



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:56 PM GMT

PDB ID : 5PRC  
Title : PHOTOSYNTHETIC REACTION CENTER FROM RHODOPSEUDOMONAS VIRIDIS (ATRAZINE COMPLEX)  
Authors : Lancaster, C.R.D.; Michel, H.  
Deposited on : 1997-08-01  
Resolution : 2.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

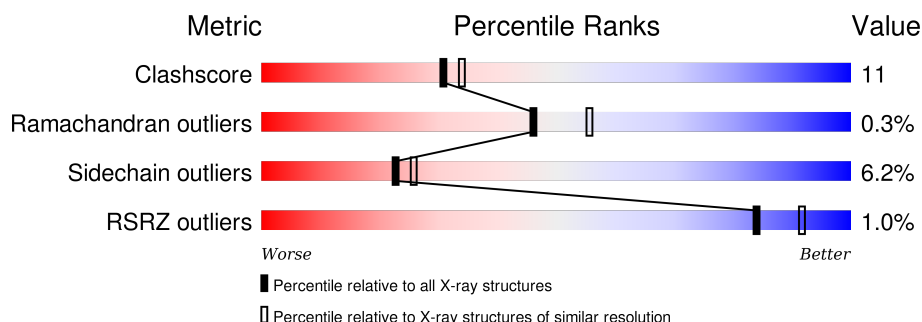
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	336	<div> <div>2%</div> <div>78%</div> <div>18%</div> <div>..</div> </div>
2	L	273	<div> <div>82%</div> <div>16%</div> <div>.</div> </div>
3	M	323	<div> <div>72%</div> <div>24%</div> <div>.</div> </div>
4	H	258	<div> <div>2%</div> <div>74%</div> <div>24%</div> <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
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 10501 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	50	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	15	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).

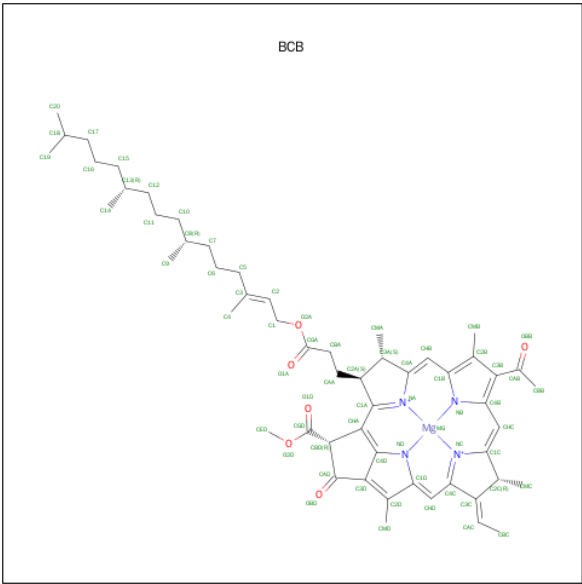
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	1	Total	Fe	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



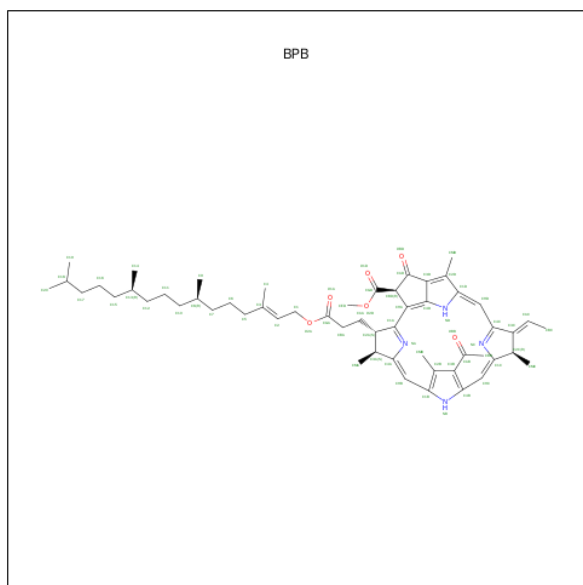
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>6</sub>).



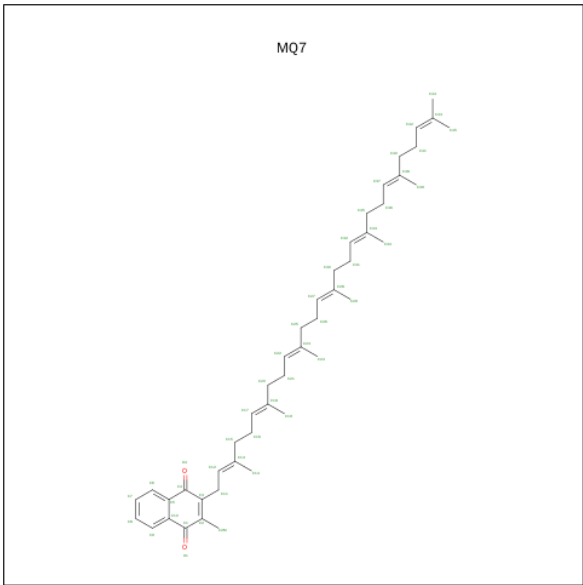
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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



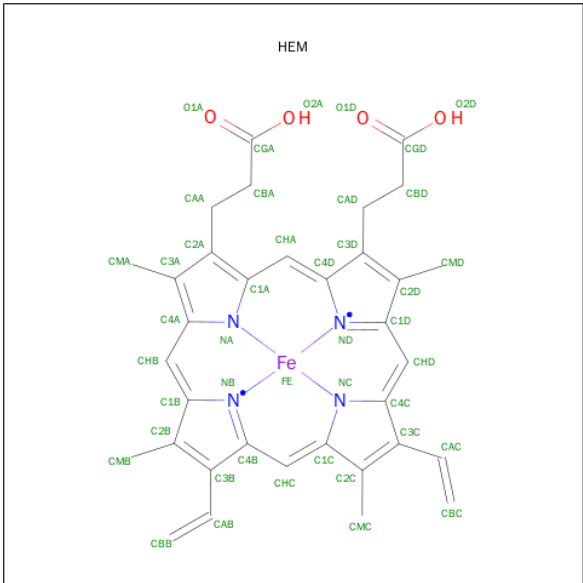
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	M	1	Total	C	N	O	7	0
			65	55	4	6		
8	L	1	Total	C	N	O	0	0
			65	55	4	6		

- 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:  $C_{34}H_{32}FeN_4O_4$ ).



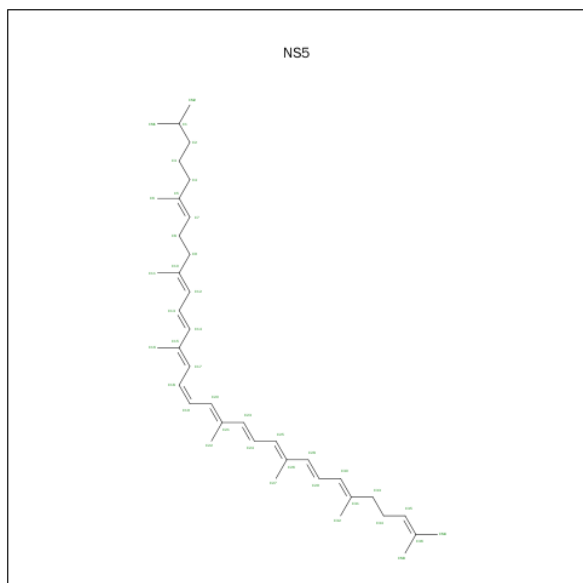
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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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	

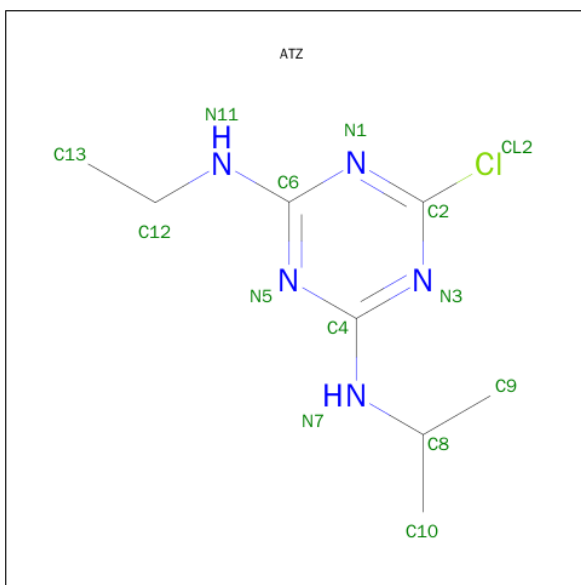
- Molecule 11 is 15-CIS-1,2-DIHYDRONEUROSPORENE (three-letter code: NS5) (formula:  $C_{40}H_{60}$ ).



