



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:04 am GMT

PDB ID : 1RZH
Title : PHOTOSYNTHETIC REACTION CENTER DOUBLE MUTANT FROM RHODOBACTER SPHAEROIDES WITH ASP L213 REPLACED WITH ASN AND ARG M233 REPLACED WITH CYS IN THE CHARGE-NEUTRAL DQAQB STATE (TRIGONAL FORM)
Authors : Xu, Q.; Axelrod, H.L.; Abresch, E.C.; Paddock, M.L.; Okamura, M.Y.; Feher, G.
Deposited on : 2003-12-24
Resolution : 1.80 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 : trunk28620
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) : recalc28949

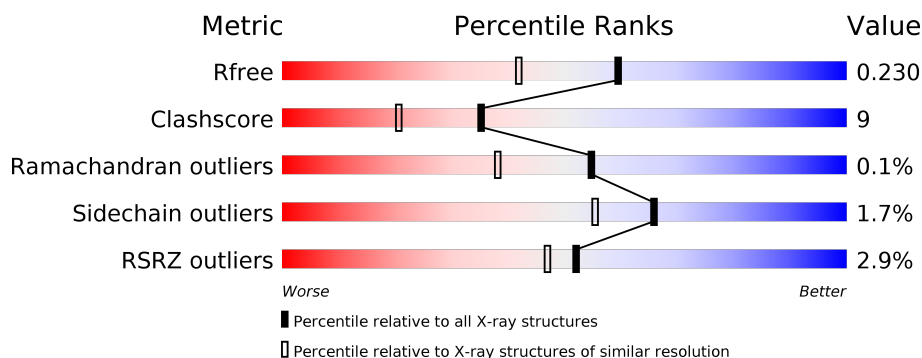
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (1.80-1.80)

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>4%</div> <div> <div></div> <div>87%</div> <div>12%</div> <div></div> </div> </div>
2	M	307	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>18%</div> <div></div> </div> </div>
3	H	260	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>8%</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	SPO	M	860	-	-	-	X
11	LDA	H	862	-	-	-	X
11	LDA	M	861	-	-	-	X
11	LDA	M	863	-	-	-	X
12	CDL	M	900	-	-	-	X
13	GOL	M	867	-	X	-	-
4	BCL	M	851	X	-	-	X
4	BCL	M	853	-	-	-	X
5	BPH	L	856	X	-	-	-
5	BPH	M	855	X	-	-	-
6	U10	L	859[A]	-	-	-	X
6	U10	M	858	-	-	-	X
7	HTO	L	865	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 7586 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	1	0
			2238	1510	357	363	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	213	ASN	ASP	ENGINEERED	UNP P02954

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	301	Total	C	N	O	S	0	0	0
			2399	1602	390	396	11			

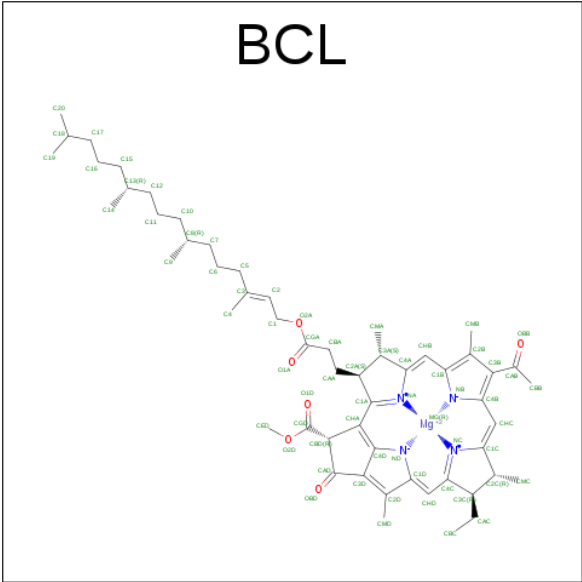
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	233	CYS	ARG	ENGINEERED	UNP P02953

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

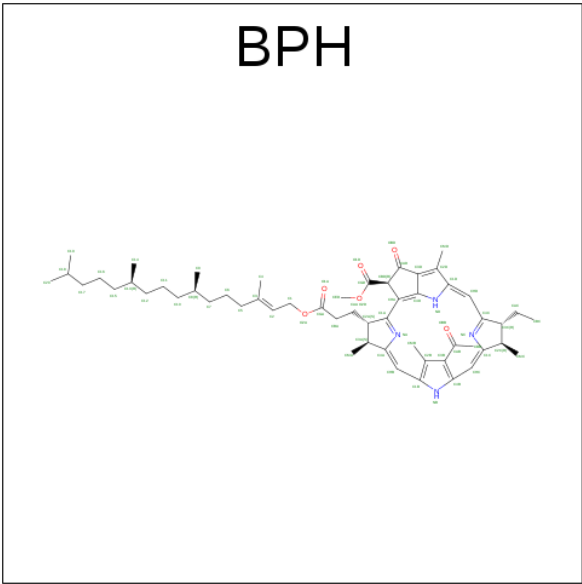
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	238	Total	C	N	O	S	0	1	0
			1822	1165	312	335	10			

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



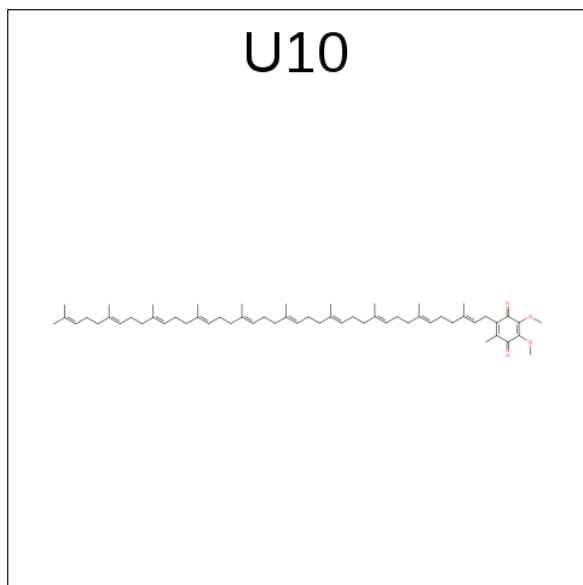
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 5 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C₅₅H₇₆N₄O₆).



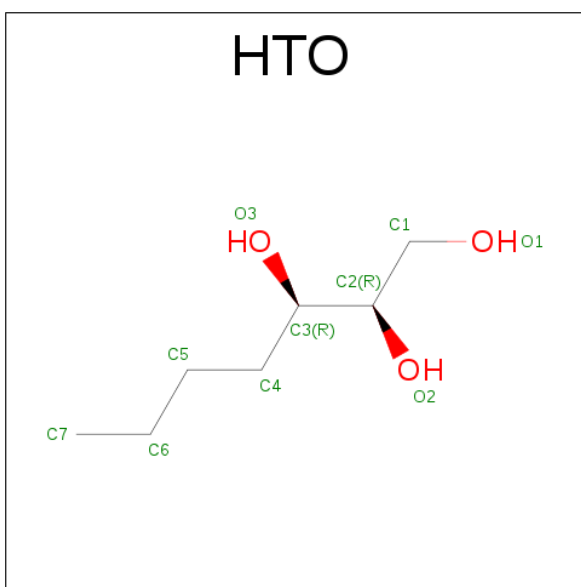
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			55	45	4	6		

- 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	1
			33	29	4		
6	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 7 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).

