



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:17 AM GMT

PDB ID : 2WJM  
Title : Lipidic sponge phase crystal structure of the photosynthetic reaction centre from *Blastochloris viridis* (low dose)  
Authors : Woehri, A.B.; Wahlgren, W.Y.; Malmerberg, E.; Johansson, L.C.; Neutze, R.; Katona, G.  
Deposited on : 2009-05-27  
Resolution : 1.95 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

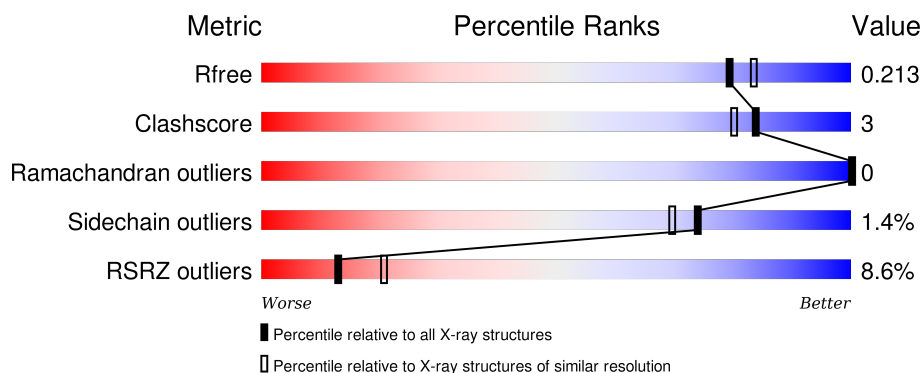
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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>4%</div> <div>92%</div> <div>7%</div> </div>
2	H	258	<div> <div>12%</div> <div>90%</div> <div>6%</div> </div>
3	L	274	<div> <div>12%</div> <div>92%</div> <div>7%</div> </div>
4	M	324	<div> <div>7%</div> <div>94%</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
12	NS5	M	1329	-	-	-	X
13	PO4	M	1331	-	-	-	X
13	PO4	M	1332	-	-	-	X
8	DGA	L	1277	-	-	-	X
9	MPG	L	1278	-	-	-	X
9	MPG	L	1279	-	-	-	X

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 10671 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
			2598	1637	465	478	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
			1880	1205	326	347	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	2	0
			2170	1458	350	355	7			

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

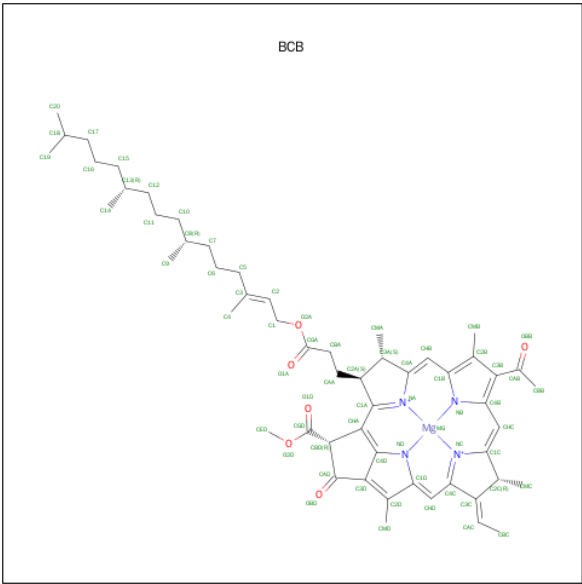
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	323	Total	C	N	O	S	0	0	0
			2548	1697	417	423	11			

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



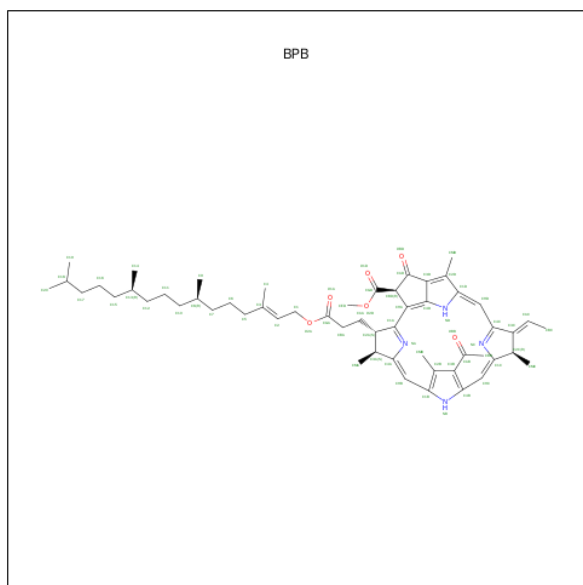
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 6 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula:  $C_{55}H_{72}MgN_4O_6$ ).



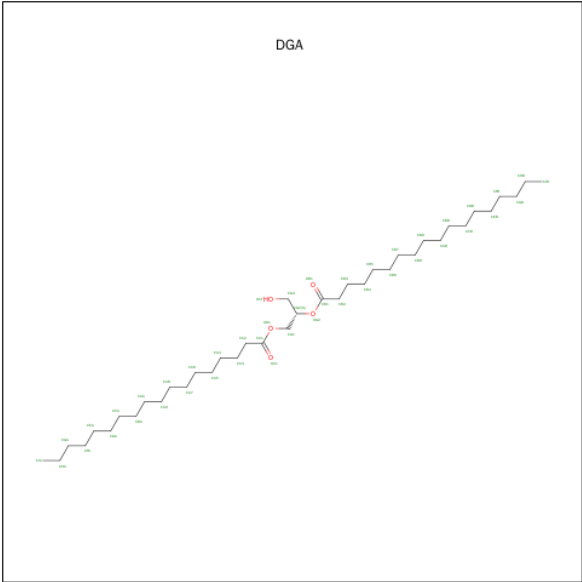
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
6	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
6	M	1	Total 65	C 54	Mg 1	N 4	O 6	0	0
6	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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



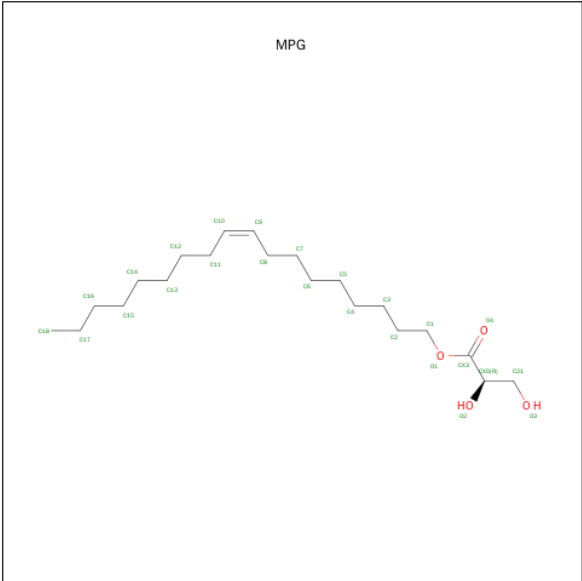
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			65	55	4	6		
7	M	1	Total	C	N	O	0	0
			61	51	4	6		

