



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 04:12 AM EDT

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 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

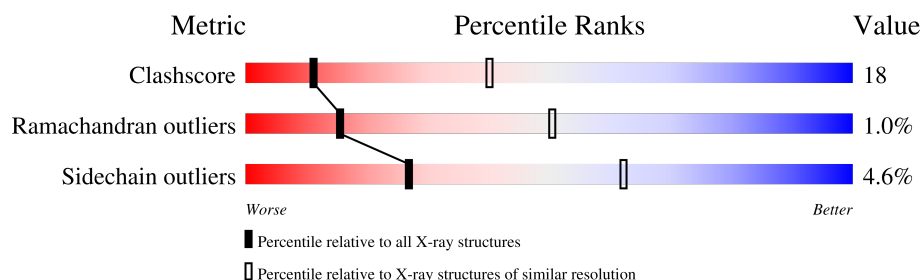
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

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 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	1607	394	398	10			

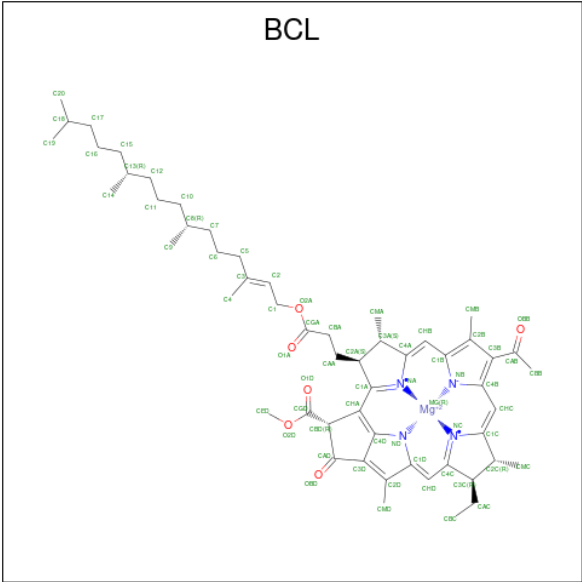
There is a discrepancy between the modelled and reference sequences:

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

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

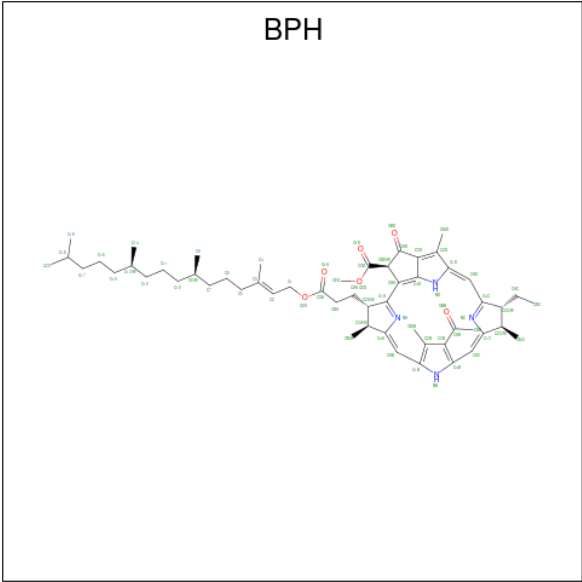
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	240	Total	C	N	O	S	0	0	0
			1829	1169	314	337	9			

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



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

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

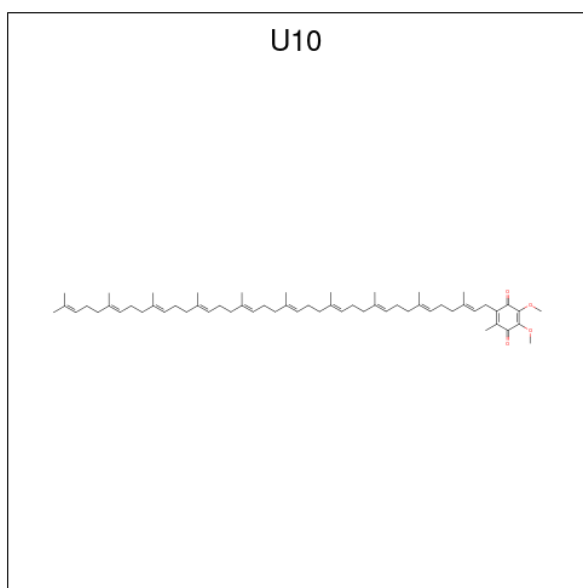


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

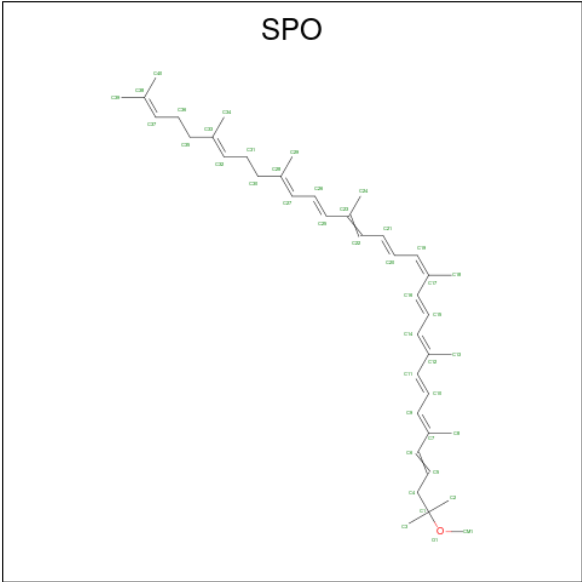
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	M	1	Total	Fe	0	0
			1	1		

- Molecule 7 is UBIQUINONE-10 (three-letter code: U10) (formula: C₅₉H₉₀O₄).



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: C₄₁H₆₀O).



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

- Molecule 9 is water.

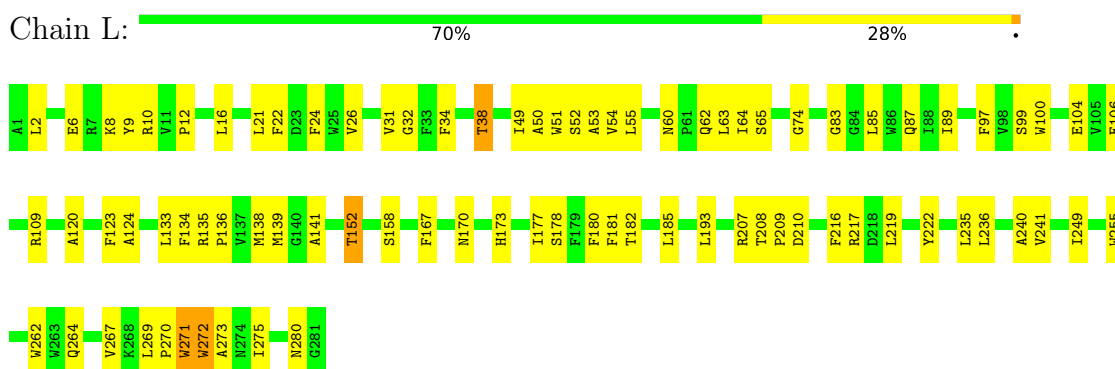
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	L	28	Total	O	0	0
			28	28		
9	M	37	Total	O	0	0
			37	37		
9	H	47	Total	O	0	0
			47	47		

