



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:05 PM GMT

PDB ID : 1JGX
Title : Photosynthetic Reaction Center Mutant With Thr M 21 Replaced With Asp
Authors : Camara-Artigas, A.; Magee, C.L.; Williams, J.C.; Allen, J.P.
Deposited on : 2001-06-27
Resolution : 3.01 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>

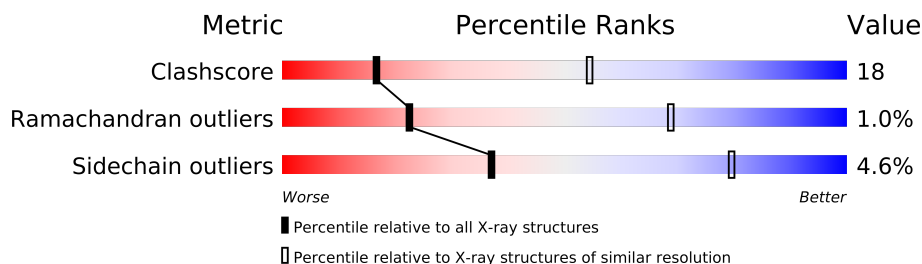
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.01 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	1732 (3.04-3.00)
Ramachandran outliers	78287	1669 (3.04-3.00)
Sidechain outliers	78261	1672 (3.04-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 9 unique types of molecules in this entry. The entry contains 7067 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	1607	394	398	10			

There is a discrepancy between the modelled and reference sequences:

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

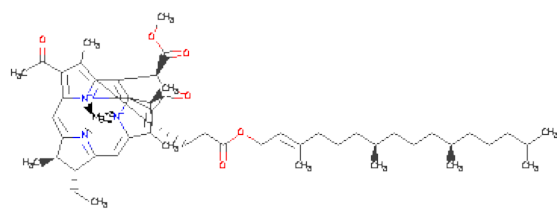
- Molecule 3 is a protein called Photosynthetic Reaction Center H subunit.

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

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

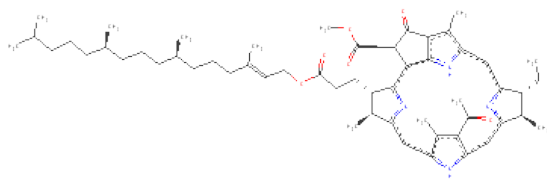
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	1	Total	Fe	0	0
			1	1		

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



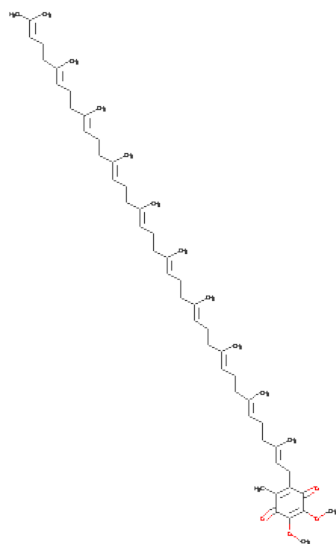
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



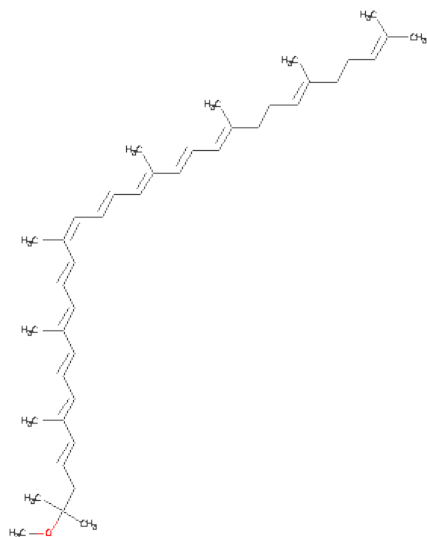
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	M	1	Total	C	N	O	0	0
			65	55	4	6		
6	L	1	Total	C	N	O	0	0
			65	55	4	6		

- 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 water.

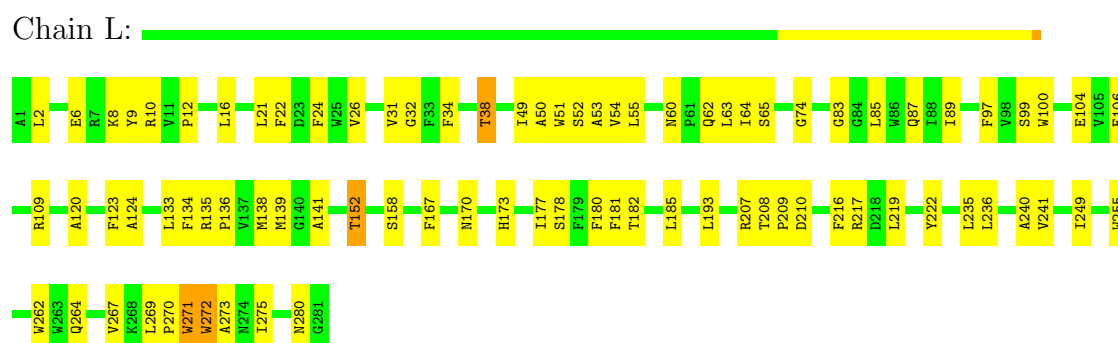
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	H	47	Total	O	0	0
			47	47		
9	L	28	Total	O	0	0
			28	28		
9	M	37	Total	O	0	0
			37	37		

3 Residue-property plots

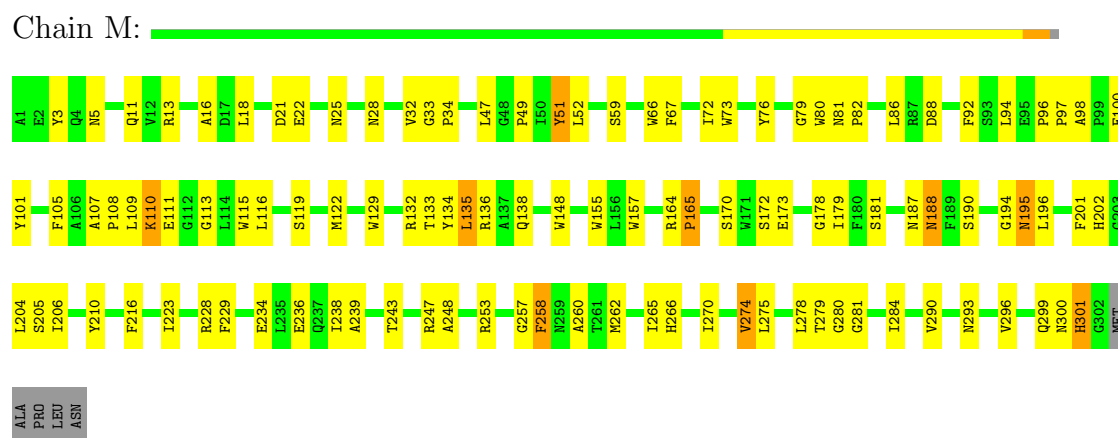
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

