



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:03 am GMT

PDB ID : 6ABP
Title : SUGAR-BINDING AND CRYSTALLOGRAPHIC STUDIES OF AN ARABINOSE-BINDING PROTEIN MUTANT (MET108LEU) WHICH EXHIBITS ENHANCED AFFINITY AND ALTERED SPECIFICITY
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Deposited on : 1991-04-25
Resolution : 1.67 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

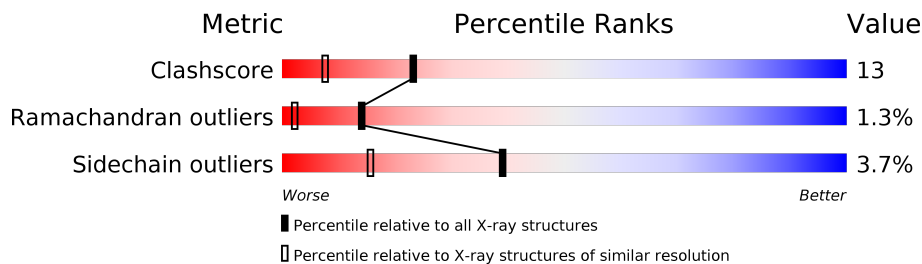
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.67 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	112137	5803 (1.70-1.66)
Ramachandran outliers	110173	5704 (1.70-1.66)
Sidechain outliers	110143	5703 (1.70-1.66)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	306	 74% 21% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2541 atoms, of which 0 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 L-ARABINOSE-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	0
			2316	1474	389	443	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	108	LEU	MET	CONFLICT	UNP P02924

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	2	Total	C	O	0	0
			20	10	10		

- Molecule 3 is water.

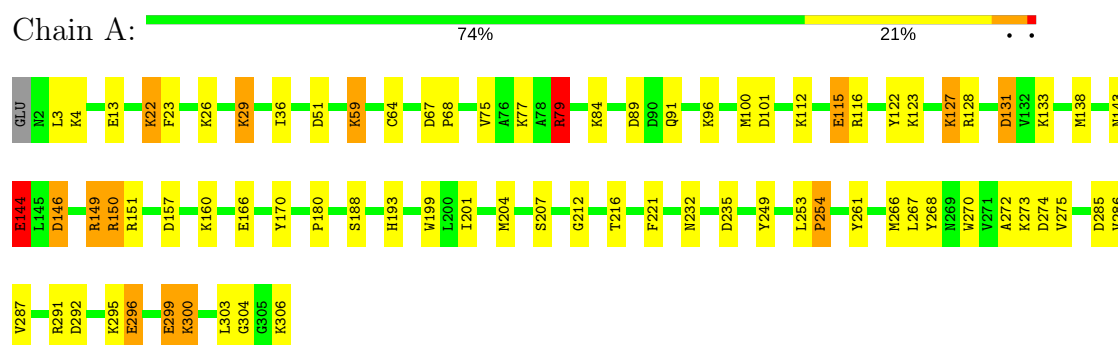
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	205	Total	O	0	0
			205	205		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: L-ARABINOSE-BINDING PROTEIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.54Å 72.12Å 78.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.67	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-1.67)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.160 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2541	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ARA, ARB

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	1.33	4/2361 (0.2%)	1.98	54/3190 (1.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	151	ARG	CZ-NH2	6.38	1.41	1.33
1	A	13	GLU	CD-OE1	-6.09	1.19	1.25
1	A	188	SER	CB-OG	5.36	1.49	1.42
1	A	207	SER	CA-CB	5.21	1.60	1.52

