



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 07:59 pm 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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

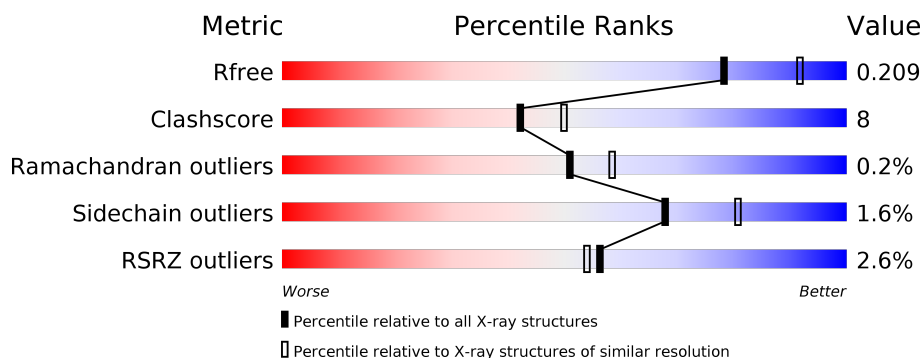
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	C	332	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>12%</div> </div> </div>
2	H	258	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>16%</div> </div> </div>
3	L	273	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>16%</div> </div> </div>
4	M	323	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>15%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	UQ7	L	502	-	-	-	X
12	NS5	M	600	-	-	-	X
13	LDA	H	701	-	-	-	X
13	LDA	H	703	-	-	-	X
13	LDA	L	702	-	-	-	X
13	LDA	M	704	-	-	-	X
6	SO4	H	806	-	-	-	X
6	SO4	H	807	-	-	X	-
8	BCB	M	401	X	-	-	-
9	BPB	M	405	X	-	-	-

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 10747 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 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).

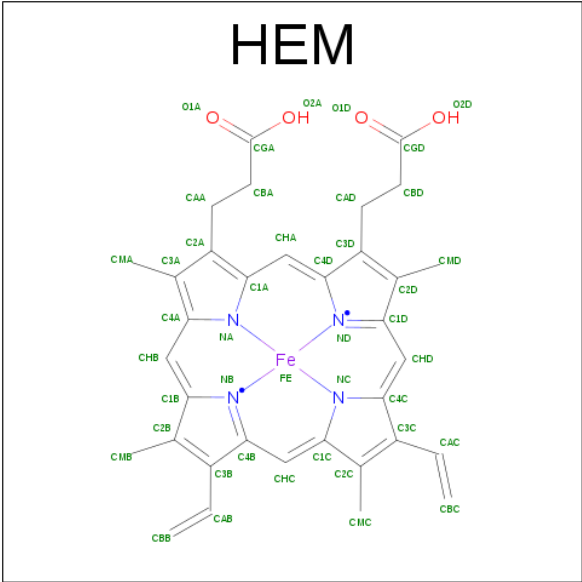
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	1	Total	Fe	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



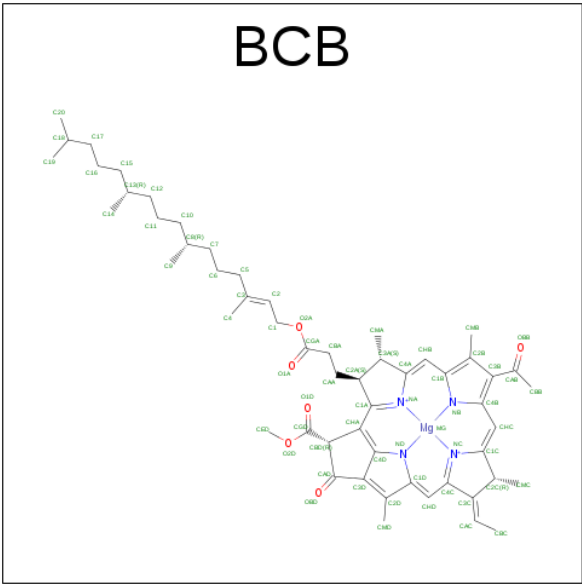
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	M	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



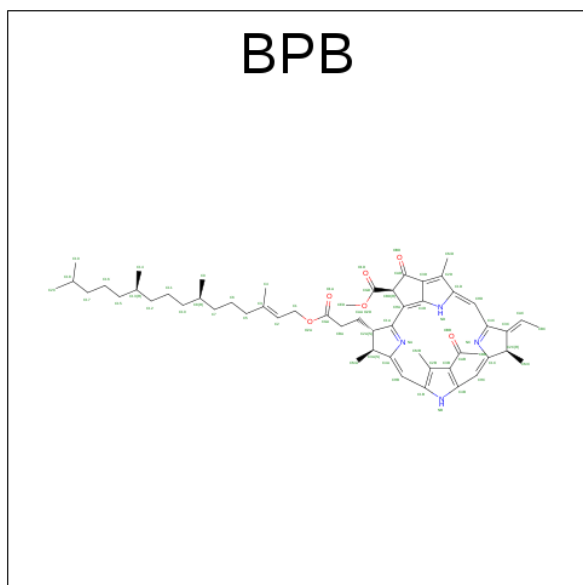
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
7	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
7	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
7	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 8 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>6</sub>).



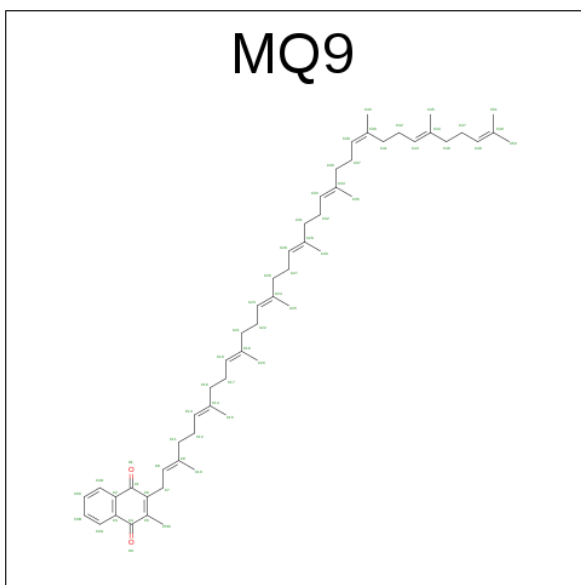
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
8	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
8	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
8	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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



