



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 27, 2024 – 11:38 AM EST

PDB ID : 1AIG
Title : PHOTOSYNTHETIC REACTION CENTER FROM RHODOBACTER SPHAEROIDES IN THE D+QB-CHARGE SEPARATED STATE
Authors : Stowell, M.H.B.; Mcphillips, T.M.; Soltis, S.M.; Rees, D.C.; Abresch, E.; Feher, G.
Deposited on : 1997-04-17
Resolution : 2.60 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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) : 2.36

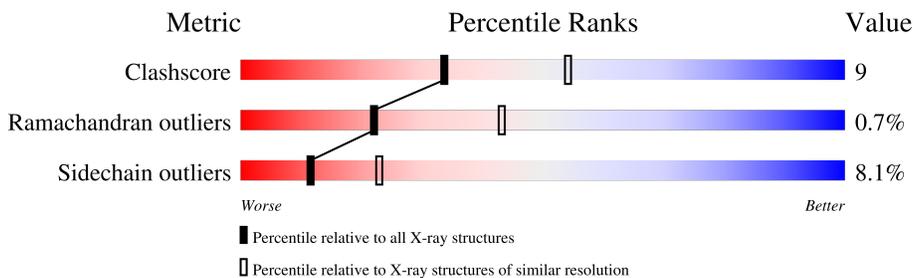
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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	
1	N	281	
2	M	307	
2	O	307	
3	H	260	
3	P	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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BCL	M	309	X	-	-	-
4	BCL	M	310	X	-	-	-
4	BCL	N	282	X	-	-	-
4	BCL	O	309	X	-	-	-
5	BPH	L	284	X	-	-	-
5	BPH	L	285	X	-	-	-
5	BPH	N	285	X	-	-	-
5	BPH	O	310	X	-	-	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 14138 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
			Total	C	N	O	S			
1	L	281	Total	C	N	O	S	0	0	0
			2232	1507	355	362	8			
1	N	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
			Total	C	N	O	S			
2	M	299	Total	C	N	O	S	0	0	0
			2390	1597	391	392	10			
2	O	299	Total	C	N	O	S	0	0	0
			2390	1597	391	392	10			

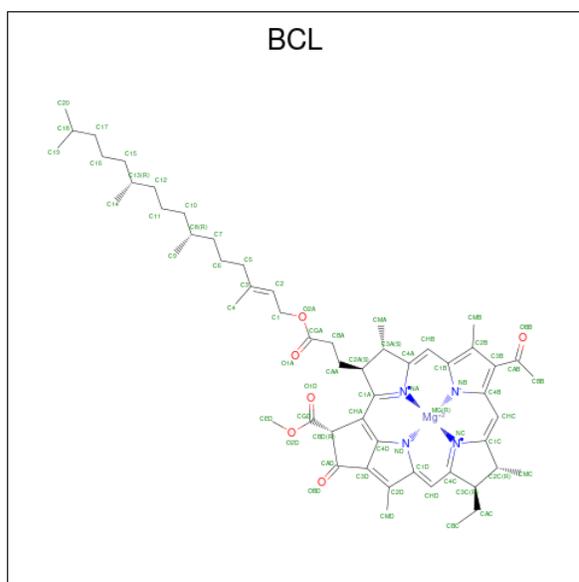
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER (H SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	248	Total	C	N	O	S	0	0	0
			1883	1204	322	347	10			
3	P	248	Total	C	N	O	S	0	0	0
			1883	1204	322	347	10			

There are 2 discrepancies between the modelled and reference sequences:

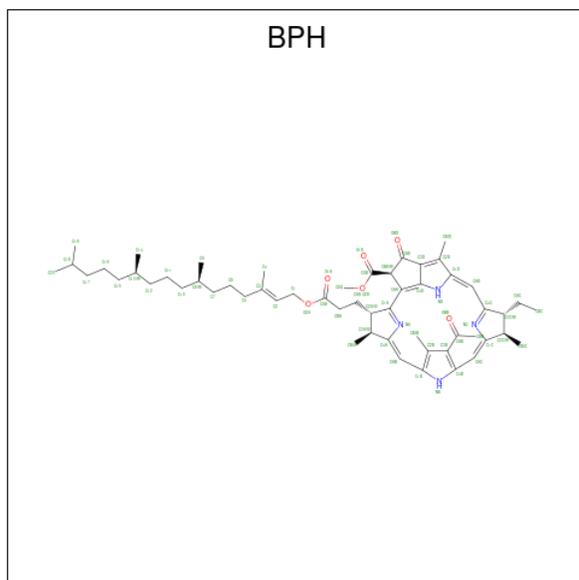
Chain	Residue	Modelled	Actual	Comment	Reference
H	8	GLN	GLY	conflict	UNP P11846
P	8	GLN	GLY	conflict	UNP P11846

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



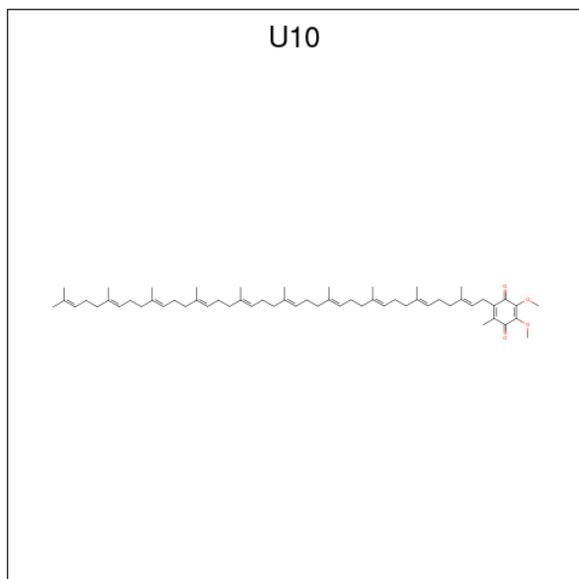
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Mg	N			O
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	N	1	Total	C	Mg	N	O	12	0
			66	55	1	4	6		
4	N	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	N	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	O	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	L	1	65	55	4	6	14	0
5	L	1	65	55	4	6	0	0
5	N	1	65	55	4	6	0	0
5	O	1	65	55	4	6	0	0

- Molecule 6 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	1	Total	C O	0	0
			63	59 4		
6	M	1	Total	C O	0	0
			63	59 4		
6	N	1	Total	C O	19	0
			63	59 4		
6	O	1	Total	C O	0	0
			63	59 4		

- Molecule 7 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 8 is water.

