Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:21 AM GMT

PDB ID	:	3I4D
Title	:	Photosynthetic reaction center from rhodobacter sphaeroides 2.4.1
Authors	:	Fujii, R.; Adachi, S.; Roszak, A.W.; Gardiner, A.T.; Cogdell, R.J.; Isaacs, N.W.; Koshihara, S.; Hashimoto, H.
Deposited on	:	2009-07-01
Resolution	:	2.01 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 ①) were used in the production of this report:

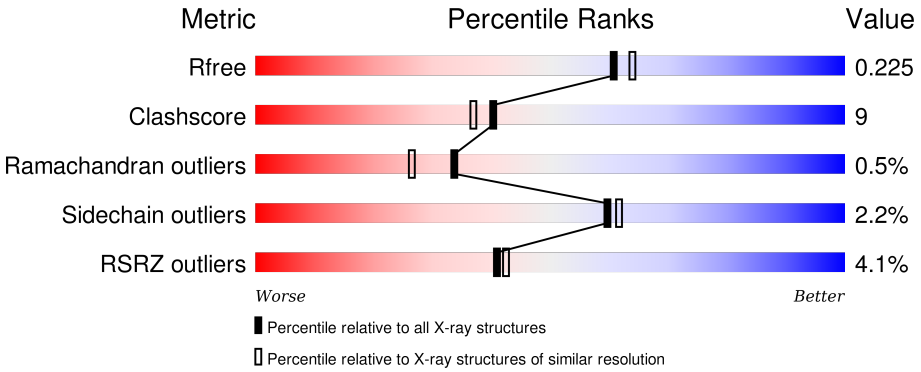
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	L	281	3% 91% 7% •
2	M	307	4% 90% 8% ••
3	H	260	5% 81% 9% • 8%

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	H	729	-	-	-	X
10	GOL	H	738	-	-	-	X
10	GOL	H	739	-	-	-	X
10	GOL	L	723	-	-	-	X
10	GOL	L	725	-	-	-	X
10	GOL	L	728	-	-	-	X
10	GOL	L	731	-	-	-	X
10	GOL	L	733	-	-	-	X
10	GOL	M	737	-	-	-	X
10	GOL	M	741	-	-	X	-
10	GOL	M	742	-	-	-	X
11	HT3	L	751	-	-	-	X
12	HTO	H	752	-	-	-	X
12	HTO	L	753	-	-	-	X
13	LDA	H	901	-	-	-	X
13	LDA	H	910	-	-	-	X
13	LDA	L	902	-	-	-	X
13	LDA	L	904	-	-	-	X
13	LDA	L	905	-	-	-	X
13	LDA	L	908	-	-	-	X
13	LDA	L	913	-	-	-	X
13	LDA	L	914	-	-	-	X
13	LDA	L	915	-	-	-	X
13	LDA	L	917	-	-	-	X
13	LDA	L	919	-	-	-	X
13	LDA	L	921	-	-	X	X
13	LDA	M	903	-	-	-	X
13	LDA	M	907	-	-	-	X
13	LDA	M	911	-	-	-	X
13	LDA	M	912	-	-	-	X
13	LDA	M	916	-	-	-	X
13	LDA	M	918	-	-	-	X
18	CDL	M	800	-	-	-	X
6	U10	L	502[A]	-	-	-	X
6	U10	L	502[B]	-	-	-	X
6	U10	M	501[A]	-	-	-	X
6	U10	M	501[B]	-	-	-	X
7	UQ1	L	503	-	-	X	X
8	PO4	L	705	-	-	-	X
8	PO4	L	708	-	-	-	X
8	PO4	M	707	-	-	-	X
9	DIO	L	711	-	-	-	X

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 8406 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 Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	281	2246	1516	358	364	8	0	2	0

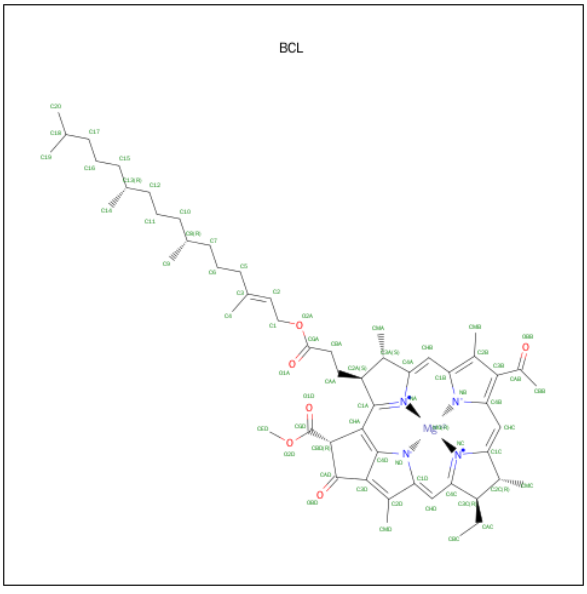
- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	M	302	2451	1635	402	402	12	0	5	0

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

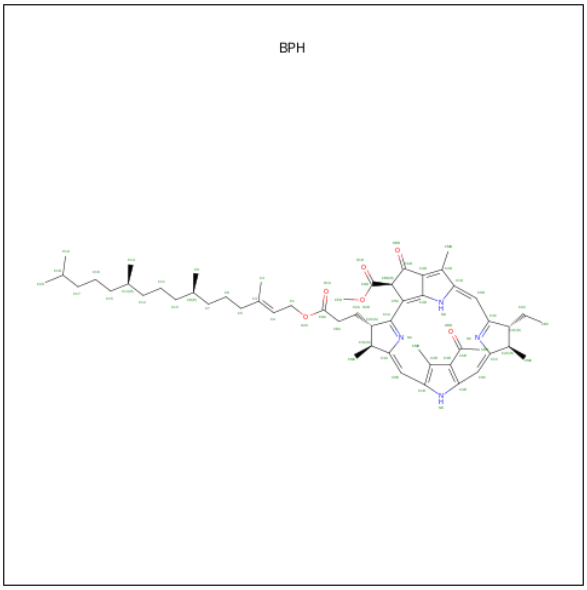
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	239	1876	1199	324	343	10	0	6	0

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



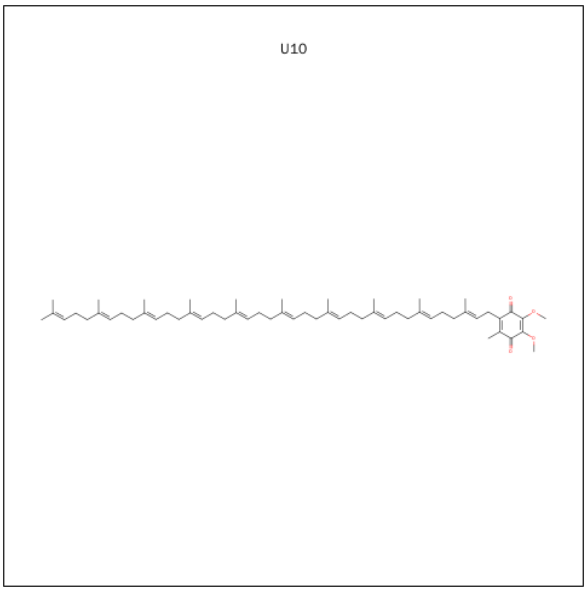
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 5 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



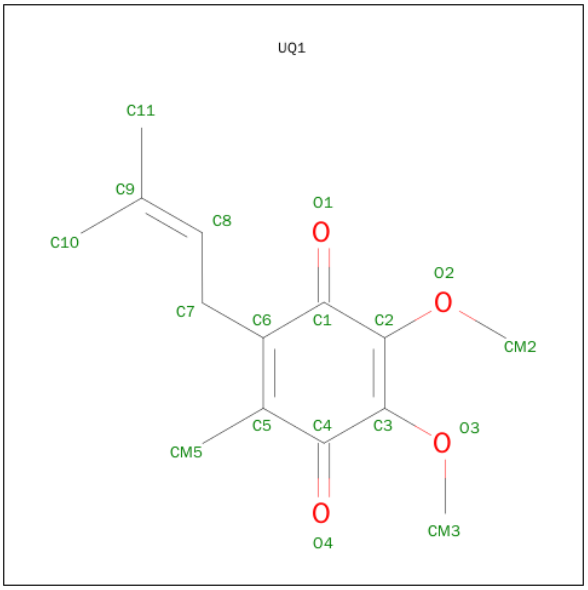
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 6 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



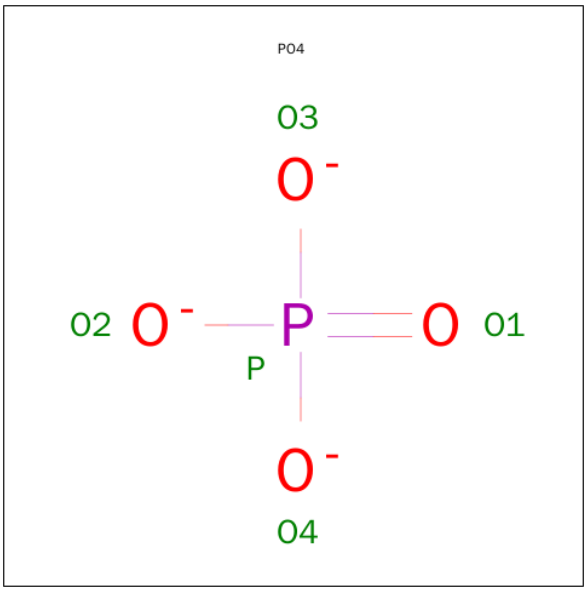
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total C O 84 80 4	0	1
6	M	1	Total C O 94 90 4	0	1

- Molecule 7 is UBIQUINONE-1 (three-letter code: UQ1) (formula: $C_{14}H_{18}O_4$).