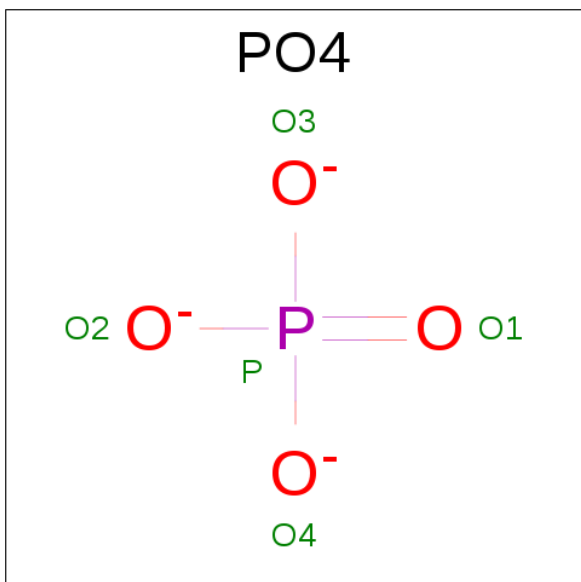


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	0
			10	7	3		
7	L	1	Total	C	O	0	0
			10	7	3		

- Molecule 8 is FE (II) ION (three-letter code: FE2) (formula: Fe).

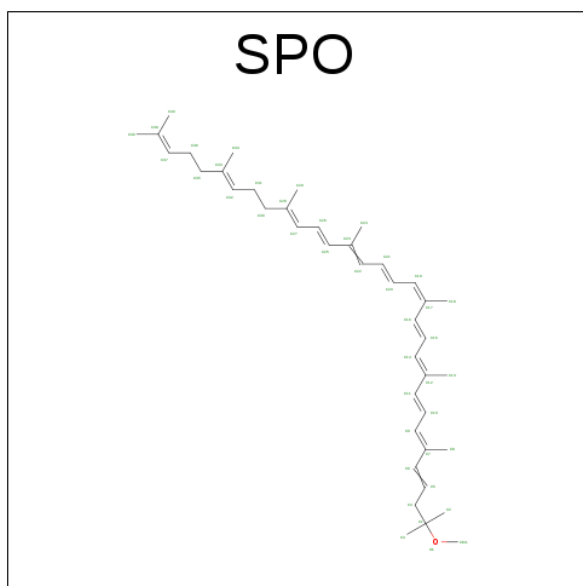
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	1	Total	Fe	0	0
			1	1		

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



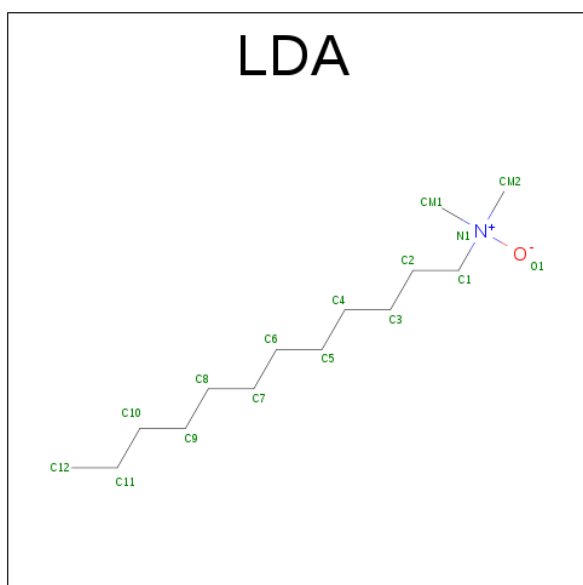
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	O	P	0	0
			5	4	1		

- Molecule 10 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).



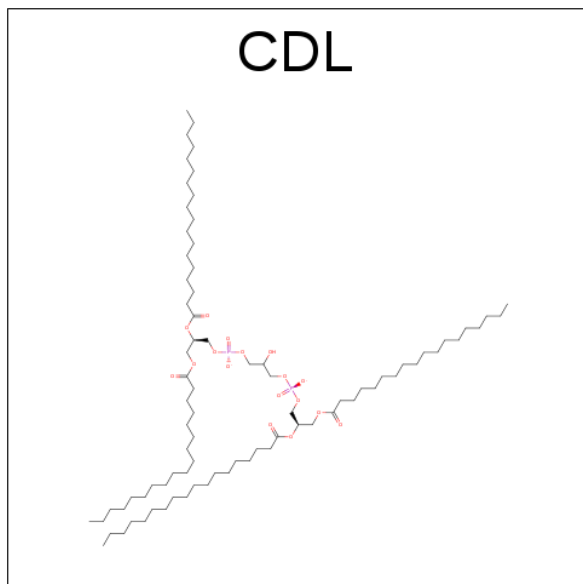
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	M	1	Total	C	O	0	0
			42	41	1		

- Molecule 11 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



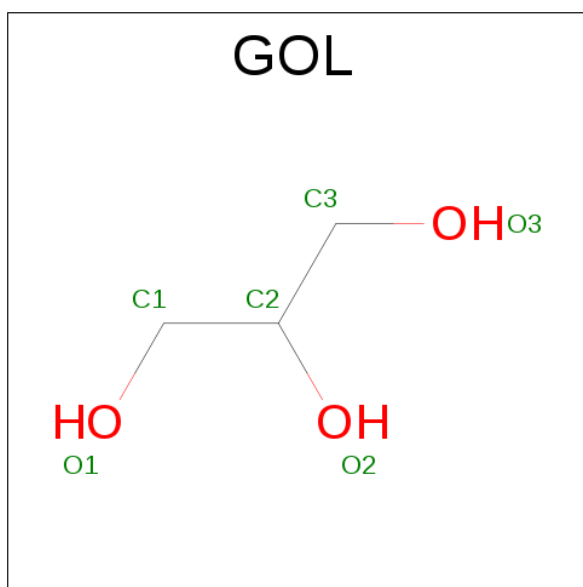
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	M	1	Total	C	N	O	0	0
			16	14	1	1		
11	M	1	Total	C	N	O	0	0
			16	14	1	1		
11	H	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 12 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	M	1	Total	C	O	P	0	0
			69	50	17	2		

- Molecule 13 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

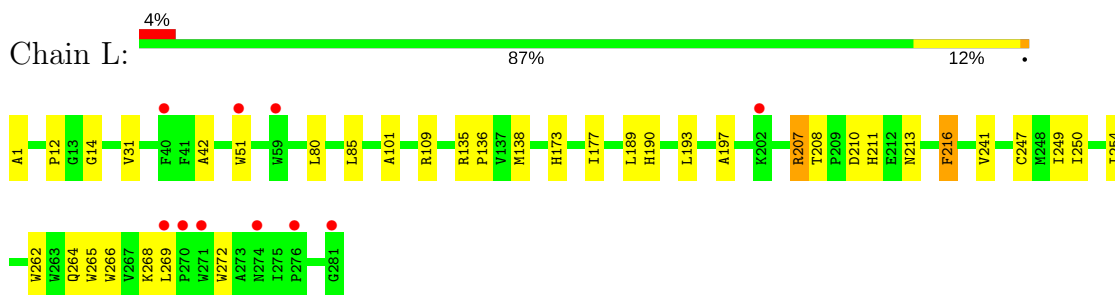
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	L	124	Total	O	0	2
			124	124		
14	M	138	Total	O	0	0
			138	138		
14	H	209	Total	O	0	0
			209	209		

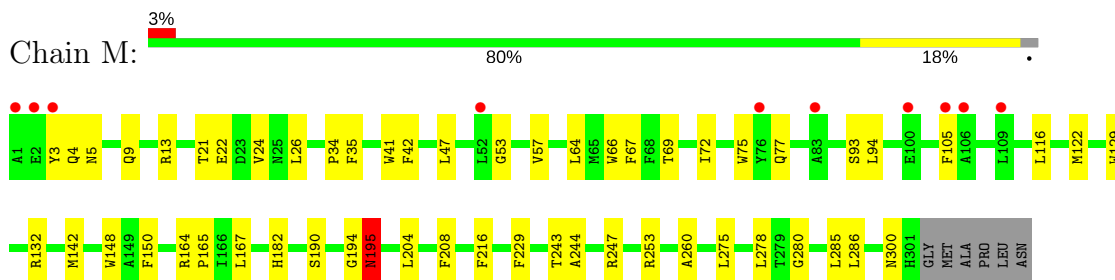
3 Residue-property plots [i](#)

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.

