



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2026 – 08:19 PM EDT

PDB ID : 1JGZ / pdb_00001jgz
Title : Photosynthetic Reaction Center Mutant With Tyr M 76 Replaced With Lys
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

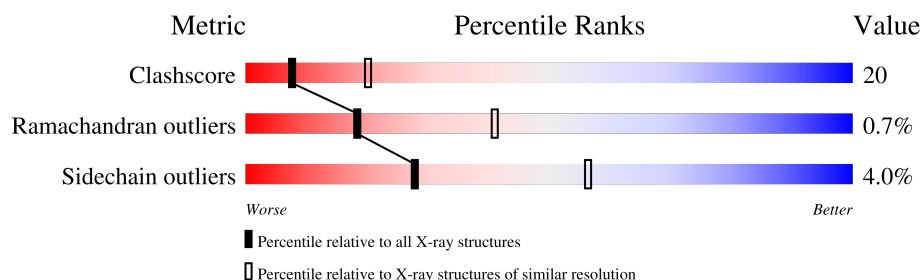
1 Overall quality at a glance

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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (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	
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 7096 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
			2405	1604	395	396	10			

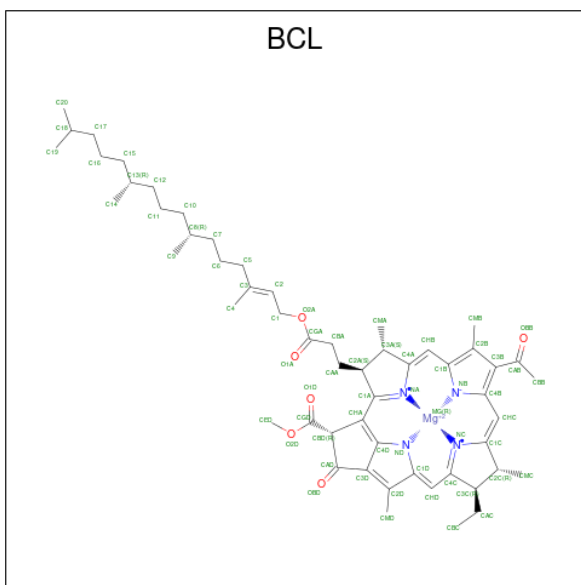
There is a discrepancy between the modelled and reference sequences:

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

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

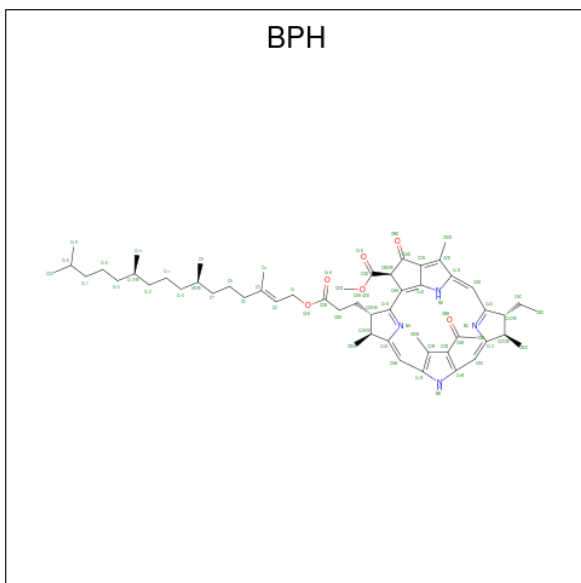
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	236	Total	C	N	O	S	0	0	0
			1794	1148	305	332	9			

- Molecule 4 is BACTERIOCHLOROPHYLL A (CCD ID: 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 (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).

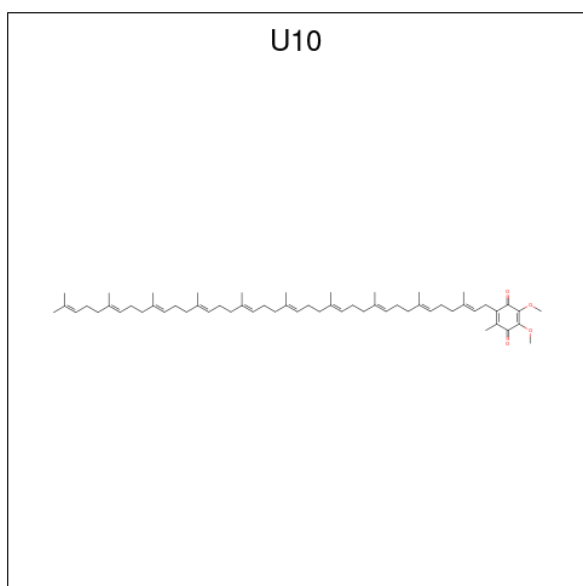


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 6 is FE (III) ION (CCD ID: FE) (formula: Fe).

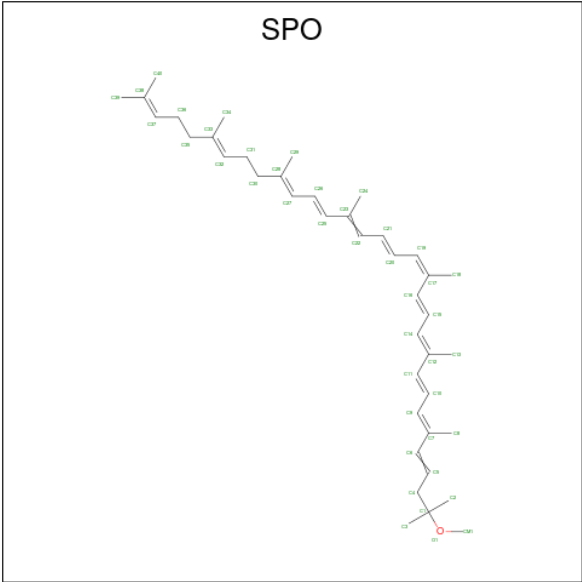
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	M	1	Total	Fe	0	0
			1	1		

- Molecule 7 is UBIQUINONE-10 (CCD ID: U10) (formula: C₅₉H₉₀O₄).



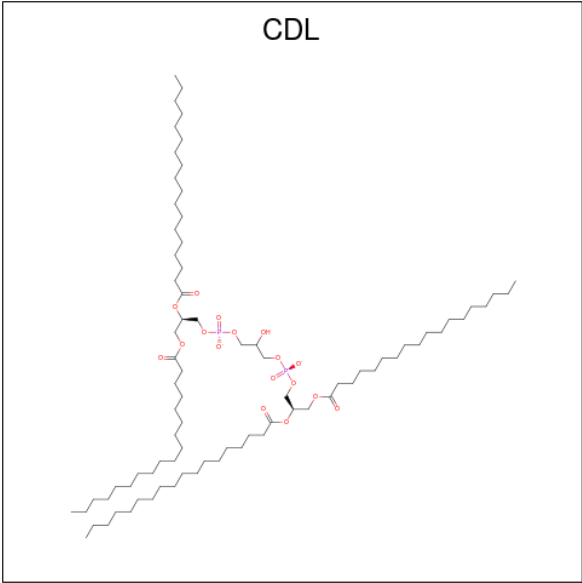
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 8 is SPHEROIDENE (CCD ID: SPO) (formula: C₄₁H₆₀O).



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

- Molecule 9 is CARDIOLIPIN (CCD ID: 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.

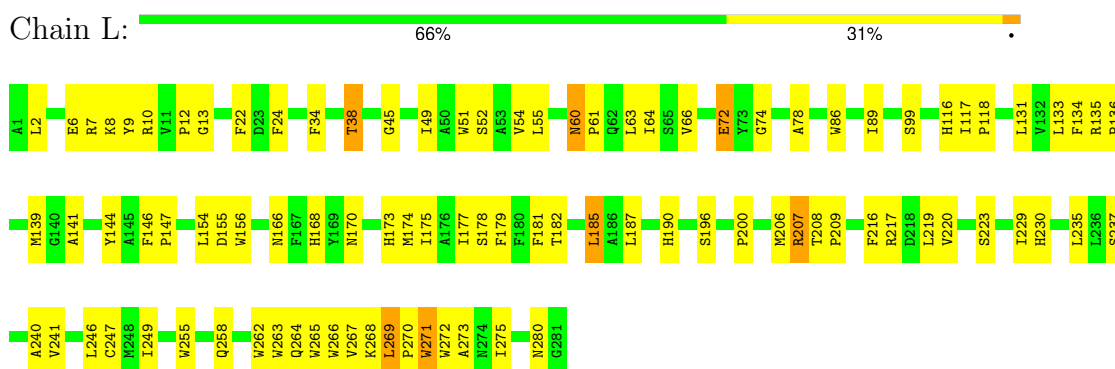
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	L	25	Total 25	O 25	0	0
10	M	36	Total 36	O 36	0	0
10	H	38	Total 38	O 38	0	0

3 Residue-property plots

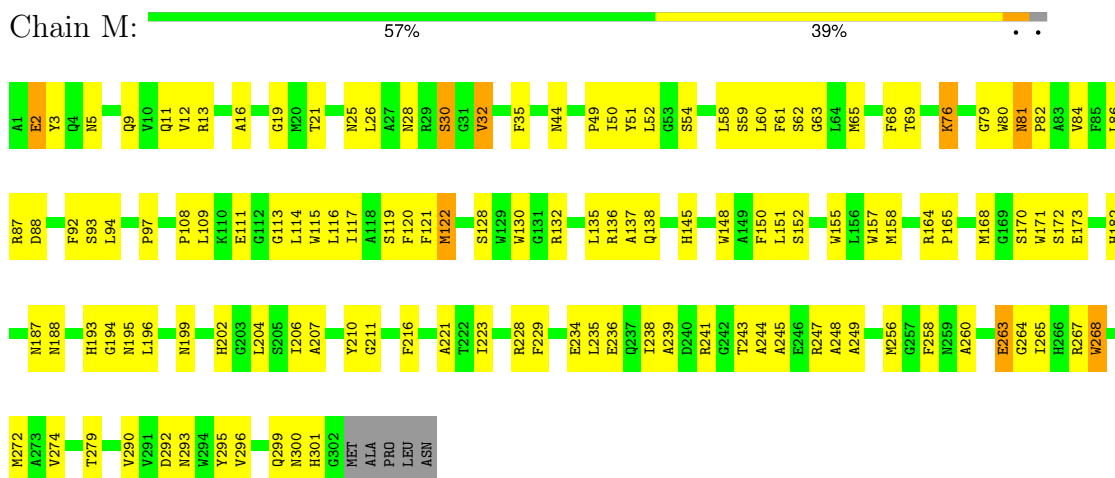
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

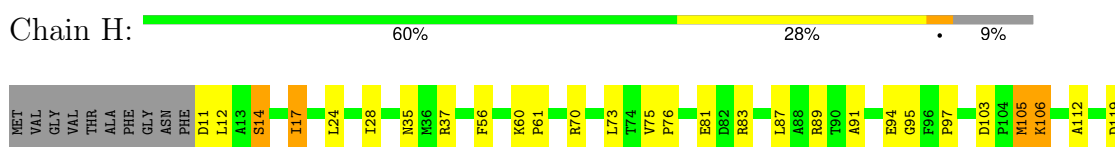
- Molecule 1: Photosynthetic Reaction Center L subunit



