



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:55 PM UTC

PDB ID : 1F6N / pdb_00001f6n
Title : CRYSTAL STRUCTURE ANALYSIS OF THE MUTANT REACTION CENTER PRO L209-> TYR FROM THE PHOTOSYNTHETIC PURPLE BACTERIUM RHODOBACTER SPHAEROIDES
Authors : Kuglstatter, A.; Ermler, U.; Michel, H.; Baciou, L.; Fritzsche, G.
Deposited on : 2000-06-22
Resolution : 2.80 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)
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)	:	2.49

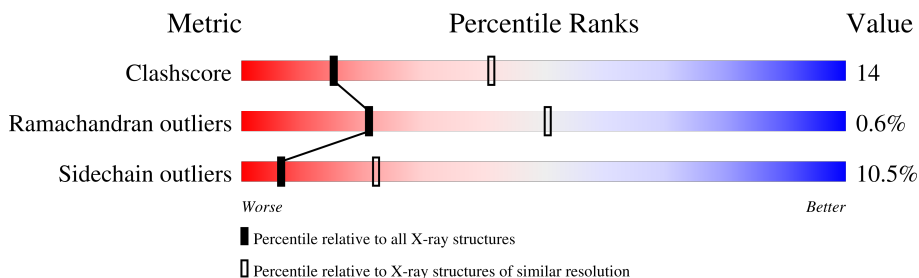
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	281	
2	M	307	
3	H	260	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BCL	L	301	X	-	-	-
4	BCL	L	304	X	-	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7186 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 REACTION CENTER PROTEIN L CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	281	Total	C	N	O	S	0	0	0
			2237	1511	355	363	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	209	TYR	PRO	engineered mutation	UNP P02954

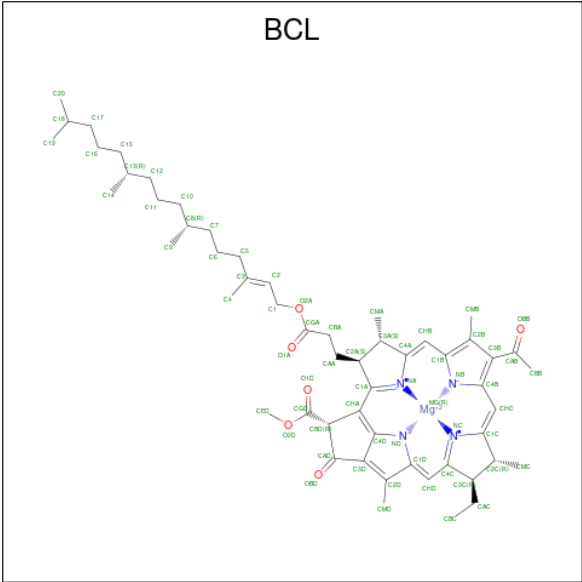
- Molecule 2 is a protein called REACTION CENTER PROTEIN M CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	0	0
			2404	1603	394	397	10			

- Molecule 3 is a protein called REACTION CENTER PROTEIN H CHAIN.

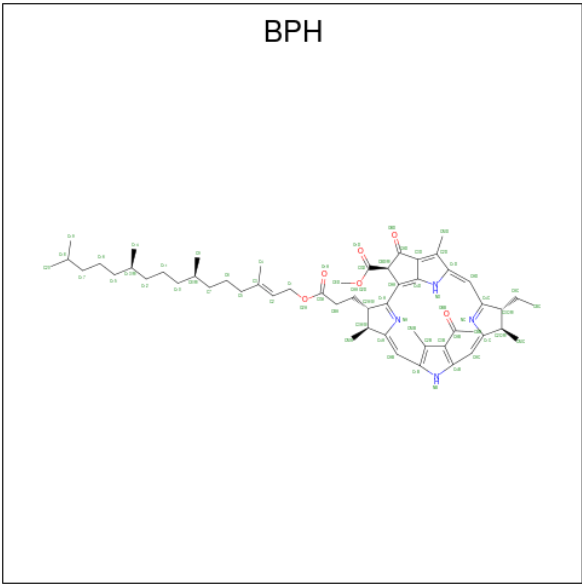
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	240	Total	C	N	O	S	0	0	0
			1829	1169	314	337	9			

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



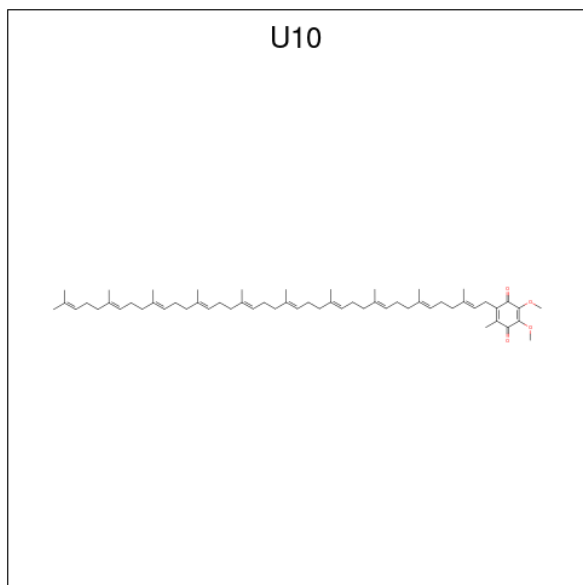
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 5 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: C₅₅H₇₆N₄O₆).



