



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2017 – 11:12 PM EDT

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
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) : rb-20029077

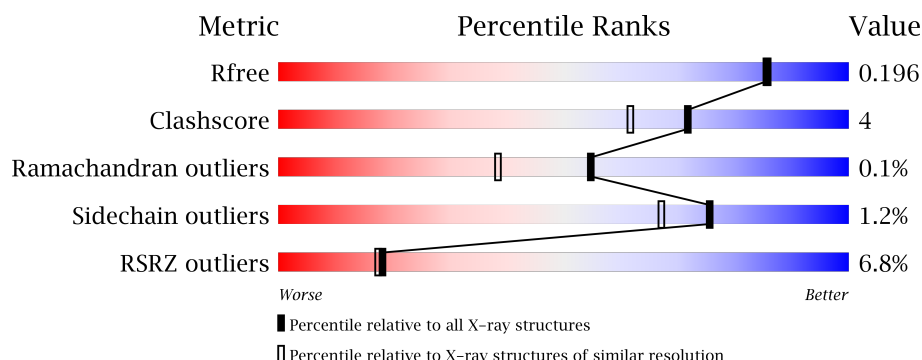
1 Overall quality at a glance

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}	100719	1923 (1.86-1.86)
Clashscore	112137	2083 (1.86-1.86)
Ramachandran outliers	110173	2060 (1.86-1.86)
Sidechain outliers	110143	2060 (1.86-1.86)
RSRZ outliers	101464	1932 (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 ≥ 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> <div></div> <div>93%</div> <div>6%</div> <div>.</div> </div> </div>
2	H	258	<div> <div>9%</div> <div> <div></div> <div>80%</div> <div>13%</div> <div>6%</div> <div>.</div> </div> </div>
3	L	274	<div> <div>9%</div> <div> <div></div> <div>95%</div> <div></div> <div>.</div> </div> </div>
4	M	324	<div> <div>5%</div> <div> <div></div> <div>95%</div> <div>5%</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	NS5	M	406	-	-	-	X
8	MPG	L	304	X	-	-	X
8	MPG	L	305	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.

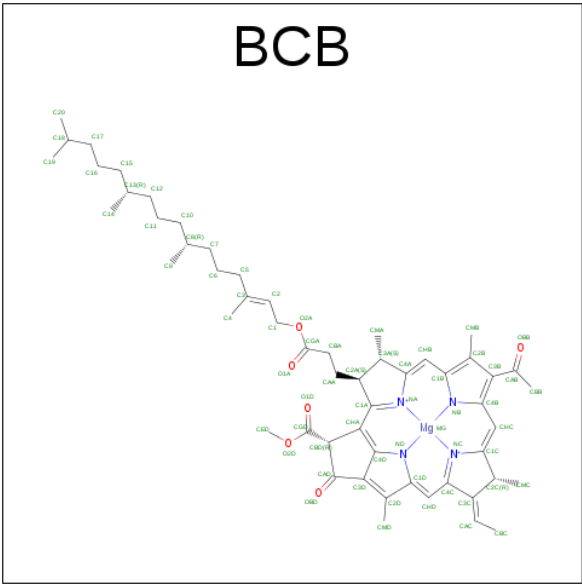
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	323	Total	C	N	O	S	0	0	0
			2548	1697	417	423	11			

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



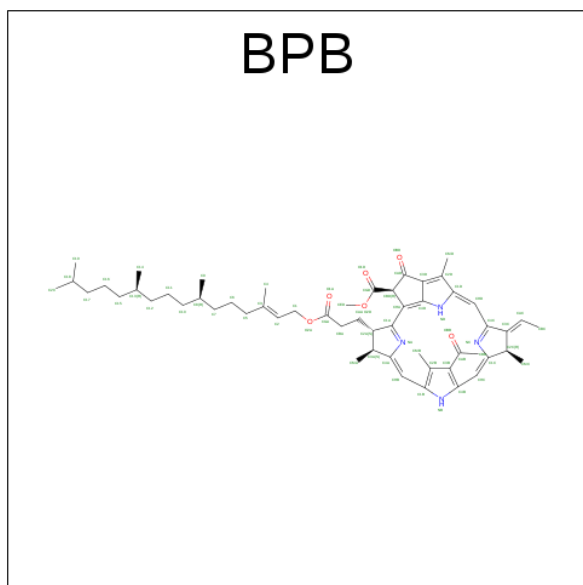
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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



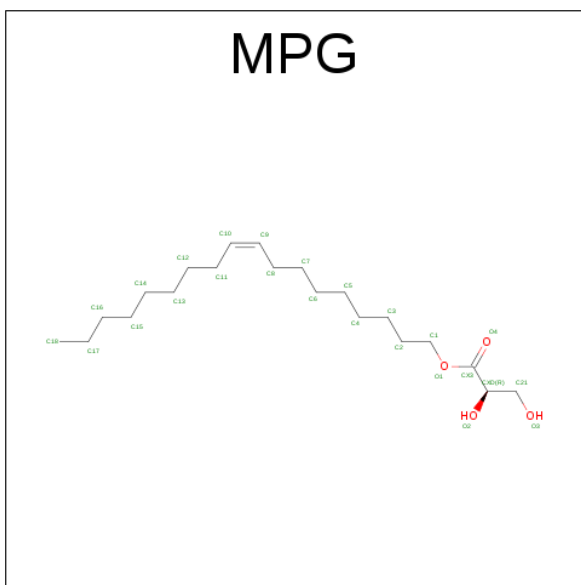
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
6	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
6	M	1	Total 65	C 54	Mg 1	N 4	O 6	0	0
6	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- 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 [(Z)-octadec-9-enyl] (2R)-2,3-bis(oxidanyl)propanoate (three-letter code: MPG) (formula: $C_{21}H_{40}O_4$).

