



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:46 PM GMT

PDB ID : 1JGW
Title : Photosynthetic Reaction Center Mutant With Thr M 21 Replaced With Leu
Authors : Camara-Artigas, A.; Magee, C.L.; Williams, J.C.; Allen, J.P.
Deposited on : 2001-06-27
Resolution : 2.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

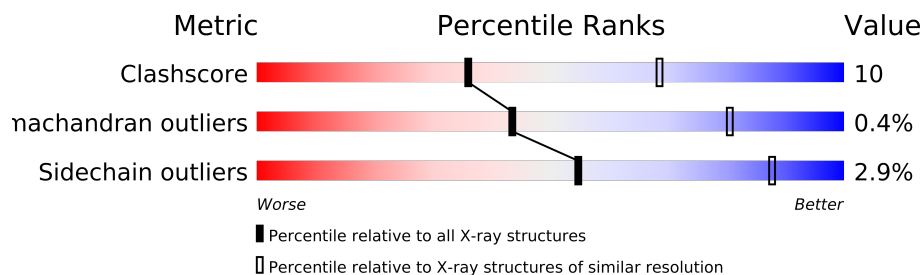
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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))
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	281	
2	M	307	
3	H	260	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 7120 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called Photosynthetic Reaction Center L subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	281	Total	C	N	O	S	0	0	0
			2232	1507	355	362	8			

- Molecule 2 is a protein called Photosynthetic Reaction Center M subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	0	0
			2409	1609	394	396	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	21	LEU	THR	ENGINEERED	UNP P02953

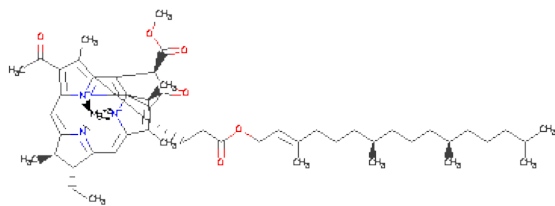
- Molecule 3 is a protein called Photosynthetic Reaction Center H subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	236	Total	C	N	O	S	0	0	0
			1794	1148	305	332	9			

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

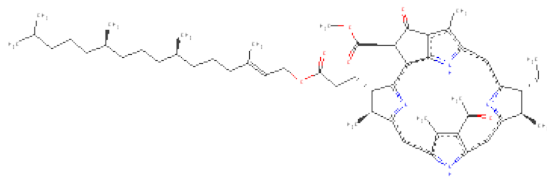
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	1	Total	Fe	0	0
			1	1		

- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



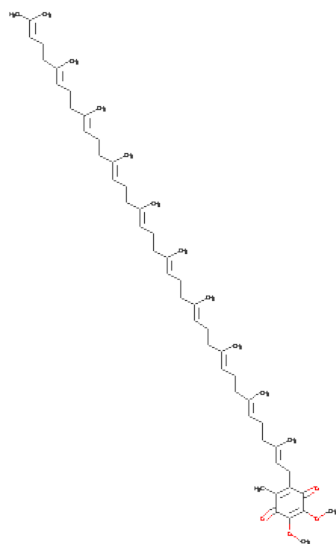
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 6 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



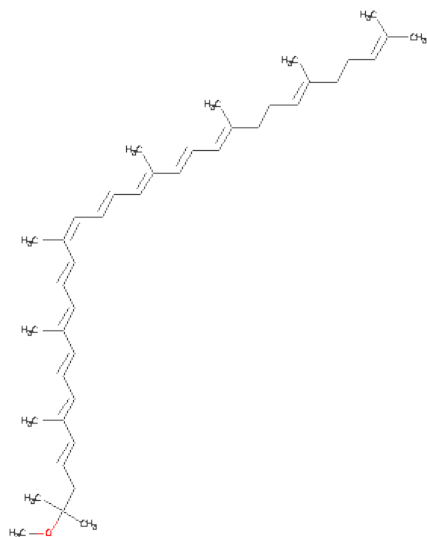
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	M	1	Total	C	N	O	0	0
			65	55	4	6		
6	L	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 7 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



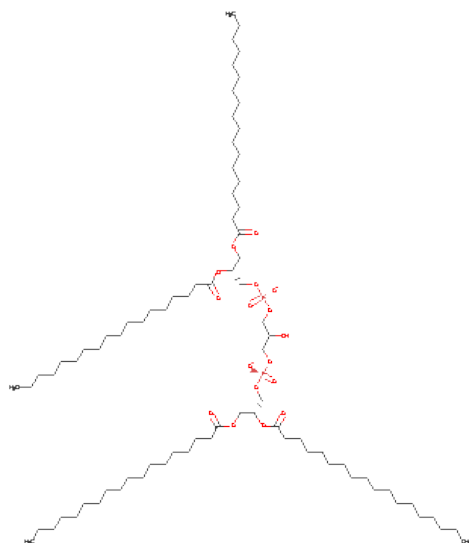
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 8 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).



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

- Molecule 9 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- Molecule 10 is water.

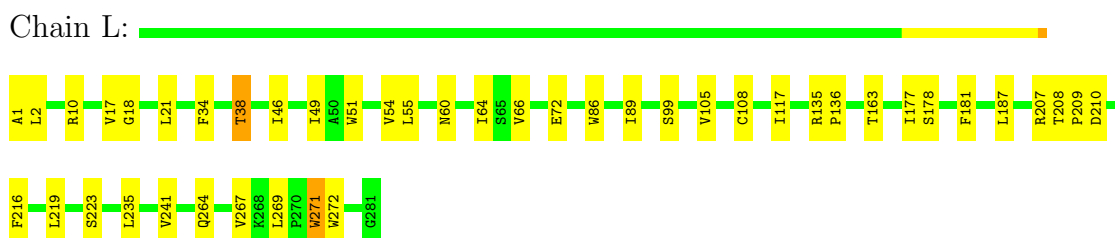
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	H	53	Total	O	0	0
			53	53		
10	L	33	Total	O	0	0
			33	33		
10	M	33	Total	O	0	0
			33	33		

