



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 05:30 AM EDT

PDB ID : 1JGY
Title : Photosynthetic Reaction Center Mutant With Tyr M 76 Replaced With Phe
Authors : Camara-Artigas, A.; Magee, C.L.; Williams, J.C.; Allen, J.P.
Deposited on : 2001-06-27
Resolution : 2.70 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

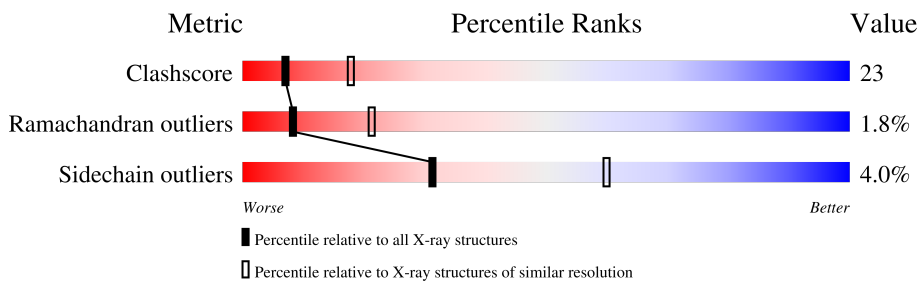
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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	 60% 37% .
2	M	307	 58% 36% . .
3	H	260	 57% 32% . 8%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 7123 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
			2407	1607	394	396	10			

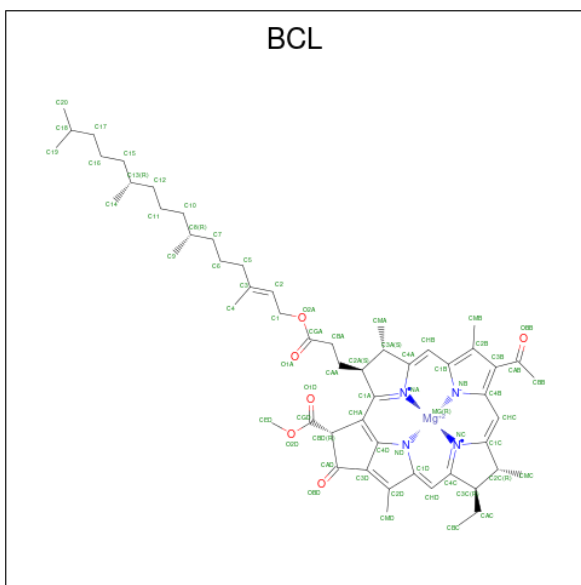
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	76	PHE	TYR	engineered mutation	UNP P02953

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

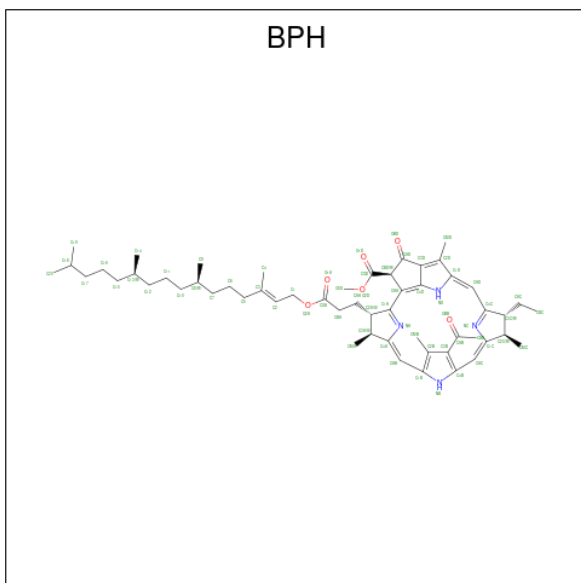
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	240	Total	C	N	O	S	0	0	0
			1829	1169	314	337	9			

- 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	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: $\text{C}_{55}\text{H}_{76}\text{N}_4\text{O}_6$).

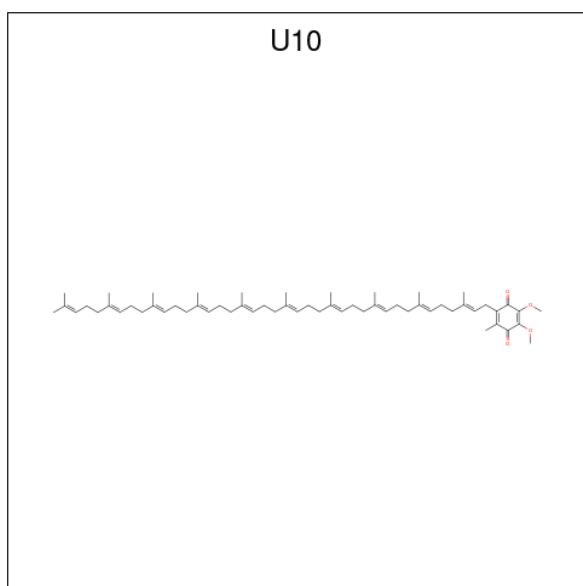


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			65	55	4	6		

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

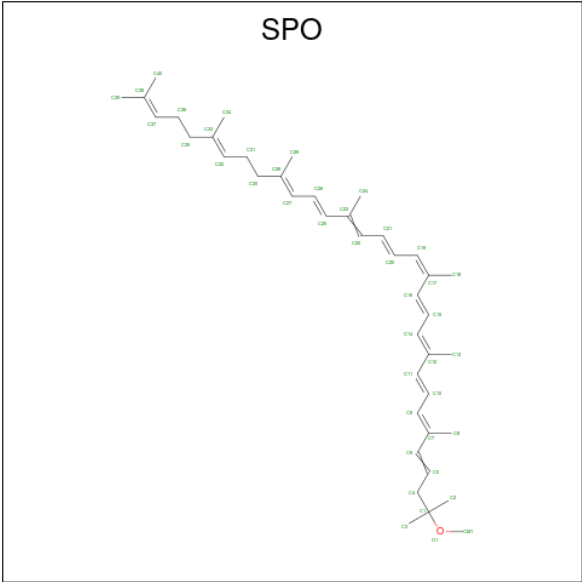
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	M	1	Total	Fe	0	0
			1	1		

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



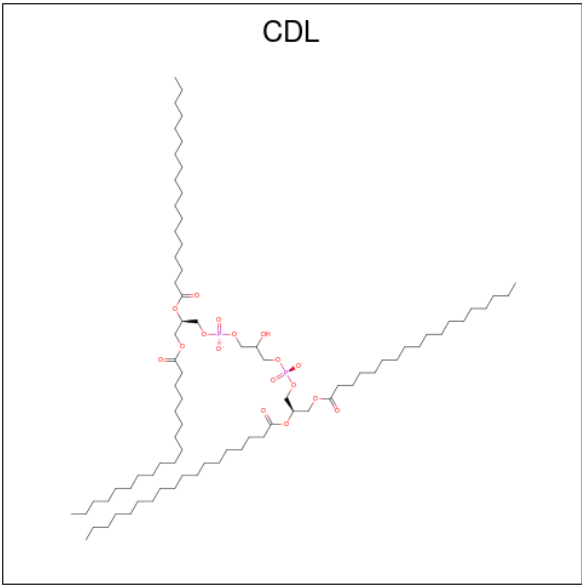
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	M	1	Total	C	O	0	0
			48	44	4		

- 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.

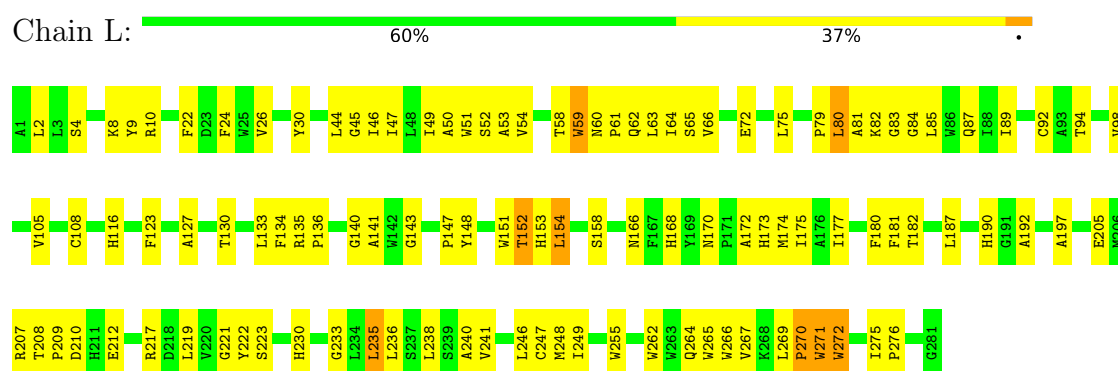
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	L	16	Total 16	O 16	0	0
10	M	33	Total 33	O 33	0	0
10	H	40	Total 40	O 40	0	0

3 Residue-property plots

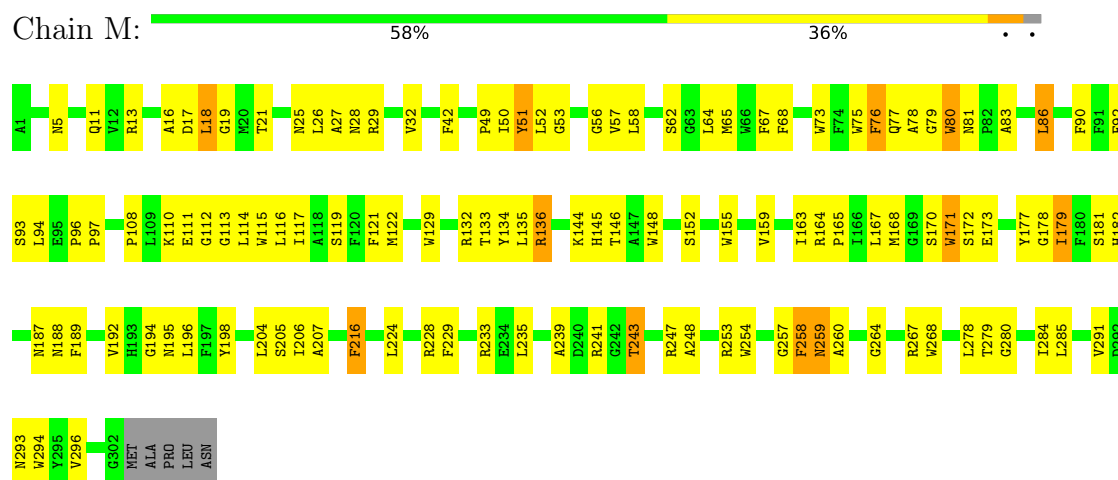
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

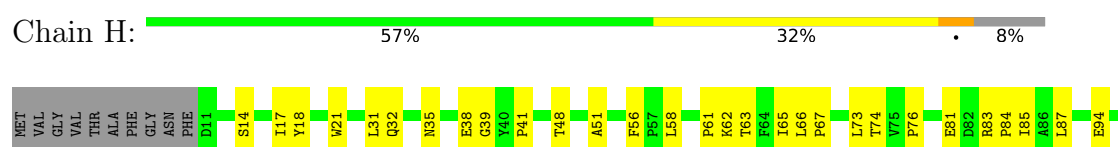
• Molecule 1: Photosynthetic Reaction Center L Subunit

