



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 09:57 AM UTC

PDB ID : 3BLM / pdb_00003blm
Title : REFINED CRYSTAL STRUCTURE OF BETA-LACTAMASE FROM STAPHYLOCOCCUS AUREUS PC1 AT 2.0
Authors : Herzberg, O.; Moulton, J.
Deposited on : 1990-12-03
Resolution : 2.00 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

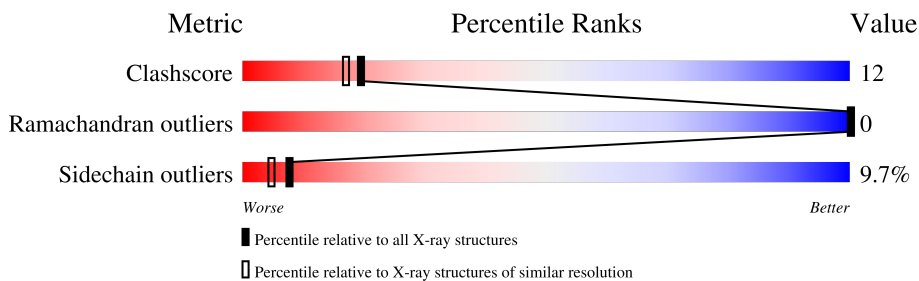
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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	257	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2236 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 BETA-LACTAMASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	257	2029	1293	341	392	3	0	0	0

- Molecule 2 is water.

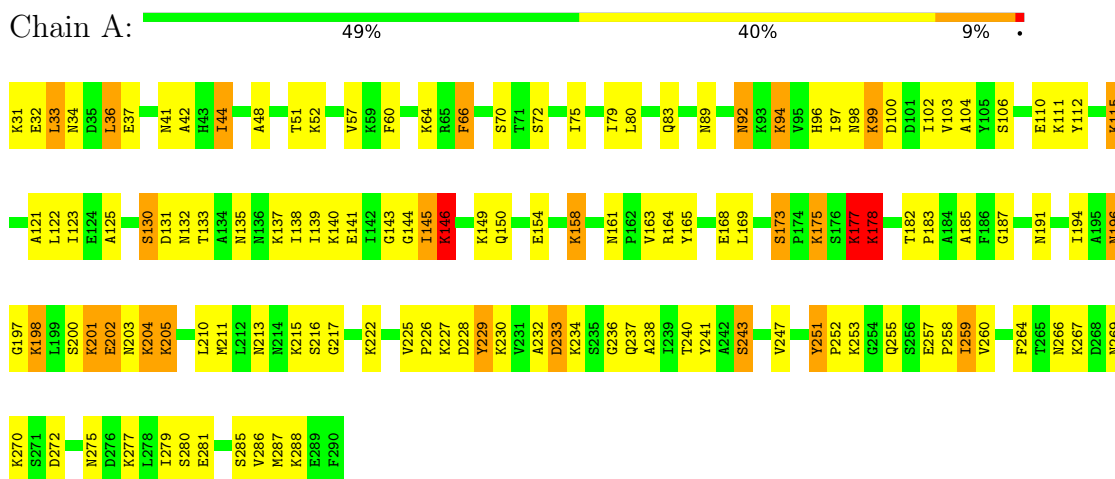
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	207	Total	O	0	0
			207	207		

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



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	53.90Å 94.00Å 139.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.163 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2236	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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	1.68	19/2059 (0.9%)	2.37	108/2764 (3.9%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	236	GLY	C-O	6.27	1.30	1.24
1	A	194	ILE	CA-CB	6.26	1.61	1.55
1	A	259	ILE	CA-C	6.03	1.60	1.52
1	A	266	ASN	N-CA	5.97	1.53	1.46
1	A	122	LEU	CA-C	5.90	1.60	1.52
1	A	103	VAL	N-CA	5.51	1.52	1.46
1	A	106	SER	N-CA	5.44	1.52	1.46
1	A	133	THR	N-CA	5.41	1.53	1.46
1	A	140	LYS	N-CA	5.38	1.52	1.46
1	A	158	LYS	C-N	-5.35	1.27	1.33
1	A	44	ILE	N-CA	5.33	1.52	1.46
1	A	251	TYR	N-CA	5.30	1.52	1.46
1	A	281	GLU	C-O	5.30	1.30	1.24
1	A	36	LEU	N-CA	5.19	1.52	1.46
1	A	100	ASP	C-O	5.09	1.30	1.24
1	A	83	GLN	C-N	-5.07	1.27	1.33
1	A	98	ASN	N-CA	5.06	1.53	1.46
1	A	104	ALA	C-N	-5.02	1.27	1.33
1	A	240	THR	CA-CB	5.01	1.61	1.53

