



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:16 PM GMT

PDB ID : 3T6D
Title : Crystal Structure of the Reaction Centre from Blastochloris viridis strain DSM 133 (ATCC 19567) substrain-08
Authors : Roszak, A.W.; Gardiner, A.T.; Isaacs, N.W.; Cogdell, R.J.
Deposited on : 2011-07-28
Resolution : 1.95 Å(reported)

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

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

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

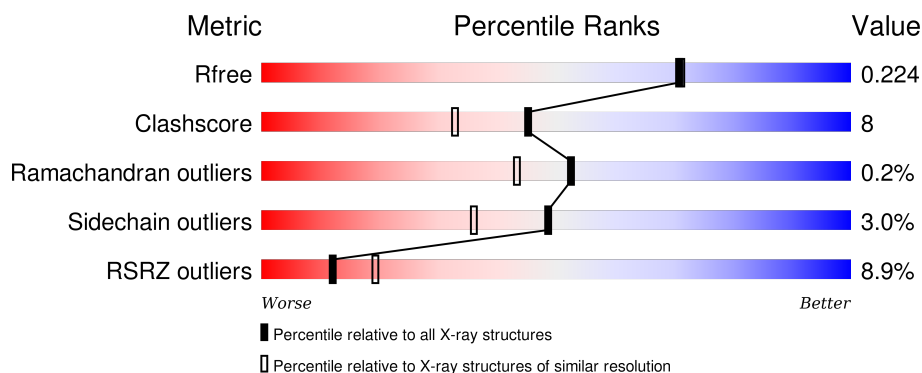
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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>12%</div> <div>86%</div> <div>8%</div> <div>6%</div> </div>
2	H	258	<div> <div>5%</div> <div>88%</div> <div>11%</div> </div>
3	L	273	<div> <div>7%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
4	M	323	<div> <div>9%</div> <div>93%</div> <div>6%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	GOL	C	359	-	-	-	X
10	GOL	C	360	-	-	-	X
10	GOL	C	362	-	-	-	X
10	GOL	C	363	-	-	-	X
10	GOL	C	364	-	-	-	X
10	GOL	C	369	-	-	-	X
10	GOL	C	371	-	-	-	X
10	GOL	C	377	-	-	X	-
10	GOL	C	378	-	-	-	X
10	GOL	H	275	-	-	-	X
10	GOL	H	276[A]	-	-	-	X
10	GOL	H	276[B]	-	-	-	X
10	GOL	H	277	-	-	-	X
10	GOL	H	279	-	-	-	X
10	GOL	H	280	-	-	-	X
10	GOL	H	282	-	-	-	X
10	GOL	H	283	-	-	X	X
10	GOL	H	289	-	-	-	X
10	GOL	L	281	-	-	-	X
10	GOL	L	285	-	-	-	X
10	GOL	L	288	-	-	-	X
10	GOL	M	334	-	-	-	X
10	GOL	M	338	-	-	-	X
13	UQ9	L	502	-	-	-	X
13	UQ9	L	503	-	-	-	X
6	LDA	C	716	-	-	-	X
6	LDA	H	701	-	-	-	X
6	LDA	H	719	-	-	-	X
6	LDA	L	702	-	-	-	X
6	LDA	L	708	-	-	-	X
6	LDA	L	709	-	-	-	X
6	LDA	L	710	-	-	-	X
6	LDA	L	711	-	-	-	X
6	LDA	L	712	-	-	-	X
6	LDA	L	723	-	-	-	X
6	LDA	L	724	-	-	-	X
6	LDA	M	705	-	-	-	X
6	LDA	M	706	-	-	-	X
6	LDA	M	707	-	-	-	X
6	LDA	M	715	-	-	-	X
6	LDA	M	717	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	DGA	C	730	-	-	-	X
8	SO4	C	338	-	-	-	X
8	SO4	C	340	-	-	-	X
8	SO4	C	343	-	-	-	X
8	SO4	C	346	-	-	-	X
8	SO4	C	347	-	-	-	X
8	SO4	C	351	-	-	-	X
8	SO4	C	354	-	-	-	X
8	SO4	H	261[A]	-	-	-	X
8	SO4	H	261[B]	-	-	X	-
8	SO4	H	263	-	-	-	X
8	SO4	H	264	-	-	-	X
8	SO4	H	266	-	-	-	X
8	SO4	H	267	-	-	-	X
8	SO4	H	268	-	-	-	X
8	SO4	H	269	-	-	-	X
8	SO4	M	326	-	-	X	-
9	HTO	C	355	-	-	X	-
9	HTO	C	356	-	-	-	X
9	HTO	C	357	-	-	-	X
9	HTO	H	273	-	-	-	X
9	HTO	L	276	-	-	-	X
9	HTO	L	279	-	-	-	X
9	HTO	M	333	-	-	-	X

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 12156 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	3	0
			2647	1667	474	486	20			

- Molecule 2 is a protein called Photosynthetic reaction center H-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	258	Total	C	N	O	S	44	4	0
			2035	1300	353	379	3			

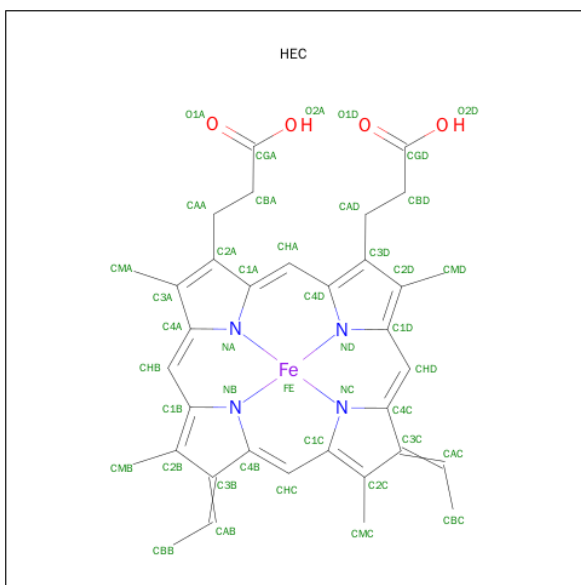
- Molecule 3 is a protein called Photosynthetic reaction center L-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	273	Total	C	N	O	S	0	2	0
			2191	1474	352	358	7			

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

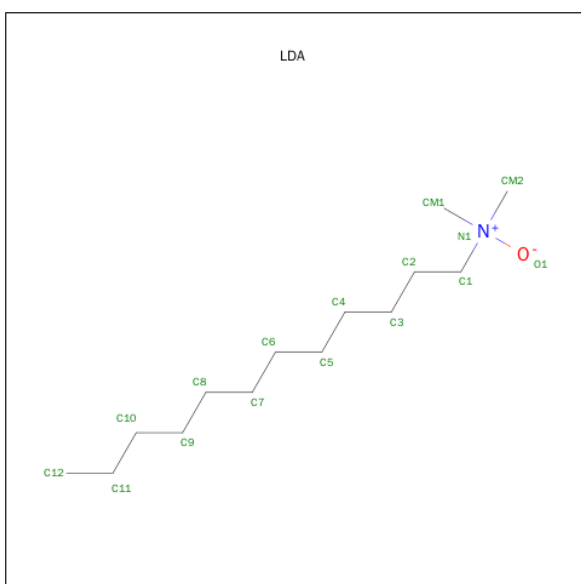
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	323	Total	C	N	O	S	0	2	0
			2574	1716	424	423	11			

- Molecule 5 is HEME C (three-letter code: HEC) (formula: C₃₄H₃₄FeN₄O₄).



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 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 6 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $\text{C}_{14}\text{H}_{31}\text{NO}$).



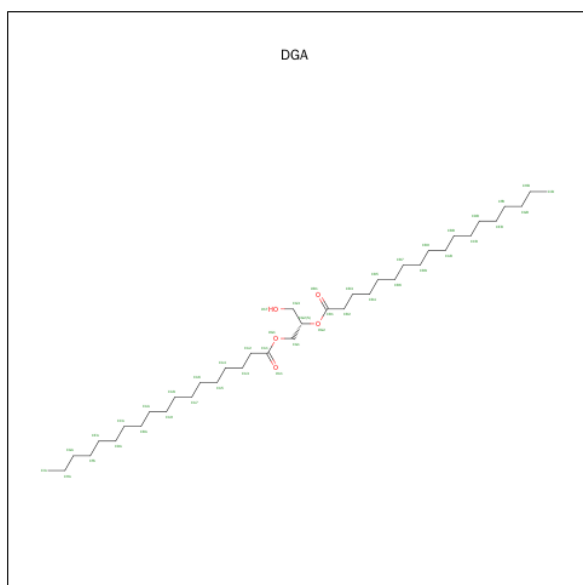
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total 16	C 14	N 1	O 1	0	0
6	C	1	Total 16	C 14	N 1	O 1	0	0
6	H	1	Total 16	C 14	N 1	O 1	0	0
6	H	1	Total 16	C 14	N 1	O 1	0	1
6	H	1	Total 16	C 14	N 1	O 1	0	0
6	H	1	Total 16	C 14	N 1	O 1	0	0
6	H	1	Total 16	C 14	N 1	O 1	0	0
6	L	1	Total 16	C 14	N 1	O 1	0	0
6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

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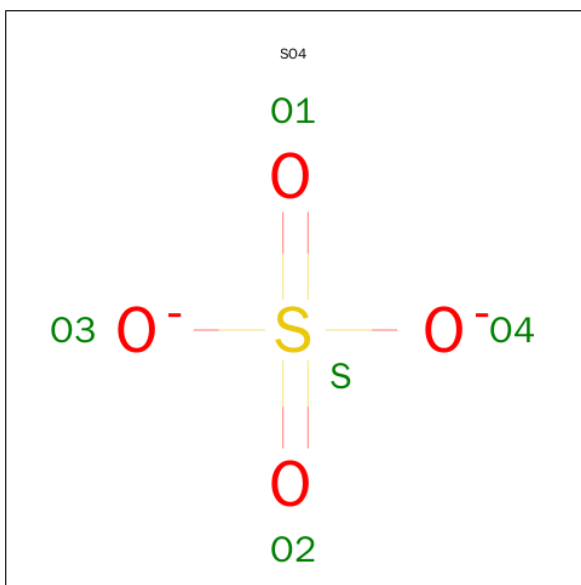
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 7 is DIACYL GLYCEROL (three-letter code: DGA) (formula: $C_{39}H_{76}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			37	33	4		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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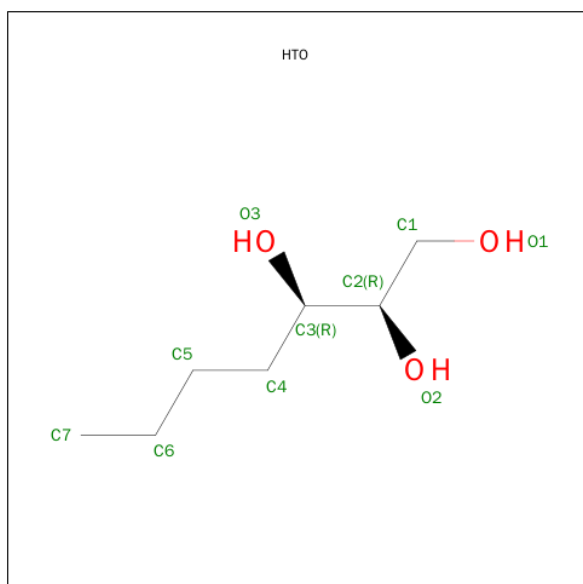
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total	O	S	0	1
			10	8	2		
8	H	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total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

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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		
8	M	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: C₇H₁₆O₃).



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	C	1	Total	C	O	0	0
			10	7	3		
9	C	1	Total	C	O	0	1
			10	7	3		
9	H	1	Total	C	O	0	0
			10	7	3		

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

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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	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	C	1	Total 6	C 3	O 3	0	1
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 8	C 4	O 4	0	1
10	H	1	Total 6	C 3	O 3	0	0
10	H	1	Total 6	C 3	O 3	0	0

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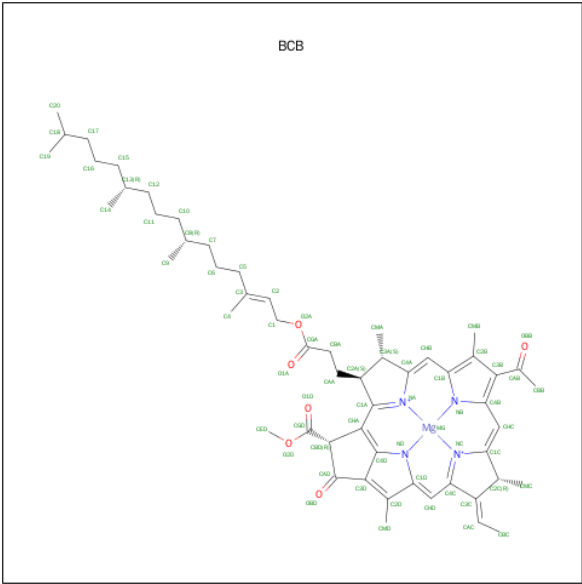
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10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

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

- Molecule 11 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: C₅₅H₇₂MgN₄O₆).