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

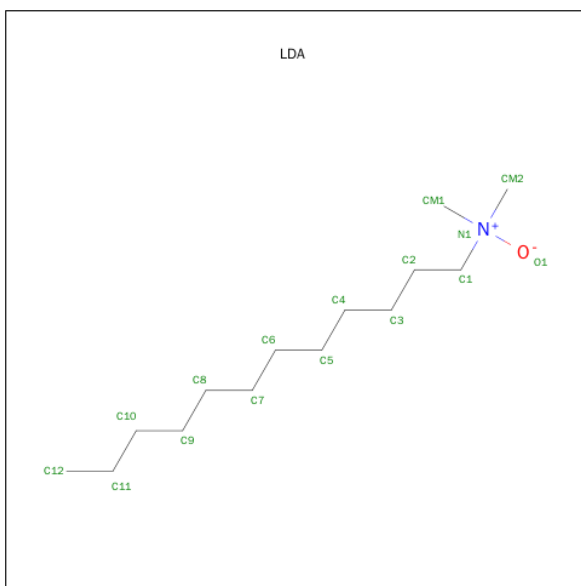
- Molecule 12 is 2-CHLORO-4-ISOPROPYLAMINO-6-ETHYLAMINO -1,3,5-TRIAZINE (three-letter code: ATZ) (formula:  $C_8H_{14}ClN_5$ ).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	L	1	Total	C	Cl	N	0	0
			14	8	1	5		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	H	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	L	1	Total	C	N	O	3	0
			16	14	1	1		
13	M	1	Total	C	N	O	4	0
			16	14	1	1		

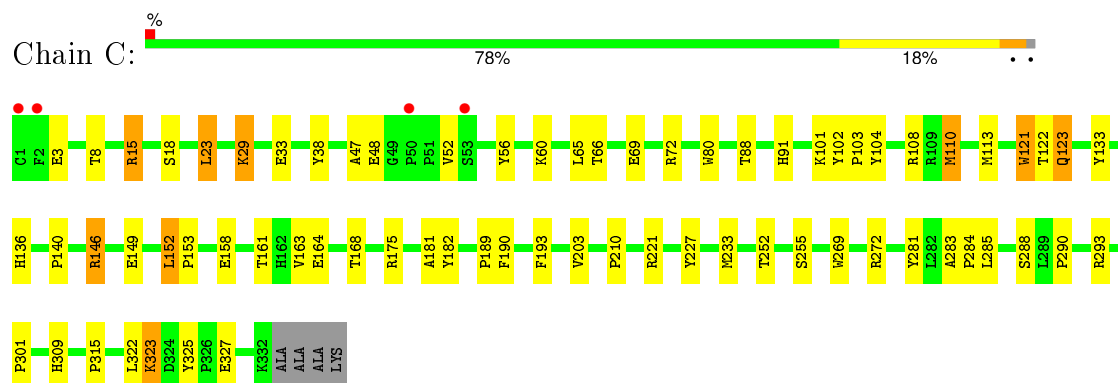
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	C	134	Total	O	0	0
			134	134		
14	H	81	Total	O	0	0
			81	81		
14	L	57	Total	O	0	0
			57	57		
14	M	71	Total	O	0	0
			71	71		

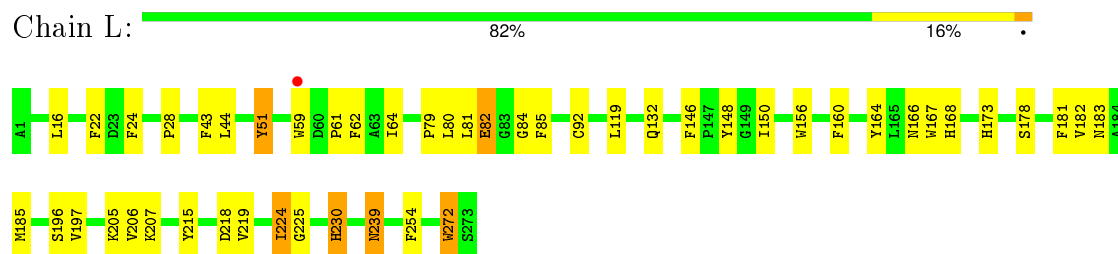
### 3 Residue-property plots [i](#)

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.

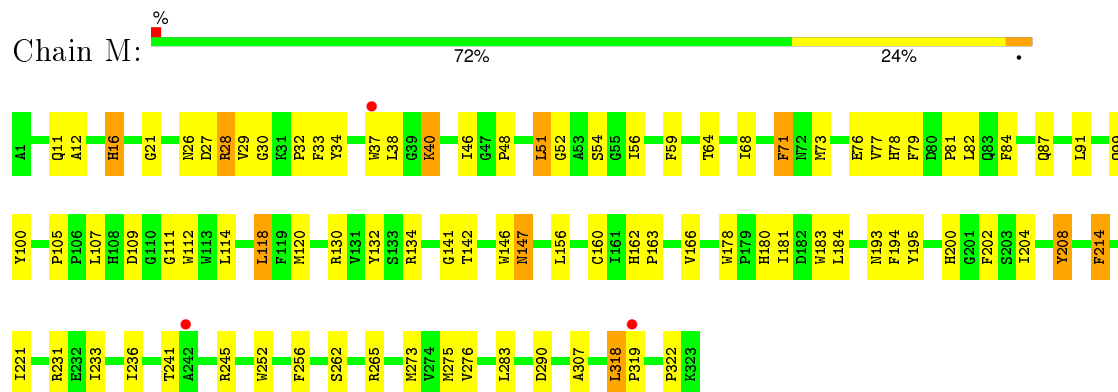
#### • Molecule 1: PHOTOSYNTHETIC REACTION CENTER

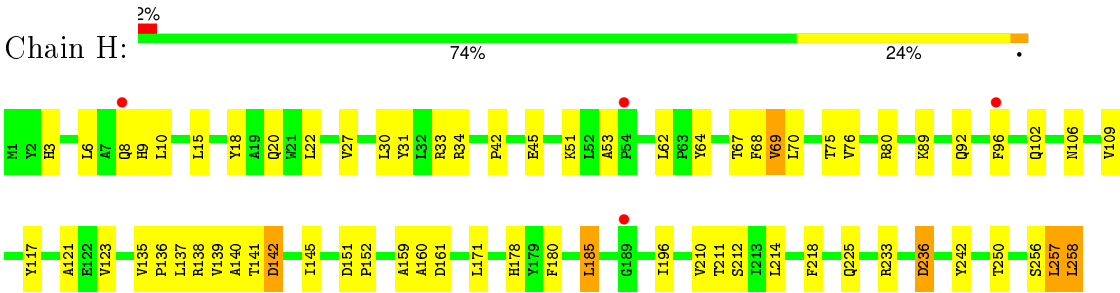


#### • Molecule 2: PHOTOSYNTHETIC REACTION CENTER



#### • Molecule 3: PHOTOSYNTHETIC REACTION CENTER





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	223.50 Å   223.50 Å   113.60 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	10.00 – 2.35 29.64 – 2.30	Depositor EDS
% Data completeness (in resolution range)	78.5 (10.00-2.35) 76.5 (29.64-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.85 (at 2.31 Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.190   ,   0.236 0.181   ,   (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	29.5	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 101.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 96950 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10501	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LDA, BPB, BCB, FE2, SO4, MQ7, HEM, FME, ATZ, 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	0.52	0/2674	0.62	0/3645
2	L	0.54	0/2259	0.58	0/3084
3	M	0.55	0/2683	0.61	1/3669 (0.0%)
4	H	0.53	0/2055	0.69	2/2807 (0.1%)
All	All	0.53	0/9671	0.62	3/13205 (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	6
2	L	0	4
3	M	0	2
4	H	0	3
All	All	0	15

