



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:56 pm GMT

PDB ID : 3T6E  
Title : Crystal Structure of the Reaction Centre from Blastochloris viridis strain DSM 133 (ATCC 19567) substrain-94  
Authors : Roszak, A.W.; Gardiner, A.T.; Isaacs, N.W.; Cogdell, R.J.  
Deposited on : 2011-07-28  
Resolution : 1.92 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

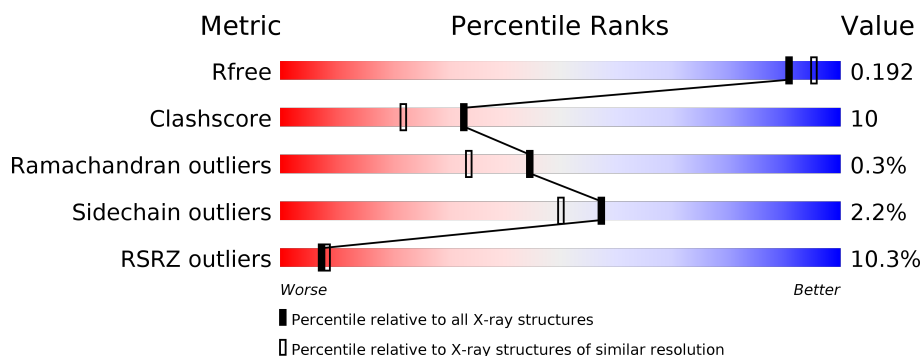
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.92 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))
$R_{free}$	100719	6276 (1.94-1.90)
Clashscore	112137	7025 (1.94-1.90)
Ramachandran outliers	110173	6947 (1.94-1.90)
Sidechain outliers	110143	6948 (1.94-1.90)
RSRZ outliers	101464	6332 (1.94-1.90)

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	356	<div> <div>7%</div> <div>86%</div> <div>8%</div> <div>6%</div> </div>
2	H	258	<div> <div>11%</div> <div>91%</div> <div>9%</div> <div>•</div> </div>
3	L	273	<div> <div>6%</div> <div>92%</div> <div>7%</div> <div>•</div> </div>
4	M	323	<div> <div>15%</div> <div>93%</div> <div>7%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	GOL	C	350	-	-	-	X
10	GOL	C	351	-	-	-	X
10	GOL	C	352	-	-	-	X
10	GOL	C	353[B]	-	-	-	X
10	GOL	C	359	-	-	X	X
10	GOL	C	360	-	-	-	X
10	GOL	H	272	-	-	-	X
10	GOL	H	274	-	-	-	X
10	GOL	H	276	-	-	-	X
10	GOL	L	277	-	-	-	X
10	GOL	L	278	-	-	-	X
10	GOL	L	279	-	-	X	X
10	GOL	L	280	-	-	-	X
10	GOL	M	335	-	-	-	X
13	UQ9	L	502	-	-	X	X
13	UQ9	L	503	-	-	-	X
16	NS5	M	600	-	-	-	X
6	LDA	C	712	-	-	-	X
6	LDA	C	722	-	-	-	X
6	LDA	H	701	-	-	-	X
6	LDA	H	707	-	-	-	X
6	LDA	L	709	-	-	-	X
6	LDA	L	720	-	-	-	X
6	LDA	M	702	-	-	X	X
6	LDA	M	706	-	-	-	X
6	LDA	M	715	-	-	-	X
7	DGA	C	730	-	-	-	X
7	DGA	H	733	-	-	-	X
7	DGA	L	731	-	-	-	X
7	DGA	M	732	-	-	X	-
8	SO4	C	337	-	-	X	-
8	SO4	C	338	-	-	X	-
8	SO4	C	342	-	-	X	X
8	SO4	C	344	-	-	X	-
8	SO4	C	345	-	-	-	X
8	SO4	H	261	-	-	X	-
8	SO4	H	262[A]	-	-	-	X
8	SO4	H	262[B]	-	-	-	X
8	SO4	H	264	-	-	-	X
8	SO4	M	329	-	-	X	-
9	HTO	C	348	-	-	X	X
9	HTO	H	266	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	HTO	H	268	-	-	-	X
9	HTO	L	274	-	-	-	X
9	HTO	M	332	-	-	-	X

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 12066 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	334	Total	C	N	O	S	0	4	0
			2651	1667	480	486	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	258	Total	C	N	O	S	45	4	0
			2034	1298	349	384	3			

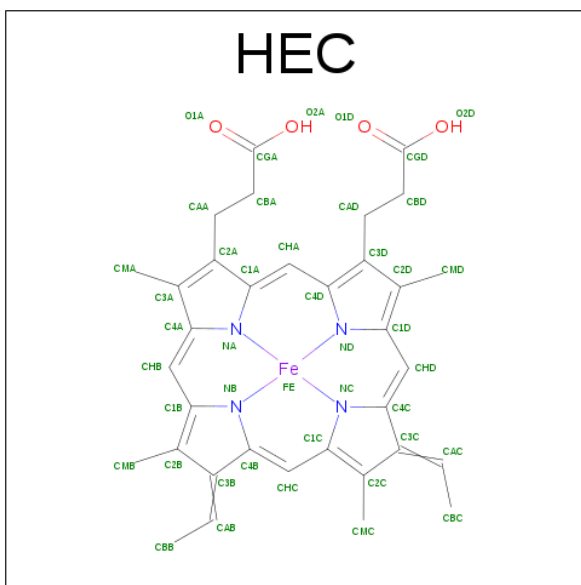
- Molecule 3 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	273	Total	C	N	O	S	0	5	0
			2207	1482	354	361	10			

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

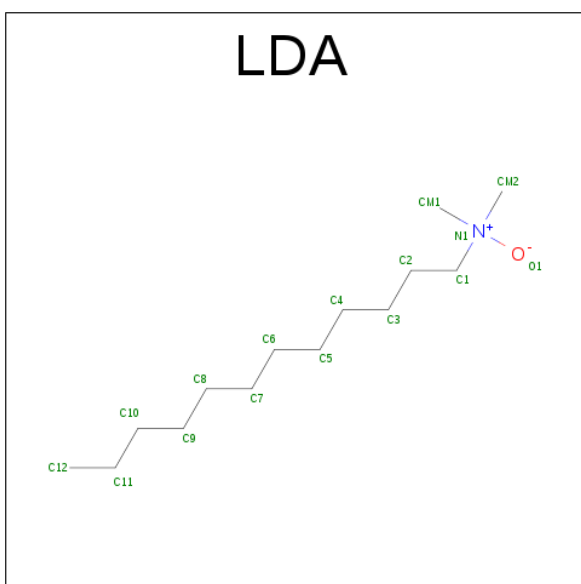
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	323	Total	C	N	O	S	0	4	0
			2591	1725	425	429	12			

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



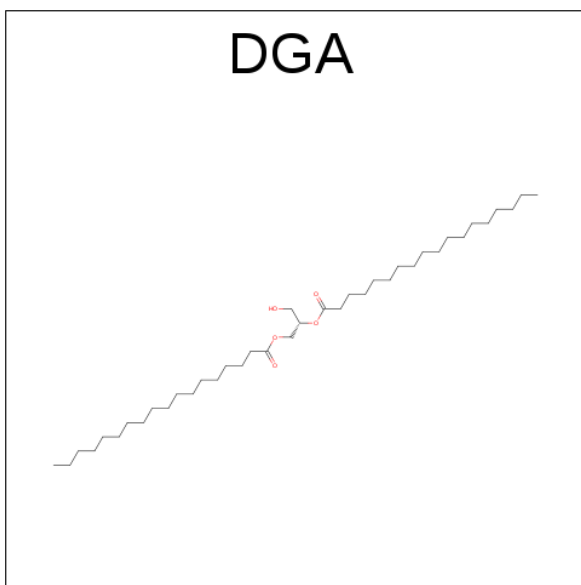
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 55	C 43	Fe 1	N 5	O 6	0	1

- Molecule 6 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).



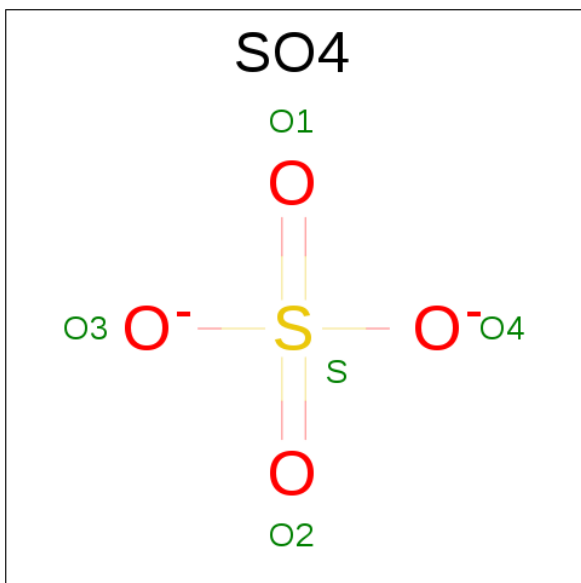
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			16	14	1	1		
6	C	1	Total	C	N	O	0	0
			16	14	1	1		
6	H	1	Total	C	N	O	0	0
			16	14	1	1		
6	H	1	Total	C	N	O	0	0
			16	14	1	1		
6	H	1	Total	C	N	O	0	0
			13	11	1	1		
6	H	1	Total	C	N	O	0	0
			16	14	1	1		
6	H	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 7 is DIACYL GLYCEROL (three-letter code: DGA) (formula: C<sub>39</sub>H<sub>76</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			37	33	4		
7	H	1	Total	C	O	0	0
			31	26	5		
7	L	1	Total	C	O	0	0
			33	28	5		
7	M	1	Total	C	O	0	0
			34	29	5		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).





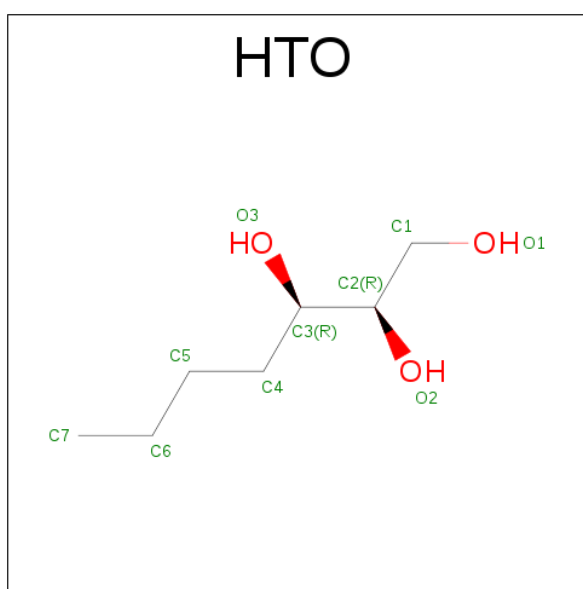
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total O S 5 4 1	0	0
8	C	1	Total O S 5 4 1	0	0
8	C	1	Total O S 5 4 1	0	0
8	C	1	Total O S 5 4 1	0	0
8	C	1	Total O S 5 4 1	0	0
8	C	1	Total O S 5 4 1	0	0
8	C	1	Total O S 5 4 1	0	0
8	C	1	Total O S 5 4 1	0	0
8	C	1	Total O S 5 4 1	0	0
8	C	1	Total O S 5 4 1	0	0
8	C	1	Total O S 5 4 1	0	0
8	H	1	Total O S 5 4 1	0	0
8	H	1	Total O S 5 4 1	0	0
8	H	1	Total O S 5 4 1	0	0
8	H	1	Total O S 10 8 2	0	1
8	H	1	Total O S 5 4 1	0	0
8	H	1	Total O S 5 4 1	0	0
8	H	1	Total O S 5 4 1	0	0
8	M	1	Total O S 5 4 1	0	0
8	M	1	Total O S 5 4 1	0	0
8	M	1	Total O S 5 4 1	0	0
8	M	1	Total O S 5 4 1	0	0

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

- Molecule 9 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: C<sub>7</sub>H<sub>16</sub>O<sub>3</sub>).



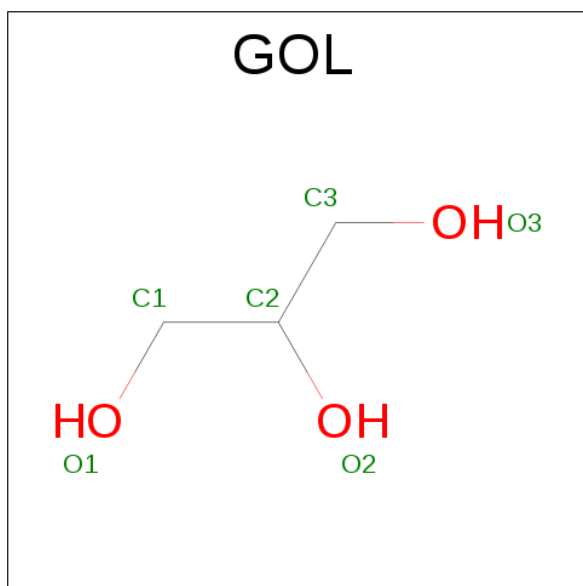
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			10	7	3		
9	C	1	Total	C	O	0	0
			10	7	3		
9	H	1	Total	C	O	0	0
			10	7	3		
9	H	1	Total	C	O	0	0
			10	7	3		
9	H	1	Total	C	O	0	0
			10	7	3		
9	L	1	Total	C	O	0	0
			10	7	3		
9	L	1	Total	C	O	0	0
			10	7	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	C	O	0	0
			10	7	3		

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	C	O	0	0
			6	3	3		
10	C	1	Total	C	O	0	0
			6	3	3		
10	C	1	Total	C	O	0	0
			6	3	3		
10	C	1	Total	C	O	0	1
			12	6	6		
10	C	1	Total	C	O	0	0
			6	3	3		
10	C	1	Total	C	O	0	0
			6	3	3		
10	C	1	Total	C	O	0	0
			6	3	3		
10	C	1	Total	C	O	0	0
			6	3	3		
10	C	1	Total	C	O	0	0
			6	3	3		