- Molecule 2: Photosynthetic Reaction Center M subunit



- Molecule 3: Photosynthetic Reaction Center H subunit



E122	L123	D124	H128	N129	K130	I131	M134	F140	S143	A144	G145	K146	M147	P148	I149	G150	L151	R154	G155	E159	I160	K163	V164	V165	D166	I167	W168	V169	D170	Q174	M175	A176	R177	F178	L190	L191	P192	M193	Q194	M195	V196	K197	V198	R202	V205	N206	A207
F213	I216	I219	K220	V225	T226	E229	F230	D231	R232	I233	C234	G235	Y236	V237	L241	M242	Y243	A244	A245	P246	LYS	ARG	LYS	SER	VAL	VAL	ALA	ALA	ALA	MET	LEU	ALA	GLU	TYR	ALA												

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	142.61Å 142.61Å 187.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.64 – 2.70	Depositor
% Data completeness (in resolution range)	72.4 (28.64-2.70)	Depositor
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.215 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7096	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: U10, BPH, FE, BCL, CDL, SPO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	L	0.54	0/2320	0.99	11/3175 (0.3%)
2	M	0.50	0/2496	0.95	9/3406 (0.3%)
3	H	0.51	0/1842	1.03	9/2509 (0.4%)
All	All	0.52	0/6658	0.98	29/9090 (0.3%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	6	GLU	N-CA-C	8.95	121.12	111.36
1	L	60	ASN	CA-C-N	7.88	127.79	119.05
1	L	60	ASN	C-N-CA	7.88	127.79	119.05
1	L	7	ARG	N-CA-C	7.11	119.64	111.11
3	H	155	GLY	N-CA-C	6.50	120.65	111.42
1	L	269	LEU	CA-C-N	6.16	127.54	119.84
1	L	269	LEU	C-N-CA	6.16	127.54	119.84
1	L	131	LEU	N-CA-C	6.02	117.84	111.28
3	H	243	TYR	N-CA-C	6.00	119.78	112.23
2	M	199	ASN	CA-C-N	5.75	125.22	119.24
2	M	199	ASN	C-N-CA	5.75	125.22	119.24
2	M	268	TRP	N-CA-C	-5.61	105.09	111.14
2	M	81	ASN	CA-C-N	5.42	125.25	119.28
2	M	81	ASN	C-N-CA	5.42	125.25	119.28
2	M	137	ALA	N-CA-C	-5.40	105.04	111.03
1	L	185	LEU	N-CA-C	-5.37	105.34	111.14
1	L	78	ALA	CA-C-N	5.36	125.28	119.76
1	L	78	ALA	C-N-CA	5.36	125.28	119.76
3	H	151	LEU	CA-C-N	5.31	126.13	120.13
3	H	151	LEU	C-N-CA	5.31	126.13	120.13
2	M	234	GLU	N-CA-C	5.30	117.47	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	60	LYS	N-CA-C	-5.29	102.92	109.64
2	M	84	VAL	N-CA-C	-5.27	105.36	110.42
3	H	56	PHE	CA-C-N	5.23	125.43	120.31
3	H	56	PHE	C-N-CA	5.23	125.43	120.31
1	L	13	GLY	N-CA-C	5.21	118.13	112.29
3	H	17	ILE	N-CA-C	5.20	116.67	111.00
3	H	95	GLY	N-CA-C	5.17	122.49	115.30
2	M	19	GLY	N-CA-C	5.09	119.27	112.65

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	98	0
2	M	2405	0	2325	141	0
3	H	1794	0	1792	63	0
4	L	132	0	148	9	0
4	M	132	0	148	10	0
5	L	65	0	76	5	0
5	M	65	0	76	3	0
6	M	1	0	0	0	0
7	M	48	0	63	5	0
8	M	42	0	60	5	0
9	M	81	0	106	3	0
10	H	38	0	0	8	0
10	L	25	0	0	3	0
10	M	36	0	0	6	0
All	All	7096	0	6981	281	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 20.

