



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 06:41 AM UTC

PDB ID : 6Z5R / pdb_00006z5r
EMDB ID : EMD-11080
Title : RC-LH1(16) complex from Rhodopseudomonas palustris
Authors : Swainsbury, D.J.K.; Qian, P.; Hitchcock, A.; Hunter, C.N.
Deposited on : 2020-05-27
Resolution : 2.80 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

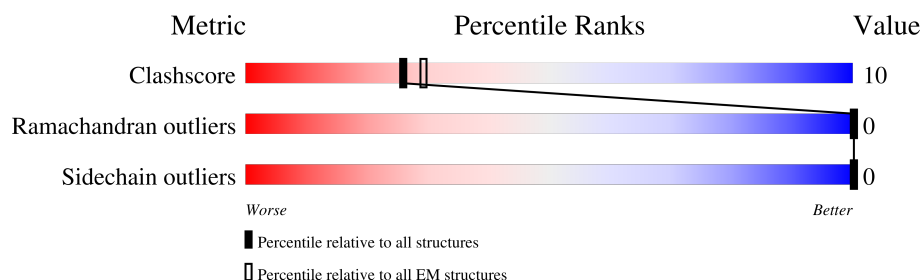
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

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.



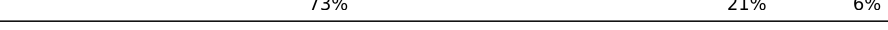
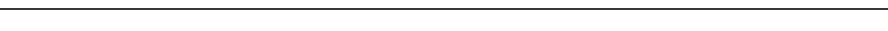
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	1	48	83% 12% .
1	3	48	75% 21% .
1	5	48	71% 23% . .
1	7	48	83% 12% .
1	9	48	50% 46% .
1	A	48	83% 12% .
1	C	48	73% 23% .
1	E	48	77% 19% .
1	G	48	75% 21% .

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Mol	Chain	Length	Quality of chain
1	J	48	
1	N	48	
1	P	48	
1	R	48	
1	T	48	
1	V	48	
1	Y	48	
2	0	52	
2	2	52	
2	4	52	
2	6	52	
2	8	52	
2	B	52	
2	D	52	
2	F	52	
2	I	52	
2	K	52	
2	O	52	
2	Q	52	
2	S	52	
2	U	52	
2	X	52	
2	Z	52	
3	H	255	
4	L	277	

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Mol	Chain	Length	Quality of chain
5	M	307	 89%11%

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
11	BPH	L	302	X	-	-	-
11	BPH	M	405	X	-	-	-
14	QAK	M	407	X	-	-	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 25048 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Light-harvesting complex 1 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	46	Total	C	N	O	S	0	0
			397	274	67	55	1		
1	E	46	Total	C	N	O	S	0	0
			397	274	67	55	1		
1	G	46	Total	C	N	O	S	0	0
			397	274	67	55	1		
1	J	45	Total	C	N	O	S	0	0
			392	271	66	54	1		
1	N	46	Total	C	N	O	S	0	0
			397	274	67	55	1		
1	R	46	Total	C	N	O	S	0	0
			397	274	67	55	1		
1	T	48	Total	C	N	O	S	0	0
			411	283	70	57	1		
1	V	46	Total	C	N	O	S	0	0
			397	274	67	55	1		
1	P	46	Total	C	N	O	S	0	0
			397	274	67	55	1		
1	Y	45	Total	C	N	O		0	0
			387	268	66	53			
1	A	46	Total	C	N	O	S	0	0
			397	274	67	55	1		
1	1	46	Total	C	N	O	S	0	0
			397	274	67	55	1		
1	3	46	Total	C	N	O	S	0	0
			397	274	67	55	1		
1	5	46	Total	C	N	O	S	0	0
			397	274	67	55	1		
1	7	46	Total	C	N	O	S	0	0
			397	274	67	55	1		
1	9	46	Total	C	N	O	S	0	0
			397	274	67	55	1		

- Molecule 2 is a protein called Light-harvesting complex 1 beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	49	Total	C	N	O	S	1	0
			403	276	62	64	1		
2	F	49	Total	C	N	O	S	1	0
			403	276	62	64	1		
2	I	47	Total	C	N	O	S	0	0
			382	262	59	60	1		
2	K	47	Total	C	N	O	S	1	0
			393	271	60	61	1		
2	O	48	Total	C	N	O	S	1	0
			399	274	61	63	1		
2	S	48	Total	C	N	O	S	1	0
			399	274	61	63	1		
2	U	47	Total	C	N	O	S	1	0
			393	271	60	61	1		
2	X	47	Total	C	N	O	S	0	0
			382	262	59	60	1		
2	Q	48	Total	C	N	O	S	1	0
			399	274	61	63	1		
2	Z	48	Total	C	N	O	S	1	0
			399	274	61	63	1		
2	B	49	Total	C	N	O	S	1	0
			403	276	62	64	1		
2	2	48	Total	C	N	O	S	1	0
			399	274	61	63	1		
2	4	48	Total	C	N	O	S	1	0
			399	274	61	63	1		
2	6	50	Total	C	N	O	S	1	0
			411	280	63	67	1		
2	8	49	Total	C	N	O	S	1	0
			403	276	62	64	1		
2	0	49	Total	C	N	O	S	1	0
			403	276	62	64	1		

- Molecule 3 is a protein called H subunit of photosynthetic reaction center complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	247	Total	C	N	O	S	0	0
			1862	1201	314	342	5		

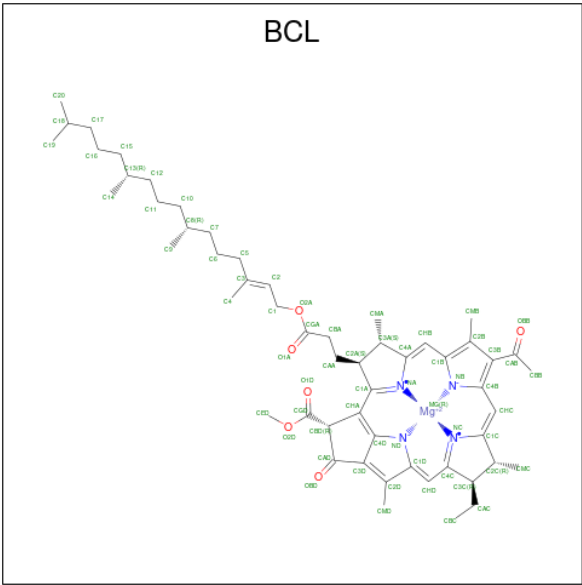
- Molecule 4 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	276	Total	C	N	O	S	0	0
			2185	1467	350	359	9		

- Molecule 5 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	M	306	2433	1615	400	406	12	0	0

- Molecule 6 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
6	C	1	Total 66	55	1	4	6	0
6	C	1	Total 66	55	1	4	6	0
6	E	1	Total 66	55	1	4	6	0
6	F	1	Total 66	55	1	4	6	0
6	G	1	Total 66	55	1	4	6	0
6	G	1	Total 66	55	1	4	6	0
6	J	1	Total 66	55	1	4	6	0
6	J	1	Total 66	55	1	4	6	0
6	N	1	Total 66	55	1	4	6	0

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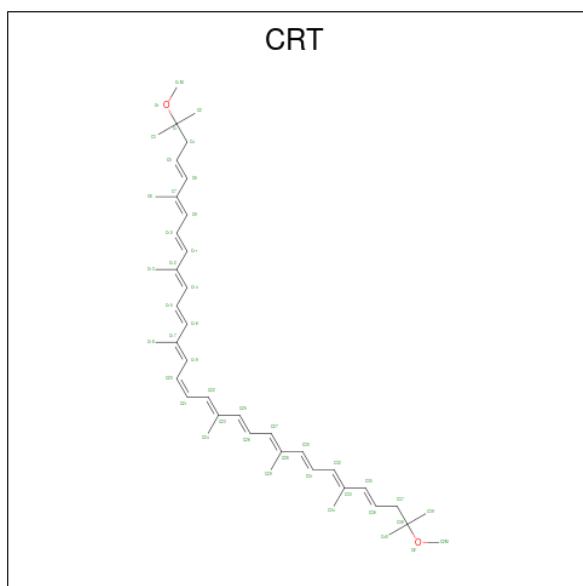
Mol	Chain	Residues	Atoms					AltConf
6	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	T	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	P	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	4	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
6	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
6	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
6	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
6	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
6	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
6	0	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 7 is SPIRILLOXANTHIN (CCD ID: CRT) (formula: $C_{42}H_{60}O_2$) (labeled as "Ligand of Interest" by depositor).



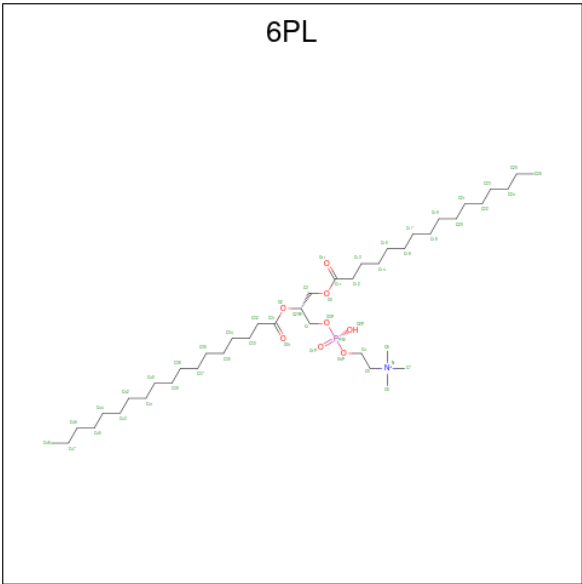
Mol	Chain	Residues	Atoms			AltConf
7	D	1	Total	C	O	0
			44	42	2	
7	G	1	Total	C	O	0
			44	42	2	
7	I	1	Total	C	O	0
			44	42	2	
7	K	1	Total	C	O	0
			44	42	2	
7	O	1	Total	C	O	0
			44	42	2	

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Mol	Chain	Residues	Atoms			AltConf
7	S	1	Total	C	O	0
			44	42	2	
7	U	1	Total	C	O	0
			44	42	2	
7	X	1	Total	C	O	0
			44	42	2	
7	Q	1	Total	C	O	0
			44	42	2	
7	Z	1	Total	C	O	0
			44	42	2	
7	B	1	Total	C	O	0
			44	42	2	
7	2	1	Total	C	O	0
			44	42	2	
7	4	1	Total	C	O	0
			44	42	2	
7	7	1	Total	C	O	0
			44	42	2	
7	8	1	Total	C	O	0
			44	42	2	
7	0	1	Total	C	O	0
			44	42	2	

- Molecule 8 is (4S,7R)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (CCD ID: 6PL) (formula: C₄₂H₈₅NO₈P) (labeled as "Ligand of Interest" by depositor).



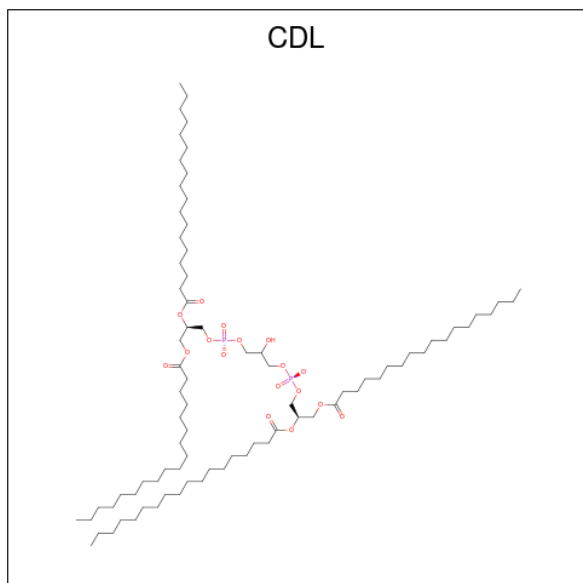
Mol	Chain	Residues	Atoms					AltConf
8	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	F	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	I	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	I	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	K	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	O	1	Total	C	N	O	P	0
			47	37	1	8	1	
8	H	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	L	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	L	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	M	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	S	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	U	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	X	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	P	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	Q	1	Total	C	N	O	P	0
			48	38	1	8	1	
8	Z	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	2	1	Total	C	N	O	P	0
			47	37	1	8	1	
8	4	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	5	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	6	1	Total	C	N	O	P	0
			52	42	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
8	8	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	0	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 9 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



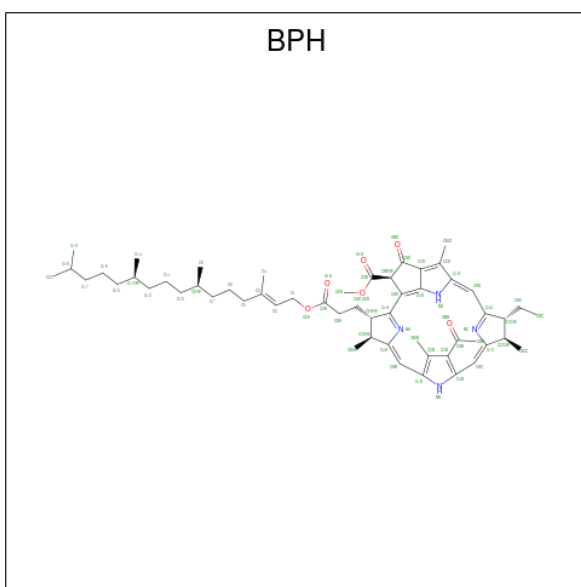
Mol	Chain	Residues	Atoms				AltConf
9	E	1	Total	C	O	P	0
			87	68	17	2	
9	G	1	Total	C	O	P	0
			100	81	17	2	
9	G	1	Total	C	O	P	0
			90	71	17	2	
9	L	1	Total	C	O	P	0
			100	81	17	2	
9	M	1	Total	C	O	P	0
			90	71	17	2	
9	M	1	Total	C	O	P	0
			84	65	17	2	

- Molecule 10 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



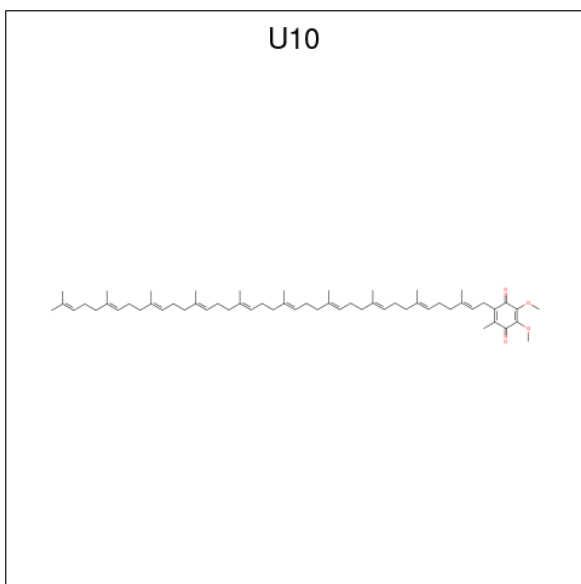
Mol	Chain	Residues	Atoms			AltConf
10	F	1	Total 35	C 24	O 11	0
10	J	1	Total 35	C 24	O 11	0
10	O	1	Total 35	C 24	O 11	0
10	H	1	Total 35	C 24	O 11	0
10	L	1	Total 35	C 24	O 11	0
10	R	1	Total 35	C 24	O 11	0
10	P	1	Total 35	C 24	O 11	0
10	Z	1	Total 35	C 24	O 11	0
10	B	1	Total 35	C 24	O 11	0
10	2	1	Total 35	C 24	O 11	0
10	4	1	Total 35	C 24	O 11	0
10	6	1	Total 35	C 24	O 11	0

- Molecule 11 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 12 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
12	L	1	Total	C	O	0
			48	44	4	

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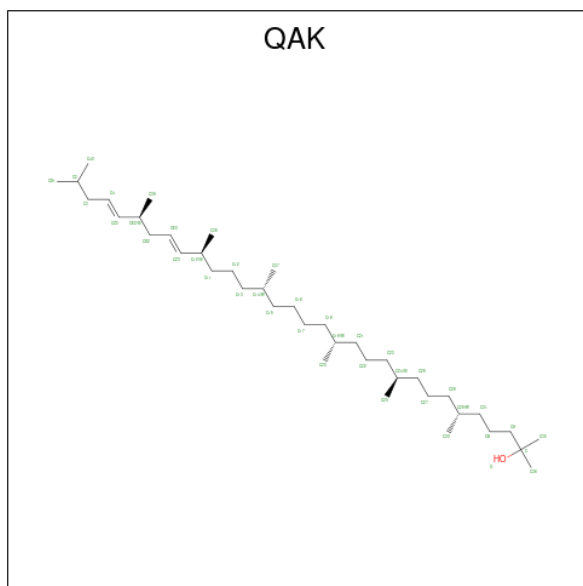
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Mol	Chain	Residues	Atoms			AltConf
12	L	1	Total	C	O	0
			63	59	4	
12	L	1	Total	C	O	0
			63	59	4	
12	M	1	Total	C	O	0
			48	44	4	
12	M	1	Total	C	O	0
			63	59	4	

- Molecule 13 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

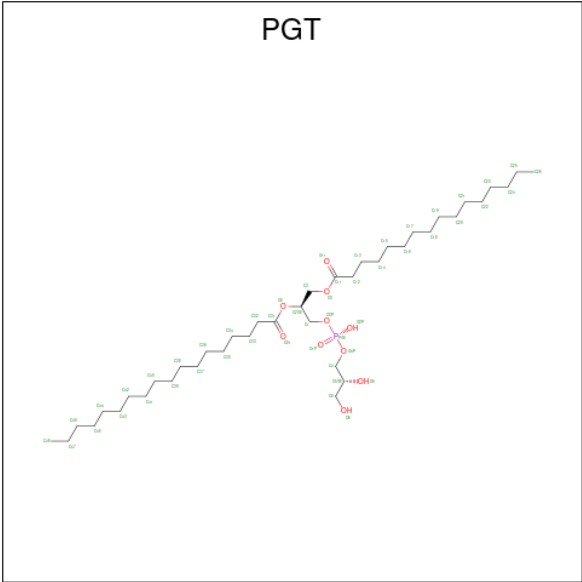
Mol	Chain	Residues	Atoms		AltConf
13	M	1	Total	Fe	0
			1	1	

- Molecule 14 is (6 {R},10 {S},14 {R},19 {R},23 {S},24 {E},27 {S},28 {E})-2,6,10,14,19,23,27,31-octamethyldotriaconta-24,28-dien-2-ol (CCD ID: QAK) (formula: C₄₀H₇₈O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
14	M	1	Total	C	O	0
			41	40	1	

- Molecule 15 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
15	7	1	Total	C	O	P	0
			51	40	10	1	
15	9	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		AltConf
16	L	1	Total	O	0
			1	1	
16	M	2	Total	O	0
			2	2	

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.

- Molecule 1: Light-harvesting complex 1 alpha chain

Chain C:  73% 23% .



- Molecule 1: Light-harvesting complex 1 alpha chain

Chain E:  77% 19% .



- Molecule 1: Light-harvesting complex 1 alpha chain

Chain G:  75% 21% .



- Molecule 1: Light-harvesting complex 1 alpha chain

Chain J:  81% 12% 6% .



- Molecule 1: Light-harvesting complex 1 alpha chain

Chain N:  73% 23% .

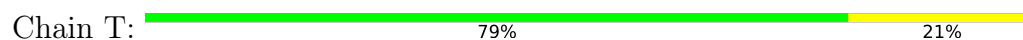


- Molecule 1: Light-harvesting complex 1 alpha chain

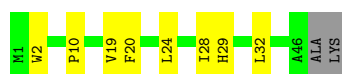
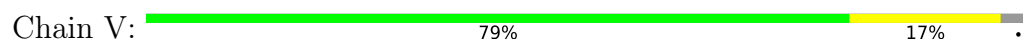
Chain R:  65% 31% .



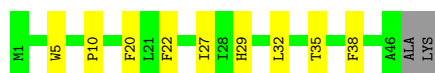
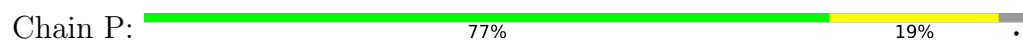
- Molecule 1: Light-harvesting complex 1 alpha chain



- Molecule 1: Light-harvesting complex 1 alpha chain



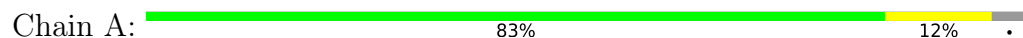
- Molecule 1: Light-harvesting complex 1 alpha chain



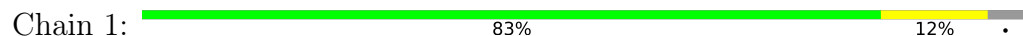
- Molecule 1: Light-harvesting complex 1 alpha chain



- Molecule 1: Light-harvesting complex 1 alpha chain



- Molecule 1: Light-harvesting complex 1 alpha chain



- Molecule 1: Light-harvesting complex 1 alpha chain

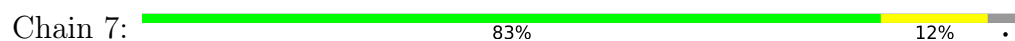




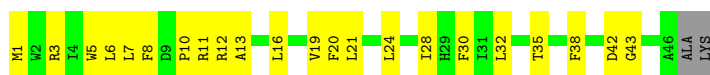
- Molecule 1: Light-harvesting complex 1 alpha chain



- Molecule 1: Light-harvesting complex 1 alpha chain



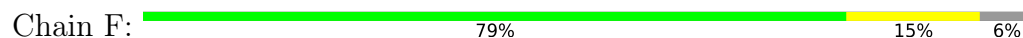
- Molecule 1: Light-harvesting complex 1 alpha chain



- Molecule 2: Light-harvesting complex 1 beta chain



- Molecule 2: Light-harvesting complex 1 beta chain



- Molecule 2: Light-harvesting complex 1 beta chain



- Molecule 2: Light-harvesting complex 1 beta chain





- Molecule 2: Light-harvesting complex 1 beta chain

Chain O: 69% 23% 8%



- Molecule 2: Light-harvesting complex 1 beta chain

Chain S: 79% 13% 8%



- Molecule 2: Light-harvesting complex 1 beta chain

Chain U: 71% 19% 10%



- Molecule 2: Light-harvesting complex 1 beta chain

Chain X: 65% 25% 10%



- Molecule 2: Light-harvesting complex 1 beta chain

Chain Q: 65% 27% 8%



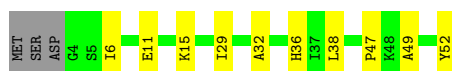
- Molecule 2: Light-harvesting complex 1 beta chain

Chain Z: 67% 25% 8%



- Molecule 2: Light-harvesting complex 1 beta chain

Chain B: 75% 19% 6%



- Molecule 2: Light-harvesting complex 1 beta chain



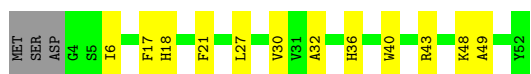
- Molecule 2: Light-harvesting complex 1 beta chain



- Molecule 2: Light-harvesting complex 1 beta chain



- Molecule 2: Light-harvesting complex 1 beta chain



- Molecule 2: Light-harvesting complex 1 beta chain



- Molecule 3: H subunit of photosynthetic reaction center complex

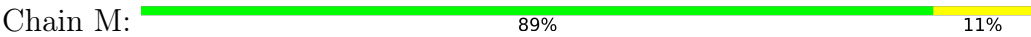


- Molecule 4: Reaction center protein L chain





• Molecule 5: Reaction center protein M chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	260752	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55.2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: QAK, FME, FE, BCL, LMT, BPH, PGT, CDL, CRT, 6PL, 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	1	0.16	0/401	0.29	0/546
1	3	0.15	0/401	0.29	0/546
1	5	0.15	0/401	0.31	0/546
1	7	0.15	0/401	0.34	0/546
1	9	0.17	0/401	0.33	0/546
1	A	0.18	0/401	0.31	0/546
1	C	0.18	0/401	0.31	0/546
1	E	0.18	0/401	0.36	0/546
1	G	0.18	0/401	0.31	0/546
1	J	0.17	0/396	0.32	0/539
1	N	0.17	0/401	0.31	0/546
1	P	0.16	0/401	0.32	0/546
1	R	0.17	0/401	0.38	0/546
1	T	0.18	0/415	0.31	0/564
1	V	0.16	0/401	0.31	0/546
1	Y	0.18	0/401	0.30	0/546
2	0	0.15	0/419	0.32	0/571
2	2	0.15	0/415	0.29	0/566
2	4	0.15	0/415	0.27	0/566
2	6	0.16	0/427	0.28	0/582
2	8	0.18	0/419	0.37	0/571
2	B	0.18	0/419	0.34	0/571
2	D	0.19	0/419	0.28	0/571
2	F	0.20	0/419	0.32	0/571
2	I	0.18	0/397	0.29	0/542
2	K	0.16	0/409	0.28	0/558
2	O	0.17	0/415	0.34	0/566
2	Q	0.17	0/415	0.28	0/566
2	S	0.18	0/415	0.28	0/566
2	U	0.17	0/409	0.32	0/558
2	X	0.17	0/397	0.33	0/542
2	Z	0.18	0/415	0.36	0/566

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	H	0.17	0/1913	0.37	0/2618
4	L	0.18	0/2271	0.32	0/3109
5	M	0.18	0/2524	0.32	0/3454
All	All	0.17	0/19757	0.32	0/26961

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	397	0	415	6	0
1	3	397	0	415	10	0
1	5	397	0	415	11	0
1	7	397	0	415	5	0
1	9	397	0	415	28	0
1	A	397	0	415	7	0
1	C	397	0	415	9	0
1	E	397	0	415	8	0
1	G	397	0	415	10	0
1	J	392	0	410	7	0
1	N	397	0	415	13	0
1	P	397	0	415	10	0
1	R	397	0	415	13	0
1	T	411	0	433	11	0
1	V	397	0	415	8	0
1	Y	387	0	404	13	0
2	0	403	0	396	12	0
2	2	399	0	393	7	0
2	4	399	0	393	21	0
2	6	411	0	400	15	0
2	8	403	0	396	16	0
2	B	403	0	396	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	403	0	396	12	0
2	F	403	0	396	9	0
2	I	382	0	380	9	0
2	K	393	0	388	7	0
2	O	399	0	393	11	0
2	Q	399	0	393	12	0
2	S	399	0	393	6	0
2	U	393	0	388	10	0
2	X	382	0	380	17	0
2	Z	399	0	393	12	0
3	H	1862	0	1873	20	0
4	L	2185	0	2130	17	0
5	M	2433	0	2379	28	0
6	0	66	0	74	4	0
6	1	132	0	148	10	0
6	3	66	0	74	2	0
6	4	66	0	74	6	0
6	5	132	0	148	10	0
6	7	132	0	148	5	0
6	9	66	0	74	1	0
6	A	66	0	74	8	0
6	B	66	0	74	6	0
6	C	132	0	148	6	0
6	E	66	0	74	1	0
6	F	66	0	74	4	0
6	G	132	0	148	8	0
6	J	132	0	148	5	0
6	L	132	0	148	5	0
6	M	132	0	148	4	0
6	N	132	0	148	4	0
6	P	66	0	74	4	0
6	Q	66	0	74	5	0
6	R	132	0	148	8	0
6	T	66	0	74	4	0
6	U	66	0	74	5	0
6	V	132	0	148	6	0
6	Y	132	0	148	12	0
7	0	44	0	60	5	0
7	2	44	0	60	5	0
7	4	44	0	60	11	0
7	7	44	0	60	2	0
7	8	44	0	60	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	44	0	60	4	0
7	D	44	0	60	5	0
7	G	44	0	60	4	0
7	I	44	0	60	2	0
7	K	44	0	60	2	0
7	O	44	0	60	4	0
7	Q	44	0	60	4	0
7	S	44	0	60	3	0
7	U	44	0	60	5	0
7	X	44	0	60	14	0
7	Z	44	0	60	7	0
8	0	52	0	84	3	0
8	2	47	0	71	7	0
8	4	52	0	84	5	0
8	5	52	0	84	2	0
8	6	52	0	84	4	0
8	8	52	0	84	4	0
8	B	52	0	84	4	0
8	D	52	0	84	5	0
8	E	52	0	84	6	0
8	F	52	0	84	3	0
8	H	52	0	84	0	0
8	I	104	0	168	10	0
8	K	52	0	84	3	0
8	L	104	0	168	10	0
8	M	52	0	84	5	0
8	O	47	0	71	4	0
8	P	52	0	84	4	0
8	Q	48	0	73	6	0
8	S	52	0	84	5	0
8	U	52	0	84	4	0
8	X	52	0	84	3	0
8	Z	52	0	84	4	0
9	E	87	0	127	7	0
9	G	190	0	289	21	0
9	L	100	0	156	9	0
9	M	174	0	251	10	0
10	2	35	0	45	2	0
10	4	35	0	45	3	0
10	6	35	0	46	3	0
10	B	35	0	45	2	0
10	F	35	0	45	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	H	35	0	45	4	0
10	J	35	0	45	7	0
10	L	35	0	45	0	0
10	O	35	0	45	1	0
10	P	35	0	44	2	0
10	R	35	0	45	3	0
10	Z	35	0	45	1	0
11	L	65	0	76	5	0
11	M	65	0	76	6	0
12	L	174	0	243	13	0
12	M	111	0	153	9	0
13	M	1	0	0	0	0
14	M	41	0	0	0	0
15	7	51	0	78	4	0
15	9	51	0	78	3	0
16	L	1	0	0	0	0
16	M	2	0	0	0	0
All	All	25048	0	26968	533	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 10.

The worst 5 of 533 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)
1:1:32:LEU:HD11	6:1:102:BCL:HHD	1.61	0.82
1:5:3:ARG:HB3	7:8:101:CRT:H23	1.65	0.77
2:8:17:PHE:HA	7:8:101:CRT:H6	1.67	0.75
9:L:310:CDL:H781	1:9:16:LEU:HD22	1.68	0.75
4:L:96:GLY:HA2	9:L:310:CDL:H632	1.67	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 PDB entries followed by that with respect to all EM entries.