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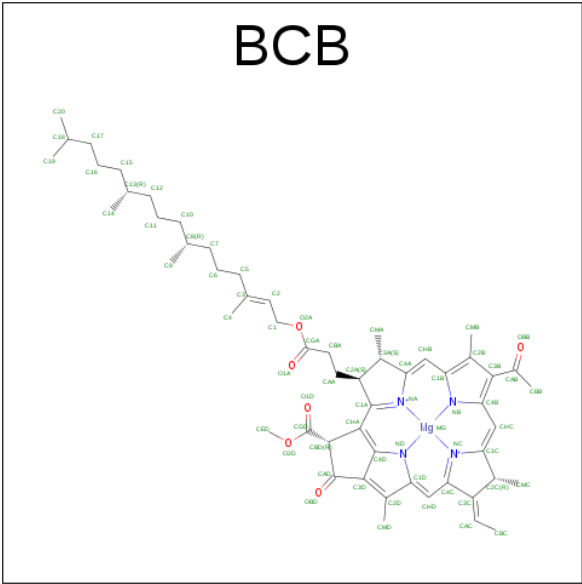
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total 6	C 3	O 3	0	0
10	C	1	Total 6	C 3	O 3	0	0
10	C	1	Total 6	C 3	O 3	0	0
10	C	1	Total 6	C 3	O 3	0	0
10	C	1	Total 6	C 3	O 3	0	0
10	C	1	Total 6	C 3	O 3	0	0
10	H	1	Total 6	C 3	O 3	0	0
10	H	1	Total 6	C 3	O 3	0	0
10	H	1	Total 6	C 3	O 3	0	0
10	H	1	Total 6	C 3	O 3	0	0
10	H	1	Total 6	C 3	O 3	0	0
10	H	1	Total 6	C 3	O 3	0	0
10	H	1	Total 6	C 3	O 3	0	0
10	H	1	Total 6	C 3	O 3	0	0
10	H	1	Total 6	C 3	O 3	0	0
10	H	1	Total 6	C 3	O 3	0	0
10	H	1	Total 6	C 3	O 3	0	0
10	L	1	Total 6	C 3	O 3	0	0
10	L	1	Total 6	C 3	O 3	0	0
10	L	1	Total 6	C 3	O 3	0	0
10	L	1	Total 6	C 3	O 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	C	O	0	0
			6	3	3		
10	L	1	Total	C	O	0	0
			6	3	3		
10	L	1	Total	C	O	0	0
			6	3	3		
10	M	1	Total	C	O	0	0
			6	3	3		
10	M	1	Total	C	O	0	0
			6	3	3		
10	M	1	Total	C	O	0	0
			6	3	3		
10	M	1	Total	C	O	0	0
			6	3	3		
10	M	1	Total	C	O	0	0
			6	3	3		
10	M	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>6</sub>).



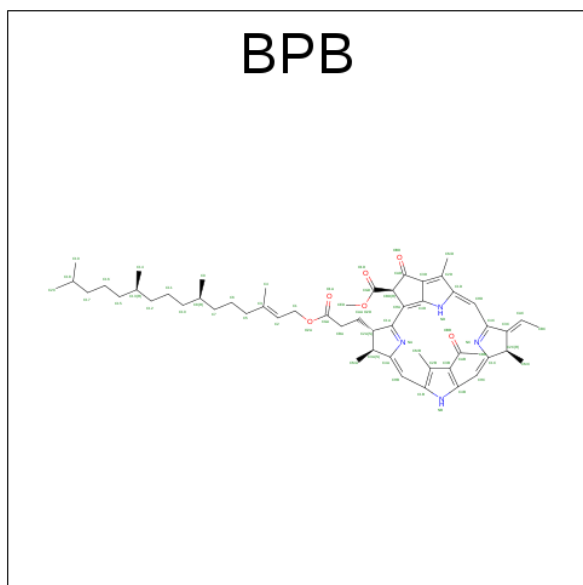
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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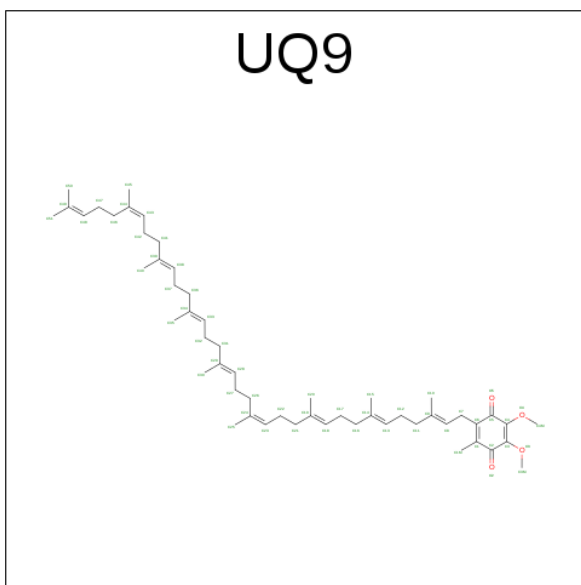
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
11	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
11	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 12 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula:  $C_{55}H_{74}N_4O_6$ ).



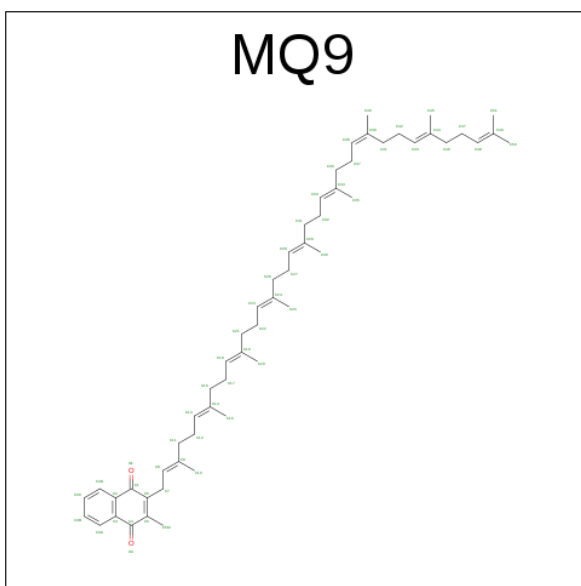
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	L	1	Total	C	N	O	0	0
			65	55	4	6		
12	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 13 is UBIQUINONE-9 (three-letter code: UQ9) (formula:  $C_{54}H_{82}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	L	1	Total	C	O	0	0
			58	54	4		
13	L	1	Total	C	O	0	0
			19	15	4		

- Molecule 14 is MENAQUINONE-9 (three-letter code: MQ9) (formula:  $C_{56}H_{80}O_2$ ).

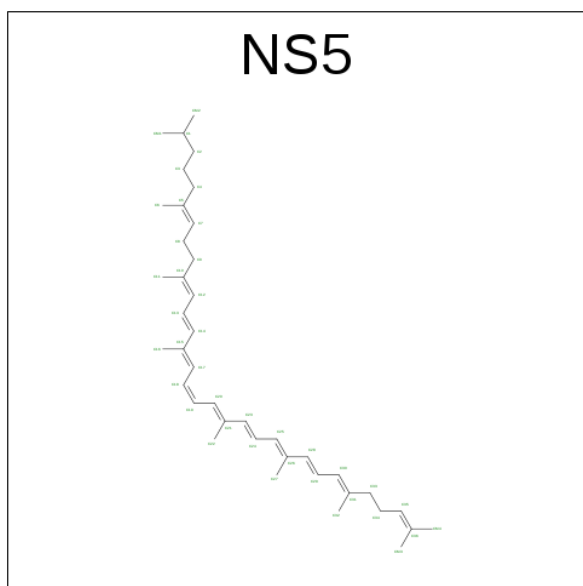


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	M	1	Total	C	O	0	0
			58	56	2		

- Molecule 15 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 16 is 15-CIS-1,2-DIHYDRONEUROSPORENE (three-letter code: NS5) (formula:  $C_{40}H_{60}$ ).



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

- Molecule 17 is water.

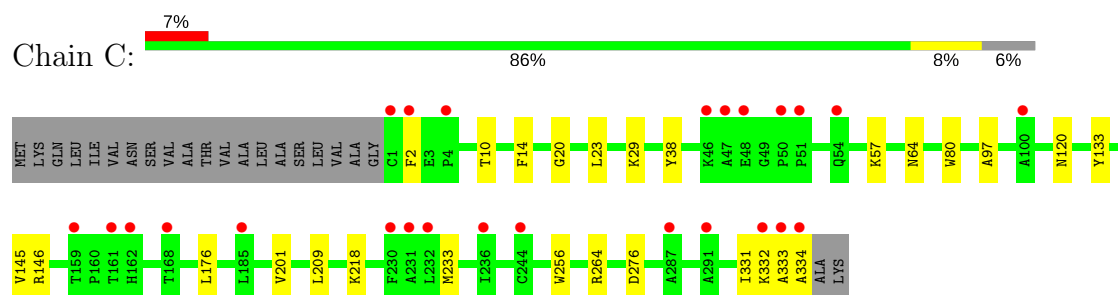
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	C	441	Total	O	0	0
			441	441		
17	H	233	Total	O	0	0
			233	233		
17	L	125	Total	O	0	0
			125	125		
17	M	175	Total	O	0	0
			175	175		



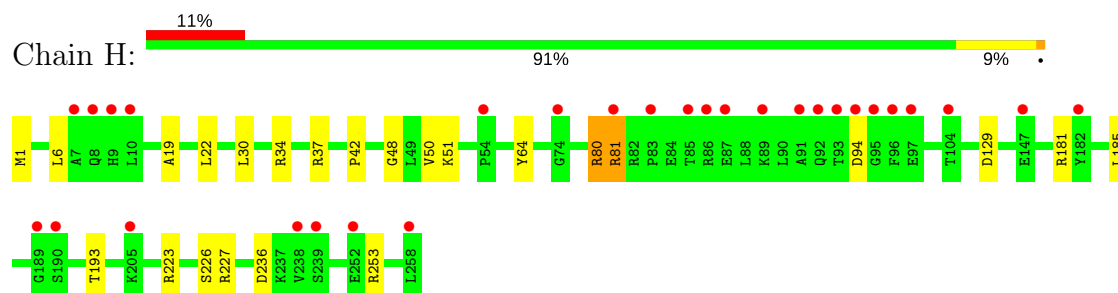
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

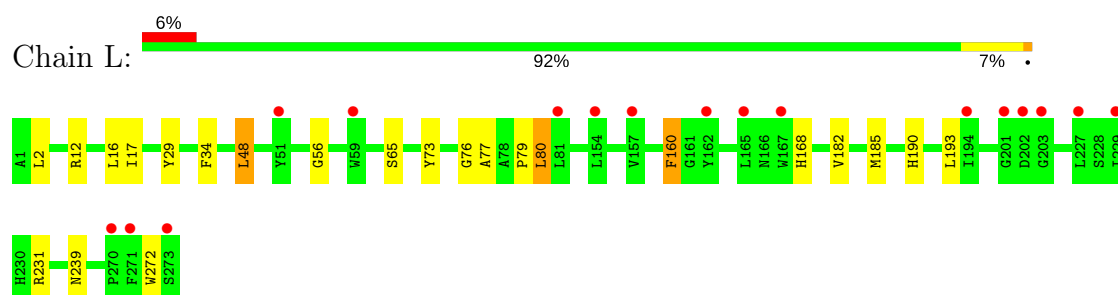
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



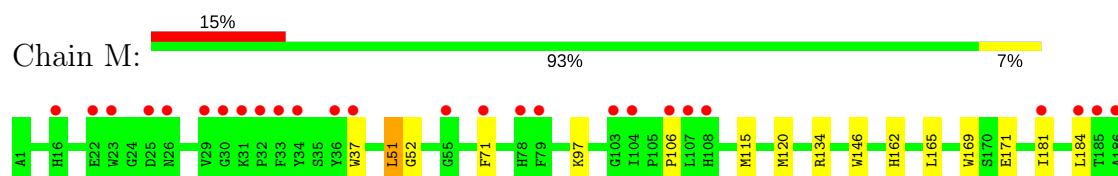
- Molecule 2: Reaction center protein H chain

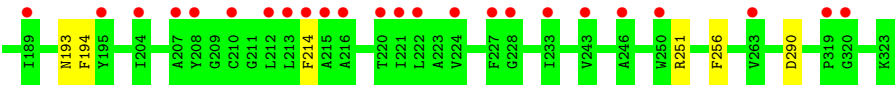


- Molecule 3: Reaction center protein L chain



- 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, $\alpha$ , $\beta$ , $\gamma$	221.58Å 221.58Å 113.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.46 – 1.92 43.46 – 1.92	Depositor EDS
% Data completeness (in resolution range)	99.4 (43.46-1.92) 99.4 (43.46-1.92)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.6.0101	Depositor
R, $R_{free}$	0.155 , 0.178 0.170 , 0.192	Depositor DCC
$R_{free}$ test set	10638 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.2	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 79.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	12066	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: GOL, LDA, BPB, HTO, CSO, BCB, UQ9, DGA, FE2, SO4, HEC, MQ9, 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	0.90	1/2718 (0.0%)	0.78	1/3702 (0.0%)
2	H	0.85	0/2064	0.81	2/2820 (0.1%)
3	L	0.90	0/2298	0.77	3/3135 (0.1%)
4	M	0.86	0/2689	0.75	1/3676 (0.0%)
All	All	0.88	1/9769 (0.0%)	0.77	7/13333 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	201	VAL	CB-CG2	5.07	1.63	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	160	PHE	CB-CG-CD1	5.77	124.84	120.80
4	M	251	ARG	NE-CZ-NH1	5.75	123.17	120.30
2	H	181	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	C	264	ARG	NE-CZ-NH2	-5.61	117.50	120.30
2	H	80	ARG	NE-CZ-NH1	5.25	122.93	120.30
3	L	12	ARG	NE-CZ-NH1	5.14	122.87	120.30
3	L	48	LEU	CA-CB-CG	5.04	126.90	115.30

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	2651	0	2624	21	0
2	H	2034	0	2011	18	0
3	L	2207	0	2134	22	0
4	M	2591	0	2478	32	0
5	C	184	0	108	2	0
6	C	32	0	62	5	0
6	H	77	0	146	25	0
6	L	64	0	124	10	0
6	M	80	0	155	22	0
7	C	37	0	58	1	0
7	H	31	0	44	6	0
7	L	33	0	48	7	0
7	M	34	0	50	23	0
8	C	55	0	0	9	0
8	H	40	0	0	8	0
8	M	40	0	0	2	0
9	C	20	0	32	13	0
9	H	30	0	48	3	0
9	L	20	0	32	0	0
9	M	10	0	16	0	0
10	C	102	0	136	15	0
10	H	66	0	88	4	0
10	L	42	0	56	7	0
10	M	42	0	56	5	0
11	L	132	0	144	7	0
11	M	132	0	144	12	0
12	L	65	0	74	2	0
12	M	65	0	74	3	0
13	L	77	0	99	37	0
14	M	58	0	80	0	0
15	M	1	0	0	0	0
16	M	40	0	60	2	0
17	C	441	0	0	3	0
17	H	233	0	0	3	0
17	L	125	0	0	1	0
17	M	175	0	0	3	0
All	All	12066	0	11181	219	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 10.

