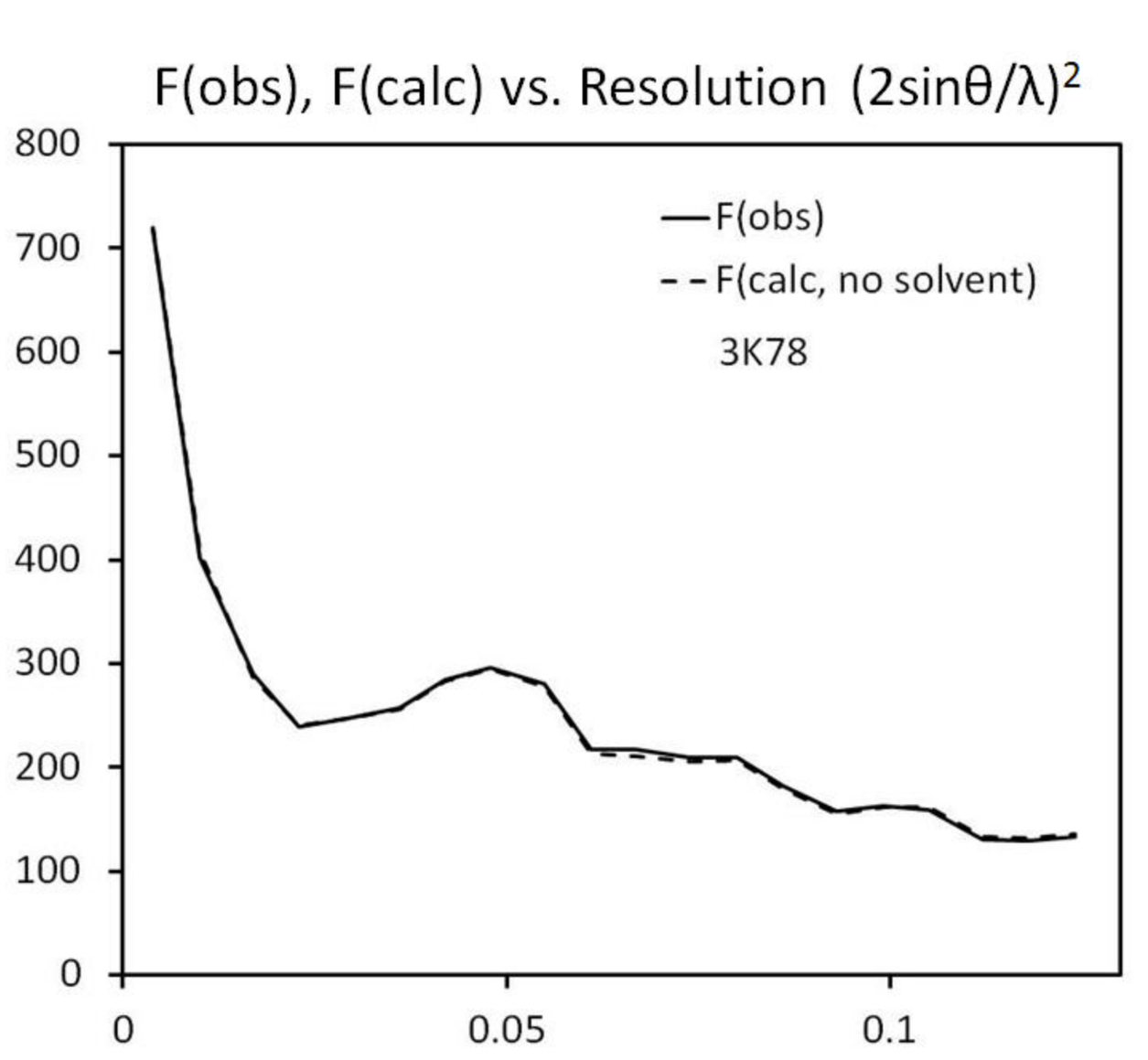

3K78 data
Y=2.6·X^0.48, R^2=0.72
I/sig(I)
Intensity I
0
20
40
60
80
100
120
140
160
180
200
0
1000
2000
3000
4000


3K78 model
Y=2.4·X^0.49, R^2=0.68
I/sig(I)
Intensity I
0
20
40
60
80
100
120
140
160
180
200
0
1000
2000
3000
4000


R-values vs. Resolution (2sinθ/λ)²
Rfree(solvent)
Rfree(no solvent)
1FM4
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.05
0.1
0.15
0.2
0.25


R-values vs. Resolution (2sinθ/λ)²
Rfree(solvent)
Rfree(no solvent)
3K78
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0.00
0
0.02
0.04
0.06
0.08
0.1
0.12


F(obs), F(calc) vs. Resolution (2sinθ/λ)²
F(obs)
F(calc, no solvent)
1FM4
500
450
400
350
300
250
200
150
100
50
0
0
0.05
0.1
0.15
0.2
0.25


F(obs), F(calc) vs. Resolution (2sinθ/λ)²
F(obs)
F(calc, no solvent)
3K78
800
700
600
500
400
300
200
100
0
0
0.05
0.1

B_sol
(Å²)
36.9
44.0
48.7

k_sol
(e⁻/Å³)
0.356
0.359
0.360

prob(k_sol,B_sol)

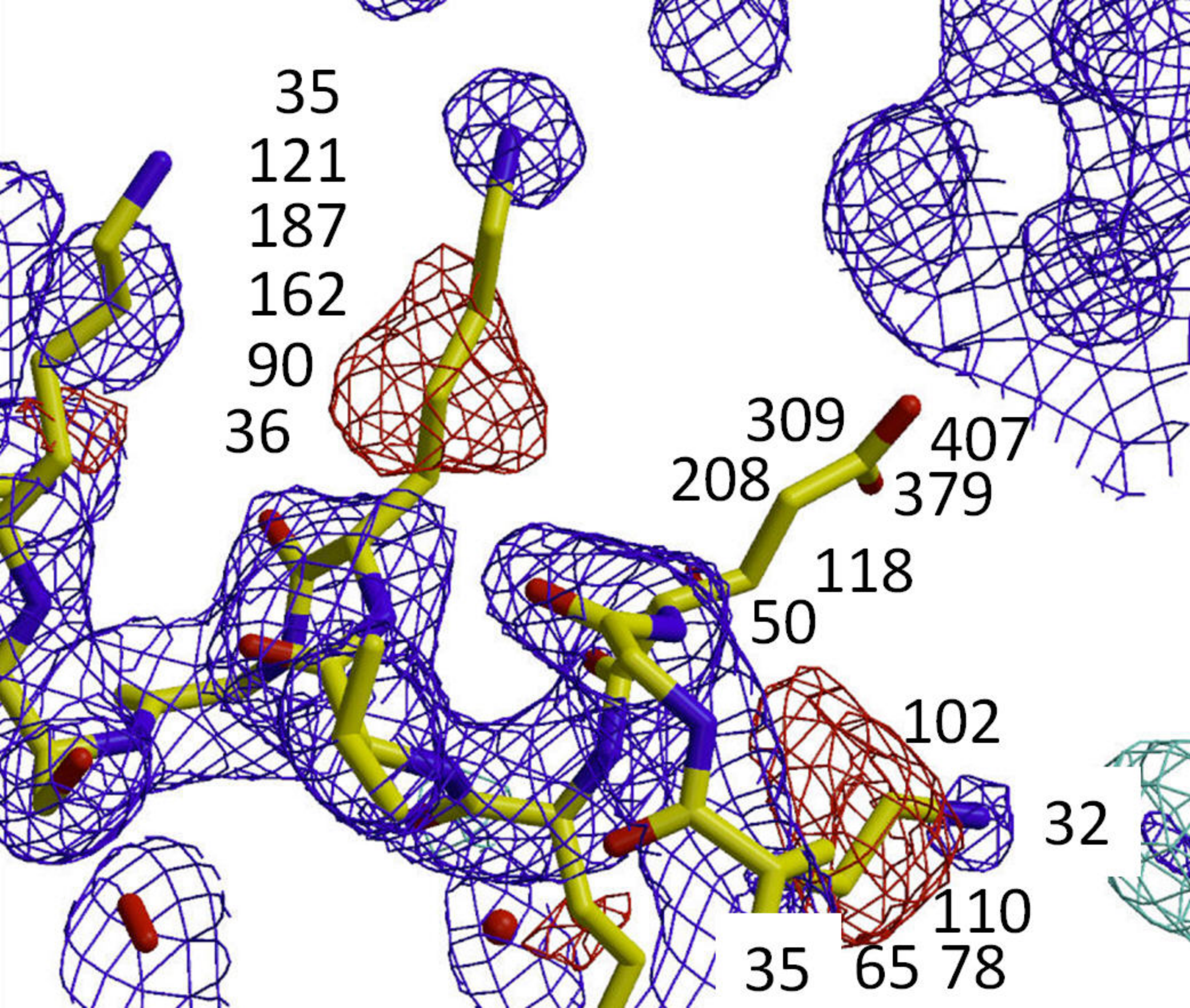
0

140

k_sol (e⁻/Å³)

0.6

B_sol (Å²)


35
121
187
162
90
36
309
407
208
379
118
50
102
32
110
35
65
78

	1FM4 deposited	1FM4 re-refined isotropic B	3K78 deposited, hybrid TLS	3K78 re-refined, hybrid TLS	3K78 re-refined, isotropic B
Space group	$P2_1$				
a (Å)	33.13		32.97		
b (Å)	57.23		57.01		
c(Å)	38.65		38.93		
β (deg)	91.94		92.27		
Resolution (Å)	28.66-1.97	28.66-1.99[1)]	32.95[2)]-2.80	25.56-2.80	
Last resolution shell (Å)	2.09-1.97	2.04-1.99	2.87-2.80		
N ref.	9658	8659	3184		
Atoms of zero occupancy	29	0	29	29	29 at 0.01
Refinement program	CNS 1.0	REFMAC 5.6.0117	REFMAC 5.2.0019 TLS	REFMAC 5.6.0117 TLS	REFMAC 5.6.0117
Riding hydrogen atoms	n.r.	yes	no	yes	no
R-free set	10% random	10% random	9.8% random[3)]	4.8% random	4.8% random[5)]
B Wilson ($Å^2$)	12.2	18.9	45.2	27.6[6)]	
B mean overall ($Å^2$)	16.3	18.7	26.8	**3.67**[7)]	15.2
B_sol ($Å^2$), k_sol	66.1, n.r.	24.0,0.37	-10.00, 0.01[10)]	**-10.00,0.03**	**no bulk solvent**
R-free, overall (last shell)	0.240(0.388)	0.213(0.400)	0.298(0.387)	**0.132 (0.250)**	**0.040(0.062)**
R-work, overall (last shell)	0.197(0.359)	0.159(0.234)	0.273(0.350)	**0.069 (0.105)**	**0.019(0.048)**
Coord. e.s.u. from Rfree (Å)	0.160	0.187	0.379	0.235	**0.072**
Correlation betw. Fc and Fo		0.962	0.934	0.993	**0.999**
Correlation, Fc and Fo free		0.929	0.919	0.968	**0.997**
Ramachandran regions %(COOT)	97.5/2.5/0	97.5/2.5/0	92.2/2.0/5.8	92.2/2.0/5.8	91.0/6.5/2.6
R.m.s.d. bonds (Å)	0.009	0.011	0.017[4)]	0.015	0.011
R.m.s.d. angles degrees	1.30	1.62	1.54[4)]	1.82	1.69
R.m.s.d. all atoms (Å)	0.247		0.705[8)]		0.640[8)]

R.m.s.d. main chain (Å)	0.081		0.352[8]		0.367[8]
R.m.s.d. Cα (Å)	0.078		0.295[8]		0.302[8]
X-ray term matrix weight[11]	n.r.	0.2	n.r.	default	**0.6**
B factor restraint (Å^2)[9]	n.r.	3/5/7/9	n.r.	default	5/7/9/11

n.r. not reported
1) deposited data extend only to 1.99 Å
2) this is a reporting error in the PDB header caused by REFMAC. Actual low resolution limit 25.56 Å
3) the deposited structure factor file contains only a 5% crossvalidation data set
4) not including the zero occupancy residues. With aero occupancy residues reset, 0.032 Å and 2.136 deg
5) a 10% a-posterior crossvalidation set gives practically the same result
6) from TRUNCATE
7) residual B-factors, some atoms show the low B-factor cutoff of 2.0 Å
8) r.m.s.d. against the original 3K78 model
9) REFMAC B-factor restraint weight sigmas (Å^2), for main chain 1-2, 1-3 neighbors, and side chain 1-2, 1-3 neighbors
10) from EDS report
11) in REFMAC, the actual X-ray term weight (Wa in CNS/XPLOR) is obtained as the product of the user-selectable X-ray matrix weight times the ratio of the trace of the geometry Hessian divided by the trace of the X-ray Hessian matrix. The REFMAC X-ray matrix weight is therefore not the same as Wa. Ian Tickle has kindly pointed me to the respective REFMAC source code for verification.

INTENSITY STATISTICS FOR DATASET # 1 r1fm4sf.hkl

Resolution	#Data	#Theory	%Complete	Redundancy	Mean I	Mean I/s	Rmerge	Rsigma
Inf - 8.23	145	154	94.2	0.94	555.0	15.48	0.0000	0.0612
8.23 - 5.49	339	342	99.1	0.99	328.1	16.20	0.0000	0.0548
5.49 - 4.36	486	489	99.4	0.99	600.3	17.50	0.0000	0.0496
4.36 - 3.80	486	487	99.8	1.00	518.1	15.39	0.0000	0.0559
3.80 - 3.45	489	489	100.0	1.00	399.2	13.90	0.0000	0.0599
3.45 - 3.20	480	482	99.6	1.00	298.8	12.97	0.0000	0.0643
3.20 - 3.01	472	473	99.8	1.00	217.0	11.65	0.0000	0.0730
3.01 - 2.86	494	494	100.0	1.00	144.3	9.89	0.0000	0.0898
2.86 - 2.73	502	502	100.0	1.00	115.2	8.83	0.0000	0.1022
2.73 - 2.63	461	462	99.8	1.00	91.7	7.70	0.0000	0.1190
2.63 - 2.54	470	470	100.0	1.00	89.2	7.61	0.0000	0.1249
2.54 - 2.46	491	493	99.6	1.00	75.2	6.18	0.0000	0.1555
2.46 - 2.38	537	537	100.0	1.00	71.6	5.92	0.0000	0.1629
2.38 - 2.32	479	479	100.0	1.00	71.4	5.50	0.0000	0.1742
2.32 - 2.26	503	504	99.8	1.00	62.1	4.89	0.0000	0.2025
2.26 - 2.21	464	465	99.8	1.00	60.4	4.30	0.0000	0.2167
2.21 - 2.16	516	518	99.6	1.00	53.1	3.89	0.0000	0.2463
2.16 - 2.12	456	459	99.3	0.99	43.0	3.18	0.0000	0.2983
2.12 - 2.08	451	469	96.2	0.96	37.9	2.70	0.0000	0.3488
2.08 - 2.04	491	525	93.5	0.94	30.7	2.38	0.0000	0.4035
2.04 - 1.99	446	743	60.0	0.60	28.2	2.10	0.0000	0.4378
2.09 - 1.99	1059	1395	75.9	0.76	30.3	2.29	0.0000	0.4102
Inf - 1.99	9658	10035	96.2	0.96	170.9	8.16	0.0000	0.0915

INTENSITY STATISTICS FOR DATASET # 1 r3k78sf.hkl

Resolution	#Data	#Theory	%Complete	Redundancy	Mean I	Mean I/s	Rmerge	Rsigma
Inf -10.67	51	75	68.0	0.68	510.0	82.26	0.0000	0.0145
0.67 - 7.65	116	120	96.7	0.97	123.4	42.28	0.0000	0.0278
7.65 - 6.13	169	176	96.0	0.96	73.8	34.78	0.0000	0.0310
6.13 - 5.36	166	167	99.4	0.99	65.2	34.31	0.0000	0.0292
5.36 - 4.88	170	171	99.4	0.99	85.6	41.88	0.0000	0.0240
4.88 - 4.53	171	175	97.7	0.98	103.4	41.60	0.0000	0.0239
4.53 - 4.27	163	164	99.4	0.99	89.2	42.22	0.0000	0.0217
4.27 - 4.06	163	164	99.4	0.99	75.6	38.27	0.0000	0.0253
4.06 - 3.88	168	169	99.4	0.99	54.2	34.31	0.0000	0.0284
3.88 - 3.73	174	176	98.9	0.99	52.0	31.69	0.0000	0.0294
3.73 - 3.60	159	160	99.4	0.99	46.7	29.52	0.0000	0.0313
3.60 - 3.49	170	170	100.0	1.00	54.9	32.33	0.0000	0.0276
3.49 - 3.39	184	184	100.0	1.00	39.0	28.91	0.0000	0.0309
3.39 - 3.29	159	166	95.8	0.96	34.2	25.06	0.0000	0.0351
3.29 - 3.21	183	192	95.3	0.95	30.8	23.29	0.0000	0.0369
3.21 - 3.13	154	172	89.5	0.90	34.1	24.97	0.0000	0.0361
3.13 - 3.06	164	193	85.0	0.85	29.6	24.69	0.0000	0.0377
3.06 - 2.99	157	182	86.3	0.86	22.5	22.23	0.0000	0.0427
2.99 - 2.92	182	229	79.5	0.79	19.9	20.45	0.0000	0.0460
2.92 - 2.86	160	196	81.6	0.82	20.6	19.14	0.0000	0.0449
2.86 - 2.80	154	224	68.8	0.69	21.4	21.29	0.0000	0.0428
2.80 - 2.79	9	42	21.4	0.21	21.8	21.67	0.0000	0.0380
2.89 - 2.79	239	360	66.4	0.66	20.5	20.27	0.0000	0.0444
Inf - 2.79	3346	3666	91.3	0.91	59.7	31.29	0.0000	0.0275

1FM4 ZERO OCCUPANCIES

```
ATOM    216  CE  LYS A  28      25.926  -2.671   8.010  0.00 23.91           C
ATOM    217  NZ  LYS A  28      26.633  -3.315   6.868  0.00 24.44           N
ATOM    490  CE  LYS A  65      18.807   1.032  29.307  0.00 20.57           C
ATOM    491  NZ  LYS A  65      19.242   0.659  30.681  0.00 20.62           N
ATOM    620  CD  LYS A  80       4.805  -6.993   0.545  0.00 15.40           C
ATOM    621  CE  LYS A  80       3.641  -7.195   1.499  0.00 16.00           C
ATOM    622  NZ  LYS A  80       2.728  -8.279   1.044  0.00 15.66           N
ATOM    797  CD  LYS A 103       2.848  -2.228  -1.464  0.00 14.05           C
ATOM    798  CE  LYS A 103       2.798  -2.525  -2.954  0.00 14.45           C
ATOM    799  NZ  LYS A 103       1.456  -3.010  -3.379  0.00 14.25           N
ATOM    992  CG  LYS A 129      -6.897   5.245  23.403  0.00 29.99           C
ATOM    993  CD  LYS A 129      -6.906   6.361  24.434  0.00 29.90           C
ATOM    994  CE  LYS A 129      -7.675   5.960  25.682  0.00 29.70           C
ATOM    995  NZ  LYS A 129      -7.679   7.044  26.703  0.00 29.58           N
ATOM   1006  CG  GLU A 131      -6.393  10.424  19.788  0.00 30.67           C
ATOM   1007  CD  GLU A 131      -7.145  11.280  20.788  0.00 30.64           C
ATOM   1008  OE1 GLU A 131      -6.626  12.352  21.164  0.00 30.54           O
ATOM   1009  OE2 GLU A 131      -8.256  10.883  21.196  0.00 30.54           O
ATOM   1015  CG  GLN A 132      -2.646   6.649  23.381  0.00 27.50           C
ATOM   1016  CD  GLN A 132      -2.803   5.577  24.442  0.00 27.45           C
ATOM   1017  OE1 GLN A 132      -1.824   5.136  25.044  0.00 27.38           O
ATOM   1018  NE2 GLN A 132      -4.038   5.152  24.677  0.00 27.38           N
ATOM   1031  CG  LYS A 134      -1.755  10.322  16.401  0.00 19.39           C
ATOM   1032  CD  LYS A 134      -2.453  11.641  16.691  0.00 19.17           C
ATOM   1033  CE  LYS A 134      -3.935  11.567  16.357  0.00 19.26           C
ATOM   1034  NZ  LYS A 134      -4.632  12.854  16.629  0.00 19.24           N
ATOM   1052  CD  LYS A 137       0.993  10.122  11.278  0.00 19.99           C
ATOM   1053  CE  LYS A 137       0.836  10.863   9.959  0.00 20.30           C
ATOM   1054  NZ  LYS A 137      -0.518  11.466   9.814  0.00 20.17           N
```

3K78 ZERO OCCUPANCIES

```
ATOM    212  CB  ASN A  29      24.578   1.000   8.850  0.00 20.00           C
ATOM    213  CG  ASN A  29      24.914  -0.474   8.951  0.00 20.00           C
ATOM    486  CG  LYS A  66      15.465   2.444  29.367  0.00 20.00           C
ATOM    487  CD  LYS A  66      16.337   1.727  30.383  0.00 20.00           C
ATOM    616  CB  LYS A  81       6.844  -5.420   0.565  0.00 20.00           C
ATOM    617  CG  LYS A  81       7.220  -6.853   0.229  0.00 20.00           C
ATOM    618  CD  LYS A  81       6.017  -7.638  -0.264  0.00 20.00           C
ATOM    793  CB  LYS A 104       4.181  -1.122   0.973  0.00 20.00           C
ATOM    794  CG  LYS A 104       4.320  -1.566  -0.586  0.00 20.00           C
ATOM    795  CD  LYS A 104       2.937  -2.049  -0.998  0.00 20.00           C
ATOM    988  O   LYS A 130      -4.110   5.815  20.168  0.00 20.00           O
ATOM    989  CB  LYS A 130      -6.498   6.168  22.237  0.00 20.00           C
ATOM    990  CG  LYS A 130      -7.388   5.691  23.371  0.00 20.00           C
ATOM    991  CD  LYS A 130      -7.902   6.857  24.199  0.00 20.00           C
ATOM   1002  O   GLU A 132      -1.642  10.106  20.349  0.00 20.00           O
ATOM   1003  CB  GLU A 132      -4.654  10.685  20.701  0.00 20.00           C
ATOM   1004  CG  GLU A 132      -5.941  11.279  20.155  0.00 20.00           C
ATOM   1005  CD  GLU A 132      -6.627  12.197  21.147  0.00 20.00           C
ATOM   1011  O   GLN A 133       0.822   7.043  20.434  0.00 20.00           O
ATOM   1012  CB  GLN A 133      -1.524   6.639  22.500  0.00 20.00           C
ATOM   1013  CG  GLN A 133      -2.041   7.280  23.805  0.00 20.00           C
ATOM   1014  CD  GLN A 133      -2.520   6.229  24.789  0.00 20.00           C
ATOM   1027  O   LYS A 135       1.505  11.182  19.279  0.00 20.00           O
ATOM   1028  CB  LYS A 135      -0.154  10.874  16.834  0.00 20.00           C
ATOM   1029  CG  LYS A 135      -1.552  10.784  17.424  0.00 20.00           C
ATOM   1030  CD  LYS A 135      -2.202  12.146  17.569  0.00 20.00           C
ATOM   1048  CB  LYS A 138       2.740   9.013  12.921  0.00 20.00           C
ATOM   1049  CG  LYS A 138       2.624   9.707  11.574  0.00 20.00           C
ATOM   1050  CD  LYS A 138       1.202  10.171  11.315  0.00 20.00           C
```

The entry 3K78 contains 4 atoms less (-1 GLY) than 1FM4. The 4 mutations add/subtract atoms as follows: (T8I, +1),(A10T, +2), M19L, 0), (K28D, -1), i.e. 3K78 gained 2 atoms from mutations and lost 4 through absence from N-terminal GLY: -4 + 2 = -2. The observed offset in zero occupancy atom numbers between 1FM4 and 3K78 is however -4.

#CCP4I VERSION CCP4Interface 2.1.0
#CCP4I SCRIPT LOG refmac5
#CCP4I DATE 09 Jan 2012 23:07:53
#CCP4I USER 'UNKNOWN'
#CCP4I PROJECT 3k78
#CCP4I JOB_ID 183
#CCP4I SCRATCH C:/Ccp4Temp
#CCP4I HOSTNAME br-server
#CCP4I PID 6244

<B><FONT COLOR="#FF0000"><!--SUMMARY_BEGIN-->
<html> <!-- CCP4 HTML LOGFILE -->
<hr>
<!--SUMMARY_END--></FONT></B>
<B><FONT COLOR="#FF0000"><!--SUMMARY_BEGIN-->
<pre>

 ##
 ##
 ##
 ### CCP4 6.2: Refmac_5.6.0117   version 5.6.0117 : 13/06/11##
 ##
 User: br Run date: 9/ 1/2012 Run time: 23:07:53

 Please reference: Collaborative Computational Project, Number 4. 1994.
 "The CCP4 Suite: Programs for Protein Crystallography". Acta Cryst. D50, 760-763.
 as well as any specific reference in the program write-up.

<!--SUMMARY_END--></FONT></B>
 $TEXT:Reference1: $$ Main reference $$
   "REFMAC5 for the refinement of macromolecular crystal structures:"
   G.N.Murshudov, P.Skubak, A.A.Lebedev, N.S.Pannu, R.A.Steiner, R.A.Nicholls, M.D.Winn,
F.Long and A.A.Vagin,(2011)
   Acta Crystallogr. D67, 355-367

 $$
 $SUMMARY :Reference1: $$ Refmac: $$
 :TEXT:Reference1: $$

 $TEXT:Reference2: $$ Secondary reference $$
   "Refinement of Macromolecular Structures by the Maximum-Likelihood Method:"
   G.N. Murshudov, A.A.Vagin and E.J.Dodson,(1997)
   Acta Crystallogr. D53, 240-255
   EU Validation contract: BIO2CT-92-0524

 $$
 $SUMMARY :Reference2: $$ Refmac: $$
 :TEXT:Reference2: $$

  Data line--- refi resolution 2.801 38.899

Data line--- make check ALL
Data line--- make hydrogen NO hout NO peptide NO cispeptide YES ssbridge YES symmetry YES sugar YES connectivity NO link NO
Data line--- refi type REST resi MLKF meth CGMAT bref ISOT
Data line--- ncyc 150
Data line--- scal type SIMP LSSC ANISO EXPE
Data line--- solvent NO
Data line--- weight MATRIX 0.6
Data line--- monitor MANY torsion 10.0 distance 10.0 angle 10.0 plane 10.0 chiral 10.0 bfactor 10.0 bsphere 10.0 rbond 10.0 ncsr 10.0
Data line--- labin FP=FP SIGFP=SIGFP FREE=FREE
Data line--- labout FC=FC FWT=FWT PHIC=PHIC PHWT=PHWT DELFWT=DELFWT PHDELWT=PHDELWT FOM=FOM
Data line--- temp 1.0 5.0 7.0 9.0 11.0
Data line--- dist 1.0
Data line--- angle 1.0
Data line--- PNAME 3k78
Data line--- DNAME 3k78
Data line--- RSIZE 80
Data line--- END

OPENED INPUT MTZ FILE
Logical Name: HKLIN Filename: c:/data/deepblue/3k78/r3k78sf.mtz

Spacegroup information obtained from library file:
Logical Name: SYMINFO Filename: C:\CCP4\6.2\lib\data\syminfo.lib

**** Input and Default parameters# ****

Input coordinate file. Logical name - XYZIN actual file name - c:/data/deepblue/3k78/3k78_iso_clean_refmac1.pdb
Output coordinate file. Logical name - XYZOUT actual file name - c:/data/deepblue/3k78/3k78_iso_clean_refmac2.pdb
Input reflection file. Logical name - HKLIN actual file name - c:/data/deepblue/3k78/r3k78sf.mtz
Output reflection file. Logical name - HKLOUT actual file name - c:/data/deepblue/3k78/3k78_iso_clean_refmac2.mtz

Cell from mtz : 32.970 57.010 38.930 90.000 92.270 90.000
Space group from mtz: number - 4; name - P 1 21 1

Refinement type : Restrained

**** Makecif parameters ****

Dictionary files for restraints : C:\CCP4\6.2\lib\data\monomers\mon*cif
Parameters for new entry and VDW: C:\CCP4\6.2\lib\data\monomers\ener_lib.cif
Program will check all entries against dictionary

Hydrogens will not be written to the output file
Links between monomers will be checked. Only those links present in the coordinate file will be used
All links to sugar will be analysed and used
For new ligands "ideal restraint" values will be taken from the energetic libary ener_lib.cif
Symmetry related links will be analysed and used
Cis peptides will be found and used automatically

Residual : Rice Maximum Likelihood for Fs

**** Least-square scaling parameters ****

Overall scale
Overall B value
Overall anisotropic B with tr(B) = 0.0

Method of minimisation : Sparse Matrix
Experimental sigmas used for weighting
Number of Bins and width: 20 0.0064
Refinement of individual isotropic Bfactors
Refinement resln : 38.8990 2.8012
Estimated number of reflections : 4939
Free R exclusion - flag equals: 0
Weighting by comparison of trace of matrix
Weighting parameters : 0.6000
Refinement cycles : 150
Scaling type :
Wilson using 1 Gaussian

Estimation of SigmaA Using 2 Gaussians:
using free set of reflns with experimental sigmas
using free set of reflns with experimental sigmas

Scaling and SigmaA resln: 38.8990 2.8012

Damping factors: 1.0000 1.0000

**** Geometry restraints and weights ****

Sigma:
Bonding distances
Weight = 1.00

Bond angles
Weight = 1.00

Planar groups
WEIGHT= 1.00

Chiral centers
Weight= 1.00

NON-BONDED CONTACTS
Overall weight = 1.00
Sigma for simple VDW = 0.20
Sigma for VDW trhough torsion angle = 0.20
Sigma for HBOND = 0.20
Sigma for metal-ion = 0.20
Sigma for DUMMY and other atom = 0.30
Distance for donor-accepetor = vdw1+vdw2+(-0.30)
Distance for acceptor - H = vdw1+ (0.10)
VDW distance through torsion = vdw1+vdw2+(-0.30)
Distance for DUMMY-others = vdw1+vdw2+(-0.70)

TORSION ANGLES
Weight= 1.00

THERMAL FACTORS
Weight= 1.00
Main chain bond (1-2 neighbour) 5.0A**2
Main chain angle (1-3 neighbour) 7.0A**2
Side chain bond 9.0A**2
Side chain angle 11.0A**2

RESTRAINTS AGAINST EXCESSIVE SHIFTS
Positional parameters 0.00A
Thermal parameters 0.00A
Occupancy parameters 0.00

RADIUS OF CONFIDENCE
Positional parameters 0.00A
Thermal parameters 0.00A**2
Occupancy parameters 0.00

Monitoring style is "MANY". Complete information will be printed out in all cycles
Sigma cutoffs for printing out outliers
If deviation of restraint parameter > alpha*sigma then information will be printed out
Distance outliers 10.000
Angle outliers 10.000
Torsion outliers 10.000
Chiral volume outliers 10.000
Plane outliers 10.000
Non-bonding outliers 10.000
B value outliers 10.000

Input file :c:/data/deepblue/3k78/3k78_iso_clean_refmac1.pdb
Size of lib_com.fh(bytes) : 117223836
NUMBER OF MONOMERS IN THE LIBRARY : 11465

```
            with complete description    : 11465
 NUMBER OF MODIFICATIONS                 :    53
 NUMBER OF LINKS                         :    66
 I am reading libraries. Please wait.
    - energy parameters
    - monomer"s description (links & mod )

FORMATTED      OLD     file opened on unit  45
<B><FONT COLOR="#FF0000"><!--SUMMARY_BEGIN-->
Logical name: ATOMSF, Filename: C:\CCP4\6.2\lib\data\atomsf.lib
<!--SUMMARY_END--></FONT></B>

 Number of atoms    :    1230
 Number of residues :     181
 Number of chains   :       2
 I am reading library. Please wait.
            mon_lib.cif
 --------------------------------
 --- title of input coord file ---

 PDB_code:xxxx
 PDB_name:----
 PDB_date:XX-XXX-XX
 --------------------------------
 Number of chains                :       2
 Total number of monomers        :     181
 Number of atoms                 :    1230
 Number of missing atoms         :       0
 Number of rebuilt atoms         :       0
 Number of unknown atoms         :       0
 Number of deleted atoms         :       0

 Number of bonds restraints    :    1229
 Number of angles restraints   :    1663
 Number of torsions restraints :     841
 Number of chiralities         :     187
 Number of planar groups       :     217


loop_
   _atom_type_symbol
   _atom_type_scat_Cromer_Mann_a1
   _atom_type_scat_Cromer_Mann_b1
   _atom_type_scat_Cromer_Mann_a2
   _atom_type_scat_Cromer_Mann_b2
   _atom_type_scat_Cromer_Mann_a3
   _atom_type_scat_Cromer_Mann_b3
   _atom_type_scat_Cromer_Mann_a4
   _atom_type_scat_Cromer_Mann_b4
   _atom_type_scat_Cromer_Mann_c
```

N	12.2126	0.0057	3.1322	9.8933	2.0125	28.9975	1.1663	0.5826	-11.5290
C	2.3100	20.8439	1.0200	10.2075	1.5886	0.5687	0.8650	51.6512	0.2156
O	3.0485	13.2771	2.2868	5.7011	1.5463	0.3239	0.8670	32.9089	0.2508
S	6.9053	1.4679	5.2034	22.2151	1.4379	0.2536	1.5863	56.1720	0.8669

	Standard	External	All
Bonds:	1229	0	1229
Angles:	1663	0	1663
Chirals:	187	0	187
Planes:	217	0	217
Torsions:	841	0	841

Number of reflections in file 3611
Number of reflections read 3611

CGMAT cycle number = 1

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
Weight matrix 0.60000002
Actual weight 4.8510904 is applied to the X-ray term
Norm of X_ray positional gradient 39.5
Norm of Geom. positional gradient 6.78
Norm of X_ray B-factor gradient 53.8
Norm of Geom. B-factor gradient 9.28
Product of X_ray and Geom posit. gradients -0.956E+06
Cosine of angle between them -0.966
Product of X_ray and Geom B-fact gradients -0.592E+06
Cosine of angle between them -0.965

Residuals: XRAY= 0.6052E+05 GEOM= 2382. TOTAL= 0.6290E+05
function value 62897.527

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.007	0.020
Bond angles : refined atoms	1663	1.255	1.966
Torsion angles, period 1. refined	155	7.216	5.000
Torsion angles, period 2. refined	54	40.727	25.741
Torsion angles, period 3. refined	214	17.640	15.000
Torsion angles, period 4. refined	3	19.926	15.000
Chiral centres: refined atoms	187	0.091	0.200

Planar groups: refined atoms 924 0.004 0.021
VDW repulsions: refined_atoms 523 0.243 0.200
VDW; torsion: refined_atoms 802 0.312 0.200
HBOND: refined_atoms 43 0.169 0.200
VDW repulsions: symmetry: refined_atoms 55 0.237 0.200
HBOND: symmetry: refined_atoms 2 0.127 0.200
Bond B values: refined atoms 1229 5.675 4.685
Angle B values: refined atoms 1663 7.363 7.169
Torsion B values: refined atoms 426 14.290 13.117
Long range B values: refined atoms 1334 5.971 15.813

Overall : scale = 1.014, B = -0.169
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 1. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 1. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 1. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 1. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 34 65.38 663.7 654.5 0.02 0.03 0 0.0 0.0****** 0.00
0.010 69 96.00 371.0 372.6 0.04 0.04 3 408.4 403.8 0.04 0.04
0.017 95 96.15 268.1 268.5 0.05 0.05 5 321.5 330.5 0.05 0.06
0.023 108 97.44 221.6 223.8 0.05 0.05 6 149.8 153.0 0.10 0.08
0.029 114 100.00 228.0 228.7 0.05 0.05 9 144.8 147.7 0.09 0.08
0.036 143 99.33 237.6 238.0 0.04 0.04 6 252.2 249.5 0.05 0.06
0.042 140 98.67 263.0 264.0 0.03 0.04 8 337.2 343.3 0.03 0.03
0.048 162 98.82 274.0 274.0 0.03 0.03 5 304.9 297.0 0.06 0.06
0.055 163 99.43 259.8 259.6 0.03 0.04 10 257.2 258.8 0.07 0.07
0.061 187 100.00 200.3 200.7 0.04 0.04 10 201.6 202.3 0.07 0.07
0.067 183 99.47 200.5 200.3 0.04 0.04 6 285.5 277.7 0.04 0.05
0.074 189 98.99 193.5 195.1 0.04 0.04 7 200.5 199.6 0.05 0.04
0.080 203 100.00 193.7 194.2 0.04 0.04 13 159.2 152.9 0.10 0.10
0.086 206 100.00 168.6 168.9 0.05 0.04 9 184.8 184.2 0.05 0.05
0.093 207 93.99 145.9 145.7 0.05 0.05 12 151.2 153.5 0.11 0.11
0.099 200 91.74 150.6 148.9 0.05 0.05 11 159.2 156.5 0.06 0.06
0.105 198 86.59 147.2 147.0 0.05 0.05 15 146.2 144.4 0.09 0.09
0.112 196 81.27 120.9 120.5 0.05 0.06 8 101.1 99.5 0.08 0.08
0.118 205 82.69 119.8 119.8 0.05 0.05 10 123.9 124.6 0.07 0.08
0.124 182 74.03 123.0 123.1 0.05 0.04 9 113.5 111.2 0.13 0.11

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 1. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 1. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.998 4 1.000 34 0.998 0.998
0.0102 62 0.997 7 1.000 69 0.997 0.998
0.0165 83 0.969 12 0.921 95 0.963 0.998
0.0228 97 0.983 11 1.000 108 0.985 0.998
0.0292 108 0.991 6 1.000 114 0.991 0.997
0.0355 126 0.988 17 0.997 143 0.989 0.997
0.0418 129 0.990 11 1.000 140 0.991 0.997
0.0482 150 0.986 12 0.999 162 0.987 0.997
0.0545 151 0.990 12 0.919 163 0.985 0.997
0.0609 172 0.971 15 0.925 187 0.967 0.997
0.0672 174 0.981 9 0.918 183 0.978 0.997
0.0735 178 0.977 11 1.000 189 0.978 0.997
0.0799 189 0.978 14 0.978 203 0.978 0.997
0.0862 197 0.960 9 0.936 206 0.959 0.997
0.0925 193 0.950 14 0.933 207 0.949 0.998
0.0989 188 0.958 12 0.975 200 0.959 0.998
0.1052 190 0.967 8 1.000 198 0.968 0.999
0.1116 183 0.954 13 0.930 196 0.952 0.999
0.1179 194 0.956 11 0.890 205 0.953 1.000
0.1242 174 0.959 8 1.000 182 0.961 1.000
$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0423
Free R factor = 0.0687
Overall weighted R factor = 0.0426
Free weighted R factor = 0.0689
Overall correlation coefficient = 0.9970
Free correlation coefficient = 0.9909
DPI based on free R factor = 0.1247
Overall figure of merit = 0.9710
ML based su of positional parameters = 0.0706
ML based su of thermal parameters = 3.4791

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 12476.088 2382.0342 61932.059 62904.664

CGMAT cycle number = 2

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
Weight matrix 0.60000002
Actual weight 3.7466385 is applied to the X-ray term
Norm of X_ray positional gradient 19.0
Norm of Geom. positional gradient 21.6
Norm of X_ray B-factor gradient 25.0
Norm of Geom. B-factor gradient 23.3
Product of X_ray and Geom posit. gradients -0.920E+06
Cosine of angle between them -0.605
Product of X_ray and Geom B-fact gradients -0.363E+06
Cosine of angle between them -0.507

Residuals: XRAY= 0.4441E+05 GEOM= 2956. TOTAL= 0.4737E+05
function value 47365.441

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.013	0.020
Bond angles : refined atoms	1663	1.517	1.966
Torsion angles, period 1. refined	155	7.560	5.000
Torsion angles, period 2. refined	54	40.983	25.741
Torsion angles, period 3. refined	214	18.121	15.000
Torsion angles, period 4. refined	3	20.282	15.000
Chiral centres: refined atoms	187	0.105	0.200
Planar groups: refined atoms	924	0.004	0.021
VDW repulsions: refined_atoms	535	0.252	0.200
VDW; torsion: refined_atoms	798	0.316	0.200
HBOND: refined_atoms	39	0.191	0.200
VDW repulsions: symmetry: refined_atoms	54	0.251	0.200
HBOND: symmetry: refined_atoms	2	0.299	0.200
Bond B values: refined atoms	1229	6.872	4.684
Angle B values: refined atoms	1663	8.829	7.122
Torsion B values: refined atoms	426	17.120	13.042
Long range B values: refined atoms	1335	6.820	15.689

Overall : scale = 1.014, B = -0.188
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 2. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 2. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 2. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 2. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 752.9 743.8 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 413.3 415.8 0.03 0.03 1 1226.2 1204.1 0.03 0.03
0.017 83 95.60 307.1 307.8 0.04 0.04 4 402.3 412.3 0.05 0.06
0.023 97 97.14 246.9 248.8 0.04 0.04 5 179.9 185.3 0.08 0.07
0.029 108 100.00 240.8 241.8 0.03 0.03 7 186.4 188.2 0.07 0.06
0.036 126 99.25 269.9 270.2 0.03 0.03 6 252.4 249.6 0.04 0.05
0.042 129 98.56 285.7 286.7 0.02 0.02 8 337.5 341.8 0.02 0.03
0.048 150 98.73 296.2 296.2 0.02 0.02 5 305.2 300.7 0.06 0.06
0.055 151 99.38 280.7 280.4 0.02 0.02 10 257.4 258.8 0.06 0.06
0.061 172 100.00 218.0 217.9 0.03 0.03 10 201.8 202.5 0.07 0.07
0.067 174 99.45 211.1 210.4 0.03 0.03 6 285.7 279.2 0.04 0.05
0.074 178 98.92 205.7 206.5 0.03 0.03 6 234.1 232.4 0.05 0.04
0.080 189 100.00 208.3 208.6 0.03 0.03 13 159.3 152.8 0.09 0.10
0.086 197 100.00 176.4 176.4 0.03 0.03 8 208.1 207.8 0.05 0.05
0.093 193 93.55 156.6 156.3 0.04 0.04 10 181.6 184.4 0.09 0.09
0.099 188 91.28 160.4 158.8 0.03 0.03 11 159.3 156.8 0.06 0.05
0.105 190 86.02 153.6 153.1 0.03 0.03 13 168.9 169.1 0.08 0.08
0.112 183 80.08 129.6 128.9 0.04 0.04 6 134.9 132.3 0.07 0.08
0.118 194 81.85 126.7 125.9 0.03 0.03 9 137.8 138.3 0.06 0.07
0.124 174 73.20 128.8 128.4 0.03 0.03 9 113.6 111.7 0.11 0.09
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 2. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 2. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.998
0.0102 62 0.997 7 1.000 69 0.998 0.998
0.0165 83 0.972 12 0.919 95 0.965 0.998
0.0228 97 0.985 11 1.000 108 0.987 0.998
0.0292 108 0.993 6 1.000 114 0.993 0.997
0.0355 126 0.990 17 0.999 143 0.991 0.997
0.0418 129 0.992 11 1.000 140 0.993 0.997
0.0482 150 0.987 12 1.000 162 0.988 0.997
0.0545 151 0.993 12 0.913 163 0.987 0.997
0.0609 172 0.973 15 0.935 187 0.970 0.997

```
 0.0672   174   0.984    9   0.919   183   0.981  0.997
 0.0735   178   0.980   11   1.000   189   0.981  0.997
 0.0799   189   0.980   14   0.984   203   0.981  0.997
 0.0862   197   0.962    9   0.957   206   0.962  0.997
 0.0925   193   0.954   14   0.936   207   0.953  0.998
 0.0989   188   0.963   12   0.976   200   0.963  0.998
 0.1052   190   0.970    8   1.000   198   0.971  0.999
 0.1116   183   0.960   13   0.930   196   0.958  0.999
 0.1179   194   0.962   11   0.898   205   0.958  1.000
 0.1242   174   0.961    8   1.000   182   0.963  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0301
Free R factor                    =     0.0606
Overall weighted R factor        =     0.0302
Free weighted R factor           =     0.0608
Overall correlation coefficient  =     0.9984
Free correlation coefficient     =     0.9929
DPI based on free R factor       =     0.1099
Overall figure of merit          =     0.9740
ML based su of positional parameters =     0.0620
ML based su of thermal parameters    =     3.0553
-------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    11857.227       2955.7837       47163.594       47380.527


    CGMAT cycle number =      3

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 Weight matrix   0.60000002
 Actual weight    3.3215556      is applied to the X-ray term
Norm of X_ray positional gradient              21.2
Norm of Geom. positional gradient              18.1
Norm of X_ray B-factor gradient                28.3
Norm of Geom. B-factor gradient                20.2
Product of X_ray and Geom posit. gradients     -0.108E+07
 Cosine of angle between them                  -0.758
Product of X_ray and Geom B-fact gradients     -0.612E+06
 Cosine of angle between them                  -0.873
```

Residuals: XRAY= 0.3872E+05 GEOM= 2948. TOTAL= 0.4167E+05
function value 41666.742

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.012	0.020
Bond angles : refined atoms	1663	1.532	1.966
Torsion angles, period 1. refined	155	7.568	5.000
Torsion angles, period 2. refined	54	41.006	25.741
Torsion angles, period 3. refined	214	18.144	15.000
Torsion angles, period 4. refined	3	20.310	15.000
Chiral centres: refined atoms	187	0.105	0.200
Planar groups: refined atoms	924	0.004	0.021
VDW repulsions: refined_atoms	535	0.255	0.200
VDW; torsion: refined_atoms	796	0.317	0.200
HBOND: refined_atoms	40	0.190	0.200
VDW repulsions: symmetry: refined_atoms	55	0.251	0.200
HBOND: symmetry: refined_atoms	3	0.234	0.200
Bond B values: refined atoms	1229	7.923	4.648
Angle B values: refined atoms	1663	10.045	7.055
Torsion B values: refined atoms	426	19.017	12.938
Long range B values: refined atoms	1335	7.361	15.480

Overall : scale = 1.013, B = -0.065
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 3. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 3. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 3. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 3. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$

0.004	30	62.50	753.2	744.4	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	413.4	415.8	0.03	0.03	1	1226.6	1204.3	0.04	0.03	
0.017	83	95.60	307.2	307.8	0.04	0.04	4	402.4	412.2	0.05	0.06	
0.023	97	97.14	247.0	248.6	0.03	0.04	5	179.9	187.7	0.07	0.06	
0.029	108	100.00	240.9	241.8	0.03	0.03	7	186.4	189.8	0.07	0.07	
0.036	126	99.25	270.0	270.1	0.03	0.03	6	252.5	249.6	0.04	0.05	
0.042	129	98.56	285.8	287.0	0.02	0.02	8	337.6	341.6	0.02	0.03	

```
 0.048    150  98.73   296.3   296.3  0.02  0.02      5   305.3   302.5  0.06  0.06
 0.055    151  99.38   280.8   280.6  0.02  0.02     10   257.5   258.8  0.05  0.05
 0.061    172 100.00   218.0   218.0  0.03  0.03     10   201.9   202.3  0.06  0.06
 0.067    174  99.45   211.1   210.7  0.03  0.03      6   285.8   280.2  0.03  0.04
 0.074    178  98.92   205.8   206.7  0.03  0.03      6   234.2   232.1  0.05  0.04
 0.080    189 100.00   208.4   208.5  0.02  0.02     13   159.4   152.7  0.08  0.09
 0.086    197 100.00   176.5   176.7  0.03  0.03      8   208.2   207.5  0.04  0.04
 0.093    193  93.55   156.7   156.4  0.03  0.03     10   181.7   185.3  0.09  0.08
 0.099    188  91.28   160.4   159.0  0.03  0.03     11   159.4   157.2  0.05  0.04
 0.105    190  86.02   153.6   153.1  0.03  0.03     13   169.0   169.5  0.08  0.07
 0.112    183  80.08   129.7   129.2  0.04  0.04      6   135.0   132.7  0.07  0.07
 0.118    194  81.85   126.8   126.5  0.03  0.03      9   137.8   138.1  0.06  0.07
 0.124    174  73.20   128.8   128.5  0.03  0.03      9   113.6   111.3  0.10  0.09
$$
```

**** Fom and SigmaA vs resolution ****

```
$TABLE: Cycle    3. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle    3. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa  FOMa  NREFc FOMc NREFall FOMall  SigmaA_Fc1 $$
$$
 0.0038    30   0.999     4   1.000    34   0.999  0.998
 0.0102    62   0.998     7   1.000    69   0.998  0.998
 0.0165    83   0.974    12   0.919    95   0.967  0.998
 0.0228    97   0.986    11   1.000   108   0.987  0.998
 0.0292   108   0.994     6   1.000   114   0.994  0.997
 0.0355   126   0.991    17   0.999   143   0.992  0.997
 0.0418   129   0.993    11   1.000   140   0.994  0.997
 0.0482   150   0.988    12   1.000   162   0.989  0.997
 0.0545   151   0.994    12   0.928   163   0.989  0.997
 0.0609   172   0.974    15   0.933   187   0.971  0.997
 0.0672   174   0.986     9   0.915   183   0.982  0.997
 0.0735   178   0.982    11   1.000   189   0.983  0.997
 0.0799   189   0.982    14   0.987   203   0.983  0.997
 0.0862   197   0.965     9   0.967   206   0.966  0.997
 0.0925   193   0.960    14   0.935   207   0.958  0.998
 0.0989   188   0.966    12   0.987   200   0.968  0.998
 0.1052   190   0.973     8   1.000   198   0.974  0.999
 0.1116   183   0.964    13   0.929   196   0.962  0.999
 0.1179   194   0.965    11   0.907   205   0.961  1.000
 0.1242   174   0.964     8   1.000   182   0.966  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0280
Free R factor                    =     0.0571
Overall weighted R factor        =     0.0280
Free weighted R factor           =     0.0574
```

Overall correlation coefficient = 0.9986
Free correlation coefficient = 0.9937
DPI based on free R factor = 0.1036
Overall figure of merit = 0.9763
ML based su of positional parameters = 0.0584
ML based su of thermal parameters = 2.8818

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 11657.598 2948.1106 41564.027 41669.469

CGMAT cycle number = 4

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
Weight matrix 0.60000002
Actual weight 2.9560583 is applied to the X-ray term
Norm of X_ray positional gradient 16.3
Norm of Geom. positional gradient 19.4
Norm of X_ray B-factor gradient 20.7
Norm of Geom. B-factor gradient 21.9
Product of X_ray and Geom posit. gradients -0.883E+06
Cosine of angle between them -0.754
Product of X_ray and Geom B-fact gradients -0.460E+06
Cosine of angle between them -0.823

Residuals: XRAY= 0.3382E+05 GEOM= 3091. TOTAL= 0.3691E+05
function value 36909.551

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.013	0.020
Bond angles : refined atoms	1663	1.569	1.966
Torsion angles, period 1. refined	155	7.658	5.000
Torsion angles, period 2. refined	54	41.039	25.741
Torsion angles, period 3. refined	214	18.662	15.000
Torsion angles, period 4. refined	3	20.570	15.000
Chiral centres: refined atoms	187	0.108	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	538	0.257	0.200
VDW; torsion: refined_atoms	794	0.319	0.200
HBOND: refined_atoms	39	0.196	0.200
VDW repulsions: symmetry: refined_atoms	58	0.247	0.200
HBOND: symmetry: refined_atoms	3	0.237	0.200

Bond B values: refined atoms 1229 8.593 4.656
Angle B values: refined atoms 1663 10.886 7.054
Torsion B values: refined atoms 426 20.483 12.946
Long range B values: refined atoms 1335 7.870 15.439

Overall : scale = 1.013, B = -0.079
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 4. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 4. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 4. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 4. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 753.6 745.4 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 413.7 416.2 0.03 0.03 1 1227.4 1205.1 0.03 0.03
0.017 83 95.60 307.4 308.1 0.04 0.03 4 402.6 411.9 0.05 0.06
0.023 97 97.14 247.2 248.5 0.03 0.03 5 180.1 187.9 0.07 0.06
0.029 108 100.00 241.1 241.9 0.03 0.03 7 186.5 189.5 0.07 0.06
0.036 126 99.25 270.1 270.4 0.03 0.02 6 252.6 250.1 0.04 0.05
0.042 129 98.56 286.0 287.2 0.02 0.02 8 337.8 341.3 0.02 0.02
0.048 150 98.73 296.5 296.5 0.02 0.02 5 305.5 303.5 0.05 0.05
0.055 151 99.38 281.0 280.8 0.02 0.02 10 257.7 259.2 0.05 0.05
0.061 172 100.00 218.2 218.1 0.02 0.02 10 202.0 202.4 0.06 0.06
0.067 174 99.45 211.3 210.7 0.02 0.03 6 286.0 280.9 0.03 0.04
0.074 178 98.92 205.9 206.7 0.02 0.02 6 234.3 232.3 0.05 0.03
0.080 189 100.00 208.5 208.7 0.02 0.02 13 159.5 153.1 0.08 0.08
0.086 197 100.00 176.6 176.6 0.03 0.03 8 208.3 207.7 0.04 0.04
0.093 193 93.55 156.8 156.6 0.03 0.03 10 181.8 185.3 0.09 0.08
0.099 188 91.28 160.5 159.2 0.03 0.03 11 159.5 157.3 0.05 0.04
0.105 190 86.02 153.7 153.2 0.03 0.03 13 169.1 170.0 0.08 0.07
0.112 183 80.08 129.8 129.2 0.03 0.03 6 135.1 133.1 0.07 0.07
0.118 194 81.85 126.8 126.2 0.03 0.03 9 137.9 138.2 0.06 0.07
0.124 174 73.20 128.9 128.5 0.02 0.02 9 113.7 111.9 0.10 0.09
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 4. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 4. M(Fom) v. resln :N:1,3,5,7,8:

$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
 0.0038   30 0.999   4 1.000   34 0.999 0.998
 0.0102   62 0.998   7 1.000   69 0.998 0.998
 0.0165   83 0.977   12 0.918   95 0.969 0.998
 0.0228   97 0.987   11 1.000 108 0.988 0.998
 0.0292 108 0.995   6 1.000 114 0.995 0.997
 0.0355 126 0.992   17 0.999 143 0.993 0.997
 0.0418 129 0.994   11 1.000 140 0.995 0.997
 0.0482 150 0.988   12 1.000 162 0.989 0.997
 0.0545 151 0.994   12 0.933 163 0.990 0.997
 0.0609 172 0.976   15 0.934 187 0.973 0.997
 0.0672 174 0.987   9 0.915 183 0.983 0.997
 0.0735 178 0.984   11 1.000 189 0.985 0.997
 0.0799 189 0.983   14 0.989 203 0.984 0.997
 0.0862 197 0.969   9 0.971 206 0.969 0.997
 0.0925 193 0.963   14 0.934 207 0.961 0.998
 0.0989 188 0.969   12 0.992 200 0.970 0.998
 0.1052 190 0.975   8 1.000 198 0.976 0.999
 0.1116 183 0.966   13 0.929 196 0.964 0.999
 0.1179 194 0.967   11 0.909 205 0.963 1.000
 0.1242 174 0.966   8 1.000 182 0.968 1.000
$$
Resolution limits   =   38.899   2.802
Number of used reflections   =   3184
Percentage observed   =   92.6870
Percentage of free reflections   =   4.8416
Overall R factor   =   0.0252
Free R factor   =   0.0540
Overall weighted R factor   =   0.0252
Free weighted R factor   =   0.0542
Overall correlation coefficient =   0.9989
Free correlation coefficient   =   0.9943
DPI based on free R factor   =   0.0981
Overall figure of merit   =   0.9779
ML based su of positional parameters =   0.0551
ML based su of thermal parameters   =   2.7217

 Trying gamma equal   0.0000000
 Convergence reached with no gamma cycles

 fvalues   11442.047   3090.7388   36980.555   36914.098

 fvalues   11442.047   3090.7388   36861.738   36914.098

    CGMAT cycle number =   5

 Limits of asymmetric unit   : 1.00 1.00 0.50

```
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    2.8403156      is applied to the X-ray term
Norm of X_ray positional gradient              16.6
Norm of Geom. positional gradient              18.9
Norm of X_ray B-factor gradient                21.0
Norm of Geom. B-factor gradient                21.2
Product of X_ray and Geom posit. gradients     -0.928E+06
 Cosine of angle between them                  -0.804
Product of X_ray and Geom B-fact gradients     -0.517E+06
 Cosine of angle between them                  -0.946


Residuals: XRAY=     0.3232E+05 GEOM=      3079.     TOTAL=     0.3540E+05
 function value    35399.730

------------------------------------------------------------------------------
          Restraint type            N restraints   Rms Delta   Av(Sigma)
Bond distances: refined atoms              1229     0.013     0.020
Bond angles  : refined atoms               1663     1.568     1.966
Torsion angles, period  1. refined          155     7.670     5.000
Torsion angles, period  2. refined           54    41.042    25.741
Torsion angles, period  3. refined          214    18.692    15.000
Torsion angles, period  4. refined            3    20.600    15.000
Chiral centres: refined atoms              187     0.108     0.200
Planar groups: refined atoms               924     0.005     0.021
VDW repulsions: refined_atoms              540     0.257     0.200
VDW; torsion: refined_atoms                794     0.319     0.200
HBOND: refined_atoms                        39     0.196     0.200
VDW repulsions: symmetry: refined_atoms     57     0.250     0.200
HBOND: symmetry: refined_atoms               3     0.238     0.200
Bond B values: refined atoms               1229     9.051     4.655
Angle B values: refined atoms              1663    11.447     7.052
Torsion B values: refined atoms             426    21.432    12.940
Long range B values: refined atoms         1337     8.277    15.386
------------------------------------------------------------------------------

------------------------------------------------------------------------------
Overall            : scale =    1.013, B  =  -0.051
Overall anisotropic scale factors
   B11 =  0.28 B22 =  0.17 B33 = -0.47 B12 =  0.00 B13 = -0.36 B23 =  0.00
------------------------------------------------------------------------------

------------------------------------------------------------------------------

    ****          Things for loggraph, R factor and others          ****
```

$TABLE: Cycle 5. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 5. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 5. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 5. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 753.6 745.4 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 413.7 416.1 0.03 0.03 1 1227.4 1204.4 0.03 0.03
0.017 83 95.60 307.4 308.1 0.03 0.03 4 402.6 412.5 0.05 0.06
0.023 97 97.14 247.1 248.6 0.03 0.03 5 180.1 188.7 0.07 0.06
0.029 108 100.00 241.1 241.9 0.03 0.03 7 186.5 189.7 0.07 0.06
0.036 126 99.25 270.1 270.3 0.02 0.02 6 252.6 250.4 0.04 0.05
0.042 129 98.56 286.0 287.3 0.02 0.02 8 337.8 341.2 0.02 0.02
0.048 150 98.73 296.4 296.5 0.02 0.02 5 305.5 304.0 0.05 0.05
0.055 151 99.38 281.0 280.8 0.02 0.02 10 257.7 259.2 0.05 0.05
0.061 172 100.00 218.2 218.1 0.02 0.02 10 202.0 202.3 0.05 0.06
0.067 174 99.45 211.3 210.7 0.02 0.03 6 286.0 281.2 0.03 0.04
0.074 178 98.92 205.9 206.7 0.02 0.02 6 234.3 232.2 0.04 0.03
0.080 189 100.00 208.5 208.7 0.02 0.02 13 159.5 153.1 0.08 0.08
0.086 197 100.00 176.6 176.7 0.03 0.03 8 208.3 207.5 0.04 0.04
0.093 193 93.55 156.8 156.6 0.03 0.03 10 181.8 185.4 0.08 0.08
0.099 188 91.28 160.5 159.2 0.03 0.03 11 159.5 157.5 0.04 0.04
0.105 190 86.02 153.7 153.2 0.03 0.03 13 169.1 170.1 0.07 0.07
0.112 183 80.08 129.8 129.3 0.03 0.03 6 135.1 133.2 0.07 0.07
0.118 194 81.85 126.8 126.3 0.03 0.03 9 137.9 138.1 0.06 0.07
0.124 174 73.20 128.9 128.5 0.02 0.02 9 113.7 111.7 0.10 0.09
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 5. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 5. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.998
0.0102 62 0.998 7 1.000 69 0.998 0.998
0.0165 83 0.978 12 0.919 95 0.970 0.998
0.0228 97 0.987 11 1.000 108 0.988 0.998
0.0292 108 0.995 6 1.000 114 0.995 0.997
0.0355 126 0.992 17 1.000 143 0.993 0.997
0.0418 129 0.994 11 1.000 140 0.995 0.997
0.0482 150 0.988 12 1.000 162 0.989 0.997
0.0545 151 0.995 12 0.937 163 0.990 0.997
0.0609 172 0.976 15 0.935 187 0.973 0.997
0.0672 174 0.987 9 0.913 183 0.984 0.997
0.0735 178 0.984 11 1.000 189 0.985 0.997

```
 0.0799   189   0.984    14   0.990   203   0.984  0.997
 0.0862   197   0.971     9   0.972   206   0.971  0.997
 0.0925   193   0.964    14   0.934   207   0.962  0.998
 0.0989   188   0.970    12   0.994   200   0.971  0.998
 0.1052   190   0.976     8   1.000   198   0.977  0.999
 0.1116   183   0.968    13   0.929   196   0.965  0.999
 0.1179   194   0.968    11   0.914   205   0.965  1.000
 0.1242   174   0.967     8   1.000   182   0.969  1.000
$$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0247
Free R factor                    =     0.0531
Overall weighted R factor        =     0.0247
Free weighted R factor           =     0.0533
Overall correlation coefficient  =     0.9989
Free correlation coefficient     =     0.9945
DPI based on free R factor       =     0.0965
Overall figure of merit          =     0.9787
ML based su of positional parameters =     0.0540
ML based su of thermal parameters    =     2.6683
--------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    11380.050       3079.3130       35465.145       35402.246

 fvalues    11380.050       3079.3130       35358.141       35402.246


    CGMAT cycle number =      6

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000008
 Actual weight    2.7238374      is applied to the X-ray term
Norm of X_ray positional gradient              16.5
Norm of Geom. positional gradient              18.5
Norm of X_ray B-factor gradient                20.9
Norm of Geom. B-factor gradient                20.9
Product of X_ray and Geom posit. gradients     -0.916E+06
 Cosine of angle between them                  -0.813
Product of X_ray and Geom B-fact gradients     -0.515E+06
```

Cosine of angle between them -0.959

Residuals: XRAY= 0.3081E+05 GEOM= 3082. TOTAL= 0.3389E+05
function value 33891.414

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.013	0.020
Bond angles : refined atoms	1663	1.573	1.966
Torsion angles, period 1. refined	155	7.685	5.000
Torsion angles, period 2. refined	54	41.043	25.741
Torsion angles, period 3. refined	214	18.689	15.000
Torsion angles, period 4. refined	3	20.642	15.000
Chiral centres: refined atoms	187	0.108	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	539	0.257	0.200
VDW; torsion: refined_atoms	791	0.320	0.200
HBOND: refined_atoms	39	0.196	0.200
VDW repulsions: symmetry: refined_atoms	57	0.251	0.200
HBOND: symmetry: refined_atoms	3	0.239	0.200
Bond B values: refined atoms	1229	9.497	4.659
Angle B values: refined atoms	1663	11.994	7.058
Torsion B values: refined atoms	426	22.400	12.948
Long range B values: refined atoms	1334	8.688	15.362

Overall : scale = 1.012, B = -0.049
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 6. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 6. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 6. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 6. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$

0.004	30	62.50	753.8	745.9	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	413.8	416.1	0.03	0.03	1	1227.6	1207.7	0.03	0.03	
0.017	83	95.60	307.5	308.1	0.03	0.03	4	402.7	411.9	0.04	0.05	
0.023	97	97.14	247.2	248.5	0.03	0.03	5	180.1	188.4	0.07	0.06	
0.029	108	100.00	241.1	241.9	0.03	0.03	7	186.6	189.6	0.07	0.06	

0.036	126	99.25	270.2	270.4	0.02	0.02	6	252.7	250.6	0.04	0.04
0.042	129	98.56	286.1	287.3	0.02	0.02	8	337.9	341.2	0.02	0.02
0.048	150	98.73	296.5	296.5	0.02	0.02	5	305.6	304.4	0.05	0.05
0.055	151	99.38	281.0	280.9	0.02	0.02	10	257.7	259.3	0.04	0.04
0.061	172	100.00	218.2	218.2	0.02	0.02	10	202.0	202.3	0.05	0.05
0.067	174	99.45	211.3	210.8	0.02	0.02	6	286.1	281.5	0.03	0.04
0.074	178	98.92	205.9	206.8	0.02	0.02	6	234.4	232.2	0.04	0.03
0.080	189	100.00	208.5	208.7	0.02	0.02	13	159.5	153.2	0.07	0.08
0.086	197	100.00	176.6	176.7	0.03	0.02	8	208.4	207.6	0.04	0.04
0.093	193	93.55	156.8	156.6	0.03	0.03	10	181.8	185.3	0.08	0.08
0.099	188	91.28	160.6	159.3	0.02	0.02	11	159.5	157.5	0.04	0.04
0.105	190	86.02	153.7	153.2	0.03	0.03	13	169.1	170.2	0.07	0.07
0.112	183	80.08	129.8	129.3	0.03	0.03	6	135.1	133.5	0.07	0.07
0.118	194	81.85	126.9	126.4	0.03	0.03	9	137.9	138.0	0.06	0.07
0.124	174	73.20	128.9	128.5	0.02	0.02	9	113.7	111.7	0.10	0.09

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 6. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 6. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.998
0.0102	62	0.998	7	1.000	69	0.998	0.998
0.0165	83	0.979	12	0.918	95	0.971	0.998
0.0228	97	0.987	11	1.000	108	0.988	0.998
0.0292	108	0.995	6	1.000	114	0.995	0.997
0.0355	126	0.993	17	1.000	143	0.994	0.997
0.0418	129	0.995	11	1.000	140	0.995	0.997
0.0482	150	0.989	12	1.000	162	0.990	0.997
0.0545	151	0.995	12	0.940	163	0.991	0.997
0.0609	172	0.977	15	0.936	187	0.974	0.997
0.0672	174	0.988	9	0.913	183	0.984	0.997
0.0735	178	0.985	11	1.000	189	0.986	0.997
0.0799	189	0.984	14	0.991	203	0.985	0.997
0.0862	197	0.972	9	0.974	206	0.972	0.997
0.0925	193	0.966	14	0.933	207	0.964	0.998
0.0989	188	0.971	12	0.994	200	0.972	0.998
0.1052	190	0.976	8	1.000	198	0.977	0.999
0.1116	183	0.968	13	0.929	196	0.966	0.999
0.1179	194	0.968	11	0.909	205	0.965	1.000
0.1242	174	0.968	8	1.000	182	0.969	1.000

$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0242
Free R factor = 0.0519

Overall weighted R factor = 0.0242
Free weighted R factor = 0.0521
Overall correlation coefficient = 0.9990
Free correlation coefficient = 0.9948
DPI based on free R factor = 0.0942
Overall figure of merit = 0.9793
ML based su of positional parameters = 0.0529
ML based su of thermal parameters = 2.6165

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 11312.007 3081.8352 33855.172 33893.902

CGMAT cycle number = 7

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 2.5373695 is applied to the X-ray term
Norm of X_ray positional gradient 16.0
Norm of Geom. positional gradient 18.4
Norm of X_ray B-factor gradient 20.5
Norm of Geom. B-factor gradient 20.7
Product of X_ray and Geom posit. gradients -0.883E+06
Cosine of angle between them -0.812
Product of X_ray and Geom B-fact gradients -0.505E+06
Cosine of angle between them -0.970

Residuals: XRAY= 0.2842E+05 GEOM= 3110. TOTAL= 0.3153E+05
function value 31531.932

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.012	0.020
Bond angles : refined atoms	1663	1.609	1.966
Torsion angles, period 1. refined	155	7.719	5.000
Torsion angles, period 2. refined	54	41.051	25.741
Torsion angles, period 3. refined	214	18.580	15.000
Torsion angles, period 4. refined	3	20.723	15.000
Chiral centres: refined atoms	187	0.110	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	539	0.257	0.200

VDW; torsion: refined_atoms 789 0.321 0.200
HBOND: refined_atoms 39 0.197 0.200
VDW repulsions: symmetry: refined_atoms 57 0.252 0.200
HBOND: symmetry: refined_atoms 3 0.244 0.200
Bond B values: refined atoms 1229 9.901 4.663
Angle B values: refined atoms 1663 12.592 7.059
Torsion B values: refined atoms 426 23.567 12.953
Long range B values: refined atoms 1333 9.125 15.359

Overall : scale = 1.012, B = -0.023
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 7. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 7. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 7. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 7. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 753.8 746.0 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 413.8 416.2 0.03 0.02 1 1227.7 1206.2 0.03 0.03
0.017 83 95.60 307.5 308.2 0.03 0.03 4 402.7 412.5 0.04 0.06
0.023 97 97.14 247.2 248.5 0.03 0.03 5 180.1 189.1 0.07 0.06
0.029 108 100.00 241.1 241.9 0.03 0.03 7 186.6 189.7 0.07 0.06
0.036 126 99.25 270.2 270.4 0.02 0.02 6 252.7 250.9 0.04 0.04
0.042 129 98.56 286.1 287.4 0.02 0.02 8 337.9 341.2 0.02 0.02
0.048 150 98.73 296.5 296.5 0.02 0.02 5 305.6 305.0 0.05 0.05
0.055 151 99.38 281.1 281.0 0.02 0.02 10 257.7 259.4 0.04 0.04
0.061 172 100.00 218.2 218.3 0.02 0.02 10 202.0 202.1 0.05 0.05
0.067 174 99.45 211.3 210.8 0.02 0.02 6 286.1 282.0 0.03 0.04
0.074 178 98.92 206.0 206.8 0.02 0.02 6 234.4 232.4 0.04 0.03
0.080 189 100.00 208.5 208.8 0.02 0.02 13 159.5 153.4 0.07 0.08
0.086 197 100.00 176.6 176.8 0.03 0.02 8 208.4 207.6 0.04 0.04
0.093 193 93.55 156.8 156.7 0.03 0.03 10 181.8 185.5 0.08 0.07
0.099 188 91.28 160.6 159.3 0.02 0.02 11 159.5 157.6 0.04 0.03
0.105 190 86.02 153.7 153.2 0.03 0.03 13 169.1 170.4 0.07 0.06
0.112 183 80.08 129.8 129.3 0.03 0.03 6 135.1 133.9 0.07 0.07
0.118 194 81.85 126.9 126.4 0.03 0.03 9 137.9 137.9 0.06 0.07
0.124 174 73.20 128.9 128.5 0.02 0.02 9 113.7 111.7 0.09 0.08
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 7. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 7. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.998
0.0102	62	0.998	7	1.000	69	0.998	0.998
0.0165	83	0.981	12	0.919	95	0.973	0.998
0.0228	97	0.987	11	1.000	108	0.989	0.998
0.0292	108	0.995	6	1.000	114	0.996	0.997
0.0355	126	0.993	17	1.000	143	0.994	0.997
0.0418	129	0.995	11	1.000	140	0.995	0.997
0.0482	150	0.989	12	1.000	162	0.990	0.997
0.0545	151	0.995	12	0.944	163	0.991	0.997
0.0609	172	0.978	15	0.937	187	0.974	0.997
0.0672	174	0.989	9	0.914	183	0.985	0.997
0.0735	178	0.985	11	1.000	189	0.986	0.997
0.0799	189	0.985	14	0.992	203	0.985	0.997
0.0862	197	0.974	9	0.976	206	0.974	0.997
0.0925	193	0.968	14	0.932	207	0.966	0.998
0.0989	188	0.972	12	0.996	200	0.973	0.998
0.1052	190	0.978	8	1.000	198	0.979	0.999
0.1116	183	0.970	13	0.929	196	0.967	0.999
0.1179	194	0.970	11	0.915	205	0.967	1.000
0.1242	174	0.970	8	1.000	182	0.971	1.000

$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0233
Free R factor = 0.0504
Overall weighted R factor = 0.0233
Free weighted R factor = 0.0505
Overall correlation coefficient = 0.9990
Free correlation coefficient = 0.9951
DPI based on free R factor = 0.0915
Overall figure of merit = 0.9804
ML based su of positional parameters = 0.0510
ML based su of thermal parameters = 2.5261

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 11201.706 3110.2126 31521.143 31533.080

CGMAT cycle number = 8

**** Bond distance outliers ****

Bond distance deviations from the ideal >10.000Sigma will be monitored

A 135 LYS CD . - A 135 LYS CE . mod.= 1.755 id.= 1.520 dev= -0.235 sig.= 0.020

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 2.3657455 is applied to the X-ray term
Norm of X_ray positional gradient 15.5
Norm of Geom. positional gradient 20.3
Norm of X_ray B-factor gradient 19.7
Norm of Geom. B-factor gradient 20.4
Product of X_ray and Geom posit. gradients -0.843E+06
Cosine of angle between them -0.725
Product of X_ray and Geom B-fact gradients -0.477E+06
Cosine of angle between them -0.964

Residuals: XRAY= 0.2625E+05 GEOM= 3158. TOTAL= 0.2940E+05
function value 29404.602

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.013	0.020
Bond angles : refined atoms	1663	1.604	1.966
Torsion angles, period 1. refined	155	7.749	5.000
Torsion angles, period 2. refined	54	41.039	25.741
Torsion angles, period 3. refined	214	18.700	15.000
Torsion angles, period 4. refined	3	20.806	15.000
Chiral centres: refined atoms	187	0.110	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	538	0.258	0.200
VDW; torsion: refined_atoms	789	0.322	0.200
HBOND: refined_atoms	39	0.198	0.200
VDW repulsions: symmetry: refined_atoms	57	0.253	0.200
HBOND: symmetry: refined_atoms	3	0.246	0.200
Bond B values: refined atoms	1229	10.352	4.671
Angle B values: refined atoms	1663	13.179	7.068
Torsion B values: refined atoms	426	24.665	12.974
Long range B values: refined atoms	1332	9.551	15.369

Overall : scale = 1.012, B = -0.023
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 8. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 8. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 8. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 8. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.0 746.3 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 413.9 416.2 0.02 0.02 1 1227.9 1208.4 0.03 0.03
0.017 83 95.60 307.6 308.3 0.03 0.03 4 402.8 412.5 0.04 0.05
0.023 97 97.14 247.3 248.5 0.03 0.03 5 180.1 189.3 0.07 0.06
0.029 108 100.00 241.2 241.9 0.02 0.03 7 186.6 189.5 0.07 0.06
0.036 126 99.25 270.2 270.5 0.02 0.02 6 252.8 251.1 0.04 0.04
0.042 129 98.56 286.1 287.4 0.02 0.02 8 337.9 341.1 0.02 0.02
0.048 150 98.73 296.6 296.5 0.02 0.02 5 305.6 305.3 0.05 0.05
0.055 151 99.38 281.1 281.1 0.02 0.02 10 257.8 259.5 0.04 0.04
0.061 172 100.00 218.3 218.3 0.02 0.02 10 202.1 202.0 0.05 0.05
0.067 174 99.45 211.4 210.8 0.02 0.02 6 286.1 282.5 0.03 0.03
0.074 178 98.92 206.0 206.8 0.02 0.02 6 234.4 232.6 0.04 0.03
0.080 189 100.00 208.6 208.8 0.02 0.02 13 159.6 153.6 0.07 0.08
0.086 197 100.00 176.7 176.8 0.02 0.02 8 208.4 207.6 0.04 0.04
0.093 193 93.55 156.8 156.7 0.03 0.03 10 181.9 185.6 0.08 0.07
0.099 188 91.28 160.6 159.4 0.02 0.02 11 159.6 157.7 0.03 0.03
0.105 190 86.02 153.8 153.2 0.02 0.03 13 169.1 170.6 0.07 0.06
0.112 183 80.08 129.8 129.4 0.03 0.03 6 135.1 134.2 0.07 0.07
0.118 194 81.85 126.9 126.4 0.03 0.03 9 138.0 137.8 0.06 0.06
0.124 174 73.20 128.9 128.6 0.02 0.02 9 113.8 111.7 0.09 0.08
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 8. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 8. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.998
0.0102 62 0.998 7 1.000 69 0.999 0.998
0.0165 83 0.984 12 0.918 95 0.975 0.998
0.0228 97 0.988 11 1.000 108 0.989 0.998

```
 0.0292   108   0.996    6   1.000   114   0.996  0.998
 0.0355   126   0.994   17   1.000   143   0.994  0.998
 0.0418   129   0.995   11   1.000   140   0.996  0.998
 0.0482   150   0.989   12   1.000   162   0.990  0.998
 0.0545   151   0.995   12   0.951   163   0.992  0.998
 0.0609   172   0.978   15   0.938   187   0.975  0.998
 0.0672   174   0.990    9   0.916   183   0.986  0.999
 0.0735   178   0.986   11   1.000   189   0.987  0.999
 0.0799   189   0.986   14   0.994   203   0.986  0.999
 0.0862   197   0.976    9   0.978   206   0.976  0.999
 0.0925   193   0.970   14   0.932   207   0.967  0.999
 0.0989   188   0.973   12   0.997   200   0.975  0.999
 0.1052   190   0.979    8   1.000   198   0.980  0.999
 0.1116   183   0.972   13   0.930   196   0.969  1.000
 0.1179   194   0.971   11   0.917   205   0.968  1.000
 0.1242   174   0.972    8   1.000   182   0.973  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0225
Free R factor                    =     0.0489
Overall weighted R factor        =     0.0225
Free weighted R factor           =     0.0490
Overall correlation coefficient  =     0.9991
Free correlation coefficient     =     0.9954
DPI based on free R factor       =     0.0887
Overall figure of merit          =     0.9814
ML based su of positional parameters =     0.0493
ML based su of thermal parameters    =     2.4412
------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    11094.459       3158.2090       29352.734       29404.875


    CGMAT cycle number =      9

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    2.2249207      is applied to the X-ray term
Norm of X_ray positional gradient              15.3
```

Norm of Geom. positional gradient 18.4
Norm of X_ray B-factor gradient 19.4
Norm of Geom. B-factor gradient 20.0
Product of X_ray and Geom posit. gradients -0.827E+06
Cosine of angle between them -0.796
Product of X_ray and Geom B-fact gradients -0.463E+06
Cosine of angle between them -0.970

Residuals: XRAY= 0.2448E+05 GEOM= 3145. TOTAL= 0.2762E+05
function value 27623.551

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.013	0.020
Bond angles : refined atoms	1663	1.607	1.966
Torsion angles, period 1. refined	155	7.771	5.000
Torsion angles, period 2. refined	54	41.027	25.741
Torsion angles, period 3. refined	214	18.743	15.000
Torsion angles, period 4. refined	3	20.884	15.000
Chiral centres: refined atoms	187	0.110	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	537	0.259	0.200
VDW; torsion: refined_atoms	788	0.322	0.200
HBOND: refined_atoms	40	0.196	0.200
VDW repulsions: symmetry: refined_atoms	57	0.254	0.200
HBOND: symmetry: refined_atoms	3	0.250	0.200
Bond B values: refined atoms	1229	10.848	4.689
Angle B values: refined atoms	1663	13.767	7.094
Torsion B values: refined atoms	426	25.720	13.013
Long range B values: refined atoms	1331	9.986	15.389

Overall : scale = 1.012, B = -0.072
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 9. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 9. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 9. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 9. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$

$$
 0.004 30 62.50 754.1 746.9 0.02 0.02 0 0.0 0.0****** 0.00
 0.010 62 95.45 413.9 416.3 0.02 0.02 1 1228.2 1213.6 0.03 0.02
 0.017 83 95.60 307.6 308.4 0.03 0.03 4 402.9 412.2 0.04 0.05
 0.023 97 97.14 247.3 248.4 0.03 0.03 5 180.2 188.9 0.07 0.06
 0.029 108 100.00 241.2 241.9 0.02 0.02 7 186.7 189.5 0.06 0.06
 0.036 126 99.25 270.3 270.5 0.02 0.02 6 252.8 251.5 0.04 0.04
 0.042 129 98.56 286.2 287.5 0.02 0.02 8 338.0 341.2 0.02 0.02
 0.048 150 98.73 296.6 296.6 0.02 0.02 5 305.7 305.7 0.05 0.04
 0.055 151 99.38 281.2 281.1 0.02 0.02 10 257.8 259.6 0.04 0.04
 0.061 172 100.00 218.3 218.3 0.02 0.02 10 202.1 202.0 0.04 0.05
 0.067 174 99.45 211.4 210.8 0.02 0.02 6 286.2 282.8 0.03 0.03
 0.074 178 98.92 206.0 206.8 0.02 0.02 6 234.5 232.8 0.04 0.03
 0.080 189 100.00 208.6 208.8 0.02 0.02 13 159.6 153.8 0.07 0.07
 0.086 197 100.00 176.7 176.8 0.02 0.02 8 208.5 207.7 0.04 0.04
 0.093 193 93.55 156.9 156.7 0.03 0.03 10 181.9 185.5 0.08 0.07
 0.099 188 91.28 160.6 159.5 0.02 0.02 11 159.6 157.8 0.03 0.03
 0.105 190 86.02 153.8 153.3 0.02 0.03 13 169.2 170.7 0.07 0.06
 0.112 183 80.08 129.8 129.4 0.03 0.03 6 135.2 134.8 0.07 0.07
 0.118 194 81.85 126.9 126.5 0.03 0.03 9 138.0 137.9 0.06 0.06
 0.124 174 73.20 129.0 128.7 0.02 0.02 9 113.8 111.8 0.09 0.08
$$

  **** Fom and SigmaA vs resolution ****

 $TABLE: Cycle 9. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
 $GRAPHS:Cycle 9. M(Fom) v. resln :N:1,3,5,7,8:
 $$
 <4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
 $$
  0.0038 30 0.999 4 1.000 34 0.999 0.998
  0.0102 62 0.999 7 1.000 69 0.999 0.998
  0.0165 83 0.985 12 0.918 95 0.977 0.998
  0.0228 97 0.988 11 1.000 108 0.989 0.998
  0.0292 108 0.996 6 1.000 114 0.996 0.998
  0.0355 126 0.994 17 1.000 143 0.995 0.998
  0.0418 129 0.996 11 1.000 140 0.996 0.998
  0.0482 150 0.990 12 1.000 162 0.990 0.998
  0.0545 151 0.996 12 0.955 163 0.993 0.998
  0.0609 172 0.979 15 0.937 187 0.976 0.998
  0.0672 174 0.990 9 0.916 183 0.987 0.999
  0.0735 178 0.987 11 1.000 189 0.988 0.999
  0.0799 189 0.986 14 0.995 203 0.987 0.999
  0.0862 197 0.977 9 0.981 206 0.977 0.999
  0.0925 193 0.971 14 0.931 207 0.969 0.999
  0.0989 188 0.974 12 0.998 200 0.976 0.999
  0.1052 190 0.981 8 1.000 198 0.981 0.999
  0.1116 183 0.973 13 0.930 196 0.970 1.000
  0.1179 194 0.972 11 0.911 205 0.969 1.000
  0.1242 174 0.973 8 1.000 182 0.974 1.000
 $$

Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0221
Free R factor = 0.0472
Overall weighted R factor = 0.0220
Free weighted R factor = 0.0473
Overall correlation coefficient = 0.9991
Free correlation coefficient = 0.9957
DPI based on free R factor = 0.0857
Overall figure of merit = 0.9822
ML based su of positional parameters = 0.0478
ML based su of thermal parameters = 2.3714

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 11003.294 3144.7041 27704.648 27626.160

fvalues 11003.294 3144.7041 27654.227 27626.160

CGMAT cycle number = 10

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000008
Actual weight 2.1975331 is applied to the X-ray term
Norm of X_ray positional gradient 15.2
Norm of Geom. positional gradient 18.3
Norm of X_ray B-factor gradient 19.3
Norm of Geom. B-factor gradient 20.0
Product of X_ray and Geom posit. gradients -0.820E+06
Cosine of angle between them -0.799
Product of X_ray and Geom B-fact gradients -0.461E+06
Cosine of angle between them -0.973

Residuals: XRAY= 0.2414E+05 GEOM= 3142. TOTAL= 0.2728E+05
function value 27277.012

Restraint type N restraints Rms Delta Av(Sigma)
Bond distances: refined atoms 1229 0.013 0.020

Bond angles : refined atoms 1663 1.604 1.966
Torsion angles, period 1. refined 155 7.776 5.000
Torsion angles, period 2. refined 54 41.017 25.741
Torsion angles, period 3. refined 214 18.744 15.000
Torsion angles, period 4. refined 3 20.897 15.000
Chiral centres: refined atoms 187 0.110 0.200
Planar groups: refined atoms 924 0.005 0.021
VDW repulsions: refined_atoms 539 0.259 0.200
VDW; torsion: refined_atoms 788 0.323 0.200
HBOND: refined_atoms 40 0.196 0.200
VDW repulsions: symmetry: refined_atoms 57 0.254 0.200
HBOND: symmetry: refined_atoms 3 0.251 0.200
Bond B values: refined atoms 1229 11.134 4.690
Angle B values: refined atoms 1663 14.037 7.096
Torsion B values: refined atoms 426 26.163 13.015
Long range B values: refined atoms 1333 10.196 15.386

Overall : scale = 1.012, B = -0.068
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 10. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 10. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 10. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 10. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.1 746.9 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 413.9 416.3 0.02 0.02 1 1228.2 1213.9 0.02 0.02
0.017 83 95.60 307.6 308.4 0.03 0.03 4 402.9 412.2 0.04 0.05
0.023 97 97.14 247.3 248.4 0.03 0.03 5 180.2 189.0 0.07 0.06
0.029 108 100.00 241.2 241.9 0.02 0.02 7 186.7 189.5 0.06 0.06
0.036 126 99.25 270.3 270.6 0.02 0.02 6 252.8 251.5 0.04 0.04
0.042 129 98.56 286.2 287.5 0.02 0.02 8 338.0 341.2 0.02 0.02
0.048 150 98.73 296.7 296.6 0.02 0.02 5 305.7 305.8 0.04 0.04
0.055 151 99.38 281.2 281.1 0.02 0.02 10 257.8 259.6 0.04 0.04
0.061 172 100.00 218.3 218.3 0.02 0.02 10 202.1 202.0 0.04 0.05
0.067 174 99.45 211.4 210.8 0.02 0.02 6 286.2 282.9 0.03 0.03
0.074 178 98.92 206.0 206.8 0.02 0.02 6 234.5 232.9 0.04 0.03
0.080 189 100.00 208.6 208.8 0.02 0.02 13 159.6 153.9 0.07 0.07
0.086 197 100.00 176.7 176.8 0.02 0.02 8 208.5 207.7 0.04 0.04

0.093	193	93.55	156.9	156.7	0.03	0.03	10	181.9	185.5	0.08	0.07
0.099	188	91.28	160.6	159.5	0.02	0.02	11	159.6	157.8	0.03	0.03
0.105	190	86.02	153.8	153.3	0.02	0.03	13	169.2	170.7	0.07	0.06
0.112	183	80.08	129.8	129.5	0.03	0.03	6	135.2	134.9	0.07	0.07
0.118	194	81.85	126.9	126.5	0.03	0.03	9	138.0	137.9	0.06	0.06
0.124	174	73.20	129.0	128.7	0.02	0.02	9	113.8	111.8	0.09	0.08

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 10. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 10. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.998
0.0102	62	0.999	7	1.000	69	0.999	0.998
0.0165	83	0.985	12	0.918	95	0.977	0.998
0.0228	97	0.988	11	1.000	108	0.989	0.998
0.0292	108	0.996	6	1.000	114	0.996	0.998
0.0355	126	0.994	17	1.000	143	0.995	0.998
0.0418	129	0.996	11	1.000	140	0.996	0.998
0.0482	150	0.990	12	1.000	162	0.991	0.998
0.0545	151	0.996	12	0.957	163	0.993	0.998
0.0609	172	0.979	15	0.937	187	0.976	0.998
0.0672	174	0.990	9	0.918	183	0.987	0.999
0.0735	178	0.987	11	1.000	189	0.988	0.999
0.0799	189	0.986	14	0.996	203	0.987	0.999
0.0862	197	0.977	9	0.981	206	0.978	0.999
0.0925	193	0.972	14	0.931	207	0.969	0.999
0.0989	188	0.975	12	0.998	200	0.976	0.999
0.1052	190	0.981	8	1.000	198	0.982	0.999
0.1116	183	0.973	13	0.930	196	0.970	1.000
0.1179	194	0.972	11	0.911	205	0.969	1.000
0.1242	174	0.973	8	1.000	182	0.974	1.000

$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0219
Free R factor = 0.0469
Overall weighted R factor = 0.0219
Free weighted R factor = 0.0470
Overall correlation coefficient = 0.9991
Free correlation coefficient = 0.9957
DPI based on free R factor = 0.0852
Overall figure of merit = 0.9824
ML based su of positional parameters = 0.0475
ML based su of thermal parameters = 2.3568

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10983.927 3141.7542 27236.453 27279.297

CGMAT cycle number = 11

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000008
Actual weight 2.1156054 is applied to the X-ray term
Norm of X_ray positional gradient 15.0
Norm of Geom. positional gradient 15.7
Norm of X_ray B-factor gradient 19.0
Norm of Geom. B-factor gradient 19.9
Product of X_ray and Geom posit. gradients -0.802E+06
Cosine of angle between them -0.927
Product of X_ray and Geom B-fact gradients -0.454E+06
Cosine of angle between them -0.973

Residuals: XRAY= 0.2312E+05 GEOM= 3125. TOTAL= 0.2624E+05
function value 26242.074

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.012	0.020
Bond angles : refined atoms	1663	1.632	1.966
Torsion angles, period 1. refined	155	7.793	5.000
Torsion angles, period 2. refined	54	40.981	25.741
Torsion angles, period 3. refined	214	18.850	15.000
Torsion angles, period 4. refined	3	20.947	15.000
Chiral centres: refined atoms	187	0.110	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	538	0.260	0.200
VDW; torsion: refined_atoms	789	0.323	0.200
HBOND: refined_atoms	40	0.196	0.200
VDW repulsions: symmetry: refined_atoms	57	0.254	0.200
HBOND: symmetry: refined_atoms	3	0.255	0.200
Bond B values: refined atoms	1229	11.721	4.691
Angle B values: refined atoms	1663	14.659	7.096
Torsion B values: refined atoms	426	27.276	13.012
Long range B values: refined atoms	1333	10.635	15.368

Overall : scale = 1.012, B = -0.043
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 11. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 11. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 11. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 11. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.1 746.8 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 413.9 416.3 0.02 0.02 1 1228.2 1212.0 0.02 0.02
0.017 83 95.60 307.6 308.4 0.03 0.03 4 402.9 412.8 0.04 0.05
0.023 97 97.14 247.3 248.5 0.02 0.03 5 180.2 189.6 0.07 0.06
0.029 108 100.00 241.2 241.9 0.02 0.02 7 186.7 189.5 0.07 0.06
0.036 126 99.25 270.3 270.6 0.02 0.02 6 252.8 251.7 0.04 0.04
0.042 129 98.56 286.2 287.5 0.02 0.02 8 338.0 341.2 0.02 0.02
0.048 150 98.73 296.6 296.5 0.02 0.02 5 305.7 306.0 0.04 0.04
0.055 151 99.38 281.2 281.1 0.02 0.02 10 257.8 259.7 0.04 0.04
0.061 172 100.00 218.3 218.4 0.02 0.02 10 202.1 201.9 0.04 0.04
0.067 174 99.45 211.4 210.8 0.02 0.02 6 286.2 283.1 0.02 0.03
0.074 178 98.92 206.0 206.8 0.02 0.02 6 234.5 233.2 0.04 0.03
0.080 189 100.00 208.6 208.9 0.02 0.02 13 159.6 154.0 0.06 0.07
0.086 197 100.00 176.7 176.8 0.02 0.02 8 208.5 207.8 0.04 0.04
0.093 193 93.55 156.9 156.8 0.03 0.03 10 181.9 185.6 0.08 0.07
0.099 188 91.28 160.6 159.5 0.02 0.02 11 159.6 157.8 0.03 0.03
0.105 190 86.02 153.8 153.3 0.02 0.02 13 169.2 170.8 0.06 0.06
0.112 183 80.08 129.8 129.5 0.03 0.03 6 135.2 135.3 0.07 0.07
0.118 194 81.85 126.9 126.5 0.03 0.03 9 138.0 137.8 0.06 0.06
0.124 174 73.20 129.0 128.7 0.02 0.02 9 113.8 111.8 0.09 0.08
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 11. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 11. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999

```
 0.0165   83  0.986   12  0.919   95  0.978  0.999
 0.0228   97  0.988   11  1.000  108  0.989  0.999
 0.0292  108  0.996    6  1.000  114  0.996  0.999
 0.0355  126  0.994   17  1.000  143  0.995  0.999
 0.0418  129  0.996   11  1.000  140  0.996  0.999
 0.0482  150  0.990   12  1.000  162  0.991  0.999
 0.0545  151  0.996   12  0.960  163  0.993  0.999
 0.0609  172  0.980   15  0.937  187  0.976  0.999
 0.0672  174  0.991    9  0.921  183  0.987  0.999
 0.0735  178  0.987   11  1.000  189  0.988  0.999
 0.0799  189  0.987   14  0.996  203  0.987  0.999
 0.0862  197  0.978    9  0.981  206  0.978  0.999
 0.0925  193  0.973   14  0.930  207  0.970  0.999
 0.0989  188  0.975   12  0.998  200  0.977  0.999
 0.1052  190  0.982    8  1.000  198  0.983  0.999
 0.1116  183  0.974   13  0.931  196  0.971  1.000
 0.1179  194  0.973   11  0.915  205  0.970  1.000
 0.1242  174  0.974    8  1.000  182  0.975  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0215
Free R factor                    =     0.0462
Overall weighted R factor        =     0.0215
Free weighted R factor           =     0.0464
Overall correlation coefficient  =     0.9992
Free correlation coefficient     =     0.9958
DPI based on free R factor       =     0.0840
Overall figure of merit          =     0.9830
ML based su of positional parameters =     0.0466
ML based su of thermal parameters    =     2.3110
--------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10927.439       3124.8875       26472.906       26243.037

 fvalues    10927.439       3124.8875       26262.107       26243.037


    CGMAT cycle number =     12

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
```

VALUE RESET TO MAXIMUM
Weight matrix 0.59999996
Actual weight 2.0951829 is applied to the X-ray term
Norm of X_ray positional gradient 14.9
Norm of Geom. positional gradient 15.8
Norm of X_ray B-factor gradient 19.0
Norm of Geom. B-factor gradient 19.8
Product of X_ray and Geom posit. gradients -0.797E+06
Cosine of angle between them -0.915
Product of X_ray and Geom B-fact gradients -0.451E+06
Cosine of angle between them -0.975

Residuals: XRAY= 0.2286E+05 GEOM= 3125. TOTAL= 0.2599E+05
function value 25989.469

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.012	0.020
Bond angles : refined atoms	1663	1.626	1.966
Torsion angles, period 1. refined	155	7.798	5.000
Torsion angles, period 2. refined	54	40.975	25.741
Torsion angles, period 3. refined	214	18.760	15.000
Torsion angles, period 4. refined	3	20.962	15.000
Chiral centres: refined atoms	187	0.110	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	538	0.260	0.200
VDW; torsion: refined_atoms	789	0.323	0.200
HBOND: refined_atoms	40	0.196	0.200
VDW repulsions: symmetry: refined_atoms	57	0.254	0.200
HBOND: symmetry: refined_atoms	3	0.254	0.200
Bond B values: refined atoms	1229	11.937	4.695
Angle B values: refined atoms	1663	14.866	7.102
Torsion B values: refined atoms	426	27.651	13.022
Long range B values: refined atoms	1333	10.774	15.369

Overall : scale = 1.012, B = -0.044
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 12. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 12. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 12. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:

:Cycle 12. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.1 746.9 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 413.9 416.3 0.02 0.02 1 1228.1 1212.4 0.02 0.02
0.017 83 95.60 307.6 308.4 0.03 0.03 4 402.9 412.8 0.04 0.05
0.023 97 97.14 247.3 248.5 0.02 0.03 5 180.2 189.5 0.07 0.06
0.029 108 100.00 241.2 241.9 0.02 0.02 7 186.7 189.4 0.07 0.06
0.036 126 99.25 270.3 270.6 0.02 0.02 6 252.8 251.7 0.04 0.04
0.042 129 98.56 286.2 287.5 0.02 0.02 8 338.0 341.3 0.02 0.02
0.048 150 98.73 296.6 296.5 0.02 0.02 5 305.7 306.1 0.04 0.04
0.055 151 99.38 281.2 281.1 0.02 0.02 10 257.8 259.7 0.04 0.04
0.061 172 100.00 218.3 218.4 0.02 0.02 10 202.1 201.9 0.04 0.04
0.067 174 99.45 211.4 210.8 0.02 0.02 6 286.2 283.2 0.02 0.03
0.074 178 98.92 206.0 206.8 0.02 0.02 6 234.5 233.3 0.04 0.03
0.080 189 100.00 208.6 208.9 0.02 0.02 13 159.6 154.1 0.06 0.07
0.086 197 100.00 176.7 176.8 0.02 0.02 8 208.5 207.8 0.04 0.04
0.093 193 93.55 156.9 156.8 0.03 0.03 10 181.9 185.6 0.08 0.07
0.099 188 91.28 160.6 159.5 0.02 0.02 11 159.6 157.8 0.03 0.03
0.105 190 86.02 153.8 153.3 0.02 0.02 13 169.2 170.8 0.06 0.06
0.112 183 80.08 129.8 129.5 0.03 0.03 6 135.2 135.4 0.07 0.06
0.118 194 81.85 126.9 126.5 0.02 0.03 9 138.0 137.8 0.06 0.06
0.124 174 73.20 129.0 128.7 0.02 0.02 9 113.8 111.8 0.09 0.08
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 12. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 12. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.987 12 0.919 95 0.978 0.999
0.0228 97 0.988 11 1.000 108 0.989 0.999
0.0292 108 0.996 6 1.000 114 0.996 0.999
0.0355 126 0.994 17 1.000 143 0.995 0.999
0.0418 129 0.996 11 1.000 140 0.996 0.999
0.0482 150 0.990 12 1.000 162 0.991 0.999
0.0545 151 0.996 12 0.962 163 0.994 0.999
0.0609 172 0.980 15 0.937 187 0.976 0.999
0.0672 174 0.991 9 0.922 183 0.987 0.999
0.0735 178 0.988 11 1.000 189 0.988 0.999
0.0799 189 0.987 14 0.996 203 0.987 0.999
0.0862 197 0.979 9 0.981 206 0.979 0.999
0.0925 193 0.973 14 0.930 207 0.970 0.999
0.0989 188 0.975 12 0.998 200 0.977 0.999
0.1052 190 0.983 8 1.000 198 0.983 0.999

```
 0.1116   183   0.974    13   0.931   196   0.971  1.000
 0.1179   194   0.974    11   0.915   205   0.971  1.000
 0.1242   174   0.975     8   1.000   182   0.976  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0215
Free R factor                    =     0.0460
Overall weighted R factor        =     0.0214
Free weighted R factor           =     0.0461
Overall correlation coefficient  =     0.9992
Free correlation coefficient     =     0.9959
DPI based on free R factor       =     0.0835
Overall figure of merit          =     0.9831
ML based su of positional parameters =     0.0464
ML based su of thermal parameters    =     2.2993
-------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10913.251       3125.1799       25962.834       25990.438


    CGMAT cycle number =     13

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    2.0291517      is applied to the X-ray term
Norm of X_ray positional gradient              14.8
Norm of Geom. positional gradient              14.5
Norm of X_ray B-factor gradient                18.8
Norm of Geom. B-factor gradient                19.6
Product of X_ray and Geom posit. gradients     -0.784E+06
 Cosine of angle between them                  -0.988
Product of X_ray and Geom B-fact gradients     -0.444E+06
 Cosine of angle between them                  -0.978


Residuals: XRAY=     0.2205E+05 GEOM=      3117.     TOTAL=     0.2516E+05
 function value    25163.809

-------------------------------------------------------------------------------
```

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.654	1.966
Torsion angles, period 1. refined	155	7.813	5.000
Torsion angles, period 2. refined	54	40.956	25.741
Torsion angles, period 3. refined	214	18.792	15.000
Torsion angles, period 4. refined	3	21.020	15.000
Chiral centres: refined atoms	187	0.110	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	538	0.261	0.200
VDW; torsion: refined_atoms	790	0.323	0.200
HBOND: refined_atoms	40	0.196	0.200
VDW repulsions: symmetry: refined_atoms	57	0.255	0.200
HBOND: symmetry: refined_atoms	3	0.254	0.200
Bond B values: refined atoms	1229	12.439	4.705
Angle B values: refined atoms	1663	15.390	7.117
Torsion B values: refined atoms	426	28.542	13.044
Long range B values: refined atoms	1333	11.210	15.371

Overall : scale = 1.012, B = -0.047

Overall anisotropic scale factors

B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 13. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 13. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 13. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 13. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$

0.004	30	62.50	754.1	747.1	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	413.9	416.3	0.02	0.02	1	1228.1	1214.4	0.02	0.02	
0.017	83	95.60	307.6	308.4	0.03	0.03	4	402.9	412.7	0.04	0.05	
0.023	97	97.14	247.3	248.5	0.02	0.02	5	180.2	189.5	0.07	0.06	
0.029	108	100.00	241.2	241.8	0.02	0.02	7	186.7	189.4	0.06	0.06	
0.036	126	99.25	270.3	270.6	0.02	0.02	6	252.8	252.0	0.04	0.04	
0.042	129	98.56	286.2	287.5	0.02	0.02	8	338.0	341.3	0.02	0.02	
0.048	150	98.73	296.6	296.5	0.02	0.02	5	305.7	306.2	0.04	0.04	
0.055	151	99.38	281.2	281.1	0.02	0.02	10	257.8	259.7	0.04	0.04	
0.061	172	100.00	218.3	218.4	0.02	0.02	10	202.1	201.8	0.04	0.04	
0.067	174	99.45	211.4	210.8	0.02	0.02	6	286.2	283.4	0.02	0.03	
0.074	178	98.92	206.0	206.8	0.02	0.02	6	234.5	233.6	0.04	0.03	

0.080	189	100.00	208.6	208.9	0.02	0.02	13	159.6	154.2	0.06	0.07
0.086	197	100.00	176.7	176.8	0.02	0.02	8	208.5	207.8	0.04	0.04
0.093	193	93.55	156.9	156.8	0.03	0.03	10	181.9	185.6	0.07	0.07
0.099	188	91.28	160.6	159.5	0.02	0.02	11	159.6	157.8	0.03	0.03
0.105	190	86.02	153.8	153.3	0.02	0.02	13	169.2	170.9	0.06	0.05
0.112	183	80.08	129.8	129.5	0.03	0.03	6	135.2	135.8	0.06	0.06
0.118	194	81.85	126.9	126.5	0.02	0.02	9	138.0	137.8	0.06	0.06
0.124	174	73.20	129.0	128.8	0.02	0.02	9	113.8	111.8	0.09	0.08

