Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:32 PM GMT

PDB ID	:	4LWY
Title	:	L(M196)H,H(M202)L Double Mutant Structure of Photosynthetic Reaction Center From Rhodobacter Sphaeroides strain RV
Authors	:	Gabdulkhakov, A.G.
Deposited on	:	2013-07-29
Resolution	:	2.90 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:

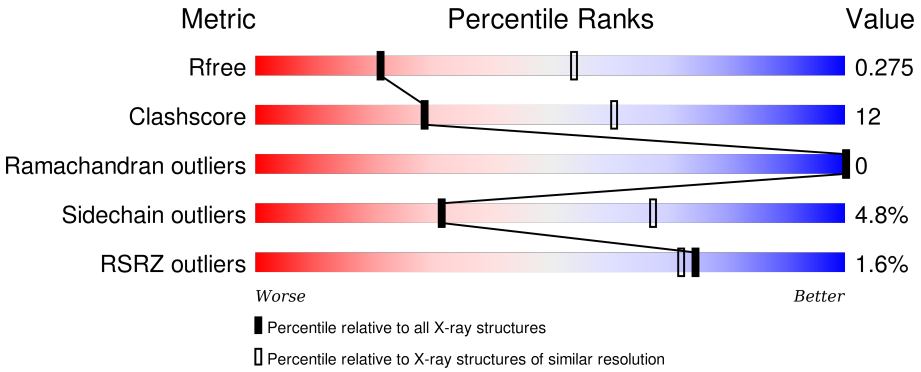
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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	H	260	2% 70% 23% 8%
2	L	282	% 72% 26%
3	M	303	% 71% 26%

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
12	BPH	L	303	X	-	-	-
12	BPH	M	402	X	-	-	-
12	BPH	M	404	X	-	-	-
14	CDL	M	401	-	-	-	X
16	SPN	M	407	-	-	-	X
4	LDA	M	409	-	-	-	X
4	LDA	M	410	-	-	-	X
4	LDA	M	411	-	-	-	X
4	LDA	M	412	-	-	-	X
5	UNL	H	304	-	-	-	X
5	UNL	L	305	-	-	-	X
5	UNL	L	306	-	-	-	X
5	UNL	L	307	-	-	-	X
5	UNL	L	308	-	-	-	X
5	UNL	M	415	-	-	-	X
7	DIO	H	307	-	-	-	X
7	DIO	L	309	-	-	-	X
8	EDO	H	310	-	-	-	X
8	EDO	H	311	-	-	-	X
8	EDO	M	419	-	-	-	X
9	TRS	L	312	-	-	-	X

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 7434 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 H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	240	Total	C	N	O	S	0	0	0
			1829	1169	314	337	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	0	0
			2233	1508	355	362	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	178	THR	SER	SEE REMARK 999	UNP P0C0Y8

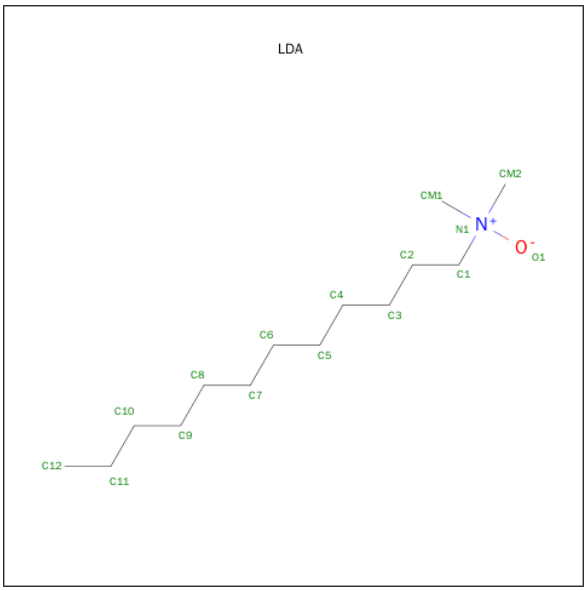
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	302	Total	C	N	O	S	0	0	0
			2409	1608	394	397	10			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	THR	SER	SEE REMARK 999	UNP P0C0Y9
M	196	HIS	LEU	ENGINEERED MUTATION	UNP P0C0Y9
M	202	LEU	HIS	ENGINEERED MUTATION	UNP P0C0Y9

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).

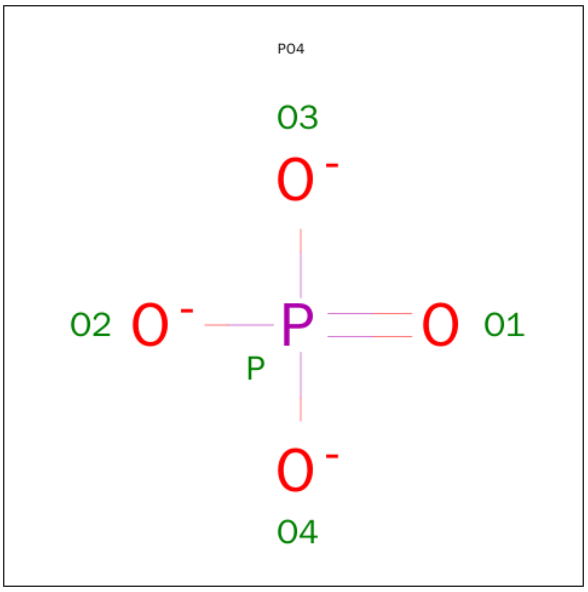


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C N O 16 14 1 1	0	0
4	M	1	Total C N O 16 14 1 1	0	0
4	M	1	Total C N O 16 14 1 1	0	0
4	M	1	Total C N O 16 14 1 1	0	0
4	M	1	Total C N O 16 14 1 1	0	0
4	M	1	Total C N O 16 14 1 1	0	0

- Molecule 5 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

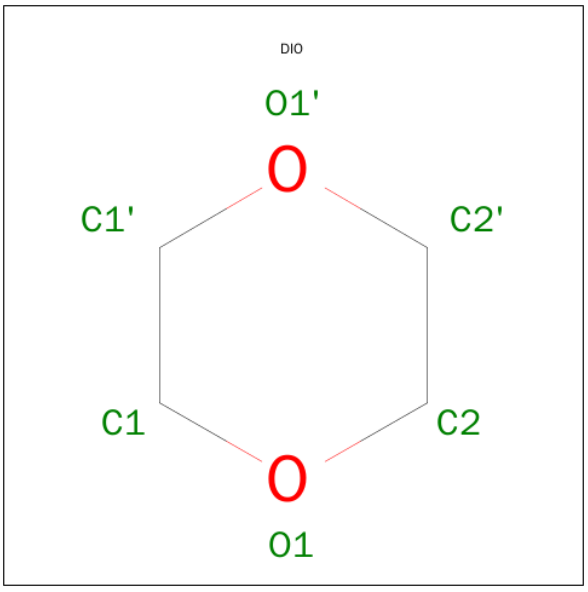
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	4	Total C 48 48	0	0
5	L	4	Total C 46 46	0	0
5	M	3	Total C 36 36	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 7 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: $C_4H_8O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	H	1	Total C O 6 4 2	0	0

