



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:15 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 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

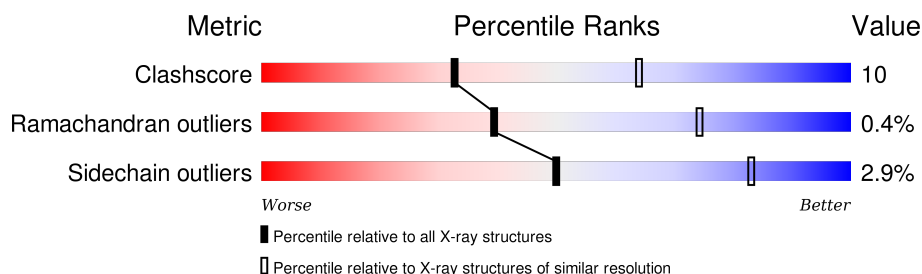
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (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. 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.

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 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 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

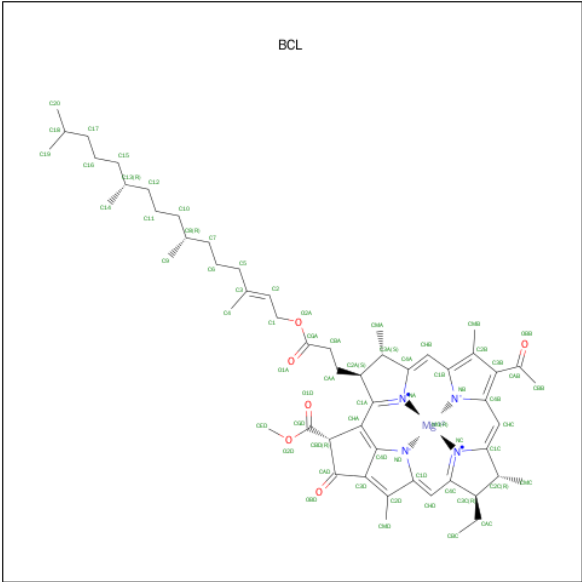
- Molecule 3 is a protein called Photosynthetic Reaction Center H subunit.

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).

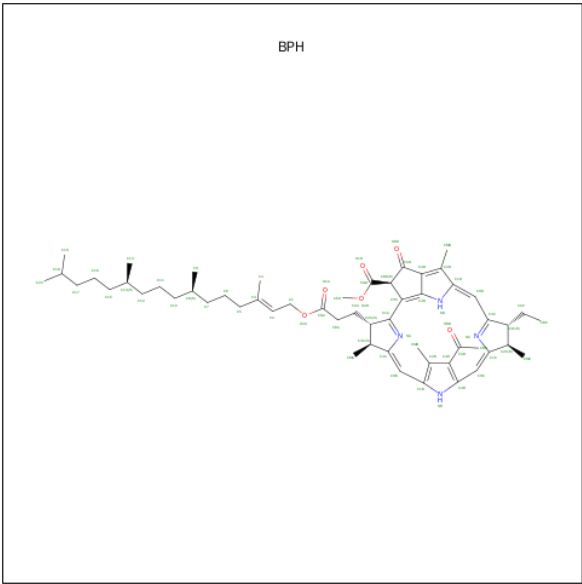
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	1	Total	Fe	0	0
			1	1		

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



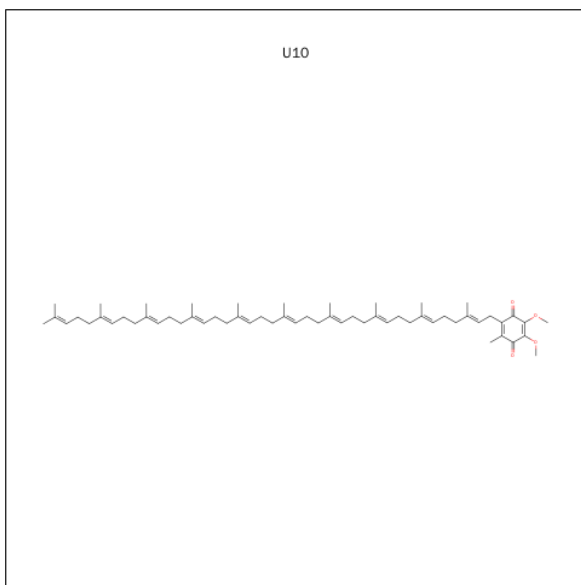
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 6 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C₅₅H₇₆N₄O₆).



