



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:55 AM GMT

PDB ID : 2JBL
Title : PHOTOSYNTHETIC REACTION CENTER FROM BLASTOCHLORIS VIRIDIS
Authors : Lancaster, C.R.D.
Deposited on : 2006-12-08
Resolution : 2.40 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 (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

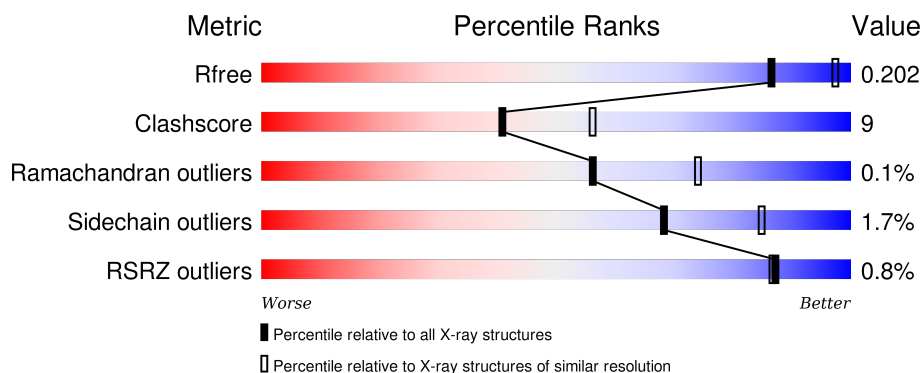
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	356	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>7%</div> </div> </div>
2	H	258	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>16%</div> </div> </div>
3	L	273	<div> <div></div> <div> <div></div> <div>87%</div> <div>13%</div> </div> </div>
4	M	323	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>17%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	NS5	M	1328	-	-	-	X
6	LDA	H	1259	-	-	-	X
6	LDA	M	1330	-	-	-	X
6	LDA	M	1331	-	-	-	X
6	LDA	M	1332	-	-	-	X
6	LDA	M	1333	-	-	-	X
8	BCB	M	1324	X	-	-	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 10512 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	51	2	0
			2618	1648	471	481	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	258	Total	C	N	O	S	124	0	0
			2018	1292	344	380	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	14	0	0
			2171	1459	350	355	7			

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

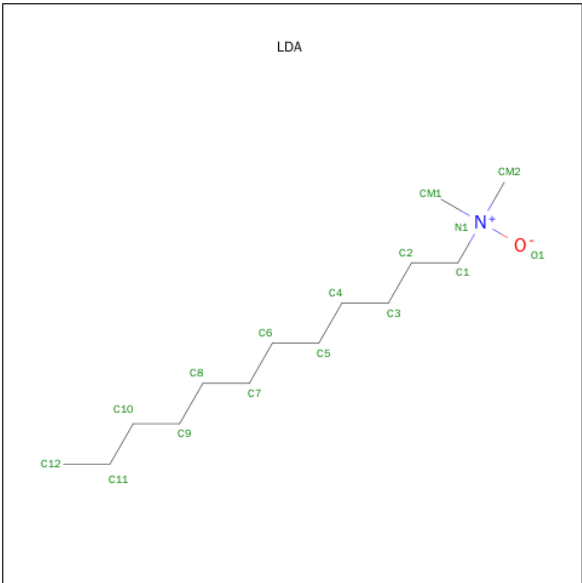
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	323	Total	C	N	O	S	19	0	0
			2555	1702	419	423	11			

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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 LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C₁₄H₃₁NO).



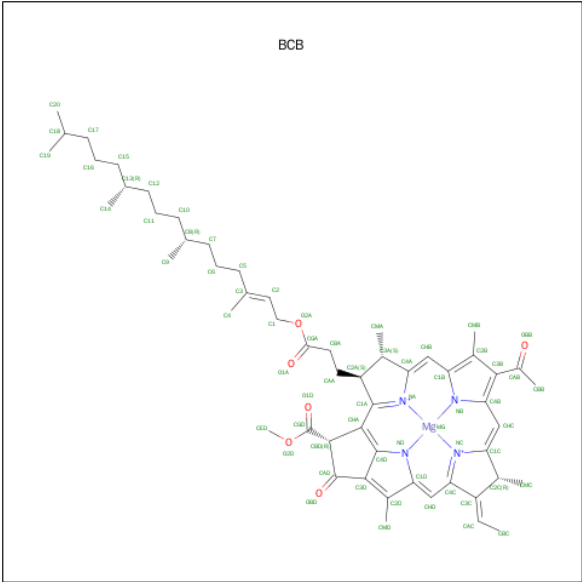
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	H	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	5	0
			16	14	1	1		
6	M	1	Total	C	N	O	4	0
			16	14	1	1		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



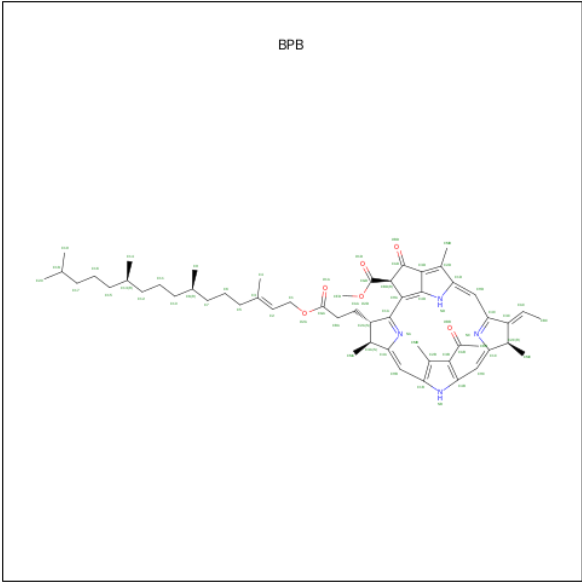
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	H	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		

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



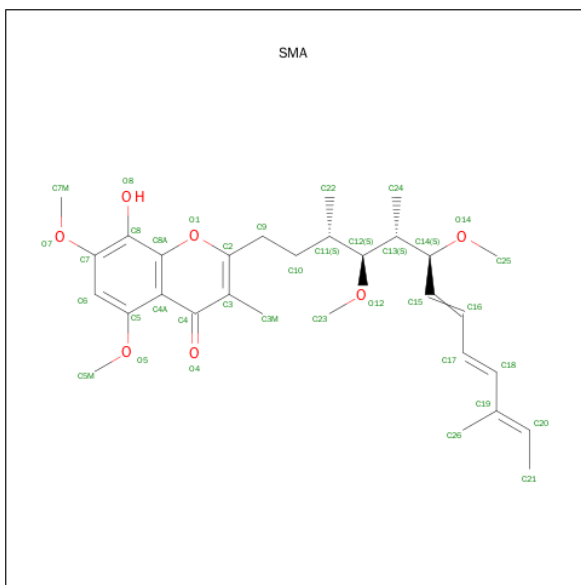
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
8	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
8	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
8	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 9 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula: C₅₅H₇₄N₄O₆).



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

- Molecule 10 is STIGMATELLIN A (three-letter code: SMA) (formula: $\text{C}_{30}\text{H}_{42}\text{O}_7$).

