Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:02 AM GMT

PDB ID	:	3D38
Title	:	Crystal structure of new trigonal form of photosynthetic reaction center from Blastochloris viridis. Crystals grown in microfluidics by detergent capture.
Authors	:	Li, L.; Nachtergaele, S.H.M.; Seddon, A.M.; Tereshko, V.; Ponomarenko, N.; Ismagilov, R.F.; Accelerated Technologies Center for Gene to 3D Structure (ATCG3D)
Deposited on	:	2008-05-09
Resolution	:	3.21 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

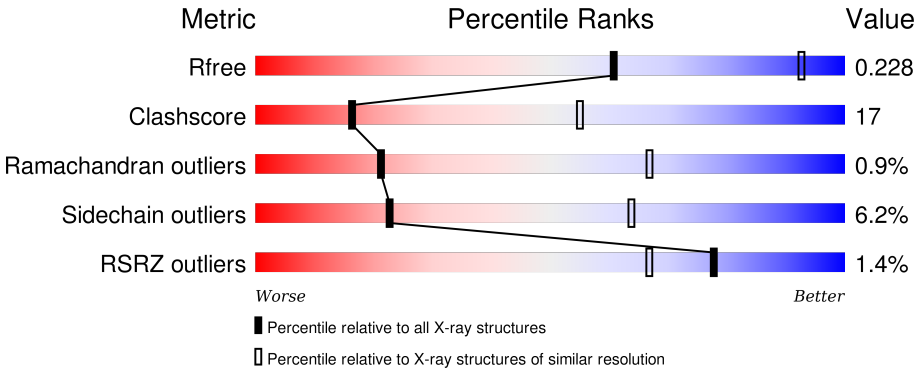
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.21 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	1095 (3.26-3.18)
Clashscore	102246	1046 (3.24-3.20)
Ramachandran outliers	100387	1026 (3.24-3.20)
Sidechain outliers	100360	1025 (3.24-3.20)
RSRZ outliers	91569	1100 (3.26-3.18)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	336	2% 73% 24%
2	H	258	% 67% 26%
3	L	273	% 72% 26%
4	M	323	% 72% 25%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	BPB	M	402	-	-	-	X
12	UQ1	L	502	-	-	-	X
12	UQ1	L	503	-	-	-	X
14	NS5	M	600	-	-	-	X
5	SO4	C	811	-	-	-	X
5	SO4	C	813	-	-	-	X
5	SO4	H	807	-	-	-	X
8	HTO	C	706	-	-	-	X
8	HTO	C	707	-	-	-	X
8	HTO	H	705	-	-	-	X
9	LDA	L	702	-	-	-	X
9	LDA	M	704	-	-	-	X

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 10311 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	250	Total	C	N	O	S	0	0	0
			1958	1251	335	370	2			

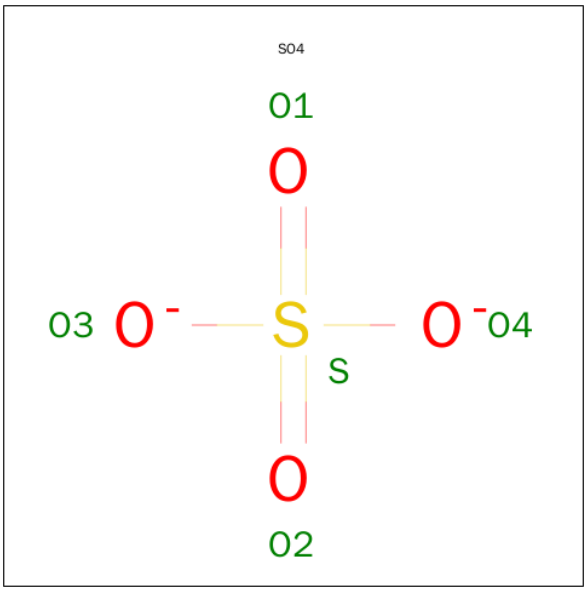
- Molecule 3 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	273	Total	C	N	O	S	0	0	0
			2171	1459	350	355	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	323	Total	C	N	O	S	0	0	0
			2555	1702	419	423	11			

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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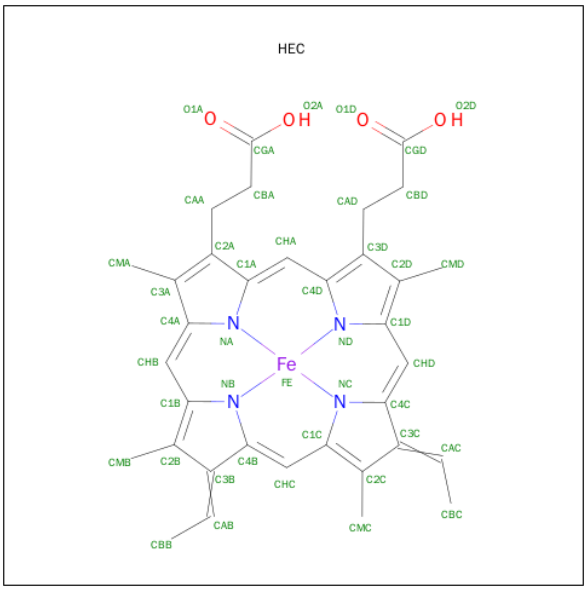
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	M	1	Total O S 5 4 1	0	0

- Molecule 6 is FE (II) ION (three-letter code: FE2) (formula: Fe).

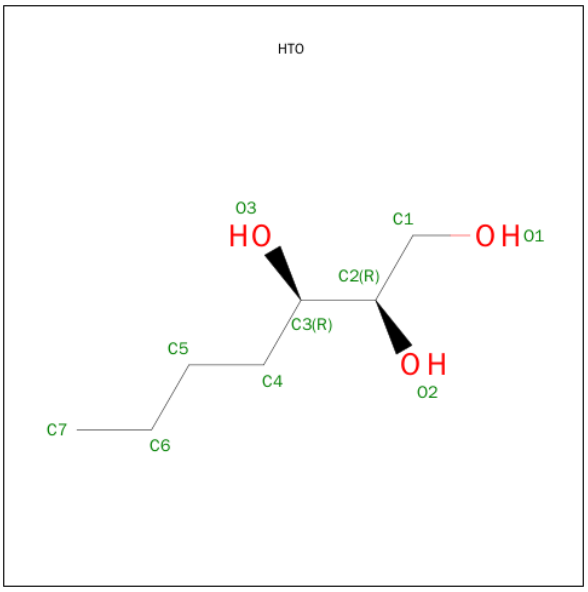
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	M	1	Total Fe 1 1	0	0

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



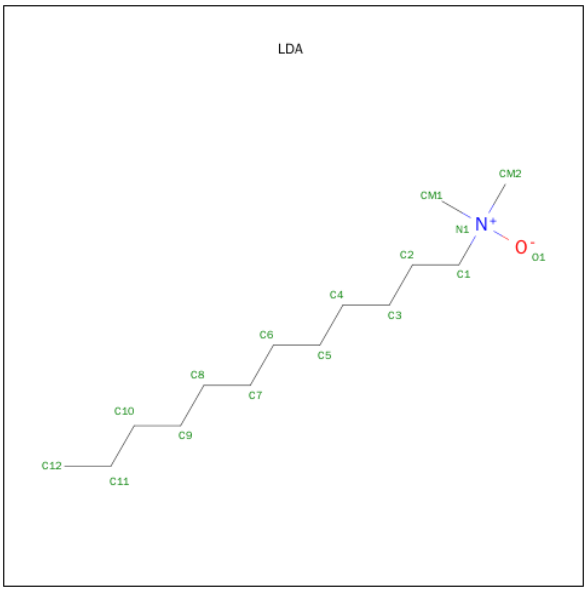
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C Fe N O 43 34 1 4 4	0	0
7	C	1	Total C Fe N O 43 34 1 4 4	0	0
7	C	1	Total C Fe N O 43 34 1 4 4	0	0
7	C	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 8 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).



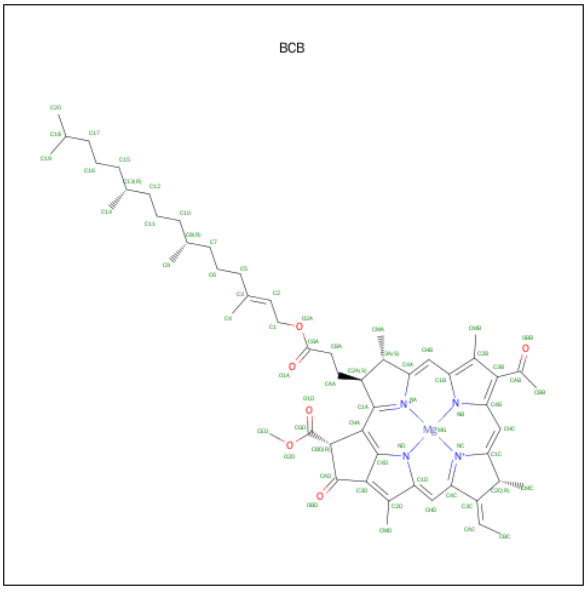
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C O 10 7 3	0	0
8	C	1	Total C O 10 7 3	0	0
8	H	1	Total C O 10 7 3	0	0

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



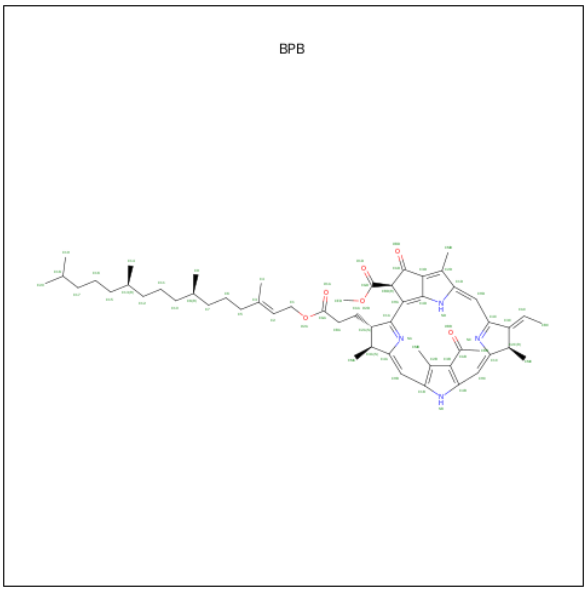
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	H	1	Total	C	N	O	0	0
			16	14	1	1		
9	H	1	Total	C	N	O	0	0
			16	14	1	1		
9	L	1	Total	C	N	O	0	0
			16	14	1	1		
9	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 10 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: $C_{55}H_{72}MgN_4O_6$).



