



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2018 – 11:39 PM EST

PDB ID : 2HJ6
Title : Reaction centre from Rhodobacter sphaeroides strain R-26.1 complexed with dibrominated phosphatidylserine
Authors : Roszak, A.W.; Gardiner, A.T.; Isaacs, N.W.; Cogdell, R.J.
Deposited on : 2006-06-30
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

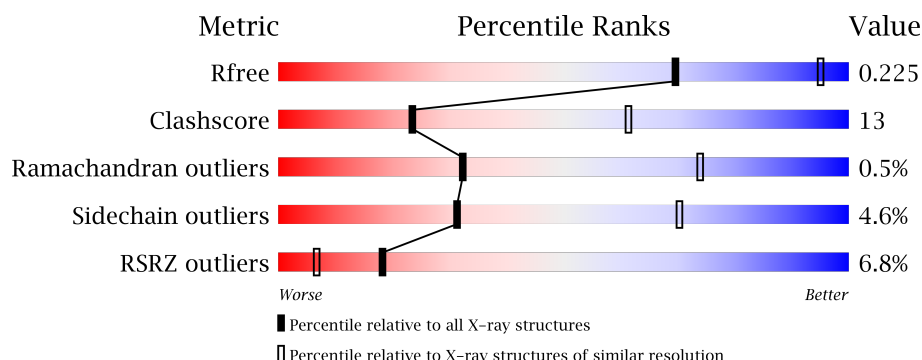
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	L	281	<div> <div>6%</div> <div> <div></div> <div>75%</div> <div>21%</div> <div>•</div> </div> </div>
2	M	307	<div> <div>6%</div> <div> <div></div> <div>76%</div> <div>20%</div> <div>••</div> </div> </div>
3	H	260	<div> <div>8%</div> <div> <div></div> <div>71%</div> <div>20%</div> <div>• 7%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CDL	M	800	-	-	-	X
11	PS2	M	802	-	-	-	X
12	LDA	H	902	-	-	-	X
12	LDA	H	905	-	-	-	X
12	LDA	M	903	-	-	-	X
12	LDA	M	906	-	-	-	X
12	LDA	M	907	-	-	-	X
12	LDA	M	920	-	-	X	X
13	GOL	M	704	-	-	-	X
6	U10	L	502	-	-	-	X

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 7685 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
1	L	281	Total	C	N	O	S	0	3	0
			2249	1520	357	364	8			

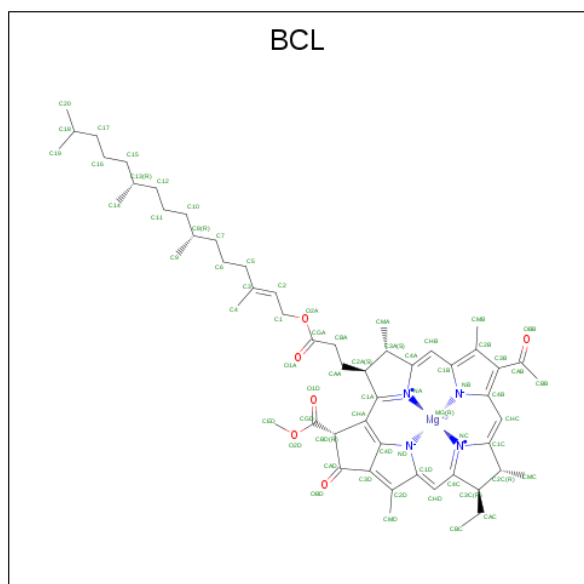
- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	5	0
			2452	1637	403	402	10			

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

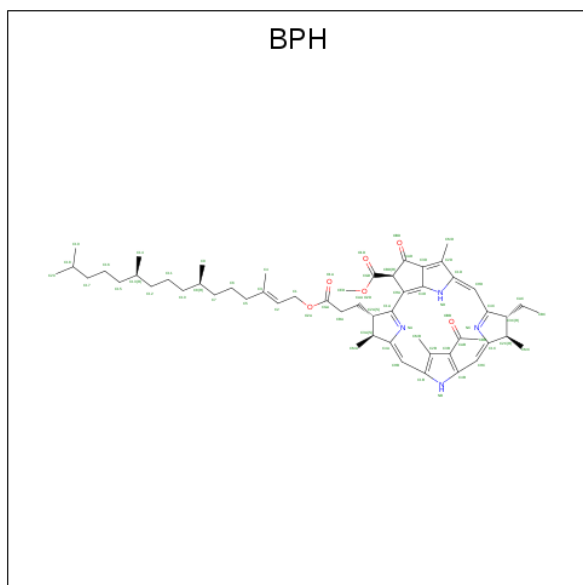
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	241	Total	C	N	O	S	0	5	0
			1846	1180	316	339	11			

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



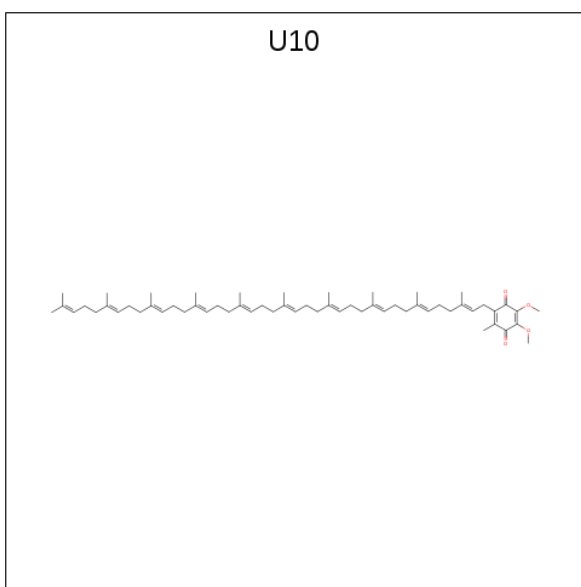
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- 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: $C_{59}H_{90}O_4$).

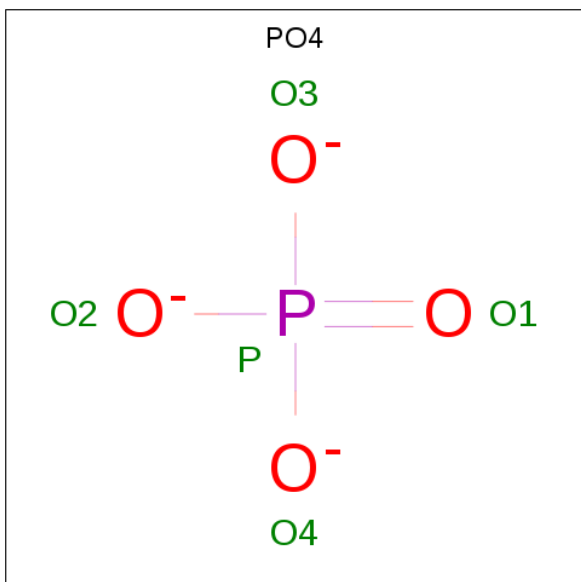


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			48	44	4		
6	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 7 is FE (III) ION (three-letter code: FE) (formula: Fe).