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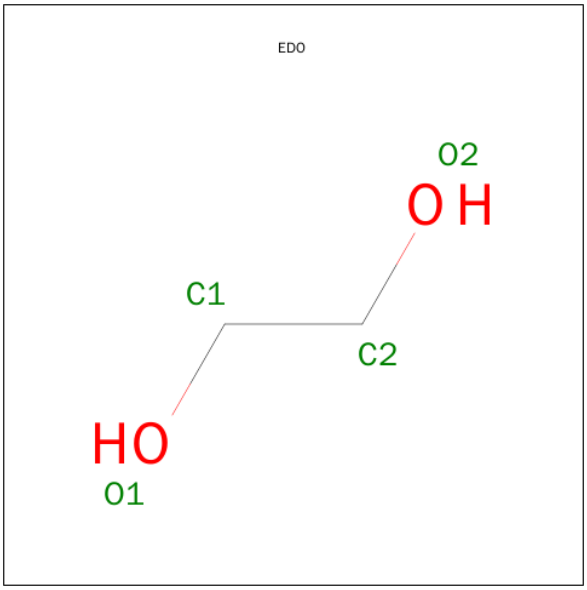
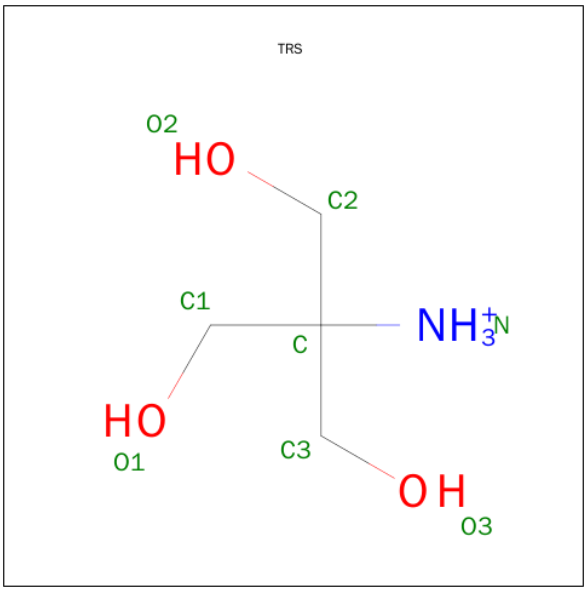
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total C O 6 4 2	0	0
7	L	1	Total C O 6 4 2	0	0
7	M	1	Total C O 6 4 2	0	0

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 9 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).

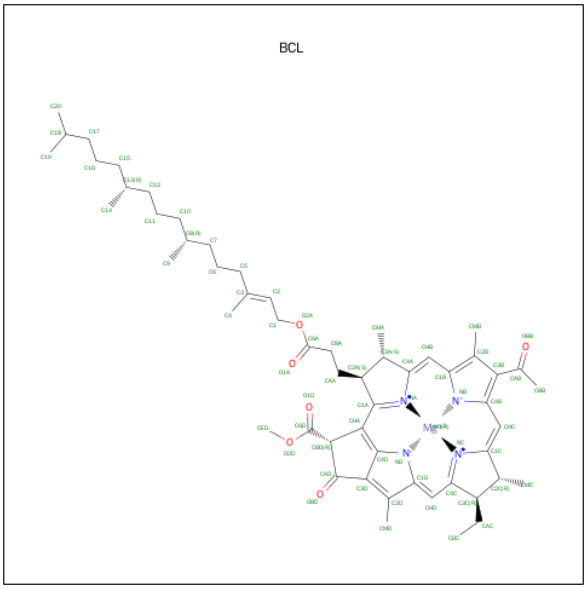


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	H	1	Total C N O 8 4 1 3	0	0
9	L	1	Total C N O 8 4 1 3	0	0

- Molecule 10 is POTASSIUM ION (three-letter code: K) (formula: K).

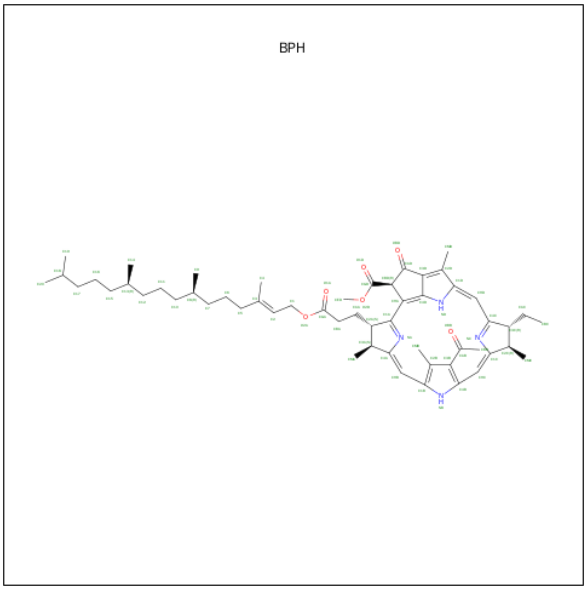
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	H	1	Total K 1 1	0	0

- Molecule 11 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



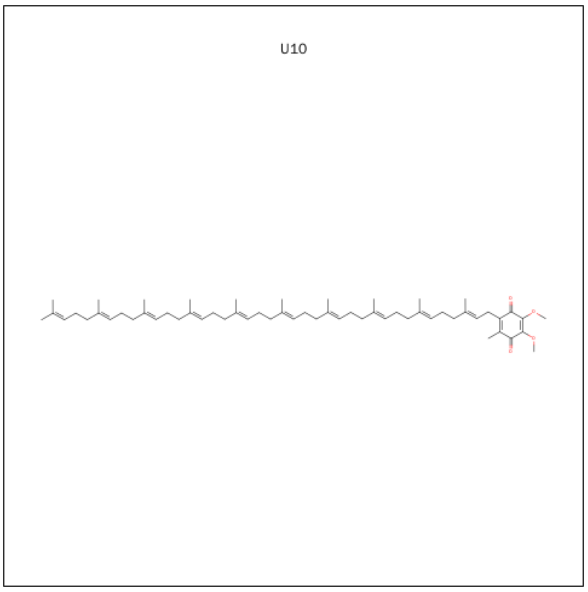
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
11	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
11	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 12 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



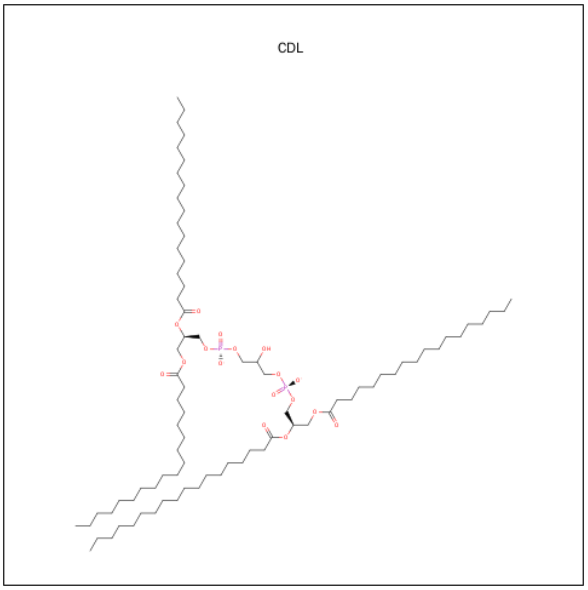
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	L	1	Total	C	N	O	0	0
			65	55	4	6		
12	M	1	Total	C	N	O	0	0
			65	55	4	6		
12	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 13 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	L	1	Total	C	O	0	0
			48	44	4		
13	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 14 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).

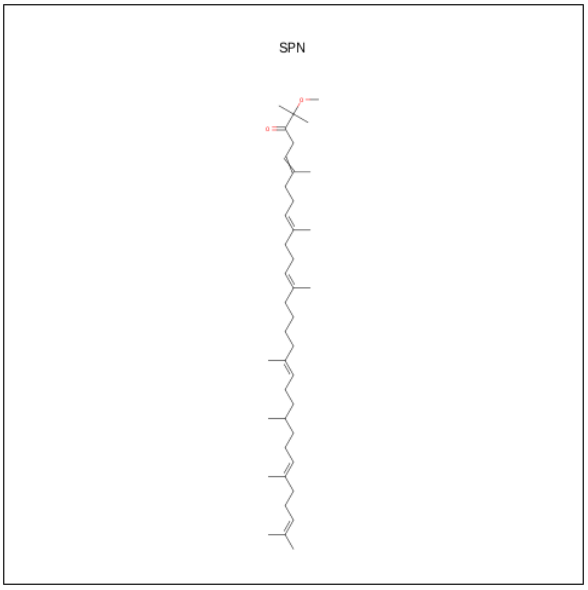


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	M	1	Total	C	O	P	0	0
			81	62	17	2		