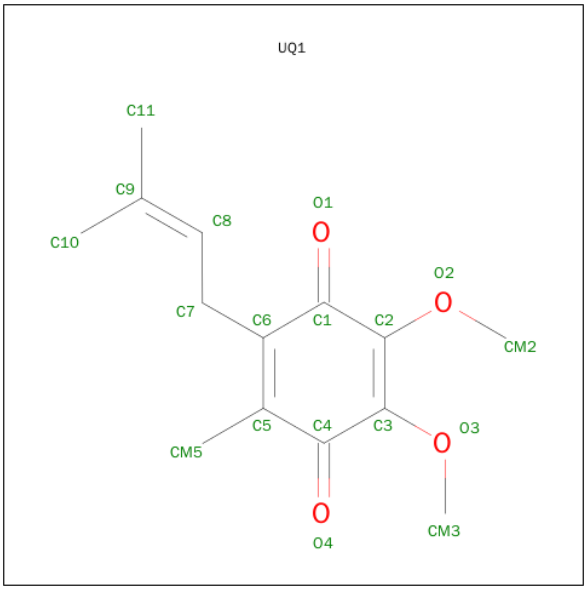
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
10	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
10	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
10	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 11 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula: $C_{55}H_{74}N_4O_6$).



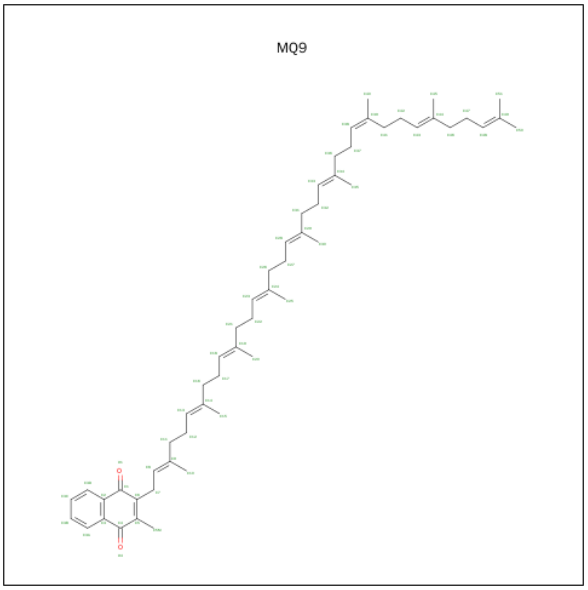
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	L	1	Total	C	N	O	0	0
			65	55	4	6		
11	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 12 is UBIQUINONE-1 (three-letter code: UQ1) (formula: $C_{14}H_{18}O_4$).



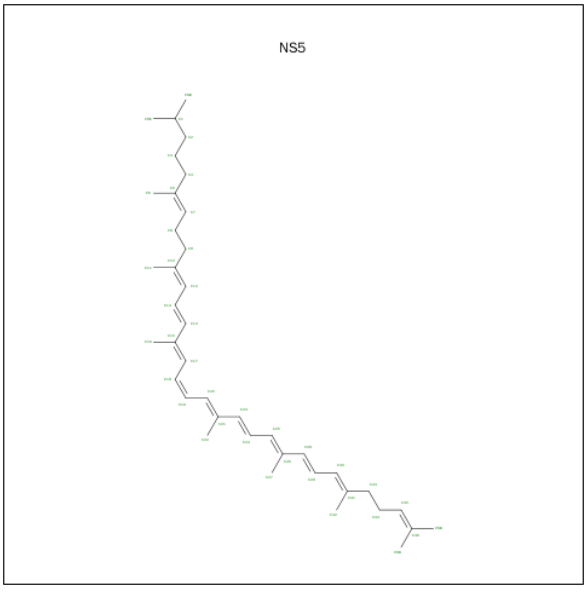
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	L	1	Total	C	O	0	0
			18	14	4		
12	L	1	Total	C	O	0	0
			18	14	4		

- Molecule 13 is MENAQUINONE-9 (three-letter code: MQ9) (formula: $C_{56}H_{80}O_2$).



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

- Molecule 14 is 15-CIS-1,2-DIHYDRONEUROSPORENE (three-letter code: NS5) (formula: $C_{40}H_{60}$).



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

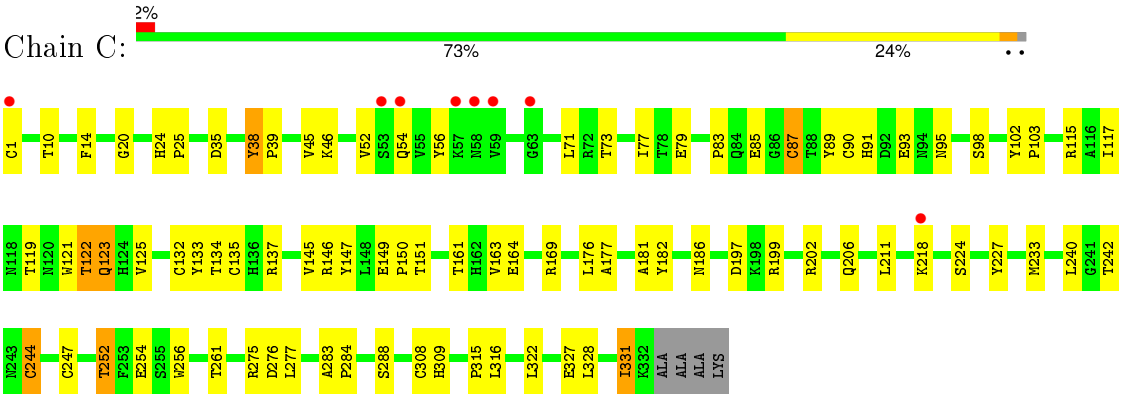
- Molecule 15 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	C	47	Total O 47 47	0	0
15	H	28	Total O 28 28	0	0
15	L	38	Total O 38 38	0	0
15	M	46	Total O 46 46	0	0

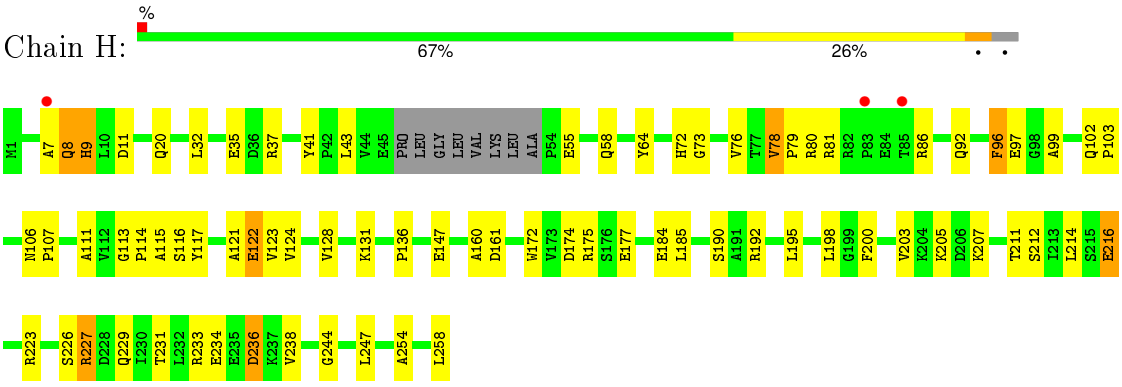
3 Residue-property plots (i)

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

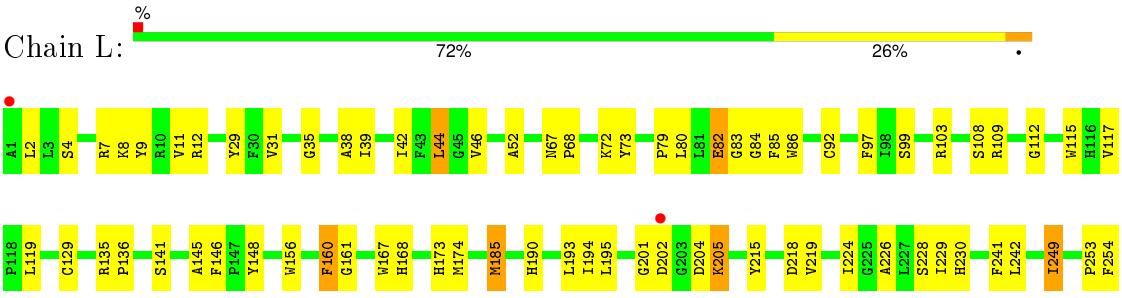
- Molecule 1: Photosynthetic reaction center cytochrome c subunit

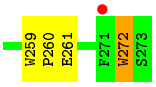


- Molecule 2: Reaction center protein H chain



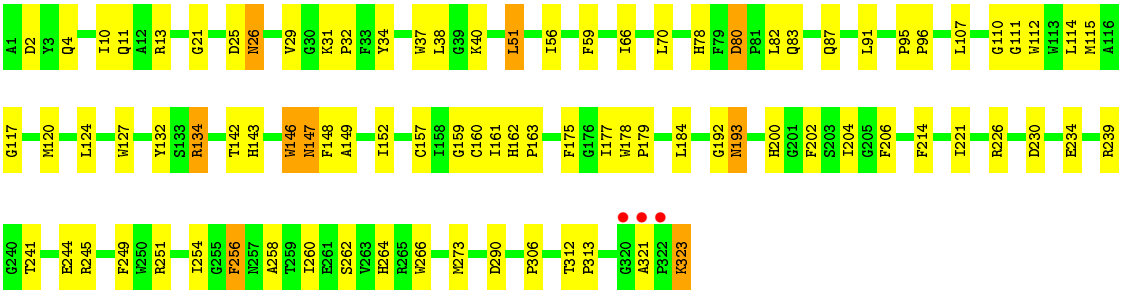
- Molecule 3: Reaction center protein L chain





• Molecule 4: Reaction center protein M chain

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	241.17Å 241.17Å 113.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.21 47.92 – 3.21	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-3.21) 99.6 (47.92-3.21)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.78 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.4.0073	Depositor
R, R_{free}	0.192 , 0.224 0.196 , 0.228	Depositor DCC
R_{free} test set	3141 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	74.4	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 68.8	EDS
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 62022 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10311	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LDA, BPB, HTO, BCB, MQ9, FE2, SO4, HEC, UQ1, FME, 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	0.53	1/2665 (0.0%)	0.64	0/3633
2	H	0.59	0/1993	0.68	0/2720
3	L	0.60	1/2259 (0.0%)	0.66	0/3084
4	M	0.57	0/2659	0.65	1/3637 (0.0%)
All	All	0.57	2/9576 (0.0%)	0.66	1/13074 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	87	CYS	CB-SG	-5.84	1.72	1.81
3	L	129	CYS	CB-SG	-5.38	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	70	LEU	CA-CB-CG	7.57	132.71	115.30

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	2598	0	2573	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1958	0	1946	65	0
3	L	2171	0	2098	64	0
4	M	2555	0	2452	76	0
5	C	35	0	0	0	0
5	H	20	0	0	1	0
5	M	20	0	0	1	0
6	M	1	0	0	0	0
7	C	172	0	125	31	0
8	C	20	0	32	1	0
8	H	10	0	16	2	0
9	H	32	0	62	6	0
9	L	16	0	31	2	0
9	M	16	0	31	0	0
10	L	132	0	144	24	0
10	M	132	0	144	27	0
11	L	65	0	74	9	0
11	M	65	0	74	20	0
12	L	36	0	36	4	0
13	M	58	0	80	3	0
14	M	40	0	60	11	0
15	C	47	0	0	9	0
15	H	28	0	0	5	0
15	L	38	0	0	3	0
15	M	46	0	0	7	0
All	All	10311	0	9978	337	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 17.