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	1	44/48 (92%)	44 (100%)	0	0	100	100
1	3	44/48 (92%)	43 (98%)	1 (2%)	0	100	100
1	5	44/48 (92%)	43 (98%)	1 (2%)	0	100	100
1	7	44/48 (92%)	42 (96%)	2 (4%)	0	100	100
1	9	44/48 (92%)	43 (98%)	1 (2%)	0	100	100
1	A	44/48 (92%)	44 (100%)	0	0	100	100
1	C	44/48 (92%)	44 (100%)	0	0	100	100
1	E	44/48 (92%)	42 (96%)	2 (4%)	0	100	100
1	G	44/48 (92%)	42 (96%)	2 (4%)	0	100	100
1	J	43/48 (90%)	42 (98%)	1 (2%)	0	100	100
1	N	44/48 (92%)	42 (96%)	2 (4%)	0	100	100
1	P	44/48 (92%)	43 (98%)	1 (2%)	0	100	100
1	R	44/48 (92%)	43 (98%)	1 (2%)	0	100	100
1	T	46/48 (96%)	45 (98%)	1 (2%)	0	100	100
1	V	44/48 (92%)	43 (98%)	1 (2%)	0	100	100
1	Y	43/48 (90%)	41 (95%)	2 (5%)	0	100	100
2	0	48/52 (92%)	45 (94%)	3 (6%)	0	100	100
2	2	47/52 (90%)	44 (94%)	3 (6%)	0	100	100
2	4	47/52 (90%)	45 (96%)	2 (4%)	0	100	100
2	6	49/52 (94%)	46 (94%)	3 (6%)	0	100	100
2	8	48/52 (92%)	44 (92%)	4 (8%)	0	100	100
2	B	48/52 (92%)	45 (94%)	3 (6%)	0	100	100
2	D	48/52 (92%)	45 (94%)	3 (6%)	0	100	100
2	F	48/52 (92%)	46 (96%)	2 (4%)	0	100	100
2	I	45/52 (86%)	42 (93%)	3 (7%)	0	100	100
2	K	46/52 (88%)	44 (96%)	2 (4%)	0	100	100
2	O	47/52 (90%)	44 (94%)	3 (6%)	0	100	100
2	Q	47/52 (90%)	45 (96%)	2 (4%)	0	100	100
2	S	47/52 (90%)	44 (94%)	3 (6%)	0	100	100
2	U	46/52 (88%)	43 (94%)	3 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	X	45/52 (86%)	42 (93%)	3 (7%)	0	100	100
2	Z	47/52 (90%)	44 (94%)	3 (6%)	0	100	100
3	H	245/255 (96%)	235 (96%)	10 (4%)	0	100	100
4	L	274/277 (99%)	270 (98%)	4 (2%)	0	100	100
5	M	304/307 (99%)	298 (98%)	6 (2%)	0	100	100
All	All	2280/2439 (94%)	2197 (96%)	83 (4%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	1	40/41 (98%)	40 (100%)	0	100	100
1	3	40/41 (98%)	40 (100%)	0	100	100
1	5	40/41 (98%)	40 (100%)	0	100	100
1	7	40/41 (98%)	40 (100%)	0	100	100
1	9	40/41 (98%)	40 (100%)	0	100	100
1	A	40/41 (98%)	40 (100%)	0	100	100
1	C	40/41 (98%)	40 (100%)	0	100	100
1	E	40/41 (98%)	40 (100%)	0	100	100
1	G	40/41 (98%)	40 (100%)	0	100	100
1	J	40/41 (98%)	40 (100%)	0	100	100
1	N	40/41 (98%)	40 (100%)	0	100	100
1	P	40/41 (98%)	40 (100%)	0	100	100
1	R	40/41 (98%)	40 (100%)	0	100	100
1	T	41/41 (100%)	41 (100%)	0	100	100
1	V	40/41 (98%)	40 (100%)	0	100	100
1	Y	40/41 (98%)	40 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	0	41/43 (95%)	41 (100%)	0	100	100
2	2	41/43 (95%)	41 (100%)	0	100	100
2	4	41/43 (95%)	41 (100%)	0	100	100
2	6	42/43 (98%)	42 (100%)	0	100	100
2	8	41/43 (95%)	41 (100%)	0	100	100
2	B	41/43 (95%)	41 (100%)	0	100	100
2	D	41/43 (95%)	41 (100%)	0	100	100
2	F	41/43 (95%)	41 (100%)	0	100	100
2	I	39/43 (91%)	39 (100%)	0	100	100
2	K	40/43 (93%)	40 (100%)	0	100	100
2	O	41/43 (95%)	41 (100%)	0	100	100
2	Q	41/43 (95%)	41 (100%)	0	100	100
2	S	41/43 (95%)	41 (100%)	0	100	100
2	U	40/43 (93%)	40 (100%)	0	100	100
2	X	39/43 (91%)	39 (100%)	0	100	100
2	Z	41/43 (95%)	41 (100%)	0	100	100
3	H	195/203 (96%)	195 (100%)	0	100	100
4	L	222/223 (100%)	222 (100%)	0	100	100
5	M	246/247 (100%)	246 (100%)	0	100	100
All	All	1955/2017 (97%)	1955 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
5	M	74	ASN
2	U	18	HIS
2	0	18	HIS
2	S	18	HIS
2	Q	18	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

15 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
1	FME	G	1	1	8,9,10	0.97	0	8,9,11	0.83	0
1	FME	C	1	1	8,9,10	0.98	0	8,9,11	0.86	0
1	FME	1	1	1	8,9,10	0.97	0	8,9,11	0.91	0
1	FME	E	1	1	8,9,10	0.97	0	8,9,11	0.81	0
1	FME	J	1	1	8,9,10	0.98	0	8,9,11	0.91	0
1	FME	T	1	1	8,9,10	0.95	0	8,9,11	0.86	0
1	FME	P	1	1	8,9,10	1.01	0	8,9,11	0.70	0
1	FME	7	1	1	8,9,10	0.93	0	8,9,11	1.26	1 (12%)
1	FME	A	1	1	8,9,10	0.98	0	8,9,11	0.86	0
1	FME	3	1	1	8,9,10	0.95	0	8,9,11	0.95	1 (12%)
1	FME	V	1	1	8,9,10	0.98	0	8,9,11	0.92	0
1	FME	5	1	1	8,9,10	0.95	0	8,9,11	1.11	1 (12%)
1	FME	R	1	1	8,9,10	0.98	0	8,9,11	0.86	0
1	FME	9	1	1	8,9,10	0.96	0	8,9,11	0.88	0
1	FME	N	1	1	8,9,10	1.00	0	8,9,11	0.91	0

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
1	FME	G	1	1	-	1/7/9/11	-
1	FME	C	1	1	-	3/7/9/11	-
1	FME	1	1	1	-	6/7/9/11	-
1	FME	E	1	1	-	3/7/9/11	-
1	FME	J	1	1	-	2/7/9/11	-
1	FME	T	1	1	-	1/7/9/11	-
1	FME	P	1	1	-	0/7/9/11	-
1	FME	7	1	1	-	3/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	A	1	1	-	3/7/9/11	-
1	FME	3	1	1	-	1/7/9/11	-
1	FME	V	1	1	-	1/7/9/11	-
1	FME	5	1	1	-	3/7/9/11	-
1	FME	R	1	1	-	5/7/9/11	-
1	FME	9	1	1	-	3/7/9/11	-
1	FME	N	1	1	-	2/7/9/11	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	7	1	FME	C-CA-N	2.70	114.71	109.50
1	5	1	FME	C-CA-N	2.27	113.88	109.50
1	3	1	FME	C-CA-N	2.03	113.42	109.50

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	1	FME	CB-CA-N-CN
1	N	1	FME	N-CA-CB-CG
1	N	1	FME	C-CA-CB-CG
1	R	1	FME	C-CA-CB-CG
1	R	1	FME	O-C-CA-CB

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	5	1	FME	1	0
1	R	1	FME	1	0
1	9	1	FME	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 105 ligands modelled in this entry, 1 is monoatomic - leaving 104 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	6PL	Z	103	-	51,51,51	0.28	0	57,59,59	0.31	0
10	LMT	O	101	-	36,36,36	1.18	6 (16%)	47,47,47	1.08	2 (4%)
15	PGT	7	103	-	50,50,50	0.26	0	53,56,56	0.33	0
7	CRT	2	102	-	43,43,43	1.50	12 (27%)	48,54,54	1.75	16 (33%)
6	BCL	1	102	-	69,74,74	1.80	17 (24%)	79,115,115	2.20	24 (30%)
9	CDL	G	101	-	99,99,99	0.27	0	105,111,111	0.35	0
10	LMT	P	101	-	36,36,36	1.15	5 (13%)	47,47,47	0.98	2 (4%)
6	BCL	M	404	-	69,74,74	1.82	17 (24%)	79,115,115	2.29	25 (31%)
8	6PL	5	102	-	51,51,51	0.27	0	57,59,59	0.31	0
10	LMT	F	101	-	36,36,36	1.18	5 (13%)	47,47,47	1.03	1 (2%)
6	BCL	Y	101	-	69,74,74	1.77	17 (24%)	79,115,115	2.35	23 (29%)
7	CRT	I	102	-	43,43,43	1.50	12 (27%)	48,54,54	1.65	14 (29%)
8	6PL	Q	102	-	47,47,51	0.28	0	53,55,59	0.31	0
14	QAK	M	407	-	39,40,40	1.48	3 (7%)	46,49,49	0.94	3 (6%)
6	BCL	E	101	-	69,74,74	1.78	18 (26%)	79,115,115	2.30	21 (26%)
6	BCL	J	103	-	69,74,74	1.79	17 (24%)	79,115,115	2.24	22 (27%)
7	CRT	X	101	-	43,43,43	1.50	12 (27%)	48,54,54	1.73	16 (33%)
6	BCL	P	102	-	69,74,74	1.78	17 (24%)	79,115,115	2.31	22 (27%)
6	BCL	L	301	-	69,74,74	1.79	17 (24%)	79,115,115	2.26	22 (27%)
12	U10	M	410	-	63,63,63	2.73	17 (26%)	78,79,79	1.78	22 (28%)
12	U10	L	303	-	48,48,63	2.75	14 (29%)	60,61,79	1.74	15 (25%)
6	BCL	5	103	-	69,74,74	1.79	17 (24%)	79,115,115	2.23	21 (26%)
6	BCL	A	100	-	69,74,74	1.78	18 (26%)	79,115,115	2.35	23 (29%)
7	CRT	G	102	-	43,43,43	1.51	12 (27%)	48,54,54	1.63	16 (33%)
6	BCL	3	100	-	69,74,74	1.79	18 (26%)	79,115,115	2.28	22 (27%)
9	CDL	M	409	-	83,83,99	0.29	0	89,95,111	0.38	0
8	6PL	P	103	-	51,51,51	0.28	0	57,59,59	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	6PL	4	104	-	51,51,51	0.28	0	57,59,59	0.35	0
7	CRT	8	101	-	43,43,43	1.52	12 (27%)	48,54,54	1.85	15 (31%)
6	BCL	R	101	-	69,74,74	1.78	17 (24%)	79,115,115	2.30	23 (29%)
10	LMT	2	101	-	36,36,36	1.15	3 (8%)	47,47,47	1.06	2 (4%)
7	CRT	U	101	-	43,43,43	1.50	12 (27%)	48,54,54	1.64	14 (29%)
6	BCL	F	102	-	69,74,74	1.80	17 (24%)	79,115,115	2.23	24 (30%)
6	BCL	U	100	-	69,74,74	1.80	17 (24%)	79,115,115	2.23	24 (30%)
8	6PL	X	102	-	51,51,51	0.28	0	57,59,59	0.34	0
8	6PL	I	101	-	51,51,51	0.28	0	57,59,59	0.37	0
8	6PL	8	102	-	51,51,51	0.28	0	57,59,59	0.31	0
8	6PL	0	102	-	51,51,51	0.28	0	57,59,59	0.40	0
8	6PL	L	305	-	51,51,51	0.30	0	57,59,59	0.34	0
8	6PL	E	102	-	51,51,51	0.29	0	57,59,59	0.28	0
12	U10	L	307	-	63,63,63	2.76	17 (26%)	78,79,79	1.74	20 (25%)
6	BCL	M	402	-	69,74,74	1.77	17 (24%)	79,115,115	2.25	23 (29%)
6	BCL	G	103	-	69,74,74	1.77	17 (24%)	79,115,115	2.36	23 (29%)
9	CDL	M	408	-	89,89,99	0.29	0	95,101,111	0.37	0
6	BCL	Y	102	-	69,74,74	1.79	17 (24%)	79,115,115	2.17	22 (27%)
7	CRT	4	103	-	43,43,43	1.50	12 (27%)	48,54,54	1.69	15 (31%)
8	6PL	2	103	-	46,46,51	0.29	0	52,54,59	0.32	0
6	BCL	J	101	-	69,74,74	1.78	17 (24%)	79,115,115	2.34	23 (29%)
6	BCL	N	101	-	69,74,74	1.78	17 (24%)	79,115,115	2.29	24 (30%)
7	CRT	Q	101	-	43,43,43	1.50	12 (27%)	48,54,54	1.61	15 (31%)
7	CRT	Z	102	-	43,43,43	1.50	12 (27%)	48,54,54	1.57	14 (29%)
6	BCL	Q	100	-	69,74,74	1.79	17 (24%)	79,115,115	2.22	22 (27%)
10	LMT	6	101	-	36,36,36	1.18	5 (13%)	47,47,47	1.05	1 (2%)
7	CRT	0	101	-	43,43,43	1.50	12 (27%)	48,54,54	1.61	14 (29%)
8	6PL	S	102	-	51,51,51	0.28	0	57,59,59	0.40	0
10	LMT	B	101	-	36,36,36	1.15	3 (8%)	47,47,47	0.99	1 (2%)
6	BCL	0	100	-	69,74,74	1.79	17 (24%)	79,115,115	2.27	24 (30%)
6	BCL	R	103	-	69,74,74	1.78	17 (24%)	79,115,115	2.21	23 (29%)
8	6PL	L	304	-	51,51,51	0.27	0	57,59,59	0.36	0
10	LMT	J	102	-	36,36,36	1.12	4 (11%)	47,47,47	1.12	3 (6%)
7	CRT	D	101	-	43,43,43	1.50	12 (27%)	48,54,54	1.63	16 (33%)
7	CRT	7	101	-	43,43,43	1.51	12 (27%)	48,54,54	1.62	14 (29%)
8	6PL	F	103	-	51,51,51	0.26	0	57,59,59	0.41	0
6	BCL	L	308	-	69,74,74	1.83	17 (24%)	79,115,115	2.23	21 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	BCL	T	100	-	69,74,74	1.78	17 (24%)	79,115,115	2.34	25 (31%)
10	LMT	4	101	-	36,36,36	1.14	5 (13%)	47,47,47	1.17	5 (10%)
10	LMT	L	306	-	36,36,36	1.12	6 (16%)	47,47,47	1.02	2 (4%)
7	CRT	K	101	-	43,43,43	1.49	12 (27%)	48,54,54	1.62	13 (27%)
7	CRT	B	103	-	43,43,43	1.51	12 (27%)	48,54,54	1.56	14 (29%)
10	LMT	Z	101	-	36,36,36	1.14	4 (11%)	47,47,47	1.04	2 (4%)
6	BCL	C	102	-	69,74,74	1.79	17 (24%)	79,115,115	2.18	23 (29%)
6	BCL	C	101	-	69,74,74	1.78	17 (24%)	79,115,115	2.30	22 (27%)
6	BCL	4	102	-	69,74,74	1.81	17 (24%)	79,115,115	2.19	23 (29%)
8	6PL	D	102	-	51,51,51	0.28	0	57,59,59	0.30	0
7	CRT	S	101	-	43,43,43	1.50	11 (25%)	48,54,54	1.61	16 (33%)
8	6PL	M	401	-	51,51,51	0.28	0	57,59,59	0.33	0
6	BCL	N	102	-	69,74,74	1.80	17 (24%)	79,115,115	2.22	21 (26%)
10	LMT	H	302	-	36,36,36	1.13	5 (13%)	47,47,47	1.07	3 (6%)
10	LMT	R	102	-	36,36,36	1.15	5 (13%)	47,47,47	1.13	3 (6%)
8	6PL	B	104	-	51,51,51	0.28	0	57,59,59	0.38	0
9	CDL	E	103	-	86,86,99	0.29	0	92,98,111	0.38	0
7	CRT	O	102	-	43,43,43	1.50	10 (23%)	48,54,54	1.61	13 (27%)
8	6PL	K	102	-	51,51,51	0.27	0	57,59,59	0.34	0
6	BCL	7	104	-	69,74,74	1.79	17 (24%)	79,115,115	2.25	22 (27%)
9	CDL	L	310	-	99,99,99	0.27	0	105,111,111	0.31	0
12	U10	L	309	-	63,63,63	2.78	17 (26%)	78,79,79	1.82	23 (29%)
11	BPH	M	405	-	59,70,70	0.76	3 (5%)	59,101,101	0.89	3 (5%)
11	BPH	L	302	-	59,70,70	0.78	3 (5%)	59,101,101	0.91	3 (5%)
8	6PL	O	103	-	46,46,51	0.29	0	52,54,59	0.33	0
6	BCL	9	102	-	69,74,74	1.78	18 (26%)	79,115,115	2.37	24 (30%)
6	BCL	B	102	-	69,74,74	1.79	17 (24%)	79,115,115	2.19	23 (29%)
8	6PL	6	102	-	51,51,51	0.27	0	57,59,59	0.34	0
6	BCL	5	101	-	69,74,74	1.78	16 (23%)	79,115,115	2.27	24 (30%)
8	6PL	I	103	-	51,51,51	0.27	0	57,59,59	0.36	0
6	BCL	V	102	-	69,74,74	1.79	17 (24%)	79,115,115	2.20	23 (29%)
6	BCL	G	104	-	69,74,74	1.79	17 (24%)	79,115,115	2.20	21 (26%)
8	6PL	U	102	-	51,51,51	0.27	0	57,59,59	0.31	0
6	BCL	7	102	-	69,74,74	1.79	17 (24%)	79,115,115	2.30	22 (27%)
8	6PL	H	301	-	51,51,51	0.28	0	57,59,59	0.42	0
12	U10	M	406	-	48,48,63	2.75	14 (29%)	60,61,79	1.61	13 (21%)
6	BCL	1	101	-	69,74,74	1.78	18 (26%)	79,115,115	2.34	23 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	BCL	V	101	-	69,74,74	1.77	17 (24%)	79,115,115	2.28	22 (27%)
15	PGT	9	101	-	50,50,50	0.27	0	53,56,56	0.35	0
9	CDL	G	105	-	89,89,99	0.30	0	95,101,111	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	6PL	Z	103	-	-	11/55/55/55	-
10	LMT	O	101	-	-	9/21/61/61	0/2/2/2
15	PGT	7	103	-	-	8/55/55/55	-
7	CRT	2	102	-	-	3/51/51/51	-
6	BCL	1	102	-	-	9/41/137/137	-
9	CDL	G	101	-	-	12/110/110/110	-
10	LMT	P	101	-	-	6/21/61/61	0/2/2/2
6	BCL	M	404	-	-	13/41/137/137	-
8	6PL	5	102	-	-	12/55/55/55	-
10	LMT	F	101	-	-	10/21/61/61	0/2/2/2
6	BCL	Y	101	-	-	11/41/137/137	-
7	CRT	I	102	-	-	0/51/51/51	-
8	6PL	Q	102	-	-	8/51/51/55	-
14	QAK	M	407	-	3/3/8/12	22/44/44/44	-
6	BCL	E	101	-	-	19/41/137/137	-
6	BCL	J	103	-	-	11/41/137/137	-
7	CRT	X	101	-	-	1/51/51/51	-
6	BCL	P	102	-	-	16/41/137/137	-
6	BCL	L	301	-	-	11/41/137/137	-
12	U10	M	410	-	-	20/63/87/87	0/1/1/1
12	U10	L	303	-	-	18/45/69/87	0/1/1/1
6	BCL	5	103	-	-	8/41/137/137	-
6	BCL	A	100	-	-	20/41/137/137	-
7	CRT	G	102	-	-	0/51/51/51	-
6	BCL	3	100	-	-	19/41/137/137	-
9	CDL	M	409	-	-	6/94/94/110	-
8	6PL	P	103	-	-	11/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	6PL	4	104	-	-	5/55/55/55	-
7	CRT	8	101	-	-	1/51/51/51	-
6	BCL	R	101	-	-	16/41/137/137	-
10	LMT	2	101	-	-	13/21/61/61	0/2/2/2
7	CRT	U	101	-	-	0/51/51/51	-
6	BCL	F	102	-	-	15/41/137/137	-
6	BCL	U	100	-	-	16/41/137/137	-
8	6PL	X	102	-	-	5/55/55/55	-
8	6PL	I	101	-	-	11/55/55/55	-
8	6PL	8	102	-	-	6/55/55/55	-
8	6PL	0	102	-	-	7/55/55/55	-
8	6PL	L	305	-	-	8/55/55/55	-
8	6PL	E	102	-	-	11/55/55/55	-
12	U10	L	307	-	-	27/63/87/87	0/1/1/1
6	BCL	M	402	-	-	9/41/137/137	-
6	BCL	G	103	-	-	15/41/137/137	-
9	CDL	M	408	-	-	8/100/100/110	-
6	BCL	Y	102	-	-	16/41/137/137	-
7	CRT	4	103	-	-	0/51/51/51	-
8	6PL	2	103	-	-	11/50/50/55	-
6	BCL	J	101	-	-	14/41/137/137	-
6	BCL	N	101	-	-	16/41/137/137	-
7	CRT	Q	101	-	-	1/51/51/51	-
7	CRT	Z	102	-	-	0/51/51/51	-
6	BCL	Q	100	-	-	10/41/137/137	-
10	LMT	6	101	-	-	7/21/61/61	0/2/2/2
7	CRT	0	101	-	-	0/51/51/51	-
8	6PL	S	102	-	-	5/55/55/55	-
10	LMT	B	101	-	-	9/21/61/61	0/2/2/2
6	BCL	0	100	-	-	13/41/137/137	-
6	BCL	R	103	-	-	9/41/137/137	-
8	6PL	L	304	-	-	6/55/55/55	-
10	LMT	J	102	-	-	6/21/61/61	0/2/2/2
7	CRT	D	101	-	-	0/51/51/51	-
7	CRT	7	101	-	-	1/51/51/51	-
8	6PL	F	103	-	-	8/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BCL	L	308	-	-	15/41/137/137	-
6	BCL	T	100	-	-	16/41/137/137	-
10	LMT	4	101	-	-	10/21/61/61	0/2/2/2
10	LMT	L	306	-	-	13/21/61/61	0/2/2/2
7	CRT	K	101	-	-	0/51/51/51	-
7	CRT	B	103	-	-	0/51/51/51	-
10	LMT	Z	101	-	-	11/21/61/61	0/2/2/2
6	BCL	C	102	-	-	12/41/137/137	-
6	BCL	C	101	-	-	15/41/137/137	-
6	BCL	4	102	-	-	9/41/137/137	-
8	6PL	D	102	-	-	4/55/55/55	-
7	CRT	S	101	-	-	0/51/51/51	-
8	6PL	M	401	-	-	8/55/55/55	-
6	BCL	N	102	-	-	8/41/137/137	-
10	LMT	H	302	-	-	10/21/61/61	0/2/2/2
10	LMT	R	102	-	-	15/21/61/61	0/2/2/2
8	6PL	B	104	-	-	7/55/55/55	-
9	CDL	E	103	-	-	10/97/97/110	-
7	CRT	O	102	-	-	1/51/51/51	-
8	6PL	K	102	-	-	11/55/55/55	-
6	BCL	7	104	-	-	15/41/137/137	-
9	CDL	L	310	-	-	18/110/110/110	-
12	U10	L	309	-	-	23/63/87/87	0/1/1/1
11	BPH	M	405	-	2/2/18/22	5/37/105/105	0/5/6/6
11	BPH	L	302	-	2/2/18/22	7/37/105/105	0/5/6/6
8	6PL	O	103	-	-	12/50/50/55	-
6	BCL	9	102	-	-	11/41/137/137	-
6	BCL	B	102	-	-	15/41/137/137	-
8	6PL	6	102	-	-	4/55/55/55	-
6	BCL	5	101	-	-	18/41/137/137	-
8	6PL	I	103	-	-	7/55/55/55	-
6	BCL	V	102	-	-	11/41/137/137	-
6	BCL	G	104	-	-	11/41/137/137	-
8	6PL	U	102	-	-	5/55/55/55	-
6	BCL	7	102	-	-	22/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	6PL	H	301	-	-	4/55/55/55	-
12	U10	M	406	-	-	10/45/69/87	0/1/1/1
6	BCL	1	101	-	-	12/41/137/137	-
6	BCL	V	101	-	-	22/41/137/137	-
15	PGT	9	101	-	-	5/55/55/55	-
9	CDL	G	105	-	-	16/100/100/110	-

The worst 5 of 949 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	410	U10	C38-C39	6.34	1.47	1.33
12	L	303	U10	C23-C24	6.34	1.47	1.33
12	L	309	U10	C38-C39	6.32	1.47	1.33
12	L	307	U10	C23-C24	6.31	1.47	1.33
12	M	410	U10	C43-C44	6.30	1.47	1.33

The worst 5 of 1183 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	9	102	BCL	CMD-C2D-C1D	8.36	139.45	124.73
6	5	101	BCL	CMD-C2D-C1D	8.35	139.43	124.73
6	T	100	BCL	CMD-C2D-C1D	8.34	139.42	124.73
6	G	103	BCL	CMD-C2D-C1D	8.32	139.37	124.73
6	Y	101	BCL	CMD-C2D-C1D	8.31	139.35	124.73

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	L	302	BPH	C13
11	L	302	BPH	C8
11	M	405	BPH	C13
11	M	405	BPH	C8
14	M	407	QAK	C19

5 of 1027 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	101	BCL	C2C-C3C-CAC-CBC
6	C	101	BCL	C4C-C3C-CAC-CBC
6	C	101	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
6	C	101	BCL	C4-C3-C5-C6
6	C	102	BCL	C1A-C2A-CAA-CBA

There are no ring outliers.

100 monomers are involved in 357 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	Z	103	6PL	4	0
10	O	101	LMT	1	0
15	7	103	PGT	4	0
7	2	102	CRT	5	0
6	1	102	BCL	7	0
9	G	101	CDL	12	0
10	P	101	LMT	2	0
6	M	404	BCL	3	0
8	5	102	6PL	2	0
10	F	101	LMT	3	0
6	Y	101	BCL	4	0
7	I	102	CRT	2	0
8	Q	102	6PL	6	0
6	E	101	BCL	1	0
6	J	103	BCL	4	0
7	X	101	CRT	14	0
6	P	102	BCL	4	0
12	M	410	U10	6	0
12	L	303	U10	1	0
6	5	103	BCL	5	0
6	A	100	BCL	8	0
7	G	102	CRT	4	0
6	3	100	BCL	2	0
9	M	409	CDL	3	0
8	P	103	6PL	4	0
8	4	104	6PL	5	0
7	8	101	CRT	5	0
6	R	101	BCL	4	0
10	2	101	LMT	2	0
7	U	101	CRT	5	0
6	F	102	BCL	4	0
6	U	100	BCL	5	0
8	X	102	6PL	3	0
8	I	101	6PL	5	0
8	8	102	6PL	4	0

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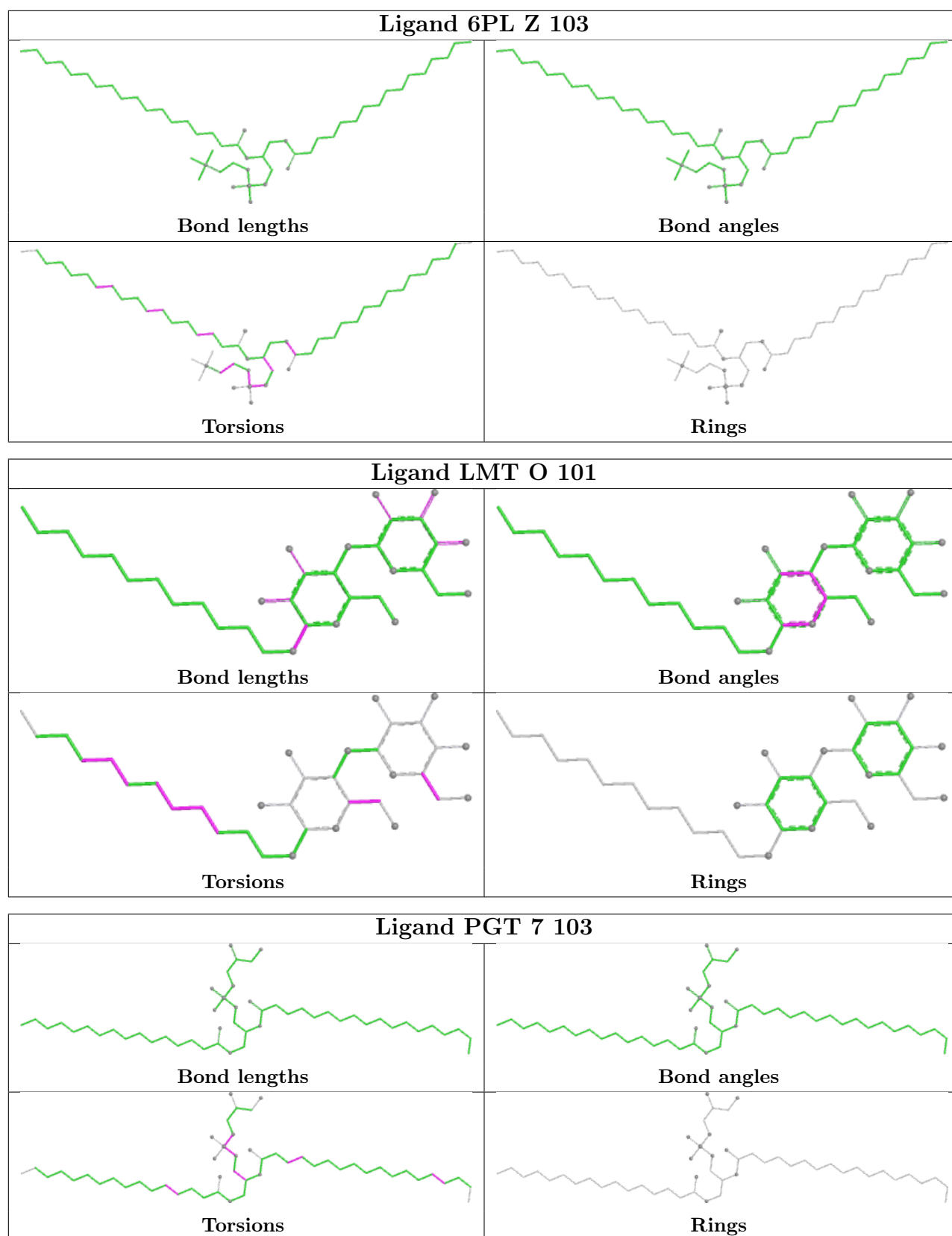
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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8	L	305	6PL	7	0
8	E	102	6PL	6	0
12	L	307	U10	8	0
6	M	402	BCL	1	0
6	G	103	BCL	3	0
9	M	408	CDL	7	0
6	Y	102	BCL	8	0
7	4	103	CRT	11	0
8	2	103	6PL	7	0
6	J	101	BCL	1	0
6	N	101	BCL	2	0
7	Q	101	CRT	4	0
7	Z	102	CRT	7	0
6	Q	100	BCL	5	0
10	6	101	LMT	3	0
7	0	101	CRT	5	0
8	S	102	6PL	5	0
10	B	101	LMT	2	0
6	0	100	BCL	4	0
6	R	103	BCL	4	0
8	L	304	6PL	4	0
10	J	102	LMT	7	0
7	D	101	CRT	5	0
7	7	101	CRT	2	0
8	F	103	6PL	3	0
6	L	308	BCL	5	0
6	T	100	BCL	4	0
10	4	101	LMT	3	0
7	K	101	CRT	2	0
7	B	103	CRT	4	0
10	Z	101	LMT	1	0
6	C	102	BCL	4	0
6	C	101	BCL	2	0
6	4	102	BCL	6	0
8	D	102	6PL	5	0
7	S	101	CRT	3	0
8	M	401	6PL	5	0
6	N	102	BCL	2	0
10	H	302	LMT	4	0
10	R	102	LMT	3	0
8	B	104	6PL	4	0