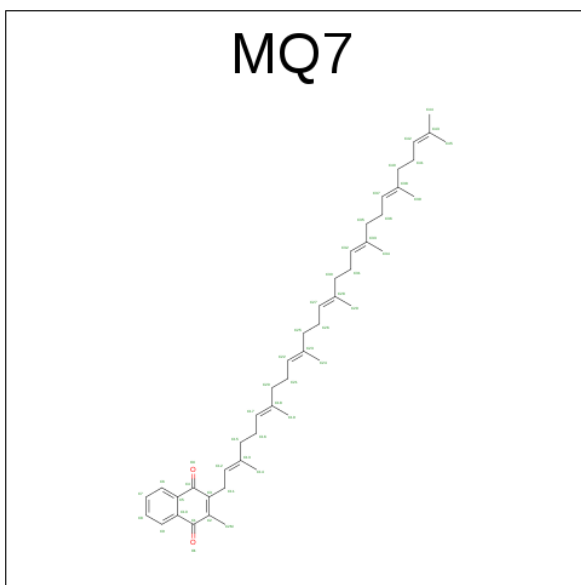


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	L	1	Total C O 21 17 4	0	0
8	L	1	Total C O 25 21 4	0	0
8	M	1	Total C 17 17	0	0

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

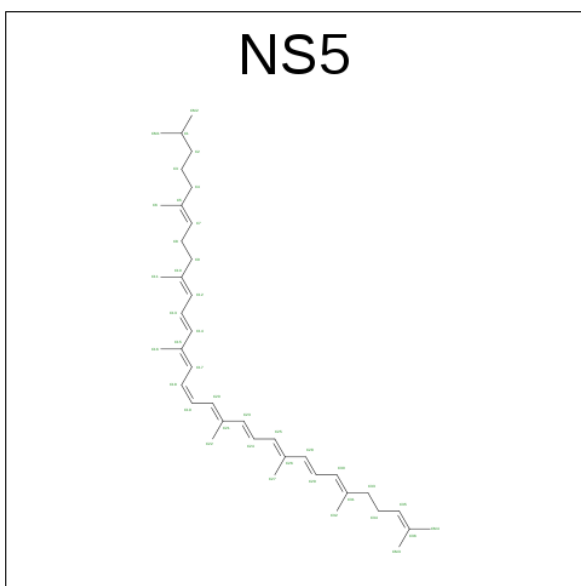
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	M	1	Total Fe 1 1	0	0

- Molecule 10 is MENAQUINONE-7 (three-letter code: MQ7) (formula: C₄₆H₆₄O₂).



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		

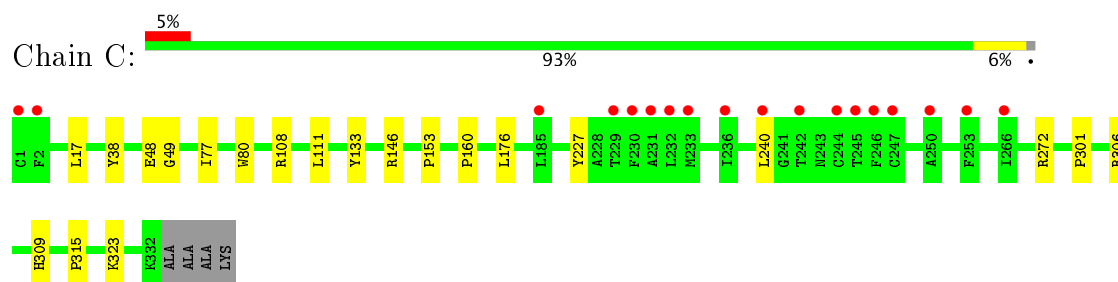
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	C	307	Total 307	O 307	0	0
12	H	149	Total 149	O 149	0	0
12	L	89	Total 89	O 89	0	0
12	M	147	Total 147	O 147	0	0

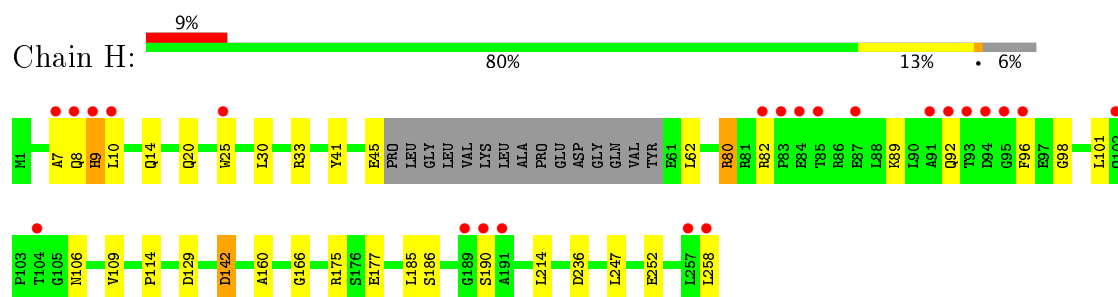
3 Residue-property plots [i](#)

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

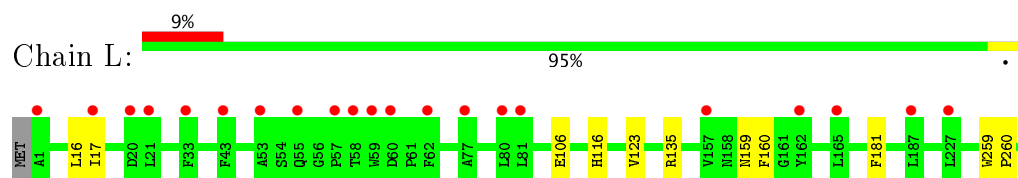
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER CYTOCHROME C SUBUNIT



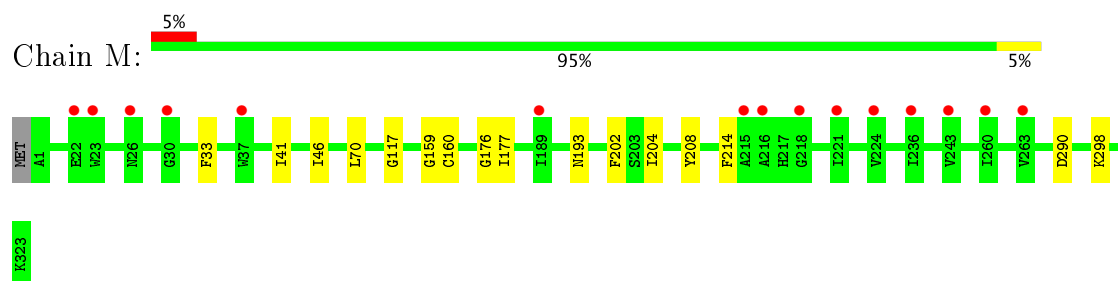
• Molecule 2: REACTION CENTER PROTEIN H CHAIN



