



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 11:52 pm GMT

PDB ID : 1IO8
Title : Thermophilic cytochrome P450 (CYP119) from *Sulfolobus solfataricus*: High resolution structural origin of its thermostability and functional properties
Authors : Park, S.-Y.; Yamane, K.; Adachi, S.; Shiro, Y.; Sligar, S.G.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2001-02-08
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

<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

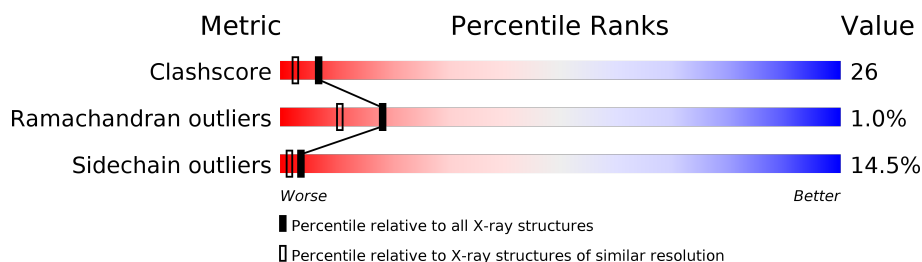
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (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 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	368	 54% 38% 7% •
1	B	368	 52% 35% 10% •

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6334 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 CYTOCHROME P450 CYP119.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			3007	1925	517	559	6			
1	B	359	Total	C	N	O	S	0	0	0
			2958	1893	509	550	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	LEU	PHE	ENGINEERED	UNP Q55080
B	524	LEU	PHE	ENGINEERED	UNP Q55080

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is water.

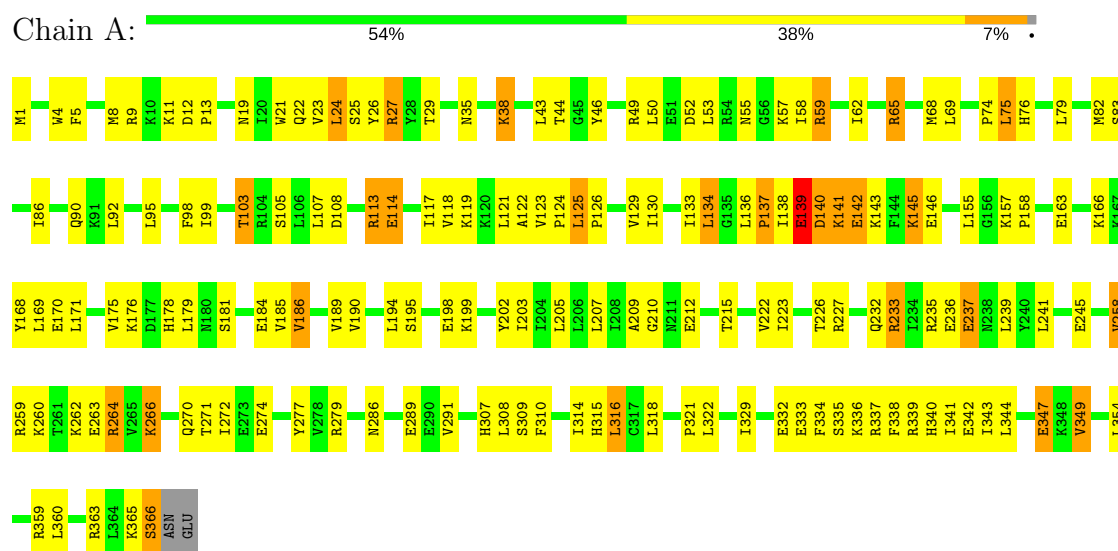
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	132	Total	O	0	0
			132	132		
3	B	151	Total	O	0	0
			151	151		

3 Residue-property plots

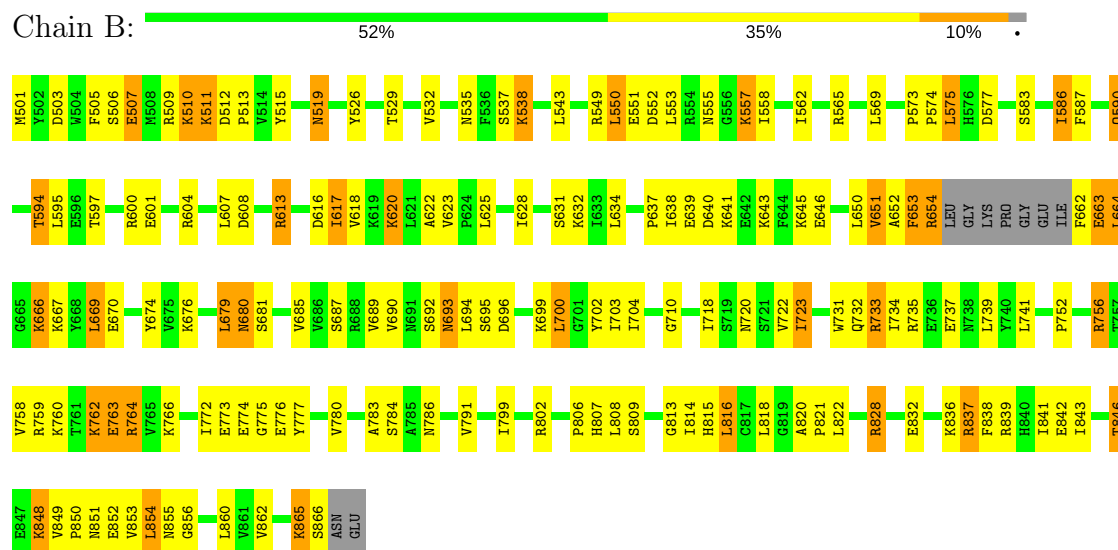
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: CYTOCHROME P450 CYP119