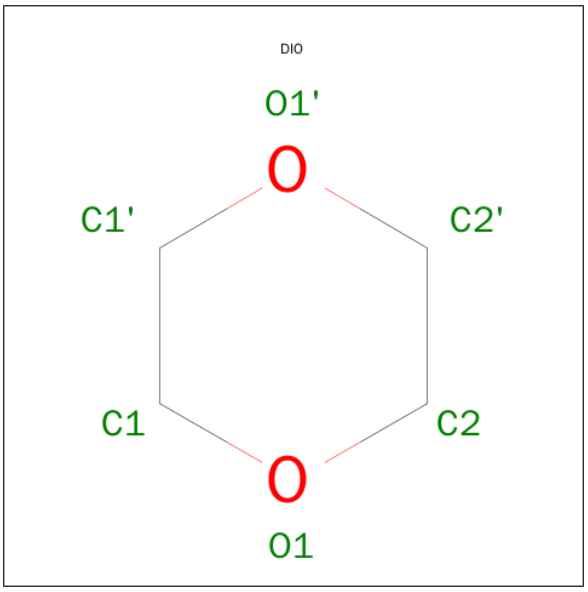
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total C O 18 14 4	0	0

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



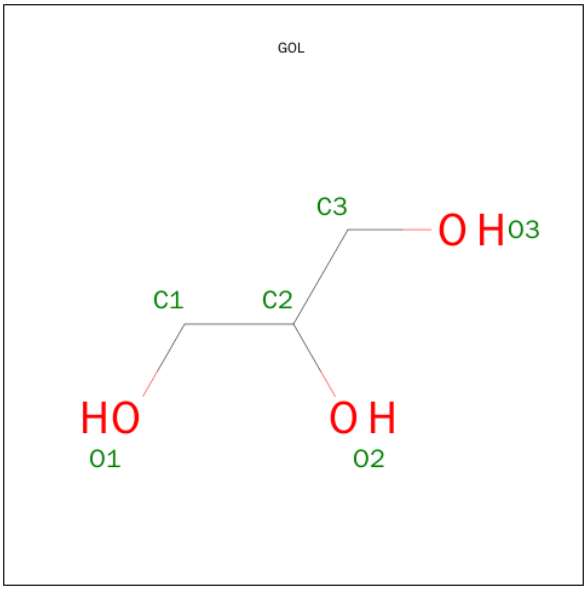
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	L	1	Total O P 5 4 1	0	0
8	L	1	Total O P 5 4 1	0	0
8	L	1	Total O P 5 4 1	0	0
8	L	1	Total O P 5 4 1	0	0
8	M	1	Total O P 5 4 1	0	0
8	M	1	Total O P 5 4 1	0	0
8	H	1	Total O P 5 4 1	0	0

- Molecule 9 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: $C_4H_8O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	L	1	Total C O 6 4 2	0	0

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



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

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

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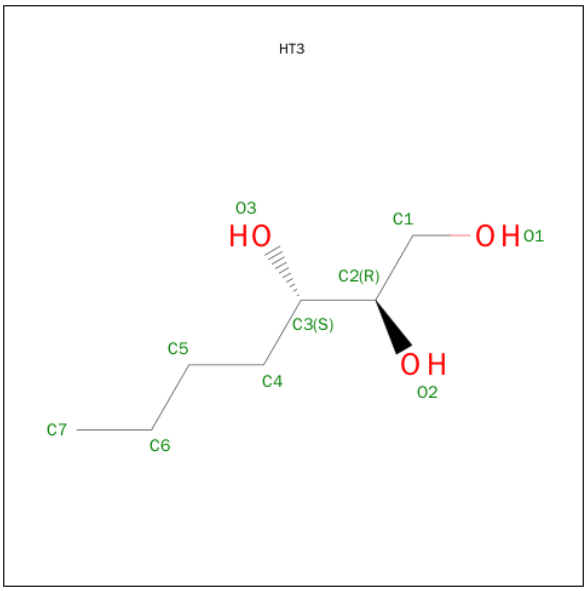
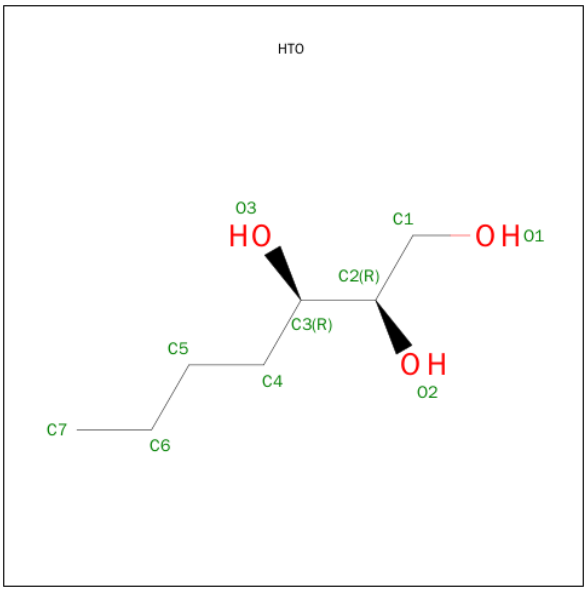
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	H	1	Total C O 6 3 3	0	0
10	H	1	Total C O 6 3 3	0	0

- Molecule 11 is (2R,3S)-HEPTANE-1,2,3-TRIOL (three-letter code: HT3) (formula: $C_7H_{16}O_3$).



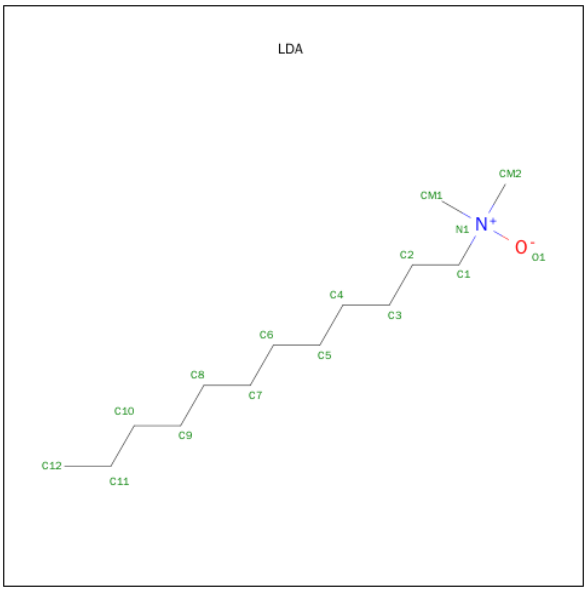
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	L	1	Total C O 10 7 3	0	0

- Molecule 12 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).



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

- Molecule 13 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



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

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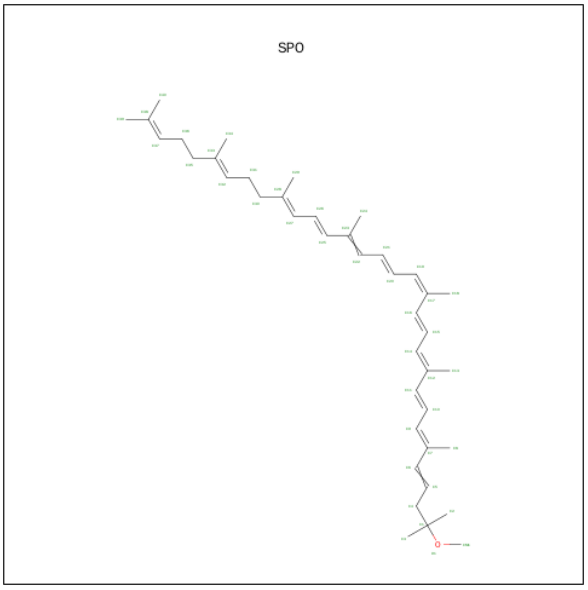
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	L	1	Total C N O 16 14 1 1	0	0
13	L	1	Total C N O 16 14 1 1	0	0
13	L	1	Total C N O 16 14 1 1	0	0
13	L	1	Total C N O 16 14 1 1	0	0
13	L	1	Total C N O 16 14 1 1	0	0
13	L	1	Total C N O 16 14 1 1	0	0
13	L	1	Total C N O 16 14 1 1	0	0
13	L	1	Total C N O 16 14 1 1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

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

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

- Molecule 15 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	M	1	Total C O 42 41 1	0	0

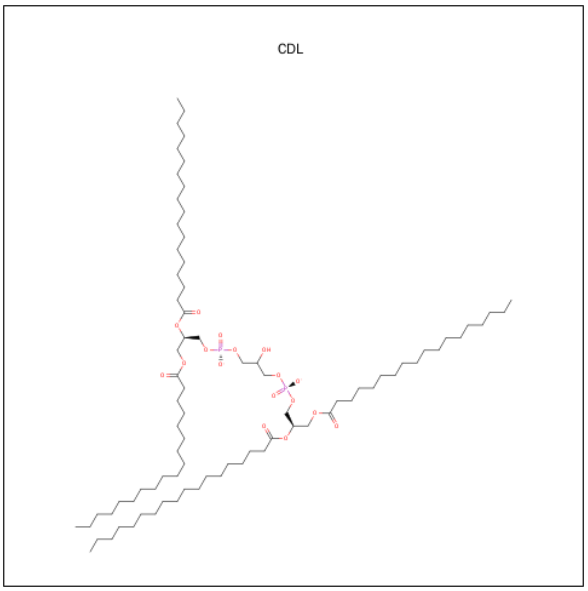
- Molecule 16 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	H	1	Total K 1 1	0	0
16	M	1	Total K 1 1	0	0

- Molecule 17 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	M	1	Total Cl 1 1	0	0

- Molecule 18 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	M	1	Total	C	O	P	0	0
			81	62	17	2		

- Molecule 19 is water.

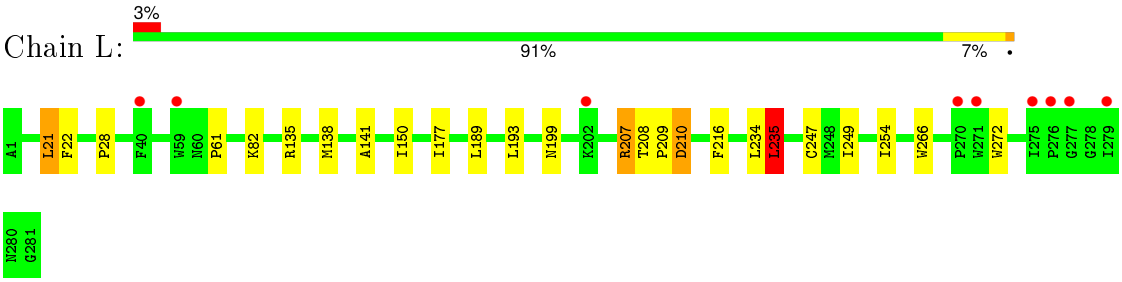
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	L	145	Total	O	0	0
			145	145		
19	M	150	Total	O	0	0
			150	150		
19	H	258	Total	O	0	0
			258	258		

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.