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 13. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 13. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.987	12	0.919	95	0.979	0.999
0.0228	97	0.988	11	1.000	108	0.989	0.999
0.0292	108	0.996	6	1.000	114	0.996	0.999
0.0355	126	0.995	17	1.000	143	0.995	0.999
0.0418	129	0.996	11	1.000	140	0.996	0.999
0.0482	150	0.990	12	1.000	162	0.991	0.999
0.0545	151	0.996	12	0.965	163	0.994	0.999
0.0609	172	0.980	15	0.936	187	0.977	0.999
0.0672	174	0.991	9	0.924	183	0.988	0.999
0.0735	178	0.988	11	1.000	189	0.989	0.999
0.0799	189	0.987	14	0.997	203	0.988	0.999
0.0862	197	0.979	9	0.981	206	0.979	0.999
0.0925	193	0.973	14	0.930	207	0.970	0.999
0.0989	188	0.976	12	0.999	200	0.977	0.999
0.1052	190	0.984	8	1.000	198	0.984	0.999
0.1116	183	0.975	13	0.931	196	0.972	1.000
0.1179	194	0.974	11	0.913	205	0.971	1.000
0.1242	174	0.975	8	1.000	182	0.977	1.000

$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0212
Free R factor = 0.0452
Overall weighted R factor = 0.0212
Free weighted R factor = 0.0454
Overall correlation coefficient = 0.9992
Free correlation coefficient = 0.9960
DPI based on free R factor = 0.0821
Overall figure of merit = 0.9836
ML based su of positional parameters = 0.0456

ML based su of thermal parameters = 2.2632

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10865.616 3117.0503 25157.977 25165.033

CGMAT cycle number = 14

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.9681515 is applied to the X-ray term
Norm of X_ray positional gradient 14.7
Norm of Geom. positional gradient 14.7
Norm of X_ray B-factor gradient 18.6
Norm of Geom. B-factor gradient 19.4
Product of X_ray and Geom posit. gradients -0.773E+06
Cosine of angle between them -0.971
Product of X_ray and Geom B-fact gradients -0.437E+06
Cosine of angle between them -0.981

Residuals: XRAY= 0.2130E+05 GEOM= 3128. TOTAL= 0.2442E+05
function value 24424.561

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.644	1.966
Torsion angles, period 1. refined	155	7.825	5.000
Torsion angles, period 2. refined	54	40.952	25.741
Torsion angles, period 3. refined	214	18.880	15.000
Torsion angles, period 4. refined	3	21.069	15.000
Chiral centres: refined atoms	187	0.110	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	539	0.261	0.200
VDW; torsion: refined_atoms	789	0.323	0.200
HBOND: refined_atoms	40	0.196	0.200
VDW repulsions: symmetry: refined_atoms	57	0.255	0.200
HBOND: symmetry: refined_atoms	3	0.256	0.200
Bond B values: refined atoms	1229	12.929	4.710
Angle B values: refined atoms	1663	15.866	7.126
Torsion B values: refined atoms	426	29.372	13.057

Long range B values: refined atoms 1333 11.551 15.368

Overall : scale = 1.012, B = -0.045
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 14. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 14. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 14. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 14. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.1 747.2 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 413.9 416.3 0.02 0.02 1 1228.2 1215.6 0.02 0.02
0.017 83 95.60 307.6 308.4 0.03 0.03 4 402.9 412.7 0.04 0.05
0.023 97 97.14 247.3 248.5 0.02 0.02 5 180.2 189.4 0.07 0.06
0.029 108 100.00 241.2 241.8 0.02 0.02 7 186.7 189.3 0.06 0.06
0.036 126 99.25 270.3 270.6 0.02 0.02 6 252.8 252.1 0.04 0.04
0.042 129 98.56 286.2 287.5 0.02 0.02 8 338.0 341.3 0.02 0.02
0.048 150 98.73 296.6 296.5 0.02 0.02 5 305.7 306.3 0.04 0.04
0.055 151 99.38 281.2 281.2 0.02 0.02 10 257.8 259.7 0.04 0.04
0.061 172 100.00 218.3 218.4 0.02 0.02 10 202.1 201.8 0.04 0.04
0.067 174 99.45 211.4 210.8 0.02 0.02 6 286.2 283.5 0.02 0.03
0.074 178 98.92 206.0 206.8 0.02 0.02 6 234.5 233.9 0.04 0.03
0.080 189 100.00 208.6 208.9 0.02 0.02 13 159.6 154.4 0.06 0.07
0.086 197 100.00 176.7 176.8 0.02 0.02 8 208.5 207.8 0.04 0.04
0.093 193 93.55 156.9 156.8 0.03 0.03 10 181.9 185.6 0.07 0.07
0.099 188 91.28 160.6 159.6 0.02 0.02 11 159.6 157.8 0.03 0.03
0.105 190 86.02 153.8 153.3 0.02 0.02 13 169.2 170.8 0.06 0.05
0.112 183 80.08 129.8 129.5 0.03 0.03 6 135.2 136.2 0.06 0.06
0.118 194 81.85 126.9 126.6 0.02 0.02 9 138.0 137.8 0.06 0.06
0.124 174 73.20 129.0 128.8 0.02 0.02 9 113.8 111.8 0.08 0.08
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 14. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 14. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.988	12	0.919	95	0.979	0.999
0.0228	97	0.988	11	1.000	108	0.989	0.999
0.0292	108	0.996	6	1.000	114	0.997	0.999
0.0355	126	0.995	17	1.000	143	0.995	0.999
0.0418	129	0.996	11	1.000	140	0.996	0.999
0.0482	150	0.990	12	1.000	162	0.991	0.999
0.0545	151	0.996	12	0.969	163	0.994	0.999
0.0609	172	0.981	15	0.935	187	0.977	0.999
0.0672	174	0.991	9	0.927	183	0.988	0.999
0.0735	178	0.988	11	1.000	189	0.989	0.999
0.0799	189	0.987	14	0.997	203	0.988	0.999
0.0862	197	0.980	9	0.981	206	0.980	0.999
0.0925	193	0.974	14	0.930	207	0.971	0.999
0.0989	188	0.976	12	0.999	200	0.978	0.999
0.1052	190	0.985	8	1.000	198	0.985	0.999
0.1116	183	0.975	13	0.932	196	0.973	1.000
0.1179	194	0.975	11	0.910	205	0.972	1.000
0.1242	174	0.976	8	1.000	182	0.977	1.000

$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0209
Free R factor = 0.0445
Overall weighted R factor = 0.0209
Free weighted R factor = 0.0447
Overall correlation coefficient = 0.9992
Free correlation coefficient = 0.9961
DPI based on free R factor = 0.0808
Overall figure of merit = 0.9840
ML based su of positional parameters = 0.0450
ML based su of thermal parameters = 2.2282

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10821.204 3128.0295 24524.139 24425.799

fvalues 10821.204 3128.0295 24433.611 24425.799

CGMAT cycle number = 15

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38

fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.9560977 is applied to the X-ray term
Norm of X_ray positional gradient 14.6
Norm of Geom. positional gradient 14.8
Norm of X_ray B-factor gradient 18.6
Norm of Geom. B-factor gradient 19.4
Product of X_ray and Geom posit. gradients -0.771E+06
Cosine of angle between them -0.965
Product of X_ray and Geom B-fact gradients -0.436E+06
Cosine of angle between them -0.981

Residuals: XRAY= 0.2115E+05 GEOM= 3128. TOTAL= 0.2428E+05
function value 24277.166

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.641	1.966
Torsion angles, period 1. refined	155	7.827	5.000
Torsion angles, period 2. refined	54	40.955	25.741
Torsion angles, period 3. refined	214	18.834	15.000
Torsion angles, period 4. refined	3	21.080	15.000
Chiral centres: refined atoms	187	0.110	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	539	0.261	0.200
VDW; torsion: refined_atoms	789	0.323	0.200
HBOND: refined_atoms	40	0.196	0.200
VDW repulsions: symmetry: refined_atoms	57	0.255	0.200
HBOND: symmetry: refined_atoms	3	0.256	0.200
Bond B values: refined atoms	1229	12.985	4.711
Angle B values: refined atoms	1663	15.925	7.127
Torsion B values: refined atoms	426	29.485	13.059
Long range B values: refined atoms	1333	11.591	15.366

Overall : scale = 1.012, B = -0.046
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 15. Rfactor analysis, F distribution v resln :

$GRAPHS:Cycle 15. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 15. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 15. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.1 747.3 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 413.9 416.3 0.02 0.02 1 1228.2 1215.7 0.02 0.02
0.017 83 95.60 307.6 308.4 0.03 0.03 4 402.9 412.7 0.04 0.05
0.023 97 97.14 247.3 248.5 0.02 0.02 5 180.2 189.4 0.07 0.06
0.029 108 100.00 241.2 241.8 0.02 0.02 7 186.7 189.3 0.07 0.06
0.036 126 99.25 270.3 270.6 0.02 0.02 6 252.8 252.2 0.04 0.04
0.042 129 98.56 286.2 287.5 0.02 0.02 8 338.0 341.4 0.02 0.02
0.048 150 98.73 296.7 296.5 0.02 0.02 5 305.7 306.3 0.04 0.04
0.055 151 99.38 281.2 281.2 0.02 0.02 10 257.8 259.7 0.04 0.04
0.061 172 100.00 218.3 218.4 0.02 0.02 10 202.1 201.8 0.04 0.04
0.067 174 99.45 211.4 210.8 0.02 0.02 6 286.2 283.6 0.02 0.03
0.074 178 98.92 206.0 206.8 0.02 0.02 6 234.5 234.0 0.04 0.03
0.080 189 100.00 208.6 208.9 0.02 0.02 13 159.6 154.4 0.06 0.07
0.086 197 100.00 176.7 176.8 0.02 0.02 8 208.5 207.8 0.04 0.04
0.093 193 93.55 156.9 156.8 0.03 0.03 10 181.9 185.6 0.07 0.07
0.099 188 91.28 160.6 159.6 0.02 0.02 11 159.6 157.8 0.03 0.03
0.105 190 86.02 153.8 153.3 0.02 0.02 13 169.2 170.8 0.06 0.05
0.112 183 80.08 129.8 129.5 0.03 0.03 6 135.2 136.3 0.06 0.06
0.118 194 81.85 126.9 126.6 0.02 0.02 9 138.0 137.8 0.06 0.06
0.124 174 73.20 129.0 128.8 0.02 0.02 9 113.8 111.8 0.08 0.08
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 15. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 15. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.988 12 0.919 95 0.979 0.999
0.0228 97 0.988 11 1.000 108 0.989 0.999
0.0292 108 0.996 6 1.000 114 0.997 0.999
0.0355 126 0.995 17 1.000 143 0.995 0.999
0.0418 129 0.996 11 1.000 140 0.996 0.999
0.0482 150 0.990 12 1.000 162 0.991 0.999
0.0545 151 0.996 12 0.970 163 0.994 0.999
0.0609 172 0.981 15 0.935 187 0.977 0.999
0.0672 174 0.991 9 0.928 183 0.988 0.999
0.0735 178 0.988 11 1.000 189 0.989 0.999
0.0799 189 0.987 14 0.997 203 0.988 0.999
0.0862 197 0.980 9 0.981 206 0.980 0.999
0.0925 193 0.974 14 0.929 207 0.971 0.999

```
 0.0989   188   0.977    12   0.999   200   0.978  0.999
 0.1052   190   0.985     8   1.000   198   0.985  0.999
 0.1116   183   0.976    13   0.932   196   0.973  1.000
 0.1179   194   0.975    11   0.910   205   0.972  1.000
 0.1242   174   0.977     8   1.000   182   0.978  1.000
$$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0209
Free R factor                    =     0.0443
Overall weighted R factor        =     0.0209
Free weighted R factor           =     0.0445
Overall correlation coefficient  =     0.9992
Free correlation coefficient     =     0.9961
DPI based on free R factor       =     0.0805
Overall figure of merit          =     0.9841
ML based su of positional parameters =     0.0448
ML based su of thermal parameters    =     2.2212
-------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10812.278       3128.4988       24266.920       24278.371


    CGMAT cycle number =     16

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    1.9117060      is applied to the X-ray term
Norm of X_ray positional gradient              14.5
Norm of Geom. positional gradient              14.3
Norm of X_ray B-factor gradient                18.5
Norm of Geom. B-factor gradient                19.3
Product of X_ray and Geom posit. gradients     -0.762E+06
 Cosine of angle between them                  -0.991
Product of X_ray and Geom B-fact gradients     -0.432E+06
 Cosine of angle between them                  -0.983


Residuals: XRAY=     0.2060E+05 GEOM=      3130.     TOTAL=     0.2373E+05
 function value    23734.334
```

```
------------------------------------------------------------------------------
          Restraint type           N restraints   Rms Delta   Av(Sigma)
Bond distances: refined atoms              1229     0.011     0.020
Bond angles  : refined atoms               1663     1.659     1.966
Torsion angles, period  1. refined          155     7.837     5.000
Torsion angles, period  2. refined           54    40.986    25.741
Torsion angles, period  3. refined          214    18.887    15.000
Torsion angles, period  4. refined            3    21.120    15.000
Chiral centres: refined atoms              187     0.110     0.200
Planar groups: refined atoms               924     0.005     0.021
VDW repulsions: refined_atoms              540     0.261     0.200
VDW; torsion: refined_atoms                788     0.323     0.200
HBOND: refined_atoms                        40     0.195     0.200
VDW repulsions: symmetry: refined_atoms     57     0.256     0.200
HBOND: symmetry: refined_atoms               3     0.257     0.200
Bond B values: refined atoms               1229    13.187     4.713
Angle B values: refined atoms              1663    16.141     7.130
Torsion B values: refined atoms             426    29.890    13.063
Long range B values: refined atoms         1333    11.972    15.377
------------------------------------------------------------------------------

------------------------------------------------------------------------------
Overall              : scale =    1.012, B  =  -0.042
Overall anisotropic scale factors
   B11 =  0.28 B22 =  0.17 B33 = -0.47 B12 =  0.00 B13 = -0.36 B23 =  0.00
------------------------------------------------------------------------------

------------------------------------------------------------------------------

    ****              Things for loggraph, R factor and others              ****


$TABLE: Cycle   16. Rfactor analysis, F distribution v resln  :
$GRAPHS:Cycle   16. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle   16. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle   16. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free   WR_free $$
$$
 0.004     30  62.50   754.2   747.3  0.02  0.02      0     0.0     0.0******  0.00
 0.010     62  95.45   414.0   416.3  0.02  0.02      1  1228.2  1216.8  0.02  0.02
 0.017     83  95.60   307.6   308.5  0.03  0.02      4   402.9   412.8  0.04  0.05
 0.023     97  97.14   247.3   248.4  0.02  0.02      5   180.2   189.3  0.07  0.06
 0.029    108 100.00   241.2   241.8  0.02  0.02      7   186.7   189.3  0.06  0.06
 0.036    126  99.25   270.3   270.6  0.02  0.02      6   252.8   252.4  0.04  0.04
 0.042    129  98.56   286.2   287.5  0.02  0.02      8   338.0   341.4  0.02  0.02
 0.048    150  98.73   296.7   296.5  0.02  0.02      5   305.7   306.4  0.04  0.04
 0.055    151  99.38   281.2   281.2  0.02  0.02     10   257.9   259.7  0.04  0.04
 0.061    172 100.00   218.3   218.5  0.02  0.02     10   202.1   201.8  0.04  0.04
```

```
 0.067    174  99.45   211.4   210.8  0.02  0.02      6   286.2   283.7  0.02  0.03
 0.074    178  98.92   206.0   206.8  0.02  0.02      6   234.5   234.2  0.04  0.03
 0.080    189 100.00   208.6   208.9  0.02  0.02     13   159.6   154.6  0.06  0.07
 0.086    197 100.00   176.7   176.8  0.02  0.02      8   208.5   207.8  0.04  0.04
 0.093    193  93.55   156.9   156.8  0.03  0.03     10   181.9   185.6  0.07  0.07
 0.099    188  91.28   160.6   159.6  0.02  0.02     11   159.6   157.8  0.03  0.02
 0.105    190  86.02   153.8   153.4  0.02  0.02     13   169.2   170.8  0.06  0.05
 0.112    183  80.08   129.9   129.5  0.03  0.03      6   135.2   136.6  0.06  0.06
 0.118    194  81.85   126.9   126.6  0.02  0.02      9   138.0   137.8  0.05  0.06
 0.124    174  73.20   129.0   128.8  0.02  0.02      9   113.8   111.7  0.08  0.08
$$
```

**** Fom and SigmaA vs resolution ****

```
$TABLE: Cycle   16. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle   16. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa  FOMa  NREFc FOMc NREFall FOMall  SigmaA_Fc1 $$
$$
 0.0038    30   0.999     4   1.000    34   0.999  0.999
 0.0102    62   0.999     7   1.000    69   0.999  0.999
 0.0165    83   0.988    12   0.920    95   0.979  0.999
 0.0228    97   0.988    11   1.000   108   0.989  0.999
 0.0292   108   0.996     6   1.000   114   0.997  0.999
 0.0355   126   0.995    17   1.000   143   0.995  0.999
 0.0418   129   0.996    11   1.000   140   0.997  0.999
 0.0482   150   0.990    12   1.000   162   0.991  0.999
 0.0545   151   0.996    12   0.973   163   0.995  0.999
 0.0609   172   0.981    15   0.934   187   0.977  0.999
 0.0672   174   0.992     9   0.929   183   0.989  0.999
 0.0735   178   0.988    11   1.000   189   0.989  0.999
 0.0799   189   0.988    14   0.998   203   0.988  0.999
 0.0862   197   0.980     9   0.981   206   0.980  0.999
 0.0925   193   0.975    14   0.929   207   0.972  0.999
 0.0989   188   0.977    12   0.999   200   0.978  0.999
 0.1052   190   0.985     8   1.000   198   0.986  0.999
 0.1116   183   0.976    13   0.933   196   0.973  1.000
 0.1179   194   0.976    11   0.908   205   0.972  1.000
 0.1242   174   0.977     8   1.000   182   0.978  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0207
Free R factor                    =     0.0439
Overall weighted R factor        =     0.0207
Free weighted R factor           =     0.0441
Overall correlation coefficient  =     0.9992
Free correlation coefficient     =     0.9962
DPI based on free R factor       =     0.0797
```

Overall figure of merit = 0.9843
ML based su of positional parameters = 0.0443
ML based su of thermal parameters = 2.1957

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10778.362 3130.4265 23728.406 23735.486

CGMAT cycle number = 17

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.59999996
Actual weight 1.8706855 is applied to the X-ray term
Norm of X_ray positional gradient 14.4
Norm of Geom. positional gradient 14.3
Norm of X_ray B-factor gradient 18.4
Norm of Geom. B-factor gradient 19.2
Product of X_ray and Geom posit. gradients -0.754E+06
Cosine of angle between them -0.991
Product of X_ray and Geom B-fact gradients -0.428E+06
Cosine of angle between them -0.985

Residuals: XRAY= 0.2010E+05 GEOM= 3134. TOTAL= 0.2324E+05
function value 23239.029

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.659	1.966
Torsion angles, period 1. refined	155	7.845	5.000
Torsion angles, period 2. refined	54	41.054	25.741
Torsion angles, period 3. refined	214	18.877	15.000
Torsion angles, period 4. refined	3	21.158	15.000
Chiral centres: refined atoms	187	0.110	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	538	0.262	0.200
VDW; torsion: refined_atoms	788	0.324	0.200
HBOND: refined_atoms	40	0.195	0.200
VDW repulsions: symmetry: refined_atoms	56	0.258	0.200
HBOND: symmetry: refined_atoms	3	0.258	0.200
Bond B values: refined atoms	1229	13.280	4.713

Angle B values: refined atoms 1663 16.250 7.130
Torsion B values: refined atoms 426 30.089 13.065
Long range B values: refined atoms 1331 12.044 15.375

Overall : scale = 1.012, B = -0.040
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 17. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 17. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 17. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 17. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.2 747.4 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.0 416.3 0.02 0.02 1 1228.3 1217.4 0.02 0.02
0.017 83 95.60 307.7 308.5 0.03 0.02 4 402.9 412.8 0.04 0.05
0.023 97 97.14 247.3 248.4 0.02 0.02 5 180.2 189.2 0.07 0.06
0.029 108 100.00 241.2 241.8 0.02 0.02 7 186.7 189.2 0.06 0.06
0.036 126 99.25 270.3 270.6 0.02 0.02 6 252.8 252.5 0.04 0.04
0.042 129 98.56 286.2 287.4 0.02 0.02 8 338.0 341.5 0.02 0.02
0.048 150 98.73 296.7 296.5 0.02 0.02 5 305.7 306.5 0.04 0.04
0.055 151 99.38 281.2 281.2 0.02 0.02 10 257.9 259.7 0.04 0.04
0.061 172 100.00 218.3 218.5 0.02 0.02 10 202.1 201.8 0.04 0.04
0.067 174 99.45 211.4 210.8 0.02 0.02 6 286.2 283.7 0.02 0.03
0.074 178 98.92 206.0 206.8 0.02 0.02 6 234.5 234.5 0.04 0.03
0.080 189 100.00 208.6 208.9 0.02 0.02 13 159.6 154.7 0.06 0.07
0.086 197 100.00 176.7 176.8 0.02 0.02 8 208.5 207.8 0.04 0.04
0.093 193 93.55 156.9 156.8 0.03 0.03 10 181.9 185.5 0.07 0.07
0.099 188 91.28 160.6 159.6 0.02 0.02 11 159.6 157.8 0.03 0.02
0.105 190 86.02 153.8 153.4 0.02 0.02 13 169.2 170.8 0.06 0.05
0.112 183 80.08 129.9 129.5 0.03 0.03 6 135.2 136.9 0.07 0.06
0.118 194 81.85 126.9 126.6 0.02 0.02 9 138.0 137.8 0.05 0.06
0.124 174 73.20 129.0 128.8 0.02 0.02 9 113.8 111.7 0.08 0.08
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 17. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 17. M(Fom) v. resln :N:1,3,5,7,8:
$$

```
<4SSQ/LL> NREFa  FOMa  NREFc FOMc NREFall FOMall  SigmaA_Fc1 $$
$$
 0.0038   30  0.999    4  1.000   34  0.999  0.999
 0.0102   62  0.999    7  1.000   69  0.999  0.999
 0.0165   83  0.988   12  0.920   95  0.980  0.999
 0.0228   97  0.988   11  1.000  108  0.989  0.999
 0.0292  108  0.997    6  1.000  114  0.997  0.999
 0.0355  126  0.995   17  1.000  143  0.996  0.999
 0.0418  129  0.996   11  1.000  140  0.997  0.999
 0.0482  150  0.990   12  1.000  162  0.991  0.999
 0.0545  151  0.996   12  0.975  163  0.995  0.999
 0.0609  172  0.981   15  0.934  187  0.977  0.999
 0.0672  174  0.992    9  0.931  183  0.989  0.999
 0.0735  178  0.989   11  1.000  189  0.989  0.999
 0.0799  189  0.988   14  0.998  203  0.989  0.999
 0.0862  197  0.981    9  0.980  206  0.981  0.999
 0.0925  193  0.975   14  0.929  207  0.972  0.999
 0.0989  188  0.977   12  0.999  200  0.979  0.999
 0.1052  190  0.986    8  1.000  198  0.986  0.999
 0.1116  183  0.977   13  0.933  196  0.974  1.000
 0.1179  194  0.976   11  0.911  205  0.973  1.000
 0.1242  174  0.978    8  1.000  182  0.979  1.000
 $$
Resolution limits                =    38.899    2.802
Number of used reflections       =      3184
Percentage observed              =   92.6870
Percentage of free reflections   =    4.8416
Overall R factor                 =    0.0205
Free R factor                    =    0.0434
Overall weighted R factor        =    0.0205
Free weighted R factor           =    0.0437
Overall correlation coefficient  =    0.9993
Free correlation coefficient     =    0.9963
DPI based on free R factor       =    0.0789
Overall figure of merit          =    0.9846
ML based su of positional parameters =    0.0438
ML based su of thermal parameters    =    2.1710
-------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10747.980       3134.0593       23257.086       23240.150

 fvalues    10747.980       3134.0593       23237.932       23240.150


    CGMAT cycle number =     18

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
```

Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.8526372 is applied to the X-ray term
Norm of X_ray positional gradient 14.4
Norm of Geom. positional gradient 14.4
Norm of X_ray B-factor gradient 18.4
Norm of Geom. B-factor gradient 19.1
Product of X_ray and Geom posit. gradients -0.750E+06
Cosine of angle between them -0.984
Product of X_ray and Geom B-fact gradients -0.426E+06
Cosine of angle between them -0.986

Residuals: XRAY= 0.1988E+05 GEOM= 3137. TOTAL= 0.2302E+05
function value 23022.225

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.653	1.966
Torsion angles, period 1. refined	155	7.849	5.000
Torsion angles, period 2. refined	54	41.095	25.741
Torsion angles, period 3. refined	214	18.970	15.000
Torsion angles, period 4. refined	3	21.173	15.000
Chiral centres: refined atoms	187	0.110	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	538	0.262	0.200
VDW; torsion: refined_atoms	788	0.324	0.200
HBOND: refined_atoms	40	0.195	0.200
VDW repulsions: symmetry: refined_atoms	56	0.258	0.200
HBOND: symmetry: refined_atoms	3	0.259	0.200
Bond B values: refined atoms	1229	13.303	4.713
Angle B values: refined atoms	1663	16.278	7.130
Torsion B values: refined atoms	426	30.129	13.066
Long range B values: refined atoms	1331	12.069	15.372

Overall : scale = 1.012, B = -0.039
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 18. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 18. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 18. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 18. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.2 747.4 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.0 416.3 0.02 0.02 1 1228.3 1217.8 0.02 0.02
0.017 83 95.60 307.7 308.5 0.03 0.02 4 402.9 412.9 0.04 0.05
0.023 97 97.14 247.3 248.4 0.02 0.02 5 180.2 189.2 0.07 0.06
0.029 108 100.00 241.3 241.8 0.02 0.02 7 186.7 189.2 0.06 0.06
0.036 126 99.25 270.3 270.6 0.02 0.02 6 252.8 252.6 0.04 0.04
0.042 129 98.56 286.2 287.4 0.02 0.02 8 338.0 341.5 0.02 0.02
0.048 150 98.73 296.7 296.5 0.02 0.02 5 305.7 306.5 0.04 0.04
0.055 151 99.38 281.2 281.2 0.02 0.02 10 257.9 259.7 0.04 0.04
0.061 172 100.00 218.3 218.5 0.02 0.02 10 202.1 201.8 0.04 0.04
0.067 174 99.45 211.4 210.9 0.02 0.02 6 286.2 283.7 0.02 0.03
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.5 234.6 0.04 0.03
0.080 189 100.00 208.6 208.9 0.02 0.02 13 159.6 154.8 0.06 0.07
0.086 197 100.00 176.7 176.8 0.02 0.02 8 208.5 207.8 0.04 0.04
0.093 193 93.55 156.9 156.8 0.03 0.03 10 181.9 185.5 0.07 0.07
0.099 188 91.28 160.6 159.6 0.02 0.02 11 159.6 157.8 0.03 0.02
0.105 190 86.02 153.8 153.4 0.02 0.02 13 169.2 170.8 0.06 0.05
0.112 183 80.08 129.9 129.5 0.03 0.03 6 135.2 137.1 0.07 0.06
0.118 194 81.85 126.9 126.6 0.02 0.02 9 138.0 137.7 0.05 0.06
0.124 174 73.20 129.0 128.8 0.02 0.02 9 113.8 111.7 0.08 0.08
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 18. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 18. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.988 12 0.920 95 0.980 0.999
0.0228 97 0.988 11 1.000 108 0.989 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.995 17 1.000 143 0.996 0.999
0.0418 129 0.996 11 1.000 140 0.997 0.999
0.0482 150 0.990 12 1.000 162 0.991 0.999
0.0545 151 0.996 12 0.976 163 0.995 0.999
0.0609 172 0.981 15 0.935 187 0.978 0.999
0.0672 174 0.992 9 0.931 183 0.989 0.999
0.0735 178 0.989 11 1.000 189 0.989 0.999
0.0799 189 0.988 14 0.998 203 0.989 0.999

```
 0.0862   197   0.981    9   0.980   206   0.981  0.999
 0.0925   193   0.975   14   0.929   207   0.972  0.999
 0.0989   188   0.977   12   0.999   200   0.979  0.999
 0.1052   190   0.986    8   1.000   198   0.987  0.999
 0.1116   183   0.977   13   0.934   196   0.974  1.000
 0.1179   194   0.977   11   0.911   205   0.973  1.000
 0.1242   174   0.978    8   1.000   182   0.979  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0204
Free R factor                    =     0.0433
Overall weighted R factor        =     0.0204
Free weighted R factor           =     0.0435
Overall correlation coefficient  =     0.9993
Free correlation coefficient     =     0.9963
DPI based on free R factor       =     0.0785
Overall figure of merit          =     0.9848
ML based su of positional parameters =     0.0436
ML based su of thermal parameters    =     2.1601
------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10733.862       3137.3892       23058.643       23023.342

 fvalues    10733.862       3137.3892       23023.883       23023.342


    CGMAT cycle number =     19

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    1.8443460      is applied to the X-ray term
Norm of X_ray positional gradient              14.3
Norm of Geom. positional gradient              14.4
Norm of X_ray B-factor gradient                18.4
Norm of Geom. B-factor gradient                19.1
Product of X_ray and Geom posit. gradients     -0.748E+06
 Cosine of angle between them                  -0.983
Product of X_ray and Geom B-fact gradients     -0.425E+06
 Cosine of angle between them                  -0.986
```

Residuals: XRAY= 0.1978E+05 GEOM= 3137. TOTAL= 0.2292E+05
function value 22921.338

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.653	1.966
Torsion angles, period 1. refined	155	7.850	5.000
Torsion angles, period 2. refined	54	41.115	25.741
Torsion angles, period 3. refined	214	18.930	15.000
Torsion angles, period 4. refined	3	21.181	15.000
Chiral centres: refined atoms	187	0.110	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	538	0.262	0.200
VDW; torsion: refined_atoms	788	0.324	0.200
HBOND: refined_atoms	40	0.195	0.200
VDW repulsions: symmetry: refined_atoms	56	0.258	0.200
HBOND: symmetry: refined_atoms	3	0.259	0.200
Bond B values: refined atoms	1229	13.311	4.713
Angle B values: refined atoms	1663	16.288	7.130
Torsion B values: refined atoms	426	30.144	13.066
Long range B values: refined atoms	1331	12.078	15.371

Overall : scale = 1.012, B = -0.039
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 19. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 19. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 19. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 19. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$

0.004	30	62.50	754.2	747.5	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	414.0	416.3	0.02	0.02	1	1228.3	1217.9	0.02	0.02	
0.017	83	95.60	307.7	308.5	0.03	0.02	4	402.9	412.9	0.04	0.05	
0.023	97	97.14	247.3	248.4	0.02	0.02	5	180.2	189.2	0.07	0.06	
0.029	108	100.00	241.3	241.8	0.02	0.02	7	186.7	189.2	0.06	0.06	
0.036	126	99.25	270.3	270.6	0.02	0.02	6	252.8	252.6	0.04	0.04	

```
 0.042    129  98.56   286.2   287.4  0.02  0.02      8   338.0   341.5  0.02  0.02
 0.048    150  98.73   296.7   296.5  0.02  0.02      5   305.7   306.5  0.04  0.04
 0.055    151  99.38   281.2   281.2  0.02  0.02     10   257.9   259.7  0.04  0.04
 0.061    172 100.00   218.3   218.5  0.02  0.02     10   202.1   201.8  0.04  0.04
 0.067    174  99.45   211.4   210.9  0.02  0.02      6   286.2   283.8  0.02  0.03
 0.074    178  98.92   206.1   206.8  0.02  0.02      6   234.5   234.6  0.04  0.03
 0.080    189 100.00   208.6   208.9  0.02  0.02     13   159.6   154.8  0.06  0.07
 0.086    197 100.00   176.7   176.8  0.02  0.02      8   208.5   207.8  0.04  0.04
 0.093    193  93.55   156.9   156.8  0.03  0.03     10   181.9   185.5  0.07  0.07
 0.099    188  91.28   160.6   159.6  0.02  0.02     11   159.6   157.8  0.03  0.02
 0.105    190  86.02   153.8   153.4  0.02  0.02     13   169.2   170.8  0.06  0.05
 0.112    183  80.08   129.9   129.5  0.03  0.03      6   135.2   137.2  0.07  0.06
 0.118    194  81.85   126.9   126.6  0.02  0.02      9   138.0   137.7  0.05  0.06
 0.124    174  73.20   129.0   128.8  0.02  0.02      9   113.8   111.7  0.08  0.08
$$
```

**** Fom and SigmaA vs resolution ****

```
$TABLE: Cycle   19. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle   19. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa  FOMa  NREFc FOMc NREFall FOMall  SigmaA_Fc1 $$
$$
 0.0038    30   0.999     4   1.000    34   0.999  0.999
 0.0102    62   0.999     7   1.000    69   0.999  0.999
 0.0165    83   0.989    12   0.920    95   0.980  0.999
 0.0228    97   0.988    11   1.000   108   0.989  0.999
 0.0292   108   0.997     6   1.000   114   0.997  0.999
 0.0355   126   0.995    17   1.000   143   0.996  0.999
 0.0418   129   0.996    11   1.000   140   0.997  0.999
 0.0482   150   0.990    12   1.000   162   0.991  0.999
 0.0545   151   0.996    12   0.977   163   0.995  0.999
 0.0609   172   0.981    15   0.935   187   0.978  0.999
 0.0672   174   0.992     9   0.932   183   0.989  0.999
 0.0735   178   0.989    11   1.000   189   0.989  0.999
 0.0799   189   0.988    14   0.998   203   0.989  0.999
 0.0862   197   0.981     9   0.980   206   0.981  0.999
 0.0925   193   0.975    14   0.929   207   0.972  0.999
 0.0989   188   0.977    12   0.999   200   0.979  0.999
 0.1052   190   0.986     8   1.000   198   0.987  0.999
 0.1116   183   0.977    13   0.934   196   0.974  1.000
 0.1179   194   0.977    11   0.911   205   0.973  1.000
 0.1242   174   0.978     8   1.000   182   0.979  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0204
Free R factor                    =     0.0432
Overall weighted R factor        =     0.0204
```

Free weighted R factor = 0.0434
Overall correlation coefficient = 0.9993
Free correlation coefficient = 0.9963
DPI based on free R factor = 0.0784
Overall figure of merit = 0.9848
ML based su of positional parameters = 0.0435
ML based su of thermal parameters = 2.1551

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10727.602 3137.0151 22915.260 22922.424

CGMAT cycle number = 20

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.59999996
Actual weight 1.8125516 is applied to the X-ray term
Norm of X_ray positional gradient 14.3
Norm of Geom. positional gradient 14.2
Norm of X_ray B-factor gradient 18.3
Norm of Geom. B-factor gradient 19.0
Product of X_ray and Geom posit. gradients -0.743E+06
Cosine of angle between them -0.994
Product of X_ray and Geom B-fact gradients -0.422E+06
Cosine of angle between them -0.987

Residuals: XRAY= 0.1940E+05 GEOM= 3137. TOTAL= 0.2254E+05
function value 22536.805

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.664	1.966
Torsion angles, period 1. refined	155	7.856	5.000
Torsion angles, period 2. refined	54	41.203	25.741
Torsion angles, period 3. refined	214	18.974	15.000
Torsion angles, period 4. refined	3	21.211	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	539	0.262	0.200
VDW; torsion: refined_atoms	787	0.324	0.200

HBOND: refined_atoms 40 0.195 0.200
VDW repulsions: symmetry: refined_atoms 56 0.258 0.200
HBOND: symmetry: refined_atoms 3 0.260 0.200
Bond B values: refined atoms 1229 13.341 4.713
Angle B values: refined atoms 1663 16.329 7.130
Torsion B values: refined atoms 426 30.200 13.064
Long range B values: refined atoms 1332 12.116 15.375

Overall : scale = 1.012, B = -0.037
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 20. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 20. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 20. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 20. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.2 747.5 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.0 416.3 0.02 0.02 1 1228.3 1218.5 0.02 0.02
0.017 83 95.60 307.7 308.5 0.03 0.02 4 402.9 413.0 0.04 0.05
0.023 97 97.14 247.3 248.4 0.02 0.02 5 180.2 189.2 0.07 0.06
0.029 108 100.00 241.3 241.9 0.02 0.02 7 186.7 189.2 0.06 0.06
0.036 126 99.25 270.3 270.6 0.02 0.02 6 252.8 252.7 0.04 0.04
0.042 129 98.56 286.2 287.4 0.02 0.02 8 338.1 341.5 0.02 0.02
0.048 150 98.73 296.7 296.4 0.02 0.02 5 305.7 306.5 0.04 0.03
0.055 151 99.38 281.2 281.3 0.02 0.02 10 257.9 259.8 0.04 0.04
0.061 172 100.00 218.3 218.5 0.02 0.02 10 202.1 201.8 0.04 0.04
0.067 174 99.45 211.4 210.9 0.02 0.02 6 286.2 283.8 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.5 234.8 0.04 0.03
0.080 189 100.00 208.7 208.9 0.02 0.02 13 159.6 154.9 0.06 0.07
0.086 197 100.00 176.7 176.8 0.02 0.02 8 208.5 207.8 0.04 0.04
0.093 193 93.55 156.9 156.8 0.03 0.02 10 181.9 185.5 0.07 0.07
0.099 188 91.28 160.6 159.6 0.02 0.02 11 159.6 157.8 0.03 0.02
0.105 190 86.02 153.8 153.4 0.02 0.02 13 169.2 170.8 0.06 0.05
0.112 183 80.08 129.9 129.5 0.03 0.03 6 135.2 137.4 0.07 0.06
0.118 194 81.85 126.9 126.6 0.02 0.02 9 138.0 137.7 0.05 0.06
0.124 174 73.20 129.0 128.8 0.02 0.02 9 113.8 111.6 0.08 0.08
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 20. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 20. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.989 12 0.921 95 0.980 0.999
0.0228 97 0.988 11 1.000 108 0.989 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.995 17 1.000 143 0.996 0.999
0.0418 129 0.996 11 1.000 140 0.997 0.999
0.0482 150 0.990 12 1.000 162 0.991 0.999
0.0545 151 0.997 12 0.979 163 0.995 0.999
0.0609 172 0.981 15 0.936 187 0.978 0.999
0.0672 174 0.992 9 0.933 183 0.989 0.999
0.0735 178 0.989 11 1.000 189 0.989 0.999
0.0799 189 0.988 14 0.998 203 0.989 0.999
0.0862 197 0.981 9 0.980 206 0.981 0.999
0.0925 193 0.976 14 0.929 207 0.973 0.999
0.0989 188 0.978 12 0.999 200 0.979 0.999
0.1052 190 0.986 8 1.000 198 0.987 0.999
0.1116 183 0.977 13 0.934 196 0.974 1.000
0.1179 194 0.977 11 0.914 205 0.974 1.000
0.1242 174 0.979 8 1.000 182 0.980 1.000
$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0203
Free R factor = 0.0428
Overall weighted R factor = 0.0203
Free weighted R factor = 0.0431
Overall correlation coefficient = 0.9993
Free correlation coefficient = 0.9964
DPI based on free R factor = 0.0778
Overall figure of merit = 0.9851
ML based su of positional parameters = 0.0431
ML based su of thermal parameters = 2.1359

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10703.355 3137.4763 22536.602 22537.861

CGMAT cycle number = 21

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.7867299 is applied to the X-ray term
Norm of X_ray positional gradient 14.2
Norm of Geom. positional gradient 14.3
Norm of X_ray B-factor gradient 18.3
Norm of Geom. B-factor gradient 18.9
Product of X_ray and Geom posit. gradients -0.738E+06
Cosine of angle between them -0.986
Product of X_ray and Geom B-fact gradients -0.419E+06
Cosine of angle between them -0.988

Residuals: XRAY= 0.1909E+05 GEOM= 3143. TOTAL= 0.2223E+05
function value 22230.414

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.661	1.966
Torsion angles, period 1. refined	155	7.861	5.000
Torsion angles, period 2. refined	54	41.274	25.741
Torsion angles, period 3. refined	214	18.967	15.000
Torsion angles, period 4. refined	3	21.234	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	541	0.262	0.200
VDW; torsion: refined_atoms	787	0.324	0.200
HBOND: refined_atoms	40	0.195	0.200
VDW repulsions: symmetry: refined_atoms	55	0.261	0.200
HBOND: symmetry: refined_atoms	3	0.261	0.200
Bond B values: refined atoms	1229	13.360	4.713
Angle B values: refined atoms	1663	16.355	7.129
Torsion B values: refined atoms	426	30.231	13.064
Long range B values: refined atoms	1334	12.140	15.370

Overall : scale = 1.012, B = -0.036
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 21. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 21. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 21. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 21. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.2 747.5 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.0 416.3 0.02 0.02 1 1228.3 1218.7 0.02 0.02
0.017 83 95.60 307.7 308.5 0.03 0.02 4 403.0 413.0 0.04 0.05
0.023 97 97.14 247.3 248.4 0.02 0.02 5 180.2 189.0 0.07 0.06
0.029 108 100.00 241.3 241.9 0.02 0.02 7 186.7 189.2 0.06 0.06
0.036 126 99.25 270.3 270.6 0.02 0.02 6 252.8 252.8 0.04 0.04
0.042 129 98.56 286.2 287.4 0.02 0.02 8 338.1 341.5 0.02 0.02
0.048 150 98.73 296.7 296.4 0.02 0.02 5 305.7 306.6 0.03 0.03
0.055 151 99.38 281.2 281.3 0.02 0.02 10 257.9 259.8 0.04 0.04
0.061 172 100.00 218.3 218.5 0.02 0.02 10 202.2 201.8 0.03 0.04
0.067 174 99.45 211.4 210.9 0.02 0.02 6 286.2 283.8 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.5 235.1 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.6 155.0 0.06 0.07
0.086 197 100.00 176.7 176.8 0.02 0.02 8 208.5 207.8 0.04 0.04
0.093 193 93.55 156.9 156.8 0.03 0.02 10 181.9 185.5 0.07 0.07
0.099 188 91.28 160.7 159.6 0.02 0.02 11 159.6 157.7 0.02 0.02
0.105 190 86.02 153.8 153.4 0.02 0.02 13 169.2 170.7 0.06 0.05
0.112 183 80.08 129.9 129.5 0.03 0.03 6 135.2 137.7 0.07 0.07
0.118 194 81.85 126.9 126.6 0.02 0.02 9 138.0 137.7 0.05 0.06
0.124 174 73.20 129.0 128.8 0.02 0.02 9 113.8 111.6 0.08 0.08
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 21. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 21. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.989 12 0.921 95 0.980 0.999
0.0228 97 0.988 11 1.000 108 0.989 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.995 17 1.000 143 0.996 0.999
0.0418 129 0.996 11 1.000 140 0.997 0.999
0.0482 150 0.990 12 1.000 162 0.991 0.999
0.0545 151 0.997 12 0.981 163 0.995 0.999
0.0609 172 0.982 15 0.938 187 0.978 0.999
0.0672 174 0.992 9 0.934 183 0.989 0.999

```
 0.0735   178   0.989    11   1.000   189   0.990  0.999
 0.0799   189   0.988    14   0.999   203   0.989  0.999
 0.0862   197   0.982     9   0.979   206   0.982  0.999
 0.0925   193   0.976    14   0.929   207   0.973  0.999
 0.0989   188   0.978    12   0.999   200   0.979  0.999
 0.1052   190   0.987     8   1.000   198   0.987  0.999
 0.1116   183   0.978    13   0.935   196   0.975  1.000
 0.1179   194   0.977    11   0.916   205   0.974  1.000
 0.1242   174   0.980     8   1.000   182   0.980  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0202
Free R factor                    =     0.0426
Overall weighted R factor        =     0.0202
Free weighted R factor           =     0.0429
Overall correlation coefficient  =     0.9993
Free correlation coefficient     =     0.9964
DPI based on free R factor       =     0.0773
Overall figure of merit          =     0.9853
ML based su of positional parameters =     0.0428
ML based su of thermal parameters    =     2.1197
------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10683.364       3143.1680       22269.098       22231.455

 fvalues    10683.364       3143.1680       22238.607       22231.455


    CGMAT cycle number =     22

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000008
 Actual weight    1.7800413      is applied to the X-ray term
Norm of X_ray positional gradient              14.2
Norm of Geom. positional gradient              14.3
Norm of X_ray B-factor gradient                18.2
Norm of Geom. B-factor gradient                18.9
Product of X_ray and Geom posit. gradients     -0.736E+06
 Cosine of angle between them                  -0.981
```

Product of X_ray and Geom B-fact gradients -0.419E+06
Cosine of angle between them -0.988

Residuals: XRAY= 0.1901E+05 GEOM= 3143. TOTAL= 0.2215E+05
function value 22149.244

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.655	1.966
Torsion angles, period 1. refined	155	7.862	5.000
Torsion angles, period 2. refined	54	41.285	25.741
Torsion angles, period 3. refined	214	18.997	15.000
Torsion angles, period 4. refined	3	21.239	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	541	0.262	0.200
VDW; torsion: refined_atoms	786	0.324	0.200
HBOND: refined_atoms	40	0.195	0.200
VDW repulsions: symmetry: refined_atoms	55	0.261	0.200
HBOND: symmetry: refined_atoms	3	0.261	0.200
Bond B values: refined atoms	1229	13.364	4.713
Angle B values: refined atoms	1663	16.361	7.129
Torsion B values: refined atoms	426	30.236	13.064
Long range B values: refined atoms	1333	12.153	15.369

Overall : scale = 1.012, B = -0.037
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 22. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 22. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 22. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 22. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$

0.004	30	62.50	754.2	747.6	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	414.0	416.3	0.02	0.02	1	1228.4	1218.9	0.02	0.02	
0.017	83	95.60	307.7	308.5	0.03	0.02	4	403.0	413.0	0.04	0.05	
0.023	97	97.14	247.4	248.4	0.02	0.02	5	180.2	189.0	0.07	0.06	

0.029	108	100.00	241.3	241.9	0.02	0.02	7	186.7	189.2	0.06	0.06
0.036	126	99.25	270.3	270.6	0.02	0.02	6	252.8	252.8	0.04	0.04
0.042	129	98.56	286.2	287.4	0.02	0.02	8	338.1	341.5	0.02	0.02
0.048	150	98.73	296.7	296.4	0.02	0.02	5	305.7	306.6	0.03	0.03
0.055	151	99.38	281.2	281.3	0.02	0.02	10	257.9	259.8	0.04	0.04
0.061	172	100.00	218.3	218.5	0.02	0.02	10	202.2	201.8	0.03	0.04
0.067	174	99.45	211.4	210.9	0.02	0.02	6	286.2	283.8	0.02	0.02
0.074	178	98.92	206.1	206.8	0.02	0.02	6	234.5	235.1	0.04	0.03
0.080	189	100.00	208.7	209.0	0.02	0.02	13	159.6	155.0	0.06	0.07
0.086	197	100.00	176.7	176.9	0.02	0.02	8	208.5	207.8	0.04	0.04
0.093	193	93.55	156.9	156.9	0.03	0.02	10	181.9	185.5	0.07	0.07
0.099	188	91.28	160.7	159.6	0.02	0.02	11	159.6	157.7	0.02	0.02
0.105	190	86.02	153.8	153.4	0.02	0.02	13	169.2	170.7	0.05	0.05
0.112	183	80.08	129.9	129.5	0.03	0.03	6	135.2	137.7	0.07	0.07
0.118	194	81.85	126.9	126.6	0.02	0.02	9	138.0	137.7	0.05	0.06
0.124	174	73.20	129.0	128.8	0.02	0.02	9	113.8	111.6	0.08	0.08

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 22. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 22. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.989	12	0.921	95	0.980	0.999
0.0228	97	0.988	11	1.000	108	0.989	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.995	17	1.000	143	0.996	0.999
0.0418	129	0.996	11	1.000	140	0.997	0.999
0.0482	150	0.991	12	1.000	162	0.991	0.999
0.0545	151	0.997	12	0.981	163	0.995	0.999
0.0609	172	0.982	15	0.938	187	0.978	0.999
0.0672	174	0.992	9	0.934	183	0.989	0.999
0.0735	178	0.989	11	1.000	189	0.990	0.999
0.0799	189	0.988	14	0.999	203	0.989	0.999
0.0862	197	0.982	9	0.979	206	0.982	0.999
0.0925	193	0.976	14	0.929	207	0.973	0.999
0.0989	188	0.978	12	0.999	200	0.979	0.999
0.1052	190	0.987	8	1.000	198	0.987	0.999
0.1116	183	0.978	13	0.935	196	0.975	1.000
0.1179	194	0.977	11	0.916	205	0.974	1.000
0.1242	174	0.980	8	1.000	182	0.981	1.000

$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0202

Free R factor = 0.0425
Overall weighted R factor = 0.0201
Free weighted R factor = 0.0428
Overall correlation coefficient = 0.9993
Free correlation coefficient = 0.9964
DPI based on free R factor = 0.0772
Overall figure of merit = 0.9853
ML based su of positional parameters = 0.0428
ML based su of thermal parameters = 2.1155

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10677.998 3143.0417 22143.439 22150.320

CGMAT cycle number = 23

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.7571279 is applied to the X-ray term
Norm of X_ray positional gradient 14.1
Norm of Geom. positional gradient 14.1
Norm of X_ray B-factor gradient 18.2
Norm of Geom. B-factor gradient 18.8
Product of X_ray and Geom posit. gradients -0.731E+06
Cosine of angle between them -0.996
Product of X_ray and Geom B-fact gradients -0.416E+06
Cosine of angle between them -0.989

Residuals: XRAY= 0.1873E+05 GEOM= 3142. TOTAL= 0.2187E+05
function value 21871.578

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.669	1.966
Torsion angles, period 1. refined	155	7.866	5.000
Torsion angles, period 2. refined	54	41.329	25.741
Torsion angles, period 3. refined	214	19.019	15.000
Torsion angles, period 4. refined	3	21.258	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021

VDW repulsions: refined_atoms 539 0.263 0.200
VDW; torsion: refined_atoms 786 0.324 0.200
HBOND: refined_atoms 40 0.195 0.200
VDW repulsions: symmetry: refined_atoms 55 0.261 0.200
HBOND: symmetry: refined_atoms 3 0.262 0.200
Bond B values: refined atoms 1229 13.374 4.712
Angle B values: refined atoms 1663 16.379 7.128
Torsion B values: refined atoms 426 30.252 13.061
Long range B values: refined atoms 1331 12.189 15.373

Overall : scale = 1.012, B = -0.034
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 23. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 23. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 23. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 23. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.2 747.6 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.0 416.3 0.02 0.02 1 1228.4 1219.5 0.02 0.02
0.017 83 95.60 307.7 308.6 0.03 0.02 4 403.0 413.1 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 189.0 0.07 0.06
0.029 108 100.00 241.3 241.9 0.02 0.02 7 186.7 189.2 0.06 0.06
0.036 126 99.25 270.3 270.6 0.02 0.02 6 252.8 253.0 0.04 0.04
0.042 129 98.56 286.2 287.4 0.02 0.02 8 338.1 341.5 0.02 0.02
0.048 150 98.73 296.7 296.4 0.02 0.02 5 305.7 306.6 0.03 0.03
0.055 151 99.38 281.2 281.3 0.02 0.02 10 257.9 259.8 0.04 0.04
0.061 172 100.00 218.3 218.5 0.02 0.02 10 202.2 201.9 0.03 0.04
0.067 174 99.45 211.4 210.9 0.02 0.02 6 286.2 283.9 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.5 235.3 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.6 155.0 0.06 0.07
0.086 197 100.00 176.7 176.8 0.02 0.02 8 208.5 207.8 0.04 0.04
0.093 193 93.55 156.9 156.9 0.02 0.02 10 181.9 185.5 0.07 0.07
0.099 188 91.28 160.7 159.6 0.02 0.02 11 159.6 157.7 0.02 0.02
0.105 190 86.02 153.8 153.4 0.02 0.02 13 169.2 170.7 0.05 0.05
0.112 183 80.08 129.9 129.5 0.03 0.03 6 135.2 137.9 0.07 0.07
0.118 194 81.85 126.9 126.6 0.02 0.02 9 138.0 137.7 0.05 0.06
0.124 174 73.20 129.0 128.8 0.02 0.02 9 113.8 111.5 0.08 0.08
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 23. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 23. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.989 12 0.921 95 0.981 0.999
0.0228 97 0.988 11 1.000 108 0.989 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.995 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.991 0.999
0.0545 151 0.997 12 0.983 163 0.996 0.999
0.0609 172 0.982 15 0.939 187 0.978 0.999
0.0672 174 0.992 9 0.935 183 0.990 0.999
0.0735 178 0.989 11 1.000 189 0.990 0.999
0.0799 189 0.988 14 0.999 203 0.989 0.999
0.0862 197 0.982 9 0.979 206 0.982 0.999
0.0925 193 0.976 14 0.929 207 0.973 0.999
0.0989 188 0.978 12 0.999 200 0.979 0.999
0.1052 190 0.987 8 1.000 198 0.987 0.999
0.1116 183 0.978 13 0.936 196 0.975 1.000
0.1179 194 0.978 11 0.917 205 0.974 1.000
0.1242 174 0.980 8 1.000 182 0.981 1.000
$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0201
Free R factor = 0.0422
Overall weighted R factor = 0.0201
Free weighted R factor = 0.0426
Overall correlation coefficient = 0.9993
Free correlation coefficient = 0.9965
DPI based on free R factor = 0.0767
Overall figure of merit = 0.9855
ML based su of positional parameters = 0.0425
ML based su of thermal parameters = 2.1014

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10659.797 3141.9307 21869.504 21872.557

CGMAT cycle number = 24

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.7391152 is applied to the X-ray term
Norm of X_ray positional gradient 14.1
Norm of Geom. positional gradient 14.0
Norm of X_ray B-factor gradient 18.2
Norm of Geom. B-factor gradient 18.7
Product of X_ray and Geom posit. gradients -0.727E+06
Cosine of angle between them -0.997
Product of X_ray and Geom B-fact gradients -0.414E+06
Cosine of angle between them -0.990

Residuals: XRAY= 0.1851E+05 GEOM= 3143. TOTAL= 0.2166E+05
function value 21656.660

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.669	1.966
Torsion angles, period 1. refined	155	7.868	5.000
Torsion angles, period 2. refined	54	41.356	25.741
Torsion angles, period 3. refined	214	19.026	15.000
Torsion angles, period 4. refined	3	21.280	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.263	0.200
VDW; torsion: refined_atoms	786	0.324	0.200
HBOND: refined_atoms	40	0.195	0.200
VDW repulsions: symmetry: refined_atoms	55	0.261	0.200
HBOND: symmetry: refined_atoms	3	0.263	0.200
Bond B values: refined atoms	1229	13.388	4.712
Angle B values: refined atoms	1663	16.399	7.127
Torsion B values: refined atoms	426	30.277	13.061
Long range B values: refined atoms	1332	12.214	15.387

Overall : scale = 1.012, B = -0.033
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 24. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 24. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 24. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 24. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.3 747.6 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.0 416.3 0.02 0.02 1 1228.4 1219.7 0.02 0.02
0.017 83 95.60 307.7 308.6 0.03 0.02 4 403.0 413.1 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.9 0.07 0.06
0.029 108 100.00 241.3 241.9 0.02 0.02 7 186.7 189.2 0.06 0.06
0.036 126 99.25 270.3 270.7 0.02 0.02 6 252.9 253.0 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.5 0.02 0.02
0.048 150 98.73 296.7 296.4 0.02 0.02 5 305.8 306.6 0.03 0.03
0.055 151 99.38 281.2 281.3 0.02 0.02 10 257.9 259.8 0.04 0.04
0.061 172 100.00 218.3 218.5 0.02 0.02 10 202.2 201.9 0.03 0.04
0.067 174 99.45 211.4 210.9 0.02 0.02 6 286.2 283.9 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.5 235.4 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.6 155.1 0.06 0.07
0.086 197 100.00 176.7 176.8 0.02 0.02 8 208.5 207.8 0.04 0.04
0.093 193 93.55 156.9 156.9 0.02 0.02 10 181.9 185.5 0.07 0.06
0.099 188 91.28 160.7 159.7 0.02 0.02 11 159.6 157.6 0.02 0.02
0.105 190 86.02 153.8 153.4 0.02 0.02 13 169.2 170.7 0.05 0.05
0.112 183 80.08 129.9 129.5 0.03 0.03 6 135.2 138.1 0.07 0.07
0.118 194 81.85 126.9 126.6 0.02 0.02 9 138.0 137.7 0.05 0.06
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.5 0.08 0.08
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 24. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 24. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.989 12 0.921 95 0.981 0.999
0.0228 97 0.988 11 1.000 108 0.989 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.995 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.991 0.999
0.0545 151 0.997 12 0.984 163 0.996 0.999

```
 0.0609   172   0.982    15   0.940   187   0.979  0.999
 0.0672   174   0.992     9   0.935   183   0.990  0.999
 0.0735   178   0.989    11   1.000   189   0.990  0.999
 0.0799   189   0.988    14   0.999   203   0.989  0.999
 0.0862   197   0.982     9   0.978   206   0.982  0.999
 0.0925   193   0.977    14   0.929   207   0.973  0.999
 0.0989   188   0.978    12   0.999   200   0.980  0.999
 0.1052   190   0.987     8   1.000   198   0.988  0.999
 0.1116   183   0.978    13   0.936   196   0.975  1.000
 0.1179   194   0.978    11   0.919   205   0.975  1.000
 0.1242   174   0.981     8   1.000   182   0.981  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0200
Free R factor                    =     0.0421
Overall weighted R factor        =     0.0200
Free weighted R factor           =     0.0424
Overall correlation coefficient  =     0.9993
Free correlation coefficient     =     0.9965
DPI based on free R factor       =     0.0764
Overall figure of merit          =     0.9856
ML based su of positional parameters =     0.0423
ML based su of thermal parameters    =     2.0898
-------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10645.769       3143.4209       21660.889       21657.639

 fvalues    10645.769       3143.4209       21659.061       21657.639


    CGMAT cycle number =     25

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    1.7353925      is applied to the X-ray term
Norm of X_ray positional gradient              14.1
Norm of Geom. positional gradient              14.0
Norm of X_ray B-factor gradient                18.1
Norm of Geom. B-factor gradient                18.7
```

Product of X_ray and Geom posit. gradients -0.726E+06
Cosine of angle between them -0.997
Product of X_ray and Geom B-fact gradients -0.413E+06
Cosine of angle between them -0.990

Residuals: XRAY= 0.1847E+05 GEOM= 3144. TOTAL= 0.2161E+05
function value 21612.055

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.668	1.966
Torsion angles, period 1. refined	155	7.869	5.000
Torsion angles, period 2. refined	54	41.360	25.741
Torsion angles, period 3. refined	214	19.045	15.000
Torsion angles, period 4. refined	3	21.284	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.263	0.200
VDW; torsion: refined_atoms	786	0.324	0.200
HBOND: refined_atoms	40	0.195	0.200
VDW repulsions: symmetry: refined_atoms	55	0.261	0.200
HBOND: symmetry: refined_atoms	3	0.264	0.200
Bond B values: refined atoms	1229	13.389	4.712
Angle B values: refined atoms	1663	16.402	7.127
Torsion B values: refined atoms	426	30.280	13.061
Long range B values: refined atoms	1332	12.218	15.386

Overall : scale = 1.012, B = -0.033
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 25. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 25. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 25. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 25. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$

0.004	30	62.50	754.3	747.6	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	414.0	416.3	0.02	0.02	1	1228.4	1219.9	0.02	0.02	

0.017	83	95.60	307.7	308.6	0.03	0.02	4	403.0	413.2	0.04	0.05
0.023	97	97.14	247.4	248.4	0.02	0.02	5	180.2	188.9	0.07	0.06
0.029	108	100.00	241.3	241.9	0.02	0.02	7	186.7	189.2	0.06	0.06
0.036	126	99.25	270.3	270.7	0.02	0.02	6	252.9	253.1	0.04	0.04
0.042	129	98.56	286.3	287.5	0.02	0.02	8	338.1	341.5	0.02	0.02
0.048	150	98.73	296.7	296.4	0.02	0.02	5	305.8	306.6	0.03	0.03
0.055	151	99.38	281.2	281.3	0.02	0.02	10	257.9	259.8	0.04	0.04
0.061	172	100.00	218.3	218.5	0.02	0.02	10	202.2	201.9	0.03	0.04
0.067	174	99.45	211.4	210.9	0.02	0.02	6	286.2	283.9	0.02	0.02
0.074	178	98.92	206.1	206.8	0.02	0.02	6	234.5	235.5	0.04	0.03
0.080	189	100.00	208.7	209.0	0.02	0.02	13	159.6	155.1	0.06	0.07
0.086	197	100.00	176.7	176.9	0.02	0.02	8	208.5	207.8	0.04	0.04
0.093	193	93.55	156.9	156.9	0.02	0.02	10	181.9	185.5	0.07	0.06
0.099	188	91.28	160.7	159.7	0.02	0.02	11	159.6	157.6	0.02	0.02
0.105	190	86.02	153.8	153.4	0.02	0.02	13	169.2	170.7	0.05	0.05
0.112	183	80.08	129.9	129.5	0.03	0.03	6	135.2	138.2	0.07	0.07
0.118	194	81.85	126.9	126.6	0.02	0.02	9	138.0	137.7	0.05	0.06
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	111.5	0.08	0.08

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 25. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 25. M(Fom) v. resln :N:1,3,5,7,8:
$$

<4SSQ/LL>	NREFa	FOMa	NREFc	FOMc	NREFall	FOMall	SigmaA_Fc1 $$
0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.989	12	0.921	95	0.981	0.999
0.0228	97	0.988	11	1.000	108	0.989	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.995	17	1.000	143	0.996	0.999
0.0418	129	0.997	11	1.000	140	0.997	0.999
0.0482	150	0.991	12	1.000	162	0.991	0.999
0.0545	151	0.997	12	0.984	163	0.996	0.999
0.0609	172	0.982	15	0.941	187	0.979	0.999
0.0672	174	0.992	9	0.935	183	0.990	0.999
0.0735	178	0.989	11	1.000	189	0.990	0.999
0.0799	189	0.988	14	0.999	203	0.989	0.999
0.0862	197	0.982	9	0.978	206	0.982	0.999
0.0925	193	0.977	14	0.929	207	0.973	0.999
0.0989	188	0.978	12	0.999	200	0.980	0.999
0.1052	190	0.987	8	1.000	198	0.988	0.999
0.1116	183	0.978	13	0.936	196	0.975	1.000
0.1179	194	0.978	11	0.919	205	0.975	1.000
0.1242	174	0.981	8	1.000	182	0.981	1.000

$$

Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870

Percentage of free reflections = 4.8416
Overall R factor = 0.0200
Free R factor = 0.0420
Overall weighted R factor = 0.0200
Free weighted R factor = 0.0423
Overall correlation coefficient = 0.9993
Free correlation coefficient = 0.9965
DPI based on free R factor = 0.0763
Overall figure of merit = 0.9856
ML based su of positional parameters = 0.0422
ML based su of thermal parameters = 2.0873

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10642.741 3143.7346 21612.650 21613.066

CGMAT cycle number = 26

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.7171758 is applied to the X-ray term
Norm of X_ray positional gradient 14.0
Norm of Geom. positional gradient 14.0
Norm of X_ray B-factor gradient 18.1
Norm of Geom. B-factor gradient 19.0
Product of X_ray and Geom posit. gradients -0.722E+06
Cosine of angle between them -0.997
Product of X_ray and Geom B-fact gradients -0.413E+06
Cosine of angle between them -0.979

Residuals: XRAY= 0.1825E+05 GEOM= 3148. TOTAL= 0.2140E+05
function value 21397.297

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.670	1.966
Torsion angles, period 1. refined	155	7.872	5.000
Torsion angles, period 2. refined	54	41.372	25.741
Torsion angles, period 3. refined	214	19.057	15.000
Torsion angles, period 4. refined	3	21.301	15.000

Chiral centres: refined atoms 187 0.111 0.200
Planar groups: refined atoms 924 0.005 0.021
VDW repulsions: refined_atoms 540 0.263 0.200
VDW; torsion: refined_atoms 786 0.324 0.200
HBOND: refined_atoms 41 0.192 0.200
VDW repulsions: symmetry: refined_atoms 55 0.261 0.200
HBOND: symmetry: refined_atoms 3 0.265 0.200
Bond B values: refined atoms 1229 13.396 4.712
Angle B values: refined atoms 1663 16.414 7.127
Torsion B values: refined atoms 426 30.295 13.060
Long range B values: refined atoms 1333 12.239 15.376

Overall : scale = 1.012, B = -0.033
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 26. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 26. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 26. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 26. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.3 747.6 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.0 416.3 0.02 0.02 1 1228.4 1220.3 0.02 0.01
0.017 83 95.60 307.7 308.6 0.03 0.02 4 403.0 413.2 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.8 0.07 0.06
0.029 108 100.00 241.3 241.9 0.02 0.02 7 186.7 189.2 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 253.2 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.5 0.02 0.02
0.048 150 98.73 296.7 296.4 0.02 0.02 5 305.8 306.6 0.03 0.03
0.055 151 99.38 281.2 281.3 0.02 0.02 10 257.9 259.9 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.0 0.03 0.04
0.067 174 99.45 211.4 210.9 0.02 0.02 6 286.3 284.0 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.5 235.6 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.6 155.2 0.06 0.07
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.5 207.7 0.04 0.04
0.093 193 93.55 156.9 156.9 0.02 0.02 10 182.0 185.6 0.07 0.06
0.099 188 91.28 160.7 159.7 0.02 0.02 11 159.6 157.6 0.02 0.02
0.105 190 86.02 153.8 153.4 0.02 0.02 13 169.2 170.6 0.05 0.05
0.112 183 80.08 129.9 129.5 0.02 0.03 6 135.2 138.3 0.07 0.07
0.118 194 81.85 126.9 126.6 0.02 0.02 9 138.0 137.7 0.05 0.06

```
 0.124    174  73.20   129.0   128.9  0.02  0.02       9   113.8   111.5  0.08  0.07
$$

   ****                Fom and SigmaA vs resolution                ****

 $TABLE: Cycle   26. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
 $GRAPHS:Cycle   26. M(Fom) v. resln :N:1,3,5,7,8:
 $$
 <4SSQ/LL> NREFa  FOMa  NREFc FOMc NREFall FOMall  SigmaA_Fc1 $$
 $$
  0.0038    30   0.999     4   1.000    34   0.999  0.999
  0.0102    62   0.999     7   1.000    69   0.999  0.999
  0.0165    83   0.990    12   0.922    95   0.981  0.999
  0.0228    97   0.988    11   1.000   108   0.989  0.999
  0.0292   108   0.997     6   1.000   114   0.997  0.999
  0.0355   126   0.995    17   1.000   143   0.996  0.999
  0.0418   129   0.997    11   1.000   140   0.997  0.999
  0.0482   150   0.991    12   1.000   162   0.991  0.999
  0.0545   151   0.997    12   0.985   163   0.996  0.999
  0.0609   172   0.982    15   0.942   187   0.979  0.999
  0.0672   174   0.993     9   0.936   183   0.990  0.999
  0.0735   178   0.989    11   1.000   189   0.990  0.999
  0.0799   189   0.988    14   0.999   203   0.989  0.999
  0.0862   197   0.982     9   0.978   206   0.982  0.999
  0.0925   193   0.977    14   0.929   207   0.974  0.999
  0.0989   188   0.979    12   0.999   200   0.980  0.999
  0.1052   190   0.987     8   1.000   198   0.988  0.999
  0.1116   183   0.978    13   0.936   196   0.976  1.000
  0.1179   194   0.978    11   0.921   205   0.975  1.000
  0.1242   174   0.981     8   1.000   182   0.982  1.000
 $$
 Resolution limits                =     38.899     2.802
 Number of used reflections       =       3184
 Percentage observed              =    92.6870
 Percentage of free reflections   =     4.8416
 Overall R factor                 =     0.0199
 Free R factor                    =     0.0418
 Overall weighted R factor        =     0.0199
 Free weighted R factor           =     0.0421
 Overall correlation coefficient  =     0.9993
 Free correlation coefficient     =     0.9965
 DPI based on free R factor       =     0.0759
 Overall figure of merit          =     0.9858
 ML based su of positional parameters =     0.0420
 ML based su of thermal parameters    =     2.0759
 ------------------------------------------------------------------------------
  Trying gamma equal    0.0000000
  Convergence reached with no gamma cycles


  fvalues    10628.313       3147.5986       21395.652       21398.281
```

CGMAT cycle number = 27

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.7096521 is applied to the X-ray term
Norm of X_ray positional gradient 14.0
Norm of Geom. positional gradient 14.0
Norm of X_ray B-factor gradient 18.2
Norm of Geom. B-factor gradient 18.7
Product of X_ray and Geom posit. gradients -0.719E+06
Cosine of angle between them -0.996
Product of X_ray and Geom B-fact gradients -0.414E+06
Cosine of angle between them -0.990

Residuals: XRAY= 0.1816E+05 GEOM= 3148. TOTAL= 0.2131E+05
function value 21306.881

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.669	1.966
Torsion angles, period 1. refined	155	7.872	5.000
Torsion angles, period 2. refined	54	41.382	25.741
Torsion angles, period 3. refined	214	19.104	15.000
Torsion angles, period 4. refined	3	21.312	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	539	0.264	0.200
VDW; torsion: refined_atoms	786	0.325	0.200
HBOND: refined_atoms	41	0.192	0.200
VDW repulsions: symmetry: refined_atoms	54	0.264	0.200
HBOND: symmetry: refined_atoms	3	0.265	0.200
Bond B values: refined atoms	1229	13.404	4.712
Angle B values: refined atoms	1663	16.428	7.126
Torsion B values: refined atoms	426	30.318	13.059
Long range B values: refined atoms	1332	12.229	15.363

Overall : scale = 1.012, B = -0.027
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 27. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 27. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 27. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 27. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$

0.004	30	62.50	754.2	747.6	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	414.0	416.3	0.02	0.02	1	1228.4	1220.6	0.02	0.01	
0.017	83	95.60	307.7	308.6	0.03	0.02	4	403.0	413.2	0.04	0.05	
0.023	97	97.14	247.4	248.4	0.02	0.02	5	180.2	188.8	0.07	0.06	
0.029	108	100.00	241.3	241.9	0.02	0.02	7	186.7	189.2	0.06	0.06	
0.036	126	99.25	270.3	270.6	0.02	0.02	6	252.8	253.2	0.04	0.04	
0.042	129	98.56	286.3	287.4	0.02	0.02	8	338.1	341.5	0.02	0.02	
0.048	150	98.73	296.7	296.4	0.02	0.02	5	305.8	306.6	0.03	0.03	
0.055	151	99.38	281.2	281.3	0.02	0.02	10	257.9	259.9	0.04	0.04	
0.061	172	100.00	218.3	218.6	0.02	0.02	10	202.2	202.0	0.03	0.04	
0.067	174	99.45	211.4	210.9	0.02	0.02	6	286.2	284.0	0.02	0.02	
0.074	178	98.92	206.1	206.7	0.02	0.02	6	234.5	235.8	0.04	0.03	
0.080	189	100.00	208.7	209.0	0.02	0.02	13	159.6	155.2	0.06	0.07	
0.086	197	100.00	176.7	176.9	0.02	0.02	8	208.5	207.7	0.04	0.04	
0.093	193	93.55	156.9	156.9	0.02	0.02	10	181.9	185.6	0.07	0.06	
0.099	188	91.28	160.7	159.7	0.02	0.02	11	159.6	157.5	0.02	0.02	
0.105	190	86.02	153.8	153.4	0.02	0.02	13	169.2	170.6	0.05	0.05	
0.112	183	80.08	129.9	129.5	0.02	0.02	6	135.2	138.5	0.07	0.07	
0.118	194	81.85	126.9	126.6	0.02	0.02	9	138.0	137.7	0.05	0.06	
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	111.5	0.08	0.07	

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 27. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 27. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.990	12	0.922	95	0.981	0.999
0.0228	97	0.988	11	1.000	108	0.989	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.995	17	1.000	143	0.996	0.999
0.0418	129	0.997	11	1.000	140	0.997	0.999

```
 0.0482   150   0.991    12   1.000   162   0.991  0.999
 0.0545   151   0.997    12   0.985   163   0.996  0.999
 0.0609   172   0.982    15   0.944   187   0.979  0.999
 0.0672   174   0.993     9   0.935   183   0.990  0.999
 0.0735   178   0.989    11   1.000   189   0.990  0.999
 0.0799   189   0.988    14   0.999   203   0.989  0.999
 0.0862   197   0.982     9   0.977   206   0.982  0.999
 0.0925   193   0.977    14   0.929   207   0.974  0.999
 0.0989   188   0.979    12   0.999   200   0.980  0.999
 0.1052   190   0.987     8   1.000   198   0.988  0.999
 0.1116   183   0.979    13   0.937   196   0.976  1.000
 0.1179   194   0.978    11   0.924   205   0.976  1.000
 0.1242   174   0.981     8   1.000   182   0.982  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0198
Free R factor                    =     0.0417
Overall weighted R factor        =     0.0198
Free weighted R factor           =     0.0420
Overall correlation coefficient  =     0.9993
Free correlation coefficient     =     0.9966
DPI based on free R factor       =     0.0757
Overall figure of merit          =     0.9859
ML based su of positional parameters =     0.0419
ML based su of thermal parameters    =     2.0705
------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10621.554       3148.4907       21319.957       21307.652

 fvalues    10621.554       3148.4907       21307.598       21307.652


    CGMAT cycle number =     28

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    1.7010095      is applied to the X-ray term
Norm of X_ray positional gradient              14.0
Norm of Geom. positional gradient              14.0
```

Norm of X_ray B-factor gradient 18.1
Norm of Geom. B-factor gradient 18.7
Product of X_ray and Geom posit. gradients -0.718E+06
Cosine of angle between them -0.992
Product of X_ray and Geom B-fact gradients -0.412E+06
Cosine of angle between them -0.990

Residuals: XRAY= 0.1805E+05 GEOM= 3150. TOTAL= 0.2121E+05
function value 21205.318

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.666	1.966
Torsion angles, period 1. refined	155	7.873	5.000
Torsion angles, period 2. refined	54	41.385	25.741
Torsion angles, period 3. refined	214	19.072	15.000
Torsion angles, period 4. refined	3	21.314	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.263	0.200
VDW; torsion: refined_atoms	787	0.324	0.200
HBOND: refined_atoms	41	0.192	0.200
VDW repulsions: symmetry: refined_atoms	54	0.264	0.200
HBOND: symmetry: refined_atoms	3	0.266	0.200
Bond B values: refined atoms	1229	13.409	4.712
Angle B values: refined atoms	1663	16.436	7.127
Torsion B values: refined atoms	426	30.331	13.062
Long range B values: refined atoms	1334	12.237	15.371

Overall : scale = 1.012, B = -0.028
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 28. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 28. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 28. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 28. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$

```
 0.004     30  62.50   754.2   747.7  0.02  0.02      0     0.0     0.0******  0.00
 0.010     62  95.45   414.0   416.3  0.02  0.02      1  1228.4  1220.5  0.02  0.01
 0.017     83  95.60   307.7   308.6  0.03  0.02      4   403.0   413.3  0.04  0.05
 0.023     97  97.14   247.4   248.4  0.02  0.02      5   180.2   188.7  0.07  0.06
 0.029    108 100.00   241.3   241.9  0.02  0.02      7   186.7   189.2  0.06  0.06
 0.036    126  99.25   270.3   270.7  0.02  0.02      6   252.8   253.2  0.04  0.04
 0.042    129  98.56   286.3   287.4  0.02  0.02      8   338.1   341.5  0.02  0.02
 0.048    150  98.73   296.7   296.4  0.02  0.02      5   305.8   306.6  0.03  0.03
 0.055    151  99.38   281.2   281.3  0.02  0.02     10   257.9   259.9  0.04  0.04
 0.061    172 100.00   218.3   218.6  0.02  0.02     10   202.2   202.0  0.03  0.04
 0.067    174  99.45   211.4   210.9  0.02  0.02      6   286.2   284.0  0.02  0.02
 0.074    178  98.92   206.1   206.7  0.02  0.02      6   234.5   235.8  0.04  0.03
 0.080    189 100.00   208.7   209.0  0.02  0.02     13   159.6   155.3  0.06  0.07
 0.086    197 100.00   176.7   176.9  0.02  0.02      8   208.5   207.7  0.04  0.04
 0.093    193  93.55   156.9   156.9  0.02  0.02     10   181.9   185.7  0.07  0.06
 0.099    188  91.28   160.7   159.7  0.02  0.02     11   159.6   157.6  0.02  0.02
 0.105    190  86.02   153.8   153.4  0.02  0.02     13   169.2   170.6  0.05  0.05
 0.112    183  80.08   129.9   129.5  0.02  0.02      6   135.2   138.6  0.07  0.07
 0.118    194  81.85   126.9   126.6  0.02  0.02      9   138.0   137.7  0.05  0.06
 0.124    174  73.20   129.0   128.9  0.02  0.02      9   113.8   111.4  0.08  0.07
$$
```

**** Fom and SigmaA vs resolution ****

```
$TABLE: Cycle   28. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle   28. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa  FOMa  NREFc FOMc NREFall FOMall  SigmaA_Fc1 $$
$$
 0.0038    30   0.999     4   1.000    34   0.999  0.999
 0.0102    62   0.999     7   1.000    69   0.999  0.999
 0.0165    83   0.990    12   0.922    95   0.981  0.999
 0.0228    97   0.988    11   1.000   108   0.989  0.999
 0.0292   108   0.997     6   1.000   114   0.997  0.999
 0.0355   126   0.995    17   1.000   143   0.996  0.999
 0.0418   129   0.997    11   1.000   140   0.997  0.999
 0.0482   150   0.991    12   1.000   162   0.991  0.999
 0.0545   151   0.997    12   0.986   163   0.996  0.999
 0.0609   172   0.982    15   0.944   187   0.979  0.999
 0.0672   174   0.993     9   0.936   183   0.990  0.999
 0.0735   178   0.989    11   1.000   189   0.990  0.999
 0.0799   189   0.989    14   0.999   203   0.989  0.999
 0.0862   197   0.982     9   0.977   206   0.982  0.999
 0.0925   193   0.977    14   0.929   207   0.974  0.999
 0.0989   188   0.979    12   0.999   200   0.980  0.999
 0.1052   190   0.987     8   1.000   198   0.988  0.999
 0.1116   183   0.979    13   0.937   196   0.976  1.000
 0.1179   194   0.979    11   0.925   205   0.976  1.000
 0.1242   174   0.981     8   1.000   182   0.982  1.000
 $$
Resolution limits                =     38.899     2.802
```

Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0198
Free R factor = 0.0416
Overall weighted R factor = 0.0198
Free weighted R factor = 0.0419
Overall correlation coefficient = 0.9993
Free correlation coefficient = 0.9966
DPI based on free R factor = 0.0755
Overall figure of merit = 0.9859
ML based su of positional parameters = 0.0418
ML based su of thermal parameters = 2.0648

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10614.729 3150.3752 21227.385 21206.131

fvalues 10614.729 3150.3752 21206.904 21206.131

CGMAT cycle number = 29

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.6983110 is applied to the X-ray term
Norm of X_ray positional gradient 14.0
Norm of Geom. positional gradient 14.0
Norm of X_ray B-factor gradient 18.1
Norm of Geom. B-factor gradient 18.7
Product of X_ray and Geom posit. gradients -0.717E+06
Cosine of angle between them -0.992
Product of X_ray and Geom B-fact gradients -0.412E+06
Cosine of angle between them -0.991

Residuals: XRAY= 0.1802E+05 GEOM= 3150. TOTAL= 0.2117E+05
function value 21172.346

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.665	1.966

Torsion angles, period 1. refined 155 7.874 5.000
Torsion angles, period 2. refined 54 41.386 25.741
Torsion angles, period 3. refined 214 19.096 15.000
Torsion angles, period 4. refined 3 21.316 15.000
Chiral centres: refined atoms 187 0.111 0.200
Planar groups: refined atoms 924 0.005 0.021
VDW repulsions: refined_atoms 538 0.264 0.200
VDW; torsion: refined_atoms 787 0.324 0.200
HBOND: refined_atoms 41 0.192 0.200
VDW repulsions: symmetry: refined_atoms 54 0.264 0.200
HBOND: symmetry: refined_atoms 3 0.266 0.200
Bond B values: refined atoms 1229 13.409 4.713
Angle B values: refined atoms 1663 16.438 7.127
Torsion B values: refined atoms 426 30.332 13.062
Long range B values: refined atoms 1332 12.248 15.375

Overall : scale = 1.012, B = -0.029
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 29. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 29. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 29. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 29. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.2 747.7 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.0 416.3 0.02 0.02 1 1228.4 1220.6 0.02 0.01
0.017 83 95.60 307.7 308.6 0.03 0.02 4 403.0 413.3 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.7 0.07 0.06
0.029 108 100.00 241.3 241.9 0.02 0.02 7 186.7 189.2 0.06 0.06
0.036 126 99.25 270.3 270.6 0.02 0.02 6 252.8 253.2 0.04 0.04
0.042 129 98.56 286.3 287.4 0.02 0.02 8 338.1 341.5 0.02 0.02
0.048 150 98.73 296.7 296.4 0.02 0.02 5 305.8 306.6 0.03 0.03
0.055 151 99.38 281.2 281.3 0.02 0.02 10 257.9 259.9 0.04 0.04
0.061 172 100.00 218.3 218.6 0.02 0.02 10 202.2 202.0 0.03 0.04
0.067 174 99.45 211.4 210.9 0.02 0.02 6 286.2 284.0 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.5 235.9 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.6 155.3 0.06 0.07
0.086 197 100.00 176.7 176.9 0.02 0.02 8 208.5 207.7 0.04 0.04
0.093 193 93.55 156.9 156.9 0.02 0.02 10 181.9 185.7 0.07 0.06

```
 0.099    188  91.28   160.7   159.7  0.02  0.02      11   159.6   157.5  0.02  0.02
 0.105    190  86.02   153.8   153.4  0.02  0.02      13   169.2   170.6  0.05  0.05
 0.112    183  80.08   129.9   129.5  0.02  0.02       6   135.2   138.6  0.07  0.07
 0.118    194  81.85   126.9   126.6  0.02  0.02       9   138.0   137.7  0.05  0.06
 0.124    174  73.20   129.0   128.9  0.02  0.02       9   113.8   111.4  0.08  0.07
$$

   ****                Fom and SigmaA vs resolution                ****

 $TABLE: Cycle   29. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
 $GRAPHS:Cycle   29. M(Fom) v. resln :N:1,3,5,7,8:
 $$
 <4SSQ/LL> NREFa  FOMa  NREFc FOMc NREFall FOMall  SigmaA_Fc1 $$
 $$
  0.0038    30   0.999     4   1.000    34   0.999  0.999
  0.0102    62   0.999     7   1.000    69   0.999  0.999
  0.0165    83   0.990    12   0.922    95   0.981  0.999
  0.0228    97   0.988    11   1.000   108   0.989  0.999
  0.0292   108   0.997     6   1.000   114   0.997  0.999
  0.0355   126   0.995    17   1.000   143   0.996  0.999
  0.0418   129   0.997    11   1.000   140   0.997  0.999
  0.0482   150   0.991    12   1.000   162   0.991  0.999
  0.0545   151   0.997    12   0.986   163   0.996  0.999
  0.0609   172   0.982    15   0.944   187   0.979  0.999
  0.0672   174   0.993     9   0.936   183   0.990  0.999
  0.0735   178   0.989    11   1.000   189   0.990  0.999
  0.0799   189   0.989    14   0.999   203   0.989  0.999
  0.0862   197   0.982     9   0.977   206   0.982  0.999
  0.0925   193   0.977    14   0.929   207   0.974  0.999
  0.0989   188   0.979    12   0.999   200   0.980  0.999
  0.1052   190   0.987     8   1.000   198   0.988  0.999
  0.1116   183   0.979    13   0.937   196   0.976  1.000
  0.1179   194   0.979    11   0.925   205   0.976  1.000
  0.1242   174   0.981     8   1.000   182   0.982  1.000
 $$
 Resolution limits                =     38.899     2.802
 Number of used reflections       =       3184
 Percentage observed              =    92.6870
 Percentage of free reflections   =     4.8416
 Overall R factor                 =     0.0198
 Free R factor                    =     0.0416
 Overall weighted R factor        =     0.0198
 Free weighted R factor           =     0.0419
 Overall correlation coefficient  =     0.9993
 Free correlation coefficient     =     0.9966
 DPI based on free R factor       =     0.0755
 Overall figure of merit          =     0.9859
 ML based su of positional parameters =     0.0418
 ML based su of thermal parameters    =     2.0630
 ------------------------------------------------------------------------
  Trying gamma equal    0.0000000
```

Convergence reached with no gamma cycles

fvalues 10612.326 3150.1484 21170.391 21173.178

CGMAT cycle number = 30

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.6852858 is applied to the X-ray term
Norm of X_ray positional gradient 13.9
Norm of Geom. positional gradient 13.9
Norm of X_ray B-factor gradient 18.0
Norm of Geom. B-factor gradient 18.6
Product of X_ray and Geom posit. gradients -0.714E+06
Cosine of angle between them -0.998
Product of X_ray and Geom B-fact gradients -0.409E+06
Cosine of angle between them -0.991

Residuals: XRAY= 0.1787E+05 GEOM= 3150. TOTAL= 0.2102E+05
function value 21017.086

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.674	1.966
Torsion angles, period 1. refined	155	7.876	5.000
Torsion angles, period 2. refined	54	41.390	25.741
Torsion angles, period 3. refined	214	19.096	15.000
Torsion angles, period 4. refined	3	21.319	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	538	0.264	0.200
VDW; torsion: refined_atoms	788	0.324	0.200
HBOND: refined_atoms	41	0.192	0.200
VDW repulsions: symmetry: refined_atoms	54	0.264	0.200
HBOND: symmetry: refined_atoms	3	0.266	0.200
Bond B values: refined atoms	1229	13.404	4.713
Angle B values: refined atoms	1663	16.438	7.128
Torsion B values: refined atoms	426	30.332	13.063
Long range B values: refined atoms	1333	12.243	15.374

Overall : scale = 1.012, B = -0.030
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 30. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 30. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 30. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 30. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004	30	62.50	754.2	747.7	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	414.0	416.3	0.02	0.02	1	1228.4	1220.9	0.02	0.01	
0.017	83	95.60	307.7	308.6	0.03	0.02	4	403.0	413.4	0.04	0.05	
0.023	97	97.14	247.4	248.4	0.02	0.02	5	180.2	188.6	0.07	0.06	
0.029	108	100.00	241.3	241.9	0.02	0.02	7	186.7	189.2	0.06	0.06	
0.036	126	99.25	270.3	270.6	0.02	0.02	6	252.9	253.3	0.04	0.04	
0.042	129	98.56	286.3	287.4	0.02	0.02	8	338.1	341.5	0.02	0.02	
0.048	150	98.73	296.7	296.4	0.02	0.02	5	305.8	306.7	0.03	0.03	
0.055	151	99.38	281.2	281.3	0.02	0.02	10	257.9	259.9	0.04	0.04	
0.061	172	100.00	218.3	218.6	0.02	0.02	10	202.2	202.0	0.03	0.03	
0.067	174	99.45	211.4	210.9	0.02	0.02	6	286.2	284.0	0.02	0.02	
0.074	178	98.92	206.1	206.7	0.02	0.02	6	234.5	236.0	0.04	0.03	
0.080	189	100.00	208.7	209.0	0.02	0.02	13	159.6	155.3	0.06	0.07	
0.086	197	100.00	176.7	176.9	0.02	0.02	8	208.5	207.7	0.04	0.04	
0.093	193	93.55	156.9	156.9	0.02	0.02	10	181.9	185.7	0.07	0.06	
0.099	188	91.28	160.7	159.7	0.02	0.02	11	159.6	157.5	0.02	0.02	
0.105	190	86.02	153.8	153.4	0.02	0.02	13	169.2	170.5	0.05	0.04	
0.112	183	80.08	129.9	129.5	0.02	0.02	6	135.2	138.8	0.07	0.07	
0.118	194	81.85	126.9	126.7	0.02	0.02	9	138.0	137.7	0.05	0.06	
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	111.4	0.07	0.07	

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 30. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 30. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.990	12	0.922	95	0.981	0.999

```
 0.0228   97  0.988   11  1.000  108  0.989  0.999
 0.0292  108  0.997    6  1.000  114  0.997  0.999
 0.0355  126  0.995   17  1.000  143  0.996  0.999
 0.0418  129  0.997   11  1.000  140  0.997  0.999
 0.0482  150  0.991   12  1.000  162  0.991  0.999
 0.0545  151  0.997   12  0.987  163  0.996  0.999
 0.0609  172  0.982   15  0.946  187  0.979  0.999
 0.0672  174  0.993    9  0.936  183  0.990  0.999
 0.0735  178  0.989   11  1.000  189  0.990  0.999
 0.0799  189  0.989   14  0.999  203  0.989  0.999
 0.0862  197  0.982    9  0.977  206  0.982  0.999
 0.0925  193  0.977   14  0.929  207  0.974  0.999
 0.0989  188  0.979   12  0.999  200  0.980  0.999
 0.1052  190  0.988    8  1.000  198  0.988  0.999
 0.1116  183  0.979   13  0.937  196  0.976  1.000
 0.1179  194  0.979   11  0.926  205  0.976  1.000
 0.1242  174  0.982    8  1.000  182  0.983  1.000
 $$
Resolution limits                 =    38.899    2.802
Number of used reflections        =      3184
Percentage observed               =   92.6870
Percentage of free reflections    =    4.8416
Overall R factor                  =    0.0197
Free R factor                     =    0.0414
Overall weighted R factor         =    0.0197
Free weighted R factor            =    0.0418
Overall correlation coefficient   =    0.9993
Free correlation coefficient      =    0.9966
DPI based on free R factor        =    0.0752
Overall figure of merit           =    0.9860
ML based su of positional parameters =    0.0416
ML based su of thermal parameters    =    2.0543
--------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10602.474       3149.7554       21016.932       21017.953


    CGMAT cycle number =     31

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :   50   90   60
 Maximuum H,K,L                 :   12   21   14
 Minimum acceptable grid spacing:   33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    1.6764749      is applied to the X-ray term
```

Norm of X_ray positional gradient 13.9
Norm of Geom. positional gradient 13.9
Norm of X_ray B-factor gradient 18.0
Norm of Geom. B-factor gradient 18.6
Product of X_ray and Geom posit. gradients -0.712E+06
Cosine of angle between them -0.997
Product of X_ray and Geom B-fact gradients -0.408E+06
Cosine of angle between them -0.992

Residuals: XRAY= 0.1776E+05 GEOM= 3152. TOTAL= 0.2091E+05
function value 20912.588

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.671	1.966
Torsion angles, period 1. refined	155	7.877	5.000
Torsion angles, period 2. refined	54	41.394	25.741
Torsion angles, period 3. refined	214	19.155	15.000
Torsion angles, period 4. refined	3	21.334	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	538	0.264	0.200
VDW; torsion: refined_atoms	789	0.324	0.200
HBOND: refined_atoms	42	0.190	0.200
VDW repulsions: symmetry: refined_atoms	54	0.264	0.200
HBOND: symmetry: refined_atoms	3	0.267	0.200
Bond B values: refined atoms	1229	13.407	4.713
Angle B values: refined atoms	1663	16.445	7.128
Torsion B values: refined atoms	426	30.344	13.063
Long range B values: refined atoms	1335	12.243	15.360

Overall : scale = 1.012, B = -0.030
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 31. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 31. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 31. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 31. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used

NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.3 747.7 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.0 416.3 0.02 0.02 1 1228.4 1221.0 0.02 0.01
0.017 83 95.60 307.7 308.6 0.03 0.02 4 403.0 413.4 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.6 0.07 0.06
0.029 108 100.00 241.3 241.9 0.02 0.02 7 186.7 189.2 0.06 0.06
0.036 126 99.25 270.3 270.7 0.02 0.02 6 252.9 253.3 0.04 0.04
0.042 129 98.56 286.3 287.4 0.02 0.02 8 338.1 341.5 0.02 0.02
0.048 150 98.73 296.7 296.4 0.02 0.02 5 305.8 306.7 0.03 0.03
0.055 151 99.38 281.2 281.3 0.01 0.02 10 257.9 259.9 0.04 0.04
0.061 172 100.00 218.3 218.6 0.02 0.02 10 202.2 202.1 0.03 0.03
0.067 174 99.45 211.4 210.9 0.02 0.02 6 286.2 284.0 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.5 236.1 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.6 155.4 0.06 0.07
0.086 197 100.00 176.7 176.9 0.02 0.02 8 208.5 207.7 0.04 0.04
0.093 193 93.55 156.9 156.9 0.02 0.02 10 181.9 185.8 0.07 0.06
0.099 188 91.28 160.7 159.7 0.02 0.02 11 159.6 157.5 0.02 0.02
0.105 190 86.02 153.8 153.4 0.02 0.02 13 169.2 170.6 0.05 0.04
0.112 183 80.08 129.9 129.5 0.02 0.02 6 135.2 138.9 0.07 0.07
0.118 194 81.85 126.9 126.6 0.02 0.02 9 138.0 137.7 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.4 0.07 0.07
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 31. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 31. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.990 12 0.922 95 0.981 0.999
0.0228 97 0.988 11 1.000 108 0.989 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.995 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.991 0.999
0.0545 151 0.997 12 0.987 163 0.996 0.999
0.0609 172 0.982 15 0.947 187 0.979 0.999
0.0672 174 0.993 9 0.936 183 0.990 0.999
0.0735 178 0.989 11 1.000 189 0.990 0.999
0.0799 189 0.989 14 0.999 203 0.989 0.999
0.0862 197 0.983 9 0.977 206 0.982 0.999
0.0925 193 0.977 14 0.929 207 0.974 0.999
0.0989 188 0.979 12 1.000 200 0.980 0.999
0.1052 190 0.988 8 1.000 198 0.988 0.999
0.1116 183 0.979 13 0.937 196 0.976 1.000
0.1179 194 0.979 11 0.928 205 0.976 1.000
0.1242 174 0.982 8 1.000 182 0.983 1.000

$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0197
Free R factor = 0.0413
Overall weighted R factor = 0.0197
Free weighted R factor = 0.0417
Overall correlation coefficient = 0.9993
Free correlation coefficient = 0.9966
DPI based on free R factor = 0.0750
Overall figure of merit = 0.9861
ML based su of positional parameters = 0.0415
ML based su of thermal parameters = 2.0487

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10594.689 3151.7124 20941.482 20913.443

fvalues 10594.689 3151.7124 20915.055 20913.443

CGMAT cycle number = 32

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.6746902 is applied to the X-ray term
Norm of X_ray positional gradient 13.9
Norm of Geom. positional gradient 13.9
Norm of X_ray B-factor gradient 18.0
Norm of Geom. B-factor gradient 18.5
Product of X_ray and Geom posit. gradients -0.711E+06
Cosine of angle between them -0.996
Product of X_ray and Geom B-fact gradients -0.408E+06
Cosine of angle between them -0.992

Residuals: XRAY= 0.1774E+05 GEOM= 3151. TOTAL= 0.2089E+05
function value 20891.016

Restraint type N restraints Rms Delta Av(Sigma)

Bond distances: refined atoms 1229 0.011 0.020
Bond angles : refined atoms 1663 1.669 1.966
Torsion angles, period 1. refined 155 7.877 5.000
Torsion angles, period 2. refined 54 41.394 25.741
Torsion angles, period 3. refined 214 19.121 15.000
Torsion angles, period 4. refined 3 21.333 15.000
Chiral centres: refined atoms 187 0.111 0.200
Planar groups: refined atoms 924 0.005 0.021
VDW repulsions: refined_atoms 538 0.264 0.200
VDW; torsion: refined_atoms 789 0.324 0.200
HBOND: refined_atoms 42 0.190 0.200
VDW repulsions: symmetry: refined_atoms 54 0.264 0.200
HBOND: symmetry: refined_atoms 3 0.267 0.200
Bond B values: refined atoms 1229 13.409 4.713
Angle B values: refined atoms 1663 16.448 7.128
Torsion B values: refined atoms 426 30.348 13.063
Long range B values: refined atoms 1335 12.245 15.360

Overall : scale = 1.012, B = -0.029
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 32. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 32. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 32. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 32. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.2 747.7 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.0 416.3 0.02 0.02 1 1228.4 1221.1 0.02 0.01
0.017 83 95.60 307.7 308.6 0.03 0.02 4 403.0 413.4 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.6 0.07 0.06
0.029 108 100.00 241.3 241.9 0.02 0.02 7 186.7 189.2 0.06 0.06
0.036 126 99.25 270.3 270.6 0.02 0.02 6 252.9 253.3 0.04 0.04
0.042 129 98.56 286.3 287.4 0.02 0.02 8 338.1 341.5 0.02 0.02
0.048 150 98.73 296.7 296.4 0.02 0.02 5 305.8 306.7 0.03 0.03
0.055 151 99.38 281.2 281.3 0.01 0.02 10 257.9 259.9 0.04 0.04
0.061 172 100.00 218.3 218.6 0.02 0.02 10 202.2 202.1 0.03 0.03
0.067 174 99.45 211.4 210.9 0.02 0.02 6 286.2 284.0 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.5 236.1 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.6 155.4 0.06 0.07

0.086	197	100.00	176.7	176.9	0.02	0.02	8	208.5	207.7	0.04	0.04
0.093	193	93.55	156.9	156.9	0.02	0.02	10	181.9	185.7	0.07	0.06
0.099	188	91.28	160.7	159.7	0.02	0.02	11	159.6	157.5	0.02	0.02
0.105	190	86.02	153.8	153.4	0.02	0.02	13	169.2	170.6	0.05	0.04
0.112	183	80.08	129.9	129.5	0.02	0.02	6	135.2	139.0	0.07	0.07
0.118	194	81.85	126.9	126.6	0.02	0.02	9	138.0	137.6	0.05	0.05
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	111.4	0.07	0.07

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 32. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 32. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.990	12	0.922	95	0.981	0.999
0.0228	97	0.988	11	1.000	108	0.989	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.995	17	1.000	143	0.996	0.999
0.0418	129	0.997	11	1.000	140	0.997	0.999
0.0482	150	0.991	12	1.000	162	0.991	0.999
0.0545	151	0.997	12	0.987	163	0.996	0.999
0.0609	172	0.982	15	0.947	187	0.979	0.999
0.0672	174	0.993	9	0.937	183	0.990	0.999
0.0735	178	0.989	11	1.000	189	0.990	0.999
0.0799	189	0.989	14	0.999	203	0.989	0.999
0.0862	197	0.983	9	0.977	206	0.982	0.999
0.0925	193	0.977	14	0.929	207	0.974	0.999
0.0989	188	0.979	12	1.000	200	0.980	0.999
0.1052	190	0.988	8	1.000	198	0.988	0.999
0.1116	183	0.979	13	0.937	196	0.976	1.000
0.1179	194	0.979	11	0.928	205	0.976	1.000
0.1242	174	0.982	8	1.000	182	0.983	1.000

$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0197
Free R factor = 0.0413
Overall weighted R factor = 0.0197
Free weighted R factor = 0.0417
Overall correlation coefficient = 0.9993
Free correlation coefficient = 0.9966
DPI based on free R factor = 0.0751
Overall figure of merit = 0.9861
ML based su of positional parameters = 0.0415
ML based su of thermal parameters = 2.0474

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10593.299 3151.3811 20889.953 20891.875

CGMAT cycle number = 33

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.6650449 is applied to the X-ray term
Norm of X_ray positional gradient 13.9
Norm of Geom. positional gradient 13.9
Norm of X_ray B-factor gradient 18.0
Norm of Geom. B-factor gradient 18.5
Product of X_ray and Geom posit. gradients -0.709E+06
Cosine of angle between them -0.998
Product of X_ray and Geom B-fact gradients -0.407E+06
Cosine of angle between them -0.992

Residuals: XRAY= 0.1762E+05 GEOM= 3152. TOTAL= 0.2078E+05
function value 20776.221

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.675	1.966
Torsion angles, period 1. refined	155	7.878	5.000
Torsion angles, period 2. refined	54	41.396	25.741
Torsion angles, period 3. refined	214	19.143	15.000
Torsion angles, period 4. refined	3	21.335	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	538	0.264	0.200
VDW; torsion: refined_atoms	788	0.324	0.200
HBOND: refined_atoms	42	0.190	0.200
VDW repulsions: symmetry: refined_atoms	54	0.264	0.200
HBOND: symmetry: refined_atoms	3	0.267	0.200
Bond B values: refined atoms	1229	13.409	4.713
Angle B values: refined atoms	1663	16.453	7.128
Torsion B values: refined atoms	426	30.358	13.063
Long range B values: refined atoms	1334	12.257	15.358

Overall : scale = 1.012, B = -0.030
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 33. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 33. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 33. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 33. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.3 747.7 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.0 416.3 0.02 0.02 1 1228.4 1221.3 0.01 0.01
0.017 83 95.60 307.7 308.6 0.03 0.02 4 403.0 413.5 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.5 0.07 0.06
0.029 108 100.00 241.3 241.9 0.02 0.02 7 186.7 189.2 0.06 0.06
0.036 126 99.25 270.3 270.7 0.02 0.02 6 252.9 253.4 0.04 0.04
0.042 129 98.56 286.3 287.4 0.02 0.02 8 338.1 341.5 0.02 0.02
0.048 150 98.73 296.7 296.4 0.02 0.02 5 305.8 306.7 0.03 0.03
0.055 151 99.38 281.2 281.3 0.01 0.02 10 257.9 260.0 0.04 0.04
0.061 172 100.00 218.3 218.6 0.02 0.02 10 202.2 202.1 0.03 0.03
0.067 174 99.45 211.4 210.9 0.02 0.02 6 286.2 284.1 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.5 236.2 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.6 155.4 0.06 0.07
0.086 197 100.00 176.7 176.9 0.02 0.02 8 208.5 207.7 0.04 0.04
0.093 193 93.55 156.9 156.9 0.02 0.02 10 181.9 185.8 0.07 0.06
0.099 188 91.28 160.7 159.7 0.02 0.02 11 159.6 157.4 0.02 0.02
0.105 190 86.02 153.8 153.4 0.02 0.02 13 169.2 170.6 0.05 0.04
0.112 183 80.08 129.9 129.5 0.02 0.02 6 135.2 139.0 0.07 0.07
0.118 194 81.85 126.9 126.7 0.02 0.02 9 138.0 137.6 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.4 0.07 0.07
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 33. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 33. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999

```
 0.0102   62  0.999    7  1.000   69  0.999  0.999
 0.0165   83  0.990   12  0.922   95  0.981  0.999
 0.0228   97  0.988   11  1.000  108  0.989  0.999
 0.0292  108  0.997    6  1.000  114  0.997  0.999
 0.0355  126  0.995   17  1.000  143  0.996  0.999
 0.0418  129  0.997   11  1.000  140  0.997  0.999
 0.0482  150  0.991   12  1.000  162  0.991  0.999
 0.0545  151  0.997   12  0.987  163  0.996  0.999
 0.0609  172  0.982   15  0.948  187  0.980  0.999
 0.0672  174  0.993    9  0.936  183  0.990  0.999
 0.0735  178  0.989   11  1.000  189  0.990  0.999
 0.0799  189  0.989   14  0.999  203  0.989  0.999
 0.0862  197  0.983    9  0.976  206  0.982  0.999
 0.0925  193  0.977   14  0.929  207  0.974  0.999
 0.0989  188  0.979   12  1.000  200  0.980  0.999
 0.1052  190  0.988    8  1.000  198  0.988  0.999
 0.1116  183  0.979   13  0.938  196  0.977  1.000
 0.1179  194  0.979   11  0.929  205  0.976  1.000
 0.1242  174  0.982    8  1.000  182  0.983  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0196
Free R factor                    =     0.0412
Overall weighted R factor        =     0.0196
Free weighted R factor           =     0.0416
Overall correlation coefficient  =     0.9993
Free correlation coefficient     =     0.9966
DPI based on free R factor       =     0.0748
Overall figure of merit          =     0.9862
ML based su of positional parameters =     0.0413
ML based su of thermal parameters    =     2.0411
------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10585.537       3151.7544       20777.715       20777.148

 fvalues    10585.537       3151.7544       20776.447       20777.148


    CGMAT cycle number =     34

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :   50   90   60
 Maximuum H,K,L                 :   12   21   14
 Minimum acceptable grid spacing:   33   56   38
 fast hessian tabulation
```