3 Residue-property plots

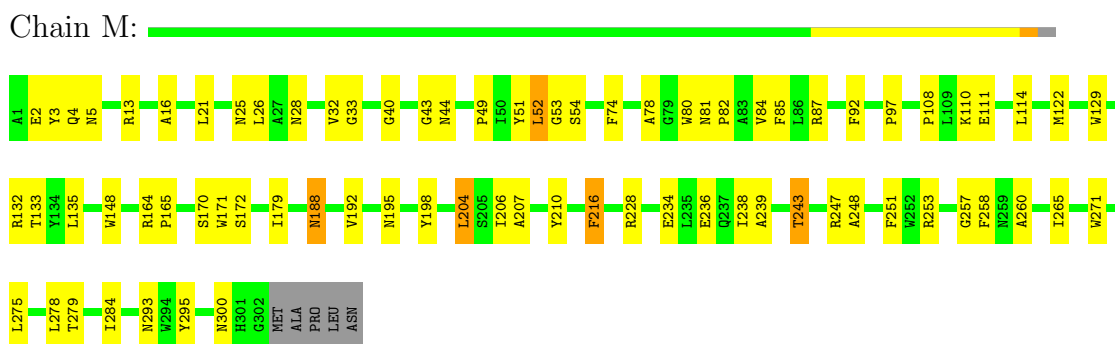
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

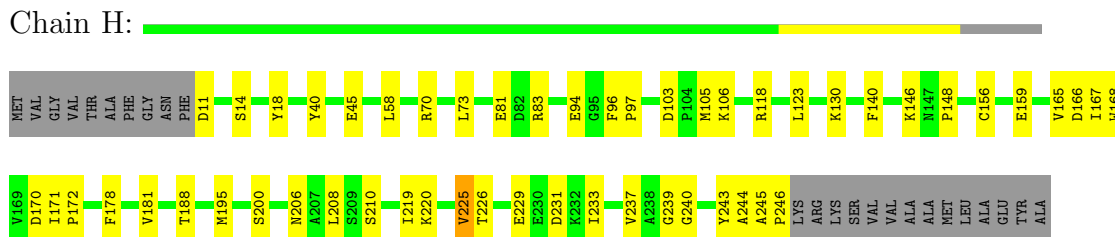
- Molecule 1: Photosynthetic Reaction Center L subunit



- Molecule 2: Photosynthetic Reaction Center M subunit



- Molecule 3: Photosynthetic Reaction Center H subunit



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.60Å 142.60Å 187.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.23 – 2.80	Depositor
% Data completeness (in resolution range)	94.4 (29.23-2.80)	Depositor
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.211 , 0.237	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7120	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, CDL, BPH, FE, 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	0.41	0/2320	0.57	0/3175
2	M	0.40	0/2501	0.56	0/3414
3	H	0.36	0/1842	0.62	0/2509
All	All	0.40	0/6663	0.58	0/9098