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

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

- Molecule 16 is SPEROIDENONE (three-letter code: SPN) (formula: $C_{41}H_{70}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	M	1	Total C O 43 41 2	0	0

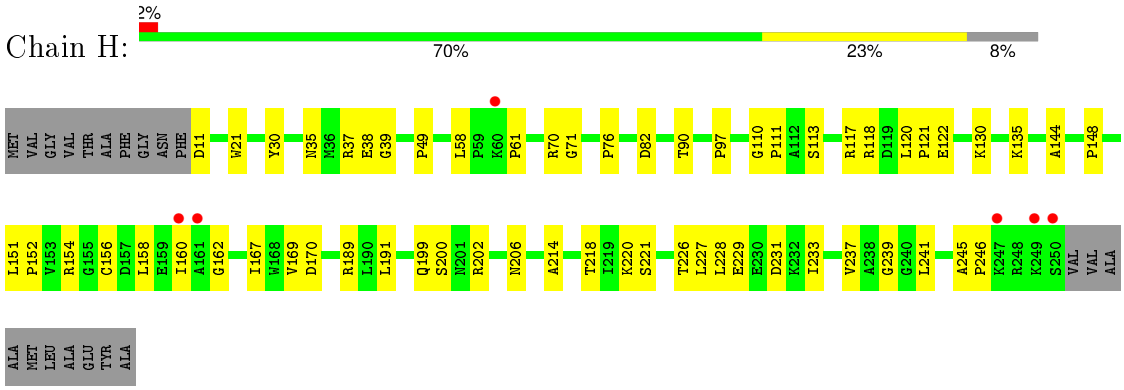
- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	H	11	Total O 11 11	0	0
17	L	10	Total O 10 10	0	0
17	M	18	Total O 18 18	0	0

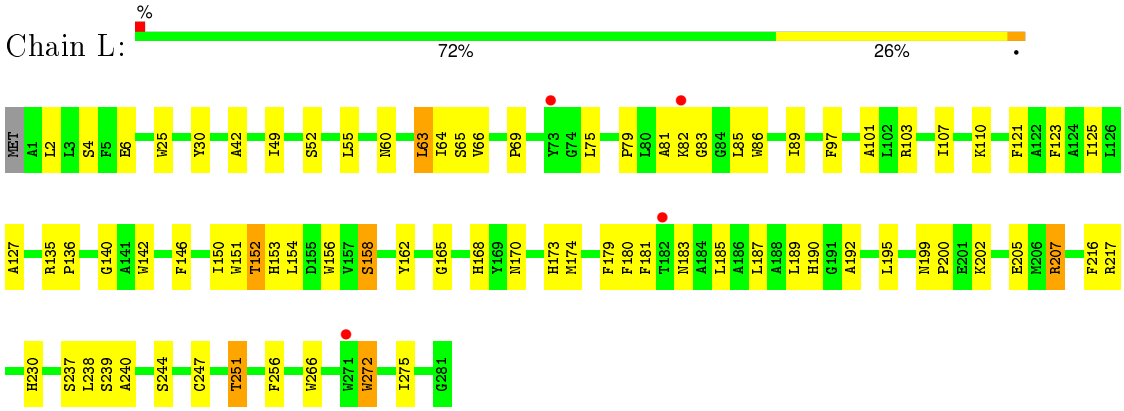
3 Residue-property plots (i)

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.

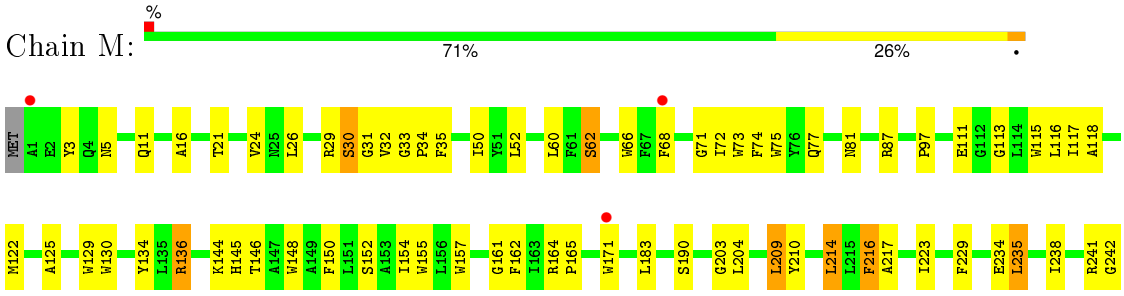
- Molecule 1: Reaction center protein H chain



- Molecule 2: Reaction center protein L chain



- Molecule 3: Reaction center protein M chain




T243
A244
R247
W254
T255
M256
G257
F258
G264
R267
W268
A269
I270
V276
T277
L278
I284
N293
V296
W297
G302

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	140.04Å 140.04Å 184.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.19 – 2.90 43.19 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.19-2.90) 99.8 (43.19-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1389)	Depositor
R, R_{free}	0.214 , 0.262 0.227 , 0.275	Depositor DCC
R_{free} test set	2335 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	53.4	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 50.4	EDS
Estimated twinning fraction	0.066 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Outliers	0 of 46696 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7434	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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, LDA, DIO, CDL, BPH, K, EDO, FE, SPN, U10, TRS, UNL, 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	H	0.43	0/1877	0.63	0/2553
2	L	0.46	0/2321	0.60	0/3177
3	M	0.44	0/2501	0.59	0/3415
All	All	0.44	0/6699	0.60	0/9145

There are no bond length outliers.

There are no bond angle outliers.

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	H	1829	0	1836	39	0
2	L	2233	0	2189	63	0
3	M	2409	0	2323	71	0
4	H	16	0	31	2	0
4	M	80	0	155	9	0
5	H	48	0	0	0	0
5	L	46	0	0	0	0
5	M	36	0	0	0	0
6	H	5	0	0	0	0
6	M	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	6	0	8	0	0
7	L	12	0	16	3	0
7	M	6	0	8	1	0
8	H	16	0	24	3	0
8	L	4	0	6	1	0
8	M	8	0	12	1	0
9	H	8	0	12	1	0
9	L	8	0	12	0	0
10	H	1	0	0	0	0
11	L	132	0	148	11	0
11	M	66	0	74	4	0
12	L	65	0	76	10	0
12	M	130	0	152	11	0
13	L	48	0	63	1	0
13	M	48	0	63	5	0
14	M	81	0	106	6	0
15	M	1	0	0	0	0
16	M	43	0	70	5	0
17	H	11	0	0	0	0
17	L	10	0	0	0	0
17	M	18	0	0	1	0
All	All	7434	0	7384	170	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 12.