- Molecule 8 is DIACYL GLYCEROL (three-letter code: DGA) (formula:  $C_{39}H_{76}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	0
			37	33	4		

- Molecule 9 is 1-MONOOLEOYL-RAC-GLYCEROL (three-letter code: MPG) (formula:  $C_{21}H_{40}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	L	1	Total	C	O	0	0
			25	21	4		
9	L	1	Total	C	O	0	0
			25	21	4		

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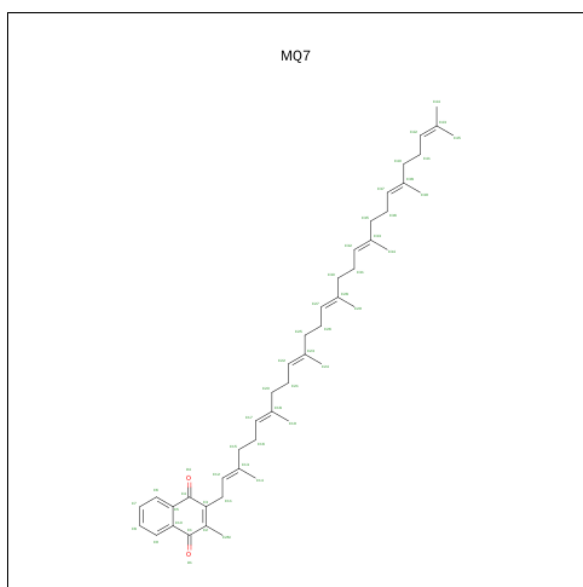
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	M	1	Total C 17 17	0	0

- Molecule 10 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

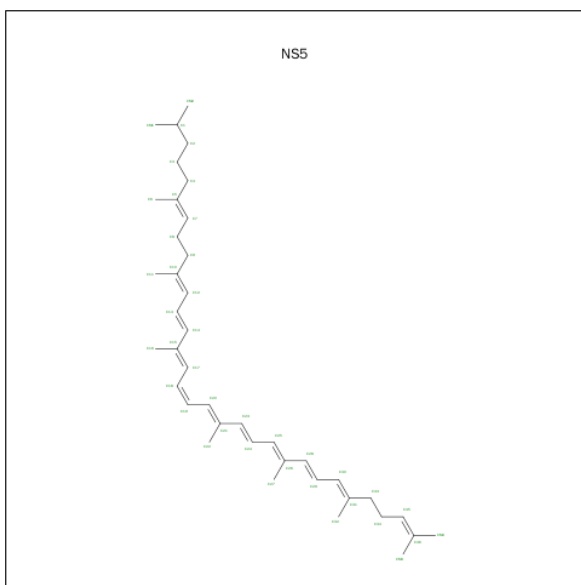
- Molecule 11 is MENAQUINONE-7 (three-letter code: MQ7) (formula: C<sub>46</sub>H<sub>64</sub>O<sub>2</sub>).



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

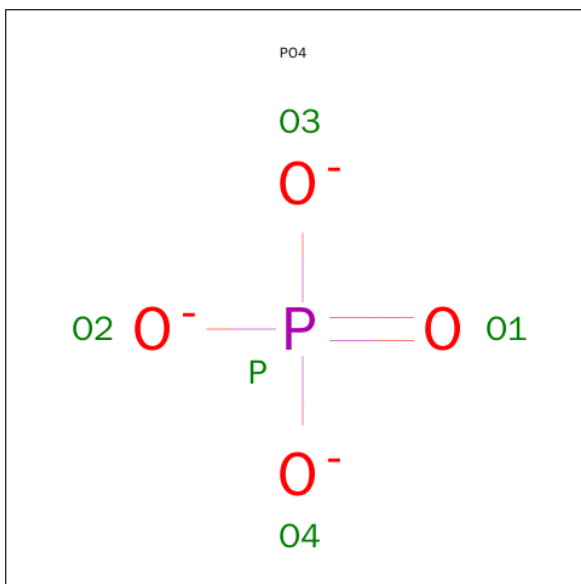
- Molecule 12 is 15-CIS-1,2-DIHYDRONEUROSPORENE (three-letter code: NS5) (formula: C<sub>40</sub>H<sub>60</sub>).





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

- Molecule 13 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	M	1	Total O P 5 4 1	0	0
13	M	1	Total O P 5 4 1	0	0

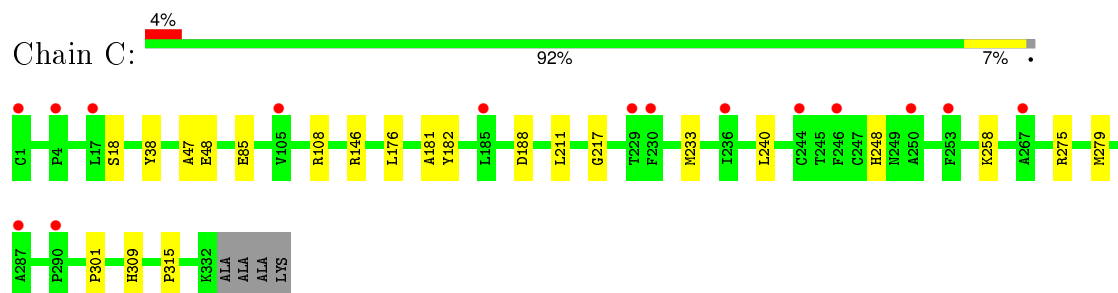
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	C	316	Total 316	O 316	0	0
14	H	148	Total 148	O 148	0	0
14	L	87	Total 87	O 87	0	0
14	M	160	Total 160	O 160	0	0

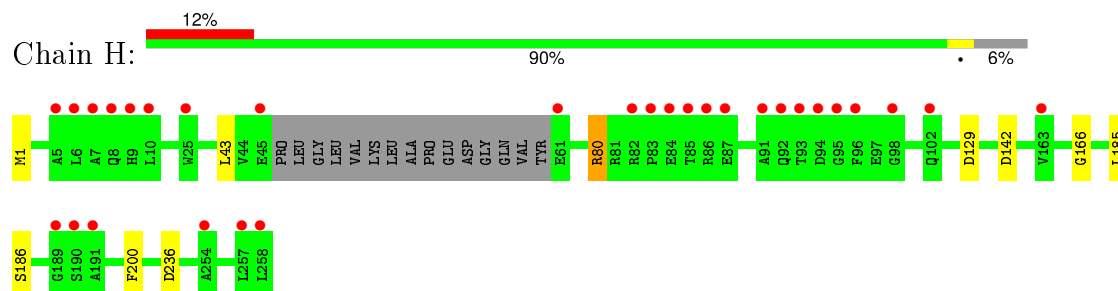
### 3 Residue-property plots [i](#)

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.