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	ARG	NE-CZ-NH1	20.74	130.67	120.30
1	A	79	ARG	NE-CZ-NH1	15.17	127.89	120.30
1	A	122	TYR	CB-CG-CD2	-11.94	113.84	121.00
1	A	291	ARG	NE-CZ-NH1	11.72	126.16	120.30
1	A	157	ASP	CB-CG-OD2	-11.62	107.84	118.30
1	A	150	ARG	NE-CZ-NH2	-11.45	114.58	120.30
1	A	291	ARG	NE-CZ-NH2	-11.39	114.61	120.30
1	A	149	ARG	NE-CZ-NH1	-11.29	114.66	120.30
1	A	123	LYS	CA-CB-CG	11.03	137.66	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	ARG	CA-CB-CG	10.07	135.56	113.40
1	A	79	ARG	NE-CZ-NH2	-8.97	115.81	120.30
1	A	67	ASP	CB-CG-OD1	8.93	126.34	118.30
1	A	116	ARG	CD-NE-CZ	8.34	135.27	123.60
1	A	150	ARG	CD-NE-CZ	8.12	134.96	123.60
1	A	146	ASP	CB-CG-OD2	7.89	125.41	118.30
1	A	261	TYR	CG-CD2-CE2	-7.86	115.01	121.30
1	A	292	ASP	CB-CG-OD2	-7.68	111.39	118.30
1	A	23	PHE	CB-CG-CD1	-7.46	115.58	120.80
1	A	51	ASP	CB-CG-OD1	7.43	124.98	118.30
1	A	170	TYR	CB-CG-CD2	-7.41	116.56	121.00
1	A	285	ASP	CB-CG-OD2	-7.26	111.76	118.30
1	A	151	ARG	NH1-CZ-NH2	-7.18	111.51	119.40
1	A	115	GLU	OE1-CD-OE2	6.89	131.57	123.30
1	A	235	ASP	CB-CG-OD1	6.60	124.24	118.30
1	A	299	GLU	CG-CD-OE1	6.58	131.46	118.30
1	A	101	ASP	CB-CG-OD1	6.50	124.15	118.30
1	A	221	PHE	CB-CG-CD2	-6.50	116.25	120.80
1	A	193	HIS	CA-CB-CG	-6.46	102.62	113.60
1	A	67	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	A	267	LEU	CB-CG-CD2	-6.38	100.15	111.00
1	A	149	ARG	NH1-CZ-NH2	6.37	126.41	119.40
1	A	151	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	180	PRO	N-CD-CG	-6.18	93.93	103.20
1	A	296	GLU	CA-CB-CG	6.08	126.78	113.40
1	A	144	GLU	CG-CD-OE1	6.07	130.44	118.30
1	A	303	LEU	C-N-CA	5.98	134.85	122.30
1	A	51	ASP	CB-CG-OD2	-5.94	112.95	118.30
1	A	296	GLU	N-CA-CB	5.86	121.14	110.60
1	A	261	TYR	CD1-CE1-CZ	-5.78	114.60	119.80
1	A	274	ASP	N-CA-CB	5.72	120.90	110.60
1	A	199	TRP	O-C-N	5.55	131.59	122.70
1	A	116	ARG	NE-CZ-NH2	5.45	123.03	120.30
1	A	296	GLU	CB-CA-C	-5.43	99.53	110.40
1	A	131	ASP	O-C-N	5.35	131.26	122.70
1	A	299	GLU	CG-CD-OE2	-5.27	107.76	118.30
1	A	77	LYS	CA-CB-CG	5.25	124.95	113.40
1	A	266	MET	CA-CB-CG	-5.20	104.47	113.30
1	A	268	TYR	CB-CG-CD2	-5.16	117.90	121.00
1	A	115	GLU	CG-CD-OE2	-5.16	107.99	118.30
1	A	249	TYR	CG-CD2-CE2	-5.13	117.20	121.30
1	A	122	TYR	CG-CD2-CE2	-5.08	117.23	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	PHE	CD1-CG-CD2	5.07	124.89	118.30
1	A	64	CYS	N-CA-CB	5.05	119.69	110.60
1	A	100	MET	CA-CB-CG	-5.02	104.76	113.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	ARG	Sidechain

5.2 Too-close contacts ⓘ

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	2316	0	2328	60	0
2	A	20	0	8	0	0
3	A	205	0	0	12	0
All	All	2541	0	2336	60	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 13.