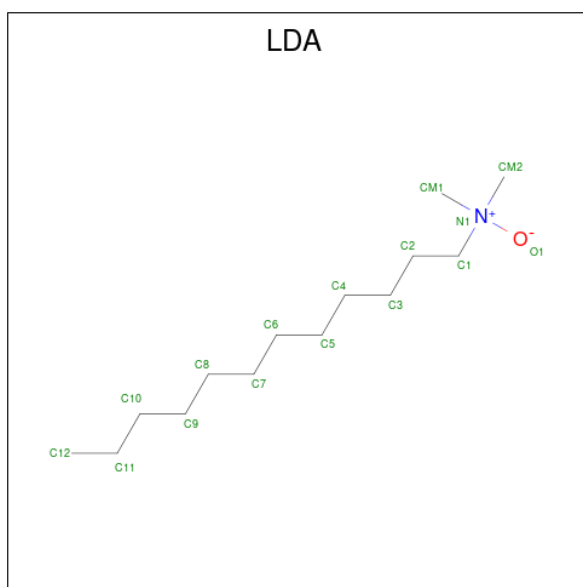
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 6 is 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
			48	44	4		
6	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 7 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: $C_{14}H_{31}NO$).

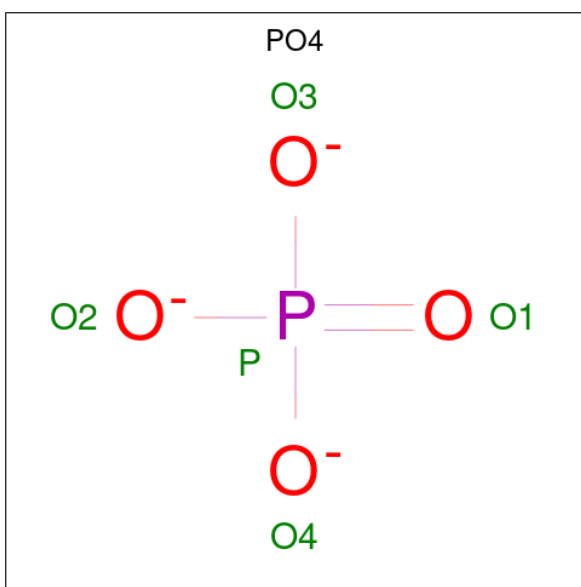


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			16	14	1	1		
7	M	1	Total	C	N	O	0	0
			16	14	1	1		
7	M	1	Total	C	N	O	0	0
			16	14	1	1		
7	H	1	Total	C	N	O	0	0
			16	14	1	1		
7	H	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 8 is FE (III) ION (CCD ID: FE) (formula: Fe).

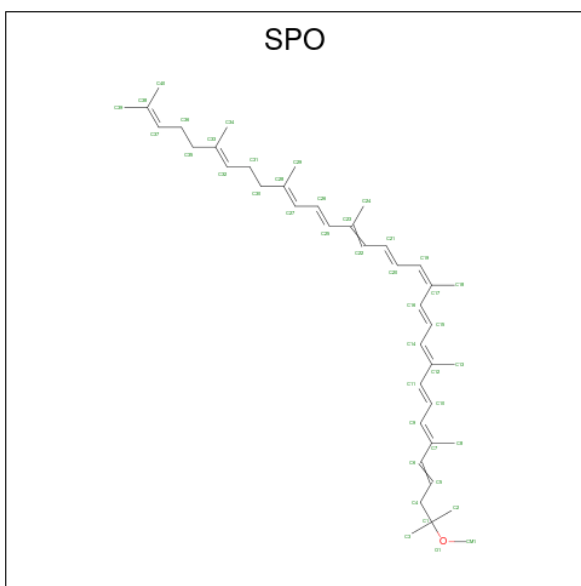
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	1	Total	Fe	0	0
			1	1		

- Molecule 9 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	O	P	0	0
			5	4	1		

- Molecule 10 is SPHEROIDENE (CCD ID: SPO) (formula: $C_{41}H_{60}O$).



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

- Molecule 11 is water.

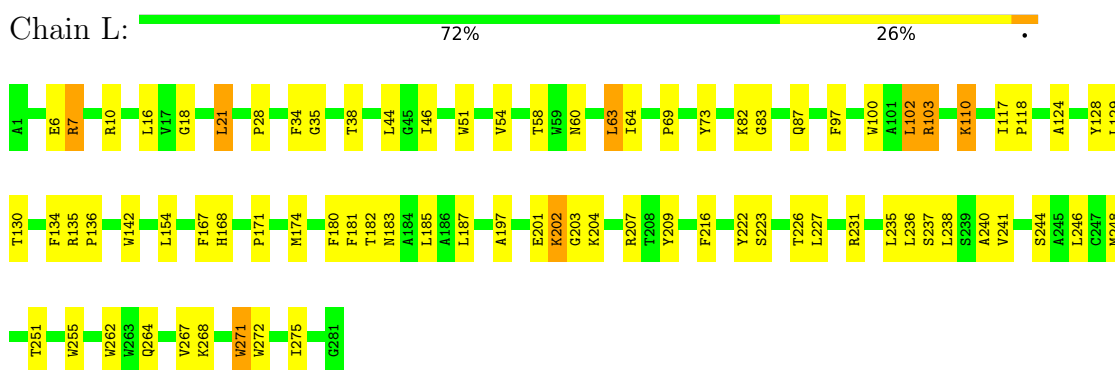
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	L	22	Total 22	O 22	0	0
11	M	27	Total 27	O 27	0	0
11	H	49	Total 49	O 49	0	0

