



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:17 AM GMT

PDB ID : 2WJN  
Title : Lipidic sponge phase crystal structure of photosynthetic reaction centre from *Blastochloris viridis* (high dose)  
Authors : Wohri, A.B.; Wahlgren, W.Y.; Malmerberg, E.; Johansson, L.C.; Neutze, R.; Katona, G.  
Deposited on : 2009-05-27  
Resolution : 1.86 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

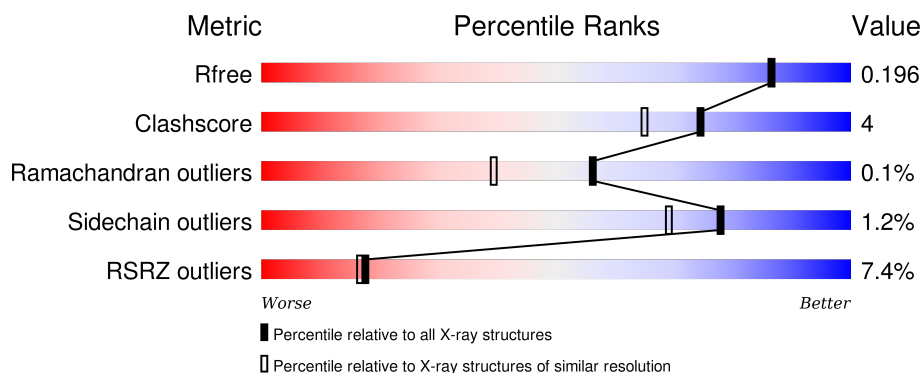
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.86 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))
$R_{free}$	91344	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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	336	<div> <div>5%</div> <div>93%</div> <div>6%</div> </div>
2	H	258	<div> <div>10%</div> <div>80%</div> <div>13%</div> <div>6%</div> </div>
3	L	274	<div> <div>9%</div> <div>95%</div> <div></div> </div>
4	M	324	<div> <div>6%</div> <div>95%</div> <div>5%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	NS5	M	1329	-	-	-	X
8	MPG	L	1277	X	-	-	X
8	MPG	L	1278	X	-	-	X

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 10590 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	0	0	0
			2590	1632	464	476	18			

- Molecule 2 is a protein called REACTION CENTER PROTEIN H CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	243	Total	C	N	O	S	0	0	0
			1886	1209	326	349	2			

- 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	0	0	0
			2161	1452	350	352	7			

- Molecule 4 is a protein called REACTION CENTER PROTEIN M CHAIN.

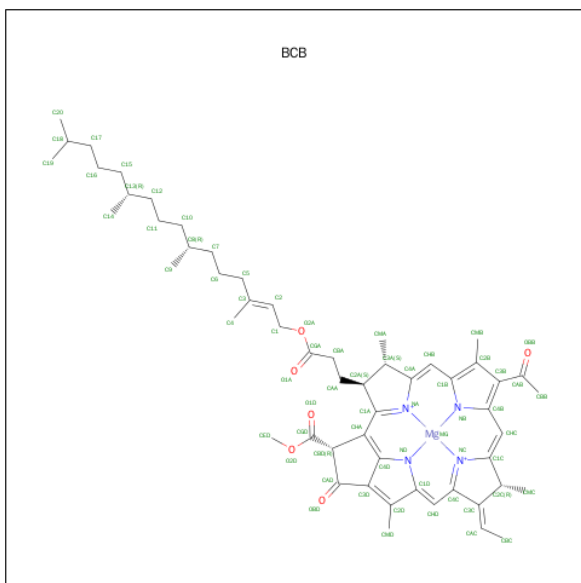
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	323	Total	C	N	O	S	0	0	0
			2548	1697	417	423	11			

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



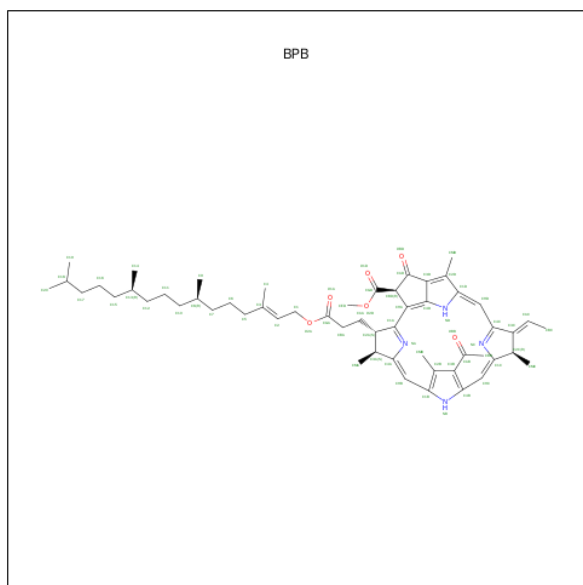
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 6 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula:  $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_6$ ).



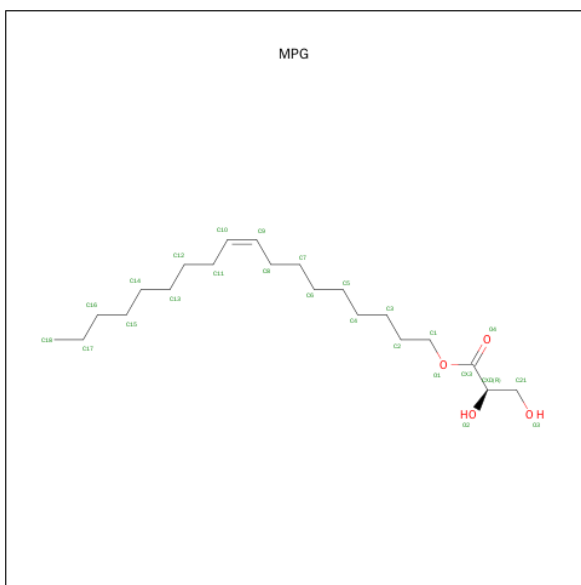
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
6	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
6	M	1	Total 65	C 54	Mg 1	N 4	O 6	0	0
6	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 7 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula:  $C_{55}H_{74}N_4O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			65	55	4	6		
7	M	1	Total	C	N	O	0	0
			61	51	4	6		

- Molecule 8 is 1-MONOOLEOYL-RAC-GLYCEROL (three-letter code: MPG) (formula:  $C_{21}H_{40}O_4$ ).