All (281) 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:21:THR:HG23	2:M:26:LEU:HD21	1.51	0.93
2:M:279:THR:HB	10:M:1024:HOH:O	1.70	0.91
3:H:148:PRO:HA	3:H:151:LEU:HD12	1.53	0.90
3:H:245:ALA:HB3	3:H:246:PRO:HD3	1.56	0.87
1:L:219:LEU:HA	2:M:132:ARG:HH12	1.40	0.86
2:M:243:THR:HG21	2:M:247:ARG:HE	1.40	0.84
2:M:243:THR:HG22	2:M:247:ARG:HE	1.43	0.83
1:L:271:TRP:H	1:L:271:TRP:CD1	1.98	0.81
1:L:51:TRP:O	1:L:54:VAL:HG22	1.81	0.79
2:M:97:PRO:HG2	2:M:171:TRP:HB2	1.62	0.79
2:M:260:ALA:HB1	10:H:1026:HOH:O	1.83	0.78
2:M:256:MET:HE3	2:M:258:PHE:CE1	2.22	0.74
2:M:265:ILE:HG22	10:M:1007:HOH:O	1.86	0.73
2:M:94:LEU:HD21	2:M:115:TRP:HA	1.71	0.72
1:L:230:HIS:CD2	2:M:223:ILE:HG13	2.24	0.71
2:M:16:ALA:CB	2:M:32:VAL:HG11	2.20	0.71
3:H:226:THR:OG1	3:H:229:GLU:HG3	1.92	0.70
1:L:264:GLN:HA	1:L:267:VAL:HG12	1.72	0.70
2:M:243:THR:HG22	2:M:247:ARG:HG3	1.74	0.69
5:L:855:BPH:HBB2	2:M:210:TYR:HB3	1.74	0.69
10:M:1082:HOH:O	3:H:175:MET:HE3	1.91	0.69
1:L:267:VAL:HG23	2:M:87:ARG:HD2	1.76	0.68
2:M:119:SER:HB3	8:M:859:SPO:H311	1.74	0.68
2:M:16:ALA:HB1	2:M:32:VAL:HG11	1.74	0.68
4:L:850:BCL:H11	5:M:854:BPH:HBB2	1.76	0.67
1:L:133:LEU:HD23	1:L:133:LEU:C	2.20	0.65
2:M:264:GLY:HA3	3:H:35:ASN:OD1	1.95	0.65
2:M:211:GLY:CA	2:M:272:MET:HE3	2.26	0.65
3:H:213:PHE:O	3:H:216:ILE:HG13	1.96	0.65
2:M:256:MET:HE3	2:M:258:PHE:CZ	2.33	0.63
1:L:271:TRP:CD1	1:L:271:TRP:N	2.65	0.62
2:M:248:ALA:HB1	7:M:857:U10:H3M2	1.81	0.62
1:L:135:ARG:HD3	10:L:1067:HOH:O	1.98	0.62
1:L:219:LEU:HD12	2:M:132:ARG:HH11	1.64	0.62
2:M:157:TRP:CE3	2:M:158:MET:HG2	2.35	0.61
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.82	0.61
2:M:204:LEU:O	2:M:207:ALA:HB3	2.00	0.61
1:L:187:LEU:HD13	2:M:216:PHE:CG	2.35	0.61
1:L:74:GLY:O	1:L:141:ALA:HA	2.01	0.60
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.36	0.60
2:M:228:ARG:HB3	3:H:195:MET:HE3	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:219:LEU:HA	2:M:132:ARG:NH1	2.14	0.60
1:L:230:HIS:HD2	2:M:223:ILE:HG13	1.65	0.60
1:L:60:ASN:ND2	1:L:63:LEU:HG	2.16	0.60
2:M:211:GLY:HA3	2:M:272:MET:HE3	1.84	0.60
1:L:269:LEU:HD12	1:L:272:TRP:HZ2	1.66	0.59
2:M:3:TYR:CZ	2:M:5:ASN:HA	2.37	0.59
1:L:60:ASN:O	1:L:64:ILE:HG13	2.01	0.59
10:L:1091:HOH:O	2:M:49:PRO:HG2	2.02	0.59
2:M:168:MET:CB	2:M:173:GLU:HG3	2.33	0.58
2:M:97:PRO:HA	2:M:111:GLU:O	2.04	0.58
1:L:12:PRO:HG3	3:H:97:PRO:CB	2.33	0.58
3:H:119:ASP:OD2	3:H:220:LYS:NZ	2.37	0.58
1:L:268:LYS:O	1:L:273:ALA:HB2	2.04	0.58
3:H:196:VAL:HG12	3:H:205:VAL:HG22	1.86	0.58
1:L:219:LEU:HD12	2:M:132:ARG:NH1	2.18	0.58
2:M:130:TRP:HD1	2:M:150:PHE:CD2	2.22	0.58
2:M:138:GLN:HA	10:M:1025:HOH:O	2.04	0.58
3:H:70:ARG:HG3	3:H:70:ARG:HH11	1.69	0.57
2:M:108:PRO:HG2	2:M:111:GLU:HB2	1.85	0.57
3:H:103:ASP:HB3	3:H:106:LYS:HB2	1.85	0.57
1:L:60:ASN:HD22	1:L:63:LEU:HG	1.69	0.57
2:M:76:LYS:HD3	2:M:76:LYS:C	2.30	0.57
3:H:11:ASP:OD1	3:H:14:SER:HB2	2.05	0.57
1:L:133:LEU:HD23	1:L:133:LEU:O	2.05	0.57
1:L:49:ILE:HG12	1:L:89:ILE:HD13	1.87	0.57
2:M:265:ILE:N	10:H:1026:HOH:O	2.38	0.57
2:M:16:ALA:HB1	2:M:32:VAL:HG21	1.87	0.57
2:M:228:ARG:CZ	3:H:195:MET:HE1	2.34	0.57
2:M:76:LYS:HD3	2:M:76:LYS:O	2.05	0.56
2:M:113:GLY:HA2	2:M:116:LEU:HD12	1.86	0.56
2:M:94:LEU:HD12	10:M:1011:HOH:O	2.04	0.56
2:M:228:ARG:CB	3:H:195:MET:HE3	2.35	0.56
1:L:269:LEU:HD12	1:L:272:TRP:CZ2	2.40	0.56
2:M:59:SER:HG	2:M:128:SER:HG	1.48	0.56
3:H:75:VAL:HA	3:H:76:PRO:C	2.30	0.55
4:L:851:BCL:HAA2	4:M:853:BCL:HBC1	1.87	0.55
1:L:45:GLY:O	1:L:49:ILE:HG13	2.06	0.55
2:M:152:SER:O	2:M:155:TRP:HB3	2.06	0.55
1:L:219:LEU:CA	2:M:132:ARG:HH12	2.16	0.55
1:L:269:LEU:HB2	1:L:272:TRP:NE1	2.21	0.55
1:L:34:PHE:O	1:L:38:THR:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:119:SER:CB	8:M:859:SPO:H342	2.37	0.55
3:H:245:ALA:CB	3:H:246:PRO:HD3	2.34	0.55
1:L:34:PHE:O	1:L:38:THR:CG2	2.54	0.54
2:M:51:TYR:O	2:M:132:ARG:NH2	2.40	0.54
4:M:853:BCL:HAA2	4:M:853:BCL:HBD	1.89	0.54
1:L:54:VAL:HG23	1:L:55:LEU:HD23	1.88	0.54
2:M:293:ASN:OD1	2:M:295:TYR:HB3	2.08	0.54
1:L:179:PHE:HB3	1:L:240:ALA:HB2	1.90	0.54
1:L:246:LEU:O	1:L:249:ILE:HG22	2.08	0.54
1:L:133:LEU:HD22	1:L:134:PHE:CD1	2.44	0.54
3:H:177:ARG:HH11	3:H:177:ARG:HG2	1.73	0.54
1:L:34:PHE:HB2	10:L:1051:HOH:O	2.08	0.53
1:L:12:PRO:HG3	3:H:97:PRO:HB2	1.89	0.53
2:M:268:TRP:HD1	10:H:1026:HOH:O	1.90	0.53
2:M:243:THR:HG22	2:M:247:ARG:NE	2.18	0.53
3:H:70:ARG:HG3	3:H:70:ARG:NH1	2.23	0.53
1:L:60:ASN:HB3	1:L:63:LEU:HD12	1.90	0.53
3:H:130:LYS:HE3	3:H:170:ASP:OD2	2.09	0.53
2:M:243:THR:HG21	2:M:247:ARG:NE	2.18	0.53
1:L:269:LEU:HD13	1:L:271:TRP:CH2	2.44	0.53
2:M:211:GLY:C	2:M:272:MET:HE3	2.34	0.53
1:L:54:VAL:HG23	1:L:55:LEU:N	2.24	0.53
5:L:855:BPH:HH1	5:L:855:BPH:HBB3	1.90	0.52
2:M:13:ARG:HD3	2:M:35:PHE:CD2	2.44	0.52
1:L:8:LYS:HA	3:H:87:LEU:HD11	1.92	0.52
3:H:37:ARG:HH11	3:H:37:ARG:HG2	1.75	0.52
1:L:223:SER:O	2:M:44:ASN:HB2	2.09	0.52
2:M:119:SER:HB2	8:M:859:SPO:H342	1.92	0.52
2:M:135:LEU:HB3	2:M:136:ARG:NH2	2.25	0.52
1:L:174:MET:HE1	1:L:263:TRP:CZ2	2.45	0.52
3:H:140:PHE:HE2	3:H:174:GLN:HG2	1.74	0.52
3:H:163:LYS:O	3:H:163:LYS:HG3	2.08	0.52
1:L:170:ASN:HB3	1:L:173:HIS:HB3	1.90	0.52
2:M:59:SER:OG	2:M:128:SER:OG	2.19	0.51
2:M:65:MET:HB3	2:M:121:PHE:CD2	2.45	0.51
3:H:207:ALA:HA	3:H:241:LEU:HD23	1.92	0.51
5:L:855:BPH:H102	4:M:853:BCL:H193	1.91	0.51
1:L:179:PHE:CB	1:L:240:ALA:HB2	2.41	0.51
2:M:290:VAL:HG21	3:H:12:LEU:HD12	1.92	0.51
3:H:177:ARG:HG2	3:H:177:ARG:NH1	2.26	0.51
1:L:133:LEU:C	1:L:133:LEU:CD2	2.84	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:159:GLU:HG3	3:H:160:ILE:N	2.26	0.50
4:L:851:BCL:H203	4:M:853:BCL:H102	1.92	0.50
2:M:109:LEU:HD22	2:M:114:LEU:HD13	1.93	0.50
3:H:89:ARG:HD3	3:H:91:ALA:O	2.12	0.50
2:M:11:GLN:HB2	3:H:144:ALA:HB3	1.93	0.50
3:H:105:MET:HA	3:H:105:MET:HE2	1.94	0.49
4:L:850:BCL:HAA2	4:L:850:BCL:HBD	1.94	0.49
2:M:300:ASN:O	2:M:301:HIS:HB2	2.13	0.49
3:H:140:PHE:CE2	3:H:174:GLN:HG2	2.47	0.49
1:L:66:VAL:HG12	1:L:86:TRP:HB2	1.94	0.49
1:L:206:MET:HE1	2:M:239:ALA:HB2	1.94	0.49
2:M:5:ASN:ND2	3:H:194:GLN:HG3	2.27	0.49
1:L:12:PRO:HG3	3:H:97:PRO:HB3	1.95	0.49
1:L:269:LEU:HD13	1:L:271:TRP:CZ3	2.48	0.49
2:M:16:ALA:HB2	2:M:32:VAL:HG11	1.93	0.49
3:H:134:MET:HE2	3:H:149:ILE:HD11	1.95	0.49
3:H:165:VAL:O	3:H:166:ASP:HB2	2.12	0.49
2:M:228:ARG:HG3	2:M:229:PHE:CE2	2.48	0.48
3:H:148:PRO:O	3:H:149:ILE:C	2.56	0.48
1:L:22:PHE:HA	1:L:24:PHE:CE2	2.48	0.48
2:M:241:ARG:HG3	2:M:245:ALA:HB3	1.95	0.48
3:H:233:ILE:O	3:H:237:VAL:HG23	2.12	0.48
2:M:97:PRO:HG2	2:M:171:TRP:CB	2.40	0.48
3:H:194:GLN:CD	3:H:194:GLN:H	2.22	0.48
2:M:268:TRP:CD1	10:H:1026:HOH:O	2.66	0.48
2:M:65:MET:HB3	2:M:121:PHE:CE2	2.48	0.48
2:M:204:LEU:HB3	2:M:279:THR:HG21	1.95	0.48
2:M:148:TRP:CD2	9:M:3000:CDL:H511	2.48	0.48
1:L:241:VAL:HG21	5:L:855:BPH:HAC1	1.95	0.48
3:H:190:LEU:O	3:H:191:LEU:HD23	2.13	0.48
3:H:131:ILE:HD11	3:H:177:ARG:HD2	1.94	0.47
2:M:68:PHE:O	2:M:69:THR:C	2.58	0.47
2:M:168:MET:HG3	2:M:173:GLU:HG3	1.96	0.47
7:M:857:U10:H222	7:M:857:U10:H201	1.64	0.47
1:L:60:ASN:HD22	1:L:63:LEU:CD1	2.28	0.47
1:L:54:VAL:CG2	1:L:55:LEU:N	2.77	0.47
1:L:139:MET:HB3	1:L:144:TYR:CE2	2.50	0.47
2:M:92:PHE:O	2:M:93:SER:HB2	2.15	0.47
2:M:206:ILE:HD12	4:M:853:BCL:OBD	2.15	0.47
1:L:268:LYS:O	1:L:269:LEU:C	2.56	0.47
1:L:208:THR:HB	1:L:209:PRO:HD2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:105:MET:HE3	3:H:243:TYR:HD2	1.79	0.47
1:L:117:ILE:HB	1:L:118:PRO:CD	2.45	0.46
2:M:260:ALA:CB	10:H:1026:HOH:O	2.54	0.46
1:L:255:TRP:HZ2	1:L:258:GLN:O	1.97	0.46
3:H:143:SER:O	3:H:144:ALA:HB2	2.16	0.46
1:L:207:ARG:NH1	1:L:207:ARG:HG3	2.30	0.46
1:L:267:VAL:HG23	2:M:87:ARG:CD	2.45	0.46
2:M:235:LEU:HA	2:M:238:ILE:HD12	1.98	0.46
7:M:857:U10:H251	7:M:857:U10:H271	1.77	0.46
2:M:80:TRP:O	2:M:82:PRO:HD3	2.16	0.46
3:H:154:ARG:CZ	3:H:202:ARG:HD2	2.46	0.46
1:L:190:HIS:CE1	1:L:230:HIS:CE1	3.04	0.46
2:M:30:SER:OG	2:M:50:ILE:HG22	2.16	0.46
2:M:157:TRP:CZ3	2:M:158:MET:HG2	2.50	0.46
1:L:60:ASN:HA	1:L:61:PRO:HD3	1.76	0.45
2:M:243:THR:CG2	2:M:247:ARG:NE	2.56	0.45
3:H:37:ARG:HG2	3:H:37:ARG:NH1	2.31	0.45
1:L:45:GLY:HA3	5:L:855:BPH:H9C1	1.98	0.45
3:H:81:GLU:O	3:H:83:ARG:HG2	2.16	0.45
4:L:851:BCL:HAA2	4:L:851:BCL:HBD	1.98	0.45
2:M:264:GLY:C	10:H:1026:HOH:O	2.58	0.45
1:L:52:SER:OG	1:L:66:VAL:HG22	2.17	0.45
1:L:177:ILE:O	1:L:177:ILE:HG22	2.17	0.45
1:L:166:ASN:OD1	1:L:168:HIS:HB2	2.17	0.45
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.99	0.45
2:M:239:ALA:O	3:H:73:LEU:HD22	2.17	0.45
2:M:243:THR:O	2:M:247:ARG:HG3	2.16	0.45
1:L:139:MET:HB3	1:L:144:TYR:CD2	2.51	0.45
4:L:850:BCL:HBB2	4:M:852:BCL:H111	1.98	0.45
3:H:219:ILE:HG21	3:H:225:VAL:HG12	1.98	0.45
3:H:14:SER:O	3:H:17:ILE:HG22	2.16	0.44
3:H:146:LYS:HD2	3:H:146:LYS:HA	1.74	0.44
1:L:230:HIS:CD2	2:M:223:ILE:HG21	2.52	0.44
2:M:296:VAL:O	2:M:299:GLN:HB2	2.17	0.44
1:L:175:ILE:O	1:L:178:SER:HB2	2.17	0.44
2:M:76:LYS:C	2:M:76:LYS:CD	2.90	0.44
2:M:119:SER:HB3	8:M:859:SPO:H342	1.99	0.44
1:L:216:PHE:O	1:L:220:VAL:HG22	2.17	0.44
2:M:267:ARG:HH11	2:M:267:ARG:HG2	1.83	0.44
3:H:35:ASN:OD1	10:H:1026:HOH:O	2.21	0.44
1:L:219:LEU:O	2:M:132:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:181:PHE:HB3	5:M:854:BPH:CBB	2.48	0.44
1:L:272:TRP:HB2	2:M:87:ARG:HD3	1.99	0.44
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.98	0.44
2:M:243:THR:HG22	2:M:247:ARG:CG	2.44	0.44
2:M:263:GLU:C	10:M:1007:HOH:O	2.60	0.44
3:H:168:TRP:HB2	3:H:178:PHE:HB2	2.00	0.44
1:L:173:HIS:O	1:L:177:ILE:HG13	2.18	0.44
1:L:181:PHE:HB3	5:M:854:BPH:HBB2	2.00	0.44
2:M:5:ASN:HD21	3:H:194:GLN:HG3	1.83	0.44
2:M:194:GLY:O	2:M:195:ASN:HB3	2.18	0.44
1:L:72:GLU:N	1:L:72:GLU:CD	2.76	0.43
2:M:58:LEU:O	2:M:62:SER:CB	2.66	0.43
4:L:851:BCL:HBC2	4:L:851:BCL:H2C	1.90	0.43
1:L:8:LYS:HE2	1:L:9:TYR:CE2	2.53	0.43
2:M:60:LEU:HD12	2:M:60:LEU:HA	1.81	0.43
2:M:211:GLY:HA3	2:M:272:MET:CE	2.48	0.43
1:L:217:ARG:HB3	2:M:49:PRO:O	2.18	0.43
2:M:13:ARG:O	3:H:140:PHE:HA	2.18	0.43
1:L:264:GLN:O	1:L:268:LYS:HG2	2.19	0.43
2:M:249:ALA:N	7:M:857:U10:H4M2	2.33	0.43
3:H:112:ALA:HA	3:H:235:GLY:O	2.18	0.43
4:L:851:BCL:CAA	4:M:853:BCL:HBC1	2.49	0.43
2:M:148:TRP:CE2	9:M:3000:CDL:H511	2.54	0.43
3:H:61:PRO:HA	3:H:76:PRO:HD2	2.01	0.43
1:L:265:TRP:CG	1:L:266:TRP:N	2.86	0.43
2:M:187:ASN:HA	4:M:852:BCL:HBC1	2.00	0.43
1:L:196:SER:HA	2:M:145:HIS:ND1	2.34	0.43
3:H:193:MET:HE3	3:H:193:MET:HA	2.00	0.43
2:M:79:GLY:C	2:M:81:ASN:H	2.27	0.42
3:H:124:ASP:OD2	3:H:128:HIS:HB2	2.19	0.42
2:M:265:ILE:HA	10:H:1026:HOH:O	2.17	0.42
2:M:61:PHE:C	2:M:63:GLY:N	2.75	0.42
1:L:2:LEU:HD21	1:L:10:ARG:CZ	2.49	0.42
2:M:25:ASN:HD22	2:M:28:ASN:ND2	2.18	0.42
2:M:59:SER:O	2:M:63:GLY:N	2.49	0.42
2:M:151:LEU:HD23	9:M:3000:CDL:H781	2.01	0.42
3:H:166:ASP:CG	3:H:167:ILE:H	2.27	0.42
2:M:122:MET:HE3	8:M:859:SPO:H25	2.01	0.42
2:M:260:ALA:HB2	7:M:857:U10:H103	2.01	0.42
1:L:272:TRP:HA	1:L:275:ILE:HD12	2.01	0.42
1:L:38:THR:HG22	1:L:99:SER:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:116:HIS:CB	2:M:221:ALA:HB1	2.50	0.42
1:L:155:ASP:O	1:L:156:TRP:C	2.63	0.42
2:M:94:LEU:HD21	2:M:115:TRP:CA	2.46	0.42
1:L:146:PHE:HB2	1:L:147:PRO:HD2	2.02	0.41
2:M:130:TRP:HD1	2:M:150:PHE:HD2	1.64	0.41
2:M:164:ARG:O	2:M:168:MET:HG2	2.20	0.41
4:M:852:BCL:HAA2	4:M:852:BCL:HBD	2.02	0.41
1:L:146:PHE:HB3	1:L:156:TRP:CD2	2.56	0.41
2:M:293:ASN:CG	2:M:296:VAL:HG23	2.45	0.41
1:L:207:ARG:HG3	1:L:207:ARG:HH11	1.84	0.41
1:L:262:TRP:O	1:L:265:TRP:HD1	2.03	0.41
2:M:9:GLN:OE1	3:H:198:VAL:HG23	2.20	0.41
2:M:109:LEU:C	2:M:111:GLU:H	2.28	0.41
2:M:114:LEU:HD12	2:M:117:ILE:HD12	2.02	0.41
1:L:182:THR:OG1	4:L:850:BCL:H42	2.21	0.41
2:M:170:SER:OG	2:M:172:SER:HB3	2.20	0.41
3:H:24:LEU:O	3:H:28:ILE:HG13	2.21	0.41
1:L:8:LYS:HE2	1:L:9:TYR:CZ	2.55	0.41
2:M:117:ILE:O	2:M:120:PHE:HB3	2.21	0.41
2:M:193:HIS:O	2:M:293:ASN:HA	2.20	0.41
1:L:60:ASN:HD22	1:L:63:LEU:CG	2.32	0.41
1:L:280:ASN:ND2	2:M:88:ASP:OD1	2.53	0.41
2:M:236:GLU:HG2	3:H:122:GLU:HG3	2.03	0.41
2:M:264:GLY:O	2:M:267:ARG:HB2	2.21	0.41
2:M:2:GLU:O	2:M:3:TYR:C	2.64	0.41
2:M:293:ASN:OD1	2:M:296:VAL:HG23	2.20	0.40
4:M:852:BCL:HBC2	4:M:852:BCL:H2C	1.95	0.40
1:L:229:ILE:HG23	1:L:230:HIS:ND1	2.37	0.40
2:M:52:LEU:HD12	2:M:52:LEU:HA	1.82	0.40
2:M:58:LEU:O	2:M:62:SER:HB3	2.22	0.40
2:M:235:LEU:O	2:M:238:ILE:HB	2.22	0.40
1:L:187:LEU:HD13	2:M:216:PHE:CD2	2.56	0.40
1:L:269:LEU:HA	1:L:270:PRO:HD3	1.90	0.40
1:L:272:TRP:HA	1:L:275:ILE:CD1	2.51	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%)	247 (88%)	30 (11%)	2 (1%)	18	41
2	M	300/307 (98%)	268 (89%)	29 (10%)	3 (1%)	12	32
3	H	234/260 (90%)	212 (91%)	21 (9%)	1 (0%)	30	54
All	All	813/848 (96%)	727 (89%)	80 (10%)	6 (1%)	18	41