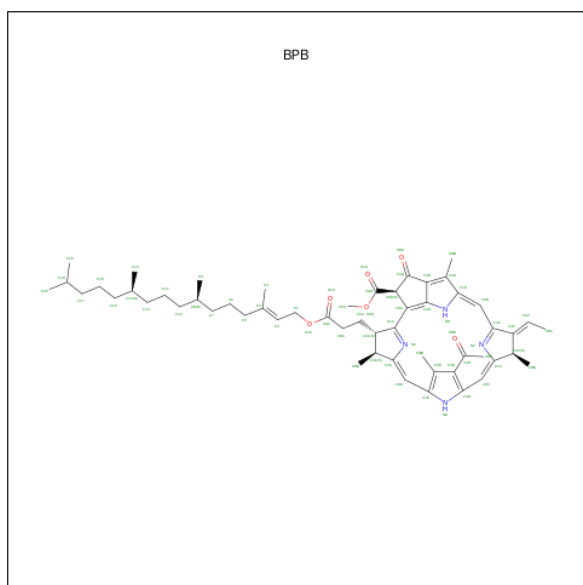
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
11	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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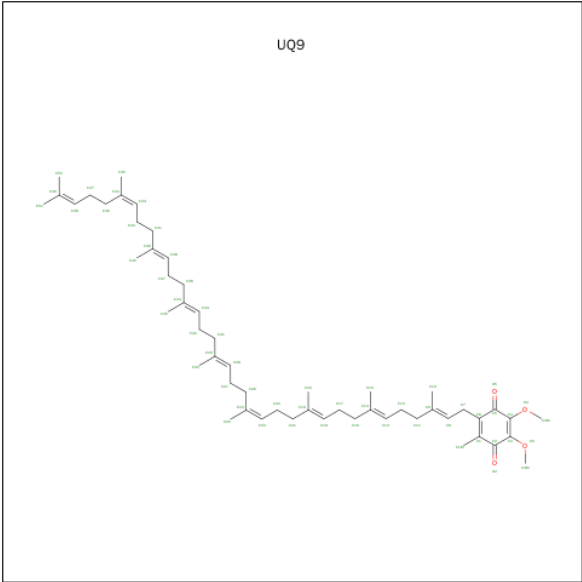
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
11	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 12 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula: C₅₅H₇₄N₄O₆).



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: C₅₄H₈₂O₄).

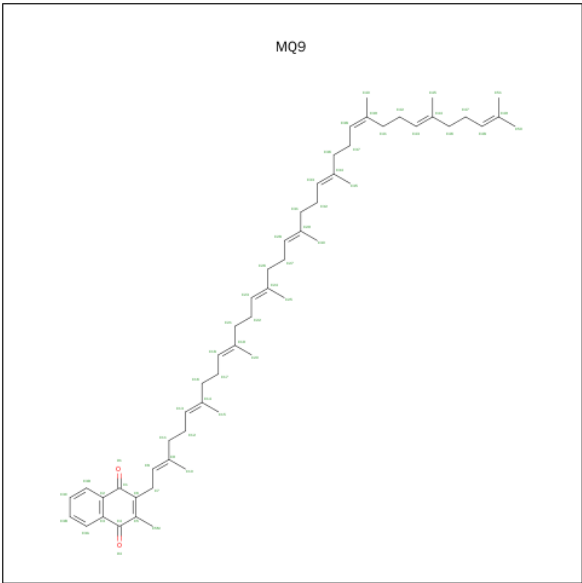


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	L	1	Total	C	O	0	0
			58	54	4		
13	L	1	Total	C	O	0	0
			23	19	4		

- Molecule 14 is FE (II) ION (three-letter code: FE2) (formula: Fe).

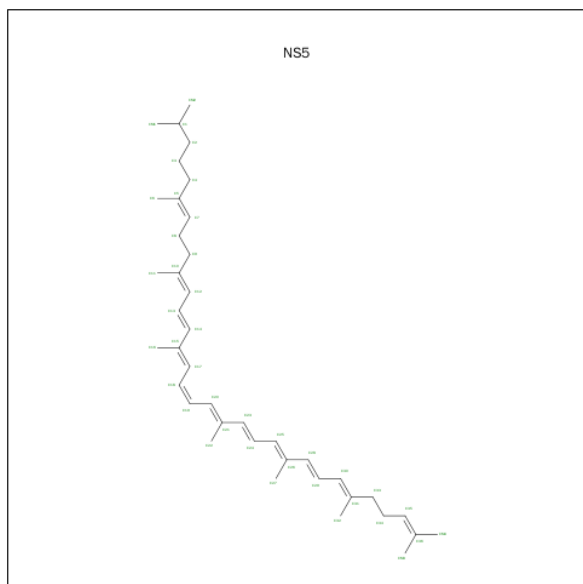
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	M	1	Total	Fe	0	0
			1	1		

- Molecule 15 is MENAQUINONE-9 (three-letter code: MQ9) (formula: C₅₆H₈₀O₂).



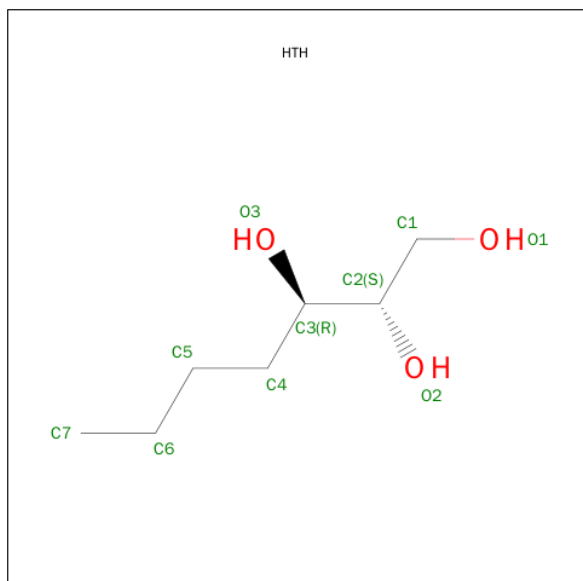
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	M	1	Total	C	O	0	0
			58	56	2		

- 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 (2S,3R)-HEPTANE-1,2,3-TRIOL (three-letter code: HTH) (formula: $C_7H_{16}O_3$).



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

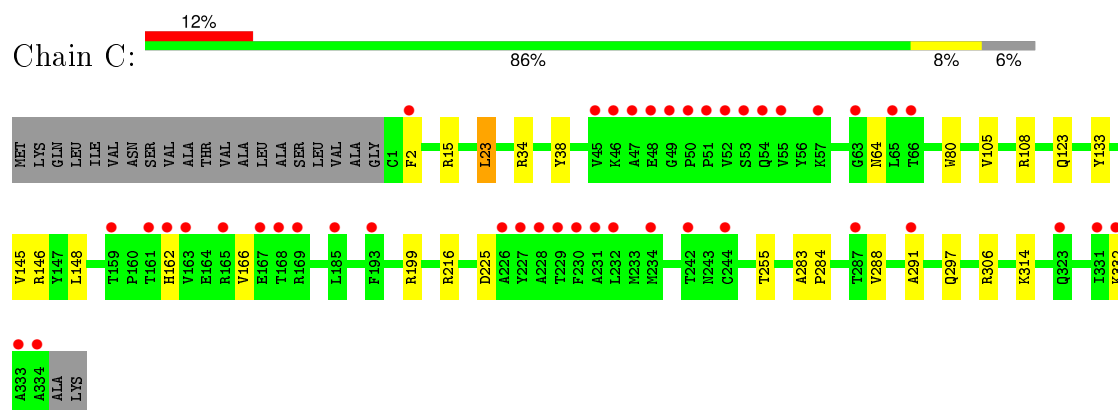
- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	C	388	Total	O	0	0
			388	388		
18	H	211	Total	O	0	0
			211	211		
18	L	109	Total	O	0	0
			109	109		
18	M	153	Total	O	0	0
			153	153		

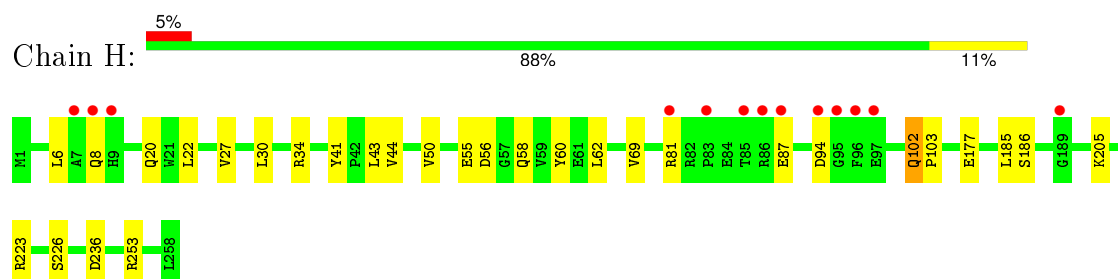
3 Residue-property plots [i](#)

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.

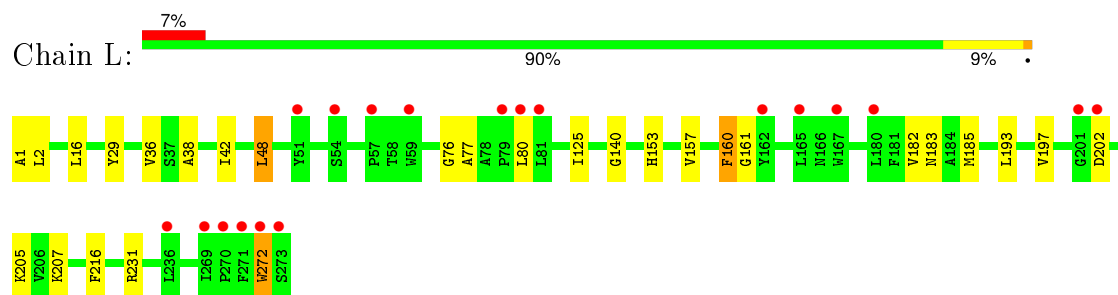
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



- Molecule 2: Photosynthetic reaction center H-subunit

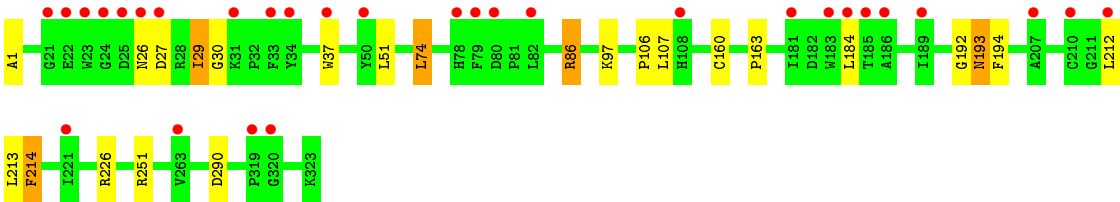


- Molecule 3: Photosynthetic reaction center L-subunit



- 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, α , β , γ	220.44Å 220.44Å 113.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.34 – 1.95 48.34 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.2 (48.34-1.95) 96.2 (48.34-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.6.0101	Depositor
R, R_{free}	0.182 , 0.216 0.192 , 0.224	Depositor DCC
R_{free} test set	9677 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	39.5	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 75.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 193178 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12156	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, LDA, BPB, HTO, BCB, HTH, 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	0.91	0/2716	0.82	3/3701 (0.1%)
2	H	0.91	2/2069 (0.1%)	0.84	0/2827
3	L	0.94	0/2280	0.81	2/3113 (0.1%)
4	M	0.94	1/2679 (0.0%)	0.79	2/3662 (0.1%)
All	All	0.93	3/9744 (0.0%)	0.81	7/13303 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	177	GLU	CD-OE1	5.52	1.31	1.25
2	H	27	VAL	CB-CG2	5.43	1.64	1.52
4	M	160	CYS	CB-SG	-5.19	1.73	1.81