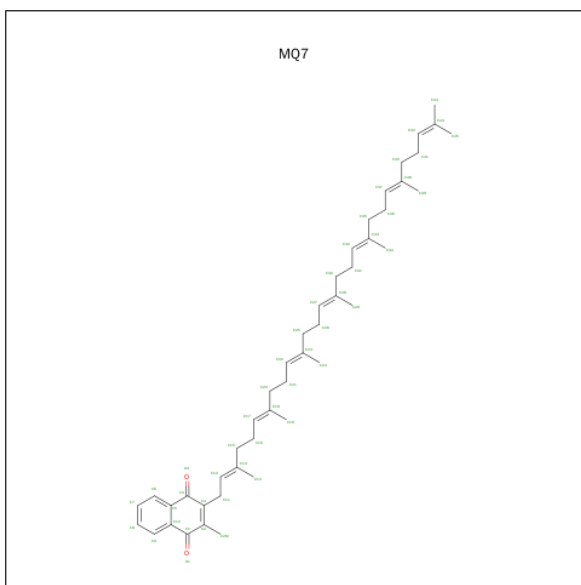


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	L	1	Total C O 21 17 4	0	0
8	L	1	Total C O 25 21 4	0	0
8	M	1	Total C 17 17	0	0

- Molecule 9 is FE (II) ION (three-letter code: FE2) (formula: Fe).

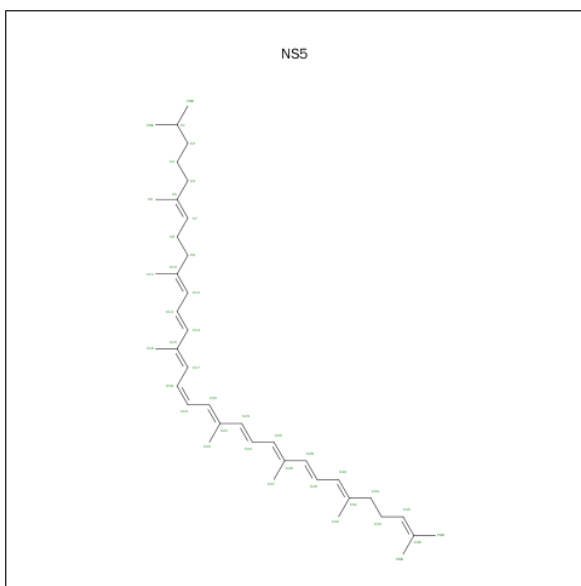
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	M	1	Total Fe 1 1	0	0

- Molecule 10 is MENAQUINONE-7 (three-letter code: MQ7) (formula: C<sub>46</sub>H<sub>64</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	M	1	Total	C	O	0	0
			48	46	2		

- Molecule 11 is 15-CIS-1,2-DIHYDRONEUROSPORENE (three-letter code: NS5) (formula:  $C_{40}H_{60}$ ).



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

- Molecule 12 is water.

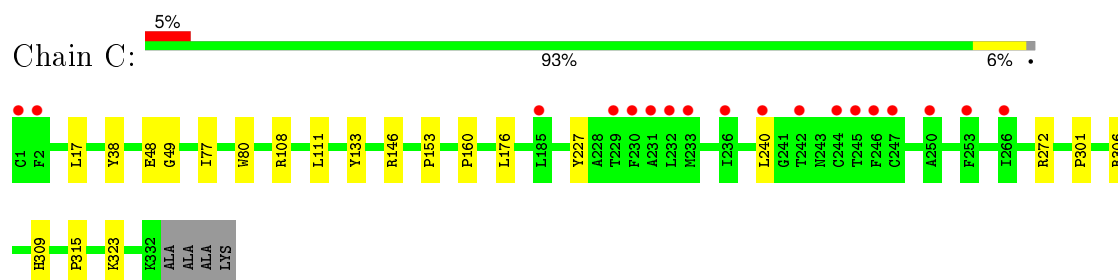


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	C	313	Total 313	O 313	0	0
12	H	148	Total 148	O 148	0	0
12	L	87	Total 87	O 87	0	0
12	M	144	Total 144	O 144	0	0

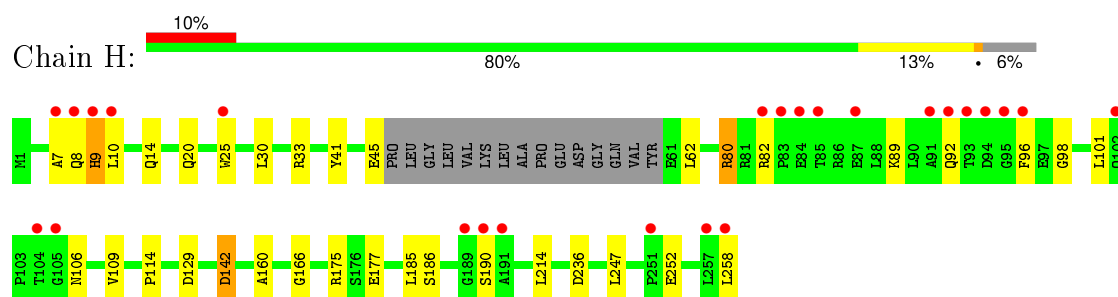
### 3 Residue-property plots [i](#)

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

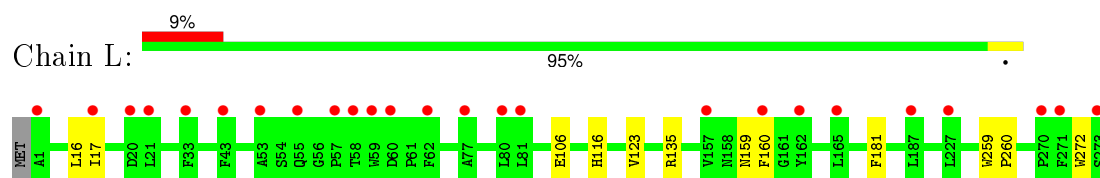
- Molecule 1: PHOTOSYNTHETIC REACTION CENTER CYTOCHROME C SUBUNIT



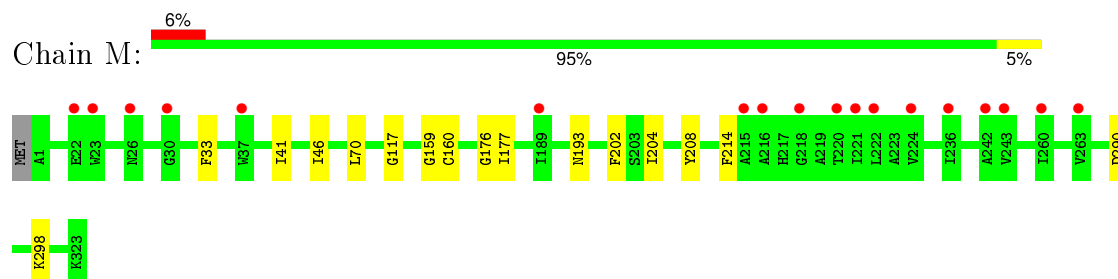
- Molecule 2: REACTION CENTER PROTEIN H CHAIN



- 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 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.76Å 139.43Å 178.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.97 – 1.86 44.97 – 1.86	Depositor EDS
% Data completeness (in resolution range)	99.4 (44.97-1.86) 99.4 (44.97-1.86)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.13 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.171 , 0.193 0.175 , 0.196	Depositor DCC
$R_{free}$ test set	8832 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.6	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 61.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 176116 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10590	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MPG, BPB, BCB, FE2, MQ7, HEM, FME, NS5

