



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 2, 2016 – 12:01 AM GMT

PDB ID : 7PRC
Title : PHOTOSYNTHETIC REACTION CENTER FROM RHODOPSEUDOMONAS VIRIDIS (DG-420315 (TRIAZINE) COMPLEX)
Authors : Lancaster, C.R.D.; Michel, H.
Deposited on : 1997-08-01
Resolution : 2.65 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

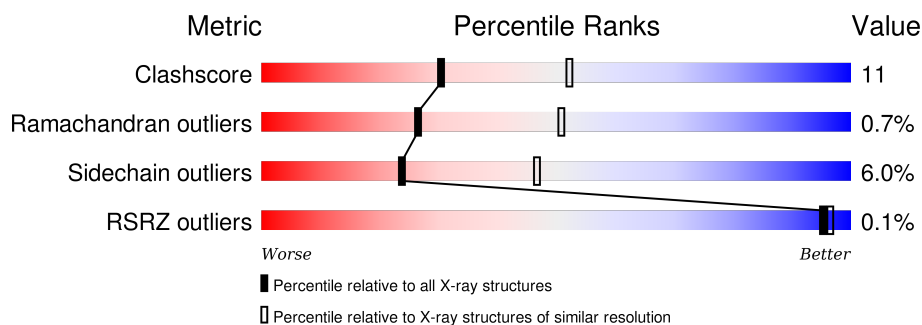
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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))
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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	
2	L	273	
3	M	323	
4	H	258	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	NS5	M	600	-	-	-	X
13	LDA	H	703	-	-	-	X
13	LDA	L	702	-	-	-	X
13	LDA	M	704	-	-	-	X
13	LDA	M	706	-	-	-	X
8	BPB	L	402	X	-	-	-

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 10476 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	332	Total	C	N	O	S	51	1	0
			2607	1642	467	480	18			

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	273	Total	C	N	O	S	14	0	0
			2171	1459	350	355	7			

- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	323	Total	C	N	O	S	19	2	0
			2577	1720	421	425	11			

- Molecule 4 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	258	Total	C	N	O	S	122	0	0
			2018	1292	344	380	2			

- Molecule 5 is FE (II) ION (three-letter code: FE2) (formula: Fe).

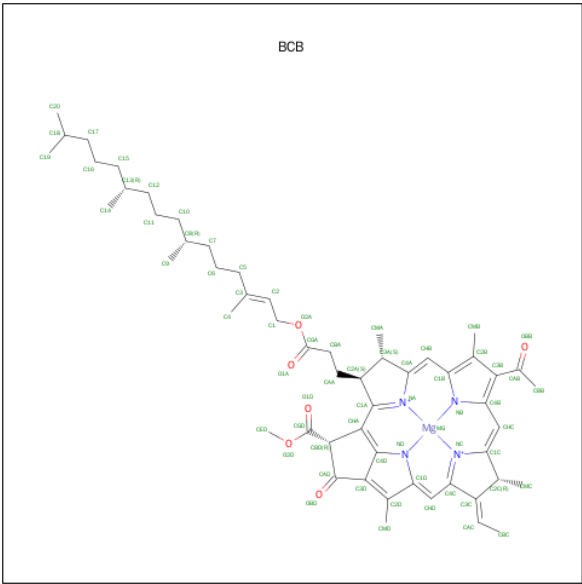
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	1	Total	Fe	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



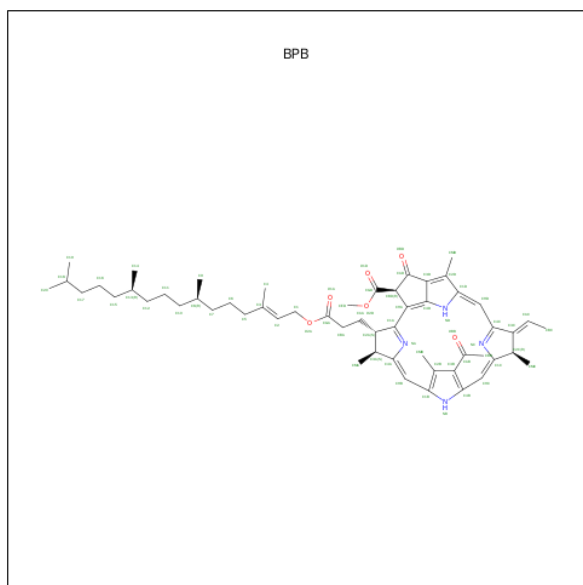
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: C₅₅H₇₂MgN₄O₆).



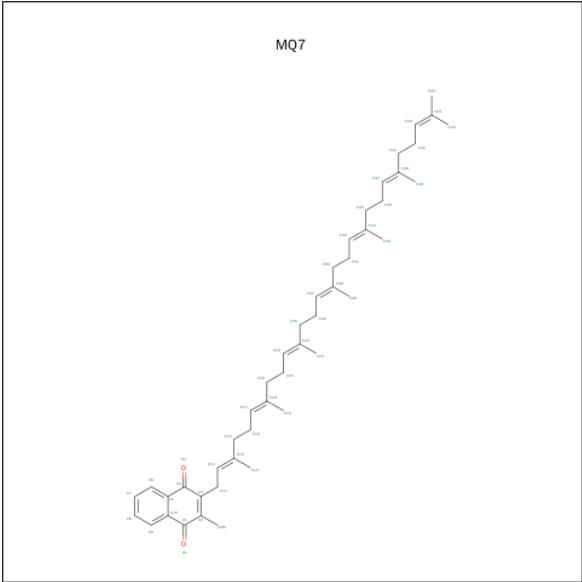
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 8 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula: $C_{55}H_{74}N_4O_6$).



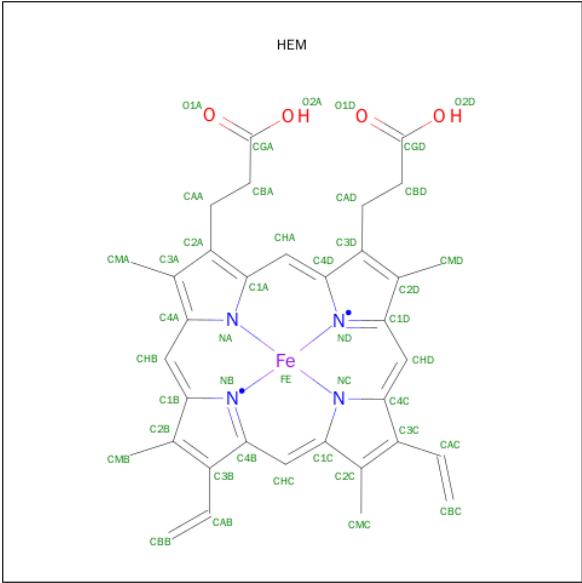
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	L	1	Total	C	N	O	7	0
			65	55	4	6		
8	L	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 9 is MENAQUINONE-7 (three-letter code: MQ7) (formula: $C_{46}H_{64}O_2$).



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

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



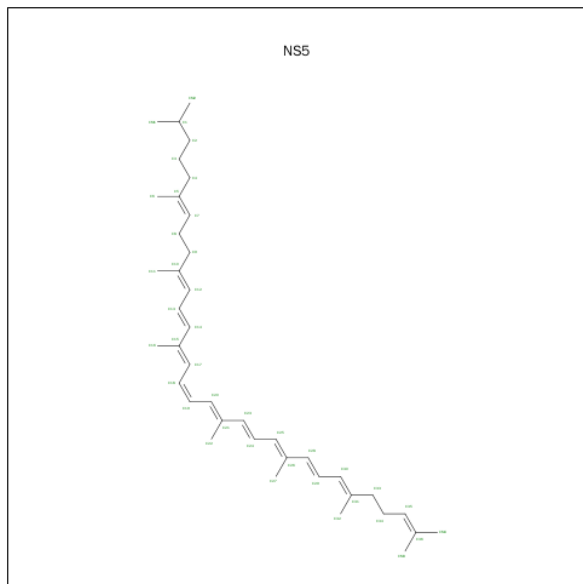
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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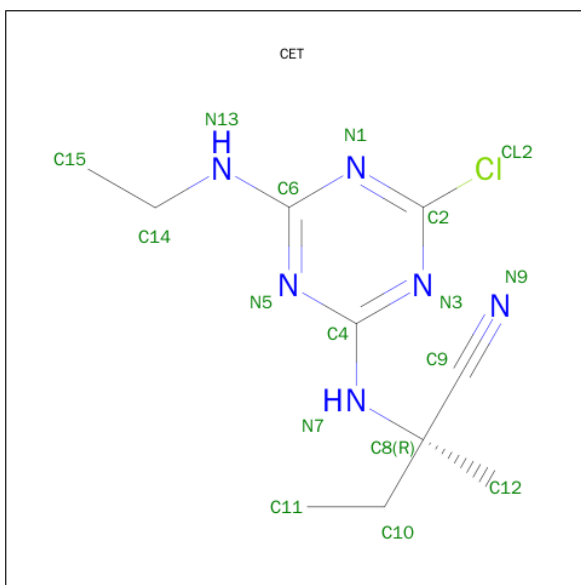
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
10	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 11 is 15-CIS-1,2-DIHYDRONEUROSPORENE (three-letter code: NS5) (formula: C₄₀H₆₀).