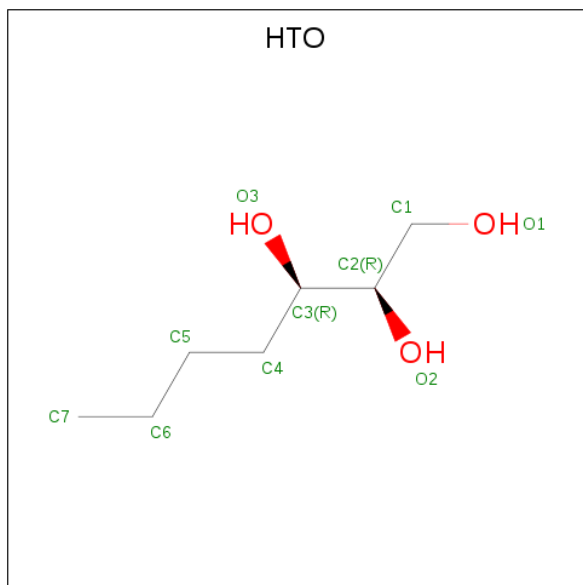
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	M	1	Total	Fe	0	0
			1	1		

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



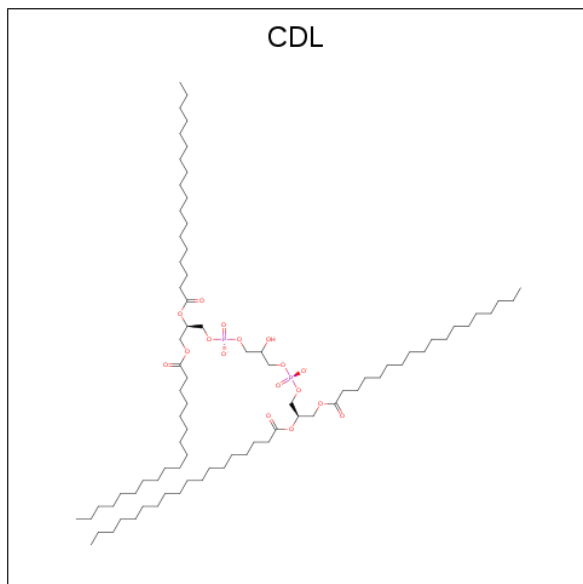
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	O	P	0	0
			5	4	1		
8	M	1	Total	O	P	0	0
			5	4	1		

- Molecule 9 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).



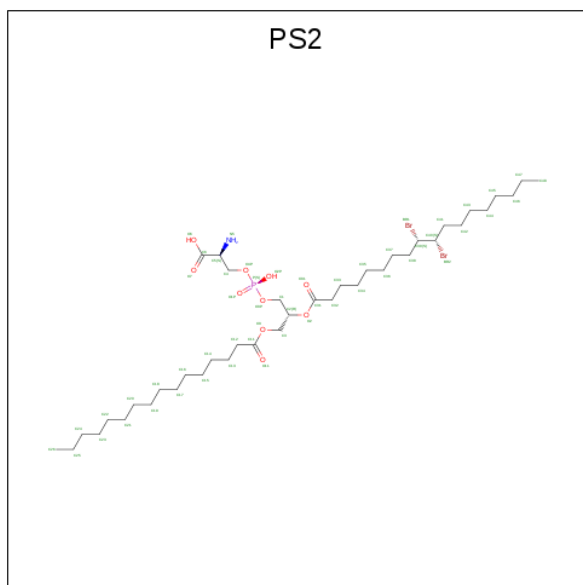
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	C	O	0	0
			10	7	3		

- Molecule 10 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



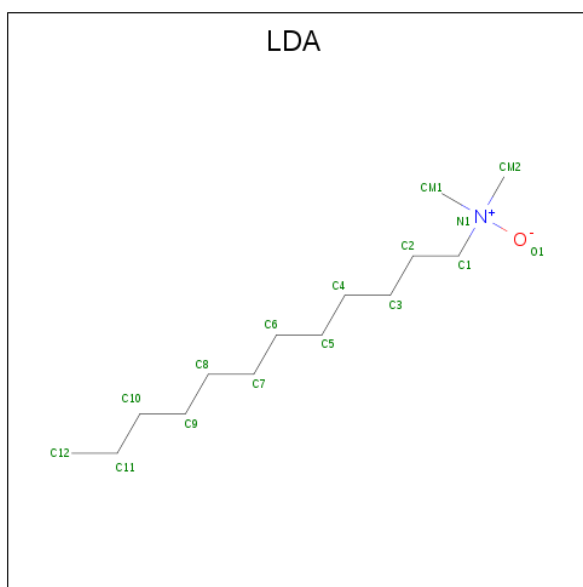
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	M	1	Total	C	O	P	0	0
			81	62	17	2		

- Molecule 11 is O-[[{(2R)-2-[[{(9S,10S)-9,10-DIBROMOOCTADECANOYL]OXY}-3-(PALM ITOYLOXY)PROPYL]OXY}(HYDROXY)PHOSPHORYL]-L-SERINE (three-letter code: PS2) (formula: C₄₀H₇₆Br₂NO₁₀P).



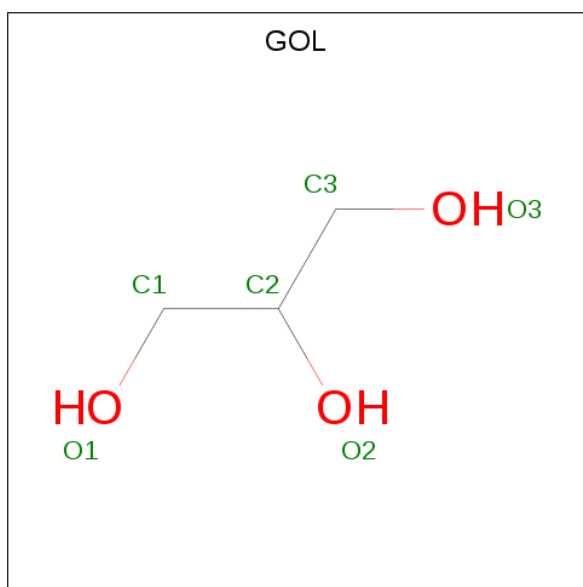
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
11	M	1	Total	Br	C	N	O	P	0	0
			54	2	40	1	10	1		

- Molecule 12 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C₁₄H₃₁NO).



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

- Molecule 13 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 14 is POTASSIUM ION (three-letter code: K) (formula: K).

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

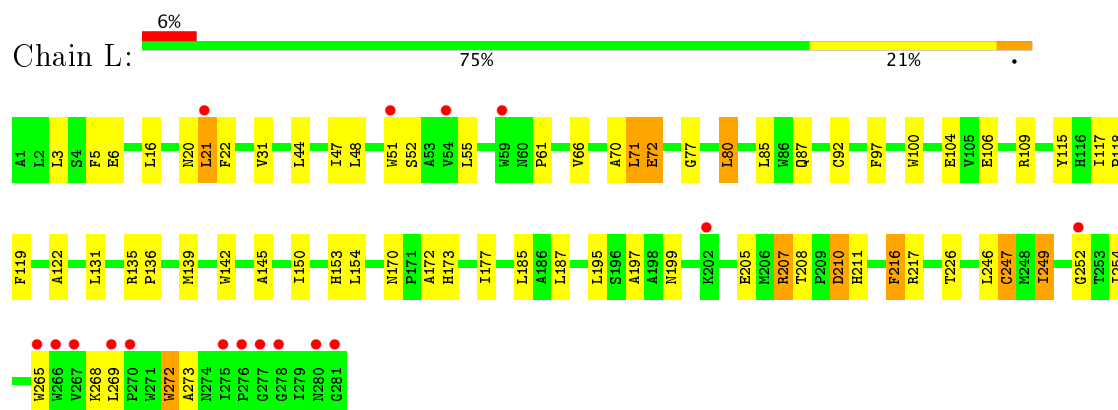
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	L	78	Total	O	0	0
			78	78		
15	M	108	Total	O	0	0
			108	108		
15	H	165	Total	O	0	0
			165	165		