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	0.81	1/2657 (0.0%)	0.92	8/3624 (0.2%)
2	H	0.74	0/1919	0.80	6/2621 (0.2%)
3	L	0.84	1/2248 (0.0%)	0.76	1/3069 (0.0%)
4	M	0.87	1/2652 (0.0%)	0.74	0/3630
All	All	0.82	3/9476 (0.0%)	0.81	15/12944 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	272	ARG	CG-CD	-6.19	1.36	1.51
4	M	160	CYS	CB-SG	-5.99	1.72	1.81
3	L	123	VAL	CB-CG1	5.19	1.63	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	108	ARG	NE-CZ-NH2	-16.96	111.82	120.30
1	C	108	ARG	NE-CZ-NH1	13.50	127.05	120.30
1	C	146	ARG	NE-CZ-NH2	-11.13	114.73	120.30
2	H	80	ARG	NE-CZ-NH1	9.45	125.03	120.30
2	H	80	ARG	NE-CZ-NH2	-9.05	115.78	120.30
1	C	146	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	C	240	LEU	CB-CG-CD2	7.34	123.48	111.00
2	H	142	ASP	CB-CG-OD1	5.99	123.69	118.30
1	C	176	LEU	CA-CB-CG	5.57	128.12	115.30
2	H	175	ARG	NE-CZ-NH1	5.57	123.09	120.30
3	L	135	ARG	NE-CZ-NH1	5.44	123.02	120.30
2	H	129	ASP	CB-CG-OD1	5.41	123.17	118.30
1	C	306	ARG	NE-CZ-NH2	-5.29	117.65	120.30
2	H	33	ARG	NE-CZ-NH1	5.23	122.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	227	TYR	CA-CB-CG	5.02	122.93	113.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-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 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	2590	0	2553	9	0
2	H	1886	0	1880	24	0
3	L	2161	0	2089	10	0
4	M	2548	0	2432	14	0
5	C	172	0	120	1	0
6	L	132	0	144	9	0
6	M	131	0	140	4	0
7	L	65	0	74	9	0
7	M	61	0	63	13	0
8	L	46	0	67	3	0
8	M	17	0	31	0	0
9	M	1	0	0	0	0
10	M	48	0	64	0	0
11	M	40	0	60	10	0
12	C	313	0	0	3	0
12	H	148	0	0	4	0
12	L	87	0	0	0	0
12	M	144	0	0	0	0
All	All	10590	0	9717	79	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 4.

All (79) 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)
7:M:1326:BPB:H14A	11:M:1329:NS5:HM43	1.37	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:1326:BPB:HHC	7:M:1326:BPB:HBBB	1.47	0.97
7:M:1326:BPB:C14	11:M:1329:NS5:HM43	1.94	0.97
7:L:1276:BPB:HHC	7:L:1276:BPB:HBBB	1.50	0.92
3:L:16:LEU:HD13	3:L:106:GLU:HG2	1.53	0.91
2:H:142:ASP:OD1	12:H:2071:HOH:O	1.91	0.89
6:L:1274:BCB:HBB3	6:L:1274:BCB:HMB1	1.69	0.74
1:C:48:GLU:O	12:C:2058:HOH:O	2.04	0.74
7:M:1326:BPB:H14A	11:M:1329:NS5:CM4	2.17	0.73
1:C:49:GLY:HA3	12:C:2058:HOH:O	1.91	0.70
4:M:117:GLY:HA3	11:M:1329:NS5:H92	1.75	0.69
7:L:1276:BPB:HHC	7:L:1276:BPB:CBB	2.23	0.65
6:M:1324:BCB:HBB2	6:M:1324:BCB:HHC	1.79	0.65
6:L:1274:BCB:CBB	6:L:1274:BCB:HMB1	2.28	0.64
2:H:96:PHE:HD2	2:H:98:GLY:H	1.39	0.64
2:H:258:LEU:HB2	3:L:17:ILE:HG22	1.83	0.60
7:M:1326:BPB:C14	11:M:1329:NS5:CM4	2.77	0.60
8:L:1278:MPG:H11	8:L:1278:MPG:O2	2.01	0.59
2:H:177:GLU:OE1	12:H:2098:HOH:O	2.17	0.59
7:M:1326:BPB:H14B	11:M:1329:NS5:HM43	1.83	0.59
7:M:1326:BPB:CHC	7:M:1326:BPB:HBBB	2.27	0.59
3:L:181:PHE:CD2	7:M:1326:BPB:HBB	2.39	0.58
3:L:181:PHE:HB3	7:M:1326:BPB:HBBA	1.84	0.57
6:M:1324:BCB:HHC	6:M:1324:BCB:CBB	2.35	0.57
1:C:301:PRO:HG2	5:C:1334:HEM:HBD1	1.87	0.56
8:L:1278:MPG:C1	8:L:1278:MPG:O2	2.54	0.55
6:M:1325:BCB:CBB	6:M:1325:BCB:HMB1	2.38	0.54
4:M:177:ILE:HD11	11:M:1329:NS5:H273	1.90	0.53
4:M:70:LEU:HD21	11:M:1329:NS5:H323	1.89	0.53
2:H:96:PHE:CD2	2:H:98:GLY:N	2.63	0.52
4:M:159:GLY:HA3	11:M:1329:NS5:C11	2.40	0.52
3:L:16:LEU:CD1	3:L:16:LEU:N	2.73	0.52
7:M:1326:BPB:CBB	7:M:1326:BPB:HHC	2.32	0.51
2:H:106:ASN:HB3	2:H:109:VAL:HG22	1.93	0.51
1:C:309:HIS:CE1	1:C:315:PRO:HD3	2.45	0.51
2:H:9:HIS:HE1	4:M:298:LYS:HG3	1.76	0.51
2:H:92:GLN:HA	2:H:101:LEU:HD23	1.92	0.51
7:L:1276:BPB:HBBA	4:M:208:TYR:HB3	1.93	0.50
7:L:1276:BPB:HBB	4:M:208:TYR:CD2	2.47	0.50
2:H:142:ASP:CG	12:H:2071:HOH:O	2.44	0.49
2:H:10:LEU:HA	2:H:14:GLN:OE1	2.13	0.48
6:M:1325:BCB:HMB1	6:M:1325:BCB:HBB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:1276:BPB:CBB	7:L:1276:BPB:CHC	2.91	0.47
6:L:1275:BCB:CBB	6:L:1275:BCB:HMB1	2.43	0.47
3:L:181:PHE:HB3	7:M:1326:BPB:CBB	2.46	0.46
3:L:259:TRP:N	3:L:260:PRO:CD	2.79	0.46
6:L:1275:BCB:C14	7:L:1276:BPB:H20B	2.46	0.45
6:L:1275:BCB:HMB2	7:L:1276:BPB:HMBA	1.98	0.45
1:C:77:ILE:HD11	1:C:111:LEU:HD21	1.98	0.45
1:C:17:LEU:O	3:L:159:ASN:HB2	2.16	0.45
2:H:252:GLU:CG	12:H:2146:HOH:O	2.64	0.44
4:M:33:PHE:CE2	4:M:46:ILE:HD12	2.52	0.44
3:L:116:HIS:CD2	8:L:1277:MPG:H31	2.53	0.44
6:L:1275:BCB:HBB2	6:L:1275:BCB:HMB1	1.99	0.44
2:H:9:HIS:CE1	4:M:298:LYS:HG3	2.53	0.43
2:H:9:HIS:CE1	4:M:298:LYS:HE3	2.54	0.43
1:C:323:LYS:HE2	12:C:2290:HOH:O	2.18	0.43
7:M:1326:BPB:CBB	7:M:1326:BPB:CHC	2.95	0.43
2:H:41:TYR:CD2	2:H:62:LEU:HD21	2.54	0.43
1:C:153:PRO:HD3	1:C:160:PRO:HB3	2.01	0.42
6:L:1275:BCB:H143	7:L:1276:BPB:H20B	2.01	0.42
2:H:166:GLY:HA3	2:H:186:SER:O	2.20	0.42
2:H:80:ARG:O	2:H:80:ARG:HG3	2.19	0.42
2:H:20:GLN:HG2	4:M:202:PHE:CE2	2.55	0.41
6:L:1275:BCB:HMD1	4:M:204:ILE:HD13	2.03	0.41
7:L:1276:BPB:ND	7:L:1276:BPB:NC	2.67	0.41
2:H:96:PHE:CE2	2:H:98:GLY:N	2.88	0.41
2:H:160:ALA:HB3	2:H:214:LEU:HD23	2.03	0.41
7:M:1326:BPB:HBCA	7:M:1326:BPB:HMC	2.02	0.41
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.56	0.41
4:M:176:GLY:H	11:M:1329:NS5:C23	2.34	0.41
3:L:16:LEU:HD12	3:L:16:LEU:N	2.35	0.41
6:L:1274:BCB:HBD	6:L:1274:BCB:HAA1	2.02	0.41
2:H:7:ALA:O	2:H:8:GLN:CB	2.69	0.41
2:H:25:TRP:CE3	2:H:25:TRP:HA	2.56	0.40
2:H:80:ARG:HD3	2:H:82:ARG:HG2	2.02	0.40
4:M:41:ILE:HD12	4:M:41:ILE:C	2.42	0.40
2:H:114:PRO:HG3	2:H:247:LEU:HD22	2.02	0.40
2:H:89:LYS:HB3	2:H:89:LYS:HE2	1.88	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	330/336 (98%)	321 (97%)	9 (3%)	0	100	100
2	H	239/258 (93%)	234 (98%)	5 (2%)	0	100	100
3	L	271/274 (99%)	264 (97%)	7 (3%)	0	100	100
4	M	321/324 (99%)	313 (98%)	7 (2%)	1 (0%)	46	29
All	All	1161/1192 (97%)	1132 (98%)	28 (2%)	1 (0%)	56	39

