



wwPDB X-ray Structure Validation Summary Report

Jul 11, 2014 – 04:24 PM EDT

PDB ID : 4LMX
Title : Light harvesting complex PE555 from the cryptophyte Hemiselmis andersenii CCMP644
Authors : Harrop, S.J.; Wilk, K.E.; Curmi, P.M.G.
Deposited on : 2013-07-11
Resolution : 1.80 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

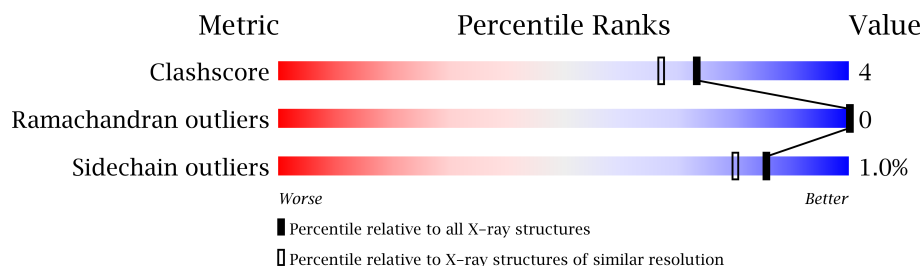
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	FAILED
Xtriage (Phenix)	:	dev-1439
EDS	:	FAILED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23161

1 Overall quality at a glance

The reported resolution of this entry is 1.80 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	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	62	
2	B	177	
2	D	177	
2	F	177	
2	H	177	
2	J	177	
2	L	177	
3	C	67	
4	E	74	
4	G	74	
4	I	74	
4	K	74	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14008 atoms, of which 0 are hydrogen and 0 are deuterium.

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 cryptophyte phycoerythrin (alpha-2 chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	62	Total	C	N	O	S	0	1	0
			466	285	80	94	7			

- Molecule 2 is a protein called cryptophyte phycoerythrin (beta chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	177	Total	C	N	O	S	0	2	0
			1292	800	220	262	10			
2	D	175	Total	C	N	O	S	0	0	0
			1267	784	217	257	9			
2	F	176	Total	C	N	O	S	0	1	0
			1284	795	220	260	9			
2	H	176	Total	C	N	O	S	0	1	0
			1284	795	220	260	9			
2	J	175	Total	C	N	O	S	0	4	0
			1294	798	222	265	9			
2	L	175	Total	C	N	O	S	0	1	0
			1276	789	219	259	9			

- Molecule 3 is a protein called cryptophyte phycoerythrin (alpha-1 chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	66	Total	C	N	O	S	0	0	0
			480	296	85	94	5			

- Molecule 4 is a protein called cryptophyte phycoerythrin (alpha-1/alpha-2 chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	66	Total	C	N	O	S	0	7	0
			536	331	94	105	6			
4	G	65	Total	C	N	O	S	0	7	0
			530	328	93	103	6			

