



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 07:19 pm GMT

PDB ID : 1C58
Title : CRYSTAL STRUCTURE OF CYCLOAMYLOSE 26
Authors : Gessler, K.; Saenger, W.; Nimz, O.
Deposited on : 1999-11-04
Resolution : 0.99 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

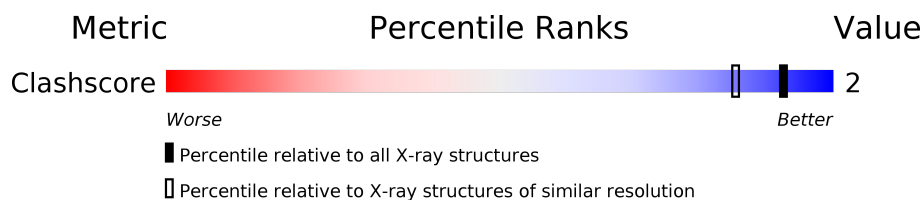
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 0.99 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	1005 (1.08-0.92)

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1307 atoms, of which 571 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 polysaccharide(D) called SUGAR (26-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
1	A	26	Total	C	H	O	0	9
			582	156	287	139		
1	B	26	Total	C	H	O	0	8
			578	156	284	138		

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	92	Total	O	0	0
			92	92		
2	B	55	Total	O	0	0
			55	55		

3 Residue-property plots

There is no protein, DNA or RNA chain in this entry to show sequence plots.

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	21.84Å 22.92Å 29.05Å 87.36° 89.51° 61.98°	Depositor
Resolution (Å)	29.02 – 0.99	Depositor
% Data completeness (in resolution range)	96.7 (29.02-0.99)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.082 , 0.100	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1307	wwPDB-VP
Average B, all atoms (Å ²)	9.0	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: GLC

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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	295	287	206	1	0
1	B	294	284	209	0	0
2	A	92	0	0	2	0
2	B	55	0	0	0	0
All	All	736	571	415	2	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 2.

All (2) 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:14:GLC:H2	2:A:292:HOH:O	2.04	0.58

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

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](#)