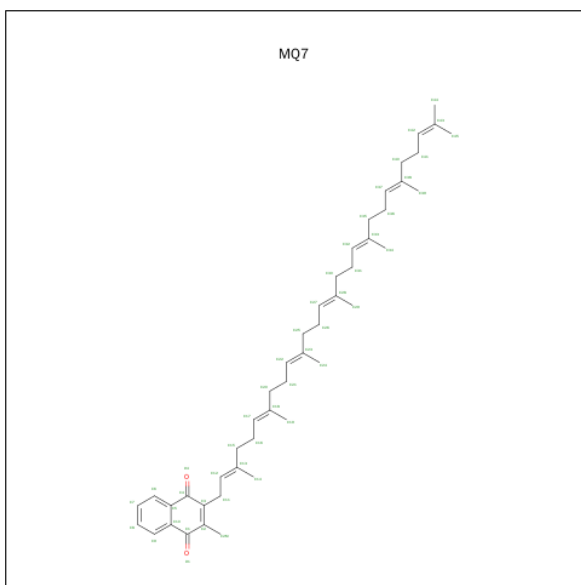


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	C	O	0	0
			37	30	7		

- Molecule 11 is FE (III) ION (three-letter code: FE) (formula: Fe).

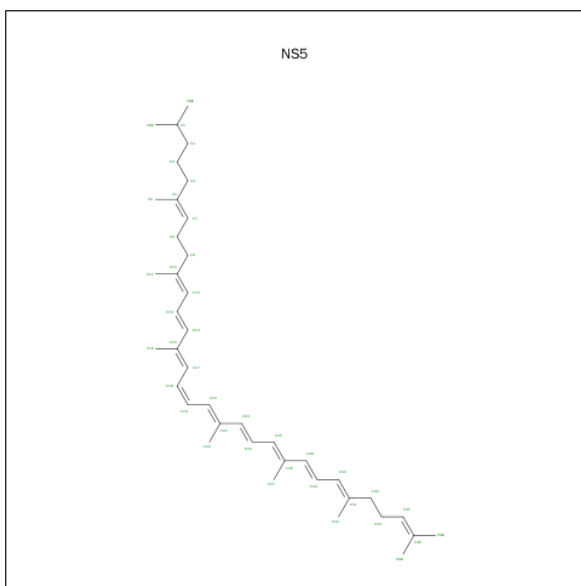
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	M	1	Total Fe 1 1	0	0

- Molecule 12 is MENAQUINONE-7 (three-letter code: MQ7) (formula: $\text{C}_{46}\text{H}_{64}\text{O}_2$).



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

- Molecule 13 is 15-CIS-1,2-DIHYDRONEUROSPORENE (three-letter code: NS5) (formula: $C_{40}H_{60}$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	M	1	Total	C	14	0
			40	40		

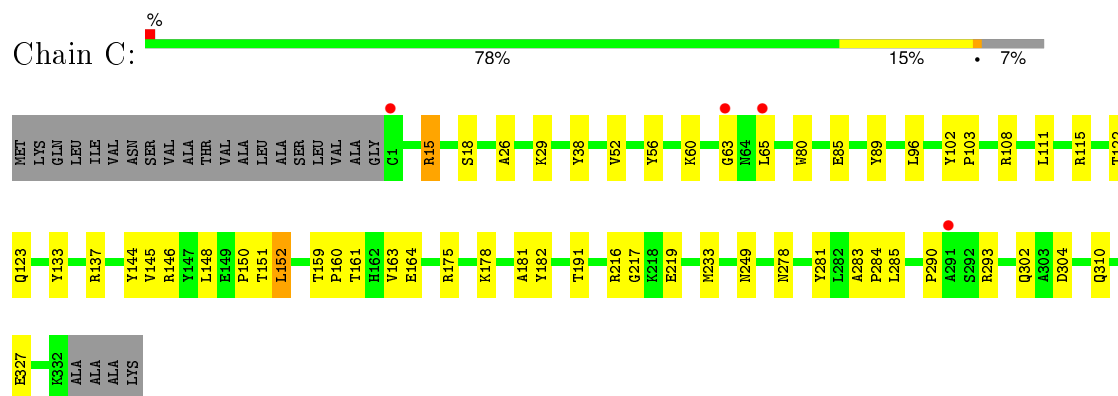
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	C	124	Total 124	O 124	0	0
14	H	76	Total 76	O 76	0	0
14	L	66	Total 66	O 66	0	0
14	M	76	Total 76	O 76	0	0

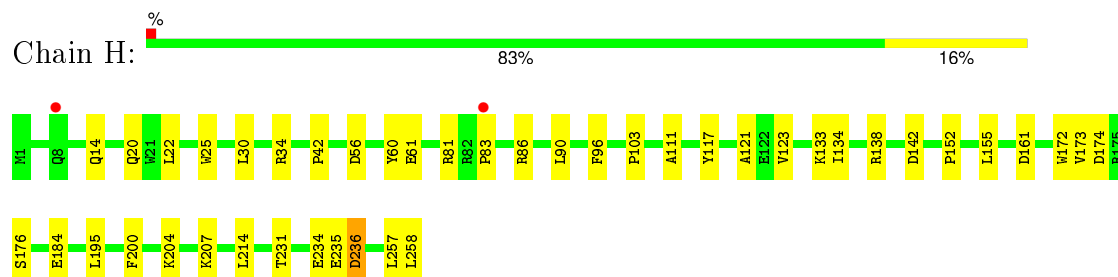
3 Residue-property plots [i](#)

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.

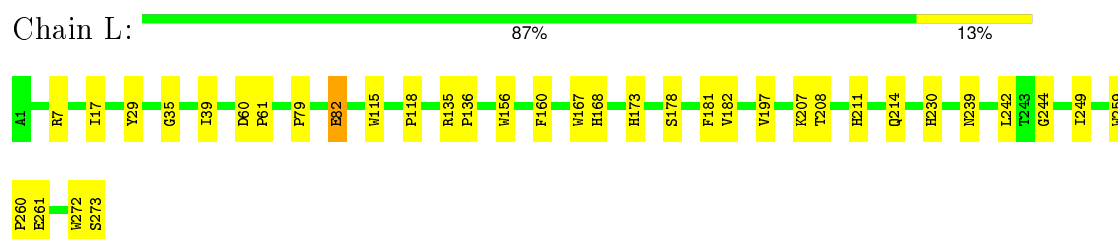
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER CYTOCHROME C SUBUNIT



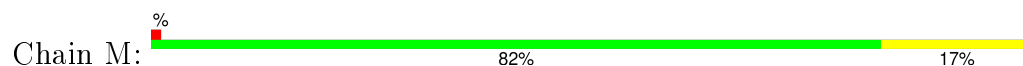
• Molecule 2: REACTION CENTER PROTEIN H CHAIN

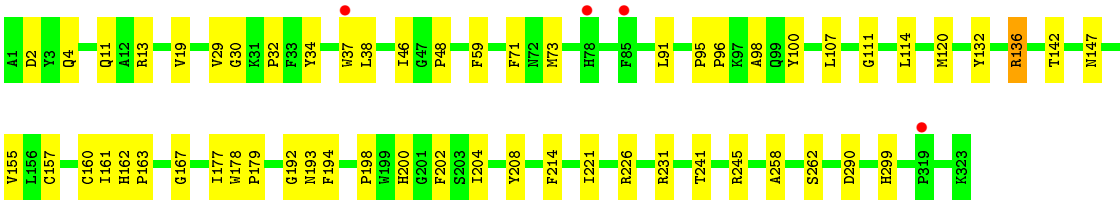


• Molecule 3: REACTION CENTER PROTEIN L CHAIN



• Molecule 4: REACTION CENTER PROTEIN M CHAIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	223.50 Å 223.50 Å 113.60 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.56 – 2.40 47.79 – 2.40	Depositor EDS
% Data completeness (in resolution range)	92.3 (26.56-2.40) 92.4 (47.79-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.39 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.190 , 0.206 0.181 , 0.202	Depositor DCC
R_{free} test set	1500 reflections (1.47%)	DCC
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 55.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 103567 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10512	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 1.77% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LDA, BPB, BCB, FE, MQ7, HEM, FME, NS5, SMA, SO4