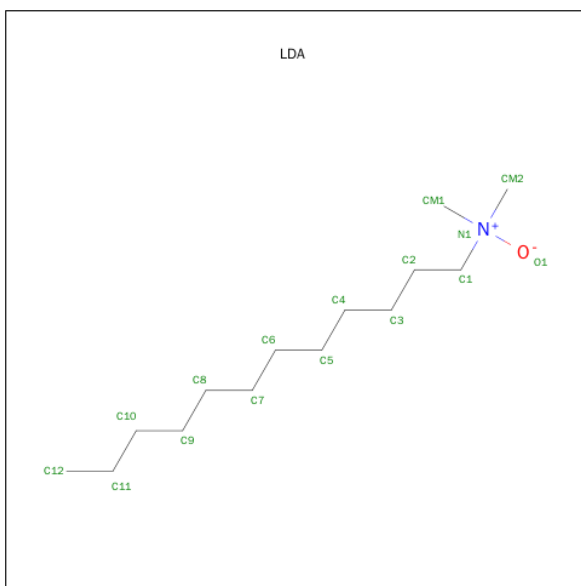
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	C		
			40	40	4	0

- Molecule 12 is 2-CHLORO-4-ETHYLAMINO-6-(R(+)-2'-CYANO-4-BUTYLAMINO)-1,3,5-TRIAZINE (three-letter code: CET) (formula: C₁₀H₁₅ClN₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	L	1	Total	C	Cl	N	0	0
			17	10	1	6		

- Molecule 13 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	M	1	Total	C	N	O	0	0
			16	14	1	1		
13	L	1	Total	C	N	O	0	0
			16	14	1	1		

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

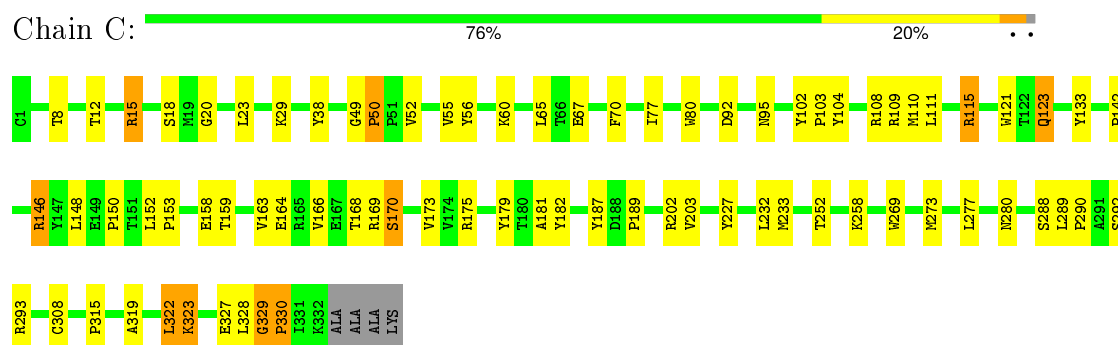
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	C	118	Total	O	0	0
			118	118		
14	H	64	Total	O	0	0
			64	64		
14	L	55	Total	O	0	0
			55	55		
14	M	78	Total	O	0	0
			78	78		

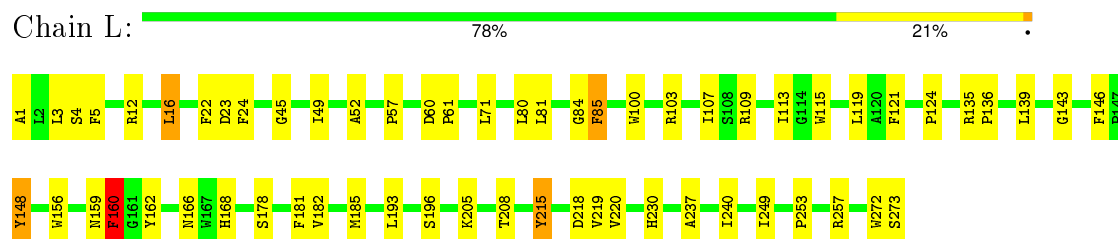
3 Residue-property plots

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.

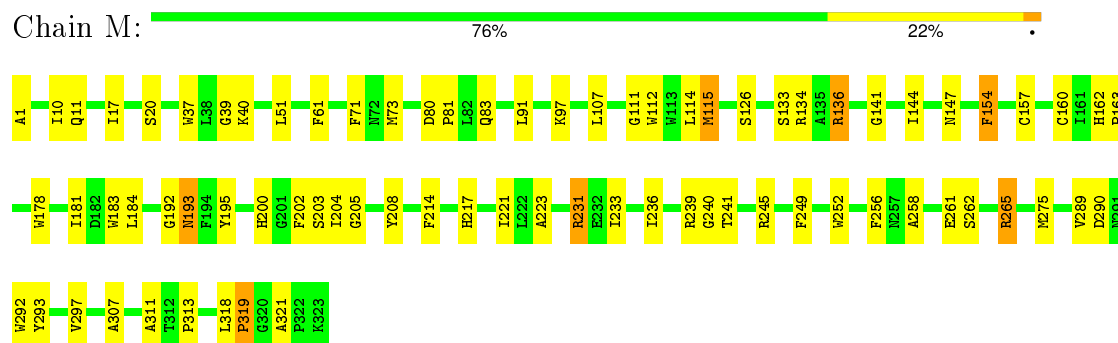
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER



• Molecule 2: PHOTOSYNTHETIC REACTION CENTER

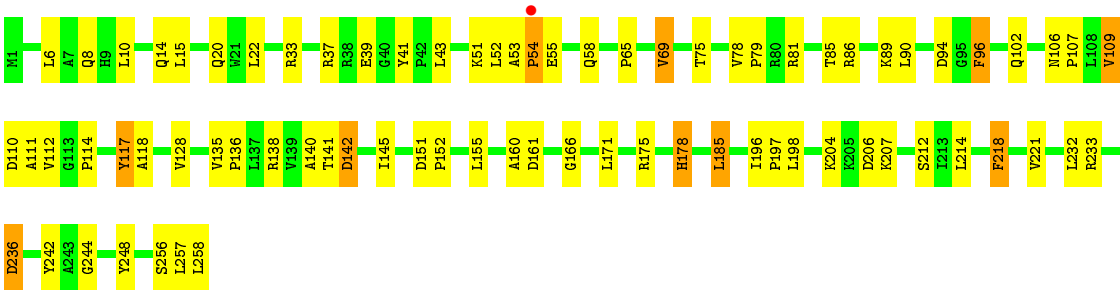


• Molecule 3: PHOTOSYNTHETIC REACTION CENTER



• Molecule 4: PHOTOSYNTHETIC REACTION CENTER





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)	10.00 – 2.65 29.74 – 2.60	Depositor EDS
% Data completeness (in resolution range)	88.3 (10.00-2.65) 87.0 (29.74-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.59 (at 2.61 Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.184 , 0.231 0.175 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 90.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 76928 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10476	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LDA, BPB, BCB, CET, FE2, SO4, 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	0.55	0/2674	0.67	2/3645 (0.1%)
2	L	0.58	0/2259	0.62	0/3084
3	M	0.58	0/2683	0.62	0/3669
4	H	0.67	2/2055 (0.1%)	0.86	4/2807 (0.1%)
All	All	0.59	2/9671 (0.0%)	0.69	6/13205 (0.0%)

