



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 16, 2021 – 02:02 pm BST

PDB ID : 7BJ9
Title : Structure of Sfh-I with 2-Mercaptomethyl-thiazolidine L-anti-1a
Authors : Hinchliffe, P.; Spencer, J.
Deposited on : 2021-01-14
Resolution : 1.21 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

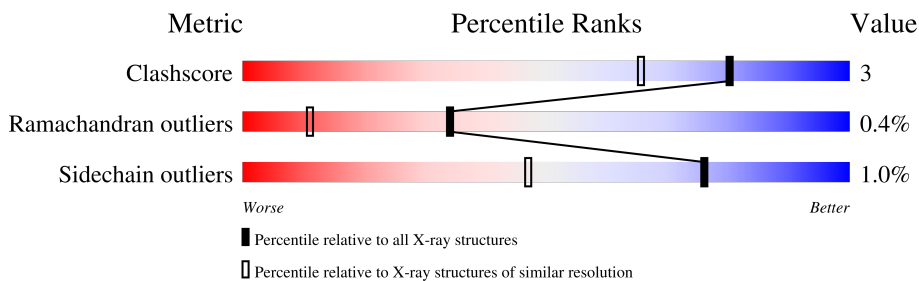
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.21 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1294 (1.24-1.20)
Ramachandran outliers	138981	1251 (1.24-1.20)
Sidechain outliers	138945	1250 (1.24-1.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	234	
1	B	234	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8190 atoms, of which 3869 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	B	230	3839	1228	1914	318	373	6	0	22	0
1	A	230	3838	1227	1920	316	368	7	0	20	0

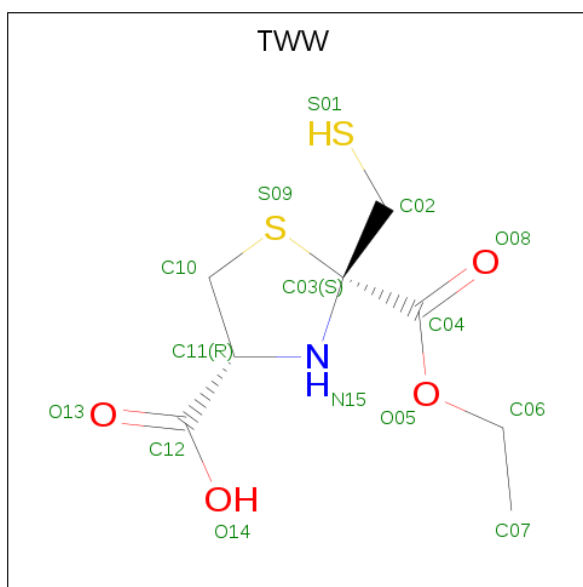
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	36	GLY	-	expression tag	UNP Q9RMI1
B	37	PRO	-	expression tag	UNP Q9RMI1
A	36	GLY	-	expression tag	UNP Q9RMI1
A	37	PRO	-	expression tag	UNP Q9RMI1

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is (2 {S},4 {R})-2-ethoxycarbonyl-2-(sulfanylmethyl)-1,3-thiazolidine-4-carboxylic acid (three-letter code: TWW) (formula: C₈H₁₃NO₄S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			S
3	B	1	26	8	11	1	4	2	0	0
3	A	1	26	8	11	1	4	2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	H			O
4	B	1	11	3	5	3	0	0
4	A	1	14	3	8	3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	249	Total 249	O 249	0	0
5	A	185	Total 185	O 185	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

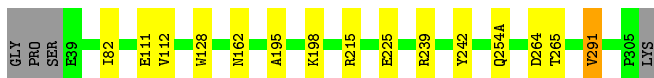
- Molecule 1: Beta-lactamase

Chain B:  93% 6%



- Molecule 1: Beta-lactamase

Chain A:  92% 6%



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	33.08Å 88.07Å 72.06Å 90.00° 90.51° 90.00°	Depositor
Resolution (Å)	72.06 – 1.21	Depositor
% Data completeness (in resolution range)	99.7 (72.06-1.21)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.136 , 0.152	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	8190	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TWW, GOL, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.40	0/2032	0.66	0/2755
1	B	0.41	0/2047	0.67	0/2776
All	All	0.41	0/4079	0.67	0/5531