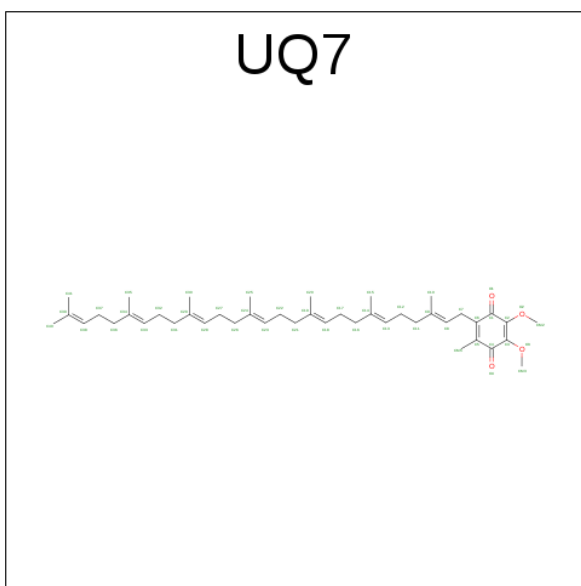
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	M	1	Total	C	N	O	9	0
			65	55	4	6		
9	L	1	Total	C	N	O	0	0
			65	55	4	6		

- 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		

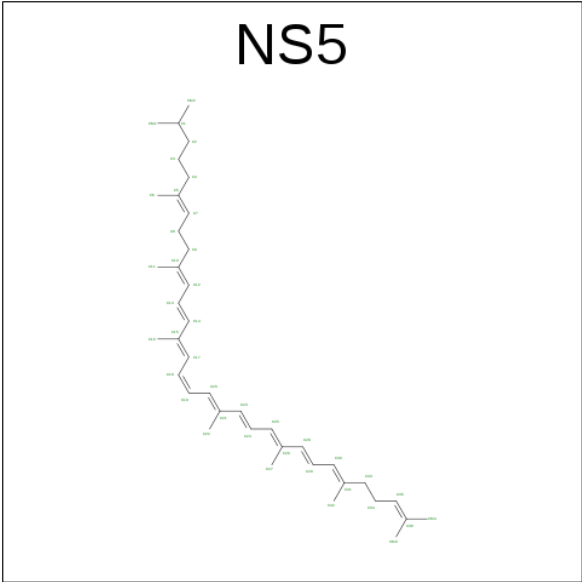
- Molecule 11 is UBIQUINONE-7 (three-letter code: UQ7) (formula:  $C_{44}H_{66}O_4$ ).



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

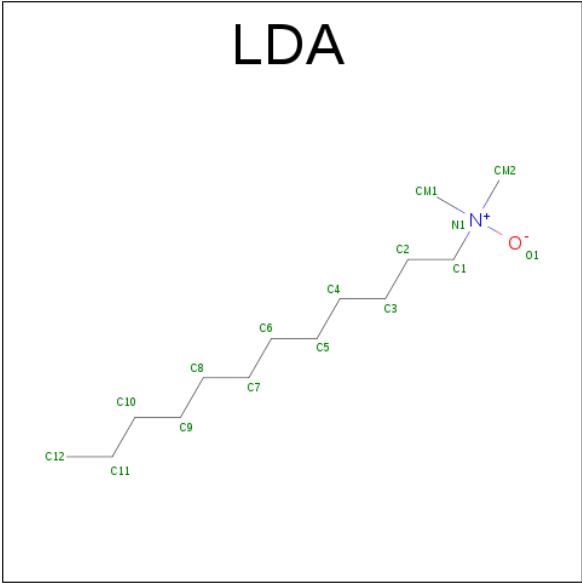
- Molecule 12 is 15-CIS-1,2-DIHYDRONEUROSPORENE (three-letter code: NS5) (formula:  $C_{40}H_{60}$ ).





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<sub>14</sub>H<sub>31</sub>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		

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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		

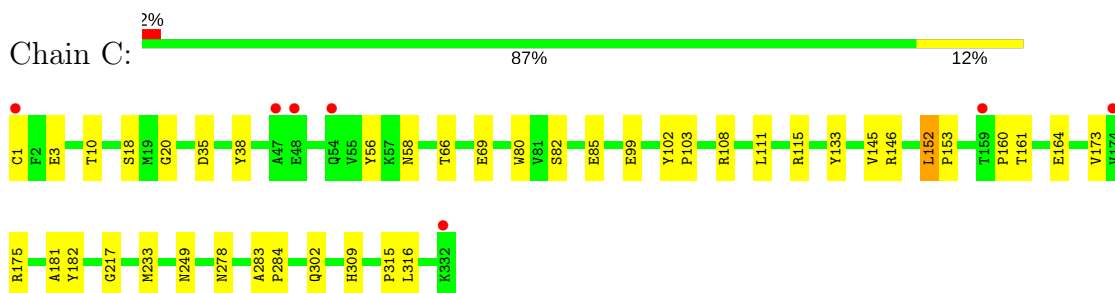
- Molecule 14 is water.

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		

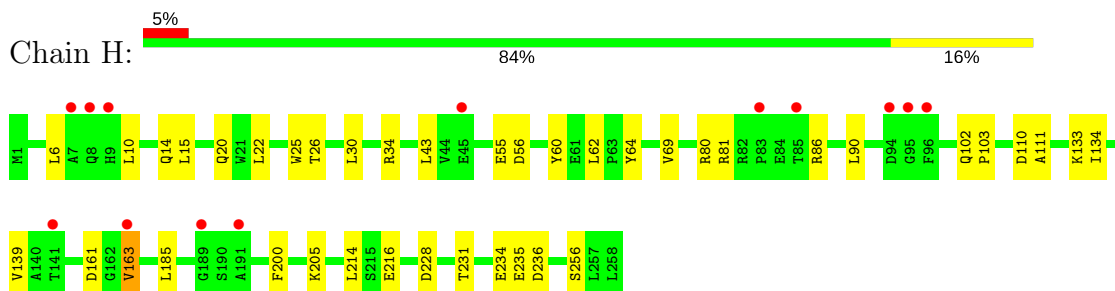
### 3 Residue-property plots [i](#)

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.