All (170) 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)
3:M:34:PRO:HA	4:M:412:LDA:H71	1.55	0.89
2:L:200:PRO:HD2	7:L:309:DIO:H22	1.64	0.80
1:H:202:ARG:HH12	9:H:312:TRS:H21	1.53	0.73
2:L:42:ALA:HA	12:L:303:BPH:H9C3	1.71	0.73
2:L:65:SER:HB2	2:L:152:THR:HG21	1.70	0.72
2:L:199:ASN:HA	7:L:309:DIO:H21	1.74	0.70
1:H:111:PRO:HB2	1:H:239:GLY:HA2	1.74	0.70
3:M:21:THR:HG23	3:M:26:LEU:HD11	1.75	0.68
3:M:62:SER:HB2	3:M:125:ALA:HB2	1.73	0.68
2:L:55:LEU:HD13	2:L:81:ALA:HB2	1.74	0.68
2:L:69:PRO:HG2	2:L:142:TRP:HB2	1.75	0.68
3:M:35:PHE:H	4:M:412:LDA:H51	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:404:BPH:HHC	12:M:404:BPH:HBB3	1.78	0.66
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.79	0.64
2:L:60:ASN:HB3	2:L:63:LEU:HB2	1.80	0.64
1:H:152:PRO:HB2	1:H:160:ILE:HD12	1.79	0.63
2:L:205:GLU:O	2:L:207:ARG:NH1	2.32	0.63
12:L:303:BPH:H7C2	11:M:403:BCL:H201	1.81	0.63
1:H:38:GLU:OE1	3:M:241:ARG:NH1	2.31	0.62
1:H:160:ILE:HG22	1:H:162:GLY:H	1.65	0.62
3:M:75:TRP:HE1	16:M:407:SPN:HMA2	1.65	0.60
2:L:266:TRP:CD2	7:M:418:DIO:H11	2.36	0.60
12:M:402:BPH:H172	12:M:404:BPH:H9C2	1.83	0.60
12:L:303:BPH:H112	11:M:403:BCL:H201	1.84	0.59
1:H:121:PRO:HA	1:H:226:THR:HA	1.84	0.58
1:H:71:GLY:H	8:H:310:EDO:H22	1.68	0.58
2:L:180:PHE:CD2	2:L:240:ALA:HB1	2.39	0.58
2:L:2:LEU:HB3	2:L:6:GLU:HB3	1.87	0.57
4:H:301:LDA:H121	4:M:408:LDA:H91	1.86	0.57
3:M:152:SER:O	3:M:155:TRP:HB3	2.05	0.57
1:H:117:ARG:O	1:H:228:LEU:HB2	2.05	0.56
2:L:146:PHE:HA	2:L:156:TRP:CD1	2.40	0.56
12:L:303:BPH:HBB2	3:M:210:TYR:HB3	1.87	0.56
3:M:97:PRO:HG2	3:M:171:TRP:HB2	1.87	0.56
12:L:303:BPH:HMA1	13:M:406:U10:H252	1.88	0.56
2:L:150:ILE:HG22	2:L:151:TRP:CD1	2.40	0.56
1:H:122:GLU:HB2	1:H:227:LEU:HD21	1.88	0.56
3:M:31:GLY:H	4:M:410:LDA:HM11	1.70	0.55
2:L:170:ASN:HB3	2:L:173:HIS:HB3	1.89	0.55
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.89	0.55
2:L:60:ASN:O	2:L:63:LEU:N	2.39	0.55
1:H:156:CYS:HB3	1:H:206:ASN:O	2.08	0.54
1:H:90:THR:OG1	1:H:97:PRO:O	2.22	0.54
1:H:167:ILE:HG22	1:H:169:VAL:HG12	1.90	0.54
1:H:11:ASP:OD2	3:M:297:TRP:NE1	2.41	0.54
3:M:134:TYR:CE2	3:M:144:LYS:HG3	2.42	0.53
2:L:49:ILE:HG12	2:L:89:ILE:HD13	1.88	0.53
3:M:190:SER:HB2	12:M:402:BPH:H3C	1.89	0.53
11:M:403:BCL:HMB1	11:M:403:BCL:HBB2	1.91	0.53
2:L:52:SER:HB2	2:L:85:LEU:HD13	1.90	0.53
2:L:179:PHE:CD2	2:L:239:SER:HB3	2.45	0.52
3:M:148:TRP:HB3	14:M:401:CDL:H761	1.92	0.52
2:L:180:PHE:HB3	3:M:209:LEU:HD21	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:157:TRP:CZ2	16:M:407:SPN:HM73	2.46	0.51
12:L:303:BPH:H152	11:M:403:BCL:H202	1.92	0.51
1:H:21:TRP:HZ2	4:M:408:LDA:HM13	1.75	0.51
2:L:230:HIS:CD2	3:M:223:ILE:HG13	2.46	0.51
2:L:180:PHE:CE2	2:L:240:ALA:HB1	2.45	0.50
4:H:301:LDA:H112	13:M:406:U10:H202	1.92	0.50
2:L:168:HIS:HB3	3:M:183:LEU:HD13	1.94	0.50
2:L:127:ALA:HB3	11:L:302:BCL:H43	1.94	0.50
1:H:113:SER:O	3:M:247:ARG:NH1	2.45	0.50
3:M:73:TRP:HE1	3:M:77:GLN:NE2	2.09	0.49
12:L:303:BPH:H3C	3:M:214:LEU:HA	1.93	0.49
2:L:181:PHE:CD2	12:M:404:BPH:HBB1	2.48	0.49
1:H:30:TYR:OH	3:M:267:ARG:NH1	2.45	0.49
11:L:301:BCL:HBB3	11:L:301:BCL:HMB1	1.94	0.49
1:H:130:LYS:HE3	1:H:170:ASP:OD2	2.12	0.49
3:M:268:TRP:CD1	13:M:406:U10:H111	2.48	0.49
2:L:190:HIS:HA	13:L:304:U10:O2	2.13	0.49
2:L:153:HIS:CE1	12:L:303:BPH:H201	2.47	0.49
2:L:97:PHE:CE1	11:L:302:BCL:H121	2.48	0.49
3:M:203:GLY:HA3	4:M:408:LDA:HM21	1.95	0.49
3:M:278:LEU:HD11	14:M:401:CDL:H811	1.94	0.49
3:M:130:TRP:HD1	3:M:150:PHE:HD2	1.61	0.49
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.95	0.48
2:L:185:LEU:HD13	12:M:404:BPH:ND	2.28	0.48
1:H:61:PRO:HA	1:H:76:PRO:HD2	1.96	0.48
11:L:301:BCL:H61	12:M:402:BPH:H203	1.95	0.47
3:M:204:LEU:HG	4:M:408:LDA:HM11	1.97	0.47
2:L:162:TYR:HA	2:L:165:GLY:O	2.13	0.47
2:L:123:PHE:CD1	2:L:238:LEU:HD13	2.48	0.47
2:L:52:SER:OG	8:L:311:EDO:O2	2.29	0.47
3:M:130:TRP:HD1	3:M:150:PHE:CD2	2.32	0.47
1:H:189:ARG:NH2	1:H:214:ALA:O	2.40	0.47
2:L:60:ASN:O	2:L:64:ILE:HG13	2.15	0.47
1:H:154:ARG:HG2	1:H:158:LEU:HA	1.97	0.47
3:M:164:ARG:HB3	3:M:165:PRO:HD3	1.96	0.47
