



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:41 AM GMT

PDB ID : 2I5N  
Title : 1.96 Å X-ray structure of photosynthetic reaction center from Rhodospseudomonas viridis: Crystals grown by microfluidic technique  
Authors : Li, L.; Mustafi, D.; Fu, Q.; Tereshko, V.; Chen, D.L.; Tice, J.D.; Ismagilov, R.F.  
Deposited on : 2006-08-25  
Resolution : 1.96 Å (reported)

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

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

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

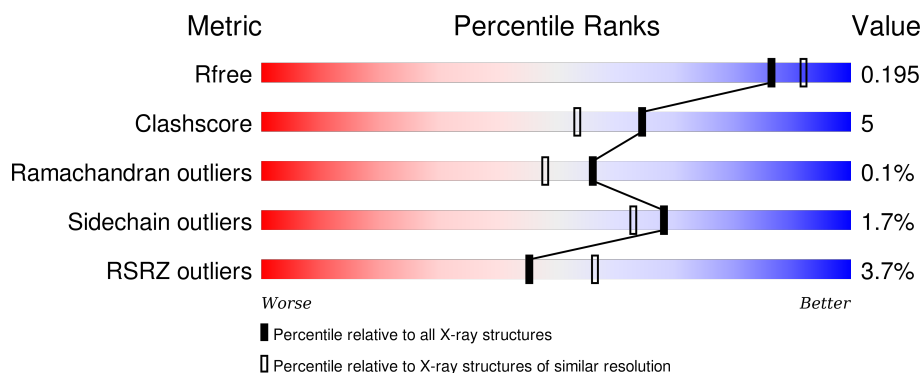
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.96 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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

Mol	Chain	Length	Quality of chain
1	C	336	<div> <div>3%</div> <div>93%</div> <div>5% ..</div> </div>
2	H	258	<div> <div>8%</div> <div>89%</div> <div>8% .</div> </div>
3	L	273	<div> <div>%</div> <div>93%</div> <div>6% .</div> </div>
4	M	323	<div> <div>3%</div> <div>91%</div> <div>8% .</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	UQ1	L	502	-	-	-	X
11	UQ1	L	503	-	-	-	X
12	NS5	M	600[A]	-	-	-	X
12	NS5	M	600[B]	-	-	-	X
13	LDA	L	702	-	-	-	X
13	LDA	M	704	-	-	-	X
14	HTO	C	706	-	-	-	X
14	HTO	C	707	-	-	-	X
14	HTO	H	705	-	-	-	X
6	SO4	C	809	-	-	-	X
6	SO4	H	807	-	-	-	X
8	BCB	M	400	-	-	-	X
9	BPB	M	402	-	-	-	X

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 11035 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	332	Total	C	N	O	S	0	0	0
			2598	1637	465	478	18			

- Molecule 2 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	250	Total	C	N	O	S	0	1	0
			1959	1251	335	371	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	1	FME	MET	MODIFIED RESIDUE	UNP P06008

- Molecule 3 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	273	Total	C	N	O	S	0	2	0
			2174	1462	350	355	7			

- Molecule 4 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	323	Total	C	N	O	S	0	2	0
			2559	1704	419	424	12			

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

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

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



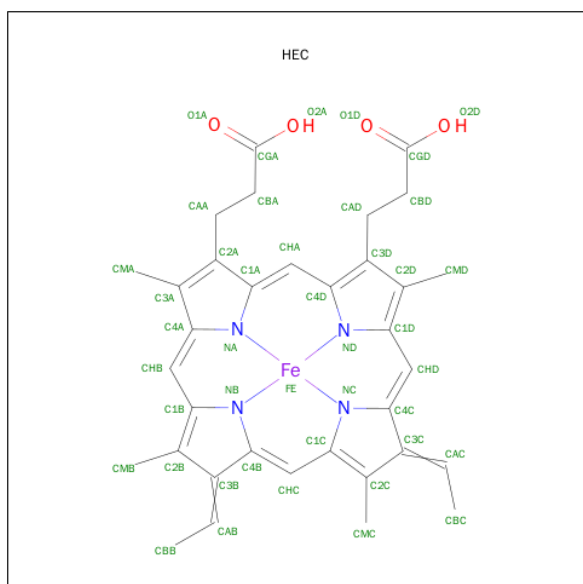
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	M	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total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

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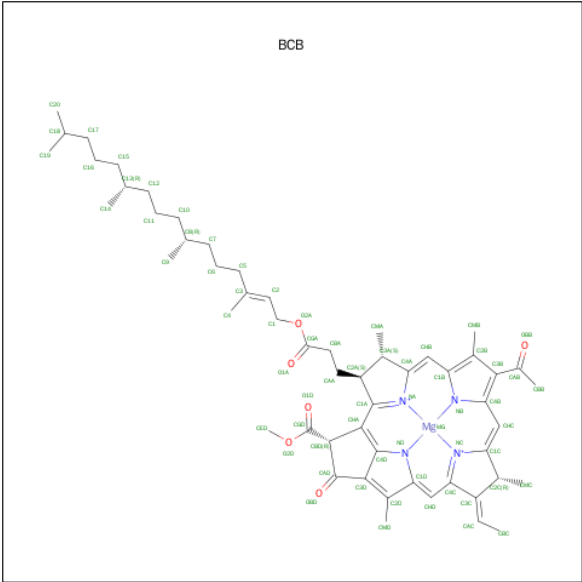
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	O	S	5	0
			5	4	1		
6	C	1	Total	O	S	5	0
			5	4	1		
6	M	1	Total	O	S	5	0
			5	4	1		
6	C	1	Total	O	S	5	0
			5	4	1		
6	M	1	Total	O	S	5	0
			5	4	1		
6	M	1	Total	O	S	5	0
			5	4	1		

- Molecule 7 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



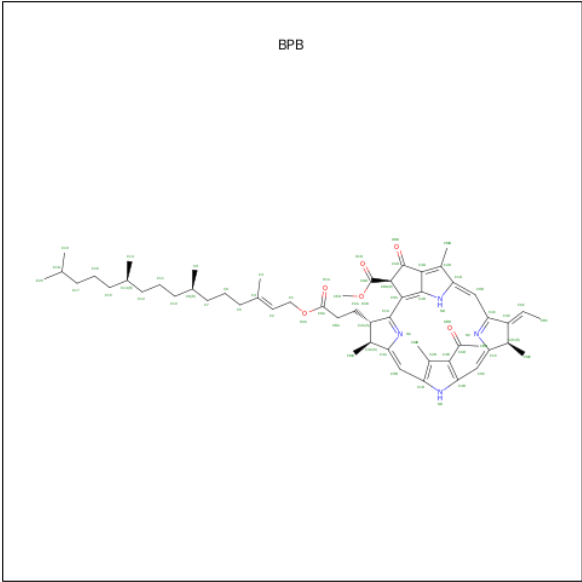
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
7	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
7	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
7	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

- Molecule 8 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula:  $C_{55}H_{72}MgN_4O_6$ ).



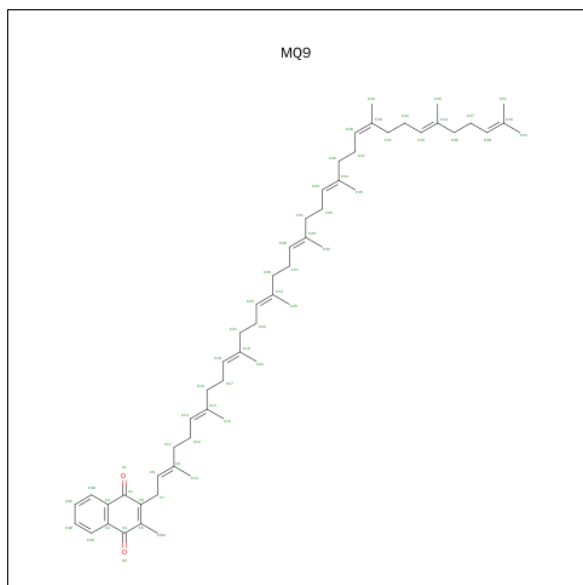
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
8	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
8	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
8	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 9 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>6</sub>).