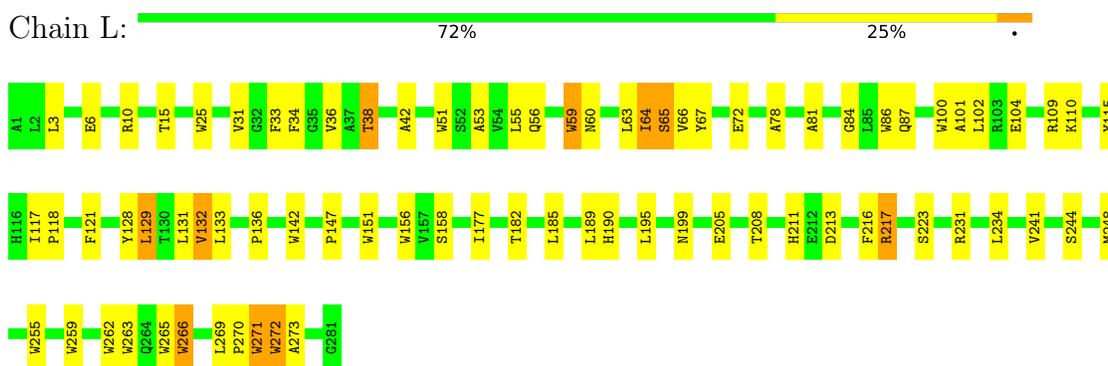
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	L	19	Total	O	0	0
			19	19		
8	M	21	Total	O	0	0
			21	21		
8	H	13	Total	O	0	0
			13	13		
8	N	13	Total	O	0	0
			13	13		
8	O	15	Total	O	0	0
			15	15		
8	P	5	Total	O	0	0
			5	5		

3 Residue-property plots

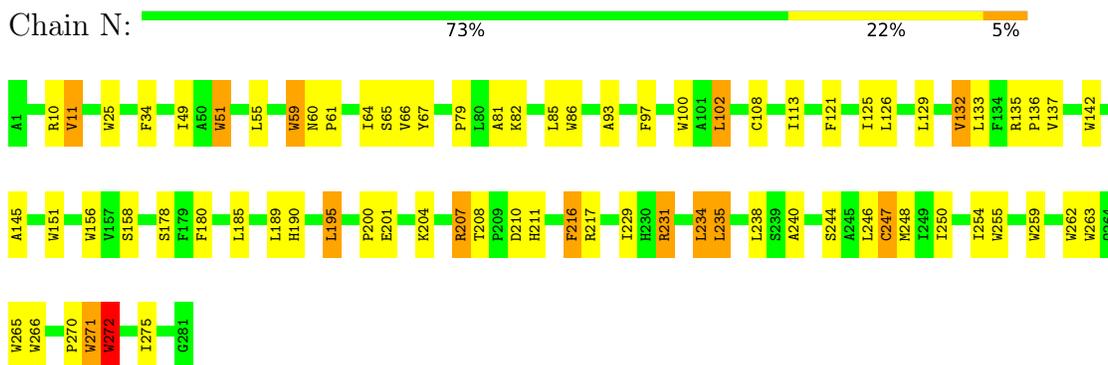
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

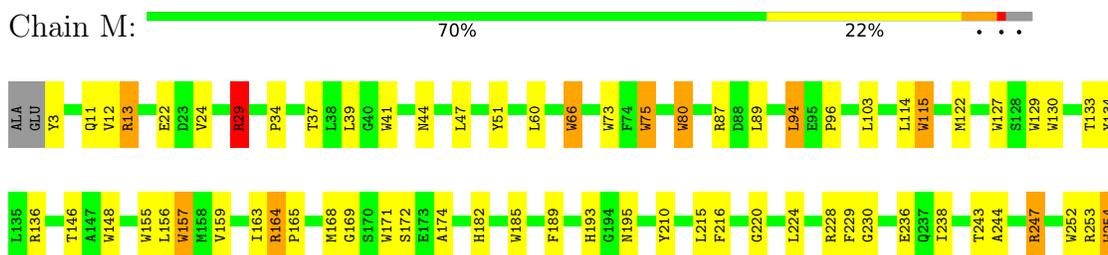
- Molecule 1: PHOTOSYNTHETIC REACTION CENTER (L SUBUNIT)



- Molecule 1: PHOTOSYNTHETIC REACTION CENTER (L SUBUNIT)

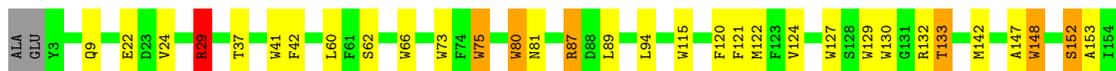


- Molecule 2: PHOTOSYNTHETIC REACTION CENTER (M SUBUNIT)





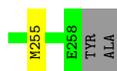
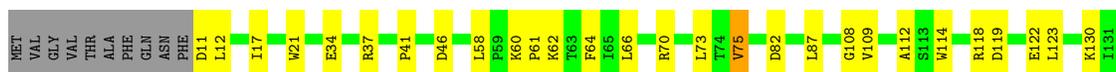
• Molecule 2: PHOTOSYNTHETIC REACTION CENTER (M SUBUNIT)



• Molecule 3: PHOTOSYNTHETIC REACTION CENTER (H SUBUNIT)



• Molecule 3: PHOTOSYNTHETIC REACTION CENTER (H SUBUNIT)



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	140.10Å 140.10Å 271.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60	Depositor
% Data completeness (in resolution range)	88.0 (30.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	X-PLOR 3.89	Depositor
R, R_{free}	0.215 , 0.299	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	14138	wwPDB-VP
Average B, all atoms (Å ²)	56.0	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: BCL, U10, BPH, FE2

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	0.87	0/2320	1.65	69/3175 (2.2%)
1	N	0.85	0/2320	1.59	53/3175 (1.7%)
2	M	0.90	0/2482	1.68	81/3389 (2.4%)
2	O	0.89	0/2482	1.60	68/3389 (2.0%)
3	H	0.76	0/1931	1.44	23/2627 (0.9%)
3	P	0.75	0/1931	1.38	15/2627 (0.6%)
All	All	0.85	0/13466	1.57	309/18382 (1.7%)

There are no bond length outliers.

The worst 5 of 309 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	217	ARG	NE-CZ-NH1	9.66	125.13	120.30
2	M	41	TRP	CD1-CG-CD2	9.54	113.93	106.30
2	O	297	TRP	CD1-CG-CD2	9.42	113.83	106.30
1	N	231	ARG	NE-CZ-NH1	9.41	125.01	120.30
3	H	37	ARG	NE-CZ-NH2	-9.33	115.64	120.30

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	39	0
1	N	2232	0	2187	40	0
2	M	2390	0	2304	36	0
2	O	2390	0	2304	47	0
3	H	1883	0	1895	30	0
3	P	1883	0	1895	30	0
4	L	132	0	148	11	0
4	M	132	0	148	12	0
4	N	198	0	222	18	0
4	O	66	0	74	9	0
5	L	130	0	152	11	0
5	N	65	0	76	7	0
5	O	65	0	76	3	0
6	L	63	0	90	4	0
6	M	63	0	90	1	0
6	N	63	0	90	6	0
6	O	63	0	90	2	0
7	M	1	0	0	0	0
7	O	1	0	0	0	0
8	H	13	0	0	3	0
8	L	19	0	0	4	0
8	M	21	0	0	0	0
8	N	13	0	0	0	0
8	O	15	0	0	1	0
8	P	5	0	0	0	0
All	All	14138	0	14028	238	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 9.