• Molecule 1: CYTOCHROME P450 CYP119



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	85.52Å 85.52Å 221.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	94.5 (20.00-2.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.230 , 0.307	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6334	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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: HEM

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	0.41	0/3070	0.65	0/4149
1	B	0.44	0/3019	0.64	0/4079
All	All	0.43	0/6089	0.64	0/8228

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	3007	0	3043	156	0
1	B	2958	0	2985	157	0
2	A	43	0	30	3	0
2	B	43	0	30	1	0
3	A	132	0	0	7	0
3	B	151	0	0	15	0
All	All	6334	0	6088	312	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 26.

All (312) 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:851:ASN:ND2	1:B:853:VAL:H	1.60	0.99
1:B:613:ARG:HB3	1:B:613:ARG:HH11	1.26	0.98
1:B:764:ARG:HB2	1:B:764:ARG:HH11	1.24	0.98
1:B:586:ILE:HD11	1:B:818:LEU:HD21	1.47	0.97
1:A:223:ILE:HD11	1:A:360:LEU:HD11	1.48	0.96
1:B:586:ILE:HG23	1:B:685:VAL:HG21	1.49	0.91
1:A:347:GLU:HB2	1:A:359:ARG:HB2	1.52	0.91
1:B:680:ASN:HD22	1:B:680:ASN:H	1.19	0.90
1:A:59:ARG:H	1:A:59:ARG:NE	1.70	0.88
1:A:58:ILE:HA	1:A:59:ARG:HH21	1.40	0.86
1:B:786:ASN:HD21	1:B:808:LEU:H	1.22	0.85
1:B:851:ASN:ND2	1:B:854:LEU:H	1.76	0.84
1:A:99:ILE:O	1:A:103:THR:HG23	1.77	0.82
1:B:652:ALA:HB3	1:B:654:ARG:HH21	1.42	0.82
1:B:763:GLU:HA	1:B:774:GLU:HB2	1.62	0.82
1:B:519:ASN:N	1:B:519:ASN:HD22	1.77	0.82
1:B:613:ARG:HB3	1:B:613:ARG:NH1	1.95	0.82
1:A:347:GLU:HG3	1:A:359:ARG:HH21	1.44	0.81
1:B:652:ALA:HB3	1:B:654:ARG:NH2	1.94	0.81
1:A:59:ARG:H	1:A:59:ARG:CZ	1.93	0.80
1:A:58:ILE:HA	1:A:59:ARG:NH2	1.96	0.79
1:B:849:VAL:HG12	1:B:856:GLY:O	1.83	0.79
1:A:136:LEU:HD12	1:A:207:LEU:HD13	1.67	0.76
1:B:828:ARG:O	1:B:832:GLU:HG3	1.84	0.76
1:A:55:ASN:HB3	1:A:57:LYS:HG2	1.67	0.75
1:B:503:ASP:OD2	1:B:506:SER:HB2	1.85	0.75
1:B:851:ASN:HD22	1:B:853:VAL:H	1.30	0.75
1:A:264:ARG:HB2	1:A:264:ARG:HH11	1.50	0.75
1:A:307:HIS:HD2	1:A:309:SER:H	1.32	0.74
1:A:166:LYS:O	1:A:170:GLU:HG3	1.87	0.74
1:B:843:ILE:HD12	1:B:860:LEU:HD21	1.70	0.73
1:B:764:ARG:CB	1:B:764:ARG:HH11	2.00	0.73
1:A:27:ARG:HG2	1:A:27:ARG:HH11	1.54	0.72
1:A:82:MET:CE	1:A:189:VAL:HA	2.19	0.72
1:A:344:LEU:HD21	1:A:363:ARG:HB2	1.72	0.72