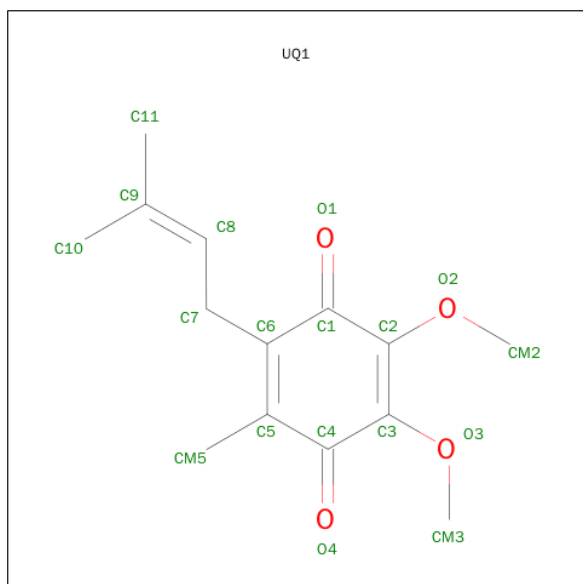
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	L	1	Total	C	N	O	0	0
			65	55	4	6		
9	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 10 is MENAQUINONE-9 (three-letter code: MQ9) (formula:  $C_{56}H_{80}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	C	O	0	0
			58	56	2		

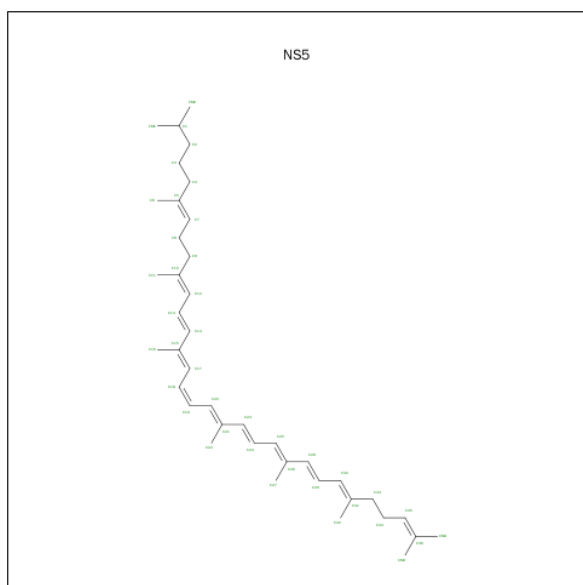
- Molecule 11 is UBIQUINONE-1 (three-letter code: UQ1) (formula:  $C_{14}H_{18}O_4$ ).





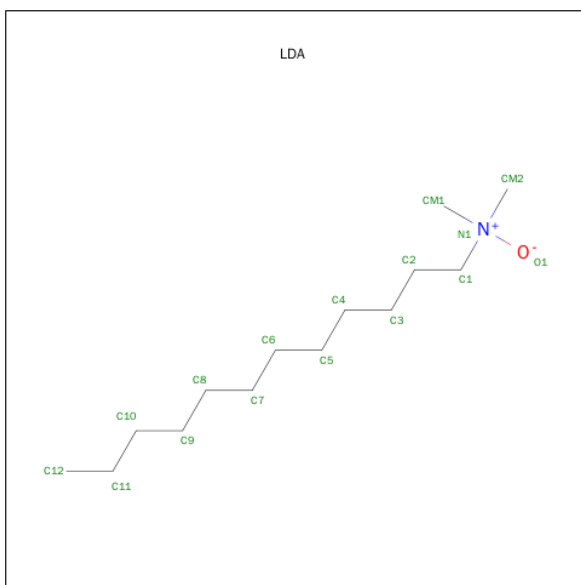
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	L	1	Total	C	O	0	0
			18	14	4		
11	L	1	Total	C	O	0	0
			18	14	4		

- Molecule 12 is 15-CIS-1,2-DIHYDRONEUROSPORENE (three-letter code: NS5) (formula:  $C_{40}H_{60}$ ).



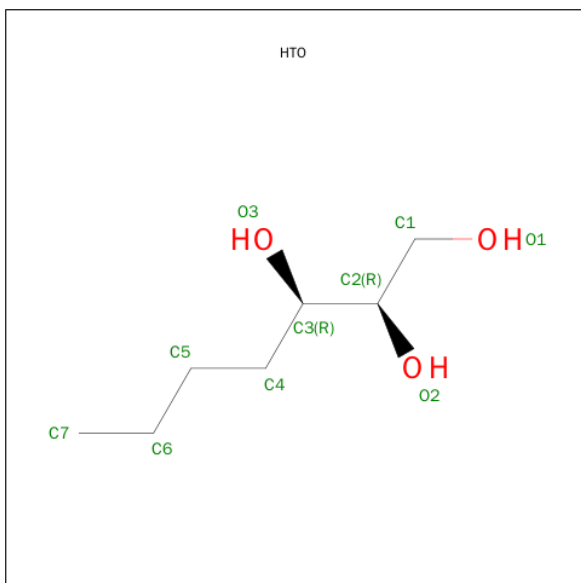
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	M	1	Total	C	0	1
			44	44		

- 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		
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		

- Molecule 14 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula:  $C_7H_{16}O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	H	1	Total C O 10 7 3	0	0
14	C	1	Total C O 10 7 3	0	0
14	C	1	Total C O 10 7 3	0	0
14	L	1	Total C O 10 7 3	10	0
14	L	1	Total C O 10 7 3	10	0

- Molecule 15 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	H	1	Total C 10 10	10	0
15	L	3	Total C 30 30	30	0
15	M	2	Total C 20 20	20	0

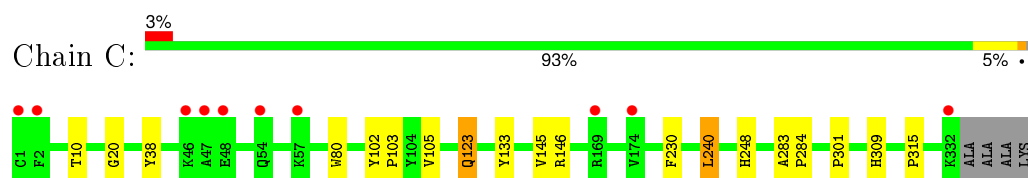
- Molecule 16 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	C	327	Total O 327 327	0	0
16	H	179	Total O 179 179	0	0
16	L	100	Total O 100 100	0	0
16	M	165	Total O 165 165	0	0

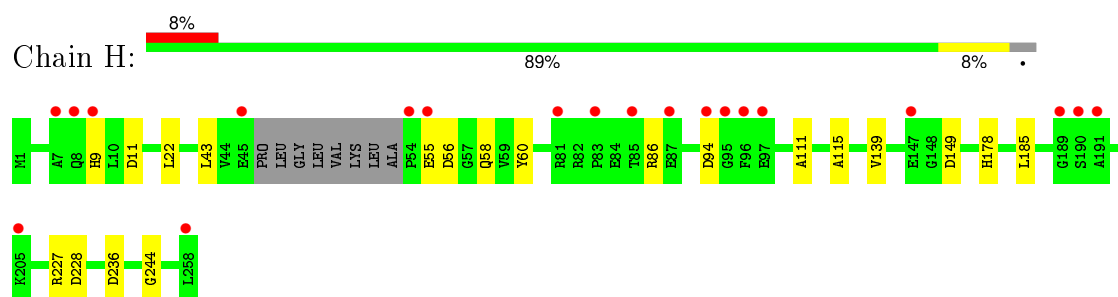
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