All (337) 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)
1:C:90:CYS:SG	7:C:401:HEC:HAC	1.31	1.69
1:C:132:CYS:SG	7:C:402:HEC:HAB	1.48	1.52
1:C:244:CYS:SG	7:C:403:HEC:HAB	1.54	1.47
1:C:132:CYS:SG	7:C:402:HEC:CAB	2.08	1.39
1:C:135:CYS:SG	7:C:402:HEC:CAC	2.12	1.37
1:C:90:CYS:SG	7:C:401:HEC:CAC	2.16	1.33
1:C:87:CYS:SG	7:C:401:HEC:HAB	1.77	1.24
1:C:135:CYS:SG	7:C:402:HEC:HAC	1.78	1.19
1:C:244:CYS:SG	7:C:403:HEC:CAB	2.37	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:CYS:SG	7:C:401:HEC:CAB	2.39	1.09
1:C:87:CYS:HG	7:C:401:HEC:HAB	1.05	1.00
3:L:193:LEU:HD23	12:L:502:UQ1:HM32	1.44	0.99
10:M:401:BCB:C2	11:M:402:BPB:HBBB	1.94	0.98
1:C:117:ILE:HD11	1:C:277:LEU:HD21	1.42	0.97
1:C:284:PRO:HA	15:C:857:HOH:O	1.65	0.96
3:L:205:LYS:H	3:L:205:LYS:HD3	1.28	0.96
1:C:132:CYS:HG	7:C:402:HEC:HAB	1.24	0.95
11:L:402:BPB:HMB	11:L:402:BPB:CBB	1.99	0.93
10:M:401:BCB:CBB	10:M:401:BCB:HMB1	1.99	0.93
1:C:123:GLN:HG2	15:C:854:HOH:O	1.69	0.93
10:L:401:BCB:HMB1	10:L:401:BCB:CBB	2.01	0.90
3:L:205:LYS:N	3:L:205:LYS:HD3	1.86	0.90
2:H:114:PRO:HG3	2:H:247:LEU:HD23	1.53	0.89
2:H:64:TYR:CE1	9:H:703:LDA:H31	2.07	0.88
10:L:400:BCB:CBB	10:L:400:BCB:HMB1	2.01	0.87
3:L:112:GLY:HA2	15:L:608:HOH:O	1.76	0.85
2:H:55:GLU:HB2	2:H:58:GLN:HE21	1.41	0.84
10:M:400:BCB:CBB	10:M:400:BCB:HHC	2.09	0.83
1:C:181:ALA:O	1:C:182:TYR:HB2	1.78	0.83
1:C:90:CYS:HG	7:C:401:HEC:HAC	1.39	0.83
7:C:401:HEC:HMB1	7:C:401:HEC:HBB3	1.62	0.82
2:H:92:GLN:HB2	15:H:901:HOH:O	1.81	0.81
4:M:260:ILE:HG22	15:M:816:HOH:O	1.81	0.81
4:M:159:GLY:HA3	14:M:600:NS5:H272	1.62	0.81
1:C:135:CYS:SG	7:C:402:HEC:C3C	2.68	0.81
3:L:83:GLY:HA2	15:L:638:HOH:O	1.82	0.80
4:M:258:ALA:HB1	4:M:262:SER:OG	1.84	0.76
2:H:227:ARG:HH11	2:H:227:ARG:CG	1.99	0.76
10:M:400:BCB:HBB2	10:M:400:BCB:HHC	1.69	0.74
10:L:400:BCB:O1A	10:L:401:BCB:HBC2	1.86	0.74
11:L:402:BPB:HBBB	11:L:402:BPB:HMB	1.69	0.73
2:H:64:TYR:HE1	9:H:703:LDA:H31	1.50	0.73
3:L:79:PRO:HG2	3:L:82:GLU:HG3	1.69	0.73
10:M:401:BCB:HMB1	10:M:401:BCB:HBB3	1.70	0.73
1:C:52:VAL:HB	1:C:56:TYR:HD2	1.53	0.73
2:H:76:VAL:HG13	2:H:80:ARG:HH12	1.55	0.72
10:L:400:BCB:HBD	10:L:400:BCB:HAA1	1.71	0.71
10:L:401:BCB:HMB1	10:L:401:BCB:HBB2	1.72	0.71
10:L:400:BCB:HBB3	10:L:400:BCB:HMB1	1.73	0.71
11:L:402:BPB:HBBA	11:L:402:BPB:HMB	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:401:BCB:HMB1	10:M:401:BCB:HBB2	1.71	0.71
7:C:403:HEC:HBC3	7:C:403:HEC:HMC1	1.72	0.71
1:C:322:LEU:HD12	15:C:834:HOH:O	1.89	0.70
11:M:402:BPB:CBB	11:M:402:BPB:HHC	2.22	0.70
2:H:203:VAL:HG11	4:M:10:ILE:HD11	1.74	0.70
10:M:400:BCB:CBB	14:M:600:NS5:H223	2.21	0.69
10:M:401:BCB:C1	11:M:402:BPB:CBB	2.71	0.69
2:H:227:ARG:HH11	2:H:227:ARG:HG3	1.56	0.69
4:M:26:ASN:OD1	15:M:840:HOH:O	2.10	0.69
10:L:401:BCB:HBB3	10:L:401:BCB:HMB1	1.73	0.69
1:C:133:TYR:CE1	1:C:137:ARG:HA	2.28	0.69
11:M:402:BPB:H7A	11:M:402:BPB:H4	1.75	0.69
3:L:205:LYS:CD	3:L:205:LYS:H	2.04	0.68
2:H:123:VAL:HG11	8:H:705:HTO:H52	1.75	0.68
10:L:400:BCB:HMB1	10:L:400:BCB:HBB2	1.74	0.68
10:M:401:BCB:H12	11:M:402:BPB:HBB	1.75	0.68
10:M:400:BCB:HBB2	14:M:600:NS5:H223	1.76	0.67
4:M:127:TRP:CD1	11:M:402:BPB:HBA	2.28	0.67
3:L:97:PHE:CE1	10:L:400:BCB:H121	2.30	0.66
4:M:107:LEU:HA	4:M:111:GLY:HA3	1.76	0.66
2:H:114:PRO:HG3	2:H:247:LEU:CD2	2.26	0.66
1:C:163:VAL:HG23	15:L:633:HOH:O	1.96	0.66
10:M:401:BCB:H12	11:M:402:BPB:CBB	2.26	0.65
1:C:77:ILE:CG2	7:C:401:HEC:HBC3	2.27	0.65
3:L:135:ARG:HB3	3:L:136:PRO:HD3	1.79	0.65
1:C:102:TYR:CD2	1:C:103:PRO:HD3	2.32	0.65
4:M:258:ALA:HB1	4:M:262:SER:HG	1.62	0.64
2:H:116:SER:HB3	3:L:8:LYS:HD2	1.80	0.64
2:H:227:ARG:HG3	2:H:227:ARG:NH1	2.11	0.64
3:L:224:ILE:HG12	3:L:228:SER:HB3	1.80	0.63
3:L:160:PHE:O	3:L:160:PHE:HD1	1.82	0.62
1:C:117:ILE:CD1	1:C:277:LEU:HD21	2.24	0.62
4:M:51:LEU:HD23	4:M:56:ILE:HD11	1.82	0.62
2:H:55:GLU:HB2	2:H:58:GLN:NE2	2.12	0.62
7:C:404:HEC:HBD2	7:C:404:HEC:HHA	1.82	0.62
10:M:401:BCB:C1	11:M:402:BPB:HBBB	2.29	0.61
4:M:147:ASN:C	4:M:147:ASN:HD22	2.04	0.61
2:H:114:PRO:CG	2:H:247:LEU:HD23	2.29	0.61
2:H:8:GLN:C	2:H:9:HIS:HD2	2.05	0.60
11:M:402:BPB:HMB	11:M:402:BPB:OBB	2.01	0.60
4:M:117:GLY:HA3	14:M:600:NS5:H28	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:123:VAL:HG12	2:H:124:VAL:N	2.17	0.59
1:C:132:CYS:SG	7:C:402:HEC:C3B	2.89	0.59
1:C:146:ARG:NH2	1:C:150:PRO:HA	2.18	0.59
1:C:242:THR:HA	15:C:843:HOH:O	2.02	0.59
2:H:64:TYR:CE1	9:H:703:LDA:H12	2.38	0.59
2:H:227:ARG:HB2	15:H:904:HOH:O	2.02	0.59
11:M:402:BPB:HBBB	11:M:402:BPB:HHC	1.83	0.58
3:L:201:GLY:O	3:L:202:ASP:HB2	2.02	0.58
1:C:161:THR:OG1	1:C:164:GLU:HG3	2.03	0.58
2:H:122:GLU:HA	2:H:122:GLU:OE1	2.04	0.58
9:H:703:LDA:HM12	15:H:574:HOH:O	2.04	0.58
1:C:117:ILE:HD11	1:C:277:LEU:CD2	2.26	0.57
10:L:400:BCB:CBD	10:L:400:BCB:HAA1	2.34	0.57
4:M:11:GLN:HB3	4:M:13:ARG:HH12	1.69	0.57
2:H:96:PHE:CE2	2:H:99:ALA:HB2	2.39	0.57
4:M:59:PHE:HA	11:M:402:BPB:H4A	1.86	0.57
1:C:283:ALA:N	1:C:284:PRO:CD	2.67	0.57
4:M:110:GLY:HA2	15:M:830:HOH:O	2.05	0.56
4:M:29:VAL:HG22	4:M:51:LEU:HD13	1.86	0.56
1:C:91:HIS:HE1	7:C:401:HEC:ND	2.00	0.56
1:C:73:THR:O	1:C:77:ILE:HG13	2.05	0.56
10:M:401:BCB:C2	11:M:402:BPB:CBB	2.76	0.56
4:M:132:TYR:CE1	4:M:142:THR:HG21	2.40	0.56
3:L:167:TRP:HE1	3:L:173:HIS:CD2	2.23	0.56
3:L:185:MET:HE3	11:M:402:BPB:NA	2.21	0.56
4:M:114:LEU:HD11	14:M:600:NS5:H351	1.87	0.56
3:L:79:PRO:CG	3:L:82:GLU:HG3	2.36	0.56
2:H:123:VAL:CG1	2:H:124:VAL:N	2.69	0.56
2:H:7:ALA:O	2:H:8:GLN:HG2	2.06	0.56
1:C:177:ALA:HA	15:C:822:HOH:O	2.06	0.55
4:M:120:MET:CE	4:M:175:PHE:HE1	2.20	0.55
4:M:226:ARG:HG3	15:M:825:HOH:O	2.06	0.55
4:M:117:GLY:CA	14:M:600:NS5:H28	2.36	0.54
1:C:95:ASN:CG	1:C:98:SER:HB2	2.28	0.54
3:L:8:LYS:HE2	3:L:9:TYR:CE2	2.42	0.54
4:M:59:PHE:HA	11:M:402:BPB:C4	2.38	0.54
10:L:400:BCB:H11	10:L:401:BCB:H2C	1.91	0.53
4:M:323:LYS:HD3	4:M:323:LYS:N	2.22	0.53
3:L:80:LEU:HD23	3:L:85:PHE:CE1	2.43	0.53
1:C:1:CYS:HA	15:C:861:HOH:O	2.07	0.53
4:M:162:HIS:HB3	4:M:163:PRO:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:ASP:HB3	1:C:275:ARG:HD3	1.91	0.53
2:H:37:ARG:HG2	2:H:41:TYR:CE1	2.45	0.52
4:M:206:PHE:CD2	4:M:273:MET:HB3	2.44	0.52
1:C:169:ARG:HE	4:M:78:HIS:CE1	2.27	0.52
1:C:115:ARG:HA	1:C:328:LEU:O	2.08	0.52
4:M:2:ASP:OD1	4:M:4:GLN:HB2	2.09	0.52
10:M:401:BCB:C3	11:M:402:BPB:HBBB	2.37	0.52
1:C:52:VAL:HB	1:C:56:TYR:CD2	2.41	0.52
2:H:136:PRO:HA	2:H:172:TRP:HA	1.91	0.52
2:H:128:VAL:O	2:H:128:VAL:HG22	2.10	0.52
3:L:195:LEU:HB3	4:M:143:HIS:CD2	2.45	0.52
1:C:182:TYR:CG	3:L:261:GLU:HA	2.45	0.52
2:H:117:TYR:HB2	2:H:236:ASP:HB3	1.91	0.52
1:C:224:SER:HA	1:C:227:TYR:HD1	1.73	0.52
1:C:182:TYR:CE1	3:L:261:GLU:HG3	2.45	0.52
10:L:400:BCB:H2C	10:M:401:BCB:H2C	1.92	0.52
2:H:121:ALA:C	2:H:123:VAL:H	2.14	0.51
10:M:400:BCB:HBB3	10:M:401:BCB:H41	1.91	0.51
4:M:95:PRO:HB2	4:M:96:PRO:HD2	1.92	0.51
10:M:400:BCB:HBB1	14:M:600:NS5:H223	1.92	0.51
1:C:206:GLN:HG2	8:C:706:HTO:H61	1.93	0.51
10:L:400:BCB:H152	11:L:402:BPB:H44	1.93	0.51
4:M:120:MET:HE3	4:M:175:PHE:HE1	1.75	0.51
4:M:34:TYR:N	4:M:34:TYR:CD1	2.79	0.51
3:L:160:PHE:HD1	3:L:160:PHE:C	2.15	0.51
3:L:86:TRP:CZ2	3:L:145:ALA:CB	2.93	0.51
2:H:161:ASP:HB3	2:H:214:LEU:HD22	1.93	0.51
2:H:72:HIS:HB2	8:H:705:HTO:H42	1.92	0.50
3:L:80:LEU:HA	3:L:84:GLY:HA3	1.94	0.50
2:H:102:GLN:HB2	2:H:103:PRO:HD2	1.93	0.50
4:M:110:GLY:CA	15:M:830:HOH:O	2.59	0.50
1:C:233:MET:HB3	7:C:403:HEC:C4B	2.41	0.50
4:M:192:GLY:O	4:M:193:ASN:HB3	2.12	0.50
3:L:39:ILE:HD12	13:M:501:MQ9:H43	1.93	0.50
1:C:102:TYR:N	1:C:103:PRO:CD	2.75	0.50
15:H:555:HOH:O	4:M:234:GLU:HB2	2.11	0.50
1:C:121:TRP:O	1:C:125:VAL:HG22	2.12	0.50
2:H:76:VAL:HG13	2:H:80:ARG:NH1	2.23	0.50