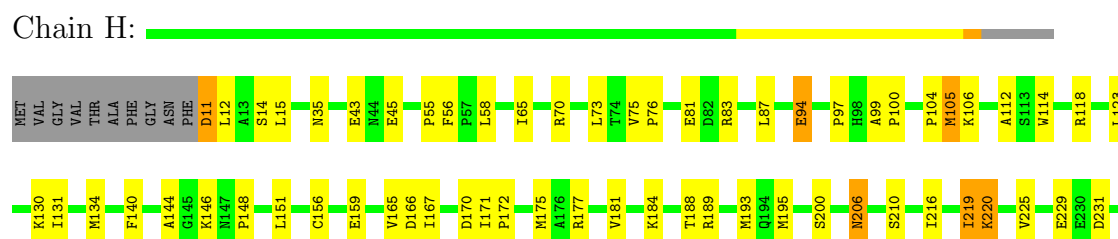
- Molecule 1: Photosynthetic Reaction Center L subunit



- Molecule 2: Photosynthetic Reaction Center M subunit



- Molecule 3: Photosynthetic Reaction Center H subunit



G235	
G239	
G240	
L241	
Y242	
Y243	
A244	
A245	
R248	
K249	
S250	
VAL	
VAL	
ALA	
ALA	
MET	
LEU	
ALA	
GLU	
TYR	
ALA	

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	142.11Å 142.11Å 187.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.97 – 3.01	Depositor
% Data completeness (in resolution range)	92.5 (29.97-3.01)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.211 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7067	wwPDB-VP
Average B, all atoms (Å ²)	50.0	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, BPH, U10, FE, SPO

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	0.59	0/3175
2	M	0.42	0/2501	0.61	1/3414 (0.0%)
3	H	0.40	0/1877	0.67	0/2553
All	All	0.41	0/6698	0.62	1/9142 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	258	PHE	N-CA-CB	-5.04	101.53	110.60

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	79	0
2	M	2409	0	2318	110	0
3	H	1829	0	1836	57	0
4	M	1	0	0	0	0
5	L	198	0	222	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	66	0	74	7	0
6	L	65	0	76	7	0
6	M	65	0	76	9	0
7	M	48	0	63	5	0
8	M	42	0	60	1	0
9	H	47	0	0	2	0
9	L	28	0	0	4	0
9	M	37	0	0	18	0
All	All	7067	0	6912	248	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 18.