1:A:349:VAL:HG21	3:A:482:HOH:O	1.88	0.72
1:A:123:VAL:HB	1:A:124:PRO:HD3	1.72	0.71
1:B:651:VAL:O	1:B:651:VAL:HG12	1.91	0.71
1:B:573:PRO:HB3	1:B:577:ASP:OD1	1.91	0.70
1:A:286:ASN:HD21	1:A:308:LEU:H	1.40	0.70
1:A:108:ASP:HA	1:A:337:ARG:NH2	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ARG:NE	1:A:59:ARG:N	2.41	0.69
1:A:49:ARG:HG3	1:A:49:ARG:HH11	1.56	0.69
1:A:264:ARG:HH11	1:A:264:ARG:CB	2.07	0.68
1:B:616:ASP:O	1:B:620:LYS:HG2	1.92	0.68
1:B:543:LEU:HD22	1:B:777:TYR:HE2	1.57	0.68
1:B:628:ILE:HG12	1:B:638:ILE:HD11	1.74	0.68
1:B:600:ARG:O	1:B:604:ARG:HG3	1.95	0.66
1:B:590:GLN:O	1:B:594:THR:HG23	1.95	0.66
1:A:113:ARG:HB3	1:A:113:ARG:NH1	2.11	0.66
1:B:848:LYS:NZ	1:B:855:ASN:HD22	1.93	0.65
1:A:74:PRO:HD2	3:A:468:HOH:O	1.96	0.65
1:B:676:LYS:HA	1:B:679:LEU:HD22	1.79	0.64
1:A:199:LYS:O	1:A:203:ILE:HG12	1.98	0.64
1:B:519:ASN:H	1:B:519:ASN:HD22	1.45	0.64
1:B:762:LYS:HD2	3:B:211:HOH:O	1.97	0.64
1:A:124:PRO:HB3	1:A:141:LYS:HE2	1.80	0.64
1:B:666:LYS:O	1:B:670:GLU:HG3	1.99	0.63
1:B:807:HIS:HD2	1:B:809:SER:H	1.46	0.63
1:B:586:ILE:HD11	1:B:818:LEU:CD2	2.27	0.63
1:B:851:ASN:HD22	1:B:853:VAL:N	1.97	0.63
1:A:95:LEU:HD11	1:A:133:ILE:HG12	1.80	0.62
1:A:142:GLU:O	1:A:146:GLU:HG3	2.00	0.62
1:A:27:ARG:HG2	1:A:27:ARG:NH1	2.14	0.62
1:A:86:ILE:HG21	1:A:185:VAL:HG13	1.82	0.62
1:B:839:ARG:HB3	1:B:866:SER:HA	1.81	0.62
1:B:510:LYS:HE2	1:B:511:LYS:HE2	1.80	0.62
1:A:58:ILE:HG23	1:A:59:ARG:NH2	2.15	0.61
1:B:510:LYS:HD3	1:B:511:LYS:HG2	1.81	0.61
1:A:49:ARG:HB3	1:A:58:ILE:HD13	1.82	0.61
1:B:507:GLU:OE1	1:B:511:LYS:HD2	2.00	0.61
1:B:692:SER:OG	1:B:694:LEU:HG	2.00	0.61
1:A:130:ILE:HG13	1:A:134:LEU:HD22	1.81	0.61
1:A:332:GLU:O	1:A:336:LYS:HG3	2.00	0.61
1:A:113:ARG:O	1:A:363:ARG:HG3	2.01	0.60
1:A:237:GLU:HB2	1:A:239:LEU:HG	1.82	0.60
1:B:618:VAL:HA	1:B:622:ALA:HB3	1.83	0.60
1:B:519:ASN:N	1:B:519:ASN:ND2	2.49	0.60
1:A:118:VAL:HG23	1:A:360:LEU:HB2	1.83	0.59
1:A:176:LYS:HA	1:A:179:LEU:CD1	2.32	0.59
1:A:264:ARG:HG3	1:A:264:ARG:O	2.03	0.59
1:A:117:ILE:HD11	1:A:222:VAL:HG11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:641:LYS:HE2	3:B:192:HOH:O	2.02	0.58
1:A:185:VAL:HG13	3:A:511:HOH:O	2.03	0.58
1:A:82:MET:HE1	1:A:189:VAL:HA	1.83	0.58
1:A:83:SER:O	1:A:86:ILE:HG12	2.04	0.58
1:A:138:ILE:C	1:A:140:ASP:H	2.06	0.58
1:B:720:ASN:O	1:B:723:ILE:HG22	2.02	0.58
1:B:552:ASP:HA	1:B:555:ASN:HB2	1.85	0.58
1:A:118:VAL:HA	1:A:122:ALA:HB3	1.85	0.58