3 Residue-property plots

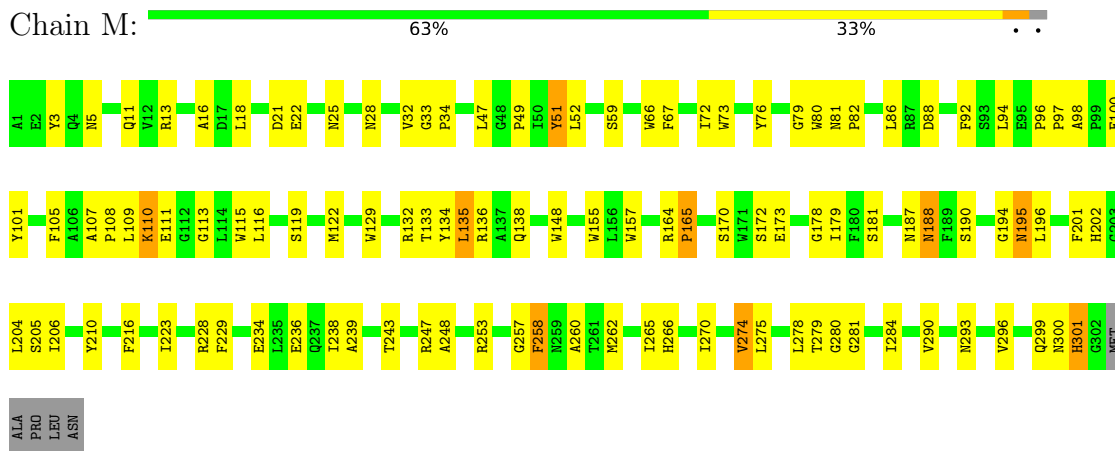
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

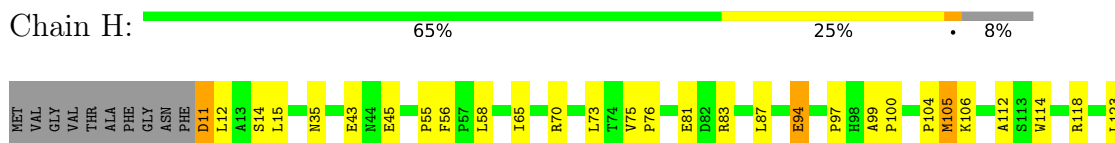
• Molecule 1: Photosynthetic Reaction Center L subunit

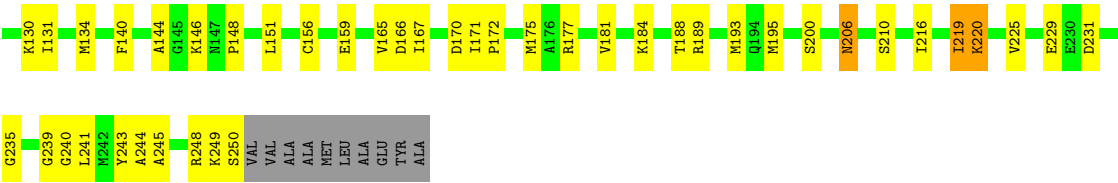


• Molecule 2: Photosynthetic Reaction Center M subunit



• Molecule 3: Photosynthetic Reaction Center H subunit





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BPH, FE, SPO, BCL, 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	0.59	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 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	79	0
2	M	2409	0	2318	110	0
3	H	1829	0	1836	57	0
4	L	198	0	222	13	0
4	M	66	0	74	7	0
5	L	65	0	76	7	0
5	M	65	0	76	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	M	1	0	0	0	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

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 18.

All (248) 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: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:HD13	3:H:219:ILE:H	1.55	0.71
3:H:131:ILE:CD1	3:H:177:ARG:HD2	2.20	0.70
1:L:271:TRP:CD1	1:L:271:TRP:N	2.53	0.70
5:L:855:BPH:HBB2	2:M:210:TYR:HB3	1.72	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	Interatomic distance (Å)	Clash overlap (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
4:L:850:BCL:H2	5:M:854:BPH:HMB2	1.78	0.65
1:L:271:TRP:H	1:L:271:TRP:HD1	1.40	0.65
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.80	0.64
2:M:67:PHE:CD1	5: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	5:M:854:BPH:HBB2	1.84	0.60
4:L:853:BCL:HMD2	4: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
2:M:73:TRP:O	2:M:76:TYR:HB2	2.03	0.58
3:H:241:LEU:O	3:H:248:ARG:NH2	2.36	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
5:L:855:BPH:HHC	5:L:855:BPH:HBB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:243:THR:HG22	2:M:247:ARG:NE	2.16	0.57
4:M:852:BCL:H203	4: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
5:M:854:BPH:H7C1	5: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
4:L:850:BCL:CBB	4:L:850:BCL:HHC	2.38	0.54
1:L:31:VAL:HG12	1:L:32:GLY:N	2.21	0.54
1:L:177:ILE:HG12	4:L:851:BCL:HMB3	1.90	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
4: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:98:ALA:HB1	2:M:100:GLU:OE1	2.08	0.52
2:M:205:SER:CB	9:M:1025:HOH:O	2.57	0.52
1:L:219:LEU:HD12	2:M:132:ARG:HH11	1.70	0.52
2:M:206:ILE:HG23	4:M:852:BCL:HMB3	1.91	0.52
1:L:34:PHE:O	1:L:38:THR:CG2	2.55	0.52
4:L:850:BCL:HHC	4: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	5: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
2:M:80:TRP:O	2:M:82:PRO:HD3	2.11	0.50
3:H:156:CYS:HB2	3:H:248:ARG:HG3	1.94	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
5:M:854:BPH:HHC	5:M:854:BPH:HBB3	1.94	0.49
1:L:74:GLY:O	1:L:141:ALA:HA	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:83:GLY:O	1:L:87:GLN:HG3	2.12	0.49
2:M:243:THR:HG22	2:M:247:ARG:CG	2.42	0.49
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
4:L:851:BCL:HAA2	4: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
1:L:2:LEU:HD22	1:L:6:GLU:HG2	1.96	0.47
5:L:855:BPH:H121	5:L:855:BPH:H8	1.70	0.47
4:L:850:BCL:HMB2	5:M:854:BPH:HMB3	1.96	0.47
1:L:34:PHE:HB2	9:L:1053:HOH:O	2.13	0.47
1:L:109:ARG:HH11	1:L:109:ARG:HG2	1.79	0.47
1:L:219:LEU:HD11	2:M:133:THR:HG22	1.94	0.47
2:M:21:ASP:O	2:M:22:GLU:C	2.53	0.47
2:M:110:LYS:O	2:M:111:GLU:HG2	2.15	0.47
1:L:170:ASN:HB3	1:L:173:HIS:HB2	1.96	0.47
2:M:66:TRP:CD1	2:M:122:MET:HB2	2.49	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	5: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:255:TRP:CZ2	1:L:262:TRP:HB2	2.50	0.47
1:L:272:TRP:HA	1:L:275:ILE:CD1	2.45	0.47
3:H:118:ARG:HD2	9:H:1106:HOH:O	2.14	0.46
3:H:175:MET:HE1	3:H:177:ARG:NH1	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:H271	7:M:857:U10:H251	1.63	0.45
3:H:165:VAL:O	3:H:166:ASP:HB2	2.16	0.45
1:L:124:ALA:HB2	5:L:855:BPH:HBC2	1.97	0.45
1:L:217:ARG:HH11	1:L:217:ARG:HG3	1.81	0.45
1:L:26:VAL:HG23	1:L:31:VAL:CG2	2.46	0.45
3:H:140:PHE:CE1	3:H:171:ILE:HD12	2.52	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:51:TYR:C	2:M:51:TYR:CD2	2.90	0.44
2:M:100:GLU:CD	2:M:100:GLU:H	2.21	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
4:L:851:BCL:H122	5:L:855:BPH:H3A	1.99	0.44
5:M:854:BPH:HMB1	5:M:854:BPH:HHB	1.75	0.44
2:M:129:TRP:O	2:M:133:THR:HG23	2.18	0.44
1:L:22:PHE:HA	1:L:24:PHE:HE2	1.82	0.43
1:L:178:SER:HA	4:L:850:BCL:O1A	2.18	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
2:M:52:LEU:HD12	2:M:52:LEU:HA	1.57	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
3:H:249:LYS:O	3:H:250:SER:HB3	2.18	0.43
1:L:49:ILE:HG13	1:L:89:ILE:HD13	2.00	0.43
4:L:850:BCL:H62	4:M:852:BCL:H202	2.01	0.43
3:H:83:ARG:NH1	3:H:114:TRP:O	2.52	0.43
1:L:269:LEU:HA	1:L:270:PRO:HD3	1.86	0.43
3:H:184:LYS:HD2	3:H:184:LYS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:L:16:LEU:HG	1:L:106:GLU:HG2	2.02	0.42
4:L:851:BCL:CAA	4:L:853:BCL:HBC1	2.48	0.42
3:H:55:PRO:HG2	3:H:56:PHE:H	1.84	0.42
3:H:130:LYS:HZ1	3:H:172:PRO:HG2	1.84	0.42
2:M:164:ARG:NH1	2:M:173:GLU:OE1	2.46	0.42
1:L:269:LEU:HB2	1:L:272:TRP:HE1	1.84	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
2:M:16:ALA:HB1	2:M:32:VAL:HG11	2.00	0.42
2:M:187:ASN:HA	4:M:852:BCL:HBC1	2.02	0.42
2:M:96:PRO:HA	2:M:115:TRP:CG	2.55	0.42
7:M:857:U10:H222	7:M:857:U10:H201	1.58	0.42
1:L:269:LEU:HB2	1:L:272:TRP:NE1	2.34	0.42
7:M:857:U10:H271	7:M:857:U10:H312	1.90	0.42
1:L:217:ARG:HG3	1:L:217:ARG:NH1	2.34	0.42
1:L:109:ARG:HG2	1:L:109:ARG:NH1	2.34	0.42
1:L:139:MET:HB3	1:L:139:MET:HE2	1.91	0.42
3:H:11:ASP:OD1	3:H:14:SER:HB2	2.20	0.41
3:H:175:MET:CE	3:H:177:ARG:NH1	2.82	0.41
2:M:170:SER:OG	2:M:172:SER:HB3	2.21	0.41
1:L:12:PRO:HG3	3:H:97:PRO:CB	2.49	0.41
1:L:241:VAL:HG21	5:L:855:BPH:HBC3	2.02	0.41
2:M:155:TRP:NE1	2:M:281:GLY:HA3	2.35	0.41
2:M:236:GLU:OE2	3:H:118:ARG:NH2	2.51	0.41
2:M:253:ARG:NE	9:M:1044:HOH:O	2.40	0.41
2:M:223:ILE:HD13	2:M:223:ILE:HA	1.89	0.41
4:M:852:BCL:HBC2	4:M:852:BCL:H2C	1.91	0.41
2:M:134:TYR:CD1	2:M:134:TYR:C	2.94	0.41
2:M:229:PHE:CE2	2:M:247:ARG:HD2	2.56	0.41
1:L:8:LYS:HA	3:H:87:LEU:HD11	2.03	0.41
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.55	0.41
2:M:3:TYR:CZ	2:M:5:ASN:HA	2.55	0.41
2:M:25:ASN:ND2	2:M:28:ASN:ND2	2.69	0.41
2:M:190:SER:HA	2:M:196:LEU:HD13	2.02	0.41
2:M:296:VAL:O	2:M:299:GLN:HB2	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:18:LEU:HB2	9:M:1084:HOH:O	2.20	0.41
3:H:58:LEU:HA	3:H:58:LEU:HD23	1.87	0.41
2:M:94:LEU:HA	9:M:1011:HOH:O	2.20	0.40
2:M:284:ILE:HG12	4:M:852:BCL:HED3	2.03	0.40
3:H:177:ARG:O	3:H:193:MET:HB2	2.20	0.40
1:L:180:PHE:CD2	1:L:240:ALA:HB1	2.56	0.40
4:L:850:BCL:HMD2	4: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:222:TYR:CD1	2:M:47:LEU:HD23	2.56	0.40
2:M:228:ARG:CZ	3:H:195:MET:HE3	2.51	0.40
1:L:9:TYR:OH	2:M:243:THR:HG23	2.21	0.40
5:L:855:BPH:HHB	5:L:855:BPH:HMB1	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	279/281 (99%)	257 (92%)	21 (8%)	1 (0%)	34	71
2	M	300/307 (98%)	270 (90%)	24 (8%)	6 (2%)	7	32
3	H	238/260 (92%)	220 (92%)	17 (7%)	1 (0%)	34	71
All	All	817/848 (96%)	747 (91%)	62 (8%)	8 (1%)	15	50