2:L:187:LEU:HD13	3:M:216:PHE:CG	2.50	0.47
3:M:164:ARG:HD2	3:M:284:ILE:HG22	1.96	0.47
2:L:75:LEU:HD11	2:L:140:GLY:HA2	1.96	0.47
2:L:79:PRO:HB2	2:L:82:LYS:HG3	1.97	0.47
11:L:301:BCL:HHC	12:M:402:BPH:H4C2	1.97	0.46
3:M:157:TRP:CE2	16:M:407:SPN:HM73	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:401:CDL:H391	14:M:401:CDL:H422	1.69	0.46
1:H:199:GLN:OE1	1:H:202:ARG:NH1	2.48	0.46
2:L:69:PRO:HD3	2:L:83:GLY:O	2.16	0.46
1:H:35:ASN:OD1	3:M:264:GLY:HA3	2.16	0.46
3:M:16:ALA:HB1	3:M:32:VAL:HG21	1.98	0.46
1:H:220:LYS:HG3	1:H:229:GLU:OE2	2.16	0.45
2:L:97:PHE:HB3	2:L:125:ILE:HD11	1.98	0.45
2:L:199:ASN:HA	7:L:309:DIO:C2	2.46	0.45
1:H:117:ARG:HD2	3:M:242:GLY:HA2	1.98	0.45
12:L:303:BPH:CBB	3:M:210:TYR:HB3	2.47	0.45
13:M:406:U10:H28	13:M:406:U10:H322	1.44	0.45
1:H:118:ARG:HG2	1:H:120:LEU:HG	1.99	0.45
3:M:234:GLU:O	3:M:238:ILE:HG13	2.17	0.45
4:M:412:LDA:HM23	4:M:412:LDA:H21	1.61	0.45
1:H:110:GLY:HA3	1:H:111:PRO:HD2	1.83	0.45
3:M:144:LYS:HB2	14:M:401:CDL:HB32	1.98	0.45
3:M:256:MET:CE	13:M:406:U10:H102	2.47	0.45
1:H:70:ARG:O	1:H:118:ARG:NH2	2.50	0.45
11:L:301:BCL:HBB2	12:M:402:BPH:H102	1.98	0.44
11:L:302:BCL:H192	11:L:302:BCL:H161	1.68	0.44
3:M:24:VAL:HG11	3:M:29:ARG:HH11	1.82	0.44
2:L:244:SER:OG	11:L:302:BCL:HMA2	2.18	0.44
1:H:241:LEU:HD13	8:M:419:EDO:H11	1.98	0.44
3:M:35:PHE:N	4:M:412:LDA:H51	2.30	0.44
2:L:237:SER:HB3	3:M:217:ALA:HB2	1.99	0.44
1:H:245:ALA:N	1:H:246:PRO:HD2	2.32	0.44
2:L:189:LEU:HD23	2:L:189:LEU:HA	1.85	0.44
2:L:66:VAL:HG12	2:L:86:TRP:HB2	2.00	0.44
3:M:113:GLY:O	3:M:117:ILE:HG13	2.17	0.43
2:L:101:ALA:HB2	2:L:121:PHE:HD2	1.83	0.43
3:M:60:LEU:HA	12:M:404:BPH:C4	2.48	0.43
3:M:162:PHE:HD1	16:M:407:SPN:H242	1.84	0.43
1:H:82:ASP:OD2	8:H:311:EDO:H12	2.18	0.43
2:L:25:TRP:CD1	2:L:30:TYR:HA	2.53	0.43
2:L:275:ILE:HG21	3:M:81:ASN:ND2	2.33	0.43
2:L:158:SER:HA	11:L:302:BCL:HBC1	2.00	0.43
3:M:32:VAL:HG12	3:M:33:GLY:O	2.18	0.43
1:H:144:ALA:HB3	3:M:11:GLN:HG3	2.00	0.43
1:H:37:ARG:O	1:H:38:GLU:HG2	2.19	0.43
2:L:179:PHE:CE2	2:L:239:SER:HB3	2.54	0.42
2:L:192:ALA:HB1	3:M:146:THR:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:49:ILE:CG1	2:L:89:ILE:HD13	2.49	0.42
2:L:127:ALA:CB	11:L:302:BCL:H43	2.49	0.42
3:M:235:LEU:HD12	17:M:506:HOH:O	2.18	0.42
3:M:209:LEU:N	3:M:276:VAL:HG22	2.35	0.42
3:M:115:TRP:CE3	3:M:116:LEU:HD23	2.55	0.42
3:M:66:TRP:HD1	3:M:118:ALA:O	2.03	0.42
2:L:181:PHE:HB3	12:M:404:BPH:HBB2	2.02	0.41
2:L:217:ARG:O	3:M:50:ILE:HA	2.20	0.41
3:M:68:PHE:O	3:M:72:ILE:HG12	2.20	0.41
2:L:153:HIS:O	2:L:156:TRP:HB3	2.21	0.41
3:M:161:GLY:HA3	16:M:407:SPN:H201	2.02	0.41
1:H:220:LYS:H	1:H:220:LYS:HG3	1.61	0.41
3:M:71:GLY:HA2	3:M:74:PHE:HB2	2.02	0.41
3:M:30:SER:OG	3:M:31:GLY:N	2.52	0.41
1:H:39:GLY:HA2	2:L:4:SER:OG	2.20	0.41
3:M:293:ASN:HB3	3:M:296:VAL:HB	2.03	0.41
1:H:148:PRO:HD2	1:H:167:ILE:HD11	2.03	0.41
2:L:174:MET:SD	11:L:301:BCL:HED3	2.61	0.41
2:L:195:LEU:HB3	3:M:145:HIS:CD2	2.56	0.41
2:L:110:LYS:HD2	3:M:254:TRP:CZ3	2.56	0.41
12:L:303:BPH:HBB1	3:M:210:TYR:CD2	2.55	0.41
14:M:401:CDL:HB31	14:M:401:CDL:HB21	2.03	0.41
2:L:103:ARG:O	2:L:107:ILE:HG13	2.21	0.41
3:M:154:ILE:HG23	3:M:157:TRP:CE3	2.56	0.41
1:H:71:GLY:N	8:H:310:EDO:H22	2.35	0.40
1:H:58:LEU:HA	1:H:58:LEU:HD23	1.85	0.40
2:L:135:ARG:HH21	2:L:251:THR:HG22	1.86	0.40
1:H:233:ILE:O	1:H:237:VAL:HG23	2.21	0.40
3:M:129:TRP:CD1	12:M:404:BPH:HBA1	2.56	0.40
3:M:148:TRP:NE1	14:M:401:CDL:OB6	2.53	0.40
3:M:136:ARG:HA	3:M:136:ARG:NH1	2.36	0.40
2:L:107:ILE:HG23	3:M:254:TRP:HE3	1.86	0.40
3:M:3:TYR:CZ	3:M:5:ASN:HA	2.56	0.40
2:L:272:TRP:CG	3:M:87:ARG:HB2	2.57	0.40
2:L:192:ALA:O	3:M:145:HIS:HB2	2.22	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	H	238/260 (92%)	233 (98%)	5 (2%)	0	100	100
2	L	279/282 (99%)	261 (94%)	18 (6%)	0	100	100
3	M	300/303 (99%)	280 (93%)	20 (7%)	0	100	100
All	All	817/845 (97%)	774 (95%)	43 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	195/208 (94%)	188 (96%)	7 (4%)	42	78
2	L	220/221 (100%)	208 (94%)	12 (6%)	27	61
3	M	236/237 (100%)	224 (95%)	12 (5%)	29	65
All	All	651/666 (98%)	620 (95%)	31 (5%)	31	67

