



wwPDB EM Validation Summary Report ⓘ

Apr 12, 2026 – 12:14 AM JST

PDB ID : 9WQV / pdb_00009wqv
EMDB ID : EMD-66181
Title : Cryo-EM structure of LH1-RC from Rhodovulum sulfidophilum
Authors : Yue, X.-Y.; Wang, G.-L.; Yu, L.-J.
Deposited on : 2025-09-11
Resolution : 1.81 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 : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.48.1

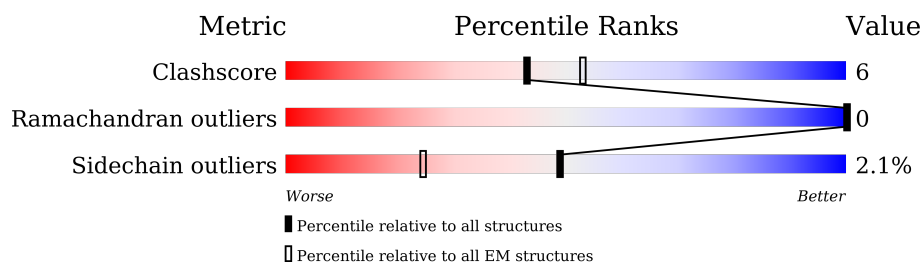
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 1.81 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.













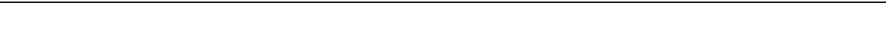

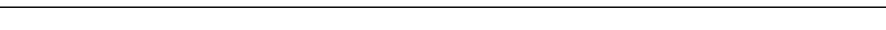
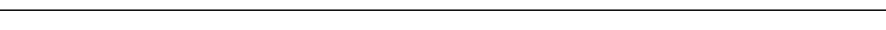











Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	0	48	83% 10% 6%
1	2	48	69% 15% • 15%
1	4	48	75% 15% 10%
1	6	48	83% 10% 6%
1	8	48	85% 8% 6%
1	B	48	83% 10% 6%
1	E	48	90% • 6%
1	G	48	90% • • 6%
1	J	48	88% 6% 6%




Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	N	48	 85% 8% 6%
1	P	48	 88% 8% .
1	R	48	 88% 6% 6%
1	T	48	 81% 10% 8%
1	V	48	 81% 12% 6%
1	X	48	 85% 6% . 6%
1	Z	48	 73% 10% 17%
2	1	54	 69% 17% 6% 9%
2	3	54	 63% 19% . 15%
2	5	54	 78% 20% .
2	7	54	 80% 19% .
2	9	54	 83% 15% .
2	A	54	 87% 11% .
2	D	54	 87% 9% . .
2	F	54	 85% 13% .
2	I	54	 85% 13% .
2	K	54	 87% 11% .
2	O	54	 89% 9% .
2	Q	54	 83% 15% .
2	S	54	 85% 13% .
2	U	54	 85% 11% . .
2	W	54	 81% 15% . .
2	Y	54	 74% 17% . 6%
3	C	356	 91% 8% .
4	H	260	 92% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	L	284	 92%8%
6	M	321	 87%11%..
7	a	229	 41%5%52%

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 28553 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 Antenna pigment protein beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	45	Total	C	N	O	S	0	0
			362	240	57	64	1		
1	2	41	Total	C	N	O	S	0	0
			326	216	53	56	1		
1	4	43	Total	C	N	O	S	0	0
			348	233	55	59	1		
1	6	45	Total	C	N	O	S	0	0
			362	240	57	64	1		
1	8	45	Total	C	N	O	S	0	0
			362	240	57	64	1		
1	B	45	Total	C	N	O	S	0	0
			362	240	57	64	1		
1	E	45	Total	C	N	O	S	0	0
			362	240	57	64	1		
1	G	45	Total	C	N	O	S	0	0
			362	240	57	64	1		
1	J	45	Total	C	N	O	S	0	0
			362	240	57	64	1		
1	N	45	Total	C	N	O	S	0	0
			362	240	57	64	1		
1	P	46	Total	C	N	O	S	0	0
			371	245	58	67	1		
1	R	45	Total	C	N	O	S	0	0
			362	240	57	64	1		
1	T	44	Total	C	N	O	S	0	0
			356	237	56	62	1		
1	V	45	Total	C	N	O	S	0	0
			362	240	57	64	1		
1	X	45	Total	C	N	O	S	0	0
			362	240	57	64	1		
1	Z	40	Total	C	N	O	S	0	0
			324	216	52	55	1		

- Molecule 2 is a protein called Antenna pigment protein alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	49	Total	C	N	O	S	0	0
			411	283	64	62	2		
2	3	46	Total	C	N	O	S	0	0
			393	272	60	58	3		
2	5	53	Total	C	N	O	S	0	0
			435	297	68	67	3		
2	7	53	Total	C	N	O	S	0	0
			435	297	68	67	3		
2	9	53	Total	C	N	O	S	1	0
			443	302	71	67	3		
2	A	53	Total	C	N	O	S	0	0
			435	297	68	67	3		
2	D	53	Total	C	N	O	S	0	0
			435	297	68	67	3		
2	F	53	Total	C	N	O	S	0	0
			435	297	68	67	3		
2	I	53	Total	C	N	O	S	0	0
			435	297	68	67	3		
2	K	53	Total	C	N	O	S	0	0
			435	297	68	67	3		
2	O	53	Total	C	N	O	S	0	0
			435	297	68	67	3		
2	Q	53	Total	C	N	O	S	0	0
			435	297	68	67	3		
2	S	53	Total	C	N	O	S	0	0
			435	297	68	67	3		
2	U	53	Total	C	N	O	S	0	0
			435	297	68	67	3		
2	W	53	Total	C	N	O	S	0	0
			435	297	68	67	3		
2	Y	51	Total	C	N	O	S	0	0
			420	288	66	64	2		

- Molecule 3 is a protein called Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	352	Total	C	N	O	S	0	0
			2715	1701	454	541	19		

- Molecule 4 is a protein called photosynthetic reaction center subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	260	Total	C	N	O	S	0	0
			2026	1303	341	371	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	283	Total	C	N	O	S	0	0
			2241	1505	357	368	11		

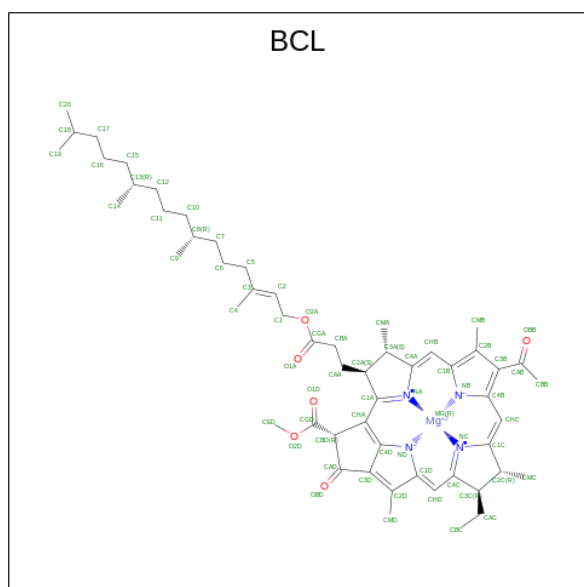
- Molecule 6 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	317	Total	C	N	O	S	1	0
			2568	1707	415	431	15		

- Molecule 7 is a protein called NADH:ubiquinone oxidoreductase 41 kd complex i subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	a	110	Total	C	N	O	S	0	0
			827	544	143	135	5		

- Molecule 8 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
8	0	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
8	3	1	Total 47	C 36	Mg 1	N 4	O 6	0
8	4	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	5	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	6	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	7	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	8	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	9	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	D	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	N	1	Total 66	C 55	Mg 1	N 4	O 6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
8	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	P	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	T	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	X	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	Z	1	Total 66	C 55	Mg 1	N 4	O 6	0

- Molecule 9 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

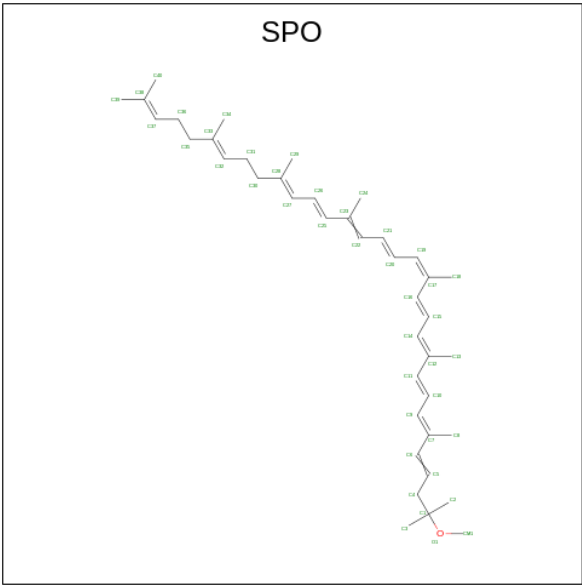
Mol	Chain	Residues	Atoms		AltConf
9	0	1	Total 18	C 18	0
9	6	1	Total 18	C 18	0
9	8	1	Total 18	C 18	0
9	B	1	Total 18	C 18	0
9	D	1	Total 18	C 18	0
9	E	1	Total 18	C 18	0
9	G	1	Total 18	C 18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
9	J	1	Total C 18 18	0
9	N	1	Total C 18 18	0
9	P	1	Total C 18 18	0
9	R	1	Total C 18 18	0
9	T	1	Total C 18 18	0
9	V	1	Total C 18 18	0

- Molecule 10 is SPHEROIDENE (CCD ID: SPO) (formula: C₄₁H₆₀O) (labeled as "Ligand of Interest" by depositor).



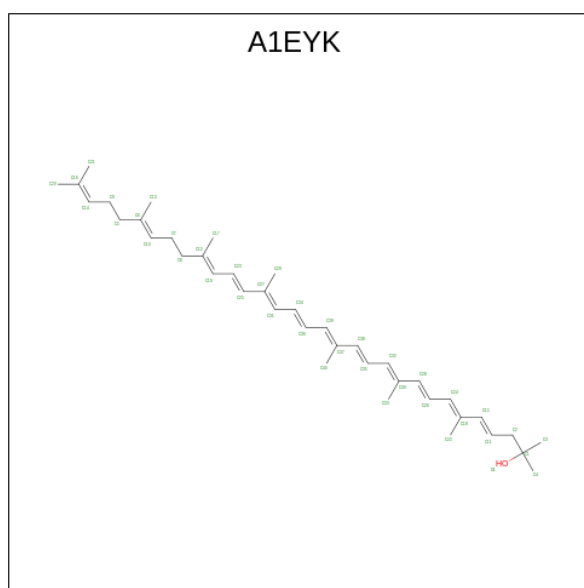
Mol	Chain	Residues	Atoms	AltConf
10	4	1	Total C O 42 41 1	0
10	5	1	Total C O 42 41 1	0
10	7	1	Total C O 42 41 1	0
10	9	1	Total C O 42 41 1	0
10	A	1	Total C O 42 41 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
10	D	1	Total	C	O	0
			42	41	1	
10	F	1	Total	C	O	0
			42	41	1	
10	I	1	Total	C	O	0
			42	41	1	
10	K	1	Total	C	O	0
			42	41	1	
10	M	1	Total	C	O	0
			42	41	1	
10	O	1	Total	C	O	0
			42	41	1	
10	Q	1	Total	C	O	0
			42	41	1	
10	S	1	Total	C	O	0
			42	41	1	
10	U	1	Total	C	O	0
			42	41	1	
10	U	1	Total	C	O	0
			42	41	1	
10	Y	1	Total	C	O	0
			42	41	1	

- Molecule 11 is (4 {E},6 {E},8 {E},10 {E},12 {E},14 {E},16 {E},18 {E},20 {E},22 {E},26 {E})-2,6,10,14,19,23,27,31-octamethyldotriaconta-4,6,8,10,12,14,16,18,20,22,26,30-dodecaen-2-ol (CCD ID: A1EYK) (formula: C₄₀H₅₈O) (labeled as "Ligand of Interest" by depositor).

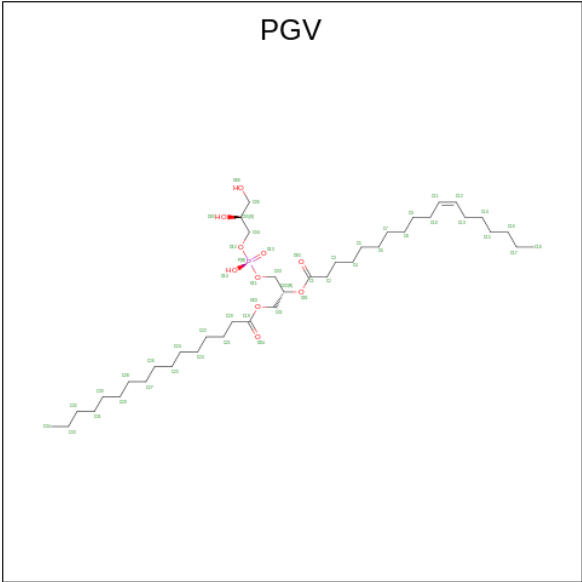


Mol	Chain	Residues	Atoms			AltConf
11	5	1	Total	C	O	0
			41	40	1	
11	7	1	Total	C	O	0
			41	40	1	
11	9	1	Total	C	O	0
			41	40	1	
11	A	1	Total	C	O	0
			41	40	1	
11	D	1	Total	C	O	0
			41	40	1	
11	F	1	Total	C	O	0
			41	40	1	
11	I	1	Total	C	O	0
			41	40	1	
11	K	1	Total	C	O	0
			41	40	1	
11	O	1	Total	C	O	0
			41	40	1	
11	Q	1	Total	C	O	0
			41	40	1	
11	S	1	Total	C	O	0
			41	40	1	
11	U	1	Total	C	O	0
			41	40	1	
11	W	1	Total	C	O	0
			41	40	1	
11	Z	1	Total	C	O	0
			41	40	1	

- Molecule 12 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



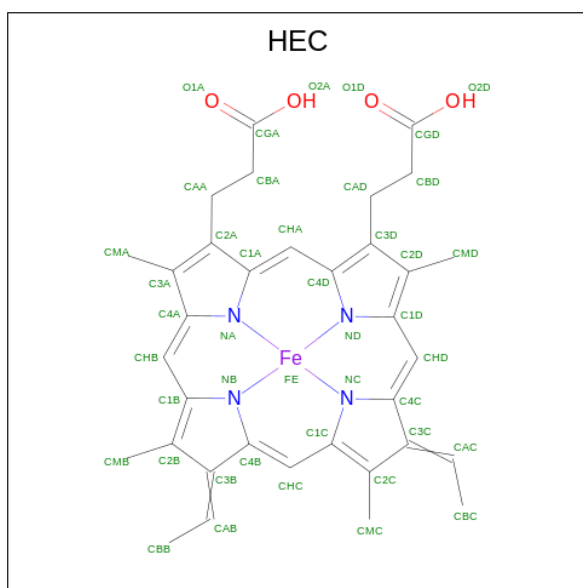
- Molecule 13 is (1R)-2-[[[(2S)-2,3-DIHYDROXYPROPYL]OXY](HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	O	P	0
			47	36	10	1	
13	D	1	Total	C	O	P	0
			32	23	8	1	
13	F	1	Total	C	O	P	0
			51	40	10	1	
13	H	1	Total	C	O	P	0
			34	23	10	1	
13	H	1	Total	C	O	P	0
			33	22	10	1	
13	H	1	Total	C	O	P	0
			42	31	10	1	
13	H	1	Total	C	O	P	0
			42	31	10	1	
13	H	1	Total	C	O	P	0
			36	27	8	1	
13	L	1	Total	C	O	P	0
			43	32	10	1	
13	M	1	Total	C	O	P	0
			40	31	8	1	
13	M	1	Total	C	O	P	0
			45	34	10	1	
13	M	1	Total	C	O	P	0
			43	32	10	1	
13	M	1	Total	C	O	P	0
			33	22	10	1	

- Molecule 14 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄) (labeled as "Ligand of

Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
14	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
14	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
14	C	1	Total 43	C 34	Fe 1	N 4	O 4	0

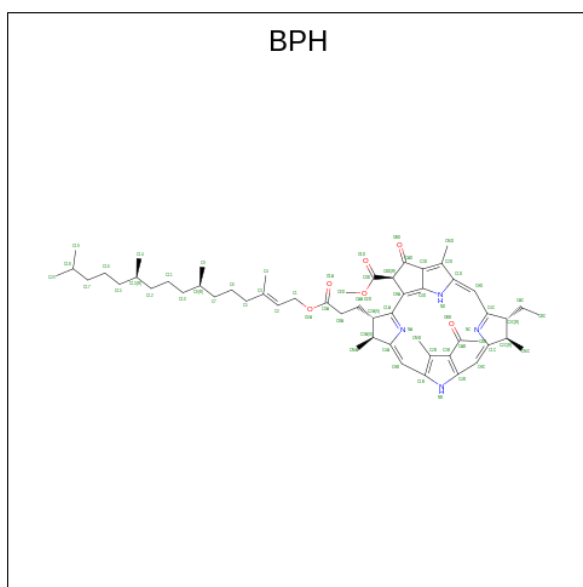
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
15	C	2	Total	Mg	0
			2	2	
15	M	2	Total	Mg	0
			2	2	

- Molecule 16 is FE (III) ION (CCD ID: FE) (formula: Fe).

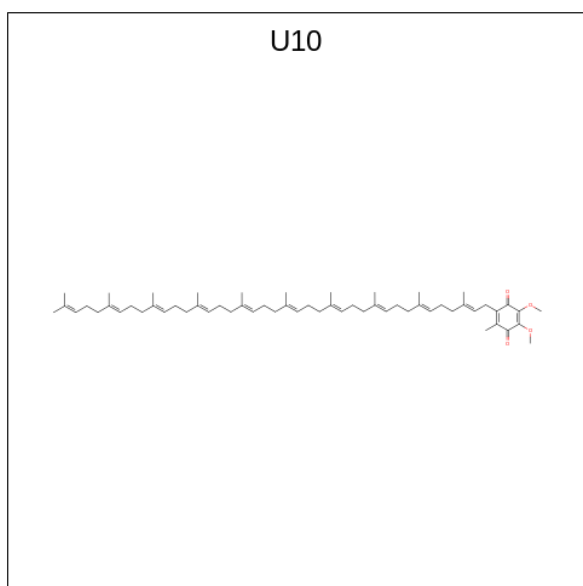
Mol	Chain	Residues	Atoms		AltConf
16	C	1	Total	Fe	0
			1	1	
16	M	1	Total	Fe	0
			1	1	

- Molecule 17 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: C₅₅H₇₆N₄O₆) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 18 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
18	L	1	Total	C	O	0
			63	59	4	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
18	M	1	Total	C	O	0
			25	21	4	
18	M	1	Total	C	O	0
			63	59	4	
18	M	1	Total	C	O	0
			28	24	4	

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		AltConf
19	0	3	Total	O	0
			3	3	
19	6	1	Total	O	0
			1	1	
19	7	3	Total	O	0
			3	3	
19	8	2	Total	O	0
			2	2	
19	9	5	Total	O	0
			5	5	
19	A	12	Total	O	0
			12	12	
19	B	7	Total	O	0
			7	7	
19	C	184	Total	O	0
			184	184	
19	D	5	Total	O	0
			5	5	
19	E	2	Total	O	0
			2	2	
19	F	6	Total	O	0
			6	6	
19	G	2	Total	O	0
			2	2	
19	H	65	Total	O	0
			65	65	
19	I	10	Total	O	0
			10	10	
19	J	4	Total	O	0
			4	4	
19	K	8	Total	O	0
			8	8	

Continued on next page...


Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
19	L	57	Total 57	O 57	0
19	M	76	Total 76	O 76	0
19	N	5	Total 5	O 5	0
19	O	5	Total 5	O 5	0
19	P	3	Total 3	O 3	0
19	Q	11	Total 11	O 11	0
19	R	2	Total 2	O 2	0
19	S	14	Total 14	O 14	0
19	T	2	Total 2	O 2	0
19	U	7	Total 7	O 7	0
19	V	1	Total 1	O 1	0

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: Antenna pigment protein beta chain

Chain 0: 



- Molecule 1: Antenna pigment protein beta chain

Chain 2: 




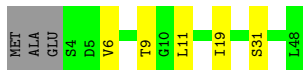
- Molecule 1: Antenna pigment protein beta chain

Chain 4: 




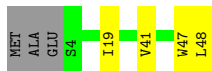
- Molecule 1: Antenna pigment protein beta chain

Chain 6: 




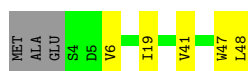
- Molecule 1: Antenna pigment protein beta chain

Chain 8: 



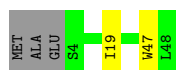
- Molecule 1: Antenna pigment protein beta chain

Chain B: 



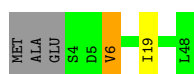
- Molecule 1: Antenna pigment protein beta chain

Chain E: 90% 6%



- Molecule 1: Antenna pigment protein beta chain

Chain G: 90% 6%



- Molecule 1: Antenna pigment protein beta chain

Chain J: 88% 6% 6%



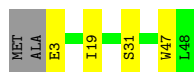
- Molecule 1: Antenna pigment protein beta chain

Chain N: 85% 8% 6%



- Molecule 1: Antenna pigment protein beta chain

Chain P: 88% 8%



- Molecule 1: Antenna pigment protein beta chain

Chain R: 88% 6% 6%

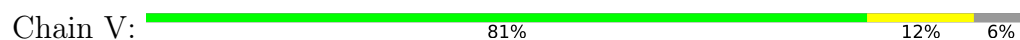


- Molecule 1: Antenna pigment protein beta chain

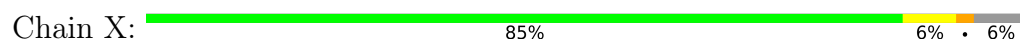
Chain T: 81% 10% 8%



- Molecule 1: Antenna pigment protein beta chain



- Molecule 1: Antenna pigment protein beta chain



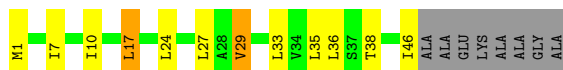
- Molecule 1: Antenna pigment protein beta chain



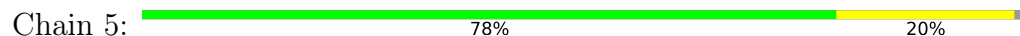
- Molecule 2: Antenna pigment protein alpha chain



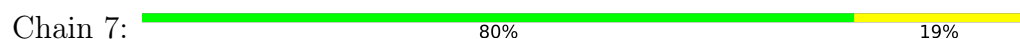
- Molecule 2: Antenna pigment protein alpha chain

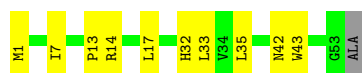


- Molecule 2: Antenna pigment protein alpha chain



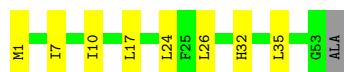
- Molecule 2: Antenna pigment protein alpha chain





- Molecule 2: Antenna pigment protein alpha chain

Chain 9: 83% 15% .



- Molecule 2: Antenna pigment protein alpha chain

Chain A: 87% 11% .



- Molecule 2: Antenna pigment protein alpha chain

Chain D: 87% 9% . .



- Molecule 2: Antenna pigment protein alpha chain

Chain F: 85% 13% .



- Molecule 2: Antenna pigment protein alpha chain

Chain I: 85% 13% .



- Molecule 2: Antenna pigment protein alpha chain

Chain K: 87% 11% .



- Molecule 2: Antenna pigment protein alpha chain

Chain O: 89% 9% .



- Molecule 2: Antenna pigment protein alpha chain

Chain Q: 83% 15% .



- Molecule 2: Antenna pigment protein alpha chain

Chain S: 85% 13% .



- Molecule 2: Antenna pigment protein alpha chain

Chain U: 85% 11% ..



- Molecule 2: Antenna pigment protein alpha chain

Chain W: 81% 15% ..



- Molecule 2: Antenna pigment protein alpha chain

Chain Y: 74% 17% 6%



- Molecule 3: Photosynthetic reaction center cytochrome c subunit

Chain C: 91% 8% .

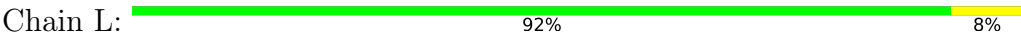


- Molecule 4: photosynthetic reaction center subunit H

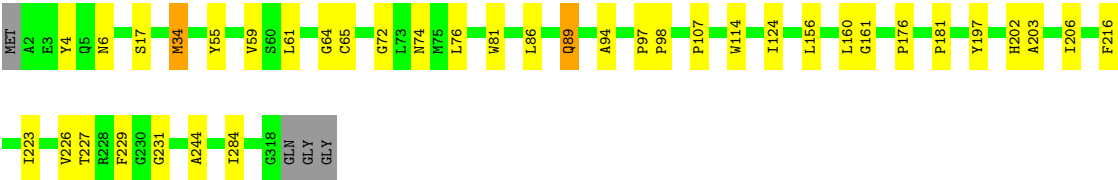
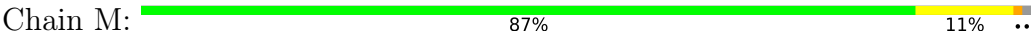
Chain H: 92% 8%



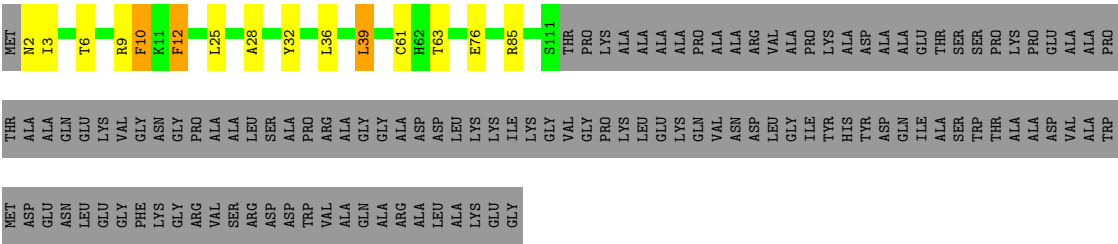
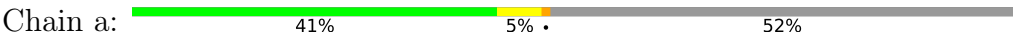
● Molecule 5: Reaction center protein L chain



● Molecule 6: Reaction center protein M chain



● Molecule 7: NADH:ubiquinone oxidoreductase 41 kd complex i subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	108964	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

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: A1EYK, HEC, MG, U10, BCL, LMT, BPH, FE, SPO, UNL, FME, PGV

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	0	0.09	0/374	0.19	0/512
1	2	0.11	0/337	0.41	0/462
1	4	0.08	0/360	0.23	0/493
1	6	0.08	0/374	0.18	0/512
1	8	0.09	0/374	0.18	0/512
1	B	0.09	0/374	0.19	0/512
1	E	0.09	0/374	0.18	0/512
1	G	0.09	0/374	0.18	0/512
1	J	0.09	0/374	0.18	0/512
1	N	0.09	0/374	0.19	0/512
1	P	0.08	0/383	0.18	0/524
1	R	0.08	0/374	0.18	0/512
1	T	0.10	0/368	0.20	0/504
1	V	0.09	0/374	0.19	0/512
1	X	0.08	0/374	0.21	0/512
1	Z	0.10	0/335	0.29	0/459
2	1	0.09	0/423	0.28	0/574
2	3	0.08	0/395	0.24	0/537
2	5	0.10	0/437	0.21	0/593
2	7	0.09	0/437	0.23	0/593
2	9	0.10	0/448	0.23	0/607
2	A	0.10	0/437	0.22	0/593
2	D	0.10	0/437	0.21	0/593
2	F	0.11	0/437	0.22	0/593
2	I	0.10	0/437	0.20	0/593
2	K	0.10	0/437	0.21	0/593
2	O	0.10	0/437	0.21	0/593
2	Q	0.11	0/437	0.25	0/593
2	S	0.09	0/437	0.22	0/593
2	U	0.08	0/437	0.22	0/593
2	W	0.08	0/437	0.25	0/593
2	Y	0.08	0/432	0.32	0/586

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	C	0.12	0/2782	0.30	0/3795
4	H	0.13	0/2084	0.26	0/2827
5	L	0.12	0/2330	0.28	0/3183
6	M	0.13	0/2667	0.29	0/3642
7	a	0.11	0/852	0.31	0/1161
All	All	0.11	0/23554	0.25	0/32102

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	0	362	0	347	4	0
1	2	326	0	308	5	0
1	4	348	0	338	8	0
1	6	362	0	347	5	0
1	8	362	0	347	7	0
1	B	362	0	347	5	0
1	E	362	0	347	3	0
1	G	362	0	347	2	0
1	J	362	0	347	4	0
1	N	362	0	347	4	0
1	P	371	0	353	3	0
1	R	362	0	347	3	0
1	T	356	0	342	5	0
1	V	362	0	347	5	0
1	X	362	0	347	4	0
1	Z	324	0	315	5	0
2	1	411	0	431	11	0
2	3	393	0	413	14	0
2	5	435	0	455	9	0
2	7	435	0	455	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	9	443	0	468	7	0
2	A	435	0	455	5	0
2	D	435	0	455	5	0
2	F	435	0	455	5	0
2	I	435	0	455	7	0
2	K	435	0	455	7	0
2	O	435	0	455	4	0
2	Q	435	0	455	7	0
2	S	435	0	455	5	0
2	U	435	0	455	6	0
2	W	435	0	455	9	0
2	Y	420	0	439	9	0
3	C	2715	0	2561	24	0
4	H	2026	0	1992	14	0
5	L	2241	0	2176	17	0
6	M	2568	0	2469	28	0
7	a	827	0	841	11	0
8	0	66	0	74	5	0
8	1	66	0	74	7	0
8	2	66	0	74	3	0
8	3	47	0	35	0	0
8	4	66	0	74	5	0
8	5	66	0	74	6	0
8	6	66	0	74	3	0
8	7	66	0	74	2	0
8	8	66	0	74	6	0
8	9	66	0	74	2	0
8	A	66	0	74	3	0
8	B	66	0	74	6	0
8	D	66	0	74	2	0
8	E	66	0	74	5	0
8	F	66	0	74	1	0
8	G	66	0	74	4	0
8	I	66	0	74	0	0
8	J	66	0	74	3	0
8	K	66	0	74	2	0
8	L	198	0	222	7	0
8	M	66	0	74	4	0
8	N	66	0	74	4	0
8	O	66	0	74	2	0
8	P	66	0	74	5	0
8	Q	66	0	74	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	R	66	0	74	5	0
8	S	66	0	74	1	0
8	T	66	0	74	6	0
8	U	66	0	74	2	0
8	V	66	0	74	5	0
8	W	66	0	74	0	0
8	X	66	0	74	8	0
8	Y	66	0	74	2	0
8	Z	66	0	74	5	0
9	0	18	0	0	0	0
9	6	18	0	0	0	0
9	8	18	0	0	0	0
9	B	18	0	0	0	0
9	D	18	0	0	0	0
9	E	18	0	0	0	0
9	G	18	0	0	0	0
9	J	18	0	0	0	0
9	N	18	0	0	0	0
9	P	18	0	0	0	0
9	R	18	0	0	0	0
9	T	18	0	0	0	0
9	V	18	0	0	0	0
10	4	42	0	60	13	0
10	5	42	0	60	4	0
10	7	42	0	60	6	0
10	9	42	0	60	4	0
10	A	42	0	60	9	0
10	D	42	0	60	7	0
10	F	42	0	60	5	0
10	I	42	0	60	4	0
10	K	42	0	60	5	0
10	M	42	0	60	4	0
10	O	42	0	60	7	0
10	Q	42	0	60	4	0
10	S	42	0	60	5	0
10	U	84	0	120	11	0
10	Y	42	0	60	10	0
11	5	41	0	0	0	0
11	7	41	0	0	0	0
11	9	41	0	0	0	0
11	A	41	0	0	0	0
11	D	41	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	F	41	0	0	0	0
11	I	41	0	0	0	0
11	K	41	0	0	0	0
11	O	41	0	0	0	0
11	Q	41	0	0	0	0
11	S	41	0	0	0	0
11	U	41	0	0	0	0
11	W	41	0	0	0	0
11	Z	41	0	0	0	0
12	7	27	0	27	4	0
12	9	27	0	27	1	0
12	D	35	0	46	2	0
12	F	28	0	29	0	0
12	K	27	0	27	1	0
12	L	54	0	54	0	0
12	M	53	0	64	0	0
12	O	27	0	27	0	0
13	A	47	0	65	3	0
13	D	32	0	38	1	0
13	F	51	0	76	2	0
13	H	187	0	229	6	0
13	L	43	0	59	2	0
13	M	161	0	200	4	0
14	C	129	0	92	8	0
15	C	2	0	0	0	0
15	M	2	0	0	0	0
16	C	1	0	0	0	0
16	M	1	0	0	0	0
17	L	65	0	76	5	0
17	M	65	0	76	6	0
18	L	63	0	90	4	0
18	M	116	0	148	6	0
19	0	3	0	0	0	0
19	6	1	0	0	0	0
19	7	3	0	0	0	0
19	8	2	0	0	0	0
19	9	5	0	0	0	0
19	A	12	0	0	0	0
19	B	7	0	0	0	0
19	C	184	0	0	1	0
19	D	5	0	0	0	0
19	E	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	F	6	0	0	0	0
19	G	2	0	0	0	0
19	H	65	0	0	0	0
19	I	10	0	0	0	0
19	J	4	0	0	0	0
19	K	8	0	0	0	0
19	L	57	0	0	0	0
19	M	76	0	0	0	0
19	N	5	0	0	0	0
19	O	5	0	0	0	0
19	P	3	0	0	0	0
19	Q	11	0	0	0	0
19	R	2	0	0	0	0
19	S	14	0	0	0	0
19	T	2	0	0	0	0
19	U	7	0	0	0	0
19	V	1	0	0	0	0
All	All	28553	0	27758	357	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 6.