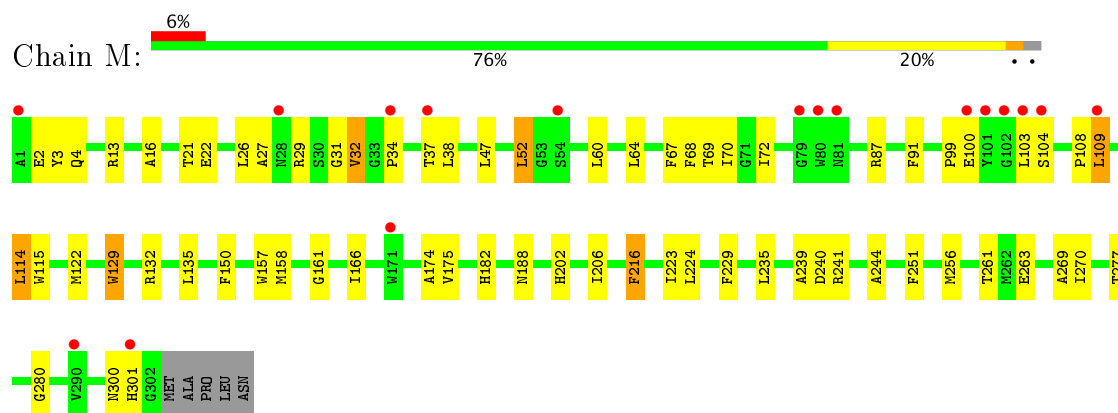
3 Residue-property plots [i](#)

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

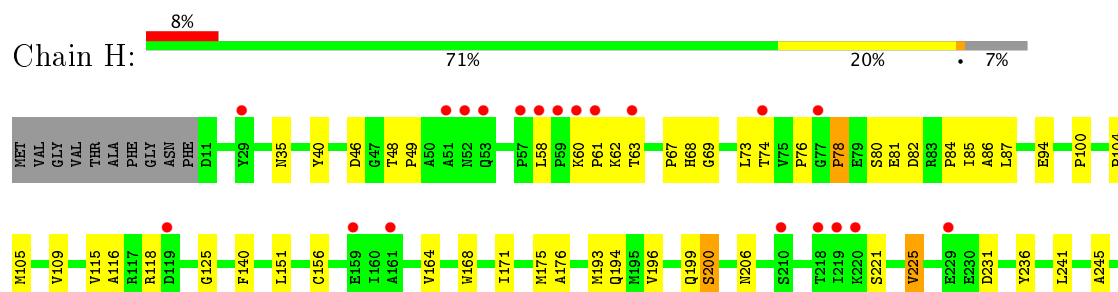
• Molecule 1: Reaction center protein L chain



• Molecule 2: Reaction center protein M chain



• Molecule 3: Reaction center protein H chain



R248			
R249			
S250			
V251			
VAL			
ALA			
ALA			
MET			
LEU			
ALA			
GLU			
TYR			
ALA			

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	139.35Å 139.35Å 183.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.29 – 3.00 38.27 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.29-3.00) 99.4 (38.27-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.174 , 0.227 0.178 , 0.225	Depositor DCC
R_{free} test set	2083 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	75.3	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 103.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7685	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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, CDL, BPH, K, HTO, FE, PS2, 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	0.85	0/2350	0.79	0/3216
2	M	0.87	1/2552 (0.0%)	0.85	4/3482 (0.1%)
3	H	0.88	1/1921 (0.1%)	0.89	0/2612
All	All	0.86	2/6823 (0.0%)	0.84	4/9310 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	129	TRP	CB-CG	-5.74	1.40	1.50
3	H	94	GLU	CG-CD	5.52	1.60	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	241	ARG	NE-CZ-NH1	-5.62	117.49	120.30
2	M	3	TYR	CB-CG-CD2	-5.47	117.72	121.00
2	M	3	TYR	CB-CG-CD1	5.18	124.11	121.00
2	M	29	ARG	NE-CZ-NH1	5.11	122.86	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	2249	0	2210	53	0
2	M	2452	0	2357	65	0
3	H	1846	0	1866	42	0
4	L	132	0	148	12	0
4	M	132	0	148	14	0
5	L	65	0	76	2	0
5	M	65	0	76	5	0
6	L	48	0	63	9	0
6	M	48	0	63	4	0
7	M	1	0	0	0	0
8	M	10	0	0	0	0
9	M	10	0	16	0	0
10	M	81	0	106	3	0
11	M	54	0	72	8	0
12	H	48	0	93	1	0
12	M	80	0	155	21	0
13	H	6	0	8	0	0
13	M	6	0	8	2	0
14	H	1	0	0	0	0
15	H	165	0	0	8	0
15	L	78	0	0	1	0
15	M	108	0	0	5	0
All	All	7685	0	7465	188	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 13.