• 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 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 1.86Å)	Xtriage
Refinement program	REFMAC	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 ²)	32.6	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 61.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10590	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	307	0	0	3	0
12	H	149	0	0	4	0
12	L	89	0	0	0	0
12	M	147	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:403:BPB:H14A	11:M:406:NS5:HM43	1.37	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:403:BPB:C14	11:M:406:NS5:HM43	1.94	0.97
7:M:403:BPB:HBBB	7:M:403:BPB:HHC	1.47	0.97
7:L:303:BPB:HHC	7:L:303: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:301:HOH:O	1.91	0.89
6:L:301:BCB:HMB1	6:L:301:BCB:HBB3	1.69	0.74
1:C:48:GLU:O	12:C:501:HOH:O	2.04	0.74
7:M:403:BPB:H14A	11:M:406:NS5:CM4	2.17	0.73
1:C:49:GLY:HA3	12:C:501:HOH:O	1.91	0.70
4:M:117:GLY:HA3	11:M:406:NS5:H92	1.75	0.69
7:L:303:BPB:HHC	7:L:303:BPB:CBB	2.23	0.65
6:M:401:BCB:HBB2	6:M:401:BCB:HHC	1.79	0.65
6:L:301:BCB:CBB	6:L:301: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:403:BPB:C14	11:M:406:NS5:CM4	2.77	0.60
8:L:305:MPG:O2	8:L:305:MPG:HX32	2.01	0.59
2:H:177:GLU:OE1	12:H:302:HOH:O	2.17	0.59
7:M:403:BPB:H14B	11:M:406:NS5:HM43	1.83	0.59
7:M:403:BPB:HBBB	7:M:403:BPB:CHC	2.27	0.59
3:L:181:PHE:CD2	7:M:403:BPB:HBB	2.39	0.58
3:L:181:PHE:HB3	7:M:403:BPB:HBBA	1.84	0.57
6:M:401:BCB:HHC	6:M:401:BCB:CBB	2.35	0.57
1:C:301:PRO:HG2	5:C:402:HEM:HBD1	1.87	0.56
8:L:305:MPG:O2	8:L:305:MPG:C1	2.54	0.55
6:M:402:BCB:CBB	6:M:402:BCB:HMB1	2.38	0.54
4:M:177:ILE:HD11	11:M:406:NS5:H273	1.90	0.53
4:M:70:LEU:HD21	11:M:406: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:406:NS5:C11	2.40	0.52
3:L:16:LEU:CD1	3:L:16:LEU:N	2.73	0.52
2:H:106:ASN:HB3	2:H:109:VAL:HG22	1.93	0.51
7:M:403:BPB:CBB	7:M:403:BPB:HHC	2.32	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:303:BPB:HBBA	4:M:208:TYR:HB3	1.93	0.50
7:L:303:BPB:HBB	4:M:208:TYR:CD2	2.47	0.50
2:H:142:ASP:CG	12:H:301:HOH:O	2.44	0.49
2:H:10:LEU:HA	2:H:14:GLN:OE1	2.13	0.48
6:M:402:BCB:HBB3	6:M:402:BCB:HMB1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:303:BPB:CHC	7:L:303:BPB:CBB	2.91	0.47
6:L:302:BCB:HMB1	6:L:302:BCB:CBB	2.43	0.47
3:L:181:PHE:HB3	7:M:403:BPB:CBB	2.46	0.46
3:L:259:TRP:N	3:L:260:PRO:CD	2.79	0.46
6:L:302:BCB:C14	7:L:303:BPB:H20B	2.46	0.45
6:L:302:BCB:HMB2	7:L:303:BPB:HMB A	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:428: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:304:MPG:H32C	2.53	0.44
6:L:302:BCB:HBB2	6:L:302:BCB:HMB1	1.99	0.44
2:H:9:HIS:CE1	4:M:298:LYS:HG3	2.53	0.43
1:C:323:LYS:HE2	12:C:744:HOH:O	2.18	0.43
2:H:9:HIS:CE1	4:M:298:LYS:HE3	2.54	0.43
7:M:403:BPB:CBB	7:M:403: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:302:BCB:H143	7:L:303: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:302:BCB:HMD1	4:M:204:ILE:HD13	2.03	0.41
7:L:303:BPB:NC	7:L:303:BPB:ND	2.67	0.41
2:H:160:ALA:HB3	2:H:214:LEU:HD23	2.03	0.41
2:H:96:PHE:CE2	2:H:98:GLY:N	2.88	0.41
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.56	0.41
7:M:403:BPB:HMC	7:M:403:BPB:HBCA	2.02	0.41
4:M:176:GLY:H	11:M:406:NS5:C23	2.34	0.41
3:L:16:LEU:HD12	3:L:16:LEU:N	2.35	0.41
6:L:301:BCB:HAA1	6:L:301:BCB:HBD	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%)	44	29
All	All	1161/1192 (97%)	1132 (98%)	28 (2%)	1 (0%)	55	38

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	91
2	H	194/212 (92%)	188 (97%)	6 (3%)	45	27
3	L	216/219 (99%)	214 (99%)	2 (1%)	82	77
4	M	247/250 (99%)	245 (99%)	2 (1%)	85	80
All	All	935/963 (97%)	924 (99%)	11 (1%)	75	67

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	9,9,10	1.02	2 (22%)	7,9,11	2.67	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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	FME	CA-C	2.02	1.52	1.50
2	H	1	FME	CN-N	2.06	1.40	1.33