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	53	ALA	CB-CA-C	-10.63	94.16	110.10
3	M	318	LEU	O-C-N	6.16	132.81	121.10
4	H	45	GLU	CB-CA-C	-5.25	99.89	110.40

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	121	TRP	Mainchain
1	C	15	ARG	Sidechain
1	C	190	PHE	Sidechain
1	C	227	TYR	Sidechain
1	C	272	ARG	Sidechain
1	C	325	TYR	Sidechain
4	H	18	TYR	Sidechain
4	H	34	ARG	Sidechain
4	H	64	TYR	Sidechain
2	L	148	TYR	Sidechain
2	L	164	TYR	Sidechain
2	L	230	HIS	Sidechain
2	L	51	TYR	Sidechain
3	M	208	TYR	Sidechain
3	M	28	ARG	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	41	0
2	L	2171	0	2098	41	0
3	M	2577	0	2468	74	0
4	H	2018	0	2020	42	0
5	M	1	0	0	0	0
6	H	5	0	0	0	0
6	M	15	0	0	1	0
7	L	132	0	144	10	0
7	M	132	0	144	20	0
8	L	65	0	74	9	0
8	M	65	0	74	10	0
9	M	48	0	64	1	0
10	C	172	0	120	3	0
11	M	40	0	60	6	0
12	L	14	0	14	2	0
13	H	32	0	62	2	0
13	L	32	0	62	4	0
13	M	32	0	62	2	0
14	C	134	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	H	81	0	0	1	0
14	L	57	0	0	0	0
14	M	71	0	0	2	0
All	All	10501	0	10041	214	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 (214) 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)
8:L:402:BPB:HBBB	8:L:402:BPB:HHC	1.32	1.09
1:C:52:VAL:HB	1:C:56:TYR:HD2	1.31	0.92
1:C:152:LEU:HD22	1:C:175:ARG:HA	1.53	0.91
8:L:402:BPB:HBBA	3:M:208:TYR:HB3	1.60	0.83
8:L:402:BPB:HHC	8:L:402:BPB:CBB	2.12	0.78
3:M:318:LEU:HB3	3:M:319:PRO:HD2	1.68	0.75
3:M:38:LEU:HD23	3:M:46:ILE:HD11	1.69	0.74
1:C:52:VAL:HB	1:C:56:TYR:CD2	2.21	0.74
2:L:181:PHE:CD2	8:M:401:BPB:HBB	2.23	0.74
8:M:401:BPB:HBBB	8:M:401:BPB:HHC	1.67	0.73
1:C:123[A]:GLN:HG3	1:C:269:TRP:CE3	2.24	0.73
13:L:702:LDA:H22	13:L:702:LDA:H62	1.71	0.73
1:C:104:TYR:HE1	1:C:108:ARG:NH2	1.87	0.72
4:H:160:ALA:HB3	4:H:214:LEU:HD23	1.74	0.70
7:M:806:BCB:H203	8:M:401:BPB:H4B	1.74	0.70
3:M:200:HIS:CE1	3:M:204:ILE:HD11	2.26	0.69
7:L:304:BCB:HMB2	8:L:402:BPB:HMBA	1.72	0.69
7:M:805:BCB:HBB3	7:M:806:BCB:H62	1.74	0.69
7:M:806:BCB:HBD	7:M:806:BCB:HAA2	1.76	0.68
3:M:71:PHE:HB3	13:M:706:LDA:H52	1.75	0.68
2:L:178:SER:O	2:L:182:VAL:HG23	1.96	0.66
4:H:42:PRO:HD3	13:H:703:LDA:H121	1.76	0.66
3:M:202:PHE:CE2	4:H:20:GLN:HG2	2.30	0.66
1:C:123[A]:GLN:HG3	1:C:269:TRP:CD2	2.31	0.65
2:L:181:PHE:HB3	8:M:401:BPB:CBB	2.27	0.65
1:C:3:GLU:O	2:L:254:PHE:HA	1.98	0.63
3:M:160:CYS:SG	11:M:600:NS5:H322	2.38	0.63
2:L:185:MET:SD	7:M:805:BCB:H41	2.40	0.62
2:L:79:PRO:HG2	2:L:82:GLU:HB2	1.82	0.62
2:L:206:VAL:HG21	4:H:68:PHE:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:87:GLN:O	3:M:91:LEU:HG	1.99	0.60
4:H:6:LEU:HB2	4:H:10:LEU:HB3	1.82	0.60
8:L:402:BPB:HBB	3:M:208:TYR:CD2	2.36	0.60
4:H:145:ILE:CD1	4:H:151:ASP:HA	2.32	0.60
4:H:70:LEU:HD11	4:H:76:VAL:HG23	1.82	0.59
1:C:8:THR:HB	1:C:23:LEU:HB2	1.84	0.59
3:M:318:LEU:HB3	3:M:319:PRO:CD	2.32	0.59
1:C:113:MET:HB2	1:C:281:TYR:CD2	2.37	0.58
2:L:59:TRP:HA	2:L:64:ILE:HD11	1.84	0.58
3:M:160:CYS:SG	11:M:600:NS5:C31	2.92	0.58
4:H:136:PRO:HG2	4:H:138:ARG:HG2	1.84	0.58
3:M:52:GLY:O	3:M:56:ILE:HD13	2.04	0.58
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.40	0.57
2:L:185:MET:SD	7:M:805:BCB:C4	2.93	0.57
2:L:218:ASP:HB3	3:M:134:ARG:HD2	1.85	0.57
4:H:196:ILE:HD13	4:H:210:VAL:HG21	1.87	0.56
2:L:272:TRP:HB3	3:M:82:LEU:HD21	1.87	0.56
3:M:79:PHE:O	3:M:81:PRO:HD3	2.06	0.56
7:L:302:BCB:OBB	7:L:302:BCB:HHC	2.04	0.56
3:M:32:PRO:HG3	3:M:48:PRO:HD3	1.88	0.56
3:M:73:MET:HE3	3:M:91:LEU:HB2	1.86	0.56
4:H:196:ILE:HD12	4:H:242:TYR:CE1	2.40	0.56
7:M:806:BCB:HAA2	7:M:806:BCB:CBD	2.32	0.55
4:H:161:ASP:HB3	4:H:214:LEU:HD22	1.88	0.55
3:M:118:LEU:HD12	3:M:118:LEU:O	2.06	0.55
6:M:804:SO4:O4	13:M:704:LDA:H22	2.06	0.55
1:C:233:MET:HB3	10:C:339:HEM:C4B	2.41	0.55
1:C:123[A]:GLN:H	1:C:123[A]:GLN:NE2	2.04	0.55
4:H:106:ASN:ND2	4:H:109:VAL:HG23	2.22	0.55
3:M:38:LEU:CD2	3:M:46:ILE:HD11	2.36	0.55
1:C:323:LYS:HD2	1:C:323:LYS:H	1.72	0.55
1:C:65:LEU:HD11	1:C:327:GLU:HG2	1.89	0.55
7:L:304:BCB:HHC	7:L:304:BCB:OBB	2.07	0.55
2:L:205:LYS:HA	4:H:69:VAL:HG22	1.89	0.55
3:M:105:PRO:HB2	3:M:109:ASP:O	2.08	0.54
8:M:401:BPB:CHC	8:M:401:BPB:HBBB	2.35	0.54
2:L:215:TYR:O	2:L:219:VAL:HG23	2.09	0.53
1:C:102:TYR:CD2	1:C:103:PRO:HD3	2.43	0.53
1:C:52:VAL:HG13	1:C:65:LEU:O	2.08	0.53
1:C:181:ALA:O	1:C:182:TYR:HB2	2.09	0.53
7:M:805:BCB:HBB2	7:M:805:BCB:HHC	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:197:VAL:HG13	2:L:207:LYS:HB2	1.90	0.53
3:M:73:MET:O	3:M:76:GLU:HB2	2.09	0.53
2:L:230:HIS:CD2	3:M:221:ILE:HG13	2.44	0.52
3:M:233:ILE:O	3:M:236:ILE:HB	2.08	0.52
3:M:241:THR:O	3:M:245:ARG:HG3	2.08	0.52
1:C:47:ALA:HB1	1:C:66:THR:HG21	1.92	0.52
7:M:805:BCB:H61	7:M:805:BCB:H111	1.92	0.52
1:C:163:VAL:HA	1:C:168:THR:HG21	1.91	0.51
3:M:64:THR:O	3:M:68:ILE:HG13	2.11	0.51
3:M:202:PHE:CZ	4:H:20:GLN:HG2	2.45	0.51
7:L:302:BCB:HMB1	7:L:302:BCB:CBB	2.41	0.51
1:C:121:TRP:HA	1:C:123[A]:GLN:HE21	1.76	0.50
3:M:160:CYS:C	3:M:163:PRO:HD2	2.32	0.50
7:M:806:BCB:HMB1	7:M:806:BCB:CBB	2.41	0.50
3:M:107:LEU:HA	3:M:111:GLY:HA3	1.92	0.50
2:L:205:LYS:HA	4:H:69:VAL:CG2	2.42	0.50
1:C:210:PRO:HB2	4:H:3:HIS:HD2	1.77	0.50
4:H:6:LEU:HD12	4:H:15:LEU:HD11	1.94	0.50
1:C:283:ALA:HB3	1:C:284:PRO:HD3	1.93	0.50
1:C:18:SER:HB2	2:L:156:TRP:CD1	2.47	0.49
4:H:257:LEU:HD12	4:H:258:LEU:HD23	1.94	0.49
3:M:120:MET:HE1	7:M:805:BCB:OBB	2.13	0.49
3:M:162:HIS:HD2	14:M:913:HOH:O	1.95	0.49
3:M:54:SER:OG	3:M:130:ARG:HB2	2.14	0.48
3:M:146:TRP:HA	3:M:146:TRP:CE3	2.49	0.48
3:M:178:TRP:HA	3:M:178:TRP:CE3	2.48	0.48
4:H:96:PHE:H	4:H:96:PHE:HD1	1.62	0.48
3:M:231:ARG:HD2	14:M:1013:HOH:O	2.13	0.48
2:L:28:PRO:O	3:M:252:TRP:HA	2.14	0.48
1:C:102:TYR:CG	1:C:103:PRO:HD3	2.49	0.47