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	245	ALA
2	M	54	SER
2	M	30	SER
1	L	237	SER
1	L	200	PRO
2	M	32	VAL

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%)	31	60
2	M	236/240 (98%)	225 (95%)	11 (5%)	23	51
3	H	191/208 (92%)	184 (96%)	7 (4%)	30	59
All	All	647/668 (97%)	621 (96%)	26 (4%)	28	56

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

Mol	Chain	Res	Type
1	L	38	THR
1	L	72	GLU
1	L	154	LEU
1	L	185	LEU
1	L	207	ARG
1	L	235	LEU
1	L	247	CYS
1	L	271	TRP
2	M	2	GLU
2	M	12	VAL
2	M	76	LYS
2	M	86	LEU
2	M	122	MET
2	M	182	HIS
2	M	188	ASN
2	M	196	LEU
2	M	263	GLU
2	M	274	VAL
2	M	292	ASP
3	H	14	SER
3	H	94	GLU
3	H	105	MET
3	H	106	LYS
3	H	206	ASN
3	H	225	VAL
3	H	231	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	60	ASN
1	L	258	GLN
1	L	264	GLN
2	M	28	ASN
2	M	195	ASN
2	M	202	HIS
2	M	299	GLN
3	H	52	ASN
3	H	206	ASN

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 oligosaccharides 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$
9	CDL	M	3000	-	80,80,99	0.76	2 (2%)	86,92,111	0.94	5 (5%)
4	BCL	L	851	1	69,74,74	1.34	11 (15%)	79,115,115	1.63	15 (18%)
8	SPO	M	859	-	41,41,41	3.33	23 (56%)	47,50,50	2.69	16 (34%)
5	BPH	M	854	-	59,70,70	1.93	11 (18%)	59,101,101	2.41	16 (27%)
4	BCL	L	850	2	69,74,74	1.39	10 (14%)	79,115,115	1.82	22 (27%)
4	BCL	M	852	2	69,74,74	1.39	9 (13%)	79,115,115	1.81	17 (21%)
5	BPH	L	855	-	59,70,70	1.80	9 (15%)	59,101,101	2.66	19 (32%)
7	U10	M	857	-	48,48,63	2.43	14 (29%)	60,61,79	2.17	18 (30%)
4	BCL	M	853	1	69,74,74	1.44	9 (13%)	79,115,115	1.91	23 (29%)

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
9	CDL	M	3000	-	-	33/91/91/110	-
4	BCL	L	851	1	-	7/41/137/137	-
8	SPO	M	859	-	-	19/47/47/47	-
5	BPH	M	854	-	-	8/37/105/105	0/5/6/6
4	BCL	L	850	2	-	5/41/137/137	-
4	BCL	M	852	2	-	10/41/137/137	-
5	BPH	L	855	-	-	4/37/105/105	0/5/6/6
7	U10	M	857	-	-	19/45/69/87	0/1/1/1
4	BCL	M	853	1	-	7/41/137/137	-