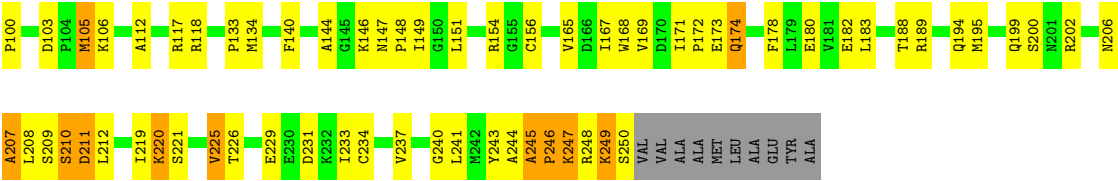


• Molecule 2: Photosynthetic Reaction Center M Subunit



• 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	141.68Å 141.68Å 186.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.10 – 2.70	Depositor
% Data completeness (in resolution range)	62.6 (29.10-2.70)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7123	wwPDB-VP
Average B, all atoms (Å ²)	49.0	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: CDL, SPO, U10, BCL, BPH, FE

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	0.60	0/3175
2	M	0.42	0/2499	0.58	0/3411
3	H	0.40	0/1877	0.64	0/2553
All	All	0.41	0/6696	0.61	0/9139

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	99	0
2	M	2407	0	2321	150	0
3	H	1829	0	1836	88	0
4	L	132	0	148	11	0
4	M	132	0	148	11	0
5	L	65	0	76	4	0
5	M	65	0	76	10	0
6	M	1	0	0	0	0
7	M	48	0	63	5	0
8	M	42	0	60	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	M	81	0	106	2	0
10	H	40	0	0	4	0
10	L	16	0	0	0	0
10	M	33	0	0	9	0
All	All	7123	0	7021	321	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 23.