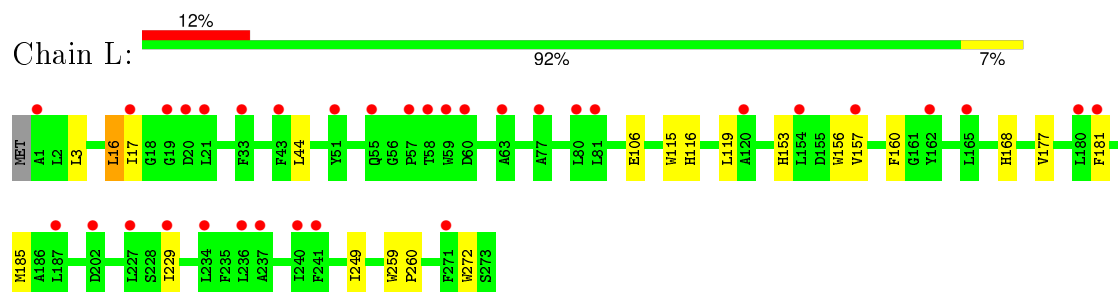
#### • Molecule 1: PHOTOSYNTHETIC REACTION CENTER CYTOCHROME C SUBUNIT



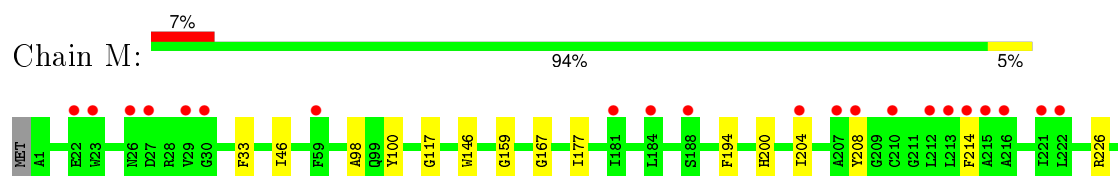
#### • Molecule 2: REACTION CENTER PROTEIN H CHAIN



#### • 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, $\alpha$ , $\beta$ , $\gamma$	84.45Å 138.50Å 177.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	176.78 – 1.95 45.87 – 1.95	Depositor EDS
% Data completeness (in resolution range)	95.8 (176.78-1.95) 95.9 (45.87-1.95)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.173 , 0.201 0.186 , 0.213	Depositor DCC
$R_{free}$ test set	7313 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.5	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 56.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 145800 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10671	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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, PO4, BCB, DGA, 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	0.70	1/2665 (0.0%)	0.76	5/3633 (0.1%)
2	H	0.61	0/1913	0.73	3/2613 (0.1%)
3	L	0.65	0/2263	0.66	0/3089
4	M	0.68	0/2652	0.66	0/3630
All	All	0.66	1/9493 (0.0%)	0.70	8/12965 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	85	GLU	CG-CD	5.87	1.60	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	80	ARG	NE-CZ-NH2	-8.81	115.89	120.30
1	C	108	ARG	NE-CZ-NH2	-8.12	116.24	120.30
2	H	80	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	C	108	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	C	146	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	C	188	ASP	CB-CG-OD1	6.34	124.01	118.30
1	C	48	GLU	N-CA-C	-6.24	94.15	111.00
2	H	129	ASP	CB-CG-OD1	6.17	123.86	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	248	HIS	Peptide
1	C	47	ALA	Peptide

## 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	2598	0	2567	11	0
2	H	1880	0	1869	6	0
3	L	2170	0	2100	13	0
4	M	2548	0	2432	14	0
5	C	172	0	120	2	0
6	L	132	0	144	11	0
6	M	131	0	140	6	0
7	L	65	0	74	8	0
7	M	61	0	63	6	0
8	L	37	0	58	0	0
9	L	50	0	80	3	0
9	M	17	0	31	0	0
10	M	1	0	0	0	0
11	M	48	0	64	0	0
12	M	40	0	60	7	0
13	M	10	0	0	0	0
14	C	316	0	0	1	0
14	H	148	0	0	2	0
14	L	87	0	0	0	0
14	M	160	0	0	0	0
All	All	10671	0	9802	60	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 3.

All (60) 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:HHC	7:M:1326:BPB:HBBB	1.44	0.98
6:M:1324:BCB:HBB2	6:M:1324:BCB:HHC	1.53	0.89
7:L:1276:BPB:HHC	7:L:1276:BPB:HBBB	1.55	0.88
2:H:142:ASP:OD1	14:H:2072:HOH:O	2.04	0.73
6:M:1324:BCB:HHC	6:M:1324:BCB:CBB	2.19	0.73
3:L:181:PHE:HB3	7:M:1326:BPB:HBBA	1.75	0.68
7:M:1326:BPB:CBB	7:M:1326:BPB:HHC	2.21	0.67
3:L:181:PHE:CD2	7:M:1326:BPB:HBB	2.33	0.63
7:L:1276:BPB:HBB	4:M:208:TYR:CD2	2.34	0.63
6:L:1274:BCB:HBB3	6:L:1274:BCB:HMB1	1.78	0.63
3:L:116:HIS:CE1	9:L:1278:MPG:H31	2.33	0.63
4:M:117:GLY:HA3	12:M:1329:NS5:H92	1.83	0.60
7:L:1276:BPB:CBB	7:L:1276:BPB:HHC	2.30	0.59
4:M:159:GLY:HA3	12:M:1329:NS5:C11	2.32	0.59
3:L:16:LEU:HD13	3:L:106:GLU:HG2	1.88	0.56
1:C:176:LEU:HD12	14:C:2194:HOH:O	2.07	0.55
7:L:1276:BPB:HBBA	4:M:208:TYR:HB3	1.88	0.55
7:M:1326:BPB:C9	12:M:1329:NS5:HM33	2.39	0.53
6:L:1274:BCB:CBB	6:L:1274:BCB:HMB1	2.38	0.53
6:M:1325:BCB:CBB	6:M:1325:BCB:HMB1	2.40	0.52
3:L:168:HIS:CE1	6:L:1274:BCB:HMC2	2.46	0.50
4:M:177:ILE:HD11	12:M:1329:NS5:H273	1.94	0.50
6:M:1324:BCB:CBB	6:M:1324:BCB:CHC	2.90	0.50
6:L:1275:BCB:CBB	6:L:1275:BCB:HMB1	2.42	0.49
6:L:1275:BCB:HMD2	6:M:1325:BCB:HBB3	1.93	0.49
6:L:1275:BCB:HMB2	7:L:1276:BPB:HMBA	1.94	0.49
4:M:159:GLY:HA3	12:M:1329:NS5:H113	1.96	0.48
4:M:98:ALA:HB3	4:M:100:TYR:CZ	2.50	0.47
3:L:259:TRP:N	3:L:260:PRO:CD	2.78	0.47
4:M:146:TRP:HA	4:M:146:TRP:CE3	2.49	0.47
2:H:43:LEU:CD2	3:L:3:LEU:HD23	2.46	0.46
1:C:309:HIS:CE1	1:C:315:PRO:HD3	2.51	0.46
1:C:240:LEU:HD22	1:C:309:HIS:CG	2.50	0.45
1:C:211:LEU:HD12	2:H:1:FME:O	2.17	0.45
3:L:177:VAL:HG13	6:L:1274:BCB:HMB3	1.98	0.45
7:M:1326:BPB:CBB	7:M:1326:BPB:CHC	2.91	0.45
6:L:1275:BCB:H142	6:L:1275:BCB:HMA1	1.99	0.44
4:M:33:PHE:CE2	4:M:46:ILE:HD12	2.53	0.44
12:M:1329:NS5:H161	12:M:1329:NS5:H18	1.78	0.44
1:C:258:LYS:HG2	4:M:307:ALA:HB2	2.00	0.44
1:C:217:GLY:HA2	4:M:167:GLY:O	2.18	0.43
1:C:233:MET:HB3	5:C:1335:HEM:C4B	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:1324:BCB:HBB3	6:M:1325:BCB:H41	2.01	0.43
6:L:1275:BCB:C1B	7:L:1276:BPB:H19A	2.49	0.43
6:L:1275:BCB:C2B	7:L:1276:BPB:H19A	2.49	0.42
4:M:200:HIS:CE1	4:M:204:ILE:HD11	2.53	0.42
6:L:1274:BCB:H203	6:L:1274:BCB:H161	1.88	0.42
2:H:80:ARG:HD2	14:H:2043:HOH:O	2.20	0.42
3:L:119:LEU:HD23	9:L:1278:MPG:H71	2.02	0.42
12:M:1329:NS5:H24	12:M:1329:NS5:H221	1.82	0.42
7:L:1276:BPB:CBB	4:M:208:TYR:CD2	3.03	0.42
1:C:181:ALA:O	1:C:182:TYR:HB2	2.20	0.41
1:C:275:ARG:O	1:C:279:MET:HE2	2.21	0.41
3:L:153:HIS:O	3:L:157:VAL:HG23	2.20	0.41
2:H:166:GLY:HA3	2:H:186:SER:O	2.21	0.40
1:C:18:SER:HB2	3:L:156:TRP:CD1	2.57	0.40
1:C:301:PRO:HG2	5:C:1334:HEM:HBD1	2.03	0.40
3:L:229:ILE:O	3:L:229:ILE:HD12	2.20	0.40
3:L:115:TRP:CE3	9:L:1278:MPG:H211	2.57	0.40
2:H:200:PHE:CZ	4:M:226:ARG:HD3	2.57	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%)	235 (98%)	4 (2%)	0	100	100
3	L	273/274 (100%)	266 (97%)	7 (3%)	0	100	100
4	M	321/324 (99%)	312 (97%)	9 (3%)	0	100	100
All	All	1163/1192 (98%)	1134 (98%)	29 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	280/282 (99%)	279 (100%)	1 (0%)	93	93
2	H	192/212 (91%)	190 (99%)	2 (1%)	82	80
3	L	218/219 (100%)	211 (97%)	7 (3%)	46	33
4	M	247/250 (99%)	244 (99%)	3 (1%)	78	75
All	All	937/963 (97%)	924 (99%)	13 (1%)	74	70