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	4
2	L	0	7
3	M	0	5
4	H	0	2
All	All	0	18

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	54	PRO	C-N	14.77	1.68	1.34
4	H	52	LEU	C-N	-6.29	1.19	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	52	LEU	O-C-N	-18.31	93.41	122.70
4	H	52	LEU	CA-C-N	13.07	145.95	117.20
4	H	52	LEU	C-N-CA	8.96	144.09	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	53	ALA	CB-CA-C	-6.78	99.92	110.10
1	C	50	PRO	CB-CA-C	-5.63	97.93	112.00
1	C	329	GLY	C-N-CD	-5.03	109.53	120.60

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	15	ARG	Sidechain
1	C	187	TYR	Sidechain
1	C	202	ARG	Sidechain
1	C	227	TYR	Sidechain
4	H	117	TYR	Sidechain
4	H	218	PHE	Sidechain
2	L	103	ARG	Sidechain
2	L	148	TYR	Sidechain
2	L	160	PHE	Sidechain
2	L	162	TYR	Sidechain
2	L	215	TYR	Sidechain
2	L	257	ARG	Sidechain
2	L	85	PHE	Sidechain
3	M	154	PHE	Sidechain
3	M	231	ARG	Sidechain
3	M	249	PHE	Sidechain
3	M	265	ARG	Sidechain
3	M	61	PHE	Sidechain

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	2607	0	2575	54	0
2	L	2171	0	2098	46	0
3	M	2577	0	2468	60	0
4	H	2018	0	2019	51	0
5	M	1	0	0	0	0
6	H	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	M	15	0	0	2	0
7	L	132	0	144	10	0
7	M	132	0	144	14	0
8	L	130	0	148	18	0
9	M	48	0	64	1	0
10	C	172	0	120	6	0
11	M	40	0	60	7	0
12	L	17	0	15	1	0
13	H	16	0	31	1	0
13	L	16	0	31	0	0
13	M	64	0	124	5	0
14	C	118	0	0	3	0
14	H	64	0	0	0	0
14	L	55	0	0	1	0
14	M	78	0	0	2	0
All	All	10476	0	10041	216	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 11.