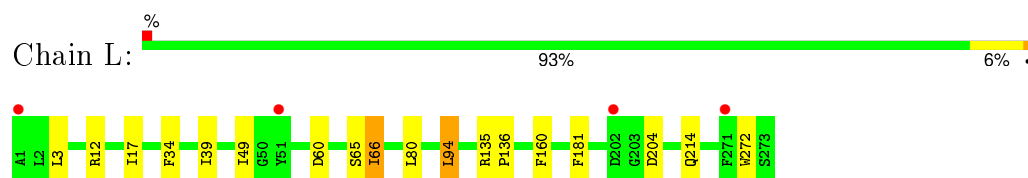
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



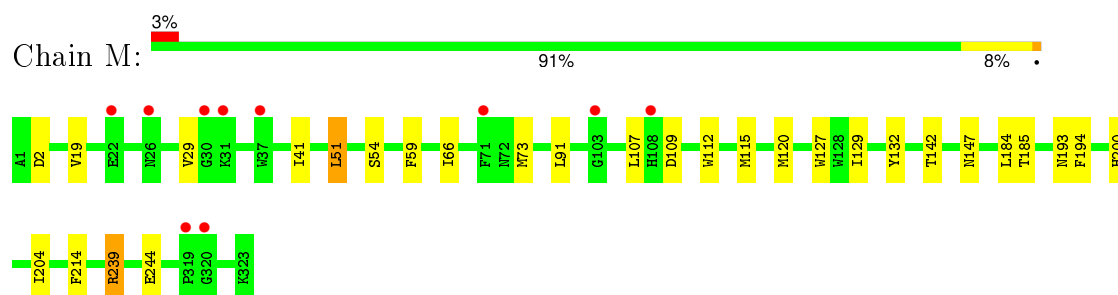
- Molecule 2: Reaction center protein H chain



- Molecule 3: Reaction center protein L chain



- Molecule 4: Reaction center protein M chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	220.40Å 220.40Å 113.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.96 19.97 – 1.96	Depositor EDS
% Data completeness (in resolution range)	96.5 (20.00-1.96) 96.5 (19.97-1.96)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.07 (at 1.96Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.172 , 0.190 0.178 , 0.195	Depositor DCC
$R_{free}$ test set	9533 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.9	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 63.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 189189 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11035	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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, HTO, BCB, MQ9, FE2, SO4, HEC, UQ1, FME, UNL, 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	0.37	0/2665	0.82	0/3633
2	H	0.37	0/1999	0.88	3/2728 (0.1%)
3	L	0.41	0/2274	0.87	6/3105 (0.2%)
4	M	0.38	0/2673	0.85	4/3655 (0.1%)
All	All	0.38	0/9611	0.85	13/13121 (0.1%)

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

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

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	239	ARG	NE-CZ-NH1	7.97	124.29	120.30
3	L	12	ARG	NE-CZ-NH2	-7.55	116.52	120.30
4	M	239	ARG	NE-CZ-NH2	-7.33	116.64	120.30
3	L	12	ARG	NE-CZ-NH1	6.46	123.53	120.30
4	M	2	ASP	CB-CG-OD2	6.36	124.02	118.30
4	M	109	ASP	CB-CG-OD2	5.78	123.50	118.30
3	L	204	ASP	CB-CG-OD2	5.64	123.38	118.30
3	L	66[A]	ILE	CB-CG1-CD1	-5.55	98.36	113.90
3	L	66[B]	ILE	CB-CG1-CD1	-5.55	98.36	113.90
3	L	60	ASP	CB-CG-OD2	5.44	123.20	118.30
2	H	94	ASP	CB-CG-OD2	5.35	123.12	118.30
2	H	11	ASP	CB-CG-OD2	5.12	122.91	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	149	ASP	CB-CG-OD2	5.07	122.86	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	248	HIS	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2598	0	2568	13	0
2	H	1959	0	1947	8	0
3	L	2174	0	2102	13	0
4	M	2559	0	2458	29	0
5	L	1	0	0	0	0
6	C	35	0	0	0	0
6	H	20	0	0	0	0
6	L	5	0	0	0	0
6	M	35	0	0	1	0
7	C	172	0	120	5	0
8	L	132	0	144	9	0
8	M	132	0	144	23	0
9	L	65	0	74	4	0
9	M	65	0	74	17	0
10	L	58	0	80	3	0
11	L	36	0	36	0	0
12	M	44	0	18	0	0
13	H	32	0	62	0	0
13	L	16	0	31	0	0
13	M	16	0	31	1	0
14	C	20	0	32	1	0
14	H	10	0	16	0	0
14	L	20	0	32	0	0
15	H	10	0	0	0	0
15	L	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	M	20	0	0	0	0
16	C	327	0	0	3	0
16	H	179	0	0	0	0
16	L	100	0	0	0	0
16	M	165	0	0	0	0
All	All	11035	0	9969	102	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 5.