1:A:13:PRO:CB	1:A:25:SER:HB3	2.34	0.57
1:B:731:TRP:O	1:B:735:ARG:HG3	2.04	0.57
1:A:334:PHE:HZ	1:A:341:ILE:HD12	1.69	0.57
1:B:773:GLU:HB2	1:B:776:GLU:OE2	2.05	0.57
1:A:49:ARG:HB3	1:A:58:ILE:CD1	2.35	0.57
1:B:586:ILE:HD12	1:B:587:PHE:CE1	2.40	0.57
1:A:233:ARG:O	1:A:237:GLU:HG3	2.05	0.56
1:A:163:GLU:HG2	3:A:448:HOH:O	2.05	0.56
1:A:44:THR:HB	1:A:65:ARG:HB3	1.87	0.56
1:B:696:ASP:HB2	3:B:143:HOH:O	2.05	0.56
1:B:693:ASN:N	1:B:693:ASN:HD22	2.04	0.55
1:A:43:LEU:CD2	1:A:260:LYS:HB2	2.36	0.55
1:A:25:SER:O	1:A:29:THR:HG23	2.07	0.55
1:A:347:GLU:CB	1:A:359:ARG:HB2	2.31	0.55
1:A:335:SER:HA	1:A:338:PHE:CE2	2.42	0.55
1:B:680:ASN:ND2	1:B:680:ASN:H	1.98	0.55
1:A:334:PHE:CZ	1:A:341:ILE:HD12	2.41	0.55
1:B:849:VAL:HG21	3:B:85:HOH:O	2.06	0.55
1:B:583:SER:O	1:B:586:ILE:HG13	2.07	0.55
1:B:764:ARG:HA	1:B:772:ILE:O	2.07	0.54
1:B:820:ALA:HB3	1:B:821:PRO:HD3	1.87	0.54
1:B:848:LYS:NZ	1:B:855:ASN:ND2	2.55	0.54
1:B:535:ASN:HB2	3:B:186:HOH:O	2.06	0.54
1:B:538:LYS:HE3	1:B:763:GLU:OE2	2.07	0.54
1:B:583:SER:O	1:B:586:ILE:CG1	2.56	0.54
1:A:226:THR:HG21	1:A:343:ILE:HG12	1.89	0.54
1:A:184:GLU:HG3	1:A:185:VAL:N	2.22	0.54
1:B:764:ARG:HG3	1:B:764:ARG:O	2.07	0.54
1:B:865:LYS:HG3	1:B:866:SER:H	1.73	0.53
1:B:617:ILE:HD11	1:B:860:LEU:HD13	1.90	0.53
1:B:505:PHE:O	1:B:509:ARG:HG3	2.08	0.53
1:A:289:GLU:CD	1:A:289:GLU:H	2.12	0.53
1:A:58:ILE:HA	1:A:59:ARG:CZ	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:758:VAL:HG22	1:B:759:ARG:N	2.23	0.53
1:B:848:LYS:HZ1	1:B:855:ASN:HD22	1.55	0.53
1:B:799:ILE:HD12	1:B:802:ARG:NH2	2.24	0.53
1:B:639:GLU:CD	1:B:639:GLU:H	2.13	0.52
1:B:685:VAL:O	1:B:689:VAL:HG23	2.08	0.52
1:B:756:ARG:NH2	1:B:852:GLU:HB3	2.25	0.52
1:B:600:ARG:HD2	1:B:604:ARG:NH2	2.24	0.52
1:A:22:GLN:HG3	3:A:525:HOH:O	2.09	0.52
1:A:35:ASN:ND2	1:A:38:LYS:HG3	2.25	0.52
1:B:763:GLU:CA	1:B:774:GLU:HB2	2.38	0.52
1:B:773:GLU:O	1:B:776:GLU:HG3	2.10	0.52
1:A:212:GLU:OE2	1:A:354:LEU:HD13	2.10	0.52
1:A:124:PRO:HA	1:A:141:LYS:HZ1	1.75	0.52
1:A:245:GLU:OE2	1:A:307:HIS:HE1	1.91	0.52
1:A:113:ARG:CZ	1:A:113:ARG:HB3	2.38	0.51
1:B:505:PHE:HB3	1:B:509:ARG:NH1	2.25	0.51
1:B:832:GLU:O	1:B:836:LYS:HG3	2.09	0.51
1:B:849:VAL:O	1:B:849:VAL:HG13	2.10	0.51
1:A:13:PRO:HB2	1:A:25:SER:HB3	1.92	0.51
1:A:171:LEU:O	1:A:175:VAL:HG23	2.11	0.51
1:A:108:ASP:HA	1:A:337:ARG:HH21	1.74	0.51
1:B:550:LEU:HD11	1:B:575:LEU:HG	1.93	0.51
1:B:851:ASN:HD22	1:B:854:LEU:H	1.57	0.51