All (219) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:71[B]:PHE:CD2	7:M:732:DGA:HA72	1.43	1.50
6:H:718:LDA:H31	6:H:718:LDA:CM1	1.39	1.38
4:M:71[B]:PHE:CE2	7:M:732:DGA:HA52	1.61	1.35
6:M:706:LDA:HM13	8:M:329:SO4:O4	1.10	1.27
6:H:718:LDA:C3	6:H:718:LDA:HM13	1.49	1.27
4:M:71[B]:PHE:CD2	7:M:732:DGA:CA7	2.27	1.17
13:L:502:UQ9:C25	13:L:502:UQ9:H28	1.71	1.17
7:L:731:DGA:OB1	7:L:731:DGA:CG1	1.91	1.16
6:M:706:LDA:CM1	8:M:329:SO4:O4	1.94	1.15
7:H:733:DGA:HA41	7:H:733:DGA:OA1	1.43	1.13
4:M:71[B]:PHE:CE2	7:M:732:DGA:CA5	2.31	1.12
7:L:731:DGA:OB1	7:L:731:DGA:HG11	1.39	1.11
13:L:502:UQ9:H47A	13:L:502:UQ9:H42A	1.22	1.10
13:L:502:UQ9:H25A	13:L:502:UQ9:H28	1.34	1.10
8:H:261:SO4:S	6:M:702:LDA:HM12	1.92	1.10
13:L:502:UQ9:O3	13:L:502:UQ9:H4MB	1.51	1.10
4:M:71[B]:PHE:CD2	7:M:732:DGA:HA52	1.87	1.09
6:M:704:LDA:HM11	6:M:704:LDA:H31	1.35	1.08
3:L:185[B]:MET:SD	11:M:400:BCB:H41	1.94	1.08
7:M:732:DGA:OB1	7:M:732:DGA:HB41	1.50	1.06
13:L:502:UQ9:H42A	13:L:502:UQ9:C47	1.85	1.05
4:M:71[B]:PHE:HE2	7:M:732:DGA:CA5	1.66	1.05
13:L:502:UQ9:C46	13:L:502:UQ9:H50	1.87	1.03
13:L:503:UQ9:O4	13:L:503:UQ9:C3M	2.05	1.02
13:L:503:UQ9:C4M	13:L:503:UQ9:O5	2.10	1.00
13:L:502:UQ9:H16A	13:L:502:UQ9:H20	1.42	0.99
13:L:502:UQ9:C25	13:L:502:UQ9:C28	2.39	0.99
1:C:332:LYS:H	9:C:349:HTO:H71	1.27	0.96
4:M:71[B]:PHE:CE2	7:M:732:DGA:CA6	2.48	0.96
6:H:707:LDA:C1	6:H:707:LDA:H51	1.95	0.96
4:M:71[B]:PHE:HD2	7:M:732:DGA:HA72	1.17	0.94
13:L:502:UQ9:H25B	13:L:502:UQ9:C28	1.99	0.92
6:M:704:LDA:C3	6:M:704:LDA:HM11	1.95	0.92
8:H:261:SO4:O1	6:M:702:LDA:HM12	1.70	0.91
4:M:115[B]:MET:CE	7:M:732:DGA:CEB	2.48	0.91
8:H:261:SO4:O2	6:M:702:LDA:HM12	1.73	0.89
13:L:502:UQ9:O3	13:L:502:UQ9:C4M	2.21	0.89
9:C:348:HTO:H72	10:C:359:GOL:H11	1.54	0.88
8:H:261:SO4:O1	6:M:702:LDA:CM1	2.22	0.88
4:M:71[B]:PHE:CD2	7:M:732:DGA:CA5	2.55	0.88
8:C:342:SO4:O3	10:M:337:GOL:H12	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:502:UQ9:H20	13:L:502:UQ9:C16	2.03	0.87
13:L:502:UQ9:H46	13:L:502:UQ9:H50	1.53	0.86
7:H:733:DGA:CA4	7:H:733:DGA:OA1	2.20	0.86
13:L:503:UQ9:O4	13:L:503:UQ9:H3MA	1.74	0.86
13:L:503:UQ9:O4	13:L:503:UQ9:H3MB	1.76	0.85
6:H:718:LDA:C3	6:H:718:LDA:CM1	2.25	0.85
8:H:261:SO4:S	6:M:702:LDA:CM1	2.65	0.84
6:H:718:LDA:H31	6:H:718:LDA:HM11	1.57	0.84
8:C:337:SO4:O1	8:C:338:SO4:O1	1.94	0.83
7:H:733:DGA:HA42	17:M:960:HOH:O	1.78	0.82
6:H:707:LDA:H12	6:H:707:LDA:H51	1.62	0.82
13:L:503:UQ9:H4MB	13:L:503:UQ9:O5	1.78	0.82
13:L:502:UQ9:H46	13:L:502:UQ9:C50	2.05	0.81
13:L:502:UQ9:H35	13:L:502:UQ9:C31	2.09	0.81
6:H:701:LDA:CM2	6:M:702:LDA:HM11	2.11	0.80
9:C:348:HTO:H71	10:C:359:GOL:H31	1.64	0.79
4:M:71[B]:PHE:CG	7:M:732:DGA:HA72	2.16	0.79
4:M:115[B]:MET:HE3	7:M:732:DGA:CEB	2.13	0.79
6:M:704:LDA:CM1	6:M:704:LDA:C3	2.59	0.79
4:M:71[B]:PHE:CD2	7:M:732:DGA:CA6	2.67	0.78
13:L:503:UQ9:O5	13:L:503:UQ9:H4MA	1.84	0.77
1:C:333:ALA:HB1	1:C:334:ALA:HB2	1.65	0.76
4:M:106:PRO:HB3	7:M:732:DGA:HB52	1.67	0.76
7:L:731:DGA:OB1	7:L:731:DGA:HG12	1.87	0.74
13:L:502:UQ9:C42	13:L:502:UQ9:H47A	2.04	0.73
13:L:502:UQ9:H15	11:M:400:BCB:C14	2.18	0.73
4:M:71[B]:PHE:CE2	7:M:732:DGA:HA61	2.22	0.73
6:C:712:LDA:H122	6:C:722:LDA:H102	1.71	0.73
13:L:502:UQ9:H46A	13:L:502:UQ9:H50	1.68	0.72
9:C:348:HTO:H72	10:C:359:GOL:C1	2.19	0.72
6:H:718:LDA:H31	6:H:718:LDA:HM13	0.75	0.72
11:M:400:BCB:HMB1	11:M:400:BCB:HBB2	1.70	0.71
6:H:707:LDA:H52	10:M:335:GOL:O1	1.89	0.71
12:L:402:BPB:HMB	12:L:402:BPB:HBBB	1.73	0.71
13:L:502:UQ9:H15	11:M:400:BCB:H143	1.72	0.71
3:L:77:ALA:O	6:L:720:LDA:HM11	1.90	0.71
6:H:701:LDA:HM21	6:M:702:LDA:HM11	1.71	0.70
1:C:2:PHE:CD2	6:C:722:LDA:HM13	2.25	0.70
1:C:120:ASN:ND2	8:C:344:SO4:O2	2.22	0.70
3:L:76:GLY:HA3	7:L:731:DGA:HG32	1.75	0.69
6:L:703:LDA:CM1	6:L:703:LDA:H32	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:707:LDA:H11	6:H:707:LDA:H51	1.72	0.69
10:C:361:GOL:O2	17:C:885:HOH:O	1.87	0.69
9:C:348:HTO:C7	10:C:359:GOL:H11	2.22	0.69
11:L:401:BCB:CBB	11:L:401:BCB:HMB1	2.23	0.68
7:M:732:DGA:CB4	7:M:732:DGA:OB1	2.15	0.68
13:L:502:UQ9:C15	11:M:400:BCB:H143	2.25	0.67
3:L:73:TYR:CE1	6:L:720:LDA:HM12	2.28	0.67
4:M:115[B]:MET:HE2	7:M:732:DGA:CEB	2.23	0.67
2:H:81:ARG:HG3	6:H:721:LDA:H122	1.75	0.67
11:M:400:BCB:HMB1	11:M:400:BCB:CBB	2.24	0.67
1:C:332:LYS:N	9:C:349:HTO:H71	2.05	0.65
13:L:502:UQ9:H31	13:L:502:UQ9:H35	1.78	0.64
6:L:703:LDA:H32	6:L:703:LDA:HM11	1.80	0.64
3:L:239:ASN:HD21	13:L:502:UQ9:C43	2.10	0.64
13:L:502:UQ9:H25B	13:L:502:UQ9:H28	1.62	0.63
6:H:707:LDA:C1	6:H:707:LDA:C5	2.76	0.63
3:L:65:SER:HB3	10:L:279:GOL:H12	1.81	0.62
6:H:701:LDA:HM23	6:M:702:LDA:HM11	1.81	0.62
9:C:348:HTO:C7	10:C:359:GOL:H31	2.28	0.62
13:L:502:UQ9:H31	13:L:502:UQ9:C35	2.29	0.61
6:L:703:LDA:CM1	6:L:703:LDA:C3	2.77	0.61
10:L:278:GOL:H11	17:L:468:HOH:O	2.00	0.61
4:M:106:PRO:CB	7:M:732:DGA:HB52	2.31	0.61
8:C:342:SO4:O3	10:M:337:GOL:C1	2.48	0.61
6:C:712:LDA:H122	6:C:722:LDA:C10	2.31	0.59
7:C:730:DGA:HA32	7:C:730:DGA:HB22	1.83	0.59
6:C:712:LDA:H122	6:C:722:LDA:C9	2.33	0.59
4:M:97:LYS:NZ	17:M:429:HOH:O	2.36	0.57
3:L:73:TYR:HE1	6:L:720:LDA:HM12	1.68	0.57
11:L:401:BCB:HMB1	11:L:401:BCB:HBB2	1.86	0.57
8:H:261:SO4:O4	8:H:262[A]:SO4:O3	2.22	0.57
3:L:29:TYR:OH	6:M:702:LDA:H22	2.04	0.56
8:C:337:SO4:O1	8:C:338:SO4:S	2.63	0.56
11:L:400:BCB:HBB3	11:L:400:BCB:HMB1	1.88	0.56
4:M:71[B]:PHE:HD2	7:M:732:DGA:CA7	1.94	0.56
9:C:348:HTO:H72	10:C:359:GOL:C2	2.35	0.55
3:L:182:VAL:HA	11:M:400:BCB:H43	1.89	0.55
4:M:256:PHE:HB3	6:M:702:LDA:HM13	1.88	0.55
13:L:502:UQ9:C20	13:L:502:UQ9:C16	2.80	0.54
3:L:17:ILE:HD12	3:L:34:PHE:CZ	2.43	0.54
10:L:276:GOL:O3	10:L:279:GOL:H31	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:402:BPB:HMB	12:L:402:BPB:CBB	2.36	0.53
13:L:502:UQ9:H35	13:L:502:UQ9:H31A	1.88	0.53
9:C:348:HTO:C6	10:C:359:GOL:H11	2.39	0.52
1:C:331:ILE:HD12	9:C:349:HTO:H2	1.91	0.52
2:H:223:ARG:NH1	10:H:274:GOL:O3	2.39	0.51
3:L:231:ARG:CG	13:L:502:UQ9:H31A	2.41	0.51
2:H:6:LEU:HD22	6:H:718:LDA:H12	1.92	0.51
1:C:209:LEU:HD12	10:C:352:GOL:H32	1.92	0.50
11:M:401:BCB:HMB1	11:M:401:BCB:HBB3	1.92	0.50
6:H:718:LDA:HM12	7:H:733:DGA:HB42	1.93	0.50
3:L:76:GLY:CA	7:L:731:DGA:HG32	2.41	0.50
6:L:703:LDA:H32	6:L:703:LDA:HM13	1.93	0.50
7:H:733:DGA:HA52	4:M:165:LEU:HD22	1.91	0.50
4:M:162[B]:HIS:HE1	4:M:171:GLU:OE1	1.95	0.50
3:L:17:ILE:HD12	3:L:34:PHE:HZ	1.77	0.50
3:L:231:ARG:HG2	13:L:502:UQ9:H27A	1.93	0.50
2:H:42:PRO:HD2	6:H:721:LDA:H121	1.94	0.49
3:L:190:HIS:HA	13:L:502:UQ9:H1M	1.94	0.49
4:M:71[B]:PHE:HD2	7:M:732:DGA:CA5	2.17	0.49
1:C:276:ASP:OD2	8:C:344:SO4:O1	2.30	0.49
6:L:703:LDA:C3	6:L:703:LDA:HM13	2.42	0.49
12:M:402:BPB:H14A	12:M:402:BPB:HMAA	1.94	0.49
1:C:218:LYS:HG3	10:C:354:GOL:H2	1.94	0.49
1:C:57:LYS:HE2	1:C:97:ALA:CB	2.42	0.48
4:M:71[B]:PHE:HE2	7:M:732:DGA:HA52	1.17	0.48
4:M:184:LEU:HD21	11:M:400:BCB:CAC	2.44	0.48
6:H:707:LDA:H62	10:M:335:GOL:H31	1.96	0.48
11:M:401:BCB:CBB	11:M:401:BCB:HMB1	2.43	0.48
2:H:227[A]:ARG:HH11	2:H:227[A]:ARG:HG3	1.79	0.47
6:M:704:LDA:H112	6:M:704:LDA:H81	1.62	0.47
9:C:348:HTO:H72	10:C:359:GOL:O2	2.13	0.47
2:H:1[B]:FME:HE1	17:H:690:HOH:O	2.14	0.47
11:L:400:BCB:CBB	11:L:400:BCB:HMB1	2.44	0.47
6:M:704:LDA:H21	6:M:704:LDA:H52	1.62	0.47
11:L:401:BCB:HMB1	11:L:401:BCB:HBB3	1.95	0.47
1:C:145:VAL:O	1:C:146:ARG:HD2	2.16	0.46
7:H:733:DGA:CB1	7:H:733:DGA:HA21	2.45	0.46
3:L:231:ARG:HD3	13:L:502:UQ9:H31A	1.97	0.46
4:M:115[B]:MET:HA	4:M:115[B]:MET:CE	2.46	0.45
7:L:731:DGA:HG11	7:L:731:DGA:HA22	1.82	0.45
1:C:256:TRP:HB2	10:C:353[B]:GOL:H2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:718:LDA:HM13	6:H:718:LDA:H32	1.75	0.45
3:L:56:GLY:CA	10:L:276:GOL:H32	2.47	0.45
13:L:502:UQ9:C3M	13:L:502:UQ9:O2	2.65	0.45
3:L:79:PRO:HD3	6:L:720:LDA:HM13	1.99	0.44
4:M:51:LEU:HB3	4:M:52:GLY:H	1.61	0.44
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.53	0.44
11:M:400:BCB:H193	12:M:402:BPB:C20	2.47	0.44
1:C:64[A]:ASN:HD21	9:C:349:HTO:C2	2.29	0.44
8:C:342:SO4:O4	10:C:352:GOL:O1	2.20	0.44
6:H:719:LDA:H21	6:H:719:LDA:HM13	1.73	0.44
10:C:358:GOL:C1	17:C:568:HOH:O	2.65	0.44
9:C:348:HTO:C7	10:C:359:GOL:C1	2.89	0.44
2:H:37:ARG:NH2	8:H:262[B]:SO4:O1	2.39	0.44
9:H:268:HTO:O1	9:H:268:HTO:O3	2.30	0.44
2:H:30:LEU:O	2:H:34:ARG:HD2	2.17	0.44
6:M:704:LDA:CM1	6:M:704:LDA:H32	2.46	0.43
6:M:706:LDA:H21	6:M:706:LDA:HM22	1.81	0.43
3:L:168:HIS:CE1	11:L:400:BCB:HMC2	2.54	0.43
1:C:2:PHE:CE2	6:C:722:LDA:HM13	2.53	0.43
3:L:65:SER:HB3	10:L:279:GOL:C1	2.47	0.43
2:H:223:ARG:NH2	17:H:558:HOH:O	2.48	0.43
2:H:253:ARG:HE	9:H:268:HTO:H11	1.84	0.43
6:H:701:LDA:HM21	6:M:702:LDA:CM1	2.47	0.43
7:L:731:DGA:HBT1	7:L:731:DGA:HB71	1.76	0.43
1:C:14:PHE:CE2	10:L:279:GOL:H2	2.54	0.43
1:C:146:ARG:HD2	1:C:146:ARG:HA	1.87	0.42
8:H:264:SO4:O1	10:H:273:GOL:H32	2.19	0.42
4:M:120:MET:CE	16:M:600:NS5:H273	2.49	0.42
1:C:64[A]:ASN:ND2	8:C:346:SO4:O3	2.52	0.42
4:M:146:TRP:HA	4:M:146:TRP:CE3	2.54	0.42
11:L:401:BCB:OBB	11:L:401:BCB:HHC	2.18	0.42
3:L:80:LEU:HD13	6:L:720:LDA:H72	2.02	0.42
12:M:402:BPB:HMB	12:M:402:BPB:HBBB	2.02	0.42
4:M:37:TRP:CE3	6:M:704:LDA:HM22	2.55	0.42
1:C:10:THR:O	1:C:20:GLY:HA3	2.20	0.41
8:C:337:SO4:O4	8:C:338:SO4:S	2.79	0.41
4:M:169:TRP:CH2	16:M:600:NS5:H342	2.55	0.41
1:C:29:LYS:NZ	17:C:608:HOH:O	2.47	0.41
2:H:64:TYR:CE2	6:H:721:LDA:HM22	2.55	0.41
2:H:81:ARG:HG3	6:H:721:LDA:C12	2.47	0.41
2:H:223:ARG:CD	10:H:274:GOL:H11	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:19:ALA:HB2	6:H:719:LDA:H122	2.01	0.41
3:L:193:LEU:HD23	13:L:502:UQ9:C2	2.51	0.41
1:C:233:MET:HB3	5:C:403:HEC:C4B	2.51	0.41
6:M:715:LDA:H22	6:M:715:LDA:HM21	1.74	0.41
2:H:193:THR:HG22	17:H:858:HOH:O	2.20	0.41
2:H:226:SER:HA	9:H:267:HTO:H73	2.03	0.41
10:M:333:GOL:C3	17:M:921:HOH:O	2.69	0.41
2:H:80:ARG:HH21	10:H:270:GOL:C2	2.34	0.40
10:L:276:GOL:O3	10:L:279:GOL:C3	2.69	0.40
2:H:1[A]:FME:HG3	2:H:1[A]:FME:H	1.58	0.40
6:H:721:LDA:H21	6:H:721:LDA:HM21	1.91	0.40
11:M:401:BCB:HHC	11:M:401:BCB:OBB	2.21	0.40
4:M:71[B]:PHE:CE2	7:M:732:DGA:CA7	2.82	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	336/356 (94%)	326 (97%)	10 (3%)	0	100	100
2	H	259/258 (100%)	249 (96%)	7 (3%)	3 (1%)	15	5
3	L	276/273 (101%)	272 (99%)	4 (1%)	0	100	100
4	M	324/323 (100%)	318 (98%)	5 (2%)	1 (0%)	44	33
All	All	1195/1210 (99%)	1165 (98%)	26 (2%)	4 (0%)	44	33