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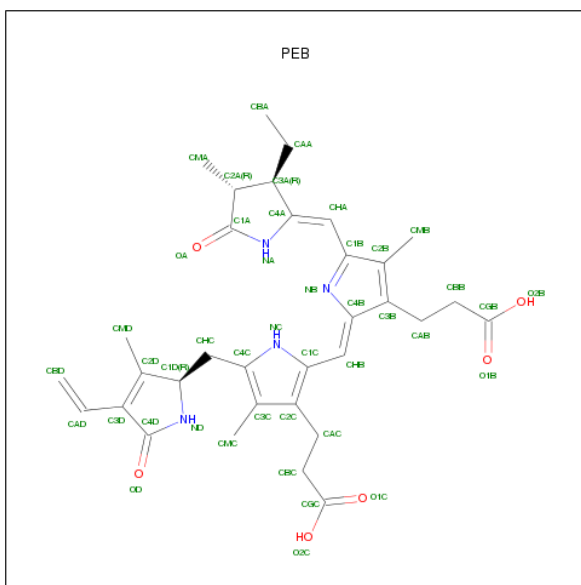
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	66	Total	C	N	O	S	0	7	0
			536	331	94	105	6			
4	K	66	Total	C	N	O	S	0	7	0
			536	331	94	105	6			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	44	LYS	GLY	MICROHETEROGENEITY	PDB 4LMX
E	45	MET	PHE	MICROHETEROGENEITY	PDB 4LMX
E	51	THR	ALA	MICROHETEROGENEITY	PDB 4LMX
E	58	ASN	GLY	MICROHETEROGENEITY	PDB 4LMX
E	59	THR	ILE	MICROHETEROGENEITY	PDB 4LMX
E	61	LEU	ARG	MICROHETEROGENEITY	PDB 4LMX
E	62	LEU	PHE	MICROHETEROGENEITY	PDB 4LMX
G	44	LYS	GLY	MICROHETEROGENEITY	PDB 4LMX
G	45	MET	PHE	MICROHETEROGENEITY	PDB 4LMX
G	51	THR	ALA	MICROHETEROGENEITY	PDB 4LMX
G	58	ASN	GLY	MICROHETEROGENEITY	PDB 4LMX
G	59	THR	ILE	MICROHETEROGENEITY	PDB 4LMX
G	61	LEU	ARG	MICROHETEROGENEITY	PDB 4LMX
G	62	LEU	PHE	MICROHETEROGENEITY	PDB 4LMX
I	44	LYS	GLY	MICROHETEROGENEITY	PDB 4LMX
I	45	MET	PHE	MICROHETEROGENEITY	PDB 4LMX
I	51	THR	ALA	MICROHETEROGENEITY	PDB 4LMX
I	58	ASN	GLY	MICROHETEROGENEITY	PDB 4LMX
I	59	THR	ILE	MICROHETEROGENEITY	PDB 4LMX
I	61	LEU	ARG	MICROHETEROGENEITY	PDB 4LMX
I	62	LEU	PHE	MICROHETEROGENEITY	PDB 4LMX
K	44	LYS	GLY	MICROHETEROGENEITY	PDB 4LMX
K	45	MET	PHE	MICROHETEROGENEITY	PDB 4LMX
K	51	THR	ALA	MICROHETEROGENEITY	PDB 4LMX
K	58	ASN	GLY	MICROHETEROGENEITY	PDB 4LMX
K	59	THR	ILE	MICROHETEROGENEITY	PDB 4LMX
K	61	LEU	ARG	MICROHETEROGENEITY	PDB 4LMX
K	62	LEU	PHE	MICROHETEROGENEITY	PDB 4LMX

- Molecule 5 is PHYCOERYTHROBILIN (three-letter code: PEB) (formula: $C_{33}H_{40}N_4O_6$).



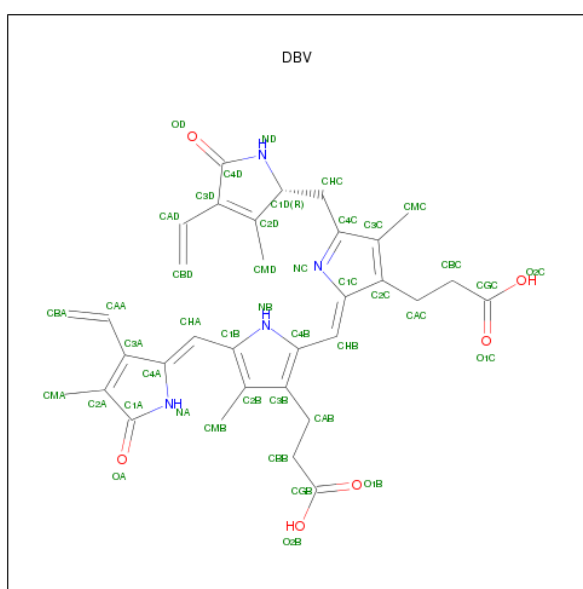
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 43	C 33	N 4	O 6	0	0
5	B	1	Total 43	C 33	N 4	O 6	0	0
5	B	1	Total 43	C 33	N 4	O 6	0	0
5	C	1	Total 43	C 33	N 4	O 6	0	0
5	D	1	Total 43	C 33	N 4	O 6	0	0
5	D	1	Total 43	C 33	N 4	O 6	0	0
5	E	1	Total 43	C 33	N 4	O 6	0	0
5	F	1	Total 43	C 33	N 4	O 6	0	0
5	F	1	Total 43	C 33	N 4	O 6	0	0
5	G	1	Total 43	C 33	N 4	O 6	0	0
5	H	1	Total 43	C 33	N 4	O 6	0	0
5	H	1	Total 43	C 33	N 4	O 6	0	0
5	I	1	Total 43	C 33	N 4	O 6	0	0
5	J	1	Total 43	C 33	N 4	O 6	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	J	1	Total	C	N	O	0	0
			43	33	4	6		
5	K	1	Total	C	N	O	0	0
			43	33	4	6		
5	L	1	Total	C	N	O	0	0
			43	33	4	6		
5	L	1	Total	C	N	O	0	0
			43	33	4	6		