All (188) 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:U10:H4M3	6:L:502:U10:H3M2	1.31	1.12
3:H:250:SER:O	3:H:251:VAL:CG2	2.11	0.99
2:M:16:ALA:HB1	2:M:32:VAL:HG11	1.46	0.97
3:H:250:SER:O	3:H:251:VAL:HG23	1.64	0.97
4:M:311:BCL:HBB2	4:M:311:BCL:HMB1	1.51	0.91
2:M:301[B]:HIS:CE1	15:M:1030:HOH:O	2.22	0.90
2:M:21:THR:HG23	2:M:26:LEU:HD21	1.54	0.88
2:M:301[B]:HIS:HE1	15:M:1030:HOH:O	1.58	0.83
6:L:502:U10:H4M3	6:L:502:U10:C3M	2.11	0.81
4:L:312:BCL:CBB	4:L:312:BCL:HMB1	2.12	0.80
4:M:311:BCL:CBB	4:M:311:BCL:HMB1	2.13	0.77
2:M:174:ALA:HB1	12:M:920:LDA:C12	2.13	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:312:BCL:HMB1	4:L:312:BCL:HBB3	1.66	0.77
2:M:135:LEU:HD13	15:M:1331:HOH:O	1.86	0.75
2:M:115:TRP:HZ2	12:M:920:LDA:H121	1.52	0.74
4:L:314:BCL:HBB2	4:L:314:BCL:HMB1	1.67	0.74
2:M:70:ILE:HG21	12:M:920:LDA:HM21	1.73	0.71
3:H:250:SER:O	3:H:251:VAL:HG22	1.92	0.69
2:M:31:GLY:H	11:M:802:PS2:H11	1.58	0.68
1:L:80:LEU:O	1:L:85:LEU:HD12	1.93	0.68
3:H:250:SER:C	3:H:251:VAL:HG23	2.13	0.67
2:M:174:ALA:HB1	12:M:920:LDA:H121	1.76	0.66
1:L:21:LEU:HD13	1:L:22:PHE:CE1	2.30	0.66
12:M:901:LDA:H121	12:M:903:LDA:C8	2.26	0.65
2:M:47:LEU:HD22	11:M:802:PS2:BR2	2.52	0.64
4:M:311:BCL:H92	4:M:313:BCL:H161	1.81	0.62
2:M:175:VAL:N	12:M:920:LDA:H122	2.15	0.62
3:H:175:MET:CE	3:H:176:ALA:O	2.49	0.61
4:L:314:BCL:HBB3	5:L:402:BPH:H141	1.83	0.60
1:L:197:ALA:HB1	2:M:235:LEU:HD11	1.83	0.60
3:H:61:PRO:HA	3:H:76:PRO:HD2	1.82	0.60
4:L:314:BCL:CBB	4:L:314:BCL:HMB1	2.32	0.59
2:M:67[A]:PHE:HD2	2:M:68[A]:PHE:CE1	2.19	0.59
2:M:69:THR:HG23	2:M:114:LEU:HD12	1.84	0.59
3:H:67:PRO:HB2	3:H:68:HIS:CD2	2.37	0.58
2:M:2:GLU:O	2:M:4:GLN:NE2	2.36	0.58
1:L:51:TRP:NE1	1:L:55:LEU:HD11	2.19	0.57
4:L:312:BCL:NA	4:M:313:BCL:HBB2	2.19	0.57
3:H:250:SER:C	3:H:251:VAL:CG2	2.73	0.57
1:L:100:TRP:CH2	6:M:501:U10:H251	2.40	0.57
1:L:216:PHE:CD2	6:L:502:U10:H102	2.39	0.57
2:M:175:VAL:O	12:M:920:LDA:H122	2.04	0.57
1:L:139:MET:HE1	1:L:252:GLY:HA3	1.88	0.56
12:M:903:LDA:H61	12:H:905:LDA:H122	1.87	0.55
4:L:312:BCL:CGA	4:L:314:BCL:HBC1	2.36	0.55
6:L:502:U10:H351	6:L:502:U10:H38	1.87	0.55
2:M:122:MET:HE1	4:M:311:BCL:HBB1	1.88	0.55
3:H:140:PHE:CE1	3:H:171:ILE:HG23	2.42	0.54
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.42	0.54
2:M:240:ASP:OD2	3:H:118:ARG:HG3	2.07	0.54
3:H:46:ASP:OD1	3:H:48:THR:HG23	2.07	0.54
3:H:193:MET:O	3:H:196:VAL:HG22	2.08	0.54
2:M:16:ALA:HB1	2:M:32:VAL:CG1	2.31	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.88	0.53
4:M:311:BCL:CAB	12:M:920:LDA:H82	2.38	0.53
12:M:901:LDA:H122	12:M:903:LDA:H102	1.89	0.53
6:L:502:U10:H351	6:L:502:U10:C38	2.39	0.53
2:M:175:VAL:H	12:M:920:LDA:H122	1.73	0.53
2:M:67[A]:PHE:HD2	2:M:68[A]:PHE:CD1	2.27	0.52
2:M:52:LEU:HD21	2:M:60:LEU:CD1	2.39	0.52
2:M:161:GLY:HA2	12:M:920:LDA:H123	1.89	0.52
3:H:105[B]:MET:HE2	3:H:236:TYR:CZ	2.45	0.52
1:L:197:ALA:CB	2:M:235:LEU:HD11	2.40	0.52
2:M:34:PRO:HG2	2:M:47:LEU:HD12	1.91	0.52
2:M:64:LEU:HD21	5:M:401:BPH:H112	1.90	0.52
2:M:67[A]:PHE:CD2	2:M:68[A]:PHE:CE1	2.97	0.52
2:M:27:ALA:HB2	15:M:1216:HOH:O	2.09	0.51
2:M:31:GLY:N	11:M:802:PS2:H11	2.22	0.51
1:L:136:PRO:HG2	1:L:145:ALA:HB2	1.92	0.51
3:H:168:TRP:CZ3	3:H:225:VAL:HG22	2.46	0.51
10:M:800:CDL:CA5	10:M:800:CDL:OA8	2.59	0.51
3:H:40:TYR:HB3	3:H:58:LEU:HD21	1.91	0.51
1:L:216:PHE:CE2	6:L:502:U10:H102	2.45	0.50
1:L:52:SER:CB	1:L:66:VAL:HG22	2.41	0.50
1:L:187:LEU:HD13	2:M:216:PHE:CG	2.47	0.50
6:M:501:U10:H4M2	6:M:501:U10:O3	2.12	0.50
3:H:175:MET:HE2	3:H:176:ALA:O	2.11	0.49
2:M:67[B]:PHE:O	2:M:68[B]:PHE:C	2.50	0.49
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.93	0.49
1:L:199:ASN:HB3	10:M:800:CDL:HA22	1.95	0.49
1:L:97:PHE:CZ	4:L:312:BCL:H112	2.48	0.49
3:H:84:PRO:O	3:H:85:ILE:HD13	2.13	0.49
2:M:280:GLY:O	4:M:313:BCL:HED3	2.13	0.48
1:L:208:THR:HG21	3:H:125:GLY:HA2	1.95	0.48
4:M:313:BCL:HAA2	4:M:313:BCL:HBD	1.94	0.48
1:L:115:TYR:HB2	12:M:906:LDA:HM13	1.96	0.48
1:L:172:ALA:HB3	1:L:247:CYS:CB	2.44	0.48
1:L:265:TRP:CZ3	1:L:269:LEU:HD11	2.48	0.48
1:L:187:LEU:HD13	2:M:216:PHE:CD2	2.48	0.48
3:H:105[B]:MET:CE	3:H:236:TYR:CZ	2.96	0.48
12:M:901:LDA:H121	12:M:903:LDA:H82	1.95	0.48
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.49	0.48
1:L:226:THR:HG22	6:L:502:U10:H4M3	1.95	0.48