All (102) 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)
9:M:402:BPB:H4	9:M:402:BPB:H7A	1.29	1.14
3:L:39:ILE:HD12	10:L:501:MQ9:H43	1.42	0.99
4:M:120:MET:HE3	8:M:401:BCB:H193	1.47	0.96
9:M:402:BPB:C7	9:M:402:BPB:H4	1.97	0.91
4:M:59:PHE:HA	9:M:402:BPB:H4A	1.54	0.86
9:M:402:BPB:CBB	9:M:402:BPB:HHC	2.11	0.80
8:M:401:BCB:C2	9:M:402:BPB:HBBB	2.13	0.78
4:M:73:MET:HE3	4:M:91:LEU:HB2	1.67	0.77
9:M:402:BPB:HBBB	9:M:402:BPB:HHC	1.70	0.73
8:M:400:BCB:CBB	8:M:400:BCB:HHC	2.20	0.71
6:M:802:SO4:O4	13:M:704:LDA:HM11	1.90	0.71
8:M:401:BCB:CBB	8:M:401:BCB:HMB1	2.21	0.70
4:M:107:LEU:CD2	4:M:115[B]:MET:CE	2.72	0.68
4:M:120:MET:HE2	8:M:401:BCB:H171	1.75	0.68
1:C:123:GLN:HE21	1:C:123:GLN:H	1.40	0.68
8:L:401:BCB:HMB1	8:L:401:BCB:CBB	2.25	0.67
9:L:402:BPB:HMB	9:L:402:BPB:CBB	2.24	0.67
4:M:107:LEU:HD21	4:M:115[B]:MET:HE2	1.77	0.65
8:L:400:BCB:CBB	8:L:400:BCB:HMB1	2.27	0.65
4:M:66:ILE:HD12	9:M:402:BPB:H9A	1.78	0.65
8:M:400:BCB:HBB2	8:M:400:BCB:HHC	1.79	0.65
4:M:120:MET:HE3	8:M:401:BCB:C19	2.25	0.64
4:M:107:LEU:HD21	4:M:115[B]:MET:CE	2.26	0.64
4:M:59:PHE:HA	9:M:402:BPB:C4	2.26	0.61
7:C:403:HEC:HBB3	7:C:403:HEC:HMB1	1.82	0.61
4:M:107:LEU:CD2	4:M:115[B]:MET:HE2	2.31	0.60
3:L:49:ILE:HG23	3:L:66[B]:ILE:HD11	1.83	0.60
4:M:239:ARG:HD3	4:M:244:GLU:CG	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:239:ARG:HD3	4:M:244:GLU:HG2	1.86	0.57
1:C:123:GLN:H	1:C:123:GLN:NE2	2.02	0.57
2:H:22:LEU:HD23	2:H:22:LEU:O	2.04	0.57
4:M:120:MET:HE2	8:M:401:BCB:C17	2.35	0.56
14:C:707:HTO:H41	16:C:1062:HOH:O	2.05	0.56
3:L:39:ILE:HD12	10:L:501:MQ9:C43	2.26	0.56
8:M:401:BCB:HMB1	8:M:401:BCB:HBB3	1.90	0.53
2:H:22:LEU:HD23	2:H:22:LEU:C	2.29	0.52
3:L:65:SER:C	3:L:66[A]:ILE:HD13	2.30	0.52
8:M:401:BCB:H12	9:M:402:BPB:HBB	1.92	0.51
3:L:135:ARG:HB3	3:L:136:PRO:HD3	1.92	0.51
9:L:402:BPB:HHC	9:L:402:BPB:OBB	2.11	0.50
9:L:402:BPB:HMB	9:L:402:BPB:HBBB	1.92	0.50
1:C:105:VAL:HG22	16:C:1106:HOH:O	2.12	0.49
9:M:402:BPB:CBB	9:M:402:BPB:CHC	2.86	0.49
8:L:400:BCB:HBB3	8:L:400:BCB:HMB1	1.93	0.49
8:L:401:BCB:HMB1	8:L:401:BCB:HBB2	1.95	0.49
8:M:401:BCB:C1	9:M:402:BPB:CBB	2.91	0.49
9:M:402:BPB:HHC	9:M:402:BPB:HBBA	1.91	0.48
9:M:402:BPB:HMB	9:M:402:BPB:OBB	2.13	0.48
8:M:400:BCB:HMB1	8:M:400:BCB:OBB	2.14	0.48
8:M:401:BCB:H12	9:M:402:BPB:CBB	2.44	0.48
2:H:86:ARG:NH2	2:H:111:ALA:HB3	2.29	0.48
2:H:55:GLU:H	2:H:58:GLN:HE21	1.60	0.48
7:C:401:HEC:HMC1	7:C:401:HEC:HBC3	1.94	0.48
7:C:403:HEC:HBC3	7:C:403:HEC:HMC1	1.96	0.47
4:M:184:LEU:HD21	8:M:400:BCB:CAC	2.44	0.47
1:C:105:VAL:HG13	16:C:1106:HOH:O	2.14	0.47
3:L:65:SER:O	3:L:66[A]:ILE:HD13	2.15	0.47
8:M:401:BCB:C1	9:M:402:BPB:HBBB	2.45	0.47
3:L:214:GLN:NE2	4:M:19:VAL:H	2.13	0.47
8:L:401:BCB:HBB3	8:L:401:BCB:HMB1	1.96	0.46
1:C:145:VAL:O	1:C:146:ARG:HD2	2.16	0.46
8:M:401:BCB:HBB2	8:M:401:BCB:HMB1	1.94	0.46
8:L:401:BCB:HBA1	8:L:401:BCB:C4A	2.45	0.46
1:C:301:PRO:HG2	7:C:402:HEC:HBD1	1.99	0.45
1:C:309:HIS:CE1	1:C:315:PRO:HD3	2.51	0.45
4:M:132:TYR:CE1	4:M:142:THR:HG21	2.51	0.44
4:M:112:TRP:CE3	4:M:115[B]:MET:HE3	2.52	0.44
4:M:29:VAL:HG22	4:M:51:LEU:HD13	1.99	0.44
1:C:102:TYR:N	1:C:103:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:THR:O	1:C:20:GLY:HA3	2.19	0.43
4:M:41:ILE:HD12	4:M:41:ILE:C	2.40	0.43
4:M:120:MET:CE	8:M:401:BCB:C17	2.96	0.42
1:C:230:PHE:CE2	4:M:185:THR:HG21	2.54	0.42
9:L:402:BPB:HBBA	9:L:402:BPB:HMB	1.98	0.42
3:L:17:ILE:HD12	3:L:34:PHE:CZ	2.54	0.42
8:L:400:BCB:HBB2	8:L:400:BCB:HMB1	2.01	0.42
1:C:240:LEU:HD22	1:C:309:HIS:CG	2.55	0.42
3:L:17:ILE:HD12	3:L:34:PHE:HZ	1.84	0.42
7:C:402:HEC:HMB1	7:C:402:HEC:HBB3	2.02	0.41
4:M:127:TRP:CD1	9:M:402:BPB:HBA	2.56	0.41
4:M:200:HIS:CE1	4:M:204:ILE:HD11	2.55	0.41
8:M:400:BCB:HHC	8:M:400:BCB:HBB3	2.00	0.41
8:M:400:BCB:HBC1	8:M:401:BCB:CAD	2.50	0.41
3:L:181:PHE:HB3	9:M:402:BPB:HBBA	2.02	0.41
4:M:107:LEU:HD21	4:M:115[B]:MET:HE1	2.02	0.41
4:M:54[B]:SER:OG	4:M:129:ILE:CG2	2.68	0.41
3:L:94:LEU:HD23	3:L:94:LEU:HA	1.91	0.41
4:M:120:MET:CE	8:M:401:BCB:H171	2.47	0.41
2:H:139:VAL:HG21	2:H:228:ASP:HB3	2.02	0.41
8:L:400:BCB:H193	10:L:501:MQ9:H252	2.03	0.41
4:M:107:LEU:CD2	4:M:115[B]:MET:HE1	2.50	0.41
2:H:43:LEU:CD2	3:L:3:LEU:HD23	2.50	0.41
1:C:283:ALA:N	1:C:284:PRO:CD	2.83	0.41
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.56	0.40
8:L:401:BCB:OBB	8:L:401:BCB:HHC	2.21	0.40
4:M:112:TRP:CE3	4:M:115[B]:MET:CE	3.04	0.40
2:H:56:ASP:HB3	2:H:60:TYR:CE2	2.57	0.40
2:H:115:ALA:HB2	2:H:244:GLY:HA3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	330/336 (98%)	318 (96%)	12 (4%)	0	100	100
2	H	247/258 (96%)	246 (100%)	1 (0%)	0	100	100
3	L	273/273 (100%)	268 (98%)	5 (2%)	0	100	100
4	M	323/323 (100%)	315 (98%)	7 (2%)	1 (0%)	46	35
All	All	1173/1190 (99%)	1147 (98%)	25 (2%)	1 (0%)	56	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	M	193	ASN

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	280/282 (99%)	277 (99%)	3 (1%)	80	77
2	H	206/212 (97%)	201 (98%)	5 (2%)	57	47
3	L	220/218 (101%)	216 (98%)	4 (2%)	66	60
4	M	251/249 (101%)	247 (98%)	4 (2%)	70	66
All	All	957/961 (100%)	941 (98%)	16 (2%)	68	63

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

Mol	Chain	Res	Type
1	C	38	TYR
1	C	123	GLN
1	C	240	LEU
2	H	9	HIS
2	H	178	HIS
2	H	185	LEU
2	H	227	ARG
2	H	236	ASP
3	L	80	LEU
3	L	94	LEU

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Mol	Chain	Res	Type
3	L	160	PHE
3	L	272	TRP
4	M	51	LEU
4	M	147	ASN
4	M	194	PHE
4	M	214	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	123	GLN
2	H	58	GLN
2	H	102	GLN
2	H	220	ASN
2	H	225	GLN
3	L	183	ASN
3	L	213	ASN
3	L	214	GLN
4	M	147	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	FME	H	1	2	8,9,10	0.77	0	6,9,11	2.99	3 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	H	1	2	-	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(°)
2	H	1	FME	CA-N-CN	-6.18	113.32	122.82
2	H	1	FME	O-C-CA	-2.26	119.46	125.44
2	H	1	FME	CE-SD-CG	2.42	108.63	100.37