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	110	LYS

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Mol	Chain	Res	Type
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%)	24	59
2	M	236/240 (98%)	227 (96%)	9 (4%)	33	68
3	H	195/208 (94%)	185 (95%)	10 (5%)	24	58
All	All	651/668 (98%)	621 (95%)	30 (5%)	27	62

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

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Mol	Chain	Res	Type
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
3	H	220	LYS
3	H	225	VAL
3	H	231	ASP

Sometimes 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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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
4	BCL	L	851	-	58,74,74	1.60	8 (13%)	69,115,115	1.85	12 (17%)
4	BCL	L	853	-	58,74,74	1.57	8 (13%)	69,115,115	2.12	19 (27%)
8	SPO	M	859	-	40,41,41	3.39	25 (62%)	47,50,50	2.82	15 (31%)
4	BCL	M	852	-	58,74,74	1.58	9 (15%)	69,115,115	1.97	15 (21%)
7	U10	M	857	-	48,48,63	2.28	13 (27%)	58,61,79	2.16	20 (34%)
5	BPH	M	854	-	64,70,70	1.44	11 (17%)	76,101,101	1.84	17 (22%)
4	BCL	L	850	-	58,74,74	2.55	11 (18%)	69,115,115	4.68	23 (33%)
5	BPH	L	855	-	64,70,70	1.37	8 (12%)	76,101,101	2.27	21 (27%)

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
4	BCL	L	851	-	-	1/37/137/137	-
4	BCL	L	853	-	-	5/37/137/137	-
8	SPO	M	859	-	-	14/47/47/47	-
4	BCL	M	852	-	-	10/37/137/137	-
7	U10	M	857	-	-	16/45/69/87	0/1/1/1
5	BPH	M	854	-	-	7/54/105/105	0/5/6/6
4	BCL	L	850	-	-	10/37/137/137	-
5	BPH	L	855	-	-	9/54/105/105	0/5/6/6

