



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 03:18 AM GMT

PDB ID : 1VRN
Title : PHOTOSYNTHETIC REACTION CENTER BLASTOCHLORIS VIRIDIS (ATCC)
Authors : Baxter, R.H.G.; Seagle, B.-L.; Norris, J.R.
Deposited on : 2005-02-23
Resolution : 2.20 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

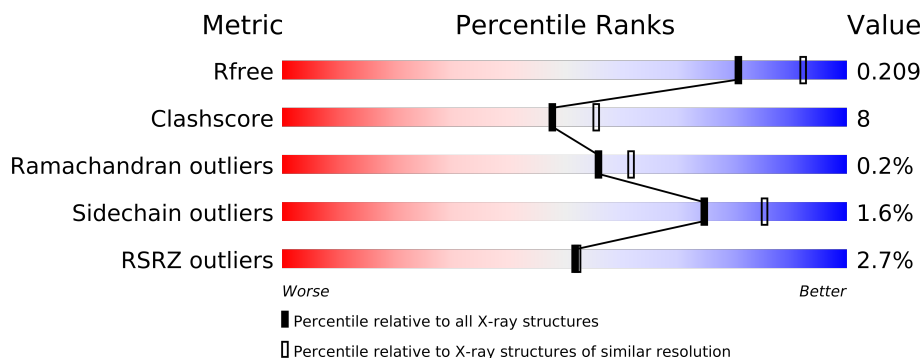
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.20 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))
R_{free}	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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.

Mol	Chain	Length	Quality of chain
1	C	332	
2	H	258	
3	L	273	
4	M	323	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
11	UQ7	L	502	-	X
12	NS5	M	600	-	X
13	LDA	H	701	-	X
13	LDA	H	703	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
13	LDA	L	702	-	X
13	LDA	L	706	-	X
13	LDA	M	704	-	X
6	SO4	H	806	-	X
6	SO4	H	807	-	X
6	SO4	M	801	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 10747 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 Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	332	Total	C	N	O	S	24	0	0
			2603	1640	466	479	18			

- Molecule 2 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	258	Total	C	N	O	S	112	0	0
			2018	1292	344	380	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	1	FME	MET	MODIFIED RESIDUE	UNP P06008

- Molecule 3 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	273	Total	C	N	O	S	5	1	0
			2177	1462	351	357	7			

- Molecule 4 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	323	Total	C	N	O	S	10	1	0
			2563	1707	420	424	12			

- Molecule 5 is FE (II) ION (three-letter code: FE2) (formula: Fe).

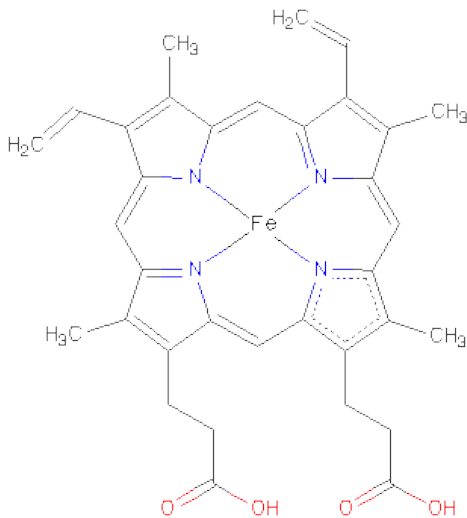
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	1	Total	Fe	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



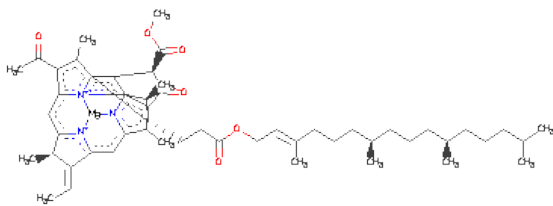
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	M	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



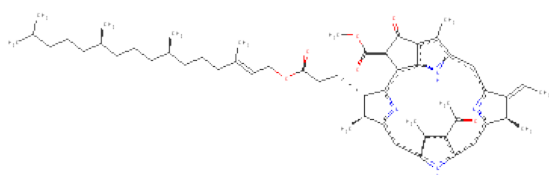
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 8 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: C₅₅H₇₂MgN₄O₆).



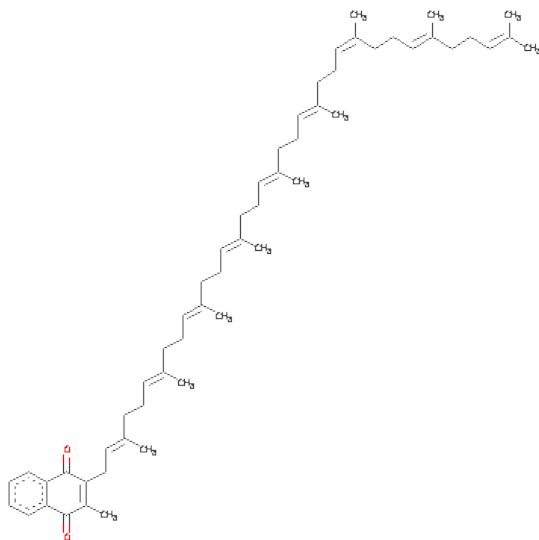
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
8	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
8	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
8	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 9 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula: $C_{55}H_{74}N_4O_6$).



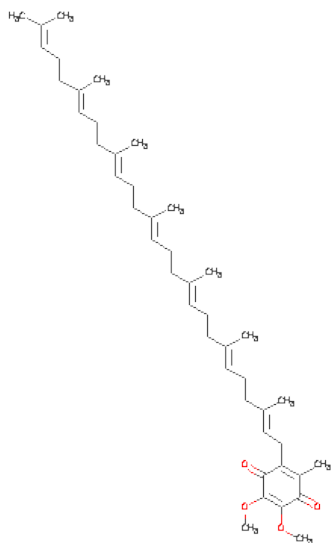
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	M	1	Total	C	N	O	9	0
			65	55	4	6		
9	L	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 10 is MENAQUINONE-9 (three-letter code: MQ9) (formula: $C_{56}H_{80}O_2$).



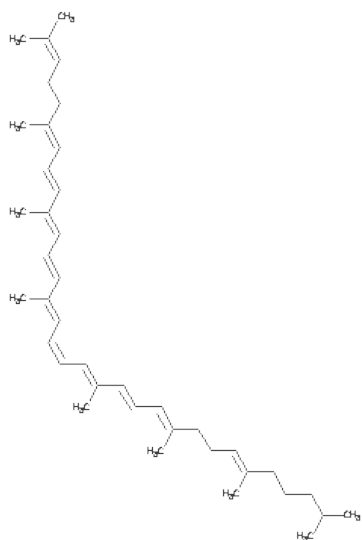
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	M	1	Total	C	O	0	0
			58	56	2		

- Molecule 11 is UBIQUINONE-7 (three-letter code: UQ7) (formula: $C_{44}H_{66}O_4$).