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	38	TYR
2	H	185	LEU
2	H	236	ASP
3	L	16	LEU
3	L	17	ILE
3	L	44	LEU
3	L	160	PHE
3	L	185	MET
3	L	249	ILE
3	L	272	TRP
4	M	194	PHE
4	M	214	PHE
4	M	290	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	302	GLN
3	L	183	ASN
3	L	239	ASN
4	M	16	HIS

### 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	3.44	3 (50%)

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	-	1/6/9/11	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	FME	CA-N-CN	-7.35	111.52	122.82
2	H	1	FME	O1-CN-N	-2.67	120.91	124.76
2	H	1	FME	CE-SD-CG	2.27	108.13	100.37

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	1	FME	O1-CN-N-CA

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	FME	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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	2.20	11 (36%)	24,82,82	2.68	11 (45%)
5	HEM	C	1334	1	30,50,50	2.32	10 (33%)	24,82,82	2.64	12 (50%)
5	HEM	C	1335	1	30,50,50	2.05	7 (23%)	24,82,82	2.51	10 (41%)
5	HEM	C	1336	1	30,50,50	2.00	9 (30%)	24,82,82	2.52	10 (41%)
6	BCB	L	1274	3	56,74,74	2.35	10 (17%)	57,115,115	2.26	21 (36%)
6	BCB	L	1275	3	56,74,74	2.28	10 (17%)	57,115,115	2.13	13 (22%)
7	BPB	L	1276	-	63,70,70	2.79	15 (23%)	63,101,101	2.00	15 (23%)
8	DGA	L	1277	1	36,36,43	1.23	2 (5%)	38,38,45	1.22	3 (7%)
9	MPG	L	1278	-	22,23,24	1.36	1 (4%)	20,23,25	1.68	2 (10%)
9	MPG	L	1279	-	22,23,24	1.44	1 (4%)	20,23,25	1.71	2 (10%)
6	BCB	M	1324	4	55,73,74	2.27	11 (20%)	55,113,115	1.96	11 (20%)
6	BCB	M	1325	4	56,74,74	2.28	9 (16%)	57,115,115	2.13	13 (22%)
7	BPB	M	1326	-	59,66,70	2.78	15 (25%)	58,96,101	2.32	14 (24%)
11	MQ7	M	1328	-	49,49,49	1.31	2 (4%)	62,63,63	1.24	9 (14%)
12	NS5	M	1329	-	39,39,39	2.10	5 (12%)	44,46,46	2.09	16 (36%)
9	MPG	M	1330	-	16,16,24	0.27	0	15,15,25	0.67	0
13	PO4	M	1331	-	4,4,4	0.49	0	6,6,6	0.35	0
13	PO4	M	1332	-	4,4,4	0.24	0	6,6,6	0.41	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	DGA	L	1277	1	-	0/37/37/45	0/0/0/0
9	MPG	L	1278	-	-	0/25/22/25	0/0/0/0
9	MPG	L	1279	-	-	0/25/22/25	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
11	MQ7	M	1328	-	-	0/41/61/61	0/2/2/2
12	NS5	M	1329	-	-	0/43/43/43	0/0/0/0
9	MPG	M	1330	-	-	0/14/14/25	0/0/0/0
13	PO4	M	1331	-	-	0/0/0/0	0/0/0/0
13	PO4	M	1332	-	-	0/0/0/0	0/0/0/0

