



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 06:38 AM EDT

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

<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

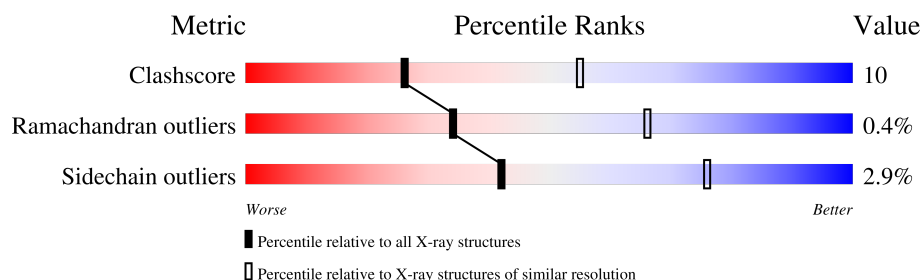
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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 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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	SPO	M	859	-	X	-	-

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			

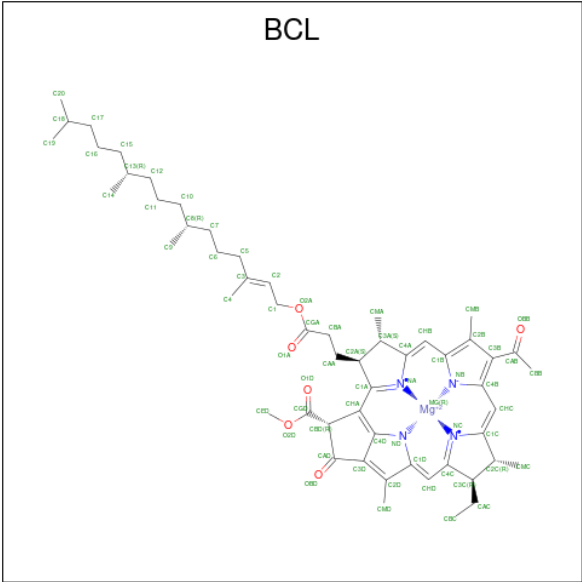
There is a discrepancy between the modelled and reference sequences:

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

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

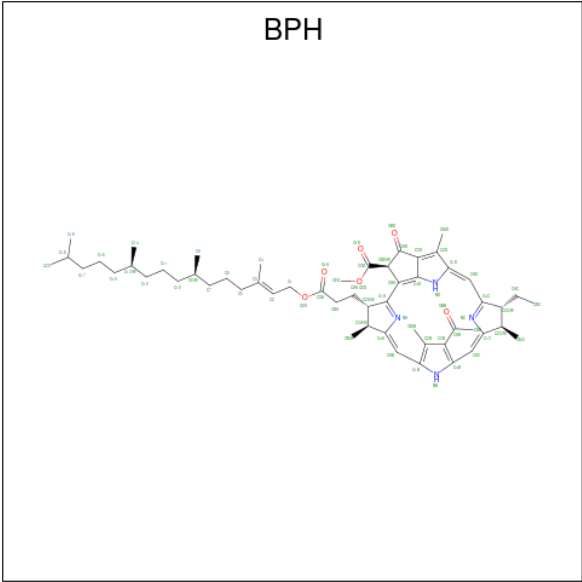
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	236	Total	C	N	O	S	0	0	0
			1794	1148	305	332	9			

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



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

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

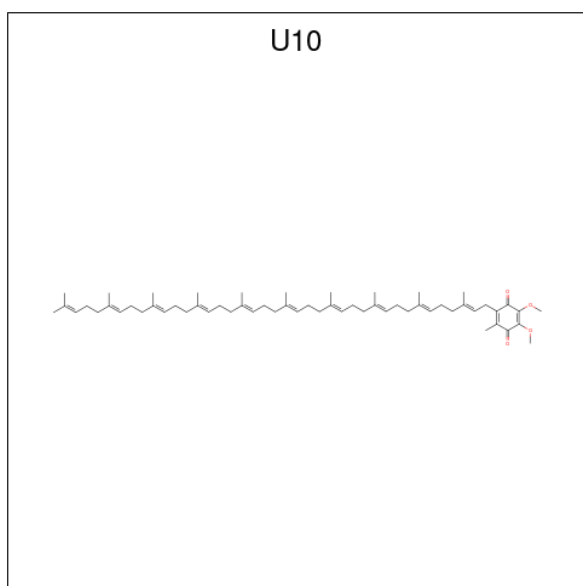


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			65	55	4	6		

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

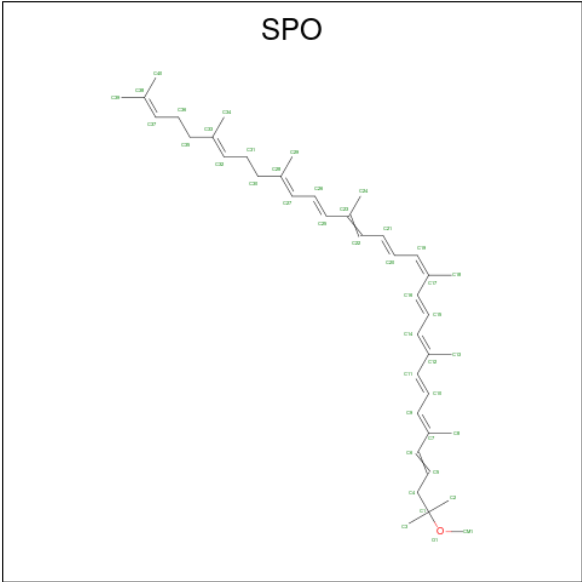
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	M	1	Total	Fe	0	0
			1	1		

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



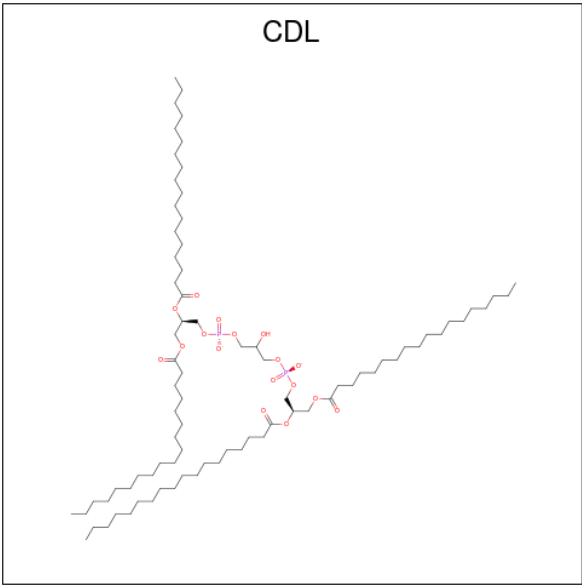
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 8 is SPHEROIDENE (three-letter code: SPO) (formula: C₄₁H₆₀O).



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

- Molecule 9 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



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

- Molecule 10 is water.

