



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2025 – 04:12 PM JST

PDB ID : 7F0L
EMDB ID : EMD-31400
Title : STRUCTURE OF PHOTOSYNTHETIC LH1-RC SUPER-COMPLEX OF RHODOBACTER SPHAEROIDES MONOMER
Authors : Tani, K.; Nagashima, V.P.; Kanno, R.; Kawamura, S.; Kikuchi, R.; Ji, X.-C.; Hall, M.; Yu, L.-J.; Kimura, Y.; Madigan, M.T.; Mizoguchi, A.; Humbel, B.M.; Wang-Otomo, Z.-Y.
Deposited on : 2021-06-05
Resolution : 2.94 Å(reported)
Based on initial model : 5Y5S

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.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.2

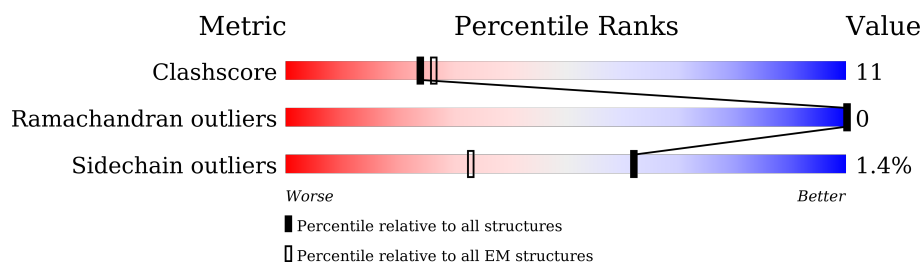
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.94 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	L	282	79% 20% .
2	M	308	77% 22% ..
3	H	260	82% 12% 5%
4	1	54	87% 13%
4	3	54	93% 6% .
4	A	54	59% 24% 17%
4	D	54	76% 24%
4	F	54	87% 11% .

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Mol	Chain	Length	Quality of chain
4	I	54	
4	K	54	
4	O	54	
4	Q	54	
4	S	54	
4	V	54	
4	Y	54	
5	2	49	
5	4	49	
5	6	49	
5	8	49	
5	B	49	
5	E	49	
5	G	49	
5	J	49	
5	N	49	
5	P	49	
5	R	49	
5	T	49	
5	W	49	
5	Z	49	
6	5	54	
6	7	54	
7	X	82	
8	U	53	

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 23458 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 Photosynthetic reaction center L subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	281	Total	C	N	O	S	0	0
			2233	1508	355	362	8		

- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	306	Total	C	N	O	S	0	0
			2437	1627	398	401	11		

- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	246	Total	C	N	O	S	0	0
			1864	1197	314	343	10		

- Molecule 4 is a protein called Light-harvesting protein B-875 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	45	Total	C	N	O	S	0	0
			386	266	59	58	3		
4	D	54	Total	C	N	O	S	0	0
			455	309	73	70	3		
4	F	54	Total	C	N	O	S	0	0
			457	311	73	70	3		
4	I	54	Total	C	N	O	S	0	0
			457	311	73	70	3		
4	K	54	Total	C	N	O	S	0	0
			457	311	73	70	3		
4	O	54	Total	C	N	O	S	0	0
			453	308	72	70	3		
4	Q	54	Total	C	N	O	S	0	0
			457	311	73	70	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	54	Total	C	N	O	S	0	0
			454	309	73	70	2		
4	V	54	Total	C	N	O	S	0	0
			457	311	73	70	3		
4	Y	54	Total	C	N	O	S	0	0
			457	311	73	70	3		
4	1	54	Total	C	N	O	S	0	0
			457	311	73	70	3		
4	3	54	Total	C	N	O	S	0	0
			457	311	73	70	3		

- Molecule 5 is a protein called Antenna pigment protein beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	44	Total	C	N	O	S	0	0
			359	240	56	62	1		
5	E	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	G	45	Total	C	N	O	S	0	0
			365	243	57	64	1		
5	J	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	N	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	P	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	R	43	Total	C	N	O	S	0	0
			347	234	55	57	1		
5	T	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	W	43	Total	C	N	O	S	0	0
			347	234	55	57	1		
5	Z	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	2	42	Total	C	N	O	S	0	0
			343	230	54	58	1		
5	4	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	6	42	Total	C	N	O	S	0	0
			332	222	54	55	1		
5	8	38	Total	C	N	O	S	0	0
			296	202	49	44	1		

- Molecule 6 is a protein called Light-harvesting protein B-875 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	53	Total	C	N	O	S	0	0
			447	305	72	68	2		
6	7	51	Total	C	N	O	S	0	0
			415	281	68	64	2		

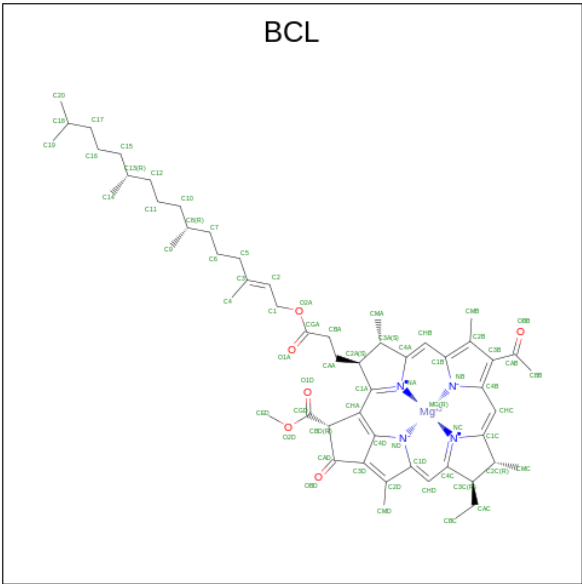
- Molecule 7 is a protein called PufX.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	X	53	Total	C	N	O	S	0	0
			405	269	69	64	3		

- Molecule 8 is a protein called protein-U.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	U	50	Total	C	N	O	S	0	0
			369	252	57	57	3		

- Molecule 9 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



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

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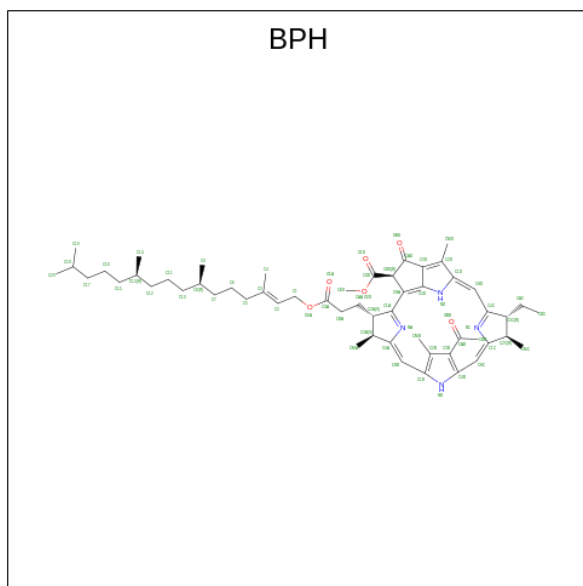
Mol	Chain	Residues	Atoms					AltConf
9	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	A	1	Total 61	C 50	Mg 1	N 4	O 6	0
9	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	D	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	P	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	T	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0

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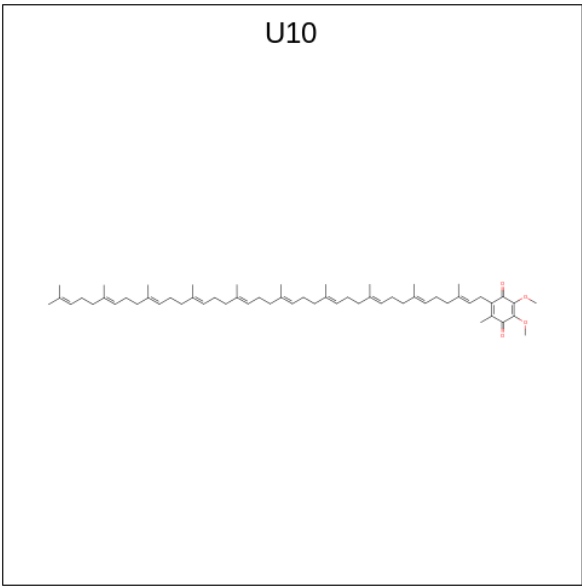
Mol	Chain	Residues	Atoms					AltConf
9	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	8	1	Total	C	Mg	N	O	0
			60	49	1	4	6	

- Molecule 10 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



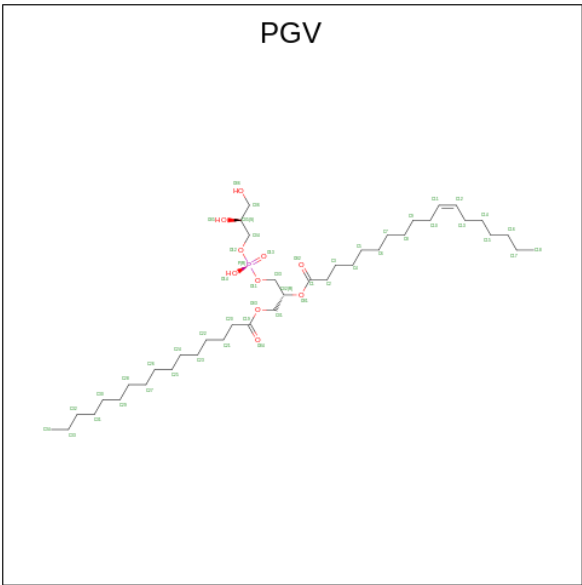
Mol	Chain	Residues	Atoms				AltConf
10	L	1	Total	C	N	O	0
			65	55	4	6	
10	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 11 is UBIQUINONE-10 (three-letter code: U10) (formula: C₅₉H₉₀O₄).



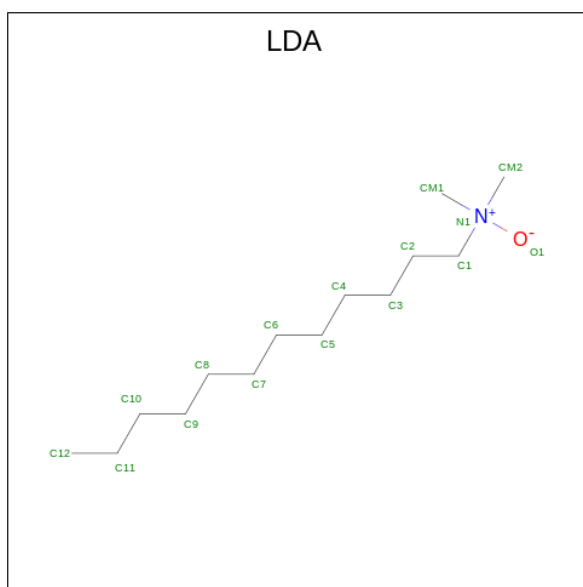
Mol	Chain	Residues	Atoms			AltConf
11	L	1	Total	C	O	0
			35	31	4	
11	L	1	Total	C	O	0
			35	31	4	
11	M	1	Total	C	O	0
			48	44	4	

- Molecule 12 is (1R)-2-{{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
12	L	1	Total	C	O	P	0
			39	28	10	1	
12	L	1	Total	C	O	P	0
			33	22	10	1	
12	L	1	Total	C	O	P	0
			45	36	8	1	
12	M	1	Total	C	O	P	0
			47	36	10	1	
12	M	1	Total	C	O	P	0
			38	27	10	1	
12	H	1	Total	C	O	P	0
			34	25	8	1	
12	H	1	Total	C	O	P	0
			40	29	10	1	
12	H	1	Total	C	O	P	0
			47	36	10	1	
12	K	1	Total	C	O	P	0
			41	34	6	1	
12	Q	1	Total	C	O	P	0
			39	28	10	1	
12	Y	1	Total	C	O	P	0
			43	32	10	1	
12	3	1	Total	C	O	P	0
			51	40	10	1	
12	X	1	Total	C	O	P	0
			39	28	10	1	

- Molecule 13 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C₁₄H₃₁NO).

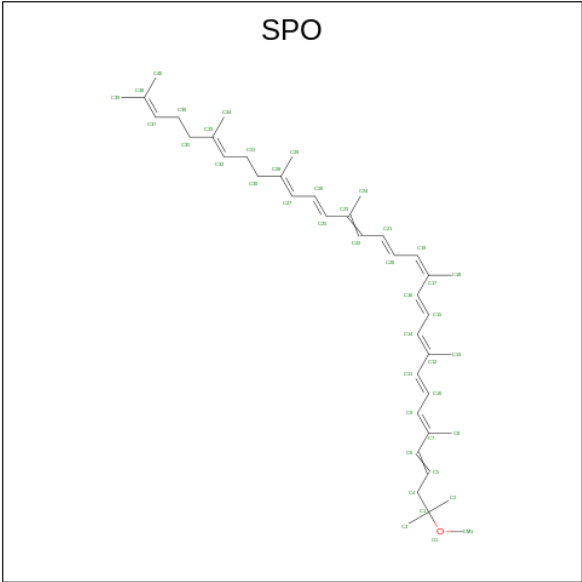


Mol	Chain	Residues	Atoms				AltConf
13	L	1	Total	C	N	O	0
			16	14	1	1	
13	L	1	Total	C	N	O	0
			16	14	1	1	
13	M	1	Total	C	N	O	0
			16	14	1	1	
13	Y	1	Total	C	N	O	0
			12	10	1	1	
13	X	1	Total	C	N	O	0
			13	11	1	1	
13	X	1	Total	C	N	O	0
			16	14	1	1	

- Molecule 14 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 15 is SPHEROIDENE (three-letter code: SPO) (formula: C₄₁H₆₀O) (labeled as "Ligand of Interest" by depositor).



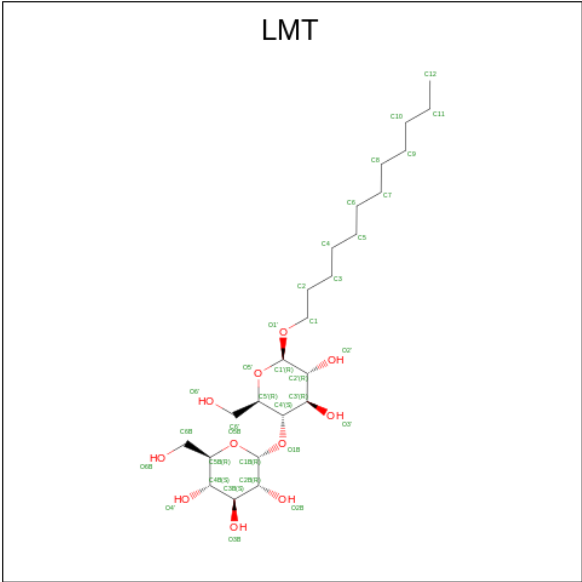
Mol	Chain	Residues	Atoms			AltConf
15	M	1	Total	C	O	0
			42	41	1	
15	D	1	Total	C	O	0
			42	41	1	
15	E	1	Total	C	O	0
			42	41	1	
15	F	1	Total	C	O	0
			42	41	1	
15	F	1	Total	C	O	0
			42	41	1	
15	G	1	Total	C	O	0
			42	41	1	
15	G	1	Total	C	O	0
			42	41	1	
15	K	1	Total	C	O	0
			42	41	1	
15	N	1	Total	C	O	0
			42	41	1	
15	O	1	Total	C	O	0
			42	41	1	
15	O	1	Total	C	O	0
			42	41	1	
15	P	1	Total	C	O	0
			42	41	1	
15	R	1	Total	C	O	0
			42	41	1	
15	S	1	Total	C	O	0
			42	41	1	

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Mol	Chain	Residues	Atoms			AltConf
15	S	1	Total	C	O	0
			42	41	1	
15	T	1	Total	C	O	0
			42	41	1	
15	V	1	Total	C	O	0
			42	41	1	
15	V	1	Total	C	O	0
			42	41	1	
15	W	1	Total	C	O	0
			42	41	1	
15	1	1	Total	C	O	0
			42	41	1	
15	1	1	Total	C	O	0
			42	41	1	
15	1	1	Total	C	O	0
			42	41	1	
15	3	1	Total	C	O	0
			42	41	1	
15	5	1	Total	C	O	0
			42	41	1	
15	5	1	Total	C	O	0
			42	41	1	
15	8	1	Total	C	O	0
			42	41	1	
15	X	1	Total	C	O	0
			42	41	1	

- Molecule 16 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



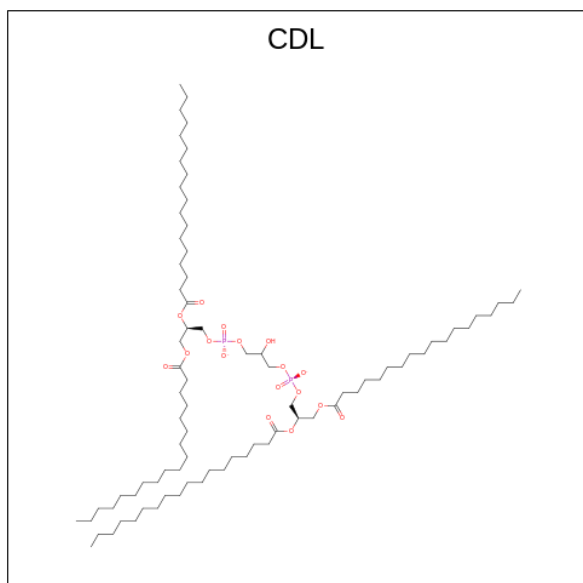
Mol	Chain	Residues	Atoms			AltConf
16	M	1	Total	C	O	0
			27	20	7	
16	M	1	Total	C	O	0
			35	24	11	
16	M	1	Total	C	O	0
			33	22	11	
16	H	1	Total	C	O	0
			35	24	11	
16	H	1	Total	C	O	0
			30	19	11	
16	A	1	Total	C	O	0
			35	24	11	
16	A	1	Total	C	O	0
			35	24	11	
16	A	1	Total	C	O	0
			27	16	11	
16	D	1	Total	C	O	0
			27	16	11	
16	F	1	Total	C	O	0
			26	16	10	
16	F	1	Total	C	O	0
			17	11	6	
16	I	1	Total	C	O	0
			27	16	11	
16	K	1	Total	C	O	0
			35	24	11	
16	Q	1	Total	C	O	0
			24	18	6	

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Mol	Chain	Residues	Atoms			AltConf
16	Q	1	Total	C	O	0
			19	13	6	
16	S	1	Total	C	O	0
			25	19	6	
16	S	1	Total	C	O	0
			30	19	11	
16	1	1	Total	C	O	0
			24	15	9	
16	3	1	Total	C	O	0
			35	24	11	
16	4	1	Total	C	O	0
			27	16	11	
16	5	1	Total	C	O	0
			33	22	11	
16	X	1	Total	C	O	0
			31	20	11	
16	U	1	Total	C	O	0
			32	21	11	
16	U	1	Total	C	O	0
			35	24	11	

- Molecule 17 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
17	M	1	Total	C	O	P	0
			79	60	17	2	

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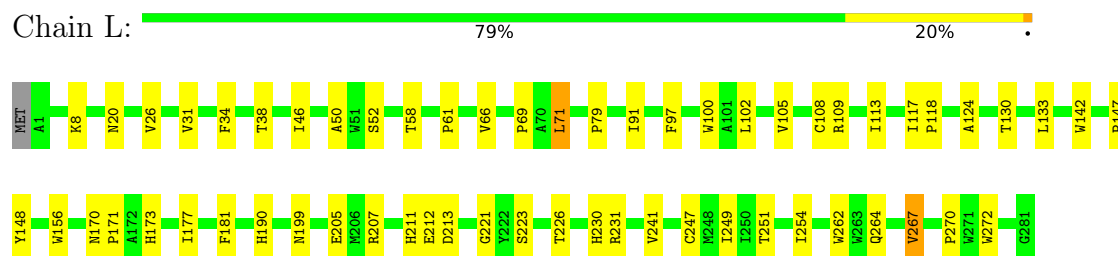
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Mol	Chain	Residues	Atoms				AltConf
17	H	1	Total	C	O	P	0
			61	42	17	2	
17	H	1	Total	C	O	P	0
			37	20	15	2	
17	Y	1	Total	C	O	P	0
			48	30	16	2	

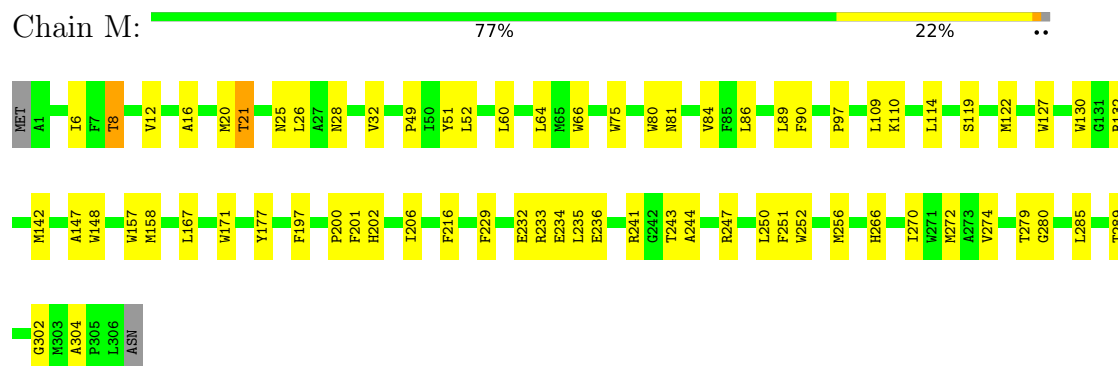
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

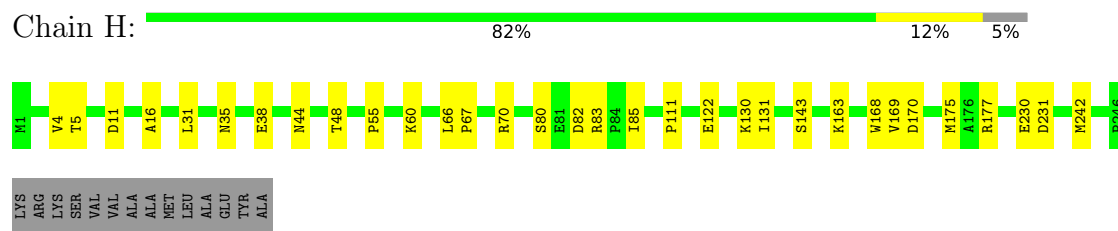
- Molecule 1: Photosynthetic reaction center L subunit



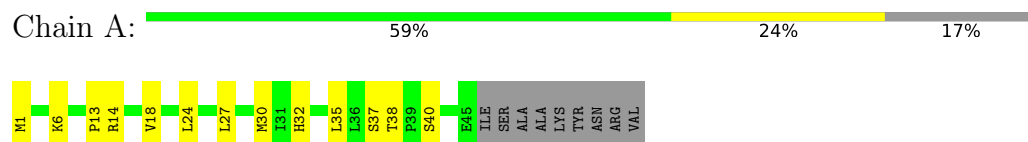
- Molecule 2: Reaction center protein M chain




- Molecule 3: Reaction center protein H chain



- Molecule 4: Light-harvesting protein B-875 alpha chain



- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain D:  76% 24%




- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain F:  87% 11%




- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain I:  80% 20%



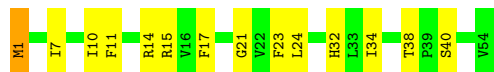
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain K:  80% 20%



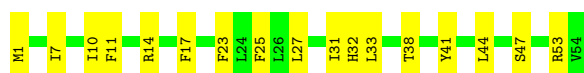
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain O:  74% 24%




- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain Q:  69% 31%




- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain S:  80% 20%




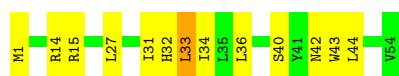
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain V:  76% 24%



- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain Y:  76% 22% .



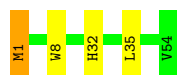
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain 1:  87% 13%




- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain 3:  93% 6% .



- Molecule 5: Antenna pigment protein beta chain

Chain B:  82% 8% 10%




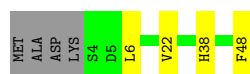
- Molecule 5: Antenna pigment protein beta chain

Chain E:  71% 16% 12%




- Molecule 5: Antenna pigment protein beta chain

Chain G:  84% 8% 8%



- Molecule 5: Antenna pigment protein beta chain

Chain J:  76% 12% 12%




- Molecule 5: Antenna pigment protein beta chain

Chain N:  73% 14% 12%




- Molecule 5: Antenna pigment protein beta chain

Chain P:  76% 12% 12%




- Molecule 5: Antenna pigment protein beta chain

Chain R:  78% 10% 12%



- Molecule 5: Antenna pigment protein beta chain

Chain T:  76% 12% 12%




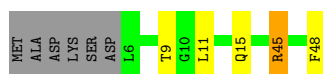
- Molecule 5: Antenna pigment protein beta chain

Chain W:  61% 27% 12%




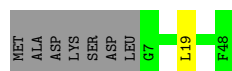
- Molecule 5: Antenna pigment protein beta chain

Chain Z:  78% 8% 12%



- Molecule 5: Antenna pigment protein beta chain

Chain 2:  84% 14%



- Molecule 5: Antenna pigment protein beta chain

Chain 4:  73% 14% 12%



- Molecule 5: Antenna pigment protein beta chain

Chain 6:  73% 12% 14%




- Molecule 5: Antenna pigment protein beta chain

Chain 8:  61% 16% 22%




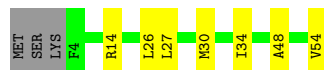
- Molecule 6: Light-harvesting protein B-875 alpha chain

Chain 5:  78% 20%



- Molecule 6: Light-harvesting protein B-875 alpha chain

Chain 7:  81% 13% 6%

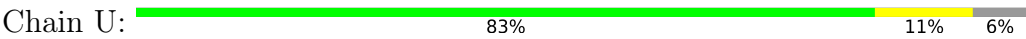


- Molecule 7: PufX

Chain X:  54% 11% 35%



- Molecule 8: protein-U



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	160448	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (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: LMT, LDA, U10, BPH, PGV, BCL, FME, CDL, SPO, FE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	L	0.34	0/2321	0.44	0/3177
2	M	0.33	0/2530	0.44	0/3455
3	H	0.30	0/1914	0.48	0/2607
4	1	0.31	0/461	0.41	0/625
4	3	0.29	0/461	0.42	0/625
4	A	0.31	0/389	0.41	0/528
4	D	0.31	0/459	0.42	0/622
4	F	0.32	0/461	0.42	0/625
4	I	0.32	0/461	0.42	0/625
4	K	0.32	0/461	0.43	0/625
4	O	0.32	0/457	0.43	0/621
4	Q	0.32	0/461	0.44	0/625
4	S	0.32	0/461	0.42	0/625
4	V	0.32	0/461	0.43	0/625
4	Y	0.33	0/461	0.43	0/625
5	2	0.28	0/356	0.40	0/488
5	4	0.28	0/364	0.42	0/499
5	6	0.25	0/344	0.37	0/472
5	8	0.25	0/308	0.33	0/424
5	B	0.28	0/372	0.38	0/510
5	E	0.32	0/364	0.40	0/499
5	G	0.30	0/378	0.41	0/518
5	J	0.28	0/364	0.40	0/499
5	N	0.28	0/364	0.38	0/499
5	P	0.29	0/364	0.40	0/499
5	R	0.30	0/360	0.43	0/494
5	T	0.28	0/364	0.40	0/499
5	W	0.29	0/360	0.38	0/494
5	Z	0.29	0/364	0.38	0/499
6	5	0.28	0/461	0.42	0/625
6	7	0.25	0/427	0.43	0/582
7	X	0.27	0/417	0.45	0/566

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	U	0.28	0/381	0.40	0/516
All	All	0.31	0/18931	0.43	0/25817

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	L	2233	0	2189	49	0
2	M	2437	0	2355	55	0
3	H	1864	0	1862	22	0
4	1	457	0	476	7	0
4	3	457	0	476	4	0
4	A	386	0	400	15	0
4	D	455	0	469	11	0
4	F	457	0	476	7	0
4	I	457	0	476	11	0
4	K	457	0	476	9	0
4	O	453	0	465	15	0
4	Q	457	0	476	16	0
4	S	454	0	469	12	0
4	V	457	0	476	16	0
4	Y	457	0	476	14	0
5	2	343	0	325	1	0
5	4	351	0	336	6	0
5	6	332	0	314	6	0
5	8	296	0	273	7	0
5	B	359	0	340	4	0
5	E	351	0	336	9	0
5	G	365	0	345	4	0
5	J	351	0	336	10	0
5	N	351	0	336	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	351	0	336	6	0
5	R	347	0	332	5	0
5	T	351	0	336	6	0
5	W	347	0	332	11	0
5	Z	351	0	336	4	0
6	5	447	0	465	12	0
6	7	415	0	422	5	0
7	X	405	0	412	6	0
8	U	369	0	366	6	0
9	1	66	0	74	6	0
9	2	66	0	74	5	0
9	3	66	0	74	4	0
9	4	66	0	74	5	0
9	5	66	0	74	6	0
9	6	66	0	74	5	0
9	7	66	0	74	6	0
9	8	60	0	58	7	0
9	A	61	0	61	2	0
9	B	66	0	74	9	0
9	D	66	0	74	6	0
9	E	66	0	74	8	0
9	F	66	0	74	4	0
9	G	66	0	74	4	0
9	I	66	0	74	9	0
9	J	66	0	74	4	0
9	K	66	0	74	7	0
9	L	198	0	222	16	0
9	M	66	0	74	3	0
9	N	66	0	74	2	0
9	O	66	0	74	6	0
9	P	66	0	74	4	0
9	Q	66	0	74	1	0
9	R	66	0	74	4	0
9	S	66	0	74	6	0
9	T	66	0	74	5	0
9	V	66	0	74	9	0
9	W	66	0	74	8	0
9	Y	66	0	74	7	0
9	Z	66	0	74	4	0
10	L	65	0	76	5	0
10	M	65	0	76	6	0
11	L	70	0	86	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	M	48	0	63	1	0
12	3	51	0	76	1	0
12	H	121	0	149	6	0
12	K	41	0	60	3	0
12	L	117	0	147	8	0
12	M	85	0	110	6	0
12	Q	39	0	48	1	0
12	X	39	0	48	3	0
12	Y	43	0	54	7	0
13	L	32	0	62	2	0
13	M	16	0	31	0	0
13	X	29	0	53	2	0
13	Y	12	0	20	5	0
14	M	1	0	0	0	0
15	1	126	0	180	13	0
15	3	42	0	60	2	0
15	5	84	0	120	10	0
15	8	42	0	60	5	0
15	D	42	0	60	4	0
15	E	42	0	60	3	0
15	F	84	0	120	7	0
15	G	84	0	120	16	0
15	K	42	0	60	7	0
15	M	42	0	60	4	0
15	N	42	0	60	8	0
15	O	84	0	120	13	0
15	P	42	0	60	2	0
15	R	42	0	60	5	0
15	S	84	0	120	11	0
15	T	42	0	60	10	0
15	V	84	0	120	9	0
15	W	42	0	60	4	0
15	X	42	0	60	5	0
16	1	24	0	21	0	0
16	3	35	0	46	3	0
16	4	27	0	27	0	0
16	5	33	0	39	2	0
16	A	97	0	119	7	0
16	D	27	0	27	0	0
16	F	43	0	40	0	0
16	H	65	0	79	5	0
16	I	27	0	27	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	K	35	0	46	2	0
16	M	95	0	121	6	0
16	Q	43	0	55	4	0
16	S	55	0	68	2	0
16	U	67	0	83	2	0
16	X	31	0	35	0	0
17	H	98	0	92	6	0
17	M	79	0	105	6	0
17	Y	48	0	46	2	0
All	All	23458	0	24489	507	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 11.