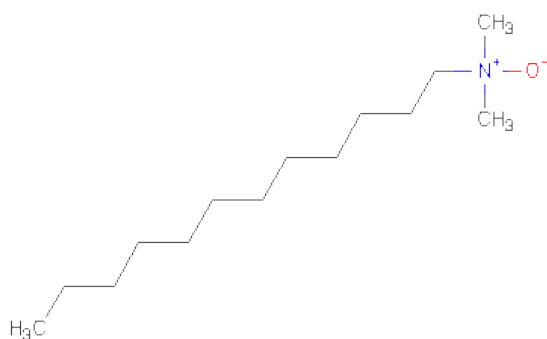
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	L	1	Total	C	O	0	0
			48	44	4		

- Molecule 12 is 15-CIS-1,2-DIHYDRONEUROSPORENE (three-letter code: NS5) (formula: $C_{40}H_{60}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total	C		0	0
			40	40			

- Molecule 13 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	H	1	Total	C	N	O	0	0
			16	14	1	1		
13	L	1	Total	C	N	O	0	0
			16	14	1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	H	1	Total	C	N	O	0	0
			16	14	1	1		
13	M	1	Total	C	N	O	0	0
			16	14	1	1		
13	M	1	Total	C	N	O	4	0
			16	14	1	1		
13	L	1	Total	C	N	O	0	0
			16	14	1	1		

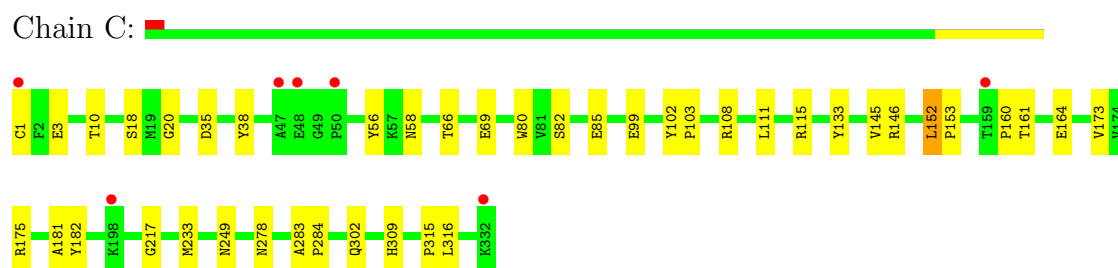
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	C	212	Total	O	0	0
			212	212		
14	H	124	Total	O	0	0
			124	124		
14	L	92	Total	O	0	0
			92	92		
14	M	114	Total	O	0	0
			114	114		

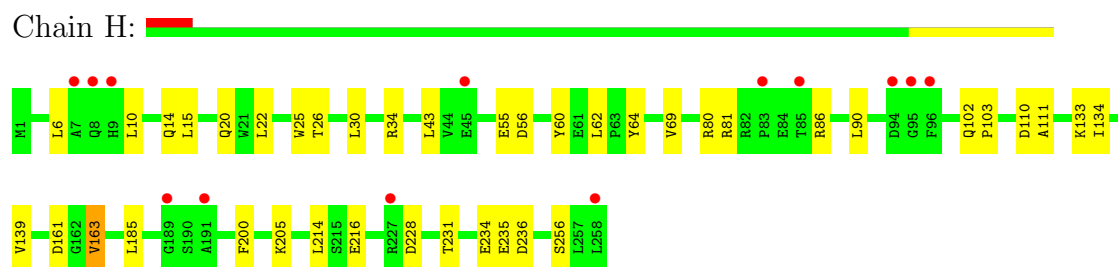
3 Residue-property plots

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.

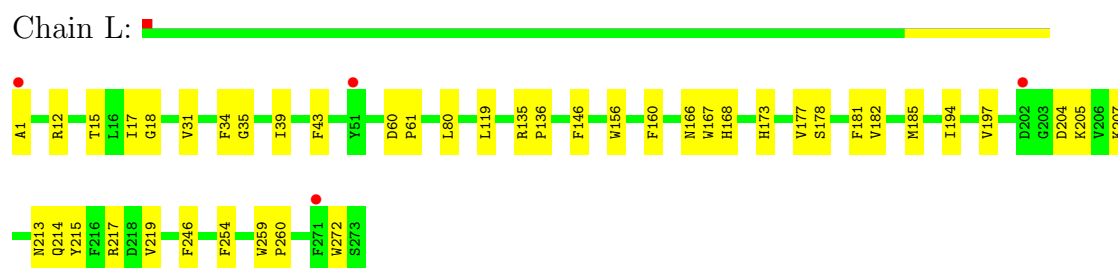
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



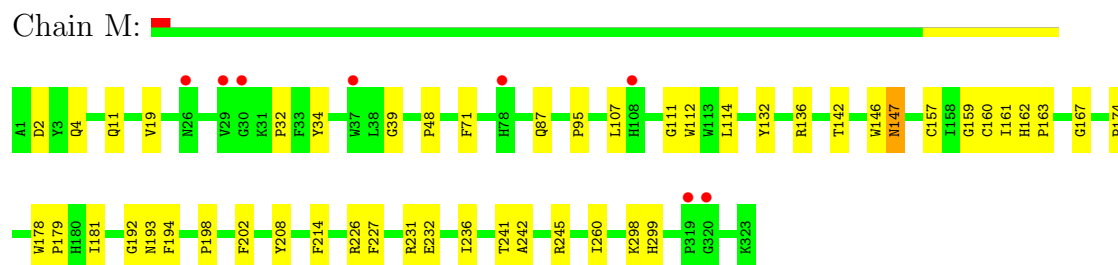
- Molecule 2: Reaction center protein H chain



- Molecule 3: Reaction center protein L chain



- Molecule 4: Reaction center protein M chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	219.40Å 219.40Å 112.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.18 – 2.20 20.13 – 2.20	Depositor EDS
% Data completeness (in resolution range)	86.2 (19.18-2.20) 86.2 (20.13-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.15 (at 2.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.191 , 0.212 0.188 , 0.209	Depositor DCC
R_{free} test set	6079 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 46.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 119616 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10747	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% of the height of the origin peak. No significant pseudotranslation is detected.*

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: LDA, BPB, BCB, FE2, SO4, MQ9, HEM, FME, NS5, UQ7

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	C	0.31	0/2670	0.60	1/3637 (0.0%)
2	H	0.29	0/2055	0.56	0/2807
3	L	0.38	0/2265	0.56	0/3092
4	M	0.35	0/2667	0.54	0/3647
All	All	0.34	0/9657	0.56	1/13183 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	249	ASN	N-CA-C	-6.30	93.99	111.00

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	C	2603	0	2579	24	0
2	H	2018	0	2020	37	0
3	L	2177	0	2102	35	0
4	M	2563	0	2460	42	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	1	0	0	0	0
6	H	15	0	0	2	0
6	M	20	0	0	1	0
7	C	172	0	120	2	0
8	L	132	0	144	10	0
8	M	132	0	144	12	0
9	L	65	0	74	6	0
9	M	65	0	74	8	0
10	M	58	0	80	2	0
11	L	48	0	66	9	0
12	M	40	0	60	4	0
13	H	32	0	62	8	0
13	L	32	0	62	4	0
13	M	32	0	62	5	0
14	C	212	0	0	0	0
14	H	124	0	0	1	0
14	L	92	0	0	1	0
14	M	114	0	0	1	0
All	All	10747	0	10109	157	0

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 8.