1:A:62:ILE:HD12	1:A:62:ILE:N	2.26	0.51
1:B:574:PRO:HD2	3:B:146:HOH:O	2.10	0.51
1:B:652:ALA:CB	1:B:654:ARG:HH21	2.17	0.51
1:A:307:HIS:CD2	1:A:309:SER:HB2	2.46	0.50
1:A:50:LEU:O	1:A:53:LEU:HB2	2.11	0.50
1:B:662:PHE:CG	1:B:663:GLU:N	2.80	0.50
1:A:13:PRO:HB3	1:A:25:SER:HB3	1.93	0.50
1:A:123:VAL:O	1:A:126:PRO:HD2	2.12	0.50
1:A:314:ILE:HG13	1:A:315:HIS:CD2	2.46	0.50
1:A:263:GLU:HA	1:A:274:GLU:HB2	1.92	0.50
1:B:600:ARG:HD3	3:B:132:HOH:O	2.12	0.50
1:A:175:VAL:O	1:A:179:LEU:HG	2.12	0.49
1:A:264:ARG:HH11	1:A:264:ARG:CG	2.25	0.49
1:A:344:LEU:HD11	1:A:363:ARG:HB2	1.94	0.49
1:B:865:LYS:HG3	1:B:866:SER:N	2.27	0.49
1:B:807:HIS:CD2	1:B:809:SER:H	2.28	0.49
1:A:35:ASN:HD21	1:A:38:LYS:HG3	1.78	0.49
1:B:763:GLU:CG	1:B:764:ARG:N	2.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ARG:HD2	1:A:237:GLU:CD	2.33	0.49
1:B:608:ASP:OD1	1:B:837:ARG:NH2	2.46	0.49
1:B:680:ASN:N	1:B:680:ASN:HD22	1.96	0.49
1:B:526:TYR:OH	1:B:806:PRO:HB2	2.13	0.49
1:A:49:ARG:HG3	1:A:49:ARG:NH1	2.27	0.48
1:B:846:THR:HG22	3:B:88:HOH:O	2.12	0.48
1:A:139:GLU:H	1:A:139:GLU:HG2	1.45	0.48
1:B:653:PHE:HE2	3:B:225:HOH:O	1.95	0.48
1:A:176:LYS:HA	1:A:179:LEU:HD12	1.94	0.48
1:A:210:GLY:HA3	2:A:401:HEM:C2C	2.49	0.48
1:B:693:ASN:ND2	1:B:693:ASN:H	2.12	0.48
1:B:693:ASN:HD22	1:B:693:ASN:H	1.60	0.48
1:B:699:LYS:O	1:B:703:ILE:HG12	2.13	0.48
1:B:839:ARG:NH2	1:B:866:SER:HB3	2.29	0.48
1:B:555:ASN:HB3	1:B:557:LYS:HD3	1.95	0.48
1:A:195:SER:O	1:A:199:LYS:HG3	2.14	0.48
1:A:232:GLN:O	1:A:236:GLU:HG3	2.14	0.48
1:B:851:ASN:ND2	1:B:853:VAL:N	2.42	0.48
1:A:107:LEU:HD13	1:A:337:ARG:HG3	1.96	0.48
1:B:760:LYS:HD3	1:B:777:TYR:CE2	2.49	0.48
1:A:82:MET:HE3	1:A:189:VAL:HA	1.96	0.47
1:A:1:MET:HA	3:B:23:HOH:O	2.13	0.47
1:B:733:ARG:HD3	1:B:737:GLU:CD	2.34	0.47
1:A:38:LYS:HE2	1:A:263:GLU:OE2	2.14	0.47
1:A:205:LEU:HD12	1:A:209:ALA:HB2	1.96	0.47
1:B:583:SER:HB2	1:B:586:ILE:HG12	1.95	0.47
1:A:21:TRP:CD1	1:A:272:ILE:HG23	2.50	0.47
1:A:75:LEU:HD22	1:A:79:LEU:CD1	2.45	0.47
1:B:718:ILE:O	1:B:722:VAL:HG23	2.14	0.47
1:B:607:LEU:HD13	1:B:837:ARG:HG3	1.97	0.47
1:B:841:ILE:HG12	1:B:842:GLU:N	2.29	0.47
1:A:241:LEU:C	1:A:241:LEU:HD23	2.34	0.47
1:A:98:PHE:HE2	1:A:129:VAL:HA	1.80	0.47
1:A:92:LEU:HD11	1:A:321:PRO:HB2	1.97	0.47
1:A:58:ILE:HA	1:A:59:ARG:NE	2.30	0.46
1:A:83:SER:HB3	3:A:511:HOH:O	2.15	0.46
1:A:86:ILE:CG2	1:A:185:VAL:HG13	2.44	0.46
1:A:129:VAL:O	1:A:133:ILE:HG13	2.15	0.46