The worst 5 of 507 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)
15:1:105:SPO:H6	9:5:102:BCL:HMB2	1.59	0.83
1:L:231:ARG:HH12	2:M:8:THR:HG22	1.49	0.77
15:5:103:SPO:H6	9:7:101:BCL:HMB2	1.67	0.77
16:H:302:LMT:H5'	4:O:38:THR:HG22	1.65	0.76
2:M:75:TRP:HE1	15:M:807:SPO:HM12	1.50	0.76

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	L	279/282 (99%)	267 (96%)	12 (4%)	0	100	100
2	M	304/308 (99%)	293 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	244/260 (94%)	231 (95%)	13 (5%)	0	100	100
4	1	52/54 (96%)	48 (92%)	4 (8%)	0	100	100
4	3	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	A	43/54 (80%)	43 (100%)	0	0	100	100
4	D	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	F	52/54 (96%)	52 (100%)	0	0	100	100
4	I	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
4	K	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	O	52/54 (96%)	52 (100%)	0	0	100	100
4	Q	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	S	52/54 (96%)	52 (100%)	0	0	100	100
4	V	52/54 (96%)	47 (90%)	5 (10%)	0	100	100
4	Y	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
5	2	40/49 (82%)	39 (98%)	1 (2%)	0	100	100
5	4	41/49 (84%)	39 (95%)	2 (5%)	0	100	100
5	6	40/49 (82%)	39 (98%)	1 (2%)	0	100	100
5	8	36/49 (74%)	36 (100%)	0	0	100	100
5	B	42/49 (86%)	42 (100%)	0	0	100	100
5	E	41/49 (84%)	41 (100%)	0	0	100	100
5	G	43/49 (88%)	42 (98%)	1 (2%)	0	100	100
5	J	41/49 (84%)	41 (100%)	0	0	100	100
5	N	41/49 (84%)	41 (100%)	0	0	100	100
5	P	41/49 (84%)	37 (90%)	4 (10%)	0	100	100
5	R	41/49 (84%)	41 (100%)	0	0	100	100
5	T	41/49 (84%)	41 (100%)	0	0	100	100
5	W	41/49 (84%)	41 (100%)	0	0	100	100
5	Z	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
6	5	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
6	7	49/54 (91%)	49 (100%)	0	0	100	100
7	X	51/82 (62%)	48 (94%)	3 (6%)	0	100	100
8	U	48/53 (91%)	47 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2211/2427 (91%)	2144 (97%)	67 (3%)	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	L	220/221 (100%)	215 (98%)	5 (2%)	45	69
2	M	239/241 (99%)	230 (96%)	9 (4%)	28	52
3	H	197/208 (95%)	194 (98%)	3 (2%)	60	78
4	1	48/48 (100%)	48 (100%)	0	100	100
4	3	48/48 (100%)	48 (100%)	0	100	100
4	A	41/48 (85%)	41 (100%)	0	100	100
4	D	47/48 (98%)	47 (100%)	0	100	100
4	F	48/48 (100%)	48 (100%)	0	100	100
4	I	48/48 (100%)	48 (100%)	0	100	100
4	K	48/48 (100%)	47 (98%)	1 (2%)	48	71
4	O	47/48 (98%)	46 (98%)	1 (2%)	48	71
4	Q	48/48 (100%)	48 (100%)	0	100	100
4	S	48/48 (100%)	48 (100%)	0	100	100
4	V	48/48 (100%)	48 (100%)	0	100	100
4	Y	48/48 (100%)	47 (98%)	1 (2%)	48	71
5	2	34/40 (85%)	34 (100%)	0	100	100
5	4	35/40 (88%)	35 (100%)	0	100	100
5	6	32/40 (80%)	32 (100%)	0	100	100
5	8	26/40 (65%)	26 (100%)	0	100	100
5	B	36/40 (90%)	36 (100%)	0	100	100
5	E	35/40 (88%)	34 (97%)	1 (3%)	37	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	G	37/40 (92%)	36 (97%)	1 (3%)	40	64
5	J	35/40 (88%)	35 (100%)	0	100	100
5	N	35/40 (88%)	35 (100%)	0	100	100
5	P	35/40 (88%)	34 (97%)	1 (3%)	37	62
5	R	34/40 (85%)	34 (100%)	0	100	100
5	T	35/40 (88%)	35 (100%)	0	100	100
5	W	34/40 (85%)	32 (94%)	2 (6%)	16	36
5	Z	35/40 (88%)	34 (97%)	1 (3%)	37	62
6	5	48/49 (98%)	48 (100%)	0	100	100
6	7	43/49 (88%)	43 (100%)	0	100	100
7	X	40/66 (61%)	39 (98%)	1 (2%)	42	66
8	U	34/37 (92%)	34 (100%)	0	100	100
All	All	1866/2007 (93%)	1839 (99%)	27 (1%)	62	79

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	83	ARG
5	E	18	GLU
4	Y	33	LEU
3	H	231	ASP
5	G	6	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	M	301	HIS
5	G	17	GLN
7	X	66	ASN
8	U	51	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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
4	FME	S	1	4	5,6,10	0.79	0	3,6,11	0.67	0
4	FME	1	1	4	8,9,10	0.51	0	7,9,11	0.99	1 (14%)
4	FME	V	1	4	8,9,10	0.52	0	7,9,11	1.03	1 (14%)
4	FME	Y	1	4	8,9,10	0.50	0	7,9,11	0.98	1 (14%)
4	FME	A	1	4	8,9,10	0.50	0	7,9,11	0.88	1 (14%)
4	FME	D	1	4	8,9,10	0.49	0	7,9,11	1.05	1 (14%)
4	FME	K	1	4	8,9,10	0.50	0	7,9,11	0.98	1 (14%)
4	FME	O	1	4	8,9,10	0.51	0	7,9,11	1.04	1 (14%)
4	FME	Q	1	4	8,9,10	0.51	0	7,9,11	0.97	1 (14%)
4	FME	F	1	4	8,9,10	0.53	0	7,9,11	0.91	1 (14%)
4	FME	I	1	4	8,9,10	0.51	0	7,9,11	0.96	1 (14%)
4	FME	3	1	4	8,9,10	0.49	0	7,9,11	0.95	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
4	FME	S	1	4	-	1/2/5/11	-
4	FME	1	1	4	-	0/7/9/11	-
4	FME	V	1	4	-	1/7/9/11	-
4	FME	Y	1	4	-	1/7/9/11	-
4	FME	A	1	4	-	3/7/9/11	-
4	FME	D	1	4	-	0/7/9/11	-
4	FME	K	1	4	-	1/7/9/11	-
4	FME	O	1	4	-	1/7/9/11	-
4	FME	Q	1	4	-	0/7/9/11	-
4	FME	F	1	4	-	1/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FME	I	1	4	-	1/7/9/11	-
4	FME	3	1	4	-	0/7/9/11	-

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	1	FME	O-C-CA	-2.53	118.14	124.78
4	D	1	FME	O-C-CA	-2.53	118.14	124.78
4	I	1	FME	O-C-CA	-2.49	118.26	124.78
4	Y	1	FME	O-C-CA	-2.48	118.28	124.78
4	1	1	FME	O-C-CA	-2.47	118.31	124.78

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1	FME	O1-CN-N-CA
4	A	1	FME	N-CA-CB-CG
4	F	1	FME	O1-CN-N-CA
4	K	1	FME	O1-CN-N-CA
4	O	1	FME	O1-CN-N-CA

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	O	1	FME	1	0
4	F	1	FME	1	0
4	3	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 112 ligands modelled in this entry, 1 is monoatomic - leaving 111 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$
9	BCL	R	102	-	64,74,74	1.69	14 (21%)	78,115,115	2.23	22 (28%)
9	BCL	L	308	-	64,74,74	1.69	13 (20%)	78,115,115	2.32	22 (28%)
13	LDA	Y	101	-	8,11,15	2.55	1 (12%)	10,13,17	0.45	0
16	LMT	3	101	-	36,36,36	0.42	0	47,47,47	0.91	3 (6%)
15	SPO	F	104	-	40,41,41	0.64	0	47,50,50	1.86	13 (27%)
15	SPO	G	102	-	40,41,41	0.64	0	47,50,50	1.80	12 (25%)
16	LMT	A	702	-	36,36,36	0.39	0	47,47,47	0.74	1 (2%)
17	CDL	H	305	-	35,35,99	1.38	3 (8%)	42,44,111	1.31	6 (14%)
15	SPO	W	102	-	40,41,41	0.67	0	47,50,50	1.72	14 (29%)
17	CDL	H	304	-	60,60,99	1.18	4 (6%)	66,72,111	1.17	4 (6%)
9	BCL	2	101	-	64,74,74	1.70	14 (21%)	78,115,115	2.26	19 (24%)
12	PGV	L	305	-	38,38,50	1.05	2 (5%)	41,44,56	1.07	3 (7%)
16	LMT	I	102	-	28,28,36	0.43	0	39,39,47	0.71	1 (2%)
9	BCL	S	102	-	64,74,74	1.68	13 (20%)	78,115,115	2.45	22 (28%)
9	BCL	K	102	-	64,74,74	1.70	12 (18%)	78,115,115	2.25	18 (23%)
9	BCL	O	101	-	64,74,74	1.66	12 (18%)	78,115,115	2.27	17 (21%)
12	PGV	H	306	-	39,39,50	1.07	2 (5%)	42,45,56	1.22	3 (7%)
15	SPO	3	104	-	40,41,41	0.64	0	47,50,50	2.02	16 (34%)
16	LMT	M	809	-	36,36,36	0.37	0	47,47,47	0.69	1 (2%)
15	SPO	S	104	-	40,41,41	0.66	0	47,50,50	1.66	16 (34%)
9	BCL	B	101	-	64,74,74	1.71	14 (21%)	78,115,115	2.16	21 (26%)
9	BCL	F	102	-	64,74,74	1.68	13 (20%)	78,115,115	2.27	22 (28%)
15	SPO	N	101	-	40,41,41	0.65	0	47,50,50	2.11	16 (34%)
12	PGV	Y	104	-	42,42,50	0.98	2 (4%)	44,48,56	1.09	3 (6%)
9	BCL	T	101	-	64,74,74	1.71	14 (21%)	78,115,115	2.19	18 (23%)
15	SPO	E	101	-	40,41,41	0.63	0	47,50,50	1.71	12 (25%)
15	SPO	R	101	-	40,41,41	0.68	0	47,50,50	2.32	15 (31%)
9	BCL	8	102	-	58,68,74	1.86	14 (24%)	70,107,115	2.31	18 (25%)
16	LMT	4	102	-	28,28,36	0.46	0	39,39,47	0.77	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BCL	G	101	-	64,74,74	1.71	14 (21%)	78,115,115	2.13	19 (24%)
15	SPO	O	102	-	40,41,41	0.66	0	47,50,50	1.82	12 (25%)
15	SPO	X	102	-	40,41,41	0.66	0	47,50,50	1.81	11 (23%)
15	SPO	5	103	-	40,41,41	0.66	0	47,50,50	1.97	15 (31%)
15	SPO	8	101	-	40,41,41	0.65	0	47,50,50	2.13	13 (27%)
16	LMT	Q	102	-	19,19,36	0.49	0	24,24,47	0.55	0
11	U10	L	304	-	35,35,63	0.77	2 (5%)	42,45,79	0.67	0
15	SPO	O	103	-	40,41,41	0.67	0	47,50,50	1.83	14 (29%)
9	BCL	I	101	-	64,74,74	1.68	13 (20%)	78,115,115	2.34	21 (26%)
10	BPH	L	302	-	51,70,70	0.60	2 (3%)	52,101,101	0.69	1 (1%)
15	SPO	G	103	-	40,41,41	0.64	0	47,50,50	2.14	14 (29%)
16	LMT	M	808	-	27,27,36	0.46	0	32,33,47	0.64	1 (3%)
12	PGV	L	306	-	32,32,50	1.10	2 (6%)	35,38,56	1.18	3 (8%)
12	PGV	H	307	-	46,46,50	0.95	2 (4%)	49,52,56	1.02	3 (6%)
9	BCL	1	101	-	64,74,74	1.68	13 (20%)	78,115,115	2.44	24 (30%)
15	SPO	V	102	-	40,41,41	0.65	0	47,50,50	1.71	12 (25%)
16	LMT	S	105	-	31,31,36	0.45	0	42,42,47	0.67	0
11	U10	L	303	-	35,35,63	0.81	2 (5%)	42,45,79	0.67	0
16	LMT	U	101	-	33,33,36	0.38	0	44,44,47	0.78	1 (2%)
17	CDL	Y	102	-	47,47,99	1.16	3 (6%)	52,58,111	1.07	3 (5%)
12	PGV	3	102	-	50,50,50	0.90	2 (4%)	53,56,56	1.05	3 (5%)
9	BCL	Y	103	-	64,74,74	1.66	13 (20%)	78,115,115	2.31	21 (26%)
15	SPO	V	103	-	40,41,41	0.68	0	47,50,50	1.82	14 (29%)
9	BCL	Q	104	-	64,74,74	1.66	12 (18%)	78,115,115	2.29	21 (26%)
13	LDA	M	802	-	12,15,15	2.08	1 (8%)	14,17,17	0.57	0
12	PGV	Q	103	-	38,38,50	1.05	2 (5%)	41,44,56	1.04	2 (4%)
9	BCL	6	101	-	64,74,74	1.73	14 (21%)	78,115,115	2.13	19 (24%)
9	BCL	P	102	-	64,74,74	1.67	14 (21%)	78,115,115	2.25	20 (25%)
12	PGV	H	303	-	33,33,50	1.14	2 (6%)	36,38,56	1.15	4 (11%)
15	SPO	1	105	-	40,41,41	0.66	0	47,50,50	1.77	13 (27%)
9	BCL	E	102	-	64,74,74	1.72	15 (23%)	78,115,115	2.21	25 (32%)
15	SPO	F	103	-	40,41,41	0.64	0	47,50,50	1.66	12 (25%)
15	SPO	D	102	-	40,41,41	0.65	0	47,50,50	1.84	15 (31%)
15	SPO	P	101	-	40,41,41	0.64	0	47,50,50	1.76	12 (25%)
9	BCL	Z	101	-	64,74,74	1.70	14 (21%)	78,115,115	2.23	21 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BCL	4	101	-	64,74,74	1.73	14 (21%)	78,115,115	2.22	20 (25%)
15	SPO	5	104	-	40,41,41	0.63	0	47,50,50	1.93	11 (23%)
17	CDL	M	811	-	78,78,99	1.03	4 (5%)	84,90,111	1.20	6 (7%)
9	BCL	L	301	-	64,74,74	1.70	14 (21%)	78,115,115	2.31	24 (30%)
15	SPO	K	103	-	40,41,41	0.66	0	47,50,50	1.81	10 (21%)
9	BCL	D	101	-	64,74,74	1.68	14 (21%)	78,115,115	2.34	23 (29%)
16	LMT	H	302	-	31,31,36	0.45	0	42,42,47	1.09	3 (7%)
16	LMT	1	104	-	24,25,36	0.61	1 (4%)	31,34,47	0.82	1 (3%)
15	SPO	M	807	-	40,41,41	0.63	0	47,50,50	1.67	10 (21%)
9	BCL	A	703	-	59,69,74	1.76	13 (22%)	72,109,115	2.31	21 (29%)
9	BCL	5	102	-	64,74,74	1.69	12 (18%)	78,115,115	2.29	20 (25%)
16	LMT	D	103	-	28,28,36	0.43	0	39,39,47	0.67	1 (2%)
16	LMT	K	101	-	36,36,36	0.41	0	47,47,47	0.96	2 (4%)
12	PGV	L	310	-	44,44,50	1.00	2 (4%)	48,49,56	1.13	4 (8%)
12	PGV	M	801	-	46,46,50	0.94	2 (4%)	49,52,56	1.17	4 (8%)
16	LMT	U	102	-	36,36,36	0.35	0	47,47,47	0.73	1 (2%)
9	BCL	L	309	-	64,74,74	1.72	14 (21%)	78,115,115	2.18	21 (26%)
9	BCL	J	101	-	64,74,74	1.73	14 (21%)	78,115,115	2.24	20 (25%)
16	LMT	5	101	-	34,34,36	0.39	0	45,45,47	0.73	0
16	LMT	Q	101	-	24,24,36	0.44	0	29,29,47	0.97	1 (3%)
13	LDA	L	311	-	12,15,15	2.09	1 (8%)	14,17,17	0.53	0
16	LMT	F	101	-	27,27,36	0.48	0	38,38,47	0.88	2 (5%)
15	SPO	S	103	-	40,41,41	0.67	0	47,50,50	1.98	15 (31%)
9	BCL	M	803	-	64,74,74	1.72	15 (23%)	78,115,115	2.36	21 (26%)
13	LDA	X	104	-	12,15,15	2.13	1 (8%)	14,17,17	0.50	0
9	BCL	N	102	-	64,74,74	1.70	15 (23%)	78,115,115	2.27	19 (24%)
16	LMT	M	810	-	34,34,36	0.42	0	45,45,47	1.15	4 (8%)
16	LMT	S	101	-	25,25,36	0.46	0	30,30,47	0.81	0
15	SPO	T	102	-	40,41,41	0.69	0	47,50,50	1.84	13 (27%)
9	BCL	7	101	-	64,74,74	1.69	12 (18%)	78,115,115	2.29	19 (24%)
10	BPH	M	804	-	51,70,70	0.57	1 (1%)	52,101,101	0.76	1 (1%)
9	BCL	W	101	-	64,74,74	1.68	15 (23%)	78,115,115	2.24	20 (25%)
9	BCL	3	103	-	64,74,74	1.71	13 (20%)	78,115,115	2.30	19 (24%)
13	LDA	X	103	-	9,12,15	2.43	1 (11%)	11,14,17	0.49	0
12	PGV	K	104	-	38,40,50	1.02	2 (5%)	40,42,56	1.16	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	SPO	1	102	-	40,41,41	0.65	0	47,50,50	2.02	14 (29%)
12	PGV	X	101	-	38,38,50	1.04	2 (5%)	41,44,56	1.10	3 (7%)
16	LMT	H	301	-	36,36,36	0.37	0	47,47,47	0.92	2 (4%)
15	SPO	1	103	-	40,41,41	0.66	0	47,50,50	1.97	17 (36%)
13	LDA	L	307	-	12,15,15	2.08	1 (8%)	14,17,17	0.50	0
16	LMT	A	701	-	36,36,36	0.34	0	47,47,47	0.71	0
9	BCL	V	101	-	64,74,74	1.68	12 (18%)	78,115,115	2.23	19 (24%)
11	U10	M	806	-	48,48,63	0.71	2 (4%)	58,61,79	0.58	0
12	PGV	M	812	-	37,37,50	1.05	2 (5%)	40,43,56	1.18	4 (10%)
16	LMT	F	105	-	17,17,36	0.45	0	22,22,47	0.57	0
16	LMT	X	105	-	32,32,36	0.40	0	43,43,47	0.80	1 (2%)
16	LMT	A	704	-	28,28,36	0.45	0	39,39,47	0.75	1 (2%)

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
9	BCL	R	102	-	-	13/37/137/137	-
9	BCL	L	308	-	-	7/37/137/137	-
13	LDA	Y	101	-	-	1/9/9/13	-
16	LMT	3	101	-	-	7/21/61/61	0/2/2/2
15	SPO	F	104	-	-	1/47/47/47	-
15	SPO	G	102	-	-	7/47/47/47	-
16	LMT	A	702	-	-	6/21/61/61	0/2/2/2
17	CDL	H	305	-	-	8/37/37/110	-
15	SPO	W	102	-	-	10/47/47/47	-
17	CDL	H	304	-	-	23/71/71/110	-
9	BCL	2	101	-	-	15/37/137/137	-
12	PGV	L	305	-	-	13/43/43/55	-
16	LMT	I	102	-	-	3/13/53/61	0/2/2/2
9	BCL	S	102	-	-	15/37/137/137	-
9	BCL	K	102	-	-	11/37/137/137	-
9	BCL	O	101	-	-	12/37/137/137	-
12	PGV	H	306	-	-	14/44/44/55	-
15	SPO	3	104	-	-	4/47/47/47	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	LMT	M	809	-	-	8/21/61/61	0/2/2/2
15	SPO	S	104	-	-	10/47/47/47	-
9	BCL	B	101	-	-	7/37/137/137	-
9	BCL	F	102	-	-	9/37/137/137	-
15	SPO	N	101	-	-	9/47/47/47	-
12	PGV	Y	104	-	-	13/47/47/55	-
9	BCL	T	101	-	-	13/37/137/137	-
15	SPO	E	101	-	-	6/47/47/47	-
15	SPO	R	101	-	-	7/47/47/47	-
9	BCL	8	102	-	-	14/29/129/137	-
16	LMT	4	102	-	-	2/13/53/61	0/2/2/2
9	BCL	G	101	-	-	15/37/137/137	-
15	SPO	O	102	-	-	5/47/47/47	-
15	SPO	X	102	-	-	4/47/47/47	-
15	SPO	5	103	-	-	5/47/47/47	-
15	SPO	8	101	-	-	2/47/47/47	-
16	LMT	Q	102	-	-	2/11/31/61	0/1/1/2
11	U10	L	304	-	-	5/30/54/87	0/1/1/1
15	SPO	O	103	-	-	10/47/47/47	-
9	BCL	I	101	-	-	10/37/137/137	-
10	BPH	L	302	-	-	3/37/105/105	0/5/6/6
15	SPO	G	103	-	-	6/47/47/47	-
16	LMT	M	808	-	-	2/19/39/61	0/1/1/2
12	PGV	L	306	-	-	13/37/37/55	-
12	PGV	H	307	-	-	13/51/51/55	-
9	BCL	1	101	-	-	12/37/137/137	-
15	SPO	V	102	-	-	3/47/47/47	-
16	LMT	S	105	-	-	5/16/56/61	0/2/2/2
11	U10	L	303	-	-	9/30/54/87	0/1/1/1
16	LMT	U	101	-	-	1/18/58/61	0/2/2/2
17	CDL	Y	102	-	-	16/56/56/110	-
12	PGV	3	102	-	-	10/55/55/55	-
9	BCL	Y	103	-	-	15/37/137/137	-
15	SPO	V	103	-	-	5/47/47/47	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	Q	104	-	-	17/37/137/137	-
13	LDA	M	802	-	-	2/13/13/13	-
12	PGV	Q	103	-	-	9/43/43/55	-
9	BCL	6	101	-	-	16/37/137/137	-
9	BCL	P	102	-	-	15/37/137/137	-
12	PGV	H	303	-	-	3/35/35/55	-
15	SPO	1	105	-	-	6/47/47/47	-
9	BCL	E	102	-	-	13/37/137/137	-
15	SPO	F	103	-	-	4/47/47/47	-
15	SPO	D	102	-	-	2/47/47/47	-
15	SPO	P	101	-	-	8/47/47/47	-
9	BCL	Z	101	-	-	12/37/137/137	-
9	BCL	4	101	-	-	9/37/137/137	-
15	SPO	5	104	-	-	8/47/47/47	-
17	CDL	M	811	-	-	30/89/89/110	-
9	BCL	L	301	-	-	20/37/137/137	-
15	SPO	K	103	-	-	4/47/47/47	-
9	BCL	D	101	-	-	9/37/137/137	-
16	LMT	H	302	-	-	6/16/56/61	0/2/2/2
16	LMT	1	104	-	-	2/11/44/61	0/2/2/2
15	SPO	M	807	-	-	8/47/47/47	-
9	BCL	A	703	-	-	9/31/131/137	-
9	BCL	5	102	-	-	12/37/137/137	-
16	LMT	D	103	-	-	2/13/53/61	0/2/2/2
16	LMT	K	101	-	-	2/21/61/61	0/2/2/2
12	PGV	L	310	-	-	7/46/46/55	-
12	PGV	M	801	-	-	14/51/51/55	-
16	LMT	U	102	-	-	3/21/61/61	0/2/2/2
9	BCL	L	309	-	-	12/37/137/137	-
9	BCL	J	101	-	-	14/37/137/137	-
16	LMT	5	101	-	-	5/19/59/61	0/2/2/2
16	LMT	Q	101	-	-	2/15/35/61	0/1/1/2
13	LDA	L	311	-	-	2/13/13/13	-
16	LMT	F	101	-	-	5/11/51/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	SPO	S	103	-	-	6/47/47/47	-
9	BCL	M	803	-	-	10/37/137/137	-
13	LDA	X	104	-	-	0/13/13/13	-
9	BCL	N	102	-	-	14/37/137/137	-
16	LMT	M	810	-	-	7/19/59/61	0/2/2/2
16	LMT	S	101	-	-	4/17/37/61	0/1/1/2
15	SPO	T	102	-	-	7/47/47/47	-
9	BCL	7	101	-	-	15/37/137/137	-
10	BPH	M	804	-	-	6/37/105/105	0/5/6/6
9	BCL	W	101	-	-	19/37/137/137	-
9	BCL	3	103	-	-	11/37/137/137	-
13	LDA	X	103	-	-	1/10/10/13	-
12	PGV	K	104	-	-	14/40/42/55	-
15	SPO	1	102	-	-	5/47/47/47	-
12	PGV	X	101	-	-	8/43/43/55	-
16	LMT	H	301	-	-	4/21/61/61	0/2/2/2
15	SPO	1	103	-	-	4/47/47/47	-
13	LDA	L	307	-	-	4/13/13/13	-
16	LMT	A	701	-	-	5/21/61/61	0/2/2/2
9	BCL	V	101	-	-	15/37/137/137	-
11	U10	M	806	-	-	1/45/69/87	0/1/1/1
12	PGV	M	812	-	-	19/42/42/55	-
16	LMT	F	105	-	-	1/9/29/61	0/1/1/2
16	LMT	X	105	-	-	4/17/57/61	0/2/2/2
16	LMT	A	704	-	-	0/13/53/61	0/2/2/2

The worst 5 of 488 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	X	104	LDA	O1-N1	-7.33	1.25	1.42
13	X	103	LDA	O1-N1	-7.27	1.25	1.42
13	L	311	LDA	O1-N1	-7.19	1.25	1.42
13	L	307	LDA	O1-N1	-7.19	1.25	1.42
13	Y	101	LDA	O1-N1	-7.18	1.25	1.42

The worst 5 of 1108 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	S	102	BCL	CHD-C1D-ND	-8.81	116.36	124.45
9	L	301	BCL	CHD-C1D-ND	-8.81	116.36	124.45
9	1	101	BCL	CHD-C1D-ND	-8.73	116.43	124.45
9	3	103	BCL	CHD-C1D-ND	-8.63	116.53	124.45
9	8	102	BCL	CHD-C1D-ND	-8.60	116.55	124.45

There are no chirality outliers.