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	251	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	C	23	LEU	CA-CB-CG	5.82	128.69	115.30
3	L	160	PHE	CB-CG-CD1	5.55	124.69	120.80
4	M	86	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	C	15	ARG	NE-CZ-NH1	5.24	122.92	120.30
3	L	48	LEU	CA-CB-CG	5.21	127.29	115.30
1	C	306	ARG	NE-CZ-NH2	-5.19	117.71	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2647	0	2610	33	0
2	H	2035	0	2017	19	0
3	L	2191	0	2116	22	0
4	M	2574	0	2470	28	0
5	C	172	0	120	4	0
6	C	32	0	62	7	0
6	H	80	0	155	9	0
6	L	144	0	279	19	0
6	M	128	0	248	12	0
7	C	37	0	58	3	0
8	C	95	0	0	3	0
8	H	70	0	0	5	0
8	L	10	0	0	0	0
8	M	40	0	0	2	0
9	C	40	0	64	8	0
9	H	30	0	48	5	0
9	L	50	0	80	3	0
9	M	10	0	16	2	0
10	C	120	0	160	15	0
10	H	104	0	135	10	0
10	L	48	0	64	1	0
10	M	54	0	72	6	0
11	L	132	0	144	9	0
11	M	132	0	144	17	0
12	L	65	0	74	2	0
12	M	65	0	74	1	0
13	L	81	0	105	16	0
14	M	1	0	0	0	0
15	M	58	0	80	2	0
16	M	40	0	60	3	0
17	M	10	0	16	0	0
18	C	388	0	0	4	0
18	H	211	0	0	4	0
18	L	109	0	0	0	0
18	M	153	0	0	1	0
All	All	12156	0	11471	178	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 (178) 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)
6:H:720:LDA:H72	6:H:720:LDA:C3	1.43	1.34
6:H:720:LDA:H32	6:H:720:LDA:C7	1.62	1.27
13:L:502:UQ9:H15A	11:M:400:BCB:C9	1.75	1.15
9:M:333:HTO:O3	9:M:333:HTO:H72	1.50	1.10
13:L:502:UQ9:H15A	11:M:400:BCB:H93	1.46	0.98
8:H:261[B]:SO4:O3	6:L:702:LDA:O1	1.81	0.96
13:L:502:UQ9:H15A	11:M:400:BCB:H91	1.49	0.94
11:M:400:BCB:HMB1	11:M:400:BCB:HBB2	1.50	0.91
9:M:333:HTO:O3	9:M:333:HTO:C7	2.23	0.85
6:C:716:LDA:H51	10:H:280:GOL:O1	1.75	0.85
3:L:272:TRP:CD1	4:M:86:ARG:HD3	2.13	0.83
6:H:720:LDA:C7	6:H:720:LDA:C3	2.21	0.81
8:H:261[B]:SO4:O3	6:L:702:LDA:HM23	1.82	0.79
4:M:29:ILE:CD1	4:M:51:LEU:HD13	2.14	0.77
1:C:199[B]:ARG:HH12	10:C:369:GOL:H12	1.48	0.77
10:C:364:GOL:H11	6:M:715:LDA:HM11	1.68	0.76
1:C:34:ARG:HD3	9:C:357:HTO:H3	1.65	0.75
8:H:261[B]:SO4:O3	6:L:702:LDA:CM2	2.34	0.75
4:M:29:ILE:HD11	4:M:51:LEU:HD13	1.70	0.74
1:C:297:GLN:HE22	10:C:365:GOL:H31	1.53	0.73
1:C:255:THR:HG23	10:C:363:GOL:H32	1.72	0.72
1:C:64[A]:ASN:HD21	9:C:355:HTO:C2	2.03	0.71
2:H:226:SER:HB3	9:H:272:HTO:H42	1.72	0.71
2:H:223[A]:ARG:HG3	10:H:283:GOL:O2	1.92	0.70
11:M:400:BCB:HMB1	11:M:400:BCB:CBB	2.22	0.69
6:C:722:LDA:H32	6:C:722:LDA:HM21	1.72	0.69
6:H:720:LDA:C7	6:H:720:LDA:H31	2.22	0.67
6:L:703:LDA:H32	6:L:703:LDA:HM21	1.76	0.67
11:L:400:BCB:HBB3	11:L:400:BCB:HMB1	1.78	0.66
1:C:148:LEU:HD13	10:C:365:GOL:H12	1.78	0.66
13:L:502:UQ9:C15	11:M:400:BCB:H91	2.26	0.65
4:M:29:ILE:HD12	4:M:51:LEU:HD22	1.78	0.65
6:C:722:LDA:C3	6:C:722:LDA:CM2	2.74	0.64
3:L:231:ARG:HG2	6:L:723:LDA:HM23	1.80	0.63
4:M:97:LYS:NZ	18:M:418:HOH:O	2.31	0.63
1:C:332:LYS:H	9:C:355:HTO:H71	1.63	0.63
10:C:364:GOL:C1	6:M:715:LDA:HM11	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:253:ARG:HE	10:H:278:GOL:H31	1.64	0.62
1:C:291:ALA:HB3	10:C:377:GOL:C3	2.29	0.62
8:H:261[B]:SO4:O3	6:L:702:LDA:N1	2.33	0.62
11:M:401:BCB:HMB1	11:M:401:BCB:HBB3	1.80	0.62
1:C:199[B]:ARG:NH1	10:C:369:GOL:H12	2.13	0.62
6:C:722:LDA:H32	6:C:722:LDA:CM2	2.30	0.62
13:L:503:UQ9:O5	13:L:503:UQ9:H4MA	2.01	0.61
6:H:720:LDA:H32	6:H:720:LDA:H72	0.67	0.61
1:C:199[A]:ARG:NH1	18:C:783:HOH:O	2.29	0.61
13:L:502:UQ9:C15	11:M:400:BCB:H93	2.27	0.61
6:L:710:LDA:H32	9:L:277:HTO:H73	1.83	0.59
2:H:253:ARG:HE	10:H:278:GOL:C3	2.16	0.59
13:L:503:UQ9:H8	13:L:503:UQ9:O5	2.03	0.59
4:M:30:GLY:HA3	10:M:342:GOL:H12	1.85	0.58
3:L:36:VAL:HG12	9:L:279:HTO:H3	1.85	0.58
12:L:402:BPB:HMB	12:L:402:BPB:HBBB	1.86	0.58
11:L:401:BCB:HMB1	11:L:401:BCB:CBB	2.34	0.57
1:C:291:ALA:HB3	10:C:377:GOL:H31	1.86	0.57
1:C:199[A]:ARG:NE	18:C:783:HOH:O	2.37	0.57
6:C:722:LDA:C3	6:C:722:LDA:HM21	2.31	0.57
11:M:401:BCB:CBB	11:M:401:BCB:HMB1	2.34	0.57
11:L:400:BCB:H193	15:M:501:MQ9:H252	1.87	0.57
5:C:401:HEC:HMB1	5:C:401:HEC:HBB3	1.87	0.57
4:M:74:LEU:CD1	16:M:600:NS5:HM23	2.36	0.56
4:M:1:ALA:N	8:M:326:SO4:O3	2.31	0.56
6:L:703:LDA:C3	6:L:703:LDA:HM21	2.33	0.56
2:H:205:LYS:O	10:H:279:GOL:O1	2.23	0.55
5:C:403:HEC:HBB3	5:C:403:HEC:HMB1	1.88	0.55
10:H:283:GOL:C1	18:H:537:HOH:O	2.55	0.55
3:L:140:GLY:HA3	6:L:712:LDA:HM13	1.88	0.55
3:L:38:ALA:O	3:L:42:ILE:HG13	2.07	0.54
4:M:37:TRP:HD1	6:M:704:LDA:CM1	2.21	0.54
1:C:123:GLN:HE21	10:M:338:GOL:H11	1.72	0.54
2:H:81[A]:ARG:HH11	2:H:81[A]:ARG:HG3	1.72	0.54
3:L:76:GLY:HA3	6:L:711:LDA:HM13	1.89	0.54
4:M:37:TRP:CD1	6:M:704:LDA:HM12	2.44	0.53
2:H:6:LEU:HD23	9:H:274[A]:HTO:H2	1.90	0.53
7:C:730:DGA:HB22	7:C:730:DGA:HA22	1.91	0.53
2:H:43:LEU:HB3	3:L:1:ALA:HB1	1.90	0.53
13:L:502:UQ9:C15	11:M:400:BCB:C9	2.67	0.53
1:C:123:GLN:HE21	10:M:338:GOL:H31	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:62:LEU:O	6:H:721:LDA:HM21	2.08	0.52
1:C:162:HIS:HB2	10:C:368:GOL:H2	1.92	0.52
1:C:291:ALA:N	10:C:377:GOL:H32	2.25	0.52
3:L:272:TRP:CG	4:M:86:ARG:HD3	2.45	0.52
3:L:193:LEU:HD22	3:L:216:PHE:CE2	2.44	0.52
4:M:37:TRP:HD1	6:M:704:LDA:HM12	1.75	0.51
1:C:283:ALA:HB3	1:C:284:PRO:HD3	1.92	0.51
1:C:225:ASP:OD1	10:C:369:GOL:O3	2.29	0.51
3:L:231:ARG:CG	6:L:723:LDA:HM23	2.40	0.50
11:L:400:BCB:CBB	11:L:400:BCB:HMB1	2.41	0.50
13:L:503:UQ9:O4	13:L:503:UQ9:H3MB	2.11	0.50
4:M:212:LEU:C	4:M:212:LEU:HD23	2.32	0.50
4:M:37:TRP:H	6:M:704:LDA:HM13	1.77	0.50
8:C:340:SO4:O3	8:C:354:SO4:O1	2.29	0.50
6:H:719:LDA:C9	6:H:720:LDA:H122	2.41	0.50
1:C:145:VAL:O	1:C:146:ARG:HD2	2.11	0.50
11:L:400:BCB:OBB	11:L:400:BCB:HHC	2.11	0.49
1:C:291:ALA:HB3	10:C:377:GOL:H32	1.95	0.49
9:H:273:HTO:C1	18:H:499:HOH:O	2.60	0.49
1:C:64[A]:ASN:ND2	9:C:355:HTO:H3	2.27	0.49
3:L:193:LEU:HD22	3:L:216:PHE:HE2	1.77	0.49
13:L:503:UQ9:C8	13:L:503:UQ9:O5	2.60	0.49
13:L:502:UQ9:H3MB	13:L:502:UQ9:O2	2.13	0.49
4:M:192:GLY:O	4:M:193:ASN:HB3	2.13	0.49
1:C:105:VAL:CG2	1:C:288:VAL:HG11	2.43	0.48
8:C:338:SO4:O4	10:M:334:GOL:O1	2.21	0.48
9:H:273:HTO:H12	18:H:499:HOH:O	2.12	0.48
7:C:730:DGA:HB62	7:C:730:DGA:HA52	1.94	0.48
2:H:223[B]:ARG:HG3	10:H:283:GOL:O2	2.14	0.47
2:H:69:VAL:HG22	3:L:205:LYS:HA	1.94	0.47
1:C:64[A]:ASN:HD21	9:C:355:HTO:C3	2.27	0.47
11:L:401:BCB:HMB1	11:L:401:BCB:HBB2	1.96	0.47
1:C:123:GLN:NE2	10:M:338:GOL:H31	2.29	0.47
3:L:161:GLY:HA3	11:L:400:BCB:HAC1	1.96	0.47
10:H:283:GOL:H11	18:H:537:HOH:O	2.14	0.47
4:M:29:ILE:HD12	4:M:51:LEU:HD13	1.96	0.46
4:M:74:LEU:HD12	16:M:600:NS5:CM2	2.45	0.46
1:C:199[A]:ARG:CZ	18:C:783:HOH:O	2.62	0.46
2:H:41:TYR:OH	8:H:261[A]:SO4:O3	2.25	0.46
2:H:223[A]:ARG:CG	10:H:283:GOL:O2	2.61	0.46
4:M:226:ARG:NH1	8:M:326:SO4:O1	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:272:TRP:CD1	4:M:86:ARG:CD	2.93	0.46
6:L:703:LDA:CM2	6:L:703:LDA:C3	2.94	0.46
1:C:108:ARG:HD2	18:C:780:HOH:O	2.15	0.46
4:M:106:PRO:HB3	6:M:714:LDA:H31	1.98	0.46
3:L:125:ILE:HG21	6:L:724:LDA:HM22	1.97	0.46
1:C:64[A]:ASN:HD21	9:C:355:HTO:H3	1.80	0.46
4:M:184:LEU:HD21	11:M:400:BCB:CAC	2.47	0.45
9:H:273:HTO:H52	9:H:273:HTO:H2	1.69	0.45
11:M:401:BCB:HAA2	11:M:401:BCB:HBD	1.98	0.45
2:H:81[A]:ARG:NH1	2:H:81[A]:ARG:HG3	2.32	0.45
12:M:402:BPB:HBBB	12:M:402:BPB:HMB	1.98	0.45
6:C:716:LDA:HM21	10:C:364:GOL:O3	2.17	0.45
4:M:107:LEU:H	6:M:714:LDA:H32	1.82	0.45
13:L:502:UQ9:O3	13:L:502:UQ9:H4MB	2.16	0.44
11:M:401:BCB:HAA2	11:M:401:BCB:CBD	2.42	0.44
13:L:502:UQ9:C51	11:M:400:BCB:H191	2.47	0.44
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.52	0.44
1:C:2[B]:PHE:O	8:C:351:SO4:O2	2.36	0.44
3:L:182:VAL:HA	11:M:400:BCB:H43	2.00	0.44
4:M:74:LEU:HD12	16:M:600:NS5:HM23	1.99	0.44
7:C:730:DGA:CA2	7:C:730:DGA:HB22	2.47	0.44
6:H:719:LDA:H91	6:H:720:LDA:H122	2.00	0.44
13:L:503:UQ9:C4M	13:L:503:UQ9:O5	2.65	0.44
6:L:723:LDA:H22	6:L:723:LDA:HM21	1.45	0.43
12:L:402:BPB:CBB	12:L:402:BPB:HMB	2.48	0.43
6:L:702:LDA:H22	6:L:702:LDA:H52	1.83	0.43
4:M:37:TRP:CD1	6:M:704:LDA:CM1	3.01	0.43
2:H:30:LEU:O	2:H:34:ARG:HD2	2.18	0.43
3:L:29:TYR:OH	6:L:702:LDA:H12	2.19	0.43
3:L:153:HIS:O	3:L:157:VAL:HG23	2.18	0.43
6:L:703:LDA:H21	6:L:703:LDA:HM11	1.60	0.43
4:M:212:LEU:O	4:M:212:LEU:HD23	2.17	0.43
3:L:77:ALA:HB1	9:L:277:HTO:O3	2.18	0.43
4:M:37:TRP:H	6:M:704:LDA:CM1	2.32	0.42
2:H:102:GLN:HA	2:H:103:PRO:HD3	1.94	0.42
1:C:314:LYS:HZ2	10:C:373:GOL:H2	1.84	0.42
15:M:501:MQ9:H33	15:M:501:MQ9:C38	2.49	0.42
11:M:401:BCB:HHC	11:M:401:BCB:OBB	2.20	0.42
11:L:401:BCB:HHC	11:L:401:BCB:OBB	2.20	0.42
1:C:146:ARG:HD2	1:C:146:ARG:HA	1.80	0.42
9:C:357:HTO:H73	10:L:286:GOL:O1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:223[B]:ARG:CG	10:H:283:GOL:O2	2.66	0.42
5:C:403:HEC:HBC3	5:C:403:HEC:HMC1	2.02	0.42
6:L:723:LDA:H52	6:L:723:LDA:H81	1.82	0.41
3:L:125:ILE:CG2	6:L:724:LDA:HM22	2.51	0.41
1:C:64[A]:ASN:HD21	9:C:355:HTO:C1	2.33	0.41
2:H:55:GLU:H	2:H:58:GLN:HE21	1.67	0.41
11:L:401:BCB:O1A	11:L:401:BCB:H43	2.21	0.41
6:M:706:LDA:H32	6:M:706:LDA:H62	1.75	0.41
1:C:216:ARG:HG3	6:C:716:LDA:HM22	2.02	0.41
3:L:197:VAL:HG13	3:L:207:LYS:HB2	2.02	0.41
6:H:719:LDA:H92	6:H:720:LDA:H122	2.04	0.40
2:H:56:ASP:HB3	2:H:60:TYR:CE2	2.56	0.40
13:L:502:UQ9:H32	13:L:502:UQ9:H35	1.95	0.40
5:C:403:HEC:HBC1	5:C:404:HEC:HMA1	2.03	0.40
3:L:183:ASN:HD21	4:M:214:PHE:HB3	1.85	0.40
6:M:707:LDA:H21	6:M:707:LDA:HM13	1.81	0.40
13:L:502:UQ9:H51A	11:M:400:BCB:H191	2.04	0.40
4:M:26:ASN:H	10:M:336:GOL:HO3	1.68	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	335/356 (94%)	326 (97%)	9 (3%)	0	100	100
2	H	259/258 (100%)	247 (95%)	11 (4%)	1 (0%)	39	27
3	L	273/273 (100%)	268 (98%)	5 (2%)	0	100	100
4	M	323/323 (100%)	315 (98%)	7 (2%)	1 (0%)	46	35
All	All	1190/1210 (98%)	1156 (97%)	32 (3%)	2 (0%)	52	43