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	0.32	0/2685	0.60	1/3659 (0.0%)
2	H	0.31	0/2055	0.59	0/2807
3	L	0.39	0/2259	0.58	0/3084
4	M	0.37	0/2659	0.55	0/3637
All	All	0.35	0/9658	0.58	1/13187 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	249	ASN	N-CA-C	-6.31	93.97	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2618	0	2587	44	0
2	H	2018	0	2020	31	0
3	L	2171	0	2098	34	0
4	M	2555	0	2452	45	0
5	C	172	0	120	3	0
6	H	16	0	31	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	M	80	0	155	7	0
7	H	5	0	0	0	0
7	M	15	0	0	0	0
8	L	198	0	216	23	0
8	M	66	0	72	10	0
9	L	65	0	74	5	0
9	M	65	0	74	7	0
10	L	37	0	42	2	0
11	M	1	0	0	0	0
12	M	48	0	64	0	0
13	M	40	0	60	3	0
14	C	124	0	0	1	0
14	H	76	0	0	1	0
14	L	66	0	0	1	0
14	M	76	0	0	1	0
All	All	10512	0	10065	169	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 9.

All (169) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:32:PRO:HG3	4:M:48:PRO:HD3	1.49	0.95
8:L:1278:BCB:H91	8:L:1278:BCB:H122	1.52	0.87
9:L:1276:BPB:HHC	9:L:1276:BPB:HBBB	1.59	0.84
8:L:1278:BCB:H141	8:L:1278:BCB:H172	1.60	0.82
4:M:136:ARG:HA	4:M:136:ARG:HE	1.45	0.81
3:L:178:SER:O	3:L:182:VAL:HG23	1.79	0.81
6:M:1331:LDA:H91	6:M:1331:LDA:H52	1.67	0.76
9:L:1276:BPB:HBBA	4:M:208:TYR:HB3	1.70	0.74
2:H:81:ARG:HG2	2:H:83:PRO:HD3	1.71	0.72
1:C:65:LEU:HD11	1:C:327:GLU:HG2	1.73	0.71
3:L:181:PHE:HB3	9:M:1325:BPB:CBB	2.21	0.71
1:C:146[B]:ARG:HB3	1:C:146[B]:ARG:HH11	1.57	0.70
1:C:152:LEU:HD21	1:C:178:LYS:HG3	1.73	0.69
3:L:181:PHE:CD2	9:M:1325:BPB:HBB	2.28	0.68
1:C:152:LEU:HD22	1:C:175:ARG:HA	1.76	0.66
2:H:42:PRO:HD3	6:H:1259:LDA:H121	1.78	0.66
2:H:86:ARG:NH2	2:H:111:ALA:HB3	2.12	0.65
4:M:38:LEU:CD2	4:M:46:ILE:HD11	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:LEU:O	1:C:115:ARG:HG3	1.97	0.64
3:L:182:VAL:HG13	8:L:1278:BCB:H42	1.80	0.64
2:H:14:GLN:HE21	6:M:1330:LDA:HM13	1.61	0.64
8:L:1278:BCB:HHC	8:L:1278:BCB:HBB2	1.80	0.64
3:L:182:VAL:HG22	8:L:1278:BCB:C1	2.28	0.63
1:C:163:VAL:HG23	14:C:2061:HOH:O	1.98	0.63
1:C:278:ASN:HB3	1:C:302:GLN:NE2	2.15	0.61
4:M:160:CYS:C	4:M:163:PRO:HD2	2.20	0.61
4:M:155:VAL:CG2	8:M:1324:BCB:H71	2.30	0.61
8:L:1275:BCB:HMB1	8:L:1275:BCB:HBB2	1.82	0.61
9:M:1325:BPB:HHC	9:M:1325:BPB:HBBB	1.83	0.61
3:L:182:VAL:HG22	8:L:1278:BCB:H12	1.83	0.60
4:M:59:PHE:HA	9:M:1325:BPB:H5	1.83	0.60
1:C:148:LEU:O	1:C:191:THR:HG21	2.01	0.59
2:H:152:PRO:HA	2:H:155:LEU:HD12	1.85	0.59
3:L:79:PRO:HG2	3:L:82:GLU:HB2	1.85	0.59
4:M:198:PRO:HG3	6:M:1330:LDA:H81	1.85	0.58
9:L:1276:BPB:HHC	9:L:1276:BPB:CBB	2.31	0.58
4:M:107:LEU:HA	4:M:111:GLY:HA3	1.86	0.58
2:H:235:GLU:CD	4:M:231:ARG:HH22	2.08	0.57
2:H:161:ASP:HB3	2:H:214:LEU:HD22	1.84	0.57
8:M:1324:BCB:HMB1	8:M:1324:BCB:CBB	2.34	0.57
4:M:299:HIS:HB3	6:M:1330:LDA:HM21	1.87	0.57
1:C:122:THR:HG22	1:C:123[B]:GLN:NE2	2.19	0.56
1:C:108:ARG:NH1	5:C:1333:HEM:O2D	2.37	0.56
1:C:145:VAL:O	1:C:146[A]:ARG:HD2	2.05	0.56
2:H:20:GLN:HG2	4:M:202:PHE:CE2	2.41	0.56
1:C:281:TYR:O	1:C:285:LEU:HG	2.06	0.56
2:H:200:PHE:CZ	4:M:226:ARG:HD3	2.41	0.56
1:C:26:ALA:O	1:C:29:LYS:HG3	2.05	0.55
3:L:135:ARG:HB3	3:L:136:PRO:HD3	1.87	0.55
1:C:60:LYS:HB2	1:C:108:ARG:NH1	2.21	0.55
9:L:1276:BPB:HBB	4:M:208:TYR:CD2	2.42	0.55
1:C:15:ARG:HG2	14:L:2020:HOH:O	2.07	0.54
1:C:52:VAL:HB	1:C:56:TYR:HD2	1.71	0.54
3:L:214:GLN:NE2	4:M:19:VAL:H	2.06	0.54
2:H:235:GLU:OE1	4:M:231:ARG:NH2	2.41	0.53
8:L:1275:BCB:HMD2	8:M:1324:BCB:HBB3	1.90	0.53
4:M:136:ARG:HA	4:M:136:ARG:NE	2.20	0.53
1:C:181:ALA:O	1:C:182:TYR:HB2	2.08	0.53
8:L:1275:BCB:CBB	8:L:1275:BCB:HMB1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:1324:BCB:HAA2	8:M:1324:BCB:HBD	1.90	0.53
1:C:278:ASN:HB3	1:C:302:GLN:HE21	1.74	0.52
1:C:123[B]:GLN:CD	1:C:123[B]:GLN:H	2.13	0.52
4:M:2:ASP:OD1	4:M:4:GLN:HB2	2.09	0.52
8:L:1274:BCB:HBB3	8:L:1274:BCB:HMB1	1.91	0.52
2:H:231:THR:OG1	2:H:234:GLU:HG3	2.09	0.52
1:C:283:ALA:HB3	1:C:284:PRO:HD3	1.91	0.52
1:C:85:GLU:HG2	1:C:89:TYR:CD1	2.45	0.52
8:L:1274:BCB:HHC	8:L:1274:BCB:OBB	2.10	0.52
3:L:182:VAL:HG13	8:L:1278:BCB:C4	2.39	0.52
2:H:142:ASP:N	2:H:142:ASP:OD1	2.40	0.52
3:L:197:VAL:HG13	3:L:207:LYS:HB2	1.91	0.51
1:C:102:TYR:CD2	1:C:103:PRO:HD3	2.45	0.51
1:C:102:TYR:CG	1:C:103:PRO:HD3	2.46	0.51
3:L:181:PHE:HB3	9:M:1325:BPB:HBBA	1.91	0.51
8:L:1274:BCB:CBB	8:L:1274:BCB:HMB1	2.41	0.51
3:L:182:VAL:HG22	8:L:1278:BCB:H11	1.93	0.51
2:H:133:LYS:HE2	2:H:176:SER:OG	2.11	0.51