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	ILE	N-CA-C	9.61	119.82	111.56
1	A	131	ASP	CA-CB-CG	-9.29	103.31	112.60
1	A	203	ASN	OD1-CG-ND2	8.88	131.48	122.60
1	A	191	ASN	OD1-CG-ND2	8.73	131.33	122.60
1	A	135	ASN	OD1-CG-ND2	-7.81	114.79	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	ILE	O-C-N	7.80	129.87	121.83
1	A	123	ILE	CA-C-O	-7.72	112.92	120.95
1	A	52	LYS	CA-C-O	7.66	128.59	120.70
1	A	132	ASN	OD1-CG-ND2	7.62	130.22	122.60
1	A	99	LYS	O-C-N	7.53	129.92	122.09
1	A	241	TYR	CA-C-O	-7.41	112.47	121.28
1	A	165	TYR	CA-C-O	-7.34	112.94	121.82
1	A	66	PHE	CA-CB-CG	7.34	121.14	113.80
1	A	57	VAL	CA-C-O	-7.33	112.68	120.53
1	A	279	ILE	O-C-N	7.22	129.41	121.90
1	A	177	LYS	CG-CD-CE	7.20	127.86	111.30
1	A	228	ASP	CA-CB-CG	-7.14	105.46	112.60
1	A	161	ASN	N-CA-CB	-7.08	100.80	111.21
1	A	210	LEU	O-C-N	6.97	129.25	122.07
1	A	99	LYS	CA-C-O	-6.96	113.45	120.90
1	A	243	SER	CA-C-N	6.74	132.28	122.77
1	A	243	SER	C-N-CA	6.74	132.28	122.77
1	A	173	SER	O-C-N	6.64	128.74	121.23
1	A	215	LYS	N-CA-CB	6.61	120.38	110.53
1	A	51	THR	CA-CB-CG2	6.55	121.64	110.50
1	A	196	ASN	CA-CB-CG	6.55	119.15	112.60
1	A	228	ASP	N-CA-CB	-6.52	100.53	110.12
1	A	92	ASN	CB-CG-ND2	6.44	126.07	116.40
1	A	275	ASN	O-C-N	6.40	130.70	123.27
1	A	89	ASN	CA-CB-CG	-6.34	106.26	112.60
1	A	252	PRO	CB-CA-C	6.33	119.27	110.98
1	A	94	LYS	CA-C-O	-6.30	114.03	120.71
1	A	121	ALA	CA-C-O	-6.27	112.76	119.97
1	A	178	LYS	CA-CB-CG	-6.26	101.57	114.10
1	A	94	LYS	CA-CB-CG	-6.23	101.64	114.10
1	A	202	GLU	CG-CD-OE1	6.19	132.64	118.40
1	A	79	ILE	CA-C-O	-6.18	114.52	120.95
1	A	233	ASP	CA-CB-CG	6.17	118.77	112.60
1	A	216	SER	CA-C-O	-6.16	112.04	119.49
1	A	96	HIS	CE1-NE2-CD2	6.14	115.14	109.00
1	A	269	ASN	CA-C-O	6.12	127.19	120.71
1	A	200	SER	N-CA-C	-6.10	102.90	110.41
1	A	144	GLY	N-CA-C	-6.08	105.48	112.29
1	A	72	SER	CA-C-O	-6.03	111.96	119.38
1	A	237	GLN	CA-C-O	-6.02	111.86	120.11
1	A	138	ILE	O-C-N	6.01	127.70	121.87
1	A	143	GLY	CA-C-O	-5.99	110.14	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	ILE	O-C-N	5.96	129.70	123.26
1	A	202	GLU	CA-CB-CG	5.96	126.03	114.10
1	A	97	ILE	CA-C-N	-5.96	112.12	123.32
1	A	97	ILE	C-N-CA	-5.96	112.12	123.32
1	A	259	ILE	CA-C-O	-5.89	113.75	120.65
1	A	183	PRO	CA-C-N	5.88	128.09	120.44