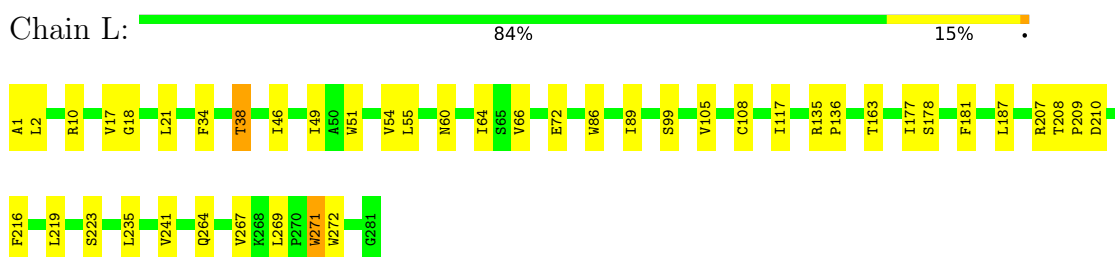
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	L	33	Total 33	O 33	0	0
10	M	33	Total 33	O 33	0	0
10	H	53	Total 53	O 53	0	0

3 Residue-property plots

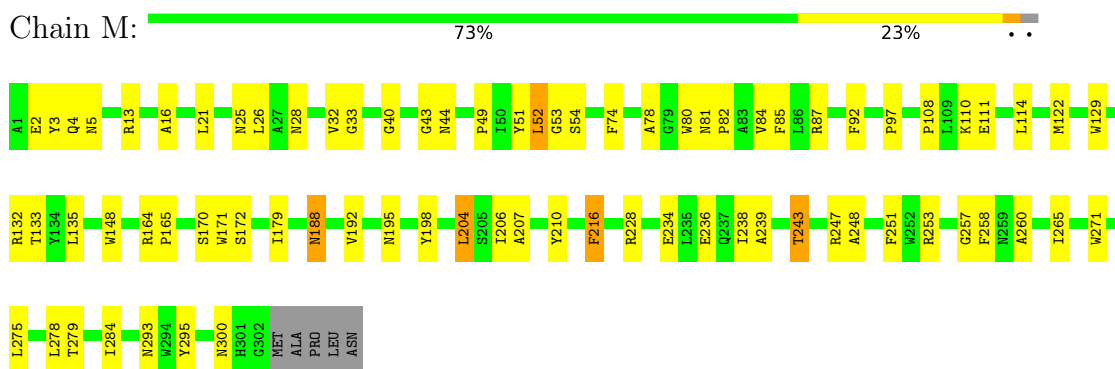
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

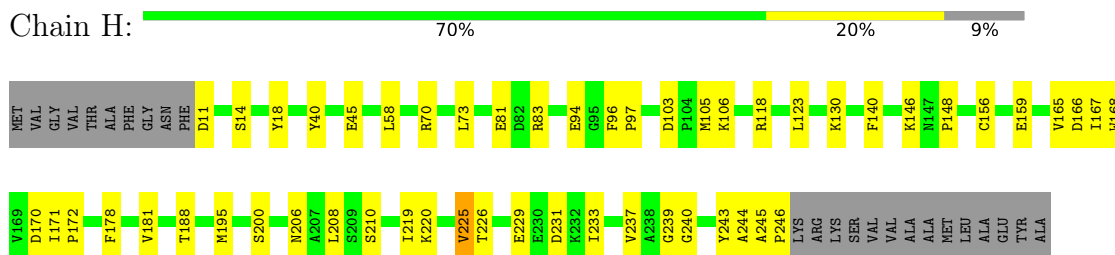
• Molecule 1: Photosynthetic Reaction Center L subunit



• 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	142.60 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	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: SPO, BPH, FE, CDL, U10, BCL

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	L	132	0	148	9	0
4	M	132	0	148	10	0
5	L	65	0	76	6	0
5	M	65	0	76	5	0
6	M	1	0	0	0	0
7	M	48	0	63	4	0
8	M	42	0	60	1	0

Continued on next page...

Continued from previous page...

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	5:L:855:BPH:HAC2	1.64	0.78
2:M:108:PRO:HG2	2:M:111:GLU:HG3	1.68	0.76
5: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	4: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:CD1	1:L:271:TRP:N	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
4:L:850:BCL:H2	5:M:854:BPH:HMB2	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:181:PHE:HB3	5: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
5:L:855:BPH:H102	4: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:2:LEU:HD21	1:L:10:ARG:CZ	2.39	0.53
1:L:34:PHE:O	1:L:38:THR:CG2	2.55	0.53
4:M:852:BCL:HBB3	4:M:853:BCL:HMD2	1.89	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
1:L:187:LEU:HD13	2:M:216:PHE:CG	2.44	0.52
3:H:245:ALA:HB3	3:H:246:PRO:HD3	1.91	0.52
1:L:181:PHE:HB3	5: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	5: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
5:L:855:BPH:HBB3	5:L:855:BPH:HHC	1.92	0.51
2:M:293:ASN:OD1	2:M:295:TYR:HB3	2.10	0.51
2:M:78:ALA:HB2	2:M:92:PHE:CZ	2.46	0.51
2:M:260:ALA:HB2	7:M:857:U10:H103	1.93	0.51
1:L:18:GLY:O	1:L:21:LEU:HD23	2.11	0.50
2:M:265:ILE:HG21	7:M:857:U10:H3M2	1.93	0.50
2:M:236:GLU:OE2	3:H:118:ARG:NH2	2.37	0.50
3:H:245:ALA:N	3:H:246:PRO:CD	2.74	0.50
2:M:40:GLY:HA2	2:M:43:GLY:O	2.12	0.49
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.93	0.49
4:L:850:BCL:HMD2	4: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:853:BCL:HAA2	4:M:853:BCL:HBD	1.95	0.48
3:H:94:GLU:H	3:H:94:GLU:CD	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:HD12	2:M:52:LEU:HA	1.61	0.47
4:L:850:BCL:HBB2	4:M:852:BCL:H111	1.97	0.46
10:L:1075:HOH:O	2:M:49:PRO:HG2	2.14	0.46
2:M:80:TRP:O	2:M:82:PRO:HD3	2.14	0.46
3:H:70:ARG:NH2	3:H:123:LEU:HG	2.31	0.46
2:M:243:THR:HG22	2:M:247:ARG:NE	2.22	0.46
2:M:284:ILE:HG12	4: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	4:M:852:BCL:HMB3	1.98	0.46
2:M:293:ASN:HB2	10:M:1023:HOH:O	2.15	0.46
3:H:45:GLU:HG3	10:H:1066: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: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
2:M:234:GLU:O	2:M:238:ILE:HG13	2.17	0.45
5:M:854:BPH:HHB	5:M:854:BPH:HMB1	1.80	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	4:L:850:BCL:HBA1	2.17	0.45
2:M:52:LEU:HB3	2:M:53:GLY:H	1.63	0.45
2:M:248:ALA:HB3	7:M:857:U10:H4M2	1.99	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:3:TYR:CZ	2:M:5:ASN:HA	2.52	0.44
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.52	0.44
1:L:267:VAL:HG23	2:M:87:ARG:HD2	2.00	0.44
2:M:192:VAL:O	2:M:192:VAL:CG1	2.65	0.44
2:M:207:ALA:HB1	4:M:853:BCL:O1A	2.17	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
1:L:51:TRP:O	1:L:54:VAL:HG22	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:850:BCL:HAA2	4:L:850:BCL:HBD	2.00	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:2:GLU:HG3	2:M:4:GLN:NE2	2.34	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
1:L:54:VAL:HG23	1:L:55:LEU:N	2.33	0.42
1:L:219:LEU:O	2:M:132:ARG:NH1	2.52	0.42
4:L:851:BCL:H122	5:L:855:BPH:H3A	1.99	0.42
3:H:96:PHE:HB3	3:H:97:PRO:CD	2.49	0.42
1:L:163:THR:HG22	1:L:163:THR:O	2.17	0.42
2:M:148:TRP:CE2	9:M:5000:CDL:H511	2.54	0.42
1:L:66:VAL:HG12	1:L:86:TRP:HB2	2.01	0.42
1:L:177:ILE:HG12	4:L:851:BCL:HMB3	2.01	0.42
3:H:156:CYS:HB3	3:H:206:ASN:O	2.19	0.42
3:H:229:GLU:O	3:H:233:ILE:HG13	2.20	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
4:L:851:BCL:HAA2	4:L:851:BCL:HBD	2.02	0.41
2:M:21:LEU:HD22	2:M:26:LEU:CD2	2.50	0.41
5:L:855:BPH:HMB1	5:L:855:BPH:HHB	1.81	0.41
4:L:850:BCL:H92	4:M:852:BCL:H202	2.03	0.41
2:M:114:LEU:HD12	2:M:114:LEU:HA	1.87	0.41
4:M:852:BCL:HAA2	4:M:852:BCL:HBD	2.03	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:195:ASN:HB3	2:M:198:TYR:HD2	1.86	0.40
1:L:223:SER:O	2:M:44:ASN:HB2	2.22	0.40
2:M:28:ASN:HB2	2:M:51:TYR:CE1	2.57	0.40
2:M:253:ARG:O	2:M:257:GLY:HA2	2.22	0.40
3:H:219:ILE:HG21	3:H:225:VAL:CG1	2.52	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%)	15	44
3	H	234/260 (90%)	227 (97%)	7 (3%)	0	100	100
All	All	813/848 (96%)	770 (95%)	40 (5%)	3 (0%)	34	66

