



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:50 AM GMT

PDB ID : 3G7F  
Title : Crystal structure of Blastochloris viridis heterodimer mutant reaction center  
Authors : Ponomarenko, N.S.; Li, L.; Tereshko, V.; Ismagilov, R.F.; Norris Jr., J.R.  
Deposited on : 2009-02-09  
Resolution : 2.50 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

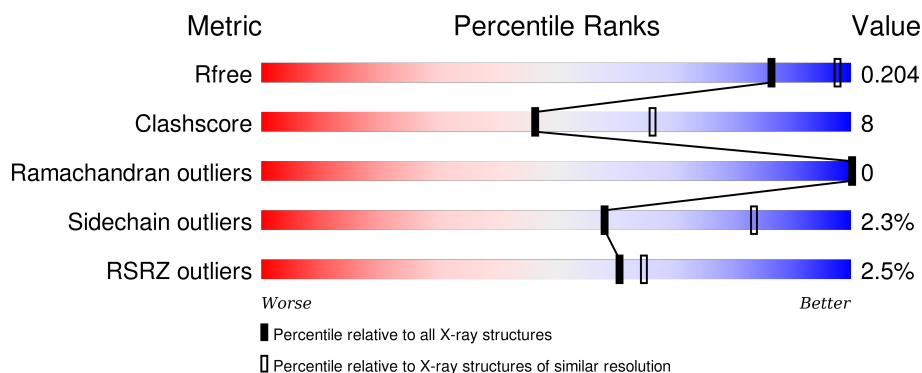
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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>92%</div> <div>7%</div> </div>
2	H	258	<div> <div>6%</div> <div>88%</div> <div>9%</div> </div>
3	L	273	<div> <div>%</div> <div>92%</div> <div>7%</div> </div>
4	M	323	<div> <div>2%</div> <div>86%</div> <div>14%</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
10	BPB	M	401	-	-	X	X
10	BPB	M	402	-	-	-	X
11	UQ1	L	502	-	-	-	X
11	UQ1	M	503	-	-	-	X
14	NS5	M	600	-	-	-	X
6	SO4	C	815	-	-	-	X
6	SO4	H	807	-	-	-	X
7	HTO	C	706	-	-	-	X
7	HTO	C	707	-	-	-	X
8	LDA	M	702	-	-	-	X
8	LDA	M	704	-	-	-	X
9	BCB	M	400	-	-	-	X

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 10922 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 Photosynthetic reaction center H subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	250	Total	C	N	O	S	0	0	0
			1956	1250	335	369	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	216	ASP	GLU	variant	UNP P06008
H	256	ALA	SER	variant	UNP P06008

- Molecule 3 is a protein called Photosynthetic reaction center L subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	273	Total	C	N	O	S	0	1	0
			2172	1460	350	355	7			

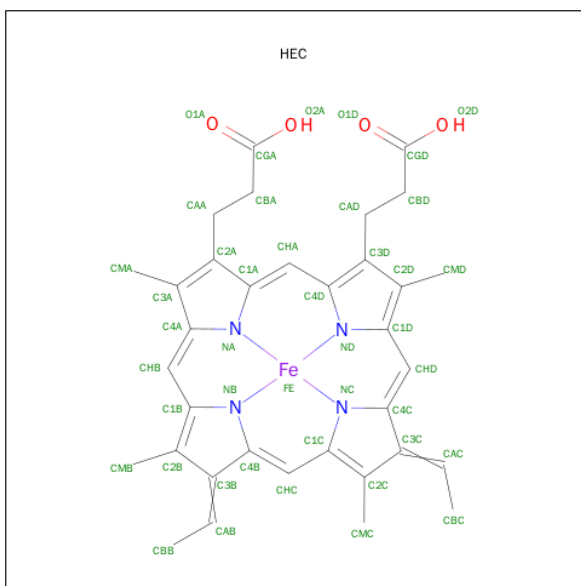
- Molecule 4 is a protein called Photosynthetic reaction center M subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	323	Total	C	N	O	S	0	2	0
			2557	1704	417	424	12			

There is a discrepancy between the modelled and reference sequences:

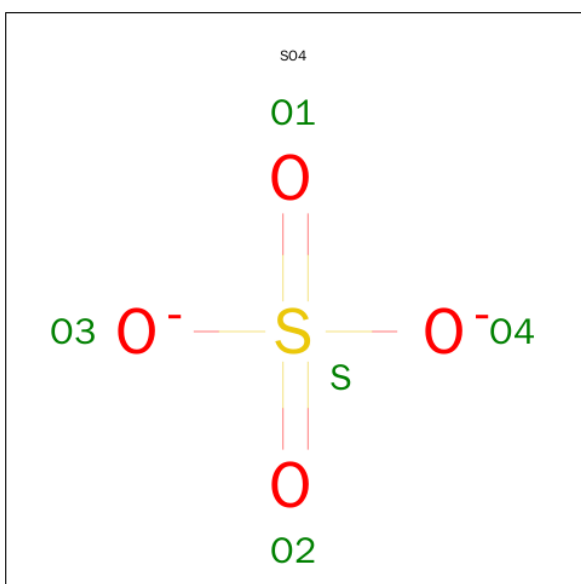
Chain	Residue	Modelled	Actual	Comment	Reference
M	200	LEU	HIS	variant	UNP P06010

- Molecule 5 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



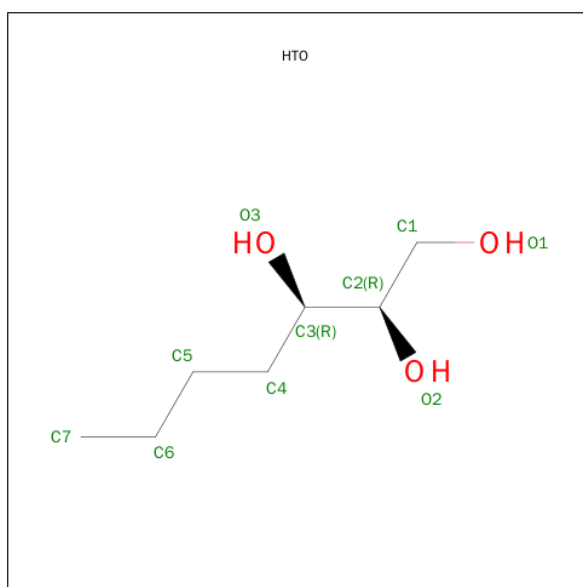
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
5	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
5	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
5	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



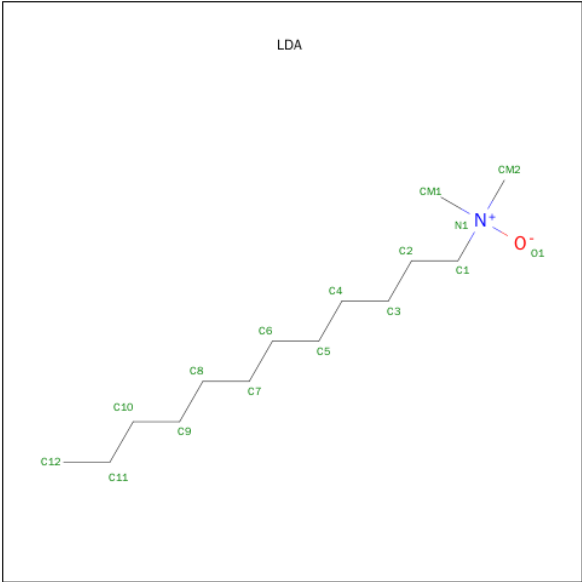
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	H	1	Total O S 5 4 1	0	0
6	H	1	Total O S 5 4 1	0	0
6	H	1	Total O S 5 4 1	0	0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

- Molecule 7 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: C<sub>7</sub>H<sub>16</sub>O<sub>3</sub>).