1:C:35:ASP:OD2	1:C:316:LEU:HA	2.13	0.49
3:L:160:PHE:CD1	3:L:160:PHE:C	2.84	0.49
3:L:109:ARG:HD3	3:L:115:TRP:CZ2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:CYS:CB	7:C:403:HEC:HAB	2.38	0.49
10:M:400:BCB:HHC	10:M:400:BCB:HBB3	1.90	0.49
4:M:200:HIS:CE1	4:M:204:ILE:HD11	2.47	0.49
2:H:8:GLN:O	2:H:9:HIS:HD2	1.96	0.49
1:C:252:THR:HA	15:C:817:HOH:O	2.12	0.49
2:H:231:THR:OG1	2:H:234:GLU:HG3	2.11	0.49
7:C:402:HEC:HBC3	7:C:402:HEC:HMC1	1.94	0.48
10:L:401:BCB:OBB	10:L:401:BCB:HHC	2.13	0.48
3:L:167:TRP:NE1	3:L:173:HIS:CD2	2.81	0.48
3:L:52:ALA:HB2	3:L:85:PHE:CD2	2.47	0.48
2:H:136:PRO:HD3	2:H:172:TRP:CZ3	2.48	0.48
7:C:401:HEC:CMB	7:C:401:HEC:HBB3	2.38	0.48
3:L:194:ILE:HG13	4:M:264:HIS:CD2	2.49	0.48
4:M:178:TRP:N	4:M:179:PRO:CD	2.76	0.48
3:L:259:TRP:O	3:L:260:PRO:C	2.52	0.48
10:M:400:BCB:HBA1	10:M:400:BCB:C4A	2.44	0.48
4:M:256:PHE:N	4:M:256:PHE:CD1	2.82	0.48
4:M:83:GLN:HB3	4:M:87:GLN:HE21	1.78	0.48
3:L:35:GLY:CA	3:L:103:ARG:HD2	2.44	0.48
2:H:8:GLN:C	2:H:9:HIS:CD2	2.87	0.48
1:C:87:CYS:C	1:C:89:TYR:H	2.16	0.47
1:C:87:CYS:SG	7:C:401:HEC:C3B	3.00	0.47
10:L:401:BCB:HBA1	10:L:401:BCB:C4A	2.44	0.47
4:M:204:ILE:HG12	10:M:401:BCB:CHB	2.44	0.47
2:H:113:GLY:C	2:H:115:ALA:H	2.16	0.47
10:M:400:BCB:HMB1	10:M:400:BCB:OBB	2.15	0.47
1:C:90:CYS:SG	7:C:401:HEC:C3C	2.97	0.47
12:L:502:UQ1:O4	12:L:502:UQ1:HM33	2.15	0.47
2:H:96:PHE:HD2	2:H:96:PHE:H	1.62	0.47
10:L:400:BCB:H203	10:L:400:BCB:H161	1.57	0.47
10:L:401:BCB:HMD2	10:M:401:BCB:HBB3	1.95	0.47
2:H:234:GLU:O	2:H:238:VAL:HG23	2.14	0.47
10:L:400:BCB:H112	10:L:401:BCB:HBB2	1.96	0.47
1:C:308:CYS:O	1:C:315:PRO:HB3	2.14	0.47
3:L:67:ASN:HB3	3:L:68:PRO:HD2	1.97	0.47
4:M:184:LEU:HD21	10:M:400:BCB:CAC	2.45	0.47
1:C:133:TYR:O	1:C:134:THR:C	2.53	0.47
2:H:190:SER:HB3	2:H:192:ARG:HG2	1.96	0.47
2:H:131:LYS:HE3	2:H:175:ARG:HH12	1.79	0.47
4:M:160:CYS:SG	14:M:600:NS5:H322	2.55	0.47
3:L:215:TYR:O	3:L:219:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:112:TRP:O	4:M:115:MET:HB2	2.15	0.47
1:C:276:ASP:O	1:C:277:LEU:C	2.52	0.47
1:C:119:THR:HG21	1:C:331:ILE:HG22	1.98	0.46
3:L:146:PHE:HB3	3:L:156:TRP:CD2	2.51	0.46
1:C:87:CYS:C	1:C:89:TYR:N	2.69	0.46
1:C:123:GLN:CG	15:C:854:HOH:O	2.43	0.46
1:C:10:THR:O	1:C:20:GLY:HA3	2.15	0.46
11:L:402:BPB:H6A	11:L:402:BPB:H2	1.60	0.46
1:C:115:ARG:NH1	1:C:327:GLU:O	2.47	0.46
3:L:35:GLY:HA2	3:L:103:ARG:HD2	1.98	0.46
3:L:242:LEU:HA	3:L:242:LEU:HD23	1.77	0.46
1:C:102:TYR:CG	1:C:103:PRO:HD3	2.51	0.46
4:M:21:GLY:HA3	15:M:835:HOH:O	2.15	0.46
3:L:52:ALA:CB	3:L:85:PHE:CD2	2.99	0.46
3:L:249:ILE:HA	3:L:249:ILE:HD13	1.80	0.46
2:H:64:TYR:CD1	9:H:703:LDA:H31	2.50	0.45
3:L:230:HIS:CD2	4:M:221:ILE:HG13	2.51	0.45
11:M:402:BPB:H55	11:M:402:BPB:HMC	1.98	0.45
2:H:20:GLN:HG2	4:M:202:PHE:CE2	2.51	0.45
9:L:702:LDA:H21	9:L:702:LDA:HM11	1.50	0.45
4:M:124:LEU:HD21	10:M:401:BCB:H112	1.98	0.45
2:H:216:GLU:HG3	2:H:216:GLU:H	1.54	0.45
4:M:239:ARG:HD3	4:M:244:GLU:HG2	1.99	0.45
1:C:79:GLU:HA	1:C:83:PRO:HB3	1.98	0.45
3:L:190:HIS:HD1	12:L:502:UQ1:HM33	1.82	0.45
3:L:241:PHE:CE2	11:L:402:BPB:H43	2.52	0.45
3:L:253:PRO:HB2	3:L:254:PHE:CD2	2.51	0.45
2:H:254:ALA:HB2	15:H:562:HOH:O	2.17	0.45
3:L:168:HIS:CE1	10:L:400:BCB:HHC	2.52	0.44
4:M:323:LYS:H	4:M:323:LYS:CD	2.29	0.44
2:H:172:TRP:HE1	2:H:184:GLU:HB2	1.82	0.44
4:M:157:CYS:HA	4:M:161:ILE:HB	1.98	0.44
3:L:272:TRP:HB3	4:M:82:LEU:HD21	1.97	0.44
1:C:150:PRO:HG3	1:C:176:LEU:HD13	1.99	0.44
2:H:172:TRP:CE2	2:H:195:LEU:HD21	2.52	0.44
2:H:113:GLY:CA	3:L:11:VAL:HG11	2.47	0.44
4:M:160:CYS:C	4:M:163:PRO:HD2	2.38	0.44
2:H:41:TYR:CE2	2:H:43:LEU:HD21	2.53	0.44
2:H:174:ASP:O	2:H:177:GLU:O	2.35	0.44
11:L:402:BPB:OBB	11:L:402:BPB:HHC	2.18	0.44
3:L:42:ILE:O	3:L:46:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:198:LEU:HA	2:H:198:LEU:HD23	1.82	0.44
1:C:38:TYR:HD1	1:C:39:PRO:HD2	1.82	0.44
1:C:202:ARG:HH12	1:C:256:TRP:HE1	1.64	0.44
3:L:38:ALA:HB2	3:L:99:SER:HB3	2.00	0.43
10:M:401:BCB:HHC	10:M:401:BCB:OBB	2.17	0.43
2:H:200:PHE:CZ	4:M:226:ARG:HD3	2.53	0.43
1:C:240:LEU:HD22	1:C:309:HIS:CG	2.53	0.43
3:L:168:HIS:HE1	10:L:400:BCB:OBB	2.01	0.43
4:M:143:HIS:ND1	4:M:143:HIS:N	2.66	0.43
10:M:401:BCB:CBB	10:M:401:BCB:CMB	2.80	0.43
3:L:174:MET:HE3	10:M:400:BCB:HED3	2.01	0.43
10:L:400:BCB:H41	10:L:400:BCB:H62	1.41	0.43
4:M:254:ILE:HD12	4:M:256:PHE:CE1	2.54	0.43
3:L:29:TYR:CG	13:M:501:MQ9:H33	2.53	0.43
3:L:226:ALA:O	3:L:229:ILE:HG22	2.18	0.43
3:L:218:ASP:HB3	4:M:134:ARG:HD2	2.01	0.43
2:H:160:ALA:HB3	2:H:214:LEU:HD23	2.00	0.43
3:L:168:HIS:HD2	15:M:809:HOH:O	2.01	0.42
2:H:8:GLN:CG	2:H:8:GLN:O	2.66	0.42
4:M:323:LYS:N	4:M:323:LYS:CD	2.82	0.42
3:L:44:LEU:HB3	3:L:92:CYS:SG	2.59	0.42
11:L:402:BPB:H55	11:L:402:BPB:HMC	2.02	0.42
4:M:323:LYS:H	4:M:323:LYS:CE	2.32	0.42
3:L:72:LYS:HE3	3:L:73:TYR:CE2	2.54	0.42
7:C:403:HEC:CMC	7:C:403:HEC:HBC3	2.45	0.42
4:M:80:ASP:C	4:M:80:ASP:OD1	2.58	0.42
4:M:241:THR:O	4:M:245:ARG:HG3	2.19	0.42
10:L:401:BCB:HBC3	10:L:401:BCB:HMC1	2.00	0.42
4:M:127:TRP:NE1	11:M:402:BPB:HBA	2.34	0.42
3:L:52:ALA:HB2	3:L:85:PHE:CG	2.54	0.42
4:M:251:ARG:HA	4:M:256:PHE:O	2.19	0.42
3:L:185:MET:HE1	11:M:402:BPB:HMAB	2.02	0.42
1:C:93:GLU:H	1:C:93:GLU:HG2	1.66	0.42
11:M:402:BPB:CHC	11:M:402:BPB:CBB	2.94	0.42
3:L:86:TRP:CZ2	3:L:145:ALA:HB3	2.55	0.42
4:M:178:TRP:HA	4:M:178:TRP:CE3	2.55	0.42
2:H:8:GLN:O	2:H:9:HIS:CD2	2.72	0.42
2:H:115:ALA:HB2	2:H:244:GLY:HA3	2.02	0.42
9:L:702:LDA:H22	9:L:702:LDA:H52	1.80	0.42
12:L:502:UQ1:HM51	12:L:502:UQ1:H71	1.72	0.42
14:M:600:NS5:H41	14:M:600:NS5:H81	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:CYS:HA	1:C:261:THR:OG1	2.20	0.42
1:C:24:HIS:O	1:C:25:PRO:C	2.58	0.42
4:M:146:TRP:O	4:M:149:ALA:HB3	2.20	0.42
11:M:402:BPB:HMC	11:M:402:BPB:CBC	2.50	0.41
1:C:102:TYR:N	1:C:103:PRO:HD2	2.35	0.41
7:C:404:HEC:CHA	7:C:404:HEC:HBD2	2.49	0.41
2:H:102:GLN:HB2	2:H:102:GLN:HE21	1.69	0.41
1:C:147:TYR:C	1:C:149:GLU:H	2.22	0.41
13:M:501:MQ9:C8	13:M:501:MQ9:H5M3	2.50	0.41
4:M:37:TRP:HD1	5:M:805:SO4:O1	2.02	0.41
1:C:132:CYS:CB	7:C:402:HEC:HAB	2.40	0.41
1:C:206:GLN:HE22	1:C:254:GLU:HB2	1.85	0.41
1:C:145:VAL:O	1:C:146:ARG:HD2	2.19	0.41
1:C:14:PHE:CD2	4:M:306:PRO:HD2	2.55	0.41
4:M:66:ILE:HG23	14:M:600:NS5:H82	2.01	0.41
1:C:85:GLU:O	1:C:85:GLU:HG3	2.20	0.41
4:M:38:LEU:HD12	4:M:38:LEU:HA	1.79	0.41
2:H:233:ARG:HD3	5:H:807:SO4:O4	2.20	0.41
1:C:132:CYS:CB	7:C:402:HEC:CAB	2.97	0.41
3:L:195:LEU:CB	4:M:143:HIS:CD2	3.04	0.41
2:H:64:TYR:OH	9:H:703:LDA:HM11	2.21	0.41
4:M:95:PRO:CB	4:M:96:PRO:HD2	2.50	0.41
2:H:86:ARG:NH2	2:H:111:ALA:HB3	2.36	0.41
1:C:71:LEU:HD23	1:C:71:LEU:HA	1.97	0.41
1:C:122:THR:HG22	15:C:847:HOH:O	2.21	0.41
2:H:32:LEU:HD13	4:M:266:TRP:CD2	2.55	0.41
3:L:148:TYR:CE1	11:L:402:BPB:H14B	2.56	0.41
2:H:113:GLY:HA2	3:L:11:VAL:HG13	2.03	0.41
2:H:106:ASN:HA	2:H:107:PRO:HD2	1.87	0.41
2:H:226:SER:HB2	2:H:229:GLN:HG2	2.03	0.41
1:C:133:TYR:CD1	1:C:137:ARG:HA	2.55	0.41
4:M:87:GLN:O	4:M:91:LEU:HG	2.20	0.41
4:M:148:PHE:CZ	4:M:152:ILE:HD11	2.56	0.41
4:M:312:THR:HA	4:M:313:PRO:HD3	1.88	0.41
10:L:400:BCB:H141	10:L:400:BCB:H162	1.92	0.40
3:L:161:GLY:HA3	10:L:400:BCB:HAC1	2.03	0.40
1:C:77:ILE:HG22	7:C:401:HEC:HBC3	2.00	0.40
4:M:239:ARG:HD3	4:M:244:GLU:CG	2.51	0.40
3:L:117:VAL:HG11	4:M:249:PHE:CE2	2.57	0.40
4:M:160:CYS:SG	14:M:600:NS5:H29	2.60	0.40
2:H:78:VAL:HA	2:H:79:PRO:C	2.41	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	330/336 (98%)	294 (89%)	35 (11%)	1 (0%)	46	84
2	H	246/258 (95%)	220 (89%)	22 (9%)	4 (2%)	12	54
3	L	271/273 (99%)	246 (91%)	24 (9%)	1 (0%)	39	80
4	M	321/323 (99%)	290 (90%)	26 (8%)	5 (2%)	12	54
All	All	1168/1190 (98%)	1050 (90%)	107 (9%)	11 (1%)	21	67