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	286/299 (96%)	283 (99%)	3 (1%)	82	80
2	H	209/211 (99%)	199 (95%)	10 (5%)	31	15
3	L	220/218 (101%)	212 (96%)	8 (4%)	42	28
4	M	249/247 (101%)	241 (97%)	8 (3%)	46	33
All	All	964/975 (99%)	935 (97%)	29 (3%)	48	36

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	23	LEU
1	C	38	TYR
1	C	166	VAL
2	H	8	GLN
2	H	20	GLN
2	H	22	LEU
2	H	44	VAL
2	H	87	GLU
2	H	94	ASP
2	H	102	GLN
2	H	185	LEU
2	H	186	SER
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	185	MET
3	L	202	ASP

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Mol	Chain	Res	Type
3	L	272	TRP
4	M	27	ASP
4	M	29	ILE
4	M	74	LEU
4	M	163	PRO
4	M	194	PHE
4	M	213	LEU
4	M	214	PHE
4	M	290	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	297	GLN
1	C	302	GLN
2	H	58	GLN
2	H	102	GLN
2	H	220	ASN
3	L	183	ASN
3	L	213	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 ⓘ

2 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]	-	8,9,10	1.17	1 (12%)	6,9,11	3.27	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FME	H	1[B]	-	8,9,10	0.90	0	6,9,11	3.33	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[A]	-	-	0/6/9/11	0/0/0/0
2	FME	H	1[B]	-	-	0/6/9/11	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1[A]	FME	CA-N	2.17	1.49	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1[B]	FME	CA-N-CN	-7.48	111.32	122.82
2	H	1[A]	FME	CA-N-CN	-7.16	111.81	122.82
2	H	1[B]	FME	O1-CN-N	-2.56	121.08	124.76
2	H	1[A]	FME	CE-SD-CG	2.28	108.14	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 152 ligands modelled in this entry, 1 is monoatomic - leaving 151 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[A]	-	4,4,4	0.36	0	6,6,6	0.14	0
8	SO4	C	337[B]	-	4,4,4	0.54	0	6,6,6	0.14	0
8	SO4	C	338	-	4,4,4	0.64	0	6,6,6	0.36	0
8	SO4	C	339	-	4,4,4	0.37	0	6,6,6	0.47	0
8	SO4	C	340	-	4,4,4	0.51	0	6,6,6	0.84	0
8	SO4	C	341	-	4,4,4	0.48	0	6,6,6	0.47	0
8	SO4	C	342	-	4,4,4	0.58	0	6,6,6	0.25	0
8	SO4	C	343	-	4,4,4	0.40	0	6,6,6	0.91	0
8	SO4	C	344	-	4,4,4	0.55	0	6,6,6	0.14	0
8	SO4	C	345	-	4,4,4	0.32	0	6,6,6	0.21	0
8	SO4	C	346	-	4,4,4	0.54	0	6,6,6	0.31	0
8	SO4	C	347	-	4,4,4	0.68	0	6,6,6	0.25	0
8	SO4	C	348	-	4,4,4	0.48	0	6,6,6	0.34	0
8	SO4	C	349	-	4,4,4	0.56	0	6,6,6	0.26	0
8	SO4	C	350	-	4,4,4	0.44	0	6,6,6	0.19	0
8	SO4	C	351	-	4,4,4	0.40	0	6,6,6	0.22	0
8	SO4	C	352	-	4,4,4	0.36	0	6,6,6	0.17	0
8	SO4	C	353	-	4,4,4	0.56	0	6,6,6	0.20	0
8	SO4	C	354	-	4,4,4	0.35	0	6,6,6	0.35	0
9	HTO	C	355	-	9,9,9	0.52	0	8,10,10	1.47	1 (12%)
9	HTO	C	356	-	9,9,9	0.70	0	8,10,10	1.98	1 (12%)
9	HTO	C	357	-	9,9,9	0.55	0	8,10,10	0.84	0
9	HTO	C	358[A]	-	9,9,9	0.69	0	8,10,10	2.85	4 (50%)
10	GOL	C	359	-	5,5,5	0.80	0	5,5,5	0.85	0
10	GOL	C	360	-	5,5,5	0.24	0	5,5,5	0.59	0
10	GOL	C	361	-	5,5,5	0.65	0	5,5,5	1.01	0
10	GOL	C	362	-	5,5,5	0.67	0	5,5,5	0.84	0
10	GOL	C	363	-	5,5,5	0.76	0	5,5,5	1.07	0
10	GOL	C	364	-	5,5,5	0.58	0	5,5,5	0.93	0
10	GOL	C	365	-	5,5,5	0.31	0	5,5,5	0.36	0
10	GOL	C	366	-	5,5,5	0.44	0	5,5,5	0.40	0
10	GOL	C	367	-	5,5,5	0.26	0	5,5,5	1.05	0
10	GOL	C	368	-	5,5,5	0.14	0	5,5,5	0.67	0
10	GOL	C	369	-	5,5,5	0.38	0	5,5,5	0.61	0
10	GOL	C	370	-	5,5,5	0.24	0	5,5,5	0.21	0
10	GOL	C	371	-	5,5,5	0.30	0	5,5,5	0.75	0
10	GOL	C	372	-	5,5,5	0.29	0	5,5,5	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	GOL	C	373	-	5,5,5	0.30	0	5,5,5	0.26	0
10	GOL	C	374[B]	-	5,5,5	0.30	0	5,5,5	0.38	0
10	GOL	C	375	-	5,5,5	0.24	0	5,5,5	0.18	0
10	GOL	C	376	-	5,5,5	0.28	0	5,5,5	0.29	0
10	GOL	C	377	-	5,5,5	0.14	0	5,5,5	0.32	0
10	GOL	C	378	-	5,5,5	0.28	0	5,5,5	0.18	0
5	HEC	C	401	1	24,50,50	1.13	1 (4%)	19,82,82	3.18	8 (42%)
5	HEC	C	402	1	24,50,50	0.82	0	19,82,82	2.46	5 (26%)
5	HEC	C	403	1	24,50,50	1.03	2 (8%)	19,82,82	2.23	4 (21%)
5	HEC	C	404	1	24,50,50	1.00	0	19,82,82	2.27	4 (21%)
6	LDA	C	716	-	15,15,15	3.65	1 (6%)	16,17,17	0.83	1 (6%)
6	LDA	C	722	-	15,15,15	3.68	2 (13%)	16,17,17	0.67	0
7	DGA	C	730	1	36,36,43	0.83	2 (5%)	38,38,45	1.49	5 (13%)
8	SO4	H	259	-	4,4,4	0.37	0	6,6,6	0.46	0
8	SO4	H	260	-	4,4,4	0.65	0	6,6,6	0.24	0
8	SO4	H	261[A]	-	4,4,4	0.45	0	6,6,6	0.25	0
8	SO4	H	261[B]	-	4,4,4	0.62	0	6,6,6	0.31	0
8	SO4	H	262	-	4,4,4	0.41	0	6,6,6	0.52	0
8	SO4	H	263	-	4,4,4	0.49	0	6,6,6	0.36	0
8	SO4	H	264	-	4,4,4	0.49	0	6,6,6	0.12	0
8	SO4	H	265	-	4,4,4	0.54	0	6,6,6	0.42	0
8	SO4	H	266	-	4,4,4	0.44	0	6,6,6	0.27	0
8	SO4	H	267	-	4,4,4	0.25	0	6,6,6	0.21	0
8	SO4	H	268	-	4,4,4	0.31	0	6,6,6	0.13	0
8	SO4	H	269	-	4,4,4	0.46	0	6,6,6	0.27	0
8	SO4	H	270	-	4,4,4	0.37	0	6,6,6	0.21	0
8	SO4	H	271	-	4,4,4	0.40	0	6,6,6	0.11	0
9	HTO	H	272	-	9,9,9	0.70	0	8,10,10	1.70	3 (37%)
9	HTO	H	273	-	9,9,9	0.41	0	8,10,10	1.10	1 (12%)
9	HTO	H	274[A]	-	9,9,9	0.31	0	8,10,10	0.79	0
10	GOL	H	275	-	5,5,5	0.63	0	5,5,5	0.42	0
10	GOL	H	276[A]	-	5,5,5	0.79	0	5,5,5	0.63	0
10	GOL	H	276[B]	-	5,5,5	0.79	0	5,5,5	0.94	0
10	GOL	H	277	-	5,5,5	0.35	0	5,5,5	0.51	0
10	GOL	H	278	-	5,5,5	0.42	0	5,5,5	0.77	0
10	GOL	H	279	-	5,5,5	0.33	0	5,5,5	0.52	0
10	GOL	H	280	-	5,5,5	0.71	0	5,5,5	1.09	1 (20%)
10	GOL	H	281	-	5,5,5	0.51	0	5,5,5	0.38	0
10	GOL	H	282	-	5,5,5	0.33	0	5,5,5	0.24	0
10	GOL	H	283	-	5,5,5	0.26	0	5,5,5	0.91	0
10	GOL	H	284	-	5,5,5	0.36	0	5,5,5	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	GOL	H	285	-	5,5,5	0.17	0	5,5,5	0.53	0
10	GOL	H	286	-	5,5,5	0.27	0	5,5,5	0.54	0
10	GOL	H	287	-	5,5,5	0.28	0	5,5,5	0.09	0
10	GOL	H	288	-	5,5,5	0.34	0	5,5,5	0.35	0
10	GOL	H	289	-	5,5,5	0.29	0	5,5,5	0.21	0
10	GOL	H	290	-	5,5,5	0.33	0	5,5,5	0.48	0
10	GOL	H	291	-	5,5,5	0.34	0	5,5,5	0.40	0
6	LDA	H	701	-	15,15,15	2.70	1 (6%)	16,17,17	1.39	3 (18%)
6	LDA	H	718[B]	-	15,15,15	3.71	1 (6%)	16,17,17	0.61	0
6	LDA	H	719	-	15,15,15	3.70	1 (6%)	16,17,17	0.50	0
6	LDA	H	720	-	15,15,15	4.22	2 (13%)	16,17,17	1.34	1 (6%)
6	LDA	H	721	-	15,15,15	3.48	2 (13%)	16,17,17	1.08	2 (12%)
8	SO4	L	274	-	4,4,4	0.35	0	6,6,6	0.28	0
8	SO4	L	275	-	4,4,4	0.29	0	6,6,6	0.18	0
9	HTO	L	276	-	9,9,9	0.45	0	8,10,10	1.60	2 (25%)
9	HTO	L	277	-	9,9,9	0.43	0	8,10,10	1.36	1 (12%)
9	HTO	L	278	-	9,9,9	0.64	0	8,10,10	1.71	3 (37%)
9	HTO	L	279	-	9,9,9	0.37	0	8,10,10	1.37	0
9	HTO	L	280	-	9,9,9	0.41	0	8,10,10	1.06	1 (12%)
10	GOL	L	281	-	5,5,5	0.19	0	5,5,5	0.40	0
10	GOL	L	282	-	5,5,5	0.86	0	5,5,5	1.23	1 (20%)
10	GOL	L	283	-	5,5,5	0.48	0	5,5,5	0.50	0
10	GOL	L	284	-	5,5,5	0.32	0	5,5,5	0.50	0
10	GOL	L	285	-	5,5,5	0.50	0	5,5,5	0.74	0
10	GOL	L	286	-	5,5,5	0.28	0	5,5,5	0.74	0
10	GOL	L	287	-	5,5,5	0.30	0	5,5,5	0.58	0
10	GOL	L	288	-	5,5,5	0.19	0	5,5,5	0.58	0
11	BCB	L	400	3	56,74,74	1.22	3 (5%)	57,115,115	1.93	14 (24%)
11	BCB	L	401	3	56,74,74	1.46	6 (10%)	57,115,115	1.82	13 (22%)
12	BPB	L	402	-	63,70,70	0.89	1 (1%)	63,101,101	1.43	11 (17%)
13	UQ9	L	502	-	58,58,58	2.43	24 (41%)	70,73,73	1.62	15 (21%)
13	UQ9	L	503	-	23,23,58	2.22	8 (34%)	28,31,73	1.41	2 (7%)
6	LDA	L	702	-	15,15,15	3.85	2 (13%)	16,17,17	1.01	1 (6%)
6	LDA	L	703	-	15,15,15	4.01	2 (13%)	16,17,17	0.77	0
6	LDA	L	708	-	15,15,15	3.61	1 (6%)	16,17,17	2.07	3 (18%)
6	LDA	L	709	-	15,15,15	3.60	1 (6%)	16,17,17	0.57	0
6	LDA	L	710	-	15,15,15	3.90	1 (6%)	16,17,17	0.63	0
6	LDA	L	711	-	15,15,15	3.84	1 (6%)	16,17,17	0.78	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	LDA	L	712	-	15,15,15	3.89	1 (6%)	16,17,17	0.62	0
6	LDA	L	723	-	15,15,15	3.85	2 (13%)	16,17,17	0.84	0
6	LDA	L	724	-	15,15,15	4.18	3 (20%)	16,17,17	0.93	2 (12%)
8	SO4	M	324	-	4,4,4	0.67	0	6,6,6	0.61	0
8	SO4	M	325	-	4,4,4	0.31	0	6,6,6	0.36	0
8	SO4	M	326	-	4,4,4	0.26	0	6,6,6	0.34	0
8	SO4	M	327	-	4,4,4	0.45	0	6,6,6	0.17	0
8	SO4	M	328	-	4,4,4	0.34	0	6,6,6	0.22	0
8	SO4	M	329	-	4,4,4	0.31	0	6,6,6	0.23	0
8	SO4	M	330	-	4,4,4	0.47	0	6,6,6	0.31	0
8	SO4	M	331	-	4,4,4	0.43	0	6,6,6	0.20	0
17	HTH	M	332	-	9,9,9	0.41	0	8,10,10	1.24	1 (12%)
9	HTO	M	333	-	9,9,9	0.44	0	8,10,10	2.78	4 (50%)
10	GOL	M	334	-	5,5,5	0.19	0	5,5,5	0.23	0
10	GOL	M	335	-	5,5,5	0.42	0	5,5,5	0.35	0
10	GOL	M	336	-	5,5,5	0.22	0	5,5,5	0.97	0
10	GOL	M	337	-	5,5,5	0.31	0	5,5,5	0.30	0
10	GOL	M	338	-	5,5,5	0.37	0	5,5,5	0.45	0
10	GOL	M	339	-	5,5,5	0.21	0	5,5,5	0.28	0
10	GOL	M	340	-	5,5,5	0.45	0	5,5,5	0.55	0
10	GOL	M	341	-	5,5,5	0.34	0	5,5,5	0.24	0
10	GOL	M	342	-	5,5,5	0.40	0	5,5,5	0.63	0
11	BCB	M	400	4	56,74,74	1.27	4 (7%)	57,115,115	1.87	14 (24%)
11	BCB	M	401	4	56,74,74	1.60	4 (7%)	57,115,115	2.36	17 (29%)
12	BPB	M	402	-	63,70,70	1.01	4 (6%)	63,101,101	1.19	6 (9%)
15	MQ9	M	501	-	59,59,59	2.45	25 (42%)	74,75,75	1.29	10 (13%)
16	NS5	M	600	-	39,39,39	1.79	12 (30%)	44,46,46	2.74	15 (34%)
6	LDA	M	704	-	15,15,15	4.62	3 (20%)	16,17,17	1.76	6 (37%)
6	LDA	M	705	-	15,15,15	3.40	1 (6%)	16,17,17	0.75	0
6	LDA	M	706	-	15,15,15	3.56	1 (6%)	16,17,17	0.61	0
6	LDA	M	707	-	15,15,15	4.00	1 (6%)	16,17,17	1.27	2 (12%)
6	LDA	M	713	-	15,15,15	3.67	1 (6%)	16,17,17	0.70	0
6	LDA	M	714	-	15,15,15	4.18	2 (13%)	16,17,17	0.53	0
6	LDA	M	715	-	15,15,15	3.78	1 (6%)	16,17,17	0.66	0
6	LDA	M	717	-	15,15,15	3.60	1 (6%)	16,17,17	0.63	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. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	SO4	C	337[A]	-	-	0/0/0/0	0/0/0/0
8	SO4	C	337[B]	-	-	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
8	SO4	C	348	-	-	0/0/0/0	0/0/0/0
8	SO4	C	349	-	-	0/0/0/0	0/0/0/0
8	SO4	C	350	-	-	0/0/0/0	0/0/0/0
8	SO4	C	351	-	-	0/0/0/0	0/0/0/0
8	SO4	C	352	-	-	0/0/0/0	0/0/0/0
8	SO4	C	353	-	-	0/0/0/0	0/0/0/0
8	SO4	C	354	-	-	0/0/0/0	0/0/0/0
9	HTO	C	355	-	-	0/10/10/10	0/0/0/0
9	HTO	C	356	-	-	0/10/10/10	0/0/0/0
9	HTO	C	357	-	-	0/10/10/10	0/0/0/0
9	HTO	C	358[A]	-	-	0/10/10/10	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
10	GOL	C	366	-	-	0/4/4/4	0/0/0/0
10	GOL	C	367	-	-	0/4/4/4	0/0/0/0
10	GOL	C	368	-	-	0/4/4/4	0/0/0/0
10	GOL	C	369	-	-	0/4/4/4	0/0/0/0
10	GOL	C	370	-	-	0/4/4/4	0/0/0/0
10	GOL	C	371	-	-	0/4/4/4	0/0/0/0
10	GOL	C	372	-	-	0/4/4/4	0/0/0/0
10	GOL	C	373	-	-	0/4/4/4	0/0/0/0
10	GOL	C	374[B]	-	-	0/4/4/4	0/0/0/0
10	GOL	C	375	-	-	0/4/4/4	0/0/0/0
10	GOL	C	376	-	-	0/4/4/4	0/0/0/0
10	GOL	C	377	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	GOL	C	378	-	-	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	1	-	0/6/54/54	0/0/8/8
6	LDA	C	716	-	-	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[A]	-	-	0/0/0/0	0/0/0/0
8	SO4	H	261[B]	-	-	0/0/0/0	0/0/0/0
8	SO4	H	262	-	-	0/0/0/0	0/0/0/0
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
8	SO4	H	266	-	-	0/0/0/0	0/0/0/0
8	SO4	H	267	-	-	0/0/0/0	0/0/0/0
8	SO4	H	268	-	-	0/0/0/0	0/0/0/0
8	SO4	H	269	-	-	0/0/0/0	0/0/0/0
8	SO4	H	270	-	-	0/0/0/0	0/0/0/0
8	SO4	H	271	-	-	0/0/0/0	0/0/0/0
9	HTO	H	272	-	-	0/10/10/10	0/0/0/0
9	HTO	H	273	-	-	0/10/10/10	0/0/0/0
9	HTO	H	274[A]	-	-	0/10/10/10	0/0/0/0
10	GOL	H	275	-	-	0/4/4/4	0/0/0/0
10	GOL	H	276[A]	-	-	0/4/4/4	0/0/0/0
10	GOL	H	276[B]	-	-	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
10	GOL	H	280	-	-	0/4/4/4	0/0/0/0
10	GOL	H	281	-	-	0/4/4/4	0/0/0/0
10	GOL	H	282	-	-	0/4/4/4	0/0/0/0
10	GOL	H	283	-	-	0/4/4/4	0/0/0/0
10	GOL	H	284	-	-	0/4/4/4	0/0/0/0
10	GOL	H	285	-	-	0/4/4/4	0/0/0/0
10	GOL	H	286	-	-	0/4/4/4	0/0/0/0
10	GOL	H	287	-	-	0/4/4/4	0/0/0/0
10	GOL	H	288	-	-	0/4/4/4	0/0/0/0
10	GOL	H	289	-	-	0/4/4/4	0/0/0/0
10	GOL	H	290	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	GOL	H	291	-	-	0/4/4/4	0/0/0/0
6	LDA	H	701	-	-	0/13/13/13	0/0/0/0
6	LDA	H	718[B]	-	-	0/13/13/13	0/0/0/0
6	LDA	H	719	-	-	0/13/13/13	0/0/0/0
6	LDA	H	720	-	-	0/13/13/13	0/0/0/0
6	LDA	H	721	-	-	0/13/13/13	0/0/0/0
8	SO4	L	274	-	-	0/0/0/0	0/0/0/0
8	SO4	L	275	-	-	0/0/0/0	0/0/0/0
9	HTO	L	276	-	-	0/10/10/10	0/0/0/0
9	HTO	L	277	-	-	0/10/10/10	0/0/0/0
9	HTO	L	278	-	-	0/10/10/10	0/0/0/0
9	HTO	L	279	-	-	0/10/10/10	0/0/0/0
9	HTO	L	280	-	-	0/10/10/10	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
10	GOL	L	283	-	-	0/4/4/4	0/0/0/0
10	GOL	L	284	-	-	0/4/4/4	0/0/0/0
10	GOL	L	285	-	-	0/4/4/4	0/0/0/0
10	GOL	L	286	-	-	0/4/4/4	0/0/0/0
10	GOL	L	287	-	-	0/4/4/4	0/0/0/0
10	GOL	L	288	-	-	0/4/4/4	0/0/0/0
11	BCB	L	400	3	-	0/37/137/137	0/0/9/9
11	BCB	L	401	3	-	0/37/137/137	0/0/9/9
12	BPB	L	402	-	-	0/46/105/105	0/1/6/6
13	UQ9	L	502	-	-	0/57/81/81	0/1/1/1
13	UQ9	L	503	-	-	0/15/39/81	0/1/1/1
6	LDA	L	702	-	-	0/13/13/13	0/0/0/0
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	710	-	-	0/13/13/13	0/0/0/0
6	LDA	L	711	-	-	0/13/13/13	0/0/0/0
6	LDA	L	712	-	-	0/13/13/13	0/0/0/0
6	LDA	L	723	-	-	0/13/13/13	0/0/0/0
6	LDA	L	724	-	-	0/13/13/13	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	SO4	M	331	-	-	0/0/0/0	0/0/0/0
17	HTH	M	332	-	-	0/10/10/10	0/0/0/0
9	HTO	M	333	-	-	0/10/10/10	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
10	GOL	M	340	-	-	0/4/4/4	0/0/0/0
10	GOL	M	341	-	-	0/4/4/4	0/0/0/0
10	GOL	M	342	-	-	0/4/4/4	0/0/0/0
11	BCB	M	400	4	-	0/37/137/137	0/0/9/9
11	BCB	M	401	4	-	0/37/137/137	0/0/9/9
12	BPB	M	402	-	-	0/46/105/105	0/1/6/6
15	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	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	707	-	-	0/13/13/13	0/0/0/0
6	LDA	M	713	-	-	0/13/13/13	0/0/0/0
6	LDA	M	714	-	-	0/13/13/13	0/0/0/0
6	LDA	M	715	-	-	0/13/13/13	0/0/0/0
6	LDA	M	717	-	-	0/13/13/13	0/0/0/0