3 Residue-property plots

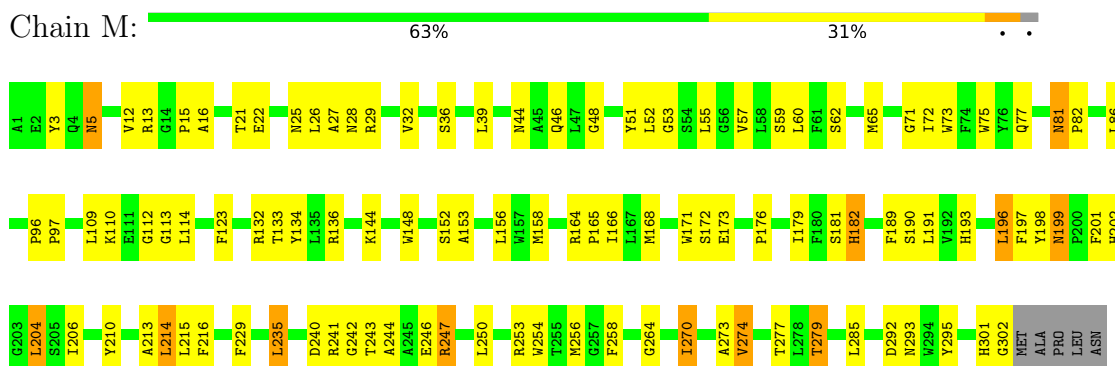
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

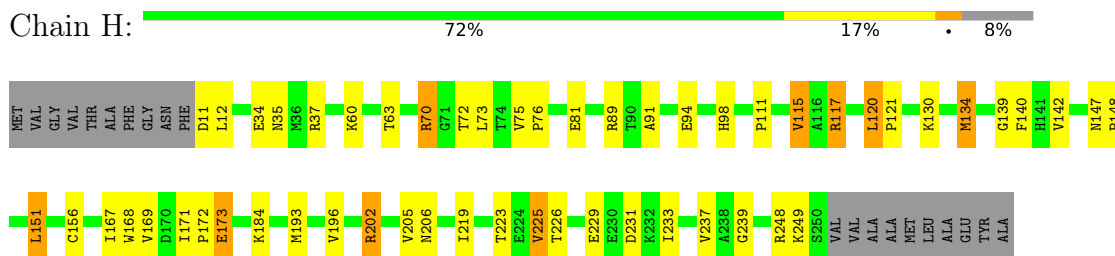
• Molecule 1: REACTION CENTER PROTEIN L CHAIN



• Molecule 2: REACTION CENTER PROTEIN M CHAIN



• Molecule 3: REACTION CENTER PROTEIN H CHAIN



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	141.53Å 141.53Å 187.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80	Depositor
% Data completeness (in resolution range)	93.1 (50.00-2.80)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.221 , 0.250	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7186	wwPDB-VP
Average B, all atoms (Å ²)	68.0	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: SPO, FE, PO4, LDA, BCL, BPH, U10

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	L	0.56	0/2325	0.80	0/3181
2	M	0.56	0/2496	0.83	2/3407 (0.1%)
3	H	0.50	0/1877	0.85	0/2553
All	All	0.54	0/6698	0.83	2/9141 (0.0%)

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	3
2	M	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	81	ASN	CA-C-N	5.54	125.89	119.47
2	M	81	ASN	C-N-CA	5.54	125.89	119.47

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	103	ARG	Sidechain
1	L	216	PHE	Sidechain
1	L	73	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	M	198	TYR	Sidechain

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	2237	0	2189	62	0
2	M	2404	0	2311	73	0
3	H	1829	0	1836	42	0
4	L	198	0	221	30	0
4	M	66	0	74	14	0
5	L	65	0	76	9	0
5	M	65	0	76	11	0
6	L	48	0	63	0	0
6	M	48	0	63	1	0
7	H	32	0	62	1	0
7	L	16	0	31	3	0
7	M	32	0	62	0	0
8	M	1	0	0	0	0
9	M	5	0	0	0	0
10	M	42	0	60	4	0
11	H	49	0	0	2	0
11	L	22	0	0	4	0
11	M	27	0	0	1	0
All	All	7186	0	7124	193	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 193 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)
4:L:301:BCL:HBB2	4:L:301:BCL:HHC	1.40	1.02
5:L:402:BPH:HHC	5:L:402:BPH:HBB3	1.42	1.01
4:L:302:BCL:HHC	4:L:302:BCL:HBB3	1.49	0.93
2:M:153:ALA:HB2	5:M:401:BPH:HAC1	1.50	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:272:TRP:HA	1:L:275:ILE:HD13	1.59	0.83