B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.6604552 is applied to the X-ray term
Norm of X_ray positional gradient 13.9
Norm of Geom. positional gradient 13.9
Norm of X_ray B-factor gradient 18.0
Norm of Geom. B-factor gradient 18.5
Product of X_ray and Geom posit. gradients -0.708E+06
Cosine of angle between them -0.998
Product of X_ray and Geom B-fact gradients -0.406E+06
Cosine of angle between them -0.993

Residuals: XRAY= 0.1757E+05 GEOM= 3152. TOTAL= 0.2072E+05
function value 20721.834

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.674	1.966
Torsion angles, period 1. refined	155	7.878	5.000
Torsion angles, period 2. refined	54	41.397	25.741
Torsion angles, period 3. refined	214	19.127	15.000
Torsion angles, period 4. refined	3	21.335	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	538	0.264	0.200
VDW; torsion: refined_atoms	788	0.324	0.200
HBOND: refined_atoms	42	0.190	0.200
VDW repulsions: symmetry: refined_atoms	54	0.264	0.200
HBOND: symmetry: refined_atoms	3	0.268	0.200
Bond B values: refined atoms	1229	13.410	4.713
Angle B values: refined atoms	1663	16.456	7.128
Torsion B values: refined atoms	426	30.364	13.063
Long range B values: refined atoms	1334	12.259	15.357

Overall : scale = 1.012, B = -0.029
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 34. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 34. <Rfactor> v. resln :N:1,6,7,11,12:

:Cycle 34. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 34. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.3 747.7 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.0 416.3 0.02 0.02 1 1228.4 1221.4 0.01 0.01
0.017 83 95.60 307.7 308.6 0.03 0.02 4 403.0 413.4 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.5 0.07 0.06
0.029 108 100.00 241.3 241.9 0.02 0.02 7 186.7 189.2 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 253.4 0.04 0.04
0.042 129 98.56 286.3 287.4 0.02 0.02 8 338.1 341.5 0.02 0.02
0.048 150 98.73 296.7 296.4 0.02 0.02 5 305.8 306.7 0.03 0.03
0.055 151 99.38 281.2 281.4 0.01 0.02 10 257.9 260.0 0.04 0.04
0.061 172 100.00 218.3 218.6 0.02 0.02 10 202.2 202.1 0.03 0.03
0.067 174 99.45 211.4 210.9 0.02 0.02 6 286.2 284.1 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.5 236.2 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.6 155.4 0.06 0.06
0.086 197 100.00 176.7 176.9 0.02 0.02 8 208.5 207.7 0.04 0.04
0.093 193 93.55 156.9 156.9 0.02 0.02 10 181.9 185.8 0.07 0.06
0.099 188 91.28 160.7 159.7 0.02 0.02 11 159.6 157.4 0.02 0.02
0.105 190 86.02 153.8 153.4 0.02 0.02 13 169.2 170.6 0.05 0.04
0.112 183 80.08 129.9 129.5 0.02 0.02 6 135.2 139.1 0.08 0.07
0.118 194 81.85 126.9 126.7 0.02 0.02 9 138.0 137.6 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.4 0.07 0.07
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 34. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 34. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.990 12 0.922 95 0.981 0.999
0.0228 97 0.988 11 1.000 108 0.989 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.995 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.991 0.999
0.0545 151 0.997 12 0.988 163 0.996 0.999
0.0609 172 0.982 15 0.948 187 0.980 0.999
0.0672 174 0.993 9 0.937 183 0.990 0.999
0.0735 178 0.990 11 1.000 189 0.990 0.999
0.0799 189 0.989 14 0.999 203 0.989 0.999
0.0862 197 0.983 9 0.976 206 0.982 0.999
0.0925 193 0.978 14 0.929 207 0.974 0.999
0.0989 188 0.979 12 1.000 200 0.980 0.999

```
 0.1052   190   0.988    8   1.000   198   0.988  0.999
 0.1116   183   0.979   13   0.938   196   0.977  1.000
 0.1179   194   0.979   11   0.929   205   0.976  1.000
 0.1242   174   0.982    8   1.000   182   0.983  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0196
Free R factor                    =     0.0412
Overall weighted R factor        =     0.0196
Free weighted R factor           =     0.0415
Overall correlation coefficient  =     0.9993
Free correlation coefficient     =     0.9966
DPI based on free R factor       =     0.0748
Overall figure of merit          =     0.9862
ML based su of positional parameters =     0.0413
ML based su of thermal parameters    =     2.0381
------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10581.767       3152.1528       20725.113       20722.703

 fvalues    10581.767       3152.1528       20722.465       20722.703


    CGMAT cycle number =     35

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    1.6575198      is applied to the X-ray term
Norm of X_ray positional gradient              13.9
Norm of Geom. positional gradient              13.9
Norm of X_ray B-factor gradient                18.0
Norm of Geom. B-factor gradient                18.5
Product of X_ray and Geom posit. gradients     -0.707E+06
 Cosine of angle between them                  -0.998
Product of X_ray and Geom B-fact gradients     -0.406E+06
 Cosine of angle between them                  -0.993


Residuals: XRAY=     0.1753E+05 GEOM=      3153.     TOTAL=     0.2069E+05
```

function value 20687.162

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.673	1.966
Torsion angles, period 1. refined	155	7.878	5.000
Torsion angles, period 2. refined	54	41.398	25.741
Torsion angles, period 3. refined	214	19.162	15.000
Torsion angles, period 4. refined	3	21.336	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	538	0.265	0.200
VDW; torsion: refined_atoms	788	0.324	0.200
HBOND: refined_atoms	42	0.190	0.200
VDW repulsions: symmetry: refined_atoms	54	0.264	0.200
HBOND: symmetry: refined_atoms	3	0.268	0.200
Bond B values: refined atoms	1229	13.408	4.713
Angle B values: refined atoms	1663	16.456	7.128
Torsion B values: refined atoms	426	30.366	13.063
Long range B values: refined atoms	1334	12.261	15.357

Overall : scale = 1.012, B = -0.029
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 35. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 35. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 35. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 35. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$

0.004	30	62.50	754.3	747.7	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	414.0	416.3	0.02	0.02	1	1228.4	1221.5	0.01	0.01	
0.017	83	95.60	307.7	308.6	0.03	0.02	4	403.0	413.5	0.04	0.05	
0.023	97	97.14	247.4	248.4	0.02	0.02	5	180.2	188.5	0.07	0.06	
0.029	108	100.00	241.3	241.9	0.02	0.02	7	186.7	189.2	0.06	0.06	
0.036	126	99.25	270.4	270.7	0.02	0.02	6	252.9	253.4	0.04	0.04	
0.042	129	98.56	286.3	287.4	0.02	0.02	8	338.1	341.5	0.02	0.02	
0.048	150	98.73	296.7	296.4	0.02	0.02	5	305.8	306.7	0.03	0.03	
0.055	151	99.38	281.2	281.4	0.01	0.02	10	257.9	260.0	0.04	0.04	

0.061	172	100.00	218.3	218.6	0.02	0.02	10	202.2	202.1	0.03	0.03
0.067	174	99.45	211.4	210.9	0.02	0.02	6	286.2	284.1	0.02	0.02
0.074	178	98.92	206.1	206.7	0.02	0.02	6	234.5	236.2	0.04	0.03
0.080	189	100.00	208.7	209.0	0.02	0.02	13	159.6	155.4	0.06	0.06
0.086	197	100.00	176.7	176.9	0.02	0.02	8	208.5	207.7	0.04	0.04
0.093	193	93.55	156.9	156.9	0.02	0.02	10	181.9	185.8	0.07	0.06
0.099	188	91.28	160.7	159.7	0.02	0.02	11	159.6	157.4	0.02	0.02
0.105	190	86.02	153.8	153.4	0.02	0.02	13	169.2	170.5	0.05	0.04
0.112	183	80.08	129.9	129.5	0.02	0.02	6	135.2	139.2	0.08	0.07
0.118	194	81.85	126.9	126.7	0.02	0.02	9	138.0	137.6	0.05	0.05
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	111.4	0.07	0.07

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 35. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 35. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.990	12	0.922	95	0.981	0.999
0.0228	97	0.988	11	1.000	108	0.989	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.995	17	1.000	143	0.996	0.999
0.0418	129	0.997	11	1.000	140	0.997	0.999
0.0482	150	0.991	12	1.000	162	0.991	0.999
0.0545	151	0.997	12	0.988	163	0.996	0.999
0.0609	172	0.982	15	0.949	187	0.980	0.999
0.0672	174	0.993	9	0.937	183	0.990	0.999
0.0735	178	0.990	11	1.000	189	0.990	0.999
0.0799	189	0.989	14	0.999	203	0.989	0.999
0.0862	197	0.983	9	0.976	206	0.982	0.999
0.0925	193	0.978	14	0.929	207	0.974	0.999
0.0989	188	0.979	12	1.000	200	0.980	0.999
0.1052	190	0.988	8	1.000	198	0.988	0.999
0.1116	183	0.979	13	0.938	196	0.977	1.000
0.1179	194	0.979	11	0.930	205	0.976	1.000
0.1242	174	0.982	8	1.000	182	0.983	1.000

$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0196
Free R factor = 0.0411
Overall weighted R factor = 0.0196
Free weighted R factor = 0.0415
Overall correlation coefficient = 0.9993
Free correlation coefficient = 0.9966

DPI based on free R factor = 0.0747
Overall figure of merit = 0.9863
ML based su of positional parameters = 0.0413
ML based su of thermal parameters = 2.0362

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10579.149 3152.8850 20693.193 20688.035

fvalues 10579.149 3152.8850 20687.895 20688.035

CGMAT cycle number = 36

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.6545693 is applied to the X-ray term
Norm of X_ray positional gradient 13.9
Norm of Geom. positional gradient 13.9
Norm of X_ray B-factor gradient 18.0
Norm of Geom. B-factor gradient 18.5
Product of X_ray and Geom posit. gradients -0.707E+06
Cosine of angle between them -0.996
Product of X_ray and Geom B-fact gradients -0.405E+06
Cosine of angle between them -0.993

Residuals: XRAY= 0.1750E+05 GEOM= 3154. TOTAL= 0.2065E+05
function value 20652.633

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.672	1.966
Torsion angles, period 1. refined	155	7.878	5.000
Torsion angles, period 2. refined	54	41.398	25.741
Torsion angles, period 3. refined	214	19.133	15.000
Torsion angles, period 4. refined	3	21.339	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	538	0.265	0.200
VDW; torsion: refined_atoms	789	0.324	0.200
HBOND: refined_atoms	42	0.190	0.200

VDW repulsions: symmetry: refined_atoms 54 0.264 0.200
HBOND: symmetry: refined_atoms 3 0.268 0.200
Bond B values: refined atoms 1229 13.410 4.713
Angle B values: refined atoms 1663 16.460 7.127
Torsion B values: refined atoms 426 30.372 13.063
Long range B values: refined atoms 1335 12.260 15.356

Overall : scale = 1.012, B = -0.029
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 36. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 36. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 36. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 36. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.3 747.7 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.0 416.3 0.02 0.02 1 1228.4 1221.5 0.01 0.01
0.017 83 95.60 307.7 308.6 0.03 0.02 4 403.0 413.5 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.5 0.07 0.06
0.029 108 100.00 241.3 241.9 0.02 0.02 7 186.7 189.2 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 253.4 0.04 0.04
0.042 129 98.56 286.3 287.4 0.02 0.02 8 338.1 341.5 0.02 0.02
0.048 150 98.73 296.7 296.4 0.02 0.02 5 305.8 306.7 0.03 0.03
0.055 151 99.38 281.2 281.4 0.01 0.02 10 257.9 260.0 0.04 0.04
0.061 172 100.00 218.3 218.6 0.02 0.02 10 202.2 202.1 0.03 0.03
0.067 174 99.45 211.4 210.9 0.02 0.02 6 286.2 284.1 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.5 236.3 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.6 155.4 0.06 0.06
0.086 197 100.00 176.7 176.9 0.02 0.02 8 208.5 207.6 0.04 0.04
0.093 193 93.55 156.9 156.9 0.02 0.02 10 182.0 185.8 0.07 0.06
0.099 188 91.28 160.7 159.7 0.02 0.02 11 159.6 157.4 0.02 0.02
0.105 190 86.02 153.8 153.4 0.02 0.02 13 169.2 170.5 0.05 0.04
0.112 183 80.08 129.9 129.5 0.02 0.02 6 135.2 139.2 0.08 0.07
0.118 194 81.85 126.9 126.7 0.02 0.02 9 138.0 137.6 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.3 0.07 0.07
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 36. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 36. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.990 12 0.922 95 0.981 0.999
0.0228 97 0.988 11 1.000 108 0.989 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.996 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.991 0.999
0.0545 151 0.997 12 0.988 163 0.996 0.999
0.0609 172 0.982 15 0.949 187 0.980 0.999
0.0672 174 0.993 9 0.936 183 0.990 0.999
0.0735 178 0.990 11 1.000 189 0.990 0.999
0.0799 189 0.989 14 0.999 203 0.989 0.999
0.0862 197 0.983 9 0.976 206 0.982 0.999
0.0925 193 0.978 14 0.929 207 0.974 0.999
0.0989 188 0.979 12 1.000 200 0.980 0.999
0.1052 190 0.988 8 1.000 198 0.988 0.999
0.1116 183 0.979 13 0.938 196 0.977 1.000
0.1179 194 0.979 11 0.931 205 0.977 1.000
0.1242 174 0.982 8 1.000 182 0.983 1.000
$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0196
Free R factor = 0.0411
Overall weighted R factor = 0.0196
Free weighted R factor = 0.0415
Overall correlation coefficient = 0.9993
Free correlation coefficient = 0.9967
DPI based on free R factor = 0.0746
Overall figure of merit = 0.9863
ML based su of positional parameters = 0.0412
ML based su of thermal parameters = 2.0342

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10576.665 3153.6279 20663.875 20653.453

fvalues 10576.665 3153.6279 20653.883 20653.453

CGMAT cycle number = 37

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000008
Actual weight 1.6520013 is applied to the X-ray term
Norm of X_ray positional gradient 13.9
Norm of Geom. positional gradient 13.9
Norm of X_ray B-factor gradient 18.0
Norm of Geom. B-factor gradient 18.5
Product of X_ray and Geom posit. gradients -0.706E+06
Cosine of angle between them -0.996
Product of X_ray and Geom B-fact gradients -0.405E+06
Cosine of angle between them -0.993

Residuals: XRAY= 0.1747E+05 GEOM= 3154. TOTAL= 0.2062E+05
function value 20621.973

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.671	1.966
Torsion angles, period 1. refined	155	7.878	5.000
Torsion angles, period 2. refined	54	41.399	25.741
Torsion angles, period 3. refined	214	19.153	15.000
Torsion angles, period 4. refined	3	21.339	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	539	0.264	0.200
VDW; torsion: refined_atoms	789	0.324	0.200
HBOND: refined_atoms	42	0.190	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.268	0.200
Bond B values: refined atoms	1229	13.412	4.713
Angle B values: refined atoms	1663	16.463	7.127
Torsion B values: refined atoms	426	30.379	13.063
Long range B values: refined atoms	1336	12.261	15.356

Overall : scale = 1.012, B = -0.029
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 37. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 37. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 37. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 37. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004	30	62.50	754.3	747.7	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	414.0	416.3	0.02	0.02	1	1228.4	1221.7	0.01	0.01	
0.017	83	95.60	307.7	308.6	0.03	0.02	4	403.0	413.5	0.04	0.05	
0.023	97	97.14	247.4	248.4	0.02	0.02	5	180.2	188.5	0.07	0.06	
0.029	108	100.00	241.3	241.9	0.02	0.02	7	186.7	189.2	0.06	0.06	
0.036	126	99.25	270.4	270.7	0.02	0.02	6	252.9	253.4	0.04	0.04	
0.042	129	98.56	286.3	287.4	0.02	0.02	8	338.1	341.5	0.02	0.02	
0.048	150	98.73	296.7	296.4	0.02	0.02	5	305.8	306.7	0.03	0.03	
0.055	151	99.38	281.2	281.4	0.01	0.02	10	257.9	260.0	0.04	0.04	
0.061	172	100.00	218.4	218.6	0.02	0.02	10	202.2	202.1	0.03	0.03	
0.067	174	99.45	211.4	210.9	0.02	0.02	6	286.3	284.1	0.02	0.02	
0.074	178	98.92	206.1	206.7	0.02	0.02	6	234.5	236.3	0.04	0.03	
0.080	189	100.00	208.7	209.0	0.02	0.02	13	159.6	155.4	0.06	0.06	
0.086	197	100.00	176.8	176.9	0.02	0.02	8	208.5	207.7	0.04	0.04	
0.093	193	93.55	156.9	156.9	0.02	0.02	10	182.0	185.8	0.07	0.06	
0.099	188	91.28	160.7	159.7	0.02	0.02	11	159.6	157.4	0.02	0.02	
0.105	190	86.02	153.8	153.4	0.02	0.02	13	169.2	170.5	0.05	0.04	
0.112	183	80.08	129.9	129.5	0.02	0.02	6	135.2	139.2	0.08	0.07	
0.118	194	81.85	126.9	126.7	0.02	0.02	9	138.0	137.6	0.05	0.05	
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	111.3	0.07	0.07	

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 37. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 37. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.990	12	0.922	95	0.981	0.999
0.0228	97	0.988	11	1.000	108	0.989	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.996	17	1.000	143	0.996	0.999
0.0418	129	0.997	11	1.000	140	0.997	0.999
0.0482	150	0.991	12	1.000	162	0.991	0.999
0.0545	151	0.997	12	0.988	163	0.996	0.999
0.0609	172	0.982	15	0.949	187	0.980	0.999

```
 0.0672   174   0.993    9   0.937   183   0.990  0.999
 0.0735   178   0.990   11   1.000   189   0.990  0.999
 0.0799   189   0.989   14   0.999   203   0.989  0.999
 0.0862   197   0.983    9   0.976   206   0.982  0.999
 0.0925   193   0.978   14   0.929   207   0.974  0.999
 0.0989   188   0.979   12   1.000   200   0.980  0.999
 0.1052   190   0.988    8   1.000   198   0.988  0.999
 0.1116   183   0.979   13   0.938   196   0.977  1.000
 0.1179   194   0.979   11   0.931   205   0.977  1.000
 0.1242   174   0.982    8   1.000   182   0.983  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0196
Free R factor                    =     0.0411
Overall weighted R factor        =     0.0196
Free weighted R factor           =     0.0414
Overall correlation coefficient  =     0.9993
Free correlation coefficient     =     0.9967
DPI based on free R factor       =     0.0746
Overall figure of merit          =     0.9863
ML based su of positional parameters =     0.0412
ML based su of thermal parameters    =     2.0326
------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10574.475       3153.7915       20621.496       20622.836


    CGMAT cycle number =     38

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    1.6461320      is applied to the X-ray term
Norm of X_ray positional gradient              13.8
Norm of Geom. positional gradient              13.8
Norm of X_ray B-factor gradient                18.0
Norm of Geom. B-factor gradient                18.4
Product of X_ray and Geom posit. gradients     -0.705E+06
 Cosine of angle between them                  -0.999
Product of X_ray and Geom B-fact gradients     -0.404E+06
```

Cosine of angle between them -0.993

Residuals: XRAY= 0.1740E+05 GEOM= 3154. TOTAL= 0.2055E+05
function value 20552.236

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.677	1.966
Torsion angles, period 1. refined	155	7.879	5.000
Torsion angles, period 2. refined	54	41.400	25.741
Torsion angles, period 3. refined	214	19.150	15.000
Torsion angles, period 4. refined	3	21.342	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	541	0.264	0.200
VDW; torsion: refined_atoms	789	0.324	0.200
HBOND: refined_atoms	42	0.190	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.268	0.200
Bond B values: refined atoms	1229	13.416	4.713
Angle B values: refined atoms	1663	16.472	7.127
Torsion B values: refined atoms	426	30.396	13.062
Long range B values: refined atoms	1338	12.261	15.363

Overall : scale = 1.012, B = -0.029
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 38. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 38. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 38. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 38. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$

0.004	30	62.50	754.3	747.7	0.02	0.02	0	0.0	0.0******	0.00	
0.010	62	95.45	414.0	416.3	0.02	0.02	1	1228.4	1221.9	0.01	0.01
0.017	83	95.60	307.7	308.7	0.03	0.02	4	403.0	413.5	0.04	0.05
0.023	97	97.14	247.4	248.4	0.02	0.02	5	180.2	188.4	0.07	0.06
0.029	108	100.00	241.3	241.9	0.02	0.02	7	186.7	189.2	0.06	0.06

0.036	126	99.25	270.4	270.7	0.02	0.02	6	252.9	253.5	0.04	0.04
0.042	129	98.56	286.3	287.4	0.02	0.02	8	338.1	341.5	0.02	0.02
0.048	150	98.73	296.7	296.4	0.02	0.02	5	305.8	306.7	0.03	0.03
0.055	151	99.38	281.2	281.4	0.01	0.02	10	257.9	260.0	0.04	0.04
0.061	172	100.00	218.4	218.6	0.02	0.02	10	202.2	202.2	0.03	0.03
0.067	174	99.45	211.4	210.9	0.02	0.02	6	286.3	284.1	0.02	0.02
0.074	178	98.92	206.1	206.7	0.02	0.02	6	234.5	236.3	0.03	0.03
0.080	189	100.00	208.7	209.0	0.02	0.02	13	159.6	155.5	0.06	0.06
0.086	197	100.00	176.8	176.9	0.02	0.02	8	208.5	207.7	0.04	0.04
0.093	193	93.55	156.9	156.9	0.02	0.02	10	182.0	185.8	0.07	0.06
0.099	188	91.28	160.7	159.7	0.02	0.02	11	159.6	157.4	0.02	0.02
0.105	190	86.02	153.8	153.5	0.02	0.02	13	169.2	170.5	0.05	0.04
0.112	183	80.08	129.9	129.5	0.02	0.02	6	135.2	139.4	0.08	0.07
0.118	194	81.85	126.9	126.7	0.02	0.02	9	138.0	137.6	0.05	0.05
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	111.3	0.07	0.07

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 38. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 38. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.990	12	0.922	95	0.981	0.999
0.0228	97	0.988	11	1.000	108	0.989	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.996	17	1.000	143	0.996	0.999
0.0418	129	0.997	11	1.000	140	0.997	0.999
0.0482	150	0.991	12	1.000	162	0.991	0.999
0.0545	151	0.997	12	0.989	163	0.996	0.999
0.0609	172	0.982	15	0.951	187	0.980	0.999
0.0672	174	0.993	9	0.937	183	0.990	0.999
0.0735	178	0.990	11	1.000	189	0.990	0.999
0.0799	189	0.989	14	0.999	203	0.989	0.999
0.0862	197	0.983	9	0.976	206	0.983	0.999
0.0925	193	0.978	14	0.929	207	0.974	0.999
0.0989	188	0.979	12	1.000	200	0.980	0.999
0.1052	190	0.988	8	1.000	198	0.988	0.999
0.1116	183	0.980	13	0.938	196	0.977	1.000
0.1179	194	0.979	11	0.931	205	0.977	1.000
0.1242	174	0.983	8	1.000	182	0.983	1.000

$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0195
Free R factor = 0.0410

Overall weighted R factor = 0.0195
Free weighted R factor = 0.0414
Overall correlation coefficient = 0.9993
Free correlation coefficient = 0.9967
DPI based on free R factor = 0.0745
Overall figure of merit = 0.9864
ML based su of positional parameters = 0.0411
ML based su of thermal parameters = 2.0287

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10569.684 3154.0061 20553.070 20553.100

CGMAT cycle number = 39

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.6417204 is applied to the X-ray term
Norm of X_ray positional gradient 13.8
Norm of Geom. positional gradient 13.8
Norm of X_ray B-factor gradient 18.0
Norm of Geom. B-factor gradient 18.4
Product of X_ray and Geom posit. gradients -0.704E+06
Cosine of angle between them -0.998
Product of X_ray and Geom B-fact gradients -0.404E+06
Cosine of angle between them -0.993

Residuals: XRAY= 0.1734E+05 GEOM= 3156. TOTAL= 0.2050E+05
function value 20500.240

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.675	1.966
Torsion angles, period 1. refined	155	7.879	5.000
Torsion angles, period 2. refined	54	41.402	25.741
Torsion angles, period 3. refined	214	19.199	15.000
Torsion angles, period 4. refined	3	21.350	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	541	0.264	0.200

VDW; torsion: refined_atoms 790 0.324 0.200
HBOND: refined_atoms 42 0.190 0.200
VDW repulsions: symmetry: refined_atoms 55 0.262 0.200
HBOND: symmetry: refined_atoms 3 0.268 0.200
Bond B values: refined atoms 1229 13.419 4.713
Angle B values: refined atoms 1663 16.478 7.127
Torsion B values: refined atoms 426 30.413 13.062
Long range B values: refined atoms 1338 12.264 15.362

Overall : scale = 1.012, B = -0.028
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 39. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 39. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 39. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 39. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.3 747.7 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.0 416.3 0.02 0.02 1 1228.5 1222.0 0.01 0.01
0.017 83 95.60 307.7 308.6 0.03 0.02 4 403.0 413.5 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.4 0.07 0.06
0.029 108 100.00 241.3 241.9 0.02 0.02 7 186.7 189.2 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 253.5 0.04 0.04
0.042 129 98.56 286.3 287.4 0.02 0.02 8 338.1 341.5 0.02 0.02
0.048 150 98.73 296.7 296.4 0.02 0.02 5 305.8 306.7 0.03 0.03
0.055 151 99.38 281.2 281.4 0.01 0.02 10 257.9 260.0 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.2 0.03 0.03
0.067 174 99.45 211.4 210.9 0.02 0.02 6 286.3 284.2 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.5 236.4 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.6 155.5 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.5 207.7 0.04 0.04
0.093 193 93.55 156.9 156.9 0.02 0.02 10 182.0 185.8 0.07 0.06
0.099 188 91.28 160.7 159.7 0.02 0.02 11 159.6 157.3 0.02 0.02
0.105 190 86.02 153.8 153.5 0.02 0.02 13 169.2 170.5 0.05 0.04
0.112 183 80.08 129.9 129.5 0.02 0.02 6 135.2 139.5 0.08 0.07
0.118 194 81.85 126.9 126.7 0.02 0.02 9 138.0 137.6 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.3 0.07 0.07
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 39. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 39. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.990	12	0.923	95	0.981	0.999
0.0228	97	0.988	11	1.000	108	0.989	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.996	17	1.000	143	0.996	0.999
0.0418	129	0.997	11	1.000	140	0.997	0.999
0.0482	150	0.991	12	1.000	162	0.991	0.999
0.0545	151	0.997	12	0.989	163	0.996	0.999
0.0609	172	0.983	15	0.951	187	0.980	0.999
0.0672	174	0.993	9	0.937	183	0.990	0.999
0.0735	178	0.990	11	1.000	189	0.990	0.999
0.0799	189	0.989	14	0.999	203	0.989	0.999
0.0862	197	0.983	9	0.975	206	0.983	0.999
0.0925	193	0.978	14	0.929	207	0.974	0.999
0.0989	188	0.979	12	1.000	200	0.980	0.999
0.1052	190	0.988	8	1.000	198	0.988	0.999
0.1116	183	0.980	13	0.938	196	0.977	1.000
0.1179	194	0.979	11	0.933	205	0.977	1.000
0.1242	174	0.983	8	1.000	182	0.983	1.000

$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0195
Free R factor = 0.0410
Overall weighted R factor = 0.0195
Free weighted R factor = 0.0414
Overall correlation coefficient = 0.9993
Free correlation coefficient = 0.9967
DPI based on free R factor = 0.0744
Overall figure of merit = 0.9864
ML based su of positional parameters = 0.0411
ML based su of thermal parameters = 2.0261

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10565.441 3155.5874 20524.148 20501.088

fvalues 10565.441 3155.5874 20502.361 20501.088

CGMAT cycle number = 40

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.6401068 is applied to the X-ray term
Norm of X_ray positional gradient 13.8
Norm of Geom. positional gradient 13.8
Norm of X_ray B-factor gradient 18.0
Norm of Geom. B-factor gradient 18.4
Product of X_ray and Geom posit. gradients -0.704E+06
Cosine of angle between them -0.997
Product of X_ray and Geom B-fact gradients -0.404E+06
Cosine of angle between them -0.993

Residuals: XRAY= 0.1733E+05 GEOM= 3155. TOTAL= 0.2048E+05
function value 20480.941

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.674	1.966
Torsion angles, period 1. refined	155	7.879	5.000
Torsion angles, period 2. refined	54	41.403	25.741
Torsion angles, period 3. refined	214	19.167	15.000
Torsion angles, period 4. refined	3	21.350	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	541	0.264	0.200
VDW; torsion: refined_atoms	790	0.324	0.200
HBOND: refined_atoms	42	0.190	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.268	0.200
Bond B values: refined atoms	1229	13.420	4.713
Angle B values: refined atoms	1663	16.481	7.127
Torsion B values: refined atoms	426	30.418	13.062
Long range B values: refined atoms	1338	12.266	15.362

Overall : scale = 1.012, B = -0.028
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 40. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 40. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 40. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 40. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.3 747.7 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.0 416.3 0.02 0.02 1 1228.5 1221.9 0.01 0.01
0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.0 413.5 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.4 0.07 0.06
0.029 108 100.00 241.3 241.9 0.02 0.02 7 186.7 189.2 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 253.5 0.04 0.04
0.042 129 98.56 286.3 287.4 0.02 0.02 8 338.1 341.5 0.02 0.02
0.048 150 98.73 296.7 296.4 0.02 0.02 5 305.8 306.7 0.03 0.03
0.055 151 99.38 281.2 281.4 0.01 0.02 10 257.9 260.0 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.2 0.03 0.03
0.067 174 99.45 211.4 210.9 0.02 0.02 6 286.3 284.2 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.5 236.4 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.6 155.5 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.5 207.7 0.04 0.04
0.093 193 93.55 156.9 156.9 0.02 0.02 10 182.0 185.8 0.07 0.06
0.099 188 91.28 160.7 159.7 0.02 0.02 11 159.6 157.3 0.02 0.02
0.105 190 86.02 153.8 153.4 0.02 0.02 13 169.2 170.5 0.05 0.04
0.112 183 80.08 129.9 129.5 0.02 0.02 6 135.2 139.5 0.08 0.07
0.118 194 81.85 126.9 126.7 0.02 0.02 9 138.0 137.6 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.3 0.07 0.07
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 40. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 40. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.990 12 0.923 95 0.981 0.999
0.0228 97 0.988 11 1.000 108 0.989 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.996 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.991 0.999

```
 0.0545   151   0.997    12   0.989   163   0.996  0.999
 0.0609   172   0.983    15   0.951   187   0.980  0.999
 0.0672   174   0.993     9   0.937   183   0.990  0.999
 0.0735   178   0.990    11   1.000   189   0.990  0.999
 0.0799   189   0.989    14   0.999   203   0.990  0.999
 0.0862   197   0.983     9   0.975   206   0.983  0.999
 0.0925   193   0.978    14   0.929   207   0.975  0.999
 0.0989   188   0.979    12   1.000   200   0.980  0.999
 0.1052   190   0.988     8   1.000   198   0.988  0.999
 0.1116   183   0.980    13   0.938   196   0.977  1.000
 0.1179   194   0.979    11   0.934   205   0.977  1.000
 0.1242   174   0.983     8   1.000   182   0.983  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0195
Free R factor                    =     0.0410
Overall weighted R factor        =     0.0195
Free weighted R factor           =     0.0414
Overall correlation coefficient  =     0.9993
Free correlation coefficient     =     0.9967
DPI based on free R factor       =     0.0744
Overall figure of merit          =     0.9864
ML based su of positional parameters =     0.0410
ML based su of thermal parameters    =     2.0249
-------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10564.213       3155.3391       20480.537       20481.777


    CGMAT cycle number =     41

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    1.6354363      is applied to the X-ray term
Norm of X_ray positional gradient              13.8
Norm of Geom. positional gradient              13.8
Norm of X_ray B-factor gradient                17.9
Norm of Geom. B-factor gradient                18.4
Product of X_ray and Geom posit. gradients     -0.702E+06
```

Cosine of angle between them -0.999
Product of X_ray and Geom B-fact gradients -0.402E+06
Cosine of angle between them -0.993

Residuals: XRAY= 0.1727E+05 GEOM= 3156. TOTAL= 0.2043E+05
function value 20425.070

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.678	1.966
Torsion angles, period 1. refined	155	7.879	5.000
Torsion angles, period 2. refined	54	41.404	25.741
Torsion angles, period 3. refined	214	19.183	15.000
Torsion angles, period 4. refined	3	21.347	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	541	0.264	0.200
VDW; torsion: refined_atoms	790	0.324	0.200
HBOND: refined_atoms	42	0.190	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.268	0.200
Bond B values: refined atoms	1229	13.422	4.713
Angle B values: refined atoms	1663	16.487	7.127
Torsion B values: refined atoms	426	30.434	13.062
Long range B values: refined atoms	1338	12.271	15.361

Overall : scale = 1.012, B = -0.029
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 41. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 41. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 41. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 41. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$

0.004	30	62.50	754.3	747.7	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	414.0	416.3	0.02	0.02	1	1228.5	1222.2	0.01	0.01	
0.017	83	95.60	307.7	308.7	0.03	0.02	4	403.0	413.5	0.04	0.05	

0.023	97	97.14	247.4	248.4	0.02	0.02	5	180.2	188.4	0.07	0.06
0.029	108	100.00	241.3	242.0	0.02	0.02	7	186.7	189.2	0.06	0.06
0.036	126	99.25	270.4	270.7	0.02	0.02	6	252.9	253.6	0.04	0.04
0.042	129	98.56	286.3	287.5	0.02	0.02	8	338.1	341.5	0.02	0.02
0.048	150	98.73	296.7	296.4	0.02	0.02	5	305.8	306.8	0.03	0.03
0.055	151	99.38	281.2	281.4	0.01	0.02	10	257.9	260.0	0.04	0.04
0.061	172	100.00	218.4	218.6	0.02	0.02	10	202.2	202.3	0.03	0.03
0.067	174	99.45	211.4	210.9	0.02	0.02	6	286.3	284.2	0.02	0.02
0.074	178	98.92	206.1	206.7	0.02	0.02	6	234.5	236.4	0.03	0.03
0.080	189	100.00	208.7	209.0	0.02	0.02	13	159.6	155.5	0.06	0.06
0.086	197	100.00	176.8	176.9	0.02	0.02	8	208.5	207.7	0.04	0.04
0.093	193	93.55	156.9	156.9	0.02	0.02	10	182.0	185.9	0.07	0.06
0.099	188	91.28	160.7	159.7	0.02	0.02	11	159.6	157.3	0.02	0.02
0.105	190	86.02	153.8	153.5	0.02	0.02	13	169.2	170.5	0.05	0.04
0.112	183	80.08	129.9	129.5	0.02	0.02	6	135.2	139.6	0.08	0.07
0.118	194	81.85	126.9	126.7	0.02	0.02	9	138.0	137.5	0.05	0.05
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	111.3	0.07	0.07

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 41. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 41. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.990	12	0.923	95	0.981	0.999
0.0228	97	0.988	11	1.000	108	0.989	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.996	17	1.000	143	0.996	0.999
0.0418	129	0.997	11	1.000	140	0.997	0.999
0.0482	150	0.991	12	1.000	162	0.991	0.999
0.0545	151	0.997	12	0.989	163	0.996	0.999
0.0609	172	0.983	15	0.952	187	0.980	0.999
0.0672	174	0.993	9	0.937	183	0.990	0.999
0.0735	178	0.990	11	1.000	189	0.990	0.999
0.0799	189	0.989	14	0.999	203	0.990	0.999
0.0862	197	0.983	9	0.975	206	0.983	0.999
0.0925	193	0.978	14	0.929	207	0.975	0.999
0.0989	188	0.979	12	1.000	200	0.980	0.999
0.1052	190	0.988	8	1.000	198	0.988	0.999
0.1116	183	0.980	13	0.938	196	0.977	1.000
0.1179	194	0.979	11	0.935	205	0.977	1.000
0.1242	174	0.983	8	1.000	182	0.984	1.000

$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416

Overall R factor = 0.0195
Free R factor = 0.0409
Overall weighted R factor = 0.0195
Free weighted R factor = 0.0413
Overall correlation coefficient = 0.9993
Free correlation coefficient = 0.9967
DPI based on free R factor = 0.0743
Overall figure of merit = 0.9865
ML based su of positional parameters = 0.0410
ML based su of thermal parameters = 2.0219

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10559.891 3155.9072 20427.170 20425.936

fvalues 10559.891 3155.9072 20425.814 20425.936

CGMAT cycle number = 42

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.6323133 is applied to the X-ray term
Norm of X_ray positional gradient 13.8
Norm of Geom. positional gradient 13.8
Norm of X_ray B-factor gradient 17.9
Norm of Geom. B-factor gradient 18.4
Product of X_ray and Geom posit. gradients -0.702E+06
Cosine of angle between them -0.999
Product of X_ray and Geom B-fact gradients -0.403E+06
Cosine of angle between them -0.994

Residuals: XRAY= 0.1723E+05 GEOM= 3156. TOTAL= 0.2039E+05
function value 20388.396

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.677	1.966
Torsion angles, period 1. refined	155	7.879	5.000
Torsion angles, period 2. refined	54	41.405	25.741
Torsion angles, period 3. refined	214	19.166	15.000

Torsion angles, period 4. refined 3 21.352 15.000
Chiral centres: refined atoms 187 0.111 0.200
Planar groups: refined atoms 924 0.005 0.021
VDW repulsions: refined_atoms 541 0.264 0.200
VDW; torsion: refined_atoms 790 0.324 0.200
HBOND: refined_atoms 42 0.190 0.200
VDW repulsions: symmetry: refined_atoms 55 0.262 0.200
HBOND: symmetry: refined_atoms 3 0.268 0.200
Bond B values: refined atoms 1229 13.424 4.713
Angle B values: refined atoms 1663 16.491 7.127
Torsion B values: refined atoms 426 30.443 13.062
Long range B values: refined atoms 1338 12.274 15.361

Overall : scale = 1.012, B = -0.028
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 42. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 42. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 42. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 42. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.3 747.7 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.0 416.3 0.02 0.02 1 1228.5 1222.3 0.01 0.01
0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.0 413.5 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.4 0.07 0.06
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.2 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 253.6 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.5 0.02 0.02
0.048 150 98.73 296.7 296.4 0.02 0.02 5 305.8 306.8 0.03 0.03
0.055 151 99.38 281.2 281.4 0.01 0.02 10 257.9 260.0 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.3 0.03 0.03
0.067 174 99.45 211.4 210.9 0.02 0.02 6 286.3 284.2 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.5 236.5 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.6 155.5 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.5 207.6 0.04 0.04
0.093 193 93.55 156.9 156.9 0.02 0.02 10 182.0 185.9 0.07 0.06
0.099 188 91.28 160.7 159.7 0.02 0.02 11 159.6 157.3 0.02 0.02
0.105 190 86.02 153.8 153.5 0.02 0.02 13 169.2 170.5 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 139.6 0.08 0.07

```
 0.118    194  81.85   126.9   126.7  0.02  0.02       9   138.0   137.5  0.05  0.05
 0.124    174  73.20   129.0   128.9  0.02  0.02       9   113.8   111.3  0.07  0.07
$$

   ****                Fom and SigmaA vs resolution                ****

 $TABLE: Cycle   42. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
 $GRAPHS:Cycle   42. M(Fom) v. resln :N:1,3,5,7,8:
 $$
 <4SSQ/LL> NREFa  FOMa  NREFc FOMc NREFall FOMall  SigmaA_Fc1 $$
 $$
  0.0038    30   0.999     4   1.000    34   0.999  0.999
  0.0102    62   0.999     7   1.000    69   0.999  0.999
  0.0165    83   0.990    12   0.923    95   0.982  0.999
  0.0228    97   0.988    11   1.000   108   0.989  0.999
  0.0292   108   0.997     6   1.000   114   0.997  0.999
  0.0355   126   0.996    17   1.000   143   0.996  0.999
  0.0418   129   0.997    11   1.000   140   0.997  0.999
  0.0482   150   0.991    12   1.000   162   0.991  0.999
  0.0545   151   0.997    12   0.989   163   0.996  0.999
  0.0609   172   0.983    15   0.952   187   0.980  0.999
  0.0672   174   0.993     9   0.938   183   0.990  0.999
  0.0735   178   0.990    11   1.000   189   0.990  0.999
  0.0799   189   0.989    14   0.999   203   0.990  0.999
  0.0862   197   0.983     9   0.975   206   0.983  0.999
  0.0925   193   0.978    14   0.929   207   0.975  0.999
  0.0989   188   0.979    12   1.000   200   0.980  0.999
  0.1052   190   0.988     8   1.000   198   0.988  0.999
  0.1116   183   0.980    13   0.938   196   0.977  1.000
  0.1179   194   0.979    11   0.935   205   0.977  1.000
  0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
 Resolution limits                =     38.899     2.802
 Number of used reflections       =       3184
 Percentage observed              =    92.6870
 Percentage of free reflections   =     4.8416
 Overall R factor                 =     0.0195
 Free R factor                    =     0.0409
 Overall weighted R factor        =     0.0195
 Free weighted R factor           =     0.0413
 Overall correlation coefficient  =     0.9993
 Free correlation coefficient     =     0.9967
 DPI based on free R factor       =     0.0743
 Overall figure of merit          =     0.9865
 ML based su of positional parameters =     0.0409
 ML based su of thermal parameters    =     2.0199
 ------------------------------------------------------------------------
  Trying gamma equal    0.0000000
  Convergence reached with no gamma cycles
```

fvalues 10557.487 3156.1392 20391.564 20389.266

fvalues 10557.487 3156.1392 20389.248 20389.266

CGMAT cycle number = 43

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.59999996
Actual weight 1.6291608 is applied to the X-ray term
Norm of X_ray positional gradient 13.8
Norm of Geom. positional gradient 13.8
Norm of X_ray B-factor gradient 17.9
Norm of Geom. B-factor gradient 18.4
Product of X_ray and Geom posit. gradients -0.701E+06
Cosine of angle between them -0.998
Product of X_ray and Geom B-fact gradients -0.402E+06
Cosine of angle between them -0.994

Residuals: XRAY= 0.1719E+05 GEOM= 3157. TOTAL= 0.2035E+05
function value 20351.518

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.676	1.966
Torsion angles, period 1. refined	155	7.879	5.000
Torsion angles, period 2. refined	54	41.406	25.741
Torsion angles, period 3. refined	214	19.198	15.000
Torsion angles, period 4. refined	3	21.353	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	541	0.264	0.200
VDW; torsion: refined_atoms	790	0.324	0.200
HBOND: refined_atoms	42	0.190	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.268	0.200
Bond B values: refined atoms	1229	13.425	4.713
Angle B values: refined atoms	1663	16.494	7.127
Torsion B values: refined atoms	426	30.451	13.061
Long range B values: refined atoms	1338	12.276	15.360

Overall : scale = 1.012, B = -0.028
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 43. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 43. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 43. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 43. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.3 747.7 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.0 416.3 0.02 0.02 1 1228.5 1222.3 0.01 0.01
0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.0 413.6 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.4 0.07 0.06
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.2 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 253.6 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.5 0.02 0.02
0.048 150 98.73 296.7 296.4 0.02 0.02 5 305.8 306.8 0.03 0.03
0.055 151 99.38 281.2 281.4 0.01 0.02 10 257.9 260.0 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.3 0.03 0.03
0.067 174 99.45 211.4 210.9 0.02 0.02 6 286.3 284.2 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.5 236.5 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.6 155.5 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.5 207.6 0.04 0.04
0.093 193 93.55 156.9 156.9 0.02 0.02 10 182.0 185.9 0.07 0.06
0.099 188 91.28 160.7 159.7 0.02 0.02 11 159.6 157.3 0.02 0.02
0.105 190 86.02 153.8 153.5 0.02 0.02 13 169.2 170.5 0.05 0.04
0.112 183 80.08 129.9 129.5 0.02 0.02 6 135.2 139.7 0.08 0.07
0.118 194 81.85 126.9 126.7 0.02 0.02 9 138.0 137.5 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.3 0.07 0.07
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 43. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 43. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.990 12 0.923 95 0.982 0.999
0.0228 97 0.988 11 1.000 108 0.989 0.999

```
 0.0292   108   0.997     6   1.000   114   0.997  0.999
 0.0355   126   0.996    17   1.000   143   0.996  0.999
 0.0418   129   0.997    11   1.000   140   0.997  0.999
 0.0482   150   0.991    12   1.000   162   0.991  0.999
 0.0545   151   0.997    12   0.990   163   0.996  0.999
 0.0609   172   0.983    15   0.953   187   0.980  0.999
 0.0672   174   0.993     9   0.937   183   0.990  0.999
 0.0735   178   0.990    11   1.000   189   0.990  0.999
 0.0799   189   0.989    14   0.999   203   0.990  0.999
 0.0862   197   0.983     9   0.975   206   0.983  0.999
 0.0925   193   0.978    14   0.929   207   0.975  0.999
 0.0989   188   0.979    12   1.000   200   0.980  0.999
 0.1052   190   0.988     8   1.000   198   0.988  0.999
 0.1116   183   0.980    13   0.938   196   0.977  1.000
 0.1179   194   0.979    11   0.936   205   0.977  1.000
 0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0194
Free R factor                    =     0.0409
Overall weighted R factor        =     0.0195
Free weighted R factor           =     0.0412
Overall correlation coefficient  =     0.9993
Free correlation coefficient     =     0.9967
DPI based on free R factor       =     0.0742
Overall figure of merit          =     0.9865
ML based su of positional parameters =     0.0409
ML based su of thermal parameters    =     2.0179
-------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10554.867       3156.8071       20356.992       20352.383

 fvalues    10554.867       3156.8071       20352.535       20352.383


    CGMAT cycle number =     44

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
```

Actual weight 1.6299514 is applied to the X-ray term
Norm of X_ray positional gradient 13.8
Norm of Geom. positional gradient 13.8
Norm of X_ray B-factor gradient 17.9
Norm of Geom. B-factor gradient 18.4
Product of X_ray and Geom posit. gradients -0.701E+06
Cosine of angle between them -0.999
Product of X_ray and Geom B-fact gradients -0.402E+06
Cosine of angle between them -0.994

Residuals: XRAY= 0.1720E+05 GEOM= 3157. TOTAL= 0.2036E+05
function value 20360.555

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.676	1.966
Torsion angles, period 1. refined	155	7.879	5.000
Torsion angles, period 2. refined	54	41.406	25.741
Torsion angles, period 3. refined	214	19.180	15.000
Torsion angles, period 4. refined	3	21.353	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	541	0.264	0.200
VDW; torsion: refined_atoms	790	0.324	0.200
HBOND: refined_atoms	42	0.190	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.268	0.200
Bond B values: refined atoms	1229	13.425	4.713
Angle B values: refined atoms	1663	16.495	7.127
Torsion B values: refined atoms	426	30.453	13.061
Long range B values: refined atoms	1338	12.276	15.360

Overall : scale = 1.012, B = -0.028
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 44. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 44. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 44. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 44. % observed v. resln :N:1,3:
$$

M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.3 747.7 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.0 416.3 0.02 0.02 1 1228.5 1222.4 0.01 0.01
0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.0 413.6 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.4 0.07 0.06
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.2 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 253.6 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.5 0.02 0.02
0.048 150 98.73 296.7 296.4 0.02 0.02 5 305.8 306.8 0.03 0.03
0.055 151 99.38 281.2 281.4 0.01 0.02 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.3 0.03 0.03
0.067 174 99.45 211.4 210.9 0.02 0.02 6 286.3 284.2 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.5 236.5 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.6 155.5 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.5 207.7 0.04 0.04
0.093 193 93.55 156.9 156.9 0.02 0.02 10 182.0 185.9 0.07 0.06
0.099 188 91.28 160.7 159.7 0.02 0.02 11 159.6 157.3 0.02 0.02
0.105 190 86.02 153.8 153.5 0.02 0.02 13 169.2 170.5 0.05 0.04
0.112 183 80.08 129.9 129.5 0.02 0.02 6 135.2 139.7 0.08 0.07
0.118 194 81.85 126.9 126.7 0.02 0.02 9 138.0 137.5 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.3 0.07 0.07
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 44. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 44. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.990 12 0.923 95 0.982 0.999
0.0228 97 0.988 11 1.000 108 0.989 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.996 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.991 0.999
0.0545 151 0.997 12 0.990 163 0.996 0.999
0.0609 172 0.983 15 0.953 187 0.980 0.999
0.0672 174 0.993 9 0.938 183 0.990 0.999
0.0735 178 0.990 11 1.000 189 0.990 0.999
0.0799 189 0.989 14 0.999 203 0.990 0.999
0.0862 197 0.983 9 0.975 206 0.983 0.999
0.0925 193 0.978 14 0.929 207 0.975 0.999
0.0989 188 0.979 12 1.000 200 0.980 0.999
0.1052 190 0.988 8 1.000 198 0.988 0.999
0.1116 183 0.980 13 0.938 196 0.977 1.000
0.1179 194 0.979 11 0.936 205 0.977 1.000

```
 0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0194
Free R factor                    =     0.0409
Overall weighted R factor        =     0.0195
Free weighted R factor           =     0.0413
Overall correlation coefficient  =     0.9993
Free correlation coefficient     =     0.9967
DPI based on free R factor       =     0.0742
Overall figure of merit          =     0.9865
ML based su of positional parameters =     0.0409
ML based su of thermal parameters    =     2.0183
------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10555.361       3156.6807       20360.674       20361.406


    CGMAT cycle number =     45

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    1.6243273      is applied to the X-ray term
Norm of X_ray positional gradient              13.8
Norm of Geom. positional gradient              13.8
Norm of X_ray B-factor gradient                17.9
Norm of Geom. B-factor gradient                18.4
Product of X_ray and Geom posit. gradients     -0.700E+06
 Cosine of angle between them                  -0.999
Product of X_ray and Geom B-fact gradients     -0.402E+06
 Cosine of angle between them                  -0.994


Residuals: XRAY=     0.1714E+05 GEOM=      3157.     TOTAL=     0.2029E+05
 function value    20294.014

------------------------------------------------------------------------------
          Restraint type            N restraints   Rms Delta   Av(Sigma)
Bond distances: refined atoms                1229     0.011      0.020
```

Bond angles : refined atoms 1663 1.679 1.966
Torsion angles, period 1. refined 155 7.879 5.000
Torsion angles, period 2. refined 54 41.407 25.741
Torsion angles, period 3. refined 214 19.193 15.000
Torsion angles, period 4. refined 3 21.358 15.000
Chiral centres: refined atoms 187 0.111 0.200
Planar groups: refined atoms 924 0.005 0.021
VDW repulsions: refined_atoms 542 0.264 0.200
VDW; torsion: refined_atoms 790 0.324 0.200
HBOND: refined_atoms 42 0.190 0.200
VDW repulsions: symmetry: refined_atoms 55 0.262 0.200
HBOND: symmetry: refined_atoms 3 0.268 0.200
Bond B values: refined atoms 1229 13.426 4.713
Angle B values: refined atoms 1663 16.499 7.126
Torsion B values: refined atoms 426 30.465 13.061
Long range B values: refined atoms 1339 12.277 15.362

Overall : scale = 1.012, B = -0.028
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 45. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 45. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 45. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 45. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.3 747.8 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.0 416.3 0.02 0.02 1 1228.5 1222.5 0.01 0.01
0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.0 413.6 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.4 0.07 0.06
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.2 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 253.6 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.5 0.02 0.02
0.048 150 98.73 296.7 296.4 0.02 0.02 5 305.8 306.8 0.03 0.03
0.055 151 99.38 281.2 281.4 0.01 0.02 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.3 0.03 0.03
0.067 174 99.45 211.4 210.9 0.02 0.02 6 286.3 284.2 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.5 236.5 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.6 155.5 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.5 207.6 0.04 0.04

```
 0.093   193  93.55   156.9   157.0  0.02  0.02     10   182.0   185.9  0.07  0.06
 0.099   188  91.28   160.7   159.7  0.02  0.02     11   159.6   157.3  0.02  0.02
 0.105   190  86.02   153.8   153.5  0.02  0.02     13   169.2   170.4  0.05  0.04
 0.112   183  80.08   129.9   129.6  0.02  0.02      6   135.2   139.8  0.08  0.07
 0.118   194  81.85   126.9   126.7  0.02  0.02      9   138.0   137.5  0.05  0.05
 0.124   174  73.20   129.0   128.9  0.02  0.02      9   113.8   111.2  0.07  0.07
$$
```

**** Fom and SigmaA vs resolution ****

```
$TABLE: Cycle   45. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle   45. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa  FOMa  NREFc FOMc NREFall FOMall  SigmaA_Fc1 $$
$$
 0.0038    30   0.999     4   1.000    34   0.999  0.999
 0.0102    62   0.999     7   1.000    69   0.999  0.999
 0.0165    83   0.990    12   0.923    95   0.982  0.999
 0.0228    97   0.988    11   1.000   108   0.989  0.999
 0.0292   108   0.997     6   1.000   114   0.997  0.999
 0.0355   126   0.996    17   1.000   143   0.996  0.999
 0.0418   129   0.997    11   1.000   140   0.997  0.999
 0.0482   150   0.991    12   1.000   162   0.991  0.999
 0.0545   151   0.997    12   0.990   163   0.996  0.999
 0.0609   172   0.983    15   0.953   187   0.980  0.999
 0.0672   174   0.993     9   0.937   183   0.990  0.999
 0.0735   178   0.990    11   1.000   189   0.990  0.999
 0.0799   189   0.989    14   0.999   203   0.990  0.999
 0.0862   197   0.983     9   0.975   206   0.983  0.999
 0.0925   193   0.978    14   0.929   207   0.975  0.999
 0.0989   188   0.979    12   1.000   200   0.981  0.999
 0.1052   190   0.988     8   1.000   198   0.989  0.999
 0.1116   183   0.980    13   0.938   196   0.977  1.000
 0.1179   194   0.980    11   0.937   205   0.977  1.000
 0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
Resolution limits                 =     38.899     2.802
Number of used reflections        =       3184
Percentage observed               =    92.6870
Percentage of free reflections    =     4.8416
Overall R factor                  =     0.0194
Free R factor                     =     0.0408
Overall weighted R factor         =     0.0194
Free weighted R factor            =     0.0412
Overall correlation coefficient   =     0.9993
Free correlation coefficient      =     0.9967
DPI based on free R factor        =     0.0741
Overall figure of merit           =     0.9865
ML based su of positional parameters =     0.0408
ML based su of thermal parameters    =     2.0148
------------------------------------------------------------------------------
```

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10550.625 3157.2397 20295.363 20294.908

fvalues 10550.625 3157.2397 20294.719 20294.908

CGMAT cycle number = 46

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.6229593 is applied to the X-ray term
Norm of X_ray positional gradient 13.8
Norm of Geom. positional gradient 13.8
Norm of X_ray B-factor gradient 17.9
Norm of Geom. B-factor gradient 18.3
Product of X_ray and Geom posit. gradients -0.700E+06
Cosine of angle between them -0.999
Product of X_ray and Geom B-fact gradients -0.402E+06
Cosine of angle between them -0.994

Residuals: XRAY= 0.1712E+05 GEOM= 3157. TOTAL= 0.2028E+05
function value 20277.838

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.679	1.966
Torsion angles, period 1. refined	155	7.879	5.000
Torsion angles, period 2. refined	54	41.408	25.741
Torsion angles, period 3. refined	214	19.180	15.000
Torsion angles, period 4. refined	3	21.360	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	542	0.264	0.200
VDW; torsion: refined_atoms	790	0.324	0.200
HBOND: refined_atoms	42	0.190	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.268	0.200
Bond B values: refined atoms	1229	13.427	4.713
Angle B values: refined atoms	1663	16.502	7.126
Torsion B values: refined atoms	426	30.473	13.060

Long range B values: refined atoms 1339 12.278 15.360

Overall : scale = 1.012, B = -0.027
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 46. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 46. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 46. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 46. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.3 747.8 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.0 416.3 0.02 0.02 1 1228.5 1222.5 0.01 0.01
0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.0 413.6 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.3 0.07 0.06
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.2 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 253.6 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.5 0.02 0.02
0.048 150 98.73 296.7 296.4 0.02 0.02 5 305.8 306.8 0.03 0.03
0.055 151 99.38 281.2 281.4 0.01 0.02 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.3 0.03 0.03
0.067 174 99.45 211.4 210.9 0.02 0.02 6 286.3 284.3 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.5 236.5 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.6 155.6 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.5 207.7 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 185.9 0.07 0.06
0.099 188 91.28 160.7 159.7 0.02 0.02 11 159.6 157.3 0.02 0.02
0.105 190 86.02 153.8 153.5 0.02 0.02 13 169.2 170.4 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 139.8 0.08 0.07
0.118 194 81.85 126.9 126.7 0.02 0.02 9 138.0 137.5 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.3 0.07 0.07
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 46. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 46. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

```
 0.0038   30  0.999    4  1.000   34  0.999  0.999
 0.0102   62  0.999    7  1.000   69  0.999  0.999
 0.0165   83  0.990   12  0.923   95  0.982  0.999
 0.0228   97  0.988   11  1.000  108  0.989  0.999
 0.0292  108  0.997    6  1.000  114  0.997  0.999
 0.0355  126  0.996   17  1.000  143  0.996  0.999
 0.0418  129  0.997   11  1.000  140  0.997  0.999
 0.0482  150  0.991   12  1.000  162  0.991  0.999
 0.0545  151  0.997   12  0.990  163  0.996  0.999
 0.0609  172  0.983   15  0.953  187  0.980  0.999
 0.0672  174  0.993    9  0.938  183  0.990  0.999
 0.0735  178  0.990   11  1.000  189  0.990  0.999
 0.0799  189  0.989   14  0.999  203  0.990  0.999
 0.0862  197  0.983    9  0.975  206  0.983  0.999
 0.0925  193  0.978   14  0.929  207  0.975  0.999
 0.0989  188  0.979   12  1.000  200  0.981  0.999
 0.1052  190  0.988    8  1.000  198  0.989  0.999
 0.1116  183  0.980   13  0.938  196  0.977  1.000
 0.1179  194  0.980   11  0.937  205  0.977  1.000
 0.1242  174  0.983    8  1.000  182  0.984  1.000
 $$
Resolution limits                =    38.899    2.802
Number of used reflections       =      3184
Percentage observed              =   92.6870
Percentage of free reflections   =    4.8416
Overall R factor                 =    0.0194
Free R factor                    =    0.0408
Overall weighted R factor        =    0.0194
Free weighted R factor           =    0.0412
Overall correlation coefficient  =    0.9993
Free correlation coefficient     =    0.9967
DPI based on free R factor       =    0.0741
Overall figure of merit          =    0.9866
ML based su of positional parameters =    0.0408
ML based su of thermal parameters    =    2.0139
-------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues   10549.383      3157.4895      20279.619      20278.707

 fvalues   10549.383      3157.4895      20278.721      20278.707


    CGMAT cycle number =    47

 Limits of asymmetric unit     : 1.00 1.00 0.50
 Grid spacing to be used       :   50   90   60
 Maximuum H,K,L                :   12   21   14
 Minimum acceptable grid spacing:   33   56   38
```

fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.6215299 is applied to the X-ray term
Norm of X_ray positional gradient 13.8
Norm of Geom. positional gradient 13.8
Norm of X_ray B-factor gradient 17.9
Norm of Geom. B-factor gradient 18.3
Product of X_ray and Geom posit. gradients -0.700E+06
Cosine of angle between them -0.999
Product of X_ray and Geom B-fact gradients -0.402E+06
Cosine of angle between them -0.994

Residuals: XRAY= 0.1710E+05 GEOM= 3158. TOTAL= 0.2026E+05
function value 20261.059

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.679	1.966
Torsion angles, period 1. refined	155	7.879	5.000
Torsion angles, period 2. refined	54	41.409	25.741
Torsion angles, period 3. refined	214	19.191	15.000
Torsion angles, period 4. refined	3	21.361	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	542	0.264	0.200
VDW; torsion: refined_atoms	790	0.324	0.200
HBOND: refined_atoms	42	0.190	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.268	0.200
Bond B values: refined atoms	1229	13.427	4.713
Angle B values: refined atoms	1663	16.503	7.126
Torsion B values: refined atoms	426	30.476	13.060
Long range B values: refined atoms	1339	12.279	15.360

Overall : scale = 1.012, B = -0.027
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 47. Rfactor analysis, F distribution v resln :

$GRAPHS:Cycle 47. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 47. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 47. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.3 747.8 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.0 416.3 0.02 0.02 1 1228.5 1222.5 0.01 0.01
0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.0 413.6 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.4 0.07 0.06
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.2 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 253.6 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.5 0.02 0.02
0.048 150 98.73 296.7 296.4 0.02 0.02 5 305.8 306.8 0.03 0.03
0.055 151 99.38 281.2 281.4 0.01 0.02 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.3 0.03 0.03
0.067 174 99.45 211.4 210.9 0.02 0.02 6 286.3 284.3 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.5 236.5 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.6 155.6 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.5 207.7 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 185.9 0.07 0.06
0.099 188 91.28 160.7 159.7 0.02 0.02 11 159.6 157.3 0.02 0.02
0.105 190 86.02 153.8 153.5 0.02 0.02 13 169.2 170.4 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 139.8 0.08 0.07
0.118 194 81.85 126.9 126.7 0.02 0.02 9 138.0 137.5 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.2 0.07 0.07
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 47. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 47. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.990 12 0.923 95 0.982 0.999
0.0228 97 0.988 11 1.000 108 0.989 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.996 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.991 0.999
0.0545 151 0.997 12 0.990 163 0.996 0.999
0.0609 172 0.983 15 0.953 187 0.980 0.999
0.0672 174 0.993 9 0.938 183 0.990 0.999
0.0735 178 0.990 11 1.000 189 0.990 0.999
0.0799 189 0.989 14 0.999 203 0.990 0.999
0.0862 197 0.983 9 0.975 206 0.983 0.999
0.0925 193 0.978 14 0.929 207 0.975 0.999

```
 0.0989   188   0.979    12   1.000   200   0.981  0.999
 0.1052   190   0.988     8   1.000   198   0.989  0.999
 0.1116   183   0.980    13   0.938   196   0.977  1.000
 0.1179   194   0.980    11   0.938   205   0.977  1.000
 0.1242   174   0.983     8   1.000   182   0.984  1.000
$$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0194
Free R factor                    =     0.0408
Overall weighted R factor        =     0.0194
Free weighted R factor           =     0.0412
Overall correlation coefficient  =     0.9993
Free correlation coefficient     =     0.9967
DPI based on free R factor       =     0.0741
Overall figure of merit          =     0.9866
ML based su of positional parameters =     0.0408
ML based su of thermal parameters    =     2.0129
---------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10548.242       3157.6052       20261.443       20261.896


    CGMAT cycle number =     48

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    1.6210023      is applied to the X-ray term
Norm of X_ray positional gradient              13.8
Norm of Geom. positional gradient              13.8
Norm of X_ray B-factor gradient                17.9
Norm of Geom. B-factor gradient                18.3
Product of X_ray and Geom posit. gradients     -0.699E+06
 Cosine of angle between them                  -0.999
Product of X_ray and Geom B-fact gradients     -0.401E+06
 Cosine of angle between them                  -0.994


Residuals: XRAY=     0.1710E+05 GEOM=      3158.     TOTAL=     0.2025E+05
 function value    20254.377
```

```
------------------------------------------------------------------------------
          Restraint type           N restraints   Rms Delta   Av(Sigma)
Bond distances: refined atoms              1229     0.011     0.020
Bond angles  : refined atoms               1663     1.680     1.966
Torsion angles, period  1. refined          155     7.879     5.000
Torsion angles, period  2. refined           54    41.410    25.741
Torsion angles, period  3. refined          214    19.190    15.000
Torsion angles, period  4. refined            3    21.364    15.000
Chiral centres: refined atoms              187     0.111     0.200
Planar groups: refined atoms               924     0.005     0.021
VDW repulsions: refined_atoms              542     0.264     0.200
VDW; torsion: refined_atoms                790     0.324     0.200
HBOND: refined_atoms                        42     0.190     0.200
VDW repulsions: symmetry: refined_atoms     55     0.262     0.200
HBOND: symmetry: refined_atoms               3     0.268     0.200
Bond B values: refined atoms               1229    13.427     4.713
Angle B values: refined atoms              1663    16.506     7.126
Torsion B values: refined atoms             426    30.487    13.060
Long range B values: refined atoms         1339    12.280    15.359
------------------------------------------------------------------------------

------------------------------------------------------------------------------
Overall              : scale =    1.012, B  =  -0.028
Overall anisotropic scale factors
   B11 =  0.28 B22 =  0.17 B33 = -0.47 B12 =  0.00 B13 = -0.36 B23 =  0.00
------------------------------------------------------------------------------

------------------------------------------------------------------------------

    ****              Things for loggraph, R factor and others              ****


$TABLE: Cycle   48. Rfactor analysis, F distribution v resln  :
$GRAPHS:Cycle   48. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle   48. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle   48. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free   WR_free $$
$$
 0.004     30  62.50   754.3   747.8  0.02  0.02      0     0.0     0.0******  0.00
 0.010     62  95.45   414.0   416.3  0.02  0.02      1  1228.5  1222.7  0.01  0.01
 0.017     83  95.60   307.7   308.7  0.03  0.02      4   403.0   413.6  0.04  0.05
 0.023     97  97.14   247.4   248.4  0.02  0.02      5   180.2   188.3  0.07  0.06
 0.029    108 100.00   241.3   242.0  0.02  0.02      7   186.7   189.2  0.06  0.06
 0.036    126  99.25   270.4   270.7  0.02  0.02      6   252.9   253.6  0.04  0.04
 0.042    129  98.56   286.3   287.5  0.02  0.02      8   338.1   341.5  0.02  0.02
 0.048    150  98.73   296.7   296.4  0.02  0.02      5   305.8   306.8  0.03  0.03
 0.055    151  99.38   281.2   281.4  0.01  0.02     10   257.9   260.1  0.04  0.04
 0.061    172 100.00   218.4   218.6  0.02  0.02     10   202.2   202.4  0.03  0.03
```

```
 0.067    174  99.45   211.4   210.9  0.02  0.02      6   286.3   284.3  0.02  0.02
 0.074    178  98.92   206.1   206.7  0.02  0.02      6   234.5   236.6  0.03  0.03
 0.080    189 100.00   208.7   209.0  0.02  0.02     13   159.6   155.6  0.06  0.06
 0.086    197 100.00   176.8   176.9  0.02  0.02      8   208.5   207.6  0.04  0.04
 0.093    193  93.55   156.9   157.0  0.02  0.02     10   182.0   185.9  0.07  0.06
 0.099    188  91.28   160.7   159.7  0.02  0.02     11   159.6   157.2  0.02  0.02
 0.105    190  86.02   153.8   153.5  0.02  0.02     13   169.2   170.4  0.05  0.04
 0.112    183  80.08   129.9   129.6  0.02  0.02      6   135.2   139.9  0.08  0.08
 0.118    194  81.85   126.9   126.7  0.02  0.02      9   138.0   137.5  0.05  0.05
 0.124    174  73.20   129.0   128.9  0.02  0.02      9   113.8   111.2  0.07  0.07
$$
```

**** Fom and SigmaA vs resolution ****

```
$TABLE: Cycle   48. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle   48. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa  FOMa  NREFc FOMc NREFall FOMall  SigmaA_Fc1 $$
$$
 0.0038    30   0.999     4   1.000    34   0.999  0.999
 0.0102    62   0.999     7   1.000    69   0.999  0.999
 0.0165    83   0.990    12   0.923    95   0.982  0.999
 0.0228    97   0.988    11   1.000   108   0.989  0.999
 0.0292   108   0.997     6   1.000   114   0.997  0.999
 0.0355   126   0.996    17   1.000   143   0.996  0.999
 0.0418   129   0.997    11   1.000   140   0.997  0.999
 0.0482   150   0.991    12   1.000   162   0.991  0.999
 0.0545   151   0.997    12   0.990   163   0.996  0.999
 0.0609   172   0.983    15   0.954   187   0.980  0.999
 0.0672   174   0.993     9   0.938   183   0.990  0.999
 0.0735   178   0.990    11   1.000   189   0.990  0.999
 0.0799   189   0.989    14   0.999   203   0.990  0.999
 0.0862   197   0.983     9   0.975   206   0.983  0.999
 0.0925   193   0.978    14   0.929   207   0.975  0.999
 0.0989   188   0.979    12   1.000   200   0.981  0.999
 0.1052   190   0.988     8   1.000   198   0.989  0.999
 0.1116   183   0.980    13   0.938   196   0.977  1.000
 0.1179   194   0.980    11   0.938   205   0.977  1.000
 0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0194
Free R factor                    =     0.0408
Overall weighted R factor        =     0.0194
Free weighted R factor           =     0.0411
Overall correlation coefficient  =     0.9993
Free correlation coefficient     =     0.9967
DPI based on free R factor       =     0.0740
```

Overall figure of merit = 0.9866
ML based su of positional parameters = 0.0408
ML based su of thermal parameters = 2.0127

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10547.261 3158.0671 20255.016 20255.201

CGMAT cycle number = 49

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.6144204 is applied to the X-ray term
Norm of X_ray positional gradient 13.8
Norm of Geom. positional gradient 13.8
Norm of X_ray B-factor gradient 17.9
Norm of Geom. B-factor gradient 18.3
Product of X_ray and Geom posit. gradients -0.698E+06
Cosine of angle between them -0.999
Product of X_ray and Geom B-fact gradients -0.400E+06
Cosine of angle between them -0.994

Residuals: XRAY= 0.1702E+05 GEOM= 3159. TOTAL= 0.2018E+05
function value 20177.148

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.679	1.966
Torsion angles, period 1. refined	155	7.879	5.000
Torsion angles, period 2. refined	54	41.411	25.741
Torsion angles, period 3. refined	214	19.215	15.000
Torsion angles, period 4. refined	3	21.371	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	542	0.264	0.200
VDW; torsion: refined_atoms	790	0.324	0.200
HBOND: refined_atoms	42	0.190	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.268	0.200
Bond B values: refined atoms	1229	13.434	4.713

Angle B values: refined atoms 1663 16.518 7.126
Torsion B values: refined atoms 426 30.511 13.060
Long range B values: refined atoms 1339 12.290 15.358

Overall : scale = 1.012, B = -0.027
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 49. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 49. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 49. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 49. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.3 747.8 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.0 416.2 0.02 0.02 1 1228.5 1222.9 0.01 0.01
0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.0 413.6 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.3 0.07 0.06
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.2 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 253.7 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.5 0.02 0.02
0.048 150 98.73 296.7 296.4 0.02 0.02 5 305.8 306.8 0.03 0.03
0.055 151 99.38 281.2 281.4 0.01 0.02 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.4 0.03 0.03
0.067 174 99.45 211.5 210.9 0.02 0.02 6 286.3 284.3 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.5 236.6 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.6 155.6 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.5 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.0 0.07 0.06
0.099 188 91.28 160.7 159.7 0.02 0.02 11 159.6 157.2 0.02 0.02
0.105 190 86.02 153.8 153.5 0.02 0.02 13 169.2 170.4 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 139.9 0.08 0.07
0.118 194 81.85 126.9 126.7 0.02 0.02 9 138.0 137.5 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.2 0.07 0.07
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 49. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 49. M(Fom) v. resln :N:1,3,5,7,8:
$$

```
<4SSQ/LL> NREFa  FOMa  NREFc FOMc NREFall FOMall  SigmaA_Fc1 $$
$$
 0.0038   30  0.999    4  1.000   34  0.999  0.999
 0.0102   62  0.999    7  1.000   69  0.999  0.999
 0.0165   83  0.990   12  0.923   95  0.982  0.999
 0.0228   97  0.988   11  1.000  108  0.989  0.999
 0.0292  108  0.997    6  1.000  114  0.997  0.999
 0.0355  126  0.996   17  1.000  143  0.996  0.999
 0.0418  129  0.997   11  1.000  140  0.997  0.999
 0.0482  150  0.991   12  1.000  162  0.991  0.999
 0.0545  151  0.997   12  0.990  163  0.996  0.999
 0.0609  172  0.983   15  0.955  187  0.981  0.999
 0.0672  174  0.993    9  0.938  183  0.990  0.999
 0.0735  178  0.990   11  1.000  189  0.990  0.999
 0.0799  189  0.989   14  0.999  203  0.990  0.999
 0.0862  197  0.983    9  0.974  206  0.983  0.999
 0.0925  193  0.978   14  0.929  207  0.975  0.999
 0.0989  188  0.979   12  1.000  200  0.981  0.999
 0.1052  190  0.988    8  1.000  198  0.989  0.999
 0.1116  183  0.980   13  0.938  196  0.977  1.000
 0.1179  194  0.980   11  0.939  205  0.977  1.000
 0.1242  174  0.983    8  1.000  182  0.984  1.000
 $$
Resolution limits                =    38.899    2.802
Number of used reflections       =      3184
Percentage observed              =   92.6870
Percentage of free reflections   =    4.8416
Overall R factor                 =    0.0194
Free R factor                    =    0.0407
Overall weighted R factor        =    0.0194
Free weighted R factor           =    0.0411
Overall correlation coefficient  =    0.9993
Free correlation coefficient     =    0.9967
DPI based on free R factor       =    0.0739
Overall figure of merit          =    0.9866
ML based su of positional parameters =    0.0407
ML based su of thermal parameters    =    2.0085
------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10541.877       3158.9412       20181.746       20177.963

 fvalues    10541.877       3158.9412       20178.117       20177.963


    CGMAT cycle number =     50

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
```

Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.6139528 is applied to the X-ray term
Norm of X_ray positional gradient 13.8
Norm of Geom. positional gradient 13.8
Norm of X_ray B-factor gradient 17.9
Norm of Geom. B-factor gradient 18.3
Product of X_ray and Geom posit. gradients -0.698E+06
Cosine of angle between them -0.999
Product of X_ray and Geom B-fact gradients -0.401E+06
Cosine of angle between them -0.994

Residuals: XRAY= 0.1701E+05 GEOM= 3159. TOTAL= 0.2017E+05
function value 20171.619

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.679	1.966
Torsion angles, period 1. refined	155	7.879	5.000
Torsion angles, period 2. refined	54	41.412	25.741
Torsion angles, period 3. refined	214	19.198	15.000
Torsion angles, period 4. refined	3	21.369	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	542	0.264	0.200
VDW; torsion: refined_atoms	790	0.324	0.200
HBOND: refined_atoms	42	0.190	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.268	0.200
Bond B values: refined atoms	1229	13.434	4.713
Angle B values: refined atoms	1663	16.519	7.126
Torsion B values: refined atoms	426	30.514	13.060
Long range B values: refined atoms	1339	12.291	15.358

Overall : scale = 1.012, B = -0.027
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 50. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 50. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 50. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 50. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.3 747.8 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.0 416.2 0.02 0.02 1 1228.5 1222.8 0.01 0.01
0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.0 413.6 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.3 0.07 0.06
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.2 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 253.7 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.5 0.02 0.02
0.048 150 98.73 296.7 296.4 0.02 0.02 5 305.8 306.8 0.03 0.03
0.055 151 99.38 281.2 281.4 0.01 0.02 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.4 0.03 0.03
0.067 174 99.45 211.5 210.9 0.02 0.02 6 286.3 284.3 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.5 236.6 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.6 155.6 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.5 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 185.9 0.07 0.06
0.099 188 91.28 160.7 159.7 0.02 0.02 11 159.6 157.2 0.02 0.02
0.105 190 86.02 153.8 153.5 0.02 0.02 13 169.2 170.4 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 139.9 0.08 0.08
0.118 194 81.85 126.9 126.7 0.02 0.02 9 138.0 137.4 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.2 0.07 0.07
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 50. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 50. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.990 12 0.923 95 0.982 0.999
0.0228 97 0.988 11 1.000 108 0.989 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.996 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.991 0.999
0.0545 151 0.997 12 0.990 163 0.996 0.999
0.0609 172 0.983 15 0.955 187 0.981 0.999
0.0672 174 0.993 9 0.938 183 0.990 0.999
0.0735 178 0.990 11 1.000 189 0.990 0.999
0.0799 189 0.989 14 0.999 203 0.990 0.999

```
 0.0862   197   0.983    9   0.974   206   0.983  0.999
 0.0925   193   0.978   14   0.929   207   0.975  0.999
 0.0989   188   0.979   12   1.000   200   0.981  0.999
 0.1052   190   0.988    8   1.000   198   0.989  0.999
 0.1116   183   0.980   13   0.938   196   0.977  1.000
 0.1179   194   0.980   11   0.939   205   0.977  1.000
 0.1242   174   0.983    8   1.000   182   0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0194
Free R factor                    =     0.0407
Overall weighted R factor        =     0.0194
Free weighted R factor           =     0.0411
Overall correlation coefficient  =     0.9993
Free correlation coefficient     =     0.9967
DPI based on free R factor       =     0.0739
Overall figure of merit          =     0.9866
ML based su of positional parameters =     0.0407
ML based su of thermal parameters    =     2.0082
------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10541.555       3158.8442       20171.932       20172.416


    CGMAT cycle number =     51

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    1.6130472      is applied to the X-ray term
Norm of X_ray positional gradient              13.8
Norm of Geom. positional gradient              13.7
Norm of X_ray B-factor gradient                17.9
Norm of Geom. B-factor gradient                18.3
Product of X_ray and Geom posit. gradients     -0.698E+06
 Cosine of angle between them                  -1.000
Product of X_ray and Geom B-fact gradients     -0.401E+06
 Cosine of angle between them                  -0.994
```

Residuals: XRAY= 0.1700E+05 GEOM= 3159. TOTAL= 0.2016E+05
function value 20160.750

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.681	1.966
Torsion angles, period 1. refined	155	7.879	5.000
Torsion angles, period 2. refined	54	41.414	25.741
Torsion angles, period 3. refined	214	19.210	15.000
Torsion angles, period 4. refined	3	21.365	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	542	0.264	0.200
VDW; torsion: refined_atoms	788	0.325	0.200
HBOND: refined_atoms	42	0.190	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.267	0.200
Bond B values: refined atoms	1229	13.431	4.713
Angle B values: refined atoms	1663	16.519	7.125
Torsion B values: refined atoms	426	30.520	13.060
Long range B values: refined atoms	1337	12.297	15.362

Overall : scale = 1.012, B = -0.027
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 51. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 51. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 51. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 51. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$

0.004	30	62.50	754.3	747.8	0.02	0.02	0	0.0	0.0******	0.00	
0.010	62	95.45	414.1	416.2	0.02	0.02	1	1228.5	1223.0	0.01	0.01
0.017	83	95.60	307.7	308.7	0.03	0.02	4	403.0	413.6	0.04	0.05
0.023	97	97.14	247.4	248.4	0.02	0.02	5	180.2	188.3	0.07	0.06
0.029	108	100.00	241.3	242.0	0.02	0.02	7	186.7	189.2	0.06	0.06
0.036	126	99.25	270.4	270.7	0.02	0.02	6	252.9	253.7	0.04	0.04
0.042	129	98.56	286.3	287.5	0.02	0.02	8	338.1	341.5	0.02	0.02
0.048	150	98.73	296.7	296.4	0.02	0.02	5	305.8	306.9	0.03	0.03

```
 0.055    151  99.38   281.2   281.4  0.01  0.02      10   257.9   260.1  0.04  0.04
 0.061    172 100.00   218.4   218.6  0.02  0.02      10   202.2   202.4  0.03  0.03
 0.067    174  99.45   211.5   210.9  0.02  0.02       6   286.3   284.3  0.02  0.02
 0.074    178  98.92   206.1   206.7  0.02  0.02       6   234.5   236.6  0.03  0.03
 0.080    189 100.00   208.7   209.0  0.02  0.02      13   159.6   155.6  0.06  0.06
 0.086    197 100.00   176.8   176.9  0.02  0.02       8   208.5   207.6  0.04  0.04
 0.093    193  93.55   156.9   157.0  0.02  0.02      10   182.0   186.0  0.07  0.06
 0.099    188  91.28   160.7   159.7  0.02  0.02      11   159.6   157.2  0.02  0.02
 0.105    190  86.02   153.8   153.5  0.02  0.02      13   169.2   170.4  0.05  0.04
 0.112    183  80.08   129.9   129.6  0.02  0.02       6   135.2   140.0  0.08  0.08
 0.118    194  81.85   127.0   126.7  0.02  0.02       9   138.0   137.4  0.05  0.05
 0.124    174  73.20   129.0   128.9  0.02  0.02       9   113.8   111.2  0.07  0.07
$$
```

**** Fom and SigmaA vs resolution ****

```
$TABLE: Cycle   51. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle   51. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa  FOMa  NREFc FOMc NREFall FOMall  SigmaA_Fc1 $$
$$
 0.0038    30   0.999     4   1.000    34   0.999  0.999
 0.0102    62   0.999     7   1.000    69   0.999  0.999
 0.0165    83   0.990    12   0.923    95   0.982  0.999
 0.0228    97   0.988    11   1.000   108   0.989  0.999
 0.0292   108   0.997     6   1.000   114   0.997  0.999
 0.0355   126   0.996    17   1.000   143   0.996  0.999
 0.0418   129   0.997    11   1.000   140   0.997  0.999
 0.0482   150   0.991    12   1.000   162   0.991  0.999
 0.0545   151   0.997    12   0.991   163   0.996  0.999
 0.0609   172   0.983    15   0.955   187   0.981  0.999
 0.0672   174   0.993     9   0.938   183   0.990  0.999
 0.0735   178   0.990    11   1.000   189   0.990  0.999
 0.0799   189   0.989    14   0.999   203   0.990  0.999
 0.0862   197   0.983     9   0.974   206   0.983  0.999
 0.0925   193   0.978    14   0.929   207   0.975  0.999
 0.0989   188   0.979    12   1.000   200   0.981  0.999
 0.1052   190   0.988     8   1.000   198   0.989  0.999
 0.1116   183   0.980    13   0.938   196   0.977  1.000
 0.1179   194   0.980    11   0.940   205   0.978  1.000
 0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
Resolution limits                =    38.899     2.802
Number of used reflections       =      3184
Percentage observed              =   92.6870
Percentage of free reflections   =    4.8416
Overall R factor                 =    0.0193
Free R factor                    =    0.0407
Overall weighted R factor        =    0.0194
Free weighted R factor           =    0.0411
Overall correlation coefficient  =    0.9993
```

Free correlation coefficient = 0.9967
DPI based on free R factor = 0.0739
Overall figure of merit = 0.9867
ML based su of positional parameters = 0.0407
ML based su of thermal parameters = 2.0075

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10540.495 3159.3052 20161.809 20161.621

fvalues 10540.495 3159.3052 20161.510 20161.621

CGMAT cycle number = 52

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.6112019 is applied to the X-ray term
Norm of X_ray positional gradient 13.8
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.9
Norm of Geom. B-factor gradient 18.3
Product of X_ray and Geom posit. gradients -0.698E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.400E+06
Cosine of angle between them -0.994

Residuals: XRAY= 0.1698E+05 GEOM= 3160. TOTAL= 0.2014E+05
function value 20138.656

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.680	1.966
Torsion angles, period 1. refined	155	7.879	5.000
Torsion angles, period 2. refined	54	41.414	25.741
Torsion angles, period 3. refined	214	19.198	15.000
Torsion angles, period 4. refined	3	21.367	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	541	0.265	0.200
VDW; torsion: refined_atoms	788	0.325	0.200

HBOND: refined_atoms 42 0.190 0.200
VDW repulsions: symmetry: refined_atoms 55 0.262 0.200
HBOND: symmetry: refined_atoms 3 0.267 0.200
Bond B values: refined atoms 1229 13.431 4.713
Angle B values: refined atoms 1663 16.521 7.125
Torsion B values: refined atoms 426 30.526 13.060
Long range B values: refined atoms 1336 12.301 15.359

Overall : scale = 1.012, B = -0.027
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 52. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 52. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 52. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 52. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.3 747.8 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.2 0.02 0.02 1 1228.5 1223.0 0.01 0.01
0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.0 413.6 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.3 0.07 0.06
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.2 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 253.7 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.5 0.02 0.02
0.048 150 98.73 296.7 296.4 0.02 0.02 5 305.8 306.9 0.03 0.03
0.055 151 99.38 281.2 281.4 0.01 0.02 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.4 0.03 0.03
0.067 174 99.45 211.5 210.9 0.02 0.02 6 286.3 284.3 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.5 236.7 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.6 155.6 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.5 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.0 0.07 0.06
0.099 188 91.28 160.7 159.7 0.02 0.02 11 159.6 157.2 0.02 0.02
0.105 190 86.02 153.8 153.5 0.02 0.02 13 169.2 170.4 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 140.0 0.08 0.08
0.118 194 81.85 126.9 126.7 0.02 0.02 9 138.0 137.4 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.2 0.07 0.07
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 52. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 52. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.990 12 0.923 95 0.982 0.999
0.0228 97 0.988 11 1.000 108 0.989 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.996 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.991 0.999
0.0545 151 0.997 12 0.991 163 0.996 0.999
0.0609 172 0.983 15 0.955 187 0.981 0.999
0.0672 174 0.993 9 0.938 183 0.990 0.999
0.0735 178 0.990 11 1.000 189 0.990 0.999
0.0799 189 0.989 14 0.999 203 0.990 0.999
0.0862 197 0.983 9 0.974 206 0.983 0.999
0.0925 193 0.978 14 0.929 207 0.975 0.999
0.0989 188 0.979 12 1.000 200 0.981 0.999
0.1052 190 0.988 8 1.000 198 0.989 0.999
0.1116 183 0.980 13 0.938 196 0.977 1.000
0.1179 194 0.980 11 0.940 205 0.978 1.000
0.1242 174 0.983 8 1.000 182 0.984 1.000
$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0193
Free R factor = 0.0407
Overall weighted R factor = 0.0194
Free weighted R factor = 0.0410
Overall correlation coefficient = 0.9993
Free correlation coefficient = 0.9967
DPI based on free R factor = 0.0738
Overall figure of merit = 0.9867
ML based su of positional parameters = 0.0407
ML based su of thermal parameters = 2.0066

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10538.688 3159.5413 20140.000 20139.496

fvalues 10538.688 3159.5413 20139.271 20139.496

CGMAT cycle number = 53

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000008
Actual weight 1.6068228 is applied to the X-ray term
Norm of X_ray positional gradient 13.8
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.9
Norm of Geom. B-factor gradient 18.3
Product of X_ray and Geom posit. gradients -0.697E+06
Cosine of angle between them -0.999
Product of X_ray and Geom B-fact gradients -0.400E+06
Cosine of angle between them -0.994

Residuals: XRAY= 0.1693E+05 GEOM= 3160. TOTAL= 0.2009E+05
function value 20087.510

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.680	1.966
Torsion angles, period 1. refined	155	7.879	5.000
Torsion angles, period 2. refined	54	41.415	25.741
Torsion angles, period 3. refined	214	19.218	15.000
Torsion angles, period 4. refined	3	21.368	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	541	0.265	0.200
VDW; torsion: refined_atoms	788	0.325	0.200
HBOND: refined_atoms	42	0.190	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.267	0.200
Bond B values: refined atoms	1229	13.431	4.713
Angle B values: refined atoms	1663	16.523	7.125
Torsion B values: refined atoms	426	30.534	13.060
Long range B values: refined atoms	1336	12.303	15.359

Overall : scale = 1.012, B = -0.027
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 53. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 53. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 53. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 53. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.3 747.8 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.2 0.02 0.02 1 1228.5 1223.0 0.01 0.01
0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.0 413.6 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.3 0.07 0.06
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.2 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 253.7 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.5 0.02 0.02
0.048 150 98.73 296.7 296.4 0.02 0.02 5 305.8 306.9 0.03 0.03
0.055 151 99.38 281.2 281.4 0.01 0.02 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.4 0.03 0.03
0.067 174 99.45 211.5 210.9 0.02 0.02 6 286.3 284.3 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.5 236.7 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.6 155.6 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.5 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.0 0.07 0.06
0.099 188 91.28 160.7 159.7 0.02 0.02 11 159.6 157.2 0.02 0.02
0.105 190 86.02 153.8 153.5 0.02 0.02 13 169.2 170.4 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 140.0 0.08 0.08
0.118 194 81.85 127.0 126.7 0.02 0.02 9 138.0 137.4 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.2 0.07 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 53. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 53. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.990 12 0.923 95 0.982 0.999
0.0228 97 0.988 11 1.000 108 0.989 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.996 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.992 0.999
0.0545 151 0.997 12 0.991 163 0.996 0.999

```
 0.0609   172   0.983    15   0.955   187   0.981  0.999
 0.0672   174   0.993     9   0.938   183   0.990  0.999
 0.0735   178   0.990    11   1.000   189   0.990  0.999
 0.0799   189   0.989    14   0.999   203   0.990  0.999
 0.0862   197   0.983     9   0.974   206   0.983  0.999
 0.0925   193   0.978    14   0.929   207   0.975  0.999
 0.0989   188   0.979    12   1.000   200   0.981  0.999
 0.1052   190   0.988     8   1.000   198   0.989  0.999
 0.1116   183   0.980    13   0.938   196   0.977  1.000
 0.1179   194   0.980    11   0.941   205   0.978  1.000
 0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0193
Free R factor                    =     0.0406
Overall weighted R factor        =     0.0193
Free weighted R factor           =     0.0410
Overall correlation coefficient  =     0.9993
Free correlation coefficient     =     0.9967
DPI based on free R factor       =     0.0737
Overall figure of merit          =     0.9867
ML based su of positional parameters =     0.0406
ML based su of thermal parameters    =     2.0036
--------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10535.283       3160.0098       20090.004       20088.344

 fvalues    10535.283       3160.0098       20088.260       20088.344


    CGMAT cycle number =     54

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    1.6064863      is applied to the X-ray term
Norm of X_ray positional gradient              13.7
Norm of Geom. positional gradient              13.7
Norm of X_ray B-factor gradient                17.9
Norm of Geom. B-factor gradient                18.3
```

Product of X_ray and Geom posit. gradients -0.697E+06
Cosine of angle between them -0.999
Product of X_ray and Geom B-fact gradients -0.400E+06
Cosine of angle between them -0.994

Residuals: XRAY= 0.1692E+05 GEOM= 3160. TOTAL= 0.2008E+05
function value 20083.602

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.680	1.966
Torsion angles, period 1. refined	155	7.879	5.000
Torsion angles, period 2. refined	54	41.415	25.741
Torsion angles, period 3. refined	214	19.198	15.000
Torsion angles, period 4. refined	3	21.370	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.265	0.200
VDW; torsion: refined_atoms	788	0.325	0.200
HBOND: refined_atoms	42	0.191	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.266	0.200
Bond B values: refined atoms	1229	13.428	4.713
Angle B values: refined atoms	1663	16.521	7.125
Torsion B values: refined atoms	426	30.532	13.060
Long range B values: refined atoms	1335	12.305	15.352

Overall : scale = 1.012, B = -0.027
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 54. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 54. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 54. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 54. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$

0.004	30	62.50	754.3	747.8	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	414.1	416.2	0.02	0.02	1	1228.5	1223.1	0.01	0.01	

0.017	83	95.60	307.7	308.7	0.03	0.02	4	403.0	413.6	0.04	0.05
0.023	97	97.14	247.4	248.4	0.02	0.02	5	180.2	188.3	0.07	0.06
0.029	108	100.00	241.3	242.0	0.02	0.02	7	186.7	189.2	0.06	0.06
0.036	126	99.25	270.4	270.7	0.02	0.02	6	252.9	253.7	0.04	0.04
0.042	129	98.56	286.3	287.5	0.02	0.02	8	338.1	341.5	0.02	0.02
0.048	150	98.73	296.7	296.4	0.02	0.02	5	305.8	306.9	0.03	0.03
0.055	151	99.38	281.2	281.4	0.01	0.02	10	257.9	260.1	0.04	0.04
0.061	172	100.00	218.4	218.6	0.02	0.02	10	202.2	202.4	0.03	0.03
0.067	174	99.45	211.5	210.9	0.02	0.02	6	286.3	284.3	0.02	0.02
0.074	178	98.92	206.1	206.7	0.02	0.02	6	234.5	236.7	0.03	0.03
0.080	189	100.00	208.7	209.0	0.02	0.02	13	159.6	155.6	0.06	0.06
0.086	197	100.00	176.8	176.9	0.02	0.02	8	208.5	207.6	0.04	0.04
0.093	193	93.55	156.9	157.0	0.02	0.02	10	182.0	186.0	0.07	0.06
0.099	188	91.28	160.7	159.7	0.02	0.02	11	159.6	157.2	0.02	0.02
0.105	190	86.02	153.8	153.5	0.02	0.02	13	169.2	170.4	0.05	0.04
0.112	183	80.08	129.9	129.6	0.02	0.02	6	135.2	140.1	0.08	0.08
0.118	194	81.85	127.0	126.7	0.02	0.02	9	138.0	137.4	0.05	0.05
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	111.2	0.07	0.06

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 54. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 54. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.990	12	0.923	95	0.982	0.999
0.0228	97	0.988	11	1.000	108	0.989	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.996	17	1.000	143	0.996	0.999
0.0418	129	0.997	11	1.000	140	0.997	0.999
0.0482	150	0.991	12	1.000	162	0.992	0.999
0.0545	151	0.997	12	0.991	163	0.996	0.999
0.0609	172	0.983	15	0.955	187	0.981	0.999
0.0672	174	0.993	9	0.938	183	0.990	0.999
0.0735	178	0.990	11	1.000	189	0.990	0.999
0.0799	189	0.989	14	0.999	203	0.990	0.999
0.0862	197	0.983	9	0.974	206	0.983	0.999
0.0925	193	0.978	14	0.930	207	0.975	0.999
0.0989	188	0.979	12	1.000	200	0.981	0.999
0.1052	190	0.988	8	1.000	198	0.989	0.999
0.1116	183	0.980	13	0.938	196	0.977	1.000
0.1179	194	0.980	11	0.941	205	0.978	1.000
0.1242	174	0.983	8	1.000	182	0.984	1.000

$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870

Percentage of free reflections = 4.8416
Overall R factor = 0.0193
Free R factor = 0.0406
Overall weighted R factor = 0.0193
Free weighted R factor = 0.0410
Overall correlation coefficient = 0.9993
Free correlation coefficient = 0.9968
DPI based on free R factor = 0.0737
Overall figure of merit = 0.9867
ML based su of positional parameters = 0.0406
ML based su of thermal parameters = 2.0034

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10534.946 3160.1819 20081.697 20084.430

CGMAT cycle number = 55

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.6032126 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.9
Norm of X_ray B-factor gradient 17.9
Norm of Geom. B-factor gradient 18.3
Product of X_ray and Geom posit. gradients -0.696E+06
Cosine of angle between them -0.991
Product of X_ray and Geom B-fact gradients -0.399E+06
Cosine of angle between them -0.991

Residuals: XRAY= 0.1688E+05 GEOM= 3159. TOTAL= 0.2004E+05
function value 20042.162

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.675	1.966
Torsion angles, period 1. refined	155	7.879	5.000
Torsion angles, period 2. refined	54	41.416	25.741
Torsion angles, period 3. refined	214	19.280	15.000
Torsion angles, period 4. refined	3	21.369	15.000

Chiral centres: refined atoms 187 0.111 0.200
Planar groups: refined atoms 924 0.005 0.021
VDW repulsions: refined_atoms 539 0.265 0.200
VDW; torsion: refined_atoms 788 0.325 0.200
HBOND: refined_atoms 42 0.191 0.200
VDW repulsions: symmetry: refined_atoms 55 0.262 0.200
HBOND: symmetry: refined_atoms 3 0.266 0.200
Bond B values: refined atoms 1229 13.428 4.713
Angle B values: refined atoms 1663 16.525 7.125
Torsion B values: refined atoms 426 30.543 13.060
Long range B values: refined atoms 1334 11.607 15.329

Overall : scale = 1.012, B = -0.027
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 55. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 55. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 55. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 55. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.3 747.8 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.2 0.02 0.02 1 1228.5 1223.2 0.01 0.01
0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.0 413.6 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.3 0.07 0.06
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.2 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 253.7 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.5 0.02 0.02
0.048 150 98.73 296.7 296.4 0.02 0.02 5 305.8 306.9 0.03 0.03
0.055 151 99.38 281.2 281.4 0.01 0.02 10 257.9 260.2 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.5 0.03 0.03
0.067 174 99.45 211.5 210.9 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.5 236.7 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.6 155.6 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.5 207.7 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.0 0.07 0.06
0.099 188 91.28 160.7 159.7 0.02 0.02 11 159.6 157.2 0.02 0.02
0.105 190 86.02 153.8 153.5 0.02 0.02 13 169.2 170.3 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 140.1 0.08 0.08
0.118 194 81.85 127.0 126.7 0.02 0.02 9 138.0 137.4 0.05 0.05

```
 0.124    174  73.20   129.0   128.9  0.02  0.02       9   113.8   111.2  0.07  0.06
$$

   ****                Fom and SigmaA vs resolution                ****

 $TABLE: Cycle   55. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
 $GRAPHS:Cycle   55. M(Fom) v. resln :N:1,3,5,7,8:
 $$
 <4SSQ/LL> NREFa  FOMa  NREFc FOMc NREFall FOMall  SigmaA_Fc1 $$
 $$
  0.0038    30   0.999     4   1.000    34   0.999  0.999
  0.0102    62   0.999     7   1.000    69   0.999  0.999
  0.0165    83   0.990    12   0.923    95   0.982  0.999
  0.0228    97   0.988    11   1.000   108   0.990  0.999
  0.0292   108   0.997     6   1.000   114   0.997  0.999
  0.0355   126   0.996    17   1.000   143   0.996  0.999
  0.0418   129   0.997    11   1.000   140   0.997  0.999
  0.0482   150   0.991    12   1.000   162   0.992  0.999
  0.0545   151   0.997    12   0.991   163   0.996  0.999
  0.0609   172   0.983    15   0.956   187   0.981  0.999
  0.0672   174   0.993     9   0.938   183   0.990  0.999
  0.0735   178   0.990    11   1.000   189   0.990  0.999
  0.0799   189   0.989    14   0.999   203   0.990  0.999
  0.0862   197   0.983     9   0.975   206   0.983  0.999
  0.0925   193   0.978    14   0.930   207   0.975  0.999
  0.0989   188   0.980    12   1.000   200   0.981  0.999
  0.1052   190   0.988     8   1.000   198   0.989  0.999
  0.1116   183   0.980    13   0.938   196   0.977  1.000
  0.1179   194   0.980    11   0.941   205   0.978  1.000
  0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
 Resolution limits                =     38.899     2.802
 Number of used reflections       =       3184
 Percentage observed              =    92.6870
 Percentage of free reflections   =     4.8416
 Overall R factor                 =     0.0193
 Free R factor                    =     0.0406
 Overall weighted R factor        =     0.0193
 Free weighted R factor           =     0.0410
 Overall correlation coefficient  =     0.9993
 Free correlation coefficient     =     0.9968
 DPI based on free R factor       =     0.0737
 Overall figure of merit          =     0.9867
 ML based su of positional parameters =     0.0406
 ML based su of thermal parameters    =     2.0016
 ------------------------------------------------------------------------------
  Trying gamma equal    0.0000000
  Convergence reached with no gamma cycles


  fvalues    10531.651       3158.5205       20162.598       20042.996
```

fvalues 10531.651 3158.5205 20052.975 20042.996

CGMAT cycle number = 56

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.6020954 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 14.0
Norm of X_ray B-factor gradient 17.9
Norm of Geom. B-factor gradient 18.3
Product of X_ray and Geom posit. gradients -0.696E+06
Cosine of angle between them -0.984
Product of X_ray and Geom B-fact gradients -0.399E+06
Cosine of angle between them -0.992

Residuals: XRAY= 0.1687E+05 GEOM= 3158. TOTAL= 0.2003E+05
function value 20027.877

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.671	1.966
Torsion angles, period 1. refined	155	7.879	5.000
Torsion angles, period 2. refined	54	41.417	25.741
Torsion angles, period 3. refined	214	19.216	15.000
Torsion angles, period 4. refined	3	21.370	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	539	0.265	0.200
VDW; torsion: refined_atoms	788	0.325	0.200
HBOND: refined_atoms	42	0.191	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.266	0.200
Bond B values: refined atoms	1229	13.437	4.714
Angle B values: refined atoms	1663	16.534	7.126
Torsion B values: refined atoms	426	30.570	13.062
Long range B values: refined atoms	1334	11.608	15.329

Overall : scale = 1.012, B = -0.027

Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 56. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 56. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 56. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 56. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.3 747.8 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.2 0.02 0.02 1 1228.5 1223.2 0.01 0.01
0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.0 413.6 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.3 0.07 0.06
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.2 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 253.7 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.5 0.02 0.02
0.048 150 98.73 296.7 296.4 0.02 0.01 5 305.8 306.9 0.03 0.03
0.055 151 99.38 281.2 281.4 0.01 0.02 10 257.9 260.2 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.5 0.03 0.03
0.067 174 99.45 211.5 210.9 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.5 236.7 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.6 155.6 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.5 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.0 0.07 0.06
0.099 188 91.28 160.7 159.7 0.02 0.02 11 159.6 157.2 0.02 0.02
0.105 190 86.02 153.8 153.5 0.02 0.02 13 169.2 170.3 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 140.2 0.08 0.08
0.118 194 81.85 127.0 126.7 0.02 0.02 9 138.0 137.4 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.2 0.07 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 56. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 56. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.990 12 0.923 95 0.982 0.999
0.0228 97 0.988 11 1.000 108 0.989 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999

```
 0.0355   126   0.996    17   1.000   143   0.996  0.999
 0.0418   129   0.997    11   1.000   140   0.997  0.999
 0.0482   150   0.991    12   1.000   162   0.992  0.999
 0.0545   151   0.997    12   0.991   163   0.996  0.999
 0.0609   172   0.983    15   0.956   187   0.981  0.999
 0.0672   174   0.993     9   0.938   183   0.990  0.999
 0.0735   178   0.990    11   1.000   189   0.990  0.999
 0.0799   189   0.989    14   0.999   203   0.990  0.999
 0.0862   197   0.983     9   0.975   206   0.983  0.999
 0.0925   193   0.978    14   0.930   207   0.975  0.999
 0.0989   188   0.980    12   1.000   200   0.981  0.999
 0.1052   190   0.988     8   1.000   198   0.989  0.999
 0.1116   183   0.980    13   0.938   196   0.977  1.000
 0.1179   194   0.980    11   0.941   205   0.978  1.000
 0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0193
Free R factor                    =     0.0406
Overall weighted R factor        =     0.0193
Free weighted R factor           =     0.0409
Overall correlation coefficient  =     0.9993
Free correlation coefficient     =     0.9968
DPI based on free R factor       =     0.0737
Overall figure of merit          =     0.9867
ML based su of positional parameters =     0.0406
ML based su of thermal parameters    =     2.0009
------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10530.335       3158.1221       20025.852       20028.723


    CGMAT cycle number =     57

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000008
 Actual weight    1.5997661      is applied to the X-ray term
Norm of X_ray positional gradient              13.7
Norm of Geom. positional gradient              13.7
```