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	-2.43	118.43	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 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	401	1	28,50,50	2.37	9 (32%)	17,82,82	1.76	4 (23%)
5	HEM	C	402	1	28,50,50	2.35	11 (39%)	17,82,82	1.88	5 (29%)
5	HEM	C	403	1	28,50,50	1.99	12 (42%)	17,82,82	1.53	4 (23%)
5	HEM	C	404	1	28,50,50	2.80	16 (57%)	17,82,82	1.73	4 (23%)
6	BCB	L	301	-	63,74,74	3.45	22 (34%)	50,115,115	2.29	15 (30%)
6	BCB	L	302	-	63,74,74	3.36	26 (41%)	50,115,115	2.02	11 (22%)
7	BPB	L	303	-	63,70,70	2.57	15 (23%)	67,101,101	2.14	20 (29%)
8	MPG	L	304	-	20,20,24	1.82	1 (5%)	19,21,25	1.92	5 (26%)
8	MPG	L	305	-	24,24,24	1.70	1 (4%)	23,25,25	1.25	3 (13%)
6	BCB	M	401	-	62,73,74	3.65	26 (41%)	48,113,115	1.95	8 (16%)
6	BCB	M	402	-	63,74,74	3.55	26 (41%)	50,115,115	2.26	13 (26%)
7	BPB	M	403	-	59,66,70	2.39	14 (23%)	62,96,101	1.96	14 (22%)
10	MQ7	M	405	-	49,49,49	1.45	3 (6%)	61,63,63	1.11	6 (9%)
11	NS5	M	406	-	39,39,39	2.12	6 (15%)	44,46,46	2.57	19 (43%)
8	MPG	M	407	-	16,16,24	0.33	0	15,15,25	0.48	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	401	1	-	0/6/54/54	0/0/8/8
5	HEM	C	402	1	-	0/6/54/54	0/0/8/8
5	HEM	C	403	1	-	0/6/54/54	0/0/8/8
5	HEM	C	404	1	-	0/6/54/54	0/0/8/8
6	BCB	L	301	-	-	0/41/177/177	0/0/9/9
6	BCB	L	302	-	-	0/41/177/177	0/0/9/9
7	BPB	L	303	-	-	0/47/105/105	0/1/6/6
8	MPG	L	304	-	1/1/2/4	0/21/21/25	0/0/0/0
8	MPG	L	305	-	1/1/2/4	1/25/25/25	0/0/0/0
6	BCB	M	401	-	-	0/40/176/177	0/0/9/9
6	BCB	M	402	-	-	0/41/177/177	0/0/9/9
7	BPB	M	403	-	-	0/43/101/105	0/1/6/6
10	MQ7	M	405	-	-	0/41/61/61	0/2/2/2
11	NS5	M	406	-	-	1/43/43/43	0/0/0/0
8	MPG	M	407	-	-	0/14/14/25	0/0/0/0