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2232	0	2187	41	0
2	M	2409	0	2325	73	0
3	H	1794	0	1792	33	0
4	M	1	0	0	0	0
5	L	132	0	148	9	0
5	M	132	0	148	10	0
6	L	65	0	76	6	0
6	M	65	0	76	5	0
7	M	48	0	63	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	M	42	0	60	1	0
9	M	81	0	106	2	0
10	H	53	0	0	1	0
10	L	33	0	0	1	0
10	M	33	0	0	2	0
All	All	7120	0	6981	145	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (145) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:M:25:ASN:HD22	2:M:28:ASN:ND2	1.68	0.91
2:M:204:LEU:HB3	2:M:279:THR:HG21	1.54	0.88
2:M:243:THR:CG2	2:M:247:ARG:HE	1.85	0.88
1:L:219:LEU:HA	2:M:132:ARG:HH12	1.39	0.87
2:M:243:THR:HG22	2:M:247:ARG:HE	1.43	0.84
1:L:34:PHE:O	1:L:38:THR:HG23	1.79	0.83
1:L:241:VAL:HG21	6:L:855:BPH:HAC2	1.64	0.78
2:M:108:PRO:HG2	2:M:111:GLU:HG3	1.68	0.76
6:L:855:BPH:HBB2	2:M:210:TYR:HB3	1.69	0.75
1:L:219:LEU:HD12	2:M:132:ARG:NH1	2.03	0.74
2:M:188:ASN:HB3	10:M:1020:HOH:O	1.89	0.72
2:M:228:ARG:NE	3:H:195:MET:HE3	2.06	0.70
2:M:16:ALA:HB1	2:M:32:VAL:HG21	1.75	0.69
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.75	0.69
2:M:108:PRO:HG2	2:M:111:GLU:CG	2.24	0.68
2:M:97:PRO:HA	2:M:111:GLU:O	1.93	0.68
2:M:243:THR:HG21	2:M:247:ARG:HE	1.61	0.66
1:L:219:LEU:HD12	2:M:132:ARG:HH11	1.61	0.65
1:L:46:ILE:HG12	5:M:853:BCL:H191	1.80	0.64
3:H:168:TRP:HB2	3:H:178:PHE:HB2	1.78	0.63
1:L:219:LEU:CA	2:M:132:ARG:HH12	2.12	0.62
3:H:81:GLU:O	3:H:83:ARG:HG2	2.00	0.62
1:L:269:LEU:HD13	1:L:271:TRP:CH2	2.34	0.62
1:L:271:TRP:N	1:L:271:TRP:CD1	2.65	0.61
2:M:32:VAL:HG12	2:M:33:GLY:O	2.01	0.61
1:L:219:LEU:HA	2:M:132:ARG:NH1	2.13	0.60
2:M:243:THR:O	2:M:247:ARG:HG3	2.01	0.60
1:L:219:LEU:HD11	2:M:133:THR:HG22	1.83	0.59
5:L:850:BCL:H2	6:M:854:BPH:HMB2	1.84	0.59
1:L:181:PHE:HB3	6:M:854:BPH:CBB	2.34	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:H:208:LEU:HD11	3:H:237:VAL:HG22	1.86	0.57
3:H:103:ASP:HB3	3:H:106:LYS:HB2	1.86	0.57
3:H:243:TYR:O	3:H:246:PRO:HD2	2.05	0.56
1:L:264:GLN:HA	1:L:267:VAL:HG12	1.88	0.56
6:L:855:BPH:H102	5:M:853:BCL:H193	1.89	0.55
1:L:38:THR:HG22	1:L:99:SER:CB	2.37	0.55
3:H:226:THR:OG1	3:H:229:GLU:HG3	2.07	0.55
1:L:38:THR:HG22	1:L:99:SER:HB3	1.89	0.55
2:M:108:PRO:HG2	2:M:111:GLU:HB2	1.89	0.54
2:M:13:ARG:O	3:H:140:PHE:HA	2.06	0.54
2:M:275:LEU:HD23	2:M:278:LEU:HD23	1.89	0.54
2:M:108:PRO:CG	2:M:111:GLU:HG3	2.36	0.54
3:H:103:ASP:CG	3:H:106:LYS:HD3	2.28	0.54
1:L:34:PHE:O	1:L:38:THR:CG2	2.55	0.53
5:M:852:BCL:HBB3	5:M:853:BCL:HMD2	1.89	0.53
1:L:2:LEU:HD21	1:L:10:ARG:CZ	2.39	0.53
2:M:228:ARG:CZ	3:H:195:MET:HE3	2.38	0.53
1:L:60:ASN:O	1:L:64:ILE:HG13	2.08	0.53
2:M:122:MET:HE1	8:M:859:SPO:H25	1.90	0.53
2:M:81:ASN:HB3	2:M:84:VAL:HB	1.90	0.53
3:H:245:ALA:HB3	3:H:246:PRO:HD3	1.91	0.52
1:L:187:LEU:HD13	2:M:216:PHE:CG	2.44	0.52
1:L:181:PHE:HB3	6:M:854:BPH:HBB2	1.91	0.52
3:H:240:GLY:O	3:H:244:ALA:HB3	2.09	0.52
1:L:181:PHE:CD2	6:M:854:BPH:HBB1	2.45	0.52
2:M:16:ALA:CB	2:M:32:VAL:HG21	2.39	0.52
3:H:130:LYS:HE3	3:H:170:ASP:OD2	2.11	0.51
6:L:855:BPH:HH3	6:L:855:BPH:HBB3	1.92	0.51
2:M:293:ASN:OD1	2:M:295:TYR:HB3	2.10	0.51
2:M:260:ALA:HB2	7:M:857:U10:H103	1.93	0.51
2:M:78:ALA:HB2	2:M:92:PHE:CZ	2.46	0.51
2:M:265:ILE:HG21	7:M:857:U10:H3M2	1.93	0.50
1:L:18:GLY:O	1:L:21:LEU:HD23	2.11	0.50
3:H:245:ALA:N	3:H:246:PRO:CD	2.74	0.50
2:M:236:GLU:OE2	3:H:118:ARG:NH2	2.37	0.50
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.93	0.49
2:M:40:GLY:HA2	2:M:43:GLY:O	2.12	0.49
5:L:850:BCL:HMD2	5:L:851:BCL:HBB3	1.95	0.49
1:L:117:ILE:HD13	2:M:251:PHE:CE1	2.47	0.49
2:M:271:TRP:CZ2	9:M:5000:CDL:H722	2.48	0.48