The worst 5 of 357 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:278:CYS:SG	14:C:402:HEC:HAC	1.77	1.24
3:C:278:CYS:SG	14:C:402:HEC:CAC	2.30	1.19
3:C:331:CYS:SG	14:C:403:HEC:CAC	2.50	1.00
3:C:331:CYS:SG	14:C:403:HEC:HAC	2.05	0.95
3:C:204:GLN:OE1	19:C:502:HOH:O	1.89	0.89

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	0	43/48 (90%)	43 (100%)	0	0	100	100
1	2	39/48 (81%)	37 (95%)	2 (5%)	0	100	100
1	4	41/48 (85%)	41 (100%)	0	0	100	100
1	6	43/48 (90%)	43 (100%)	0	0	100	100
1	8	43/48 (90%)	43 (100%)	0	0	100	100
1	B	43/48 (90%)	43 (100%)	0	0	100	100
1	E	43/48 (90%)	42 (98%)	1 (2%)	0	100	100
1	G	43/48 (90%)	42 (98%)	1 (2%)	0	100	100
1	J	43/48 (90%)	42 (98%)	1 (2%)	0	100	100
1	N	43/48 (90%)	42 (98%)	1 (2%)	0	100	100
1	P	44/48 (92%)	43 (98%)	1 (2%)	0	100	100
1	R	43/48 (90%)	43 (100%)	0	0	100	100
1	T	42/48 (88%)	42 (100%)	0	0	100	100
1	V	43/48 (90%)	43 (100%)	0	0	100	100
1	X	43/48 (90%)	43 (100%)	0	0	100	100
1	Z	38/48 (79%)	35 (92%)	3 (8%)	0	100	100
2	1	47/54 (87%)	47 (100%)	0	0	100	100
2	3	44/54 (82%)	44 (100%)	0	0	100	100
2	5	51/54 (94%)	51 (100%)	0	0	100	100
2	7	51/54 (94%)	51 (100%)	0	0	100	100
2	9	52/54 (96%)	52 (100%)	0	0	100	100
2	A	51/54 (94%)	51 (100%)	0	0	100	100
2	D	51/54 (94%)	51 (100%)	0	0	100	100
2	F	51/54 (94%)	51 (100%)	0	0	100	100
2	I	51/54 (94%)	51 (100%)	0	0	100	100
2	K	51/54 (94%)	51 (100%)	0	0	100	100
2	O	51/54 (94%)	51 (100%)	0	0	100	100
2	Q	51/54 (94%)	51 (100%)	0	0	100	100
2	S	51/54 (94%)	51 (100%)	0	0	100	100
2	U	51/54 (94%)	51 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	W	51/54 (94%)	51 (100%)	0	0	100	100
2	Y	49/54 (91%)	49 (100%)	0	0	100	100
3	C	350/356 (98%)	341 (97%)	9 (3%)	0	100	100
4	H	258/260 (99%)	254 (98%)	4 (2%)	0	100	100
5	L	281/284 (99%)	275 (98%)	6 (2%)	0	100	100
6	M	316/321 (98%)	308 (98%)	8 (2%)	0	100	100
7	a	108/229 (47%)	107 (99%)	1 (1%)	0	100	100
All	All	2794/3082 (91%)	2756 (99%)	38 (1%)	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	0	37/39 (95%)	37 (100%)	0	100	100
1	2	31/39 (80%)	28 (90%)	3 (10%)	6	0
1	4	35/39 (90%)	35 (100%)	0	100	100
1	6	37/39 (95%)	37 (100%)	0	100	100
1	8	37/39 (95%)	37 (100%)	0	100	100
1	B	37/39 (95%)	37 (100%)	0	100	100
1	E	37/39 (95%)	37 (100%)	0	100	100
1	G	37/39 (95%)	36 (97%)	1 (3%)	40	22
1	J	37/39 (95%)	37 (100%)	0	100	100
1	N	37/39 (95%)	37 (100%)	0	100	100
1	P	38/39 (97%)	37 (97%)	1 (3%)	41	24
1	R	37/39 (95%)	36 (97%)	1 (3%)	40	22
1	T	36/39 (92%)	35 (97%)	1 (3%)	38	21
1	V	37/39 (95%)	37 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	X	37/39 (95%)	36 (97%)	1 (3%)	40	22
1	Z	32/39 (82%)	32 (100%)	0	100	100
2	1	43/43 (100%)	37 (86%)	6 (14%)	3	0
2	3	41/43 (95%)	37 (90%)	4 (10%)	6	0
2	5	43/43 (100%)	42 (98%)	1 (2%)	45	29
2	7	43/43 (100%)	43 (100%)	0	100	100
2	9	44/43 (102%)	43 (98%)	1 (2%)	45	29
2	A	43/43 (100%)	43 (100%)	0	100	100
2	D	43/43 (100%)	42 (98%)	1 (2%)	45	29
2	F	43/43 (100%)	43 (100%)	0	100	100
2	I	43/43 (100%)	43 (100%)	0	100	100
2	K	43/43 (100%)	43 (100%)	0	100	100
2	O	43/43 (100%)	43 (100%)	0	100	100
2	Q	43/43 (100%)	43 (100%)	0	100	100
2	S	43/43 (100%)	42 (98%)	1 (2%)	45	29
2	U	43/43 (100%)	42 (98%)	1 (2%)	45	29
2	W	43/43 (100%)	43 (100%)	0	100	100
2	Y	43/43 (100%)	39 (91%)	4 (9%)	7	0
3	C	295/298 (99%)	289 (98%)	6 (2%)	50	35
4	H	210/210 (100%)	207 (99%)	3 (1%)	62	50
5	L	224/225 (100%)	221 (99%)	3 (1%)	65	52
6	M	256/257 (100%)	252 (98%)	4 (2%)	58	45
7	a	80/162 (49%)	73 (91%)	7 (9%)	8	1
All	All	2331/2464 (95%)	2281 (98%)	50 (2%)	49	32

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	L	248	CYS
2	S	26	LEU
7	a	76	GLU
6	M	34	MET
6	M	216	PHE

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

Mol	Chain	Res	Type
7	a	2	ASN
1	T	15	GLN
6	M	25	ASN
5	L	240	ASN
6	M	74	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

14 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	$\# Z > 2$
2	FME	Q	1	2	8,9,10	0.51	0	7,9,11	1.04	1 (14%)
2	FME	S	1	2	8,9,10	0.50	0	7,9,11	0.96	1 (14%)
2	FME	I	1	2	8,9,10	0.50	0	7,9,11	0.95	1 (14%)
2	FME	A	1	2	8,9,10	0.51	0	7,9,11	0.98	1 (14%)
2	FME	F	1	2	8,9,10	0.52	0	7,9,11	0.96	1 (14%)
2	FME	3	1	2	8,9,10	0.51	0	7,9,11	1.26	1 (14%)
2	FME	K	1	2	8,9,10	0.51	0	7,9,11	0.98	1 (14%)
2	FME	7	1	2	8,9,10	0.52	0	7,9,11	1.00	1 (14%)
2	FME	O	1	2	8,9,10	0.52	0	7,9,11	0.97	1 (14%)
2	FME	U	1	2	8,9,10	0.52	0	7,9,11	0.94	1 (14%)
2	FME	9	1	2	8,9,10	0.51	0	7,9,11	0.96	1 (14%)
2	FME	W	1	2	8,9,10	0.52	0	7,9,11	1.00	1 (14%)
2	FME	5	1	2	8,9,10	0.52	0	7,9,11	0.94	1 (14%)
2	FME	D	1	2	8,9,10	0.50	0	7,9,11	0.98	1 (14%)

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
2	FME	Q	1	2	-	0/7/9/11	-
2	FME	S	1	2	-	0/7/9/11	-
2	FME	I	1	2	-	0/7/9/11	-
2	FME	A	1	2	-	1/7/9/11	-
2	FME	F	1	2	-	0/7/9/11	-
2	FME	3	1	2	-	1/7/9/11	-
2	FME	K	1	2	-	1/7/9/11	-
2	FME	7	1	2	-	2/7/9/11	-
2	FME	O	1	2	-	0/7/9/11	-
2	FME	U	1	2	-	0/7/9/11	-
2	FME	9	1	2	-	1/7/9/11	-
2	FME	W	1	2	-	2/7/9/11	-
2	FME	5	1	2	-	0/7/9/11	-
2	FME	D	1	2	-	1/7/9/11	-

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	1	FME	O-C-CA	-2.57	118.05	124.78
2	Q	1	FME	O-C-CA	-2.56	118.07	124.78
2	W	1	FME	O-C-CA	-2.52	118.18	124.78
2	7	1	FME	O-C-CA	-2.51	118.21	124.78
2	K	1	FME	O-C-CA	-2.50	118.24	124.78

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	3	1	FME	CB-CA-N-CN
2	7	1	FME	O1-CN-N-CA
2	7	1	FME	CB-CA-N-CN
2	9	1	FME	O1-CN-N-CA
2	A	1	FME	O1-CN-N-CA

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	W	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 117 ligands modelled in this entry, 13 are unknown and 6 are monoatomic - leaving 98 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	$\# Z > 2$
11	A1EYK	Q	103	-	39,40,40	1.70	11 (28%)	47,49,49	0.77	0
8	BCL	U	101	2	64,74,74	1.68	12 (18%)	78,115,115	2.34	23 (29%)
8	BCL	W	101	2	64,74,74	1.69	14 (21%)	78,115,115	2.33	20 (25%)
8	BCL	M	403	6	64,74,74	1.72	14 (21%)	78,115,115	2.31	22 (28%)
8	BCL	F	101	2	64,74,74	1.68	12 (18%)	78,115,115	2.31	23 (29%)
13	PGV	H	305	-	35,35,50	1.11	2 (5%)	38,40,56	1.23	4 (10%)
8	BCL	S	101	2	64,74,74	1.66	13 (20%)	78,115,115	2.30	22 (28%)
8	BCL	3	101	2	45,55,74	2.17	14 (31%)	55,92,115	2.58	16 (29%)
10	SPO	U	104	-	40,41,41	0.64	0	47,50,50	1.73	13 (27%)
8	BCL	O	101	2	64,74,74	1.68	12 (18%)	78,115,115	2.32	22 (28%)
8	BCL	9	101	2	64,74,74	1.68	13 (20%)	78,115,115	2.31	23 (29%)
11	A1EYK	S	103	-	39,40,40	1.69	11 (28%)	47,49,49	0.83	0
8	BCL	0	101	1	64,74,74	1.68	14 (21%)	78,115,115	2.17	21 (26%)
8	BCL	P	101	1	64,74,74	1.68	14 (21%)	78,115,115	2.16	19 (24%)
8	BCL	5	101	2	64,74,74	1.70	14 (21%)	78,115,115	2.20	23 (29%)
18	U10	L	303	-	63,63,63	0.58	2 (3%)	76,79,79	0.50	0
13	PGV	M	411	-	31,31,50	1.15	2 (6%)	33,36,56	1.22	3 (9%)
10	SPO	9	102	-	40,41,41	0.62	0	47,50,50	1.66	10 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	PGV	L	304	-	42,42,50	0.99	2 (4%)	45,48,56	1.04	4 (8%)
10	SPO	K	102	-	40,41,41	0.62	0	47,50,50	1.70	11 (23%)
10	SPO	U	102	-	40,41,41	0.63	0	47,50,50	1.76	13 (27%)
10	SPO	Y	102	-	40,41,41	0.64	0	47,50,50	1.84	11 (23%)
14	HEC	C	402	3	32,50,50	1.56	4 (12%)	24,82,82	1.35	1 (4%)
17	BPH	M	404	-	51,70,70	0.50	1 (1%)	52,101,101	0.68	1 (1%)
13	PGV	A	104	-	46,46,50	0.95	2 (4%)	49,52,56	1.03	3 (6%)
18	U10	M	402	-	25,25,63	0.90	2 (8%)	30,33,79	0.73	0
8	BCL	Q	101	2	64,74,74	1.68	13 (20%)	78,115,115	2.42	23 (29%)
8	BCL	E	101	1	64,74,74	1.68	14 (21%)	78,115,115	2.17	18 (23%)
12	LMT	L	306	-	28,28,36	0.44	0	39,39,47	0.75	1 (2%)
11	A1EYK	I	103	-	39,40,40	1.71	11 (28%)	47,49,49	0.86	2 (4%)
8	BCL	L	308	6	64,74,74	1.71	14 (21%)	78,115,115	2.24	22 (28%)
10	SPO	I	102	-	40,41,41	0.62	0	47,50,50	1.73	11 (23%)
8	BCL	4	102	1	64,74,74	1.82	14 (21%)	78,115,115	2.24	20 (25%)
12	LMT	K	104	-	28,28,36	0.45	0	39,39,47	0.79	1 (2%)
12	LMT	M	414	-	29,29,36	0.46	0	40,40,47	0.69	1 (2%)
10	SPO	S	102	-	40,41,41	0.63	0	47,50,50	1.70	10 (21%)
13	PGV	M	408	-	44,44,50	0.96	2 (4%)	47,50,56	1.09	3 (6%)
12	LMT	F	104	-	29,29,36	0.48	0	40,40,47	1.16	4 (10%)
10	SPO	A	102	-	40,41,41	0.63	0	47,50,50	1.63	10 (21%)
13	PGV	F	105	-	50,50,50	0.91	2 (4%)	53,56,56	0.95	2 (3%)
8	BCL	K	101	2	64,74,74	1.69	13 (20%)	78,115,115	2.31	20 (25%)
12	LMT	D	101	-	36,36,36	0.37	0	47,47,47	0.84	2 (4%)
8	BCL	J	101	1	64,74,74	1.67	14 (21%)	78,115,115	2.18	19 (24%)
12	LMT	M	413	-	25,25,36	0.44	0	30,30,47	0.56	0
8	BCL	D	102	2	64,74,74	1.67	13 (20%)	78,115,115	2.31	23 (29%)
8	BCL	6	101	1	64,74,74	1.69	14 (21%)	78,115,115	2.17	21 (26%)
8	BCL	1	101	2	64,74,74	1.77	14 (21%)	78,115,115	2.18	19 (24%)
8	BCL	2	101	1	64,74,74	1.83	14 (21%)	78,115,115	2.16	19 (24%)
11	A1EYK	O	103	-	39,40,40	1.70	11 (28%)	47,49,49	0.81	0
12	LMT	L	305	-	28,28,36	0.49	0	39,39,47	1.13	5 (12%)
11	A1EYK	9	103	-	39,40,40	1.73	10 (25%)	47,49,49	1.30	4 (8%)
10	SPO	O	102	-	40,41,41	0.62	0	47,50,50	1.70	11 (23%)
11	A1EYK	D	104	-	39,40,40	1.71	11 (28%)	47,49,49	0.79	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BCL	X	101	1	64,74,74	1.71	14 (21%)	78,115,115	2.15	19 (24%)
13	PGV	M	407	-	39,39,50	1.06	2 (5%)	43,44,56	1.22	4 (9%)
8	BCL	N	101	1	64,74,74	1.67	13 (20%)	78,115,115	2.21	20 (25%)
12	LMT	7	104	-	28,28,36	0.50	0	39,39,47	1.08	2 (5%)
8	BCL	V	101	1	64,74,74	1.69	14 (21%)	78,115,115	2.21	20 (25%)
13	PGV	H	301	-	33,33,50	1.12	2 (6%)	36,39,56	1.19	3 (8%)
12	LMT	O	104	-	28,28,36	0.48	0	39,39,47	0.94	1 (2%)
13	PGV	H	302	-	32,32,50	1.13	2 (6%)	35,38,56	1.14	3 (8%)
13	PGV	M	409	-	42,42,50	1.02	2 (4%)	45,48,56	1.01	2 (4%)
11	A1EYK	K	103	-	39,40,40	1.71	11 (28%)	47,49,49	0.80	0
12	LMT	9	104	-	28,28,36	0.51	0	39,39,47	0.98	2 (5%)
11	A1EYK	A	103	-	39,40,40	1.68	11 (28%)	47,49,49	0.81	1 (2%)
8	BCL	7	101	2	64,74,74	1.68	12 (18%)	78,115,115	2.25	23 (29%)
8	BCL	Y	101	2	64,74,74	1.74	14 (21%)	78,115,115	2.23	19 (24%)
11	A1EYK	5	103	-	39,40,40	1.73	11 (28%)	47,49,49	0.85	0
8	BCL	Z	102	1	64,74,74	1.80	15 (23%)	78,115,115	2.19	22 (28%)
8	BCL	T	101	1	64,74,74	1.67	14 (21%)	78,115,115	2.20	20 (25%)
10	SPO	Q	102	-	40,41,41	0.62	0	47,50,50	1.69	10 (21%)
8	BCL	8	101	1	64,74,74	1.67	14 (21%)	78,115,115	2.20	21 (26%)
14	HEC	C	401	3	32,50,50	1.57	4 (12%)	24,82,82	1.47	4 (16%)
17	BPH	L	302	-	51,70,70	0.51	0	52,101,101	0.60	0
10	SPO	4	101	-	40,41,41	0.66	0	47,50,50	2.01	15 (31%)
10	SPO	D	103	-	40,41,41	0.62	0	47,50,50	1.65	11 (23%)
8	BCL	R	101	1	64,74,74	1.67	13 (20%)	78,115,115	2.16	20 (25%)
8	BCL	L	307	5	64,74,74	1.68	14 (21%)	78,115,115	2.21	20 (25%)
11	A1EYK	Z	101	-	39,40,40	1.69	10 (25%)	47,49,49	1.31	3 (6%)
11	A1EYK	F	103	-	39,40,40	1.69	11 (28%)	47,49,49	0.82	1 (2%)
13	PGV	H	304	-	41,41,50	1.00	2 (4%)	44,47,56	1.16	4 (9%)
13	PGV	H	303	-	41,41,50	1.01	2 (4%)	44,47,56	1.09	3 (6%)
10	SPO	M	406	-	40,41,41	0.62	0	47,50,50	1.71	8 (17%)
8	BCL	L	301	5	64,74,74	1.68	14 (21%)	78,115,115	2.25	20 (25%)
11	A1EYK	U	103	-	39,40,40	1.70	10 (25%)	47,49,49	1.30	5 (10%)
8	BCL	I	101	2	64,74,74	1.67	12 (18%)	78,115,115	2.35	23 (29%)
14	HEC	C	403	3	32,50,50	1.56	4 (12%)	24,82,82	1.29	1 (4%)
10	SPO	F	102	-	40,41,41	0.61	0	47,50,50	1.65	10 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BCL	G	101	1	64,74,74	1.67	14 (21%)	78,115,115	2.16	20 (25%)
8	BCL	B	101	1	64,74,74	1.68	14 (21%)	78,115,115	2.16	17 (21%)
18	U10	M	405	-	63,63,63	0.61	2 (3%)	76,79,79	0.52	0
10	SPO	5	102	-	40,41,41	0.63	0	47,50,50	1.71	11 (23%)
13	PGV	D	105	-	31,31,50	1.14	2 (6%)	34,36,56	1.07	3 (8%)
8	BCL	A	101	2	64,74,74	1.69	12 (18%)	78,115,115	2.29	23 (29%)
18	U10	M	410	-	28,28,63	0.83	2 (7%)	34,37,79	0.72	0
11	A1EYK	W	102	-	39,40,40	1.80	10 (25%)	47,49,49	1.56	6 (12%)
11	A1EYK	7	103	-	39,40,40	1.69	11 (28%)	47,49,49	0.81	0
10	SPO	7	102	-	40,41,41	0.62	0	47,50,50	1.70	10 (21%)

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
11	A1EYK	Q	103	-	-	2/44/44/44	-
8	BCL	U	101	2	-	9/37/137/137	-
8	BCL	W	101	2	-	16/37/137/137	-
8	BCL	M	403	6	-	11/37/137/137	-
8	BCL	F	101	2	-	6/37/137/137	-
13	PGV	H	305	-	-	5/37/37/55	-
8	BCL	S	101	2	-	6/37/137/137	-
8	BCL	3	101	2	-	8/15/115/137	-
10	SPO	U	104	-	-	4/47/47/47	-
8	BCL	O	101	2	-	8/37/137/137	-
8	BCL	9	101	2	-	11/37/137/137	-
11	A1EYK	S	103	-	-	2/44/44/44	-
8	BCL	0	101	1	-	9/37/137/137	-
8	BCL	P	101	1	-	10/37/137/137	-
8	BCL	5	101	2	-	12/37/137/137	-
18	U10	L	303	-	-	12/63/87/87	0/1/1/1
13	PGV	M	411	-	-	10/35/35/55	-
10	SPO	9	102	-	-	3/47/47/47	-
13	PGV	L	304	-	-	12/47/47/55	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	SPO	K	102	-	-	3/47/47/47	-
10	SPO	U	102	-	-	3/47/47/47	-
10	SPO	Y	102	-	-	4/47/47/47	-
14	HEC	C	402	3	-	2/10/54/54	-
17	BPH	M	404	-	-	6/37/105/105	0/5/6/6
13	PGV	A	104	-	-	9/51/51/55	-
18	U10	M	402	-	-	5/18/42/87	0/1/1/1
8	BCL	Q	101	2	-	11/37/137/137	-
8	BCL	E	101	1	-	9/37/137/137	-
12	LMT	L	306	-	-	1/13/53/61	0/2/2/2
11	A1EYK	I	103	-	-	1/44/44/44	-
8	BCL	L	308	6	-	9/37/137/137	-
10	SPO	I	102	-	-	3/47/47/47	-
8	BCL	4	102	1	-	10/37/137/137	-
12	LMT	K	104	-	-	3/13/53/61	0/2/2/2
12	LMT	M	414	-	-	4/14/54/61	0/2/2/2
10	SPO	S	102	-	-	3/47/47/47	-
13	PGV	M	408	-	-	12/49/49/55	-
12	LMT	F	104	-	-	5/14/54/61	0/2/2/2
10	SPO	A	102	-	-	1/47/47/47	-
13	PGV	F	105	-	-	23/55/55/55	-
8	BCL	K	101	2	-	13/37/137/137	-
12	LMT	D	101	-	-	3/21/61/61	0/2/2/2
8	BCL	J	101	1	-	8/37/137/137	-
12	LMT	M	413	-	-	5/17/37/61	0/1/1/2
8	BCL	D	102	2	-	8/37/137/137	-
8	BCL	6	101	1	-	11/37/137/137	-
8	BCL	1	101	2	-	15/37/137/137	-
8	BCL	2	101	1	-	14/37/137/137	-
11	A1EYK	O	103	-	-	2/44/44/44	-
12	LMT	L	305	-	-	3/13/53/61	0/2/2/2
11	A1EYK	9	103	-	-	4/44/44/44	-
10	SPO	O	102	-	-	3/47/47/47	-
11	A1EYK	D	104	-	-	2/44/44/44	-
8	BCL	X	101	1	-	14/37/137/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	PGV	M	407	-	-	4/41/41/55	-
8	BCL	N	101	1	-	6/37/137/137	-
12	LMT	7	104	-	-	4/13/53/61	0/2/2/2
8	BCL	V	101	1	-	10/37/137/137	-
13	PGV	H	301	-	-	13/38/38/55	-
12	LMT	O	104	-	-	2/13/53/61	0/2/2/2
13	PGV	H	302	-	-	17/37/37/55	-
13	PGV	M	409	-	-	16/47/47/55	-
11	A1EYK	K	103	-	-	1/44/44/44	-
12	LMT	9	104	-	-	1/13/53/61	0/2/2/2
11	A1EYK	A	103	-	-	1/44/44/44	-
8	BCL	7	101	2	-	11/37/137/137	-
8	BCL	Y	101	2	-	10/37/137/137	-
11	A1EYK	5	103	-	-	2/44/44/44	-
8	BCL	Z	102	1	-	7/37/137/137	-
8	BCL	T	101	1	-	6/37/137/137	-
10	SPO	Q	102	-	-	3/47/47/47	-
8	BCL	8	101	1	-	9/37/137/137	-
14	HEC	C	401	3	-	2/10/54/54	-
17	BPH	L	302	-	-	5/37/105/105	0/5/6/6
10	SPO	4	101	-	-	11/47/47/47	-
10	SPO	D	103	-	-	1/47/47/47	-
8	BCL	R	101	1	-	10/37/137/137	-
8	BCL	L	307	5	-	8/37/137/137	-
11	A1EYK	Z	101	-	-	1/44/44/44	-
11	A1EYK	F	103	-	-	1/44/44/44	-
13	PGV	H	304	-	-	11/46/46/55	-
13	PGV	H	303	-	-	15/46/46/55	-
10	SPO	M	406	-	-	5/47/47/47	-
8	BCL	L	301	5	-	12/37/137/137	-
11	A1EYK	U	103	-	-	4/44/44/44	-
8	BCL	I	101	2	-	10/37/137/137	-
14	HEC	C	403	3	-	0/10/54/54	-
10	SPO	F	102	-	-	3/47/47/47	-
8	BCL	G	101	1	-	8/37/137/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	B	101	1	-	10/37/137/137	-
18	U10	M	405	-	-	9/63/87/87	0/1/1/1
10	SPO	5	102	-	-	3/47/47/47	-
13	PGV	D	105	-	-	9/35/35/55	-
8	BCL	A	101	2	-	16/37/137/137	-
18	U10	M	410	-	-	2/21/45/87	0/1/1/1
11	A1EYK	W	102	-	-	6/44/44/44	-
11	A1EYK	7	103	-	-	1/44/44/44	-
10	SPO	7	102	-	-	2/47/47/47	-

The worst 5 of 683 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	403	BCL	O2D-CGD	5.30	1.46	1.33
8	1	101	BCL	O2D-CGD	5.23	1.46	1.33
8	4	102	BCL	C3B-C2B	5.21	1.48	1.39
8	L	301	BCL	O2D-CGD	5.20	1.45	1.33
8	3	101	BCL	C3B-C2B	5.20	1.48	1.39

The worst 5 of 1010 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	2	101	BCL	CHD-C1D-ND	-9.17	116.03	124.45
8	4	102	BCL	CHD-C1D-ND	-9.16	116.04	124.45
8	3	101	BCL	CHD-C1D-ND	-9.00	116.19	124.45
8	5	101	BCL	CHD-C1D-ND	-8.71	116.45	124.45
8	1	101	BCL	CHD-C1D-ND	-8.69	116.47	124.45

There are no chirality outliers.

5 of 676 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	0	101	BCL	C3A-C2A-CAA-CBA
8	1	101	BCL	C1A-C2A-CAA-CBA
8	1	101	BCL	C4C-C3C-CAC-CBC
8	1	101	BCL	C2-C3-C5-C6
8	1	101	BCL	C4-C3-C5-C6

There are no ring outliers.

72 monomers are involved in 257 short contacts:

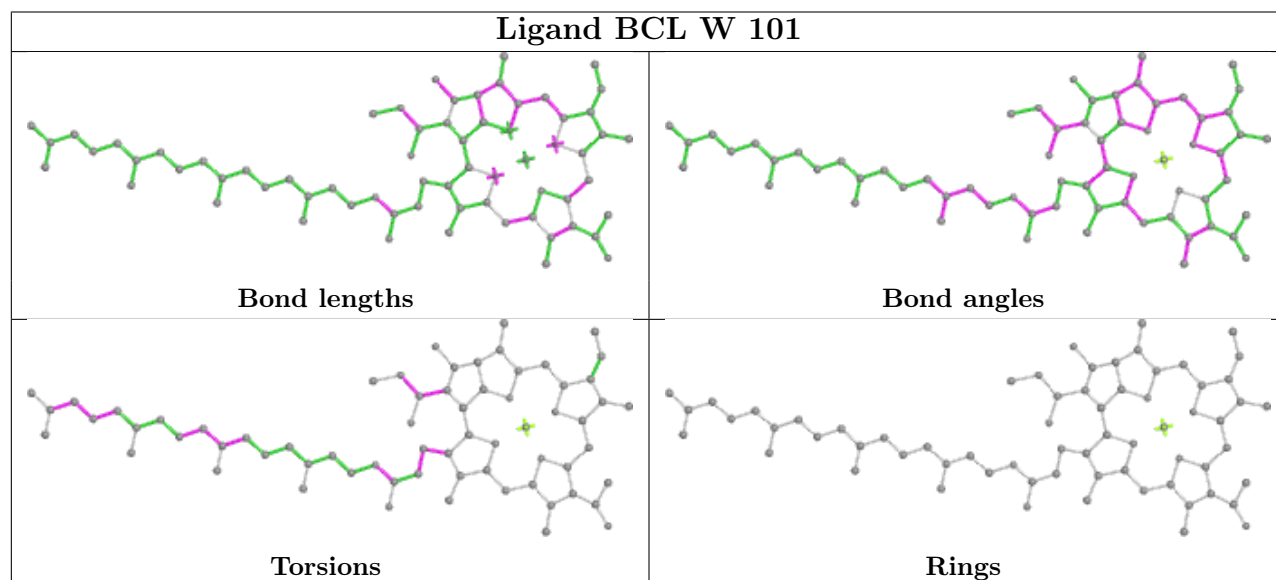
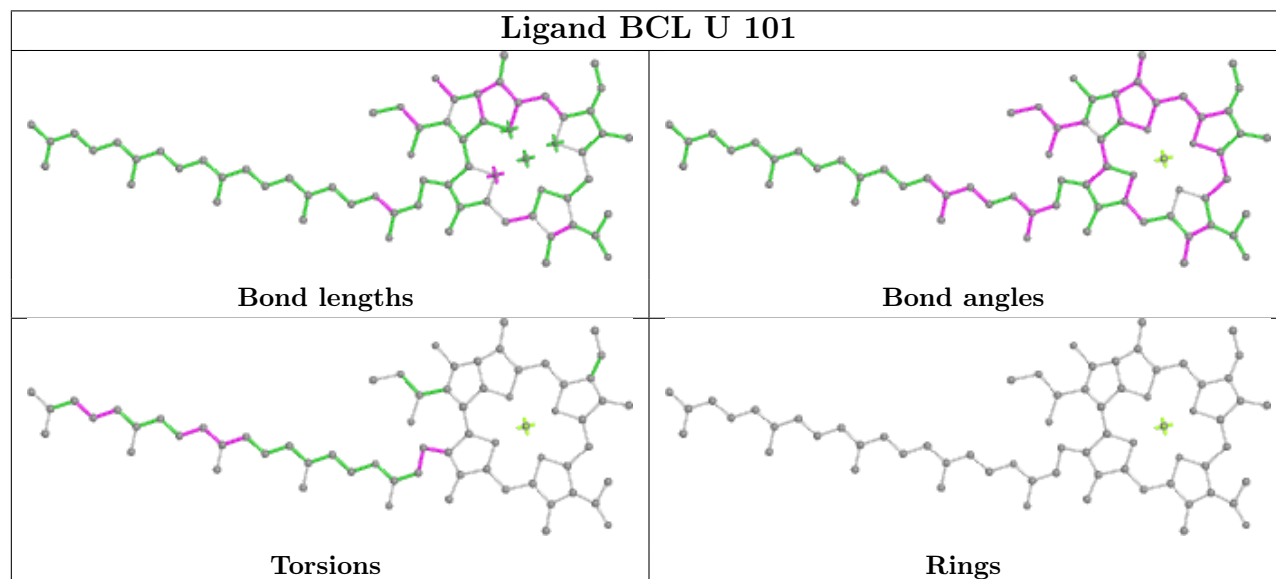
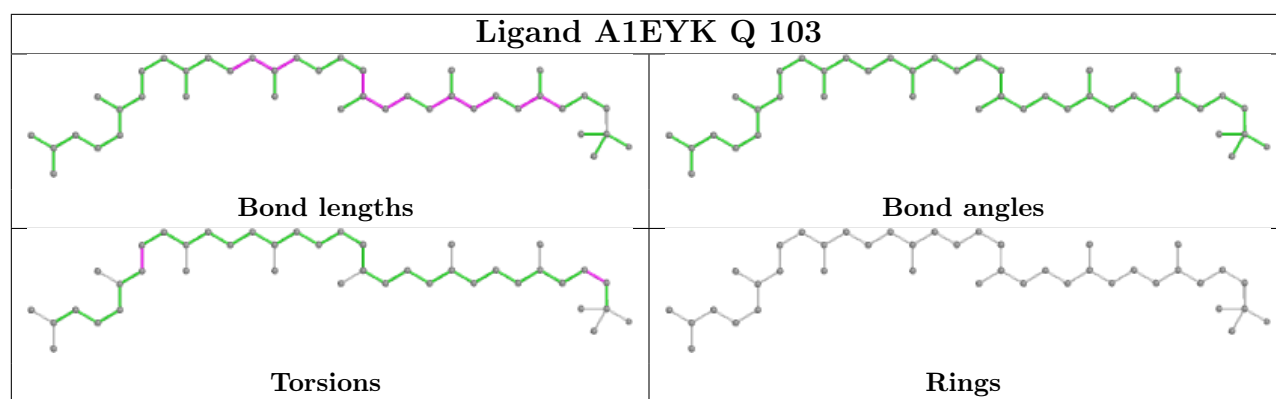
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	U	101	BCL	2	0
8	M	403	BCL	4	0
8	F	101	BCL	1	0
13	H	305	PGV	2	0
8	S	101	BCL	1	0
10	U	104	SPO	6	0
8	O	101	BCL	2	0
8	9	101	BCL	2	0
8	0	101	BCL	5	0
8	P	101	BCL	5	0
8	5	101	BCL	6	0
18	L	303	U10	4	0
13	M	411	PGV	2	0
10	9	102	SPO	4	0
13	L	304	PGV	2	0
10	K	102	SPO	5	0
10	U	102	SPO	5	0
10	Y	102	SPO	10	0
14	C	402	HEC	3	0
17	M	404	BPH	6	0
13	A	104	PGV	3	0
8	Q	101	BCL	3	0
8	E	101	BCL	5	0
8	L	308	BCL	2	0
10	I	102	SPO	4	0
8	4	102	BCL	5	0
12	K	104	LMT	1	0
10	S	102	SPO	5	0
13	M	408	PGV	1	0
10	A	102	SPO	9	0
13	F	105	PGV	2	0
8	K	101	BCL	2	0
12	D	101	LMT	2	0
8	J	101	BCL	3	0
8	D	102	BCL	2	0
8	6	101	BCL	3	0
8	1	101	BCL	7	0
8	2	101	BCL	3	0
10	O	102	SPO	7	0
8	X	101	BCL	8	0
8	N	101	BCL	4	0
12	7	104	LMT	4	0

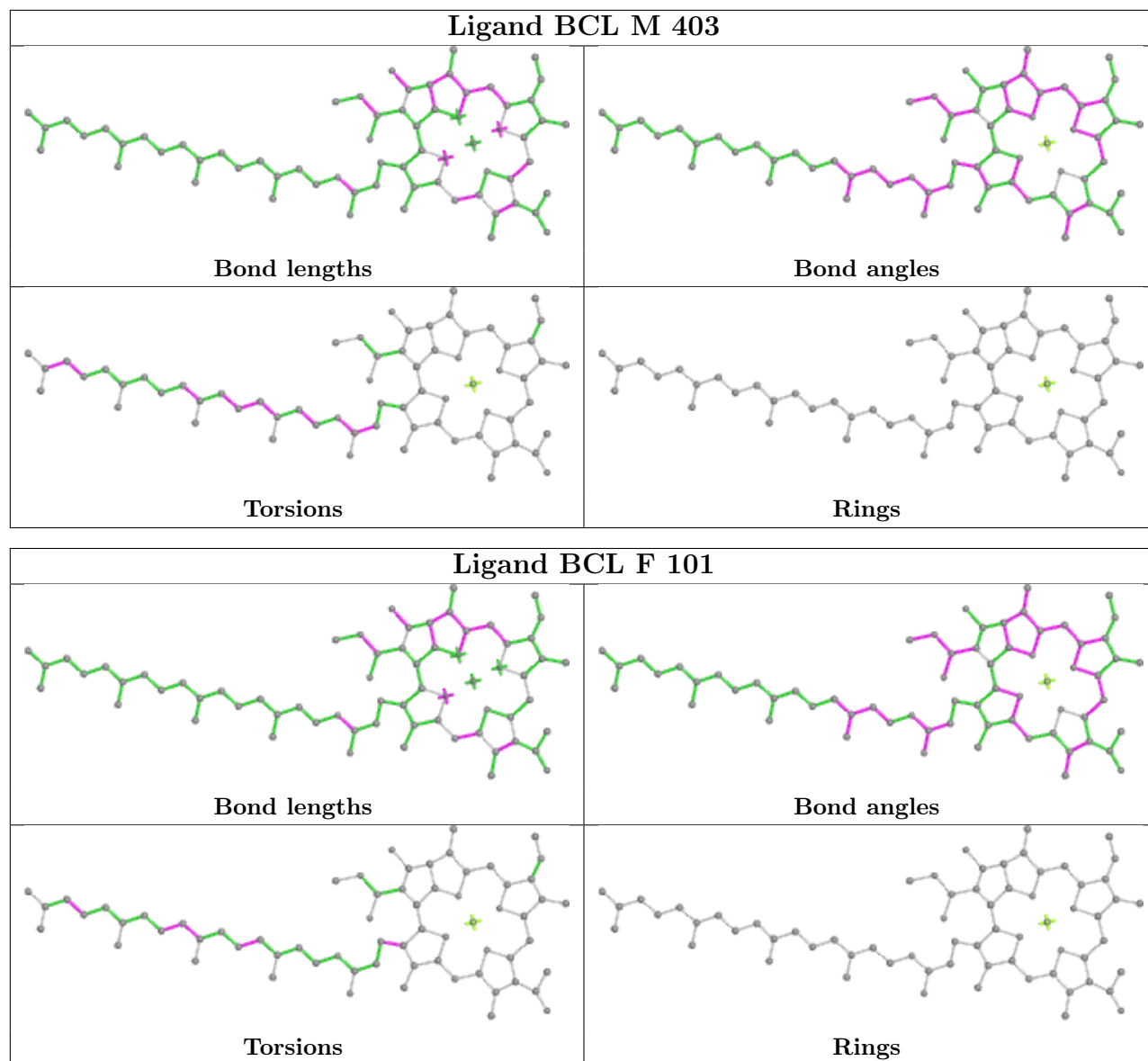
Continued on next page...