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	50	VAL
4	M	193	ASN

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Mol	Chain	Res	Type
2	H	51	LYS
2	H	48	GLY

### 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	285/297 (96%)	282 (99%)	3 (1%)	78	76
2	H	210/212 (99%)	204 (97%)	6 (3%)	48	37
3	L	223/218 (102%)	217 (97%)	6 (3%)	50	41
4	M	252/248 (102%)	246 (98%)	6 (2%)	54	46
All	All	970/975 (100%)	949 (98%)	21 (2%)	57	50

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	23	LEU
1	C	38	TYR
1	C	176	LEU
2	H	22	LEU
2	H	81	ARG
2	H	94	ASP
2	H	129	ASP
2	H	185	LEU
2	H	236	ASP
3	L	2	LEU
3	L	16	LEU
3	L	48	LEU
3	L	80	LEU
3	L	160	PHE
3	L	272	TRP
4	M	51	LEU
4	M	134	ARG
4	M	181	ILE
4	M	194	PHE

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Mol	Chain	Res	Type
4	M	214	PHE
4	M	290	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	206	GLN
1	C	302	GLN
2	H	58	GLN
2	H	178	HIS
2	H	220	ASN
3	L	183	ASN
3	L	239	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are 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[A]	2	9,9,10	0.80	0	7,9,11	2.23	2 (28%)
2	FME	H	1[B]	2	9,9,10	0.87	0	7,9,11	2.66	2 (28%)
4	CSO	M	160	4	4,6,7	0.72	0	1,6,8	2.64	1 (100%)

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[A]	2	-	0/6/9/11	0/0/0/0
2	FME	H	1[B]	2	-	0/6/9/11	0/0/0/0
4	CSO	M	160	4	-	0/1/5/7	0/0/0/0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1[B]	FME	CA-N-CN	-6.06	113.50	122.82
2	H	1[A]	FME	CA-N-CN	-5.04	115.06	122.82
4	M	160	CSO	O-C-CA	-2.64	117.72	125.02
2	H	1[B]	FME	O-C-CA	-2.41	119.53	125.15
2	H	1[A]	FME	O-C-CA	-2.12	120.21	125.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1[A]	FME	1	0
2	H	1[B]	FME	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 113 ligands modelled in this entry, 1 is monoatomic - leaving 112 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
8	SO4	C	337	-	4,4,4	0.40	0	6,6,6	0.16	0
8	SO4	C	338	-	4,4,4	0.38	0	6,6,6	0.27	0
8	SO4	C	339	-	4,4,4	0.38	0	6,6,6	0.22	0
8	SO4	C	340	-	4,4,4	0.37	0	6,6,6	0.35	0
8	SO4	C	341	-	4,4,4	0.42	0	6,6,6	0.27	0
8	SO4	C	342	-	4,4,4	0.41	0	6,6,6	0.22	0
8	SO4	C	343	-	4,4,4	0.30	0	6,6,6	0.39	0
8	SO4	C	344	-	4,4,4	0.49	0	6,6,6	0.28	0
8	SO4	C	345	-	4,4,4	0.65	0	6,6,6	0.42	0
8	SO4	C	346	-	4,4,4	0.49	0	6,6,6	0.26	0
8	SO4	C	347	-	4,4,4	0.40	0	6,6,6	0.07	0
9	HTO	C	348	-	9,9,9	0.42	0	9,10,10	1.30	1 (11%)
9	HTO	C	349	-	9,9,9	0.57	0	9,10,10	0.99	0
10	GOL	C	350	-	5,5,5	1.04	1 (20%)	5,5,5	1.13	0
10	GOL	C	351	-	5,5,5	0.62	0	5,5,5	1.18	0
10	GOL	C	352	-	5,5,5	0.35	0	5,5,5	0.52	0
10	GOL	C	353[A]	-	5,5,5	0.53	0	5,5,5	0.72	0
10	GOL	C	353[B]	-	5,5,5	0.50	0	5,5,5	0.37	0
10	GOL	C	354	-	5,5,5	0.70	0	5,5,5	0.54	0
10	GOL	C	355	-	5,5,5	0.26	0	5,5,5	0.37	0
10	GOL	C	356	-	5,5,5	0.92	0	5,5,5	1.47	1 (20%)
10	GOL	C	357	-	5,5,5	0.54	0	5,5,5	0.34	0
10	GOL	C	358	-	5,5,5	0.50	0	5,5,5	0.52	0
10	GOL	C	359	-	5,5,5	0.41	0	5,5,5	0.35	0
10	GOL	C	360	-	5,5,5	0.26	0	5,5,5	0.29	0
10	GOL	C	361	-	5,5,5	0.23	0	5,5,5	0.32	0
10	GOL	C	362	-	5,5,5	0.24	0	5,5,5	0.50	0
10	GOL	C	363	-	5,5,5	0.29	0	5,5,5	0.48	0
10	GOL	C	364	-	5,5,5	0.77	0	5,5,5	2.08	2 (40%)
10	GOL	C	365	-	5,5,5	0.21	0	5,5,5	0.45	0
5	HEC	C	401	1	28,50,50	1.11	1 (3%)	16,82,82	1.70	4 (25%)
5	HEC	C	402	1	28,50,50	1.19	3 (10%)	16,82,82	1.35	3 (18%)
5	HEC	C	403	1	28,50,50	0.96	1 (3%)	16,82,82	1.10	2 (12%)
5	HEC	C	404[A]	-	28,50,50	1.03	1 (3%)	16,82,82	1.91	5 (31%)
5	HEC	C	404[B]	-	28,50,50	0.98	1 (3%)	16,82,82	1.63	4 (25%)
6	LDA	C	712	-	13,15,15	2.50	1 (7%)	14,17,17	0.55	0
6	LDA	C	722	-	13,15,15	2.31	1 (7%)	14,17,17	0.56	0
7	DGA	C	730	1	36,36,43	0.80	2 (5%)	38,38,45	1.46	3 (7%)
8	SO4	H	259	-	4,4,4	0.35	0	6,6,6	0.25	0
8	SO4	H	260	-	4,4,4	0.37	0	6,6,6	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	SO4	H	261	-	4,4,4	0.45	0	6,6,6	1.04	1 (16%)
8	SO4	H	262[A]	-	4,4,4	0.52	0	6,6,6	0.46	0
8	SO4	H	262[B]	-	4,4,4	0.47	0	6,6,6	0.52	0
8	SO4	H	263	-	4,4,4	0.45	0	6,6,6	0.34	0
8	SO4	H	264	-	4,4,4	0.49	0	6,6,6	0.28	0
8	SO4	H	265	-	4,4,4	0.42	0	6,6,6	0.07	0
9	HTO	H	266	-	9,9,9	0.36	0	9,10,10	1.10	1 (11%)
9	HTO	H	267	-	9,9,9	0.52	0	9,10,10	0.96	0
9	HTO	H	268	-	9,9,9	0.32	0	9,10,10	1.79	1 (11%)
10	GOL	H	269	-	5,5,5	0.19	0	5,5,5	0.61	0
10	GOL	H	270	-	5,5,5	0.30	0	5,5,5	0.56	0
10	GOL	H	271	-	5,5,5	0.59	0	5,5,5	1.14	0
10	GOL	H	272	-	5,5,5	0.25	0	5,5,5	0.58	0
10	GOL	H	273	-	5,5,5	0.27	0	5,5,5	0.61	0
10	GOL	H	274	-	5,5,5	0.20	0	5,5,5	0.40	0
10	GOL	H	275	-	5,5,5	0.30	0	5,5,5	0.34	0
10	GOL	H	276	-	5,5,5	0.19	0	5,5,5	0.40	0
10	GOL	H	277	-	5,5,5	0.30	0	5,5,5	0.33	0
10	GOL	H	278	-	5,5,5	0.17	0	5,5,5	0.66	0
10	GOL	H	279	-	5,5,5	0.23	0	5,5,5	0.48	0
6	LDA	H	701	-	13,15,15	1.70	1 (7%)	14,17,17	1.18	1 (7%)
6	LDA	H	707	-	13,15,15	2.31	1 (7%)	14,17,17	0.55	0
6	LDA	H	718	-	10,12,15	2.81	1 (10%)	11,14,17	0.61	0
6	LDA	H	719	-	13,15,15	2.37	1 (7%)	14,17,17	0.70	0
6	LDA	H	721	-	13,15,15	2.17	2 (15%)	14,17,17	1.04	1 (7%)
7	DGA	H	733	-	30,30,43	0.64	1 (3%)	32,32,45	1.92	8 (25%)
9	HTO	L	274	-	9,9,9	0.66	0	9,10,10	1.52	2 (22%)
9	HTO	L	275	-	9,9,9	0.87	0	9,10,10	3.23	3 (33%)
10	GOL	L	276	-	5,5,5	0.40	0	5,5,5	0.50	0
10	GOL	L	277	-	5,5,5	0.36	0	5,5,5	1.01	0
10	GOL	L	278	-	5,5,5	0.96	0	5,5,5	1.28	1 (20%)
10	GOL	L	279	-	5,5,5	0.78	0	5,5,5	1.04	0
10	GOL	L	280	-	5,5,5	0.27	0	5,5,5	0.17	0
10	GOL	L	281	-	5,5,5	0.26	0	5,5,5	0.32	0
10	GOL	L	282	-	5,5,5	0.35	0	5,5,5	0.21	0
11	BCB	L	400	3	63,74,74	3.88	22 (34%)	50,115,115	2.42	17 (34%)
11	BCB	L	401	3	63,74,74	3.80	20 (31%)	50,115,115	2.20	11 (22%)
12	BPB	L	402	-	63,70,70	0.86	1 (1%)	67,101,101	1.42	8 (11%)
13	UQ9	L	502	-	58,58,58	2.16	21 (36%)	70,73,73	1.37	11 (15%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	UQ9	L	503	-	19,19,58	2.25	5 (26%)	23,26,73	1.58	4 (17%)
6	LDA	L	703	-	13,15,15	2.47	2 (15%)	14,17,17	0.62	0
6	LDA	L	708	-	13,15,15	1.87	1 (7%)	14,17,17	0.92	1 (7%)
6	LDA	L	709	-	13,15,15	2.31	1 (7%)	14,17,17	0.32	0
6	LDA	L	720	-	13,15,15	2.22	1 (7%)	14,17,17	1.34	3 (21%)
7	DGA	L	731	-	32,32,43	0.66	0	34,34,45	1.65	6 (17%)
8	SO4	M	324	-	4,4,4	0.42	0	6,6,6	0.96	0
8	SO4	M	325	-	4,4,4	0.25	0	6,6,6	0.27	0
8	SO4	M	326	-	4,4,4	0.16	0	6,6,6	0.36	0
8	SO4	M	327	-	4,4,4	0.40	0	6,6,6	0.16	0
8	SO4	M	328	-	4,4,4	0.33	0	6,6,6	0.59	0
8	SO4	M	329	-	4,4,4	0.30	0	6,6,6	0.33	0
8	SO4	M	330	-	4,4,4	0.48	0	6,6,6	0.38	0
8	SO4	M	331	-	4,4,4	0.40	0	6,6,6	0.77	0
9	HTO	M	332	-	9,9,9	0.54	0	9,10,10	3.50	5 (55%)
10	GOL	M	333	-	5,5,5	0.26	0	5,5,5	0.27	0
10	GOL	M	334	-	5,5,5	0.35	0	5,5,5	1.05	0
10	GOL	M	335	-	5,5,5	0.59	0	5,5,5	1.71	2 (40%)
10	GOL	M	336	-	5,5,5	0.20	0	5,5,5	0.58	0
10	GOL	M	337	-	5,5,5	0.26	0	5,5,5	0.35	0
10	GOL	M	338	-	5,5,5	0.39	0	5,5,5	1.37	0
10	GOL	M	339	-	5,5,5	0.32	0	5,5,5	0.46	0
11	BCB	M	400	4	63,74,74	3.63	20 (31%)	50,115,115	2.05	13 (26%)
11	BCB	M	401	4	63,74,74	3.97	24 (38%)	50,115,115	2.47	16 (32%)
12	BPB	M	402	-	63,70,70	1.19	4 (6%)	67,101,101	1.34	12 (17%)
14	MQ9	M	501	-	59,59,59	2.05	25 (42%)	73,75,75	1.22	9 (12%)
16	NS5	M	600	-	39,39,39	2.15	17 (43%)	44,46,46	2.12	11 (25%)
6	LDA	M	702	-	13,15,15	2.32	1 (7%)	14,17,17	0.82	0
6	LDA	M	704	-	13,15,15	2.32	1 (7%)	14,17,17	0.60	0
6	LDA	M	705	-	13,15,15	2.08	1 (7%)	14,17,17	0.76	0
6	LDA	M	706	-	13,15,15	2.36	1 (7%)	14,17,17	0.74	0
6	LDA	M	715	-	13,15,15	2.27	1 (7%)	14,17,17	0.61	0
7	DGA	M	732	-	33,33,43	0.64	0	35,35,45	1.63	4 (11%)