1:A:260:LYS:NZ	1:A:277:TYR:CZ	2.83	0.46
1:A:347:GLU:HG3	1:A:359:ARG:NH2	2.22	0.46
1:A:235:ARG:HH11	1:A:235:ARG:HG2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:731:TRP:CD2	1:B:838:PHE:HZ	2.34	0.46
1:B:815:HIS:O	1:B:816:LEU:C	2.54	0.46
1:B:838:PHE:CE1	1:B:841:ILE:HB	2.51	0.46
1:B:758:VAL:O	1:B:759:ARG:HD3	2.16	0.45
1:B:543:LEU:HD22	1:B:777:TYR:CE2	2.44	0.45
1:B:529:THR:HG23	1:B:780:VAL:HB	1.98	0.45
1:A:24:LEU:HD22	1:A:24:LEU:N	2.32	0.45
1:A:23:VAL:HG12	1:A:29:THR:HG23	1.98	0.45
1:A:338:PHE:CE1	1:A:341:ILE:HG22	2.52	0.45
1:B:597:THR:O	1:B:601:GLU:HB2	2.16	0.45
1:B:590:GLN:H	1:B:590:GLN:HE21	1.65	0.45
1:B:652:ALA:HB3	1:B:654:ARG:CZ	2.47	0.45
1:B:652:ALA:O	1:B:654:ARG:N	2.44	0.45
1:A:258:VAL:CG2	1:A:259:ARG:N	2.80	0.45
1:B:512:ASP:HB3	1:B:515:TYR:HB2	1.98	0.45
1:B:623:VAL:HG11	1:B:645:LYS:HD3	1.97	0.45
1:B:620:LYS:NZ	3:B:215:HOH:O	2.49	0.45
1:B:653:PHE:N	1:B:653:PHE:CD1	2.85	0.45
1:B:741:LEU:HD22	1:B:828:ARG:HD3	1.98	0.45
1:A:137:PRO:HG2	1:A:178:HIS:CD2	2.52	0.45
1:B:849:VAL:HG11	3:B:85:HOH:O	2.17	0.45
1:A:74:PRO:O	1:A:75:LEU:C	2.55	0.44
1:B:551:GLU:HB3	3:B:61:HOH:O	2.16	0.44
1:B:679:LEU:HA	1:B:679:LEU:HD12	1.79	0.44
1:A:176:LYS:HA	1:A:179:LEU:HD11	1.98	0.44
1:A:92:LEU:CD1	1:A:321:PRO:HB2	2.47	0.44
1:A:117:ILE:HD11	1:A:360:LEU:HD23	1.98	0.44
1:A:266:LYS:HA	1:A:270:GLN:O	2.18	0.44
1:B:505:PHE:CG	1:B:784:SER:HB2	2.53	0.44
1:A:179:LEU:O	1:A:190:VAL:HG21	2.17	0.44
1:A:186:VAL:HG22	3:A:455:HOH:O	2.18	0.44
1:A:136:LEU:CD1	1:A:207:LEU:HD13	2.42	0.44
1:A:76:HIS:HE2	2:A:401:HEM:CGD	2.31	0.44
1:B:505:PHE:HB3	1:B:509:ARG:HH12	1.82	0.44
1:B:839:ARG:CB	1:B:866:SER:HA	2.45	0.44
1:A:58:ILE:HA	1:A:59:ARG:HE	1.83	0.44
1:B:532:VAL:HG11	1:B:780:VAL:HG11	2.00	0.44
1:B:543:LEU:HD11	1:B:758:VAL:HG13	2.00	0.44
1:B:552:ASP:C	1:B:558:ILE:HD12	2.38	0.43
1:B:848:LYS:HZ2	1:B:855:ASN:HD22	1.65	0.43
1:A:340:HIS:CE1	1:A:342:GLU:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:773:GLU:HA	1:B:773:GLU:OE1	2.18	0.43
1:B:695:SER:O	1:B:699:LYS:HG3	2.17	0.43
1:B:733:ARG:NH2	3:B:89:HOH:O	2.43	0.43
1:A:22:GLN:OE1	1:A:279:ARG:HD2	2.18	0.43
1:B:700:LEU:O	1:B:704:ILE:HG13	2.17	0.43
1:A:194:LEU:HD13	1:A:198:GLU:HB3	2.01	0.43
1:A:23:VAL:HG12	1:A:29:THR:CG2	2.49	0.43
1:A:95:LEU:HD11	1:A:133:ILE:CG1	2.49	0.43
1:B:646:GLU:OE2	1:B:667:LYS:HD3	2.19	0.43
1:A:108:ASP:OD1	1:A:337:ARG:NH2	2.52	0.43