All (131) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	704	LDA	O1-N1	-16.80	1.23	1.39
6	H	720	LDA	O1-N1	-16.06	1.24	1.39
6	M	714	LDA	O1-N1	-15.93	1.24	1.39
6	L	724	LDA	O1-N1	-15.73	1.24	1.39
6	M	707	LDA	O1-N1	-15.36	1.24	1.39
6	L	703	LDA	O1-N1	-15.13	1.25	1.39
6	L	710	LDA	O1-N1	-14.92	1.25	1.39
6	L	712	LDA	O1-N1	-14.90	1.25	1.39
6	L	702	LDA	O1-N1	-14.75	1.25	1.39
6	L	711	LDA	O1-N1	-14.72	1.25	1.39
6	L	723	LDA	O1-N1	-14.41	1.25	1.39
6	M	715	LDA	O1-N1	-14.41	1.25	1.39
6	H	718[B]	LDA	O1-N1	-14.11	1.26	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	719	LDA	O1-N1	-14.09	1.26	1.39
6	M	713	LDA	O1-N1	-14.05	1.26	1.39
6	C	716	LDA	O1-N1	-14.03	1.26	1.39
6	L	708	LDA	O1-N1	-13.93	1.26	1.39
6	C	722	LDA	O1-N1	-13.91	1.26	1.39
6	L	709	LDA	O1-N1	-13.80	1.26	1.39
6	M	717	LDA	O1-N1	-13.73	1.26	1.39
6	M	706	LDA	O1-N1	-13.61	1.26	1.39
6	H	721	LDA	O1-N1	-13.04	1.27	1.39
6	M	705	LDA	O1-N1	-12.95	1.27	1.39
6	H	701	LDA	O1-N1	-10.12	1.30	1.39
11	M	401	BCB	C4D-CHA	-9.32	1.33	1.45
11	L	401	BCB	C4D-CHA	-7.24	1.36	1.45
11	L	400	BCB	C4D-CHA	-6.49	1.37	1.45
11	M	400	BCB	C4D-CHA	-6.36	1.37	1.45
13	L	502	UQ9	C7-C8	-6.28	1.41	1.50
13	L	503	UQ9	C7-C8	-6.26	1.41	1.50
6	M	704	LDA	CM1-N1	-5.23	1.41	1.49
15	M	501	MQ9	C7-C8	-4.80	1.43	1.50
15	M	501	MQ9	C2-C1	-4.54	1.39	1.48
13	L	502	UQ9	C42-C43	-3.99	1.39	1.50
13	L	502	UQ9	C32-C33	-3.87	1.39	1.50
13	L	502	UQ9	C47-C48	-3.82	1.39	1.50
15	M	501	MQ9	C37-C38	-3.79	1.39	1.50
13	L	502	UQ9	C22-C23	-3.77	1.39	1.50
15	M	501	MQ9	C5-C4	-3.73	1.39	1.48
13	L	502	UQ9	C27-C28	-3.71	1.40	1.50
13	L	502	UQ9	C12-C13	-3.68	1.40	1.50
12	M	402	BPB	C1C-NC	-3.58	1.31	1.38
15	M	501	MQ9	C27-C28	-3.56	1.40	1.50
15	M	501	MQ9	C47-C48	-3.54	1.40	1.50
13	L	503	UQ9	C12-C13	-3.51	1.40	1.50
15	M	501	MQ9	C32-C33	-3.46	1.40	1.50
15	M	501	MQ9	C22-C23	-3.45	1.40	1.50
13	L	502	UQ9	C17-C18	-3.45	1.40	1.50
13	L	502	UQ9	C37-C38	-3.41	1.41	1.50
13	L	502	UQ9	C4-C5	-3.29	1.39	1.48
15	M	501	MQ9	C42-C43	-3.26	1.41	1.50
13	L	502	UQ9	C3-C2	-3.22	1.39	1.48
15	M	501	MQ9	C12-C13	-3.14	1.41	1.50
6	L	723	LDA	C1-N1	-2.99	1.45	1.51
13	L	503	UQ9	C3-C2	-2.88	1.40	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	M	501	MQ9	C17-C18	-2.85	1.42	1.50
6	L	703	LDA	C1-N1	-2.81	1.46	1.51
15	M	501	MQ9	C6-C1	-2.77	1.40	1.47
13	L	503	UQ9	C4-C5	-2.75	1.41	1.48
6	L	724	LDA	CM2-N1	-2.74	1.45	1.49
13	L	502	UQ9	C6-C5	-2.64	1.38	1.46
6	H	721	LDA	CM1-N1	-2.56	1.45	1.49
11	M	401	BCB	CAA-CBA	-2.51	1.44	1.52
6	M	714	LDA	C1-N1	-2.49	1.46	1.51
12	M	402	BPB	C1D-C2D	-2.48	1.40	1.45
6	C	722	LDA	C1-N1	-2.46	1.46	1.51
5	C	403	HEC	CAA-C2A	-2.46	1.47	1.52
6	H	720	LDA	C1-N1	-2.42	1.47	1.51
5	C	401	HEC	CAD-C3D	-2.38	1.47	1.52
6	M	704	LDA	C1-N1	-2.24	1.47	1.51
6	L	724	LDA	C1-N1	-2.12	1.47	1.51
12	M	402	BPB	C3D-C4D	-2.01	1.37	1.43
6	L	702	LDA	C1-N1	-2.01	1.47	1.51
7	C	730	DGA	CA2-CA1	2.00	1.56	1.50
11	L	401	BCB	C4C-NC	2.04	1.41	1.37
11	M	400	BCB	CHD-C4C	2.06	1.41	1.35
13	L	502	UQ9	C25-C24	2.10	1.55	1.50
16	M	600	NS5	C13-C12	2.13	1.50	1.43
11	M	401	BCB	OBD-CAD	2.17	1.25	1.22
11	L	400	BCB	CAC-C3C	2.17	1.35	1.33
15	M	501	MQ9	O4-C4	2.18	1.27	1.23
13	L	502	UQ9	C7-C6	2.18	1.55	1.51
15	M	501	MQ9	C46-C44	2.19	1.56	1.51
5	C	403	HEC	C2A-C3A	2.19	1.44	1.37
16	M	600	NS5	C19-C20	2.24	1.50	1.43
16	M	600	NS5	C34-C35	2.25	1.56	1.50
15	M	501	MQ9	C41-C39	2.28	1.56	1.51
16	M	600	NS5	C16-C15	2.29	1.55	1.50
13	L	503	UQ9	C6-C1	2.29	1.40	1.35
13	L	503	UQ9	C7-C6	2.29	1.55	1.51
16	M	600	NS5	C22-C21	2.30	1.55	1.50
11	L	401	BCB	C3D-C4D	2.32	1.45	1.41
13	L	502	UQ9	C6-C1	2.42	1.40	1.35
7	C	730	DGA	CG1-CG2	2.47	1.56	1.50
16	M	600	NS5	C28-C26	2.48	1.51	1.45
11	M	400	BCB	CMD-C2D	2.49	1.56	1.51
11	L	401	BCB	CMA-C3A	2.49	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	L	401	BCB	CHD-C4C	2.50	1.43	1.35
15	M	501	MQ9	C48-C49	2.59	1.40	1.32
13	L	503	UQ9	C13-C14	2.62	1.40	1.32
11	L	400	BCB	O2D-CGD	2.64	1.39	1.33
16	M	600	NS5	C17-C15	2.66	1.39	1.35
16	M	600	NS5	C29-C30	2.69	1.52	1.43
11	L	401	BCB	CAC-C3C	2.75	1.36	1.33
11	M	400	BCB	CAC-C3C	2.76	1.36	1.33
13	L	502	UQ9	C48-C49	2.76	1.40	1.32
16	M	600	NS5	C23-C21	2.81	1.52	1.45
16	M	600	NS5	C24-C25	2.85	1.52	1.43
12	L	402	BPB	C3B-C4B	2.87	1.45	1.41
15	M	501	MQ9	C23-C24	2.95	1.38	1.33
13	L	502	UQ9	C43-C44	3.14	1.39	1.33
12	M	402	BPB	C3B-C4B	3.18	1.45	1.41
11	M	401	BCB	O2D-CGD	3.22	1.41	1.33
13	L	502	UQ9	C33-C34	3.25	1.39	1.33
13	L	502	UQ9	C23-C24	3.38	1.39	1.33
15	M	501	MQ9	C5M-C5	3.42	1.58	1.50
15	M	501	MQ9	C6-C5	3.45	1.43	1.35
13	L	502	UQ9	C13-C14	3.49	1.39	1.33
16	M	600	NS5	C30-C31	3.62	1.38	1.34
15	M	501	MQ9	C18-C19	3.63	1.40	1.33
13	L	502	UQ9	C18-C19	3.80	1.40	1.33
13	L	502	UQ9	C38-C39	3.83	1.40	1.33
13	L	502	UQ9	C28-C29	3.86	1.40	1.33
13	L	503	UQ9	C8-C9	3.87	1.40	1.33
15	M	501	MQ9	C28-C29	3.98	1.40	1.33
13	L	502	UQ9	C8-C9	4.08	1.41	1.33
15	M	501	MQ9	C38-C39	4.13	1.41	1.33
16	M	600	NS5	C20-C21	4.15	1.41	1.35
15	M	501	MQ9	C8-C9	4.24	1.41	1.33
15	M	501	MQ9	C33-C34	4.49	1.41	1.33
15	M	501	MQ9	C43-C44	4.56	1.41	1.33