1:L:44:LEU:HA	1:L:47:ILE:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:502:U10:C4M	6:L:502:U10:H3M2	2.23	0.47
2:M:52:LEU:HD21	2:M:60:LEU:HD11	1.96	0.47
3:H:241:LEU:HB2	15:H:1089:HOH:O	2.14	0.47
1:L:16:LEU:N	1:L:106:GLU:OE2	2.35	0.47
12:M:901:LDA:H121	12:M:903:LDA:C9	2.45	0.47
3:H:115:VAL:CG1	3:H:116:ALA:N	2.77	0.46
1:L:210:ASP:OD1	1:L:210:ASP:N	2.47	0.46
3:H:69:GLY:N	15:H:1165:HOH:O	2.41	0.46
1:L:272:TRP:HB2	2:M:87:ARG:HD3	1.98	0.46
2:M:175:VAL:HB	12:M:920:LDA:H101	1.97	0.46
2:M:256:MET:CE	6:M:501:U10:H102	2.45	0.46
2:M:239:ALA:HA	3:H:73:LEU:HD23	1.98	0.46
2:M:277:THR:CG2	5:M:401:BPH:HAC2	2.46	0.46
4:L:312:BCL:H52	5:L:402:BPH:HBB2	1.98	0.45
2:M:263:GLU:OE1	3:H:62:LYS:NZ	2.46	0.45
2:M:13:ARG:O	3:H:140:PHE:HA	2.16	0.45
1:L:48:LEU:HD22	1:L:85:LEU:CD2	2.47	0.45
3:H:87:LEU:HD23	3:H:100:PRO:HA	1.98	0.45
1:L:131:LEU:HD21	4:L:312:BCL:CED	2.47	0.45
1:L:119:PHE:O	1:L:122:ALA:HB3	2.17	0.45
10:M:800:CDL:OB7	10:M:800:CDL:C31	2.65	0.45
4:M:313:BCL:HMB1	4:M:313:BCL:CBB	2.47	0.44
3:H:199:GLN:O	3:H:200:SER:C	2.53	0.44
1:L:172:ALA:HB3	1:L:247:CYS:HB2	1.99	0.44
2:M:21:THR:O	2:M:22:GLU:C	2.55	0.44
2:M:300:ASN:O	2:M:301[B]:HIS:CG	2.69	0.44
2:M:175:VAL:H	12:M:920:LDA:C12	2.30	0.44
3:H:60:LYS:N	15:H:1285:HOH:O	2.46	0.44
1:L:217:ARG:NH2	15:L:1047:HOH:O	2.50	0.44
1:L:87:GLN:NE2	1:L:142:TRP:CD1	2.86	0.44
1:L:195:LEU:O	1:L:199:ASN:HB2	2.17	0.44
2:M:261:THR:HG23	3:H:35:ASN:O	2.18	0.44
4:M:311:BCL:H72	4:M:311:BCL:H41	1.99	0.44
2:M:223:ILE:O	2:M:224:LEU:C	2.54	0.44
11:M:802:PS2:H322	11:M:802:PS2:O11	2.18	0.44
1:L:139:MET:CE	1:L:252:GLY:HA3	2.46	0.43
2:M:13:ARG:NH2	15:M:1107:HOH:O	2.49	0.43
1:L:3:LEU:HB2	1:L:6:GLU:HB2	1.99	0.43
6:L:502:U10:H153	11:M:802:PS2:H483	2.00	0.43
12:M:907:LDA:H71	12:M:907:LDA:H101	1.84	0.43
3:H:200:SER:HB3	15:H:1280:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:77:GLY:HA2	1:L:87:GLN:OE1	2.18	0.43
4:M:311:BCL:HMB2	5:M:401:BPH:HMB3	2.01	0.43
2:M:70:ILE:HG21	12:M:920:LDA:CM2	2.42	0.43
1:L:5:PHE:HA	3:H:81:GLU:OE2	2.19	0.43
1:L:117:ILE:N	1:L:118:PRO:HD2	2.34	0.43
11:M:802:PS2:C31	11:M:802:PS2:O11	2.66	0.43
2:M:150:PHE:N	5:M:401:BPH:HMD3	2.33	0.43
3:H:49:PRO:HD3	15:H:1324:HOH:O	2.18	0.43
1:L:117:ILE:HB	1:L:118:PRO:HD3	2.00	0.43
4:L:314:BCL:HMD1	2:M:206:ILE:HD13	2.00	0.43
12:M:901:LDA:C12	12:M:903:LDA:H102	2.48	0.43
4:M:311:BCL:C7	4:M:311:BCL:H41	2.48	0.43
4:M:313:BCL:HMB1	4:M:313:BCL:HBB3	2.00	0.42
2:M:157:TRP:CE3	2:M:158:MET:HG2	2.53	0.42
4:M:311:BCL:HBA1	4:M:311:BCL:H3A	1.85	0.42
3:H:82:ASP:N	15:H:1348:HOH:O	2.52	0.42
1:L:71:LEU:H	1:L:71:LEU:HD12	1.84	0.42
3:H:63:THR:OG1	3:H:74:THR:HG23	2.19	0.42
1:L:61:PRO:O	1:L:150:ILE:HD12	2.19	0.42
3:H:245:ALA:HA	3:H:248:ARG:NH1	2.34	0.42
1:L:44:LEU:HD23	1:L:92:CYS:SG	2.59	0.42
2:M:108:PRO:O	2:M:109:LEU:C	2.58	0.42
2:M:99:PRO:HD2	2:M:100:GLU:OE2	2.19	0.42
3:H:115:VAL:HG12	3:H:116:ALA:N	2.35	0.42
3:H:151:LEU:O	3:H:164:VAL:HG23	2.20	0.42
1:L:70:ALA:HB1	1:L:72:GLU:HG3	2.02	0.42
2:M:251:PHE:CD1	2:M:251:PHE:C	2.94	0.42
2:M:60:LEU:HA	5:M:401:BPH:H4C1	2.02	0.41
2:M:2:GLU:HG3	13:M:704:GOL:H31	2.02	0.41
1:L:246:LEU:HA	1:L:249:ILE:HG22	2.03	0.41
2:M:269:ALA:O	2:M:270:ILE:C	2.58	0.41
2:M:2:GLU:HG3	13:M:704:GOL:C3	2.50	0.41
2:M:129:TRP:CZ2	11:M:802:PS2:H263	2.56	0.41
3:H:104:PRO:HA	3:H:109:VAL:HG22	2.02	0.41
11:M:802:PS2:H263	11:M:802:PS2:H232	1.61	0.41
1:L:269:LEU:O	1:L:273:ALA:HB2	2.21	0.41
1:L:207:ARG:HG2	1:L:211:HIS:CG	2.55	0.41
2:M:91:PHE:N	2:M:91:PHE:CD2	2.89	0.41
1:L:3:LEU:HD13	1:L:5:PHE:CZ	2.55	0.41
3:H:156[A]:CYS:HB3	3:H:206:ASN:O	2.21	0.40
3:H:156[B]:CYS:HB3	3:H:206:ASN:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:170:ASN:HB3	1:L:173:HIS:HB3	2.03	0.40
6:M:501:U10:H202	12:M:901:LDA:H111	2.04	0.40
3:H:194:GLN:NE2	15:H:1050:HOH:O	2.54	0.40
1:L:100:TRP:O	1:L:104:GLU:HG3	2.21	0.40
1:L:20:ASN:C	1:L:20:ASN:ND2	2.74	0.40
4:L:312:BCL:HBB2	4:L:312:BCL:HMB1	1.97	0.40
2:M:239:ALA:O	3:H:73:LEU:HD22	2.21	0.40
1:L:153:HIS:CE1	1:L:154:LEU:CD1	3.04	0.40
1:L:268:LYS:O	1:L:269:LEU:C	2.59	0.40
1:L:16:LEU:HD23	1:L:109:ARG:CZ	2.52	0.40
2:M:103:LEU:HD21	2:M:166:ILE:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	282/281 (100%)	263 (93%)	18 (6%)	1 (0%)	38	78
2	M	305/307 (99%)	283 (93%)	21 (7%)	1 (0%)	44	81
3	H	244/260 (94%)	237 (97%)	5 (2%)	2 (1%)	22	64
All	All	831/848 (98%)	783 (94%)	44 (5%)	4 (0%)	32	74