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	850	BCL	C1B-NB	-12.34	1.24	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	850	BCL	C3B-C2B	9.44	1.56	1.39
7	M	857	U10	C6-C1	9.39	1.52	1.35
8	M	859	SPO	C15-C16	9.03	1.57	1.34
8	M	859	SPO	C6-C5	6.95	1.50	1.32
8	M	859	SPO	C10-C11	6.88	1.52	1.34
4	L	850	BCL	C3D-C2D	5.57	1.49	1.39
8	M	859	SPO	C21-C20	5.56	1.50	1.36
4	L	851	BCL	C3D-C2D	5.56	1.49	1.39
4	M	852	BCL	C3D-C2D	5.54	1.49	1.39
4	M	852	BCL	C3B-C2B	5.17	1.48	1.39
4	L	853	BCL	C3D-C2D	5.12	1.48	1.39
4	L	851	BCL	C3B-C2B	4.95	1.48	1.39
8	M	859	SPO	C26-C25	4.83	1.47	1.34
8	M	859	SPO	C27-C28	4.83	1.39	1.34
5	M	854	BPH	C3D-C2D	4.83	1.48	1.39
5	L	855	BPH	C3D-C2D	4.83	1.48	1.39
4	L	853	BCL	C3B-C2B	4.45	1.47	1.39
4	L	853	BCL	C2-C3	4.33	1.43	1.33
4	L	850	BCL	C3B-CAB	4.17	1.60	1.49
7	M	857	U10	C4-C3	4.14	1.53	1.36
8	M	859	SPO	C13-C12	4.07	1.59	1.50
4	L	851	BCL	C4B-NB	3.97	1.38	1.35
8	M	859	SPO	O1-CM1	3.90	1.55	1.43
8	M	859	SPO	C11-C12	-3.85	1.37	1.45
7	M	857	U10	C7-C6	3.79	1.57	1.51
8	M	859	SPO	C4-C5	-3.77	1.44	1.50
7	M	857	U10	C7-C8	-3.75	1.45	1.50
8	M	859	SPO	C15-C14	3.65	1.54	1.43
5	M	854	BPH	CMB-C2B	3.60	1.58	1.50
4	L	850	BCL	C2-C3	3.57	1.41	1.33
7	M	857	U10	C6-C5	3.47	1.56	1.46
8	M	859	SPO	C37-C38	3.36	1.42	1.32
8	M	859	SPO	C14-C12	3.28	1.40	1.35
8	M	859	SPO	O1-C1	3.26	1.59	1.41
5	L	855	BPH	CMB-C2B	3.21	1.57	1.50
4	L	853	BCL	C4B-NB	3.18	1.38	1.35
7	M	857	U10	C18-C19	3.11	1.40	1.33
8	M	859	SPO	C31-C32	-3.07	1.40	1.50
4	M	852	BCL	C2-C3	3.00	1.40	1.33
8	M	859	SPO	C32-C33	2.97	1.40	1.33
5	M	854	BPH	C2-C3	2.97	1.40	1.33
7	M	857	U10	C38-C39	2.94	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	857	U10	C33-C34	2.91	1.40	1.33
7	M	857	U10	C13-C14	2.89	1.39	1.33
5	L	855	BPH	C2-C3	2.87	1.39	1.33
4	L	850	BCL	CMB-C2B	2.84	1.57	1.51
8	M	859	SPO	C10-C9	2.83	1.52	1.43
8	M	859	SPO	C25-C23	-2.83	1.39	1.45
5	M	854	BPH	CMD-C2D	2.83	1.57	1.51
5	L	855	BPH	C3D-CAD	-2.82	1.41	1.47
7	M	857	U10	C23-C24	2.82	1.39	1.33
8	M	859	SPO	C8-C7	2.82	1.56	1.50
4	L	850	BCL	CAA-C2A	2.80	1.59	1.54
4	M	852	BCL	C4B-NB	2.77	1.37	1.35
4	L	853	BCL	CMB-C2B	2.76	1.57	1.51
5	M	854	BPH	C1B-C2B	-2.74	1.39	1.45
4	M	852	BCL	C3B-CAB	2.74	1.56	1.49
4	M	852	BCL	CMB-C2B	2.70	1.57	1.51
8	M	859	SPO	C6-C7	-2.68	1.40	1.45
8	M	859	SPO	C19-C17	2.68	1.39	1.35
4	L	851	BCL	CMB-C2B	2.67	1.57	1.51
7	M	857	U10	C28-C29	2.66	1.39	1.33
5	L	855	BPH	C3B-C2B	2.61	1.46	1.39
4	L	851	BCL	C2-C3	2.58	1.39	1.33
5	M	854	BPH	C3D-CAD	-2.54	1.42	1.47
4	L	850	BCL	C3A-C2A	-2.53	1.47	1.54
4	L	851	BCL	O2A-CGA	-2.53	1.25	1.33
4	L	853	BCL	C3B-CAB	2.51	1.55	1.49
8	M	859	SPO	C24-C23	2.49	1.56	1.50
4	M	852	BCL	CBB-CAB	2.46	1.57	1.49
5	L	855	BPH	O2A-CGA	-2.45	1.26	1.33
4	L	850	BCL	O2A-CGA	-2.40	1.26	1.33
4	M	852	BCL	C3D-CAD	-2.39	1.40	1.46
4	L	851	BCL	C3C-C4C	-2.36	1.48	1.51
4	L	851	BCL	C3B-CAB	2.35	1.55	1.49
4	L	853	BCL	C3A-C2A	-2.35	1.47	1.54
8	M	859	SPO	C29-C28	2.33	1.56	1.50
5	L	855	BPH	C1B-C2B	-2.33	1.40	1.45
4	L	850	BCL	O2D-CGD	-2.32	1.27	1.33
5	M	854	BPH	C3A-C2A	-2.31	1.48	1.54
8	M	859	SPO	C35-C33	2.31	1.56	1.51
7	M	857	U10	O4-C4	2.30	1.42	1.36
7	M	857	U10	C8-C9	2.29	1.38	1.33
5	L	855	BPH	C3B-CAB	2.22	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	854	BPH	C3B-C2B	2.14	1.45	1.39
4	L	853	BCL	CBB-CAB	2.13	1.56	1.49
5	M	854	BPH	C2A-C1A	2.11	1.55	1.51
4	M	852	BCL	OBD-CAD	2.05	1.25	1.22
5	M	854	BPH	O2D-CGD	-2.05	1.28	1.33
5	M	854	BPH	CHA-C1A	2.01	1.42	1.38
8	M	859	SPO	C39-C38	2.01	1.55	1.50
4	L	850	BCL	CBA-CGA	2.01	1.56	1.50