1:B:693:ASN:N	1:B:693:ASN:ND2	2.66	0.43
1:B:700:LEU:HA	1:B:700:LEU:HD12	1.77	0.43
1:A:334:PHE:CE1	1:A:338:PHE:CE2	3.07	0.43
1:A:49:ARG:CG	1:A:49:ARG:NH1	2.82	0.43
1:A:68:MET:O	1:A:76:HIS:HD2	2.01	0.43
1:B:549:ARG:HH12	1:B:565:ARG:NH2	2.17	0.43
1:A:223:ILE:CD1	1:A:360:LEU:HD11	2.34	0.42
1:A:38:LYS:HE2	1:A:263:GLU:CD	2.40	0.42
1:B:562:ILE:HG21	1:B:662:PHE:CE2	2.55	0.42
1:B:640:ASP:O	1:B:643:LYS:HB2	2.19	0.42
1:B:666:LYS:HG2	1:B:666:LYS:H	1.52	0.42
1:A:52:ASP:HA	1:A:55:ASN:HB2	2.00	0.42
1:A:5:PHE:O	1:A:9:ARG:HG3	2.18	0.42
1:A:55:ASN:CB	1:A:57:LYS:HG2	2.44	0.42
1:B:851:ASN:HD21	1:B:853:VAL:H	1.59	0.42
1:B:550:LEU:O	1:B:553:LEU:HB2	2.19	0.42
1:B:664:LEU:HD21	1:B:669:LEU:HD22	2.00	0.42
1:B:848:LYS:O	1:B:850:PRO:HD3	2.19	0.42
1:A:122:ALA:HB1	1:A:215:THR:HG23	2.01	0.42
1:A:142:GLU:OE1	1:A:145:LYS:HE2	2.19	0.42
1:A:4:TRP:HB2	1:B:681:SER:O	2.20	0.42
1:A:264:ARG:NH1	1:A:264:ARG:CG	2.81	0.42
1:A:310:PHE:CE2	2:A:401:HEM:HBB2	2.55	0.42
1:A:315:HIS:O	1:A:316:LEU:C	2.57	0.42
1:B:664:LEU:CD2	1:B:669:LEU:HD22	2.50	0.42
1:B:813:GLY:O	1:B:816:LEU:HB2	2.19	0.42
1:A:82:MET:HE2	1:A:189:VAL:HG22	2.01	0.41
1:A:118:VAL:HG23	1:A:360:LEU:CB	2.50	0.41
1:B:637:PRO:HD2	1:B:674:TYR:OH	2.20	0.41
1:B:662:PHE:CD2	1:B:663:GLU:N	2.83	0.41
1:B:758:VAL:CG2	1:B:759:ARG:N	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:814:ILE:HG12	3:B:279:HOH:O	2.21	0.41
1:B:620:LYS:HE2	1:B:620:LYS:HB3	1.55	0.41
1:A:79:LEU:CD2	1:A:194:LEU:HD11	2.50	0.41
1:B:734:ILE:HA	1:B:739:LEU:HB2	2.03	0.41
1:B:814:ILE:HG13	1:B:815:HIS:CD2	2.55	0.41
1:B:710:GLY:HA3	2:B:901:HEM:C2C	2.56	0.41
1:A:329:ILE:O	1:A:333:GLU:HG2	2.21	0.41
1:A:340:HIS:HE1	1:A:342:GLU:HB2	1.84	0.41
1:B:670:GLU:HG3	1:B:670:GLU:H	1.57	0.41
1:B:752:PRO:HG3	1:B:783:ALA:HA	2.02	0.41
1:B:774:GLU:HG3	1:B:775:GLY:N	2.36	0.41
1:A:334:PHE:CD1	1:A:338:PHE:HE2	2.39	0.41
1:A:339:ARG:HG3	1:A:366:SER:C	2.41	0.41
1:A:344:LEU:HD21	1:A:363:ARG:CB	2.47	0.41
1:B:526:TYR:CD2	1:B:791:VAL:HG21	2.56	0.41
1:B:848:LYS:HZ2	1:B:855:ASN:ND2	2.17	0.41
1:A:125:LEU:HB3	1:A:126:PRO:HD3	2.03	0.40
1:A:130:ILE:HD12	1:A:130:ILE:HA	1.94	0.40
1:A:262:LYS:O	1:A:263:GLU:HB3	2.22	0.40
1:B:843:ILE:HD13	1:B:862:VAL:HG12	2.02	0.40
1:A:8:MET:O	1:A:12:ASP:N	2.50	0.40
1:A:22:GLN:HG2	1:A:279:ARG:HB3	2.03	0.40
1:A:26:TYR:CD2	1:A:291:VAL:HG21	2.57	0.40
1:A:354:LEU:HA	1:A:354:LEU:HD23	1.90	0.40
1:A:108:ASP:HA	1:A:337:ARG:HH22	1.85	0.40