All (157) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:M:32:PRO:HG3	4:M:48:PRO:HD3	1.46	0.95
9:L:406:BPB:HBBB	9:L:406:BPB:HHC	1.52	0.92
9:M:405:BPB:HHC	9:M:405:BPB:HBBB	1.56	0.87
4:M:114:LEU:HG	12:M:600:NS5:HM43	1.64	0.79
2:H:69:VAL:HG13	3:L:205:LYS:HA	1.66	0.78
8:M:401:BCB:HBB2	8:M:401:BCB:HHC	1.66	0.77
1:C:152:LEU:HD22	1:C:175:ARG:HA	1.66	0.76
2:H:102:GLN:OE1	3:L:12:ARG:HD3	1.91	0.71
11:L:502:UQ7:H171	8:M:401:BCB:H91	1.73	0.70
4:M:71:PHE:HB3	13:M:705:LDA:H61	1.75	0.68
3:L:181:PHE:HB3	9:M:405:BPB:HBBA	1.74	0.68
3:L:214:GLN:NE2	4:M:19:VAL:H	1.91	0.68
1:C:153:PRO:HD3	1:C:160:PRO:HB3	1.77	0.67
9:L:406:BPB:HHC	9:L:406:BPB:CBB	2.24	0.66
2:H:86:ARG:NH2	2:H:111:ALA:HB3	2.11	0.65
8:M:401:BCB:H142	8:M:401:BCB:H102	1.77	0.65
8:L:402:BCB:HMB1	8:L:402:BCB:HBB3	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:69:VAL:HG12	14:H:1292:HOH:O	1.95	0.64
11:L:502:UQ7:H153	8:M:401:BCB:H101	1.78	0.64
2:H:81:ARG:H	13:H:703:LDA:H112	1.63	0.64
3:L:178:SER:HB3	11:L:502:UQ7:H261	1.79	0.64
9:L:406:BPB:HBBA	4:M:208:TYR:HB3	1.80	0.63
4:M:231:ARG:HD2	14:M:1383:HOH:O	1.98	0.62
13:L:702:LDA:H72	13:L:702:LDA:H31	1.81	0.62
3:L:181:PHE:CD2	9:M:405:BPB:HBB	2.35	0.62
2:H:231:THR:OG1	2:H:234:GLU:HG3	1.99	0.61
6:H:807:SO4:S	13:H:703:LDA:HM23	2.42	0.59
2:H:86:ARG:HH22	2:H:111:ALA:HB3	1.66	0.59
6:H:807:SO4:O3	13:H:703:LDA:HM23	2.03	0.58
1:C:1:CYS:HB2	14:L:1204:HOH:O	2.03	0.58
3:L:181:PHE:HB3	9:M:405:BPB:CBB	2.34	0.57
1:C:145:VAL:O	1:C:146:ARG:HD2	2.03	0.57
4:M:132:TYR:CE1	4:M:142:THR:HG21	2.39	0.56
8:L:404:BCB:HBB2	8:L:404:BCB:HMB1	1.87	0.56
4:M:71:PHE:HB3	13:M:705:LDA:C6	2.35	0.56
8:L:404:BCB:CBB	8:L:404:BCB:HMB1	2.36	0.55
3:L:182:VAL:HG11	11:L:502:UQ7:H253	1.88	0.55
13:H:701:LDA:H52	10:M:501:MQ9:H202	1.89	0.55
4:M:95:PRO:HD3	4:M:174:PRO:HB3	1.88	0.55
9:L:406:BPB:HBB	4:M:208:TYR:CD2	2.41	0.55
2:H:133:LYS:HG2	2:H:134:ILE:HD12	1.89	0.55
2:H:30:LEU:O	2:H:34:ARG:HD2	2.07	0.55
2:H:20:GLN:HG2	4:M:202:PHE:CE2	2.42	0.54
3:L:214:GLN:HE21	4:M:19:VAL:H	1.55	0.54
4:M:112:TRP:CZ3	13:M:705:LDA:H81	2.42	0.54
4:M:162:HIS:HB3	4:M:163:PRO:HD3	1.90	0.54
2:H:139:VAL:HG21	2:H:228:ASP:HB3	1.89	0.54
2:H:6:LEU:HD12	2:H:10:LEU:HD12	1.90	0.54
8:M:403:BCB:H203	9:M:405:BPB:C4	2.38	0.54
3:L:135:ARG:HB3	3:L:136:PRO:HD3	1.88	0.54
8:M:403:BCB:HMB1	8:M:403:BCB:HBB3	1.89	0.53
13:L:702:LDA:H111	4:M:198:PRO:HA	1.91	0.52
8:M:403:BCB:H203	9:M:405:BPB:H4	1.92	0.52
8:M:403:BCB:CBB	8:M:403:BCB:HMB1	2.40	0.51
2:H:235:GLU:OE1	4:M:231:ARG:NH2	2.38	0.51
2:H:81:ARG:N	13:H:703:LDA:H112	2.25	0.51
3:L:213:ASN:OD1	11:L:502:UQ7:HM21	2.11	0.50
1:C:18:SER:HB2	3:L:156:TRP:CD1	2.47	0.50
4:M:241:THR:O	4:M:245:ARG:HG3	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:L:177:VAL:HG13	8:L:402:BCB:HMB3	1.93	0.50
2:H:134:ILE:N	2:H:134:ILE:HD12	2.27	0.50
4:M:146:TRP:HA	4:M:146:TRP:CE3	2.47	0.50
2:H:6:LEU:HD12	2:H:10:LEU:CD1	2.42	0.50
4:M:157:CYS:HA	4:M:161:ILE:HB	1.93	0.50
2:H:80:ARG:HA	13:H:703:LDA:H101	1.93	0.50
1:C:102:TYR:CG	1:C:103:PRO:HD3	2.47	0.49
4:M:178:TRP:HB2	4:M:179:PRO:HD3	1.94	0.49
1:C:35:ASP:OD2	1:C:316:LEU:HA	2.13	0.49
8:L:402:BCB:CBB	8:L:402:BCB:HMB1	2.43	0.49
4:M:298:LYS:HE3	4:M:299:HIS:NE2	2.28	0.48
8:L:404:BCB:HHC	8:L:404:BCB:OBB	2.13	0.48
1:C:283:ALA:HB3	1:C:284:PRO:HD3	1.96	0.48
3:L:246:PHE:CD1	11:L:502:UQ7:H412	2.49	0.48
1:C:111:LEU:O	1:C:115:ARG:HG3	2.14	0.48
1:C:278:ASN:HB3	1:C:302:GLN:NE2	2.29	0.47
11:L:502:UQ7:H171	8:M:401:BCB:C9	2.43	0.47
9:M:405:BPB:HMC	9:M:405:BPB:H55	1.95	0.47
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.49	0.47
3:L:43:PHE:CD1	10:M:501:MQ9:H512	2.50	0.47
3:L:167:TRP:HE1	3:L:173:HIS:CD2	2.33	0.47
1:C:161:THR:OG1	1:C:164:GLU:HG3	2.15	0.47
8:L:402:BCB:H11	8:L:404:BCB:H2C	1.97	0.47
2:H:133:LYS:CG	2:H:134:ILE:HD12	2.45	0.46
3:L:197:VAL:HG13	3:L:207:LYS:HB2	1.95	0.46
4:M:192:GLY:O	4:M:193:ASN:HB3	2.14	0.46
4:M:107:LEU:HA	4:M:111:GLY:HA3	1.96	0.46
2:H:22:LEU:HD13	2:H:22:LEU:C	2.35	0.46
3:L:146:PHE:HB3	3:L:156:TRP:CD2	2.50	0.46
2:H:62:LEU:O	13:H:703:LDA:HM13	2.15	0.46
8:M:401:BCB:C10	8:M:401:BCB:H142	2.45	0.46
2:H:86:ARG:NH2	2:H:110:ASP:O	2.49	0.46
1:C:66:THR:OG1	1:C:69:GLU:HG3	2.16	0.46
8:L:404:BCB:H172	9:L:406:BPB:H11A	1.98	0.46
1:C:181:ALA:O	1:C:182:TYR:HB2	2.15	0.46
2:H:26:THR:O	2:H:30:LEU:HB2	2.16	0.45
3:L:35:GLY:O	3:L:39:ILE:HG12	2.16	0.45
12:M:600:NS5:H271	12:M:600:NS5:H29	1.82	0.45
2:H:90:LEU:HD23	2:H:103:PRO:HA	1.98	0.45
8:M:403:BCB:OBB	8:M:403:BCB:HHC	2.17	0.45
4:M:160:CYS:C	4:M:163:PRO:HD2	2.37	0.45
8:M:401:BCB:HHC	8:M:401:BCB:CBB	2.43	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:56:ASP:HB3	2:H:60:TYR:CE2	2.52	0.45
4:M:112:TRP:CH2	13:M:705:LDA:H81	2.52	0.45
13:L:702:LDA:C7	13:L:702:LDA:H31	2.46	0.45
1:C:102:TYR:CD2	1:C:103:PRO:HD3	2.52	0.44
2:H:43:LEU:HB3	3:L:1:ALA:H2	1.81	0.44
3:L:17:ILE:HG13	3:L:18:GLY:N	2.32	0.44
2:H:69:VAL:CG1	3:L:204:ASP:O	2.65	0.44
4:M:34:TYR:CD1	4:M:34:TYR:N	2.85	0.44
2:H:256:SER:HA	3:L:15:THR:O	2.18	0.44
2:H:161:ASP:HB3	2:H:214:LEU:HD22	1.99	0.44
2:H:25:TRP:HA	2:H:25:TRP:CE3	2.51	0.44
8:L:402:BCB:OBB	8:L:402:BCB:HHC	2.16	0.44
2:H:216:GLU:H	2:H:216:GLU:CD	2.20	0.44
1:C:10:THR:O	1:C:20:GLY:HA3	2.18	0.43
4:M:132:TYR:CZ	4:M:136:ARG:HD2	2.53	0.43
4:M:178:TRP:O	4:M:181:ILE:HB	2.18	0.43
2:H:161:ASP:CG	2:H:163:VAL:HG13	2.38	0.43
4:M:147:ASN:C	4:M:147:ASN:HD22	2.20	0.43
3:L:60:ASP:OD2	13:L:702:LDA:HM12	2.19	0.43
1:C:233:MET:HB3	7:C:403:HEM:C4B	2.53	0.43
3:L:214:GLN:HG2	4:M:19:VAL:HB	2.00	0.43
1:C:217:GLY:HA2	4:M:167:GLY:O	2.18	0.42
1:C:99:GLU:OE2	1:C:108:ARG:NH2	2.51	0.42
4:M:227:PHE:HB2	4:M:242:ALA:HB2	2.01	0.42
3:L:215:TYR:O	3:L:219:VAL:HG23	2.20	0.42
3:L:213:ASN:O	3:L:217:ARG:HG3	2.19	0.42
3:L:259:TRP:N	3:L:260:PRO:CD	2.83	0.42
6:M:804:SO4:O4	13:M:704:LDA:HM11	2.19	0.42
2:H:200:PHE:CZ	4:M:226:ARG:HD3	2.54	0.42
3:L:166:ASN:OD1	3:L:168:HIS:HB2	2.19	0.42
9:L:406:BPB:CBB	4:M:208:TYR:CD2	3.02	0.42
1:C:82:SER:HB2	1:C:85:GLU:HB2	2.01	0.42
1:C:309:HIS:CE1	1:C:315:PRO:HD3	2.55	0.42
11:L:502:UQ7:H312	11:L:502:UQ7:H352	2.02	0.42
4:M:178:TRP:N	4:M:179:PRO:CD	2.83	0.42
9:M:405:BPB:CHC	9:M:405:BPB:HBBB	2.37	0.42
2:H:6:LEU:HB2	2:H:10:LEU:HD12	2.02	0.42
2:H:10:LEU:HD13	2:H:15:LEU:HD21	2.01	0.42
4:M:159:GLY:HA3	12:M:600:NS5:H272	2.02	0.42
3:L:194:ILE:HD11	11:L:502:UQ7:HM31	2.01	0.42
1:C:173:VAL:HB	4:M:87:GLN:OE1	2.19	0.41
3:L:146:PHE:HB3	3:L:156:TRP:CE3	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:M:178:TRP:CE3	4:M:178:TRP:HA	2.55	0.41
4:M:11:GLN:OE1	4:M:39:GLY:HA3	2.21	0.41
2:H:10:LEU:HB2	2:H:14:GLN:OE1	2.21	0.41
4:M:236:ILE:HG12	4:M:260:ILE:HG23	2.01	0.41
1:C:3:GLU:O	3:L:254:PHE:HA	2.20	0.41
12:M:600:NS5:H22	12:M:600:NS5:H7	2.02	0.41
2:H:22:LEU:HD13	2:H:22:LEU:O	2.21	0.41
4:M:2:ASP:OD1	4:M:4:GLN:HB2	2.20	0.41
3:L:60:ASP:HA	3:L:61:PRO:HD3	1.89	0.40
3:L:168:HIS:CE1	8:L:402:BCB:HMC2	2.55	0.40
3:L:17:ILE:HG22	3:L:34:PHE:CE2	2.56	0.40
1:C:56:TYR:HB3	7:C:401:HEM:CGA	2.51	0.40
2:H:64:TYR:CZ	13:H:703:LDA:HM22	2.56	0.40
4:M:232:GLU:O	4:M:236:ILE:HG13	2.21	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	C	330/332 (99%)	320 (97%)	10 (3%)	0	100	100
2	H	256/258 (99%)	249 (97%)	6 (2%)	1 (0%)	43	45
3	L	272/273 (100%)	267 (98%)	4 (2%)	1 (0%)	43	45
4	M	322/323 (100%)	310 (96%)	12 (4%)	0	100	100
All	All	1180/1186 (100%)	1146 (97%)	32 (3%)	2 (0%)	56	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	55	GLU
3	L	31	VAL