- Molecule 6 is 15,16-DIHYDROBILIVERDIN (three-letter code: DBV) (formula: $C_{33}H_{36}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			43	33	4	6		
6	D	1	Total	C	N	O	0	0
			43	33	4	6		
6	F	1	Total	C	N	O	0	0
			43	33	4	6		
6	H	1	Total	C	N	O	0	0
			43	33	4	6		
6	J	1	Total	C	N	O	0	0
			43	33	4	6		
6	L	1	Total	C	N	O	0	0
			43	33	4	6		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	111	Total 111	O 111	0	0
7	B	282	Total 282	O 282	0	0
7	C	136	Total 136	O 136	0	0
7	D	248	Total 248	O 248	0	0
7	E	129	Total 129	O 129	0	0
7	F	274	Total 274	O 274	0	0
7	G	97	Total 97	O 97	0	0
7	H	254	Total 254	O 254	0	0
7	I	116	Total 116	O 116	0	0
7	J	271	Total 271	O 271	0	0
7	K	104	Total 104	O 104	0	0
7	L	173	Total 173	O 173	0	0

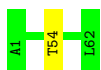
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 failed to run properly.

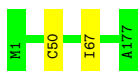
- Molecule 1: cryptophyte phycoerythrin (alpha-2 chain)

Chain A: 



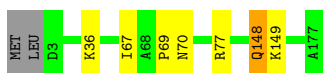
- Molecule 2: cryptophyte phycoerythrin (beta chain)

Chain B: 



- Molecule 2: cryptophyte phycoerythrin (beta chain)

Chain D: 



- Molecule 2: cryptophyte phycoerythrin (beta chain)

Chain F: 



- Molecule 2: cryptophyte phycoerythrin (beta chain)

Chain H: 



- Molecule 2: cryptophyte phycoerythrin (beta chain)

Chain J: 



- Molecule 2: cryptophyte phycoerythrin (beta chain)

Chain L: 



- Molecule 3: cryptophyte phycoerythrin (alpha-1 chain)

Chain C: 



- Molecule 4: cryptophyte phycoerythrin (alpha-1/alpha-2 chain)

Chain E: 



- Molecule 4: cryptophyte phycoerythrin (alpha-1/alpha-2 chain)

Chain G: 



- Molecule 4: cryptophyte phycoerythrin (alpha-1/alpha-2 chain)

Chain I: 



- Molecule 4: cryptophyte phycoerythrin (alpha-1/alpha-2 chain)

Chain K: 



4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.07Å 76.74Å 142.59Å 90.00° 92.86° 90.00°	Depositor
Resolution (Å)	18.64 – 1.80	Depositor
% Data completeness (in resolution range)	99.8 (18.64-1.80)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 1.80Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2.867)	Depositor
R, R_{free}	0.158 , 0.214	Depositor
Wilson B-factor (Å ²)	16.5	Xtriage
Anisotropy	0.535	Xtriage
Estimated twinning fraction	0.015 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	4 of 131573 reflections (0.003%)	Xtriage
Total number of atoms	14008	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.03 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.2047e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PEB, LYZ, DBV