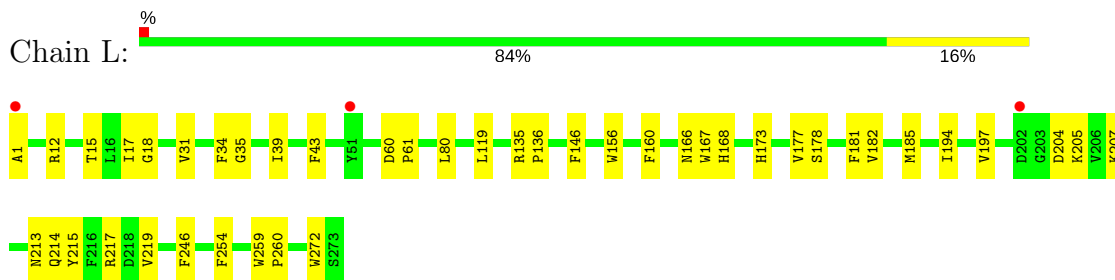
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



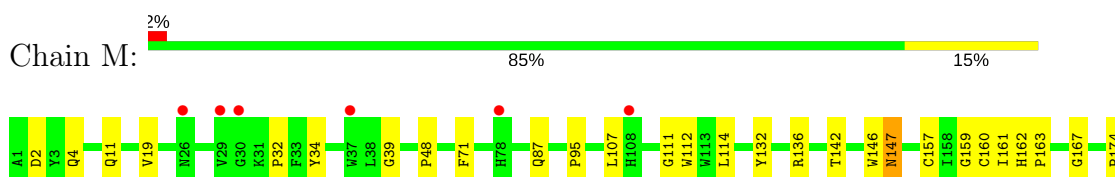
- Molecule 2: Reaction center protein H chain



- 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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	6074 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.8	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.44 , 69.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10747	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: 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 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	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
5	M	1	0	0	0	0
6	H	15	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 8.

All (157) 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)
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
2:H:69:VAL:HG12	14:H:1292:HOH:O	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:402:BCB:HMB1	8:L:402:BCB:HBB3	1.79	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
13:L:702:LDA:H72	13:L:702:LDA:H31	1.81	0.62
4:M:231:ARG:HD2	14:M:1383:HOH:O	1.98	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
1:C:1:CYS:HB2	14:L:1204:HOH:O	2.03	0.58
6:H:807:SO4:O3	13:H:703:LDA:HM23	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
3:L:135:ARG:HB3	3:L:136:PRO:HD3	1.88	0.54
8:M:403:BCB:H203	9:M:405:BPB:C4	2.38	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
2:H:235:GLU:OE1	4:M:231:ARG:NH2	2.38	0.51
8:M:403:BCB:CBB	8:M:403:BCB:HMB1	2.40	0.51
2:H:81:ARG:N	13:H:703:LDA:H112	2.25	0.51
1:C:18:SER:HB2	3:L:156:TRP:CD1	2.47	0.50
3:L:213:ASN:OD1	11:L:502:UQ7:HM21	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:241:THR:O	4:M:245:ARG:HG3	2.12	0.50
2:H:134:ILE:N	2:H:134:ILE:HD12	2.27	0.50
3:L:177:VAL:HG13	8:L:402:BCB:HMB3	1.93	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
1:C:283:ALA:HB3	1:C:284:PRO:HD3	1.96	0.48
8:L:404:BCB:HHC	8:L:404:BCB:OBB	2.13	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:167:TRP:HE1	3:L:173:HIS:CD2	2.33	0.47
3:L:43:PHE:CD1	10:M:501:MQ9:H512	2.50	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
2:H:22:LEU:HD13	2:H:22:LEU:C	2.35	0.46
3:L:197:VAL:HG13	3:L:207:LYS:HB2	1.95	0.46
4:M:107:LEU:HA	4:M:111:GLY:HA3	1.96	0.46
4:M:192:GLY:O	4:M:193:ASN:HB3	2.14	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
1:C:66:THR:OG1	1:C:69:GLU:HG3	2.16	0.46
2:H:86:ARG:NH2	2:H:110:ASP:O	2.49	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
2:H:90:LEU:HD23	2:H:103:PRO:HA	1.98	0.45
12:M:600:NS5:H271	12:M:600:NS5:H29	1.82	0.45
4:M:160:CYS:C	4:M:163:PRO:HD2	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:403:BCB:OBB	8:M:403:BCB:HHC	2.17	0.45
2:H:56:ASP:HB3	2:H:60:TYR:CE2	2.52	0.45
8:M:401:BCB:HHC	8:M:401:BCB:CBB	2.43	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:N	4:M:34:TYR:CD1	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
2:H:216:GLU:H	2:H:216:GLU:CD	2.20	0.44
8:L:402:BCB:HHC	8:L:402:BCB:OBB	2.16	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
1:C:233:MET:HB3	7:C:403:HEM:C4B	2.53	0.43
3:L:60:ASP:OD2	13:L:702:LDA:HM12	2.19	0.43
3:L:214:GLN:HG2	4:M:19:VAL:HB	2.00	0.43
1:C:99:GLU:OE2	1:C:108:ARG:NH2	2.51	0.42
1:C:217:GLY:HA2	4:M:167:GLY:O	2.18	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
2:H:200:PHE:CZ	4:M:226:ARG:HD3	2.54	0.42
6:M:804:SO4:O4	13:M:704:LDA:HM11	2.19	0.42
1:C:309:HIS:CE1	1:C:315:PRO:HD3	2.55	0.42
1:C:82:SER:HB2	1:C:85:GLU:HB2	2.01	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
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
2:H:6:LEU:HB2	2:H:10:LEU:HD12	2.02	0.42
9:M:405:BPB:CHC	9:M:405:BPB:HBBB	2.37	0.42
2:H:10:LEU:HD13	2:H:15:LEU:HD21	2.01	0.42
3:L:194:ILE:HD11	11:L:502:UQ7:HM31	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:159:GLY:HA3	12:M:600:NS5:H272	2.02	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
4:M:11:GLN:OE1	4:M:39:GLY:HA3	2.21	0.41
4:M:178:TRP:CE3	4:M:178:TRP:HA	2.55	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
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
12:M:600:NS5:H7	12:M:600:NS5:H22	2.02	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
1:C:56:TYR:HB3	7:C:401:HEM:CGA	2.51	0.40
3:L:17:ILE:HG22	3:L:34:PHE:CE2	2.56	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%)	38	41
3	L	272/273 (100%)	267 (98%)	4 (2%)	1 (0%)	38	41
4	M	322/323 (100%)	310 (96%)	12 (4%)	0	100	100
All	All	1180/1186 (100%)	1146 (97%)	32 (3%)	2 (0%)	51	58