69 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	$\# Z > 2$
1	GLC	A	1	1	11,11,12	0.76	0	13,15,17	0.96	1 (7%)
1	GLC	A	10[1]	-	11,11,12	0.90	1 (9%)	13,15,17	0.82	0
1	GLC	A	10[2]	-	11,11,12	0.88	1 (9%)	13,15,17	0.79	0
1	GLC	A	11[1]	-	11,11,12	1.28	1 (9%)	13,15,17	0.89	0
1	GLC	A	11[2]	-	11,11,12	1.26	1 (9%)	13,15,17	0.90	0
1	GLC	A	12	1	11,11,12	0.75	0	13,15,17	0.62	0
1	GLC	A	13	1	11,11,12	0.89	1 (9%)	13,15,17	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	GLC	A	14	1	11,11,12	1.03	1 (9%)	13,15,17	1.43	1 (7%)
1	GLC	A	15	1	11,11,12	1.23	1 (9%)	13,15,17	1.32	1 (7%)
1	GLC	A	16[1]	-	11,11,12	0.97	1 (9%)	13,15,17	1.00	1 (7%)
1	GLC	A	16[2]	-	11,11,12	0.97	1 (9%)	13,15,17	0.98	1 (7%)
1	GLC	A	17	1	11,11,12	0.70	0	13,15,17	0.70	0
1	GLC	A	18	1	11,11,12	1.00	0	13,15,17	0.91	0
1	GLC	A	19	1	11,11,12	0.78	0	13,15,17	0.74	0
1	GLC	A	2	1	11,11,12	0.89	1 (9%)	13,15,17	1.31	2 (15%)
1	GLC	A	20	1	11,11,12	0.68	0	13,15,17	0.77	0
1	GLC	A	21	1	11,11,12	0.89	1 (9%)	13,15,17	0.81	1 (7%)
1	GLC	A	22[1]	-	11,11,12	0.72	0	13,15,17	0.91	0
1	GLC	A	22[2]	-	11,11,12	0.71	0	13,15,17	0.91	0
1	GLC	A	23[1]	-	11,11,12	0.80	0	13,15,17	0.79	0
1	GLC	A	23[2]	-	11,11,12	0.89	0	13,15,17	0.88	0
1	GLC	A	24[1]	-	11,11,12	0.90	1 (9%)	13,15,17	0.72	0
1	GLC	A	24[2]	-	11,11,12	0.90	1 (9%)	13,15,17	0.72	0
1	GLC	A	25	1	11,11,12	0.72	0	13,15,17	0.70	0
1	GLC	A	26	1	11,11,12	0.73	0	13,15,17	1.18	1 (7%)
1	GLC	A	3	1	11,11,12	0.99	0	13,15,17	0.98	0
1	GLC	A	4[1]	-	11,11,12	1.09	1 (9%)	13,15,17	0.89	1 (7%)
1	GLC	A	4[2]	-	11,11,12	1.11	1 (9%)	13,15,17	0.90	1 (7%)
1	GLC	A	5[1]	-	11,11,12	0.87	0	13,15,17	0.83	0
1	GLC	A	5[2]	-	11,11,12	0.91	0	13,15,17	0.83	0
1	GLC	A	6	1	11,11,12	0.83	0	13,15,17	0.86	0
1	GLC	A	7	1	11,11,12	0.75	0	13,15,17	0.81	0
1	GLC	A	8	1	11,11,12	0.70	0	13,15,17	0.85	0
1	GLC	A	9[1]	-	11,11,12	0.93	0	13,15,17	0.79	0
1	GLC	A	9[2]	-	11,11,12	0.94	0	13,15,17	0.86	0
1	GLC	B	101	1	11,11,12	1.05	1 (9%)	13,15,17	0.77	0
1	GLC	B	102	1	11,11,12	1.32	1 (9%)	13,15,17	1.36	1 (7%)
1	GLC	B	103	1	11,11,12	1.03	1 (9%)	13,15,17	0.98	1 (7%)
1	GLC	B	104	1	11,11,12	0.79	1 (9%)	13,15,17	0.72	0
1	GLC	B	105	1	11,11,12	0.87	0	13,15,17	0.88	0
1	GLC	B	106	1	11,11,12	0.84	0	13,15,17	0.88	1 (7%)
1	GLC	B	107	1	11,11,12	0.83	0	13,15,17	0.73	0
1	GLC	B	108	1	11,11,12	1.14	1 (9%)	13,15,17	1.08	1 (7%)
1	GLC	B	109	1	11,11,12	0.94	1 (9%)	13,15,17	0.82	0
1	GLC	B	110	1	11,11,12	0.86	1 (9%)	13,15,17	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	GLC	B	111[1]	-	11,11,12	0.78	0	13,15,17	0.93	0
1	GLC	B	111[2]	-	11,11,12	0.78	0	13,15,17	0.92	0
1	GLC	B	112[1]	-	11,11,12	0.90	0	13,15,17	0.75	0
1	GLC	B	112[2]	-	11,11,12	0.81	0	13,15,17	0.66	0
1	GLC	B	113[1]	-	11,11,12	1.06	0	13,15,17	1.08	0
1	GLC	B	113[2]	-	11,11,12	1.00	0	13,15,17	1.04	0
1	GLC	B	114	1	11,11,12	0.80	0	13,15,17	1.19	0
1	GLC	B	115	1	11,11,12	0.82	0	13,15,17	0.82	0
1	GLC	B	116	1	11,11,12	1.08	1 (9%)	13,15,17	1.14	0
1	GLC	B	117[1]	-	11,11,12	1.06	1 (9%)	13,15,17	1.06	1 (7%)
1	GLC	B	117[2]	-	11,11,12	1.02	1 (9%)	13,15,17	1.04	1 (7%)
1	GLC	B	118	1	11,11,12	0.75	0	13,15,17	0.65	0
1	GLC	B	119[1]	-	11,11,12	1.02	1 (9%)	13,15,17	0.89	0
1	GLC	B	119[2]	-	11,11,12	1.02	1 (9%)	13,15,17	0.85	0
1	GLC	B	120	1	11,11,12	0.90	1 (9%)	13,15,17	0.86	0
1	GLC	B	121	1	11,11,12	0.90	1 (9%)	13,15,17	0.69	0
1	GLC	B	122	1	11,11,12	0.80	0	13,15,17	0.83	0
1	GLC	B	123	1	11,11,12	0.90	0	13,15,17	1.15	1 (7%)
1	GLC	B	124[1]	-	11,11,12	1.24	1 (9%)	13,15,17	0.82	1 (7%)
1	GLC	B	124[2]	-	11,11,12	1.21	1 (9%)	13,15,17	0.88	1 (7%)
1	GLC	B	125[1]	-	11,11,12	0.81	0	13,15,17	0.88	1 (7%)
1	GLC	B	125[2]	-	11,11,12	0.81	0	13,15,17	0.87	1 (7%)
1	GLC	B	126[1]	-	11,11,12	1.02	1 (9%)	13,15,17	0.62	0
1	GLC	B	126[2]	-	11,11,12	1.02	1 (9%)	13,15,17	0.62	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