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	M	193	ASN

### 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	278/282 (99%)	277 (100%)	1 (0%)	93	92
2	H	194/212 (92%)	188 (97%)	6 (3%)	47	28
3	L	216/219 (99%)	214 (99%)	2 (1%)	84	79
4	M	247/250 (99%)	245 (99%)	2 (1%)	86	82
All	All	935/963 (97%)	924 (99%)	11 (1%)	78	69

All (11) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	C	38	TYR
2	H	9	HIS
2	H	30	LEU
2	H	45	GLU
2	H	185	LEU
2	H	190	SER
2	H	236	ASP
3	L	160	PHE
3	L	272	TRP
4	M	214	PHE
4	M	290	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	8	GLN
2	H	9	HIS
2	H	220	ASN
3	L	183	ASN
3	L	239	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	8,9,10	0.75	0	6,9,11	3.17	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	-	0/6/9/11	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	FME	CA-N-CN	-5.77	113.94	122.82
2	H	1	FME	O1-CN-N	-4.40	118.43	124.76

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 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 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
5	HEM	C	1333	1	30,50,50	2.47	9 (30%)	24,82,82	3.12	12 (50%)
5	HEM	C	1334	1	30,50,50	2.27	13 (43%)	24,82,82	3.29	14 (58%)
5	HEM	C	1335	1	30,50,50	2.06	10 (33%)	24,82,82	2.78	11 (45%)
5	HEM	C	1336	1	30,50,50	2.49	9 (30%)	24,82,82	2.70	11 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	BCB	L	1274	3	56,74,74	2.16	8 (14%)	57,115,115	2.01	15 (26%)
6	BCB	L	1275	3	56,74,74	2.21	10 (17%)	57,115,115	1.97	11 (19%)
7	BPB	L	1276	-	63,70,70	2.57	16 (25%)	63,101,101	2.04	17 (26%)
8	MPG	L	1277	-	18,19,24	1.85	1 (5%)	15,19,25	1.94	3 (20%)
8	MPG	L	1278	-	22,23,24	1.66	1 (4%)	20,23,25	1.12	2 (10%)
6	BCB	M	1324	4	55,73,74	1.91	9 (16%)	55,113,115	1.75	9 (16%)
6	BCB	M	1325	4	56,74,74	2.10	10 (17%)	57,115,115	2.15	16 (28%)
7	BPB	M	1326	-	59,66,70	2.44	14 (23%)	58,96,101	1.92	12 (20%)
10	MQ7	M	1328	-	49,49,49	1.49	3 (6%)	62,63,63	1.19	7 (11%)
11	NS5	M	1329	-	39,39,39	2.09	6 (15%)	44,46,46	2.52	19 (43%)
8	MPG	M	1330	-	16,16,24	0.34	0	15,15,25	0.50	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
5	HEM	C	1333	1	-	0/10/54/54	0/0/8/8
5	HEM	C	1334	1	-	0/10/54/54	0/0/8/8
5	HEM	C	1335	1	-	0/10/54/54	0/0/8/8
5	HEM	C	1336	1	-	0/10/54/54	0/0/8/8
6	BCB	L	1274	3	-	0/37/137/137	0/0/9/9
6	BCB	L	1275	3	-	0/37/137/137	0/0/9/9
7	BPB	L	1276	-	-	0/46/105/105	0/1/6/6
8	MPG	L	1277	-	1/1/1/4	0/21/18/25	0/0/0/0
8	MPG	L	1278	-	1/1/1/4	1/25/22/25	0/0/0/0
6	BCB	M	1324	4	-	0/36/136/137	0/0/9/9
6	BCB	M	1325	4	-	0/37/137/137	0/0/9/9
7	BPB	M	1326	-	-	0/42/101/105	0/1/6/6
10	MQ7	M	1328	-	-	0/41/61/61	0/2/2/2
11	NS5	M	1329	-	-	1/43/43/43	0/0/0/0
8	MPG	M	1330	-	-	0/14/14/25	0/0/0/0