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	147	GLU
2	H	73	GLY
4	M	32	PRO
4	M	51	LEU
4	M	193	ASN
1	C	186	ASN
4	M	321	ALA
2	H	35	GLU
2	H	122	GLU
4	M	177	ILE
3	L	31	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	280/282 (99%)	266 (95%)	14 (5%)	30 71
2	H	205/212 (97%)	188 (92%)	17 (8%)	14 49
3	L	218/218 (100%)	203 (93%)	15 (7%)	19 59
4	M	249/249 (100%)	236 (95%)	13 (5%)	29 69
All	All	952/961 (99%)	893 (94%)	59 (6%)	23 64

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	38	TYR
1	C	45	VAL
1	C	46	LYS
1	C	54	GLN
1	C	122	THR
1	C	123	GLN
1	C	151	THR
1	C	199	ARG
1	C	211	LEU
1	C	218	LYS
1	C	244	CYS
1	C	252	THR
1	C	288	SER
1	C	331	ILE
2	H	8	GLN
2	H	9	HIS
2	H	11	ASP
2	H	78	VAL
2	H	81	ARG
2	H	96	PHE
2	H	97	GLU
2	H	185	LEU
2	H	205	LYS
2	H	207	LYS
2	H	211	THR
2	H	212	SER
2	H	216	GLU
2	H	223	ARG
2	H	227	ARG
2	H	236	ASP
2	H	258	LEU
3	L	2	LEU
3	L	4	SER