1	A	183	PRO	C-N-CA	5.88	128.09	120.44
1	A	182	THR	CA-CB-CG2	5.86	120.46	110.50
1	A	213	ASN	OD1-CG-ND2	-5.85	116.75	122.60
1	A	123	ILE	CA-C-N	5.84	128.03	120.44
1	A	123	ILE	C-N-CA	5.84	128.03	120.44
1	A	141	GLU	CG-CD-OE2	-5.79	105.09	118.40
1	A	70	SER	CA-C-O	-5.71	111.63	119.05
1	A	237	GLN	OE1-CD-NE2	-5.70	116.90	122.60
1	A	279	ILE	CA-C-O	-5.70	114.73	121.05
1	A	286	VAL	O-C-N	5.69	127.39	121.87
1	A	266	ASN	CA-CB-CG	5.67	118.28	112.60
1	A	264	PHE	CA-C-O	-5.65	114.72	120.71
1	A	104	ALA	CA-C-O	-5.59	115.62	121.55
1	A	211	MET	CB-CA-C	5.59	120.08	110.79
1	A	130	SER	CB-CA-C	5.56	119.63	111.73
1	A	125	ALA	CA-C-O	-5.55	115.00	120.82
1	A	60	PHE	O-C-N	5.47	129.93	123.36
1	A	270	LYS	CA-C-O	-5.47	114.75	120.55
1	A	217	GLY	O-C-N	5.46	127.16	121.97
1	A	200	SER	CA-C-N	5.43	127.56	120.28
1	A	200	SER	C-N-CA	5.43	127.56	120.28
1	A	66	PHE	CA-C-O	-5.42	114.92	120.99
1	A	145	ILE	CA-C-O	5.40	126.66	121.05
1	A	213	ASN	CA-C-N	5.38	128.41	120.82
1	A	213	ASN	C-N-CA	5.38	128.41	120.82
1	A	102	ILE	N-CA-C	5.38	116.19	108.93
1	A	92	ASN	OD1-CG-ND2	-5.35	117.25	122.60
1	A	96	HIS	CG-CD2-NE2	-5.33	101.87	107.20
1	A	44	ILE	CB-CG1-CD1	-5.31	102.65	113.80
1	A	75	ILE	O-C-N	5.29	127.28	121.83
1	A	216	SER	CA-CB-OG	-5.29	100.52	111.10
1	A	146	LYS	CB-CG-CD	5.26	123.39	111.30
1	A	41	ASN	O-C-N	5.25	128.88	122.58
1	A	182	THR	CA-CB-OG1	-5.23	101.75	109.60
1	A	37	GLU	CB-CG-CD	5.20	121.44	112.60
1	A	229	TYR	CA-C-O	-5.20	115.34	121.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	HIS	CA-CB-CG	-5.20	108.60	113.80
1	A	185	ALA	CA-C-N	5.20	127.51	120.44
1	A	185	ALA	C-N-CA	5.20	127.51	120.44
1	A	232	ALA	CA-C-N	-5.20	114.09	122.82
1	A	232	ALA	C-N-CA	-5.20	114.09	122.82
1	A	215	LYS	N-CA-C	-5.19	107.00	113.38
1	A	187	GLY	CA-C-O	-5.18	115.17	120.66
1	A	247	VAL	CB-CA-C	5.18	118.80	110.82
1	A	34	ASN	CA-CB-CG	-5.16	107.44	112.60
1	A	196	ASN	CA-C-O	-5.14	113.00	122.62
1	A	234	LYS	CA-C-O	-5.13	113.94	120.20
1	A	80	LEU	O-C-N	5.11	127.98	122.15
1	A	259	ILE	O-C-N	5.10	129.17	122.94
1	A	70	SER	O-C-N	5.05	129.43	122.46
1	A	280	SER	CA-CB-OG	-5.05	101.01	111.10
1	A	37	GLU	CG-CD-OE1	5.03	129.97	118.40
1	A	42	ALA	CA-C-O	-5.03	115.88	121.51
1	A	149	LYS	CA-CB-CG	-5.03	104.04	114.10
1	A	98	ASN	CA-C-O	5.02	127.67	121.60