All (118) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1333	HEM	C3B-C4B	-7.09	1.45	1.51
5	C	1335	HEM	C3B-C4B	-6.82	1.45	1.51
5	C	1334	HEM	C3B-C4B	-6.54	1.46	1.51
5	C	1336	HEM	C3B-C4B	-5.93	1.46	1.51
5	C	1334	HEM	C3D-C4D	-5.66	1.44	1.51
12	M	1329	NS5	C9-C8	-5.39	1.35	1.53
5	C	1333	HEM	C3D-C4D	-4.99	1.45	1.51
5	C	1336	HEM	C3D-C4D	-4.46	1.45	1.51
5	C	1334	HEM	C2C-C1C	-4.23	1.44	1.52
7	M	1326	BPB	C4C-NC	-4.06	1.27	1.37
7	M	1326	BPB	C1A-NA	-4.00	1.28	1.36
5	C	1336	HEM	C2C-C1C	-3.97	1.45	1.52
5	C	1335	HEM	C3D-C4D	-3.77	1.46	1.51
6	M	1325	BCB	C2C-C1C	-3.70	1.48	1.51
5	C	1335	HEM	C2C-C1C	-3.67	1.45	1.52
7	L	1276	BPB	C1A-NA	-3.62	1.29	1.36
5	C	1333	HEM	C2C-C1C	-3.56	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	1276	BPB	C4C-NC	-3.23	1.29	1.37
7	M	1326	BPB	C1C-NC	-2.64	1.33	1.38
6	M	1324	BCB	C2C-C1C	-2.63	1.49	1.51
5	C	1333	HEM	C2D-C1D	-2.52	1.43	1.51
6	L	1274	BCB	CHB-C4A	-2.35	1.34	1.41
6	M	1324	BCB	CHB-C4A	-2.32	1.34	1.41
5	C	1335	HEM	C2B-C1B	-2.30	1.44	1.51
5	C	1336	HEM	C2D-C1D	-2.29	1.44	1.51
7	L	1276	BPB	C1D-ND	-2.27	1.33	1.38
5	C	1334	HEM	C2B-C1B	-2.27	1.44	1.51
6	L	1275	BCB	CHB-C4A	-2.26	1.34	1.41
5	C	1335	HEM	C2D-C1D	-2.20	1.44	1.51
5	C	1333	HEM	C2B-C1B	-2.17	1.44	1.51
5	C	1334	HEM	C2D-C1D	-2.13	1.44	1.51
7	M	1326	BPB	C1D-ND	-2.01	1.34	1.38
6	M	1324	BCB	CHC-C1C	2.02	1.47	1.41
5	C	1334	HEM	C4C-NC	2.04	1.38	1.36
5	C	1333	HEM	C4C-NC	2.04	1.38	1.36
7	M	1326	BPB	CHD-C4C	2.07	1.45	1.40
7	L	1276	BPB	C1B-CHB	2.08	1.48	1.40
6	M	1324	BCB	C3B-C2B	2.11	1.45	1.40
5	C	1336	HEM	C3C-CAC	2.15	1.55	1.51
5	C	1336	HEM	FE-NB	2.25	2.09	1.97
5	C	1336	HEM	C1C-NC	2.27	1.38	1.36
5	C	1336	HEM	C4C-NC	2.28	1.38	1.36
7	L	1276	BPB	C4C-C3C	2.31	1.50	1.45
5	C	1334	HEM	C3C-CAC	2.31	1.55	1.51
5	C	1333	HEM	FE-ND	2.32	2.09	1.97
5	C	1334	HEM	FE-ND	2.34	2.09	1.97
5	C	1333	HEM	CMA-C3A	2.38	1.56	1.51
6	L	1274	BCB	C3D-C2D	2.39	1.45	1.40
5	C	1336	HEM	C3B-CAB	2.40	1.55	1.51
5	C	1333	HEM	FE-NC	2.42	2.05	1.95
5	C	1333	HEM	C3B-CAB	2.42	1.55	1.51
6	M	1324	BCB	CHD-C4C	2.44	1.42	1.35
6	L	1274	BCB	CHC-C1C	2.48	1.48	1.41
7	L	1276	BPB	C4B-CHC	2.49	1.49	1.40
5	C	1333	HEM	C3C-CAC	2.50	1.56	1.51
7	M	1326	BPB	C1B-CHB	2.51	1.49	1.40
6	M	1325	BCB	C3B-C2B	2.64	1.46	1.40
12	M	1329	NS5	C30-C31	2.64	1.37	1.34
5	C	1334	HEM	FE-NB	2.71	2.11	1.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	1274	BCB	C3B-C2B	2.73	1.46	1.40
12	M	1329	NS5	C29-C30	2.74	1.52	1.43
5	C	1335	HEM	FE-ND	2.83	2.12	1.97
6	L	1275	BCB	CHC-C1C	2.86	1.49	1.41
6	M	1325	BCB	C3D-C2D	2.92	1.47	1.40
6	L	1275	BCB	C3D-C2D	2.97	1.47	1.40
7	M	1326	BPB	C3B-C2B	2.98	1.47	1.40
6	L	1274	BCB	CHD-C4C	2.99	1.44	1.35
6	M	1325	BCB	O2A-CGA	3.02	1.42	1.33
7	M	1326	BPB	C3D-C2D	3.07	1.47	1.38
6	L	1274	BCB	O2A-CGA	3.08	1.42	1.33
7	L	1276	BPB	O2A-CGA	3.13	1.42	1.33
7	M	1326	BPB	O2A-CGA	3.17	1.42	1.33
6	L	1275	BCB	OBD-CAD	3.18	1.27	1.22
5	C	1335	HEM	C1C-NC	3.23	1.40	1.36
6	L	1275	BCB	CHD-C4C	3.25	1.45	1.35
6	M	1325	BCB	CHD-C4C	3.31	1.45	1.35
7	L	1276	BPB	C3B-C2B	3.32	1.48	1.40
6	L	1275	BCB	O2A-CGA	3.41	1.43	1.33
6	L	1275	BCB	C3B-C2B	3.44	1.48	1.40
6	M	1324	BCB	O2D-CGD	3.45	1.42	1.33
7	L	1276	BPB	OBD-CAD	3.50	1.28	1.22
6	L	1275	BCB	O2D-CGD	3.52	1.42	1.33
7	L	1276	BPB	CHD-C1D	3.53	1.45	1.38
7	M	1326	BPB	O2D-CGD	3.59	1.42	1.33
6	M	1324	BCB	O2A-CGA	3.61	1.44	1.33
7	M	1326	BPB	CHD-C1D	3.65	1.45	1.38
6	M	1324	BCB	C3D-C2D	3.66	1.48	1.40
5	C	1334	HEM	C1C-NC	3.68	1.40	1.36
7	M	1326	BPB	OBD-CAD	3.70	1.29	1.22
7	L	1276	BPB	C3D-C2D	3.80	1.49	1.38
7	L	1276	BPB	O2D-CGD	4.10	1.43	1.33
6	M	1324	BCB	OBD-CAD	4.18	1.28	1.22
6	M	1325	BCB	O2D-CGD	4.56	1.44	1.33
8	L	1277	DGA	OG1-CA1	4.65	1.47	1.33
6	L	1274	BCB	O2D-CGD	4.73	1.45	1.33
8	L	1277	DGA	OG2-CB1	4.84	1.48	1.34
7	M	1326	BPB	C3B-C4B	5.03	1.48	1.41
6	L	1274	BCB	OBD-CAD	5.03	1.30	1.22
6	M	1325	BCB	C1A-CHA	5.15	1.47	1.37
11	M	1328	MQ7	C10-C5	5.17	1.48	1.40
6	M	1324	BCB	C1A-CHA	5.18	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	1274	BCB	C1A-CHA	5.26	1.48	1.37
6	L	1275	BCB	C1A-CHA	5.41	1.48	1.37
6	M	1325	BCB	OBD-CAD	5.56	1.30	1.22
11	M	1328	MQ7	C3-C2	5.74	1.48	1.35
7	L	1276	BPB	C3B-C4B	5.83	1.49	1.41
9	L	1278	MPG	O1-CX3	6.04	1.46	1.33
9	L	1279	MPG	O1-CX3	6.23	1.46	1.33
7	M	1326	BPB	C1A-CHA	7.00	1.49	1.36
12	M	1329	NS5	C29-C28	7.06	1.53	1.34
7	L	1276	BPB	C1A-CHA	7.23	1.50	1.36
12	M	1329	NS5	C35-C36	7.25	1.54	1.32
6	M	1325	BCB	CAC-C3C	12.00	1.48	1.33
6	M	1324	BCB	CAC-C3C	12.09	1.48	1.33
6	L	1275	BCB	CAC-C3C	12.76	1.49	1.33
6	L	1274	BCB	CAC-C3C	13.12	1.49	1.33
7	M	1326	BPB	CAC-C3C	15.06	1.51	1.33
7	L	1276	BPB	CAC-C3C	15.86	1.52	1.33