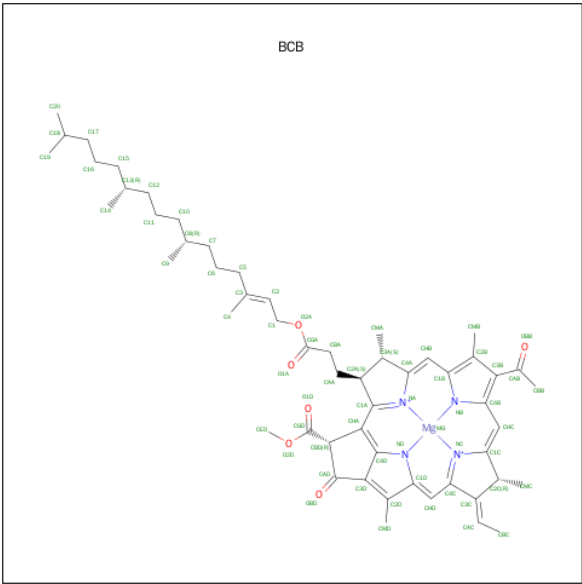
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			10	7	3		
7	C	1	Total	C	O	0	0
			10	7	3		
7	H	1	Total	C	O	0	0
			10	7	3		
7	L	1	Total	C	O	0	0
			10	7	3		
7	L	1	Total	C	O	0	0
			10	7	3		

- Molecule 8 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).



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

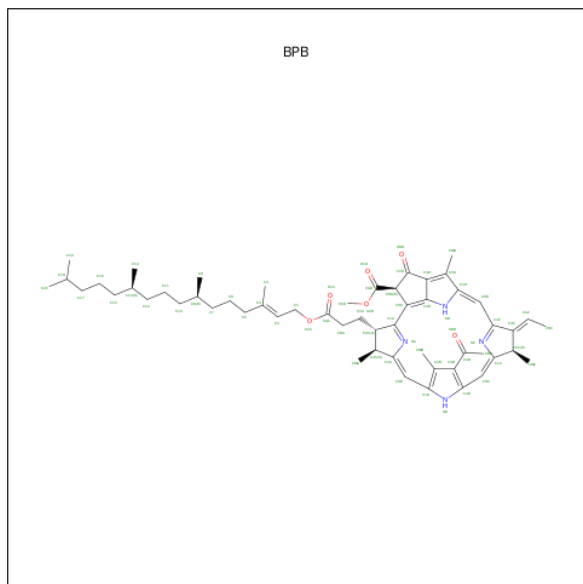
- Molecule 9 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>6</sub>).





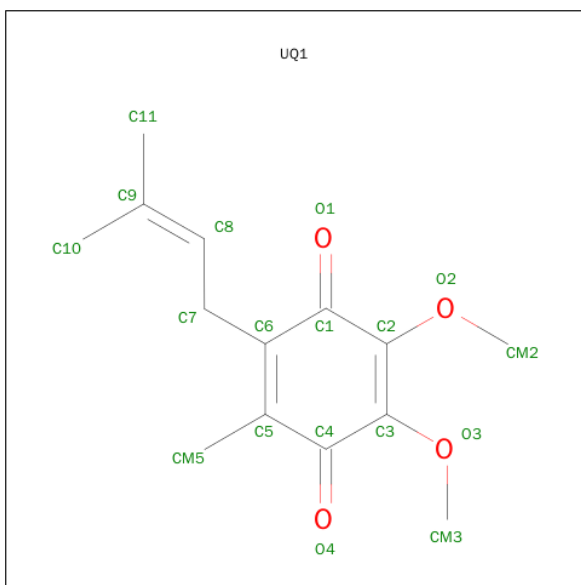
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 10 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula:  $C_{55}H_{74}N_4O_6$ ).



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

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

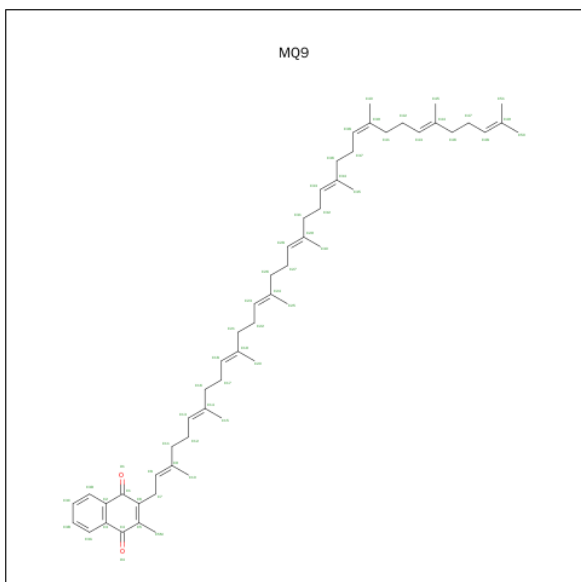


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	L	1	Total	C	O	0	0
			18	14	4		
11	M	1	Total	C	O	0	0
			18	14	4		

- Molecule 12 is FE (II) ION (three-letter code: FE2) (formula: Fe).

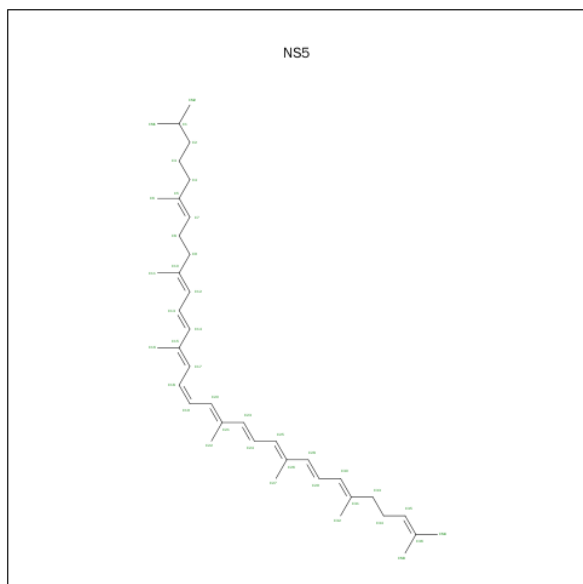
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	M	1	Total Fe 1 1	0	0

- Molecule 13 is MENAQUINONE-9 (three-letter code: MQ9) (formula:  $\text{C}_{56}\text{H}_{80}\text{O}_2$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	M	1	Total	C O	0	0
			58	56 2		

- Molecule 14 is 15-CIS-1,2-DIHYDRONEUROSPORENE (three-letter code: NS5) (formula: C<sub>40</sub>H<sub>60</sub>).



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

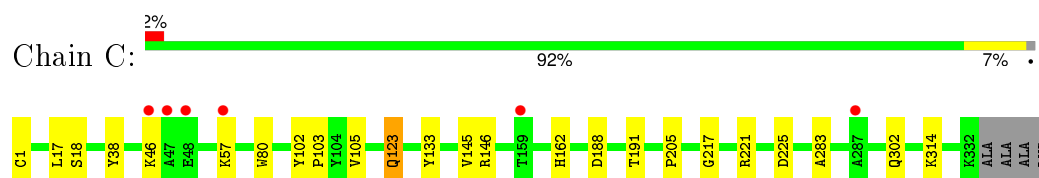
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	C	292	Total	O	0	0
			292	292		
15	H	172	Total	O	1	0
			172	172		
15	L	94	Total	O	0	0
			94	94		
15	M	172	Total	O	2	0
			172	172		

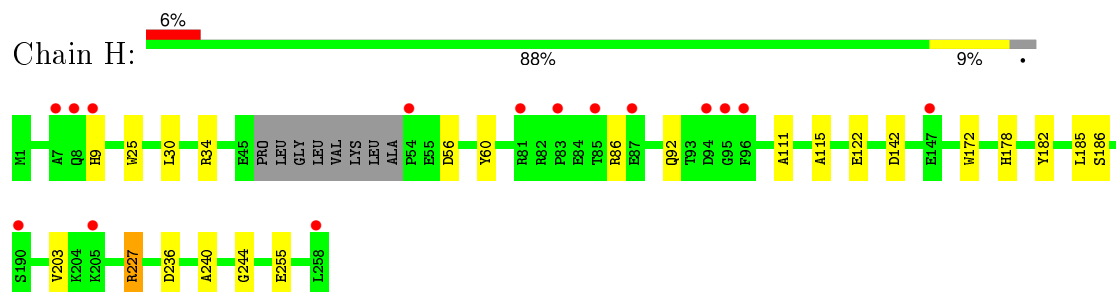
### 3 Residue-property plots [i](#)

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.