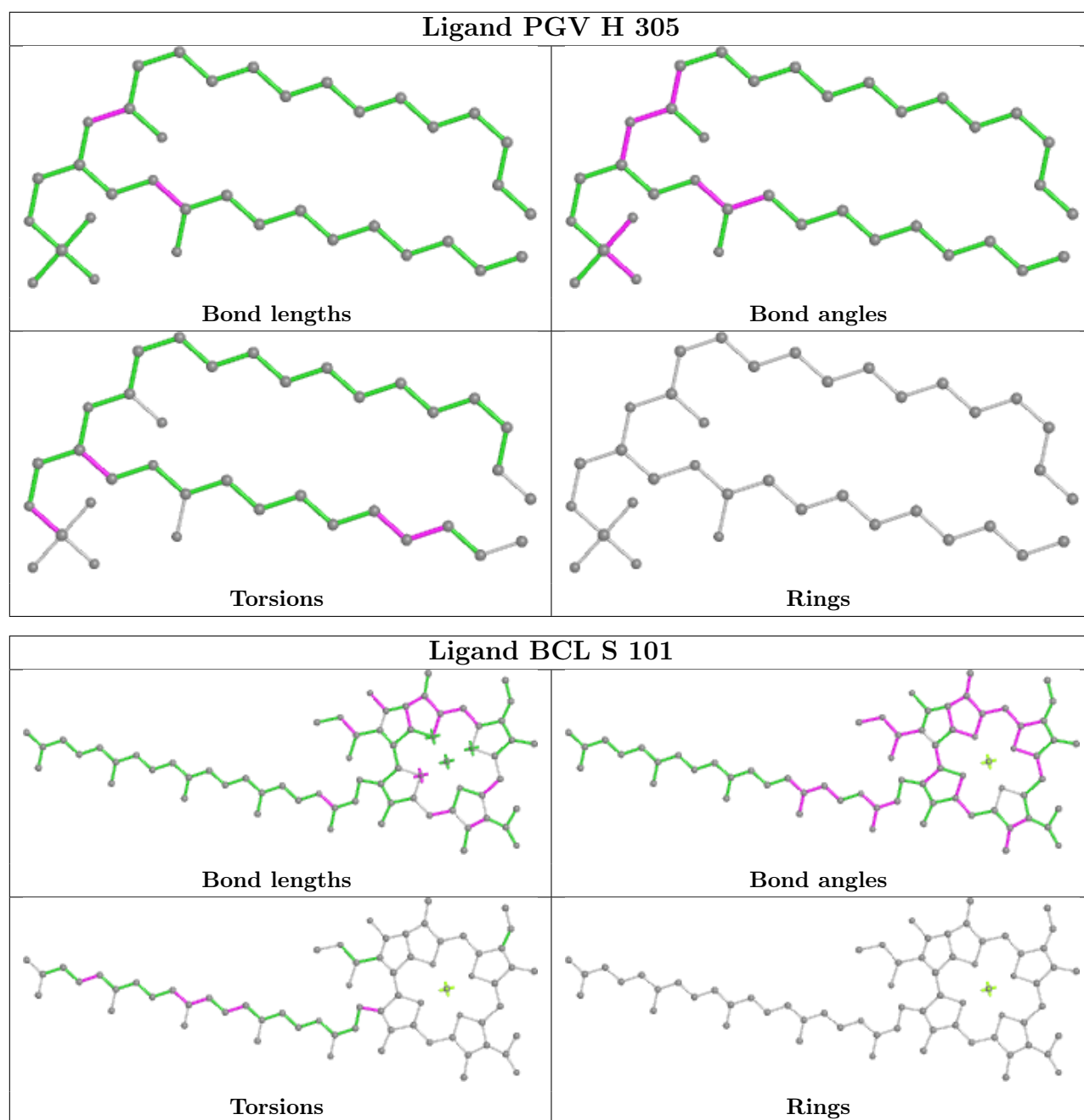
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	V	101	BCL	5	0
13	H	301	PGV	1	0
13	M	409	PGV	1	0
12	9	104	LMT	1	0
8	7	101	BCL	2	0
8	Y	101	BCL	2	0
8	Z	102	BCL	5	0
8	T	101	BCL	6	0
10	Q	102	SPO	4	0
8	8	101	BCL	6	0
14	C	401	HEC	3	0
17	L	302	BPH	5	0
10	4	101	SPO	13	0
10	D	103	SPO	7	0
8	R	101	BCL	5	0
8	L	307	BCL	3	0
13	H	304	PGV	1	0
13	H	303	PGV	3	0
10	M	406	SPO	4	0
8	L	301	BCL	2	0
14	C	403	HEC	2	0
10	F	102	SPO	5	0
8	G	101	BCL	4	0
8	B	101	BCL	6	0
18	M	405	U10	5	0
10	5	102	SPO	4	0
13	D	105	PGV	1	0
8	A	101	BCL	3	0
18	M	410	U10	1	0
10	7	102	SPO	6	0

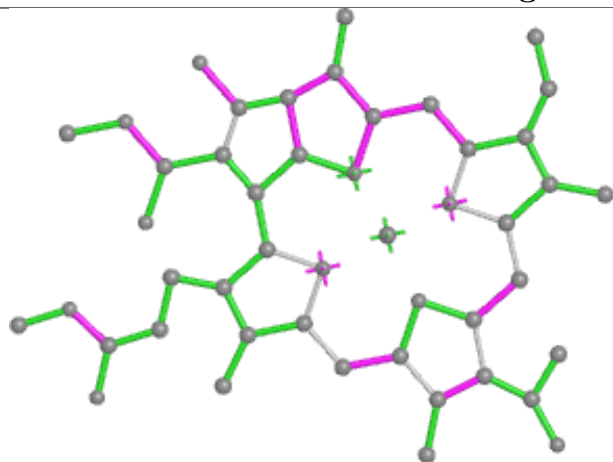
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



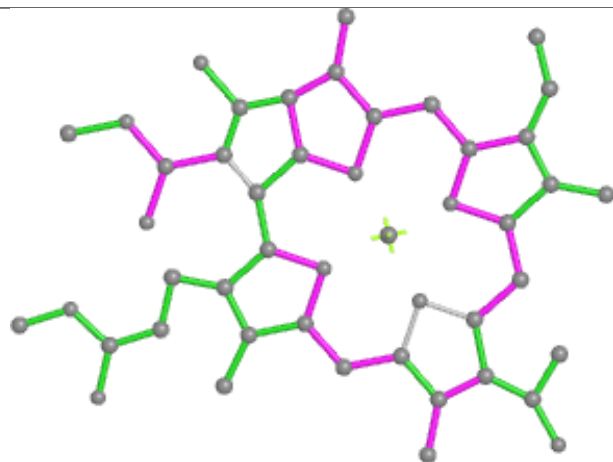




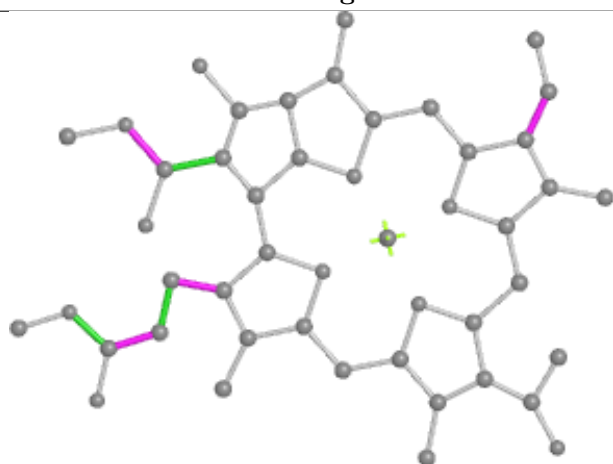
Ligand BCL 3 101



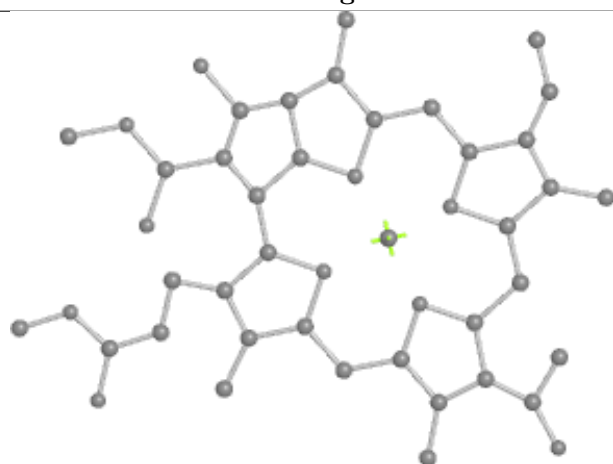
Bond lengths



Bond angles

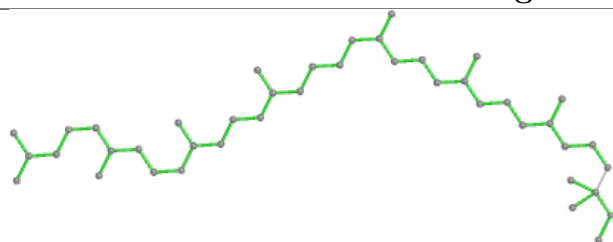


Torsions

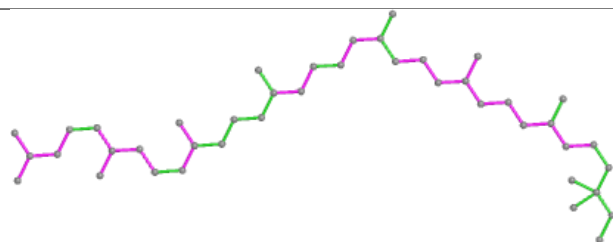


Rings

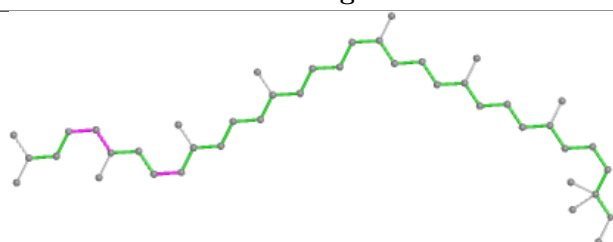
Ligand SPO U 104



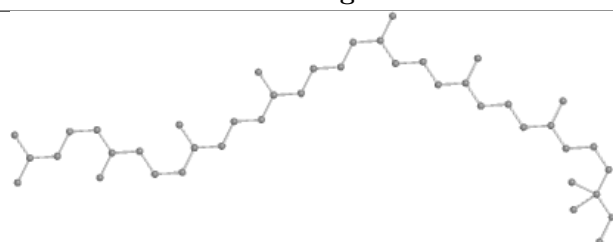
Bond lengths



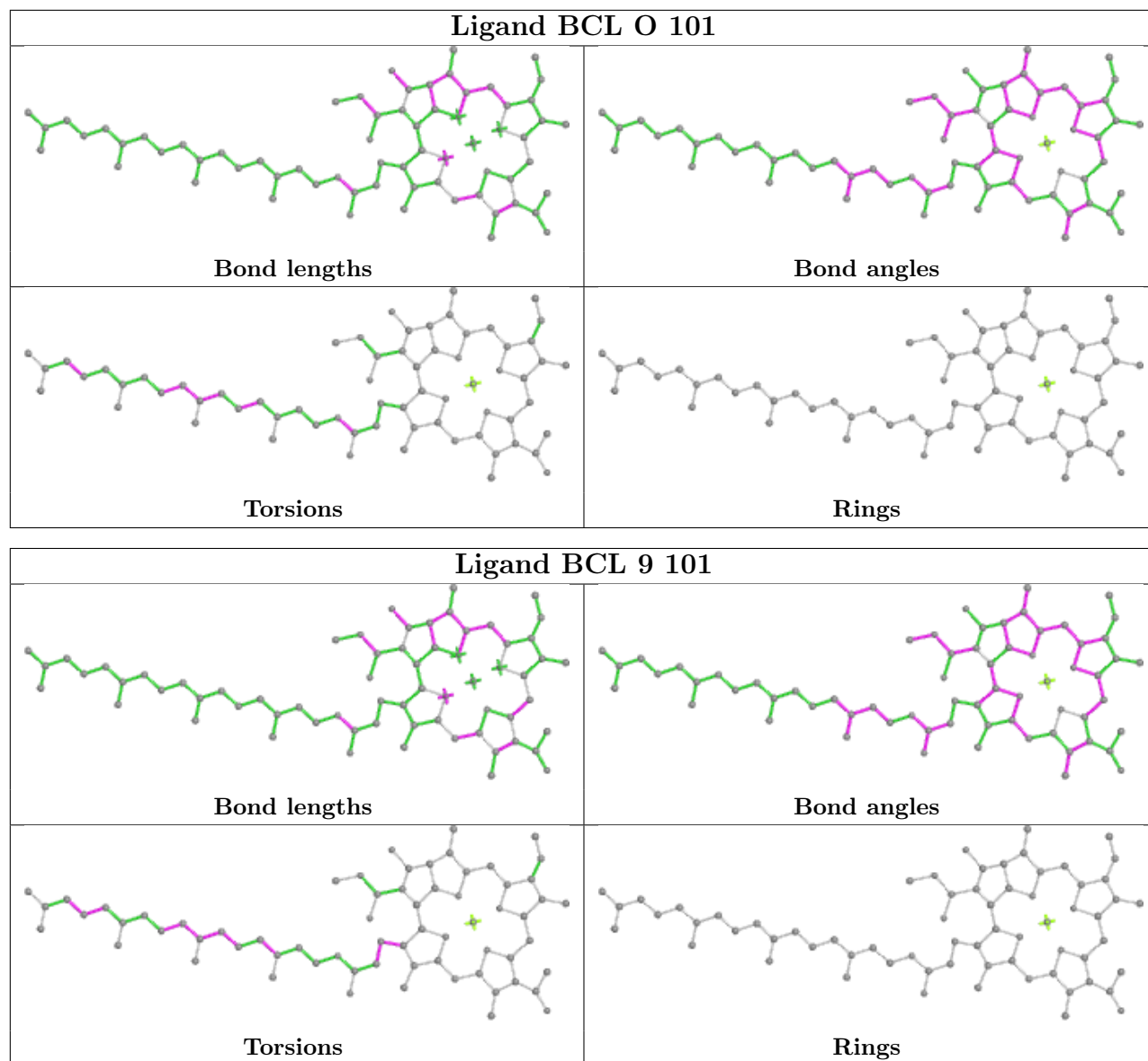
Bond angles

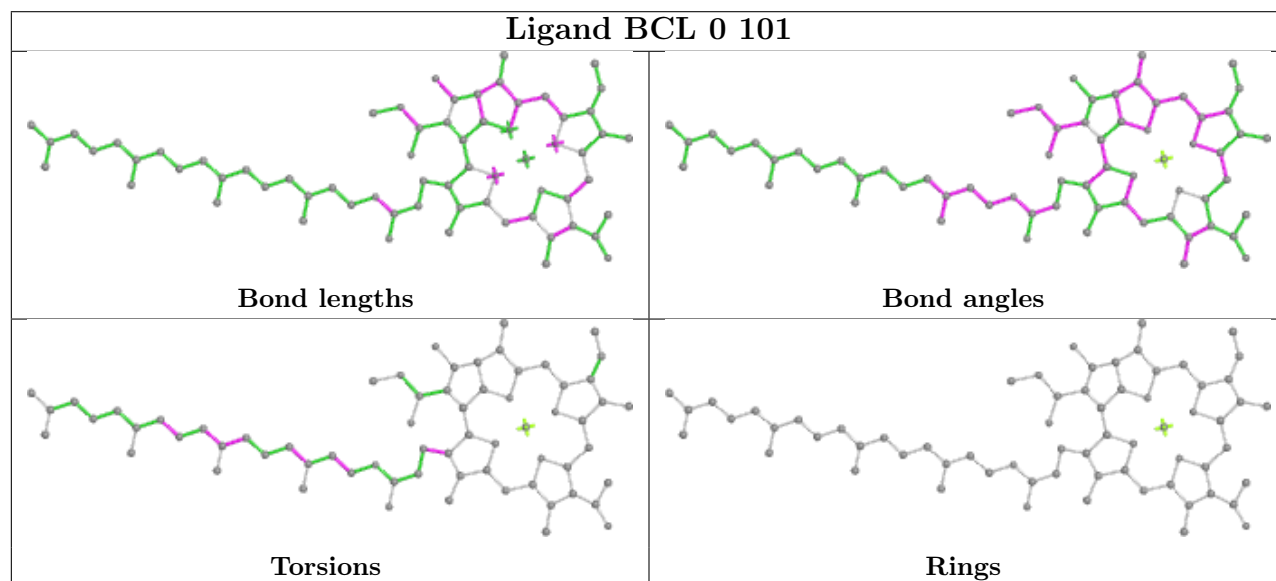
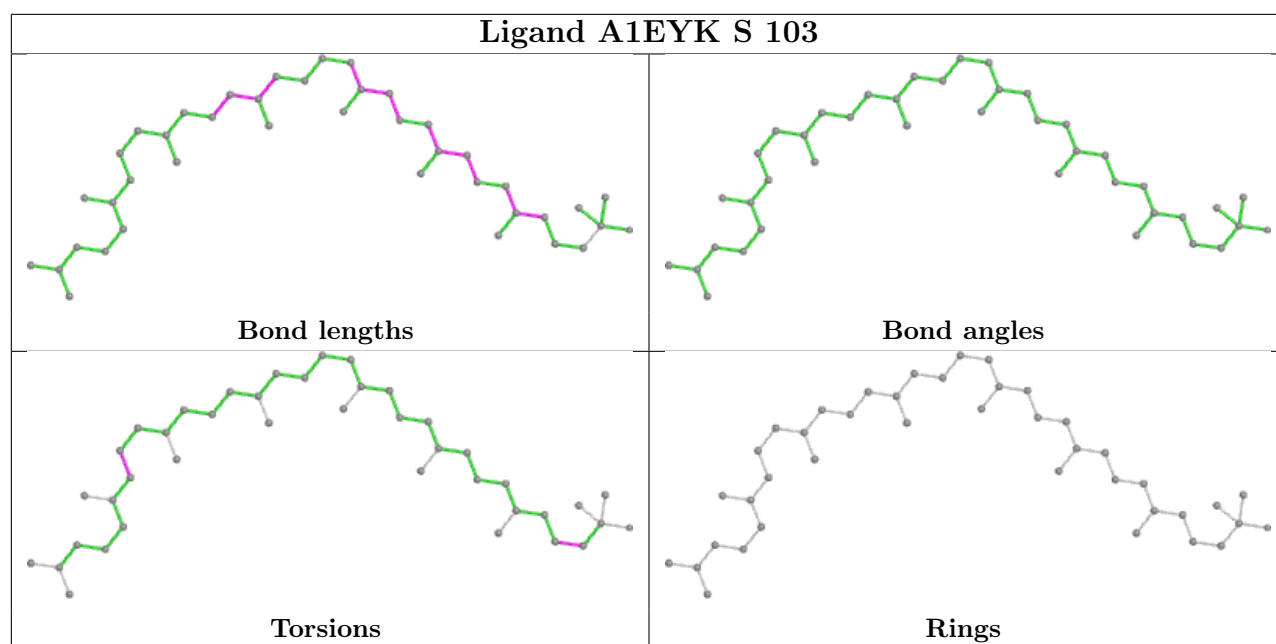


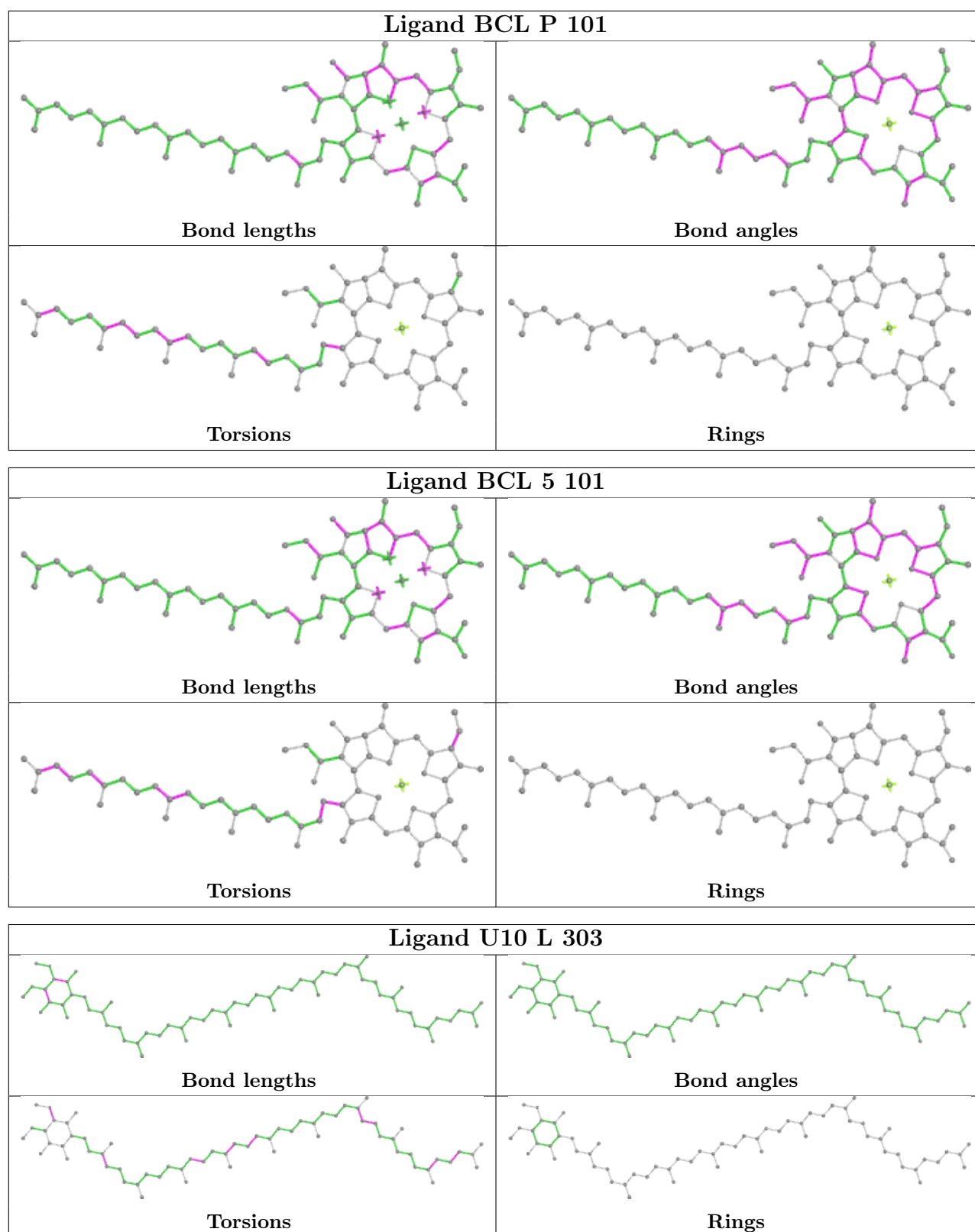
Torsions

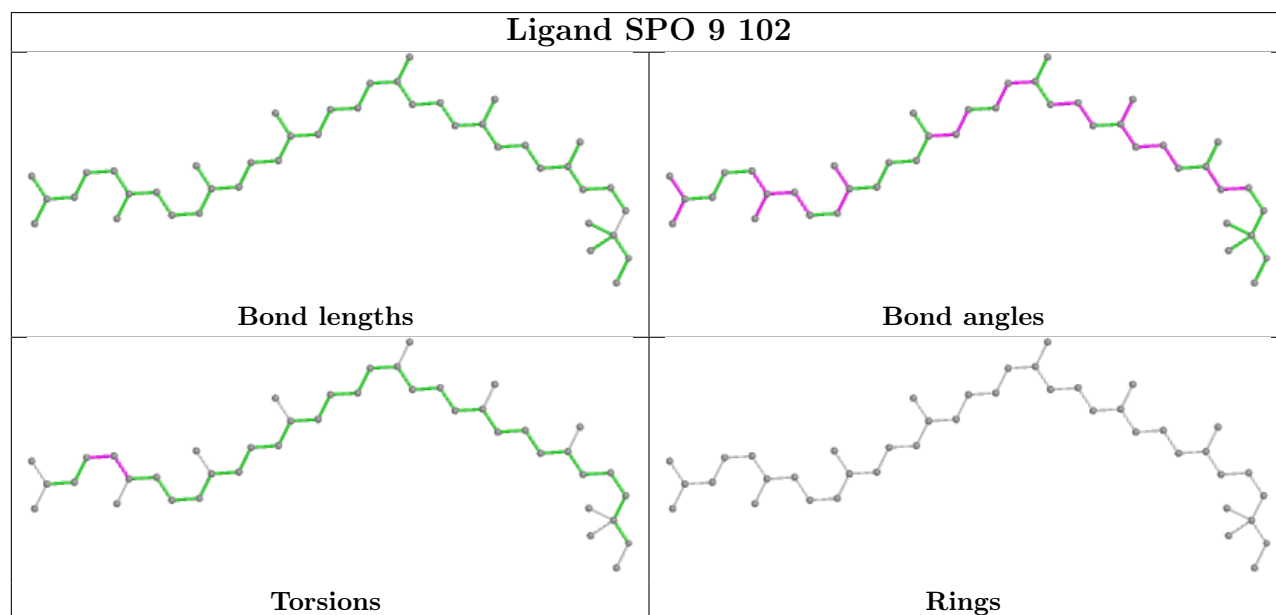
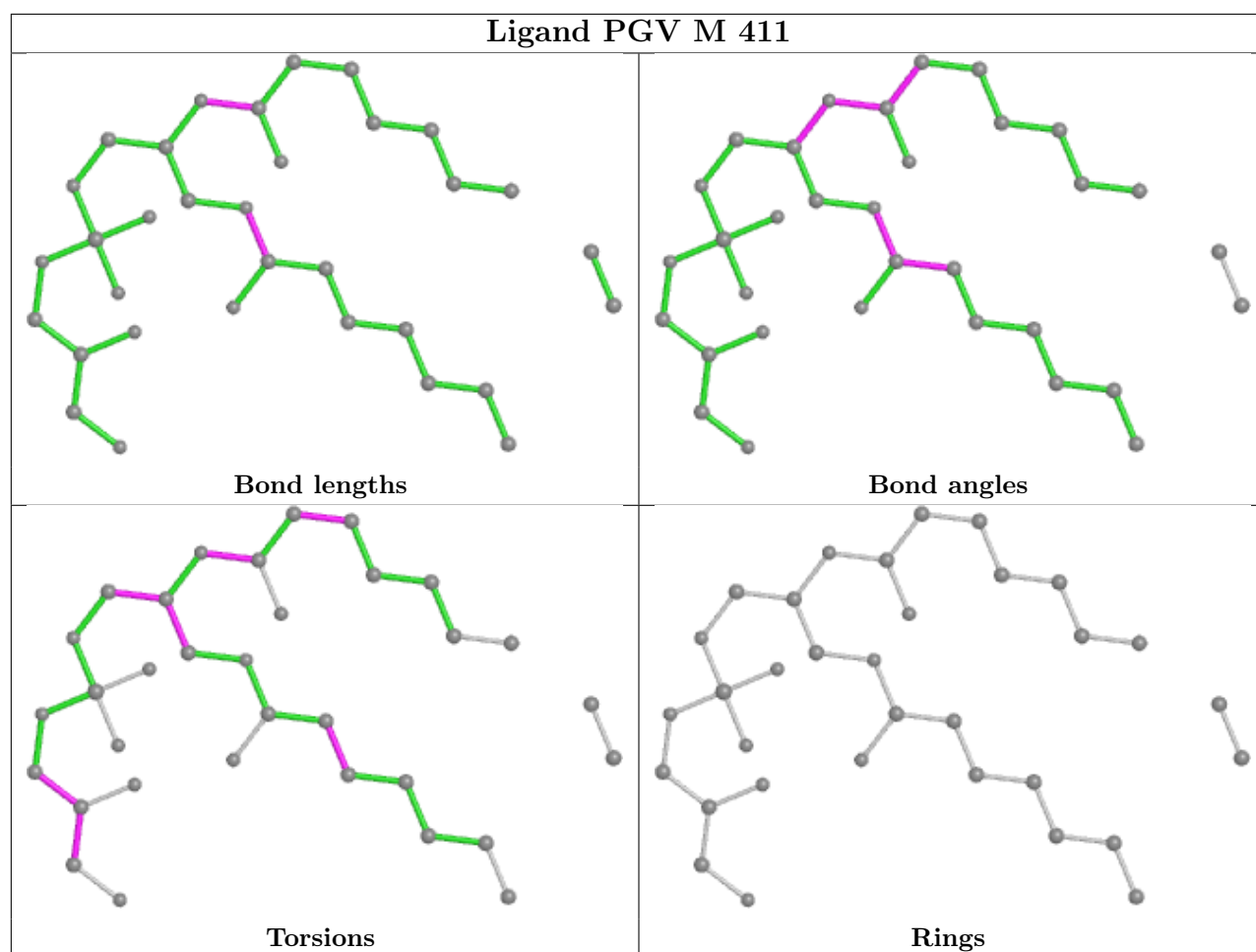


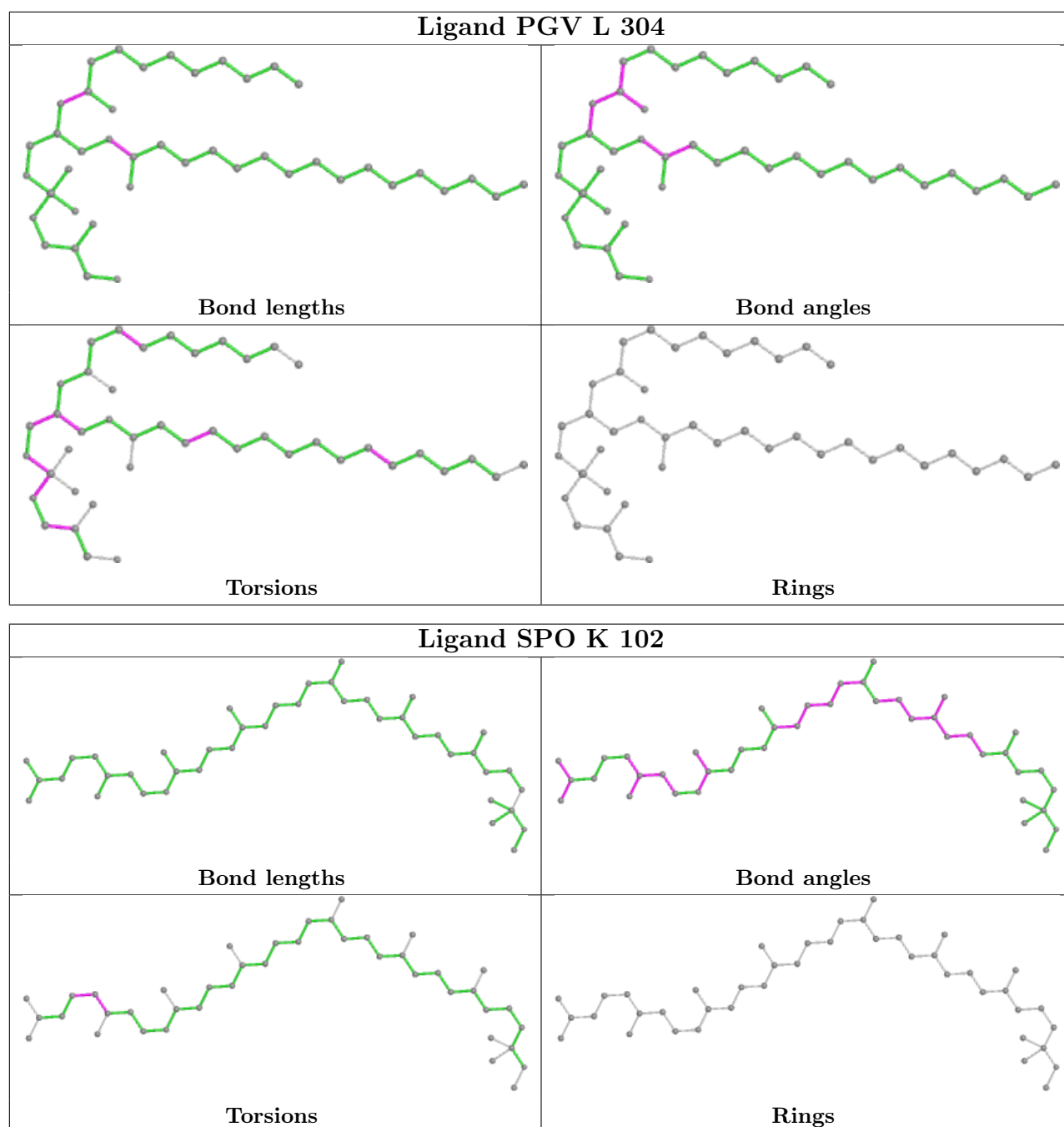
Rings

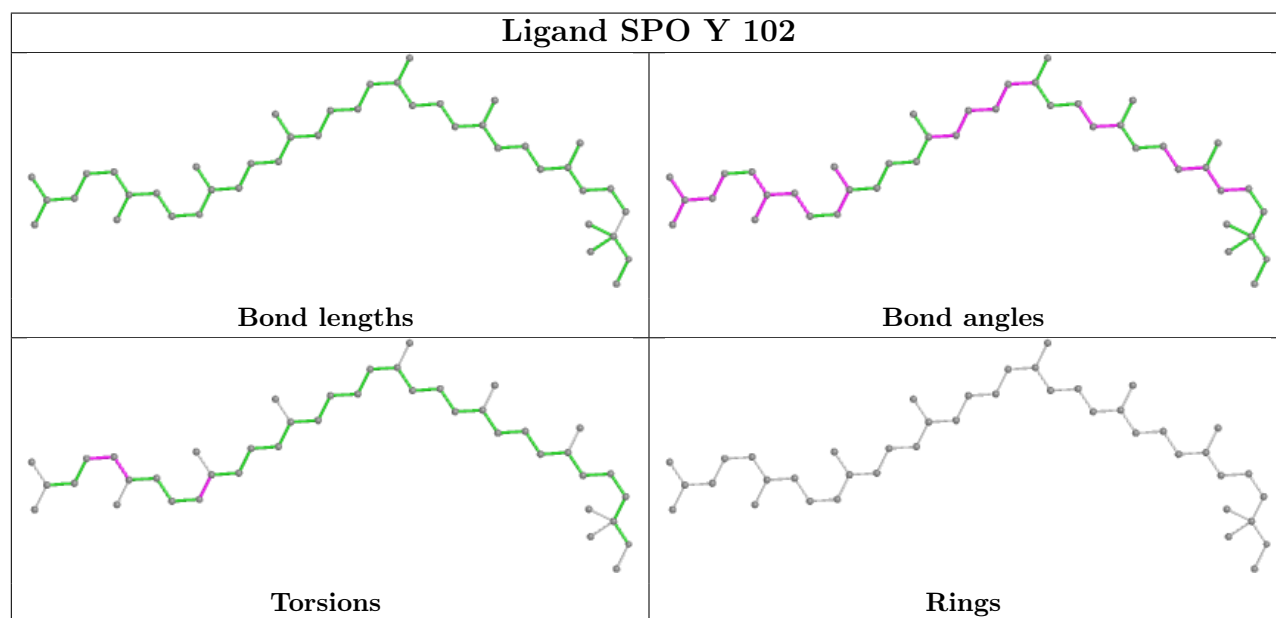
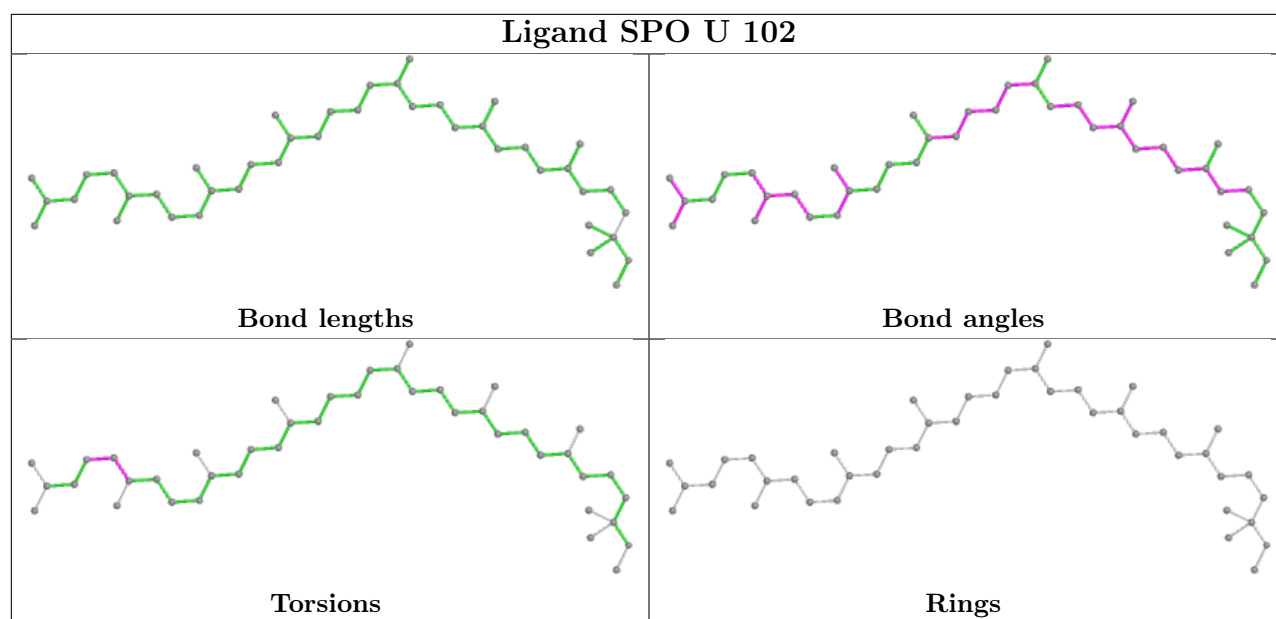