5 of 915 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	L	301	BCL	C2C-C3C-CAC-CBC
9	L	301	BCL	C4C-C3C-CAC-CBC
9	A	703	BCL	C2A-CAA-CBA-CGA
9	B	101	BCL	C1A-C2A-CAA-CBA
9	B	101	BCL	C3A-C2A-CAA-CBA

There are no ring outliers.

97 monomers are involved in 363 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	R	102	BCL	4	0
9	L	308	BCL	6	0
13	Y	101	LDA	5	0
16	3	101	LMT	3	0
15	F	104	SPO	3	0
15	G	102	SPO	8	0
16	A	702	LMT	6	0
15	W	102	SPO	4	0
17	H	304	CDL	6	0
9	2	101	BCL	5	0
12	L	305	PGV	4	0
9	S	102	BCL	6	0
9	K	102	BCL	7	0
9	O	101	BCL	6	0
12	H	306	PGV	3	0
15	3	104	SPO	2	0
16	M	809	LMT	2	0
15	S	104	SPO	5	0
9	B	101	BCL	9	0
9	F	102	BCL	4	0
15	N	101	SPO	8	0
12	Y	104	PGV	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	T	101	BCL	5	0
15	E	101	SPO	3	0
15	R	101	SPO	5	0
9	8	102	BCL	7	0
9	G	101	BCL	4	0
15	O	102	SPO	8	0
15	X	102	SPO	5	0
15	5	103	SPO	4	0
15	8	101	SPO	5	0
16	Q	102	LMT	1	0
11	L	304	U10	4	0
15	O	103	SPO	5	0
9	I	101	BCL	9	0
10	L	302	BPH	5	0
15	G	103	SPO	8	0
16	M	808	LMT	2	0
12	L	306	PGV	3	0
12	H	307	PGV	3	0
9	1	101	BCL	6	0
15	V	102	SPO	4	0
16	S	105	LMT	1	0
11	L	303	U10	3	0
17	Y	102	CDL	2	0
12	3	102	PGV	1	0
9	Y	103	BCL	7	0
15	V	103	SPO	5	0
9	Q	104	BCL	1	0
12	Q	103	PGV	1	0
9	6	101	BCL	5	0
9	P	102	BCL	4	0
15	1	105	SPO	6	0
9	E	102	BCL	8	0
15	F	103	SPO	5	0
15	D	102	SPO	4	0
15	P	101	SPO	2	0
9	Z	101	BCL	4	0
9	4	101	BCL	5	0
15	5	104	SPO	7	0
17	M	811	CDL	6	0
9	L	301	BCL	6	0
15	K	103	SPO	7	0
9	D	101	BCL	6	0

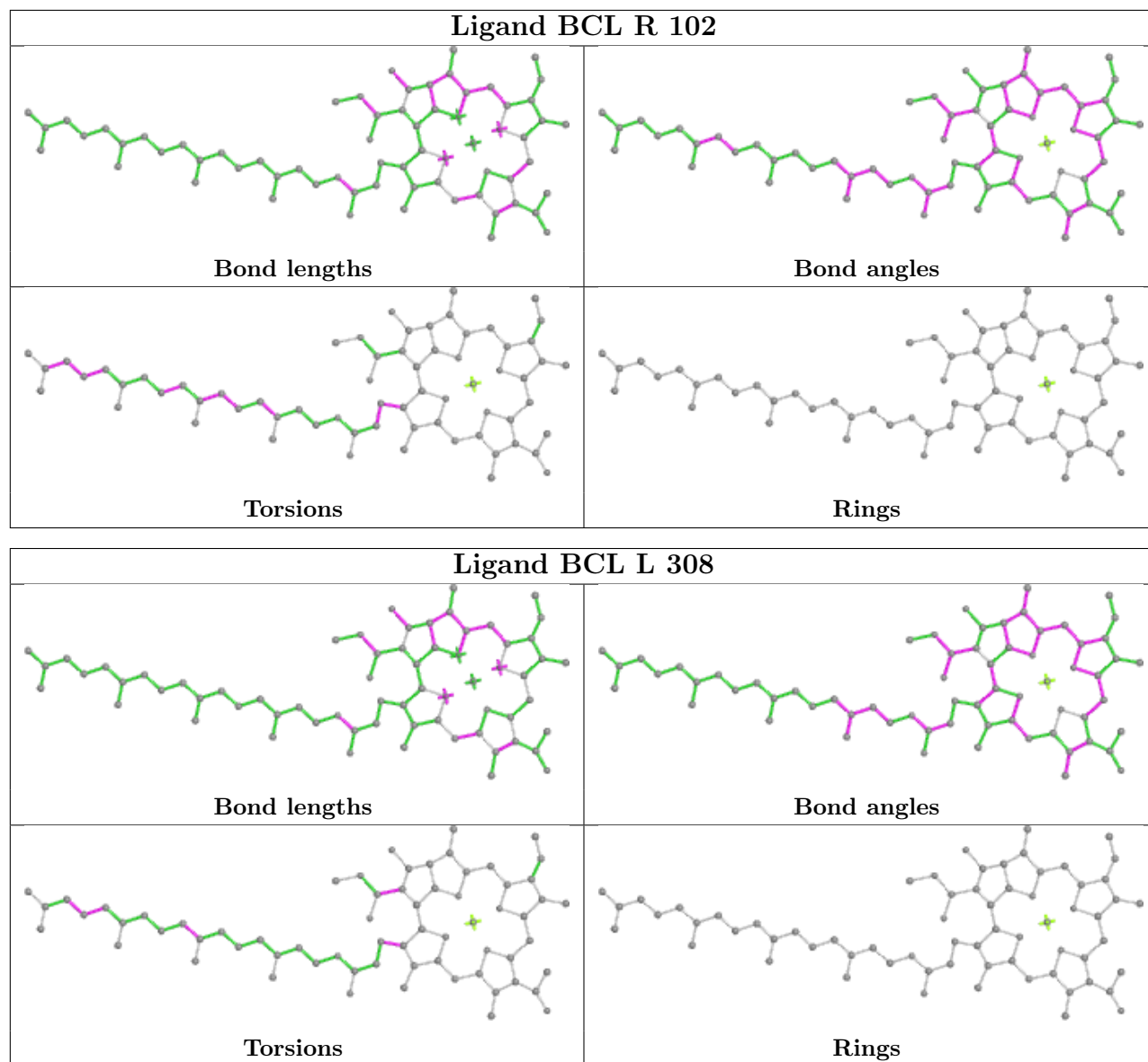
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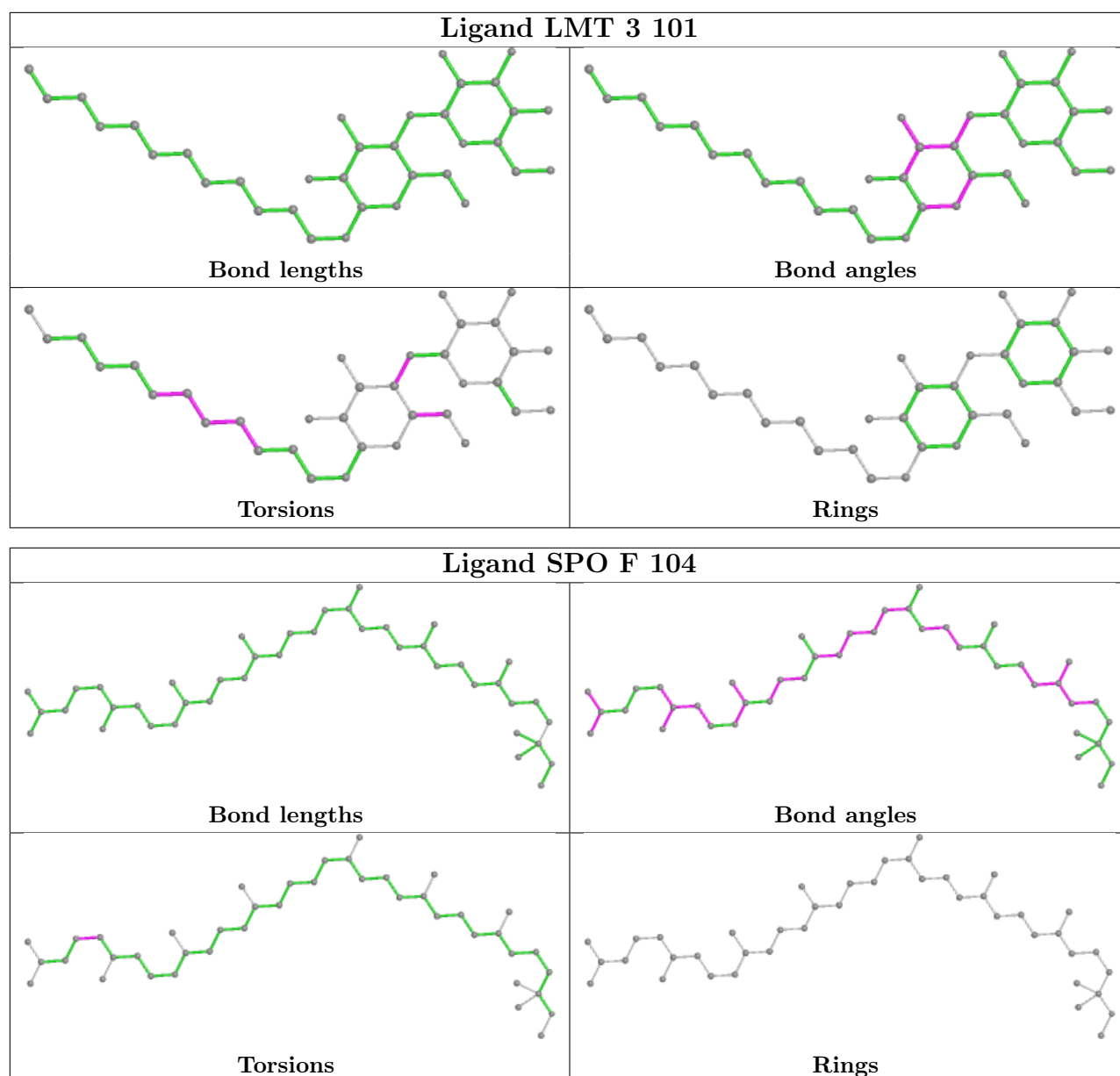
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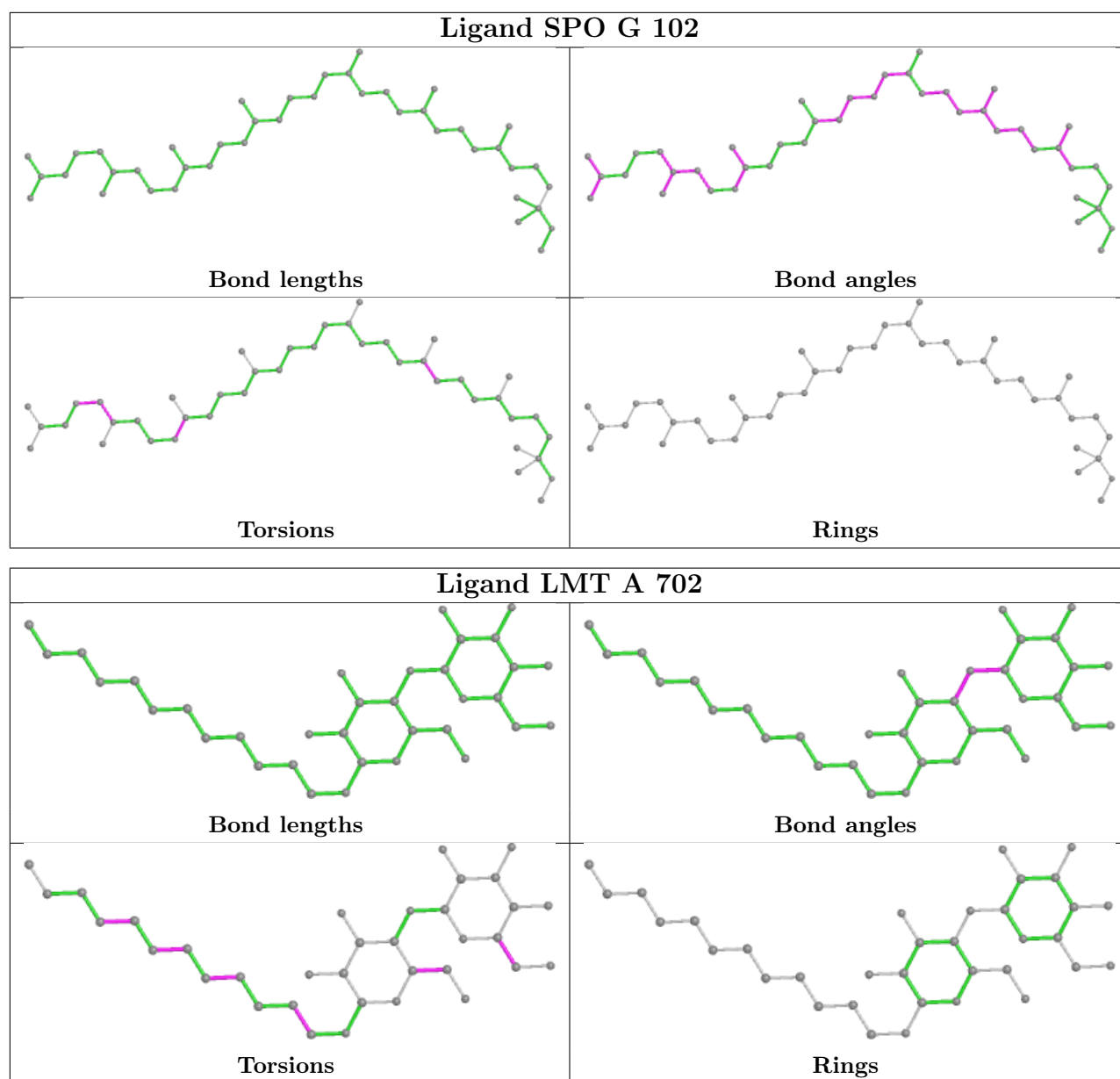
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	H	302	LMT	4	0
15	M	807	SPO	4	0
9	A	703	BCL	2	0
9	5	102	BCL	6	0
16	K	101	LMT	2	0
12	L	310	PGV	1	0
12	M	801	PGV	2	0
16	U	102	LMT	2	0
9	L	309	BCL	5	0
9	J	101	BCL	4	0
16	5	101	LMT	2	0
16	Q	101	LMT	3	0
13	L	311	LDA	2	0
15	S	103	SPO	6	0
9	M	803	BCL	3	0
9	N	102	BCL	2	0
16	M	810	LMT	2	0
16	S	101	LMT	1	0
15	T	102	SPO	10	0
9	7	101	BCL	6	0
10	M	804	BPH	6	0
9	W	101	BCL	8	0
9	3	103	BCL	4	0
13	X	103	LDA	2	0
12	K	104	PGV	3	0
15	1	102	SPO	3	0
12	X	101	PGV	3	0
16	H	301	LMT	1	0
15	1	103	SPO	4	0
16	A	701	LMT	1	0
9	V	101	BCL	9	0
11	M	806	U10	1	0
12	M	812	PGV	4	0

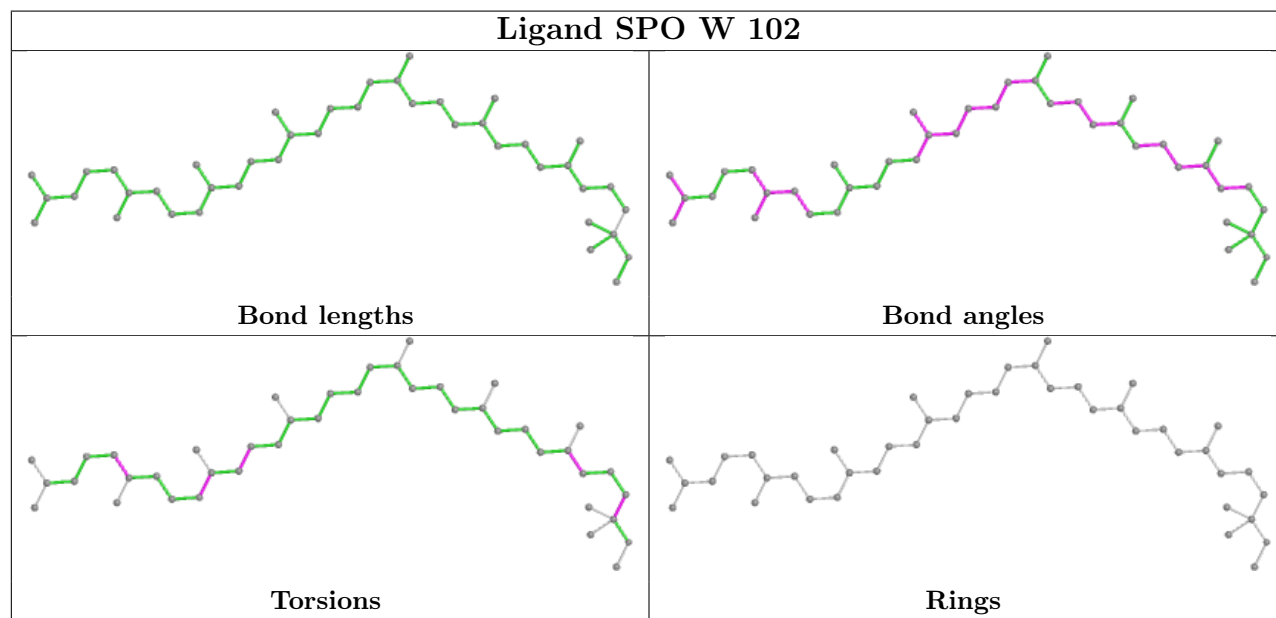
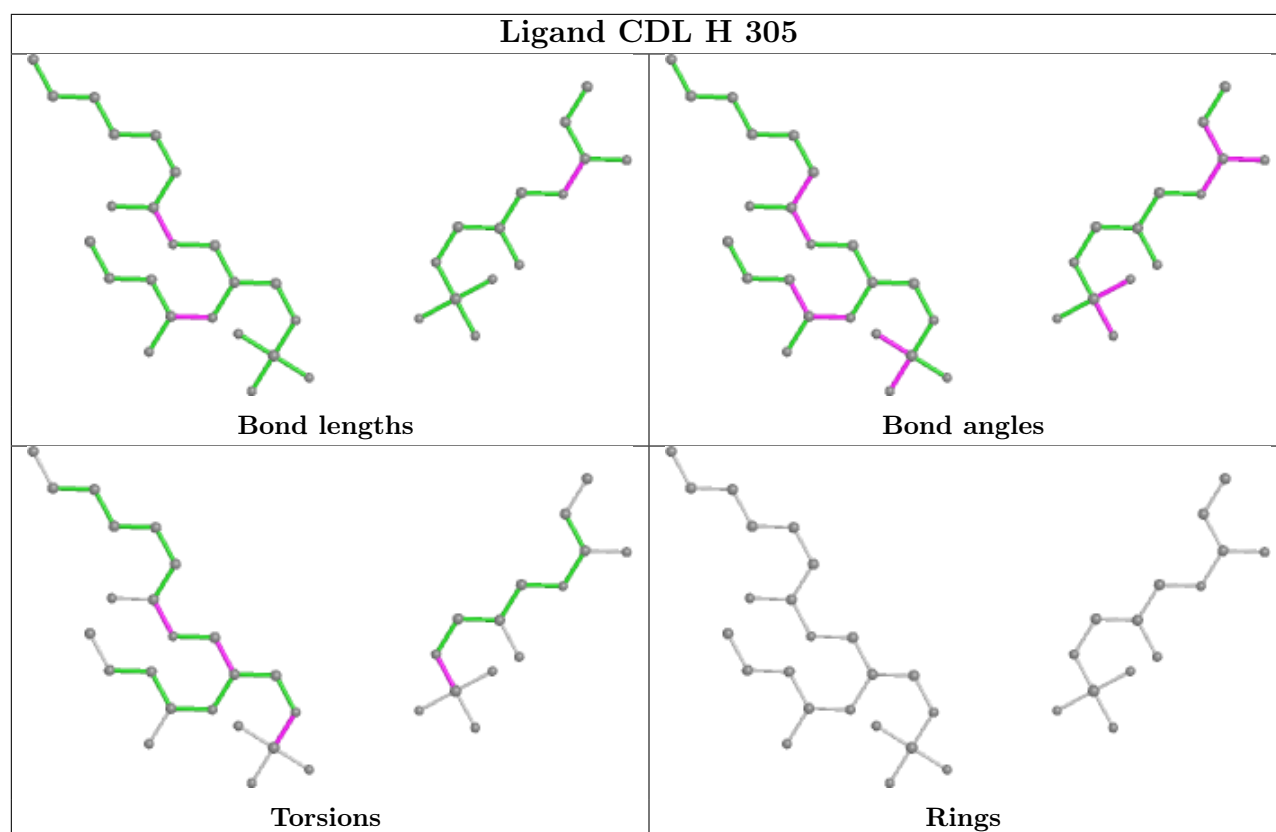
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

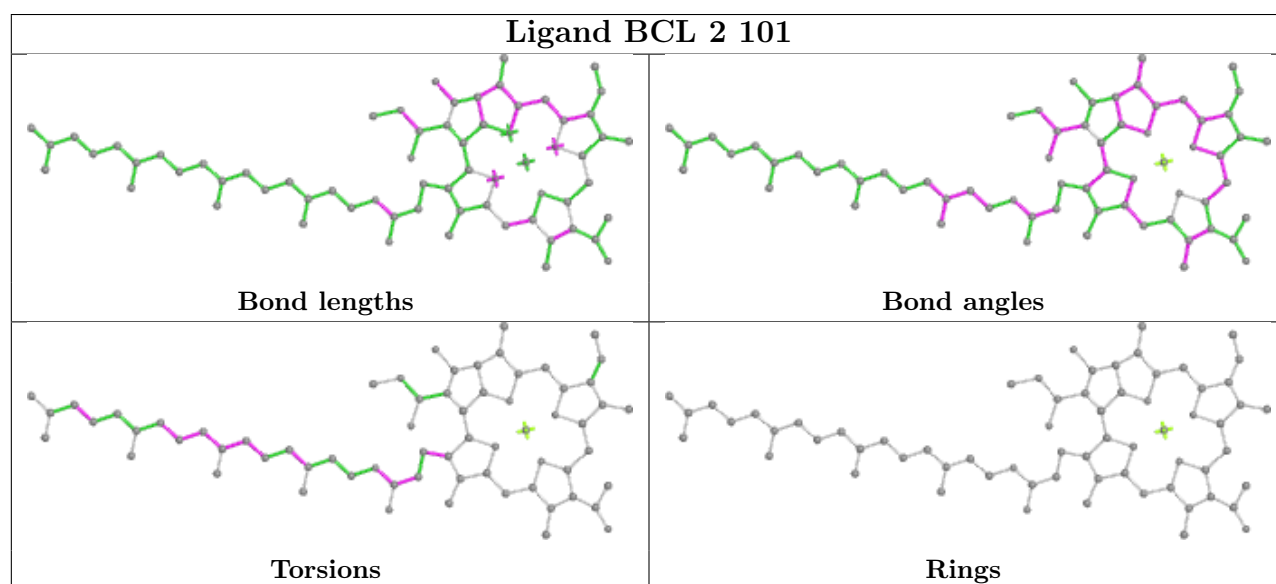
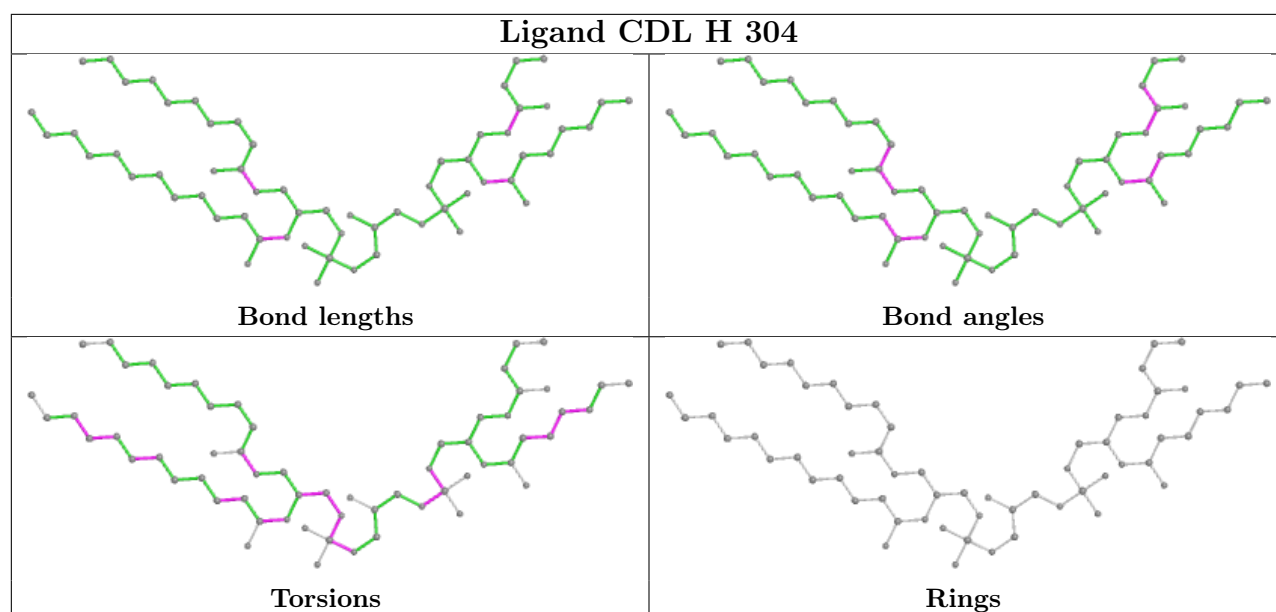
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