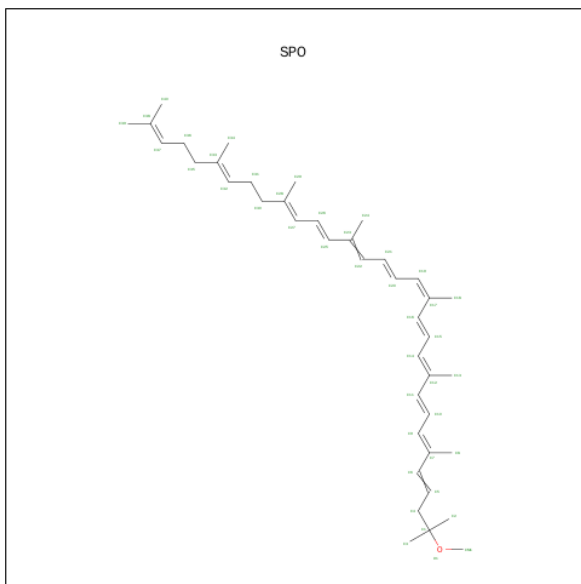
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	M	1	Total	C	N	O	0	0
			65	55	4	6		
6	L	1	Total	C	N	O	0	0
			65	55	4	6		

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



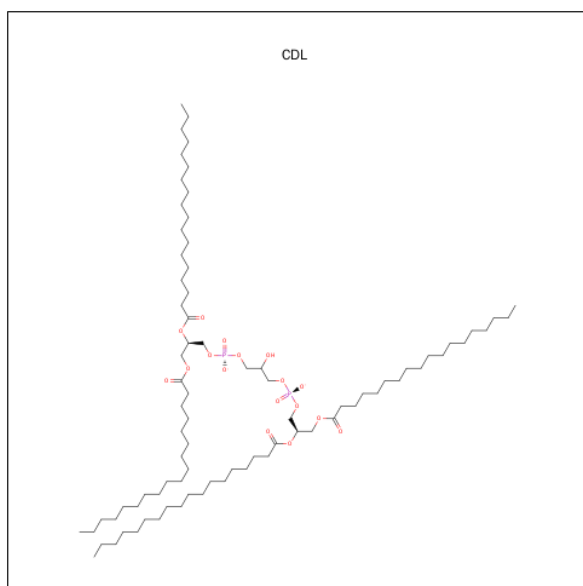
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	M	1	Total	C	O	0	0
			48	44	4		

- 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.

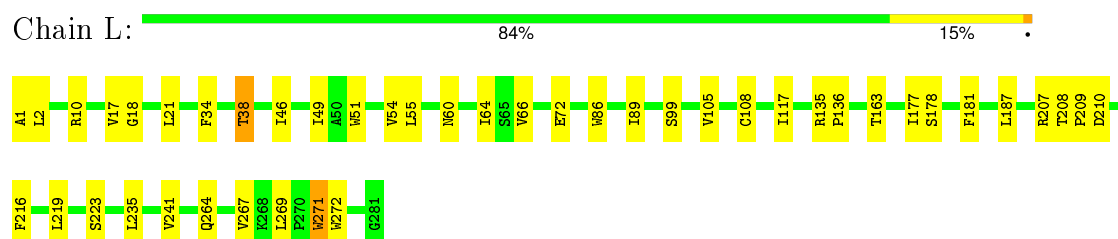
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	H	53	Total	O	0	0
			53	53		
10	L	33	Total	O	0	0
			33	33		
10	M	33	Total	O	0	0
			33	33		