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%)	35	69
2	M	236/240 (98%)	228 (97%)	8 (3%)	37	71
3	H	191/208 (92%)	188 (98%)	3 (2%)	62	88
All	All	647/668 (97%)	628 (97%)	19 (3%)	42	76

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

Sometimes 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 monosaccharides 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	BPH	L	855	-	64,70,70	1.32	12 (18%)	76,101,101	1.91	20 (26%)
7	U10	M	857	-	48,48,63	2.35	13 (27%)	58,61,79	2.19	22 (37%)
9	CDL	M	5000	-	80,80,99	0.58	1 (1%)	86,92,111	0.95	5 (5%)
4	BCL	L	851	1	58,74,74	1.58	8 (13%)	69,115,115	1.83	14 (20%)
4	BCL	L	850	2	58,74,74	1.62	11 (18%)	69,115,115	1.95	18 (26%)
4	BCL	M	852	2	58,74,74	1.61	12 (20%)	69,115,115	1.96	15 (21%)
5	BPH	M	854	-	64,70,70	1.39	11 (17%)	76,101,101	1.85	18 (23%)
8	SPO	M	859	-	40,41,41	3.59	26 (65%)	47,50,50	2.74	15 (31%)
4	BCL	M	853	1	58,74,74	1.56	8 (13%)	69,115,115	2.08	17 (24%)

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	BPH	L	855	-	-	5/54/105/105	0/5/6/6
7	U10	M	857	-	-	13/45/69/87	0/1/1/1
9	CDL	M	5000	-	-	32/91/91/110	-
4	BCL	L	851	1	-	6/37/137/137	-
4	BCL	L	850	2	-	7/37/137/137	-
4	BCL	M	852	2	-	10/37/137/137	-
5	BPH	M	854	-	-	10/54/105/105	0/5/6/6
8	SPO	M	859	-	-	18/47/47/47	-
4	BCL	M	853	1	-	6/37/137/137	-

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	857	U10	C6-C1	9.53	1.52	1.35
8	M	859	SPO	C15-C16	9.46	1.58	1.34
8	M	859	SPO	C6-C5	7.20	1.50	1.32
8	M	859	SPO	C10-C11	7.11	1.52	1.34
8	M	859	SPO	C27-C28	6.00	1.40	1.34
4	L	851	BCL	C3D-C2D	6.00	1.50	1.39
8	M	859	SPO	C21-C20	5.55	1.50	1.36
4	L	850	BCL	C3D-C2D	5.44	1.49	1.39
4	M	852	BCL	C3B-C2B	5.38	1.49	1.39
8	M	859	SPO	C26-C25	5.33	1.48	1.34
4	M	852	BCL	C3D-C2D	5.24	1.48	1.39
4	M	853	BCL	C3D-C2D	4.91	1.48	1.39
4	L	851	BCL	C3B-C2B	4.90	1.48	1.39
5	M	854	BPH	C3D-C2D	4.77	1.48	1.39
4	M	853	BCL	C3B-C2B	4.72	1.47	1.39
4	L	850	BCL	C3B-C2B	4.59	1.47	1.39
7	M	857	U10	C7-C6	4.50	1.58	1.51
8	M	859	SPO	C13-C12	4.43	1.60	1.50
7	M	857	U10	C4-C3	4.20	1.53	1.36
8	M	859	SPO	C14-C12	4.10	1.41	1.35
8	M	859	SPO	O1-CM1	4.09	1.56	1.43
7	M	857	U10	C7-C8	-4.01	1.44	1.50
5	L	855	BPH	C3D-C2D	3.97	1.46	1.39
4	M	853	BCL	C2-C3	3.96	1.42	1.33
8	M	859	SPO	C15-C14	3.94	1.55	1.43
8	M	859	SPO	C32-C33	3.60	1.41	1.33
4	M	852	BCL	C2-C3	3.58	1.41	1.33
4	L	850	BCL	C2-C3	3.57	1.41	1.33
7	M	857	U10	C6-C5	3.51	1.56	1.46
5	M	854	BPH	CMB-C2B	3.48	1.58	1.50
7	M	857	U10	C28-C29	3.48	1.41	1.33
8	M	859	SPO	C4-C5	-3.45	1.44	1.50
8	M	859	SPO	C19-C17	3.44	1.40	1.35
8	M	859	SPO	C11-C12	-3.41	1.38	1.45
4	L	851	BCL	C4B-NB	3.37	1.38	1.35
7	M	857	U10	C18-C19	3.26	1.40	1.33
8	M	859	SPO	O1-C1	3.21	1.59	1.41
5	L	855	BPH	C3D-CAD	-3.18	1.40	1.47
8	M	859	SPO	C37-C38	3.18	1.41	1.32
5	L	855	BPH	CMB-C2B	3.14	1.57	1.50
8	M	859	SPO	C35-C33	3.07	1.57	1.51
7	M	857	U10	C33-C34	3.04	1.40	1.33
4	L	850	BCL	C4B-NB	3.00	1.37	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	851	BCL	C2-C3	2.98	1.40	1.33
5	M	854	BPH	C2-C3	2.98	1.40	1.33
7	M	857	U10	C13-C14	2.96	1.40	1.33
4	L	850	BCL	CMB-C2B	2.94	1.57	1.51
8	M	859	SPO	C31-C32	-2.94	1.40	1.50
8	M	859	SPO	C8-C7	2.92	1.56	1.50
4	L	851	BCL	CMB-C2B	2.89	1.57	1.51
8	M	859	SPO	C10-C9	2.89	1.52	1.43
4	M	852	BCL	C3B-CAB	2.89	1.56	1.49
4	M	852	BCL	C4B-NB	2.87	1.37	1.35
4	M	853	BCL	C4B-NB	2.87	1.37	1.35
5	M	854	BPH	C3D-CAD	-2.86	1.41	1.47
4	L	850	BCL	C3B-CAB	2.82	1.56	1.49
7	M	857	U10	C38-C39	2.82	1.40	1.32
4	L	850	BCL	OBD-CAD	2.76	1.26	1.22
4	M	852	BCL	C3C-C4C	-2.71	1.48	1.51
4	M	852	BCL	CMB-C2B	2.70	1.57	1.51
4	M	853	BCL	OBD-CAD	2.68	1.26	1.22
5	L	855	BPH	C2-C3	2.67	1.39	1.33
7	M	857	U10	C23-C24	2.66	1.39	1.33
4	M	853	BCL	C3B-CAB	2.63	1.56	1.49
5	L	855	BPH	O2A-CGA	-2.59	1.25	1.33
7	M	857	U10	O4-C4	2.57	1.43	1.36
4	L	850	BCL	CAA-C2A	2.52	1.58	1.54
4	M	853	BCL	CMB-C2B	2.51	1.56	1.51
4	M	853	BCL	C3C-C4C	-2.51	1.48	1.51
5	M	854	BPH	CMD-C2D	2.49	1.56	1.51
4	L	851	BCL	C3B-CAB	2.48	1.55	1.49
4	L	850	BCL	O2D-CGD	-2.46	1.27	1.33
8	M	859	SPO	C22-C23	2.44	1.39	1.35
8	M	859	SPO	C25-C23	-2.43	1.40	1.45
5	L	855	BPH	C3B-C2B	2.43	1.45	1.39
5	M	854	BPH	C3B-C2B	2.42	1.45	1.39
8	M	859	SPO	C29-C28	2.41	1.56	1.50
8	M	859	SPO	C24-C23	2.40	1.55	1.50
4	L	850	BCL	C3A-C2A	-2.38	1.47	1.54
4	L	850	BCL	CBB-CAB	2.29	1.56	1.49
5	M	854	BPH	C1B-C2B	-2.25	1.41	1.45
5	M	854	BPH	C3A-C2A	-2.25	1.48	1.54
5	L	855	BPH	C3A-C2A	-2.22	1.48	1.54
8	M	859	SPO	C6-C7	-2.22	1.41	1.45
5	L	855	BPH	OBD-CAD	2.21	1.25	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	854	BPH	O2A-CGA	-2.19	1.26	1.33
5	M	854	BPH	O2D-CGD	-2.19	1.27	1.33
4	M	852	BCL	CMD-C2D	2.17	1.56	1.51
8	M	859	SPO	C26-C27	2.15	1.50	1.43
5	L	855	BPH	C3B-CAB	2.15	1.53	1.46
5	L	855	BPH	C1B-C2B	-2.13	1.41	1.45
4	M	852	BCL	CBB-CAB	2.12	1.56	1.49
9	M	5000	CDL	CB3-CB4	2.12	1.57	1.50
4	M	852	BCL	C3D-CAD	-2.08	1.40	1.46
4	M	852	BCL	OBD-CAD	2.07	1.25	1.22
4	L	851	BCL	CMD-C2D	2.04	1.56	1.51
5	L	855	BPH	CHA-C1A	2.04	1.42	1.38
4	L	851	BCL	CBB-CAB	2.03	1.55	1.49
7	M	857	U10	C8-C9	2.02	1.37	1.33
4	M	852	BCL	CHD-C4C	-2.02	1.35	1.41
5	L	855	BPH	CMD-C2D	2.01	1.55	1.51
5	M	854	BPH	C5-C3	2.00	1.55	1.51