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	C	281/281 (100%)	278 (99%)	3 (1%)	84	92
2	H	212/212 (100%)	208 (98%)	4 (2%)	69	81
3	L	219/218 (100%)	214 (98%)	5 (2%)	63	74
4	M	250/249 (100%)	247 (99%)	3 (1%)	82	90
All	All	962/960 (100%)	947 (98%)	15 (2%)	75	85

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	38	TYR
1	C	58	ASN
1	C	152	LEU
2	H	163	VAL
2	H	185	LEU
2	H	205	LYS
2	H	236	ASP
3	L	80	LEU
3	L	119	LEU
3	L	160	PHE
3	L	185	MET
3	L	272	TRP
4	M	147	ASN
4	M	194	PHE
4	M	214	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	54	GLN
1	C	58	ASN
1	C	94	ASN
1	C	127	GLN
1	C	206	GLN
2	H	8	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	58	GLN
3	L	214	GLN
4	M	147	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	FME	H	1	2	9,9,10	5.98	2 (22%)	6,9,11	2.18	2 (33%)

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	FME	H	1	2	-	0/7/9/11	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	FME	O-C	17.70	1.23	1.11
2	H	1	FME	CA-C	2.55	1.53	1.48

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	FME	CA-N-CN	-3.97	116.40	122.97
2	H	1	FME	O1-CN-N	-3.27	115.12	125.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 1 is monoatomic - leaving 26 for Mogul analysis.