5:M:853:BCL:HBD	5:M:853:BCL:HAA2	1.95	0.48
3:H:94:GLU:CD	3:H:94:GLU:H	2.15	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:208:THR:HB	1:L:209:PRO:HD2	1.95	0.48
3:H:165:VAL:O	3:H:166:ASP:HB2	2.13	0.48
1:L:105:VAL:O	1:L:108:CYS:HB2	2.14	0.47
2:M:239:ALA:O	3:H:73:LEU:HD22	2.14	0.47
2:M:108:PRO:HG2	2:M:111:GLU:CB	2.45	0.47
2:M:243:THR:HG22	2:M:247:ARG:HG3	1.97	0.47
2:M:52:LEU:HA	2:M:52:LEU:HD12	1.61	0.47
5:L:850:BCL:HBB2	5:M:852:BCL:H111	1.97	0.46
10:L:1075:HOH:O	2:M:49:PRO:HG2	2.14	0.46
3:H:70:ARG:NH2	3:H:123:LEU:HG	2.31	0.46
2:M:80:TRP:O	2:M:82:PRO:HD3	2.14	0.46
2:M:243:THR:HG22	2:M:247:ARG:NE	2.22	0.46
2:M:284:ILE:HG12	5:M:852:BCL:HED3	1.97	0.46
3:H:105:MET:HE3	3:H:239:GLY:C	2.35	0.46
2:M:206:ILE:HG23	5:M:852:BCL:HMB3	1.98	0.46
2:M:293:ASN:HB2	10:M:1023:HOH:O	2.15	0.46
3:H:148:PRO:HD2	3:H:167:ILE:HD11	1.97	0.46
3:H:181:VAL:O	3:H:188:THR:HA	2.16	0.46
3:H:45:GLU:HG3	10:H:1066:HOH:O	2.15	0.46
3:H:159:GLU:HB3	3:H:210:SER:HB3	1.98	0.45
1:L:17:VAL:HG12	1:L:18:GLY:N	2.32	0.45
6:M:854:BPH:HMB1	6:M:854:BPH:HHB	1.80	0.45
2:M:234:GLU:O	2:M:238:ILE:HG13	2.17	0.45
3:H:171:ILE:HB	3:H:172:PRO:CD	2.46	0.45
2:M:51:TYR:O	2:M:132:ARG:NH2	2.49	0.45
1:L:178:SER:OG	5:L:850:BCL:HBA1	2.17	0.45
2:M:248:ALA:HB3	7:M:857:U10:H4M2	1.99	0.45
2:M:52:LEU:HB3	2:M:53:GLY:H	1.63	0.45
7:M:857:U10:H222	7:M:857:U10:H201	1.64	0.44
2:M:195:ASN:HB3	2:M:198:TYR:CD2	2.52	0.44
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.52	0.44
2:M:3:TYR:CZ	2:M:5:ASN:HA	2.52	0.44
2:M:207:ALA:HB1	5:M:853:BCL:O1A	2.17	0.44
1:L:267:VAL:HG23	2:M:87:ARG:HD2	2.00	0.44
2:M:192:VAL:CG1	2:M:192:VAL:O	2.65	0.44
3:H:40:TYR:HB3	3:H:58:LEU:HD21	2.00	0.43
1:L:2:LEU:CD2	1:L:10:ARG:CZ	2.96	0.43
3:H:146:LYS:HE2	3:H:200:SER:O	2.18	0.43
5:L:850:BCL:HAA2	5:L:850:BCL:HBD	2.00	0.43
1:L:51:TRP:O	1:L:54:VAL:HG22	2.17	0.43
2:M:170:SER:C	2:M:172:SER:H	2.21	0.43
2:M:97:PRO:HG2	2:M:171:TRP:HB2	2.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:M:21:LEU:HD22	2:M:26:LEU:HD21	2.01	0.43
3:H:11:ASP:OD1	3:H:14:SER:HB2	2.17	0.43
2:M:2:GLU:HG3	2:M:4:GLN:NE2	2.34	0.43
1:L:219:LEU:O	2:M:132:ARG:NH1	2.52	0.42
1:L:54:VAL:HG23	1:L:55:LEU:N	2.33	0.42
5:L:851:BCL:H122	6:L:855:BPH:H3A	1.99	0.42
3:H:96:PHE:HB3	3:H:97:PRO:CD	2.49	0.42
2:M:148:TRP:CE2	9:M:5000:CDL:H511	2.54	0.42
1:L:163:THR:HG22	1:L:163:THR:O	2.17	0.42
1:L:66:VAL:HG12	1:L:86:TRP:HB2	2.01	0.42
1:L:177:ILE:HG12	5:L:851:BCL:HMB3	2.01	0.42
3:H:229:GLU:O	3:H:233:ILE:HG13	2.20	0.42
3:H:156:CYS:HB3	3:H:206:ASN:O	2.19	0.42
1:L:1:ALA:O	1:L:2:LEU:HD23	2.20	0.41
2:M:129:TRP:O	2:M:132:ARG:HB3	2.19	0.41
1:L:17:VAL:CG1	1:L:18:GLY:N	2.83	0.41
1:L:267:VAL:HG23	2:M:87:ARG:CD	2.51	0.41
3:H:14:SER:O	3:H:18:TYR:CD2	2.74	0.41
5:L:851:BCL:HAA2	5:L:851:BCL:HBD	2.02	0.41
2:M:21:LEU:HD22	2:M:26:LEU:CD2	2.50	0.41
6:L:855:BPH:HHB	6:L:855:BPH:HMB1	1.81	0.41
5:L:850:BCL:H92	5:M:852:BCL:H202	2.03	0.41
2:M:114:LEU:HA	2:M:114:LEU:HD12	1.87	0.41
5:M:852:BCL:HBD	5:M:852:BCL:HAA2	2.03	0.40
2:M:195:ASN:HB3	2:M:198:TYR:HD2	1.86	0.40
1:L:49:ILE:HG12	1:L:89:ILE:HD13	2.03	0.40
2:M:74:PHE:HB3	2:M:85:PHE:CE1	2.57	0.40
2:M:28:ASN:HB2	2:M:51:TYR:CE1	2.57	0.40
3:H:219:ILE:HG21	3:H:225:VAL:CG1	2.52	0.40
2:M:253:ARG:O	2:M:257:GLY:HA2	2.22	0.40
1:L:223:SER:O	2:M:44:ASN: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	L	279/281 (99%)	265 (95%)	14 (5%)	0	100	100
2	M	300/307 (98%)	278 (93%)	19 (6%)	3 (1%)	22	60
3	H	234/260 (90%)	227 (97%)	7 (3%)	0	100	100
All	All	813/848 (96%)	770 (95%)	40 (5%)	3 (0%)	43	80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	179	ILE
2	M	54	SER
2	M	110	LYS