All (2) Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	281/281 (100%)	278 (99%)	3 (1%)	78	88
2	H	212/212 (100%)	208 (98%)	4 (2%)	62	76
3	L	219/218 (100%)	214 (98%)	5 (2%)	56	69
4	M	250/249 (100%)	247 (99%)	3 (1%)	75	86
All	All	962/960 (100%)	947 (98%)	15 (2%)	68	81

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
2	H	58	GLN
3	L	214	GLN
4	M	147	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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	0.92	1 (11%)	7,9,11	2.34	2 (28%)

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	-	0/6/9/11	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	FME	CA-C	2.14	1.53	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	FME	CA-N-CN	-4.17	116.40	122.82
2	H	1	FME	O1-CN-N	-3.61	115.12	125.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	28,50,50	1.69	6 (21%)	17,82,82	0.73	0
7	HEM	C	402	1	28,50,50	1.70	6 (21%)	17,82,82	1.03	1 (5%)
7	HEM	C	403	1	28,50,50	1.75	6 (21%)	17,82,82	0.80	0
7	HEM	C	404	1	28,50,50	1.73	6 (21%)	17,82,82	1.23	1 (5%)
13	LDA	H	701	-	13,15,15	2.47	1 (7%)	14,17,17	0.65	0
13	LDA	H	703	-	13,15,15	2.58	1 (7%)	14,17,17	0.68	0
6	SO4	H	802	-	4,4,4	0.36	0	6,6,6	0.17	0
6	SO4	H	806	-	4,4,4	0.29	0	6,6,6	0.14	0
6	SO4	H	807	-	4,4,4	0.54	0	6,6,6	0.35	0
8	BCB	L	402	3	63,74,74	3.68	24 (38%)	50,115,115	2.41	16 (32%)
8	BCB	L	404	3	63,74,74	3.78	25 (39%)	50,115,115	2.86	19 (38%)
9	BPB	L	406	-	63,70,70	1.39	7 (11%)	67,101,101	1.65	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	UQ7	L	502	-	48,48,48	1.60	10 (20%)	58,61,61	1.18	6 (10%)
13	LDA	L	702	-	13,15,15	2.76	2 (15%)	14,17,17	0.64	0
13	LDA	L	706	-	13,15,15	2.70	2 (15%)	14,17,17	0.69	0
8	BCB	M	401	4	63,74,74	3.77	25 (39%)	50,115,115	2.62	18 (36%)
8	BCB	M	403	4	63,74,74	3.69	24 (38%)	50,115,115	2.41	15 (30%)
9	BPB	M	405	-	63,70,70	1.33	6 (9%)	67,101,101	1.54	7 (10%)
10	MQ9	M	501	-	59,59,59	1.49	9 (15%)	73,75,75	1.01	5 (6%)
12	NS5	M	600	-	39,39,39	0.52	0	44,46,46	0.89	3 (6%)
13	LDA	M	704	-	13,15,15	2.79	2 (15%)	14,17,17	0.71	0
13	LDA	M	705	-	13,15,15	2.85	2 (15%)	14,17,17	0.67	0
6	SO4	M	801	-	4,4,4	0.45	0	6,6,6	0.20	0
6	SO4	M	803	-	4,4,4	0.49	0	6,6,6	0.38	0
6	SO4	M	804	-	4,4,4	0.45	0	6,6,6	0.33	0
6	SO4	M	805	-	4,4,4	0.40	0	6,6,6	0.30	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	-	0/6/54/54	0/0/8/8
7	HEM	C	402	1	-	0/6/54/54	0/0/8/8
7	HEM	C	403	1	-	0/6/54/54	0/0/8/8
7	HEM	C	404	1	-	0/6/54/54	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	-	0/41/177/177	0/0/9/9
8	BCB	L	404	3	-	0/41/177/177	0/0/9/9
9	BPB	L	406	-	-	0/47/105/105	0/1/6/6
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	1/1/31/36	0/41/177/177	0/0/9/9
8	BCB	M	403	4	-	0/41/177/177	0/0/9/9
9	BPB	M	405	-	2/2/18/23	0/47/105/105	0/1/6/6
10	MQ9	M	501	-	-	0/53/73/73	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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 (164) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	403	BCB	C3D-C4D	-10.16	1.42	1.54
8	M	401	BCB	C3D-C4D	-10.03	1.43	1.54