3 Residue-property plots

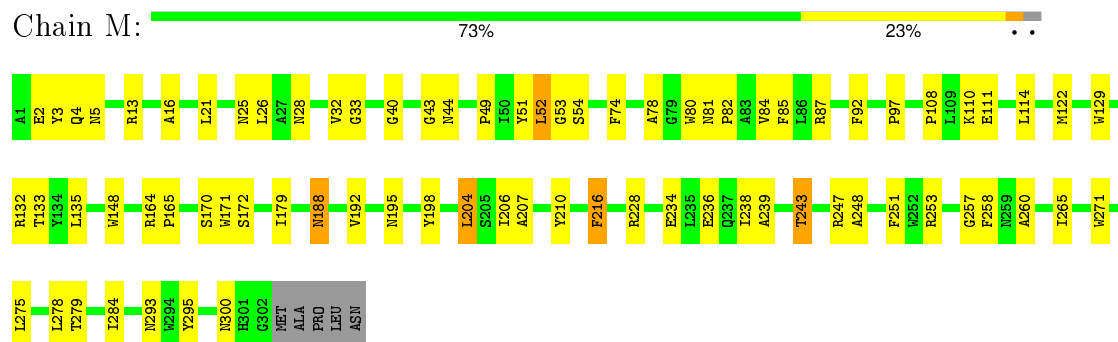
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

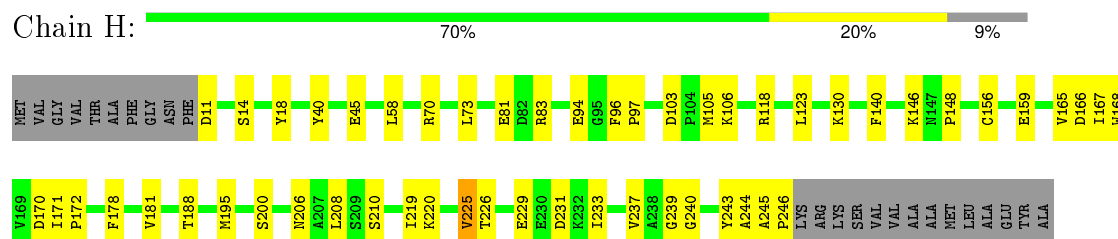
• Molecule 1: Photosynthetic Reaction Center L subunit



• 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	142.60 Å 142.60 Å 187.40 Å 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 [i](#)

5.1 Standard geometry [i](#)

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 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	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
8	M	42	0	60	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 10.

All (145) 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)
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:181:PHE:HB3	6:M:854:BPH:CBB	2.34	0.58
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:HHC	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	19	52
3	H	234/260 (90%)	227 (97%)	7 (3%)	0	100	100
All	All	813/848 (96%)	770 (95%)	40 (5%)	3 (0%)	39	74

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%)	42	76
2	M	236/240 (98%)	228 (97%)	8 (3%)	44	78
3	H	191/208 (92%)	188 (98%)	3 (2%)	70	93
All	All	647/668 (97%)	628 (97%)	19 (3%)	50	83

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
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 molecules 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	53,74,74	1.49	11 (20%)	57,115,115	1.82	11 (19%)
5	BCL	L	851	1	53,74,74	1.37	6 (11%)	57,115,115	1.63	9 (15%)
6	BPH	L	855	-	64,70,70	1.28	11 (17%)	73,101,101	1.93	17 (23%)
9	CDL	M	5000	-	80,80,99	0.59	1 (1%)	82,92,111	0.97	4 (4%)
5	BCL	M	852	2	53,74,74	1.45	9 (16%)	57,115,115	1.78	10 (17%)
5	BCL	M	853	1	53,74,74	1.44	7 (13%)	57,115,115	2.00	13 (22%)
6	BPH	M	854	-	64,70,70	1.34	10 (15%)	73,101,101	1.72	14 (19%)
7	U10	M	857	-	48,48,63	2.28	14 (29%)	58,61,79	2.43	24 (41%)
8	SPO	M	859	-	40,41,41	3.51	25 (62%)	45,50,50	2.74	15 (33%)