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	220/220 (100%)	212 (96%)	8 (4%)	47	82
2	M	236/240 (98%)	228 (97%)	8 (3%)	49	84
3	H	191/208 (92%)	188 (98%)	3 (2%)	75	96
All	All	647/668 (97%)	628 (97%)	19 (3%)	55	88

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	38	THR
1	L	72	GLU
1	L	207	ARG
1	L	210	ASP
1	L	216	PHE
1	L	235	LEU
1	L	271	TRP
1	L	272	TRP
2	M	52	LEU
2	M	135	LEU
2	M	188	ASN
2	M	204	LEU

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Mol	Chain	Res	Type
2	M	216	PHE
2	M	243	THR
2	M	258	PHE
2	M	300	ASN
3	H	220	LYS
3	H	225	VAL
3	H	231	ASP

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

Mol	Chain	Res	Type
2	M	4	GLN
2	M	28	ASN
2	M	299	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 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
5	BCL	L	850	2	74,74,74	1.46	15 (20%)	97,115,115	2.03	25 (25%)
5	BCL	L	851	1	74,74,74	1.45	11 (14%)	97,115,115	1.89	23 (23%)
6	BPH	L	855	-	70,70,70	1.41	9 (12%)	94,101,101	2.07	23 (24%)
9	CDL	M	5000	-	80,80,99	1.28	5 (6%)	92,92,111	1.04	6 (6%)
5	BCL	M	852	2	74,74,74	1.49	11 (14%)	97,115,115	1.95	23 (23%)
5	BCL	M	853	1	74,74,74	1.48	13 (17%)	97,115,115	2.15	27 (27%)
6	BPH	M	854	-	70,70,70	1.53	8 (11%)	94,101,101	1.99	21 (22%)
7	U10	M	857	-	48,48,63	2.25	15 (31%)	59,61,79	2.45	24 (40%)
8	SPO	M	859	-	41,41,41	3.50	27 (65%)	50,50,50	2.87	16 (32%)