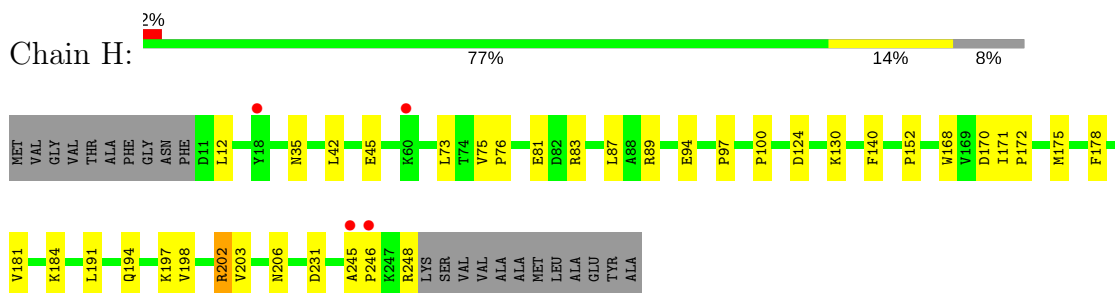
• Molecule 1: Reaction center protein L chain



• Molecule 2: Reaction center protein M chain



• Molecule 3: Reaction center protein H chain



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 184.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.31 – 1.80 39.31 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (39.31-1.80) 98.3 (39.31-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 1.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.221 , 0.233 0.218 , 0.230	Depositor DCC
R_{free} test set	9418 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7586	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, GOL, LDA, CDL, BPH, PO4, HTO, FE2, SPO, U10

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	0.36	0/2326	0.55	0/3183
2	M	0.35	0/2491	0.53	0/3402
3	H	0.30	0/1870	0.59	0/2544
All	All	0.34	0/6687	0.56	0/9129

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 [i](#)