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%)	263 (94%)	15 (5%)	1 (0%)	30	60
2	M	300/307 (98%)	283 (94%)	13 (4%)	4 (1%)	9	31
3	H	238/260 (92%)	228 (96%)	10 (4%)	0	100	100
All	All	817/848 (96%)	774 (95%)	38 (5%)	5 (1%)	21	51

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	113	GLY
2	M	301	HIS
1	L	202	LYS
2	M	5	ASN
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	220/220 (100%)	200 (91%)	20 (9%)	9	28
2	M	235/240 (98%)	205 (87%)	30 (13%)	4	15
3	H	195/208 (94%)	177 (91%)	18 (9%)	8	27
All	All	650/668 (97%)	582 (90%)	68 (10%)	6	22

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	120	LEU
3	H	151	LEU
3	H	225	VAL
2	M	60	LEU
2	M	59	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	193	HIS
2	M	199	ASN
3	H	206	ASN
3	H	98	HIS
3	H	128	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 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 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	304	1	69,74,74	2.03	11 (15%)	79,115,115	3.33	17 (21%)
5	BPH	M	401	-	59,70,70	1.89	13 (22%)	59,101,101	2.39	14 (23%)
7	LDA	H	705	-	13,15,15	2.28	2 (15%)	14,17,17	0.46	0
6	U10	M	501	-	48,48,63	2.16	15 (31%)	60,61,79	1.03	4 (6%)
5	BPH	L	402	-	59,70,70	1.72	9 (15%)	59,101,101	2.38	11 (18%)
7	LDA	L	703	-	13,15,15	2.11	1 (7%)	14,17,17	0.59	0
7	LDA	H	702	-	13,15,15	2.87	2 (15%)	14,17,17	0.57	0
10	SPO	M	600	-	41,41,41	2.99	20 (48%)	47,50,50	2.33	14 (29%)
4	BCL	L	301	2	69,74,74	1.33	7 (10%)	79,115,115	1.89	9 (11%)
7	LDA	M	704	-	13,15,15	2.55	2 (15%)	14,17,17	0.54	0
4	BCL	M	801	2	69,74,74	1.25	7 (10%)	79,115,115	1.88	12 (15%)
6	U10	L	502	-	48,48,63	1.84	16 (33%)	60,61,79	1.15	6 (10%)
7	LDA	M	701	-	13,15,15	2.35	2 (15%)	14,17,17	0.48	0
9	PO4	M	800	-	4,4,4	1.99	1 (25%)	6,6,6	0.54	0
4	BCL	L	302	1	69,74,74	1.39	9 (13%)	79,115,115	1.75	8 (10%)

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	304	1	1/1/21/25	16/41/137/137	-
5	BPH	M	401	-	-	19/37/105/105	0/5/6/6
7	LDA	H	705	-	-	4/13/13/13	-
6	U10	M	501	-	-	4/45/69/87	0/1/1/1
5	BPH	L	402	-	-	7/37/105/105	0/5/6/6
7	LDA	L	703	-	-	2/13/13/13	-
7	LDA	H	702	-	-	5/13/13/13	-
10	SPO	M	600	-	-	19/47/47/47	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BCL	L	301	2	1/1/21/25	9/41/137/137	-
7	LDA	M	704	-	-	1/13/13/13	-
4	BCL	M	801	2	-	7/41/137/137	-
6	U10	L	502	-	-	12/45/69/87	0/1/1/1
7	LDA	M	701	-	-	2/13/13/13	-
4	BCL	L	302	1	-	8/41/137/137	-

The worst 5 of 117 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	304	BCL	MG-NA	9.71	2.29	2.06
7	H	702	LDA	O1-N1	-8.54	1.21	1.42
10	M	600	SPO	C6-C5	8.06	1.54	1.32
10	M	600	SPO	C10-C11	7.89	1.55	1.34
7	M	701	LDA	O1-N1	-7.72	1.23	1.42

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	304	BCL	CHB-C4A-NA	-15.84	101.53	124.40
4	L	304	BCL	CHB-C1B-NB	-13.71	103.48	124.05
5	L	402	BPH	O2D-CGD-CBD	12.37	124.53	110.95
5	M	401	BPH	O2D-CGD-CBD	11.71	123.82	110.95
4	L	304	BCL	C4A-NA-C1A	8.88	110.73	106.68

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	L	301	BCL	C8
4	L	304	BCL	C13

5 of 115 torsion outliers are listed below:

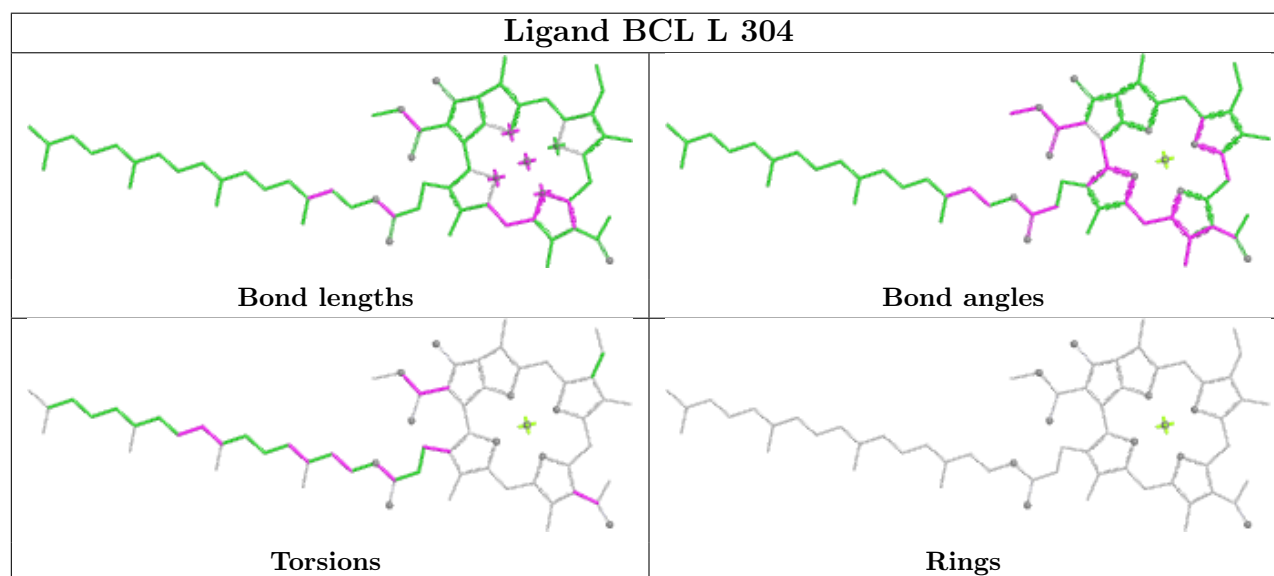
Mol	Chain	Res	Type	Atoms
4	L	301	BCL	CHA-CBD-CGD-O1D
4	L	301	BCL	CHA-CBD-CGD-O2D
4	L	304	BCL	CBD-CGD-O2D-CED
4	L	304	BCL	O2A-C1-C2-C3
4	L	304	BCL	C11-C10-C8-C9

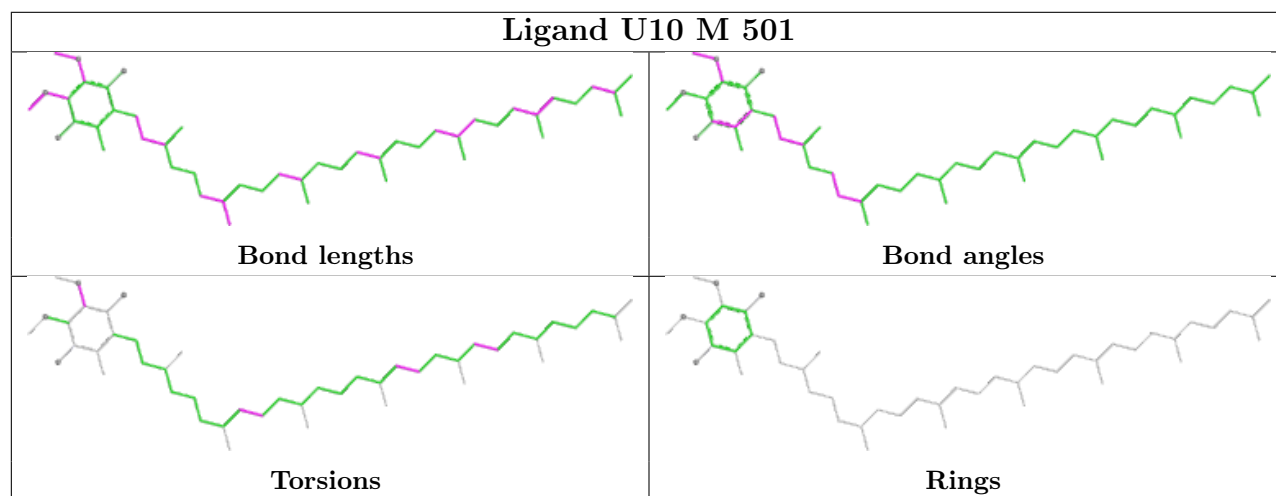
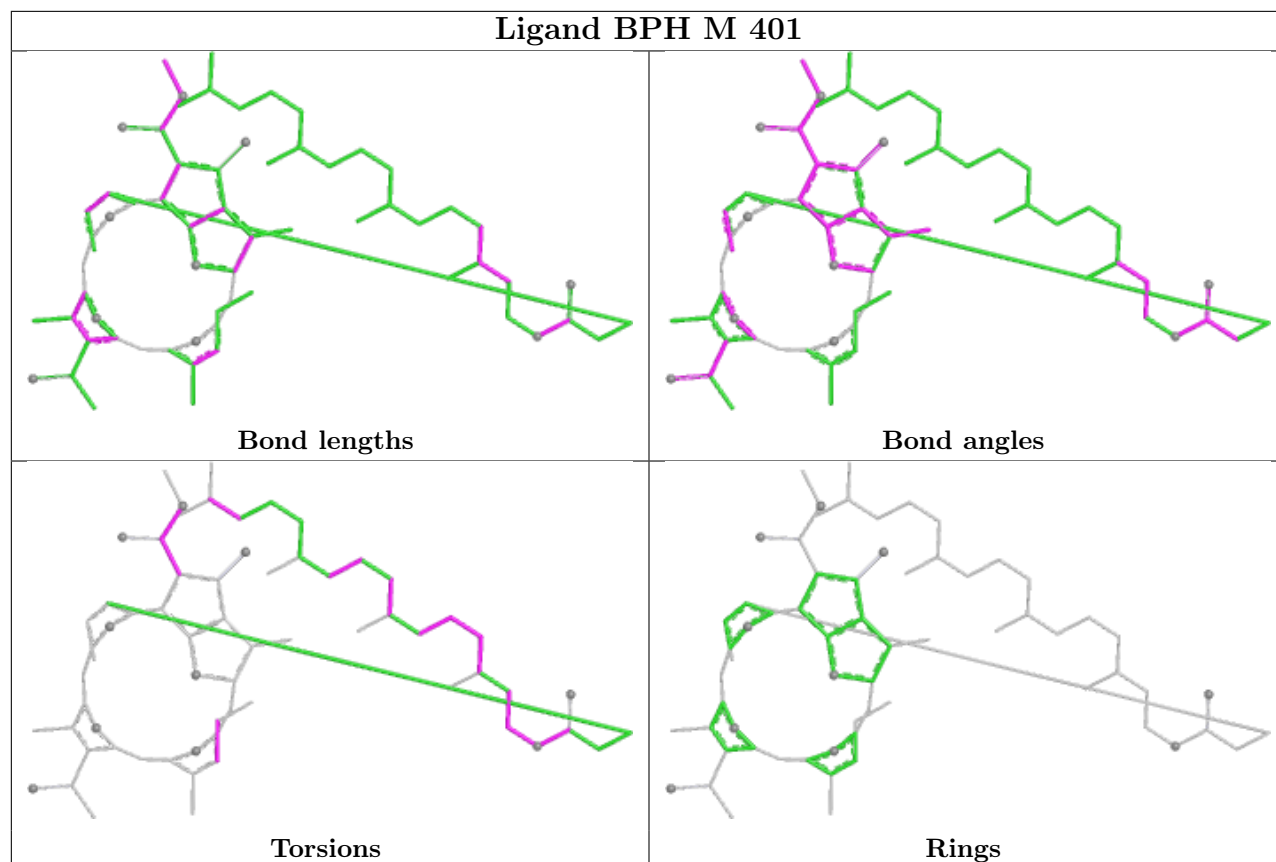
There are no ring outliers.