All (162) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	1326	BPB	C2C-C3C-C4C	-7.72	100.19	107.24
7	L	1276	BPB	C2C-C3C-C4C	-7.24	100.63	107.24
7	M	1326	BPB	CBC-CAC-C3C	-6.84	111.30	127.07
12	M	1329	NS5	C29-C28-C26	-5.45	110.28	126.32
7	L	1276	BPB	CBC-CAC-C3C	-5.33	114.77	127.07
6	M	1325	BCB	C4D-C3D-CAD	-5.25	99.93	107.86
6	M	1324	BCB	OBD-CAD-C3D	-5.25	117.64	128.35
6	L	1274	BCB	OBD-CAD-C3D	-5.19	117.76	128.35
6	L	1275	BCB	C4D-C3D-CAD	-5.07	100.22	107.86
7	L	1276	BPB	C4D-C3D-C2D	-5.05	101.02	106.74
6	M	1324	BCB	C4D-C3D-CAD	-4.90	100.46	107.86
6	M	1325	BCB	O2D-CGD-O1D	-4.83	113.81	123.79
5	C	1333	HEM	C3C-CAC-CBC	-4.78	117.13	124.46
6	M	1324	BCB	CHC-C1C-NC	-4.75	119.55	125.06
6	L	1275	BCB	OBD-CAD-C3D	-4.65	118.86	128.35
6	L	1274	BCB	CHC-C1C-NC	-4.65	119.66	125.06
5	C	1336	HEM	C3B-CAB-CBB	-4.60	117.40	124.46
6	M	1325	BCB	OBD-CAD-C3D	-4.53	119.12	128.35
6	L	1275	BCB	CHC-C1C-NC	-4.46	119.89	125.06
12	M	1329	NS5	C18-C17-C15	-4.38	120.87	127.20
5	C	1334	HEM	C3B-CAB-CBB	-4.35	117.79	124.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	1325	BCB	C1D-CHD-C4C	-4.30	120.03	129.26
7	M	1326	BPB	C4D-C3D-C2D	-4.19	101.99	106.74
6	M	1325	BCB	CHC-C1C-NC	-3.99	120.43	125.06
5	C	1335	HEM	C3B-CAB-CBB	-3.99	118.34	124.46
6	M	1324	BCB	C2C-C1C-CHC	-3.97	114.14	123.29
5	C	1333	HEM	C3B-CAB-CBB	-3.88	118.50	124.46
6	L	1274	BCB	C4D-C3D-CAD	-3.87	102.01	107.86
9	L	1278	MPG	O1-CX3-O11	-3.73	116.43	124.05
6	L	1275	BCB	C1D-CHD-C4C	-3.73	121.25	129.26
7	M	1326	BPB	CMD-C2D-C3D	-3.71	119.41	128.04
7	L	1276	BPB	OBD-CAD-C3D	-3.66	118.48	128.37
6	L	1275	BCB	O1D-CGD-CBD	-3.66	119.38	124.62
12	M	1329	NS5	CM3-C36-C35	-3.62	110.96	122.61
12	M	1329	NS5	C24-C25-C26	-3.52	122.12	127.20
7	M	1326	BPB	O2D-CGD-O1D	-3.49	116.59	123.79
6	L	1274	BCB	C1D-CHD-C4C	-3.45	121.84	129.26
12	M	1329	NS5	C34-C35-C36	-3.30	115.04	127.73
6	M	1325	BCB	C2C-C1C-CHC	-3.29	115.70	123.29
5	C	1334	HEM	C3C-CAC-CBC	-3.22	119.52	124.46
6	L	1275	BCB	C2C-C1C-CHC	-3.21	115.89	123.29
9	L	1279	MPG	O1-CX3-O11	-3.18	117.57	124.05
5	C	1333	HEM	CBD-CAD-C3D	-3.14	104.42	113.55
6	L	1274	BCB	O2D-CGD-O1D	-3.11	117.36	123.79
6	L	1274	BCB	C2C-C1C-CHC	-3.11	116.12	123.29
5	C	1336	HEM	CAA-CBA-CGA	-3.02	107.20	112.75
6	L	1274	BCB	CMD-C2D-C3D	-3.02	119.19	125.09
5	C	1333	HEM	CAA-C2A-C1A	-2.96	123.79	127.01
5	C	1335	HEM	C3B-C4B-NB	-2.84	106.19	111.63
12	M	1329	NS5	CM4-C36-C35	-2.75	113.75	122.61
6	M	1324	BCB	C1D-CHD-C4C	-2.75	123.35	129.26
5	C	1335	HEM	CAA-C2A-C1A	-2.75	124.02	127.01
6	L	1274	BCB	O2A-CGA-O1A	-2.74	116.43	123.49
6	L	1275	BCB	CHD-C4C-C3C	-2.70	121.47	129.02
6	L	1274	BCB	CHD-C4C-C3C	-2.64	121.62	129.02
5	C	1336	HEM	C3C-CAC-CBC	-2.63	120.42	124.46
7	M	1326	BPB	OBD-CAD-C3D	-2.55	121.49	128.37
5	C	1336	HEM	CMA-C3A-C4A	-2.53	124.18	128.36
11	M	1328	MQ7	C21-C22-C23	-2.52	122.28	127.76
12	M	1329	NS5	C30-C29-C28	-2.49	115.53	123.13
5	C	1334	HEM	CBA-CAA-C2A	-2.46	108.13	112.53
5	C	1334	HEM	C3B-C4B-NB	-2.44	106.96	111.63
11	M	1328	MQ7	C30-C31-C32	-2.42	105.36	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	1276	BPB	CMD-C2D-C3D	-2.41	122.43	128.04
6	M	1324	BCB	O2D-CGD-O1D	-2.38	118.88	123.79
11	M	1328	MQ7	C26-C27-C28	-2.38	122.60	127.76
12	M	1329	NS5	CM4-C36-CM3	-2.35	108.86	114.64
6	L	1275	BCB	C5-C3-C2	-2.32	116.65	121.05
6	L	1274	BCB	C5-C3-C2	-2.32	116.65	121.05
12	M	1329	NS5	C23-C21-C20	-2.30	115.28	118.98
6	M	1324	BCB	C4-C3-C2	-2.28	119.03	123.50
7	L	1276	BPB	CBA-CAA-C2A	-2.26	107.36	113.73
6	M	1325	BCB	CHD-C4C-C3C	-2.24	122.74	129.02
5	C	1334	HEM	CBD-CAD-C3D	-2.24	107.03	113.55
5	C	1333	HEM	CBA-CAA-C2A	-2.18	108.62	112.53
7	M	1326	BPB	CBB-CAB-C3B	-2.14	113.99	120.33
11	M	1328	MQ7	C16-C17-C18	-2.12	123.15	127.76