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	-	0/37/137/137	0/0/9/9
5	BCL	L	851	1	-	0/37/137/137	0/0/9/9
6	BPH	L	855	-	-	0/54/105/105	0/1/6/6
9	CDL	M	5000	-	-	0/91/91/110	0/0/0/0
5	BCL	M	852	2	-	0/37/137/137	0/0/9/9
5	BCL	M	853	1	-	0/37/137/137	0/0/9/9
6	BPH	M	854	-	-	0/54/105/105	0/1/6/6
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 (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	859	SPO	C4-C5	-3.80	1.44	1.50
7	M	857	U10	C7-C8	-3.80	1.44	1.50
8	M	859	SPO	C31-C32	-3.44	1.40	1.50
8	M	859	SPO	C11-C12	-3.29	1.38	1.45
6	L	855	BPH	C3D-CAD	-2.95	1.40	1.46
5	M	852	BCL	C3C-C4C	-2.65	1.48	1.51
6	M	854	BPH	C3D-CAD	-2.62	1.41	1.46
6	L	855	BPH	O2A-CGA	-2.50	1.25	1.33
5	M	853	BCL	C3C-C4C	-2.45	1.48	1.51
8	M	859	SPO	C25-C23	-2.34	1.40	1.45
5	L	850	BCL	O2D-CGD	-2.32	1.27	1.33
5	L	850	BCL	C3A-C2A	-2.26	1.47	1.54
6	M	854	BPH	C1B-C2B	-2.16	1.41	1.45
8	M	859	SPO	C6-C7	-2.14	1.41	1.45
6	M	854	BPH	C3A-C2A	-2.14	1.48	1.54
6	L	855	BPH	C3A-C2A	-2.12	1.48	1.54
7	M	857	U10	C22-C23	-2.11	1.44	1.50
6	M	854	BPH	O2A-CGA	-2.11	1.26	1.33
6	M	854	BPH	O2D-CGD	-2.06	1.27	1.33
6	L	855	BPH	C1B-C2B	-2.04	1.41	1.45
5	M	852	BCL	CHD-C4C	-2.00	1.35	1.41
6	L	855	BPH	CMD-C2D	2.02	1.55	1.51
8	M	859	SPO	C26-C27	2.05	1.50	1.43
5	M	852	BCL	CBB-CAB	2.08	1.56	1.49
6	L	855	BPH	C3B-CAB	2.09	1.53	1.46
5	L	850	BCL	CMD-C2D	2.09	1.56	1.51
5	L	851	BCL	CMD-C2D	2.22	1.56	1.51
5	L	850	BCL	CBB-CAB	2.25	1.56	1.49
6	L	855	BPH	CHA-C1A	2.26	1.42	1.37
9	M	5000	CDL	CB3-CB4	2.30	1.57	1.50
8	M	859	SPO	C24-C23	2.30	1.55	1.50
7	M	857	U10	O4-C4	2.33	1.43	1.37
5	L	850	BCL	CAA-C2A	2.34	1.58	1.54
5	M	852	BCL	CMD-C2D	2.36	1.56	1.51
5	M	853	BCL	OBD-CAD	2.41	1.26	1.22
8	M	859	SPO	C22-C23	2.47	1.39	1.35
5	L	851	BCL	C3B-CAB	2.47	1.55	1.49
7	M	857	U10	C8-C9	2.49	1.37	1.33
5	L	850	BCL	OBD-CAD	2.49	1.26	1.22
6	M	854	BPH	CMD-C2D	2.51	1.56	1.51
8	M	859	SPO	C29-C28	2.53	1.56	1.50
5	M	853	BCL	CMB-C2B	2.53	1.56	1.51