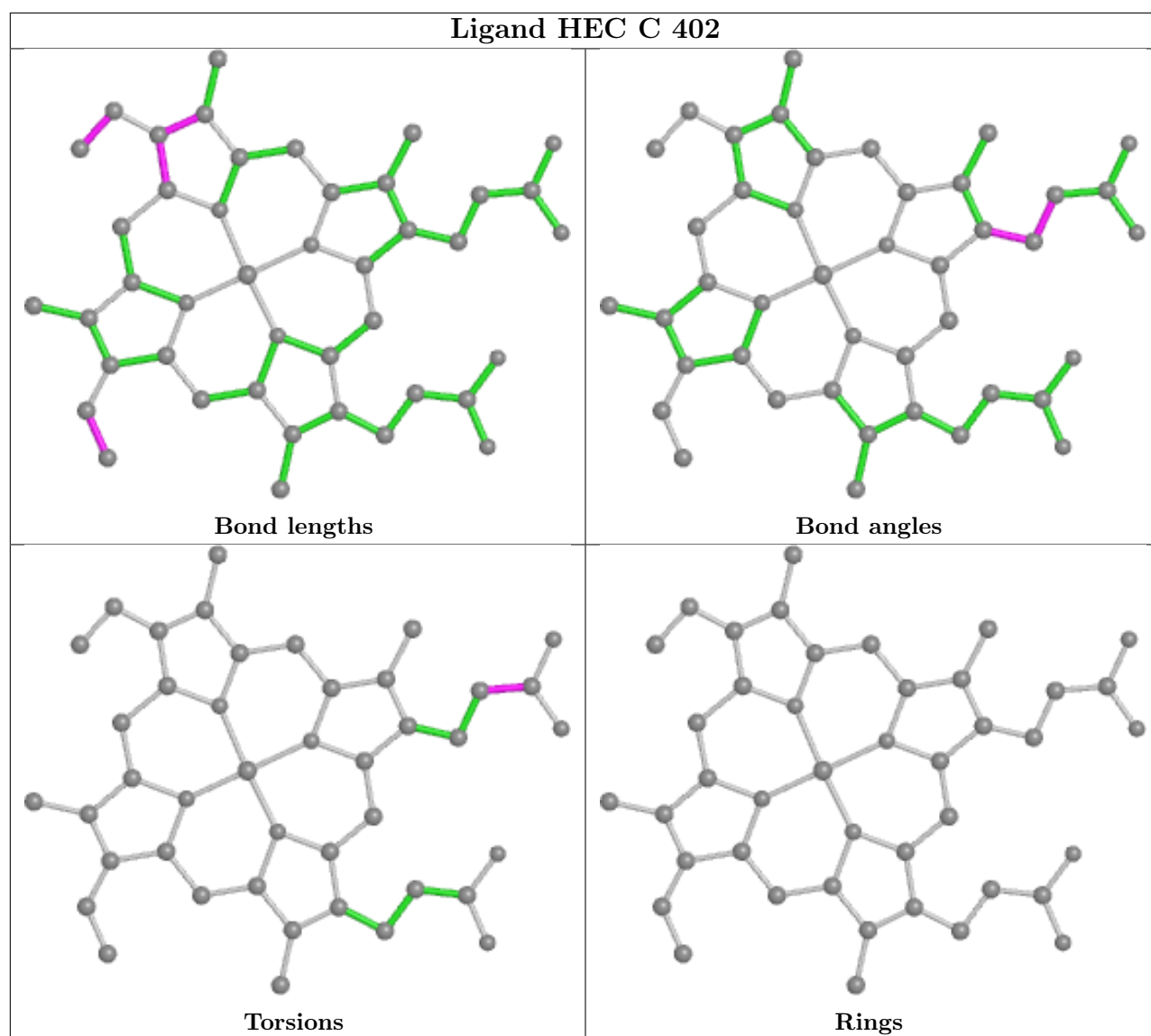


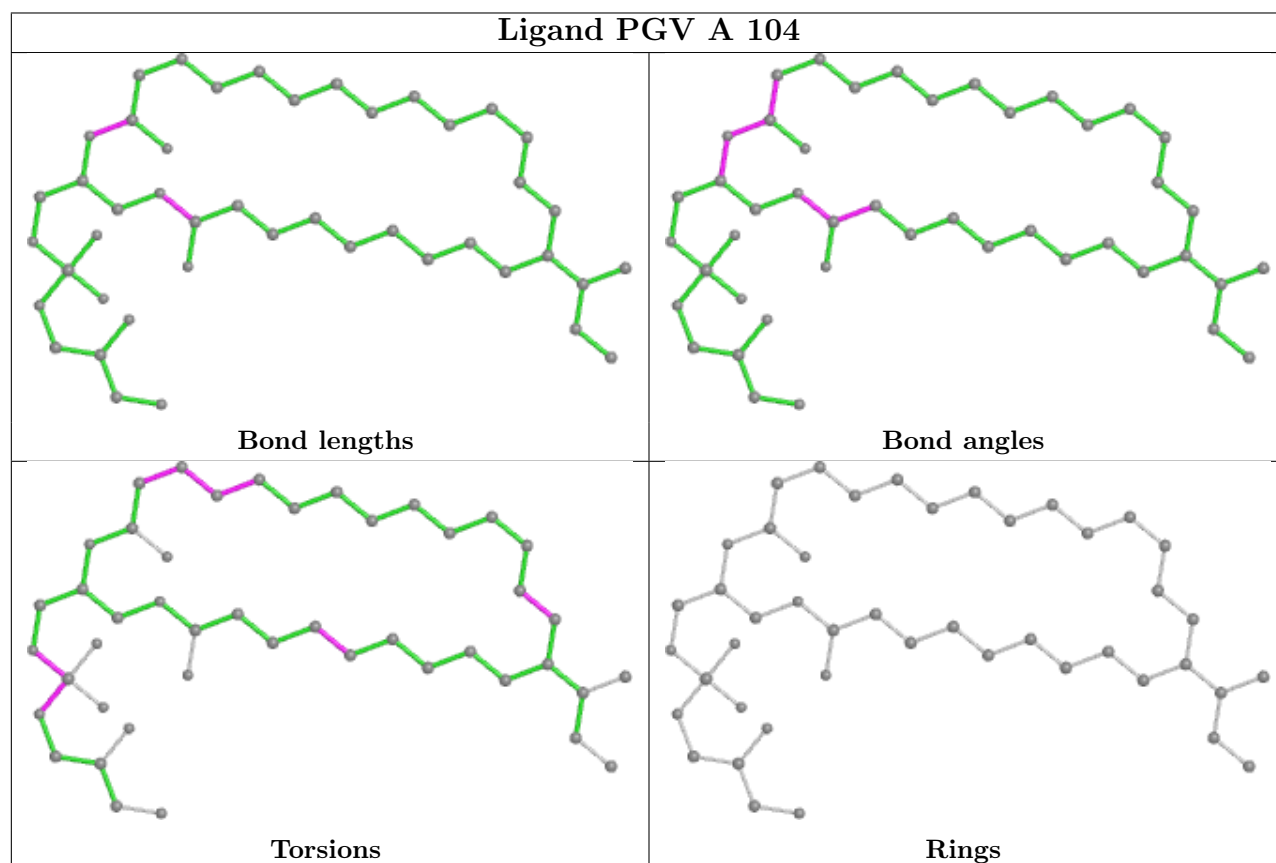
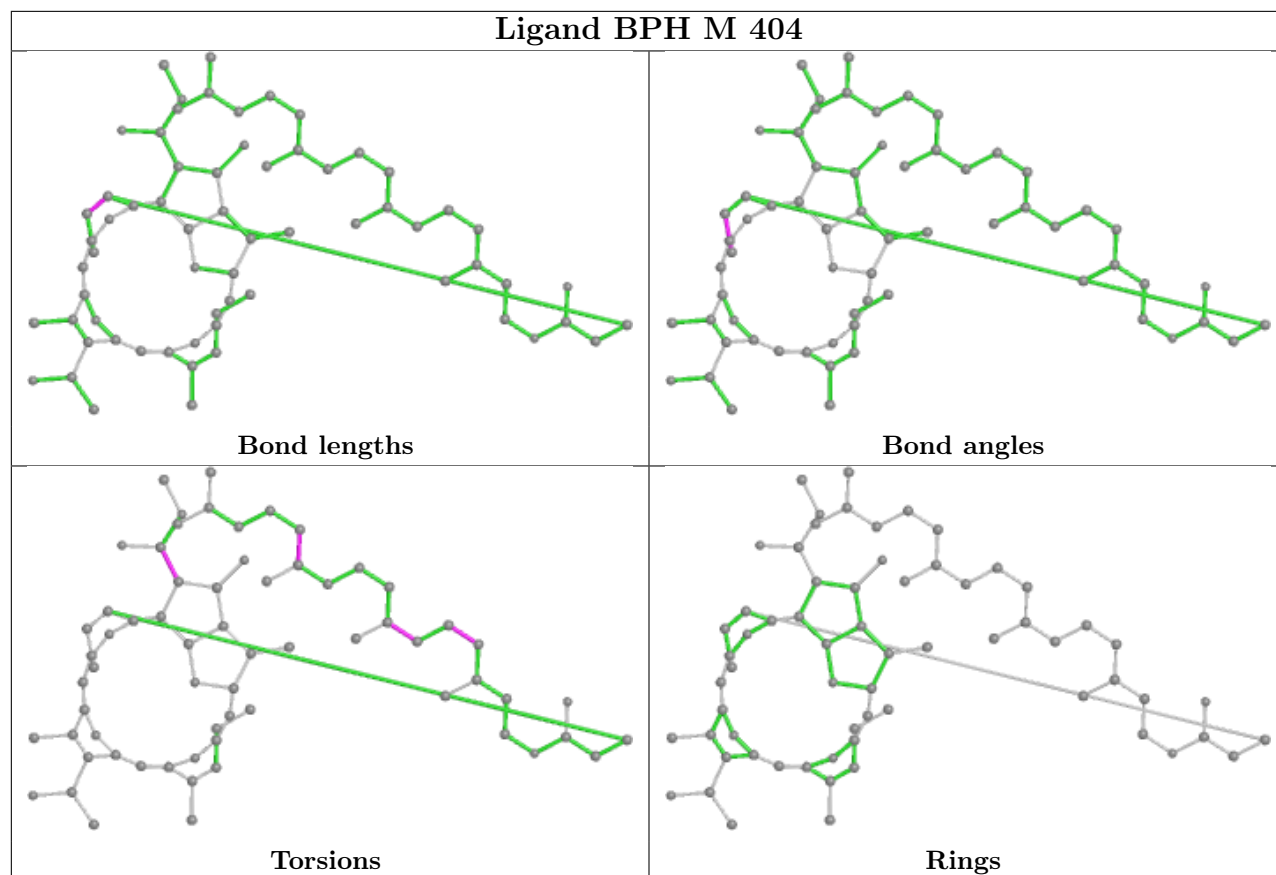


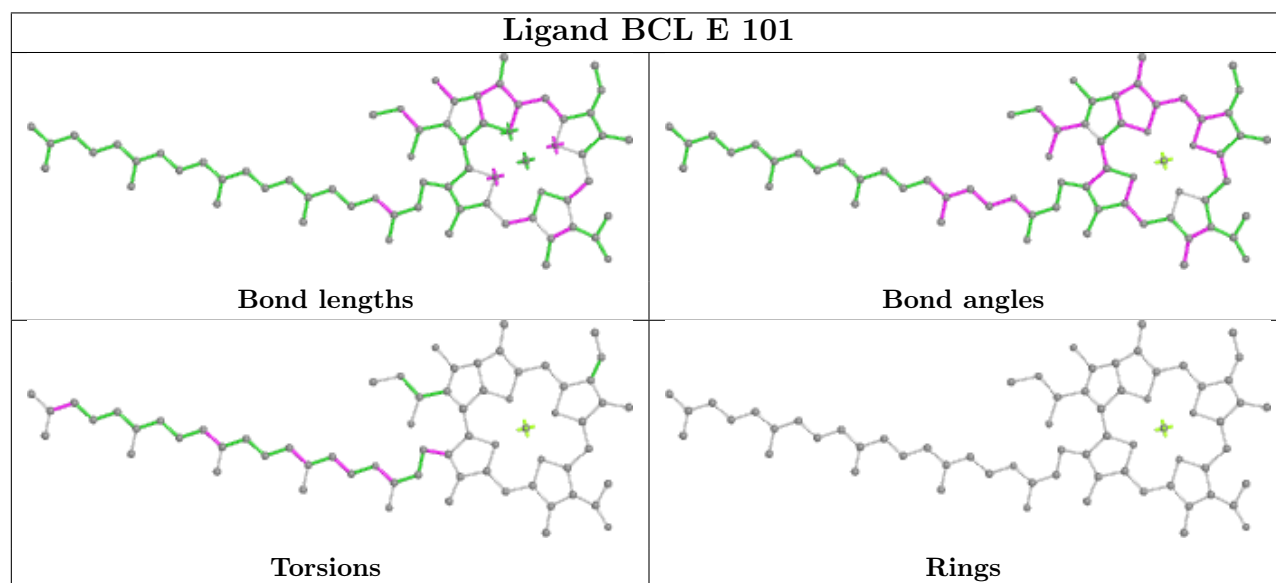
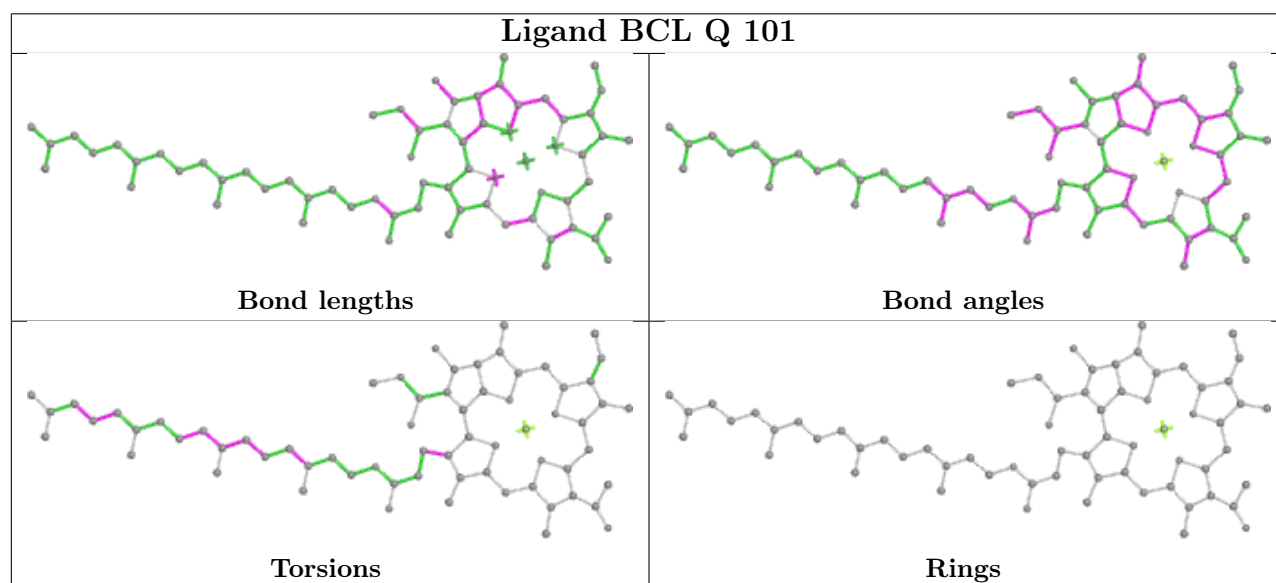
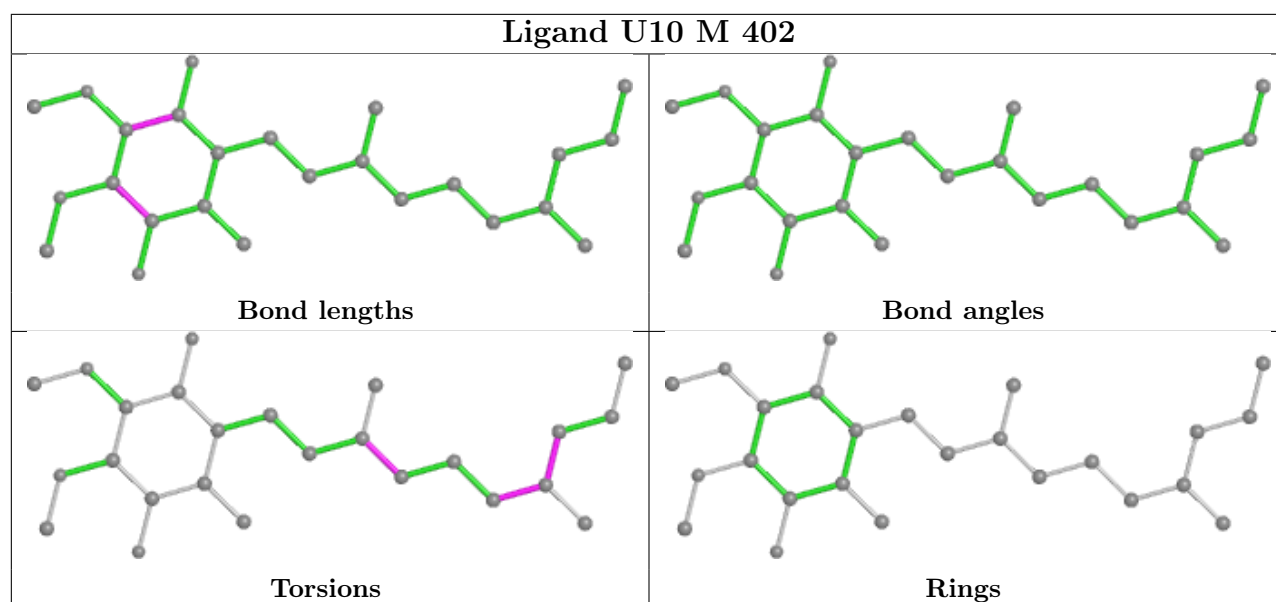


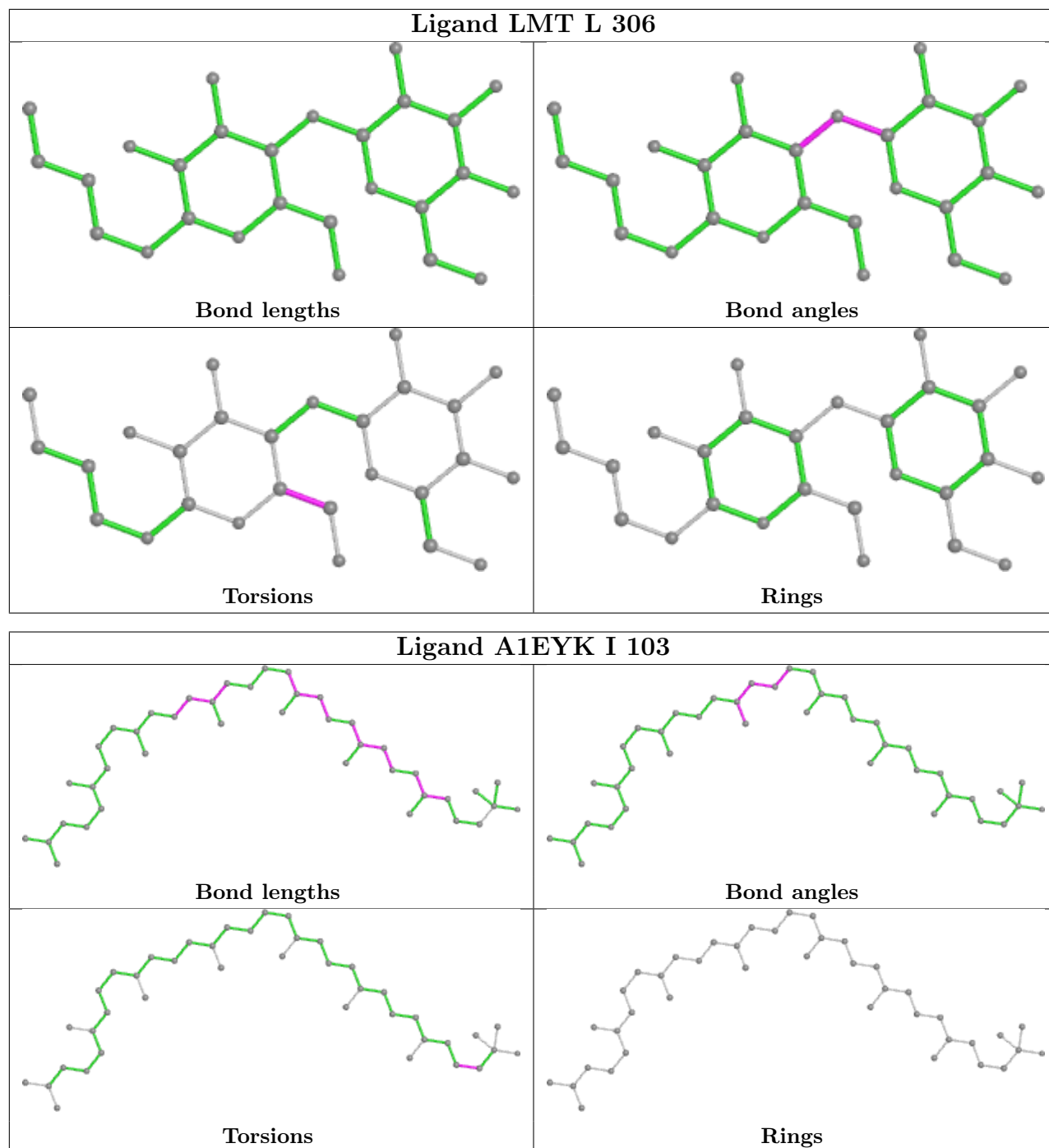


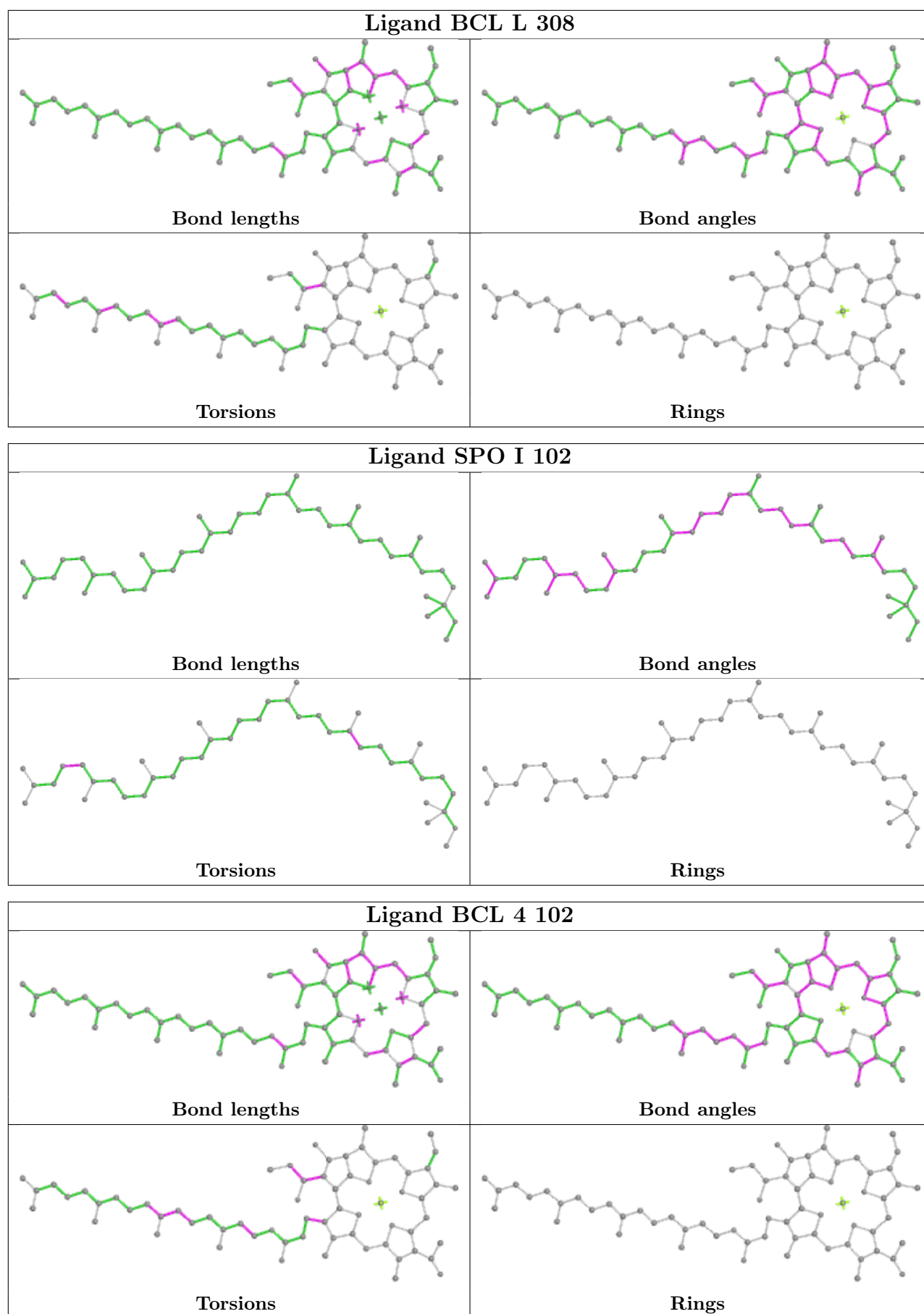


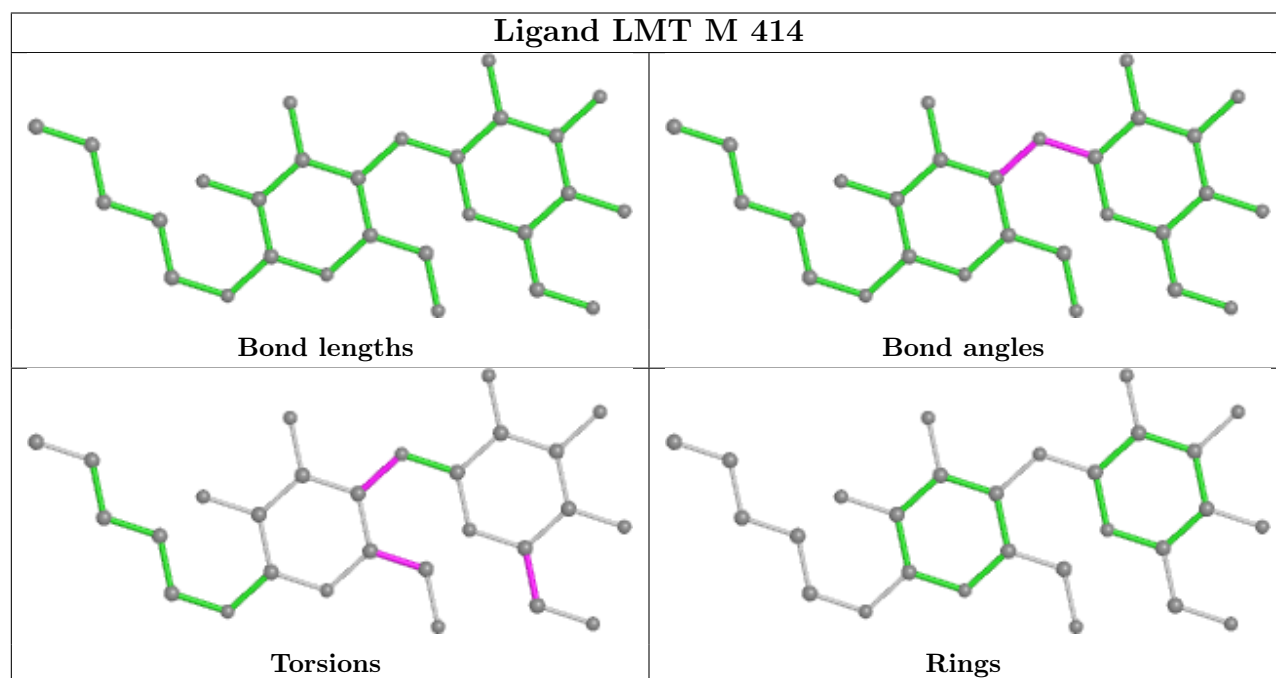
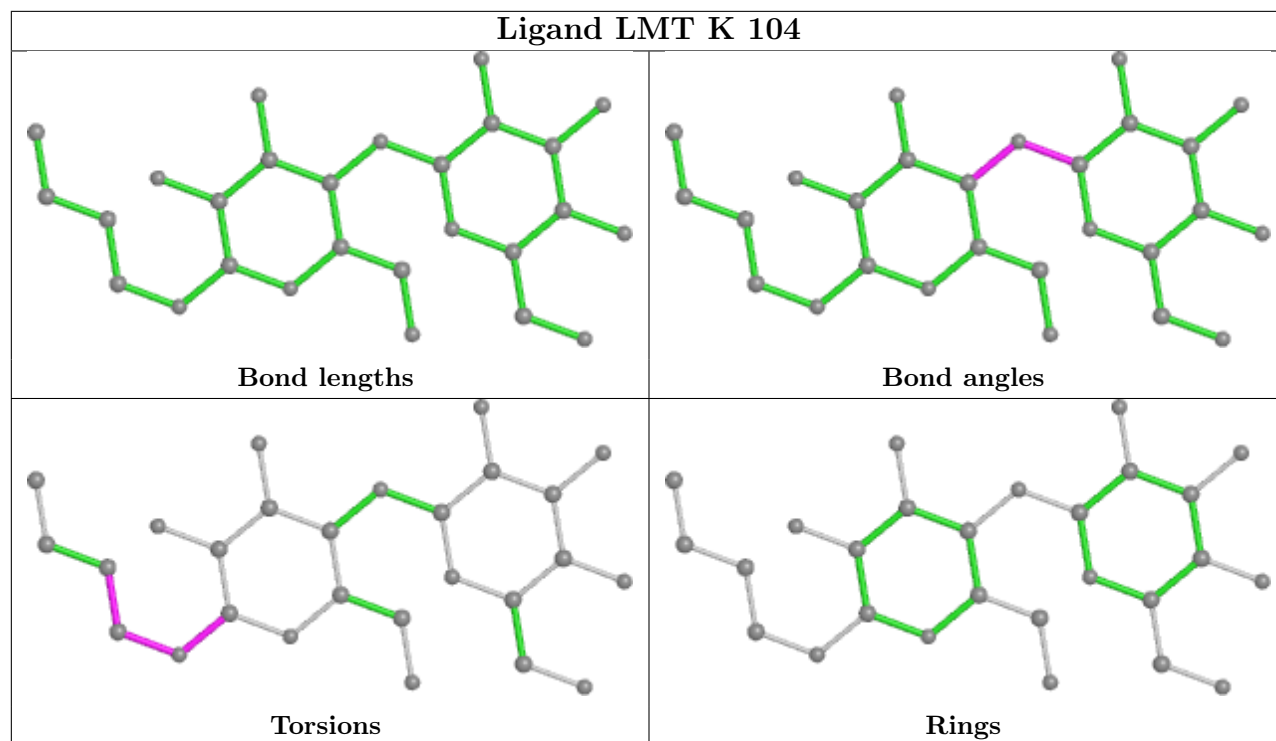


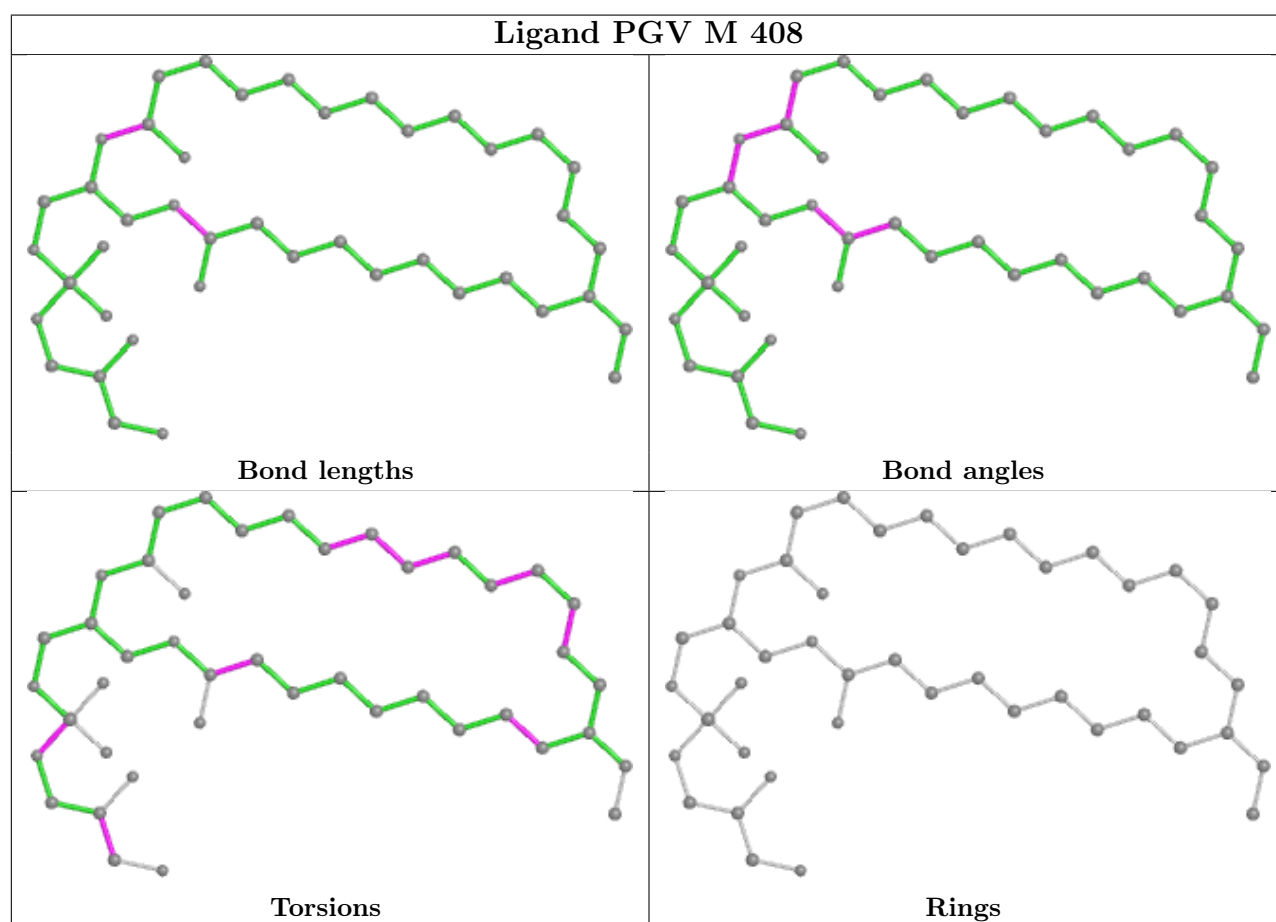
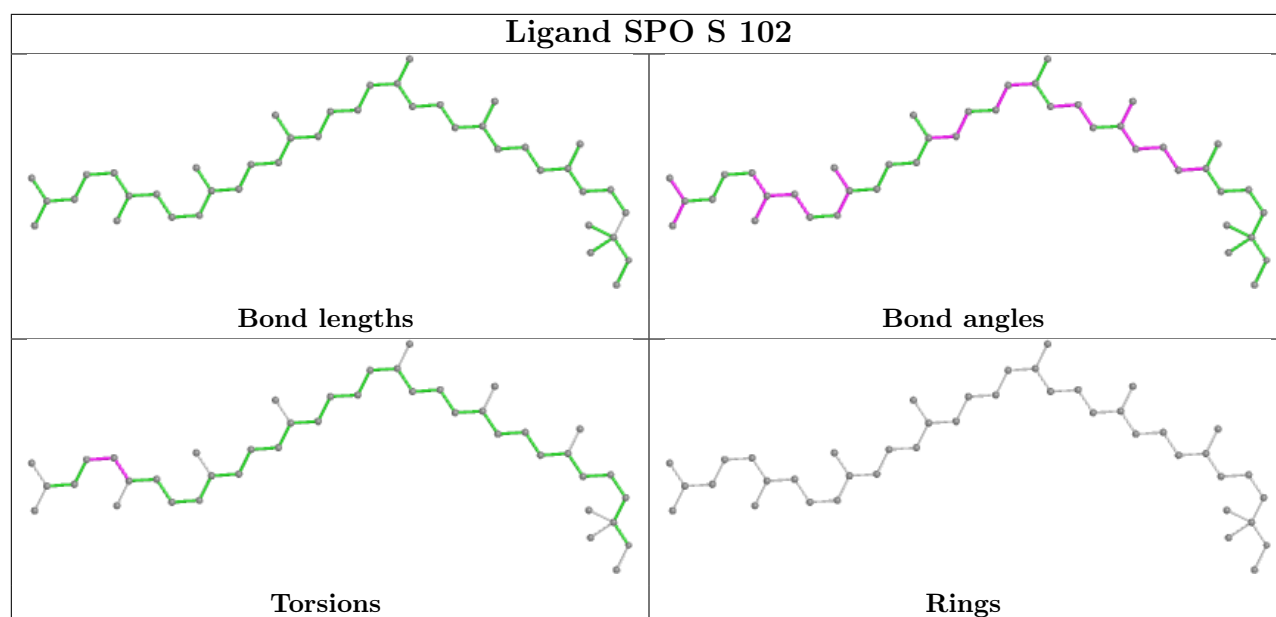