The worst 5 of 238 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:275:LEU:O	2:M:279:THR:HB	1.86	0.75
4:N:282:BCL:HBB3	4:O:309:BCL:H41	1.71	0.72
4:N:284:BCL:HED2	2:O:203:GLY:HA3	1.72	0.70
2:M:261:THR:HG22	2:M:264:GLY:H	1.55	0.70
3:H:226:THR:HG22	3:H:229:GLU:H	1.55	0.70

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%)	261 (94%)	14 (5%)	4 (1%)	11	22
1	N	279/281 (99%)	261 (94%)	15 (5%)	3 (1%)	14	30
2	M	297/307 (97%)	284 (96%)	11 (4%)	2 (1%)	22	43
2	O	297/307 (97%)	284 (96%)	11 (4%)	2 (1%)	22	43
3	H	246/260 (95%)	238 (97%)	8 (3%)	0	100	100
3	P	246/260 (95%)	238 (97%)	7 (3%)	1 (0%)	34	57
All	All	1644/1696 (97%)	1566 (95%)	66 (4%)	12 (1%)	22	43

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	270	PRO
2	M	259	ASN
2	O	259	ASN
1	L	271	TRP
2	M	195	ASN

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%)	208 (94%)	12 (6%)	21	43
1	N	220/220 (100%)	201 (91%)	19 (9%)	10	20
2	M	235/240 (98%)	218 (93%)	17 (7%)	14	29

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	O	235/240 (98%)	220 (94%)	15 (6%)	17	35
3	H	200/209 (96%)	179 (90%)	21 (10%)	7	13
3	P	200/209 (96%)	178 (89%)	22 (11%)	6	11
All	All	1310/1338 (98%)	1204 (92%)	106 (8%)	11	23

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	132	VAL
2	O	37	THR
3	P	219	ILE
1	N	189	LEU
1	N	235	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	O	11	GLN
3	P	199	GLN
3	P	204	HIS
2	O	193	HIS
1	N	87	GLN

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

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	N	284	1	64,74,74	1.24	9 (14%)	78,115,115	2.20	26 (33%)
4	BCL	M	309	2	64,74,74	1.29	9 (14%)	78,115,115	2.27	26 (33%)
5	BPH	N	285	-	51,70,70	1.20	4 (7%)	52,101,101	2.19	14 (26%)
4	BCL	O	309	2,4	64,74,74	1.21	8 (12%)	78,115,115	1.78	18 (23%)
6	U10	M	311	-	63,63,63	1.73	15 (23%)	76,79,79	1.31	6 (7%)
4	BCL	N	283	1,4	64,74,74	1.20	7 (10%)	78,115,115	2.07	25 (32%)
6	U10	O	311	-	63,63,63	1.58	14 (22%)	76,79,79	1.19	10 (13%)
5	BPH	L	284	-	51,70,70	1.60	5 (9%)	52,101,101	1.94	14 (26%)
4	BCL	M	310	2	64,74,74	1.16	7 (10%)	78,115,115	2.08	22 (28%)
6	U10	N	286	-	63,63,63	1.70	14 (22%)	76,79,79	1.52	9 (11%)
4	BCL	L	282	1	64,74,74	1.25	9 (14%)	78,115,115	1.81	21 (26%)
4	BCL	N	282	2	64,74,74	1.41	11 (17%)	78,115,115	1.93	21 (26%)
4	BCL	L	283	1	64,74,74	1.24	9 (14%)	78,115,115	2.11	24 (30%)
5	BPH	L	285	-	51,70,70	1.50	5 (9%)	52,101,101	1.85	13 (25%)
6	U10	L	286	-	63,63,63	1.73	14 (22%)	76,79,79	1.34	8 (10%)
5	BPH	O	310	-	51,70,70	1.18	5 (9%)	52,101,101	2.09	12 (23%)

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	N	284	1	-	5/37/137/137	-
4	BCL	M	309	2	2/2/21/25	12/37/137/137	-
5	BPH	N	285	-	1/1/18/22	10/37/105/105	0/5/6/6
4	BCL	O	309	2,4	1/1/21/25	5/37/137/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	U10	M	311	-	-	16/63/87/87	0/1/1/1
4	BCL	N	283	1,4	-	12/37/137/137	-
6	U10	O	311	-	-	14/63/87/87	0/1/1/1
5	BPH	L	284	-	2/2/18/22	10/37/105/105	0/5/6/6
4	BCL	M	310	2	2/2/21/25	5/37/137/137	-
6	U10	N	286	-	-	20/63/87/87	0/1/1/1
4	BCL	L	282	1	-	3/37/137/137	-
4	BCL	N	282	2	2/2/21/25	6/37/137/137	-
4	BCL	L	283	1	-	6/37/137/137	-
5	BPH	L	285	-	1/1/18/22	11/37/105/105	0/5/6/6
6	U10	L	286	-	-	13/63/87/87	0/1/1/1
5	BPH	O	310	-	1/1/18/22	11/37/105/105	0/5/6/6

The worst 5 of 145 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	285	BPH	C3A-C2A	-7.46	1.47	1.54
5	L	284	BPH	C2C-C3C	-6.54	1.48	1.54
5	L	284	BPH	C3A-C2A	-5.45	1.49	1.54
6	L	286	U10	C7-C8	-5.03	1.43	1.50
6	M	311	U10	C7-C8	-4.86	1.43	1.50

The worst 5 of 269 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	285	BPH	O2D-CGD-CBD	8.45	121.70	111.00
5	O	310	BPH	O2D-CGD-CBD	8.25	121.44	111.00
4	M	309	BCL	C1C-NC-C4C	8.06	110.33	106.71
4	N	284	BCL	C1C-NC-C4C	7.38	110.02	106.71
4	L	283	BCL	C1C-NC-C4C	6.74	109.73	106.71

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	M	309	BCL	C8
4	M	309	BCL	C13
4	M	310	BCL	C8
4	M	310	BCL	C13
4	N	282	BCL	C8

5 of 159 torsion outliers are listed below:

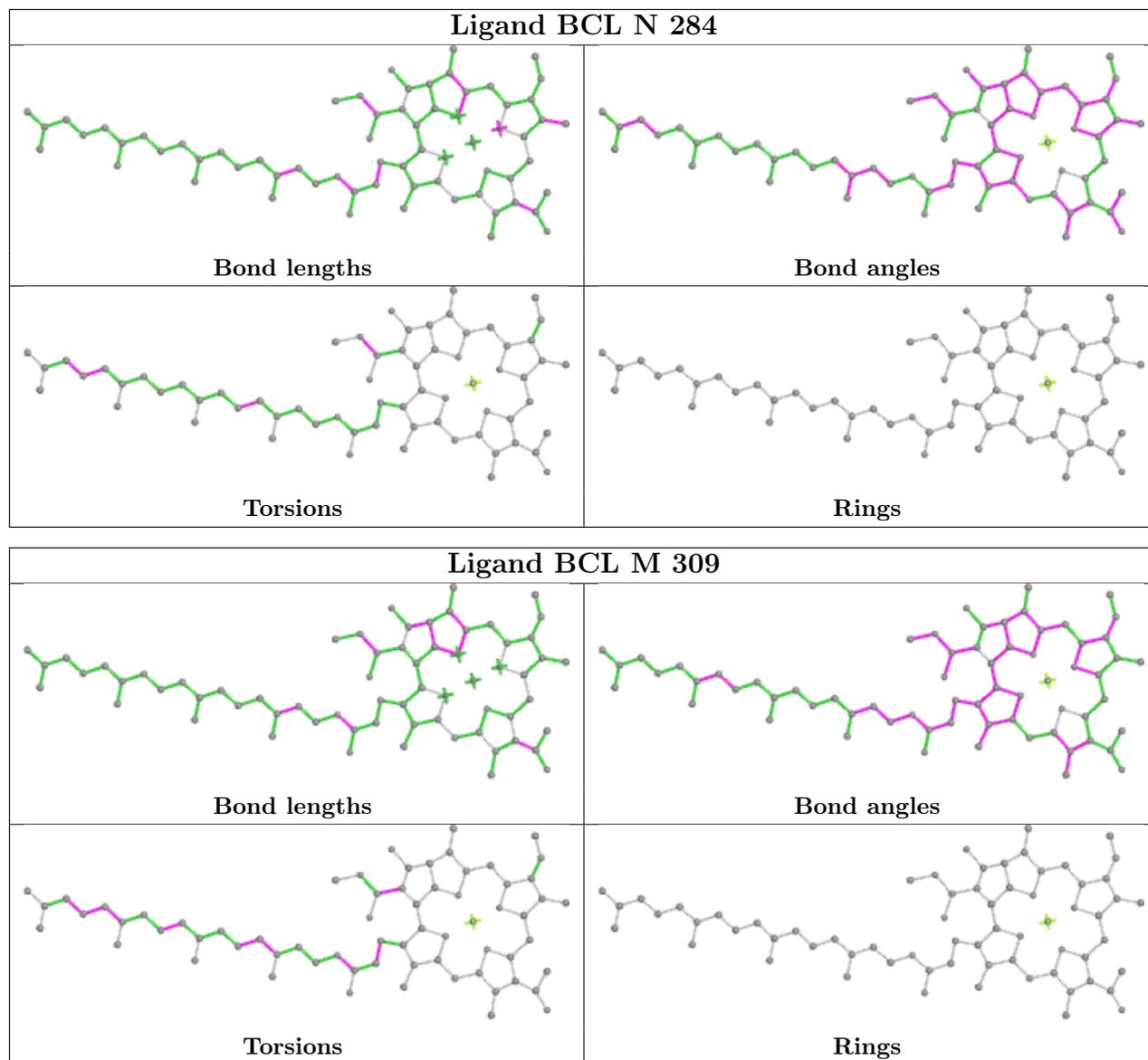
Mol	Chain	Res	Type	Atoms
4	L	283	BCL	CBD-CGD-O2D-CED
4	M	309	BCL	C2-C3-C5-C6
4	M	309	BCL	C4-C3-C5-C6
4	N	283	BCL	CBD-CGD-O2D-CED
4	N	284	BCL	CBD-CGD-O2D-CED

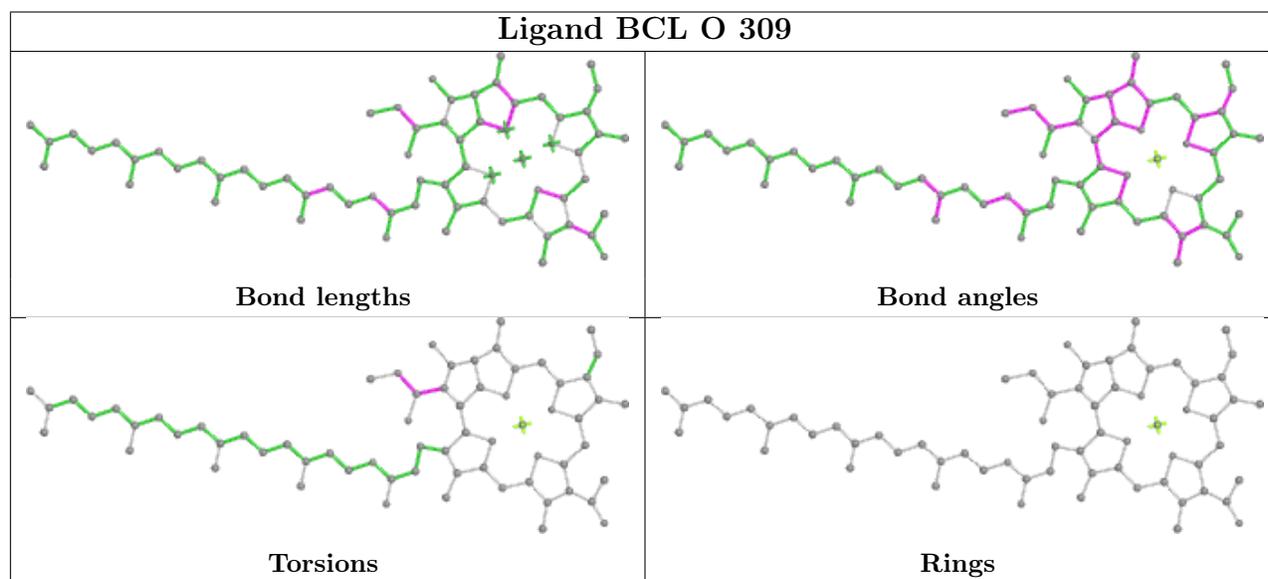
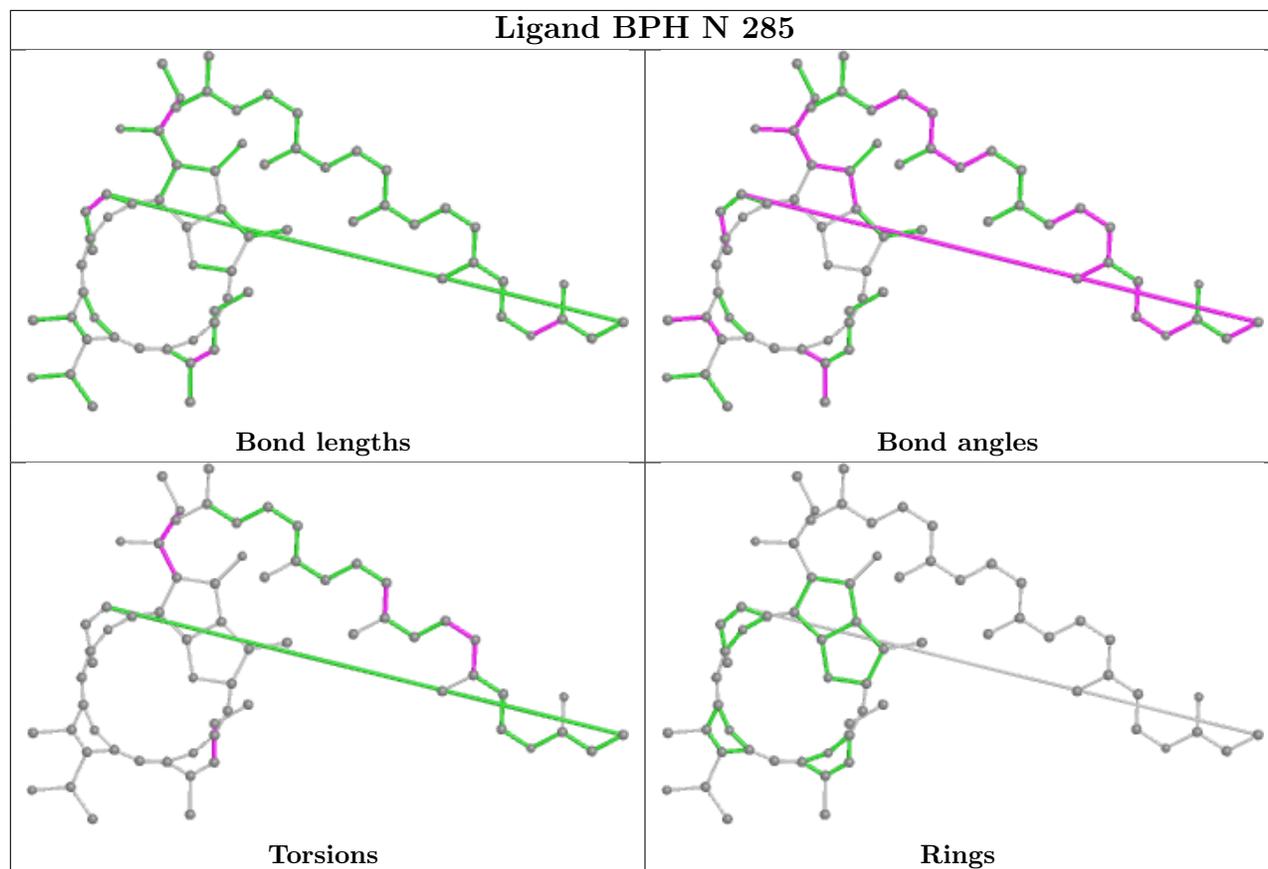
There are no ring outliers.