All (216) 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:H:54:PRO:C	4:H:55:GLU:N	1.68	1.44
8:L:402:BPB:HBBB	8:L:402:BPB:HHC	1.54	0.90
7:M:805:BCB:HBB2	7:M:805:BCB:HHC	1.57	0.85
8:L:402:BPB:HHC	8:L:402:BPB:CBB	2.09	0.83
2:L:181:PHE:HB3	8:L:401:BPB:CBB	2.10	0.81
1:C:65:LEU:HD11	1:C:327:GLU:HG2	1.65	0.78
4:H:152:PRO:HA	4:H:155:LEU:HD12	1.67	0.76
1:C:152:LEU:HB3	1:C:164:GLU:HG2	1.69	0.75
8:L:401:BPB:H4B	7:M:806:BCB:H172	1.69	0.75
13:M:701:LDA:HM21	13:M:705:LDA:H22	1.71	0.73
1:C:123[A]:GLN:HG3	1:C:269:TRP:CE3	2.24	0.73
3:M:107:LEU:HD22	3:M:112:TRP:CE2	2.26	0.71
2:L:178:SER:O	2:L:182:VAL:HG23	1.91	0.70
3:M:160:CYS:SG	11:M:600:NS5:C31	2.80	0.69
3:M:160:CYS:SG	11:M:600:NS5:H332	2.34	0.68
4:H:160:ALA:HB3	4:H:214:LEU:HD23	1.76	0.68
2:L:80:LEU:HA	2:L:84:GLY:HA3	1.73	0.67
4:H:161:ASP:HB3	4:H:214:LEU:HD22	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:LYS:HG2	3:M:307:ALA:HB2	1.77	0.66
1:C:52:VAL:HB	1:C:56:TYR:HD2	1.60	0.65
1:C:323:LYS:HD3	1:C:323:LYS:H	1.62	0.65
7:M:805:BCB:CBB	7:M:805:BCB:HHC	2.26	0.64
4:H:117:TYR:HB2	4:H:236:ASP:HB3	1.80	0.64
2:L:208:THR:HG21	4:H:128:VAL:HG23	1.79	0.64
1:C:52:VAL:HG13	1:C:65:LEU:O	1.98	0.64
1:C:290:PRO:HG2	1:C:293:ARG:HG2	1.79	0.64
3:M:202:PHE:CE2	4:H:20:GLN:HG2	2.32	0.63
3:M:195:TYR:CE2	7:M:806:BCB:HMC2	2.34	0.63
8:L:401:BPB:HHC	8:L:401:BPB:HBBB	1.80	0.63
7:L:302:BCB:OBB	7:L:302:BCB:HHC	1.99	0.63
3:M:107:LEU:HA	3:M:111:GLY:HA3	1.80	0.63
2:L:205:LYS:HA	4:H:69:VAL:HG22	1.80	0.63
1:C:152:LEU:HD22	1:C:175:ARG:HA	1.81	0.62
4:H:107:PRO:HA	4:H:110:ASP:HB2	1.82	0.62
3:M:160:CYS:SG	11:M:600:NS5:H322	2.40	0.61
1:C:323:LYS:H	1:C:323:LYS:CD	2.14	0.61
3:M:195:TYR:CZ	7:M:806:BCB:HMC2	2.36	0.61
3:M:178:TRP:HA	3:M:178:TRP:CE3	2.36	0.60
1:C:102:TYR:CG	1:C:103:PRO:HD3	2.36	0.60
2:L:185:MET:SD	7:M:805:BCB:H41	2.41	0.60
7:M:805:BCB:HBB3	7:M:806:BCB:H41	1.83	0.60
3:M:231:ARG:HD2	14:M:1013:HOH:O	2.02	0.59
2:L:230:HIS:CD2	3:M:221:ILE:HG13	2.37	0.59
8:L:401:BPB:HBBB	8:L:401:BPB:CHC	2.33	0.58
3:M:136:ARG:HE	3:M:136:ARG:HA	1.69	0.58
1:C:8:THR:HB	1:C:23:LEU:HB2	1.86	0.58
4:H:86:ARG:NH2	4:H:111:ALA:O	2.36	0.57
2:L:215:TYR:O	2:L:219:VAL:HG23	2.03	0.57
4:H:37:ARG:HG2	4:H:41:TYR:CZ	2.39	0.57
1:C:56:TYR:HB3	10:C:337:HEM:O2A	2.04	0.57
2:L:181:PHE:HB3	8:L:401:BPB:HBB	1.86	0.57
8:L:402:BPB:HBB	3:M:208:TYR:CD2	2.40	0.57
1:C:121:TRP:HA	1:C:123[A]:GLN:HE21	1.70	0.57
4:H:136:PRO:HG2	4:H:138:ARG:HG2	1.86	0.57
1:C:189:PRO:HB3	1:C:232:LEU:HA	1.86	0.56
7:L:302:BCB:HMC1	7:L:302:BCB:HBC3	1.88	0.56
2:L:181:PHE:CD2	8:L:401:BPB:HBB	2.41	0.56
12:L:502:CET:H101	12:L:502:CET:N3	2.21	0.56
8:L:401:BPB:HMDA	3:M:147:ASN:HD22	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:55:GLU:HB3	4:H:58:GLN:HG3	1.88	0.55
4:H:90:LEU:HA	4:H:102:GLN:O	2.06	0.55
1:C:52:VAL:HB	1:C:56:TYR:CD2	2.41	0.55
2:L:124:PRO:HB2	7:L:302:BCB:H93	1.89	0.54
7:L:304:BCB:HHC	7:L:304:BCB:OBB	2.07	0.54
3:M:192:GLY:O	3:M:193:ASN:HB3	2.06	0.54
4:H:166:GLY:HA3	4:H:185:LEU:HD12	1.89	0.54
2:L:220:VAL:HG11	8:L:401:BPB:HEDA	1.89	0.54
3:M:204:ILE:HG12	7:M:806:BCB:HMB3	1.90	0.54
4:H:218:PHE:HA	4:H:221:VAL:HG23	1.89	0.54
3:M:178:TRP:HA	3:M:178:TRP:HE3	1.72	0.53
4:H:114:PRO:HB2	4:H:244:GLY:HA2	1.90	0.53
2:L:109:ARG:HD2	14:L:1243:HOH:O	2.08	0.53
8:L:401:BPB:HBCA	3:M:275:MET:HG2	1.90	0.53
4:H:152:PRO:HD2	4:H:171:LEU:HD11	1.90	0.53
1:C:170:SER:HB2	3:M:83:GLN:HG3	1.90	0.53
2:L:185:MET:SD	7:M:805:BCB:C4	2.97	0.52
1:C:323:LYS:HD3	1:C:323:LYS:N	2.25	0.52
2:L:139:LEU:HD21	2:L:253:PRO:HD3	1.92	0.52
2:L:12:ARG:HD3	4:H:102:GLN:NE2	2.26	0.51
7:L:304:BCB:HMB1	7:L:304:BCB:CBB	2.41	0.51
1:C:319:ALA:HB2	14:C:1169:HOH:O	2.11	0.51
4:H:233:ARG:O	4:H:233:ARG:HG2	2.11	0.50
1:C:50:PRO:HB2	1:C:55:VAL:HG23	1.91	0.50
2:L:22:PHE:HA	2:L:24:PHE:CE1	2.47	0.50
2:L:193:LEU:HB2	3:M:144:ILE:HD11	1.94	0.50
4:H:155:LEU:HD22	4:H:206:ASP:C	2.32	0.50
3:M:160:CYS:SG	11:M:600:NS5:C30	3.00	0.50
2:L:81:LEU:HD23	2:L:85:PHE:CE2	2.47	0.50
3:M:289:VAL:HG11	3:M:292:TRP:CD2	2.47	0.50
2:L:124:PRO:HB2	7:L:302:BCB:C9	2.42	0.50
3:M:160:CYS:SG	11:M:600:NS5:C32	2.99	0.50
1:C:252:THR:HG23	1:C:252:THR:O	2.11	0.49
2:L:166:ASN:OD1	2:L:168:HIS:HB2	2.12	0.49
7:L:302:BCB:HMB1	7:L:302:BCB:CBB	2.42	0.49
1:C:123[A]:GLN:HG3	1:C:269:TRP:CD2	2.47	0.49
4:H:106:ASN:ND2	4:H:109:VAL:HG23	2.28	0.49
4:H:145:ILE:HD13	4:H:151:ASP:HA	1.95	0.49
3:M:160:CYS:SG	11:M:600:NS5:C33	2.99	0.49
4:H:65:PRO:HA	4:H:79:PRO:HD2	1.95	0.49
2:L:205:LYS:HA	4:H:69:VAL:CG2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:256:PHE:HB2	4:H:33:ARG:NH2	2.27	0.49
4:H:65:PRO:HG3	13:H:703:LDA:H82	1.95	0.48
1:C:146:ARG:NH2	1:C:150:PRO:HA	2.28	0.48
4:H:54:PRO:C	4:H:55:GLU:CA	2.73	0.48
4:H:37:ARG:HG2	4:H:41:TYR:CE1	2.48	0.48
4:H:204:LYS:HB2	4:H:207:LYS:O	2.13	0.48
4:H:96:PHE:H	4:H:96:PHE:HD1	1.61	0.48
1:C:65:LEU:HD11	1:C:327:GLU:CG	2.40	0.48
8:L:402:BPB:HBBA	3:M:208:TYR:HB3	1.95	0.48
3:M:73:MET:HE3	3:M:91:LEU:HB2	1.95	0.48
2:L:148:TYR:CE1	8:L:402:BPB:H14	2.48	0.48
3:M:200:HIS:CE1	3:M:204:ILE:HD11	2.48	0.48
7:M:806:BCB:HBD	7:M:806:BCB:HAA2	1.97	0.47
1:C:102:TYR:CD2	1:C:103:PRO:HD3	2.49	0.47
3:M:160:CYS:C	3:M:163:PRO:HD2	2.35	0.47
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.97	0.47
4:H:145:ILE:CD1	4:H:151:ASP:HA	2.45	0.47
1:C:52:VAL:HA	1:C:55:VAL:HB	1.97	0.47
2:L:22:PHE:HA	2:L:24:PHE:HE1	1.79	0.47
2:L:1:ALA:N	4:H:43:LEU:HB3	2.30	0.47
7:L:302:BCB:HBB3	7:M:805:BCB:HMD2	1.96	0.47
2:L:16:LEU:HD12	2:L:16:LEU:HA	1.63	0.47
3:M:154:PHE:O	3:M:157:CYS:HB2	2.14	0.47
7:M:806:BCB:HMB1	7:M:806:BCB:HBB3	1.96	0.47
3:M:289:VAL:HG11	3:M:292:TRP:CE3	2.50	0.46
1:C:115:ARG:HA	1:C:328:LEU:O	2.15	0.46
3:M:293:TYR:O	3:M:297:VAL:HG23	2.16	0.46
2:L:237:ALA:HA	2:L:240:ILE:HD12	1.97	0.46
2:L:196:SER:HB2	3:M:141:GLY:O	2.15	0.46
1:C:123[A]:GLN:H	1:C:123[A]:GLN:NE2	2.14	0.46
4:H:78:VAL:HA	4:H:79:PRO:C	2.36	0.46
2:L:113:ILE:HB	3:M:223:ALA:O	2.16	0.46
1:C:179:TYR:HB2	14:C:914:HOH:O	2.14	0.46
2:L:45:GLY:O	2:L:49:ILE:HG13	2.16	0.46
1:C:233:MET:HB3	10:C:339:HEM:C4B	2.51	0.46
8:L:401:BPB:C1B	7:M:805:BCB:H42	2.46	0.46
2:L:3:LEU:HD13	2:L:5:PHE:CZ	2.51	0.46
3:M:133:SER:OG	13:M:704:LDA:HM12	2.17	0.45
1:C:49:GLY:HA3	1:C:50:PRO:HD3	1.63	0.45
2:L:81:LEU:HD23	2:L:85:PHE:HE2	1.80	0.45
4:H:96:PHE:CD1	4:H:96:PHE:N	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:MET:O	1:C:277:LEU:HG	2.16	0.45
1:C:50:PRO:HB2	1:C:55:VAL:CG2	2.47	0.45
2:L:71:LEU:HD23	2:L:143:GLY:HA3	1.98	0.45
1:C:104:TYR:HE1	1:C:108:ARG:NH2	2.15	0.45
4:H:90:LEU:HD21	4:H:112:VAL:HB	1.99	0.45
1:C:110:MET:HB3	10:C:338:HEM:C4B	2.52	0.44
1:C:70:PHE:HE2	10:C:337:HEM:C2A	2.35	0.44
1:C:108:ARG:NH1	10:C:337:HEM:O2D	2.50	0.44
4:H:6:LEU:HA	4:H:6:LEU:HD23	1.77	0.44
2:L:218:ASP:HB3	3:M:134:ARG:HD2	1.99	0.44
1:C:163:VAL:HB	2:L:273:SER:O	2.17	0.44
3:M:10:ILE:CG2	4:H:145:ILE:HG23	2.48	0.44
1:C:181:ALA:O	1:C:182:TYR:HB2	2.18	0.44
2:L:107:ILE:HG23	3:M:252:TRP:HE3	1.83	0.44
7:M:805:BCB:HBA2	7:M:805:BCB:C4A	2.47	0.44
1:C:18:SER:HB2	2:L:156:TRP:CD1	2.53	0.44
3:M:112:TRP:CZ2	13:M:706:LDA:H51	2.53	0.43
1:C:92:ASP:HB3	1:C:95:ASN:O	2.18	0.43
3:M:241:THR:O	3:M:245:ARG:HG3	2.18	0.43
4:H:106:ASN:CG	4:H:109:VAL:HG23	2.39	0.43
3:M:262:SER:O	3:M:265:ARG:HB2	2.18	0.43
4:H:196:ILE:HD12	4:H:242:TYR:CE1	2.53	0.43
1:C:173:VAL:HG13	14:C:1137:HOH:O	2.18	0.43
2:L:115:TRP:CD1	2:L:115:TRP:N	2.86	0.43
1:C:109:ARG:NH2	1:C:280:ASN:O	2.52	0.43
11:M:600:NS5:H29	11:M:600:NS5:H271	1.71	0.43
4:H:114:PRO:HD2	4:H:248:TYR:CE2	2.53	0.43
1:C:308:CYS:O	1:C:315:PRO:HB3	2.18	0.43
8:L:401:BPB:H7A	8:L:401:BPB:H4	2.00	0.43
3:M:162:HIS:HD2	14:M:913:HOH:O	2.02	0.43
4:H:142:ASP:OD1	4:H:142:ASP:N	2.50	0.43
3:M:240:GLY:HA2	4:H:118:ALA:CB	2.49	0.43
3:M:183:TRP:CE3	3:M:184:LEU:HD23	2.53	0.43
3:M:239:ARG:HD3	4:H:39:GLU:OE1	2.18	0.43
3:M:112:TRP:O	3:M:115:MET:HB2	2.19	0.43
2:L:52:ALA:HB2	2:L:85:PHE:CG	2.53	0.43
1:C:111:LEU:HD23	10:C:338:HEM:CBB	2.49	0.43
3:M:233:ILE:O	3:M:236:ILE:HB	2.19	0.42
4:H:10:LEU:HD21	4:H:15:LEU:HD21	2.01	0.42
1:C:12:THR:OG1	1:C:20:GLY:HA2	2.19	0.42
2:L:80:LEU:HD12	2:L:80:LEU:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:217:HIS:CE1	3:M:221:ILE:HD11	2.55	0.42
1:C:322:LEU:HD11	1:C:330:PRO:HD3	2.00	0.42
4:H:69:VAL:HA	4:H:75:THR:HG22	2.01	0.42
4:H:135:VAL:HG23	4:H:140:ALA:HB2	2.01	0.42
3:M:11:GLN:OE1	3:M:39:GLY:HA3	2.20	0.42
2:L:60:ASP:HA	2:L:61:PRO:HD3	1.80	0.42
2:L:100:TRP:CH2	9:M:501:MQ7:H301	2.55	0.42
7:L:304:BCB:H62	7:L:304:BCB:H92	1.75	0.42
6:M:804:SO4:O4	13:M:704:LDA:H22	2.20	0.42
3:M:1:ALA:N	6:M:803:SO4:S	2.85	0.42
2:L:121:PHE:O	2:L:124:PRO:HG2	2.19	0.42
3:M:318:LEU:HB2	3:M:321:ALA:HB2	2.02	0.42
3:M:17:ILE:HG13	4:H:178:HIS:CE1	2.55	0.42
1:C:77:ILE:HD11	1:C:111:LEU:HD21	2.02	0.41
2:L:146:PHE:HB3	2:L:156:TRP:CD2	2.56	0.41
3:M:236:ILE:HG12	3:M:261:GLU:HB2	2.01	0.41
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.55	0.41
7:L:304:BCB:HBB3	7:L:304:BCB:HMB1	2.02	0.41
3:M:311:ALA:O	3:M:313:PRO:HD3	2.20	0.41
1:C:329:GLY:HA2	1:C:330:PRO:C	2.41	0.41
1:C:153:PRO:HG2	1:C:158:GLU:HB2	2.03	0.41
8:L:401:BPB:H4	8:L:401:BPB:C7	2.50	0.41
1:C:123[A]:GLN:CD	1:C:123[A]:GLN:H	2.24	0.41
1:C:289:LEU:HD22	1:C:293:ARG:HG3	2.01	0.41
3:M:258:ALA:HB1	3:M:262:SER:OG	2.21	0.41
3:M:205:GLY:HA3	13:M:701:LDA:H121	2.03	0.40
4:H:232:LEU:HA	4:H:232:LEU:HD23	1.89	0.40
3:M:318:LEU:HA	3:M:319:PRO:HD2	1.64	0.40
3:M:80:ASP:HA	3:M:81:PRO:HD2	1.87	0.40
8:L:401:BPB:H6	8:L:401:BPB:H4	1.96	0.40
4:H:196:ILE:HG13	4:H:197:PRO:HD2	2.03	0.40
2:L:159:ASN:O	2:L:160:PHE:C	2.58	0.40
1:C:60:LYS:HB2	1:C:108:ARG:NH1	2.36	0.40
3:M:202:PHE:CZ	4:H:20:GLN:HG2	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	331/336 (98%)	314 (95%)	14 (4%)	3 (1%)	21	44
2	L	271/273 (99%)	255 (94%)	14 (5%)	2 (1%)	26	51
3	M	323/323 (100%)	308 (95%)	12 (4%)	3 (1%)	21	44
4	H	256/258 (99%)	241 (94%)	15 (6%)	0	100	100
All	All	1181/1190 (99%)	1118 (95%)	55 (5%)	8 (1%)	26	51