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 50 ligands modelled in this entry, 6 are unknown and 1 is monoatomic - leaving 43 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	$\# Z  > 2$
7	HEC	C	401	1	24,50,50	1.70	2 (8%)	19,82,82	2.65	5 (26%)
7	HEC	C	402	1	24,50,50	1.69	3 (12%)	19,82,82	2.72	5 (26%)
7	HEC	C	403	1	24,50,50	1.54	2 (8%)	19,82,82	2.64	5 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	HEC	C	404	1	24,50,50	1.58	3 (12%)	19,82,82	2.62	6 (31%)
14	HTO	C	706	-	9,9,9	0.36	0	8,10,10	0.48	0
14	HTO	C	707	-	9,9,9	0.44	0	8,10,10	0.76	0
6	SO4	C	808	-	4,4,4	0.15	0	6,6,6	0.28	0
6	SO4	C	809	-	4,4,4	0.23	0	6,6,6	0.11	0
6	SO4	C	810	-	4,4,4	0.29	0	6,6,6	0.13	0
6	SO4	C	811	-	4,4,4	0.30	0	6,6,6	0.13	0
6	SO4	C	813	-	4,4,4	0.32	0	6,6,6	0.09	0
6	SO4	C	815	-	4,4,4	0.24	0	6,6,6	0.14	0
6	SO4	C	817	-	4,4,4	0.17	0	6,6,6	0.12	0
13	LDA	H	701	-	15,15,15	3.40	2 (13%)	16,17,17	0.85	1 (6%)
13	LDA	H	703	-	15,15,15	3.51	2 (13%)	16,17,17	0.67	0
14	HTO	H	705	-	9,9,9	0.41	0	8,10,10	0.81	0
6	SO4	H	803	-	4,4,4	0.18	0	6,6,6	0.24	0
6	SO4	H	806	-	4,4,4	0.34	0	6,6,6	0.20	0
6	SO4	H	807	-	4,4,4	0.15	0	6,6,6	0.10	0
6	SO4	H	812	-	4,4,4	0.27	0	6,6,6	0.08	0
8	BCB	L	400	3	56,74,74	2.44	8 (14%)	57,115,115	1.64	9 (15%)
8	BCB	L	401	3	56,74,74	2.52	8 (14%)	57,115,115	1.62	8 (14%)
9	BPB	L	402	-	63,70,70	2.38	8 (12%)	63,101,101	2.68	16 (25%)
10	MQ9	L	501	-	59,59,59	1.92	21 (35%)	74,75,75	1.42	12 (16%)
11	UQ1	L	502	-	18,18,18	1.66	2 (11%)	22,25,25	0.98	0
11	UQ1	L	503	-	18,18,18	1.78	2 (11%)	22,25,25	1.00	1 (4%)
13	LDA	L	702	-	15,15,15	3.66	2 (13%)	16,17,17	0.69	1 (6%)
14	HTO	L	708	-	9,9,9	0.31	0	8,10,10	0.65	0
14	HTO	L	709	-	9,9,9	0.30	0	8,10,10	0.71	0
6	SO4	L	814	-	4,4,4	0.29	0	6,6,6	0.37	0
8	BCB	M	400	4	56,74,74	2.32	8 (14%)	57,115,115	1.65	9 (15%)
8	BCB	M	401	4	56,74,74	2.49	7 (12%)	57,115,115	1.71	11 (19%)
9	BPB	M	402	-	63,70,70	2.40	8 (12%)	63,101,101	2.73	15 (23%)
12	NS5	M	600[A]	-	39,39,39	1.41	1 (2%)	44,46,46	1.90	13 (29%)
12	NS5	M	600[B]	-	39,39,39	1.42	1 (2%)	44,46,46	1.89	13 (29%)
13	LDA	M	704	-	15,15,15	3.80	2 (13%)	16,17,17	0.72	0
6	SO4	M	801	-	4,4,4	0.41	0	6,6,6	0.33	0
6	SO4	M	802	-	4,4,4	0.47	0	6,6,6	0.21	0
6	SO4	M	804	-	4,4,4	0.32	0	6,6,6	0.17	0
6	SO4	M	805	-	4,4,4	0.29	0	6,6,6	0.22	0
6	SO4	M	816	-	4,4,4	0.24	0	6,6,6	0.10	0
6	SO4	M	818	-	4,4,4	0.21	0	6,6,6	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	SO4	M	819	-	4,4,4	0.23	0	6,6,6	0.29	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	HEC	C	401	1	-	0/6/54/54	0/0/8/8
7	HEC	C	402	1	-	0/6/54/54	0/0/8/8
7	HEC	C	403	1	-	0/6/54/54	0/0/8/8
7	HEC	C	404	1	-	0/6/54/54	0/0/8/8
14	HTO	C	706	-	-	0/10/10/10	0/0/0/0
14	HTO	C	707	-	-	0/10/10/10	0/0/0/0
6	SO4	C	808	-	-	0/0/0/0	0/0/0/0
6	SO4	C	809	-	-	0/0/0/0	0/0/0/0
6	SO4	C	810	-	-	0/0/0/0	0/0/0/0
6	SO4	C	811	-	-	0/0/0/0	0/0/0/0
6	SO4	C	813	-	-	0/0/0/0	0/0/0/0
6	SO4	C	815	-	-	0/0/0/0	0/0/0/0
6	SO4	C	817	-	-	0/0/0/0	0/0/0/0
13	LDA	H	701	-	-	0/13/13/13	0/0/0/0
13	LDA	H	703	-	-	0/13/13/13	0/0/0/0
14	HTO	H	705	-	-	0/10/10/10	0/0/0/0
6	SO4	H	803	-	-	0/0/0/0	0/0/0/0
6	SO4	H	806	-	-	0/0/0/0	0/0/0/0
6	SO4	H	807	-	-	0/0/0/0	0/0/0/0
6	SO4	H	812	-	-	0/0/0/0	0/0/0/0
8	BCB	L	400	3	-	0/37/137/137	0/0/9/9
8	BCB	L	401	3	-	0/37/137/137	0/0/9/9
9	BPB	L	402	-	-	0/46/105/105	0/1/6/6
10	MQ9	L	501	-	-	0/53/73/73	0/2/2/2
11	UQ1	L	502	-	-	0/9/33/33	0/1/1/1
11	UQ1	L	503	-	-	0/9/33/33	0/1/1/1
13	LDA	L	702	-	-	0/13/13/13	0/0/0/0
14	HTO	L	708	-	-	0/10/10/10	0/0/0/0
14	HTO	L	709	-	-	0/10/10/10	0/0/0/0
6	SO4	L	814	-	-	0/0/0/0	0/0/0/0
8	BCB	M	400	4	-	0/37/137/137	0/0/9/9
8	BCB	M	401	4	-	0/37/137/137	0/0/9/9
9	BPB	M	402	-	-	0/46/105/105	0/1/6/6
12	NS5	M	600[A]	-	-	0/43/43/43	0/0/0/0
12	NS5	M	600[B]	-	-	0/43/43/43	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	LDA	M	704	-	-	0/13/13/13	0/0/0/0
6	SO4	M	801	-	-	0/0/0/0	0/0/0/0
6	SO4	M	802	-	-	0/0/0/0	0/0/0/0
6	SO4	M	804	-	-	0/0/0/0	0/0/0/0
6	SO4	M	805	-	-	0/0/0/0	0/0/0/0
6	SO4	M	816	-	-	0/0/0/0	0/0/0/0
6	SO4	M	818	-	-	0/0/0/0	0/0/0/0
6	SO4	M	819	-	-	0/0/0/0	0/0/0/0