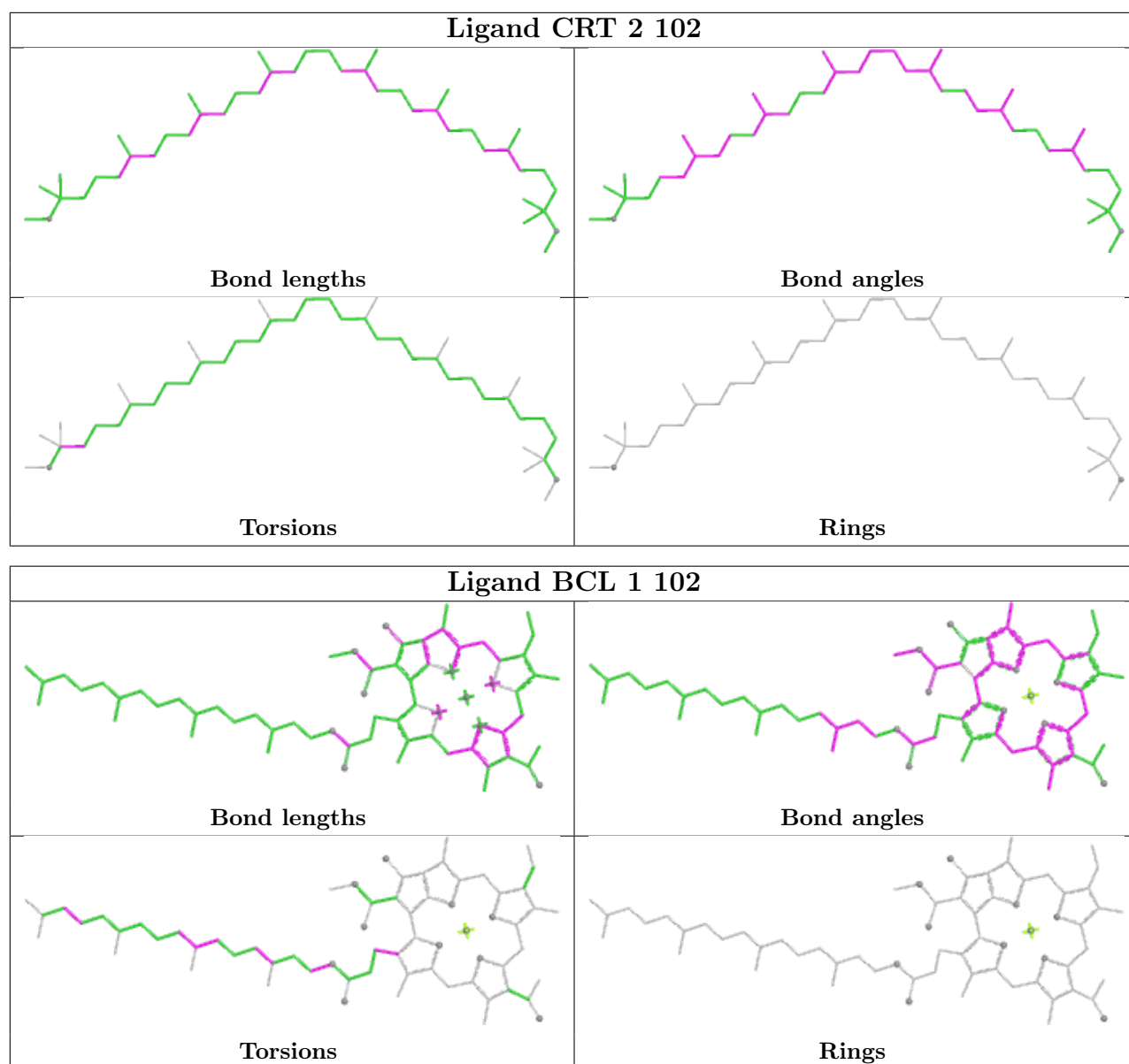
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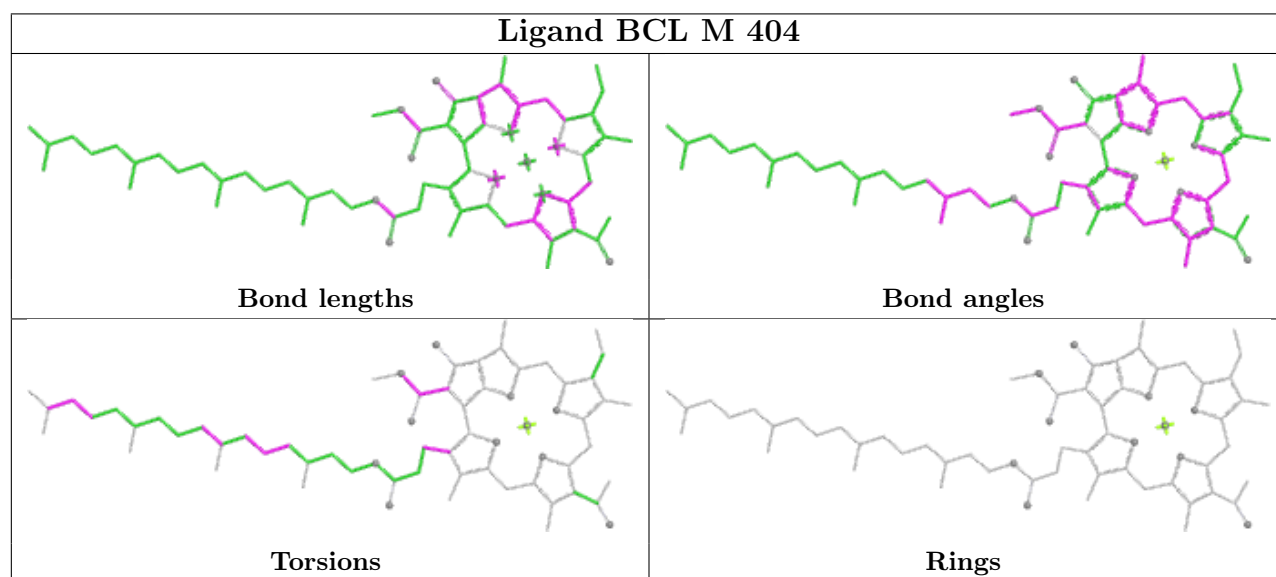
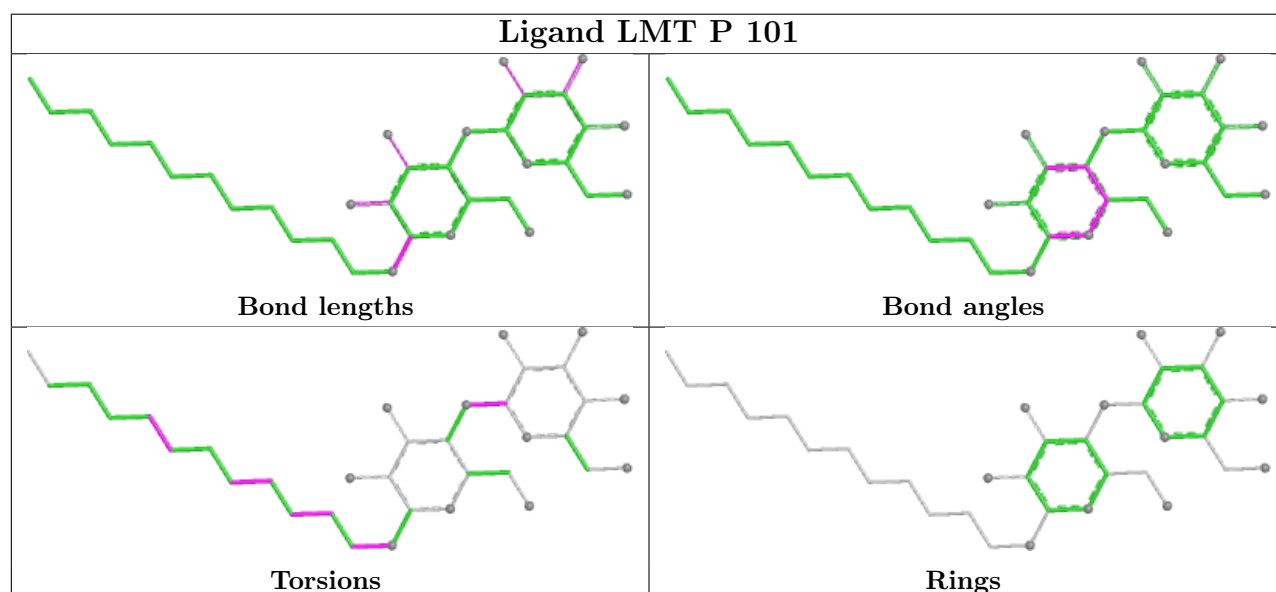
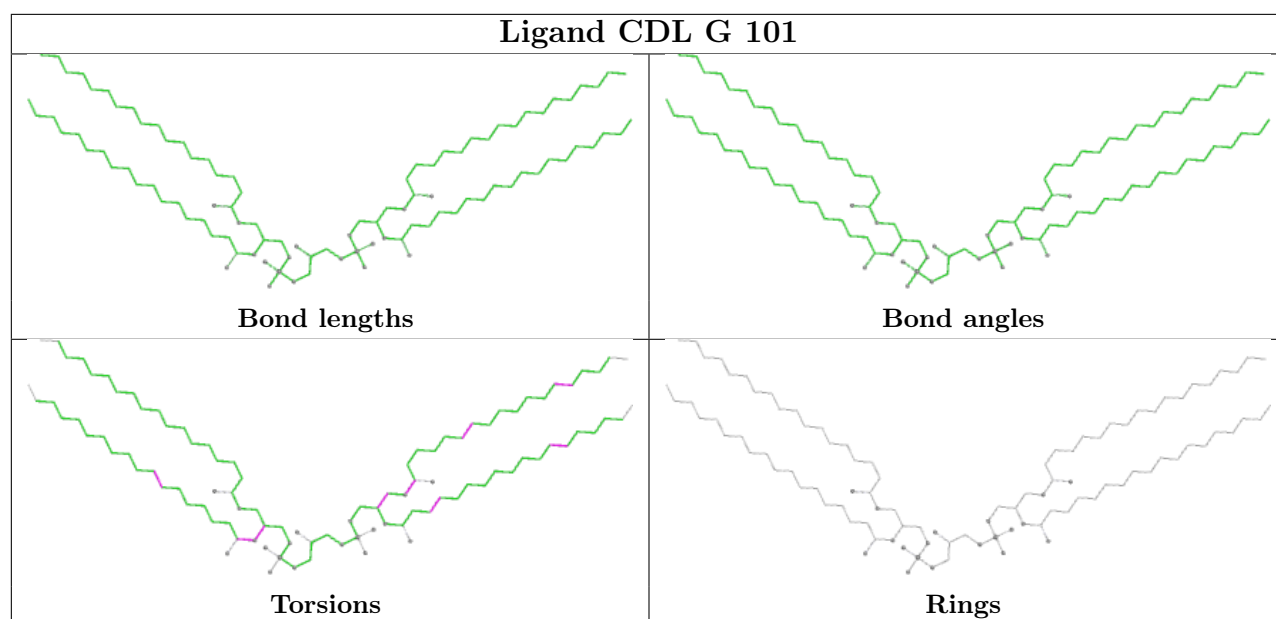
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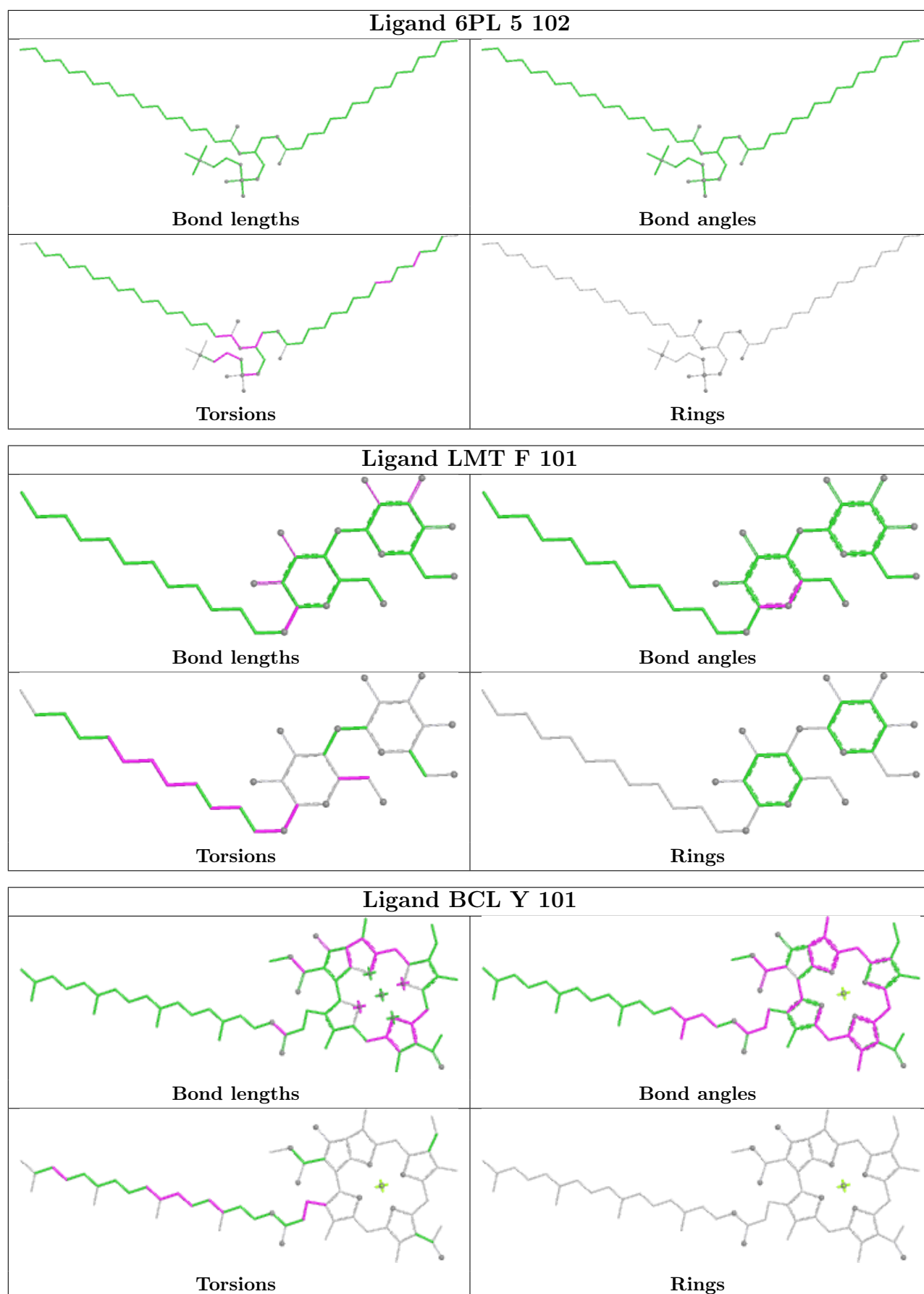
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	E	103	CDL	7	0
7	O	102	CRT	4	0
8	K	102	6PL	3	0
6	7	104	BCL	4	0
9	L	310	CDL	9	0
12	L	309	U10	4	0
11	M	405	BPH	6	0
11	L	302	BPH	5	0
8	O	103	6PL	4	0
6	9	102	BCL	1	0
6	B	102	BCL	6	0
8	6	102	6PL	4	0
6	5	101	BCL	5	0
8	I	103	6PL	5	0
6	V	102	BCL	4	0
6	G	104	BCL	5	0
8	U	102	6PL	4	0
6	7	102	BCL	1	0
12	M	406	U10	3	0
6	1	101	BCL	3	0
6	V	101	BCL	2	0
15	9	101	PGT	3	0
9	G	105	CDL	9	0

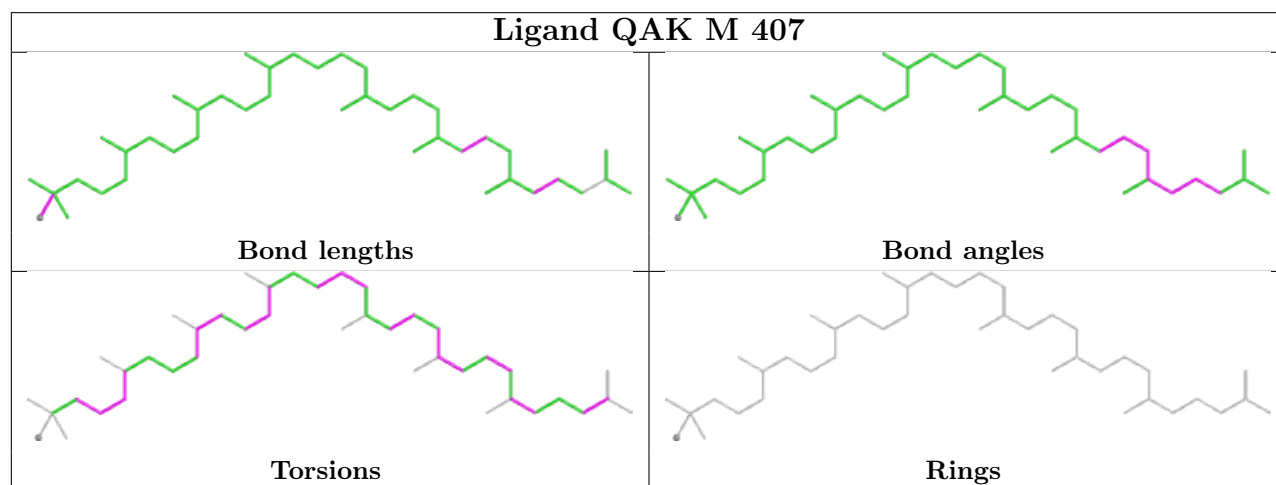
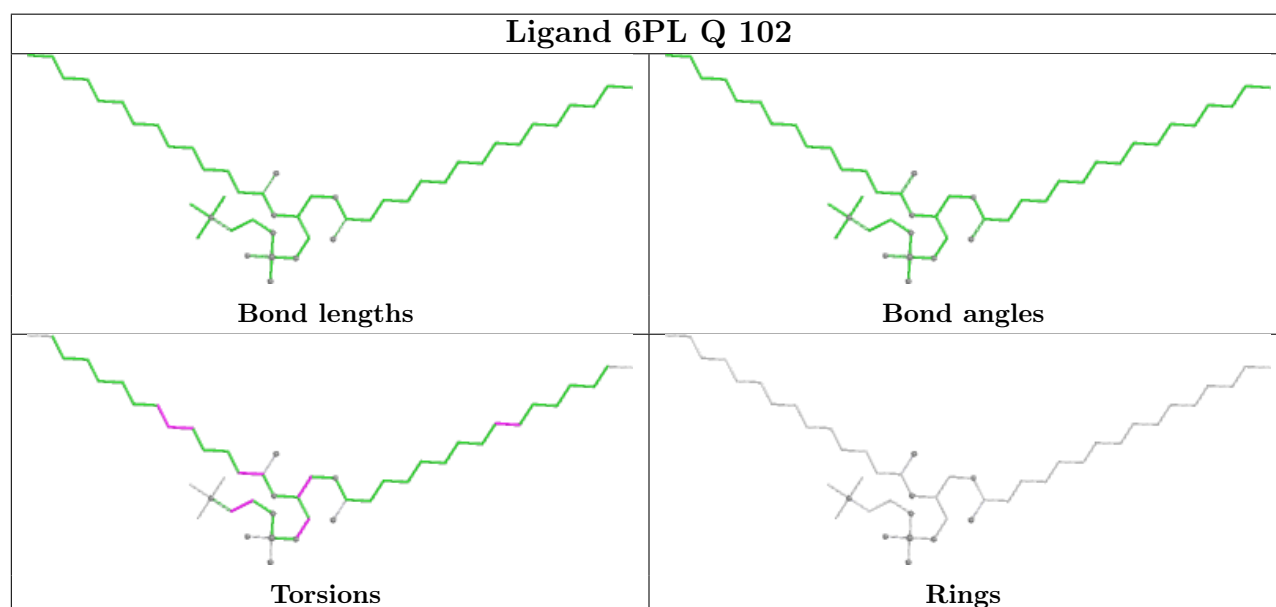
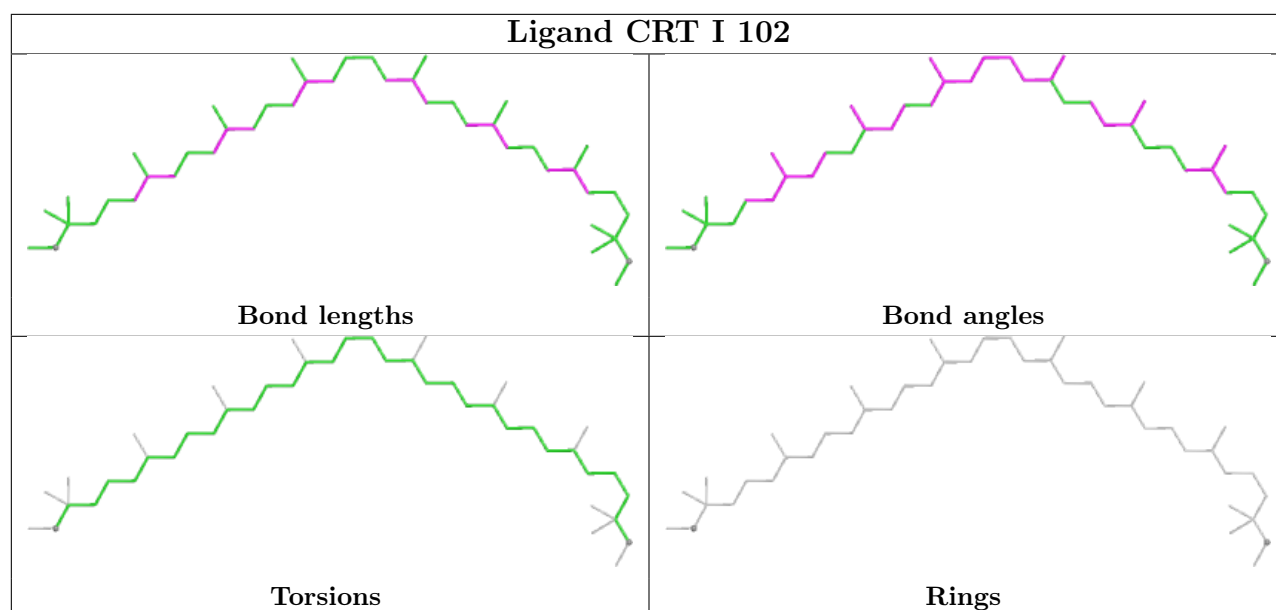
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