All (248) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:M:243:THR:CG2	2:M:247:ARG:HE	1.71	1.03
2:M:260:ALA:CB	9:M:1027:HOH:O	2.12	0.97
1:L:60:ASN:HD22	1:L:63:LEU:HG	1.27	0.96
2:M:260:ALA:HB3	9:M:1027:HOH:O	1.68	0.93
1:L:97:PHE:HA	9:L:1014:HOH:O	1.71	0.91
1:L:100:TRP:HB3	9:L:1014:HOH:O	1.71	0.89
2:M:279:THR:HB	9:M:1025:HOH:O	1.72	0.88
2:M:188:ASN:HB3	9:M:1024:HOH:O	1.73	0.88
2:M:122:MET:HE1	2:M:157:TRP:HE1	1.37	0.87
2:M:243:THR:HG21	2:M:247:ARG:HE	1.39	0.84
2:M:243:THR:HG22	2:M:247:ARG:HE	1.40	0.84
1:L:219:LEU:HD12	2:M:132:ARG:NH1	1.93	0.83
2:M:122:MET:CE	2:M:157:TRP:HE1	1.90	0.83
1:L:60:ASN:ND2	1:L:63:LEU:HG	1.96	0.81
2:M:265:ILE:HB	9:M:1027:HOH:O	1.80	0.80
1:L:34:PHE:O	1:L:38:THR:HG23	1.84	0.77
1:L:65:SER:HB2	1:L:152:THR:HG21	1.66	0.76
2:M:262:MET:O	9:M:1007:HOH:O	2.05	0.75
1:L:38:THR:HG22	1:L:99:SER:HB3	1.69	0.73
2:M:266:HIS:ND1	9:M:1007:HOH:O	2.22	0.73
2:M:248:ALA:HB1	7:M:857:U10:H3M2	1.72	0.72
3:H:219:ILE:H	3:H:219:ILE:HD13	1.55	0.71
3:H:131:ILE:CD1	3:H:177:ARG:HD2	2.20	0.70
6:L:855:BPH:HBB2	2:M:210:TYR:HB3	1.72	0.70
1:L:271:TRP:CD1	1:L:271:TRP:N	2.53	0.70
3:H:131:ILE:HD13	3:H:170:ASP:HA	1.73	0.70
2:M:204:LEU:HB3	2:M:279:THR:HG21	1.73	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:M:265:ILE:HG22	9:M:1007:HOH:O	1.93	0.68
2:M:293:ASN:HB2	9:M:1031:HOH:O	1.93	0.67
2:M:243:THR:HG22	2:M:247:ARG:HG3	1.75	0.67
2:M:280:GLY:N	9:M:1025:HOH:O	2.27	0.67
3:H:131:ILE:HD11	3:H:177:ARG:HD2	1.77	0.67
2:M:260:ALA:HB1	9:M:1027:HOH:O	1.87	0.67
1:L:50:ALA:O	1:L:53:ALA:HB3	1.95	0.66
3:H:105:MET:HE3	3:H:105:MET:HA	1.76	0.66
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.76	0.66
1:L:219:LEU:HA	2:M:132:ARG:HH12	1.61	0.65
1:L:60:ASN:HD22	1:L:63:LEU:CG	2.05	0.65
2:M:119:SER:HB3	8:M:859:SPO:H311	1.77	0.65
2:M:260:ALA:HB1	3:H:35:ASN:OD1	1.96	0.65
5:L:850:BCL:H2	6:M:854:BPH:HMB2	1.78	0.65
1:L:271:TRP:HD1	1:L:271:TRP:H	1.40	0.65
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.80	0.64
2:M:67:PHE:CD1	6:M:854:BPH:H9C1	2.32	0.64
1:L:208:THR:HB	1:L:209:PRO:HD2	1.79	0.64
1:L:22:PHE:HA	1:L:24:PHE:CE2	2.33	0.64
2:M:13:ARG:O	3:H:140:PHE:HA	1.98	0.63
3:H:156:CYS:HB3	3:H:206:ASN:O	1.98	0.62
2:M:253:ARG:O	2:M:257:GLY:HA2	1.99	0.62
2:M:196:LEU:HD23	2:M:202:HIS:CD2	2.35	0.62
2:M:108:PRO:HG2	2:M:111:GLU:HG3	1.82	0.62
2:M:300:ASN:O	2:M:301:HIS:ND1	2.32	0.61
1:L:38:THR:HG22	1:L:99:SER:CB	2.30	0.61
1:L:65:SER:CB	1:L:152:THR:HG21	2.30	0.61
2:M:108:PRO:HG2	2:M:111:GLU:HB2	1.82	0.61
2:M:76:TYR:HE1	2:M:110:LYS:HZ1	1.49	0.61
2:M:138:GLN:HA	9:M:1026:HOH:O	2.00	0.61
3:H:130:LYS:HE3	3:H:170:ASP:OD2	2.00	0.61
1:L:182:THR:HG22	1:L:236:LEU:HD13	1.82	0.60
1:L:181:PHE:HB3	6:M:854:BPH:HBB2	1.84	0.60
5:L:853:BCL:HMD2	5:M:852:BCL:HBB3	1.85	0.59
1:L:219:LEU:HD12	2:M:132:ARG:HH12	1.68	0.59
1:L:51:TRP:O	1:L:54:VAL:HG22	2.02	0.59
3:H:241:LEU:O	3:H:248:ARG:NH2	2.36	0.58
2:M:73:TRP:O	2:M:76:TYR:HB2	2.03	0.58
1:L:272:TRP:HA	1:L:275:ILE:HD12	1.86	0.58
2:M:11:GLN:HB2	3:H:144:ALA:HB3	1.86	0.57
6:L:855:BPH:HH1	6:L:855:BPH:HBB3	1.87	0.57
2:M:243:THR:HG22	2:M:247:ARG:NE	2.16	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:M:852:BCL:H203	5:M:852:BCL:H152	1.87	0.56
1:L:264:GLN:HA	1:L:267:VAL:HG12	1.88	0.56
2:M:243:THR:HG21	2:M:247:ARG:NE	2.16	0.56
6:M:854:BPH:H7C1	6:M:854:BPH:H121	1.88	0.56
1:L:280:ASN:ND2	2:M:88:ASP:OD1	2.39	0.55
2:M:228:ARG:NE	3:H:195:MET:HE3	2.21	0.55
3:H:81:GLU:O	3:H:83:ARG:HG2	2.06	0.55
3:H:131:ILE:HD12	3:H:177:ARG:HD2	1.89	0.55
3:H:148:PRO:HA	3:H:151:LEU:HD12	1.89	0.55
1:L:12:PRO:HG3	3:H:97:PRO:HB2	1.89	0.54
5:L:850:BCL:CBB	5:L:850:BCL:HHC	2.38	0.54
1:L:177:ILE:HG12	5:L:851:BCL:HMB3	1.90	0.54
1:L:31:VAL:HG12	1:L:32:GLY:N	2.21	0.54
1:L:60:ASN:O	1:L:64:ILE:HG13	2.07	0.54
1:L:138:MET:SD	1:L:249:ILE:HD11	2.48	0.54
3:H:94:GLU:HG3	9:H:1110:HOH:O	2.07	0.54
3:H:219:ILE:H	3:H:219:ILE:CD1	2.20	0.54
2:M:25:ASN:HD22	2:M:28:ASN:ND2	2.06	0.53
5:L:853:BCL:H61	7:M:857:U10:H203	1.91	0.53
2:M:135:LEU:HB3	2:M:136:ARG:HH21	1.73	0.53
2:M:290:VAL:HG21	3:H:12:LEU:HD12	1.90	0.53
2:M:205:SER:CB	9:M:1025:HOH:O	2.57	0.52
2:M:98:ALA:HB1	2:M:100:GLU:OE1	2.08	0.52
1:L:219:LEU:HD12	2:M:132:ARG:HH11	1.70	0.52
2:M:206:ILE:HG23	5:M:852:BCL:HMB3	1.91	0.52
1:L:34:PHE:O	1:L:38:THR:CG2	2.55	0.52
5:L:850:BCL:HHC	5:L:850:BCL:HBB3	1.92	0.52
2:M:76:TYR:HE1	2:M:110:LYS:NZ	2.07	0.52
3:H:189:ARG:HD2	3:H:216:ILE:HB	1.91	0.51
3:H:220:LYS:HG2	3:H:229:GLU:OE2	2.11	0.51
1:L:181:PHE:HB3	6:M:854:BPH:CBB	2.41	0.51
1:L:60:ASN:ND2	1:L:62:GLN:HB2	2.27	0.50
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.47	0.50
3:H:55:PRO:HG2	3:H:56:PHE:CD2	2.47	0.50
3:H:156:CYS:HB2	3:H:248:ARG:HG3	1.94	0.50
2:M:80:TRP:O	2:M:82:PRO:HD3	2.11	0.50
3:H:112:ALA:HB2	3:H:239:GLY:HA3	1.93	0.49
2:M:243:THR:O	2:M:247:ARG:HG3	2.12	0.49
6:M:854:BPH:HHC	6:M:854:BPH:HBB3	1.94	0.49
2:M:243:THR:HG22	2:M:247:ARG:CG	2.42	0.49
1:L:74:GLY:O	1:L:141:ALA:HA	2.11	0.49
1:L:83:GLY:O	1:L:87:GLN:HG3	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:M:205:SER:HB2	9:M:1025:HOH:O	2.12	0.49
3:H:181:VAL:O	3:H:188:THR:HA	2.12	0.49
2:M:101:TYR:CG	2:M:107:ALA:HB2	2.48	0.49
1:L:100:TRP:O	1:L:104:GLU:HG3	2.13	0.49
3:H:112:ALA:HA	3:H:235:GLY:O	2.13	0.49
1:L:267:VAL:HG21	1:L:280:ASN:ND2	2.28	0.48
5:L:851:BCL:HAA2	5:L:853:BCL:HBC1	1.95	0.48
2:M:79:GLY:C	2:M:81:ASN:H	2.15	0.48
2:M:122:MET:HE3	2:M:157:TRP:HE1	1.77	0.48
3:H:12:LEU:O	3:H:15:LEU:N	2.45	0.48
1:L:60:ASN:HD21	1:L:62:GLN:HB2	1.78	0.48
2:M:94:LEU:HD21	2:M:115:TRP:HA	1.96	0.48
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.48	0.48
2:M:201:PHE:HD1	2:M:279:THR:HG23	1.79	0.48