Norm of X_ray B-factor gradient 17.9
Norm of Geom. B-factor gradient 18.3
Product of X_ray and Geom posit. gradients -0.696E+06
Cosine of angle between them -0.999
Product of X_ray and Geom B-fact gradients -0.399E+06
Cosine of angle between them -0.994

Residuals: XRAY= 0.1684E+05 GEOM= 3156. TOTAL= 0.2000E+05
function value 19997.453

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.683	1.966
Torsion angles, period 1. refined	155	7.878	5.000
Torsion angles, period 2. refined	54	41.419	25.741
Torsion angles, period 3. refined	214	19.219	15.000
Torsion angles, period 4. refined	3	21.373	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	539	0.265	0.200
VDW; torsion: refined_atoms	788	0.325	0.200
HBOND: refined_atoms	42	0.191	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.265	0.200
Bond B values: refined atoms	1229	13.469	4.715
Angle B values: refined atoms	1663	16.565	7.126
Torsion B values: refined atoms	426	30.656	13.066
Long range B values: refined atoms	1334	11.612	15.327

Overall : scale = 1.012, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 57. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 57. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 57. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 57. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$

```
 0.004     30  62.50   754.3   747.8  0.02  0.02      0     0.0     0.0******  0.00
 0.010     62  95.45   414.1   416.2  0.02  0.02      1  1228.5  1223.3  0.01  0.01
 0.017     83  95.60   307.7   308.7  0.03  0.02      4   403.0   413.6  0.04  0.05
 0.023     97  97.14   247.4   248.4  0.02  0.02      5   180.2   188.4  0.07  0.06
 0.029    108 100.00   241.3   242.0  0.02  0.02      7   186.7   189.3  0.06  0.06
 0.036    126  99.25   270.4   270.7  0.02  0.02      6   252.9   253.8  0.04  0.04
 0.042    129  98.56   286.3   287.5  0.02  0.02      8   338.1   341.4  0.02  0.02
 0.048    150  98.73   296.7   296.4  0.02  0.01      5   305.8   306.9  0.03  0.03
 0.055    151  99.38   281.2   281.4  0.01  0.02     10   257.9   260.2  0.04  0.04
 0.061    172 100.00   218.4   218.6  0.02  0.02     10   202.2   202.5  0.03  0.03
 0.067    174  99.45   211.5   210.9  0.02  0.02      6   286.3   284.3  0.02  0.02
 0.074    178  98.92   206.1   206.7  0.02  0.02      6   234.5   236.7  0.03  0.03
 0.080    189 100.00   208.7   209.0  0.02  0.02     13   159.6   155.7  0.06  0.06
 0.086    197 100.00   176.8   176.9  0.02  0.02      8   208.5   207.6  0.04  0.04
 0.093    193  93.55   156.9   157.0  0.02  0.02     10   182.0   186.0  0.07  0.06
 0.099    188  91.28   160.7   159.7  0.02  0.02     11   159.6   157.2  0.02  0.02
 0.105    190  86.02   153.8   153.5  0.02  0.02     13   169.2   170.3  0.05  0.04
 0.112    183  80.08   129.9   129.6  0.02  0.02      6   135.2   140.2  0.08  0.08
 0.118    194  81.85   127.0   126.7  0.02  0.02      9   138.0   137.4  0.05  0.05
 0.124    174  73.20   129.0   128.9  0.02  0.02      9   113.8   111.2  0.07  0.06
$$
```

**** Fom and SigmaA vs resolution ****

```
$TABLE: Cycle   57. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle   57. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa  FOMa  NREFc FOMc NREFall FOMall  SigmaA_Fc1 $$
$$
 0.0038    30   0.999     4   1.000    34   0.999  0.999
 0.0102    62   0.999     7   1.000    69   0.999  0.999
 0.0165    83   0.990    12   0.923    95   0.982  0.999
 0.0228    97   0.988    11   1.000   108   0.990  0.999
 0.0292   108   0.997     6   1.000   114   0.997  0.999
 0.0355   126   0.996    17   1.000   143   0.996  0.999
 0.0418   129   0.997    11   1.000   140   0.997  0.999
 0.0482   150   0.991    12   1.000   162   0.992  0.999
 0.0545   151   0.997    12   0.991   163   0.996  0.999
 0.0609   172   0.983    15   0.956   187   0.981  0.999
 0.0672   174   0.993     9   0.937   183   0.990  0.999
 0.0735   178   0.990    11   1.000   189   0.990  0.999
 0.0799   189   0.989    14   0.999   203   0.990  0.999
 0.0862   197   0.983     9   0.974   206   0.983  0.999
 0.0925   193   0.978    14   0.930   207   0.975  0.999
 0.0989   188   0.980    12   1.000   200   0.981  0.999
 0.1052   190   0.988     8   1.000   198   0.989  0.999
 0.1116   183   0.980    13   0.938   196   0.977  1.000
 0.1179   194   0.980    11   0.940   205   0.978  1.000
 0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
Resolution limits               =     38.899     2.802
```

Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0193
Free R factor = 0.0405
Overall weighted R factor = 0.0193
Free weighted R factor = 0.0409
Overall correlation coefficient = 0.9993
Free correlation coefficient = 0.9968
DPI based on free R factor = 0.0735
Overall figure of merit = 0.9867
ML based su of positional parameters = 0.0405
ML based su of thermal parameters = 1.9996

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10527.709 3156.3953 19998.031 19998.268

CGMAT cycle number = 58

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5995183 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.9
Norm of Geom. B-factor gradient 18.3
Product of X_ray and Geom posit. gradients -0.696E+06
Cosine of angle between them -0.999
Product of X_ray and Geom B-fact gradients -0.399E+06
Cosine of angle between them -0.994

Residuals: XRAY= 0.1684E+05 GEOM= 3157. TOTAL= 0.1999E+05
function value 19994.234

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.682	1.966
Torsion angles, period 1. refined	155	7.877	5.000
Torsion angles, period 2. refined	54	41.420	25.741

Torsion angles, period 3. refined 214 19.205 15.000
Torsion angles, period 4. refined 3 21.371 15.000
Chiral centres: refined atoms 187 0.111 0.200
Planar groups: refined atoms 924 0.005 0.021
VDW repulsions: refined_atoms 539 0.265 0.200
VDW; torsion: refined_atoms 788 0.325 0.200
HBOND: refined_atoms 42 0.191 0.200
VDW repulsions: symmetry: refined_atoms 55 0.262 0.200
HBOND: symmetry: refined_atoms 3 0.266 0.200
Bond B values: refined atoms 1229 13.501 4.717
Angle B values: refined atoms 1663 16.596 7.127
Torsion B values: refined atoms 426 30.723 13.070
Long range B values: refined atoms 1334 11.627 15.328

Overall : scale = 1.012, B = -0.026
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 58. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 58. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 58. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 58. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.3 747.8 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.2 0.02 0.02 1 1228.5 1223.3 0.01 0.01
0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.0 413.5 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.4 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.3 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 253.8 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.4 0.02 0.02
0.048 150 98.73 296.7 296.4 0.02 0.01 5 305.8 306.9 0.03 0.03
0.055 151 99.38 281.3 281.4 0.01 0.02 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.5 0.03 0.03
0.067 174 99.45 211.5 210.9 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.5 236.8 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.6 155.7 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.5 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.0 0.07 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.6 157.2 0.02 0.02
0.105 190 86.02 153.8 153.5 0.02 0.02 13 169.2 170.3 0.05 0.04

```
 0.112    183  80.08   129.9   129.6  0.02  0.02      6   135.2   140.3  0.08  0.08
 0.118    194  81.85   127.0   126.7  0.02  0.02      9   138.0   137.4  0.05  0.05
 0.124    174  73.20   129.0   128.9  0.02  0.02      9   113.8   111.2  0.07  0.06
$$
```

**** Fom and SigmaA vs resolution ****

```
 $TABLE: Cycle   58. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
 $GRAPHS:Cycle   58. M(Fom) v. resln :N:1,3,5,7,8:
 $$
 <4SSQ/LL> NREFa  FOMa  NREFc FOMc NREFall FOMall  SigmaA_Fc1 $$
 $$
  0.0038    30   0.999     4   1.000    34   0.999  0.999
  0.0102    62   0.999     7   1.000    69   0.999  0.999
  0.0165    83   0.990    12   0.923    95   0.982  0.999
  0.0228    97   0.988    11   1.000   108   0.990  0.999
  0.0292   108   0.997     6   1.000   114   0.997  0.999
  0.0355   126   0.996    17   1.000   143   0.996  0.999
  0.0418   129   0.997    11   1.000   140   0.997  0.999
  0.0482   150   0.991    12   1.000   162   0.992  0.999
  0.0545   151   0.997    12   0.992   163   0.996  0.999
  0.0609   172   0.983    15   0.955   187   0.981  0.999
  0.0672   174   0.993     9   0.937   183   0.990  0.999
  0.0735   178   0.990    11   1.000   189   0.990  0.999
  0.0799   189   0.989    14   0.999   203   0.990  0.999
  0.0862   197   0.983     9   0.974   206   0.983  0.999
  0.0925   193   0.978    14   0.930   207   0.975  0.999
  0.0989   188   0.980    12   1.000   200   0.981  0.999
  0.1052   190   0.988     8   1.000   198   0.989  0.999
  0.1116   183   0.980    13   0.938   196   0.977  1.000
  0.1179   194   0.980    11   0.940   205   0.978  1.000
  0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0193
Free R factor                    =     0.0405
Overall weighted R factor        =     0.0193
Free weighted R factor           =     0.0408
Overall correlation coefficient  =     0.9993
Free correlation coefficient     =     0.9968
DPI based on free R factor       =     0.0735
Overall figure of merit          =     0.9867
ML based su of positional parameters =     0.0405
ML based su of thermal parameters    =     1.9996
------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles
```

fvalues 10526.821 3157.1929 20000.330 19995.037

fvalues 10526.821 3157.1929 19995.002 19995.037

CGMAT cycle number = 59

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5976536 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.8
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.3
Product of X_ray and Geom posit. gradients -0.696E+06
Cosine of angle between them -0.998
Product of X_ray and Geom B-fact gradients -0.398E+06
Cosine of angle between them -0.994

Residuals: XRAY= 0.1681E+05 GEOM= 3158. TOTAL= 0.1997E+05
function value 19972.252

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.679	1.966
Torsion angles, period 1. refined	155	7.877	5.000
Torsion angles, period 2. refined	54	41.421	25.741
Torsion angles, period 3. refined	214	19.245	15.000
Torsion angles, period 4. refined	3	21.368	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	539	0.265	0.200
VDW; torsion: refined_atoms	788	0.325	0.200
HBOND: refined_atoms	42	0.191	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.266	0.200
Bond B values: refined atoms	1229	13.512	4.717
Angle B values: refined atoms	1663	16.607	7.128
Torsion B values: refined atoms	426	30.745	13.071
Long range B values: refined atoms	1334	11.634	15.327

Overall : scale = 1.012, B = -0.026
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 59. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 59. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 59. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 59. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004	30	62.50	754.4	747.8	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	414.1	416.2	0.02	0.02	1	1228.6	1223.4	0.01	0.01	
0.017	83	95.60	307.7	308.7	0.03	0.02	4	403.0	413.5	0.04	0.05	
0.023	97	97.14	247.4	248.4	0.02	0.02	5	180.2	188.5	0.07	0.07	
0.029	108	100.00	241.3	242.0	0.02	0.02	7	186.7	189.3	0.06	0.06	
0.036	126	99.25	270.4	270.7	0.02	0.02	6	252.9	253.8	0.04	0.04	
0.042	129	98.56	286.3	287.5	0.02	0.02	8	338.1	341.4	0.02	0.02	
0.048	150	98.73	296.7	296.4	0.02	0.01	5	305.8	306.9	0.03	0.03	
0.055	151	99.38	281.3	281.5	0.01	0.02	10	257.9	260.1	0.04	0.04	
0.061	172	100.00	218.4	218.6	0.02	0.02	10	202.2	202.5	0.03	0.03	
0.067	174	99.45	211.5	210.9	0.02	0.02	6	286.3	284.4	0.02	0.02	
0.074	178	98.92	206.1	206.7	0.02	0.02	6	234.5	236.8	0.03	0.03	
0.080	189	100.00	208.7	209.0	0.02	0.02	13	159.6	155.7	0.06	0.06	
0.086	197	100.00	176.8	176.9	0.02	0.02	8	208.5	207.6	0.04	0.04	
0.093	193	93.55	156.9	157.0	0.02	0.02	10	182.0	186.0	0.07	0.06	
0.099	188	91.28	160.7	159.8	0.02	0.02	11	159.6	157.2	0.02	0.02	
0.105	190	86.02	153.8	153.5	0.02	0.02	13	169.2	170.2	0.05	0.04	
0.112	183	80.08	129.9	129.6	0.02	0.02	6	135.2	140.4	0.08	0.08	
0.118	194	81.85	127.0	126.7	0.02	0.02	9	138.0	137.4	0.05	0.05	
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	111.2	0.07	0.06	

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 59. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 59. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.990	12	0.923	95	0.982	0.999

```
 0.0228   97  0.988   11  1.000  108  0.990  0.999
 0.0292  108  0.997    6  1.000  114  0.997  0.999
 0.0355  126  0.996   17  1.000  143  0.996  0.999
 0.0418  129  0.997   11  1.000  140  0.997  0.999
 0.0482  150  0.991   12  1.000  162  0.992  0.999
 0.0545  151  0.997   12  0.992  163  0.997  0.999
 0.0609  172  0.983   15  0.955  187  0.981  0.999
 0.0672  174  0.993    9  0.937  183  0.990  0.999
 0.0735  178  0.990   11  1.000  189  0.990  0.999
 0.0799  189  0.989   14  0.999  203  0.990  0.999
 0.0862  197  0.983    9  0.974  206  0.983  0.999
 0.0925  193  0.978   14  0.930  207  0.975  0.999
 0.0989  188  0.980   12  1.000  200  0.981  0.999
 0.1052  190  0.988    8  1.000  198  0.989  0.999
 0.1116  183  0.980   13  0.938  196  0.977  1.000
 0.1179  194  0.980   11  0.940  205  0.978  1.000
 0.1242  174  0.983    8  1.000  182  0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0192
Free R factor                    =     0.0404
Overall weighted R factor        =     0.0193
Free weighted R factor           =     0.0408
Overall correlation coefficient  =     0.9993
Free correlation coefficient     =     0.9968
DPI based on free R factor       =     0.0734
Overall figure of merit          =     0.9868
ML based su of positional parameters =     0.0405
ML based su of thermal parameters    =     1.9985
--------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10524.740       3158.1543       19983.664       19973.043

 fvalues    10524.740       3158.1543       19973.672       19973.043


    CGMAT cycle number =     60

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :   50   90   60
 Maximuum H,K,L                 :   12   21   14
 Minimum acceptable grid spacing:   33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
```

Weight matrix 0.60000002
Actual weight 1.5971302 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.8
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.3
Product of X_ray and Geom posit. gradients -0.695E+06
Cosine of angle between them -0.998
Product of X_ray and Geom B-fact gradients -0.398E+06
Cosine of angle between them -0.994

Residuals: XRAY= 0.1681E+05 GEOM= 3158. TOTAL= 0.1997E+05
function value 19966.193

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.679	1.966
Torsion angles, period 1. refined	155	7.877	5.000
Torsion angles, period 2. refined	54	41.422	25.741
Torsion angles, period 3. refined	214	19.220	15.000
Torsion angles, period 4. refined	3	21.368	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	539	0.265	0.200
VDW; torsion: refined_atoms	788	0.325	0.200
HBOND: refined_atoms	42	0.191	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.266	0.200
Bond B values: refined atoms	1229	13.516	4.717
Angle B values: refined atoms	1663	16.612	7.128
Torsion B values: refined atoms	426	30.756	13.071
Long range B values: refined atoms	1334	11.637	15.327

Overall : scale = 1.012, B = -0.026
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 60. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 60. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 60. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 60. % observed v. resln :N:1,3:

$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 747.8 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.2 0.02 0.02 1 1228.6 1223.3 0.01 0.01
0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.0 413.5 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.5 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.3 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 253.8 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.4 0.02 0.02
0.048 150 98.73 296.7 296.4 0.02 0.01 5 305.8 306.9 0.03 0.03
0.055 151 99.38 281.3 281.5 0.01 0.02 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.5 0.03 0.03
0.067 174 99.45 211.5 210.9 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.5 236.8 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.6 155.7 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.5 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.0 0.07 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.6 157.2 0.02 0.02
0.105 190 86.02 153.8 153.5 0.02 0.02 13 169.2 170.2 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 140.4 0.08 0.08
0.118 194 81.85 127.0 126.7 0.02 0.02 9 138.0 137.4 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.2 0.07 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 60. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 60. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.990 12 0.923 95 0.982 0.999
0.0228 97 0.988 11 1.000 108 0.990 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.996 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.992 0.999
0.0545 151 0.997 12 0.992 163 0.997 0.999
0.0609 172 0.983 15 0.955 187 0.981 0.999
0.0672 174 0.993 9 0.937 183 0.990 0.999
0.0735 178 0.990 11 1.000 189 0.990 0.999
0.0799 189 0.989 14 0.999 203 0.990 0.999
0.0862 197 0.983 9 0.974 206 0.983 0.999
0.0925 193 0.978 14 0.930 207 0.975 0.999
0.0989 188 0.980 12 1.000 200 0.981 0.999
0.1052 190 0.988 8 1.000 198 0.989 0.999
0.1116 183 0.980 13 0.938 196 0.977 1.000

```
 0.1179   194   0.980    11   0.940   205   0.978  1.000
 0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0192
Free R factor                    =     0.0404
Overall weighted R factor        =     0.0193
Free weighted R factor           =     0.0408
Overall correlation coefficient  =     0.9993
Free correlation coefficient     =     0.9968
DPI based on free R factor       =     0.0734
Overall figure of merit          =     0.9868
ML based su of positional parameters =     0.0405
ML based su of thermal parameters    =     1.9979
---------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10524.569       3157.9031       19966.527       19967.010


    CGMAT cycle number =     61

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    1.5951693      is applied to the X-ray term
Norm of X_ray positional gradient              13.7
Norm of Geom. positional gradient              13.7
Norm of X_ray B-factor gradient                17.8
Norm of Geom. B-factor gradient                18.2
Product of X_ray and Geom posit. gradients     -0.695E+06
 Cosine of angle between them                  -1.000
Product of X_ray and Geom B-fact gradients     -0.398E+06
 Cosine of angle between them                  -0.994


Residuals: XRAY=     0.1678E+05 GEOM=      3158.     TOTAL=     0.1994E+05
 function value    19942.641

---------------------------------------------------------------------------
          Restraint type            N restraints   Rms Delta    Av(Sigma)
```

Bond distances: refined atoms 1229 0.011 0.020
Bond angles : refined atoms 1663 1.683 1.966
Torsion angles, period 1. refined 155 7.877 5.000
Torsion angles, period 2. refined 54 41.423 25.741
Torsion angles, period 3. refined 214 19.231 15.000
Torsion angles, period 4. refined 3 21.370 15.000
Chiral centres: refined atoms 187 0.111 0.200
Planar groups: refined atoms 924 0.005 0.021
VDW repulsions: refined_atoms 539 0.265 0.200
VDW; torsion: refined_atoms 788 0.325 0.200
HBOND: refined_atoms 42 0.191 0.200
VDW repulsions: symmetry: refined_atoms 55 0.262 0.200
HBOND: symmetry: refined_atoms 3 0.266 0.200
Bond B values: refined atoms 1229 13.531 4.718
Angle B values: refined atoms 1663 16.628 7.128
Torsion B values: refined atoms 426 30.789 13.072
Long range B values: refined atoms 1334 11.647 15.326

Overall : scale = 1.012, B = -0.026
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 61. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 61. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 61. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 61. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 747.8 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.2 0.02 0.02 1 1228.6 1223.4 0.01 0.01
0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.0 413.5 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.5 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.3 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 253.8 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.4 0.02 0.02
0.048 150 98.73 296.7 296.4 0.02 0.01 5 305.8 307.0 0.03 0.03
0.055 151 99.38 281.3 281.5 0.01 0.02 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.6 0.03 0.03
0.067 174 99.45 211.5 210.9 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.5 236.8 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 155.7 0.06 0.06

0.086	197	100.00	176.8	176.9	0.02	0.02	8	208.5	207.6	0.04	0.04
0.093	193	93.55	156.9	157.0	0.02	0.02	10	182.0	186.1	0.07	0.06
0.099	188	91.28	160.7	159.8	0.02	0.02	11	159.7	157.2	0.02	0.02
0.105	190	86.02	153.9	153.5	0.02	0.02	13	169.2	170.2	0.05	0.04
0.112	183	80.08	129.9	129.6	0.02	0.02	6	135.2	140.4	0.08	0.08
0.118	194	81.85	127.0	126.7	0.02	0.02	9	138.0	137.3	0.05	0.05
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	111.2	0.07	0.06

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 61. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 61. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.990	12	0.923	95	0.982	0.999
0.0228	97	0.988	11	1.000	108	0.990	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.996	17	1.000	143	0.996	0.999
0.0418	129	0.997	11	1.000	140	0.997	0.999
0.0482	150	0.991	12	1.000	162	0.992	0.999
0.0545	151	0.997	12	0.992	163	0.997	0.999
0.0609	172	0.983	15	0.955	187	0.981	0.999
0.0672	174	0.993	9	0.936	183	0.990	0.999
0.0735	178	0.990	11	1.000	189	0.990	0.999
0.0799	189	0.989	14	0.999	203	0.990	0.999
0.0862	197	0.983	9	0.974	206	0.983	0.999
0.0925	193	0.978	14	0.930	207	0.975	0.999
0.0989	188	0.980	12	1.000	200	0.981	0.999
0.1052	190	0.988	8	1.000	198	0.989	0.999
0.1116	183	0.980	13	0.938	196	0.977	1.000
0.1179	194	0.980	11	0.939	205	0.978	1.000
0.1242	174	0.983	8	1.000	182	0.984	1.000

$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0192
Free R factor = 0.0404
Overall weighted R factor = 0.0192
Free weighted R factor = 0.0408
Overall correlation coefficient = 0.9993
Free correlation coefficient = 0.9968
DPI based on free R factor = 0.0733
Overall figure of merit = 0.9868
ML based su of positional parameters = 0.0405
ML based su of thermal parameters = 1.9968

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10522.585 3158.1025 19944.621 19943.406

fvalues 10522.585 3158.1025 19943.377 19943.406

CGMAT cycle number = 62

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5942730 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.695E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.398E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1677E+05 GEOM= 3158. TOTAL= 0.1993E+05
function value 19932.039

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.682	1.966
Torsion angles, period 1. refined	155	7.876	5.000
Torsion angles, period 2. refined	54	41.424	25.741
Torsion angles, period 3. refined	214	19.214	15.000
Torsion angles, period 4. refined	3	21.367	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	539	0.265	0.200
VDW; torsion: refined_atoms	788	0.325	0.200
HBOND: refined_atoms	42	0.191	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.266	0.200
Bond B values: refined atoms	1229	13.538	4.718
Angle B values: refined atoms	1663	16.636	7.128

Torsion B values: refined atoms 426 30.806 13.073
Long range B values: refined atoms 1334 11.652 15.326

Overall : scale = 1.012, B = -0.026
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 62. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 62. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 62. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 62. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 747.8 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.2 0.02 0.02 1 1228.6 1223.4 0.01 0.01
0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.0 413.5 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.5 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.3 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 253.8 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.4 0.02 0.02
0.048 150 98.73 296.7 296.4 0.02 0.01 5 305.8 307.0 0.03 0.03
0.055 151 99.38 281.3 281.5 0.01 0.02 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.6 0.03 0.03
0.067 174 99.45 211.5 210.9 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.5 236.8 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.6 155.7 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.5 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.1 0.07 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.6 157.2 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.2 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 140.4 0.08 0.08
0.118 194 81.85 127.0 126.7 0.02 0.02 9 138.0 137.3 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.2 0.07 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 62. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 62. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$

$$
 0.0038 30 0.999 4 1.000 34 0.999 0.999
 0.0102 62 0.999 7 1.000 69 0.999 0.999
 0.0165 83 0.990 12 0.924 95 0.982 0.999
 0.0228 97 0.988 11 1.000 108 0.990 0.999
 0.0292 108 0.997 6 1.000 114 0.997 0.999
 0.0355 126 0.996 17 1.000 143 0.996 0.999
 0.0418 129 0.997 11 1.000 140 0.997 0.999
 0.0482 150 0.991 12 1.000 162 0.992 0.999
 0.0545 151 0.997 12 0.992 163 0.997 0.999
 0.0609 172 0.983 15 0.955 187 0.981 0.999
 0.0672 174 0.993 9 0.936 183 0.990 0.999
 0.0735 178 0.990 11 1.000 189 0.990 0.999
 0.0799 189 0.989 14 0.999 203 0.990 0.999
 0.0862 197 0.983 9 0.974 206 0.983 0.999
 0.0925 193 0.978 14 0.930 207 0.975 0.999
 0.0989 188 0.980 12 1.000 200 0.981 0.999
 0.1052 190 0.988 8 1.000 198 0.989 0.999
 0.1116 183 0.980 13 0.938 196 0.977 1.000
 0.1179 194 0.980 11 0.939 205 0.978 1.000
 0.1242 174 0.983 8 1.000 182 0.984 1.000
$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0192
Free R factor = 0.0404
Overall weighted R factor = 0.0192
Free weighted R factor = 0.0407
Overall correlation coefficient = 0.9993
Free correlation coefficient = 0.9968
DPI based on free R factor = 0.0733
Overall figure of merit = 0.9868
ML based su of positional parameters = 0.0405
ML based su of thermal parameters = 1.9962

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10521.729 3158.3279 19934.746 19932.836

fvalues 10521.729 3158.3279 19932.793 19932.836

CGMAT cycle number = 63

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14

Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5917969 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.695E+06
Cosine of angle between them -0.999
Product of X_ray and Geom B-fact gradients -0.398E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1674E+05 GEOM= 3159. TOTAL= 0.1990E+05
function value 19903.125

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.681	1.966
Torsion angles, period 1. refined	155	7.876	5.000
Torsion angles, period 2. refined	54	41.425	25.741
Torsion angles, period 3. refined	214	19.241	15.000
Torsion angles, period 4. refined	3	21.366	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	539	0.265	0.200
VDW; torsion: refined_atoms	788	0.325	0.200
HBOND: refined_atoms	42	0.191	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.266	0.200
Bond B values: refined atoms	1229	13.543	4.719
Angle B values: refined atoms	1663	16.643	7.128
Torsion B values: refined atoms	426	30.820	13.074
Long range B values: refined atoms	1334	11.655	15.326

Overall : scale = 1.012, B = -0.026
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 63. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 63. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 63. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 63. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 747.8 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.2 0.02 0.02 1 1228.6 1223.5 0.01 0.01
0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.0 413.5 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.5 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.3 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 253.8 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.3 0.02 0.02
0.048 150 98.73 296.7 296.4 0.02 0.01 5 305.8 307.0 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.02 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.6 0.03 0.03
0.067 174 99.45 211.5 210.9 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.5 236.8 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 155.7 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.5 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.1 0.07 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.2 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.2 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 140.5 0.08 0.08
0.118 194 81.85 127.0 126.7 0.02 0.02 9 138.0 137.3 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.2 0.07 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 63. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 63. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.990 12 0.924 95 0.982 0.999
0.0228 97 0.988 11 1.000 108 0.990 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.996 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.992 0.999
0.0545 151 0.997 12 0.992 163 0.997 0.999
0.0609 172 0.983 15 0.955 187 0.981 0.999
0.0672 174 0.993 9 0.936 183 0.990 0.999
0.0735 178 0.990 11 1.000 189 0.990 0.999
0.0799 189 0.989 14 0.999 203 0.990 0.999
0.0862 197 0.983 9 0.974 206 0.983 0.999

```
 0.0925   193   0.979    14   0.930   207   0.975  0.999
 0.0989   188   0.980    12   1.000   200   0.981  0.999
 0.1052   190   0.988     8   1.000   198   0.989  0.999
 0.1116   183   0.980    13   0.938   196   0.978  1.000
 0.1179   194   0.980    11   0.939   205   0.978  1.000
 0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0192
Free R factor                    =     0.0403
Overall weighted R factor        =     0.0192
Free weighted R factor           =     0.0407
Overall correlation coefficient  =     0.9993
Free correlation coefficient     =     0.9968
DPI based on free R factor       =     0.0733
Overall figure of merit          =     0.9868
ML based su of positional parameters =     0.0404
ML based su of thermal parameters    =     1.9947
 ---------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10519.602       3158.8455       19907.695       19903.914

 fvalues    10519.602       3158.8455       19904.025       19903.914


    CGMAT cycle number =     64

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    1.5918106      is applied to the X-ray term
Norm of X_ray positional gradient              13.7
Norm of Geom. positional gradient              13.7
Norm of X_ray B-factor gradient                17.8
Norm of Geom. B-factor gradient                18.2
Product of X_ray and Geom posit. gradients     -0.695E+06
 Cosine of angle between them                  -0.999
Product of X_ray and Geom B-fact gradients     -0.398E+06
 Cosine of angle between them                  -0.995
```

Residuals: XRAY= 0.1674E+05 GEOM= 3159. TOTAL= 0.1990E+05
function value 19902.924

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.681	1.966
Torsion angles, period 1. refined	155	7.876	5.000
Torsion angles, period 2. refined	54	41.426	25.741
Torsion angles, period 3. refined	214	19.224	15.000
Torsion angles, period 4. refined	3	21.366	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	539	0.265	0.200
VDW; torsion: refined_atoms	788	0.325	0.200
HBOND: refined_atoms	42	0.191	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.266	0.200
Bond B values: refined atoms	1229	13.544	4.719
Angle B values: refined atoms	1663	16.644	7.128
Torsion B values: refined atoms	426	30.823	13.074
Long range B values: refined atoms	1334	11.656	15.326

Overall : scale = 1.012, B = -0.026
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 64. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 64. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 64. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 64. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$

0.004	30	62.50	754.4	747.8	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	414.1	416.2	0.02	0.02	1	1228.6	1223.5	0.01	0.01	
0.017	83	95.60	307.7	308.7	0.03	0.02	4	403.0	413.5	0.04	0.05	
0.023	97	97.14	247.4	248.4	0.02	0.02	5	180.2	188.5	0.07	0.07	
0.029	108	100.00	241.3	242.0	0.02	0.02	7	186.7	189.3	0.06	0.06	
0.036	126	99.25	270.4	270.7	0.02	0.02	6	252.9	253.8	0.04	0.04	
0.042	129	98.56	286.3	287.5	0.02	0.02	8	338.1	341.3	0.02	0.02	

```
 0.048    150  98.73   296.7   296.4  0.02  0.01      5   305.8   307.0  0.03  0.02
 0.055    151  99.38   281.3   281.5  0.01  0.02     10   257.9   260.1  0.04  0.04
 0.061    172 100.00   218.4   218.6  0.02  0.02     10   202.2   202.6  0.03  0.03
 0.067    174  99.45   211.5   210.9  0.02  0.02      6   286.3   284.4  0.02  0.02
 0.074    178  98.92   206.1   206.7  0.02  0.02      6   234.5   236.8  0.03  0.03
 0.080    189 100.00   208.7   209.0  0.02  0.02     13   159.7   155.7  0.06  0.06
 0.086    197 100.00   176.8   176.9  0.02  0.02      8   208.5   207.6  0.04  0.04
 0.093    193  93.55   156.9   157.0  0.02  0.02     10   182.0   186.1  0.07  0.06
 0.099    188  91.28   160.7   159.8  0.02  0.02     11   159.7   157.2  0.02  0.02
 0.105    190  86.02   153.9   153.5  0.02  0.02     13   169.2   170.2  0.05  0.04
 0.112    183  80.08   129.9   129.6  0.02  0.02      6   135.2   140.5  0.08  0.08
 0.118    194  81.85   127.0   126.7  0.02  0.02      9   138.0   137.3  0.05  0.05
 0.124    174  73.20   129.0   128.9  0.02  0.02      9   113.8   111.1  0.07  0.06
$$
```

**** Fom and SigmaA vs resolution ****

```
$TABLE: Cycle   64. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle   64. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa  FOMa  NREFc FOMc NREFall FOMall  SigmaA_Fc1 $$
$$
 0.0038    30   0.999     4   1.000    34   0.999  0.999
 0.0102    62   0.999     7   1.000    69   0.999  0.999
 0.0165    83   0.990    12   0.924    95   0.982  0.999
 0.0228    97   0.988    11   1.000   108   0.990  0.999
 0.0292   108   0.997     6   1.000   114   0.997  0.999
 0.0355   126   0.996    17   1.000   143   0.996  0.999
 0.0418   129   0.997    11   1.000   140   0.997  0.999
 0.0482   150   0.991    12   1.000   162   0.992  0.999
 0.0545   151   0.997    12   0.992   163   0.997  0.999
 0.0609   172   0.983    15   0.955   187   0.981  0.999
 0.0672   174   0.993     9   0.936   183   0.990  0.999
 0.0735   178   0.990    11   1.000   189   0.990  0.999
 0.0799   189   0.989    14   0.999   203   0.990  0.999
 0.0862   197   0.983     9   0.974   206   0.983  0.999
 0.0925   193   0.979    14   0.930   207   0.975  0.999
 0.0989   188   0.980    12   1.000   200   0.981  0.999
 0.1052   190   0.988     8   1.000   198   0.989  0.999
 0.1116   183   0.980    13   0.938   196   0.978  1.000
 0.1179   194   0.980    11   0.939   205   0.978  1.000
 0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0192
Free R factor                    =     0.0403
Overall weighted R factor        =     0.0192
Free weighted R factor           =     0.0407
```

Overall correlation coefficient = 0.9993
Free correlation coefficient = 0.9968
DPI based on free R factor = 0.0733
Overall figure of merit = 0.9868
ML based su of positional parameters = 0.0404
ML based su of thermal parameters = 1.9948

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10519.460 3158.7095 19903.516 19903.697

CGMAT cycle number = 65

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5909051 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.695E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.397E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1673E+05 GEOM= 3159. TOTAL= 0.1989E+05
function value 19892.135

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.683	1.966
Torsion angles, period 1. refined	155	7.876	5.000
Torsion angles, period 2. refined	54	41.428	25.741
Torsion angles, period 3. refined	214	19.233	15.000
Torsion angles, period 4. refined	3	21.367	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	539	0.265	0.200
VDW; torsion: refined_atoms	788	0.325	0.200
HBOND: refined_atoms	42	0.191	0.200

VDW repulsions: symmetry: refined_atoms 55 0.262 0.200
HBOND: symmetry: refined_atoms 3 0.265 0.200
Bond B values: refined atoms 1229 13.550 4.719
Angle B values: refined atoms 1663 16.653 7.129
Torsion B values: refined atoms 426 30.843 13.075
Long range B values: refined atoms 1334 11.662 15.326

Overall : scale = 1.012, B = -0.026
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 65. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 65. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 65. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 65. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 747.8 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.2 0.02 0.02 1 1228.6 1223.6 0.01 0.01
0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.0 413.5 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.6 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.3 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 253.8 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.3 0.02 0.02
0.048 150 98.73 296.7 296.4 0.02 0.01 5 305.8 307.0 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.02 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.6 0.03 0.03
0.067 174 99.45 211.5 210.9 0.02 0.02 6 286.3 284.3 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.6 236.9 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 155.7 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.5 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.1 0.07 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.2 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.2 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 140.5 0.08 0.08
0.118 194 81.85 127.0 126.7 0.02 0.02 9 138.0 137.3 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.2 0.07 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 65. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 65. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.990 12 0.924 95 0.982 0.999
0.0228 97 0.988 11 1.000 108 0.990 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.996 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.992 0.999
0.0545 151 0.997 12 0.992 163 0.997 0.999
0.0609 172 0.983 15 0.955 187 0.981 0.999
0.0672 174 0.993 9 0.936 183 0.990 0.999
0.0735 178 0.990 11 1.000 189 0.990 0.999
0.0799 189 0.989 14 0.999 203 0.990 0.999
0.0862 197 0.983 9 0.974 206 0.983 0.999
0.0925 193 0.979 14 0.930 207 0.975 0.999
0.0989 188 0.980 12 1.000 200 0.981 0.999
0.1052 190 0.988 8 1.000 198 0.989 0.999
0.1116 183 0.980 13 0.938 196 0.978 1.000
0.1179 194 0.980 11 0.939 205 0.978 1.000
0.1242 174 0.983 8 1.000 182 0.984 1.000
$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0192
Free R factor = 0.0403
Overall weighted R factor = 0.0192
Free weighted R factor = 0.0407
Overall correlation coefficient = 0.9993
Free correlation coefficient = 0.9968
DPI based on free R factor = 0.0732
Overall figure of merit = 0.9868
ML based su of positional parameters = 0.0404
ML based su of thermal parameters = 1.9942

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10518.464 3159.0776 19893.229 19892.955

fvalues 10518.464 3159.0776 19892.813 19892.955

CGMAT cycle number = 66

```
 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    1.5894438      is applied to the X-ray term
Norm of X_ray positional gradient              13.7
Norm of Geom. positional gradient              13.7
Norm of X_ray B-factor gradient                17.8
Norm of Geom. B-factor gradient                18.2
Product of X_ray and Geom posit. gradients     -0.695E+06
 Cosine of angle between them                  -1.000
Product of X_ray and Geom B-fact gradients     -0.397E+06
 Cosine of angle between them                  -0.995


Residuals: XRAY=     0.1672E+05 GEOM=      3159.     TOTAL=     0.1987E+05
 function value    19874.885

------------------------------------------------------------------------------
          Restraint type            N restraints   Rms Delta   Av(Sigma)
Bond distances: refined atoms               1229     0.011     0.020
Bond angles  : refined atoms                1663     1.683     1.966
Torsion angles, period  1. refined           155     7.875     5.000
Torsion angles, period  2. refined            54    41.428    25.741
Torsion angles, period  3. refined           214    19.220    15.000
Torsion angles, period  4. refined             3    21.368    15.000
Chiral centres: refined atoms               187     0.111     0.200
Planar groups: refined atoms                924     0.005     0.021
VDW repulsions: refined_atoms               539     0.265     0.200
VDW; torsion: refined_atoms                 788     0.325     0.200
HBOND: refined_atoms                         42     0.191     0.200
VDW repulsions: symmetry: refined_atoms      55     0.262     0.200
HBOND: symmetry: refined_atoms                3     0.265     0.200
Bond B values: refined atoms                1229    13.553     4.719
Angle B values: refined atoms               1663    16.658     7.129
Torsion B values: refined atoms              426    30.856    13.076
Long range B values: refined atoms          1334    11.663    15.326
------------------------------------------------------------------------------

------------------------------------------------------------------------------
Overall              : scale =    1.012, B  =  -0.026
Overall anisotropic scale factors
   B11 =  0.28 B22 =  0.17 B33 = -0.47 B12 =  0.00 B13 = -0.36 B23 =  0.00
------------------------------------------------------------------------------

------------------------------------------------------------------------------
```

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 66. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 66. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 66. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 66. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 747.8 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.2 0.02 0.02 1 1228.6 1223.6 0.01 0.01
0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.0 413.5 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.6 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.3 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 253.8 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.3 0.02 0.02
0.048 150 98.73 296.7 296.4 0.02 0.01 5 305.8 307.0 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.02 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.6 0.03 0.03
0.067 174 99.45 211.5 210.9 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.6 236.9 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 155.7 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.5 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.1 0.07 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.2 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.2 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 140.6 0.08 0.08
0.118 194 81.85 127.0 126.7 0.02 0.02 9 138.0 137.3 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.1 0.07 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 66. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 66. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.990 12 0.924 95 0.982 0.999
0.0228 97 0.988 11 1.000 108 0.990 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.996 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.992 0.999
0.0545 151 0.997 12 0.992 163 0.997 0.999
0.0609 172 0.983 15 0.955 187 0.981 0.999

```
 0.0672   174   0.993    9   0.936   183   0.990  0.999
 0.0735   178   0.990   11   1.000   189   0.990  0.999
 0.0799   189   0.989   14   0.999   203   0.990  0.999
 0.0862   197   0.983    9   0.974   206   0.983  0.999
 0.0925   193   0.979   14   0.930   207   0.975  0.999
 0.0989   188   0.980   12   1.000   200   0.981  0.999
 0.1052   190   0.988    8   1.000   198   0.989  0.999
 0.1116   183   0.980   13   0.938   196   0.978  1.000
 0.1179   194   0.980   11   0.939   205   0.978  1.000
 0.1242   174   0.983    8   1.000   182   0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0192
Free R factor                    =     0.0403
Overall weighted R factor        =     0.0192
Free weighted R factor           =     0.0407
Overall correlation coefficient  =     0.9993
Free correlation coefficient     =     0.9968
DPI based on free R factor       =     0.0732
Overall figure of merit          =     0.9868
ML based su of positional parameters =     0.0404
ML based su of thermal parameters    =     1.9934
-------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10517.164       3159.2637       19876.525       19875.705

 fvalues    10517.164       3159.2637       19875.555       19875.705


    CGMAT cycle number =     67

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000008
 Actual weight    1.5886469      is applied to the X-ray term
Norm of X_ray positional gradient              13.7
Norm of Geom. positional gradient              13.7
Norm of X_ray B-factor gradient                17.8
Norm of Geom. B-factor gradient                18.2
Product of X_ray and Geom posit. gradients     -0.695E+06
```

Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.397E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1671E+05 GEOM= 3160. TOTAL= 0.1987E+05
function value 19865.359

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.682	1.966
Torsion angles, period 1. refined	155	7.875	5.000
Torsion angles, period 2. refined	54	41.428	25.741
Torsion angles, period 3. refined	214	19.240	15.000
Torsion angles, period 4. refined	3	21.368	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	539	0.265	0.200
VDW; torsion: refined_atoms	788	0.325	0.200
HBOND: refined_atoms	42	0.191	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.265	0.200
Bond B values: refined atoms	1229	13.555	4.719
Angle B values: refined atoms	1663	16.663	7.129
Torsion B values: refined atoms	426	30.866	13.076
Long range B values: refined atoms	1334	11.667	15.325

Overall : scale = 1.012, B = -0.026
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 67. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 67. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 67. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 67. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$

0.004	30	62.50	754.4	747.9	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	414.1	416.2	0.02	0.02	1	1228.6	1223.7	0.01	0.01	
0.017	83	95.60	307.7	308.7	0.03	0.02	4	403.0	413.5	0.04	0.05	

```
 0.023     97  97.14   247.4   248.4  0.02  0.02       5   180.2   188.6  0.07  0.07
 0.029    108 100.00   241.3   242.0  0.02  0.02       7   186.7   189.3  0.06  0.06
 0.036    126  99.25   270.4   270.7  0.02  0.02       6   252.9   253.8  0.04  0.04
 0.042    129  98.56   286.3   287.5  0.02  0.02       8   338.1   341.3  0.02  0.02
 0.048    150  98.73   296.7   296.4  0.02  0.01       5   305.8   307.0  0.03  0.02
 0.055    151  99.38   281.3   281.5  0.01  0.02      10   257.9   260.1  0.04  0.04
 0.061    172 100.00   218.4   218.6  0.02  0.02      10   202.2   202.6  0.03  0.03
 0.067    174  99.45   211.5   210.9  0.02  0.02       6   286.3   284.4  0.02  0.02
 0.074    178  98.92   206.1   206.7  0.02  0.02       6   234.6   236.9  0.03  0.03
 0.080    189 100.00   208.7   209.0  0.02  0.02      13   159.7   155.7  0.06  0.06
 0.086    197 100.00   176.8   176.9  0.02  0.02       8   208.5   207.6  0.04  0.04
 0.093    193  93.55   156.9   157.0  0.02  0.02      10   182.0   186.1  0.07  0.06
 0.099    188  91.28   160.7   159.8  0.02  0.02      11   159.7   157.2  0.02  0.02
 0.105    190  86.02   153.9   153.5  0.02  0.02      13   169.2   170.2  0.05  0.04
 0.112    183  80.08   129.9   129.6  0.02  0.02       6   135.2   140.6  0.08  0.08
 0.118    194  81.85   127.0   126.7  0.02  0.02       9   138.0   137.3  0.05  0.05
 0.124    174  73.20   129.0   128.9  0.02  0.02       9   113.8   111.1  0.07  0.06
$$
```

**** Fom and SigmaA vs resolution ****

```
$TABLE: Cycle   67. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle   67. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa  FOMa  NREFc FOMc NREFall FOMall  SigmaA_Fc1 $$
$$
 0.0038    30   0.999     4   1.000    34   0.999  0.999
 0.0102    62   0.999     7   1.000    69   0.999  0.999
 0.0165    83   0.990    12   0.924    95   0.982  0.999
 0.0228    97   0.988    11   1.000   108   0.990  0.999
 0.0292   108   0.997     6   1.000   114   0.997  0.999
 0.0355   126   0.996    17   1.000   143   0.996  0.999
 0.0418   129   0.997    11   1.000   140   0.997  0.999
 0.0482   150   0.991    12   1.000   162   0.992  0.999
 0.0545   151   0.997    12   0.993   163   0.997  0.999
 0.0609   172   0.983    15   0.955   187   0.981  0.999
 0.0672   174   0.993     9   0.935   183   0.990  0.999
 0.0735   178   0.990    11   1.000   189   0.990  0.999
 0.0799   189   0.989    14   0.999   203   0.990  0.999
 0.0862   197   0.983     9   0.974   206   0.983  0.999
 0.0925   193   0.979    14   0.930   207   0.975  0.999
 0.0989   188   0.980    12   1.000   200   0.981  0.999
 0.1052   190   0.988     8   1.000   198   0.989  0.999
 0.1116   183   0.980    13   0.938   196   0.978  1.000
 0.1179   194   0.980    11   0.940   205   0.978  1.000
 0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
```

Overall R factor = 0.0192
Free R factor = 0.0403
Overall weighted R factor = 0.0192
Free weighted R factor = 0.0407
Overall correlation coefficient = 0.9993
Free correlation coefficient = 0.9968
DPI based on free R factor = 0.0732
Overall figure of merit = 0.9868
ML based su of positional parameters = 0.0404
ML based su of thermal parameters = 1.9929

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10516.178 3159.6636 19868.072 19866.156

fvalues 10516.178 3159.6636 19866.359 19866.156

CGMAT cycle number = 68

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5875049 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.694E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.397E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1669E+05 GEOM= 3160. TOTAL= 0.1985E+05
function value 19852.094

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.682	1.966
Torsion angles, period 1. refined	155	7.875	5.000
Torsion angles, period 2. refined	54	41.429	25.741
Torsion angles, period 3. refined	214	19.228	15.000

Torsion angles, period 4. refined 3 21.368 15.000
Chiral centres: refined atoms 187 0.111 0.200
Planar groups: refined atoms 924 0.005 0.021
VDW repulsions: refined_atoms 539 0.265 0.200
VDW; torsion: refined_atoms 788 0.325 0.200
HBOND: refined_atoms 42 0.191 0.200
VDW repulsions: symmetry: refined_atoms 55 0.262 0.200
HBOND: symmetry: refined_atoms 3 0.264 0.200
Bond B values: refined atoms 1229 13.556 4.719
Angle B values: refined atoms 1663 16.665 7.129
Torsion B values: refined atoms 426 30.871 13.076
Long range B values: refined atoms 1334 11.668 15.325

Overall : scale = 1.012, B = -0.026
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 68. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 68. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 68. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 68. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 747.9 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.2 0.02 0.02 1 1228.6 1223.7 0.01 0.01
0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.0 413.5 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.6 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.3 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 253.8 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.3 0.02 0.02
0.048 150 98.73 296.7 296.4 0.02 0.01 5 305.8 307.0 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.02 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.6 0.03 0.03
0.067 174 99.45 211.5 210.9 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.6 236.9 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 155.7 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.5 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.1 0.07 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.2 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.2 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 140.6 0.08 0.08

```
 0.118    194  81.85   127.0   126.7  0.02  0.02       9   138.0   137.3  0.05  0.05
 0.124    174  73.20   129.0   128.9  0.02  0.02       9   113.8   111.1  0.07  0.06
$$

   ****                Fom and SigmaA vs resolution                ****

 $TABLE: Cycle   68. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
 $GRAPHS:Cycle   68. M(Fom) v. resln :N:1,3,5,7,8:
 $$
 <4SSQ/LL> NREFa  FOMa  NREFc FOMc NREFall FOMall  SigmaA_Fc1 $$
 $$
  0.0038    30   0.999     4   1.000    34   0.999  0.999
  0.0102    62   0.999     7   1.000    69   0.999  0.999
  0.0165    83   0.991    12   0.924    95   0.982  0.999
  0.0228    97   0.988    11   1.000   108   0.990  0.999
  0.0292   108   0.997     6   1.000   114   0.997  0.999
  0.0355   126   0.996    17   1.000   143   0.996  0.999
  0.0418   129   0.997    11   1.000   140   0.997  0.999
  0.0482   150   0.991    12   1.000   162   0.992  0.999
  0.0545   151   0.997    12   0.993   163   0.997  0.999
  0.0609   172   0.983    15   0.955   187   0.981  0.999
  0.0672   174   0.993     9   0.935   183   0.990  0.999
  0.0735   178   0.990    11   1.000   189   0.990  0.999
  0.0799   189   0.989    14   0.999   203   0.990  0.999
  0.0862   197   0.983     9   0.974   206   0.983  0.999
  0.0925   193   0.979    14   0.930   207   0.975  0.999
  0.0989   188   0.980    12   1.000   200   0.981  0.999
  0.1052   190   0.988     8   1.000   198   0.989  0.999
  0.1116   183   0.980    13   0.938   196   0.978  1.000
  0.1179   194   0.980    11   0.940   205   0.978  1.000
  0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
 Resolution limits                =     38.899     2.802
 Number of used reflections       =       3184
 Percentage observed              =    92.6870
 Percentage of free reflections   =     4.8416
 Overall R factor                 =     0.0192
 Free R factor                    =     0.0403
 Overall weighted R factor        =     0.0192
 Free weighted R factor           =     0.0407
 Overall correlation coefficient  =     0.9993
 Free correlation coefficient     =     0.9968
 DPI based on free R factor       =     0.0731
 Overall figure of merit          =     0.9868
 ML based su of positional parameters =     0.0404
 ML based su of thermal parameters    =     1.9921
 ------------------------------------------------------------------------
  Trying gamma equal    0.0000000
  Convergence reached with no gamma cycles
```

fvalues 10515.440 3159.6111 19852.791 19852.924

CGMAT cycle number = 69

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5866987 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.694E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.397E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1668E+05 GEOM= 3160. TOTAL= 0.1984E+05
function value 19842.266

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.684	1.966
Torsion angles, period 1. refined	155	7.875	5.000
Torsion angles, period 2. refined	54	41.430	25.741
Torsion angles, period 3. refined	214	19.235	15.000
Torsion angles, period 4. refined	3	21.371	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	539	0.265	0.200
VDW; torsion: refined_atoms	788	0.325	0.200
HBOND: refined_atoms	42	0.191	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.263	0.200
Bond B values: refined atoms	1229	13.559	4.720
Angle B values: refined atoms	1663	16.672	7.129
Torsion B values: refined atoms	426	30.891	13.077
Long range B values: refined atoms	1334	11.670	15.324

Overall : scale = 1.012, B = -0.025
Overall anisotropic scale factors

B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 69. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 69. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 69. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 69. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$

0.004	30	62.50	754.4	747.9	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	414.1	416.2	0.02	0.02	1	1228.6	1223.8	0.01	0.01	
0.017	83	95.60	307.7	308.7	0.03	0.02	4	403.0	413.5	0.04	0.05	
0.023	97	97.14	247.4	248.4	0.02	0.02	5	180.2	188.6	0.07	0.07	
0.029	108	100.00	241.3	242.0	0.02	0.02	7	186.7	189.3	0.06	0.06	
0.036	126	99.25	270.4	270.7	0.02	0.02	6	252.9	253.9	0.04	0.04	
0.042	129	98.56	286.3	287.5	0.02	0.02	8	338.1	341.3	0.02	0.02	
0.048	150	98.73	296.7	296.4	0.02	0.01	5	305.8	307.0	0.03	0.02	
0.055	151	99.38	281.3	281.5	0.01	0.02	10	257.9	260.1	0.04	0.04	
0.061	172	100.00	218.4	218.6	0.02	0.02	10	202.2	202.6	0.03	0.03	
0.067	174	99.45	211.5	210.9	0.02	0.02	6	286.3	284.4	0.02	0.02	
0.074	178	98.92	206.1	206.7	0.02	0.02	6	234.6	236.9	0.03	0.03	
0.080	189	100.00	208.7	209.0	0.02	0.02	13	159.7	155.7	0.06	0.06	
0.086	197	100.00	176.8	176.9	0.02	0.02	8	208.5	207.6	0.04	0.04	
0.093	193	93.55	156.9	157.0	0.02	0.02	10	182.0	186.1	0.07	0.06	
0.099	188	91.28	160.7	159.8	0.02	0.02	11	159.7	157.1	0.02	0.02	
0.105	190	86.02	153.9	153.5	0.02	0.02	13	169.2	170.2	0.05	0.04	
0.112	183	80.08	129.9	129.6	0.02	0.02	6	135.2	140.6	0.08	0.08	
0.118	194	81.85	127.0	126.7	0.02	0.02	9	138.0	137.3	0.05	0.05	
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	111.1	0.07	0.06	

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 69. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 69. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.991	12	0.924	95	0.982	0.999
0.0228	97	0.988	11	1.000	108	0.990	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.996	17	1.000	143	0.996	0.999

```
 0.0418   129   0.997    11   1.000   140   0.997  0.999
 0.0482   150   0.991    12   1.000   162   0.992  0.999
 0.0545   151   0.997    12   0.993   163   0.997  0.999
 0.0609   172   0.983    15   0.955   187   0.981  0.999
 0.0672   174   0.993     9   0.935   183   0.990  0.999
 0.0735   178   0.990    11   1.000   189   0.990  0.999
 0.0799   189   0.989    14   0.999   203   0.990  0.999
 0.0862   197   0.983     9   0.974   206   0.983  0.999
 0.0925   193   0.979    14   0.930   207   0.975  0.999
 0.0989   188   0.980    12   1.000   200   0.981  0.999
 0.1052   190   0.988     8   1.000   198   0.989  0.999
 0.1116   183   0.980    13   0.938   196   0.978  1.000
 0.1179   194   0.980    11   0.940   205   0.978  1.000
 0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0192
Free R factor                    =     0.0403
Overall weighted R factor        =     0.0192
Free weighted R factor           =     0.0406
Overall correlation coefficient  =     0.9993
Free correlation coefficient     =     0.9968
DPI based on free R factor       =     0.0731
Overall figure of merit          =     0.9868
ML based su of positional parameters =     0.0404
ML based su of thermal parameters    =     1.9918
-------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10514.354       3159.9417       19843.215       19843.055

 fvalues    10514.354       3159.9417       19842.967       19843.055


    CGMAT cycle number =     70

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    1.5868512      is applied to the X-ray term
Norm of X_ray positional gradient              13.7
```

Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.694E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.397E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1668E+05 GEOM= 3160. TOTAL= 0.1984E+05
function value 19844.018

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.684	1.966
Torsion angles, period 1. refined	155	7.875	5.000
Torsion angles, period 2. refined	54	41.431	25.741
Torsion angles, period 3. refined	214	19.225	15.000
Torsion angles, period 4. refined	3	21.369	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	539	0.265	0.200
VDW; torsion: refined_atoms	788	0.325	0.200
HBOND: refined_atoms	42	0.191	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.263	0.200
Bond B values: refined atoms	1229	13.561	4.720
Angle B values: refined atoms	1663	16.677	7.129
Torsion B values: refined atoms	426	30.902	13.077
Long range B values: refined atoms	1334	11.673	15.324

Overall : scale = 1.012, B = -0.026
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 70. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 70. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 70. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 70. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$

$$
 0.004 30 62.50 754.4 747.9 0.02 0.02 0 0.0 0.0****** 0.00
 0.010 62 95.45 414.1 416.2 0.02 0.02 1 1228.6 1223.8 0.01 0.01
 0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.0 413.5 0.04 0.05
 0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.6 0.07 0.07
 0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.3 0.06 0.06
 0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 253.9 0.04 0.04
 0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.3 0.02 0.02
 0.048 150 98.73 296.7 296.4 0.02 0.01 5 305.8 307.0 0.03 0.02
 0.055 151 99.38 281.3 281.5 0.01 0.02 10 257.9 260.1 0.04 0.04
 0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.6 0.03 0.03
 0.067 174 99.45 211.5 210.9 0.02 0.02 6 286.3 284.3 0.02 0.02
 0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.6 236.9 0.03 0.03
 0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 155.7 0.06 0.06
 0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.5 207.6 0.04 0.04
 0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.1 0.07 0.06
 0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
 0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.2 0.05 0.04
 0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 140.7 0.08 0.08
 0.118 194 81.85 127.0 126.7 0.02 0.02 9 138.0 137.3 0.05 0.05
 0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.1 0.07 0.06
$$

 **** Fom and SigmaA vs resolution ****

 $TABLE: Cycle 70. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
 $GRAPHS:Cycle 70. M(Fom) v. resln :N:1,3,5,7,8:
 $$
 <4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
 $$
  0.0038 30 0.999 4 1.000 34 0.999 0.999
  0.0102 62 0.999 7 1.000 69 0.999 0.999
  0.0165 83 0.991 12 0.924 95 0.982 0.999
  0.0228 97 0.988 11 1.000 108 0.990 0.999
  0.0292 108 0.997 6 1.000 114 0.997 0.999
  0.0355 126 0.996 17 1.000 143 0.996 0.999
  0.0418 129 0.997 11 1.000 140 0.997 0.999
  0.0482 150 0.991 12 1.000 162 0.992 0.999
  0.0545 151 0.997 12 0.993 163 0.997 0.999
  0.0609 172 0.983 15 0.955 187 0.981 0.999
  0.0672 174 0.993 9 0.935 183 0.990 0.999
  0.0735 178 0.990 11 1.000 189 0.990 0.999
  0.0799 189 0.989 14 0.999 203 0.990 0.999
  0.0862 197 0.983 9 0.974 206 0.983 0.999
  0.0925 193 0.979 14 0.930 207 0.975 0.999
  0.0989 188 0.980 12 1.000 200 0.981 0.999
  0.1052 190 0.988 8 1.000 198 0.989 0.999
  0.1116 183 0.980 13 0.938 196 0.978 1.000
  0.1179 194 0.980 11 0.940 205 0.978 1.000
  0.1242 174 0.983 8 1.000 182 0.984 1.000
 $$

Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0192
Free R factor = 0.0403
Overall weighted R factor = 0.0192
Free weighted R factor = 0.0406
Overall correlation coefficient = 0.9994
Free correlation coefficient = 0.9968
DPI based on free R factor = 0.0731
Overall figure of merit = 0.9868
ML based su of positional parameters = 0.0404
ML based su of thermal parameters = 1.9918

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10514.388 3160.1050 19845.305 19844.875

fvalues 10514.388 3160.1050 19844.953 19844.875

CGMAT cycle number = 71

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5858252 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.694E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.397E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1667E+05 GEOM= 3160. TOTAL= 0.1983E+05
function value 19832.131

Restraint type N restraints Rms Delta Av(Sigma)
Bond distances: refined atoms 1229 0.011 0.020

Bond angles : refined atoms 1663 1.683 1.966
Torsion angles, period 1. refined 155 7.875 5.000
Torsion angles, period 2. refined 54 41.431 25.741
Torsion angles, period 3. refined 214 19.232 15.000
Torsion angles, period 4. refined 3 21.369 15.000
Chiral centres: refined atoms 187 0.111 0.200
Planar groups: refined atoms 924 0.005 0.021
VDW repulsions: refined_atoms 539 0.265 0.200
VDW; torsion: refined_atoms 788 0.325 0.200
HBOND: refined_atoms 42 0.191 0.200
VDW repulsions: symmetry: refined_atoms 55 0.262 0.200
HBOND: symmetry: refined_atoms 3 0.263 0.200
Bond B values: refined atoms 1229 13.563 4.720
Angle B values: refined atoms 1663 16.681 7.129
Torsion B values: refined atoms 426 30.910 13.078
Long range B values: refined atoms 1334 11.675 15.324

Overall : scale = 1.012, B = -0.026
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 71. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 71. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 71. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 71. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 747.9 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.2 0.02 0.02 1 1228.6 1223.8 0.01 0.01
0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.0 413.5 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.6 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.3 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 253.9 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.3 0.02 0.02
0.048 150 98.73 296.7 296.4 0.02 0.01 5 305.8 307.0 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.02 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.6 0.03 0.03
0.067 174 99.45 211.5 210.9 0.02 0.02 6 286.3 284.3 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.6 236.9 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 155.7 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04

0.093	193	93.55	156.9	157.0	0.02	0.02	10	182.0	186.1	0.07	0.06
0.099	188	91.28	160.7	159.8	0.02	0.02	11	159.7	157.1	0.02	0.02
0.105	190	86.02	153.9	153.5	0.02	0.02	13	169.2	170.1	0.05	0.04
0.112	183	80.08	129.9	129.6	0.02	0.02	6	135.2	140.7	0.08	0.08
0.118	194	81.85	127.0	126.7	0.02	0.02	9	138.0	137.3	0.05	0.05
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	111.1	0.07	0.06

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 71. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 71. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.991	12	0.924	95	0.982	0.999
0.0228	97	0.988	11	1.000	108	0.990	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.996	17	1.000	143	0.996	0.999
0.0418	129	0.997	11	1.000	140	0.997	0.999
0.0482	150	0.991	12	1.000	162	0.992	0.999
0.0545	151	0.997	12	0.993	163	0.997	0.999
0.0609	172	0.983	15	0.955	187	0.981	0.999
0.0672	174	0.993	9	0.935	183	0.990	0.999
0.0735	178	0.990	11	1.000	189	0.990	0.999
0.0799	189	0.989	14	0.999	203	0.990	0.999
0.0862	197	0.983	9	0.974	206	0.983	0.999
0.0925	193	0.979	14	0.930	207	0.975	0.999
0.0989	188	0.980	12	1.000	200	0.981	0.999
0.1052	190	0.988	8	1.000	198	0.989	0.999
0.1116	183	0.980	13	0.938	196	0.978	1.000
0.1179	194	0.980	11	0.940	205	0.978	1.000
0.1242	174	0.983	8	1.000	182	0.984	1.000

$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0192
Free R factor = 0.0402
Overall weighted R factor = 0.0192
Free weighted R factor = 0.0406
Overall correlation coefficient = 0.9993
Free correlation coefficient = 0.9968
DPI based on free R factor = 0.0731
Overall figure of merit = 0.9868
ML based su of positional parameters = 0.0404
ML based su of thermal parameters = 1.9912

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10513.573 3160.2009 19832.588 19832.891

CGMAT cycle number = 72

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5834808 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.694E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.397E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1664E+05 GEOM= 3161. TOTAL= 0.1980E+05
function value 19804.406

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.684	1.966
Torsion angles, period 1. refined	155	7.874	5.000
Torsion angles, period 2. refined	54	41.432	25.741
Torsion angles, period 3. refined	214	19.229	15.000
Torsion angles, period 4. refined	3	21.371	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	539	0.266	0.200
VDW; torsion: refined_atoms	788	0.325	0.200
HBOND: refined_atoms	42	0.191	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.262	0.200
Bond B values: refined atoms	1229	13.568	4.720
Angle B values: refined atoms	1663	16.690	7.129
Torsion B values: refined atoms	426	30.933	13.078
Long range B values: refined atoms	1334	11.680	15.324

Overall : scale = 1.012, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 72. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 72. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 72. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 72. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 747.9 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.2 0.02 0.02 1 1228.6 1223.9 0.01 0.01
0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.0 413.5 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.6 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.3 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 253.9 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.3 0.02 0.02
0.048 150 98.73 296.7 296.4 0.02 0.01 5 305.8 307.1 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.02 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.6 0.03 0.03
0.067 174 99.45 211.5 210.9 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.6 237.0 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 155.8 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.1 0.07 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.1 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 140.7 0.08 0.08
0.118 194 81.85 127.0 126.7 0.02 0.02 9 138.0 137.3 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.1 0.07 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 72. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 72. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999

```
 0.0165   83  0.991   12  0.924   95  0.982  0.999
 0.0228   97  0.988   11  1.000  108  0.990  0.999
 0.0292  108  0.997    6  1.000  114  0.997  0.999
 0.0355  126  0.996   17  1.000  143  0.996  0.999
 0.0418  129  0.997   11  1.000  140  0.997  0.999
 0.0482  150  0.991   12  1.000  162  0.992  0.999
 0.0545  151  0.997   12  0.993  163  0.997  0.999
 0.0609  172  0.983   15  0.956  187  0.981  0.999
 0.0672  174  0.993    9  0.934  183  0.990  0.999
 0.0735  178  0.990   11  1.000  189  0.990  0.999
 0.0799  189  0.989   14  0.999  203  0.990  0.999
 0.0862  197  0.983    9  0.974  206  0.983  0.999
 0.0925  193  0.979   14  0.930  207  0.975  0.999
 0.0989  188  0.980   12  1.000  200  0.981  0.999
 0.1052  190  0.988    8  1.000  198  0.989  0.999
 0.1116  183  0.980   13  0.938  196  0.978  1.000
 0.1179  194  0.980   11  0.940  205  0.978  1.000
 0.1242  174  0.983    8  1.000  182  0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0192
Free R factor                    =     0.0402
Overall weighted R factor        =     0.0192
Free weighted R factor           =     0.0406
Overall correlation coefficient  =     0.9993
Free correlation coefficient     =     0.9968
DPI based on free R factor       =     0.0730
Overall figure of merit          =     0.9868
ML based su of positional parameters =     0.0403
ML based su of thermal parameters    =     1.9897
------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10511.420       3160.5662       19805.164       19805.197


    CGMAT cycle number =     73

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
```

Actual weight 1.5830604 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.694E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1664E+05 GEOM= 3161. TOTAL= 0.1980E+05
function value 19799.346

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.684	1.966
Torsion angles, period 1. refined	155	7.875	5.000
Torsion angles, period 2. refined	54	41.433	25.741
Torsion angles, period 3. refined	214	19.244	15.000
Torsion angles, period 4. refined	3	21.370	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	539	0.266	0.200
VDW; torsion: refined_atoms	789	0.325	0.200
HBOND: refined_atoms	42	0.191	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.260	0.200
Bond B values: refined atoms	1229	13.567	4.720
Angle B values: refined atoms	1663	16.695	7.129
Torsion B values: refined atoms	426	30.945	13.080
Long range B values: refined atoms	1335	11.677	15.320

Overall : scale = 1.012, B = -0.026
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 73. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 73. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 73. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 73. % observed v. resln :N:1,3:
$$

M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 747.9 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.2 0.02 0.02 1 1228.6 1224.0 0.01 0.01
0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.0 413.5 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.7 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.3 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 253.9 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.3 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.1 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.02 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.7 0.03 0.03
0.067 174 99.45 211.5 210.9 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.6 237.0 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 155.8 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.1 0.07 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.1 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 140.8 0.08 0.08
0.118 194 81.85 127.0 126.7 0.02 0.02 9 138.0 137.3 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.1 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 73. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 73. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.991 12 0.924 95 0.982 0.999
0.0228 97 0.988 11 1.000 108 0.990 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.996 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.992 0.999
0.0545 151 0.997 12 0.993 163 0.997 0.999
0.0609 172 0.983 15 0.956 187 0.981 0.999
0.0672 174 0.993 9 0.934 183 0.990 0.999
0.0735 178 0.990 11 1.000 189 0.990 0.999
0.0799 189 0.989 14 0.999 203 0.990 0.999
0.0862 197 0.983 9 0.974 206 0.983 0.999
0.0925 193 0.979 14 0.930 207 0.975 0.999
0.0989 188 0.980 12 1.000 200 0.981 0.999
0.1052 190 0.988 8 1.000 198 0.989 0.999
0.1116 183 0.980 13 0.938 196 0.978 1.000
0.1179 194 0.980 11 0.940 205 0.978 1.000

```
 0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0192
Free R factor                    =     0.0402
Overall weighted R factor        =     0.0192
Free weighted R factor           =     0.0405
Overall correlation coefficient  =     0.9993
Free correlation coefficient     =     0.9968
DPI based on free R factor       =     0.0730
Overall figure of merit          =     0.9868
ML based su of positional parameters =     0.0403
ML based su of thermal parameters    =     1.9895
---------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10510.774       3160.9602       19801.230       19800.150

 fvalues    10510.774       3160.9602       19800.229       19800.150


    CGMAT cycle number =     74

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    1.5825143      is applied to the X-ray term
Norm of X_ray positional gradient              13.7
Norm of Geom. positional gradient              13.7
Norm of X_ray B-factor gradient                17.8
Norm of Geom. B-factor gradient                18.2
Product of X_ray and Geom posit. gradients     -0.694E+06
 Cosine of angle between them                  -1.000
Product of X_ray and Geom B-fact gradients     -0.396E+06
 Cosine of angle between them                  -0.995


Residuals: XRAY=     0.1663E+05 GEOM=      3161.     TOTAL=     0.1979E+05
 function value    19792.824

---------------------------------------------------------------------------
```

```
          Restraint type            N restraints   Rms Delta   Av(Sigma)
Bond distances: refined atoms              1229     0.011     0.020
Bond angles  : refined atoms               1663     1.684     1.966
Torsion angles, period  1. refined          155     7.874     5.000
Torsion angles, period  2. refined           54    41.433    25.741
Torsion angles, period  3. refined          214    19.232    15.000
Torsion angles, period  4. refined            3    21.369    15.000
Chiral centres: refined atoms              187     0.111     0.200
Planar groups: refined atoms               924     0.005     0.021
VDW repulsions: refined_atoms              539     0.266     0.200
VDW; torsion: refined_atoms                789     0.325     0.200
HBOND: refined_atoms                        42     0.191     0.200
VDW repulsions: symmetry: refined_atoms     55     0.262     0.200
HBOND: symmetry: refined_atoms               3     0.260     0.200
Bond B values: refined atoms               1229    13.567     4.721
Angle B values: refined atoms              1663    16.697     7.129
Torsion B values: refined atoms             426    30.951    13.080
Long range B values: refined atoms         1335    11.678    15.319
------------------------------------------------------------------------------

------------------------------------------------------------------------------
Overall              : scale =    1.012, B  =  -0.026
Overall anisotropic scale factors
  B11 =  0.28 B22 =  0.17 B33 = -0.47 B12 =  0.00 B13 = -0.36 B23 =  0.00
------------------------------------------------------------------------------

------------------------------------------------------------------------------

   ****            Things for loggraph, R factor and others            ****


$TABLE: Cycle   74. Rfactor analysis, F distribution v resln  :
$GRAPHS:Cycle   74. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle   74. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle   74. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free   WR_free $$
$$
 0.004     30  62.50   754.4   747.9  0.02  0.02       0     0.0     0.0******  0.00
 0.010     62  95.45   414.1   416.2  0.02  0.02       1  1228.6  1224.0  0.01  0.01
 0.017     83  95.60   307.7   308.7  0.03  0.02       4   403.0   413.5  0.04  0.05
 0.023     97  97.14   247.4   248.4  0.02  0.02       5   180.2   188.7  0.07  0.07
 0.029    108 100.00   241.3   242.0  0.02  0.02       7   186.7   189.3  0.06  0.06
 0.036    126  99.25   270.4   270.7  0.02  0.02       6   252.9   253.9  0.04  0.04
 0.042    129  98.56   286.3   287.5  0.02  0.02       8   338.1   341.3  0.02  0.02
 0.048    150  98.73   296.8   296.4  0.02  0.01       5   305.8   307.1  0.03  0.02
 0.055    151  99.38   281.3   281.5  0.01  0.02      10   257.9   260.1  0.04  0.04
 0.061    172 100.00   218.4   218.6  0.02  0.02      10   202.2   202.7  0.03  0.03
 0.067    174  99.45   211.5   210.9  0.02  0.02       6   286.3   284.4  0.02  0.02
 0.074    178  98.92   206.1   206.7  0.02  0.02       6   234.6   237.0  0.03  0.03
```

0.080	189	100.00	208.7	209.0	0.02	0.02	13	159.7	155.8	0.06	0.06
0.086	197	100.00	176.8	176.9	0.02	0.02	8	208.6	207.6	0.04	0.04
0.093	193	93.55	156.9	157.0	0.02	0.02	10	182.0	186.1	0.07	0.06
0.099	188	91.28	160.7	159.8	0.02	0.02	11	159.7	157.1	0.02	0.02
0.105	190	86.02	153.9	153.5	0.02	0.02	13	169.2	170.1	0.05	0.04
0.112	183	80.08	129.9	129.6	0.02	0.02	6	135.2	140.8	0.08	0.08
0.118	194	81.85	127.0	126.7	0.02	0.02	9	138.0	137.3	0.05	0.05
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	111.1	0.06	0.06

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 74. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 74. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.991	12	0.924	95	0.982	0.999
0.0228	97	0.988	11	1.000	108	0.990	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.996	17	1.000	143	0.996	0.999
0.0418	129	0.997	11	1.000	140	0.997	0.999
0.0482	150	0.991	12	1.000	162	0.992	0.999
0.0545	151	0.997	12	0.993	163	0.997	0.999
0.0609	172	0.983	15	0.956	187	0.981	0.999
0.0672	174	0.993	9	0.934	183	0.990	0.999
0.0735	178	0.990	11	1.000	189	0.990	0.999
0.0799	189	0.989	14	0.999	203	0.990	0.999
0.0862	197	0.983	9	0.974	206	0.983	0.999
0.0925	193	0.979	14	0.930	207	0.975	0.999
0.0989	188	0.980	12	1.000	200	0.981	0.999
0.1052	190	0.988	8	1.000	198	0.989	0.999
0.1116	183	0.980	13	0.937	196	0.978	1.000
0.1179	194	0.980	11	0.939	205	0.978	1.000
0.1242	174	0.983	8	1.000	182	0.984	1.000

$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0192
Free R factor = 0.0402
Overall weighted R factor = 0.0192
Free weighted R factor = 0.0405
Overall correlation coefficient = 0.9993
Free correlation coefficient = 0.9968
DPI based on free R factor = 0.0729
Overall figure of merit = 0.9869
ML based su of positional parameters = 0.0403

ML based su of thermal parameters = 1.9892

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10510.312 3160.9041 19793.240 19793.623

CGMAT cycle number = 75

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5803857 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.694E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.397E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1661E+05 GEOM= 3161. TOTAL= 0.1977E+05
function value 19767.523

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.684	1.966
Torsion angles, period 1. refined	155	7.874	5.000
Torsion angles, period 2. refined	54	41.434	25.741
Torsion angles, period 3. refined	214	19.238	15.000
Torsion angles, period 4. refined	3	21.368	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	539	0.266	0.200
VDW; torsion: refined_atoms	789	0.325	0.200
HBOND: refined_atoms	41	0.193	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.259	0.200
Bond B values: refined atoms	1229	13.567	4.721
Angle B values: refined atoms	1663	16.702	7.129
Torsion B values: refined atoms	426	30.967	13.080

Long range B values: refined atoms 1334 11.658 15.309

Overall : scale = 1.012, B = -0.026
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 75. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 75. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 75. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 75. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 747.9 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.2 0.02 0.02 1 1228.6 1224.1 0.01 0.01
0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.0 413.5 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.7 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.3 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 253.9 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.3 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.1 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.02 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.6 0.03 0.03
0.067 174 99.45 211.5 210.9 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.6 237.0 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 155.8 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.1 0.07 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.1 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 140.8 0.08 0.08
0.118 194 81.85 127.0 126.7 0.02 0.02 9 138.0 137.3 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.1 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 75. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 75. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.991	12	0.924	95	0.982	0.999
0.0228	97	0.988	11	1.000	108	0.990	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.996	17	1.000	143	0.996	0.999
0.0418	129	0.997	11	1.000	140	0.997	0.999
0.0482	150	0.991	12	1.000	162	0.992	0.999
0.0545	151	0.997	12	0.993	163	0.997	0.999
0.0609	172	0.983	15	0.956	187	0.981	0.999
0.0672	174	0.993	9	0.934	183	0.990	0.999
0.0735	178	0.990	11	1.000	189	0.990	0.999
0.0799	189	0.989	14	0.999	203	0.990	0.999
0.0862	197	0.983	9	0.974	206	0.983	0.999
0.0925	193	0.979	14	0.930	207	0.975	0.999
0.0989	188	0.980	12	1.000	200	0.981	0.999
0.1052	190	0.988	8	1.000	198	0.989	0.999
0.1116	183	0.981	13	0.938	196	0.978	1.000
0.1179	194	0.980	11	0.940	205	0.978	1.000
0.1242	174	0.983	8	1.000	182	0.984	1.000

$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0191
Free R factor = 0.0401
Overall weighted R factor = 0.0192
Free weighted R factor = 0.0405
Overall correlation coefficient = 0.9993
Free correlation coefficient = 0.9968
DPI based on free R factor = 0.0729
Overall figure of merit = 0.9869
ML based su of positional parameters = 0.0403
ML based su of thermal parameters = 1.9879

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10508.557 3160.7095 19768.266 19768.281

CGMAT cycle number = 76

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG

VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5785915 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1659E+05 GEOM= 3161. TOTAL= 0.1975E+05
function value 19746.504

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.684	1.966
Torsion angles, period 1. refined	155	7.874	5.000
Torsion angles, period 2. refined	54	41.435	25.741
Torsion angles, period 3. refined	214	19.221	15.000
Torsion angles, period 4. refined	3	21.371	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	539	0.266	0.200
VDW; torsion: refined_atoms	790	0.325	0.200
HBOND: refined_atoms	41	0.193	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.258	0.200
Bond B values: refined atoms	1229	13.570	4.721
Angle B values: refined atoms	1663	16.711	7.129
Torsion B values: refined atoms	426	30.990	13.081
Long range B values: refined atoms	1335	11.657	15.307

Overall : scale = 1.012, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 76. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 76. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 76. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:

:Cycle 76. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 747.9 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.2 0.02 0.02 1 1228.6 1224.1 0.01 0.01
0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.0 413.5 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.7 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.3 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 253.9 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.3 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.1 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.02 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.6 0.03 0.03
0.067 174 99.45 211.5 210.9 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.6 237.0 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 155.8 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.1 0.07 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.1 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 140.8 0.08 0.08
0.118 194 81.85 127.0 126.7 0.02 0.02 9 138.0 137.2 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.1 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 76. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 76. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.991 12 0.924 95 0.982 0.999
0.0228 97 0.988 11 1.000 108 0.990 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.996 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.992 0.999
0.0545 151 0.997 12 0.993 163 0.997 0.999
0.0609 172 0.983 15 0.956 187 0.981 0.999
0.0672 174 0.993 9 0.934 183 0.990 0.999
0.0735 178 0.990 11 1.000 189 0.990 0.999
0.0799 189 0.989 14 0.999 203 0.990 0.999
0.0862 197 0.983 9 0.974 206 0.983 0.999
0.0925 193 0.979 14 0.930 207 0.975 0.999
0.0989 188 0.980 12 1.000 200 0.981 0.999
0.1052 190 0.988 8 1.000 198 0.989 0.999

```
 0.1116   183   0.981    13   0.938   196   0.978  1.000
 0.1179   194   0.980    11   0.941   205   0.978  1.000
 0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0191
Free R factor                    =     0.0401
Overall weighted R factor        =     0.0192
Free weighted R factor           =     0.0405
Overall correlation coefficient  =     0.9993
Free correlation coefficient     =     0.9968
DPI based on free R factor       =     0.0728
Overall figure of merit          =     0.9869
ML based su of positional parameters =     0.0403
ML based su of thermal parameters    =     1.9868
---------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10506.789       3161.3530       19753.230       19747.281

 fvalues    10506.789       3161.3530       19747.475       19747.281


    CGMAT cycle number =     77

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    1.5791590      is applied to the X-ray term
Norm of X_ray positional gradient              13.7
Norm of Geom. positional gradient              13.7
Norm of X_ray B-factor gradient                17.8
Norm of Geom. B-factor gradient                18.2
Product of X_ray and Geom posit. gradients     -0.693E+06
 Cosine of angle between them                  -1.000
Product of X_ray and Geom B-fact gradients     -0.396E+06
 Cosine of angle between them                  -0.995


Residuals: XRAY=     0.1659E+05 GEOM=      3161.     TOTAL=     0.1975E+05
 function value    19752.547
```

```
------------------------------------------------------------------------------
          Restraint type           N restraints   Rms Delta   Av(Sigma)
Bond distances: refined atoms              1229     0.011     0.020
Bond angles  : refined atoms               1663     1.683     1.966
Torsion angles, period  1. refined          155     7.874     5.000
Torsion angles, period  2. refined           54    41.436    25.741
Torsion angles, period  3. refined          214    19.237    15.000
Torsion angles, period  4. refined            3    21.371    15.000
Chiral centres: refined atoms              187     0.111     0.200
Planar groups: refined atoms               924     0.005     0.021
VDW repulsions: refined_atoms              539     0.266     0.200
VDW; torsion: refined_atoms                790     0.325     0.200
HBOND: refined_atoms                        41     0.193     0.200
VDW repulsions: symmetry: refined_atoms     55     0.262     0.200
HBOND: symmetry: refined_atoms               3     0.257     0.200
Bond B values: refined atoms               1229    13.570     4.721
Angle B values: refined atoms              1663    16.713     7.129
Torsion B values: refined atoms             426    30.995    13.081
Long range B values: refined atoms         1335    11.657    15.307
------------------------------------------------------------------------------

------------------------------------------------------------------------------
Overall              : scale =    1.012, B  =  -0.025
Overall anisotropic scale factors
   B11 =  0.28 B22 =  0.17 B33 = -0.47 B12 =  0.00 B13 = -0.36 B23 =  0.00
------------------------------------------------------------------------------

------------------------------------------------------------------------------

    ****              Things for loggraph, R factor and others              ****


$TABLE: Cycle   77. Rfactor analysis, F distribution v resln  :
$GRAPHS:Cycle   77. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle   77. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle   77. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free   WR_free $$
$$
 0.004     30  62.50   754.4   747.9  0.02  0.02      0     0.0     0.0******  0.00
 0.010     62  95.45   414.1   416.2  0.02  0.02      1  1228.6  1224.1  0.01  0.01
 0.017     83  95.60   307.7   308.7  0.03  0.02      4   403.0   413.5  0.04  0.05
 0.023     97  97.14   247.4   248.4  0.02  0.02      5   180.2   188.7  0.07  0.07
 0.029    108 100.00   241.3   242.0  0.02  0.02      7   186.7   189.3  0.06  0.06
 0.036    126  99.25   270.4   270.7  0.02  0.02      6   252.9   253.9  0.04  0.04
 0.042    129  98.56   286.3   287.5  0.02  0.02      8   338.1   341.3  0.02  0.02
 0.048    150  98.73   296.8   296.4  0.02  0.01      5   305.8   307.1  0.03  0.02
 0.055    151  99.38   281.3   281.5  0.01  0.02     10   257.9   260.1  0.04  0.04
 0.061    172 100.00   218.4   218.6  0.02  0.02     10   202.2   202.6  0.03  0.03
```

0.067	174	99.45	211.5	210.9	0.02	0.02	6	286.3	284.4	0.02	0.02
0.074	178	98.92	206.1	206.7	0.02	0.02	6	234.6	237.0	0.03	0.03
0.080	189	100.00	208.7	209.0	0.02	0.02	13	159.7	155.8	0.06	0.06
0.086	197	100.00	176.8	176.9	0.02	0.02	8	208.6	207.6	0.04	0.04
0.093	193	93.55	156.9	157.0	0.02	0.02	10	182.0	186.1	0.07	0.06
0.099	188	91.28	160.7	159.8	0.02	0.02	11	159.7	157.1	0.02	0.02
0.105	190	86.02	153.9	153.5	0.02	0.02	13	169.2	170.1	0.05	0.04
0.112	183	80.08	129.9	129.6	0.02	0.02	6	135.2	140.8	0.08	0.08
0.118	194	81.85	127.0	126.7	0.02	0.02	9	138.0	137.3	0.05	0.05
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	111.1	0.06	0.06

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 77. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 77. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.991	12	0.924	95	0.982	0.999
0.0228	97	0.988	11	1.000	108	0.990	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.996	17	1.000	143	0.996	0.999
0.0418	129	0.997	11	1.000	140	0.997	0.999
0.0482	150	0.991	12	1.000	162	0.992	0.999
0.0545	151	0.997	12	0.993	163	0.997	0.999
0.0609	172	0.983	15	0.956	187	0.981	0.999
0.0672	174	0.993	9	0.934	183	0.990	0.999
0.0735	178	0.990	11	1.000	189	0.990	0.999
0.0799	189	0.989	14	0.999	203	0.990	0.999
0.0862	197	0.983	9	0.974	206	0.983	0.999
0.0925	193	0.979	14	0.930	207	0.975	0.999
0.0989	188	0.980	12	1.000	200	0.981	0.999
0.1052	190	0.988	8	1.000	198	0.989	0.999
0.1116	183	0.981	13	0.938	196	0.978	1.000
0.1179	194	0.980	11	0.941	205	0.978	1.000
0.1242	174	0.983	8	1.000	182	0.984	1.000

$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0191
Free R factor = 0.0401
Overall weighted R factor = 0.0191
Free weighted R factor = 0.0405
Overall correlation coefficient = 0.9993
Free correlation coefficient = 0.9968
DPI based on free R factor = 0.0728

Overall figure of merit = 0.9869
ML based su of positional parameters = 0.0403
ML based su of thermal parameters = 1.9873

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10506.902 3161.2554 19753.221 19753.324

CGMAT cycle number = 78

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5762259 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1656E+05 GEOM= 3161. TOTAL= 0.1972E+05
function value 19718.385

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.685	1.966
Torsion angles, period 1. refined	155	7.874	5.000
Torsion angles, period 2. refined	54	41.437	25.741
Torsion angles, period 3. refined	214	19.228	15.000
Torsion angles, period 4. refined	3	21.370	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	539	0.266	0.200
VDW; torsion: refined_atoms	790	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.256	0.200
Bond B values: refined atoms	1229	13.573	4.721

Angle B values: refined atoms 1663 16.723 7.130
Torsion B values: refined atoms 426 31.022 13.083
Long range B values: refined atoms 1335 11.660 15.307

Overall : scale = 1.012, B = -0.026
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 78. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 78. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 78. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 78. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 747.9 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.1 0.02 0.02 1 1228.6 1224.2 0.01 0.01
0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.0 413.5 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.8 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.3 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 253.9 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.3 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.1 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.02 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.6 0.03 0.03
0.067 174 99.45 211.5 210.9 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.6 237.1 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 155.8 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.1 0.07 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.1 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 140.9 0.08 0.08
0.118 194 81.85 127.0 126.7 0.02 0.02 9 138.0 137.2 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.1 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 78. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 78. M(Fom) v. resln :N:1,3,5,7,8:
$$

```
<4SSQ/LL> NREFa  FOMa  NREFc FOMc NREFall FOMall  SigmaA_Fc1 $$
$$
 0.0038   30  0.999    4  1.000   34  0.999  0.999
 0.0102   62  0.999    7  1.000   69  0.999  0.999
 0.0165   83  0.991   12  0.924   95  0.982  0.999
 0.0228   97  0.988   11  1.000  108  0.990  0.999
 0.0292  108  0.997    6  1.000  114  0.997  0.999
 0.0355  126  0.996   17  1.000  143  0.996  0.999
 0.0418  129  0.997   11  1.000  140  0.997  0.999
 0.0482  150  0.991   12  1.000  162  0.992  0.999
 0.0545  151  0.997   12  0.993  163  0.997  0.999
 0.0609  172  0.983   15  0.956  187  0.981  0.999
 0.0672  174  0.993    9  0.934  183  0.990  0.999
 0.0735  178  0.990   11  1.000  189  0.990  0.999
 0.0799  189  0.989   14  0.999  203  0.990  0.999
 0.0862  197  0.984    9  0.974  206  0.983  0.999
 0.0925  193  0.979   14  0.930  207  0.975  0.999
 0.0989  188  0.980   12  1.000  200  0.981  0.999
 0.1052  190  0.988    8  1.000  198  0.989  0.999
 0.1116  183  0.981   13  0.938  196  0.978  1.000
 0.1179  194  0.980   11  0.941  205  0.978  1.000
 0.1242  174  0.983    8  1.000  182  0.984  1.000
 $$
Resolution limits                =    38.899    2.802
Number of used reflections       =      3184
Percentage observed              =   92.6870
Percentage of free reflections   =    4.8416
Overall R factor                 =    0.0191
Free R factor                    =    0.0401
Overall weighted R factor        =    0.0191
Free weighted R factor           =    0.0405
Overall correlation coefficient  =    0.9993
Free correlation coefficient     =    0.9968
DPI based on free R factor       =    0.0728
Overall figure of merit          =    0.9869
ML based su of positional parameters =    0.0402
ML based su of thermal parameters    =    1.9853
------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10504.752       3161.3198       19719.549       19719.182

 fvalues    10504.752       3161.3198       19719.102       19719.182


    CGMAT cycle number =     79

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
```

Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5761292 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1656E+05 GEOM= 3162. TOTAL= 0.1972E+05
function value 19716.865

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.684	1.966
Torsion angles, period 1. refined	155	7.873	5.000
Torsion angles, period 2. refined	54	41.437	25.741
Torsion angles, period 3. refined	214	19.242	15.000
Torsion angles, period 4. refined	3	21.369	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	539	0.266	0.200
VDW; torsion: refined_atoms	790	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.255	0.200
Bond B values: refined atoms	1229	13.569	4.721
Angle B values: refined atoms	1663	16.721	7.129
Torsion B values: refined atoms	426	31.022	13.083
Long range B values: refined atoms	1335	11.657	15.307

Overall : scale = 1.012, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 79. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 79. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 79. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 79. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 747.9 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.1 0.02 0.02 1 1228.6 1224.3 0.01 0.01
0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.0 413.5 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.8 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.3 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.0 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.3 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.1 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.02 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.7 0.03 0.03
0.067 174 99.45 211.5 210.9 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.6 237.1 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 155.8 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.1 0.07 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.1 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 140.9 0.08 0.08
0.118 194 81.85 127.0 126.7 0.02 0.02 9 138.0 137.2 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.1 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 79. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 79. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.991 12 0.924 95 0.982 0.999
0.0228 97 0.988 11 1.000 108 0.990 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.996 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.992 0.999
0.0545 151 0.997 12 0.993 163 0.997 0.999
0.0609 172 0.983 15 0.956 187 0.981 0.999
0.0672 174 0.993 9 0.934 183 0.990 0.999
0.0735 178 0.990 11 1.000 189 0.990 0.999
0.0799 189 0.989 14 0.999 203 0.990 0.999

```
 0.0862   197   0.984    9   0.974   206   0.983  0.999
 0.0925   193   0.979   14   0.930   207   0.975  0.999
 0.0989   188   0.980   12   1.000   200   0.981  0.999
 0.1052   190   0.988    8   1.000   198   0.989  0.999
 0.1116   183   0.981   13   0.938   196   0.978  1.000
 0.1179   194   0.980   11   0.941   205   0.978  1.000
 0.1242   174   0.983    8   1.000   182   0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0191
Free R factor                    =     0.0401
Overall weighted R factor        =     0.0191
Free weighted R factor           =     0.0405
Overall correlation coefficient  =     0.9993
Free correlation coefficient     =     0.9968
DPI based on free R factor       =     0.0728
Overall figure of merit          =     0.9869
ML based su of positional parameters =     0.0402
ML based su of thermal parameters    =     1.9855
------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10504.293       3161.5574       19718.203       19717.680

 fvalues    10504.293       3161.5574       19717.600       19717.680


    CGMAT cycle number =     80

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    1.5758502      is applied to the X-ray term
Norm of X_ray positional gradient              13.7
Norm of Geom. positional gradient              13.7
Norm of X_ray B-factor gradient                17.8
Norm of Geom. B-factor gradient                18.2
Product of X_ray and Geom posit. gradients     -0.693E+06
 Cosine of angle between them                  -1.000
Product of X_ray and Geom B-fact gradients     -0.396E+06
 Cosine of angle between them                  -0.995
```

Residuals: XRAY= 0.1655E+05 GEOM= 3162. TOTAL= 0.1971E+05
function value 19713.379

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.684	1.966
Torsion angles, period 1. refined	155	7.873	5.000
Torsion angles, period 2. refined	54	41.438	25.741
Torsion angles, period 3. refined	214	19.226	15.000
Torsion angles, period 4. refined	3	21.369	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	539	0.266	0.200
VDW; torsion: refined_atoms	790	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.255	0.200
Bond B values: refined atoms	1229	13.567	4.722
Angle B values: refined atoms	1663	16.723	7.129
Torsion B values: refined atoms	426	31.029	13.083
Long range B values: refined atoms	1335	11.656	15.307

Overall : scale = 1.012, B = -0.026
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 80. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 80. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 80. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 80. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$

0.004	30	62.50	754.4	747.9	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	414.1	416.1	0.02	0.02	1	1228.6	1224.3	0.01	0.01	
0.017	83	95.60	307.7	308.7	0.03	0.02	4	403.0	413.5	0.04	0.05	
0.023	97	97.14	247.4	248.4	0.02	0.02	5	180.2	188.8	0.07	0.07	
0.029	108	100.00	241.3	242.0	0.02	0.02	7	186.7	189.3	0.06	0.06	
0.036	126	99.25	270.4	270.7	0.02	0.02	6	252.9	254.0	0.04	0.04	

```
 0.042    129  98.56   286.3   287.5  0.02  0.02      8   338.1   341.3  0.02  0.02
 0.048    150  98.73   296.8   296.4  0.02  0.01      5   305.8   307.1  0.03  0.02
 0.055    151  99.38   281.3   281.5  0.01  0.02     10   257.9   260.1  0.04  0.04
 0.061    172 100.00   218.4   218.6  0.02  0.02     10   202.2   202.7  0.03  0.03
 0.067    174  99.45   211.5   210.9  0.02  0.02      6   286.3   284.4  0.02  0.02
 0.074    178  98.92   206.1   206.7  0.02  0.02      6   234.6   237.1  0.03  0.03
 0.080    189 100.00   208.7   209.0  0.02  0.02     13   159.7   155.8  0.06  0.06
 0.086    197 100.00   176.8   176.9  0.02  0.02      8   208.6   207.6  0.04  0.04
 0.093    193  93.55   156.9   157.0  0.02  0.02     10   182.0   186.1  0.07  0.06
 0.099    188  91.28   160.7   159.8  0.02  0.02     11   159.7   157.1  0.02  0.02
 0.105    190  86.02   153.9   153.5  0.02  0.02     13   169.2   170.1  0.05  0.04
 0.112    183  80.08   129.9   129.6  0.02  0.02      6   135.2   140.9  0.08  0.08
 0.118    194  81.85   127.0   126.7  0.02  0.02      9   138.0   137.2  0.05  0.05
 0.124    174  73.20   129.0   128.9  0.02  0.02      9   113.8   111.1  0.06  0.06
$$

   ****                Fom and SigmaA vs resolution                ****

 $TABLE: Cycle   80. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
 $GRAPHS:Cycle   80. M(Fom) v. resln :N:1,3,5,7,8:
 $$
 <4SSQ/LL> NREFa  FOMa  NREFc FOMc NREFall FOMall  SigmaA_Fc1 $$
 $$
  0.0038    30   0.999     4   1.000    34   0.999  0.999
  0.0102    62   0.999     7   1.000    69   0.999  0.999
  0.0165    83   0.991    12   0.924    95   0.982  0.999
  0.0228    97   0.988    11   1.000   108   0.990  0.999
  0.0292   108   0.997     6   1.000   114   0.997  0.999
  0.0355   126   0.996    17   1.000   143   0.996  0.999
  0.0418   129   0.997    11   1.000   140   0.997  0.999
  0.0482   150   0.991    12   1.000   162   0.992  0.999
  0.0545   151   0.997    12   0.993   163   0.997  0.999
  0.0609   172   0.983    15   0.956   187   0.981  0.999
  0.0672   174   0.993     9   0.933   183   0.990  0.999
  0.0735   178   0.990    11   1.000   189   0.990  0.999
  0.0799   189   0.989    14   0.999   203   0.990  0.999
  0.0862   197   0.984     9   0.974   206   0.983  0.999
  0.0925   193   0.979    14   0.930   207   0.975  0.999
  0.0989   188   0.980    12   1.000   200   0.981  0.999
  0.1052   190   0.988     8   1.000   198   0.989  0.999
  0.1116   183   0.981    13   0.937   196   0.978  1.000
  0.1179   194   0.980    11   0.942   205   0.978  1.000
  0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
 Resolution limits                =     38.899     2.802
 Number of used reflections       =       3184
 Percentage observed              =    92.6870
 Percentage of free reflections   =     4.8416
 Overall R factor                 =     0.0191
 Free R factor                    =     0.0401
 Overall weighted R factor        =     0.0191
```

Free weighted R factor = 0.0404
Overall correlation coefficient = 0.9993
Free correlation coefficient = 0.9968
DPI based on free R factor = 0.0728
Overall figure of merit = 0.9869
ML based su of positional parameters = 0.0402
ML based su of thermal parameters = 1.9854

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10503.837 3161.6831 19715.408 19714.156

fvalues 10503.837 3161.6831 19714.098 19714.156

CGMAT cycle number = 81

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5747390 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1654E+05 GEOM= 3162. TOTAL= 0.1970E+05
function value 19700.402

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.683	1.966
Torsion angles, period 1. refined	155	7.873	5.000
Torsion angles, period 2. refined	54	41.438	25.741
Torsion angles, period 3. refined	214	19.248	15.000
Torsion angles, period 4. refined	3	21.368	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021

VDW repulsions: refined_atoms 539 0.266 0.200
VDW; torsion: refined_atoms 789 0.325 0.200
HBOND: refined_atoms 41 0.194 0.200
VDW repulsions: symmetry: refined_atoms 55 0.262 0.200
HBOND: symmetry: refined_atoms 3 0.254 0.200
Bond B values: refined atoms 1229 13.566 4.722
Angle B values: refined atoms 1663 16.725 7.129
Torsion B values: refined atoms 426 31.036 13.083
Long range B values: refined atoms 1334 11.659 15.308

Overall : scale = 1.012, B = -0.026
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 81. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 81. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 81. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 81. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 747.9 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.1 0.02 0.02 1 1228.6 1224.3 0.01 0.01
0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.0 413.4 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.8 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.0 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.3 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.1 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.02 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.7 0.03 0.03
0.067 174 99.45 211.5 210.9 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.6 237.1 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 155.8 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.1 0.07 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.1 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 140.9 0.08 0.08
0.118 194 81.85 127.0 126.7 0.02 0.02 9 138.0 137.2 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.1 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 81. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 81. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.991 12 0.924 95 0.982 0.999
0.0228 97 0.988 11 1.000 108 0.990 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.996 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.992 0.999
0.0545 151 0.997 12 0.993 163 0.997 0.999
0.0609 172 0.983 15 0.956 187 0.981 0.999
0.0672 174 0.993 9 0.933 183 0.990 0.999
0.0735 178 0.990 11 1.000 189 0.990 0.999
0.0799 189 0.989 14 0.999 203 0.990 0.999
0.0862 197 0.984 9 0.974 206 0.983 0.999
0.0925 193 0.979 14 0.930 207 0.975 0.999
0.0989 188 0.980 12 1.000 200 0.981 0.999
0.1052 190 0.988 8 1.000 198 0.989 0.999
0.1116 183 0.981 13 0.938 196 0.978 1.000
0.1179 194 0.980 11 0.942 205 0.978 1.000
0.1242 174 0.983 8 1.000 182 0.984 1.000
$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0191
Free R factor = 0.0401
Overall weighted R factor = 0.0191
Free weighted R factor = 0.0404
Overall correlation coefficient = 0.9994
Free correlation coefficient = 0.9968
DPI based on free R factor = 0.0727
Overall figure of merit = 0.9869
ML based su of positional parameters = 0.0402
ML based su of thermal parameters = 1.9847

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10502.811 3161.9968 19703.498 19701.182

fvalues 10502.811 3161.9968 19701.273 19701.182

CGMAT cycle number = 82

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000008
Actual weight 1.5745326 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1654E+05 GEOM= 3162. TOTAL= 0.1970E+05
function value 19697.998

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.683	1.966
Torsion angles, period 1. refined	155	7.873	5.000
Torsion angles, period 2. refined	54	41.439	25.741
Torsion angles, period 3. refined	214	19.233	15.000
Torsion angles, period 4. refined	3	21.368	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	539	0.266	0.200
VDW; torsion: refined_atoms	789	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.254	0.200
Bond B values: refined atoms	1229	13.565	4.722
Angle B values: refined atoms	1663	16.726	7.129
Torsion B values: refined atoms	426	31.041	13.084
Long range B values: refined atoms	1334	11.659	15.308

Overall : scale = 1.012, B = -0.026
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 82. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 82. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 82. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 82. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 747.9 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.1 0.02 0.02 1 1228.6 1224.3 0.01 0.01
0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.0 413.5 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.8 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.3 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.0 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.3 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.2 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.02 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.7 0.03 0.03
0.067 174 99.45 211.5 210.9 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.7 0.02 0.02 6 234.6 237.1 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 155.8 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.1 0.07 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.1 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 140.9 0.08 0.08
0.118 194 81.85 127.0 126.7 0.02 0.02 9 138.0 137.2 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.1 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 82. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 82. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.991 12 0.924 95 0.982 0.999
0.0228 97 0.988 11 1.000 108 0.990 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.996 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999

```
 0.0482   150   0.991    12   1.000   162   0.992  0.999
 0.0545   151   0.997    12   0.993   163   0.997  0.999
 0.0609   172   0.983    15   0.956   187   0.981  0.999
 0.0672   174   0.993     9   0.933   183   0.990  0.999
 0.0735   178   0.990    11   1.000   189   0.990  0.999
 0.0799   189   0.989    14   0.999   203   0.990  0.999
 0.0862   197   0.984     9   0.974   206   0.983  0.999
 0.0925   193   0.979    14   0.930   207   0.975  0.999
 0.0989   188   0.980    12   1.000   200   0.981  0.999
 0.1052   190   0.988     8   1.000   198   0.989  0.999
 0.1116   183   0.981    13   0.938   196   0.978  1.000
 0.1179   194   0.980    11   0.941   205   0.978  1.000
 0.1242   174   0.983     8   1.000   182   0.984  1.000
$$
Resolution limits                 =     38.899     2.802
Number of used reflections        =       3184
Percentage observed               =    92.6870
Percentage of free reflections    =     4.8416
Overall R factor                  =     0.0191
Free R factor                     =     0.0401
Overall weighted R factor         =     0.0191
Free weighted R factor            =     0.0404
Overall correlation coefficient   =     0.9994
Free correlation coefficient      =     0.9968
DPI based on free R factor        =     0.0727
Overall figure of merit           =     0.9869
ML based su of positional parameters =     0.0402
ML based su of thermal parameters    =     1.9845
------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10502.752       3161.8579       19698.629       19698.783


    CGMAT cycle number =     83

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000008
 Actual weight    1.5730371      is applied to the X-ray term
Norm of X_ray positional gradient              13.7
Norm of Geom. positional gradient              13.7
Norm of X_ray B-factor gradient                17.8
Norm of Geom. B-factor gradient                18.2
```

Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1652E+05 GEOM= 3162. TOTAL= 0.1968E+05
function value 19679.992

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.685	1.966
Torsion angles, period 1. refined	155	7.873	5.000
Torsion angles, period 2. refined	54	41.440	25.741
Torsion angles, period 3. refined	214	19.240	15.000
Torsion angles, period 4. refined	3	21.367	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	539	0.266	0.200
VDW; torsion: refined_atoms	789	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.252	0.200
Bond B values: refined atoms	1229	13.564	4.722
Angle B values: refined atoms	1663	16.731	7.129
Torsion B values: refined atoms	426	31.058	13.084
Long range B values: refined atoms	1334	11.657	15.307