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	850	BCL	OBB-CAB-C3B	24.18	162.90	119.99
4	L	850	BCL	OBB-CAB-CBB	-18.66	78.19	120.17
4	L	850	BCL	CBB-CAB-C3B	-12.00	84.71	120.34
8	M	859	SPO	C25-C23-C22	-11.54	101.23	118.94
4	L	850	BCL	C4B-C3B-CAB	9.87	146.17	127.13
4	L	850	BCL	CMB-C2B-C1B	-9.09	114.50	128.46
5	L	855	BPH	C6-C5-C3	6.94	131.65	113.45
5	L	855	BPH	C4-C3-C5	6.76	126.64	115.27
4	M	852	BCL	CMB-C2B-C1B	-6.72	118.13	128.46
4	L	853	BCL	CAA-C2A-C1A	-6.66	90.16	111.97
4	L	851	BCL	CMB-C2B-C1B	-6.45	118.55	128.46
8	M	859	SPO	C18-C17-C19	-6.33	114.06	122.92
4	M	852	BCL	C4D-C3D-CAD	-6.25	104.98	108.47
5	L	855	BPH	C1-O2A-CGA	6.19	132.69	116.44
4	L	853	BCL	CMB-C2B-C1B	-6.12	119.06	128.46
5	L	855	BPH	C5-C3-C2	-6.11	108.75	121.12
5	M	854	BPH	C1-O2A-CGA	5.78	131.60	116.44
4	L	850	BCL	CAA-C2A-C1A	-5.78	93.05	111.97
8	M	859	SPO	C20-C21-C22	-5.70	111.80	123.47
4	L	851	BCL	C4D-C3D-CAD	-5.43	105.44	108.47
5	L	855	BPH	C7-C6-C5	-5.32	98.90	113.36
7	M	857	U10	C7-C6-C5	5.30	124.86	118.48
4	L	850	BCL	C4D-C3D-CAD	-5.30	105.52	108.47
4	L	853	BCL	C4D-C3D-CAD	-5.09	105.63	108.47
4	M	852	BCL	CMB-C2B-C3B	5.07	134.16	124.68
5	L	855	BPH	C4D-C3D-CAD	-5.06	104.66	107.87
7	M	857	U10	C15-C14-C16	4.97	123.64	115.27
5	M	854	BPH	C4D-C3D-CAD	-4.97	104.72	107.87
4	L	851	BCL	CMB-C2B-C3B	4.78	133.62	124.68
4	L	853	BCL	CMB-C2B-C3B	4.64	133.36	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	855	BPH	CHD-C4C-NC	-4.61	119.73	125.20
4	M	852	BCL	CED-O2D-CGD	4.58	126.29	115.94
8	M	859	SPO	C24-C23-C22	-4.50	116.61	122.92
7	M	857	U10	C7-C8-C9	4.50	134.29	126.79
7	M	857	U10	C15-C14-C13	-4.50	112.14	123.68
5	M	854	BPH	CHD-C4C-NC	-4.29	120.10	125.20
7	M	857	U10	C10-C9-C8	-4.27	112.73	123.68
4	L	851	BCL	CED-O2D-CGD	4.27	125.58	115.94
4	L	851	BCL	OBD-CAD-C3D	-4.24	120.94	127.98
5	M	854	BPH	C4-C3-C5	4.06	122.10	115.27
8	M	859	SPO	C15-C14-C12	-4.02	121.57	127.31
8	M	859	SPO	C8-C7-C9	4.01	128.53	122.92
8	M	859	SPO	C11-C12-C14	-4.00	112.80	118.94
4	M	852	BCL	OBD-CAD-C3D	-3.98	121.37	127.98
4	M	852	BCL	C6-C5-C3	3.93	123.76	113.45
4	L	850	BCL	OBD-CAD-C3D	-3.90	121.50	127.98
4	L	853	BCL	OBD-CAD-C3D	-3.86	121.57	127.98
4	L	853	BCL	CED-O2D-CGD	3.86	124.66	115.94
4	L	850	BCL	CBA-CAA-C2A	3.85	125.23	113.86
7	M	857	U10	C11-C9-C8	3.85	128.90	121.12
4	L	850	BCL	C4B-CHC-C1C	3.81	137.67	130.12
5	M	854	BPH	O2A-C1-C2	-3.73	98.83	108.64
5	M	854	BPH	O2D-CGD-CBD	3.69	117.82	111.27
4	L	853	BCL	CBA-CAA-C2A	3.68	124.72	113.86
4	L	850	BCL	C4A-NA-C1A	3.65	108.34	106.71
8	M	859	SPO	C2-C1-C4	-3.58	105.36	110.86
5	L	855	BPH	CMB-C2B-C1B	-3.54	119.62	125.06
4	L	851	BCL	C2A-C3A-C4A	3.54	107.58	101.87
4	L	850	BCL	O2A-C1-C2	-3.47	99.52	108.64
5	M	854	BPH	CHC-C1C-NC	-3.46	121.09	125.20
4	L	850	BCL	CED-O2D-CGD	3.46	123.75	115.94
7	M	857	U10	C35-C34-C33	-3.43	114.88	123.68
4	M	852	BCL	C2A-C3A-C4A	3.41	107.38	101.87
8	M	859	SPO	C15-C16-C17	-3.40	116.87	126.42
5	M	854	BPH	O1D-CGD-CBD	-3.39	117.54	124.48
4	L	853	BCL	C4A-NA-C1A	3.36	108.22	106.71
5	M	854	BPH	CMB-C2B-C1B	-3.34	119.92	125.06
5	L	855	BPH	O2D-CGD-CBD	3.26	117.07	111.27
5	L	855	BPH	C6-C7-C8	3.19	126.25	115.92
4	L	853	BCL	C16-C15-C13	-3.18	105.62	115.92
4	L	853	BCL	CAC-C3C-C2C	-3.17	106.33	114.26
4	M	852	BCL	CHA-C1A-NA	-3.15	119.18	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	850	BCL	C2A-C3A-C4A	3.11	106.90	101.87
5	L	855	BPH	CHC-C4B-NB	-3.11	118.43	124.93
4	L	850	BCL	C2A-C1A-CHA	3.11	129.29	123.86
4	L	853	BCL	O2A-CGA-CBA	3.07	121.54	111.91
5	M	854	BPH	CHC-C4B-NB	-3.06	118.54	124.93
4	L	850	BCL	C1-O2A-CGA	3.05	124.45	116.44
7	M	857	U10	C25-C24-C26	3.01	120.33	115.27
7	M	857	U10	C35-C34-C36	3.00	120.32	115.27
5	L	855	BPH	C3D-CAD-CBD	3.00	111.55	107.61
7	M	857	U10	C4M-O4-C4	2.96	126.95	116.47
7	M	857	U10	C20-C19-C18	-2.95	116.12	123.68
4	M	852	BCL	C4A-NA-C1A	2.94	108.03	106.71
4	L	853	BCL	C2A-C3A-C4A	2.90	106.55	101.87
8	M	859	SPO	C16-C17-C19	2.90	123.38	118.94
5	M	854	BPH	C3D-CAD-CBD	2.87	111.39	107.61
4	M	852	BCL	C2A-C1A-CHA	2.87	128.87	123.86
5	L	855	BPH	O1D-CGD-CBD	-2.85	118.65	124.48
8	M	859	SPO	C18-C17-C16	2.84	122.56	118.08
7	M	857	U10	C25-C24-C23	-2.82	116.43	123.68
4	L	853	BCL	CAA-C2A-C3A	-2.81	105.08	112.78
4	L	851	BCL	CHA-C1A-NA	-2.81	119.97	126.40
7	M	857	U10	C30-C29-C31	2.79	119.97	115.27
7	M	857	U10	C8-C7-C6	-2.76	104.61	112.05
5	L	855	BPH	CHC-C1C-NC	-2.75	121.94	125.20
4	L	851	BCL	C2A-C1A-CHA	2.73	128.62	123.86
5	L	855	BPH	C1-C2-C3	2.71	130.73	126.04
7	M	857	U10	C21-C19-C18	2.70	126.59	121.12
4	L	850	BCL	CAA-C2A-C3A	-2.70	105.39	112.78
4	M	852	BCL	C4B-CHC-C1C	2.70	135.45	130.12
5	L	855	BPH	CED-O2D-CGD	2.65	121.94	115.94
5	M	854	BPH	CMB-C2B-C3B	2.63	133.67	127.61
7	M	857	U10	O5-C5-C4	-2.63	115.35	120.93
5	L	855	BPH	CMB-C2B-C3B	2.61	133.62	127.61
5	M	854	BPH	CED-O2D-CGD	2.60	121.82	115.94
4	L	850	BCL	CHA-C1A-NA	-2.57	120.52	126.40
4	L	853	BCL	C4B-CHC-C1C	2.56	135.19	130.12
4	L	851	BCL	C4B-CHC-C1C	2.54	135.15	130.12
4	L	853	BCL	C2A-C1A-CHA	2.51	128.26	123.86
4	M	852	BCL	C15-C13-C12	-2.48	99.10	112.13
4	L	851	BCL	C4A-NA-C1A	2.47	107.82	106.71
5	M	854	BPH	C1C-NC-C4C	-2.46	108.38	110.54
5	M	854	BPH	CBB-CAB-C3B	-2.43	115.23	120.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	855	BPH	CBB-CAB-C3B	-2.42	115.25	120.43
8	M	859	SPO	C13-C12-C11	2.41	121.87	118.08
4	L	853	BCL	C2C-C3C-C4C	2.40	104.94	101.34
4	M	852	BCL	C3D-CAD-CBD	2.39	110.75	107.61
4	L	851	BCL	C3D-CAD-CBD	2.34	110.69	107.61
8	M	859	SPO	C9-C10-C11	-2.34	115.92	123.22
7	M	857	U10	C1M-C1-C6	-2.33	120.59	124.40
4	L	853	BCL	O1D-CGD-CBD	-2.33	119.73	124.48
8	M	859	SPO	C10-C9-C7	-2.32	124.00	127.31
4	L	853	BCL	CHA-C1A-NA	-2.28	121.17	126.40
4	L	850	BCL	C15-C13-C12	-2.25	100.27	112.13
5	M	854	BPH	C2A-C3A-C4A	2.25	105.78	101.34
4	L	853	BCL	O2D-CGD-CBD	2.19	115.17	111.27
4	L	850	BCL	O2D-CGD-CBD	2.16	115.11	111.27
5	M	854	BPH	C2A-C1A-CHA	2.15	130.92	125.22
5	L	855	BPH	CAC-C3C-C4C	2.13	118.14	112.67
4	L	850	BCL	C3D-CAD-CBD	2.12	110.40	107.61
4	M	852	BCL	CGD-CBD-CAD	-2.11	103.90	110.73
7	M	857	U10	C11-C12-C13	2.10	118.78	111.88
4	M	852	BCL	O2A-CGA-CBA	2.09	118.48	111.91
4	L	851	BCL	C6-C5-C3	2.08	118.92	113.45
5	L	855	BPH	C2A-C3A-C4A	2.07	105.43	101.34
5	L	855	BPH	C1C-NC-C4C	-2.06	108.73	110.54
4	L	850	BCL	O1D-CGD-CBD	-2.06	120.28	124.48
4	L	850	BCL	C1C-NC-C4C	2.04	107.62	106.71
7	M	857	U10	C31-C32-C33	-2.03	105.22	111.88
7	M	857	U10	C30-C29-C28	-2.01	118.53	123.68
8	M	859	SPO	C8-C7-C6	-2.00	114.92	118.08