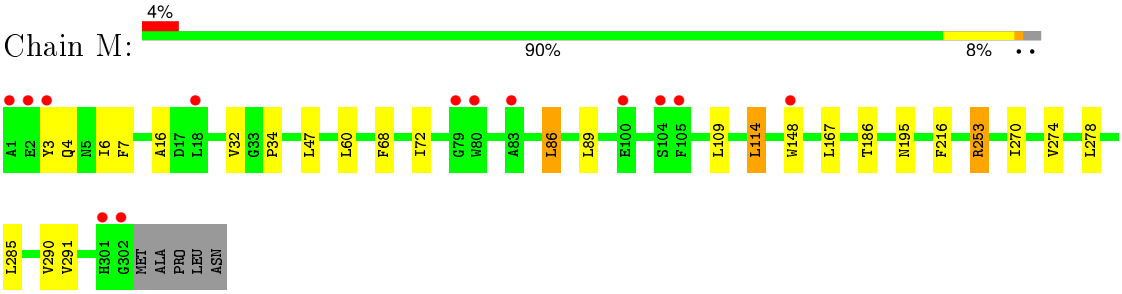
- Molecule 1: Reaction center protein L chain

Chain L:



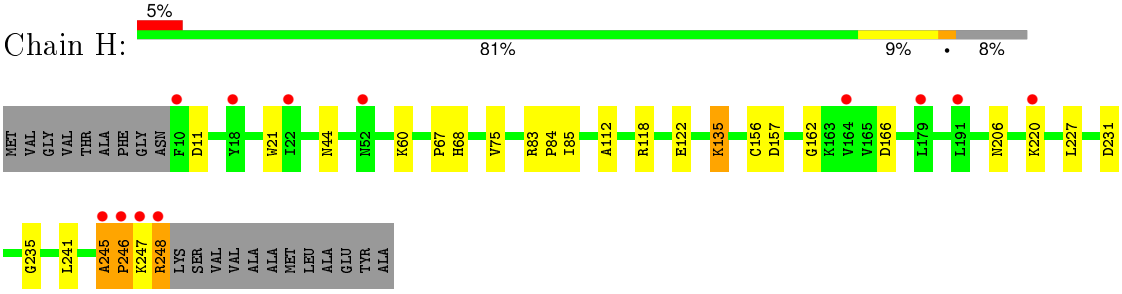
- Molecule 2: Reaction center protein M chain

Chain M:



- Molecule 3: Reaction center protein H chain

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	138.80Å 138.80Å 184.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.25 – 2.01 30.25 – 2.01	Depositor EDS
% Data completeness (in resolution range)	90.9 (30.25-2.01) 90.9 (30.25-2.01)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.181 , 0.207 0.206 , 0.225	Depositor DCC
R_{free} test set	6134 reflections (5.21%)	DCC
Wilson B-factor (Å^2)	34.2	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 98.4	EDS
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	1 of 123965 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8406	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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: BCL, GOL, LDA, DIO, CL, CDL, BPH, K, HTO, HT3, FE, SPO, UQ1, U10, PO4

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	L	0.94	0/2334	0.78	4/3194 (0.1%)
2	M	0.89	1/2543 (0.0%)	0.79	2/3469 (0.1%)
3	H	0.96	0/1925	0.86	5/2616 (0.2%)
All	All	0.93	1/6802 (0.0%)	0.81	11/9279 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	274	VAL	CB-CG2	-5.07	1.42	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	118[A]	ARG	NE-CZ-NH2	-5.96	117.32	120.30
3	H	118[B]	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	L	235	LEU	CA-CB-CG	5.83	128.72	115.30
3	H	83	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	L	135	ARG	NE-CZ-NH2	5.57	123.08	120.30
1	L	210	ASP	CB-CG-OD1	5.29	123.06	118.30
2	M	253[A]	ARG	NE-CZ-NH2	-5.12	117.74	120.30
2	M	253[B]	ARG	NE-CZ-NH2	-5.12	117.74	120.30
3	H	135[A]	LYS	CD-CE-NZ	5.07	123.36	111.70
3	H	135[B]	LYS	CD-CE-NZ	5.07	123.36	111.70
1	L	207	ARG	NE-CZ-NH1	-5.03	117.78	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	L	2246	0	2203	28	0
2	M	2451	0	2369	27	0
3	H	1876	0	1882	19	0
4	L	132	0	148	5	0
4	M	132	0	148	12	0
5	L	65	0	75	0	0
5	M	65	0	76	4	0
6	L	84	0	70	14	0
6	M	94	0	102	7	0
7	L	18	0	18	13	0
8	H	5	0	0	0	0
8	L	20	0	0	1	0
8	M	10	0	0	1	0
9	L	6	0	8	0	0
10	H	54	0	72	4	0
10	L	72	0	96	3	0
10	M	30	0	40	6	0
11	L	10	0	16	0	0
12	H	10	0	16	3	0
12	L	10	0	16	0	0
13	H	64	0	124	9	0
13	L	176	0	341	27	0
13	M	96	0	186	6	0
14	M	1	0	0	0	0
15	M	42	0	60	1	0
16	H	1	0	0	0	0
16	M	1	0	0	0	0
17	M	1	0	0	0	0
18	M	81	0	106	9	0
19	H	258	0	0	1	0
19	L	145	0	0	2	0
19	M	150	0	0	1	0
All	All	8406	0	8172	138	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 9.

All (138) 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:L:502[B]:U10:H502	2:M:86:LEU:HD11	1.25	1.14
6:L:502[B]:U10:C50	2:M:86:LEU:HD11	1.89	1.02
10:M:740:GOL:O1	10:M:742:GOL:O3	1.83	0.96
1:L:235:LEU:HA	13:L:921:LDA:HM21	1.47	0.94
2:M:253[A]:ARG:NH2	19:M:415:HOH:O	2.04	0.89
10:L:724:GOL:H2	3:H:241:LEU:HD13	1.56	0.88
3:H:245:ALA:HB3	3:H:246:PRO:HD3	1.54	0.86
1:L:235:LEU:HD23	13:L:921:LDA:HM11	1.58	0.84
6:M:501[B]:U10:H501	6:M:501[B]:U10:C53	2.09	0.82
4:M:601:BCL:C7	4:M:601:BCL:H41	2.07	0.82
1:L:235:LEU:HA	13:L:921:LDA:CM2	2.10	0.81
6:M:501[B]:U10:H501	6:M:501[B]:U10:H53	1.62	0.81
13:H:906:LDA:HM23	13:H:910:LDA:O1	1.82	0.80
4:M:601:BCL:H72	4:M:601:BCL:H41	1.63	0.78
10:H:739:GOL:H2	12:H:752:HTO:H72	1.64	0.77
4:M:601:BCL:CBB	4:M:601:BCL:HMB1	2.15	0.77
2:M:16:ALA:HB1	2:M:32:VAL:HG11	1.69	0.74
7:L:503:UQ1:H102	13:L:920:LDA:H121	1.71	0.73
10:H:739:GOL:H2	12:H:752:HTO:C7	2.18	0.73
13:H:906:LDA:CM2	13:H:910:LDA:O1	2.38	0.72
7:L:503:UQ1:HM53	2:M:89:LEU:HD23	1.72	0.72
13:M:903:LDA:H91	13:H:901:LDA:H121	1.72	0.72
4:M:601:BCL:HBB2	4:M:601:BCL:HMB1	1.73	0.70
6:L:502[B]:U10:H502	2:M:86:LEU:CD1	2.15	0.69
1:L:235:LEU:CA	13:L:921:LDA:CM2	2.72	0.67
3:H:162:GLY:HA2	12:H:752:HTO:H2	1.77	0.67
1:L:82[A]:LYS:NZ	19:L:448:HOH:O	2.28	0.66
13:H:909:LDA:H123	13:H:910:LDA:H111	1.77	0.65
1:L:28:PRO:HG3	13:L:902:LDA:HM21	1.79	0.64
7:L:503:UQ1:CM5	2:M:89:LEU:HD23	2.28	0.64
1:L:61:PRO:O	1:L:150:ILE:HD12	1.97	0.64
13:L:921:LDA:O1	2:M:6:ILE:HD12	2.00	0.62
13:L:905:LDA:H122	13:L:917:LDA:HM11	1.82	0.61
13:L:905:LDA:H122	13:L:917:LDA:CM1	2.30	0.61
4:L:602:BCL:HBB3	4:L:602:BCL:HMB1	1.83	0.60
4:L:604:BCL:HMB1	4:L:604:BCL:HBB2	1.84	0.60
7:L:503:UQ1:H102	13:L:920:LDA:C12	2.31	0.60
2:M:278[B]:LEU:HD11	18:M:800:CDL:H811	1.83	0.59
7:L:503:UQ1:CM2	7:L:503:UQ1:O1	2.49	0.59