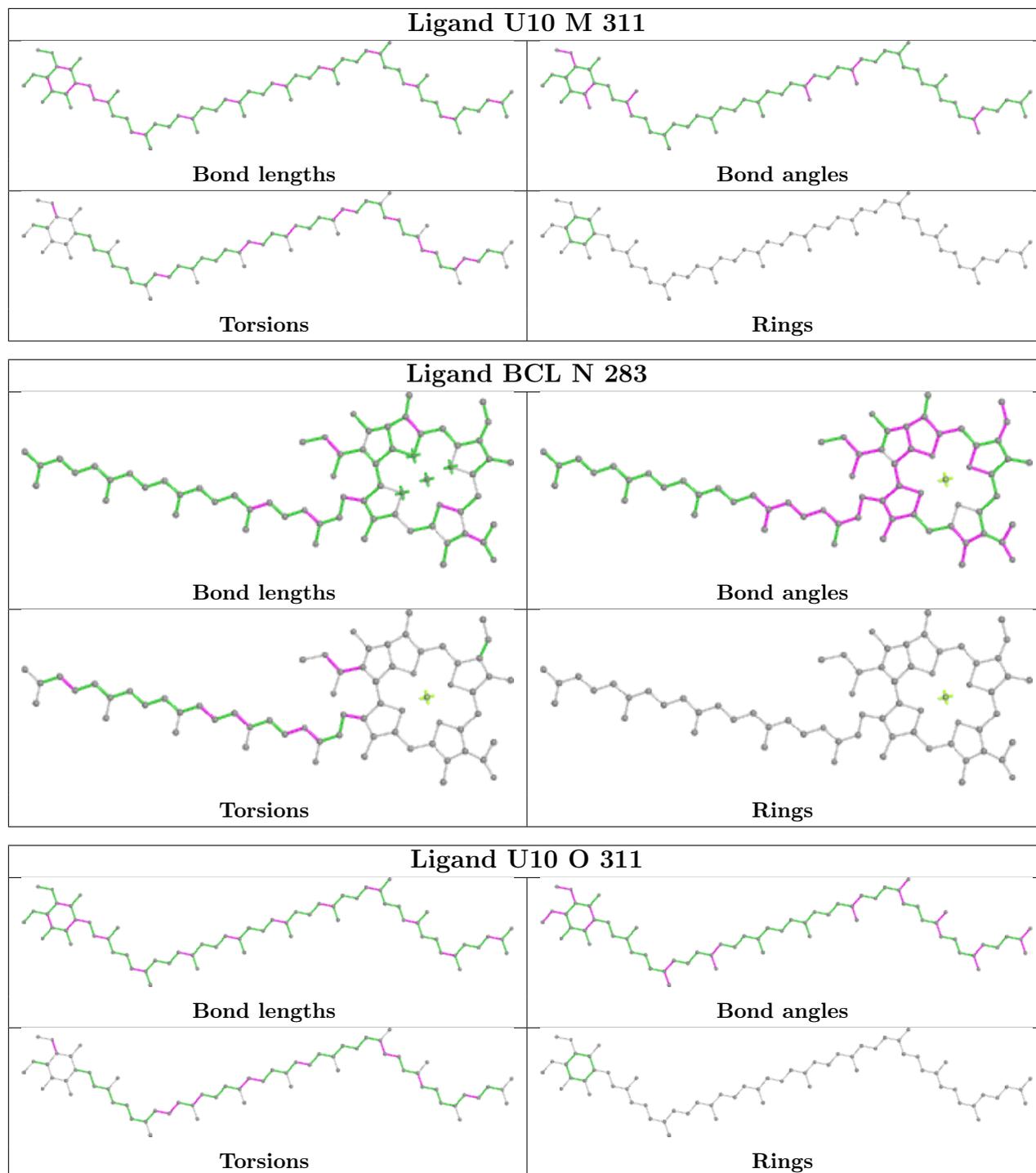
16 monomers are involved in 75 short contacts:

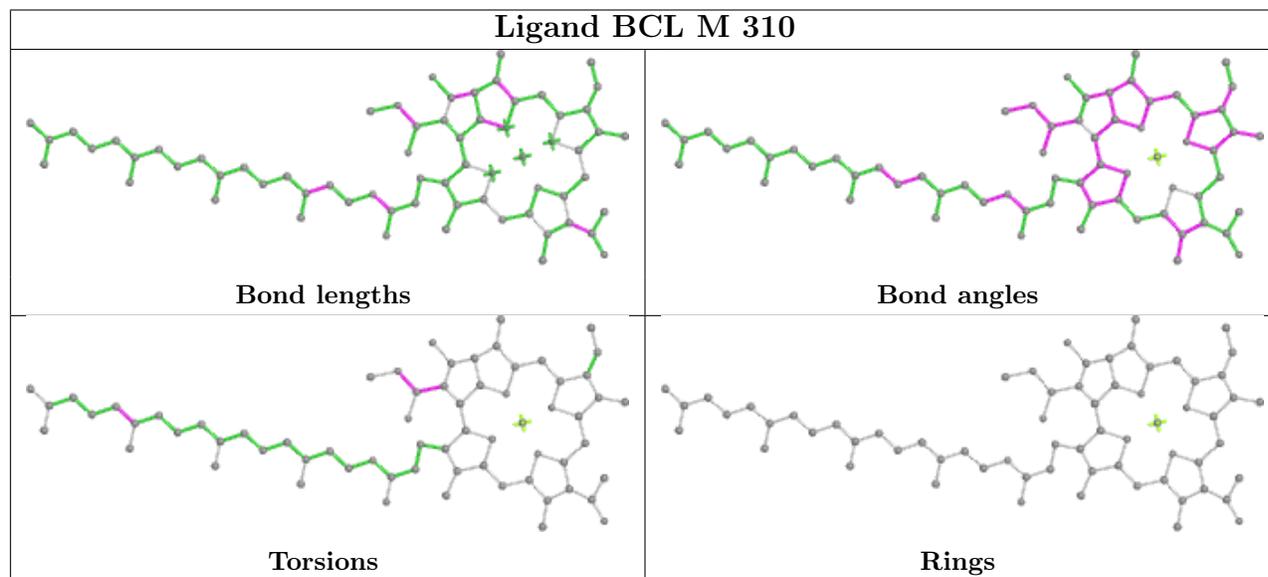
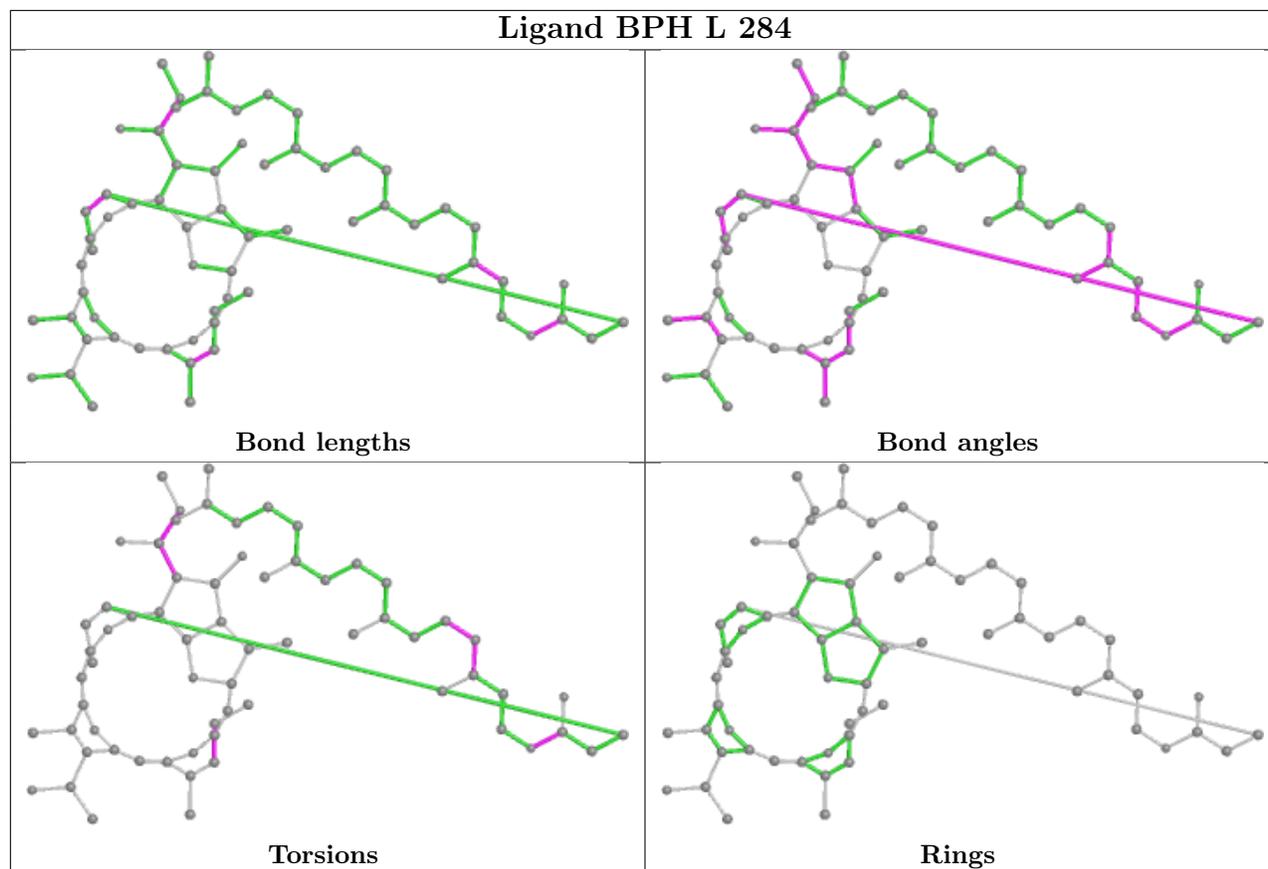
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	284	BCL	7	0
4	M	309	BCL	7	0
5	N	285	BPH	7	0
4	O	309	BCL	9	0
6	M	311	U10	1	0
4	N	283	BCL	6	0
6	O	311	U10	2	0
5	L	284	BPH	2	0
4	M	310	BCL	5	0
6	N	286	U10	6	0
4	L	282	BCL	8	0
4	N	282	BCL	7	0
4	L	283	BCL	6	0
5	L	285	BPH	9	0
6	L	286	U10	4	0
5	O	310	BPH	3	0