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	859	SPO	C25-C23-C22	-10.98	102.09	118.94
4	M	853	BCL	CMB-C2B-C1B	-6.50	118.47	128.46
4	L	850	BCL	CMB-C2B-C1B	-6.47	118.52	128.46
4	M	852	BCL	CMB-C2B-C1B	-6.44	118.56	128.46
4	M	852	BCL	C4D-C3D-CAD	-6.19	105.02	108.47
4	L	851	BCL	CMB-C2B-C1B	-6.17	118.99	128.46
4	M	853	BCL	CAA-C2A-C1A	-6.04	92.18	111.97
8	M	859	SPO	C18-C17-C19	-6.03	114.48	122.92
5	L	855	BPH	C4-C3-C5	5.90	125.19	115.27
7	M	857	U10	C7-C6-C5	5.81	125.47	118.48
5	M	854	BPH	C1-O2A-CGA	5.67	131.33	116.44
4	L	851	BCL	C4D-C3D-CAD	-5.58	105.36	108.47
5	L	855	BPH	C1-O2A-CGA	5.57	131.07	116.44
4	L	850	BCL	C4D-C3D-CAD	-5.39	105.47	108.47
4	M	853	BCL	C4D-C3D-CAD	-5.31	105.51	108.47
8	M	859	SPO	C20-C21-C22	-5.19	112.84	123.47
5	M	854	BPH	C4D-C3D-CAD	-5.13	104.62	107.87
8	M	859	SPO	C24-C23-C22	-5.10	115.78	122.92
4	L	850	BCL	CAA-C2A-C1A	-5.03	95.50	111.97
7	M	857	U10	C15-C14-C16	4.95	123.60	115.27
4	M	853	BCL	CMB-C2B-C3B	4.93	133.89	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	852	BCL	CMB-C2B-C3B	4.87	133.79	124.68
4	L	850	BCL	CMB-C2B-C3B	4.86	133.77	124.68
5	L	855	BPH	C6-C5-C3	4.72	125.83	113.45
4	L	851	BCL	CMB-C2B-C3B	4.66	133.41	124.68
7	M	857	U10	C15-C14-C13	-4.49	112.17	123.68
4	M	852	BCL	CED-O2D-CGD	4.48	126.06	115.94
5	L	855	BPH	C4D-C3D-CAD	-4.47	105.04	107.87
7	M	857	U10	C10-C9-C8	-4.40	112.39	123.68
7	M	857	U10	C7-C8-C9	4.39	134.09	126.79
5	M	854	BPH	CHD-C4C-NC	-4.38	120.00	125.20
8	M	859	SPO	C15-C14-C12	-4.30	121.18	127.31
5	M	854	BPH	C4-C3-C5	4.18	122.31	115.27
4	L	851	BCL	OBD-CAD-C3D	-4.17	121.06	127.98
4	L	851	BCL	CED-O2D-CGD	4.10	125.20	115.94
5	L	855	BPH	C5-C3-C2	-4.02	112.97	121.12
8	M	859	SPO	C8-C7-C9	3.92	128.41	122.92
9	M	5000	CDL	OB8-CB6-CB4	3.86	119.68	108.43
5	M	854	BPH	O2A-C1-C2	-3.82	98.58	108.64
4	L	851	BCL	C2A-C3A-C4A	3.81	108.03	101.87
4	M	852	BCL	OBD-CAD-C3D	-3.80	121.68	127.98
8	M	859	SPO	C2-C1-C4	-3.80	105.03	110.86
4	M	853	BCL	C4A-NA-C1A	3.78	108.41	106.71
5	L	855	BPH	CHD-C4C-NC	-3.78	120.71	125.20
5	M	854	BPH	O2D-CGD-CBD	3.78	117.98	111.27
4	M	852	BCL	C6-C5-C3	3.73	123.24	113.45
7	M	857	U10	C11-C9-C8	3.73	128.66	121.12
4	M	853	BCL	OBD-CAD-C3D	-3.72	121.81	127.98
7	M	857	U10	C25-C24-C23	-3.66	114.29	123.68
4	L	850	BCL	OBD-CAD-C3D	-3.64	121.94	127.98
4	M	853	BCL	CED-O2D-CGD	3.62	124.12	115.94
5	L	855	BPH	CHC-C4B-NB	-3.47	117.68	124.93
8	M	859	SPO	C11-C12-C14	-3.44	113.66	118.94
5	M	854	BPH	O1D-CGD-CBD	-3.42	117.48	124.48
4	M	853	BCL	CAC-C3C-C2C	-3.36	105.86	114.26
4	L	850	BCL	CBA-CAA-C2A	3.33	123.71	113.86
4	M	853	BCL	C2A-C3A-C4A	3.30	107.20	101.87
5	L	855	BPH	CMB-C2B-C1B	-3.30	119.98	125.06
4	M	853	BCL	CBA-CAA-C2A	3.28	123.54	113.86
4	M	852	BCL	C2A-C3A-C4A	3.23	107.09	101.87
7	M	857	U10	C35-C34-C33	-3.20	115.48	123.68
5	M	854	BPH	CMB-C2B-C1B	-3.18	120.16	125.06
5	M	854	BPH	C3D-CAD-CBD	3.16	111.77	107.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	852	BCL	C4A-NA-C1A	3.16	108.13	106.71
4	L	850	BCL	CED-O2D-CGD	3.15	123.06	115.94
8	M	859	SPO	C15-C16-C17	-3.13	117.61	126.42
5	L	855	BPH	O2D-CGD-CBD	3.12	116.82	111.27
5	M	854	BPH	CHC-C4B-NB	-3.11	118.42	124.93
5	M	854	BPH	CBB-CAB-C3B	-3.10	113.80	120.43
4	M	852	BCL	CHA-C1A-NA	-3.10	119.30	126.40
5	M	854	BPH	CHC-C1C-NC	-3.09	121.53	125.20
5	L	855	BPH	O1D-CGD-CBD	-3.05	118.24	124.48
7	M	857	U10	C4M-O4-C4	3.01	127.14	116.47
4	L	850	BCL	C2A-C3A-C4A	2.94	106.62	101.87
7	M	857	U10	C20-C19-C18	-2.93	116.16	123.68
4	M	853	BCL	O2D-CGD-CBD	2.88	116.38	111.27
4	L	851	BCL	CHA-C1A-NA	-2.87	119.82	126.40
4	M	852	BCL	C4B-CHC-C1C	2.81	135.68	130.12
8	M	859	SPO	C18-C17-C16	2.80	122.48	118.08
4	L	850	BCL	O2A-C1-C2	-2.80	101.28	108.64
4	M	853	BCL	O2A-CGA-CBA	2.78	120.63	111.91
7	M	857	U10	C25-C24-C26	2.77	119.93	115.27
4	L	851	BCL	C2A-C1A-CHA	2.72	128.61	123.86
7	M	857	U10	O5-C5-C4	-2.68	115.25	120.93
5	L	855	BPH	C3D-CAD-CBD	2.67	111.13	107.61
7	M	857	U10	C21-C19-C18	2.67	126.52	121.12
8	M	859	SPO	C16-C17-C19	2.67	123.03	118.94
5	L	855	BPH	CED-O2D-CGD	2.66	121.95	115.94
5	M	854	BPH	CED-O2D-CGD	2.64	121.91	115.94
4	L	850	BCL	C6-C5-C3	2.60	120.26	113.45
4	M	852	BCL	C15-C13-C12	-2.59	98.51	112.13
4	M	852	BCL	C2A-C1A-CHA	2.58	128.37	123.86
9	M	5000	CDL	CB4-OB6-CB5	2.57	124.11	117.79
4	L	851	BCL	C4B-CHC-C1C	2.56	135.18	130.12
5	M	854	BPH	CMB-C2B-C3B	2.55	133.48	127.61
9	M	5000	CDL	CB6-CB4-CB3	-2.55	105.77	111.79
4	M	853	BCL	O1D-CGD-CBD	-2.53	119.30	124.48
5	L	855	BPH	C7-C6-C5	-2.52	106.53	113.36
4	M	853	BCL	C2C-C3C-C4C	2.51	105.11	101.34
5	L	855	BPH	CHC-C1C-NC	-2.51	122.22	125.20
5	L	855	BPH	C1C-NC-C4C	-2.51	108.34	110.54
4	M	852	BCL	C3D-CAD-CBD	2.50	110.89	107.61
7	M	857	U10	C35-C34-C36	2.50	119.47	115.27
4	L	850	BCL	C4B-CHC-C1C	2.49	135.04	130.12
7	M	857	U10	C30-C29-C31	2.47	119.43	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	850	BCL	CHA-C1A-NA	-2.44	120.81	126.40
4	M	852	BCL	CGD-CBD-CAD	-2.43	102.86	110.73
4	L	851	BCL	C3D-CAD-CBD	2.43	110.80	107.61
4	M	853	BCL	C4B-CHC-C1C	2.39	134.84	130.12
5	M	854	BPH	C1C-NC-C4C	-2.36	108.47	110.54
4	L	850	BCL	C1-O2A-CGA	2.35	122.61	116.44
4	L	850	BCL	C4A-NA-C1A	2.34	107.76	106.71
8	M	859	SPO	C10-C9-C7	-2.33	123.98	127.31
5	L	855	BPH	CBB-CAB-C3B	-2.33	115.46	120.43
5	L	855	BPH	CMB-C2B-C3B	2.33	132.96	127.61
7	M	857	U10	C26-C24-C23	2.30	125.78	121.12
5	L	855	BPH	CAC-C3C-C2C	-2.28	108.55	114.26
5	L	855	BPH	C2A-C3A-C4A	2.28	105.85	101.34
4	L	850	BCL	C2A-C1A-CHA	2.26	127.81	123.86
9	M	5000	CDL	CA6-CA4-CA3	-2.26	106.44	111.79
5	M	854	BPH	C2A-C3A-C4A	2.25	105.79	101.34
4	L	851	BCL	C6-C5-C3	2.25	119.36	113.45
4	L	850	BCL	O2D-CGD-CBD	2.25	115.26	111.27
7	M	857	U10	C1-C6-C5	-2.25	117.47	119.58
7	M	857	U10	C8-C7-C6	-2.22	106.06	112.05
4	L	851	BCL	O2A-CGA-CBA	2.20	118.80	111.91
7	M	857	U10	C10-C9-C11	2.19	118.95	115.27
4	L	850	BCL	C2C-C3C-C4C	2.17	104.59	101.34
4	L	851	BCL	C4A-NA-C1A	2.16	107.68	106.71
7	M	857	U10	C27-C28-C29	-2.13	122.53	127.66
4	L	851	BCL	CBC-CAC-C3C	2.13	118.21	113.47
7	M	857	U10	C1M-C1-C6	-2.13	120.93	124.40
5	M	854	BPH	C6-C5-C3	2.11	118.99	113.45
4	L	850	BCL	O1D-CGD-CBD	-2.11	120.17	124.48
4	M	853	BCL	C2A-C1A-CHA	2.10	127.53	123.86
4	M	853	BCL	CHA-C1A-NA	-2.09	121.60	126.40
5	L	855	BPH	OBD-CAD-C3D	-2.09	124.52	127.98
8	M	859	SPO	C9-C10-C11	-2.07	116.76	123.22
8	M	859	SPO	C13-C12-C11	2.07	121.33	118.08
9	M	5000	CDL	C52-C51-CB5	2.06	121.11	113.62
4	M	852	BCL	CAC-C3C-C2C	-2.06	109.12	114.26
8	M	859	SPO	C34-C33-C35	-2.03	111.85	115.27
7	M	857	U10	C11-C12-C13	2.03	118.54	111.88
5	M	854	BPH	OBD-CAD-C3D	-2.02	124.62	127.98