5	C	1335	HEM	CBA-CAA-C2A	-2.05	108.86	112.53
11	M	1328	MQ7	C31-C32-C33	-2.02	123.37	127.76
6	L	1274	BCB	OBB-CAB-C3B	-2.02	116.81	120.00
6	L	1274	BCB	C4-C3-C2	-2.02	119.54	123.50
12	M	1329	NS5	C25-C24-C23	-2.00	117.02	123.13
6	L	1274	BCB	CED-O2D-CGD	2.00	120.69	115.99
7	M	1326	BPB	C3D-C4D-ND	2.10	116.42	109.65
11	M	1328	MQ7	C39-C38-C40	2.11	118.63	115.41
11	M	1328	MQ7	C19-C18-C20	2.14	118.68	115.41
6	M	1325	BCB	CMD-C2D-C1D	2.16	131.94	128.36
7	L	1276	BPB	CBD-CAD-C3D	2.18	111.55	107.56
8	L	1277	DGA	CG1-OG1-CA1	2.18	122.94	116.85
12	M	1329	NS5	C11-C10-C9	2.19	118.75	115.41
7	M	1326	BPB	C2B-C1B-NB	2.20	113.90	110.29
6	L	1274	BCB	O2A-CGA-CBA	2.24	118.73	111.90
7	L	1276	BPB	C3D-C4D-ND	2.25	116.90	109.65
7	L	1276	BPB	CED-O2D-CGD	2.27	121.31	115.99
12	M	1329	NS5	C18-C19-C20	2.30	128.48	123.39
5	C	1333	HEM	CMD-C2D-C3D	2.40	124.95	114.35
6	M	1324	BCB	CMB-C2B-C3B	2.48	129.94	125.09
7	L	1276	BPB	C2B-C1B-NB	2.58	114.51	110.29
6	L	1274	BCB	CMB-C2B-C3B	2.61	130.19	125.09
7	M	1326	BPB	CAD-C3D-C2D	2.64	153.52	140.80
5	C	1334	HEM	C2D-C3D-C4D	2.69	106.07	101.50
12	M	1329	NS5	C8-C9-C10	2.73	121.61	112.71
5	C	1336	HEM	C3B-C4B-CHC	2.77	127.06	123.16
6	L	1274	BCB	CAA-C2A-C1A	2.80	122.35	112.47
5	C	1335	HEM	CMD-C2D-C3D	2.82	126.82	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	1326	BPB	OBB-CAB-C3B	2.83	124.48	120.00
5	C	1335	HEM	C3B-C4B-CHC	2.85	127.17	123.16
6	M	1324	BCB	CMD-C2D-C1D	2.86	133.10	128.36
5	C	1334	HEM	CMD-C2D-C3D	2.86	127.00	114.35
8	L	1277	DGA	OG1-CA1-CA2	2.88	120.68	111.90
11	M	1328	MQ7	C34-C33-C35	2.88	119.81	115.41
7	L	1276	BPB	CMB-C2B-C3B	2.89	130.74	125.09
6	M	1325	BCB	CAA-C2A-C1A	2.91	122.74	112.47
11	M	1328	MQ7	C24-C23-C25	2.97	119.94	115.41
12	M	1329	NS5	C22-C21-C20	2.98	127.30	122.90
7	L	1276	BPB	CAD-C3D-C2D	3.06	155.55	140.80
6	L	1275	BCB	C3C-C4C-NC	3.06	112.52	110.24
6	M	1325	BCB	C4-C3-C5	3.11	120.16	115.41
5	C	1333	HEM	C2D-C3D-C4D	3.23	106.98	101.50
5	C	1336	HEM	CMD-C2D-C3D	3.28	128.84	114.35
5	C	1336	HEM	CMC-C2C-C3C	3.29	124.73	116.53
12	M	1329	NS5	C9-C8-C7	3.32	120.38	111.69
5	C	1334	HEM	C3B-C4B-CHC	3.32	127.84	123.16
6	L	1274	BCB	C3C-C4C-NC	3.42	112.79	110.24
7	L	1276	BPB	C3C-C4C-NC	3.51	115.57	109.52
7	L	1276	BPB	O2D-CGD-CBD	3.56	116.18	111.30
7	M	1326	BPB	C4-C3-C5	3.77	121.17	115.41
12	M	1329	NS5	C19-C18-C17	3.85	131.91	123.39
5	C	1334	HEM	CAD-C3D-C4D	3.91	126.25	112.47
5	C	1333	HEM	CAD-C3D-C2D	4.03	124.80	113.22
5	C	1336	HEM	CAD-C3D-C4D	4.07	126.82	112.47
6	M	1325	BCB	CMB-C2B-C3B	4.11	133.12	125.09
6	M	1324	BCB	O2D-CGD-CBD	4.23	117.11	111.30
7	L	1276	BPB	CMD-C2D-C1D	4.26	131.99	125.06
5	C	1334	HEM	CMB-C2B-C3B	4.27	127.19	116.53
5	C	1333	HEM	CMB-C2B-C3B	4.29	127.24	116.53
5	C	1335	HEM	CAD-C3D-C2D	4.30	125.59	113.22
6	L	1275	BCB	O2D-CGD-CBD	4.35	117.27	111.30
6	M	1325	BCB	C3D-CAD-CBD	4.36	113.76	107.60
5	C	1335	HEM	CMC-C2C-C3C	4.37	127.43	116.53
5	C	1334	HEM	CMC-C2C-C3C	4.41	127.53	116.53
5	C	1333	HEM	CAD-C3D-C4D	4.44	128.13	112.47
6	L	1275	BCB	CMB-C2B-C3B	4.45	133.79	125.09
5	C	1335	HEM	CMB-C2B-C3B	4.52	127.82	116.53
6	L	1274	BCB	C3D-CAD-CBD	4.57	114.05	107.60
8	L	1277	DGA	OG2-CB1-CB2	4.58	121.47	111.53
6	L	1275	BCB	CMD-C2D-C1D	4.58	135.94	128.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1333	HEM	CMC-C2C-C3C	4.61	128.04	116.53
5	C	1336	HEM	CMB-C2B-C3B	4.66	128.17	116.53
6	L	1274	BCB	CMD-C2D-C1D	4.78	136.28	128.36
6	L	1274	BCB	O2D-CGD-CBD	4.81	117.90	111.30
5	C	1335	HEM	CAD-C3D-C4D	4.87	129.63	112.47
5	C	1334	HEM	CAD-C3D-C2D	5.03	127.68	113.22
5	C	1336	HEM	CAD-C3D-C2D	5.21	128.21	113.22
6	L	1274	BCB	C4-C3-C5	5.50	123.80	115.41
9	L	1278	MPG	O1-CX3-CXD	5.86	122.46	111.79
6	L	1275	BCB	C3D-CAD-CBD	5.97	116.03	107.60
