



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:02 PM UTC

PDB ID : 1PST / pdb_00001pst
Title : CRYSTALLOGRAPHIC ANALYSES OF SITE-DIRECTED MUTANTS OF THE PHOTOSYNTHETIC REACTION CENTER FROM RHODOBACTER SPHAEROIDES
Authors : Chirino, A.J.; Feher, G.; Rees, D.C.
Deposited on : 1993-12-13
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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)
Xtrriage (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) : 2.49

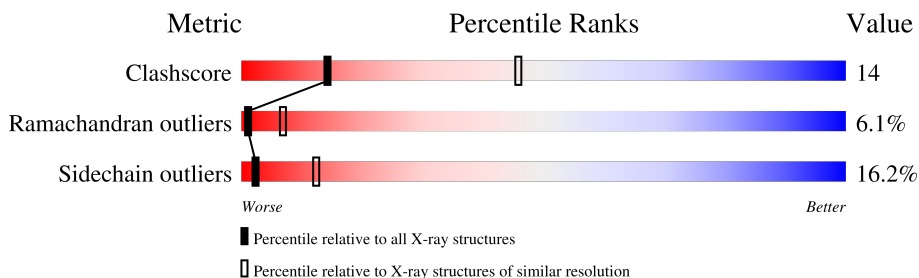
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	266	
2	M	296	
3	H	237	

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
5	BPH	M	5	X	-	-	-
8	CRT	M	304	-	X	-	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6786 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	266	2121	1433	336	344	8	0	0	0

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	M	296	2360	1579	384	387	10	0	0	0

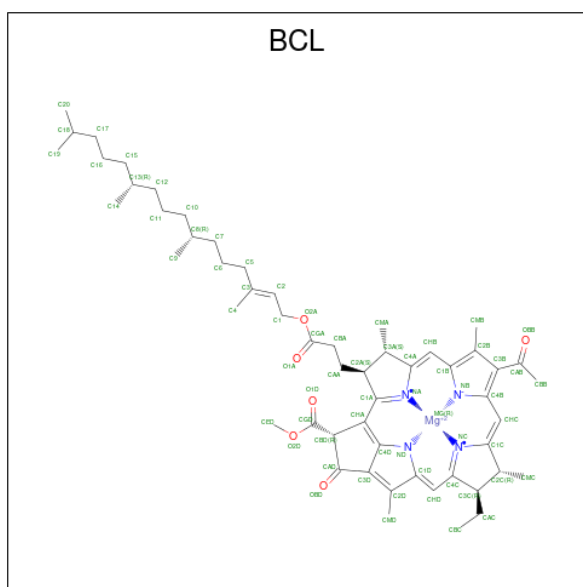
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	202	LEU	HIS	conflict	UNP P02953

- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER.

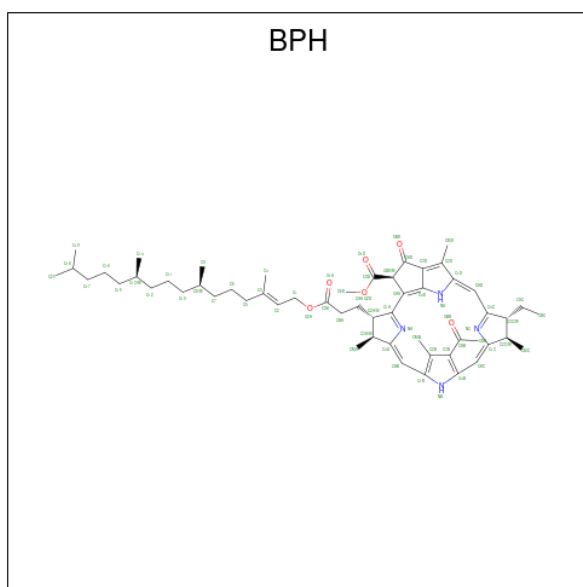
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	237	1807	1156	310	332	9	0	0	0

- Molecule 4 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	L	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		

- Molecule 5 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



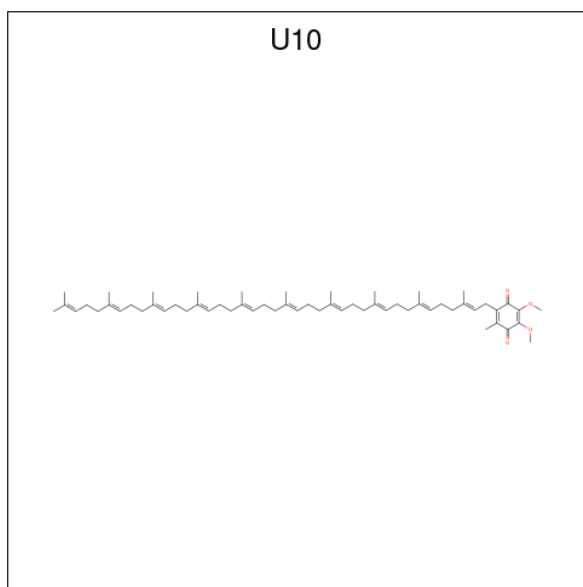
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O		
			65	55	4	6	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	M	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 UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).