13	M	705	LDA	O1-N1	-9.94	1.22	1.42
8	L	404	BCB	C3D-C4D	-9.78	1.43	1.54
8	L	402	BCB	C3D-C4D	-9.76	1.43	1.54
13	M	704	LDA	O1-N1	-9.73	1.23	1.42
13	L	702	LDA	O1-N1	-9.66	1.23	1.42
13	L	706	LDA	O1-N1	-9.44	1.23	1.42
13	H	703	LDA	O1-N1	-9.18	1.24	1.42
13	H	701	LDA	O1-N1	-8.66	1.25	1.42
8	L	402	BCB	CHD-C1D	-8.31	1.40	1.53
8	L	404	BCB	CHD-C1D	-8.28	1.40	1.53
8	M	401	BCB	CHB-C1B	-8.28	1.40	1.53
8	L	404	BCB	CHB-C1B	-8.27	1.40	1.53
8	M	403	BCB	CHB-C1B	-8.21	1.40	1.53
8	M	401	BCB	CHD-C1D	-8.13	1.40	1.53
8	M	401	BCB	C1A-CHA	-8.11	1.40	1.53
8	L	404	BCB	C1A-CHA	-8.10	1.41	1.53
8	M	403	BCB	CHD-C1D	-8.02	1.40	1.53
8	M	401	BCB	CHC-C4B	-8.00	1.40	1.53
8	M	403	BCB	CHC-C4B	-7.95	1.40	1.53
8	L	402	BCB	CHB-C1B	-7.88	1.40	1.53
8	L	404	BCB	CHC-C4B	-7.78	1.41	1.53
8	M	403	BCB	C1A-CHA	-7.77	1.41	1.53
8	L	402	BCB	CHC-C4B	-7.73	1.41	1.53
8	L	402	BCB	C1A-CHA	-7.51	1.41	1.53
8	M	401	BCB	C3B-C2B	-7.37	1.35	1.55
8	L	402	BCB	CHD-C4C	-7.03	1.40	1.53
8	L	404	BCB	C3B-C2B	-6.98	1.36	1.55
8	L	402	BCB	C3B-C2B	-6.96	1.36	1.55
8	L	402	BCB	C3B-C4B	-6.90	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	402	BCB	C3D-C2D	-6.90	1.36	1.55
8	L	404	BCB	C3D-C2D	-6.88	1.36	1.55
8	M	403	BCB	C3B-C2B	-6.84	1.37	1.55
8	M	401	BCB	CHD-C4C	-6.82	1.41	1.53
8	M	403	BCB	CHD-C4C	-6.79	1.41	1.53
8	M	403	BCB	C3D-C2D	-6.73	1.37	1.55
8	M	401	BCB	C3D-C2D	-6.72	1.37	1.55
8	L	404	BCB	CHD-C4C	-6.68	1.41	1.53
8	M	401	BCB	C3B-C4B	-6.64	1.46	1.54
8	M	403	BCB	C3B-C4B	-6.62	1.46	1.54
8	L	404	BCB	C3B-C4B	-6.62	1.46	1.54
8	L	402	BCB	C4D-ND	-6.27	1.36	1.50
8	M	403	BCB	C4D-ND	-6.27	1.36	1.50
8	M	401	BCB	C4D-ND	-6.19	1.37	1.50
8	L	404	BCB	C4D-ND	-6.09	1.37	1.50
8	M	401	BCB	C1D-ND	-5.83	1.37	1.50
8	M	403	BCB	C1D-ND	-5.80	1.37	1.50
8	L	404	BCB	C1D-ND	-5.79	1.37	1.50
8	M	403	BCB	C4B-NB	-5.76	1.37	1.50
8	M	401	BCB	C4B-NB	-5.74	1.38	1.50
8	L	402	BCB	C1D-ND	-5.73	1.38	1.50
8	L	402	BCB	C4B-NB	-5.64	1.38	1.50
8	M	401	BCB	C3B-CAB	-5.64	1.46	1.52
8	L	404	BCB	C4B-NB	-5.57	1.38	1.50
8	M	401	BCB	C1B-NB	-5.55	1.38	1.50
8	L	404	BCB	C3B-CAB	-5.53	1.46	1.52
8	M	401	BCB	CHC-C1C	-5.53	1.39	1.52
8	M	403	BCB	C1B-NB	-5.49	1.38	1.50
8	L	404	BCB	CHB-C4A	-5.47	1.39	1.52
8	L	404	BCB	C1B-NB	-5.44	1.38	1.50
8	M	403	BCB	CHB-C4A	-5.42	1.39	1.52
8	L	402	BCB	C1B-NB	-5.42	1.38	1.50
8	M	401	BCB	CHB-C4A	-5.36	1.39	1.52
8	L	402	BCB	C3B-CAB	-5.30	1.46	1.52
8	M	403	BCB	CHC-C1C	-5.29	1.40	1.52
8	L	404	BCB	CHC-C1C	-5.23	1.40	1.52
8	L	402	BCB	CHC-C1C	-5.21	1.40	1.52
8	L	402	BCB	CHB-C4A	-5.20	1.40	1.52
8	M	403	BCB	C3B-CAB	-5.12	1.46	1.52
8	L	404	BCB	C2B-C1B	-4.44	1.44	1.53
8	M	401	BCB	C2B-C1B	-4.40	1.44	1.53
8	L	402	BCB	C2B-C1B	-4.29	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	403	BCB	C2B-C1B	-4.14	1.45	1.53
8	M	401	BCB	C2D-C1D	-3.77	1.45	1.53
8	M	403	BCB	C2D-C1D	-3.75	1.45	1.53
8	L	402	BCB	C2D-C1D	-3.61	1.46	1.53
11	L	502	UQ7	C7-C8	-3.60	1.45	1.50
8	L	402	BCB	C3D-CAD	-3.58	1.44	1.51
8	L	404	BCB	C2D-C1D	-3.56	1.46	1.53
7	C	403	HEM	C3B-C2B	-3.54	1.35	1.40
7	C	404	HEM	C3B-C2B	-3.54	1.35	1.40
7	C	401	HEM	C3C-C2C	-3.54	1.35	1.40