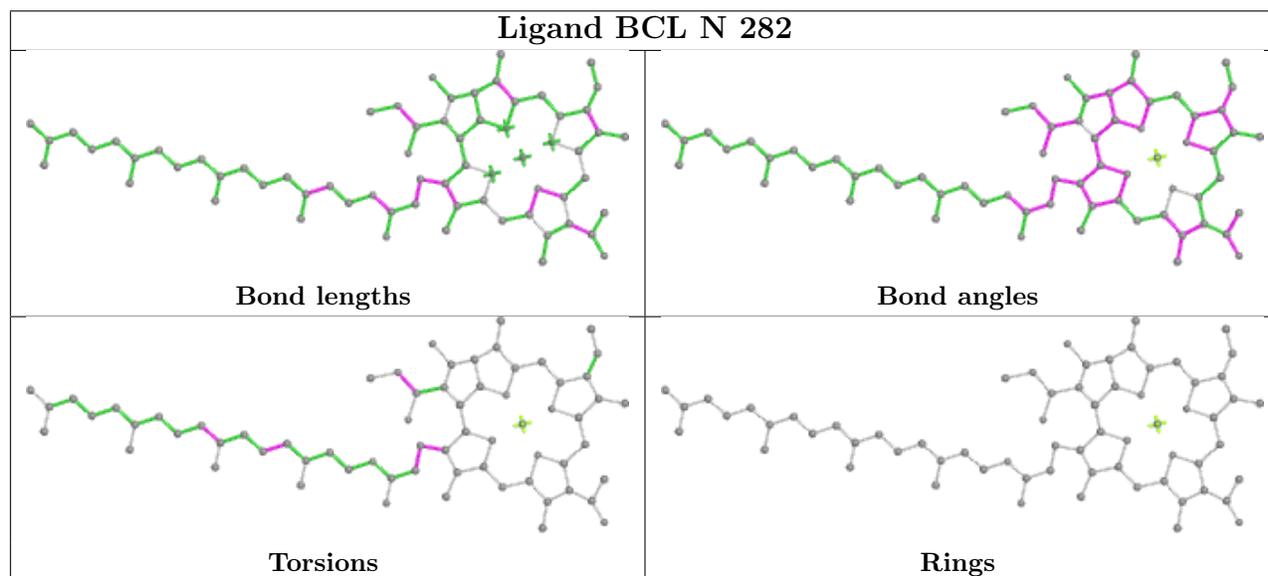
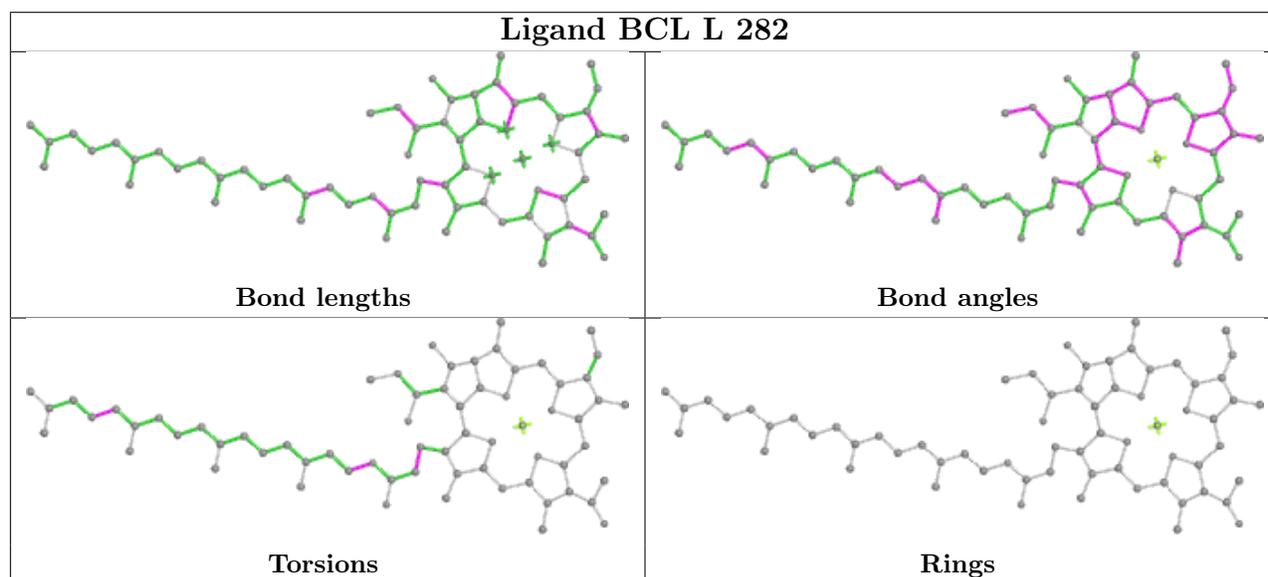
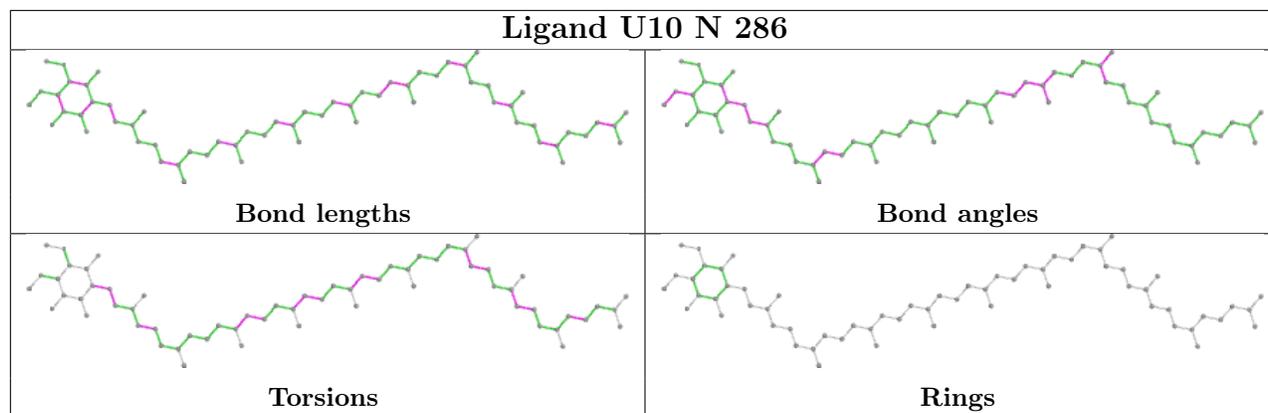
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