All (188) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	401	BCB	C3D-C4D	-15.81	1.36	1.54
6	M	402	BCB	C3D-C4D	-13.65	1.39	1.54
6	L	301	BCB	C3D-C4D	-12.43	1.40	1.54
6	L	302	BCB	C3D-C4D	-11.44	1.41	1.54
6	L	302	BCB	CHB-C4A	-8.74	1.31	1.52
6	M	401	BCB	C4B-NB	-8.26	1.32	1.50
6	L	301	BCB	CHD-C1D	-8.25	1.40	1.53
6	L	301	BCB	C3B-C4B	-8.03	1.45	1.54
6	L	302	BCB	C4D-ND	-7.98	1.33	1.50
6	M	402	BCB	C4B-NB	-7.97	1.33	1.50
6	M	401	BCB	C1D-ND	-7.63	1.33	1.50
6	L	302	BCB	C1D-ND	-7.29	1.34	1.50
6	L	301	BCB	C4D-ND	-7.12	1.35	1.50
6	M	402	BCB	C4D-ND	-7.03	1.35	1.50
6	L	302	BCB	C4B-NB	-6.98	1.35	1.50
6	M	401	BCB	C1B-NB	-6.91	1.35	1.50
6	M	402	BCB	CHB-C4A	-6.91	1.36	1.52
6	M	402	BCB	C3B-C4B	-6.80	1.46	1.54
6	M	401	BCB	CHD-C1D	-6.79	1.42	1.53
6	M	402	BCB	CHD-C1D	-6.77	1.42	1.53
6	M	402	BCB	C1D-ND	-6.71	1.35	1.50
6	L	301	BCB	CHB-C4A	-6.70	1.36	1.52
6	M	402	BCB	C1B-NB	-6.53	1.36	1.50
6	M	401	BCB	CHB-C4A	-6.51	1.37	1.52
6	M	402	BCB	CHB-C1B	-6.47	1.43	1.53
6	L	301	BCB	C1D-ND	-6.42	1.36	1.50
6	L	301	BCB	C1B-NB	-6.23	1.36	1.50
6	L	302	BCB	CHD-C1D	-6.19	1.43	1.53
6	L	301	BCB	C4B-NB	-6.11	1.37	1.50
6	L	301	BCB	CHB-C1B	-6.05	1.43	1.53
11	M	406	NS5	C9-C8	-5.78	1.33	1.53
6	L	301	BCB	C1A-CHA	-5.67	1.44	1.53
6	L	302	BCB	C1B-NB	-5.56	1.38	1.50
6	M	401	BCB	C4D-ND	-5.53	1.38	1.50
6	M	402	BCB	C1A-CHA	-5.40	1.45	1.53
6	M	401	BCB	C3B-C4B	-5.29	1.48	1.54
6	L	302	BCB	C3B-C4B	-5.27	1.48	1.54
6	M	402	BCB	CHD-C4C	-5.17	1.44	1.53
6	L	302	BCB	CHB-C1B	-5.13	1.45	1.53
5	C	404	HEM	C3B-C2B	-5.00	1.33	1.40
6	M	401	BCB	C2D-C1D	-5.00	1.43	1.53
6	M	401	BCB	CHD-C4C	-4.88	1.44	1.53
6	M	401	BCB	C4A-C3A	-4.78	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	401	BCB	C3B-C2B	-4.38	1.43	1.55
6	M	402	BCB	C2D-C1D	-4.17	1.45	1.53
6	M	401	BCB	CHC-C4B	-4.14	1.47	1.53
6	L	302	BCB	C3B-CAB	-4.12	1.47	1.52
6	M	401	BCB	CHB-C1B	-4.10	1.47	1.53
5	C	401	HEM	C3C-C2C	-4.08	1.35	1.40
5	C	404	HEM	C3C-C2C	-4.07	1.35	1.40
7	M	403	BPB	C4C-NC	-4.05	1.27	1.36
6	L	302	BCB	CHD-C4C	-3.93	1.46	1.53
6	L	301	BCB	C3D-CAD	-3.85	1.44	1.51
6	L	301	BCB	C2D-C1D	-3.78	1.45	1.53
6	L	302	BCB	C2D-C1D	-3.74	1.45	1.53
6	M	401	BCB	C1A-CHA	-3.70	1.48	1.53
6	L	302	BCB	C4A-C3A	-3.70	1.49	1.53
6	M	401	BCB	CBD-CAD	-3.65	1.47	1.53
6	L	302	BCB	C1A-CHA	-3.55	1.48	1.53
5	C	402	HEM	C3B-C2B	-3.51	1.35	1.40
7	L	303	BPB	C1A-NA	-3.50	1.29	1.36
6	L	302	BCB	C3B-C2B	-3.40	1.46	1.55
6	L	302	BCB	CBD-CAD	-3.38	1.48	1.53
6	M	402	BCB	CBD-CAD	-3.31	1.48	1.53
6	L	301	BCB	C3B-C2B	-3.31	1.46	1.55
6	L	301	BCB	C3D-C2D	-3.30	1.46	1.55
6	M	402	BCB	CHA-CBD	-3.28	1.45	1.53
6	M	401	BCB	C3D-CAD	-3.26	1.45	1.51
6	L	301	BCB	CHD-C4C	-3.25	1.47	1.53
6	M	402	BCB	C3B-C2B	-3.22	1.46	1.55
5	C	403	HEM	C3B-C2B	-3.17	1.36	1.40
5	C	401	HEM	C3B-C2B	-3.16	1.36	1.40
6	M	401	BCB	C3D-C2D	-3.13	1.46	1.55
6	L	302	BCB	C3D-C2D	-3.09	1.47	1.55
6	M	402	BCB	C3D-C2D	-3.02	1.47	1.55
6	L	302	BCB	C2B-C1B	-3.02	1.47	1.53
6	L	301	BCB	CBD-CAD	-3.02	1.48	1.53
7	M	403	BPB	C1A-NA	-2.96	1.30	1.36
6	L	302	BCB	CHC-C4B	-2.91	1.49	1.53
5	C	403	HEM	C3C-C2C	-2.89	1.36	1.40
6	M	402	BCB	C2B-C1B	-2.83	1.47	1.53
6	M	401	BCB	CBD-CGD	-2.71	1.47	1.52
6	M	401	BCB	C2B-C1B	-2.69	1.47	1.53
6	L	301	BCB	CHC-C4B	-2.69	1.49	1.53
6	M	402	BCB	CHC-C4B	-2.68	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	402	BCB	C3D-CAD	-2.63	1.46	1.51
5	C	404	HEM	C1D-CHD	-2.52	1.33	1.40
6	L	302	BCB	C3D-CAD	-2.51	1.46	1.51
7	M	403	BPB	CBB-CAB	-2.51	1.41	1.49
6	L	301	BCB	CHC-C1C	-2.42	1.46	1.52
5	C	402	HEM	C3C-C2C	-2.39	1.37	1.40
6	M	402	BCB	CHC-C1C	-2.33	1.47	1.52