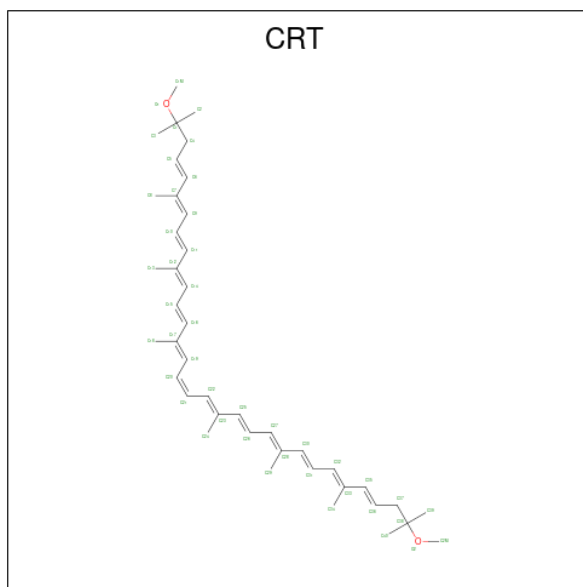


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			41	37	4		
6	M	1	Total	C	O	0	0
			51	47	4		

- Molecule 7 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 8 is SPIRILLOXANTHIN (CCD ID: CRT) (formula: $C_{42}H_{60}O_2$).



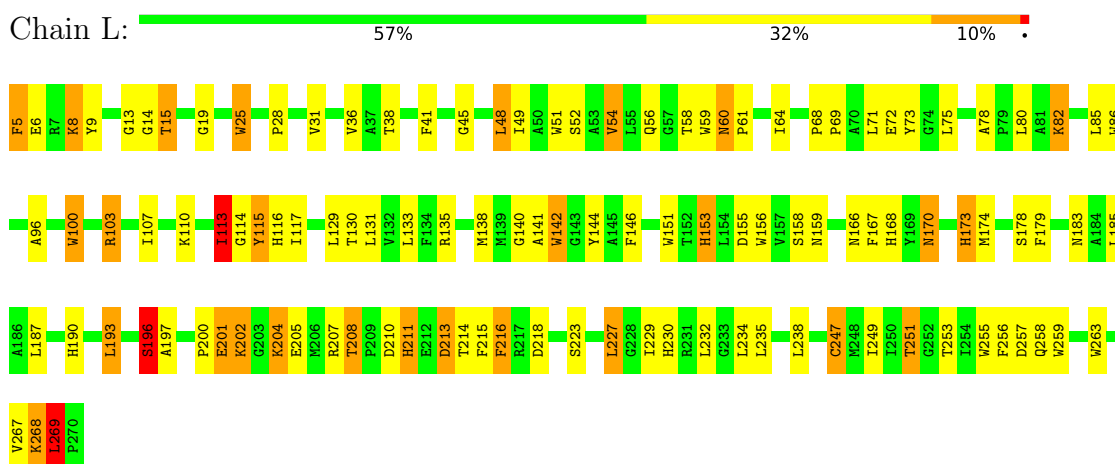
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	C	O	0	0
			42	41	1		

3 Residue-property plots [i](#)

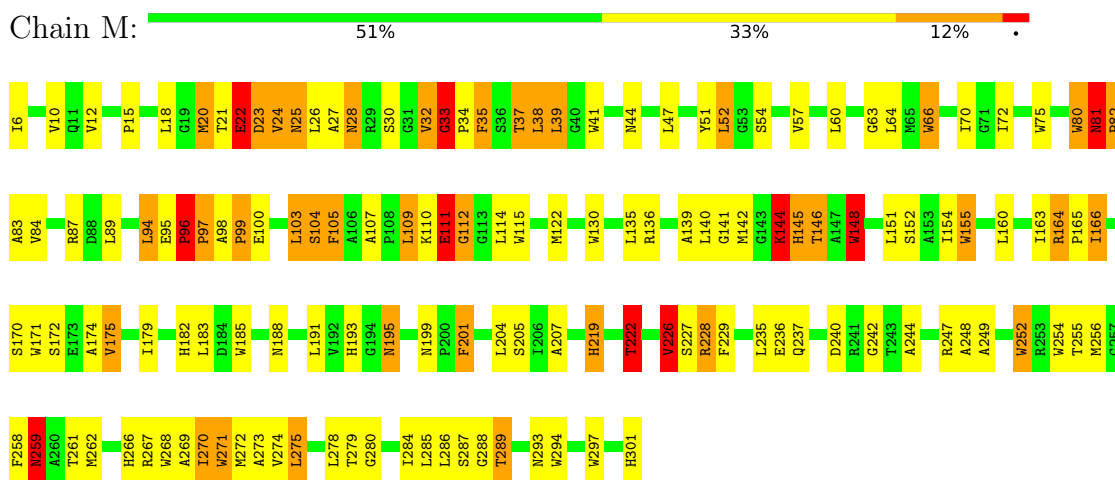
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

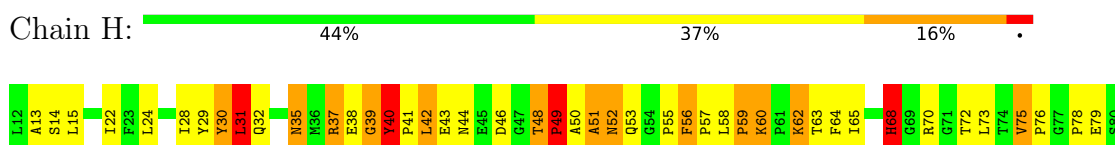
- Molecule 1: PHOTOSYNTHETIC REACTION CENTER