All (119) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1333	HEM	C3B-C4B	-9.08	1.43	1.51
11	M	1329	NS5	C9-C8	-5.82	1.33	1.53
5	C	1335	HEM	C3B-C4B	-5.56	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1336	HEM	C3B-C4B	-5.25	1.47	1.51
5	C	1336	HEM	C2C-C1C	-4.92	1.43	1.52
5	C	1335	HEM	C2C-C1C	-4.75	1.43	1.52
5	C	1334	HEM	C3D-C4D	-4.49	1.45	1.51
5	C	1334	HEM	C2C-C1C	-4.49	1.44	1.52
5	C	1333	HEM	C3D-C4D	-4.23	1.46	1.51
5	C	1336	HEM	C3D-C4D	-4.03	1.46	1.51
7	M	1326	BPB	C4C-NC	-4.03	1.27	1.37
7	L	1276	BPB	C1A-NA	-3.49	1.29	1.36
6	L	1275	BCB	CHB-C4A	-3.26	1.31	1.41
6	M	1324	BCB	C3D-C4D	-3.16	1.36	1.41
7	M	1326	BPB	C1A-NA	-2.95	1.30	1.36
6	M	1325	BCB	C4C-NC	-2.78	1.33	1.37
5	C	1333	HEM	C2C-C1C	-2.64	1.47	1.52
5	C	1335	HEM	C2B-C1B	-2.54	1.43	1.51
5	C	1334	HEM	C3B-C4B	-2.51	1.49	1.51
7	M	1326	BPB	CBB-CAB	-2.50	1.41	1.49
5	C	1335	HEM	C3D-C4D	-2.26	1.48	1.51
7	L	1276	BPB	C4C-NC	-2.24	1.31	1.37
5	C	1333	HEM	C2D-C1D	-2.23	1.44	1.51
7	M	1326	BPB	C1D-ND	-2.23	1.33	1.38
7	L	1276	BPB	CBB-CAB	-2.09	1.43	1.49
5	C	1333	HEM	C2B-C1B	-2.07	1.45	1.51
5	C	1335	HEM	C2D-C1D	-2.04	1.45	1.51
5	C	1336	HEM	C3B-CAB	2.01	1.55	1.51
6	L	1275	BCB	CHC-C1C	2.04	1.47	1.41
11	M	1329	NS5	C30-C31	2.11	1.36	1.34
6	M	1324	BCB	CHC-C1C	2.12	1.47	1.41
5	C	1334	HEM	CMB-C2B	2.13	1.58	1.53
5	C	1334	HEM	C1C-NC	2.13	1.38	1.36
7	L	1276	BPB	C4B-CHC	2.15	1.48	1.40
5	C	1335	HEM	CMA-C3A	2.20	1.56	1.51
11	M	1329	NS5	C28-C26	2.22	1.50	1.45
5	C	1336	HEM	CMA-C3A	2.22	1.56	1.51
5	C	1334	HEM	C3B-CAB	2.24	1.55	1.51
5	C	1335	HEM	FE-NB	2.28	2.09	1.97
6	L	1274	BCB	C2C-C1C	2.30	1.53	1.51
7	L	1276	BPB	C1B-CHB	2.33	1.49	1.40
7	L	1276	BPB	CHD-C4C	2.35	1.46	1.40
5	C	1335	HEM	FE-ND	2.37	2.10	1.97
10	M	1328	MQ7	O4-C4	2.40	1.28	1.23
5	C	1333	HEM	C4C-NC	2.42	1.39	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	1324	BCB	O2A-CGA	2.43	1.40	1.33
6	L	1275	BCB	O2A-CGA	2.46	1.40	1.33
7	M	1326	BPB	CHD-C4C	2.48	1.46	1.40
6	M	1325	BCB	C4D-CHA	2.49	1.48	1.45
5	C	1335	HEM	CAA-C2A	2.50	1.56	1.52
5	C	1335	HEM	C1C-NC	2.50	1.39	1.36
6	L	1275	BCB	C3B-C2B	2.54	1.46	1.40
7	L	1276	BPB	OBD-CAD	2.55	1.27	1.22
7	M	1326	BPB	C1B-CHB	2.59	1.50	1.40
6	L	1274	BCB	C3B-C2B	2.64	1.46	1.40
6	L	1274	BCB	C3D-C2D	2.65	1.46	1.40
6	M	1324	BCB	OBD-CAD	2.69	1.26	1.22
6	M	1325	BCB	O2A-CGA	2.72	1.41	1.33
6	M	1325	BCB	C3B-C2B	2.74	1.46	1.40
7	L	1276	BPB	O2D-CGD	2.76	1.40	1.33
6	M	1325	BCB	CHD-C4C	2.78	1.44	1.35
5	C	1334	HEM	CAA-C2A	2.79	1.56	1.52
6	M	1324	BCB	C3D-C2D	2.84	1.46	1.40
5	C	1334	HEM	FE-ND	2.87	2.12	1.97
6	L	1275	BCB	C3D-C2D	2.88	1.47	1.40
11	M	1329	NS5	C29-C30	2.89	1.52	1.43
7	L	1276	BPB	OBB-CAB	2.89	1.32	1.22
7	L	1276	BPB	C3B-C2B	2.92	1.47	1.40
6	M	1324	BCB	CHD-C4C	2.94	1.44	1.35
6	M	1325	BCB	C3D-C2D	2.96	1.47	1.40
7	M	1326	BPB	C3D-C2D	2.96	1.46	1.38
7	M	1326	BPB	O2D-CGD	3.01	1.40	1.33
5	C	1334	HEM	CMA-C3A	3.04	1.57	1.51
7	L	1276	BPB	CHD-C1D	3.07	1.44	1.38
7	L	1276	BPB	C3D-C2D	3.11	1.47	1.38
7	M	1326	BPB	OBD-CAD	3.21	1.28	1.22
5	C	1333	HEM	FE-NC	3.23	2.08	1.95
5	C	1334	HEM	FE-NB	3.25	2.14	1.97
6	L	1275	BCB	O2D-CGD	3.26	1.41	1.33
7	L	1276	BPB	O2A-CGA	3.28	1.43	1.33
5	C	1334	HEM	C4C-NC	3.36	1.40	1.36
5	C	1336	HEM	CAA-C2A	3.39	1.57	1.52
7	M	1326	BPB	CHD-C1D	3.40	1.45	1.38
6	L	1275	BCB	CHD-C4C	3.46	1.46	1.35
6	M	1325	BCB	O2D-CGD	3.48	1.42	1.33
7	M	1326	BPB	O2A-CGA	3.50	1.43	1.33
6	L	1274	BCB	C1A-CHA	3.57	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1336	HEM	C3C-CAC	3.60	1.58	1.51
5	C	1334	HEM	FE-NC	3.67	2.10	1.95
5	C	1334	HEM	C3C-CAC	3.69	1.58	1.51
6	M	1325	BCB	C1A-CHA	3.78	1.45	1.37
6	M	1324	BCB	O2D-CGD	3.80	1.42	1.33
6	L	1274	BCB	CHD-C4C	3.84	1.47	1.35
6	L	1274	BCB	O2D-CGD	3.85	1.43	1.33
5	C	1333	HEM	CMA-C3A	3.86	1.59	1.51
5	C	1333	HEM	C3C-CAC	4.23	1.59	1.51
6	L	1275	BCB	OBD-CAD	4.80	1.29	1.22
5	C	1336	HEM	C1C-NC	4.97	1.42	1.36
7	M	1326	BPB	C3B-C4B	5.05	1.48	1.41
6	M	1324	BCB	C1A-CHA	5.18	1.48	1.37
6	M	1325	BCB	OBD-CAD	5.20	1.30	1.22
5	C	1336	HEM	C4C-NC	5.22	1.42	1.36
6	L	1275	BCB	C1A-CHA	5.30	1.48	1.37
7	L	1276	BPB	C1A-CHA	5.57	1.47	1.36
10	M	1328	MQ7	C10-C5	5.60	1.49	1.40
6	L	1274	BCB	OBD-CAD	6.00	1.31	1.22
10	M	1328	MQ7	C3-C2	6.12	1.49	1.35
7	M	1326	BPB	C1A-CHA	6.26	1.48	1.36
7	L	1276	BPB	C3B-C4B	6.54	1.50	1.41
11	M	1329	NS5	C29-C28	6.92	1.52	1.34
11	M	1329	NS5	C35-C36	7.07	1.54	1.32
8	L	1278	MPG	O1-CX3	7.35	1.48	1.33
8	L	1277	MPG	O1-CX3	7.41	1.49	1.33
6	M	1324	BCB	CAC-C3C	9.17	1.44	1.33
6	M	1325	BCB	CAC-C3C	10.96	1.46	1.33
6	L	1274	BCB	CAC-C3C	11.44	1.47	1.33
6	L	1275	BCB	CAC-C3C	11.98	1.48	1.33
7	M	1326	BPB	CAC-C3C	12.44	1.48	1.33
7	L	1276	BPB	CAC-C3C	14.66	1.51	1.33