7	C	404	HEM	C3C-C2C	-3.50	1.35	1.40
8	L	404	BCB	C3D-CAD	-3.50	1.44	1.51
7	C	402	HEM	C3C-C2C	-3.39	1.35	1.40
7	C	401	HEM	C3B-C2B	-3.37	1.35	1.40
7	C	402	HEM	C3B-C2B	-3.36	1.35	1.40
8	M	403	BCB	C3D-CAD	-3.31	1.45	1.51
7	C	403	HEM	C3C-C2C	-3.31	1.36	1.40
8	M	401	BCB	C3D-CAD	-3.25	1.45	1.51
8	L	404	BCB	C1-C2	-3.20	1.39	1.49
8	L	404	BCB	O2D-CED	-2.94	1.38	1.45
8	L	402	BCB	C4C-C3C	-2.84	1.41	1.50
8	M	401	BCB	C4C-C3C	-2.75	1.41	1.50
8	M	401	BCB	O2D-CED	-2.74	1.38	1.45
11	L	502	UQ7	O3-CM3	-2.67	1.38	1.45
8	M	403	BCB	C4C-C3C	-2.65	1.42	1.50
8	L	404	BCB	C4C-C3C	-2.65	1.42	1.50
13	M	704	LDA	C1-N1	-2.48	1.45	1.51
13	M	705	LDA	C1-N1	-2.47	1.45	1.51
11	L	502	UQ7	O2-CM2	-2.36	1.39	1.45
13	L	706	LDA	C1-N1	-2.35	1.46	1.51
8	M	401	BCB	C1-C2	-2.34	1.41	1.49
13	L	702	LDA	C1-N1	-2.23	1.46	1.51
8	L	402	BCB	C1-C2	-2.22	1.42	1.49
9	L	406	BPB	O2D-CED	-2.17	1.40	1.45
9	M	405	BPB	O2D-CED	-2.17	1.40	1.45
8	M	403	BCB	O2D-CED	-2.14	1.40	1.45
8	L	402	BCB	O2D-CED	-2.02	1.40	1.45
9	L	406	BPB	C3B-C2B	-2.01	1.35	1.39
8	L	402	BCB	C2-C3	2.22	1.38	1.33
8	M	403	BCB	O2A-CGA	2.34	1.40	1.33
10	M	501	MQ9	C13-C14	2.34	1.38	1.33
7	C	402	HEM	C3C-CAC	2.39	1.52	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	401	BCB	C2-C3	2.40	1.39	1.33
7	C	403	HEM	C3C-CAC	2.40	1.52	1.47
8	L	404	BCB	C2-C3	2.43	1.39	1.33
10	M	501	MQ9	C18-C19	2.44	1.39	1.33
9	M	405	BPB	C2-C3	2.44	1.39	1.33
8	M	403	BCB	C2-C3	2.49	1.39	1.33
10	M	501	MQ9	C48-C49	2.51	1.39	1.32
10	M	501	MQ9	C23-C24	2.51	1.39	1.33
10	M	501	MQ9	C8-C9	2.55	1.39	1.33
11	L	502	UQ7	C38-C39	2.58	1.39	1.32
10	M	501	MQ9	C38-C39	2.58	1.39	1.33
11	L	502	UQ7	C18-C19	2.62	1.39	1.33
11	L	502	UQ7	C23-C24	2.64	1.39	1.33
7	C	401	HEM	C3B-CAB	2.64	1.53	1.47
11	L	502	UQ7	C28-C29	2.65	1.39	1.33
10	M	501	MQ9	C28-C29	2.65	1.39	1.33
11	L	502	UQ7	C8-C9	2.67	1.39	1.33
11	L	502	UQ7	C33-C34	2.67	1.39	1.33
9	L	406	BPB	C2-C3	2.69	1.39	1.33
9	M	405	BPB	O2A-CGA	2.71	1.41	1.33
10	M	501	MQ9	C33-C34	2.71	1.39	1.33
10	M	501	MQ9	C43-C44	2.71	1.39	1.33
11	L	502	UQ7	C13-C14	2.74	1.39	1.33
7	C	401	HEM	C3C-CAC	2.76	1.53	1.47
8	M	403	BCB	O2D-CGD	2.92	1.40	1.33
9	L	406	BPB	O2A-CGA	2.94	1.42	1.33
8	M	401	BCB	O2A-CGA	3.02	1.42	1.33
7	C	404	HEM	C3B-CAB	3.05	1.53	1.47
7	C	402	HEM	C3B-CAB	3.10	1.54	1.47
9	M	405	BPB	O2D-CGD	3.17	1.41	1.33
7	C	404	HEM	C3C-CAC	3.22	1.54	1.47
8	M	401	BCB	O2D-CGD	3.35	1.41	1.33
8	L	404	BCB	O2D-CGD	3.42	1.41	1.33
7	C	404	HEM	CBB-CAB	3.45	1.53	1.28
7	C	404	HEM	CBC-CAC	3.46	1.53	1.28
7	C	401	HEM	CBC-CAC	3.48	1.53	1.28
7	C	402	HEM	CBB-CAB	3.49	1.53	1.28
7	C	401	HEM	CBB-CAB	3.52	1.53	1.28
8	L	402	BCB	O2D-CGD	3.52	1.42	1.33
7	C	402	HEM	CBC-CAC	3.55	1.53	1.28
7	C	403	HEM	CBC-CAC	3.58	1.54	1.28
7	C	403	HEM	CBB-CAB	3.59	1.54	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	403	HEM	C3B-CAB	3.61	1.55	1.47
9	L	406	BPB	O2D-CGD	3.63	1.42	1.33
9	M	405	BPB	C3B-C4B	4.62	1.47	1.41
8	L	404	BCB	O2A-CGA	4.72	1.47	1.33
9	L	406	BPB	CAC-C3C	5.07	1.39	1.33
9	L	406	BPB	C3B-C4B	5.12	1.47	1.41
9	M	405	BPB	CAC-C3C	5.54	1.39	1.33