Overall : scale = 1.012, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 83. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 83. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 83. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 83. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$

0.004	30	62.50	754.4	747.9	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	414.1	416.1	0.02	0.02	1	1228.6	1224.4	0.01	0.01	

0.017	83	95.60	307.7	308.7	0.03	0.02	4	403.0	413.4	0.04	0.05
0.023	97	97.14	247.4	248.4	0.02	0.02	5	180.2	188.8	0.07	0.07
0.029	108	100.00	241.3	242.0	0.02	0.02	7	186.7	189.4	0.06	0.06
0.036	126	99.25	270.4	270.7	0.02	0.02	6	252.9	254.0	0.04	0.04
0.042	129	98.56	286.3	287.5	0.02	0.02	8	338.1	341.2	0.02	0.02
0.048	150	98.73	296.8	296.4	0.02	0.01	5	305.8	307.2	0.03	0.02
0.055	151	99.38	281.3	281.5	0.01	0.01	10	257.9	260.1	0.04	0.04
0.061	172	100.00	218.4	218.6	0.02	0.02	10	202.2	202.7	0.03	0.03
0.067	174	99.45	211.5	210.9	0.02	0.02	6	286.3	284.4	0.02	0.02
0.074	178	98.92	206.1	206.7	0.02	0.02	6	234.6	237.1	0.03	0.03
0.080	189	100.00	208.7	209.0	0.02	0.02	13	159.7	155.8	0.06	0.06
0.086	197	100.00	176.8	176.9	0.02	0.02	8	208.6	207.6	0.04	0.04
0.093	193	93.55	156.9	157.0	0.02	0.02	10	182.0	186.1	0.07	0.06
0.099	188	91.28	160.7	159.8	0.02	0.02	11	159.7	157.1	0.02	0.02
0.105	190	86.02	153.9	153.5	0.02	0.02	13	169.2	170.1	0.05	0.04
0.112	183	80.08	129.9	129.6	0.02	0.02	6	135.2	140.9	0.08	0.08
0.118	194	81.85	127.0	126.7	0.02	0.02	9	138.0	137.2	0.05	0.05
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	111.1	0.06	0.06

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 83. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 83. M(Fom) v. resln :N:1,3,5,7,8:
$$

<4SSQ/LL>	NREFa	FOMa	NREFc	FOMc	NREFall	FOMall	SigmaA_Fc1 $$
$$							
0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.991	12	0.924	95	0.982	0.999
0.0228	97	0.988	11	1.000	108	0.990	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.996	17	1.000	143	0.996	0.999
0.0418	129	0.997	11	1.000	140	0.997	0.999
0.0482	150	0.991	12	1.000	162	0.992	0.999
0.0545	151	0.997	12	0.993	163	0.997	0.999
0.0609	172	0.983	15	0.956	187	0.981	0.999
0.0672	174	0.993	9	0.934	183	0.990	0.999
0.0735	178	0.990	11	1.000	189	0.990	0.999
0.0799	189	0.989	14	0.999	203	0.990	0.999
0.0862	197	0.984	9	0.974	206	0.983	0.999
0.0925	193	0.979	14	0.930	207	0.975	0.999
0.0989	188	0.980	12	1.000	200	0.981	0.999
0.1052	190	0.988	8	1.000	198	0.989	0.999
0.1116	183	0.981	13	0.937	196	0.978	1.000
0.1179	194	0.980	11	0.942	205	0.978	1.000
0.1242	174	0.983	8	1.000	182	0.984	1.000

$$

Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870

Percentage of free reflections = 4.8416
Overall R factor = 0.0191
Free R factor = 0.0400
Overall weighted R factor = 0.0191
Free weighted R factor = 0.0404
Overall correlation coefficient = 0.9994
Free correlation coefficient = 0.9968
DPI based on free R factor = 0.0727
Overall figure of merit = 0.9869
ML based su of positional parameters = 0.0402
ML based su of thermal parameters = 1.9838

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10501.195 3161.9973 19681.248 19680.768

fvalues 10501.195 3161.9973 19680.826 19680.768

CGMAT cycle number = 84

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5740055 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1653E+05 GEOM= 3162. TOTAL= 0.1969E+05
function value 19691.178

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.685	1.966
Torsion angles, period 1. refined	155	7.873	5.000
Torsion angles, period 2. refined	54	41.440	25.741

Torsion angles, period 3. refined 214 19.233 15.000
Torsion angles, period 4. refined 3 21.366 15.000
Chiral centres: refined atoms 187 0.111 0.200
Planar groups: refined atoms 924 0.005 0.021
VDW repulsions: refined_atoms 539 0.266 0.200
VDW; torsion: refined_atoms 789 0.325 0.200
HBOND: refined_atoms 41 0.194 0.200
VDW repulsions: symmetry: refined_atoms 55 0.262 0.200
HBOND: symmetry: refined_atoms 3 0.252 0.200
Bond B values: refined atoms 1229 13.564 4.722
Angle B values: refined atoms 1663 16.733 7.129
Torsion B values: refined atoms 426 31.065 13.085
Long range B values: refined atoms 1334 11.657 15.307

Overall : scale = 1.012, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 84. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 84. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 84. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 84. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 747.9 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.1 0.02 0.02 1 1228.6 1224.4 0.01 0.01
0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.0 413.4 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.8 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.3 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.0 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.2 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.2 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.7 0.03 0.03
0.067 174 99.45 211.5 210.9 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.1 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 155.8 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.1 0.07 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.1 0.05 0.04

```
 0.112    183  80.08   129.9   129.6  0.02  0.02      6   135.2   140.9  0.08  0.08
 0.118    194  81.85   127.0   126.7  0.02  0.02      9   138.0   137.2  0.05  0.05
 0.124    174  73.20   129.0   128.9  0.02  0.02      9   113.8   111.0  0.06  0.06
$$

   ****                Fom and SigmaA vs resolution                ****

 $TABLE: Cycle   84. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
 $GRAPHS:Cycle   84. M(Fom) v. resln :N:1,3,5,7,8:
 $$
 <4SSQ/LL> NREFa  FOMa  NREFc FOMc NREFall FOMall  SigmaA_Fc1 $$
 $$
  0.0038    30   0.999     4   1.000    34   0.999  0.999
  0.0102    62   0.999     7   1.000    69   0.999  0.999
  0.0165    83   0.991    12   0.924    95   0.982  0.999
  0.0228    97   0.988    11   1.000   108   0.990  0.999
  0.0292   108   0.997     6   1.000   114   0.997  0.999
  0.0355   126   0.996    17   1.000   143   0.996  0.999
  0.0418   129   0.997    11   1.000   140   0.997  0.999
  0.0482   150   0.991    12   1.000   162   0.992  0.999
  0.0545   151   0.997    12   0.994   163   0.997  0.999
  0.0609   172   0.983    15   0.956   187   0.981  0.999
  0.0672   174   0.993     9   0.934   183   0.990  0.999
  0.0735   178   0.990    11   1.000   189   0.990  0.999
  0.0799   189   0.989    14   0.999   203   0.990  0.999
  0.0862   197   0.984     9   0.974   206   0.983  0.999
  0.0925   193   0.979    14   0.930   207   0.975  0.999
  0.0989   188   0.980    12   1.000   200   0.981  0.999
  0.1052   190   0.988     8   1.000   198   0.989  0.999
  0.1116   183   0.981    13   0.937   196   0.978  1.000
  0.1179   194   0.980    11   0.942   205   0.978  1.000
  0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
 Resolution limits                =     38.899     2.802
 Number of used reflections       =       3184
 Percentage observed              =    92.6870
 Percentage of free reflections   =     4.8416
 Overall R factor                 =     0.0191
 Free R factor                    =     0.0400
 Overall weighted R factor        =     0.0191
 Free weighted R factor           =     0.0404
 Overall correlation coefficient  =     0.9994
 Free correlation coefficient     =     0.9968
 DPI based on free R factor       =     0.0727
 Overall figure of merit          =     0.9869
 ML based su of positional parameters =     0.0402
 ML based su of thermal parameters    =     1.9845
 ------------------------------------------------------------------------
  Trying gamma equal    0.0000000
  Convergence reached with no gamma cycles
```

fvalues 10501.855 3162.0066 19691.992 19691.984

fvalues 10501.855 3162.0066 19692.025 19691.984

CGMAT cycle number = 85

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000008
Actual weight 1.5730649 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1652E+05 GEOM= 3162. TOTAL= 0.1968E+05
function value 19680.285

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.685	1.966
Torsion angles, period 1. refined	155	7.873	5.000
Torsion angles, period 2. refined	54	41.439	25.741
Torsion angles, period 3. refined	214	19.234	15.000
Torsion angles, period 4. refined	3	21.366	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	539	0.266	0.200
VDW; torsion: refined_atoms	789	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.251	0.200
Bond B values: refined atoms	1229	13.564	4.722
Angle B values: refined atoms	1663	16.735	7.129
Torsion B values: refined atoms	426	31.072	13.085
Long range B values: refined atoms	1334	11.657	15.307

Overall : scale = 1.012, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 85. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 85. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 85. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 85. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004	30	62.50	754.4	747.9	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	414.1	416.1	0.02	0.02	1	1228.6	1224.5	0.01	0.01	
0.017	83	95.60	307.7	308.7	0.03	0.02	4	403.1	413.4	0.04	0.05	
0.023	97	97.14	247.4	248.4	0.02	0.02	5	180.2	188.8	0.07	0.07	
0.029	108	100.00	241.3	242.0	0.02	0.02	7	186.7	189.3	0.06	0.06	
0.036	126	99.25	270.4	270.7	0.02	0.02	6	252.9	254.0	0.04	0.04	
0.042	129	98.56	286.3	287.5	0.02	0.02	8	338.1	341.2	0.02	0.02	
0.048	150	98.73	296.8	296.4	0.02	0.01	5	305.8	307.2	0.03	0.02	
0.055	151	99.38	281.3	281.5	0.01	0.01	10	257.9	260.1	0.04	0.04	
0.061	172	100.00	218.4	218.6	0.02	0.02	10	202.2	202.7	0.03	0.03	
0.067	174	99.45	211.5	210.9	0.02	0.02	6	286.3	284.4	0.02	0.02	
0.074	178	98.92	206.1	206.8	0.02	0.02	6	234.6	237.1	0.03	0.03	
0.080	189	100.00	208.7	209.0	0.02	0.02	13	159.7	155.8	0.06	0.06	
0.086	197	100.00	176.8	176.9	0.02	0.02	8	208.6	207.6	0.04	0.04	
0.093	193	93.55	156.9	157.0	0.02	0.02	10	182.0	186.1	0.07	0.06	
0.099	188	91.28	160.7	159.8	0.02	0.02	11	159.7	157.1	0.02	0.02	
0.105	190	86.02	153.9	153.5	0.02	0.02	13	169.2	170.0	0.05	0.04	
0.112	183	80.08	129.9	129.6	0.02	0.02	6	135.2	140.9	0.08	0.08	
0.118	194	81.85	127.0	126.7	0.02	0.02	9	138.0	137.2	0.05	0.05	
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	111.0	0.06	0.06	

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 85. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 85. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.991	12	0.924	95	0.982	0.999

```
 0.0228   97  0.988   11  1.000  108  0.990  0.999
 0.0292  108  0.997    6  1.000  114  0.997  0.999
 0.0355  126  0.996   17  1.000  143  0.996  0.999
 0.0418  129  0.997   11  1.000  140  0.997  0.999
 0.0482  150  0.991   12  1.000  162  0.992  0.999
 0.0545  151  0.997   12  0.994  163  0.997  0.999
 0.0609  172  0.983   15  0.956  187  0.981  0.999
 0.0672  174  0.993    9  0.934  183  0.990  0.999
 0.0735  178  0.990   11  1.000  189  0.990  0.999
 0.0799  189  0.989   14  0.999  203  0.990  0.999
 0.0862  197  0.984    9  0.975  206  0.983  0.999
 0.0925  193  0.979   14  0.930  207  0.975  0.999
 0.0989  188  0.980   12  1.000  200  0.981  0.999
 0.1052  190  0.988    8  1.000  198  0.989  0.999
 0.1116  183  0.981   13  0.937  196  0.978  1.000
 0.1179  194  0.980   11  0.942  205  0.978  1.000
 0.1242  174  0.983    8  1.000  182  0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0191
Free R factor                    =     0.0400
Overall weighted R factor        =     0.0191
Free weighted R factor           =     0.0404
Overall correlation coefficient  =     0.9993
Free correlation coefficient     =     0.9968
DPI based on free R factor       =     0.0727
Overall figure of merit          =     0.9869
ML based su of positional parameters =     0.0402
ML based su of thermal parameters    =     1.9838
------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10501.127       3162.0920       19681.133       19681.047

 fvalues    10501.127       3162.0920       19681.174       19681.047


    CGMAT cycle number =     86

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :   50   90   60
 Maximuum H,K,L                 :   12   21   14
 Minimum acceptable grid spacing:   33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
```

Weight matrix 0.60000002
Actual weight 1.5717542 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1650E+05 GEOM= 3162. TOTAL= 0.1967E+05
function value 19665.117

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.685	1.966
Torsion angles, period 1. refined	155	7.873	5.000
Torsion angles, period 2. refined	54	41.439	25.741
Torsion angles, period 3. refined	214	19.234	15.000
Torsion angles, period 4. refined	3	21.365	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	539	0.266	0.200
VDW; torsion: refined_atoms	789	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.251	0.200
Bond B values: refined atoms	1229	13.565	4.722
Angle B values: refined atoms	1663	16.737	7.129
Torsion B values: refined atoms	426	31.078	13.085
Long range B values: refined atoms	1334	11.657	15.307

Overall : scale = 1.012, B = -0.026
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 86. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 86. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 86. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 86. % observed v. resln :N:1,3:

$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 747.9 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.1 0.02 0.02 1 1228.6 1224.5 0.01 0.01
0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.1 413.4 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.8 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.3 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.0 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.2 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.2 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.7 0.03 0.03
0.067 174 99.45 211.5 210.9 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.1 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 155.8 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.1 0.07 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.0 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 140.9 0.08 0.08
0.118 194 81.85 127.0 126.7 0.02 0.02 9 138.0 137.2 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.0 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 86. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 86. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.991 12 0.924 95 0.982 0.999
0.0228 97 0.988 11 1.000 108 0.990 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.996 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.992 0.999
0.0545 151 0.997 12 0.994 163 0.997 0.999
0.0609 172 0.983 15 0.956 187 0.981 0.999
0.0672 174 0.993 9 0.934 183 0.990 0.999
0.0735 178 0.990 11 1.000 189 0.990 0.999
0.0799 189 0.989 14 0.999 203 0.990 0.999
0.0862 197 0.984 9 0.975 206 0.983 0.999
0.0925 193 0.979 14 0.930 207 0.976 0.999
0.0989 188 0.980 12 1.000 200 0.981 0.999
0.1052 190 0.988 8 1.000 198 0.989 0.999
0.1116 183 0.981 13 0.937 196 0.978 1.000

```
 0.1179   194   0.980    11   0.942   205   0.978  1.000
 0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0191
Free R factor                    =     0.0400
Overall weighted R factor        =     0.0191
Free weighted R factor           =     0.0404
Overall correlation coefficient  =     0.9993
Free correlation coefficient     =     0.9968
DPI based on free R factor       =     0.0727
Overall figure of merit          =     0.9869
ML based su of positional parameters =     0.0402
ML based su of thermal parameters    =     1.9830
------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10500.216       3162.1575       19665.801       19665.916


    CGMAT cycle number =     87

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    1.5711654      is applied to the X-ray term
Norm of X_ray positional gradient              13.7
Norm of Geom. positional gradient              13.7
Norm of X_ray B-factor gradient                17.8
Norm of Geom. B-factor gradient                18.2
Product of X_ray and Geom posit. gradients     -0.693E+06
 Cosine of angle between them                  -1.000
Product of X_ray and Geom B-fact gradients     -0.396E+06
 Cosine of angle between them                  -0.995


Residuals: XRAY=     0.1650E+05 GEOM=      3162.     TOTAL=     0.1966E+05
 function value    19658.268

------------------------------------------------------------------------------
          Restraint type            N restraints   Rms Delta   Av(Sigma)
```

Bond distances: refined atoms 1229 0.011 0.020
Bond angles : refined atoms 1663 1.686 1.966
Torsion angles, period 1. refined 155 7.872 5.000
Torsion angles, period 2. refined 54 41.439 25.741
Torsion angles, period 3. refined 214 19.234 15.000
Torsion angles, period 4. refined 3 21.362 15.000
Chiral centres: refined atoms 187 0.111 0.200
Planar groups: refined atoms 924 0.005 0.021
VDW repulsions: refined_atoms 539 0.266 0.200
VDW; torsion: refined_atoms 789 0.325 0.200
HBOND: refined_atoms 41 0.194 0.200
VDW repulsions: symmetry: refined_atoms 55 0.262 0.200
HBOND: symmetry: refined_atoms 3 0.250 0.200
Bond B values: refined atoms 1229 13.562 4.722
Angle B values: refined atoms 1663 16.742 7.129
Torsion B values: refined atoms 426 31.096 13.086
Long range B values: refined atoms 1334 11.654 15.307

Overall : scale = 1.012, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 87. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 87. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 87. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 87. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 747.9 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.1 0.02 0.02 1 1228.6 1224.6 0.01 0.01
0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.1 413.4 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.9 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.3 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.0 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.2 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.2 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.7 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.2 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 155.9 0.06 0.06

0.086	197	100.00	176.8	176.9	0.02	0.02	8	208.6	207.6	0.04	0.04
0.093	193	93.55	156.9	157.0	0.02	0.02	10	182.0	186.1	0.07	0.06
0.099	188	91.28	160.7	159.8	0.02	0.02	11	159.7	157.1	0.02	0.02
0.105	190	86.02	153.9	153.5	0.02	0.02	13	169.2	170.0	0.05	0.04
0.112	183	80.08	129.9	129.6	0.02	0.02	6	135.2	141.0	0.08	0.08
0.118	194	81.85	127.0	126.7	0.02	0.02	9	138.0	137.2	0.05	0.05
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	111.0	0.06	0.06

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 87. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 87. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.991	12	0.924	95	0.982	0.999
0.0228	97	0.988	11	1.000	108	0.990	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.996	17	1.000	143	0.996	0.999
0.0418	129	0.997	11	1.000	140	0.997	0.999
0.0482	150	0.991	12	1.000	162	0.992	0.999
0.0545	151	0.997	12	0.994	163	0.997	0.999
0.0609	172	0.983	15	0.956	187	0.981	0.999
0.0672	174	0.993	9	0.934	183	0.990	0.999
0.0735	178	0.990	11	1.000	189	0.990	0.999
0.0799	189	0.989	14	0.999	203	0.990	0.999
0.0862	197	0.984	9	0.975	206	0.983	0.999
0.0925	193	0.979	14	0.930	207	0.976	0.999
0.0989	188	0.980	12	1.000	200	0.981	0.999
0.1052	190	0.988	8	1.000	198	0.989	0.999
0.1116	183	0.981	13	0.937	196	0.978	1.000
0.1179	194	0.980	11	0.942	205	0.978	1.000
0.1242	174	0.983	8	1.000	182	0.984	1.000

$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0191
Free R factor = 0.0400
Overall weighted R factor = 0.0191
Free weighted R factor = 0.0404
Overall correlation coefficient = 0.9994
Free correlation coefficient = 0.9968
DPI based on free R factor = 0.0726
Overall figure of merit = 0.9869
ML based su of positional parameters = 0.0402
ML based su of thermal parameters = 1.9825

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10499.578 3162.4607 19659.004 19659.035

CGMAT cycle number = 88

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5686036 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1647E+05 GEOM= 3163. TOTAL= 0.1963E+05
function value 19628.104

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.686	1.966
Torsion angles, period 1. refined	155	7.872	5.000
Torsion angles, period 2. refined	54	41.440	25.741
Torsion angles, period 3. refined	214	19.233	15.000
Torsion angles, period 4. refined	3	21.364	15.000
Chiral centres: refined atoms	187	0.111	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	539	0.266	0.200
VDW; torsion: refined_atoms	789	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.248	0.200
Bond B values: refined atoms	1229	13.560	4.723
Angle B values: refined atoms	1663	16.747	7.130
Torsion B values: refined atoms	426	31.115	13.087
Long range B values: refined atoms	1334	11.651	15.306

Overall : scale = 1.012, B = -0.026
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 88. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 88. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 88. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 88. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 747.9 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.1 0.02 0.02 1 1228.6 1224.6 0.01 0.01
0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.1 413.4 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.9 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.0 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.2 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.2 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.7 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.2 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 155.9 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.1 0.07 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.0 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 141.0 0.08 0.08
0.118 194 81.85 127.0 126.8 0.02 0.02 9 138.0 137.2 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.0 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 88. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 88. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999

```
 0.0102   62  0.999    7  1.000   69  0.999  0.999
 0.0165   83  0.991   12  0.924   95  0.982  0.999
 0.0228   97  0.988   11  1.000  108  0.990  0.999
 0.0292  108  0.997    6  1.000  114  0.997  0.999
 0.0355  126  0.996   17  1.000  143  0.996  0.999
 0.0418  129  0.997   11  1.000  140  0.997  0.999
 0.0482  150  0.991   12  1.000  162  0.992  0.999
 0.0545  151  0.997   12  0.994  163  0.997  0.999
 0.0609  172  0.983   15  0.956  187  0.981  0.999
 0.0672  174  0.993    9  0.934  183  0.990  0.999
 0.0735  178  0.990   11  1.000  189  0.991  0.999
 0.0799  189  0.989   14  0.999  203  0.990  0.999
 0.0862  197  0.984    9  0.975  206  0.983  0.999
 0.0925  193  0.979   14  0.930  207  0.976  0.999
 0.0989  188  0.980   12  1.000  200  0.981  0.999
 0.1052  190  0.988    8  1.000  198  0.989  0.999
 0.1116  183  0.981   13  0.937  196  0.978  1.000
 0.1179  194  0.980   11  0.943  205  0.978  1.000
 0.1242  174  0.983    8  1.000  182  0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0191
Free R factor                    =     0.0400
Overall weighted R factor        =     0.0191
Free weighted R factor           =     0.0403
Overall correlation coefficient  =     0.9993
Free correlation coefficient     =     0.9969
DPI based on free R factor       =     0.0726
Overall figure of merit          =     0.9870
ML based su of positional parameters =     0.0401
ML based su of thermal parameters    =     1.9811
------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10497.459       3162.5806       19628.754       19628.934


    CGMAT cycle number =     89

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :   50   90   60
 Maximuum H,K,L                 :   12   21   14
 Minimum acceptable grid spacing:   33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
```

Weight matrix 0.60000002
Actual weight 1.5672158 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1645E+05 GEOM= 3163. TOTAL= 0.1961E+05
function value 19612.066

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.686	1.966
Torsion angles, period 1. refined	155	7.872	5.000
Torsion angles, period 2. refined	54	41.441	25.741
Torsion angles, period 3. refined	214	19.234	15.000
Torsion angles, period 4. refined	3	21.365	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	539	0.266	0.200
VDW; torsion: refined_atoms	789	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.246	0.200
Bond B values: refined atoms	1229	13.555	4.723
Angle B values: refined atoms	1663	16.748	7.129
Torsion B values: refined atoms	426	31.129	13.087
Long range B values: refined atoms	1334	11.645	15.306

Overall : scale = 1.012, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 89. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 89. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 89. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 89. % observed v. resln :N:1,3:

$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 747.9 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.1 0.02 0.02 1 1228.6 1224.7 0.01 0.01
0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.1 413.4 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.9 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.0 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.2 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.2 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.7 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.2 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 155.9 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.1 0.07 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.0 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 141.0 0.08 0.08
0.118 194 81.85 127.0 126.7 0.02 0.02 9 138.0 137.2 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.1 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 89. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 89. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.991 12 0.925 95 0.982 0.999
0.0228 97 0.988 11 1.000 108 0.990 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.996 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.992 0.999
0.0545 151 0.997 12 0.994 163 0.997 0.999
0.0609 172 0.983 15 0.956 187 0.981 0.999
0.0672 174 0.993 9 0.934 183 0.990 0.999
0.0735 178 0.990 11 1.000 189 0.990 0.999
0.0799 189 0.989 14 0.999 203 0.990 0.999
0.0862 197 0.984 9 0.975 206 0.983 0.999
0.0925 193 0.979 14 0.930 207 0.976 0.999
0.0989 188 0.980 12 1.000 200 0.981 0.999
0.1052 190 0.988 8 1.000 198 0.989 0.999
0.1116 183 0.981 13 0.937 196 0.978 1.000

```
 0.1179   194   0.980    11   0.943   205   0.978  1.000
 0.1242   174   0.984     8   1.000   182   0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0191
Free R factor                    =     0.0399
Overall weighted R factor        =     0.0191
Free weighted R factor           =     0.0403
Overall correlation coefficient  =     0.9993
Free correlation coefficient     =     0.9969
DPI based on free R factor       =     0.0725
Overall figure of merit          =     0.9870
ML based su of positional parameters =     0.0401
ML based su of thermal parameters    =     1.9800
---------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10496.278       3162.9036       19612.785       19612.836


    CGMAT cycle number =     90

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    1.5680692      is applied to the X-ray term
Norm of X_ray positional gradient              13.7
Norm of Geom. positional gradient              13.7
Norm of X_ray B-factor gradient                17.8
Norm of Geom. B-factor gradient                18.2
Product of X_ray and Geom posit. gradients     -0.693E+06
 Cosine of angle between them                  -1.000
Product of X_ray and Geom B-fact gradients     -0.396E+06
 Cosine of angle between them                  -0.995


Residuals: XRAY=     0.1646E+05 GEOM=      3163.     TOTAL=     0.1962E+05
 function value    19621.621

---------------------------------------------------------------------------
          Restraint type            N restraints   Rms Delta    Av(Sigma)
```

Bond distances: refined atoms 1229 0.011 0.020
Bond angles : refined atoms 1663 1.686 1.966
Torsion angles, period 1. refined 155 7.872 5.000
Torsion angles, period 2. refined 54 41.440 25.741
Torsion angles, period 3. refined 214 19.231 15.000
Torsion angles, period 4. refined 3 21.363 15.000
Chiral centres: refined atoms 187 0.111 0.200
Planar groups: refined atoms 924 0.005 0.021
VDW repulsions: refined_atoms 539 0.266 0.200
VDW; torsion: refined_atoms 789 0.325 0.200
HBOND: refined_atoms 41 0.194 0.200
VDW repulsions: symmetry: refined_atoms 55 0.262 0.200
HBOND: symmetry: refined_atoms 3 0.245 0.200
Bond B values: refined atoms 1229 13.551 4.723
Angle B values: refined atoms 1663 16.751 7.129
Torsion B values: refined atoms 426 31.144 13.088
Long range B values: refined atoms 1334 11.639 15.306

Overall : scale = 1.012, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 90. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 90. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 90. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 90. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 747.9 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.1 0.02 0.02 1 1228.6 1224.7 0.01 0.01
0.017 83 95.60 307.7 308.7 0.03 0.02 4 403.1 413.4 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 188.9 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.1 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.2 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.2 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.7 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.2 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 155.9 0.06 0.06

0.086	197	100.00	176.8	176.9	0.02	0.02	8	208.6	207.6	0.04	0.04
0.093	193	93.55	156.9	157.0	0.02	0.02	10	182.0	186.1	0.07	0.06
0.099	188	91.28	160.7	159.8	0.02	0.02	11	159.7	157.1	0.02	0.02
0.105	190	86.02	153.9	153.5	0.02	0.02	13	169.2	170.0	0.05	0.04
0.112	183	80.08	129.9	129.6	0.02	0.02	6	135.2	141.0	0.08	0.08
0.118	194	81.85	127.0	126.7	0.02	0.02	9	138.0	137.2	0.05	0.05
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	111.0	0.06	0.06

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 90. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 90. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.991	12	0.925	95	0.982	0.999
0.0228	97	0.988	11	1.000	108	0.990	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.996	17	1.000	143	0.996	0.999
0.0418	129	0.997	11	1.000	140	0.997	0.999
0.0482	150	0.991	12	1.000	162	0.992	0.999
0.0545	151	0.997	12	0.994	163	0.997	0.999
0.0609	172	0.983	15	0.957	187	0.981	0.999
0.0672	174	0.993	9	0.933	183	0.990	0.999
0.0735	178	0.990	11	1.000	189	0.990	0.999
0.0799	189	0.989	14	0.999	203	0.990	0.999
0.0862	197	0.984	9	0.975	206	0.983	0.999
0.0925	193	0.979	14	0.930	207	0.976	0.999
0.0989	188	0.980	12	1.000	200	0.981	0.999
0.1052	190	0.988	8	1.000	198	0.989	0.999
0.1116	183	0.981	13	0.937	196	0.978	1.000
0.1179	194	0.980	11	0.943	205	0.978	1.000
0.1242	174	0.983	8	1.000	182	0.984	1.000

$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0191
Free R factor = 0.0399
Overall weighted R factor = 0.0191
Free weighted R factor = 0.0403
Overall correlation coefficient = 0.9994
Free correlation coefficient = 0.9969
DPI based on free R factor = 0.0725
Overall figure of merit = 0.9870
ML based su of positional parameters = 0.0401
ML based su of thermal parameters = 1.9808

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10496.663 3162.8884 19622.201 19622.383

CGMAT cycle number = 91

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5650843 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.692E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.395E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1642E+05 GEOM= 3163. TOTAL= 0.1959E+05
function value 19586.520

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.686	1.966
Torsion angles, period 1. refined	155	7.872	5.000
Torsion angles, period 2. refined	54	41.441	25.741
Torsion angles, period 3. refined	214	19.243	15.000
Torsion angles, period 4. refined	3	21.360	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	539	0.266	0.200
VDW; torsion: refined_atoms	789	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.243	0.200
Bond B values: refined atoms	1229	13.560	4.724
Angle B values: refined atoms	1663	16.767	7.130
Torsion B values: refined atoms	426	31.184	13.090
Long range B values: refined atoms	1334	11.646	15.306

Overall : scale = 1.012, B = -0.026
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 91. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 91. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 91. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 91. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 747.9 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.1 0.02 0.02 1 1228.7 1224.8 0.01 0.01
0.017 83 95.60 307.8 308.7 0.03 0.02 4 403.1 413.3 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 189.0 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.1 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.2 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.2 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.7 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.3 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 155.9 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.1 0.07 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.0 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 141.1 0.08 0.08
0.118 194 81.85 127.0 126.8 0.02 0.02 9 138.0 137.2 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.1 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 91. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 91. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999

```
 0.0102   62  0.999    7  1.000   69  0.999  0.999
 0.0165   83  0.991   12  0.925   95  0.982  0.999
 0.0228   97  0.988   11  1.000  108  0.990  0.999
 0.0292  108  0.997    6  1.000  114  0.997  0.999
 0.0355  126  0.996   17  1.000  143  0.996  0.999
 0.0418  129  0.997   11  1.000  140  0.997  0.999
 0.0482  150  0.991   12  1.000  162  0.992  0.999
 0.0545  151  0.997   12  0.994  163  0.997  0.999
 0.0609  172  0.983   15  0.956  187  0.981  0.999
 0.0672  174  0.993    9  0.933  183  0.990  0.999
 0.0735  178  0.990   11  1.000  189  0.990  0.999
 0.0799  189  0.989   14  0.999  203  0.990  0.999
 0.0862  197  0.984    9  0.975  206  0.983  0.999
 0.0925  193  0.979   14  0.930  207  0.976  0.999
 0.0989  188  0.980   12  1.000  200  0.981  0.999
 0.1052  190  0.988    8  1.000  198  0.989  0.999
 0.1116  183  0.981   13  0.937  196  0.978  1.000
 0.1179  194  0.980   11  0.944  205  0.978  1.000
 0.1242  174  0.983    8  1.000  182  0.984  1.000
 $$
Resolution limits                =    38.899    2.802
Number of used reflections       =      3184
Percentage observed              =   92.6870
Percentage of free reflections   =    4.8416
Overall R factor                 =    0.0191
Free R factor                    =    0.0399
Overall weighted R factor        =    0.0191
Free weighted R factor           =    0.0403
Overall correlation coefficient  =    0.9993
Free correlation coefficient     =    0.9969
DPI based on free R factor       =    0.0725
Overall figure of merit          =    0.9870
ML based su of positional parameters =    0.0401
ML based su of thermal parameters    =    1.9790
-------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10493.949       3163.4226       19588.537       19587.338

 fvalues    10493.949       3163.4226       19587.461       19587.338


    CGMAT cycle number =     92

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :   50   90   60
 Maximuum H,K,L                 :   12   21   14
 Minimum acceptable grid spacing:   33   56   38
 fast hessian tabulation
```

B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5648897 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.692E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1642E+05 GEOM= 3163. TOTAL= 0.1958E+05
function value 19584.230

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.686	1.966
Torsion angles, period 1. refined	155	7.872	5.000
Torsion angles, period 2. refined	54	41.441	25.741
Torsion angles, period 3. refined	214	19.232	15.000
Torsion angles, period 4. refined	3	21.360	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.265	0.200
VDW; torsion: refined_atoms	789	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.243	0.200
Bond B values: refined atoms	1229	13.558	4.724
Angle B values: refined atoms	1663	16.768	7.130
Torsion B values: refined atoms	426	31.186	13.090
Long range B values: refined atoms	1335	11.640	15.309

Overall : scale = 1.012, B = -0.026
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 92. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 92. <Rfactor> v. resln :N:1,6,7,11,12:

:Cycle 92. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 92. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 747.9 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.1 0.02 0.02 1 1228.7 1224.8 0.01 0.01
0.017 83 95.60 307.8 308.7 0.03 0.02 4 403.1 413.3 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 189.0 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.1 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.2 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.2 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.7 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.3 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 155.9 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.1 0.07 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.0 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 141.1 0.08 0.08
0.118 194 81.85 127.0 126.8 0.02 0.02 9 138.0 137.1 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.0 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 92. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 92. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.991 12 0.925 95 0.982 0.999
0.0228 97 0.988 11 1.000 108 0.990 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.996 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.992 0.999
0.0545 151 0.997 12 0.994 163 0.997 0.999
0.0609 172 0.983 15 0.956 187 0.981 0.999
0.0672 174 0.993 9 0.933 183 0.990 0.999
0.0735 178 0.990 11 1.000 189 0.991 0.999
0.0799 189 0.989 14 0.999 203 0.990 0.999
0.0862 197 0.984 9 0.975 206 0.983 0.999
0.0925 193 0.979 14 0.930 207 0.976 0.999
0.0989 188 0.980 12 1.000 200 0.981 0.999

```
 0.1052   190   0.988    8   1.000   198   0.989  0.999
 0.1116   183   0.981   13   0.937   196   0.978  1.000
 0.1179   194   0.980   11   0.944   205   0.978  1.000
 0.1242   174   0.983    8   1.000   182   0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0191
Free R factor                    =     0.0399
Overall weighted R factor        =     0.0191
Free weighted R factor           =     0.0403
Overall correlation coefficient  =     0.9993
Free correlation coefficient     =     0.9969
DPI based on free R factor       =     0.0724
Overall figure of merit          =     0.9870
ML based su of positional parameters =     0.0401
ML based su of thermal parameters    =     1.9788
------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10493.790       3163.3687       19585.035       19584.992

 fvalues    10493.790       3163.3687       19584.941       19584.992


    CGMAT cycle number =     93

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    1.5637804      is applied to the X-ray term
Norm of X_ray positional gradient              13.7
Norm of Geom. positional gradient              13.7
Norm of X_ray B-factor gradient                17.8
Norm of Geom. B-factor gradient                18.2
Product of X_ray and Geom posit. gradients     -0.692E+06
 Cosine of angle between them                  -1.000
Product of X_ray and Geom B-fact gradients     -0.396E+06
 Cosine of angle between them                  -0.995


Residuals: XRAY=     0.1641E+05 GEOM=      3163.     TOTAL=     0.1957E+05
```

function value 19571.377

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.686	1.966
Torsion angles, period 1. refined	155	7.872	5.000
Torsion angles, period 2. refined	54	41.441	25.741
Torsion angles, period 3. refined	214	19.234	15.000
Torsion angles, period 4. refined	3	21.360	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.265	0.200
VDW; torsion: refined_atoms	789	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.242	0.200
Bond B values: refined atoms	1229	13.556	4.724
Angle B values: refined atoms	1663	16.769	7.130
Torsion B values: refined atoms	426	31.193	13.090
Long range B values: refined atoms	1335	11.638	15.309

Overall : scale = 1.012, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 93. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 93. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 93. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 93. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$

0.004	30	62.50	754.4	747.9	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	414.1	416.1	0.02	0.02	1	1228.7	1224.8	0.01	0.01	
0.017	83	95.60	307.8	308.8	0.03	0.02	4	403.1	413.3	0.04	0.05	
0.023	97	97.14	247.4	248.4	0.02	0.02	5	180.2	189.0	0.07	0.07	
0.029	108	100.00	241.3	242.0	0.02	0.02	7	186.7	189.4	0.06	0.06	
0.036	126	99.25	270.4	270.7	0.02	0.02	6	252.9	254.1	0.04	0.04	
0.042	129	98.56	286.3	287.5	0.02	0.02	8	338.1	341.2	0.02	0.02	
0.048	150	98.73	296.8	296.4	0.02	0.01	5	305.8	307.3	0.03	0.02	
0.055	151	99.38	281.3	281.5	0.01	0.01	10	257.9	260.1	0.04	0.04	

0.061	172	100.00	218.4	218.6	0.02	0.02	10	202.2	202.7	0.03	0.03
0.067	174	99.45	211.5	211.0	0.02	0.02	6	286.3	284.4	0.02	0.02
0.074	178	98.92	206.1	206.8	0.02	0.02	6	234.6	237.3	0.03	0.03
0.080	189	100.00	208.7	209.0	0.02	0.02	13	159.7	155.9	0.06	0.06
0.086	197	100.00	176.8	176.9	0.02	0.02	8	208.6	207.6	0.04	0.04
0.093	193	93.55	156.9	157.0	0.02	0.02	10	182.0	186.1	0.07	0.06
0.099	188	91.28	160.7	159.8	0.02	0.02	11	159.7	157.1	0.02	0.02
0.105	190	86.02	153.9	153.5	0.02	0.02	13	169.2	170.0	0.05	0.04
0.112	183	80.08	129.9	129.6	0.02	0.02	6	135.2	141.1	0.08	0.08
0.118	194	81.85	127.0	126.8	0.02	0.02	9	138.0	137.1	0.05	0.05
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	111.0	0.06	0.06

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 93. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 93. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.991	12	0.925	95	0.982	0.999
0.0228	97	0.988	11	1.000	108	0.990	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.996	17	1.000	143	0.996	0.999
0.0418	129	0.997	11	1.000	140	0.997	0.999
0.0482	150	0.991	12	1.000	162	0.992	0.999
0.0545	151	0.997	12	0.994	163	0.997	0.999
0.0609	172	0.983	15	0.956	187	0.981	0.999
0.0672	174	0.993	9	0.933	183	0.990	0.999
0.0735	178	0.990	11	1.000	189	0.990	0.999
0.0799	189	0.989	14	0.999	203	0.990	0.999
0.0862	197	0.984	9	0.975	206	0.983	0.999
0.0925	193	0.979	14	0.930	207	0.976	0.999
0.0989	188	0.980	12	1.000	200	0.981	0.999
0.1052	190	0.988	8	1.000	198	0.989	0.999
0.1116	183	0.981	13	0.937	196	0.978	1.000
0.1179	194	0.980	11	0.944	205	0.978	1.000
0.1242	174	0.984	8	1.000	182	0.984	1.000

$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0191
Free R factor = 0.0399
Overall weighted R factor = 0.0191
Free weighted R factor = 0.0403
Overall correlation coefficient = 0.9994
Free correlation coefficient = 0.9969

DPI based on free R factor = 0.0724
Overall figure of merit = 0.9870
ML based su of positional parameters = 0.0401
ML based su of thermal parameters = 1.9780

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10492.994 3163.4224 19572.154 19572.162

CGMAT cycle number = 94

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5644822 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1642E+05 GEOM= 3164. TOTAL= 0.1958E+05
function value 19579.365

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.686	1.966
Torsion angles, period 1. refined	155	7.871	5.000
Torsion angles, period 2. refined	54	41.441	25.741
Torsion angles, period 3. refined	214	19.227	15.000
Torsion angles, period 4. refined	3	21.359	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.265	0.200
VDW; torsion: refined_atoms	789	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.240	0.200

Bond B values: refined atoms 1229 13.552 4.724
Angle B values: refined atoms 1663 16.772 7.130
Torsion B values: refined atoms 426 31.210 13.091
Long range B values: refined atoms 1335 11.632 15.308

Overall : scale = 1.012, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 94. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 94. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 94. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 94. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 747.9 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.1 0.02 0.02 1 1228.7 1224.9 0.01 0.01
0.017 83 95.60 307.8 308.8 0.03 0.02 4 403.1 413.3 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 189.0 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.1 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.2 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.3 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.7 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.3 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 155.9 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.1 0.07 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.0 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 141.1 0.08 0.08
0.118 194 81.85 127.0 126.8 0.02 0.02 9 138.0 137.1 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.0 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 94. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 94. M(Fom) v. resln :N:1,3,5,7,8:

$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
 0.0038   30 0.999   4 1.000   34 0.999 0.999
 0.0102   62 0.999   7 1.000   69 0.999 0.999
 0.0165   83 0.991   12 0.925   95 0.982 0.999
 0.0228   97 0.988   11 1.000 108 0.990 0.999
 0.0292 108 0.997   6 1.000 114 0.997 0.999
 0.0355 126 0.996   17 1.000 143 0.996 0.999
 0.0418 129 0.997   11 1.000 140 0.997 0.999
 0.0482 150 0.991   12 1.000 162 0.992 0.999
 0.0545 151 0.997   12 0.994 163 0.997 0.999
 0.0609 172 0.983   15 0.957 187 0.981 0.999
 0.0672 174 0.993   9 0.934 183 0.990 0.999
 0.0735 178 0.990   11 1.000 189 0.991 0.999
 0.0799 189 0.989   14 0.999 203 0.990 0.999
 0.0862 197 0.984   9 0.975 206 0.983 0.999
 0.0925 193 0.979   14 0.930 207 0.976 0.999
 0.0989 188 0.980   12 1.000 200 0.981 0.999
 0.1052 190 0.988   8 1.000 198 0.989 0.999
 0.1116 183 0.981   13 0.937 196 0.978 1.000
 0.1179 194 0.980   11 0.944 205 0.978 1.000
 0.1242 174 0.983   8 1.000 182 0.984 1.000
$$
Resolution limits   =   38.899   2.802
Number of used reflections   =   3184
Percentage observed   =   92.6870
Percentage of free reflections   =   4.8416
Overall R factor   =   0.0191
Free R factor   =   0.0399
Overall weighted R factor   =   0.0191
Free weighted R factor   =   0.0403
Overall correlation coefficient   =   0.9994
Free correlation coefficient   =   0.9969
DPI based on free R factor   =   0.0724
Overall figure of merit   =   0.9870
ML based su of positional parameters =   0.0401
ML based su of thermal parameters   =   1.9786

 Trying gamma equal   0.0000000
 Convergence reached with no gamma cycles

 fvalues   10493.314   3163.5151   19580.342   19580.119

 fvalues   10493.314   3163.5151   19580.027   19580.119

    CGMAT cycle number =   95

 Limits of asymmetric unit   : 1.00 1.00 0.50

```
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    1.5633849      is applied to the X-ray term
Norm of X_ray positional gradient              13.7
Norm of Geom. positional gradient              13.7
Norm of X_ray B-factor gradient                17.8
Norm of Geom. B-factor gradient                18.2
Product of X_ray and Geom posit. gradients     -0.692E+06
 Cosine of angle between them                  -1.000
Product of X_ray and Geom B-fact gradients     -0.396E+06
 Cosine of angle between them                  -0.995


Residuals: XRAY=     0.1640E+05 GEOM=      3164.     TOTAL=     0.1957E+05
 function value    19566.389

------------------------------------------------------------------------------
          Restraint type            N restraints   Rms Delta   Av(Sigma)
Bond distances: refined atoms              1229     0.011     0.020
Bond angles  : refined atoms               1663     1.686     1.966
Torsion angles, period  1. refined          155     7.871     5.000
Torsion angles, period  2. refined           54    41.441    25.741
Torsion angles, period  3. refined          214    19.239    15.000
Torsion angles, period  4. refined            3    21.357    15.000
Chiral centres: refined atoms              187     0.112     0.200
Planar groups: refined atoms               924     0.005     0.021
VDW repulsions: refined_atoms              540     0.265     0.200
VDW; torsion: refined_atoms                789     0.325     0.200
HBOND: refined_atoms                        41     0.194     0.200
VDW repulsions: symmetry: refined_atoms     55     0.262     0.200
HBOND: symmetry: refined_atoms               3     0.240     0.200
Bond B values: refined atoms               1229    13.553     4.724
Angle B values: refined atoms              1663    16.776     7.130
Torsion B values: refined atoms             426    31.223    13.092
Long range B values: refined atoms         1335    11.633    15.308
------------------------------------------------------------------------------


------------------------------------------------------------------------------
Overall          : scale =    1.012, B  =  -0.025
Overall anisotropic scale factors
   B11 =  0.28 B22 =  0.17 B33 = -0.47 B12 =  0.00 B13 = -0.36 B23 =  0.00
------------------------------------------------------------------------------


------------------------------------------------------------------------------

    ****          Things for loggraph, R factor and others          ****
```

$TABLE: Cycle 95. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 95. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 95. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 95. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 747.9 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.1 0.02 0.02 1 1228.7 1224.9 0.01 0.01
0.017 83 95.60 307.8 308.7 0.03 0.02 4 403.1 413.3 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 189.0 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.1 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.2 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.3 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.7 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.3 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.3 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 155.9 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.1 0.07 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.0 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 141.1 0.08 0.08
0.118 194 81.85 127.0 126.8 0.02 0.02 9 138.0 137.1 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.0 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 95. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 95. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.991 12 0.925 95 0.982 0.999
0.0228 97 0.988 11 1.000 108 0.990 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.996 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.992 0.999
0.0545 151 0.997 12 0.994 163 0.997 0.999
0.0609 172 0.983 15 0.957 187 0.981 0.999
0.0672 174 0.993 9 0.933 183 0.990 0.999
0.0735 178 0.990 11 1.000 189 0.991 0.999

```
 0.0799   189   0.989    14   0.999   203   0.990  0.999
 0.0862   197   0.984     9   0.976   206   0.983  0.999
 0.0925   193   0.979    14   0.930   207   0.976  0.999
 0.0989   188   0.980    12   1.000   200   0.981  0.999
 0.1052   190   0.988     8   1.000   198   0.989  0.999
 0.1116   183   0.981    13   0.937   196   0.978  1.000
 0.1179   194   0.980    11   0.944   205   0.978  1.000
 0.1242   174   0.983     8   1.000   182   0.984  1.000
$$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0191
Free R factor                    =     0.0399
Overall weighted R factor        =     0.0191
Free weighted R factor           =     0.0403
Overall correlation coefficient  =     0.9994
Free correlation coefficient     =     0.9969
DPI based on free R factor       =     0.0724
Overall figure of merit          =     0.9870
ML based su of positional parameters =     0.0401
ML based su of thermal parameters    =     1.9780
-------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10492.264       3163.7300       19567.867       19567.176

 fvalues    10492.264       3163.7300       19567.186       19567.176


    CGMAT cycle number =     96

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000008
 Actual weight    1.5626702      is applied to the X-ray term
Norm of X_ray positional gradient              13.7
Norm of Geom. positional gradient              13.7
Norm of X_ray B-factor gradient                17.8
Norm of Geom. B-factor gradient                18.2
Product of X_ray and Geom posit. gradients     -0.692E+06
 Cosine of angle between them                  -1.000
Product of X_ray and Geom B-fact gradients     -0.396E+06
```

Cosine of angle between them -0.995

Residuals: XRAY= 0.1639E+05 GEOM= 3164. TOTAL= 0.1956E+05
function value 19558.014

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.686	1.966
Torsion angles, period 1. refined	155	7.871	5.000
Torsion angles, period 2. refined	54	41.441	25.741
Torsion angles, period 3. refined	214	19.231	15.000
Torsion angles, period 4. refined	3	21.357	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.265	0.200
VDW; torsion: refined_atoms	789	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.239	0.200
Bond B values: refined atoms	1229	13.553	4.724
Angle B values: refined atoms	1663	16.778	7.130
Torsion B values: refined atoms	426	31.228	13.092
Long range B values: refined atoms	1335	11.632	15.308

Overall : scale = 1.012, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 96. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 96. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 96. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 96. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$

0.004	30	62.50	754.4	747.9	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	414.1	416.1	0.02	0.02	1	1228.7	1224.9	0.01	0.01	
0.017	83	95.60	307.8	308.8	0.03	0.02	4	403.1	413.3	0.04	0.05	
0.023	97	97.14	247.4	248.4	0.02	0.02	5	180.2	189.0	0.07	0.07	
0.029	108	100.00	241.3	242.0	0.02	0.02	7	186.7	189.4	0.06	0.06	

0.036	126	99.25	270.4	270.7	0.02	0.02	6	252.9	254.1	0.04	0.04
0.042	129	98.56	286.3	287.5	0.02	0.02	8	338.1	341.2	0.02	0.02
0.048	150	98.73	296.8	296.4	0.02	0.01	5	305.8	307.3	0.03	0.02
0.055	151	99.38	281.3	281.5	0.01	0.01	10	257.9	260.1	0.04	0.04
0.061	172	100.00	218.4	218.6	0.02	0.02	10	202.2	202.7	0.03	0.03
0.067	174	99.45	211.5	211.0	0.02	0.02	6	286.3	284.4	0.02	0.02
0.074	178	98.92	206.1	206.8	0.02	0.02	6	234.6	237.3	0.03	0.03
0.080	189	100.00	208.7	209.0	0.02	0.02	13	159.7	155.9	0.06	0.06
0.086	197	100.00	176.8	176.9	0.02	0.02	8	208.6	207.6	0.04	0.04
0.093	193	93.55	156.9	157.0	0.02	0.02	10	182.0	186.1	0.07	0.06
0.099	188	91.28	160.7	159.8	0.02	0.02	11	159.7	157.1	0.02	0.02
0.105	190	86.02	153.9	153.5	0.02	0.02	13	169.2	170.0	0.05	0.04
0.112	183	80.08	129.9	129.6	0.02	0.02	6	135.2	141.1	0.08	0.08
0.118	194	81.85	127.0	126.8	0.02	0.02	9	138.0	137.1	0.05	0.05
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	111.0	0.06	0.06

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 96. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 96. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.991	12	0.925	95	0.983	0.999
0.0228	97	0.988	11	1.000	108	0.990	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.996	17	1.000	143	0.996	0.999
0.0418	129	0.997	11	1.000	140	0.997	0.999
0.0482	150	0.991	12	1.000	162	0.992	0.999
0.0545	151	0.997	12	0.994	163	0.997	0.999
0.0609	172	0.983	15	0.956	187	0.981	0.999
0.0672	174	0.993	9	0.933	183	0.990	0.999
0.0735	178	0.990	11	1.000	189	0.991	0.999
0.0799	189	0.989	14	0.999	203	0.990	0.999
0.0862	197	0.984	9	0.976	206	0.983	0.999
0.0925	193	0.979	14	0.930	207	0.976	0.999
0.0989	188	0.980	12	1.000	200	0.981	0.999
0.1052	190	0.988	8	1.000	198	0.989	0.999
0.1116	183	0.981	13	0.937	196	0.978	1.000
0.1179	194	0.980	11	0.944	205	0.978	1.000
0.1242	174	0.983	8	1.000	182	0.984	1.000

$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0191
Free R factor = 0.0399

Overall weighted R factor = 0.0191
Free weighted R factor = 0.0403
Overall correlation coefficient = 0.9994
Free correlation coefficient = 0.9969
DPI based on free R factor = 0.0724
Overall figure of merit = 0.9870
ML based su of positional parameters = 0.0401
ML based su of thermal parameters = 1.9775

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10491.698 3163.7036 19558.895 19558.768

fvalues 10491.698 3163.7036 19558.936 19558.768

CGMAT cycle number = 97

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5620717 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.692E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.395E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1639E+05 GEOM= 3164. TOTAL= 0.1955E+05
function value 19551.031

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.686	1.966
Torsion angles, period 1. refined	155	7.871	5.000
Torsion angles, period 2. refined	54	41.441	25.741
Torsion angles, period 3. refined	214	19.232	15.000
Torsion angles, period 4. refined	3	21.357	15.000
Chiral centres: refined atoms	187	0.112	0.200

Planar groups: refined atoms 924 0.005 0.021
VDW repulsions: refined_atoms 539 0.266 0.200
VDW; torsion: refined_atoms 789 0.325 0.200
HBOND: refined_atoms 41 0.194 0.200
VDW repulsions: symmetry: refined_atoms 55 0.262 0.200
HBOND: symmetry: refined_atoms 3 0.239 0.200
Bond B values: refined atoms 1229 13.553 4.724
Angle B values: refined atoms 1663 16.780 7.130
Torsion B values: refined atoms 426 31.234 13.092
Long range B values: refined atoms 1334 11.636 15.310

Overall : scale = 1.012, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 97. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 97. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 97. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 97. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 747.9 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.1 0.02 0.02 1 1228.7 1224.9 0.01 0.01
0.017 83 95.60 307.8 308.8 0.03 0.02 4 403.1 413.3 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 189.1 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.1 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.2 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.3 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.7 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.3 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 155.9 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.1 0.07 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.0 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 141.1 0.08 0.08
0.118 194 81.85 127.0 126.8 0.02 0.02 9 138.0 137.1 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.0 0.06 0.06

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 97. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 97. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.991 12 0.925 95 0.983 0.999
0.0228 97 0.988 11 1.000 108 0.990 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.996 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.992 0.999
0.0545 151 0.997 12 0.994 163 0.997 0.999
0.0609 172 0.983 15 0.956 187 0.981 0.999
0.0672 174 0.993 9 0.933 183 0.990 0.999
0.0735 178 0.990 11 1.000 189 0.991 0.999
0.0799 189 0.989 14 0.999 203 0.990 0.999
0.0862 197 0.984 9 0.976 206 0.983 0.999
0.0925 193 0.979 14 0.930 207 0.976 0.999
0.0989 188 0.980 12 1.000 200 0.981 0.999
0.1052 190 0.988 8 1.000 198 0.989 0.999
0.1116 183 0.981 13 0.937 196 0.978 1.000
0.1179 194 0.980 11 0.944 205 0.978 1.000
0.1242 174 0.984 8 1.000 182 0.984 1.000
$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0190
Free R factor = 0.0399
Overall weighted R factor = 0.0191
Free weighted R factor = 0.0402
Overall correlation coefficient = 0.9994
Free correlation coefficient = 0.9969
DPI based on free R factor = 0.0724
Overall figure of merit = 0.9870
ML based su of positional parameters = 0.0400
ML based su of thermal parameters = 1.9771

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10491.225 3163.7324 19551.826 19551.777

fvalues 10491.225 3163.7324 19551.896 19551.777

CGMAT cycle number = 98

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5611560 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.692E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1638E+05 GEOM= 3164. TOTAL= 0.1954E+05
function value 19540.248

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.686	1.966
Torsion angles, period 1. refined	155	7.871	5.000
Torsion angles, period 2. refined	54	41.441	25.741
Torsion angles, period 3. refined	214	19.232	15.000
Torsion angles, period 4. refined	3	21.356	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	539	0.266	0.200
VDW; torsion: refined_atoms	789	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.238	0.200
Bond B values: refined atoms	1229	13.553	4.724
Angle B values: refined atoms	1663	16.782	7.130
Torsion B values: refined atoms	426	31.240	13.093
Long range B values: refined atoms	1334	11.635	15.310

Overall : scale = 1.012, B = -0.025
Overall anisotropic scale factors

B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 98. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 98. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 98. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 98. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$

0.004	30	62.50	754.4	747.9	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	414.1	416.1	0.02	0.02	1	1228.7	1224.9	0.01	0.01	
0.017	83	95.60	307.8	308.8	0.03	0.02	4	403.1	413.3	0.04	0.05	
0.023	97	97.14	247.4	248.4	0.02	0.02	5	180.2	189.1	0.07	0.07	
0.029	108	100.00	241.3	242.0	0.02	0.02	7	186.7	189.4	0.06	0.06	
0.036	126	99.25	270.4	270.7	0.02	0.02	6	252.9	254.1	0.04	0.04	
0.042	129	98.56	286.3	287.5	0.02	0.02	8	338.1	341.2	0.02	0.02	
0.048	150	98.73	296.8	296.4	0.02	0.01	5	305.8	307.3	0.03	0.02	
0.055	151	99.38	281.3	281.5	0.01	0.01	10	257.9	260.1	0.04	0.04	
0.061	172	100.00	218.4	218.6	0.02	0.02	10	202.2	202.7	0.03	0.03	
0.067	174	99.45	211.5	211.0	0.02	0.02	6	286.3	284.3	0.02	0.02	
0.074	178	98.92	206.1	206.8	0.02	0.02	6	234.6	237.3	0.03	0.03	
0.080	189	100.00	208.7	209.0	0.02	0.02	13	159.7	155.9	0.06	0.06	
0.086	197	100.00	176.8	176.9	0.02	0.02	8	208.6	207.6	0.04	0.04	
0.093	193	93.55	156.9	157.0	0.02	0.02	10	182.0	186.1	0.07	0.06	
0.099	188	91.28	160.7	159.8	0.02	0.02	11	159.7	157.1	0.02	0.02	
0.105	190	86.02	153.9	153.5	0.02	0.02	13	169.2	170.0	0.05	0.04	
0.112	183	80.08	129.9	129.6	0.02	0.02	6	135.2	141.1	0.08	0.08	
0.118	194	81.85	127.0	126.8	0.02	0.02	9	138.0	137.1	0.05	0.05	
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	111.0	0.06	0.06	

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 98. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 98. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.991	12	0.925	95	0.983	0.999
0.0228	97	0.988	11	1.000	108	0.990	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.996	17	1.000	143	0.996	0.999

```
 0.0418   129   0.997    11   1.000   140   0.997  0.999
 0.0482   150   0.991    12   1.000   162   0.992  0.999
 0.0545   151   0.997    12   0.994   163   0.997  0.999
 0.0609   172   0.983    15   0.957   187   0.981  0.999
 0.0672   174   0.993     9   0.934   183   0.990  0.999
 0.0735   178   0.990    11   1.000   189   0.991  0.999
 0.0799   189   0.989    14   0.999   203   0.990  0.999
 0.0862   197   0.984     9   0.976   206   0.983  0.999
 0.0925   193   0.979    14   0.930   207   0.976  0.999
 0.0989   188   0.980    12   1.000   200   0.981  0.999
 0.1052   190   0.988     8   1.000   198   0.989  0.999
 0.1116   183   0.981    13   0.937   196   0.978  1.000
 0.1179   194   0.980    11   0.944   205   0.978  1.000
 0.1242   174   0.984     8   1.000   182   0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0190
Free R factor                    =     0.0399
Overall weighted R factor        =     0.0191
Free weighted R factor           =     0.0402
Overall correlation coefficient  =     0.9994
Free correlation coefficient     =     0.9969
DPI based on free R factor       =     0.0724
Overall figure of merit          =     0.9870
ML based su of positional parameters =     0.0400
ML based su of thermal parameters    =     1.9766
-------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10490.474       3163.7568       19541.117       19541.023

 fvalues    10490.474       3163.7568       19541.061       19541.023


    CGMAT cycle number =     99

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    1.5611620      is applied to the X-ray term
Norm of X_ray positional gradient              13.7
```

Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1638E+05 GEOM= 3164. TOTAL= 0.1954E+05
function value 19540.506

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.686	1.966
Torsion angles, period 1. refined	155	7.871	5.000
Torsion angles, period 2. refined	54	41.441	25.741
Torsion angles, period 3. refined	214	19.232	15.000
Torsion angles, period 4. refined	3	21.356	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	539	0.266	0.200
VDW; torsion: refined_atoms	789	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.238	0.200
Bond B values: refined atoms	1229	13.553	4.724
Angle B values: refined atoms	1663	16.783	7.130
Torsion B values: refined atoms	426	31.246	13.093
Long range B values: refined atoms	1334	11.634	15.310

Overall : scale = 1.012, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 99. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 99. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 99. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 99. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$

$$
 0.004 30 62.50 754.4 747.9 0.02 0.02 0 0.0 0.0****** 0.00
 0.010 62 95.45 414.1 416.1 0.02 0.02 1 1228.7 1224.9 0.01 0.01
 0.017 83 95.60 307.8 308.8 0.03 0.02 4 403.1 413.3 0.04 0.05
 0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 189.1 0.07 0.07
 0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
 0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.1 0.04 0.04
 0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.2 0.02 0.02
 0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.3 0.03 0.02
 0.055 151 99.38 281.3 281.5 0.01 0.01 10 257.9 260.1 0.04 0.04
 0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.7 0.03 0.03
 0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.4 0.02 0.02
 0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.3 0.03 0.03
 0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 155.9 0.06 0.06
 0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
 0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.1 0.07 0.06
 0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
 0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.0 0.05 0.04
 0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 141.1 0.08 0.08
 0.118 194 81.85 127.0 126.8 0.02 0.02 9 138.0 137.1 0.05 0.05
 0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.0 0.06 0.06
$$

 **** Fom and SigmaA vs resolution ****

$TABLE: Cycle 99. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 99. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
 0.0038 30 0.999 4 1.000 34 0.999 0.999
 0.0102 62 0.999 7 1.000 69 0.999 0.999
 0.0165 83 0.991 12 0.925 95 0.983 0.999
 0.0228 97 0.988 11 1.000 108 0.990 0.999
 0.0292 108 0.997 6 1.000 114 0.997 0.999
 0.0355 126 0.996 17 1.000 143 0.996 0.999
 0.0418 129 0.997 11 1.000 140 0.997 0.999
 0.0482 150 0.991 12 1.000 162 0.992 0.999
 0.0545 151 0.997 12 0.994 163 0.997 0.999
 0.0609 172 0.983 15 0.957 187 0.981 0.999
 0.0672 174 0.993 9 0.934 183 0.990 0.999
 0.0735 178 0.990 11 1.000 189 0.991 0.999
 0.0799 189 0.989 14 0.999 203 0.990 0.999
 0.0862 197 0.984 9 0.976 206 0.983 0.999
 0.0925 193 0.979 14 0.930 207 0.976 0.999
 0.0989 188 0.980 12 1.000 200 0.981 0.999
 0.1052 190 0.988 8 1.000 198 0.989 0.999
 0.1116 183 0.981 13 0.937 196 0.978 1.000
 0.1179 194 0.980 11 0.945 205 0.978 1.000
 0.1242 174 0.984 8 1.000 182 0.984 1.000
$$

Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0190
Free R factor = 0.0399
Overall weighted R factor = 0.0191
Free weighted R factor = 0.0402
Overall correlation coefficient = 0.9994
Free correlation coefficient = 0.9969
DPI based on free R factor = 0.0724
Overall figure of merit = 0.9870
ML based su of positional parameters = 0.0400
ML based su of thermal parameters = 1.9766

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10490.570 3163.7922 19541.209 19541.271

CGMAT cycle number = 100

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5606605 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.692E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1637E+05 GEOM= 3164. TOTAL= 0.1953E+05
function value 19534.500

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.687	1.966
Torsion angles, period 1. refined	155	7.871	5.000

Torsion angles, period 2. refined 54 41.442 25.741
Torsion angles, period 3. refined 214 19.232 15.000
Torsion angles, period 4. refined 3 21.355 15.000
Chiral centres: refined atoms 187 0.112 0.200
Planar groups: refined atoms 924 0.005 0.021
VDW repulsions: refined_atoms 539 0.266 0.200
VDW; torsion: refined_atoms 790 0.325 0.200
HBOND: refined_atoms 41 0.194 0.200
VDW repulsions: symmetry: refined_atoms 55 0.262 0.200
HBOND: symmetry: refined_atoms 3 0.236 0.200
Bond B values: refined atoms 1229 13.553 4.725
Angle B values: refined atoms 1663 16.790 7.130
Torsion B values: refined atoms 426 31.271 13.094
Long range B values: refined atoms 1335 11.627 15.305

Overall : scale = 1.012, B = -0.025
Overall anisotropic scale factors
  B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 100. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 100. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 100. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 100. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
 0.004 30 62.50 754.4 748.0 0.02 0.02 0 0.0 0.0****** 0.00
 0.010 62 95.45 414.1 416.1 0.02 0.02 1 1228.7 1225.0 0.01 0.01
 0.017 83 95.60 307.8 308.8 0.03 0.02 4 403.1 413.3 0.04 0.05
 0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 189.1 0.07 0.07
 0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
 0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.1 0.04 0.04
 0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.1 0.02 0.02
 0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.3 0.03 0.02
 0.055 151 99.38 281.3 281.5 0.01 0.01 10 257.9 260.1 0.04 0.04
 0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.7 0.03 0.03
 0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.4 0.02 0.02
 0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.3 0.03 0.03
 0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 155.9 0.06 0.06
 0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
 0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.1 0.07 0.06
 0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02

```
 0.105    190  86.02   153.9   153.5  0.02  0.02      13   169.2   170.0  0.05  0.04
 0.112    183  80.08   129.9   129.6  0.02  0.02       6   135.2   141.1  0.08  0.08
 0.118    194  81.85   127.0   126.8  0.02  0.02       9   138.0   137.1  0.05  0.05
 0.124    174  73.20   129.0   128.9  0.02  0.02       9   113.8   111.0  0.06  0.06
$$
```

**** Fom and SigmaA vs resolution ****

```
$TABLE: Cycle  100. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle  100. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa  FOMa  NREFc FOMc NREFall FOMall  SigmaA_Fc1 $$
$$
 0.0038    30   0.999     4   1.000    34   0.999  0.999
 0.0102    62   0.999     7   1.000    69   0.999  0.999
 0.0165    83   0.991    12   0.925    95   0.983  0.999
 0.0228    97   0.988    11   1.000   108   0.990  0.999
 0.0292   108   0.997     6   1.000   114   0.997  0.999
 0.0355   126   0.996    17   1.000   143   0.996  0.999
 0.0418   129   0.997    11   1.000   140   0.997  0.999
 0.0482   150   0.991    12   1.000   162   0.992  0.999
 0.0545   151   0.997    12   0.994   163   0.997  0.999
 0.0609   172   0.983    15   0.957   187   0.981  0.999
 0.0672   174   0.993     9   0.933   183   0.990  0.999
 0.0735   178   0.990    11   1.000   189   0.991  0.999
 0.0799   189   0.989    14   0.999   203   0.990  0.999
 0.0862   197   0.984     9   0.976   206   0.983  0.999
 0.0925   193   0.979    14   0.930   207   0.976  0.999
 0.0989   188   0.980    12   1.000   200   0.981  0.999
 0.1052   190   0.988     8   1.000   198   0.989  0.999
 0.1116   183   0.981    13   0.937   196   0.978  1.000
 0.1179   194   0.980    11   0.945   205   0.978  1.000
 0.1242   174   0.984     8   1.000   182   0.984  1.000
 $$
Resolution limits                 =     38.899     2.802
Number of used reflections        =       3184
Percentage observed               =    92.6870
Percentage of free reflections    =     4.8416
Overall R factor                  =     0.0190
Free R factor                     =     0.0398
Overall weighted R factor         =     0.0191
Free weighted R factor            =     0.0402
Overall correlation coefficient   =     0.9994
Free correlation coefficient      =     0.9969
DPI based on free R factor        =     0.0723
Overall figure of merit           =     0.9870
ML based su of positional parameters =     0.0400
ML based su of thermal parameters    =     1.9763
-------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles
```

fvalues 10489.948 3164.0322 19535.182 19535.279

CGMAT cycle number = 101

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.59999996
Actual weight 1.5603367 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1637E+05 GEOM= 3164. TOTAL= 0.1953E+05
function value 19530.389

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.687	1.966
Torsion angles, period 1. refined	155	7.871	5.000
Torsion angles, period 2. refined	54	41.442	25.741
Torsion angles, period 3. refined	214	19.231	15.000
Torsion angles, period 4. refined	3	21.353	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	789	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.235	0.200
Bond B values: refined atoms	1229	13.556	4.725
Angle B values: refined atoms	1663	16.802	7.130
Torsion B values: refined atoms	426	31.305	13.095
Long range B values: refined atoms	1335	11.625	15.313

Overall : scale = 1.012, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 101. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 101. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 101. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 101. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 748.0 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.1 0.02 0.02 1 1228.7 1225.0 0.01 0.01
0.017 83 95.60 307.8 308.8 0.03 0.02 4 403.1 413.3 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 189.1 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.1 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.1 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.3 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.7 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.4 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 155.9 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.1 0.07 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.0 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 141.1 0.08 0.08
0.118 194 81.85 127.0 126.8 0.02 0.02 9 138.0 137.1 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.0 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 101. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 101. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.991 12 0.925 95 0.983 0.999
0.0228 97 0.988 11 1.000 108 0.990 0.999

```
 0.0292   108   0.997     6   1.000   114   0.997  0.999
 0.0355   126   0.996    17   1.000   143   0.996  0.999
 0.0418   129   0.997    11   1.000   140   0.997  0.999
 0.0482   150   0.991    12   1.000   162   0.992  0.999
 0.0545   151   0.997    12   0.994   163   0.997  0.999
 0.0609   172   0.983    15   0.957   187   0.981  0.999
 0.0672   174   0.993     9   0.934   183   0.990  0.999
 0.0735   178   0.990    11   1.000   189   0.991  0.999
 0.0799   189   0.989    14   0.999   203   0.990  0.999
 0.0862   197   0.984     9   0.976   206   0.983  0.999
 0.0925   193   0.979    14   0.930   207   0.976  0.999
 0.0989   188   0.980    12   1.000   200   0.981  0.999
 0.1052   190   0.988     8   1.000   198   0.989  0.999
 0.1116   183   0.981    13   0.937   196   0.978  1.000
 0.1179   194   0.980    11   0.945   205   0.978  1.000
 0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0190
Free R factor                    =     0.0398
Overall weighted R factor        =     0.0191
Free weighted R factor           =     0.0402
Overall correlation coefficient  =     0.9994
Free correlation coefficient     =     0.9969
DPI based on free R factor       =     0.0723
Overall figure of merit          =     0.9870
ML based su of positional parameters =     0.0400
ML based su of thermal parameters    =     1.9763
------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10489.393       3164.1697       19531.100       19531.154


    CGMAT cycle number =    102

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    1.5581931      is applied to the X-ray term
Norm of X_ray positional gradient              13.7
```

Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.692E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1634E+05 GEOM= 3164. TOTAL= 0.1951E+05
function value 19505.707

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.687	1.966
Torsion angles, period 1. refined	155	7.871	5.000
Torsion angles, period 2. refined	54	41.442	25.741
Torsion angles, period 3. refined	214	19.231	15.000
Torsion angles, period 4. refined	3	21.351	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	790	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.233	0.200
Bond B values: refined atoms	1229	13.561	4.725
Angle B values: refined atoms	1663	16.814	7.130
Torsion B values: refined atoms	426	31.336	13.097
Long range B values: refined atoms	1336	11.624	15.309

Overall : scale = 1.012, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 102. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 102. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 102. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 102. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$

$$
 0.004 30 62.50 754.4 748.0 0.02 0.02 0 0.0 0.0****** 0.00
 0.010 62 95.45 414.1 416.1 0.02 0.02 1 1228.7 1225.0 0.01 0.01
 0.017 83 95.60 307.8 308.8 0.03 0.02 4 403.1 413.2 0.04 0.05
 0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 189.2 0.07 0.07
 0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
 0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.1 0.04 0.04
 0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.1 0.02 0.02
 0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.3 0.03 0.02
 0.055 151 99.38 281.3 281.5 0.01 0.01 10 257.9 260.1 0.04 0.04
 0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.8 0.03 0.03
 0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.4 0.02 0.02
 0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.4 0.03 0.03
 0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 155.9 0.06 0.06
 0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
 0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.1 0.07 0.06
 0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
 0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.0 0.05 0.04
 0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 141.2 0.08 0.08
 0.118 194 81.85 127.0 126.8 0.02 0.02 9 138.0 137.1 0.05 0.05
 0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.0 0.06 0.06
$$

 **** Fom and SigmaA vs resolution ****

$TABLE: Cycle 102. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 102. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
 0.0038 30 0.999 4 1.000 34 0.999 0.999
 0.0102 62 0.999 7 1.000 69 0.999 0.999
 0.0165 83 0.991 12 0.925 95 0.983 0.999
 0.0228 97 0.988 11 1.000 108 0.990 0.999
 0.0292 108 0.997 6 1.000 114 0.997 0.999
 0.0355 126 0.996 17 1.000 143 0.996 0.999
 0.0418 129 0.997 11 1.000 140 0.997 0.999
 0.0482 150 0.991 12 1.000 162 0.992 0.999
 0.0545 151 0.997 12 0.994 163 0.997 0.999
 0.0609 172 0.983 15 0.957 187 0.981 0.999
 0.0672 174 0.993 9 0.933 183 0.990 0.999
 0.0735 178 0.990 11 1.000 189 0.991 0.999
 0.0799 189 0.989 14 0.999 203 0.990 0.999
 0.0862 197 0.984 9 0.976 206 0.983 0.999
 0.0925 193 0.979 14 0.930 207 0.976 0.999
 0.0989 188 0.980 12 1.000 200 0.981 0.999
 0.1052 190 0.988 8 1.000 198 0.989 0.999
 0.1116 183 0.981 13 0.937 196 0.978 1.000
 0.1179 194 0.980 11 0.946 205 0.978 1.000
 0.1242 174 0.984 8 1.000 182 0.984 1.000
$$

Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0190
Free R factor = 0.0398
Overall weighted R factor = 0.0190
Free weighted R factor = 0.0402
Overall correlation coefficient = 0.9994
Free correlation coefficient = 0.9969
DPI based on free R factor = 0.0723
Overall figure of merit = 0.9870
ML based su of positional parameters = 0.0400
ML based su of thermal parameters = 1.9747

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10487.792 3164.4851 19506.357 19506.490

CGMAT cycle number = 103

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5578890 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1634E+05 GEOM= 3164. TOTAL= 0.1950E+05
function value 19501.350

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.687	1.966
Torsion angles, period 1. refined	155	7.871	5.000

Torsion angles, period 2. refined 54 41.442 25.741
Torsion angles, period 3. refined 214 19.231 15.000
Torsion angles, period 4. refined 3 21.351 15.000
Chiral centres: refined atoms 187 0.112 0.200
Planar groups: refined atoms 924 0.005 0.021
VDW repulsions: refined_atoms 540 0.266 0.200
VDW; torsion: refined_atoms 789 0.325 0.200
HBOND: refined_atoms 41 0.194 0.200
VDW repulsions: symmetry: refined_atoms 55 0.262 0.200
HBOND: symmetry: refined_atoms 3 0.232 0.200
Bond B values: refined atoms 1229 13.555 4.726
Angle B values: refined atoms 1663 16.814 7.130
Torsion B values: refined atoms 426 31.348 13.098
Long range B values: refined atoms 1335 11.620 15.313

Overall : scale = 1.012, B = -0.025
Overall anisotropic scale factors
  B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 103. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 103. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 103. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 103. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
 0.004 30 62.50 754.4 748.0 0.02 0.02 0 0.0 0.0****** 0.00
 0.010 62 95.45 414.1 416.1 0.02 0.02 1 1228.7 1225.1 0.01 0.01
 0.017 83 95.60 307.8 308.8 0.03 0.02 4 403.1 413.2 0.04 0.05
 0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 189.2 0.07 0.07
 0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
 0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.2 0.04 0.04
 0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.1 0.02 0.02
 0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.3 0.03 0.02
 0.055 151 99.38 281.3 281.5 0.01 0.01 10 257.9 260.1 0.04 0.04
 0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.8 0.03 0.03
 0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.4 0.02 0.02
 0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.4 0.03 0.03
 0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 155.9 0.06 0.06
 0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
 0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.1 0.07 0.06
 0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02

```
 0.105    190  86.02   153.9   153.5  0.02  0.02      13   169.2   170.0  0.05  0.04
 0.112    183  80.08   129.9   129.6  0.02  0.02       6   135.2   141.2  0.08  0.08
 0.118    194  81.85   127.0   126.8  0.02  0.02       9   138.0   137.1  0.05  0.05
 0.124    174  73.20   129.0   128.9  0.02  0.02       9   113.8   111.0  0.06  0.06
$$
```

**** Fom and SigmaA vs resolution ****

```
$TABLE: Cycle  103. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle  103. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa  FOMa  NREFc FOMc NREFall FOMall  SigmaA_Fc1 $$
$$
 0.0038    30   0.999     4   1.000    34   0.999  0.999
 0.0102    62   0.999     7   1.000    69   0.999  0.999
 0.0165    83   0.991    12   0.925    95   0.983  0.999
 0.0228    97   0.988    11   1.000   108   0.990  0.999
 0.0292   108   0.997     6   1.000   114   0.997  0.999
 0.0355   126   0.996    17   1.000   143   0.996  0.999
 0.0418   129   0.997    11   1.000   140   0.997  0.999
 0.0482   150   0.991    12   1.000   162   0.992  0.999
 0.0545   151   0.997    12   0.994   163   0.997  0.999
 0.0609   172   0.983    15   0.957   187   0.981  0.999
 0.0672   174   0.993     9   0.933   183   0.990  0.999
 0.0735   178   0.990    11   1.000   189   0.991  0.999
 0.0799   189   0.989    14   0.999   203   0.990  0.999
 0.0862   197   0.984     9   0.976   206   0.983  0.999
 0.0925   193   0.979    14   0.930   207   0.976  0.999
 0.0989   188   0.980    12   1.000   200   0.981  0.999
 0.1052   190   0.988     8   1.000   198   0.989  0.999
 0.1116   183   0.981    13   0.937   196   0.978  1.000
 0.1179   194   0.980    11   0.945   205   0.978  1.000
 0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0190
Free R factor                    =     0.0398
Overall weighted R factor        =     0.0190
Free weighted R factor           =     0.0402
Overall correlation coefficient  =     0.9993
Free correlation coefficient     =     0.9969
DPI based on free R factor       =     0.0723
Overall figure of merit          =     0.9870
ML based su of positional parameters =     0.0400
ML based su of thermal parameters    =     1.9749
-------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles
```

fvalues 10487.052 3164.4685 19502.164 19502.131

fvalues 10487.052 3164.4685 19502.129 19502.131

CGMAT cycle number = 104

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000008
Actual weight 1.5589101 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.395E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1635E+05 GEOM= 3165. TOTAL= 0.1951E+05
function value 19513.217

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.687	1.966
Torsion angles, period 1. refined	155	7.870	5.000
Torsion angles, period 2. refined	54	41.442	25.741
Torsion angles, period 3. refined	214	19.230	15.000
Torsion angles, period 4. refined	3	21.349	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	790	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.231	0.200
Bond B values: refined atoms	1229	13.558	4.726
Angle B values: refined atoms	1663	16.821	7.131
Torsion B values: refined atoms	426	31.365	13.098
Long range B values: refined atoms	1336	11.617	15.309

Overall : scale = 1.012, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 104. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 104. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 104. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 104. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 748.0 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.1 0.02 0.02 1 1228.7 1225.1 0.01 0.01
0.017 83 95.60 307.8 308.8 0.03 0.02 4 403.1 413.2 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 189.2 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.2 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.1 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.3 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.8 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.4 0.03 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 155.9 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.1 0.07 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.0 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 141.2 0.08 0.08
0.118 194 81.85 127.0 126.8 0.02 0.02 9 138.0 137.1 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.0 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 104. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 104. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999

```
 0.0165   83  0.991   12  0.925   95  0.983  0.999
 0.0228   97  0.988   11  1.000  108  0.990  0.999
 0.0292  108  0.997    6  1.000  114  0.997  0.999
 0.0355  126  0.996   17  1.000  143  0.996  0.999
 0.0418  129  0.997   11  1.000  140  0.997  0.999
 0.0482  150  0.991   12  1.000  162  0.992  0.999
 0.0545  151  0.997   12  0.994  163  0.997  0.999
 0.0609  172  0.983   15  0.957  187  0.981  0.999
 0.0672  174  0.993    9  0.934  183  0.990  0.999
 0.0735  178  0.990   11  1.000  189  0.990  0.999
 0.0799  189  0.989   14  0.999  203  0.990  0.999
 0.0862  197  0.984    9  0.976  206  0.983  0.999
 0.0925  193  0.979   14  0.930  207  0.976  0.999
 0.0989  188  0.980   12  1.000  200  0.981  0.999
 0.1052  190  0.988    8  1.000  198  0.989  0.999
 0.1116  183  0.981   13  0.937  196  0.978  1.000
 0.1179  194  0.980   11  0.946  205  0.978  1.000
 0.1242  174  0.983    8  1.000  182  0.984  1.000
 $$
Resolution limits                 =    38.899    2.802
Number of used reflections        =      3184
Percentage observed               =   92.6870
Percentage of free reflections    =    4.8416
Overall R factor                  =    0.0190
Free R factor                     =    0.0398
Overall weighted R factor         =    0.0190
Free weighted R factor            =    0.0402
Overall correlation coefficient   =    0.9994
Free correlation coefficient      =    0.9969
DPI based on free R factor        =    0.0723
Overall figure of merit           =    0.9870
ML based su of positional parameters =    0.0400
ML based su of thermal parameters    =    1.9756
--------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10487.714       3164.6279       19514.010       19514.031


    CGMAT cycle number =    105

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :   50   90   60
 Maximuum H,K,L                 :   12   21   14
 Minimum acceptable grid spacing:   33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
```

Actual weight 1.5562689 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1632E+05 GEOM= 3165. TOTAL= 0.1948E+05
function value 19482.170

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.687	1.966
Torsion angles, period 1. refined	155	7.870	5.000
Torsion angles, period 2. refined	54	41.442	25.741
Torsion angles, period 3. refined	214	19.232	15.000
Torsion angles, period 4. refined	3	21.345	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	790	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.230	0.200
Bond B values: refined atoms	1229	13.565	4.726
Angle B values: refined atoms	1663	16.835	7.131
Torsion B values: refined atoms	426	31.401	13.100
Long range B values: refined atoms	1336	11.619	15.309

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 105. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 105. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 105. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 105. % observed v. resln :N:1,3:
$$

M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 748.0 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.1 0.02 0.02 1 1228.7 1225.1 0.01 0.01
0.017 83 95.60 307.8 308.8 0.03 0.02 4 403.1 413.2 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 189.2 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.2 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.1 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.3 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.8 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.3 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.4 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 156.0 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.1 0.07 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.0 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 141.2 0.08 0.08
0.118 194 81.85 127.0 126.8 0.02 0.02 9 138.0 137.1 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.0 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 105. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 105. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.991 12 0.925 95 0.983 0.999
0.0228 97 0.989 11 1.000 108 0.990 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.996 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.992 0.999
0.0545 151 0.997 12 0.994 163 0.997 0.999
0.0609 172 0.983 15 0.957 187 0.981 0.999
0.0672 174 0.993 9 0.934 183 0.990 0.999
0.0735 178 0.990 11 1.000 189 0.991 0.999
0.0799 189 0.989 14 1.000 203 0.990 0.999
0.0862 197 0.984 9 0.977 206 0.984 0.999
0.0925 193 0.979 14 0.930 207 0.976 0.999
0.0989 188 0.980 12 1.000 200 0.981 0.999
0.1052 190 0.988 8 1.000 198 0.989 0.999
0.1116 183 0.981 13 0.937 196 0.978 1.000
0.1179 194 0.980 11 0.946 205 0.978 1.000

```
 0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0190
Free R factor                    =     0.0398
Overall weighted R factor        =     0.0190
Free weighted R factor           =     0.0402
Overall correlation coefficient  =     0.9994
Free correlation coefficient     =     0.9969
DPI based on free R factor       =     0.0722
Overall figure of merit          =     0.9871
ML based su of positional parameters =     0.0400
ML based su of thermal parameters    =     1.9741
------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10485.396       3164.8855       19482.918       19482.982


    CGMAT cycle number =     106

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    1.5552186      is applied to the X-ray term
Norm of X_ray positional gradient              13.7
Norm of Geom. positional gradient              13.7
Norm of X_ray B-factor gradient                17.8
Norm of Geom. B-factor gradient                18.2
Product of X_ray and Geom posit. gradients     -0.693E+06
 Cosine of angle between them                  -1.000
Product of X_ray and Geom B-fact gradients     -0.396E+06
 Cosine of angle between them                  -0.995


Residuals: XRAY=     0.1630E+05 GEOM=      3165.     TOTAL=     0.1947E+05
 function value    19470.100

------------------------------------------------------------------------------
          Restraint type            N restraints   Rms Delta   Av(Sigma)
Bond distances: refined atoms                1229     0.011      0.020
```

Bond angles : refined atoms 1663 1.687 1.966
Torsion angles, period 1. refined 155 7.870 5.000
Torsion angles, period 2. refined 54 41.442 25.741
Torsion angles, period 3. refined 214 19.223 15.000
Torsion angles, period 4. refined 3 21.338 15.000
Chiral centres: refined atoms 187 0.112 0.200
Planar groups: refined atoms 924 0.005 0.021
VDW repulsions: refined_atoms 540 0.266 0.200
VDW; torsion: refined_atoms 790 0.325 0.200
HBOND: refined_atoms 41 0.194 0.200
VDW repulsions: symmetry: refined_atoms 55 0.262 0.200
HBOND: symmetry: refined_atoms 3 0.228 0.200
Bond B values: refined atoms 1229 13.563 4.726
Angle B values: refined atoms 1663 16.840 7.131
Torsion B values: refined atoms 426 31.421 13.101
Long range B values: refined atoms 1336 11.615 15.309

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 106. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 106. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 106. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 106. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 748.0 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.0 0.02 0.02 1 1228.7 1225.2 0.01 0.01
0.017 83 95.60 307.8 308.8 0.03 0.02 4 403.1 413.2 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 189.3 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.2 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.1 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.3 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 257.9 260.0 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.8 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.5 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 156.0 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04

```
 0.093   193  93.55   156.9   157.0  0.02  0.02     10   182.0   186.0  0.07  0.06
 0.099   188  91.28   160.7   159.8  0.02  0.02     11   159.7   157.1  0.02  0.02
 0.105   190  86.02   153.9   153.5  0.02  0.02     13   169.2   170.0  0.05  0.04
 0.112   183  80.08   129.9   129.6  0.02  0.02      6   135.2   141.2  0.08  0.08
 0.118   194  81.85   127.0   126.8  0.02  0.02      9   138.0   137.1  0.05  0.05
 0.124   174  73.20   129.0   128.9  0.02  0.02      9   113.8   111.0  0.06  0.06
$$
```

**** Fom and SigmaA vs resolution ****

```
$TABLE: Cycle  106. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle  106. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa  FOMa  NREFc FOMc NREFall FOMall  SigmaA_Fc1 $$
$$
 0.0038    30   0.999     4   1.000    34   0.999  0.999
 0.0102    62   0.999     7   1.000    69   0.999  0.999
 0.0165    83   0.991    12   0.925    95   0.983  0.999
 0.0228    97   0.989    11   1.000   108   0.990  0.999
 0.0292   108   0.997     6   1.000   114   0.997  0.999
 0.0355   126   0.996    17   1.000   143   0.996  0.999
 0.0418   129   0.997    11   1.000   140   0.997  0.999
 0.0482   150   0.991    12   1.000   162   0.992  0.999
 0.0545   151   0.997    12   0.994   163   0.997  0.999
 0.0609   172   0.983    15   0.957   187   0.981  0.999
 0.0672   174   0.993     9   0.934   183   0.990  0.999
 0.0735   178   0.990    11   1.000   189   0.990  0.999
 0.0799   189   0.989    14   0.999   203   0.990  0.999
 0.0862   197   0.984     9   0.977   206   0.984  0.999
 0.0925   193   0.979    14   0.930   207   0.976  0.999
 0.0989   188   0.980    12   1.000   200   0.981  0.999
 0.1052   190   0.988     8   1.000   198   0.989  0.999
 0.1116   183   0.981    13   0.937   196   0.978  1.000
 0.1179   194   0.980    11   0.946   205   0.978  1.000
 0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
Resolution limits                 =     38.899     2.802
Number of used reflections        =       3184
Percentage observed               =    92.6870
Percentage of free reflections    =     4.8416
Overall R factor                  =     0.0190
Free R factor                     =     0.0397
Overall weighted R factor         =     0.0190
Free weighted R factor            =     0.0401
Overall correlation coefficient   =     0.9994
Free correlation coefficient      =     0.9969
DPI based on free R factor        =     0.0722
Overall figure of merit           =     0.9871
ML based su of positional parameters =      0.0400
ML based su of thermal parameters    =     1.9733
------------------------------------------------------------------------------
```

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10484.525 3165.1553 19471.541 19470.885

fvalues 10484.525 3165.1553 19470.891 19470.885

CGMAT cycle number = 107

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5559398 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.692E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1631E+05 GEOM= 3165. TOTAL= 0.1948E+05
function value 19478.393

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.687	1.966
Torsion angles, period 1. refined	155	7.870	5.000
Torsion angles, period 2. refined	54	41.442	25.741
Torsion angles, period 3. refined	214	19.230	15.000
Torsion angles, period 4. refined	3	21.340	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	791	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.228	0.200
Bond B values: refined atoms	1229	13.563	4.727
Angle B values: refined atoms	1663	16.842	7.131
Torsion B values: refined atoms	426	31.429	13.101

Long range B values: refined atoms 1337 11.610 15.308

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 107. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 107. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 107. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 107. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 748.0 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.0 0.02 0.02 1 1228.7 1225.1 0.01 0.01
0.017 83 95.60 307.8 308.8 0.03 0.02 4 403.1 413.2 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 189.3 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.2 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.1 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.3 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.8 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.5 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 156.0 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.0 0.07 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.0 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 141.2 0.08 0.08
0.118 194 81.85 127.0 126.8 0.02 0.02 9 138.0 137.1 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.0 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 107. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 107. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.991	12	0.925	95	0.983	0.999
0.0228	97	0.989	11	1.000	108	0.990	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.996	17	1.000	143	0.996	0.999
0.0418	129	0.997	11	1.000	140	0.997	0.999
0.0482	150	0.991	12	1.000	162	0.992	0.999
0.0545	151	0.997	12	0.994	163	0.997	0.999
0.0609	172	0.983	15	0.957	187	0.981	0.999
0.0672	174	0.993	9	0.933	183	0.990	0.999
0.0735	178	0.990	11	1.000	189	0.990	0.999
0.0799	189	0.989	14	0.999	203	0.990	0.999
0.0862	197	0.984	9	0.977	206	0.984	0.999
0.0925	193	0.979	14	0.930	207	0.976	0.999
0.0989	188	0.980	12	1.000	200	0.981	0.999
0.1052	190	0.988	8	1.000	198	0.989	0.999
0.1116	183	0.981	13	0.937	196	0.978	1.000
0.1179	194	0.980	11	0.947	205	0.978	1.000
0.1242	174	0.983	8	1.000	182	0.984	1.000

$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0190
Free R factor = 0.0398
Overall weighted R factor = 0.0190
Free weighted R factor = 0.0402
Overall correlation coefficient = 0.9994
Free correlation coefficient = 0.9969
DPI based on free R factor = 0.0722
Overall figure of merit = 0.9871
ML based su of positional parameters = 0.0400
ML based su of thermal parameters = 1.9737

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10484.956 3165.2004 19479.096 19479.160

CGMAT cycle number = 108

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG

VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5538298 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.692E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1629E+05 GEOM= 3165. TOTAL= 0.1945E+05
function value 19453.764

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.687	1.966
Torsion angles, period 1. refined	155	7.870	5.000
Torsion angles, period 2. refined	54	41.443	25.741
Torsion angles, period 3. refined	214	19.226	15.000
Torsion angles, period 4. refined	3	21.344	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	791	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.226	0.200
Bond B values: refined atoms	1229	13.566	4.727
Angle B values: refined atoms	1663	16.852	7.131
Torsion B values: refined atoms	426	31.459	13.102
Long range B values: refined atoms	1337	11.609	15.308

Overall : scale = 1.012, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 108. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 108. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 108. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:

:Cycle 108. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 748.0 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.0 0.02 0.02 1 1228.7 1225.2 0.01 0.01
0.017 83 95.60 307.8 308.8 0.03 0.02 4 403.1 413.2 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 189.3 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.2 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.1 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.4 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 257.9 260.1 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.8 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.3 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.5 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 156.0 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.0 0.07 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.0 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 141.2 0.08 0.08
0.118 194 81.85 127.0 126.8 0.02 0.02 9 138.0 137.1 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 111.0 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 108. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 108. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.991 12 0.925 95 0.983 0.999
0.0228 97 0.989 11 1.000 108 0.990 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.996 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.992 0.999
0.0545 151 0.997 12 0.994 163 0.997 0.999
0.0609 172 0.983 15 0.957 187 0.981 0.999
0.0672 174 0.993 9 0.933 183 0.990 0.999
0.0735 178 0.990 11 1.000 189 0.990 0.999
0.0799 189 0.989 14 0.999 203 0.990 0.999
0.0862 197 0.984 9 0.977 206 0.984 0.999
0.0925 193 0.979 14 0.930 207 0.976 0.999
0.0989 188 0.980 12 1.000 200 0.981 0.999
0.1052 190 0.988 8 1.000 198 0.989 0.999

```
 0.1116   183   0.981    13   0.937   196   0.978  1.000
 0.1179   194   0.980    11   0.947   205   0.978  1.000
 0.1242   174   0.984     8   1.000   182   0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0190
Free R factor                    =     0.0397
Overall weighted R factor        =     0.0190
Free weighted R factor           =     0.0401
Overall correlation coefficient  =     0.9994
Free correlation coefficient     =     0.9969
DPI based on free R factor       =     0.0721
Overall figure of merit          =     0.9871
ML based su of positional parameters =     0.0399
ML based su of thermal parameters    =     1.9723
------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10483.288       3165.3047       19454.738       19454.551

 fvalues    10483.288       3165.3047       19454.545       19454.551


    CGMAT cycle number =    109

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    1.5536827      is applied to the X-ray term
Norm of X_ray positional gradient              13.7
Norm of Geom. positional gradient              13.7
Norm of X_ray B-factor gradient                17.8
Norm of Geom. B-factor gradient                18.2
Product of X_ray and Geom posit. gradients     -0.692E+06
 Cosine of angle between them                  -1.000
Product of X_ray and Geom B-fact gradients     -0.396E+06
 Cosine of angle between them                  -0.995


Residuals: XRAY=     0.1629E+05 GEOM=      3165.     TOTAL=     0.1945E+05
 function value    19451.699
```

```
------------------------------------------------------------------------------
          Restraint type           N restraints   Rms Delta   Av(Sigma)
Bond distances: refined atoms              1229     0.011     0.020
Bond angles  : refined atoms               1663     1.687     1.966
Torsion angles, period  1. refined          155     7.870     5.000
Torsion angles, period  2. refined           54    41.443    25.741
Torsion angles, period  3. refined          214    19.232    15.000
Torsion angles, period  4. refined            3    21.342    15.000
Chiral centres: refined atoms              187     0.112     0.200
Planar groups: refined atoms               924     0.005     0.021
VDW repulsions: refined_atoms              540     0.266     0.200
VDW; torsion: refined_atoms                791     0.325     0.200
HBOND: refined_atoms                        41     0.194     0.200
VDW repulsions: symmetry: refined_atoms     55     0.262     0.200
HBOND: symmetry: refined_atoms               3     0.226     0.200
Bond B values: refined atoms               1229    13.566     4.727
Angle B values: refined atoms              1663    16.855     7.131
Torsion B values: refined atoms             426    31.468    13.103
Long range B values: refined atoms         1337    11.607    15.308
------------------------------------------------------------------------------

------------------------------------------------------------------------------
Overall              : scale =    1.011, B  =  -0.025
Overall anisotropic scale factors
   B11 =  0.28 B22 =  0.17 B33 = -0.47 B12 =  0.00 B13 = -0.36 B23 =  0.00
------------------------------------------------------------------------------

------------------------------------------------------------------------------

    ****              Things for loggraph, R factor and others              ****


$TABLE: Cycle  109. Rfactor analysis, F distribution v resln  :
$GRAPHS:Cycle  109. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle  109. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle  109. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free   WR_free $$
$$
 0.004     30  62.50   754.4   748.0  0.02  0.02      0     0.0     0.0******  0.00
 0.010     62  95.45   414.1   416.0  0.02  0.02      1  1228.7  1225.2  0.01  0.01
 0.017     83  95.60   307.8   308.8  0.03  0.02      4   403.1   413.2  0.04  0.05
 0.023     97  97.14   247.4   248.4  0.02  0.02      5   180.2   189.3  0.07  0.07
 0.029    108 100.00   241.3   242.0  0.02  0.02      7   186.7   189.4  0.06  0.06
 0.036    126  99.25   270.4   270.7  0.02  0.02      6   252.9   254.2  0.04  0.04
 0.042    129  98.56   286.3   287.5  0.02  0.02      8   338.2   341.1  0.02  0.02
 0.048    150  98.73   296.8   296.4  0.02  0.01      5   305.8   307.4  0.03  0.02
 0.055    151  99.38   281.3   281.5  0.01  0.01     10   257.9   260.0  0.04  0.04
 0.061    172 100.00   218.4   218.6  0.02  0.02     10   202.2   202.8  0.03  0.03
```

```
 0.067    174  99.45   211.5   211.0  0.02  0.02      6   286.3   284.4  0.02  0.02
 0.074    178  98.92   206.1   206.8  0.02  0.02      6   234.6   237.5  0.04  0.03
 0.080    189 100.00   208.7   209.0  0.02  0.02     13   159.7   156.0  0.06  0.06
 0.086    197 100.00   176.8   176.9  0.02  0.02      8   208.6   207.6  0.04  0.04
 0.093    193  93.55   156.9   157.0  0.02  0.02     10   182.0   186.0  0.07  0.06
 0.099    188  91.28   160.7   159.8  0.02  0.02     11   159.7   157.1  0.02  0.02
 0.105    190  86.02   153.9   153.5  0.02  0.02     13   169.2   170.0  0.05  0.04
 0.112    183  80.08   129.9   129.6  0.02  0.02      6   135.2   141.2  0.08  0.08
 0.118    194  81.85   127.0   126.8  0.02  0.02      9   138.0   137.1  0.05  0.05
 0.124    174  73.20   129.0   128.9  0.02  0.02      9   113.8   111.0  0.06  0.06
$$
```

**** Fom and SigmaA vs resolution ****

```
$TABLE: Cycle  109. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle  109. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa  FOMa  NREFc FOMc NREFall FOMall  SigmaA_Fc1 $$
$$
 0.0038    30   0.999     4   1.000    34   0.999  0.999
 0.0102    62   0.999     7   1.000    69   0.999  0.999
 0.0165    83   0.991    12   0.925    95   0.983  0.999
 0.0228    97   0.989    11   1.000   108   0.990  0.999
 0.0292   108   0.997     6   1.000   114   0.997  0.999
 0.0355   126   0.996    17   1.000   143   0.996  0.999
 0.0418   129   0.997    11   1.000   140   0.997  0.999
 0.0482   150   0.991    12   1.000   162   0.992  0.999
 0.0545   151   0.997    12   0.995   163   0.997  0.999
 0.0609   172   0.983    15   0.957   187   0.981  0.999
 0.0672   174   0.993     9   0.933   183   0.990  0.999
 0.0735   178   0.990    11   1.000   189   0.990  0.999
 0.0799   189   0.989    14   0.999   203   0.990  0.999
 0.0862   197   0.984     9   0.977   206   0.984  0.999
 0.0925   193   0.979    14   0.930   207   0.976  0.999
 0.0989   188   0.980    12   1.000   200   0.981  0.999
 0.1052   190   0.988     8   1.000   198   0.989  0.999
 0.1116   183   0.981    13   0.937   196   0.978  1.000
 0.1179   194   0.980    11   0.947   205   0.978  1.000
 0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0190
Free R factor                    =     0.0397
Overall weighted R factor        =     0.0190
Free weighted R factor           =     0.0401
Overall correlation coefficient  =     0.9994
Free correlation coefficient     =     0.9969
DPI based on free R factor       =     0.0721
```

Overall figure of merit = 0.9871
ML based su of positional parameters = 0.0399
ML based su of thermal parameters = 1.9725

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10482.905 3165.3945 19452.658 19452.504

fvalues 10482.905 3165.3945 19452.398 19452.504

CGMAT cycle number = 110

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5541888 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1629E+05 GEOM= 3165. TOTAL= 0.1946E+05
function value 19457.348

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.687	1.966
Torsion angles, period 1. refined	155	7.869	5.000
Torsion angles, period 2. refined	54	41.443	25.741
Torsion angles, period 3. refined	214	19.223	15.000
Torsion angles, period 4. refined	3	21.341	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	791	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200

HBOND: symmetry: refined_atoms 3 0.225 0.200
Bond B values: refined atoms 1229 13.567 4.727
Angle B values: refined atoms 1663 16.860 7.131
Torsion B values: refined atoms 426 31.483 13.103
Long range B values: refined atoms 1337 11.607 15.308

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 110. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 110. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 110. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 110. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 748.0 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.0 0.02 0.02 1 1228.7 1225.2 0.01 0.01
0.017 83 95.60 307.8 308.8 0.03 0.02 4 403.1 413.2 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 189.3 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.2 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.1 341.1 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.4 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 257.9 260.0 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.8 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.3 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.5 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 156.0 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.0 0.07 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.0 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 141.2 0.08 0.08
0.118 194 81.85 127.0 126.8 0.02 0.02 9 138.0 137.1 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 110.9 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 110. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:

$GRAPHS:Cycle 110. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
 0.0038   30 0.999   4 1.000   34 0.999 0.999
 0.0102   62 0.999   7 1.000   69 0.999 0.999
 0.0165   83 0.991   12 0.925   95 0.983 0.999
 0.0228   97 0.989   11 1.000 108 0.990 0.999
 0.0292 108 0.997   6 1.000 114 0.997 0.999
 0.0355 126 0.996   17 1.000 143 0.996 0.999
 0.0418 129 0.997   11 1.000 140 0.997 0.999
 0.0482 150 0.991   12 1.000 162 0.992 0.999
 0.0545 151 0.997   12 0.994 163 0.997 0.999
 0.0609 172 0.983   15 0.957 187 0.981 0.999
 0.0672 174 0.993   9 0.933 183 0.990 0.999
 0.0735 178 0.990   11 1.000 189 0.991 0.999
 0.0799 189 0.989   14 0.999 203 0.990 0.999
 0.0862 197 0.984   9 0.977 206 0.984 0.999
 0.0925 193 0.979   14 0.930 207 0.976 0.999
 0.0989 188 0.980   12 1.000 200 0.981 0.999
 0.1052 190 0.988   8 1.000 198 0.989 0.999
 0.1116 183 0.981   13 0.937 196 0.978 1.000
 0.1179 194 0.980   11 0.947 205 0.978 1.000
 0.1242 174 0.983   8 1.000 182 0.984 1.000
$$
Resolution limits   =   38.899   2.802
Number of used reflections   =   3184
Percentage observed   =   92.6870
Percentage of free reflections   =   4.8416
Overall R factor   =   0.0190
Free R factor   =   0.0397
Overall weighted R factor   =   0.0190
Free weighted R factor   =   0.0401
Overall correlation coefficient =   0.9994
Free correlation coefficient   =   0.9969
DPI based on free R factor   =   0.0721
Overall figure of merit   =   0.9871
ML based su of positional parameters =   0.0399
ML based su of thermal parameters   =   1.9729