7:M:806:BCB:HHC	7:M:806:BCB:OBB	2.14	0.47
3:M:160:CYS:SG	11:M:600:NS5:C30	3.02	0.47
4:H:117:TYR:HB2	4:H:236:ASP:HB3	1.95	0.47
3:M:29:VAL:HG23	3:M:51:LEU:HD13	1.95	0.47
3:M:11:GLN:NE2	3:M:40:LYS:HG2	2.29	0.47
4:H:62:LEU:O	13:H:703:LDA:H11	2.14	0.47
4:H:137:LEU:HA	4:H:140:ALA:HB3	1.95	0.47
1:C:189:PRO:O	1:C:193:PHE:HB2	2.15	0.47
3:M:107:LEU:HD22	3:M:112:TRP:CE2	2.49	0.47
2:L:224:ILE:HG13	2:L:224:ILE:O	2.15	0.47
2:L:80:LEU:HA	2:L:84:GLY:HA3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:195:TYR:CZ	7:M:806:BCB:HMC2	2.50	0.47
1:C:203:VAL:HG12	1:C:221:ARG:NH2	2.30	0.47
1:C:210:PRO:HB2	4:H:3:HIS:CD2	2.50	0.47
4:H:233:ARG:O	4:H:233:ARG:HG2	2.15	0.47
7:M:805:BCB:HBB2	7:M:806:BCB:H41	1.98	0.46
3:M:160:CYS:SG	11:M:600:NS5:C32	3.03	0.46
4:H:152:PRO:HD2	4:H:171:LEU:HD11	1.97	0.46
3:M:132:TYR:CE1	3:M:142:THR:HG21	2.51	0.46
2:L:51:TYR:HD1	2:L:85:PHE:CZ	2.33	0.46
1:C:290:PRO:HG2	1:C:293:ARG:HG2	1.96	0.46
3:M:318:LEU:CB	3:M:319:PRO:HD2	2.41	0.46
2:L:81:LEU:HA	2:L:81:LEU:HD23	1.79	0.46
3:M:162:HIS:O	3:M:166:VAL:HG22	2.17	0.45
4:H:102:GLN:NE2	14:H:1204:HOH:O	2.49	0.45
3:M:38:LEU:HD23	3:M:46:ILE:CD1	2.44	0.45
4:H:33:ARG:HD2	4:H:33:ARG:HA	1.72	0.45
3:M:99:GLN:HA	3:M:99:GLN:OE1	2.16	0.45
2:L:225:GLY:HA2	12:L:502:ATZ:H132	1.98	0.45
1:C:309:HIS:CE1	1:C:315:PRO:HD3	2.51	0.45
1:C:252:THR:HG23	1:C:255:SER:HB2	1.98	0.45
3:M:318:LEU:CB	3:M:319:PRO:CD	2.84	0.45
4:H:138:ARG:CG	4:H:139:VAL:N	2.79	0.45
4:H:185:LEU:HD11	4:H:218:PHE:CD2	2.52	0.45
3:M:12:ALA:HB2	4:H:180:PHE:CE2	2.52	0.45
7:L:304:BCB:HMB2	8:L:402:BPB:CMB	2.45	0.44
4:H:135:VAL:HB	4:H:136:PRO:HD2	1.99	0.44
4:H:145:ILE:HD12	4:H:151:ASP:HA	1.99	0.44
4:H:142:ASP:OD1	4:H:142:ASP:N	2.50	0.44
2:L:239:ASN:HD22	2:L:239:ASN:HA	1.56	0.44
2:L:224:ILE:HG22	12:L:502:ATZ:C4	2.47	0.44
2:L:62:PHE:HE2	13:L:702:LDA:HM21	1.83	0.44
1:C:146:ARG:HA	1:C:146:ARG:HD2	1.67	0.44
8:M:401:BPB:H6	8:M:401:BPB:H4	1.68	0.44
3:M:107:LEU:HB3	3:M:112:TRP:CD1	2.52	0.44
3:M:77:VAL:HG21	3:M:84:PHE:CA	2.48	0.44
2:L:22:PHE:HA	2:L:24:PHE:CE2	2.53	0.44
3:M:318:LEU:HA	3:M:319:PRO:HD3	1.58	0.43
3:M:16:HIS:CD2	3:M:32:PRO:HG2	2.53	0.43
2:L:196:SER:HB2	3:M:141:GLY:O	2.18	0.43
1:C:136:HIS:CE1	1:C:140:PRO:O	2.72	0.43
4:H:27:VAL:O	4:H:31:TYR:HB3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:178:TRP:HA	3:M:178:TRP:HE3	1.82	0.43
2:L:51:TYR:CD1	2:L:85:PHE:CZ	3.06	0.43
2:L:206:VAL:CG2	4:H:68:PHE:HB3	2.46	0.43
1:C:283:ALA:N	1:C:284:PRO:CD	2.81	0.43
8:L:402:BPB:CHC	8:L:402:BPB:CBB	2.83	0.43
3:M:147:ASN:HD22	8:M:401:BPB:HMDA	1.83	0.43
7:M:805:BCB:HBB2	7:M:805:BCB:CHC	2.49	0.43
13:L:705:LDA:H21	3:M:256:PHE:HD1	1.84	0.43
2:L:62:PHE:CD2	13:L:702:LDA:HM11	2.54	0.43
3:M:100:TYR:HD2	3:M:105:PRO:HB3	1.83	0.43
1:C:301:PRO:HG2	10:C:338:HEM:HBD1	2.00	0.43
2:L:183:ASN:HD21	3:M:214:PHE:HB3	1.84	0.43
2:L:44:LEU:HB3	2:L:92:CYS:SG	2.58	0.43
2:L:61:PRO:O	2:L:150:ILE:HD12	2.18	0.43
4:H:136:PRO:HG2	4:H:139:VAL:HG23	2.01	0.42
3:M:262:SER:O	3:M:265:ARG:HB2	2.19	0.42
2:L:146:PHE:HB3	2:L:156:TRP:CD2	2.54	0.42
3:M:262:SER:HA	3:M:265:ARG:HG3	2.02	0.42
3:M:183:TRP:CE3	3:M:184:LEU:HD23	2.54	0.42
1:C:110:MET:HB3	10:C:338:HEM:C4B	2.55	0.42
7:M:806:BCB:H141	7:M:806:BCB:H162	1.68	0.42
3:M:34:TYR:N	3:M:34:TYR:CD1	2.87	0.42
4:H:159:ALA:HB3	4:H:161:ASP:OD1	2.19	0.42
2:L:167:TRP:HE1	2:L:173:HIS:CD2	2.38	0.42
3:M:283:LEU:HD23	3:M:283:LEU:HA	1.93	0.42
1:C:29:LYS:HE2	1:C:33:GLU:OE2	2.20	0.42
2:L:168:HIS:HB3	3:M:181:ILE:CG2	2.50	0.41
7:L:302:BCB:HBB3	7:M:805:BCB:HMD2	2.01	0.41
3:M:78:HIS:ND1	3:M:78:HIS:O	2.53	0.41
1:C:153:PRO:HG2	1:C:158:GLU:HB2	2.03	0.41
8:L:402:BPB:H6	8:L:402:BPB:H2	1.85	0.41
7:L:302:BCB:H2C	7:M:806:BCB:H2C	2.02	0.41
3:M:59[B]:PHE:HA	8:M:401:BPB:H5	2.03	0.41
1:C:281:TYR:O	1:C:285:LEU:HG	2.20	0.41
4:H:138:ARG:HG3	4:H:139:VAL:N	2.35	0.41
2:L:168:HIS:CE1	7:L:302:BCB:HMC2	2.56	0.41
7:M:806:BCB:HBB3	7:M:806:BCB:HMB1	2.02	0.41
2:L:80:LEU:HD12	2:L:80:LEU:HA	1.85	0.41
4:H:67:THR:CG2	4:H:75:THR:HB	2.50	0.41
3:M:21:GLY:H	3:M:28:ARG:HH22	1.69	0.41
11:M:600:NS5:H18	11:M:600:NS5:H161	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:600:NS5:H29	11:M:600:NS5:H271	1.64	0.41
3:M:29:VAL:HG21	3:M:51:LEU:HD22	2.03	0.41
14:C:1190:HOH:O	3:M:307:ALA:HA	2.20	0.41
3:M:275:MET:HG2	8:M:401:BPB:HBCA	2.02	0.41
7:L:304:BCB:HMD2	7:M:806:BCB:HBB3	2.03	0.41
4:H:121:ALA:HB1	4:H:123:VAL:HG22	2.02	0.41
7:L:304:BCB:HMB1	7:L:304:BCB:CBB	2.50	0.40
4:H:76:VAL:CG1	4:H:80:ARG:HH12	2.34	0.40
2:L:166:ASN:OD1	2:L:168:HIS:HB2	2.21	0.40
8:L:402:BPB:CBB	3:M:208:TYR:CD2	3.03	0.40
2:L:132:GLN:OE1	2:L:146:PHE:CD2	2.75	0.40
8:M:401:BPB:HMC	8:M:401:BPB:H55	2.04	0.40
3:M:29:VAL:HG12	3:M:30:GLY:N	2.35	0.40
3:M:195:TYR:CE2	7:M:806:BCB:HMC2	2.57	0.40
1:C:91:HIS:O	1:C:101:LYS:HE3	2.20	0.40
3:M:273:MET:HA	3:M:276:VAL:HB	2.03	0.40
9:M:501:MQ7:H111	9:M:501:MQ7:H2M1	1.83	0.40
4:H:137:LEU:HD12	4:H:171:LEU:HB2	2.03	0.40
1:C:69:GLU:O	1:C:72:ARG:HB3	2.22	0.40
1:C:161:THR:OG1	1:C:164:GLU:HG3	2.21	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	331/336 (98%)	313 (95%)	18 (5%)	0	100	100
2	L	271/273 (99%)	257 (95%)	14 (5%)	0	100	100
3	M	323/323 (100%)	309 (96%)	11 (3%)	3 (1%)	21	22
4	H	256/258 (99%)	237 (93%)	19 (7%)	0	100	100
All	All	1181/1190 (99%)	1116 (94%)	62 (5%)	3 (0%)	46	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	51	LEU
3	M	322	PRO
3	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	281/282 (100%)	264 (94%)	17 (6%)	24	28
2	L	218/218 (100%)	210 (96%)	8 (4%)	41	53
3	M	251/249 (101%)	236 (94%)	15 (6%)	24	28
4	H	212/212 (100%)	192 (91%)	20 (9%)	11	10
All	All	962/961 (100%)	902 (94%)	60 (6%)	23	26