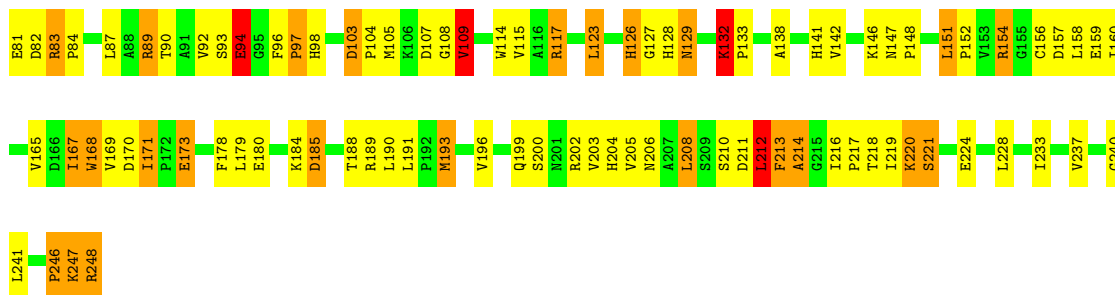


- Molecule 2: PHOTOSYNTHETIC REACTION CENTER



- Molecule 3: PHOTOSYNTHETIC REACTION CENTER





4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	138.00Å 77.50Å 141.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.218 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6786	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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, CRT, FE, BPH, 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	0.98	9/2204 (0.4%)	1.86	58/3014 (1.9%)
2	M	1.02	10/2450 (0.4%)	1.96	77/3344 (2.3%)
3	H	0.99	6/1855 (0.3%)	1.91	62/2523 (2.5%)
All	All	1.00	25/6509 (0.4%)	1.91	197/8881 (2.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1
2	M	0	2
3	H	0	4
All	All	0	7

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	116	HIS	CD2-NE2	-7.54	1.29	1.37
1	L	211	HIS	CD2-NE2	-7.21	1.29	1.37
1	L	153	HIS	CD2-NE2	-7.06	1.30	1.37
2	M	145	HIS	CD2-NE2	-7.06	1.30	1.37
2	M	193	HIS	CD2-NE2	-6.94	1.30	1.37

The worst 5 of 197 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	148	TRP	N-CA-C	-12.78	91.60	111.02
2	M	270	ILE	CB-CA-C	-11.08	97.78	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	5	PHE	CA-CB-CG	11.04	124.84	113.80
2	M	226	VAL	N-CA-CB	-10.71	98.19	112.22
2	M	270	ILE	N-CA-CB	10.59	122.94	110.55

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	40	TYR	Peptide
3	H	56	PHE	Peptide
1	L	269	LEU	Peptide
2	M	81	ASN	Peptide
2	M	96	PRO	Peptide

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	2121	0	2077	56	0
2	M	2360	0	2285	79	0
3	H	1807	0	1814	64	0
4	L	117	0	115	10	0
4	M	51	0	41	6	0
5	L	65	0	76	6	0
5	M	130	0	152	8	0
6	L	41	0	52	4	0
6	M	51	0	68	5	0
7	M	1	0	0	0	0
8	M	42	0	57	2	0
All	All	6786	0	6737	192	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 14.

The worst 5 of 192 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)
3:H:154:ARG:HD2	3:H:160:ILE:HG12	1.52	0.92
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.58	0.84
1:L:205:GLU:HA	3:H:65:ILE:HG13	1.63	0.79
2:M:261:THR:HG22	3:H:40:TYR:HD1	1.49	0.76
2:M:27:ALA:HB2	2:M:51:TYR:HD1	1.50	0.74

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	264/266 (99%)	237 (90%)	20 (8%)	7 (3%)	4	22
2	M	294/296 (99%)	242 (82%)	30 (10%)	22 (8%)	1	4
3	H	235/237 (99%)	188 (80%)	28 (12%)	19 (8%)	1	3
All	All	793/799 (99%)	667 (84%)	78 (10%)	48 (6%)	1	7

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	71	LEU
1	L	115	TYR
1	L	201	GLU
1	L	269	LEU
2	M	22	GLU

5.3.2 Protein sidechains [i](#)

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	210/210 (100%)	181 (86%)	29 (14%)	3	17
2	M	232/232 (100%)	197 (85%)	35 (15%)	3	14
3	H	192/192 (100%)	153 (80%)	39 (20%)	1	7
All	All	634/634 (100%)	531 (84%)	103 (16%)	2	12

5 of 103 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	262	MET
3	H	68	HIS
3	H	228	LEU
2	M	270	ILE
3	H	15	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
3	H	204	HIS
3	H	147	ASN
2	M	77	GLN
2	M	28	ASN
3	H	141	HIS