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	51	LEU
3	M	193	ASN
2	L	57	PRO
1	C	67	GLU
2	L	23	ASP
1	C	148	LEU
3	M	319	PRO
1	C	330	PRO

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	281/282 (100%)	263 (94%)	18 (6%)	22	43
2	L	218/218 (100%)	212 (97%)	6 (3%)	51	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	M	251/249 (101%)	238 (95%)	13 (5%)	29	54
4	H	212/212 (100%)	190 (90%)	22 (10%)	9	18
All	All	962/961 (100%)	903 (94%)	59 (6%)	24	46

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	15	ARG
1	C	29	LYS
1	C	38	TYR
1	C	115	ARG
1	C	123[A]	GLN
1	C	123[B]	GLN
1	C	142	PRO
1	C	146	ARG
1	C	159	THR
1	C	166	VAL
1	C	168	THR
1	C	169	ARG
1	C	170	SER
1	C	203	VAL
1	C	288	SER
1	C	292	SER
1	C	322	LEU
1	C	323	LYS
2	L	4	SER
2	L	16	LEU
2	L	119	LEU
2	L	160	PHE
2	L	249	ILE
2	L	272	TRP
3	M	20	SER
3	M	37	TRP
3	M	40	LYS
3	M	71	PHE
3	M	97	LYS
3	M	114	LEU
3	M	115	MET
3	M	126	SER
3	M	136	ARG
3	M	181	ILE

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Mol	Chain	Res	Type
3	M	203	SER
3	M	214	PHE
3	M	290	ASP
4	H	8	GLN
4	H	14	GLN
4	H	22	LEU
4	H	51	LYS
4	H	69	VAL
4	H	81	ARG
4	H	85	THR
4	H	89	LYS
4	H	94	ASP
4	H	96	PHE
4	H	109	VAL
4	H	141	THR
4	H	142	ASP
4	H	175	ARG
4	H	178	HIS
4	H	185	LEU
4	H	198	LEU
4	H	212	SER
4	H	236	ASP
4	H	256	SER
4	H	257	LEU
4	H	258	LEU

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

Mol	Chain	Res	Type
2	L	183	ASN
2	L	214	GLN
2	L	239	ASN
3	M	147	ASN
4	H	102	GLN

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	$\# Z > 2$
4	FME	H	1	4	8,9,10	0.55	0	6,9,11	4.50	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
4	FME	H	1	4	-	0/6/9/11	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(°)
4	H	1	FME	O1-CN-N	-9.94	110.45	124.76
4	H	1	FME	CA-N-CN	-4.04	116.60	122.82
4	H	1	FME	O-C-CA	-2.09	119.92	125.44

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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
10	HEM	C	337	1	30,50,50	2.86	7 (23%)	24,82,82	2.94	10 (41%)
10	HEM	C	338	1	30,50,50	2.67	9 (30%)	24,82,82	3.14	9 (37%)
10	HEM	C	339	1	30,50,50	2.61	8 (26%)	24,82,82	3.48	10 (41%)
10	HEM	C	340	1	30,50,50	2.79	11 (36%)	24,82,82	2.64	10 (41%)
13	LDA	H	703	-	15,15,15	4.46	3 (20%)	16,17,17	0.82	0
6	SO4	H	801	-	4,4,4	1.19	0	6,6,6	0.35	0
7	BCB	L	302	2	56,74,74	1.47	6 (10%)	57,115,115	1.75	9 (15%)
7	BCB	L	304	2	56,74,74	1.34	7 (12%)	57,115,115	2.16	11 (19%)
8	BPB	L	401	-	63,70,70	1.39	8 (12%)	63,101,101	2.28	12 (19%)
8	BPB	L	402	-	63,70,70	1.42	9 (14%)	63,101,101	1.84	9 (14%)
12	CET	L	502	-	16,17,17	1.14	1 (6%)	16,23,23	0.89	1 (6%)
13	LDA	L	702	-	15,15,15	4.32	2 (13%)	16,17,17	0.49	0
9	MQ7	M	501	-	49,49,49	1.63	12 (24%)	62,63,63	1.84	14 (22%)
11	NS5	M	600	-	39,39,39	0.80	1 (2%)	44,46,46	1.17	5 (11%)
13	LDA	M	701	-	15,15,15	4.99	4 (26%)	16,17,17	0.99	0
13	LDA	M	704	-	15,15,15	3.66	2 (13%)	16,17,17	0.54	0
13	LDA	M	705	-	15,15,15	4.26	4 (26%)	16,17,17	0.62	0
13	LDA	M	706	-	15,15,15	4.24	4 (26%)	16,17,17	0.62	0
6	SO4	M	802	-	4,4,4	1.19	0	6,6,6	0.79	0
6	SO4	M	803	-	4,4,4	1.39	0	6,6,6	1.23	1 (16%)
6	SO4	M	804	-	4,4,4	1.74	1 (25%)	6,6,6	0.59	0
7	BCB	M	805	3	56,74,74	1.81	7 (12%)	57,115,115	1.89	10 (17%)
7	BCB	M	806	3	56,74,74	1.55	8 (14%)	57,115,115	2.25	12 (21%)