1	GLC	A	1	1	-	0/2/19/22	0/1/1/1
1	GLC	A	10[1]	-	-	0/2/19/22	0/1/1/1
1	GLC	A	10[2]	-	-	0/2/19/22	0/1/1/1
1	GLC	A	11[1]	-	-	0/2/19/22	0/1/1/1
1	GLC	A	11[2]	-	-	0/2/19/22	0/1/1/1
1	GLC	A	12	1	-	0/2/19/22	0/1/1/1
1	GLC	A	13	1	-	0/2/19/22	0/1/1/1
1	GLC	A	14	1	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GLC	A	15	1	-	0/2/19/22	0/1/1/1
1	GLC	A	16[1]	-	-	0/2/19/22	0/1/1/1
1	GLC	A	16[2]	-	-	0/2/19/22	0/1/1/1
1	GLC	A	17	1	-	0/2/19/22	0/1/1/1
1	GLC	A	18	1	-	0/2/19/22	0/1/1/1
1	GLC	A	19	1	-	0/2/19/22	0/1/1/1
1	GLC	A	2	1	-	0/2/19/22	0/1/1/1
1	GLC	A	20	1	-	0/2/19/22	0/1/1/1
1	GLC	A	21	1	-	0/2/19/22	0/1/1/1
1	GLC	A	22[1]	-	-	0/2/19/22	0/1/1/1
1	GLC	A	22[2]	-	-	0/2/19/22	0/1/1/1
1	GLC	A	23[1]	-	-	0/2/19/22	0/1/1/1
1	GLC	A	23[2]	-	-	0/2/19/22	0/1/1/1
1	GLC	A	24[1]	-	-	0/2/19/22	0/1/1/1
1	GLC	A	24[2]	-	-	0/2/19/22	0/1/1/1
1	GLC	A	25	1	-	0/2/19/22	0/1/1/1
1	GLC	A	26	1	-	0/2/19/22	0/1/1/1
1	GLC	A	3	1	-	0/2/19/22	0/1/1/1
1	GLC	A	4[1]	-	-	0/2/19/22	0/1/1/1
1	GLC	A	4[2]	-	-	0/2/19/22	0/1/1/1
1	GLC	A	5[1]	-	-	0/2/19/22	0/1/1/1
1	GLC	A	5[2]	-	-	0/2/19/22	0/1/1/1
1	GLC	A	6	1	-	0/2/19/22	0/1/1/1
1	GLC	A	7	1	-	0/2/19/22	0/1/1/1
1	GLC	A	8	1	-	0/2/19/22	0/1/1/1
1	GLC	A	9[1]	-	-	0/2/19/22	0/1/1/1
1	GLC	A	9[2]	-	-	0/2/19/22	0/1/1/1
1	GLC	B	101	1	-	0/2/19/22	0/1/1/1
1	GLC	B	102	1	-	0/2/19/22	0/1/1/1
1	GLC	B	103	1	-	0/2/19/22	0/1/1/1
1	GLC	B	104	1	-	0/2/19/22	0/1/1/1
1	GLC	B	105	1	-	0/2/19/22	0/1/1/1
1	GLC	B	106	1	-	0/2/19/22	0/1/1/1
1	GLC	B	107	1	-	0/2/19/22	0/1/1/1
1	GLC	B	108	1	-	0/2/19/22	0/1/1/1
1	GLC	B	109	1	-	0/2/19/22	0/1/1/1
1	GLC	B	110	1	-	0/2/19/22	0/1/1/1
1	GLC	B	111[1]	-	-	0/2/19/22	0/1/1/1
1	GLC	B	111[2]	-	-	0/2/19/22	0/1/1/1
1	GLC	B	112[1]	-	-	0/2/19/22	0/1/1/1
1	GLC	B	112[2]	-	-	0/2/19/22	0/1/1/1
1	GLC	B	113[1]	-	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GLC	B	113[2]	-	-	0/2/19/22	0/1/1/1
1	GLC	B	114	1	-	0/2/19/22	0/1/1/1
1	GLC	B	115	1	-	0/2/19/22	0/1/1/1
1	GLC	B	116	1	-	0/2/19/22	0/1/1/1
1	GLC	B	117[1]	-	-	0/2/19/22	0/1/1/1
1	GLC	B	117[2]	-	-	0/2/19/22	0/1/1/1
1	GLC	B	118	1	-	0/2/19/22	0/1/1/1
1	GLC	B	119[1]	-	-	0/2/19/22	0/1/1/1
1	GLC	B	119[2]	-	-	0/2/19/22	0/1/1/1
1	GLC	B	120	1	-	0/2/19/22	0/1/1/1
1	GLC	B	121	1	-	0/2/19/22	0/1/1/1
1	GLC	B	122	1	-	0/2/19/22	0/1/1/1
1	GLC	B	123	1	-	0/2/19/22	0/1/1/1
1	GLC	B	124[1]	-	-	0/2/19/22	0/1/1/1
1	GLC	B	124[2]	-	-	0/2/19/22	0/1/1/1
1	GLC	B	125[1]	-	-	0/2/19/22	0/1/1/1
1	GLC	B	125[2]	-	-	0/2/19/22	0/1/1/1
1	GLC	B	126[1]	-	-	0/2/19/22	0/1/1/1
1	GLC	B	126[2]	-	-	0/2/19/22	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	102	GLC	O5-C1	-3.38	1.38	1.43
1	B	124[2]	GLC	O5-C1	-3.14	1.38	1.43
1	B	124[1]	GLC	O5-C1	-3.14	1.38	1.43
1	A	15	GLC	O5-C1	-3.10	1.38	1.43
1	A	11[2]	GLC	O5-C1	-3.04	1.38	1.43
1	A	11[1]	GLC	O5-C1	-3.04	1.38	1.43
1	A	4[2]	GLC	O5-C1	-2.97	1.38	1.43
1	A	4[1]	GLC	O5-C1	-2.97	1.38	1.43
1	A	14	GLC	C2-C3	-2.92	1.48	1.52
1	B	108	GLC	O5-C1	-2.58	1.39	1.43
1	B	101	GLC	O5-C1	-2.51	1.39	1.43
1	B	126[2]	GLC	O5-C1	-2.45	1.39	1.43
1	B	126[1]	GLC	O5-C1	-2.45	1.39	1.43
1	A	16[1]	GLC	O5-C1	-2.43	1.39	1.43
1	A	16[2]	GLC	O5-C1	-2.43	1.39	1.43
1	B	103	GLC	O5-C1	-2.41	1.39	1.43
1	B	116	GLC	O5-C1	-2.37	1.39	1.43
1	B	117[1]	GLC	O5-C1	-2.37	1.39	1.43
1	B	117[2]	GLC	O5-C1	-2.37	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	13	GLC	O5-C1	-2.33	1.39	1.43
1	B	109	GLC	O5-C1	-2.32	1.39	1.43
1	B	104	GLC	O5-C1	-2.17	1.40	1.43
1	B	120	GLC	O5-C1	-2.17	1.40	1.43
1	A	2	GLC	O5-C1	-2.13	1.40	1.43
1	B	119[2]	GLC	O5-C1	-2.13	1.40	1.43
1	B	119[1]	GLC	O5-C1	-2.13	1.40	1.43
1	A	24[1]	GLC	O5-C1	-2.12	1.40	1.43
1	A	24[2]	GLC	O5-C1	-2.12	1.40	1.43
1	A	21	GLC	O5-C1	-2.09	1.40	1.43
1	B	121	GLC	C2-C3	-2.08	1.49	1.52
1	B	110	GLC	O5-C1	-2.08	1.40	1.43
1	A	10[2]	GLC	O5-C1	-2.06	1.40	1.43
1	A	10[1]	GLC	O5-C1	-2.06	1.40	1.43