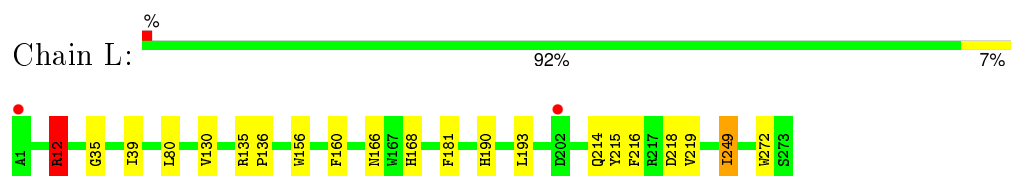
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



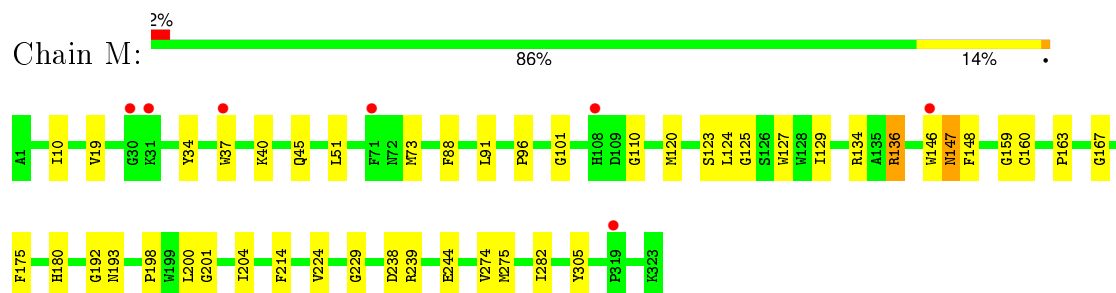
- Molecule 2: Photosynthetic reaction center H subunit



- Molecule 3: Photosynthetic reaction center L subunit



- Molecule 4: Photosynthetic reaction center M subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	220.13Å 220.13Å 112.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.99 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-2.50) 99.2 (19.99-2.50)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.92 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.176 , 0.206 0.175 , 0.204	Depositor DCC
$R_{free}$ test set	4754 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.3	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 60.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	2 of 95151 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10922	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	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 [i](#)

### 5.1 Standard geometry [i](#)

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, 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	0.62	0/2665	0.66	0/3633
2	H	0.65	0/1991	0.65	0/2718
3	L	0.72	0/2267	0.68	2/3095 (0.1%)
4	M	0.71	0/2670	0.63	0/3651
All	All	0.67	0/9593	0.65	2/13097 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	12	ARG	NE-CZ-NH2	-6.70	116.95	120.30
3	L	12	ARG	CG-CD-NE	-5.23	100.82	111.80

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2598	0	2568	16	0
2	H	1956	0	1944	14	0
3	L	2172	0	2097	22	0
4	M	2557	0	2462	48	0
5	C	172	0	120	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	35	0	0	1	0
6	H	20	0	0	0	0
6	L	5	0	0	0	0
6	M	35	0	0	1	0
7	C	20	0	32	2	0
7	H	10	0	16	1	0
7	L	20	0	32	0	0
8	H	32	0	62	0	0
8	M	32	0	62	3	0
9	L	132	0	144	27	0
9	M	66	0	72	7	0
10	L	65	0	74	6	0
10	M	130	0	148	40	0
11	L	18	0	18	4	0
11	M	18	0	18	0	0
12	M	1	0	0	0	0
13	M	58	0	80	4	0
14	M	40	0	60	4	0
15	C	292	0	0	2	0
15	H	172	0	0	4	0
15	L	94	0	0	0	0
15	M	172	0	0	3	0
All	All	10922	0	10009	152	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 8.