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	401	HEC	CBB-CAB-C3B	-9.85	105.45	127.35
5	C	402	HEC	CBB-CAB-C3B	-7.55	110.58	127.35
5	C	403	HEC	CBB-CAB-C3B	-7.04	111.70	127.35
16	M	600	NS5	C19-C20-C21	-6.54	117.75	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	404	HEC	CBC-CAC-C3C	-6.44	113.03	127.35
16	M	600	NS5	C14-C15-C17	-6.41	108.65	118.98
11	M	401	BCB	O2D-CGD-O1D	-6.29	110.80	123.79
9	M	333	HTO	C5-C4-C3	-6.07	103.33	114.20
5	C	401	HEC	CBC-CAC-C3C	-6.04	113.93	127.35
9	C	358[A]	HTO	C5-C4-C3	-5.37	104.58	114.20
7	C	730	DGA	CG2-OG2-CB1	-5.24	111.15	117.92
5	C	403	HEC	CBC-CAC-C3C	-5.14	115.93	127.35
5	C	404	HEC	CBB-CAB-C3B	-5.13	115.96	127.35
6	L	708	LDA	O1-N1-CM2	-4.90	102.50	109.05
5	C	402	HEC	CBC-CAC-C3C	-4.73	116.85	127.35
6	H	720	LDA	O1-N1-C1	-4.56	105.14	110.27
12	L	402	BPB	CBD-CHA-C4D	-4.41	103.51	108.46
9	C	356	HTO	O3-C3-C2	-4.40	100.80	109.79
16	M	600	NS5	C24-C25-C26	-4.39	120.85	127.20
15	M	501	MQ9	C40-C39-C38	-4.07	115.52	123.50
16	M	600	NS5	C8-C7-C5	-4.05	118.95	127.76
11	M	401	BCB	CAA-C2A-C1A	-4.05	98.20	112.47
16	M	600	NS5	C12-C13-C14	-3.89	111.28	123.13
11	M	400	BCB	CHC-C1C-NC	-3.86	120.58	125.06
9	C	358[A]	HTO	O3-C3-C4	-3.78	100.95	109.35
12	L	402	BPB	O1D-CGD-CBD	-3.73	119.27	124.62
11	M	401	BCB	C4D-C3D-CAD	-3.66	102.33	107.86
9	C	358[A]	HTO	O1-C1-C2	-3.62	103.22	111.10
11	L	401	BCB	O1D-CGD-CBD	-3.58	119.49	124.62
12	L	402	BPB	C2B-C1B-NB	-3.54	104.49	110.29
11	L	400	BCB	O2A-CGA-O1A	-3.51	114.43	123.49
5	C	401	HEC	CMC-C2C-C1C	-3.48	122.61	128.36
11	M	401	BCB	OBD-CAD-CBD	-3.44	120.75	125.94
11	L	400	BCB	C4D-C3D-CAD	-3.42	102.70	107.86
9	L	277	HTO	C5-C4-C3	-3.41	108.09	114.20
11	M	400	BCB	OBD-CAD-CBD	-3.39	120.82	125.94
9	M	333	HTO	O1-C1-C2	-3.27	103.98	111.10
11	M	400	BCB	C4D-C3D-CAD	-3.27	102.93	107.86
11	M	401	BCB	CHC-C1C-NC	-3.22	121.33	125.06
11	M	400	BCB	CBA-CAA-C2A	-3.16	104.82	113.73
13	L	503	UQ9	C1-C6-C5	-3.13	116.55	120.12
6	M	704	LDA	O1-N1-CM2	-3.09	104.92	109.05
12	L	402	BPB	CBC-CAC-C3C	-3.08	119.97	127.07
11	L	401	BCB	OBD-CAD-C3D	-3.06	122.10	128.35
13	L	502	UQ9	C7-C6-C5	-3.01	115.02	118.56
6	L	702	LDA	O1-N1-C1	-3.00	106.90	110.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	M	600	NS5	C9-C10-C12	-2.96	113.94	122.35
9	L	278	HTO	O2-C2-C1	-2.94	102.35	109.22
17	M	332	HTH	O3-C3-C2	-2.93	103.81	109.79
13	L	502	UQ9	C45-C44-C43	-2.91	117.79	123.50
11	L	400	BCB	OBD-CAD-CBD	-2.90	121.55	125.94
11	M	400	BCB	O1D-CGD-CBD	-2.90	120.47	124.62
9	H	272	HTO	C5-C4-C3	-2.87	109.05	114.20
11	L	401	BCB	C6-C5-C3	-2.87	106.18	112.48
5	C	404	HEC	C4B-C3B-C2B	-2.73	103.40	106.35
9	L	278	HTO	O1-C1-C2	-2.73	105.16	111.10
9	H	272	HTO	O1-C1-C2	-2.73	105.16	111.10
5	C	401	HEC	CMB-C2B-C1B	-2.71	123.87	128.36
5	C	402	HEC	CMC-C2C-C1C	-2.71	123.88	128.36
12	L	402	BPB	C2C-C3C-C4C	-2.70	104.77	107.24
5	C	401	HEC	C4C-C3C-C2C	-2.68	103.46	106.35
6	H	721	LDA	O1-N1-C1	-2.67	107.27	110.27
5	C	404	HEC	CMB-C2B-C1B	-2.65	123.98	128.36
9	C	358[A]	HTO	O2-C2-C1	-2.64	103.06	109.22
13	L	502	UQ9	C1-C6-C5	-2.62	117.14	120.12
9	L	276	HTO	O2-C2-C3	-2.60	104.47	109.79
11	L	400	BCB	C5-C3-C2	-2.57	116.17	121.05
13	L	502	UQ9	C25-C24-C23	-2.57	118.46	123.50
6	M	704	LDA	CM1-N1-C1	-2.56	101.52	109.77
5	C	403	HEC	CAA-C2A-C1A	-2.54	124.25	127.01
5	C	402	HEC	CMB-C2B-C1B	-2.53	124.17	128.36
11	L	401	BCB	C4D-C3D-CAD	-2.50	104.09	107.86
11	L	401	BCB	C5-C3-C2	-2.49	116.32	121.05
5	C	401	HEC	CBD-CAD-C3D	-2.47	108.11	112.53
13	L	502	UQ9	C1M-C1-C6	-2.45	118.86	124.10
11	M	401	BCB	CAA-C2A-C3A	-2.44	106.20	113.22
13	L	502	UQ9	O5-C5-C6	-2.42	117.12	121.68
6	M	704	LDA	CM2-N1-CM1	-2.36	106.17	108.83
11	M	400	BCB	C4-C3-C2	-2.35	118.88	123.50
9	H	272	HTO	O2-C2-C1	-2.34	103.76	109.22
15	M	501	MQ9	C35-C34-C33	-2.28	119.02	123.50
11	M	401	BCB	CBC-CAC-C3C	-2.25	121.88	127.07
12	M	402	BPB	CBD-CHA-C4D	-2.25	105.94	108.46
9	M	333	HTO	O3-C3-C4	-2.25	104.34	109.35
15	M	501	MQ9	C5M-C5-C6	-2.22	119.34	124.10
13	L	502	UQ9	C15-C14-C13	-2.19	119.21	123.50
16	M	600	NS5	C24-C23-C21	-2.18	119.92	126.32
13	L	502	UQ9	O2-C2-C3	-2.17	116.10	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	401	BCB	C4-C3-C2	-2.16	119.25	123.50
11	L	401	BCB	C1D-CHD-C4C	-2.16	124.62	129.26
6	M	707	LDA	O1-N1-CM1	-2.14	106.19	109.05
6	H	701	LDA	CM2-N1-CM1	-2.10	106.46	108.83
12	L	402	BPB	CHD-C1D-ND	-2.10	120.75	124.66
11	L	400	BCB	O1D-CGD-CBD	-2.09	121.62	124.62
16	M	600	NS5	C4-C5-C7	-2.09	117.08	121.05
11	M	400	BCB	CHD-C4C-C3C	-2.09	123.18	129.02
16	M	600	NS5	C28-C26-C25	-2.08	115.64	118.98
12	L	402	BPB	CHD-C4C-NC	-2.07	120.96	124.91
9	L	280	HTO	C5-C4-C3	-2.07	110.49	114.20
11	M	401	BCB	CAA-CBA-CGA	-2.07	107.26	113.32
11	L	400	BCB	O2D-CGD-O1D	-2.06	119.53	123.79
13	L	502	UQ9	C31-C29-C28	-2.03	117.21	121.05
6	L	724	LDA	O1-N1-CM2	-2.03	106.34	109.05
11	L	401	BCB	CHC-C1C-NC	-2.02	122.71	125.06
12	L	402	BPB	C3C-C4C-NC	2.01	112.99	109.52
15	M	501	MQ9	C5M-C5-C4	2.07	119.63	116.27
5	C	401	HEC	CAD-C3D-C4D	2.07	129.26	127.01
6	L	711	LDA	O1-N1-CM1	2.07	111.83	109.05
10	H	280	GOL	C3-C2-C1	2.10	119.34	111.12
7	C	730	DGA	OG1-CG1-CG2	2.11	114.27	108.61
9	M	333	HTO	O3-C3-C2	2.11	114.11	109.79
15	M	501	MQ9	C41-C39-C38	2.12	125.06	121.05
5	C	403	HEC	CMA-C3A-C2A	2.15	129.72	125.24
16	M	600	NS5	C27-C26-C28	2.15	121.68	118.10
6	L	724	LDA	O1-N1-CM1	2.18	111.96	109.05
6	M	704	LDA	CM2-N1-C1	2.18	116.78	109.77
9	H	273	HTO	O1-C1-C2	2.19	115.85	111.10
12	M	402	BPB	O2D-CGD-CBD	2.19	114.31	111.30
12	M	402	BPB	C6-C5-C3	2.23	117.37	112.48
10	L	282	GOL	C3-C2-C1	2.23	119.86	111.12
12	L	402	BPB	CMB-C2B-C3B	2.26	129.51	125.09
9	L	276	HTO	O3-C3-C4	2.28	114.41	109.35
15	M	501	MQ9	C3D-C2-C3	2.29	121.86	119.26
13	L	502	UQ9	C15-C14-C16	2.30	118.92	115.41
11	L	400	BCB	CMD-C2D-C1D	2.31	132.18	128.36
9	C	355	HTO	O2-C2-C1	2.31	114.61	109.22
6	C	716	LDA	O1-N1-C1	2.33	112.90	110.27
9	L	278	HTO	O2-C2-C3	2.37	114.64	109.79
12	L	402	BPB	CHD-C1D-C2D	2.38	131.00	125.61
11	M	401	BCB	C3D-CAD-CBD	2.39	110.97	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	400	BCB	C4B-CHC-C1C	2.39	129.72	126.07
12	M	402	BPB	CHD-C1D-C2D	2.44	131.12	125.61
11	M	401	BCB	C4-C3-C5	2.46	119.17	115.41
11	M	400	BCB	O2A-CGA-CBA	2.50	119.52	111.90
11	L	401	BCB	C3D-CAD-CBD	2.50	111.13	107.60
5	C	402	HEC	CAA-C2A-C1A	2.52	129.74	127.01
6	H	721	LDA	O1-N1-CM2	2.55	112.46	109.05
11	M	400	BCB	C4A-NA-C1A	2.56	109.05	106.04
6	M	704	LDA	O1-N1-CM1	2.60	112.53	109.05
15	M	501	MQ9	C40-C39-C41	2.61	119.40	115.41
11	L	400	BCB	O2A-CGA-CBA	2.64	119.93	111.90
11	L	401	BCB	C4B-CHC-C1C	2.65	130.12	126.07
5	C	401	HEC	CAD-CBD-CGD	2.68	117.66	112.75
15	M	501	MQ9	C25-C24-C26	2.76	119.62	115.41
13	L	502	UQ9	C45-C44-C46	2.79	119.66	115.41
12	M	402	BPB	C4D-C3D-C2D	2.83	109.94	106.74
12	L	402	BPB	CED-O2D-CGD	2.94	122.87	115.99
11	L	400	BCB	CMB-C2B-C3B	2.98	130.92	125.09
6	L	708	LDA	CM2-N1-CM1	2.98	112.20	108.83
15	M	501	MQ9	C35-C34-C36	3.06	120.08	115.41
11	M	401	BCB	CMB-C2B-C3B	3.07	131.10	125.09
11	L	400	BCB	C4A-NA-C1A	3.08	109.67	106.04
6	H	701	LDA	O1-N1-C1	3.09	113.75	110.27
7	C	730	DGA	OG1-CA1-CA2	3.10	121.33	111.90
7	C	730	DGA	OG2-CG2-CG1	3.10	112.93	105.90
13	L	502	UQ9	C7-C8-C9	3.14	132.01	126.70
11	M	401	BCB	O2A-CGA-CBA	3.22	121.71	111.90
11	M	401	BCB	CED-O2D-CGD	3.22	123.55	115.99
15	M	501	MQ9	C15-C14-C16	3.24	120.35	115.41
6	H	701	LDA	O1-N1-CM1	3.26	113.41	109.05
6	M	707	LDA	O1-N1-CM2	3.29	113.45	109.05
16	M	600	NS5	C32-C31-C33	3.34	120.50	115.41
11	L	400	BCB	C3D-CAD-CBD	3.37	112.36	107.60
11	M	400	BCB	C4-C3-C5	3.59	120.89	115.41
11	L	401	BCB	O2D-CGD-CBD	3.73	116.41	111.30
12	M	402	BPB	CMB-C2B-C3B	3.73	132.37	125.09
13	L	502	UQ9	C35-C34-C36	3.77	121.16	115.41
11	M	401	BCB	C4A-NA-C1A	3.85	110.58	106.04
11	L	400	BCB	C4-C3-C5	3.88	121.33	115.41
11	L	401	BCB	C4-C3-C5	3.93	121.41	115.41
11	L	401	BCB	CMB-C2B-C3B	3.96	132.83	125.09
7	C	730	DGA	OG2-CB1-CB2	3.96	120.13	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	704	LDA	O1-N1-C1	4.02	114.80	110.27
11	M	400	BCB	C3D-CAD-CBD	4.03	113.29	107.60
11	M	401	BCB	C3C-C4C-NC	4.06	113.27	110.24
13	L	502	UQ9	C30-C29-C31	4.21	121.84	115.41
16	M	600	NS5	C6-C5-C4	4.36	122.07	115.41
11	M	400	BCB	O2D-CGD-CBD	4.47	117.43	111.30
13	L	503	UQ9	C7-C8-C9	4.49	134.30	126.70
13	L	502	UQ9	C25-C24-C26	4.64	122.49	115.41
16	M	600	NS5	C18-C19-C20	4.93	134.29	123.39
6	L	708	LDA	O1-N1-C1	5.13	116.04	110.27
11	L	400	BCB	O2D-CGD-CBD	5.50	118.84	111.30
16	M	600	NS5	C16-C15-C17	5.54	131.08	122.90
11	L	400	BCB	C3C-C4C-NC	5.94	114.67	110.24
11	M	400	BCB	C3C-C4C-NC	6.55	115.12	110.24
11	L	401	BCB	C3C-C4C-NC	6.90	115.38	110.24
16	M	600	NS5	C11-C10-C9	7.30	126.55	115.41
11	M	401	BCB	O2D-CGD-CBD	9.67	124.57	111.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