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
5	BCL	L	850	2	-	0/41/137/137	0/0/9/9
5	BCL	L	851	1	-	0/41/137/137	0/0/9/9
6	BPH	L	855	-	2/2/18/22	0/49/105/105	0/0/6/6
9	CDL	M	5000	-	1/1/9/9	0/91/91/110	0/0/0/0
5	BCL	M	852	2	-	0/41/137/137	0/0/9/9
5	BCL	M	853	1	-	0/41/137/137	0/0/9/9
6	BPH	M	854	-	2/2/18/22	0/49/105/105	0/0/6/6
7	U10	M	857	-	-	0/45/69/87	0/1/1/1
8	SPO	M	859	-	-	0/47/47/47	0/0/0/0

All (114) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	859	SPO	C15-C16	9.02	1.58	1.34
7	M	857	U10	C6-C1	7.05	1.52	1.35
6	M	854	BPH	C1D-CHD	6.93	1.43	1.35
8	M	859	SPO	C10-C11	6.79	1.52	1.34
9	M	5000	CDL	C43-C42	-6.53	1.52	1.55
8	M	859	SPO	C6-C5	6.46	1.50	1.31
8	M	859	SPO	C27-C28	5.94	1.40	1.34
8	M	859	SPO	C21-C20	5.53	1.50	1.35
6	L	855	BPH	C1D-CHD	5.49	1.41	1.35
8	M	859	SPO	C13-C12	5.19	1.60	1.51
9	M	5000	CDL	C58-C57	-5.16	1.53	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	859	SPO	C26-C25	5.09	1.48	1.34
6	L	855	BPH	C3B-C4B	4.94	1.47	1.40
5	L	851	BCL	C1A-NA	4.80	1.42	1.32
5	M	853	BCL	C2-C3	4.73	1.42	1.32
6	M	854	BPH	C3B-C4B	4.62	1.47	1.40
9	M	5000	CDL	C84-C83	-4.46	1.53	1.55
5	M	853	BCL	C1A-NA	4.44	1.42	1.32
9	M	5000	CDL	C24-C23	-4.42	1.53	1.55
5	M	852	BCL	C1A-NA	4.41	1.42	1.32
8	M	859	SPO	C32-C33	4.30	1.41	1.32
5	M	852	BCL	C2-C3	4.27	1.41	1.32
5	L	850	BCL	C2-C3	4.26	1.41	1.32
8	M	859	SPO	C14-C12	4.16	1.41	1.35
7	M	857	U10	C28-C29	4.16	1.41	1.32
5	M	853	BCL	C3B-C4B	4.02	1.46	1.40
8	M	859	SPO	C15-C14	4.00	1.55	1.43
8	M	859	SPO	O1-CM1	4.00	1.56	1.43
7	M	857	U10	C4-C3	3.99	1.53	1.35
5	L	850	BCL	C3B-C4B	3.93	1.46	1.40
7	M	857	U10	C18-C19	3.90	1.40	1.32
7	M	857	U10	C7-C6	3.85	1.58	1.51
5	L	850	BCL	C1A-NA	3.77	1.40	1.32
5	L	851	BCL	C3B-C4B	3.77	1.46	1.40
5	M	852	BCL	C3B-C4B	3.68	1.45	1.40
5	M	852	BCL	C4C-NC	3.66	1.40	1.32
7	M	857	U10	C7-C8	-3.66	1.44	1.50
7	M	857	U10	C33-C34	3.64	1.40	1.32
6	M	854	BPH	C2-C3	3.56	1.40	1.32
5	L	851	BCL	C2-C3	3.56	1.40	1.32
7	M	857	U10	C13-C14	3.54	1.40	1.32
8	M	859	SPO	C19-C17	3.49	1.40	1.35
7	M	857	U10	C6-C5	3.43	1.56	1.46
8	M	859	SPO	C8-C7	3.40	1.56	1.51
8	M	859	SPO	C4-C5	-3.37	1.44	1.50
8	M	859	SPO	C31-C32	-3.34	1.40	1.50
8	M	859	SPO	C11-C12	-3.30	1.38	1.45
5	L	851	BCL	C3D-C2D	3.24	1.50	1.40
5	L	850	BCL	C4C-NC	3.22	1.39	1.32
5	M	852	BCL	C3D-CAD	-3.22	1.40	1.47
5	L	851	BCL	C4C-NC	3.20	1.39	1.32
6	L	855	BPH	C2-C3	3.20	1.39	1.32
6	L	855	BPH	C3D-CAD	-3.19	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	857	U10	C23-C24	3.18	1.39	1.32
6	M	854	BPH	CMB-C2B	3.11	1.58	1.51
7	M	857	U10	C38-C39	2.98	1.40	1.34
8	M	859	SPO	C10-C9	2.92	1.52	1.43
5	L	850	BCL	CMB-C2B	2.92	1.57	1.51
5	L	850	BCL	C3D-C2D	2.92	1.49	1.40
5	L	851	BCL	C4B-NB	2.88	1.38	1.34
5	M	852	BCL	C3B-C2B	2.88	1.49	1.40
5	L	851	BCL	CMB-C2B	2.87	1.57	1.51
6	M	854	BPH	C3D-CAD	-2.85	1.41	1.47
8	M	859	SPO	C37-C38	2.84	1.41	1.32
8	M	859	SPO	O1-C1	2.84	1.59	1.41
5	M	852	BCL	C3D-C2D	2.79	1.48	1.40
5	M	852	BCL	C3B-CAB	2.79	1.56	1.49
8	M	859	SPO	C24-C23	2.79	1.55	1.51
6	L	855	BPH	CMB-C2B	2.76	1.57	1.51
5	L	850	BCL	C3B-CAB	2.73	1.56	1.49
5	M	852	BCL	CMB-C2B	2.68	1.57	1.51
8	M	859	SPO	C35-C33	2.67	1.57	1.51
5	M	852	BCL	C3C-C4C	-2.65	1.48	1.51
5	L	850	BCL	OBD-CAD	2.62	1.26	1.22
5	L	850	BCL	CAA-C2A	2.61	1.58	1.54
5	L	850	BCL	C4B-NB	2.60	1.37	1.34
5	M	853	BCL	C3D-C2D	2.60	1.48	1.40
5	L	851	BCL	C3B-C2B	2.60	1.48	1.40
5	L	851	BCL	C3D-CAD	-2.55	1.42	1.47
5	M	853	BCL	C3B-CAB	2.54	1.56	1.49
5	M	853	BCL	OBD-CAD	2.54	1.26	1.22
5	M	853	BCL	C4C-NC	2.52	1.37	1.32
6	M	854	BPH	C3D-C2D	2.52	1.48	1.40
7	M	857	U10	O4-C4	2.51	1.43	1.36
5	M	852	BCL	C4B-NB	2.50	1.37	1.34
5	M	853	BCL	C4B-NB	2.50	1.37	1.34
5	M	853	BCL	CMB-C2B	2.49	1.56	1.51
5	M	853	BCL	C3B-C2B	2.49	1.47	1.40
8	M	859	SPO	C22-C23	2.48	1.39	1.35
5	M	853	BCL	C3C-C4C	-2.45	1.48	1.51
7	M	857	U10	C8-C9	2.43	1.37	1.32
5	L	850	BCL	C3B-C2B	2.41	1.47	1.40
8	M	859	SPO	C29-C28	2.41	1.56	1.50
5	L	851	BCL	C3B-CAB	2.40	1.55	1.49
6	L	855	BPH	O2A-CGA	-2.37	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	859	SPO	C25-C23	-2.35	1.40	1.45
9	M	5000	CDL	CB3-CB4	2.32	1.57	1.50
8	M	859	SPO	C18-C17	2.30	1.55	1.51
5	L	850	BCL	C3A-C2A	-2.28	1.47	1.54
7	M	857	U10	C41-C39	2.26	1.52	1.40
5	L	850	BCL	O2D-CGD	-2.23	1.27	1.33
6	M	854	BPH	C3A-C2A	-2.16	1.48	1.54
8	M	859	SPO	C26-C27	2.15	1.50	1.43
5	L	850	BCL	C3D-CAD	-2.14	1.43	1.47
8	M	859	SPO	C6-C7	-2.14	1.41	1.45
5	L	850	BCL	CBB-CAB	2.14	1.56	1.49
6	L	855	BPH	C3A-C2A	-2.14	1.48	1.54
5	M	853	BCL	C3D-CAD	-2.10	1.43	1.47
6	L	855	BPH	OBD-CAD	2.10	1.25	1.22
7	M	857	U10	C22-C23	-2.05	1.44	1.50
6	M	854	BPH	C1B-CHB	-2.05	1.38	1.46
6	L	855	BPH	C3D-C2D	2.04	1.46	1.40
5	M	853	BCL	MG-NB	2.03	2.09	2.05
5	L	851	BCL	C1B-C2B	2.01	1.42	1.40