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1333	HEM	C3C-CAC-CBC	-7.24	113.35	124.46
7	L	1276	BPB	C2C-C3C-C4C	-6.59	101.21	107.24
5	C	1334	HEM	C3C-CAC-CBC	-6.29	114.81	124.46
5	C	1333	HEM	C3B-CAB-CBB	-6.26	114.86	124.46
7	M	1326	BPB	C2C-C3C-C4C	-6.11	101.66	107.24
7	M	1326	BPB	CBC-CAC-C3C	-5.80	113.69	127.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	1274	BCB	OBD-CAD-C3D	-5.74	116.65	128.35
11	M	1329	NS5	C29-C28-C26	-5.58	109.90	126.32
5	C	1335	HEM	C3B-CAB-CBB	-5.37	116.22	124.46
5	C	1336	HEM	C3B-CAB-CBB	-5.35	116.25	124.46
6	M	1325	BCB	O2D-CGD-O1D	-5.34	112.76	123.79
6	M	1325	BCB	C4D-C3D-CAD	-4.96	100.38	107.86
6	L	1275	BCB	CHC-C1C-NC	-4.84	119.45	125.06
7	L	1276	BPB	CBC-CAC-C3C	-4.71	116.20	127.07
6	L	1275	BCB	C4D-C3D-CAD	-4.53	101.03	107.86
11	M	1329	NS5	C34-C35-C36	-4.52	110.34	127.73
6	M	1325	BCB	OBD-CAD-C3D	-4.23	119.73	128.35
5	C	1334	HEM	C3B-CAB-CBB	-4.22	117.98	124.46
6	M	1324	BCB	C1D-CHD-C4C	-4.17	120.31	129.26
6	M	1324	BCB	CHC-C1C-NC	-4.12	120.28	125.06
6	L	1274	BCB	C1D-CHD-C4C	-4.09	120.48	129.26
6	L	1275	BCB	OBD-CAD-C3D	-4.02	120.16	128.35
5	C	1334	HEM	CAA-C2A-C1A	-4.00	122.67	127.01
6	L	1275	BCB	O1D-CGD-CBD	-3.71	119.31	124.62
11	M	1329	NS5	C18-C17-C15	-3.67	121.89	127.20
5	C	1334	HEM	C3B-C4B-NB	-3.66	104.62	111.63
7	L	1276	BPB	C4D-C3D-C2D	-3.65	102.61	106.74
11	M	1329	NS5	CM4-C36-C35	-3.64	110.89	122.61
11	M	1329	NS5	C24-C25-C26	-3.61	121.98	127.20
6	L	1274	BCB	C4D-C3D-CAD	-3.60	102.44	107.86
10	M	1328	MQ7	C26-C27-C28	-3.52	120.10	127.76
5	C	1335	HEM	CAA-C2A-C1A	-3.48	123.23	127.01
5	C	1333	HEM	CBD-CAD-C3D	-3.47	103.44	113.55
7	M	1326	BPB	C4D-C3D-C2D	-3.47	102.82	106.74
6	L	1275	BCB	C2C-C1C-CHC	-3.44	115.36	123.29
7	M	1326	BPB	CBB-CAB-C3B	-3.37	110.33	120.33
5	C	1335	HEM	C3B-C4B-NB	-3.32	105.27	111.63
6	M	1325	BCB	C1D-CHD-C4C	-3.32	122.14	129.26
11	M	1329	NS5	CM3-C36-C35	-3.30	111.99	122.61
11	M	1329	NS5	C16-C15-C14	-3.28	112.64	118.10
6	M	1325	BCB	CHC-C1C-NC	-3.27	121.26	125.06
6	L	1274	BCB	CHC-C1C-NC	-3.27	121.27	125.06
6	M	1324	BCB	C2C-C1C-CHC	-3.26	115.78	123.29
5	C	1336	HEM	C3B-C4B-NB	-3.24	105.43	111.63
6	M	1324	BCB	OBD-CAD-C3D	-3.20	121.83	128.35
7	M	1326	BPB	OBD-CAD-C3D	-3.17	119.82	128.37
7	L	1276	BPB	CMD-C2D-C3D	-3.12	120.79	128.04
11	M	1329	NS5	C8-C7-C5	-3.11	121.01	127.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	1324	BCB	C4D-C3D-CAD	-3.06	103.25	107.86
5	C	1334	HEM	CBA-CAA-C2A	-2.95	107.24	112.53
7	L	1276	BPB	CBB-CAB-C3B	-2.93	111.62	120.33
11	M	1329	NS5	C23-C21-C20	-2.87	114.36	118.98
6	L	1275	BCB	C1D-CHD-C4C	-2.85	123.14	129.26
7	L	1276	BPB	OBD-CAD-C3D	-2.81	120.78	128.37
6	M	1325	BCB	CMD-C2D-C3D	-2.73	119.75	125.09
6	L	1274	BCB	O2D-CGD-O1D	-2.72	118.18	123.79
6	L	1274	BCB	C2C-C1C-CHC	-2.71	117.04	123.29
6	M	1325	BCB	C2C-C1C-CHC	-2.71	117.05	123.29
5	C	1335	HEM	C3C-CAC-CBC	-2.68	120.34	124.46
5	C	1336	HEM	C3C-CAC-CBC	-2.67	120.36	124.46
11	M	1329	NS5	C30-C29-C28	-2.52	115.45	123.13
6	L	1274	BCB	CHD-C4C-C3C	-2.51	121.99	129.02
5	C	1336	HEM	CMA-C3A-C4A	-2.41	124.37	128.36
7	M	1326	BPB	O2D-CGD-O1D	-2.39	118.85	123.79
7	L	1276	BPB	O2A-CGA-O1A	-2.33	117.48	123.49
5	C	1333	HEM	CAA-C2A-C1A	-2.27	124.55	127.01
11	M	1329	NS5	C22-C21-C23	-2.25	114.35	118.10
6	L	1274	BCB	C4-C3-C2	-2.23	119.11	123.50
7	L	1276	BPB	O2D-CGD-O1D	-2.23	119.19	123.79
11	M	1329	NS5	C24-C23-C21	-2.20	119.85	126.32
6	M	1325	BCB	CHD-C4C-C3C	-2.12	123.10	129.02
10	M	1328	MQ7	C30-C31-C32	-2.10	106.19	111.69
10	M	1328	MQ7	C44-C43-C42	-2.05	116.01	122.61
7	L	1276	BPB	C4D-ND-C1D	-2.05	103.29	107.05
5	C	1333	HEM	C3B-C4B-NB	-2.01	107.79	111.63
7	L	1276	BPB	C2D-C1D-ND	2.07	112.83	109.73
10	M	1328	MQ7	C45-C43-C44	2.08	119.76	114.64
6	L	1274	BCB	OBD-CAD-CBD	2.12	129.13	125.94