62 monomers are involved in 144 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	338	SO4	1	0
8	C	340	SO4	1	0
8	C	351	SO4	1	0
8	C	354	SO4	1	0
9	C	355	HTO	6	0
9	C	357	HTO	2	0
10	C	363	GOL	1	0
10	C	364	GOL	3	0
10	C	365	GOL	2	0
10	C	368	GOL	1	0
10	C	369	GOL	3	0
10	C	373	GOL	1	0
10	C	377	GOL	4	0
5	C	401	HEC	1	0
5	C	403	HEC	3	0
5	C	404	HEC	1	0
6	C	716	LDA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	722	LDA	4	0
7	C	730	DGA	3	0
8	H	261[A]	SO4	1	0
8	H	261[B]	SO4	4	0
9	H	272	HTO	1	0
9	H	273	HTO	3	0
9	H	274[A]	HTO	1	0
10	H	278	GOL	2	0
10	H	279	GOL	1	0
10	H	280	GOL	1	0
10	H	283	GOL	6	0
6	H	719	LDA	3	0
6	H	720	LDA	8	0
6	H	721	LDA	1	0
9	L	277	HTO	2	0
9	L	279	HTO	1	0
10	L	286	GOL	1	0
11	L	400	BCB	5	0
11	L	401	BCB	4	0
12	L	402	BPB	2	0
13	L	502	UQ9	11	0
13	L	503	UQ9	5	0
6	L	702	LDA	6	0
6	L	703	LDA	4	0
6	L	710	LDA	1	0
6	L	711	LDA	1	0
6	L	712	LDA	1	0
6	L	723	LDA	4	0
6	L	724	LDA	2	0
8	M	326	SO4	2	0
9	M	333	HTO	2	0
10	M	334	GOL	1	0
10	M	336	GOL	1	0
10	M	338	GOL	3	0
10	M	342	GOL	1	0
11	M	400	BCB	12	0
11	M	401	BCB	5	0
12	M	402	BPB	1	0
15	M	501	MQ9	2	0
16	M	600	NS5	3	0
6	M	704	LDA	6	0
6	M	706	LDA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	707	LDA	1	0
6	M	714	LDA	2	0
6	M	715	LDA	2	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	C	334/356 (93%)	0.42	43 (12%) 5 8	34, 46, 68, 125	0
2	H	249/258 (96%)	0.01	13 (5%) 31 42	35, 51, 81, 119	0
3	L	273/273 (100%)	0.12	19 (6%) 19 29	33, 42, 58, 82	0
4	M	323/323 (100%)	0.31	30 (9%) 11 17	32, 43, 65, 83	0
All	All	1179/1210 (97%)	0.23	105 (8%) 12 19	32, 45, 69, 125	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	333	ALA	9.3
1	C	334	ALA	8.7
1	C	47	ALA	5.8
3	L	273	SER	5.2
1	C	332	LYS	5.0
2	H	85	THR	4.6
3	L	51[A]	TYR	4.4
3	L	271	PHE	4.3
3	L	202	ASP	4.2
1	C	230	PHE	4.2
4	M	78	HIS	4.2
2	H	8	GLN	4.1
4	M	26	ASN	4.0
3	L	81	LEU	4.0
1	C	48	GLU	4.0
3	L	270	PRO	3.9
4	M	23	TRP	3.9
2	H	7	ALA	3.8
4	M	319	PRO	3.8
4	M	37	TRP	3.7
4	M	31	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
3	L	165	LEU	3.7
1	C	168	THR	3.7
4	M	189	ILE	3.6
2	H	9	HIS	3.6
1	C	52	VAL	3.6
1	C	162	HIS	3.5
3	L	59	TRP	3.4
4	M	181	ILE	3.4
3	L	201	GLY	3.4
1	C	232	LEU	3.2
4	M	184	LEU	3.1
1	C	46	LYS	3.1
4	M	186	ALA	3.0
1	C	54	GLN	3.0
1	C	51	PRO	3.0
1	C	185	LEU	3.0
4	M	185	THR	2.9
3	L	162	TYR	2.9
1	C	66	THR	2.9
1	C	231	ALA	2.9
1	C	228	ALA	2.8
1	C	2[A]	PHE	2.8
4	M	33	PHE	2.8
1	C	244	CYS	2.8
2	H	83	PRO	2.8
4	M	80	ASP	2.7
1	C	159	THR	2.7
2	H	94	ASP	2.7
1	C	63	GLY	2.6
2	H	95	GLY	2.6
1	C	229	THR	2.6
2	H	96	PHE	2.6
4	M	82	LEU	2.6
1	C	291	ALA	2.6
1	C	331	ILE	2.6
1	C	163	VAL	2.6
1	C	167	GLU	2.5
3	L	272	TRP	2.5
1	C	169	ARG	2.5
2	H	81[A]	ARG	2.5
1	C	65	LEU	2.5
3	L	269	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
4	M	108	HIS	2.5
4	M	22	GLU	2.5
4	M	27	ASP	2.4
1	C	287	THR	2.4
4	M	212	LEU	2.4
2	H	189	GLY	2.4
3	L	79	PRO	2.4
4	M	25	ASP	2.4
3	L	167	TRP	2.4
3	L	236	LEU	2.4
1	C	161	THR	2.4
4	M	207	ALA	2.3
3	L	80	LEU	2.3
1	C	226	ALA	2.3
4	M	24	GLY	2.3
1	C	165	ARG	2.3
1	C	234	MET	2.3
1	C	50	PRO	2.3
4	M	320	GLY	2.2
1	C	53	SER	2.2
4	M	263	VAL	2.2
1	C	193	PHE	2.2
4	M	79	PHE	2.2
3	L	57	PRO	2.1
3	L	54	SER	2.1
3	L	180	LEU	2.1
1	C	55	VAL	2.1
4	M	34	TYR	2.1
2	H	97	GLU	2.1
4	M	50	TYR	2.1
2	H	86	ARG	2.1
2	H	87	GLU	2.1
4	M	21	GLY	2.1
1	C	57	LYS	2.0
4	M	221	ILE	2.0
4	M	183	TRP	2.0
4	M	210	CYS	2.0
1	C	49	GLY	2.0
1	C	242	THR	2.0
1	C	323	GLN	2.0
1	C	227	TYR	2.0
1	C	45	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	FME	H	1[A]	10/11	0.97	0.09	-	47,50,54,56	7
2	FME	H	1[B]	10/11	0.97	0.09	-	47,53,59,61	7