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	$\# Z > 2$
7	HEM	C	401	1	49,50,50	2.10	14 (28%)	46,82,82	1.21	2 (4%)
7	HEM	C	402	1	49,50,50	2.08	15 (30%)	46,82,82	1.22	2 (4%)
7	HEM	C	403	1	49,50,50	2.04	13 (26%)	46,82,82	1.18	2 (4%)
7	HEM	C	404	1	49,50,50	2.05	11 (22%)	46,82,82	1.29	3 (6%)
13	LDA	H	701	-	15,15,15	4.05	3 (20%)	17,17,17	1.32	1 (5%)
13	LDA	H	703	-	15,15,15	4.28	3 (20%)	17,17,17	0.92	1 (5%)
6	SO4	H	802	-	4,4,4	1.01	0	6,6,6	0.17	0
6	SO4	H	806	-	4,4,4	0.85	0	6,6,6	0.11	0
6	SO4	H	807	-	4,4,4	1.37	0	6,6,6	0.24	0
8	BCB	L	402	3	74,74,74	1.67	14 (18%)	94,115,115	1.67	17 (18%)
8	BCB	L	404	3	74,74,74	1.80	15 (20%)	94,115,115	2.07	19 (20%)
9	BPB	L	406	-	70,70,70	1.91	11 (15%)	93,101,101	1.71	18 (19%)
11	UQ7	L	502	-	48,48,48	1.75	12 (25%)	61,61,61	1.28	8 (13%)
13	LDA	L	702	-	15,15,15	4.58	4 (26%)	17,17,17	2.75	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	LDA	L	706	-	15,15,15	4.45	3 (20%)	17,17,17	1.82	1 (5%)
8	BCB	M	401	4	74,74,74	1.68	14 (18%)	94,115,115	1.62	17 (18%)
8	BCB	M	403	4	74,74,74	1.64	15 (20%)	94,115,115	1.67	17 (18%)
9	BPB	M	405	-	70,70,70	1.84	11 (15%)	93,101,101	1.65	16 (17%)
10	MQ9	M	501	-	59,59,59	1.65	10 (16%)	75,75,75	1.10	7 (9%)
12	NS5	M	600	-	39,39,39	0.54	0	46,46,46	0.97	4 (8%)
13	LDA	M	704	-	15,15,15	4.64	4 (26%)	17,17,17	1.87	1 (5%)
13	LDA	M	705	-	15,15,15	4.74	4 (26%)	17,17,17	1.51	1 (5%)
6	SO4	M	801	-	4,4,4	1.21	0	6,6,6	0.17	0
6	SO4	M	803	-	4,4,4	1.28	0	6,6,6	0.37	0
6	SO4	M	804	-	4,4,4	1.19	0	6,6,6	0.40	0
6	SO4	M	805	-	4,4,4	1.09	0	6,6,6	0.38	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
7	HEM	C	401	1	-	0/14/114/114	0/0/8/8
7	HEM	C	402	1	-	0/14/114/114	0/0/8/8
7	HEM	C	403	1	-	0/14/114/114	0/0/8/8
7	HEM	C	404	1	-	0/14/114/114	0/0/8/8
13	LDA	H	701	-	-	0/13/13/13	0/0/0/0
13	LDA	H	703	-	-	0/13/13/13	0/0/0/0
6	SO4	H	802	-	-	0/0/0/0	0/0/0/0
6	SO4	H	806	-	-	0/0/0/0	0/0/0/0
6	SO4	H	807	-	-	0/0/0/0	0/0/0/0
8	BCB	L	402	3	-	0/41/137/137	0/0/9/9
8	BCB	L	404	3	-	0/41/137/137	0/0/9/9
9	BPB	L	406	-	-	0/52/105/105	0/0/6/6
11	UQ7	L	502	-	-	0/45/69/69	0/1/1/1
13	LDA	L	702	-	-	0/13/13/13	0/0/0/0
13	LDA	L	706	-	-	0/13/13/13	0/0/0/0
8	BCB	M	401	4	1/1/21/26	0/41/137/137	0/0/9/9
8	BCB	M	403	4	-	0/41/137/137	0/0/9/9
9	BPB	M	405	-	2/2/18/23	0/52/105/105	0/0/6/6
10	MQ9	M	501	-	-	0/53/73/73	0/0/2/2
12	NS5	M	600	-	-	0/43/43/43	0/0/0/0
13	LDA	M	704	-	-	0/13/13/13	0/0/0/0
13	LDA	M	705	-	-	0/13/13/13	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SO4	M	801	-	-	0/0/0/0	0/0/0/0
6	SO4	M	803	-	-	0/0/0/0	0/0/0/0
6	SO4	M	804	-	-	0/0/0/0	0/0/0/0
6	SO4	M	805	-	-	0/0/0/0	0/0/0/0