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	15	ARG
1	C	23	LEU
1	C	29	LYS
1	C	38	TYR
1	C	48	GLU
1	C	60	LYS
1	C	88	THR
1	C	110	MET
1	C	122	THR
1	C	123[A]	GLN
1	C	123[B]	GLN
1	C	146	ARG
1	C	149	GLU
1	C	152	LEU
1	C	288	SER
1	C	322	LEU
1	C	323	LYS

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Mol	Chain	Res	Type
2	L	16	LEU
2	L	43	PHE
2	L	82	GLU
2	L	119	LEU
2	L	160	PHE
2	L	224	ILE
2	L	239	ASN
2	L	272	TRP
3	M	16	HIS
3	M	26	ASN
3	M	27	ASP
3	M	33	PHE
3	M	37	TRP
3	M	40	LYS
3	M	71	PHE
3	M	114	LEU
3	M	118	LEU
3	M	147	ASN
3	M	156	LEU
3	M	180	HIS
3	M	194	PHE
3	M	214	PHE
3	M	290	ASP
4	H	8	GLN
4	H	9	HIS
4	H	22	LEU
4	H	30	LEU
4	H	51	LYS
4	H	69	VAL
4	H	89	LYS
4	H	92	GLN
4	H	141	THR
4	H	142	ASP
4	H	178	HIS
4	H	185	LEU
4	H	211	THR
4	H	212	SER
4	H	225	GLN
4	H	236	ASP
4	H	250	THR
4	H	256	SER
4	H	257	LEU

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Mol	Chain	Res	Type
4	H	258	LEU

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

Mol	Chain	Res	Type
1	C	58	ASN
2	L	183	ASN
2	L	239	ASN
3	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	$\# Z  > 2$
4	FME	H	1	4	8,9,10	0.55	0	6,9,11	4.19	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	-7.71	113.65	124.76
4	H	1	FME	CA-N-CN	-6.20	113.28	122.82
4	H	1	FME	O-C-CA	-2.27	119.43	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 [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	$\# Z  > 2$
10	HEM	C	337	1	30,50,50	2.72	7 (23%)	24,82,82	3.30	9 (37%)
10	HEM	C	338	1	30,50,50	2.80	9 (30%)	24,82,82	2.96	9 (37%)
10	HEM	C	339	1	30,50,50	2.40	8 (26%)	24,82,82	3.23	10 (41%)
10	HEM	C	340	1	30,50,50	2.75	11 (36%)	24,82,82	2.78	9 (37%)
13	LDA	H	701	-	15,15,15	4.77	4 (26%)	16,17,17	0.65	0
13	LDA	H	703	-	15,15,15	4.73	3 (20%)	16,17,17	0.73	1 (6%)
6	SO4	H	801	-	4,4,4	1.25	0	6,6,6	0.68	0
7	BCB	L	302	2	56,74,74	1.53	7 (12%)	57,115,115	1.88	11 (19%)
7	BCB	L	304	2	56,74,74	1.52	9 (16%)	57,115,115	2.03	9 (15%)
8	BPB	L	402	-	63,70,70	1.33	9 (14%)	63,101,101	1.87	10 (15%)
12	ATZ	L	502	-	14,14,14	0.65	0	17,18,18	1.55	1 (5%)
13	LDA	L	702	-	15,15,15	4.99	4 (26%)	16,17,17	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	LDA	L	705	-	15,15,15	4.53	4 (26%)	16,17,17	0.75	0
8	BPB	M	401	-	63,70,70	1.51	7 (11%)	63,101,101	1.99	12 (19%)
9	MQ7	M	501	-	49,49,49	1.85	12 (24%)	62,63,63	1.61	13 (20%)
11	NS5	M	600	-	39,39,39	0.84	1 (2%)	44,46,46	1.34	6 (13%)
13	LDA	M	704	-	15,15,15	3.56	4 (26%)	16,17,17	0.54	0
13	LDA	M	706	-	15,15,15	4.44	4 (26%)	16,17,17	0.60	0
6	SO4	M	802	-	4,4,4	1.08	0	6,6,6	0.48	0
6	SO4	M	803	-	4,4,4	0.97	0	6,6,6	0.86	0
6	SO4	M	804	-	4,4,4	1.41	0	6,6,6	0.97	0
7	BCB	M	805	3	56,74,74	1.65	6 (10%)	57,115,115	2.05	9 (15%)
7	BCB	M	806	3	56,74,74	1.61	8 (14%)	57,115,115	2.15	15 (26%)