6:L:855:BPH:H8	6:L:855:BPH:H121	1.70	0.47
1:L:2:LEU:HD22	1:L:6:GLU:HG2	1.96	0.47
5:L:850:BCL:HMB2	6:M:854:BPH:HMB3	1.96	0.47
1:L:34:PHE:HB2	9:L:1053:HOH:O	2.13	0.47
1:L:219:LEU:HD11	2:M:133:THR:HG22	1.94	0.47
2:M:110:LYS:O	2:M:111:GLU:HG2	2.15	0.47
2:M:21:ASP:O	2:M:22:GLU:C	2.53	0.47
1:L:109:ARG:HH11	1:L:109:ARG:HG2	1.79	0.47
2:M:66:TRP:CD1	2:M:122:MET:HB2	2.49	0.47
1:L:170:ASN:HB3	1:L:173:HIS:HB2	1.96	0.47
2:M:234:GLU:O	2:M:238:ILE:HG13	2.15	0.47
3:H:104:PRO:HB2	3:H:243:TYR:CE2	2.50	0.47
1:L:135:ARG:HD3	9:L:1077:HOH:O	2.14	0.47
2:M:96:PRO:HB2	2:M:97:PRO:HD2	1.95	0.47
2:M:270:ILE:O	2:M:274:VAL:HB	2.15	0.47
1:L:8:LYS:HE2	1:L:9:TYR:CZ	2.50	0.47
1:L:181:PHE:CD2	6:M:854:BPH:HBB1	2.49	0.47
3:H:156:CYS:SG	3:H:248:ARG:HB2	2.55	0.47
2:M:109:LEU:C	2:M:111:GLU:H	2.16	0.47
2:M:178:GLY:HA3	2:M:181:SER:HB3	1.97	0.47
1:L:133:LEU:HD23	1:L:134:PHE:CE1	2.49	0.47
1:L:272:TRP:HA	1:L:275:ILE:CD1	2.45	0.47
1:L:255:TRP:CZ2	1:L:262:TRP:HB2	2.50	0.47
3:H:175:MET:HE1	3:H:177:ARG:NH1	2.29	0.46
3:H:118:ARG:HD2	9:H:1106:HOH:O	2.14	0.46
2:M:113:GLY:HA2	2:M:116:LEU:HD12	1.97	0.46
1:L:170:ASN:HB3	1:L:173:HIS:CB	2.45	0.46
1:L:52:SER:HB2	1:L:85:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:54:VAL:HG23	1:L:55:LEU:N	2.31	0.45
2:M:32:VAL:HG22	2:M:49:PRO:HD3	1.97	0.45
7:M:857:U10:H251	7:M:857:U10:H271	1.63	0.45
3:H:165:VAL:O	3:H:166:ASP:HB2	2.16	0.45
1:L:124:ALA:HB2	6:L:855:BPH:HBC2	1.97	0.45
1:L:217:ARG:HH11	1:L:217:ARG:HG3	1.81	0.45
3:H:140:PHE:CE1	3:H:171:ILE:HD12	2.52	0.45
1:L:26:VAL:HG23	1:L:31:VAL:CG2	2.46	0.45
2:M:105:PHE:N	2:M:105:PHE:CD1	2.83	0.45
2:M:243:THR:HG21	2:M:247:ARG:HH21	1.80	0.45
2:M:265:ILE:CG2	9:M:1007:HOH:O	2.60	0.45
3:H:131:ILE:CD1	3:H:170:ASP:HA	2.46	0.45
3:H:159:GLU:HB3	3:H:210:SER:HB3	1.98	0.45
2:M:100:GLU:H	2:M:100:GLU:CD	2.21	0.44
2:M:51:TYR:CD2	2:M:51:TYR:C	2.90	0.44
1:L:2:LEU:HD12	3:H:45:GLU:HA	1.97	0.44
3:H:99:ALA:HA	3:H:100:PRO:HD3	1.78	0.44
2:M:194:GLY:O	2:M:195:ASN:HB3	2.17	0.44
3:H:65:ILE:HD12	3:H:65:ILE:N	2.31	0.44
1:L:193:LEU:HD13	1:L:216:PHE:CE2	2.52	0.44
5:L:851:BCL:H122	6:L:855:BPH:H3A	1.99	0.44
6:M:854:BPH:HHB	6:M:854:BPH:HMB1	1.75	0.44
2:M:129:TRP:O	2:M:133:THR:HG23	2.18	0.44
1:L:178:SER:HA	5:L:850:BCL:O1A	2.18	0.43
1:L:22:PHE:HA	1:L:24:PHE:HE2	1.82	0.43
2:M:148:TRP:HA	2:M:148:TRP:HE3	1.83	0.43
1:L:2:LEU:HD21	1:L:10:ARG:NE	2.33	0.43
2:M:275:LEU:HD23	2:M:278:LEU:HD23	2.00	0.43
2:M:32:VAL:HG12	2:M:33:GLY:O	2.18	0.43
3:H:75:VAL:HA	3:H:76:PRO:C	2.39	0.43
3:H:146:LYS:HE2	3:H:200:SER:O	2.18	0.43
2:M:52:LEU:HD12	2:M:52:LEU:HA	1.57	0.43
3:H:249:LYS:O	3:H:250:SER:HB3	2.18	0.43
5:L:850:BCL:H62	5:M:852:BCL:H202	2.01	0.43
3:H:83:ARG:NH1	3:H:114:TRP:O	2.52	0.43
1:L:49:ILE:HG13	1:L:89:ILE:HD13	2.00	0.43
1:L:269:LEU:HA	1:L:270:PRO:HD3	1.86	0.43
3:H:184:LYS:O	3:H:184:LYS:HD2	2.18	0.43
1:L:8:LYS:HE2	1:L:9:TYR:CE2	2.53	0.43
1:L:120:ALA:O	1:L:123:PHE:HB2	2.19	0.43
2:M:108:PRO:HG2	2:M:111:GLU:CG	2.49	0.43
1:L:182:THR:HG22	1:L:236:LEU:CD1	2.46	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:L:851:BCL:CAA	5:L:853:BCL:HBC1	2.48	0.42
3:H:130:LYS:HZ1	3:H:172:PRO:HG2	1.84	0.42
3:H:55:PRO:HG2	3:H:56:PHE:H	1.84	0.42
1:L:16:LEU:HG	1:L:106:GLU:HG2	2.02	0.42
2:M:164:ARG:NH1	2:M:173:GLU:OE1	2.46	0.42
2:M:243:THR:CG2	2:M:247:ARG:NE	2.57	0.42
2:M:300:ASN:O	2:M:301:HIS:CB	2.68	0.42
1:L:269:LEU:HB2	1:L:272:TRP:HE1	1.84	0.42
2:M:187:ASN:HA	5:M:852:BCL:HBC1	2.02	0.42
2:M:16:ALA:HB1	2:M:32:VAL:HG11	2.00	0.42
7:M:857:U10:H201	7:M:857:U10:H222	1.58	0.42
2:M:96:PRO:HA	2:M:115:TRP:CG	2.55	0.42
7:M:857:U10:H312	7:M:857:U10:H271	1.90	0.42
1:L:269:LEU:HB2	1:L:272:TRP:NE1	2.34	0.42
1:L:217:ARG:HG3	1:L:217:ARG:NH1	2.34	0.42
1:L:109:ARG:NH1	1:L:109:ARG:HG2	2.34	0.42
1:L:139:MET:HB3	1:L:139:MET:HE2	1.91	0.42
3:H:175:MET:CE	3:H:177:ARG:NH1	2.82	0.41
3:H:11:ASP:OD1	3:H:14:SER:HB2	2.20	0.41
2:M:170:SER:OG	2:M:172:SER:HB3	2.21	0.41
1:L:241:VAL:HG21	6:L:855:BPH:HBC3	2.02	0.41
1:L:12:PRO:HG3	3:H:97:PRO:CB	2.49	0.41
2:M:236:GLU:OE2	3:H:118:ARG:NH2	2.51	0.41
2:M:155:TRP:NE1	2:M:281:GLY:HA3	2.35	0.41
2:M:253:ARG:NE	9:M:1044:HOH:O	2.40	0.41
5:M:852:BCL:H2C	5:M:852:BCL:HBC2	1.91	0.41
2:M:223:ILE:HA	2:M:223:ILE:HD13	1.89	0.41
2:M:229:PHE:CE2	2:M:247:ARG:HD2	2.56	0.41
2:M:134:TYR:CD1	2:M:134:TYR:C	2.94	0.41
1:L:8:LYS:HA	3:H:87:LEU:HD11	2.03	0.41
2:M:190:SER:HA	2:M:196:LEU:HD13	2.02	0.41
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.55	0.41
2:M:25:ASN:ND2	2:M:28:ASN:ND2	2.69	0.41
3:H:70:ARG:NH2	3:H:123:LEU:HG	2.36	0.41
3:H:240:GLY:O	3:H:244:ALA:HB3	2.19	0.41
2:M:296:VAL:O	2:M:299:GLN:HB2	2.20	0.41
2:M:3:TYR:CZ	2:M:5:ASN:HA	2.55	0.41
3:H:58:LEU:HD23	3:H:58:LEU:HA	1.87	0.41
2:M:18:LEU:HB2	9:M:1084:HOH:O	2.20	0.41
2:M:284:ILE:HG12	5:M:852:BCL:HED3	2.03	0.40
3:H:177:ARG:O	3:H:193:MET:HB2	2.20	0.40
2:M:94:LEU:HA	9:M:1011:HOH:O	2.20	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:L:850:BCL:HMD2	5:L:851:BCL:HBB3	2.02	0.40
2:M:108:PRO:HG2	2:M:111:GLU:CB	2.50	0.40
2:M:239:ALA:HA	3:H:73:LEU:HD22	2.02	0.40
1:L:180:PHE:CD2	1:L:240:ALA:HB1	2.56	0.40
2:M:228:ARG:CZ	3:H:195:MET:HE3	2.51	0.40
1:L:222:TYR:CD1	2:M:47:LEU:HD23	2.56	0.40
1:L:9:TYR:OH	2:M:243:THR:HG23	2.21	0.40
6:L:855:BPH:HMB1	6:L:855:BPH:HBB	1.80	0.40
2:M:300:ASN:O	2:M:301:HIS:HB2	2.21	0.40
2:M:72:ILE:HD13	2:M:72:ILE:HA	1.97	0.40
3:H:134:MET:HB2	3:H:167:ILE:O	2.21	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%)	257 (92%)	21 (8%)	1 (0%)	43	85
2	M	300/307 (98%)	270 (90%)	24 (8%)	6 (2%)	11	47
3	H	238/260 (92%)	220 (92%)	17 (7%)	1 (0%)	43	85
All	All	817/848 (96%)	747 (91%)	62 (8%)	8 (1%)	22	69