There are no chirality outliers.

All (107) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	850	BCL	C14-C13-C15-C16
4	L	851	BCL	C2C-C3C-CAC-CBC
4	L	851	BCL	C4C-C3C-CAC-CBC
4	M	852	BCL	C4-C3-C5-C6
5	L	855	BPH	C4C-C3C-CAC-CBC
5	L	855	BPH	C2C-C3C-CAC-CBC
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
7	M	857	U10	C20-C19-C21-C22
7	M	857	U10	C19-C21-C22-C23
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	C20-C21-C22-C23
8	M	859	SPO	C21-C22-C23-C24
8	M	859	SPO	C36-C37-C38-C39
9	M	5000	CDL	CA3-OA5-PA1-OA2
9	M	5000	CDL	CA3-OA5-PA1-OA3
9	M	5000	CDL	CA3-OA5-PA1-OA4
8	M	859	SPO	C36-C37-C38-C40
4	M	852	BCL	C2-C3-C5-C6
7	M	857	U10	C18-C19-C21-C22
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
8	M	859	SPO	C24-C23-C25-C26
9	M	5000	CDL	C11-CA5-OA6-CA4
9	M	5000	CDL	CB7-C71-C72-C73
4	L	850	BCL	C2A-CAA-CBA-CGA
4	M	853	BCL	C5-C6-C7-C8
7	M	857	U10	C29-C31-C32-C33
9	M	5000	CDL	CA5-C11-C12-C13
9	M	5000	CDL	OA7-CA5-OA6-CA4
4	L	851	BCL	C2A-CAA-CBA-CGA
9	M	5000	CDL	C79-C80-C81-C82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	M	5000	CDL	C11-C12-C13-C14
9	M	5000	CDL	C36-C37-C38-C39
9	M	5000	CDL	C54-C55-C56-C57
9	M	5000	CDL	C51-C52-C53-C54
9	M	5000	CDL	C20-C21-C22-C23
9	M	5000	CDL	C39-C40-C41-C42
4	M	853	BCL	C3-C5-C6-C7
9	M	5000	CDL	C78-C79-C80-C81
9	M	5000	CDL	C34-C35-C36-C37
4	M	853	BCL	C14-C13-C15-C16
9	M	5000	CDL	OA5-CA3-CA4-CA6
5	M	854	BPH	C2C-C3C-CAC-CBC
9	M	5000	CDL	CA3-CA4-CA6-OA8
8	M	859	SPO	C4-C1-O1-CM1
9	M	5000	CDL	C40-C41-C42-C43
9	M	5000	CDL	C80-C81-C82-C83
8	M	859	SPO	C2-C1-O1-CM1
8	M	859	SPO	C3-C1-O1-CM1
9	M	5000	CDL	C55-C56-C57-C58
9	M	5000	CDL	C52-C53-C54-C55
4	M	853	BCL	C12-C13-C15-C16
5	M	854	BPH	C11-C10-C8-C9
7	M	857	U10	C12-C11-C9-C10
4	L	850	BCL	C2-C1-O2A-CGA
9	M	5000	CDL	C38-C39-C40-C41
4	L	850	BCL	C12-C13-C15-C16
4	M	852	BCL	C11-C10-C8-C7
4	M	852	BCL	C12-C13-C15-C16
5	M	854	BPH	C11-C10-C8-C7
4	L	851	BCL	CAD-CBD-CGD-O2D
4	M	852	BCL	C15-C16-C17-C18
9	M	5000	CDL	OA5-CA3-CA4-OA6
4	M	852	BCL	C11-C10-C8-C9
4	M	852	BCL	C14-C13-C15-C16
4	M	853	BCL	C2A-CAA-CBA-CGA
4	L	851	BCL	C5-C6-C7-C8
8	M	859	SPO	C34-C33-C35-C36
4	M	852	BCL	C3-C5-C6-C7
7	M	857	U10	C12-C11-C9-C8
9	M	5000	CDL	CB3-OB5-PB2-OB2
5	M	854	BPH	C2A-CAA-CBA-CGA
5	M	854	BPH	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	M	5000	CDL	C31-C32-C33-C34
8	M	859	SPO	C17-C19-C20-C21
7	M	857	U10	C9-C11-C12-C13
9	M	5000	CDL	C21-C22-C23-C24
8	M	859	SPO	C18-C17-C19-C20
9	M	5000	CDL	CA7-C31-C32-C33
4	L	850	BCL	C4-C3-C5-C6
8	M	859	SPO	C16-C17-C19-C20
9	M	5000	CDL	OA6-CA4-CA6-OA8
8	M	859	SPO	C33-C35-C36-C37
4	L	850	BCL	C2-C3-C5-C6
9	M	5000	CDL	C81-C82-C83-C84
8	M	859	SPO	C32-C33-C35-C36
4	L	850	BCL	CHA-CBD-CGD-O1D
4	M	852	BCL	CHA-CBD-CGD-O2D
4	M	853	BCL	CHA-CBD-CGD-O1D
5	L	855	BPH	CHA-CBD-CGD-O2D
9	M	5000	CDL	C72-C71-CB7-OB8
8	M	859	SPO	C29-C28-C30-C31
9	M	5000	CDL	C72-C71-CB7-OB9
4	L	851	BCL	C14-C13-C15-C16
4	M	852	BCL	CAA-CBA-CGA-O2A