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	49	PRO
1	H	135	LYS
1	H	191	LEU
1	H	200	SER
1	H	218	THR

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Mol	Chain	Res	Type
1	H	221	SER
1	H	231	ASP
2	L	63	LEU
2	L	152	THR
2	L	154	LEU
2	L	158	SER
2	L	183	ASN
2	L	202	LYS
2	L	207	ARG
2	L	216	PHE
2	L	247	CYS
2	L	251	THR
2	L	256	PHE
2	L	272	TRP
3	M	30	SER
3	M	52	LEU
3	M	62	SER
3	M	111	GLU
3	M	122	MET
3	M	136	ARG
3	M	209	LEU
3	M	214	LEU
3	M	216	PHE
3	M	235	LEU
3	M	258	PHE
3	M	270	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	M	77	GLN

5.3.3 RNA (i)

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 45 ligands modelled in this entry, 11 are unknown and 2 are monoatomic - leaving 32 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	$\#\|Z\| > 2$
4	LDA	H	301	-	15,15,15	3.81	2 (13%)	16,17,17	0.55	0
6	PO4	H	306	-	4,4,4	0.47	0	6,6,6	0.26	0
7	DIO	H	307	-	6,6,6	0.84	0	6,6,6	0.76	0
8	EDO	H	308	-	3,3,3	0.48	0	2,2,2	0.37	0
8	EDO	H	309	-	3,3,3	0.45	0	2,2,2	0.64	0
8	EDO	H	310	-	3,3,3	0.47	0	2,2,2	0.57	0
8	EDO	H	311	-	3,3,3	0.55	0	2,2,2	0.26	0
9	TRS	H	312	-	7,7,7	0.96	1 (14%)	9,9,9	0.52	0
11	BCL	L	301	-	53,74,74	0.61	0	57,115,115	1.59	8 (14%)
11	BCL	L	302	-	53,74,74	0.60	1 (1%)	57,115,115	1.63	10 (17%)
12	BPH	L	303	-	64,70,70	1.47	8 (12%)	73,101,101	1.49	10 (13%)
13	U10	L	304	-	48,48,63	2.94	13 (27%)	58,61,79	1.96	15 (25%)
7	DIO	L	309	-	6,6,6	0.80	0	6,6,6	0.79	0
7	DIO	L	310	-	6,6,6	0.69	0	6,6,6	1.06	0
8	EDO	L	311	-	3,3,3	0.55	0	2,2,2	0.18	0
9	TRS	L	312	-	7,7,7	1.02	1 (14%)	9,9,9	0.42	0
14	CDL	M	401	-	80,80,99	0.88	4 (5%)	82,92,111	1.33	7 (8%)
12	BPH	M	402	-	64,70,70	1.41	7 (10%)	73,101,101	1.52	8 (10%)
11	BCL	M	403	-	53,74,74	0.67	1 (1%)	57,115,115	1.74	11 (19%)
12	BPH	M	404	-	64,70,70	1.40	7 (10%)	73,101,101	1.62	8 (10%)
13	U10	M	406	-	48,48,63	3.00	12 (25%)	58,61,79	1.94	16 (27%)
16	SPN	M	407	-	41,42,42	1.26	6 (14%)	41,52,52	2.02	17 (41%)
4	LDA	M	408	-	15,15,15	3.91	2 (13%)	16,17,17	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	LDA	M	409	-	15,15,15	3.80	2 (13%)	16,17,17	0.41	0
4	LDA	M	410	-	15,15,15	3.91	2 (13%)	16,17,17	0.56	0
4	LDA	M	411	-	15,15,15	3.88	2 (13%)	16,17,17	0.42	0
4	LDA	M	412	-	15,15,15	3.81	2 (13%)	16,17,17	0.71	0
6	PO4	M	416	-	4,4,4	0.39	0	6,6,6	0.27	0
6	PO4	M	417	-	4,4,4	0.41	0	6,6,6	0.27	0
7	DIO	M	418	-	6,6,6	0.83	0	6,6,6	0.84	0
8	EDO	M	419	-	3,3,3	0.52	0	2,2,2	0.36	0
8	EDO	M	420	-	3,3,3	0.53	0	2,2,2	0.28	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
4	LDA	H	301	-	-	0/13/13/13	0/0/0/0
6	PO4	H	306	-	-	0/0/0/0	0/0/0/0
7	DIO	H	307	-	-	0/0/6/6	0/1/1/1
8	EDO	H	308	-	-	0/1/1/1	0/0/0/0
8	EDO	H	309	-	-	0/1/1/1	0/0/0/0
8	EDO	H	310	-	-	0/1/1/1	0/0/0/0
8	EDO	H	311	-	-	0/1/1/1	0/0/0/0
9	TRS	H	312	-	-	0/9/9/9	0/0/0/0
11	BCL	L	301	-	-	0/37/137/137	0/0/9/9
11	BCL	L	302	-	-	0/37/137/137	0/0/9/9
12	BPH	L	303	-	2/2/18/22	0/54/105/105	0/1/6/6
13	U10	L	304	-	-	0/45/69/87	0/1/1/1
7	DIO	L	309	-	-	0/0/6/6	0/1/1/1
7	DIO	L	310	-	-	0/0/6/6	0/1/1/1
8	EDO	L	311	-	-	0/1/1/1	0/0/0/0
9	TRS	L	312	-	-	0/9/9/9	0/0/0/0
14	CDL	M	401	-	-	0/91/91/110	0/0/0/0
12	BPH	M	402	-	2/2/18/22	0/54/105/105	0/1/6/6
11	BCL	M	403	-	-	0/37/137/137	0/0/9/9
12	BPH	M	404	-	2/2/18/22	0/54/105/105	0/1/6/6
13	U10	M	406	-	-	0/45/69/87	0/1/1/1
16	SPN	M	407	-	-	0/50/51/51	0/0/0/0
4	LDA	M	408	-	-	0/13/13/13	0/0/0/0
4	LDA	M	409	-	-	0/13/13/13	0/0/0/0
4	LDA	M	410	-	-	0/13/13/13	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LDA	M	411	-	-	0/13/13/13	0/0/0/0
4	LDA	M	412	-	-	0/13/13/13	0/0/0/0
6	PO4	M	416	-	-	0/0/0/0	0/0/0/0
6	PO4	M	417	-	-	0/0/0/0	0/0/0/0
7	DIO	M	418	-	-	0/0/6/6	0/1/1/1
8	EDO	M	419	-	-	0/1/1/1	0/0/0/0
8	EDO	M	420	-	-	0/1/1/1	0/0/0/0

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	408	LDA	O1-N1	-14.78	1.25	1.39
4	M	410	LDA	O1-N1	-14.74	1.25	1.39
4	M	411	LDA	O1-N1	-14.65	1.25	1.39
4	H	301	LDA	O1-N1	-14.40	1.25	1.39
4	M	412	LDA	O1-N1	-14.38	1.25	1.39
4	M	409	LDA	O1-N1	-14.38	1.25	1.39
13	M	406	U10	O4-C4	-4.68	1.24	1.37
13	L	304	U10	O4-C4	-4.47	1.25	1.37
13	L	304	U10	O3-C3	-4.37	1.25	1.37
13	M	406	U10	O3-C3	-4.32	1.25	1.37
12	M	402	BPH	C1B-C2B	-3.86	1.37	1.45
12	M	404	BPH	C4C-NC	-3.85	1.28	1.37
12	M	402	BPH	CHB-C4A	-3.75	1.33	1.40
12	L	303	BPH	C1B-C2B	-3.63	1.37	1.45
12	M	404	BPH	C1B-C2B	-3.48	1.38	1.45
12	M	402	BPH	C4C-NC	-3.38	1.29	1.37
12	M	402	BPH	C1A-NA	-3.10	1.30	1.37
12	L	303	BPH	CHB-C4A	-3.10	1.34	1.40
12	L	303	BPH	C4C-NC	-2.93	1.30	1.37
12	M	404	BPH	CHB-C4A	-2.92	1.35	1.40
12	L	303	BPH	C1A-NA	-2.89	1.31	1.37
13	L	304	U10	C4-C5	-2.88	1.40	1.48
12	M	404	BPH	C1A-NA	-2.82	1.31	1.37
4	M	410	LDA	C1-N1	-2.75	1.46	1.51
4	M	412	LDA	C1-N1	-2.73	1.46	1.51
4	H	301	LDA	C1-N1	-2.72	1.46	1.51
4	M	408	LDA	C1-N1	-2.71	1.46	1.51
4	M	411	LDA	C1-N1	-2.70	1.46	1.51
9	L	312	TRS	C-N	-2.64	1.46	1.50
4	M	409	LDA	C1-N1	-2.61	1.46	1.51
13	M	406	U10	C4-C5	-2.54	1.41	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	L	304	U10	C3-C2	-2.52	1.41	1.48
9	H	312	TRS	C-N	-2.44	1.47	1.50
11	L	302	BCL	CHD-C4C	-2.35	1.34	1.41
11	M	403	BCL	CHD-C4C	-2.22	1.34	1.41
13	M	406	U10	C3-C2	-2.14	1.42	1.48
13	L	304	U10	C6-C5	-2.10	1.40	1.46
12	M	404	BPH	C3D-C4D	2.00	1.43	1.41
12	M	402	BPH	C3D-C4D	2.05	1.44	1.41
14	M	401	CDL	OA6-CA5	2.09	1.40	1.34
12	L	303	BPH	CHB-C1B	2.12	1.42	1.38
13	L	304	U10	C6-C1	2.19	1.40	1.35
16	M	407	SPN	C29-C30	2.20	1.39	1.32
13	M	406	U10	C6-C1	2.24	1.40	1.35
12	L	303	BPH	C3D-C4D	2.42	1.44	1.41
16	M	407	SPN	C4-C5	2.46	1.37	1.33
16	M	407	SPN	C12-C13	2.53	1.37	1.33
14	M	401	CDL	OB6-CB5	2.65	1.42	1.34
14	M	401	CDL	OA8-CA7	2.86	1.41	1.33
16	M	407	SPN	C19-C18	3.17	1.39	1.33
16	M	407	SPN	C8-C9	3.28	1.39	1.33
14	M	401	CDL	OB8-CB7	3.29	1.43	1.33
16	M	407	SPN	C25-C26	3.57	1.40	1.33
12	M	404	BPH	CHD-C4C	3.99	1.48	1.38
12	M	402	BPH	CHD-C4C	4.02	1.48	1.38
13	M	406	U10	C38-C39	4.82	1.47	1.32
12	M	402	BPH	CHA-C1A	4.86	1.48	1.37
12	L	303	BPH	CHD-C4C	4.98	1.50	1.38
12	M	404	BPH	CHA-C1A	5.05	1.49	1.37
13	L	304	U10	C38-C39	5.44	1.49	1.32
12	L	303	BPH	CHA-C1A	5.49	1.50	1.37
13	L	304	U10	C8-C9	6.47	1.45	1.33
13	M	406	U10	C8-C9	6.89	1.46	1.33
13	L	304	U10	C28-C29	7.08	1.46	1.33
13	L	304	U10	C23-C24	7.19	1.47	1.33
13	L	304	U10	C33-C34	7.34	1.47	1.33
13	M	406	U10	C28-C29	7.36	1.47	1.33
13	L	304	U10	C18-C19	7.42	1.47	1.33
13	M	406	U10	C18-C19	7.42	1.47	1.33
13	M	406	U10	C33-C34	7.57	1.47	1.33
13	L	304	U10	C13-C14	7.57	1.47	1.33
13	M	406	U10	C13-C14	7.68	1.48	1.33
13	M	406	U10	C23-C24	7.75	1.48	1.33