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	110	LYS
2	M	301	HIS
1	L	273	ALA
2	M	179	ILE
2	M	92	PHE
2	M	34	PRO
2	M	195	ASN
3	H	245	ALA

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%)	209 (95%)	11 (5%)	34	76
2	M	236/240 (98%)	227 (96%)	9 (4%)	44	85
3	H	195/208 (94%)	185 (95%)	10 (5%)	33	75
All	All	651/668 (98%)	621 (95%)	30 (5%)	37	79

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	21	LEU
1	L	38	THR
1	L	152	THR
1	L	158	SER
1	L	167	PHE
1	L	185	LEU
1	L	207	ARG
1	L	210	ASP
1	L	235	LEU
1	L	271	TRP
1	L	272	TRP
2	M	51	TYR
2	M	59	SER
2	M	86	LEU
2	M	135	LEU
2	M	165	PRO
2	M	188	ASN
2	M	216	PHE
2	M	258	PHE
2	M	274	VAL
3	H	11	ASP
3	H	43	GLU
3	H	94	GLU
3	H	105	MET
3	H	106	LYS
3	H	206	ASN
3	H	219	ILE

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Mol	Chain	Res	Type
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 (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	60	ASN
1	L	173	HIS
1	L	280	ASN
2	M	28	ASN
2	M	202	HIS
2	M	299	GLN
3	H	206	ASN

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 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	-	74,74,74	2.33	16 (21%)	97,115,115	5.14	30 (30%)
5	BCL	L	851	-	74,74,74	1.48	12 (16%)	97,115,115	1.92	23 (23%)
5	BCL	L	853	-	74,74,74	1.51	14 (18%)	97,115,115	2.18	27 (27%)
6	BPH	L	855	-	70,70,70	1.50	7 (10%)	94,101,101	2.35	23 (24%)
5	BCL	M	852	-	74,74,74	1.45	11 (14%)	97,115,115	1.95	25 (25%)
6	BPH	M	854	-	70,70,70	1.53	9 (12%)	94,101,101	1.95	22 (23%)
7	U10	M	857	-	48,48,63	2.18	15 (31%)	59,61,79	2.41	22 (37%)
8	SPO	M	859	-	41,41,41	3.32	25 (60%)	50,50,50	2.98	18 (36%)