3:H:135[A]:LYS:HE3	3:H:166:ASP:OD2	2.03	0.58
6:L:502[B]:U10:H402	15:M:600:SPO:H133	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:60:LEU:HD23	5:M:401:BPH:H4C1	1.85	0.57
2:M:34:PRO:HG2	2:M:47[A]:LEU:HD12	1.86	0.57
7:L:503:UQ1:HM22	7:L:503:UQ1:O1	2.03	0.57
3:H:246:PRO:HA	3:H:247:LYS:O	2.05	0.56
7:L:503:UQ1:C10	13:L:920:LDA:C12	2.83	0.56
6:M:501[B]:U10:C50	6:M:501[B]:U10:C53	2.84	0.55
1:L:28:PRO:HD3	13:L:902:LDA:HM21	1.88	0.55
1:L:141:ALA:HB2	8:L:708:PO4:O4	2.05	0.55
3:H:245:ALA:CB	3:H:246:PRO:HD3	2.30	0.55
4:L:602:BCL:HMB1	4:L:602:BCL:CBB	2.37	0.55
4:M:603:BCL:HMB1	4:M:603:BCL:CBB	2.36	0.55
2:M:290:VAL:HG12	2:M:291:VAL:HG23	1.89	0.54
6:L:502[A]:U10:H502	4:M:603:BCL:H171	1.90	0.53
7:L:503:UQ1:HM51	7:L:503:UQ1:C8	2.39	0.53
13:M:903:LDA:H82	13:H:910:LDA:H123	1.90	0.53
1:L:21:LEU:HD13	1:L:22:PHE:CE1	2.44	0.53
2:M:278[A]:LEU:CD2	18:M:800:CDL:H791	2.38	0.53
2:M:68:PHE:O	2:M:72:ILE:HG12	2.09	0.53
6:M:501[B]:U10:H371	6:M:501[B]:U10:H312	1.91	0.53
1:L:28:PRO:CD	13:L:902:LDA:HM21	2.40	0.52
1:L:235:LEU:CA	13:L:921:LDA:HM23	2.39	0.52
1:L:235:LEU:HB2	13:L:921:LDA:HM23	1.92	0.52
2:M:278[A]:LEU:HD21	18:M:800:CDL:H791	1.92	0.51
6:M:501[B]:U10:C50	6:M:501[B]:U10:H53	2.37	0.51
7:L:503:UQ1:O4	7:L:503:UQ1:CM3	2.59	0.50
1:L:28:PRO:CG	13:L:902:LDA:HM21	2.42	0.50
1:L:235:LEU:CA	13:L:921:LDA:HM21	2.31	0.49
4:M:601:BCL:HBB3	4:M:601:BCL:HMB1	1.93	0.49
1:L:266:TRP:CD1	7:L:503:UQ1:HM33	2.48	0.48
4:L:604:BCL:HMB1	4:L:604:BCL:CBB	2.43	0.48
3:H:67:PRO:HB2	3:H:68:HIS:CD2	2.48	0.48
13:H:909:LDA:H123	13:H:910:LDA:C11	2.43	0.48
1:L:21:LEU:HD13	1:L:22:PHE:CZ	2.48	0.48
1:L:177:ILE:HG12	4:L:602:BCL:HMB3	1.96	0.48
6:M:501[B]:U10:H472	6:M:501[B]:U10:H451	1.60	0.47
2:M:167:LEU:HD12	2:M:285:LEU:HD11	1.96	0.47
5:M:401:BPH:CBC	5:M:401:BPH:HHD	2.45	0.47
2:M:270:ILE:HD13	18:M:800:CDL:H712	1.97	0.47
2:M:186:THR:HG23	4:M:603:BCL:HMD2	1.95	0.47
4:M:603:BCL:H201	13:M:918:LDA:H111	1.97	0.46
13:H:906:LDA:HM21	13:H:910:LDA:O1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:603:BCL:HMB1	4:M:603:BCL:HBB3	1.96	0.46
1:L:234:LEU:HG	13:L:921:LDA:HM22	1.97	0.46
2:M:278[B]:LEU:CD1	18:M:800:CDL:H811	2.46	0.46
6:L:502[A]:U10:C38	7:L:503:UQ1:H112	2.46	0.46
1:L:235:LEU:HD23	13:L:921:LDA:CM1	2.38	0.46
1:L:199:ASN:HB3	18:M:800:CDL:CA2	2.46	0.46
3:H:122:GLU:HB2	3:H:227:LEU:HD21	1.98	0.45
10:L:728:GOL:HO3	10:L:733:GOL:HO1	1.61	0.45
3:H:247:LYS:HA	3:H:248:ARG:HA	1.81	0.45
1:L:208:THR:HB	1:L:209:PRO:HD2	1.99	0.45
3:H:44:ASN:HD21	10:H:729:GOL:H32	1.82	0.45
2:M:4:GLN:H	10:M:741:GOL:C1	2.29	0.44
13:M:903:LDA:C9	13:H:901:LDA:H121	2.45	0.44
1:L:199:ASN:HB3	18:M:800:CDL:HA21	2.00	0.44
2:M:4:GLN:H	10:M:741:GOL:H12	1.83	0.44
3:H:75:VAL:HG12	10:H:738:GOL:H11	1.99	0.44
1:L:138:MET:SD	1:L:249:ILE:HD11	2.58	0.44
4:M:603:BCL:HBD	4:M:603:BCL:HAA2	1.99	0.43
10:L:728:GOL:O3	10:L:733:GOL:O1	2.31	0.43
3:H:112:ALA:HA	3:H:235:GLY:O	2.19	0.43
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.54	0.43
1:L:254:ILE:HD13	1:L:254:ILE:HG21	1.72	0.43
2:M:3:TYR:CD1	10:M:741:GOL:H12	2.54	0.43
13:L:914:LDA:H122	13:L:919:LDA:H52	2.00	0.43
8:M:707:PO4:O1	10:M:740:GOL:O2	2.37	0.43
3:H:156:CYS:HB3	3:H:206[A]:ASN:O	2.19	0.42
2:M:278[B]:LEU:HD11	18:M:800:CDL:C81	2.49	0.42
2:M:109:LEU:HD22	2:M:114:LEU:HD13	2.01	0.42
1:L:189:LEU:HD23	5:M:401:BPH:HMD2	2.01	0.42
3:H:246:PRO:HA	3:H:247:LYS:C	2.39	0.42
3:H:157:ASP:N	3:H:157:ASP:OD1	2.52	0.42
6:L:502[A]:U10:C43	5:M:401:BPH:H201	2.49	0.42
3:H:135[A]:LYS:CE	3:H:166:ASP:OD2	2.66	0.42
7:L:503:UQ1:C10	13:L:920:LDA:H121	2.44	0.42
6:L:502[B]:U10:H421	6:L:502[B]:U10:H401	1.80	0.42
6:M:501[A]:U10:H412	6:M:501[A]:U10:H371	1.92	0.41
2:M:278[B]:LEU:CD1	18:M:800:CDL:C81	2.98	0.41
3:H:84:PRO:O	3:H:85:ILE:HD13	2.20	0.41
3:H:21:TRP:CD2	13:H:906:LDA:HM22	2.55	0.41
6:L:502[A]:U10:H372	7:L:503:UQ1:C11	2.50	0.41
2:M:7:PHE:H	10:M:741:GOL:H32	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:601:BCL:C7	4:M:601:BCL:C4	2.90	0.41
13:M:903:LDA:HM12	19:H:280:HOH:O	2.20	0.41
13:L:915:LDA:HM21	13:M:918:LDA:O1	2.22	0.40
1:L:235:LEU:N	13:L:921:LDA:HM23	2.36	0.40
3:H:245:ALA:HB3	3:H:246:PRO:CD	2.39	0.40
13:L:908:LDA:HM22	19:L:447:HOH:O	2.20	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	L	281/281 (100%)	276 (98%)	5 (2%)	0	100 100
2	M	305/307 (99%)	299 (98%)	5 (2%)	1 (0%)	46 41
3	H	243/260 (94%)	238 (98%)	2 (1%)	3 (1%)	16 8
All	All	829/848 (98%)	813 (98%)	12 (1%)	4 (0%)	34 26