All (321) 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:21:THR:HG23	2:M:26:LEU:HD21	1.39	1.05
3:H:249:LYS:HG3	3:H:250:SER:H	1.23	1.03
3:H:148:PRO:HA	3:H:151:LEU:HD12	1.43	1.00
2:M:114:LEU:HA	2:M:117:ILE:HD12	1.47	0.97
2:M:279:THR:HB	10:M:1024:HOH:O	1.65	0.95
2:M:243:THR:CG2	2:M:247:ARG:HE	1.81	0.93
3:H:41:PRO:HG3	3:H:58:LEU:HD11	1.49	0.93
2:M:114:LEU:HD12	2:M:117:ILE:HD12	1.58	0.84
2:M:243:THR:HG22	2:M:247:ARG:HE	1.42	0.83
2:M:204:LEU:HB3	2:M:279:THR:HG21	1.59	0.83
2:M:108:PRO:HG2	2:M:111:GLU:HB2	1.60	0.83
2:M:136:ARG:HA	2:M:136:ARG:HH11	1.47	0.79
3:H:148:PRO:HA	3:H:151:LEU:CD1	2.14	0.77
3:H:103:ASP:HB3	3:H:106:LYS:HB2	1.66	0.76
1:L:269:LEU:HB2	1:L:272:TRP:NE1	2.02	0.75
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.69	0.74
1:L:60:ASN:O	1:L:64:ILE:HG13	1.89	0.73
1:L:180:PHE:CD2	1:L:240:ALA:HB1	2.23	0.73
2:M:253:ARG:HH11	2:M:259:ASN:ND2	1.88	0.72
3:H:249:LYS:HG3	3:H:250:SER:N	2.03	0.71
2:M:32:VAL:HG22	2:M:49:PRO:HD3	1.72	0.71
1:L:52:SER:OG	1:L:66:VAL:HG22	1.92	0.70
1:L:208:THR:HB	1:L:209:PRO:HD2	1.73	0.69
1:L:264:GLN:HA	1:L:267:VAL:HG12	1.75	0.69
2:M:113:GLY:HA2	2:M:116:LEU:HD12	1.75	0.68
3:H:226:THR:OG1	3:H:229:GLU:HG3	1.93	0.68
2:M:248:ALA:HB1	7:M:857:U10:H3M2	1.75	0.68
2:M:25:ASN:HD21	2:M:27:ALA:HB3	1.59	0.68
2:M:243:THR:HG21	2:M:247:ARG:HE	1.56	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:18:LEU:HD22	2:M:18:LEU:N	2.08	0.68
3:H:183:LEU:HB2	10:H:1090:HOH:O	1.94	0.68
2:M:25:ASN:HD22	2:M:28:ASN:ND2	1.93	0.67
1:L:187:LEU:HD13	2:M:216:PHE:CG	2.30	0.67
2:M:243:THR:HG21	2:M:247:ARG:HH21	1.60	0.67
3:H:61:PRO:HA	3:H:76:PRO:HD2	1.76	0.67
4:M:852:BCL:HBB3	4:M:853:BCL:HMD2	1.75	0.66
2:M:11:GLN:HB2	3:H:144:ALA:HB3	1.77	0.66
2:M:253:ARG:O	2:M:257:GLY:HA2	1.93	0.66
1:L:94:THR:O	1:L:98:VAL:HG23	1.95	0.66
2:M:259:ASN:N	2:M:259:ASN:HD22	1.94	0.66
2:M:253:ARG:HH11	2:M:259:ASN:HD21	1.41	0.66
2:M:228:ARG:NE	3:H:195:MET:HE3	2.12	0.65
3:H:148:PRO:CG	3:H:167:ILE:HD11	2.26	0.65
2:M:136:ARG:HH11	2:M:136:ARG:CA	2.10	0.65
1:L:45:GLY:HA3	5:L:855:BPH:H9C1	1.79	0.64
1:L:75:LEU:HD11	1:L:140:GLY:HA2	1.81	0.63
2:M:53:GLY:O	2:M:57:VAL:HG23	1.98	0.63
1:L:30:TYR:HB2	2:M:254:TRP:HB3	1.81	0.62
1:L:271:TRP:CD1	1:L:271:TRP:N	2.58	0.62
4:L:850:BCL:HBB2	4:M:852:BCL:H111	1.82	0.62
1:L:269:LEU:HD12	1:L:272:TRP:CZ2	2.34	0.62
3:H:14:SER:O	3:H:18:TYR:HD2	1.82	0.62
1:L:269:LEU:HD12	1:L:272:TRP:HZ2	1.65	0.61
4:L:850:BCL:H2	5:M:854:BPH:HMB2	1.82	0.61
3:H:245:ALA:HB2	3:H:248:ARG:NH2	2.16	0.61
3:H:219:ILE:HG21	3:H:225:VAL:HG13	1.83	0.61
2:M:18:LEU:HD22	2:M:18:LEU:H	1.66	0.61
2:M:108:PRO:HG2	2:M:111:GLU:CB	2.31	0.60
3:H:245:ALA:HB3	3:H:246:PRO:HD3	1.84	0.60
2:M:178:GLY:HA3	2:M:181:SER:HB3	1.84	0.60
2:M:25:ASN:ND2	2:M:27:ALA:HB3	2.16	0.60
2:M:119:SER:HB3	8:M:859:SPO:H311	1.84	0.59
2:M:64:LEU:HB3	2:M:68:PHE:CE2	2.37	0.59
2:M:67:PHE:CD1	5:M:854:BPH:H9C1	2.38	0.59
1:L:127:ALA:O	1:L:130:THR:HB	2.02	0.59
3:H:154:ARG:HD3	10:H:1020:HOH:O	2.03	0.59
3:H:240:GLY:O	3:H:244:ALA:HB3	2.03	0.59
2:M:280:GLY:HA2	4:M:852:BCL:HED2	1.85	0.58
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.85	0.58
1:L:174:MET:HG2	4:L:850:BCL:O1D	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:113:GLY:O	2:M:117:ILE:HG13	2.03	0.58
2:M:228:ARG:CD	3:H:195:MET:HE3	2.34	0.58
2:M:243:THR:O	2:M:247:ARG:HG3	2.04	0.58
3:H:210:SER:O	3:H:212:LEU:N	2.37	0.57
2:M:135:LEU:HB3	2:M:136:ARG:HH12	1.68	0.57
2:M:135:LEU:HB3	2:M:136:ARG:NH1	2.19	0.56
1:L:65:SER:HB2	1:L:152:THR:HG21	1.87	0.56
2:M:241:ARG:HD3	3:H:38:GLU:OE1	2.05	0.56
3:H:48:THR:HA	10:H:1044:HOH:O	2.06	0.56
3:H:81:GLU:O	3:H:83:ARG:HG2	2.04	0.56
2:M:206:ILE:HD12	4:M:853:BCL:OBD	2.04	0.56
1:L:170:ASN:HB3	1:L:173:HIS:HB3	1.86	0.56
2:M:239:ALA:HA	3:H:73:LEU:HD22	1.87	0.56
2:M:114:LEU:HD12	2:M:117:ILE:CD1	2.34	0.56
2:M:51:TYR:HD2	2:M:51:TYR:C	2.09	0.55
2:M:97:PRO:HA	2:M:112:GLY:HA3	1.87	0.55
1:L:52:SER:HB2	1:L:85:LEU:HD13	1.88	0.55
3:H:105:MET:HE3	3:H:112:ALA:HB2	1.89	0.55
4:L:851:BCL:H122	5:L:855:BPH:H3A	1.89	0.55
2:M:16:ALA:HB1	2:M:32:VAL:HG11	1.88	0.54
2:M:205:SER:HA	10:M:1024:HOH:O	2.07	0.54
3:H:168:TRP:NE1	3:H:180:GLU:HB2	2.22	0.54
2:M:76:PHE:CZ	2:M:110:LYS:HE3	2.42	0.54
2:M:51:TYR:C	2:M:51:TYR:CD2	2.81	0.54
1:L:151:TRP:O	1:L:154:LEU:HB2	2.08	0.54
3:H:229:GLU:O	3:H:233:ILE:HG13	2.07	0.54
3:H:156:CYS:HB2	3:H:248:ARG:HG3	1.89	0.54
3:H:199:GLN:OE1	3:H:202:ARG:HD2	2.07	0.54
3:H:245:ALA:C	3:H:247:LYS:H	2.11	0.54
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.43	0.54
3:H:156:CYS:SG	3:H:248:ARG:HB2	2.47	0.54
3:H:156:CYS:HB3	3:H:206:ASN:O	2.06	0.54
2:M:78:ALA:HB2	2:M:92:PHE:CZ	2.42	0.54
3:H:165:VAL:HG11	3:H:182:GLU:HB2	1.90	0.54
1:L:51:TRP:O	1:L:54:VAL:HG22	2.08	0.54
1:L:60:ASN:HD22	1:L:63:LEU:HG	1.73	0.54
1:L:75:LEU:CD1	1:L:140:GLY:HA2	2.38	0.54
1:L:262:TRP:O	1:L:265:TRP:HD1	1.90	0.54
1:L:235:LEU:HD22	2:M:42:PHE:CZ	2.43	0.53
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.43	0.53
2:M:163:ILE:O	2:M:167:LEU:HG	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:182:THR:HG22	1:L:236:LEU:HD13	1.91	0.53
2:M:90:PHE:HD1	2:M:179:ILE:HG21	1.73	0.53
3:H:243:TYR:O	3:H:246:PRO:HD2	2.09	0.53
1:L:49:ILE:HG12	1:L:89:ILE:HD13	1.90	0.53
2:M:170:SER:OG	2:M:172:SER:HB3	2.07	0.53
1:L:275:ILE:HD12	2:M:83:ALA:HB1	1.90	0.53
2:M:58:LEU:O	2:M:62:SER:HB2	2.08	0.53
1:L:58:THR:HG23	1:L:64:ILE:HG12	1.91	0.53
1:L:272:TRP:HA	1:L:275:ILE:CD1	2.39	0.53
2:M:25:ASN:ND2	2:M:28:ASN:ND2	2.57	0.53
1:L:219:LEU:HD12	2:M:132:ARG:NH1	2.24	0.53
1:L:133:LEU:HD23	1:L:133:LEU:C	2.30	0.52
1:L:181:PHE:HB3	5:M:854:BPH:HBB2	1.90	0.52
4:M:853:BCL:HAA2	4:M:853:BCL:HBD	1.92	0.52
3:H:248:ARG:HB2	3:H:248:ARG:HH11	1.74	0.52
1:L:60:ASN:HB3	1:L:63:LEU:HD12	1.90	0.52
3:H:63:THR:HA	3:H:73:LEU:O	2.10	0.52
1:L:79:PRO:O	1:L:82:LYS:N	2.40	0.52
2:M:134:TYR:CE2	2:M:144:LYS:HG3	2.45	0.52
2:M:264:GLY:HA3	3:H:35:ASN:OD1	2.10	0.52
3:H:65:ILE:O	3:H:65:ILE:HG22	2.09	0.52
1:L:59:TRP:HA	1:L:59:TRP:CE3	2.45	0.52
1:L:272:TRP:HA	1:L:275:ILE:HG13	1.91	0.51
2:M:5:ASN:ND2	3:H:194:GLN:HG3	2.25	0.51
2:M:187:ASN:HA	4:M:852:BCL:HBC1	1.92	0.51
1:L:181:PHE:CD2	5:M:854:BPH:HBB1	2.46	0.51
1:L:271:TRP:O	1:L:275:ILE:HD11	2.10	0.51
2:M:56:GLY:HA2	2:M:132:ARG:HD2	1.92	0.51
3:H:245:ALA:HB2	3:H:248:ARG:HH22	1.74	0.51
1:L:133:LEU:HD22	1:L:134:PHE:CD1	2.46	0.51
2:M:280:GLY:N	10:M:1024:HOH:O	2.43	0.51
2:M:108:PRO:HG2	2:M:111:GLU:CG	2.40	0.51
2:M:94:LEU:HD11	2:M:114:LEU:HB3	1.93	0.51
1:L:233:GLY:HA3	2:M:216:PHE:CE1	2.46	0.51
2:M:205:SER:CB	10:M:1024:HOH:O	2.59	0.51
3:H:173:GLU:O	3:H:174:GLN:C	2.50	0.50
1:L:8:LYS:HA	3:H:87:LEU:HD11	1.92	0.50
4:L:850:BCL:HAA2	4:L:850:BCL:HBD	1.93	0.50
3:H:207:ALA:HA	3:H:241:LEU:HD23	1.94	0.50
3:H:209:SER:O	3:H:210:SER:C	2.49	0.50
1:L:116:HIS:CD2	2:M:224:LEU:HB3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:141:ALA:C	1:L:143:GLY:H	2.15	0.50
3:H:208:LEU:HD11	3:H:237:VAL:HG22	1.94	0.49
1:L:22:PHE:HA	1:L:24:PHE:CE2	2.47	0.49
2:M:258:PHE:HE2	3:H:32:GLN:OE1	1.95	0.49
4:L:850:BCL:H11	5:M:854:BPH:HBB2	1.95	0.49
3:H:248:ARG:O	3:H:248:ARG:HG2	2.13	0.49
1:L:172:ALA:HB3	1:L:247:CYS:CB	2.43	0.49
2:M:168:MET:HG3	2:M:173:GLU:HG3	1.94	0.49
2:M:68:PHE:HE1	8:M:859:SPO:H31	1.78	0.49
2:M:167:LEU:CD1	2:M:285:LEU:HD11	2.43	0.49
2:M:189:PHE:HA	10:M:1023:HOH:O	2.12	0.49
2:M:243:THR:HG21	2:M:247:ARG:NH2	2.27	0.48
1:L:83:GLY:O	1:L:87:GLN:HG3	2.14	0.48
3:H:248:ARG:HB2	3:H:248:ARG:NH1	2.28	0.48
1:L:105:VAL:O	1:L:108:CYS:HB2	2.14	0.48
2:M:136:ARG:NH1	2:M:136:ARG:N	2.62	0.48
3:H:168:TRP:HE1	3:H:180:GLU:HB2	1.79	0.48
2:M:192:VAL:HG12	2:M:192:VAL:O	2.13	0.48
2:M:243:THR:HG22	2:M:247:ARG:NE	2.19	0.48
1:L:44:LEU:HD23	1:L:92:CYS:SG	2.54	0.48
2:M:92:PHE:O	2:M:93:SER:HB2	2.14	0.48
1:L:265:TRP:CG	1:L:266:TRP:N	2.82	0.48
2:M:187:ASN:HA	4:M:852:BCL:HAC1	1.95	0.48
2:M:243:THR:CG2	2:M:247:ARG:NE	2.64	0.48
2:M:148:TRP:CE2	9:M:3000:CDL:H511	2.49	0.47
2:M:159:VAL:HA	2:M:163:ILE:HB	1.95	0.47
1:L:133:LEU:HD22	1:L:134:PHE:CE1	2.49	0.47
2:M:267:ARG:HH11	2:M:267:ARG:HG2	1.79	0.47
1:L:50:ALA:O	1:L:53:ALA:HB3	2.14	0.47
2:M:194:GLY:O	2:M:195:ASN:HB3	2.14	0.47
1:L:9:TYR:OH	2:M:243:THR:HG23	2.14	0.47
4:L:851:BCL:HAA2	4:L:851:BCL:HBD	1.96	0.47
2:M:253:ARG:O	2:M:257:GLY:CA	2.63	0.47
2:M:51:TYR:HE2	2:M:53:GLY:HA3	1.80	0.47
2:M:171:TRP:HA	2:M:171:TRP:CE3	2.50	0.46
1:L:79:PRO:O	1:L:81:ALA:N	2.48	0.46
2:M:228:ARG:HB3	3:H:195:MET:CE	2.45	0.46
3:H:171:ILE:N	3:H:172:PRO:HD2	2.31	0.46
2:M:73:TRP:O	2:M:77:GLN:HG3	2.16	0.46
2:M:267:ARG:HG2	2:M:267:ARG:NH1	2.31	0.46
2:M:284:ILE:HG12	4:M:852:BCL:HED3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:135:ARG:HD2	1:L:248:MET:O	2.16	0.46
2:M:259:ASN:ND2	2:M:259:ASN:N	2.63	0.46
5:M:854:BPH:H7C1	5:M:854:BPH:H121	1.97	0.46
3:H:180:GLU:OE2	3:H:188:THR:HG21	2.15	0.46
1:L:187:LEU:HD13	2:M:216:PHE:CD2	2.51	0.46
2:M:65:MET:HB3	2:M:121:PHE:CE2	2.51	0.46
2:M:188:ASN:ND2	10:M:1023:HOH:O	2.49	0.46
5:L:855:BPH:HHB	5:L:855:BPH:HMB1	1.79	0.46
2:M:259:ASN:HD22	2:M:259:ASN:H	1.62	0.46
1:L:180:PHE:CE2	1:L:240:ALA:HB1	2.51	0.45
2:M:96:PRO:HA	2:M:115:TRP:CG	2.52	0.45
2:M:239:ALA:HB1	3:H:66:LEU:HD22	1.98	0.45
2:M:268:TRP:CE3	3:H:31:LEU:HD13	2.51	0.45
1:L:2:LEU:HD21	1:L:10:ARG:CZ	2.47	0.45
1:L:272:TRP:HA	1:L:275:ILE:HD12	1.99	0.45
3:H:220:LYS:HG3	3:H:221:SER:H	1.82	0.45
1:L:221:GLY:HA2	2:M:50:ILE:HB	1.98	0.45
4:L:850:BCL:HMD2	4:L:851:BCL:HBB3	1.99	0.45
2:M:18:LEU:N	2:M:18:LEU:CD2	2.78	0.45
2:M:205:SER:CA	10:M:1024:HOH:O	2.65	0.45
1:L:181:PHE:HB3	5:M:854:BPH:CBB	2.47	0.45
2:M:114:LEU:HA	2:M:117:ILE:CD1	2.32	0.45
2:M:187:ASN:HA	4:M:852:BCL:CAC	2.47	0.45
5:M:854:BPH:HMB1	5:M:854:BPH:HHB	1.77	0.45
1:L:45:GLY:O	1:L:46:ILE:C	2.56	0.44
1:L:264:GLN:O	1:L:265:TRP:C	2.55	0.44
2:M:29:ARG:HA	2:M:51:TYR:HA	1.99	0.44
2:M:90:PHE:CD1	2:M:179:ILE:HG21	2.53	0.44
2:M:136:ARG:HH11	2:M:136:ARG:N	2.15	0.44
3:H:14:SER:O	3:H:17:ILE:HG22	2.17	0.44
3:H:210:SER:C	3:H:212:LEU:H	2.20	0.44
2:M:52:LEU:HD21	2:M:57:VAL:HG22	1.99	0.44
2:M:228:ARG:HB3	3:H:195:MET:HE3	1.99	0.44
3:H:208:LEU:HD23	3:H:240:GLY:HA3	1.99	0.44
1:L:60:ASN:ND2	1:L:63:LEU:HG	2.32	0.44
1:L:141:ALA:C	1:L:143:GLY:N	2.71	0.44
1:L:166:ASN:OD1	1:L:168:HIS:HB2	2.17	0.44
2:M:129:TRP:O	2:M:132:ARG:HB3	2.18	0.44
2:M:187:ASN:HA	4:M:852:BCL:CBC	2.47	0.44
5:M:854:BPH:HHB	5:M:854:BPH:HBB3	2.00	0.44
3:H:246:PRO:C	3:H:247:LYS:HG3	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:192:ALA:HB1	2:M:146:THR:N	2.32	0.44
2:M:291:VAL:HG21	2:M:294:TRP:CH2	2.52	0.44
3:H:32:GLN:HG2	3:H:56:PHE:CE2	2.53	0.44
3:H:66:LEU:HD13	3:H:118:ARG:NH1	2.32	0.44
1:L:80:LEU:HA	1:L:84:GLY:HA3	2.00	0.43
2:M:13:ARG:O	3:H:140:PHE:HA	2.18	0.43
3:H:17:ILE:O	3:H:21:TRP:HD1	2.00	0.43
1:L:52:SER:HB2	1:L:85:LEU:CD1	2.48	0.43
1:L:147:PRO:HG2	1:L:153:HIS:HA	2.00	0.43
2:M:75:TRP:HE3	2:M:80:TRP:HA	1.82	0.43
2:M:243:THR:HG21	2:M:247:ARG:NE	2.26	0.43
3:H:210:SER:OG	3:H:211:ASP:N	2.51	0.43
2:M:79:GLY:C	2:M:81:ASN:H	2.21	0.43
7:M:857:U10:H1M1	7:M:857:U10:H71	1.74	0.43
3:H:168:TRP:HB2	3:H:178:PHE:HB2	1.99	0.43
2:M:18:LEU:H	2:M:18:LEU:CD2	2.31	0.43
2:M:94:LEU:HD12	10:M:1010:HOH:O	2.18	0.43
2:M:97:PRO:CA	2:M:112:GLY:HA3	2.49	0.43
2:M:145:HIS:HE1	9:M:3000:CDL:HB21	1.84	0.43
2:M:233:ARG:HA	10:M:1085:HOH:O	2.19	0.43
1:L:270:PRO:HB2	1:L:271:TRP:CD1	2.53	0.43
2:M:79:GLY:O	2:M:81:ASN:N	2.51	0.43
3:H:148:PRO:HG2	3:H:167:ILE:HD11	2.00	0.43
3:H:94:GLU:OE1	3:H:94:GLU:N	2.52	0.43
1:L:272:TRP:HA	1:L:275:ILE:CG1	2.49	0.42
4:L:850:BCL:HMB2	5:M:854:BPH:HMB3	2.01	0.42
2:M:122:MET:HE1	2:M:177:TYR:HE1	1.84	0.42
1:L:65:SER:HA	1:L:148:TYR:O	2.18	0.42
2:M:167:LEU:HD12	2:M:285:LEU:HD11	2.01	0.42
1:L:172:ALA:O	1:L:175:ILE:N	2.52	0.42
2:M:241:ARG:NH1	3:H:38:GLU:OE1	2.47	0.42
1:L:4:SER:OG	3:H:39:GLY:HA2	2.19	0.42
1:L:60:ASN:HA	1:L:61:PRO:HD3	1.79	0.42
1:L:123:PHE:CD1	1:L:238:LEU:HD13	2.55	0.42
1:L:222:TYR:CG	1:L:223:SER:N	2.87	0.42
2:M:5:ASN:ND2	3:H:194:GLN:CG	2.82	0.42
2:M:228:ARG:CB	3:H:195:MET:HE3	2.50	0.42
2:M:253:ARG:NH1	2:M:259:ASN:HD21	2.14	0.42
7:M:857:U10:H312	7:M:857:U10:H271	1.84	0.42
7:M:857:U10:H271	7:M:857:U10:H251	1.68	0.42
3:H:134:MET:CE	3:H:149:ILE:HD11	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:190:HIS:CE1	1:L:230:HIS:CE1	3.08	0.42
2:M:86:LEU:HD22	2:M:86:LEU:HA	1.89	0.42
2:M:73:TRP:CG	2:M:94:LEU:HD13	2.55	0.42
2:M:148:TRP:HA	2:M:148:TRP:HE3	1.83	0.42
2:M:293:ASN:HB3	2:M:296:VAL:HB	2.02	0.42
3:H:183:LEU:HD11	3:H:189:ARG:HG3	2.01	0.42
1:L:246:LEU:O	1:L:249:ILE:HG22	2.19	0.42
1:L:275:ILE:HA	1:L:276:PRO:HD2	1.81	0.42
3:H:165:VAL:CG1	3:H:182:GLU:HB2	2.50	0.42
1:L:44:LEU:O	1:L:47:ILE:HB	2.20	0.41
1:L:269:LEU:HB2	1:L:272:TRP:HE1	1.79	0.41
4:L:851:BCL:H2C	4:M:852:BCL:H2C	2.02	0.41
3:H:84:PRO:O	3:H:85:ILE:HD13	2.20	0.41
1:L:217:ARG:HB3	2:M:49:PRO:O	2.20	0.41
2:M:155:TRP:HD1	2:M:278:LEU:HA	1.85	0.41
3:H:87:LEU:HD23	3:H:100:PRO:HA	2.02	0.41
3:H:169:VAL:HG23	3:H:171:ILE:HD13	2.03	0.41
1:L:85:LEU:O	1:L:89:ILE:HG13	2.20	0.41
2:M:260:ALA:HB2	7:M:857:U10:H103	2.03	0.41
3:H:156:CYS:SG	3:H:248:ARG:HA	2.59	0.41
1:L:49:ILE:CG1	1:L:89:ILE:HD13	2.50	0.41
1:L:177:ILE:HG12	4:L:851:BCL:HMB3	2.02	0.41
2:M:171:TRP:HA	2:M:171:TRP:HE3	1.86	0.41
2:M:229:PHE:HD1	3:H:234:CYS:HB3	1.86	0.41
2:M:204:LEU:O	2:M:207:ALA:HB3	2.20	0.41
3:H:62:LYS:O	3:H:74:THR:HA	2.21	0.41
3:H:156:CYS:SG	3:H:209:SER:HB3	2.60	0.41
1:L:205:GLU:OE2	3:H:67:PRO:HA	2.21	0.41
1:L:264:GLN:HA	1:L:267:VAL:CG1	2.48	0.41
2:M:5:ASN:HD21	3:H:194:GLN:HG3	1.84	0.41
1:L:197:ALA:CB	2:M:235:LEU:HD11	2.51	0.41
2:M:16:ALA:HB1	2:M:32:VAL:HG21	2.03	0.41
3:H:117:ARG:HA	10:H:1048:HOH:O	2.21	0.41
3:H:133:PRO:HB3	3:H:168:TRP:CE2	2.55	0.41
1:L:270:PRO:HB2	1:L:271:TRP:HD1	1.86	0.40
2:M:17:ASP:OD1	2:M:19:GLY:N	2.46	0.40
2:M:152:SER:O	2:M:155:TRP:HB3	2.20	0.40
1:L:209:PRO:O	1:L:212:GLU:HB2	2.20	0.40
2:M:196:LEU:C	2:M:198:TYR:N	2.75	0.40
1:L:255:TRP:CZ2	1:L:262:TRP:HB2	2.57	0.40
3:H:146:LYS:HE3	3:H:147:ASN:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:60:ASN:HD21	1:L:62:GLN:HB2	1.87	0.40
1:L:79:PRO:HD2	1:L:82:LYS:HB2	2.03	0.40
1:L:140:GLY:O	1:L:141:ALA:HB2	2.22	0.40
1:L:241:VAL:HG21	5:L:855:BPH:H2C	2.03	0.40
3:H:156:CYS:SG	3:H:248:ARG:CB	3.09	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%)	243 (87%)	33 (12%)	3 (1%)	14	34
2	M	300/307 (98%)	268 (89%)	30 (10%)	2 (1%)	22	46
3	H	238/260 (92%)	214 (90%)	14 (6%)	10 (4%)	3	5
All	All	817/848 (96%)	725 (89%)	77 (9%)	15 (2%)	8	21