6:M:1330:LDA:HM21	6:M:1330:LDA:H32	1.92	0.50
1:C:182:TYR:CE1	3:L:261:GLU:HG3	2.47	0.50
2:H:134:ILE:N	2:H:134:ILE:HD12	2.27	0.50
3:L:167:TRP:HE1	3:L:173:HIS:CD2	2.30	0.49
1:C:161:THR:OG1	1:C:164:GLU:HG3	2.12	0.49
3:L:29:TYR:OH	6:M:1332:LDA:H32	2.13	0.49
3:L:230:HIS:CD2	4:M:221:ILE:HG13	2.48	0.49
4:M:29:VAL:HG12	4:M:30:GLY:N	2.27	0.49
2:H:138:ARG:NH2	2:H:184:GLU:OE1	2.41	0.49
8:L:1278:BCB:HBB3	8:M:1324:BCB:H62	1.95	0.49
8:M:1324:BCB:H203	9:M:1325:BPB:H4B	1.95	0.49
4:M:120:MET:CE	13:M:1328:NS5:H273	2.43	0.49
3:L:79:PRO:HG2	3:L:82:GLU:CB	2.43	0.49
1:C:182:TYR:CD1	3:L:261:GLU:HG3	2.48	0.49
3:L:214:GLN:HE21	4:M:19:VAL:H	1.60	0.49
2:H:184:GLU:HG3	2:H:195:LEU:HD23	1.95	0.48
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.49	0.48
8:M:1324:BCB:HBB3	8:M:1324:BCB:HMB1	1.96	0.48
4:M:132:TYR:CE1	4:M:142:THR:HG21	2.48	0.48
4:M:34:TYR:CD1	4:M:34:TYR:N	2.81	0.48
8:L:1278:BCB:H91	8:L:1278:BCB:C12	2.35	0.48
4:M:155:VAL:HG21	8:M:1324:BCB:H71	1.96	0.47
4:M:2:ASP:OD2	4:M:226:ARG:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:258:LEU:HB2	3:L:17:ILE:HG22	1.96	0.47
2:H:134:ILE:HG22	2:H:172:TRP:HE3	1.78	0.47
1:C:146[B]:ARG:HB3	1:C:146[B]:ARG:NH1	2.26	0.47
4:M:160:CYS:SG	13:M:1328:NS5:H322	2.55	0.46
4:M:241:THR:O	4:M:245:ARG:HG3	2.15	0.46
2:H:90:LEU:HD23	2:H:103:PRO:HA	1.96	0.46
2:H:96:PHE:HD1	2:H:96:PHE:H	1.62	0.46
4:M:231:ARG:HD2	14:M:2050:HOH:O	2.16	0.46
4:M:147:ASN:HD22	9:M:1325:BPB:HMDA	1.81	0.46
4:M:38:LEU:HD22	4:M:46:ILE:HD11	1.97	0.45
10:L:1277:SMA:H19	8:L:1278:BCB:H92	1.98	0.45
4:M:98:ALA:HB3	4:M:100:TYR:CZ	2.51	0.45
2:H:86:ARG:HH22	2:H:111:ALA:HB3	1.82	0.45
2:H:34:ARG:HG2	2:H:61:GLU:O	2.17	0.45
8:L:1274:BCB:H11	8:L:1275:BCB:H2C	1.99	0.45
4:M:155:VAL:HG23	8:M:1324:BCB:H71	1.97	0.45
3:L:35:GLY:O	3:L:39:ILE:HG12	2.17	0.45
8:L:1275:BCB:HHC	8:L:1275:BCB:OBB	2.16	0.44
8:L:1278:BCB:H141	8:L:1278:BCB:C17	2.40	0.44
3:L:168:HIS:CE1	8:L:1274:BCB:HMC2	2.53	0.44
2:H:56:ASP:HB3	2:H:60:TYR:CE2	2.52	0.44
1:C:96:LEU:O	5:C:1333:HEM:HBA1	2.17	0.44
1:C:216:ARG:O	1:C:219:GLU:HG3	2.18	0.44
4:M:73:MET:HE3	4:M:91:LEU:HB2	1.99	0.44
8:M:1324:BCB:OBB	8:M:1324:BCB:HHC	2.17	0.44
2:H:117:TYR:HB2	2:H:236:ASP:HB3	2.00	0.43
14:H:2032:HOH:O	4:M:231:ARG:HD2	2.18	0.43
3:L:244:GLY:O	8:L:1274:BCB:HED3	2.18	0.43
2:H:138:ARG:HH22	2:H:184:GLU:CD	2.19	0.43
2:H:121:ALA:HB1	2:H:123:VAL:HG13	2.00	0.43
1:C:146[A]:ARG:NH2	1:C:150:PRO:HA	2.34	0.43
1:C:18:SER:HB2	3:L:156:TRP:CD1	2.54	0.43
4:M:258:ALA:HB1	4:M:262:SER:OG	2.19	0.43
4:M:162:HIS:HB3	4:M:163:PRO:HD3	2.01	0.42
3:L:208:THR:OG1	3:L:211:HIS:HD2	2.02	0.42
2:H:173:VAL:HG22	2:H:174:ASP:N	2.33	0.42
1:C:144:TYR:CD2	1:C:310:GLN:HG2	2.54	0.42
1:C:146[A]:ARG:HH21	1:C:150:PRO:HA	1.85	0.42
9:L:1276:BPB:H44	9:L:1276:BPB:HBAA	1.92	0.42
2:H:204:LYS:HB2	2:H:207:LYS:O	2.20	0.42
1:C:65:LEU:CD1	1:C:327:GLU:HG2	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:THR:HA	1:C:160:PRO:HD3	1.87	0.42
1:C:290:PRO:HG2	1:C:293:ARG:HG2	2.01	0.42
1:C:163:VAL:HB	3:L:273:SER:O	2.20	0.42
13:M:1328:NS5:H29	13:M:1328:NS5:H271	1.81	0.42
3:L:239:ASN:HD22	3:L:242:LEU:HB2	1.85	0.41
4:M:192:GLY:O	4:M:193:ASN:HB3	2.19	0.41
4:M:11:GLN:HB3	4:M:13:ARG:HH12	1.85	0.41
1:C:217:GLY:HA2	4:M:167:GLY:O	2.19	0.41
1:C:146[A]:ARG:NH2	1:C:151:THR:H	2.19	0.41
2:H:14:GLN:HE21	6:M:1330:LDA:CM1	2.29	0.41
3:L:239:ASN:HD22	3:L:239:ASN:HA	1.76	0.41
3:L:259:TRP:N	3:L:260:PRO:CD	2.84	0.41
1:C:304:ASP:OD1	1:C:304:ASP:C	2.59	0.41
4:M:95:PRO:HB2	4:M:96:PRO:HD2	2.02	0.41
1:C:133:TYR:CE1	1:C:137:ARG:HA	2.55	0.41
3:L:60:ASP:HA	3:L:61:PRO:HD3	1.88	0.41
2:H:30:LEU:O	2:H:34:ARG:HD2	2.21	0.41
10:L:1277:SMA:C15	8:L:1278:BCB:H92	2.50	0.41
4:M:162:HIS:N	4:M:163:PRO:CD	2.84	0.41
4:M:157:CYS:HA	4:M:161:ILE:HB	2.02	0.41
4:M:200:HIS:CE1	4:M:204:ILE:HD11	2.56	0.41
3:L:115:TRP:O	3:L:118:PRO:HG2	2.21	0.40
3:L:249:ILE:HA	3:L:249:ILE:HD13	1.98	0.40
2:H:25:TRP:CE3	2:H:25:TRP:HA	2.56	0.40
1:C:233:MET:HB3	5:C:1335:HEM:C4B	2.55	0.40
4:M:178:TRP:N	4:M:179:PRO:CD	2.85	0.40
1:C:52:VAL:HG23	1:C:63:GLY:HA2	2.02	0.40
3:L:7:ARG:HH11	3:L:7:ARG:HG3	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	332/356 (93%)	317 (96%)	15 (4%)	0	100	100
2	H	256/258 (99%)	242 (94%)	14 (6%)	0	100	100
3	L	271/273 (99%)	262 (97%)	9 (3%)	0	100	100
4	M	321/323 (99%)	310 (97%)	10 (3%)	1 (0%)	46	63
All	All	1180/1210 (98%)	1131 (96%)	48 (4%)	1 (0%)	56	74