7	M	1326	BPB	CBD-CAD-C3D	2.17	111.53	107.56
6	M	1325	BCB	C4A-NA-C1A	2.19	108.62	106.04
10	M	1328	MQ7	C34-C33-C35	2.24	118.82	115.41
10	M	1328	MQ7	C19-C18-C20	2.25	118.84	115.41
8	L	1277	MPG	O1-C1-C2	2.28	115.57	108.59
6	L	1274	BCB	C1B-CHB-C4A	2.29	129.57	126.07
5	C	1335	HEM	C2D-C3D-C4D	2.31	105.41	101.50
6	M	1325	BCB	O1D-CGD-CBD	2.31	127.93	124.62
10	M	1328	MQ7	C39-C38-C40	2.32	118.94	115.41
5	C	1333	HEM	C2D-C3D-C4D	2.34	105.46	101.50
5	C	1333	HEM	C1D-CHD-C4C	2.35	129.74	125.82
7	L	1276	BPB	CAD-C3D-C2D	2.41	152.41	140.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	1276	BPB	CBD-CAD-C3D	2.47	112.09	107.56
5	C	1333	HEM	CMD-C2D-C3D	2.49	125.37	114.35
6	M	1325	BCB	CAA-C2A-C1A	2.50	121.30	112.47
7	M	1326	BPB	C4-C3-C5	2.54	119.29	115.41
7	M	1326	BPB	CAD-C3D-C2D	2.54	153.07	140.80
11	M	1329	NS5	C6-C5-C4	2.57	119.33	115.41
5	C	1335	HEM	C2C-C1C-CHC	2.65	127.71	123.68
6	L	1274	BCB	CMD-C2D-C1D	2.73	132.88	128.36
5	C	1334	HEM	C2D-C3D-C4D	2.82	106.28	101.50
5	C	1334	HEM	CMD-C2D-C3D	2.86	127.00	114.35
5	C	1336	HEM	CMD-C2D-C3D	2.89	127.12	114.35
5	C	1335	HEM	CMD-C2D-C3D	2.92	127.24	114.35
11	M	1329	NS5	C16-C15-C17	2.95	127.25	122.90
11	M	1329	NS5	C11-C10-C9	2.99	119.97	115.41
8	L	1278	MPG	O1-CX3-CXD	3.01	117.28	111.79
5	C	1334	HEM	C2C-C1C-CHC	3.11	128.41	123.68
5	C	1334	HEM	C1D-CHD-C4C	3.11	131.02	125.82
5	C	1336	HEM	C2D-C3D-C4D	3.17	106.87	101.50
7	M	1326	BPB	OBB-CAB-C3B	3.18	125.04	120.00
8	L	1278	MPG	O1-C1-C2	3.22	118.43	108.59
6	M	1324	BCB	CMD-C2D-C1D	3.23	133.70	128.36
5	C	1334	HEM	CAD-C3D-C4D	3.24	123.90	112.47
11	M	1329	NS5	C9-C8-C7	3.24	120.19	111.69
6	L	1275	BCB	C3C-C4C-NC	3.25	112.66	110.24
6	M	1325	BCB	C4-C3-C5	3.28	120.42	115.41
7	L	1276	BPB	C3C-C4C-NC	3.30	115.20	109.52
7	L	1276	BPB	CED-O2D-CGD	3.34	123.82	115.99
6	M	1325	BCB	CMB-C2B-C3B	3.37	131.68	125.09
6	M	1324	BCB	O2D-CGD-CBD	3.40	115.97	111.30
5	C	1336	HEM	C3B-C4B-CHC	3.45	128.01	123.16
6	L	1275	BCB	CMD-C2D-C1D	3.54	134.22	128.36
6	L	1274	BCB	C3C-C4C-NC	3.56	112.89	110.24
5	C	1334	HEM	C3B-C4B-CHC	3.67	128.34	123.16
7	L	1276	BPB	O2D-CGD-CBD	3.68	116.35	111.30
11	M	1329	NS5	C18-C19-C20	3.70	131.57	123.39
7	L	1276	BPB	OBB-CAB-C3B	3.72	125.89	120.00
5	C	1333	HEM	CMB-C2B-C3B	3.73	125.83	116.53
5	C	1336	HEM	CAD-C3D-C4D	3.85	126.05	112.47
7	M	1326	BPB	CMD-C2D-C1D	3.86	131.34	125.06
7	M	1326	BPB	O2D-CGD-CBD	4.08	116.90	111.30
6	M	1324	BCB	CMB-C2B-C3B	4.09	133.08	125.09
5	C	1335	HEM	CAD-C3D-C4D	4.09	126.89	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1333	HEM	CAD-C3D-C4D	4.11	126.98	112.47
5	C	1336	HEM	CMC-C2C-C3C	4.18	126.97	116.53
6	L	1275	BCB	CMB-C2B-C3B	4.21	133.32	125.09
8	L	1277	MPG	C1-O1-CX3	4.31	126.23	116.59
6	L	1275	BCB	O2D-CGD-CBD	4.40	117.34	111.30
5	C	1336	HEM	CMB-C2B-C3B	4.42	127.58	116.53
6	L	1274	BCB	O2D-CGD-CBD	4.61	117.62	111.30
6	L	1274	BCB	C3D-CAD-CBD	4.66	114.18	107.60
6	L	1274	BCB	C4-C3-C5	4.73	122.63	115.41
5	C	1336	HEM	CAD-C3D-C2D	4.78	126.96	113.22
5	C	1335	HEM	CMB-C2B-C3B	4.82	128.56	116.53
5	C	1335	HEM	CMC-C2C-C3C	4.91	128.79	116.53
5	C	1334	HEM	CMB-C2B-C3B	4.93	128.83	116.53
5	C	1333	HEM	CAD-C3D-C2D	4.98	127.52	113.22
11	M	1329	NS5	C19-C18-C17	4.99	134.43	123.39
6	M	1325	BCB	O2D-CGD-CBD	5.02	118.19	111.30
5	C	1335	HEM	CAD-C3D-C2D	5.04	127.70	113.22
6	M	1325	BCB	C3D-CAD-CBD	5.09	114.80	107.60
6	M	1324	BCB	C3D-CAD-CBD	5.34	115.14	107.60
8	L	1277	MPG	O1-CX3-CXD	5.50	121.82	111.79
6	L	1275	BCB	C3D-CAD-CBD	5.52	115.40	107.60
5	C	1333	HEM	CMC-C2C-C3C	5.55	130.38	116.53
7	L	1276	BPB	CMD-C2D-C1D	5.58	134.14	125.06
11	M	1329	NS5	C22-C21-C20	5.64	131.23	122.90
5	C	1334	HEM	CAD-C3D-C2D	5.78	129.82	113.22
6	M	1325	BCB	CMD-C2D-C1D	5.83	138.01	128.36
5	C	1334	HEM	CMC-C2C-C3C	6.02	131.56	116.53