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	245	ALA
2	M	195	ASN
3	H	246	PRO
3	H	11	ASP

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	L	222/220 (101%)	215 (97%)	7 (3%)	46	44
2	M	241/240 (100%)	238 (99%)	3 (1%)	78	81
3	H	200/208 (96%)	195 (98%)	5 (2%)	55	55
All	All	663/668 (99%)	648 (98%)	15 (2%)	60	60

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	21	LEU
1	L	207	ARG
1	L	210	ASP
1	L	216	PHE
1	L	235	LEU
1	L	247	CYS
1	L	272	TRP
2	M	86	LEU
2	M	114	LEU
2	M	216	PHE
3	H	60	LYS
3	H	220[A]	LYS
3	H	220[B]	LYS
3	H	231	ASP
3	H	248	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	M	28	ASN
3	H	44	ASN
3	H	68	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 75 ligands modelled in this entry, 4 are monoatomic - leaving 71 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	PO4	H	709	-	4,4,4	0.51	0	6,6,6	0.31	0
10	GOL	H	721	-	5,5,5	0.23	0	5,5,5	0.85	0
10	GOL	H	729	-	5,5,5	0.30	0	5,5,5	0.46	0
10	GOL	H	735	-	5,5,5	0.59	0	5,5,5	0.55	0
10	GOL	H	736	-	5,5,5	0.39	0	5,5,5	0.29	0
10	GOL	H	738	-	5,5,5	0.37	0	5,5,5	0.28	0
10	GOL	H	739	-	5,5,5	0.44	0	5,5,5	0.31	0
10	GOL	H	743	-	5,5,5	0.64	0	5,5,5	0.83	0
10	GOL	H	745	-	5,5,5	0.38	0	5,5,5	0.46	0
10	GOL	H	746	-	5,5,5	0.57	0	5,5,5	0.56	0
12	HTO	H	752	-	9,9,9	0.45	0	8,10,10	1.37	1 (12%)
13	LDA	H	901	-	15,15,15	3.94	2 (13%)	16,17,17	0.52	0
13	LDA	H	906	-	15,15,15	3.84	2 (13%)	16,17,17	0.90	1 (6%)
13	LDA	H	909	-	15,15,15	3.87	2 (13%)	16,17,17	0.86	1 (6%)
13	LDA	H	910	-	15,15,15	3.59	1 (6%)	16,17,17	1.13	2 (12%)
5	BPH	L	402	-	64,70,70	0.85	3 (4%)	73,101,101	1.50	12 (16%)
6	U10	L	502[A]	-	63,63,63	2.43	24 (38%)	76,79,79	1.77	16 (21%)
6	U10	L	502[B]	-	63,63,63	2.43	24 (38%)	76,79,79	1.60	15 (19%)
7	UQ1	L	503	-	18,18,18	2.16	5 (27%)	22,25,25	1.73	4 (18%)
4	BCL	L	602	-	53,74,74	0.77	1 (1%)	57,115,115	1.17	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	BCL	L	604	-	53,74,74	0.98	1 (1%)	57,115,115	1.70	14 (24%)
8	PO4	L	703	-	4,4,4	0.42	0	6,6,6	0.28	0
8	PO4	L	705	-	4,4,4	0.55	0	6,6,6	0.30	0
8	PO4	L	706	-	4,4,4	0.50	0	6,6,6	0.32	0
8	PO4	L	708	-	4,4,4	0.52	0	6,6,6	0.26	0
9	DIO	L	711	-	6,6,6	0.41	0	6,6,6	0.67	0
10	GOL	L	722	-	5,5,5	0.39	0	5,5,5	0.67	0
10	GOL	L	723	-	5,5,5	0.47	0	5,5,5	0.84	0
10	GOL	L	724	-	5,5,5	0.60	0	5,5,5	0.45	0
10	GOL	L	725	-	5,5,5	0.43	0	5,5,5	0.96	0
10	GOL	L	727	-	5,5,5	0.44	0	5,5,5	0.64	0
10	GOL	L	728	-	5,5,5	0.39	0	5,5,5	0.27	0
10	GOL	L	730	-	5,5,5	0.50	0	5,5,5	0.59	0
10	GOL	L	731	-	5,5,5	0.79	0	5,5,5	0.69	0
10	GOL	L	732	-	5,5,5	0.40	0	5,5,5	0.39	0
10	GOL	L	733	-	5,5,5	0.41	0	5,5,5	0.63	0
10	GOL	L	734	-	5,5,5	0.16	0	5,5,5	0.52	0
10	GOL	L	744	-	5,5,5	0.71	0	5,5,5	0.52	0
11	HT3	L	751	-	9,9,9	0.91	0	8,10,10	1.75	3 (37%)
12	HTO	L	753	-	9,9,9	0.51	0	8,10,10	1.67	2 (25%)
13	LDA	L	902	-	15,15,15	3.72	2 (13%)	16,17,17	0.94	1 (6%)
13	LDA	L	904	-	15,15,15	3.77	2 (13%)	16,17,17	0.74	0
13	LDA	L	905	-	15,15,15	3.72	2 (13%)	16,17,17	0.74	1 (6%)
13	LDA	L	908	-	15,15,15	3.52	1 (6%)	16,17,17	1.00	2 (12%)
13	LDA	L	913	-	15,15,15	3.67	2 (13%)	16,17,17	0.66	1 (6%)
13	LDA	L	914	-	15,15,15	3.39	1 (6%)	16,17,17	1.48	3 (18%)
13	LDA	L	915	-	15,15,15	3.48	2 (13%)	16,17,17	0.87	1 (6%)
13	LDA	L	917	-	15,15,15	3.57	1 (6%)	16,17,17	0.77	1 (6%)
13	LDA	L	919	-	15,15,15	3.88	2 (13%)	16,17,17	0.82	1 (6%)
13	LDA	L	920	-	15,15,15	3.75	2 (13%)	16,17,17	0.87	1 (6%)
13	LDA	L	921	-	15,15,15	4.17	3 (20%)	16,17,17	0.96	1 (6%)
5	BPH	M	401	-	64,70,70	0.75	0	73,101,101	1.67	14 (19%)
6	U10	M	501[A]	-	63,63,63	2.37	26 (41%)	76,79,79	1.75	14 (18%)
6	U10	M	501[B]	-	63,63,63	2.41	25 (39%)	76,79,79	1.47	11 (14%)
15	SPO	M	600	-	40,41,41	1.16	3 (7%)	45,50,50	1.60	10 (22%)
4	BCL	M	601	-	53,74,74	0.77	0	57,115,115	1.81	11 (19%)
4	BCL	M	603	-	53,74,74	0.96	3 (5%)	57,115,115	1.41	9 (15%)
8	PO4	M	704	-	4,4,4	0.50	0	6,6,6	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	PO4	M	707	-	4,4,4	0.40	0	6,6,6	0.32	0
10	GOL	M	726	-	5,5,5	0.56	0	5,5,5	0.51	0
10	GOL	M	737	-	5,5,5	0.35	0	5,5,5	0.30	0
10	GOL	M	740	-	5,5,5	0.51	0	5,5,5	0.18	0
10	GOL	M	741	-	5,5,5	0.52	0	5,5,5	1.46	1 (20%)
10	GOL	M	742	-	5,5,5	0.51	0	5,5,5	0.55	0
18	CDL	M	800	-	80,80,99	1.12	4 (5%)	82,92,111	1.24	7 (8%)
13	LDA	M	903	-	15,15,15	4.00	1 (6%)	16,17,17	1.86	3 (18%)
13	LDA	M	907	-	15,15,15	3.68	2 (13%)	16,17,17	1.06	2 (12%)
13	LDA	M	911	-	15,15,15	3.79	2 (13%)	16,17,17	0.53	0
13	LDA	M	912	-	15,15,15	3.62	2 (13%)	16,17,17	0.70	1 (6%)
13	LDA	M	916	-	15,15,15	3.64	2 (13%)	16,17,17	0.64	0
13	LDA	M	918	-	15,15,15	3.90	2 (13%)	16,17,17	0.95	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PO4	H	709	-	-	0/0/0/0	0/0/0/0
10	GOL	H	721	-	-	0/4/4/4	0/0/0/0
10	GOL	H	729	-	-	0/4/4/4	0/0/0/0
10	GOL	H	735	-	-	0/4/4/4	0/0/0/0
10	GOL	H	736	-	-	0/4/4/4	0/0/0/0
10	GOL	H	738	-	-	0/4/4/4	0/0/0/0
10	GOL	H	739	-	-	0/4/4/4	0/0/0/0
10	GOL	H	743	-	-	0/4/4/4	0/0/0/0
10	GOL	H	745	-	-	0/4/4/4	0/0/0/0
10	GOL	H	746	-	-	0/4/4/4	0/0/0/0
12	HTO	H	752	-	-	0/10/10/10	0/0/0/0
13	LDA	H	901	-	-	0/13/13/13	0/0/0/0
13	LDA	H	906	-	-	0/13/13/13	0/0/0/0
13	LDA	H	909	-	-	0/13/13/13	0/0/0/0
13	LDA	H	910	-	-	0/13/13/13	0/0/0/0
5	BPH	L	402	-	-	0/54/105/105	0/1/6/6
6	U10	L	502[A]	-	-	0/63/87/87	0/1/1/1
6	U10	L	502[B]	-	-	0/63/87/87	0/1/1/1
7	UQ1	L	503	-	-	0/9/33/33	0/1/1/1
4	BCL	L	602	-	-	0/37/137/137	0/0/9/9
4	BCL	L	604	-	-	0/37/137/137	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PO4	L	703	-	-	0/0/0/0	0/0/0/0
8	PO4	L	705	-	-	0/0/0/0	0/0/0/0
8	PO4	L	706	-	-	0/0/0/0	0/0/0/0
8	PO4	L	708	-	-	0/0/0/0	0/0/0/0
9	DIO	L	711	-	-	0/0/6/6	0/1/1/1
10	GOL	L	722	-	-	0/4/4/4	0/0/0/0
10	GOL	L	723	-	-	0/4/4/4	0/0/0/0
10	GOL	L	724	-	-	0/4/4/4	0/0/0/0
10	GOL	L	725	-	-	0/4/4/4	0/0/0/0
10	GOL	L	727	-	-	0/4/4/4	0/0/0/0
10	GOL	L	728	-	-	0/4/4/4	0/0/0/0
10	GOL	L	730	-	-	0/4/4/4	0/0/0/0
10	GOL	L	731	-	-	0/4/4/4	0/0/0/0
10	GOL	L	732	-	-	0/4/4/4	0/0/0/0
10	GOL	L	733	-	-	0/4/4/4	0/0/0/0
10	GOL	L	734	-	-	0/4/4/4	0/0/0/0
10	GOL	L	744	-	-	0/4/4/4	0/0/0/0
11	HT3	L	751	-	-	0/10/10/10	0/0/0/0
12	HTO	L	753	-	-	0/10/10/10	0/0/0/0
13	LDA	L	902	-	-	0/13/13/13	0/0/0/0
13	LDA	L	904	-	-	0/13/13/13	0/0/0/0
13	LDA	L	905	-	-	0/13/13/13	0/0/0/0
13	LDA	L	908	-	-	0/13/13/13	0/0/0/0
13	LDA	L	913	-	-	0/13/13/13	0/0/0/0
13	LDA	L	914	-	-	0/13/13/13	0/0/0/0
13	LDA	L	915	-	-	0/13/13/13	0/0/0/0
13	LDA	L	917	-	-	0/13/13/13	0/0/0/0
13	LDA	L	919	-	-	0/13/13/13	0/0/0/0
13	LDA	L	920	-	-	0/13/13/13	0/0/0/0
13	LDA	L	921	-	-	0/13/13/13	0/0/0/0
5	BPH	M	401	-	-	0/54/105/105	0/1/6/6
6	U10	M	501[A]	-	-	0/63/87/87	0/1/1/1
6	U10	M	501[B]	-	-	0/63/87/87	0/1/1/1
15	SPO	M	600	-	-	0/47/47/47	0/0/0/0
4	BCL	M	601	-	-	0/37/137/137	0/0/9/9
4	BCL	M	603	-	-	0/37/137/137	0/0/9/9
8	PO4	M	704	-	-	0/0/0/0	0/0/0/0
8	PO4	M	707	-	-	0/0/0/0	0/0/0/0
10	GOL	M	726	-	-	0/4/4/4	0/0/0/0
10	GOL	M	737	-	-	0/4/4/4	0/0/0/0
10	GOL	M	740	-	-	0/4/4/4	0/0/0/0
10	GOL	M	741	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	GOL	M	742	-	-	0/4/4/4	0/0/0/0
18	CDL	M	800	-	-	0/91/91/110	0/0/0/0
13	LDA	M	903	-	-	0/13/13/13	0/0/0/0
13	LDA	M	907	-	-	0/13/13/13	0/0/0/0
13	LDA	M	911	-	-	0/13/13/13	0/0/0/0
13	LDA	M	912	-	-	0/13/13/13	0/0/0/0
13	LDA	M	916	-	-	0/13/13/13	0/0/0/0
13	LDA	M	918	-	-	0/13/13/13	0/0/0/0