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	2238	0	2193	36	0
2	M	2399	0	2310	53	0
3	H	1822	0	1826	29	0
4	L	132	0	148	4	0
4	M	132	0	148	21	0
5	L	65	0	74	5	0
5	M	55	0	53	3	0
6	L	33	0	39	8	0
6	M	48	0	61	3	0
7	L	20	0	32	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	M	1	0	0	0	0
9	M	5	0	0	0	0
10	M	42	0	60	7	0
11	H	16	0	31	2	0
11	M	32	0	62	5	0
12	M	69	0	82	2	0
13	M	6	0	4	0	0
14	H	209	0	0	1	0
14	L	124	0	0	0	0
14	M	138	0	0	0	0
All	All	7586	0	7123	132	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 (132) 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)
4:M:851:BCL:H121	4:M:851:BCL:C9	1.41	1.43
4:M:851:BCL:C12	4:M:851:BCL:H91	1.36	1.39
1:L:241:VAL:HG21	5:L:856:BPH:HAC1	1.46	0.97
4:M:851:BCL:H91	4:M:851:BCL:H122	1.54	0.90
2:M:21:THR:HG23	2:M:26:LEU:HD11	1.53	0.90
3:H:206:ASN:HD21	3:H:248:ARG:HD3	1.49	0.76
2:M:13:ARG:HD2	2:M:35:PHE:CD2	2.21	0.76
1:L:216:PHE:CG	6:L:859[A]:U10:H3M2	2.21	0.74
4:M:851:BCL:H92	4:M:851:BCL:H121	1.67	0.72
4:M:851:BCL:H112	4:M:853:BCL:H171	1.72	0.72
1:L:189:LEU:HB3	6:L:859[A]:U10:H4M3	1.74	0.70
3:H:89:ARG:NH1	3:H:94:GLU:HG2	2.07	0.70
2:M:77:GLN:HE22	2:M:93:SER:H	1.38	0.70
2:M:9:GLN:NE2	3:H:198:VAL:H	1.90	0.68
2:M:9:GLN:HE22	3:H:198:VAL:H	1.43	0.67
4:M:851:BCL:C12	4:M:851:BCL:C9	2.16	0.66
4:M:853:BCL:HMB1	4:M:853:BCL:CBB	2.27	0.65
3:H:171:ILE:HB	3:H:172:PRO:HD3	1.78	0.64
4:M:851:BCL:H91	4:M:851:BCL:H121	0.66	0.64
2:M:64:LEU:HD23	5:M:855:BPH:H9C3	1.79	0.64
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.80	0.63
1:L:193:LEU:HD22	6:L:859[A]:U10:H3M3	1.79	0.62
3:H:202:ARG:HG2	3:H:203:VAL:N	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:181:VAL:HG21	3:H:191:LEU:HD12	1.83	0.61
2:M:41:TRP:CG	11:M:863:LDA:HM13	2.36	0.61
2:M:75:TRP:HE1	10:M:860:SPO:HM13	1.66	0.61
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.82	0.60
2:M:3:TYR:CZ	2:M:5:ASN:HA	2.37	0.60
3:H:87:LEU:HD23	3:H:100:PRO:HA	1.84	0.59
2:M:286:LEU:HD21	3:H:12:LEU:HD12	1.83	0.59
4:M:851:BCL:HMB1	4:M:851:BCL:CBB	2.32	0.59
1:L:266:TRP:O	1:L:269:LEU:HD23	2.02	0.59
2:M:69:THR:O	2:M:72:ILE:HG22	2.02	0.59
2:M:148:TRP:HB3	12:M:900:CDL:H741	1.85	0.58
4:M:851:BCL:HMB1	4:M:851:BCL:HBB2	1.85	0.58
1:L:211:HIS:HE1	2:M:22:GLU:OE1	1.86	0.58
1:L:207:ARG:HG2	2:M:142:MET:HG2	1.84	0.58
1:L:189:LEU:CB	6:L:859[A]:U10:H4M3	2.34	0.57
1:L:241:VAL:CG2	5:L:856:BPH:HAC1	2.30	0.56
4:M:853:BCL:HBB3	4:M:853:BCL:HMB1	1.88	0.56
1:L:265:TRP:O	1:L:269:LEU:HD22	2.05	0.56
4:L:854:BCL:HMB1	4:L:854:BCL:HBB2	1.87	0.56
1:L:208:THR:H	1:L:211:HIS:CD2	2.24	0.56
2:M:204:LEU:HG	11:M:861:LDA:HM22	1.88	0.56
2:M:105:PHE:HD1	2:M:116:LEU:HD13	1.73	0.54
4:L:854:BCL:H61	6:M:858:U10:H203	1.89	0.54
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.88	0.54
1:L:193:LEU:CD2	6:L:859[A]:U10:H3M3	2.38	0.53
3:H:206:ASN:HD21	3:H:248:ARG:CD	2.21	0.53
2:M:253:ARG:HH12	11:H:862:LDA:HM23	1.73	0.52
1:L:31:VAL:HG22	6:M:858:U10:H403	1.91	0.52
2:M:253:ARG:HH12	11:H:862:LDA:CM2	2.21	0.52
1:L:51:TRP:CZ3	1:L:80:LEU:HD13	2.46	0.51
2:M:66:TRP:CD1	2:M:122:MET:HB2	2.46	0.51
1:L:216:PHE:CD1	6:L:859[A]:U10:H3M2	2.45	0.51
3:H:81:GLU:O	3:H:83:ARG:HG2	2.11	0.50
7:L:866:HTO:H61	6:M:858:U10:H23	1.92	0.50
2:M:275:LEU:HD23	2:M:278:LEU:HD23	1.94	0.50
1:L:189:LEU:HB3	6:L:859[A]:U10:C4M	2.40	0.49
2:M:9:GLN:HE22	3:H:197:LYS:HA	1.76	0.49
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.48	0.48
4:L:852:BCL:H122	5:L:856:BPH:H3A	1.95	0.48
3:H:75:VAL:HA	3:H:76:PRO:C	2.34	0.48
2:M:24:VAL:O	2:M:26:LEU:HD12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:194:GLY:O	2:M:195:ASN:HB3	2.13	0.48
2:M:167:LEU:HD12	2:M:285:LEU:HD11	1.95	0.48
3:H:45:GLU:HG3	3:H:94:GLU:OE2	2.14	0.48
1:L:266:TRP:HA	1:L:269:LEU:CD2	2.43	0.47
2:M:26:LEU:N	2:M:26:LEU:HD12	2.29	0.47
3:H:152:PRO:HG2	3:H:202:ARG:HB2	1.96	0.47
1:L:14:GLY:O	1:L:109:ARG:HD3	2.15	0.47
2:M:53:GLY:O	2:M:57:VAL:HG23	2.15	0.47
2:M:190:SER:HB2	4:M:853:BCL:H3C	1.97	0.47
1:L:208:THR:H	1:L:211:HIS:HD2	1.63	0.46
2:M:260:ALA:HB1	3:H:35:ASN:OD1	2.15	0.46
1:L:138:MET:SD	1:L:249:ILE:HD11	2.56	0.46
10:M:860:SPO:H5	10:M:860:SPO:HM12	1.97	0.46
2:M:26:LEU:HD12	2:M:26:LEU:H	1.81	0.46
1:L:264:GLN:O	1:L:268:LYS:HG2	2.16	0.46
2:M:150:PHE:N	5:M:855:BPH:HMD3	2.31	0.46
2:M:286:LEU:CD2	3:H:12:LEU:HD12	2.45	0.45
4:M:851:BCL:H61	4:M:851:BCL:H102	1.40	0.45
3:H:12:LEU:HD13	3:H:12:LEU:O	2.15	0.45
2:M:13:ARG:O	3:H:140:PHE:HA	2.17	0.45
3:H:245:ALA:HA	3:H:248:ARG:NH2	2.32	0.45
2:M:41:TRP:CD2	11:M:863:LDA:CM1	3.00	0.45
4:M:853:BCL:OBB	4:M:853:BCL:HHC	2.17	0.45
1:L:42:ALA:HA	5:L:856:BPH:H9C3	1.97	0.44
2:M:300:ASN:N	2:M:300:ASN:HD22	2.14	0.44
2:M:194:GLY:O	2:M:195:ASN:CB	2.66	0.44
1:L:51:TRP:CE3	1:L:85:LEU:HD21	2.53	0.44
10:M:860:SPO:H15	10:M:860:SPO:H131	1.82	0.43
2:M:243:THR:O	2:M:247:ARG:HG3	2.18	0.43
3:H:130:LYS:NZ	3:H:170:ASP:OD2	2.52	0.43
1:L:262:TRP:O	1:L:265:TRP:HD1	2.02	0.43
1:L:12:PRO:HG3	3:H:97:PRO:HB2	2.00	0.43
4:M:851:BCL:H192	10:M:860:SPO:H81	2.01	0.43
4:M:851:BCL:C19	10:M:860:SPO:C8	2.97	0.43
3:H:194:GLN:CD	3:H:194:GLN:H	2.22	0.43
2:M:208:PHE:CE1	11:M:861:LDA:H92	2.54	0.42
2:M:182:HIS:CG	10:M:860:SPO:H181	2.54	0.42
2:M:190:SER:CB	4:M:853:BCL:H3C	2.49	0.42
1:L:250:ILE:HB	1:L:254:ILE:HD11	2.01	0.42
4:L:854:BCL:C4A	4:L:854:BCL:HBA1	2.49	0.42
2:M:67:PHE:CG	5:M:855:BPH:H9C2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:210:ASP:OD1	3:H:124:ASP:HB2	2.20	0.42
3:H:184:LYS:HD3	14:H:913:HOH:O	2.20	0.42
1:L:208:THR:OG1	1:L:211:HIS:HD2	2.03	0.42
2:M:34:PRO:HG2	2:M:47:LEU:HD22	2.01	0.42
2:M:280:GLY:O	4:M:853:BCL:HED3	2.20	0.42
1:L:101:ALA:CB	7:L:865:HTO:H72	2.50	0.42
2:M:129:TRP:O	2:M:132:ARG:HB3	2.19	0.41
2:M:42:PHE:HB2	11:M:863:LDA:H72	2.01	0.41
2:M:75:TRP:HE1	10:M:860:SPO:H32A	1.86	0.41
2:M:195:ASN:HD22	2:M:195:ASN:C	2.24	0.41
4:M:851:BCL:H72	4:M:851:BCL:C4	2.49	0.41
4:M:851:BCL:HHC	4:M:851:BCL:OBB	2.21	0.41
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.55	0.41
1:L:197:ALA:HA	1:L:207:ARG:HB2	2.02	0.41
1:L:1:ALA:HB1	3:H:42:LEU:HB3	2.02	0.41
3:H:168:TRP:HB2	3:H:178:PHE:HB2	2.02	0.41
2:M:300:ASN:N	2:M:300:ASN:ND2	2.68	0.41
3:H:89:ARG:HH12	3:H:94:GLU:HG2	1.82	0.41
2:M:148:TRP:CE2	12:M:900:CDL:H511	2.56	0.41
4:M:851:BCL:C4	4:M:851:BCL:C7	2.99	0.40
1:L:190:HIS:HA	6:L:859[A]:U10:H4M1	2.04	0.40
2:M:4:GLN:OE1	2:M:4:GLN:HA	2.21	0.40
3:H:245:ALA:N	3:H:246:PRO:CD	2.84	0.40
1:L:213:ASN:HD22	1:L:213:ASN:HA	1.73	0.40
2:M:26:LEU:CD1	2:M:26:LEU:H	2.34	0.40
1:L:269:LEU:HD13	1:L:269:LEU:HA	1.92	0.40
5:L:856:BPH:OBB	5:L:856:BPH:HHC	2.21	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	280/281 (100%)	273 (98%)	7 (2%)	0	100	100
2	M	299/307 (97%)	292 (98%)	6 (2%)	1 (0%)	44	29
3	H	237/260 (91%)	236 (100%)	1 (0%)	0	100	100
All	All	816/848 (96%)	801 (98%)	14 (2%)	1 (0%)	55	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	195	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	221/220 (100%)	217 (98%)	4 (2%)	64	53
2	M	236/240 (98%)	233 (99%)	3 (1%)	73	66
3	H	194/208 (93%)	190 (98%)	4 (2%)	59	46
All	All	651/668 (98%)	640 (98%)	11 (2%)	66	55