6	L	302	BCB	CBD-CGD	-2.32	1.48	1.52
6	L	301	BCB	C2B-C1B	-2.26	1.48	1.53
7	L	303	BPB	C4C-NC	-2.24	1.31	1.36
6	M	402	BCB	CMB-C2B	-2.22	1.48	1.53
7	M	403	BPB	C1D-ND	-2.22	1.33	1.38
6	L	302	BCB	CHC-C1C	-2.21	1.47	1.52
6	M	401	BCB	C2A-C3A	-2.12	1.50	1.55
6	M	401	BCB	CHC-C1C	-2.12	1.47	1.52
6	M	402	BCB	C3B-CAB	-2.09	1.49	1.52
7	L	303	BPB	CBB-CAB	-2.09	1.43	1.49
5	C	403	HEM	C1B-NB	2.01	1.39	1.36
5	C	404	HEM	C1B-NB	2.05	1.39	1.36
5	C	403	HEM	C4A-NA	2.06	1.40	1.36
7	L	303	BPB	C4B-CHC	2.15	1.48	1.40
11	M	406	NS5	C30-C31	2.15	1.36	1.34
5	C	403	HEM	CMC-C2C	2.18	1.56	1.51
7	M	403	BPB	C3B-C2B	2.20	1.44	1.39
5	C	403	HEM	CMA-C3A	2.24	1.56	1.51
5	C	404	HEM	C1A-NA	2.25	1.40	1.36
5	C	404	HEM	CMA-C3A	2.25	1.56	1.51
11	M	406	NS5	C28-C26	2.26	1.50	1.45
5	C	403	HEM	CMD-C2D	2.27	1.56	1.51
5	C	401	HEM	CMB-C2B	2.29	1.56	1.51
7	L	303	BPB	C1B-CHB	2.33	1.49	1.40
10	M	405	MQ7	O4-C4	2.34	1.28	1.23
5	C	404	HEM	C4D-ND	2.39	1.39	1.36
7	L	303	BPB	CHD-C4C	2.43	1.46	1.40
6	M	401	BCB	O2A-CGA	2.48	1.40	1.33
6	L	302	BCB	O2A-CGA	2.51	1.40	1.33
5	C	403	HEM	CAA-C2A	2.52	1.56	1.52
7	M	403	BPB	CHD-C4C	2.56	1.46	1.40
7	L	303	BPB	OBD-CAD	2.59	1.27	1.22
7	M	403	BPB	C1B-CHB	2.59	1.50	1.40
5	C	404	HEM	CMD-C2D	2.60	1.56	1.51
5	C	403	HEM	CMB-C2B	2.65	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	402	HEM	CMD-C2D	2.69	1.57	1.51
7	L	303	BPB	O2D-CGD	2.77	1.40	1.33
6	M	402	BCB	O2A-CGA	2.78	1.41	1.33
5	C	402	HEM	CAA-C2A	2.82	1.56	1.52
5	C	404	HEM	CMB-C2B	2.82	1.57	1.51
5	C	404	HEM	C4A-NA	2.84	1.42	1.36
5	C	401	HEM	C1D-ND	2.86	1.42	1.36
5	C	402	HEM	C4C-NC	2.87	1.40	1.36
6	M	401	BCB	OBD-CAD	2.88	1.26	1.21
11	M	406	NS5	C29-C30	2.98	1.52	1.43
7	L	303	BPB	OBB-CAB	3.02	1.32	1.22
7	M	403	BPB	O2D-CGD	3.03	1.40	1.33
7	M	403	BPB	C3D-C2D	3.03	1.46	1.38
5	C	402	HEM	CMB-C2B	3.05	1.58	1.51
5	C	403	HEM	C3B-CAB	3.06	1.54	1.47
7	L	303	BPB	CHD-C1D	3.08	1.44	1.38
5	C	402	HEM	CMA-C3A	3.08	1.57	1.51
5	C	401	HEM	C1B-NB	3.09	1.40	1.36
5	C	401	HEM	C3B-CAB	3.18	1.54	1.47
7	L	303	BPB	C3D-C2D	3.18	1.47	1.38
5	C	403	HEM	C3C-CAC	3.20	1.54	1.47
7	M	403	BPB	OBD-CAD	3.27	1.28	1.22
6	L	302	BCB	O2D-CGD	3.28	1.41	1.33
7	L	303	BPB	C3B-C2B	3.35	1.47	1.39
7	L	303	BPB	O2A-CGA	3.35	1.43	1.33
7	M	403	BPB	CHD-C1D	3.40	1.45	1.38
6	M	401	BCB	CAC-C3C	3.41	1.44	1.33
5	C	404	HEM	CAA-C2A	3.42	1.57	1.52
6	M	402	BCB	O2D-CGD	3.50	1.42	1.33
7	M	403	BPB	O2A-CGA	3.58	1.43	1.33
5	C	404	HEM	C3B-CAB	3.63	1.55	1.47
6	M	401	BCB	O2D-CGD	3.82	1.42	1.33
5	C	402	HEM	C3B-CAB	3.85	1.55	1.47
6	L	301	BCB	O2D-CGD	3.87	1.43	1.33
5	C	401	HEM	CMA-C3A	3.91	1.59	1.51
5	C	402	HEM	C4A-NA	3.94	1.44	1.36
6	M	402	BCB	CAC-C3C	4.09	1.46	1.33
5	C	403	HEM	C3D-C2D	4.26	1.50	1.37
6	L	301	BCB	CAC-C3C	4.27	1.47	1.33
6	L	302	BCB	CAC-C3C	4.47	1.48	1.33
5	C	402	HEM	C3D-C2D	4.52	1.51	1.37
5	C	404	HEM	C3D-C2D	4.54	1.51	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	404	HEM	C1C-NC	4.56	1.42	1.36
6	L	302	BCB	OBD-CAD	4.77	1.29	1.21
5	C	404	HEM	C4C-NC	4.83	1.42	1.36
5	C	401	HEM	C3D-C2D	5.04	1.52	1.37
10	M	405	MQ7	C10-C5	5.07	1.49	1.40
6	M	402	BCB	OBD-CAD	5.13	1.30	1.21
5	C	404	HEM	C3C-CAC	5.20	1.58	1.47
5	C	402	HEM	C3C-CAC	5.29	1.58	1.47
7	M	403	BPB	C3B-C4B	5.38	1.48	1.41
5	C	401	HEM	C3C-CAC	5.80	1.59	1.47
6	L	301	BCB	OBD-CAD	5.86	1.31	1.21
10	M	405	MQ7	C3-C2	6.56	1.49	1.35
7	L	303	BPB	C3B-C4B	6.97	1.50	1.41
11	M	406	NS5	C29-C28	7.02	1.52	1.34
11	M	406	NS5	C35-C36	7.41	1.54	1.32
8	L	305	MPG	O1-CX3	7.60	1.48	1.33
8	L	304	MPG	O1-CX3	7.66	1.49	1.33
7	M	403	BPB	CAC-C3C	12.96	1.48	1.33
7	L	303	BPB	CAC-C3C	15.28	1.51	1.33