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	405	BPB	O1D-CGD-CBD	-5.24	115.18	124.60
9	L	406	BPB	O1D-CGD-CBD	-5.23	115.20	124.60
8	M	401	BCB	O1D-CGD-CBD	-4.63	114.98	124.53
8	L	404	BCB	O1D-CGD-CBD	-4.53	115.17	124.53
8	M	403	BCB	CHA-CBD-CGD	-4.48	104.62	115.00
8	L	402	BCB	CHA-CBD-CGD	-4.47	104.62	115.00
8	L	404	BCB	C4-C3-C2	-4.28	112.27	123.69
8	M	403	BCB	O1D-CGD-CBD	-4.19	115.88	124.53
8	M	401	BCB	CHA-CBD-CGD	-4.09	105.52	115.00
8	L	402	BCB	O1D-CGD-CBD	-3.98	116.31	124.53
8	L	404	BCB	CHA-CBD-CGD	-3.97	105.78	115.00
8	M	401	BCB	OBb-CAB-C3B	-3.89	117.39	121.55
8	L	402	BCB	O2A-CGA-O1A	-3.08	115.90	123.55
9	M	405	BPB	C2C-C3C-C4C	-2.91	104.53	107.35
8	M	401	BCB	OBD-CAD-CBD	-2.89	120.52	127.52
8	M	403	BCB	OBD-CAD-CBD	-2.78	120.79	127.52
8	L	402	BCB	OBD-CAD-CBD	-2.70	120.97	127.52
9	L	406	BPB	C2C-C3C-C4C	-2.63	104.80	107.35
8	L	404	BCB	OBD-CAD-CBD	-2.59	121.25	127.52
11	L	502	UQ7	C12-C11-C9	-2.54	104.32	112.93
9	L	406	BPB	O2A-CGA-O1A	-2.49	117.36	123.55
9	L	406	BPB	CBC-CAC-C3C	-2.48	121.53	127.00
11	L	502	UQ7	C25-C24-C26	-2.44	111.04	115.29
9	M	405	BPB	CBD-CHA-C4D	-2.40	105.83	108.54
12	M	600	NS5	C16-C15-C14	-2.25	114.51	118.10
8	M	401	BCB	CBC-CAC-C3C	-2.25	121.44	126.49
10	M	501	MQ9	C45-C44-C46	-2.16	111.53	115.29
9	L	406	BPB	CBD-CHA-C4D	-2.15	106.11	108.54
12	M	600	NS5	C19-C20-C21	-2.12	124.28	127.31
10	M	501	MQ9	C30-C29-C31	-2.03	111.77	115.29
8	L	404	BCB	CED-O2D-CGD	2.06	120.81	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	502	UQ7	CM3-O3-C3	2.12	124.01	116.44
11	L	502	UQ7	C37-C36-C34	2.16	120.24	112.93
8	M	401	BCB	C15-C13-C12	2.24	122.86	112.10
11	L	502	UQ7	C7-C8-C9	2.27	130.51	126.71
9	L	406	BPB	C2A-C1A-NA	2.28	109.76	107.83
12	M	600	NS5	C19-C18-C17	2.37	128.53	123.46
8	M	403	BCB	O2A-CGA-CBA	2.45	119.03	111.90
10	M	501	MQ9	C32-C33-C34	2.46	133.85	127.68
9	M	405	BPB	O2A-CGA-CBA	2.47	119.10	111.90
8	L	402	BCB	OBD-CAD-C3D	2.48	131.07	126.75
8	L	404	BCB	OBD-CAD-C3D	2.51	131.12	126.75
9	M	405	BPB	C5-C3-C2	2.53	126.28	121.10
8	M	401	BCB	C3B-C4B-NB	2.54	108.16	103.57
8	M	403	BCB	OBD-CAD-C3D	2.55	131.20	126.75
10	M	501	MQ9	C7-C8-C9	2.58	131.02	126.71
8	L	404	BCB	C3B-C4B-NB	2.59	108.25	103.57
8	L	402	BCB	C3B-C4B-NB	2.60	108.28	103.57
8	M	401	BCB	C6-C5-C3	2.61	118.57	112.66
11	L	502	UQ7	C17-C18-C19	2.64	134.31	127.68
8	L	404	BCB	CHB-C1B-C2B	2.65	124.34	116.99
8	M	403	BCB	C3B-C4B-NB	2.67	108.40	103.57
8	M	401	BCB	CHB-C1B-C2B	2.69	124.43	116.99
8	L	404	BCB	OBB-CAB-C3B	2.69	124.43	121.55
8	M	401	BCB	OBD-CAD-C3D	2.70	131.45	126.75
8	M	403	BCB	CHB-C1B-C2B	2.71	124.50	116.99
8	L	402	BCB	CHB-C1B-C2B	2.76	124.64	116.99
7	C	402	HEM	CBD-CAD-C3D	2.98	118.14	112.47
8	L	404	BCB	O2A-CGA-CBA	2.98	120.56	111.90
10	M	501	MQ9	C37-C38-C39	2.98	135.17	127.68
8	M	401	BCB	CHB-C4A-C3A	3.05	125.38	117.08
8	L	404	BCB	CHB-C4A-C3A	3.08	125.47	117.08
7	C	404	HEM	CBD-CAD-C3D	3.31	118.78	112.47
8	M	403	BCB	CHB-C4A-C3A	3.31	126.10	117.08
9	L	406	BPB	O2A-CGA-CBA	3.38	121.72	111.90
9	M	405	BPB	C3C-C2C-C1C	3.41	105.36	100.59
8	L	404	BCB	CHC-C4B-C3B	3.41	126.51	118.09
8	L	402	BCB	CHB-C4A-C3A	3.41	126.36	117.08
8	L	402	BCB	CHD-C1D-C2D	3.43	126.50	116.99
8	M	401	BCB	CHC-C4B-C3B	3.45	126.62	118.09
9	L	406	BPB	C3C-C2C-C1C	3.47	105.45	100.59
8	L	402	BCB	OBB-CAB-C3B	3.48	125.27	121.55
8	L	404	BCB	CHD-C1D-C2D	3.50	126.69	116.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	402	BCB	CHC-C4B-C3B	3.51	126.77	118.09
8	M	403	BCB	CHC-C4B-C3B	3.51	126.78	118.09
8	M	401	BCB	CHD-C1D-C2D	3.61	126.98	116.99
8	M	403	BCB	CHD-C1D-C2D	3.61	126.99	116.99
8	L	402	BCB	O2A-CGA-CBA	3.88	123.18	111.90
8	L	402	BCB	O2D-CGD-CBD	3.88	120.67	111.20
9	L	406	BPB	C1-C2-C3	3.99	133.30	125.96
8	M	403	BCB	OBB-CAB-C3B	4.16	126.00	121.55
8	M	403	BCB	O2D-CGD-CBD	4.37	121.86	111.20
8	M	401	BCB	O2D-CGD-CBD	4.71	122.70	111.20
8	M	401	BCB	CMB-C2B-C3B	4.74	126.27	114.27
8	L	404	BCB	O2D-CGD-CBD	4.79	122.88	111.20
8	L	404	BCB	CMD-C2D-C3D	5.38	127.89	114.27
8	L	404	BCB	C5-C3-C2	5.53	132.43	121.10
8	L	402	BCB	CMB-C2B-C3B	5.66	128.59	114.27
8	L	402	BCB	CMD-C2D-C3D	5.69	128.66	114.27
8	L	404	BCB	CMB-C2B-C3B	5.75	128.82	114.27
8	M	401	BCB	CMD-C2D-C3D	5.77	128.87	114.27
8	M	403	BCB	CMD-C2D-C3D	6.06	129.62	114.27
8	M	403	BCB	CMB-C2B-C3B	6.25	130.08	114.27
9	L	406	BPB	O2D-CGD-CBD	6.37	122.67	111.30
9	M	405	BPB	O2D-CGD-CBD	6.46	122.85	111.30
8	M	403	BCB	C1D-CHD-C4C	6.95	127.19	112.37
8	M	401	BCB	C1D-CHD-C4C	7.14	127.59	112.37
8	L	402	BCB	C1D-CHD-C4C	7.21	127.73	112.37
8	M	401	BCB	CBB-CAB-C3B	7.24	124.25	116.82
8	L	404	BCB	C1D-CHD-C4C	7.34	128.01	112.37
8	L	404	BCB	C1-C2-C3	9.28	143.04	125.96