6	M	854	BPH	C3B-C2B	2.55	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	855	BPH	C3B-C2B	2.56	1.45	1.38
5	M	853	BCL	C3B-CAB	2.62	1.56	1.49
6	L	855	BPH	C3D-C2D	2.68	1.46	1.40
7	M	857	U10	C38-C39	2.68	1.40	1.32
5	M	852	BCL	CMB-C2B	2.73	1.57	1.51
8	M	859	SPO	C10-C9	2.79	1.52	1.43
8	M	859	SPO	C8-C7	2.80	1.56	1.50
5	L	850	BCL	C3B-CAB	2.81	1.56	1.49
8	M	859	SPO	C35-C33	2.83	1.57	1.51
5	M	852	BCL	C3B-CAB	2.87	1.56	1.49
5	L	851	BCL	CMB-C2B	2.92	1.57	1.51
5	L	850	BCL	CMB-C2B	2.97	1.57	1.51
8	M	859	SPO	C37-C38	3.01	1.41	1.32
6	L	855	BPH	CMB-C2B	3.12	1.57	1.50
5	L	850	BCL	C3B-C2B	3.14	1.47	1.40
5	M	853	BCL	C3B-C2B	3.23	1.47	1.40
7	M	857	U10	C23-C24	3.26	1.39	1.33
6	L	855	BPH	C2-C3	3.27	1.39	1.33
6	M	854	BPH	C3D-C2D	3.28	1.48	1.40
5	L	851	BCL	C3B-C2B	3.37	1.48	1.40
5	M	853	BCL	C3D-C2D	3.38	1.48	1.40
8	M	859	SPO	C19-C17	3.47	1.40	1.35
6	M	854	BPH	CMB-C2B	3.47	1.58	1.50
7	M	857	U10	C6-C5	3.50	1.56	1.46
5	M	852	BCL	C3D-C2D	3.62	1.48	1.40
7	M	857	U10	C13-C14	3.63	1.40	1.33
6	M	854	BPH	C2-C3	3.65	1.40	1.33
5	L	851	BCL	C2-C3	3.65	1.40	1.33
5	M	852	BCL	C3B-C2B	3.73	1.49	1.40
7	M	857	U10	C33-C34	3.73	1.40	1.33
5	L	850	BCL	C3D-C2D	3.78	1.49	1.40
8	M	859	SPO	C15-C14	3.83	1.55	1.43
7	M	857	U10	C18-C19	4.00	1.40	1.33
8	M	859	SPO	O1-CM1	4.06	1.56	1.43
7	M	857	U10	C7-C6	4.06	1.58	1.51
7	M	857	U10	C4-C3	4.07	1.53	1.35
8	M	859	SPO	C14-C12	4.14	1.41	1.35
5	L	851	BCL	C3D-C2D	4.19	1.50	1.40
7	M	857	U10	C28-C29	4.27	1.41	1.33
8	M	859	SPO	C13-C12	4.27	1.60	1.50
5	L	850	BCL	C2-C3	4.37	1.41	1.33
5	M	852	BCL	C2-C3	4.39	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	859	SPO	C32-C33	4.41	1.41	1.33
5	M	853	BCL	C2-C3	4.85	1.42	1.33
8	M	859	SPO	C26-C25	5.28	1.48	1.34
8	M	859	SPO	C21-C20	5.44	1.50	1.35
8	M	859	SPO	C27-C28	5.68	1.40	1.34
8	M	859	SPO	C6-C5	6.79	1.50	1.31
8	M	859	SPO	C10-C11	7.04	1.52	1.34
7	M	857	U10	C6-C1	7.35	1.52	1.35
8	M	859	SPO	C15-C16	9.34	1.58	1.34