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	2029	0	2115	48	0
2	A	207	0	0	9	0
All	All	2236	0	2115	48	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 12.

All (48) 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:285:SER:HB3	2:A:458:HOH:O	1.23	1.29
1:A:177:LYS:HD3	1:A:177:LYS:H	1.07	1.14
1:A:196:ASN:HA	2:A:488:HOH:O	1.62	0.99
1:A:146:LYS:HD2	1:A:146:LYS:H	1.37	0.88
1:A:201:LYS:HE3	1:A:205:LYS:NZ	1.89	0.88
1:A:201:LYS:HE3	1:A:205:LYS:HZ1	1.43	0.81
1:A:229:TYR:CE2	1:A:287:MET:HE2	2.19	0.78
1:A:229:TYR:HE2	1:A:287:MET:CE	2.00	0.74
1:A:201:LYS:O	1:A:205:LYS:HE3	1.91	0.70
1:A:229:TYR:HE2	1:A:287:MET:HE2	1.53	0.70
1:A:177:LYS:HD3	1:A:177:LYS:N	1.92	0.70
1:A:173:SER:OG	1:A:175:LYS:HG3	1.91	0.69
1:A:111:LYS:HE3	2:A:343:HOH:O	1.94	0.67
1:A:229:TYR:N	1:A:229:TYR:HD1	1.94	0.66
1:A:177:LYS:H	1:A:177:LYS:CD	1.97	0.65
1:A:229:TYR:N	1:A:229:TYR:CD1	2.65	0.64
1:A:110:GLU:HG3	1:A:111:LYS:HE2	1.82	0.61
1:A:222:LYS:HG3	2:A:294:HOH:O	2.04	0.57
1:A:64:LYS:HE3	1:A:66:PHE:CZ	2.40	0.56
1:A:175:LYS:C	1:A:175:LYS:HD2	2.31	0.55
1:A:197:GLY:N	2:A:392:HOH:O	2.01	0.55
1:A:198:LYS:HE2	1:A:198:LYS:N	2.21	0.54
1:A:178:LYS:NZ	2:A:460:HOH:O	2.39	0.54
1:A:201:LYS:HE3	1:A:205:LYS:HZ2	1.73	0.54
1:A:33:LEU:HD12	1:A:36:LEU:HD12	1.92	0.51
1:A:169:LEU:HD12	1:A:169:LEU:C	2.36	0.50
1:A:146:LYS:H	1:A:146:LYS:CD	2.04	0.50
1:A:164:ARG:HD2	1:A:168:GLU:HB3	1.94	0.49
1:A:259:ILE:CD1	1:A:287:MET:HE1	2.43	0.49
1:A:238:ALA:HB3	1:A:243:SER:HB2	1.94	0.48
1:A:255:GLN:HG2	1:A:257:GLU:O	2.14	0.48
1:A:229:TYR:CD2	1:A:287:MET:HE2	2.49	0.47
1:A:145:ILE:N	1:A:146:LYS:HD2	2.30	0.46
1:A:44:ILE:HD13	1:A:44:ILE:HG21	1.67	0.46
1:A:163:VAL:HG11	1:A:178:LYS:HG2	1.96	0.46
1:A:225:VAL:HB	1:A:226:PRO:HD2	1.97	0.46
1:A:267:LYS:HD3	1:A:272:ASP:HB3	1.97	0.46
1:A:277:LYS:NZ	2:A:353:HOH:O	2.47	0.45
1:A:137:LYS:NZ	2:A:477:HOH:O	2.32	0.44
1:A:112:TYR:O	1:A:115:LYS:HB2	2.18	0.43
1:A:259:ILE:HD12	1:A:287:MET:HE1	2.00	0.43
1:A:204:LYS:HB3	1:A:205:LYS:HE2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:LYS:HD2	1:A:146:LYS:N	2.19	0.42
1:A:48:ALA:HA	1:A:260:VAL:O	2.20	0.42
1:A:150:GLN:O	1:A:154:GLU:HG3	2.20	0.41
1:A:229:TYR:CE2	1:A:287:MET:CE	2.86	0.41
1:A:251:TYR:CZ	1:A:258:PRO:HB3	2.56	0.41
1:A:288:LYS:NZ	2:A:359:HOH:O	2.52	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	255/257 (99%)	247 (97%)	8 (3%)	0	100 100

There are no Ramachandran outliers to report.

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	227/227 (100%)	205 (90%)	22 (10%)	8 5

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LYS
1	A	32	GLU
1	A	33	LEU
1	A	92	ASN
1	A	94	LYS
1	A	99	LYS
1	A	115	LYS
1	A	130	SER
1	A	146	LYS
1	A	158	LYS
1	A	175	LYS
1	A	177	LYS
1	A	178	LYS
1	A	198	LYS
1	A	201	LYS
1	A	202	GLU
1	A	204	LYS
1	A	205	LYS
1	A	227	LYS
1	A	230	LYS
1	A	233	ASP
1	A	253	LYS

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

Mol	Chain	Res	Type
1	A	34	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.