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 oligosaccharides 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
4	BCL	L	2	1	69,74,74	1.19	7 (10%)	79,115,115	1.82	17 (21%)
6	U10	M	303	-	51,51,63	1.60	13 (25%)	63,64,79	1.61	13 (20%)
4	BCL	M	1	2	54,59,74	1.21	4 (7%)	61,97,115	2.14	21 (34%)
4	BCL	L	4	1	54,59,74	1.32	8 (14%)	61,97,115	2.31	20 (32%)
6	U10	L	272	-	41,41,63	1.78	10 (24%)	51,52,79	1.52	12 (23%)
5	BPH	M	3	-	59,70,70	1.64	8 (13%)	59,101,101	2.55	19 (32%)
5	BPH	M	5	-	59,70,70	1.62	8 (13%)	59,101,101	2.51	19 (32%)
5	BPH	L	271	-	59,70,70	1.54	7 (11%)	59,101,101	2.64	19 (32%)
8	CRT	M	304	-	40,41,43	3.95	23 (57%)	47,50,54	3.00	17 (36%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BCL	L	2	1	-	8/41/137/137	-
6	U10	M	303	-	-	15/49/73/87	0/1/1/1
4	BCL	M	1	2	-	5/23/119/137	-
4	BCL	L	4	1	-	3/23/119/137	-
6	U10	L	272	-	-	8/37/61/87	0/1/1/1
5	BPH	M	5	-	2/2/18/22	3/37/105/105	0/5/6/6
5	BPH	M	3	-	-	10/37/105/105	0/5/6/6
5	BPH	L	271	-	-	7/37/105/105	0/5/6/6
8	CRT	M	304	-	-	26/47/47/51	-

The worst 5 of 88 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	304	CRT	C6-C5	8.47	1.55	1.32
5	M	5	BPH	C3A-C2A	-8.21	1.47	1.54
5	L	271	BPH	C3A-C2A	-7.91	1.47	1.54
8	M	304	CRT	C26-C25	7.90	1.55	1.34
8	M	304	CRT	C10-C11	7.64	1.54	1.34

The worst 5 of 157 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	271	BPH	O2D-CGD-CBD	9.32	121.19	110.95
8	M	304	CRT	C37-C36-C35	-9.20	106.03	125.93
5	M	5	BPH	C4D-CHA-CBD	-7.71	104.76	108.45
5	M	3	BPH	C4D-CHA-CBD	-7.70	104.76	108.45
5	M	3	BPH	C3D-C4D-ND	7.52	117.34	107.71

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	M	5	BPH	C8
5	M	5	BPH	C13

5 of 85 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	1	BCL	CHA-CBD-CGD-O1D
4	M	1	BCL	CHA-CBD-CGD-O2D
5	L	271	BPH	C4C-C3C-CAC-CBC
5	M	3	BPH	C2C-C3C-CAC-CBC
6	L	272	U10	C29-C31-C32-C33

There are no ring outliers.

9 monomers are involved in 35 short contacts:

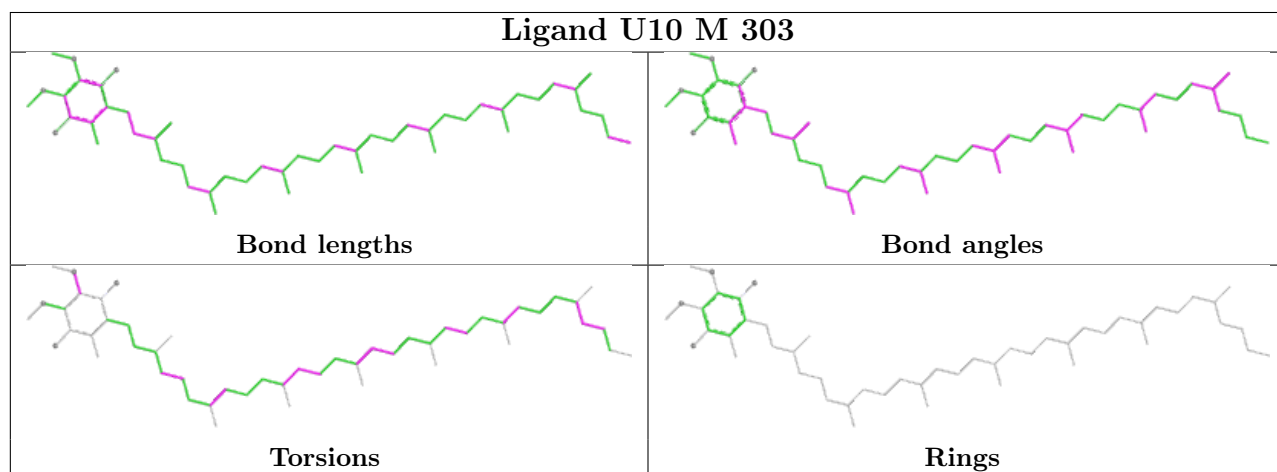
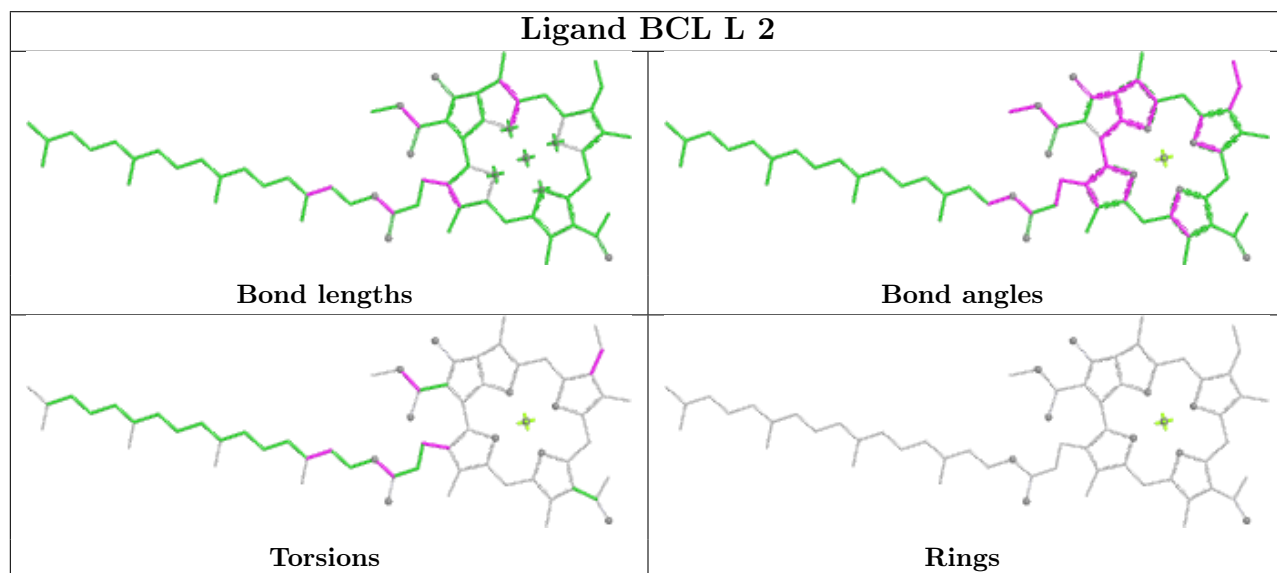
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	2	BCL	7	0
6	M	303	U10	5	0
4	M	1	BCL	6	0
4	L	4	BCL	5	0
6	L	272	U10	4	0
5	M	3	BPH	7	0
5	M	5	BPH	1	0
5	L	271	BPH	6	0