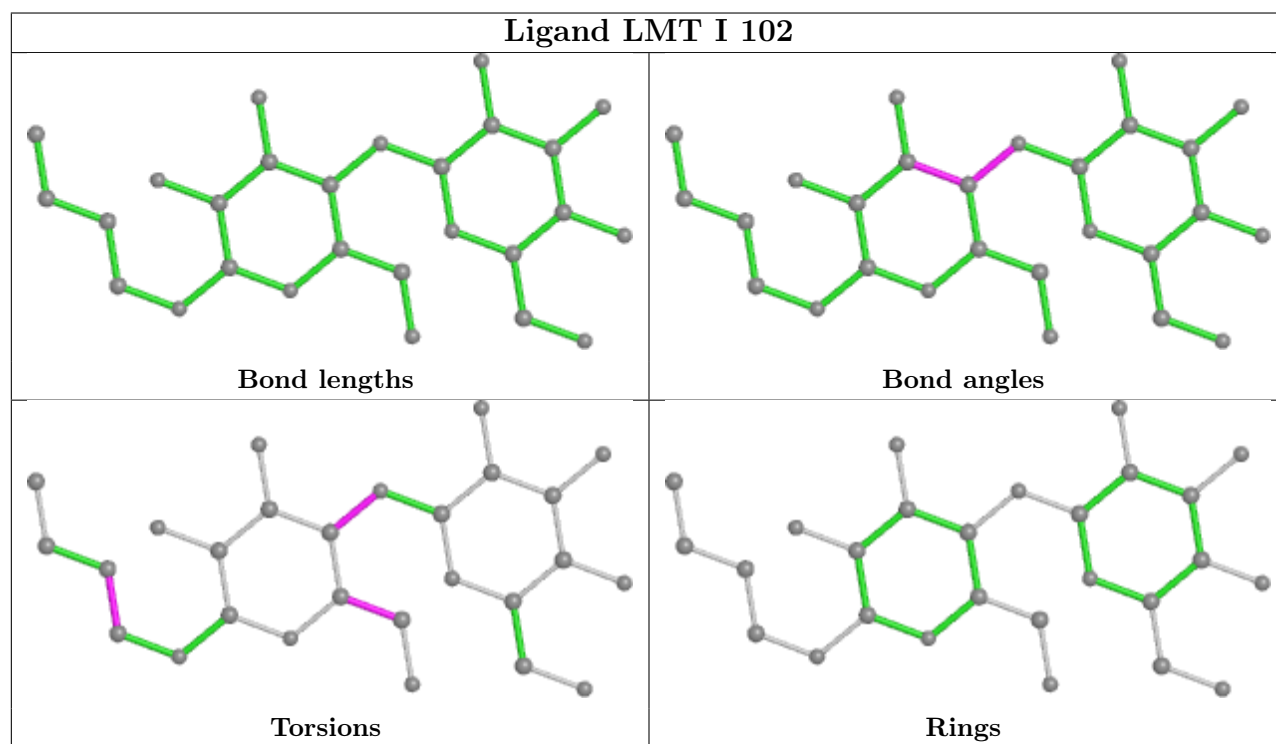
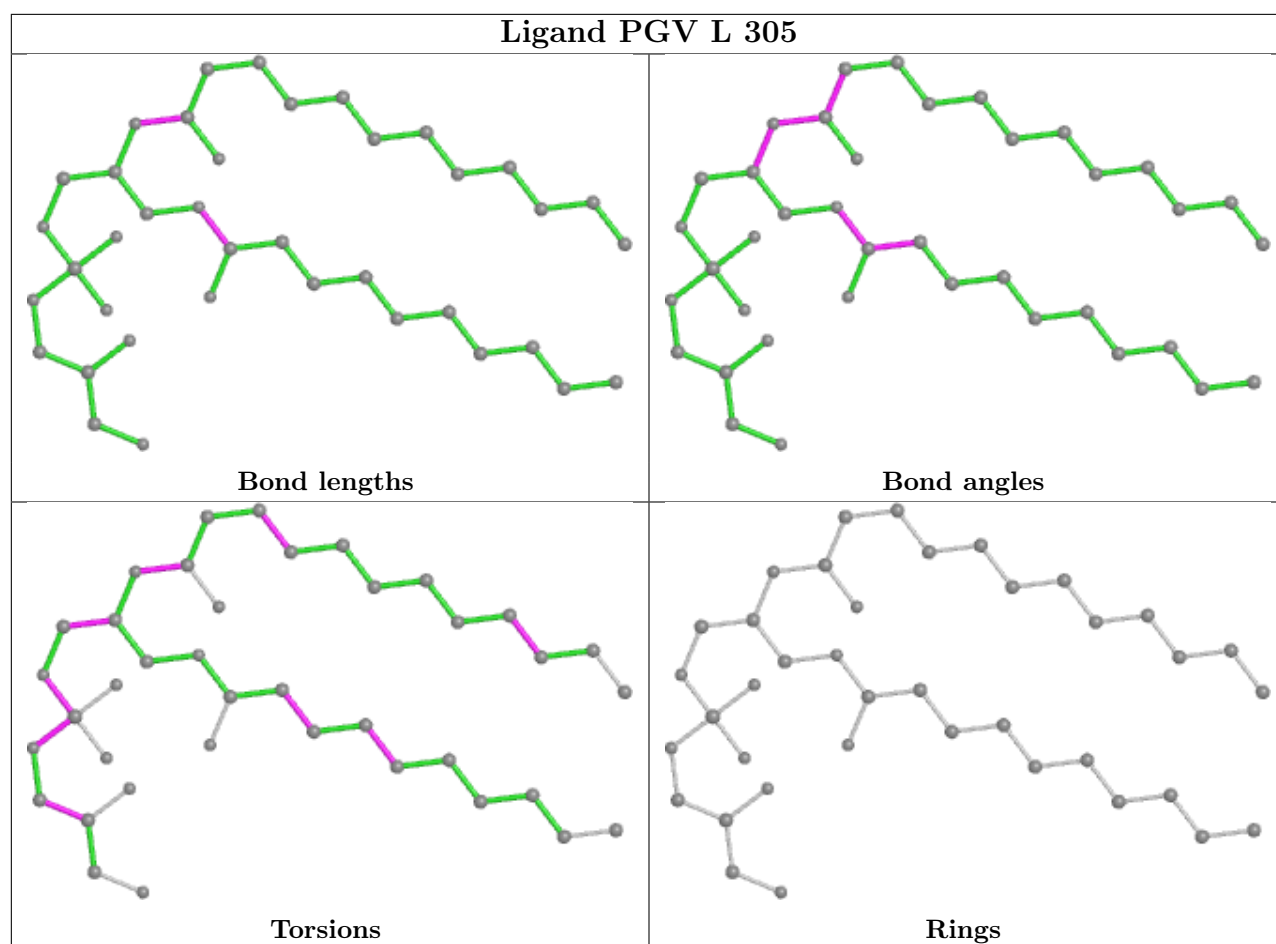


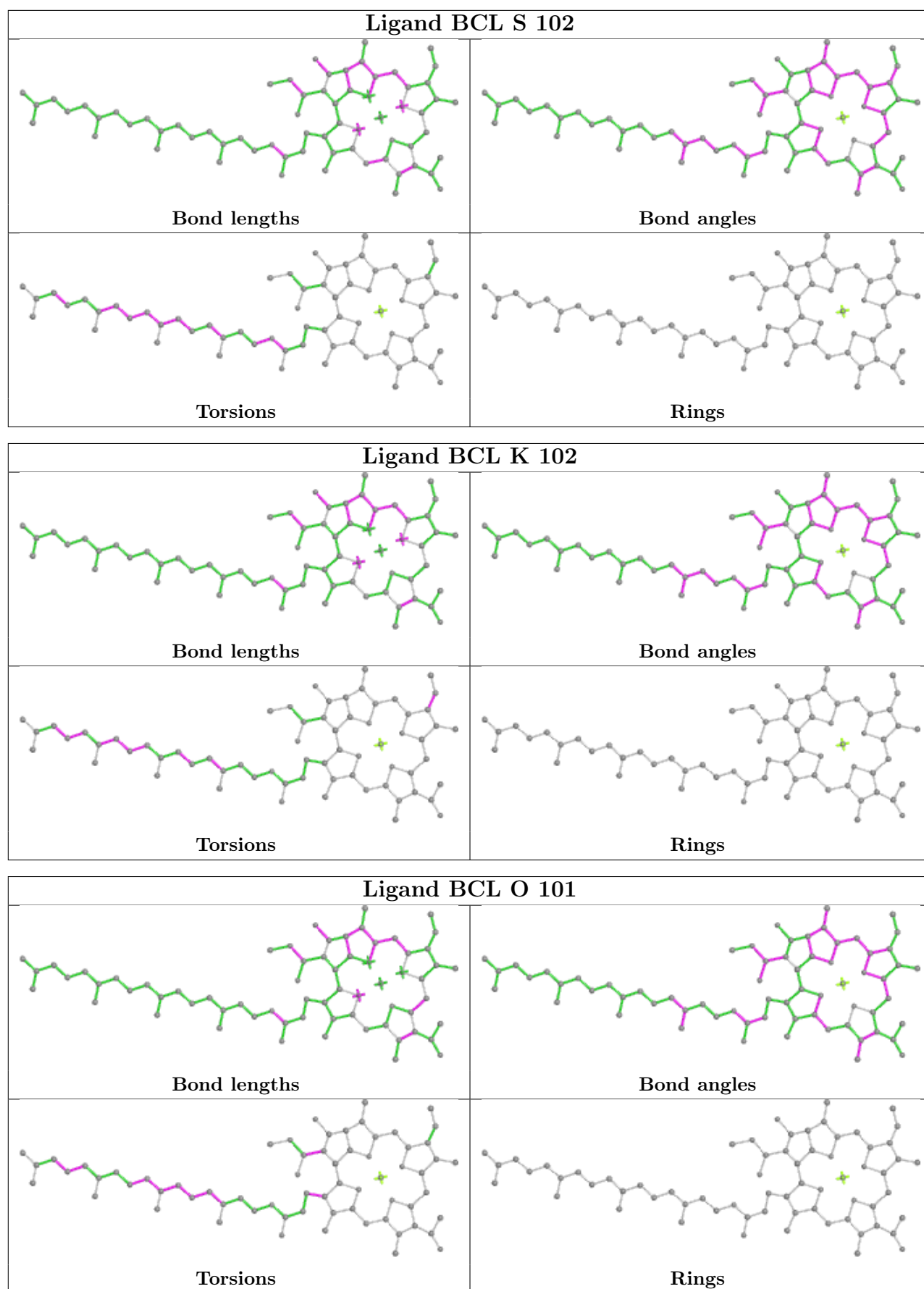


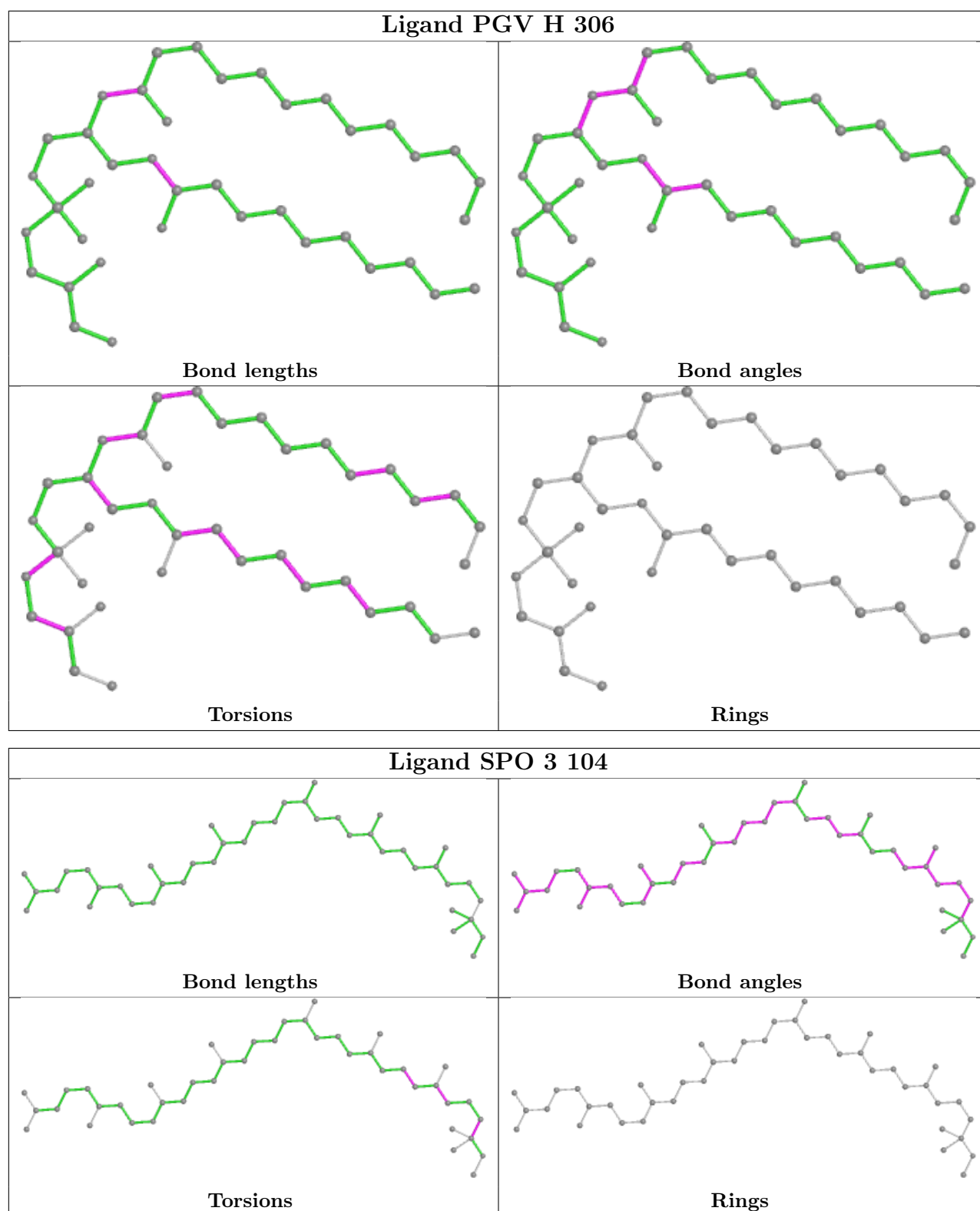


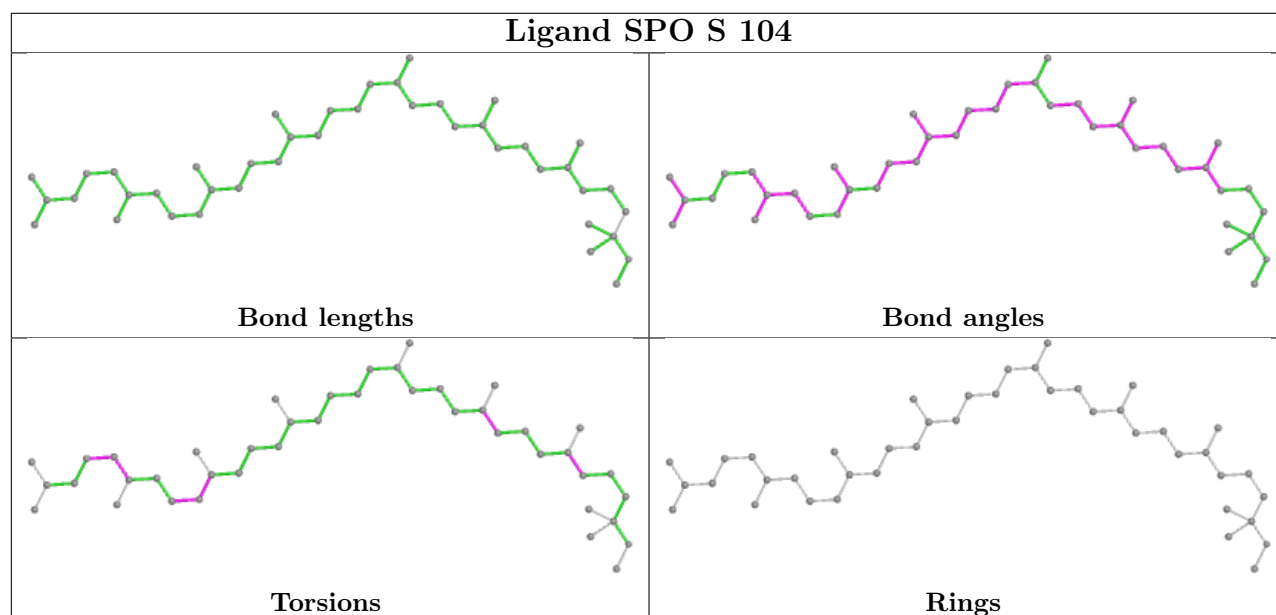
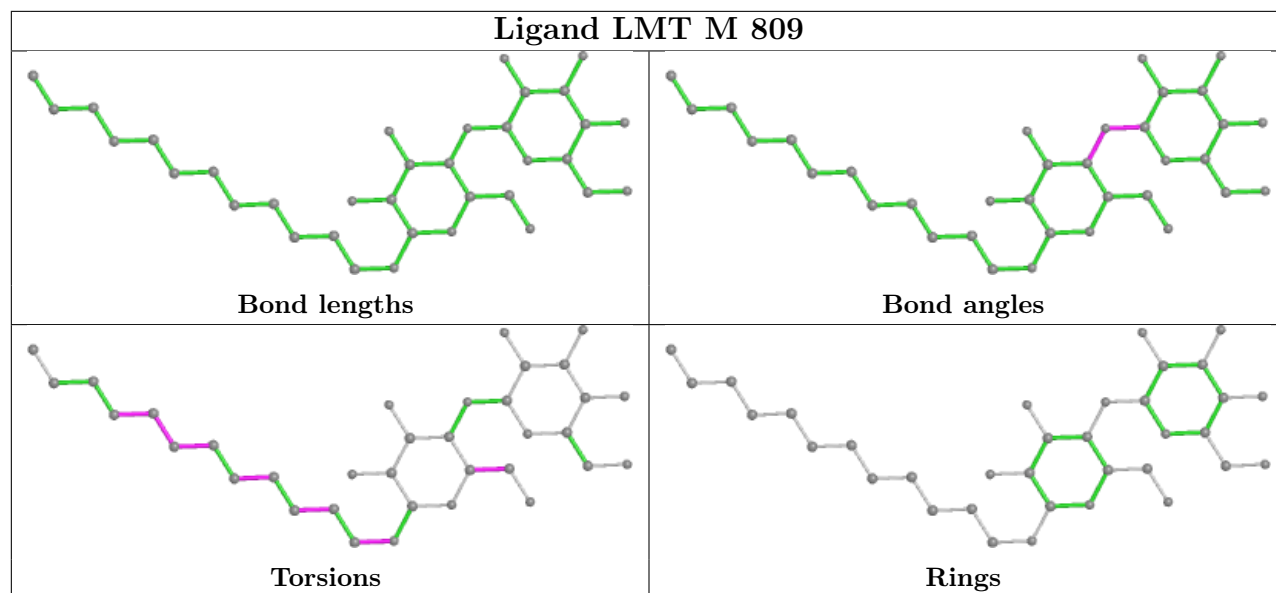


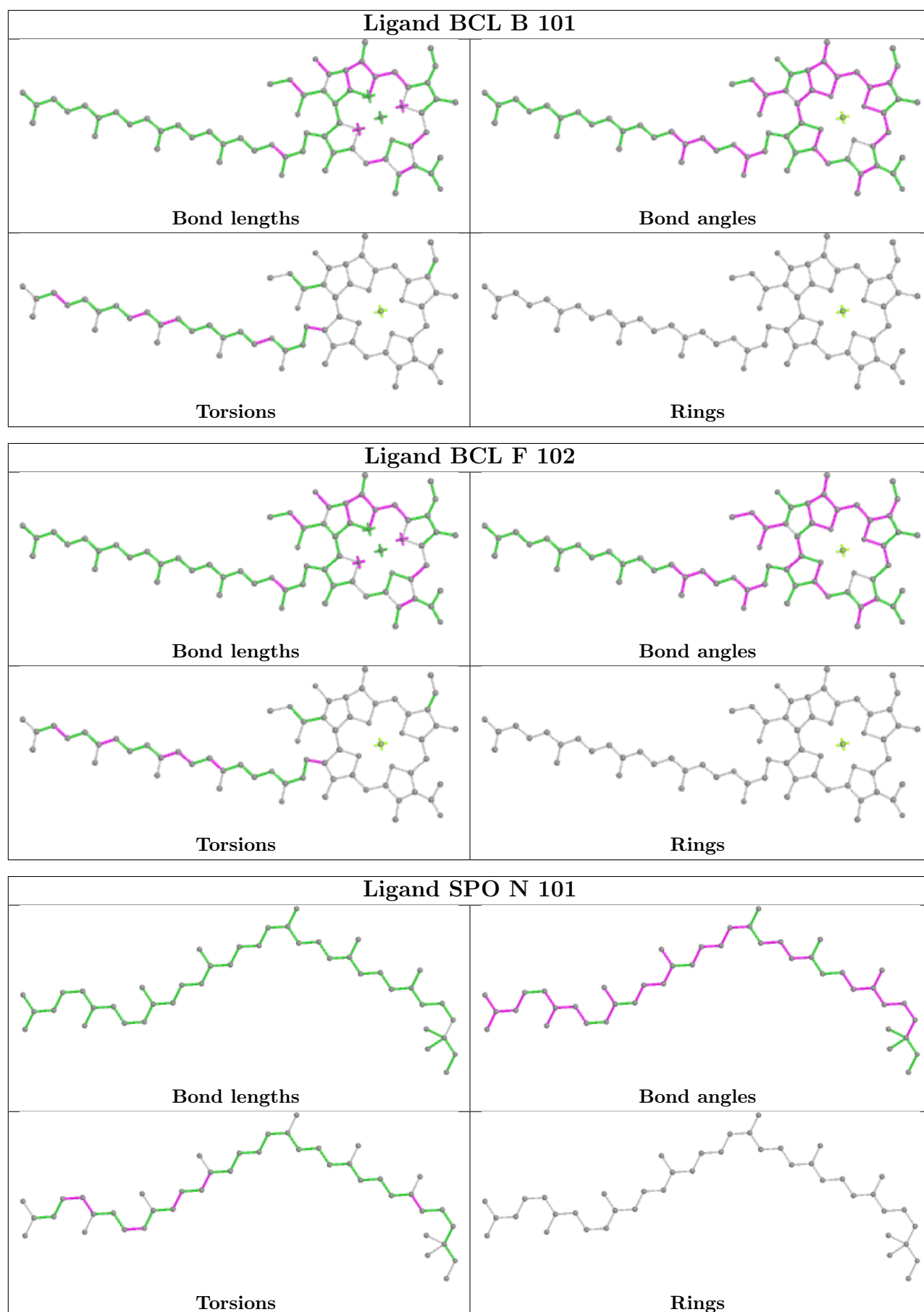


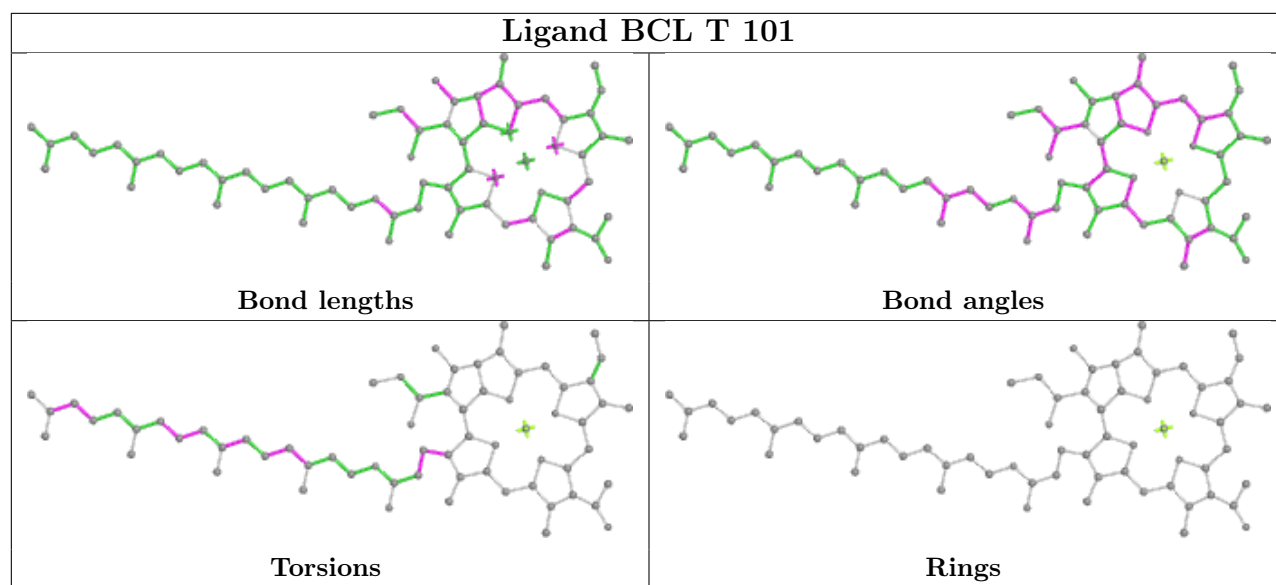
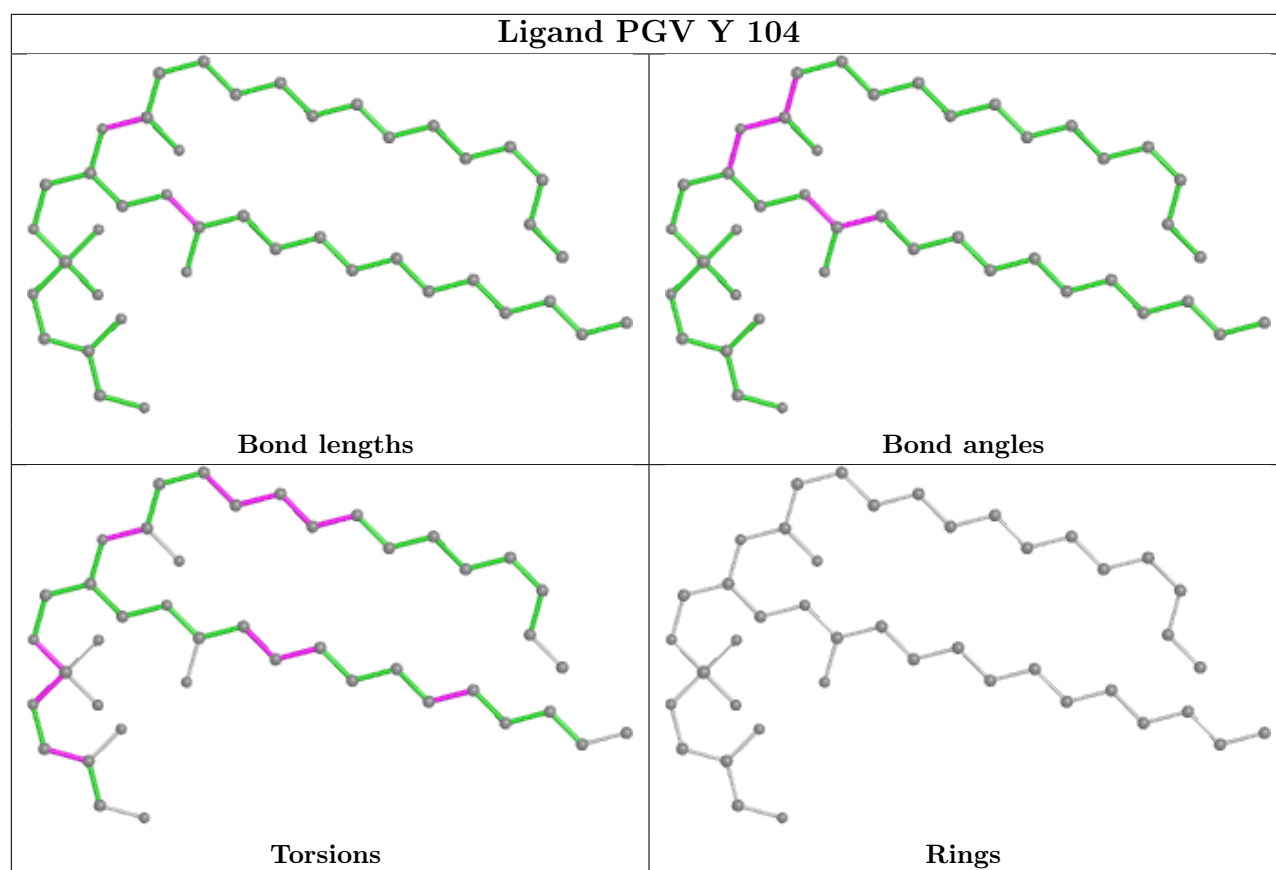


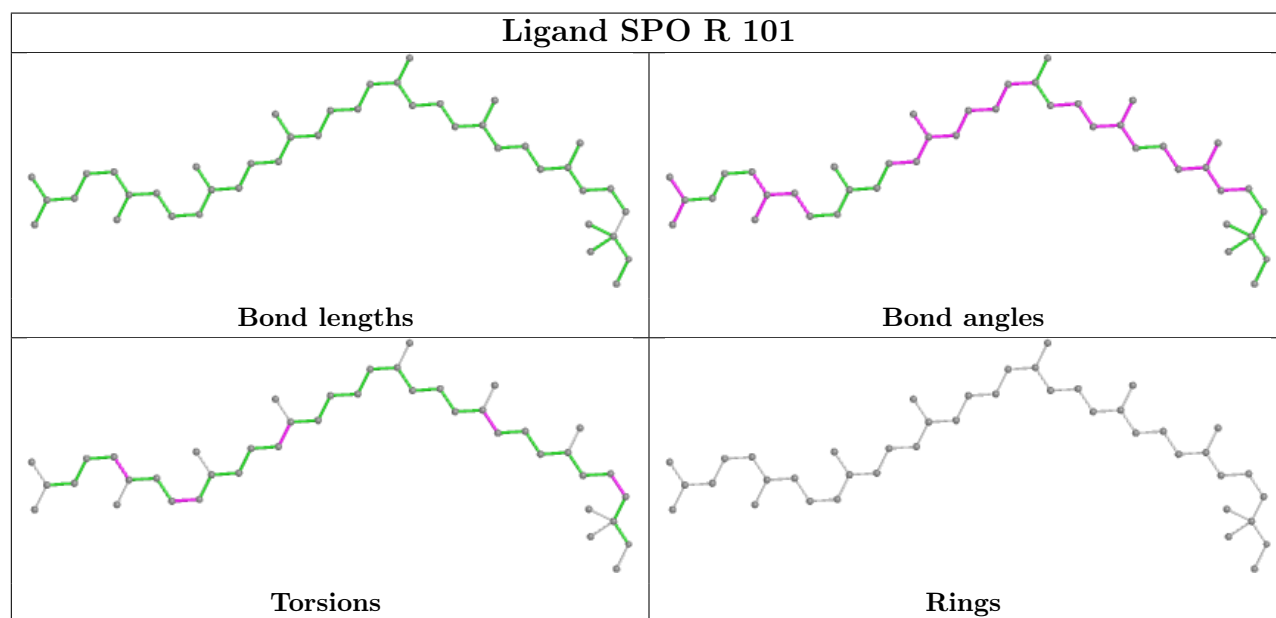
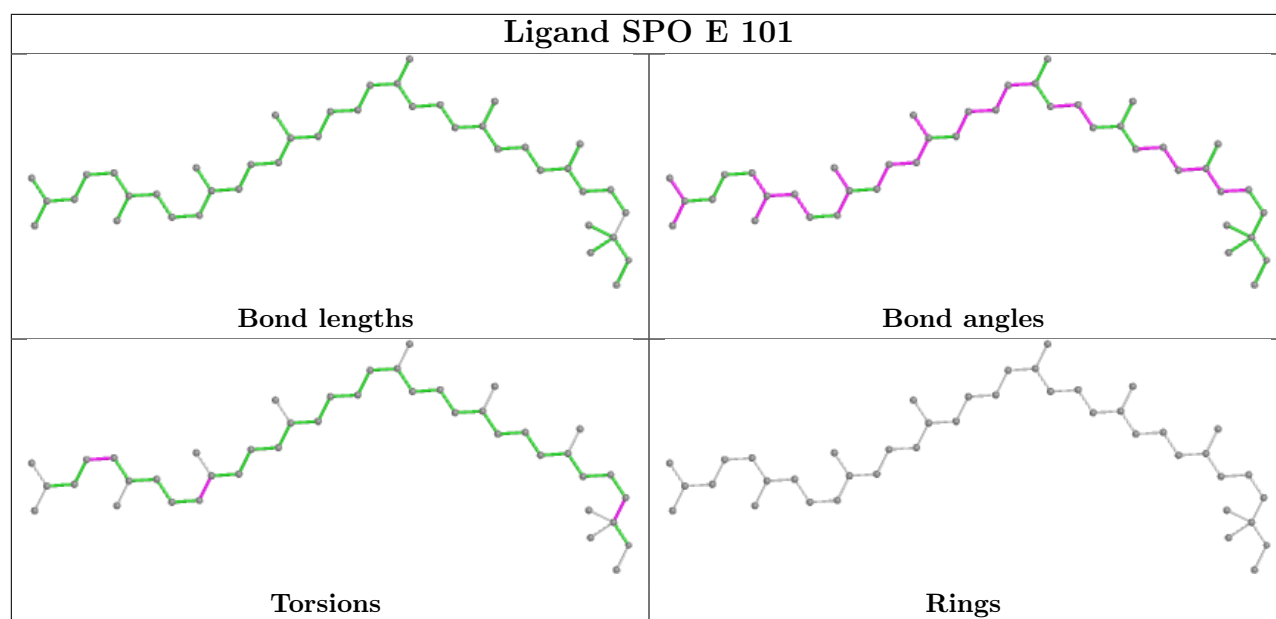