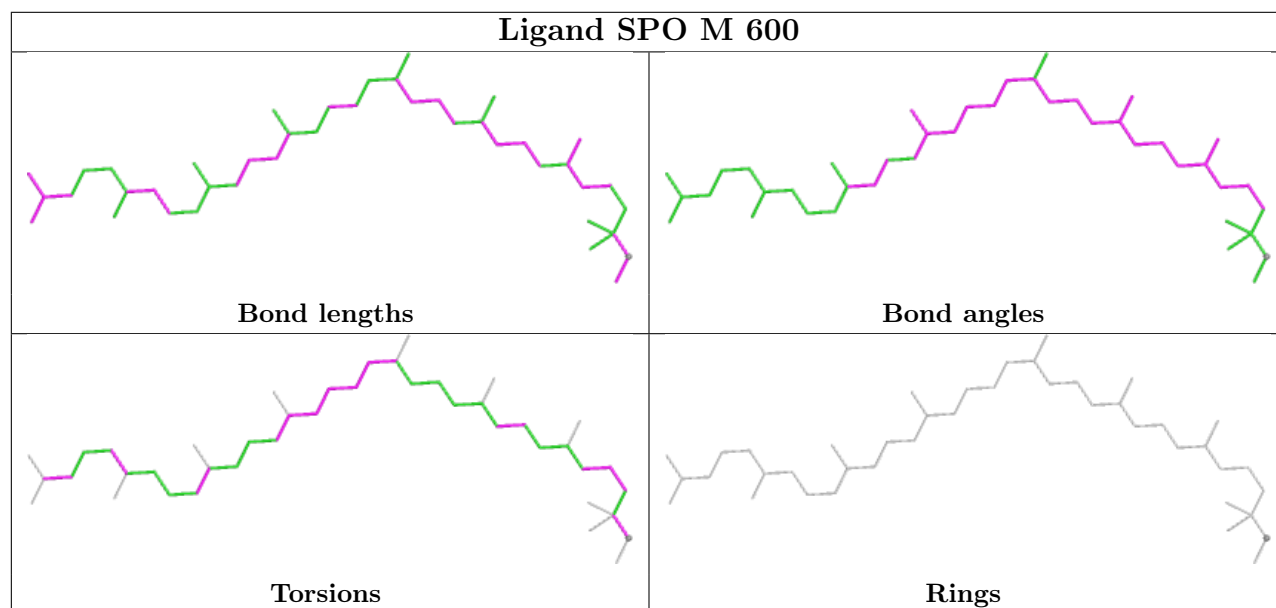
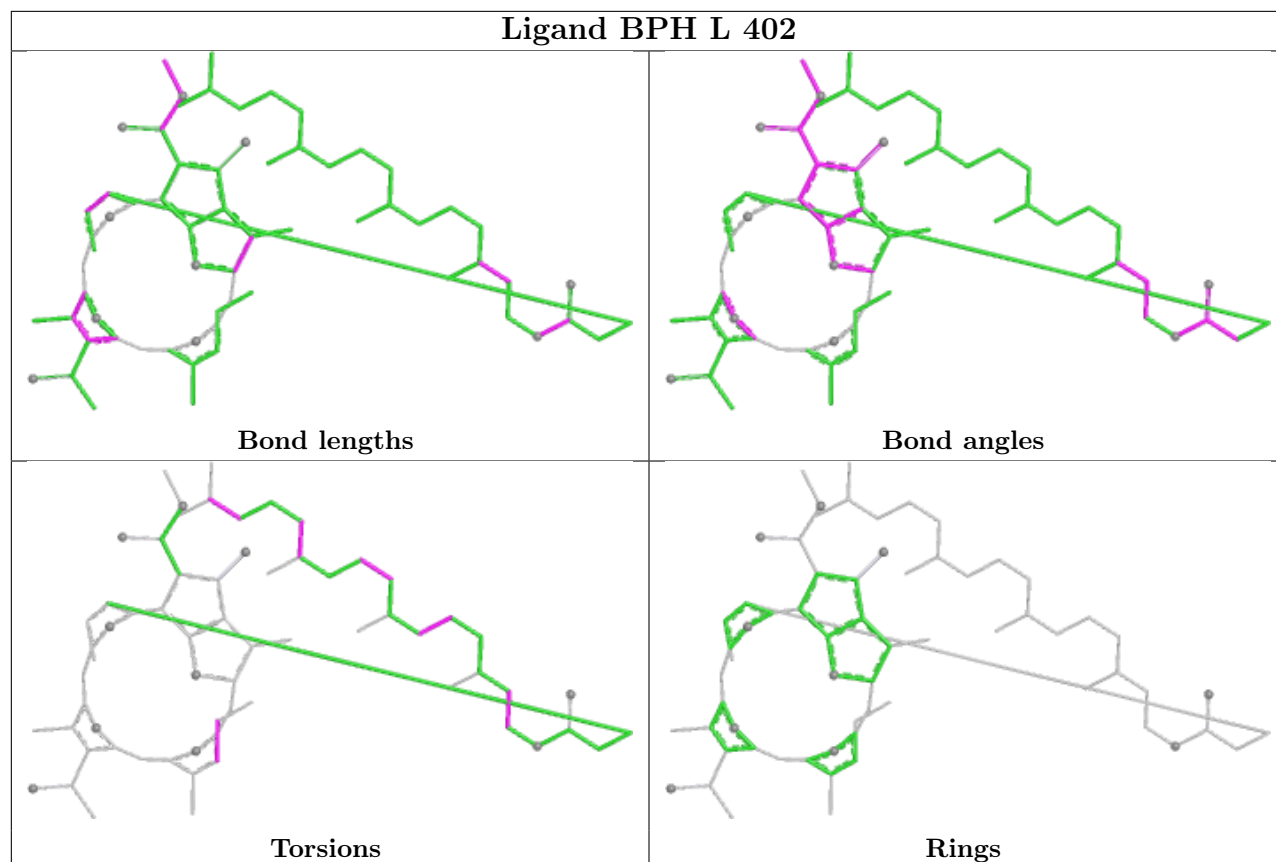
10 monomers are involved in 63 short contacts:

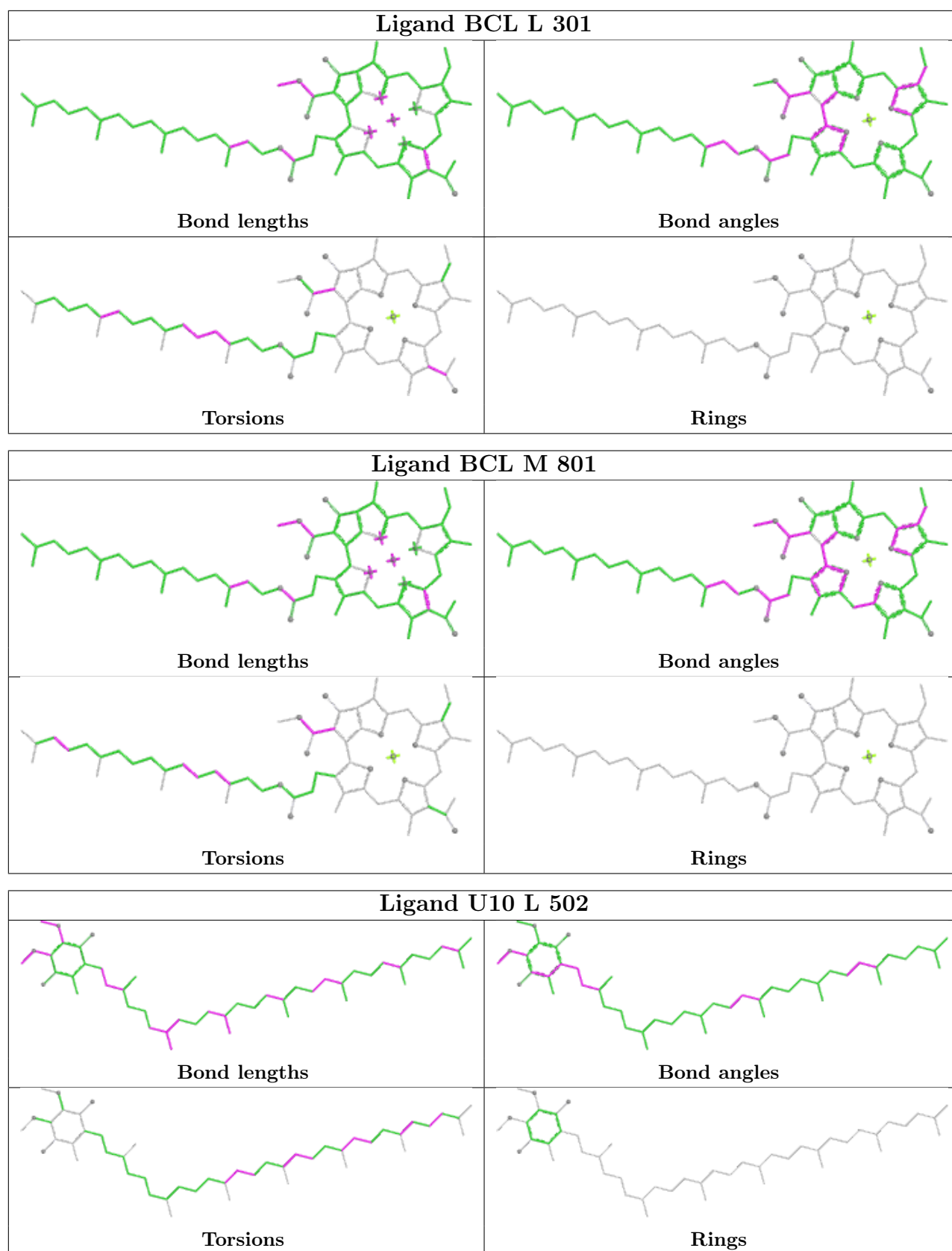
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	304	BCL	7	0
5	M	401	BPH	11	0
6	M	501	U10	1	0
5	L	402	BPH	9	0
7	L	703	LDA	3	0
7	H	702	LDA	1	0
10	M	600	SPO	4	0
4	L	301	BCL	12	0
4	M	801	BCL	14	0
4	L	302	BCL	12	0