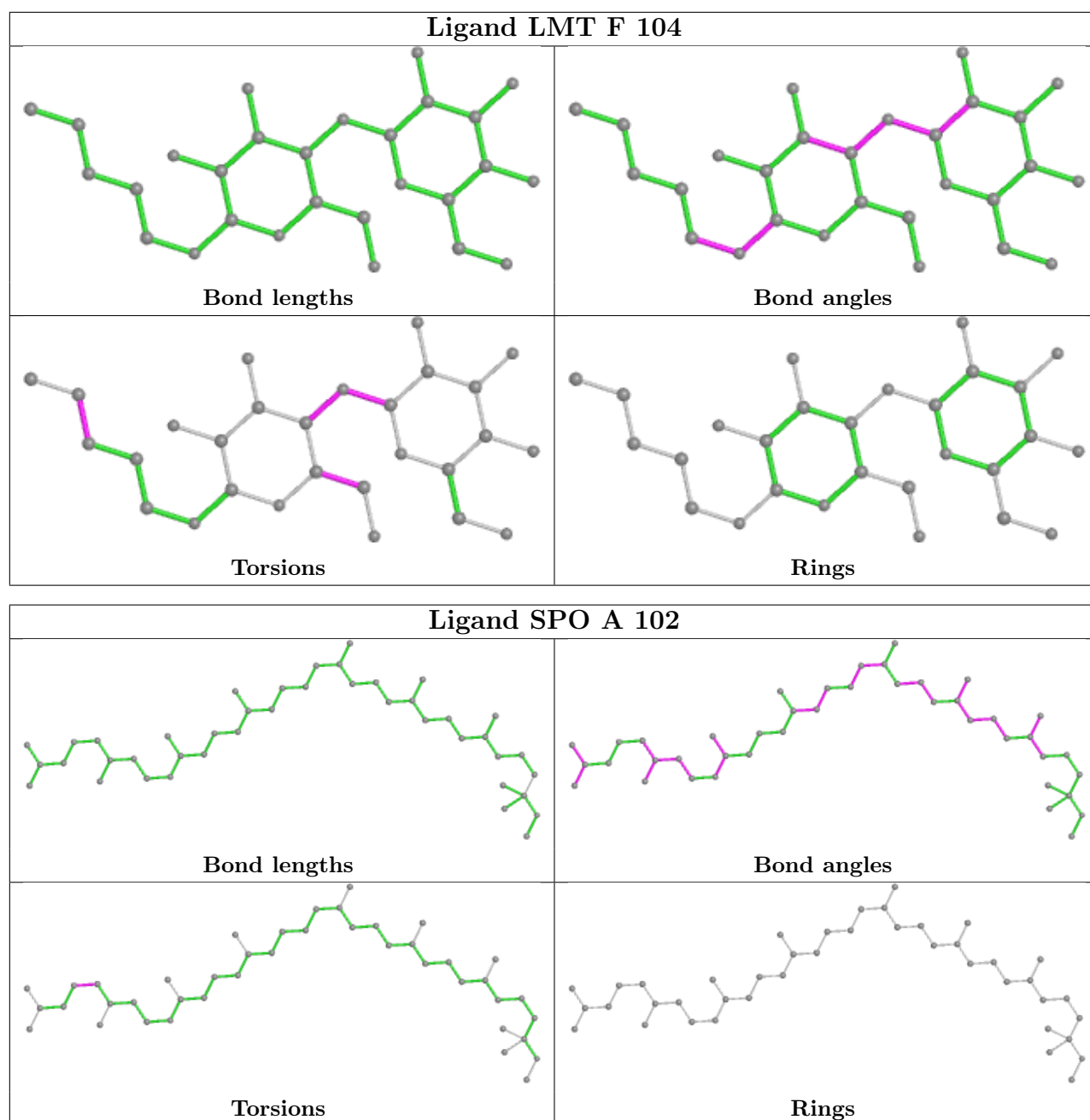


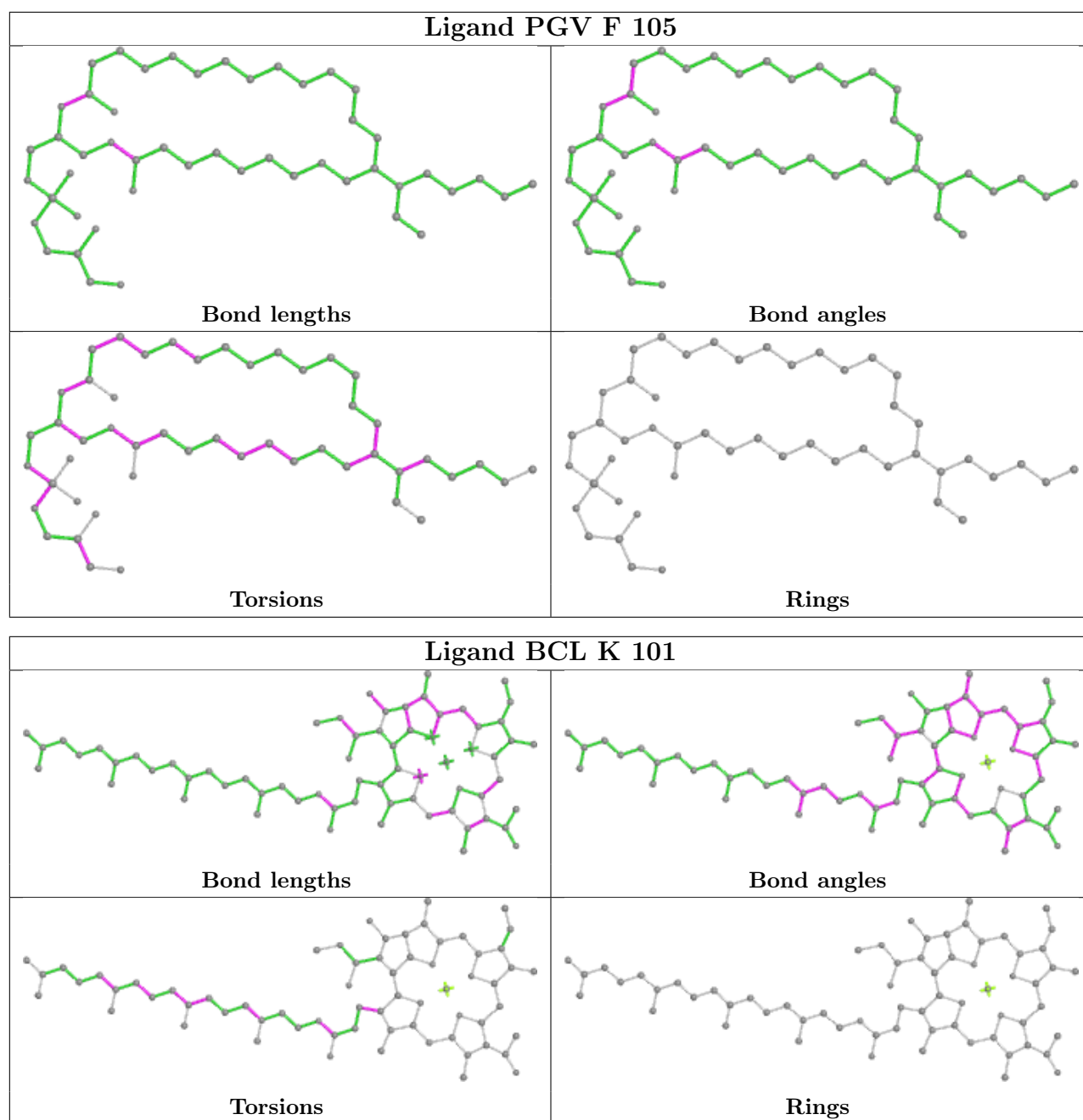


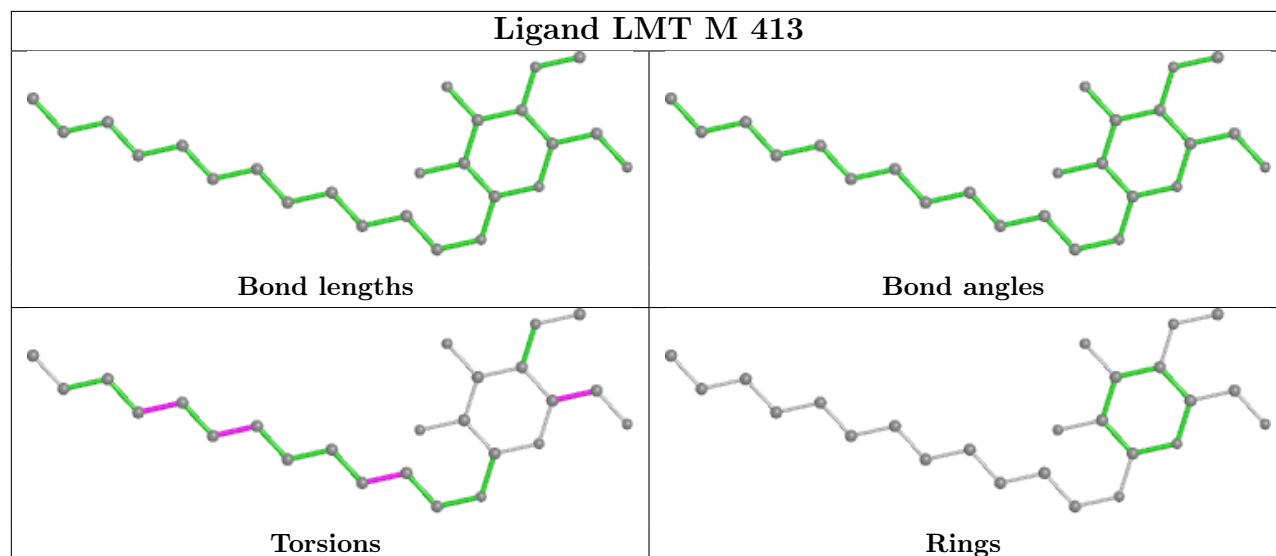
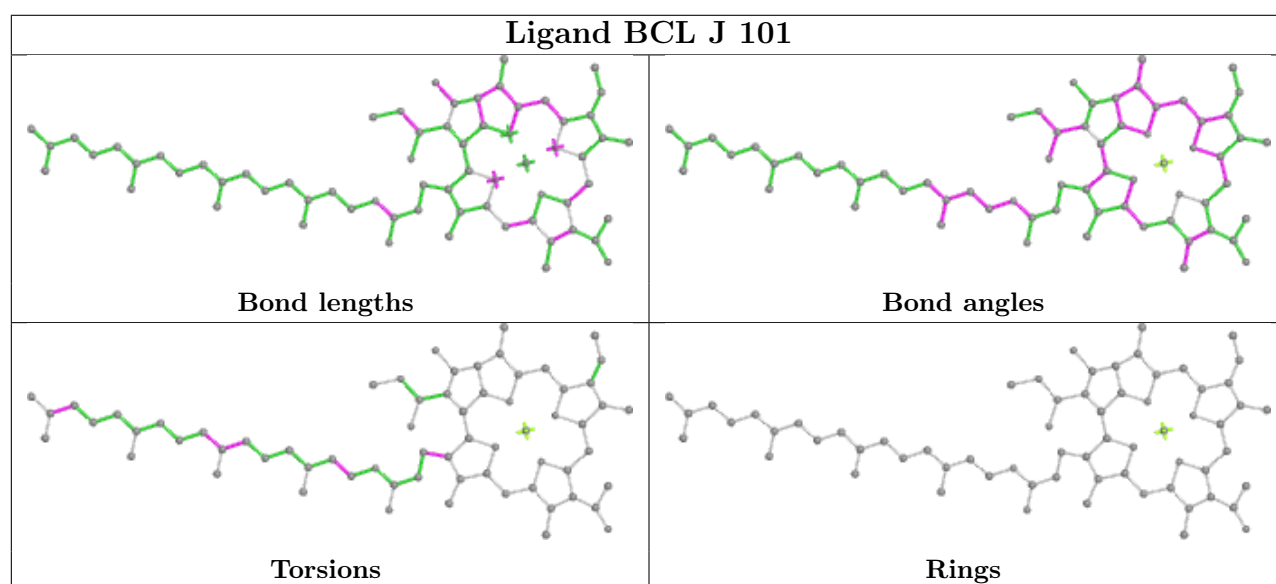
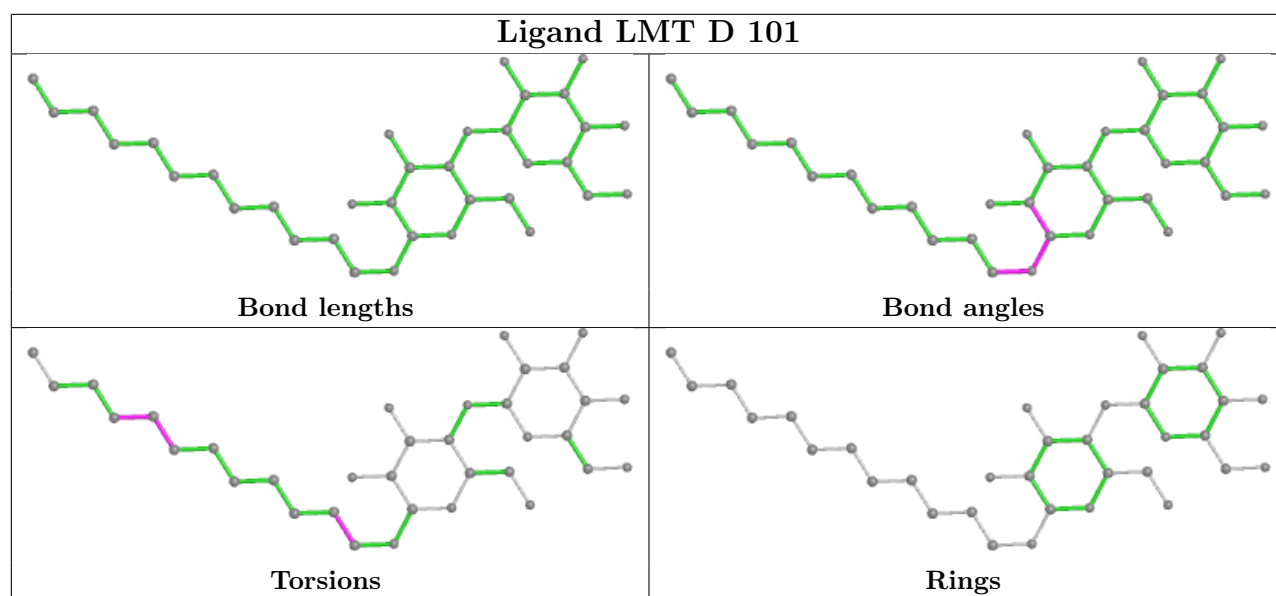


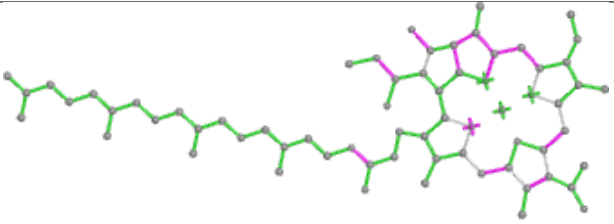
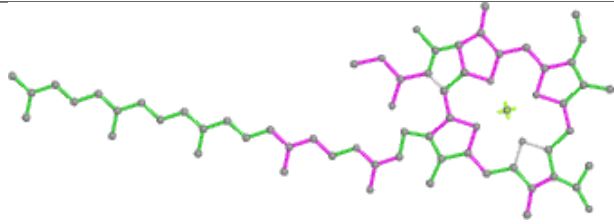
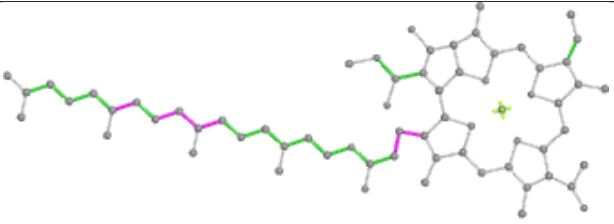
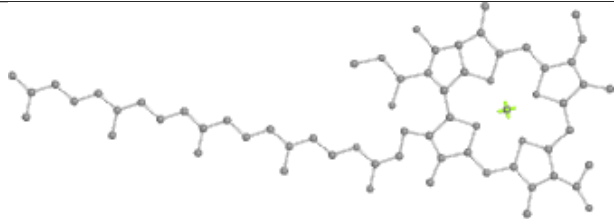
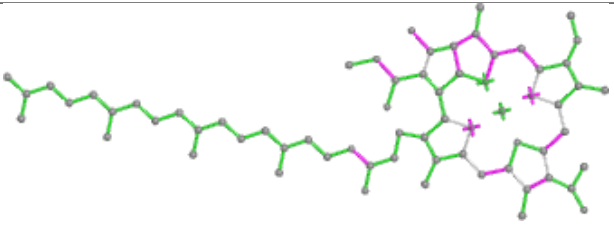
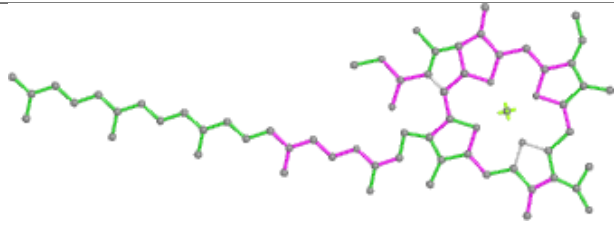
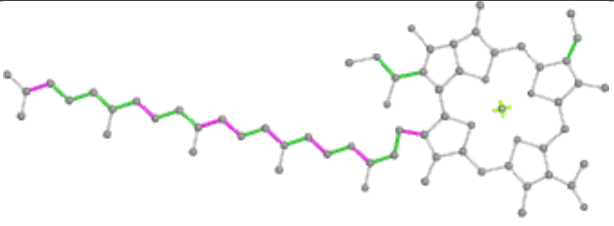
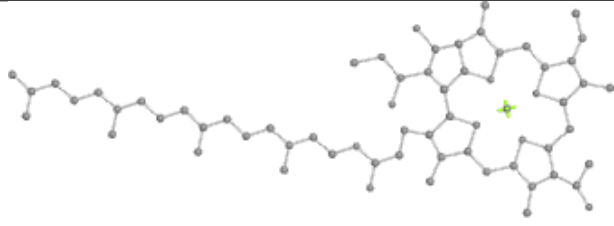
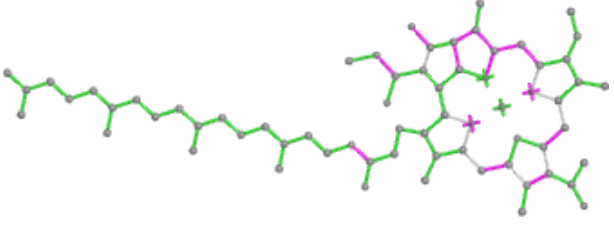
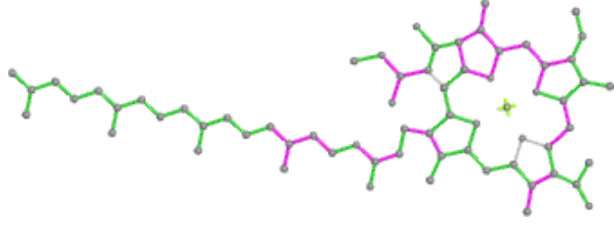
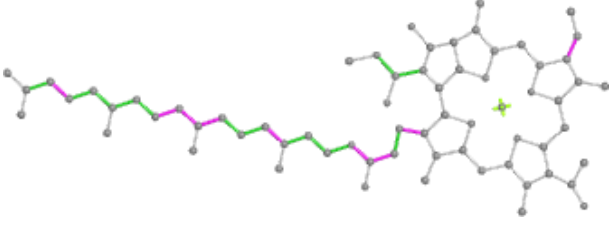
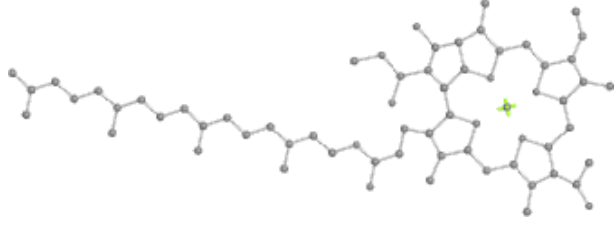


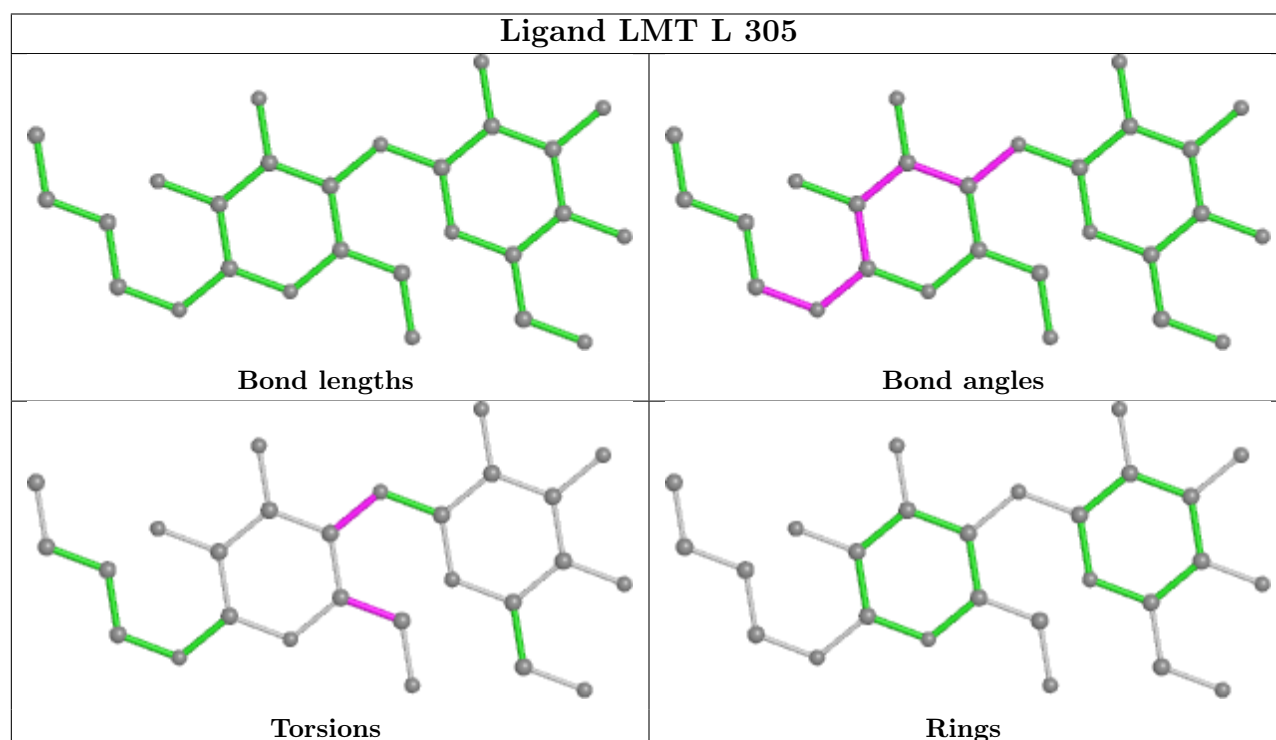
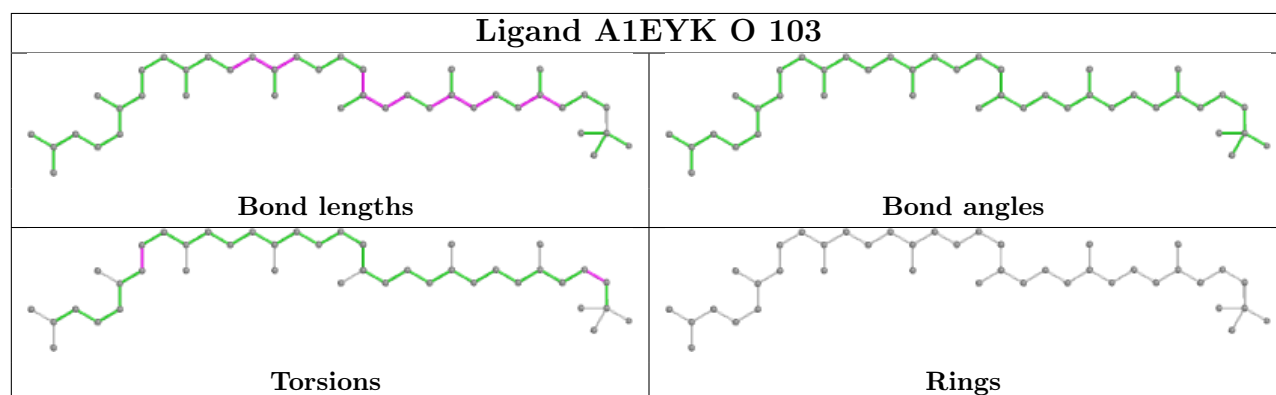
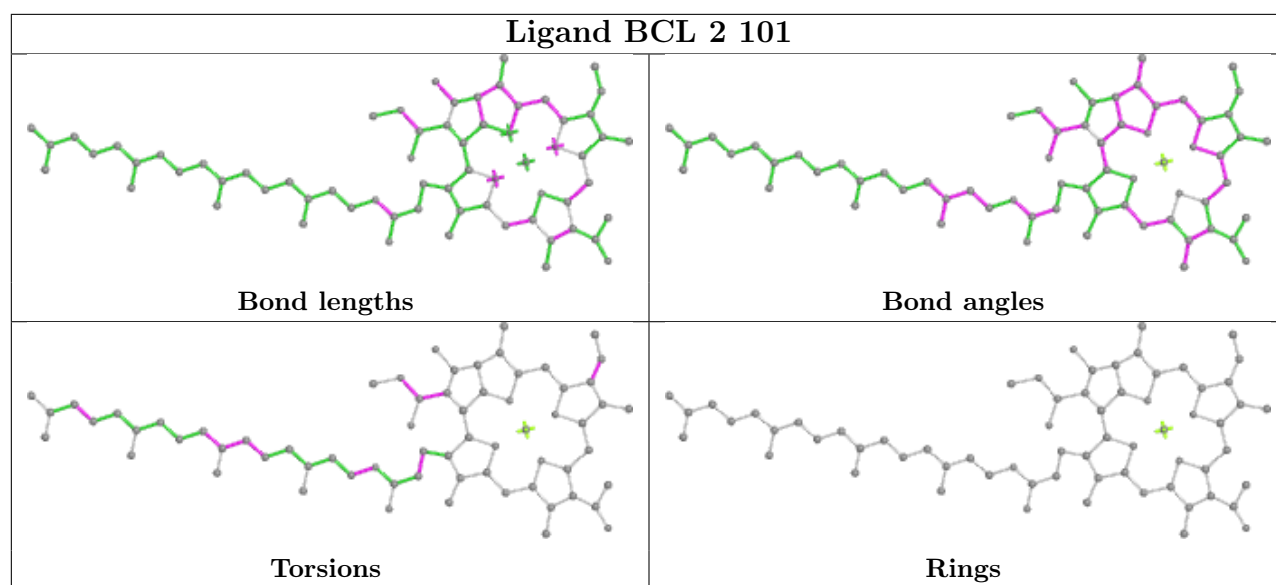




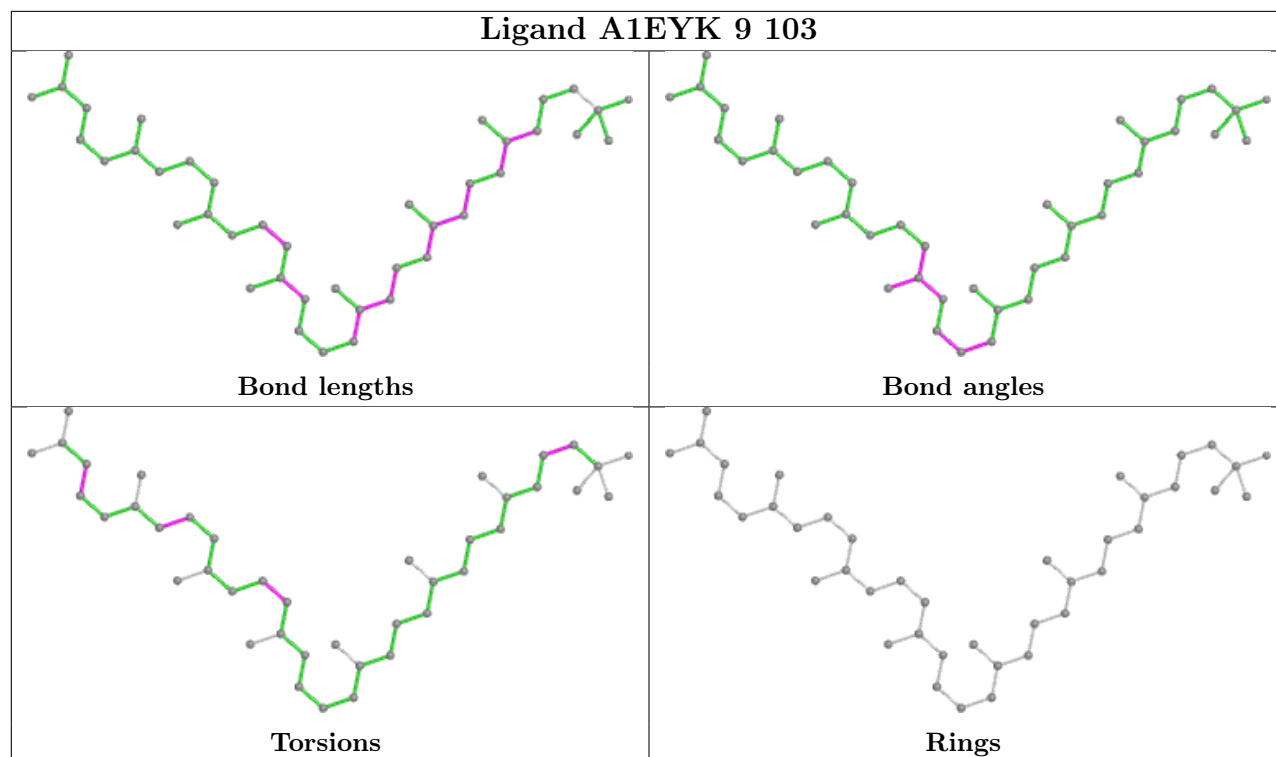




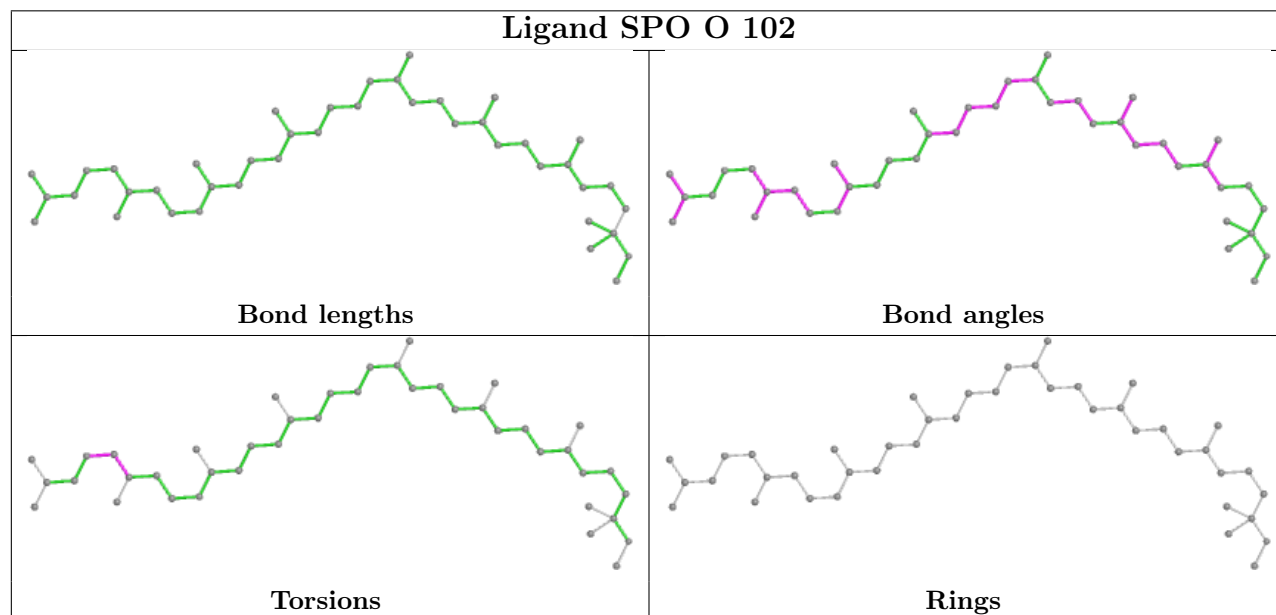
Ligand BCL D 102	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCL 6 101	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCL 1 101	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

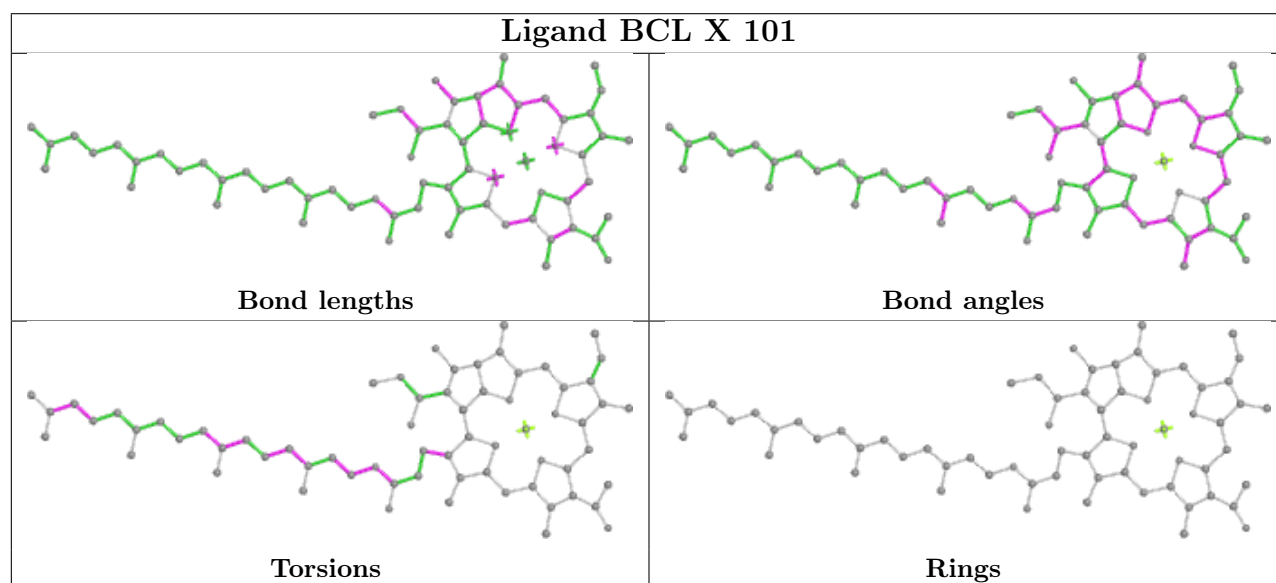
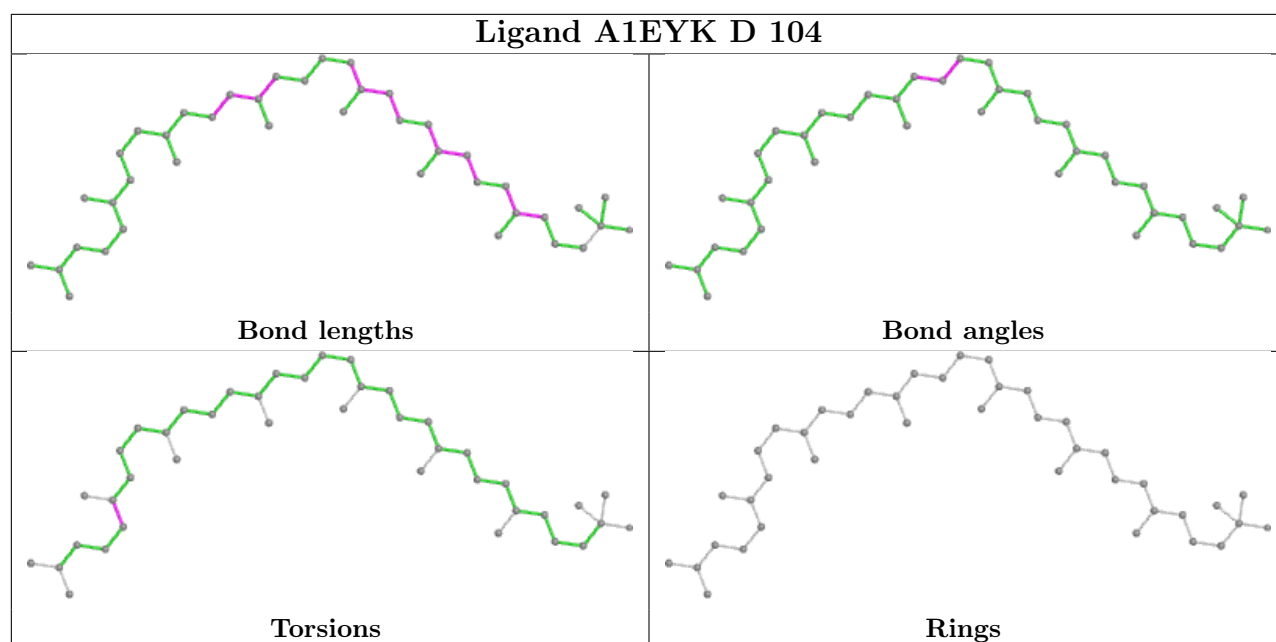