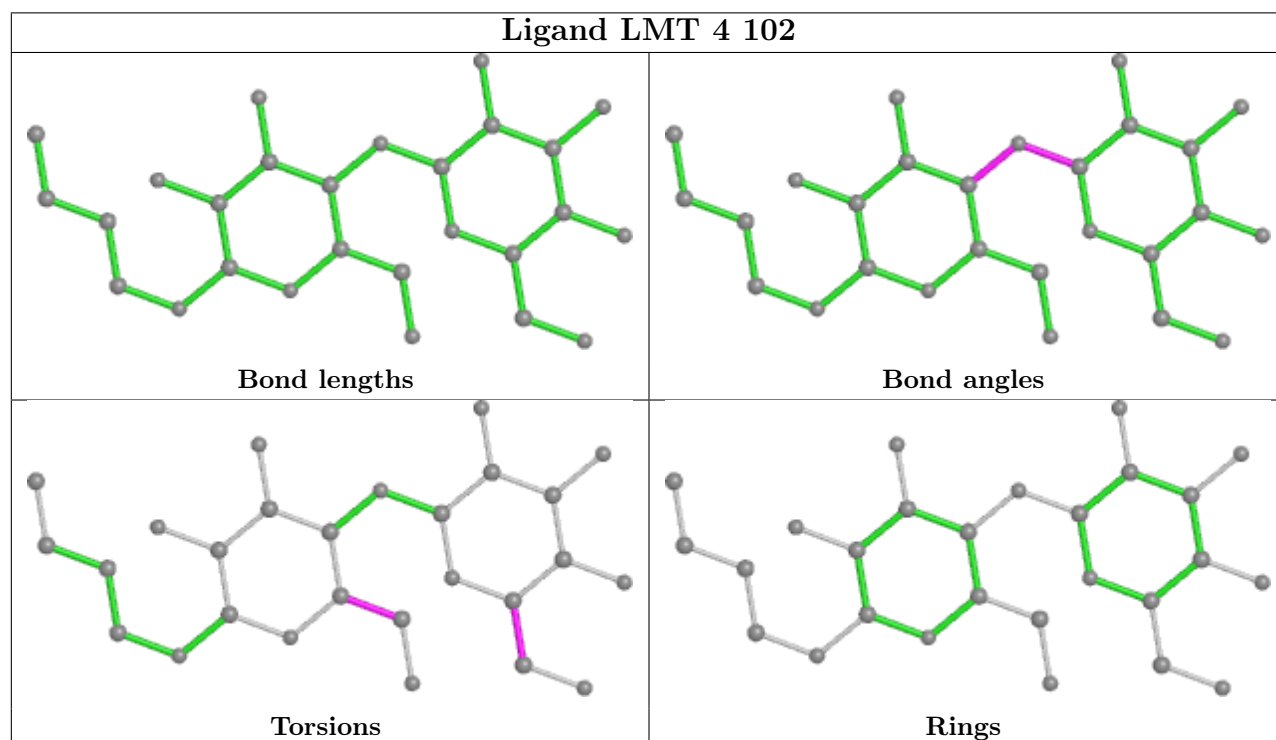
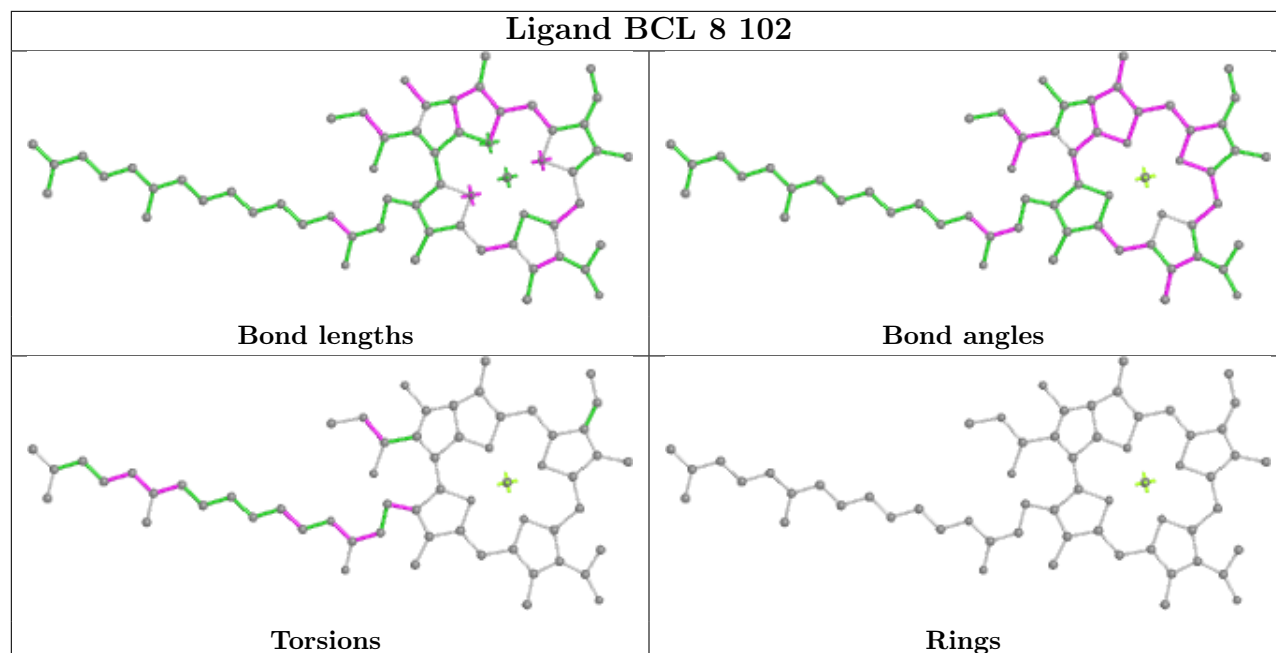


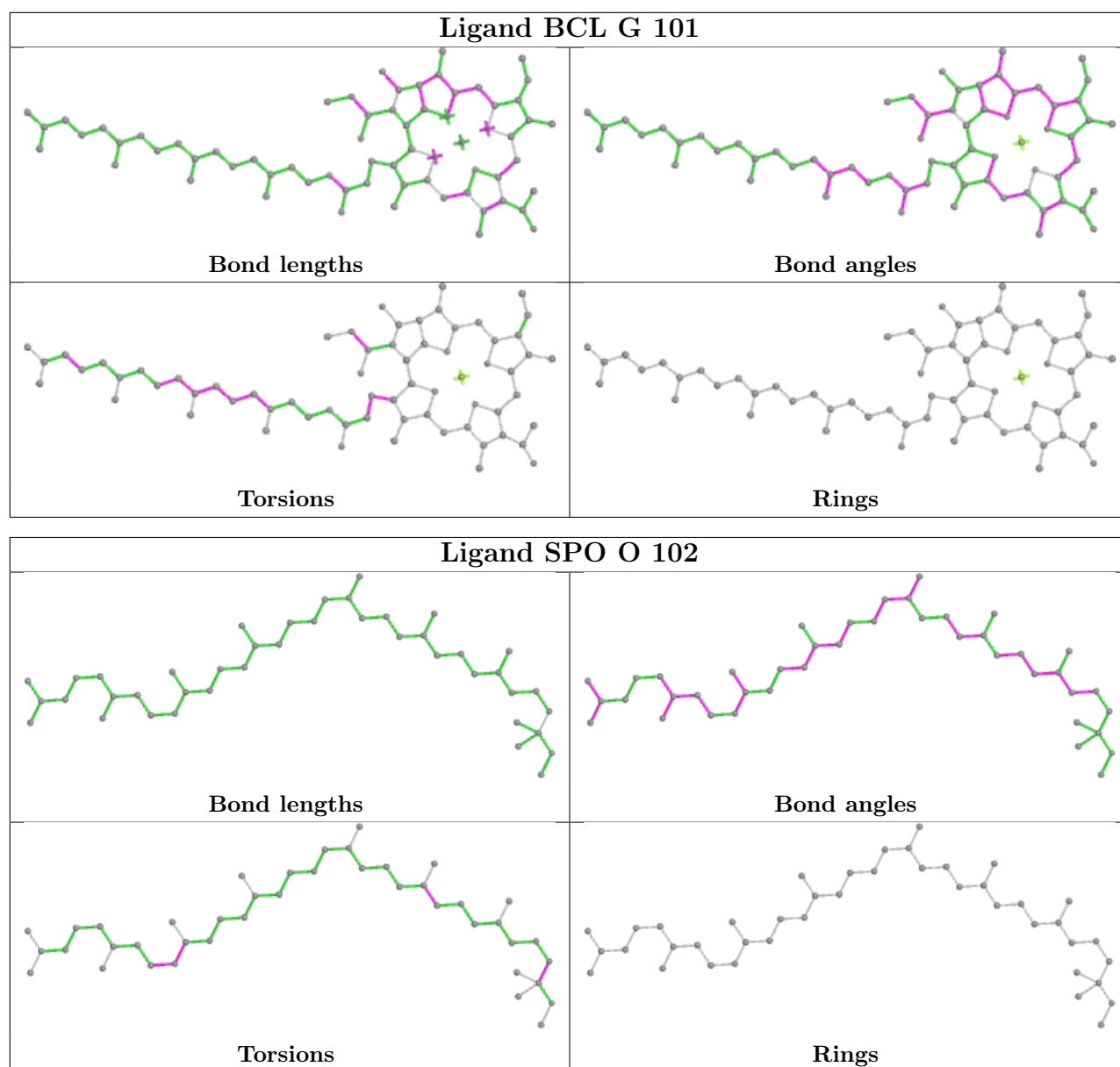


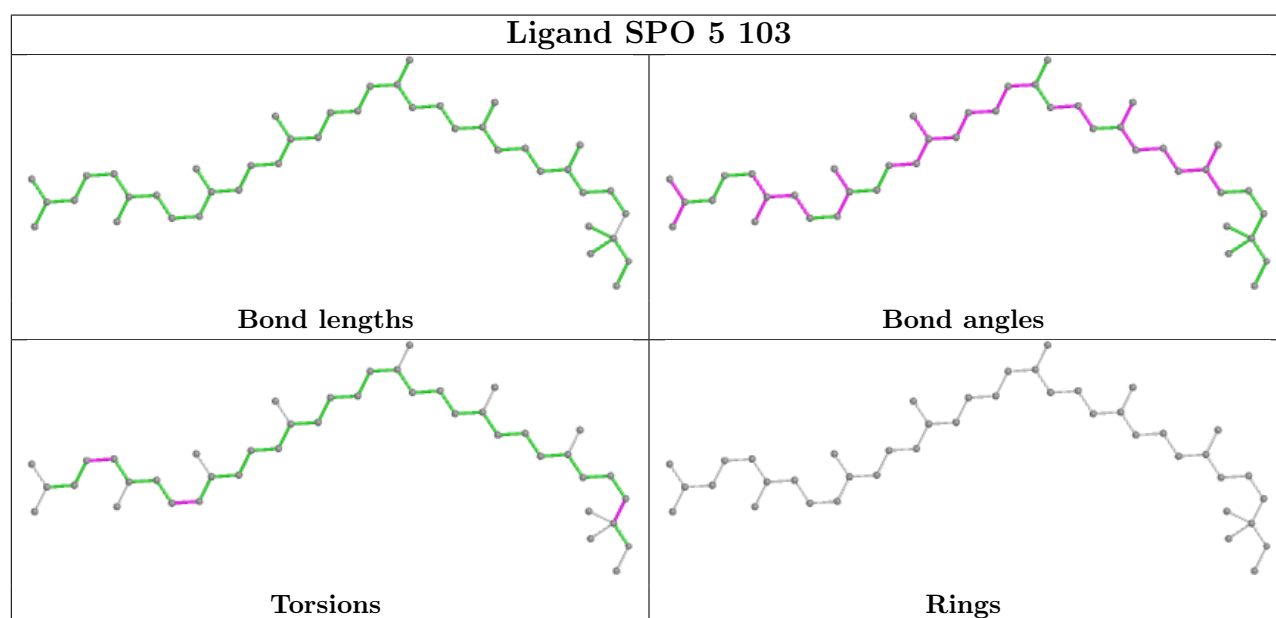
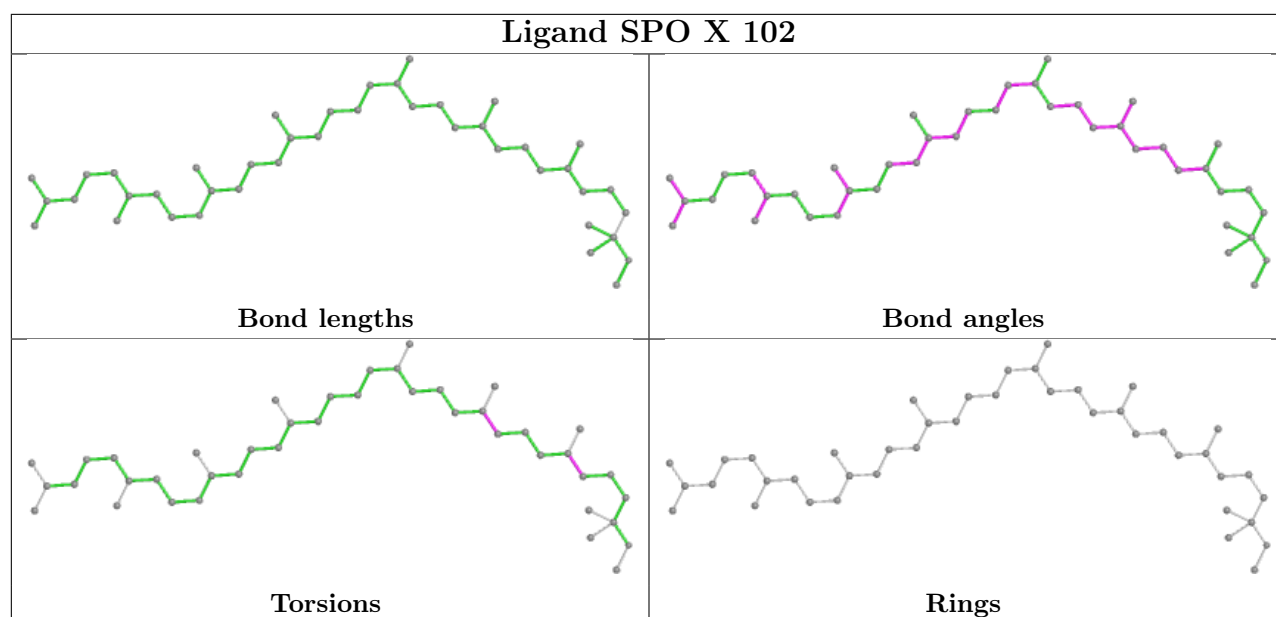


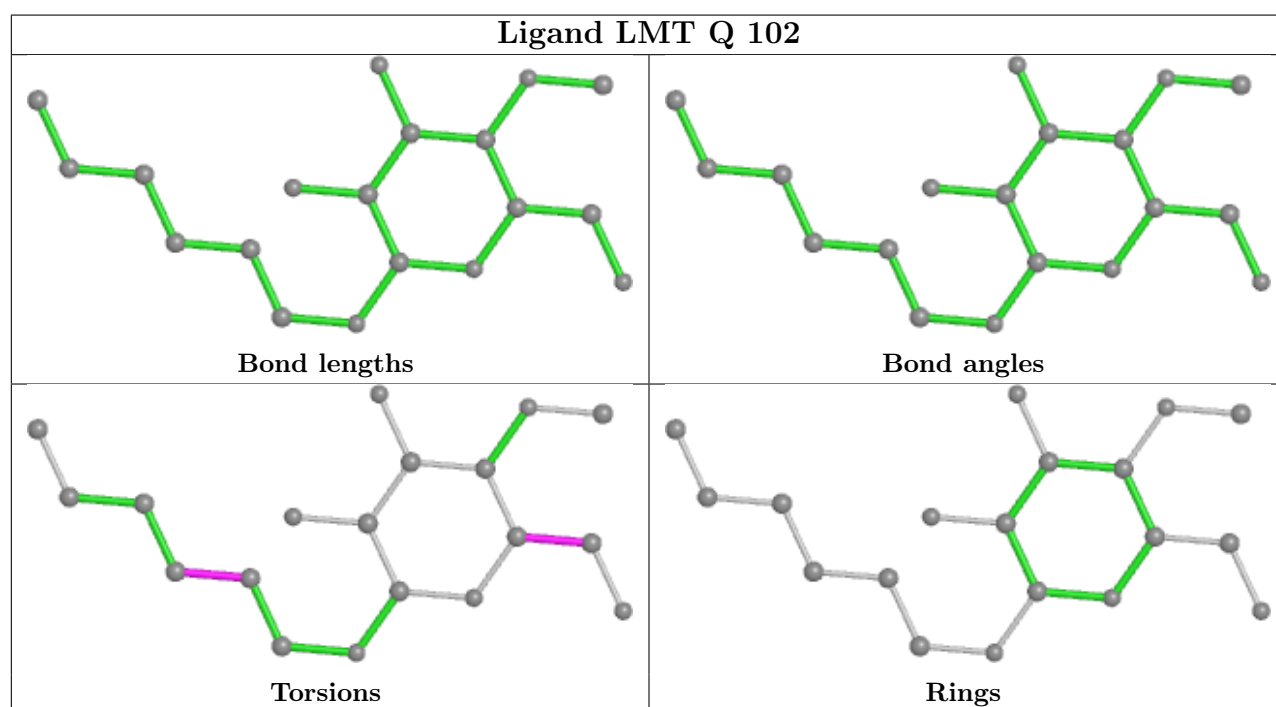
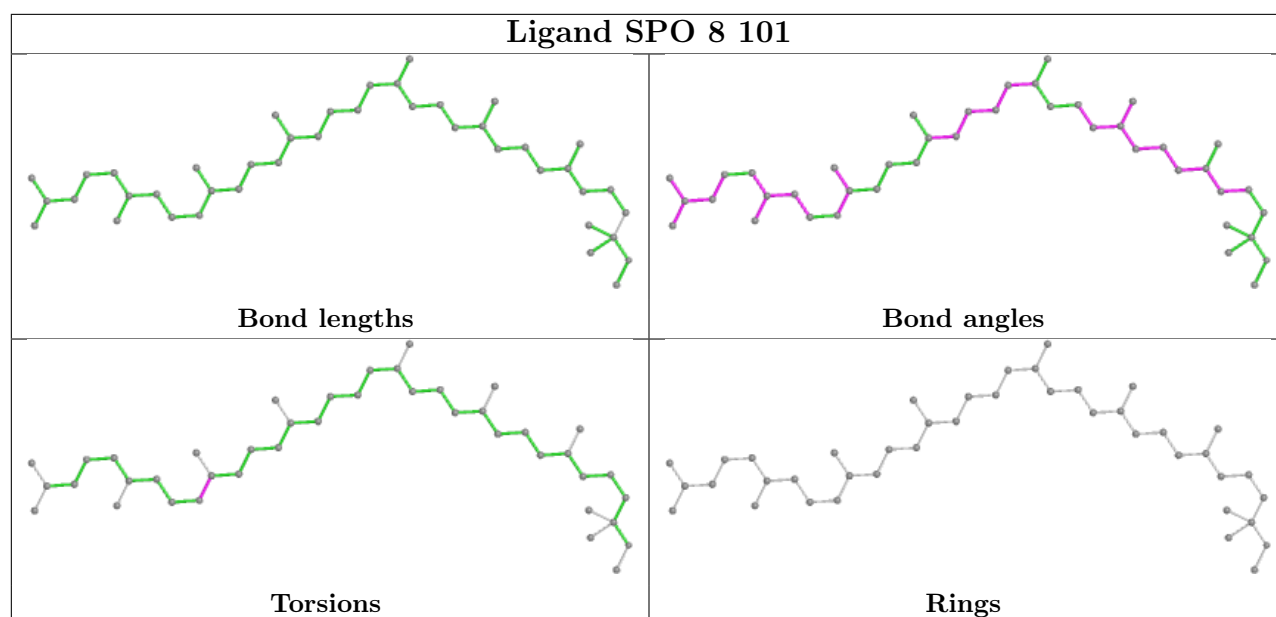


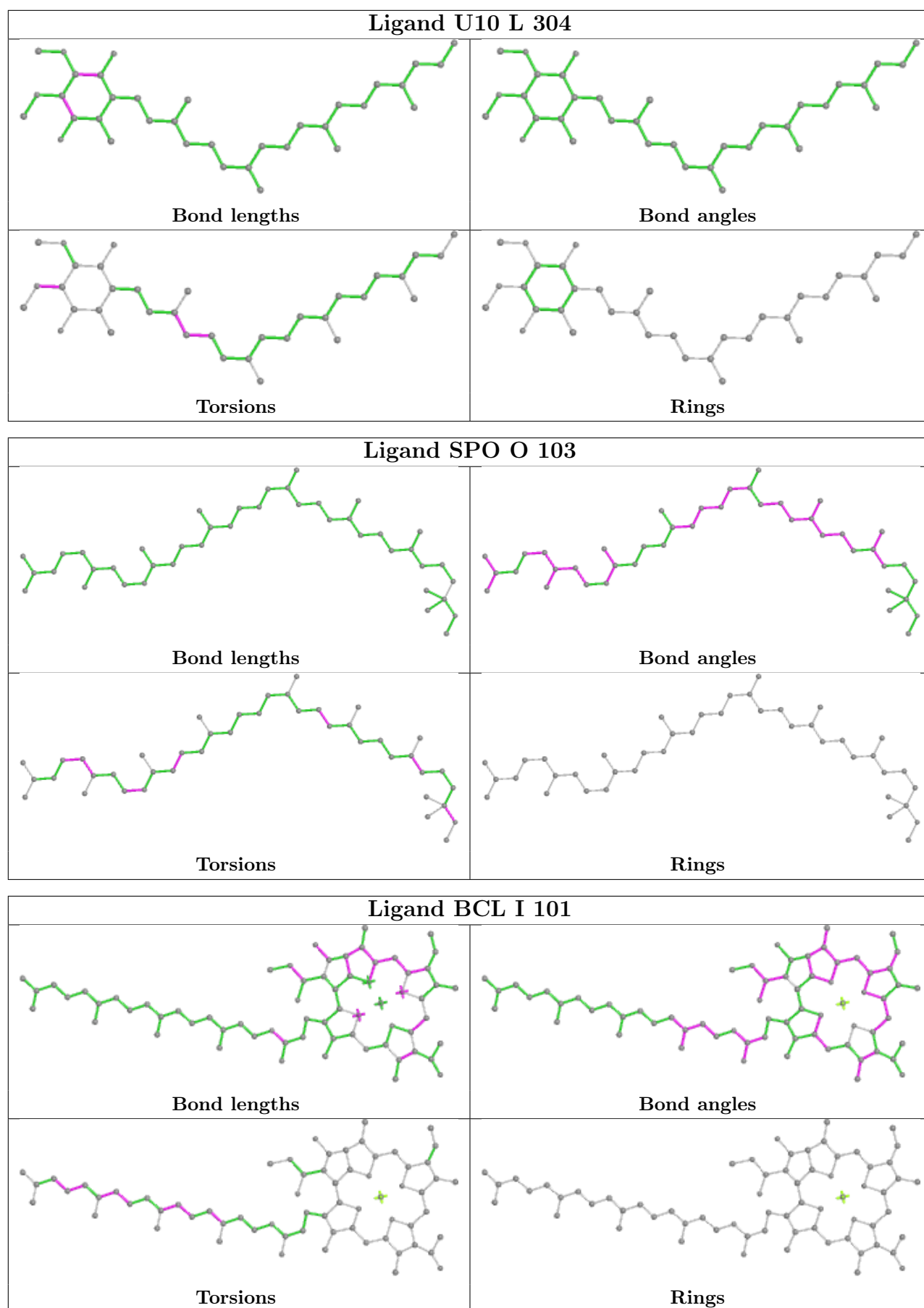


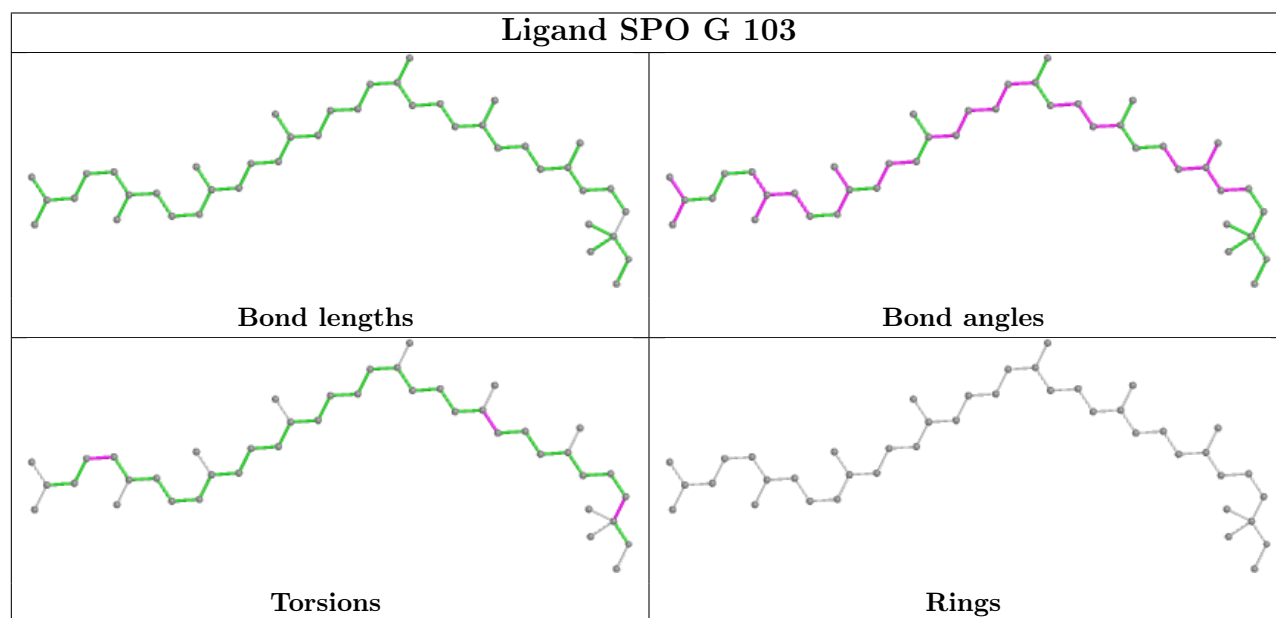
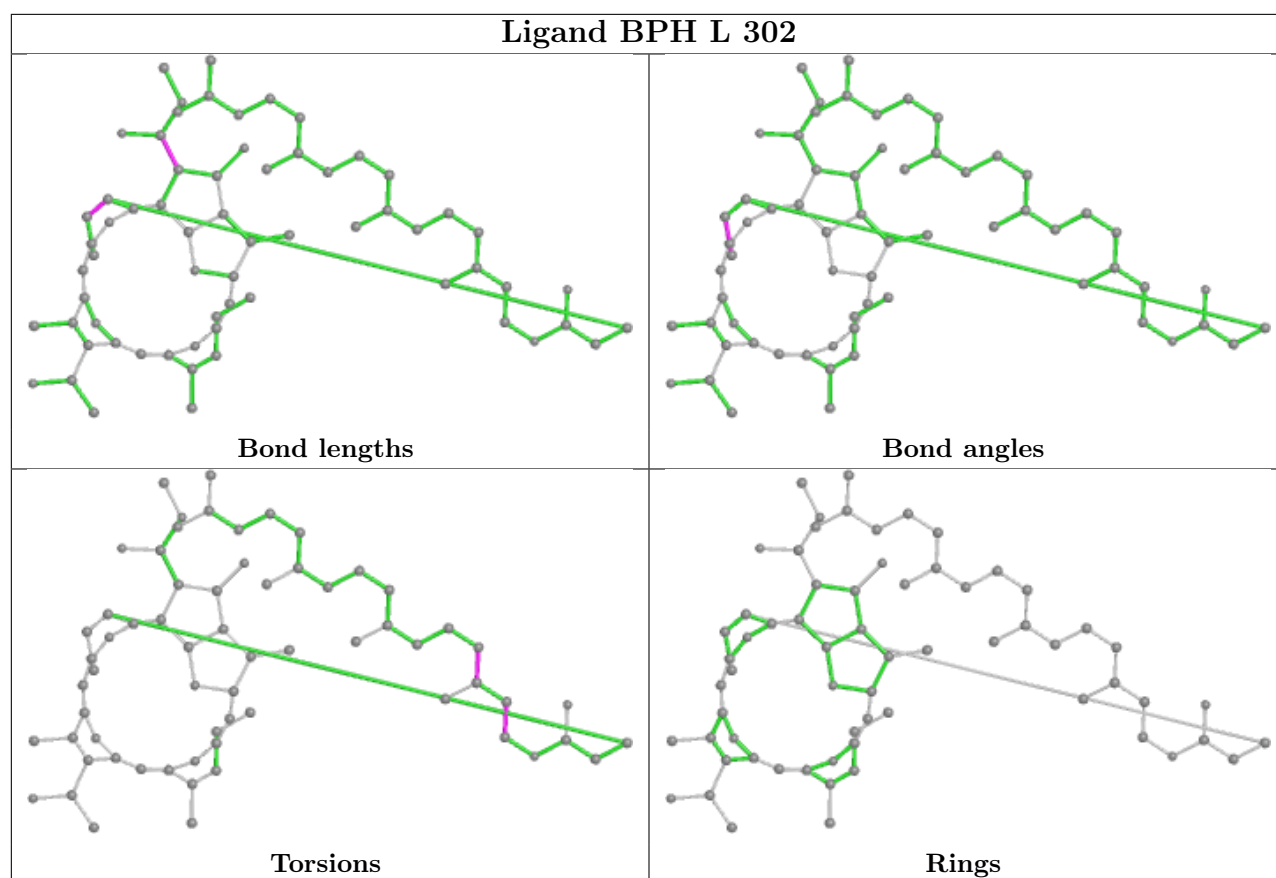