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	GLC	O3-C3-C2	-2.33	105.78	110.02
1	A	1	GLC	C1-C2-C3	2.02	112.21	109.65
1	A	4[2]	GLC	C3-C4-C5	2.03	113.79	110.22
1	A	4[1]	GLC	C3-C4-C5	2.03	113.79	110.22
1	B	117[1]	GLC	C1-O5-C5	2.06	115.01	112.17
1	B	117[2]	GLC	C1-O5-C5	2.06	115.01	112.17
1	B	123	GLC	C1-O5-C5	2.07	115.02	112.17
1	A	21	GLC	C1-O5-C5	2.10	115.06	112.17
1	A	16[1]	GLC	C1-O5-C5	2.18	115.17	112.17
1	A	16[2]	GLC	C1-O5-C5	2.18	115.17	112.17
1	B	125[1]	GLC	C1-O5-C5	2.21	115.22	112.17
1	B	125[2]	GLC	C1-O5-C5	2.21	115.22	112.17
1	A	2	GLC	C1-O5-C5	2.26	115.29	112.17
1	B	106	GLC	C1-O5-C5	2.27	115.30	112.17
1	B	103	GLC	C1-O5-C5	2.33	115.37	112.17
1	B	124[2]	GLC	C1-O5-C5	2.36	115.41	112.17
1	B	124[1]	GLC	C1-O5-C5	2.36	115.41	112.17
1	B	108	GLC	C3-C4-C5	2.39	114.43	110.22
1	A	2	GLC	C1-C2-C3	2.59	112.94	109.65
1	B	102	GLC	C1-O5-C5	2.78	116.00	112.17
1	A	15	GLC	C1-O5-C5	3.36	116.79	112.17
1	A	14	GLC	C1-C2-C3	3.80	114.47	109.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	14	GLC	1	0

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

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.