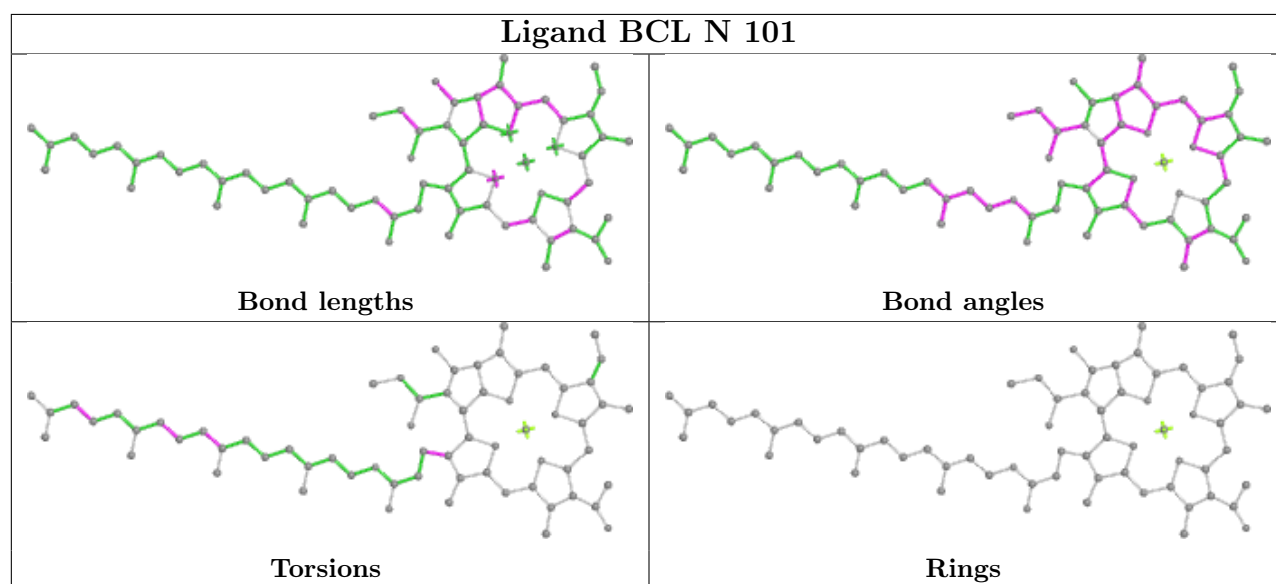
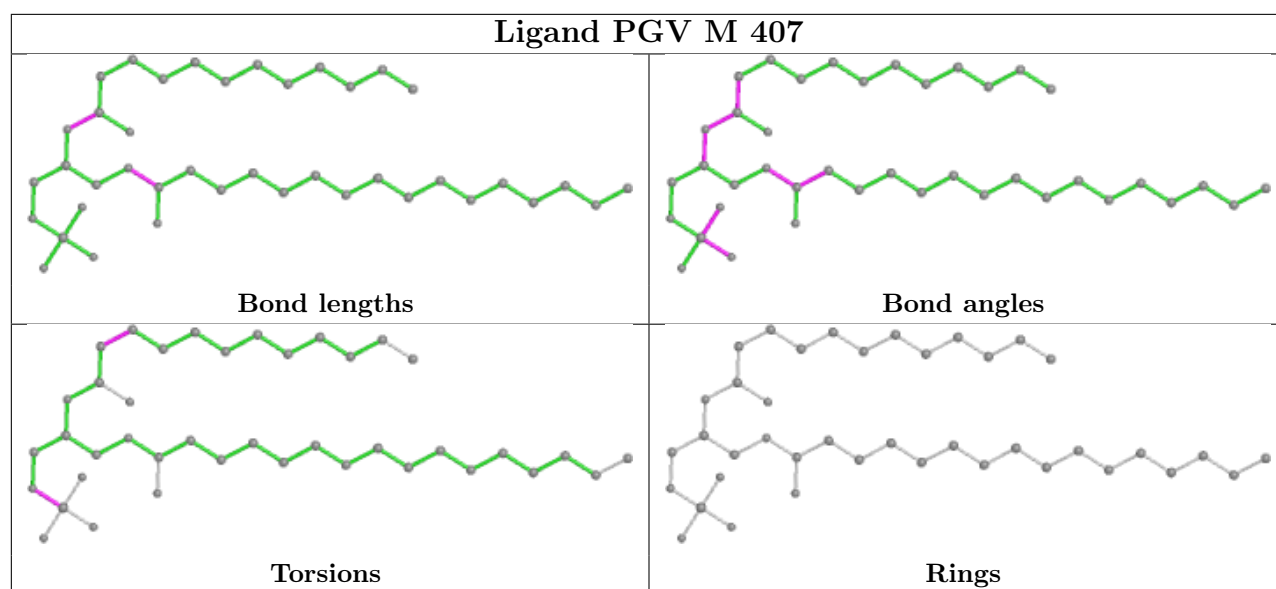
Ligand A1EYK 9 103



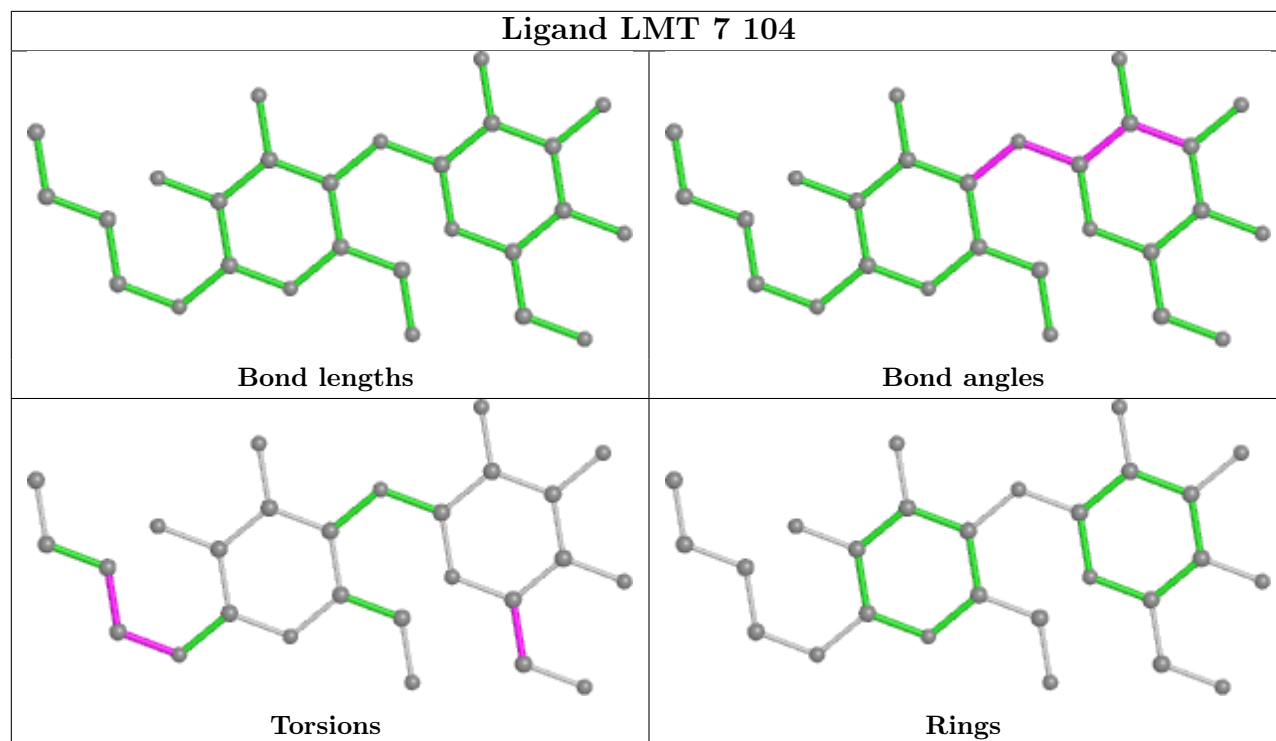
Ligand SPO O 102



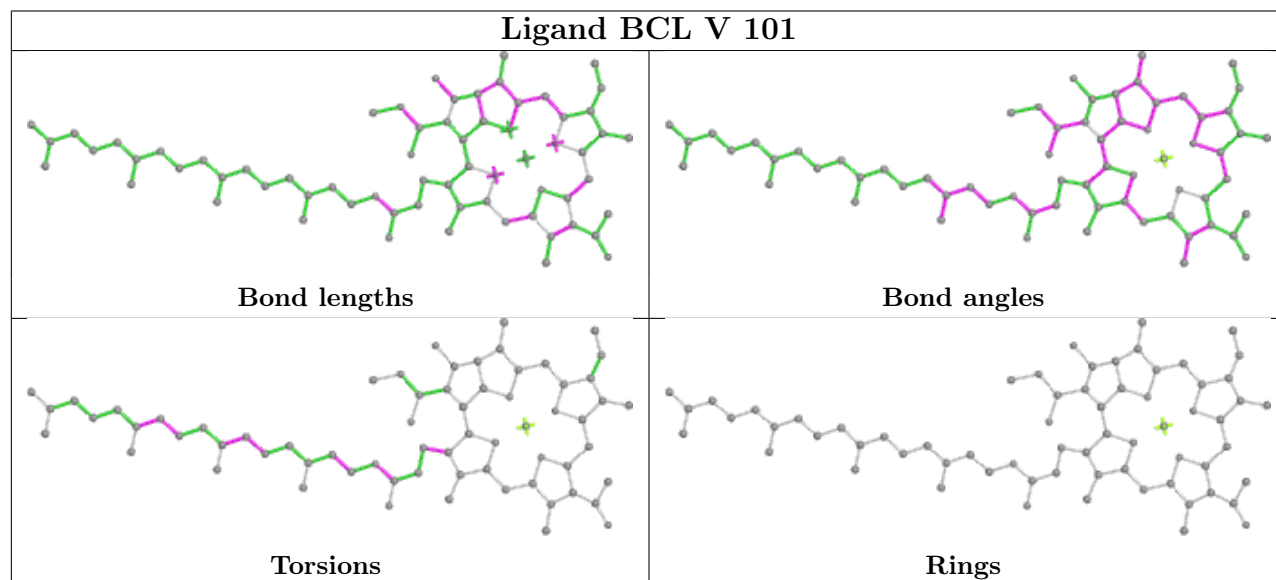


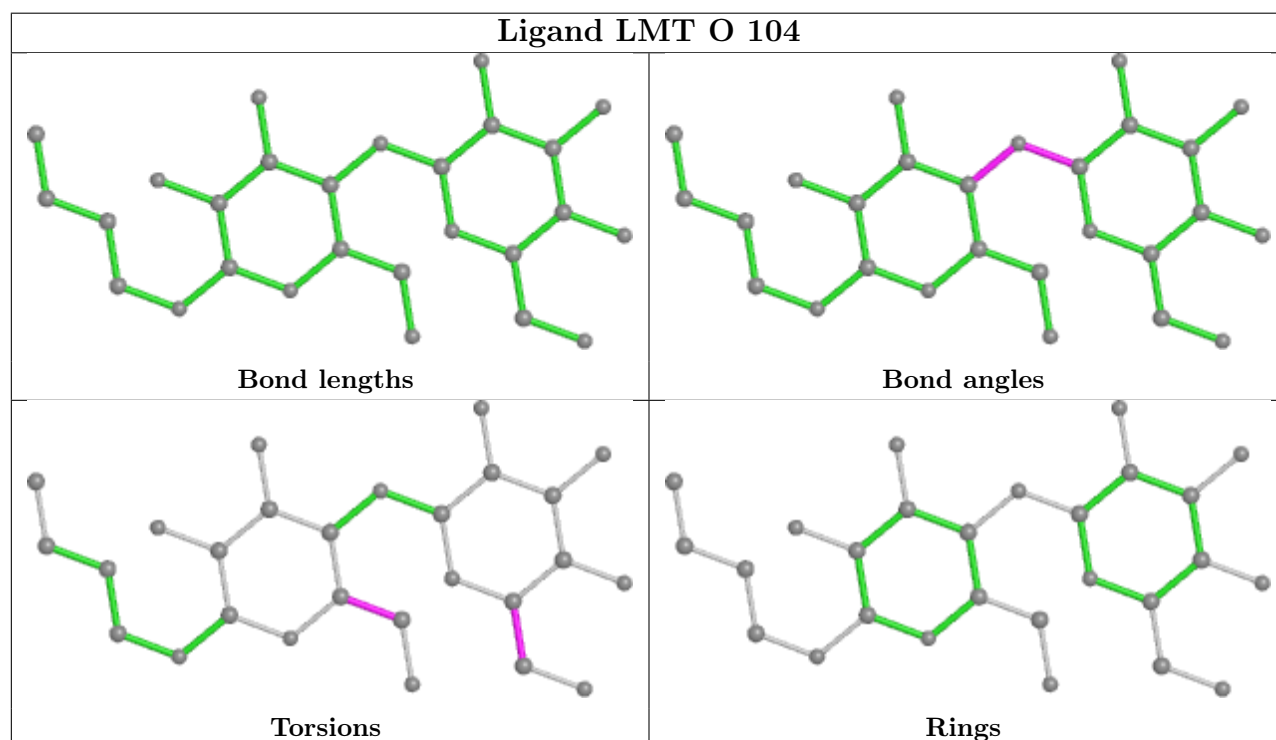
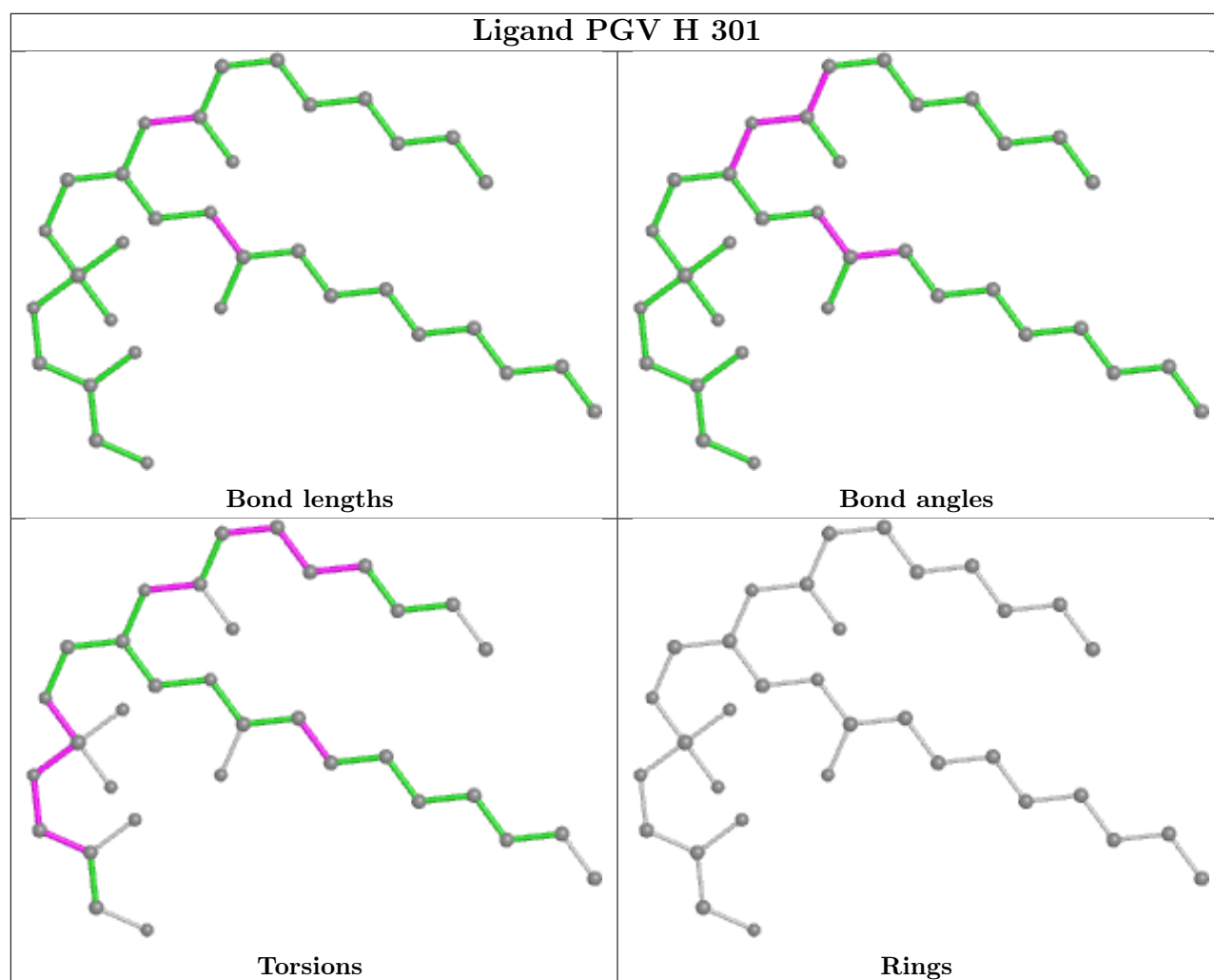


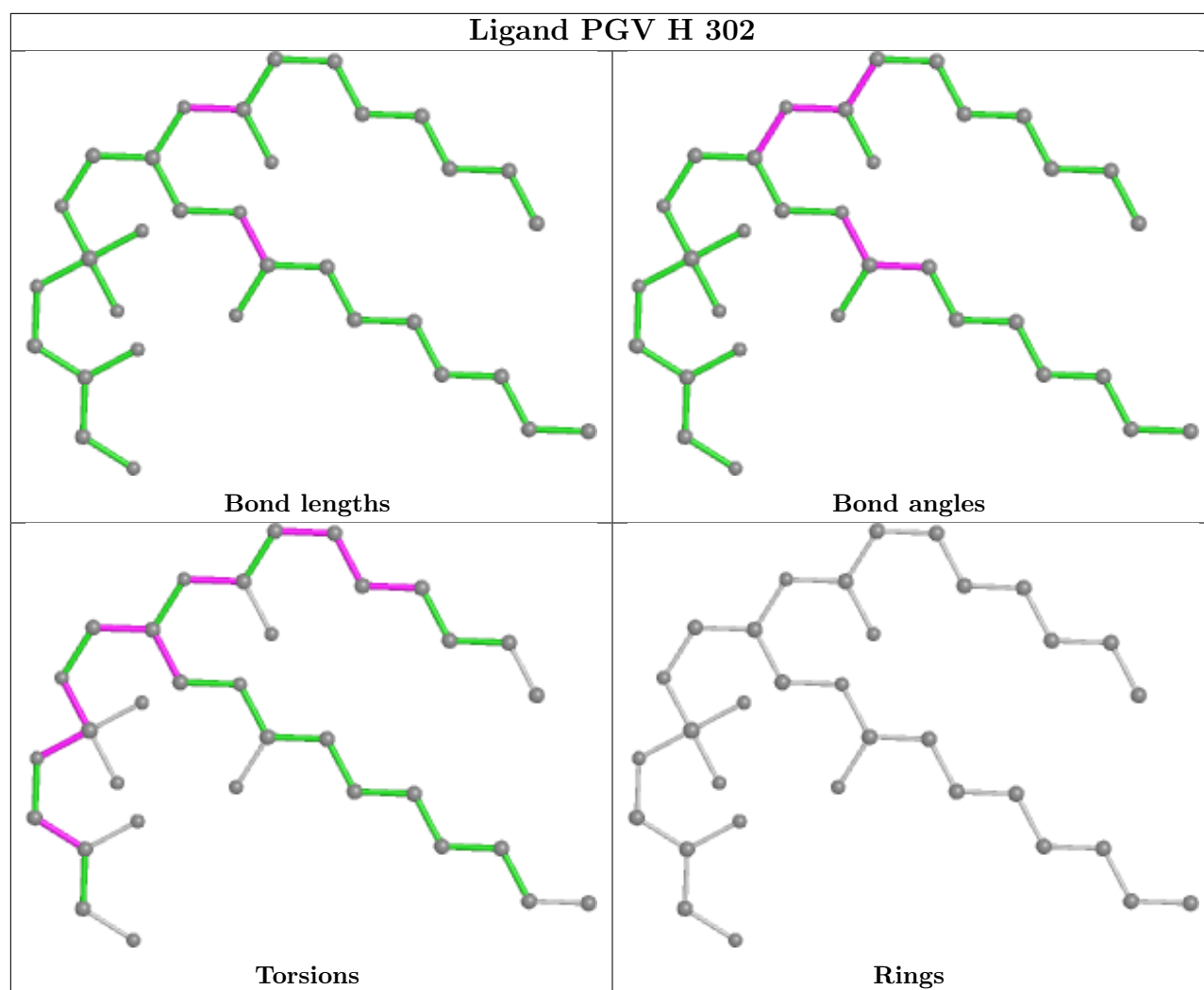
Ligand LMT 7 104

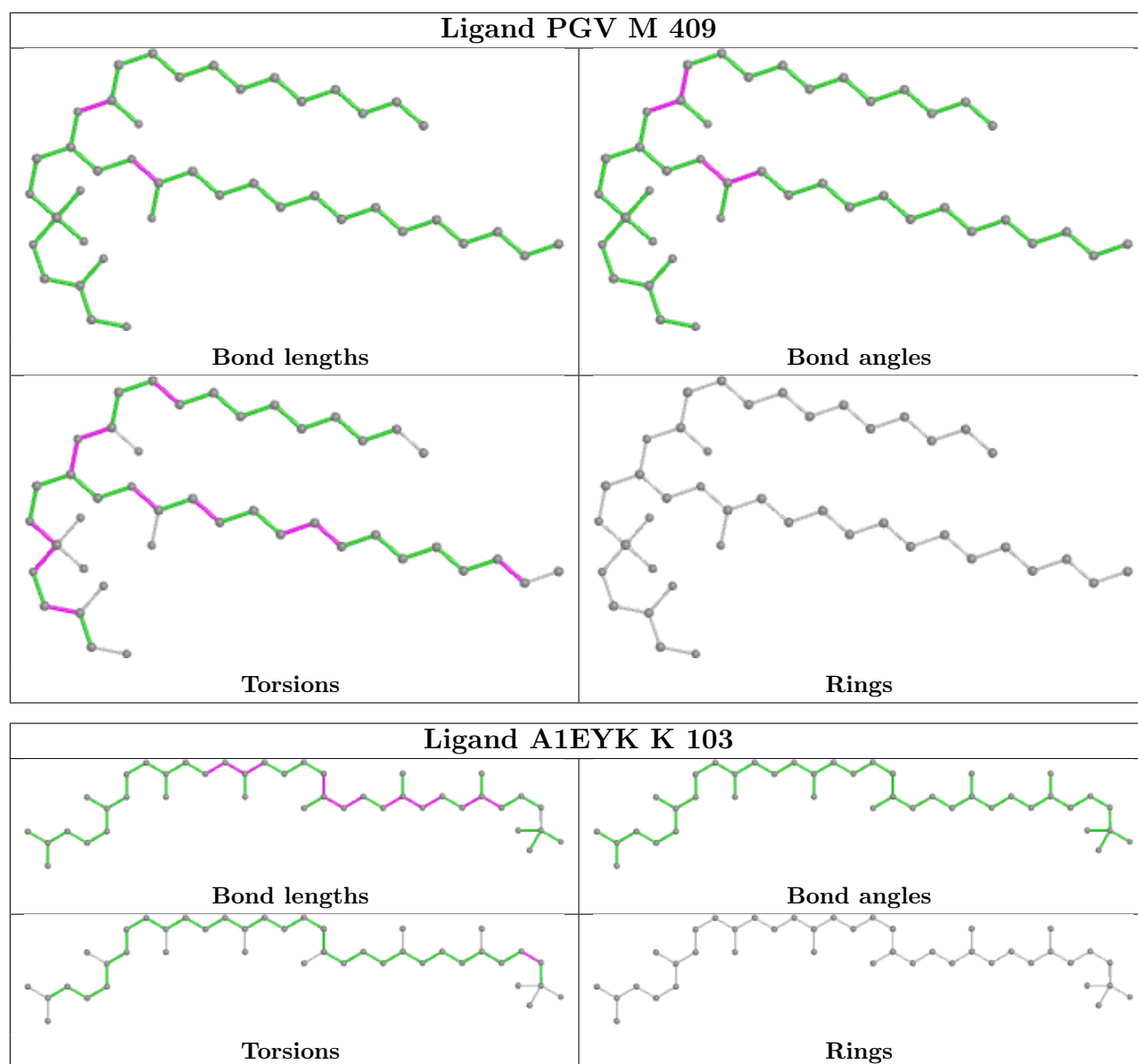


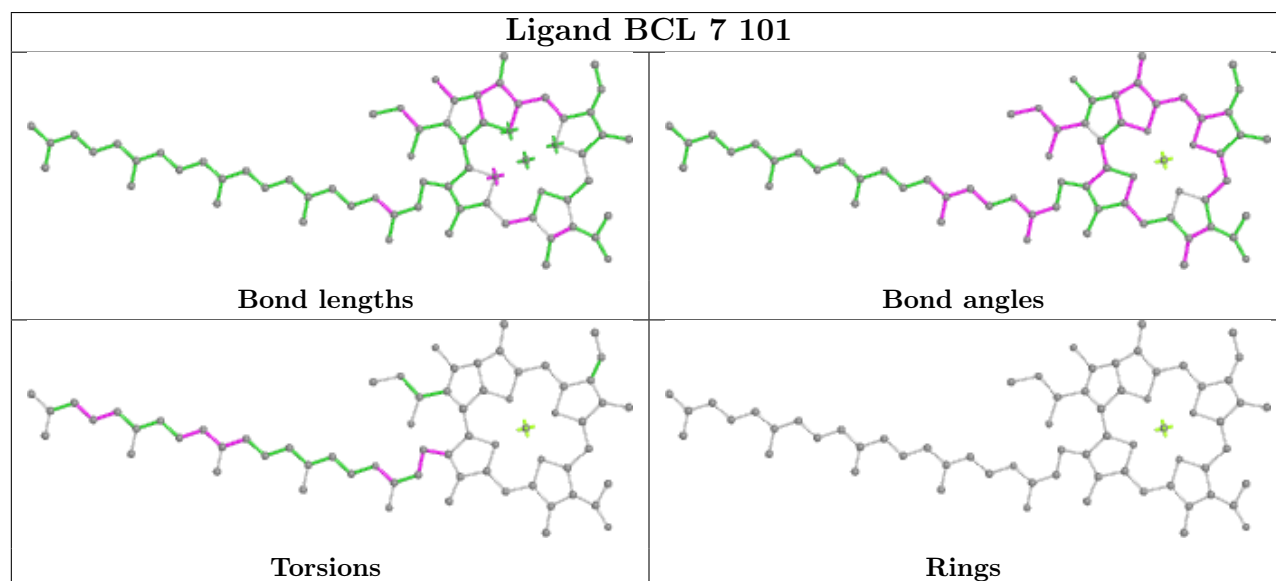
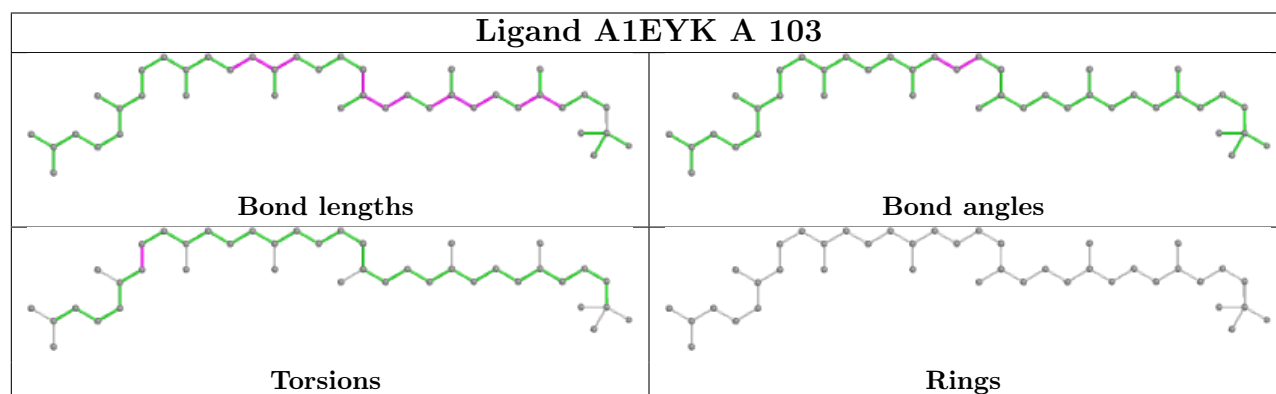
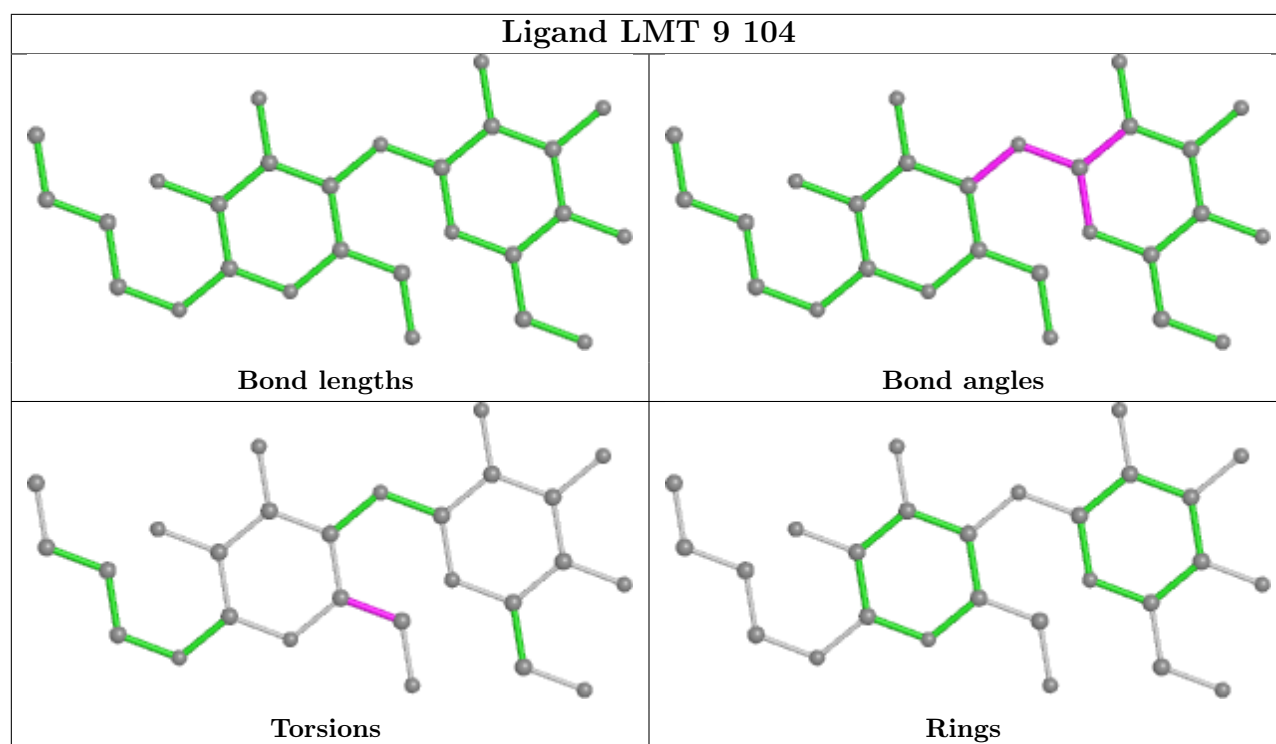
Ligand BCL V 101

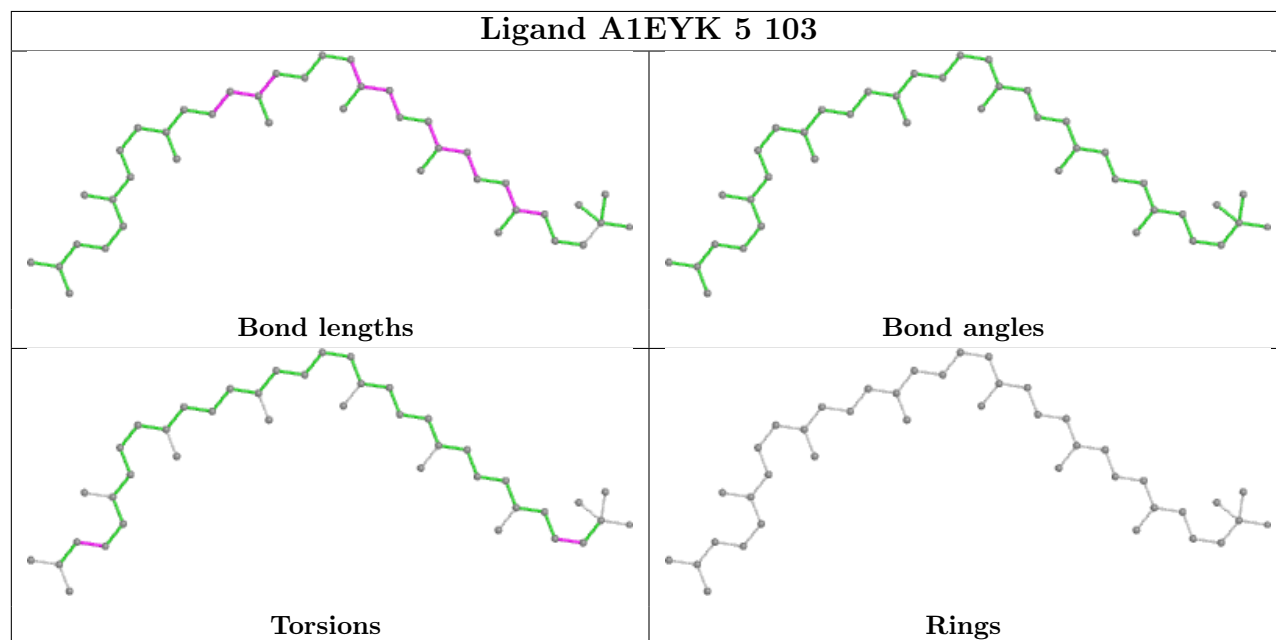
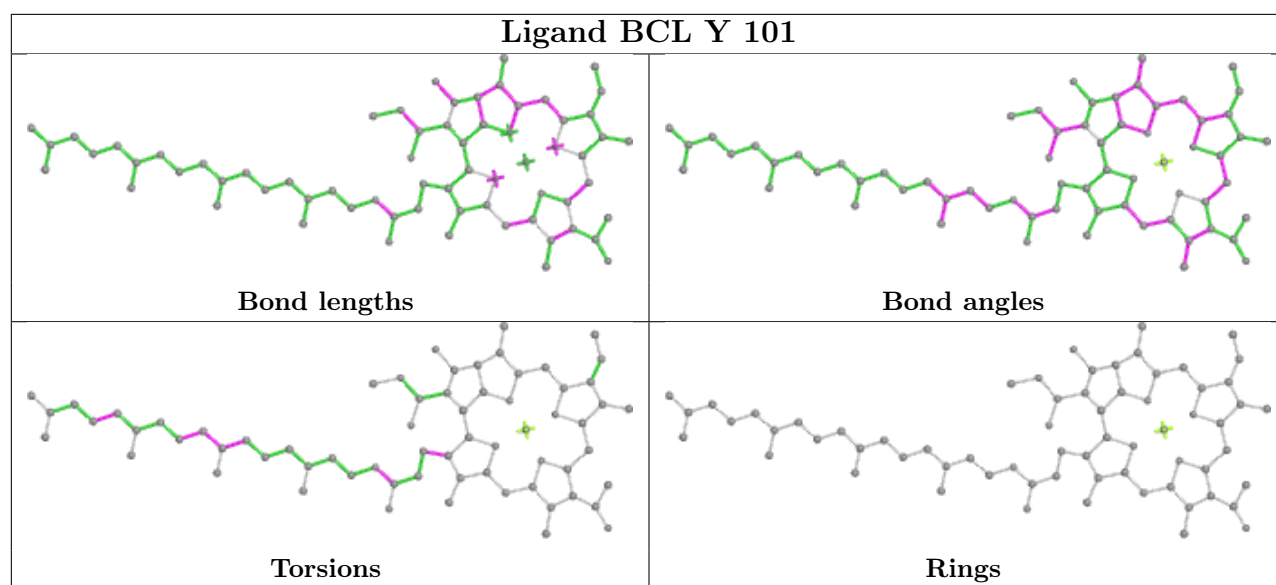