All (152) 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)
10:M:401:BPB:H4A	10:M:402:BPB:CBB	1.98	0.92
10:M:401:BPB:H4A	10:M:402:BPB:HBBB	1.53	0.90
10:M:402:BPB:CBB	10:M:402:BPB:HHC	2.04	0.88
4:M:204:ILE:HG12	10:M:401:BPB:CHB	2.03	0.87
4:M:200:LEU:HD13	4:M:204:ILE:HD12	1.60	0.81
9:L:401:BCB:HMD2	10:M:401:BPB:HBBB	1.62	0.81
9:M:400:BCB:CBB	9:M:400:BCB:HHC	2.11	0.81
9:L:400:BCB:CHB	10:M:401:BPB:HMBA	2.15	0.76
5:C:403:HEC:HBB3	5:C:403:HEC:HMB1	1.67	0.76
9:L:400:BCB:CBB	9:L:400:BCB:HMB1	2.16	0.76
9:L:401:BCB:HMB1	9:L:401:BCB:CBB	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:402:BPB:HBBB	10:M:402:BPB:HHC	1.69	0.74
2:H:86:ARG:NH1	15:H:569:HOH:O	2.20	0.74
1:C:123:GLN:HE21	1:C:123:GLN:H	1.35	0.73
10:M:401:BPB:HMB	10:M:401:BPB:CBB	2.19	0.73
10:M:401:BPB:H4A	10:M:402:BPB:CAB	2.19	0.72
3:L:168:HIS:CE1	9:L:400:BCB:HMC2	2.26	0.70
9:M:400:BCB:HBB2	14:M:600:NS5:H223	1.76	0.67
4:M:120:MET:CE	4:M:175:PHE:HE1	2.07	0.67
10:L:402:BPB:HMB	10:L:402:BPB:CBB	2.24	0.67
3:L:39:ILE:HD12	13:M:501:MQ9:H43	1.76	0.67
9:M:400:BCB:HBB2	9:M:400:BCB:HHC	1.76	0.66
5:C:403:HEC:HBC3	5:C:403:HEC:HMC1	1.78	0.64
4:M:127:TRP:CD1	10:M:402:BPB:HBAA	2.33	0.64
4:M:274:VAL:HG12	4:M:275:MET:HE2	1.80	0.63
4:M:101:GLY:O	15:M:797:HOH:O	2.15	0.63
2:H:122:GLU:OE2	15:H:605:HOH:O	2.16	0.63
3:L:214:GLN:NE2	4:M:19:VAL:H	1.97	0.62
3:L:193:LEU:HD23	11:L:502:UQ1:HM32	1.82	0.62
4:M:200:LEU:HD13	4:M:204:ILE:CD1	2.30	0.62
3:L:181:PHE:HB3	10:M:402:BPB:HBBA	1.82	0.62
1:C:221:ARG:NE	1:C:225:ASP:OD2	2.33	0.62
1:C:123:GLN:NE2	1:C:123:GLN:H	1.98	0.61
10:M:402:BPB:HBBA	10:M:402:BPB:HHC	1.81	0.61
9:L:400:BCB:H193	13:M:501:MQ9:H252	1.83	0.59
4:M:127:TRP:CD1	10:M:402:BPB:CBA	2.85	0.59
9:L:400:BCB:HMB2	10:M:401:BPB:CHB	2.32	0.59
9:L:400:BCB:HBB3	9:L:400:BCB:HMB1	1.84	0.58
9:L:401:BCB:HMB1	9:L:401:BCB:HBB2	1.85	0.57
3:L:181:PHE:CD2	10:M:402:BPB:HBB	2.39	0.57
10:M:401:BPB:C4	10:M:402:BPB:HBBB	2.31	0.57
4:M:120:MET:HE1	4:M:175:PHE:HE1	1.70	0.56
9:L:400:BCB:CHB	10:M:401:BPB:CMB	2.84	0.55
4:M:204:ILE:CG1	10:M:401:BPB:CHB	2.82	0.55
3:L:35:GLY:O	3:L:39:ILE:HG12	2.07	0.55
9:M:400:BCB:HBB3	9:M:400:BCB:HHC	1.87	0.55
1:C:314:LYS:HG2	5:C:404:HEC:HBD2	1.88	0.54
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.43	0.54
3:L:168:HIS:NE2	9:L:400:BCB:HMC2	2.23	0.54
10:M:401:BPB:HMB	10:M:401:BPB:HBBB	1.89	0.53
2:H:227:ARG:H	2:H:227:ARG:NE	2.06	0.53
4:M:200:LEU:CD1	4:M:204:ILE:CD1	2.87	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:400:BCB:HBB	10:M:401:BPB:HMB A	1.91	0.52
9:L:401:BCB:HBB3	9:L:401:BCB:HMB1	1.89	0.52
1:C:18:SER:HB2	3:L:156:TRP:CD1	2.44	0.52
4:M:200:LEU:CD1	4:M:204:ILE:HD12	2.36	0.52
1:C:102:TYR:CG	1:C:103:PRO:HD3	2.44	0.52
10:M:401:BPB:HBBA	10:M:401:BPB:HMB	1.90	0.52
4:M:120:MET:HE3	4:M:175:PHE:HE1	1.74	0.52
9:L:401:BCB:HMD2	10:M:401:BPB:CBB	2.35	0.52
1:C:217:GLY:HA2	4:M:167:GLY:O	2.09	0.52
10:L:402:BPB:HMB	10:L:402:BPB:HBBB	1.91	0.51
9:M:400:BCB:CBB	14:M:600:NS5:H223	2.38	0.51
1:C:162:HIS:N	6:C:813:SO4:O3	2.42	0.51
9:L:400:BCB:HBB2	9:L:400:BCB:HMB1	1.92	0.51
4:M:146:TRP:HZ2	15:M:829:HOH:O	1.92	0.51
2:H:30:LEU:O	2:H:34:ARG:HD2	2.11	0.51
2:H:115:ALA:HB2	2:H:244:GLY:HA3	1.93	0.51
9:L:401:BCB:HHC	9:L:401:BCB:OBB	2.11	0.50
3:L:166:ASN:OD1	3:L:168:HIS:HB2	2.12	0.50
10:M:402:BPB:CBB	10:M:402:BPB:CHC	2.82	0.50
9:L:400:BCB:HBD	9:L:400:BCB:HAA1	1.94	0.50
3:L:190:HIS:HD1	11:L:502:UQ1:HM33	1.77	0.49
2:H:92:GLN:NE2	15:H:637:HOH:O	2.45	0.49
9:L:400:BCB:H151	10:L:402:BPB:H5A	1.93	0.49
4:M:204:ILE:HG12	10:M:401:BPB:C1B	2.43	0.49
4:M:148:PHE:HE1	10:M:401:BPB:H9B	1.78	0.49
1:C:205:PRO:HB3	7:C:706:HTO:H12	1.93	0.49
11:L:502:UQ1:HM33	11:L:502:UQ1:O4	2.12	0.49
2:H:142:ASP:OD1	15:H:551:HOH:O	2.20	0.49
7:C:707:HTO:H42	15:C:764:HOH:O	2.13	0.49