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
8	SO4	C	337	-	-	0/0/0/0	0/0/0/0
8	SO4	C	338	-	-	0/0/0/0	0/0/0/0
8	SO4	C	339	-	-	0/0/0/0	0/0/0/0
8	SO4	C	340	-	-	0/0/0/0	0/0/0/0
8	SO4	C	341	-	-	0/0/0/0	0/0/0/0
8	SO4	C	342	-	-	0/0/0/0	0/0/0/0
8	SO4	C	343	-	-	0/0/0/0	0/0/0/0
8	SO4	C	344	-	-	0/0/0/0	0/0/0/0
8	SO4	C	345	-	-	0/0/0/0	0/0/0/0
8	SO4	C	346	-	-	0/0/0/0	0/0/0/0
8	SO4	C	347	-	-	0/0/0/0	0/0/0/0
9	HTO	C	348	-	-	0/10/10/10	0/0/0/0
9	HTO	C	349	-	-	0/10/10/10	0/0/0/0
10	GOL	C	350	-	-	0/4/4/4	0/0/0/0
10	GOL	C	351	-	-	0/4/4/4	0/0/0/0
10	GOL	C	352	-	-	0/4/4/4	0/0/0/0
10	GOL	C	353[A]	-	-	0/4/4/4	0/0/0/0
10	GOL	C	353[B]	-	-	0/4/4/4	0/0/0/0
10	GOL	C	354	-	-	0/4/4/4	0/0/0/0
10	GOL	C	355	-	-	0/4/4/4	0/0/0/0
10	GOL	C	356	-	-	0/4/4/4	0/0/0/0
10	GOL	C	357	-	-	0/4/4/4	0/0/0/0
10	GOL	C	358	-	-	0/4/4/4	0/0/0/0
10	GOL	C	359	-	-	0/4/4/4	0/0/0/0
10	GOL	C	360	-	-	0/4/4/4	0/0/0/0
10	GOL	C	361	-	-	0/4/4/4	0/0/0/0
10	GOL	C	362	-	-	0/4/4/4	0/0/0/0
10	GOL	C	363	-	-	0/4/4/4	0/0/0/0
10	GOL	C	364	-	-	0/4/4/4	0/0/0/0
10	GOL	C	365	-	-	0/4/4/4	0/0/0/0
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[A]	-	-	0/6/54/54	0/0/8/8
5	HEC	C	404[B]	-	-	0/6/54/54	0/0/8/8
6	LDA	C	712	-	-	0/13/13/13	0/0/0/0
6	LDA	C	722	-	-	0/13/13/13	0/0/0/0
7	DGA	C	730	1	-	0/37/37/45	0/0/0/0
8	SO4	H	259	-	-	0/0/0/0	0/0/0/0
8	SO4	H	260	-	-	0/0/0/0	0/0/0/0
8	SO4	H	261	-	-	0/0/0/0	0/0/0/0
8	SO4	H	262[A]	-	-	0/0/0/0	0/0/0/0
8	SO4	H	262[B]	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	SO4	H	263	-	-	0/0/0/0	0/0/0/0
8	SO4	H	264	-	-	0/0/0/0	0/0/0/0
8	SO4	H	265	-	-	0/0/0/0	0/0/0/0
9	HTO	H	266	-	-	0/10/10/10	0/0/0/0
9	HTO	H	267	-	-	0/10/10/10	0/0/0/0
9	HTO	H	268	-	-	0/10/10/10	0/0/0/0
10	GOL	H	269	-	-	0/4/4/4	0/0/0/0
10	GOL	H	270	-	-	0/4/4/4	0/0/0/0
10	GOL	H	271	-	-	0/4/4/4	0/0/0/0
10	GOL	H	272	-	-	0/4/4/4	0/0/0/0
10	GOL	H	273	-	-	0/4/4/4	0/0/0/0
10	GOL	H	274	-	-	0/4/4/4	0/0/0/0
10	GOL	H	275	-	-	0/4/4/4	0/0/0/0
10	GOL	H	276	-	-	0/4/4/4	0/0/0/0
10	GOL	H	277	-	-	0/4/4/4	0/0/0/0
10	GOL	H	278	-	-	0/4/4/4	0/0/0/0
10	GOL	H	279	-	-	0/4/4/4	0/0/0/0
6	LDA	H	701	-	-	0/13/13/13	0/0/0/0
6	LDA	H	707	-	-	0/13/13/13	0/0/0/0
6	LDA	H	718	-	-	0/10/10/13	0/0/0/0
6	LDA	H	719	-	-	0/13/13/13	0/0/0/0
6	LDA	H	721	-	-	0/13/13/13	0/0/0/0
7	DGA	H	733	-	-	0/32/32/45	0/0/0/0
9	HTO	L	274	-	-	0/10/10/10	0/0/0/0
9	HTO	L	275	-	-	0/10/10/10	0/0/0/0
10	GOL	L	276	-	-	0/4/4/4	0/0/0/0
10	GOL	L	277	-	-	0/4/4/4	0/0/0/0
10	GOL	L	278	-	-	0/4/4/4	0/0/0/0
10	GOL	L	279	-	-	0/4/4/4	0/0/0/0
10	GOL	L	280	-	-	0/4/4/4	0/0/0/0
10	GOL	L	281	-	-	0/4/4/4	0/0/0/0
10	GOL	L	282	-	-	0/4/4/4	0/0/0/0
11	BCB	L	400	3	-	0/41/177/177	0/0/9/9
11	BCB	L	401	3	-	0/41/177/177	0/0/9/9
12	BPB	L	402	-	-	0/47/105/105	0/1/6/6
13	UQ9	L	502	-	-	0/57/81/81	0/1/1/1
13	UQ9	L	503	-	-	0/11/35/81	0/1/1/1
6	LDA	L	703	-	-	0/13/13/13	0/0/0/0
6	LDA	L	708	-	-	0/13/13/13	0/0/0/0
6	LDA	L	709	-	-	0/13/13/13	0/0/0/0
6	LDA	L	720	-	-	0/13/13/13	0/0/0/0
7	DGA	L	731	-	-	0/34/34/45	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	SO4	M	324	-	-	0/0/0/0	0/0/0/0
8	SO4	M	325	-	-	0/0/0/0	0/0/0/0
8	SO4	M	326	-	-	0/0/0/0	0/0/0/0
8	SO4	M	327	-	-	0/0/0/0	0/0/0/0
8	SO4	M	328	-	-	0/0/0/0	0/0/0/0
8	SO4	M	329	-	-	0/0/0/0	0/0/0/0
8	SO4	M	330	-	-	0/0/0/0	0/0/0/0
8	SO4	M	331	-	-	0/0/0/0	0/0/0/0
9	HTO	M	332	-	-	0/10/10/10	0/0/0/0
10	GOL	M	333	-	-	0/4/4/4	0/0/0/0
10	GOL	M	334	-	-	0/4/4/4	0/0/0/0
10	GOL	M	335	-	-	0/4/4/4	0/0/0/0
10	GOL	M	336	-	-	0/4/4/4	0/0/0/0
10	GOL	M	337	-	-	0/4/4/4	0/0/0/0
10	GOL	M	338	-	-	0/4/4/4	0/0/0/0
10	GOL	M	339	-	-	0/4/4/4	0/0/0/0
11	BCB	M	400	4	-	0/41/177/177	0/0/9/9
11	BCB	M	401	4	-	0/41/177/177	0/0/9/9
12	BPB	M	402	-	-	0/47/105/105	0/1/6/6
14	MQ9	M	501	-	-	0/53/73/73	0/2/2/2
16	NS5	M	600	-	-	0/43/43/43	0/0/0/0
6	LDA	M	702	-	-	0/13/13/13	0/0/0/0
6	LDA	M	704	-	-	0/13/13/13	0/0/0/0
6	LDA	M	705	-	-	0/13/13/13	0/0/0/0
6	LDA	M	706	-	-	0/13/13/13	0/0/0/0
6	LDA	M	715	-	-	0/13/13/13	0/0/0/0
7	DGA	M	732	-	-	2/35/35/45	0/0/0/0