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Mol	Chain	Res	Type
3	L	7	ARG
3	L	12	ARG
3	L	44	LEU
3	L	82	GLU
3	L	108	SER
3	L	119	LEU
3	L	141	SER
3	L	160	PHE
3	L	185	MET
3	L	204	ASP
3	L	205	LYS
3	L	249	ILE
3	L	272	TRP
4	M	25	ASP
4	M	26	ASN
4	M	31	LYS
4	M	40	LYS
4	M	80	ASP
4	M	134	ARG
4	M	146	TRP
4	M	147	ASN
4	M	214	PHE
4	M	230	ASP
4	M	256	PHE
4	M	290	ASP
4	M	323	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	37	GLN
1	C	54	GLN
1	C	123	GLN
1	C	206	GLN
1	C	302	GLN
2	H	9	HIS
2	H	58	GLN
2	H	102	GLN
2	H	106	ASN
2	H	225	GLN
3	L	55	GLN
3	L	168	HIS

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Mol	Chain	Res	Type
3	L	183	ASN
3	L	239	ASN
4	M	4	GLN
4	M	9	GLN
4	M	78	HIS
4	M	147	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FME	H	1	2	8,9,10	0.76	0	6,9,11	4.06	3 (50%)

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

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	1	FME	CA-N-CN	-9.15	108.76	122.82
2	H	1	FME	O1-CN-N	-2.66	120.92	124.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	1	FME	CE-SD-CG	2.42	108.62	100.37

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	1	FME	O1-CN-N-CA

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 37 ligands modelled in this entry, 1 is monoatomic - leaving 36 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	HEC	C	401	1	24,50,50	2.12	2 (8%)	19,82,82	2.89	3 (15%)
7	HEC	C	402	1	24,50,50	1.91	2 (8%)	19,82,82	2.91	5 (26%)
7	HEC	C	403	1	24,50,50	1.87	3 (12%)	19,82,82	2.69	3 (15%)
7	HEC	C	404	1	24,50,50	1.89	3 (12%)	19,82,82	2.87	6 (31%)
8	HTO	C	706	-	9,9,9	0.26	0	8,10,10	0.65	0
8	HTO	C	707	-	9,9,9	0.62	0	8,10,10	0.56	0
5	SO4	C	808	-	4,4,4	0.17	0	6,6,6	0.22	0
5	SO4	C	809	-	4,4,4	0.19	0	6,6,6	0.09	0
5	SO4	C	810	-	4,4,4	0.18	0	6,6,6	0.07	0
5	SO4	C	811	-	4,4,4	0.16	0	6,6,6	0.16	0
5	SO4	C	813	-	4,4,4	0.21	0	6,6,6	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	SO4	C	814	-	4,4,4	0.09	0	6,6,6	0.36	0
5	SO4	C	815	-	4,4,4	0.11	0	6,6,6	0.20	0
9	LDA	H	701	-	15,15,15	3.77	2 (13%)	16,17,17	0.79	1 (6%)
9	LDA	H	703	-	15,15,15	3.66	2 (13%)	16,17,17	1.16	2 (12%)
8	HTO	H	705	-	9,9,9	0.65	0	8,10,10	0.83	0
5	SO4	H	803	-	4,4,4	0.21	0	6,6,6	0.25	0
5	SO4	H	806	-	4,4,4	0.18	0	6,6,6	0.27	0
5	SO4	H	807	-	4,4,4	0.20	0	6,6,6	0.26	0
5	SO4	H	812	-	4,4,4	0.13	0	6,6,6	0.12	0
10	BCB	L	400	3	56,74,74	2.55	7 (12%)	57,115,115	1.66	12 (21%)
10	BCB	L	401	3	56,74,74	2.46	6 (10%)	57,115,115	1.83	9 (15%)
11	BPB	L	402	-	63,70,70	2.44	8 (12%)	63,101,101	2.87	18 (28%)
12	UQ1	L	502	-	18,18,18	1.80	2 (11%)	22,25,25	1.17	3 (13%)
12	UQ1	L	503	-	18,18,18	1.85	2 (11%)	22,25,25	1.07	1 (4%)
9	LDA	L	702	-	15,15,15	3.93	2 (13%)	16,17,17	0.68	0
10	BCB	M	400	4	56,74,74	2.50	7 (12%)	57,115,115	1.73	10 (17%)
10	BCB	M	401	4	56,74,74	2.67	7 (12%)	57,115,115	1.69	13 (22%)
11	BPB	M	402	-	63,70,70	2.39	9 (14%)	63,101,101	2.93	16 (25%)
13	MQ9	M	501	-	59,59,59	1.95	20 (33%)	74,75,75	1.64	20 (27%)
14	NS5	M	600	-	39,39,39	1.51	3 (7%)	44,46,46	1.91	12 (27%)
9	LDA	M	704	-	15,15,15	4.07	2 (13%)	16,17,17	1.34	2 (12%)
5	SO4	M	801	-	4,4,4	0.26	0	6,6,6	0.48	0
5	SO4	M	802	-	4,4,4	0.22	0	6,6,6	0.32	0
5	SO4	M	804	-	4,4,4	0.18	0	6,6,6	0.18	0
5	SO4	M	805	-	4,4,4	0.25	0	6,6,6	0.33	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	HEC	C	401	1	-	0/6/54/54	0/0/8/8
7	HEC	C	402	1	-	0/6/54/54	0/0/8/8
7	HEC	C	403	1	-	0/6/54/54	0/0/8/8
7	HEC	C	404	1	-	0/6/54/54	0/0/8/8
8	HTO	C	706	-	-	0/10/10/10	0/0/0/0
8	HTO	C	707	-	-	0/10/10/10	0/0/0/0
5	SO4	C	808	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	C	809	-	-	0/0/0/0	0/0/0/0
5	SO4	C	810	-	-	0/0/0/0	0/0/0/0
5	SO4	C	811	-	-	0/0/0/0	0/0/0/0
5	SO4	C	813	-	-	0/0/0/0	0/0/0/0
5	SO4	C	814	-	-	0/0/0/0	0/0/0/0
5	SO4	C	815	-	-	0/0/0/0	0/0/0/0
9	LDA	H	701	-	-	0/13/13/13	0/0/0/0
9	LDA	H	703	-	-	0/13/13/13	0/0/0/0
8	HTO	H	705	-	-	0/10/10/10	0/0/0/0
5	SO4	H	803	-	-	0/0/0/0	0/0/0/0
5	SO4	H	806	-	-	0/0/0/0	0/0/0/0
5	SO4	H	807	-	-	0/0/0/0	0/0/0/0
5	SO4	H	812	-	-	0/0/0/0	0/0/0/0
10	BCB	L	400	3	-	0/37/137/137	0/0/9/9
10	BCB	L	401	3	-	0/37/137/137	0/0/9/9
11	BPB	L	402	-	-	0/46/105/105	0/1/6/6
12	UQ1	L	502	-	-	0/9/33/33	0/1/1/1
12	UQ1	L	503	-	-	0/9/33/33	0/1/1/1
9	LDA	L	702	-	-	0/13/13/13	0/0/0/0
10	BCB	M	400	4	-	0/37/137/137	0/0/9/9
10	BCB	M	401	4	-	0/37/137/137	0/0/9/9
11	BPB	M	402	-	-	0/46/105/105	0/1/6/6
13	MQ9	M	501	-	-	0/53/73/73	0/2/2/2
14	NS5	M	600	-	-	0/43/43/43	0/0/0/0
9	LDA	M	704	-	-	0/13/13/13	0/0/0/0
5	SO4	M	801	-	-	0/0/0/0	0/0/0/0
5	SO4	M	802	-	-	0/0/0/0	0/0/0/0
5	SO4	M	804	-	-	0/0/0/0	0/0/0/0
5	SO4	M	805	-	-	0/0/0/0	0/0/0/0