All (157) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	L	921	LDA	O1-N1	-15.72	1.24	1.39
13	M	903	LDA	O1-N1	-14.85	1.25	1.39
13	H	901	LDA	O1-N1	-14.81	1.25	1.39
13	M	918	LDA	O1-N1	-14.78	1.25	1.39
13	H	909	LDA	O1-N1	-14.76	1.25	1.39
13	L	919	LDA	O1-N1	-14.61	1.25	1.39
13	H	906	LDA	O1-N1	-14.46	1.25	1.39
13	M	911	LDA	O1-N1	-14.25	1.26	1.39
13	L	904	LDA	O1-N1	-14.21	1.26	1.39
13	L	920	LDA	O1-N1	-14.21	1.26	1.39
13	L	902	LDA	O1-N1	-14.14	1.26	1.39
13	L	905	LDA	O1-N1	-14.10	1.26	1.39
13	L	913	LDA	O1-N1	-13.85	1.26	1.39
13	M	907	LDA	O1-N1	-13.79	1.26	1.39
13	M	916	LDA	O1-N1	-13.74	1.26	1.39
13	H	910	LDA	O1-N1	-13.71	1.26	1.39
13	M	912	LDA	O1-N1	-13.71	1.26	1.39
13	L	917	LDA	O1-N1	-13.60	1.26	1.39
13	L	908	LDA	O1-N1	-13.41	1.26	1.39
13	L	915	LDA	O1-N1	-13.13	1.27	1.39
13	L	914	LDA	O1-N1	-12.85	1.27	1.39
6	L	502[B]	U10	C7-C8	-8.13	1.38	1.50
6	L	502[A]	U10	C7-C8	-8.13	1.38	1.50
7	L	503	UQ1	C7-C8	-6.18	1.41	1.50
6	M	501[B]	U10	C7-C8	-5.43	1.42	1.50
6	M	501[A]	U10	C7-C8	-5.43	1.42	1.50
6	M	501[A]	U10	C27-C28	-4.90	1.36	1.50
6	M	501[B]	U10	C27-C28	-4.55	1.37	1.50
6	M	501[B]	U10	C22-C23	-4.54	1.37	1.50
6	M	501[A]	U10	C22-C23	-4.54	1.37	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	502[A]	U10	C47-C48	-4.49	1.37	1.50
4	L	604	BCL	C3C-C4C	-4.35	1.46	1.51
6	L	502[B]	U10	C27-C28	-4.26	1.38	1.50
6	L	502[A]	U10	C27-C28	-4.26	1.38	1.50
6	L	502[A]	U10	C52-C53	-4.16	1.38	1.50
6	M	501[B]	U10	C42-C43	-4.11	1.39	1.50
6	L	502[A]	U10	C42-C43	-4.09	1.39	1.50
6	M	501[B]	U10	C47-C48	-4.06	1.39	1.50
6	M	501[B]	U10	C37-C38	-4.01	1.39	1.50
6	M	501[A]	U10	C37-C38	-3.96	1.39	1.50
6	L	502[B]	U10	C52-C53	-3.87	1.39	1.50
6	L	502[B]	U10	C17-C18	-3.87	1.39	1.50
6	L	502[A]	U10	C17-C18	-3.87	1.39	1.50
6	L	502[B]	U10	C42-C43	-3.85	1.39	1.50
6	M	501[B]	U10	C17-C18	-3.73	1.40	1.50
6	M	501[A]	U10	C17-C18	-3.73	1.40	1.50
6	M	501[B]	U10	C32-C33	-3.72	1.40	1.50
6	L	502[B]	U10	C37-C38	-3.67	1.40	1.50
6	L	502[B]	U10	C47-C48	-3.67	1.40	1.50
6	M	501[B]	U10	C52-C53	-3.66	1.40	1.50
6	M	501[A]	U10	C42-C43	-3.64	1.40	1.50
6	M	501[A]	U10	C47-C48	-3.56	1.40	1.50
15	M	600	SPO	C4-C1	-3.54	1.48	1.53
6	M	501[A]	U10	C52-C53	-3.51	1.40	1.50
6	L	502[B]	U10	C22-C23	-3.48	1.40	1.50
6	L	502[A]	U10	C22-C23	-3.48	1.40	1.50
6	M	501[B]	U10	C12-C13	-3.48	1.40	1.50
6	M	501[A]	U10	C12-C13	-3.48	1.40	1.50
6	M	501[A]	U10	C32-C33	-3.45	1.40	1.50
6	L	502[A]	U10	C37-C38	-3.43	1.40	1.50
6	L	502[B]	U10	C32-C33	-3.35	1.41	1.50
6	L	502[A]	U10	C32-C33	-3.35	1.41	1.50
7	L	503	UQ1	C3-C4	-3.34	1.39	1.48
6	L	502[B]	U10	C3-C2	-3.32	1.39	1.48
6	L	502[A]	U10	C3-C2	-3.32	1.39	1.48
6	M	501[B]	U10	C4-C5	-3.20	1.39	1.48
6	M	501[A]	U10	C4-C5	-3.20	1.39	1.48
13	M	911	LDA	C1-N1	-3.15	1.45	1.51
13	H	901	LDA	C1-N1	-3.10	1.45	1.51
6	L	502[B]	U10	C12-C13	-3.01	1.42	1.50
6	L	502[A]	U10	C12-C13	-3.01	1.42	1.50
13	M	907	LDA	C1-N1	-2.90	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	H	906	LDA	C1-N1	-2.83	1.46	1.51
13	L	919	LDA	C1-N1	-2.82	1.46	1.51
4	M	603	BCL	C3B-C2B	-2.80	1.33	1.40
13	L	913	LDA	C1-N1	-2.58	1.46	1.51
13	L	921	LDA	CM2-N1	-2.52	1.45	1.49
13	L	920	LDA	C1-N1	-2.52	1.46	1.51
13	M	912	LDA	C1-N1	-2.37	1.47	1.51
7	L	503	UQ1	C2-C1	-2.37	1.42	1.48
13	L	904	LDA	C1-N1	-2.30	1.47	1.51
13	L	915	LDA	C1-N1	-2.26	1.47	1.51
13	M	916	LDA	C1-N1	-2.25	1.47	1.51
13	L	905	LDA	C1-N1	-2.23	1.47	1.51
13	M	918	LDA	C1-N1	-2.23	1.47	1.51
6	L	502[B]	U10	C4-C5	-2.22	1.42	1.48
6	L	502[A]	U10	C4-C5	-2.22	1.42	1.48
13	L	921	LDA	C1-N1	-2.20	1.47	1.51
13	L	902	LDA	C1-N1	-2.20	1.47	1.51
6	M	501[B]	U10	C3-C2	-2.17	1.42	1.48
6	M	501[A]	U10	C3-C2	-2.17	1.42	1.48
4	M	603	BCL	C2C-C3C	-2.13	1.48	1.54
13	H	909	LDA	C1-N1	-2.11	1.47	1.51
6	L	502[B]	U10	C31-C29	2.04	1.55	1.51
6	L	502[A]	U10	C31-C29	2.04	1.55	1.51
7	L	503	UQ1	C7-C6	2.05	1.55	1.51
5	L	402	BPH	C3D-C4D	2.06	1.44	1.41
6	M	501[A]	U10	C46-C44	2.07	1.56	1.51
5	L	402	BPH	CHC-C1C	2.09	1.40	1.36
6	L	502[A]	U10	C48-C49	2.13	1.37	1.33
4	M	603	BCL	OBD-CAD	2.28	1.25	1.22
6	M	501[B]	U10	C53-C54	2.31	1.39	1.32
6	M	501[A]	U10	C30-C29	2.33	1.56	1.50
5	L	402	BPH	C3B-C4B	2.33	1.48	1.43
6	M	501[B]	U10	C23-C24	2.39	1.37	1.33
6	M	501[A]	U10	C23-C24	2.39	1.37	1.33
6	L	502[B]	U10	C8-C9	2.40	1.37	1.33
6	L	502[A]	U10	C8-C9	2.40	1.37	1.33
6	M	501[B]	U10	C28-C29	2.41	1.37	1.33
15	M	600	SPO	C4-C5	2.51	1.53	1.50
6	M	501[A]	U10	C38-C39	2.52	1.37	1.33
6	M	501[B]	U10	C13-C14	2.53	1.37	1.33
6	M	501[A]	U10	C13-C14	2.53	1.37	1.33
6	L	502[B]	U10	C53-C54	2.54	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	501[A]	U10	C35-C34	2.58	1.57	1.50
6	M	501[B]	U10	C6-C1	2.62	1.41	1.35
6	M	501[A]	U10	C6-C1	2.62	1.41	1.35
6	L	502[A]	U10	C53-C54	2.62	1.40	1.32
6	L	502[B]	U10	C6-C1	2.68	1.41	1.35
6	L	502[A]	U10	C6-C1	2.68	1.41	1.35
6	L	502[A]	U10	C43-C44	2.77	1.38	1.33
6	M	501[A]	U10	C53-C54	2.79	1.40	1.32
6	M	501[B]	U10	C36-C34	2.90	1.57	1.51
4	L	602	BCL	CMB-C2B	3.01	1.57	1.51
7	L	503	UQ1	C8-C9	3.10	1.41	1.32
6	M	501[B]	U10	C8-C9	3.22	1.39	1.33
6	M	501[A]	U10	C8-C9	3.22	1.39	1.33
15	M	600	SPO	C21-C22	3.29	1.54	1.43
6	L	502[B]	U10	C43-C44	3.31	1.39	1.33
6	L	502[B]	U10	C18-C19	3.38	1.39	1.33
6	L	502[A]	U10	C18-C19	3.38	1.39	1.33
6	M	501[B]	U10	C48-C49	3.41	1.39	1.33
6	M	501[B]	U10	C18-C19	3.43	1.39	1.33
6	M	501[A]	U10	C18-C19	3.43	1.39	1.33
6	M	501[B]	U10	C33-C34	3.49	1.39	1.33
6	L	502[B]	U10	C23-C24	3.55	1.39	1.33
6	L	502[A]	U10	C23-C24	3.55	1.39	1.33
6	M	501[A]	U10	C43-C44	3.56	1.39	1.33
6	L	502[B]	U10	C33-C34	3.58	1.40	1.33
6	L	502[A]	U10	C33-C34	3.58	1.40	1.33
6	L	502[A]	U10	C38-C39	3.60	1.40	1.33
6	L	502[B]	U10	C38-C39	3.61	1.40	1.33
6	M	501[A]	U10	C33-C34	3.61	1.40	1.33
6	M	501[A]	U10	C48-C49	3.63	1.40	1.33
6	M	501[B]	U10	C43-C44	3.66	1.40	1.33
6	L	502[B]	U10	C48-C49	3.68	1.40	1.33
6	L	502[B]	U10	C13-C14	3.87	1.40	1.33
6	L	502[A]	U10	C13-C14	3.87	1.40	1.33
18	M	800	CDL	OB8-CB7	3.93	1.45	1.33
6	M	501[B]	U10	C38-C39	3.98	1.40	1.33
18	M	800	CDL	OA6-CA5	4.30	1.47	1.34
18	M	800	CDL	OB6-CB5	4.38	1.47	1.34
6	L	502[B]	U10	C28-C29	4.39	1.41	1.33
6	L	502[A]	U10	C28-C29	4.39	1.41	1.33
18	M	800	CDL	OA8-CA7	4.49	1.46	1.33
6	M	501[B]	U10	O4-C4M	4.94	1.57	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	501[A]	U10	O4-C4M	4.94	1.57	1.45