All (188) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	L	401	BCB	C3B-C4B	-12.16	1.40	1.54
11	M	401	BCB	C3B-C4B	-11.96	1.41	1.54
11	L	400	BCB	C3B-C4B	-11.43	1.41	1.54
11	M	400	BCB	C3B-C4B	-10.69	1.42	1.54
11	M	401	BCB	C3D-C4D	-10.07	1.43	1.54
11	L	400	BCB	C3D-C4D	-9.71	1.43	1.54
11	M	400	BCB	CHD-C1D	-9.38	1.38	1.53
11	L	401	BCB	C3D-C4D	-9.23	1.44	1.54
11	L	400	BCB	CHD-C1D	-9.15	1.38	1.53
11	L	401	BCB	CHD-C1D	-8.94	1.39	1.53
6	C	712	LDA	O1-N1	-8.93	1.24	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	L	400	BCB	CHC-C4B	-8.86	1.39	1.53
6	H	718	LDA	O1-N1	-8.68	1.25	1.42
11	M	401	BCB	C1A-CHA	-8.65	1.40	1.53
6	L	703	LDA	O1-N1	-8.58	1.25	1.42
11	M	401	BCB	C4D-ND	-8.56	1.31	1.50
6	M	706	LDA	O1-N1	-8.39	1.25	1.42
11	M	400	BCB	C1A-CHA	-8.37	1.40	1.53
6	H	719	LDA	O1-N1	-8.31	1.25	1.42
11	M	401	BCB	CHB-C1B	-8.29	1.40	1.53
11	L	401	BCB	CHB-C1B	-8.26	1.40	1.53
6	L	709	LDA	O1-N1	-8.22	1.26	1.42
11	L	400	BCB	C4D-ND	-8.20	1.32	1.50
6	M	704	LDA	O1-N1	-8.17	1.26	1.42
11	M	400	BCB	C3D-C4D	-8.16	1.45	1.54
6	M	702	LDA	O1-N1	-8.13	1.26	1.42
11	M	401	BCB	CHC-C4B	-8.09	1.40	1.53
6	H	707	LDA	O1-N1	-8.07	1.26	1.42
6	C	722	LDA	O1-N1	-8.04	1.26	1.42
11	L	400	BCB	C1A-CHA	-8.03	1.41	1.53
6	M	715	LDA	O1-N1	-7.99	1.26	1.42
11	L	401	BCB	CHC-C4B	-7.98	1.40	1.53
6	L	720	LDA	O1-N1	-7.89	1.26	1.42
11	M	401	BCB	CHD-C1D	-7.50	1.41	1.53
11	M	401	BCB	C2D-C1D	-7.49	1.38	1.53
6	H	721	LDA	O1-N1	-7.44	1.27	1.42
11	M	400	BCB	CHC-C4B	-7.37	1.41	1.53
11	L	401	BCB	C4D-ND	-7.34	1.34	1.50
6	M	705	LDA	O1-N1	-7.26	1.27	1.42
13	L	503	UQ9	C7-C8	-7.05	1.39	1.50
13	L	502	UQ9	C7-C8	-7.05	1.39	1.50
11	M	400	BCB	C4D-ND	-7.03	1.35	1.50
11	M	400	BCB	CHB-C1B	-6.95	1.42	1.53
11	L	401	BCB	CHD-C4C	-6.92	1.40	1.53
11	M	401	BCB	C2B-C1B	-6.79	1.40	1.53
11	L	401	BCB	C2D-C1D	-6.72	1.40	1.53
6	L	708	LDA	O1-N1	-6.67	1.29	1.42
11	L	401	BCB	C1A-CHA	-6.59	1.43	1.53
11	L	400	BCB	CHD-C4C	-6.50	1.41	1.53
11	M	401	BCB	C1D-ND	-6.47	1.36	1.50
11	M	400	BCB	C2D-C1D	-6.46	1.40	1.53
11	M	400	BCB	C3B-C2B	-6.39	1.38	1.55
11	L	400	BCB	C1D-ND	-6.36	1.36	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	L	400	BCB	C2B-C1B	-6.34	1.40	1.53
11	L	400	BCB	CHB-C1B	-6.19	1.43	1.53
11	M	401	BCB	CHD-C4C	-6.19	1.42	1.53
11	M	400	BCB	C2B-C1B	-6.13	1.41	1.53
11	L	401	BCB	CHB-C4A	-5.98	1.38	1.52
11	L	400	BCB	C3D-C2D	-5.94	1.39	1.55
11	L	401	BCB	C2B-C1B	-5.89	1.41	1.53
11	L	400	BCB	C2D-C1D	-5.88	1.41	1.53
6	H	701	LDA	O1-N1	-5.84	1.30	1.42
11	L	401	BCB	C3B-C2B	-5.69	1.40	1.55
11	M	400	BCB	C1D-ND	-5.65	1.38	1.50
11	L	400	BCB	CHB-C4A	-5.49	1.39	1.52
11	L	400	BCB	C3B-C2B	-5.48	1.40	1.55
11	M	401	BCB	CHB-C4A	-5.46	1.39	1.52
11	M	401	BCB	C4B-NB	-5.46	1.38	1.50
11	L	401	BCB	C1B-NB	-5.41	1.38	1.50
11	M	401	BCB	C3D-C2D	-5.36	1.41	1.55
11	L	400	BCB	C1B-NB	-5.33	1.38	1.50
11	L	401	BCB	CHC-C1C	-5.30	1.40	1.52
11	M	401	BCB	C1B-NB	-5.29	1.38	1.50
11	M	401	BCB	C3B-C2B	-5.25	1.41	1.55
11	M	401	BCB	CHC-C1C	-5.10	1.40	1.52
11	M	400	BCB	CHD-C4C	-5.08	1.44	1.53
11	L	400	BCB	CHC-C1C	-5.07	1.40	1.52
11	M	400	BCB	CHC-C1C	-5.01	1.40	1.52
11	M	400	BCB	C4B-NB	-4.90	1.39	1.50
11	L	401	BCB	C4B-NB	-4.84	1.39	1.50
11	L	400	BCB	C4B-NB	-4.83	1.39	1.50
11	M	400	BCB	C1B-NB	-4.73	1.40	1.50
11	M	400	BCB	C3D-C2D	-4.68	1.42	1.55
11	M	400	BCB	CHB-C4A	-4.40	1.42	1.52
11	L	401	BCB	C3D-C2D	-4.11	1.44	1.55
11	L	401	BCB	C1D-ND	-4.09	1.41	1.50
13	L	502	UQ9	C4-C5	-4.06	1.37	1.48
13	L	502	UQ9	C3-C2	-3.35	1.39	1.48
11	L	401	BCB	C3D-CAD	-3.33	1.45	1.51
13	L	502	UQ9	C27-C28	-3.29	1.39	1.50
13	L	502	UQ9	C37-C38	-3.28	1.39	1.50
14	M	501	MQ9	C5-C4	-3.24	1.41	1.48
13	L	502	UQ9	C47-C48	-3.23	1.39	1.50
13	L	502	UQ9	C17-C18	-3.21	1.39	1.50
14	M	501	MQ9	C37-C38	-3.20	1.39	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	L	502	UQ9	C22-C23	-3.16	1.39	1.50
11	L	400	BCB	C3D-CAD	-3.16	1.45	1.51
13	L	502	UQ9	C32-C33	-3.07	1.40	1.50
11	M	401	BCB	CHA-CBD	-3.06	1.46	1.53
14	M	501	MQ9	C3-C4	-3.06	1.42	1.48
13	L	502	UQ9	C12-C13	-3.04	1.40	1.50
5	C	402	HEC	CAA-C2A	-2.95	1.46	1.52
14	M	501	MQ9	C7-C8	-2.91	1.46	1.50
13	L	503	UQ9	C4-C5	-2.87	1.40	1.48
13	L	502	UQ9	C42-C43	-2.84	1.40	1.50
14	M	501	MQ9	C2-C1	-2.84	1.42	1.48
14	M	501	MQ9	C22-C23	-2.82	1.40	1.50
13	L	503	UQ9	C3-C2	-2.82	1.40	1.48
14	M	501	MQ9	C47-C48	-2.72	1.41	1.50
11	L	400	BCB	C2A-C3A	-2.71	1.49	1.55
7	H	733	DGA	OG1-CG1	-2.63	1.39	1.45
14	M	501	MQ9	C42-C43	-2.62	1.41	1.50
11	M	400	BCB	C4C-C3C	-2.53	1.42	1.50
13	L	502	UQ9	C6-C5	-2.49	1.39	1.46
11	M	400	BCB	C3D-CAD	-2.42	1.46	1.51
14	M	501	MQ9	C27-C28	-2.31	1.42	1.50
6	H	721	LDA	C1-N1	-2.30	1.46	1.51
6	L	703	LDA	C1-N1	-2.25	1.46	1.51
14	M	501	MQ9	C32-C33	-2.25	1.42	1.50
11	M	400	BCB	C2A-C3A	-2.25	1.50	1.55
11	L	400	BCB	C4C-C3C	-2.25	1.43	1.50
11	M	401	BCB	C4C-C3C	-2.23	1.43	1.50
11	L	401	BCB	C4C-C3C	-2.20	1.43	1.50
11	M	401	BCB	C3D-CAD	-2.10	1.47	1.51
11	M	401	BCB	CBD-CAD	-2.05	1.50	1.53
14	M	501	MQ9	C12-C13	-2.00	1.43	1.50
10	C	350	GOL	O3-C3	2.01	1.50	1.42
16	M	600	NS5	C34-C35	2.02	1.57	1.50
5	C	404[A]	HEC	CBC-CAC	2.05	1.57	1.49
5	C	404[B]	HEC	CBC-CAC	2.05	1.57	1.49
16	M	600	NS5	C19-C20	2.08	1.50	1.43
12	L	402	BPB	C1-C2	2.08	1.55	1.49
16	M	600	NS5	C29-C28	2.08	1.39	1.34
12	M	402	BPB	C1-C2	2.09	1.55	1.49
16	M	600	NS5	C25-C26	2.09	1.38	1.35
11	M	401	BCB	O2D-CGD	2.11	1.38	1.33
16	M	600	NS5	C35-C36	2.12	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	401	BCB	OBD-CAD	2.14	1.25	1.21
16	M	600	NS5	C23-C21	2.15	1.50	1.45
7	C	730	DGA	OG1-CG1	2.20	1.50	1.45
5	C	402	HEC	CBB-CAB	2.21	1.58	1.49
7	C	730	DGA	CG1-CG2	2.22	1.56	1.50
11	M	401	BCB	CBD-CGD	2.23	1.55	1.52
5	C	403	HEC	CBB-CAB	2.23	1.58	1.49
14	M	501	MQ9	C18-C19	2.25	1.38	1.33
16	M	600	NS5	C24-C25	2.25	1.50	1.43
14	M	501	MQ9	C25-C24	2.28	1.56	1.50
14	M	501	MQ9	C23-C24	2.28	1.38	1.33
16	M	600	NS5	C8-C7	2.29	1.58	1.50
12	M	402	BPB	CAC-C3C	2.29	1.35	1.33
11	L	401	BCB	OBD-CAD	2.32	1.25	1.21
11	L	400	BCB	O2D-CGD	2.34	1.39	1.33
13	L	502	UQ9	C7-C6	2.34	1.55	1.51
14	M	501	MQ9	C8-C9	2.36	1.38	1.33
16	M	600	NS5	C22-C21	2.36	1.55	1.50
13	L	503	UQ9	C6-C1	2.41	1.40	1.35
11	L	400	BCB	C1A-C2A	2.46	1.56	1.53
14	M	501	MQ9	C41-C39	2.47	1.56	1.51
13	L	502	UQ9	C8-C9	2.50	1.39	1.33
16	M	600	NS5	C20-C21	2.52	1.39	1.35
14	M	501	MQ9	C11-C9	2.53	1.56	1.51
13	L	503	UQ9	C8-C9	2.56	1.39	1.33
5	C	402	HEC	C3C-C2C	2.58	1.43	1.40
12	M	402	BPB	CMB-C2B	2.58	1.56	1.51
13	L	502	UQ9	C33-C34	2.59	1.39	1.33
14	M	501	MQ9	C46-C44	2.63	1.57	1.51
13	L	502	UQ9	C13-C14	2.69	1.39	1.33
16	M	600	NS5	C17-C15	2.71	1.39	1.35
13	L	502	UQ9	C43-C44	2.71	1.39	1.33
14	M	501	MQ9	C48-C49	2.72	1.40	1.32
13	L	502	UQ9	C23-C24	2.73	1.39	1.33
5	C	401	HEC	C1A-NA	2.79	1.40	1.36
16	M	600	NS5	C28-C26	2.91	1.52	1.45
16	M	600	NS5	C4-C5	2.93	1.57	1.51
13	L	502	UQ9	C38-C39	2.93	1.40	1.33
13	L	502	UQ9	C28-C29	2.94	1.40	1.33
14	M	501	MQ9	C28-C29	2.95	1.40	1.33
13	L	502	UQ9	C18-C19	2.97	1.40	1.33
14	M	501	MQ9	C33-C34	3.02	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	M	600	NS5	C29-C30	3.03	1.52	1.43
16	M	600	NS5	C13-C12	3.04	1.52	1.43
14	M	501	MQ9	C38-C39	3.13	1.40	1.33
14	M	501	MQ9	C5M-C5	3.47	1.58	1.50
14	M	501	MQ9	C43-C44	3.56	1.41	1.33
14	M	501	MQ9	C6-C5	4.31	1.44	1.35
16	M	600	NS5	C12-C10	4.66	1.39	1.34
16	M	600	NS5	C30-C31	5.55	1.40	1.34
12	M	402	BPB	C3B-C4B	5.87	1.48	1.41