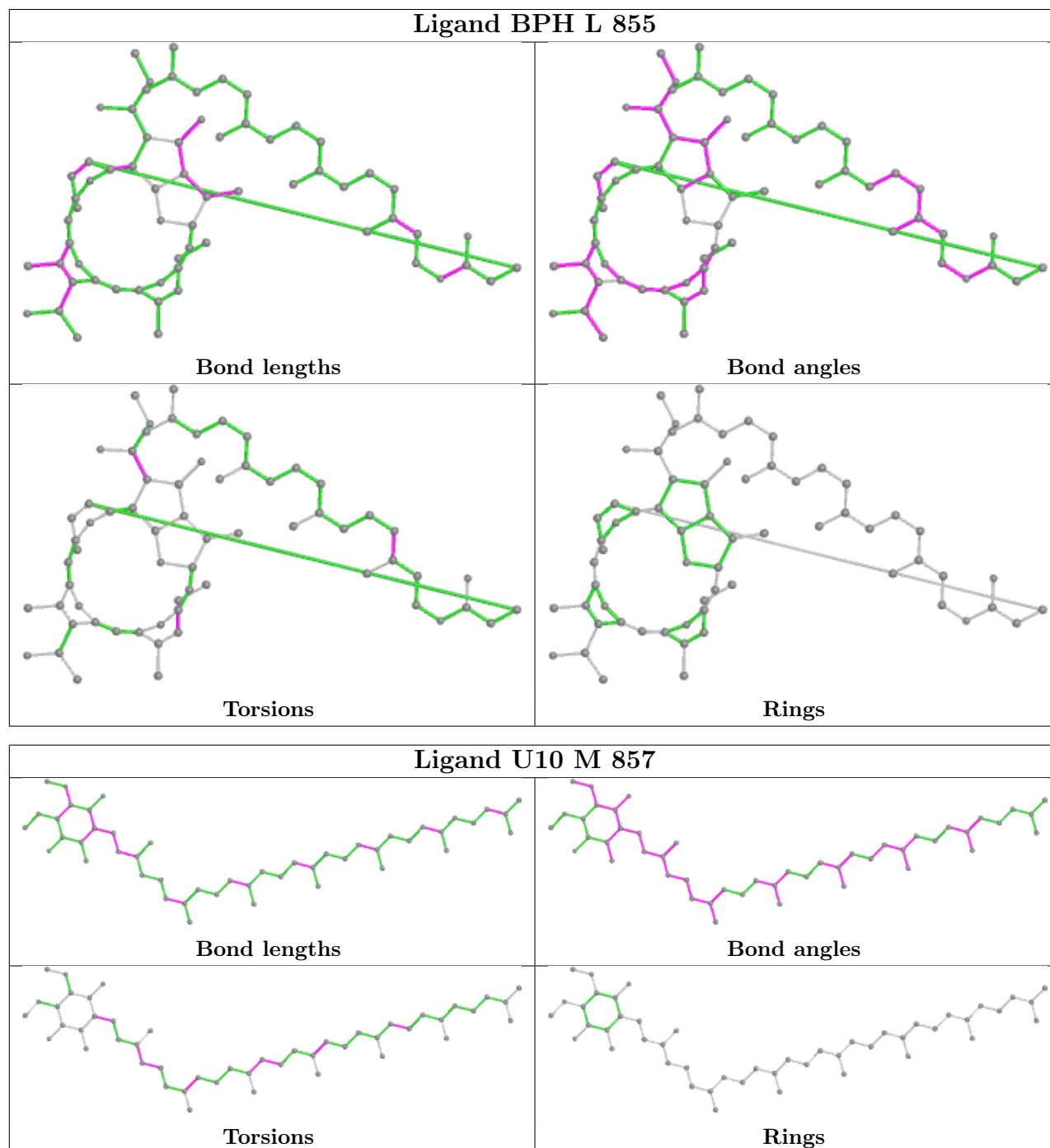
There are no ring outliers.