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	704	LDA	O1-N1	-15.43	1.24	1.39
9	L	702	LDA	O1-N1	-14.96	1.25	1.39
9	H	701	LDA	O1-N1	-14.28	1.26	1.39
9	H	703	LDA	O1-N1	-13.49	1.26	1.39
7	C	401	HEC	C3B-C2B	-6.89	1.33	1.40
7	C	402	HEC	C3B-C2B	-6.72	1.33	1.40
7	C	401	HEC	C3C-C2C	-6.12	1.34	1.40
10	M	401	BCB	C4D-CHA	-5.94	1.37	1.45
10	L	401	BCB	C4D-CHA	-5.87	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	403	HEC	C3C-C2C	-5.75	1.34	1.40
7	C	404	HEC	C3C-C2C	-5.74	1.34	1.40
7	C	404	HEC	C3B-C2B	-5.60	1.34	1.40
10	M	400	BCB	C4D-CHA	-5.49	1.38	1.45
7	C	403	HEC	C3B-C2B	-5.43	1.35	1.40
10	L	400	BCB	C4D-CHA	-5.04	1.38	1.45
10	M	400	BCB	C2C-C1C	-4.92	1.47	1.51
7	C	402	HEC	C3C-C2C	-4.69	1.35	1.40
13	M	501	MQ9	C3-C4	-4.42	1.39	1.48
13	M	501	MQ9	C7-C8	-4.17	1.44	1.50
13	M	501	MQ9	C2-C1	-3.60	1.41	1.48
9	H	703	LDA	C1-N1	-3.55	1.44	1.51
13	M	501	MQ9	C5-C4	-3.49	1.40	1.48
13	M	501	MQ9	C6-C1	-3.26	1.38	1.47
13	M	501	MQ9	C32-C33	-2.73	1.42	1.50
10	L	400	BCB	C2C-C1C	-2.70	1.49	1.51
13	M	501	MQ9	C27-C28	-2.66	1.43	1.50
9	M	704	LDA	C1-N1	-2.64	1.46	1.51
13	M	501	MQ9	C22-C23	-2.53	1.43	1.50
13	M	501	MQ9	C17-C18	-2.47	1.43	1.50
11	L	402	BPB	C3D-C4D	-2.41	1.35	1.43
11	M	402	BPB	C3D-C4D	-2.41	1.35	1.43
9	H	701	LDA	C1-N1	-2.39	1.47	1.51
9	L	702	LDA	C1-N1	-2.35	1.47	1.51
11	L	402	BPB	C4D-CHA	-2.32	1.38	1.44
10	M	401	BCB	C3A-C2A	-2.28	1.47	1.54
11	M	402	BPB	C3D-C2D	-2.20	1.32	1.38
11	M	402	BPB	C4D-CHA	-2.06	1.39	1.44
13	M	501	MQ9	C37-C38	-2.02	1.44	1.50
13	M	501	MQ9	C47-C48	-2.01	1.44	1.50
7	C	404	HEC	C4C-NC	2.02	1.39	1.36
10	L	401	BCB	C2-C3	2.04	1.37	1.33
11	L	402	BPB	C4C-C3C	2.07	1.50	1.45
10	M	400	BCB	C4C-C3C	2.17	1.49	1.45
10	L	400	BCB	C4C-NC	2.18	1.41	1.37
7	C	403	HEC	C3B-C4B	2.20	1.47	1.42
13	M	501	MQ9	C33-C34	2.28	1.37	1.33
10	M	401	BCB	C4C-C3C	2.28	1.49	1.45
10	M	401	BCB	C2-C3	2.36	1.37	1.33
11	M	402	BPB	C1D-ND	2.39	1.43	1.38
11	L	402	BPB	C1D-ND	2.42	1.43	1.38
11	M	402	BPB	C3B-C4B	2.45	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	401	BCB	C4C-NC	2.49	1.42	1.37
13	M	501	MQ9	C48-C49	2.55	1.40	1.32
10	M	400	BCB	C2-C3	2.64	1.38	1.33
14	M	600	NS5	C4-C5	2.73	1.57	1.51
10	L	400	BCB	C2-C3	2.86	1.38	1.33
11	M	402	BPB	C2-C3	3.00	1.38	1.33
13	M	501	MQ9	C8-C9	3.03	1.38	1.33
14	M	600	NS5	C7-C5	3.05	1.38	1.33
13	M	501	MQ9	C23-C24	3.25	1.39	1.33
13	M	501	MQ9	C28-C29	3.29	1.39	1.33
12	L	502	UQ1	C3-C2	3.37	1.50	1.35
11	L	402	BPB	C2-C3	3.39	1.39	1.33
13	M	501	MQ9	C13-C14	3.44	1.39	1.33
13	M	501	MQ9	C38-C39	3.46	1.39	1.33
12	L	503	UQ1	C3-C2	3.54	1.51	1.35
13	M	501	MQ9	C18-C19	3.61	1.40	1.33
10	L	400	BCB	O2D-CGD	3.67	1.42	1.33
11	M	402	BPB	O2D-CGD	3.79	1.42	1.33
10	M	400	BCB	O2D-CGD	3.90	1.43	1.33
10	L	401	BCB	O2A-CGA	3.95	1.45	1.33
11	L	402	BPB	O2A-CGA	4.00	1.45	1.33
10	L	400	BCB	O2A-CGA	4.02	1.45	1.33
13	M	501	MQ9	C43-C44	4.11	1.41	1.33
10	M	401	BCB	O2A-CGA	4.28	1.46	1.33
10	L	401	BCB	O2D-CGD	4.33	1.44	1.33
10	M	401	BCB	O2D-CGD	4.34	1.44	1.33
10	M	400	BCB	O2A-CGA	4.41	1.46	1.33
11	M	402	BPB	O2A-CGA	4.47	1.46	1.33
11	L	402	BPB	O2D-CGD	4.65	1.45	1.33
12	L	503	UQ1	C6-C5	6.22	1.50	1.35
12	L	502	UQ1	C6-C5	6.26	1.50	1.35
14	M	600	NS5	C35-C36	6.99	1.53	1.32
10	M	400	BCB	CAC-C3C	14.83	1.51	1.33
10	L	401	BCB	CAC-C3C	14.88	1.51	1.33
11	M	402	BPB	CAC-C3C	16.15	1.53	1.33
10	L	400	BCB	CAC-C3C	16.17	1.53	1.33
11	L	402	BPB	CAC-C3C	16.21	1.53	1.33
10	M	401	BCB	CAC-C3C	16.38	1.53	1.33

All (136) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	402	HEC	CBB-CAB-C3B	-8.70	108.01	127.35
7	C	401	HEC	CBC-CAC-C3C	-8.64	108.15	127.35
7	C	404	HEC	CBB-CAB-C3B	-7.79	110.03	127.35
7	C	403	HEC	CBB-CAB-C3B	-7.55	110.57	127.35
7	C	401	HEC	CBB-CAB-C3B	-7.38	110.94	127.35
7	C	403	HEC	CBC-CAC-C3C	-7.09	111.60	127.35
7	C	402	HEC	CBC-CAC-C3C	-6.82	112.20	127.35
7	C	404	HEC	CBC-CAC-C3C	-6.77	112.31	127.35
11	M	402	BPB	C3D-C2D-C1D	-6.09	95.98	105.77
11	L	402	BPB	C3D-C2D-C1D	-5.82	96.42	105.77
14	M	600	NS5	C19-C20-C21	-5.16	119.75	127.20
10	L	401	BCB	O1D-CGD-CBD	-4.09	118.76	124.62
11	L	402	BPB	O1D-CGD-CBD	-4.09	118.76	124.62
13	M	501	MQ9	C32-C33-C34	-3.96	119.15	127.76
11	M	402	BPB	O1D-CGD-CBD	-3.93	118.98	124.62
10	L	401	BCB	CBC-CAC-C3C	-3.86	118.17	127.07
10	M	400	BCB	CBC-CAC-C3C	-3.77	118.37	127.07
11	M	402	BPB	CAD-C3D-C2D	-3.65	123.19	140.80
14	M	600	NS5	C34-C35-C36	-3.65	113.69	127.73
14	M	600	NS5	CM4-C36-C35	-3.62	110.97	122.61
14	M	600	NS5	CM3-C36-C35	-3.57	111.13	122.61
10	M	401	BCB	CBC-CAC-C3C	-3.57	118.84	127.07
11	L	402	BPB	CAD-C3D-C2D	-3.47	124.05	140.80
7	C	404	HEC	CAD-CBD-CGD	-3.39	106.53	112.75
11	M	402	BPB	C3D-C4D-ND	-3.35	98.86	109.65
10	M	400	BCB	C3C-C4C-NC	-3.35	107.75	110.24
10	L	400	BCB	CBC-CAC-C3C	-3.30	119.45	127.07
10	L	400	BCB	C1D-CHD-C4C	-3.20	122.39	129.26
11	L	402	BPB	C3D-C4D-ND	-3.18	99.41	109.65
11	M	402	BPB	CBC-CAC-C3C	-3.09	119.95	127.07
13	M	501	MQ9	C12-C13-C14	-3.08	121.06	127.76
11	L	402	BPB	CBC-CAC-C3C	-3.03	120.07	127.07
14	M	600	NS5	C6-C5-C7	-3.00	117.61	123.50
10	M	401	BCB	C1D-CHD-C4C	-2.93	122.97	129.26
13	M	501	MQ9	C17-C18-C19	-2.91	121.43	127.76
14	M	600	NS5	C18-C17-C15	-2.90	123.00	127.20
10	L	401	BCB	C1D-CHD-C4C	-2.88	123.08	129.26
13	M	501	MQ9	C27-C28-C29	-2.85	121.57	127.76
9	H	703	LDA	CM2-N1-CM1	-2.77	105.71	108.83
9	M	704	LDA	O1-N1-CM1	-2.74	105.39	109.05
10	M	401	BCB	C3C-C4C-NC	-2.73	108.21	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	M	501	MQ9	C22-C23-C24	-2.73	121.83	127.76
10	L	400	BCB	CAA-CBA-CGA	-2.72	105.35	113.32
10	L	400	BCB	C3C-C4C-NC	-2.72	108.22	110.24
13	M	501	MQ9	C37-C38-C39	-2.71	121.86	127.76
7	C	404	HEC	CBA-CAA-C2A	-2.71	107.67	112.53
10	M	400	BCB	O2D-CGD-O1D	-2.68	118.25	123.79
14	M	600	NS5	C12-C13-C14	-2.67	115.00	123.13
10	L	401	BCB	C3C-C4C-NC	-2.62	108.30	110.24
7	C	402	HEC	CBA-CAA-C2A	-2.57	107.91	112.53
13	M	501	MQ9	C35-C34-C33	-2.56	118.47	123.50
10	M	400	BCB	O1D-CGD-CBD	-2.56	120.95	124.62
12	L	502	UQ1	C7-C8-C9	-2.54	117.36	127.16
13	M	501	MQ9	C7-C8-C9	-2.47	122.51	126.70
10	M	401	BCB	O1D-CGD-CBD	-2.47	121.08	124.62
10	M	401	BCB	C6-C5-C3	-2.47	107.07	112.48
11	L	402	BPB	C6-C7-C8	-2.44	107.38	115.49
10	L	400	BCB	C6-C5-C3	-2.44	107.14	112.48
7	C	403	HEC	CBA-CAA-C2A	-2.42	108.19	112.53
10	M	401	BCB	O2D-CGD-O1D	-2.39	118.86	123.79
10	L	400	BCB	C6-C7-C8	-2.34	107.71	115.49
14	M	600	NS5	C30-C29-C28	-2.31	116.08	123.13
13	M	501	MQ9	C42-C43-C44	-2.31	122.74	127.76
11	M	402	BPB	CAA-CBA-CGA	-2.30	106.57	113.32
13	M	501	MQ9	C5M-C5-C6	-2.29	119.20	124.10
7	C	402	HEC	CMC-C2C-C1C	-2.25	124.63	128.36
14	M	600	NS5	C24-C25-C26	-2.25	123.94	127.20
10	M	401	BCB	CGD-CBD-CAD	-2.25	103.00	110.62
7	C	404	HEC	CMC-C2C-C1C	-2.23	124.68	128.36
13	M	501	MQ9	C40-C39-C38	-2.23	119.13	123.50
11	L	402	BPB	CAA-CBA-CGA	-2.22	106.81	113.32
10	L	400	BCB	CGD-CBD-CAD	-2.21	103.13	110.62
10	L	400	BCB	O2D-CGD-O1D	-2.21	119.23	123.79
7	C	404	HEC	CAA-CBA-CGA	-2.16	108.79	112.75
10	M	401	BCB	C6-C7-C8	-2.16	108.33	115.49
10	L	401	BCB	O2A-CGA-O1A	-2.12	118.01	123.49
13	M	501	MQ9	C10-C9-C8	-2.10	119.38	123.50
7	C	402	HEC	CMB-C2B-C1B	-2.10	124.89	128.36
11	M	402	BPB	C4-C3-C2	-2.04	119.50	123.50
12	L	502	UQ1	CM5-C5-C6	-2.03	119.75	124.10
10	M	400	BCB	CGD-CBD-CAD	-2.03	103.75	110.62
10	M	401	BCB	C11-C10-C8	-2.03	108.77	115.49
11	M	402	BPB	O2D-CGD-O1D	-2.01	119.64	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	M	400	BCB	C4-C3-C2	-2.01	119.56	123.50
7	C	401	HEC	CMC-C2C-C1C	-2.01	125.05	128.36
9	H	701	LDA	O1-N1-CM2	2.04	111.78	109.05
11	L	402	BPB	CHD-C1D-C2D	2.13	130.43	125.61
11	L	402	BPB	CMD-C2D-C3D	2.15	133.04	128.04
12	L	502	UQ1	C7-C6-C1	2.21	121.16	118.56
11	L	402	BPB	CED-O2D-CGD	2.24	121.24	115.99
11	M	402	BPB	C4-C3-C5	2.25	118.84	115.41
12	L	503	UQ1	C11-C9-C10	2.29	120.26	114.64
13	M	501	MQ9	C25-C24-C26	2.32	118.95	115.41
13	M	501	MQ9	C5M-C5-C4	2.40	120.17	116.27
13	M	501	MQ9	C40-C39-C41	2.42	119.10	115.41
13	M	501	MQ9	C30-C29-C31	2.46	119.17	115.41
11	L	402	BPB	C4-C3-C5	2.49	119.22	115.41
11	M	402	BPB	CMD-C2D-C3D	2.51	133.89	128.04
11	L	402	BPB	C3C-C2C-C1C	2.58	104.81	100.99
11	L	402	BPB	CBD-CHA-C1A	2.59	131.15	126.78
10	L	400	BCB	C4-C3-C5	2.67	119.48	115.41
13	M	501	MQ9	C10-C9-C11	2.73	119.57	115.41
10	M	401	BCB	O2A-CGA-CBA	2.74	120.25	111.90
11	M	402	BPB	CBD-CHA-C1A	2.76	131.43	126.78
13	M	501	MQ9	C15-C14-C16	2.76	119.62	115.41
11	L	402	BPB	C4D-C3D-CAD	2.78	110.50	105.51
11	M	402	BPB	C4D-C3D-CAD	2.79	110.52	105.51
10	M	401	BCB	C4A-NA-C1A	2.82	109.37	106.04
13	M	501	MQ9	C20-C19-C21	2.83	119.73	115.41
9	H	703	LDA	O1-N1-CM2	2.88	112.90	109.05
11	M	402	BPB	O2A-CGA-CBA	2.89	120.69	111.90
10	L	401	BCB	O2A-CGA-CBA	2.90	120.73	111.90
14	M	600	NS5	C11-C10-C9	2.90	119.84	115.41
10	L	400	BCB	O2A-CGA-CBA	2.91	120.76	111.90
14	M	600	NS5	C32-C31-C33	3.01	120.00	115.41
11	M	402	BPB	CMD-C2D-C1D	3.12	130.13	125.06
11	L	402	BPB	O2A-CGA-CBA	3.12	121.41	111.90
10	M	400	BCB	O2A-CGA-CBA	3.13	121.45	111.90
10	M	401	BCB	C4-C3-C5	3.16	120.23	115.41
10	L	401	BCB	C4A-NA-C1A	3.18	109.79	106.04
10	M	400	BCB	C4A-NA-C1A	3.24	109.86	106.04
10	L	400	BCB	C4A-NA-C1A	3.28	109.91	106.04
11	L	402	BPB	CMD-C2D-C1D	3.36	130.53	125.06
14	M	600	NS5	C6-C5-C4	3.57	120.86	115.41
10	M	400	BCB	C4-C3-C5	3.62	120.94	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	M	501	MQ9	C35-C34-C36	3.73	121.11	115.41
10	L	401	BCB	C4-C3-C5	3.87	121.31	115.41
9	M	704	LDA	CM2-N1-CM1	4.10	113.46	108.83
10	L	400	BCB	O2D-CGD-CBD	5.46	118.78	111.30
11	L	402	BPB	O2D-CGD-CBD	6.13	119.71	111.30
10	M	401	BCB	O2D-CGD-CBD	6.38	120.05	111.30
10	M	400	BCB	O2D-CGD-CBD	6.90	120.76	111.30
10	L	401	BCB	O2D-CGD-CBD	7.15	121.11	111.30
11	M	402	BPB	O2D-CGD-CBD	7.34	121.37	111.30
11	L	402	BPB	C4D-C3D-C2D	16.55	125.45	106.74
11	M	402	BPB	C4D-C3D-C2D	17.29	126.29	106.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