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	704	LDA	O1-N1	-14.41	1.25	1.39
13	L	702	LDA	O1-N1	-13.82	1.26	1.39
13	H	703	LDA	O1-N1	-13.17	1.27	1.39
13	H	701	LDA	O1-N1	-12.83	1.27	1.39
8	L	400	BCB	C4D-CHA	-5.31	1.38	1.45
8	L	401	BCB	C4D-CHA	-5.23	1.38	1.45
8	M	400	BCB	C4D-CHA	-5.05	1.38	1.45
7	C	401	HEC	C3B-C2B	-5.01	1.35	1.40
7	C	403	HEC	C3B-C2B	-4.97	1.35	1.40
8	M	401	BCB	C4D-CHA	-4.87	1.39	1.45
7	C	402	HEC	C3B-C2B	-4.82	1.35	1.40
7	C	404	HEC	C3B-C2B	-4.72	1.35	1.40
7	C	402	HEC	C3C-C2C	-4.61	1.35	1.40
7	C	401	HEC	C3C-C2C	-4.32	1.36	1.40
7	C	404	HEC	C3C-C2C	-4.30	1.36	1.40
10	L	501	MQ9	C3-C4	-4.03	1.40	1.48
7	C	403	HEC	C3C-C2C	-3.64	1.37	1.40
10	L	501	MQ9	C2-C1	-3.61	1.41	1.48
8	M	401	BCB	C2C-C1C	-3.41	1.48	1.51
10	L	501	MQ9	C5-C4	-3.23	1.41	1.48
13	H	703	LDA	C1-N1	-2.87	1.46	1.51
9	L	402	BPB	C4D-CHA	-2.84	1.36	1.44
8	M	400	BCB	C2C-C1C	-2.78	1.49	1.51
8	L	400	BCB	C2C-C1C	-2.72	1.49	1.51
9	M	402	BPB	C4D-CHA	-2.64	1.37	1.44
13	L	702	LDA	C1-N1	-2.63	1.46	1.51
10	L	501	MQ9	C6-C1	-2.62	1.40	1.47
13	M	704	LDA	C1-N1	-2.53	1.46	1.51
13	H	701	LDA	C1-N1	-2.41	1.47	1.51
10	L	501	MQ9	C7-C8	-2.40	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	501	MQ9	C47-C48	-2.40	1.43	1.50
10	L	501	MQ9	C37-C38	-2.39	1.43	1.50
10	L	501	MQ9	C42-C43	-2.26	1.44	1.50
10	L	501	MQ9	C32-C33	-2.13	1.44	1.50
9	L	402	BPB	C3D-C4D	-2.10	1.36	1.43
9	M	402	BPB	C3D-C4D	-2.03	1.37	1.43
10	L	501	MQ9	C12-C13	-2.02	1.44	1.50
10	L	501	MQ9	O1-C1	2.01	1.27	1.23
8	L	401	BCB	CHD-C4C	2.01	1.41	1.35
8	L	400	BCB	C3D-C4D	2.05	1.44	1.41
7	C	402	HEC	C3C-C4C	2.05	1.47	1.42
8	M	400	BCB	C4C-C3C	2.07	1.48	1.45
8	M	400	BCB	C3D-C4D	2.07	1.44	1.41
8	L	400	BCB	C4C-C3C	2.09	1.48	1.45
8	L	400	BCB	C2-C3	2.10	1.37	1.33
10	L	501	MQ9	C48-C49	2.15	1.38	1.32
7	C	404	HEC	C3C-C4C	2.16	1.47	1.42
8	M	401	BCB	C4C-C3C	2.18	1.49	1.45
8	L	401	BCB	C4C-C3C	2.19	1.49	1.45
9	M	402	BPB	C1D-ND	2.22	1.43	1.38
9	L	402	BPB	C1D-ND	2.26	1.43	1.38
8	L	401	BCB	C3D-C4D	2.33	1.45	1.41
9	M	402	BPB	C3B-C4B	2.89	1.45	1.41
9	L	402	BPB	C3B-C4B	2.91	1.45	1.41
8	M	400	BCB	C2-C3	2.94	1.38	1.33
10	L	501	MQ9	C6-C5	2.94	1.42	1.35
8	M	401	BCB	C2-C3	2.97	1.38	1.33
11	L	502	UQ1	C3-C2	3.07	1.49	1.35
10	L	501	MQ9	C23-C24	3.07	1.39	1.33
8	L	400	BCB	O2A-CGA	3.19	1.42	1.33
11	L	503	UQ1	C3-C2	3.19	1.49	1.35
8	L	401	BCB	C2-C3	3.28	1.39	1.33
10	L	501	MQ9	C38-C39	3.29	1.39	1.33
9	M	402	BPB	C2-C3	3.35	1.39	1.33
10	L	501	MQ9	C43-C44	3.37	1.39	1.33
10	L	501	MQ9	C13-C14	3.39	1.39	1.33
10	L	501	MQ9	C18-C19	3.42	1.39	1.33
10	L	501	MQ9	C28-C29	3.48	1.39	1.33
8	M	400	BCB	O2D-CGD	3.48	1.42	1.33
8	M	401	BCB	O2A-CGA	3.54	1.44	1.33
10	L	501	MQ9	C33-C34	3.54	1.39	1.33
9	L	402	BPB	C2-C3	3.55	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	401	BCB	O2A-CGA	3.62	1.44	1.33
9	M	402	BPB	O2D-CGD	3.73	1.42	1.33
8	L	401	BCB	O2D-CGD	3.78	1.42	1.33
9	M	402	BPB	O2A-CGA	3.78	1.44	1.33
9	L	402	BPB	O2D-CGD	3.79	1.42	1.33
8	L	400	BCB	O2D-CGD	3.88	1.43	1.33
8	M	400	BCB	O2A-CGA	3.90	1.45	1.33
9	L	402	BPB	O2A-CGA	3.92	1.45	1.33
8	M	401	BCB	O2D-CGD	4.03	1.43	1.33
10	L	501	MQ9	C8-C9	4.25	1.41	1.33
11	L	502	UQ1	C6-C5	5.94	1.49	1.35
11	L	503	UQ1	C6-C5	6.21	1.49	1.35
12	M	600[A]	NS5	C35-C36	6.76	1.53	1.32
12	M	600[B]	NS5	C35-C36	6.85	1.53	1.32
8	M	400	BCB	CAC-C3C	14.05	1.50	1.33
8	L	400	BCB	CAC-C3C	15.16	1.51	1.33
8	M	401	BCB	CAC-C3C	15.29	1.52	1.33
8	L	401	BCB	CAC-C3C	15.78	1.52	1.33
9	L	402	BPB	CAC-C3C	15.92	1.52	1.33
9	M	402	BPB	CAC-C3C	16.29	1.53	1.33