All (176) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	705	LDA	O1-N1	-17.76	1.22	1.39
13	M	704	LDA	O1-N1	-17.33	1.23	1.39
13	L	702	LDA	O1-N1	-17.19	1.23	1.39
13	L	706	LDA	O1-N1	-16.74	1.23	1.39
13	H	703	LDA	O1-N1	-16.21	1.24	1.39
13	H	701	LDA	O1-N1	-15.17	1.25	1.39
9	L	406	BPB	CHD-C4C	7.90	1.40	1.35
9	M	405	BPB	CHD-C4C	7.89	1.40	1.35
8	L	402	BCB	C4D-CHA	-5.27	1.38	1.45
8	L	404	BCB	C4D-CHA	-5.17	1.38	1.45
9	M	405	BPB	CAC-C3C	5.14	1.39	1.33
9	L	406	BPB	C4B-CHC	5.08	1.41	1.35
8	M	401	BCB	C4D-CHA	-5.04	1.38	1.45
9	M	405	BPB	C4B-CHC	4.98	1.40	1.35
9	L	406	BPB	C4B-C3B	4.91	1.47	1.41
8	L	404	BCB	C1D-C2D	4.88	1.46	1.40
8	L	402	BCB	C1D-C2D	4.79	1.46	1.40
8	M	403	BCB	C4D-CHA	-4.72	1.39	1.45
9	L	406	BPB	CAC-C3C	4.70	1.39	1.33
7	C	404	HEM	C3D-C2D	-4.69	1.35	1.43
7	C	403	HEM	C3B-CAB	4.65	1.55	1.40
9	L	406	BPB	C4D-CHA	-4.62	1.39	1.45
7	C	403	HEM	C3B-C2B	-4.62	1.35	1.43
7	C	404	HEM	C3B-C2B	-4.62	1.35	1.43
7	C	401	HEM	C3C-C2C	-4.62	1.35	1.43
7	C	404	HEM	C3C-C2C	-4.59	1.35	1.43
8	M	403	BCB	C1D-C2D	4.58	1.45	1.40
8	M	401	BCB	C1D-C2D	4.55	1.45	1.40
7	C	402	HEM	C3D-C2D	-4.54	1.35	1.43
7	C	402	HEM	C3C-C2C	-4.51	1.35	1.43
7	C	401	HEM	C3B-C2B	-4.50	1.35	1.43
7	C	402	HEM	C3B-C2B	-4.49	1.35	1.43
7	C	403	HEM	C3C-C2C	-4.45	1.36	1.43
8	L	404	BCB	O2A-CGA	4.44	1.47	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	404	BCB	CAC-C3C	4.44	1.38	1.33
7	C	401	HEM	C3D-C2D	-4.41	1.36	1.43
9	M	405	BPB	C4B-C3B	4.41	1.47	1.41
7	C	404	HEM	C3C-CAC	4.37	1.54	1.40
7	C	403	HEM	C3D-C2D	-4.36	1.36	1.43
7	C	403	HEM	CBB-CAB	4.33	1.54	1.28
7	C	403	HEM	CBC-CAC	4.33	1.54	1.28
7	C	402	HEM	C3B-CAB	4.33	1.54	1.40
7	C	404	HEM	C3B-CAB	4.30	1.53	1.40
7	C	402	HEM	CBC-CAC	4.29	1.53	1.28
7	C	401	HEM	CBB-CAB	4.25	1.53	1.28
8	L	404	BCB	C4B-C3B	4.22	1.46	1.41
8	M	403	BCB	C4B-C3B	4.22	1.46	1.41
7	C	402	HEM	CBB-CAB	4.22	1.53	1.28
7	C	401	HEM	CBC-CAC	4.21	1.53	1.28
8	M	401	BCB	C4B-C3B	4.21	1.46	1.41
7	C	404	HEM	CBC-CAC	4.19	1.53	1.28
9	L	406	BPB	C1B-CHB	4.18	1.40	1.35
7	C	404	HEM	CBB-CAB	4.18	1.53	1.28
8	M	403	BCB	CAC-C3C	4.14	1.38	1.33
8	L	404	BCB	MG-NA	4.09	2.19	2.07
7	C	401	HEM	C3C-CAC	4.08	1.53	1.40
7	C	401	HEM	C3B-CAB	4.05	1.53	1.40
7	C	401	HEM	C4A-C3A	4.04	1.45	1.40
8	L	402	BCB	C4B-C3B	3.97	1.46	1.41
8	L	402	BCB	CAC-C3C	3.95	1.38	1.33
8	M	401	BCB	CAC-C3C	3.91	1.38	1.33
8	M	403	BCB	C4C-NC	3.88	1.40	1.38
9	M	405	BPB	C1B-CHB	3.87	1.39	1.35
7	C	403	HEM	C3C-CAC	3.85	1.52	1.40
7	C	402	HEM	C3C-CAC	3.85	1.52	1.40
8	M	401	BCB	MG-NA	3.84	2.18	2.07
8	M	403	BCB	MG-NA	3.83	2.18	2.07
9	M	405	BPB	C4D-CHA	-3.73	1.40	1.45
8	M	401	BCB	C4C-NC	3.69	1.40	1.38
7	C	404	HEM	C4A-C3A	3.62	1.44	1.40
7	C	402	HEM	C4A-C3A	3.55	1.44	1.40
7	C	403	HEM	C4A-C3A	3.50	1.44	1.40
9	L	406	BPB	O2D-CGD	3.49	1.42	1.33
11	L	502	UQ7	C7-C8	-3.47	1.45	1.50
11	L	502	UQ7	C13-C14	3.41	1.39	1.32
8	L	402	BCB	MG-NA	3.39	2.17	2.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	402	BCB	O2D-CGD	3.39	1.42	1.33
10	M	501	MQ9	C43-C44	3.38	1.39	1.32
10	M	501	MQ9	C33-C34	3.38	1.39	1.32
8	L	402	BCB	C4C-NC	3.36	1.40	1.38
9	L	406	BPB	C2-C3	3.35	1.39	1.32
11	L	502	UQ7	C33-C34	3.33	1.39	1.32
11	L	502	UQ7	C8-C9	3.32	1.39	1.32
10	M	501	MQ9	C28-C29	3.30	1.39	1.32
11	L	502	UQ7	C28-C29	3.30	1.39	1.32
8	L	404	BCB	O2D-CGD	3.30	1.41	1.33
11	L	502	UQ7	C23-C24	3.29	1.39	1.32
11	L	502	UQ7	C18-C19	3.27	1.39	1.32
8	L	404	BCB	C4C-NC	3.27	1.40	1.38
8	L	402	BCB	C4A-NA	3.24	1.39	1.32
8	M	401	BCB	O2D-CGD	3.22	1.41	1.33
10	M	501	MQ9	C38-C39	3.22	1.39	1.32
8	M	401	BCB	C4A-NA	3.20	1.39	1.32
10	M	501	MQ9	C8-C9	3.18	1.39	1.32
8	L	402	BCB	C1C-NC	3.17	1.39	1.32
8	L	404	BCB	C4A-NA	3.13	1.39	1.32
10	M	501	MQ9	C23-C24	3.12	1.39	1.32
8	M	403	BCB	C4A-NA	3.12	1.39	1.32
8	M	403	BCB	C2-C3	3.11	1.39	1.32
8	L	404	BCB	C1C-NC	3.09	1.39	1.32
9	M	405	BPB	O2D-CGD	3.05	1.41	1.33
8	M	403	BCB	C1C-NC	3.05	1.39	1.32
9	M	405	BPB	C2-C3	3.05	1.39	1.32
10	M	501	MQ9	C18-C19	3.04	1.39	1.32
8	L	404	BCB	C2-C3	3.03	1.39	1.32
8	M	401	BCB	C1C-NC	3.00	1.38	1.32
8	M	401	BCB	C2-C3	2.99	1.39	1.32
13	M	704	LDA	C1-N1	-2.97	1.45	1.51
13	M	705	LDA	C1-N1	-2.95	1.45	1.51
10	M	501	MQ9	C13-C14	2.92	1.38	1.32
8	L	404	BCB	C1-C2	-2.89	1.39	1.49
8	M	401	BCB	O2A-CGA	2.86	1.42	1.33
8	L	404	BCB	O2D-CED	-2.83	1.38	1.45
8	M	403	BCB	O2D-CGD	2.81	1.40	1.33
7	C	404	HEM	CHA-C4D	2.81	1.39	1.35
13	L	706	LDA	C1-N1	-2.81	1.46	1.51
7	C	403	HEM	CHA-C4D	2.81	1.39	1.35
7	C	402	HEM	CHB-C1B	2.79	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	406	BPB	O2A-CGA	2.78	1.42	1.33
8	L	402	BCB	C2-C3	2.77	1.38	1.32
7	C	402	HEM	CHA-C4D	2.75	1.39	1.35
7	C	401	HEM	CHA-C4D	2.72	1.39	1.35
7	C	401	HEM	CHB-C1B	2.72	1.39	1.35
13	M	704	LDA	CM2-N1	-2.69	1.45	1.49
8	L	402	BCB	C1D-ND	2.69	1.38	1.34
13	H	701	LDA	CM2-N1	-2.68	1.45	1.49
13	L	702	LDA	C1-N1	-2.67	1.46	1.51
8	M	401	BCB	O2D-CED	-2.64	1.38	1.45
8	L	404	BCB	C1D-ND	2.58	1.37	1.34
7	C	404	HEM	FE-NA	2.58	2.03	1.92
7	C	401	HEM	C2D-C1D	2.58	1.45	1.44
13	M	704	LDA	CM1-N1	-2.58	1.45	1.49
7	C	403	HEM	CHB-C1B	2.57	1.39	1.35
13	M	705	LDA	CM1-N1	-2.57	1.45	1.49
11	L	502	UQ7	O3-CM3	-2.57	1.38	1.45
8	M	403	BCB	C1D-ND	2.56	1.37	1.34
9	M	405	BPB	O2A-CGA	2.56	1.41	1.33
13	L	702	LDA	CM2-N1	-2.51	1.45	1.49
13	M	705	LDA	CM2-N1	-2.51	1.45	1.49
8	M	401	BCB	C1D-ND	2.50	1.37	1.34
7	C	402	HEM	FE-NA	2.48	2.03	1.92
13	L	702	LDA	CM1-N1	-2.36	1.45	1.49
7	C	404	HEM	CHB-C1B	2.36	1.39	1.35
10	M	501	MQ9	C32-C33	-2.35	1.43	1.50
8	L	402	BCB	C1A-CHA	2.35	1.41	1.37
11	L	502	UQ7	C38-C39	2.34	1.39	1.32
9	L	406	BPB	C3D-C4D	2.31	1.43	1.40
13	H	701	LDA	C1-N1	-2.28	1.47	1.51
10	M	501	MQ9	C48-C49	2.28	1.39	1.32
8	M	403	BCB	MG-ND	-2.27	2.00	2.05
11	L	502	UQ7	O2-CM2	-2.27	1.39	1.45
7	C	401	HEM	FE-NA	2.26	2.02	1.92
13	H	703	LDA	CM2-N1	-2.25	1.46	1.49
7	C	403	HEM	CMD-C2D	2.24	1.54	1.47
7	C	401	HEM	CHD-C4C	2.24	1.40	1.36
7	C	402	HEM	CMC-C2C	2.21	1.54	1.47
8	M	403	BCB	O2A-CGA	2.21	1.40	1.33
8	L	402	BCB	MG-ND	-2.21	2.00	2.05
9	M	405	BPB	C3D-C4D	2.20	1.43	1.40
7	C	402	HEM	C2D-C1D	2.18	1.45	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	403	BCB	C1A-CHA	2.14	1.41	1.37
7	C	402	HEM	CHD-C4C	2.12	1.40	1.36
13	H	703	LDA	CM1-N1	-2.11	1.46	1.49
8	M	401	BCB	C1-C2	-2.11	1.41	1.49
9	L	406	BPB	O2D-CED	-2.10	1.40	1.45
9	M	405	BPB	O2D-CED	-2.09	1.40	1.45
7	C	403	HEM	FE-NA	2.09	2.01	1.92
13	L	706	LDA	CM2-N1	-2.08	1.46	1.49
7	C	403	HEM	CMC-C2C	2.07	1.53	1.47
8	M	403	BCB	O2D-CED	-2.06	1.40	1.45
11	L	502	UQ7	C12-C13	-2.05	1.44	1.50
8	L	404	BCB	C4D-ND	2.05	1.37	1.34
7	C	401	HEM	C2B-C1B	2.04	1.45	1.44
7	C	402	HEM	CMB-C2B	2.03	1.53	1.47
8	L	402	BCB	C1-C2	-2.00	1.42	1.49
11	L	502	UQ7	C17-C18	-2.00	1.44	1.50