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	207	ARG
1	L	216	PHE
1	L	247	CYS
1	L	272	TRP
2	M	94	LEU
2	M	195	ASN
2	M	216	PHE
3	H	73	LEU
3	H	175	MET
3	H	202	ARG
3	H	231	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	87	GLN
1	L	211	HIS
1	L	213	ASN
2	M	9	GLN
2	M	77	GLN
2	M	195	ASN
2	M	299	GLN
2	M	300	ASN
3	H	206	ASN

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 18 ligands modelled in this entry, 1 is monoatomic - leaving 17 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	$\# Z > 2$
11	LDA	H	862	-	13,15,15	2.44	1 (7%)	14,17,17	2.33	5 (35%)
4	BCL	L	852	-	55,74,74	1.24	4 (7%)	65,115,115	1.74	16 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BCL	L	854	-	55,74,74	1.75	11 (20%)	65,115,115	1.99	20 (30%)
5	BPH	L	856	-	65,70,70	1.45	9 (13%)	75,101,101	2.13	19 (25%)
6	U10	L	859[A]	-	33,33,63	1.98	11 (33%)	40,43,79	1.85	9 (22%)
7	HTO	L	865	-	9,9,9	1.26	1 (11%)	9,10,10	0.37	0
7	HTO	L	866	-	9,9,9	1.26	1 (11%)	9,10,10	0.37	0
4	BCL	M	851	-	55,74,74	1.72	9 (16%)	65,115,115	2.38	23 (35%)
4	BCL	M	853	-	55,74,74	1.57	9 (16%)	65,115,115	1.87	17 (26%)
5	BPH	M	855	-	55,60,70	1.35	7 (12%)	63,89,101	2.28	20 (31%)
6	U10	M	858	-	48,48,63	2.05	18 (37%)	58,61,79	3.16	17 (29%)
10	SPO	M	860	-	40,41,41	3.37	23 (57%)	49,50,50	3.95	17 (34%)
11	LDA	M	861	-	13,15,15	2.41	1 (7%)	14,17,17	2.03	5 (35%)
11	LDA	M	863	-	13,15,15	2.29	1 (7%)	14,17,17	2.20	5 (35%)
9	PO4	M	864	-	4,4,4	1.41	0	6,6,6	0.39	0
13	GOL	M	867	-	5,5,5	4.90	5 (100%)	5,5,5	5.50	3 (60%)
12	CDL	M	900	-	68,68,99	0.74	2 (2%)	70,80,111	1.01	4 (5%)

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
11	LDA	H	862	-	-	0/13/13/13	0/0/0/0
4	BCL	L	852	-	-	0/37/137/137	0/0/9/9
4	BCL	L	854	-	-	0/37/137/137	0/0/9/9
5	BPH	L	856	-	2/2/18/22	0/54/105/105	0/1/6/6
6	U10	L	859[A]	-	-	0/27/51/87	0/1/1/1
7	HTO	L	865	-	-	0/10/10/10	0/0/0/0
7	HTO	L	866	-	-	0/10/10/10	0/0/0/0
4	BCL	M	851	-	2/2/21/25	0/37/137/137	0/0/9/9
4	BCL	M	853	-	-	0/37/137/137	0/0/9/9
5	BPH	M	855	-	1/1/16/22	0/42/93/105	0/1/6/6
6	U10	M	858	-	-	0/45/69/87	0/1/1/1
10	SPO	M	860	-	-	0/47/47/47	0/0/0/0
11	LDA	M	861	-	-	0/13/13/13	0/0/0/0
11	LDA	M	863	-	-	0/13/13/13	0/0/0/0
9	PO4	M	864	-	-	0/0/0/0	0/0/0/0
13	GOL	M	867	-	-	0/4/4/4	0/0/0/0
12	CDL	M	900	-	-	0/79/79/110	0/0/0/0