All (98) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	857	U10	C6-C1	9.64	1.52	1.35
8	M	859	SPO	C15-C16	9.25	1.58	1.34
5	M	854	BPH	C3A-C2A	-8.07	1.47	1.54
5	L	855	BPH	C3A-C2A	-7.54	1.48	1.54
8	M	859	SPO	C10-C11	6.93	1.52	1.34
8	M	859	SPO	C6-C5	6.78	1.50	1.32
8	M	859	SPO	C21-C20	5.51	1.51	1.36
7	M	857	U10	C4-C3	5.00	1.54	1.36
8	M	859	SPO	C26-C25	4.93	1.47	1.34
4	M	853	BCL	C2-C3	4.87	1.44	1.33
8	M	859	SPO	C13-C12	4.85	1.60	1.50
5	L	855	BPH	C3D-C2D	4.56	1.47	1.39
8	M	859	SPO	C15-C14	4.51	1.57	1.43
5	M	854	BPH	C3B-C4B	4.29	1.48	1.41
5	M	854	BPH	C3D-C2D	4.24	1.46	1.39
4	L	851	BCL	C3D-C2D	4.19	1.50	1.39
4	L	850	BCL	C3D-C2D	4.12	1.50	1.39
4	M	852	BCL	C3D-C2D	4.04	1.50	1.39
5	L	855	BPH	C3B-C4B	3.89	1.47	1.41
4	L	850	BCL	C2-C3	3.88	1.42	1.33
8	M	859	SPO	C32-C33	3.83	1.41	1.33
5	L	855	BPH	C3D-CAD	-3.82	1.40	1.47
4	M	853	BCL	C3D-C2D	3.79	1.49	1.39
5	M	854	BPH	C2-C3	3.78	1.41	1.33
7	M	857	U10	C6-C5	3.75	1.57	1.46
5	M	854	BPH	C3B-C2B	3.63	1.45	1.39
7	M	857	U10	C18-C19	3.61	1.41	1.33
7	M	857	U10	C33-C34	3.60	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	852	BCL	C2-C3	3.56	1.41	1.33
8	M	859	SPO	C4-C5	-3.54	1.44	1.50
7	M	857	U10	C28-C29	3.52	1.41	1.33
7	M	857	U10	C7-C8	-3.51	1.45	1.50
8	M	859	SPO	O1-CM1	3.51	1.54	1.43
7	M	857	U10	C13-C14	3.49	1.41	1.33
5	M	854	BPH	C3D-CAD	-3.47	1.41	1.47
4	L	850	BCL	C3B-CAB	3.47	1.57	1.46
8	M	859	SPO	C8-C7	3.45	1.57	1.50
5	L	855	BPH	C3B-C2B	3.44	1.45	1.39
4	L	851	BCL	CMB-C2B	3.41	1.57	1.50
7	M	857	U10	C7-C6	3.39	1.57	1.51
4	M	853	BCL	C3B-CAB	3.37	1.57	1.46
4	M	853	BCL	CMB-C2B	3.30	1.57	1.50
4	M	852	BCL	CBB-CAB	3.28	1.56	1.50
4	M	852	BCL	CMB-C2B	3.28	1.57	1.50
5	L	855	BPH	CMB-C2B	3.27	1.58	1.51
4	M	852	BCL	C3B-CAB	3.26	1.56	1.46
4	M	852	BCL	C1D-C2D	-3.25	1.38	1.45
5	L	855	BPH	C2-C3	3.24	1.40	1.33
8	M	859	SPO	C10-C9	3.21	1.53	1.43
4	L	850	BCL	CMB-C2B	3.18	1.57	1.50
8	M	859	SPO	C37-C38	3.18	1.42	1.32
4	M	852	BCL	CMD-C2D	3.08	1.57	1.50
8	M	859	SPO	O1-C1	3.08	1.58	1.41
5	M	854	BPH	CMB-C2B	3.02	1.57	1.51
4	L	851	BCL	CBB-CAB	3.00	1.56	1.50
8	M	859	SPO	C35-C33	2.98	1.57	1.51
7	M	857	U10	O3-C3	2.97	1.43	1.36
7	M	857	U10	C23-C24	2.94	1.39	1.33
8	M	859	SPO	C14-C12	2.93	1.42	1.35
4	L	851	BCL	C3B-C4B	2.91	1.46	1.41
4	L	850	BCL	CBB-CAB	2.90	1.55	1.50
8	M	859	SPO	C31-C32	-2.87	1.41	1.50
4	L	851	BCL	C2-C3	2.85	1.39	1.33
7	M	857	U10	O4-C4	2.78	1.43	1.36
4	L	850	BCL	C3B-C4B	2.77	1.46	1.41
5	L	855	BPH	CMD-C2D	2.76	1.57	1.51
4	M	853	BCL	CBB-CAB	2.75	1.55	1.50
5	M	854	BPH	C2C-C3C	-2.72	1.52	1.54
4	L	851	BCL	C3B-CAB	2.64	1.55	1.46
8	M	859	SPO	C29-C28	2.62	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	859	SPO	C11-C12	-2.59	1.40	1.46
5	M	854	BPH	CMD-C2D	2.57	1.56	1.51
7	M	857	U10	C38-C39	2.50	1.40	1.32
4	L	851	BCL	C1D-C2D	-2.49	1.40	1.45
8	M	859	SPO	C24-C23	2.49	1.55	1.50
8	M	859	SPO	C25-C23	-2.49	1.40	1.46
8	M	859	SPO	C19-C17	2.48	1.41	1.35
9	M	3000	CDL	OA8-CA7	2.43	1.40	1.33
4	L	850	BCL	CMD-C2D	2.41	1.55	1.50
7	M	857	U10	C8-C9	2.38	1.38	1.33
4	L	850	BCL	OBD-CAD	2.38	1.26	1.22
4	M	853	BCL	C1D-C2D	-2.36	1.40	1.45
4	L	850	BCL	C3A-C2A	-2.35	1.48	1.54
4	M	852	BCL	C3B-C4B	2.24	1.45	1.41
5	M	854	BPH	C1A-C2A	2.24	1.54	1.51
5	L	855	BPH	O2A-CGA	-2.20	1.27	1.33
4	L	851	BCL	MG-NB	2.16	2.10	2.05
4	M	852	BCL	C3C-C4C	-2.16	1.48	1.51
4	L	850	BCL	MG-NB	2.16	2.10	2.05
4	M	853	BCL	CMD-C2D	2.15	1.55	1.50
9	M	3000	CDL	CB3-CB4	2.14	1.57	1.50
4	M	853	BCL	C3B-C4B	2.13	1.45	1.41
5	M	854	BPH	C5-C3	2.13	1.55	1.51
4	M	853	BCL	C3A-C2A	-2.13	1.48	1.54
4	L	851	BCL	CHC-C4B	2.12	1.44	1.39
8	M	859	SPO	C26-C27	2.12	1.49	1.43
4	L	851	BCL	CMD-C2D	2.09	1.55	1.50
4	L	851	BCL	O2A-CGA	-2.02	1.27	1.33

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	859	SPO	C25-C23-C22	-11.27	101.28	119.01
5	L	855	BPH	C4D-CHA-CBD	-9.22	104.03	108.45
5	M	854	BPH	C4D-CHA-CBD	-8.16	104.54	108.45
5	L	855	BPH	C1-O2A-CGA	6.57	132.56	116.65
5	M	854	BPH	C1-O2A-CGA	6.13	131.49	116.65
5	L	855	BPH	O2D-CGD-CBD	5.98	117.52	110.95
4	M	853	BCL	CAA-C2A-C1A	-5.93	92.53	111.97
5	M	854	BPH	O2D-CGD-CBD	5.83	117.35	110.95
7	M	857	U10	C7-C6-C5	5.74	125.19	118.52
5	M	854	BPH	C3D-C4D-ND	5.72	115.04	107.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	855	BPH	C3D-C4D-ND	5.44	114.69	107.71
5	L	855	BPH	C6-C5-C3	5.35	126.49	113.47
8	M	859	SPO	C20-C21-C22	-5.21	112.86	123.52
5	L	855	BPH	C4-C3-C5	5.20	124.26	115.23
8	M	859	SPO	C18-C17-C19	-5.06	114.62	122.82
4	L	850	BCL	CAA-C2A-C1A	-5.03	95.48	111.97
4	M	852	BCL	C4D-CHA-C1A	4.76	126.93	121.24
4	L	850	BCL	CMB-C2B-C1B	-4.74	118.20	125.42
4	M	852	BCL	CED-O2D-CGD	4.71	126.60	115.92
5	M	854	BPH	C2B-C1B-NB	4.68	112.81	109.43
7	M	857	U10	C7-C6-C1	-4.66	116.89	124.89
7	M	857	U10	C7-C8-C9	4.58	134.72	126.83
4	M	852	BCL	CMB-C2B-C1B	-4.49	118.58	125.42
5	L	855	BPH	CMB-C2B-C3B	4.49	133.65	124.68
4	L	850	BCL	CHC-C4B-NB	-4.46	117.36	124.05
5	L	855	BPH	O1D-CGD-CBD	-4.43	118.00	124.72
7	M	857	U10	C10-C9-C8	-4.42	112.28	123.63
4	M	853	BCL	CHC-C4B-NB	-4.42	117.42	124.05
4	L	851	BCL	CMB-C2B-C1B	-4.38	118.75	125.42
7	M	857	U10	C15-C14-C13	-4.34	112.47	123.63
5	M	854	BPH	O1D-CGD-CBD	-4.33	118.16	124.72
4	M	852	BCL	CHC-C4B-NB	-4.32	117.57	124.05
5	M	854	BPH	CMB-C2B-C3B	4.31	133.29	124.68
7	M	857	U10	C15-C14-C16	4.29	122.68	115.23
4	M	852	BCL	C6-C5-C3	4.22	123.75	113.47
4	L	851	BCL	CHC-C4B-NB	-4.22	117.72	124.05
4	M	853	BCL	CMB-C2B-C1B	-4.19	119.04	125.42
8	M	859	SPO	C26-C27-C28	-4.17	121.83	127.69
8	M	859	SPO	C24-C23-C22	-4.16	116.07	122.82
4	M	853	BCL	CED-O2D-CGD	4.14	125.32	115.92
4	L	851	BCL	CED-O2D-CGD	4.04	125.09	115.92
4	L	851	BCL	C2A-C3A-C4A	4.02	108.37	101.87
4	L	850	BCL	CED-O2D-CGD	4.00	125.00	115.92
5	L	855	BPH	C2B-C1B-NB	4.00	112.32	109.43
4	L	850	BCL	C3D-C4D-ND	3.88	116.30	109.99
4	M	853	BCL	CBA-CAA-C2A	3.84	125.22	113.79
9	M	3000	CDL	OB8-CB6-CB4	3.69	119.04	108.40
5	M	854	BPH	C4D-ND-C1D	-3.68	104.47	108.87
5	L	855	BPH	C5-C3-C2	-3.65	112.98	121.17
4	M	853	BCL	C3D-C4D-ND	3.64	115.90	109.99
7	M	857	U10	C11-C9-C8	3.63	129.31	121.17
4	L	850	BCL	C4D-CHA-C1A	3.63	125.57	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	853	BCL	C4A-NA-C1A	3.61	108.32	106.68
5	L	855	BPH	C7-C6-C5	-3.57	103.74	113.26
4	M	853	BCL	C4D-CHA-C1A	3.55	125.47	121.24
8	M	859	SPO	C10-C9-C7	-3.52	122.34	127.28
5	L	855	BPH	C4D-ND-C1D	-3.52	104.66	108.87
4	M	853	BCL	C2A-C3A-C4A	3.51	107.54	101.87
4	L	850	BCL	CBA-CAA-C2A	3.49	124.16	113.79
8	M	859	SPO	C15-C14-C12	-3.45	122.44	127.28
4	M	852	BCL	C4A-NA-C1A	3.44	108.25	106.68
8	M	859	SPO	C4-C5-C6	-3.42	120.11	124.91
5	M	854	BPH	C4A-C3A-C2A	3.41	106.08	102.84
5	M	854	BPH	C4-C3-C5	3.33	121.01	115.23
4	M	852	BCL	C2A-C3A-C4A	3.29	107.18	101.87
8	M	859	SPO	C11-C12-C14	-3.27	113.87	119.01
4	L	850	BCL	C2A-C3A-C4A	3.25	107.12	101.87
4	L	851	BCL	C4D-CHA-C1A	3.25	125.12	121.24
7	M	857	U10	C35-C34-C33	-3.24	115.29	123.63
7	M	857	U10	C25-C24-C23	-3.21	115.38	123.63
7	M	857	U10	C25-C24-C26	3.20	120.78	115.23
4	M	852	BCL	C3D-C4D-ND	3.18	115.16	109.99
4	M	852	BCL	CHA-C1A-NA	-3.09	119.39	126.39
7	M	857	U10	C8-C7-C6	-3.05	104.58	112.08
4	M	852	BCL	OBD-CAD-C3D	-3.03	121.33	128.42
5	M	854	BPH	C3D-CAD-CBD	3.01	111.57	107.61
4	L	851	BCL	C3D-C4D-ND	3.00	114.86	109.99
8	M	859	SPO	C15-C16-C17	-2.97	118.21	126.36
4	M	852	BCL	C4D-C3D-CAD	-2.97	104.88	108.11
8	M	859	SPO	C8-C7-C9	2.91	127.53	122.82
5	L	855	BPH	C3D-CAD-CBD	2.90	111.43	107.61
4	L	851	BCL	OBD-CAD-C3D	-2.89	121.67	128.42
4	M	853	BCL	CMD-C2D-C1D	2.86	129.76	124.73
4	L	851	BCL	CHA-C1A-NA	-2.79	120.07	126.39
4	M	853	BCL	OBD-CAD-C3D	-2.79	121.89	128.42
7	M	857	U10	O5-C5-C4	-2.78	115.14	121.03
9	M	3000	CDL	CB4-OB6-CB5	2.77	124.42	117.80
5	L	855	BPH	C4A-C3A-C2A	2.76	105.47	102.84
4	M	853	BCL	O2D-CGD-CBD	2.75	116.04	111.23
8	M	859	SPO	C16-C17-C19	2.69	123.24	119.01
4	L	851	BCL	C4A-NA-C1A	2.67	107.90	106.68
4	L	850	BCL	C4A-NA-C1A	2.67	107.90	106.68
4	M	853	BCL	O2A-CGA-CBA	2.67	119.97	111.83
4	M	853	BCL	C3B-C4B-NB	2.67	113.28	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	853	BCL	O1D-CGD-CBD	-2.66	119.28	124.52
9	M	3000	CDL	CB6-CB4-CB3	-2.65	105.60	111.78
8	M	859	SPO	C18-C17-C16	2.65	122.14	118.09
4	L	851	BCL	C4D-C3D-CAD	-2.65	105.23	108.11
4	L	850	BCL	CMB-C2B-C3B	2.64	134.01	125.67
5	M	854	BPH	CED-O2D-CGD	2.63	121.88	115.92
5	L	855	BPH	C2D-C1D-ND	2.61	111.32	109.43
7	M	857	U10	C20-C19-C18	-2.61	116.93	123.63
4	L	851	BCL	C2A-C1A-CHA	2.58	128.34	123.87
5	M	854	BPH	C3B-C4B-NB	2.54	111.74	108.05
4	M	852	BCL	CMB-C2B-C3B	2.53	133.65	125.67
4	M	853	BCL	CMD-C2D-C3D	-2.53	121.89	127.69
4	L	850	BCL	CMD-C2D-C1D	2.51	129.15	124.73
4	M	852	BCL	C15-C13-C12	-2.50	99.41	112.07
4	M	852	BCL	CMD-C2D-C1D	2.48	129.09	124.73
4	M	852	BCL	C2A-C1A-CHA	2.46	128.14	123.87
4	L	850	BCL	C2A-C1A-CHA	2.45	128.12	123.87
4	M	853	BCL	CMB-C2B-C3B	2.45	133.40	125.67
4	L	851	BCL	CMB-C2B-C3B	2.42	133.31	125.67
5	L	855	BPH	CED-O2D-CGD	2.41	121.38	115.92
7	M	857	U10	C4M-O4-C4	2.40	124.89	116.47
4	L	850	BCL	CMD-C2D-C3D	-2.38	122.22	127.69
5	M	854	BPH	C2D-C1D-ND	2.37	111.14	109.43
5	M	854	BPH	OBD-CAD-C3D	-2.33	124.25	127.89
7	M	857	U10	C30-C29-C31	2.33	119.27	115.23
4	L	850	BCL	CHA-C1A-NA	-2.32	121.15	126.39
4	L	850	BCL	O1D-CGD-CBD	-2.31	119.95	124.52
4	L	850	BCL	C4D-C3D-CAD	-2.31	105.59	108.11
9	M	3000	CDL	C52-C51-CB5	2.31	122.16	113.69
4	M	853	BCL	CHA-C1A-NA	-2.31	121.17	126.39
7	M	857	U10	C1M-C1-C6	-2.31	120.66	124.45
4	L	851	BCL	CMD-C2D-C1D	2.28	128.74	124.73
4	M	852	BCL	CGD-CBD-CAD	-2.28	103.47	110.85
8	M	859	SPO	C13-C12-C11	2.27	121.56	118.09
4	L	850	BCL	OBD-CAD-C3D	-2.25	123.15	128.42
4	M	852	BCL	C1-O2A-CGA	2.22	122.02	116.65
4	L	850	BCL	C6-C5-C3	2.21	118.85	113.47
8	M	859	SPO	C8-C7-C6	-2.21	114.71	118.09
5	L	855	BPH	OBD-CAD-C3D	-2.21	124.45	127.89
5	L	855	BPH	C3B-C4B-NB	2.20	111.26	108.05
4	M	853	BCL	C4D-C3D-CAD	-2.17	105.75	108.11
4	M	853	BCL	C2C-C3C-C4C	2.17	104.59	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	853	BCL	CMA-C3A-C2A	-2.17	105.61	113.98
4	L	851	BCL	CMD-C2D-C3D	-2.16	122.74	127.69
4	L	850	BCL	CHA-C4D-ND	-2.15	128.12	132.55
7	M	857	U10	C35-C34-C36	2.14	118.94	115.23
9	M	3000	CDL	CA6-CA4-CA3	-2.13	106.81	111.78
5	L	855	BPH	C6-C7-C8	2.10	122.96	115.97
4	L	851	BCL	C2C-C3C-C4C	2.10	104.48	101.34
4	M	853	BCL	C6-C5-C3	2.09	118.56	113.47
4	M	853	BCL	CAB-C3B-C2B	2.09	132.09	127.74
4	L	850	BCL	O2A-CGA-CBA	2.07	118.15	111.83
4	L	850	BCL	C3D-C2D-C1D	2.05	108.63	105.83
7	M	857	U10	C36-C34-C33	2.05	125.77	121.17
5	M	854	BPH	CMA-C3A-C2A	-2.03	106.28	114.13
4	L	850	BCL	C3B-C4B-NB	2.02	112.43	109.76
8	M	859	SPO	C27-C26-C25	-2.01	117.38	123.20