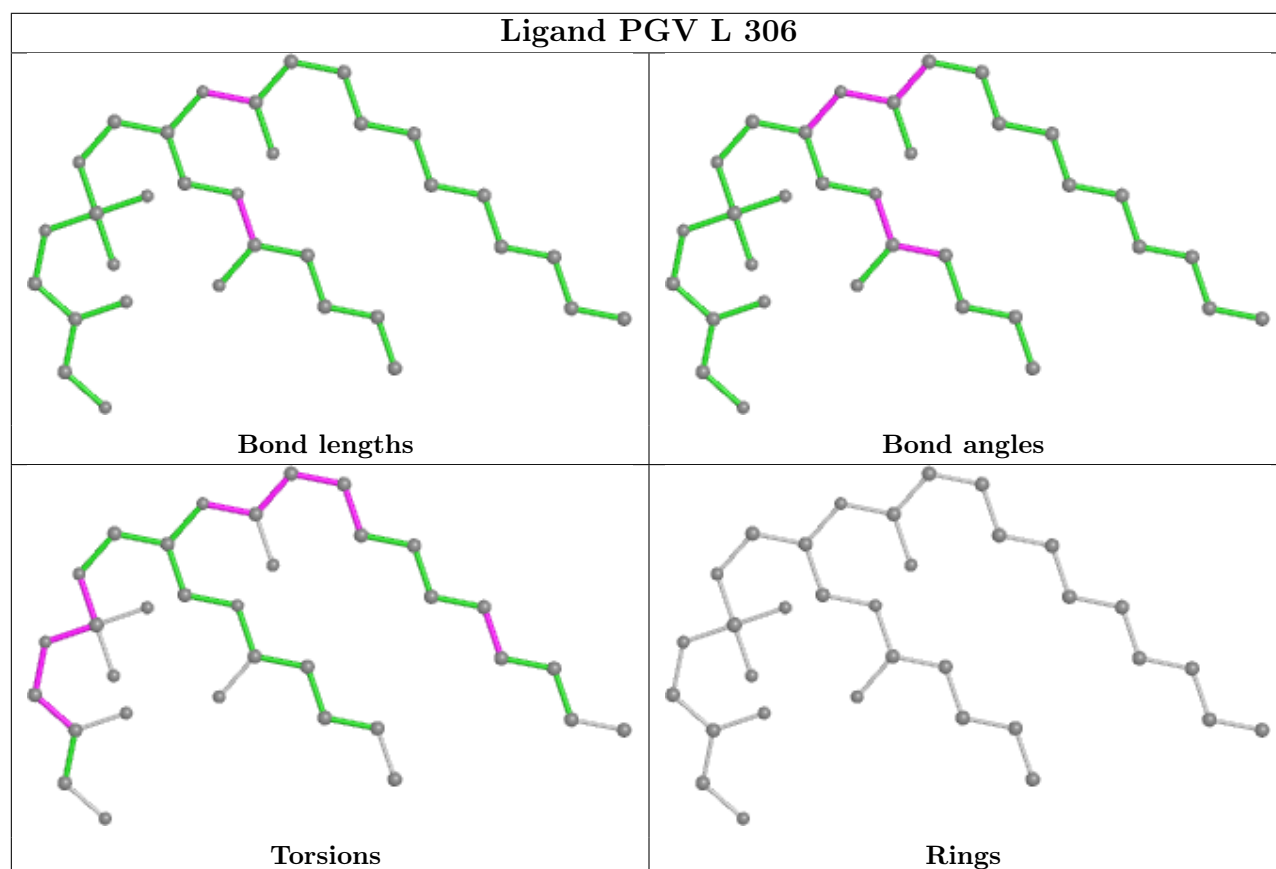
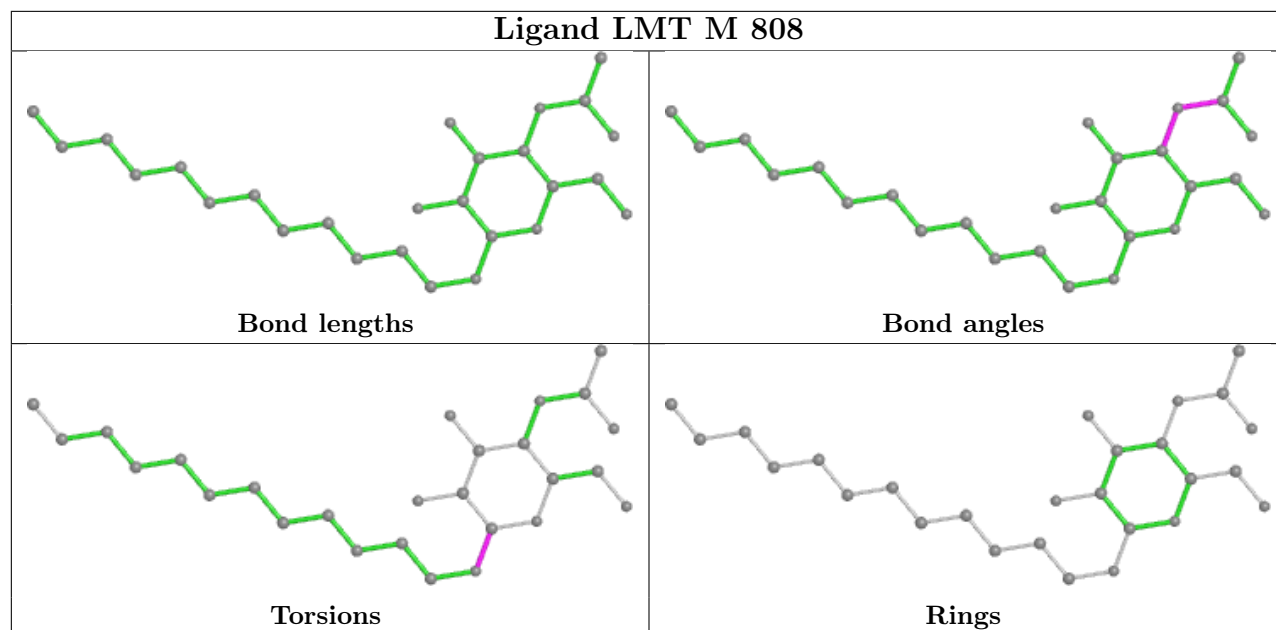


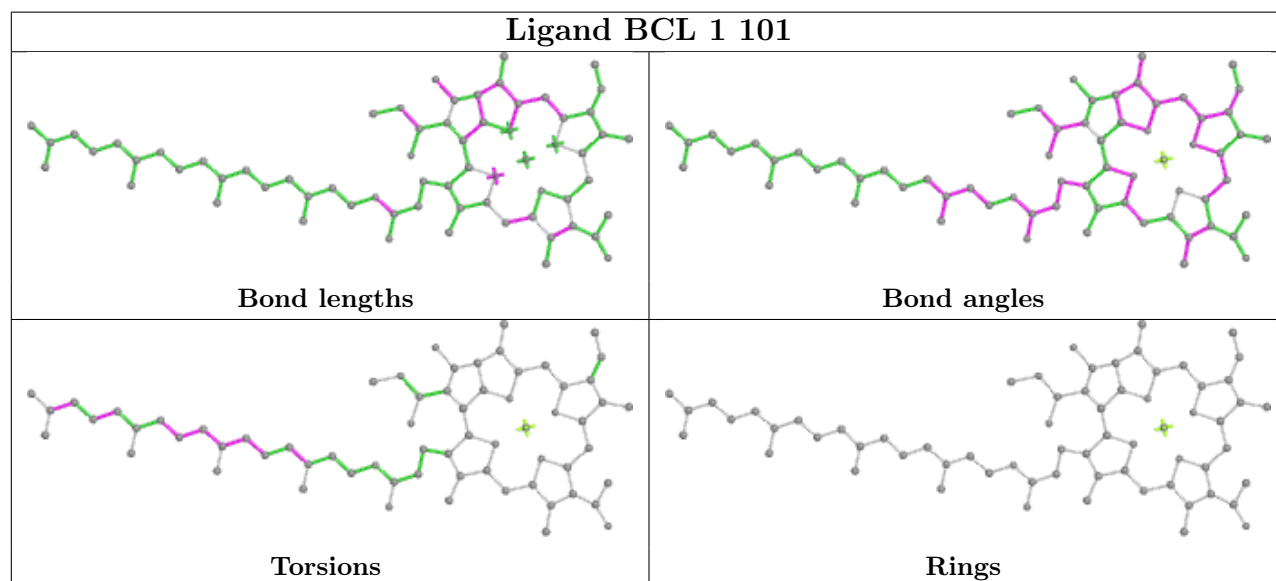
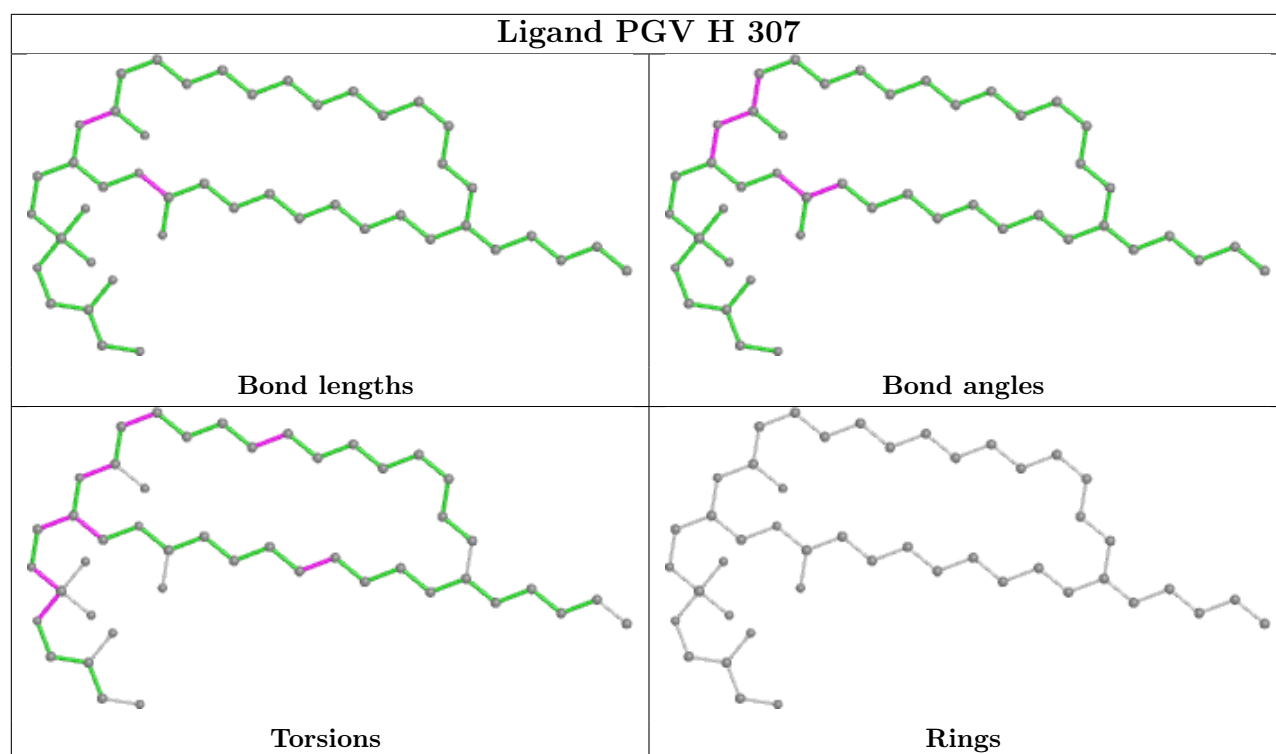


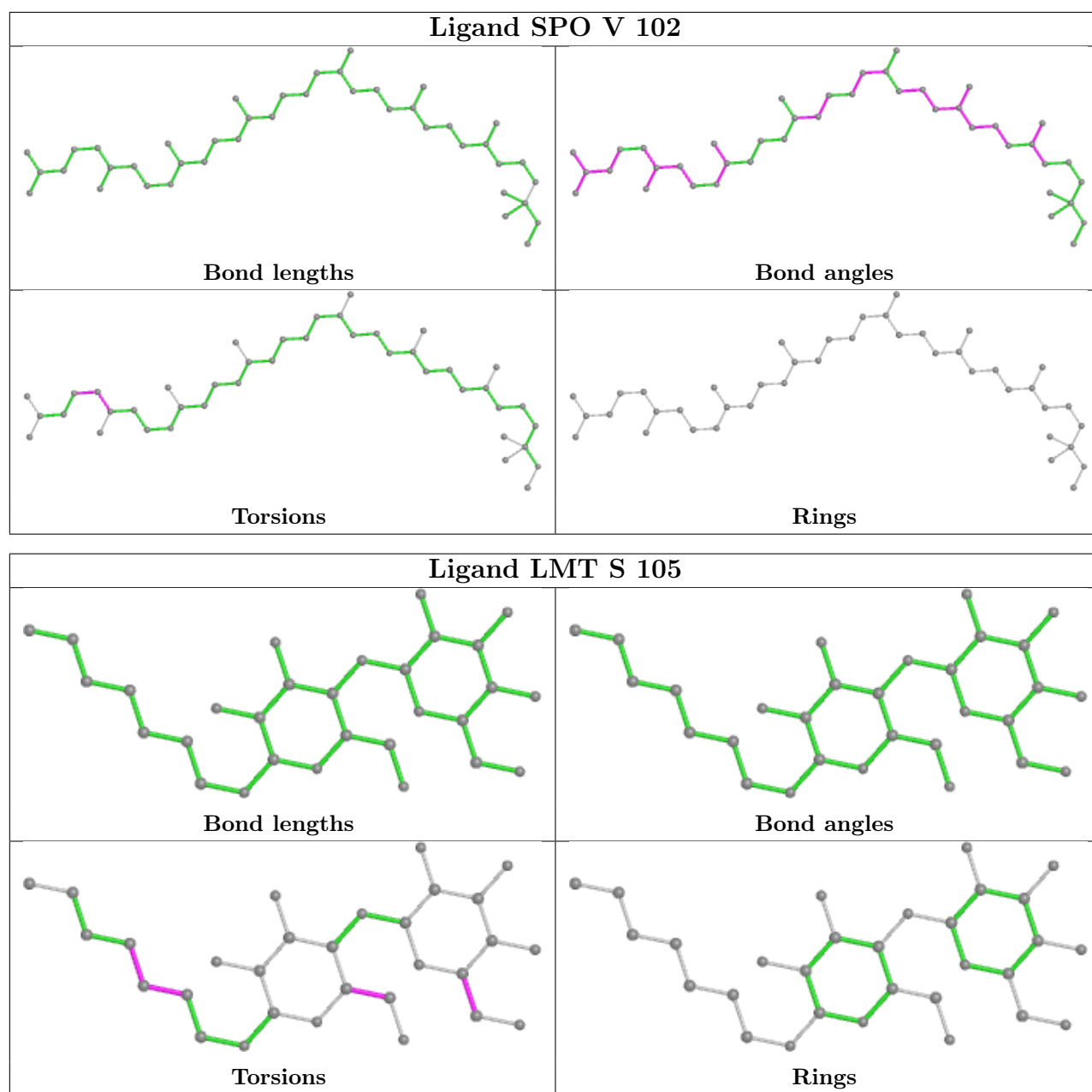


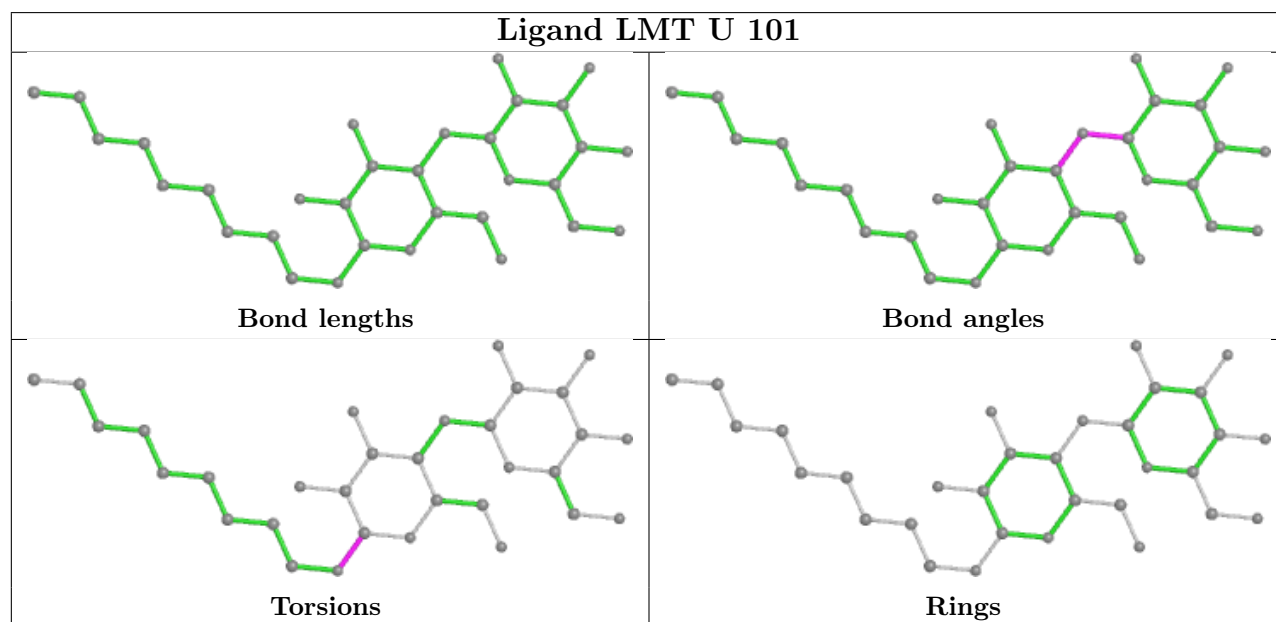
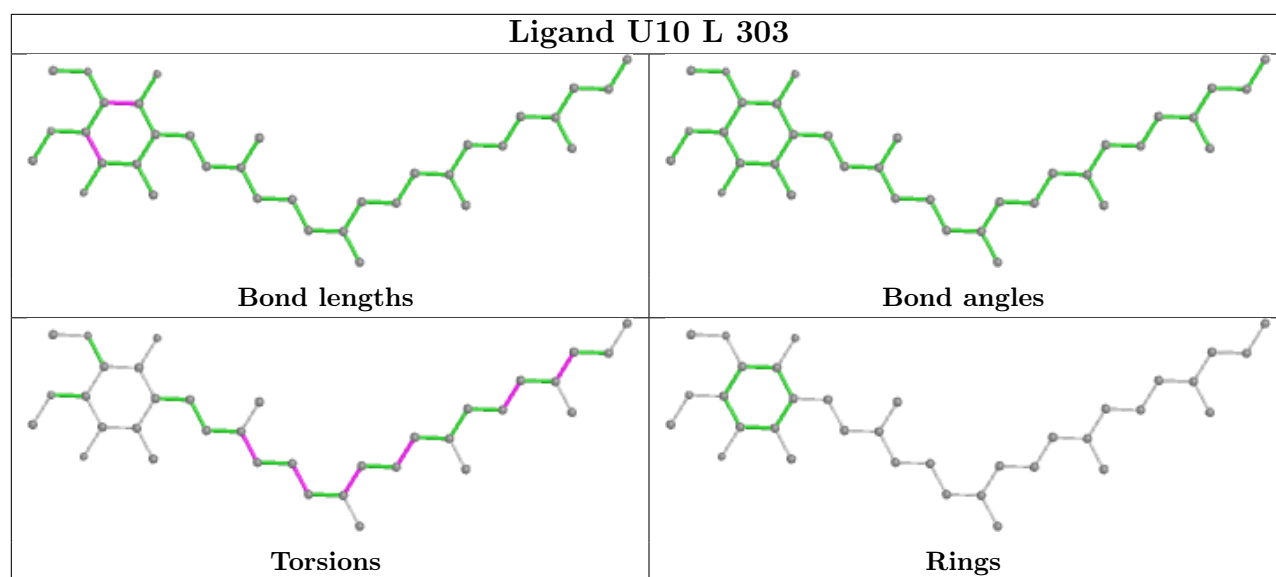


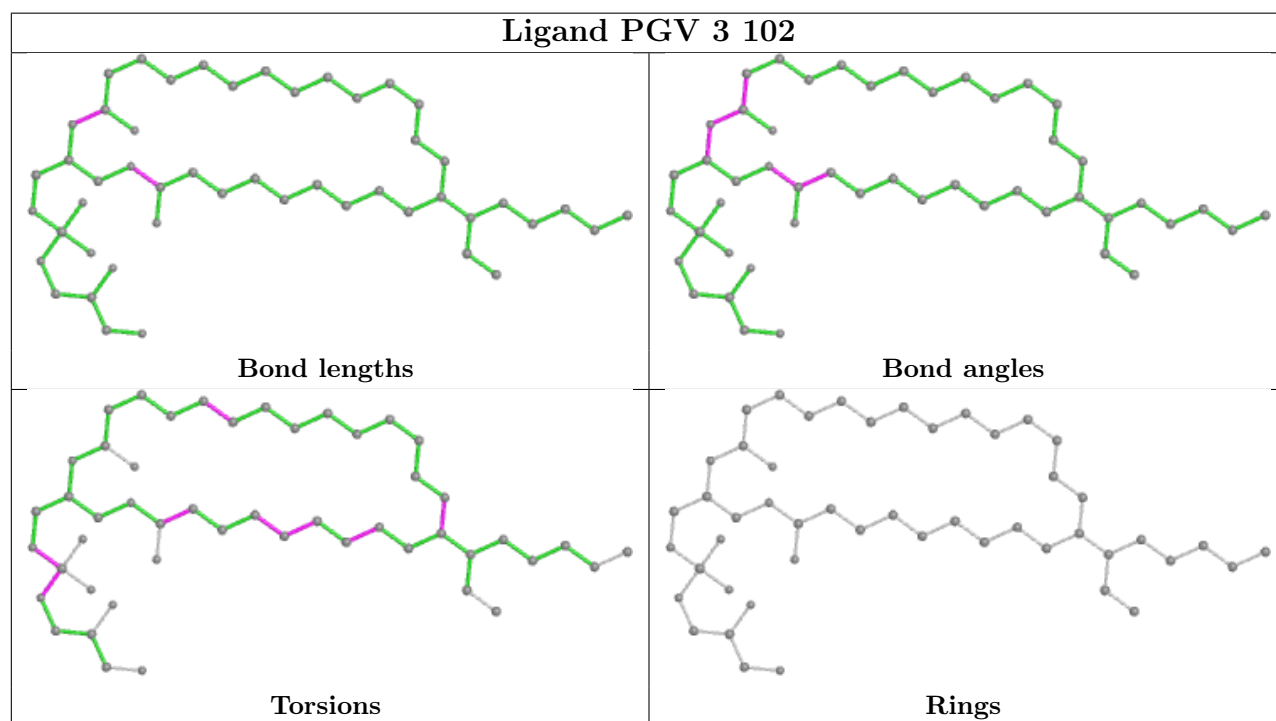
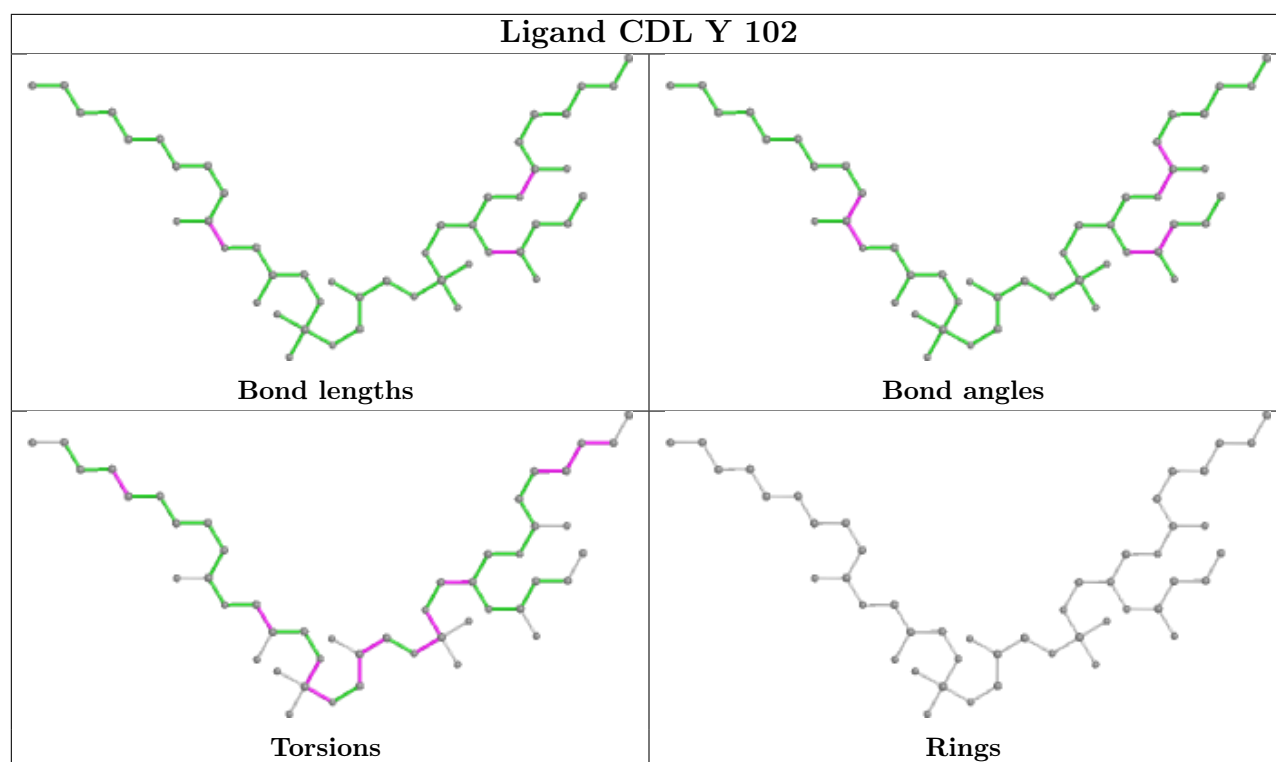