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	-	-	0/41/137/137	0/0/9/9
5	BCL	L	851	-	-	0/41/137/137	0/0/9/9
5	BCL	L	853	-	-	0/41/137/137	0/0/9/9
6	BPH	L	855	-	2/2/18/22	0/49/105/105	0/0/6/6
5	BCL	M	852	-	-	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 (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	850	BCL	C3B-C4B	11.85	1.58	1.40
5	L	850	BCL	C1B-NB	-9.00	1.24	1.34
8	M	859	SPO	C15-C16	8.61	1.57	1.34
7	M	857	U10	C6-C1	6.95	1.52	1.35
6	M	854	BPH	C1D-CHD	6.80	1.43	1.35
6	L	855	BPH	C1D-CHD	6.78	1.42	1.35
8	M	859	SPO	C10-C11	6.57	1.52	1.34
8	M	859	SPO	C6-C5	6.25	1.50	1.31
8	M	859	SPO	C21-C20	5.54	1.50	1.35
5	L	850	BCL	C3B-C2B	5.28	1.56	1.40
5	L	853	BCL	C2-C3	5.16	1.43	1.32
6	L	855	BPH	C3B-C4B	4.94	1.47	1.40
5	L	851	BCL	C1A-NA	4.87	1.43	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	859	SPO	C27-C28	4.78	1.39	1.34
8	M	859	SPO	C13-C12	4.76	1.59	1.51
8	M	859	SPO	C26-C25	4.62	1.47	1.34
5	M	852	BCL	C1A-NA	4.51	1.42	1.32
5	L	853	BCL	C1A-NA	4.32	1.41	1.32
6	M	854	BPH	C3B-C4B	4.30	1.46	1.40
5	L	850	BCL	C2-C3	4.26	1.41	1.32
5	L	850	BCL	C1A-NA	4.12	1.41	1.32
5	L	853	BCL	C3B-C4B	4.03	1.46	1.40
5	L	850	BCL	C3B-CAB	4.02	1.60	1.49
7	M	857	U10	C4-C3	3.93	1.53	1.35
5	M	852	BCL	C3B-C4B	3.93	1.46	1.40
5	L	851	BCL	C3B-C4B	3.82	1.46	1.40
8	M	859	SPO	O1-CM1	3.81	1.55	1.43
7	M	857	U10	C18-C19	3.72	1.40	1.32
8	M	859	SPO	C11-C12	-3.72	1.37	1.45
8	M	859	SPO	C15-C14	3.70	1.54	1.43
8	M	859	SPO	C4-C5	-3.68	1.44	1.50
5	M	852	BCL	C3D-CAD	-3.59	1.40	1.47
5	M	852	BCL	C4C-NC	3.59	1.40	1.32
5	M	852	BCL	C2-C3	3.59	1.40	1.32
8	M	859	SPO	C32-C33	3.56	1.40	1.32
6	M	854	BPH	C2-C3	3.55	1.40	1.32
8	M	859	SPO	C31-C32	-3.49	1.40	1.50
7	M	857	U10	C33-C34	3.48	1.40	1.32
7	M	857	U10	C13-C14	3.46	1.39	1.32
6	L	855	BPH	C2-C3	3.44	1.39	1.32
7	M	857	U10	C7-C8	-3.43	1.45	1.50
5	L	851	BCL	C4C-NC	3.42	1.39	1.32
7	M	857	U10	C6-C5	3.38	1.56	1.46
7	M	857	U10	C23-C24	3.38	1.39	1.32
5	L	851	BCL	C4B-NB	3.33	1.38	1.34
8	M	859	SPO	C14-C12	3.33	1.40	1.35
8	M	859	SPO	C8-C7	3.28	1.56	1.51
5	L	850	BCL	C4C-NC	3.25	1.39	1.32
6	M	854	BPH	CMB-C2B	3.23	1.58	1.51
7	M	857	U10	C7-C6	3.23	1.57	1.51
7	M	857	U10	C28-C29	3.19	1.39	1.32
7	M	857	U10	C38-C39	3.15	1.40	1.34
5	L	851	BCL	C2-C3	3.09	1.39	1.32
5	L	853	BCL	C4C-NC	3.07	1.39	1.32
5	L	853	BCL	C3D-CAD	-3.02	1.41	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	851	BCL	C3D-CAD	-3.00	1.41	1.47
8	M	859	SPO	C37-C38	3.00	1.42	1.32
5	L	850	BCL	C3D-C2D	2.99	1.49	1.40
5	L	851	BCL	C3D-C2D	2.98	1.49	1.40
5	M	852	BCL	C3D-C2D	2.98	1.49	1.40
5	L	850	BCL	CAA-C2A	2.90	1.59	1.54
8	M	859	SPO	C24-C23	2.89	1.56	1.51
8	M	859	SPO	O1-C1	2.88	1.59	1.41
8	M	859	SPO	C10-C9	2.86	1.52	1.43
6	L	855	BPH	CMB-C2B	2.83	1.57	1.51
6	L	855	BPH	C3D-CAD	-2.82	1.41	1.47
5	L	850	BCL	CMB-C2B	2.81	1.57	1.51
7	M	857	U10	C8-C9	2.75	1.38	1.32
5	M	852	BCL	C3B-C2B	2.75	1.48	1.40
5	L	853	BCL	CMB-C2B	2.74	1.57	1.51
5	L	853	BCL	C4B-NB	2.74	1.38	1.34
5	L	850	BCL	C3D-CAD	-2.73	1.41	1.47
8	M	859	SPO	C25-C23	-2.73	1.39	1.45
5	L	853	BCL	C3D-C2D	2.72	1.48	1.40
8	M	859	SPO	C19-C17	2.72	1.39	1.35
5	M	852	BCL	CMB-C2B	2.68	1.57	1.51
5	M	852	BCL	C3B-CAB	2.65	1.56	1.49
5	L	851	BCL	CMB-C2B	2.64	1.57	1.51
5	L	851	BCL	C3B-C2B	2.62	1.48	1.40
8	M	859	SPO	C6-C7	-2.58	1.40	1.45
6	L	855	BPH	C3D-C2D	2.55	1.48	1.40
6	M	854	BPH	C3D-C2D	2.55	1.48	1.40
6	M	854	BPH	C3D-CAD	-2.53	1.42	1.47
6	M	854	BPH	C1B-CHB	-2.43	1.36	1.46
5	M	852	BCL	C4B-NB	2.43	1.37	1.34
5	L	853	BCL	C3B-CAB	2.43	1.55	1.49
5	L	850	BCL	C3A-C2A	-2.41	1.47	1.54
8	M	859	SPO	C4-C1	-2.41	1.51	1.54
8	M	859	SPO	C29-C28	2.33	1.56	1.50
5	L	853	BCL	C3B-C2B	2.33	1.47	1.40
5	L	851	BCL	C3C-C4C	-2.31	1.48	1.51
5	L	851	BCL	O2A-CGA	-2.30	1.25	1.33
5	L	850	BCL	C4B-CHC	2.30	1.46	1.39
5	M	852	BCL	CBB-CAB	2.29	1.57	1.49
5	L	851	BCL	C3B-CAB	2.28	1.55	1.49
7	M	857	U10	O4-C4	2.25	1.42	1.36
7	M	857	U10	C41-C39	2.25	1.52	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	853	BCL	C3A-C2A	-2.25	1.47	1.54
6	L	855	BPH	O2A-CGA	-2.24	1.26	1.33
6	M	854	BPH	C3A-C2A	-2.22	1.48	1.54
5	L	850	BCL	O2A-CGA	-2.19	1.26	1.33
6	M	854	BPH	C1C-NC	-2.11	1.33	1.38
5	L	850	BCL	O2D-CGD	-2.10	1.27	1.33
5	L	853	BCL	MG-NB	2.08	2.09	2.05
5	L	853	BCL	CAA-C2A	2.06	1.57	1.54
5	L	853	BCL	C1B-C2B	2.05	1.42	1.40
5	L	850	BCL	MG-NB	2.05	2.09	2.05
7	M	857	U10	C12-C13	-2.01	1.44	1.50
8	M	859	SPO	C35-C33	2.01	1.56	1.51