19 monomers are involved in 129 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	401	HEC	13	0
7	C	402	HEC	10	0
7	C	403	HEC	6	0
7	C	404	HEC	2	0
8	C	706	HTO	1	0
9	H	703	LDA	6	0
8	H	705	HTO	2	0
5	H	807	SO4	1	0
10	L	400	BCB	17	0
10	L	401	BCB	10	0
11	L	402	BPB	9	0
12	L	502	UQ1	4	0
9	L	702	LDA	2	0
10	M	400	BCB	11	0
10	M	401	BCB	17	0
11	M	402	BPB	20	0
13	M	501	MQ9	3	0
14	M	600	NS5	11	0
5	M	805	SO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	332/336 (98%)	-0.22	8 (2%)	62	50	46, 74, 113, 124	0
2	H	249/258 (96%)	-0.17	3 (1%)	81	71	50, 73, 99, 105	0
3	L	273/273 (100%)	-0.57	3 (1%)	82	73	37, 54, 74, 85	0
4	M	323/323 (100%)	-0.50	3 (0%)	85	79	42, 60, 89, 117	0
All	All	1177/1190 (98%)	-0.37	17 (1%)	78	67	37, 66, 102, 124	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	85	THR	3.8
1	C	59	VAL	3.7
1	C	54	GLN	3.0
1	C	53	SER	2.9
2	H	83	PRO	2.8
3	L	271	PHE	2.6
1	C	218	LYS	2.4
1	C	58	ASN	2.4
4	M	322	PRO	2.4
1	C	63	GLY	2.3
2	H	7	ALA	2.2
3	L	1	ALA	2.1
1	C	57	LYS	2.1
4	M	321	ALA	2.1
1	C	1	CYS	2.0
3	L	202	ASP	2.0
4	M	320	GLY	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^{th} 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	10/11	0.77	0.37	-	104,105,115,117	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^{th} 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
8	HTO	C	706	10/10	0.88	0.71	11.55	56,57,58,58	10
9	LDA	M	704	16/16	0.91	0.41	11.44	68,70,73,73	16
8	HTO	H	705	10/10	0.55	0.59	7.00	56,59,61,61	10
12	UQ1	L	502	18/18	0.89	0.40	5.83	63,65,66,66	18
8	HTO	C	707	10/10	0.77	0.39	5.67	44,48,49,49	10
5	SO4	C	811	5/5	0.85	0.60	5.56	76,76,76,77	5
9	LDA	L	702	16/16	0.95	0.36	5.15	67,73,79,80	0
14	NS5	M	600	40/40	0.87	0.28	4.97	65,71,100,101	4
12	UQ1	L	503	18/18	0.62	0.59	3.92	73,76,78,78	18
11	BPB	M	402	65/65	0.89	0.28	3.04	61,67,123,124	0
5	SO4	C	813	5/5	0.82	0.43	2.34	79,79,80,80	5
5	SO4	H	807	5/5	0.81	0.42	2.22	108,108,108,109	5
13	MQ9	M	501	58/58	0.91	0.25	1.87	40,64,102,103	0
9	LDA	H	703	16/16	0.94	0.39	1.47	54,58,60,61	16
7	HEC	C	403	43/43	0.98	0.19	0.81	46,48,52,54	0
11	BPB	L	402	65/65	0.96	0.19	0.79	38,51,60,60	0
10	BCB	M	401	66/66	0.98	0.18	0.77	36,41,63,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
10	BCB	M	400	66/66	0.97	0.18	0.66	37,48,107,108	0
10	BCB	L	400	66/66	0.97	0.18	0.56	37,40,45,49	0
10	BCB	L	401	66/66	0.97	0.19	0.44	41,44,59,64	0
7	HEC	C	404	43/43	0.98	0.16	0.17	52,55,68,73	0
7	HEC	C	402	43/43	0.98	0.19	0.09	73,76,80,81	0
9	LDA	H	701	16/16	0.96	0.17	-0.03	54,57,68,68	0
7	HEC	C	401	43/43	0.96	0.27	-0.34	99,110,118,120	0
5	SO4	H	806	5/5	0.95	0.14	-0.57	72,72,73,73	5
5	SO4	M	802	5/5	0.99	0.09	-1.07	89,89,90,90	0
6	FE2	M	500	1/1	1.00	0.16	-1.74	50,50,50,50	0
5	SO4	C	814	5/5	0.92	0.37	-	48,48,49,50	5
5	SO4	M	801	5/5	0.96	0.11	-	61,62,63,63	0
5	SO4	C	808	5/5	0.47	0.40	-	104,104,104,104	5
5	SO4	M	804	5/5	0.95	0.18	-	94,95,96,96	0
5	SO4	H	803	5/5	0.76	0.34	-	82,82,83,83	5
5	SO4	C	810	5/5	0.80	0.42	-	88,88,88,88	5
5	SO4	C	809	5/5	0.48	0.54	-	109,110,110,110	5
5	SO4	C	815	5/5	0.92	0.25	-	40,40,41,41	5
5	SO4	M	805	5/5	0.96	0.09	-	64,65,65,67	5
5	SO4	H	812	5/5	0.76	0.33	-	92,92,93,93	5

6.5 Other polymers (i)

There are no such residues in this entry.