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	701	-	-	0/13/13/13	0/0/0/0
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	402	-	1/1/18/23	0/46/105/105	0/1/6/6
12	ATZ	L	502	-	-	0/7/7/7	0/1/1/1
13	LDA	L	702	-	-	0/13/13/13	0/0/0/0
13	LDA	L	705	-	-	0/13/13/13	0/0/0/0
8	BPB	M	401	-	-	0/46/105/105	0/1/6/6
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	704	-	-	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 (117) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	L	702	LDA	O1-N1	-18.52	1.21	1.39
13	H	703	LDA	O1-N1	-17.41	1.22	1.39
13	H	701	LDA	O1-N1	-17.17	1.23	1.39
13	L	705	LDA	O1-N1	-16.88	1.23	1.39
13	M	706	LDA	O1-N1	-16.60	1.23	1.39
13	M	704	LDA	O1-N1	-13.21	1.27	1.39
10	C	337	HEM	C3B-C4B	-8.65	1.44	1.51
10	C	338	HEM	C3B-C4B	-8.43	1.44	1.51
7	M	806	BCB	C4D-CHA	-7.27	1.36	1.45
10	C	340	HEM	C3B-C4B	-7.09	1.45	1.51
7	L	302	BCB	C4D-CHA	-6.97	1.36	1.45
7	L	304	BCB	C4D-CHA	-6.91	1.36	1.45
10	C	340	HEM	C2D-C3D	-6.23	1.35	1.54
10	C	337	HEM	C2D-C3D	-6.19	1.35	1.54
10	C	338	HEM	C2D-C3D	-6.08	1.36	1.54
10	C	339	HEM	C2D-C3D	-6.05	1.36	1.54
10	C	339	HEM	C3B-C4B	-5.98	1.46	1.51
10	C	340	HEM	C3D-C4D	-5.49	1.44	1.51
10	C	338	HEM	C3D-C4D	-5.36	1.44	1.51
10	C	337	HEM	C3D-C4D	-5.36	1.44	1.51
13	H	701	LDA	CM1-N1	-5.35	1.41	1.49
10	C	339	HEM	C3D-C4D	-5.24	1.44	1.51
10	C	337	HEM	C2C-C1C	-4.86	1.43	1.52
7	M	805	BCB	C4D-CHA	-4.84	1.39	1.45
13	H	703	LDA	C1-N1	-4.40	1.43	1.51
10	C	338	HEM	C2C-C1C	-4.35	1.44	1.52
9	M	501	MQ7	C11-C12	-4.22	1.44	1.50
10	C	340	HEM	C2C-C1C	-4.19	1.44	1.52
13	L	702	LDA	CM1-N1	-3.92	1.43	1.49
7	L	302	BCB	O2D-CED	-3.75	1.36	1.45
9	M	501	MQ7	C26-C27	-3.60	1.40	1.50
10	C	339	HEM	C2C-C1C	-3.58	1.45	1.52
9	M	501	MQ7	C21-C22	-3.50	1.40	1.50
10	C	340	HEM	CAD-C3D	-3.49	1.47	1.54
7	M	806	BCB	O2D-CED	-3.45	1.36	1.45
9	M	501	MQ7	C10-C5	-3.40	1.35	1.40
13	H	703	LDA	CM1-N1	-3.32	1.44	1.49
7	L	304	BCB	O2D-CED	-3.28	1.37	1.45
10	C	340	HEM	CAA-C2A	-3.22	1.46	1.52
13	H	701	LDA	C1-N1	-3.02	1.45	1.51
13	L	705	LDA	CM2-N1	-2.88	1.45	1.49
13	L	702	LDA	C1-N1	-2.83	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	L	705	LDA	C1-N1	-2.82	1.46	1.51
7	M	805	BCB	O2D-CED	-2.76	1.38	1.45
13	H	701	LDA	CM2-N1	-2.71	1.45	1.49
7	L	304	BCB	C1-C2	-2.66	1.40	1.49
7	L	302	BCB	C1-C2	-2.66	1.40	1.49
13	M	706	LDA	C1-N1	-2.62	1.46	1.51
8	L	402	BPB	C4C-C3C	-2.60	1.39	1.45
8	M	401	BPB	C3B-C2B	-2.60	1.33	1.40
13	L	702	LDA	CM2-N1	-2.59	1.45	1.49
7	M	805	BCB	C2C-C1C	-2.56	1.49	1.51
13	M	706	LDA	CM2-N1	-2.55	1.45	1.49
13	L	705	LDA	CM1-N1	-2.48	1.45	1.49
10	C	338	HEM	CMC-C2C	-2.46	1.47	1.53
7	M	806	BCB	C4C-C3C	-2.39	1.40	1.45
13	M	706	LDA	CM1-N1	-2.37	1.45	1.49
7	L	304	BCB	C4C-C3C	-2.36	1.40	1.45
13	M	704	LDA	CM1-N1	-2.35	1.45	1.49
7	M	806	BCB	CAA-CBA	-2.32	1.44	1.52
8	L	402	BPB	O2D-CED	-2.22	1.39	1.45
10	C	340	HEM	C2D-C1D	-2.19	1.44	1.51
10	C	337	HEM	C2B-C1B	-2.16	1.44	1.51
13	M	704	LDA	C1-N1	-2.15	1.47	1.51
7	L	304	BCB	C3D-C2D	-2.14	1.34	1.40
8	M	401	BPB	O2D-CED	-2.13	1.40	1.45
8	L	402	BPB	C1-C2	-2.10	1.42	1.49
9	M	501	MQ7	C16-C17	-2.08	1.44	1.50
10	C	339	HEM	C2B-C1B	-2.08	1.45	1.51
13	M	704	LDA	CM2-N1	-2.06	1.46	1.49
7	L	302	BCB	C2C-C1C	-2.01	1.50	1.51
7	M	806	BCB	CMD-C2D	2.01	1.55	1.51
7	M	806	BCB	O2A-CGA	2.06	1.39	1.33
7	L	302	BCB	CMB-C2B	2.06	1.56	1.51
7	L	304	BCB	C2-C3	2.14	1.37	1.33
10	C	339	HEM	C1C-NC	2.16	1.38	1.36
7	L	304	BCB	O2A-CGA	2.24	1.40	1.33
7	L	304	BCB	O2D-CGD	2.28	1.39	1.33
10	C	340	HEM	C3B-CAB	2.30	1.55	1.51
8	L	402	BPB	CMD-C2D	2.31	1.55	1.50
8	L	402	BPB	CAC-C3C	2.33	1.36	1.33
10	C	338	HEM	C1C-NC	2.36	1.38	1.36
10	C	340	HEM	FE-NC	2.41	2.05	1.95
8	L	402	BPB	O2D-CGD	2.51	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	501	MQ7	C42-C43	2.51	1.40	1.32
9	M	501	MQ7	C12-C13	2.62	1.38	1.33
7	L	302	BCB	O2D-CGD	2.66	1.40	1.33
9	M	501	MQ7	C22-C23	2.68	1.38	1.33
7	L	302	BCB	C2-C3	2.83	1.38	1.33
7	M	805	BCB	C2-C3	2.87	1.38	1.33
11	M	600	NS5	C30-C31	2.87	1.37	1.34
7	M	806	BCB	C2-C3	2.98	1.38	1.33
9	M	501	MQ7	C27-C28	3.06	1.39	1.33
8	M	401	BPB	C3B-C4B	3.15	1.45	1.41
7	L	304	BCB	CAC-C3C	3.15	1.37	1.33
8	L	402	BPB	C2-C3	3.15	1.39	1.33
10	C	338	HEM	FE-NC	3.28	2.08	1.95
9	M	501	MQ7	C17-C18	3.36	1.39	1.33
9	M	501	MQ7	C37-C38	3.47	1.39	1.33
9	M	501	MQ7	C32-C33	3.68	1.40	1.33
10	C	339	HEM	CBB-CAB	3.77	1.51	1.29
10	C	338	HEM	CBC-CAC	3.82	1.51	1.29
10	C	337	HEM	CBB-CAB	3.92	1.51	1.29
8	M	401	BPB	C2-C3	3.98	1.40	1.33
8	L	402	BPB	C1A-CHA	3.99	1.44	1.36
10	C	337	HEM	CBC-CAC	4.01	1.52	1.29
8	M	401	BPB	O2D-CGD	4.06	1.43	1.33
10	C	338	HEM	CBB-CAB	4.13	1.53	1.29
10	C	340	HEM	CBB-CAB	4.21	1.53	1.29
8	M	401	BPB	O2A-CGA	4.29	1.46	1.33
10	C	340	HEM	CBC-CAC	4.34	1.54	1.29
10	C	339	HEM	CBC-CAC	4.44	1.54	1.29
8	L	402	BPB	C3B-C4B	4.51	1.47	1.41
7	M	805	BCB	O2A-CGA	4.56	1.47	1.33
7	M	806	BCB	CAC-C3C	4.68	1.39	1.33
8	M	401	BPB	CAC-C3C	5.86	1.40	1.33
7	M	805	BCB	CAC-C3C	7.12	1.42	1.33