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	859	SPO	C25-C23-C22	-10.48	102.09	118.98
5	M	853	BCL	CMB-C2B-C1B	-5.98	118.47	128.36
5	L	850	BCL	CMB-C2B-C1B	-5.95	118.52	128.36
5	M	852	BCL	CMB-C2B-C1B	-5.93	118.56	128.36
7	M	857	U10	C15-C14-C13	-5.77	112.17	123.50
5	M	853	BCL	CAA-C2A-C1A	-5.75	92.18	112.47
8	M	859	SPO	C18-C17-C19	-5.70	114.48	122.90
5	L	851	BCL	CMB-C2B-C1B	-5.67	118.99	128.36
7	M	857	U10	C10-C9-C8	-5.66	112.39	123.50
6	M	854	BPH	O1D-CGD-CBD	-4.98	117.48	124.62
8	M	859	SPO	C24-C23-C22	-4.82	115.78	122.90
5	L	850	BCL	CAA-C2A-C1A	-4.81	95.50	112.47
8	M	859	SPO	C20-C21-C22	-4.77	112.84	123.39
8	M	859	SPO	C4-C5-C6	-4.72	117.95	124.67
7	M	857	U10	C25-C24-C23	-4.69	114.29	123.50
6	L	855	BPH	O1D-CGD-CBD	-4.46	118.24	124.62
6	L	855	BPH	C5-C3-C2	-4.26	112.97	121.05
8	M	859	SPO	C15-C14-C12	-4.17	121.18	127.20
6	L	855	BPH	C4D-C3D-C2D	-4.15	101.72	107.08
7	M	857	U10	C35-C34-C33	-4.09	115.48	123.50
6	M	854	BPH	C4D-C3D-C2D	-4.00	101.92	107.08
6	L	855	BPH	CHC-C4B-NB	-3.80	117.68	124.91
7	M	857	U10	C20-C19-C18	-3.74	116.16	123.50
5	M	853	BCL	O1D-CGD-CBD	-3.71	119.30	124.62
5	L	851	BCL	OBD-CAD-C3D	-3.58	121.06	128.35
6	M	854	BPH	CHC-C4B-NB	-3.41	118.42	124.91
8	M	859	SPO	C11-C12-C14	-3.30	113.66	118.98
5	M	853	BCL	CAC-C3C-C2C	-3.29	105.86	114.13
5	M	852	BCL	OBD-CAD-C3D	-3.27	121.68	128.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	853	BCL	OBD-CAD-C3D	-3.21	121.81	128.35
5	L	850	BCL	OBD-CAD-C3D	-3.15	121.94	128.35
6	L	855	BPH	CMB-C2B-C1B	-3.12	119.98	125.06
5	L	850	BCL	O1D-CGD-CBD	-3.11	120.17	124.62
6	M	854	BPH	CBB-CAB-C3B	-3.02	113.80	120.52
6	M	854	BPH	CMB-C2B-C1B	-3.01	120.16	125.06
8	M	859	SPO	C15-C16-C17	-2.96	117.61	126.32
5	M	852	BCL	CHA-C1A-NA	-2.75	119.30	126.06
9	M	5000	CDL	CB6-CB4-CB3	-2.70	105.77	112.07
7	M	857	U10	O5-C5-C4	-2.56	115.25	120.79
5	L	851	BCL	CHA-C1A-NA	-2.54	119.82	126.06
7	M	857	U10	C27-C28-C29	-2.41	122.53	127.76
9	M	5000	CDL	CA6-CA4-CA3	-2.41	106.44	112.07
8	M	859	SPO	C34-C33-C35	-2.33	111.85	115.41
7	M	857	U10	C1-C6-C5	-2.33	117.47	120.12
5	M	852	BCL	C15-C13-C12	-2.31	98.51	112.27
5	M	852	BCL	CGD-CBD-CAD	-2.29	102.86	110.62
6	L	855	BPH	CBB-CAB-C3B	-2.28	115.46	120.52
7	M	857	U10	C30-C29-C28	-2.26	119.06	123.50
8	M	859	SPO	C10-C9-C7	-2.23	123.98	127.20
6	L	855	BPH	CAC-C3C-C2C	-2.22	108.55	114.13
6	L	855	BPH	C7-C6-C5	-2.21	106.53	113.06
7	M	857	U10	C21-C22-C23	-2.21	105.91	111.69
7	M	857	U10	C31-C32-C33	-2.20	105.94	111.69
5	L	850	BCL	CHA-C1A-NA	-2.13	120.81	126.06
8	M	859	SPO	C9-C10-C11	-2.09	116.76	123.13
6	L	855	BPH	C1C-NC-C4C	-2.05	108.34	110.44
5	M	853	BCL	CAA-C2A-C3A	-2.04	107.36	113.22
6	M	854	BPH	C4-C3-C2	-2.01	119.56	123.50
6	M	854	BPH	C2A-C3A-C4A	2.05	105.79	101.10
6	L	855	BPH	C2A-C3A-C4A	2.08	105.85	101.10
7	M	857	U10	C36-C34-C33	2.11	125.05	121.05