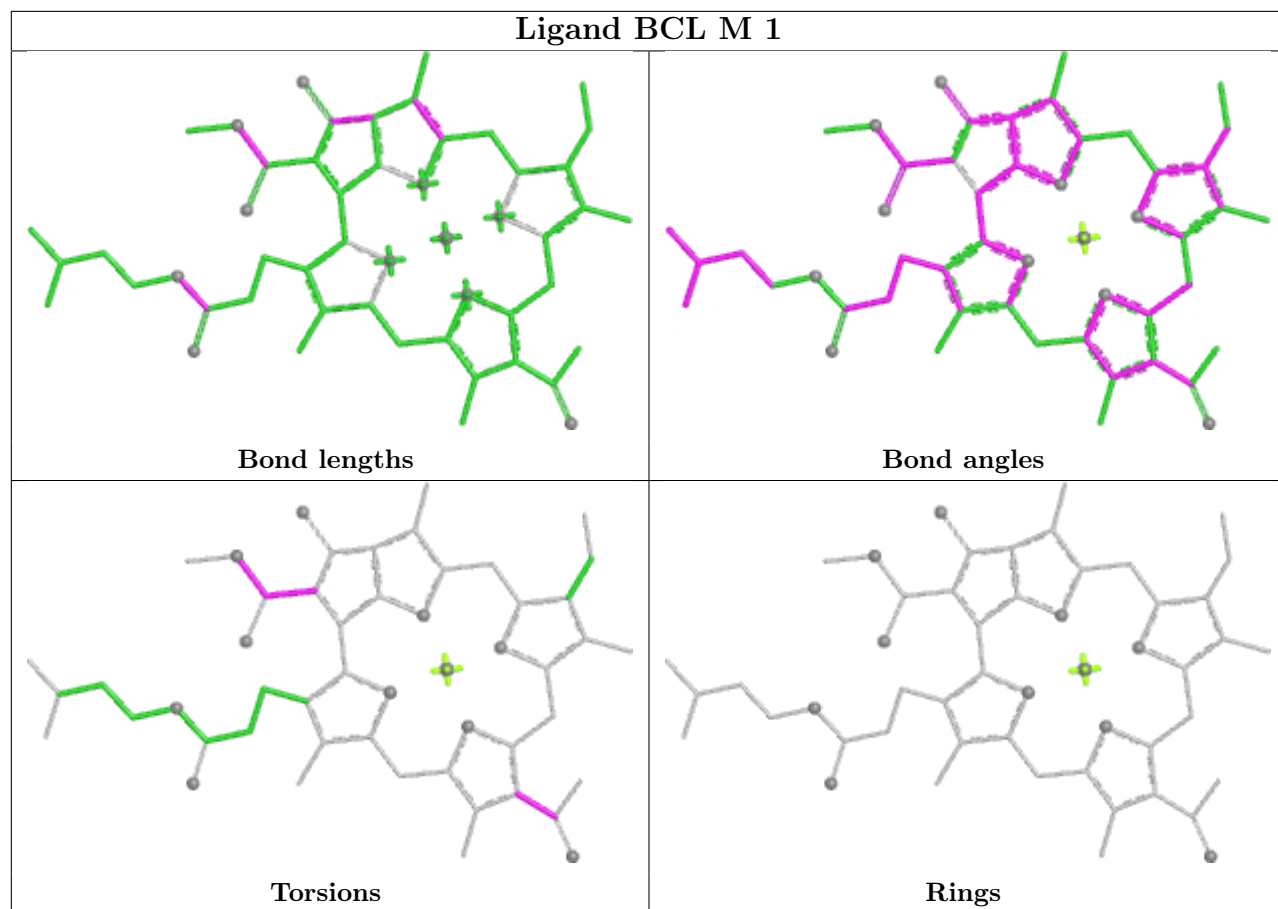
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