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	337	HEM	C3B-CAB-CBB	-9.81	109.41	124.46
10	C	339	HEM	C3B-CAB-CBB	-8.86	110.86	124.46
10	C	338	HEM	C3B-CAB-CBB	-7.29	113.28	124.46
10	C	338	HEM	C3C-CAC-CBC	-7.27	113.30	124.46
10	C	340	HEM	C3B-CAB-CBB	-7.21	113.40	124.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	805	BCB	O1D-CGD-CBD	-6.97	114.63	124.62
10	C	337	HEM	C3C-CAC-CBC	-6.90	113.86	124.46
8	M	401	BPB	O1D-CGD-CBD	-6.67	115.07	124.62
7	L	304	BCB	O1D-CGD-CBD	-6.65	115.09	124.62
8	L	402	BPB	O1D-CGD-CBD	-6.48	115.33	124.62
10	C	339	HEM	C3C-CAC-CBC	-6.27	114.84	124.46
7	M	806	BCB	O1D-CGD-CBD	-5.80	116.30	124.62
7	L	302	BCB	O1D-CGD-CBD	-5.74	116.40	124.62
10	C	340	HEM	C3C-CAC-CBC	-5.42	116.14	124.46
11	M	600	NS5	C19-C20-C21	-4.11	121.26	127.20
7	M	806	BCB	OBD-CAD-CBD	-3.78	120.24	125.94
7	M	805	BCB	OBD-CAD-CBD	-3.70	120.36	125.94
9	M	501	MQ7	C34-C33-C35	-3.55	109.99	115.41
10	C	338	HEM	CBA-CAA-C2A	-3.52	106.22	112.53
7	M	806	BCB	O2A-CGA-O1A	-3.47	114.55	123.49
9	M	501	MQ7	C19-C18-C20	-3.44	110.16	115.41
7	M	806	BCB	CAA-C2A-C1A	-3.44	100.35	112.47
7	L	304	BCB	OBD-CAD-CBD	-3.31	120.94	125.94
10	C	339	HEM	CMA-C3A-C4A	-3.29	122.93	128.36
9	M	501	MQ7	C40-C41-C42	-3.27	103.13	111.69
11	M	600	NS5	C16-C15-C14	-3.26	112.68	118.10
8	M	401	BPB	C2C-C3C-C4C	-3.21	104.31	107.24
7	L	302	BCB	OBD-CAD-CBD	-3.20	121.11	125.94
8	M	401	BPB	CBB-CAB-C3B	-3.19	110.85	120.33
8	L	402	BPB	O2A-CGA-O1A	-3.11	115.48	123.49
7	L	302	BCB	O2A-CGA-O1A	-2.93	115.92	123.49
7	L	302	BCB	CBC-CAC-C3C	-2.70	120.85	127.07
8	L	402	BPB	CBD-CHA-C4D	-2.67	105.47	108.46
7	L	304	BCB	CBC-CAC-C3C	-2.65	120.95	127.07
9	M	501	MQ7	C16-C15-C13	-2.61	104.20	112.71
9	M	501	MQ7	C21-C22-C23	-2.60	122.11	127.76
7	M	806	BCB	C4-C3-C2	-2.59	118.42	123.50
7	M	805	BCB	C4-C3-C2	-2.55	118.50	123.50
8	L	402	BPB	CBC-CAC-C3C	-2.41	121.52	127.07
8	L	402	BPB	C2C-C3C-C4C	-2.37	105.07	107.24
8	M	401	BPB	CMB-C2B-C3B	-2.29	120.61	125.09
11	M	600	NS5	C18-C17-C15	-2.27	123.91	127.20
9	M	501	MQ7	C25-C26-C27	-2.25	105.79	111.69
9	M	501	MQ7	C21-C20-C18	-2.22	105.47	112.71
10	C	337	HEM	CBD-CAD-C3D	-2.17	107.25	113.55
7	M	806	BCB	CED-O2D-CGD	-2.16	110.92	115.99
7	L	302	BCB	CBB-CAB-C3B	-2.05	114.24	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	501	MQ7	C26-C25-C23	-2.05	106.05	112.71
8	M	401	BPB	CHD-C4C-NC	-2.03	121.04	124.91
7	M	806	BCB	CMD-C2D-C3D	2.00	129.00	125.09
8	M	401	BPB	O2A-CGA-CBA	2.02	118.05	111.90
10	C	337	HEM	CMD-C2D-C3D	2.04	123.38	114.35
13	H	703	LDA	O1-N1-CM2	2.05	111.79	109.05
7	M	805	BCB	C3C-C4C-NC	2.07	111.78	110.24
9	M	501	MQ7	C16-C17-C18	2.13	132.39	127.76
9	M	501	MQ7	C19-C18-C17	2.14	127.70	123.50
10	C	339	HEM	CMA-C3A-C2A	2.14	129.72	125.24
10	C	340	HEM	CBA-CAA-C2A	2.15	116.39	112.53
11	M	600	NS5	C14-C15-C17	2.16	122.47	118.98
7	M	805	BCB	C6-C5-C3	2.18	117.27	112.48
7	M	806	BCB	C5-C3-C2	2.18	125.19	121.05
9	M	501	MQ7	C35-C33-C32	2.19	125.20	121.05
7	M	806	BCB	C3C-C4C-NC	2.33	111.98	110.24
8	L	402	BPB	C4-C3-C2	2.39	128.19	123.50
8	M	401	BPB	CBD-CHA-C1A	2.59	131.15	126.78
7	L	304	BCB	O2A-CGA-CBA	2.65	119.97	111.90
8	M	401	BPB	C3C-C2C-C1C	2.67	104.94	100.99
8	M	401	BPB	CED-O2D-CGD	2.68	122.27	115.99
7	M	805	BCB	O2A-CGA-CBA	2.69	120.09	111.90
10	C	338	HEM	CMD-C2D-C3D	2.72	126.36	114.35
11	M	600	NS5	C18-C19-C20	2.82	129.63	123.39
7	L	302	BCB	C3C-C4C-NC	2.86	112.37	110.24
10	C	339	HEM	CMD-C2D-C3D	2.88	127.09	114.35
9	M	501	MQ7	C41-C42-C43	2.94	139.06	127.73
7	M	806	BCB	C6-C5-C3	2.96	118.98	112.48
10	C	337	HEM	C2D-C3D-C4D	3.00	106.59	101.50
10	C	340	HEM	CMD-C2D-C3D	3.02	127.72	114.35
7	L	302	BCB	CMB-C2B-C3B	3.05	131.06	125.09
10	C	339	HEM	C2D-C3D-C4D	3.06	106.68	101.50
10	C	338	HEM	C2D-C3D-C4D	3.13	106.80	101.50
8	L	402	BPB	C3C-C2C-C1C	3.15	105.64	100.99
7	L	304	BCB	C3C-C4C-NC	3.20	112.62	110.24
7	L	302	BCB	O2A-CGA-CBA	3.31	122.00	111.90
7	L	304	BCB	C4A-NA-C1A	3.33	109.97	106.04
8	L	402	BPB	OBB-CAB-C3B	3.40	125.39	120.00
10	C	340	HEM	C2D-C3D-C4D	3.42	107.30	101.50
10	C	338	HEM	CMB-C2B-C3B	3.45	125.14	116.53
8	L	402	BPB	O2A-CGA-CBA	3.47	122.48	111.90
11	M	600	NS5	C19-C18-C17	3.49	131.12	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	805	BCB	C4-C3-C5	3.53	120.81	115.41
10	C	337	HEM	CMB-C2B-C3B	3.66	125.66	116.53
8	M	401	BPB	C6-C5-C3	3.66	120.51	112.48
7	M	805	BCB	C4A-NA-C1A	3.67	110.36	106.04
7	M	806	BCB	CMB-C2B-C3B	3.69	132.30	125.09
7	L	304	BCB	OBB-CAB-C3B	3.69	125.84	120.00
10	C	339	HEM	CAD-C3D-C4D	3.72	125.60	112.47
7	L	302	BCB	C4A-NA-C1A	3.77	110.48	106.04
10	C	340	HEM	CMB-C2B-C3B	3.83	126.10	116.53
10	C	340	HEM	CAD-C3D-C4D	3.86	126.07	112.47
10	C	338	HEM	CAD-C3D-C2D	3.87	124.36	113.22
7	M	806	BCB	C4A-NA-C1A	3.93	110.67	106.04
7	L	302	BCB	OBB-CAB-C3B	4.00	126.33	120.00
10	C	338	HEM	CMC-C2C-C3C	4.04	126.62	116.53
7	L	304	BCB	CMB-C2B-C3B	4.05	133.00	125.09
10	C	339	HEM	CMC-C2C-C3C	4.14	126.88	116.53
10	C	337	HEM	CAD-C3D-C2D	4.15	125.14	113.22
10	C	340	HEM	CAD-C3D-C2D	4.46	126.03	113.22
10	C	337	HEM	CAD-C3D-C4D	4.46	128.22	112.47
10	C	340	HEM	CMC-C2C-C3C	4.56	127.92	116.53
10	C	338	HEM	CAD-C3D-C4D	4.59	128.68	112.47
7	M	806	BCB	OBB-CAB-C3B	4.64	127.36	120.00
7	M	806	BCB	O2A-CGA-CBA	4.66	126.09	111.90
12	L	502	ATZ	C4-N7-C8	4.77	129.44	123.92
10	C	339	HEM	CAD-C3D-C2D	5.00	127.59	113.22
8	M	401	BPB	OBB-CAB-C3B	5.18	128.20	120.00
10	C	339	HEM	CMB-C2B-C3B	6.03	131.57	116.53
10	C	337	HEM	CMC-C2C-C3C	6.30	132.26	116.53
9	M	501	MQ7	C11-C12-C13	6.31	137.38	126.70
7	L	302	BCB	O2D-CGD-CBD	6.59	120.34	111.30
7	M	806	BCB	O2D-CGD-CBD	7.18	121.15	111.30
8	L	402	BPB	O2D-CGD-CBD	8.30	122.69	111.30
7	L	304	BCB	O2D-CGD-CBD	8.86	123.46	111.30
8	M	401	BPB	O2D-CGD-CBD	8.87	123.47	111.30
7	M	805	BCB	O2D-CGD-CBD	9.59	124.45	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.