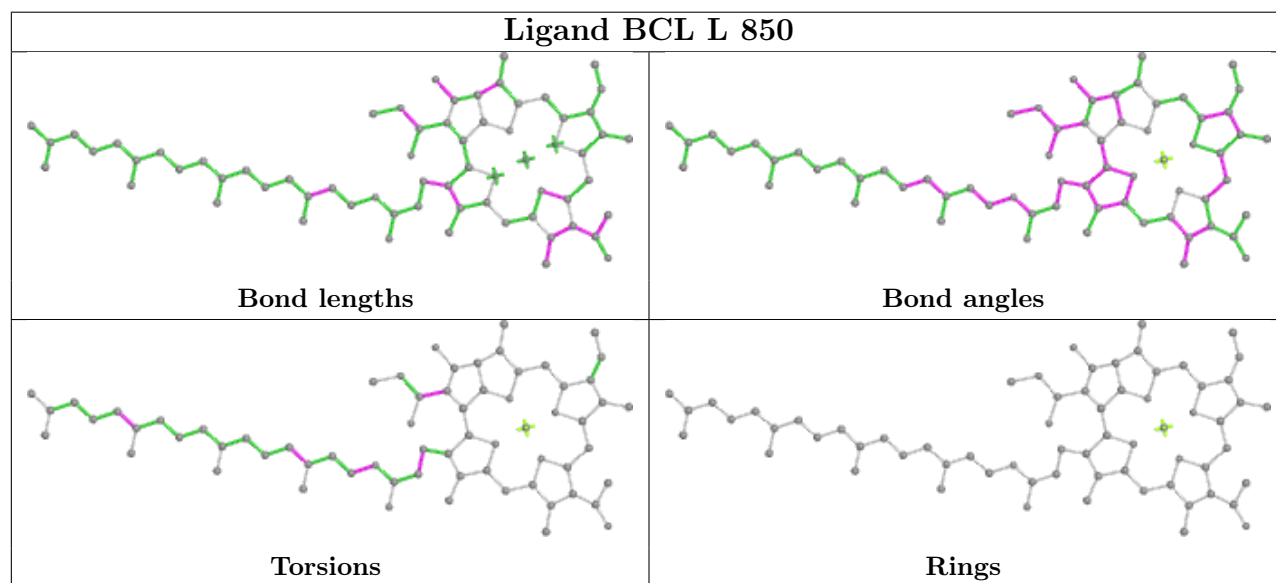
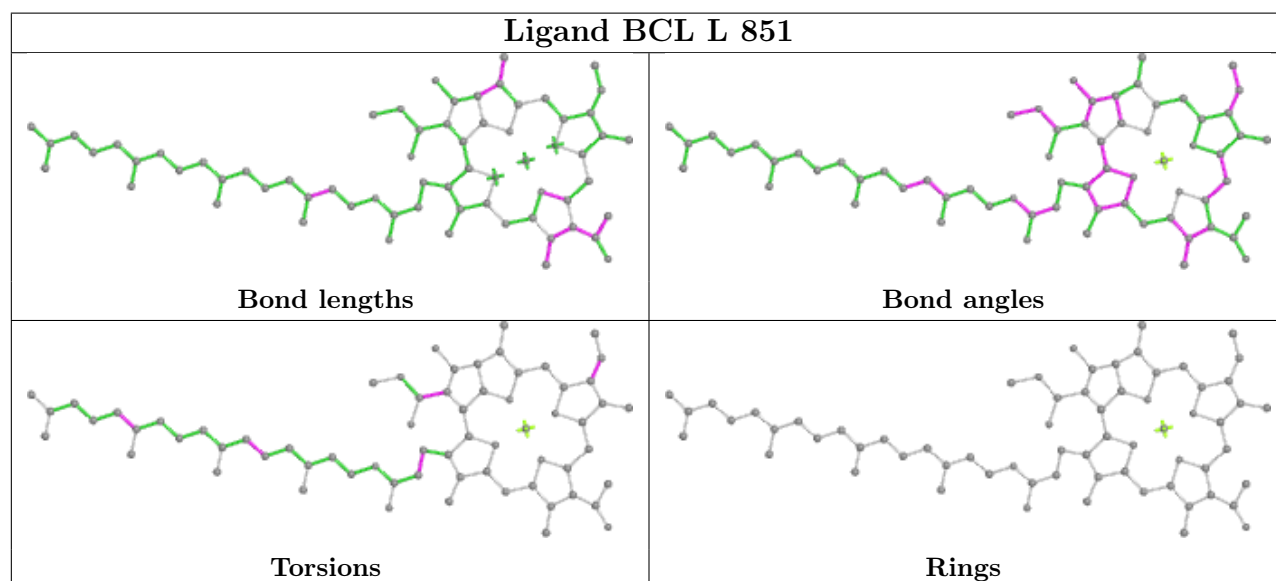
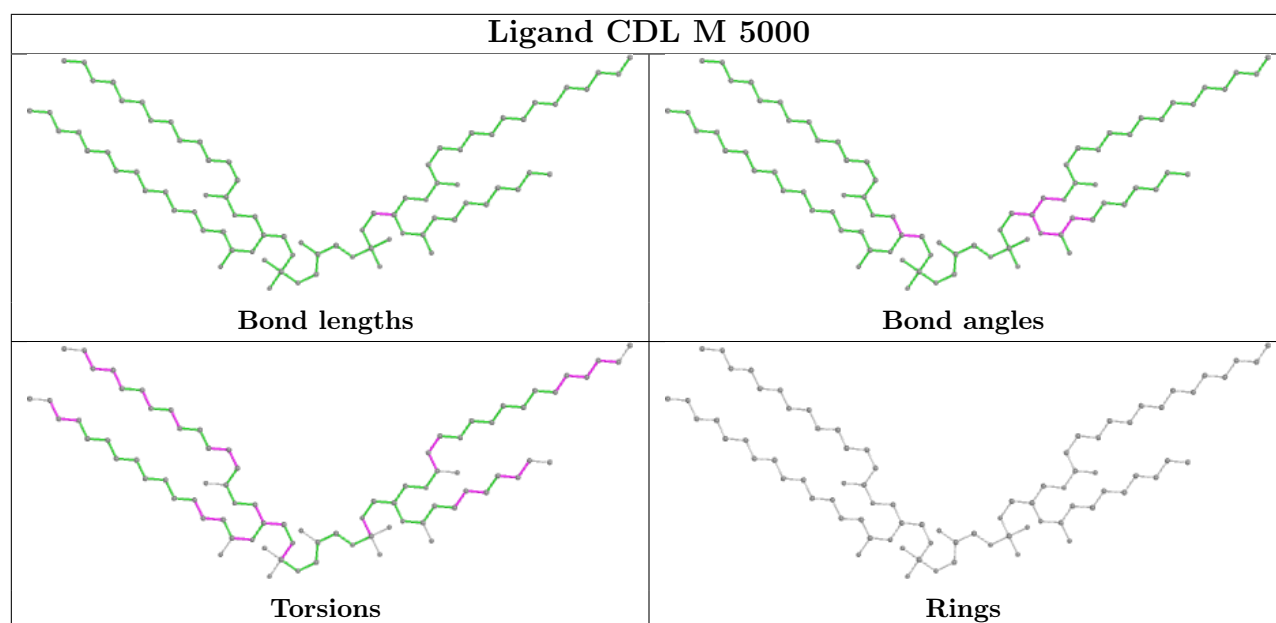
9 monomers are involved in 32 short contacts:

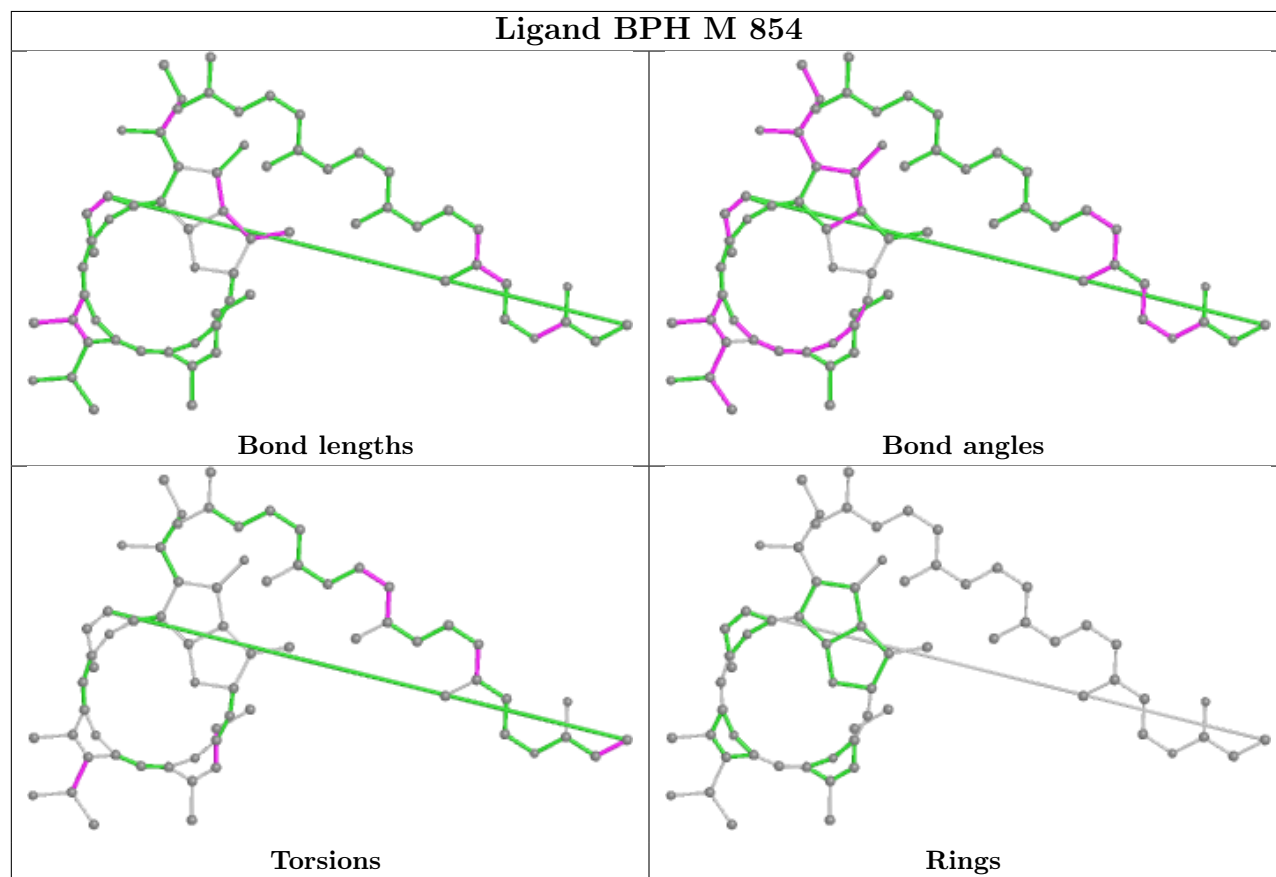
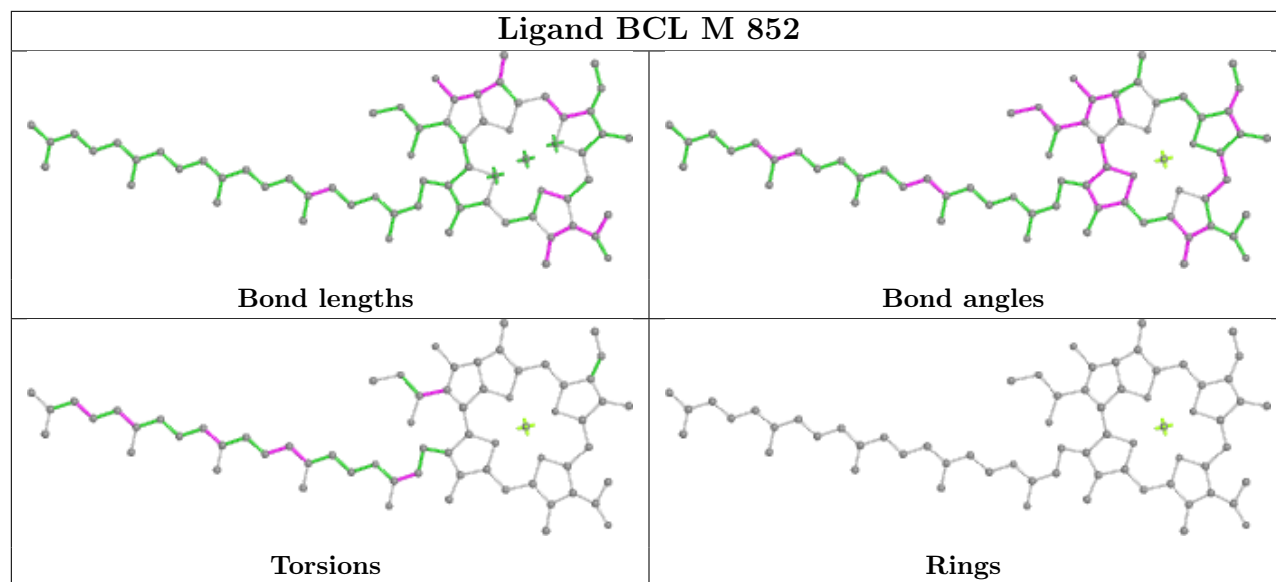
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	855	BPH	6	0
7	M	857	U10	4	0
9	M	5000	CDL	2	0
4	L	851	BCL	4	0
4	L	850	BCL	6	0
4	M	852	BCL	6	0
5	M	854	BPH	5	0
8	M	859	SPO	1	0
4	M	853	BCL	5	0

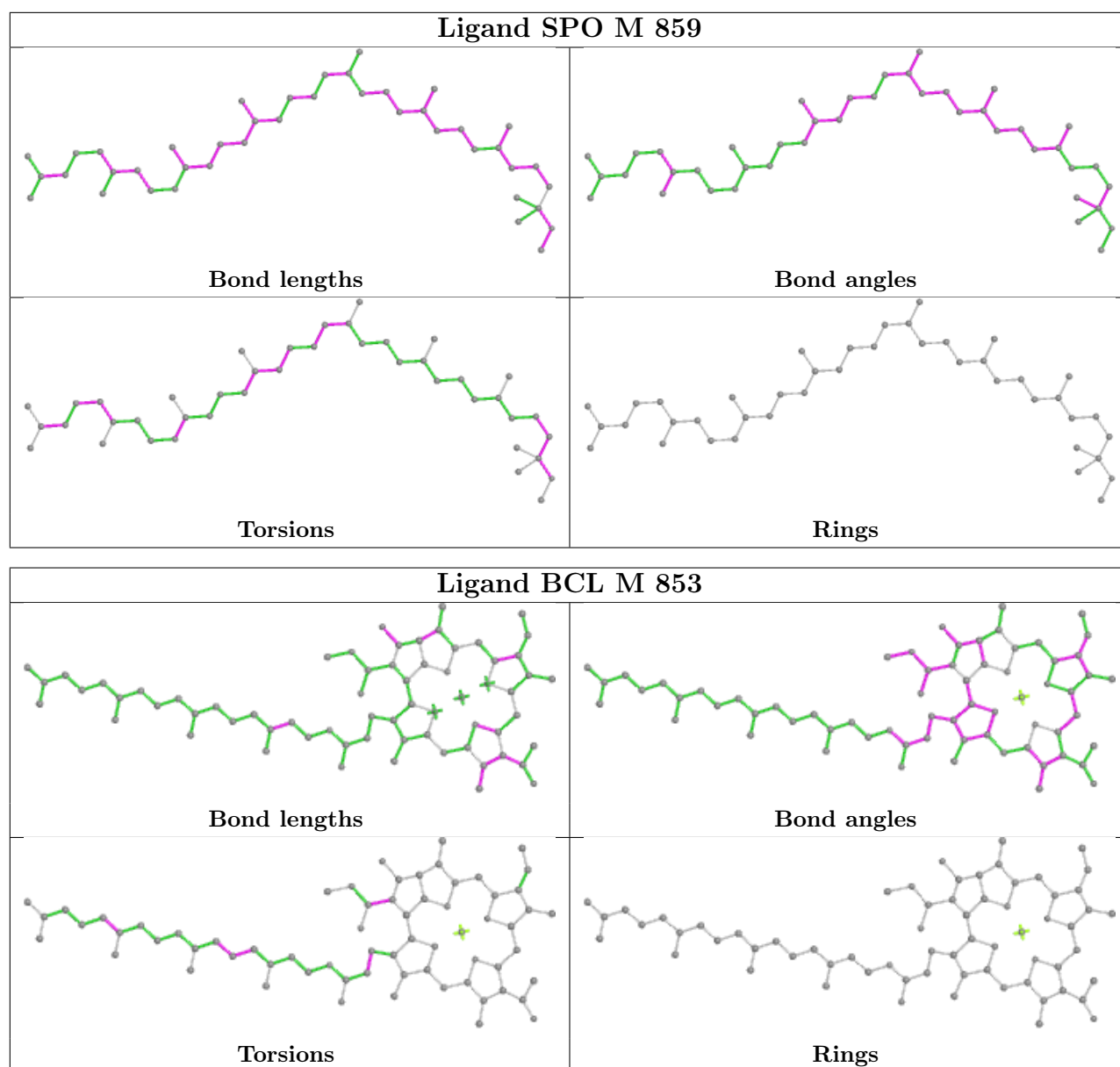
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.