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	303	BPB	C2C-C3C-C4C	-6.33	101.21	107.35
7	M	403	BPB	CBC-CAC-C3C	-6.04	113.69	127.00
11	M	406	NS5	C29-C28-C26	-5.88	109.90	126.42
7	M	403	BPB	C2C-C3C-C4C	-5.88	101.66	107.35
6	L	301	BCB	OBD-CAD-C3D	-5.80	116.65	126.75
6	M	402	BCB	O2D-CGD-O1D	-5.50	112.76	123.82
7	L	303	BPB	CBC-CAC-C3C	-4.90	116.20	127.00
11	M	406	NS5	C34-C35-C36	-4.89	110.34	127.80
6	M	402	BCB	CHA-CBD-CGD	-4.87	103.71	115.00
5	C	401	HEM	CBD-CAD-C3D	-4.73	103.44	112.47
7	L	303	BPB	CHD-C4C-C3C	-4.51	117.95	125.26
6	L	301	BCB	C1-C2-C3	-4.43	117.80	125.96
6	L	301	BCB	CHA-CBD-CGD	-4.06	105.58	115.00
6	L	302	BCB	CBA-CAA-C2A	-4.06	110.16	115.76
6	M	402	BCB	OBD-CAD-C3D	-4.03	119.73	126.75
11	M	406	NS5	CM4-C36-C35	-3.90	110.89	122.65
11	M	406	NS5	C18-C17-C15	-3.80	121.89	127.31
6	L	302	BCB	OBD-CAD-C3D	-3.79	120.16	126.75
11	M	406	NS5	C24-C25-C26	-3.73	121.98	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	304	MPG	O4-CX3-CXD	-3.63	114.81	123.60
5	C	402	HEM	C3B-C4B-NB	-3.55	104.62	109.21
11	M	406	NS5	CM3-C36-C35	-3.53	111.99	122.65
7	M	403	BPB	OBD-CAD-C3D	-3.50	119.82	128.43
7	M	403	BPB	CBB-CAB-C3B	-3.46	110.33	120.39
11	M	406	NS5	C16-C15-C14	-3.43	112.64	118.10
5	C	404	HEM	C1D-C2D-C3D	-3.42	104.61	107.00
6	M	401	BCB	CBA-CAA-C2A	-3.41	111.06	115.76
7	L	303	BPB	C1-C2-C3	-3.13	120.19	125.96
7	L	303	BPB	OBD-CAD-C3D	-3.11	120.78	128.43
5	C	403	HEM	C3B-C4B-NB	-3.05	105.27	109.21
10	M	405	MQ7	C26-C27-C28	-3.02	120.10	127.68
7	L	303	BPB	CBB-CAB-C3B	-3.02	111.62	120.39
11	M	406	NS5	C23-C21-C20	-2.98	114.36	118.94
5	C	404	HEM	C3B-C4B-NB	-2.92	105.43	109.21
7	L	303	BPB	CMD-C2D-C3D	-2.92	120.79	127.86
6	M	401	BCB	OBD-CAD-C3D	-2.83	121.83	126.75
6	L	301	BCB	O2D-CGD-O1D	-2.80	118.18	123.82
5	C	402	HEM	CBA-CAA-C2A	-2.74	107.24	112.48
5	C	404	HEM	CMA-C3A-C4A	-2.66	124.37	128.46
11	M	406	NS5	C8-C7-C5	-2.66	121.01	127.68
8	L	305	MPG	O3-C21-CXD	-2.61	105.10	111.97
11	M	406	NS5	C30-C29-C28	-2.54	115.45	123.23
6	L	302	BCB	O1D-CGD-CBD	-2.53	119.31	124.53
8	L	304	MPG	O3-C21-CXD	-2.50	105.37	111.97
6	L	301	BCB	OBB-CAB-C3B	-2.47	118.91	121.55
5	C	402	HEM	C1D-C2D-C3D	-2.47	105.28	107.00
7	M	403	BPB	O2D-CGD-O1D	-2.47	118.85	123.82
5	C	404	HEM	CAD-CBD-CGD	-2.46	108.45	112.66
7	L	303	BPB	O2A-CGA-O1A	-2.44	117.48	123.55
11	M	406	NS5	C22-C21-C23	-2.36	114.35	118.10
11	M	406	NS5	C24-C23-C21	-2.34	119.85	126.42
7	L	303	BPB	O2D-CGD-O1D	-2.30	119.19	123.82
5	C	403	HEM	C3C-C4C-NC	-2.25	106.70	110.94
10	M	405	MQ7	C44-C43-C42	-2.20	116.01	122.65
6	L	301	BCB	C15-C13-C12	-2.19	101.60	112.10
5	C	401	HEM	C1D-C2D-C3D	-2.18	105.48	107.00
5	C	401	HEM	C3C-C4C-NC	-2.13	106.93	110.94
6	L	302	BCB	C4A-C3A-C2A	-2.07	100.70	103.86
7	L	303	BPB	C4D-ND-C1D	-2.04	103.29	106.98
7	M	403	BPB	C1-C2-C3	-2.00	122.27	125.96
7	L	303	BPB	C2D-C1D-ND	2.03	112.83	109.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	405	MQ7	C34-C33-C35	2.04	118.82	115.29
6	L	302	BCB	C1-O2A-CGA	2.05	121.68	116.77
10	M	405	MQ7	C19-C18-C20	2.05	118.84	115.29
7	L	303	BPB	C3C-C2C-C1C	2.06	103.48	100.59
6	M	401	BCB	CHC-C4B-C3B	2.07	123.20	118.09
5	C	403	HEM	CMC-C2C-C3C	2.10	128.79	124.89
6	M	402	BCB	CHD-C1D-C2D	2.10	122.81	116.99
5	C	403	HEM	C4C-C3C-C2C	2.10	108.37	106.90
10	M	405	MQ7	C39-C38-C40	2.11	118.94	115.29
5	C	402	HEM	CMB-C2B-C3B	2.12	128.83	124.89
7	M	403	BPB	CMB-C2B-C3B	2.13	128.85	124.89
6	M	402	BCB	CMD-C2D-C3D	2.17	119.75	114.27
7	M	403	BPB	CBD-CAD-C3D	2.17	111.53	107.56
6	L	301	BCB	CHB-C4A-C3A	2.20	123.06	117.08
10	M	405	MQ7	C45-C43-C44	2.21	119.76	114.60
6	L	302	BCB	CHD-C1D-C2D	2.24	123.20	116.99
7	M	403	BPB	C4-C3-C5	2.31	119.29	115.29
11	M	406	NS5	C6-C5-C4	2.33	119.33	115.29
11	M	406	NS5	C9-C8-C7	2.40	120.19	111.97
7	L	303	BPB	CAD-C3D-C2D	2.41	152.41	140.80
7	L	303	BPB	CBD-CAD-C3D	2.47	112.09	107.56
6	L	302	BCB	O2D-CGD-CBD	2.51	117.34	111.20
7	M	403	BPB	CAD-C3D-C2D	2.54	153.07	140.80
6	L	301	BCB	O2D-CGD-CBD	2.63	117.62	111.20
7	M	403	BPB	OBB-CAB-C3B	2.67	125.04	119.95
6	M	402	BCB	CHC-C4B-C3B	2.70	124.76	118.09
11	M	406	NS5	C11-C10-C9	2.70	119.97	115.29
6	M	402	BCB	CBB-CAB-C3B	2.70	119.59	116.82
8	L	305	MPG	O1-C1-C2	2.75	118.43	108.73
6	L	301	BCB	CHC-C4B-C3B	2.82	125.06	118.09
7	L	303	BPB	O2D-CGD-CBD	2.82	116.35	111.30
6	L	302	BCB	CMD-C2D-C3D	2.84	121.45	114.27
6	M	402	BCB	O2D-CGD-CBD	2.86	118.19	111.20
8	L	305	MPG	O2-CXD-CX3	2.92	117.61	109.29
6	M	402	BCB	C4-C3-C5	2.96	120.42	115.29
5	C	401	HEM	CMC-C2C-C3C	2.96	130.38	124.89
6	M	401	BCB	CMD-C2D-C3D	3.07	122.05	114.27
11	M	406	NS5	C16-C15-C17	3.09	127.25	122.92
7	L	303	BPB	OBB-CAB-C3B	3.12	125.89	119.95
6	M	402	BCB	C1-O2A-CGA	3.13	124.28	116.77
7	M	403	BPB	O2D-CGD-CBD	3.14	116.90	111.30
7	L	303	BPB	C3C-C4C-NC	3.32	115.20	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	304	MPG	O2-CXD-C21	3.32	117.46	110.00
7	L	303	BPB	CED-O2D-CGD	3.35	123.82	115.97
5	C	402	HEM	CMC-C2C-C3C	3.59	131.56	124.89
8	L	304	MPG	O2-CXD-CX3	3.64	119.65	109.29
6	M	401	BCB	CBB-CAB-C3B	3.69	120.60	116.82
6	M	401	BCB	C1D-CHD-C4C	3.72	120.31	112.37
11	M	406	NS5	C18-C19-C20	3.80	131.57	123.46
6	L	301	BCB	C1D-CHD-C4C	3.80	120.48	112.37
7	M	403	BPB	CMD-C2D-C1D	4.04	131.34	125.04
6	L	301	BCB	CMD-C2D-C3D	4.13	124.73	114.27
6	L	301	BCB	C4-C3-C5	4.23	122.63	115.29
6	L	301	BCB	CBB-CAB-C3B	4.24	121.17	116.82
6	L	302	BCB	C3B-C4B-NB	4.30	111.36	103.57
8	L	304	MPG	C1-O1-CX3	4.51	126.23	116.64
6	M	402	BCB	C1D-CHD-C4C	4.58	122.14	112.37
6	L	301	BCB	C3B-C4B-NB	4.93	112.50	103.57
6	M	401	BCB	C3B-C4B-NB	5.02	112.66	103.57
6	L	302	BCB	C1D-CHD-C4C	5.05	123.14	112.37
11	M	406	NS5	C19-C18-C17	5.14	134.43	123.46
6	M	402	BCB	C3B-C4B-NB	5.25	113.08	103.57
6	L	301	BCB	CMB-C2B-C3B	5.43	128.00	114.27
7	L	303	BPB	C2A-C1A-NA	5.80	112.74	107.83
7	L	303	BPB	CMD-C2D-C1D	5.84	134.14	125.04
7	M	403	BPB	C2A-C1A-NA	5.90	112.83	107.83
11	M	406	NS5	C22-C21-C20	5.93	131.23	122.92
6	M	402	BCB	CMB-C2B-C3B	6.88	131.68	114.27
6	M	401	BCB	CMB-C2B-C3B	7.43	133.08	114.27
6	L	302	BCB	CMB-C2B-C3B	7.53	133.32	114.27