All (190) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	850	BCL	OBB-CAB-C3B	28.54	162.90	120.07
5	L	850	BCL	C4B-C3B-C2B	-22.97	79.19	106.97
5	L	850	BCL	C3B-C4B-NB	16.98	125.15	108.64
5	L	850	BCL	OBB-CAB-CBB	-16.88	78.19	120.13
5	L	850	BCL	CBB-CAB-C3B	-12.18	84.71	120.30
8	M	859	SPO	C25-C23-C22	-11.55	101.23	118.97
5	L	850	BCL	CMB-C2B-C1B	-9.18	114.50	128.62
5	L	853	BCL	CAA-C2A-C1A	-8.60	90.16	111.62
6	L	855	BPH	C6-C5-C3	7.94	131.65	112.78
8	M	859	SPO	C26-C27-C28	-7.92	120.33	127.91
5	L	850	BCL	CAA-C2A-C1A	-7.44	93.05	111.62
6	L	855	BPH	C4-C3-C5	7.40	126.64	115.39
5	L	850	BCL	CHC-C4B-NB	-7.24	112.49	124.58
5	M	852	BCL	CMB-C2B-C1B	-6.82	118.13	128.62
5	L	851	BCL	CMB-C2B-C1B	-6.55	118.55	128.62
6	L	855	BPH	C4B-C3B-C2B	-6.44	102.93	107.60
6	L	855	BPH	C5-C3-C2	-6.41	108.75	121.08
8	M	859	SPO	C18-C17-C19	-6.24	114.06	122.92
5	L	853	BCL	CMB-C2B-C1B	-6.21	119.06	128.62
6	L	855	BPH	CMB-C2B-C1B	-5.94	119.62	128.65
5	L	850	BCL	C4D-C3D-C2D	-5.91	100.19	107.42
5	L	853	BCL	C4D-C3D-C2D	-5.86	100.26	107.42
6	M	854	BPH	C4B-C3B-C2B	-5.85	103.36	107.60
5	M	852	BCL	CMB-C2B-C3B	5.84	134.16	124.97
7	M	857	U10	C15-C14-C13	-5.75	112.14	123.52
6	M	854	BPH	CMB-C2B-C1B	-5.74	119.92	128.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	851	BCL	C4D-C3D-C2D	-5.69	100.47	107.42
7	M	857	U10	C7-C6-C5	5.63	124.86	118.75
6	L	855	BPH	C1-O2A-CGA	5.61	132.69	116.98
6	M	854	BPH	CMB-C2B-C3B	5.52	133.67	124.97
6	L	855	BPH	CMB-C2B-C3B	5.49	133.62	124.97
5	L	851	BCL	CMB-C2B-C3B	5.49	133.62	124.97
7	M	857	U10	C10-C9-C8	-5.45	112.73	123.52
7	M	857	U10	C15-C14-C16	5.42	123.64	115.39
5	M	852	BCL	C4D-C3D-C2D	-5.42	100.80	107.42
5	L	853	BCL	CMB-C2B-C3B	5.33	133.36	124.97
8	M	859	SPO	C20-C21-C22	-5.22	111.80	123.36
6	M	854	BPH	C1-O2A-CGA	5.22	131.60	116.98
6	L	855	BPH	C4D-C3D-C2D	-4.86	101.49	107.37
6	L	855	BPH	C7-C6-C5	-4.79	98.90	113.01
6	M	854	BPH	C4D-C3D-C2D	-4.70	101.68	107.37
5	M	852	BCL	C6-C5-C3	4.62	123.76	112.78
5	L	853	BCL	CHC-C4B-NB	-4.50	117.07	124.58
5	L	853	BCL	C4B-C3B-C2B	-4.49	101.54	106.97
5	L	851	BCL	C4B-C3B-C2B	-4.49	101.54	106.97
6	M	854	BPH	O2A-C1-C2	-4.48	98.83	108.55
5	M	852	BCL	C4B-C3B-C2B	-4.47	101.56	106.97
7	M	857	U10	C7-C8-C9	4.46	134.29	126.76
8	M	859	SPO	C24-C23-C22	-4.44	116.61	122.92
6	M	854	BPH	C4-C3-C5	4.41	122.10	115.39
7	M	857	U10	C35-C34-C33	-4.36	114.88	123.52
5	L	850	BCL	C4B-C3B-CAB	4.35	146.17	127.09
5	M	852	BCL	CED-O2D-CGD	4.32	126.29	116.02
5	M	852	BCL	CHC-C4B-NB	-4.28	117.42	124.58
5	L	850	BCL	O2A-C1-C2	-4.17	99.52	108.55
5	L	853	BCL	C3B-C4B-NB	4.15	112.67	108.64
5	L	851	BCL	CHC-C4B-NB	-4.10	117.74	124.58
7	M	857	U10	C11-C9-C8	4.06	128.90	121.08
5	L	851	BCL	C2A-C3A-C4A	4.02	107.58	101.40
5	L	851	BCL	CED-O2D-CGD	4.02	125.58	116.02
8	M	859	SPO	C11-C12-C14	-4.02	112.80	118.97
8	M	859	SPO	C15-C14-C12	-3.97	121.57	127.29
8	M	859	SPO	C8-C7-C9	3.96	128.53	122.92
6	M	854	BPH	C3B-C4B-NB	3.91	111.51	107.10
5	M	852	BCL	C2A-C3A-C4A	3.89	107.38	101.40
6	L	855	BPH	C3B-C4B-NB	3.87	111.47	107.10
8	M	859	SPO	C4-C5-C6	-3.86	118.56	124.95
6	L	855	BPH	C6-C7-C8	3.86	126.25	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	855	BPH	C4B-CHC-C1C	3.78	139.63	127.62
5	L	850	BCL	CBA-CAA-C2A	3.78	125.23	114.01
5	L	851	BCL	OBD-CAD-C3D	-3.74	120.94	127.91
7	M	857	U10	C20-C19-C18	-3.74	116.12	123.52
5	L	851	BCL	C3B-C4B-NB	3.67	112.20	108.64
5	L	850	BCL	C4B-CHC-C1C	3.65	137.67	130.06
5	L	853	BCL	CED-O2D-CGD	3.63	124.66	116.02
5	L	853	BCL	CBA-CAA-C2A	3.61	124.72	114.01
7	M	857	U10	C25-C24-C23	-3.58	116.43	123.52
5	M	852	BCL	C3B-C4B-NB	3.58	112.12	108.64
5	L	850	BCL	C2A-C3A-C4A	3.57	106.90	101.40
5	M	852	BCL	OBD-CAD-C3D	-3.52	121.37	127.91
5	L	850	BCL	C3B-C2B-C1B	3.47	120.17	109.98
5	L	850	BCL	OBD-CAD-C3D	-3.44	121.50	127.91
5	M	852	BCL	CHA-C1A-NA	-3.43	119.18	126.22
5	L	853	BCL	OBD-CAD-C3D	-3.41	121.57	127.91
8	M	859	SPO	C2-C1-C4	-3.39	105.36	110.97
5	L	851	BCL	CGD-CBD-CHA	3.38	122.43	110.96
5	L	853	BCL	CAA-C2A-C3A	-3.37	105.08	113.04
6	M	854	BPH	O1D-CGD-CBD	-3.36	117.54	124.42
5	L	853	BCL	C2A-C3A-C4A	3.35	106.55	101.40
8	M	859	SPO	C15-C16-C17	-3.33	116.87	126.38
6	M	854	BPH	C4B-CHC-C1C	3.33	138.18	127.62
5	L	853	BCL	C16-C15-C13	-3.30	105.62	115.14
5	L	853	BCL	CAC-C3C-C2C	-3.29	106.33	113.89
7	M	857	U10	C25-C24-C26	3.25	120.33	115.39
5	L	850	BCL	CED-O2D-CGD	3.25	123.75	116.02
7	M	857	U10	C35-C34-C36	3.24	120.32	115.39