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	859	SPO	C25-C23-C22	-10.99	102.09	118.97
5	M	853	BCL	CAA-C2A-C1A	-7.79	92.18	111.62
8	M	859	SPO	C26-C27-C28	-6.93	121.28	127.91
6	L	855	BPH	C4B-C3B-C2B	-6.86	102.62	107.60
5	M	853	BCL	CMB-C2B-C1B	-6.60	118.47	128.62
5	L	850	BCL	CMB-C2B-C1B	-6.57	118.52	128.62
5	M	852	BCL	CMB-C2B-C1B	-6.54	118.56	128.62
6	M	854	BPH	C4B-C3B-C2B	-6.49	102.89	107.60
5	L	850	BCL	CAA-C2A-C1A	-6.46	95.50	111.62
6	L	855	BPH	C4-C3-C5	6.44	125.19	115.39
5	M	853	BCL	C4D-C3D-C2D	-6.34	99.67	107.42
5	L	851	BCL	CMB-C2B-C1B	-6.26	118.99	128.62
7	M	857	U10	C7-C6-C5	6.18	125.47	118.75
5	L	850	BCL	C4D-C3D-C2D	-6.16	99.89	107.42
8	M	859	SPO	C18-C17-C19	-5.94	114.48	122.92
7	M	857	U10	C15-C14-C13	-5.73	112.17	123.52
6	L	855	BPH	CMB-C2B-C1B	-5.69	119.98	128.65
5	M	853	BCL	CMB-C2B-C3B	5.67	133.89	124.97
7	M	857	U10	C10-C9-C8	-5.62	112.39	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	852	BCL	CMB-C2B-C3B	5.60	133.79	124.97
5	L	850	BCL	CMB-C2B-C3B	5.58	133.77	124.97
6	M	854	BPH	CMB-C2B-C1B	-5.58	120.16	128.65
5	M	852	BCL	C4D-C3D-C2D	-5.55	100.64	107.42
5	L	851	BCL	C4D-C3D-C2D	-5.50	100.70	107.42
6	L	855	BPH	C6-C5-C3	5.49	125.83	112.78
6	M	854	BPH	CMB-C2B-C3B	5.40	133.48	124.97
7	M	857	U10	C15-C14-C16	5.40	123.60	115.39
5	L	851	BCL	CMB-C2B-C3B	5.36	133.41	124.97
6	M	854	BPH	C1-O2A-CGA	5.12	131.33	116.98
6	L	855	BPH	CMB-C2B-C3B	5.08	132.96	124.97
6	L	855	BPH	C1-O2A-CGA	5.03	131.07	116.98
8	M	859	SPO	C24-C23-C22	-5.03	115.78	122.92
8	M	859	SPO	C20-C21-C22	-4.75	112.84	123.36
5	M	853	BCL	C4B-C3B-C2B	-4.72	101.26	106.97
6	L	855	BPH	C4D-C3D-C2D	-4.67	101.72	107.37
7	M	857	U10	C25-C24-C23	-4.66	114.29	123.52
6	M	854	BPH	O2A-C1-C2	-4.60	98.58	108.55
6	M	854	BPH	C4-C3-C5	4.55	122.31	115.39
5	M	852	BCL	C4B-C3B-C2B	-4.54	101.47	106.97
5	L	850	BCL	C4B-C3B-C2B	-4.51	101.52	106.97
6	M	854	BPH	C4D-C3D-C2D	-4.51	101.92	107.37
5	M	853	BCL	CHC-C4B-NB	-4.41	117.21	124.58
5	M	852	BCL	C6-C5-C3	4.40	123.24	112.78
7	M	857	U10	C7-C8-C9	4.34	134.09	126.76
5	L	851	BCL	C2A-C3A-C4A	4.31	108.03	101.40
5	L	851	BCL	C4B-C3B-C2B	-4.28	101.80	106.97
6	M	854	BPH	C3B-C4B-NB	4.26	111.91	107.10
8	M	859	SPO	C15-C14-C12	-4.24	121.18	127.29
5	L	850	BCL	CHC-C4B-NB	-4.24	117.50	124.58
8	M	859	SPO	C4-C5-C6	-4.23	117.95	124.95
5	M	852	BCL	CHC-C4B-NB	-4.22	117.53	124.58
5	M	852	BCL	CED-O2D-CGD	4.22	126.06	116.02
6	L	855	BPH	C5-C3-C2	-4.22	112.97	121.08
9	M	5000	CDL	OB8-CB6-CB4	4.14	119.68	108.83
5	M	853	BCL	C3B-C4B-NB	4.10	112.63	108.64
6	L	855	BPH	C3B-C4B-NB	4.06	111.69	107.10
7	M	857	U10	C35-C34-C33	-4.06	115.48	123.52
5	L	851	BCL	CHC-C4B-NB	-4.04	117.83	124.58
7	M	857	U10	C11-C9-C8	3.93	128.66	121.08
5	M	852	BCL	C3B-C4B-NB	3.90	112.44	108.64
8	M	859	SPO	C8-C7-C9	3.87	128.41	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	851	BCL	CED-O2D-CGD	3.86	125.20	116.02
5	M	853	BCL	C2A-C3A-C4A	3.77	107.20	101.40
5	L	851	BCL	C3B-C4B-NB	3.75	112.29	108.64
7	M	857	U10	C20-C19-C18	-3.72	116.16	123.52
5	M	852	BCL	C2A-C3A-C4A	3.70	107.09	101.40
5	L	851	BCL	OBD-CAD-C3D	-3.68	121.06	127.91
6	M	854	BPH	C4B-CHC-C1C	3.68	139.30	127.62
8	M	859	SPO	C2-C1-C4	-3.60	105.03	110.97
5	L	850	BCL	C3B-C4B-NB	3.56	112.10	108.64
5	L	851	BCL	CGD-CBD-CHA	3.53	122.97	110.96
5	M	853	BCL	CAC-C3C-C2C	-3.50	105.86	113.89
6	L	855	BPH	C4B-CHC-C1C	3.46	138.59	127.62
8	M	859	SPO	C11-C12-C14	-3.45	113.66	118.97
5	M	853	BCL	CED-O2D-CGD	3.40	124.12	116.02
5	L	850	BCL	C2A-C3A-C4A	3.40	106.62	101.40
6	M	854	BPH	O1D-CGD-CBD	-3.39	117.48	124.42
5	M	852	BCL	CHA-C1A-NA	-3.37	119.30	126.22
5	L	850	BCL	O2A-C1-C2	-3.35	101.28	108.55
5	M	852	BCL	OBD-CAD-C3D	-3.35	121.68	127.91
5	M	853	BCL	OBD-CAD-C3D	-3.28	121.81	127.91
5	L	850	BCL	CBA-CAA-C2A	3.27	123.71	114.01
6	M	854	BPH	O2D-CGD-CBD	3.27	117.98	111.33
5	M	853	BCL	CBA-CAA-C2A	3.21	123.54	114.01
5	L	850	BCL	OBD-CAD-C3D	-3.21	121.94	127.91
5	L	850	BCL	C6-C5-C3	3.15	120.26	112.78
7	M	857	U10	C4M-O4-C4	3.14	127.14	116.48
5	L	851	BCL	CHA-C1A-NA	-3.12	119.82	126.22
8	M	859	SPO	C15-C16-C17	-3.07	117.61	126.38
6	L	855	BPH	O1D-CGD-CBD	-3.02	118.24	124.42
7	M	857	U10	C25-C24-C26	2.99	119.93	115.39
5	L	850	BCL	CED-O2D-CGD	2.96	123.06	116.02
6	M	854	BPH	C3D-CAD-CBD	2.95	111.77	107.60
5	M	853	BCL	C2C-C3C-C4C	2.93	105.11	101.05
7	M	857	U10	C21-C19-C18	2.83	126.52	121.08
5	L	851	BCL	C6-C5-C3	2.77	119.36	112.78