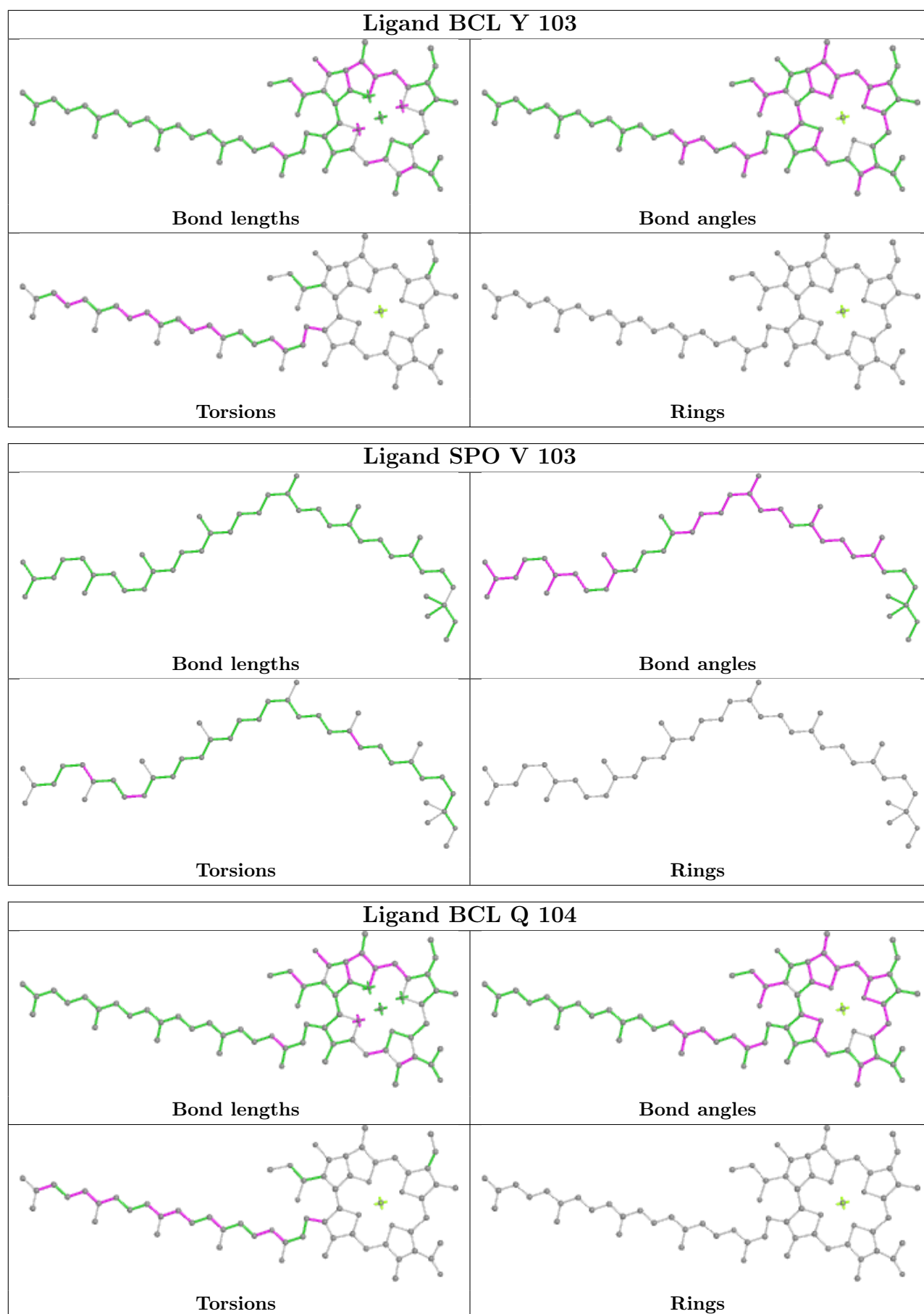


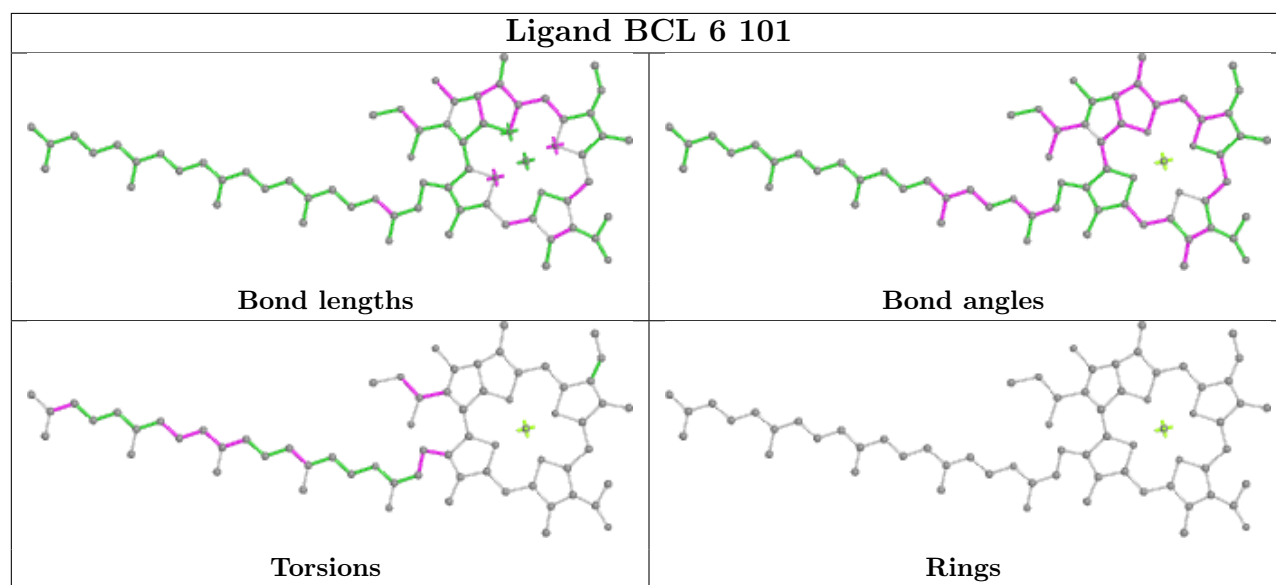
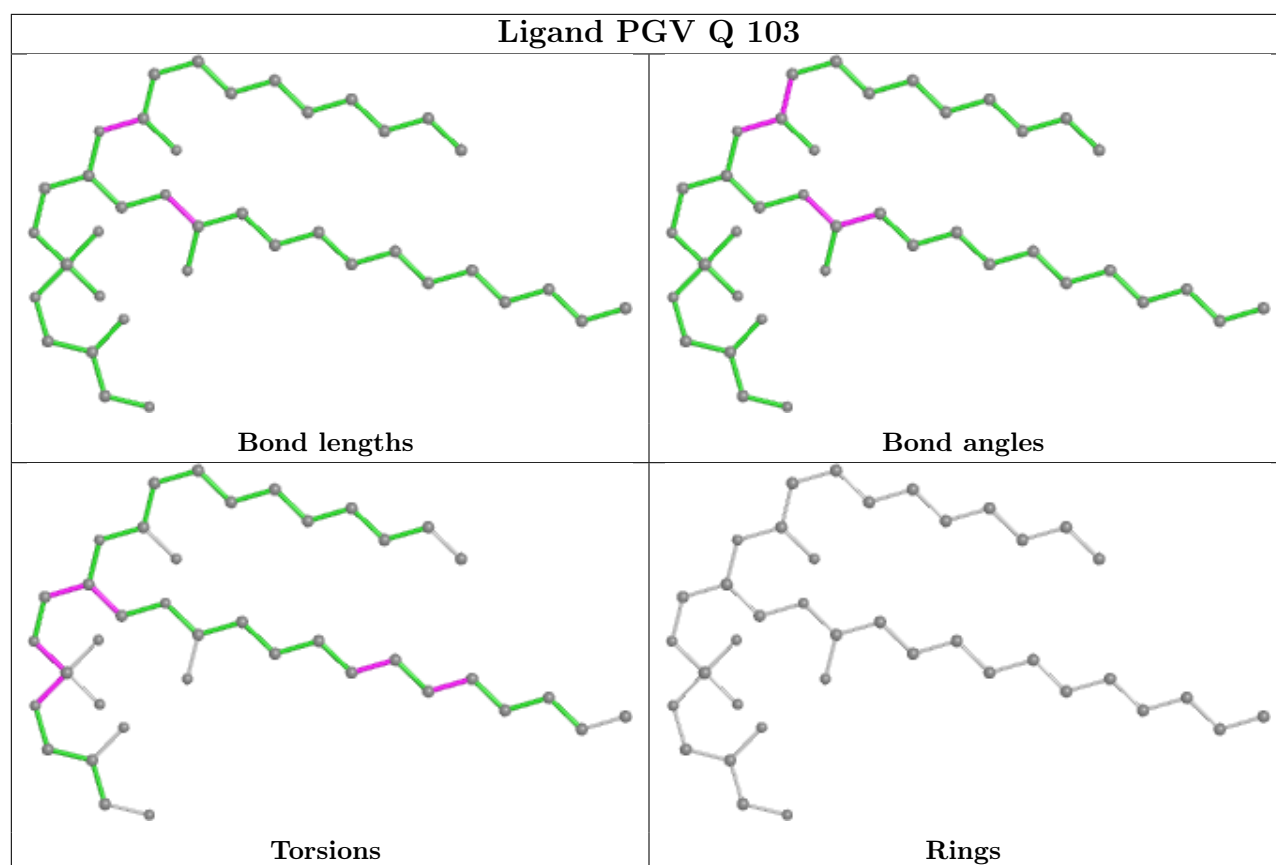


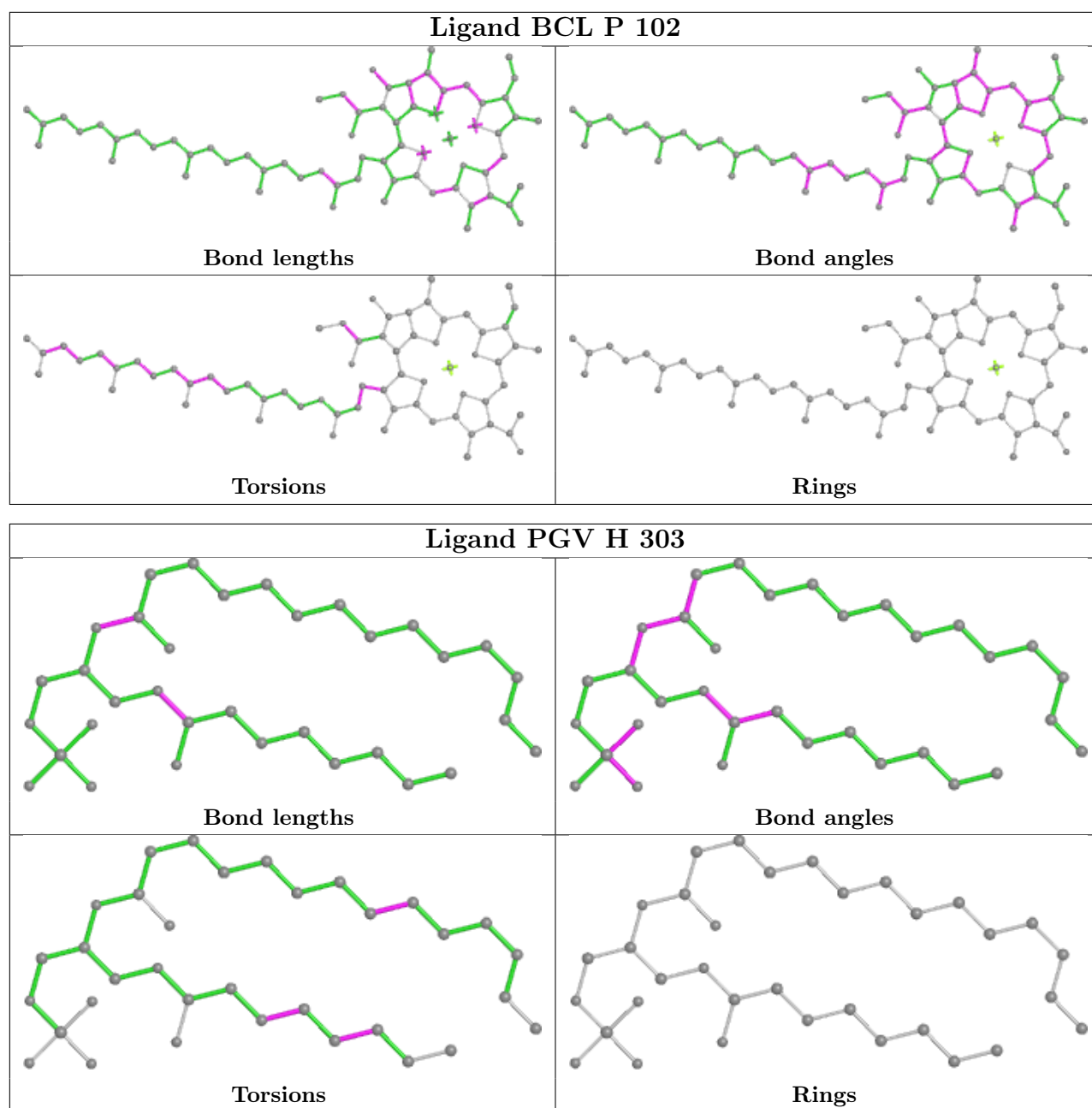


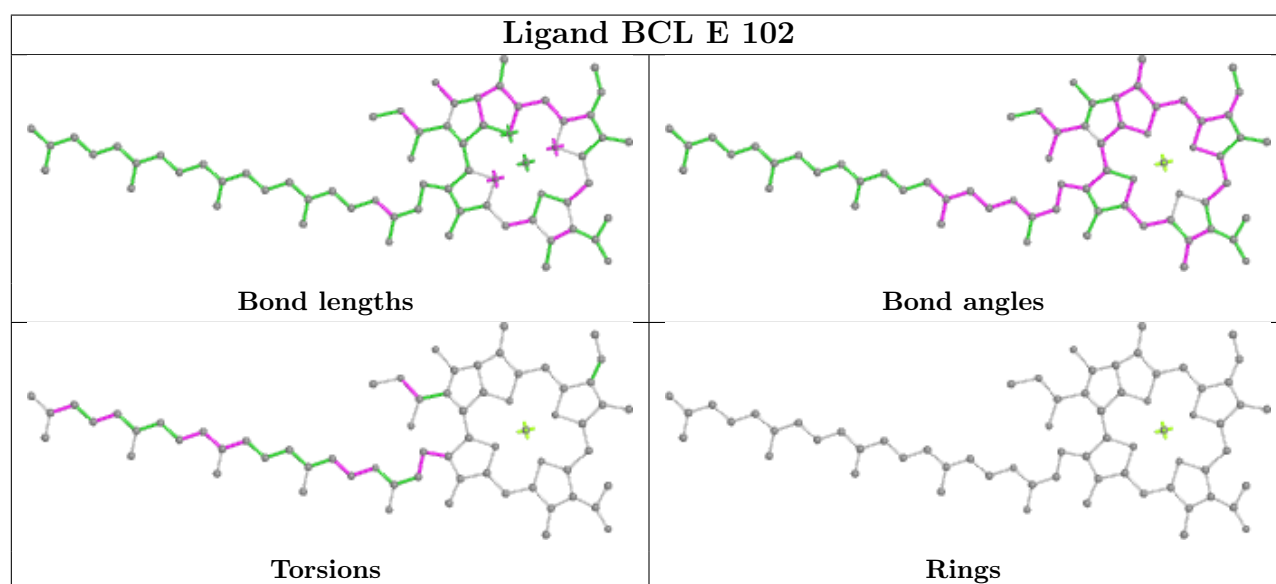
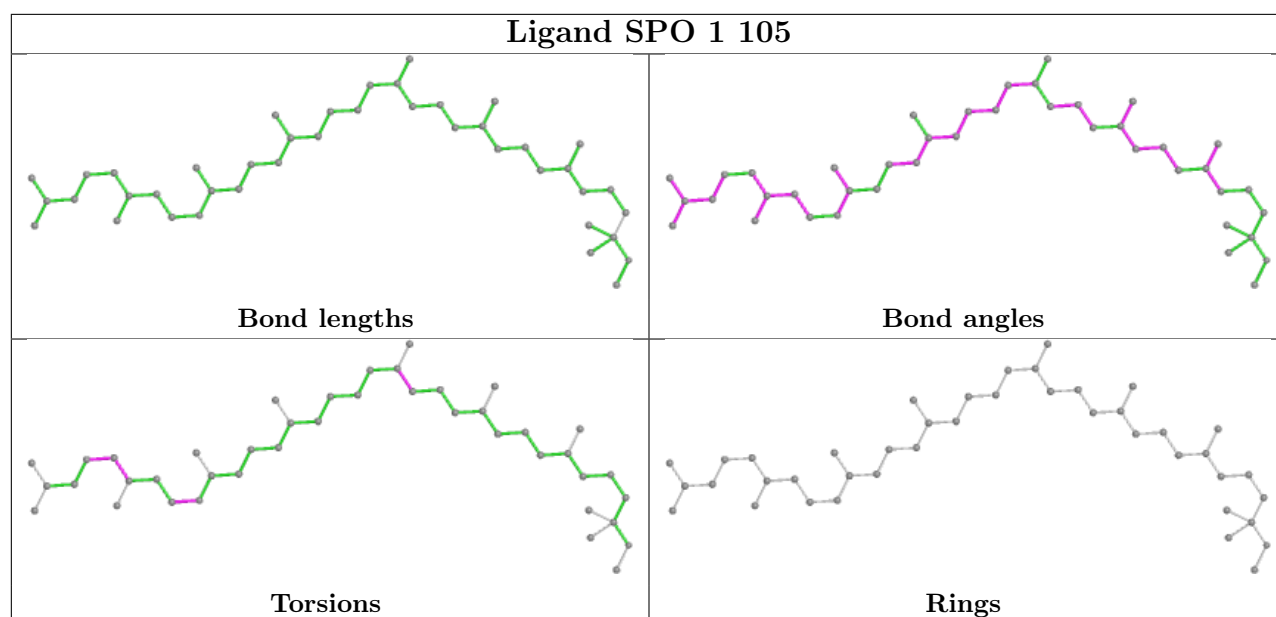


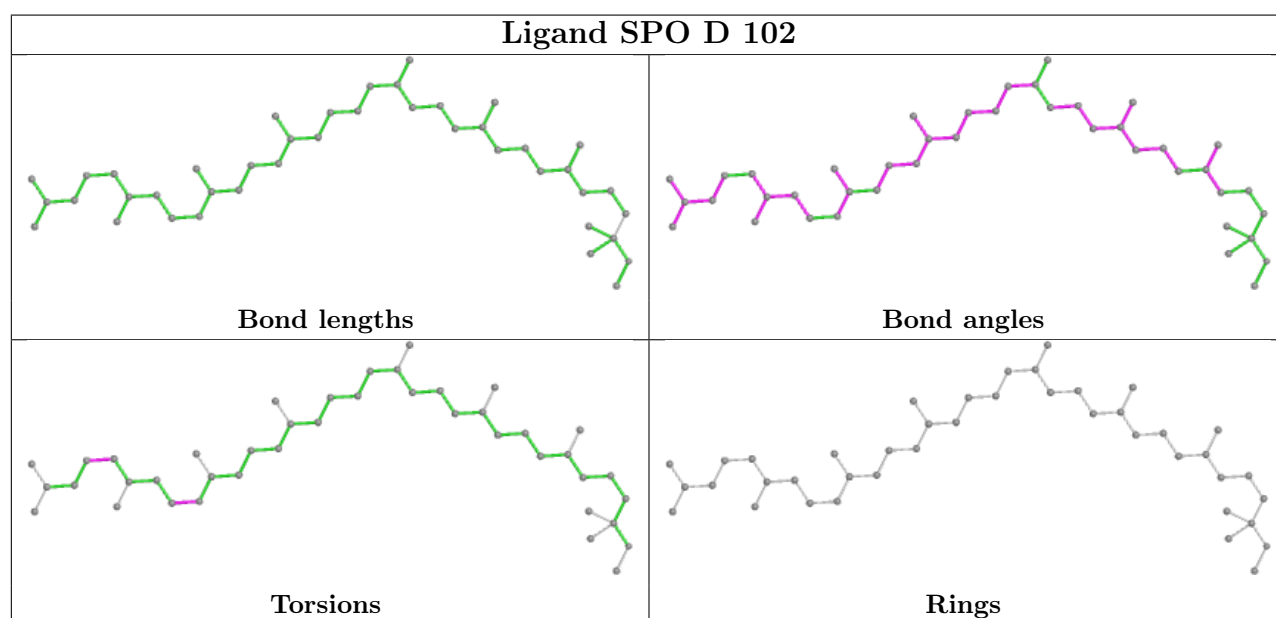
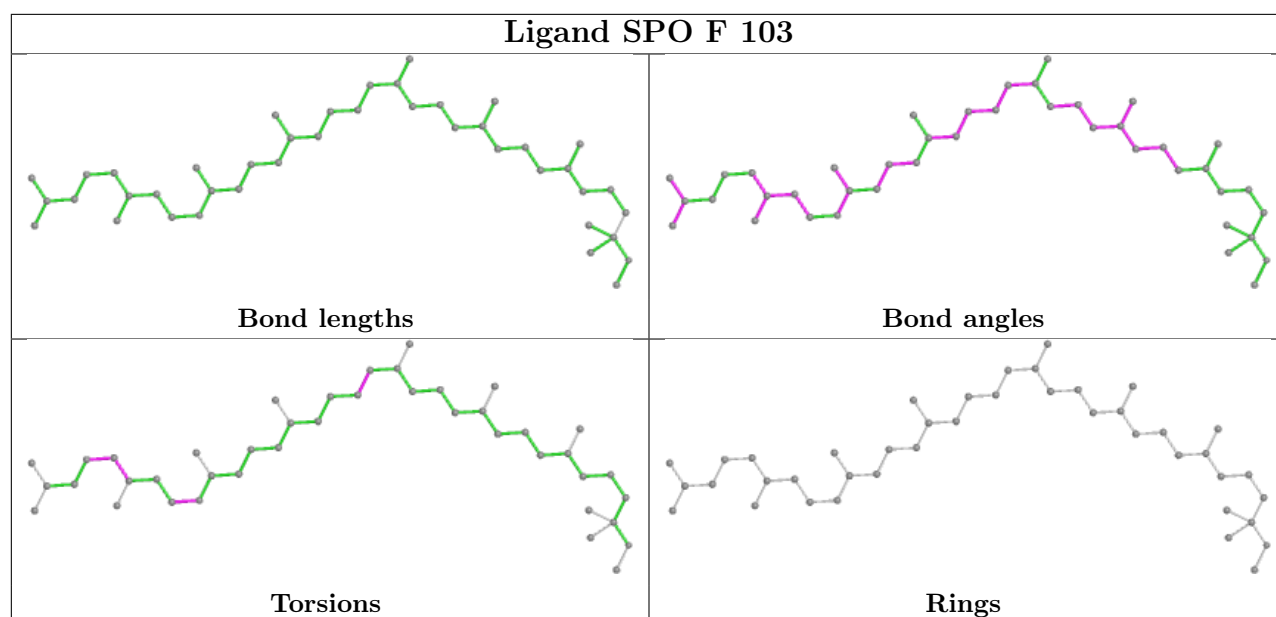


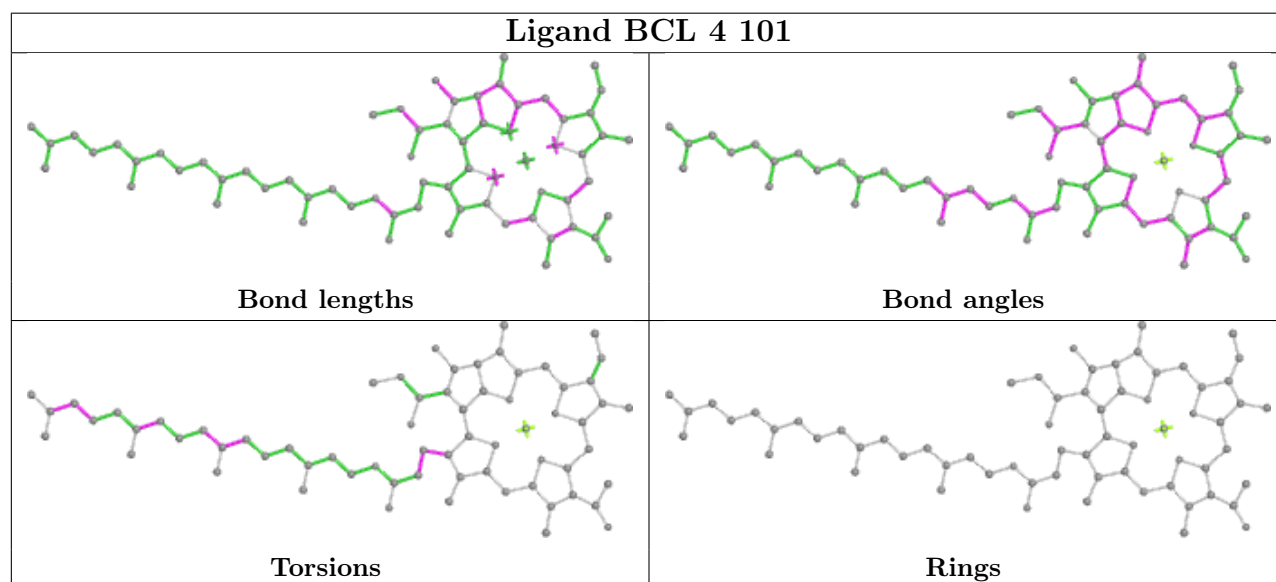
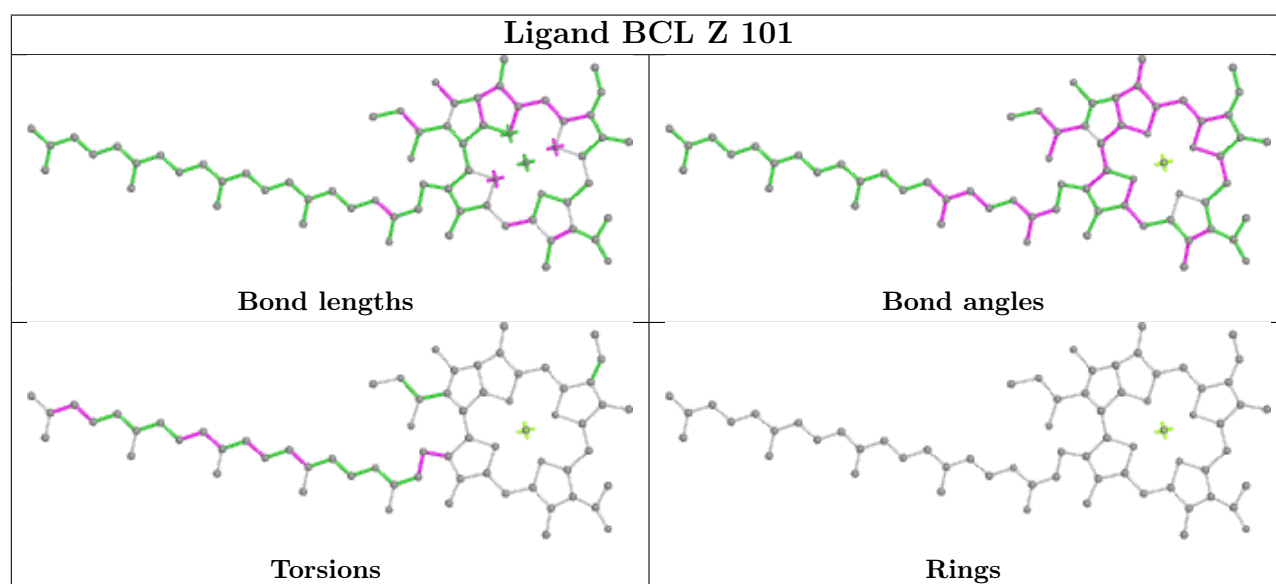
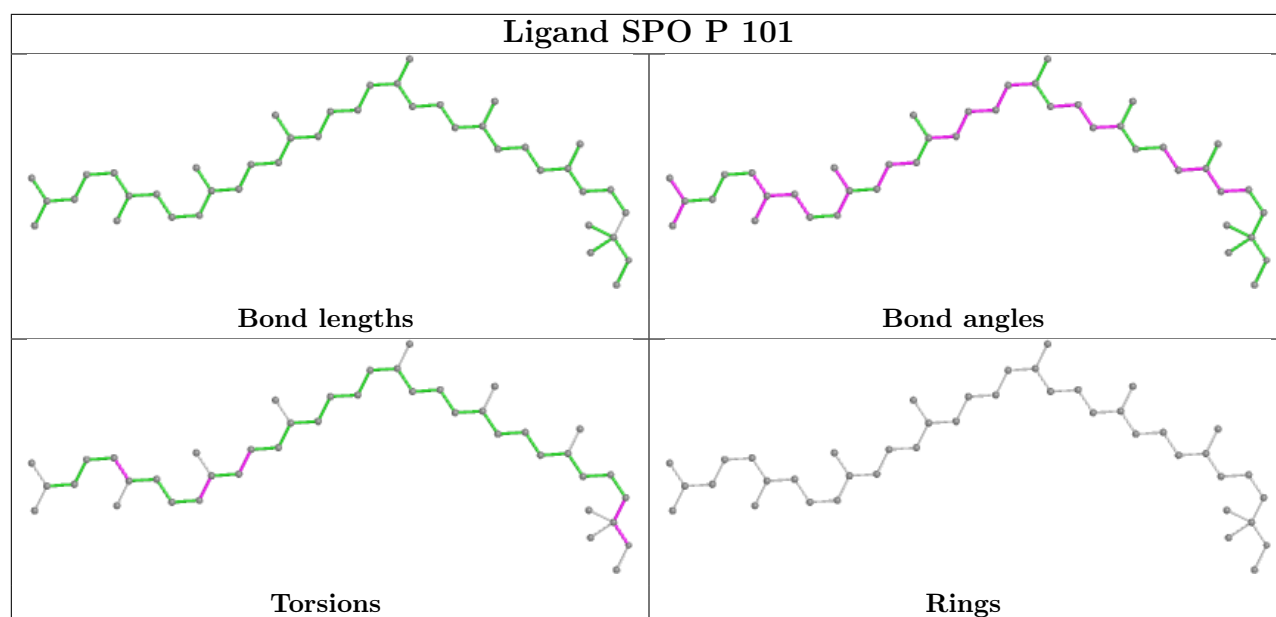