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	109	LEU
1	L	31	VAL
3	H	86	ALA
3	H	78	PRO

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	223/220 (101%)	210 (94%)	13 (6%)	23	61
2	M	241/240 (100%)	230 (95%)	11 (5%)	31	70
3	H	201/208 (97%)	194 (96%)	7 (4%)	41	78
All	All	665/668 (100%)	634 (95%)	31 (5%)	31	69

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

Mol	Chain	Res	Type
1	L	21	LEU
1	L	71	LEU
1	L	72	GLU
1	L	80	LEU
1	L	185	LEU
1	L	205	GLU
1	L	207	ARG
1	L	210	ASP
1	L	216	PHE
1	L	247	CYS
1	L	249	ILE
1	L	254	ILE
1	L	272	TRP
2	M	32	VAL
2	M	37	THR
2	M	38	LEU
2	M	52	LEU
2	M	72	ILE
2	M	104	SER
2	M	114	LEU
2	M	132	ARG
2	M	182	HIS
2	M	188	ASN
2	M	216	PHE
3	H	78	PRO
3	H	80	SER

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Mol	Chain	Res	Type
3	H	200	SER
3	H	221[A]	SER
3	H	221[B]	SER
3	H	225	VAL
3	H	231	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	20	ASN
2	M	202	HIS
3	H	68	HIS
3	H	141	HIS