All (177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	275	HTO	O2-C2-C3	-7.17	95.50	109.77
16	M	600	NS5	C19-C20-C21	-6.30	118.32	127.31
11	M	401	BCB	O2D-CGD-O1D	-5.85	112.05	123.82
9	M	332	HTO	O1-C1-C2	-5.76	98.39	111.11
9	L	275	HTO	O3-C3-C2	-5.69	98.44	109.77
9	M	332	HTO	C5-C4-C3	-5.69	104.64	114.22
16	M	600	NS5	C24-C25-C26	-5.53	119.41	127.31
7	H	733	DGA	CG1-CG2-CG3	-5.41	99.80	111.87
7	C	730	DGA	CG2-OG2-CB1	-4.79	111.83	117.90
11	M	401	BCB	CHA-CBD-CGD	-4.47	104.64	115.00
16	M	600	NS5	C12-C13-C14	-4.43	109.65	123.23
9	M	332	HTO	O3-C3-C4	-4.31	99.87	109.25
7	H	733	DGA	OG1-CG1-CG2	-4.30	97.84	108.66
11	M	400	BCB	CBA-CAA-C2A	-4.25	109.90	115.76
9	M	332	HTO	O2-C2-C1	-4.22	99.45	109.21
9	H	268	HTO	C5-C4-C3	-4.18	107.18	114.22
5	C	404[A]	HEC	C1D-C2D-C3D	-4.09	104.15	107.00
11	L	401	BCB	CBA-CAA-C2A	-4.04	110.19	115.76
11	L	400	BCB	CHA-CBD-CGD	-4.03	105.66	115.00
7	M	732	DGA	CB3-CB2-CB1	-3.99	99.01	113.58
11	L	400	BCB	C1-C2-C3	-3.81	118.94	125.96
5	C	401	HEC	CMB-C2B-C1B	-3.79	122.64	128.46
9	C	348	HTO	O3-C3-C2	-3.72	102.38	109.77
10	C	364	GOL	O3-C3-C2	-3.51	92.38	110.07
12	L	402	BPB	CBD-CHA-C4D	-3.48	104.62	108.54
14	M	501	MQ9	C40-C39-C38	-3.40	114.61	123.69
11	L	400	BCB	OBB-CAB-C3B	-3.33	117.99	121.55
11	L	401	BCB	C5-C3-C2	-3.32	114.31	121.10
16	M	600	NS5	C14-C15-C17	-3.25	113.95	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	731	DGA	CG1-CG2-CG3	-3.18	104.77	111.87
12	M	402	BPB	CBC-CAC-C3C	-3.17	120.02	127.00
7	H	733	DGA	CG2-OG2-CB1	-3.15	110.44	117.88
7	L	731	DGA	CG2-OG2-CB1	-3.13	110.48	117.88
13	L	502	UQ9	C1M-C1-C6	-3.10	117.92	124.20
6	H	721	LDA	CM2-N1-C1	-3.00	103.93	110.23
5	C	404[A]	HEC	C4C-C3C-C2C	-2.97	103.14	106.35
5	C	404[B]	HEC	C4C-C3C-C2C	-2.97	103.14	106.35
5	C	404[A]	HEC	CMB-C2B-C1B	-2.89	124.03	128.46
5	C	404[B]	HEC	CMB-C2B-C1B	-2.89	124.03	128.46
11	L	400	BCB	CBA-CAA-C2A	-2.86	111.81	115.76
7	H	733	DGA	CG1-OG1-CA1	-2.85	108.55	117.13
5	C	402	HEC	C1D-C2D-C3D	-2.84	105.02	107.00
6	L	720	LDA	CM2-N1-CM1	-2.83	105.57	110.99
7	L	731	DGA	CG1-OG1-CA1	-2.81	108.67	117.13
12	M	402	BPB	C2A-C3A-C4A	-2.63	97.61	101.87
9	L	274	HTO	C4-C3-C2	-2.62	107.36	113.10
11	M	401	BCB	CBA-CAA-C2A	-2.60	112.17	115.76
10	M	335	GOL	O2-C2-C3	-2.59	96.61	108.84
7	M	732	DGA	OB1-CB1-CB2	-2.56	113.56	123.68
11	L	400	BCB	O2D-CGD-O1D	-2.55	118.69	123.82
16	M	600	NS5	C24-C23-C21	-2.55	119.26	126.42
9	L	274	HTO	O2-C2-C1	-2.54	103.32	109.21
6	H	701	LDA	CM2-N1-C1	-2.53	104.91	110.23
6	L	720	LDA	CM1-N1-C1	-2.52	104.93	110.23
11	M	401	BCB	C5-C3-C2	-2.52	115.95	121.10
10	L	278	GOL	O2-C2-C1	-2.43	97.37	108.84
14	M	501	MQ9	C5M-C5-C6	-2.38	119.37	124.20
12	L	402	BPB	CBC-CAC-C3C	-2.36	121.80	127.00
12	M	402	BPB	C1-C2-C3	-2.33	121.66	125.96
6	L	708	LDA	CM1-N1-C1	-2.33	105.34	110.23
13	L	503	UQ9	C4M-O4-C4	-2.32	108.14	116.44
5	C	401	HEC	CBA-CAA-C2A	-2.29	108.10	112.47
11	M	401	BCB	OBD-CAD-CBD	-2.29	121.98	127.52
12	M	402	BPB	CBD-CHA-C4D	-2.26	105.99	108.54
16	M	600	NS5	C25-C24-C23	-2.25	116.31	123.23
13	L	502	UQ9	C4M-O4-C4	-2.20	108.58	116.44
7	H	733	DGA	OXT-CG3-CG2	-2.19	105.71	111.76
13	L	502	UQ9	O2-C2-C3	-2.18	116.32	120.95
5	C	401	HEC	CMC-C2C-C1C	-2.17	125.12	128.46
5	C	404[B]	HEC	C1D-C2D-C3D	-2.12	105.52	107.00
5	C	403	HEC	CMB-C2B-C1B	-2.11	125.22	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	400	BCB	C15-C13-C12	-2.11	101.96	112.10
12	L	402	BPB	CHD-C1D-ND	-2.10	120.52	124.64
11	M	400	BCB	OBD-CAD-CBD	-2.10	122.44	127.52
5	C	404[A]	HEC	CAD-CBD-CGD	-2.06	109.14	112.66
5	C	401	HEC	CBD-CAD-C3D	-2.05	108.57	112.48
12	M	402	BPB	CHD-C1D-ND	-2.04	120.63	124.64
7	H	733	DGA	CA3-CA2-CA1	-2.04	106.14	113.58
5	C	402	HEC	CMC-C2C-C1C	-2.03	125.35	128.46
10	C	364	GOL	O2-C2-C3	-2.02	99.32	108.84
5	C	402	HEC	CMB-C2B-C1B	-2.01	125.37	128.46
10	M	335	GOL	O1-C1-C2	2.01	120.19	110.07
12	M	402	BPB	C4D-ND-C1D	2.04	110.66	106.98
8	H	261	SO4	O3-S-O1	2.05	120.54	109.26
14	M	501	MQ9	C45-C44-C46	2.05	118.85	115.29
11	M	401	BCB	CMD-C2D-C3D	2.08	119.52	114.27
13	L	503	UQ9	O3-C3-C2	2.09	123.09	116.60
14	M	501	MQ9	C37-C38-C39	2.12	133.00	127.68
12	M	402	BPB	O2D-CGD-CBD	2.13	115.10	111.30
16	M	600	NS5	C27-C26-C28	2.13	121.49	118.10
12	M	402	BPB	C5-C3-C2	2.16	125.53	121.10
5	C	403	HEC	CMA-C3A-C2A	2.18	129.06	124.94
7	H	733	DGA	OG1-CA1-CA2	2.20	118.30	111.90
12	L	402	BPB	C3D-C4D-CHA	2.21	115.69	109.97
11	L	401	BCB	CHB-C1B-C2B	2.24	123.20	116.99
11	M	400	BCB	O2A-CGA-CBA	2.26	118.47	111.90
13	L	502	UQ9	C25-C24-C26	2.27	119.23	115.29
11	L	400	BCB	CHB-C1B-C2B	2.27	123.28	116.99
11	M	400	BCB	CED-O2D-CGD	2.30	121.36	115.97
12	M	402	BPB	CHD-C1D-C2D	2.32	130.94	125.62
12	L	402	BPB	CHD-C1D-C2D	2.32	130.94	125.62
11	M	400	BCB	CHB-C4A-C3A	2.33	123.41	117.08
13	L	502	UQ9	C15-C14-C16	2.33	119.33	115.29
14	M	501	MQ9	C40-C39-C41	2.36	119.38	115.29
14	M	501	MQ9	C41-C39-C38	2.38	125.98	121.10
11	M	401	BCB	CHB-C4A-C3A	2.39	123.58	117.08
16	M	600	NS5	C6-C5-C4	2.41	119.47	115.29
9	M	332	HTO	C4-C3-C2	2.43	118.43	113.10
11	M	401	BCB	CHB-C1B-C2B	2.44	123.75	116.99
10	C	356	GOL	C3-C2-C1	2.49	121.40	111.52
11	M	401	BCB	CED-O2D-CGD	2.52	121.87	115.97
11	M	400	BCB	CBB-CAB-C3B	2.54	119.42	116.82
13	L	502	UQ9	O3-C3-C2	2.54	124.49	116.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	400	BCB	C4-C3-C5	2.55	119.71	115.29
12	M	402	BPB	C3D-C4D-CHA	2.57	116.63	109.97
11	M	400	BCB	CHC-C4B-C3B	2.61	124.54	118.09
9	L	275	HTO	O1-C1-C2	2.61	116.87	111.11
13	L	502	UQ9	C50-C49-C51	2.62	120.71	114.60
11	L	401	BCB	CMD-C2D-C3D	2.68	121.05	114.27
14	M	501	MQ9	C30-C29-C31	2.69	119.95	115.29
11	M	400	BCB	CHB-C1B-C2B	2.71	124.50	116.99
6	L	720	LDA	CM2-N1-C1	2.75	116.01	110.23
11	L	400	BCB	CHB-C4A-C3A	2.75	124.57	117.08
13	L	502	UQ9	C3M-O3-C3	2.80	126.47	116.44
5	C	404[A]	HEC	CMA-C3A-C2A	2.81	130.25	124.94
5	C	404[B]	HEC	CMA-C3A-C2A	2.81	130.25	124.94
12	L	402	BPB	CMB-C2B-C3B	2.82	130.12	124.89
7	L	731	DGA	OG1-CA1-CA2	2.82	120.11	111.90
13	L	503	UQ9	C7-C6-C5	2.83	122.10	118.47
13	L	502	UQ9	C10-C9-C11	2.84	120.21	115.29
11	M	400	BCB	CMD-C2D-C3D	2.89	121.59	114.27
9	H	266	HTO	O2-C2-C3	2.92	115.58	109.77
7	C	730	DGA	OG1-CA1-CA2	2.94	120.44	111.90
16	M	600	NS5	C18-C19-C20	2.94	129.73	123.46
12	L	402	BPB	C4B-CHC-C1C	2.99	132.42	128.53
13	L	502	UQ9	C30-C29-C31	3.07	120.61	115.29
11	L	401	BCB	CHC-C4B-C3B	3.07	125.68	118.09
11	L	400	BCB	O2D-CGD-CBD	3.07	118.69	111.20
16	M	600	NS5	C16-C15-C17	3.12	127.29	122.92
12	M	402	BPB	C2A-C1A-NA	3.17	110.51	107.83
7	M	732	DGA	OG1-CA1-CA2	3.19	121.19	111.90
11	L	401	BCB	CHB-C4A-C3A	3.33	126.13	117.08
11	L	400	BCB	CHD-C1D-C2D	3.34	126.24	116.99
11	M	401	BCB	CHC-C4B-C3B	3.44	126.58	118.09
14	M	501	MQ9	C35-C34-C36	3.48	121.33	115.29
13	L	502	UQ9	C35-C34-C36	3.50	121.36	115.29
7	L	731	DGA	OG2-CG2-CG3	3.50	121.01	108.39
14	M	501	MQ9	C25-C24-C26	3.55	121.46	115.29
11	L	400	BCB	CMD-C2D-C3D	3.64	123.47	114.27
11	M	401	BCB	CBB-CAB-C3B	3.64	120.56	116.82
11	M	401	BCB	CHD-C1D-C2D	3.68	127.19	116.99
11	L	400	BCB	CHC-C4B-C3B	3.70	127.23	118.09
12	M	402	BPB	CMB-C2B-C3B	3.75	131.86	124.89
11	M	400	BCB	CHD-C1D-C2D	3.84	127.62	116.99
11	M	400	BCB	C3B-C4B-NB	3.84	110.53	103.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	503	UQ9	C10-C9-C11	4.10	120.70	115.85
11	L	401	BCB	C3B-C4B-NB	4.15	111.09	103.57
11	M	401	BCB	C3B-C4B-NB	4.27	111.31	103.57
16	M	600	NS5	C11-C10-C9	4.28	122.71	115.29
7	H	733	DGA	OG2-CB1-CB2	4.36	120.60	111.55
11	L	401	BCB	CHD-C1D-C2D	4.57	129.65	116.99
11	L	400	BCB	C3B-C4B-NB	4.58	111.87	103.57
11	M	401	BCB	O2D-CGD-CBD	4.69	122.65	111.20
7	L	731	DGA	OG2-CB1-CB2	4.85	121.63	111.55
11	L	401	BCB	C4-C3-C5	4.87	123.74	115.29
7	C	730	DGA	OG2-CB1-CB2	5.01	121.95	111.55
11	L	400	BCB	CBB-CAB-C3B	5.11	122.06	116.82
11	M	400	BCB	CMB-C2B-C3B	5.53	128.25	114.27
12	L	402	BPB	C2A-C1A-NA	5.88	112.81	107.83
11	L	400	BCB	CMB-C2B-C3B	6.06	129.61	114.27
7	M	732	DGA	OG2-CB1-CB2	6.14	124.30	111.55
11	L	401	BCB	CMB-C2B-C3B	6.24	130.08	114.27
11	M	401	BCB	C1D-CHD-C4C	6.85	126.97	112.37
11	M	401	BCB	CMB-C2B-C3B	6.91	131.77	114.27
11	L	400	BCB	C1D-CHD-C4C	6.92	127.11	112.37
11	L	401	BCB	C1D-CHD-C4C	7.09	127.48	112.37
11	M	400	BCB	C1D-CHD-C4C	7.14	127.58	112.37

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	M	732	DGA	CG2-OG2-CB1-OB1
7	M	732	DGA	CG2-OG2-CB1-CB2

There are no ring outliers.

56 monomers are involved in 199 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	337	SO4	3	0
8	C	338	SO4	3	0
8	C	342	SO4	3	0
8	C	344	SO4	2	0
8	C	346	SO4	1	0
9	C	348	HTO	9	0
9	C	349	HTO	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	352	GOL	2	0
10	C	353[B]	GOL	1	0
10	C	354	GOL	1	0
10	C	358	GOL	1	0
10	C	359	GOL	9	0
10	C	361	GOL	1	0
5	C	403	HEC	2	0
6	C	712	LDA	3	0
6	C	722	LDA	5	0
7	C	730	DGA	1	0
8	H	261	SO4	6	0
8	H	262[A]	SO4	1	0
8	H	262[B]	SO4	1	0
8	H	264	SO4	1	0
9	H	267	HTO	1	0
9	H	268	HTO	2	0
10	H	270	GOL	1	0
10	H	273	GOL	1	0
10	H	274	GOL	2	0
6	H	701	LDA	4	0
6	H	707	LDA	6	0
6	H	718	LDA	8	0
6	H	719	LDA	2	0
6	H	721	LDA	5	0
7	H	733	DGA	6	0
10	L	276	GOL	3	0
10	L	278	GOL	1	0
10	L	279	GOL	5	0
11	L	400	BCB	3	0
11	L	401	BCB	4	0
12	L	402	BPB	2	0
13	L	502	UQ9	31	0
13	L	503	UQ9	6	0
6	L	703	LDA	5	0
6	L	720	LDA	5	0
7	L	731	DGA	7	0
8	M	329	SO4	2	0
10	M	333	GOL	1	0
10	M	335	GOL	2	0
10	M	337	GOL	2	0
11	M	400	BCB	9	0
11	M	401	BCB	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	M	402	BPB	3	0
16	M	600	NS5	2	0
6	M	702	LDA	11	0
6	M	704	LDA	7	0
6	M	706	LDA	3	0
6	M	715	LDA	1	0
7	M	732	DGA	23	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	334/356 (93%)	0.30	25 (7%) 15 17	38, 49, 70, 123	0
2	H	249/258 (96%)	0.43	29 (11%) 5 6	42, 58, 85, 120	1 (0%)
3	L	273/273 (100%)	0.28	17 (6%) 21 25	37, 47, 62, 88	0
4	M	322/323 (99%)	0.52	50 (15%) 2 2	38, 49, 70, 91	0
All	All	1178/1210 (97%)	0.39	121 (10%) 7 8	37, 50, 73, 123	1 (0%)