10:M:401:BPB:NC	10:M:401:BPB:ND	2.59	0.48
4:M:282:ILE:HD11	10:M:401:BPB:OBD	2.13	0.48
4:M:136:ARG:NH1	15:M:853:HOH:O	2.41	0.48
2:H:25:TRP:CE3	2:H:25:TRP:HA	2.49	0.48
3:L:130:VAL:HG13	3:L:249:ILE:HG12	1.95	0.48
3:L:214:GLN:HE21	4:M:19:VAL:H	1.62	0.48
4:M:73:MET:HE1	4:M:88:PHE:CE1	2.48	0.48
3:L:39:ILE:HD11	13:M:501:MQ9:H372	1.97	0.47
10:M:401:BPB:H20A	10:M:401:BPB:H16	1.75	0.47
13:M:501:MQ9:H421	13:M:501:MQ9:H403	1.75	0.47
10:L:402:BPB:HHC	10:L:402:BPB:OBB	2.15	0.47
4:M:73:MET:HE3	4:M:91:LEU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:198:PRO:HA	8:M:702:LDA:H112	1.97	0.47
4:M:96:PRO:HD3	4:M:110:GLY:HA3	1.96	0.47
4:M:274:VAL:HG12	4:M:275:MET:CE	2.44	0.46
10:M:402:BPB:H9	10:M:402:BPB:H11	1.72	0.46
2:H:255:GLU:CD	3:L:12:ARG:HH22	2.18	0.46
4:M:127:TRP:CD1	10:M:402:BPB:HBA	2.51	0.46
14:M:600:NS5:H18	14:M:600:NS5:H161	1.81	0.45
10:M:402:BPB:HMB	10:M:402:BPB:OBB	2.16	0.45
4:M:239:ARG:HD3	4:M:244:GLU:HG2	1.99	0.45
8:M:704:LDA:HM11	8:M:704:LDA:H22	1.74	0.45
10:M:402:BPB:CBC	10:M:402:BPB:HMC	2.47	0.45
4:M:159:GLY:HA3	14:M:600:NS5:H272	1.99	0.45
1:C:145:VAL:O	1:C:146:ARG:HD2	2.17	0.45
11:L:502:UQ1:O4	11:L:502:UQ1:CM3	2.65	0.45
4:M:37:TRP:HD1	6:M:805:SO4:O2	1.99	0.45
9:M:400:BCB:CBB	9:M:400:BCB:CHC	2.86	0.44
2:H:56:ASP:HB3	2:H:60:TYR:CE2	2.52	0.44
4:M:160:CYS:C	4:M:163:PRO:HD2	2.38	0.44
2:H:172:TRP:HB2	2:H:182:TYR:HB2	1.99	0.44
4:M:204:ILE:HD11	10:M:401:BPB:C1B	2.48	0.44
2:H:203:VAL:HG11	4:M:10:ILE:HD11	2.00	0.44
1:C:188:ASP:OD2	1:C:191:THR:HG23	2.18	0.44
10:L:402:BPB:HBBA	10:L:402:BPB:HMB	1.98	0.43
9:L:400:BCB:H203	9:L:400:BCB:H161	1.64	0.43
3:L:160:PHE:CD2	9:L:400:BCB:HMD1	2.53	0.43
1:C:105:VAL:HG13	15:C:510:HOH:O	2.17	0.43
1:C:17:LEU:HD21	4:M:305:TYR:CZ	2.54	0.43
4:M:192:GLY:O	4:M:193:ASN:HB3	2.19	0.43
4:M:120:MET:HE1	4:M:175:PHE:CE1	2.53	0.43
4:M:34:TYR:CE2	4:M:45:GLN:HB2	2.53	0.43
9:L:401:BCB:HBA1	9:L:401:BCB:C4A	2.48	0.43
10:M:401:BPB:H16A	10:M:401:BPB:H14	1.64	0.43
9:M:400:BCB:HMB1	9:M:400:BCB:OBB	2.19	0.43
2:H:86:ARG:NH2	2:H:111:ALA:O	2.52	0.43
4:M:224:VAL:HG23	4:M:229:GLY:HA3	2.00	0.42
4:M:148:PHE:HE1	10:M:401:BPB:C9	2.32	0.42
4:M:200:LEU:HD11	4:M:204:ILE:HD11	2.01	0.42
9:L:400:BCB:CAD	9:L:401:BCB:HBC1	2.49	0.42
3:L:193:LEU:HD22	3:L:216:PHE:HE2	1.84	0.42
4:M:201:GLY:HA3	8:M:702:LDA:H122	2.02	0.42
3:L:218:ASP:HB3	4:M:134:ARG:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:400:BCB:C1B	10:M:401:BPB:C2B	2.97	0.42
9:L:400:BCB:HHC	9:L:400:BCB:OBB	2.19	0.42
2:H:115:ALA:HA	2:H:240:ALA:O	2.20	0.42
3:L:135:ARG:HB3	3:L:136:PRO:HD3	2.02	0.42
10:L:402:BPB:NC	10:L:402:BPB:ND	2.68	0.41
9:L:400:BCB:CMB	10:M:401:BPB:CHB	2.98	0.41
1:C:146:ARG:HD2	1:C:146:ARG:HA	1.87	0.41
9:L:400:BCB:HMB2	10:M:401:BPB:HHB	2.02	0.41
4:M:147:ASN:C	4:M:147:ASN:HD22	2.24	0.41
4:M:123:SER:OG	10:M:402:BPB:H1	2.21	0.41
7:H:705:HTO:H73	4:M:238:ASP:HB2	2.02	0.41
9:L:400:BCB:H2C	10:M:401:BPB:H43	2.03	0.41
3:L:215:TYR:O	3:L:219:VAL:HG23	2.21	0.40
3:L:214:GLN:HG2	4:M:19:VAL:HB	2.03	0.40
4:M:146:TRP:HA	4:M:146:TRP:CE3	2.56	0.40
3:L:193:LEU:HD22	3:L:216:PHE:CE2	2.57	0.40
4:M:125:GLY:O	4:M:129:ILE:HG13	2.21	0.40
1:C:283:ALA:HB2	1:C:302:GLN:NE2	2.36	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	330/336 (98%)	318 (96%)	12 (4%)	0	100	100
2	H	246/258 (95%)	240 (98%)	6 (2%)	0	100	100
3	L	272/273 (100%)	267 (98%)	5 (2%)	0	100	100
4	M	323/323 (100%)	314 (97%)	9 (3%)	0	100	100
All	All	1171/1190 (98%)	1139 (97%)	32 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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%)	275 (98%)	5 (2%)	66	88
2	H	204/211 (97%)	198 (97%)	6 (3%)	50	77
3	L	219/218 (100%)	215 (98%)	4 (2%)	66	88
4	M	251/249 (101%)	244 (97%)	7 (3%)	51	78
All	All	954/960 (99%)	932 (98%)	22 (2%)	58	83