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1918	1920	1837	12	0
1	B	1925	1914	1815	11	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	15	11	0	0	0
3	B	15	11	0	0	0
4	A	6	8	8	0	0
4	B	6	5	8	0	0
5	A	185	0	0	7	0
5	B	249	0	0	7	0
All	All	4321	3869	3668	21	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (21) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168[B]:GLU:OE1	5:B:501:HOH:O	1.94	0.85
1:A:111:GLU:OE2	5:A:501:HOH:O	2.12	0.67
1:A:162:ASN:ND2	5:A:502:HOH:O	2.26	0.62
1:A:239:ARG:HD2	5:A:663:HOH:O	2.02	0.60
1:B:264:ASP:HB2	5:B:579:HOH:O	2.00	0.59
1:A:264:ASP:HB2	5:A:541:HOH:O	2.05	0.56
1:A:254(A):GLN:NE2	5:A:503:HOH:O	2.27	0.56
1:B:162[A]:ASN:ND2	5:B:506:HOH:O	2.39	0.55
1:B:196:HIS:HE1	5:B:513:HOH:O	1.91	0.54
1:B:162[B]:ASN:ND2	1:B:162[B]:ASN:O	2.40	0.53
1:A:225:GLU:OE2	1:A:265[B]:THR:HG22	2.08	0.53
1:B:196:HIS:CE1	5:B:513:HOH:O	2.63	0.52
1:A:82[B]:ILE:CD1	1:A:128:TRP:CH2	2.98	0.46
1:B:215[A]:ARG:NH2	5:B:504:HOH:O	2.32	0.46
1:A:291[A]:VAL:HG22	5:A:543:HOH:O	2.17	0.45
1:B:159:GLN:HG3	1:A:215[B]:ARG:HH22	1.81	0.44
1:B:111:GLU:OE2	5:B:502:HOH:O	2.20	0.44
1:B:155:ASN:HB3	1:A:215[B]:ARG:NH2	2.34	0.42
1:A:198:LYS:NZ	5:A:509:HOH:O	2.48	0.42
1:A:112:VAL:HG21	1:A:128:TRP:CG	2.54	0.42
1:B:239:ARG:HH22	1:B:304:ALA:HB1	1.85	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	248/234 (106%)	239 (96%)	8 (3%)	1 (0%)	34 11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	250/234 (107%)	241 (96%)	8 (3%)	1 (0%)	34 11
All	All	498/468 (106%)	480 (96%)	16 (3%)	2 (0%)	34 11

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	195	ALA
1	A	195	ALA

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	218/202 (108%)	215 (99%)	3 (1%)	67 32
1	B	220/202 (109%)	217 (99%)	3 (1%)	67 32
All	All	438/404 (108%)	432 (99%)	6 (1%)	76 32

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	242	TYR
1	B	291[A]	VAL
1	B	291[B]	VAL
1	A	242	TYR
1	A	291[A]	VAL
1	A	291[B]	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	159	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TWW	A	402	2	10,15,15	6.50	4 (40%)	8,21,21	4.57	5 (62%)
3	TWW	B	402	2	10,15,15	6.50	4 (40%)	8,21,21	4.21	5 (62%)
4	GOL	A	403	-	5,5,5	0.52	0	5,5,5	0.49	0
4	GOL	B	403	-	5,5,5	0.60	0	5,5,5	0.49	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TWW	A	402	2	-	2/9/27/27	0/1/1/1
3	TWW	B	402	2	-	1/9/27/27	0/1/1/1
4	GOL	A	403	-	-	0/4/4/4	-
4	GOL	B	403	-	-	0/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	TWW	C02-C03	17.96	1.68	1.53
3	A	402	TWW	C02-C03	17.36	1.68	1.53
3	A	402	TWW	C03-N15	-6.75	1.37	1.45
3	A	402	TWW	C02-S01	6.59	1.95	1.81
3	B	402	TWW	C03-S09	-6.07	1.73	1.85
3	B	402	TWW	C03-N15	-6.05	1.38	1.45
3	A	402	TWW	C03-S09	-5.16	1.74	1.85
3	B	402	TWW	C02-S01	4.99	1.92	1.81

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	TWW	O05-C04-C03	8.72	119.83	111.76
3	A	402	TWW	O05-C04-C03	6.96	118.20	111.76
3	A	402	TWW	C02-C03-C04	-6.93	93.79	110.62
3	A	402	TWW	C04-C03-N15	6.62	124.58	110.39
3	B	402	TWW	C02-C03-C04	-4.77	99.02	110.62
3	A	402	TWW	C03-C02-S01	4.37	119.11	114.19
3	B	402	TWW	C04-C03-N15	4.03	119.02	110.39
3	B	402	TWW	C03-C02-S01	3.91	118.59	114.19
3	B	402	TWW	O05-C04-O08	-3.06	118.26	124.54
3	A	402	TWW	O05-C04-O08	-2.52	119.37	124.54

There are no chirality outliers.