There are no chirality outliers.

All (112) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	851	BCL	C2C-C3C-CAC-CBC
4	L	851	BCL	C4C-C3C-CAC-CBC
5	M	854	BPH	C4C-C3C-CAC-CBC
5	M	854	BPH	C2C-C3C-CAC-CBC
8	M	859	SPO	O1-C1-C4-C5
8	M	859	SPO	C2-C1-C4-C5
8	M	859	SPO	C21-C22-C23-C24
9	M	3000	CDL	CA3-OA5-PA1-OA2
9	M	3000	CDL	CA3-OA5-PA1-OA3
9	M	3000	CDL	CA3-OA5-PA1-OA4
9	M	3000	CDL	CB2-OB2-PB2-OB3
9	M	3000	CDL	CB3-OB5-PB2-OB2
8	M	859	SPO	C36-C37-C38-C39
8	M	859	SPO	C36-C37-C38-C40
4	M	852	BCL	C4-C3-C5-C6
7	M	857	U10	C12-C11-C9-C10
4	M	852	BCL	C2-C3-C5-C6
7	M	857	U10	C12-C11-C9-C8
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	C20-C19-C21-C22

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Mol	Chain	Res	Type	Atoms
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	C18-C19-C21-C22
7	M	857	U10	C23-C24-C26-C27
8	M	859	SPO	C28-C30-C31-C32
8	M	859	SPO	C24-C23-C25-C26
8	M	859	SPO	C20-C21-C22-C23
7	M	857	U10	C19-C21-C22-C23
7	M	857	U10	C29-C31-C32-C33
4	L	850	BCL	C5-C6-C7-C8
9	M	3000	CDL	CB7-C71-C72-C73
4	M	852	BCL	C15-C16-C17-C18
4	M	853	BCL	C5-C6-C7-C8
5	M	854	BPH	C10-C11-C12-C13
7	M	857	U10	C24-C26-C27-C28
4	L	851	BCL	C2A-CAA-CBA-CGA
9	M	3000	CDL	C36-C37-C38-C39
8	M	859	SPO	C9-C10-C11-C12
7	M	857	U10	C35-C34-C36-C37
9	M	3000	CDL	C34-C35-C36-C37
4	M	853	BCL	C12-C13-C15-C16
8	M	859	SPO	C3-C1-C4-C5
9	M	3000	CDL	C19-C20-C21-C22
4	L	850	BCL	C2A-CAA-CBA-CGA
4	M	853	BCL	C14-C13-C15-C16
9	M	3000	CDL	CA3-CA4-CA6-OA8
8	M	859	SPO	C4-C1-O1-CM1
9	M	3000	CDL	C39-C40-C41-C42
9	M	3000	CDL	C33-C34-C35-C36
9	M	3000	CDL	OA5-CA3-CA4-CA6
4	M	852	BCL	C11-C10-C8-C7
5	L	855	BPH	C6-C7-C8-C10
9	M	3000	CDL	C21-C22-C23-C24
4	M	853	BCL	C2A-CAA-CBA-CGA
4	M	852	BCL	C3-C5-C6-C7
9	M	3000	CDL	OA5-CA3-CA4-OA6
9	M	3000	CDL	C78-C79-C80-C81
4	M	853	BCL	C3-C5-C6-C7
4	M	852	BCL	C11-C10-C8-C9
9	M	3000	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
7	M	857	U10	C9-C11-C12-C13
7	M	857	U10	C33-C34-C36-C37
9	M	3000	CDL	C55-C56-C57-C58
7	M	857	U10	C1-C6-C7-C8
7	M	857	U10	C5-C6-C7-C8
4	M	852	BCL	C12-C13-C15-C16
4	M	852	BCL	C2C-C3C-CAC-CBC
9	M	3000	CDL	OA7-CA5-OA6-CA4
5	L	855	BPH	C3-C5-C6-C7
4	M	853	BCL	CHA-CBD-CGD-O1D
4	M	853	BCL	CHA-CBD-CGD-O2D
9	M	3000	CDL	CB2-OB2-PB2-OB4
9	M	3000	CDL	CB2-OB2-PB2-OB5
9	M	3000	CDL	C11-CA5-OA6-CA4
9	M	3000	CDL	C81-C82-C83-C84
4	L	851	BCL	C12-C13-C15-C16
9	M	3000	CDL	C38-C39-C40-C41
8	M	859	SPO	C2-C1-O1-CM1
7	M	857	U10	C14-C16-C17-C18
9	M	3000	CDL	C79-C80-C81-C82
9	M	3000	CDL	OA6-CA4-CA6-OA8
8	M	859	SPO	C18-C17-C19-C20
4	L	850	BCL	C4-C3-C5-C6
4	M	852	BCL	C14-C13-C15-C16
9	M	3000	CDL	C71-C72-C73-C74
8	M	859	SPO	C16-C17-C19-C20
8	M	859	SPO	C29-C28-C30-C31
4	L	850	BCL	C2-C3-C5-C6
7	M	857	U10	C5-C4-O4-C4M
5	M	854	BPH	C11-C10-C8-C9
9	M	3000	CDL	C72-C73-C74-C75
9	M	3000	CDL	C80-C81-C82-C83
5	M	854	BPH	C2A-CAA-CBA-CGA
4	M	852	BCL	CAA-CBA-CGA-O2A
9	M	3000	CDL	C51-C52-C53-C54
4	L	851	BCL	C14-C13-C15-C16
5	M	854	BPH	C11-C10-C8-C7
8	M	859	SPO	C3-C1-O1-CM1
9	M	3000	CDL	C40-C41-C42-C43
8	M	859	SPO	C17-C19-C20-C21
8	M	859	SPO	C1-C4-C5-C6
4	L	851	BCL	C5-C6-C7-C8