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
10	HEM	C	337	1	-	0/10/54/54	0/0/8/8
10	HEM	C	338	1	-	0/10/54/54	0/0/8/8
10	HEM	C	339	1	-	0/10/54/54	0/0/8/8
10	HEM	C	340	1	-	0/10/54/54	0/0/8/8
13	LDA	H	703	-	-	0/13/13/13	0/0/0/0
6	SO4	H	801	-	-	0/0/0/0	0/0/0/0
7	BCB	L	302	2	-	0/37/137/137	0/0/9/9
7	BCB	L	304	2	-	0/37/137/137	0/0/9/9
8	BPB	L	401	-	-	0/46/105/105	0/1/6/6
8	BPB	L	402	-	1/1/18/23	0/46/105/105	0/1/6/6
12	CET	L	502	-	-	0/11/14/14	0/1/1/1
13	LDA	L	702	-	-	0/13/13/13	0/0/0/0
9	MQ7	M	501	-	-	0/41/61/61	0/2/2/2
11	NS5	M	600	-	-	0/43/43/43	0/0/0/0
13	LDA	M	701	-	-	0/13/13/13	0/0/0/0
13	LDA	M	704	-	-	0/13/13/13	0/0/0/0
13	LDA	M	705	-	-	0/13/13/13	0/0/0/0
13	LDA	M	706	-	-	0/13/13/13	0/0/0/0
6	SO4	M	802	-	-	0/0/0/0	0/0/0/0
6	SO4	M	803	-	-	0/0/0/0	0/0/0/0
6	SO4	M	804	-	-	0/0/0/0	0/0/0/0
7	BCB	M	805	3	-	0/37/137/137	0/0/9/9
7	BCB	M	806	3	-	0/37/137/137	0/0/9/9

All (114) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	701	LDA	O1-N1	-18.26	1.22	1.39
13	H	703	LDA	O1-N1	-16.44	1.23	1.39
13	L	702	LDA	O1-N1	-16.37	1.23	1.39
13	M	705	LDA	O1-N1	-15.83	1.24	1.39
13	M	706	LDA	O1-N1	-15.76	1.24	1.39
13	M	704	LDA	O1-N1	-13.56	1.26	1.39
10	C	337	HEM	C3B-C4B	-9.62	1.43	1.51
10	C	338	HEM	C3B-C4B	-7.97	1.44	1.51
10	C	339	HEM	C3B-C4B	-6.95	1.45	1.51
10	C	340	HEM	C3B-C4B	-6.39	1.46	1.51
7	L	302	BCB	C4D-CHA	-6.31	1.37	1.45
7	M	805	BCB	C4D-CHA	-6.27	1.37	1.45
10	C	340	HEM	C2D-C3D	-6.27	1.35	1.54
10	C	340	HEM	C3D-C4D	-6.24	1.43	1.51
10	C	338	HEM	C2D-C3D	-6.12	1.36	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	338	HEM	C3D-C4D	-6.12	1.43	1.51
10	C	339	HEM	C2D-C3D	-6.04	1.36	1.54
10	C	337	HEM	C2D-C3D	-6.00	1.36	1.54
7	M	806	BCB	C4D-CHA	-5.81	1.37	1.45
7	L	304	BCB	C4D-CHA	-5.62	1.38	1.45
10	C	339	HEM	C3D-C4D	-5.39	1.44	1.51
10	C	337	HEM	C3D-C4D	-5.11	1.45	1.51
10	C	337	HEM	C2C-C1C	-4.66	1.43	1.52
10	C	340	HEM	CAD-C3D	-4.63	1.44	1.54
8	L	402	BPB	O2D-CED	-4.47	1.34	1.45
13	M	701	LDA	C1-N1	-4.46	1.43	1.51
10	C	339	HEM	C2C-C1C	-4.31	1.44	1.52
10	C	340	HEM	C2C-C1C	-4.11	1.44	1.52
7	M	805	BCB	O2D-CED	-3.98	1.35	1.45
7	L	302	BCB	O2D-CED	-3.96	1.35	1.45
10	C	338	HEM	C2C-C1C	-3.82	1.45	1.52
7	M	805	BCB	C1-C2	-3.80	1.36	1.49
13	H	703	LDA	CM1-N1	-3.69	1.43	1.49
13	M	701	LDA	CM1-N1	-3.54	1.44	1.49
13	H	703	LDA	C1-N1	-3.51	1.45	1.51
9	M	501	MQ7	C21-C22	-3.35	1.41	1.50
9	M	501	MQ7	C11-C12	-3.28	1.45	1.50
13	M	705	LDA	C1-N1	-3.18	1.45	1.51
13	M	704	LDA	CM1-N1	-3.01	1.44	1.49
7	L	302	BCB	C1-C2	-2.80	1.39	1.49
13	M	706	LDA	C1-N1	-2.72	1.46	1.51
11	M	600	NS5	C22-C21	-2.61	1.45	1.50
13	M	706	LDA	CM2-N1	-2.59	1.45	1.49
13	M	701	LDA	CM2-N1	-2.58	1.45	1.49
9	M	501	MQ7	C16-C17	-2.55	1.43	1.50
9	M	501	MQ7	C10-C5	-2.54	1.36	1.40
7	L	302	BCB	C4C-C3C	-2.51	1.40	1.45
7	M	806	BCB	C4C-C3C	-2.45	1.40	1.45
7	M	806	BCB	CAA-CBA	-2.44	1.44	1.52
13	M	705	LDA	CM1-N1	-2.42	1.45	1.49
13	M	706	LDA	CM1-N1	-2.41	1.45	1.49
13	M	705	LDA	CM2-N1	-2.38	1.45	1.49
7	L	304	BCB	O2D-CED	-2.35	1.39	1.45
6	M	804	SO4	O1-S	-2.34	1.39	1.47
8	L	402	BPB	C4C-C3C	-2.30	1.40	1.45
7	L	304	BCB	C3D-C2D	-2.23	1.34	1.40
10	C	340	HEM	C2D-C1D	-2.23	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	337	HEM	C2B-C1B	-2.15	1.44	1.51
8	L	401	BPB	C4C-C3C	-2.14	1.40	1.45
10	C	338	HEM	C2B-C1B	-2.12	1.44	1.51
7	L	304	BCB	C2C-C1C	-2.11	1.50	1.51
13	L	702	LDA	CM2-N1	-2.09	1.46	1.49
10	C	339	HEM	C2B-C1B	-2.02	1.45	1.51
10	C	338	HEM	C2D-C1D	-2.02	1.45	1.51
10	C	340	HEM	C1C-NC	2.02	1.38	1.36
7	L	304	BCB	CAC-C3C	2.04	1.35	1.33
7	M	806	BCB	C1A-CHA	2.05	1.41	1.37
10	C	340	HEM	C4C-NC	2.07	1.38	1.36
10	C	340	HEM	FE-NC	2.07	2.04	1.95
7	M	806	BCB	CMD-C2D	2.14	1.56	1.51
7	M	806	BCB	O2D-CGD	2.16	1.38	1.33
8	L	401	BPB	C4D-ND	2.21	1.41	1.36
8	L	402	BPB	CMB-C2B	2.22	1.56	1.51
7	M	805	BCB	O2D-CGD	2.22	1.38	1.33
8	L	402	BPB	O2A-CGA	2.32	1.40	1.33
10	C	338	HEM	FE-NC	2.33	2.05	1.95
9	M	501	MQ7	C42-C43	2.34	1.39	1.32
9	M	501	MQ7	C19-C18	2.35	1.56	1.50
7	L	302	BCB	C2-C3	2.46	1.37	1.33
9	M	501	MQ7	C12-C13	2.47	1.37	1.33
9	M	501	MQ7	C22-C23	2.49	1.37	1.33
7	M	805	BCB	C2-C3	2.60	1.38	1.33
7	L	304	BCB	O2D-CGD	2.60	1.39	1.33
8	L	401	BPB	O2D-CGD	2.63	1.39	1.33
8	L	402	BPB	O2D-CGD	2.66	1.40	1.33
8	L	401	BPB	C1A-CHA	2.79	1.42	1.36
7	M	805	BCB	O2A-CGA	2.81	1.41	1.33
10	C	339	HEM	C4C-NC	2.81	1.39	1.36
8	L	401	BPB	C3B-C4B	2.89	1.45	1.41
7	L	304	BCB	C2-C3	2.93	1.38	1.33
9	M	501	MQ7	C17-C18	2.96	1.38	1.33
9	M	501	MQ7	C27-C28	3.01	1.38	1.33
9	M	501	MQ7	C37-C38	3.05	1.39	1.33
7	M	806	BCB	C2-C3	3.07	1.39	1.33
8	L	402	BPB	CAC-C3C	3.13	1.37	1.33
7	L	302	BCB	O2D-CGD	3.18	1.41	1.33
8	L	402	BPB	CMD-C2D	3.19	1.57	1.50
8	L	402	BPB	C2-C3	3.21	1.39	1.33
12	L	502	CET	C9-N9	3.27	1.19	1.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	401	BPB	C2-C3	3.44	1.39	1.33
10	C	338	HEM	CBB-CAB	3.64	1.50	1.29
10	C	340	HEM	CBB-CAB	3.75	1.51	1.29
9	M	501	MQ7	C32-C33	3.90	1.40	1.33
10	C	338	HEM	CBC-CAC	4.01	1.52	1.29
10	C	337	HEM	CBC-CAC	4.06	1.52	1.29
10	C	337	HEM	CBB-CAB	4.14	1.53	1.29
10	C	339	HEM	CBB-CAB	4.38	1.54	1.29
8	L	401	BPB	O2A-CGA	4.43	1.46	1.33
10	C	339	HEM	CBC-CAC	4.48	1.55	1.29
7	M	806	BCB	CAC-C3C	4.58	1.38	1.33
10	C	340	HEM	CBC-CAC	4.74	1.56	1.29
8	L	402	BPB	C3B-C4B	5.06	1.48	1.41
8	L	401	BPB	CAC-C3C	5.32	1.39	1.33
7	M	805	BCB	CAC-C3C	7.93	1.43	1.33