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	852	BCL	C2C-C3C-CAC-CBC
4	M	852	BCL	C4C-C3C-CAC-CBC
4	M	852	BCL	C2-C3-C5-C6
4	M	852	BCL	C4-C3-C5-C6
5	M	854	BPH	C4C-C3C-CAC-CBC
5	M	854	BPH	C4B-C3B-CAB-CBB
5	M	854	BPH	C4B-C3B-CAB-OB
7	M	857	U10	C1-C6-C7-C8
7	M	857	U10	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
7	M	857	U10	C20-C19-C21-C22
7	M	857	U10	C19-C21-C22-C23
7	M	857	U10	C24-C26-C27-C28
8	M	859	SPO	O1-C1-C4-C5
8	M	859	SPO	C2-C1-C4-C5
8	M	859	SPO	C3-C1-C4-C5
8	M	859	SPO	C1-C4-C5-C6
8	M	859	SPO	C21-C22-C23-C24
7	M	857	U10	C12-C11-C9-C10
7	M	857	U10	C18-C19-C21-C22
8	M	859	SPO	C20-C21-C22-C23
5	L	855	BPH	C4-C3-C5-C6
5	M	854	BPH	C4-C3-C5-C6
7	M	857	U10	C15-C14-C16-C17
7	M	857	U10	C25-C24-C26-C27
5	L	855	BPH	C2-C3-C5-C6
5	M	854	BPH	C2-C3-C5-C6
7	M	857	U10	C13-C14-C16-C17
7	M	857	U10	C23-C24-C26-C27
7	M	857	U10	C29-C31-C32-C33
7	M	857	U10	C12-C11-C9-C8
4	M	852	BCL	C14-C13-C15-C16
8	M	859	SPO	C24-C23-C25-C26
4	L	850	BCL	C15-C16-C17-C18
4	L	850	BCL	C5-C6-C7-C8
5	L	855	BPH	C6-C7-C8-C10
4	L	851	BCL	C2A-CAA-CBA-CGA
4	L	853	BCL	C14-C13-C15-C16
4	L	853	BCL	C12-C13-C15-C16
5	L	855	BPH	C8-C10-C11-C12
5	M	854	BPH	C2C-C3C-CAC-CBC
4	L	850	BCL	C2A-CAA-CBA-CGA
8	M	859	SPO	C2-C1-O1-CM1
4	M	852	BCL	C11-C10-C8-C7
4	M	852	BCL	C12-C13-C15-C16
5	L	855	BPH	C11-C10-C8-C7
4	M	852	BCL	C11-C10-C8-C9
5	L	855	BPH	C6-C7-C8-C9
5	L	855	BPH	C11-C10-C8-C9
4	L	850	BCL	CAD-CBD-CGD-O2D
4	L	850	BCL	C4-C3-C5-C6
4	L	850	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
4	L	850	BCL	C12-C13-C15-C16
8	M	859	SPO	C3-C1-O1-CM1
4	L	850	BCL	C14-C13-C15-C16
8	M	859	SPO	C18-C17-C19-C20
8	M	859	SPO	C16-C17-C19-C20
7	M	857	U10	C35-C34-C36-C37
8	M	859	SPO	C29-C28-C30-C31
4	L	853	BCL	C2A-CAA-CBA-CGA
4	M	852	BCL	C15-C16-C17-C18
8	M	859	SPO	C27-C28-C30-C31
5	L	855	BPH	C4B-C3B-CAB-OBB
4	L	853	BCL	CAD-CBD-CGD-O2D
5	M	854	BPH	CAD-CBD-CGD-O2D
4	L	850	BCL	CAA-CBA-CGA-O2A
4	M	852	BCL	CAA-CBA-CGA-O2A
5	L	855	BPH	CHA-CBD-CGD-O1D
4	L	853	BCL	C5-C6-C7-C8
4	L	850	BCL	CAA-CBA-CGA-O1A
8	M	859	SPO	C35-C36-C37-C38
7	M	857	U10	C33-C34-C36-C37
7	M	857	U10	C9-C11-C12-C13

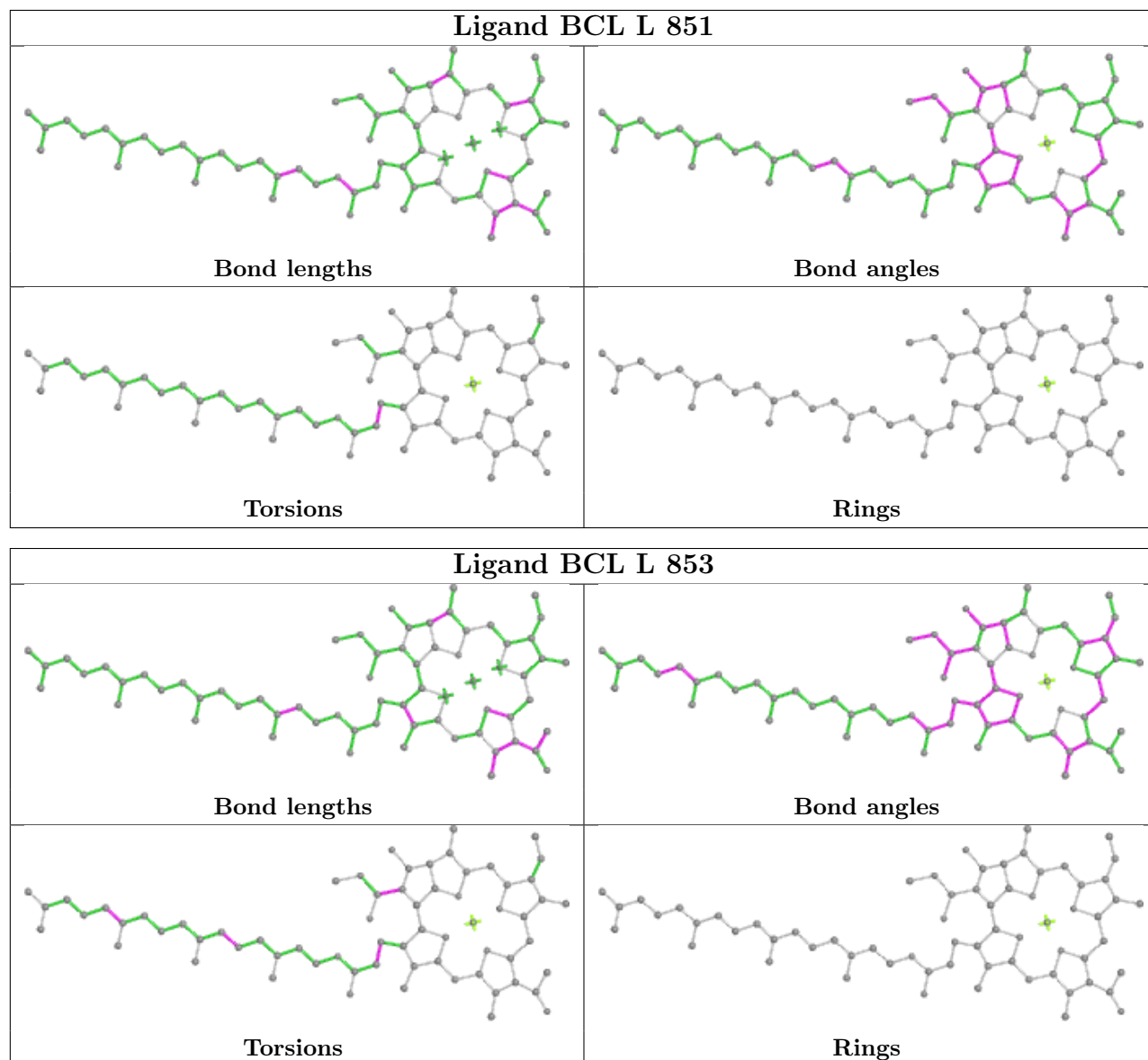
There are no ring outliers.