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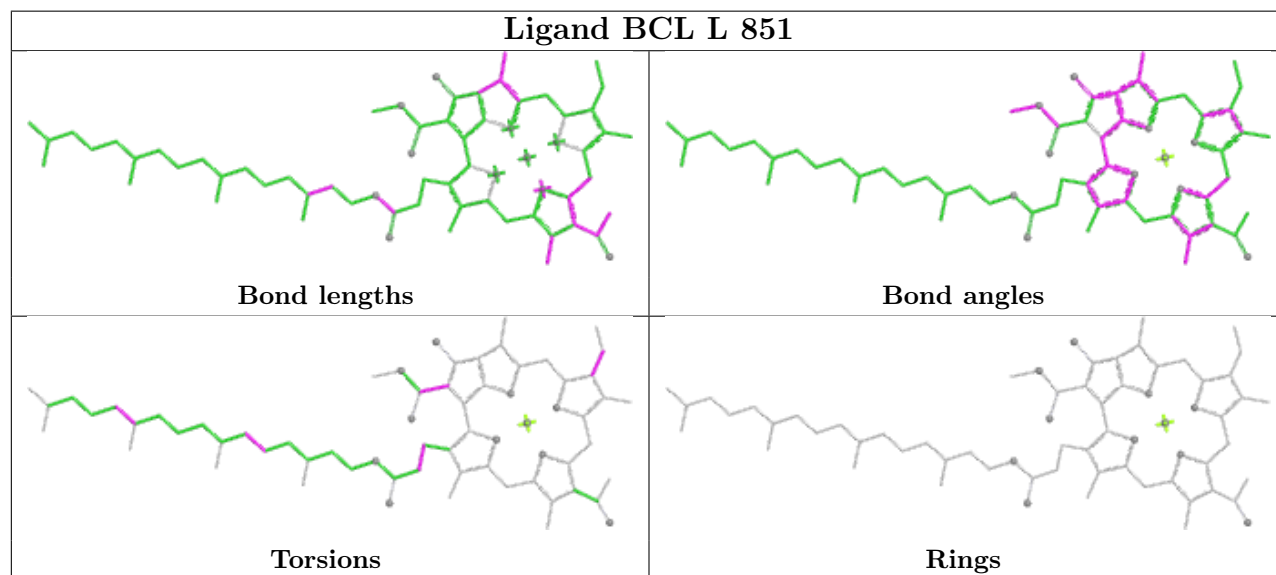
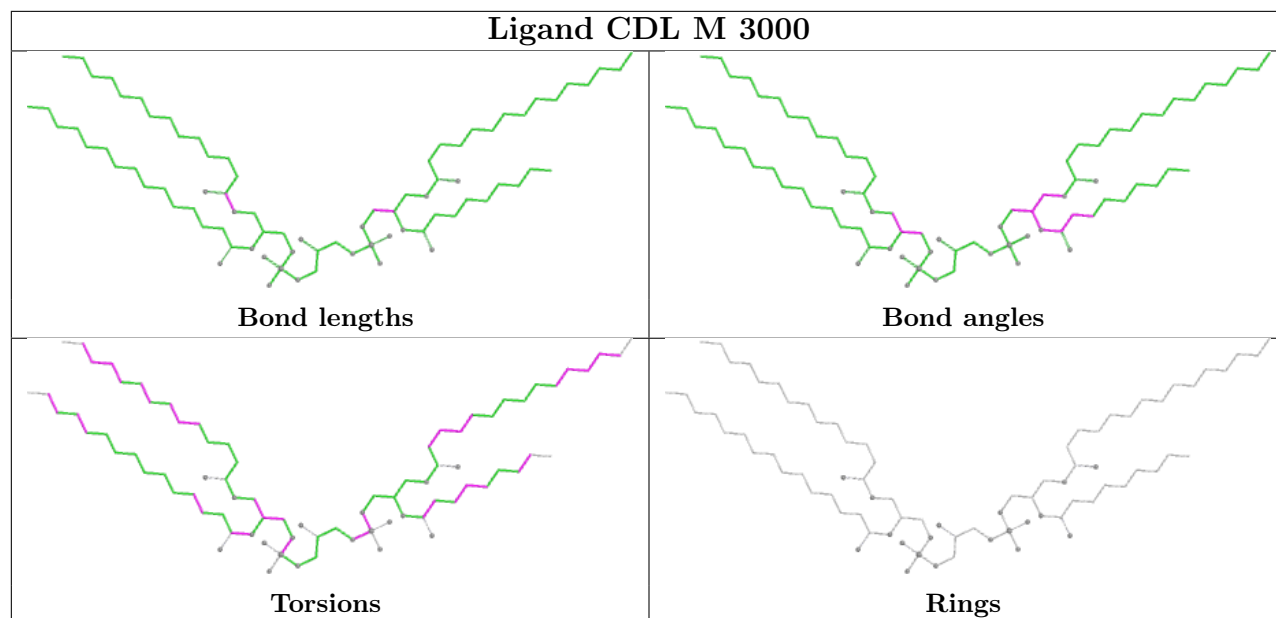
Mol	Chain	Res	Type	Atoms
9	M	3000	CDL	C52-C53-C54-C55
7	M	857	U10	C34-C36-C37-C38
8	M	859	SPO	C27-C28-C30-C31
4	L	851	BCL	CAD-CBD-CGD-O2D
4	L	850	BCL	C2-C1-O2A-CGA
9	M	3000	CDL	C52-C51-CB5-OB6

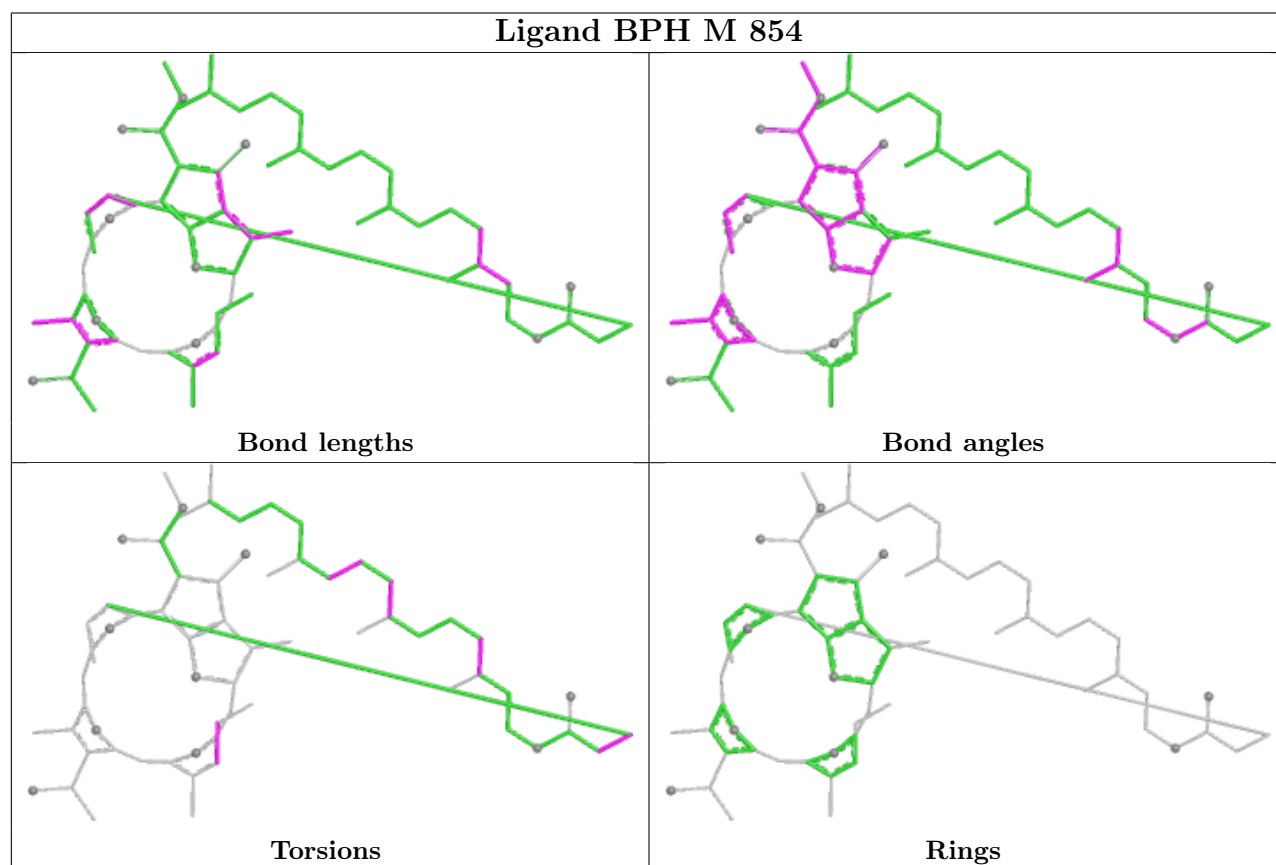
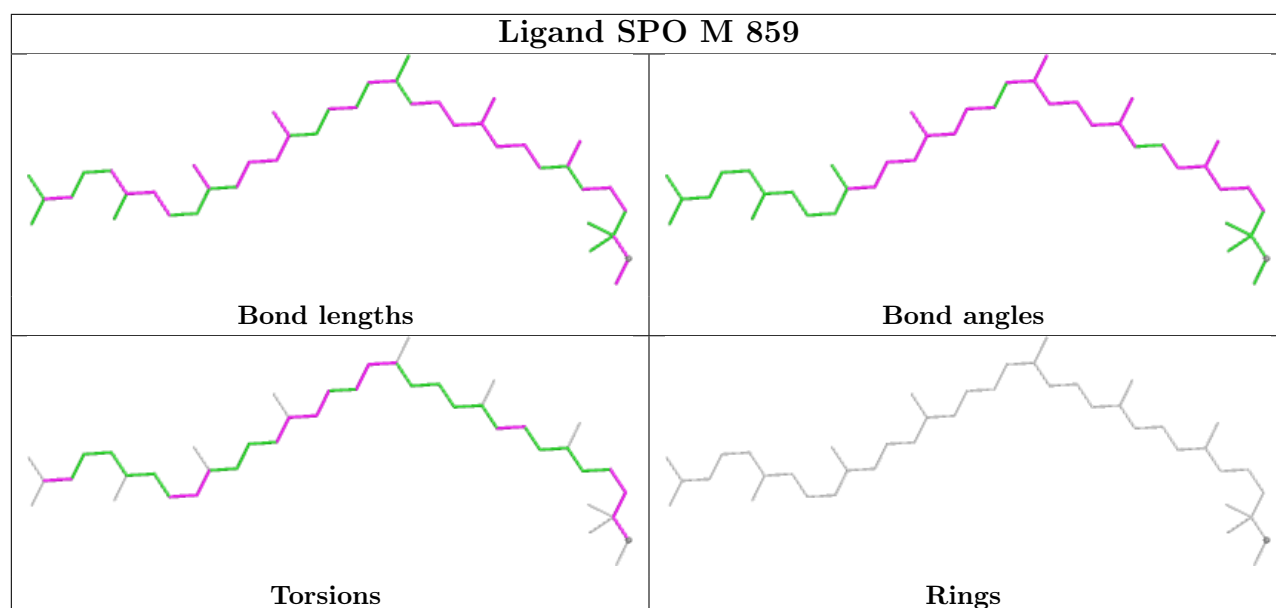
There are no ring outliers.