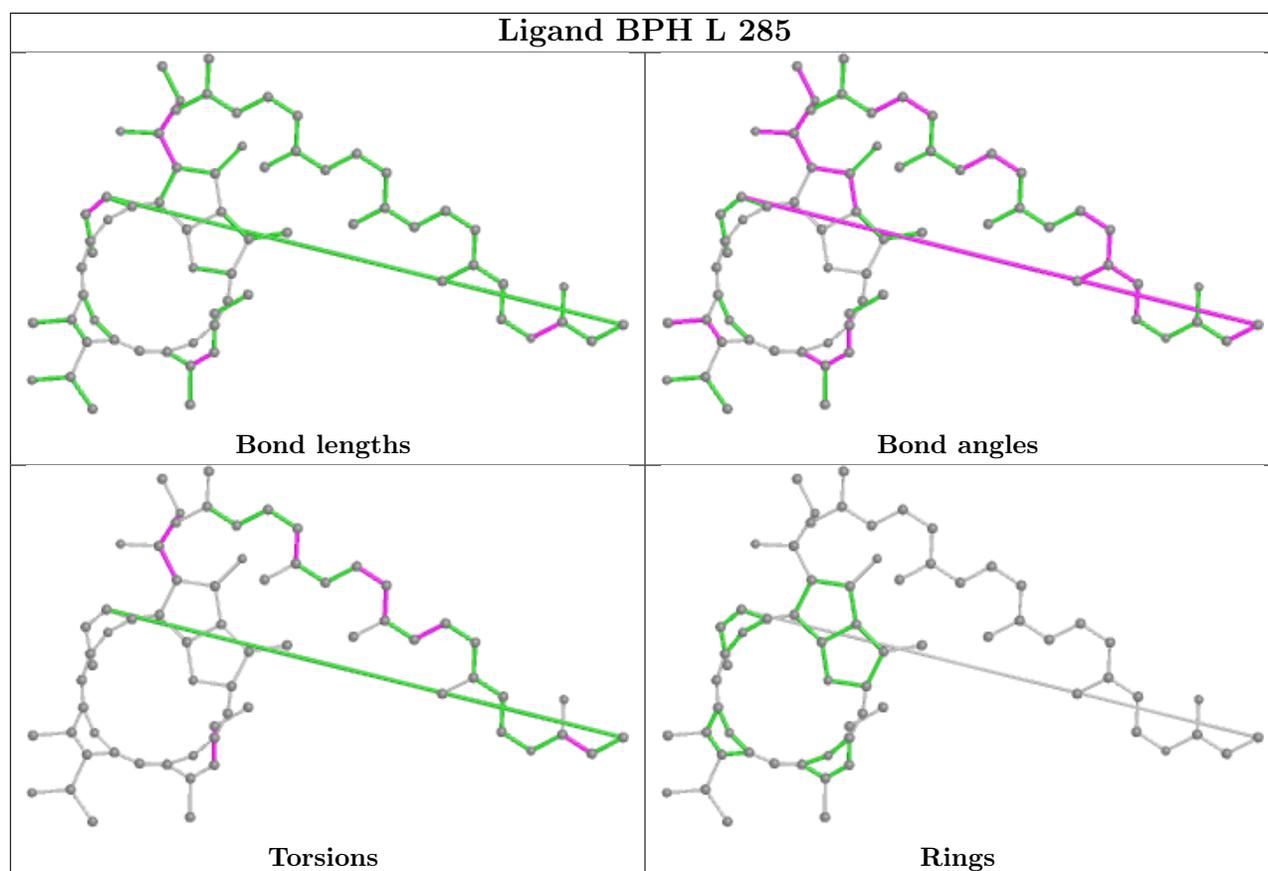
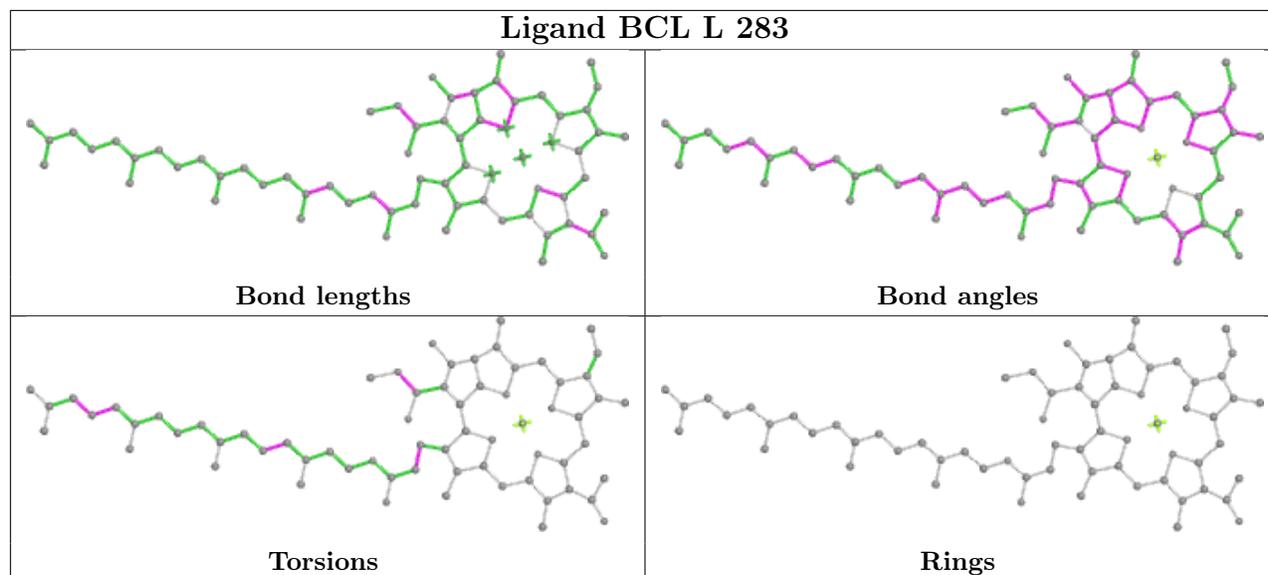


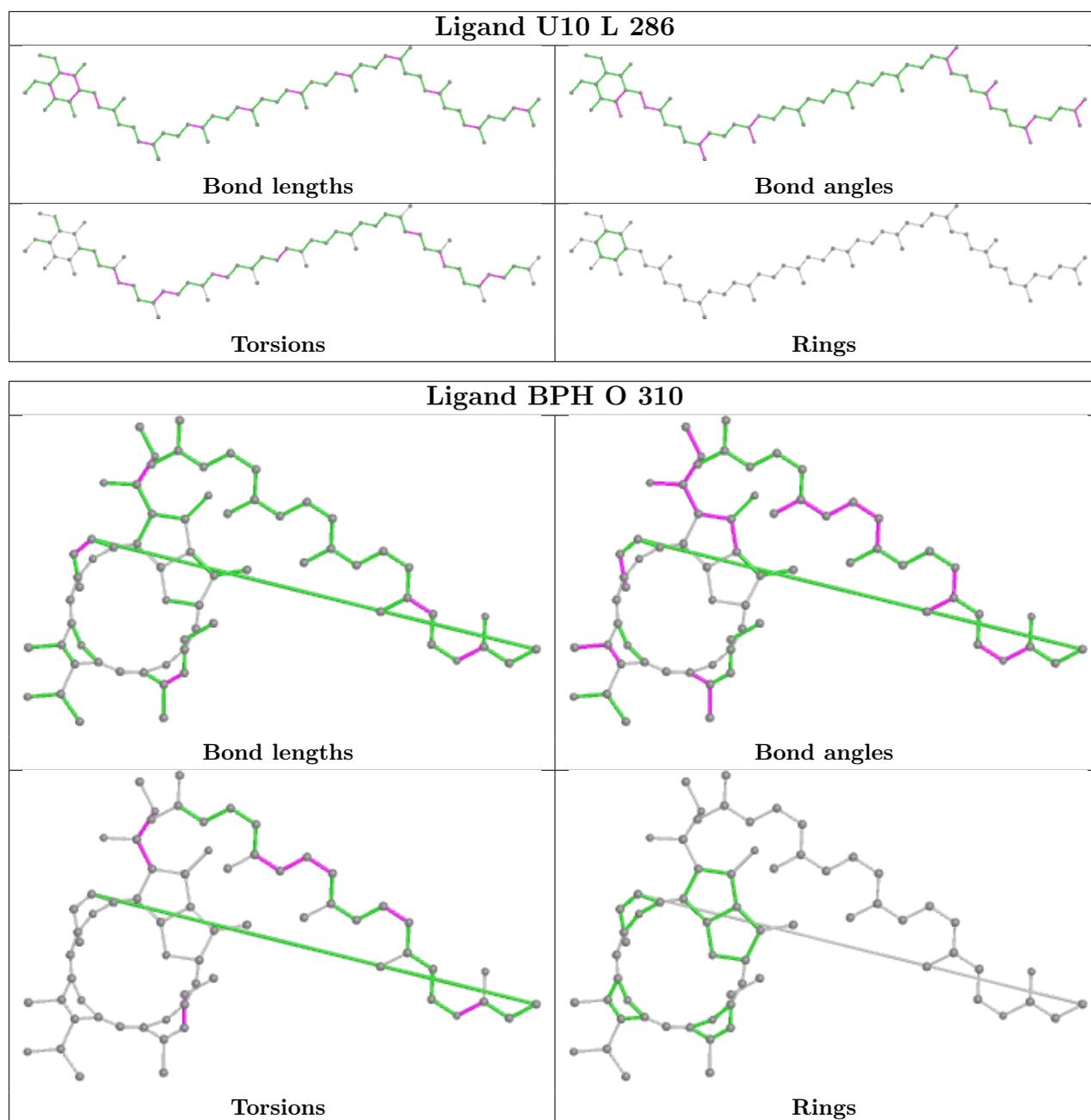












5.7 Other polymers [i](#)

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.