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	702	LDA	C2-C1-N1	11.13	132.98	113.80
8	L	404	BCB	C1-C2-C3	9.48	143.04	126.19
13	M	704	LDA	C2-C1-N1	7.24	126.28	113.80
13	L	706	LDA	C2-C1-N1	7.06	125.97	113.80
8	L	404	BCB	C5-C3-C2	5.89	132.43	121.08
7	C	402	HEM	C3B-C4B-NB	-5.80	109.85	114.00
7	C	404	HEM	C3B-C4B-NB	-5.75	109.89	114.00
7	C	403	HEM	C3B-C4B-NB	-5.71	109.91	114.00
13	M	705	LDA	C2-C1-N1	5.71	123.64	113.80
7	C	401	HEM	C3B-C4B-NB	-5.69	109.93	114.00
8	L	404	BCB	C4-C3-C2	-5.68	112.27	123.52
8	L	404	BCB	O2D-CGD-CBD	5.67	122.88	111.33
9	M	405	BPB	O2D-CGD-CBD	5.66	122.85	111.33
8	M	401	BCB	O2D-CGD-CBD	5.58	122.70	111.33
9	L	406	BPB	O2D-CGD-CBD	5.57	122.67	111.33
8	M	403	BCB	O2D-CGD-CBD	5.17	121.86	111.33
13	H	701	LDA	C2-C1-N1	4.92	122.29	113.80
9	L	406	BPB	C3D-C4D-CHA	4.74	114.43	109.18
8	M	401	BCB	O1D-CGD-CBD	-4.61	114.98	124.42
9	M	405	BPB	C3D-C4D-CHA	4.59	114.26	109.18
8	L	402	BCB	O2D-CGD-CBD	4.59	120.67	111.33
8	L	404	BCB	O1D-CGD-CBD	-4.51	115.17	124.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	405	BPB	O1D-CGD-CBD	-4.51	115.18	124.42
9	L	406	BPB	O1D-CGD-CBD	-4.50	115.20	124.42
8	M	403	BCB	C3D-C4D-CHA	4.29	115.16	108.91
8	M	401	BCB	C3D-C4D-CHA	4.24	115.09	108.91
8	L	402	BCB	C3D-C4D-CHA	4.24	115.08	108.91
8	M	403	BCB	O1D-CGD-CBD	-4.17	115.88	124.42
8	L	402	BCB	C3A-C4A-CHB	4.11	126.36	122.11
8	L	404	BCB	C3D-C4D-CHA	4.06	114.83	108.91
9	L	406	BPB	C1-C2-C3	4.00	133.30	126.19
8	L	402	BCB	O1D-CGD-CBD	-3.96	116.31	124.42
8	M	403	BCB	OBB-CAB-C3B	3.91	126.00	120.04
8	M	403	BCB	C3A-C4A-CHB	3.86	126.10	122.11
9	M	405	BPB	CHD-C4C-NC	-3.82	121.54	128.59
8	M	403	BCB	C4A-NA-C1A	3.75	110.82	106.13
9	L	406	BPB	CHD-C4C-NC	-3.74	121.70	128.59
9	L	406	BPB	C3C-C2C-C1C	3.69	105.45	101.05
8	L	404	BCB	C4A-NA-C1A	3.63	110.66	106.13
9	M	405	BPB	C3C-C2C-C1C	3.62	105.36	101.05
8	L	402	BCB	C4A-NA-C1A	3.60	110.63	106.13
8	M	401	BCB	C4A-NA-C1A	3.60	110.63	106.13
8	M	401	BCB	OBD-CAD-CBD	-3.59	120.52	125.94
8	L	402	BCB	O2A-CGA-CBA	3.57	123.18	111.94
9	M	405	BPB	OBD-CAD-CBD	-3.47	120.71	125.94
9	L	406	BPB	C3D-C2D-C1D	-3.44	104.95	107.01
8	L	402	BCB	OBB-CAB-C3B	3.43	125.27	120.04
10	M	501	MQ9	C37-C38-C39	3.42	135.17	127.80
8	M	403	BCB	OBD-CAD-CBD	-3.41	120.79	125.94
9	L	406	BPB	OBD-CAD-CBD	-3.31	120.94	125.94
8	L	402	BCB	C3C-C4C-NC	3.30	112.22	109.98
8	L	404	BCB	C3C-C4C-NC	3.30	112.22	109.98
8	L	402	BCB	OBD-CAD-CBD	-3.29	120.97	125.94
8	L	404	BCB	C3A-C4A-CHB	3.25	125.47	122.11
8	M	403	BCB	CMB-C2B-C3B	3.24	130.08	124.97
8	M	401	BCB	C3A-C4A-CHB	3.16	125.38	122.11
9	M	405	BPB	C3D-C2D-C1D	-3.14	105.13	107.01
13	H	703	LDA	C2-C1-N1	3.13	119.20	113.80
8	L	404	BCB	OBD-CAD-CBD	-3.11	121.25	125.94
9	L	406	BPB	O2A-CGA-CBA	3.11	121.72	111.94
8	L	402	BCB	C3A-C4A-NA	-3.09	108.55	111.79
7	C	404	HEM	C2D-C1D-ND	-3.06	109.31	112.93
7	C	401	HEM	C2D-C1D-ND	-3.04	109.34	112.93
11	L	502	UQ7	C17-C18-C19	3.02	134.31	127.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	404	BCB	C3A-C4A-NA	-2.99	108.65	111.79
8	M	403	BCB	C2C-C1C-NC	-2.98	107.89	111.65
8	L	404	BCB	C2C-C1C-NC	-2.96	107.91	111.65
12	M	600	NS5	C13-C12-C10	2.96	130.74	127.91
8	M	403	BCB	CMD-C2D-C3D	2.95	129.62	124.97
8	M	401	BCB	C3C-C4C-NC	2.91	111.96	109.98
8	L	404	BCB	OBB-CAB-C3B	2.88	124.43	120.04
9	L	406	BPB	C2C-C1C-NC	-2.86	108.12	113.50
11	L	502	UQ7	C25-C24-C26	-2.86	111.04	115.39
7	C	402	HEM	C2D-C1D-ND	-2.85	109.56	112.93
8	M	403	BCB	C3A-C4A-NA	-2.84	108.81	111.79
9	M	405	BPB	C2C-C3C-C4C	-2.84	104.53	108.73
8	L	402	BCB	C2C-C1C-NC	-2.83	108.08	111.65
9	M	405	BPB	C2C-C1C-NC	-2.81	108.21	113.50
10	M	501	MQ9	C32-C33-C34	2.80	133.85	127.80
8	M	401	BCB	C3A-C4A-NA	-2.79	108.87	111.79
8	M	403	BCB	C2C-C3C-C4C	-2.78	104.62	108.73
8	L	402	BCB	O2A-CGA-O1A	-2.76	115.90	123.43
8	L	404	BCB	O2A-CGA-CBA	2.74	120.56	111.94
9	M	405	BPB	C3A-C4A-NA	-2.74	108.87	113.57
9	M	405	BPB	C5-C3-C2	2.70	126.28	121.08
8	L	404	BCB	C2C-C3C-C4C	-2.68	104.77	108.73
8	M	401	BCB	C2C-C1C-NC	-2.67	108.29	111.65
9	L	406	BPB	C2C-C3C-C4C	-2.66	104.80	108.73
8	M	401	BCB	C2C-C3C-C4C	-2.62	104.85	108.73
9	L	406	BPB	C3A-C4A-NA	-2.62	109.07	113.57
8	L	402	BCB	C2C-C3C-C4C	-2.61	104.87	108.73
7	C	403	HEM	C2D-C1D-ND	-2.57	109.90	112.93
11	L	502	UQ7	C12-C11-C9	-2.54	104.32	112.74
10	M	501	MQ9	C45-C44-C46	-2.54	111.53	115.39
8	M	403	BCB	CMD-C2D-C1D	-2.53	124.72	128.62
10	M	501	MQ9	C7-C8-C9	2.53	131.02	126.76
8	M	401	BCB	CMD-C2D-C3D	2.48	128.87	124.97
8	L	404	BCB	CMB-C2B-C3B	2.44	128.82	124.97
8	M	401	BCB	C6-C5-C3	2.43	118.57	112.78
11	L	502	UQ7	C26-C27-C28	2.42	118.53	111.62
8	M	401	BCB	CBC-CAC-C3C	-2.42	121.44	126.93
9	L	406	BPB	C3D-C4D-ND	2.41	110.99	106.97
10	M	501	MQ9	C30-C29-C31	-2.38	111.77	115.39
9	L	406	BPB	CBC-CAC-C3C	-2.38	121.53	126.93
8	L	402	BCB	CMD-C2D-C3D	2.34	128.66	124.97
8	L	404	BCB	C3D-C4D-ND	2.34	110.95	108.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	403	BCB	C3C-C4C-NC	2.34	111.57	109.98
9	M	405	BPB	C3D-C4D-ND	2.34	110.87	106.97
12	M	600	NS5	C19-C18-C17	2.34	128.53	123.36
9	M	405	BPB	CMD-C2D-C3D	2.31	128.62	124.97
8	M	401	BCB	C3D-C4D-ND	2.31	110.91	108.61
9	L	406	BPB	CMD-C2D-C3D	2.30	128.60	124.97
8	L	402	BCB	CMB-C2B-C3B	2.30	128.59	124.97
8	L	402	BCB	C3D-C4D-ND	2.30	110.90	108.61
9	M	405	BPB	O2A-CGA-CBA	2.28	119.10	111.94
11	L	502	UQ7	C37-C36-C34	2.27	120.24	112.74
8	M	403	BCB	O2A-CGA-CBA	2.25	119.03	111.94
8	M	403	BCB	C3D-C4D-ND	2.25	110.85	108.61
11	L	502	UQ7	C7-C8-C9	2.22	130.51	126.76
9	L	406	BPB	O2A-CGA-O1A	-2.22	117.36	123.43
12	M	600	NS5	C16-C15-C14	-2.22	114.51	118.09
11	L	502	UQ7	CM3-O3-C3	2.22	124.01	116.48
8	M	401	BCB	C15-C13-C12	2.12	122.86	111.92
9	M	405	BPB	C1D-CHD-C4C	-2.09	125.84	129.92
12	M	600	NS5	C19-C20-C21	-2.09	124.28	127.29
8	M	401	BCB	C3A-C2A-C1A	2.09	104.04	101.08
10	M	501	MQ9	C37-C36-C34	2.08	119.61	112.74
9	L	406	BPB	C3A-C4A-CHB	2.05	125.74	121.69
11	L	502	UQ7	C16-C14-C13	2.05	125.02	121.08
8	M	403	BCB	CMB-C2B-C1B	-2.04	122.13	126.16
8	L	402	BCB	C4-C3-C5	2.04	118.48	115.39
9	L	406	BPB	C1D-CHD-C4C	-2.03	125.97	129.92
9	M	405	BPB	C3A-C4A-CHB	2.02	125.69	121.69
7	C	404	HEM	CBD-CAD-C3D	2.02	118.78	114.37
8	L	404	BCB	CED-O2D-CGD	2.01	120.81	116.02
8	L	404	BCB	C3A-C2A-C1A	2.01	103.92	101.08
10	M	501	MQ9	C36-C37-C38	2.00	117.34	111.62
8	M	401	BCB	C2A-C3A-C4A	2.00	104.48	101.40