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	M	177	ILE

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	282/297 (95%)	279 (99%)	3 (1%)	80	92
2	H	212/212 (100%)	209 (99%)	3 (1%)	74	88
3	L	218/218 (100%)	215 (99%)	3 (1%)	74	88
4	M	249/249 (100%)	242 (97%)	7 (3%)	51	72
All	All	961/976 (98%)	945 (98%)	16 (2%)	68	85

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	15	ARG
1	C	38	TYR
1	C	152	LEU
2	H	22	LEU
2	H	236	ASP
2	H	257	LEU
3	L	82	GLU
3	L	160	PHE
3	L	272	TRP
4	M	37	TRP

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Mol	Chain	Res	Type
4	M	71	PHE
4	M	114	LEU
4	M	136	ARG
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 (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	302	GLN
2	H	58	GLN
2	H	220	ASN
3	L	211	HIS
3	L	214	GLN
3	L	239	ASN
4	M	147	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FME	H	1	2	8,9,10	0.56	0	6,9,11	4.65	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	O1-CN-N	-9.64	110.88	124.76
2	H	1	FME	CA-N-CN	-5.79	113.91	122.82

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 24 ligands modelled in this entry, 1 is monoatomic - leaving 23 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	2.61	9 (30%)	24,82,82	3.22	8 (33%)
5	HEM	C	1334	1	30,50,50	2.62	8 (26%)	24,82,82	3.21	9 (37%)
5	HEM	C	1335	1	30,50,50	2.60	9 (30%)	24,82,82	3.32	9 (37%)
5	HEM	C	1336	1	30,50,50	2.64	9 (30%)	24,82,82	3.06	9 (37%)
6	LDA	H	1259	-	15,15,15	4.65	4 (26%)	16,17,17	0.64	0
7	SO4	H	1260	-	4,4,4	1.11	0	6,6,6	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BCB	L	1274	3	56,74,74	1.49	6 (10%)	57,115,115	1.97	12 (21%)
8	BCB	L	1275	3	56,74,74	1.53	6 (10%)	57,115,115	2.04	8 (14%)
9	BPB	L	1276	-	63,70,70	1.43	6 (9%)	63,101,101	1.81	9 (14%)
10	SMA	L	1277	-	35,38,38	1.93	8 (22%)	40,52,52	1.40	4 (10%)
8	BCB	L	1278	4	56,74,74	1.58	6 (10%)	57,115,115	2.03	9 (15%)
8	BCB	M	1324	4	56,74,74	1.52	7 (12%)	57,115,115	2.14	12 (21%)
9	BPB	M	1325	-	63,70,70	1.44	8 (12%)	63,101,101	1.92	8 (12%)
12	MQ7	M	1327	-	49,49,49	1.62	9 (18%)	62,63,63	1.26	7 (11%)
13	NS5	M	1328	-	39,39,39	0.66	0	44,46,46	1.06	4 (9%)
6	LDA	M	1329	-	15,15,15	4.30	4 (26%)	16,17,17	0.70	0
6	LDA	M	1330	-	15,15,15	4.57	4 (26%)	16,17,17	0.54	0
6	LDA	M	1331	-	15,15,15	4.35	4 (26%)	16,17,17	0.49	0
6	LDA	M	1332	-	15,15,15	4.76	4 (26%)	16,17,17	0.63	0
6	LDA	M	1333	-	15,15,15	4.74	4 (26%)	16,17,17	0.59	0
7	SO4	M	1334	-	4,4,4	1.72	0	6,6,6	0.45	0
7	SO4	M	1335	-	4,4,4	1.29	0	6,6,6	0.08	0
7	SO4	M	1336	-	4,4,4	1.20	0	6,6,6	0.37	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	LDA	H	1259	-	-	0/13/13/13	0/0/0/0
7	SO4	H	1260	-	-	0/0/0/0	0/0/0/0
8	BCB	L	1274	3	-	0/37/137/137	0/0/9/9
8	BCB	L	1275	3	-	0/37/137/137	0/0/9/9
9	BPB	L	1276	-	-	0/46/105/105	0/1/6/6
10	SMA	L	1277	-	-	0/33/34/34	0/2/2/2
8	BCB	L	1278	4	-	0/37/137/137	0/0/9/9
8	BCB	M	1324	4	1/1/21/26	0/37/137/137	0/0/9/9
9	BPB	M	1325	-	-	0/46/105/105	0/1/6/6
12	MQ7	M	1327	-	-	0/41/61/61	0/2/2/2
13	NS5	M	1328	-	-	0/43/43/43	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	LDA	M	1329	-	-	0/13/13/13	0/0/0/0
6	LDA	M	1330	-	-	0/13/13/13	0/0/0/0
6	LDA	M	1331	-	-	0/13/13/13	0/0/0/0
6	LDA	M	1332	-	-	0/13/13/13	0/0/0/0
6	LDA	M	1333	-	-	0/13/13/13	0/0/0/0
7	SO4	M	1334	-	-	0/0/0/0	0/0/0/0
7	SO4	M	1335	-	-	0/0/0/0	0/0/0/0
7	SO4	M	1336	-	-	0/0/0/0	0/0/0/0