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	601	BCL	C4-C3-C2	-5.83	112.06	123.50
4	M	601	BCL	OBD-CAD-CBD	-5.19	118.11	125.94
6	M	501[A]	U10	C31-C29-C28	-4.97	111.62	121.05
6	L	502[A]	U10	C51-C49-C48	-4.33	112.84	121.05
15	M	600	SPO	C4-C5-C6	-4.32	118.52	124.67
4	L	604	BCL	CMB-C2B-C1B	-4.28	121.28	128.36
6	M	501[A]	U10	C26-C27-C28	-4.27	100.50	111.69
5	M	401	BPH	O1D-CGD-CBD	-4.17	118.64	124.62
4	M	603	BCL	CMB-C2B-C1B	-3.82	122.04	128.36
13	M	903	LDA	O1-N1-CM2	-3.76	104.02	109.05
4	M	601	BCL	CMB-C2B-C1B	-3.72	122.21	128.36
4	L	604	BCL	CAC-C3C-C4C	-3.68	104.42	112.58
5	M	401	BPH	CAA-C2A-C1A	-3.59	103.40	112.86
5	L	402	BPH	C1C-NC-C4C	-3.58	106.77	110.44
15	M	600	SPO	C20-C19-C17	-3.53	122.09	127.20
6	L	502[B]	U10	C30-C29-C28	-3.47	116.68	123.50
6	L	502[A]	U10	C30-C29-C28	-3.47	116.68	123.50
7	L	503	UQ1	CM5-C5-C6	-3.39	116.85	124.10
15	M	600	SPO	C5-C6-C7	-3.36	120.62	125.75
13	L	914	LDA	O1-N1-CM2	-3.36	104.56	109.05
4	M	603	BCL	CAC-C3C-C2C	-3.35	105.70	114.13
4	L	604	BCL	CAC-C3C-C2C	-3.35	105.72	114.13
5	M	401	BPH	C1C-NC-C4C	-3.35	107.01	110.44
5	L	402	BPH	CAA-C2A-C3A	-3.33	103.65	113.22
18	M	800	CDL	CA4-OA6-CA5	-3.32	109.92	117.89
4	L	602	BCL	CMB-C2B-C1B	-3.32	122.88	128.36
18	M	800	CDL	OB8-CB7-OB9	-3.29	115.01	123.49
4	L	604	BCL	O1D-CGD-CBD	-3.24	119.98	124.62
12	H	752	HTO	C5-C4-C3	-3.17	108.52	114.20
4	M	603	BCL	O2A-CGA-O1A	-3.13	115.42	123.49
13	H	906	LDA	CM2-N1-CM1	-3.08	105.35	108.83
6	M	501[B]	U10	C35-C34-C33	-3.02	117.56	123.50
13	H	909	LDA	O1-N1-CM2	-3.01	105.03	109.05
13	L	914	LDA	CM2-N1-CM1	-2.99	105.45	108.83
4	M	603	BCL	OBD-CAD-CBD	-2.99	121.43	125.94
4	M	601	BCL	O1D-CGD-CBD	-2.96	120.38	124.62
6	M	501[B]	U10	C22-C21-C19	-2.88	103.33	112.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	501[A]	U10	C22-C21-C19	-2.88	103.33	112.71
12	L	753	HTO	O1-C1-C2	-2.86	104.88	111.10
6	L	502[B]	U10	C40-C39-C38	-2.82	117.97	123.50
6	L	502[A]	U10	C46-C47-C48	-2.79	104.39	111.69
13	M	907	LDA	O1-N1-CM2	-2.78	105.34	109.05
13	L	920	LDA	CM2-N1-CM1	-2.77	105.70	108.83
15	M	600	SPO	C25-C23-C22	-2.70	114.64	118.98
6	M	501[A]	U10	C26-C24-C23	-2.64	116.05	121.05
7	L	503	UQ1	C5-C6-C1	-2.64	117.11	120.12
4	L	604	BCL	CAA-C2A-C3A	-2.62	105.67	113.22
5	M	401	BPH	CMA-C3A-C2A	-2.59	102.90	114.35
13	L	921	LDA	O1-N1-CM2	-2.58	105.61	109.05
6	L	502[A]	U10	C47-C46-C44	-2.58	104.32	112.71
4	L	604	BCL	OBD-CAD-CBD	-2.56	122.07	125.94
5	L	402	BPH	CMB-C2B-C1B	-2.56	120.89	125.06
5	L	402	BPH	CMA-C3A-C2A	-2.56	103.04	114.35
4	L	602	BCL	CAA-C2A-C3A	-2.55	105.89	113.22
5	M	401	BPH	CAA-C2A-C3A	-2.52	105.96	113.22
5	L	402	BPH	C3B-C4B-NB	-2.52	104.62	109.98
5	M	401	BPH	C4-C3-C2	-2.50	118.60	123.50
6	M	501[A]	U10	C35-C34-C33	-2.49	118.62	123.50
5	M	401	BPH	CMB-C2B-C1B	-2.48	121.01	125.06
12	L	753	HTO	O2-C2-C1	-2.48	103.43	109.22
13	L	905	LDA	CM2-N1-CM1	-2.47	106.05	108.83
6	L	502[B]	U10	C27-C26-C24	-2.42	104.83	112.71
6	L	502[A]	U10	C27-C26-C24	-2.42	104.83	112.71
15	M	600	SPO	C16-C17-C19	-2.40	115.11	118.98
4	L	602	BCL	CAA-C2A-C1A	-2.39	104.04	112.47
6	M	501[B]	U10	C30-C29-C28	-2.39	118.82	123.50
4	M	601	BCL	C6-C5-C3	-2.36	107.30	112.48
6	L	502[B]	U10	C36-C34-C33	-2.36	116.58	121.05
18	M	800	CDL	OA6-CA5-OA7	-2.35	117.36	123.67
4	M	601	BCL	CAA-C2A-C3A	-2.33	106.53	113.22
4	M	603	BCL	CHA-C1A-NA	-2.32	120.35	126.06
13	M	903	LDA	O1-N1-CM1	-2.32	105.96	109.05
4	L	602	BCL	OBD-CAD-CBD	-2.31	122.46	125.94
13	L	902	LDA	O1-N1-CM2	-2.31	105.97	109.05
13	L	915	LDA	O1-N1-CM2	-2.30	105.97	109.05
5	M	401	BPH	OBD-CAD-CBD	-2.30	122.47	125.94
6	L	502[A]	U10	C40-C39-C38	-2.30	118.99	123.50
6	L	502[B]	U10	O2-C2-C3	-2.29	115.82	120.79
6	L	502[A]	U10	O2-C2-C3	-2.29	115.82	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	604	BCL	CMA-C3A-C2A	-2.27	104.30	114.35
15	M	600	SPO	C27-C26-C25	-2.25	116.26	123.13
13	H	910	LDA	CM2-N1-CM1	-2.24	106.30	108.83
4	L	604	BCL	CHA-C1A-NA	-2.24	120.56	126.06
13	L	913	LDA	O1-N1-C1	-2.23	107.76	110.27
13	M	912	LDA	O1-N1-CM1	-2.23	106.07	109.05
6	M	501[B]	U10	C50-C49-C48	-2.21	119.15	123.50
4	M	601	BCL	CAA-C2A-C1A	-2.21	104.69	112.47
4	L	602	BCL	CMA-C3A-C2A	-2.15	104.83	114.35
6	L	502[B]	U10	C21-C22-C23	-2.14	106.08	111.69
6	L	502[A]	U10	C21-C22-C23	-2.14	106.08	111.69
4	L	604	BCL	CMC-C2C-C3C	-2.14	104.90	114.35
13	L	908	LDA	CM2-N1-CM1	-2.12	106.44	108.83
13	L	919	LDA	CM2-N1-CM1	-2.10	106.46	108.83
13	L	917	LDA	CM2-N1-CM1	-2.09	106.48	108.83
6	L	502[B]	U10	C45-C44-C43	-2.08	119.43	123.50
11	L	751	HT3	O2-C2-C1	-2.07	104.40	109.22
4	M	603	BCL	CAC-C3C-C4C	-2.06	108.00	112.58
4	L	604	BCL	C5-C3-C2	-2.06	117.14	121.05
5	L	402	BPH	OBD-CAD-CBD	-2.01	122.90	125.94
5	L	402	BPH	CAC-C3C-C2C	2.06	119.30	114.13
6	M	501[B]	U10	C56-C54-C55	2.11	119.84	114.64
6	L	502[B]	U10	C40-C39-C41	2.12	118.64	115.41
5	L	402	BPH	CMB-C2B-C3B	2.12	132.99	128.04
5	M	401	BPH	C5-C3-C2	2.14	125.12	121.05
13	M	907	LDA	O1-N1-C1	2.15	112.69	110.27
13	L	908	LDA	O1-N1-C1	2.17	112.72	110.27
15	M	600	SPO	C34-C33-C35	2.23	118.82	115.41
4	M	601	BCL	CMB-C2B-C3B	2.24	129.47	125.09
4	L	604	BCL	C4-C3-C5	2.26	118.85	115.41
6	L	502[B]	U10	C3M-O3-C3	2.26	124.64	116.61
6	L	502[A]	U10	C3M-O3-C3	2.26	124.64	116.61
4	M	603	BCL	O2D-CGD-CBD	2.26	114.40	111.30
4	M	601	BCL	O2D-CGD-CBD	2.28	114.42	111.30
6	L	502[B]	U10	C17-C16-C14	2.28	120.14	112.71
6	L	502[A]	U10	C17-C16-C14	2.28	120.14	112.71
6	L	502[B]	U10	C22-C21-C19	2.29	120.18	112.71
6	L	502[A]	U10	C22-C21-C19	2.29	120.18	112.71
4	M	603	BCL	CMB-C2B-C3B	2.29	129.58	125.09
5	M	401	BPH	CMC-C2C-C1C	2.31	119.36	112.33
10	M	741	GOL	O2-C2-C1	2.33	119.35	108.65
11	L	751	HT3	O3-C3-C2	2.39	114.67	109.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	604	BCL	C2C-C3C-C4C	2.40	105.56	101.50
6	M	501[B]	U10	C10-C9-C11	2.40	119.07	115.41
6	M	501[A]	U10	C10-C9-C11	2.40	119.07	115.41
15	M	600	SPO	C24-C23-C22	2.43	126.49	122.90
15	M	600	SPO	C18-C17-C19	2.46	126.54	122.90
6	L	502[A]	U10	C35-C34-C36	2.57	119.34	115.41
13	M	918	LDA	O1-N1-C1	2.58	113.18	110.27
6	L	502[A]	U10	C40-C39-C41	2.60	119.37	115.41
6	L	502[B]	U10	C30-C29-C31	2.72	119.56	115.41
6	L	502[A]	U10	C30-C29-C31	2.72	119.56	115.41
5	L	402	BPH	CMC-C2C-C1C	2.74	120.67	112.33
6	M	501[A]	U10	C50-C49-C51	2.79	119.66	115.41
6	L	502[B]	U10	C45-C44-C46	2.84	119.74	115.41
4	M	603	BCL	CMD-C2D-C3D	2.84	130.65	125.09
6	M	501[A]	U10	C45-C44-C46	2.88	119.80	115.41
15	M	600	SPO	C21-C20-C19	2.88	129.76	123.39
4	L	602	BCL	CMB-C2B-C3B	2.93	130.83	125.09
5	M	401	BPH	C3A-C2A-C1A	2.94	105.57	101.84
7	L	503	UQ1	CM3-O3-C3	2.96	127.14	116.61
11	L	751	HT3	O2-C2-C3	2.97	115.85	109.79
5	L	402	BPH	C1B-NB-C4B	2.97	112.39	106.51
18	M	800	CDL	OB8-CB7-C71	3.08	121.28	111.90
6	L	502[B]	U10	C25-C24-C26	3.09	120.12	115.41
6	L	502[A]	U10	C25-C24-C26	3.09	120.12	115.41
13	H	910	LDA	O1-N1-C1	3.15	113.82	110.27
6	M	501[A]	U10	C25-C24-C26	3.16	120.23	115.41
6	M	501[B]	U10	C50-C49-C51	3.17	120.25	115.41
4	M	601	BCL	OBB-CAB-C3B	3.18	125.04	120.00
6	M	501[A]	U10	C40-C39-C41	3.18	120.27	115.41
6	M	501[A]	U10	C27-C28-C29	3.20	134.72	127.76
18	M	800	CDL	OA8-CA7-C31	3.26	121.83	111.90
5	M	401	BPH	C3C-C4C-NC	3.28	111.22	107.93
13	L	914	LDA	O1-N1-C1	3.30	113.98	110.27
18	M	800	CDL	OB6-CB5-C51	3.34	118.78	111.53
4	L	604	BCL	CMB-C2B-C3B	3.41	131.76	125.09
6	M	501[B]	U10	C15-C14-C16	3.52	120.78	115.41
6	M	501[A]	U10	C15-C14-C16	3.52	120.78	115.41
6	M	501[B]	U10	C45-C44-C46	3.56	120.85	115.41
4	L	604	BCL	O2D-CGD-CBD	3.63	116.27	111.30
5	L	402	BPH	CAC-C3C-C4C	3.68	122.13	112.67
6	M	501[B]	U10	C35-C34-C36	3.71	121.08	115.41
6	M	501[A]	U10	C35-C34-C36	3.92	121.40	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	L	503	UQ1	C7-C6-C1	4.20	123.50	118.56
5	M	401	BPH	CAC-C3C-C4C	4.56	124.39	112.67
6	M	501[B]	U10	C30-C29-C31	4.65	122.51	115.41
13	M	903	LDA	O1-N1-C1	4.88	115.77	110.27
5	L	402	BPH	C3C-C4C-NC	5.07	113.00	107.93
18	M	800	CDL	OA6-CA5-C11	5.15	122.72	111.53
6	L	502[B]	U10	C35-C34-C36	5.32	123.53	115.41
5	M	401	BPH	O2D-CGD-CBD	5.43	118.75	111.30
4	M	601	BCL	C5-C3-C2	5.64	131.75	121.05
6	M	501[A]	U10	C30-C29-C31	6.03	124.61	115.41
6	L	502[A]	U10	C50-C49-C51	6.49	125.32	115.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