All (113) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	862	LDA	O1-N1	-8.60	1.25	1.42
11	M	861	LDA	O1-N1	-8.40	1.25	1.42
13	M	867	GOL	C3-C2	-8.30	1.21	1.52
11	M	863	LDA	O1-N1	-8.05	1.26	1.42
5	L	856	BPH	C11-C10	-5.26	1.28	1.52
6	M	858	U10	C37-C38	-4.53	1.35	1.50
6	M	858	U10	C7-C8	-3.38	1.45	1.50
13	M	867	GOL	C1-C2	-3.26	1.40	1.52
6	L	859[A]	U10	C7-C8	-3.09	1.46	1.50
10	M	860	SPO	C25-C23	-2.90	1.39	1.45
4	L	854	BCL	C2C-C3C	-2.85	1.46	1.54
6	L	859[A]	U10	O3-C3M	-2.80	1.38	1.45
13	M	867	GOL	O2-C2	-2.80	1.35	1.43
10	M	860	SPO	C11-C12	-2.61	1.40	1.45
5	M	855	BPH	O2D-CED	-2.54	1.39	1.45
5	L	856	BPH	O2D-CED	-2.49	1.39	1.45
6	M	858	U10	O3-C3M	-2.48	1.39	1.45
4	M	851	BCL	C2C-C3C	-2.31	1.47	1.54
10	M	860	SPO	C6-C7	-2.29	1.40	1.45
4	M	853	BCL	O2D-CED	-2.27	1.39	1.45
4	L	854	BCL	C3B-C2B	-2.16	1.35	1.39
5	M	855	BPH	C2C-C3C	-2.11	1.48	1.54
4	M	851	BCL	C3B-C2B	-2.04	1.35	1.39
4	M	853	BCL	O1D-CGD	2.01	1.26	1.21
4	M	853	BCL	C3C-C4C	2.03	1.54	1.51
5	L	856	BPH	C2A-C1A	2.04	1.54	1.51
4	M	853	BCL	C4-C3	2.04	1.55	1.50
6	M	858	U10	C6-C5	2.12	1.52	1.46
12	M	900	CDL	OA8-CA7	2.16	1.39	1.33
4	L	854	BCL	CMB-C2B	2.18	1.56	1.51
6	M	858	U10	C30-C29	2.19	1.56	1.50
6	M	858	U10	C36-C34	2.20	1.56	1.51
6	L	859[A]	U10	C7-C6	2.20	1.55	1.51
5	L	856	BPH	CHC-C1C	2.20	1.40	1.36
5	M	855	BPH	O1D-CGD	2.26	1.26	1.21
12	M	900	CDL	CB3-CB4	2.27	1.57	1.50
4	M	851	BCL	C2-C3	2.28	1.38	1.33
5	L	856	BPH	C4C-NC	2.29	1.42	1.37
4	M	851	BCL	CMA-C3A	2.32	1.58	1.53
10	M	860	SPO	C22-C23	2.32	1.38	1.35
6	M	858	U10	C28-C29	2.33	1.38	1.33
6	L	859[A]	U10	C15-C14	2.34	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	858	U10	C15-C14	2.34	1.56	1.50
5	M	855	BPH	CAA-C2A	2.34	1.58	1.54
4	L	852	BCL	CBB-CAB	2.34	1.56	1.49
4	L	854	BCL	O1D-CGD	2.35	1.27	1.21
6	M	858	U10	C25-C24	2.38	1.56	1.50
6	M	858	U10	C18-C19	2.40	1.39	1.33
6	M	858	U10	C23-C24	2.41	1.39	1.33
6	M	858	U10	C8-C9	2.41	1.39	1.33
4	L	854	BCL	C2-C3	2.43	1.39	1.33
4	L	854	BCL	CMC-C2C	2.46	1.58	1.53
4	L	854	BCL	CAA-C2A	2.49	1.58	1.54
4	L	852	BCL	C4-C3	2.53	1.57	1.50
5	L	856	BPH	CAA-C2A	2.54	1.59	1.54
10	M	860	SPO	C13-C12	2.58	1.56	1.50
10	M	860	SPO	C24-C23	2.60	1.56	1.50
5	L	856	BPH	C2-C3	2.60	1.39	1.33
4	M	851	BCL	CAA-C2A	2.61	1.59	1.54
5	M	855	BPH	C2-C3	2.65	1.39	1.33
10	M	860	SPO	C8-C7	2.65	1.56	1.50
10	M	860	SPO	O1-C1	2.66	1.57	1.41
6	L	859[A]	U10	C18-C19	2.66	1.39	1.33
10	M	860	SPO	C26-C27	2.67	1.51	1.43
4	L	854	BCL	O2A-CGA	2.69	1.41	1.33
10	M	860	SPO	C15-C14	2.70	1.51	1.43
10	M	860	SPO	C32-C33	2.80	1.40	1.33
10	M	860	SPO	C37-C38	2.82	1.40	1.32
10	M	860	SPO	C10-C9	2.84	1.52	1.43
6	L	859[A]	U10	C6-C1	2.88	1.41	1.35
7	L	865	HTO	C3-C2	2.89	1.60	1.53
7	L	866	HTO	C3-C2	2.91	1.60	1.53
6	L	859[A]	U10	C8-C9	2.93	1.40	1.33
4	L	852	BCL	CHB-C4A	2.94	1.37	1.33
6	M	858	U10	C6-C1	2.94	1.41	1.35
6	M	858	U10	C31-C29	3.03	1.57	1.51
6	L	859[A]	U10	C23-C24	3.04	1.41	1.32
4	M	853	BCL	C2-C3	3.07	1.40	1.33
4	M	853	BCL	O2A-CGA	3.29	1.43	1.33
6	L	859[A]	U10	O3-C3	3.31	1.45	1.36
6	M	858	U10	C13-C14	3.40	1.41	1.33
13	M	867	GOL	O3-C3	3.46	1.57	1.42
6	M	858	U10	O3-C3	3.49	1.45	1.36
10	M	860	SPO	C9-C7	3.55	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	851	BCL	O2A-CGA	3.70	1.44	1.33
10	M	860	SPO	C19-C17	3.70	1.40	1.35
5	L	856	BPH	O2D-CGD	3.72	1.42	1.33
6	L	859[A]	U10	C13-C14	3.78	1.42	1.33
5	M	855	BPH	O2D-CGD	3.79	1.42	1.33
5	L	856	BPH	O2A-CGA	3.85	1.44	1.33
5	M	855	BPH	O2A-CGA	3.99	1.45	1.33
10	M	860	SPO	O1-CM1	4.04	1.56	1.43
4	L	852	BCL	CHC-C1C	4.08	1.38	1.33
4	M	853	BCL	CHB-C4A	4.23	1.38	1.33
6	M	858	U10	C33-C34	4.26	1.43	1.33
10	M	860	SPO	C14-C12	4.31	1.41	1.35
13	M	867	GOL	O1-C1	4.54	1.61	1.42
4	M	851	BCL	O2D-CGD	4.58	1.44	1.33
6	L	859[A]	U10	O4-C4	4.67	1.48	1.36
4	M	853	BCL	O2D-CGD	4.68	1.45	1.33
6	M	858	U10	O4-C4	4.83	1.48	1.36
10	M	860	SPO	C26-C25	4.85	1.47	1.34
4	L	854	BCL	O2D-CGD	5.00	1.45	1.33
10	M	860	SPO	C21-C20	5.12	1.49	1.35
4	M	851	BCL	CHB-C4A	5.31	1.40	1.33
10	M	860	SPO	C27-C28	5.36	1.39	1.34
4	L	854	BCL	CHC-C1C	5.44	1.40	1.33
4	M	853	BCL	CHC-C1C	5.45	1.40	1.33
4	L	854	BCL	CHB-C4A	5.63	1.40	1.33
4	M	851	BCL	CHC-C1C	6.83	1.42	1.33
10	M	860	SPO	C15-C16	7.66	1.54	1.34
10	M	860	SPO	C10-C11	7.90	1.54	1.34
10	M	860	SPO	C6-C5	8.60	1.54	1.31