All (115) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	1332	LDA	O1-N1	-17.76	1.22	1.39
6	M	1333	LDA	O1-N1	-17.74	1.22	1.39
6	H	1259	LDA	O1-N1	-17.45	1.22	1.39
6	M	1330	LDA	O1-N1	-17.24	1.23	1.39
6	M	1331	LDA	O1-N1	-16.38	1.23	1.39
6	M	1329	LDA	O1-N1	-16.10	1.24	1.39
5	C	1335	HEM	C3B-C4B	-7.70	1.45	1.51
5	C	1333	HEM	C3B-C4B	-7.60	1.45	1.51
5	C	1336	HEM	C3B-C4B	-7.50	1.45	1.51
5	C	1334	HEM	C3B-C4B	-7.43	1.45	1.51
5	C	1336	HEM	C2D-C3D	-6.33	1.35	1.54
8	M	1324	BCB	C4D-CHA	-6.31	1.37	1.45
5	C	1333	HEM	C2D-C3D	-6.22	1.35	1.54
5	C	1334	HEM	C2D-C3D	-6.12	1.36	1.54
5	C	1335	HEM	C2D-C3D	-5.97	1.36	1.54
8	L	1274	BCB	C4D-CHA	-5.75	1.37	1.45
5	C	1336	HEM	C3D-C4D	-5.40	1.44	1.51
5	C	1333	HEM	C3D-C4D	-5.39	1.44	1.51
5	C	1335	HEM	C3D-C4D	-5.22	1.44	1.51
8	L	1275	BCB	C4D-CHA	-5.12	1.38	1.45
5	C	1334	HEM	C3D-C4D	-5.07	1.45	1.51
8	L	1278	BCB	C4D-CHA	-5.04	1.38	1.45
5	C	1334	HEM	C2C-C1C	-4.39	1.44	1.52
8	L	1275	BCB	O2D-CED	-4.13	1.35	1.45
5	C	1333	HEM	C2C-C1C	-4.01	1.45	1.52
5	C	1336	HEM	C2C-C1C	-3.99	1.45	1.52
8	M	1324	BCB	O2D-CED	-3.91	1.35	1.45
9	L	1276	BPB	O2D-CED	-3.91	1.35	1.45
5	C	1335	HEM	C2C-C1C	-3.90	1.45	1.52
9	M	1325	BPB	O2D-CED	-3.87	1.35	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	1278	BCB	O2D-CED	-3.84	1.35	1.45
8	L	1274	BCB	O2D-CED	-3.68	1.36	1.45
6	M	1332	LDA	C1-N1	-3.17	1.45	1.51
12	M	1327	MQ7	C11-C12	-3.11	1.45	1.50
6	M	1333	LDA	C1-N1	-3.02	1.45	1.51
6	M	1329	LDA	C1-N1	-2.98	1.46	1.51
8	L	1274	BCB	C1-C2	-2.84	1.39	1.49
6	M	1330	LDA	CM1-N1	-2.81	1.45	1.49
6	H	1259	LDA	C1-N1	-2.78	1.46	1.51
6	H	1259	LDA	CM1-N1	-2.71	1.45	1.49
6	M	1332	LDA	CM1-N1	-2.68	1.45	1.49
6	M	1332	LDA	CM2-N1	-2.67	1.45	1.49
6	M	1333	LDA	CM1-N1	-2.58	1.45	1.49
6	M	1333	LDA	CM2-N1	-2.49	1.45	1.49
6	M	1331	LDA	C1-N1	-2.31	1.47	1.51
5	C	1336	HEM	C2D-C1D	-2.28	1.44	1.51
6	M	1329	LDA	CM1-N1	-2.26	1.46	1.49
8	M	1324	BCB	C4C-C3C	-2.26	1.40	1.45
6	M	1331	LDA	CM1-N1	-2.22	1.46	1.49
9	M	1325	BPB	C4C-C3C	-2.16	1.40	1.45
5	C	1335	HEM	C2B-C1B	-2.15	1.44	1.51
12	M	1327	MQ7	C10-C5	-2.12	1.37	1.40
5	C	1336	HEM	C2B-C1B	-2.10	1.45	1.51
5	C	1334	HEM	C2D-C1D	-2.10	1.45	1.51
5	C	1334	HEM	C2B-C1B	-2.09	1.45	1.51
5	C	1333	HEM	C2D-C1D	-2.07	1.45	1.51
5	C	1333	HEM	C2B-C1B	-2.06	1.45	1.51
5	C	1335	HEM	C2D-C1D	-2.06	1.45	1.51
6	M	1329	LDA	CM2-N1	-2.05	1.46	1.49
6	M	1331	LDA	CM2-N1	-2.02	1.46	1.49
6	H	1259	LDA	CM2-N1	-2.01	1.46	1.49
6	M	1330	LDA	CM2-N1	-2.00	1.46	1.49
6	M	1330	LDA	C1-N1	-2.00	1.47	1.51
10	L	1277	SMA	O1-C8A	2.02	1.40	1.36
5	C	1333	HEM	C1C-NC	2.03	1.38	1.36
10	L	1277	SMA	C6-C7	2.04	1.42	1.38
5	C	1335	HEM	C4C-NC	2.15	1.38	1.36
5	C	1336	HEM	C3C-CAC	2.16	1.55	1.51
10	L	1277	SMA	C7-C8	2.20	1.43	1.40
9	M	1325	BPB	C1A-CHA	2.31	1.41	1.36
10	L	1277	SMA	O7-C7	2.33	1.40	1.37
8	M	1324	BCB	O2D-CGD	2.42	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	1277	SMA	C4A-C8A	2.44	1.44	1.41
9	M	1325	BPB	O2A-CGA	2.53	1.40	1.33
12	M	1327	MQ7	C42-C43	2.56	1.40	1.32
9	L	1276	BPB	O2A-CGA	2.67	1.41	1.33
8	L	1278	BCB	O2D-CGD	2.86	1.40	1.33
8	L	1274	BCB	C2-C3	2.86	1.38	1.33
8	L	1275	BCB	O2A-CGA	2.88	1.42	1.33
8	M	1324	BCB	O2A-CGA	2.96	1.42	1.33
8	L	1275	BCB	O2D-CGD	2.99	1.40	1.33
12	M	1327	MQ7	C22-C23	3.00	1.38	1.33
12	M	1327	MQ7	C17-C18	3.01	1.38	1.33
12	M	1327	MQ7	C12-C13	3.03	1.38	1.33
12	M	1327	MQ7	C27-C28	3.10	1.39	1.33
9	M	1325	BPB	O2D-CGD	3.11	1.41	1.33
8	M	1324	BCB	C2-C3	3.27	1.39	1.33
12	M	1327	MQ7	C32-C33	3.28	1.39	1.33
8	L	1275	BCB	C2-C3	3.32	1.39	1.33
12	M	1327	MQ7	C37-C38	3.33	1.39	1.33
9	L	1276	BPB	C2-C3	3.38	1.39	1.33
10	L	1277	SMA	C4-C3	3.38	1.51	1.41
8	L	1274	BCB	O2D-CGD	3.48	1.42	1.33
9	M	1325	BPB	C2-C3	3.50	1.39	1.33
9	M	1325	BPB	C3B-C4B	3.59	1.46	1.41
8	L	1278	BCB	C2-C3	3.59	1.40	1.33
9	L	1276	BPB	O2D-CGD	3.78	1.42	1.33
9	L	1276	BPB	C3B-C4B	4.07	1.46	1.41
5	C	1336	HEM	CBB-CAB	4.09	1.52	1.29
5	C	1333	HEM	CBC-CAC	4.10	1.53	1.29
5	C	1335	HEM	CBB-CAB	4.11	1.53	1.29
8	L	1274	BCB	CAC-C3C	4.12	1.38	1.33
5	C	1334	HEM	CBB-CAB	4.13	1.53	1.29
5	C	1336	HEM	CBC-CAC	4.13	1.53	1.29
8	M	1324	BCB	CAC-C3C	4.16	1.38	1.33
5	C	1334	HEM	CBC-CAC	4.19	1.53	1.29
5	C	1333	HEM	CBB-CAB	4.23	1.53	1.29
5	C	1335	HEM	CBC-CAC	4.47	1.55	1.29
8	L	1278	BCB	O2A-CGA	4.61	1.47	1.33
8	L	1275	BCB	CAC-C3C	4.87	1.39	1.33
8	L	1278	BCB	CAC-C3C	4.88	1.39	1.33
10	L	1277	SMA	O1-C2	5.09	1.41	1.35
9	L	1276	BPB	CAC-C3C	5.33	1.39	1.33
9	M	1325	BPB	CAC-C3C	6.15	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	1277	SMA	C4-C4A	7.05	1.51	1.41