39 monomers are involved in 108 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	H	729	GOL	1	0
10	H	738	GOL	1	0
10	H	739	GOL	2	0
12	H	752	HTO	3	0
13	H	901	LDA	2	0
13	H	906	LDA	4	0
13	H	909	LDA	2	0
13	H	910	LDA	6	0
6	L	502[A]	U10	9	0
6	L	502[B]	U10	5	0
7	L	503	UQ1	13	0
4	L	602	BCL	3	0
4	L	604	BCL	2	0
8	L	708	PO4	1	0
10	L	724	GOL	1	0
10	L	728	GOL	2	0
10	L	733	GOL	2	0
13	L	902	LDA	4	0
13	L	905	LDA	2	0
13	L	908	LDA	1	0
13	L	914	LDA	1	0
13	L	915	LDA	1	0
13	L	917	LDA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	L	919	LDA	4	0
13	L	920	LDA	4	0
13	L	921	LDA	11	0
5	M	401	BPH	4	0
6	M	501[A]	U10	1	0
6	M	501[B]	U10	6	0
15	M	600	SPO	1	0
4	M	601	BCL	6	0
4	M	603	BCL	6	0
8	M	707	PO4	1	0
10	M	740	GOL	2	0
10	M	741	GOL	4	0
10	M	742	GOL	1	0
18	M	800	CDL	9	0
13	M	903	LDA	4	0
13	M	918	LDA	2	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	L	281/281 (100%)	-0.37	9 (3%)	51	52	27, 35, 57, 81	0
2	M	302/307 (98%)	-0.17	13 (4%)	39	40	25, 40, 64, 83	0
3	H	239/260 (91%)	0.07	12 (5%)	32	34	31, 40, 52, 98	0
All	All	822/848 (96%)	-0.17	34 (4%)	41	42	25, 38, 60, 98	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	10	PHE	9.7
2	M	1	ALA	7.3
3	H	246	PRO	5.6
3	H	248	ARG	5.2
3	H	245	ALA	5.1
2	M	2	GLU	5.1
3	H	18	TYR	5.0
2	M	302	GLY	4.5
2	M	3	TYR	4.0
3	H	52	ASN	3.7
3	H	247	LYS	3.6
3	H	220[A]	LYS	3.6
1	L	59	TRP	3.5
1	L	279	ILE	3.4
1	L	277	GLY	3.3
2	M	105	PHE	3.2
2	M	301	HIS	2.9
1	L	270	PRO	2.7
3	H	22	ILE	2.6
2	M	83	ALA	2.6
1	L	275	ILE	2.4
2	M	18	LEU	2.4
2	M	100	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	M	79	GLY	2.3
2	M	80	TRP	2.3
2	M	148	TRP	2.3
3	H	191	LEU	2.3
2	M	104	SER	2.2
1	L	276	PRO	2.2
1	L	202	LYS	2.2
3	H	179	LEU	2.2
1	L	271	TRP	2.1
3	H	164	VAL	2.1
1	L	40	PHE	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

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
13	LDA	L	919	16/16	0.51	0.71	33.02	46,58,86,93	16
10	GOL	L	733	6/6	0.72	0.58	27.81	51,52,52,53	6
13	LDA	M	916	16/16	0.37	0.41	27.67	47,56,79,89	16
13	LDA	L	904	16/16	-0.06	0.73	26.65	43,50,83,85	16
13	LDA	M	903	16/16	0.44	0.76	21.48	46,52,73,82	16
13	LDA	L	914	16/16	0.41	0.45	20.73	41,54,82,85	16
10	GOL	L	728	6/6	0.81	0.77	19.64	59,62,63,63	6
13	LDA	M	918	16/16	0.19	0.64	18.50	42,57,77,85	16
13	LDA	L	915	16/16	0.56	0.47	17.18	44,59,85,94	16
8	PO4	L	708	5/5	0.70	0.40	15.63	65,66,67,67	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
13	LDA	L	908	16/16	0.04	0.53	12.07	44,54,87,88	16
8	PO4	M	707	5/5	0.89	0.25	10.95	48,53,55,58	5
10	GOL	L	725	6/6	0.69	0.33	10.89	41,55,59,61	6
7	UQ1	L	503	18/18	0.55	0.40	10.77	44,55,60,61	18
6	U10	L	502[B]	63/63	0.73	0.33	9.96	26,55,59,62	63
6	U10	L	502[A]	63/63	0.73	0.33	9.96	26,47,58,59	63
9	DIO	L	711	6/6	0.95	0.20	9.70	51,52,53,55	6
10	GOL	M	737	6/6	0.90	0.57	9.21	62,66,68,70	6
18	CDL	M	800	81/100	0.63	0.49	8.52	32,52,69,72	81
10	GOL	H	738	6/6	0.89	0.36	8.50	42,45,48,49	6
13	LDA	L	917	16/16	0.49	0.33	8.35	34,52,77,82	16
13	LDA	L	905	16/16	0.63	0.35	8.35	41,54,85,89	16
13	LDA	L	902	16/16	0.53	0.51	8.05	42,56,83,83	16
10	GOL	L	731	6/6	0.82	0.34	7.75	52,55,56,57	6
12	HTO	H	752	10/10	0.72	0.45	5.80	62,66,67,68	10
10	GOL	H	729	6/6	0.71	0.31	5.31	50,57,59,61	6
13	LDA	L	921	16/16	0.76	0.25	5.18	44,60,88,99	16
10	GOL	M	742	6/6	0.75	0.35	5.17	55,56,57,57	6
13	LDA	L	913	16/16	0.50	0.34	4.69	46,55,81,82	16
13	LDA	H	910	16/16	0.11	0.62	4.64	39,55,79,88	16
10	GOL	L	723	6/6	0.90	0.19	4.61	39,47,50,55	6
13	LDA	M	911	16/16	0.77	0.33	4.46	45,58,92,102	16
13	LDA	H	901	16/16	0.81	0.28	4.01	45,52,63,70	0
12	HTO	L	753	10/10	0.81	0.35	3.59	50,57,58,58	10
13	LDA	M	912	16/16	0.66	0.31	3.55	47,64,94,108	16
11	HT3	L	751	10/10	0.51	0.27	2.84	53,56,58,58	10
6	U10	M	501[A]	63/63	0.91	0.17	2.83	24,38,68,69	31
6	U10	M	501[B]	63/63	0.91	0.17	2.83	24,40,67,71	31
13	LDA	M	907	16/16	0.70	0.25	2.63	40,47,64,65	16
10	GOL	H	739	6/6	0.66	0.35	2.62	57,62,62,62	6
8	PO4	L	705	5/5	0.84	0.19	2.07	47,51,54,56	5
10	GOL	H	735	6/6	0.92	0.34	1.86	48,53,54,56	6
15	SPO	M	600	42/42	0.87	0.19	1.76	34,39,74,89	0
8	PO4	M	704	5/5	0.97	0.17	1.58	56,58,67,67	5
4	BCL	M	603	66/66	0.96	0.12	1.19	27,31,52,63	0
4	BCL	M	601	66/66	0.94	0.13	1.01	28,34,103,107	0
10	GOL	H	745	6/6	0.50	0.31	1.00	60,60,61,61	6
5	BPH	M	401	65/65	0.94	0.11	0.88	29,34,85,86	0
4	BCL	L	604	66/66	0.96	0.11	0.82	24,29,53,57	0
4	BCL	L	602	66/66	0.96	0.10	0.72	24,29,39,44	0
10	GOL	H	721	6/6	0.96	0.17	0.66	42,44,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	BPH	L	402	65/65	0.95	0.10	0.66	23,28,39,40	0
10	GOL	L	722	6/6	0.91	0.14	0.54	47,51,56,62	0
10	GOL	L	744	6/6	0.84	0.26	0.49	44,45,46,49	6
10	GOL	M	741	6/6	0.62	0.29	0.45	35,41,42,44	6
8	PO4	L	703	5/5	0.96	0.13	0.14	55,62,65,66	0
10	GOL	L	724	6/6	0.93	0.14	0.07	39,41,42,45	6
16	K	H	700	1/1	0.98	0.11	-0.69	48,48,48,48	0
14	FE	M	500	1/1	1.00	0.01	-2.76	28,28,28,28	0
17	CL	M	702	1/1	0.98	0.11	-	47,47,47,47	0
13	LDA	L	920	16/16	0.32	0.35	-	47,70,102,104	16
8	PO4	L	706	5/5	0.84	0.23	-	53,57,59,60	5
10	GOL	H	736	6/6	0.79	0.21	-	61,62,62,62	6
10	GOL	L	727	6/6	0.52	0.47	-	55,56,60,60	6
10	GOL	L	734	6/6	0.66	0.52	-	54,56,59,62	6
10	GOL	L	732	6/6	0.72	1.65	-	56,57,57,57	6
8	PO4	H	709	5/5	0.80	0.35	-	61,61,63,63	5
10	GOL	H	743	6/6	0.78	0.27	-	40,52,53,58	6
13	LDA	H	909	16/16	0.55	0.29	-	46,56,80,83	16
16	K	M	701	1/1	0.94	0.08	-	57,57,57,57	0
13	LDA	H	906	16/16	0.50	0.64	-	48,57,68,72	16
10	GOL	L	730	6/6	0.87	0.23	-	56,62,64,66	6
10	GOL	H	746	6/6	0.67	0.27	-	49,52,54,55	6
10	GOL	M	726	6/6	0.90	0.23	-	52,53,54,55	6
10	GOL	M	740	6/6	0.72	0.56	-	59,60,60,61	6

6.5 Other polymers (i)

There are no such residues in this entry.