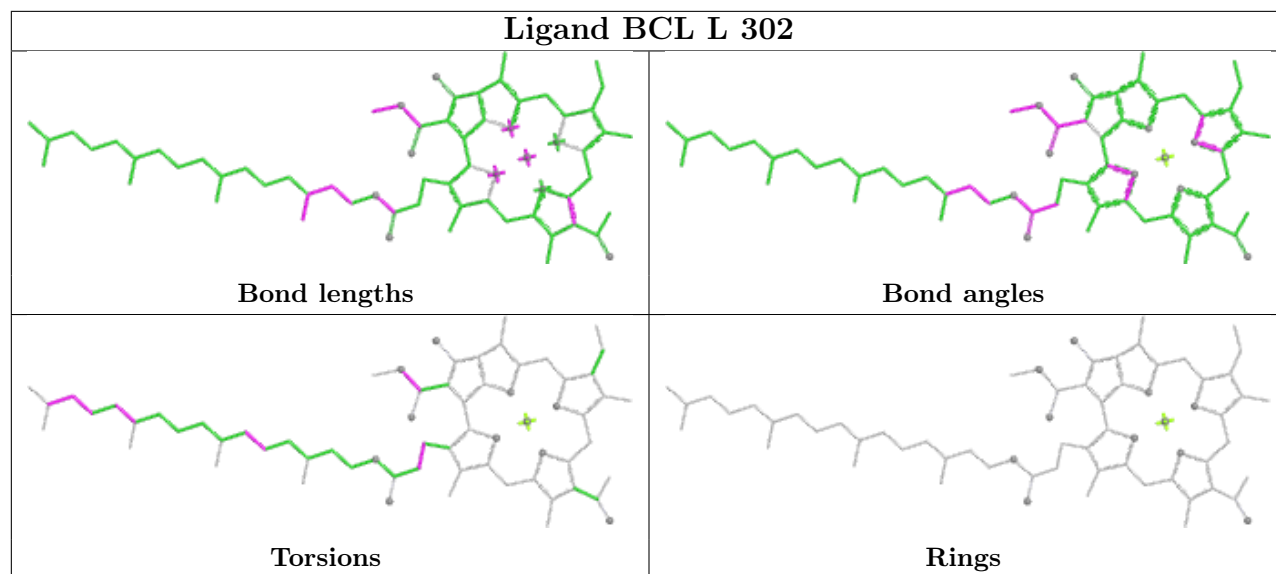
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.