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	0.35	0/458	0.53	0/607
2	B	0.34	0/1308	0.47	0/1764
2	D	0.34	0/1280	0.47	0/1727
2	F	0.34	0/1297	0.46	0/1750
2	H	0.34	0/1297	0.45	0/1750
2	J	0.34	0/1307	0.49	0/1763
2	L	0.30	0/1289	0.44	0/1739
3	C	0.34	0/474	0.54	0/628
4	E	0.35	0/522	0.56	0/678
4	G	0.56	2/516 (0.4%)	0.55	0/670
4	I	0.34	0/522	0.63	1/678 (0.1%)
4	K	0.38	0/522	0.52	0/678
All	All	0.35	2/10792 (0.0%)	0.49	1/14432 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	58[B]	GLY	C-N	-7.35	1.17	1.34
4	G	44[B]	GLY	C-N	-7.28	1.17	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	61[B]	ARG	NE-CZ-NH1	5.84	123.22	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	466	0	473	1	0
2	B	1292	0	1305	1	0
2	D	1267	0	1273	5	0
2	F	1284	0	1288	6	0
2	H	1284	0	1287	8	0
2	J	1294	0	1289	3	0
2	L	1276	0	1277	10	0
3	C	480	0	480	4	0
4	E	536	0	531	8	0
4	G	530	0	526	7	0
4	I	536	0	530	6	0
4	K	536	0	532	9	0
5	A	43	0	37	1	0
5	B	86	0	74	2	0
5	C	43	0	37	0	0
5	D	86	0	74	2	0
5	E	43	0	37	2	0
5	F	86	0	74	4	0
5	G	43	0	37	2	0
5	H	86	0	74	2	0
5	I	43	0	37	2	0
5	J	86	0	74	2	0
5	K	43	0	37	0	0
5	L	86	0	74	3	0
6	B	43	0	32	1	0
6	D	43	0	32	5	0
6	F	43	0	32	1	0
6	H	43	0	32	2	0
6	J	43	0	32	0	0
6	L	43	0	32	0	0
7	A	111	0	0	0	0
7	B	282	0	0	0	0
7	C	136	0	0	1	0
7	D	248	0	0	0	0
7	E	129	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	F	274	0	0	3	1
7	G	97	0	0	2	0
7	H	254	0	0	0	0
7	I	116	0	0	0	1
7	J	271	0	0	3	0
7	K	104	0	0	4	0
7	L	173	0	0	0	0
All	All	14008	0	11649	70	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

The worst 5 of 70 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:K:63:GLY:N	2:L:148[A]:GLN:NE2	1.67	1.39
4:G:63:GLY:N	2:H:148[A]:GLN:NE2	1.73	1.34
4:I:62[A]:LEU:HD12	2:L:148[A]:GLN:HG3	1.60	0.82
4:E:62[A]:LEU:HD12	2:H:148[A]:GLN:NE2	2.03	0.73
2:J:129:ARG:NH1	7:J:458:HOH:O	2.21	0.73

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:F:504:HOH:O	7:I:279:HOH:O[2_756]	2.11	0.09

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	60/62 (97%)	60 (100%)	0	0	100	100
2	B	177/177 (100%)	175 (99%)	2 (1%)	0	100	100
2	D	173/177 (98%)	171 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
2	H	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
2	J	177/177 (100%)	175 (99%)	2 (1%)	0	100	100
2	L	174/177 (98%)	172 (99%)	2 (1%)	0	100	100
3	C	63/67 (94%)	63 (100%)	0	0	100	100
4	E	56/74 (76%)	56 (100%)	0	0	100	100
4	G	55/74 (74%)	55 (100%)	0	0	100	100
4	I	56/74 (76%)	56 (100%)	0	0	100	100
4	K	56/74 (76%)	55 (98%)	1 (2%)	0	100	100
All	All	1397/1487 (94%)	1382 (99%)	15 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	49/48 (102%)	49 (100%)	0	100	100
2	B	142/140 (101%)	141 (99%)	1 (1%)	91	88
2	D	138/140 (99%)	136 (99%)	2 (1%)	78	69
2	F	140/140 (100%)	138 (99%)	2 (1%)	78	69
2	H	140/140 (100%)	139 (99%)	1 (1%)	91	88
2	J	142/140 (101%)	141 (99%)	1 (1%)	91	88
2	L	139/140 (99%)	137 (99%)	2 (1%)	78	69
3	C	47/48 (98%)	47 (100%)	0	100	100
4	E	54/55 (98%)	54 (100%)	0	100	100
4	G	53/55 (96%)	53 (100%)	0	100	100
4	I	54/55 (98%)	52 (96%)	2 (4%)	45	26
4	K	54/55 (98%)	54 (100%)	0	100	100
All	All	1152/1156 (100%)	1141 (99%)	11 (1%)	85	80

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	144	ASN
2	H	50	CYS
2	J	50	CYS
2	F	50	CYS
4	I	62[B]	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.5 Carbohydrates ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.6 Ligand geometry ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.7 Other polymers ⓘ

Mogul failed to run properly - this section will therefore be empty.

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 failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.