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	L	305	MPG	CXD
8	L	304	MPG	CXD

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	M	406	NS5	C30-C29-C28-C26
8	L	305	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	402	HEM	1	0
6	L	301	BCB	3	0
6	L	302	BCB	6	0
7	L	303	BPB	9	0
8	L	304	MPG	1	0
8	L	305	MPG	2	0
6	M	401	BCB	2	0
6	M	402	BCB	2	0
7	M	403	BPB	13	0
11	M	406	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	C	332/336 (98%)	0.15	18 (5%) 26 26	31, 35, 44, 69	0
2	H	242/258 (93%)	0.30	23 (9%) 9 8	28, 35, 48, 65	0
3	L	273/274 (99%)	0.36	24 (8%) 11 10	31, 35, 46, 59	0
4	M	323/324 (99%)	0.12	15 (4%) 33 32	32, 35, 44, 52	0
All	All	1170/1192 (98%)	0.22	80 (6%) 18 17	28, 35, 46, 69	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	CYS	6.9
2	H	7	ALA	6.4
2	H	9	HIS	6.2
2	H	258	LEU	6.1
3	L	59	TRP	5.7
2	H	85	THR	5.6
2	H	8	GLN	5.6
2	H	93	THR	5.2
2	H	94	ASP	5.0
2	H	96	PHE	4.7
2	H	91	ALA	4.6
1	C	2	PHE	4.4
3	L	271	PHE	4.4
2	H	83	PRO	4.3
3	L	21	LEU	4.0
1	C	244	CYS	3.7
2	H	191	ALA	3.5
3	L	165	LEU	3.5
3	L	58	THR	3.5
2	H	92	GLN	3.3
2	H	10	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
3	L	80	LEU	3.1
1	C	236	ILE	3.1
3	L	162	TYR	3.1
3	L	81	LEU	3.1
2	H	95	GLY	3.1
4	M	260	ILE	3.0
2	H	84	GLU	3.0
4	M	26	ASN	3.0
2	H	87	GLU	2.9
4	M	37	TRP	2.9
1	C	230	PHE	2.9
4	M	243	VAL	2.9
1	C	246	PHE	2.9
3	L	20	ASP	2.8
2	H	25	TRP	2.8
3	L	1	ALA	2.8
1	C	250	ALA	2.7
1	C	253	PHE	2.7
2	H	102	GLN	2.7
4	M	224	VAL	2.6
4	M	22	GLU	2.6
1	C	229	THR	2.6
4	M	221	ILE	2.6
3	L	55	GLN	2.6
3	L	60	ASP	2.5
3	L	270	PRO	2.5
1	C	240	LEU	2.5
2	H	189	GLY	2.5
2	H	257	LEU	2.5
1	C	242	THR	2.5
4	M	30	GLY	2.4
1	C	245	THR	2.4
3	L	53	ALA	2.4
2	H	82	ARG	2.3
3	L	187	LEU	2.3
1	C	185	LEU	2.3
3	L	57	PRO	2.3
3	L	33	PHE	2.3
3	L	62	PHE	2.3
4	M	216	ALA	2.3
2	H	190	SER	2.2
2	H	104	THR	2.2

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Mol	Chain	Res	Type	RSRZ
3	L	77	ALA	2.2
4	M	236	ILE	2.2
4	M	23	TRP	2.2
4	M	218	GLY	2.2
4	M	263	VAL	2.2
3	L	273	SER	2.2
4	M	215	ALA	2.1
3	L	157	VAL	2.1
4	M	189	ILE	2.1
1	C	232	LEU	2.1
1	C	266	ILE	2.1
3	L	17	ILE	2.0
3	L	227	LEU	2.0
1	C	231	ALA	2.0
3	L	43	PHE	2.0
1	C	233	MET	2.0
1	C	247	CYS	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	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 [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, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
11	NS5	M	406	40/40	0.76	0.24	5.91	42,62,77,77	0
8	MPG	L	305	25/25	0.73	0.25	4.64	36,47,54,54	25
8	MPG	L	304	21/25	0.66	0.20	2.70	56,63,69,71	0
8	MPG	M	407	17/25	0.74	0.19	1.27	62,64,65,65	0
5	HEM	C	402	43/43	0.98	0.08	-0.05	27,30,37,38	0
5	HEM	C	401	43/43	0.98	0.09	-0.40	28,32,37,41	0
7	BPB	M	403	61/65	0.95	0.09	-0.53	17,28,59,62	0
6	BCB	M	401	65/66	0.94	0.11	-0.59	23,27,73,75	0
10	MQ7	M	405	48/48	0.93	0.10	-0.90	28,34,53,57	0
7	BPB	L	303	65/65	0.95	0.08	-1.01	22,31,37,40	0
5	HEM	C	404	43/43	0.97	0.07	-1.08	20,27,36,48	0
6	BCB	M	402	66/66	0.97	0.07	-1.42	20,26,37,39	0
6	BCB	L	302	66/66	0.96	0.08	-1.53	22,27,51,56	0
6	BCB	L	301	66/66	0.96	0.07	-1.75	19,26,38,42	0
5	HEM	C	403	43/43	0.99	0.08	-2.43	21,25,27,29	0
9	FE2	M	404	1/1	1.00	0.02	-7.03	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.