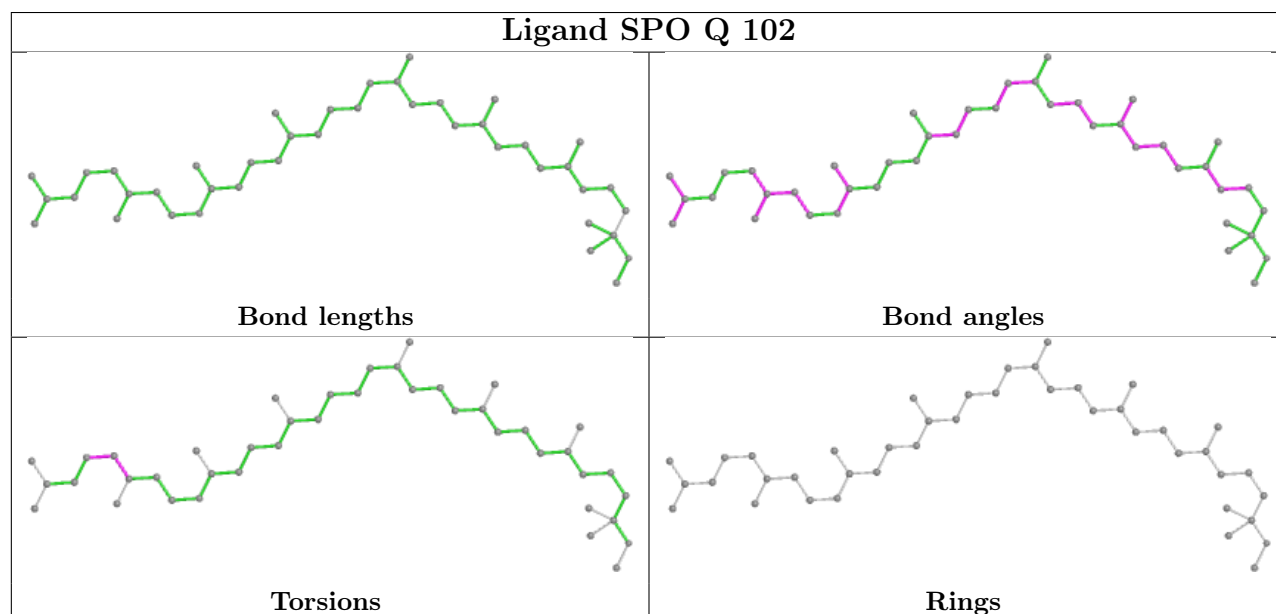
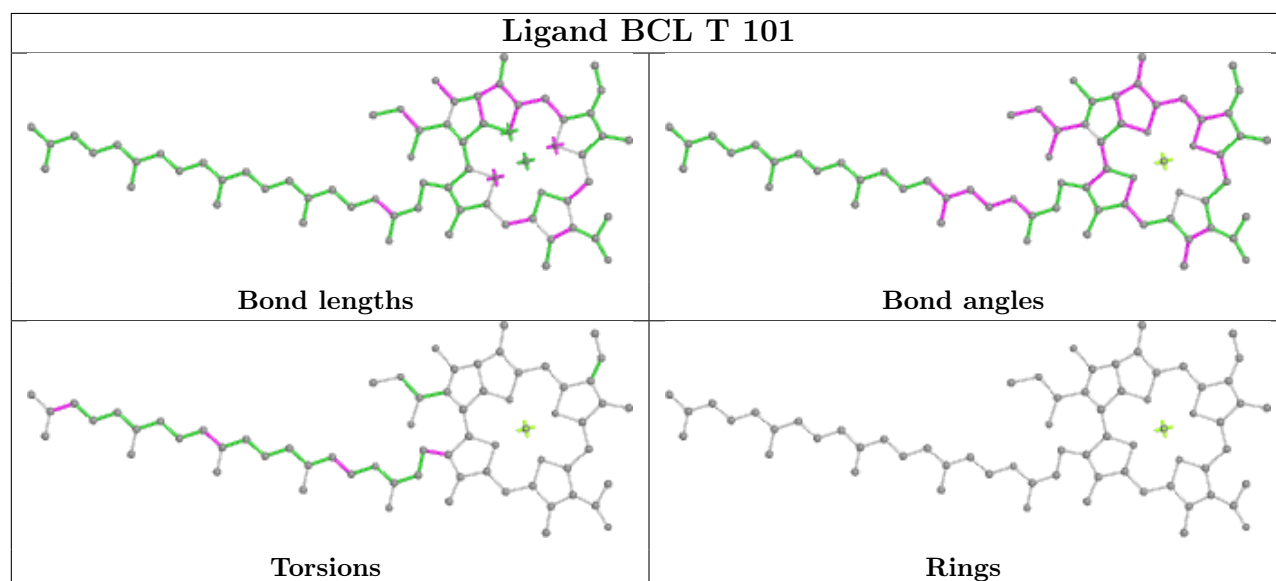
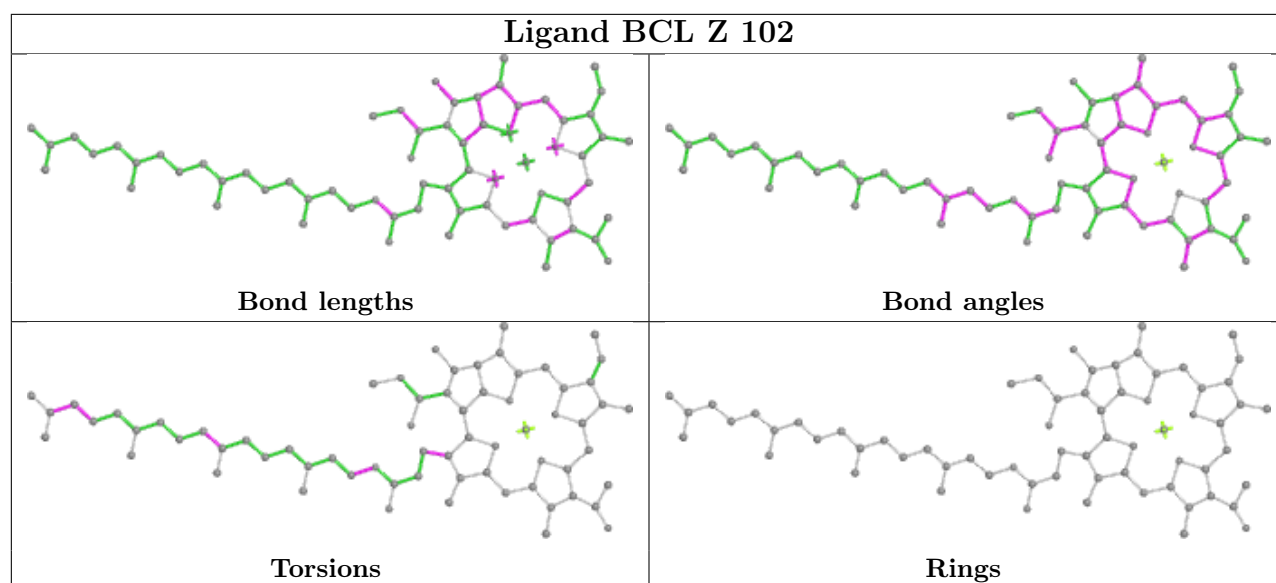


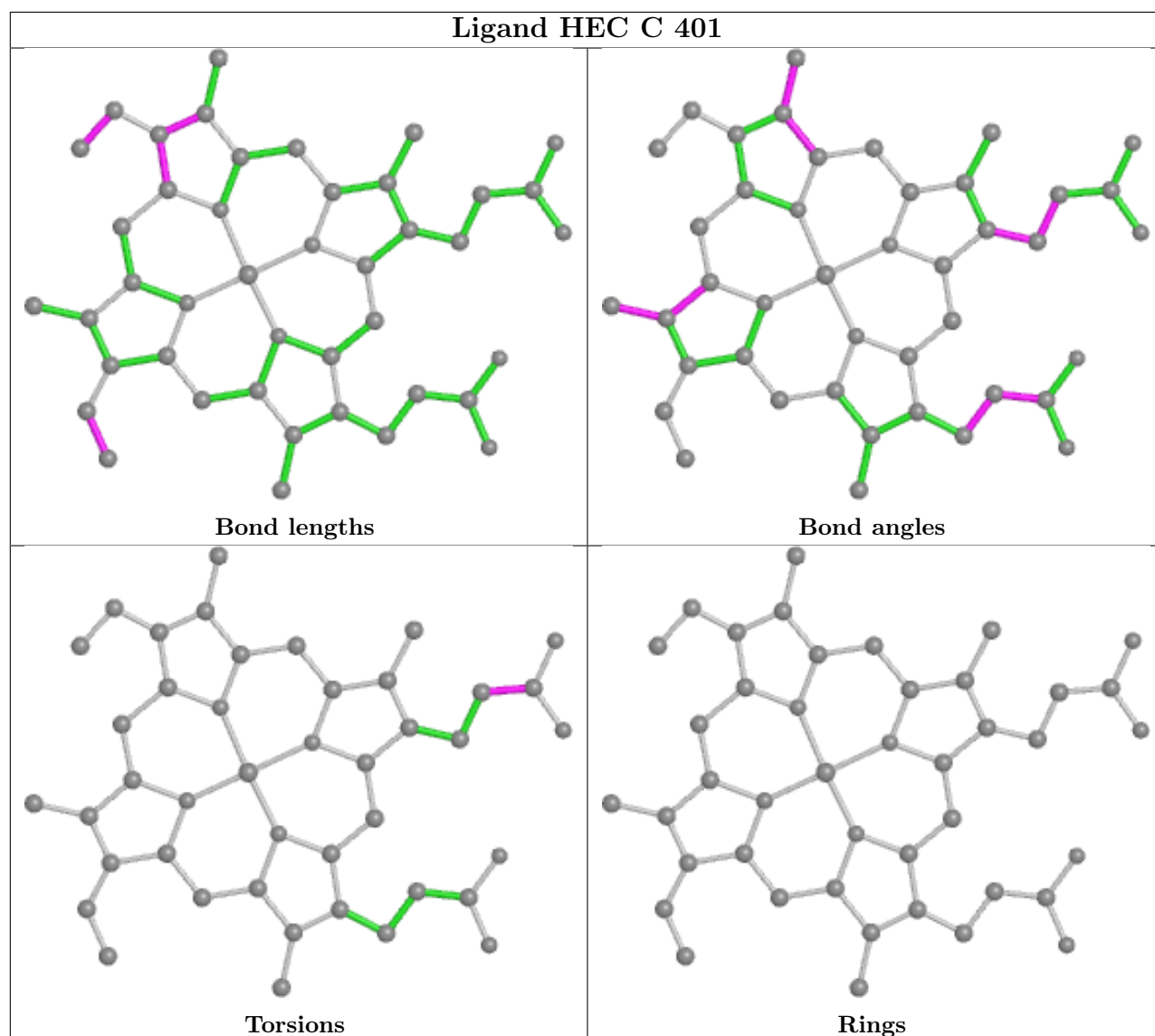
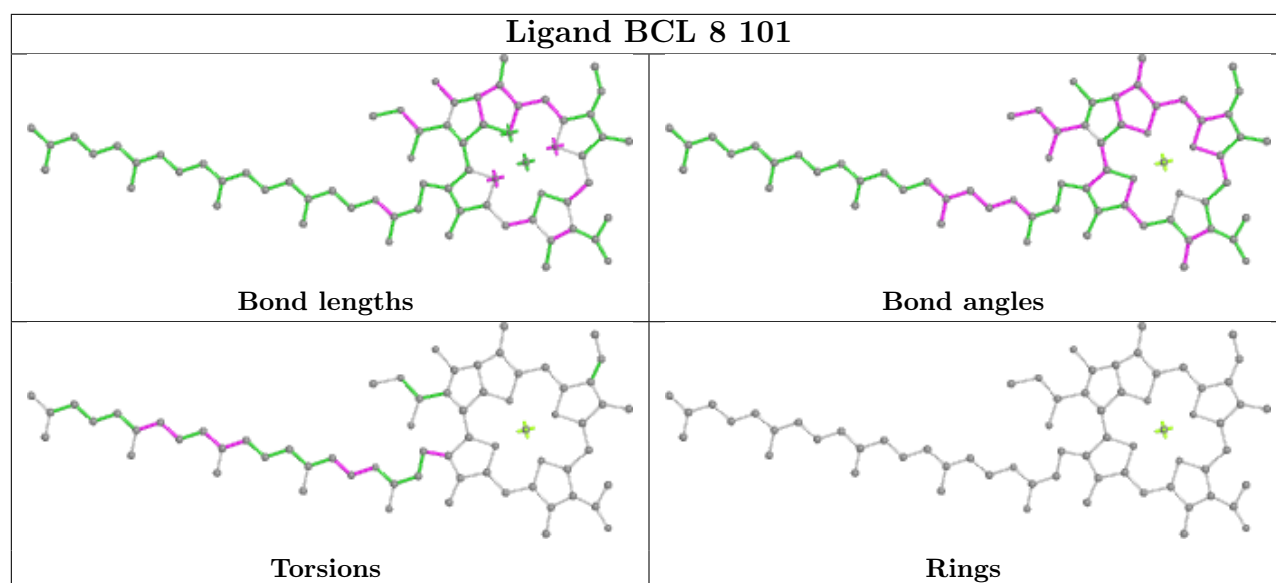


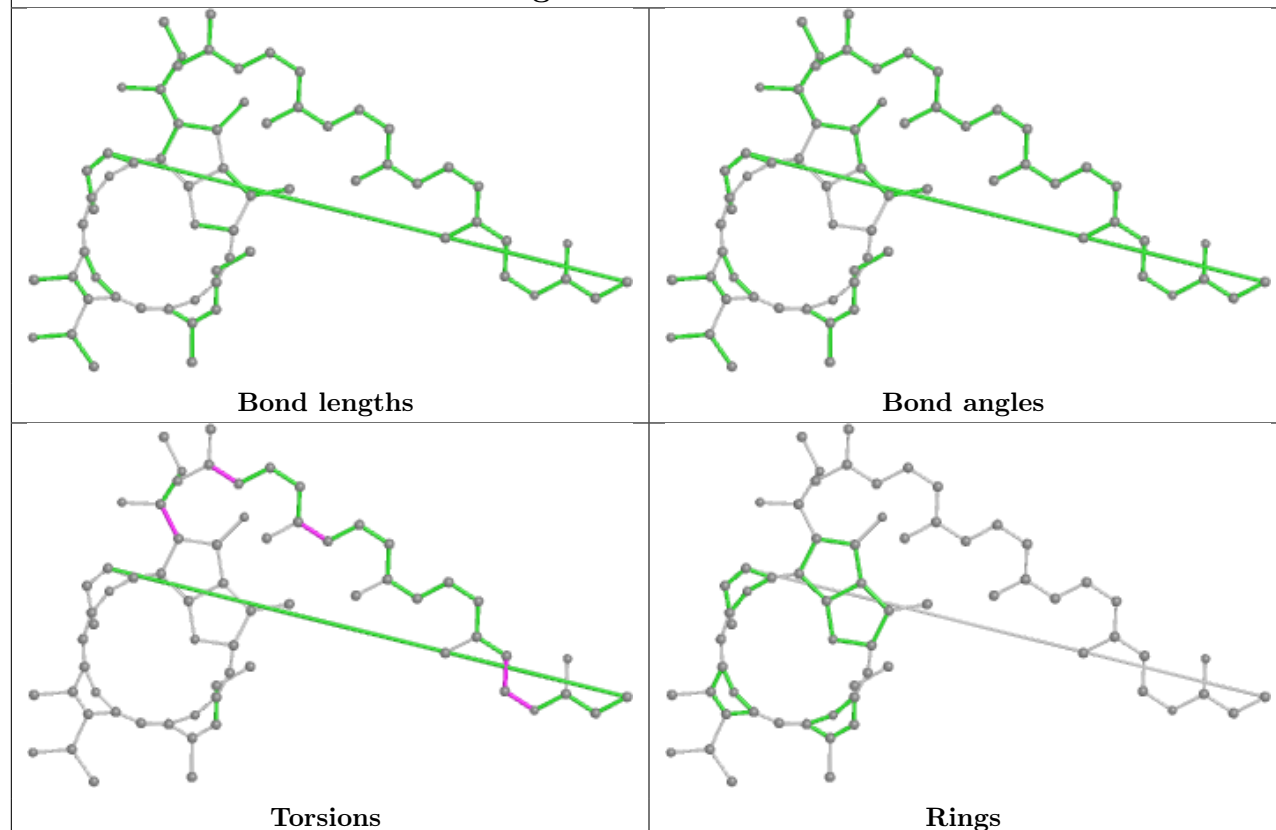
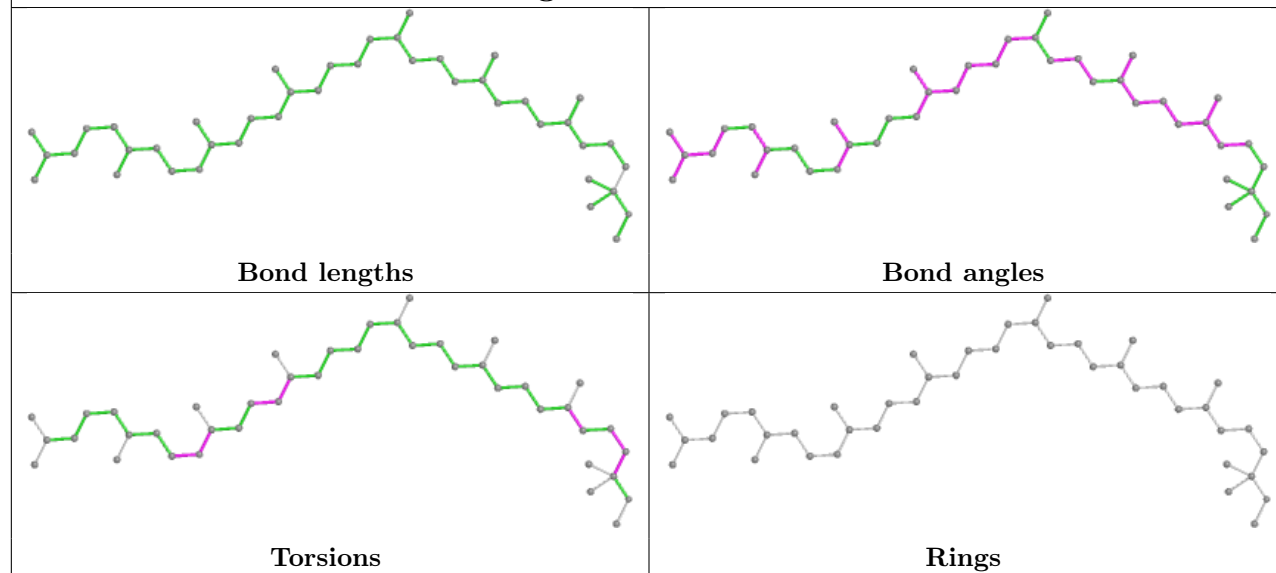


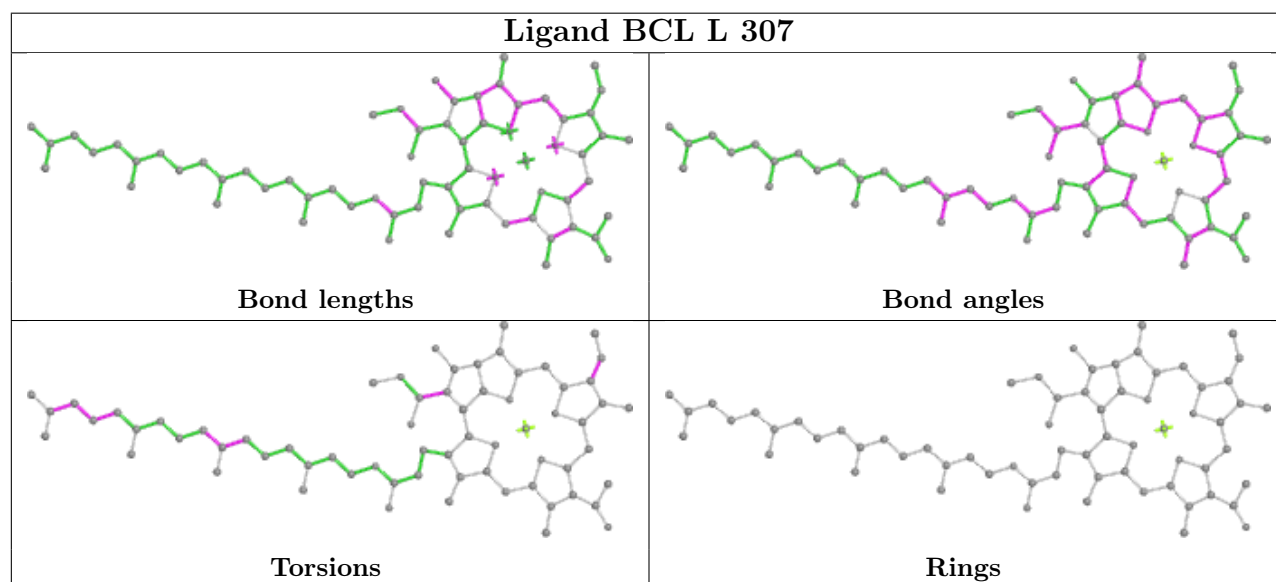
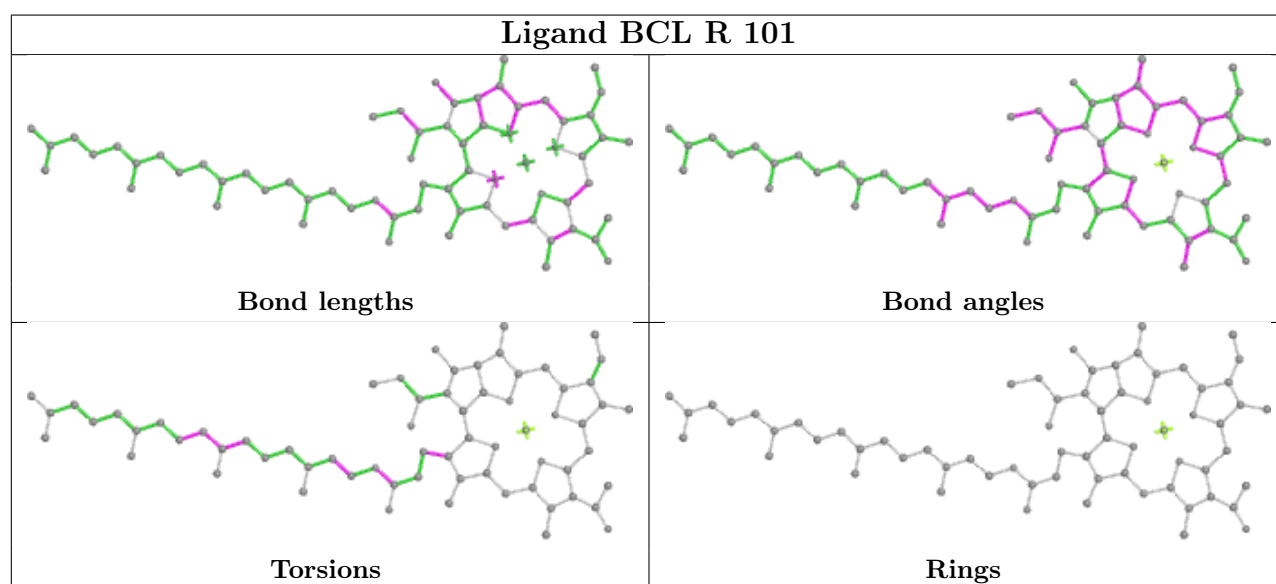
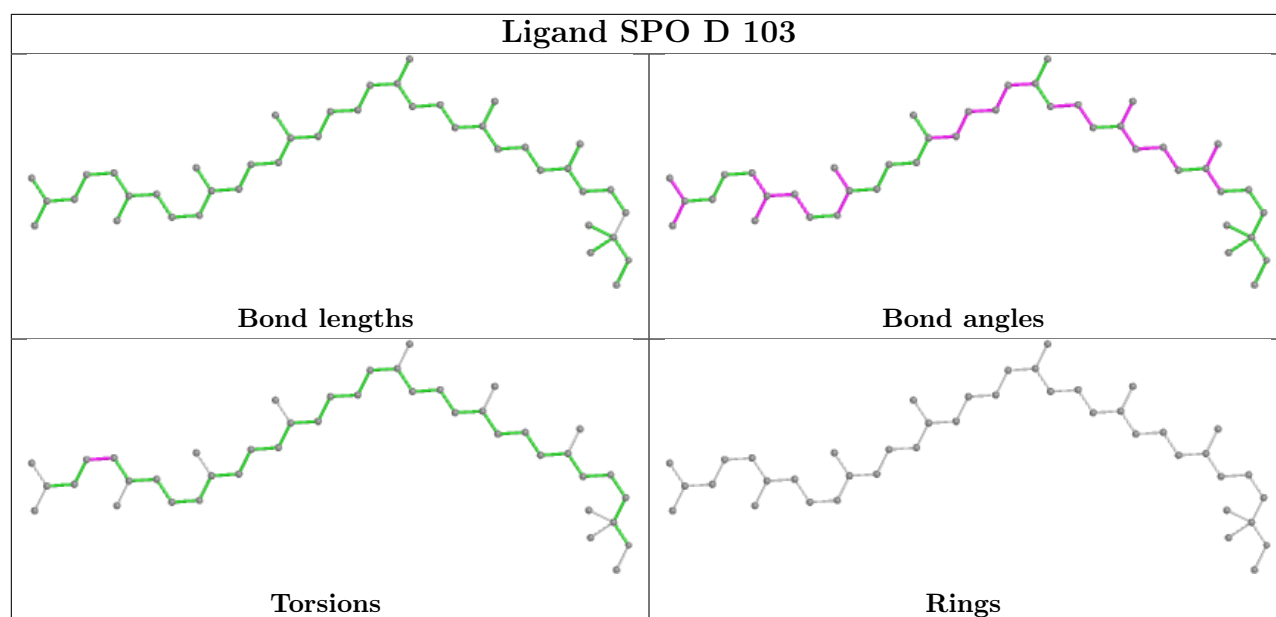


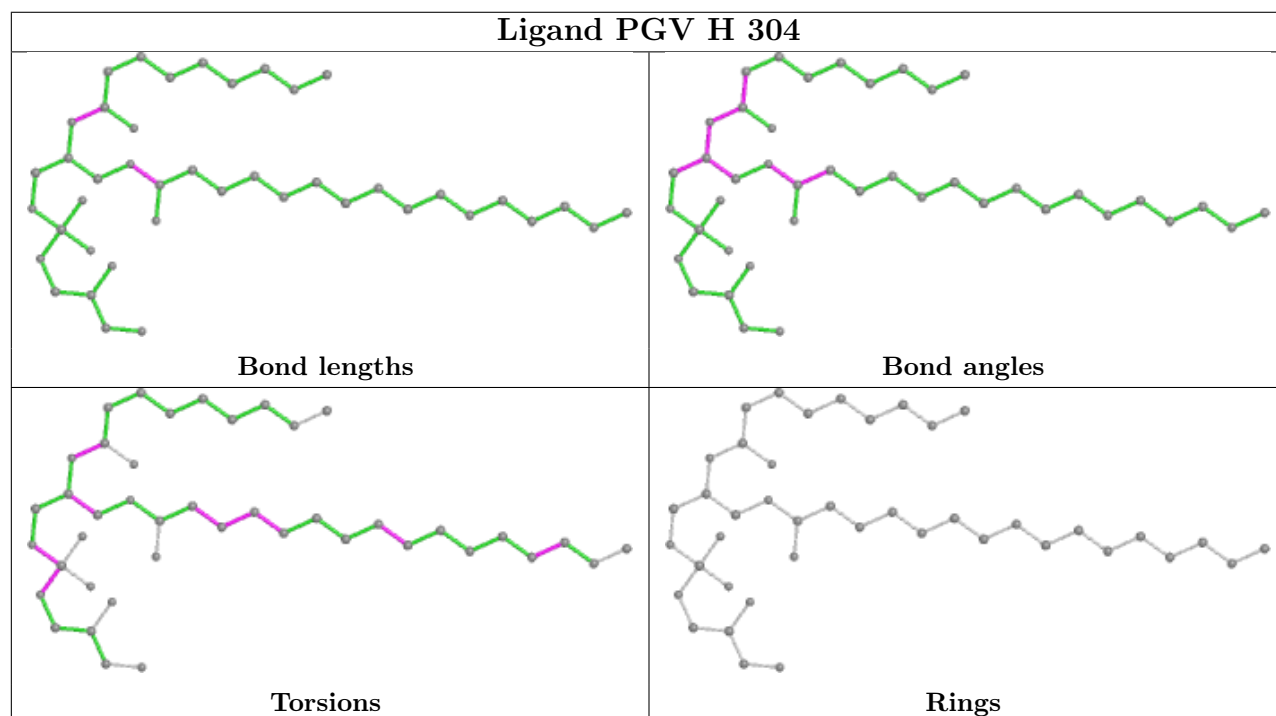
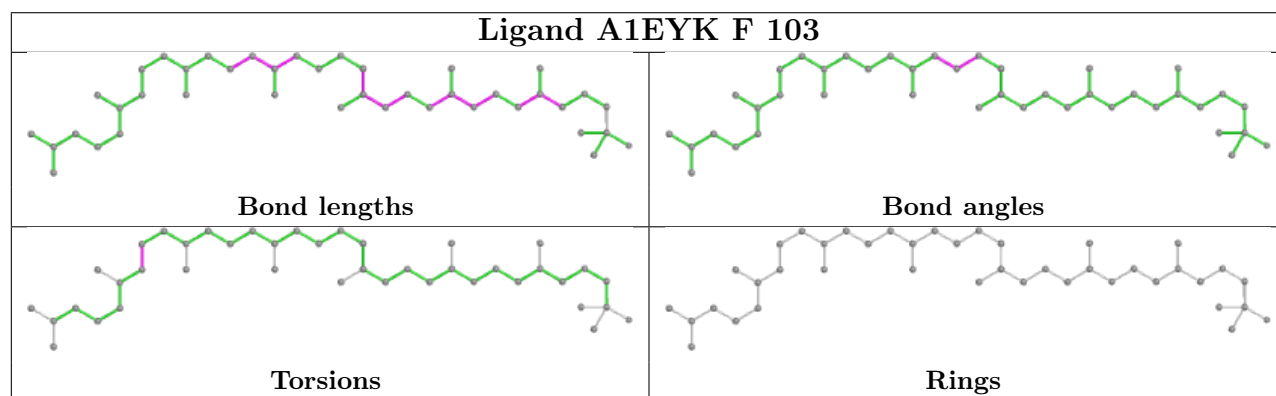
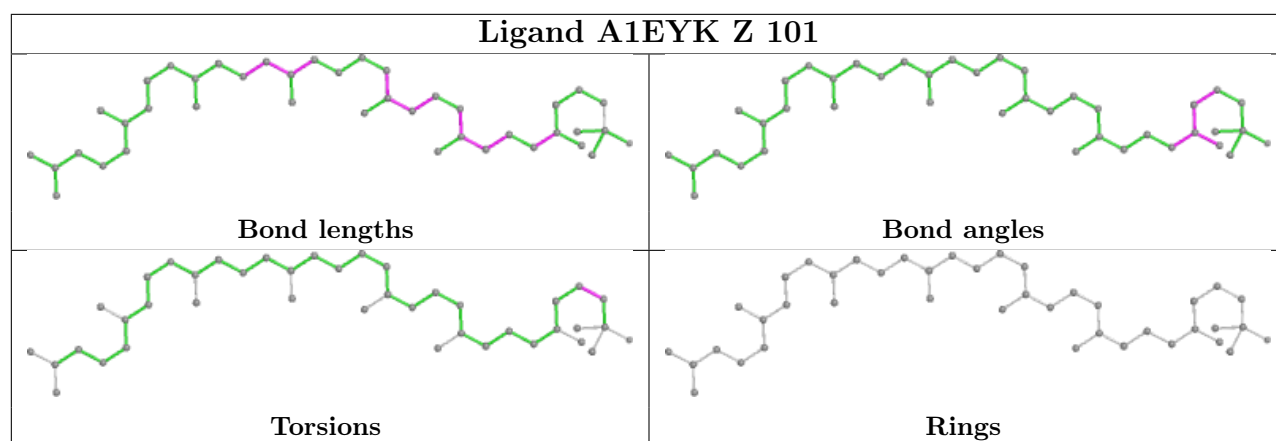


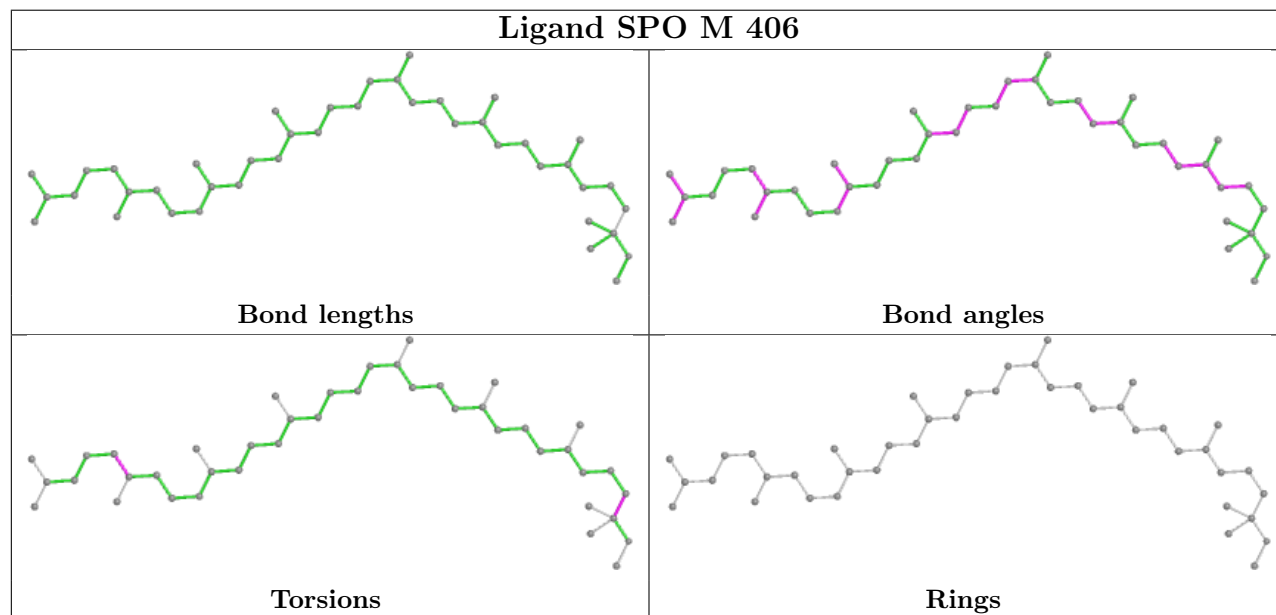
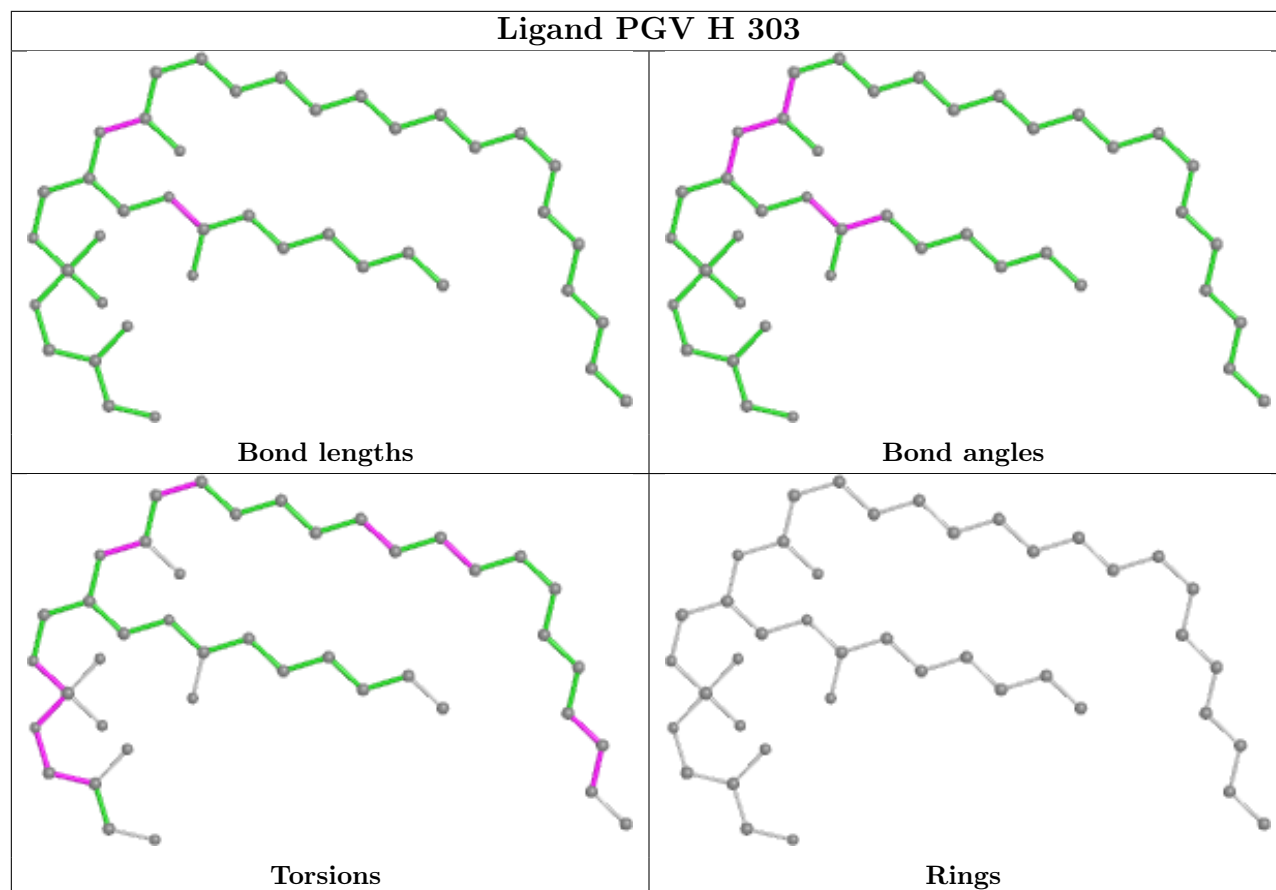