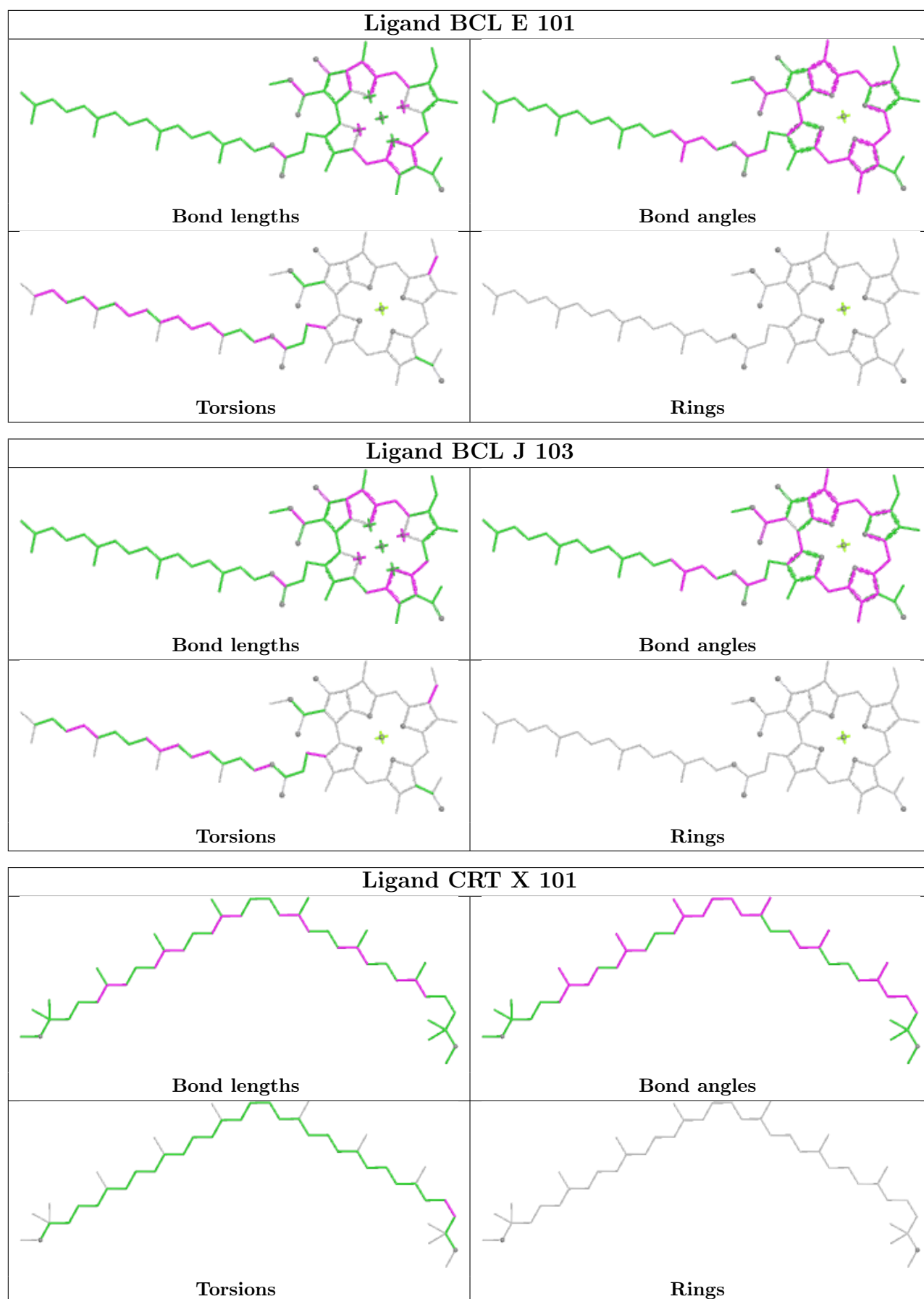


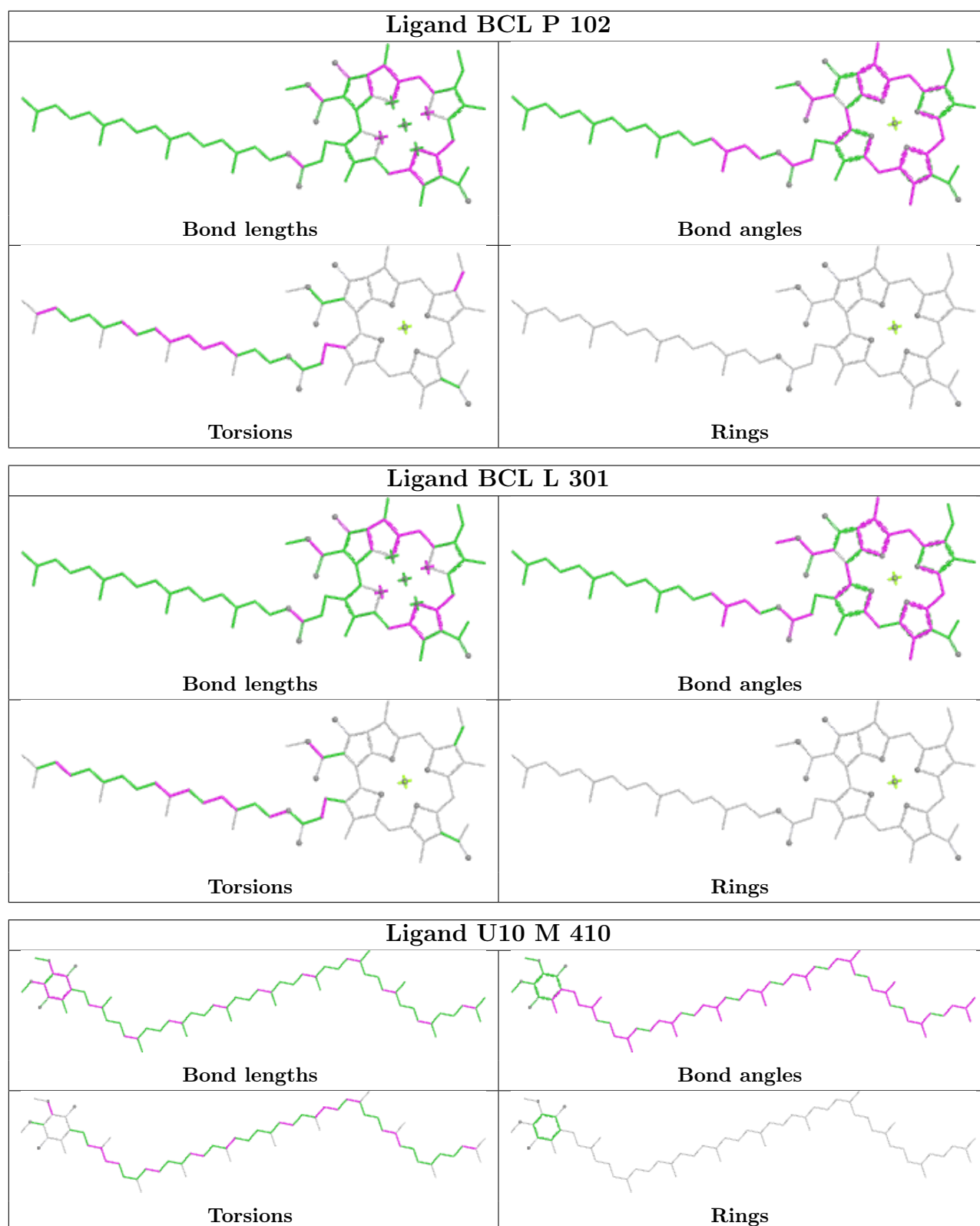


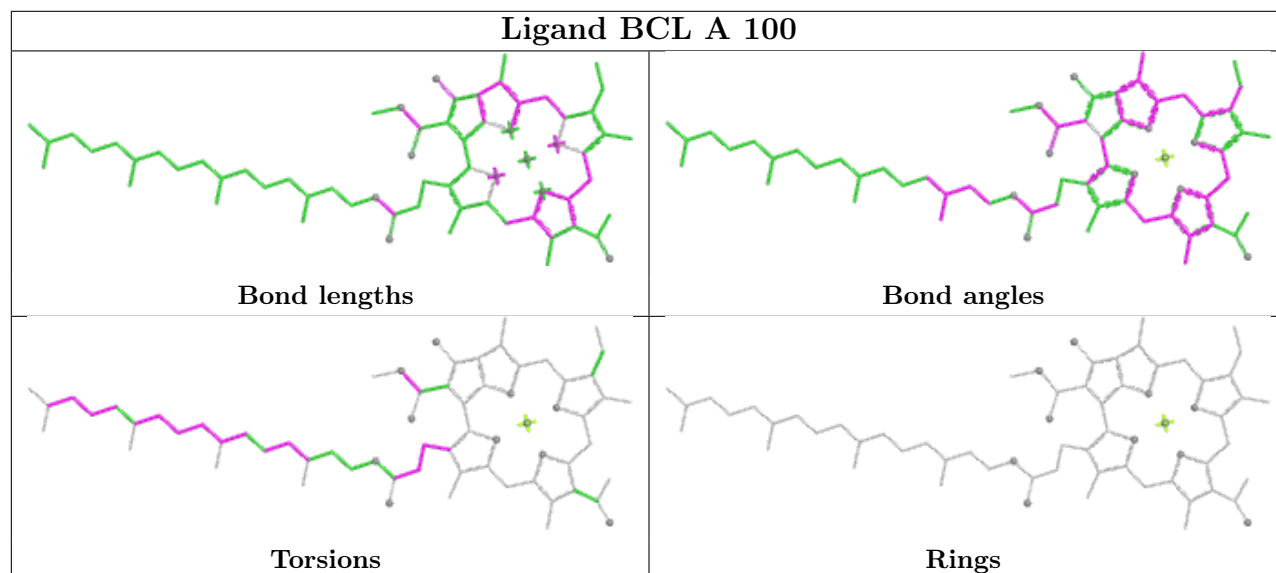
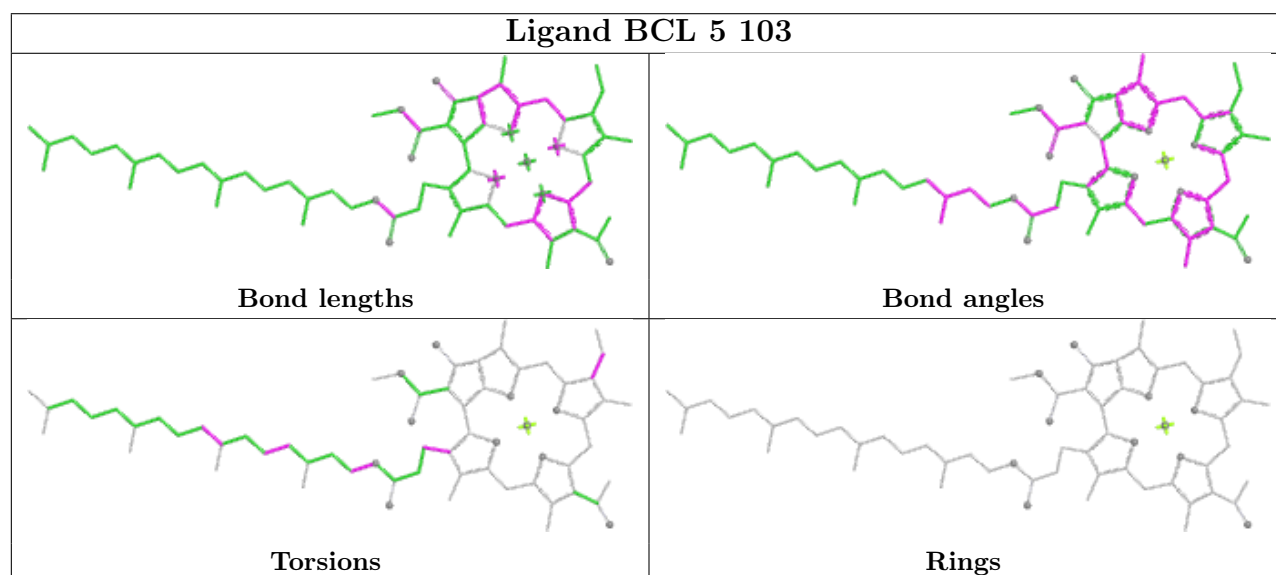
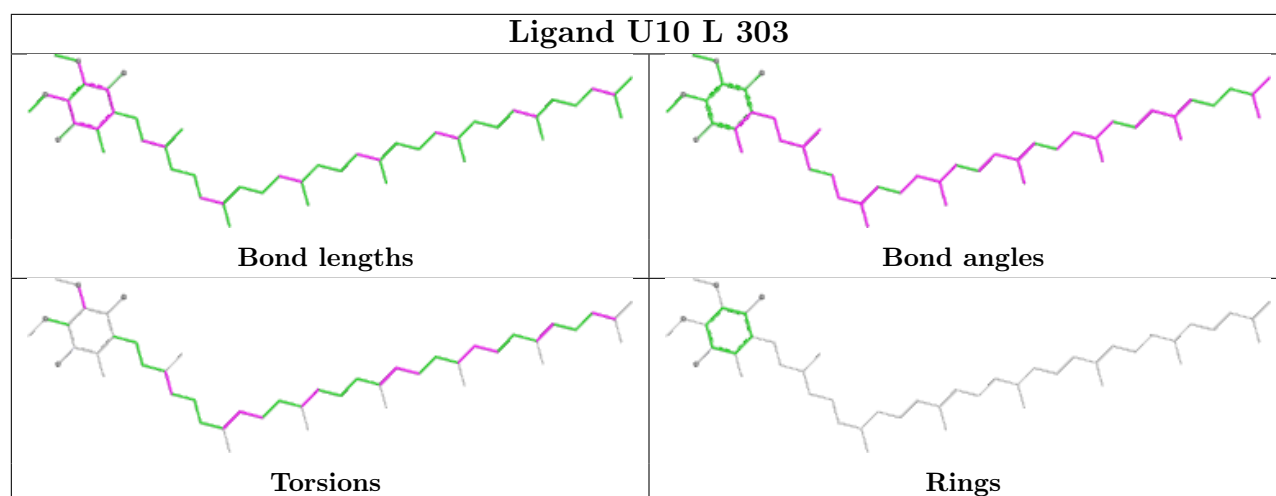


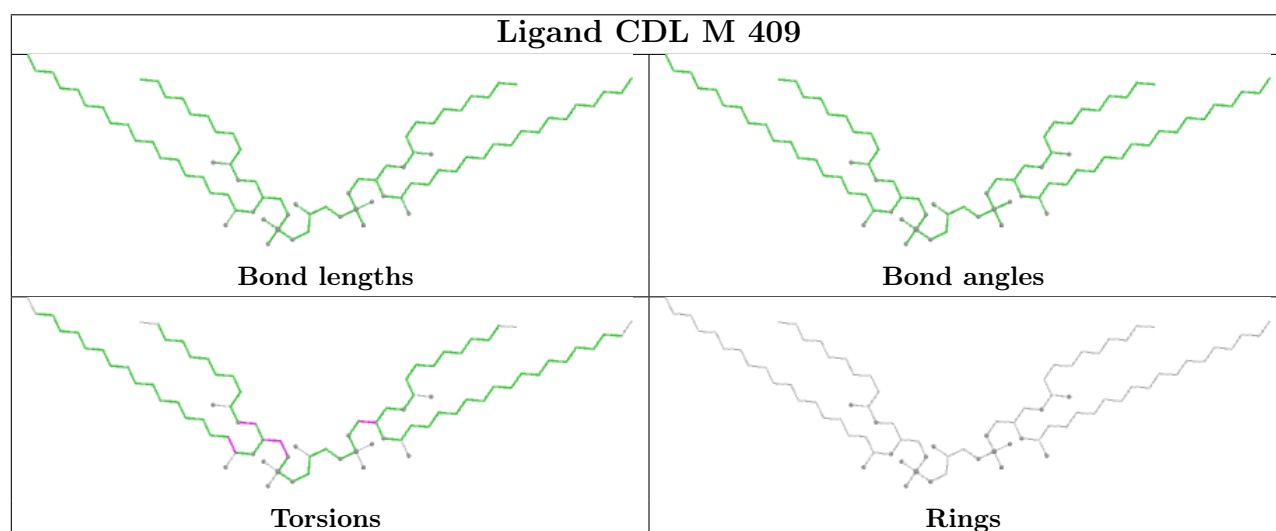
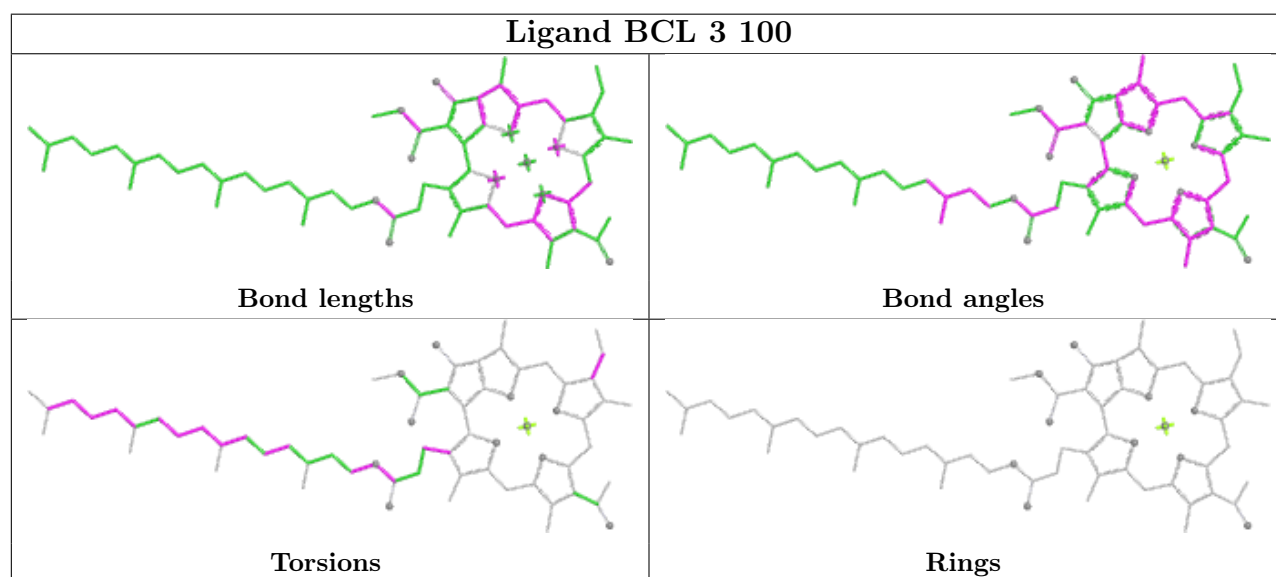
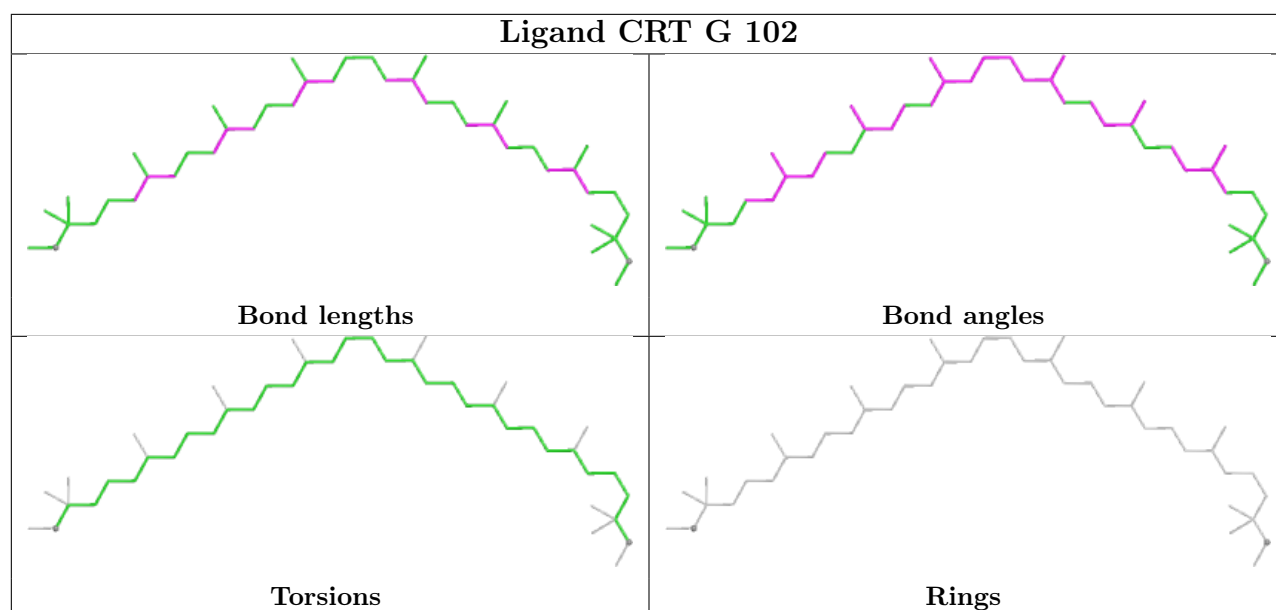


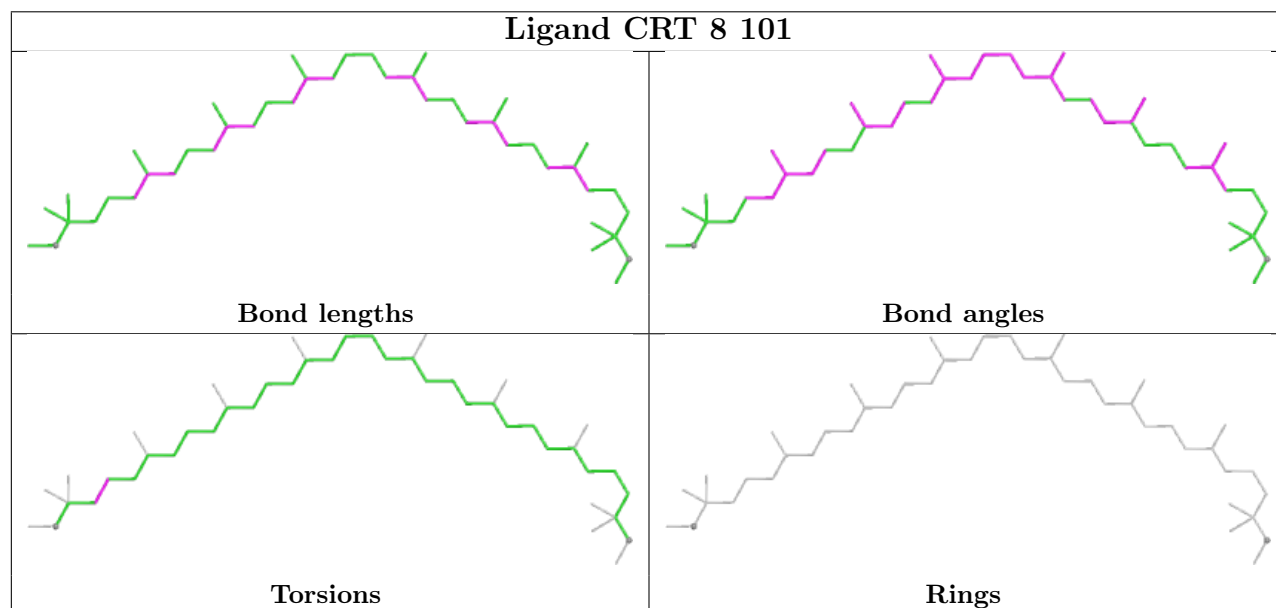
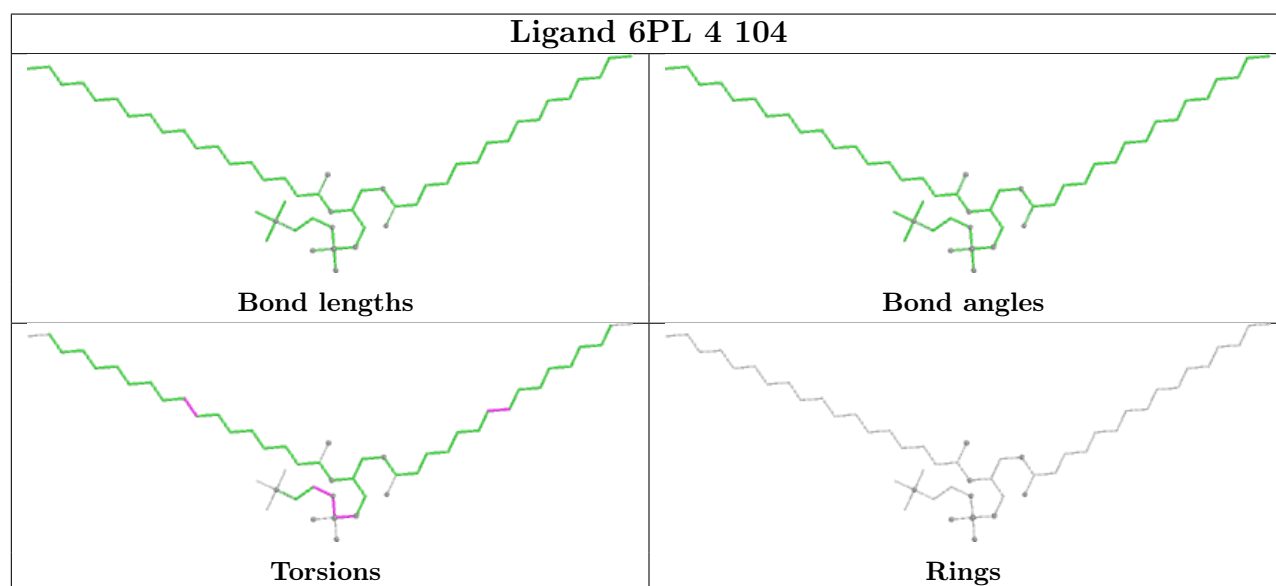
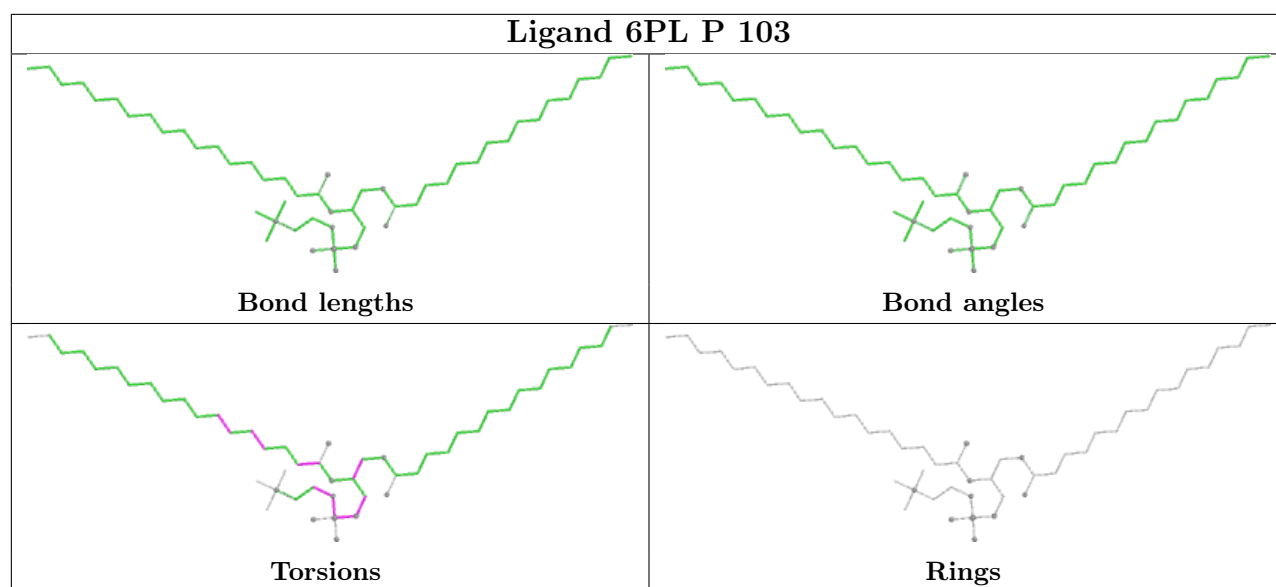


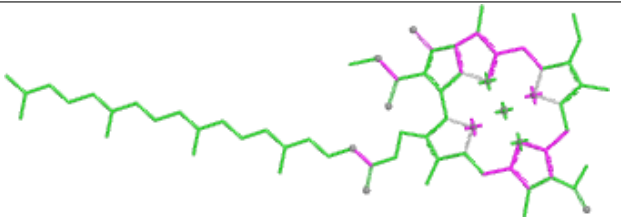
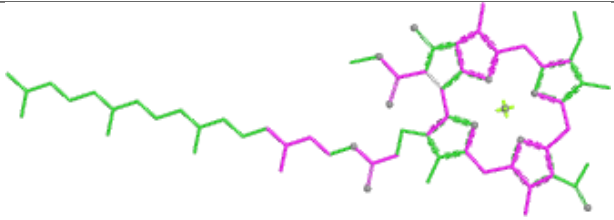
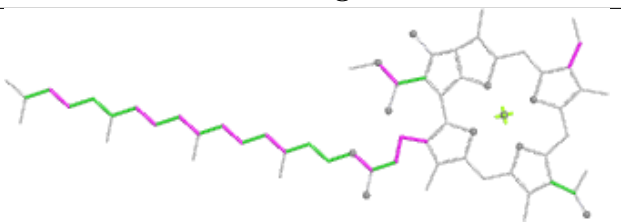
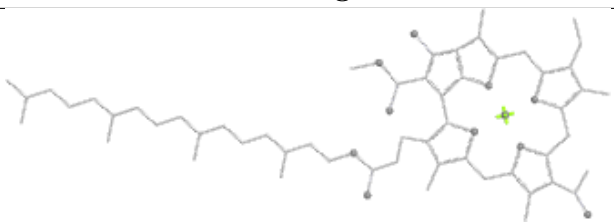


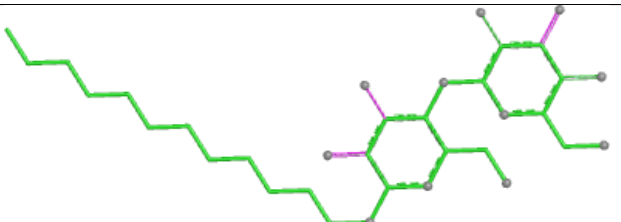
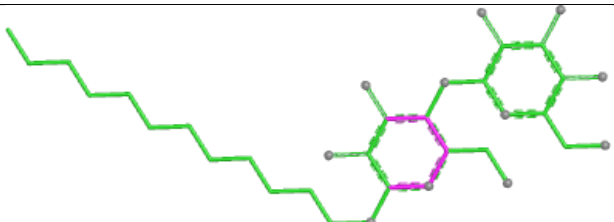
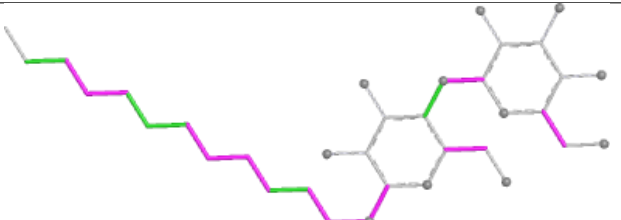
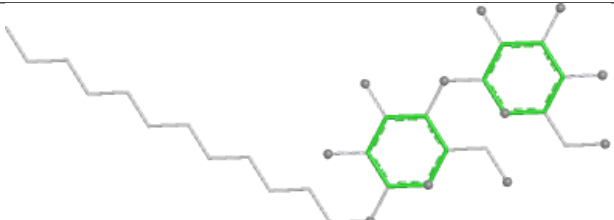


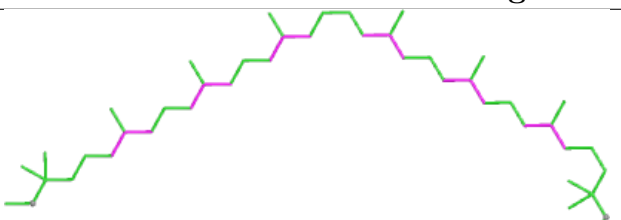
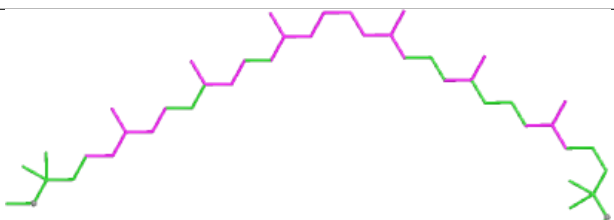
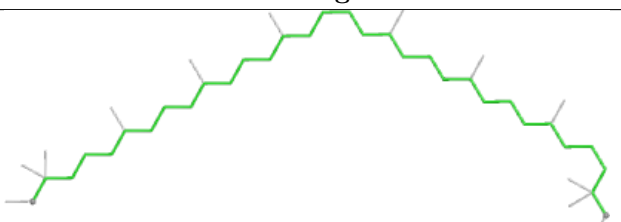
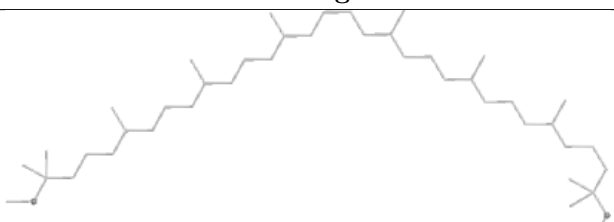


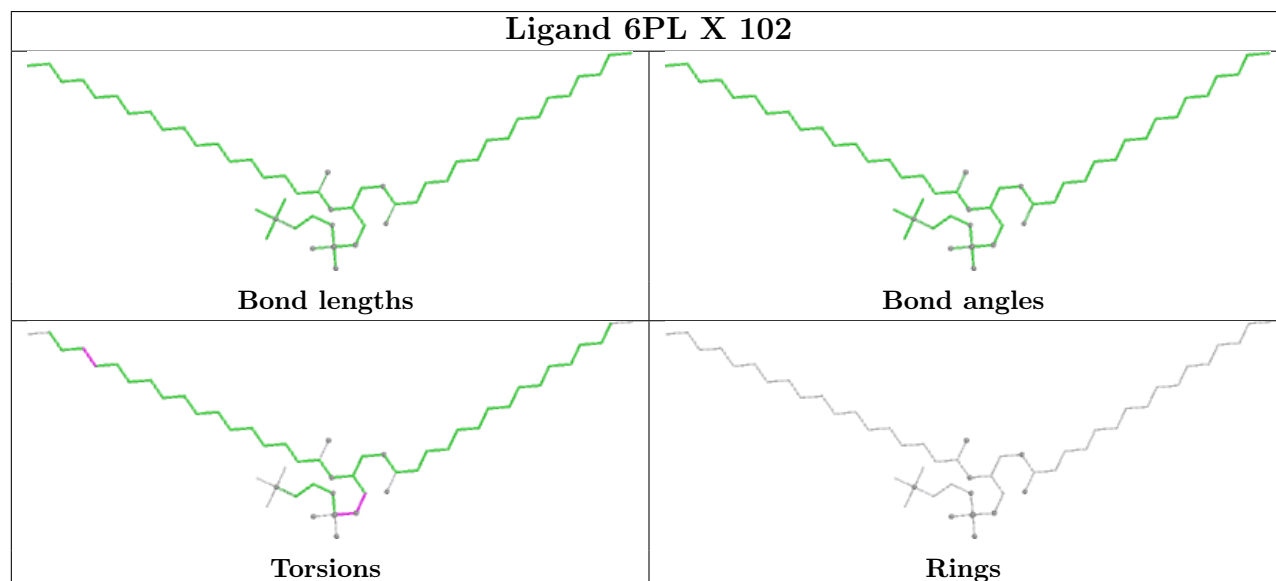
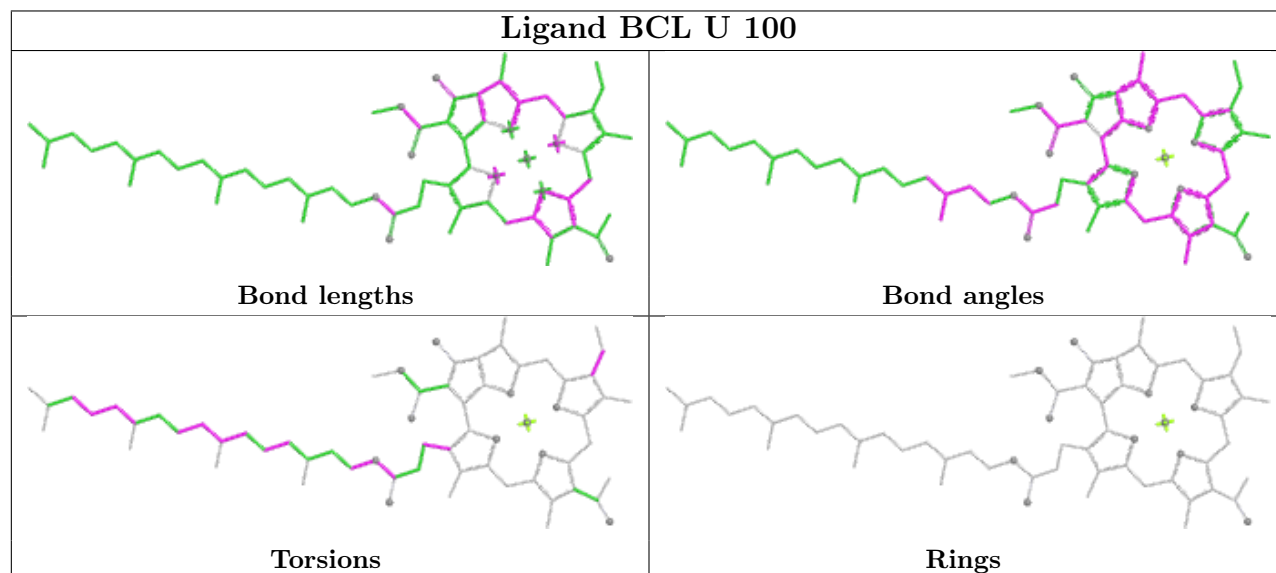
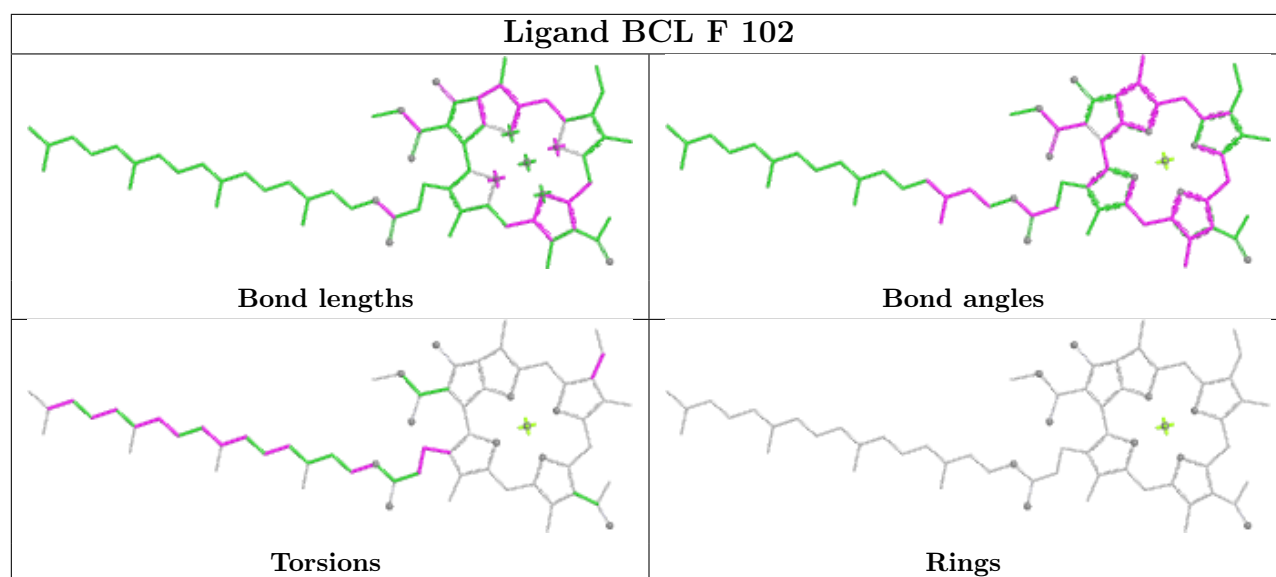