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 25 ligands modelled in this entry, 2 are monoatomic - leaving 23 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
13	GOL	H	705	-	5,5,5	0.37	0	5,5,5	0.28	0
12	LDA	H	902	-	13,15,15	2.20	1 (7%)	14,17,17	0.88	1 (7%)
12	LDA	H	904	-	13,15,15	2.29	1 (7%)	14,17,17	0.81	1 (7%)
12	LDA	H	905	-	13,15,15	2.38	1 (7%)	14,17,17	0.58	0
4	BCL	L	312	1	55,74,74	1.26	2 (3%)	65,115,115	1.26	9 (13%)
4	BCL	L	314	1	55,74,74	1.51	5 (9%)	65,115,115	1.78	18 (27%)
5	BPH	L	402	-	65,70,70	0.73	0	75,101,101	1.59	12 (16%)
6	U10	L	502	-	48,48,63	1.11	2 (4%)	58,61,79	1.55	10 (17%)
4	BCL	M	311	2	55,74,74	1.40	4 (7%)	65,115,115	1.79	16 (24%)
4	BCL	M	313	2	55,74,74	1.41	2 (3%)	65,115,115	1.31	9 (13%)
5	BPH	M	401	-	65,70,70	0.81	1 (1%)	75,101,101	1.70	14 (18%)
6	U10	M	501	-	48,48,63	1.10	4 (8%)	58,61,79	1.34	7 (12%)
8	PO4	M	701	-	4,4,4	0.43	0	6,6,6	0.92	0
8	PO4	M	702	-	4,4,4	0.66	0	6,6,6	0.86	0
9	HTO	M	703	-	9,9,9	0.86	0	9,10,10	2.16	4 (44%)
13	GOL	M	704	-	5,5,5	0.48	0	5,5,5	0.42	0
10	CDL	M	800	-	80,80,99	1.25	5 (6%)	82,92,111	1.40	10 (12%)
11	PS2	M	802	-	49,53,53	1.13	4 (8%)	50,62,62	2.51	13 (26%)
12	LDA	M	901	-	13,15,15	2.51	1 (7%)	14,17,17	0.55	0
12	LDA	M	903	-	13,15,15	2.29	1 (7%)	14,17,17	1.37	2 (14%)
12	LDA	M	906	-	13,15,15	1.79	1 (7%)	14,17,17	1.19	2 (14%)
12	LDA	M	907	-	13,15,15	1.97	1 (7%)	14,17,17	1.05	1 (7%)
12	LDA	M	920	-	13,15,15	1.99	1 (7%)	14,17,17	0.98	1 (7%)

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
13	GOL	H	705	-	-	0/4/4/4	0/0/0/0
12	LDA	H	902	-	-	0/13/13/13	0/0/0/0
12	LDA	H	904	-	-	0/13/13/13	0/0/0/0
12	LDA	H	905	-	-	0/13/13/13	0/0/0/0
4	BCL	L	312	1	-	0/37/137/137	0/0/9/9
4	BCL	L	314	1	-	0/37/137/137	0/0/9/9
5	BPH	L	402	-	-	0/54/105/105	0/1/6/6
6	U10	L	502	-	-	0/45/69/87	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BCL	M	311	2	-	0/37/137/137	0/0/9/9
4	BCL	M	313	2	-	0/37/137/137	0/0/9/9
5	BPH	M	401	-	-	0/54/105/105	0/1/6/6
6	U10	M	501	-	-	0/45/69/87	0/1/1/1
8	PO4	M	701	-	-	0/0/0/0	0/0/0/0
8	PO4	M	702	-	-	0/0/0/0	0/0/0/0
9	HTO	M	703	-	-	0/10/10/10	0/0/0/0
13	GOL	M	704	-	-	0/4/4/4	0/0/0/0
10	CDL	M	800	-	-	0/91/91/110	0/0/0/0
11	PS2	M	802	-	-	0/58/62/62	0/0/0/0
12	LDA	M	901	-	-	0/13/13/13	0/0/0/0
12	LDA	M	903	-	-	0/13/13/13	0/0/0/0
12	LDA	M	906	-	-	0/13/13/13	0/0/0/0
12	LDA	M	907	-	-	0/13/13/13	0/0/0/0
12	LDA	M	920	-	-	0/13/13/13	0/0/0/0

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	901	LDA	O1-N1	-8.86	1.24	1.42
12	H	905	LDA	O1-N1	-8.32	1.25	1.42
12	H	904	LDA	O1-N1	-8.00	1.26	1.42
12	M	903	LDA	O1-N1	-7.71	1.27	1.42
12	H	902	LDA	O1-N1	-7.65	1.27	1.42
12	M	920	LDA	O1-N1	-7.06	1.28	1.42
12	M	907	LDA	O1-N1	-6.77	1.28	1.42
12	M	906	LDA	O1-N1	-6.14	1.30	1.42
4	L	314	BCL	C3C-C4C	-2.99	1.47	1.51
11	M	802	PS2	BR2-C40	-2.65	1.90	1.97
4	M	311	BCL	C1A-CHA	-2.39	1.33	1.43
10	M	800	CDL	CA3-CA4	2.08	1.56	1.50
4	L	314	BCL	OBD-CAD	2.13	1.25	1.22
6	M	501	U10	C18-C19	2.14	1.38	1.33
6	M	501	U10	C31-C29	2.17	1.56	1.51
11	M	802	PS2	P-O4P	2.27	1.68	1.59
4	L	314	BCL	C1-C2	2.38	1.56	1.49
4	M	311	BCL	OBD-CAD	2.71	1.26	1.22
6	M	501	U10	O4-C4	2.86	1.44	1.36
11	M	802	PS2	C32-C31	3.12	1.59	1.50
6	M	501	U10	O3-C3	3.29	1.45	1.36
6	L	502	U10	O4-C4	3.41	1.45	1.36
10	M	800	CDL	OB8-CB7	3.43	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	401	BPH	CHC-C1C	3.54	1.43	1.36
4	L	312	BCL	CHB-C4A	3.95	1.38	1.33
11	M	802	PS2	P-O1P	4.04	1.66	1.50
6	L	502	U10	O3-C3	4.23	1.47	1.36
10	M	800	CDL	OB6-CB5	4.38	1.47	1.34
4	M	313	BCL	CHC-C1C	4.77	1.39	1.33
4	M	311	BCL	CHC-C1C	5.09	1.40	1.33
10	M	800	CDL	OA8-CA7	5.19	1.48	1.33
10	M	800	CDL	OA6-CA5	5.38	1.49	1.34
4	M	311	BCL	CHB-C4A	5.53	1.40	1.33
4	L	314	BCL	CHB-C4A	5.58	1.40	1.33
4	L	314	BCL	CHC-C1C	6.23	1.41	1.33
4	L	312	BCL	CHC-C1C	6.60	1.41	1.33
4	M	313	BCL	CHB-C4A	6.86	1.42	1.33