All (60) 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:A:146:ASP:HB2	3:A:464:HOH:O	1.23	1.38
1:A:295:LYS:HE3	1:A:306:LYS:O	1.46	1.15
1:A:295:LYS:CE	1:A:306:LYS:O	1.96	1.13
1:A:127:LYS:HB2	1:A:127:LYS:NZ	1.56	1.12
1:A:22:LYS:HB2	1:A:22:LYS:NZ	1.51	1.11
1:A:127:LYS:HZ3	1:A:127:LYS:CB	1.68	1.05
1:A:22:LYS:HB2	1:A:22:LYS:HZ3	1.20	0.99
1:A:127:LYS:HZ3	1:A:127:LYS:HB2	0.80	0.96
1:A:3:LEU:HD11	1:A:59:LYS:CG	1.96	0.95
1:A:3:LEU:HD11	1:A:59:LYS:HG3	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LYS:HD3	1:A:166:GLU:HG2	1.53	0.91
1:A:127:LYS:NZ	1:A:127:LYS:CB	2.23	0.90
1:A:3:LEU:CD1	1:A:59:LYS:CG	2.50	0.88
1:A:3:LEU:CD1	1:A:59:LYS:HG3	2.04	0.86
1:A:146:ASP:CB	3:A:464:HOH:O	1.93	0.85
1:A:3:LEU:CD1	1:A:59:LYS:HG2	2.13	0.77
1:A:295:LYS:HE2	1:A:306:LYS:O	1.83	0.76
1:A:22:LYS:NZ	1:A:22:LYS:CB	2.36	0.75
1:A:26:LYS:HA	1:A:29:LYS:HD2	1.70	0.73
1:A:295:LYS:HE3	1:A:306:LYS:C	2.09	0.72
1:A:115:GLU:OE1	3:A:434:HOH:O	2.13	0.65
1:A:3:LEU:HD11	1:A:59:LYS:HG2	1.71	0.63
1:A:273:LYS:HB2	1:A:275:VAL:HG23	1.81	0.63
1:A:160:LYS:HD3	1:A:166:GLU:CG	2.28	0.61
1:A:75:VAL:O	1:A:79:ARG:HG2	1.99	0.61
1:A:22:LYS:HE3	3:A:475:HOH:O	2.02	0.60
1:A:3:LEU:HD12	1:A:59:LYS:HG2	1.82	0.59
1:A:4:LYS:HD2	1:A:36:ILE:HD11	1.88	0.56
1:A:84:LYS:HE2	3:A:487:HOH:O	2.05	0.55
1:A:127:LYS:HE2	3:A:360:HOH:O	2.07	0.54
1:A:127:LYS:HZ2	1:A:127:LYS:CB	2.17	0.52
1:A:144:GLU:CD	1:A:144:GLU:H	2.13	0.52
1:A:59:LYS:HD3	3:A:422:HOH:O	2.11	0.51
1:A:146:ASP:CG	3:A:464:HOH:O	2.34	0.51
1:A:306:LYS:C	3:A:435:HOH:O	2.49	0.50
1:A:131:ASP:OD2	1:A:133:LYS:HE3	2.11	0.50
1:A:296:GLU:HG3	3:A:337:HOH:O	2.11	0.50
1:A:84:LYS:HD2	1:A:270:TRP:CE2	2.47	0.49
1:A:59:LYS:HZ2	1:A:59:LYS:HB3	1.77	0.49
1:A:138:MET:CE	1:A:201:ILE:HG12	2.41	0.49
1:A:300:LYS:CB	1:A:300:LYS:NZ	2.77	0.48
1:A:212:GLY:O	1:A:216:THR:HG23	2.15	0.46
1:A:112:LYS:HD3	1:A:112:LYS:HA	1.25	0.45
1:A:68:PRO:HB3	1:A:91:GLN:O	2.16	0.45
1:A:143:ASN:OD1	1:A:149:ARG:HG3	2.18	0.44
1:A:146:ASP:OD2	1:A:150:ARG:HD3	2.17	0.44
1:A:112:LYS:HE2	1:A:115:GLU:OE1	2.18	0.44
1:A:201:ILE:HD11	1:A:216:THR:HG21	1.99	0.44
1:A:286:VAL:HG22	1:A:287:VAL:N	2.33	0.43
1:A:272:ALA:C	1:A:273:LYS:HG3	2.39	0.43
1:A:300:LYS:HB2	1:A:300:LYS:HZ2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:LYS:HB2	1:A:96:LYS:HE3	1.29	0.43
1:A:59:LYS:NZ	1:A:59:LYS:HB3	2.34	0.42
1:A:22:LYS:HE2	1:A:22:LYS:HB3	1.49	0.42
1:A:138:MET:HE3	1:A:201:ILE:HG12	2.01	0.42
1:A:150:ARG:CG	3:A:465:HOH:O	2.68	0.41
1:A:253:LEU:HA	1:A:254:PRO:HD3	1.92	0.41
1:A:84:LYS:HD2	1:A:270:TRP:CZ2	2.56	0.41
1:A:22:LYS:CE	3:A:475:HOH:O	2.65	0.40
1:A:270:TRP:HA	1:A:275:VAL:O	2.21	0.40