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	403	HEC	CBB-CAB-C3B	-7.81	109.98	127.35
7	C	402	HEC	CBB-CAB-C3B	-7.62	110.42	127.35
7	C	401	HEC	CBB-CAB-C3B	-7.39	110.92	127.35
7	C	404	HEC	CBC-CAC-C3C	-6.68	112.50	127.35
7	C	404	HEC	CBB-CAB-C3B	-6.64	112.61	127.35
7	C	402	HEC	CBC-CAC-C3C	-6.55	112.79	127.35
7	C	401	HEC	CBC-CAC-C3C	-6.18	113.61	127.35
9	L	402	BPB	C3D-C2D-C1D	-6.14	95.91	105.77
9	M	402	BPB	C3D-C2D-C1D	-5.94	96.23	105.77
7	C	403	HEC	CBC-CAC-C3C	-5.49	115.16	127.35
12	M	600[A]	NS5	C19-C20-C21	-5.40	119.39	127.20
12	M	600[B]	NS5	C19-C20-C21	-5.40	119.39	127.20
12	M	600[A]	NS5	C34-C35-C36	-4.24	111.40	127.73
8	M	401	BCB	C3C-C4C-NC	-4.15	107.15	110.24
12	M	600[B]	NS5	C34-C35-C36	-4.08	112.04	127.73
8	L	401	BCB	O1D-CGD-CBD	-3.87	119.07	124.62
8	M	400	BCB	O1D-CGD-CBD	-3.66	119.38	124.62
12	M	600[B]	NS5	CM4-C36-C35	-3.65	110.86	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	600[A]	NS5	CM3-C36-C35	-3.60	111.02	122.61
12	M	600[A]	NS5	CM4-C36-C35	-3.59	111.07	122.61
9	M	402	BPB	O1D-CGD-CBD	-3.51	119.60	124.62
12	M	600[B]	NS5	CM3-C36-C35	-3.50	111.34	122.61
8	M	400	BCB	CBC-CAC-C3C	-3.50	119.00	127.07
9	L	402	BPB	O1D-CGD-CBD	-3.32	119.86	124.62
9	M	402	BPB	C4-C3-C2	-3.32	116.98	123.50
7	C	403	HEC	CMC-C2C-C1C	-3.31	122.89	128.36
8	M	400	BCB	C3C-C4C-NC	-3.22	107.85	110.24
9	L	402	BPB	CBC-CAC-C3C	-3.17	119.75	127.07
9	M	402	BPB	CAD-C3D-C2D	-3.13	125.69	140.80
9	M	402	BPB	C3D-C4D-ND	-3.08	99.75	109.65
9	L	402	BPB	CAD-C3D-C2D	-3.03	126.15	140.80
7	C	402	HEC	CMC-C2C-C1C	-2.95	123.49	128.36
9	L	402	BPB	C3D-C4D-ND	-2.93	100.23	109.65
8	L	400	BCB	O1D-CGD-CBD	-2.93	120.43	124.62
10	L	501	MQ9	C37-C38-C39	-2.90	121.45	127.76
7	C	404	HEC	CMC-C2C-C1C	-2.85	123.65	128.36
10	L	501	MQ9	C40-C39-C38	-2.84	117.93	123.50
8	L	400	BCB	C3C-C4C-NC	-2.76	108.19	110.24
8	L	401	BCB	CBC-CAC-C3C	-2.73	120.76	127.07
8	M	401	BCB	CBC-CAC-C3C	-2.73	120.76	127.07
10	L	501	MQ9	C22-C23-C24	-2.71	121.88	127.76
8	M	401	BCB	O2D-CGD-O1D	-2.70	118.22	123.79
7	C	401	HEC	CBD-CAD-C3D	-2.69	107.70	112.53
10	L	501	MQ9	C42-C43-C44	-2.68	121.93	127.76
8	L	400	BCB	CBC-CAC-C3C	-2.66	120.94	127.07
8	L	401	BCB	C1D-CHD-C4C	-2.65	123.57	129.26
12	M	600[A]	NS5	C12-C13-C14	-2.62	115.13	123.13
12	M	600[B]	NS5	C12-C13-C14	-2.62	115.13	123.13
10	L	501	MQ9	C17-C18-C19	-2.62	122.06	127.76
7	C	401	HEC	CMC-C2C-C1C	-2.62	124.03	128.36
8	M	401	BCB	C1D-CHD-C4C	-2.58	123.72	129.26
8	L	400	BCB	C1D-CHD-C4C	-2.58	123.73	129.26
12	M	600[A]	NS5	C6-C5-C7	-2.49	118.61	123.50
12	M	600[B]	NS5	C6-C5-C7	-2.49	118.61	123.50
8	L	401	BCB	C3C-C4C-NC	-2.45	108.42	110.24
7	C	404	HEC	CMB-C2B-C1B	-2.42	124.36	128.36
12	M	600[A]	NS5	C18-C17-C15	-2.40	123.73	127.20
12	M	600[B]	NS5	C18-C17-C15	-2.40	123.73	127.20
9	L	402	BPB	CHD-C1D-ND	-2.36	120.26	124.66
9	M	402	BPB	CBC-CAC-C3C	-2.34	121.66	127.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	401	BCB	O1D-CGD-CBD	-2.27	121.37	124.62
10	L	501	MQ9	C27-C28-C29	-2.26	122.86	127.76
12	M	600[A]	NS5	C24-C25-C26	-2.24	123.96	127.20
12	M	600[B]	NS5	C24-C25-C26	-2.24	123.96	127.20
7	C	404	HEC	CAD-CBD-CGD	-2.22	108.67	112.75
7	C	403	HEC	CMB-C2B-C1B	-2.22	124.69	128.36
12	M	600[A]	NS5	C8-C7-C5	-2.18	123.02	127.76
12	M	600[B]	NS5	C8-C7-C5	-2.18	123.02	127.76
7	C	401	HEC	CMB-C2B-C1B	-2.18	124.75	128.36
8	M	400	BCB	C1D-CHD-C4C	-2.11	124.74	129.26
7	C	403	HEC	CBA-CAA-C2A	-2.10	108.77	112.53
12	M	600[A]	NS5	C22-C21-C20	-2.08	119.83	122.90
12	M	600[B]	NS5	C22-C21-C20	-2.08	119.83	122.90
7	C	402	HEC	CBA-CAA-C2A	-2.06	108.84	112.53
8	L	400	BCB	C6-C7-C8	-2.03	108.77	115.49
9	M	402	BPB	CAA-C2A-C1A	-2.02	105.33	112.47
7	C	402	HEC	CAA-C2A-C1A	-2.02	124.82	127.01
7	C	404	HEC	CAA-C2A-C1A	-2.01	124.83	127.01
9	L	402	BPB	O2A-CGA-CBA	2.00	118.00	111.90
11	L	503	UQ1	C11-C9-C10	2.01	119.59	114.64
9	L	402	BPB	CHD-C1D-C2D	2.02	130.17	125.61
13	L	702	LDA	O1-N1-C1	2.02	112.55	110.27
9	M	402	BPB	C3C-C2C-C1C	2.11	104.10	100.99
8	M	401	BCB	CAA-C2A-C1A	2.13	119.99	112.47
8	M	400	BCB	CED-O2D-CGD	2.15	121.04	115.99
9	M	402	BPB	CMD-C2D-C1D	2.16	128.57	125.06
9	L	402	BPB	C4D-C3D-CAD	2.17	109.42	105.51
9	L	402	BPB	CBD-CHA-C1A	2.18	130.46	126.78
10	L	501	MQ9	C10-C9-C11	2.18	118.74	115.41
8	M	400	BCB	O2A-CGA-CBA	2.22	118.68	111.90
8	L	401	BCB	O2A-CGA-CBA	2.23	118.69	111.90
10	L	501	MQ9	C30-C29-C31	2.24	118.83	115.41
8	M	401	BCB	CED-O2D-CGD	2.30	121.38	115.99
9	M	402	BPB	C4-C3-C5	2.33	118.96	115.41
9	M	402	BPB	C4D-C3D-CAD	2.36	109.75	105.51
8	M	401	BCB	C3A-C2A-C1A	2.41	105.59	101.50
10	L	501	MQ9	C25-C24-C26	2.41	119.09	115.41
9	L	402	BPB	CED-O2D-CGD	2.43	121.68	115.99
12	M	600[A]	NS5	C11-C10-C9	2.52	119.26	115.41
12	M	600[B]	NS5	C11-C10-C9	2.52	119.26	115.41
8	L	400	BCB	O2A-CGA-CBA	2.53	119.61	111.90
9	L	402	BPB	CMD-C2D-C1D	2.55	129.20	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	501	MQ9	C35-C34-C36	2.58	119.34	115.41
9	M	402	BPB	CBD-CHA-C1A	2.62	131.21	126.78
10	L	501	MQ9	C40-C39-C41	2.63	119.42	115.41
12	M	600[A]	NS5	C32-C31-C33	2.69	119.51	115.41
12	M	600[B]	NS5	C32-C31-C33	2.69	119.51	115.41
8	M	401	BCB	C4-C3-C5	2.71	119.55	115.41
8	L	401	BCB	C4-C3-C5	2.72	119.56	115.41
9	L	402	BPB	C3C-C2C-C1C	2.74	105.05	100.99
10	L	501	MQ9	C20-C19-C21	2.77	119.64	115.41
8	M	400	BCB	C4-C3-C5	2.77	119.64	115.41
13	H	701	LDA	O1-N1-C1	2.80	113.42	110.27
8	M	400	BCB	C4A-NA-C1A	2.85	109.40	106.04
9	L	402	BPB	CMD-C2D-C3D	2.94	134.88	128.04
12	M	600[A]	NS5	C6-C5-C4	3.04	120.05	115.41
12	M	600[B]	NS5	C6-C5-C4	3.04	120.05	115.41
9	M	402	BPB	CMD-C2D-C3D	3.07	135.19	128.04
8	M	401	BCB	C4A-NA-C1A	3.34	109.98	106.04
8	L	400	BCB	C4A-NA-C1A	3.37	110.01	106.04
8	L	401	BCB	C4A-NA-C1A	3.66	110.35	106.04
8	L	400	BCB	C4-C3-C5	4.22	121.85	115.41
8	L	400	BCB	O2D-CGD-CBD	5.82	119.28	111.30
9	L	402	BPB	O2D-CGD-CBD	5.95	119.46	111.30
8	L	401	BCB	O2D-CGD-CBD	6.23	119.84	111.30
8	M	400	BCB	O2D-CGD-CBD	6.40	120.08	111.30
9	M	402	BPB	O2D-CGD-CBD	6.61	120.37	111.30
8	M	401	BCB	O2D-CGD-CBD	6.63	120.39	111.30
9	L	402	BPB	C4D-C3D-C2D	15.64	124.42	106.74
9	M	402	BPB	C4D-C3D-C2D	15.75	124.54	106.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	401	HEC	1	0
7	C	402	HEC	2	0
7	C	403	HEC	2	0
14	C	707	HTO	1	0
8	L	400	BCB	4	0
8	L	401	BCB	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	L	402	BPB	4	0
10	L	501	MQ9	3	0
8	M	400	BCB	9	0
8	M	401	BCB	15	0
9	M	402	BPB	17	0
13	M	704	LDA	1	0
6	M	802	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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%)	-0.25	10 (3%) 54 64	16, 24, 40, 54	0
2	H	249/258 (96%)	-0.01	20 (8%) 15 24	16, 25, 44, 60	0
3	L	273/273 (100%)	-0.49	4 (1%) 76 84	15, 20, 31, 41	0
4	M	323/323 (100%)	-0.34	10 (3%) 52 62	14, 22, 37, 47	0
All	All	1177/1190 (98%)	-0.28	44 (3%) 45 56	14, 23, 39, 60	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	85	THR	8.5
2	H	8	GLN	5.6
2	H	54	PRO	5.6
2	H	7	ALA	5.6
2	H	83	PRO	4.8
2	H	81	ARG	4.1
2	H	96	PHE	4.0
4	M	319	PRO	3.5
2	H	9	HIS	3.5
3	L	202	ASP	3.4
3	L	271	PHE	3.3
2	H	94	ASP	3.3
1	C	48	GLU	3.2
3	L	51	TYR	3.2
4	M	31	LYS	3.2
1	C	57	LYS	3.0
4	M	71	PHE	3.0
2	H	45	GLU	2.9
4	M	108	HIS	2.9
4	M	37	TRP	2.8
2	H	87	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	47	ALA	2.6
4	M	26	ASN	2.6
3	L	1	ALA	2.5
4	M	320	GLY	2.5
2	H	191	ALA	2.4
2	H	147	GLU	2.4
2	H	258	LEU	2.4
4	M	30	GLY	2.4
2	H	95	GLY	2.4
2	H	205	LYS	2.4
1	C	332	LYS	2.3
4	M	22	GLU	2.3
2	H	55	GLU	2.2
2	H	189	GLY	2.2
1	C	46	LYS	2.2
2	H	190	SER	2.2
4	M	103	GLY	2.1
1	C	2	PHE	2.1
1	C	174	VAL	2.1
1	C	54	GLN	2.0
2	H	97	GLU	2.0
1	C	169	ARG	2.0
1	C	1	CYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	FME	H	1	10/11	0.94	0.08	-	24,27,40,48	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.



## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
13	LDA	M	704	16/16	0.77	0.23	6.81	56,59,67,68	0
14	HTO	C	707	10/10	0.86	0.18	5.17	27,38,44,45	0
11	UQ1	L	503	18/18	0.82	0.23	4.27	44,46,52,53	0
9	BPB	M	402	65/65	0.89	0.17	4.14	14,19,91,92	0
12	NS5	M	600[B]	40/40	0.89	0.17	3.86	20,29,57,58	4
12	NS5	M	600[A]	40/40	0.89	0.17	3.86	20,29,57,58	4
14	HTO	C	706	10/10	0.82	0.22	3.50	28,40,44,45	0
13	LDA	L	702	16/16	0.86	0.17	3.36	29,34,38,39	0
6	SO4	C	809	5/5	0.87	0.25	2.67	37,46,48,50	5
11	UQ1	L	502	18/18	0.94	0.11	2.53	33,34,38,40	0
6	SO4	H	807	5/5	0.94	0.24	2.41	44,49,51,51	5
8	BCB	M	400	66/66	0.94	0.11	2.23	14,18,69,71	0
14	HTO	H	705	10/10	0.94	0.12	2.22	26,32,35,37	0
6	SO4	H	806	5/5	0.94	0.12	1.56	45,46,50,50	5
8	BCB	M	401	66/66	0.96	0.09	1.44	12,16,36,38	0
8	BCB	L	400	66/66	0.97	0.10	1.43	12,15,25,32	0
10	MQ9	L	501	58/58	0.94	0.11	1.30	13,20,66,68	0
9	BPB	L	402	65/65	0.97	0.09	0.89	13,16,22,25	0
13	LDA	H	703	16/16	0.92	0.19	0.79	35,49,60,62	0
13	LDA	H	701	16/16	0.94	0.10	0.06	24,33,42,44	0
7	HEC	C	403	43/43	0.98	0.09	0.03	12,16,19,24	0
7	HEC	C	404	43/43	0.98	0.08	0.02	15,18,27,37	0
7	HEC	C	401	43/43	0.98	0.10	-0.07	19,25,34,39	0
6	SO4	M	802	5/5	0.99	0.09	-0.27	38,41,45,46	0
7	HEC	C	402	43/43	0.98	0.09	-0.28	18,21,26,28	0
8	BCB	L	401	66/66	0.97	0.07	-0.33	12,16,35,43	0
5	FE2	L	500	1/1	1.00	0.03	-4.48	16,16,16,16	0
6	SO4	C	813	5/5	0.91	0.23	-	41,41,42,44	5
6	SO4	C	808	5/5	0.92	0.16	-	39,39,45,46	5
15	UNL	L	711	10/-	-	-	-	35,45,52,53	10
6	SO4	M	801	5/5	0.99	0.08	-	23,30,32,37	0
14	HTO	L	709	10/10	-	-	-	20,36,41,42	10
6	SO4	M	816	5/5	-	-	-	35,36,38,39	5
6	SO4	C	810	5/5	0.97	0.08	-	36,38,38,39	5
6	SO4	H	803	5/5	0.98	0.19	-	40,41,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	SO4	C	817	5/5	-	-	-	32,32,39,39	5
6	SO4	L	814	5/5	-	-	-	29,30,35,37	5
6	SO4	M	804	5/5	0.98	0.15	-	43,45,48,49	0
6	SO4	M	805	5/5	0.94	0.17	-	38,39,45,47	5
15	UNL	L	712	10/-	-	-	-	44,49,53,55	10
15	UNL	H	710	10/-	-	-	-	30,42,49,49	10
6	SO4	M	819	5/5	-	-	-	38,40,42,42	5
6	SO4	H	812	5/5	0.94	0.15	-	45,46,46,47	5
6	SO4	M	818	5/5	-	-	-	50,52,52,54	5
6	SO4	C	815	5/5	-	-	-	27,31,34,37	5
15	UNL	M	715	10/-	-	-	-	41,53,63,64	10
14	HTO	L	708	10/10	-	-	-	25,33,35,35	10
6	SO4	C	811	5/5	0.94	0.14	-	41,42,42,45	5
15	UNL	L	713	10/-	-	-	-	38,43,54,54	10
15	UNL	M	714	10/-	-	-	-	48,52,60,60	10

## 6.5 Other polymers [i](#)

There are no such residues in this entry.