6	L	855	BPH	CMB-C2B-C3B	2.11	132.96	128.04
5	M	853	BCL	C2C-C3C-C4C	2.13	105.11	101.50
5	L	850	BCL	C2A-C1A-CHA	2.13	127.81	123.89
5	L	851	BCL	O2A-CGA-CBA	2.27	118.80	111.90
5	L	851	BCL	C3D-CAD-CBD	2.27	110.80	107.60
7	M	857	U10	C10-C9-C11	2.32	118.95	115.41
5	M	852	BCL	C3D-CAD-CBD	2.33	110.89	107.60
6	M	854	BPH	CMB-C2B-C3B	2.34	133.48	128.04
5	M	852	BCL	C2A-C1A-CHA	2.44	128.37	123.89
7	M	857	U10	C26-C24-C23	2.49	125.78	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	855	BPH	C3D-CAD-CBD	2.50	111.13	107.60
8	M	859	SPO	C16-C17-C19	2.51	123.03	118.98
6	M	854	BPH	CED-O2D-CGD	2.52	121.91	115.99
6	L	855	BPH	CED-O2D-CGD	2.54	121.95	115.99
5	L	851	BCL	C2A-C1A-CHA	2.56	128.61	123.89
9	M	5000	CDL	CB4-OB6-CB5	2.59	124.11	117.89
7	M	857	U10	C11-C12-C13	2.62	118.54	111.69
5	M	853	BCL	C6-C5-C3	2.63	118.27	112.48
8	M	859	SPO	C18-C17-C16	2.64	122.48	118.10
7	M	857	U10	C30-C29-C31	2.64	119.43	115.41
7	M	857	U10	C35-C34-C36	2.66	119.47	115.41
8	M	859	SPO	O1-C1-C4	2.66	112.39	105.87
5	M	853	BCL	O2A-CGA-CBA	2.86	120.63	111.90
7	M	857	U10	C21-C19-C18	2.88	126.52	121.05
5	L	850	BCL	O2D-CGD-CBD	2.89	115.26	111.30
6	M	854	BPH	C3D-CAD-CBD	2.95	111.77	107.60
7	M	857	U10	C4M-O4-C4	2.96	127.14	116.61
7	M	857	U10	C25-C24-C26	2.96	119.93	115.41
6	M	854	BPH	C6-C5-C3	2.96	118.99	112.48
5	L	850	BCL	CED-O2D-CGD	3.02	123.06	115.99
5	L	851	BCL	C6-C5-C3	3.13	119.36	112.48
5	M	853	BCL	CED-O2D-CGD	3.47	124.12	115.99
5	M	853	BCL	CBA-CAA-C2A	3.48	123.54	113.73
5	L	850	BCL	CBA-CAA-C2A	3.54	123.71	113.73
5	L	850	BCL	C6-C5-C3	3.55	120.26	112.48
5	M	853	BCL	O2D-CGD-CBD	3.70	116.38	111.30
8	M	859	SPO	C8-C7-C9	3.73	128.41	122.90
5	L	851	BCL	CED-O2D-CGD	3.93	125.20	115.99
7	M	857	U10	C11-C9-C8	4.01	128.66	121.05
6	L	855	BPH	O2D-CGD-CBD	4.02	116.82	111.30
9	M	5000	CDL	OB8-CB6-CB4	4.08	119.68	108.69
5	L	851	BCL	CMB-C2B-C3B	4.25	133.41	125.09
5	M	852	BCL	CED-O2D-CGD	4.29	126.06	115.99
7	M	857	U10	C7-C8-C9	4.36	134.09	126.70
5	L	850	BCL	CMB-C2B-C3B	4.44	133.77	125.09
5	M	852	BCL	CMB-C2B-C3B	4.45	133.79	125.09
5	M	853	BCL	CMB-C2B-C3B	4.50	133.89	125.09
6	M	854	BPH	C3C-C4C-NC	4.51	112.45	107.93
6	M	854	BPH	C4-C3-C5	4.52	122.31	115.41
6	L	855	BPH	C3C-C4C-NC	4.71	112.65	107.93
6	M	854	BPH	O2D-CGD-CBD	4.87	117.98	111.30
5	M	852	BCL	C6-C5-C3	4.90	123.24	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	857	U10	C15-C14-C16	5.37	123.60	115.41
7	M	857	U10	C7-C6-C5	5.87	125.47	118.56
6	L	855	BPH	C6-C5-C3	6.08	125.83	112.48
6	L	855	BPH	C4-C3-C5	6.40	125.19	115.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	850	BCL	6	0
5	L	851	BCL	4	0
6	L	855	BPH	6	0
9	M	5000	CDL	2	0
5	M	852	BCL	6	0
5	M	853	BCL	5	0
6	M	854	BPH	5	0
7	M	857	U10	4	0
8	M	859	SPO	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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