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	LDA	L	724	16/16	0.77	0.47	40.82	53,63,68,69	16
10	GOL	L	288	6/6	0.70	0.52	31.67	54,57,58,60	6
6	LDA	L	723	16/16	0.85	1.01	31.08	55,58,64,68	16
6	LDA	M	706	16/16	0.34	0.59	29.52	49,55,65,68	16
9	HTO	C	357	10/10	0.65	0.61	26.51	59,65,73,80	10
9	HTO	M	333	10/10	0.78	0.72	23.28	44,51,55,55	10
8	SO4	H	268	5/5	0.90	0.54	21.55	63,66,70,72	5
6	LDA	L	702	16/16	0.56	0.80	21.36	51,53,57,57	16
6	LDA	L	712	16/16	0.55	0.42	19.88	51,64,70,71	16
10	GOL	C	369	6/6	0.80	1.19	18.95	49,56,61,61	6
8	SO4	C	346	5/5	0.93	0.25	17.46	57,65,71,72	5
10	GOL	C	363	6/6	0.68	0.29	15.44	46,59,65,69	6
10	GOL	H	275	6/6	0.95	0.26	13.10	59,62,64,67	0
10	GOL	H	276[A]	6/6	0.79	0.26	13.07	50,60,62,62	2
10	GOL	H	276[B]	6/6	0.79	0.26	13.07	50,59,60,62	2
6	LDA	M	717	16/16	0.60	0.39	13.05	50,59,89,91	16

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
9	HTO	L	276	10/10	0.85	0.48	12.84	50,67,70,71	10
10	GOL	H	277	6/6	0.74	0.31	12.72	55,59,62,62	6
8	SO4	H	266	5/5	0.84	0.33	12.45	65,66,68,71	5
6	LDA	C	716	16/16	0.61	0.34	11.52	50,65,72,74	16
6	LDA	M	715	16/16	0.71	0.39	10.75	58,71,77,79	16
9	HTO	L	279	10/10	0.60	0.32	10.54	65,66,69,75	10
13	UQ9	L	502	58/58	0.81	0.52	10.42	44,80,97,99	58
8	SO4	C	338	5/5	0.96	0.19	10.19	53,57,60,64	5
8	SO4	H	263	5/5	0.87	0.49	9.51	75,76,78,79	5
10	GOL	L	281	6/6	0.94	0.41	8.96	54,58,66,68	6
10	GOL	C	378	6/6	0.75	0.43	8.85	78,80,81,81	6
8	SO4	C	347	5/5	0.75	0.40	8.55	78,82,83,90	5
10	GOL	C	364	6/6	0.83	0.24	7.67	52,67,67,68	6
7	DGA	C	730	37/44	0.33	0.41	7.33	112,125,144,151	0
9	HTO	H	273	10/10	0.76	0.34	7.02	48,51,60,62	10
10	GOL	C	362	6/6	0.90	0.38	6.98	51,57,63,63	6
8	SO4	H	261[A]	5/5	0.90	0.19	6.15	52,58,64,65	5
10	GOL	C	359	6/6	0.96	0.44	5.65	44,50,54,55	6
13	UQ9	L	503	23/58	0.77	0.30	4.90	59,73,85,87	23
8	SO4	C	354	5/5	0.74	0.37	4.68	66,69,70,71	5
8	SO4	H	269	5/5	0.81	0.29	4.60	71,72,75,76	5
6	LDA	H	701	16/16	0.91	0.26	4.59	43,57,71,73	0
8	SO4	H	267	5/5	0.88	0.26	4.57	56,64,65,65	5
8	SO4	C	351	5/5	0.67	0.40	4.29	60,60,63,67	5
6	LDA	L	710	16/16	0.73	0.28	4.23	52,60,81,82	16
8	SO4	C	343	5/5	0.83	0.40	4.02	52,62,65,66	5
10	GOL	C	360	6/6	0.87	0.23	3.93	44,56,62,71	6
6	LDA	L	711	16/16	0.55	0.31	3.88	60,68,76,77	16
10	GOL	M	334	6/6	0.94	0.18	3.74	40,56,66,69	6
6	LDA	M	707	16/16	0.69	0.31	3.68	42,58,72,81	16
10	GOL	H	280	6/6	0.79	0.23	3.48	52,60,65,66	6
6	LDA	L	709	16/16	0.55	0.28	3.41	39,63,93,97	16
6	LDA	L	708	16/16	0.82	0.21	3.24	40,56,68,76	0
8	SO4	C	340	5/5	0.88	0.29	3.06	57,71,76,82	5
10	GOL	H	283	6/6	0.75	0.21	3.05	59,60,61,61	6
10	GOL	H	289	6/6	0.74	0.35	2.84	62,66,66,67	6
6	LDA	H	719	16/16	0.74	0.23	2.63	58,63,71,72	16
10	GOL	M	338	6/6	0.56	0.36	2.56	57,60,62,63	6
10	GOL	C	371	6/6	0.64	0.43	2.36	55,62,62,63	6
6	LDA	M	705	16/16	0.76	0.25	2.34	61,69,87,87	16
10	GOL	H	279	6/6	0.73	0.28	2.26	63,68,71,72	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
10	GOL	L	285	6/6	0.82	0.21	2.22	51,67,70,71	6
8	SO4	H	264	5/5	0.86	0.18	2.18	61,67,72,73	5
10	GOL	H	282	6/6	0.87	0.37	2.16	59,66,68,69	6
9	HTO	C	356	10/10	0.81	0.27	2.11	59,72,76,77	10
6	LDA	C	722	16/16	0.69	0.24	1.83	53,63,66,66	16
8	SO4	H	261[B]	5/5	0.90	0.19	1.82	47,54,61,61	5
8	SO4	M	324	5/5	0.99	0.11	1.60	47,52,61,63	0
16	NS5	M	600	40/40	0.90	0.14	1.42	42,54,95,96	0
6	LDA	M	704	16/16	0.90	0.22	1.18	49,80,87,87	16
15	MQ9	M	501	58/58	0.91	0.17	1.05	31,41,92,98	0
10	GOL	H	290	6/6	0.88	0.19	1.02	49,59,63,67	6
12	BPB	M	402	65/65	0.96	0.13	1.02	33,41,124,132	0
6	LDA	M	714	16/16	0.87	0.20	1.00	70,75,81,82	16
11	BCB	L	400	66/66	0.97	0.18	0.98	28,36,48,52	0
6	LDA	M	713	16/16	0.87	0.18	0.92	63,69,84,86	16
10	GOL	M	342	6/6	0.67	0.24	0.85	66,67,69,70	6
11	BCB	M	400	66/66	0.95	0.18	0.84	34,40,109,121	0
12	BPB	L	402	65/65	0.96	0.13	0.77	32,39,48,51	0
11	BCB	M	401	66/66	0.95	0.17	0.70	28,34,58,66	0
9	HTO	L	277	10/10	0.82	0.17	0.60	57,64,69,76	10
9	HTO	C	355	10/10	0.75	0.24	0.46	62,66,71,72	10
9	HTO	L	278	10/10	0.79	0.20	0.26	57,65,67,69	10
11	BCB	L	401	66/66	0.96	0.14	0.26	27,35,64,75	0
8	SO4	M	325	5/5	0.99	0.17	0.13	64,67,78,79	0
6	LDA	H	721	16/16	0.95	0.14	0.06	50,66,69,69	0
5	HEC	C	402	43/43	0.98	0.09	-0.12	39,44,52,60	0
10	GOL	M	335	6/6	0.93	0.10	-0.13	44,54,60,68	6
5	HEC	C	401	43/43	0.98	0.10	-0.14	41,46,55,58	0
14	FE2	M	500	1/1	1.00	0.14	-0.16	37,37,37,37	0
5	HEC	C	403	43/43	0.98	0.15	-0.33	32,36,41,42	0
10	GOL	L	282	6/6	0.87	0.14	-0.44	53,59,59,63	6
5	HEC	C	404	43/43	0.98	0.09	-0.46	32,38,51,64	0
10	GOL	C	361	6/6	0.91	0.24	-0.89	60,64,72,75	6
10	GOL	M	336	6/6	0.86	0.17	-2.56	68,69,70,71	6
10	GOL	H	291	6/6	0.85	0.26	-	74,78,80,81	6
8	SO4	M	326	5/5	0.97	0.18	-	56,61,62,62	5
8	SO4	H	265	5/5	0.79	0.22	-	69,74,75,81	5
10	GOL	C	375	6/6	0.76	0.37	-	66,69,70,72	6
6	LDA	H	720	16/16	0.84	0.24	-	55,69,73,73	16
8	SO4	C	339	5/5	0.93	0.36	-	69,71,75,80	5
10	GOL	H	285	6/6	0.83	0.28	-	68,70,71,71	6
8	SO4	H	262	5/5	0.99	0.12	-	41,43,45,47	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
9	HTO	L	280	10/10	0.47	0.39	-	63,69,71,72	10
10	GOL	M	340	6/6	0.75	0.29	-	60,64,65,66	6
10	GOL	C	376	6/6	0.64	0.34	-	63,74,77,83	6
6	LDA	L	703	16/16	0.83	0.40	-	52,57,61,63	16
10	GOL	L	283	6/6	0.89	0.13	-	59,63,68,70	6
10	GOL	M	341	6/6	0.37	0.44	-	68,71,74,75	6
8	SO4	C	341	5/5	0.95	0.17	-	67,74,80,81	5
8	SO4	M	330	5/5	0.66	0.46	-	67,68,68,69	5
8	SO4	C	345	5/5	0.94	0.23	-	66,68,72,72	5
10	GOL	H	278	6/6	0.85	0.19	-	63,67,68,71	6
10	GOL	L	284	6/6	0.82	0.21	-	52,65,67,67	6
10	GOL	M	337	6/6	0.84	0.13	-	68,69,69,70	6
8	SO4	C	353	5/5	0.83	0.38	-	66,69,72,76	5
10	GOL	H	288	6/6	0.61	0.19	-	60,68,68,73	6
17	HTH	M	332	10/10	0.36	0.31	-	58,68,76,77	10
10	GOL	C	372	6/6	0.75	0.22	-	56,62,65,65	6
8	SO4	C	350	5/5	0.76	0.39	-	64,67,69,72	5
8	SO4	L	274	5/5	0.82	0.26	-	62,62,65,68	5
9	HTO	H	272	10/10	0.90	0.17	-	61,67,75,80	10
8	SO4	L	275	5/5	0.69	0.44	-	66,66,67,68	5
10	GOL	H	286	6/6	0.90	0.33	-	67,67,69,70	6
8	SO4	C	344	5/5	0.88	0.38	-	74,76,79,82	5
10	GOL	H	281	6/6	0.71	0.39	-	64,67,72,76	6
8	SO4	H	259	5/5	0.97	0.13	-	60,62,67,69	5
10	GOL	L	286	6/6	0.88	0.65	-	58,63,64,68	6
10	GOL	H	284	6/6	0.82	0.21	-	58,63,65,68	6
8	SO4	C	352	5/5	0.87	0.35	-	78,78,81,82	5
10	GOL	C	373	6/6	0.86	1.85	-	60,63,64,65	6
8	SO4	C	337[A]	5/5	0.85	0.23	-	59,62,67,67	5
8	SO4	H	270	5/5	0.71	0.33	-	60,61,63,63	5
8	SO4	M	328	5/5	0.83	0.34	-	61,62,64,69	5
8	SO4	C	337[B]	5/5	0.85	0.23	-	59,64,69,70	5
10	GOL	L	287	6/6	0.77	0.25	-	54,55,57,57	6
8	SO4	M	329	5/5	0.73	0.42	-	57,58,63,67	5
10	GOL	C	374[B]	6/6	0.61	0.49	-	66,67,68,68	6
9	HTO	H	274[A]	10/10	0.54	0.57	-	53,69,72,75	10
8	SO4	M	327	5/5	0.94	0.22	-	53,58,68,75	5
10	GOL	C	365	6/6	0.87	0.18	-	60,67,69,72	6
10	GOL	C	367	6/6	0.81	1.39	-	50,58,59,60	6
10	GOL	C	377	6/6	0.88	0.12	-	63,65,67,67	6
8	SO4	C	348	5/5	0.82	0.20	-	70,73,77,80	5
10	GOL	C	368	6/6	0.89	0.19	-	62,63,68,70	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	LDA	H	718[B]	16/16	0.30	0.54	-	50,80,89,90	16
8	SO4	M	331	5/5	0.83	0.20	-	60,60,61,62	5
10	GOL	C	366	6/6	0.82	0.22	-	56,62,63,71	6
10	GOL	H	287	6/6	0.72	0.17	-	65,71,72,73	6
10	GOL	M	339	6/6	0.79	0.39	-	60,65,66,66	6
8	SO4	H	260	5/5	0.96	0.09	-	59,63,68,71	5
8	SO4	H	271	5/5	0.44	0.34	-	64,64,65,68	5
8	SO4	C	349	5/5	0.84	0.42	-	63,64,71,71	5
9	HTO	C	358[A]	10/10	0.66	0.31	-	58,62,67,68	10
8	SO4	C	342	5/5	0.90	0.25	-	63,68,71,75	5
10	GOL	C	370	6/6	0.66	0.42	-	64,66,68,68	6

6.5 Other polymers [i](#)

There are no such residues in this entry.