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	210	SER
3	H	211	ASP
2	M	80	TRP
3	H	51	ALA
1	L	26	VAL
1	L	80	LEU
3	H	207	ALA
3	H	249	LYS
3	H	174	GLN
3	H	220	LYS
3	H	247	LYS
1	L	270	PRO

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Mol	Chain	Res	Type
2	M	179	ILE
3	H	245	ALA
3	H	246	PRO

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%)	210 (96%)	10 (4%)	27	55
2	M	236/240 (98%)	224 (95%)	12 (5%)	24	50
3	H	195/208 (94%)	191 (98%)	4 (2%)	53	80
All	All	651/668 (98%)	625 (96%)	26 (4%)	31	60

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	59	TRP
1	L	72	GLU
1	L	152	THR
1	L	154	LEU
1	L	158	SER
1	L	207	ARG
1	L	210	ASP
1	L	235	LEU
1	L	271	TRP
1	L	272	TRP
2	M	18	LEU
2	M	51	TYR
2	M	76	PHE
2	M	86	LEU
2	M	133	THR
2	M	136	ARG
2	M	171	TRP
2	M	182	HIS
2	M	216	PHE

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Mol	Chain	Res	Type
2	M	243	THR
2	M	258	PHE
2	M	259	ASN
3	H	105	MET
3	H	200	SER
3	H	225	VAL
3	H	231	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	60	ASN
2	M	25	ASN
2	M	28	ASN
2	M	202	HIS
2	M	259	ASN
2	M	299	GLN
3	H	129	ASN
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 [i](#)

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
8	SPO	M	859	-	40,41,41	3.59	24 (60%)	47,50,50	2.72	13 (27%)
9	CDL	M	3000	-	80,80,99	0.65	2 (2%)	86,92,111	0.90	4 (4%)
4	BCL	L	850	2	58,74,74	1.55	8 (13%)	69,115,115	2.03	21 (30%)
5	BPH	M	854	-	64,70,70	1.48	13 (20%)	76,101,101	1.83	16 (21%)
4	BCL	M	853	1	58,74,74	1.67	9 (15%)	69,115,115	2.11	18 (26%)
7	U10	M	857	-	48,48,63	2.28	12 (25%)	58,61,79	2.16	21 (36%)
5	BPH	L	855	-	64,70,70	1.27	8 (12%)	76,101,101	1.91	17 (22%)
4	BCL	L	851	1	58,74,74	1.74	11 (18%)	69,115,115	1.88	13 (18%)
4	BCL	M	852	2	58,74,74	1.50	10 (17%)	69,115,115	1.98	13 (18%)

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
8	SPO	M	859	-	-	18/47/47/47	-
9	CDL	M	3000	-	-	25/91/91/110	-
4	BCL	L	850	2	-	6/37/137/137	-
5	BPH	M	854	-	-	9/54/105/105	0/5/6/6
4	BCL	M	853	1	-	6/37/137/137	-
7	U10	M	857	-	-	17/45/69/87	0/1/1/1
5	BPH	L	855	-	-	4/54/105/105	0/5/6/6
4	BCL	L	851	1	-	4/37/137/137	-
4	BCL	M	852	2	-	9/37/137/137	-