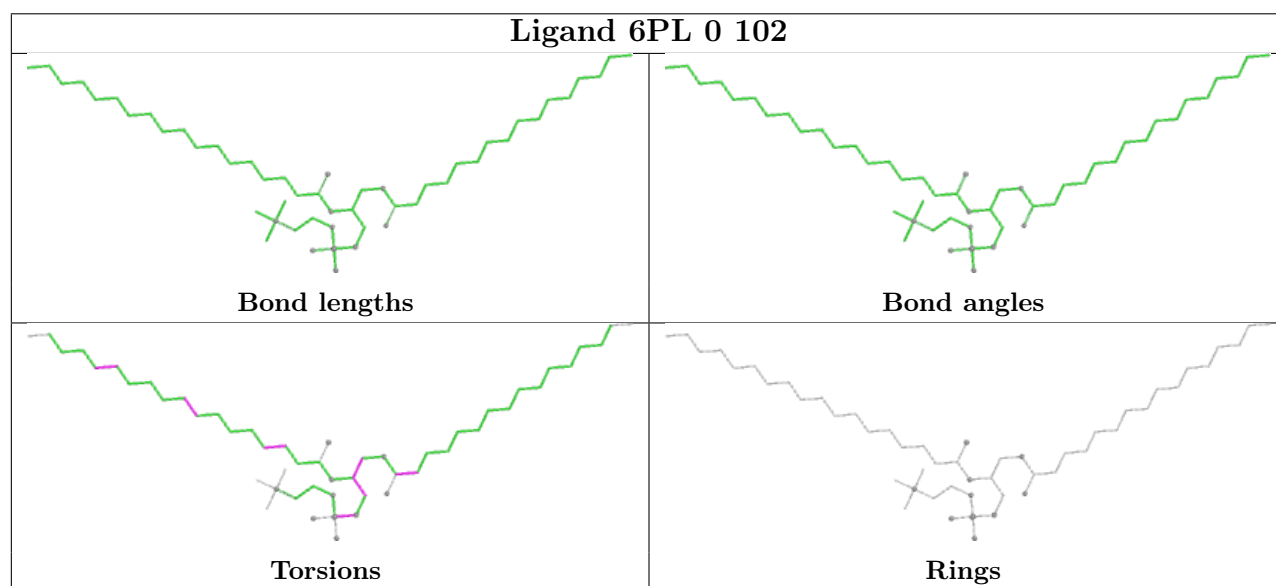
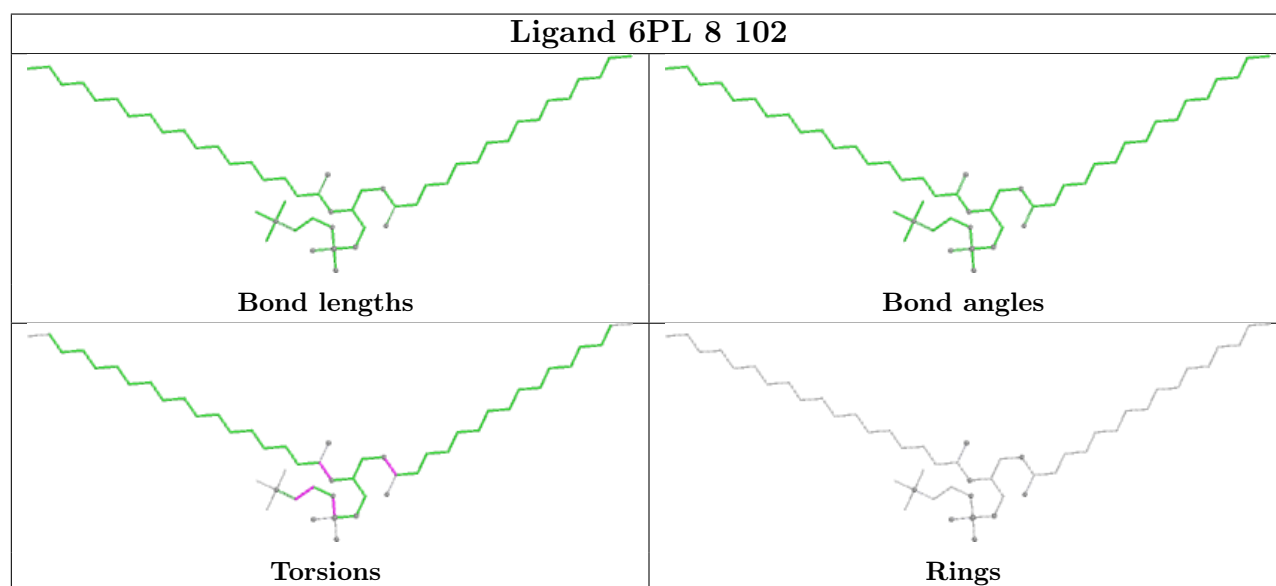
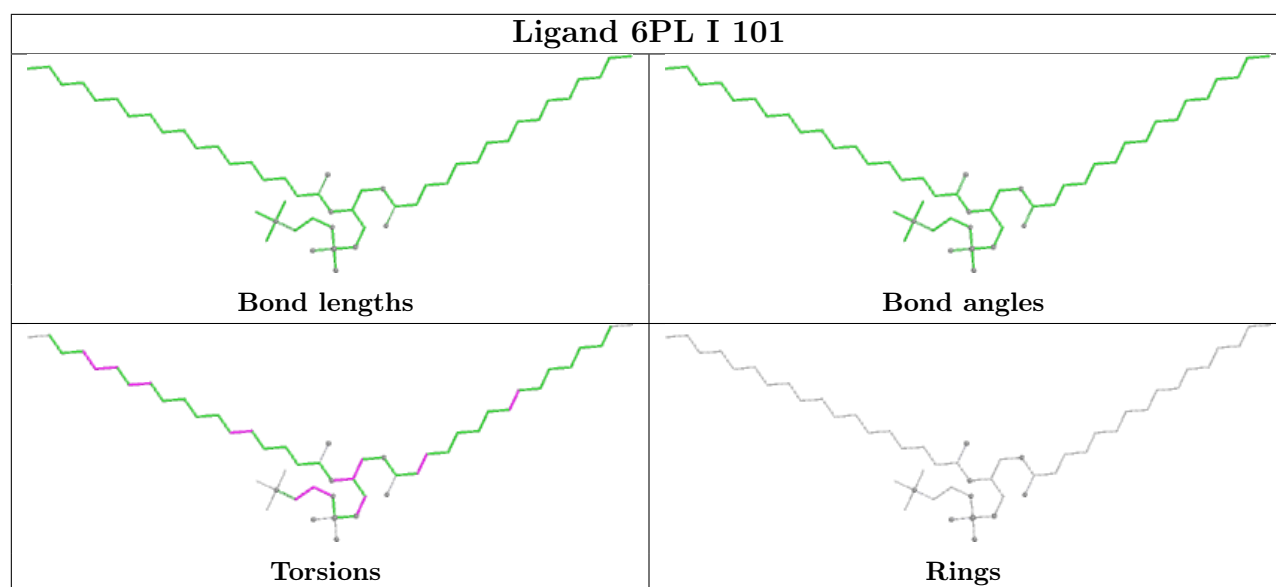


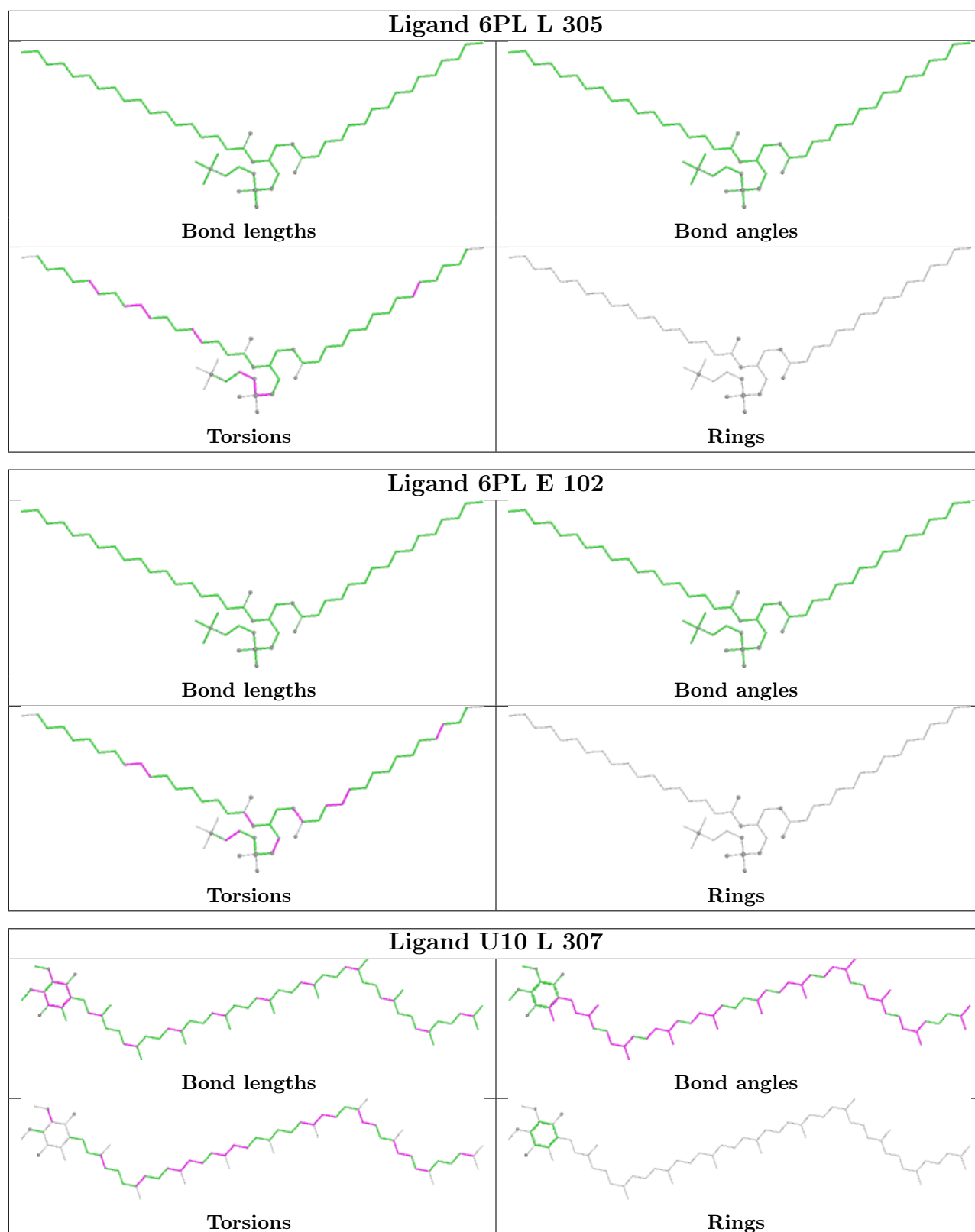
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Bond lengths	Bond angles
	
Torsions	Rings

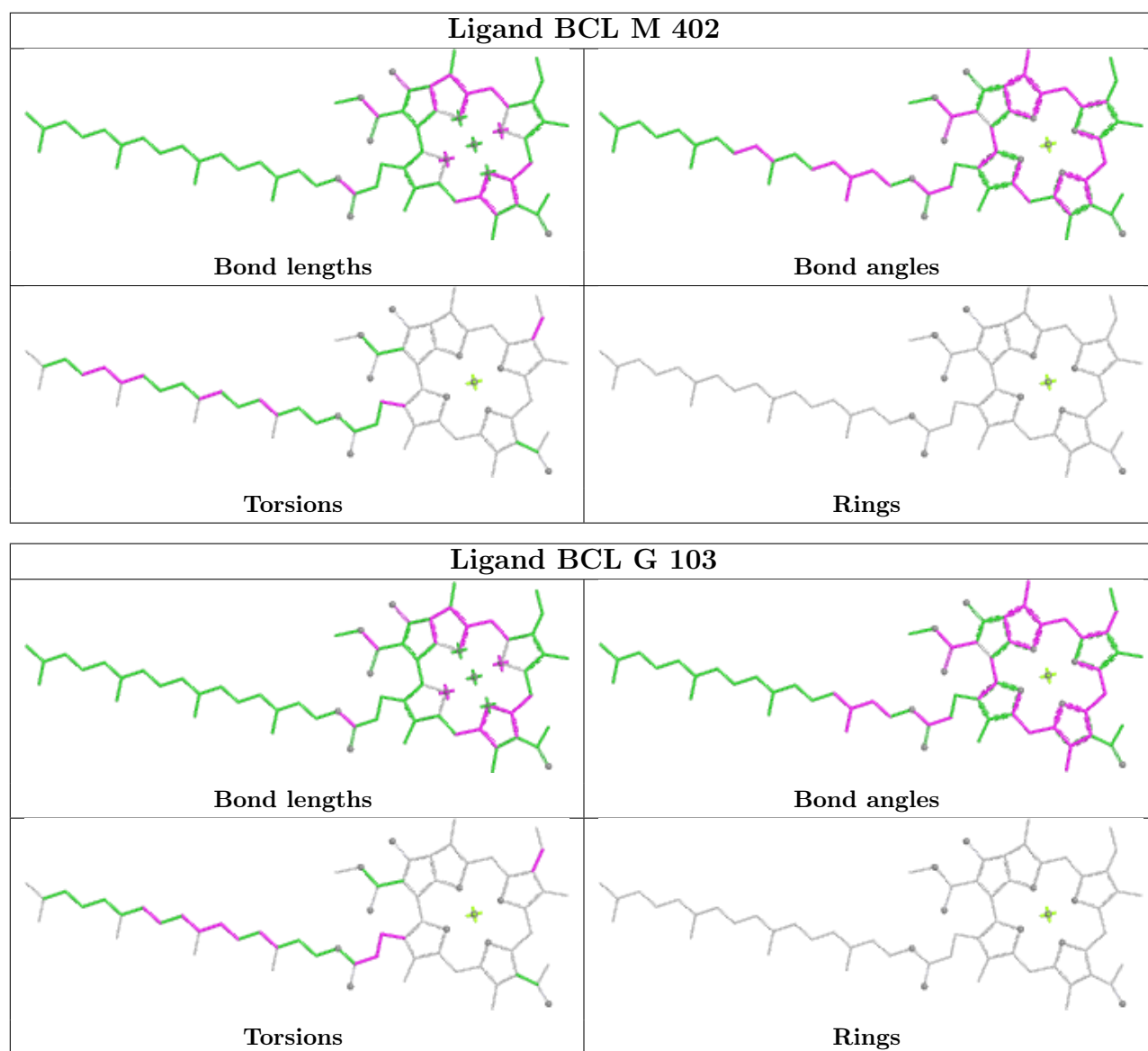
Ligand LMT 2 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

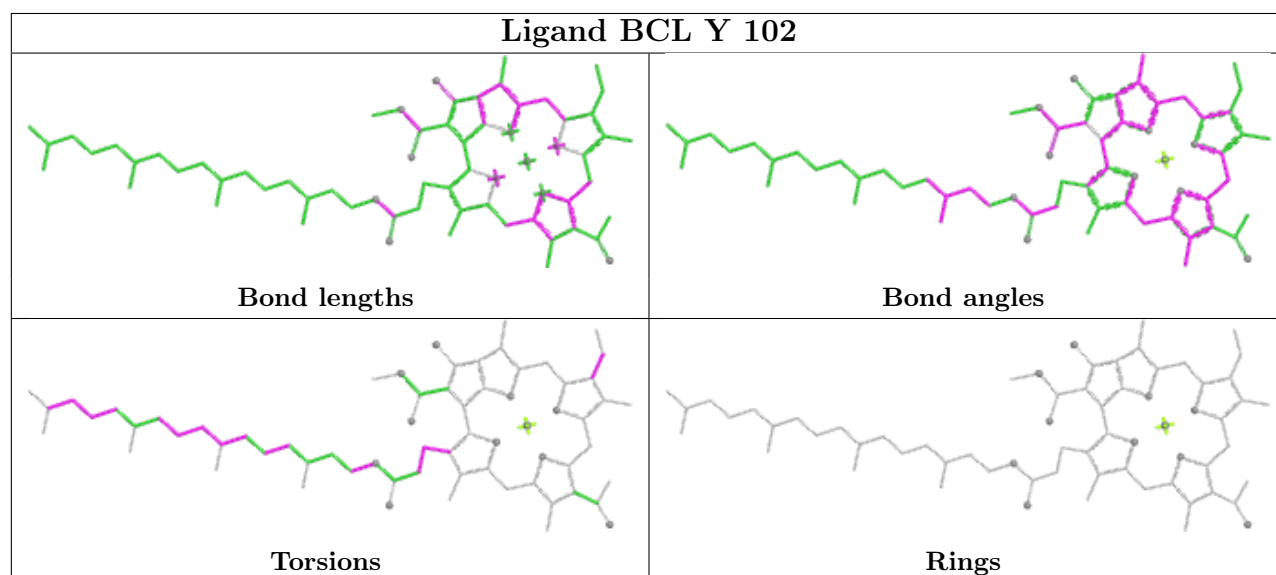
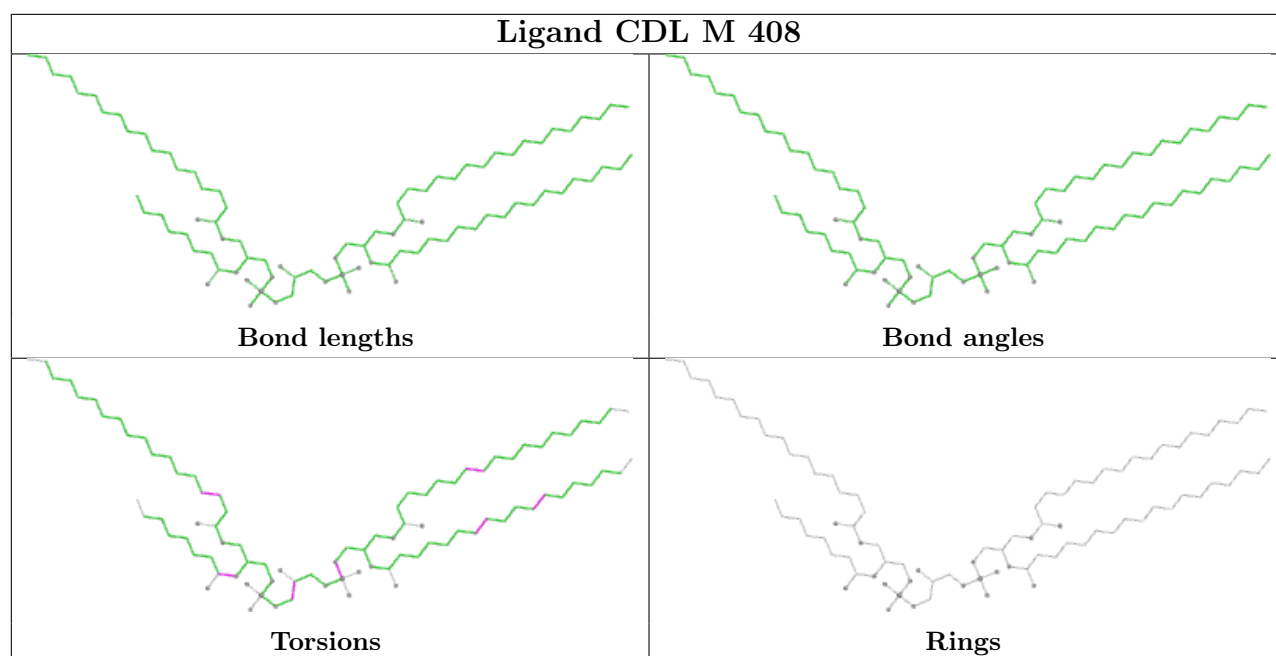
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Bond lengths	Bond angles
	