17 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	338	HEM	2	0
10	C	339	HEM	1	0
13	H	703	LDA	2	0
7	L	302	BCB	5	0
7	L	304	BCB	5	0
8	L	402	BPB	9	0
12	L	502	ATZ	2	0
13	L	702	LDA	3	0
13	L	705	LDA	1	0
8	M	401	BPB	10	0
9	M	501	MQ7	1	0
11	M	600	NS5	6	0
13	M	704	LDA	1	0
13	M	706	LDA	1	0
6	M	804	SO4	1	0
7	M	805	BCB	9	0
7	M	806	BCB	13	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	C	332/336 (98%)	-0.66	4 (1%) 81 89	13, 30, 57, 82	18 (5%)
2	L	273/273 (100%)	-0.74	1 (0%) 93 97	11, 25, 49, 67	7 (2%)
3	M	323/323 (100%)	-0.55	3 (0%) 85 92	10, 28, 59, 72	10 (3%)
4	H	249/258 (96%)	-0.46	4 (1%) 74 84	16, 39, 70, 90	19 (7%)
All	All	1177/1190 (98%)	-0.61	12 (1%) 84 92	10, 30, 60, 90	54 (4%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	54	PRO	3.8
3	M	319	PRO	3.0
2	L	59	TRP	2.8
3	M	37	TRP	2.8
1	C	2	PHE	2.3
1	C	53	SER	2.3
4	H	189	GLY	2.3
1	C	50	PRO	2.2
4	H	96	PHE	2.2
3	M	242	ALA	2.2
4	H	8	GLN	2.1
1	C	1	CYS	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	FME	H	1	10/11	0.97	0.09	-	34,38,46,54	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
13	LDA	M	704	16/16	0.80	0.29	5.11	67,73,102,103	0
13	LDA	M	706	16/16	0.65	0.33	4.69	77,82,87,87	4
13	LDA	L	702	16/16	0.84	0.21	3.97	34,54,73,75	0
11	NS5	M	600	40/40	0.91	0.16	3.18	34,51,70,70	14
13	LDA	H	703	16/16	0.96	0.18	2.68	30,40,65,67	0
9	MQ7	M	501	48/48	0.94	0.13	0.73	12,18,46,48	0
7	BCB	M	806	66/66	0.99	0.12	0.66	6,16,31,36	0
10	HEM	C	338	43/43	0.98	0.13	0.52	15,30,38,47	0
10	HEM	C	340	43/43	0.99	0.10	0.45	10,23,36,53	0
6	SO4	M	802	5/5	0.99	0.09	0.40	37,41,47,51	0
7	BCB	L	304	66/66	0.99	0.12	0.38	8,17,29,44	0
13	LDA	L	705	16/16	0.86	0.16	0.33	62,70,78,79	3
7	BCB	M	805	66/66	0.95	0.10	0.32	8,27,61,62	0
13	LDA	H	701	16/16	0.97	0.12	0.23	18,28,36,37	0
6	SO4	H	801	5/5	0.98	0.08	0.19	62,65,65,66	0
8	BPB	L	402	65/65	0.98	0.08	0.17	2,17,22,26	0
8	BPB	M	401	65/65	0.96	0.10	0.11	14,32,81,82	7
12	ATZ	L	502	14/14	0.98	0.12	0.10	21,33,35,36	0
7	BCB	L	302	66/66	0.99	0.10	0.03	3,13,21,24	0
6	SO4	M	804	5/5	0.98	0.10	-0.25	45,49,53,54	0
10	HEM	C	339	43/43	0.99	0.08	-0.29	6,19,24,34	0
10	HEM	C	337	43/43	0.98	0.08	-0.54	25,31,44,49	0
5	FE2	M	500	1/1	0.99	0.08	-2.15	24,24,24,24	0
6	SO4	M	803	5/5	0.95	0.11	-	84,88,90,90	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.