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1	CYS
1	C	38	TYR
1	C	46	LYS
1	C	57	LYS
1	C	123	GLN
2	H	9	HIS
2	H	178	HIS
2	H	185	LEU
2	H	186	SER
2	H	227	ARG
2	H	236	ASP
3	L	12	ARG
3	L	80	LEU
3	L	249	ILE
3	L	272	TRP
4	M	40	LYS
4	M	51	LEU
4	M	124	LEU
4	M	136	ARG
4	M	147	ASN
4	M	180	HIS
4	M	214	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	54	GLN
1	C	123	GLN
1	C	206	GLN
1	C	302	GLN
2	H	58	GLN
2	H	220	ASN
2	H	225	GLN
3	L	183	ASN
3	L	214	GLN
3	L	239	ASN
4	M	147	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FME	H	1	2	8,9,10	0.77	0	6,9,11	3.62	2 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	H	1	2	-	0/6/9/11	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	FME	CA-N-CN	-7.98	110.55	122.82
2	H	1	FME	CE-SD-CG	2.45	108.73	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 43 ligands modelled in this entry, 1 is monoatomic - leaving 42 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	HEC	C	401	1	24,50,50	2.00	2 (8%)	19,82,82	2.70	4 (21%)
5	HEC	C	402	1	24,50,50	1.81	3 (12%)	19,82,82	2.41	5 (26%)
5	HEC	C	403	1	24,50,50	1.65	2 (8%)	19,82,82	2.60	4 (21%)
5	HEC	C	404	1	24,50,50	1.51	2 (8%)	19,82,82	2.62	6 (31%)
7	HTO	C	706	-	9,9,9	0.41	0	8,10,10	0.48	0
7	HTO	C	707	-	9,9,9	0.73	0	8,10,10	0.86	0
6	SO4	C	808	-	4,4,4	0.17	0	6,6,6	0.26	0
6	SO4	C	809	-	4,4,4	0.18	0	6,6,6	0.20	0
6	SO4	C	810	-	4,4,4	0.30	0	6,6,6	0.18	0
6	SO4	C	811	-	4,4,4	0.30	0	6,6,6	0.22	0
6	SO4	C	813	-	4,4,4	0.38	0	6,6,6	0.51	0
6	SO4	C	815	-	4,4,4	0.26	0	6,6,6	0.08	0
6	SO4	C	817	-	4,4,4	0.26	0	6,6,6	0.07	0
8	LDA	H	701	-	15,15,15	3.36	1 (6%)	16,17,17	1.05	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	LDA	H	703	-	15,15,15	3.30	2 (13%)	16,17,17	1.00	1 (6%)
7	HTO	H	705	-	9,9,9	0.39	0	8,10,10	0.72	0
6	SO4	H	803	-	4,4,4	0.10	0	6,6,6	0.36	0
6	SO4	H	806	-	4,4,4	0.25	0	6,6,6	0.17	0
6	SO4	H	807	-	4,4,4	0.10	0	6,6,6	0.26	0
6	SO4	H	812	-	4,4,4	0.24	0	6,6,6	0.14	0
9	BCB	L	400	3	56,74,74	2.59	6 (10%)	57,115,115	1.69	10 (17%)
9	BCB	L	401	3	56,74,74	2.61	5 (8%)	57,115,115	1.68	8 (14%)
10	BPB	L	402	-	63,70,70	2.32	9 (14%)	63,101,101	2.86	17 (26%)
11	UQ1	L	502	-	18,18,18	1.85	2 (11%)	22,25,25	1.05	1 (4%)
7	HTO	L	708	-	9,9,9	0.21	0	8,10,10	0.73	0
7	HTO	L	709	-	9,9,9	0.22	0	8,10,10	0.66	0
6	SO4	L	814	-	4,4,4	0.26	0	6,6,6	0.09	0
9	BCB	M	400	4	56,74,74	2.54	7 (12%)	57,115,115	1.64	8 (14%)
10	BPB	M	401	-	63,70,70	2.43	9 (14%)	63,101,101	3.09	20 (31%)
10	BPB	M	402	-	63,70,70	2.40	8 (12%)	63,101,101	2.92	18 (28%)
13	MQ9	M	501	-	59,59,59	2.00	19 (32%)	74,75,75	1.48	17 (22%)
11	UQ1	M	503	-	18,18,18	1.92	2 (11%)	22,25,25	1.06	0
14	NS5	M	600	-	39,39,39	1.45	3 (7%)	44,46,46	1.83	9 (20%)
8	LDA	M	702	-	15,15,15	3.60	2 (13%)	16,17,17	0.82	1 (6%)
8	LDA	M	704	-	15,15,15	3.83	1 (6%)	16,17,17	1.20	2 (12%)
6	SO4	M	801	-	4,4,4	0.31	0	6,6,6	0.66	0
6	SO4	M	802	-	4,4,4	0.31	0	6,6,6	0.49	0
6	SO4	M	804	-	4,4,4	0.39	0	6,6,6	0.28	0
6	SO4	M	805	-	4,4,4	0.25	0	6,6,6	0.39	0
6	SO4	M	816	-	4,4,4	0.26	0	6,6,6	0.08	0
6	SO4	M	818	-	4,4,4	0.25	0	6,6,6	0.08	0
6	SO4	M	819	-	4,4,4	0.25	0	6,6,6	0.10	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEC	C	401	1	-	0/6/54/54	0/0/8/8
5	HEC	C	402	1	-	0/6/54/54	0/0/8/8
5	HEC	C	403	1	-	0/6/54/54	0/0/8/8
5	HEC	C	404	1	-	0/6/54/54	0/0/8/8
7	HTO	C	706	-	-	0/10/10/10	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	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
8	LDA	H	701	-	-	0/13/13/13	0/0/0/0
8	LDA	H	703	-	-	0/13/13/13	0/0/0/0
7	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
9	BCB	L	400	3	-	0/37/137/137	0/0/9/9
9	BCB	L	401	3	-	0/37/137/137	0/0/9/9
10	BPB	L	402	-	-	0/46/105/105	0/1/6/6
11	UQ1	L	502	-	-	0/9/33/33	0/1/1/1
7	HTO	L	708	-	-	0/10/10/10	0/0/0/0
7	HTO	L	709	-	-	0/10/10/10	0/0/0/0
6	SO4	L	814	-	-	0/0/0/0	0/0/0/0
9	BCB	M	400	4	-	0/37/137/137	0/0/9/9
10	BPB	M	401	-	-	0/46/105/105	0/1/6/6
10	BPB	M	402	-	-	0/46/105/105	0/1/6/6
13	MQ9	M	501	-	-	0/53/73/73	0/2/2/2
11	UQ1	M	503	-	-	0/9/33/33	0/1/1/1
14	NS5	M	600	-	-	0/43/43/43	0/0/0/0
8	LDA	M	702	-	-	0/13/13/13	0/0/0/0
8	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 (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	704	LDA	O1-N1	-14.65	1.25	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	702	LDA	O1-N1	-13.69	1.26	1.39
8	H	701	LDA	O1-N1	-12.73	1.27	1.39
8	H	703	LDA	O1-N1	-12.37	1.27	1.39
5	C	401	HEC	C3B-C2B	-6.34	1.34	1.40
9	L	401	BCB	C4D-CHA	-6.16	1.37	1.45
5	C	401	HEC	C3C-C2C	-6.00	1.34	1.40
9	L	400	BCB	C4D-CHA	-5.83	1.37	1.45
9	M	400	BCB	C4D-CHA	-5.36	1.38	1.45
5	C	402	HEC	C3C-C2C	-5.35	1.35	1.40
5	C	402	HEC	C3B-C2B	-4.92	1.35	1.40
5	C	403	HEC	C3B-C2B	-4.82	1.35	1.40
13	M	501	MQ9	C2-C1	-4.61	1.39	1.48
5	C	403	HEC	C3C-C2C	-4.46	1.36	1.40
5	C	404	HEC	C3B-C2B	-4.35	1.36	1.40
13	M	501	MQ9	C3-C4	-3.97	1.40	1.48
5	C	404	HEC	C3C-C2C	-3.88	1.36	1.40
13	M	501	MQ9	C5-C4	-3.73	1.39	1.48
13	M	501	MQ9	C7-C8	-3.19	1.45	1.50
8	H	703	LDA	C1-N1	-2.83	1.46	1.51
10	L	402	BPB	C4D-CHA	-2.75	1.37	1.44
13	M	501	MQ9	C32-C33	-2.50	1.43	1.50
10	M	402	BPB	C3D-C4D	-2.49	1.35	1.43
13	M	501	MQ9	C6-C1	-2.43	1.41	1.47
9	M	400	BCB	C2C-C1C	-2.39	1.49	1.51
10	M	401	BPB	C3D-C2D	-2.38	1.31	1.38
13	M	501	MQ9	C47-C48	-2.29	1.44	1.50
10	M	401	BPB	C3D-C4D	-2.27	1.36	1.43
10	L	402	BPB	C3D-C4D	-2.20	1.36	1.43
10	M	402	BPB	C4D-CHA	-2.20	1.38	1.44
13	M	501	MQ9	C37-C38	-2.20	1.44	1.50
8	M	702	LDA	C1-N1	-2.15	1.47	1.51
13	M	501	MQ9	C42-C43	-2.11	1.44	1.50
10	L	402	BPB	C4C-NC	2.01	1.41	1.37
5	C	402	HEC	C4A-NA	2.14	1.39	1.36
14	M	600	NS5	C7-C5	2.22	1.37	1.33
9	L	400	BCB	C3D-C4D	2.24	1.44	1.41
13	M	501	MQ9	C48-C49	2.27	1.39	1.32
14	M	600	NS5	C4-C5	2.27	1.56	1.51
10	M	401	BPB	C2-C3	2.35	1.37	1.33
9	M	400	BCB	C4C-C3C	2.40	1.49	1.45
10	M	402	BPB	C3B-C4B	2.53	1.44	1.41
10	L	402	BPB	C1D-ND	2.59	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	402	BPB	C3B-C4B	2.69	1.44	1.41
10	M	401	BPB	C1D-ND	2.69	1.44	1.38
10	M	402	BPB	C1D-ND	2.70	1.44	1.38
13	M	501	MQ9	C6-C5	2.91	1.42	1.35
10	M	401	BPB	C1A-CHA	3.05	1.42	1.36
9	L	401	BCB	C2-C3	3.10	1.39	1.33
11	L	502	UQ1	C3-C2	3.11	1.49	1.35
9	L	401	BCB	O2D-CGD	3.14	1.41	1.33
13	M	501	MQ9	C18-C19	3.27	1.39	1.33
13	M	501	MQ9	C23-C24	3.33	1.39	1.33
10	L	402	BPB	C2-C3	3.34	1.39	1.33
9	M	400	BCB	C2-C3	3.39	1.39	1.33
13	M	501	MQ9	C43-C44	3.43	1.39	1.33
9	L	400	BCB	C2-C3	3.51	1.39	1.33
11	M	503	UQ1	C3-C2	3.59	1.51	1.35
10	L	402	BPB	O2A-CGA	3.61	1.44	1.33
13	M	501	MQ9	C33-C34	3.63	1.40	1.33
13	M	501	MQ9	C38-C39	3.70	1.40	1.33
9	M	400	BCB	O2D-CGD	3.72	1.42	1.33
13	M	501	MQ9	C13-C14	3.73	1.40	1.33
10	M	401	BPB	C3B-C4B	3.79	1.46	1.41
13	M	501	MQ9	C28-C29	3.81	1.40	1.33
10	M	401	BPB	O2A-CGA	3.87	1.45	1.33
9	L	400	BCB	O2A-CGA	3.87	1.45	1.33
9	L	401	BCB	O2A-CGA	3.97	1.45	1.33
10	M	402	BPB	C2-C3	3.99	1.40	1.33
10	M	402	BPB	O2A-CGA	4.00	1.45	1.33
10	L	402	BPB	O2D-CGD	4.03	1.43	1.33
10	M	402	BPB	O2D-CGD	4.06	1.43	1.33
9	L	400	BCB	O2D-CGD	4.28	1.44	1.33
9	M	400	BCB	O2A-CGA	4.28	1.46	1.33
13	M	501	MQ9	C8-C9	4.36	1.41	1.33
10	M	401	BPB	O2D-CGD	5.00	1.46	1.33
11	M	503	UQ1	C6-C5	6.36	1.50	1.35
11	L	502	UQ1	C6-C5	6.40	1.50	1.35
14	M	600	NS5	C35-C36	6.72	1.53	1.32
10	L	402	BPB	CAC-C3C	15.36	1.52	1.33
9	M	400	BCB	CAC-C3C	15.65	1.52	1.33
10	M	401	BPB	CAC-C3C	15.84	1.52	1.33
10	M	402	BPB	CAC-C3C	16.03	1.53	1.33
9	L	400	BCB	CAC-C3C	16.18	1.53	1.33
9	L	401	BCB	CAC-C3C	16.61	1.53	1.33