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1335	HEM	C3B-CAB-CBB	-10.50	108.35	124.46
5	C	1333	HEM	C3B-CAB-CBB	-9.16	110.40	124.46
5	C	1336	HEM	C3B-CAB-CBB	-9.14	110.44	124.46
5	C	1333	HEM	C3C-CAC-CBC	-8.66	111.17	124.46
5	C	1334	HEM	C3C-CAC-CBC	-8.48	111.45	124.46
5	C	1334	HEM	C3B-CAB-CBB	-8.41	111.55	124.46
5	C	1335	HEM	C3C-CAC-CBC	-7.99	112.20	124.46
8	L	1275	BCB	O1D-CGD-CBD	-7.45	113.94	124.62
9	M	1325	BPB	O1D-CGD-CBD	-7.16	114.35	124.62
9	L	1276	BPB	O1D-CGD-CBD	-6.87	114.78	124.62
8	L	1278	BCB	O1D-CGD-CBD	-6.80	114.87	124.62
5	C	1336	HEM	C3C-CAC-CBC	-6.77	114.08	124.46
8	L	1274	BCB	O1D-CGD-CBD	-6.51	115.29	124.62
8	M	1324	BCB	O1D-CGD-CBD	-6.37	115.49	124.62
8	L	1278	BCB	C4-C3-C5	-4.51	108.52	115.41
10	L	1277	SMA	C3-C4-C4A	-4.05	115.73	121.35
8	M	1324	BCB	O2A-CGA-O1A	-3.31	114.94	123.49
8	L	1278	BCB	OBD-CAD-CBD	-3.30	120.96	125.94
8	M	1324	BCB	OBD-CAD-CBD	-3.27	121.01	125.94
8	L	1274	BCB	OBD-CAD-CBD	-3.24	121.05	125.94
8	L	1275	BCB	OBD-CAD-CBD	-3.23	121.06	125.94
9	M	1325	BPB	C2C-C3C-C4C	-3.06	104.45	107.24
13	M	1328	NS5	C16-C15-C14	-2.90	113.27	118.10
8	M	1324	BCB	C15-C13-C12	-2.85	95.25	112.27
8	M	1324	BCB	C4-C3-C5	-2.76	111.19	115.41
8	L	1275	BCB	C4-C3-C5	-2.75	111.21	115.41
9	L	1276	BPB	C2C-C3C-C4C	-2.68	104.79	107.24
8	L	1274	BCB	O2A-CGA-O1A	-2.55	116.90	123.49
12	M	1327	MQ7	C39-C38-C40	-2.50	111.58	115.41
9	M	1325	BPB	CBD-CHA-C4D	-2.42	105.75	108.46
8	L	1278	BCB	O2A-CGA-O1A	-2.41	117.26	123.49
9	L	1276	BPB	C4-C3-C5	-2.38	111.78	115.41
8	L	1274	BCB	C15-C13-C12	-2.35	98.22	112.27
12	M	1327	MQ7	C34-C33-C35	-2.35	111.81	115.41
5	C	1336	HEM	CAA-C2A-C1A	-2.29	124.53	127.01
9	L	1276	BPB	CBD-CHA-C4D	-2.27	105.92	108.46
10	L	1277	SMA	O12-C12-C13	-2.22	104.27	107.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1335	HEM	CAA-C2A-C1A	-2.14	124.69	127.01
8	M	1324	BCB	CMD-C2D-C3D	2.01	129.01	125.09
8	L	1275	BCB	CMB-C2B-C3B	2.01	129.01	125.09
9	M	1325	BPB	CBD-CHA-C1A	2.05	130.24	126.78
13	M	1328	NS5	C14-C15-C17	2.09	122.35	118.98
9	L	1276	BPB	C6-C5-C3	2.15	117.20	112.48
12	M	1327	MQ7	C20-C21-C22	2.17	117.37	111.69
9	L	1276	BPB	CED-O2D-CGD	2.17	121.08	115.99
8	L	1275	BCB	C3C-C4C-NC	2.17	111.86	110.24
10	L	1277	SMA	C11-C12-C13	2.18	119.15	114.36
8	L	1274	BCB	CMD-C2D-C3D	2.20	129.39	125.09
8	L	1274	BCB	C4-C3-C5	2.22	118.80	115.41
8	L	1278	BCB	C5-C3-C2	2.24	125.31	121.05
9	M	1325	BPB	O2A-CGA-CBA	2.30	118.92	111.90
5	C	1333	HEM	CMD-C2D-C3D	2.32	124.59	114.35
8	L	1274	BCB	CMB-C2B-C3B	2.35	129.69	125.09
13	M	1328	NS5	C18-C19-C20	2.39	128.68	123.39
12	M	1327	MQ7	C36-C37-C38	2.46	133.12	127.76
12	M	1327	MQ7	C40-C38-C37	2.49	125.77	121.05
5	C	1334	HEM	CMD-C2D-C3D	2.52	125.49	114.35
5	C	1334	HEM	CAA-C2A-C1A	2.53	129.75	127.01
8	M	1324	BCB	C3C-C4C-NC	2.58	112.16	110.24
5	C	1336	HEM	CMD-C2D-C3D	2.65	126.07	114.35
9	L	1276	BPB	O2A-CGA-CBA	2.70	120.13	111.90
5	C	1335	HEM	CMD-C2D-C3D	2.73	126.43	114.35
8	L	1274	BCB	C3C-C4C-NC	2.73	112.28	110.24
8	L	1278	BCB	C3C-C4C-NC	2.73	112.28	110.24
5	C	1335	HEM	CMC-C2C-C3C	2.76	123.42	116.53
9	M	1325	BPB	C3C-C2C-C1C	2.79	105.11	100.99
8	M	1324	BCB	C5-C3-C2	2.80	126.35	121.05
8	L	1275	BCB	OBB-CAB-C3B	2.91	124.61	120.00
8	L	1274	BCB	OBB-CAB-C3B	2.91	124.62	120.00
12	M	1327	MQ7	C41-C42-C43	2.91	138.95	127.73
9	L	1276	BPB	C3C-C2C-C1C	3.11	105.59	100.99
5	C	1333	HEM	C2D-C3D-C4D	3.13	106.80	101.50
5	C	1334	HEM	C2D-C3D-C4D	3.24	107.00	101.50
5	C	1336	HEM	C2D-C3D-C4D	3.25	107.01	101.50
5	C	1335	HEM	C2D-C3D-C4D	3.33	107.14	101.50
5	C	1333	HEM	CMB-C2B-C3B	3.38	124.98	116.53
13	M	1328	NS5	C19-C18-C17	3.42	130.96	123.39
8	L	1274	BCB	O2A-CGA-CBA	3.46	122.44	111.90
5	C	1336	HEM	CMC-C2C-C3C	3.57	125.43	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	1278	BCB	O2A-CGA-CBA	3.58	122.80	111.90
8	M	1324	BCB	OBB-CAB-C3B	3.64	125.76	120.00
8	L	1275	BCB	C4A-NA-C1A	3.74	110.45	106.04
5	C	1334	HEM	CAD-C3D-C2D	3.82	124.19	113.22
8	L	1274	BCB	C4A-NA-C1A	3.84	110.56	106.04
5	C	1336	HEM	CMB-C2B-C3B	3.85	126.15	116.53
5	C	1336	HEM	CAD-C3D-C4D	3.87	126.13	112.47
5	C	1335	HEM	CAD-C3D-C4D	3.91	126.24	112.47
5	C	1335	HEM	CMB-C2B-C3B	3.91	126.30	116.53
5	C	1334	HEM	CMB-C2B-C3B	3.92	126.31	116.53
5	C	1333	HEM	CAD-C3D-C2D	3.94	124.55	113.22
8	L	1278	BCB	C4A-NA-C1A	4.00	110.75	106.04
12	M	1327	MQ7	C11-C12-C13	4.00	133.47	126.70
5	C	1334	HEM	CMC-C2C-C3C	4.02	126.58	116.53
5	C	1333	HEM	CMC-C2C-C3C	4.12	126.82	116.53
8	M	1324	BCB	C4A-NA-C1A	4.21	111.00	106.04
5	C	1333	HEM	CAD-C3D-C4D	4.57	128.58	112.47
5	C	1334	HEM	CAD-C3D-C4D	4.63	128.79	112.47
5	C	1335	HEM	CAD-C3D-C2D	4.66	126.61	113.22
8	M	1324	BCB	O2A-CGA-CBA	4.69	126.20	111.90
5	C	1336	HEM	CAD-C3D-C2D	4.72	126.78	113.22
10	L	1277	SMA	C9-C2-C3	5.18	127.39	120.56
9	M	1325	BPB	C6-C5-C3	5.54	124.64	112.48
8	L	1274	BCB	O2D-CGD-CBD	8.14	122.47	111.30
9	L	1276	BPB	O2D-CGD-CBD	8.32	122.71	111.30
8	M	1324	BCB	O2D-CGD-CBD	8.40	122.82	111.30
8	L	1278	BCB	O2D-CGD-CBD	8.56	123.04	111.30
9	M	1325	BPB	O2D-CGD-CBD	8.97	123.61	111.30
8	L	1275	BCB	O2D-CGD-CBD	9.60	124.47	111.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	M	1324	BCB	C8