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	859	SPO	C15-C16	9.32	1.58	1.34
7	M	857	U10	C6-C1	8.73	1.51	1.35
8	M	859	SPO	C6-C5	7.48	1.51	1.32
8	M	859	SPO	C10-C11	7.25	1.53	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	851	BCL	C3D-C2D	6.44	1.51	1.39
8	M	859	SPO	C27-C28	6.23	1.40	1.34
8	M	859	SPO	C21-C20	5.75	1.50	1.36
4	M	853	BCL	C3D-C2D	5.72	1.49	1.39
4	M	852	BCL	C3D-C2D	5.56	1.49	1.39
4	L	851	BCL	C3B-C2B	5.41	1.49	1.39
4	L	850	BCL	C3D-C2D	5.31	1.49	1.39
5	M	854	BPH	C3D-C2D	5.16	1.48	1.39
8	M	859	SPO	C26-C25	5.06	1.47	1.34
4	M	853	BCL	C3B-C2B	4.96	1.48	1.39
4	M	852	BCL	C3B-C2B	4.82	1.48	1.39
4	M	853	BCL	C2-C3	4.69	1.44	1.33
4	L	850	BCL	C3B-C2B	4.64	1.47	1.39
8	M	859	SPO	C13-C12	4.54	1.60	1.50
7	M	857	U10	C4-C3	4.34	1.53	1.36
5	L	855	BPH	C3D-C2D	4.30	1.47	1.39
8	M	859	SPO	C14-C12	4.01	1.41	1.35
8	M	859	SPO	C15-C14	4.01	1.55	1.43
4	L	851	BCL	C4B-NB	4.00	1.38	1.35
7	M	857	U10	C7-C8	-3.92	1.45	1.50
7	M	857	U10	C7-C6	3.83	1.57	1.51
8	M	859	SPO	O1-CM1	3.79	1.55	1.43
7	M	857	U10	C6-C5	3.59	1.56	1.46
8	M	859	SPO	C19-C17	3.53	1.40	1.35
8	M	859	SPO	C32-C33	3.48	1.41	1.33
7	M	857	U10	C28-C29	3.47	1.41	1.33
8	M	859	SPO	C4-C5	-3.46	1.44	1.50
4	L	851	BCL	C2-C3	3.41	1.41	1.33
7	M	857	U10	C33-C34	3.38	1.41	1.33
5	M	854	BPH	CMB-C2B	3.37	1.57	1.50
8	M	859	SPO	C37-C38	3.35	1.42	1.32
4	L	850	BCL	C2-C3	3.31	1.40	1.33
4	M	852	BCL	CMB-C2B	3.22	1.58	1.51
5	L	855	BPH	CMB-C2B	3.20	1.57	1.50
4	L	850	BCL	C4B-NB	3.19	1.38	1.35
8	M	859	SPO	O1-C1	3.10	1.58	1.41
7	M	857	U10	C38-C39	3.10	1.41	1.32
5	M	854	BPH	C2-C3	3.09	1.40	1.33
7	M	857	U10	C13-C14	3.09	1.40	1.33
8	M	859	SPO	C10-C9	3.07	1.53	1.43
8	M	859	SPO	C11-C12	-3.07	1.39	1.45
4	L	851	BCL	C3C-C4C	-3.05	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	857	U10	C18-C19	3.04	1.40	1.33
8	M	859	SPO	C8-C7	3.00	1.57	1.50
4	M	852	BCL	C2-C3	2.96	1.40	1.33
8	M	859	SPO	C35-C33	2.92	1.57	1.51
4	M	853	BCL	C3C-C4C	-2.90	1.47	1.51
5	M	854	BPH	CMD-C2D	2.87	1.57	1.51
7	M	857	U10	C23-C24	2.84	1.39	1.33
4	M	853	BCL	C3B-CAB	2.82	1.56	1.49
7	M	857	U10	O4-C4	2.81	1.43	1.36
8	M	859	SPO	C31-C32	-2.79	1.41	1.50
4	L	851	BCL	CMB-C2B	2.76	1.57	1.51
4	M	853	BCL	CMB-C2B	2.76	1.57	1.51
4	L	850	BCL	CMB-C2B	2.76	1.57	1.51
5	L	855	BPH	C3D-CAD	-2.76	1.41	1.47
4	M	853	BCL	C4B-NB	2.66	1.37	1.35
4	M	853	BCL	OBD-CAD	2.65	1.26	1.22
8	M	859	SPO	C25-C23	-2.64	1.40	1.45
5	M	854	BPH	C1B-C2B	-2.61	1.40	1.45
4	L	851	BCL	C3B-CAB	2.56	1.56	1.49
8	M	859	SPO	C24-C23	2.49	1.56	1.50
8	M	859	SPO	C29-C28	2.48	1.57	1.50
5	L	855	BPH	C2-C3	2.47	1.38	1.33
4	M	852	BCL	C3B-CAB	2.47	1.55	1.49
9	M	3000	CDL	CB3-CB4	2.43	1.58	1.50
5	M	854	BPH	CHC-C4B	2.38	1.46	1.40
8	M	859	SPO	C9-C7	2.37	1.38	1.35
4	L	850	BCL	C3A-C2A	-2.36	1.47	1.54
5	L	855	BPH	C3B-C2B	2.36	1.45	1.39
5	M	854	BPH	C3B-C2B	2.35	1.45	1.39
5	M	854	BPH	C3D-CAD	-2.35	1.42	1.47
5	L	855	BPH	C3B-CAB	2.29	1.53	1.46
4	L	850	BCL	C3B-CAB	2.26	1.55	1.49
4	L	851	BCL	CBB-CAB	2.24	1.56	1.49
5	M	854	BPH	O2A-CGA	-2.21	1.26	1.33
4	L	850	BCL	CAA-C2A	2.21	1.58	1.54
5	M	854	BPH	C2A-C1A	2.20	1.55	1.51
4	L	851	BCL	C3A-C2A	-2.18	1.48	1.54
5	L	855	BPH	C3A-C2A	-2.16	1.48	1.54
9	M	3000	CDL	OA8-CA7	2.15	1.39	1.33
4	L	851	BCL	CMD-C2D	2.14	1.56	1.51
4	M	853	BCL	C3A-C2A	-2.13	1.48	1.54
4	M	852	BCL	C4B-NB	2.13	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	852	BCL	CMD-C2D	2.12	1.56	1.51
5	L	855	BPH	C1B-C2B	-2.08	1.41	1.45
4	M	852	BCL	OBD-CAD	2.08	1.25	1.22
4	M	852	BCL	C3D-CAD	-2.04	1.40	1.46
5	M	854	BPH	C4-C3	2.03	1.55	1.50
5	M	854	BPH	C3B-CAB	2.02	1.53	1.46
4	M	852	BCL	CBB-CAB	2.01	1.55	1.49
5	M	854	BPH	C5-C3	2.01	1.55	1.51
4	L	851	BCL	OBD-CAD	2.01	1.25	1.22

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	859	SPO	C25-C23-C22	-10.83	102.32	118.94
4	L	851	BCL	CMB-C2B-C1B	-6.62	118.30	128.46
4	M	853	BCL	CMB-C2B-C1B	-6.53	118.43	128.46
4	M	852	BCL	C4D-C3D-CAD	-6.40	104.90	108.47
4	L	850	BCL	CMB-C2B-C1B	-6.29	118.80	128.46
4	M	852	BCL	CMB-C2B-C1B	-6.26	118.84	128.46
4	M	853	BCL	CAA-C2A-C1A	-6.20	91.66	111.97
4	L	851	BCL	C4D-C3D-CAD	-6.03	105.11	108.47
8	M	859	SPO	C24-C23-C22	-5.99	114.54	122.92
5	L	855	BPH	C1-O2A-CGA	5.97	132.10	116.44
7	M	857	U10	C7-C6-C5	5.94	125.63	118.48
8	M	859	SPO	C18-C17-C19	-5.89	114.67	122.92
4	M	853	BCL	C4D-C3D-CAD	-5.53	105.39	108.47
5	M	854	BPH	C1-O2A-CGA	5.40	130.62	116.44
4	L	850	BCL	C4D-C3D-CAD	-5.30	105.51	108.47
5	M	854	BPH	C4D-C3D-CAD	-5.18	104.59	107.87
5	L	855	BPH	C4D-C3D-CAD	-5.10	104.64	107.87
5	L	855	BPH	C4-C3-C5	5.09	123.84	115.27
8	M	859	SPO	C20-C21-C22	-5.06	113.12	123.47
4	L	850	BCL	CAA-C2A-C1A	-5.01	95.56	111.97
4	M	852	BCL	CMB-C2B-C3B	4.94	133.91	124.68
4	L	851	BCL	CMB-C2B-C3B	4.92	133.89	124.68
4	M	853	BCL	CMB-C2B-C3B	4.88	133.80	124.68
4	L	850	BCL	CMB-C2B-C3B	4.72	133.52	124.68
7	M	857	U10	C15-C14-C16	4.67	123.12	115.27
5	M	854	BPH	CHD-C4C-NC	-4.66	119.67	125.20
4	M	852	BCL	CED-O2D-CGD	4.61	126.36	115.94
4	L	851	BCL	CED-O2D-CGD	4.44	125.97	115.94
4	M	853	BCL	CED-O2D-CGD	4.39	125.87	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	857	U10	C10-C9-C8	-4.35	112.51	123.68
7	M	857	U10	C15-C14-C13	-4.14	113.06	123.68
7	M	857	U10	C7-C8-C9	4.13	133.66	126.79
4	M	852	BCL	OBD-CAD-C3D	-4.03	121.30	127.98
5	M	854	BPH	C4-C3-C5	3.98	121.96	115.27
8	M	859	SPO	C11-C12-C14	-3.90	112.96	118.94
5	L	855	BPH	CHC-C4B-NB	-3.85	116.88	124.93
5	L	855	BPH	CHD-C4C-NC	-3.84	120.64	125.20
4	M	853	BCL	C4A-NA-C1A	3.83	108.43	106.71
5	L	855	BPH	O2A-C1-C2	-3.83	98.57	108.64
5	M	854	BPH	O2A-C1-C2	-3.82	98.60	108.64
8	M	859	SPO	C15-C14-C12	-3.77	121.92	127.31
5	L	855	BPH	C6-C5-C3	3.74	123.26	113.45
4	L	851	BCL	C2A-C3A-C4A	3.73	107.90	101.87
4	L	850	BCL	CED-O2D-CGD	3.72	124.35	115.94
4	M	853	BCL	CBA-CAA-C2A	3.64	124.59	113.86
4	M	852	BCL	C6-C5-C3	3.59	122.86	113.45
7	M	857	U10	C25-C24-C23	-3.56	114.53	123.68
8	M	859	SPO	C8-C7-C9	3.55	127.89	122.92
5	M	854	BPH	O2D-CGD-CBD	3.54	117.56	111.27
4	L	850	BCL	OBD-CAD-C3D	-3.54	122.11	127.98
5	L	855	BPH	O2D-CGD-CBD	3.53	117.53	111.27
4	L	851	BCL	OBD-CAD-C3D	-3.51	122.15	127.98
4	M	853	BCL	CAC-C3C-C2C	-3.50	105.50	114.26
7	M	857	U10	C11-C9-C8	3.48	128.16	121.12
4	L	850	BCL	CBA-CAA-C2A	3.46	124.08	113.86
5	L	855	BPH	CMB-C2B-C1B	-3.44	119.76	125.06
8	M	859	SPO	C2-C1-C4	-3.44	105.58	110.86
5	M	854	BPH	CMB-C2B-C1B	-3.44	119.77	125.06
4	M	853	BCL	C2A-C3A-C4A	3.43	107.42	101.87
7	M	857	U10	C35-C34-C33	-3.42	114.91	123.68
4	M	852	BCL	C2A-C3A-C4A	3.41	107.38	101.87
4	L	850	BCL	C2A-C3A-C4A	3.35	107.28	101.87
4	M	853	BCL	OBD-CAD-C3D	-3.34	122.44	127.98
5	L	855	BPH	C5-C3-C2	-3.32	114.40	121.12
4	M	852	BCL	C4A-NA-C1A	3.26	108.17	106.71
7	M	857	U10	C25-C24-C26	3.24	120.71	115.27
9	M	3000	CDL	OB8-CB6-CB4	3.22	117.79	108.43
5	M	854	BPH	CHC-C1C-NC	-3.20	121.40	125.20
5	M	854	BPH	C3D-CAD-CBD	3.16	111.76	107.61
5	M	854	BPH	CHC-C4B-NB	-3.13	118.38	124.93
4	M	852	BCL	CHA-C1A-NA	-3.08	119.35	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	855	BPH	O1D-CGD-CBD	-3.04	118.27	124.48
5	M	854	BPH	O1D-CGD-CBD	-3.03	118.28	124.48
4	M	852	BCL	C4B-CHC-C1C	2.90	135.87	130.12
4	L	851	BCL	C6-C5-C3	2.90	121.06	113.45
4	L	851	BCL	CHA-C1A-NA	-2.90	119.77	126.40
4	M	852	BCL	C15-C13-C12	-2.89	96.93	112.13
8	M	859	SPO	C15-C16-C17	-2.84	118.44	126.42
7	M	857	U10	C20-C19-C18	-2.82	116.44	123.68
8	M	859	SPO	C18-C17-C16	2.77	122.45	118.08
4	L	850	BCL	C4A-NA-C1A	2.73	107.93	106.71
7	M	857	U10	O5-C5-C4	-2.72	115.16	120.93
4	L	850	BCL	O2A-C1-C2	-2.72	101.49	108.64
5	L	855	BPH	C3D-CAD-CBD	2.72	111.18	107.61
5	M	854	BPH	CED-O2D-CGD	2.69	122.03	115.94
7	M	857	U10	C4M-O4-C4	2.64	125.84	116.47
4	M	852	BCL	C2A-C1A-CHA	2.64	128.47	123.86
4	M	853	BCL	O2A-CGA-CBA	2.62	120.11	111.91
5	M	854	BPH	CBB-CAB-C3B	-2.61	114.86	120.43
5	L	855	BPH	CHC-C1C-NC	-2.60	122.11	125.20
4	L	851	BCL	C4B-CHC-C1C	2.60	135.26	130.12
9	M	3000	CDL	CB4-OB6-CB5	2.59	124.17	117.79
7	M	857	U10	C8-C7-C6	-2.58	105.08	112.05
4	L	850	BCL	C15-C13-C12	-2.58	98.58	112.13
8	M	859	SPO	C10-C9-C7	-2.58	123.63	127.31
8	M	859	SPO	C16-C17-C19	2.57	122.88	118.94
5	L	855	BPH	C1C-NC-C4C	-2.56	108.28	110.54
4	L	850	BCL	C4B-CHC-C1C	2.52	135.11	130.12
7	M	857	U10	C36-C34-C33	2.51	126.20	121.12
5	M	854	BPH	CMB-C2B-C3B	2.50	133.37	127.61
4	M	852	BCL	C3D-CAD-CBD	2.50	110.90	107.61
4	M	853	BCL	C4B-CHC-C1C	2.50	135.06	130.12
7	M	857	U10	C21-C19-C18	2.50	126.17	121.12
7	M	857	U10	C30-C29-C31	2.49	119.47	115.27
5	L	855	BPH	C7-C6-C5	-2.46	106.67	113.36
4	M	853	BCL	C2C-C3C-C4C	2.45	105.01	101.34
8	M	859	SPO	C13-C12-C11	2.45	121.94	118.08
5	L	855	BPH	CED-O2D-CGD	2.44	121.46	115.94
4	L	851	BCL	C2A-C1A-CHA	2.44	128.13	123.86
4	L	850	BCL	CHA-C1A-NA	-2.43	120.84	126.40
5	L	855	BPH	CMB-C2B-C3B	2.42	133.18	127.61
4	L	850	BCL	C9-C8-C10	-2.42	102.55	111.29
7	M	857	U10	C10-C9-C11	2.41	119.32	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	850	BCL	C6-C5-C3	2.39	119.73	113.45
7	M	857	U10	C1M-C1-C6	-2.35	120.56	124.40
4	L	850	BCL	O2D-CGD-CBD	2.31	115.36	111.27
9	M	3000	CDL	CB6-CB4-CB3	-2.30	106.34	111.79
4	L	850	BCL	O2A-CGA-CBA	2.28	119.07	111.91
5	M	854	BPH	C2A-C3A-C4A	2.28	105.84	101.34
4	M	853	BCL	O1D-CGD-CBD	-2.26	119.86	124.48
4	L	851	BCL	CBC-CAC-C3C	2.26	118.49	113.47
9	M	3000	CDL	C52-C51-CB5	2.24	121.78	113.62
4	M	853	BCL	CHA-C1A-NA	-2.22	121.32	126.40
4	M	853	BCL	C16-C15-C13	-2.20	108.81	115.92
7	M	857	U10	C11-C12-C13	2.18	119.05	111.88
4	L	850	BCL	O1D-CGD-CBD	-2.17	120.05	124.48
4	L	850	BCL	C3D-CAD-CBD	2.16	110.45	107.61
7	M	857	U10	C35-C34-C36	2.15	118.89	115.27
4	L	850	BCL	C2A-C1A-CHA	2.12	127.56	123.86
4	M	853	BCL	C2A-C1A-CHA	2.11	127.55	123.86
4	M	853	BCL	C6-C5-C3	2.09	118.94	113.45
5	M	854	BPH	C6-C5-C3	2.05	118.83	113.45
4	L	850	BCL	C12-C11-C10	-2.05	103.83	113.24
4	L	851	BCL	C4A-NA-C1A	2.05	107.63	106.71
7	M	857	U10	C27-C28-C29	-2.01	122.81	127.66
4	L	851	BCL	C2C-C3C-C4C	2.01	104.35	101.34