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	403	HEC	CBB-CAB-C3B	-7.96	109.66	127.35
5	C	401	HEC	CBB-CAB-C3B	-7.72	110.20	127.35
5	C	401	HEC	CBC-CAC-C3C	-7.04	111.72	127.35
5	C	404	HEC	CBC-CAC-C3C	-6.89	112.05	127.35
5	C	402	HEC	CBB-CAB-C3B	-6.56	112.77	127.35
5	C	404	HEC	CBB-CAB-C3B	-6.45	113.03	127.35
10	L	402	BPB	C3D-C2D-C1D	-6.24	95.75	105.77
10	M	401	BPB	C3D-C2D-C1D	-6.21	95.79	105.77
5	C	403	HEC	CBC-CAC-C3C	-6.07	113.87	127.35
5	C	402	HEC	CBC-CAC-C3C	-6.05	113.91	127.35
10	M	402	BPB	C3D-C2D-C1D	-5.97	96.18	105.77
14	M	600	NS5	C19-C20-C21	-4.57	120.59	127.20
9	M	400	BCB	O1D-CGD-CBD	-4.36	118.38	124.62
14	M	600	NS5	C34-C35-C36	-4.22	111.50	127.73
10	M	401	BPB	CAD-C3D-C2D	-3.92	121.89	140.80
10	M	402	BPB	O1D-CGD-CBD	-3.87	119.08	124.62
10	M	401	BPB	C3D-C4D-ND	-3.70	97.75	109.65
10	M	402	BPB	C4-C3-C2	-3.65	116.34	123.50
14	M	600	NS5	CM4-C36-C35	-3.64	110.90	122.61
14	M	600	NS5	CM3-C36-C35	-3.58	111.09	122.61
10	L	402	BPB	CBC-CAC-C3C	-3.52	118.96	127.07
14	M	600	NS5	C18-C17-C15	-3.51	122.12	127.20
10	M	401	BPB	O1D-CGD-CBD	-3.51	119.59	124.62
10	M	402	BPB	CBC-CAC-C3C	-3.51	118.96	127.07
10	L	402	BPB	CAD-C3D-C2D	-3.40	124.38	140.80
10	M	402	BPB	CAD-C3D-C2D	-3.35	124.63	140.80
10	M	401	BPB	C2C-C3C-C4C	-3.35	104.18	107.24
10	L	402	BPB	O1D-CGD-CBD	-3.24	119.98	124.62
5	C	404	HEC	CAD-CBD-CGD	-3.23	106.82	112.75
9	M	400	BCB	CBC-CAC-C3C	-3.23	119.63	127.07
10	M	402	BPB	C3D-C4D-ND	-3.19	99.38	109.65
9	L	400	BCB	O1D-CGD-CBD	-3.18	120.07	124.62
9	L	400	BCB	CBC-CAC-C3C	-3.14	119.82	127.07
10	L	402	BPB	C3D-C4D-ND	-3.08	99.75	109.65
8	M	704	LDA	O1-N1-CM1	-3.05	104.98	109.05
13	M	501	MQ9	C40-C39-C38	-2.98	117.64	123.50
9	L	401	BCB	C1D-CHD-C4C	-2.93	122.97	129.26
5	C	403	HEC	CMB-C2B-C1B	-2.91	123.54	128.36
9	M	400	BCB	C1D-CHD-C4C	-2.91	123.00	129.26
9	L	401	BCB	O1D-CGD-CBD	-2.91	120.46	124.62
9	L	401	BCB	O2D-CGD-O1D	-2.87	117.86	123.79
13	M	501	MQ9	C32-C33-C34	-2.87	121.52	127.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	401	BPB	CBC-CAC-C3C	-2.82	120.57	127.07
9	L	401	BCB	CBC-CAC-C3C	-2.80	120.62	127.07
13	M	501	MQ9	C22-C23-C24	-2.72	121.84	127.76
14	M	600	NS5	C6-C5-C7	-2.66	118.27	123.50
5	C	404	HEC	CMC-C2C-C1C	-2.64	124.00	128.36
5	C	401	HEC	CMC-C2C-C1C	-2.63	124.02	128.36
10	M	402	BPB	CAA-C2A-C1A	-2.62	103.22	112.47
9	M	400	BCB	C3C-C4C-NC	-2.61	108.30	110.24
13	M	501	MQ9	C42-C43-C44	-2.59	122.13	127.76
9	L	400	BCB	C1D-CHD-C4C	-2.59	123.70	129.26
10	M	402	BPB	CAA-C2A-C3A	-2.54	105.92	113.22
10	M	401	BPB	CGD-CBD-CAD	-2.52	102.10	110.62
13	M	501	MQ9	C17-C18-C19	-2.48	122.37	127.76
5	C	404	HEC	CMB-C2B-C1B	-2.48	124.26	128.36
8	H	703	LDA	CM2-N1-CM1	-2.44	106.08	108.83
10	M	402	BPB	C2C-C3C-C4C	-2.43	105.02	107.24
10	M	401	BPB	C6-C5-C3	-2.38	107.25	112.48
13	M	501	MQ9	C37-C38-C39	-2.37	122.62	127.76
5	C	402	HEC	CBA-CAA-C2A	-2.29	108.43	112.53
5	C	402	HEC	CMB-C2B-C1B	-2.29	124.58	128.36
5	C	402	HEC	CMC-C2C-C1C	-2.28	124.60	128.36
10	M	401	BPB	CBD-CHA-C4D	-2.27	105.91	108.46
9	L	400	BCB	C6-C7-C8	-2.27	107.95	115.49
5	C	401	HEC	CBD-CAD-C3D	-2.25	108.50	112.53
10	L	402	BPB	O2D-CGD-O1D	-2.20	119.25	123.79
10	M	401	BPB	C6-C7-C8	-2.19	108.21	115.49
10	L	402	BPB	O2A-CGA-O1A	-2.18	117.86	123.49
13	M	501	MQ9	C12-C13-C14	-2.17	123.05	127.76
13	M	501	MQ9	C7-C8-C9	-2.13	123.08	126.70
10	M	402	BPB	CAA-CBA-CGA	-2.13	107.08	113.32
13	M	501	MQ9	C45-C44-C43	-2.12	119.33	123.50
13	M	501	MQ9	C27-C28-C29	-2.08	123.25	127.76
5	C	404	HEC	CAD-C3D-C4D	-2.04	124.79	127.01
5	C	403	HEC	CMC-C2C-C1C	-2.03	125.00	128.36
10	L	402	BPB	CHD-C1D-ND	-2.03	120.87	124.66
9	L	400	BCB	CED-O2D-CGD	2.04	120.77	115.99
13	M	501	MQ9	C45-C44-C46	2.13	118.66	115.41
11	L	502	UQ1	CM3-O3-C3	2.16	124.28	116.61
10	L	402	BPB	C4-C3-C5	2.20	118.77	115.41
10	M	402	BPB	C3C-C2C-C1C	2.20	104.24	100.99
10	M	401	BPB	O2A-CGA-CBA	2.22	118.65	111.90
10	M	402	BPB	C4-C3-C5	2.24	118.83	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	401	BPB	C4-C3-C5	2.27	118.87	115.41
10	M	401	BPB	CED-O2D-CGD	2.29	121.36	115.99
9	L	400	BCB	C3A-C2A-C1A	2.33	105.44	101.50
10	M	401	BPB	CMD-C2D-C3D	2.34	133.48	128.04
13	M	501	MQ9	C30-C29-C31	2.36	119.01	115.41
8	M	704	LDA	CM2-N1-CM1	2.38	111.51	108.83
13	M	501	MQ9	C20-C19-C21	2.42	119.11	115.41
14	M	600	NS5	C11-C10-C9	2.43	119.11	115.41
13	M	501	MQ9	C15-C14-C16	2.45	119.15	115.41
13	M	501	MQ9	C40-C39-C41	2.45	119.16	115.41
10	M	402	BPB	C4D-C3D-CAD	2.46	109.94	105.51
10	L	402	BPB	C4D-C3D-CAD	2.53	110.07	105.51
9	M	400	BCB	O2A-CGA-CBA	2.55	119.68	111.90
10	L	402	BPB	O2A-CGA-CBA	2.57	119.74	111.90
9	L	401	BCB	O2A-CGA-CBA	2.58	119.76	111.90
10	M	401	BPB	C2A-C1A-CHA	2.66	133.47	126.22
8	M	702	LDA	O1-N1-C1	2.68	113.29	110.27
10	L	402	BPB	CMD-C2D-C1D	2.75	129.53	125.06
13	M	501	MQ9	C35-C34-C36	2.76	119.63	115.41
8	H	701	LDA	O1-N1-C1	2.78	113.40	110.27