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	339	HEM	C3B-CAB-CBB	-8.80	110.95	124.46
10	C	338	HEM	C3C-CAC-CBC	-8.32	111.70	124.46
10	C	339	HEM	C3C-CAC-CBC	-8.01	112.17	124.46
10	C	337	HEM	C3B-CAB-CBB	-7.96	112.24	124.46
7	L	304	BCB	O1D-CGD-CBD	-7.32	114.14	124.62
8	L	402	BPB	O1D-CGD-CBD	-7.30	114.15	124.62
10	C	338	HEM	C3B-CAB-CBB	-7.03	113.67	124.46
8	L	401	BPB	O1D-CGD-CBD	-7.01	114.58	124.62
7	M	806	BCB	O1D-CGD-CBD	-6.39	115.47	124.62
10	C	337	HEM	C3C-CAC-CBC	-5.97	115.30	124.46
7	M	805	BCB	O1D-CGD-CBD	-5.80	116.31	124.62
7	L	302	BCB	O1D-CGD-CBD	-5.77	116.36	124.62
10	C	340	HEM	C3B-CAB-CBB	-5.56	115.92	124.46
9	M	501	MQ7	C29-C28-C30	-5.27	107.36	115.41
8	L	401	BPB	CBB-CAB-C3B	-4.23	107.77	120.33
9	M	501	MQ7	C40-C41-C42	-4.10	100.96	111.69
11	M	600	NS5	C19-C20-C21	-4.04	121.36	127.20
9	M	501	MQ7	C34-C33-C35	-3.96	109.36	115.41
10	C	340	HEM	CAA-C2A-C1A	-3.78	122.91	127.01
9	M	501	MQ7	C24-C23-C25	-3.75	109.68	115.41
7	L	302	BCB	CED-O2D-CGD	-3.59	107.56	115.99
7	L	302	BCB	OBD-CAD-CBD	-3.51	120.64	125.94
7	M	805	BCB	OBD-CAD-CBD	-3.42	120.78	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	304	BCB	OBD-CAD-CBD	-3.39	120.83	125.94
7	M	806	BCB	OBD-CAD-CBD	-3.36	120.87	125.94
7	M	806	BCB	O2A-CGA-O1A	-3.27	115.05	123.49
7	M	805	BCB	C5-C3-C2	-3.12	115.13	121.05
8	L	401	BPB	C2C-C3C-C4C	-3.11	104.39	107.24
10	C	338	HEM	CBA-CAA-C2A	-3.06	107.05	112.53
7	L	304	BCB	CBC-CAC-C3C	-3.05	120.04	127.07
10	C	340	HEM	C3C-CAC-CBC	-3.05	119.78	124.46
10	C	339	HEM	CAA-C2A-C3A	-2.94	120.60	129.00
6	M	803	SO4	O2-S-O1	-2.91	100.27	109.50
8	L	402	BPB	C4-C3-C5	-2.89	111.00	115.41
7	M	806	BCB	CBB-CAB-C3B	-2.64	112.48	120.33
9	M	501	MQ7	C21-C20-C18	-2.60	104.23	112.71
7	M	806	BCB	CAA-C2A-C1A	-2.60	103.31	112.47
7	L	304	BCB	C4-C3-C5	-2.46	111.66	115.41
11	M	600	NS5	C22-C21-C23	-2.43	114.05	118.10
7	L	302	BCB	CBC-CAC-C3C	-2.43	121.46	127.07
8	L	402	BPB	O2A-CGA-O1A	-2.41	117.28	123.49
9	M	501	MQ7	C21-C22-C23	-2.38	122.59	127.76
12	L	502	CET	C11-C10-C8	-2.33	108.98	115.16
8	L	401	BPB	CBD-CHA-C4D	-2.29	105.90	108.46
7	M	806	BCB	CBC-CAC-C3C	-2.27	121.83	127.07
8	L	402	BPB	CBD-CHA-C4D	-2.25	105.94	108.46
9	M	501	MQ7	C36-C37-C38	-2.21	122.95	127.76
9	M	501	MQ7	C14-C13-C12	-2.21	119.16	123.50
8	L	402	BPB	C2C-C3C-C4C	-2.20	105.23	107.24
7	M	805	BCB	OBB-CAB-C3B	-2.11	116.67	120.00
8	L	401	BPB	CHD-C4C-NC	-2.05	121.00	124.91
7	L	304	BCB	O2A-CGA-O1A	-2.04	118.23	123.49
10	C	337	HEM	CAA-C2A-C3A	-2.01	123.26	129.00
7	M	806	BCB	C3C-C4C-NC	2.00	111.73	110.24
8	L	401	BPB	C10-C8-C7	2.02	124.30	112.27
8	L	402	BPB	CBD-CHA-C1A	2.03	130.21	126.78
10	C	340	HEM	CBD-CAD-C3D	2.14	119.78	113.55
10	C	337	HEM	CAA-C2A-C1A	2.15	129.34	127.01
9	M	501	MQ7	C44-C43-C42	2.16	129.56	122.61
10	C	337	HEM	CMD-C2D-C3D	2.19	124.03	114.35
11	M	600	NS5	C18-C19-C20	2.19	128.24	123.39
8	L	401	BPB	CBD-CHA-C1A	2.28	130.63	126.78
11	M	600	NS5	C19-C18-C17	2.34	128.56	123.39
8	L	402	BPB	O2A-CGA-CBA	2.51	119.55	111.90
8	L	401	BPB	C3C-C2C-C1C	2.55	104.75	100.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	340	HEM	CBA-CAA-C2A	2.56	117.11	112.53
11	M	600	NS5	C23-C21-C20	2.61	123.18	118.98
10	C	340	HEM	CMB-C2B-C3B	2.64	123.12	116.53
7	L	304	BCB	C3C-C4C-NC	2.66	112.22	110.24
9	M	501	MQ7	C31-C32-C33	2.72	133.69	127.76
7	M	805	BCB	C3C-C4C-NC	2.73	112.28	110.24
7	L	302	BCB	CMB-C2B-C3B	2.82	130.60	125.09
10	C	338	HEM	CAD-C3D-C4D	2.86	122.56	112.47
7	L	304	BCB	CMB-C2B-C3B	2.87	130.70	125.09
10	C	340	HEM	CMD-C2D-C3D	2.87	127.06	114.35
10	C	337	HEM	C2D-C3D-C4D	2.90	106.41	101.50
10	C	338	HEM	CMD-C2D-C3D	2.96	127.44	114.35
8	L	402	BPB	C3C-C2C-C1C	2.98	105.39	100.99
7	L	304	BCB	OBB-CAB-C3B	3.01	124.78	120.00
10	C	339	HEM	C2D-C3D-C4D	3.03	106.63	101.50
7	L	302	BCB	C3C-C4C-NC	3.06	112.52	110.24
10	C	338	HEM	C2D-C3D-C4D	3.14	106.82	101.50
7	M	805	BCB	O2A-CGA-CBA	3.20	121.66	111.90
7	M	805	BCB	CMB-C2B-C3B	3.26	131.46	125.09
9	M	501	MQ7	C30-C28-C27	3.30	127.31	121.05
7	L	302	BCB	C4A-NA-C1A	3.31	109.94	106.04
10	C	339	HEM	CMD-C2D-C3D	3.35	129.19	114.35
10	C	340	HEM	C2D-C3D-C4D	3.41	107.28	101.50
7	L	302	BCB	OBB-CAB-C3B	3.47	125.50	120.00
7	L	304	BCB	O2A-CGA-CBA	3.49	122.53	111.90
8	L	401	BPB	C6-C5-C3	3.54	120.25	112.48
7	L	304	BCB	C4A-NA-C1A	3.59	110.27	106.04
7	M	805	BCB	C4A-NA-C1A	3.60	110.28	106.04
10	C	337	HEM	CMB-C2B-C3B	3.65	125.63	116.53
10	C	337	HEM	CAD-C3D-C2D	3.69	123.82	113.22
10	C	339	HEM	CAD-C3D-C4D	3.71	125.55	112.47
7	M	806	BCB	C4A-NA-C1A	4.04	110.81	106.04
9	M	501	MQ7	C41-C42-C43	4.10	143.52	127.73
10	C	340	HEM	CMC-C2C-C3C	4.10	126.77	116.53
10	C	339	HEM	CMC-C2C-C3C	4.21	127.03	116.53
10	C	338	HEM	CMC-C2C-C3C	4.22	127.07	116.53
9	M	501	MQ7	C35-C33-C32	4.31	129.23	121.05
9	M	501	MQ7	C25-C23-C22	4.32	129.24	121.05
7	M	806	BCB	O2A-CGA-CBA	4.33	125.10	111.90
10	C	338	HEM	CMB-C2B-C3B	4.55	127.89	116.53
10	C	339	HEM	CAA-C2A-C1A	4.59	131.99	127.01
7	M	805	BCB	C4-C3-C5	4.63	122.47	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	337	HEM	CAD-C3D-C4D	4.88	129.69	112.47
7	L	302	BCB	O2D-CGD-CBD	5.06	118.24	111.30
10	C	339	HEM	CAD-C3D-C2D	5.07	127.80	113.22
8	L	401	BPB	CED-O2D-CGD	5.13	128.01	115.99
10	C	337	HEM	CMC-C2C-C3C	5.45	130.12	116.53
10	C	339	HEM	CMB-C2B-C3B	5.76	130.90	116.53
7	M	806	BCB	CMB-C2B-C3B	5.85	136.54	125.09
7	M	806	BCB	OBB-CAB-C3B	5.89	129.34	120.00
10	C	338	HEM	CAD-C3D-C2D	6.02	130.53	113.22
7	M	805	BCB	O2D-CGD-CBD	6.94	120.82	111.30
10	C	340	HEM	CAD-C3D-C2D	7.02	133.39	113.22
8	L	401	BPB	OBB-CAB-C3B	7.30	131.56	120.00
7	M	806	BCB	O2D-CGD-CBD	7.79	121.99	111.30
8	L	402	BPB	O2D-CGD-CBD	8.36	122.77	111.30
7	L	304	BCB	O2D-CGD-CBD	9.32	124.09	111.30
8	L	401	BPB	O2D-CGD-CBD	9.71	124.63	111.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	L	402	BPB	C13