 Trying gamma equal   0.0000000
 Convergence reached with no gamma cycles

 fvalues   10483.063   3165.4609   19458.469   19458.119

 fvalues   10483.063   3165.4609   19458.211   19458.119

    CGMAT cycle number =   111

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5537741 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1629E+05 GEOM= 3166. TOTAL= 0.1945E+05
function value 19452.410

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.687	1.966
Torsion angles, period 1. refined	155	7.869	5.000
Torsion angles, period 2. refined	54	41.443	25.741
Torsion angles, period 3. refined	214	19.228	15.000
Torsion angles, period 4. refined	3	21.340	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	791	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.225	0.200
Bond B values: refined atoms	1229	13.569	4.727
Angle B values: refined atoms	1663	16.864	7.131
Torsion B values: refined atoms	426	31.492	13.104
Long range B values: refined atoms	1337	11.608	15.308

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 111. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 111. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 111. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 111. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$

0.004	30	62.50	754.4	748.0	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	414.1	416.0	0.02	0.02	1	1228.7	1225.3	0.01	0.01	
0.017	83	95.60	307.8	308.8	0.03	0.02	4	403.1	413.1	0.04	0.05	
0.023	97	97.14	247.4	248.4	0.02	0.02	5	180.2	189.4	0.07	0.07	
0.029	108	100.00	241.3	242.0	0.02	0.02	7	186.7	189.4	0.06	0.06	
0.036	126	99.25	270.4	270.7	0.02	0.02	6	252.9	254.2	0.04	0.04	
0.042	129	98.56	286.3	287.5	0.02	0.02	8	338.1	341.1	0.02	0.02	
0.048	150	98.73	296.8	296.4	0.02	0.01	5	305.8	307.4	0.03	0.02	
0.055	151	99.38	281.3	281.5	0.01	0.01	10	257.9	260.0	0.04	0.04	
0.061	172	100.00	218.4	218.6	0.02	0.02	10	202.2	202.8	0.03	0.03	
0.067	174	99.45	211.5	211.0	0.02	0.02	6	286.3	284.3	0.02	0.02	
0.074	178	98.92	206.1	206.8	0.02	0.02	6	234.6	237.5	0.04	0.03	
0.080	189	100.00	208.7	209.0	0.02	0.02	13	159.7	156.0	0.06	0.06	
0.086	197	100.00	176.8	176.9	0.02	0.02	8	208.6	207.6	0.04	0.04	
0.093	193	93.55	156.9	157.0	0.02	0.02	10	182.0	186.0	0.07	0.06	
0.099	188	91.28	160.7	159.8	0.02	0.02	11	159.7	157.1	0.02	0.02	
0.105	190	86.02	153.9	153.5	0.02	0.02	13	169.2	170.0	0.05	0.04	
0.112	183	80.08	129.9	129.6	0.02	0.02	6	135.2	141.2	0.08	0.08	
0.118	194	81.85	127.0	126.8	0.02	0.02	9	138.0	137.1	0.05	0.05	
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	110.9	0.06	0.06	

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 111. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 111. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.991	12	0.925	95	0.983	0.999
0.0228	97	0.989	11	1.000	108	0.990	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.996	17	1.000	143	0.996	0.999
0.0418	129	0.997	11	1.000	140	0.997	0.999
0.0482	150	0.991	12	1.000	162	0.992	0.999
0.0545	151	0.997	12	0.994	163	0.997	0.999
0.0609	172	0.983	15	0.957	187	0.981	0.999
0.0672	174	0.993	9	0.933	183	0.990	0.999

```
 0.0735   178   0.990    11   1.000   189   0.991  0.999
 0.0799   189   0.989    14   0.999   203   0.990  0.999
 0.0862   197   0.984     9   0.977   206   0.984  0.999
 0.0925   193   0.979    14   0.930   207   0.976  0.999
 0.0989   188   0.980    12   1.000   200   0.981  0.999
 0.1052   190   0.988     8   1.000   198   0.989  0.999
 0.1116   183   0.981    13   0.937   196   0.978  1.000
 0.1179   194   0.980    11   0.947   205   0.978  1.000
 0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0190
Free R factor                    =     0.0397
Overall weighted R factor        =     0.0190
Free weighted R factor           =     0.0401
Overall correlation coefficient  =     0.9994
Free correlation coefficient     =     0.9969
DPI based on free R factor       =     0.0721
Overall figure of merit          =     0.9871
ML based su of positional parameters =     0.0399
ML based su of thermal parameters    =     1.9728
------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10482.663       3165.5232       19453.199       19453.213


    CGMAT cycle number =    112

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    1.5526797      is applied to the X-ray term
Norm of X_ray positional gradient              13.7
Norm of Geom. positional gradient              13.7
Norm of X_ray B-factor gradient                17.8
Norm of Geom. B-factor gradient                18.2
Product of X_ray and Geom posit. gradients     -0.693E+06
 Cosine of angle between them                  -1.000
Product of X_ray and Geom B-fact gradients     -0.396E+06
 Cosine of angle between them                  -0.995
```

Residuals: XRAY= 0.1627E+05 GEOM= 3166. TOTAL= 0.1944E+05
function value 19439.781

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.688	1.966
Torsion angles, period 1. refined	155	7.870	5.000
Torsion angles, period 2. refined	54	41.444	25.741
Torsion angles, period 3. refined	214	19.225	15.000
Torsion angles, period 4. refined	3	21.336	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	791	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.223	0.200
Bond B values: refined atoms	1229	13.576	4.728
Angle B values: refined atoms	1663	16.878	7.132
Torsion B values: refined atoms	426	31.528	13.105
Long range B values: refined atoms	1337	11.611	15.308

Overall : scale = 1.011, B = -0.026
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 112. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 112. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 112. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 112. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$

0.004	30	62.50	754.4	748.0	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	414.1	416.0	0.02	0.02	1	1228.7	1225.3	0.01	0.01	
0.017	83	95.60	307.8	308.8	0.03	0.02	4	403.1	413.1	0.04	0.05	
0.023	97	97.14	247.4	248.4	0.02	0.02	5	180.2	189.4	0.07	0.07	
0.029	108	100.00	241.3	242.0	0.02	0.02	7	186.7	189.4	0.06	0.06	
0.036	126	99.25	270.4	270.7	0.02	0.02	6	252.9	254.2	0.04	0.04	

0.042	129	98.56	286.3	287.5	0.02	0.02	8	338.2	341.1	0.02	0.02
0.048	150	98.73	296.8	296.4	0.02	0.01	5	305.8	307.4	0.03	0.02
0.055	151	99.38	281.3	281.5	0.01	0.01	10	257.9	260.1	0.04	0.04
0.061	172	100.00	218.4	218.6	0.02	0.02	10	202.2	202.8	0.03	0.03
0.067	174	99.45	211.5	211.0	0.02	0.02	6	286.3	284.4	0.02	0.02
0.074	178	98.92	206.1	206.8	0.02	0.02	6	234.6	237.5	0.04	0.03
0.080	189	100.00	208.7	209.0	0.02	0.02	13	159.7	156.0	0.06	0.06
0.086	197	100.00	176.8	176.9	0.02	0.02	8	208.6	207.6	0.04	0.04
0.093	193	93.55	156.9	157.0	0.02	0.02	10	182.0	186.0	0.07	0.06
0.099	188	91.28	160.7	159.8	0.02	0.02	11	159.7	157.1	0.02	0.02
0.105	190	86.02	153.9	153.5	0.02	0.02	13	169.2	170.0	0.05	0.04
0.112	183	80.08	129.9	129.6	0.02	0.02	6	135.2	141.2	0.08	0.08
0.118	194	81.85	127.0	126.8	0.02	0.02	9	138.0	137.1	0.05	0.05
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	110.9	0.06	0.06

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 112. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 112. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.991	12	0.925	95	0.983	0.999
0.0228	97	0.989	11	1.000	108	0.990	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.996	17	1.000	143	0.996	0.999
0.0418	129	0.997	11	1.000	140	0.997	0.999
0.0482	150	0.991	12	1.000	162	0.992	0.999
0.0545	151	0.997	12	0.995	163	0.997	0.999
0.0609	172	0.983	15	0.957	187	0.981	0.999
0.0672	174	0.993	9	0.933	183	0.990	0.999
0.0735	178	0.990	11	1.000	189	0.991	0.999
0.0799	189	0.989	14	1.000	203	0.990	0.999
0.0862	197	0.984	9	0.977	206	0.984	0.999
0.0925	193	0.979	14	0.930	207	0.976	0.999
0.0989	188	0.980	12	1.000	200	0.981	0.999
0.1052	190	0.988	8	1.000	198	0.989	0.999
0.1116	183	0.981	13	0.937	196	0.978	1.000
0.1179	194	0.980	11	0.947	205	0.978	1.000
0.1242	174	0.983	8	1.000	182	0.984	1.000

$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0190
Free R factor = 0.0397
Overall weighted R factor = 0.0190

Free weighted R factor = 0.0401
Overall correlation coefficient = 0.9994
Free correlation coefficient = 0.9969
DPI based on free R factor = 0.0721
Overall figure of merit = 0.9871
ML based su of positional parameters = 0.0399
ML based su of thermal parameters = 1.9720

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10481.785 3165.7371 19440.402 19440.592

CGMAT cycle number = 113

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000008
Actual weight 1.5512633 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.692E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1626E+05 GEOM= 3166. TOTAL= 0.1942E+05
function value 19422.969

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.687	1.966
Torsion angles, period 1. refined	155	7.870	5.000
Torsion angles, period 2. refined	54	41.443	25.741
Torsion angles, period 3. refined	214	19.235	15.000
Torsion angles, period 4. refined	3	21.338	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	791	0.325	0.200

HBOND: refined_atoms 41 0.194 0.200
VDW repulsions: symmetry: refined_atoms 55 0.262 0.200
HBOND: symmetry: refined_atoms 3 0.222 0.200
Bond B values: refined atoms 1229 13.578 4.728
Angle B values: refined atoms 1663 16.887 7.131
Torsion B values: refined atoms 426 31.554 13.105
Long range B values: refined atoms 1337 11.609 15.307

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 113. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 113. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 113. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 113. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 748.0 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.0 0.02 0.02 1 1228.7 1225.4 0.01 0.01
0.017 83 95.60 307.8 308.8 0.03 0.02 4 403.1 413.1 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 189.4 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.2 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.2 341.0 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.4 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 257.9 260.0 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.8 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.6 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 156.0 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.0 0.06 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.0 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 141.2 0.08 0.08
0.118 194 81.85 127.0 126.8 0.02 0.02 9 138.0 137.1 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 110.9 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 113. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 113. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.991 12 0.925 95 0.983 0.999
0.0228 97 0.989 11 1.000 108 0.990 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.996 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.992 0.999
0.0545 151 0.997 12 0.995 163 0.997 0.999
0.0609 172 0.983 15 0.957 187 0.981 0.999
0.0672 174 0.993 9 0.933 183 0.990 0.999
0.0735 178 0.990 11 1.000 189 0.990 0.999
0.0799 189 0.989 14 1.000 203 0.990 0.999
0.0862 197 0.984 9 0.977 206 0.984 0.999
0.0925 193 0.979 14 0.930 207 0.976 0.999
0.0989 188 0.980 12 1.000 200 0.981 0.999
0.1052 190 0.988 8 1.000 198 0.989 0.999
0.1116 183 0.981 13 0.937 196 0.978 1.000
0.1179 194 0.980 11 0.948 205 0.978 1.000
0.1242 174 0.983 8 1.000 182 0.984 1.000
$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0190
Free R factor = 0.0397
Overall weighted R factor = 0.0190
Free weighted R factor = 0.0401
Overall correlation coefficient = 0.9994
Free correlation coefficient = 0.9969
DPI based on free R factor = 0.0721
Overall figure of merit = 0.9871
ML based su of positional parameters = 0.0399
ML based su of thermal parameters = 1.9712

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10480.333 3166.0034 19424.637 19423.760

fvalues 10480.333 3166.0034 19423.816 19423.760

CGMAT cycle number = 114

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5517062 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.692E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1626E+05 GEOM= 3166. TOTAL= 0.1943E+05
function value 19428.027

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.687	1.966
Torsion angles, period 1. refined	155	7.870	5.000
Torsion angles, period 2. refined	54	41.443	25.741
Torsion angles, period 3. refined	214	19.225	15.000
Torsion angles, period 4. refined	3	21.338	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	791	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.222	0.200
Bond B values: refined atoms	1229	13.579	4.728
Angle B values: refined atoms	1663	16.889	7.131
Torsion B values: refined atoms	426	31.561	13.106
Long range B values: refined atoms	1337	11.609	15.307

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 114. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 114. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 114. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 114. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$

0.004	30	62.50	754.4	748.0	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	414.1	416.0	0.02	0.02	1	1228.7	1225.4	0.01	0.01	
0.017	83	95.60	307.8	308.8	0.03	0.02	4	403.1	413.1	0.04	0.05	
0.023	97	97.14	247.4	248.4	0.02	0.02	5	180.2	189.4	0.07	0.07	
0.029	108	100.00	241.3	242.0	0.02	0.02	7	186.7	189.4	0.06	0.06	
0.036	126	99.25	270.4	270.7	0.02	0.02	6	252.9	254.2	0.04	0.04	
0.042	129	98.56	286.3	287.5	0.02	0.02	8	338.2	341.0	0.02	0.02	
0.048	150	98.73	296.8	296.4	0.02	0.01	5	305.8	307.4	0.03	0.02	
0.055	151	99.38	281.3	281.5	0.01	0.01	10	257.9	260.0	0.04	0.04	
0.061	172	100.00	218.4	218.6	0.02	0.02	10	202.2	202.8	0.03	0.03	
0.067	174	99.45	211.5	211.0	0.02	0.02	6	286.3	284.4	0.02	0.02	
0.074	178	98.92	206.1	206.8	0.02	0.02	6	234.6	237.6	0.04	0.03	
0.080	189	100.00	208.7	209.0	0.02	0.02	13	159.7	156.0	0.06	0.06	
0.086	197	100.00	176.8	176.9	0.02	0.02	8	208.6	207.6	0.04	0.04	
0.093	193	93.55	156.9	157.0	0.02	0.02	10	182.0	186.0	0.06	0.06	
0.099	188	91.28	160.7	159.8	0.02	0.02	11	159.7	157.1	0.02	0.02	
0.105	190	86.02	153.9	153.5	0.02	0.02	13	169.2	170.0	0.05	0.04	
0.112	183	80.08	129.9	129.6	0.02	0.02	6	135.2	141.3	0.08	0.08	
0.118	194	81.85	127.0	126.8	0.02	0.02	9	138.0	137.1	0.05	0.05	
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	110.9	0.06	0.06	

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 114. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 114. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.991	12	0.925	95	0.983	0.999
0.0228	97	0.989	11	1.000	108	0.990	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.996	17	1.000	143	0.996	0.999
0.0418	129	0.997	11	1.000	140	0.997	0.999
0.0482	150	0.991	12	1.000	162	0.992	0.999
0.0545	151	0.997	12	0.995	163	0.997	0.999

```
 0.0609   172   0.983    15   0.957   187   0.981  0.999
 0.0672   174   0.993     9   0.933   183   0.990  0.999
 0.0735   178   0.990    11   1.000   189   0.990  0.999
 0.0799   189   0.989    14   0.999   203   0.990  0.999
 0.0862   197   0.984     9   0.977   206   0.984  0.999
 0.0925   193   0.979    14   0.930   207   0.976  0.999
 0.0989   188   0.980    12   1.000   200   0.981  0.999
 0.1052   190   0.988     8   1.000   198   0.989  0.999
 0.1116   183   0.981    13   0.937   196   0.978  1.000
 0.1179   194   0.980    11   0.948   205   0.978  1.000
 0.1242   174   0.983     8   1.000   182   0.984  1.000
$$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0190
Free R factor                    =     0.0397
Overall weighted R factor        =     0.0190
Free weighted R factor           =     0.0401
Overall correlation coefficient  =     0.9994
Free correlation coefficient     =     0.9969
DPI based on free R factor       =     0.0721
Overall figure of merit          =     0.9871
ML based su of positional parameters =     0.0399
ML based su of thermal parameters    =     1.9715
--------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10480.645       3165.9360       19428.672       19428.816


    CGMAT cycle number =     115

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000008
 Actual weight    1.5500388      is applied to the X-ray term
Norm of X_ray positional gradient              13.7
Norm of Geom. positional gradient              13.7
Norm of X_ray B-factor gradient                17.8
Norm of Geom. B-factor gradient                18.2
Product of X_ray and Geom posit. gradients     -0.692E+06
 Cosine of angle between them                  -1.000
```

Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1624E+05 GEOM= 3166. TOTAL= 0.1941E+05
function value 19408.248

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.688	1.966
Torsion angles, period 1. refined	155	7.869	5.000
Torsion angles, period 2. refined	54	41.443	25.741
Torsion angles, period 3. refined	214	19.229	15.000
Torsion angles, period 4. refined	3	21.336	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	791	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.220	0.200
Bond B values: refined atoms	1229	13.583	4.728
Angle B values: refined atoms	1663	16.899	7.132
Torsion B values: refined atoms	426	31.590	13.107
Long range B values: refined atoms	1337	11.608	15.307

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 115. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 115. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 115. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 115. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$

0.004	30	62.50	754.4	748.0	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	414.1	416.0	0.02	0.02	1	1228.7	1225.4	0.01	0.01	
0.017	83	95.60	307.8	308.8	0.03	0.02	4	403.1	413.1	0.04	0.05	
0.023	97	97.14	247.4	248.4	0.02	0.02	5	180.2	189.5	0.07	0.07	

0.029	108	100.00	241.3	242.0	0.02	0.02	7	186.7	189.4	0.06	0.06
0.036	126	99.25	270.4	270.7	0.02	0.02	6	252.9	254.2	0.04	0.04
0.042	129	98.56	286.3	287.5	0.02	0.02	8	338.2	341.0	0.02	0.02
0.048	150	98.73	296.8	296.4	0.02	0.01	5	305.8	307.4	0.03	0.02
0.055	151	99.38	281.3	281.5	0.01	0.01	10	257.9	260.0	0.04	0.04
0.061	172	100.00	218.4	218.6	0.02	0.02	10	202.2	202.8	0.03	0.03
0.067	174	99.45	211.5	211.0	0.02	0.02	6	286.3	284.3	0.02	0.02
0.074	178	98.92	206.1	206.8	0.02	0.02	6	234.6	237.6	0.04	0.03
0.080	189	100.00	208.7	209.0	0.02	0.02	13	159.7	156.0	0.06	0.06
0.086	197	100.00	176.8	176.9	0.02	0.02	8	208.6	207.6	0.04	0.04
0.093	193	93.55	156.9	157.0	0.02	0.02	10	182.0	186.0	0.06	0.06
0.099	188	91.28	160.7	159.8	0.02	0.02	11	159.7	157.1	0.02	0.02
0.105	190	86.02	153.9	153.5	0.02	0.02	13	169.2	170.0	0.05	0.04
0.112	183	80.08	129.9	129.6	0.02	0.02	6	135.2	141.3	0.08	0.08
0.118	194	81.85	127.0	126.8	0.02	0.02	9	138.0	137.1	0.05	0.05
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	110.9	0.06	0.06

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 115. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 115. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.991	12	0.925	95	0.983	0.999
0.0228	97	0.989	11	1.000	108	0.990	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.996	17	1.000	143	0.996	0.999
0.0418	129	0.997	11	1.000	140	0.997	0.999
0.0482	150	0.991	12	1.000	162	0.992	0.999
0.0545	151	0.997	12	0.995	163	0.997	0.999
0.0609	172	0.983	15	0.957	187	0.981	0.999
0.0672	174	0.993	9	0.933	183	0.990	0.999
0.0735	178	0.990	11	1.000	189	0.990	0.999
0.0799	189	0.989	14	1.000	203	0.990	0.999
0.0862	197	0.984	9	0.977	206	0.984	0.999
0.0925	193	0.979	14	0.930	207	0.976	0.999
0.0989	188	0.980	12	1.000	200	0.981	0.999
0.1052	190	0.988	8	1.000	198	0.989	0.999
0.1116	183	0.981	13	0.937	196	0.978	1.000
0.1179	194	0.980	11	0.948	205	0.979	1.000
0.1242	174	0.983	8	1.000	182	0.984	1.000

$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0190

Free R factor = 0.0397
Overall weighted R factor = 0.0190
Free weighted R factor = 0.0401
Overall correlation coefficient = 0.9994
Free correlation coefficient = 0.9969
DPI based on free R factor = 0.0721
Overall figure of merit = 0.9871
ML based su of positional parameters = 0.0399
ML based su of thermal parameters = 1.9705

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10479.063 3166.0808 19409.174 19409.035

fvalues 10479.063 3166.0808 19408.975 19409.035

CGMAT cycle number = 116

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5506107 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.692E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1625E+05 GEOM= 3166. TOTAL= 0.1942E+05
function value 19415.047

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.688	1.966
Torsion angles, period 1. refined	155	7.869	5.000
Torsion angles, period 2. refined	54	41.443	25.741
Torsion angles, period 3. refined	214	19.221	15.000
Torsion angles, period 4. refined	3	21.336	15.000

Chiral centres: refined atoms 187 0.112 0.200
Planar groups: refined atoms 924 0.005 0.021
VDW repulsions: refined_atoms 540 0.266 0.200
VDW; torsion: refined_atoms 791 0.325 0.200
HBOND: refined_atoms 41 0.194 0.200
VDW repulsions: symmetry: refined_atoms 55 0.262 0.200
HBOND: symmetry: refined_atoms 3 0.220 0.200
Bond B values: refined atoms 1229 13.585 4.729
Angle B values: refined atoms 1663 16.905 7.132
Torsion B values: refined atoms 426 31.605 13.108
Long range B values: refined atoms 1337 11.608 15.307

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 116. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 116. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 116. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 116. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 748.0 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.0 0.02 0.02 1 1228.7 1225.4 0.01 0.01
0.017 83 95.60 307.8 308.8 0.03 0.02 4 403.1 413.1 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 189.5 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.3 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.2 341.0 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.4 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 257.9 260.0 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.8 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.6 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 156.0 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.0 0.06 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.0 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 141.3 0.08 0.08
0.118 194 81.85 127.0 126.8 0.02 0.02 9 138.0 137.1 0.05 0.05

```
 0.124    174  73.20   129.0   128.9  0.02  0.02       9   113.8   110.9  0.06  0.06
$$
```

**** Fom and SigmaA vs resolution ****

```
$TABLE: Cycle  116. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle  116. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa  FOMa  NREFc FOMc NREFall FOMall  SigmaA_Fc1 $$
$$
 0.0038    30   0.999     4   1.000    34   0.999  0.999
 0.0102    62   0.999     7   1.000    69   0.999  0.999
 0.0165    83   0.991    12   0.925    95   0.983  0.999
 0.0228    97   0.989    11   1.000   108   0.990  0.999
 0.0292   108   0.997     6   1.000   114   0.997  0.999
 0.0355   126   0.996    17   1.000   143   0.996  0.999
 0.0418   129   0.997    11   1.000   140   0.997  0.999
 0.0482   150   0.991    12   1.000   162   0.992  0.999
 0.0545   151   0.997    12   0.995   163   0.997  0.999
 0.0609   172   0.983    15   0.957   187   0.981  0.999
 0.0672   174   0.993     9   0.933   183   0.990  0.999
 0.0735   178   0.990    11   1.000   189   0.991  0.999
 0.0799   189   0.989    14   1.000   203   0.990  0.999
 0.0862   197   0.984     9   0.977   206   0.984  0.999
 0.0925   193   0.979    14   0.930   207   0.976  0.999
 0.0989   188   0.980    12   1.000   200   0.981  0.999
 0.1052   190   0.988     8   1.000   198   0.989  0.999
 0.1116   183   0.981    13   0.937   196   0.978  1.000
 0.1179   194   0.980    11   0.948   205   0.979  1.000
 0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
Resolution limits                 =     38.899     2.802
Number of used reflections        =       3184
Percentage observed               =    92.6870
Percentage of free reflections    =     4.8416
Overall R factor                  =     0.0190
Free R factor                     =     0.0397
Overall weighted R factor         =     0.0190
Free weighted R factor            =     0.0401
Overall correlation coefficient   =     0.9994
Free correlation coefficient      =     0.9969
DPI based on free R factor        =     0.0721
Overall figure of merit           =     0.9871
ML based su of positional parameters =     0.0399
ML based su of thermal parameters    =     1.9708
---------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10479.555       3166.1409       19416.227       19415.850
```

fvalues 10479.555 3166.1409 19415.791 19415.850

CGMAT cycle number = 117

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5502332 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.692E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1624E+05 GEOM= 3166. TOTAL= 0.1941E+05
function value 19410.494

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.687	1.966
Torsion angles, period 1. refined	155	7.869	5.000
Torsion angles, period 2. refined	54	41.443	25.741
Torsion angles, period 3. refined	214	19.231	15.000
Torsion angles, period 4. refined	3	21.335	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	791	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.219	0.200
Bond B values: refined atoms	1229	13.585	4.729
Angle B values: refined atoms	1663	16.908	7.132
Torsion B values: refined atoms	426	31.616	13.108
Long range B values: refined atoms	1337	11.606	15.307

Overall : scale = 1.011, B = -0.025

Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 117. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 117. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 117. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 117. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004	30	62.50	754.4	748.0	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	414.1	416.0	0.02	0.02	1	1228.7	1225.5	0.01	0.01	
0.017	83	95.60	307.8	308.8	0.03	0.02	4	403.1	413.1	0.04	0.05	
0.023	97	97.14	247.4	248.4	0.02	0.02	5	180.2	189.5	0.07	0.07	
0.029	108	100.00	241.3	242.0	0.02	0.02	7	186.7	189.4	0.06	0.06	
0.036	126	99.25	270.4	270.7	0.02	0.02	6	252.9	254.3	0.04	0.04	
0.042	129	98.56	286.3	287.5	0.02	0.02	8	338.2	341.0	0.02	0.02	
0.048	150	98.73	296.8	296.4	0.02	0.01	5	305.8	307.4	0.03	0.02	
0.055	151	99.38	281.3	281.5	0.01	0.01	10	257.9	260.0	0.04	0.04	
0.061	172	100.00	218.4	218.6	0.02	0.02	10	202.2	202.8	0.03	0.03	
0.067	174	99.45	211.5	211.0	0.02	0.02	6	286.3	284.4	0.02	0.02	
0.074	178	98.92	206.1	206.8	0.02	0.02	6	234.6	237.6	0.04	0.03	
0.080	189	100.00	208.7	209.0	0.02	0.02	13	159.7	156.0	0.06	0.06	
0.086	197	100.00	176.8	176.9	0.02	0.02	8	208.6	207.6	0.04	0.04	
0.093	193	93.55	156.9	157.0	0.02	0.02	10	182.0	186.0	0.06	0.06	
0.099	188	91.28	160.7	159.8	0.02	0.02	11	159.7	157.1	0.02	0.02	
0.105	190	86.02	153.9	153.5	0.02	0.02	13	169.2	170.0	0.05	0.04	
0.112	183	80.08	129.9	129.6	0.02	0.02	6	135.2	141.3	0.08	0.08	
0.118	194	81.85	127.0	126.8	0.02	0.02	9	138.0	137.1	0.05	0.05	
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	110.9	0.06	0.06	

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 117. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 117. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.991	12	0.925	95	0.983	0.999
0.0228	97	0.989	11	1.000	108	0.990	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999

```
 0.0355   126   0.996    17   1.000   143   0.996  0.999
 0.0418   129   0.997    11   1.000   140   0.997  0.999
 0.0482   150   0.991    12   1.000   162   0.992  0.999
 0.0545   151   0.997    12   0.995   163   0.997  0.999
 0.0609   172   0.983    15   0.957   187   0.981  0.999
 0.0672   174   0.993     9   0.933   183   0.990  0.999
 0.0735   178   0.990    11   1.000   189   0.991  0.999
 0.0799   189   0.989    14   1.000   203   0.990  0.999
 0.0862   197   0.984     9   0.977   206   0.984  0.999
 0.0925   193   0.979    14   0.930   207   0.976  0.999
 0.0989   188   0.980    12   1.000   200   0.981  0.999
 0.1052   190   0.988     8   1.000   198   0.989  0.999
 0.1116   183   0.981    13   0.937   196   0.978  1.000
 0.1179   194   0.980    11   0.948   205   0.979  1.000
 0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0190
Free R factor                    =     0.0397
Overall weighted R factor        =     0.0190
Free weighted R factor           =     0.0401
Overall correlation coefficient  =     0.9994
Free correlation coefficient     =     0.9969
DPI based on free R factor       =     0.0721
Overall figure of merit          =     0.9871
ML based su of positional parameters =     0.0399
ML based su of thermal parameters    =     1.9707
------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10479.059       3166.2815       19411.779       19411.266

 fvalues    10479.059       3166.2815       19411.324       19411.266


    CGMAT cycle number =    118

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    1.5500413      is applied to the X-ray term
```

Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.692E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1624E+05 GEOM= 3166. TOTAL= 0.1941E+05
function value 19408.221

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.687	1.966
Torsion angles, period 1. refined	155	7.869	5.000
Torsion angles, period 2. refined	54	41.443	25.741
Torsion angles, period 3. refined	214	19.224	15.000
Torsion angles, period 4. refined	3	21.335	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	791	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.219	0.200
Bond B values: refined atoms	1229	13.586	4.729
Angle B values: refined atoms	1663	16.911	7.132
Torsion B values: refined atoms	426	31.624	13.109
Long range B values: refined atoms	1337	11.606	15.307

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 118. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 118. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 118. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 118. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used

NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 748.0 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.0 0.02 0.02 1 1228.7 1225.5 0.01 0.01
0.017 83 95.60 307.8 308.8 0.03 0.02 4 403.1 413.1 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 189.5 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.3 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.2 341.0 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.4 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 257.9 260.0 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.8 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.6 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 156.0 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.0 0.06 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.0 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 141.3 0.08 0.08
0.118 194 81.85 127.0 126.8 0.02 0.02 9 138.0 137.1 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 110.9 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 118. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 118. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.991 12 0.925 95 0.983 0.999
0.0228 97 0.989 11 1.000 108 0.990 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.996 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.992 0.999
0.0545 151 0.997 12 0.995 163 0.997 0.999
0.0609 172 0.983 15 0.957 187 0.981 0.999
0.0672 174 0.993 9 0.933 183 0.990 0.999
0.0735 178 0.990 11 1.000 189 0.990 0.999
0.0799 189 0.989 14 1.000 203 0.990 0.999
0.0862 197 0.984 9 0.977 206 0.984 0.999
0.0925 193 0.979 14 0.930 207 0.976 0.999
0.0989 188 0.980 12 1.000 200 0.981 0.999
0.1052 190 0.988 8 1.000 198 0.989 0.999
0.1116 183 0.981 13 0.937 196 0.978 1.000
0.1179 194 0.980 11 0.948 205 0.979 1.000
0.1242 174 0.983 8 1.000 182 0.984 1.000

$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0190
Free R factor = 0.0397
Overall weighted R factor = 0.0190
Free weighted R factor = 0.0401
Overall correlation coefficient = 0.9994
Free correlation coefficient = 0.9969
DPI based on free R factor = 0.0721
Overall figure of merit = 0.9871
ML based su of positional parameters = 0.0399
ML based su of thermal parameters = 1.9705

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10478.911 3166.2590 19409.066 19409.004

fvalues 10478.911 3166.2590 19409.059 19409.004

CGMAT cycle number = 119

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5506598 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.692E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1625E+05 GEOM= 3166. TOTAL= 0.1942E+05
function value 19415.377

Restraint type N restraints Rms Delta Av(Sigma)

Bond distances: refined atoms 1229 0.011 0.020
Bond angles : refined atoms 1663 1.688 1.966
Torsion angles, period 1. refined 155 7.869 5.000
Torsion angles, period 2. refined 54 41.443 25.741
Torsion angles, period 3. refined 214 19.225 15.000
Torsion angles, period 4. refined 3 21.334 15.000
Chiral centres: refined atoms 187 0.112 0.200
Planar groups: refined atoms 924 0.005 0.021
VDW repulsions: refined_atoms 540 0.266 0.200
VDW; torsion: refined_atoms 791 0.325 0.200
HBOND: refined_atoms 41 0.194 0.200
VDW repulsions: symmetry: refined_atoms 55 0.262 0.200
HBOND: symmetry: refined_atoms 3 0.219 0.200
Bond B values: refined atoms 1229 13.587 4.729
Angle B values: refined atoms 1663 16.913 7.132
Torsion B values: refined atoms 426 31.630 13.109
Long range B values: refined atoms 1337 11.606 15.307

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 119. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 119. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 119. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 119. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 748.0 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.0 0.02 0.02 1 1228.7 1225.5 0.01 0.01
0.017 83 95.60 307.8 308.8 0.03 0.02 4 403.1 413.1 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 189.5 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.3 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.2 341.0 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.4 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 257.9 260.0 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.8 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.6 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 156.0 0.06 0.06

0.086	197	100.00	176.8	176.9	0.02	0.02	8	208.6	207.6	0.04	0.04
0.093	193	93.55	156.9	157.0	0.02	0.02	10	182.0	186.0	0.06	0.06
0.099	188	91.28	160.7	159.8	0.02	0.02	11	159.7	157.1	0.02	0.02
0.105	190	86.02	153.9	153.5	0.02	0.02	13	169.2	170.0	0.05	0.04
0.112	183	80.08	129.9	129.6	0.02	0.02	6	135.2	141.3	0.08	0.08
0.118	194	81.85	127.0	126.8	0.02	0.02	9	138.0	137.1	0.05	0.05
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	110.9	0.06	0.06

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 119. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 119. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.991	12	0.925	95	0.983	0.999
0.0228	97	0.989	11	1.000	108	0.990	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.996	17	1.000	143	0.996	0.999
0.0418	129	0.997	11	1.000	140	0.997	0.999
0.0482	150	0.991	12	1.000	162	0.992	0.999
0.0545	151	0.997	12	0.995	163	0.997	0.999
0.0609	172	0.983	15	0.957	187	0.981	0.999
0.0672	174	0.993	9	0.933	183	0.990	0.999
0.0735	178	0.990	11	1.000	189	0.990	0.999
0.0799	189	0.989	14	1.000	203	0.990	0.999
0.0862	197	0.984	9	0.978	206	0.984	0.999
0.0925	193	0.979	14	0.930	207	0.976	0.999
0.0989	188	0.980	12	1.000	200	0.981	0.999
0.1052	190	0.988	8	1.000	198	0.989	0.999
0.1116	183	0.981	13	0.937	196	0.978	1.000
0.1179	194	0.980	11	0.948	205	0.979	1.000
0.1242	174	0.983	8	1.000	182	0.984	1.000

$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0190
Free R factor = 0.0397
Overall weighted R factor = 0.0190
Free weighted R factor = 0.0401
Overall correlation coefficient = 0.9994
Free correlation coefficient = 0.9969
DPI based on free R factor = 0.0721
Overall figure of merit = 0.9871
ML based su of positional parameters = 0.0399
ML based su of thermal parameters = 1.9709

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10479.329 3166.2834 19416.207 19416.158

fvalues 10479.329 3166.2834 19416.182 19416.158

CGMAT cycle number = 120

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5500172 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.692E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1624E+05 GEOM= 3166. TOTAL= 0.1941E+05
function value 19407.881

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.688	1.966
Torsion angles, period 1. refined	155	7.869	5.000
Torsion angles, period 2. refined	54	41.443	25.741
Torsion angles, period 3. refined	214	19.225	15.000
Torsion angles, period 4. refined	3	21.334	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	791	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.218	0.200
Bond B values: refined atoms	1229	13.588	4.729
Angle B values: refined atoms	1663	16.916	7.132

Torsion B values: refined atoms 426 31.638 13.109
Long range B values: refined atoms 1337 11.606 15.307

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 120. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 120. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 120. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 120. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 748.0 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.0 0.02 0.02 1 1228.7 1225.5 0.01 0.01
0.017 83 95.60 307.8 308.8 0.03 0.02 4 403.1 413.1 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.2 189.5 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.3 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.2 341.0 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.4 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 257.9 260.0 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.8 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.6 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 156.0 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.0 0.06 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.0 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 141.3 0.08 0.08
0.118 194 81.85 127.0 126.8 0.02 0.02 9 138.0 137.1 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 110.9 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 120. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 120. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$

$$
 0.0038 30 0.999 4 1.000 34 0.999 0.999
 0.0102 62 0.999 7 1.000 69 0.999 0.999
 0.0165 83 0.991 12 0.925 95 0.983 0.999
 0.0228 97 0.989 11 1.000 108 0.990 0.999
 0.0292 108 0.997 6 1.000 114 0.997 0.999
 0.0355 126 0.996 17 1.000 143 0.996 0.999
 0.0418 129 0.997 11 1.000 140 0.997 0.999
 0.0482 150 0.991 12 1.000 162 0.992 0.999
 0.0545 151 0.997 12 0.995 163 0.997 0.999
 0.0609 172 0.983 15 0.957 187 0.981 0.999
 0.0672 174 0.993 9 0.933 183 0.990 0.999
 0.0735 178 0.990 11 1.000 189 0.990 0.999
 0.0799 189 0.989 14 1.000 203 0.990 0.999
 0.0862 197 0.984 9 0.978 206 0.984 0.999
 0.0925 193 0.979 14 0.930 207 0.976 0.999
 0.0989 188 0.980 12 1.000 200 0.981 0.999
 0.1052 190 0.988 8 1.000 198 0.989 0.999
 0.1116 183 0.981 13 0.937 196 0.978 1.000
 0.1179 194 0.980 11 0.948 205 0.979 1.000
 0.1242 174 0.983 8 1.000 182 0.984 1.000
$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0190
Free R factor = 0.0397
Overall weighted R factor = 0.0190
Free weighted R factor = 0.0401
Overall correlation coefficient = 0.9994
Free correlation coefficient = 0.9969
DPI based on free R factor = 0.0721
Overall figure of merit = 0.9871
ML based su of positional parameters = 0.0399
ML based su of thermal parameters = 1.9706

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10478.831 3166.3259 19408.648 19408.695

CGMAT cycle number = 121

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation

B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5488243 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.692E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1623E+05 GEOM= 3166. TOTAL= 0.1939E+05
function value 19394.125

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.688	1.966
Torsion angles, period 1. refined	155	7.869	5.000
Torsion angles, period 2. refined	54	41.443	25.741
Torsion angles, period 3. refined	214	19.224	15.000
Torsion angles, period 4. refined	3	21.330	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	791	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.217	0.200
Bond B values: refined atoms	1229	13.590	4.729
Angle B values: refined atoms	1663	16.924	7.132
Torsion B values: refined atoms	426	31.662	13.110
Long range B values: refined atoms	1337	11.604	15.307

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 121. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 121. <Rfactor> v. resln :N:1,6,7,11,12:

:Cycle 121. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 121. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 748.0 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.0 0.02 0.02 1 1228.7 1225.5 0.01 0.01
0.017 83 95.60 307.8 308.8 0.03 0.02 4 403.1 413.0 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.3 189.6 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.3 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.2 341.0 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.4 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 257.9 260.0 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.8 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.3 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.6 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 156.0 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.0 0.06 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.0 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 141.3 0.08 0.08
0.118 194 81.85 127.0 126.8 0.02 0.02 9 138.0 137.1 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 110.9 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 121. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 121. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.991 12 0.925 95 0.983 0.999
0.0228 97 0.989 11 1.000 108 0.990 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.996 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.992 0.999
0.0545 151 0.997 12 0.995 163 0.997 0.999
0.0609 172 0.983 15 0.957 187 0.981 0.999
0.0672 174 0.993 9 0.933 183 0.990 0.999
0.0735 178 0.990 11 1.000 189 0.990 0.999
0.0799 189 0.989 14 1.000 203 0.990 0.999
0.0862 197 0.984 9 0.978 206 0.984 0.999
0.0925 193 0.979 14 0.930 207 0.976 0.999
0.0989 188 0.980 12 1.000 200 0.981 0.999

```
 0.1052   190   0.988    8   1.000   198   0.989  0.999
 0.1116   183   0.981   13   0.937   196   0.978  1.000
 0.1179   194   0.980   11   0.949   205   0.979  1.000
 0.1242   174   0.983    8   1.000   182   0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0190
Free R factor                    =     0.0397
Overall weighted R factor        =     0.0190
Free weighted R factor           =     0.0401
Overall correlation coefficient  =     0.9994
Free correlation coefficient     =     0.9969
DPI based on free R factor       =     0.0721
Overall figure of merit          =     0.9871
ML based su of positional parameters =     0.0399
ML based su of thermal parameters    =     1.9697
--------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10477.924       3166.4497       19394.947       19394.912

 fvalues    10477.924       3166.4497       19394.969       19394.912


    CGMAT cycle number =    122

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000008
 Actual weight    1.5486791      is applied to the X-ray term
Norm of X_ray positional gradient              13.7
Norm of Geom. positional gradient              13.7
Norm of X_ray B-factor gradient                17.8
Norm of Geom. B-factor gradient                18.2
Product of X_ray and Geom posit. gradients     -0.693E+06
 Cosine of angle between them                  -1.000
Product of X_ray and Geom B-fact gradients     -0.396E+06
 Cosine of angle between them                  -0.995


Residuals: XRAY=     0.1623E+05 GEOM=      3166.     TOTAL=     0.1939E+05
```

function value 19392.182

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.688	1.966
Torsion angles, period 1. refined	155	7.869	5.000
Torsion angles, period 2. refined	54	41.443	25.741
Torsion angles, period 3. refined	214	19.224	15.000
Torsion angles, period 4. refined	3	21.330	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	791	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.217	0.200
Bond B values: refined atoms	1229	13.591	4.729
Angle B values: refined atoms	1663	16.925	7.132
Torsion B values: refined atoms	426	31.668	13.110
Long range B values: refined atoms	1337	11.603	15.307

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 122. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 122. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 122. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 122. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$

0.004	30	62.50	754.4	748.0	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	414.1	416.0	0.02	0.02	1	1228.7	1225.5	0.01	0.01	
0.017	83	95.60	307.8	308.8	0.03	0.02	4	403.1	413.0	0.04	0.05	
0.023	97	97.14	247.4	248.4	0.02	0.02	5	180.3	189.6	0.07	0.07	
0.029	108	100.00	241.3	242.0	0.02	0.02	7	186.7	189.4	0.06	0.06	
0.036	126	99.25	270.4	270.7	0.02	0.02	6	252.9	254.3	0.04	0.04	
0.042	129	98.56	286.3	287.5	0.02	0.02	8	338.2	341.0	0.02	0.02	
0.048	150	98.73	296.8	296.4	0.02	0.01	5	305.8	307.4	0.03	0.02	
0.055	151	99.38	281.3	281.5	0.01	0.01	10	257.9	260.0	0.04	0.04	

0.061	172	100.00	218.4	218.6	0.02	0.02	10	202.2	202.8	0.03	0.03
0.067	174	99.45	211.5	211.0	0.02	0.02	6	286.3	284.3	0.02	0.02
0.074	178	98.92	206.1	206.8	0.02	0.02	6	234.6	237.7	0.04	0.03
0.080	189	100.00	208.7	209.0	0.02	0.02	13	159.7	156.0	0.06	0.06
0.086	197	100.00	176.8	176.9	0.02	0.02	8	208.6	207.6	0.04	0.04
0.093	193	93.55	156.9	157.0	0.02	0.02	10	182.0	186.0	0.06	0.06
0.099	188	91.28	160.7	159.8	0.02	0.02	11	159.7	157.1	0.02	0.02
0.105	190	86.02	153.9	153.5	0.02	0.02	13	169.2	170.0	0.05	0.04
0.112	183	80.08	129.9	129.6	0.02	0.02	6	135.2	141.3	0.08	0.08
0.118	194	81.85	127.0	126.8	0.02	0.02	9	138.0	137.1	0.05	0.05
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	110.9	0.06	0.06

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 122. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 122. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.991	12	0.925	95	0.983	0.999
0.0228	97	0.989	11	1.000	108	0.990	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.996	17	1.000	143	0.996	0.999
0.0418	129	0.997	11	1.000	140	0.997	0.999
0.0482	150	0.991	12	1.000	162	0.992	0.999
0.0545	151	0.997	12	0.995	163	0.997	0.999
0.0609	172	0.983	15	0.957	187	0.981	0.999
0.0672	174	0.993	9	0.933	183	0.990	0.999
0.0735	178	0.990	11	1.000	189	0.990	0.999
0.0799	189	0.989	14	1.000	203	0.990	0.999
0.0862	197	0.984	9	0.978	206	0.984	0.999
0.0925	193	0.979	14	0.930	207	0.976	0.999
0.0989	188	0.980	12	1.000	200	0.981	0.999
0.1052	190	0.988	8	1.000	198	0.989	0.999
0.1116	183	0.981	13	0.937	196	0.978	1.000
0.1179	194	0.980	11	0.949	205	0.979	1.000
0.1242	174	0.983	8	1.000	182	0.984	1.000

$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0190
Free R factor = 0.0397
Overall weighted R factor = 0.0190
Free weighted R factor = 0.0401
Overall correlation coefficient = 0.9994
Free correlation coefficient = 0.9969

DPI based on free R factor = 0.0721
Overall figure of merit = 0.9871
ML based su of positional parameters = 0.0399
ML based su of thermal parameters = 1.9698

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10477.628 3166.4758 19393.090 19392.959

fvalues 10477.628 3166.4758 19392.975 19392.959

CGMAT cycle number = 123

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5485406 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1622E+05 GEOM= 3167. TOTAL= 0.1939E+05
function value 19390.605

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.688	1.966
Torsion angles, period 1. refined	155	7.869	5.000
Torsion angles, period 2. refined	54	41.443	25.741
Torsion angles, period 3. refined	214	19.223	15.000
Torsion angles, period 4. refined	3	21.330	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	791	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200

VDW repulsions: symmetry: refined_atoms 55 0.262 0.200
HBOND: symmetry: refined_atoms 3 0.217 0.200
Bond B values: refined atoms 1229 13.591 4.729
Angle B values: refined atoms 1663 16.927 7.132
Torsion B values: refined atoms 426 31.674 13.111
Long range B values: refined atoms 1337 11.602 15.307

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 123. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 123. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 123. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 123. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 748.0 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.0 0.02 0.02 1 1228.7 1225.5 0.01 0.01
0.017 83 95.60 307.8 308.8 0.03 0.02 4 403.1 413.0 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.3 189.6 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.3 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.2 341.0 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.4 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 257.9 260.0 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.8 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.3 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.7 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 156.0 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.0 0.06 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.0 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 141.3 0.08 0.08
0.118 194 81.85 127.0 126.8 0.02 0.02 9 138.0 137.1 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 110.9 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 123. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 123. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
 0.0038   30 0.999   4 1.000   34 0.999 0.999
 0.0102   62 0.999   7 1.000   69 0.999 0.999
 0.0165   83 0.991   12 0.925   95 0.983 0.999
 0.0228   97 0.989   11 1.000 108 0.990 0.999
 0.0292 108 0.997   6 1.000 114 0.997 0.999
 0.0355 126 0.996   17 1.000 143 0.996 0.999
 0.0418 129 0.997   11 1.000 140 0.997 0.999
 0.0482 150 0.991   12 1.000 162 0.992 0.999
 0.0545 151 0.997   12 0.995 163 0.997 0.999
 0.0609 172 0.983   15 0.957 187 0.981 0.999
 0.0672 174 0.993   9 0.933 183 0.990 0.999
 0.0735 178 0.990   11 1.000 189 0.990 0.999
 0.0799 189 0.989   14 1.000 203 0.990 0.999
 0.0862 197 0.984   9 0.978 206 0.984 0.999
 0.0925 193 0.979   14 0.930 207 0.976 0.999
 0.0989 188 0.980   12 1.000 200 0.981 0.999
 0.1052 190 0.988   8 1.000 198 0.989 0.999
 0.1116 183 0.981   13 0.937 196 0.978 1.000
 0.1179 194 0.980   11 0.949 205 0.979 1.000
 0.1242 174 0.983   8 1.000 182 0.984 1.000
 $$
Resolution limits   =   38.899   2.802
Number of used reflections   =   3184
Percentage observed   =   92.6870
Percentage of free reflections   =   4.8416
Overall R factor   =   0.0190
Free R factor   =   0.0397
Overall weighted R factor   =   0.0190
Free weighted R factor   =   0.0401
Overall correlation coefficient =   0.9994
Free correlation coefficient   =   0.9969
DPI based on free R factor   =   0.0721
Overall figure of merit   =   0.9871
ML based su of positional parameters =   0.0399
ML based su of thermal parameters   =   1.9697

 Trying gamma equal   0.0000000
 Convergence reached with no gamma cycles

 fvalues   10477.519   3166.5171   19391.533   19391.379

 fvalues   10477.519   3166.5171   19391.408   19391.379

    CGMAT cycle number =   124

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000008
Actual weight 1.5486761 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1623E+05 GEOM= 3167. TOTAL= 0.1939E+05
function value 19391.980

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.688	1.966
Torsion angles, period 1. refined	155	7.869	5.000
Torsion angles, period 2. refined	54	41.443	25.741
Torsion angles, period 3. refined	214	19.223	15.000
Torsion angles, period 4. refined	3	21.330	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	791	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.216	0.200
Bond B values: refined atoms	1229	13.592	4.729
Angle B values: refined atoms	1663	16.929	7.132
Torsion B values: refined atoms	426	31.680	13.111
Long range B values: refined atoms	1337	11.602	15.306

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 124. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 124. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 124. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 124. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 748.0 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.0 0.02 0.02 1 1228.7 1225.5 0.01 0.01
0.017 83 95.60 307.8 308.8 0.03 0.02 4 403.1 413.0 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.3 189.6 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.3 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.2 341.0 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.4 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 257.9 260.0 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.8 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.3 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.6 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 156.0 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.0 0.06 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.0 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 141.3 0.08 0.08
0.118 194 81.85 127.0 126.8 0.02 0.02 9 138.0 137.1 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 110.9 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 124. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 124. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.991 12 0.925 95 0.983 0.999
0.0228 97 0.989 11 1.000 108 0.990 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.996 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.992 0.999
0.0545 151 0.997 12 0.995 163 0.997 0.999
0.0609 172 0.983 15 0.957 187 0.981 0.999

```
 0.0672   174   0.993    9   0.933   183   0.990  0.999
 0.0735   178   0.990   11   1.000   189   0.990  0.999
 0.0799   189   0.989   14   1.000   203   0.990  0.999
 0.0862   197   0.984    9   0.978   206   0.984  0.999
 0.0925   193   0.979   14   0.930   207   0.976  0.999
 0.0989   188   0.980   12   1.000   200   0.981  0.999
 0.1052   190   0.988    8   1.000   198   0.989  0.999
 0.1116   183   0.981   13   0.937   196   0.978  1.000
 0.1179   194   0.980   11   0.949   205   0.979  1.000
 0.1242   174   0.983    8   1.000   182   0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0190
Free R factor                    =     0.0397
Overall weighted R factor        =     0.0190
Free weighted R factor           =     0.0401
Overall correlation coefficient  =     0.9994
Free correlation coefficient     =     0.9969
DPI based on free R factor       =     0.0721
Overall figure of merit          =     0.9871
ML based su of positional parameters =     0.0399
ML based su of thermal parameters    =     1.9699
------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10477.473       3166.5562       19392.824       19392.768

 fvalues    10477.473       3166.5562       19392.893       19392.768


    CGMAT cycle number =    125

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    1.5483088      is applied to the X-ray term
Norm of X_ray positional gradient              13.7
Norm of Geom. positional gradient              13.7
Norm of X_ray B-factor gradient                17.8
Norm of Geom. B-factor gradient                18.2
Product of X_ray and Geom posit. gradients     -0.693E+06
```

Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1622E+05 GEOM= 3167. TOTAL= 0.1939E+05
function value 19387.783

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.688	1.966
Torsion angles, period 1. refined	155	7.869	5.000
Torsion angles, period 2. refined	54	41.443	25.741
Torsion angles, period 3. refined	214	19.223	15.000
Torsion angles, period 4. refined	3	21.330	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	791	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.216	0.200
Bond B values: refined atoms	1229	13.593	4.729
Angle B values: refined atoms	1663	16.932	7.132
Torsion B values: refined atoms	426	31.687	13.111
Long range B values: refined atoms	1337	11.602	15.306

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 125. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 125. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 125. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 125. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$

0.004	30	62.50	754.4	748.0	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	414.1	416.0	0.02	0.02	1	1228.7	1225.5	0.01	0.01	
0.017	83	95.60	307.8	308.8	0.03	0.02	4	403.1	413.0	0.04	0.05	

0.023	97	97.14	247.4	248.4	0.02	0.02	5	180.3	189.6	0.07	0.07
0.029	108	100.00	241.3	242.0	0.02	0.02	7	186.7	189.4	0.06	0.06
0.036	126	99.25	270.4	270.7	0.02	0.02	6	252.9	254.3	0.04	0.04
0.042	129	98.56	286.3	287.5	0.02	0.02	8	338.2	341.0	0.02	0.02
0.048	150	98.73	296.8	296.4	0.02	0.01	5	305.8	307.4	0.03	0.02
0.055	151	99.38	281.3	281.5	0.01	0.01	10	257.9	260.0	0.04	0.04
0.061	172	100.00	218.4	218.6	0.02	0.02	10	202.2	202.8	0.03	0.03
0.067	174	99.45	211.5	211.0	0.02	0.02	6	286.3	284.3	0.02	0.02
0.074	178	98.92	206.1	206.8	0.02	0.02	6	234.6	237.7	0.04	0.03
0.080	189	100.00	208.7	209.0	0.02	0.02	13	159.7	156.0	0.06	0.06
0.086	197	100.00	176.8	176.9	0.02	0.02	8	208.6	207.6	0.04	0.04
0.093	193	93.55	156.9	157.0	0.02	0.02	10	182.0	186.0	0.06	0.06
0.099	188	91.28	160.7	159.8	0.02	0.02	11	159.7	157.1	0.02	0.02
0.105	190	86.02	153.9	153.5	0.02	0.02	13	169.2	170.0	0.05	0.04
0.112	183	80.08	129.9	129.6	0.02	0.02	6	135.2	141.3	0.08	0.08
0.118	194	81.85	127.0	126.8	0.02	0.02	9	138.0	137.1	0.05	0.05
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	110.9	0.06	0.06

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 125. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 125. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.991	12	0.925	95	0.983	0.999
0.0228	97	0.989	11	1.000	108	0.990	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.996	17	1.000	143	0.996	0.999
0.0418	129	0.997	11	1.000	140	0.997	0.999
0.0482	150	0.991	12	1.000	162	0.992	0.999
0.0545	151	0.997	12	0.995	163	0.997	0.999
0.0609	172	0.983	15	0.957	187	0.981	0.999
0.0672	174	0.993	9	0.933	183	0.990	0.999
0.0735	178	0.990	11	1.000	189	0.990	0.999
0.0799	189	0.989	14	1.000	203	0.990	0.999
0.0862	197	0.984	9	0.978	206	0.984	0.999
0.0925	193	0.979	14	0.930	207	0.976	0.999
0.0989	188	0.980	12	1.000	200	0.981	0.999
0.1052	190	0.988	8	1.000	198	0.989	0.999
0.1116	183	0.981	13	0.937	196	0.978	1.000
0.1179	194	0.980	11	0.949	205	0.979	1.000
0.1242	174	0.983	8	1.000	182	0.984	1.000

$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416

Overall R factor = 0.0190
Free R factor = 0.0397
Overall weighted R factor = 0.0190
Free weighted R factor = 0.0401
Overall correlation coefficient = 0.9994
Free correlation coefficient = 0.9969
DPI based on free R factor = 0.0721
Overall figure of merit = 0.9871
ML based su of positional parameters = 0.0399
ML based su of thermal parameters = 1.9697

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10477.189 3166.6169 19388.570 19388.543

fvalues 10477.189 3166.6169 19388.484 19388.543

CGMAT cycle number = 126

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5483186 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1622E+05 GEOM= 3167. TOTAL= 0.1939E+05
function value 19387.707

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.688	1.966
Torsion angles, period 1. refined	155	7.869	5.000
Torsion angles, period 2. refined	54	41.443	25.741
Torsion angles, period 3. refined	214	19.223	15.000

Torsion angles, period 4. refined 3 21.330 15.000
Chiral centres: refined atoms 187 0.112 0.200
Planar groups: refined atoms 924 0.005 0.021
VDW repulsions: refined_atoms 540 0.266 0.200
VDW; torsion: refined_atoms 791 0.325 0.200
HBOND: refined_atoms 41 0.194 0.200
VDW repulsions: symmetry: refined_atoms 55 0.262 0.200
HBOND: symmetry: refined_atoms 3 0.216 0.200
Bond B values: refined atoms 1229 13.595 4.730
Angle B values: refined atoms 1663 16.937 7.132
Torsion B values: refined atoms 426 31.702 13.112
Long range B values: refined atoms 1337 11.601 15.306

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 126. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 126. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 126. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 126. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 748.0 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.0 0.02 0.02 1 1228.7 1225.6 0.01 0.01
0.017 83 95.60 307.8 308.8 0.03 0.02 4 403.1 413.0 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.3 189.6 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.3 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.2 341.0 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.4 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 257.9 260.0 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.8 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.3 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.7 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 156.0 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.0 0.06 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.0 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 141.3 0.08 0.08

```
 0.118    194  81.85   127.0   126.8  0.02  0.02      9   138.0   137.1  0.05  0.05
 0.124    174  73.20   129.0   128.9  0.02  0.02      9   113.8   110.9  0.06  0.06
$$

   ****                Fom and SigmaA vs resolution                ****

 $TABLE: Cycle  126. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
 $GRAPHS:Cycle  126. M(Fom) v. resln :N:1,3,5,7,8:
 $$
 <4SSQ/LL> NREFa  FOMa  NREFc FOMc NREFall FOMall  SigmaA_Fc1 $$
 $$
  0.0038    30   0.999     4   1.000    34   0.999  0.999
  0.0102    62   0.999     7   1.000    69   0.999  0.999
  0.0165    83   0.991    12   0.925    95   0.983  0.999
  0.0228    97   0.989    11   1.000   108   0.990  0.999
  0.0292   108   0.997     6   1.000   114   0.997  0.999
  0.0355   126   0.996    17   1.000   143   0.996  0.999
  0.0418   129   0.997    11   1.000   140   0.997  0.999
  0.0482   150   0.991    12   1.000   162   0.992  0.999
  0.0545   151   0.997    12   0.995   163   0.997  0.999
  0.0609   172   0.983    15   0.957   187   0.981  0.999
  0.0672   174   0.993     9   0.933   183   0.990  0.999
  0.0735   178   0.990    11   1.000   189   0.990  0.999
  0.0799   189   0.989    14   1.000   203   0.990  0.999
  0.0862   197   0.984     9   0.978   206   0.984  0.999
  0.0925   193   0.979    14   0.930   207   0.976  0.999
  0.0989   188   0.980    12   1.000   200   0.981  0.999
  0.1052   190   0.988     8   1.000   198   0.989  0.999
  0.1116   183   0.981    13   0.937   196   0.978  1.000
  0.1179   194   0.980    11   0.949   205   0.979  1.000
  0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
 Resolution limits                =     38.899     2.802
 Number of used reflections       =       3184
 Percentage observed              =    92.6870
 Percentage of free reflections   =     4.8416
 Overall R factor                 =     0.0190
 Free R factor                    =     0.0397
 Overall weighted R factor        =     0.0190
 Free weighted R factor           =     0.0401
 Overall correlation coefficient  =     0.9994
 Free correlation coefficient     =     0.9969
 DPI based on free R factor       =     0.0721
 Overall figure of merit          =     0.9871
 ML based su of positional parameters =     0.0399
 ML based su of thermal parameters    =     1.9698
 ------------------------------------------------------------------------
  Trying gamma equal    0.0000000
  Convergence reached with no gamma cycles
```

fvalues 10477.022 3166.7271 19388.625 19388.496

fvalues 10477.022 3166.7271 19388.557 19388.496

CGMAT cycle number = 127

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5478252 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1622E+05 GEOM= 3167. TOTAL= 0.1938E+05
function value 19381.949

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.688	1.966
Torsion angles, period 1. refined	155	7.869	5.000
Torsion angles, period 2. refined	54	41.444	25.741
Torsion angles, period 3. refined	214	19.223	15.000
Torsion angles, period 4. refined	3	21.330	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	791	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.216	0.200
Bond B values: refined atoms	1229	13.598	4.730
Angle B values: refined atoms	1663	16.941	7.132
Torsion B values: refined atoms	426	31.711	13.112
Long range B values: refined atoms	1337	11.602	15.306

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 127. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 127. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 127. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 127. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 748.0 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.0 0.02 0.02 1 1228.7 1225.6 0.01 0.01
0.017 83 95.60 307.8 308.8 0.03 0.02 4 403.1 413.0 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.3 189.6 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.3 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.2 341.0 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.4 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 257.9 260.0 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.8 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.3 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.7 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 156.0 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.0 0.06 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.0 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 141.3 0.08 0.08
0.118 194 81.85 127.0 126.8 0.02 0.02 9 138.0 137.1 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 110.9 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 127. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 127. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.991 12 0.925 95 0.983 0.999
0.0228 97 0.989 11 1.000 108 0.990 0.999

```
 0.0292   108   0.997     6   1.000   114   0.997  0.999
 0.0355   126   0.996    17   1.000   143   0.996  0.999
 0.0418   129   0.997    11   1.000   140   0.997  0.999
 0.0482   150   0.991    12   1.000   162   0.992  0.999
 0.0545   151   0.997    12   0.995   163   0.997  0.999
 0.0609   172   0.983    15   0.957   187   0.981  0.999
 0.0672   174   0.993     9   0.933   183   0.990  0.999
 0.0735   178   0.990    11   1.000   189   0.991  0.999
 0.0799   189   0.989    14   1.000   203   0.990  0.999
 0.0862   197   0.984     9   0.978   206   0.984  0.999
 0.0925   193   0.979    14   0.930   207   0.976  0.999
 0.0989   188   0.980    12   1.000   200   0.981  0.999
 0.1052   190   0.988     8   1.000   198   0.989  0.999
 0.1116   183   0.981    13   0.937   196   0.978  1.000
 0.1179   194   0.980    11   0.949   205   0.979  1.000
 0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
Resolution limits                 =     38.899     2.802
Number of used reflections        =       3184
Percentage observed               =    92.6870
Percentage of free reflections    =     4.8416
Overall R factor                  =     0.0190
Free R factor                     =     0.0397
Overall weighted R factor         =     0.0190
Free weighted R factor            =     0.0401
Overall correlation coefficient   =     0.9994
Free correlation coefficient      =     0.9969
DPI based on free R factor        =     0.0720
Overall figure of merit           =     0.9871
ML based su of positional parameters =     0.0399
ML based su of thermal parameters    =     1.9695
------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10476.591       3166.7881       19382.750       19382.719

 fvalues    10476.591       3166.7881       19382.795       19382.719


    CGMAT cycle number =    128

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
```

Actual weight 1.5477890 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1621E+05 GEOM= 3167. TOTAL= 0.1938E+05
function value 19381.729

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.688	1.966
Torsion angles, period 1. refined	155	7.869	5.000
Torsion angles, period 2. refined	54	41.444	25.741
Torsion angles, period 3. refined	214	19.223	15.000
Torsion angles, period 4. refined	3	21.329	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	791	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.215	0.200
Bond B values: refined atoms	1229	13.599	4.730
Angle B values: refined atoms	1663	16.944	7.132
Torsion B values: refined atoms	426	31.719	13.112
Long range B values: refined atoms	1337	11.603	15.306

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 128. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 128. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 128. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 128. % observed v. resln :N:1,3:
$$

M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 748.0 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.0 0.02 0.02 1 1228.7 1225.6 0.01 0.01
0.017 83 95.60 307.8 308.8 0.03 0.02 4 403.1 413.0 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.3 189.6 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.3 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.2 341.0 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.4 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 257.9 260.0 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.8 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.3 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.7 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 156.0 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.0 0.06 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.2 170.0 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 141.3 0.08 0.08
0.118 194 81.85 127.0 126.8 0.02 0.02 9 138.0 137.1 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 110.9 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 128. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 128. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.991 12 0.925 95 0.983 0.999
0.0228 97 0.989 11 1.000 108 0.990 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.996 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.992 0.999
0.0545 151 0.997 12 0.995 163 0.997 0.999
0.0609 172 0.983 15 0.957 187 0.981 0.999
0.0672 174 0.993 9 0.933 183 0.990 0.999
0.0735 178 0.990 11 1.000 189 0.990 0.999
0.0799 189 0.989 14 1.000 203 0.990 0.999
0.0862 197 0.984 9 0.978 206 0.984 0.999
0.0925 193 0.979 14 0.930 207 0.976 0.999
0.0989 188 0.980 12 1.000 200 0.981 0.999
0.1052 190 0.988 8 1.000 198 0.989 0.999
0.1116 183 0.981 13 0.937 196 0.978 1.000
0.1179 194 0.980 11 0.949 205 0.979 1.000

```
 0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0190
Free R factor                    =     0.0397
Overall weighted R factor        =     0.0190
Free weighted R factor           =     0.0401
Overall correlation coefficient  =     0.9994
Free correlation coefficient     =     0.9969
DPI based on free R factor       =     0.0721
Overall figure of merit          =     0.9871
ML based su of positional parameters =     0.0399
ML based su of thermal parameters    =     1.9694
------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10476.665       3166.8396       19382.482       19382.506


    CGMAT cycle number =    129

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    1.5474682      is applied to the X-ray term
Norm of X_ray positional gradient              13.7
Norm of Geom. positional gradient              13.7
Norm of X_ray B-factor gradient                17.8
Norm of Geom. B-factor gradient                18.2
Product of X_ray and Geom posit. gradients     -0.693E+06
 Cosine of angle between them                  -1.000
Product of X_ray and Geom B-fact gradients     -0.396E+06
 Cosine of angle between them                  -0.995


Residuals: XRAY=     0.1621E+05 GEOM=      3167.     TOTAL=     0.1938E+05
 function value    19377.840

------------------------------------------------------------------------------
          Restraint type            N restraints   Rms Delta   Av(Sigma)
Bond distances: refined atoms                1229     0.011      0.020
```

Bond angles : refined atoms 1663 1.688 1.966
Torsion angles, period 1. refined 155 7.869 5.000
Torsion angles, period 2. refined 54 41.444 25.741
Torsion angles, period 3. refined 214 19.222 15.000
Torsion angles, period 4. refined 3 21.330 15.000
Chiral centres: refined atoms 187 0.112 0.200
Planar groups: refined atoms 924 0.005 0.021
VDW repulsions: refined_atoms 540 0.266 0.200
VDW; torsion: refined_atoms 791 0.325 0.200
HBOND: refined_atoms 41 0.194 0.200
VDW repulsions: symmetry: refined_atoms 55 0.262 0.200
HBOND: symmetry: refined_atoms 3 0.214 0.200
Bond B values: refined atoms 1229 13.604 4.730
Angle B values: refined atoms 1663 16.954 7.132
Torsion B values: refined atoms 426 31.746 13.113
Long range B values: refined atoms 1337 11.603 15.306

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 129. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 129. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 129. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 129. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 748.0 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.0 0.02 0.02 1 1228.7 1225.6 0.01 0.01
0.017 83 95.60 307.8 308.8 0.03 0.02 4 403.1 413.0 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.3 189.6 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.3 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.2 341.0 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.4 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 258.0 260.0 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.8 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.3 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.7 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 156.0 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04

0.093	193	93.55	156.9	157.0	0.02	0.02	10	182.0	186.0	0.06	0.06
0.099	188	91.28	160.7	159.8	0.02	0.02	11	159.7	157.1	0.02	0.02
0.105	190	86.02	153.9	153.5	0.02	0.02	13	169.3	170.0	0.05	0.04
0.112	183	80.08	129.9	129.6	0.02	0.02	6	135.2	141.4	0.08	0.08
0.118	194	81.85	127.0	126.8	0.02	0.02	9	138.0	137.1	0.05	0.05
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	110.9	0.06	0.06

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 129. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 129. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.991	12	0.925	95	0.983	0.999
0.0228	97	0.989	11	1.000	108	0.990	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.996	17	1.000	143	0.996	0.999
0.0418	129	0.997	11	1.000	140	0.997	0.999
0.0482	150	0.991	12	1.000	162	0.992	0.999
0.0545	151	0.997	12	0.995	163	0.997	0.999
0.0609	172	0.983	15	0.957	187	0.981	0.999
0.0672	174	0.993	9	0.933	183	0.990	0.999
0.0735	178	0.990	11	1.000	189	0.990	0.999
0.0799	189	0.989	14	1.000	203	0.990	0.999
0.0862	197	0.984	9	0.978	206	0.984	0.999
0.0925	193	0.979	14	0.930	207	0.976	0.999
0.0989	188	0.980	12	1.000	200	0.981	0.999
0.1052	190	0.988	8	1.000	198	0.989	0.999
0.1116	183	0.981	13	0.937	196	0.978	1.000
0.1179	194	0.980	11	0.949	205	0.979	1.000
0.1242	174	0.983	8	1.000	182	0.984	1.000

$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0190
Free R factor = 0.0397
Overall weighted R factor = 0.0190
Free weighted R factor = 0.0401
Overall correlation coefficient = 0.9994
Free correlation coefficient = 0.9969
DPI based on free R factor = 0.0721
Overall figure of merit = 0.9871
ML based su of positional parameters = 0.0399
ML based su of thermal parameters = 1.9693

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10476.188 3167.0298 19378.600 19378.598

fvalues 10476.188 3167.0298 19378.643 19378.598

CGMAT cycle number = 130

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5484583 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1622E+05 GEOM= 3167. TOTAL= 0.1939E+05
function value 19389.338

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.688	1.966
Torsion angles, period 1. refined	155	7.868	5.000
Torsion angles, period 2. refined	54	41.444	25.741
Torsion angles, period 3. refined	214	19.222	15.000
Torsion angles, period 4. refined	3	21.330	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	791	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.214	0.200
Bond B values: refined atoms	1229	13.605	4.730
Angle B values: refined atoms	1663	16.956	7.132
Torsion B values: refined atoms	426	31.753	13.113

Long range B values: refined atoms 1337 11.603 15.306

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 130. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 130. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 130. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 130. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 748.0 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.0 0.02 0.02 1 1228.7 1225.6 0.01 0.01
0.017 83 95.60 307.8 308.8 0.03 0.02 4 403.1 413.0 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.3 189.6 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.3 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.2 341.0 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.4 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 258.0 260.0 0.04 0.04
0.061 172 100.00 218.4 218.6 0.02 0.02 10 202.2 202.8 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.3 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.7 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 156.0 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.0 0.06 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.3 170.0 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 141.4 0.08 0.08
0.118 194 81.85 127.0 126.8 0.02 0.02 9 138.0 137.1 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 110.9 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 130. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 130. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.991	12	0.925	95	0.983	0.999
0.0228	97	0.989	11	1.000	108	0.990	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.996	17	1.000	143	0.996	0.999
0.0418	129	0.997	11	1.000	140	0.997	0.999
0.0482	150	0.991	12	1.000	162	0.992	0.999
0.0545	151	0.997	12	0.995	163	0.997	0.999
0.0609	172	0.983	15	0.957	187	0.981	0.999
0.0672	174	0.993	9	0.933	183	0.990	0.999
0.0735	178	0.990	11	1.000	189	0.990	0.999
0.0799	189	0.989	14	1.000	203	0.990	0.999
0.0862	197	0.984	9	0.978	206	0.984	0.999
0.0925	193	0.979	14	0.930	207	0.976	0.999
0.0989	188	0.980	12	1.000	200	0.981	0.999
0.1052	190	0.988	8	1.000	198	0.989	0.999
0.1116	183	0.981	13	0.937	196	0.978	1.000
0.1179	194	0.980	11	0.949	205	0.979	1.000
0.1242	174	0.983	8	1.000	182	0.984	1.000

$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0190
Free R factor = 0.0397
Overall weighted R factor = 0.0190
Free weighted R factor = 0.0401
Overall correlation coefficient = 0.9994
Free correlation coefficient = 0.9969
DPI based on free R factor = 0.0721
Overall figure of merit = 0.9871
ML based su of positional parameters = 0.0399
ML based su of thermal parameters = 1.9700

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10476.913 3167.0681 19389.971 19390.131

CGMAT cycle number = 131

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG

VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5463698 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1620E+05 GEOM= 3167. TOTAL= 0.1936E+05
function value 19364.916

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.688	1.966
Torsion angles, period 1. refined	155	7.868	5.000
Torsion angles, period 2. refined	54	41.444	25.741
Torsion angles, period 3. refined	214	19.221	15.000
Torsion angles, period 4. refined	3	21.330	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	791	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.213	0.200
Bond B values: refined atoms	1229	13.610	4.730
Angle B values: refined atoms	1663	16.967	7.133
Torsion B values: refined atoms	426	31.782	13.115
Long range B values: refined atoms	1337	11.603	15.306

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 131. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 131. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 131. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:

:Cycle 131. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004	30	62.50	754.4	748.0	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	414.1	416.0	0.02	0.02	1	1228.7	1225.6	0.01	0.01	
0.017	83	95.60	307.8	308.8	0.03	0.02	4	403.1	412.9	0.04	0.05	
0.023	97	97.14	247.4	248.4	0.02	0.02	5	180.3	189.7	0.07	0.07	
0.029	108	100.00	241.3	242.0	0.02	0.02	7	186.7	189.4	0.06	0.06	
0.036	126	99.25	270.4	270.7	0.02	0.02	6	252.9	254.3	0.04	0.04	
0.042	129	98.56	286.3	287.5	0.02	0.02	8	338.2	341.0	0.02	0.02	
0.048	150	98.73	296.8	296.4	0.02	0.01	5	305.8	307.4	0.03	0.02	
0.055	151	99.38	281.3	281.5	0.01	0.01	10	258.0	260.0	0.04	0.04	
0.061	172	100.00	218.4	218.7	0.02	0.02	10	202.2	202.8	0.03	0.03	
0.067	174	99.45	211.5	211.0	0.02	0.02	6	286.3	284.3	0.02	0.02	
0.074	178	98.92	206.1	206.8	0.02	0.02	6	234.6	237.7	0.04	0.03	
0.080	189	100.00	208.7	209.0	0.02	0.02	13	159.7	156.0	0.06	0.06	
0.086	197	100.00	176.8	176.9	0.02	0.02	8	208.6	207.6	0.04	0.04	
0.093	193	93.55	156.9	157.0	0.02	0.02	10	182.0	186.0	0.06	0.06	
0.099	188	91.28	160.7	159.8	0.02	0.02	11	159.7	157.0	0.02	0.02	
0.105	190	86.02	153.9	153.5	0.02	0.02	13	169.3	170.0	0.05	0.04	
0.112	183	80.08	129.9	129.6	0.02	0.02	6	135.2	141.3	0.08	0.08	
0.118	194	81.85	127.0	126.8	0.02	0.02	9	138.0	137.1	0.05	0.05	
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	110.9	0.06	0.06	

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 131. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 131. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.991	12	0.925	95	0.983	0.999
0.0228	97	0.989	11	1.000	108	0.990	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.996	17	1.000	143	0.996	0.999
0.0418	129	0.997	11	1.000	140	0.997	0.999
0.0482	150	0.991	12	1.000	162	0.992	0.999
0.0545	151	0.997	12	0.995	163	0.997	0.999
0.0609	172	0.983	15	0.957	187	0.981	0.999
0.0672	174	0.993	9	0.933	183	0.990	0.999
0.0735	178	0.990	11	1.000	189	0.990	0.999
0.0799	189	0.989	14	1.000	203	0.990	0.999
0.0862	197	0.984	9	0.978	206	0.984	0.999
0.0925	193	0.979	14	0.930	207	0.976	0.999
0.0989	188	0.980	12	1.000	200	0.981	0.999
0.1052	190	0.988	8	1.000	198	0.989	0.999

```
 0.1116   183   0.981    13   0.937   196   0.978  1.000
 0.1179   194   0.980    11   0.950   205   0.979  1.000
 0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0190
Free R factor                    =     0.0397
Overall weighted R factor        =     0.0190
Free weighted R factor           =     0.0401
Overall correlation coefficient  =     0.9994
Free correlation coefficient     =     0.9969
DPI based on free R factor       =     0.0720
Overall figure of merit          =     0.9871
ML based su of positional parameters =     0.0398
ML based su of thermal parameters    =     1.9686
-------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10475.104       3167.2900       19365.576       19365.674


    CGMAT cycle number =    132

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000008
 Actual weight    1.5453080      is applied to the X-ray term
Norm of X_ray positional gradient              13.7
Norm of Geom. positional gradient              13.7
Norm of X_ray B-factor gradient                17.8
Norm of Geom. B-factor gradient                18.2
Product of X_ray and Geom posit. gradients     -0.693E+06
 Cosine of angle between them                  -1.000
Product of X_ray and Geom B-fact gradients     -0.396E+06
 Cosine of angle between them                  -0.995


Residuals: XRAY=     0.1618E+05 GEOM=      3167.     TOTAL=     0.1935E+05
 function value    19352.236

-------------------------------------------------------------------------------
```

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.689	1.966
Torsion angles, period 1. refined	155	7.868	5.000
Torsion angles, period 2. refined	54	41.443	25.741
Torsion angles, period 3. refined	214	19.220	15.000
Torsion angles, period 4. refined	3	21.331	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	791	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.212	0.200
Bond B values: refined atoms	1229	13.611	4.731
Angle B values: refined atoms	1663	16.972	7.133
Torsion B values: refined atoms	426	31.800	13.115
Long range B values: refined atoms	1337	11.599	15.306

Overall : scale = 1.011, B = -0.025

Overall anisotropic scale factors

B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 132. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 132. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 132. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 132. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$

0.004	30	62.50	754.4	748.0	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	414.1	416.0	0.02	0.02	1	1228.7	1225.7	0.01	0.01	
0.017	83	95.60	307.8	308.8	0.03	0.02	4	403.1	412.9	0.04	0.05	
0.023	97	97.14	247.4	248.4	0.02	0.02	5	180.3	189.7	0.07	0.07	
0.029	108	100.00	241.3	242.0	0.02	0.02	7	186.7	189.4	0.06	0.06	
0.036	126	99.25	270.4	270.7	0.02	0.02	6	252.9	254.3	0.04	0.04	
0.042	129	98.56	286.3	287.5	0.02	0.02	8	338.2	341.0	0.02	0.02	
0.048	150	98.73	296.8	296.4	0.02	0.01	5	305.8	307.4	0.03	0.02	
0.055	151	99.38	281.3	281.5	0.01	0.01	10	258.0	260.0	0.04	0.04	
0.061	172	100.00	218.4	218.7	0.02	0.02	10	202.2	202.8	0.03	0.03	
0.067	174	99.45	211.5	211.0	0.02	0.02	6	286.3	284.3	0.02	0.02	
0.074	178	98.92	206.1	206.8	0.02	0.02	6	234.6	237.7	0.04	0.03	

0.080	189	100.00	208.7	209.0	0.02	0.02	13	159.7	156.0	0.06	0.06
0.086	197	100.00	176.8	176.9	0.02	0.02	8	208.6	207.6	0.04	0.04
0.093	193	93.55	156.9	157.0	0.02	0.02	10	182.0	186.0	0.06	0.06
0.099	188	91.28	160.7	159.8	0.02	0.02	11	159.7	157.1	0.02	0.02
0.105	190	86.02	153.9	153.5	0.02	0.02	13	169.3	169.9	0.05	0.04
0.112	183	80.08	129.9	129.6	0.02	0.02	6	135.2	141.3	0.08	0.08
0.118	194	81.85	127.0	126.8	0.02	0.02	9	138.0	137.1	0.05	0.05
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	110.9	0.06	0.06

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 132. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 132. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.991	12	0.925	95	0.983	0.999
0.0228	97	0.989	11	1.000	108	0.990	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.996	17	1.000	143	0.996	0.999
0.0418	129	0.997	11	1.000	140	0.997	0.999
0.0482	150	0.991	12	1.000	162	0.992	0.999
0.0545	151	0.997	12	0.995	163	0.997	0.999
0.0609	172	0.983	15	0.957	187	0.981	0.999
0.0672	174	0.993	9	0.933	183	0.990	0.999
0.0735	178	0.990	11	1.000	189	0.990	0.999
0.0799	189	0.989	14	1.000	203	0.990	0.999
0.0862	197	0.984	9	0.978	206	0.984	0.999
0.0925	193	0.979	14	0.930	207	0.976	0.999
0.0989	188	0.980	12	1.000	200	0.981	0.999
0.1052	190	0.988	8	1.000	198	0.989	0.999
0.1116	183	0.981	13	0.937	196	0.978	1.000
0.1179	194	0.980	11	0.950	205	0.979	1.000
0.1242	174	0.983	8	1.000	182	0.984	1.000

$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0190
Free R factor = 0.0397
Overall weighted R factor = 0.0190
Free weighted R factor = 0.0401
Overall correlation coefficient = 0.9994
Free correlation coefficient = 0.9969
DPI based on free R factor = 0.0720
Overall figure of merit = 0.9871
ML based su of positional parameters = 0.0398

ML based su of thermal parameters = 1.9680

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10474.065 3167.3994 19353.086 19353.057

fvalues 10474.065 3167.3994 19353.070 19353.057

CGMAT cycle number = 133

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5446839 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1618E+05 GEOM= 3167. TOTAL= 0.1935E+05
function value 19345.057

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.689	1.966
Torsion angles, period 1. refined	155	7.868	5.000
Torsion angles, period 2. refined	54	41.443	25.741
Torsion angles, period 3. refined	214	19.220	15.000
Torsion angles, period 4. refined	3	21.330	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	791	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.262	0.200
HBOND: symmetry: refined_atoms	3	0.212	0.200
Bond B values: refined atoms	1229	13.612	4.731

Angle B values: refined atoms 1663 16.975 7.133
Torsion B values: refined atoms 426 31.807 13.116
Long range B values: refined atoms 1337 11.600 15.306

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 133. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 133. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 133. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 133. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 748.0 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.0 0.02 0.02 1 1228.7 1225.7 0.01 0.01
0.017 83 95.60 307.8 308.8 0.03 0.02 4 403.1 413.0 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.3 189.7 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.3 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.2 341.0 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.4 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 258.0 260.0 0.04 0.04
0.061 172 100.00 218.4 218.7 0.02 0.02 10 202.2 202.8 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.3 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.7 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 156.0 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.0 0.06 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.3 169.9 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 141.3 0.08 0.08
0.118 194 81.85 127.0 126.8 0.02 0.02 9 138.0 137.1 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 110.9 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 133. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 133. M(Fom) v. resln :N:1,3,5,7,8:
$$

<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.991 12 0.925 95 0.983 0.999
0.0228 97 0.989 11 1.000 108 0.990 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.996 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.992 0.999
0.0545 151 0.997 12 0.995 163 0.997 0.999
0.0609 172 0.983 15 0.957 187 0.981 0.999
0.0672 174 0.993 9 0.933 183 0.990 0.999
0.0735 178 0.990 11 1.000 189 0.990 0.999
0.0799 189 0.989 14 1.000 203 0.990 0.999
0.0862 197 0.984 9 0.978 206 0.984 0.999
0.0925 193 0.979 14 0.930 207 0.976 0.999
0.0989 188 0.980 12 1.000 200 0.981 0.999
0.1052 190 0.988 8 1.000 198 0.989 0.999
0.1116 183 0.981 13 0.937 196 0.978 1.000
0.1179 194 0.980 11 0.950 205 0.979 1.000
0.1242 174 0.983 8 1.000 182 0.984 1.000
$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0190
Free R factor = 0.0397
Overall weighted R factor = 0.0190
Free weighted R factor = 0.0401
Overall correlation coefficient = 0.9994
Free correlation coefficient = 0.9969
DPI based on free R factor = 0.0720
Overall figure of merit = 0.9871
ML based su of positional parameters = 0.0398
ML based su of thermal parameters = 1.9676

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10473.631 3167.4421 19345.863 19345.891

CGMAT cycle number = 134

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38

fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5457927 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1619E+05 GEOM= 3168. TOTAL= 0.1936E+05
function value 19357.801

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.689	1.966
Torsion angles, period 1. refined	155	7.868	5.000
Torsion angles, period 2. refined	54	41.443	25.741
Torsion angles, period 3. refined	214	19.219	15.000
Torsion angles, period 4. refined	3	21.329	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	791	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.261	0.200
HBOND: symmetry: refined_atoms	3	0.211	0.200
Bond B values: refined atoms	1229	13.615	4.731
Angle B values: refined atoms	1663	16.983	7.133
Torsion B values: refined atoms	426	31.828	13.116
Long range B values: refined atoms	1337	11.600	15.305

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 134. Rfactor analysis, F distribution v resln :

$GRAPHS:Cycle 134. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 134. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 134. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 748.0 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.0 0.02 0.02 1 1228.7 1225.7 0.01 0.01
0.017 83 95.60 307.8 308.8 0.03 0.02 4 403.1 412.9 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.3 189.7 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.5 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.3 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.2 341.0 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.5 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 258.0 260.0 0.04 0.04
0.061 172 100.00 218.4 218.7 0.02 0.02 10 202.2 202.8 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.3 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.7 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 156.0 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.0 0.06 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.3 169.9 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 141.4 0.08 0.08
0.118 194 81.85 127.0 126.8 0.02 0.02 9 138.0 137.1 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 110.9 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 134. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 134. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.991 12 0.925 95 0.983 0.999
0.0228 97 0.989 11 1.000 108 0.990 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.996 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.992 0.999
0.0545 151 0.997 12 0.995 163 0.997 0.999
0.0609 172 0.983 15 0.957 187 0.981 0.999
0.0672 174 0.993 9 0.933 183 0.990 0.999
0.0735 178 0.990 11 1.000 189 0.990 0.999
0.0799 189 0.989 14 1.000 203 0.990 0.999
0.0862 197 0.984 9 0.979 206 0.984 0.999
0.0925 193 0.979 14 0.930 207 0.976 0.999

```
 0.0989   188   0.980    12   1.000   200   0.981  0.999
 0.1052   190   0.988     8   1.000   198   0.989  0.999
 0.1116   183   0.981    13   0.936   196   0.978  1.000
 0.1179   194   0.980    11   0.950   205   0.979  1.000
 0.1242   174   0.983     8   1.000   182   0.984  1.000
$$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0189
Free R factor                    =     0.0397
Overall weighted R factor        =     0.0190
Free weighted R factor           =     0.0401
Overall correlation coefficient  =     0.9994
Free correlation coefficient     =     0.9969
DPI based on free R factor       =     0.0720
Overall figure of merit          =     0.9871
ML based su of positional parameters =     0.0398
ML based su of thermal parameters    =     1.9685
-------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10474.239       3167.5854       19358.613       19358.588

 fvalues    10474.239       3167.5854       19358.529       19358.588


    CGMAT cycle number =    135

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    1.5446254      is applied to the X-ray term
Norm of X_ray positional gradient              13.7
Norm of Geom. positional gradient              13.7
Norm of X_ray B-factor gradient                17.8
Norm of Geom. B-factor gradient                18.2
Product of X_ray and Geom posit. gradients     -0.693E+06
 Cosine of angle between them                  -1.000
Product of X_ray and Geom B-fact gradients     -0.396E+06
 Cosine of angle between them                  -0.995
```

Residuals: XRAY= 0.1618E+05 GEOM= 3168. TOTAL= 0.1934E+05
function value 19344.416

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.689	1.966
Torsion angles, period 1. refined	155	7.868	5.000
Torsion angles, period 2. refined	54	41.442	25.741
Torsion angles, period 3. refined	214	19.218	15.000
Torsion angles, period 4. refined	3	21.327	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	791	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.261	0.200
HBOND: symmetry: refined_atoms	3	0.211	0.200
Bond B values: refined atoms	1229	13.620	4.731
Angle B values: refined atoms	1663	16.990	7.133
Torsion B values: refined atoms	426	31.845	13.117
Long range B values: refined atoms	1337	11.602	15.305

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 135. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 135. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 135. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 135. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$

0.004	30	62.50	754.4	748.0	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	414.1	416.0	0.02	0.02	1	1228.7	1225.8	0.01	0.01	
0.017	83	95.60	307.8	308.8	0.03	0.02	4	403.1	412.9	0.04	0.05	
0.023	97	97.14	247.4	248.4	0.02	0.02	5	180.3	189.7	0.07	0.07	
0.029	108	100.00	241.3	242.0	0.02	0.02	7	186.7	189.4	0.06	0.06	
0.036	126	99.25	270.4	270.7	0.02	0.02	6	252.9	254.3	0.04	0.04	
0.042	129	98.56	286.3	287.5	0.02	0.02	8	338.2	341.0	0.02	0.02	
0.048	150	98.73	296.8	296.4	0.02	0.01	5	305.8	307.5	0.03	0.02	

```
 0.055    151  99.38   281.3   281.5  0.01  0.01      10   258.0   260.0  0.04  0.04
 0.061    172 100.00   218.4   218.7  0.02  0.02      10   202.2   202.8  0.03  0.03
 0.067    174  99.45   211.5   211.0  0.02  0.02       6   286.3   284.3  0.02  0.02
 0.074    178  98.92   206.1   206.8  0.02  0.02       6   234.6   237.7  0.04  0.03
 0.080    189 100.00   208.7   209.0  0.02  0.02      13   159.7   156.0  0.06  0.06
 0.086    197 100.00   176.8   176.9  0.02  0.02       8   208.6   207.6  0.04  0.04
 0.093    193  93.55   156.9   157.0  0.02  0.02      10   182.0   186.0  0.06  0.06
 0.099    188  91.28   160.7   159.8  0.02  0.02      11   159.7   157.1  0.02  0.02
 0.105    190  86.02   153.9   153.5  0.02  0.02      13   169.3   169.9  0.05  0.04
 0.112    183  80.08   129.9   129.6  0.02  0.02       6   135.2   141.4  0.08  0.08
 0.118    194  81.85   127.0   126.8  0.02  0.02       9   138.0   137.1  0.05  0.05
 0.124    174  73.20   129.0   128.9  0.02  0.02       9   113.8   110.9  0.06  0.06
$$
```

**** Fom and SigmaA vs resolution ****

```
$TABLE: Cycle  135. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle  135. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa  FOMa  NREFc FOMc NREFall FOMall  SigmaA_Fc1 $$
$$
 0.0038    30   0.999     4   1.000    34   0.999  0.999
 0.0102    62   0.999     7   1.000    69   0.999  0.999
 0.0165    83   0.991    12   0.926    95   0.983  0.999
 0.0228    97   0.989    11   1.000   108   0.990  0.999
 0.0292   108   0.997     6   1.000   114   0.997  0.999
 0.0355   126   0.996    17   1.000   143   0.996  0.999
 0.0418   129   0.997    11   1.000   140   0.997  0.999
 0.0482   150   0.991    12   1.000   162   0.992  0.999
 0.0545   151   0.997    12   0.995   163   0.997  0.999
 0.0609   172   0.983    15   0.957   187   0.981  0.999
 0.0672   174   0.993     9   0.933   183   0.990  0.999
 0.0735   178   0.990    11   1.000   189   0.990  0.999
 0.0799   189   0.989    14   1.000   203   0.990  0.999
 0.0862   197   0.984     9   0.979   206   0.984  0.999
 0.0925   193   0.979    14   0.930   207   0.976  0.999
 0.0989   188   0.980    12   1.000   200   0.981  0.999
 0.1052   190   0.988     8   1.000   198   0.989  0.999
 0.1116   183   0.981    13   0.936   196   0.978  1.000
 0.1179   194   0.980    11   0.950   205   0.979  1.000
 0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0189
Free R factor                    =     0.0397
Overall weighted R factor        =     0.0190
Free weighted R factor           =     0.0400
Overall correlation coefficient  =     0.9994
```

Free correlation coefficient = 0.9969
DPI based on free R factor = 0.0720
Overall figure of merit = 0.9872
ML based su of positional parameters = 0.0398
ML based su of thermal parameters = 1.9675

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10473.442 3167.6741 19345.146 19345.219

CGMAT cycle number = 136

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000008
Actual weight 1.5434026 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1616E+05 GEOM= 3168. TOTAL= 0.1933E+05
function value 19329.676

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.689	1.966
Torsion angles, period 1. refined	155	7.868	5.000
Torsion angles, period 2. refined	54	41.442	25.741
Torsion angles, period 3. refined	214	19.218	15.000
Torsion angles, period 4. refined	3	21.325	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	791	0.325	0.200
HBOND: refined_atoms	40	0.197	0.200
VDW repulsions: symmetry: refined_atoms	55	0.261	0.200

HBOND: symmetry: refined_atoms 3 0.210 0.200
Bond B values: refined atoms 1229 13.623 4.731
Angle B values: refined atoms 1663 16.998 7.133
Torsion B values: refined atoms 426 31.869 13.117
Long range B values: refined atoms 1336 11.603 15.310

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 136. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 136. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 136. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 136. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 748.0 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.0 0.02 0.02 1 1228.7 1225.7 0.02 0.01
0.017 83 95.60 307.8 308.8 0.03 0.02 4 403.1 412.9 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.3 189.7 0.07 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.3 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.2 341.0 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.5 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 258.0 260.0 0.04 0.04
0.061 172 100.00 218.4 218.7 0.02 0.02 10 202.2 202.8 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.3 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.8 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 156.0 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 186.0 0.06 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.3 170.0 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 141.3 0.08 0.08
0.118 194 81.85 127.0 126.8 0.02 0.02 9 138.0 137.1 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 110.9 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 136. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:

$GRAPHS:Cycle 136. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.991 12 0.925 95 0.983 0.999
0.0228 97 0.989 11 1.000 108 0.990 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.996 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.992 0.999
0.0545 151 0.997 12 0.995 163 0.997 0.999
0.0609 172 0.983 15 0.957 187 0.981 0.999
0.0672 174 0.993 9 0.933 183 0.990 0.999
0.0735 178 0.990 11 1.000 189 0.990 0.999
0.0799 189 0.989 14 1.000 203 0.990 0.999
0.0862 197 0.984 9 0.979 206 0.984 0.999
0.0925 193 0.979 14 0.930 207 0.976 0.999
0.0989 188 0.980 12 1.000 200 0.981 0.999
0.1052 190 0.988 8 1.000 198 0.989 0.999
0.1116 183 0.981 13 0.937 196 0.978 1.000
0.1179 194 0.980 11 0.951 205 0.979 1.000
0.1242 174 0.983 8 1.000 182 0.984 1.000
$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0189
Free R factor = 0.0397
Overall weighted R factor = 0.0190
Free weighted R factor = 0.0400
Overall correlation coefficient = 0.9994
Free correlation coefficient = 0.9969
DPI based on free R factor = 0.0720
Overall figure of merit = 0.9872
ML based su of positional parameters = 0.0398
ML based su of thermal parameters = 1.9671

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10472.193 3167.7051 19330.533 19330.516

fvalues 10472.193 3167.7051 19330.541 19330.516

CGMAT cycle number = 137

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5426372 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1615E+05 GEOM= 3168. TOTAL= 0.1932E+05
function value 19320.775

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.689	1.966
Torsion angles, period 1. refined	155	7.868	5.000
Torsion angles, period 2. refined	54	41.442	25.741
Torsion angles, period 3. refined	214	19.218	15.000
Torsion angles, period 4. refined	3	21.324	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	791	0.325	0.200
HBOND: refined_atoms	40	0.197	0.200
VDW repulsions: symmetry: refined_atoms	55	0.261	0.200
HBOND: symmetry: refined_atoms	3	0.210	0.200
Bond B values: refined atoms	1229	13.624	4.731
Angle B values: refined atoms	1663	16.999	7.133
Torsion B values: refined atoms	426	31.874	13.118
Long range B values: refined atoms	1336	11.603	15.310

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 137. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 137. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 137. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 137. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$

0.004	30	62.50	754.4	748.0	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	414.1	416.0	0.02	0.02	1	1228.7	1225.7	0.01	0.01	
0.017	83	95.60	307.8	308.8	0.03	0.02	4	403.1	412.9	0.04	0.05	
0.023	97	97.14	247.4	248.4	0.02	0.02	5	180.3	189.8	0.07	0.07	
0.029	108	100.00	241.3	242.0	0.02	0.02	7	186.7	189.4	0.06	0.06	
0.036	126	99.25	270.4	270.7	0.02	0.02	6	252.9	254.3	0.04	0.04	
0.042	129	98.56	286.3	287.5	0.02	0.02	8	338.2	341.0	0.02	0.02	
0.048	150	98.73	296.8	296.4	0.02	0.01	5	305.8	307.5	0.03	0.02	
0.055	151	99.38	281.3	281.5	0.01	0.01	10	258.0	260.0	0.04	0.04	
0.061	172	100.00	218.4	218.7	0.02	0.02	10	202.2	202.8	0.03	0.03	
0.067	174	99.45	211.5	211.0	0.02	0.02	6	286.3	284.3	0.02	0.02	
0.074	178	98.92	206.1	206.8	0.02	0.02	6	234.6	237.8	0.04	0.03	
0.080	189	100.00	208.7	209.0	0.02	0.02	13	159.7	156.0	0.06	0.06	
0.086	197	100.00	176.8	176.9	0.02	0.02	8	208.6	207.6	0.04	0.04	
0.093	193	93.55	156.9	157.0	0.02	0.02	10	182.0	186.0	0.06	0.06	
0.099	188	91.28	160.7	159.8	0.02	0.02	11	159.7	157.1	0.02	0.02	
0.105	190	86.02	153.9	153.5	0.02	0.02	13	169.3	170.0	0.05	0.04	
0.112	183	80.08	129.9	129.6	0.02	0.02	6	135.2	141.3	0.08	0.08	
0.118	194	81.85	127.0	126.8	0.02	0.02	9	138.0	137.1	0.05	0.05	
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	110.9	0.06	0.06	

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 137. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 137. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.991	12	0.926	95	0.983	0.999
0.0228	97	0.989	11	1.000	108	0.990	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.996	17	1.000	143	0.996	0.999
0.0418	129	0.997	11	1.000	140	0.997	0.999
0.0482	150	0.991	12	1.000	162	0.992	0.999
0.0545	151	0.997	12	0.995	163	0.997	0.999
0.0609	172	0.983	15	0.957	187	0.981	0.999
0.0672	174	0.993	9	0.933	183	0.990	0.999

```
 0.0735   178   0.990    11   1.000   189   0.990  0.999
 0.0799   189   0.989    14   1.000   203   0.990  0.999
 0.0862   197   0.984     9   0.979   206   0.984  0.999
 0.0925   193   0.979    14   0.930   207   0.976  0.999
 0.0989   188   0.980    12   1.000   200   0.981  0.999
 0.1052   190   0.988     8   1.000   198   0.989  0.999
 0.1116   183   0.981    13   0.937   196   0.978  1.000
 0.1179   194   0.980    11   0.950   205   0.979  1.000
 0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0189
Free R factor                    =     0.0396
Overall weighted R factor        =     0.0190
Free weighted R factor           =     0.0400
Overall correlation coefficient  =     0.9994
Free correlation coefficient     =     0.9969
DPI based on free R factor       =     0.0720
Overall figure of merit          =     0.9872
ML based su of positional parameters =     0.0398
ML based su of thermal parameters    =     1.9665
------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10471.552       3167.7520       19321.680       19321.557

 fvalues    10471.552       3167.7520       19321.631       19321.557


    CGMAT cycle number =    138

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    1.5434952      is applied to the X-ray term
Norm of X_ray positional gradient              13.7
Norm of Geom. positional gradient              13.7
Norm of X_ray B-factor gradient                17.8
Norm of Geom. B-factor gradient                18.2
Product of X_ray and Geom posit. gradients     -0.693E+06
 Cosine of angle between them                  -1.000
```

Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1616E+05 GEOM= 3168. TOTAL= 0.1933E+05
function value 19330.709

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.689	1.966
Torsion angles, period 1. refined	155	7.868	5.000
Torsion angles, period 2. refined	54	41.442	25.741
Torsion angles, period 3. refined	214	19.218	15.000
Torsion angles, period 4. refined	3	21.324	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	791	0.325	0.200
HBOND: refined_atoms	40	0.197	0.200
VDW repulsions: symmetry: refined_atoms	55	0.261	0.200
HBOND: symmetry: refined_atoms	3	0.210	0.200
Bond B values: refined atoms	1229	13.624	4.731
Angle B values: refined atoms	1663	17.001	7.133
Torsion B values: refined atoms	426	31.878	13.118
Long range B values: refined atoms	1336	11.603	15.310

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 138. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 138. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 138. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 138. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$

0.004	30	62.50	754.4	748.0	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	414.1	416.0	0.02	0.02	1	1228.7	1225.7	0.01	0.01	
0.017	83	95.60	307.8	308.8	0.03	0.02	4	403.1	412.9	0.04	0.05	
0.023	97	97.14	247.4	248.4	0.02	0.02	5	180.3	189.8	0.07	0.07	

0.029	108	100.00	241.3	242.0	0.02	0.02	7	186.7	189.4	0.06	0.06
0.036	126	99.25	270.4	270.7	0.02	0.02	6	252.9	254.3	0.04	0.04
0.042	129	98.56	286.3	287.5	0.02	0.02	8	338.2	341.0	0.02	0.02
0.048	150	98.73	296.8	296.4	0.02	0.01	5	305.8	307.5	0.03	0.02
0.055	151	99.38	281.3	281.5	0.01	0.01	10	258.0	260.0	0.04	0.04
0.061	172	100.00	218.4	218.7	0.02	0.02	10	202.2	202.8	0.03	0.03
0.067	174	99.45	211.5	211.0	0.02	0.02	6	286.3	284.3	0.02	0.02
0.074	178	98.92	206.1	206.8	0.02	0.02	6	234.6	237.8	0.04	0.03
0.080	189	100.00	208.7	209.0	0.02	0.02	13	159.7	156.0	0.06	0.06
0.086	197	100.00	176.8	176.9	0.02	0.02	8	208.6	207.6	0.04	0.04
0.093	193	93.55	156.9	157.0	0.02	0.02	10	182.0	186.0	0.06	0.06
0.099	188	91.28	160.7	159.8	0.02	0.02	11	159.7	157.1	0.02	0.02
0.105	190	86.02	153.9	153.5	0.02	0.02	13	169.3	169.9	0.05	0.04
0.112	183	80.08	129.9	129.6	0.02	0.02	6	135.2	141.3	0.08	0.08
0.118	194	81.85	127.0	126.8	0.02	0.02	9	138.0	137.1	0.05	0.05
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	110.9	0.06	0.06

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 138. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 138. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.991	12	0.925	95	0.983	0.999
0.0228	97	0.989	11	1.000	108	0.990	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.996	17	1.000	143	0.996	0.999
0.0418	129	0.997	11	1.000	140	0.997	0.999
0.0482	150	0.991	12	1.000	162	0.992	0.999
0.0545	151	0.997	12	0.995	163	0.997	0.999
0.0609	172	0.983	15	0.957	187	0.981	0.999
0.0672	174	0.993	9	0.933	183	0.990	0.999
0.0735	178	0.990	11	1.000	189	0.990	0.999
0.0799	189	0.989	14	1.000	203	0.990	0.999
0.0862	197	0.984	9	0.979	206	0.984	0.999
0.0925	193	0.979	14	0.930	207	0.976	0.999
0.0989	188	0.980	12	1.000	200	0.981	0.999
0.1052	190	0.988	8	1.000	198	0.989	0.999
0.1116	183	0.981	13	0.937	196	0.978	1.000
0.1179	194	0.980	11	0.950	205	0.979	1.000
0.1242	174	0.983	8	1.000	182	0.984	1.000