14	M	600	NS5	C32-C31-C33	2.80	119.68	115.41
10	L	402	BPB	CMD-C2D-C3D	2.87	134.72	128.04
10	M	401	BPB	C4D-C3D-CAD	2.90	110.72	105.51
10	L	402	BPB	C3C-C2C-C1C	2.94	105.33	100.99
10	L	402	BPB	CBD-CHA-C1A	2.96	131.78	126.78
9	M	400	BCB	C4A-NA-C1A	2.97	109.54	106.04
9	M	400	BCB	C4-C3-C5	3.08	120.11	115.41
9	L	400	BCB	O2A-CGA-CBA	3.10	121.34	111.90
9	L	400	BCB	C4-C3-C5	3.18	120.27	115.41
14	M	600	NS5	C6-C5-C4	3.28	120.42	115.41
10	M	402	BPB	CBD-CHA-C1A	3.29	132.34	126.78
10	M	402	BPB	CMD-C2D-C3D	3.31	135.74	128.04
9	L	401	BCB	C4-C3-C5	3.32	120.48	115.41
9	L	400	BCB	C4A-NA-C1A	3.33	109.97	106.04
13	M	501	MQ9	C25-C24-C26	3.36	120.55	115.41
10	M	401	BPB	CBD-CHA-C1A	3.44	132.58	126.78
10	M	401	BPB	CMD-C2D-C1D	3.48	130.73	125.06
9	L	401	BCB	C4A-NA-C1A	3.54	110.21	106.04
10	M	402	BPB	O2A-CGA-CBA	3.70	123.18	111.90
9	L	400	BCB	O2D-CGD-CBD	6.10	119.67	111.30
9	M	400	BCB	O2D-CGD-CBD	6.51	120.22	111.30
10	M	401	BPB	O2D-CGD-CBD	6.78	120.60	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	402	BPB	O2D-CGD-CBD	6.86	120.71	111.30
10	M	402	BPB	O2D-CGD-CBD	7.09	121.03	111.30
9	L	401	BCB	O2D-CGD-CBD	7.44	121.50	111.30
10	M	402	BPB	C4D-C3D-C2D	16.52	125.42	106.74
10	L	402	BPB	C4D-C3D-C2D	16.64	125.56	106.74
10	M	401	BPB	C4D-C3D-C2D	18.26	127.38	106.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 89 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	403	HEC	2	0
5	C	404	HEC	1	0
7	C	706	HTO	1	0
7	C	707	HTO	1	0
6	C	813	SO4	1	0
7	H	705	HTO	1	0
9	L	400	BCB	20	0
9	L	401	BCB	8	0
10	L	402	BPB	6	0
11	L	502	UQ1	4	0
9	M	400	BCB	7	0
10	M	401	BPB	27	0
10	M	402	BPB	17	0
13	M	501	MQ9	4	0
14	M	600	NS5	4	0
8	M	702	LDA	2	0
8	M	704	LDA	1	0
6	M	805	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%)	-0.51	6 (1%) 71 75	21, 31, 49, 61	0
2	H	249/258 (96%)	-0.37	15 (6%) 25 28	18, 32, 50, 60	0
3	L	273/273 (100%)	-0.75	2 (0%) 89 90	20, 26, 41, 47	0
4	M	323/323 (100%)	-0.64	7 (2%) 65 69	17, 28, 45, 50	0
All	All	1177/1190 (98%)	-0.57	30 (2%) 61 65	17, 29, 46, 61	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	85	THR	5.7
2	H	83	PRO	3.9
4	M	319	PRO	3.9
2	H	8	GLN	3.9
1	C	47	ALA	3.6
2	H	81	ARG	3.4
2	H	9	HIS	3.4
3	L	202	ASP	3.4
4	M	108	HIS	3.2
2	H	54	PRO	3.2
2	H	7	ALA	3.0
4	M	31	LYS	2.9
1	C	48	GLU	2.9
1	C	57	LYS	2.8
2	H	95	GLY	2.8
3	L	1	ALA	2.7
4	M	37	TRP	2.6
1	C	46	LYS	2.5
4	M	30	GLY	2.4
2	H	205	LYS	2.4
2	H	87	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	94	ASP	2.3
2	H	258	LEU	2.3
2	H	147	GLU	2.3
2	H	190	SER	2.3
4	M	71	PHE	2.3
1	C	159	THR	2.3
1	C	287	ALA	2.2
2	H	96	PHE	2.1
4	M	146	TRP	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	0.97	0.10	-	36,38,49,53	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(Å <sup>2</sup> )	Q<0.9
6	SO4	C	815	5/5	0.12	1.74	18.96	2,2,2,2	5
10	BPB	M	401	65/65	0.77	0.34	11.01	28,39,45,47	65
8	LDA	M	702	16/16	0.76	0.32	8.36	47,57,67,67	0
11	UQ1	M	503	18/18	0.33	0.48	7.86	93,94,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	HTO	C	707	10/10	0.85	0.22	7.20	50,54,57,57	0
8	LDA	M	704	16/16	0.81	0.27	6.31	55,58,68,69	0
6	SO4	H	807	5/5	0.94	0.34	4.19	64,65,66,66	5
14	NS5	M	600	40/40	0.81	0.23	4.08	35,45,74,74	4
10	BPB	M	402	65/65	0.87	0.21	3.88	21,27,97,99	0
11	UQ1	L	502	18/18	0.91	0.14	2.35	45,46,49,50	0
9	BCB	M	400	66/66	0.93	0.14	2.28	23,27,85,86	0
7	HTO	C	706	10/10	0.87	0.21	2.07	45,50,51,51	0
7	HTO	H	705	10/10	0.94	0.13	1.26	41,42,44,45	0
13	MQ9	M	501	58/58	0.94	0.13	0.95	16,22,74,75	0
8	LDA	H	703	16/16	0.90	0.22	0.85	47,53,60,62	0
9	BCB	L	400	66/66	0.97	0.11	0.78	23,26,33,38	0
5	HEC	C	402	43/43	0.97	0.12	0.28	26,30,37,39	0
8	LDA	H	701	16/16	0.95	0.12	0.18	36,41,47,48	0
5	HEC	C	401	43/43	0.98	0.12	-0.11	30,33,45,51	0
10	BPB	L	402	65/65	0.98	0.09	-0.41	14,20,28,29	0
5	HEC	C	403	43/43	0.99	0.09	-0.47	14,21,27,31	0
5	HEC	C	404	43/43	0.98	0.09	-0.55	21,24,34,41	0
9	BCB	L	401	66/66	0.97	0.08	-0.96	18,24,40,44	0
6	SO4	H	806	5/5	0.98	0.07	-1.09	48,49,50,50	5
6	SO4	M	802	5/5	0.99	0.06	-2.10	47,48,49,50	0
12	FE2	M	500	1/1	1.00	0.03	-4.31	21,21,21,21	0
6	SO4	M	804	5/5	0.98	0.18	-	53,54,55,56	0
6	SO4	H	812	5/5	0.94	0.17	-	47,47,48,48	5
6	SO4	C	817	5/5	0.21	1.94	-	2,2,2,2	5
6	SO4	C	813	5/5	0.92	0.29	-	39,39,41,41	5
6	SO4	C	808	5/5	0.92	0.14	-	55,56,57,58	5
7	HTO	L	709	10/10	-0.19	1.80	-	2,2,2,2	10
6	SO4	M	816	5/5	-0.13	1.86	-	2,2,2,2	5
6	SO4	H	803	5/5	0.96	0.26	-	67,68,68,69	0
6	SO4	M	818	5/5	0.21	1.58	-	2,2,2,2	5
7	HTO	L	708	10/10	0.22	1.90	-	2,2,2,2	10
6	SO4	M	805	5/5	0.93	0.23	-	48,49,49,50	5
6	SO4	L	814	5/5	0.08	1.95	-	2,2,2,2	5
6	SO4	C	810	5/5	0.95	0.16	-	46,47,47,47	5
6	SO4	C	811	5/5	0.93	0.23	-	42,43,44,44	5
6	SO4	M	819	5/5	0.01	1.41	-	2,2,2,2	5
6	SO4	C	809	5/5	0.91	0.36	-	66,67,67,68	5
6	SO4	M	801	5/5	0.99	0.13	-	29,29,32,32	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.