There are no chirality outliers.

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	C2C-C3C-CAC-CBC
5	M	854	BPH	C4B-C3B-CAB-CBB
5	M	854	BPH	C4B-C3B-CAB-OB
7	M	857	U10	C18-C19-C21-C22
7	M	857	U10	C20-C19-C21-C22
8	M	859	SPO	C1-C4-C5-C6
8	M	859	SPO	C4-C5-C6-C7
8	M	859	SPO	C9-C10-C11-C12
8	M	859	SPO	C21-C22-C23-C24
8	M	859	SPO	C36-C37-C38-C40
9	M	3000	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
9	M	3000	CDL	CA3-OA5-PA1-OA3
9	M	3000	CDL	CA3-OA5-PA1-OA4
8	M	859	SPO	C36-C37-C38-C39
5	L	855	BPH	C3-C5-C6-C7
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	C24-C26-C27-C28
7	M	857	U10	C29-C31-C32-C33
8	M	859	SPO	C24-C23-C25-C26
4	M	852	BCL	C15-C16-C17-C18
9	M	3000	CDL	CB7-C71-C72-C73
4	L	850	BCL	C2A-CAA-CBA-CGA
7	M	857	U10	C19-C21-C22-C23
5	M	854	BPH	C10-C11-C12-C13
9	M	3000	CDL	C39-C40-C41-C42
9	M	3000	CDL	C34-C35-C36-C37
9	M	3000	CDL	C78-C79-C80-C81
9	M	3000	CDL	C36-C37-C38-C39
9	M	3000	CDL	C79-C80-C81-C82
9	M	3000	CDL	C80-C81-C82-C83
9	M	3000	CDL	C11-C12-C13-C14
9	M	3000	CDL	C54-C55-C56-C57
9	M	3000	CDL	C20-C21-C22-C23
9	M	3000	CDL	C51-C52-C53-C54
4	M	852	BCL	C12-C13-C15-C16
4	L	851	BCL	C2A-CAA-CBA-CGA
9	M	3000	CDL	C11-CA5-OA6-CA4
4	M	852	BCL	C14-C13-C15-C16
4	M	853	BCL	C2A-CAA-CBA-CGA
9	M	3000	CDL	OA7-CA5-OA6-CA4
9	M	3000	CDL	C38-C39-C40-C41
5	M	854	BPH	C2A-CAA-CBA-CGA
9	M	3000	CDL	CA3-CA4-CA6-OA8
9	M	3000	CDL	C55-C56-C57-C58
8	M	859	SPO	C4-C1-O1-CM1

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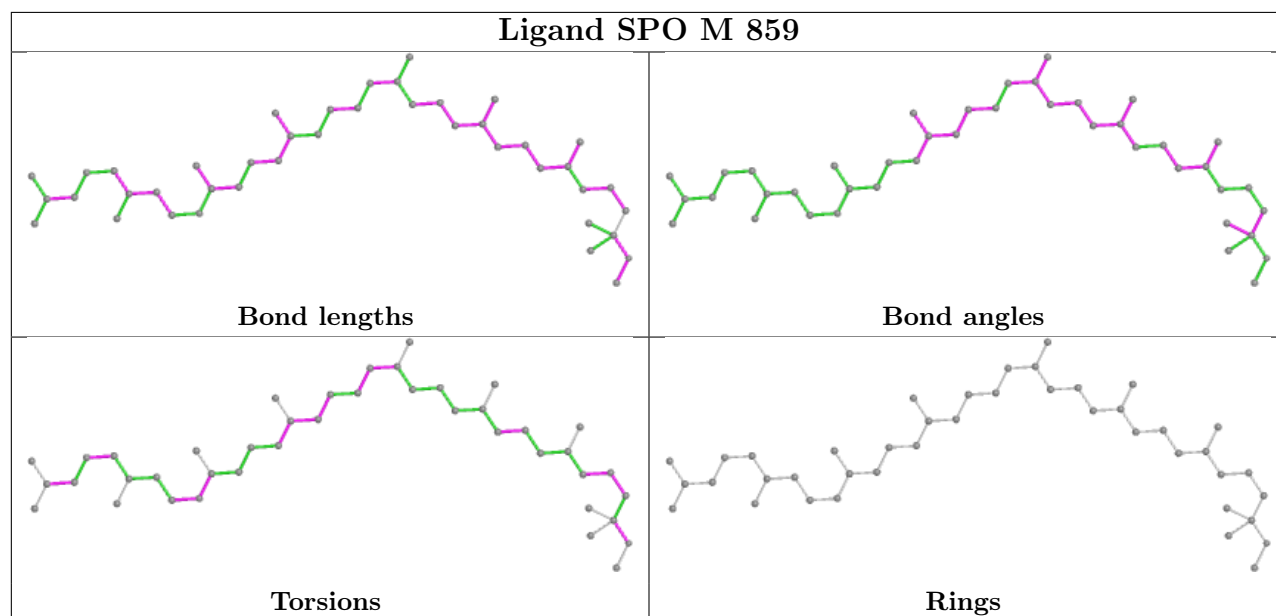
Mol	Chain	Res	Type	Atoms
7	M	857	U10	C5-C6-C7-C8
8	M	859	SPO	C2-C1-O1-CM1
8	M	859	SPO	C3-C1-O1-CM1
9	M	3000	CDL	OA5-CA3-CA4-CA6
7	M	857	U10	C12-C11-C9-C10
9	M	3000	CDL	C40-C41-C42-C43
4	M	852	BCL	C11-C10-C8-C9
4	M	853	BCL	C14-C13-C15-C16
4	M	853	BCL	C5-C6-C7-C8
4	M	852	BCL	C11-C10-C8-C7
4	L	851	BCL	CAD-CBD-CGD-O2D
5	M	854	BPH	CAD-CBD-CGD-O2D
9	M	3000	CDL	OA5-CA3-CA4-OA6
4	M	852	BCL	C3-C5-C6-C7
7	M	857	U10	C9-C11-C12-C13
9	M	3000	CDL	C31-C32-C33-C34
7	M	857	U10	C1-C6-C7-C8
8	M	859	SPO	C33-C35-C36-C37
4	L	850	BCL	C4-C3-C5-C6
7	M	857	U10	C12-C11-C9-C8
8	M	859	SPO	C18-C17-C19-C20
4	M	853	BCL	C12-C13-C15-C16
7	M	857	U10	C3-C4-O4-C4M
8	M	859	SPO	C16-C17-C19-C20
8	M	859	SPO	C17-C19-C20-C21
4	L	850	BCL	C2-C3-C5-C6
7	M	857	U10	C14-C16-C17-C18
4	L	850	BCL	C11-C10-C8-C7
8	M	859	SPO	C29-C28-C30-C31
4	L	850	BCL	CAD-CBD-CGD-O2D
4	M	852	BCL	CAD-CBD-CGD-O2D
8	M	859	SPO	C27-C28-C30-C31
4	M	853	BCL	CHA-CBD-CGD-O1D
4	M	853	BCL	CHA-CBD-CGD-O2D
5	L	855	BPH	CHA-CBD-CGD-O2D
9	M	3000	CDL	C52-C51-CB5-OB6
4	L	850	BCL	C11-C10-C8-C9
7	M	857	U10	C5-C4-O4-C4M
9	M	3000	CDL	C52-C51-CB5-OB7
4	L	851	BCL	C14-C13-C15-C16
4	L	851	BCL	C12-C13-C15-C16
8	M	859	SPO	C28-C30-C31-C32