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	L	304	U10	C7-C8-C9	-5.53	117.32	126.70
11	L	302	BCL	CMB-C2B-C1B	-4.57	120.80	128.36
11	L	301	BCL	O1D-CGD-CBD	-4.14	118.68	124.62
13	L	304	U10	C17-C18-C19	-4.14	118.75	127.76
13	M	406	U10	C22-C23-C24	-4.00	119.06	127.76
12	M	404	BPH	C4-C3-C5	-3.89	109.47	115.41
16	M	407	SPN	C24-C25-C26	-3.84	119.40	127.76
13	M	406	U10	C17-C18-C19	-3.75	119.61	127.76
13	M	406	U10	C27-C28-C29	-3.59	119.96	127.76
11	M	403	BCL	O1D-CGD-CBD	-3.56	119.52	124.62
16	M	407	SPN	C7-C8-C9	-3.55	120.04	127.76
13	L	304	U10	C22-C23-C24	-3.49	120.18	127.76
16	M	407	SPN	C6-C5-C4	-3.44	114.53	121.05
13	M	406	U10	C32-C33-C34	-3.43	120.30	127.76
16	M	407	SPN	C3-C4-C5	-3.38	120.98	126.70
13	L	304	U10	C32-C33-C34	-3.38	120.42	127.76
13	L	304	U10	C12-C13-C14	-3.33	120.52	127.76
11	L	302	BCL	C1D-CHD-C4C	-3.26	121.10	126.07
16	M	407	SPN	C20-C19-C18	-3.25	120.69	127.76
13	L	304	U10	C27-C28-C29	-3.11	120.99	127.76
13	L	304	U10	C35-C34-C33	-3.07	117.48	123.50
16	M	407	SPN	C11-C12-C13	-2.97	121.31	127.76
11	L	301	BCL	CMB-C2B-C1B	-2.95	123.48	128.36
12	M	402	BPH	OBB-CAB-CBB	-2.95	112.77	119.69
12	M	402	BPH	C2D-C1D-ND	-2.87	105.58	110.29
12	L	303	BPH	C2D-C1D-ND	-2.87	105.59	110.29
11	M	403	BCL	C1D-CHD-C4C	-2.80	121.80	126.07
12	M	404	BPH	C2D-C1D-ND	-2.74	105.80	110.29
13	L	304	U10	C10-C9-C8	-2.68	118.25	123.50
12	L	303	BPH	C2B-C1B-NB	-2.67	105.72	109.73
12	M	404	BPH	C1C-NC-C4C	-2.66	107.71	110.44
11	L	301	BCL	C1D-CHD-C4C	-2.56	122.16	126.07
13	M	406	U10	C26-C27-C28	-2.53	105.05	111.69
11	L	301	BCL	C6-C5-C3	-2.53	106.94	112.48
12	L	303	BPH	C3B-C4B-NB	-2.52	104.63	109.98
11	M	403	BCL	C2A-C1A-CHA	-2.40	119.47	123.89
13	L	304	U10	C20-C19-C18	-2.39	118.80	123.50
11	M	403	BCL	C3C-C4C-CHD	-2.38	118.03	123.33
13	M	406	U10	C7-C8-C9	-2.32	122.76	126.70
11	M	403	BCL	CMB-C2B-C1B	-2.31	124.54	128.36
12	M	402	BPH	CMB-C2B-C1B	-2.31	121.30	125.06
12	M	402	BPH	C4-C3-C5	-2.20	112.05	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	M	407	SPN	CM4-C9-C8	-2.19	119.20	123.50
11	L	302	BCL	C3C-C4C-CHD	-2.18	118.47	123.33
13	M	406	U10	C37-C38-C39	-2.18	119.36	127.73
13	M	406	U10	C30-C29-C28	-2.14	119.31	123.50
13	M	406	U10	C20-C19-C18	-2.13	119.31	123.50
16	M	407	SPN	CM8-C26-C25	-2.09	119.40	123.50
12	M	402	BPH	C1D-CHD-C4C	-2.07	119.71	127.23
12	M	404	BPH	C1B-NB-C4B	2.06	110.59	106.51
12	L	303	BPH	OBB-CAB-C3B	2.08	124.33	120.31
11	M	403	BCL	O2A-CGA-CBA	2.09	118.26	111.90
11	M	403	BCL	CHC-C1C-NC	2.19	127.54	124.51
16	M	407	SPN	CM4-C9-C10	2.23	118.81	115.41
16	M	407	SPN	CM5-C13-C14	2.24	118.83	115.41
16	M	407	SPN	C7-C6-C5	2.33	120.32	112.71
12	L	303	BPH	C4D-C3D-C2D	2.34	110.10	107.08
12	M	402	BPH	CMD-C2D-C3D	2.36	129.71	125.09
12	L	303	BPH	CMD-C2D-C3D	2.37	129.73	125.09
11	L	302	BCL	CHB-C4A-NA	2.38	127.81	124.51
12	M	404	BPH	C4D-C3D-C2D	2.46	110.27	107.08
13	L	304	U10	C15-C14-C16	2.47	119.19	115.41
12	L	303	BPH	O2D-CGD-O1D	2.50	128.94	123.79
14	M	401	CDL	OA8-CA7-C31	2.50	119.53	111.90
16	M	407	SPN	CMA-O1-C1	2.52	125.61	112.20
13	M	406	U10	C25-C24-C26	2.57	119.33	115.41
16	M	407	SPN	CM6-C18-C17	2.58	119.35	115.41
16	M	407	SPN	CM8-C26-C27	2.65	119.45	115.41
16	M	407	SPN	C15-C14-C13	2.71	118.43	112.48
16	M	407	SPN	C27-C28-C29	2.73	118.84	111.69
11	L	301	BCL	CED-O2D-CGD	2.73	122.39	115.99
12	L	303	BPH	C1B-NB-C4B	2.73	111.92	106.51
11	L	301	BCL	C4-C3-C5	2.83	119.73	115.41
11	L	302	BCL	CED-O2D-CGD	2.84	122.65	115.99
11	M	403	BCL	C4-C3-C5	2.85	119.76	115.41
13	M	406	U10	C41-C39-C40	2.89	121.76	114.64
13	M	406	U10	C20-C19-C21	3.00	119.99	115.41
14	M	401	CDL	CB4-OB6-CB5	3.04	125.17	117.89
14	M	401	CDL	OB8-CB7-C71	3.05	121.20	111.90
12	M	404	BPH	CMD-C2D-C3D	3.08	131.11	125.09
13	L	304	U10	C35-C34-C36	3.10	120.14	115.41
11	L	302	BCL	O2D-CGD-CBD	3.11	115.57	111.30
16	M	407	SPN	CM3-C5-C6	3.14	120.20	115.41
11	L	302	BCL	CMB-C2B-C3B	3.15	131.25	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	L	304	U10	C30-C29-C31	3.17	120.25	115.41
11	L	302	BCL	C4-C3-C5	3.18	120.27	115.41
11	L	301	BCL	CHD-C4C-NC	3.19	128.76	125.06
13	L	304	U10	C20-C19-C21	3.27	120.40	115.41
11	L	302	BCL	O2A-CGA-CBA	3.29	121.91	111.90
14	M	401	CDL	OA6-CA5-C11	3.35	118.80	111.53
12	L	303	BPH	C6-C5-C3	3.35	119.84	112.48
12	M	402	BPH	C6-C5-C3	3.37	119.88	112.48
13	L	304	U10	C25-C24-C26	3.39	120.59	115.41
11	M	403	BCL	CHB-C4A-NA	3.46	129.30	124.51
12	M	404	BPH	C5-C3-C2	3.53	127.74	121.05
14	M	401	CDL	OA8-CA6-CA4	3.60	118.38	108.69
14	M	401	CDL	OB6-CB5-C51	3.67	119.49	111.53
13	M	406	U10	C35-C34-C36	3.68	121.02	115.41
11	L	302	BCL	CHD-C4C-NC	3.72	129.38	125.06
13	M	406	U10	C10-C9-C11	3.81	121.23	115.41
13	M	406	U10	C15-C14-C16	3.95	121.44	115.41
13	L	304	U10	C10-C9-C11	4.15	121.74	115.41
14	M	401	CDL	OB8-CB6-CB4	4.24	120.09	108.69
11	M	403	BCL	CHD-C4C-NC	4.68	130.49	125.06
13	M	406	U10	C30-C29-C31	4.97	123.00	115.41
11	M	403	BCL	O2D-CGD-CBD	6.31	119.95	111.30
11	L	301	BCL	O2D-CGD-CBD	6.31	119.96	111.30
12	L	303	BPH	C3C-C4C-NC	6.51	114.45	107.93
12	M	402	BPH	C3C-C4C-NC	8.01	115.95	107.93
12	M	404	BPH	C3C-C4C-NC	8.17	116.11	107.93