All (3) torsion outliers are listed below:

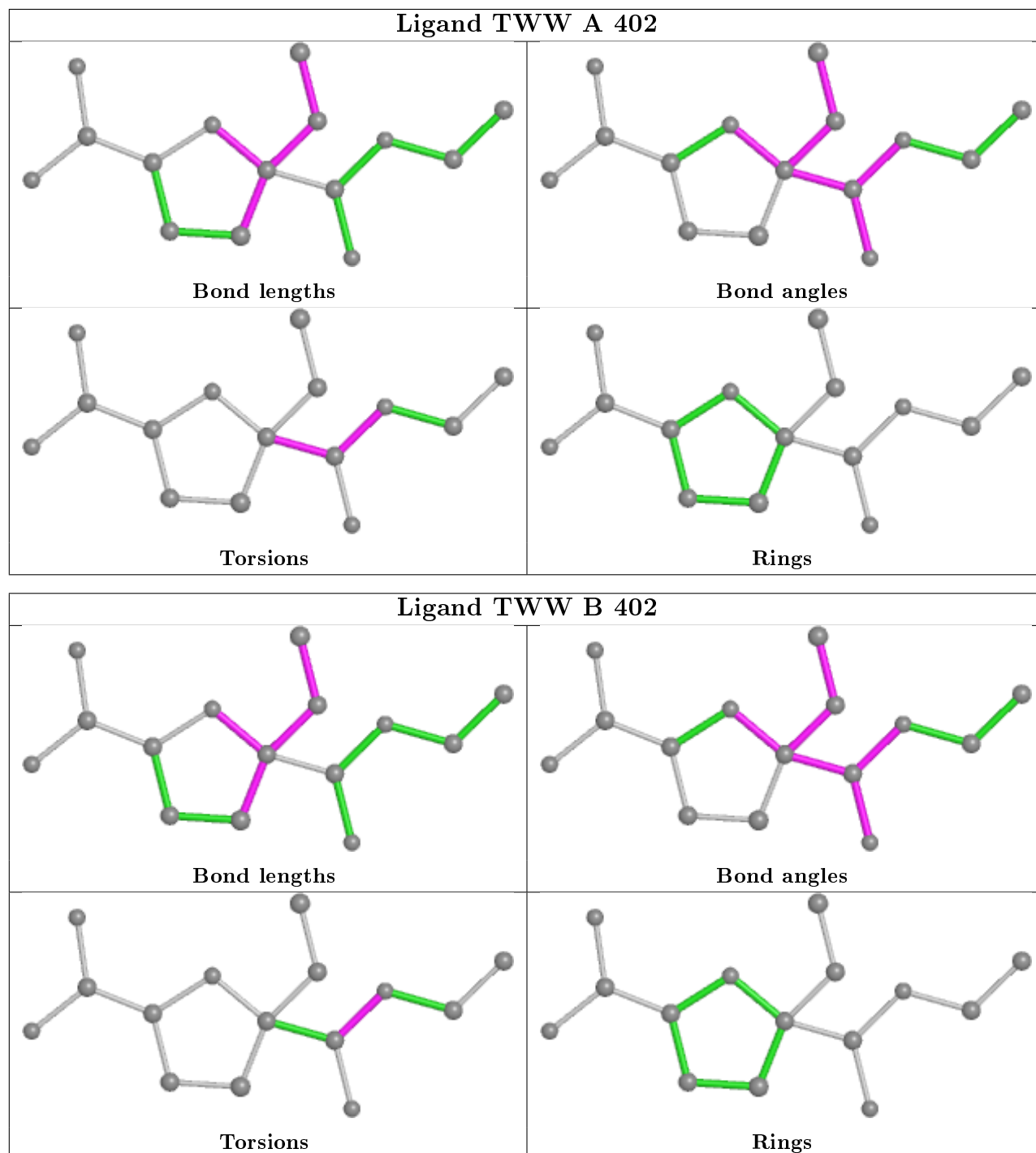
Mol	Chain	Res	Type	Atoms
3	A	402	TWW	N15-C03-C04-O08
3	B	402	TWW	C03-C04-O05-C06
3	A	402	TWW	C03-C04-O05-C06

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.