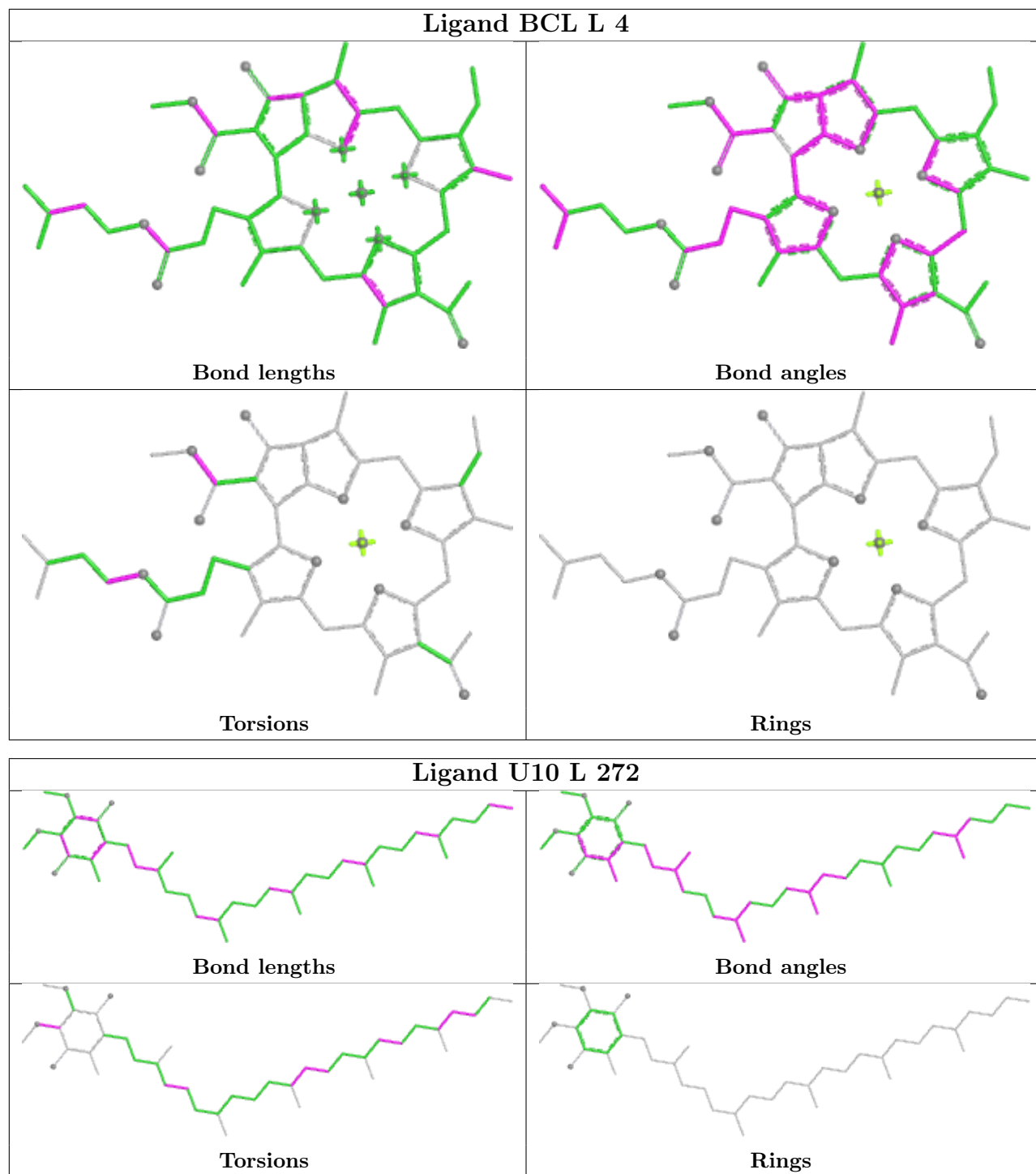
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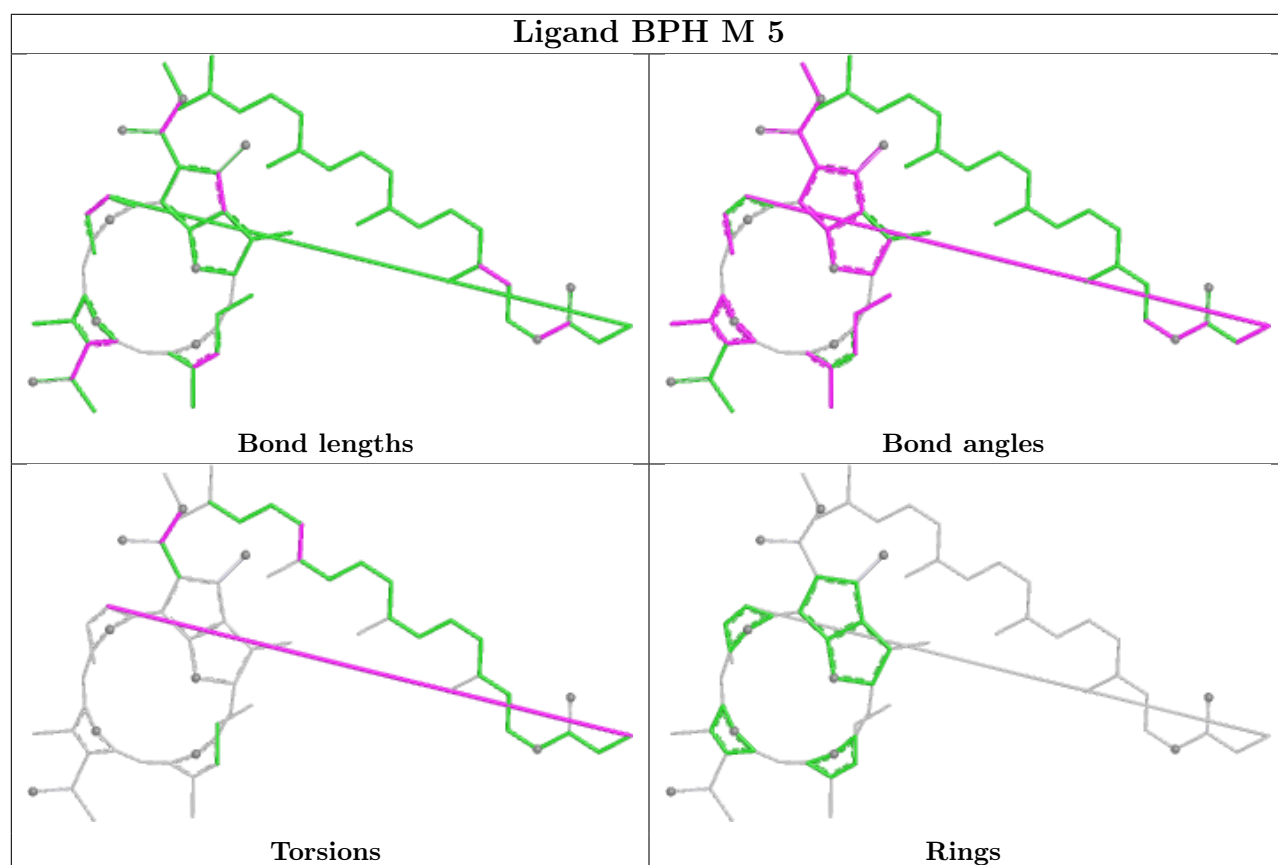