5	M	853	BCL	O2A-CGA-CBA	2.76	120.63	111.94
5	L	851	BCL	C2A-C1A-CHA	2.76	128.61	123.83
6	M	854	BPH	C3C-C4C-CHD	2.75	127.56	121.83
8	M	859	SPO	C18-C17-C16	2.72	122.48	118.09
5	M	852	BCL	C4B-CHC-C1C	2.69	135.68	130.06
6	L	855	BPH	O2D-CGD-CBD	2.69	116.82	111.33
7	M	857	U10	C35-C34-C36	2.69	119.47	115.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	5000	CDL	CB6-CB4-CB3	-2.67	105.77	111.86
7	M	857	U10	C30-C29-C31	2.66	119.43	115.39
8	M	859	SPO	C16-C17-C19	2.65	123.03	118.97
5	L	850	BCL	CHA-C1A-NA	-2.63	120.81	126.22
5	M	852	BCL	C2A-C1A-CHA	2.62	128.37	123.83
6	M	854	BPH	C6-C5-C3	2.61	118.99	112.78
5	L	850	BCL	C2B-C1B-NB	2.61	111.38	109.41
5	M	852	BCL	C15-C13-C12	-2.60	98.51	111.92
9	M	5000	CDL	OB4-PB2-OB3	-2.58	110.94	118.72
7	M	857	U10	O5-C5-C4	-2.58	115.25	120.96
7	M	857	U10	C7-C6-C1	-2.56	117.07	123.35
5	L	850	BCL	C2C-C3C-C4C	2.56	104.59	101.05
9	M	5000	CDL	CB4-OB6-CB5	2.51	124.11	117.92
6	M	854	BPH	CHD-C4C-NC	-2.51	120.00	124.54
5	M	853	BCL	O1D-CGD-CBD	-2.50	119.30	124.42
6	L	855	BPH	C3D-CAD-CBD	2.50	111.13	107.60
6	L	855	BPH	CED-O2D-CGD	2.49	121.95	116.02
5	M	853	BCL	C2D-C1D-ND	2.49	111.29	109.41
5	M	853	BCL	O2D-CGD-CBD	2.48	116.38	111.33
6	M	854	BPH	CED-O2D-CGD	2.48	121.91	116.02
5	M	852	BCL	C4D-C3D-CAD	-2.47	105.02	108.05
5	L	851	BCL	C4B-CHC-C1C	2.46	135.18	130.06
5	M	853	BCL	C2B-C1B-NB	2.45	111.26	109.41
5	M	852	BCL	C2D-C1D-ND	2.45	111.26	109.41
9	M	5000	CDL	OA4-PA1-OA3	-2.45	111.34	118.72
6	M	854	BPH	C4D-CHA-CBD	-2.44	104.10	110.15
7	M	857	U10	C27-C28-C29	-2.44	122.53	127.80
7	M	857	U10	C26-C24-C23	2.44	125.78	121.08
5	M	853	BCL	C2D-C3D-CAD	2.43	154.82	138.46
7	M	857	U10	C11-C12-C13	2.42	118.54	111.62
5	L	850	BCL	C2D-C3D-CAD	2.41	154.65	138.46
5	M	853	BCL	CAA-C2A-C3A	-2.40	107.36	113.04
5	L	850	BCL	C4B-CHC-C1C	2.39	135.04	130.06
5	M	852	BCL	CGD-CBD-CAD	-2.38	102.86	110.96
9	M	5000	CDL	CA6-CA4-CA3	-2.38	106.44	111.86
6	L	855	BPH	C4D-CHA-CBD	-2.37	104.28	110.15
5	M	852	BCL	C2D-C3D-CAD	2.36	154.34	138.46
5	L	851	BCL	C2C-C3C-C4C	2.35	104.31	101.05
7	M	857	U10	C10-C9-C11	2.34	118.95	115.39
5	M	852	BCL	C3D-CAD-CBD	2.33	110.89	107.60
6	L	855	BPH	O2A-C1-C2	-2.33	103.50	108.55
8	M	859	SPO	C34-C33-C35	-2.33	111.85	115.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	855	BPH	CAC-C3C-C2C	-2.33	108.55	113.89
5	L	850	BCL	C3B-C4B-CHC	2.32	130.40	126.00
6	L	855	BPH	C3C-C4C-CHD	2.31	126.64	121.83
5	M	853	BCL	C6-C5-C3	2.31	118.27	112.78
5	L	851	BCL	C2D-C3D-CAD	2.30	153.94	138.46
5	L	850	BCL	C2A-C1A-CHA	2.30	127.81	123.83
8	M	859	SPO	C10-C9-C7	-2.30	123.98	127.29
5	M	853	BCL	C4B-CHC-C1C	2.29	134.84	130.06
5	M	852	BCL	C4D-CHA-C1A	2.29	126.96	120.32
5	L	850	BCL	CAA-C2A-C3A	-2.29	107.63	113.04
5	L	851	BCL	C2D-C1D-ND	2.28	111.13	109.41
5	M	853	BCL	CGD-CBD-CHA	2.27	118.67	110.96
5	L	851	BCL	C3D-CAD-CBD	2.27	110.80	107.60
5	L	851	BCL	C4D-CHA-CBD	-2.26	104.04	109.37
7	M	857	U10	C30-C29-C28	-2.25	119.06	123.52
5	M	853	BCL	CHA-C1A-NA	-2.25	121.60	126.22
6	M	854	BPH	C2B-C1B-NB	2.24	112.51	108.16
6	M	854	BPH	C2D-C3D-CAD	2.23	153.46	138.46
6	M	854	BPH	CBB-CAB-C3B	-2.22	113.80	120.30
7	M	857	U10	C1-C6-C5	-2.22	117.47	120.26
6	L	855	BPH	C7-C6-C5	-2.20	106.53	113.01
6	L	855	BPH	C2D-C3D-CAD	2.20	153.23	138.46
5	L	851	BCL	C4D-C3D-CAD	-2.19	105.36	108.05
5	M	853	BCL	C3B-C4B-CHC	2.19	130.15	126.00
7	M	857	U10	C40-C39-C38	-2.18	118.39	123.62
5	L	851	BCL	O2A-CGA-CBA	2.18	118.80	111.94
5	M	853	BCL	C2A-C1A-CHA	2.13	127.53	123.83
6	L	855	BPH	C3D-C4D-ND	2.13	115.20	108.80
5	M	852	BCL	C3B-C4B-CHC	2.12	130.02	126.00
6	L	855	BPH	CHD-C4C-NC	-2.11	120.71	124.54
5	L	850	BCL	C4D-C3D-CAD	-2.10	105.47	108.05
6	L	855	BPH	C2A-C3A-C4A	2.10	105.85	101.11
5	M	852	BCL	C4D-CHA-CBD	-2.08	104.48	109.37
5	M	852	BCL	CAC-C3C-C2C	-2.08	109.12	113.89
6	M	854	BPH	C2A-C3A-C4A	2.08	105.79	101.11
5	L	850	BCL	O1D-CGD-CBD	-2.08	120.17	124.42
5	M	853	BCL	C4D-C3D-CAD	-2.07	105.51	108.05
5	L	851	BCL	C2C-C1C-NC	2.07	113.46	110.95
7	M	857	U10	C36-C34-C33	2.06	125.05	121.08
5	L	851	BCL	C3B-C4B-CHC	2.03	129.86	126.00
5	L	850	BCL	C1-O2A-CGA	2.01	122.61	116.98
5	L	850	BCL	CMD-C2D-C3D	-2.01	121.81	124.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	859	SPO	C13-C12-C11	2.00	121.33	118.09

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	M	5000	CDL	CA4
6	M	854	BPH	C8
6	M	854	BPH	C13
6	L	855	BPH	C8
6	L	855	BPH	C13

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.