7	M	1326	BPB	O2D-CGD-CBD	6.05	119.59	111.30
9	L	1279	MPG	O1-CX3-CXD	6.10	122.90	111.79
7	M	1326	BPB	CMD-C2D-C1D	6.27	135.26	125.06
6	M	1324	BCB	C3D-CAD-CBD	6.44	116.71	107.60
6	M	1325	BCB	O2D-CGD-CBD	6.64	120.41	111.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1334	HEM	1	0
5	C	1335	HEM	1	0
6	L	1274	BCB	5	0
6	L	1275	BCB	6	0
7	L	1276	BPB	8	0
9	L	1278	MPG	3	0
6	M	1324	BCB	4	0
6	M	1325	BCB	3	0
7	M	1326	BPB	6	0
12	M	1329	NS5	7	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%)	0.41	15 (4%) 37 48	27, 32, 38, 53	0
2	H	242/258 (93%)	0.67	30 (12%) 5 9	26, 31, 43, 58	0
3	L	273/274 (99%)	0.80	34 (12%) 5 9	28, 32, 41, 54	0
4	M	323/324 (99%)	0.54	22 (6%) 20 30	27, 31, 40, 43	0
All	All	1170/1192 (98%)	0.59	101 (8%) 13 21	26, 32, 41, 58	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	85	THR	7.4
2	H	7	ALA	6.0
2	H	8	GLN	5.9
2	H	9	HIS	5.5
3	L	21	LEU	5.2
3	L	59	TRP	4.9
2	H	258	LEU	4.7
1	C	1	CYS	4.7
3	L	1	ALA	4.3
3	L	58	THR	4.3
3	L	81	LEU	4.1
3	L	271	PHE	4.1
2	H	91	ALA	3.8
2	H	84	GLU	3.8
2	H	87	GLU	3.8
2	H	257	LEU	3.7
2	H	95	GLY	3.7
3	L	20	ASP	3.6
2	H	96	PHE	3.5
3	L	236	LEU	3.5
4	M	216	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
2	H	83	PRO	3.4
2	H	102	GLN	3.4
2	H	190	SER	3.3
2	H	10	LEU	3.3
3	L	17	ILE	3.3
4	M	212	LEU	3.3
3	L	57	PRO	3.2
3	L	77	ALA	3.2
2	H	93	THR	3.2
1	C	185	LEU	3.2
4	M	213	LEU	3.1
3	L	43	PHE	3.1
2	H	82	ARG	3.1
3	L	154	LEU	3.1
2	H	189	GLY	3.1
3	L	60	ASP	3.0
3	L	162	TYR	3.0
4	M	215	ALA	3.0
1	C	105	VAL	2.9
4	M	214	PHE	2.9
3	L	80	LEU	2.9
1	C	236	ILE	2.9
4	M	184	LEU	2.9
3	L	157	VAL	2.9
4	M	23	TRP	2.9
4	M	26	ASN	2.8
2	H	94	ASP	2.8
4	M	22	GLU	2.8
3	L	33	PHE	2.8
4	M	221	ILE	2.8
4	M	208	TYR	2.7
3	L	240	ILE	2.7
1	C	244	CYS	2.6
3	L	63	ALA	2.6
2	H	45	GLU	2.6
2	H	86	ARG	2.6
3	L	165	LEU	2.6
3	L	180	LEU	2.6
1	C	229	THR	2.6
4	M	210	CYS	2.5
3	L	227	LEU	2.5
4	M	29	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
4	M	30	GLY	2.5
3	L	187	LEU	2.5
3	L	229	ILE	2.4
2	H	254	ALA	2.4
3	L	55	GLN	2.4
1	C	230	PHE	2.4
2	H	25	TRP	2.4
1	C	250	ALA	2.4
2	H	61	GLU	2.3
3	L	202	ASP	2.3
2	H	191	ALA	2.3
4	M	27	ASP	2.3
1	C	290	PRO	2.3
3	L	237	ALA	2.3
1	C	17	LEU	2.3
4	M	59	PHE	2.3
2	H	5	ALA	2.2
4	M	204	ILE	2.2
4	M	207	ALA	2.2
2	H	92	GLN	2.2
2	H	98	GLY	2.2
1	C	253	PHE	2.2
4	M	188	SER	2.2
3	L	51	TYR	2.2
2	H	6	LEU	2.2
3	L	234	LEU	2.2
4	M	260	ILE	2.2
1	C	4	PRO	2.1
1	C	246	PHE	2.1
3	L	181	PHE	2.1
2	H	163	VAL	2.1
3	L	19	GLY	2.1
3	L	241	PHE	2.0
3	L	120	ALA	2.0
4	M	181	ILE	2.0
4	M	222	LEU	2.0
1	C	267	ALA	2.0
1	C	287	ALA	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	0.69	0.32	-	31,36,49,51	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
13	PO4	M	1332	5/5	0.91	0.33	9.50	42,45,49,54	0
13	PO4	M	1331	5/5	0.81	0.27	5.07	50,52,60,61	0
12	NS5	M	1329	40/40	0.79	0.25	4.97	38,50,65,66	0
8	DGA	L	1277	37/44	0.52	0.35	4.28	54,66,76,76	0
9	MPG	L	1278	25/25	0.49	0.27	4.15	47,56,76,76	0
9	MPG	L	1279	25/25	0.78	0.28	3.22	34,43,48,49	25
9	MPG	M	1330	17/25	0.80	0.16	0.37	53,56,57,57	0
5	HEM	C	1333	43/43	0.97	0.12	0.10	26,30,32,33	0
7	BPB	M	1326	61/65	0.93	0.12	-0.34	19,25,56,58	0
5	HEM	C	1334	43/43	0.97	0.10	-0.50	23,26,32,35	0
11	MQ7	M	1328	48/48	0.93	0.11	-0.69	26,30,44,46	0
7	BPB	L	1276	65/65	0.95	0.09	-1.27	22,29,34,36	0
5	HEM	C	1336	43/43	0.97	0.09	-1.33	20,24,35,43	0
6	BCB	M	1324	65/66	0.95	0.11	-1.41	20,23,65,67	0
6	BCB	M	1325	66/66	0.96	0.09	-1.47	19,22,35,36	0
6	BCB	L	1275	66/66	0.95	0.10	-1.59	22,25,49,52	0
6	BCB	L	1274	66/66	0.96	0.10	-2.09	19,25,35,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	HEM	C	1335	43/43	0.98	0.08	-2.41	19,23,25,27	0
10	FE2	M	1327	1/1	1.00	0.03	-5.05	26,26,26,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.