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.

18 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	401	HEM	1	0
7	C	403	HEM	1	0
13	H	701	LDA	1	0
13	H	703	LDA	7	0
6	H	807	SO4	2	0
8	L	402	BCB	6	0
8	L	404	BCB	5	0
9	L	406	BPB	6	0
11	L	502	UQ7	9	0
13	L	702	LDA	4	0
8	M	401	BCB	7	0
8	M	403	BCB	5	0
9	M	405	BPB	8	0
10	M	501	MQ9	2	0
12	M	600	NS5	4	0
13	M	704	LDA	1	0
13	M	705	LDA	4	0
6	M	804	SO4	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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	C	332/332 (100%)	-0.40	7 (2%) 64 61	16, 27, 44, 59	9 (2%)
2	H	248/258 (96%)	-0.17	13 (5%) 28 27	19, 32, 49, 58	20 (8%)
3	L	273/273 (100%)	-0.68	3 (1%) 80 79	16, 23, 35, 52	5 (1%)
4	M	323/323 (100%)	-0.54	8 (2%) 58 55	16, 26, 44, 58	7 (2%)
All	All	1176/1186 (99%)	-0.46	31 (2%) 56 54	16, 27, 45, 59	41 (3%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	85	THR	5.1
2	H	45	GLU	4.7
2	H	8	GLN	4.1
1	C	332	LYS	4.1
1	C	47	ALA	4.0
2	H	96	PHE	3.9
4	M	30	GLY	3.9
1	C	1	CYS	3.8
2	H	9	HIS	3.7
4	M	319	PRO	3.7
4	M	320	GLY	3.5
2	H	95	GLY	3.2
4	M	29	VAL	2.9
4	M	108	HIS	2.8
2	H	7	ALA	2.7
2	H	189	GLY	2.7
2	H	83	PRO	2.7
3	L	202	ASP	2.6
3	L	1	ALA	2.4
2	H	141	THR	2.4
4	M	78	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	159	THR	2.4
4	M	37	TRP	2.4
2	H	191	ALA	2.4
4	M	26	ASN	2.4
2	H	94	ASP	2.3
1	C	54	GLN	2.2
3	L	51	TYR	2.1
1	C	174	VAL	2.1
2	H	163	VAL	2.0
1	C	48	GLU	2.0

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

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, 95<sup>th</sup> 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	FME	H	1	10/11	0.96	0.08	-	28,32,49,55	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
11	UQ7	L	502	48/48	0.65	0.34	14.09	23,36,44,44	48
13	LDA	L	702	16/16	0.73	0.26	6.66	29,50,54,54	0
12	NS5	M	600	40/40	0.78	0.20	3.79	24,35,65,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
13	LDA	H	701	16/16	0.89	0.15	3.62	23,36,50,52	0
6	SO4	H	806	5/5	0.96	0.26	3.19	58,61,63,63	0
13	LDA	H	703	16/16	0.80	0.22	2.39	38,48,61,62	0
13	LDA	M	704	16/16	0.82	0.18	2.22	52,54,65,65	0
10	MQ9	M	501	58/58	0.90	0.15	1.93	15,20,62,64	0
6	SO4	H	802	5/5	0.97	0.14	1.78	57,59,60,61	0
8	BCB	M	401	66/66	0.92	0.13	1.63	15,22,68,71	0
13	LDA	M	705	16/16	0.83	0.22	1.06	57,60,62,63	4
8	BCB	L	402	66/66	0.96	0.12	0.91	13,17,23,30	0
9	BPB	L	406	65/65	0.96	0.11	0.72	14,18,23,26	0
8	BCB	M	403	66/66	0.96	0.11	0.51	12,18,40,41	0
9	BPB	M	405	65/65	0.94	0.11	0.48	14,24,57,59	9
7	HEM	C	402	43/43	0.96	0.13	0.27	18,27,32,34	0
7	HEM	C	404	43/43	0.97	0.10	-0.29	14,21,33,43	0
7	HEM	C	401	43/43	0.97	0.11	-0.31	23,30,37,39	0
7	HEM	C	403	43/43	0.98	0.09	-0.35	14,19,22,26	0
8	BCB	L	404	66/66	0.96	0.08	-0.35	10,16,41,48	0
6	SO4	M	804	5/5	0.99	0.07	-1.41	40,41,42,44	0
5	FE2	M	500	1/1	1.00	0.02	-6.03	17,17,17,17	0
6	SO4	M	801	5/5	0.99	0.10	-	31,32,33,38	0
6	SO4	M	803	5/5	0.96	0.12	-	46,47,53,55	0
6	SO4	M	805	5/5	0.96	0.23	-	55,57,59,60	0
13	LDA	L	706	16/16	0.68	0.33	-	48,58,69,69	0
6	SO4	H	807	5/5	0.93	0.20	-	31,32,32,38	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.