There are no symmetry-related clashes.

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	364/368 (99%)	338 (93%)	22 (6%)	4 (1%)	17 9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	355/368 (96%)	333 (94%)	19 (5%)	3 (1%)	22	15
All	All	719/736 (98%)	671 (93%)	41 (6%)	7 (1%)	18	10

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	GLU
1	B	653	PHE
1	A	139	GLU
1	B	513	PRO
1	A	137	PRO
1	B	651	VAL
1	A	158	PRO

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	336/338 (99%)	290 (86%)	46 (14%)	4	2
1	B	331/338 (98%)	280 (85%)	51 (15%)	3	1
All	All	667/676 (99%)	570 (86%)	97 (14%)	4	2

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	19	ASN
1	A	24	LEU
1	A	27	ARG
1	A	38	LYS
1	A	46	TYR
1	A	59	ARG
1	A	65	ARG
1	A	69	LEU

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Mol	Chain	Res	Type
1	A	75	LEU
1	A	90	GLN
1	A	103	THR
1	A	105	SER
1	A	113	ARG
1	A	114	GLU
1	A	119	LYS
1	A	121	LEU
1	A	125	LEU
1	A	134	LEU
1	A	139	GLU
1	A	140	ASP
1	A	141	LYS
1	A	142	GLU
1	A	143	LYS
1	A	145	LYS
1	A	155	LEU
1	A	157	LYS
1	A	168	TYR
1	A	169	LEU
1	A	181	SER
1	A	186	VAL
1	A	202	TYR
1	A	227	ARG
1	A	233	ARG
1	A	237	GLU
1	A	258	VAL
1	A	264	ARG
1	A	266	LYS
1	A	271	THR
1	A	316	LEU
1	A	318	LEU
1	A	322	LEU
1	A	347	GLU
1	A	349	VAL
1	A	365	LYS
1	A	366	SER
1	B	501	MET
1	B	507	GLU
1	B	510	LYS
1	B	511	LYS
1	B	519	ASN

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Mol	Chain	Res	Type
1	B	537	SER
1	B	538	LYS
1	B	550	LEU
1	B	557	LYS
1	B	569	LEU
1	B	575	LEU
1	B	586	ILE
1	B	590	GLN
1	B	594	THR
1	B	595	LEU
1	B	613	ARG
1	B	617	ILE
1	B	620	LYS
1	B	625	LEU
1	B	631	SER
1	B	632	LYS
1	B	634	LEU
1	B	650	LEU
1	B	654	ARG
1	B	663	GLU
1	B	664	LEU
1	B	666	LYS
1	B	669	LEU
1	B	679	LEU
1	B	680	ASN
1	B	687	SER
1	B	690	VAL
1	B	693	ASN
1	B	700	LEU
1	B	702	TYR
1	B	723	ILE
1	B	732	GLN
1	B	733	ARG
1	B	756	ARG
1	B	762	LYS
1	B	763	GLU
1	B	764	ARG
1	B	766	LYS
1	B	816	LEU
1	B	822	LEU
1	B	828	ARG
1	B	837	ARG

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Mol	Chain	Res	Type
1	B	846	THR
1	B	848	LYS
1	B	854	LEU
1	B	865	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	ASN
1	A	307	HIS
1	A	355	ASN
1	B	519	ASN
1	B	590	GLN
1	B	680	ASN
1	B	691	ASN
1	B	693	ASN
1	B	729	ASN
1	B	732	GLN
1	B	786	ASN
1	B	807	HIS
1	B	851	ASN
1	B	855	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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	HEM	A	401	1,3	28,50,50	2.35	12 (42%)	17,82,82	1.33	3 (17%)
2	HEM	B	901	1,3	28,50,50	2.48	9 (32%)	17,82,82	1.75	5 (29%)

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	HEM	A	401	1,3	-	0/6/54/54	0/0/8/8
2	HEM	B	901	1,3	-	0/6/54/54	0/0/8/8

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	HEM	C3B-CAB	-4.10	1.39	1.47
2	A	401	HEM	C3C-CAC	-4.09	1.39	1.47
2	B	901	HEM	C3B-CAB	-3.81	1.40	1.47
2	B	901	HEM	C3C-CAC	-3.31	1.41	1.47
2	A	401	HEM	C3C-C2C	-2.95	1.36	1.40
2	B	901	HEM	C3B-C2B	-2.42	1.37	1.40
2	A	401	HEM	C3B-C2B	-2.26	1.37	1.40
2	A	401	HEM	CMB-C2B	2.03	1.55	1.51
2	A	401	HEM	C1D-ND	2.07	1.40	1.36
2	A	401	HEM	C1A-NA	2.17	1.40	1.36
2	B	901	HEM	C1D-ND	2.61	1.41	1.36
2	A	401	HEM	C1B-NB	2.63	1.39	1.36
2	A	401	HEM	C4A-NA	2.64	1.41	1.36
2	B	901	HEM	C4A-NA	2.96	1.42	1.36
2	A	401	HEM	C4D-ND	3.90	1.41	1.36
2	B	901	HEM	C4D-ND	4.28	1.41	1.36
2	B	901	HEM	C1C-NC	4.93	1.42	1.36
2	A	401	HEM	C4C-NC	5.03	1.42	1.36
2	B	901	HEM	C1B-NB	5.20	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	HEM	C1C-NC	5.39	1.43	1.36
2	B	901	HEM	C4C-NC	5.51	1.43	1.36

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	HEM	CBD-CAD-C3D	-3.95	104.93	112.47
2	B	901	HEM	C4A-C3A-C2A	-3.33	104.68	107.00
2	B	901	HEM	CMD-C2D-C1D	-2.98	123.89	128.46
2	A	401	HEM	CMD-C2D-C1D	-2.91	124.00	128.46
2	A	401	HEM	C4A-C3A-C2A	-2.41	105.32	107.00
2	B	901	HEM	C4C-C3C-C2C	2.05	108.33	106.90
2	A	401	HEM	CMD-C2D-C3D	2.09	128.89	124.94
2	B	901	HEM	CMD-C2D-C3D	2.25	129.18	124.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	HEM	3	0
2	B	901	HEM	1	0

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.