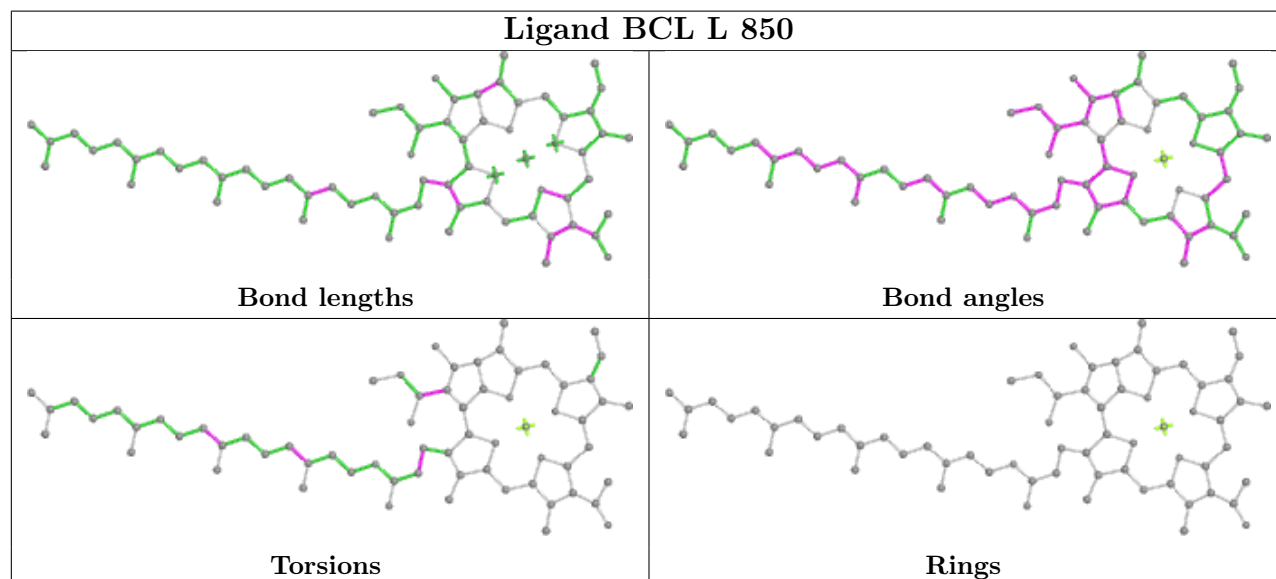
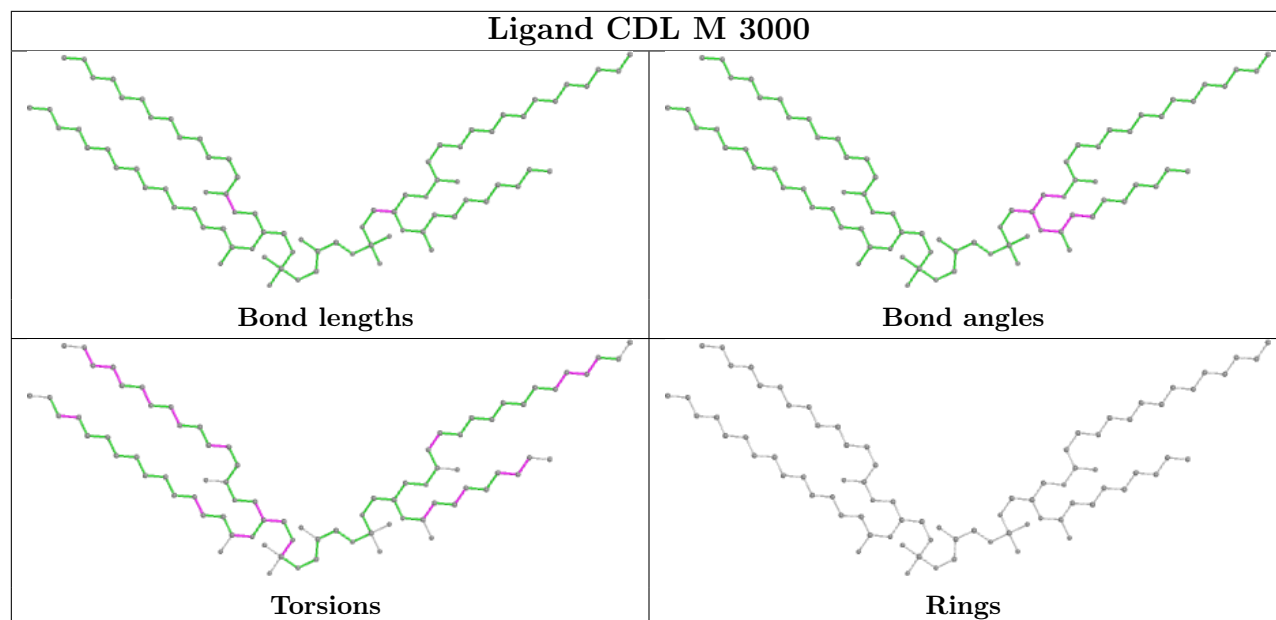
There are no ring outliers.

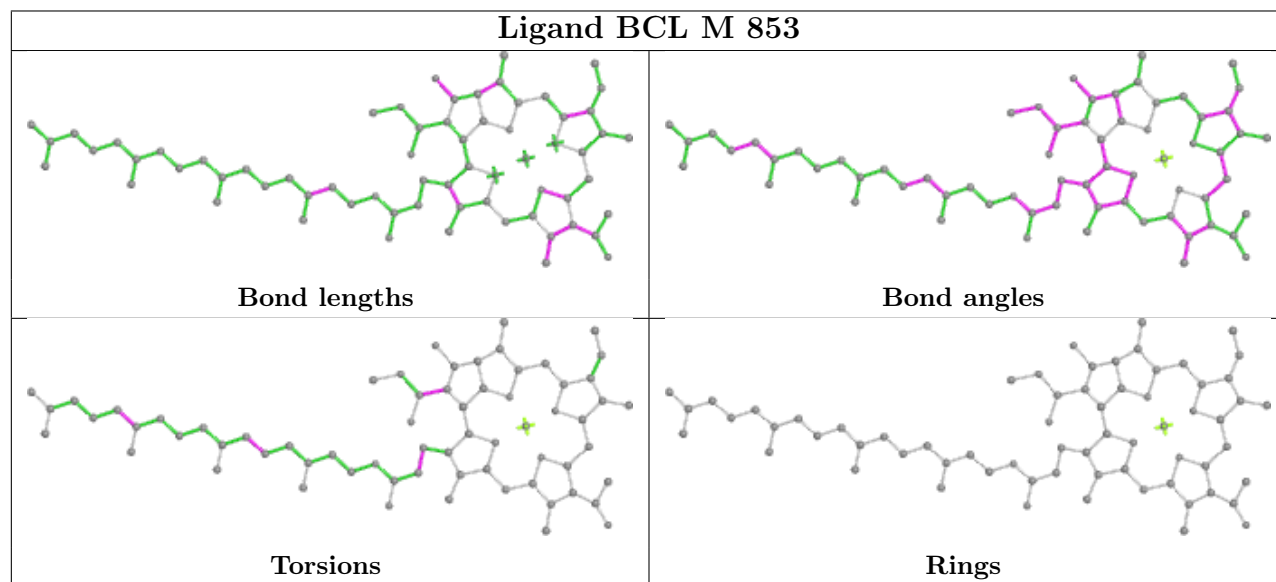
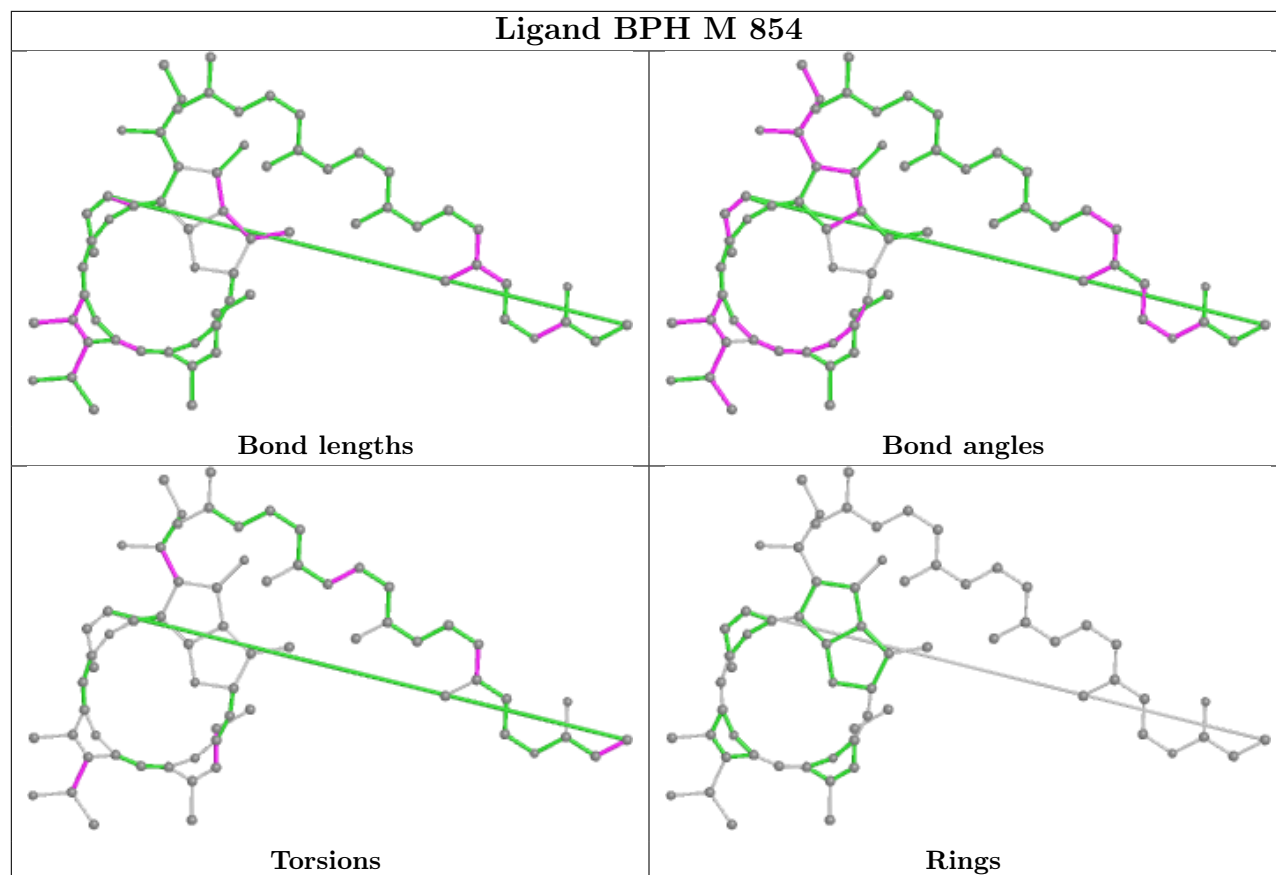
9 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	859	SPO	2	0
9	M	3000	CDL	2	0
4	L	850	BCL	7	0
5	M	854	BPH	10	0
4	M	853	BCL	3	0
7	M	857	U10	5	0
5	L	855	BPH	4	0
4	L	851	BCL	5	0
4	M	852	BCL	9	0