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	M	405	BPB	C8
9	M	405	BPB	C13
8	M	401	BCB	C8

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	C	332/332 (100%)	-0.43	7 (2%) 60 61	16, 27, 44, 59	9 (2%)
2	H	249/258 (96%)	-0.20	13 (5%) 26 26	19, 32, 49, 58	20 (8%)
3	L	273/273 (100%)	-0.73	4 (1%) 70 71	16, 23, 35, 52	5 (1%)
4	M	323/323 (100%)	-0.56	8 (2%) 54 55	16, 26, 44, 58	7 (2%)
All	All	1177/1186 (99%)	-0.49	32 (2%) 52 52	16, 27, 45, 59	41 (3%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	45	GLU	6.1
4	M	319	PRO	4.5
1	C	332	LYS	4.4
2	H	8	GLN	4.4
2	H	85	THR	4.4
2	H	96	PHE	4.4
1	C	1	CYS	4.3
2	H	9	HIS	4.2
4	M	320	GLY	4.0
1	C	47	ALA	3.8
4	M	30	GLY	3.8
2	H	95	GLY	3.4
3	L	1	ALA	3.2
3	L	202	ASP	2.9
4	M	78	HIS	2.8
2	H	191	ALA	2.7
2	H	189	GLY	2.7
2	H	7	ALA	2.7
2	H	94	ASP	2.6
4	M	108	HIS	2.6
2	H	83	PRO	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	M	26	ASN	2.5
1	C	159	THR	2.4
4	M	29	VAL	2.4
3	L	271	PHE	2.4
4	M	37	TRP	2.3
1	C	48	GLU	2.3
3	L	51	TYR	2.2
2	H	227	ARG	2.1
1	C	198	LYS	2.0
2	H	258	LEU	2.0
1	C	50	PRO	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	FME	H	1	10/11	0.09	1.37	28,32,49,55	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
11	UQ7	L	502	48/48	0.39	16.86	23,36,44,44	48
13	LDA	L	706	16/16	0.32	9.06	48,58,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
13	LDA	L	702	16/16	0.24	6.54	29,50,54,54	0
12	NS5	M	600	40/40	0.21	4.61	24,35,65,66	0
6	SO4	H	806	5/5	0.29	3.97	58,61,63,63	0
13	LDA	H	701	16/16	0.15	3.81	23,36,50,52	0
6	SO4	M	801	5/5	0.08	3.73	31,32,33,38	0
13	LDA	M	704	16/16	0.22	3.62	52,54,65,65	0
13	LDA	H	703	16/16	0.23	3.14	38,48,61,62	0
6	SO4	H	807	5/5	0.20	2.91	31,32,32,38	5
10	MQ9	M	501	58/58	0.14	1.93	15,20,62,64	0
8	BCB	M	401	66/66	0.12	1.93	15,22,68,71	0
13	LDA	M	705	16/16	0.26	1.84	57,60,62,63	4
6	SO4	M	805	5/5	0.21	1.53	55,57,59,60	0
9	BPB	M	405	65/65	0.11	1.03	14,24,57,59	9
6	SO4	H	802	5/5	0.11	0.99	57,59,60,61	0
8	BCB	L	402	66/66	0.11	0.94	13,17,23,30	0
7	HEM	C	402	43/43	0.12	0.67	18,27,32,34	0
9	BPB	L	406	65/65	0.09	0.61	14,18,23,26	0
6	SO4	M	803	5/5	0.11	0.47	46,47,53,55	0
8	BCB	M	403	66/66	0.09	0.39	12,18,40,41	0
7	HEM	C	401	43/43	0.10	-0.20	23,30,37,39	0
8	BCB	L	404	66/66	0.07	-0.21	10,16,41,48	0
7	HEM	C	403	43/43	0.08	-0.25	14,19,22,26	0
7	HEM	C	404	43/43	0.09	-0.37	14,21,33,43	0
6	SO4	M	804	5/5	0.08	-1.23	40,41,42,44	0
5	FE2	M	500	1/1	0.02	-7.43	17,17,17,17	0

6.5 Other polymers ⓘ

There are no such residues in this entry.