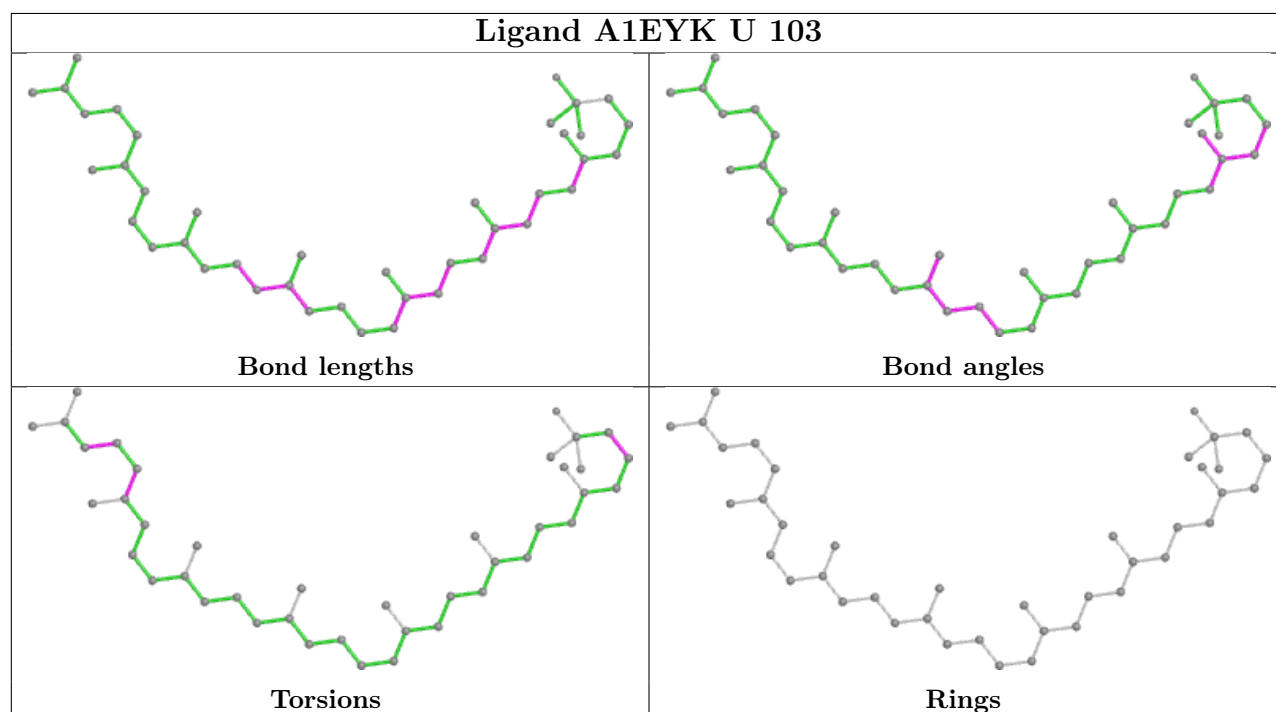
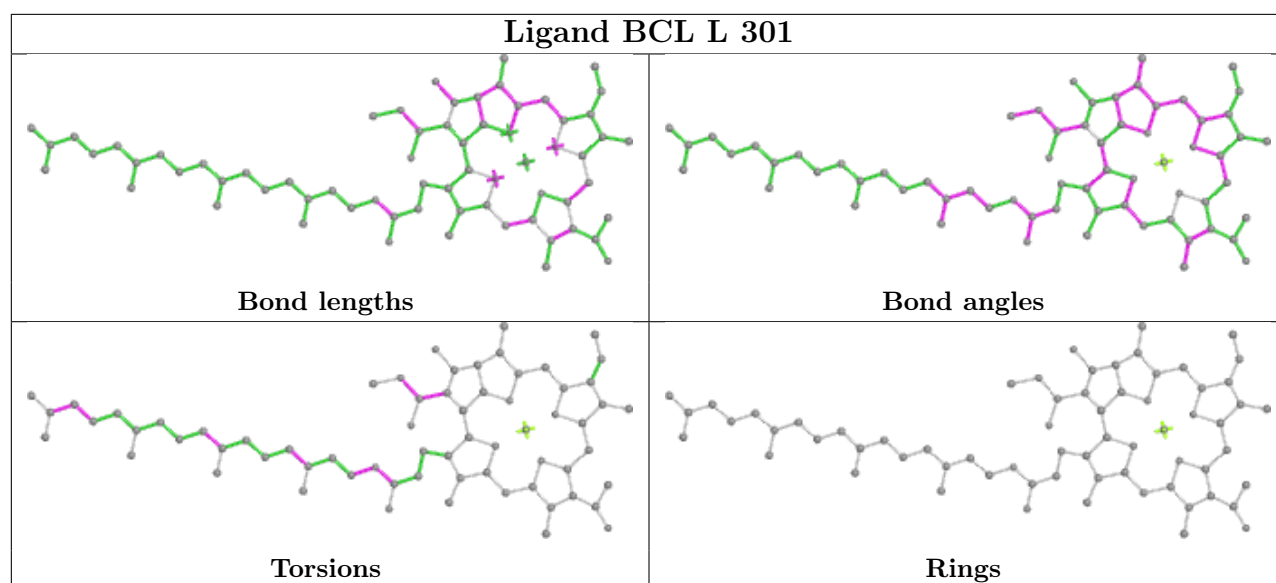


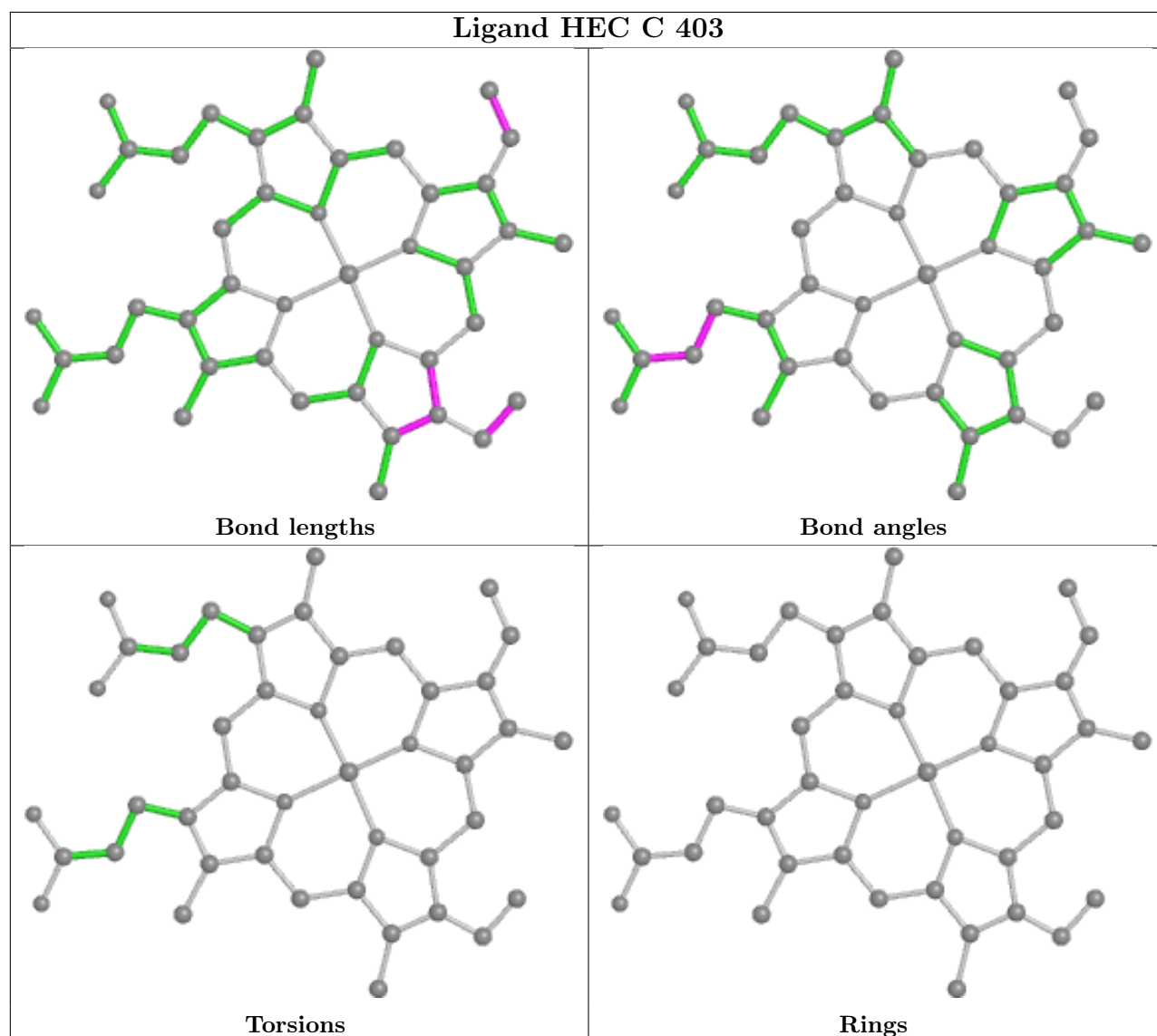
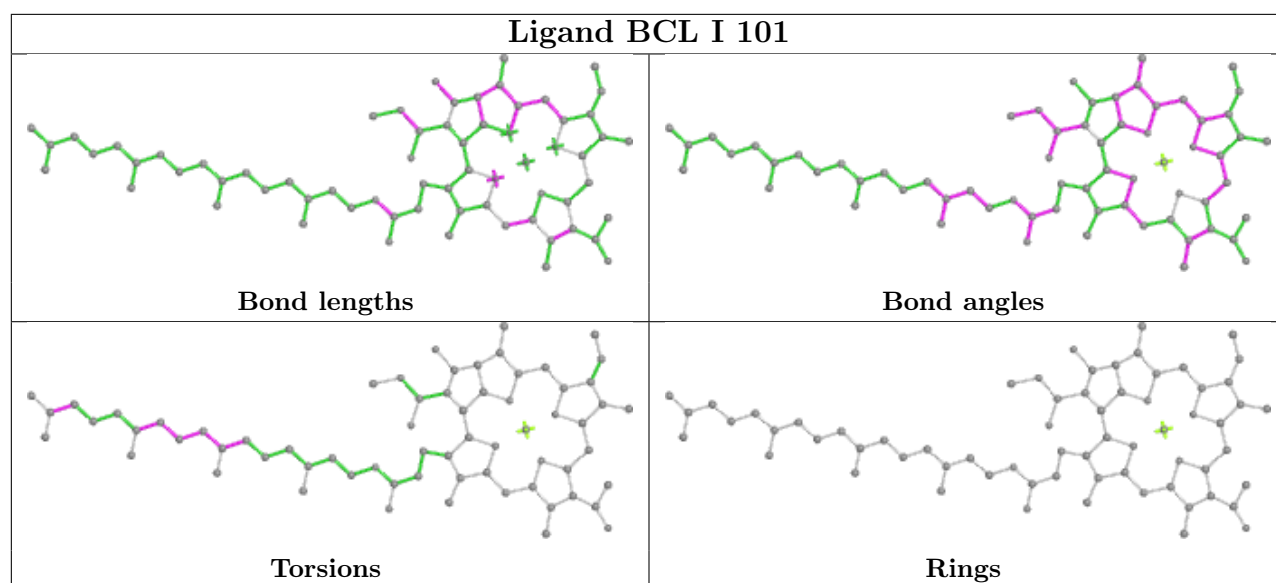
Ligand BPH L 302**Ligand SPO 4 101**

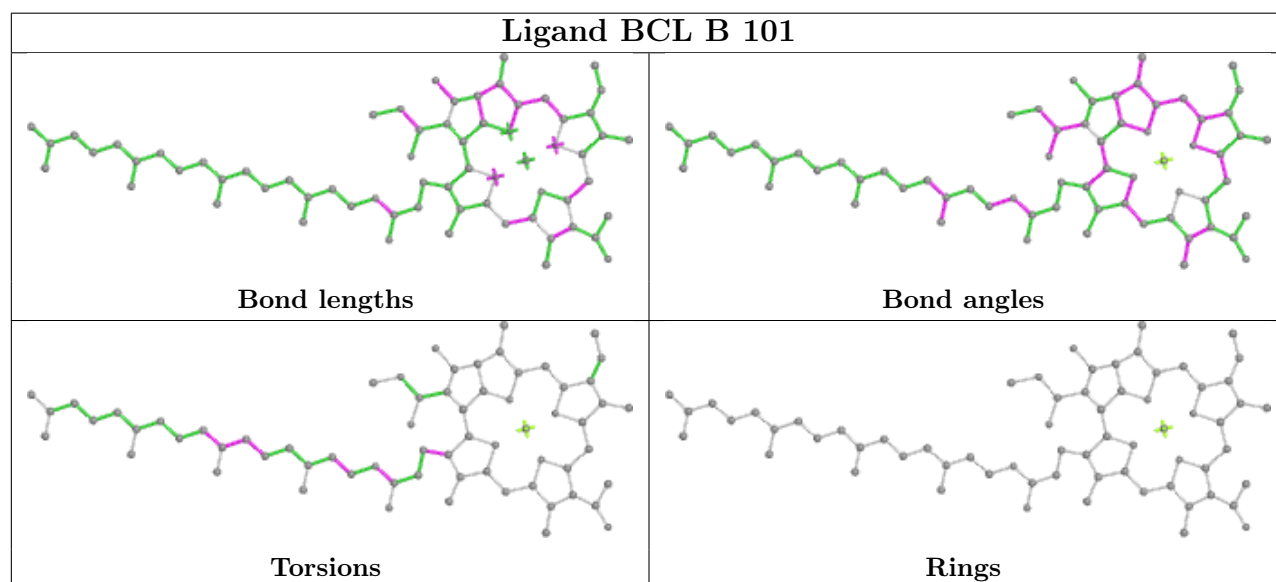
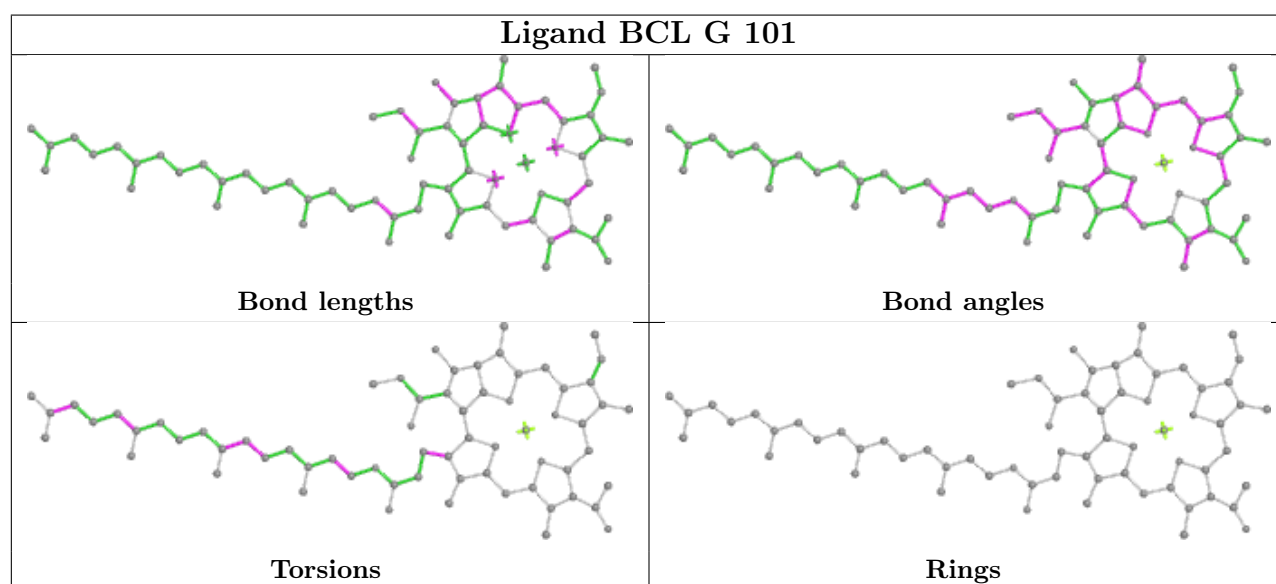
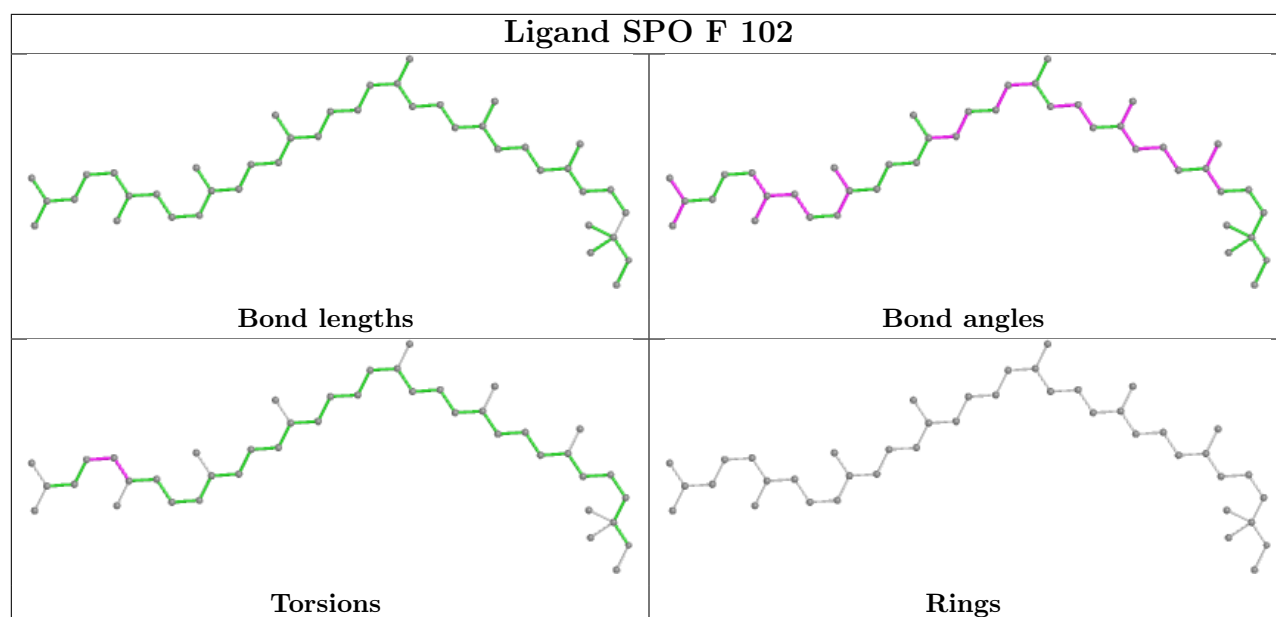


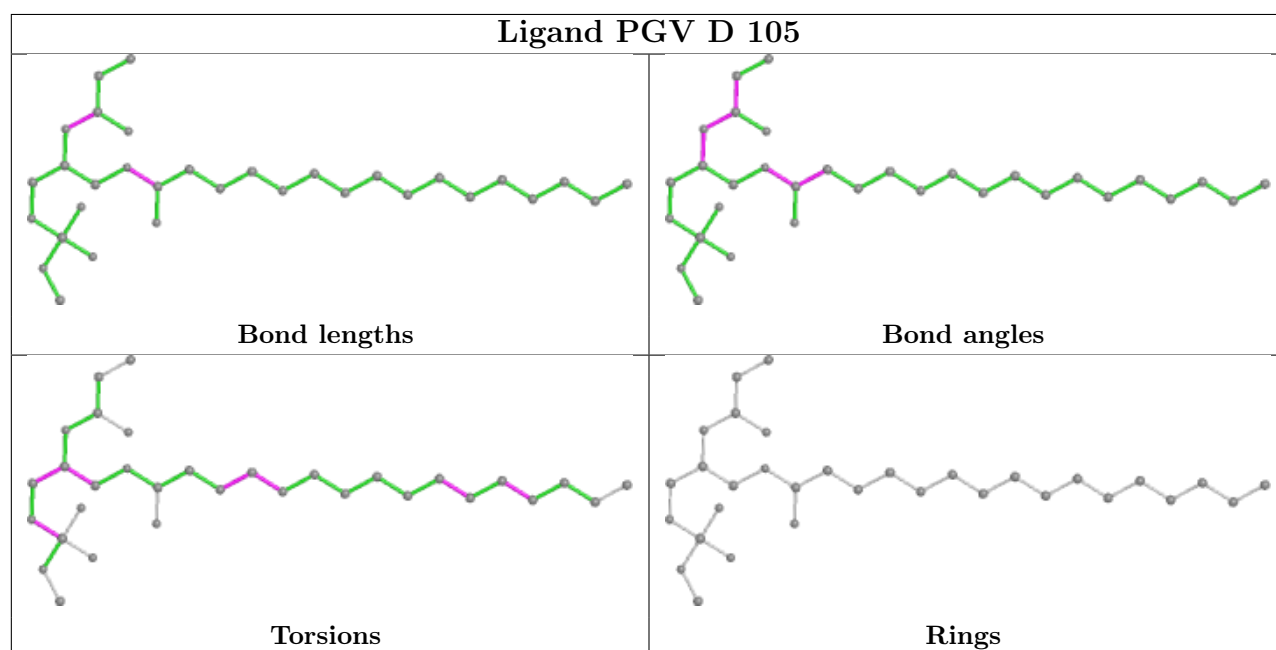
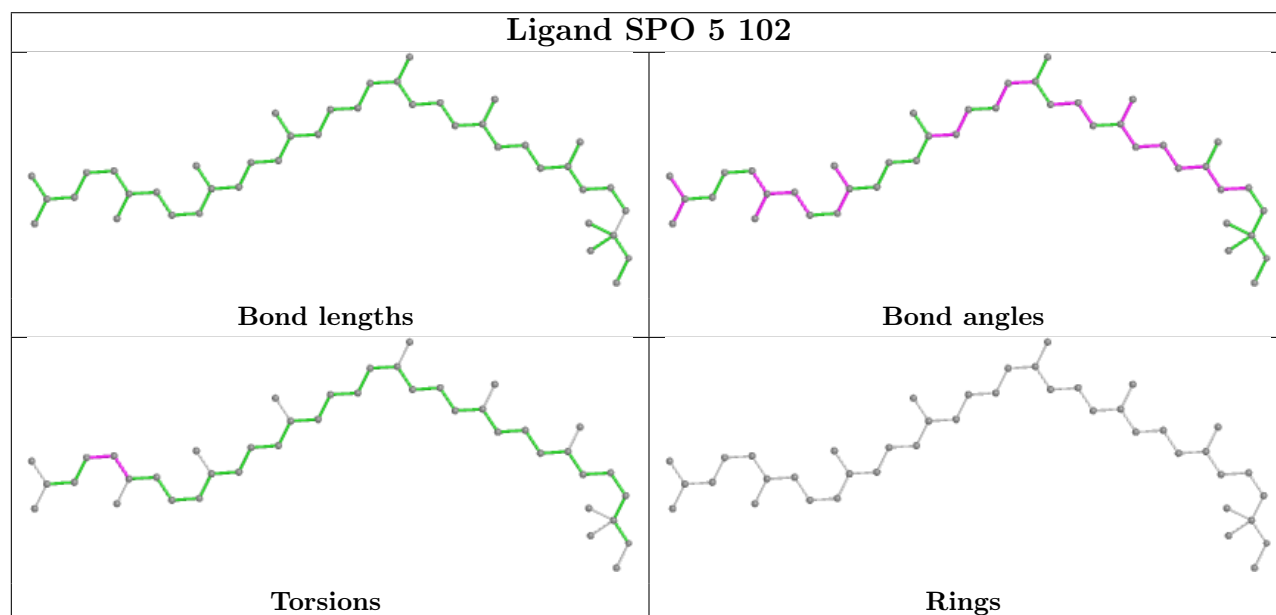
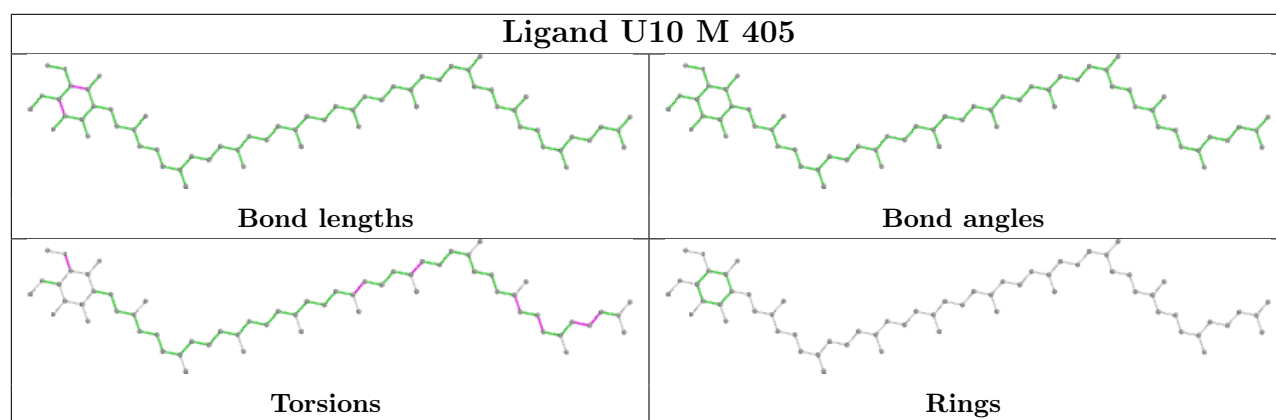


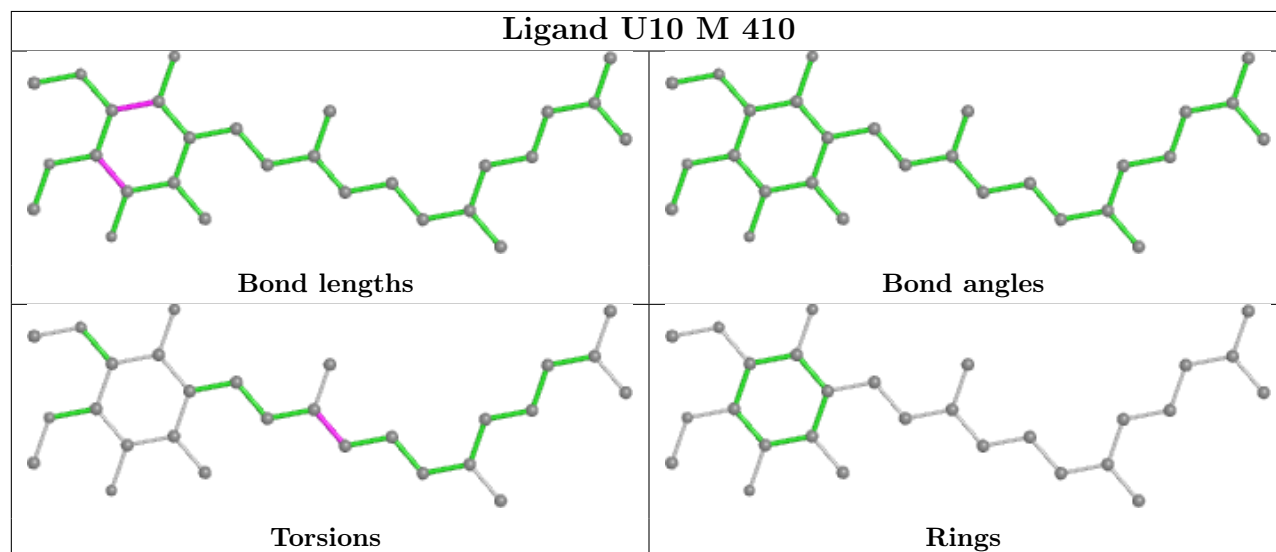
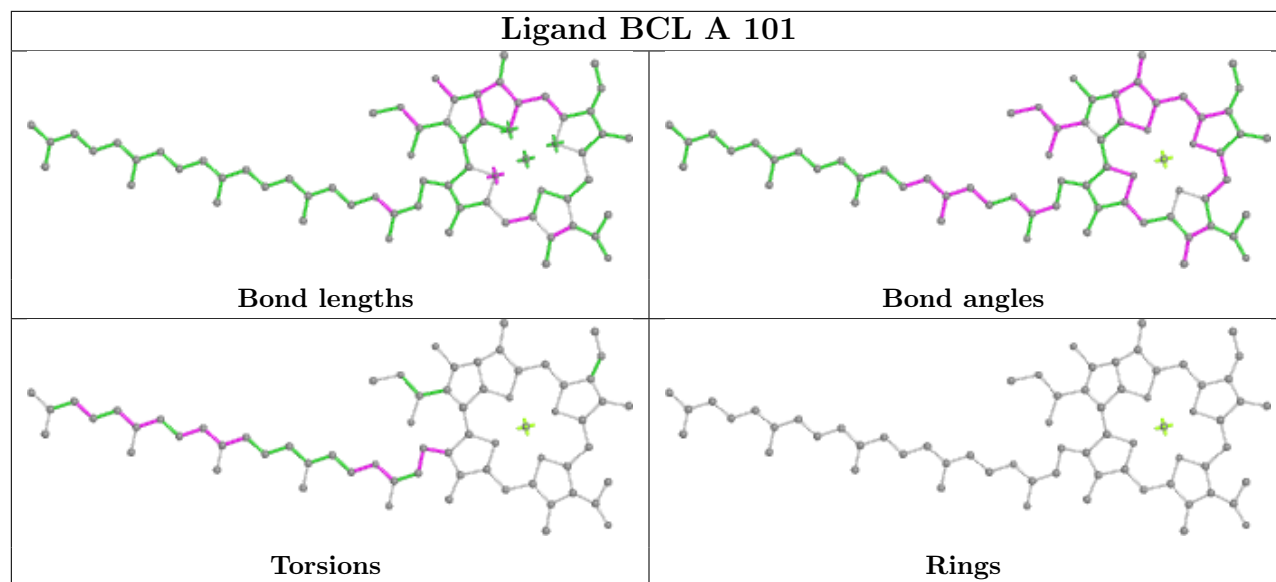


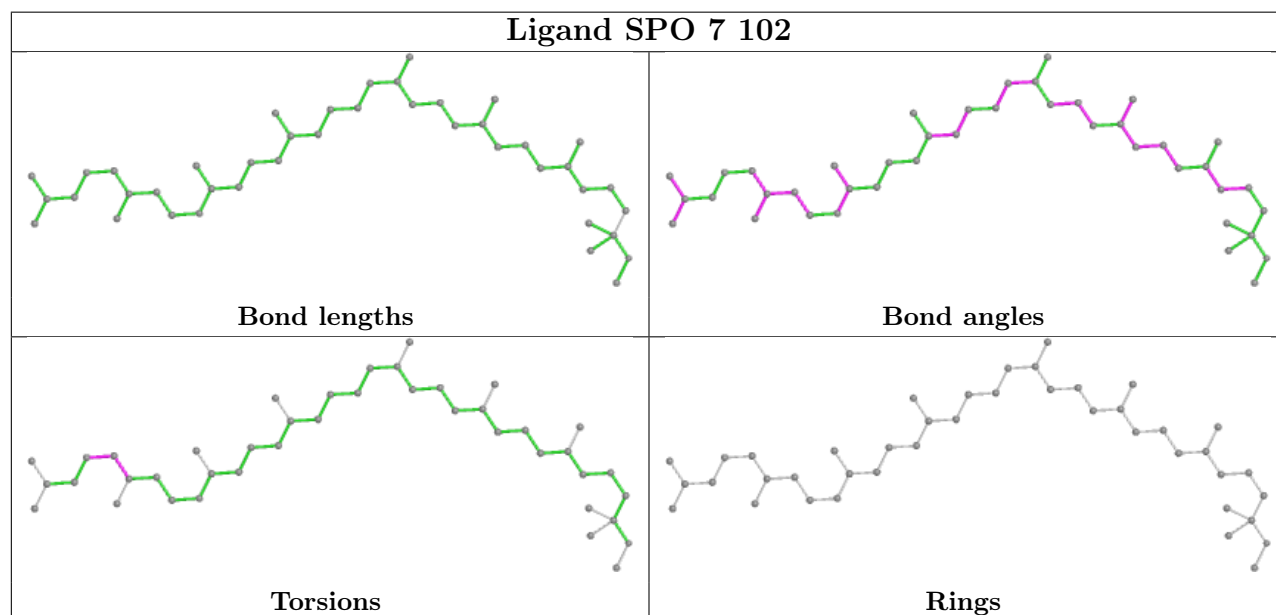
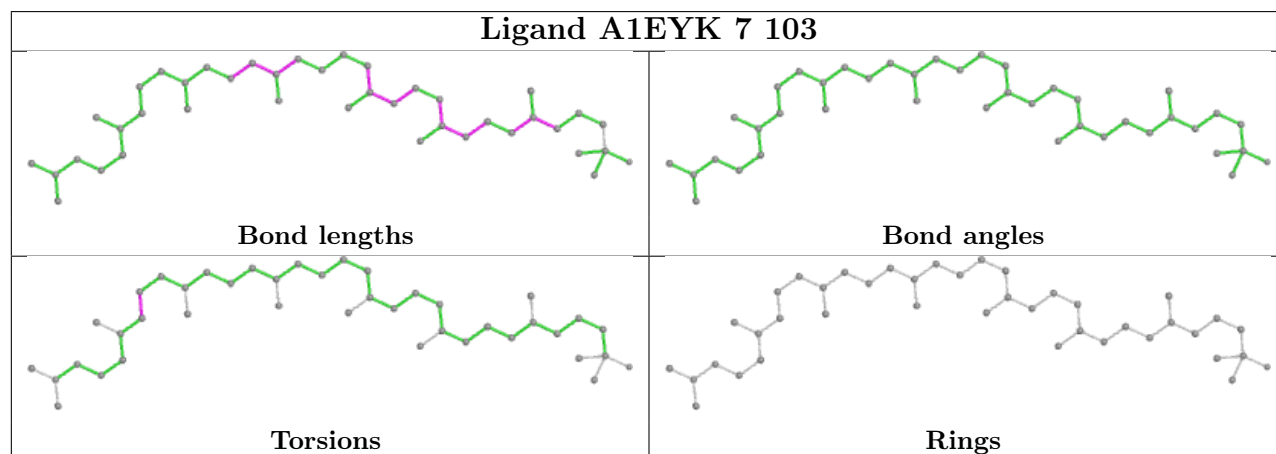
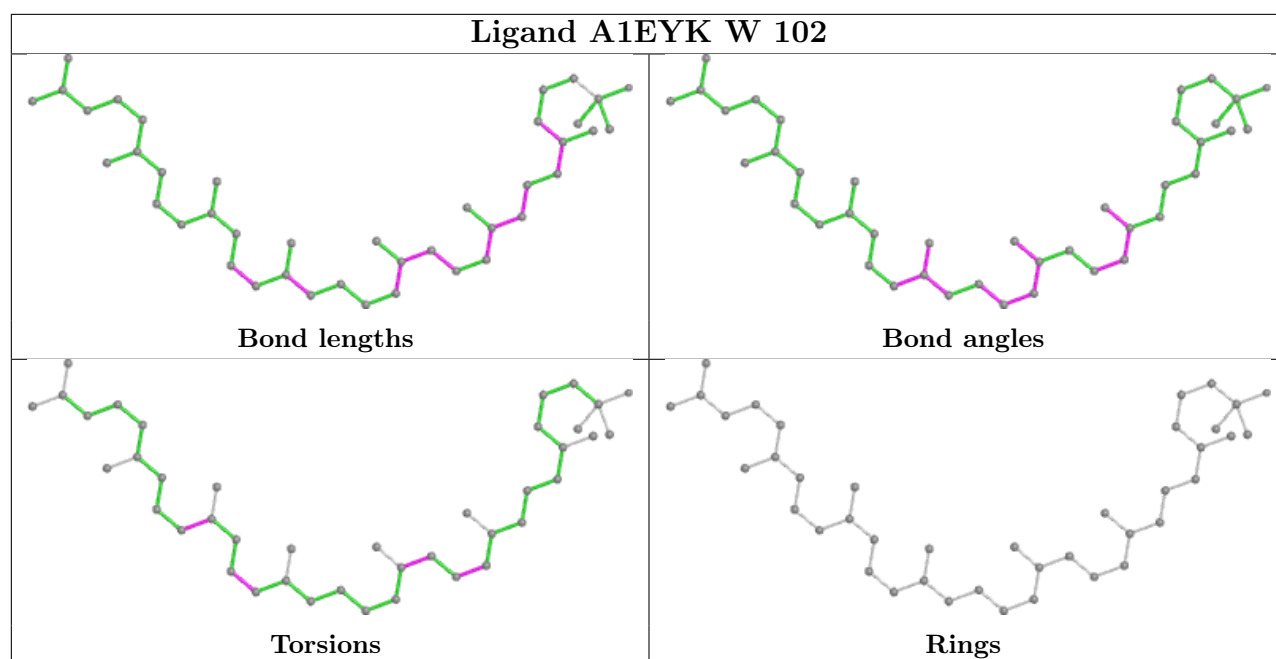












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.