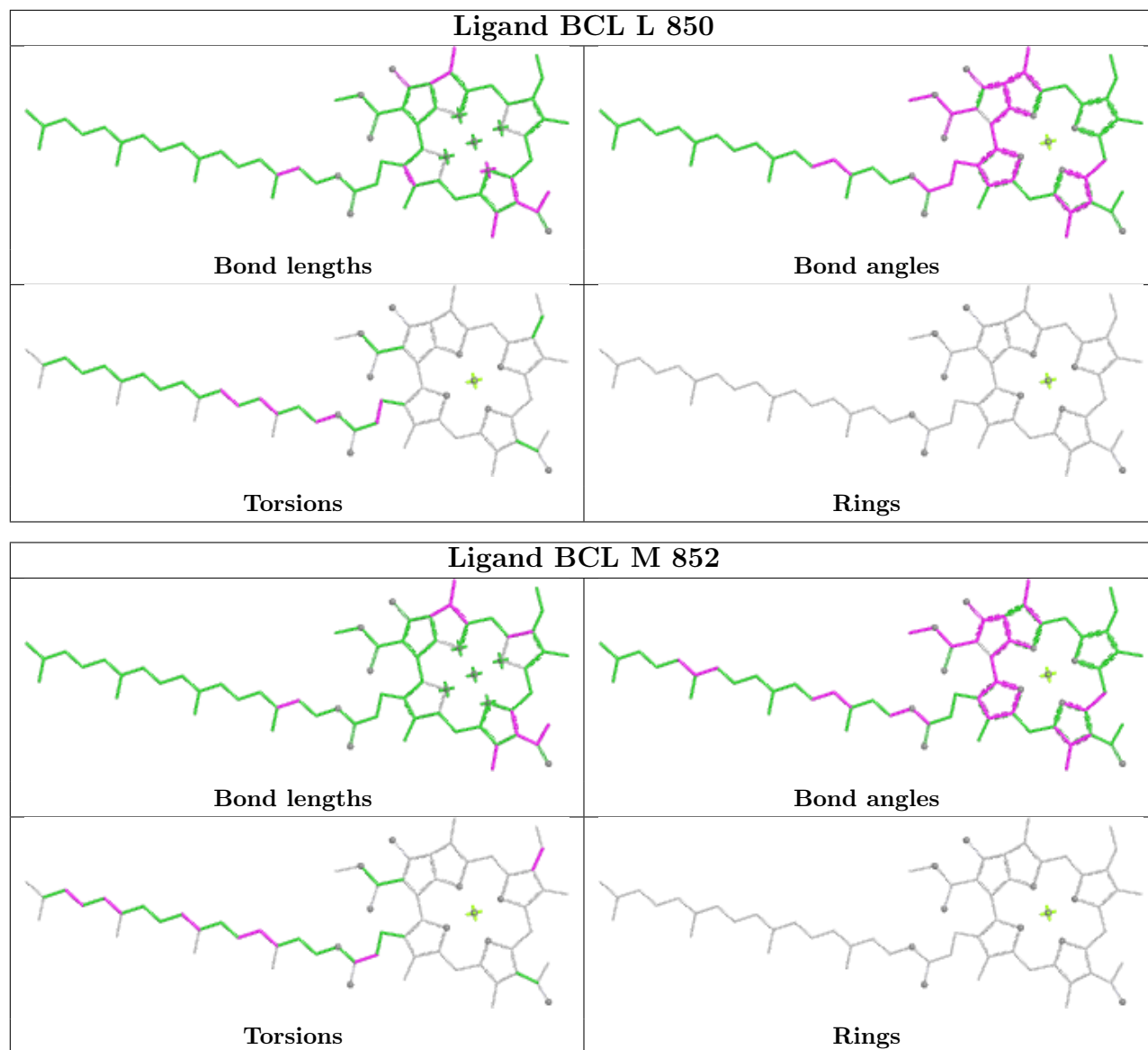
9 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	M	3000	CDL	3	0
4	L	851	BCL	5	0
8	M	859	SPO	5	0
5	M	854	BPH	3	0
4	L	850	BCL	4	0
4	M	852	BCL	4	0
5	L	855	BPH	5	0
7	M	857	U10	5	0
4	M	853	BCL	6	0

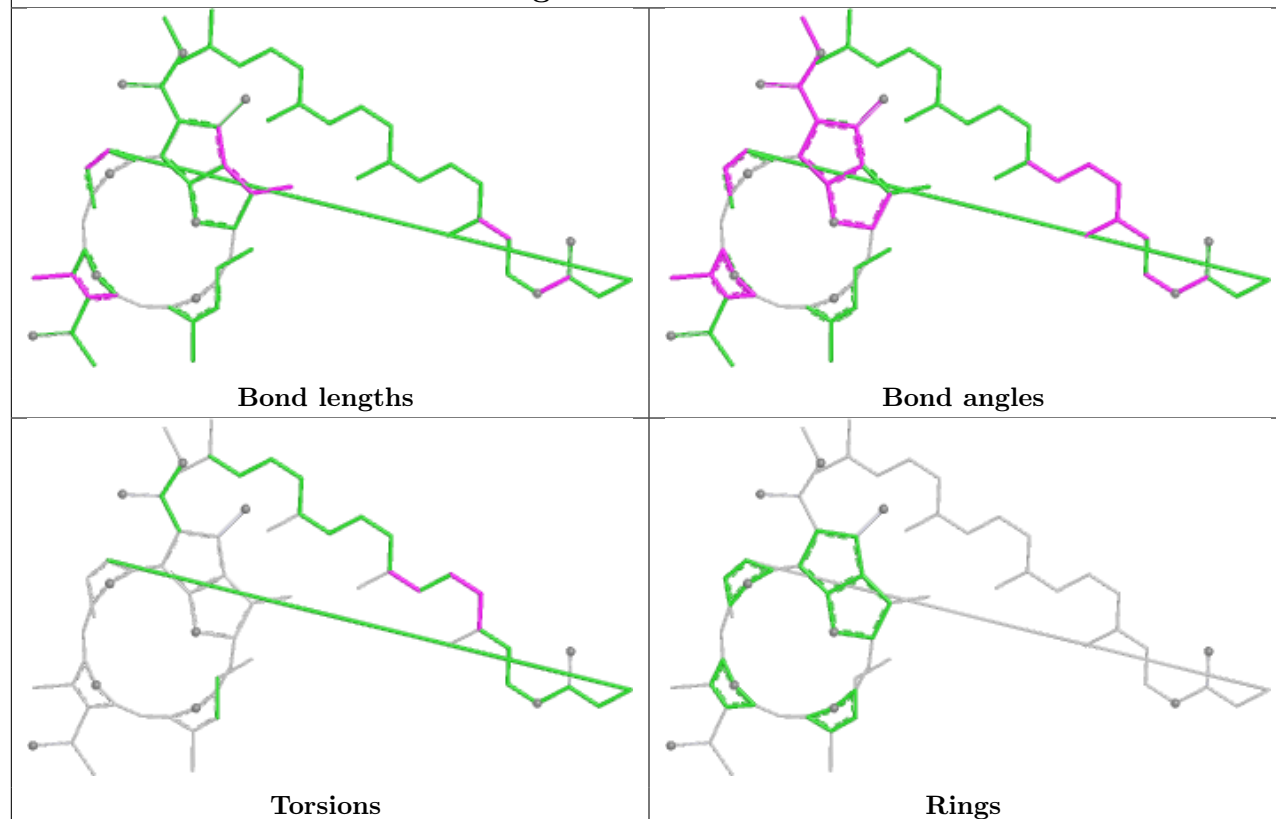
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



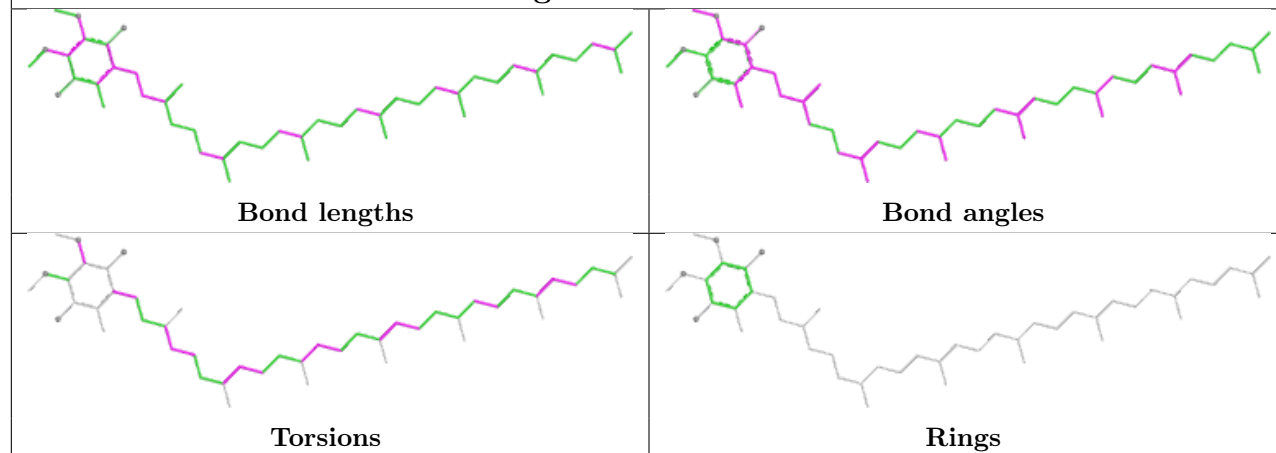


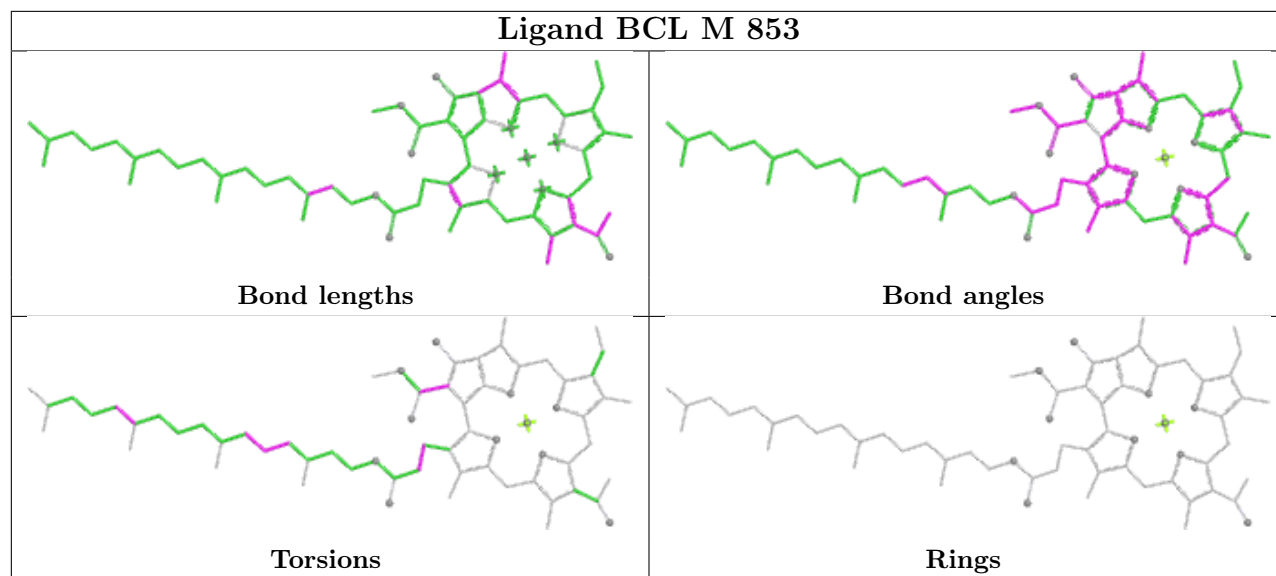


Ligand BPH L 855



Ligand U10 M 857





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.