$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0189

Free R factor = 0.0396
Overall weighted R factor = 0.0190
Free weighted R factor = 0.0400
Overall correlation coefficient = 0.9994
Free correlation coefficient = 0.9969
DPI based on free R factor = 0.0720
Overall figure of merit = 0.9872
ML based su of positional parameters = 0.0398
ML based su of thermal parameters = 1.9671

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10472.177 3167.7725 19331.523 19331.527

CGMAT cycle number = 139

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.59999996
Actual weight 1.5430776 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1616E+05 GEOM= 3168. TOTAL= 0.1933E+05
function value 19325.717

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.689	1.966
Torsion angles, period 1. refined	155	7.867	5.000
Torsion angles, period 2. refined	54	41.442	25.741
Torsion angles, period 3. refined	214	19.217	15.000
Torsion angles, period 4. refined	3	21.324	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021

VDW repulsions: refined_atoms 540 0.266 0.200
VDW; torsion: refined_atoms 791 0.325 0.200
HBOND: refined_atoms 41 0.194 0.200
VDW repulsions: symmetry: refined_atoms 55 0.261 0.200
HBOND: symmetry: refined_atoms 3 0.209 0.200
Bond B values: refined atoms 1229 13.628 4.732
Angle B values: refined atoms 1663 17.009 7.133
Torsion B values: refined atoms 426 31.899 13.119
Long range B values: refined atoms 1337 11.599 15.305

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 139. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 139. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 139. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 139. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 748.0 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.0 0.02 0.02 1 1228.7 1225.8 0.02 0.01
0.017 83 95.60 307.8 308.8 0.03 0.02 4 403.1 412.9 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.3 189.8 0.08 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.3 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.2 340.9 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.5 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 258.0 260.0 0.04 0.04
0.061 172 100.00 218.4 218.7 0.02 0.02 10 202.2 202.8 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.8 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 156.0 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 185.9 0.06 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.0 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.3 169.9 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 141.4 0.08 0.08
0.118 194 81.85 127.0 126.8 0.02 0.02 9 138.0 137.1 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 110.9 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 139. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 139. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.991 12 0.926 95 0.983 0.999
0.0228 97 0.989 11 1.000 108 0.990 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.996 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.992 0.999
0.0545 151 0.997 12 0.995 163 0.997 0.999
0.0609 172 0.983 15 0.957 187 0.981 0.999
0.0672 174 0.993 9 0.933 183 0.990 0.999
0.0735 178 0.990 11 1.000 189 0.990 0.999
0.0799 189 0.989 14 1.000 203 0.990 0.999
0.0862 197 0.984 9 0.979 206 0.984 0.999
0.0925 193 0.979 14 0.930 207 0.976 0.999
0.0989 188 0.980 12 1.000 200 0.981 0.999
0.1052 190 0.988 8 1.000 198 0.989 0.999
0.1116 183 0.981 13 0.936 196 0.978 1.000
0.1179 194 0.980 11 0.950 205 0.979 1.000
0.1242 174 0.983 8 1.000 182 0.984 1.000
$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0189
Free R factor = 0.0396
Overall weighted R factor = 0.0189
Free weighted R factor = 0.0400
Overall correlation coefficient = 0.9994
Free correlation coefficient = 0.9969
DPI based on free R factor = 0.0720
Overall figure of merit = 0.9872
ML based su of positional parameters = 0.0398
ML based su of thermal parameters = 1.9670

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10471.636 3167.9565 19326.514 19326.504

fvalues 10471.636 3167.9565 19326.469 19326.504

CGMAT cycle number = 140

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000008
Actual weight 1.5427153 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1615E+05 GEOM= 3168. TOTAL= 0.1932E+05
function value 19321.275

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.689	1.966
Torsion angles, period 1. refined	155	7.867	5.000
Torsion angles, period 2. refined	54	41.442	25.741
Torsion angles, period 3. refined	214	19.217	15.000
Torsion angles, period 4. refined	3	21.323	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	791	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.261	0.200
HBOND: symmetry: refined_atoms	3	0.209	0.200
Bond B values: refined atoms	1229	13.631	4.732
Angle B values: refined atoms	1663	17.014	7.133
Torsion B values: refined atoms	426	31.912	13.120
Long range B values: refined atoms	1337	11.599	15.305

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 140. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 140. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 140. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 140. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 748.0 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.0 0.02 0.02 1 1228.7 1225.8 0.01 0.01
0.017 83 95.60 307.8 308.8 0.03 0.02 4 403.1 412.9 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.3 189.8 0.08 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.3 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.2 341.0 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.5 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 258.0 260.0 0.04 0.04
0.061 172 100.00 218.4 218.7 0.02 0.02 10 202.2 202.8 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.8 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 156.0 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 185.9 0.06 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.3 169.9 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 141.4 0.08 0.08
0.118 194 81.85 127.0 126.8 0.02 0.02 9 138.0 137.1 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 110.9 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 140. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 140. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.991 12 0.926 95 0.983 0.999
0.0228 97 0.989 11 1.000 108 0.990 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.996 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999

```
 0.0482   150   0.991    12   1.000   162   0.992  0.999
 0.0545   151   0.997    12   0.995   163   0.997  0.999
 0.0609   172   0.983    15   0.957   187   0.981  0.999
 0.0672   174   0.993     9   0.933   183   0.990  0.999
 0.0735   178   0.990    11   1.000   189   0.990  0.999
 0.0799   189   0.989    14   1.000   203   0.990  0.999
 0.0862   197   0.984     9   0.979   206   0.984  0.999
 0.0925   193   0.979    14   0.930   207   0.976  0.999
 0.0989   188   0.980    12   1.000   200   0.981  0.999
 0.1052   190   0.988     8   1.000   198   0.989  0.999
 0.1116   183   0.981    13   0.937   196   0.978  1.000
 0.1179   194   0.980    11   0.951   205   0.979  1.000
 0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
Resolution limits                 =     38.899     2.802
Number of used reflections        =       3184
Percentage observed               =    92.6870
Percentage of free reflections    =     4.8416
Overall R factor                  =     0.0189
Free R factor                     =     0.0396
Overall weighted R factor         =     0.0189
Free weighted R factor            =     0.0400
Overall correlation coefficient   =     0.9994
Free correlation coefficient      =     0.9969
DPI based on free R factor        =     0.0720
Overall figure of merit           =     0.9872
ML based su of positional parameters =     0.0398
ML based su of thermal parameters    =     1.9669
------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10471.156       3168.0396       19321.998       19322.053


    CGMAT cycle number =    141

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    1.5421122      is applied to the X-ray term
Norm of X_ray positional gradient              13.7
Norm of Geom. positional gradient              13.7
Norm of X_ray B-factor gradient                17.8
Norm of Geom. B-factor gradient                18.2
```

Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1615E+05 GEOM= 3168. TOTAL= 0.1931E+05
function value 19314.031

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.689	1.966
Torsion angles, period 1. refined	155	7.867	5.000
Torsion angles, period 2. refined	54	41.442	25.741
Torsion angles, period 3. refined	214	19.216	15.000
Torsion angles, period 4. refined	3	21.319	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	791	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.261	0.200
HBOND: symmetry: refined_atoms	3	0.208	0.200
Bond B values: refined atoms	1229	13.637	4.732
Angle B values: refined atoms	1663	17.024	7.134
Torsion B values: refined atoms	426	31.940	13.120
Long range B values: refined atoms	1337	11.601	15.305

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 141. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 141. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 141. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 141. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.4 748.0 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.0 0.02 0.02 1 1228.7 1225.8 0.02 0.01

0.017	83	95.60	307.8	308.8	0.03	0.02	4	403.1	412.9	0.04	0.05
0.023	97	97.14	247.4	248.4	0.02	0.02	5	180.3	189.8	0.08	0.07
0.029	108	100.00	241.3	242.0	0.02	0.02	7	186.7	189.4	0.06	0.06
0.036	126	99.25	270.4	270.7	0.02	0.02	6	252.9	254.3	0.04	0.04
0.042	129	98.56	286.3	287.5	0.02	0.02	8	338.2	340.9	0.02	0.02
0.048	150	98.73	296.8	296.4	0.02	0.01	5	305.8	307.5	0.03	0.02
0.055	151	99.38	281.3	281.5	0.01	0.01	10	258.0	260.0	0.04	0.04
0.061	172	100.00	218.4	218.7	0.02	0.02	10	202.2	202.8	0.03	0.03
0.067	174	99.45	211.5	211.0	0.02	0.02	6	286.3	284.3	0.02	0.02
0.074	178	98.92	206.1	206.8	0.02	0.02	6	234.6	237.8	0.04	0.03
0.080	189	100.00	208.7	209.0	0.02	0.02	13	159.7	156.0	0.06	0.06
0.086	197	100.00	176.8	176.9	0.02	0.02	8	208.6	207.6	0.04	0.04
0.093	193	93.55	156.9	157.0	0.02	0.02	10	182.0	185.9	0.06	0.06
0.099	188	91.28	160.7	159.8	0.02	0.02	11	159.7	157.1	0.02	0.02
0.105	190	86.02	153.9	153.5	0.02	0.02	13	169.3	169.9	0.05	0.04
0.112	183	80.08	129.9	129.6	0.02	0.02	6	135.2	141.4	0.08	0.08
0.118	194	81.85	127.0	126.8	0.02	0.02	9	138.0	137.1	0.05	0.05
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	110.9	0.06	0.06

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 141. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 141. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.991	12	0.926	95	0.983	0.999
0.0228	97	0.989	11	1.000	108	0.990	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.996	17	1.000	143	0.996	0.999
0.0418	129	0.997	11	1.000	140	0.997	0.999
0.0482	150	0.991	12	1.000	162	0.992	0.999
0.0545	151	0.997	12	0.995	163	0.997	0.999
0.0609	172	0.983	15	0.957	187	0.981	0.999
0.0672	174	0.993	9	0.933	183	0.990	0.999
0.0735	178	0.990	11	1.000	189	0.990	0.999
0.0799	189	0.989	14	1.000	203	0.990	0.999
0.0862	197	0.984	9	0.979	206	0.984	0.999
0.0925	193	0.979	14	0.930	207	0.976	0.999
0.0989	188	0.980	12	1.000	200	0.981	0.999
0.1052	190	0.988	8	1.000	198	0.989	0.999
0.1116	183	0.981	13	0.937	196	0.978	1.000
0.1179	194	0.980	11	0.950	205	0.979	1.000
0.1242	174	0.983	8	1.000	182	0.984	1.000

$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870

Percentage of free reflections = 4.8416
Overall R factor = 0.0189
Free R factor = 0.0396
Overall weighted R factor = 0.0189
Free weighted R factor = 0.0400
Overall correlation coefficient = 0.9994
Free correlation coefficient = 0.9969
DPI based on free R factor = 0.0720
Overall figure of merit = 0.9872
ML based su of positional parameters = 0.0398
ML based su of thermal parameters = 1.9666

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10470.415 3168.2629 19314.760 19314.818

CGMAT cycle number = 142

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.59999996
Actual weight 1.5413374 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1614E+05 GEOM= 3168. TOTAL= 0.1930E+05
function value 19304.965

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.689	1.966
Torsion angles, period 1. refined	155	7.867	5.000
Torsion angles, period 2. refined	54	41.443	25.741
Torsion angles, period 3. refined	214	19.214	15.000
Torsion angles, period 4. refined	3	21.318	15.000

Chiral centres: refined atoms 187 0.112 0.200
Planar groups: refined atoms 924 0.005 0.021
VDW repulsions: refined_atoms 540 0.266 0.200
VDW; torsion: refined_atoms 791 0.325 0.200
HBOND: refined_atoms 41 0.194 0.200
VDW repulsions: symmetry: refined_atoms 55 0.261 0.200
HBOND: symmetry: refined_atoms 3 0.208 0.200
Bond B values: refined atoms 1229 13.640 4.732
Angle B values: refined atoms 1663 17.031 7.134
Torsion B values: refined atoms 426 31.961 13.121
Long range B values: refined atoms 1337 11.599 15.305

Overall : scale = 1.011, B = -0.026
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 142. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 142. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 142. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 142. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.5 748.0 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.0 0.02 0.02 1 1228.7 1225.8 0.02 0.01
0.017 83 95.60 307.8 308.8 0.03 0.02 4 403.1 412.8 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.3 189.8 0.08 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.4 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.4 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.2 340.9 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.5 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 258.0 259.9 0.04 0.04
0.061 172 100.00 218.4 218.7 0.02 0.02 10 202.2 202.8 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.3 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.8 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 156.0 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 185.9 0.06 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.0 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.3 169.9 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 141.4 0.08 0.08
0.118 194 81.85 127.0 126.8 0.02 0.02 9 138.0 137.1 0.05 0.05

```
 0.124    174  73.20   129.0   128.9  0.02  0.02       9   113.8   110.9  0.06  0.06
$$

   ****                Fom and SigmaA vs resolution                ****

 $TABLE: Cycle  142. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
 $GRAPHS:Cycle  142. M(Fom) v. resln :N:1,3,5,7,8:
 $$
 <4SSQ/LL> NREFa  FOMa  NREFc FOMc NREFall FOMall  SigmaA_Fc1 $$
 $$
  0.0038    30   0.999     4   1.000    34   0.999  0.999
  0.0102    62   0.999     7   1.000    69   0.999  0.999
  0.0165    83   0.991    12   0.926    95   0.983  0.999
  0.0228    97   0.989    11   1.000   108   0.990  0.999
  0.0292   108   0.997     6   1.000   114   0.997  0.999
  0.0355   126   0.996    17   1.000   143   0.996  0.999
  0.0418   129   0.997    11   1.000   140   0.997  0.999
  0.0482   150   0.991    12   1.000   162   0.992  0.999
  0.0545   151   0.997    12   0.995   163   0.997  0.999
  0.0609   172   0.983    15   0.957   187   0.981  0.999
  0.0672   174   0.993     9   0.933   183   0.990  0.999
  0.0735   178   0.990    11   1.000   189   0.990  0.999
  0.0799   189   0.989    14   1.000   203   0.990  0.999
  0.0862   197   0.984     9   0.979   206   0.984  0.999
  0.0925   193   0.979    14   0.930   207   0.976  0.999
  0.0989   188   0.980    12   1.000   200   0.981  0.999
  0.1052   190   0.988     8   1.000   198   0.989  0.999
  0.1116   183   0.981    13   0.937   196   0.978  1.000
  0.1179   194   0.980    11   0.951   205   0.979  1.000
  0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
 Resolution limits                =     38.899     2.802
 Number of used reflections       =       3184
 Percentage observed              =    92.6870
 Percentage of free reflections   =     4.8416
 Overall R factor                 =     0.0189
 Free R factor                    =     0.0396
 Overall weighted R factor        =     0.0189
 Free weighted R factor           =     0.0400
 Overall correlation coefficient  =     0.9994
 Free correlation coefficient     =     0.9969
 DPI based on free R factor       =     0.0719
 Overall figure of merit          =     0.9872
 ML based su of positional parameters =     0.0398
 ML based su of thermal parameters    =     1.9662
 ------------------------------------------------------------------------------
  Trying gamma equal    0.0000000
  Convergence reached with no gamma cycles


  fvalues    10469.733       3168.3564       19305.631       19305.748
```

CGMAT cycle number = 143

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000008
Actual weight 1.5411818 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1613E+05 GEOM= 3169. TOTAL= 0.1930E+05
function value 19303.027

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.689	1.966
Torsion angles, period 1. refined	155	7.867	5.000
Torsion angles, period 2. refined	54	41.442	25.741
Torsion angles, period 3. refined	214	19.214	15.000
Torsion angles, period 4. refined	3	21.318	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	790	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.261	0.200
HBOND: symmetry: refined_atoms	3	0.207	0.200
Bond B values: refined atoms	1229	13.646	4.733
Angle B values: refined atoms	1663	17.042	7.134
Torsion B values: refined atoms	426	31.986	13.122
Long range B values: refined atoms	1337	11.601	15.304

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 143. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 143. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 143. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 143. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$

0.004	30	62.50	754.4	748.1	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	414.1	416.0	0.02	0.02	1	1228.7	1225.9	0.02	0.01	
0.017	83	95.60	307.8	308.8	0.03	0.02	4	403.1	412.8	0.04	0.05	
0.023	97	97.14	247.4	248.4	0.02	0.02	5	180.3	189.8	0.08	0.07	
0.029	108	100.00	241.3	242.0	0.02	0.02	7	186.7	189.4	0.06	0.06	
0.036	126	99.25	270.4	270.7	0.02	0.02	6	252.9	254.4	0.04	0.04	
0.042	129	98.56	286.3	287.5	0.02	0.02	8	338.2	340.9	0.02	0.02	
0.048	150	98.73	296.8	296.4	0.02	0.01	5	305.8	307.5	0.03	0.02	
0.055	151	99.38	281.3	281.5	0.01	0.01	10	258.0	259.9	0.04	0.04	
0.061	172	100.00	218.4	218.7	0.02	0.02	10	202.2	202.8	0.03	0.03	
0.067	174	99.45	211.5	211.0	0.02	0.02	6	286.3	284.3	0.02	0.02	
0.074	178	98.92	206.1	206.8	0.02	0.02	6	234.6	237.8	0.04	0.03	
0.080	189	100.00	208.7	209.0	0.02	0.02	13	159.7	156.0	0.06	0.06	
0.086	197	100.00	176.8	176.9	0.02	0.02	8	208.6	207.6	0.04	0.04	
0.093	193	93.55	156.9	157.0	0.02	0.02	10	182.0	185.9	0.06	0.06	
0.099	188	91.28	160.7	159.8	0.02	0.02	11	159.7	157.1	0.02	0.02	
0.105	190	86.02	153.9	153.5	0.02	0.02	13	169.3	169.9	0.05	0.04	
0.112	183	80.08	129.9	129.6	0.02	0.02	6	135.2	141.4	0.08	0.08	
0.118	194	81.85	127.0	126.8	0.02	0.02	9	138.0	137.1	0.05	0.05	
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	110.9	0.06	0.06	

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 143. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 143. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.991	12	0.926	95	0.983	0.999
0.0228	97	0.989	11	1.000	108	0.990	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.996	17	1.000	143	0.996	0.999
0.0418	129	0.997	11	1.000	140	0.997	0.999

```
 0.0482   150   0.991    12   1.000   162   0.992  0.999
 0.0545   151   0.997    12   0.995   163   0.997  0.999
 0.0609   172   0.983    15   0.957   187   0.981  0.999
 0.0672   174   0.993     9   0.932   183   0.990  0.999
 0.0735   178   0.990    11   1.000   189   0.990  0.999
 0.0799   189   0.989    14   1.000   203   0.990  0.999
 0.0862   197   0.984     9   0.979   206   0.984  0.999
 0.0925   193   0.979    14   0.930   207   0.976  0.999
 0.0989   188   0.980    12   1.000   200   0.981  0.999
 0.1052   190   0.988     8   1.000   198   0.989  0.999
 0.1116   183   0.981    13   0.937   196   0.978  1.000
 0.1179   194   0.980    11   0.951   205   0.979  1.000
 0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
Resolution limits                 =     38.899     2.802
Number of used reflections        =       3184
Percentage observed               =    92.6870
Percentage of free reflections    =     4.8416
Overall R factor                  =     0.0189
Free R factor                     =     0.0396
Overall weighted R factor         =     0.0189
Free weighted R factor            =     0.0400
Overall correlation coefficient   =     0.9994
Free correlation coefficient      =     0.9969
DPI based on free R factor        =     0.0720
Overall figure of merit           =     0.9872
ML based su of positional parameters =     0.0398
ML based su of thermal parameters    =     1.9660
------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10469.404       3168.5457       19303.822       19303.801

 fvalues    10469.404       3168.5457       19303.875       19303.801


    CGMAT cycle number =    144

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    1.5407250      is applied to the X-ray term
Norm of X_ray positional gradient              13.7
Norm of Geom. positional gradient              13.7
```

Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1613E+05 GEOM= 3169. TOTAL= 0.1930E+05
function value 19297.701

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.689	1.966
Torsion angles, period 1. refined	155	7.867	5.000
Torsion angles, period 2. refined	54	41.442	25.741
Torsion angles, period 3. refined	214	19.214	15.000
Torsion angles, period 4. refined	3	21.318	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	790	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.261	0.200
HBOND: symmetry: refined_atoms	3	0.207	0.200
Bond B values: refined atoms	1229	13.647	4.733
Angle B values: refined atoms	1663	17.044	7.134
Torsion B values: refined atoms	426	31.991	13.122
Long range B values: refined atoms	1337	11.601	15.304

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 144. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 144. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 144. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 144. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$

```
 0.004     30  62.50   754.5   748.1  0.02  0.02      0     0.0     0.0******  0.00
 0.010     62  95.45   414.1   416.0  0.02  0.02      1  1228.7  1225.9  0.02  0.01
 0.017     83  95.60   307.8   308.8  0.03  0.02      4   403.1   412.8  0.04  0.05
 0.023     97  97.14   247.4   248.4  0.02  0.02      5   180.3   189.8  0.08  0.07
 0.029    108 100.00   241.3   242.0  0.02  0.02      7   186.7   189.4  0.06  0.06
 0.036    126  99.25   270.4   270.7  0.02  0.02      6   252.9   254.4  0.04  0.04
 0.042    129  98.56   286.3   287.5  0.02  0.02      8   338.2   340.9  0.02  0.02
 0.048    150  98.73   296.8   296.4  0.02  0.01      5   305.8   307.5  0.03  0.02
 0.055    151  99.38   281.3   281.5  0.01  0.01     10   258.0   259.9  0.04  0.04
 0.061    172 100.00   218.4   218.7  0.02  0.02     10   202.2   202.8  0.03  0.03
 0.067    174  99.45   211.5   211.0  0.02  0.02      6   286.3   284.3  0.02  0.02
 0.074    178  98.92   206.1   206.8  0.02  0.02      6   234.6   237.8  0.04  0.03
 0.080    189 100.00   208.7   209.0  0.02  0.02     13   159.7   156.0  0.06  0.06
 0.086    197 100.00   176.8   176.9  0.02  0.02      8   208.6   207.6  0.04  0.04
 0.093    193  93.55   156.9   157.0  0.02  0.02     10   182.0   185.9  0.06  0.06
 0.099    188  91.28   160.7   159.8  0.02  0.02     11   159.7   157.1  0.02  0.02
 0.105    190  86.02   153.9   153.5  0.02  0.02     13   169.3   169.9  0.05  0.04
 0.112    183  80.08   129.9   129.6  0.02  0.02      6   135.2   141.4  0.08  0.08
 0.118    194  81.85   127.0   126.8  0.02  0.02      9   138.0   137.1  0.05  0.05
 0.124    174  73.20   129.0   128.9  0.02  0.02      9   113.8   110.9  0.06  0.06
$$
```

**** Fom and SigmaA vs resolution ****

```
$TABLE: Cycle  144. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle  144. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa  FOMa  NREFc FOMc NREFall FOMall  SigmaA_Fc1 $$
$$
 0.0038   30   0.999    4   1.000   34   0.999  0.999
 0.0102   62   0.999    7   1.000   69   0.999  0.999
 0.0165   83   0.991   12   0.926   95   0.983  0.999
 0.0228   97   0.989   11   1.000  108   0.990  0.999
 0.0292  108   0.997    6   1.000  114   0.997  0.999
 0.0355  126   0.996   17   1.000  143   0.996  0.999
 0.0418  129   0.997   11   1.000  140   0.997  0.999
 0.0482  150   0.991   12   1.000  162   0.992  0.999
 0.0545  151   0.997   12   0.995  163   0.997  0.999
 0.0609  172   0.983   15   0.957  187   0.981  0.999
 0.0672  174   0.993    9   0.932  183   0.990  0.999
 0.0735  178   0.990   11   1.000  189   0.990  0.999
 0.0799  189   0.989   14   1.000  203   0.990  0.999
 0.0862  197   0.984    9   0.979  206   0.984  0.999
 0.0925  193   0.979   14   0.930  207   0.976  0.999
 0.0989  188   0.980   12   1.000  200   0.981  0.999
 0.1052  190   0.988    8   1.000  198   0.989  0.999
 0.1116  183   0.981   13   0.937  196   0.978  1.000
 0.1179  194   0.980   11   0.951  205   0.979  1.000
 0.1242  174   0.983    8   1.000  182   0.984  1.000
 $$
Resolution limits          =    38.899     2.802
```

Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0189
Free R factor = 0.0396
Overall weighted R factor = 0.0189
Free weighted R factor = 0.0400
Overall correlation coefficient = 0.9994
Free correlation coefficient = 0.9969
DPI based on free R factor = 0.0719
Overall figure of merit = 0.9872
ML based su of positional parameters = 0.0398
ML based su of thermal parameters = 1.9658

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10469.058 3168.5542 19298.438 19298.492

CGMAT cycle number = 145

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5411060 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1613E+05 GEOM= 3169. TOTAL= 0.1930E+05
function value 19302.002

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.689	1.966
Torsion angles, period 1. refined	155	7.866	5.000
Torsion angles, period 2. refined	54	41.443	25.741

Torsion angles, period 3. refined 214 19.212 15.000
Torsion angles, period 4. refined 3 21.316 15.000
Chiral centres: refined atoms 187 0.112 0.200
Planar groups: refined atoms 924 0.005 0.021
VDW repulsions: refined_atoms 540 0.266 0.200
VDW; torsion: refined_atoms 790 0.325 0.200
HBOND: refined_atoms 41 0.194 0.200
VDW repulsions: symmetry: refined_atoms 55 0.261 0.200
HBOND: symmetry: refined_atoms 3 0.207 0.200
Bond B values: refined atoms 1229 13.650 4.733
Angle B values: refined atoms 1663 17.050 7.134
Torsion B values: refined atoms 426 32.007 13.123
Long range B values: refined atoms 1337 11.601 15.304

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 145. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 145. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 145. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 145. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.5 748.1 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.0 0.02 0.02 1 1228.7 1225.9 0.02 0.01
0.017 83 95.60 307.8 308.8 0.03 0.02 4 403.1 412.8 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.3 189.9 0.08 0.07
0.029 108 100.00 241.3 242.1 0.02 0.02 7 186.7 189.4 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.4 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.2 340.9 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.5 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 258.0 259.9 0.04 0.04
0.061 172 100.00 218.4 218.7 0.02 0.02 10 202.2 202.8 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.8 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 156.0 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 185.9 0.06 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.0 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.3 169.9 0.05 0.04

```
 0.112    183  80.08   129.9   129.6  0.02  0.02      6   135.2   141.4  0.08  0.08
 0.118    194  81.85   127.0   126.8  0.02  0.02      9   138.0   137.1  0.05  0.05
 0.124    174  73.20   129.0   128.9  0.02  0.02      9   113.8   110.9  0.06  0.06
$$

   ****                Fom and SigmaA vs resolution                ****

 $TABLE: Cycle  145. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
 $GRAPHS:Cycle  145. M(Fom) v. resln :N:1,3,5,7,8:
 $$
 <4SSQ/LL> NREFa  FOMa  NREFc FOMc NREFall FOMall  SigmaA_Fc1 $$
 $$
  0.0038    30   0.999     4   1.000    34   0.999  0.999
  0.0102    62   0.999     7   1.000    69   0.999  0.999
  0.0165    83   0.991    12   0.926    95   0.983  0.999
  0.0228    97   0.989    11   1.000   108   0.990  0.999
  0.0292   108   0.997     6   1.000   114   0.997  0.999
  0.0355   126   0.996    17   1.000   143   0.996  0.999
  0.0418   129   0.997    11   1.000   140   0.997  0.999
  0.0482   150   0.991    12   1.000   162   0.992  0.999
  0.0545   151   0.997    12   0.995   163   0.997  0.999
  0.0609   172   0.983    15   0.957   187   0.981  0.999
  0.0672   174   0.993     9   0.932   183   0.990  0.999
  0.0735   178   0.990    11   1.000   189   0.990  0.999
  0.0799   189   0.989    14   1.000   203   0.990  0.999
  0.0862   197   0.984     9   0.979   206   0.984  0.999
  0.0925   193   0.979    14   0.930   207   0.976  0.999
  0.0989   188   0.980    12   1.000   200   0.981  0.999
  0.1052   190   0.988     8   1.000   198   0.989  0.999
  0.1116   183   0.981    13   0.937   196   0.978  1.000
  0.1179   194   0.980    11   0.951   205   0.979  1.000
  0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
 Resolution limits                =     38.899     2.802
 Number of used reflections       =       3184
 Percentage observed              =    92.6870
 Percentage of free reflections   =     4.8416
 Overall R factor                 =     0.0189
 Free R factor                    =     0.0396
 Overall weighted R factor        =     0.0189
 Free weighted R factor           =     0.0400
 Overall correlation coefficient  =     0.9994
 Free correlation coefficient     =     0.9969
 DPI based on free R factor       =     0.0719
 Overall figure of merit          =     0.9872
 ML based su of positional parameters =     0.0398
 ML based su of thermal parameters    =     1.9661
 ------------------------------------------------------------------------
  Trying gamma equal    0.0000000
  Convergence reached with no gamma cycles
```

fvalues 10469.206 3168.6621 19302.902 19302.818

fvalues 10469.206 3168.6621 19302.844 19302.818

CGMAT cycle number = 146

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.59999996
Actual weight 1.5407065 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1613E+05 GEOM= 3169. TOTAL= 0.1930E+05
function value 19297.357

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.689	1.966
Torsion angles, period 1. refined	155	7.866	5.000
Torsion angles, period 2. refined	54	41.443	25.741
Torsion angles, period 3. refined	214	19.212	15.000
Torsion angles, period 4. refined	3	21.316	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	790	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.261	0.200
HBOND: symmetry: refined_atoms	3	0.206	0.200
Bond B values: refined atoms	1229	13.650	4.733
Angle B values: refined atoms	1663	17.051	7.134
Torsion B values: refined atoms	426	32.012	13.123
Long range B values: refined atoms	1337	11.601	15.304

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 146. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 146. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 146. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 146. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used
NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004	30	62.50	754.5	748.1	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	414.1	416.0	0.02	0.02	1	1228.7	1225.9	0.02	0.01	
0.017	83	95.60	307.8	308.8	0.03	0.02	4	403.1	412.8	0.04	0.05	
0.023	97	97.14	247.4	248.4	0.02	0.02	5	180.3	189.9	0.08	0.07	
0.029	108	100.00	241.3	242.1	0.02	0.02	7	186.7	189.4	0.06	0.06	
0.036	126	99.25	270.4	270.7	0.02	0.02	6	252.9	254.4	0.04	0.04	
0.042	129	98.56	286.3	287.5	0.02	0.02	8	338.2	340.9	0.02	0.02	
0.048	150	98.73	296.8	296.4	0.02	0.01	5	305.8	307.5	0.03	0.02	
0.055	151	99.38	281.3	281.5	0.01	0.01	10	258.0	259.9	0.04	0.04	
0.061	172	100.00	218.4	218.7	0.02	0.02	10	202.2	202.8	0.03	0.03	
0.067	174	99.45	211.5	211.0	0.02	0.02	6	286.3	284.3	0.02	0.02	
0.074	178	98.92	206.1	206.8	0.02	0.02	6	234.6	237.8	0.04	0.03	
0.080	189	100.00	208.7	209.0	0.02	0.02	13	159.7	156.0	0.06	0.06	
0.086	197	100.00	176.8	176.9	0.02	0.02	8	208.6	207.6	0.04	0.04	
0.093	193	93.55	156.9	157.0	0.02	0.02	10	182.0	185.9	0.06	0.06	
0.099	188	91.28	160.7	159.8	0.02	0.02	11	159.7	157.0	0.02	0.02	
0.105	190	86.02	153.9	153.5	0.02	0.02	13	169.3	169.9	0.05	0.04	
0.112	183	80.08	129.9	129.6	0.02	0.02	6	135.2	141.4	0.08	0.08	
0.118	194	81.85	127.0	126.8	0.02	0.02	9	138.0	137.1	0.05	0.05	
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	110.9	0.06	0.06	

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 146. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 146. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.991	12	0.926	95	0.983	0.999

```
 0.0228   97  0.989   11  1.000  108  0.990  0.999
 0.0292  108  0.997    6  1.000  114  0.997  0.999
 0.0355  126  0.996   17  1.000  143  0.996  0.999
 0.0418  129  0.997   11  1.000  140  0.997  0.999
 0.0482  150  0.991   12  1.000  162  0.992  0.999
 0.0545  151  0.997   12  0.995  163  0.997  0.999
 0.0609  172  0.983   15  0.957  187  0.981  0.999
 0.0672  174  0.993    9  0.932  183  0.990  0.999
 0.0735  178  0.990   11  1.000  189  0.990  0.999
 0.0799  189  0.989   14  1.000  203  0.990  0.999
 0.0862  197  0.984    9  0.979  206  0.984  0.999
 0.0925  193  0.979   14  0.930  207  0.976  0.999
 0.0989  188  0.980   12  1.000  200  0.981  0.999
 0.1052  190  0.988    8  1.000  198  0.989  0.999
 0.1116  183  0.981   13  0.937  196  0.978  1.000
 0.1179  194  0.980   11  0.951  205  0.979  1.000
 0.1242  174  0.983    8  1.000  182  0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0189
Free R factor                    =     0.0396
Overall weighted R factor        =     0.0189
Free weighted R factor           =     0.0400
Overall correlation coefficient  =     0.9994
Free correlation coefficient     =     0.9969
DPI based on free R factor       =     0.0719
Overall figure of merit          =     0.9872
ML based su of positional parameters =     0.0398
ML based su of thermal parameters    =     1.9659
-------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10468.892       3168.6882       19298.436       19298.178

 fvalues    10468.892       3168.6882       19298.236       19298.178


    CGMAT cycle number =    147

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
```

Weight matrix 0.60000002
Actual weight 1.5402669 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1612E+05 GEOM= 3169. TOTAL= 0.1929E+05
function value 19292.297

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.689	1.966
Torsion angles, period 1. refined	155	7.866	5.000
Torsion angles, period 2. refined	54	41.443	25.741
Torsion angles, period 3. refined	214	19.212	15.000
Torsion angles, period 4. refined	3	21.316	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	790	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.261	0.200
HBOND: symmetry: refined_atoms	3	0.206	0.200
Bond B values: refined atoms	1229	13.651	4.733
Angle B values: refined atoms	1663	17.053	7.134
Torsion B values: refined atoms	426	32.017	13.123
Long range B values: refined atoms	1337	11.600	15.304

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 147. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 147. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 147. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 147. % observed v. resln :N:1,3:

$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.5 748.1 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.0 0.02 0.02 1 1228.7 1225.9 0.02 0.01
0.017 83 95.60 307.8 308.8 0.03 0.02 4 403.1 412.8 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.3 189.9 0.08 0.07
0.029 108 100.00 241.3 242.1 0.02 0.02 7 186.7 189.5 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.4 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.2 340.9 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.5 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 258.0 259.9 0.04 0.04
0.061 172 100.00 218.4 218.7 0.02 0.02 10 202.2 202.8 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.8 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 156.0 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 185.9 0.06 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.0 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.3 169.9 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 141.4 0.08 0.08
0.118 194 81.85 127.0 126.8 0.02 0.02 9 138.0 137.1 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 110.9 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 147. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 147. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.991 12 0.926 95 0.983 0.999
0.0228 97 0.989 11 1.000 108 0.990 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.996 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.992 0.999
0.0545 151 0.997 12 0.995 163 0.997 0.999
0.0609 172 0.983 15 0.957 187 0.981 0.999
0.0672 174 0.993 9 0.932 183 0.990 0.999
0.0735 178 0.990 11 1.000 189 0.990 0.999
0.0799 189 0.989 14 1.000 203 0.990 0.999
0.0862 197 0.984 9 0.979 206 0.984 0.999
0.0925 193 0.979 14 0.930 207 0.976 0.999
0.0989 188 0.980 12 1.000 200 0.981 0.999
0.1052 190 0.988 8 1.000 198 0.989 0.999
0.1116 183 0.981 13 0.936 196 0.978 1.000

```
 0.1179   194   0.980    11   0.951   205   0.979  1.000
 0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0189
Free R factor                    =     0.0396
Overall weighted R factor        =     0.0189
Free weighted R factor           =     0.0400
Overall correlation coefficient  =     0.9994
Free correlation coefficient     =     0.9969
DPI based on free R factor       =     0.0719
Overall figure of merit          =     0.9872
ML based su of positional parameters =     0.0398
ML based su of thermal parameters    =     1.9656
------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10468.581       3168.7107       19293.348       19293.119

 fvalues    10468.581       3168.7107       19293.170       19293.119


    CGMAT cycle number =    148

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.59999996
 Actual weight    1.5397651      is applied to the X-ray term
Norm of X_ray positional gradient              13.7
Norm of Geom. positional gradient              13.7
Norm of X_ray B-factor gradient                17.8
Norm of Geom. B-factor gradient                18.2
Product of X_ray and Geom posit. gradients     -0.693E+06
 Cosine of angle between them                  -1.000
Product of X_ray and Geom B-fact gradients     -0.396E+06
 Cosine of angle between them                  -0.995


Residuals: XRAY=     0.1612E+05 GEOM=      3169.     TOTAL=     0.1929E+05
 function value    19286.396
```

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.689	1.966
Torsion angles, period 1. refined	155	7.866	5.000
Torsion angles, period 2. refined	54	41.443	25.741
Torsion angles, period 3. refined	214	19.211	15.000
Torsion angles, period 4. refined	3	21.315	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	790	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.261	0.200
HBOND: symmetry: refined_atoms	3	0.206	0.200
Bond B values: refined atoms	1229	13.652	4.733
Angle B values: refined atoms	1663	17.054	7.134
Torsion B values: refined atoms	426	32.021	13.123
Long range B values: refined atoms	1337	11.600	15.304

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 148. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 148. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 148. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 148. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$

0.004	30	62.50	754.5	748.1	0.02	0.02	0	0.0	0.0******	0.00	
0.010	62	95.45	414.1	416.0	0.02	0.02	1	1228.7	1225.9	0.02	0.01
0.017	83	95.60	307.8	308.8	0.03	0.02	4	403.1	412.8	0.04	0.05
0.023	97	97.14	247.4	248.4	0.02	0.02	5	180.3	189.9	0.08	0.07
0.029	108	100.00	241.3	242.0	0.02	0.02	7	186.7	189.5	0.06	0.06
0.036	126	99.25	270.4	270.7	0.02	0.02	6	252.9	254.4	0.04	0.04
0.042	129	98.56	286.3	287.5	0.02	0.02	8	338.2	340.9	0.02	0.02
0.048	150	98.73	296.8	296.4	0.02	0.01	5	305.8	307.5	0.03	0.02
0.055	151	99.38	281.3	281.5	0.01	0.01	10	258.0	259.9	0.04	0.04
0.061	172	100.00	218.4	218.7	0.02	0.02	10	202.2	202.8	0.03	0.03
0.067	174	99.45	211.5	211.0	0.02	0.02	6	286.3	284.4	0.02	0.02

```
 0.074    178  98.92   206.1   206.8  0.02  0.02      6   234.6   237.8  0.04  0.03
 0.080    189 100.00   208.7   209.0  0.02  0.02     13   159.7   156.1  0.06  0.06
 0.086    197 100.00   176.8   176.9  0.02  0.02      8   208.6   207.6  0.04  0.04
 0.093    193  93.55   156.9   157.0  0.02  0.02     10   182.0   185.9  0.06  0.06
 0.099    188  91.28   160.7   159.8  0.02  0.02     11   159.7   157.0  0.02  0.02
 0.105    190  86.02   153.9   153.5  0.02  0.02     13   169.3   169.9  0.05  0.04
 0.112    183  80.08   129.9   129.6  0.02  0.02      6   135.2   141.4  0.08  0.08
 0.118    194  81.85   127.0   126.8  0.02  0.02      9   138.0   137.1  0.05  0.05
 0.124    174  73.20   129.0   128.9  0.02  0.02      9   113.8   110.9  0.06  0.06
$$
```

**** Fom and SigmaA vs resolution ****

```
$TABLE: Cycle  148. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle  148. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa  FOMa  NREFc FOMc NREFall FOMall  SigmaA_Fc1 $$
$$
 0.0038    30   0.999     4   1.000    34   0.999  0.999
 0.0102    62   0.999     7   1.000    69   0.999  0.999
 0.0165    83   0.991    12   0.926    95   0.983  0.999
 0.0228    97   0.989    11   1.000   108   0.990  0.999
 0.0292   108   0.997     6   1.000   114   0.997  0.999
 0.0355   126   0.996    17   1.000   143   0.996  0.999
 0.0418   129   0.997    11   1.000   140   0.997  0.999
 0.0482   150   0.991    12   1.000   162   0.992  0.999
 0.0545   151   0.997    12   0.995   163   0.997  0.999
 0.0609   172   0.983    15   0.957   187   0.981  0.999
 0.0672   174   0.993     9   0.932   183   0.990  0.999
 0.0735   178   0.990    11   1.000   189   0.990  0.999
 0.0799   189   0.989    14   1.000   203   0.990  0.999
 0.0862   197   0.984     9   0.979   206   0.984  0.999
 0.0925   193   0.979    14   0.930   207   0.976  0.999
 0.0989   188   0.980    12   1.000   200   0.981  0.999
 0.1052   190   0.988     8   1.000   198   0.989  0.999
 0.1116   183   0.981    13   0.937   196   0.978  1.000
 0.1179   194   0.980    11   0.951   205   0.979  1.000
 0.1242   174   0.983     8   1.000   182   0.984  1.000
 $$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0189
Free R factor                    =     0.0396
Overall weighted R factor        =     0.0189
Free weighted R factor           =     0.0400
Overall correlation coefficient  =     0.9994
Free correlation coefficient     =     0.9969
DPI based on free R factor       =     0.0719
Overall figure of merit          =     0.9872
```

ML based su of positional parameters = 0.0398
ML based su of thermal parameters = 1.9653

Trying gamma equal 0.0000000
Convergence reached with no gamma cycles

fvalues 10468.122 3168.7312 19287.367 19287.180

fvalues 10468.122 3168.7312 19287.379 19287.180

CGMAT cycle number = 149

Limits of asymmetric unit : 1.00 1.00 0.50
Grid spacing to be used : 50 90 60
Maximuum H,K,L : 12 21 14
Minimum acceptable grid spacing: 33 56 38
fast hessian tabulation
B ARRAY FOR HESSIAN TABULATION TOO BIG
VALUE RESET TO MAXIMUM
Weight matrix 0.60000002
Actual weight 1.5390190 is applied to the X-ray term
Norm of X_ray positional gradient 13.7
Norm of Geom. positional gradient 13.7
Norm of X_ray B-factor gradient 17.8
Norm of Geom. B-factor gradient 18.2
Product of X_ray and Geom posit. gradients -0.693E+06
Cosine of angle between them -1.000
Product of X_ray and Geom B-fact gradients -0.396E+06
Cosine of angle between them -0.995

Residuals: XRAY= 0.1611E+05 GEOM= 3169. TOTAL= 0.1928E+05
function value 19277.662

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.689	1.966
Torsion angles, period 1. refined	155	7.866	5.000
Torsion angles, period 2. refined	54	41.443	25.741
Torsion angles, period 3. refined	214	19.211	15.000
Torsion angles, period 4. refined	3	21.316	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	540	0.266	0.200
VDW; torsion: refined_atoms	790	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.261	0.200
HBOND: symmetry: refined_atoms	3	0.206	0.200

Bond B values: refined atoms 1229 13.652 4.733
Angle B values: refined atoms 1663 17.055 7.134
Torsion B values: refined atoms 426 32.025 13.123
Long range B values: refined atoms 1337 11.599 15.304

Overall : scale = 1.011, B = -0.025
Overall anisotropic scale factors
B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 149. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 149. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 149. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 149. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.5 748.1 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.0 0.02 0.02 1 1228.7 1225.9 0.02 0.01
0.017 83 95.60 307.8 308.8 0.03 0.02 4 403.1 412.8 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.3 189.9 0.08 0.07
0.029 108 100.00 241.3 242.0 0.02 0.02 7 186.7 189.5 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.4 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.2 340.9 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.5 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 258.0 259.9 0.04 0.04
0.061 172 100.00 218.4 218.7 0.02 0.02 10 202.2 202.8 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.3 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.8 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 156.1 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 185.9 0.06 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.0 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.3 169.9 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 141.4 0.08 0.08
0.118 194 81.85 127.0 126.8 0.02 0.02 9 138.0 137.1 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 110.9 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 149. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 149. M(Fom) v. resln :N:1,3,5,7,8:

$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
 0.0038   30 0.999   4 1.000   34 0.999 0.999
 0.0102   62 0.999   7 1.000   69 0.999 0.999
 0.0165   83 0.991   12 0.926   95 0.983 0.999
 0.0228   97 0.989   11 1.000 108 0.990 0.999
 0.0292 108 0.997   6 1.000 114 0.997 0.999
 0.0355 126 0.996   17 1.000 143 0.996 0.999
 0.0418 129 0.997   11 1.000 140 0.997 0.999
 0.0482 150 0.991   12 1.000 162 0.992 0.999
 0.0545 151 0.997   12 0.995 163 0.997 0.999
 0.0609 172 0.983   15 0.957 187 0.981 0.999
 0.0672 174 0.993   9 0.932 183 0.990 0.999
 0.0735 178 0.990   11 1.000 189 0.990 0.999
 0.0799 189 0.989   14 1.000 203 0.990 0.999
 0.0862 197 0.984   9 0.979 206 0.984 0.999
 0.0925 193 0.979   14 0.930 207 0.976 0.999
 0.0989 188 0.980   12 1.000 200 0.981 0.999
 0.1052 190 0.988   8 1.000 198 0.989 0.999
 0.1116 183 0.981   13 0.936 196 0.978 1.000
 0.1179 194 0.980   11 0.951 205 0.979 1.000
 0.1242 174 0.983   8 1.000 182 0.984 1.000
$$
Resolution limits   =   38.899   2.802
Number of used reflections   =   3184
Percentage observed   =   92.6870
Percentage of free reflections   =   4.8416
Overall R factor   =   0.0189
Free R factor   =   0.0396
Overall weighted R factor   =   0.0189
Free weighted R factor   =   0.0400
Overall correlation coefficient =   0.9994
Free correlation coefficient   =   0.9969
DPI based on free R factor   =   0.0719
Overall figure of merit   =   0.9872
ML based su of positional parameters =   0.0398
ML based su of thermal parameters   =   1.9649

 Trying gamma equal   0.0000000
 Convergence reached with no gamma cycles

 fvalues   10467.497   3168.7734   19278.695   19278.449

 fvalues   10467.497   3168.7734   19278.629   19278.449

    CGMAT cycle number =   150

 Limits of asymmetric unit   : 1.00 1.00 0.50

```
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38
 fast hessian tabulation
 B ARRAY FOR HESSIAN TABULATION TOO BIG
 VALUE RESET TO MAXIMUM
 Weight matrix   0.60000002
 Actual weight    1.5393107      is applied to the X-ray term
Norm of X_ray positional gradient              13.7
Norm of Geom. positional gradient              13.7
Norm of X_ray B-factor gradient                17.8
Norm of Geom. B-factor gradient                18.2
Product of X_ray and Geom posit. gradients     -0.693E+06
 Cosine of angle between them                  -1.000
Product of X_ray and Geom B-fact gradients     -0.396E+06
 Cosine of angle between them                  -0.995


Residuals: XRAY=     0.1611E+05 GEOM=      3169.     TOTAL=     0.1928E+05
 function value    19281.186

------------------------------------------------------------------------------
          Restraint type            N restraints   Rms Delta   Av(Sigma)
Bond distances: refined atoms              1229     0.011     0.020
Bond angles  : refined atoms               1663     1.690     1.966
Torsion angles, period  1. refined          155     7.866     5.000
Torsion angles, period  2. refined           54    41.443    25.741
Torsion angles, period  3. refined          214    19.211    15.000
Torsion angles, period  4. refined            3    21.316    15.000
Chiral centres: refined atoms              187     0.112     0.200
Planar groups: refined atoms               924     0.005     0.021
VDW repulsions: refined_atoms              541     0.265     0.200
VDW; torsion: refined_atoms                790     0.325     0.200
HBOND: refined_atoms                        41     0.194     0.200
VDW repulsions: symmetry: refined_atoms     55     0.261     0.200
HBOND: symmetry: refined_atoms               3     0.206     0.200
Bond B values: refined atoms               1229    13.652     4.733
Angle B values: refined atoms              1663    17.056     7.134
Torsion B values: refined atoms             426    32.029    13.123
Long range B values: refined atoms         1338    11.595    15.300
------------------------------------------------------------------------------

------------------------------------------------------------------------------
Overall          : scale =    1.011, B  =  -0.025
Overall anisotropic scale factors
   B11 =  0.28 B22 =  0.17 B33 = -0.47 B12 =  0.00 B13 = -0.36 B23 =  0.00
------------------------------------------------------------------------------

------------------------------------------------------------------------------

    ****          Things for loggraph, R factor and others          ****
```

$TABLE: Cycle 150. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 150. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 150. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 150. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$
0.004 30 62.50 754.5 748.1 0.02 0.02 0 0.0 0.0****** 0.00
0.010 62 95.45 414.1 416.0 0.02 0.02 1 1228.7 1225.9 0.02 0.01
0.017 83 95.60 307.8 308.8 0.03 0.02 4 403.1 412.8 0.04 0.05
0.023 97 97.14 247.4 248.4 0.02 0.02 5 180.3 189.9 0.08 0.07
0.029 108 100.00 241.3 242.1 0.02 0.02 7 186.7 189.5 0.06 0.06
0.036 126 99.25 270.4 270.7 0.02 0.02 6 252.9 254.4 0.04 0.04
0.042 129 98.56 286.3 287.5 0.02 0.02 8 338.2 340.9 0.02 0.02
0.048 150 98.73 296.8 296.4 0.02 0.01 5 305.8 307.5 0.03 0.02
0.055 151 99.38 281.3 281.5 0.01 0.01 10 258.0 259.9 0.04 0.04
0.061 172 100.00 218.4 218.7 0.02 0.02 10 202.2 202.8 0.03 0.03
0.067 174 99.45 211.5 211.0 0.02 0.02 6 286.3 284.4 0.02 0.02
0.074 178 98.92 206.1 206.8 0.02 0.02 6 234.6 237.8 0.04 0.03
0.080 189 100.00 208.7 209.0 0.02 0.02 13 159.7 156.1 0.06 0.06
0.086 197 100.00 176.8 176.9 0.02 0.02 8 208.6 207.6 0.04 0.04
0.093 193 93.55 156.9 157.0 0.02 0.02 10 182.0 185.9 0.06 0.06
0.099 188 91.28 160.7 159.8 0.02 0.02 11 159.7 157.1 0.02 0.02
0.105 190 86.02 153.9 153.5 0.02 0.02 13 169.3 169.9 0.05 0.04
0.112 183 80.08 129.9 129.6 0.02 0.02 6 135.2 141.4 0.08 0.08
0.118 194 81.85 127.0 126.8 0.02 0.02 9 138.0 137.1 0.05 0.05
0.124 174 73.20 129.0 128.9 0.02 0.02 9 113.8 110.9 0.06 0.06
$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 150. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 150. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$
0.0038 30 0.999 4 1.000 34 0.999 0.999
0.0102 62 0.999 7 1.000 69 0.999 0.999
0.0165 83 0.991 12 0.926 95 0.983 0.999
0.0228 97 0.989 11 1.000 108 0.990 0.999
0.0292 108 0.997 6 1.000 114 0.997 0.999
0.0355 126 0.996 17 1.000 143 0.996 0.999
0.0418 129 0.997 11 1.000 140 0.997 0.999
0.0482 150 0.991 12 1.000 162 0.992 0.999
0.0545 151 0.997 12 0.995 163 0.997 0.999
0.0609 172 0.983 15 0.957 187 0.981 0.999
0.0672 174 0.993 9 0.932 183 0.990 0.999
0.0735 178 0.990 11 1.000 189 0.990 0.999

```
 0.0799   189   0.989    14   1.000   203   0.990  0.999
 0.0862   197   0.984     9   0.979   206   0.984  0.999
 0.0925   193   0.979    14   0.930   207   0.976  0.999
 0.0989   188   0.980    12   1.000   200   0.981  0.999
 0.1052   190   0.988     8   1.000   198   0.989  0.999
 0.1116   183   0.981    13   0.937   196   0.978  1.000
 0.1179   194   0.980    11   0.952   205   0.979  1.000
 0.1242   174   0.983     8   1.000   182   0.984  1.000
$$
Resolution limits                =     38.899     2.802
Number of used reflections       =       3184
Percentage observed              =    92.6870
Percentage of free reflections   =     4.8416
Overall R factor                 =     0.0189
Free R factor                    =     0.0396
Overall weighted R factor        =     0.0189
Free weighted R factor           =     0.0400
Overall correlation coefficient  =     0.9994
Free correlation coefficient     =     0.9969
DPI based on free R factor       =     0.0719
Overall figure of merit          =     0.9872
ML based su of positional parameters =     0.0398
ML based su of thermal parameters    =     1.9651
------------------------------------------------------------------------------
 Trying gamma equal    0.0000000
 Convergence reached with no gamma cycles


 fvalues    10467.650       3168.9944       19281.813       19281.961

 Limits of asymmetric unit      : 1.00 1.00 0.50
 Grid spacing to be used        :    50   90   60
 Maximuum H,K,L                 :    12   21   14
 Minimum acceptable grid spacing:    33   56   38

 WRITTEN OUTPUT MTZ FILE
 Logical Name: HKLOUT   Filename: c:/data/deepblue/3k78/3k78_iso_clean_refmac2.mtz

Norm of X_ray positional gradient              0.00
Norm of Geom. positional gradient              0.00
Norm of X_ray B-factor gradient                0.00
Norm of Geom. B-factor gradient                0.00
Product of X_ray and Geom posit. gradients     0.00
 Cosine of angle between them                  0.000
Product of X_ray and Geom B-fact gradients     0.00
 Cosine of angle between them                  0.000


Residuals: XRAY=     0.1611E+05 GEOM=      3169.     TOTAL=     0.1928E+05

------------------------------------------------------------------------------
```

Restraint type	N restraints	Rms Delta	Av(Sigma)
Bond distances: refined atoms	1229	0.011	0.020
Bond angles : refined atoms	1663	1.690	1.966
Torsion angles, period 1. refined	155	7.866	5.000
Torsion angles, period 2. refined	54	41.443	25.741
Torsion angles, period 3. refined	214	19.210	15.000
Torsion angles, period 4. refined	3	21.317	15.000
Chiral centres: refined atoms	187	0.112	0.200
Planar groups: refined atoms	924	0.005	0.021
VDW repulsions: refined_atoms	541	0.265	0.200
VDW; torsion: refined_atoms	790	0.325	0.200
HBOND: refined_atoms	41	0.194	0.200
VDW repulsions: symmetry: refined_atoms	55	0.261	0.200
HBOND: symmetry: refined_atoms	3	0.206	0.200
Bond B values: refined atoms	1229	13.656	4.733
Angle B values: refined atoms	1663	17.064	7.134
Torsion B values: refined atoms	426	32.048	13.124
Long range B values: refined atoms	1338	11.595	15.299

Overall : scale = 1.011, B = -0.025

Overall anisotropic scale factors

B11 = 0.28 B22 = 0.17 B33 = -0.47 B12 = 0.00 B13 = -0.36 B23 = 0.00

**** Things for loggraph, R factor and others ****

$TABLE: Cycle 151. Rfactor analysis, F distribution v resln :
$GRAPHS:Cycle 151. <Rfactor> v. resln :N:1,6,7,11,12:
:Cycle 151. <Fobs> and <Fc> v. resln :N:1,4,5,9,10:
:Cycle 151. % observed v. resln :N:1,3:
$$
M(4SSQ/LL) NR_used %_obs M(Fo_used) M(Fc_used) Rf_used WR_used NR_free M(Fo_free) M(Fc_free) Rf_free WR_free $$
$$

0.004	30	62.50	754.5	748.1	0.02	0.02	0	0.0	0.0******	0.00		
0.010	62	95.45	414.1	416.0	0.02	0.02	1	1228.7	1226.0	0.02	0.01	
0.017	83	95.60	307.8	308.8	0.03	0.02	4	403.1	412.8	0.04	0.05	
0.023	97	97.14	247.4	248.4	0.02	0.02	5	180.3	189.9	0.08	0.07	
0.029	108	100.00	241.3	242.0	0.02	0.02	7	186.7	189.5	0.06	0.06	
0.036	126	99.25	270.4	270.7	0.02	0.02	6	252.9	254.4	0.04	0.04	
0.042	129	98.56	286.3	287.5	0.02	0.02	8	338.2	340.9	0.02	0.02	
0.048	150	98.73	296.8	296.4	0.02	0.01	5	305.8	307.5	0.03	0.02	
0.055	151	99.38	281.3	281.5	0.01	0.01	10	258.0	259.9	0.04	0.04	
0.061	172	100.00	218.4	218.7	0.02	0.02	10	202.2	202.8	0.03	0.03	
0.067	174	99.45	211.5	211.0	0.02	0.02	6	286.3	284.3	0.02	0.02	
0.074	178	98.92	206.1	206.8	0.02	0.02	6	234.6	237.9	0.04	0.03	

0.080	189	100.00	208.7	209.0	0.02	0.02	13	159.7	156.1	0.06	0.06
0.086	197	100.00	176.8	176.9	0.02	0.02	8	208.6	207.6	0.04	0.04
0.093	193	93.55	156.9	157.0	0.02	0.02	10	182.0	185.9	0.06	0.06
0.099	188	91.28	160.7	159.8	0.02	0.02	11	159.7	157.1	0.02	0.02
0.105	190	86.02	153.9	153.5	0.02	0.02	13	169.3	169.9	0.05	0.04
0.112	183	80.08	129.9	129.6	0.02	0.02	6	135.2	141.4	0.08	0.08
0.118	194	81.85	127.0	126.8	0.02	0.02	9	138.0	137.1	0.05	0.05
0.124	174	73.20	129.0	128.9	0.02	0.02	9	113.8	110.9	0.06	0.06

$$

**** Fom and SigmaA vs resolution ****

$TABLE: Cycle 151. Fom(<cos(DelPhi)>-acentric, centric, overall v resln:
$GRAPHS:Cycle 151. M(Fom) v. resln :N:1,3,5,7,8:
$$
<4SSQ/LL> NREFa FOMa NREFc FOMc NREFall FOMall SigmaA_Fc1 $$
$$

0.0038	30	0.999	4	1.000	34	0.999	0.999
0.0102	62	0.999	7	1.000	69	0.999	0.999
0.0165	83	0.991	12	0.926	95	0.983	0.999
0.0228	97	0.989	11	1.000	108	0.990	0.999
0.0292	108	0.997	6	1.000	114	0.997	0.999
0.0355	126	0.996	17	1.000	143	0.996	0.999
0.0418	129	0.997	11	1.000	140	0.997	0.999
0.0482	150	0.991	12	1.000	162	0.992	0.999
0.0545	151	0.997	12	0.995	163	0.997	0.999
0.0609	172	0.983	15	0.957	187	0.981	0.999
0.0672	174	0.993	9	0.932	183	0.990	0.999
0.0735	178	0.990	11	1.000	189	0.990	0.999
0.0799	189	0.989	14	1.000	203	0.990	0.999
0.0862	197	0.984	9	0.979	206	0.984	0.999
0.0925	193	0.979	14	0.930	207	0.976	0.999
0.0989	188	0.980	12	1.000	200	0.981	0.999
0.1052	190	0.988	8	1.000	198	0.989	0.999
0.1116	183	0.981	13	0.936	196	0.978	1.000
0.1179	194	0.980	11	0.951	205	0.979	1.000
0.1242	174	0.983	8	1.000	182	0.984	1.000

$$
Resolution limits = 38.899 2.802
Number of used reflections = 3184
Percentage observed = 92.6870
Percentage of free reflections = 4.8416
Overall R factor = 0.0189
Free R factor = 0.0396
Overall weighted R factor = 0.0189
Free weighted R factor = 0.0400
Overall correlation coefficient = 0.9994
Free correlation coefficient = 0.9969
DPI based on free R factor = 0.0719
Overall figure of merit = 0.9872
ML based su of positional parameters = 0.0398

ML based su of thermal parameters = 1.9651

Time in seconds: CPU = 0.00
Elapsed = 775.00

**** Things for loggraph, R factor and others vs cycle ****

$TABLE: Rfactor analysis, stats vs cycle :
$GRAPHS:<Rfactor> vs cycle :N:1,2,3:
:FOM vs cycle :N:1,4:
:-LL vs cycle :N:1,5:
:-LLfree vs cycle :N:1,6:
:Geometry vs cycle:N:1,7,8,9,10,11:
$$

Ncyc	Rfact	Rfree	FOM	-LL	-LLfree	rmsBOND	zBOND	rmsANGL	zANGL	rmsCHIRAL
$$										
0	0.0423	0.0687	0.971	12475.	684.0	0.0068	0.340	1.255	0.570	0.091
1	0.0301	0.0606	0.974	11853.	662.8	0.0128	0.643	1.517	0.699	0.105
2	0.0280	0.0571	0.976	11657.	653.6	0.0119	0.593	1.532	0.704	0.105
3	0.0252	0.0540	0.978	11441.	644.8	0.0131	0.652	1.569	0.724	0.108
4	0.0247	0.0531	0.979	11379.	641.7	0.0127	0.635	1.568	0.724	0.108
5	0.0242	0.0519	0.979	11311.	638.3	0.0125	0.623	1.573	0.726	0.108
6	0.0233	0.0504	0.980	11201.	632.9	0.0125	0.621	1.609	0.740	0.110
7	0.0225	0.0489	0.981	11094.	628.0	0.0134	0.667	1.604	0.739	0.110
8	0.0221	0.0472	0.982	11002.	623.2	0.0128	0.636	1.607	0.744	0.110
9	0.0219	0.0469	0.982	10983.	622.3	0.0126	0.630	1.604	0.742	0.110
10	0.0215	0.0462	0.983	10927.	619.6	0.0116	0.578	1.632	0.752	0.110
11	0.0215	0.0460	0.983	10913.	618.9	0.0117	0.583	1.626	0.750	0.110
12	0.0212	0.0452	0.984	10865.	616.5	0.0110	0.547	1.654	0.760	0.110
13	0.0209	0.0445	0.984	10821.	614.3	0.0112	0.560	1.644	0.757	0.110
14	0.0209	0.0443	0.984	10812.	613.8	0.0113	0.562	1.641	0.756	0.110
15	0.0207	0.0439	0.984	10778.	612.1	0.0109	0.544	1.659	0.763	0.110
16	0.0205	0.0434	0.985	10747.	610.5	0.0110	0.547	1.659	0.763	0.110
17	0.0204	0.0433	0.985	10733.	609.8	0.0111	0.552	1.653	0.761	0.110
18	0.0204	0.0432	0.985	10727.	609.5	0.0111	0.552	1.653	0.761	0.110
19	0.0203	0.0428	0.985	10703.	608.3	0.0109	0.542	1.664	0.765	0.111
20	0.0202	0.0426	0.985	10683.	607.3	0.0111	0.551	1.661	0.764	0.111
21	0.0202	0.0425	0.985	10677.	607.0	0.0111	0.553	1.655	0.763	0.111
22	0.0201	0.0422	0.985	10659.	606.1	0.0109	0.540	1.669	0.767	0.111
23	0.0200	0.0421	0.986	10645.	605.3	0.0109	0.541	1.669	0.767	0.111
24	0.0200	0.0420	0.986	10642.	605.2	0.0109	0.541	1.668	0.767	0.111
25	0.0199	0.0418	0.986	10628.	604.4	0.0108	0.540	1.670	0.768	0.111
26	0.0198	0.0417	0.986	10621.	604.0	0.0109	0.541	1.669	0.768	0.111
27	0.0198	0.0416	0.986	10614.	603.7	0.0110	0.545	1.666	0.767	0.111
28	0.0198	0.0416	0.986	10612.	603.6	0.0110	0.545	1.665	0.767	0.111
29	0.0197	0.0414	0.986	10602.	603.0	0.0108	0.538	1.674	0.770	0.111
30	0.0197	0.0413	0.986	10594.	602.6	0.0109	0.540	1.671	0.769	0.111
31	0.0197	0.0413	0.986	10593.	602.5	0.0109	0.542	1.669	0.768	0.111
32	0.0196	0.0412	0.986	10585.	602.1	0.0108	0.538	1.675	0.770	0.111

33	0.0196	0.0412	0.986	10581.	601.9	0.0108	0.539	1.674	0.770	0.111
34	0.0196	0.0411	0.986	10579.	601.7	0.0108	0.539	1.673	0.770	0.111
35	0.0196	0.0411	0.986	10576.	601.6	0.0109	0.542	1.672	0.770	0.111
36	0.0196	0.0411	0.986	10574.	601.4	0.0109	0.541	1.671	0.769	0.111
37	0.0195	0.0410	0.986	10569.	601.2	0.0108	0.537	1.677	0.771	0.111
38	0.0195	0.0410	0.986	10565.	600.9	0.0108	0.539	1.675	0.771	0.111
39	0.0195	0.0410	0.986	10564.	600.9	0.0109	0.540	1.674	0.770	0.111
40	0.0195	0.0409	0.986	10559.	600.6	0.0108	0.537	1.678	0.772	0.111
41	0.0195	0.0409	0.986	10557.	600.5	0.0108	0.538	1.677	0.772	0.111
42	0.0194	0.0409	0.987	10554.	600.3	0.0108	0.538	1.676	0.771	0.111
43	0.0194	0.0409	0.987	10555.	600.4	0.0108	0.539	1.676	0.771	0.111
44	0.0194	0.0408	0.987	10550.	600.1	0.0108	0.536	1.679	0.772	0.111
45	0.0194	0.0408	0.987	10549.	600.0	0.0108	0.537	1.679	0.772	0.111
46	0.0194	0.0408	0.987	10548.	600.0	0.0108	0.537	1.679	0.772	0.111
47	0.0194	0.0408	0.987	10547.	599.9	0.0108	0.536	1.680	0.773	0.111
48	0.0194	0.0407	0.987	10541.	599.6	0.0108	0.537	1.679	0.773	0.111
49	0.0194	0.0407	0.987	10541.	599.6	0.0108	0.537	1.679	0.772	0.111
50	0.0193	0.0407	0.987	10540.	599.5	0.0108	0.536	1.681	0.773	0.111
51	0.0193	0.0407	0.987	10538.	599.4	0.0108	0.537	1.680	0.773	0.111
52	0.0193	0.0406	0.987	10535.	599.2	0.0108	0.537	1.680	0.773	0.111
53	0.0193	0.0406	0.987	10534.	599.2	0.0108	0.538	1.680	0.773	0.111
54	0.0193	0.0406	0.987	10531.	599.0	0.0109	0.543	1.675	0.771	0.111
55	0.0193	0.0406	0.987	10530.	599.0	0.0110	0.547	1.671	0.770	0.111
56	0.0193	0.0405	0.987	10527.	598.8	0.0108	0.536	1.683	0.774	0.111
57	0.0193	0.0405	0.987	10526.	598.7	0.0108	0.537	1.682	0.774	0.111
58	0.0192	0.0404	0.987	10524.	598.6	0.0108	0.539	1.679	0.773	0.111
59	0.0192	0.0404	0.987	10524.	598.6	0.0108	0.539	1.679	0.773	0.111
60	0.0192	0.0404	0.987	10522.	598.4	0.0108	0.536	1.683	0.774	0.111
61	0.0192	0.0404	0.987	10521.	598.4	0.0108	0.537	1.682	0.774	0.111
62	0.0192	0.0403	0.987	10519.	598.2	0.0108	0.537	1.681	0.773	0.111
63	0.0192	0.0403	0.987	10519.	598.2	0.0108	0.538	1.681	0.773	0.111
64	0.0192	0.0403	0.987	10518.	598.2	0.0108	0.536	1.683	0.774	0.111
65	0.0192	0.0403	0.987	10517.	598.1	0.0108	0.536	1.683	0.774	0.111
66	0.0192	0.0403	0.987	10516.	598.0	0.0108	0.537	1.682	0.774	0.111
67	0.0192	0.0403	0.987	10515.	598.0	0.0108	0.537	1.682	0.774	0.111
68	0.0192	0.0403	0.987	10514.	597.9	0.0108	0.536	1.684	0.775	0.111
69	0.0192	0.0403	0.987	10514.	597.9	0.0108	0.536	1.684	0.775	0.111
70	0.0192	0.0402	0.987	10513.	597.9	0.0108	0.536	1.683	0.775	0.111
71	0.0192	0.0402	0.987	10511.	597.7	0.0108	0.536	1.684	0.775	0.111
72	0.0192	0.0402	0.987	10510.	597.7	0.0108	0.536	1.684	0.775	0.111
73	0.0192	0.0402	0.987	10510.	597.7	0.0108	0.536	1.684	0.775	0.111
74	0.0191	0.0401	0.987	10508.	597.6	0.0108	0.536	1.684	0.775	0.111
75	0.0191	0.0401	0.987	10506.	597.5	0.0108	0.537	1.684	0.775	0.111
76	0.0191	0.0401	0.987	10506.	597.5	0.0108	0.537	1.683	0.774	0.111
77	0.0191	0.0401	0.987	10504.	597.4	0.0108	0.536	1.685	0.775	0.111
78	0.0191	0.0401	0.987	10504.	597.4	0.0108	0.536	1.684	0.775	0.111
79	0.0191	0.0401	0.987	10503.	597.3	0.0108	0.536	1.684	0.775	0.111
80	0.0191	0.0401	0.987	10502.	597.3	0.0108	0.537	1.683	0.775	0.111
81	0.0191	0.0401	0.987	10502.	597.3	0.0108	0.537	1.683	0.775	0.111
82	0.0191	0.0400	0.987	10501.	597.2	0.0108	0.535	1.685	0.775	0.111
83	0.0191	0.0400	0.987	10501.	597.2	0.0108	0.536	1.685	0.775	0.111

84	0.0191	0.0400	0.987	10501.	597.2	0.0108	0.536	1.685	0.775	0.111
85	0.0191	0.0400	0.987	10500.	597.1	0.0108	0.536	1.685	0.775	0.111
86	0.0191	0.0400	0.987	10499.	597.1	0.0108	0.536	1.686	0.776	0.111
87	0.0191	0.0400	0.987	10497.	597.0	0.0108	0.536	1.686	0.776	0.111
88	0.0191	0.0399	0.987	10496.	596.9	0.0108	0.536	1.686	0.776	0.112
89	0.0191	0.0399	0.987	10496.	596.9	0.0108	0.536	1.686	0.776	0.111
90	0.0191	0.0399	0.987	10493.	596.8	0.0108	0.536	1.686	0.776	0.112
91	0.0191	0.0399	0.987	10493.	596.8	0.0108	0.536	1.686	0.776	0.112
92	0.0191	0.0399	0.987	10492.	596.7	0.0108	0.536	1.686	0.776	0.112
93	0.0191	0.0399	0.987	10493.	596.7	0.0108	0.536	1.686	0.776	0.112
94	0.0191	0.0399	0.987	10492.	596.7	0.0108	0.536	1.686	0.776	0.112
95	0.0191	0.0399	0.987	10491.	596.6	0.0108	0.536	1.686	0.776	0.112
96	0.0190	0.0399	0.987	10491.	596.6	0.0108	0.536	1.686	0.776	0.112
97	0.0190	0.0399	0.987	10490.	596.6	0.0108	0.536	1.686	0.776	0.112
98	0.0190	0.0399	0.987	10490.	596.6	0.0108	0.536	1.686	0.776	0.112
99	0.0190	0.0398	0.987	10489.	596.5	0.0108	0.536	1.687	0.776	0.112
100	0.0190	0.0398	0.987	10489.	596.5	0.0108	0.535	1.687	0.776	0.112
101	0.0190	0.0398	0.987	10487.	596.4	0.0108	0.536	1.687	0.776	0.112
102	0.0190	0.0398	0.987	10487.	596.4	0.0108	0.535	1.687	0.776	0.112
103	0.0190	0.0398	0.987	10487.	596.4	0.0108	0.536	1.687	0.776	0.112
104	0.0190	0.0398	0.987	10485.	596.3	0.0108	0.535	1.687	0.776	0.112
105	0.0190	0.0397	0.987	10484.	596.2	0.0108	0.536	1.687	0.776	0.112
106	0.0190	0.0398	0.987	10484.	596.3	0.0108	0.536	1.687	0.776	0.112
107	0.0190	0.0397	0.987	10483.	596.2	0.0108	0.536	1.687	0.777	0.112
108	0.0190	0.0397	0.987	10482.	596.1	0.0108	0.536	1.687	0.777	0.112
109	0.0190	0.0397	0.987	10483.	596.1	0.0108	0.536	1.687	0.777	0.112
110	0.0190	0.0397	0.987	10482.	596.1	0.0108	0.536	1.687	0.777	0.112
111	0.0190	0.0397	0.987	10481.	596.1	0.0108	0.536	1.688	0.777	0.112
112	0.0190	0.0397	0.987	10480.	596.0	0.0108	0.536	1.687	0.777	0.112
113	0.0190	0.0397	0.987	10480.	596.0	0.0108	0.536	1.687	0.777	0.112
114	0.0190	0.0397	0.987	10479.	595.9	0.0108	0.536	1.688	0.777	0.112
115	0.0190	0.0397	0.987	10479.	596.0	0.0108	0.536	1.688	0.777	0.112
116	0.0190	0.0397	0.987	10479.	595.9	0.0108	0.536	1.687	0.777	0.112
117	0.0190	0.0397	0.987	10478.	595.9	0.0108	0.536	1.687	0.777	0.112
118	0.0190	0.0397	0.987	10479.	595.9	0.0108	0.536	1.688	0.777	0.112
119	0.0190	0.0397	0.987	10478.	595.9	0.0108	0.536	1.688	0.777	0.112
120	0.0190	0.0397	0.987	10477.	595.9	0.0108	0.536	1.688	0.777	0.112
121	0.0190	0.0397	0.987	10477.	595.9	0.0108	0.536	1.688	0.777	0.112
122	0.0190	0.0397	0.987	10477.	595.8	0.0108	0.536	1.688	0.777	0.112
123	0.0190	0.0397	0.987	10477.	595.8	0.0108	0.536	1.688	0.777	0.112
124	0.0190	0.0397	0.987	10477.	595.8	0.0108	0.536	1.688	0.777	0.112
125	0.0190	0.0397	0.987	10477.	595.8	0.0108	0.536	1.688	0.777	0.112
126	0.0190	0.0397	0.987	10476.	595.8	0.0108	0.536	1.688	0.777	0.112
127	0.0190	0.0397	0.987	10476.	595.8	0.0108	0.536	1.688	0.777	0.112
128	0.0190	0.0397	0.987	10476.	595.7	0.0108	0.536	1.688	0.777	0.112
129	0.0190	0.0397	0.987	10476.	595.8	0.0108	0.536	1.688	0.777	0.112
130	0.0190	0.0397	0.987	10475.	595.7	0.0108	0.536	1.688	0.777	0.112
131	0.0190	0.0397	0.987	10474.	595.6	0.0108	0.536	1.689	0.777	0.112
132	0.0190	0.0397	0.987	10473.	595.6	0.0108	0.536	1.689	0.777	0.112
133	0.0189	0.0397	0.987	10474.	595.6	0.0108	0.536	1.689	0.777	0.112
134	0.0189	0.0397	0.987	10473.	595.6	0.0108	0.536	1.689	0.777	0.112

```
   135  0.0189  0.0397  0.987    10472.    595.5  0.0108  0.536   1.689  0.777   0.112
   136  0.0189  0.0396  0.987    10471.    595.5  0.0108  0.536   1.689  0.777   0.112
   137  0.0189  0.0396  0.987    10472.    595.5  0.0108  0.536   1.689  0.777   0.112
   138  0.0189  0.0396  0.987    10471.    595.5  0.0108  0.536   1.689  0.777   0.112
   139  0.0189  0.0396  0.987    10471.    595.5  0.0108  0.536   1.689  0.777   0.112
   140  0.0189  0.0396  0.987    10470.    595.4  0.0108  0.536   1.689  0.777   0.112
   141  0.0189  0.0396  0.987    10469.    595.4  0.0108  0.536   1.689  0.778   0.112
   142  0.0189  0.0396  0.987    10469.    595.4  0.0108  0.536   1.689  0.778   0.112
   143  0.0189  0.0396  0.987    10469.    595.4  0.0108  0.536   1.689  0.778   0.112
   144  0.0189  0.0396  0.987    10469.    595.4  0.0108  0.536   1.689  0.778   0.112
   145  0.0189  0.0396  0.987    10468.    595.4  0.0108  0.536   1.689  0.778   0.112
   146  0.0189  0.0396  0.987    10468.    595.3  0.0108  0.536   1.689  0.778   0.112
   147  0.0189  0.0396  0.987    10468.    595.3  0.0108  0.536   1.689  0.778   0.112
   148  0.0189  0.0396  0.987    10467.    595.3  0.0108  0.536   1.689  0.778   0.112
   149  0.0189  0.0396  0.987    10467.    595.3  0.0108  0.536   1.690  0.778   0.112
   150  0.0189  0.0396  0.987    10468.    595.3  0.0108  0.536   1.690  0.778   0.112
 $$
 $TEXT:Result: $$ Final results $$
                 Initial    Final
         R factor    0.0423   0.0189
           R free    0.0687   0.0396
    Rms BondLength    0.0068   0.0108
     Rms BondAngle    1.2547   1.6897
    Rms ChirVolume    0.0910   0.1118
 $$
<B><FONT COLOR="#FF0000"><!--SUMMARY_BEGIN-->
 Refmac_5.6.0117:  End of Refmac_5.6.0117
Times: User:       0.0s System:    0.0s Elapsed:    13:08
</pre>
</html>
<!--SUMMARY_END--></FONT></B>
**************************************************************************
* Information from CCP4Interface script
**************************************************************************
Writing final coordinates (XYZOUT) to c:/data/deepblue/3k78/3k78_iso_clean_refmac2.pdb
**************************************************************************

**************************************************************************
* Information from CCP4Interface script
**************************************************************************
Writing final phases (HKLOUT) to c:/data/deepblue/3k78/3k78_iso_clean_refmac2.mtz
**************************************************************************


#CCP4I TERMINATION STATUS 1
#CCP4I TERMINATION TIME 09 Jan 2012  23:21:01
#CCP4I TERMINATION OUTPUT_FILES  c:/data/deepblue/3k78/3k78_183_3k78.refmac.cif
3k78
#CCP4I MESSAGE Task completed successfully
```

```
HEADER    ----                                    XX-XXX-XX   xxxx
COMPND    ---
REMARK   3
REMARK   3 REFINEMENT.
REMARK   3   PROGRAM     : REFMAC 5.6.0117
REMARK   3   AUTHORS     : MURSHUDOV,VAGIN,DODSON
REMARK   3
REMARK   3    REFINEMENT TARGET : MAXIMUM LIKELIHOOD
REMARK   3
REMARK   3  DATA USED IN REFINEMENT.
REMARK   3   RESOLUTION RANGE HIGH (ANGSTROMS) :   2.80
REMARK   3   RESOLUTION RANGE LOW  (ANGSTROMS) :  38.90
REMARK   3   DATA CUTOFF            (SIGMA(F)) : NONE
REMARK   3   COMPLETENESS FOR RANGE        (%) :  92.69
REMARK   3   NUMBER OF REFLECTIONS             :    3184
REMARK   3
REMARK   3  FIT TO DATA USED IN REFINEMENT.
REMARK   3   CROSS-VALIDATION METHOD          : THROUGHOUT
REMARK   3   FREE R VALUE TEST SET SELECTION  : RANDOM
REMARK   3   R VALUE     (WORKING + TEST SET) : 0.01989
REMARK   3   R VALUE           (WORKING SET) :  0.01891
REMARK   3   FREE R VALUE                     :  0.03962
REMARK   3   FREE R VALUE TEST SET SIZE   (%) :  4.8
REMARK   3   FREE R VALUE TEST SET COUNT      :   162
REMARK   3
REMARK   3  FIT IN THE HIGHEST RESOLUTION BIN.
REMARK   3   TOTAL NUMBER OF BINS USED           :      20
REMARK   3   BIN RESOLUTION RANGE HIGH           :    2.802
REMARK   3   BIN RESOLUTION RANGE LOW            :    2.874
REMARK   3   REFLECTION IN BIN     (WORKING SET) :      174
REMARK   3   BIN COMPLETENESS (WORKING+TEST) (%) :    73.20
REMARK   3   BIN R VALUE           (WORKING SET) :    0.019
REMARK   3   BIN FREE R VALUE SET COUNT          :        9
REMARK   3   BIN FREE R VALUE                    :    0.062
REMARK   3
REMARK   3  NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK   3   ALL ATOMS                :     1230
REMARK   3
REMARK   3  B VALUES.
REMARK   3   FROM WILSON PLOT           (A**2) : NULL
REMARK   3   MEAN B VALUE      (OVERALL, A**2) :  15.223
REMARK   3   OVERALL ANISOTROPIC B VALUE.
REMARK   3    B11 (A**2) :     0.28
REMARK   3    B22 (A**2) :     0.17
REMARK   3    B33 (A**2) :    -0.47
REMARK   3    B12 (A**2) :     0.00
REMARK   3    B13 (A**2) :    -0.36
REMARK   3    B23 (A**2) :     0.00
REMARK   3
REMARK   3  ESTIMATED OVERALL COORDINATE ERROR.
REMARK   3   ESU BASED ON R VALUE                            (A): NULL
REMARK   3   ESU BASED ON FREE R VALUE                       (A):   0.072
REMARK   3   ESU BASED ON MAXIMUM LIKELIHOOD                 (A):   0.040
REMARK   3   ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD (A**2):   1.965
REMARK   3
REMARK   3 CORRELATION COEFFICIENTS.
REMARK   3   CORRELATION COEFFICIENT FO-FC      :   0.999
REMARK   3   CORRELATION COEFFICIENT FO-FC FREE :   0.997
REMARK   3
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REMARK   3  RMS DEVIATIONS FROM IDEAL VALUES        COUNT    RMS
WEIGHT
REMARK   3   BOND LENGTHS REFINED ATOMS        (A):  1229 ; 0.011 ; 0.020
REMARK   3   BOND ANGLES REFINED ATOMS   (DEGREES):  1663 ; 1.690 ; 1.966
REMARK   3   TORSION ANGLES, PERIOD 1    (DEGREES):   155 ; 7.866 ; 5.000
REMARK   3   TORSION ANGLES, PERIOD 2    (DEGREES):    54 ;41.443 ;25.741
REMARK   3   TORSION ANGLES, PERIOD 3    (DEGREES):   214 ;19.210 ;15.000
REMARK   3   TORSION ANGLES, PERIOD 4    (DEGREES):     3 ;21.317 ;15.000
REMARK   3   CHIRAL-CENTER RESTRAINTS       (A**3):   187 ; 0.112 ; 0.200
REMARK   3   GENERAL PLANES REFINED ATOMS      (A):   924 ; 0.005 ; 0.021
REMARK   3
REMARK   3  ISOTROPIC THERMAL FACTOR RESTRAINTS.     COUNT   RMS
WEIGHT
REMARK   3
REMARK   3  NCS RESTRAINTS STATISTICS
REMARK   3   NUMBER OF NCS GROUPS : NULL
REMARK   3
REMARK   3  TWIN DETAILS
REMARK   3   NUMBER OF TWIN DOMAINS  : NULL
REMARK   3
REMARK   3
REMARK   3  TLS DETAILS
REMARK   3   NUMBER OF TLS GROUPS  : NULL
REMARK   3
REMARK   3
REMARK   3  BULK SOLVENT MODELLING.
REMARK   3   METHOD USED : NONE
REMARK   3   PARAMETERS FOR MASK CACLULATION
REMARK   3   VDW PROBE RADIUS   : NULL
REMARK   3   ION PROBE RADIUS   : NULL
REMARK   3   SHRINKAGE RADIUS   : NULL
REMARK   3
REMARK   3  OTHER REFINEMENT REMARKS:
REMARK   3  U VALUES      : REFINED INDIVIDUALLY
REMARK   3
CRYST1   32.970   57.010   38.930  90.00  92.27  90.00 P 1 21 1
SCALE1      0.030331  0.000000  0.001202        0.00000
SCALE2     -0.000000  0.017541  0.000000        0.00000
SCALE3      0.000000 -0.000000  0.025707        0.00000
ATOM      1  N   VAL A   3      -6.709  -7.341  17.884  1.00 10.30      A
N
ATOM      2  CA  VAL A   3      -5.902  -6.485  16.952  1.00 10.36      A
C
ATOM      3  CB  VAL A   3      -5.658  -7.209  15.616  1.00 10.23      A
C
ATOM      4  CG1 VAL A   3      -4.723  -6.396  14.731  1.00  9.43      A
C
ATOM      5  CG2 VAL A   3      -5.113  -8.607  15.860  1.00 11.19      A
C
ATOM      6  C   VAL A   3      -6.515  -5.103  16.640  1.00 10.37      A
C
ATOM      7  O   VAL A   3      -7.708  -4.991  16.318  1.00  9.44      A
O
ATOM      8  N   PHE A   4      -5.678  -4.069  16.737  1.00 10.33      A
N
ATOM      9  CA  PHE A   4      -5.986  -2.706  16.273  1.00 11.25      A
C
ATOM     10  CB  PHE A   4      -5.680  -1.690  17.380  1.00 11.69      A
C
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ATOM     11  CG  PHE A   4      -6.584  -1.775  18.579  1.00 12.63      A
C
ATOM     12  CD1 PHE A   4      -6.380  -2.751  19.568  1.00 12.85      A
C
ATOM     13  CE1 PHE A   4      -7.207  -2.814  20.693  1.00 10.63      A
C
ATOM     14  CZ  PHE A   4      -8.238  -1.890  20.847  1.00 11.42      A
C
ATOM     15  CE2 PHE A   4      -8.443  -0.903  19.881  1.00 12.80      A
C
ATOM     16  CD2 PHE A   4      -7.620  -0.846  18.755  1.00 12.68      A
C
ATOM     17  C   PHE A   4      -5.138  -2.336  15.034  1.00 10.92      A
C
ATOM     18  O   PHE A   4      -3.904  -2.310  15.103  1.00 10.21      A
O
ATOM     19  N   ASN A   5      -5.788  -2.027  13.916  1.00 11.43      A
N
ATOM     20  CA  ASN A   5      -5.080  -1.732  12.659  1.00 11.68      A
C
ATOM     21  CB  ASN A   5      -5.629  -2.607  11.529  1.00 12.18      A
C
ATOM     22  CG  ASN A   5      -5.548  -4.074  11.860  1.00 15.39      A
C
ATOM     23  OD1 ASN A   5      -4.479  -4.670  11.794  1.00 16.23      A
O
ATOM     24  ND2 ASN A   5      -6.670  -4.659  12.261  1.00 19.25      A
N
ATOM     25  C   ASN A   5      -5.097  -0.258  12.253  1.00 10.89      A
C
ATOM     26  O   ASN A   5      -6.155   0.355  12.190  1.00  9.21      A
O
ATOM     27  N   TYR A   6      -3.919   0.304  11.987  1.00 12.17      A
N
ATOM     28  CA  TYR A   6      -3.801   1.711  11.572  1.00 13.03      A
C
ATOM     29  CB  TYR A   6      -3.253   2.562  12.713  1.00 12.23      A
C
ATOM     30  CG  TYR A   6      -4.079   2.641  13.990  1.00 12.32      A
C
ATOM     31  CD1 TYR A   6      -3.760   1.860  15.087  1.00 11.72      A
C
ATOM     32  CE1 TYR A   6      -4.459   1.965  16.274  1.00 12.54      A
C
ATOM     33  CZ  TYR A   6      -5.496   2.865  16.379  1.00 13.33      A
C
ATOM     34  OH  TYR A   6      -6.195   2.933  17.562  1.00 14.13      A
O
ATOM     35  CE2 TYR A   6      -5.834   3.666  15.308  1.00 12.92      A
C
ATOM     36  CD2 TYR A   6      -5.115   3.561  14.127  1.00 12.44      A
C
ATOM     37  C   TYR A   6      -2.878   1.895  10.362  1.00 12.33      A
C
ATOM     38  O   TYR A   6      -1.898   1.146  10.213  1.00 11.27      A
O
ATOM     39  N   GLU A   7      -3.168   2.900   9.524  1.00 11.23      A
N
ATOM     40  CA  GLU A   7      -2.324   3.197   8.341  1.00 12.21      A
C
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ATOM     41  CB  GLU A   7      -2.941   2.612   7.072  1.00 12.51      A
C
ATOM     42  CG  GLU A   7      -3.391   1.167   7.178  1.00 12.41      A
C
ATOM     43  CD  GLU A   7      -4.287   0.771   6.027  1.00 15.28      A
C
ATOM     44  OE1 GLU A   7      -4.642   1.649   5.221  1.00 19.34      A
O
ATOM     45  OE2 GLU A   7      -4.626  -0.423   5.906  1.00 20.92      A
O
ATOM     46  C   GLU A   7      -1.996   4.677   8.084  1.00 12.25      A
C
ATOM     47  O   GLU A   7      -2.811   5.549   8.348  1.00 13.28      A
O
ATOM     48  N   ILE A   8      -0.800   4.938   7.548  1.00 15.54      A
N
ATOM     49  CA  ILE A   8      -0.389   6.271   7.048  1.00 13.67      A
C
ATOM     50  CB  ILE A   8       0.701   7.001   7.903  1.00 14.52      A
C
ATOM     51  CG1 ILE A   8       1.050   6.266   9.201  1.00 14.59      A
C
ATOM     52  CD1 ILE A   8       2.146   5.250   8.992  1.00 13.93      A
C
ATOM     53  CG2 ILE A   8       0.398   8.498   8.079  1.00 12.83      A
C
ATOM     54  C   ILE A   8       0.311   6.087   5.732  1.00 13.01      A
C
ATOM     55  O   ILE A   8       0.896   5.034   5.461  1.00 12.25      A
O
ATOM     56  N   GLU A   9       0.278   7.142   4.930  1.00 14.05      A
N
ATOM     57  CA  GLU A   9       1.175   7.263   3.805  1.00 13.60      A
C
ATOM     58  CB  GLU A   9       0.405   7.621   2.539  1.00 14.03      A
C
ATOM     59  CG  GLU A   9      -0.848   6.789   2.334  1.00 15.99      A
C
ATOM     60  CD  GLU A   9      -1.083   6.417   0.890  1.00 19.68      A
C
ATOM     61  OE1 GLU A   9      -0.451   7.015  -0.013  1.00 22.50      A
O
ATOM     62  OE2 GLU A   9      -1.909   5.511   0.665  1.00 24.46      A
O
ATOM     63  C   GLU A   9       2.143   8.369   4.136  1.00 14.43      A
C
ATOM     64  O   GLU A   9       1.804   9.302   4.859  1.00 18.33      A
O
ATOM     65  N   THR A  10       3.361   8.265   3.633  1.00 17.16      A
N
ATOM     66  CA  THR A  10       4.206   9.450   3.551  1.00 19.05      A
C
ATOM     67  CB  THR A  10       5.245   9.532   4.672  1.00 20.55      A
C
ATOM     68  OG1 THR A  10       5.950  10.774   4.538  1.00 23.77      A
O
ATOM     69  CG2 THR A  10       6.223   8.341   4.613  1.00 21.48      A
C
ATOM     70  C   THR A  10       4.884   9.595   2.200  1.00 17.93      A
C
```