5	L	850	BCL	CAA-C2A-C3A	-3.24	105.39	113.04
5	L	850	BCL	C2B-C3B-CAB	-3.24	116.39	127.43
6	M	854	BPH	O2D-CGD-CBD	3.19	117.82	111.33
5	L	850	BCL	C2A-C1A-CHA	3.15	129.29	123.83
7	M	857	U10	C4M-O4-C4	3.08	126.95	116.48
5	L	853	BCL	O2A-CGA-CBA	3.05	121.54	111.94
5	L	851	BCL	CHA-C1A-NA	-3.04	119.97	126.22
7	M	857	U10	C30-C29-C31	3.01	119.97	115.39
5	M	852	BCL	C2A-C1A-CHA	2.91	128.87	123.83
8	M	859	SPO	C16-C17-C19	2.87	123.38	118.97
7	M	857	U10	C21-C19-C18	2.86	126.59	121.08
6	L	855	BPH	O1D-CGD-CBD	-2.81	118.65	124.42
6	L	855	BPH	O2D-CGD-CBD	2.82	117.07	111.33
5	L	853	BCL	C2C-C3C-C4C	2.80	104.94	101.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	855	BPH	C3D-CAD-CBD	2.80	111.55	107.60
5	L	850	BCL	CHA-C1A-NA	-2.78	120.52	126.22
5	L	851	BCL	C2A-C1A-CHA	2.77	128.62	123.83
8	M	859	SPO	C18-C17-C16	2.76	122.56	118.09
6	L	855	BPH	C3C-C4C-CHD	2.70	127.44	121.83
5	L	851	BCL	C2D-C1D-ND	2.70	111.45	109.41
6	M	854	BPH	C3D-CAD-CBD	2.68	111.39	107.60
5	L	850	BCL	C1-O2A-CGA	2.67	124.45	116.98
6	L	855	BPH	CHD-C4C-NC	-2.66	119.73	124.54
6	M	854	BPH	C3C-C4C-CHD	2.61	127.26	121.83
5	M	852	BCL	C4B-CHC-C1C	2.59	135.45	130.06
5	L	851	BCL	C6-C5-C3	2.58	118.92	112.78
6	L	855	BPH	C1-C2-C3	2.56	130.73	126.19
5	L	853	BCL	C2A-C1A-CHA	2.55	128.26	123.83
7	M	857	U10	O5-C5-C4	-2.53	115.35	120.96
7	M	857	U10	C30-C29-C28	-2.52	118.53	123.52
7	M	857	U10	C11-C12-C13	2.51	118.78	111.62
5	M	852	BCL	C4D-C3D-CAD	-2.50	104.98	108.05
6	L	855	BPH	CED-O2D-CGD	2.49	121.94	116.02
5	M	852	BCL	C15-C13-C12	-2.49	99.10	111.92
5	L	853	BCL	C4B-CHC-C1C	2.46	135.19	130.06
5	L	853	BCL	CHA-C1A-NA	-2.46	121.17	126.22
5	L	853	BCL	C2B-C1B-NB	2.46	111.27	109.41
6	M	854	BPH	CHD-C4C-NC	-2.45	120.10	124.54
7	M	857	U10	C7-C6-C1	-2.44	117.35	123.35
5	L	851	BCL	C4B-CHC-C1C	2.44	135.15	130.06
6	M	854	BPH	CED-O2D-CGD	2.44	121.82	116.02
5	L	850	BCL	C6-C5-C3	2.43	118.57	112.78
5	L	851	BCL	CAA-C2A-C1A	-2.43	105.56	111.62
6	M	854	BPH	C4D-CHA-CBD	-2.43	104.14	110.15
6	L	855	BPH	C4D-CHA-CBD	-2.41	104.17	110.15
6	M	854	BPH	C2B-C1B-NB	2.37	112.77	108.16
5	L	850	BCL	C2D-C3D-CAD	2.36	154.29	138.46
5	M	852	BCL	C3B-C4B-CHC	2.35	130.46	126.00
5	M	852	BCL	C2D-C3D-CAD	2.34	154.22	138.46
8	M	859	SPO	C13-C12-C11	2.34	121.87	118.09
5	L	853	BCL	O2A-C1-C2	-2.33	103.49	108.55
5	L	853	BCL	C2D-C3D-CAD	2.33	154.11	138.46
5	L	851	BCL	C2D-C3D-CAD	2.33	154.09	138.46
5	L	851	BCL	C4D-CHA-CBD	-2.32	103.91	109.37
6	M	854	BPH	C2A-C1A-CHA	2.30	130.92	125.03
5	L	853	BCL	O1D-CGD-CBD	-2.29	119.73	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	855	BPH	C2D-C3D-CAD	2.29	153.85	138.46
8	M	859	SPO	C10-C9-C7	-2.28	124.00	127.29
5	L	850	BCL	C15-C13-C12	-2.26	100.27	111.92
6	M	854	BPH	C2D-C3D-CAD	2.25	153.59	138.46
5	M	852	BCL	C4D-CHA-C1A	2.25	126.84	120.32
5	L	853	BCL	C3B-C4B-CHC	2.24	130.26	126.00
7	M	857	U10	C31-C32-C33	-2.24	105.22	111.62
5	L	850	BCL	C2C-C3C-C4C	2.24	104.15	101.05
5	M	852	BCL	C3D-CAD-CBD	2.23	110.75	107.60
7	M	857	U10	C40-C39-C38	-2.22	118.30	123.62
5	L	851	BCL	C2C-C3C-C4C	2.22	104.13	101.05
5	L	853	BCL	C3A-C2A-C1A	2.20	104.20	101.08
6	M	854	BPH	C6-C5-C3	2.20	118.01	112.78
7	M	857	U10	C8-C7-C6	-2.19	104.61	111.61
5	L	850	BCL	C4B-NB-C1B	-2.19	103.88	106.76
5	L	851	BCL	C3D-CAD-CBD	2.19	110.69	107.60
5	L	851	BCL	C2B-C1B-NB	2.19	111.06	109.41
8	M	859	SPO	C9-C10-C11	-2.17	115.92	123.24
5	L	851	BCL	C3B-C4B-CHC	2.13	130.05	126.00
5	L	851	BCL	C4D-C3D-CAD	-2.12	105.44	108.05
5	L	853	BCL	CMD-C2D-C1D	2.11	130.32	126.16
6	M	854	BPH	C4-C3-C2	-2.10	119.35	123.52
5	M	852	BCL	C2D-C1D-ND	2.10	111.00	109.41
5	M	852	BCL	O2A-CGA-CBA	2.08	118.48	111.94
5	M	852	BCL	CGD-CBD-CAD	-2.08	103.90	110.96
6	M	854	BPH	C2A-C3A-C4A	2.07	105.78	101.11
5	L	853	BCL	CMD-C2D-C3D	-2.07	121.71	124.97
5	M	852	BCL	C2C-C3C-C4C	2.07	103.92	101.05
8	M	859	SPO	C31-C32-C33	2.07	132.25	127.80
5	L	850	BCL	C4D-C3D-CAD	-2.06	105.52	108.05
6	L	855	BPH	C2B-C1B-NB	2.06	112.16	108.16
8	M	859	SPO	C34-C33-C35	-2.05	112.26	115.39
7	M	857	U10	C27-C28-C29	-2.05	123.37	127.80
5	L	850	BCL	CMD-C2D-C3D	-2.04	121.75	124.97
6	L	855	BPH	C3D-C4D-ND	2.04	114.93	108.80
5	M	852	BCL	C2B-C1B-NB	2.04	110.95	109.41
5	L	850	BCL	O1D-CGD-CBD	-2.02	120.28	124.42
5	M	852	BCL	C4D-CHA-CBD	-2.01	104.63	109.37

All (4) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
6	L	855	BPH	C8
6	L	855	BPH	C13
6	M	854	BPH	C8
6	M	854	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.