All (180) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	860	SPO	C2-C1-C4	-18.59	79.29	110.90
10	M	860	SPO	C3-C1-C4	-10.38	93.25	110.90
10	M	860	SPO	O1-C1-C4	-7.47	86.23	106.29
10	M	860	SPO	C15-C14-C12	-6.19	118.47	127.31
11	H	862	LDA	CM2-N1-CM1	-5.91	99.69	110.99
4	M	851	BCL	C4-C3-C5	-5.78	105.25	115.29
10	M	860	SPO	C20-C21-C22	-5.68	111.34	123.46
11	M	863	LDA	CM2-N1-CM1	-5.53	100.41	110.99
10	M	860	SPO	C25-C23-C22	-5.04	111.21	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	861	LDA	CM2-N1-CM1	-4.90	101.62	110.99
6	M	858	U10	C36-C37-C38	-4.79	95.52	111.97
4	M	851	BCL	O2A-CGA-O1A	-4.67	111.94	123.55
4	M	851	BCL	OBD-CAD-CBD	-4.45	119.23	125.94
4	L	852	BCL	OBB-CAB-CBB	-4.17	110.64	120.16
5	M	855	BPH	O1D-CGD-CBD	-4.08	117.27	124.60
4	L	854	BCL	CMB-C2B-C1B	-4.03	122.27	128.46
4	M	853	BCL	CAC-C3C-C2C	-4.01	104.17	114.24
4	M	851	BCL	CAA-C2A-C3A	-3.92	102.07	112.81
6	M	858	U10	C35-C34-C36	-3.85	108.60	115.29
6	L	859[A]	U10	O5-C5-C6	-3.84	114.74	121.82
4	L	852	BCL	C1-C2-C3	-3.80	118.96	125.96
4	L	854	BCL	C4B-CHC-C1C	-3.79	122.61	130.12
4	L	854	BCL	C1B-CHB-C4A	-3.79	122.62	130.12
10	M	860	SPO	C18-C17-C19	-3.78	117.63	122.92
4	L	852	BCL	CAA-C2A-C3A	-3.77	102.46	112.81
10	M	860	SPO	C4-C5-C6	-3.75	119.19	124.57
5	L	856	BPH	O1D-CGD-CBD	-3.75	117.87	124.60
4	L	854	BCL	CAC-C3C-C2C	-3.66	105.05	114.24
4	M	851	BCL	CMB-C2B-C1B	-3.60	122.93	128.46
4	L	852	BCL	C7-C6-C5	-3.47	103.45	113.11
11	H	862	LDA	CM1-N1-C1	-3.43	103.02	110.23
10	M	860	SPO	C6-C7-C9	-3.43	113.67	118.94
11	M	863	LDA	CM1-N1-C1	-3.36	103.17	110.23
10	M	860	SPO	C15-C16-C17	-3.36	116.98	126.42
6	L	859[A]	U10	O2-C2-C3	-3.33	113.87	120.95
5	M	855	BPH	O2D-CGD-O1D	-3.30	117.17	123.82
5	L	856	BPH	O2D-CGD-O1D	-3.29	117.21	123.82
4	M	853	BCL	C1-C2-C3	-3.24	119.99	125.96
4	L	854	BCL	O2D-CGD-O1D	-3.17	117.44	123.82
4	M	851	BCL	OBB-CAB-CBB	-3.17	112.94	120.16
4	M	853	BCL	CAC-C3C-C4C	-3.13	105.65	112.58
4	L	852	BCL	CMB-C2B-C1B	-3.12	123.67	128.46
6	M	858	U10	O5-C5-C6	-3.12	116.08	121.82
4	M	851	BCL	O2D-CGD-O1D	-3.11	117.56	123.82
4	M	853	BCL	O1D-CGD-CBD	-3.09	119.06	124.60
4	M	853	BCL	C4B-CHC-C1C	-3.06	124.06	130.12
6	M	858	U10	O2-C2-C3	-3.06	114.45	120.95
4	M	851	BCL	C4B-CHC-C1C	-3.04	124.10	130.12
6	M	858	U10	C20-C19-C21	-3.03	110.02	115.29
10	M	860	SPO	C20-C19-C17	-2.95	123.10	127.31
6	M	858	U10	C30-C29-C31	-2.87	110.31	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	854	BCL	OBD-CAD-CBD	-2.78	121.74	125.94
4	L	852	BCL	OBD-CAD-CBD	-2.78	121.75	125.94
11	M	861	LDA	CM1-N1-C1	-2.77	104.41	110.23
4	M	851	BCL	CMA-C3A-C2A	-2.77	102.54	113.77
6	L	859[A]	U10	C20-C19-C21	-2.75	110.52	115.29
5	L	856	BPH	C7-C6-C5	-2.74	105.50	113.11
5	L	856	BPH	C4B-C3B-CAB	-2.73	120.00	130.09
5	M	855	BPH	C4B-C3B-CAB	-2.65	120.33	130.09
4	M	853	BCL	O2D-CGD-O1D	-2.61	118.56	123.82
4	L	854	BCL	OB B-CAB-CBB	-2.61	114.21	120.16
5	M	855	BPH	C4D-CHA-C1A	-2.56	123.71	130.23
4	L	854	BCL	O1D-CGD-CBD	-2.53	120.06	124.60
5	L	856	BPH	O2A-CGA-O1A	-2.50	117.33	123.55
4	L	854	BCL	CAA-C2A-C3A	-2.50	105.95	112.81
4	L	852	BCL	O2D-CGD-CBD	-2.49	106.85	111.30
10	M	860	SPO	C10-C9-C7	-2.48	123.77	127.31
5	L	856	BPH	OBD-CAD-CBD	-2.47	122.20	125.94
4	M	851	BCL	O1D-CGD-CBD	-2.44	120.21	124.60
5	M	855	BPH	C5-C3-C2	-2.39	116.20	121.10
5	M	855	BPH	CAA-C2A-C3A	-2.39	106.27	112.81
5	L	856	BPH	CAA-C2A-C3A	-2.37	106.32	112.81
12	M	900	CDL	CB6-CB4-CB3	-2.36	106.53	111.86
11	M	863	LDA	C9-C8-C7	-2.36	102.30	114.45
4	L	852	BCL	CAC-C3C-C4C	-2.34	107.38	112.58
11	H	862	LDA	C9-C8-C7	-2.30	102.63	114.45
4	L	852	BCL	CHA-C1A-NA	-2.29	120.85	126.18
5	L	856	BPH	C4D-CHA-C1A	-2.29	124.40	130.23
5	M	855	BPH	C2A-C1A-NA	-2.27	109.15	111.91
4	M	851	BCL	C1B-CHB-C4A	-2.25	125.66	130.12
6	L	859[A]	U10	C7-C6-C5	-2.25	115.59	118.47
4	M	853	BCL	OBD-CAD-CBD	-2.21	122.60	125.94
5	M	855	BPH	O2A-CGA-O1A	-2.20	118.09	123.55
4	M	853	BCL	O2A-CGA-O1A	-2.19	118.12	123.55
4	M	853	BCL	CMB-C2B-C1B	-2.13	125.18	128.46
4	M	853	BCL	C1B-CHB-C4A	-2.12	125.91	130.12
10	M	860	SPO	C10-C11-C12	-2.11	120.48	126.42
4	M	851	BCL	CHA-C1A-NA	-2.11	121.29	126.18
4	L	852	BCL	C12-C11-C10	-2.11	103.07	113.25
4	L	852	BCL	C11-C12-C13	-2.09	108.86	115.73
11	M	861	LDA	C9-C8-C7	-2.07	103.78	114.45
4	M	851	BCL	CMA-C3A-C4A	-2.05	106.26	111.77
4	L	854	BCL	O2A-CGA-O1A	-2.04	118.48	123.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	858	U10	C41-C39-C38	-2.04	116.50	122.65
5	M	855	BPH	CAC-C3C-C2C	-2.02	109.16	114.24
6	M	858	U10	C7-C8-C9	2.01	130.08	126.71
4	M	851	BCL	C3C-C2C-C1C	2.02	105.13	101.87
4	M	851	BCL	CMB-C2B-C3B	2.04	128.69	124.89
4	M	851	BCL	C6-C5-C3	2.08	117.38	112.66
6	L	859[A]	U10	C21-C19-C18	2.09	125.37	121.10
11	M	861	LDA	CM2-N1-C1	2.10	114.64	110.23
4	L	854	BCL	C2A-C3A-C4A	2.10	105.26	101.87
4	M	853	BCL	C3A-C2A-C1A	2.12	104.52	101.34
12	M	900	CDL	C52-C51-CB5	2.12	121.34	113.58
6	L	859[A]	U10	C7-C6-C1	2.13	127.67	123.47
5	L	856	BPH	CAC-C3C-C4C	2.18	118.28	112.67
5	M	855	BPH	C4-C3-C5	2.21	119.12	115.29
6	M	858	U10	C21-C19-C18	2.27	125.75	121.10
5	L	856	BPH	CMD-C2D-C3D	2.30	129.16	124.89
6	L	859[A]	U10	C17-C18-C19	2.32	133.51	127.68
6	M	858	U10	C16-C14-C13	2.33	125.87	121.10
11	M	863	LDA	CM2-N1-C1	2.33	115.13	110.23
4	M	853	BCL	C3C-C2C-C1C	2.38	105.71	101.87
4	L	854	BCL	CHB-C4A-NA	2.38	127.80	124.51
6	M	858	U10	C31-C29-C28	2.39	125.99	121.10
5	M	855	BPH	CMD-C2D-C3D	2.39	129.33	124.89
12	M	900	CDL	CB4-OB6-CB5	2.45	123.67	117.88
11	H	862	LDA	CM2-N1-C1	2.47	115.42	110.23
4	M	851	BCL	CMD-C2D-C3D	2.48	129.49	124.89
4	L	854	BCL	C3C-C2C-C1C	2.48	105.88	101.87
4	L	852	BCL	C2C-C3C-C4C	2.49	105.07	101.34
5	L	856	BPH	C3C-C2C-C1C	2.49	105.90	101.87
5	M	855	BPH	C3C-C2C-C1C	2.50	105.91	101.87
4	L	854	BCL	C4A-NA-C1A	2.54	109.60	106.45
4	L	852	BCL	O1D-CGD-CBD	2.54	129.17	124.60
11	M	861	LDA	O1-N1-C1	2.57	115.58	109.27
11	M	863	LDA	O1-N1-C1	2.64	115.76	109.27
4	L	852	BCL	CBB-CAB-C3B	2.65	128.11	120.39
4	M	853	BCL	C5-C3-C2	2.69	126.60	121.10
4	L	854	BCL	O2A-CGA-CBA	2.73	119.86	111.90
5	M	855	BPH	C2C-C3C-C4C	2.85	105.61	101.34
6	L	859[A]	U10	C16-C14-C13	2.86	126.95	121.10
4	L	854	BCL	CMB-C2B-C3B	2.90	130.28	124.89
11	H	862	LDA	O1-N1-C1	2.95	116.52	109.27
4	M	851	BCL	C2C-C3C-C4C	3.02	105.87	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	856	BPH	C2C-C3C-C4C	3.04	105.90	101.34
13	M	867	GOL	O1-C1-C2	3.11	125.74	110.07
10	M	860	SPO	C8-C7-C6	3.18	123.17	118.10
10	M	860	SPO	C3-C1-C2	3.20	116.64	110.31
4	L	852	BCL	CMD-C2D-C3D	3.27	130.95	124.89
4	L	852	BCL	CMB-C2B-C3B	3.27	130.96	124.89
4	M	853	BCL	O2A-CGA-CBA	3.29	121.47	111.90
4	M	853	BCL	CHC-C1C-NC	3.31	129.09	124.51
4	L	854	BCL	C1-O2A-CGA	3.39	124.90	116.77
4	L	854	BCL	OBB-CAB-C3B	3.40	126.43	119.95
5	M	855	BPH	C7-C6-C5	3.58	123.08	113.11
4	L	854	BCL	CHC-C1C-NC	3.62	129.52	124.51
5	M	855	BPH	CBC-CAC-C3C	3.65	121.79	113.51
5	L	856	BPH	C11-C10-C8	3.72	127.94	115.73
10	M	860	SPO	C1-C4-C5	3.79	122.65	112.87
10	M	860	SPO	C24-C23-C25	3.85	124.23	118.10
12	M	900	CDL	OB8-CB6-CB4	3.88	118.41	108.66
4	M	851	BCL	C5-C3-C2	3.90	129.08	121.10
5	L	856	BPH	CED-O2D-CGD	4.02	125.39	115.97
4	M	853	BCL	C4A-NA-C1A	4.06	111.49	106.45
5	M	855	BPH	CED-O2D-CGD	4.16	125.73	115.97
6	M	858	U10	C36-C34-C33	4.19	129.67	121.10
5	M	855	BPH	C6-C5-C3	4.27	122.33	112.66
5	L	856	BPH	C4A-NA-C1A	4.43	111.75	108.16
6	M	858	U10	C31-C32-C33	4.50	127.42	111.97
4	M	851	BCL	O2D-CGD-CBD	4.54	119.41	111.30
6	M	858	U10	C37-C38-C39	4.69	144.53	127.80
5	M	855	BPH	C4A-NA-C1A	4.95	112.17	108.16
4	M	851	BCL	O2A-CGA-CBA	4.96	126.34	111.90
5	L	856	BPH	CBC-CAC-C3C	5.19	125.28	113.51
5	L	856	BPH	C6-C5-C3	5.39	124.86	112.66
5	L	856	BPH	C1-C2-C3	5.43	135.96	125.96
5	M	855	BPH	C1-C2-C3	5.56	136.20	125.96
4	M	851	BCL	OBB-CAB-C3B	5.57	130.56	119.95
6	M	858	U10	C3M-O3-C3	5.67	136.72	116.44
6	M	858	U10	C27-C28-C29	6.04	142.84	127.68
4	L	854	BCL	O2D-CGD-CBD	6.07	122.15	111.30
4	M	853	BCL	O2D-CGD-CBD	6.08	122.16	111.30
6	L	859[A]	U10	C3M-O3-C3	6.26	138.85	116.44
13	M	867	GOL	O2-C2-C3	6.40	139.06	108.84
4	M	851	BCL	C1-C2-C3	7.41	139.61	125.96
5	L	856	BPH	O2D-CGD-CBD	7.60	124.89	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	855	BPH	O2D-CGD-CBD	7.97	125.55	111.30
13	M	867	GOL	O3-C3-C2	10.00	160.46	110.07
6	M	858	U10	C32-C33-C34	17.61	171.91	127.68