There are no torsion outliers.

There are no ring outliers.

19 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	337	HEM	3	0
10	C	338	HEM	2	0
10	C	339	HEM	1	0
13	H	703	LDA	1	0
7	L	302	BCB	6	0
7	L	304	BCB	4	0
8	L	401	BPB	13	0
8	L	402	BPB	5	0
12	L	502	CET	1	0
9	M	501	MQ7	1	0
11	M	600	NS5	7	0
13	M	701	LDA	2	0
13	M	704	LDA	2	0
13	M	705	LDA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	706	LDA	1	0
6	M	803	SO4	1	0
6	M	804	SO4	1	0
7	M	805	BCB	8	0
7	M	806	BCB	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 [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(Å²)	Q<0.9	
1	C	332/336 (98%)	-0.75	0	100	100	4, 20, 44, 66	18 (5%)
2	L	273/273 (100%)	-0.88	0	100	100	4, 16, 41, 61	6 (2%)
3	M	323/323 (100%)	-0.76	0	100	100	4, 18, 48, 60	10 (3%)
4	H	249/258 (96%)	-0.62	1 (0%)	93	94	6, 27, 58, 76	19 (7%)
All	All	1177/1190 (98%)	-0.76	1 (0%)	95	96	4, 20, 48, 76	53 (4%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	54	PRO	3.4

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
4	FME	H	1	10/11	0.96	0.10	-	23,30,40,42	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(Å ²)	Q<0.9
13	LDA	M	704	16/16	0.80	0.34	6.01	55,59,79,81	0
13	LDA	M	706	16/16	0.77	0.36	5.83	68,71,72,73	4
13	LDA	L	702	16/16	0.73	0.38	5.38	17,45,71,72	0
11	NS5	M	600	40/40	0.84	0.23	4.29	23,40,76,76	4
13	LDA	H	703	16/16	0.93	0.22	2.05	27,38,57,58	0
13	LDA	M	705	16/16	0.80	0.23	0.84	53,58,69,69	5
8	BPB	L	402	65/65	0.97	0.10	0.47	2,6,13,17	0
7	BCB	M	806	66/66	0.97	0.12	0.43	2,10,25,29	0
9	MQ7	M	501	48/48	0.94	0.13	0.42	3,15,34,38	0
8	BPB	L	401	65/65	0.95	0.13	0.37	2,21,70,70	7
10	HEM	C	338	43/43	0.97	0.14	0.33	11,22,28,33	0
10	HEM	C	340	43/43	0.97	0.11	0.21	5,13,30,44	0
7	BCB	M	805	66/66	0.95	0.12	0.17	2,15,44,46	0
7	BCB	L	304	66/66	0.98	0.12	0.16	2,6,21,27	0
7	BCB	L	302	66/66	0.97	0.11	0.15	2,8,15,19	0
6	SO4	M	804	5/5	0.98	0.12	0.02	39,39,44,44	0
13	LDA	M	701	16/16	0.96	0.11	-0.13	11,21,24,27	0
10	HEM	C	339	43/43	0.98	0.10	-0.14	2,10,15,23	0
6	SO4	H	801	5/5	0.98	0.09	-0.36	56,56,57,57	0
12	CET	L	502	17/17	0.98	0.11	-0.36	10,18,21,25	0
6	SO4	M	802	5/5	0.99	0.09	-0.60	21,24,27,28	0
10	HEM	C	337	43/43	0.97	0.10	-0.77	8,21,30,39	0
5	FE2	M	500	1/1	0.99	0.04	-3.48	16,16,16,16	0
6	SO4	M	803	5/5	0.95	0.18	-	73,74,76,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.