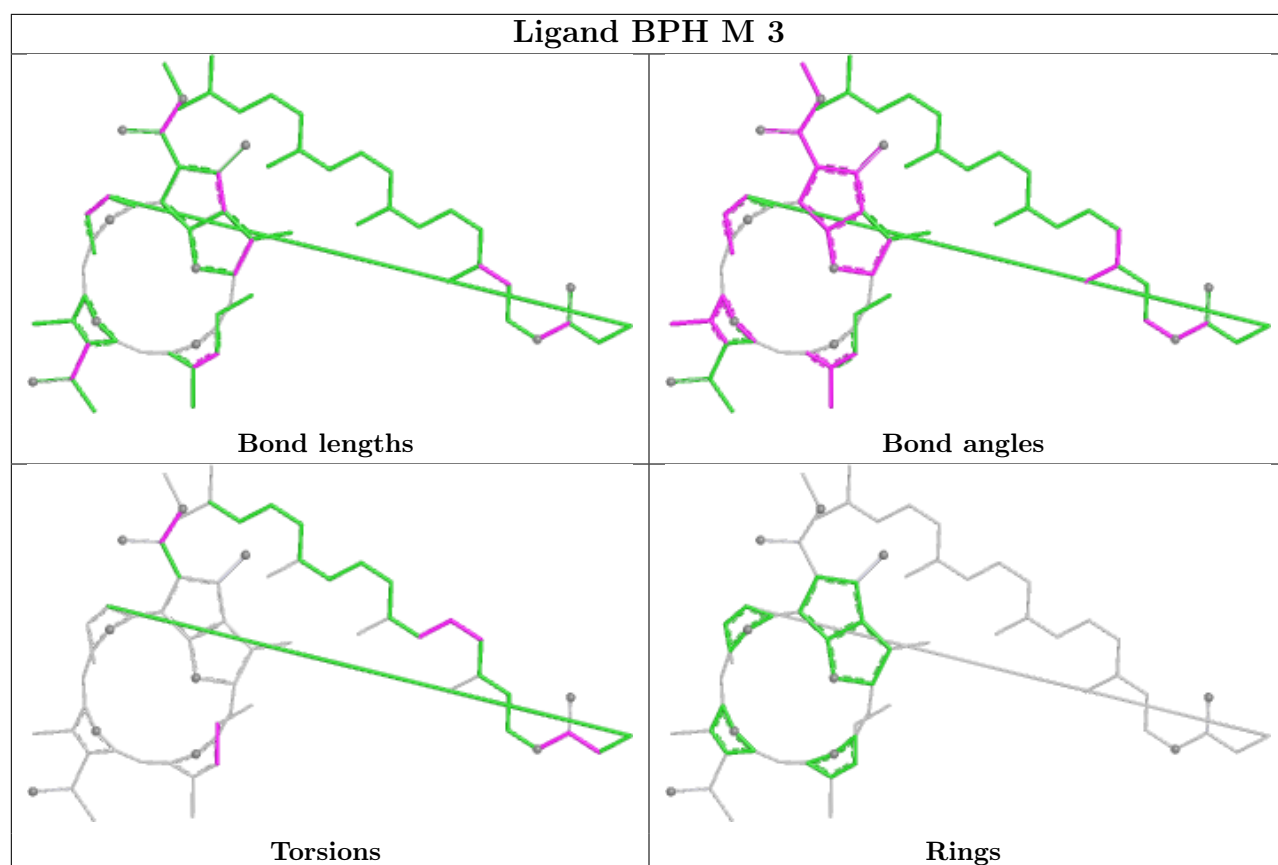
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	304	CRT	2	0