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	303/306 (99%)	296 (98%)	3 (1%)	4 (1%)	14 2

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	232	ASN
1	A	254	PRO
1	A	89	ASP
1	A	304	GLY

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	243/246 (99%)	234 (96%)	9 (4%)	39 16

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	29	LYS
1	A	59	LYS
1	A	79	ARG
1	A	127	LYS
1	A	144	GLU
1	A	204	MET
1	A	299	GLU
1	A	300	LYS

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

Mol	Chain	Res	Type
1	A	126	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](#)

2 carbohydrates are modelled in this entry.

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
2	ARA	A	307	2	10,10,10	2.83	4 (40%)	14,14,14	1.85	4 (28%)
2	ARB	A	308	2	10,10,10	2.02	6 (60%)	14,14,14	2.21	4 (28%)

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
2	ARA	A	307	2	-	0/0/17/17	0/1/1/1
2	ARB	A	308	2	-	0/0/17/17	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	307	ARA	C3-C2	-5.50	1.38	1.52
2	A	308	ARB	C3-C2	-2.20	1.46	1.52
2	A	307	ARA	O3-C3	2.10	1.47	1.43
2	A	308	ARB	O2-C2	2.12	1.47	1.43
2	A	308	ARB	O5-C1	2.17	1.46	1.43
2	A	308	ARB	O4-C4	2.44	1.48	1.43
2	A	308	ARB	C5-C4	2.51	1.58	1.52
2	A	308	ARB	C4-C3	3.13	1.56	1.52
2	A	307	ARA	O5-C5	4.13	1.50	1.43
2	A	307	ARA	C4-C3	4.74	1.58	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	307	ARA	O5-C1-C2	-3.22	104.99	109.31
2	A	308	ARB	O2-C2-C3	-3.03	103.75	110.36
2	A	307	ARA	O3-C3-C4	-2.85	104.84	110.02
2	A	308	ARB	O5-C5-C4	-2.24	107.28	110.79
2	A	307	ARA	C4-C3-C2	2.09	114.51	110.88
2	A	307	ARA	O3-C3-C2	2.58	115.97	110.36
2	A	308	ARB	O5-C1-C2	2.88	113.17	109.31
2	A	308	ARB	C5-O5-C1	5.66	122.60	112.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

There are no ligands in this entry.

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.