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	L	303	BPH	C8
12	L	303	BPH	C13
12	M	402	BPH	C8
12	M	402	BPH	C13
12	M	404	BPH	C8
12	M	404	BPH	C13

There are no torsion outliers.

There are no ring outliers.

21 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	301	LDA	2	0
8	H	310	EDO	2	0
8	H	311	EDO	1	0
9	H	312	TRS	1	0
11	L	301	BCL	5	0
11	L	302	BCL	6	0
12	L	303	BPH	10	0
13	L	304	U10	1	0
7	L	309	DIO	3	0
8	L	311	EDO	1	0
14	M	401	CDL	6	0
12	M	402	BPH	5	0
11	M	403	BCL	4	0
12	M	404	BPH	7	0
13	M	406	U10	5	0
16	M	407	SPN	5	0
4	M	408	LDA	4	0
4	M	410	LDA	1	0
4	M	412	LDA	4	0
7	M	418	DIO	1	0
8	M	419	EDO	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	H	240/260 (92%)	-0.40	6 (2%)	61	55	19, 45, 74, 127	0
2	L	281/282 (99%)	-0.31	4 (1%)	78	76	13, 42, 83, 130	0
3	M	302/303 (99%)	-0.30	3 (0%)	84	82	18, 45, 84, 118	0
All	All	823/845 (97%)	-0.34	13 (1%)	74	72	13, 44, 82, 130	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	250	SER	4.7
1	H	247	LYS	3.2
3	M	1	ALA	2.6
2	L	82	LYS	2.3
2	L	271	TRP	2.3
3	M	68	PHE	2.2
1	H	60	LYS	2.2
2	L	73	TYR	2.2
1	H	161	ALA	2.2
2	L	182	THR	2.0
1	H	249	LYS	2.0
1	H	160	ILE	2.0
3	M	171	TRP	2.0

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

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

6.3 Carbohydrates

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
5	UNL	L	307	10/-	0.76	0.92	34.01	53,79,104,107	0
5	UNL	M	415	12/-	0.82	0.69	23.35	70,82,90,92	0
5	UNL	L	306	12/-	0.85	0.38	14.75	35,54,67,68	0
4	LDA	M	411	16/16	0.64	0.93	13.76	63,106,135,139	0
5	UNL	L	305	12/-	0.76	0.83	10.66	67,78,91,94	0
5	UNL	H	304	12/-	0.81	0.51	9.70	39,53,80,83	0
8	EDO	H	311	4/4	0.72	0.37	9.41	58,60,62,63	0
8	EDO	H	310	4/4	0.88	0.34	8.39	61,65,68,70	0
7	DIO	H	307	6/6	0.75	0.60	7.76	100,102,102,102	0
4	LDA	M	412	16/16	0.80	0.34	7.44	63,87,99,105	0
14	CDL	M	401	81/100	0.80	0.48	7.30	58,97,140,158	0
9	TRS	L	312	8/8	0.85	0.39	6.47	73,77,88,89	0
5	UNL	L	308	12/-	0.73	0.36	5.94	39,70,76,79	0
4	LDA	M	409	16/16	0.86	0.46	5.55	34,45,80,83	0
4	LDA	M	410	16/16	0.85	0.29	5.53	48,66,88,98	0
7	DIO	L	309	6/6	0.93	0.32	4.44	34,36,40,46	6
8	EDO	M	419	4/4	0.84	0.29	3.86	60,73,77,78	0
16	SPN	M	407	43/43	0.92	0.40	2.94	30,52,74,78	0
4	LDA	H	301	16/16	0.94	0.18	1.66	48,58,63,69	0
13	U10	M	406	48/63	0.91	0.24	1.56	28,39,57,64	0
12	BPH	M	404	65/65	0.93	0.26	1.51	39,54,101,113	0
8	EDO	H	309	4/4	0.95	0.17	1.49	55,56,59,61	0
13	U10	L	304	48/63	0.88	0.24	1.16	53,70,84,90	0
12	BPH	L	303	65/65	0.95	0.18	0.56	25,31,44,51	0
8	EDO	M	420	4/4	0.96	0.19	0.55	37,40,46,47	0
4	LDA	M	408	16/16	0.95	0.17	0.27	45,55,64,66	0
10	K	H	313	1/1	0.88	0.15	0.25	64,64,64,64	0
11	BCL	L	302	66/66	0.97	0.16	0.17	24,32,42,46	0
12	BPH	M	402	65/65	0.97	0.16	0.06	27,33,55,67	0
6	PO4	M	417	5/5	0.86	0.22	0.06	94,102,115,118	0
8	EDO	L	311	4/4	0.90	0.20	0.05	68,73,73,81	0
11	BCL	L	301	66/66	0.97	0.17	-0.17	21,34,65,72	0
11	BCL	M	403	66/66	0.97	0.16	-0.36	19,24,37,41	0
6	PO4	H	306	5/5	0.89	0.16	-0.88	94,105,115,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
15	FE	M	405	1/1	1.00	0.15	-1.81	25,25,25,25	0
5	UNL	M	413	12/-	0.86	0.25	-	32,47,55,58	0
5	UNL	H	302	12/-	0.87	0.41	-	53,59,78,82	0
5	UNL	H	303	12/-	0.84	0.55	-	43,54,70,73	0
9	TRS	H	312	8/8	0.83	0.26	-	76,84,92,102	0
7	DIO	M	418	6/6	0.91	0.36	-	99,104,105,112	0
5	UNL	H	305	12/-	0.86	0.38	-	54,66,81,82	0
8	EDO	H	308	4/4	0.89	0.18	-	79,79,82,86	0
7	DIO	L	310	6/6	0.87	0.23	-	64,68,73,82	0
6	PO4	M	416	5/5	0.85	0.13	-	95,108,121,134	0
5	UNL	M	414	12/-	0.79	0.32	-	45,66,80,85	0

6.5 Other polymers (i)

There are no such residues in this entry.