Torsions	Rings

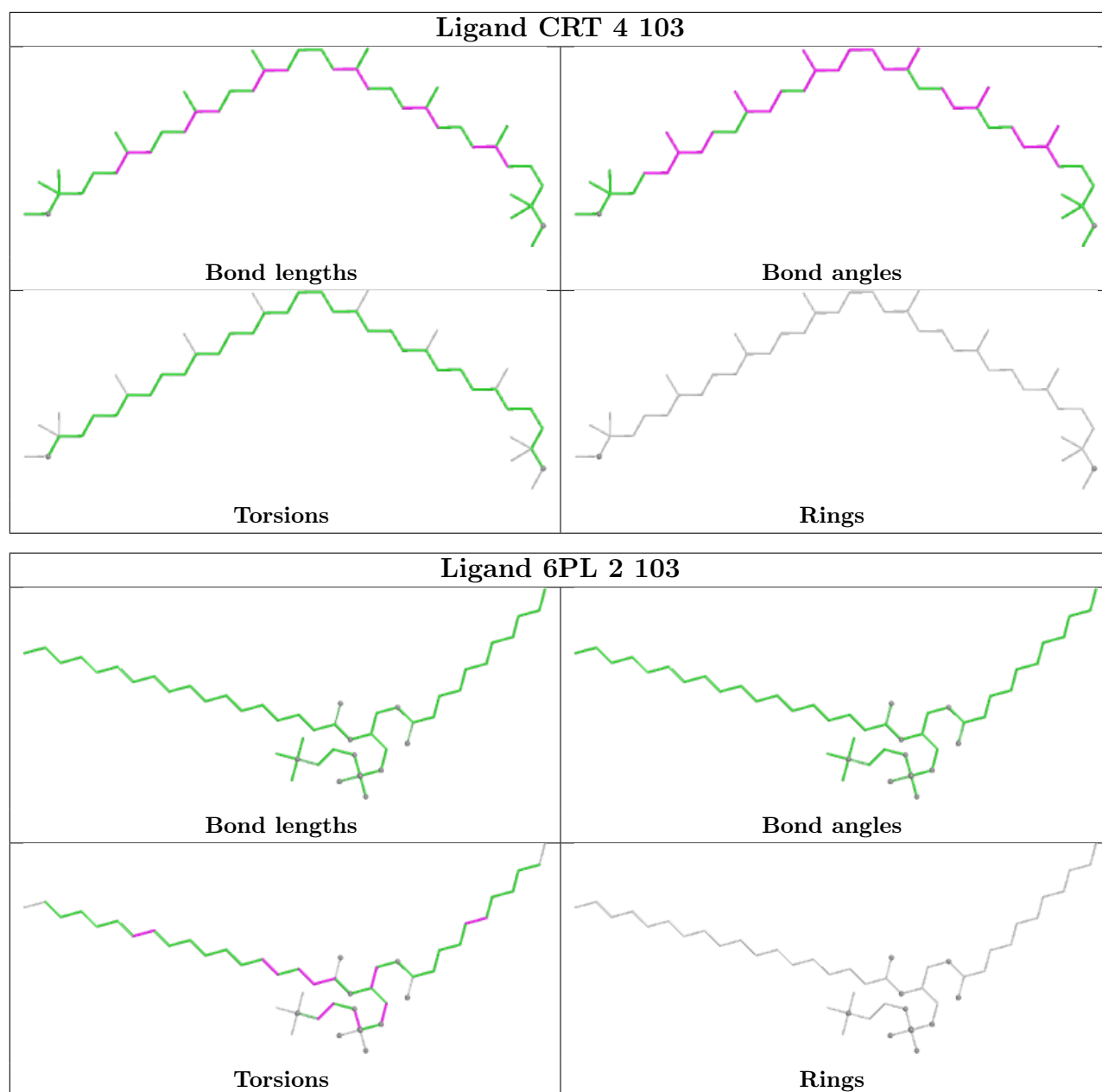


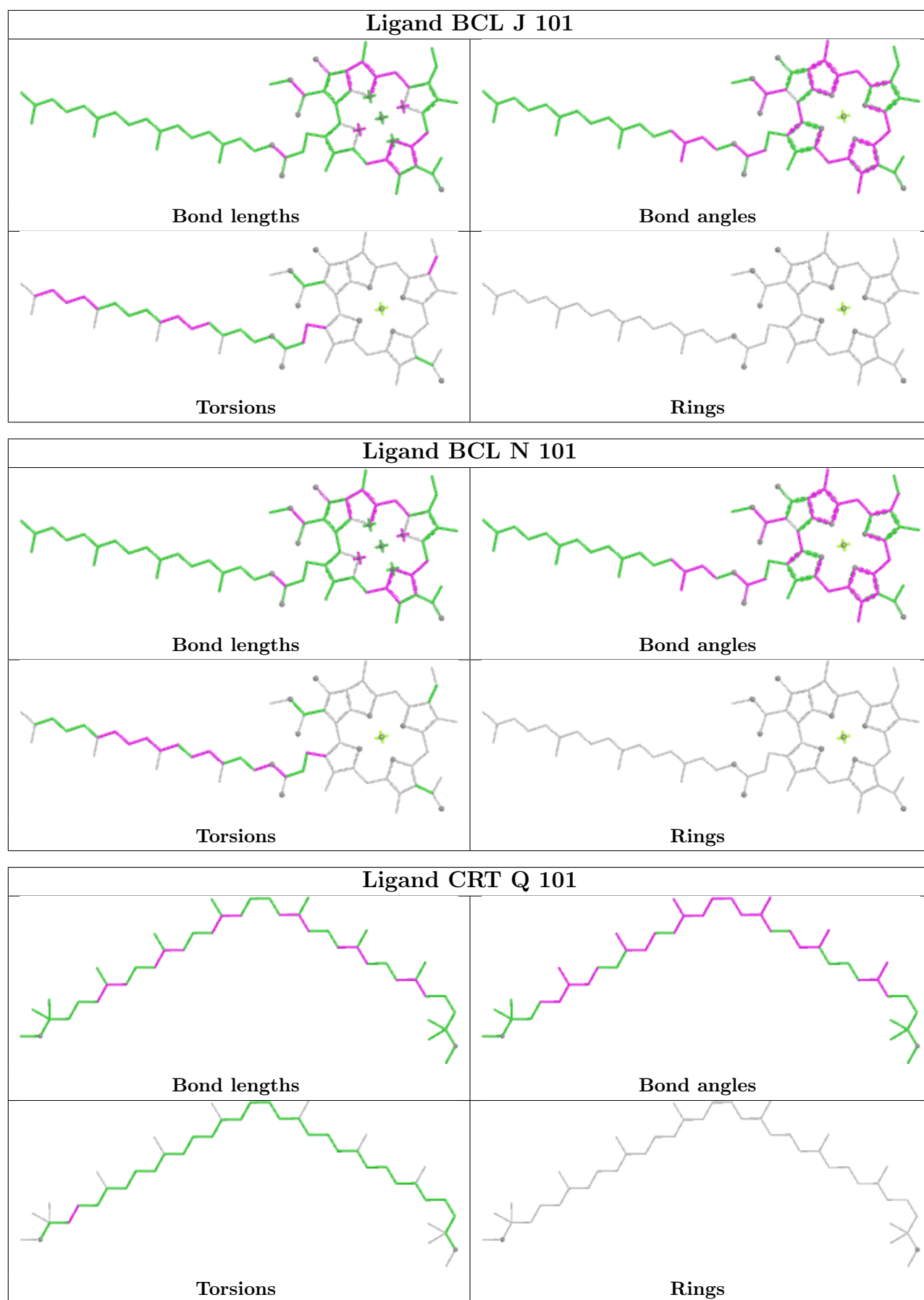


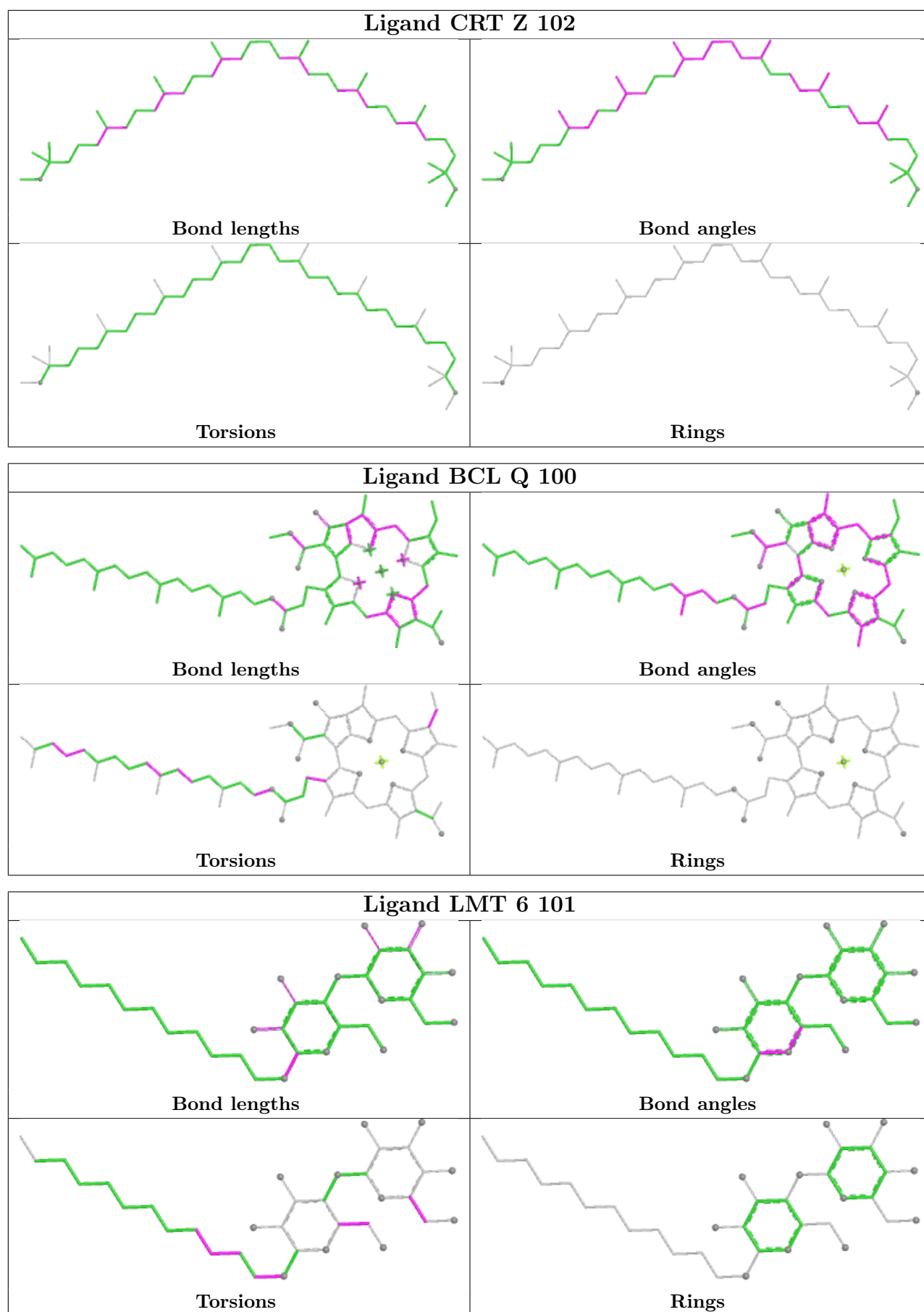


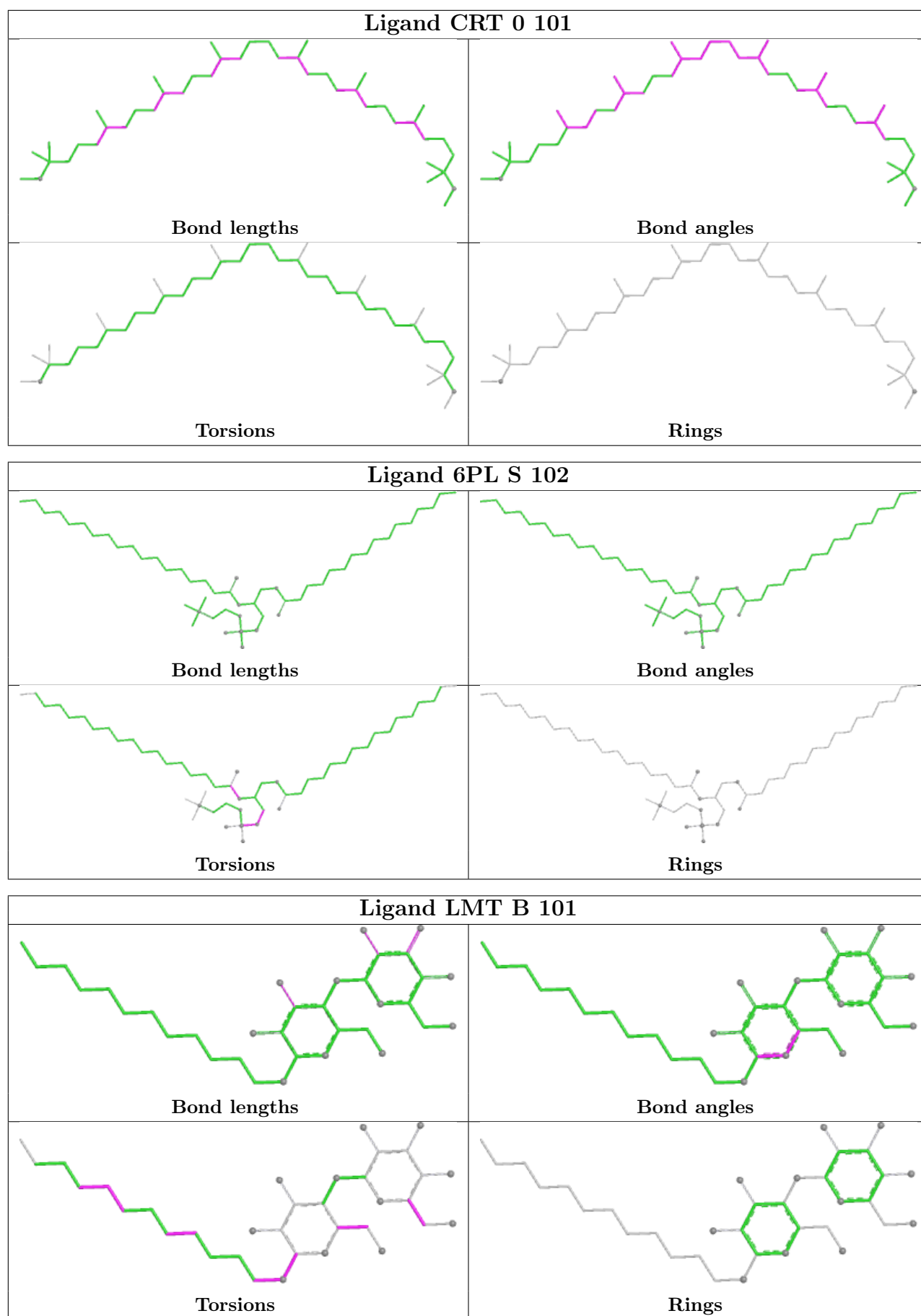


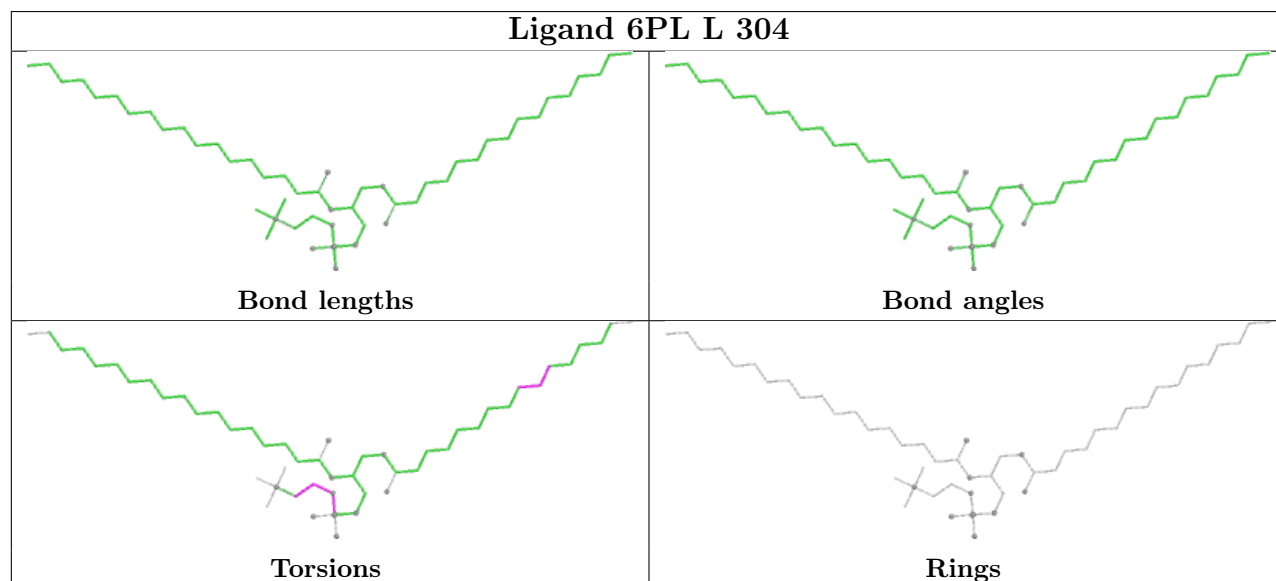
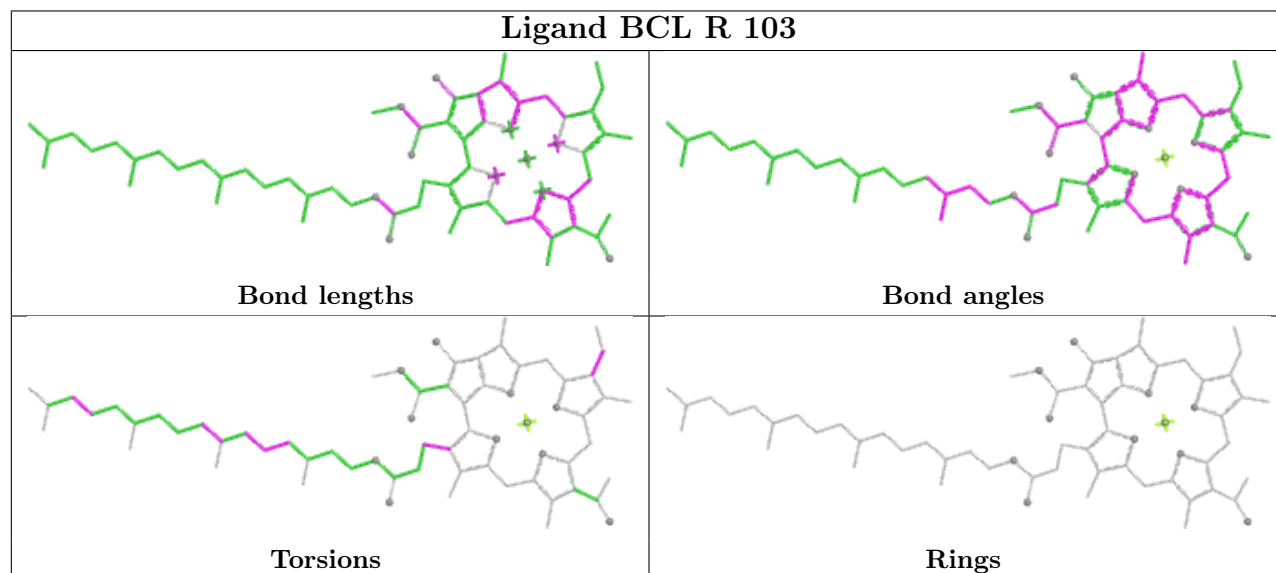
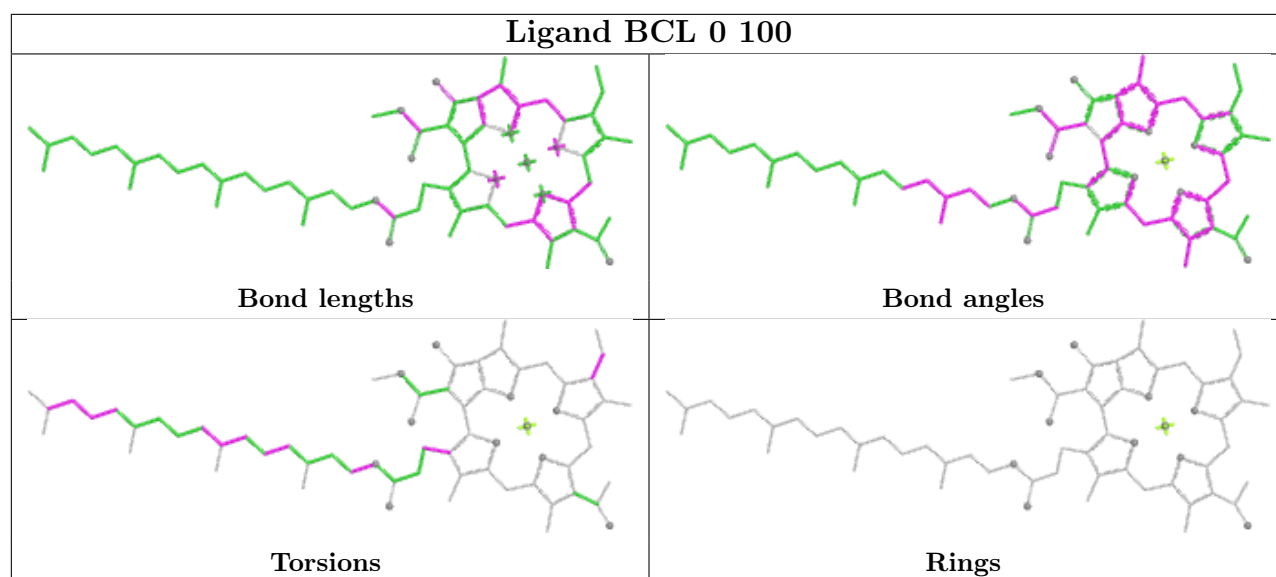


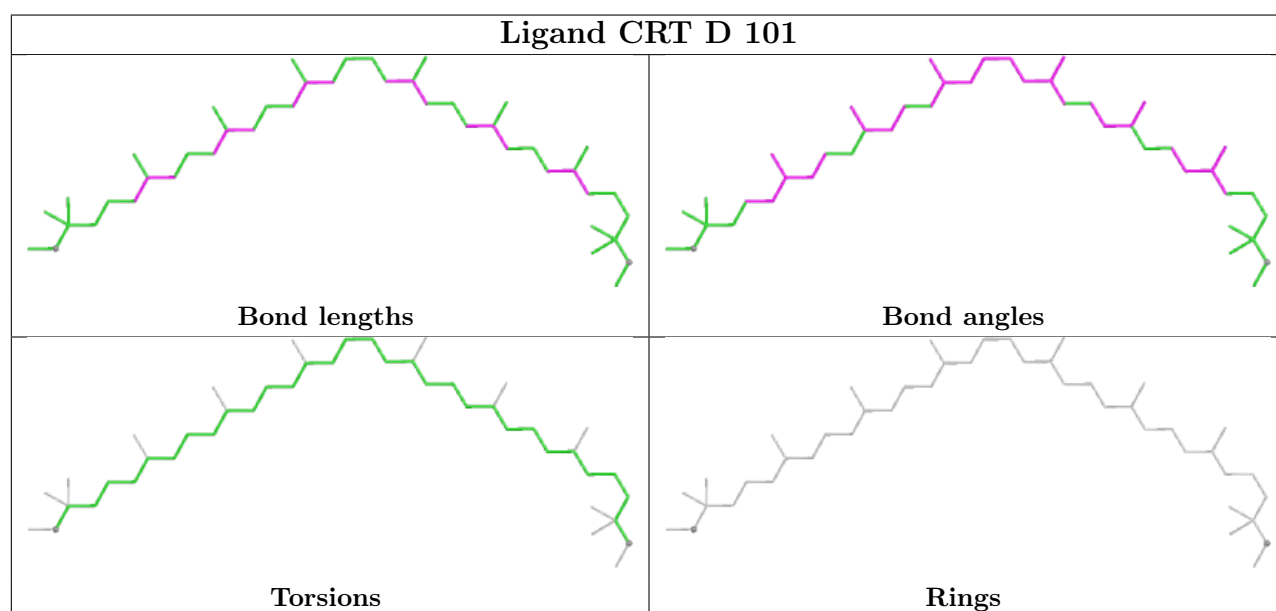
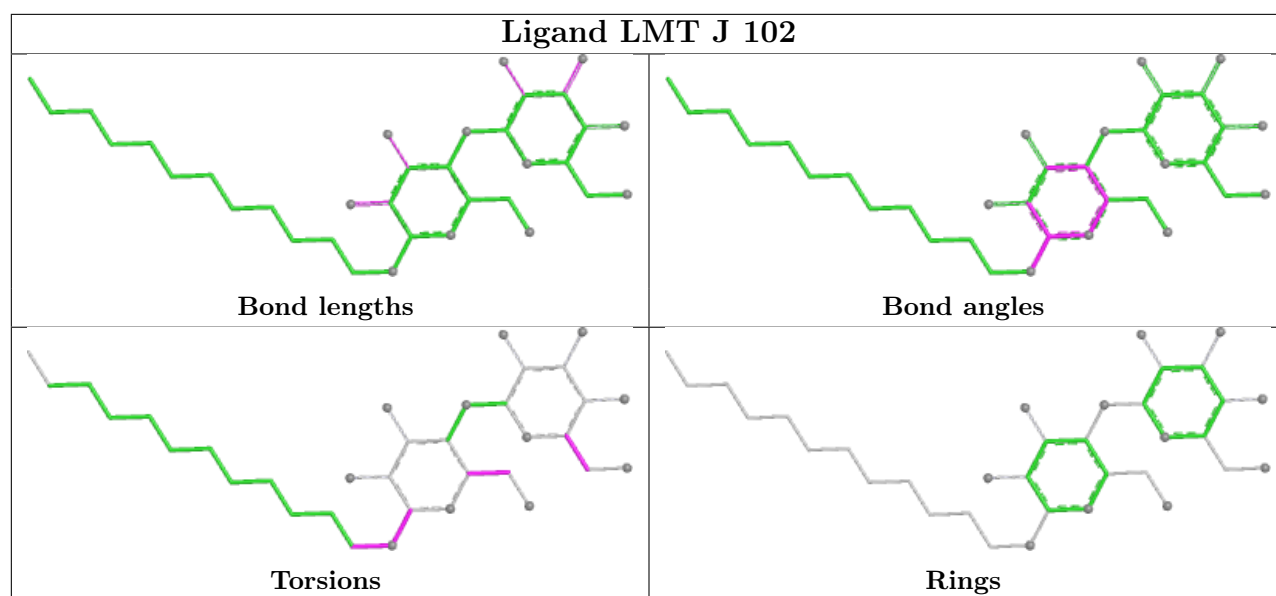


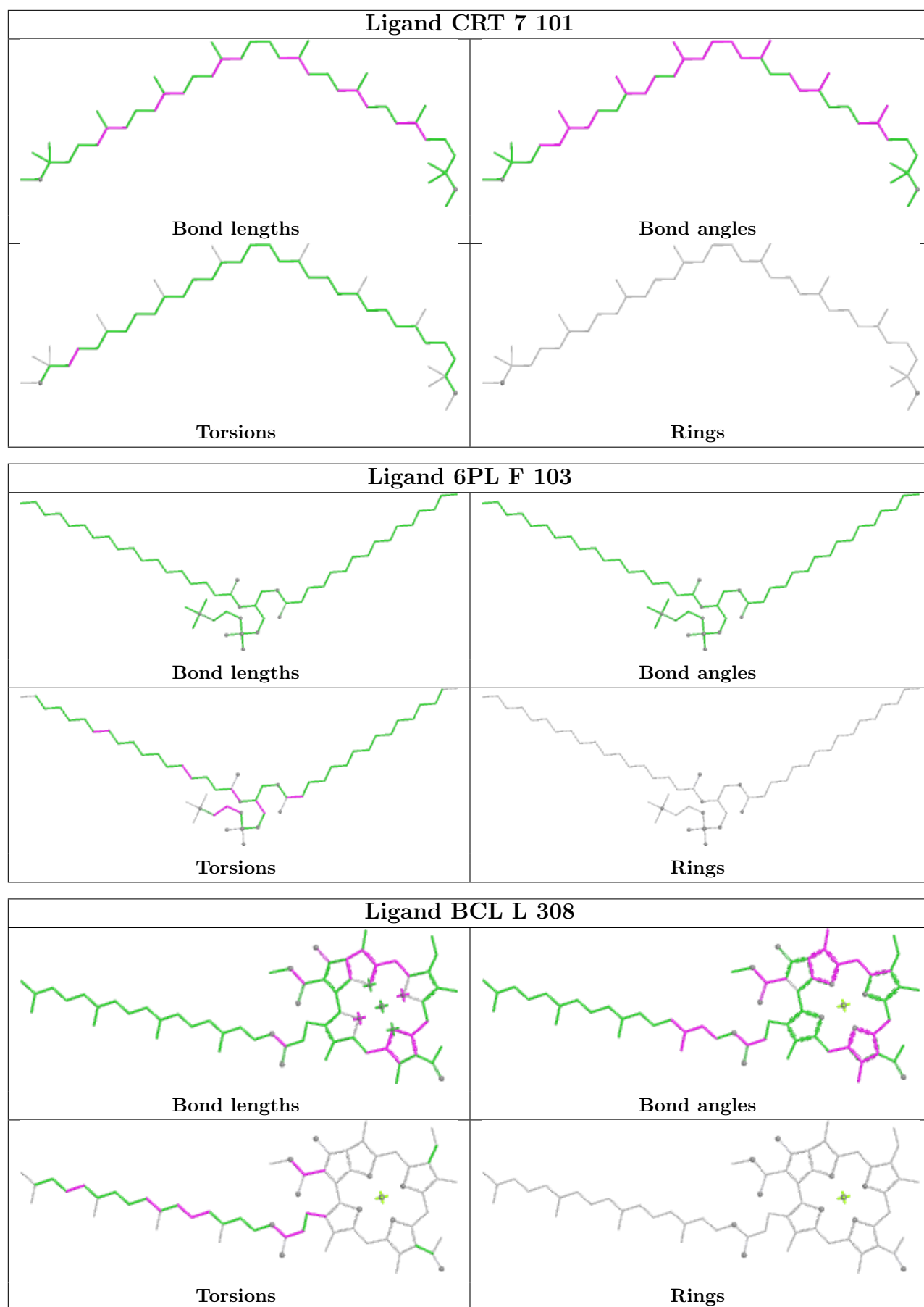


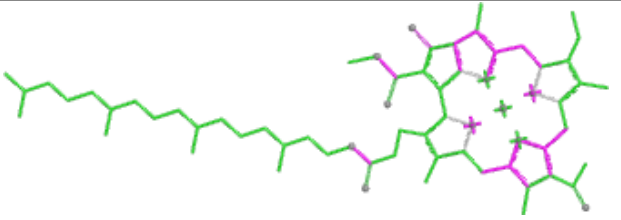
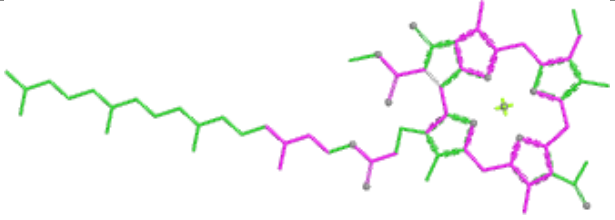
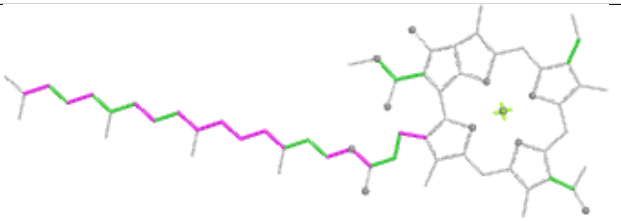
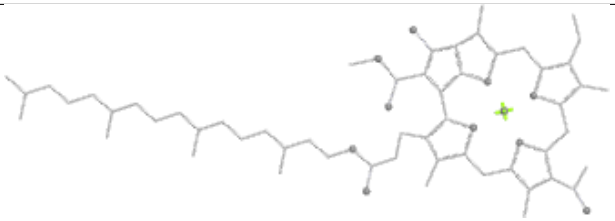
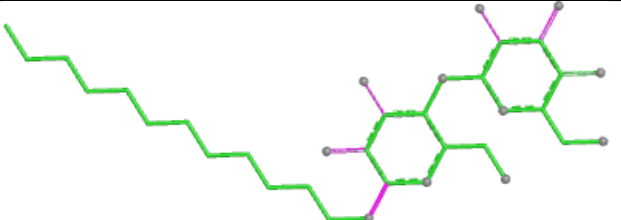
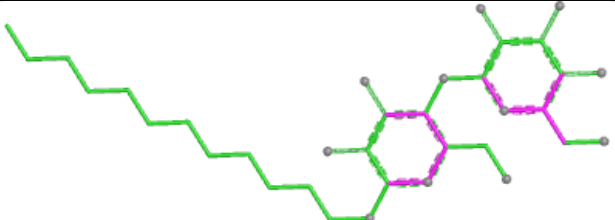
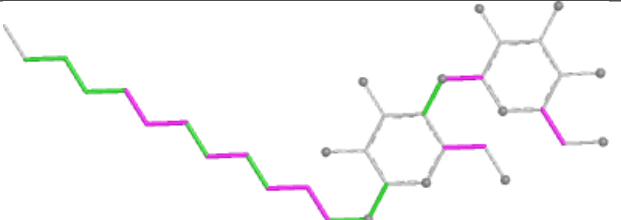
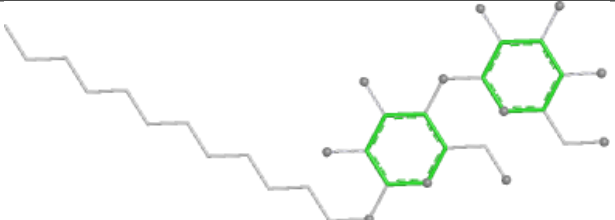
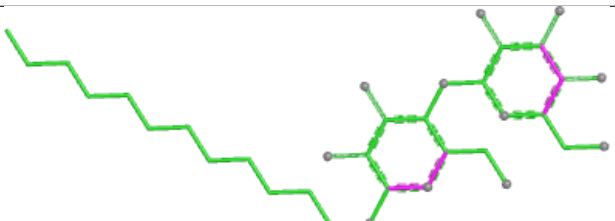
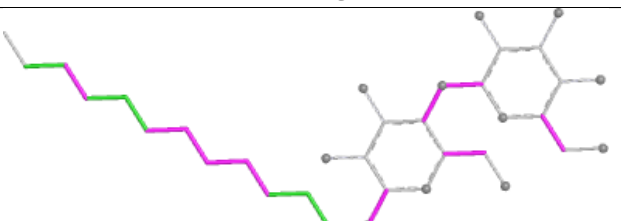
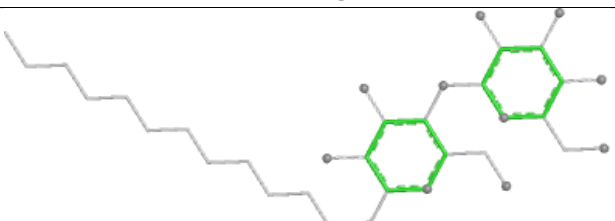


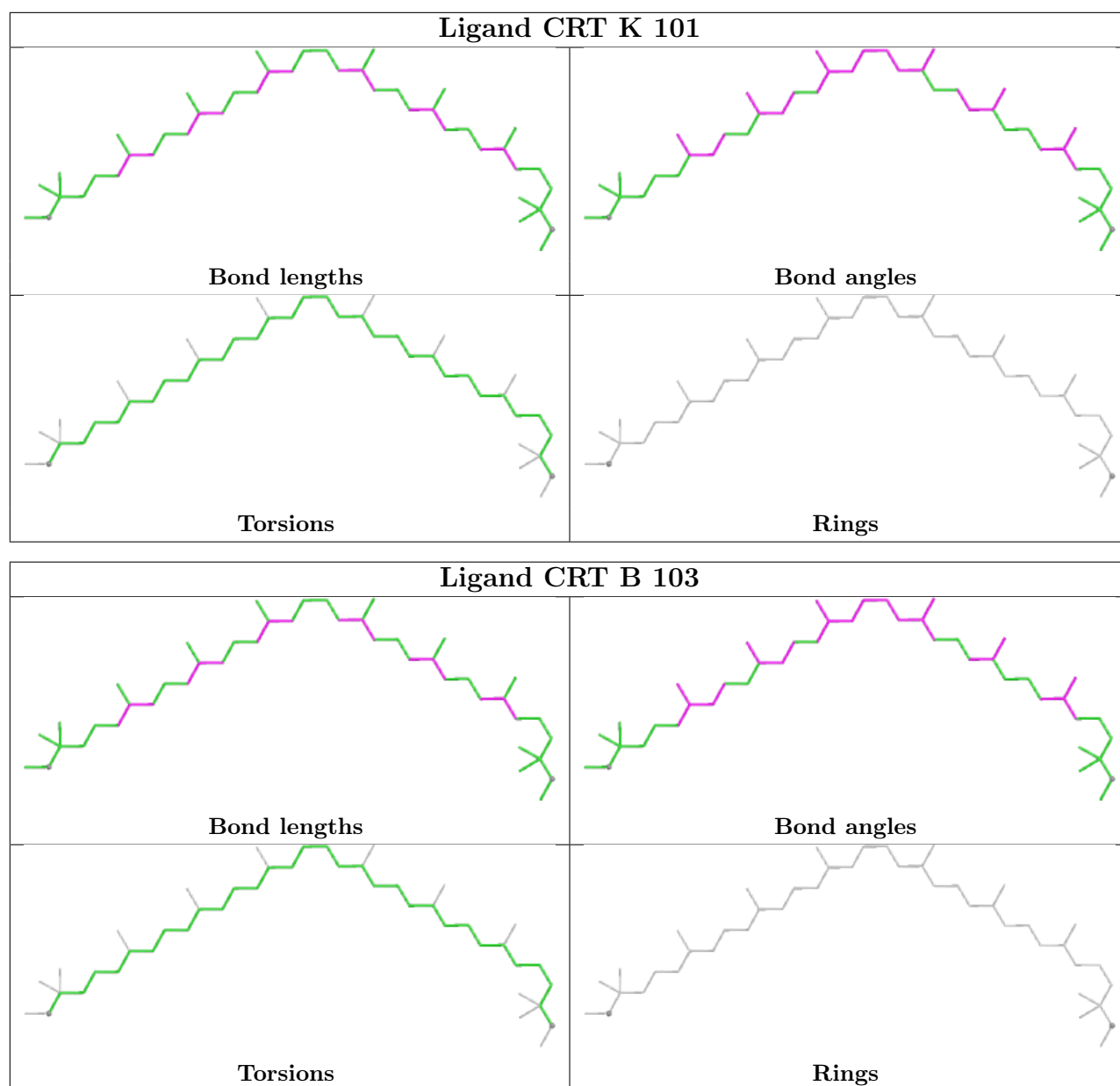


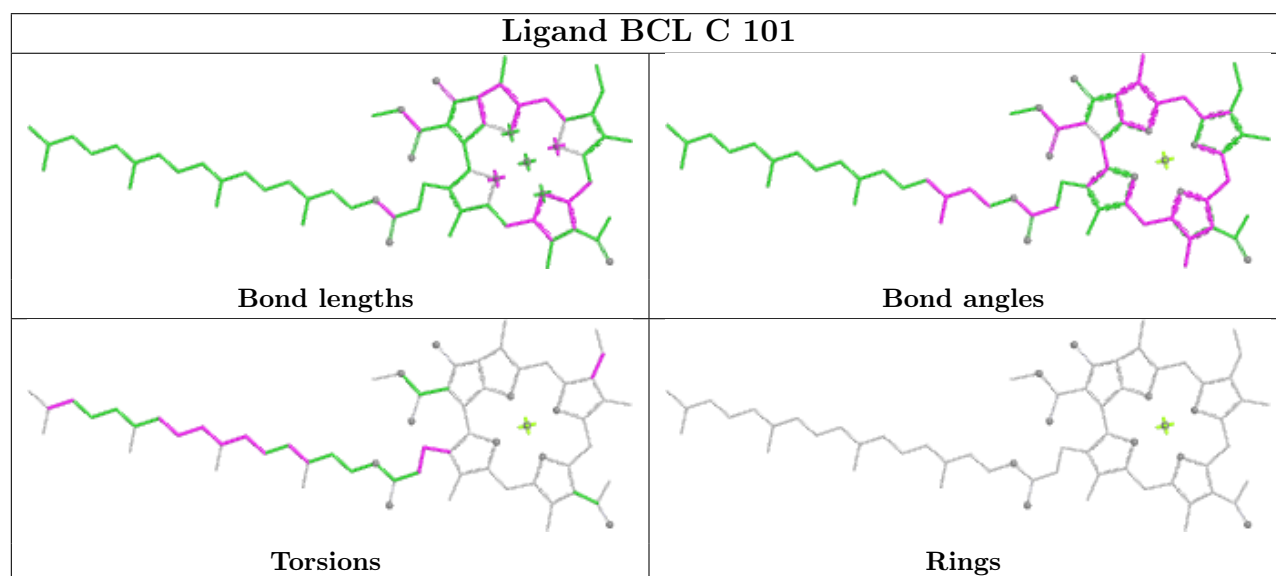
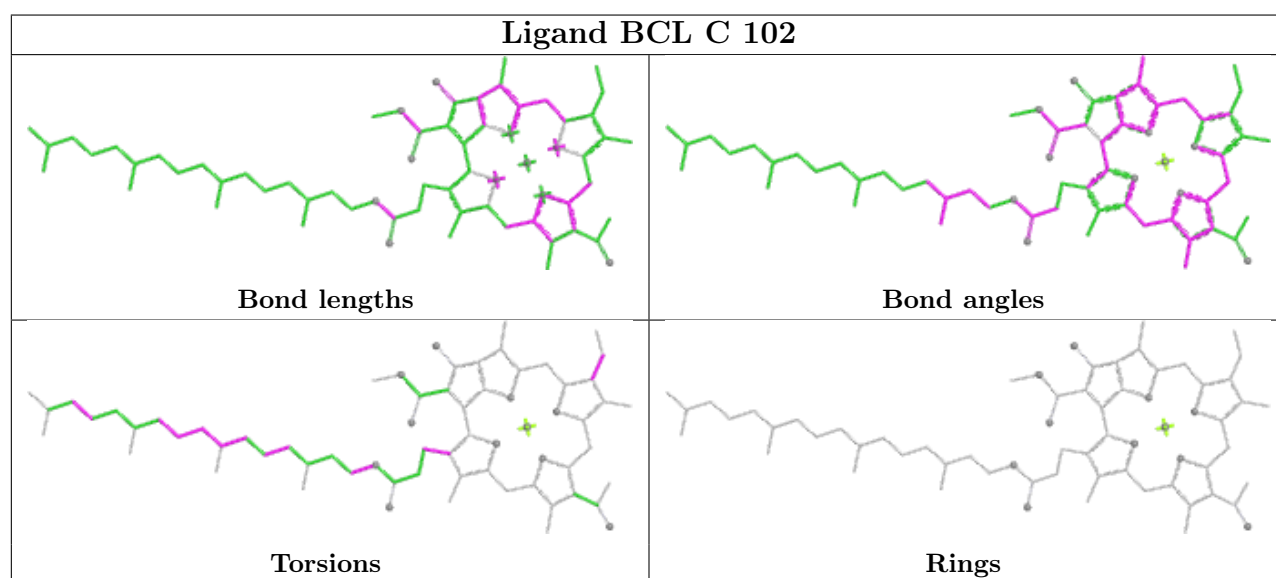
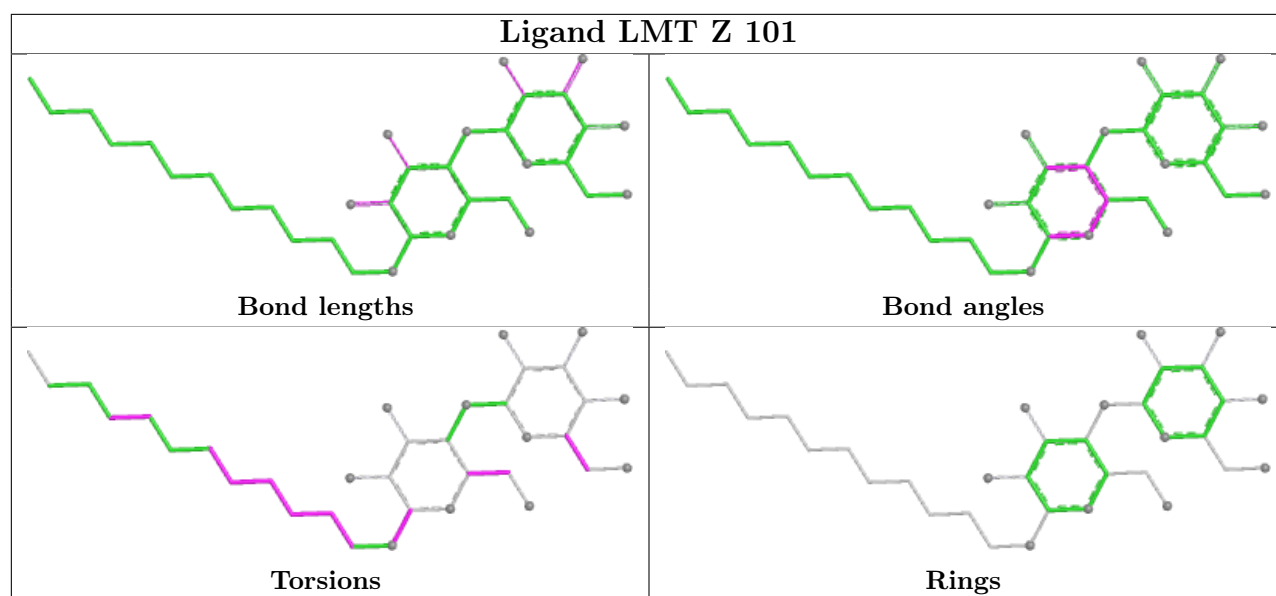