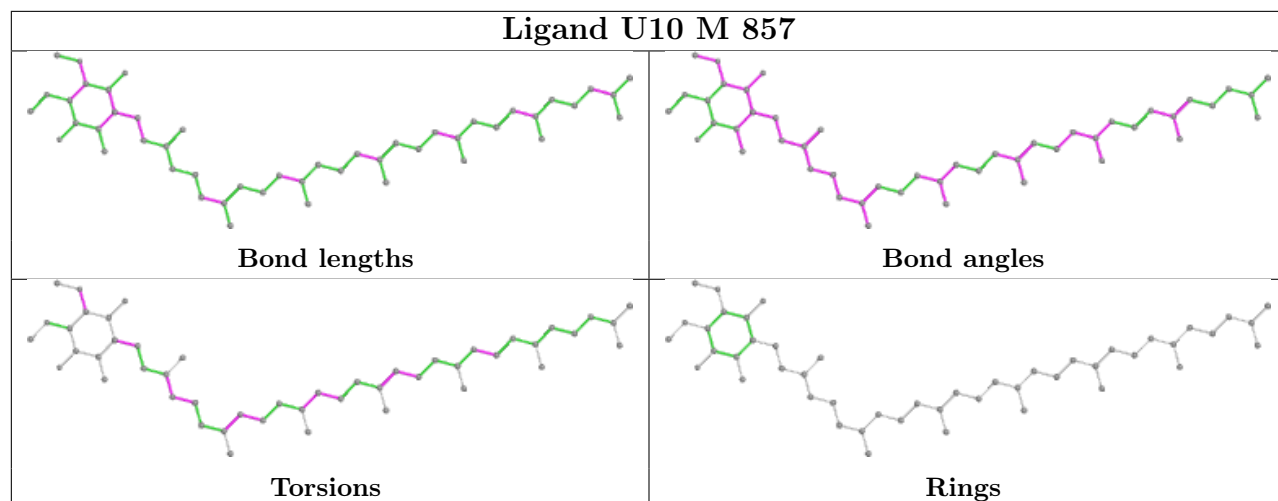
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



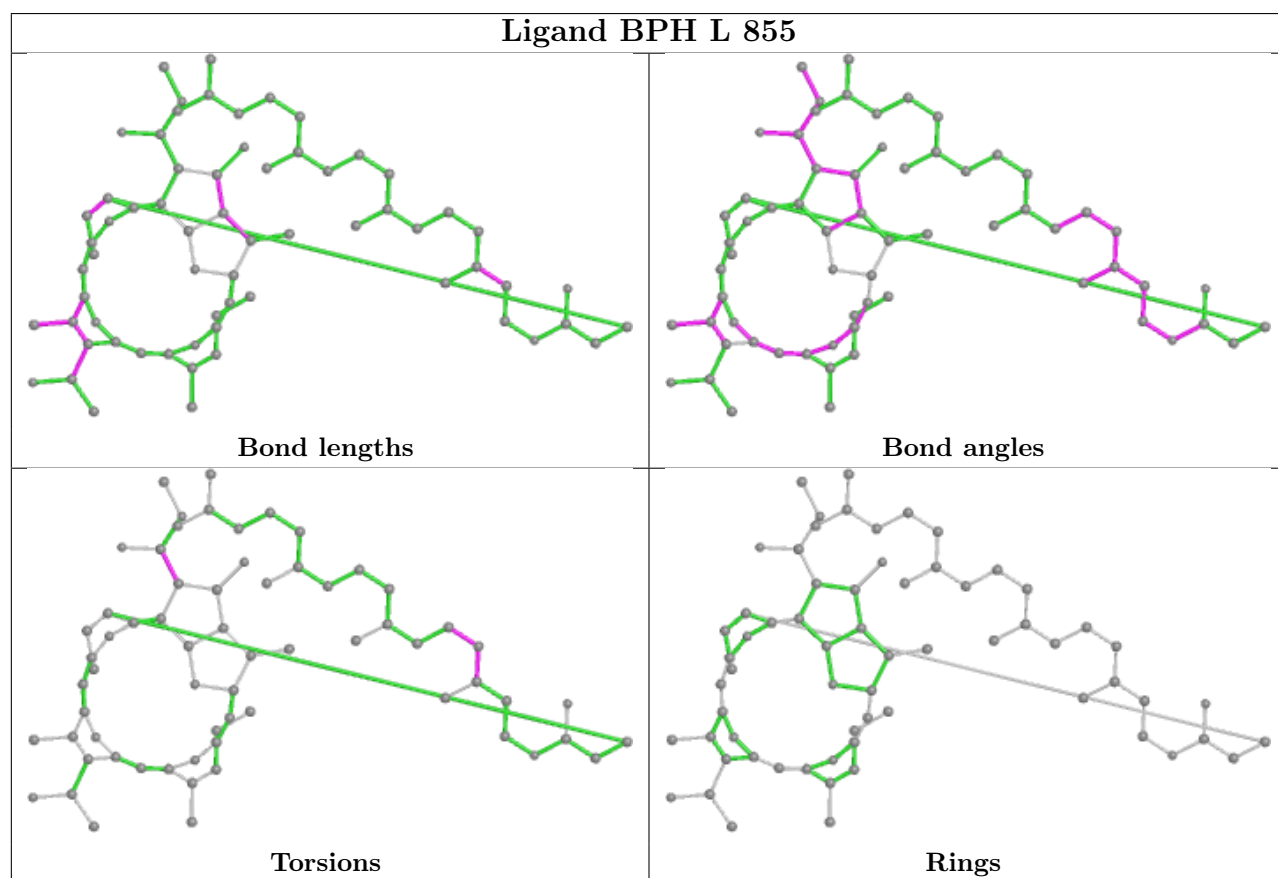


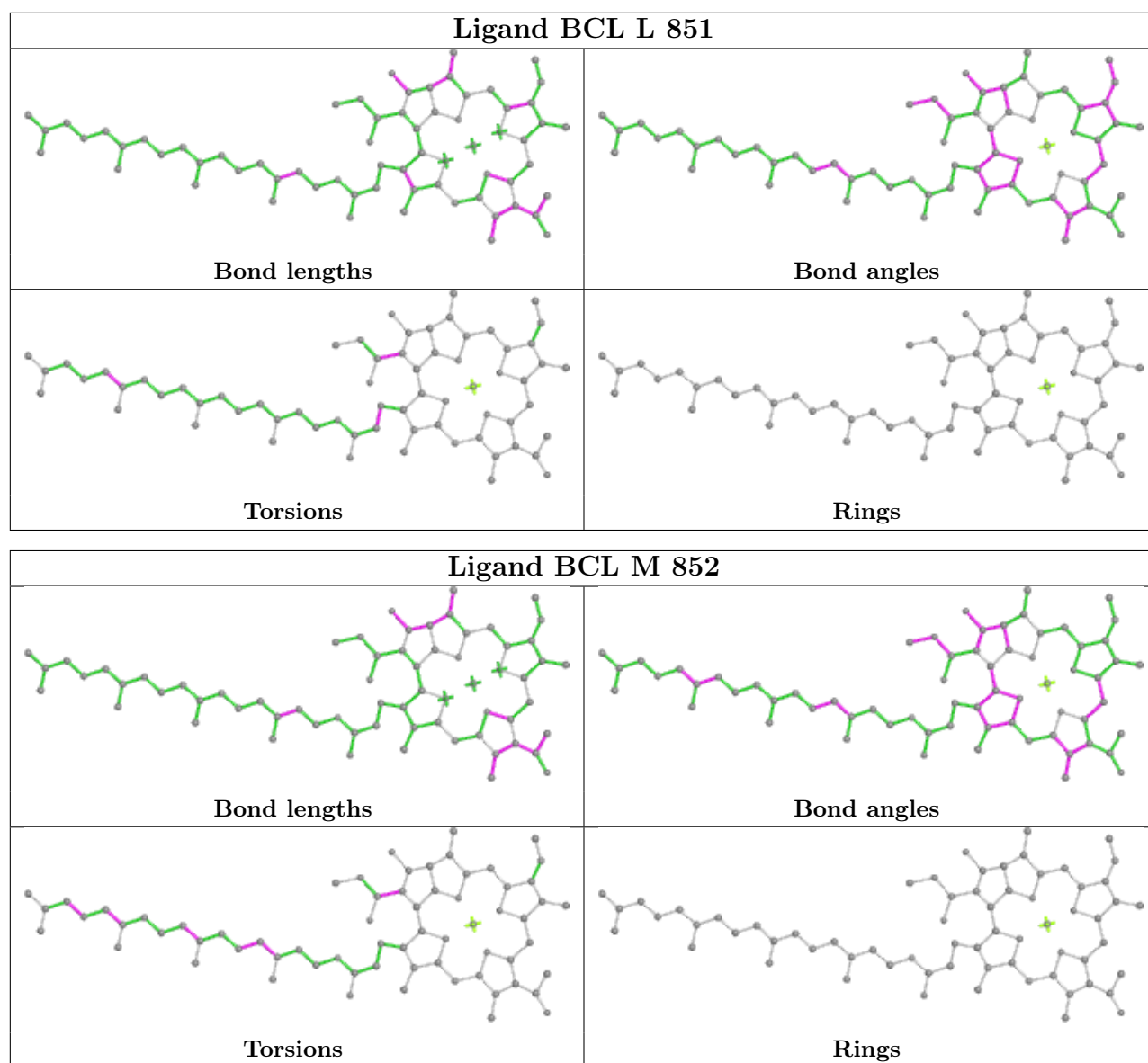


Ligand U10 M 857



Ligand BPH L 855





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.