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	856	BPH	C8
5	L	856	BPH	C13
4	M	851	BCL	C8
4	M	851	BCL	C13
5	M	855	BPH	C8

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	H	862	LDA	2	0
4	L	852	BCL	1	0
4	L	854	BCL	3	0
5	L	856	BPH	5	0
6	L	859[A]	U10	8	0
7	L	865	HTO	1	0
7	L	866	HTO	1	0
4	M	851	BCL	15	0
4	M	853	BCL	7	0
5	M	855	BPH	3	0
6	M	858	U10	3	0
10	M	860	SPO	7	0
11	M	861	LDA	2	0
11	M	863	LDA	3	0
12	M	900	CDL	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, 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%)	-0.09	10 (3%) 43 38	15, 22, 46, 59	0
2	M	301/307 (98%)	-0.02	10 (3%) 47 41	13, 25, 47, 63	0
3	H	238/260 (91%)	-0.27	4 (1%) 70 67	17, 25, 38, 51	0
All	All	820/848 (96%)	-0.12	24 (2%) 52 47	13, 24, 45, 63	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	ALA	10.2
1	L	281	GLY	4.9
1	L	51	TRP	4.2
1	L	276	PRO	3.7
2	M	2	GLU	3.6
1	L	270	PRO	3.5
2	M	105	PHE	3.3
1	L	271	TRP	3.3
3	H	246	PRO	3.1
3	H	245	ALA	3.0
2	M	106	ALA	2.9
1	L	202	LYS	2.8
1	L	274	ASN	2.8
2	M	76	TYR	2.5
1	L	59	TRP	2.5
2	M	83	ALA	2.5
2	M	109	LEU	2.4
3	H	60	LYS	2.4
1	L	269	LEU	2.4
2	M	3	TYR	2.3
2	M	100	GLU	2.3
3	H	18	TYR	2.2
2	M	52	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	40	PHE	2.0

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	U10	L	859[A]	33/63	0.71	0.65	14.40	45,50,52,53	33
11	LDA	M	861	16/16	0.63	0.31	13.98	57,63,67,68	0
7	HTO	L	865	10/10	0.69	0.25	13.07	61,63,64,64	0
12	CDL	M	900	69/100	0.68	0.37	4.90	49,71,77,78	0
11	LDA	M	863	16/16	0.70	0.27	4.90	70,70,74,74	0
11	LDA	H	862	16/16	0.75	0.22	4.67	61,62,66,67	0
6	U10	M	858	48/63	0.89	0.19	2.88	16,29,61,63	0
4	BCL	M	851	66/66	0.91	0.16	2.51	17,22,66,68	0
10	SPO	M	860	42/42	0.75	0.19	2.44	25,32,50,52	0
4	BCL	M	853	66/66	0.92	0.14	2.20	13,18,38,44	0
4	BCL	L	852	66/66	0.93	0.12	1.48	15,17,29,32	0
9	PO4	M	864	5/5	0.89	0.17	1.38	72,73,73,73	0
5	BPH	L	856	65/65	0.92	0.13	1.33	13,17,33,36	0
4	BCL	L	854	66/66	0.93	0.12	1.12	12,17,40,44	0
5	BPH	M	855	55/65	0.93	0.13	0.96	19,22,63,66	0
8	FE2	M	857	1/1	0.98	0.09	-4.56	14,14,14,14	0
7	HTO	L	866	10/10	0.58	0.35	-	66,68,69,69	0
13	GOL	M	867	6/6	0.86	0.20	-	51,55,56,58	0

6.5 Other polymers ⓘ

There are no such residues in this entry.