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1333	HEM	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1335	HEM	1	0
6	H	1259	LDA	1	0
8	L	1274	BCB	6	0
8	L	1275	BCB	5	0
9	L	1276	BPB	5	0
10	L	1277	SMA	2	0
8	L	1278	BCB	13	0
8	M	1324	BCB	10	0
9	M	1325	BPB	7	0
13	M	1328	NS5	3	0
6	M	1330	LDA	5	0
6	M	1331	LDA	1	0
6	M	1332	LDA	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	332/356 (93%)	-0.48	4 (1%) 81 81	21, 36, 58, 76	19 (5%)
2	H	249/258 (96%)	-0.59	2 (0%) 87 87	24, 41, 66, 81	20 (8%)
3	L	273/273 (100%)	-0.62	0 100 100	21, 30, 51, 62	7 (2%)
4	M	323/323 (100%)	-0.51	4 (1%) 81 81	20, 34, 58, 64	12 (3%)
All	All	1177/1210 (97%)	-0.55	10 (0%) 87 87	20, 35, 59, 81	58 (4%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	M	85	PHE	3.3
1	C	1	CYS	3.3
1	C	65	LEU	2.3
4	M	319	PRO	2.3
1	C	291	ALA	2.3
2	H	8	GLN	2.2
4	M	37	TRP	2.2
1	C	63	GLY	2.2
2	H	83	PRO	2.1
4	M	78	HIS	2.1

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(\AA^2)	Q<0.9
2	FME	H	1	10/11	0.96	0.12	-	41,44,53,61	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	LDA	M	1332	16/16	0.72	0.36	7.89	86,88,90,90	5
6	LDA	M	1330	16/16	0.60	0.33	7.34	52,71,83,83	0
6	LDA	M	1331	16/16	0.71	0.41	5.85	83,84,93,93	0
13	NS5	M	1328	40/40	0.92	0.18	3.59	50,58,79,80	14
6	LDA	M	1333	16/16	0.81	0.25	2.59	86,90,90,90	4
6	LDA	H	1259	16/16	0.93	0.22	2.41	52,60,66,67	0
8	BCB	L	1278	66/66	0.95	0.18	1.67	20,29,49,50	20
10	SMA	L	1277	37/37	0.96	0.15	1.31	28,36,66,69	0
8	BCB	M	1324	66/66	0.97	0.17	1.06	17,24,47,49	0
8	BCB	L	1274	66/66	0.98	0.17	0.99	16,21,34,39	0
6	LDA	M	1329	16/16	0.97	0.16	0.78	41,44,46,47	0
12	MQ7	M	1327	48/48	0.96	0.13	0.57	24,27,54,58	0
9	BPB	L	1276	65/65	0.98	0.14	0.55	19,27,32,34	0
9	BPB	M	1325	65/65	0.94	0.13	0.46	25,35,61,62	7
7	SO4	H	1260	5/5	0.98	0.11	0.29	75,76,76,77	0
8	BCB	L	1275	66/66	0.97	0.14	0.04	15,22,46,50	0
5	HEM	C	1336	43/43	0.98	0.10	0.02	24,29,42,49	0
5	HEM	C	1334	43/43	0.98	0.10	0.00	29,35,40,42	0
7	SO4	M	1336	5/5	0.99	0.13	-0.24	57,57,58,59	0
5	HEM	C	1333	43/43	0.98	0.10	-0.54	34,39,49,53	0
5	HEM	C	1335	43/43	0.99	0.11	-0.66	21,25,29,34	0
11	FE	M	1326	1/1	1.00	0.08	-3.25	25,25,25,25	0
7	SO4	M	1334	5/5	0.99	0.10	-	39,41,42,44	0
7	SO4	M	1335	5/5	0.97	0.11	-	85,86,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.