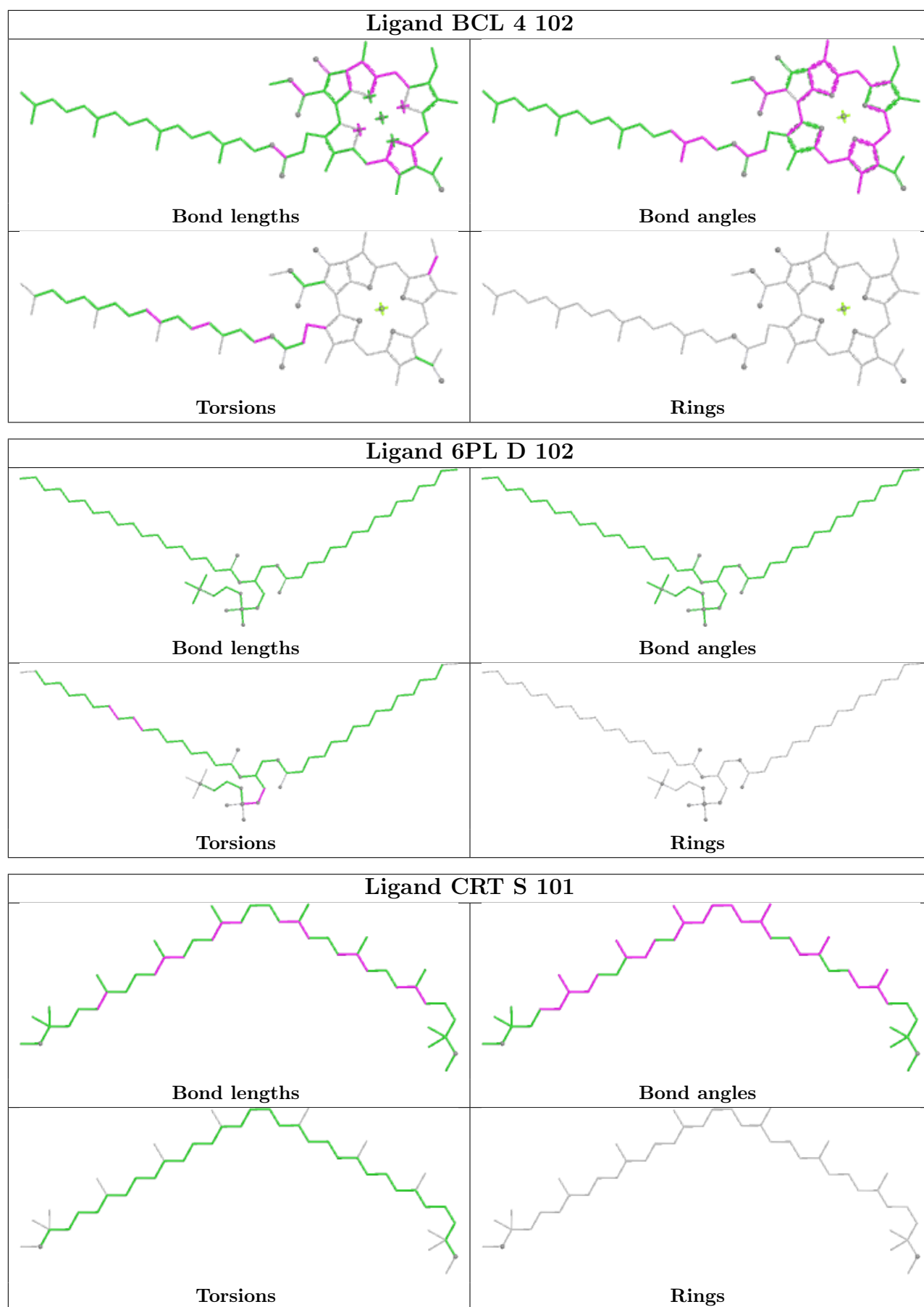


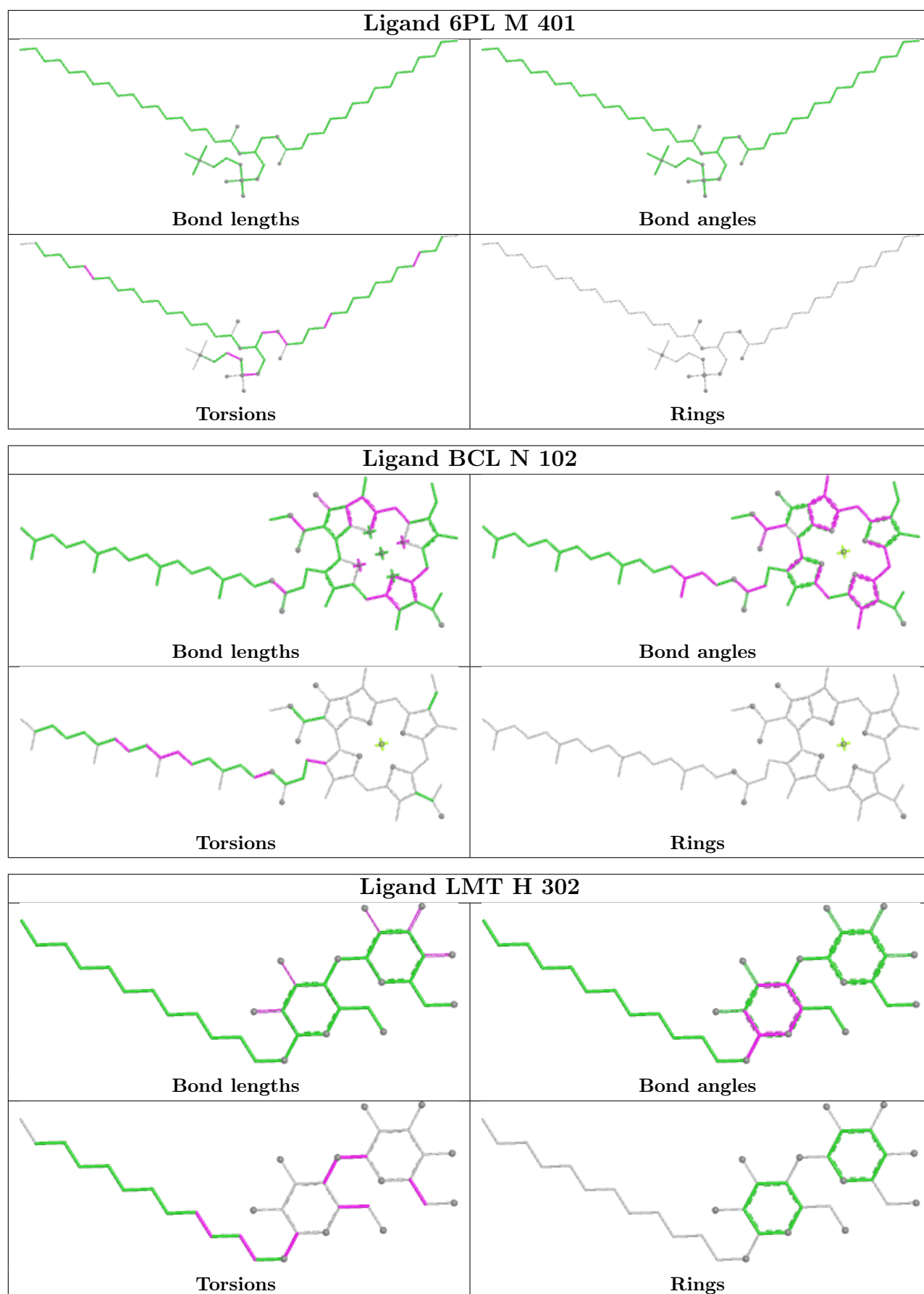


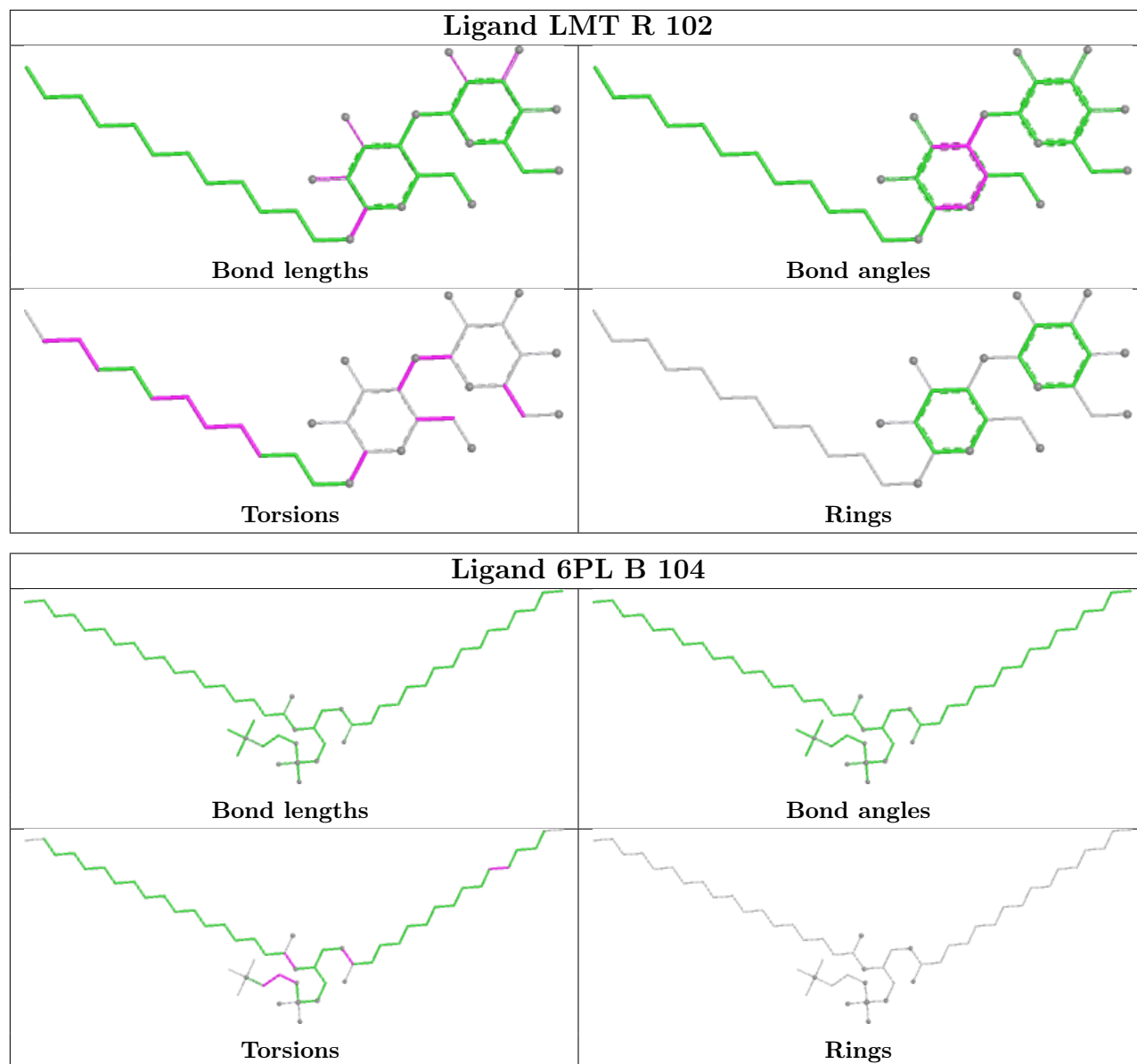
Ligand BCL T 100	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMT 4 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMT L 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

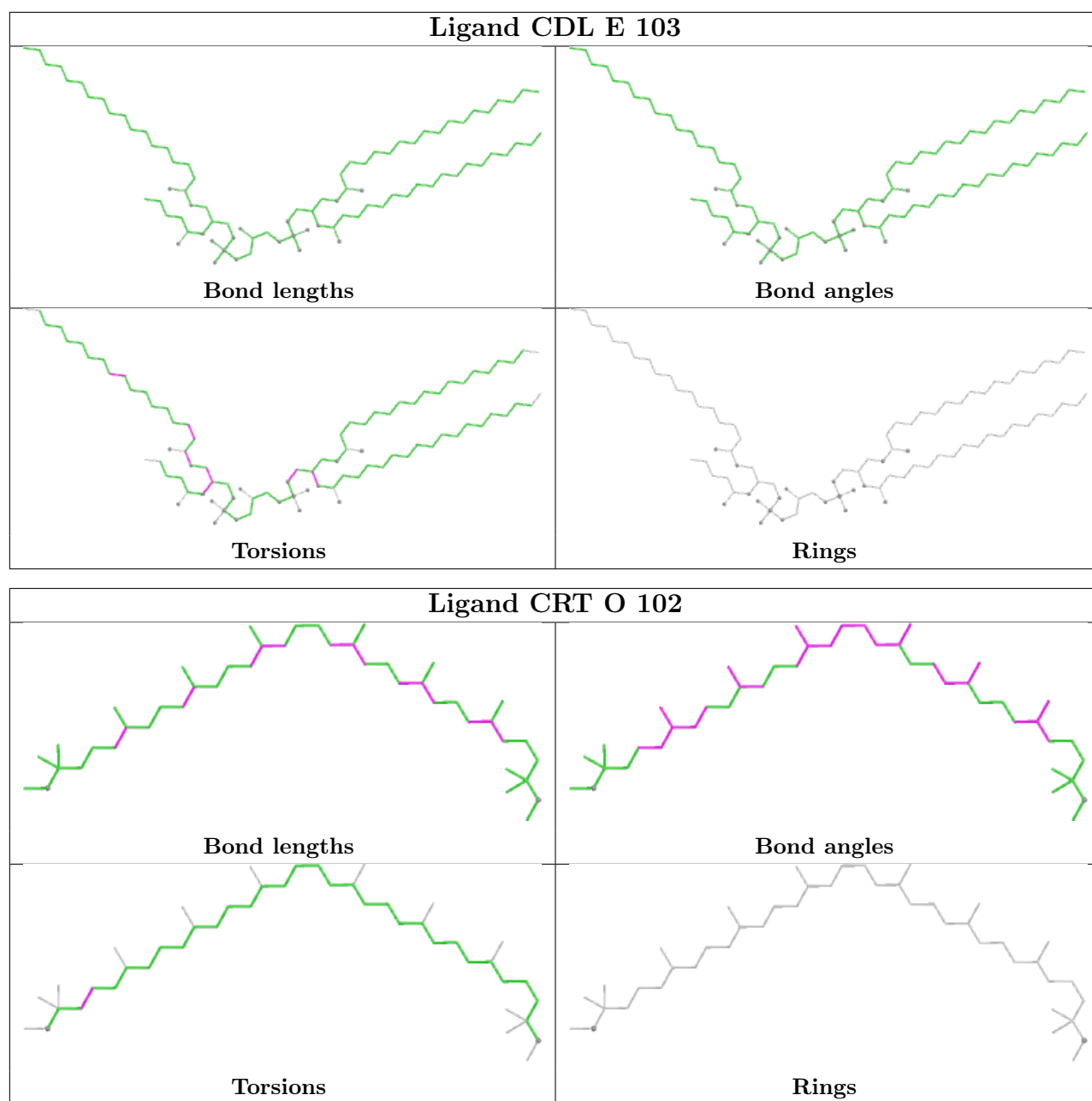


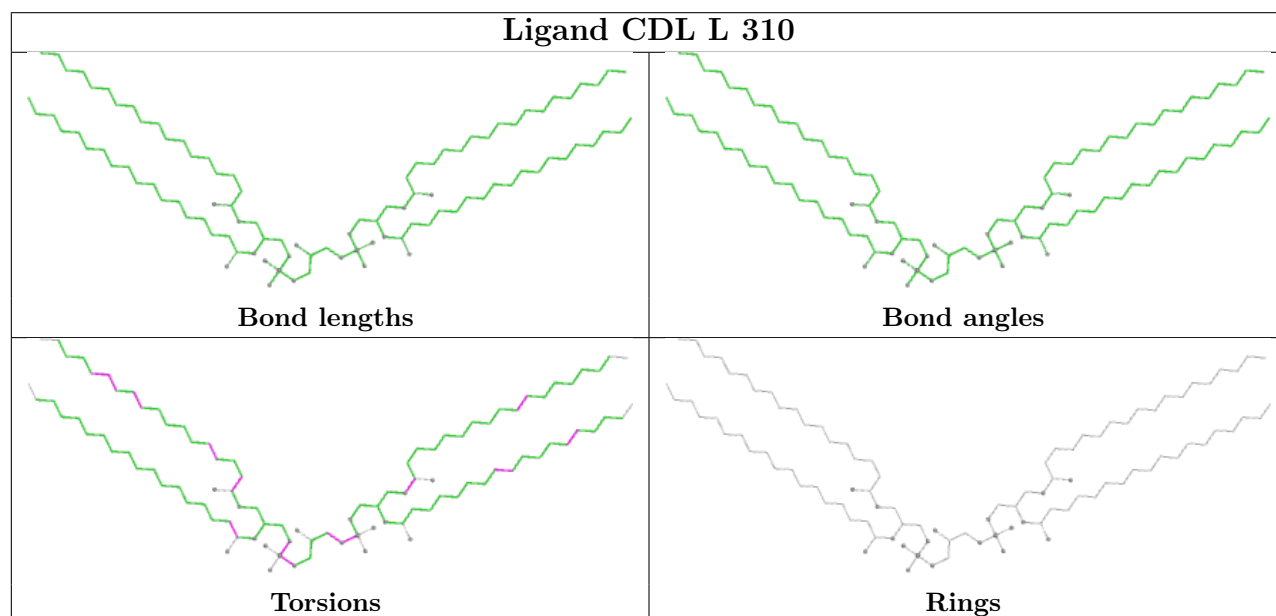
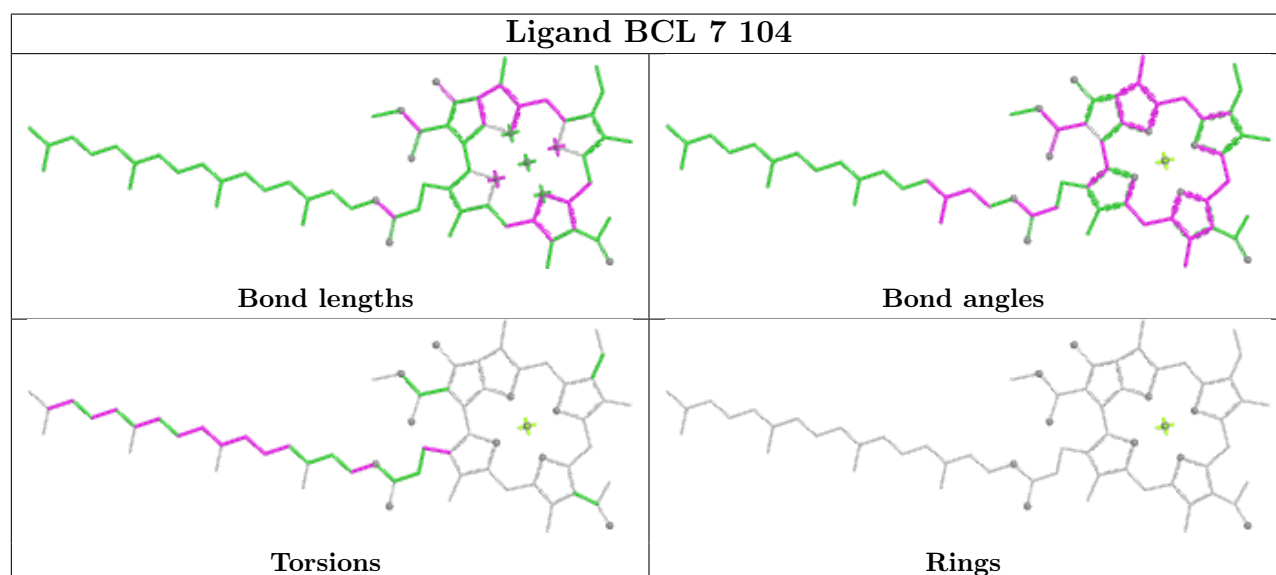
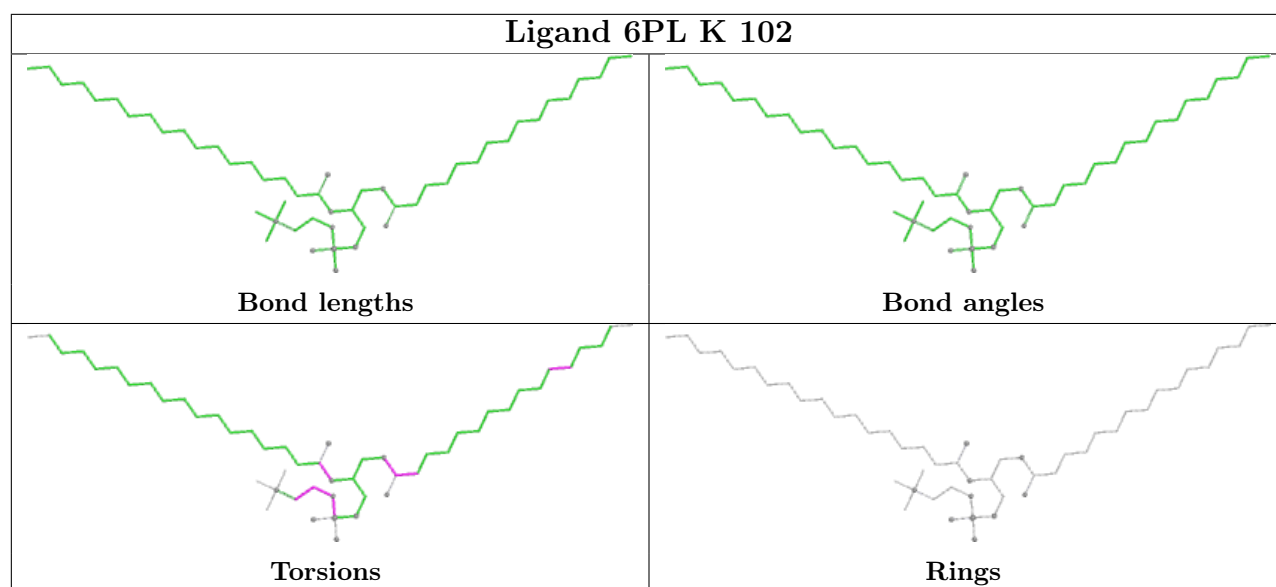


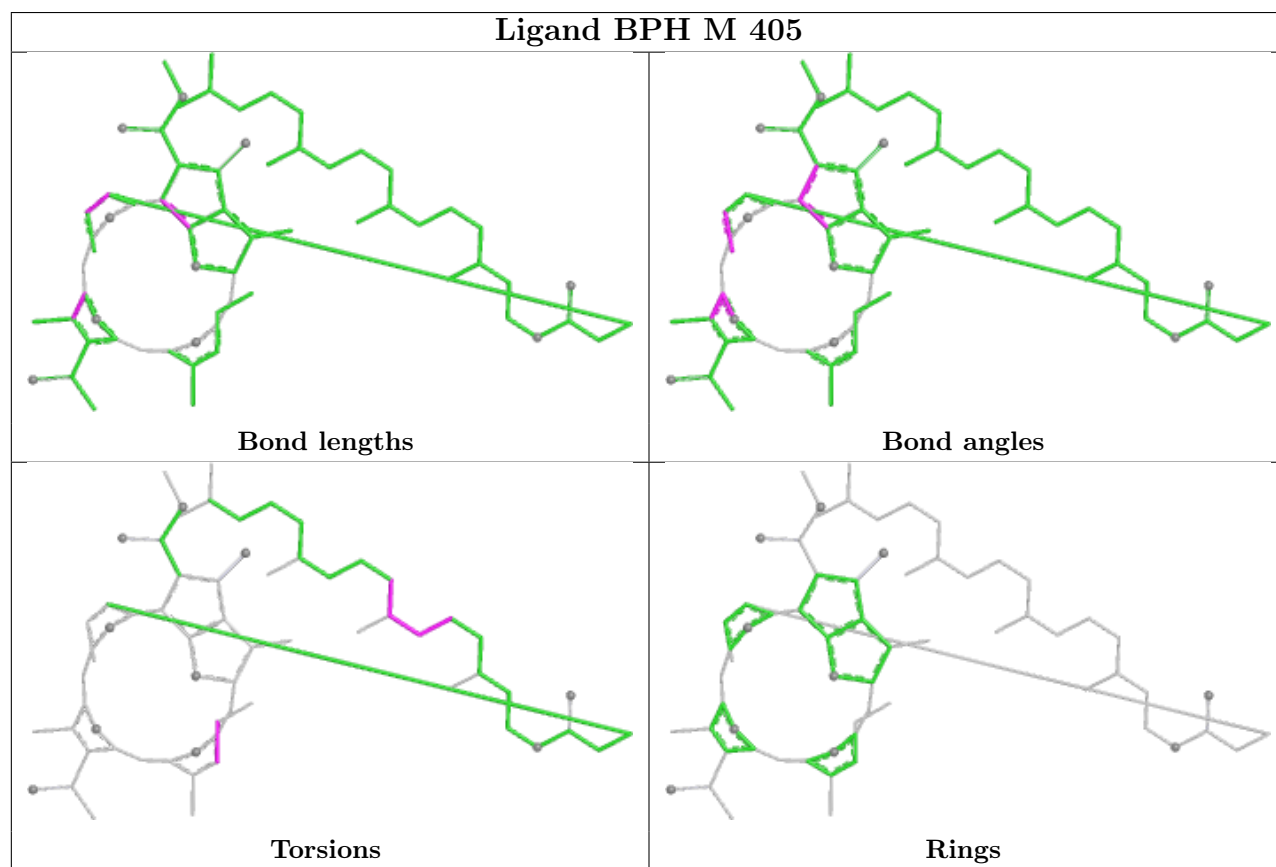
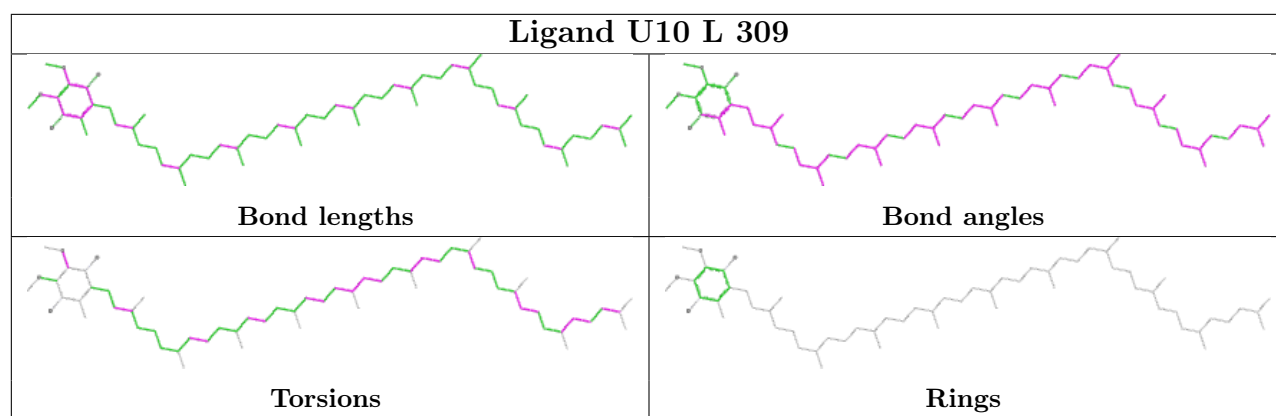