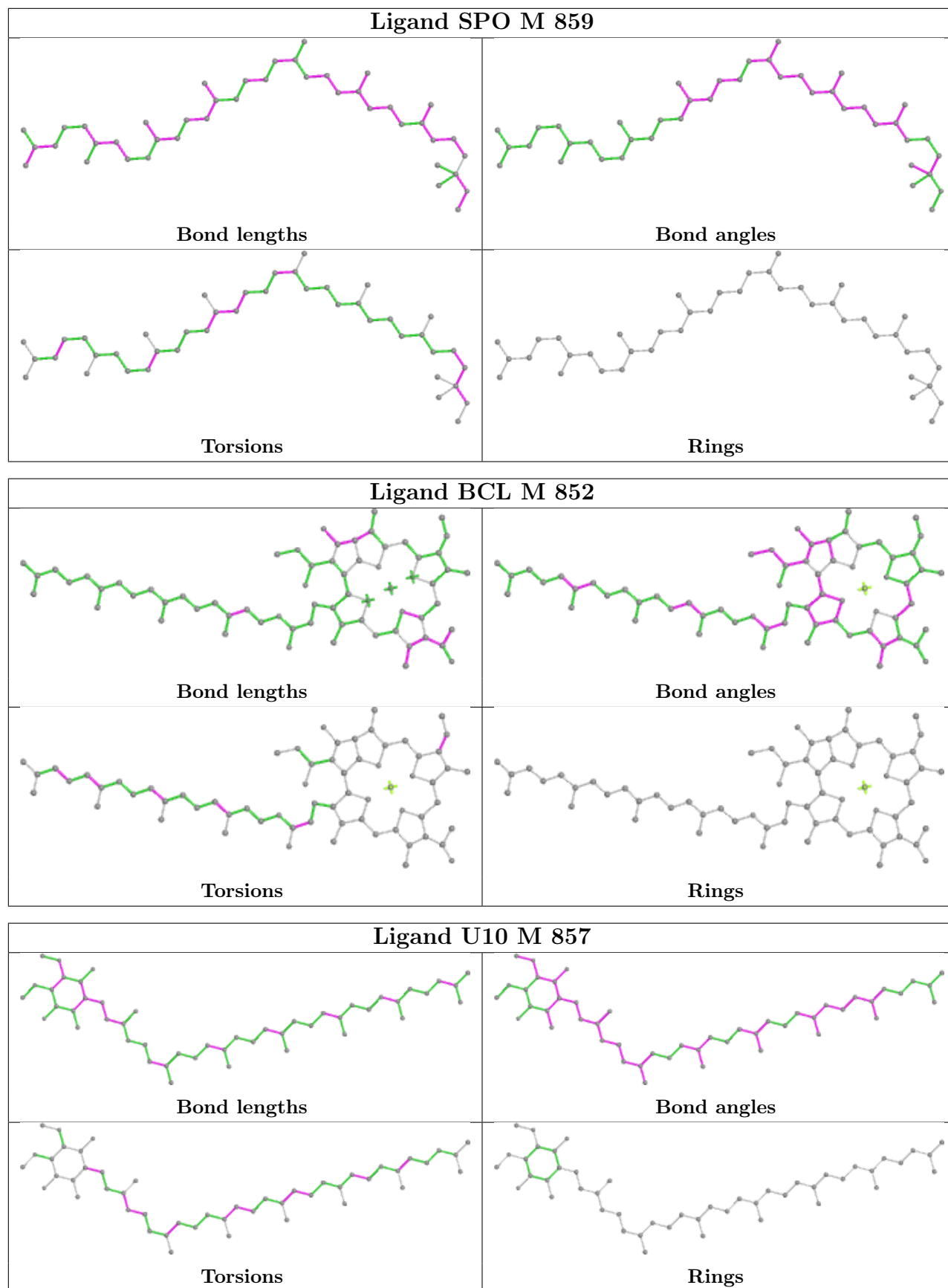
8 monomers are involved in 36 short contacts:

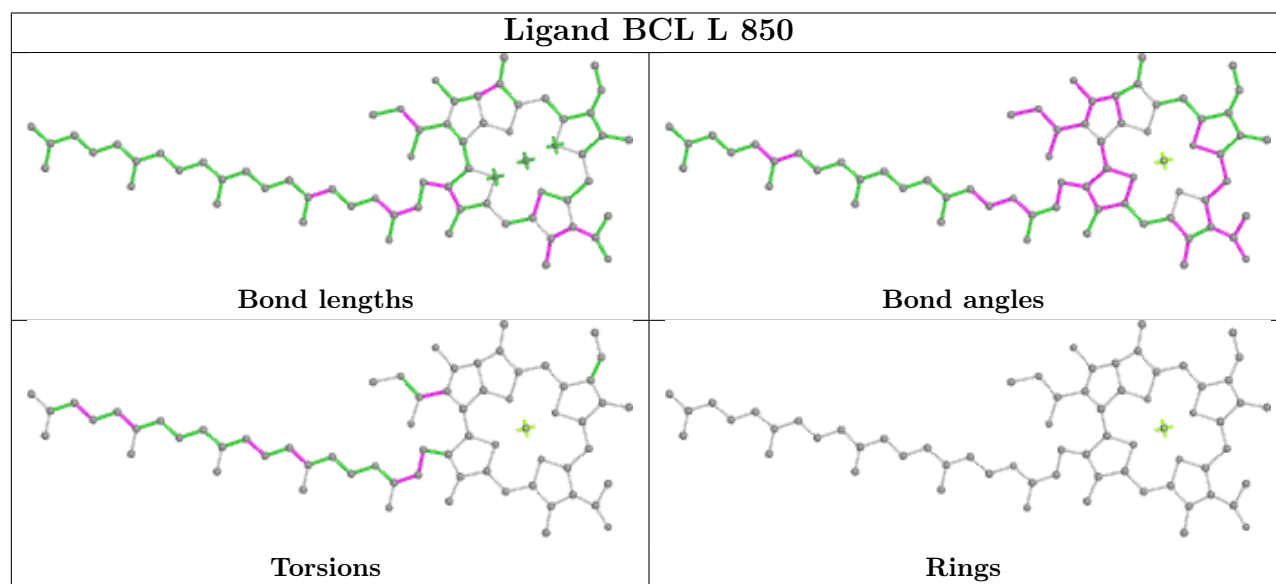
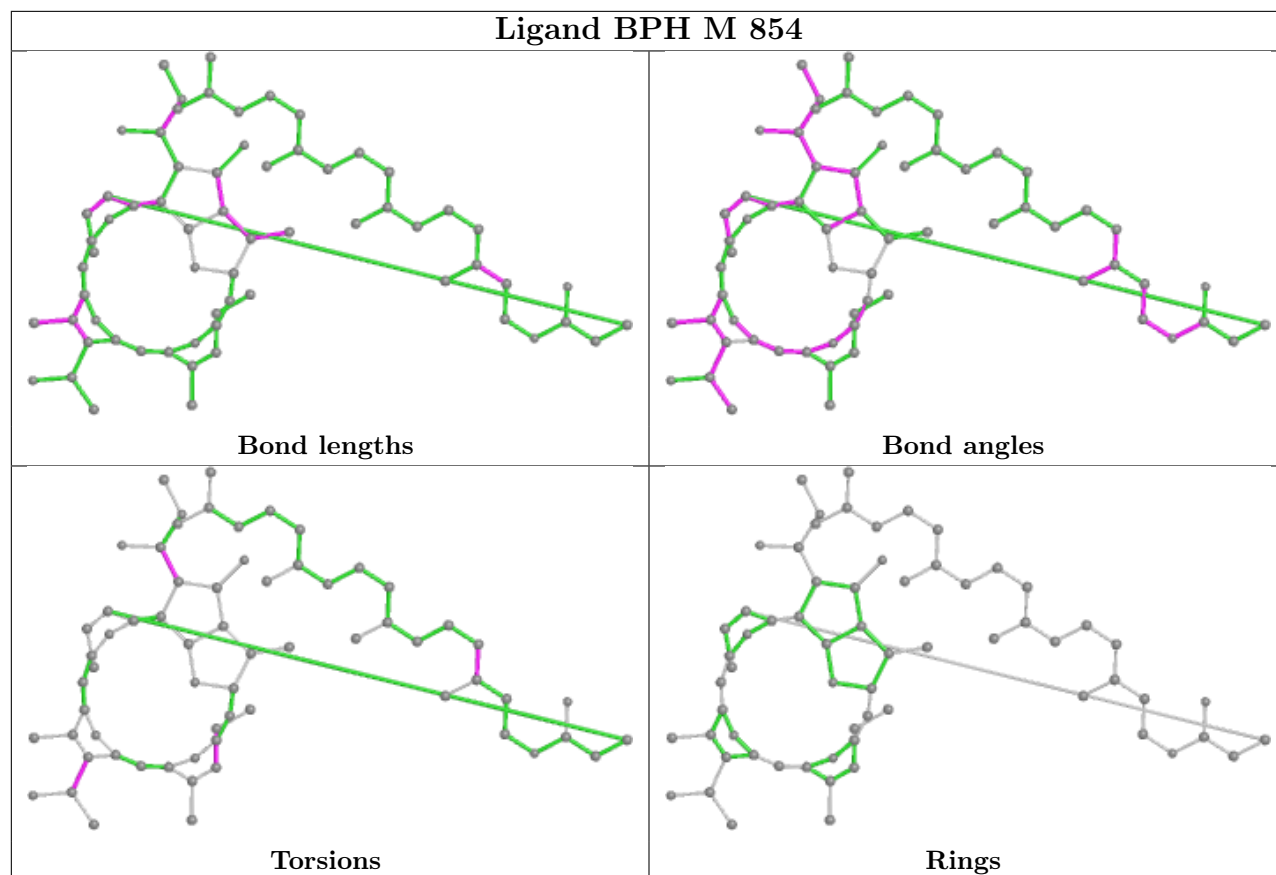
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	851	BCL	5	0
4	L	853	BCL	4	0
8	M	859	SPO	1	0
4	M	852	BCL	7	0
7	M	857	U10	5	0
5	M	854	BPH	9	0
4	L	850	BCL	7	0
5	L	855	BPH	7	0

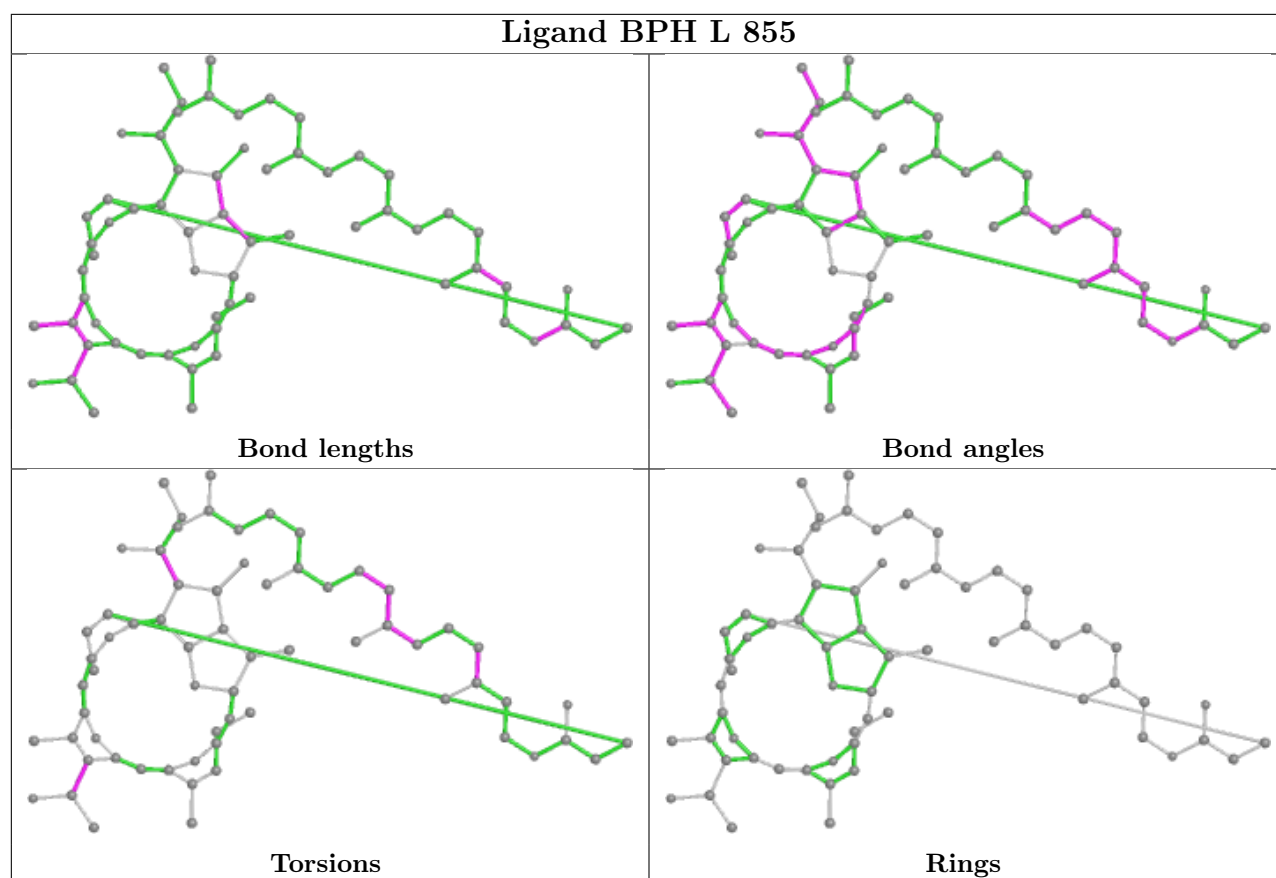
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.