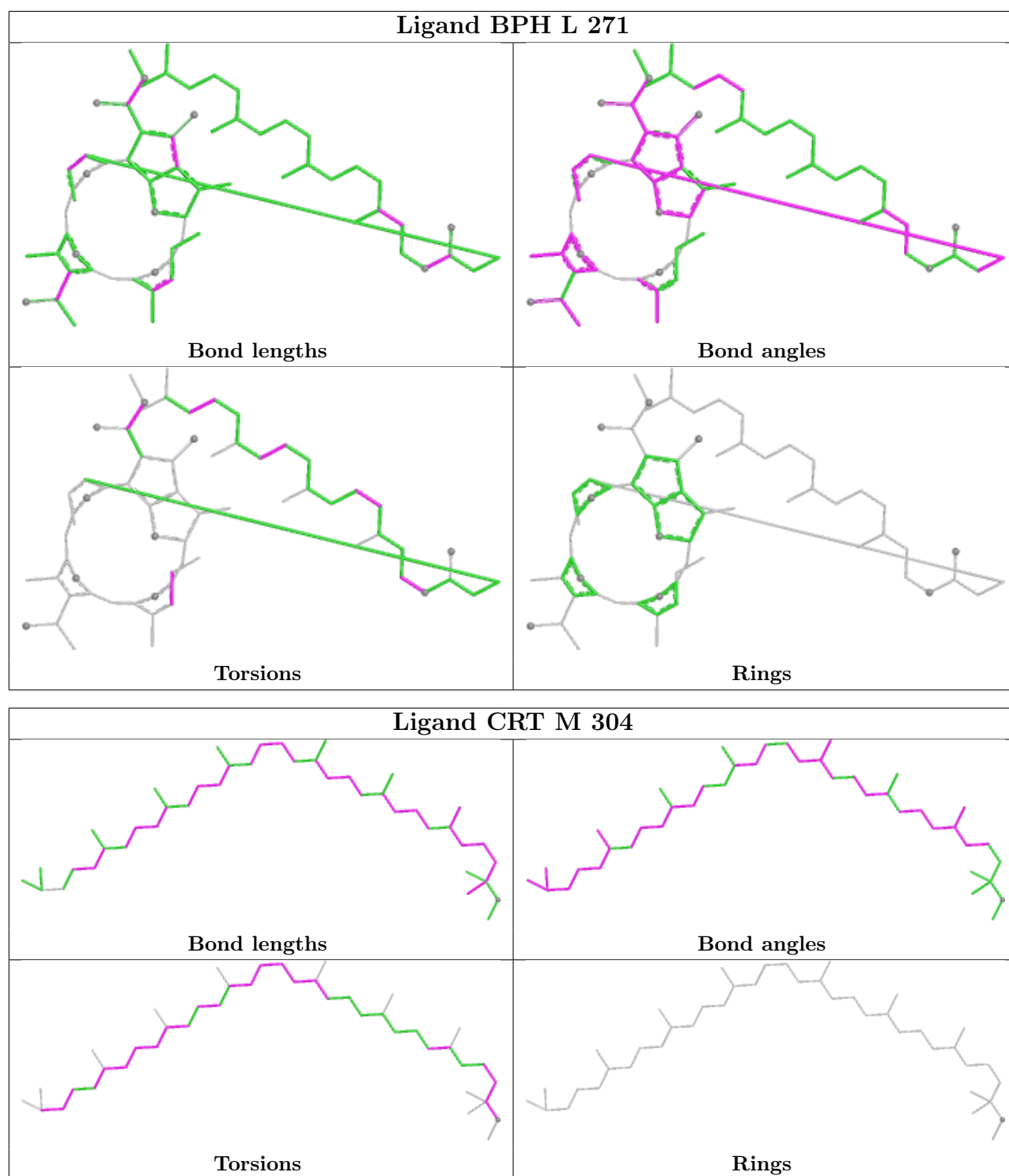
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.