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	L	1278	MPG	CXD
8	L	1277	MPG	CXD

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	M	1329	NS5	C30-C29-C28-C26
8	L	1278	MPG	C1-O1-CX3-CXD

There are no ring outliers.

10 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1334	HEM	1	0
6	L	1274	BCB	3	0
6	L	1275	BCB	6	0
7	L	1276	BPB	9	0
8	L	1277	MPG	1	0
8	L	1278	MPG	2	0
6	M	1324	BCB	2	0
6	M	1325	BCB	2	0
7	M	1326	BPB	13	0
11	M	1329	NS5	10	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	332/336 (98%)	0.19	18 (5%) 29 28	31, 35, 44, 69	0
2	H	242/258 (93%)	0.34	25 (10%) 9 8	28, 35, 48, 65	0
3	L	273/274 (99%)	0.40	25 (9%) 11 11	31, 35, 46, 59	0
4	M	323/324 (99%)	0.16	18 (5%) 28 26	32, 35, 44, 52	0
All	All	1170/1192 (98%)	0.26	86 (7%) 17 17	28, 35, 46, 69	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	CYS	7.0
2	H	7	ALA	6.5
2	H	9	HIS	6.3
2	H	258	LEU	6.2
3	L	59	TRP	5.8
2	H	85	THR	5.7
2	H	8	GLN	5.6
2	H	93	THR	5.3
2	H	94	ASP	5.1
2	H	96	PHE	4.8
2	H	91	ALA	4.8
1	C	2	PHE	4.5
3	L	271	PHE	4.5
2	H	83	PRO	4.3
3	L	21	LEU	4.1
1	C	244	CYS	3.7
2	H	191	ALA	3.6
3	L	165	LEU	3.6
3	L	58	THR	3.6
2	H	10	LEU	3.4
2	H	92	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
3	L	80	LEU	3.2
1	C	236	ILE	3.2
3	L	81	LEU	3.2
2	H	95	GLY	3.1
3	L	162	TYR	3.1
4	M	260	ILE	3.1
2	H	84	GLU	3.0
4	M	26	ASN	3.0
4	M	37	TRP	3.0
1	C	230	PHE	3.0
4	M	243	VAL	3.0
2	H	87	GLU	3.0
1	C	246	PHE	3.0
3	L	1	ALA	2.9
3	L	20	ASP	2.9
2	H	25	TRP	2.9
1	C	250	ALA	2.8
1	C	253	PHE	2.8
4	M	224	VAL	2.7
2	H	102	GLN	2.7
4	M	22	GLU	2.7
4	M	221	ILE	2.7
1	C	229	THR	2.6
3	L	55	GLN	2.6
3	L	60	ASP	2.6
1	C	240	LEU	2.6
2	H	257	LEU	2.6
3	L	270	PRO	2.6
2	H	189	GLY	2.5
1	C	242	THR	2.5
4	M	30	GLY	2.5
3	L	53	ALA	2.5
1	C	245	THR	2.4
3	L	187	LEU	2.4
1	C	185	LEU	2.4
2	H	82	ARG	2.4
3	L	57	PRO	2.4
3	L	33	PHE	2.4
3	L	62	PHE	2.4
4	M	216	ALA	2.3
2	H	190	SER	2.3
4	M	236	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	104	THR	2.3
3	L	77	ALA	2.3
4	M	263	VAL	2.3
4	M	23	TRP	2.2
4	M	218	GLY	2.2
3	L	273	SER	2.2
3	L	157	VAL	2.2
4	M	215	ALA	2.2
4	M	189	ILE	2.2
1	C	232	LEU	2.2
1	C	266	ILE	2.1
3	L	17	ILE	2.1
3	L	227	LEU	2.1
3	L	43	PHE	2.1
1	C	231	ALA	2.1
1	C	247	CYS	2.1
4	M	222	LEU	2.1
2	H	251	PRO	2.1
3	L	160	PHE	2.0
2	H	105	GLY	2.0
1	C	233	MET	2.0
4	M	242	ALA	2.0
4	M	220	THR	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	0.76	0.27	-	33,40,56,58	0

## 6.3 Carbohydrates [i](#)

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, 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	NS5	M	1329	40/40	0.76	0.24	5.91	42,62,77,77	0
8	MPG	L	1278	25/25	0.73	0.25	4.62	36,47,54,54	25
8	MPG	L	1277	21/25	0.66	0.20	2.70	56,63,69,71	0
8	MPG	M	1330	17/25	0.74	0.19	1.27	62,64,65,65	0
5	HEM	C	1334	43/43	0.98	0.08	-0.05	27,30,37,38	0
5	HEM	C	1333	43/43	0.98	0.09	-0.40	28,32,37,41	0
7	BPB	M	1326	61/65	0.95	0.09	-0.53	17,28,59,62	0
6	BCB	M	1324	65/66	0.94	0.11	-0.60	23,27,73,75	0
10	MQ7	M	1328	48/48	0.93	0.10	-0.90	28,34,53,57	0
7	BPB	L	1276	65/65	0.95	0.08	-1.01	22,31,37,40	0
5	HEM	C	1336	43/43	0.97	0.07	-1.08	20,27,36,48	0
6	BCB	M	1325	66/66	0.97	0.07	-1.42	20,26,37,39	0
6	BCB	L	1275	66/66	0.96	0.08	-1.53	22,27,51,56	0
6	BCB	L	1274	66/66	0.96	0.07	-1.75	19,26,38,42	0
5	HEM	C	1335	43/43	0.99	0.08	-2.43	21,25,27,29	0
9	FE2	M	1327	1/1	1.00	0.02	-7.03	27,27,27,27	0

## 6.5 Other polymers

There are no such residues in this entry.