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ATOM     71  O   THR A  10       5.235   8.602   1.558  1.00 17.39      A
O
ATOM     72  N   THR A  11       5.057  10.839   1.770  1.00 18.21      A
N
ATOM     73  CA  THR A  11       5.648  11.094   0.466  1.00 16.54      A
C
ATOM     74  CB  THR A  11       4.911  12.190  -0.338  1.00 15.64      A
C
ATOM     75  OG1 THR A  11       5.023  13.448   0.335  1.00 19.34      A
O
ATOM     76  CG2 THR A  11       3.443  11.839  -0.495  1.00 15.17      A
C
ATOM     77  C   THR A  11       7.103  11.435   0.627  1.00 13.56      A
C
ATOM     78  O   THR A  11       7.498  12.100   1.586  1.00 13.44      A
O
ATOM     79  N   SER A  12       7.887  10.936  -0.318  1.00 13.28      A
N
ATOM     80  CA  SER A  12       9.294  11.256  -0.442  1.00 11.65      A
C
ATOM     81  CB  SER A  12      10.179  10.047  -0.090  1.00 13.33      A
C
ATOM     82  OG  SER A  12      11.564  10.320  -0.291  1.00 12.01      A
O
ATOM     83  C   SER A  12       9.573  11.736  -1.857  1.00 11.53      A
C
ATOM     84  O   SER A  12       8.864  11.401  -2.822  1.00 11.87      A
O
ATOM     85  N   VAL A  13      10.631  12.526  -1.941  1.00 11.64      A
N
ATOM     86  CA  VAL A  13      11.069  13.232  -3.126  1.00 10.26      A
C
ATOM     87  CB  VAL A  13      11.503  14.653  -2.685  1.00 10.69      A
C
ATOM     88  CG1 VAL A  13      12.951  14.958  -3.026  1.00 11.72      A
C
ATOM     89  CG2 VAL A  13      10.526  15.720  -3.185  1.00 10.93      A
C
ATOM     90  C   VAL A  13      12.197  12.428  -3.795  1.00 10.33      A
C
ATOM     91  O   VAL A  13      12.571  12.673  -4.955  1.00 10.79      A
O
ATOM     92  N   ILE A  14      12.704  11.454  -3.034  1.00  8.96      A
N
ATOM     93  CA  ILE A  14      13.749  10.512  -3.438  1.00  8.08      A
C
ATOM     94  CB  ILE A  14      14.643  10.152  -2.206  1.00  8.08      A
C
ATOM     95  CG1 ILE A  14      15.543  11.349  -1.802  1.00  7.30      A
C
ATOM     96  CD1 ILE A  14      16.935  11.410  -2.390  1.00  6.30      A
C
ATOM     97  CG2 ILE A  14      15.416   8.843  -2.388  1.00  7.57      A
C
ATOM     98  C   ILE A  14      13.047   9.280  -4.017  1.00  7.83      A
C
ATOM     99  O   ILE A  14      11.981   8.897  -3.513  1.00  7.96      A
O
ATOM    100  N   PRO A  15      13.619   8.667  -5.083  1.00  6.69      A
N
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ATOM    101  CA  PRO A  15      13.001   7.511  -5.780  1.00  6.30      A
C
ATOM    102  CB  PRO A  15      13.865   7.341  -7.032  1.00  5.77      A
C
ATOM    103  CG  PRO A  15      15.167   7.971  -6.682  1.00  6.13      A
C
ATOM    104  CD  PRO A  15      14.870   9.094  -5.732  1.00  6.22      A
C
ATOM    105  C   PRO A  15      12.915   6.187  -4.985  1.00  5.87      A
C
ATOM    106  O   PRO A  15      13.847   5.803  -4.270  1.00  5.50      A
O
ATOM    107  N   ALA A  16      11.795   5.489  -5.156  1.00  6.04      A
N
ATOM    108  CA  ALA A  16      11.472   4.282  -4.385  1.00  5.64      A
C
ATOM    109  CB  ALA A  16      10.328   3.534  -5.050  1.00  5.17      A
C
ATOM    110  C   ALA A  16      12.648   3.336  -4.092  1.00  5.27      A
C
ATOM    111  O   ALA A  16      12.751   2.798  -3.006  1.00  5.89      A
O
ATOM    112  N   ALA A  17      13.531   3.137  -5.054  1.00  5.11      A
N
ATOM    113  CA  ALA A  17      14.587   2.136  -4.906  1.00  5.24      A
C
ATOM    114  CB  ALA A  17      15.016   1.582  -6.272  1.00  4.81      A
C
ATOM    115  C   ALA A  17      15.794   2.661  -4.127  1.00  5.05      A
C
ATOM    116  O   ALA A  17      16.484   1.889  -3.443  1.00  5.11      A
O
ATOM    117  N   ARG A  18      16.069   3.958  -4.238  1.00  4.30      A
N
ATOM    118  CA  ARG A  18      17.192   4.492  -3.508  1.00  4.16      A
C
ATOM    119  CB  ARG A  18      17.579   5.878  -3.989  1.00  4.43      A
C
ATOM    120  CG  ARG A  18      19.012   6.222  -3.629  1.00  4.69      A
C
ATOM    121  CD  ARG A  18      19.300   7.683  -3.880  1.00  5.36      A
C
ATOM    122  NE  ARG A  18      20.651   8.007  -3.444  1.00  6.79      A
N
ATOM    123  CZ  ARG A  18      21.079   9.231  -3.150  1.00  7.74      A
C
ATOM    124  NH1 ARG A  18      20.252  10.264  -3.250  1.00  7.60      A
N
ATOM    125  NH2 ARG A  18      22.338   9.417  -2.752  1.00  9.41      A
N
ATOM    126  C   ARG A  18      16.826   4.555  -2.052  1.00  3.96      A
C
ATOM    127  O   ARG A  18      17.643   4.249  -1.183  1.00  3.84      A
O
ATOM    128  N   LEU A  19      15.587   4.950  -1.789  1.00  3.71      A
N
ATOM    129  CA  LEU A  19      15.153   5.089  -0.422  1.00  3.84      A
C
ATOM    130  CB  LEU A  19      14.118   6.216  -0.281  1.00  3.82      A
C
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ATOM    131  CG  LEU A  19      13.614   6.468   1.141  1.00  3.41      A
C
ATOM    132  CD1 LEU A  19      13.650   7.908   1.605  1.00  3.04      A
C
ATOM    133  CD2 LEU A  19      12.209   5.907   1.146  1.00  3.83      A
C
ATOM    134  C   LEU A  19      14.727   3.785   0.259  1.00  3.57      A
C
ATOM    135  O   LEU A  19      14.652   3.713   1.473  1.00  3.57      A
O
ATOM    136  N   PHE A  20      14.486   2.741  -0.507  1.00  3.70      A
N
ATOM    137  CA  PHE A  20      14.250   1.465   0.128  1.00  4.35      A
C
ATOM    138  CB  PHE A  20      13.568   0.451  -0.812  1.00  4.74      A
C
ATOM    139  CG  PHE A  20      13.150  -0.840  -0.128  1.00  5.29      A
C
ATOM    140  CD1 PHE A  20      12.006  -0.891   0.684  1.00  5.58      A
C
ATOM    141  CE1 PHE A  20      11.619  -2.083   1.306  1.00  5.44      A
C
ATOM    142  CZ  PHE A  20      12.376  -3.242   1.122  1.00  5.53      A
C
ATOM    143  CE2 PHE A  20      13.502  -3.212   0.322  1.00  5.63      A
C
ATOM    144  CD2 PHE A  20      13.889  -2.018  -0.302  1.00  5.45      A
C
ATOM    145  C   PHE A  20      15.554   0.930   0.705  1.00  4.36      A
C
ATOM    146  O   PHE A  20      15.561   0.450   1.825  1.00  4.42      A
O
ATOM    147  N   LYS A  21      16.645   1.045  -0.057  1.00  5.04      A
N
ATOM    148  CA  LYS A  21      17.977   0.514   0.299  1.00  5.69      A
C
ATOM    149  CB  LYS A  21      18.890   0.485  -0.950  1.00  6.92      A
C
ATOM    150  CG  LYS A  21      20.361   0.153  -0.672  1.00  7.84      A
C
ATOM    151  CD  LYS A  21      20.705  -1.256  -1.146  1.00 11.27      A
C
ATOM    152  CE  LYS A  21      20.878  -2.267  -0.033  1.00 13.01      A
C
ATOM    153  NZ  LYS A  21      20.881  -3.643  -0.594  1.00  8.91      A
N
ATOM    154  C   LYS A  21      18.631   1.327   1.433  1.00  5.07      A
C
ATOM    155  O   LYS A  21      19.257   0.772   2.333  1.00  4.79      A
O
ATOM    156  N   ALA A  22      18.475   2.644   1.374  1.00  4.86      A
N
ATOM    157  CA  ALA A  22      18.988   3.530   2.404  1.00  5.74      A
C
ATOM    158  CB  ALA A  22      18.929   4.963   1.914  1.00  6.42      A
C
ATOM    159  C   ALA A  22      18.226   3.414   3.725  1.00  6.34      A
C
ATOM    160  O   ALA A  22      18.822   3.211   4.787  1.00  6.08      A
O
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ATOM    161  N   PHE A  23      16.905   3.550   3.631  1.00  6.60      A
N
ATOM    162  CA  PHE A  23      16.046   3.720   4.784  1.00  8.12      A
C
ATOM    163  CB  PHE A  23      14.820   4.568   4.384  1.00  8.76      A
C
ATOM    164  CG  PHE A  23      13.875   4.865   5.524  1.00  9.71      A
C
ATOM    165  CD1 PHE A  23      14.356   5.376   6.743  1.00  9.47      A
C
ATOM    166  CE1 PHE A  23      13.498   5.640   7.798  1.00  9.50      A
C
ATOM    167  CZ  PHE A  23      12.135   5.419   7.635  1.00 11.48      A
C
ATOM    168  CE2 PHE A  23      11.637   4.928   6.420  1.00 11.27      A
C
ATOM    169  CD2 PHE A  23      12.504   4.653   5.373  1.00 10.28      A
C
ATOM    170  C   PHE A  23      15.625   2.415   5.474  1.00  8.66      A
C
ATOM    171  O   PHE A  23      15.387   2.381   6.678  1.00  8.34      A
O
ATOM    172  N   ILE A  24      15.540   1.338   4.714  1.00  9.08      A
N
ATOM    173  CA  ILE A  24      14.997   0.107   5.248  1.00  9.63      A
C
ATOM    174  CB  ILE A  24      13.761  -0.330   4.456  1.00 10.16      A
C
ATOM    175  CG1 ILE A  24      12.661   0.746   4.517  1.00  9.87      A
C
ATOM    176  CD1 ILE A  24      12.164   1.087   5.912  1.00 10.53      A
C
ATOM    177  CG2 ILE A  24      13.303  -1.699   4.933  1.00 11.72      A
C
ATOM    178  C   ILE A  24      16.023  -1.019   5.279  1.00 10.30      A
C
ATOM    179  O   ILE A  24      16.252  -1.616   6.335  1.00 10.22      A
O
ATOM    180  N   LEU A  25      16.634  -1.293   4.126  1.00 10.18      A
N
ATOM    181  CA  LEU A  25      17.705  -2.277   4.031  1.00 11.13      A
C
ATOM    182  CB  LEU A  25      18.049  -2.594   2.574  1.00 10.23      A
C
ATOM    183  CG  LEU A  25      16.889  -3.255   1.816  1.00 13.03      A
C
ATOM    184  CD1 LEU A  25      17.344  -3.879   0.502  1.00 12.76      A
C
ATOM    185  CD2 LEU A  25      16.122  -4.277   2.658  1.00 12.44      A
C
ATOM    186  C   LEU A  25      18.958  -1.886   4.814  1.00 11.73      A
C
ATOM    187  O   LEU A  25      19.593  -2.753   5.411  1.00 13.11      A
O
ATOM    188  N   ASP A  26      19.315  -0.601   4.815  1.00 11.09      A
N
ATOM    189  CA  ASP A  26      20.466  -0.146   5.603  1.00 13.24      A
C
ATOM    190  CB  ASP A  26      21.619   0.318   4.699  1.00 13.29      A
C
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ATOM    191  CG  ASP A  26      21.971  -0.723   3.633  1.00 16.77      A
C
ATOM    192  OD1 ASP A  26      21.984  -1.937   3.952  1.00 16.09      A
O
ATOM    193  OD2 ASP A  26      22.194  -0.336   2.460  1.00 20.66      A
O
ATOM    194  C   ASP A  26      20.064   0.870   6.678  1.00 13.32      A
C
ATOM    195  O   ASP A  26      20.813   1.800   7.013  1.00 11.30      A
O
ATOM    196  N   GLY A  27      18.860   0.650   7.216  1.00 14.34      A
N
ATOM    197  CA  GLY A  27      18.317   1.411   8.334  1.00 14.15      A
C
ATOM    198  C   GLY A  27      19.277   1.342   9.495  1.00 15.48      A
C
ATOM    199  O   GLY A  27      19.709   2.385   9.983  1.00 18.64      A
O
ATOM    200  N   ASP A  28      19.600   0.111   9.921  1.00 16.21      A
N
ATOM    201  CA  ASP A  28      20.764  -0.212  10.782  1.00 16.51      A
C
ATOM    202  CB  ASP A  28      21.444  -1.438  10.229  1.00 18.00      A
C
ATOM    203  CG  ASP A  28      20.709  -2.637  10.496  1.00 21.76      A
C
ATOM    204  OD1 ASP A  28      19.764  -2.541  11.311  1.00 28.66      A
O
ATOM    205  OD2 ASP A  28      21.085  -3.658   9.891  1.00 24.93      A
O
ATOM    206  C   ASP A  28      21.883   0.789  10.755  1.00 17.01      A
C
ATOM    207  O   ASP A  28      22.194   1.442  11.755  1.00 14.45      A
O
ATOM    208  N   ASN A  29      22.517   0.798   9.577  1.00 16.89      A
N
ATOM    209  CA  ASN A  29      23.633   1.625   9.224  1.00 12.31      A
C
ATOM    210  CB  ASN A  29      24.238   1.087   7.909  0.01 12.65      A
C
ATOM    211  CG  ASN A  29      24.929  -0.211   8.189  0.01 12.27      A
C
ATOM    212  OD1 ASN A  29      25.152  -0.388   9.341  1.00  8.08      A
O
ATOM    213  ND2 ASN A  29      25.193  -1.130   7.233  1.00 17.53      A
N
ATOM    214  C   ASN A  29      23.340   3.126   9.289  1.00 12.80      A
C
ATOM    215  O   ASN A  29      23.946   3.809  10.112  1.00 10.62      A
O
ATOM    216  N   LEU A  30      22.366   3.614   8.514  1.00 11.36      A
N
ATOM    217  CA  LEU A  30      22.259   5.062   8.247  1.00 12.84      A
C
ATOM    218  CB  LEU A  30      21.679   5.326   6.847  1.00 11.42      A
C
ATOM    219  CG  LEU A  30      21.678   6.781   6.359  1.00 10.14      A
C
ATOM    220  CD1 LEU A  30      23.098   7.318   6.242  1.00  9.78      A
C
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ATOM    221  CD2 LEU A  30      20.914   6.930   5.055  1.00 10.87      A
C
ATOM    222  C   LEU A  30      21.572   5.969   9.301  1.00 13.32      A
C
ATOM    223  O   LEU A  30      22.006   7.121   9.501  1.00 11.66      A
O
ATOM    224  N   VAL A  31      20.535   5.450   9.962  1.00 12.96      A
N
ATOM    225  CA  VAL A  31      19.662   6.243  10.865  1.00 12.87      A
C
ATOM    226  CB  VAL A  31      18.351   5.487  11.208  1.00 12.77      A
C
ATOM    227  CG1 VAL A  31      17.359   6.414  11.878  1.00 12.54      A
C
ATOM    228  CG2 VAL A  31      17.730   4.892   9.951  1.00 13.14      A
C
ATOM    229  C   VAL A  31      20.327   6.807  12.150  1.00 12.90      A
C
ATOM    230  O   VAL A  31      20.210   8.018  12.423  1.00 11.03      A
O
ATOM    231  N   PRO A  32      21.019   5.948  12.939  1.00 12.22      A
N
ATOM    232  CA  PRO A  32      21.780   6.463  14.094  1.00 12.87      A
C
ATOM    233  CB  PRO A  32      22.535   5.218  14.599  1.00 12.84      A
C
ATOM    234  CG  PRO A  32      21.696   4.060  14.171  1.00 12.65      A
C
ATOM    235  CD  PRO A  32      21.092   4.475  12.849  1.00 11.99      A
C
ATOM    236  C   PRO A  32      22.785   7.567  13.710  1.00 13.00      A
C
ATOM    237  O   PRO A  32      23.092   8.454  14.520  1.00 14.17      A
O
ATOM    238  N   LYS A  33      23.285   7.493  12.480  1.00 12.47      A
N
ATOM    239  CA  LYS A  33      24.224   8.465  11.945  1.00 12.85      A
C
ATOM    240  CB  LYS A  33      24.917   7.929  10.690  1.00 15.75      A
C
ATOM    241  CG  LYS A  33      25.030   6.407  10.616  1.00 18.40      A
C
ATOM    242  CD  LYS A  33      25.813   5.850  11.796  1.00 22.18      A
C
ATOM    243  CE  LYS A  33      25.471   4.402  12.076  1.00 16.60      A
C
ATOM    244  NZ  LYS A  33      26.648   3.541  11.818  1.00 17.23      A
N
ATOM    245  C   LYS A  33      23.493   9.722  11.577  1.00 12.22      A
C
ATOM    246  O   LYS A  33      24.011  10.811  11.789  1.00 14.45      A
O
ATOM    247  N   VAL A  34      22.294   9.574  11.012  1.00 12.38      A
N
ATOM    248  CA  VAL A  34      21.551  10.732  10.512  1.00 11.90      A
C
ATOM    249  CB  VAL A  34      20.863  10.504   9.146  1.00 12.19      A
C
ATOM    250  CG1 VAL A  34      21.882  10.150   8.081  1.00 13.16      A
C
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ATOM    251  CG2 VAL A  34      19.763   9.462   9.227  1.00 13.05      A
C
ATOM    252  C   VAL A  34      20.547  11.294  11.497  1.00 12.84      A
C
ATOM    253  O   VAL A  34      20.142  12.449  11.348  1.00 13.14      A
O
ATOM    254  N   ALA A  35      20.152  10.497  12.495  1.00 11.71      A
N
ATOM    255  CA  ALA A  35      19.207  10.976  13.515  1.00 10.51      A
C
ATOM    256  CB  ALA A  35      17.786  10.571  13.142  1.00  9.38      A
C
ATOM    257  C   ALA A  35      19.540  10.572  14.965  1.00  9.55      A
C
ATOM    258  O   ALA A  35      18.702   9.959  15.641  1.00  8.65      A
O
ATOM    259  N   PRO A  36      20.746  10.945  15.462  1.00  9.28      A
N
ATOM    260  CA  PRO A  36      21.247  10.423  16.750  1.00 10.35      A
C
ATOM    261  CB  PRO A  36      22.642  11.039  16.861  1.00 10.26      A
C
ATOM    262  CG  PRO A  36      22.606  12.256  16.013  1.00  9.27      A
C
ATOM    263  CD  PRO A  36      21.647  11.964  14.896  1.00  9.32      A
C
ATOM    264  C   PRO A  36      20.376  10.831  17.947  1.00 10.98      A
C
ATOM    265  O   PRO A  36      20.274  10.118  18.946  1.00 11.03      A
O
ATOM    266  N   GLN A  37      19.746  11.985  17.802  1.00 12.66      A
N
ATOM    267  CA  GLN A  37      18.818  12.551  18.760  1.00 12.14      A
C
ATOM    268  CB  GLN A  37      18.511  13.976  18.301  1.00 13.09      A
C
ATOM    269  CG  GLN A  37      18.848  14.160  16.832  1.00 16.08      A
C
ATOM    270  CD  GLN A  37      19.206  15.575  16.466  1.00 23.83      A
C
ATOM    271  OE1 GLN A  37      18.329  16.436  16.353  1.00 32.57      A
O
ATOM    272  NE2 GLN A  37      20.502  15.826  16.250  1.00 22.49      A
N
ATOM    273  C   GLN A  37      17.534  11.731  18.923  1.00 10.80      A
C
ATOM    274  O   GLN A  37      16.744  12.012  19.815  1.00 12.51      A
O
ATOM    275  N   ALA A  38      17.353  10.708  18.082  1.00 10.45      A
N
ATOM    276  CA  ALA A  38      16.116   9.898  18.044  1.00  8.95      A
C
ATOM    277  CB  ALA A  38      15.320  10.225  16.789  1.00  9.33      A
C
ATOM    278  C   ALA A  38      16.334   8.370  18.162  1.00  7.85      A
C
ATOM    279  O   ALA A  38      15.570   7.680  18.840  1.00  6.83      A
O
ATOM    280  N   ILE A  39      17.356   7.854  17.473  1.00  7.09      A
N
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ATOM    281  CA  ILE A  39      17.815   6.468  17.644  1.00  5.88      A
C
ATOM    282  CB  ILE A  39      17.538   5.585  16.385  1.00  5.41      A
C
ATOM    283  CG1 ILE A  39      16.086   5.727  15.889  1.00  5.28      A
C
ATOM    284  CD1 ILE A  39      15.020   5.001  16.689  1.00  4.89      A
C
ATOM    285  CG2 ILE A  39      17.903   4.118  16.626  1.00  5.12      A
C
ATOM    286  C   ILE A  39      19.315   6.509  17.989  1.00  5.59      A
C
ATOM    287  O   ILE A  39      20.148   6.878  17.142  1.00  5.41      A
O
ATOM    288  N   SER A  40      19.651   6.160  19.234  1.00  5.38      A
N
ATOM    289  CA  SER A  40      21.053   6.149  19.682  1.00  5.52      A
C
ATOM    290  CB  SER A  40      21.170   6.101  21.208  1.00  5.85      A
C
ATOM    291  OG  SER A  40      20.478   4.980  21.756  1.00  6.79      A
O
ATOM    292  C   SER A  40      21.836   4.995  19.061  1.00  5.11      A
C
ATOM    293  O   SER A  40      23.001   5.162  18.681  1.00  5.62      A
O
ATOM    294  N   SER A  41      21.206   3.829  18.971  1.00  4.24      A
N
ATOM    295  CA  SER A  41      21.850   2.699  18.353  1.00  4.13      A
C
ATOM    296  CB  SER A  41      22.912   2.135  19.286  1.00  4.08      A
C
ATOM    297  OG  SER A  41      22.299   1.492  20.374  1.00  4.22      A
O
ATOM    298  C   SER A  41      20.885   1.606  17.944  1.00  4.07      A
C
ATOM    299  O   SER A  41      19.807   1.472  18.510  1.00  3.89      A
O
ATOM    300  N   VAL A  42      21.301   0.836  16.940  1.00  4.44      A
N
ATOM    301  CA  VAL A  42      20.643  -0.414  16.530  1.00  4.71      A
C
ATOM    302  CB  VAL A  42      20.169  -0.359  15.063  1.00  4.61      A
C
ATOM    303  CG1 VAL A  42      19.697  -1.721  14.599  1.00  5.22      A
C
ATOM    304  CG2 VAL A  42      19.087   0.696  14.856  1.00  4.32      A
C
ATOM    305  C   VAL A  42      21.651  -1.560  16.703  1.00  5.15      A
C
ATOM    306  O   VAL A  42      22.774  -1.486  16.205  1.00  5.32      A
O
ATOM    307  N   GLU A  43      21.256  -2.607  17.422  1.00  5.48      A
N
ATOM    308  CA  GLU A  43      22.145  -3.736  17.702  1.00  5.90      A
C
ATOM    309  CB  GLU A  43      22.269  -3.937  19.210  1.00  6.24      A
C
ATOM    310  CG  GLU A  43      23.348  -4.908  19.671  1.00  6.18      A
C
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ATOM    311  CD  GLU A  43      23.201  -5.216  21.150  1.00  7.93      A
C
ATOM    312  OE1 GLU A  43      24.126  -5.828  21.752  1.00  7.87      A
O
ATOM    313  OE2 GLU A  43      22.140  -4.832  21.717  1.00  8.87      A
O
ATOM    314  C   GLU A  43      21.630  -5.013  17.046  1.00  6.07      A
C
ATOM    315  O   GLU A  43      20.439  -5.317  17.128  1.00  5.83      A
O
ATOM    316  N   ASN A  44      22.528  -5.753  16.396  1.00  6.45      A
N
ATOM    317  CA  ASN A  44      22.136  -6.963  15.663  1.00  7.11      A
C
ATOM    318  CB  ASN A  44      22.925  -7.087  14.348  1.00  6.65      A
C
ATOM    319  CG  ASN A  44      22.328  -8.095  13.385  1.00  6.37      A
C
ATOM    320  OD1 ASN A  44      21.409  -7.799  12.624  1.00  5.69      A
O
ATOM    321  ND2 ASN A  44      22.887  -9.289  13.386  1.00  7.55      A
N
ATOM    322  C   ASN A  44      22.299  -8.185  16.567  1.00  7.36      A
C
ATOM    323  O   ASN A  44      23.401  -8.682  16.769  1.00  8.30      A
O
ATOM    324  N   ILE A  45      21.179  -8.635  17.125  1.00  8.61      A
N
ATOM    325  CA  ILE A  45      21.142  -9.702  18.120  1.00  8.78      A
C
ATOM    326  CB  ILE A  45      19.753  -9.828  18.769  1.00  8.05      A
C
ATOM    327  CG1 ILE A  45      19.288  -8.473  19.282  1.00  8.29      A
C
ATOM    328  CD1 ILE A  45      20.280  -7.807  20.221  1.00 10.10      A
C
ATOM    329  CG2 ILE A  45      19.791 -10.838  19.906  1.00  9.08      A
C
ATOM    330  C   ILE A  45      21.532 -11.030  17.508  1.00 10.04      A
C
ATOM    331  O   ILE A  45      22.524 -11.638  17.933  1.00 11.13      A
O
ATOM    332  N   GLU A  46      20.748 -11.457  16.512  1.00 11.91      A
N
ATOM    333  CA  GLU A  46      20.938 -12.719  15.777  1.00 11.62      A
C
ATOM    334  CB  GLU A  46      20.243 -13.870  16.519  1.00 11.47      A
C
ATOM    335  CG  GLU A  46      18.721 -13.862  16.425  1.00 12.69      A
C
ATOM    336  CD  GLU A  46      18.212 -14.567  15.185  1.00 14.43      A
C
ATOM    337  OE1 GLU A  46      18.940 -15.457  14.697  1.00 14.98      A
O
ATOM    338  OE2 GLU A  46      17.098 -14.241  14.711  1.00 15.38      A
O
ATOM    339  C   GLU A  46      20.408 -12.626  14.337  1.00 11.12      A
C
ATOM    340  O   GLU A  46      19.584 -11.761  14.028  1.00 10.58      A
O
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ATOM    341  N   GLY A  47      20.857 -13.541  13.478  1.00 11.16      A
N
ATOM    342  CA  GLY A  47      20.365 -13.636  12.101  1.00 11.80      A
C
ATOM    343  C   GLY A  47      21.098 -12.707  11.160  1.00 11.63      A
C
ATOM    344  O   GLY A  47      21.757 -11.777  11.607  1.00 12.45      A
O
ATOM    345  N   ASN A  48      20.979 -12.944   9.857  1.00 14.60      A
N
ATOM    346  CA  ASN A  48      21.812 -12.229   8.882  1.00 16.21      A
C
ATOM    347  CB  ASN A  48      22.755 -13.206   8.160  1.00 18.86      A
C
ATOM    348  CG  ASN A  48      22.026 -14.135   7.213  1.00 18.72      A
C
ATOM    349  OD1 ASN A  48      21.801 -13.804   6.050  1.00 16.10      A
O
ATOM    350  ND2 ASN A  48      21.648 -15.303   7.709  1.00 18.45      A
N
ATOM    351  C   ASN A  48      21.041 -11.360   7.888  1.00 14.84      A
C
ATOM    352  O   ASN A  48      21.529 -11.072   6.790  1.00 14.97      A
O
ATOM    353  N   GLY A  49      19.851 -10.925   8.292  1.00 13.78      A
N
ATOM    354  CA  GLY A  49      18.954 -10.187   7.404  1.00 13.04      A
C
ATOM    355  C   GLY A  49      17.957 -11.137   6.778  1.00 10.99      A
C
ATOM    356  O   GLY A  49      18.261 -12.296   6.543  1.00 13.56      A
O
ATOM    357  N   GLY A  50      16.758 -10.672   6.494  1.00  9.67      A
N
ATOM    358  CA  GLY A  50      15.755 -11.621   6.055  1.00 10.28      A
C
ATOM    359  C   GLY A  50      15.248 -12.421   7.244  1.00  9.86      A
C
ATOM    360  O   GLY A  50      15.782 -12.278   8.352  1.00 10.75      A
O
ATOM    361  N   PRO A  51      14.245 -13.288   7.009  1.00  9.05      A
N
ATOM    362  CA  PRO A  51      13.270 -13.741   8.011  1.00 10.08      A
C
ATOM    363  CB  PRO A  51      12.577 -14.924   7.315  1.00 11.19      A
C
ATOM    364  CG  PRO A  51      12.650 -14.576   5.859  1.00  9.56      A
C
ATOM    365  CD  PRO A  51      14.000 -13.919   5.694  1.00  9.40      A
C
ATOM    366  C   PRO A  51      13.736 -14.084   9.444  1.00 10.03      A
C
ATOM    367  O   PRO A  51      13.046 -13.749  10.408  1.00 12.26      A
O
ATOM    368  N   GLY A  52      14.878 -14.704   9.637  1.00  8.50      A
N
ATOM    369  CA  GLY A  52      15.265 -14.915  11.034  1.00 11.16      A
C
ATOM    370  C   GLY A  52      15.430 -13.721  11.992  1.00 10.57      A
C
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ATOM    371  O   GLY A  52      15.209 -13.851  13.205  1.00 11.10      A
O
ATOM    372  N   THR A  53      15.781 -12.562  11.434  1.00 10.54      A
N
ATOM    373  CA  THR A  53      16.656 -11.574  12.094  1.00  9.66      A
C
ATOM    374  CB  THR A  53      17.326 -10.641  11.054  1.00  9.79      A
C
ATOM    375  OG1 THR A  53      18.256 -11.394  10.258  1.00 10.14      A
O
ATOM    376  CG2 THR A  53      18.075  -9.502  11.741  1.00  8.84      A
C
ATOM    377  C   THR A  53      16.061 -10.732  13.207  1.00  9.56      A
C
ATOM    378  O   THR A  53      15.029 -10.091  13.037  1.00  9.78      A
O
ATOM    379  N   ILE A  54      16.757 -10.721  14.338  1.00  9.48      A
N
ATOM    380  CA  ILE A  54      16.392  -9.879  15.469  1.00  9.77      A
C
ATOM    381  CB  ILE A  54      16.294 -10.714  16.770  1.00 10.04      A
C
ATOM    382  CG1 ILE A  54      15.335 -11.901  16.558  1.00 10.13      A
C
ATOM    383  CD1 ILE A  54      14.946 -12.632  17.832  1.00 10.72      A
C
ATOM    384  CG2 ILE A  54      15.905  -9.831  17.957  1.00  8.93      A
C
ATOM    385  C   ILE A  54      17.357  -8.691  15.649  1.00  9.58      A
C
ATOM    386  O   ILE A  54      18.577  -8.856  15.642  1.00  7.99      A
O
ATOM    387  N   LYS A  55      16.790  -7.496  15.808  1.00 10.55      A
N
ATOM    388  CA  LYS A  55      17.561  -6.275  16.082  1.00 10.50      A
C
ATOM    389  CB  LYS A  55      17.548  -5.361  14.861  1.00 11.20      A
C
ATOM    390  CG  LYS A  55      18.458  -5.811  13.732  1.00 12.64      A
C
ATOM    391  CD  LYS A  55      18.035  -5.223  12.392  1.00 10.68      A
C
ATOM    392  CE  LYS A  55      18.945  -5.784  11.319  1.00 11.42      A
C
ATOM    393  NZ  LYS A  55      18.645  -5.252   9.965  1.00 15.90      A
N
ATOM    394  C   LYS A  55      17.021  -5.502  17.287  1.00 10.08      A
C
ATOM    395  O   LYS A  55      15.817  -5.457  17.524  1.00 11.49      A
O
ATOM    396  N   LYS A  56      17.912  -4.875  18.035  1.00  8.98      A
N
ATOM    397  CA  LYS A  56      17.516  -4.110  19.213  1.00  8.52      A
C
ATOM    398  CB  LYS A  56      18.365  -4.512  20.417  1.00  8.59      A
C
ATOM    399  CG  LYS A  56      17.928  -3.919  21.735  1.00  9.18      A
C
ATOM    400  CD  LYS A  56      18.964  -4.252  22.788  1.00 11.00      A
C
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ATOM    401  CE  LYS A  56      18.542  -3.818  24.176  1.00 10.31      A
C
ATOM    402  NZ  LYS A  56      18.674  -4.983  25.088  1.00 10.84      A
N
ATOM    403  C   LYS A  56      17.672  -2.623  18.932  1.00  8.06      A
C
ATOM    404  O   LYS A  56      18.769  -2.138  18.665  1.00  8.24      A
O
ATOM    405  N   ILE A  57      16.564  -1.903  18.991  1.00  8.00      A
N
ATOM    406  CA  ILE A  57      16.563  -0.484  18.709  1.00  7.24      A
C
ATOM    407  CB  ILE A  57      15.289  -0.065  17.921  1.00  7.86      A
C
ATOM    408  CG1 ILE A  57      14.943  -1.075  16.804  1.00  8.57      A
C
ATOM    409  CD1 ILE A  57      16.069  -1.406  15.821  1.00  7.45      A
C
ATOM    410  CG2 ILE A  57      15.425   1.338  17.346  1.00  7.96      A
C
ATOM    411  C   ILE A  57      16.657   0.202  20.065  1.00  6.93      A
C
ATOM    412  O   ILE A  57      15.762   0.061  20.899  1.00  6.24      A
O
ATOM    413  N   ASN A  58      17.769   0.902  20.286  1.00  6.85      A
N
ATOM    414  CA  ASN A  58      18.018   1.636  21.524  1.00  6.62      A
C
ATOM    415  CB  ASN A  58      19.456   1.446  22.007  1.00  6.83      A
C
ATOM    416  CG  ASN A  58      19.766   0.018  22.347  1.00  6.89      A
C
ATOM    417  OD1 ASN A  58      19.247  -0.527  23.323  1.00  7.61      A
O
ATOM    418  ND2 ASN A  58      20.615  -0.605  21.542  1.00  6.85      A
N
ATOM    419  C   ASN A  58      17.739   3.120  21.387  1.00  6.61      A
C
ATOM    420  O   ASN A  58      18.339   3.817  20.569  1.00  5.96      A
O
ATOM    421  N   PHE A  59      16.830   3.590  22.225  1.00  7.17      A
N
ATOM    422  CA  PHE A  59      16.420   4.969  22.217  1.00  7.66      A
C
ATOM    423  CB  PHE A  59      14.932   5.053  22.544  1.00  7.34      A
C
ATOM    424  CG  PHE A  59      14.082   4.363  21.539  1.00  7.94      A
C
ATOM    425  CD1 PHE A  59      13.596   3.087  21.783  1.00  8.37      A
C
ATOM    426  CE1 PHE A  59      12.825   2.426  20.835  1.00  7.75      A
C
ATOM    427  CZ  PHE A  59      12.552   3.038  19.624  1.00  8.48      A
C
ATOM    428  CE2 PHE A  59      13.041   4.310  19.363  1.00  8.75      A
C
ATOM    429  CD2 PHE A  59      13.807   4.965  20.315  1.00  8.57      A
C
ATOM    430  C   PHE A  59      17.260   5.766  23.195  1.00  7.79      A
C
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ATOM    431  O   PHE A  59      17.687   5.224  24.212  1.00  7.40      A
O
ATOM    432  N   PRO A  60      17.485   7.063  22.894  1.00  9.28      A
N
ATOM    433  CA  PRO A  60      18.258   7.981  23.752  1.00  9.58      A
C
ATOM    434  CB  PRO A  60      18.231   9.298  22.974  1.00 10.48      A
C
ATOM    435  CG  PRO A  60      17.036   9.199  22.079  1.00 10.16      A
C
ATOM    436  CD  PRO A  60      16.960   7.752  21.697  1.00  9.70      A
C
ATOM    437  C   PRO A  60      17.628   8.215  25.117  1.00  9.81      A
C
ATOM    438  O   PRO A  60      16.402   8.080  25.283  1.00  9.64      A
O
ATOM    439  N   GLU A  61      18.467   8.590  26.077  1.00  9.40      A
N
ATOM    440  CA  GLU A  61      17.998   8.930  27.413  1.00 10.11      A
C
ATOM    441  CB  GLU A  61      19.142   9.491  28.235  1.00 11.74      A
C
ATOM    442  CG  GLU A  61      18.865   9.584  29.718  1.00 12.69      A
C
ATOM    443  CD  GLU A  61      19.992  10.266  30.452  1.00 15.29      A
C
ATOM    444  OE1 GLU A  61      19.742  10.810  31.547  1.00 18.57      A
O
ATOM    445  OE2 GLU A  61      21.130  10.255  29.928  1.00 16.54      A
O
ATOM    446  C   GLU A  61      16.858   9.940  27.345  1.00  9.52      A
C
ATOM    447  O   GLU A  61      16.836  10.811  26.475  1.00  9.97      A
O
ATOM    448  N   GLY A  62      15.904   9.792  28.256  1.00  9.19      A
N
ATOM    449  CA  GLY A  62      14.751  10.664  28.315  1.00  9.15      A
C
ATOM    450  C   GLY A  62      13.505  10.025  27.776  1.00  8.75      A
C
ATOM    451  O   GLY A  62      12.430  10.232  28.311  1.00  9.31      A
O
ATOM    452  N   PHE A  63      13.664   9.241  26.713  1.00  9.69      A
N
ATOM    453  CA  PHE A  63      12.549   8.583  26.023  1.00  8.87      A
C
ATOM    454  CB  PHE A  63      13.065   7.822  24.798  1.00 10.68      A
C
ATOM    455  CG  PHE A  63      13.245   8.691  23.577  1.00 12.69      A
C
ATOM    456  CD1 PHE A  63      14.001   9.869  23.639  1.00 13.15      A
C
ATOM    457  CE1 PHE A  63      14.152  10.686  22.524  1.00 12.55      A
C
ATOM    458  CZ  PHE A  63      13.556  10.320  21.330  1.00 13.18      A
C
ATOM    459  CE2 PHE A  63      12.798   9.153  21.252  1.00 12.95      A
C
ATOM    460  CD2 PHE A  63      12.647   8.344  22.366  1.00 12.38      A
C
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ATOM    461  C   PHE A  63      11.789   7.662  26.957  1.00  7.78      A
C
ATOM    462  O   PHE A  63      12.400   6.982  27.775  1.00  8.04      A
O
ATOM    463  N   PRO A  64      10.446   7.663  26.863  1.00  7.80      A
N
ATOM    464  CA  PRO A  64       9.604   6.851  27.763  1.00  7.64      A
C
ATOM    465  CB  PRO A  64       8.216   6.927  27.107  1.00  6.67      A
C
ATOM    466  CG  PRO A  64       8.231   8.202  26.340  1.00  6.28      A
C
ATOM    467  CD  PRO A  64       9.641   8.438  25.895  1.00  7.04      A
C
ATOM    468  C   PRO A  64      10.079   5.386  27.912  1.00  7.20      A
C
ATOM    469  O   PRO A  64      10.188   4.880  29.027  1.00  7.24      A
O
ATOM    470  N   PHE A  65      10.370   4.732  26.791  1.00  7.42      A
N
ATOM    471  CA  PHE A  65      10.851   3.351  26.781  1.00  7.90      A
C
ATOM    472  CB  PHE A  65       9.984   2.524  25.814  1.00  7.36      A
C
ATOM    473  CG  PHE A  65       8.524   2.503  26.185  1.00  7.00      A
C
ATOM    474  CD1 PHE A  65       7.565   3.087  25.352  1.00  7.28      A
C
ATOM    475  CE1 PHE A  65       6.202   3.080  25.720  1.00  7.99      A
C
ATOM    476  CZ  PHE A  65       5.790   2.488  26.920  1.00  6.07      A
C
ATOM    477  CE2 PHE A  65       6.735   1.898  27.749  1.00  6.22      A
C
ATOM    478  CD2 PHE A  65       8.093   1.910  27.392  1.00  6.65      A
C
ATOM    479  C   PHE A  65      12.344   3.277  26.431  1.00  7.30      A
C
ATOM    480  O   PHE A  65      12.819   4.047  25.601  1.00  7.48      A
O
ATOM    481  N   LYS A  66      13.093   2.379  27.059  1.00  8.16      A
N
ATOM    482  CA  LYS A  66      14.534   2.291  26.743  1.00 10.66      A
C
ATOM    483  CB  LYS A  66      15.343   1.715  27.912  1.00 15.40      A
C
ATOM    484  CG  LYS A  66      15.399   2.648  29.114  0.01 40.95      A
C
ATOM    485  CD  LYS A  66      16.559   2.333  30.042  0.01 75.71      A
C
ATOM    486  CE  LYS A  66      16.713   3.419  31.096  1.00196.07      A
C
ATOM    487  NZ  LYS A  66      17.880   3.183  31.991  1.00376.00      A
N
ATOM    488  C   LYS A  66      14.878   1.614  25.381  1.00  7.91      A
C
ATOM    489  O   LYS A  66      15.871   1.952  24.761  1.00  7.58      A
O
ATOM    490  N   TYR A  67      14.045   0.694  24.908  1.00  6.62      A
N
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ATOM    491  CA  TYR A  67      14.338  -0.089  23.706  1.00  6.97      A
C
ATOM    492  CB  TYR A  67      15.545  -1.035  23.925  1.00  7.71      A
C
ATOM    493  CG  TYR A  67      15.202  -2.276  24.727  1.00  8.27      A
C
ATOM    494  CD1 TYR A  67      14.823  -3.463  24.096  1.00  8.13      A
C
ATOM    495  CE1 TYR A  67      14.483  -4.591  24.834  1.00  8.76      A
C
ATOM    496  CZ  TYR A  67      14.516  -4.538  26.226  1.00  9.66      A
C
ATOM    497  OH  TYR A  67      14.196  -5.647  26.984  1.00  9.87      A
O
ATOM    498  CE2 TYR A  67      14.890  -3.370  26.874  1.00  9.90      A
C
ATOM    499  CD2 TYR A  67      15.228  -2.250  26.127  1.00  9.45      A
C
ATOM    500  C   TYR A  67      13.141  -0.929  23.248  1.00  7.29      A
C
ATOM    501  O   TYR A  67      12.194  -1.185  24.006  1.00  8.83      A
O
ATOM    502  N   VAL A  68      13.186  -1.361  21.996  1.00  6.77      A
N
ATOM    503  CA  VAL A  68      12.250  -2.360  21.493  1.00  5.91      A
C
ATOM    504  CB  VAL A  68      11.007  -1.743  20.735  1.00  5.30      A
C
ATOM    505  CG1 VAL A  68      10.240  -0.739  21.589  1.00  4.63      A
C
ATOM    506  CG2 VAL A  68      11.394  -1.104  19.412  1.00  5.28      A
C
ATOM    507  C   VAL A  68      13.099  -3.307  20.630  1.00  5.39      A
C
ATOM    508  O   VAL A  68      14.165  -2.910  20.153  1.00  4.54      A
O
ATOM    509  N   LYS A  69      12.648  -4.555  20.468  1.00  6.06      A
N
ATOM    510  CA  LYS A  69      13.318  -5.529  19.583  1.00  6.09      A
C
ATOM    511  CB  LYS A  69      13.771  -6.801  20.325  1.00  6.75      A
C
ATOM    512  CG  LYS A  69      14.801  -6.531  21.406  1.00  7.53      A
C
ATOM    513  CD  LYS A  69      15.285  -7.784  22.098  1.00  8.44      A
C
ATOM    514  CE  LYS A  69      16.133  -7.395  23.307  1.00 11.62      A
C
ATOM    515  NZ  LYS A  69      16.935  -8.512  23.900  1.00 12.91      A
N
ATOM    516  C   LYS A  69      12.461  -5.877  18.389  1.00  5.61      A
C
ATOM    517  O   LYS A  69      11.361  -6.426  18.517  1.00  5.24      A
O
ATOM    518  N   ASP A  70      12.984  -5.520  17.223  1.00  6.16      A
N
ATOM    519  CA  ASP A  70      12.352  -5.820  15.947  1.00  6.49      A
C
ATOM    520  CB  ASP A  70      12.697  -4.730  14.922  1.00  5.71      A
C
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ATOM    521  CG  ASP A  70      12.038  -3.392  15.238  1.00  5.27      A
C
ATOM    522  OD1 ASP A  70      11.319  -3.284  16.262  1.00  4.76      A
O
ATOM    523  OD2 ASP A  70      12.238  -2.448  14.450  1.00  4.39      A
O
ATOM    524  C   ASP A  70      12.791  -7.189  15.432  1.00  7.18      A
C
ATOM    525  O   ASP A  70      13.994  -7.472  15.376  1.00  7.48      A
O
ATOM    526  N   ARG A  71      11.815  -8.033  15.082  1.00  7.95      A
N
ATOM    527  CA  ARG A  71      12.060  -9.271  14.327  1.00  8.46      A
C
ATOM    528  CB  ARG A  71      11.320 -10.448  14.979  1.00 10.40      A
C
ATOM    529  CG  ARG A  71      10.954 -11.630  14.082  1.00 12.36      A
C
ATOM    530  CD  ARG A  71      10.689 -12.877  14.918  1.00 15.59      A
C
ATOM    531  NE  ARG A  71      11.909 -13.682  15.063  1.00 25.39      A
N
ATOM    532  CZ  ARG A  71      12.209 -14.468  16.104  1.00 30.46      A
C
ATOM    533  NH1 ARG A  71      11.386 -14.569  17.141  1.00 28.00      A
N
ATOM    534  NH2 ARG A  71      13.354 -15.149  16.112  1.00 25.40      A
N
ATOM    535  C   ARG A  71      11.655  -9.075  12.864  1.00  8.08      A
C
ATOM    536  O   ARG A  71      10.524  -8.702  12.594  1.00  8.07      A
O
ATOM    537  N   VAL A  72      12.584  -9.308  11.931  1.00  8.56      A
N
ATOM    538  CA  VAL A  72      12.321  -9.158  10.475  1.00  9.42      A
C
ATOM    539  CB  VAL A  72      13.625  -9.041   9.627  1.00  9.34      A
C
ATOM    540  CG1 VAL A  72      13.305  -8.728   8.164  1.00  8.44      A
C
ATOM    541  CG2 VAL A  72      14.574  -8.004  10.202  1.00  9.84      A
C
ATOM    542  C   VAL A  72      11.568 -10.366   9.923  1.00  8.71      A
C
ATOM    543  O   VAL A  72      12.152 -11.434   9.812  1.00  8.33      A
O
ATOM    544  N   ASP A  73      10.306 -10.175   9.538  1.00  8.10      A
N
ATOM    545  CA  ASP A  73       9.453 -11.269   9.045  1.00  9.00      A
C
ATOM    546  CB  ASP A  73       7.975 -10.997   9.370  1.00  9.57      A
C
ATOM    547  CG  ASP A  73       7.730 -10.748  10.854  1.00 12.15      A
C
ATOM    548  OD1 ASP A  73       8.058 -11.641  11.676  1.00 15.55      A
O
ATOM    549  OD2 ASP A  73       7.192  -9.663  11.206  1.00 11.45      A
O
ATOM    550  C   ASP A  73       9.611 -11.613   7.547  1.00  9.16      A
C
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ATOM    551  O   ASP A  73       9.579 -12.789   7.178  1.00  8.74      A
O
ATOM    552  N   GLU A  74       9.776 -10.599   6.696  1.00  9.52      A
N
ATOM    553  CA  GLU A  74       9.816 -10.805   5.250  1.00  9.69      A
C
ATOM    554  CB  GLU A  74       8.403 -11.080   4.740  1.00 10.03      A
C
ATOM    555  CG  GLU A  74       8.270 -12.298   3.841  1.00 11.05      A
C
ATOM    556  CD  GLU A  74       6.822 -12.716   3.651  1.00 12.26      A
C
ATOM    557  OE1 GLU A  74       5.973 -11.826   3.416  1.00 12.79      A
O
ATOM    558  OE2 GLU A  74       6.527 -13.929   3.749  1.00 12.36      A
O
ATOM    559  C   GLU A  74      10.372  -9.575   4.535  1.00 10.07      A
C
ATOM    560  O   GLU A  74      10.060  -8.454   4.940  1.00  8.85      A
O
ATOM    561  N   VAL A  75      11.182  -9.799   3.482  1.00 10.53      A
N
ATOM    562  CA  VAL A  75      11.783  -8.729   2.639  1.00 11.03      A
C
ATOM    563  CB  VAL A  75      13.274  -8.478   2.960  1.00  9.96      A
C
ATOM    564  CG1 VAL A  75      13.736  -7.199   2.284  1.00 10.97      A
C
ATOM    565  CG2 VAL A  75      13.528  -8.401   4.453  1.00 10.91      A
C
ATOM    566  C   VAL A  75      11.705  -8.999   1.117  1.00 11.86      A
C
ATOM    567  O   VAL A  75      12.264  -9.984   0.627  1.00 11.86      A
O
ATOM    568  N   ASP A  76      11.055  -8.103   0.371  1.00 11.01      A
N
ATOM    569  CA  ASP A  76      10.885  -8.277  -1.072  1.00 12.31      A
C
ATOM    570  CB  ASP A  76       9.406  -8.107  -1.464  1.00 13.03      A
C
ATOM    571  CG  ASP A  76       9.140  -8.364  -2.951  1.00 14.99      A
C
ATOM    572  OD1 ASP A  76      10.095  -8.446  -3.752  1.00 17.74      A
O
ATOM    573  OD2 ASP A  76       7.960  -8.482  -3.330  1.00 15.29      A
O
ATOM    574  C   ASP A  76      11.747  -7.285  -1.837  1.00 12.95      A
C
ATOM    575  O   ASP A  76      11.289  -6.190  -2.131  1.00 16.01      A
O
ATOM    576  N   HIS A  77      12.975  -7.675  -2.183  1.00 12.59      A
N
ATOM    577  CA  HIS A  77      13.949  -6.746  -2.793  1.00 14.45      A
C
ATOM    578  CB  HIS A  77      15.338  -7.366  -2.876  1.00 16.34      A
C
ATOM    579  CG  HIS A  77      16.018  -7.548  -1.545  1.00 14.67      A
C
ATOM    580  ND1 HIS A  77      17.281  -7.127  -1.315  1.00 13.66      A
N
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ATOM    581  CE1 HIS A  77      17.628  -7.440  -0.063  1.00 15.67      A
C
ATOM    582  NE2 HIS A  77      16.583  -8.070   0.516  1.00 18.05      A
N
ATOM    583  CD2 HIS A  77      15.581  -8.155  -0.373  1.00 14.15      A
C
ATOM    584  C   HIS A  77      13.560  -6.281  -4.168  1.00 15.70      A
C
ATOM    585  O   HIS A  77      14.101  -5.296  -4.673  1.00 15.70      A
O
ATOM    586  N   THR A  78      12.643  -7.011  -4.792  1.00 13.13      A
N
ATOM    587  CA  THR A  78      12.063  -6.598  -6.041  1.00 11.34      A
C
ATOM    588  CB  THR A  78      11.504  -7.806  -6.784  1.00 11.08      A
C
ATOM    589  OG1 THR A  78      12.592  -8.667  -7.140  1.00 13.14      A
O
ATOM    590  CG2 THR A  78      10.766  -7.380  -8.035  1.00 12.64      A
C
ATOM    591  C   THR A  78      10.989  -5.528  -5.816  1.00 13.16      A
C
ATOM    592  O   THR A  78      11.177  -4.374  -6.227  1.00 14.98      A
O
ATOM    593  N   ASN A  79       9.893  -5.887  -5.139  1.00 11.90      A
N
ATOM    594  CA  ASN A  79       8.730  -4.989  -5.028  1.00 11.97      A
C
ATOM    595  CB  ASN A  79       7.445  -5.788  -5.021  1.00 11.57      A
C
ATOM    596  CG  ASN A  79       7.141  -6.397  -6.360  1.00 11.84      A
C
ATOM    597  OD1 ASN A  79       7.725  -6.023  -7.388  1.00 11.44      A
O
ATOM    598  ND2 ASN A  79       6.210  -7.346  -6.362  1.00 13.79      A
N
ATOM    599  C   ASN A  79       8.684  -3.945  -3.904  1.00 11.76      A
C
ATOM    600  O   ASN A  79       7.662  -3.284  -3.723  1.00 11.97      A
O
ATOM    601  N   PHE A  80       9.795  -3.781  -3.190  1.00 12.05      A
N
ATOM    602  CA  PHE A  80       9.933  -2.828  -2.076  1.00 12.19      A
C
ATOM    603  CB  PHE A  80       9.941  -1.368  -2.574  1.00 11.58      A
C
ATOM    604  CG  PHE A  80      10.847  -1.112  -3.748  1.00 10.45      A
C
ATOM    605  CD1 PHE A  80      10.389  -0.387  -4.839  1.00 11.30      A
C
ATOM    606  CE1 PHE A  80      11.205  -0.132  -5.937  1.00  9.44      A
C
ATOM    607  CZ  PHE A  80      12.493  -0.618  -5.954  1.00 10.01      A
C
ATOM    608  CE2 PHE A  80      12.976  -1.337  -4.868  1.00 12.39      A
C
ATOM    609  CD2 PHE A  80      12.155  -1.581  -3.769  1.00 12.20      A
C
ATOM    610  C   PHE A  80       8.898  -3.008  -0.944  1.00 13.56      A
C
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ATOM    611  O   PHE A  80       8.430  -2.010  -0.388  1.00 11.54      A
O
ATOM    612  N   LYS A  81       8.544  -4.275  -0.644  1.00 14.70      A
N
ATOM    613  CA  LYS A  81       7.748  -4.684   0.526  1.00 12.94      A
C
ATOM    614  CB  LYS A  81       6.776  -5.825   0.188  0.01 16.62      A
C
ATOM    615  CG  LYS A  81       7.297  -7.188   0.635  0.01 20.03      A
C
ATOM    616  CD  LYS A  81       6.279  -8.310   0.686  0.01 24.92      A
C
ATOM    617  CE  LYS A  81       6.900  -9.511   1.394  1.00 34.17      A
C
ATOM    618  NZ  LYS A  81       6.433 -10.800   0.811  1.00 40.49      A
N
ATOM    619  C   LYS A  81       8.710  -5.173   1.615  1.00 12.98      A
C
ATOM    620  O   LYS A  81       9.721  -5.804   1.304  1.00 11.68      A
O
ATOM    621  N   TYR A  82       8.366  -4.925   2.880  1.00 12.15      A
N
ATOM    622  CA  TYR A  82       9.206  -5.281   4.031  1.00 10.40      A
C
ATOM    623  CB  TYR A  82      10.200  -4.150   4.270  1.00 11.01      A
C
ATOM    624  CG  TYR A  82      11.109  -4.336   5.464  1.00 12.59      A
C
ATOM    625  CD1 TYR A  82      12.112  -5.303   5.443  1.00 14.55      A
C
ATOM    626  CE1 TYR A  82      12.960  -5.478   6.517  1.00 13.08      A
C
ATOM    627  CZ  TYR A  82      12.824  -4.671   7.620  1.00 12.04      A
C
ATOM    628  OH  TYR A  82      13.692  -4.880   8.650  1.00 14.36      A
O
ATOM    629  CE2 TYR A  82      11.848  -3.689   7.680  1.00 10.89      A
C
ATOM    630  CD2 TYR A  82      10.993  -3.526   6.602  1.00 11.23      A
C
ATOM    631  C   TYR A  82       8.391  -5.546   5.323  1.00 10.83      A
C
ATOM    632  O   TYR A  82       7.738  -4.641   5.863  1.00 11.68      A
O
ATOM    633  N   ASN A  83       8.425  -6.774   5.831  1.00 10.16      A
N
ATOM    634  CA  ASN A  83       7.671  -7.080   7.057  1.00 10.81      A
C
ATOM    635  CB  ASN A  83       6.608  -8.159   6.808  1.00 11.09      A
C
ATOM    636  CG  ASN A  83       5.747  -7.862   5.574  1.00 13.56      A
C
ATOM    637  OD1 ASN A  83       6.273  -7.659   4.474  1.00 14.94      A
O
ATOM    638  ND2 ASN A  83       4.422  -7.855   5.746  1.00 11.30      A
N
ATOM    639  C   ASN A  83       8.529  -7.386   8.293  1.00 10.01      A
C
ATOM    640  O   ASN A  83       9.462  -8.186   8.243  1.00 10.98      A
O
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ATOM    641  N   TYR A  84       8.229  -6.693   9.388  1.00  9.45      A
N
ATOM    642  CA  TYR A  84       8.843  -6.963  10.691  1.00  8.78      A
C
ATOM    643  CB  TYR A  84       9.988  -5.982  10.989  1.00  7.95      A
C
ATOM    644  CG  TYR A  84       9.558  -4.566  11.305  1.00  6.79      A
C
ATOM    645  CD1 TYR A  84       9.308  -3.655  10.280  1.00  6.47      A
C
ATOM    646  CE1 TYR A  84       8.926  -2.356  10.554  1.00  6.29      A
C
ATOM    647  CZ  TYR A  84       8.788  -1.943  11.869  1.00  6.24      A
C
ATOM    648  OH  TYR A  84       8.391  -0.654  12.114  1.00  5.74      A
O
ATOM    649  CE2 TYR A  84       9.041  -2.822  12.912  1.00  6.51      A
C
ATOM    650  CD2 TYR A  84       9.432  -4.128  12.626  1.00  6.40      A
C
ATOM    651  C   TYR A  84       7.797  -6.909  11.795  1.00  8.32      A
C
ATOM    652  O   TYR A  84       6.751  -6.277  11.636  1.00 10.00      A
O
ATOM    653  N   SER A  85       8.083  -7.579  12.902  1.00  8.08      A
N
ATOM    654  CA  SER A  85       7.281  -7.455  14.109  1.00  9.13      A
C
ATOM    655  CB  SER A  85       6.753  -8.828  14.532  1.00 10.21      A
C
ATOM    656  OG  SER A  85       5.839  -9.337  13.573  1.00 12.15      A
O
ATOM    657  C   SER A  85       8.069  -6.833  15.257  1.00  8.86      A
C
ATOM    658  O   SER A  85       9.279  -7.002  15.349  1.00  9.51      A
O
ATOM    659  N   VAL A  86       7.389  -6.118  16.143  1.00  9.57      A
N
ATOM    660  CA  VAL A  86       8.019  -5.710  17.398  1.00  9.94      A
C
ATOM    661  CB  VAL A  86       7.485  -4.361  17.910  1.00  9.34      A
C
ATOM    662  CG1 VAL A  86       8.063  -4.023  19.283  1.00  9.56      A
C
ATOM    663  CG2 VAL A  86       7.821  -3.265  16.921  1.00  9.86      A
C
ATOM    664  C   VAL A  86       7.754  -6.800  18.425  1.00 10.78      A
C
ATOM    665  O   VAL A  86       6.633  -6.945  18.906  1.00 13.21      A
O
ATOM    666  N   ILE A  87       8.777  -7.565  18.772  1.00 11.49      A
N
ATOM    667  CA  ILE A  87       8.542  -8.718  19.639  1.00 13.01      A
C
ATOM    668  CB  ILE A  87       9.268  -9.978  19.117  1.00 12.31      A
C
ATOM    669  CG1 ILE A  87      10.672  -9.634  18.604  1.00 13.66      A
C
ATOM    670  CD1 ILE A  87      11.663 -10.791  18.636  1.00 13.91      A
C
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ATOM    671  CG2 ILE A  87       8.427 -10.653  18.047  1.00 10.37      A
C
ATOM    672  C   ILE A  87       8.745  -8.541  21.169  1.00 15.12      A
C
ATOM    673  O   ILE A  87       8.322  -9.390  21.960  1.00 15.38      A
O
ATOM    674  N   GLU A  88       9.348  -7.428  21.580  1.00 17.11      A
N
ATOM    675  CA  GLU A  88       9.731  -7.207  22.978  1.00 16.42      A
C
ATOM    676  CB  GLU A  88      10.932  -8.100  23.334  1.00 18.45      A
C
ATOM    677  CG  GLU A  88      11.545  -7.880  24.712  1.00 18.36      A
C
ATOM    678  CD  GLU A  88      12.835  -8.656  24.918  1.00 19.56      A
C
ATOM    679  OE1 GLU A  88      12.872  -9.858  24.564  1.00 20.88      A
O
ATOM    680  OE2 GLU A  88      13.812  -8.069  25.441  1.00 18.20      A
O
ATOM    681  C   GLU A  88      10.088  -5.741  23.238  1.00 17.27      A
C
ATOM    682  O   GLU A  88      10.367  -4.982  22.310  1.00 17.38      A
O
ATOM    683  N   GLY A  89      10.097  -5.359  24.512  1.00 17.26      A
N
ATOM    684  CA  GLY A  89      10.445  -4.011  24.908  1.00 17.82      A
C
ATOM    685  C   GLY A  89       9.213  -3.155  24.871  1.00 18.12      A
C
ATOM    686  O   GLY A  89       8.154  -3.611  24.458  1.00 20.97      A
O
ATOM    687  N   GLY A  90       9.346  -1.910  25.306  1.00 19.61      A
N
ATOM    688  CA  GLY A  90       8.183  -1.037  25.474  1.00 19.95      A
C
ATOM    689  C   GLY A  90       6.970  -1.661  26.164  1.00 18.40      A
C
ATOM    690  O   GLY A  90       7.108  -2.432  27.137  1.00 18.31      A
O
ATOM    691  N   PRO A  91       5.769  -1.321  25.668  1.00 17.97      A
N
ATOM    692  CA  PRO A  91       4.471  -1.812  26.155  1.00 20.04      A
C
ATOM    693  CB  PRO A  91       3.453  -1.028  25.317  1.00 19.71      A
C
ATOM    694  CG  PRO A  91       4.201   0.146  24.784  1.00 20.17      A
C
ATOM    695  CD  PRO A  91       5.609  -0.325  24.596  1.00 17.26      A
C
ATOM    696  C   PRO A  91       4.267  -3.304  25.915  1.00 21.19      A
C
ATOM    697  O   PRO A  91       3.375  -3.912  26.521  1.00 18.91      A
O
ATOM    698  N   VAL A  92       5.078  -3.891  25.037  1.00 21.15      A
N
ATOM    699  CA  VAL A  92       4.896  -5.289  24.686  1.00 21.81      A
C
ATOM    700  CB  VAL A  92       5.966  -5.808  23.721  1.00 21.89      A
C
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ATOM    701  CG1 VAL A  92       5.765  -7.289  23.461  1.00 23.09      A
C
ATOM    702  CG2 VAL A  92       5.899  -5.043  22.406  1.00 22.55      A
C
ATOM    703  C   VAL A  92       4.785  -6.125  25.951  1.00 21.72      A
C
ATOM    704  O   VAL A  92       3.821  -6.854  26.115  1.00 26.63      A
O
ATOM    705  N   GLY A  93       5.739  -5.982  26.861  1.00 27.31      A
N
ATOM    706  CA  GLY A  93       5.598  -6.538  28.220  1.00 31.41      A
C
ATOM    707  C   GLY A  93       4.175  -6.618  28.777  1.00 27.25      A
C
ATOM    708  O   GLY A  93       3.685  -7.712  29.041  1.00 25.44      A
O
ATOM    709  N   ASP A  94       3.502  -5.473  28.932  1.00 27.73      A
N
ATOM    710  CA  ASP A  94       2.187  -5.412  29.599  1.00 25.30      A
C
ATOM    711  CB  ASP A  94       1.944  -4.050  30.280  1.00 25.25      A
C
ATOM    712  CG  ASP A  94       3.122  -3.547  31.050  1.00 24.53      A
C
ATOM    713  OD1 ASP A  94       4.248  -3.563  30.518  1.00 32.13      A
O
ATOM    714  OD2 ASP A  94       2.908  -3.095  32.187  1.00 28.31      A
O
ATOM    715  C   ASP A  94       1.012  -5.594  28.659  1.00 25.43      A
C
ATOM    716  O   ASP A  94       0.495  -6.695  28.459  1.00 24.87      A
O
ATOM    717  N   THR A  95       0.600  -4.456  28.108  1.00 23.84      A
N
ATOM    718  CA  THR A  95      -0.672  -4.283  27.433  1.00 23.15      A
C
ATOM    719  CB  THR A  95      -1.017  -2.782  27.353  1.00 21.59      A
C
ATOM    720  OG1 THR A  95       0.060  -2.079  26.738  1.00 18.44      A
O
ATOM    721  CG2 THR A  95      -1.245  -2.199  28.740  1.00 20.27      A
C
ATOM    722  C   THR A  95      -0.747  -4.920  26.035  1.00 22.93      A
C
ATOM    723  O   THR A  95      -1.827  -5.301  25.585  1.00 20.82      A
O
ATOM    724  N   LEU A  96       0.396  -5.028  25.360  1.00 24.76      A
N
ATOM    725  CA  LEU A  96       0.457  -5.599  24.013  1.00 21.81      A
C
ATOM    726  CB  LEU A  96       1.263  -4.677  23.100  1.00 21.00      A
C
ATOM    727  CG  LEU A  96       0.733  -3.257  22.903  1.00 21.47      A
C
ATOM    728  CD1 LEU A  96       1.765  -2.382  22.204  1.00 18.81      A
C
ATOM    729  CD2 LEU A  96      -0.581  -3.292  22.134  1.00 22.83      A
C
ATOM    730  C   LEU A  96       1.059  -7.009  23.979  1.00 23.96      A
C
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ATOM    731  O   LEU A  96       1.619  -7.492  24.961  1.00 25.69      A
O
ATOM    732  N   GLU A  97       0.936  -7.676  22.842  1.00 23.53      A
N
ATOM    733  CA  GLU A  97       1.614  -8.951  22.647  1.00 20.98      A
C
ATOM    734  CB  GLU A  97       0.612 -10.050  22.323  1.00 21.69      A
C
ATOM    735  CG  GLU A  97      -0.305 -10.346  23.487  1.00 21.04      A
C
ATOM    736  CD  GLU A  97      -1.160 -11.560  23.266  1.00 23.83      A
C
ATOM    737  OE1 GLU A  97      -1.369 -11.931  22.094  1.00 26.19      A
O
ATOM    738  OE2 GLU A  97      -1.634 -12.129  24.269  1.00 26.93      A
O
ATOM    739  C   GLU A  97       2.651  -8.810  21.546  1.00 20.56      A
C
ATOM    740  O   GLU A  97       3.827  -9.143  21.743  1.00 16.80      A
O
ATOM    741  N   LYS A  98       2.200  -8.298  20.397  1.00 17.79      A
N
ATOM    742  CA  LYS A  98       3.062  -7.991  19.258  1.00 13.99      A
C
ATOM    743  CB  LYS A  98       2.955  -9.065  18.148  1.00 15.42      A
C
ATOM    744  CG  LYS A  98       3.341 -10.482  18.530  1.00 18.43      A
C
ATOM    745  CD  LYS A  98       4.806 -10.548  18.934  1.00 24.84      A
C
ATOM    746  CE  LYS A  98       5.019 -11.482  20.118  1.00 24.66      A
C
ATOM    747  NZ  LYS A  98       6.042 -10.918  21.049  1.00 24.30      A
N
ATOM    748  C   LYS A  98       2.631  -6.673  18.655  1.00 13.07      A
C
ATOM    749  O   LYS A  98       1.550  -6.137  18.951  1.00 11.77      A
O
ATOM    750  N   ILE A  99       3.511  -6.162  17.807  1.00 12.11      A
N
ATOM    751  CA  ILE A  99       3.180  -5.183  16.798  1.00 10.43      A
C
ATOM    752  CB  ILE A  99       3.889  -3.821  17.060  1.00  9.67      A
C
ATOM    753  CG1 ILE A  99       3.382  -3.185  18.368  1.00  8.54      A
C
ATOM    754  CD1 ILE A  99       4.093  -1.914  18.781  1.00  8.36      A
C
ATOM    755  CG2 ILE A  99       3.703  -2.868  15.882  1.00  8.82      A
C
ATOM    756  C   ILE A  99       3.648  -5.831  15.491  1.00 10.27      A
C
ATOM    757  O   ILE A  99       4.812  -6.212  15.368  1.00 10.48      A
O
ATOM    758  N   SER A 100       2.733  -6.005  14.544  1.00  9.62      A
N
ATOM    759  CA  SER A 100       3.088  -6.500  13.223  1.00  9.09      A
C
ATOM    760  CB  SER A 100       2.241  -7.713  12.861  1.00  8.85      A
C
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ATOM    761  OG  SER A 100       2.765  -8.876  13.460  1.00  9.62      A
O
ATOM    762  C   SER A 100       2.941  -5.408  12.170  1.00  8.98      A
C
ATOM    763  O   SER A 100       1.843  -4.901  11.935  1.00  8.46      A
O
ATOM    764  N   ASN A 101       4.056  -5.062  11.533  1.00  9.08      A
N
ATOM    765  CA  ASN A 101       4.094  -3.935  10.605  1.00  8.93      A
C
ATOM    766  CB  ASN A 101       5.098  -2.895  11.072  1.00  8.92      A
C
ATOM    767  CG  ASN A 101       4.850  -2.452  12.483  1.00  9.61      A
C
ATOM    768  OD1 ASN A 101       3.728  -2.099  12.853  1.00  9.08      A
O
ATOM    769  ND2 ASN A 101       5.901  -2.481  13.293  1.00 10.42      A
N
ATOM    770  C   ASN A 101       4.436  -4.303   9.183  1.00  8.76      A
C
ATOM    771  O   ASN A 101       4.915  -5.400   8.918  1.00  9.51      A
O
ATOM    772  N   GLU A 102       4.207  -3.352   8.281  1.00  7.99      A
N
ATOM    773  CA  GLU A 102       4.499  -3.521   6.868  1.00  7.82      A
C
ATOM    774  CB  GLU A 102       3.297  -4.142   6.151  1.00  7.14      A
C
ATOM    775  CG  GLU A 102       3.687  -4.912   4.908  1.00  7.46      A
C
ATOM    776  CD  GLU A 102       2.607  -4.908   3.859  1.00  7.65      A
C
ATOM    777  OE1 GLU A 102       1.869  -5.925   3.786  1.00  6.81      A
O
ATOM    778  OE2 GLU A 102       2.507  -3.891   3.114  1.00  7.72      A
O
ATOM    779  C   GLU A 102       4.855  -2.188   6.211  1.00  7.72      A
C
ATOM    780  O   GLU A 102       4.249  -1.155   6.513  1.00  7.89      A
O
ATOM    781  N   ILE A 103       5.833  -2.206   5.309  1.00  7.84      A
N
ATOM    782  CA  ILE A 103       6.118  -1.017   4.494  1.00  8.71      A
C
ATOM    783  CB  ILE A 103       7.410  -0.285   4.955  1.00  9.52      A
C
ATOM    784  CG1 ILE A 103       7.349  -0.007   6.474  1.00  8.29      A
C
ATOM    785  CD1 ILE A 103       8.688   0.092   7.160  1.00  8.06      A
C
ATOM    786  CG2 ILE A 103       7.599   1.021   4.171  1.00  8.39      A
C
ATOM    787  C   ILE A 103       6.156  -1.355   3.004  1.00  8.41      A
C
ATOM    788  O   ILE A 103       6.853  -2.274   2.595  1.00  9.19      A
O
ATOM    789  N   LYS A 104       5.375  -0.639   2.210  1.00  8.28      A
N
ATOM    790  CA  LYS A 104       5.396  -0.803   0.783  1.00 10.54      A
C
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ATOM    791  CB  LYS A 104       4.005  -1.188   0.268  0.01 22.56      A
C
ATOM    792  CG  LYS A 104       3.970  -1.678  -1.172  0.01 42.15      A
C
ATOM    793  CD  LYS A 104       2.554  -2.049  -1.589  0.01 76.34      A
C
ATOM    794  CE  LYS A 104       2.512  -2.595  -3.008  1.00195.58      A
C
ATOM    795  NZ  LYS A 104       1.125  -2.943  -3.433  1.00262.91      A
N
ATOM    796  C   LYS A 104       5.820   0.538   0.238  1.00  8.40      A
C
ATOM    797  O   LYS A 104       5.176   1.544   0.504  1.00  7.52      A
O
ATOM    798  N   ILE A 105       6.918   0.571  -0.508  1.00  7.42      A
N
ATOM    799  CA  ILE A 105       7.349   1.823  -1.144  1.00  6.36      A
C
ATOM    800  CB  ILE A 105       8.820   2.174  -0.843  1.00  6.28      A
C
ATOM    801  CG1 ILE A 105       9.174   1.800   0.619  1.00  5.43      A
C
ATOM    802  CD1 ILE A 105      10.371   2.509   1.208  1.00  4.88      A
C
ATOM    803  CG2 ILE A 105       9.085   3.635  -1.201  1.00  6.03      A
C
ATOM    804  C   ILE A 105       7.055   1.839  -2.648  1.00  5.84      A
C
ATOM    805  O   ILE A 105       7.531   0.988  -3.408  1.00  5.41      A
O
ATOM    806  N   VAL A 106       6.247   2.811  -3.055  1.00  5.89      A
N
ATOM    807  CA  VAL A 106       5.725   2.876  -4.421  1.00  6.32      A
C
ATOM    808  CB  VAL A 106       4.199   2.708  -4.446  1.00  5.90      A
C
ATOM    809  CG1 VAL A 106       3.830   1.378  -3.811  1.00  6.56      A
C
ATOM    810  CG2 VAL A 106       3.530   3.844  -3.702  1.00  5.88      A
C
ATOM    811  C   VAL A 106       6.119   4.142  -5.183  1.00  6.77      A
C
ATOM    812  O   VAL A 106       6.081   5.264  -4.642  1.00  6.90      A
O
ATOM    813  N   ALA A 107       6.483   3.950  -6.448  1.00  6.43      A
N
ATOM    814  CA  ALA A 107       6.963   5.040  -7.280  1.00  7.55      A
C
ATOM    815  CB  ALA A 107       7.650   4.485  -8.513  1.00  7.60      A
C
ATOM    816  C   ALA A 107       5.902   6.060  -7.692  1.00  8.47      A
C
ATOM    817  O   ALA A 107       4.820   5.692  -8.166  1.00  9.14      A
O
ATOM    818  N   THR A 108       6.223   7.342  -7.526  1.00  9.87      A
N
ATOM    819  CA  THR A 108       5.499   8.390  -8.264  1.00 12.89      A
C
ATOM    820  CB  THR A 108       5.431   9.741  -7.496  1.00 12.13      A
C
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ATOM    821  OG1 THR A 108       6.653  10.467  -7.676  1.00 13.49      A
O
ATOM    822  CG2 THR A 108       5.188   9.533  -6.008  1.00 12.58      A
C
ATOM    823  C   THR A 108       6.175   8.598  -9.650  1.00 13.28      A
C
ATOM    824  O   THR A 108       7.380   8.339  -9.784  1.00 11.42      A
O
ATOM    825  N   PRO A 109       5.407   9.065 -10.668  1.00 11.82      A
N
ATOM    826  CA  PRO A 109       5.945   9.583 -11.943  1.00 12.03      A
C
ATOM    827  CB  PRO A 109       4.701  10.072 -12.692  1.00 11.68      A
C
ATOM    828  CG  PRO A 109       3.562   9.373 -12.063  1.00 12.76      A
C
ATOM    829  CD  PRO A 109       3.937   9.147 -10.627  1.00 12.49      A
C
ATOM    830  C   PRO A 109       6.915  10.769 -11.792  1.00 12.08      A
C
ATOM    831  O   PRO A 109       7.606  11.093 -12.752  1.00 12.10      A
O
ATOM    832  N   ASP A 110       6.923  11.411 -10.616  1.00 13.99      A
N
ATOM    833  CA  ASP A 110       7.895  12.452 -10.208  1.00 14.67      A
C
ATOM    834  CB  ASP A 110       7.712  12.806  -8.718  1.00 16.40      A
C
ATOM    835  CG  ASP A 110       6.515  13.656  -8.443  1.00 16.90      A
C
ATOM    836  OD1 ASP A 110       6.334  14.678  -9.135  1.00 21.54      A
O
ATOM    837  OD2 ASP A 110       5.775  13.314  -7.501  1.00 15.73      A
O
ATOM    838  C   ASP A 110       9.346  12.016 -10.284  1.00 13.61      A
C
ATOM    839  O   ASP A 110      10.242  12.850 -10.449  1.00 12.86      A
O
ATOM    840  N   GLY A 111       9.572  10.717 -10.078  1.00 13.43      A
N
ATOM    841  CA  GLY A 111      10.874  10.208  -9.655  1.00 12.02      A
C
ATOM    842  C   GLY A 111      10.971  10.274  -8.137  1.00 13.38      A
C
ATOM    843  O   GLY A 111      12.052  10.133  -7.558  1.00 13.71      A
O
ATOM    844  N   GLY A 112       9.831  10.515  -7.492  1.00 12.90      A
N
ATOM    845  CA  GLY A 112       9.736  10.493  -6.040  1.00 12.59      A
C
ATOM    846  C   GLY A 112       9.143   9.165  -5.609  1.00 12.65      A
C
ATOM    847  O   GLY A 112       9.223   8.174  -6.337  1.00 12.27      A
O
ATOM    848  N   CYS A 113       8.541   9.130  -4.428  1.00 11.19      A
N
ATOM    849  CA  CYS A 113       7.929   7.894  -3.986  1.00 11.22      A
C
ATOM    850  CB  CYS A 113       8.994   6.825  -3.638  1.00 11.46      A
C
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ATOM    851  SG  CYS A 113       9.942   7.002  -2.097  1.00 11.28      A
S
ATOM    852  C   CYS A 113       6.971   8.142  -2.845  1.00 10.69      A
C
ATOM    853  O   CYS A 113       6.985   9.219  -2.250  1.00 10.00      A
O
ATOM    854  N   VAL A 114       6.118   7.150  -2.591  1.00 10.97      A
N
ATOM    855  CA  VAL A 114       5.194   7.130  -1.453  1.00 11.47      A
C
ATOM    856  CB  VAL A 114       3.706   7.153  -1.905  1.00 10.24      A
C
ATOM    857  CG1 VAL A 114       2.771   6.961  -0.724  1.00  9.87      A
C
ATOM    858  CG2 VAL A 114       3.358   8.443  -2.632  1.00  9.55      A
C
ATOM    859  C   VAL A 114       5.463   5.847  -0.661  1.00 11.30      A
C
ATOM    860  O   VAL A 114       5.648   4.777  -1.246  1.00 11.21      A
O
ATOM    861  N   LEU A 115       5.481   5.963   0.666  1.00 11.87      A
N
ATOM    862  CA  LEU A 115       5.664   4.810   1.564  1.00 10.54      A
C
ATOM    863  CB  LEU A 115       6.732   5.109   2.635  1.00 10.85      A
C
ATOM    864  CG  LEU A 115       8.205   5.431   2.281  1.00 10.17      A
C
ATOM    865  CD1 LEU A 115       8.372   6.561   1.267  1.00 12.22      A
C
ATOM    866  CD2 LEU A 115       9.009   5.762   3.528  1.00  9.34      A
C
ATOM    867  C   LEU A 115       4.327   4.456   2.214  1.00  9.12      A
C
ATOM    868  O   LEU A 115       3.663   5.318   2.762  1.00 10.37      A
O
ATOM    869  N   LYS A 116       3.915   3.199   2.118  1.00  8.59      A
N
ATOM    870  CA  LYS A 116       2.656   2.753   2.724  1.00  8.80      A
C
ATOM    871  CB  LYS A 116       1.814   1.938   1.723  1.00  9.67      A
C
ATOM    872  CG  LYS A 116       1.415   2.697   0.459  1.00  9.19      A
C
ATOM    873  CD  LYS A 116       0.431   1.906  -0.391  1.00  9.57      A
C
ATOM    874  CE  LYS A 116       0.178   2.553  -1.754  1.00  9.88      A
C
ATOM    875  NZ  LYS A 116      -0.562   3.848  -1.684  1.00 10.25      A
N
ATOM    876  C   LYS A 116       2.951   1.958   3.999  1.00  8.23      A
C
ATOM    877  O   LYS A 116       3.694   0.976   3.983  1.00  8.33      A
O
ATOM    878  N   ILE A 117       2.389   2.401   5.115  1.00  7.66      A
N
ATOM    879  CA  ILE A 117       2.767   1.847   6.410  1.00  7.09      A
C
ATOM    880  CB  ILE A 117       3.573   2.870   7.274  1.00  7.57      A
C
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ATOM    881  CG1 ILE A 117       4.664   3.591   6.434  1.00  6.58      A
C
ATOM    882  CD1 ILE A 117       5.641   4.472   7.190  1.00  5.53      A
C
ATOM    883  CG2 ILE A 117       4.124   2.204   8.537  1.00  7.36      A
C
ATOM    884  C   ILE A 117       1.525   1.349   7.147  1.00  6.99      A
C
ATOM    885  O   ILE A 117       0.617   2.119   7.460  1.00  6.84      A
O
ATOM    886  N   SER A 118       1.481   0.043   7.385  1.00  6.95      A
N
ATOM    887  CA  SER A 118       0.416  -0.580   8.175  1.00  6.49      A
C
ATOM    888  CB  SER A 118      -0.213  -1.767   7.412  1.00  6.78      A
C
ATOM    889  OG  SER A 118      -0.674  -2.796   8.284  1.00  6.15      A
O
ATOM    890  C   SER A 118       1.006  -1.017   9.508  1.00  5.97      A
C
ATOM    891  O   SER A 118       2.082  -1.611   9.536  1.00  5.46      A
O
ATOM    892  N   ASN A 119       0.320  -0.672  10.601  1.00  5.95      A
N
ATOM    893  CA  ASN A 119       0.676  -1.137  11.943  1.00  5.95      A
C
ATOM    894  CB  ASN A 119       0.961   0.031  12.909  1.00  5.95      A
C
ATOM    895  CG  ASN A 119       1.979   1.043  12.372  1.00  6.54      A
C
ATOM    896  OD1 ASN A 119       1.714   2.259  12.357  1.00  6.16      A
O
ATOM    897  ND2 ASN A 119       3.165   0.558  11.969  1.00  6.59      A
N
ATOM    898  C   ASN A 119      -0.473  -1.961  12.510  1.00  6.10      A
C
ATOM    899  O   ASN A 119      -1.562  -1.433  12.710  1.00  6.17      A
O
ATOM    900  N   LYS A 120      -0.242  -3.246  12.766  1.00  7.06      A
N
ATOM    901  CA  LYS A 120      -1.197  -4.053  13.530  1.00  7.81      A
C
ATOM    902  CB  LYS A 120      -1.357  -5.443  12.919  1.00  9.21      A
C
ATOM    903  CG  LYS A 120      -1.715  -5.452  11.442  1.00 11.96      A
C
ATOM    904  CD  LYS A 120      -2.330  -6.786  11.028  1.00 15.40      A
C
ATOM    905  CE  LYS A 120      -2.942  -6.721   9.633  1.00 16.92      A
C
ATOM    906  NZ  LYS A 120      -4.360  -7.201   9.585  1.00 17.62      A
N
ATOM    907  C   LYS A 120      -0.767  -4.157  15.004  1.00  7.27      A
C
ATOM    908  O   LYS A 120       0.347  -4.582  15.305  1.00  6.62      A
O
ATOM    909  N   TYR A 121      -1.639  -3.753  15.921  1.00  7.48      A
N
ATOM    910  CA  TYR A 121      -1.319  -3.872  17.346  1.00  9.44      A
C
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ATOM    911  CB  TYR A 121      -1.562  -2.556  18.094  1.00  9.63      A
C
ATOM    912  CG  TYR A 121      -0.782  -1.378  17.573  1.00  9.28      A
C
ATOM    913  CD1 TYR A 121      -1.288  -0.597  16.544  1.00  9.86      A
C
ATOM    914  CE1 TYR A 121      -0.591   0.495  16.056  1.00 10.64      A
C
ATOM    915  CZ  TYR A 121       0.630   0.829  16.611  1.00 12.65      A
C
ATOM    916  OH  TYR A 121       1.309   1.934  16.114  1.00 13.15      A
O
ATOM    917  CE2 TYR A 121       1.154   0.064  17.651  1.00 10.83      A
C
ATOM    918  CD2 TYR A 121       0.444  -1.027  18.125  1.00  9.87      A
C
ATOM    919  C   TYR A 121      -2.088  -5.003  18.020  1.00  9.51      A
C
ATOM    920  O   TYR A 121      -3.317  -4.954  18.105  1.00 11.45      A
O
ATOM    921  N   HIS A 122      -1.356  -6.009  18.500  1.00  9.76      A
N
ATOM    922  CA  HIS A 122      -1.955  -7.177  19.131  1.00 11.54      A
C
ATOM    923  CB  HIS A 122      -1.169  -8.446  18.779  1.00 13.05      A
C
ATOM    924  CG  HIS A 122      -1.330  -8.899  17.338  1.00 14.51      A
C
ATOM    925  ND1 HIS A 122      -0.493  -8.511  16.351  1.00 15.61      A
N
ATOM    926  CE1 HIS A 122      -0.882  -9.066  15.182  1.00 14.34      A
C
ATOM    927  NE2 HIS A 122      -1.965  -9.817  15.421  1.00 15.47      A
N
ATOM    928  CD2 HIS A 122      -2.269  -9.737  16.743  1.00 15.19      A
C
ATOM    929  C   HIS A 122      -2.027  -6.968  20.613  1.00 12.31      A
C
ATOM    930  O   HIS A 122      -1.034  -7.101  21.315  1.00 15.87      A
O
ATOM    931  N   THR A 123      -3.206  -6.617  21.111  1.00 15.17      A
N
ATOM    932  CA  THR A 123      -3.357  -6.295  22.537  1.00 16.19      A
C
ATOM    933  CB  THR A 123      -4.611  -5.462  22.812  1.00 14.85      A
C
ATOM    934  OG1 THR A 123      -5.757  -6.165  22.326  1.00 18.73      A
O
ATOM    935  CG2 THR A 123      -4.510  -4.117  22.135  1.00 16.04      A
C
ATOM    936  C   THR A 123      -3.414  -7.518  23.439  1.00 17.75      A
C
ATOM    937  O   THR A 123      -3.703  -8.633  22.991  1.00 18.47      A
O
ATOM    938  N   LYS A 124      -3.122  -7.293  24.716  1.00 20.30      A
N
ATOM    939  CA  LYS A 124      -3.205  -8.327  25.738  1.00 20.58      A
C
ATOM    940  CB  LYS A 124      -2.015  -8.242  26.696  1.00 22.30      A
C
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ATOM    941  CG  LYS A 124      -0.778  -9.006  26.274  1.00 21.83      A
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ATOM    942  CD  LYS A 124       0.283  -8.975  27.361  1.00 21.11      A
C
ATOM    943  CE  LYS A 124       0.165 -10.151  28.312  1.00 26.43      A
C
ATOM    944  NZ  LYS A 124       0.655 -11.416  27.683  1.00 44.62      A
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ATOM    945  C   LYS A 124      -4.468  -8.065  26.516  1.00 22.03      A
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ATOM    946  O   LYS A 124      -4.750  -6.914  26.861  1.00 25.72      A
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ATOM    947  N   GLY A 125      -5.225  -9.119  26.805  1.00 21.51      A
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ATOM    948  CA  GLY A 125      -6.416  -8.969  27.623  1.00 22.31      A
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ATOM    949  C   GLY A 125      -7.336  -8.002  26.918  1.00 24.38      A
C
ATOM    950  O   GLY A 125      -7.651  -8.207  25.740  1.00 26.41      A
O
ATOM    951  N   ASN A 126      -7.735  -6.934  27.614  1.00 22.20      A
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ATOM    952  CA  ASN A 126      -8.710  -5.978  27.061  1.00 22.40      A
C
ATOM    953  CB  ASN A 126     -10.040  -6.060  27.807  1.00 21.89      A
C
ATOM    954  CG  ASN A 126      -9.950  -5.494  29.210  1.00 22.43      A
C
ATOM    955  OD1 ASN A 126      -8.857  -5.217  29.706  1.00 20.64      A
O
ATOM    956  ND2 ASN A 126     -11.102  -5.316  29.857  1.00 25.60      A
N
ATOM    957  C   ASN A 126      -8.261  -4.523  27.023  1.00 21.44      A
C
ATOM    958  O   ASN A 126      -9.103  -3.624  26.992  1.00 20.70      A
O
ATOM    959  N   HIS A 127      -6.948  -4.300  27.044  1.00 20.27      A
N
ATOM    960  CA  HIS A 127      -6.359  -2.999  26.732  1.00 19.59      A
C
ATOM    961  CB  HIS A 127      -4.837  -3.129  26.696  1.00 23.09      A
C
ATOM    962  CG  HIS A 127      -4.090  -1.820  26.482  1.00 20.72      A
C
ATOM    963  ND1 HIS A 127      -4.073  -0.832  27.395  1.00 19.56      A
N
ATOM    964  CE1 HIS A 127      -3.309   0.181  26.950  1.00 17.65      A
C
ATOM    965  NE2 HIS A 127      -2.817  -0.166  25.752  1.00 18.22      A
N
ATOM    966  CD2 HIS A 127      -3.274  -1.397  25.436  1.00 20.31      A
C
ATOM    967  C   HIS A 127      -6.866  -2.561  25.389  1.00 21.11      A
C
ATOM    968  O   HIS A 127      -7.222  -3.408  24.546  1.00 19.19      A
O
ATOM    969  N   GLU A 128      -6.895  -1.240  25.177  1.00 21.07      A
N
ATOM    970  CA  GLU A 128      -7.390  -0.638  23.933  1.00 19.50      A
C
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ATOM    971  CB  GLU A 128      -8.373   0.489  24.244  1.00 18.87      A
C
ATOM    972  CG  GLU A 128      -8.908   1.248  23.043  1.00 19.90      A
C
ATOM    973  CD  GLU A 128      -9.922   2.307  23.427  1.00 17.74      A
C
ATOM    974  OE1 GLU A 128     -10.292   3.118  22.555  1.00 17.13      A
O
ATOM    975  OE2 GLU A 128     -10.346   2.332  24.601  1.00 20.26      A
O
ATOM    976  C   GLU A 128      -6.275  -0.173  22.971  1.00 21.88      A
C
ATOM    977  O   GLU A 128      -5.945  -0.865  22.008  1.00 22.49      A
O
ATOM    978  N   VAL A 129      -5.674   0.972  23.258  1.00 18.66      A
N
ATOM    979  CA  VAL A 129      -4.783   1.694  22.321  1.00 20.11      A
C
ATOM    980  CB  VAL A 129      -3.834   0.835  21.370  1.00 20.61      A
C
ATOM    981  CG1 VAL A 129      -3.179  -0.373  22.058  1.00 19.56      A
C
ATOM    982  CG2 VAL A 129      -4.501   0.436  20.061  1.00 18.84      A
C
ATOM    983  C   VAL A 129      -5.642   2.687  21.545  1.00 18.50      A
C
ATOM    984  O   VAL A 129      -6.262   2.335  20.544  1.00 21.43      A
O
ATOM    985  N   LYS A 130      -5.717   3.914  22.062  1.00 20.39      A
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ATOM    986  CA  LYS A 130      -6.360   5.022  21.362  1.00 22.36      A
C
ATOM    987  CB  LYS A 130      -6.802   6.158  22.347  0.01 23.39      A
C
ATOM    988  CG  LYS A 130      -8.277   6.179  22.837  0.01 25.60      A
C
ATOM    989  CD  LYS A 130      -8.531   7.050  24.101  0.01 27.36      A
C
ATOM    990  CE  LYS A 130      -9.981   7.580  24.282  1.00 36.99      A
C
ATOM    991  NZ  LYS A 130     -10.475   8.029  25.652  1.00 19.28      A
N
ATOM    992  C   LYS A 130      -5.404   5.519  20.248  1.00 16.90      A
C
ATOM    993  O   LYS A 130      -4.181   5.522  20.409  0.01 18.81      A
O
ATOM    994  N   ALA A 131      -6.004   5.932  19.133  1.00 19.98      A
N
ATOM    995  CA  ALA A 131      -5.329   6.472  17.941  1.00 21.42      A
C
ATOM    996  CB  ALA A 131      -6.343   6.686  16.820  1.00 22.10      A
C
ATOM    997  C   ALA A 131      -4.516   7.752  18.149  1.00 21.81      A
C
ATOM    998  O   ALA A 131      -3.715   8.113  17.282  1.00 23.19      A
O
ATOM    999  N   GLU A 132      -4.740   8.443  19.267  1.00 21.99      A
N
ATOM   1000  CA  GLU A 132      -3.904   9.569  19.676  1.00 25.68      A
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ATOM   1001  CB  GLU A 132      -4.607  10.407  20.749  0.01 62.80      A
C
ATOM   1002  CG  GLU A 132      -5.783  11.226  20.233  0.01120.70      A
C
ATOM   1003  CD  GLU A 132      -6.420  12.098  21.302  0.01207.36      A
C
ATOM   1004  OE1 GLU A 132      -5.681  12.767  22.060  1.00457.21      A
O
ATOM   1005  OE2 GLU A 132      -7.667  12.126  21.376  1.00441.48      A
O
ATOM   1006  C   GLU A 132      -2.529   9.115  20.174  1.00 21.54      A
C
ATOM   1007  O   GLU A 132      -1.571   9.890  20.133  0.01 21.67      A
O
ATOM   1008  N   GLN A 133      -2.434   7.866  20.643  1.00 19.04      A
N
ATOM   1009  CA  GLN A 133      -1.154   7.297  21.077  1.00 21.01      A
C
ATOM   1010  CB  GLN A 133      -1.331   6.142  22.051  0.01 28.62      A
C
ATOM   1011  CG  GLN A 133      -1.806   6.567  23.418  0.01 41.06      A
C
ATOM   1012  CD  GLN A 133      -3.273   6.308  23.592  0.01 53.57      A
C
ATOM   1013  OE1 GLN A 133      -3.651   5.417  24.341  1.00166.00      A
O
ATOM   1014  NE2 GLN A 133      -4.109   7.057  22.871  1.00 27.75      A
N
ATOM   1015  C   GLN A 133      -0.341   6.818  19.900  1.00 21.05      A
C
ATOM   1016  O   GLN A 133       0.871   6.622  20.008  0.01 21.55      A
O
ATOM   1017  N   VAL A 134      -1.013   6.610  18.773  1.00 23.41      A
N
ATOM   1018  CA  VAL A 134      -0.297   6.266  17.559  1.00 21.63      A
C
ATOM   1019  CB  VAL A 134      -1.074   5.301  16.609  1.00 21.46      A
C
ATOM   1020  CG1 VAL A 134      -1.621   4.100  17.378  1.00 19.68      A
C
ATOM   1021  CG2 VAL A 134      -2.176   6.013  15.822  1.00 21.53      A
C
ATOM   1022  C   VAL A 134       0.209   7.502  16.823  1.00 21.06      A
C
ATOM   1023  O   VAL A 134       1.058   7.349  15.942  1.00 23.55      A
O
ATOM   1024  N   LYS A 135      -0.294   8.705  17.159  1.00 18.26      A
N
ATOM   1025  CA  LYS A 135       0.165   9.928  16.452  1.00 24.92      A
C
ATOM   1026  CB  LYS A 135      -0.843  11.146  16.471  0.01 32.38      A
C
ATOM   1027  CG  LYS A 135      -1.568  11.505  15.123  0.01 41.93      A
C
ATOM   1028  CD  LYS A 135      -2.386  12.845  15.062  0.01 52.27      A
C
ATOM   1029  CE  LYS A 135      -3.047  13.185  13.678  1.00112.39      A
C
ATOM   1030  NZ  LYS A 135      -3.895  14.425  13.372  1.00 24.13      A
N
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ATOM   1031  C   LYS A 135       1.561  10.233  16.998  1.00 22.11      A
C
ATOM   1032  O   LYS A 135       2.017  11.378  16.988  0.01 22.22      A
O
ATOM   1033  N   ALA A 136       2.222   9.172  17.472  1.00 19.11      A
N
ATOM   1034  CA  ALA A 136       3.571   9.231  18.048  1.00 22.50      A
C
ATOM   1035  CB  ALA A 136       3.566   8.770  19.504  1.00 20.08      A
C
ATOM   1036  C   ALA A 136       4.573   8.403  17.243  1.00 22.79      A
C
ATOM   1037  O   ALA A 136       5.674   8.879  16.951  1.00 22.80      A
O
ATOM   1038  N   SER A 137       4.202   7.161  16.916  1.00 20.22      A
N
ATOM   1039  CA  SER A 137       5.013   6.298  16.038  1.00 22.60      A
C
ATOM   1040  CB  SER A 137       4.405   4.883  15.934  1.00 21.42      A
C
ATOM   1041  OG  SER A 137       3.064   4.882  15.461  1.00 19.18      A
O
ATOM   1042  C   SER A 137       5.177   6.937  14.647  1.00 21.61      A
C
ATOM   1043  O   SER A 137       6.228   6.841  14.000  1.00 19.93      A
O
ATOM   1044  N   LYS A 138       4.109   7.601  14.231  1.00 19.11      A
N
ATOM   1045  CA  LYS A 138       4.030   8.367  13.018  1.00 20.11      A
C
ATOM   1046  CB  LYS A 138       2.664   9.010  13.006  0.01 22.21      A
C
ATOM   1047  CG  LYS A 138       1.546   8.146  12.469  0.01 24.94      A
C
ATOM   1048  CD  LYS A 138       0.725   9.100  11.650  0.01 27.80      A
C
ATOM   1049  CE  LYS A 138       1.673  10.235  11.311  1.00 27.23      A
C
ATOM   1050  NZ  LYS A 138       1.122  11.137  10.285  1.00 64.20      A
N
ATOM   1051  C   LYS A 138       5.089   9.466  13.008  1.00 19.47      A
C
ATOM   1052  O   LYS A 138       6.002   9.469  12.191  1.00 16.62      A
O
ATOM   1053  N   GLU A 139       4.946  10.392  13.947  1.00 20.90      A
N
ATOM   1054  CA  GLU A 139       5.862  11.496  14.157  1.00 17.39      A
C
ATOM   1055  CB  GLU A 139       5.546  12.109  15.510  1.00 18.85      A
C
ATOM   1056  CG  GLU A 139       5.815  13.588  15.621  1.00 21.34      A
C
ATOM   1057  CD  GLU A 139       4.670  14.298  16.303  1.00 22.49      A
C
ATOM   1058  OE1 GLU A 139       4.181  13.787  17.337  1.00 18.27      A
O
ATOM   1059  OE2 GLU A 139       4.259  15.361  15.789  1.00 23.20      A
O
ATOM   1060  C   GLU A 139       7.319  11.046  14.125  1.00 17.31      A
C
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ATOM   1061  O   GLU A 139       8.145  11.661  13.458  1.00 19.94      A
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ATOM   1062  N   MET A 140       7.621   9.978  14.860  1.00 15.83      A
N
ATOM   1063  CA  MET A 140       8.951   9.381  14.881  1.00 15.10      A
C
ATOM   1064  CB  MET A 140       8.977   8.167  15.817  1.00 16.05      A
C
ATOM   1065  CG  MET A 140      10.255   7.350  15.747  1.00 17.81      A
C
ATOM   1066  SD  MET A 140      11.698   8.150  16.485  1.00 21.47      A
S
ATOM   1067  CE  MET A 140      11.575   7.568  18.177  1.00 19.11      A
C
ATOM   1068  C   MET A 140       9.403   8.980  13.476  1.00 13.02      A
C
ATOM   1069  O   MET A 140      10.476   9.373  13.035  1.00 11.72      A
O
ATOM   1070  N   GLY A 141       8.574   8.204  12.783  1.00 11.99      A
N
ATOM   1071  CA  GLY A 141       8.856   7.783  11.417  1.00 10.95      A
C
ATOM   1072  C   GLY A 141       9.116   8.969  10.510  1.00 11.33      A
C
ATOM   1073  O   GLY A 141      10.113   8.994   9.778  1.00 12.19      A
O
ATOM   1074  N   GLU A 142       8.219   9.955  10.571  1.00 11.05      A
N
ATOM   1075  CA  GLU A 142       8.384  11.217   9.852  1.00 10.94      A
C
ATOM   1076  CB  GLU A 142       7.327  12.246  10.285  1.00 11.27      A
C
ATOM   1077  CG  GLU A 142       6.090  12.314   9.400  1.00 11.40      A
C
ATOM   1078  CD  GLU A 142       6.403  12.412   7.907  1.00 13.13      A
C
ATOM   1079  OE1 GLU A 142       7.132  13.333   7.442  1.00 10.39      A
O
ATOM   1080  OE2 GLU A 142       5.883  11.545   7.188  1.00 17.53      A
O
ATOM   1081  C   GLU A 142       9.776  11.787  10.079  1.00  9.90      A
C
ATOM   1082  O   GLU A 142      10.477  12.114   9.132  1.00  9.51      A
O
ATOM   1083  N   THR A 143      10.162  11.880  11.347  1.00  9.39      A
N
ATOM   1084  CA  THR A 143      11.450  12.418  11.741  1.00  8.93      A
C
ATOM   1085  CB  THR A 143      11.608  12.386  13.273  1.00  8.43      A
C
ATOM   1086  OG1 THR A 143      10.507  13.071  13.876  1.00  7.72      A
O
ATOM   1087  CG2 THR A 143      12.924  13.042  13.697  1.00  9.14      A
C
ATOM   1088  C   THR A 143      12.566  11.614  11.100  1.00  8.27      A
C
ATOM   1089  O   THR A 143      13.485  12.165  10.496  1.00  8.74      A
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ATOM   1090  N   LEU A 144      12.465  10.302  11.233  1.00  6.96      A
N
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ATOM   1091  CA  LEU A 144      13.466   9.407  10.699  1.00  6.51      A
C
ATOM   1092  CB  LEU A 144      13.176   7.973  11.136  1.00  5.37      A
C
ATOM   1093  CG  LEU A 144      13.320   7.726  12.629  1.00  4.71      A
C
ATOM   1094  CD1 LEU A 144      13.494   6.241  12.867  1.00  4.63      A
C
ATOM   1095  CD2 LEU A 144      14.476   8.510  13.234  1.00  4.44      A
C
ATOM   1096  C   LEU A 144      13.547   9.521   9.180  1.00  6.56      A
C
ATOM   1097  O   LEU A 144      14.640   9.514   8.617  1.00  6.71      A
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ATOM   1098  N   LEU A 145      12.390   9.663   8.541  1.00  6.22      A
N
ATOM   1099  CA  LEU A 145      12.302   9.865   7.090  1.00  7.15      A
C
ATOM   1100  CB  LEU A 145      10.844   9.790   6.646  1.00  6.86      A
C
ATOM   1101  CG  LEU A 145      10.552   9.894   5.163  1.00  6.09      A
C
ATOM   1102  CD1 LEU A 145      11.174   8.716   4.440  1.00  6.22      A
C
ATOM   1103  CD2 LEU A 145       9.054   9.930   4.989  1.00  6.45      A
C
ATOM   1104  C   LEU A 145      12.918  11.167   6.554  1.00  7.70      A
C
ATOM   1105  O   LEU A 145      13.654  11.166   5.559  1.00  7.18      A
O
ATOM   1106  N   ARG A 146      12.593  12.282   7.196  1.00  9.17      A
N
ATOM   1107  CA  ARG A 146      13.069  13.562   6.715  1.00  9.76      A
C
ATOM   1108  CB  ARG A 146      12.406  14.742   7.437  1.00 10.61      A
C
ATOM   1109  CG  ARG A 146      10.885  14.842   7.202  1.00 12.43      A
C
ATOM   1110  CD  ARG A 146      10.458  14.590   5.752  1.00 11.99      A
C
ATOM   1111  NE  ARG A 146       9.075  14.101   5.668  1.00 17.35      A
N
ATOM   1112  CZ  ARG A 146       8.474  13.685   4.547  1.00 18.06      A
C
ATOM   1113  NH1 ARG A 146       9.122  13.692   3.392  1.00 17.54      A
N
ATOM   1114  NH2 ARG A 146       7.216  13.258   4.572  1.00 17.52      A
N
ATOM   1115  C   ARG A 146      14.566  13.565   6.838  1.00  9.82      A
C
ATOM   1116  O   ARG A 146      15.265  13.894   5.861  1.00 10.17      A
O
ATOM   1117  N   ALA A 147      15.046  13.120   8.006  1.00  9.65      A
N
ATOM   1118  CA  ALA A 147      16.482  13.053   8.306  1.00  9.08      A
C
ATOM   1119  CB  ALA A 147      16.736  12.394   9.650  1.00  8.95      A
C
ATOM   1120  C   ALA A 147      17.225  12.320   7.202  1.00  9.46      A
C
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ATOM   1121  O   ALA A 147      18.176  12.862   6.640  1.00  9.30      A
O
ATOM   1122  N   VAL A 148      16.749  11.116   6.878  1.00  9.32      A
N
ATOM   1123  CA  VAL A 148      17.334  10.268   5.843  1.00  9.28      A
C
ATOM   1124  CB  VAL A 148      16.751   8.844   5.913  1.00 10.48      A
C
ATOM   1125  CG1 VAL A 148      16.997   8.091   4.598  1.00  9.52      A
C
ATOM   1126  CG2 VAL A 148      17.327   8.088   7.115  1.00 10.21      A
C
ATOM   1127  C   VAL A 148      17.142  10.801   4.425  1.00  9.48      A
C
ATOM   1128  O   VAL A 148      17.974  10.572   3.556  1.00  9.16      A
O
ATOM   1129  N   GLU A 149      16.026  11.479   4.191  1.00 11.57      A
N
ATOM   1130  CA  GLU A 149      15.767  12.114   2.903  1.00 11.29      A
C
ATOM   1131  CB  GLU A 149      14.337  12.651   2.852  1.00 10.90      A
C
ATOM   1132  CG  GLU A 149      13.973  13.261   1.517  1.00 10.01      A
C
ATOM   1133  CD  GLU A 149      12.479  13.390   1.324  1.00  9.79      A
C
ATOM   1134  OE1 GLU A 149      11.877  14.362   1.820  1.00  8.46      A
O
ATOM   1135  OE2 GLU A 149      11.913  12.517   0.648  1.00 10.24      A
O
ATOM   1136  C   GLU A 149      16.765  13.246   2.650  1.00 11.18      A
C
ATOM   1137  O   GLU A 149      17.373  13.312   1.580  1.00 10.16      A
O
ATOM   1138  N   SER A 150      16.918  14.128   3.641  1.00 11.08      A
N
ATOM   1139  CA  SER A 150      17.831  15.268   3.558  1.00 12.15      A
C
ATOM   1140  CB  SER A 150      17.751  16.091   4.850  1.00 12.64      A
C
ATOM   1141  OG  SER A 150      18.505  17.295   4.770  1.00 13.11      A
O
ATOM   1142  C   SER A 150      19.275  14.812   3.283  1.00 13.33      A
C
ATOM   1143  O   SER A 150      19.982  15.413   2.473  1.00 14.95      A
O
ATOM   1144  N   TYR A 151      19.680  13.731   3.949  1.00 13.35      A
N
ATOM   1145  CA  TYR A 151      21.004  13.137   3.806  1.00 13.11      A
C
ATOM   1146  CB  TYR A 151      21.213  12.000   4.834  1.00 13.92      A
C
ATOM   1147  CG  TYR A 151      22.532  11.258   4.662  1.00 17.05      A
C
ATOM   1148  CD1 TYR A 151      23.671  11.645   5.367  1.00 16.08      A
C
ATOM   1149  CE1 TYR A 151      24.881  10.983   5.191  1.00 16.35      A
C
ATOM   1150  CZ  TYR A 151      24.960   9.915   4.305  1.00 18.23      A
C
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ATOM   1151  OH  TYR A 151      26.156   9.253   4.135  1.00 17.78      A
O
ATOM   1152  CE2 TYR A 151      23.846   9.509   3.588  1.00 18.26      A
C
ATOM   1153  CD2 TYR A 151      22.643  10.175   3.768  1.00 18.69      A
C
ATOM   1154  C   TYR A 151      21.246  12.633   2.383  1.00 14.35      A
C
ATOM   1155  O   TYR A 151      22.374  12.666   1.893  1.00 14.99      A
O
ATOM   1156  N   LEU A 152      20.186  12.168   1.725  1.00 16.76      A
N
ATOM   1157  CA  LEU A 152      20.290  11.573   0.388  1.00 15.22      A
C
ATOM   1158  CB  LEU A 152      19.234  10.477   0.203  1.00 14.01      A
C
ATOM   1159  CG  LEU A 152      19.477   9.158   0.938  1.00 12.28      A
C
ATOM   1160  CD1 LEU A 152      18.349   8.175   0.661  1.00 10.73      A
C
ATOM   1161  CD2 LEU A 152      20.817   8.573   0.519  1.00 12.86      A
C
ATOM   1162  C   LEU A 152      20.222  12.604  -0.748  1.00 15.74      A
C
ATOM   1163  O   LEU A 152      20.736  12.368  -1.841  1.00 15.54      A
O
ATOM   1164  N   LEU A 153      19.607  13.753  -0.490  1.00 15.21      A
N
ATOM   1165  CA  LEU A 153      19.665  14.849  -1.451  1.00 15.97      A
C
ATOM   1166  CB  LEU A 153      18.645  15.933  -1.097  1.00 15.48      A
C
ATOM   1167  CG  LEU A 153      17.176  15.499  -1.126  1.00 13.37      A
C
ATOM   1168  CD1 LEU A 153      16.299  16.559  -0.488  1.00 13.97      A
C
ATOM   1169  CD2 LEU A 153      16.746  15.209  -2.553  1.00 12.67      A
C
ATOM   1170  C   LEU A 153      21.082  15.408  -1.458  1.00 15.98      A
C
ATOM   1171  O   LEU A 153      21.668  15.637  -2.518  1.00 14.95      A
O
ATOM   1172  N   ALA A 154      21.637  15.567  -0.258  1.00 16.06      A
N
ATOM   1173  CA  ALA A 154      23.000  16.061  -0.069  1.00 17.59      A
C
ATOM   1174  CB  ALA A 154      23.199  16.510   1.380  1.00 14.07      A
C
ATOM   1175  C   ALA A 154      24.124  15.094  -0.514  1.00 17.66      A
C
ATOM   1176  O   ALA A 154      25.290  15.493  -0.595  1.00 20.30      A
O
ATOM   1177  N   HIS A 155      23.781  13.846  -0.829  1.00 18.92      A
N
ATOM   1178  CA  HIS A 155      24.808  12.843  -1.159  1.00 21.49      A
C
ATOM   1179  CB  HIS A 155      25.080  11.944   0.049  1.00 20.27      A
C
ATOM   1180  CG  HIS A 155      25.633  12.684   1.245  1.00 18.09      A
C
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ATOM   1181  ND1 HIS A 155      26.948  12.892   1.422  1.00 20.97      A
N
ATOM   1182  CE1 HIS A 155      27.146  13.573   2.560  1.00 16.57      A
C
ATOM   1183  NE2 HIS A 155      25.956  13.806   3.112  1.00 18.86      A
N
ATOM   1184  CD2 HIS A 155      25.000  13.272   2.326  1.00 16.72      A
C
ATOM   1185  C   HIS A 155      24.647  12.024  -2.435  1.00 24.07      A
C
ATOM   1186  O   HIS A 155      25.476  11.164  -2.705  1.00 28.81      A
O
ATOM   1187  N   SER A 156      23.602  12.279  -3.223  1.00 24.32      A
N
ATOM   1188  CA  SER A 156      23.480  11.777  -4.616  1.00 25.43      A
C
ATOM   1189  CB  SER A 156      23.976  12.840  -5.608  1.00 25.74      A
C
ATOM   1190  OG  SER A 156      25.396  12.920  -5.623  1.00 20.68      A
O
ATOM   1191  C   SER A 156      24.161  10.438  -4.954  1.00 24.58      A
C
ATOM   1192  O   SER A 156      23.510   9.485  -5.404  1.00 21.70      A
O
ATOM   1193  N   ASP A 157      25.477  10.390  -4.759  1.00 23.40      A
N
ATOM   1194  CA  ASP A 157      26.298   9.244  -5.158  1.00 27.82      A
C
ATOM   1195  CB  ASP A 157      27.791   9.594  -5.018  1.00 26.27      A
C
ATOM   1196  CG  ASP A 157      28.386  10.181  -6.297  1.00 28.79      A
C
ATOM   1197  OD1 ASP A 157      27.892  11.216  -6.800  1.00 31.44      A
O
ATOM   1198  OD2 ASP A 157      29.369   9.601  -6.799  1.00 31.40      A
O
ATOM   1199  C   ASP A 157      25.963   7.938  -4.417  1.00 26.97      A
C
ATOM   1200  O   ASP A 157      26.344   6.849  -4.864  1.00 24.63      A
O
ATOM   1201  N   ALA A 158      25.245   8.062  -3.298  1.00 24.96      A
N
ATOM   1202  CA  ALA A 158      24.935   6.932  -2.427  1.00 21.85      A
C
ATOM   1203  CB  ALA A 158      24.864   7.376  -0.972  1.00 22.36      A
C
ATOM   1204  C   ALA A 158      23.640   6.261  -2.853  1.00 19.21      A
C
ATOM   1205  O   ALA A 158      22.644   6.283  -2.138  1.00 20.85      A
O
ATOM   1206  O   HOH A 161      14.007  14.588  10.817  1.00 17.77      A
O
ATOM   1207  O   HOH A 162      19.383 -16.566   8.548  1.00  5.69      A
O
ATOM   1208  O   HOH A 163       1.146   6.884  24.049  1.00 21.27      A
O
ATOM   1209  O   HOH A 164       4.504   3.367  20.820  1.00 13.32      A
O
ATOM   1210  O   HOH A 165       8.932 -15.181   8.847  1.00 27.66      A
O
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ATOM   1211  O   HOH A 166       4.283 -10.455  24.219  1.00  9.06      A
O
ATOM   1212  O   HOH A 167       9.539   5.362  21.876  1.00 11.98      A
O
ATOM   1213  O   HOH A 168      23.145   7.863  17.546  1.00 15.89      A
O
ATOM   1214  O   HOH A 169      10.896  11.778  26.459  1.00 18.42      A
O
ATOM   1215  O   HOH A 170      15.741  -2.325  -3.731  1.00 38.86      A
O
ATOM   1216  O   HOH A 171      -0.496   0.709  24.427  1.00  2.99      A
O
ATOM   1217  O   HOH A 172       0.752   2.784  22.368  1.00 15.89      A
O
ATOM   1218  O   HOH A 173      14.545   2.205  11.137  1.00 19.76      A
O
ATOM   1219  O   HOH A 174      12.131  -0.017  13.728  1.00  3.72      A
O
ATOM   1220  O   HOH A 175      11.431   2.224  14.001  1.00  8.26      A
O
ATOM   1221  O   HOH A 176      24.805   1.620  12.999  1.00  7.32      A
O
ATOM   1222  O   HOH A 177      13.504 -10.314  -1.999  1.00  3.88      A
O
ATOM   1223  O   HOH A 178      21.757  13.929  18.924  1.00 17.33
O
ATOM   1224  O   HOH A 179      18.420  14.125  12.117  1.00 18.80
O
ATOM   1225  O   HOH A 180      22.718   2.932  -5.991  1.00 45.45
O
ATOM   1226  O   HOH A 181      19.546 -14.221   7.458  1.00 13.58
O
ATOM   1227  O   HOH A 182       1.428   8.384  21.986  1.00 23.25
O
ATOM   1228  O   HOH A 183      -0.595  -0.900  33.881  1.00 69.63
O
ATOM   1229  O   HOH A 184      -6.492   9.380  24.998  1.00 25.05
O
ATOM   1230  O   HOH A 186      22.871   4.104  -4.513  1.00 32.32
O
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