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	802	PS2	C3-C2-C1	-6.67	96.81	111.86
5	L	402	BPH	C4D-C3D-CAD	-6.22	104.22	107.78
11	M	802	PS2	BR1-C39-C40	-6.06	98.40	110.28
5	M	401	BPH	OBD-CAD-CBD	-4.87	118.58	125.94
5	M	401	BPH	C4D-C3D-CAD	-4.70	105.09	107.78
5	L	402	BPH	OBD-CAD-CBD	-4.39	119.32	125.94
4	L	314	BCL	O1D-CGD-CBD	-4.35	116.79	124.60
4	L	314	BCL	CAC-C3C-C2C	-4.18	103.74	114.24
11	M	802	PS2	C3-O3-C11	-4.16	104.62	117.13
6	M	501	U10	C17-C18-C19	-3.86	117.98	127.68
4	L	314	BCL	CAA-C2A-C3A	-3.83	102.30	112.81
6	L	502	U10	C7-C8-C9	-3.74	120.46	126.71
4	M	311	BCL	CED-O2D-CGD	-3.58	107.58	115.97
4	M	313	BCL	CAC-C3C-C2C	-3.54	105.35	114.24
4	M	313	BCL	CMB-C2B-C1B	-3.51	123.06	128.46
4	M	311	BCL	CMB-C2B-C1B	-3.45	123.16	128.46
9	M	703	HTO	O2-C2-C1	-3.42	101.29	109.21
12	M	906	LDA	CM2-N1-CM1	-3.41	104.47	110.99
4	L	314	BCL	CAC-C3C-C4C	-3.33	105.19	112.58
11	M	802	PS2	O2-C31-O31	-3.18	115.74	123.68
4	M	311	BCL	O1D-CGD-CBD	-3.18	118.89	124.60
10	M	800	CDL	OB8-CB7-OB9	-3.18	115.66	123.55
4	M	311	BCL	CMA-C3A-C4A	-3.18	103.23	111.77
12	M	907	LDA	CM2-N1-CM1	-3.17	104.93	110.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	402	BPH	C1-C2-C3	-3.05	120.33	125.96
4	L	314	BCL	CMB-C2B-C1B	-3.05	123.78	128.46
12	M	903	LDA	CM2-N1-CM1	-2.89	105.45	110.99
4	L	312	BCL	CAA-C2A-C3A	-2.89	104.88	112.81
4	L	314	BCL	C5-C3-C2	-2.88	115.22	121.10
4	M	313	BCL	O2D-CGD-O1D	-2.87	118.04	123.82
4	L	314	BCL	C6-C5-C3	-2.82	106.27	112.66
4	M	313	BCL	CHA-C1A-NA	-2.79	119.71	126.18
4	M	311	BCL	CHA-C1A-NA	-2.77	119.75	126.18
4	M	311	BCL	CAA-C2A-C3A	-2.75	105.26	112.81
5	L	402	BPH	CAA-C2A-C3A	-2.71	105.39	112.81
10	M	800	CDL	CA4-OA6-CA5	-2.69	111.52	117.88
4	M	311	BCL	C1B-CHB-C4A	-2.63	124.90	130.12
11	M	802	PS2	BR2-C40-C39	-2.61	105.16	110.28
12	M	920	LDA	CM2-N1-CM1	-2.60	106.02	110.99
4	M	313	BCL	CAC-C3C-C4C	-2.60	106.81	112.58
4	L	314	BCL	CHA-C1A-NA	-2.60	120.15	126.18
4	L	312	BCL	C5-C3-C2	-2.59	115.79	121.10
4	M	311	BCL	C3D-CAD-CBD	-2.58	103.95	107.60
9	M	703	HTO	C5-C4-C3	-2.57	109.89	114.22
5	M	401	BPH	CAA-C2A-C3A	-2.56	105.80	112.81
6	L	502	U10	C35-C34-C33	-2.53	116.95	123.69
6	L	502	U10	C12-C11-C9	-2.52	104.40	112.93
5	M	401	BPH	O1D-CGD-CBD	-2.48	120.15	124.60
6	L	502	U10	C15-C14-C13	-2.46	117.12	123.69
4	M	313	BCL	CMC-C2C-C3C	-2.45	103.82	113.77
4	L	312	BCL	O1D-CGD-CBD	-2.43	120.23	124.60
10	M	800	CDL	CB6-CB4-CB3	-2.43	106.37	111.86
4	L	312	BCL	CMB-C2B-C1B	-2.41	124.76	128.46
6	L	502	U10	C31-C29-C28	-2.41	116.18	121.10
5	L	402	BPH	C4B-C3B-CAB	-2.36	121.37	130.09
4	L	314	BCL	CAA-C2A-C1A	-2.35	104.26	111.97
12	H	902	LDA	CM1-N1-C1	-2.34	105.31	110.23
6	M	501	U10	O5-C5-C6	-2.31	117.56	121.82
4	M	311	BCL	CAC-C3C-C4C	-2.29	107.51	112.58
6	M	501	U10	C37-C38-C39	-2.26	119.73	127.80
12	H	904	LDA	CM2-N1-CM1	-2.26	106.67	110.99
4	L	312	BCL	CHA-C1A-NA	-2.25	120.95	126.18
4	L	314	BCL	C3D-CAD-CBD	-2.25	104.42	107.60
5	M	401	BPH	C1-C2-C3	-2.24	121.83	125.96
4	L	314	BCL	O2A-CGA-O1A	-2.20	118.09	123.55
5	M	401	BPH	CMA-C3A-C4A	-2.19	105.78	112.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	311	BCL	C4-C3-C5	-2.19	111.49	115.29
11	M	802	PS2	O3-C11-O11	-2.17	118.16	123.55
4	L	312	BCL	C6-C7-C8	-2.17	108.62	115.73
11	M	802	PS2	BR2-C40-C41	-2.16	105.26	108.92
5	L	402	BPH	C4D-CHA-C1A	-2.14	124.78	130.23
4	M	311	BCL	CHD-C4C-NC	-2.13	122.71	125.08
4	M	313	BCL	O2A-CGA-O1A	-2.12	118.29	123.55
6	L	502	U10	C12-C13-C14	-2.11	122.39	127.68
9	M	703	HTO	O3-C3-C2	-2.10	105.60	109.77
4	L	312	BCL	CBC-CAC-C3C	-2.09	108.78	113.51
6	M	501	U10	C7-C6-C5	-2.08	115.81	118.47
10	M	800	CDL	OB6-CB5-OB7	-2.07	118.51	123.68
5	L	402	BPH	O2D-CGD-O1D	-2.06	119.68	123.82
5	M	401	BPH	C2B-C1B-NB	-2.02	106.82	109.82
11	M	802	PS2	C2-O2-C31	-2.01	113.14	117.88
12	M	906	LDA	O1-N1-C1	2.05	114.29	109.27
10	M	800	CDL	OA6-CA4-CA3	2.11	116.09	108.44
6	L	502	U10	C36-C34-C33	2.11	125.43	121.10
4	L	312	BCL	OBB-CAB-C3B	2.12	123.99	119.95
11	M	802	PS2	O3-C3-C2	2.14	114.02	108.66
5	L	402	BPH	CAC-C3C-C2C	2.24	119.86	114.24
6	L	502	U10	C15-C14-C16	2.29	119.27	115.29
6	M	501	U10	C31-C32-C33	2.30	119.86	111.97
10	M	800	CDL	OB8-CB7-C71	2.31	118.61	111.90
6	M	501	U10	C21-C19-C18	2.31	125.84	121.10
5	L	402	BPH	C1B-NB-C4B	2.46	111.39	106.52
5	M	401	BPH	OBD-CAD-C3D	2.48	132.60	128.03
4	M	311	BCL	CMB-C2B-C3B	2.49	129.52	124.89
4	L	314	BCL	C3A-C2A-C1A	2.49	105.08	101.34
4	M	313	BCL	CMB-C2B-C3B	2.56	129.64	124.89
4	L	314	BCL	C4-C3-C5	2.58	119.77	115.29
4	M	311	BCL	OBD-CAD-C3D	2.59	132.79	128.03
6	M	501	U10	C41-C39-C40	2.59	120.64	114.60
12	M	903	LDA	CM1-N1-C1	2.68	115.86	110.23
5	M	401	BPH	CMC-C2C-C1C	2.68	119.59	112.09
5	L	402	BPH	CMD-C2D-C3D	2.69	129.89	124.89
5	L	402	BPH	CED-O2D-CGD	2.71	122.32	115.97
4	L	314	BCL	C2A-C1A-CHA	2.76	128.82	123.92
4	L	314	BCL	CAA-CBA-CGA	2.82	121.83	113.35
5	M	401	BPH	CMD-C2D-C3D	3.03	130.51	124.89
5	M	401	BPH	C1B-NB-C4B	3.03	112.52	106.52
10	M	800	CDL	CA6-OA8-CA7	3.09	126.42	117.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	402	BPH	O2D-CGD-CBD	3.14	116.91	111.30
4	M	313	BCL	O2D-CGD-CBD	3.18	116.98	111.30
10	M	800	CDL	OA8-CA7-C31	3.26	121.39	111.90
4	L	314	BCL	CBC-CAC-C3C	3.32	121.02	113.51
6	L	502	U10	C30-C29-C31	3.42	121.23	115.29
11	M	802	PS2	O3-C11-C12	3.48	122.04	111.90
4	L	314	BCL	C2C-C3C-C4C	3.50	106.57	101.34
4	L	312	BCL	C4-C3-C5	3.57	121.48	115.29
4	L	314	BCL	O2D-CGD-CBD	3.63	117.78	111.30
4	M	311	BCL	C5-C3-C2	3.67	128.62	121.10
9	M	703	HTO	C4-C3-C2	3.94	121.72	113.10
5	M	401	BPH	C3C-C4C-NC	3.96	111.70	107.97
10	M	800	CDL	OB6-CB5-C51	4.15	120.17	111.55
4	M	311	BCL	O2D-CGD-CBD	4.26	118.92	111.30
4	M	311	BCL	C1-O2A-CGA	4.41	127.35	116.77
6	L	502	U10	C25-C24-C26	4.48	123.07	115.29
5	M	401	BPH	C1-O2A-CGA	4.54	127.65	116.77
5	M	401	BPH	O2D-CGD-CBD	4.58	119.48	111.30
11	M	802	PS2	BR1-C39-C38	5.45	118.17	108.92
11	M	802	PS2	O2-C31-C32	6.04	124.09	111.55
10	M	800	CDL	OA6-CA5-C11	6.26	124.54	111.55
11	M	802	PS2	O4P-C4-C5	8.88	115.94	108.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 73 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	H	905	LDA	1	0
4	L	312	BCL	8	0
4	L	314	BCL	5	0
5	L	402	BPH	2	0
6	L	502	U10	9	0
4	M	311	BCL	9	0
4	M	313	BCL	6	0
5	M	401	BPH	5	0
6	M	501	U10	4	0
13	M	704	GOL	2	0
10	M	800	CDL	3	0
11	M	802	PS2	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	M	901	LDA	6	0
12	M	903	LDA	6	0
12	M	906	LDA	1	0
12	M	907	LDA	1	0
12	M	920	LDA	12	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	L	281/281 (100%)	0.15	17 (6%)	23 9	61, 70, 78, 86	0
2	M	302/307 (98%)	0.28	17 (5%)	25 10	62, 69, 78, 113	0
3	H	241/260 (92%)	0.34	22 (9%)	10 4	59, 69, 80, 100	0
All	All	824/848 (97%)	0.25	56 (6%)	18 7	59, 69, 79, 113	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	77	GLY	4.7
2	M	1	ALA	3.8
3	H	219	ILE	3.7
3	H	218	THR	3.6
2	M	104	SER	3.6
3	H	52	ASN	3.6
1	L	280	ASN	3.6
2	M	171	TRP	3.6
1	L	202	LYS	3.5
1	L	277	GLY	3.5
3	H	74	THR	3.4
2	M	80	TRP	3.3
3	H	60	LYS	3.2
1	L	276[A]	PRO	3.2
2	M	301[A]	HIS	3.2
2	M	290	VAL	3.1
3	H	220	LYS	3.1
3	H	53	GLN	3.0
1	L	281	GLY	3.0
1	L	54	VAL	3.0
1	L	265	TRP	2.9
2	M	102	GLY	2.8
2	M	28	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
3	H	57	PRO	2.8
1	L	270	PRO	2.7
1	L	51	TRP	2.7
3	H	210	SER	2.7
1	L	267	VAL	2.6
3	H	250	SER	2.6
3	H	159	GLU	2.5
3	H	61	PRO	2.5
3	H	63	THR	2.4
3	H	251	VAL	2.4
3	H	59	PRO	2.4
3	H	119	ASP	2.4
2	M	103	LEU	2.4
2	M	100	GLU	2.3
1	L	59	TRP	2.3
1	L	269	LEU	2.3
1	L	252	GLY	2.3
2	M	34	PRO	2.3
3	H	51	ALA	2.2
2	M	81	ASN	2.2
2	M	37	THR	2.2
2	M	54	SER	2.2
2	M	101	TYR	2.1
2	M	109	LEU	2.1
3	H	29	TYR	2.1
1	L	275	ILE	2.1
3	H	229	GLU	2.1
3	H	58	LEU	2.1
1	L	266	TRP	2.0
1	L	278	GLY	2.0
3	H	161	ALA	2.0
2	M	79	GLY	2.0
1	L	21	LEU	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 ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
12	LDA	M	906	16/16	0.72	0.58	13.30	57,61,68,70	16
13	GOL	M	704	6/6	0.71	1.20	11.69	68,71,72,74	6
12	LDA	M	903	16/16	0.83	0.49	5.23	41,60,71,72	16
12	LDA	M	907	16/16	0.75	0.56	4.99	63,67,78,78	16
10	CDL	M	800	81/100	0.61	0.52	4.15	57,70,81,82	81
12	LDA	H	905	16/16	0.50	0.58	3.81	65,69,74,75	16
12	LDA	M	920	16/16	0.69	0.48	3.50	65,70,85,87	16
12	LDA	H	902	16/16	0.55	0.73	3.02	55,59,73,73	16
11	PS2	M	802	54/54	0.48	0.62	2.83	48,62,75,77	54
6	U10	L	502	48/63	0.70	0.44	2.75	52,57,69,71	48
6	U10	M	501	48/63	0.83	0.38	1.26	64,72,91,92	0
5	BPH	M	401	65/65	0.84	0.31	1.12	61,71,110,111	0
4	BCL	L	312	66/66	0.89	0.26	1.02	60,66,77,82	0
12	LDA	M	901	16/16	0.84	0.33	0.65	67,70,73,74	16
4	BCL	M	313	66/66	0.95	0.24	0.53	55,65,80,84	0
4	BCL	M	311	66/66	0.95	0.23	0.17	52,66,113,114	0
8	PO4	M	701	5/5	0.92	0.33	0.10	61,62,63,64	5
5	BPH	L	402	65/65	0.94	0.22	0.08	61,71,74,75	0
4	BCL	L	314	66/66	0.95	0.21	0.02	62,69,74,78	0
14	K	H	700	1/1	0.97	0.10	-1.27	63,63,63,63	0
7	FE	M	500	1/1	0.99	0.19	-1.52	70,70,70,70	0
9	HTO	M	703	10/10	0.53	0.52	-	58,61,63,63	10
12	LDA	H	904	16/16	0.32	1.04	-	53,57,61,62	16
8	PO4	M	702	5/5	0.62	0.39	-	64,66,68,68	5
13	GOL	H	705	6/6	0.58	0.23	-	56,58,60,61	6

6.5 Other polymers ⓘ

There are no such residues in this entry.