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	333	ALA	8.1
1	C	334	ALA	7.9
4	M	37	TRP	7.8
3	L	51	TYR	5.9
2	H	7	ALA	5.7
2	H	8	GLN	5.6
3	L	202	ASP	5.5
2	H	85	THR	5.3
4	M	319	PRO	4.9
2	H	96	PHE	4.8
4	M	33	PHE	4.8
4	M	221	ILE	4.7
3	L	201	GLY	4.6
2	H	81	ARG	4.4
4	M	320	GLY	4.2
1	C	47	ALA	3.9
3	L	271	PHE	3.9
2	H	9	HIS	3.9
4	M	23	TRP	3.7
3	L	273	SER	3.7
4	M	108	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
2	H	94	ASP	3.6
2	H	258	LEU	3.5
4	M	243	VAL	3.5
2	H	83	PRO	3.4
2	H	182	TYR	3.4
4	M	26	ASN	3.4
3	L	165	LEU	3.4
4	M	246	ALA	3.3
1	C	1	CYS	3.2
4	M	31	LYS	3.2
1	C	236	ILE	3.2
3	L	157	VAL	3.2
4	M	107	LEU	3.1
2	H	147	GLU	3.1
4	M	189	ILE	3.1
4	M	78	HIS	3.1
4	M	71[A]	PHE	3.1
3	L	81	LEU	3.0
4	M	224	VAL	3.0
4	M	212	LEU	3.0
1	C	230	PHE	3.0
3	L	154	LEU	2.9
2	H	89	LYS	2.9
4	M	214	PHE	2.9
4	M	36	TYR	2.9
3	L	203	GLY	2.9
4	M	34	TYR	2.8
2	H	54	PRO	2.8
3	L	162	TYR	2.8
4	M	195	TYR	2.8
1	C	287	ALA	2.8
1	C	244	CYS	2.8
4	M	213	LEU	2.7
4	M	204	ILE	2.7
2	H	86	ARG	2.7
4	M	186	ALA	2.7
2	H	87	GLU	2.7
1	C	54	GLN	2.7
4	M	103	GLY	2.7
1	C	162	HIS	2.7
3	L	227	LEU	2.7
4	M	104	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
4	M	227	PHE	2.6
4	M	106	PRO	2.6
4	M	185	THR	2.6
2	H	205	LYS	2.6
1	C	231	ALA	2.5
2	H	97	GLU	2.5
4	M	32	PRO	2.5
1	C	332	LYS	2.5
4	M	263	VAL	2.4
4	M	222	LEU	2.4
1	C	4	PRO	2.4
2	H	93	THR	2.4
3	L	167	TRP	2.4
2	H	74	GLY	2.4
4	M	220	THR	2.4
2	H	10	LEU	2.4
4	M	181	ILE	2.4
4	M	29	VAL	2.4
1	C	2	PHE	2.3
2	H	104	THR	2.3
3	L	59	TRP	2.3
1	C	232	LEU	2.3
4	M	215	ALA	2.3
4	M	228	GLY	2.3
3	L	229	ILE	2.3
2	H	189	GLY	2.3
1	C	48	GLU	2.3
2	H	252	GLU	2.3
4	M	207	ALA	2.2
4	M	216	ALA	2.2
3	L	270	PRO	2.2
1	C	185	LEU	2.2
2	H	190	SER	2.2
1	C	46	LYS	2.2
2	H	238	VAL	2.2
3	L	194	ILE	2.2
4	M	25	ASP	2.2
1	C	50	PRO	2.2
4	M	184	LEU	2.2
2	H	91	ALA	2.2
2	H	95	GLY	2.1
1	C	100	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
4	M	250	TRP	2.1
4	M	22	GLU	2.1
4	M	30	GLY	2.1
4	M	79	PHE	2.1
1	C	168	THR	2.1
4	M	233	ILE	2.1
4	M	208	TYR	2.1
1	C	161	THR	2.1
4	M	210	CYS	2.1
2	H	92	GLN	2.1
4	M	55	GLY	2.0
1	C	159	THR	2.0
2	H	239[A]	SER	2.0
1	C	51	PRO	2.0
1	C	291	ALA	2.0
4	M	16	HIS	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[B]	10/11	0.93	0.13	-	49,52,54,64	10
2	FME	H	1[A]	10/11	0.93	0.13	-	50,54,59,61	10
4	CSO	M	160	7/8	0.90	0.13	-	46,49,73,77	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
13	UQ9	L	502	58/58	0.52	1.40	28.43	38,58,69,73	58
10	GOL	M	335	6/6	0.77	0.46	21.81	50,57,62,64	6
9	HTO	M	332	10/10	0.89	0.85	21.69	52,59,68,70	10
6	LDA	M	706	16/16	0.49	0.53	20.94	61,65,73,73	16
6	LDA	H	707	16/16	0.67	0.45	19.63	53,67,77,85	16
8	SO4	H	262[A]	5/5	0.92	0.20	14.66	55,56,67,71	5
10	GOL	L	280	6/6	0.87	0.34	13.11	60,65,70,74	6
10	GOL	L	279	6/6	0.86	0.39	12.01	48,50,60,61	6
6	LDA	M	702	16/16	0.53	0.79	11.79	52,56,62,65	16
9	HTO	C	348	10/10	0.57	0.61	11.53	52,62,68,74	10
8	SO4	C	345	5/5	0.70	0.37	10.92	71,79,83,86	5
10	GOL	H	272	6/6	0.71	0.40	10.42	66,72,75,76	6
10	GOL	C	359	6/6	0.82	0.73	9.81	47,54,60,68	6
10	GOL	C	353[B]	6/6	0.74	0.33	9.18	42,56,71,73	6
8	SO4	H	264	5/5	0.52	0.35	9.15	63,65,67,73	5
7	DGA	L	731	33/44	0.42	0.33	9.03	47,69,78,82	33
9	HTO	H	268	10/10	0.69	0.41	8.67	71,76,80,80	10
16	NS5	M	600	40/40	0.76	0.24	8.31	53,76,118,126	0
13	UQ9	L	503	19/58	0.48	0.38	8.13	49,70,84,86	19
7	DGA	H	733	31/44	0.74	0.32	7.63	45,62,78,79	31
6	LDA	C	722	16/16	0.74	0.39	6.47	54,61,65,65	16
6	LDA	L	720	16/16	0.48	0.41	6.29	58,70,76,78	16
6	LDA	L	709	16/16	0.45	0.36	5.96	49,67,91,92	16
10	GOL	L	277	6/6	0.92	0.41	5.73	55,61,63,65	6
8	SO4	C	342	5/5	0.92	0.23	5.61	47,56,60,62	5
6	LDA	C	712	16/16	0.60	0.31	5.35	56,62,74,74	16
10	GOL	H	274	6/6	0.88	0.32	5.27	59,71,78,81	6
10	GOL	C	351	6/6	0.83	0.29	4.85	51,58,65,67	6
9	HTO	L	274	10/10	0.82	0.28	4.35	58,67,76,80	10
10	GOL	C	350	6/6	0.93	0.38	4.26	49,56,58,60	0
7	DGA	C	730	37/44	0.64	0.31	4.16	58,76,94,99	37
10	GOL	C	352	6/6	0.91	0.21	4.11	37,56,61,61	6
8	SO4	H	262[B]	5/5	0.92	0.20	4.00	58,63,71,72	5
9	HTO	H	266	10/10	0.83	0.19	3.45	60,68,76,78	0
10	GOL	C	360	6/6	0.72	0.26	3.43	71,73,75,78	6
6	LDA	M	715	16/16	-0.06	0.47	3.15	63,77,84,85	16
6	LDA	H	701	16/16	0.86	0.25	2.75	47,57,69,70	0
10	GOL	L	278	6/6	0.89	0.27	2.19	46,54,56,58	6
10	GOL	H	276	6/6	0.75	0.20	2.00	71,79,85,85	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
9	HTO	H	267	10/10	0.72	0.26	1.77	74,77,89,91	10
6	LDA	M	704	16/16	0.56	0.39	1.76	64,67,86,88	16
6	LDA	H	719	16/16	0.84	0.20	1.62	55,61,81,83	16
7	DGA	M	732	34/44	0.59	0.27	1.40	58,72,80,84	34
6	LDA	L	708	16/16	0.84	0.18	1.35	47,58,66,76	0
6	LDA	M	705	16/16	0.72	0.21	1.35	63,70,77,78	16
10	GOL	C	354	6/6	0.74	0.21	1.29	57,68,78,86	6
9	HTO	L	275	10/10	0.86	0.23	1.01	64,69,72,74	10
9	HTO	C	349	10/10	0.72	0.22	0.96	59,68,74,75	10
8	SO4	H	261	5/5	0.88	0.21	0.81	46,55,72,75	5
11	BCB	L	400	66/66	0.96	0.18	0.80	34,39,49,57	0
11	BCB	M	400	66/66	0.95	0.15	0.76	37,46,109,115	0
10	GOL	C	362	6/6	0.78	0.22	0.75	70,75,75,75	6
11	BCB	M	401	66/66	0.95	0.17	0.71	33,39,62,67	0
12	BPB	L	402	65/65	0.96	0.15	0.69	37,41,51,53	0
14	MQ9	M	501	58/58	0.86	0.20	0.69	38,46,92,98	0
10	GOL	C	356	6/6	0.93	0.26	0.67	60,69,74,75	0
10	GOL	H	275	6/6	0.91	0.18	0.45	51,66,74,75	6
8	SO4	M	325	5/5	0.99	0.18	0.23	69,70,77,82	0
11	BCB	L	401	66/66	0.96	0.17	0.16	35,39,69,79	0
6	LDA	H	721	16/16	0.95	0.13	0.07	53,63,80,87	16
10	GOL	L	276	6/6	0.92	0.14	-0.05	55,56,58,60	0
5	HEC	C	402	43/43	0.96	0.10	-0.11	41,46,55,61	0
5	HEC	C	404[A]	43/43	0.97	0.12	-0.13	38,41,49,51	12
5	HEC	C	404[B]	43/43	0.97	0.12	-0.13	38,41,46,49	12
12	BPB	M	402	65/65	0.96	0.11	-0.25	39,46,101,105	0
5	HEC	C	403	43/43	0.97	0.15	-0.31	36,40,43,49	0
5	HEC	C	401	43/43	0.97	0.09	-0.47	46,52,61,67	0
8	SO4	H	259	5/5	0.98	0.08	-0.95	64,65,69,71	5
15	FE2	M	500	1/1	0.99	0.12	-1.26	42,42,42,42	0
8	SO4	C	338	5/5	0.88	0.17	-	66,66,73,74	5
8	SO4	C	343	5/5	0.92	0.20	-	66,66,70,74	5
10	GOL	C	364	6/6	0.89	0.17	-	53,55,61,62	6
10	GOL	H	277	6/6	0.58	0.35	-	65,69,71,72	6
10	GOL	M	334	6/6	0.79	0.53	-	63,65,67,68	6
8	SO4	C	346	5/5	0.73	0.32	-	73,73,82,82	5
10	GOL	L	281	6/6	0.85	0.22	-	60,62,66,67	6
8	SO4	M	330	5/5	0.75	0.67	-	58,64,67,70	5
8	SO4	M	331	5/5	0.94	0.27	-	75,77,81,85	5
8	SO4	H	260	5/5	0.94	0.13	-	82,82,83,88	5
8	SO4	C	341	5/5	0.94	0.24	-	62,70,77,79	5
10	GOL	M	333	6/6	0.36	0.30	-	70,70,73,78	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	LDA	L	703	16/16	0.75	0.68	-	56,61,69,72	16
8	SO4	M	328	5/5	0.96	0.19	-	59,65,67,71	5
8	SO4	M	324	5/5	1.00	0.11	-	54,54,60,71	0
10	GOL	L	282	6/6	0.88	0.20	-	60,67,75,75	6
8	SO4	C	339	5/5	0.95	0.15	-	62,67,67,69	5
8	SO4	M	329	5/5	0.93	0.15	-	62,73,75,76	5
10	GOL	C	365	6/6	0.76	0.27	-	59,60,61,65	6
10	GOL	H	273	6/6	0.70	0.32	-	71,75,79,80	6
8	SO4	C	347	5/5	0.81	0.15	-	71,73,76,77	5
10	GOL	C	355	6/6	0.82	0.21	-	67,70,71,71	6
10	GOL	H	279	6/6	0.59	0.25	-	80,86,88,91	6
6	LDA	H	718	13/16	0.69	0.27	-	55,61,79,84	13
10	GOL	H	269	6/6	0.82	0.20	-	68,76,79,83	6
8	SO4	M	327	5/5	0.71	0.26	-	79,82,83,86	5
10	GOL	C	363	6/6	0.80	0.30	-	72,75,78,78	6
8	SO4	C	344	5/5	0.92	0.22	-	61,69,77,79	5
10	GOL	M	336	6/6	0.81	0.18	-	81,82,84,87	6
10	GOL	M	337	6/6	0.67	0.29	-	56,64,66,69	6
10	GOL	H	270	6/6	0.67	0.32	-	63,69,69,71	6
10	GOL	C	357	6/6	0.85	0.15	-	69,69,76,78	6
10	GOL	M	338	6/6	0.70	0.26	-	67,71,72,73	6
8	SO4	H	265	5/5	0.71	0.39	-	71,74,75,76	5
10	GOL	M	339	6/6	0.84	0.21	-	37,53,62,67	6
8	SO4	C	340	5/5	0.79	0.17	-	72,73,77,79	5
8	SO4	H	263	5/5	0.99	0.15	-	47,50,52,52	5
10	GOL	H	278	6/6	0.88	0.16	-	75,77,78,79	6
10	GOL	H	271	6/6	0.86	0.28	-	54,63,65,75	6
10	GOL	C	361	6/6	0.78	0.46	-	66,71,76,80	6
8	SO4	C	337	5/5	0.92	0.16	-	70,73,78,84	5
8	SO4	M	326	5/5	0.98	0.24	-	57,65,67,67	5
10	GOL	C	358	6/6	0.90	0.14	-	48,64,67,68	6
10	GOL	C	353[A]	6/6	0.74	0.33	-	44,55,59,61	6

## 6.5 Other polymers [i](#)

There are no such residues in this entry.