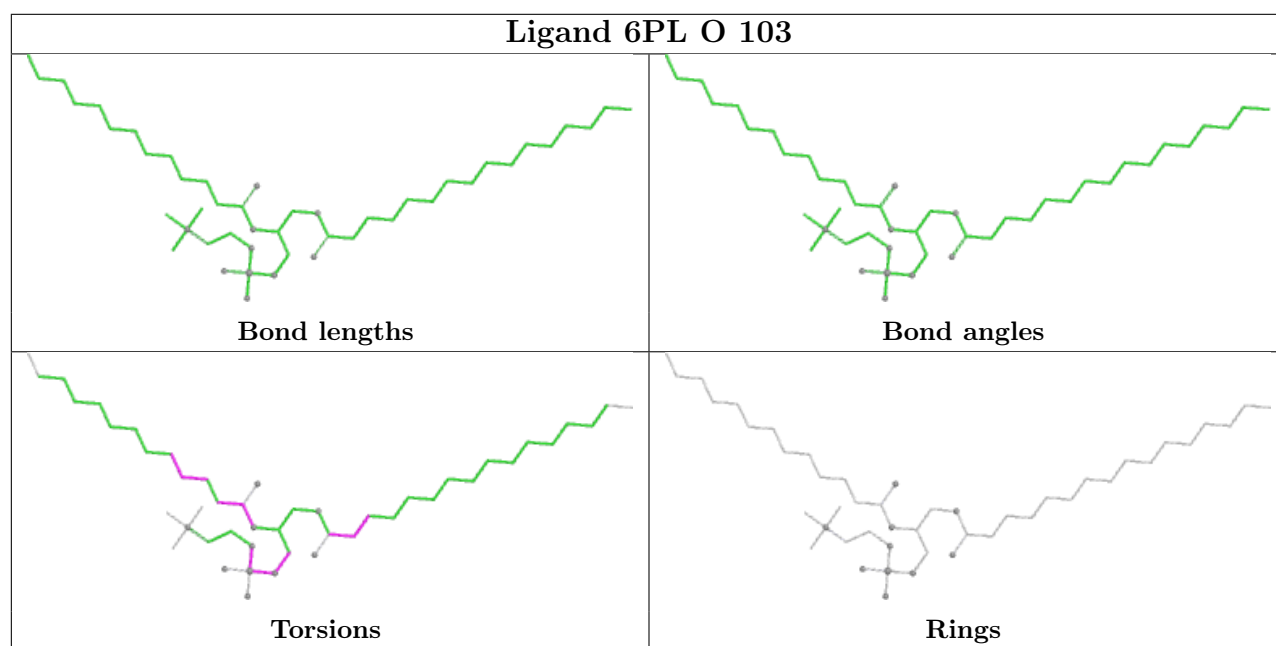
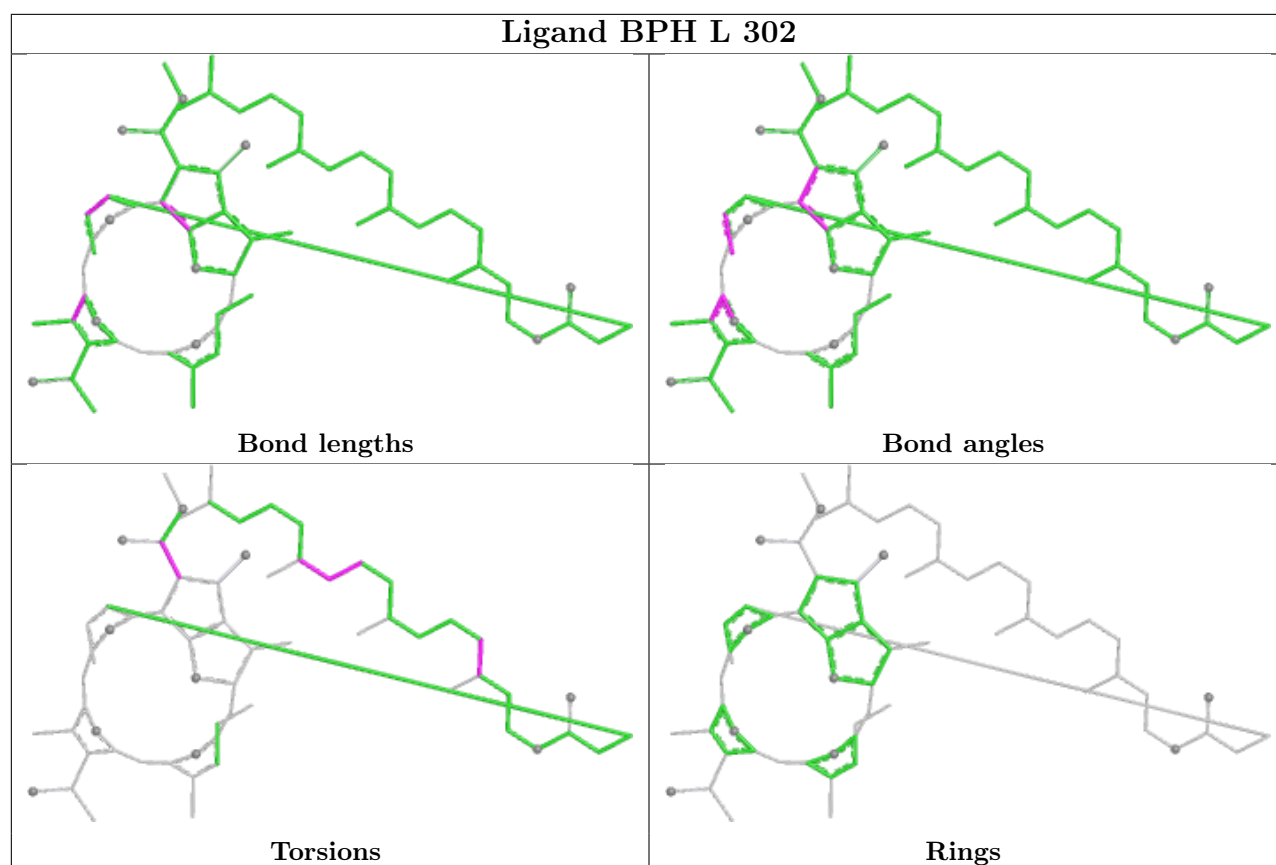


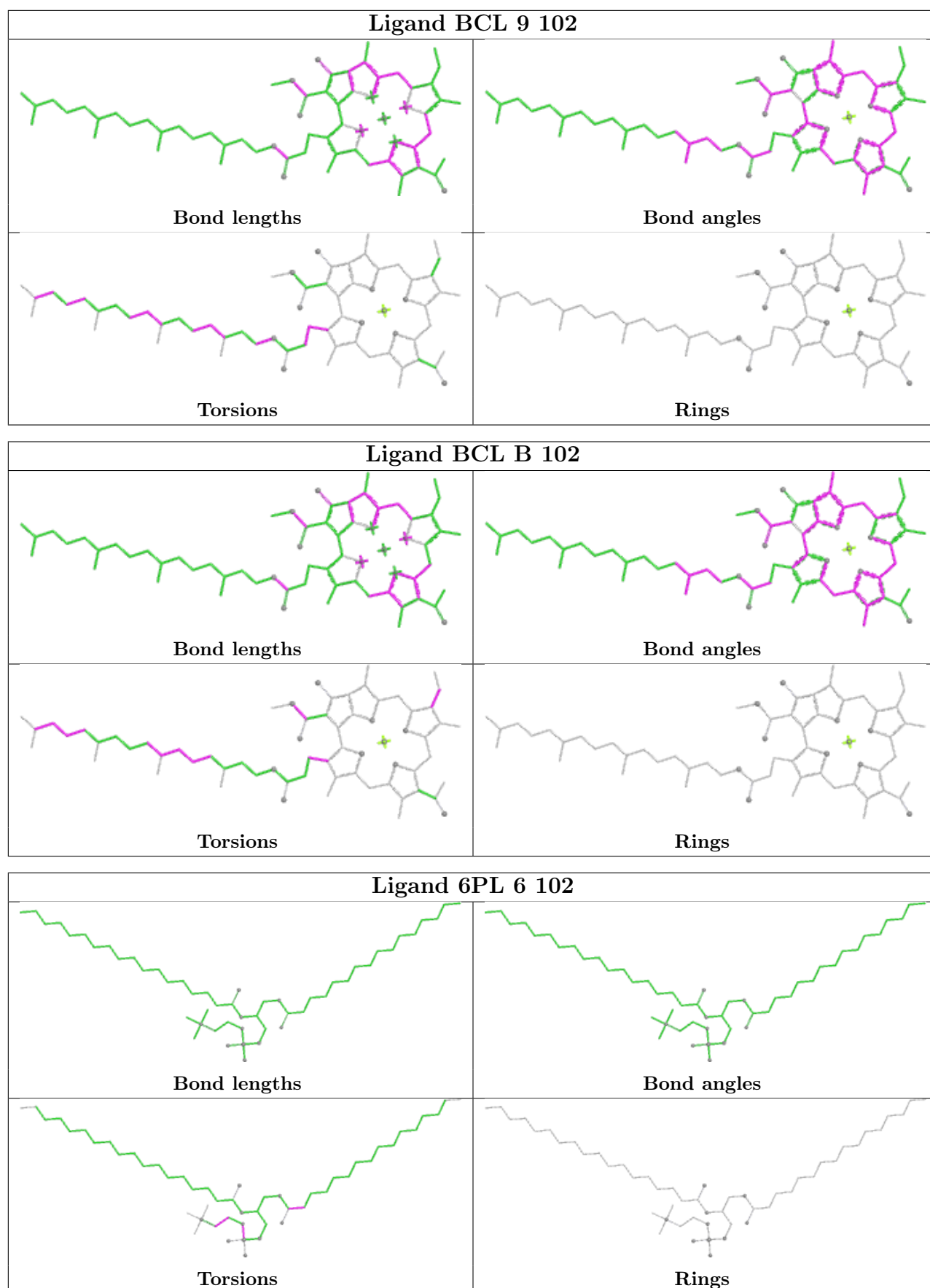


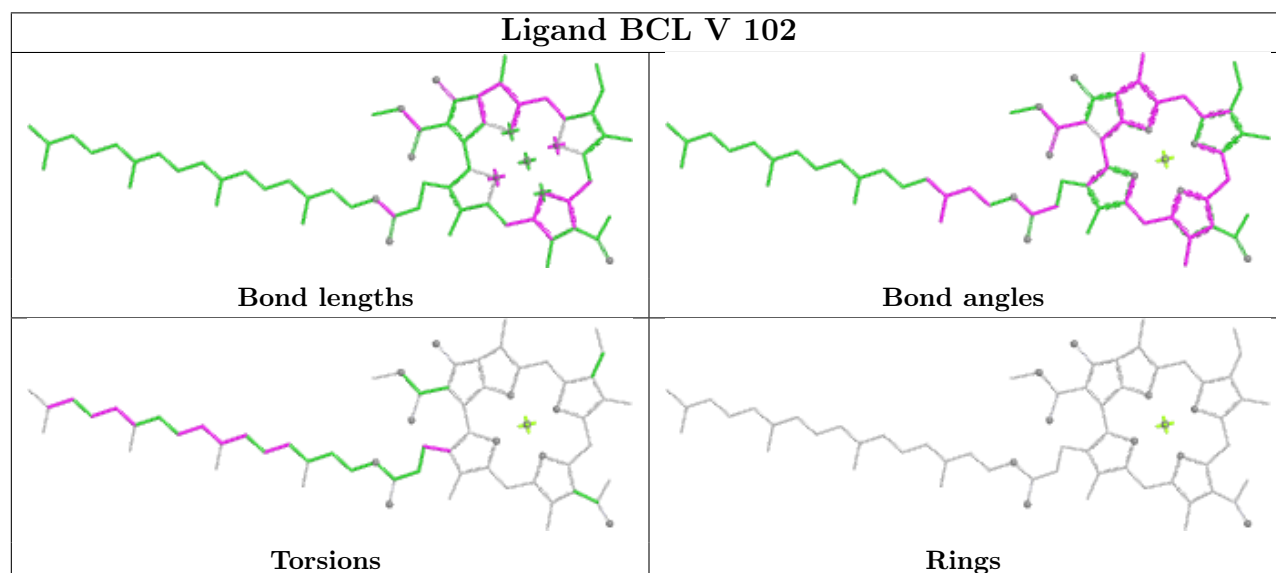
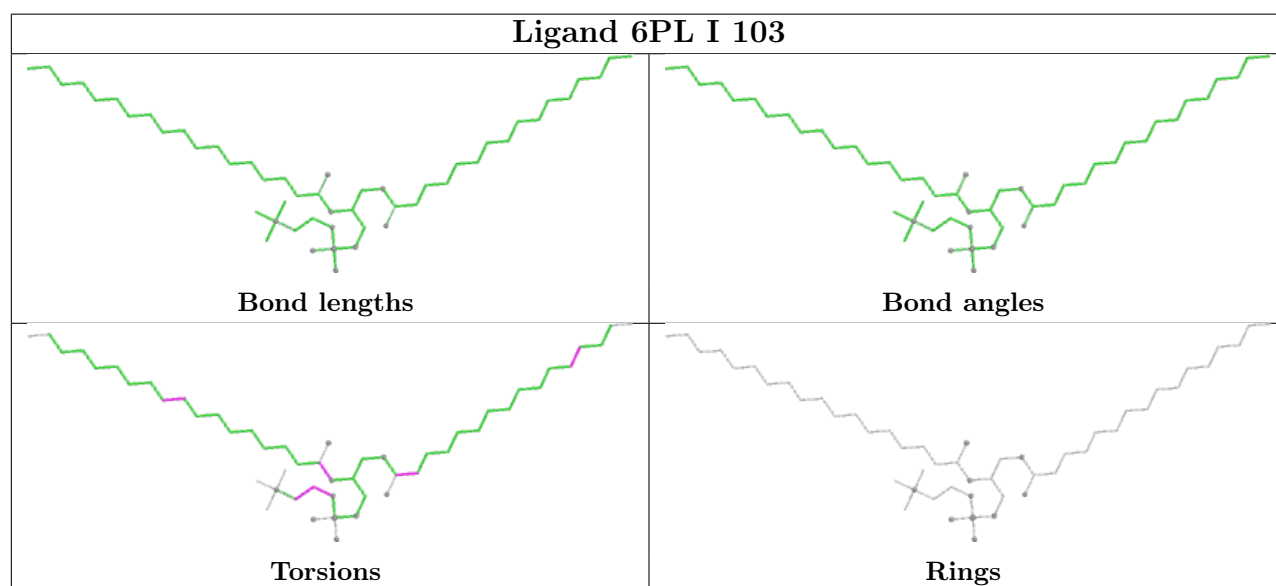
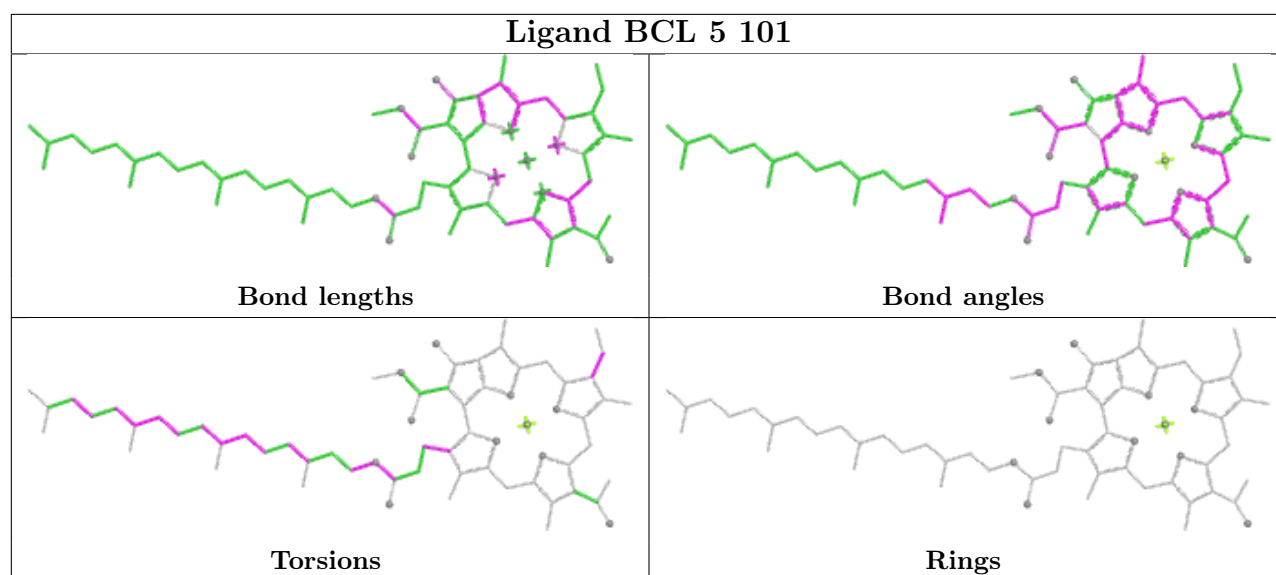


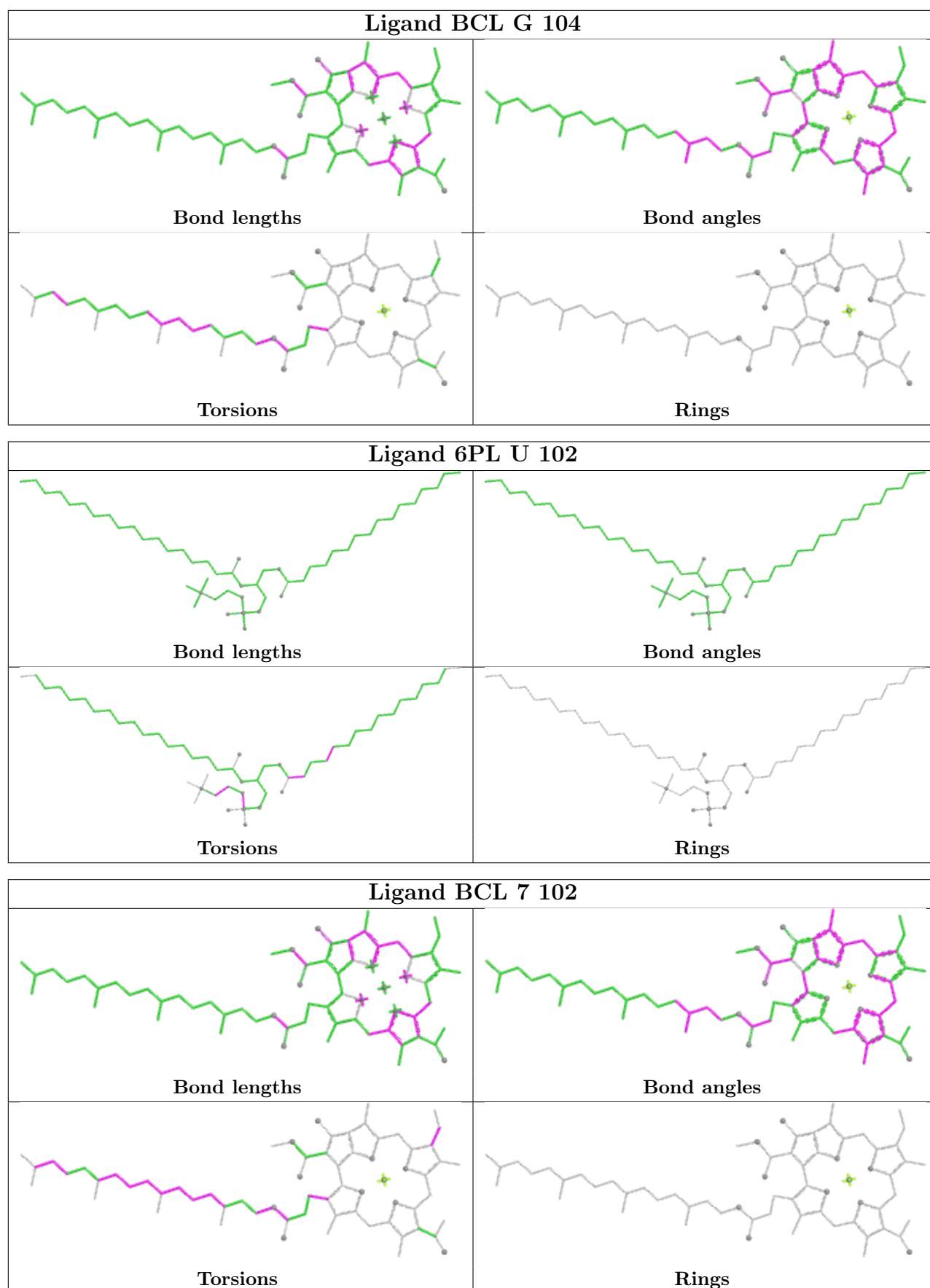


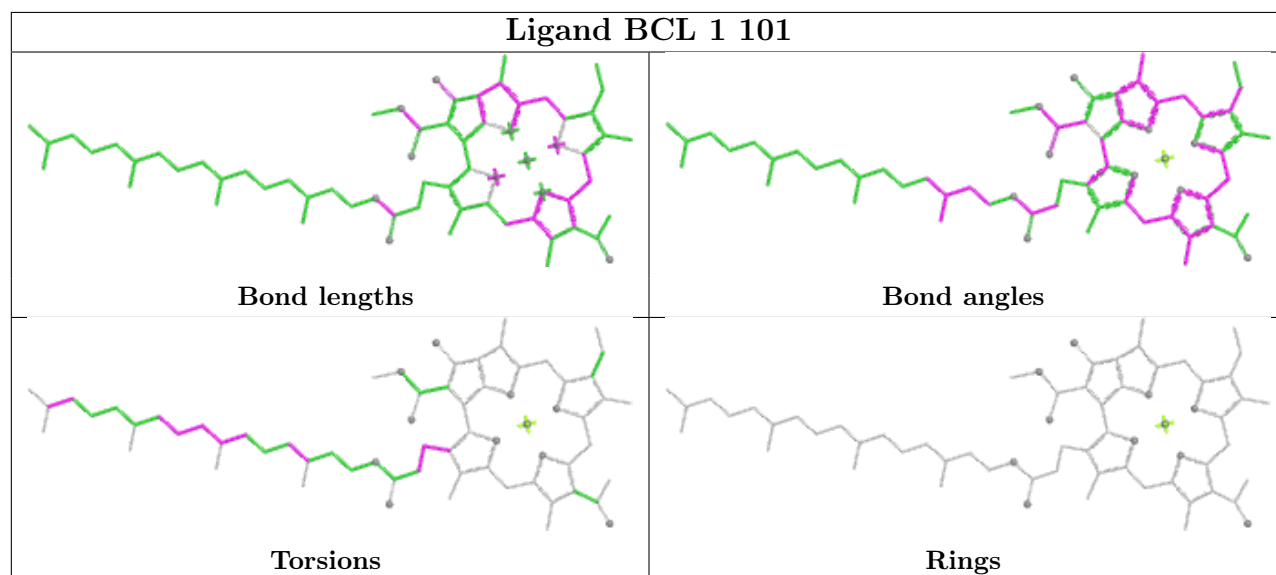
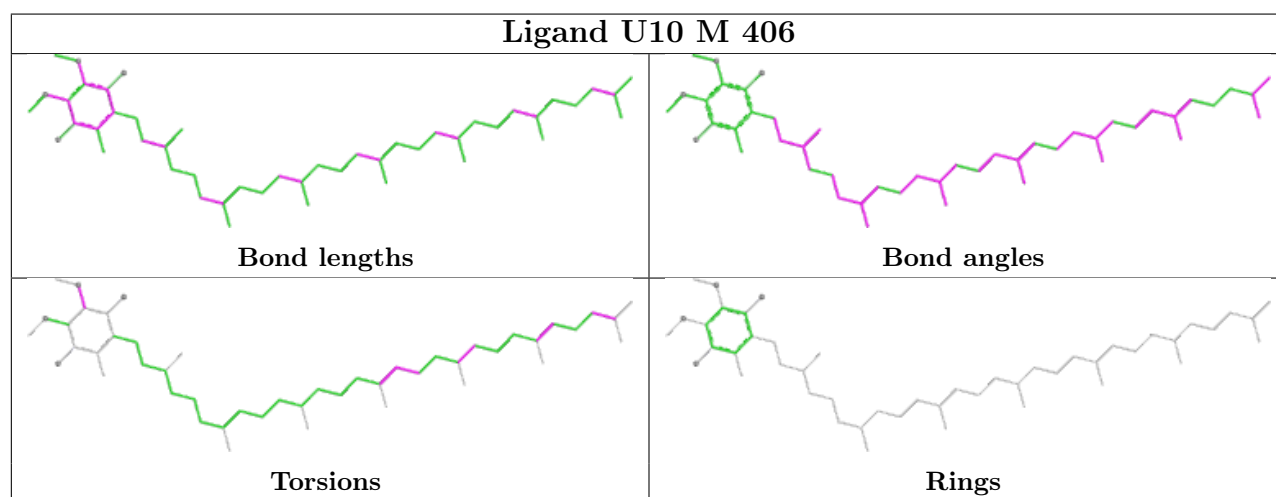
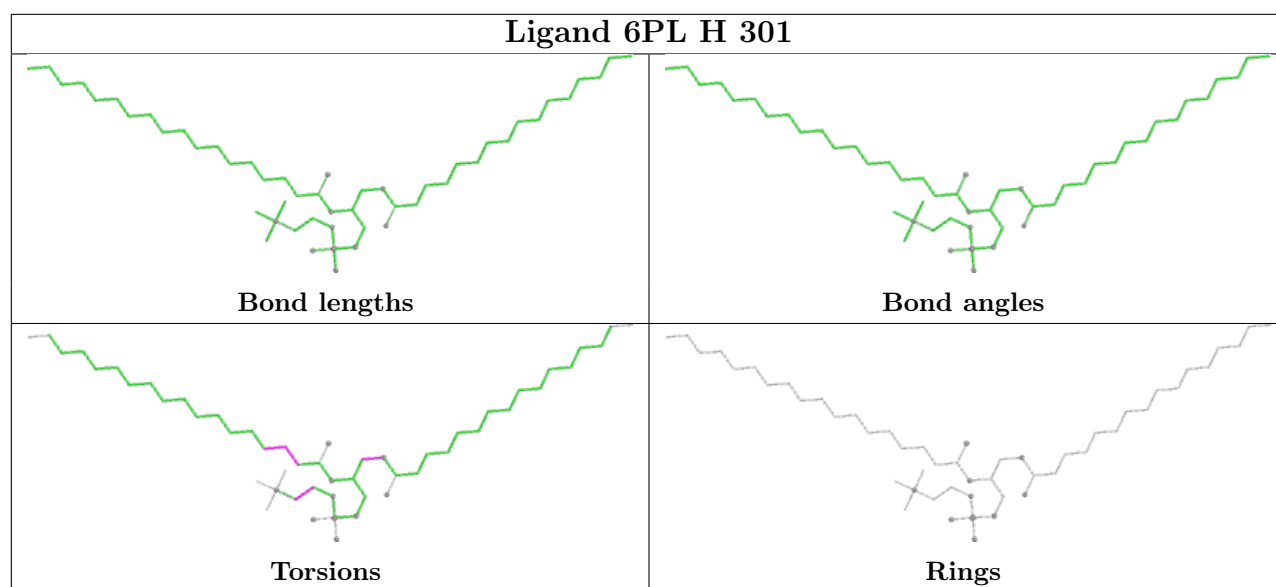


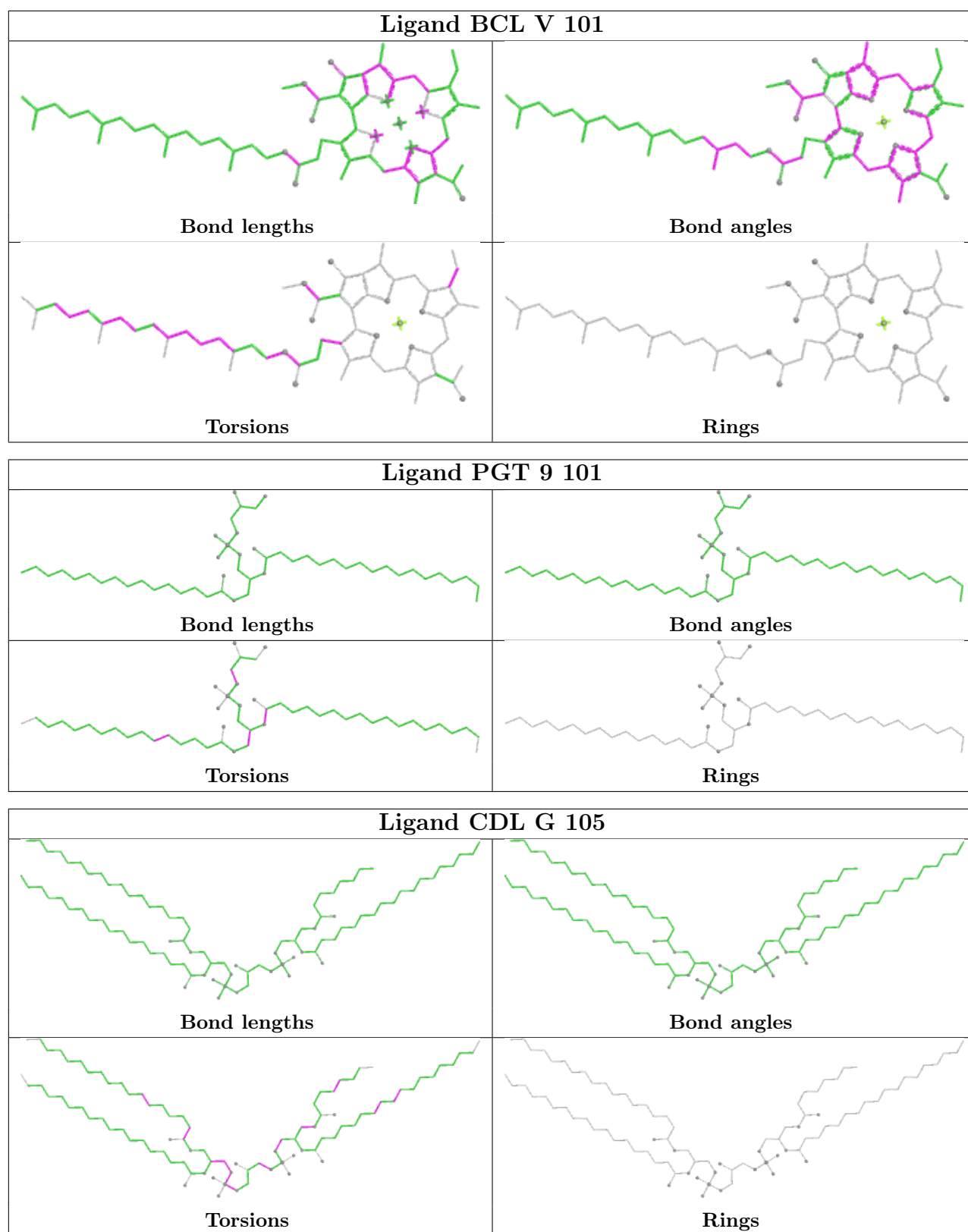












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11080. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.