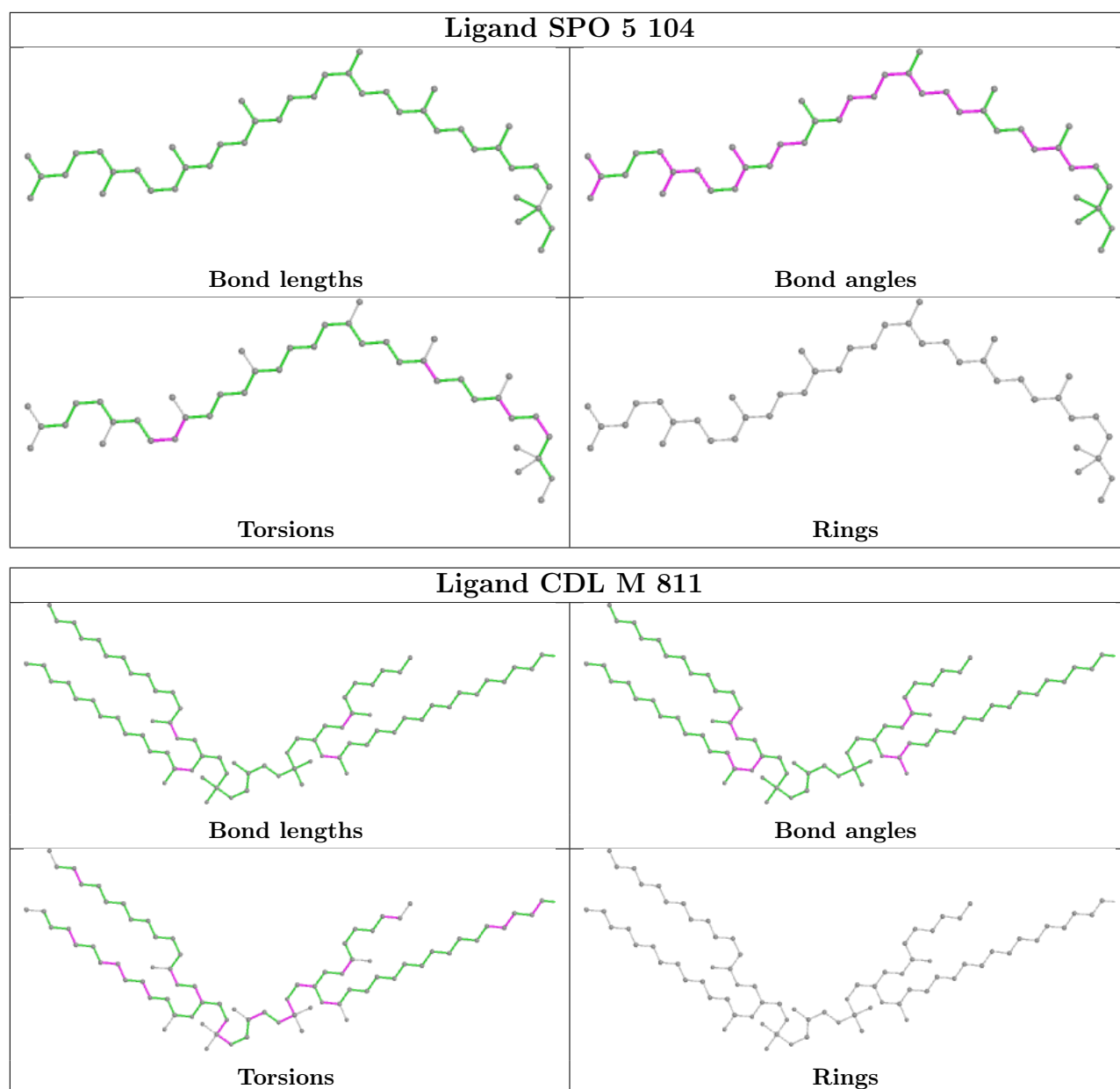


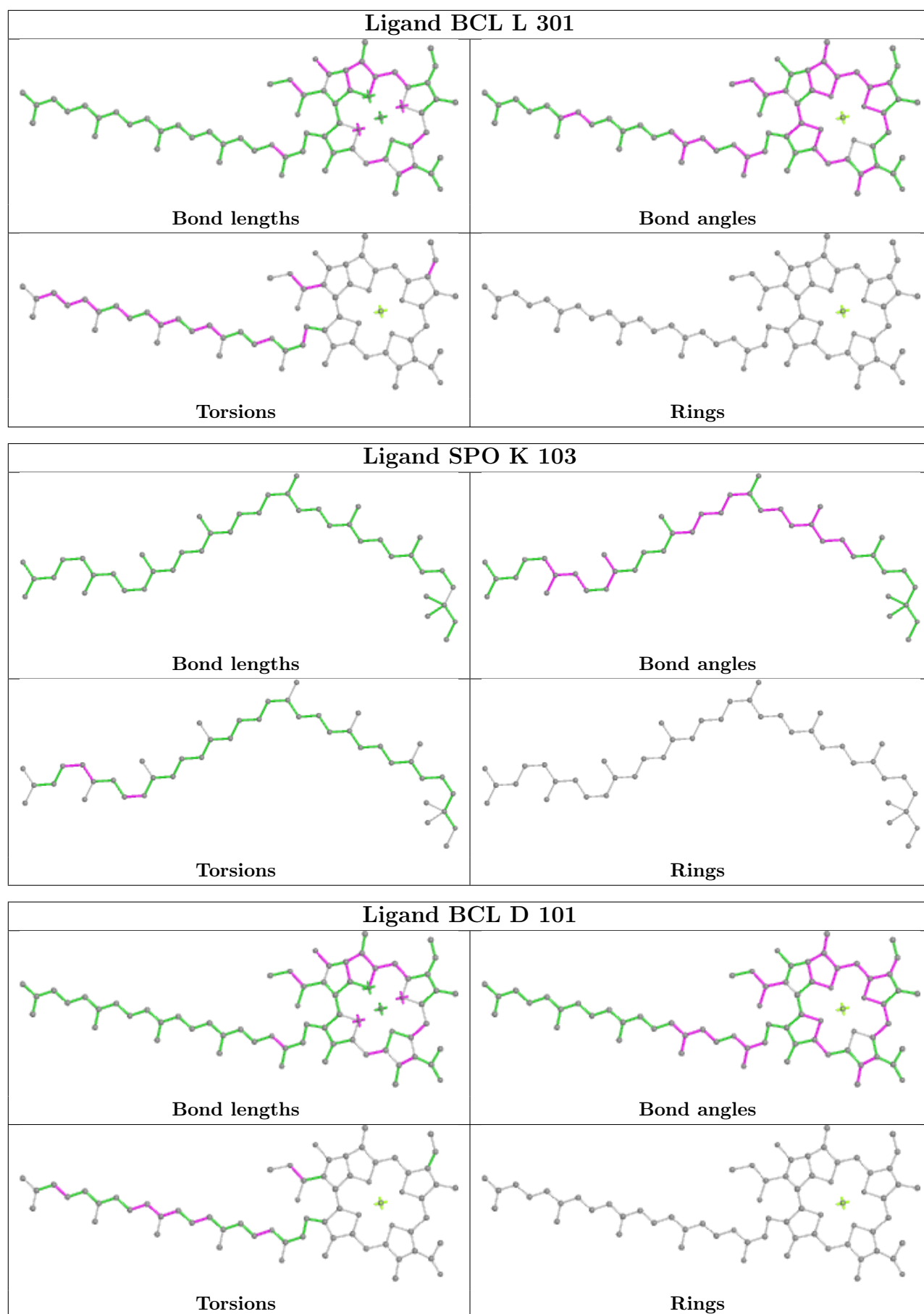


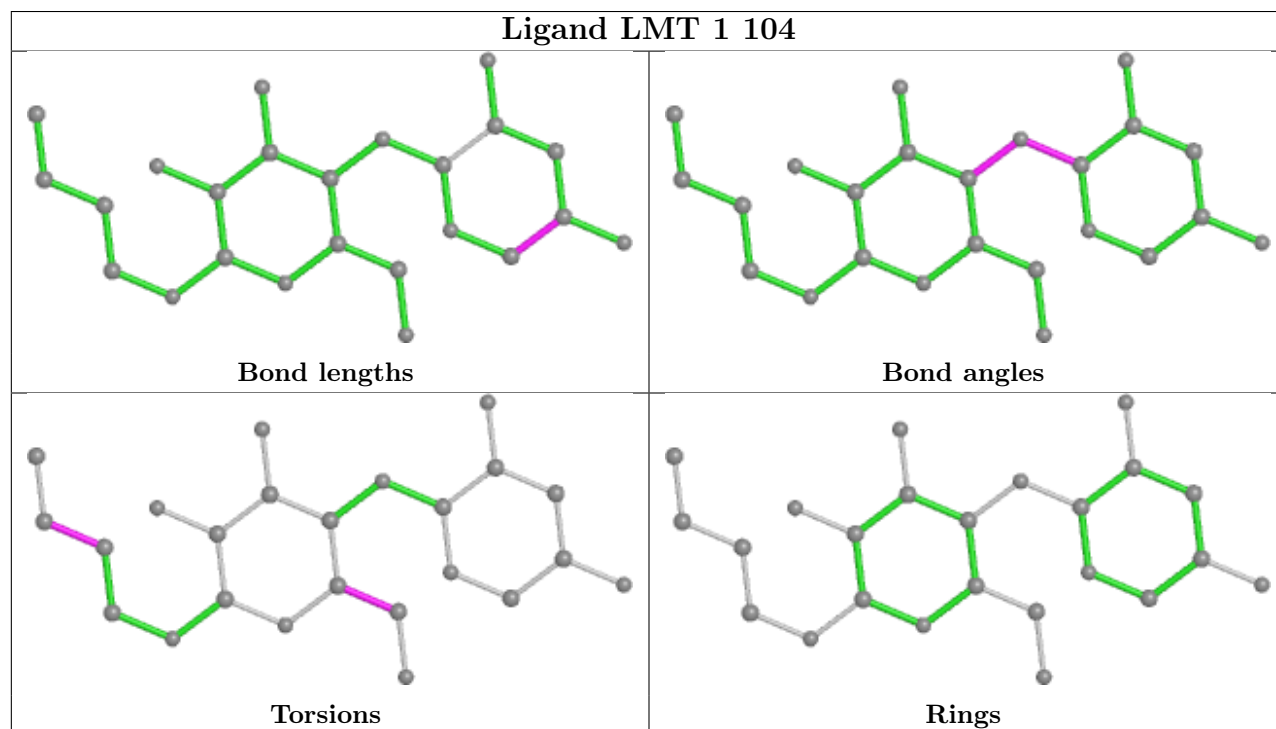
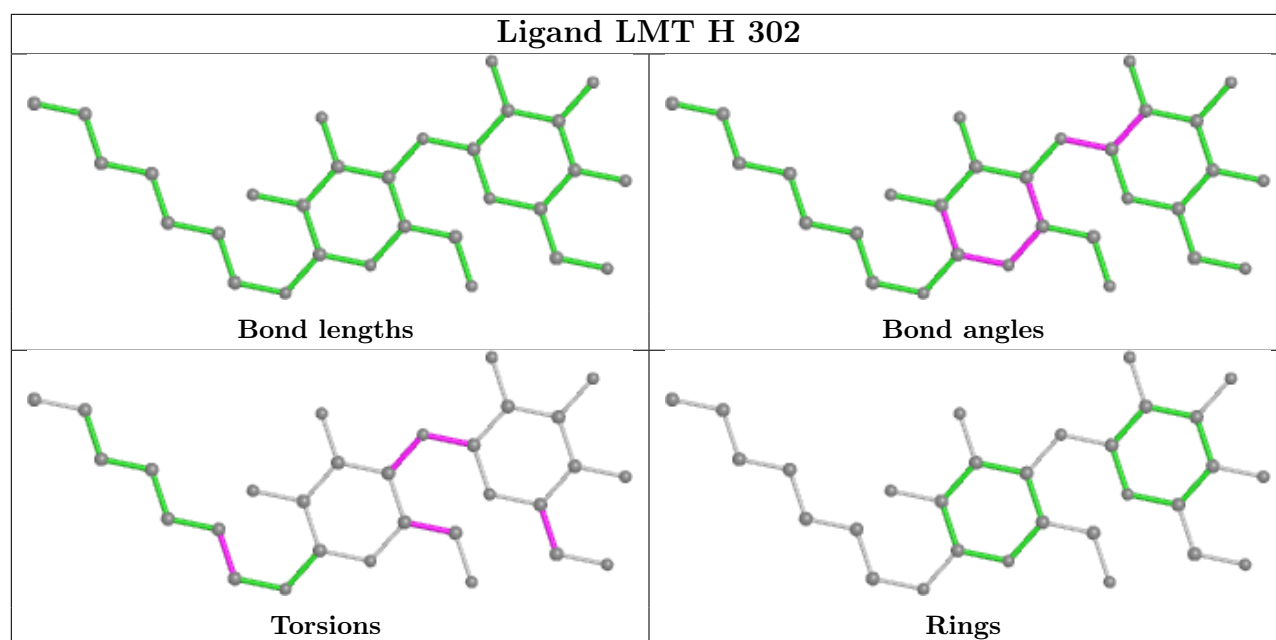


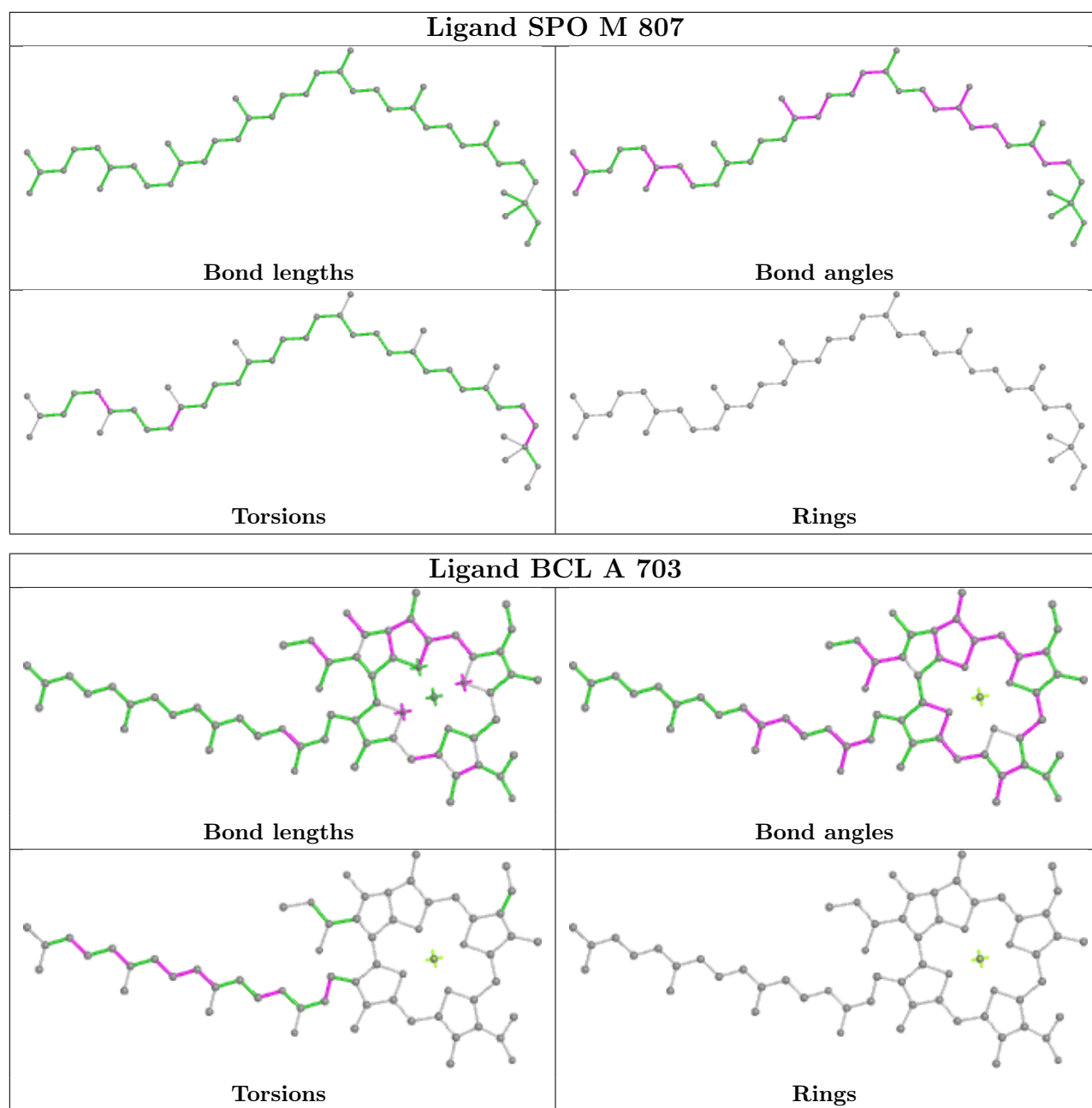


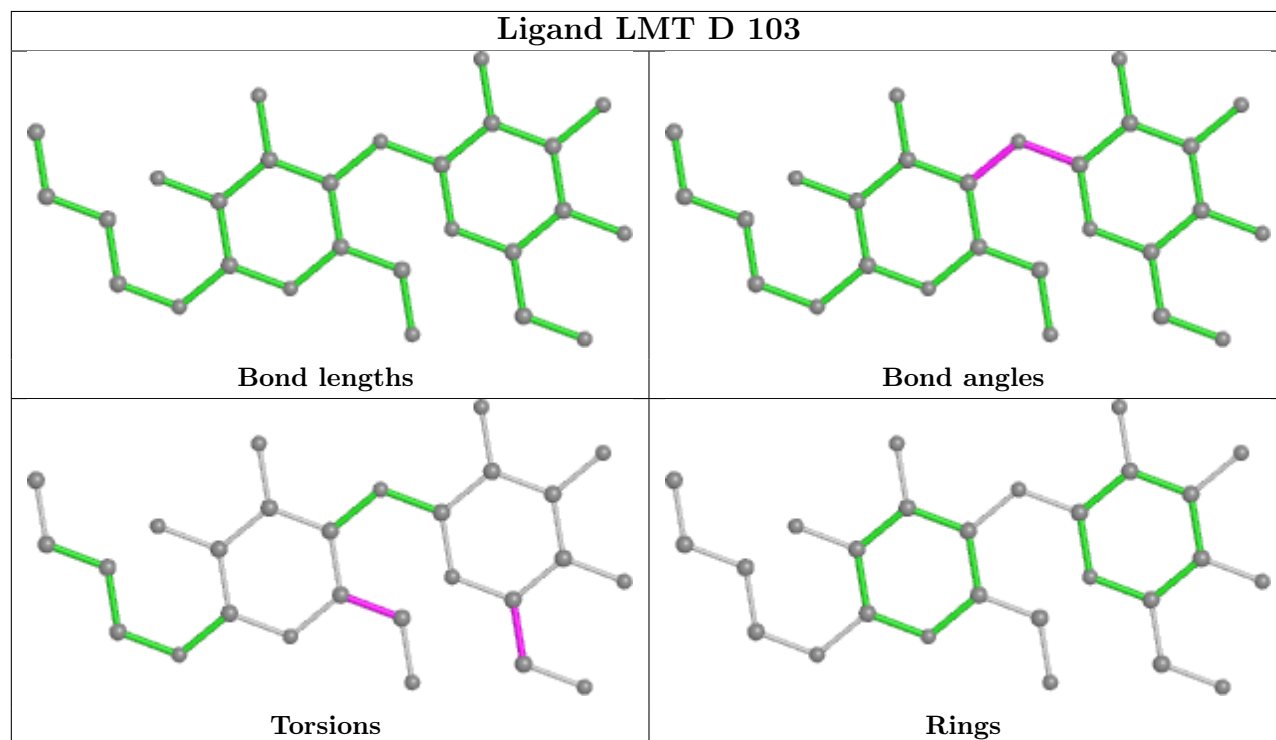
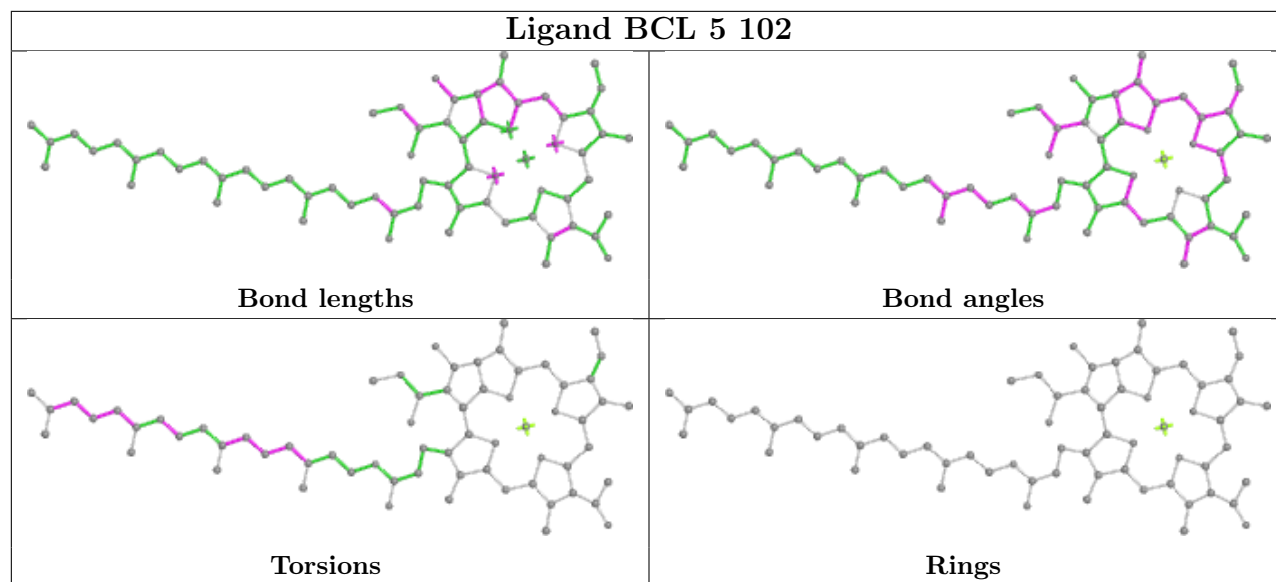


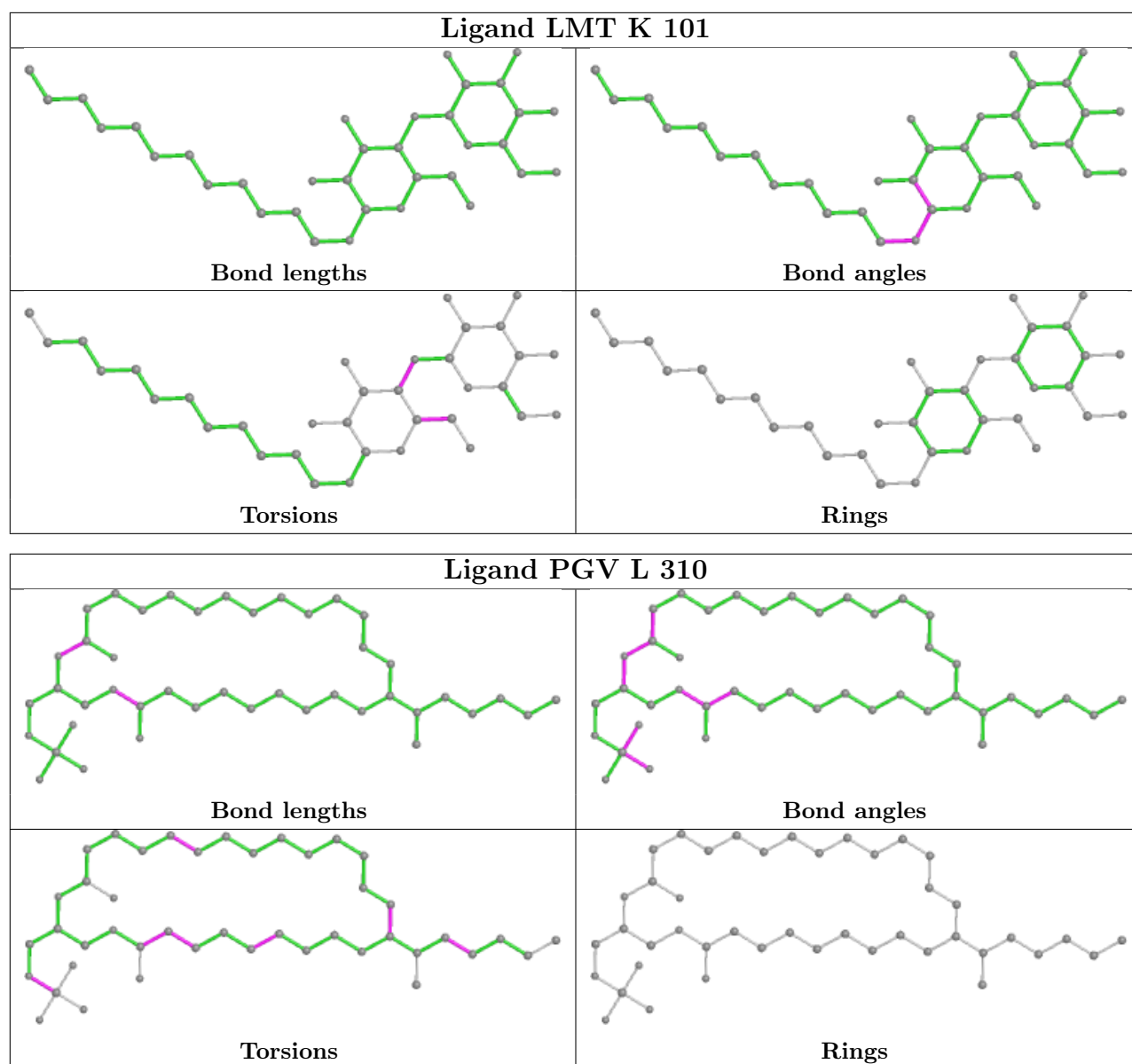


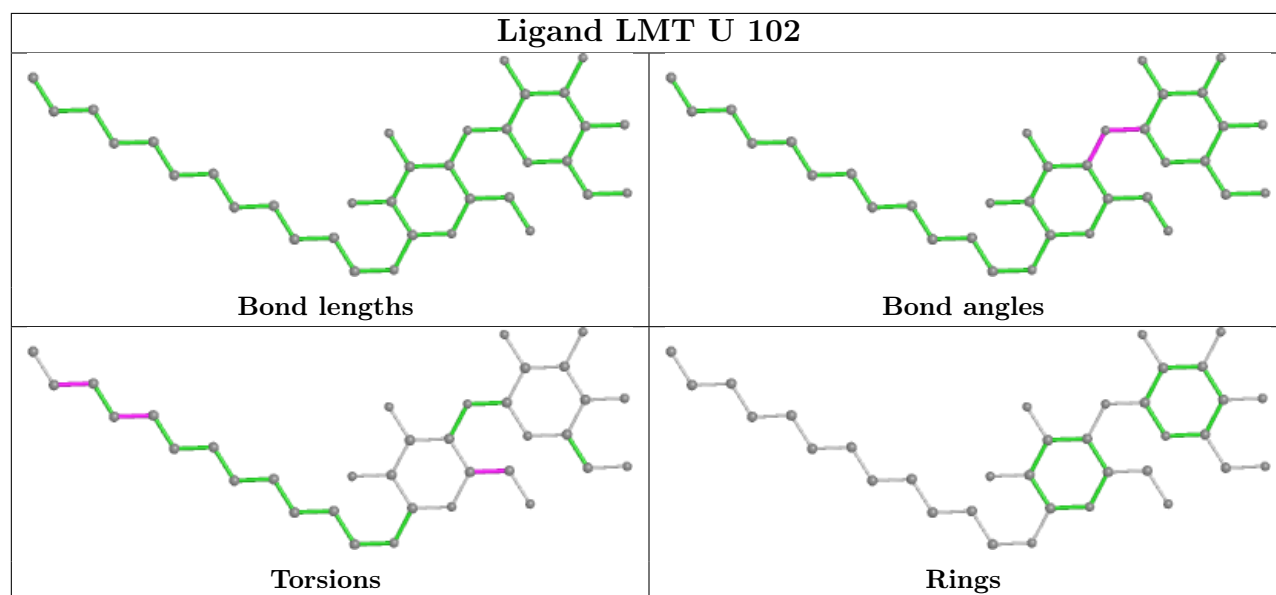
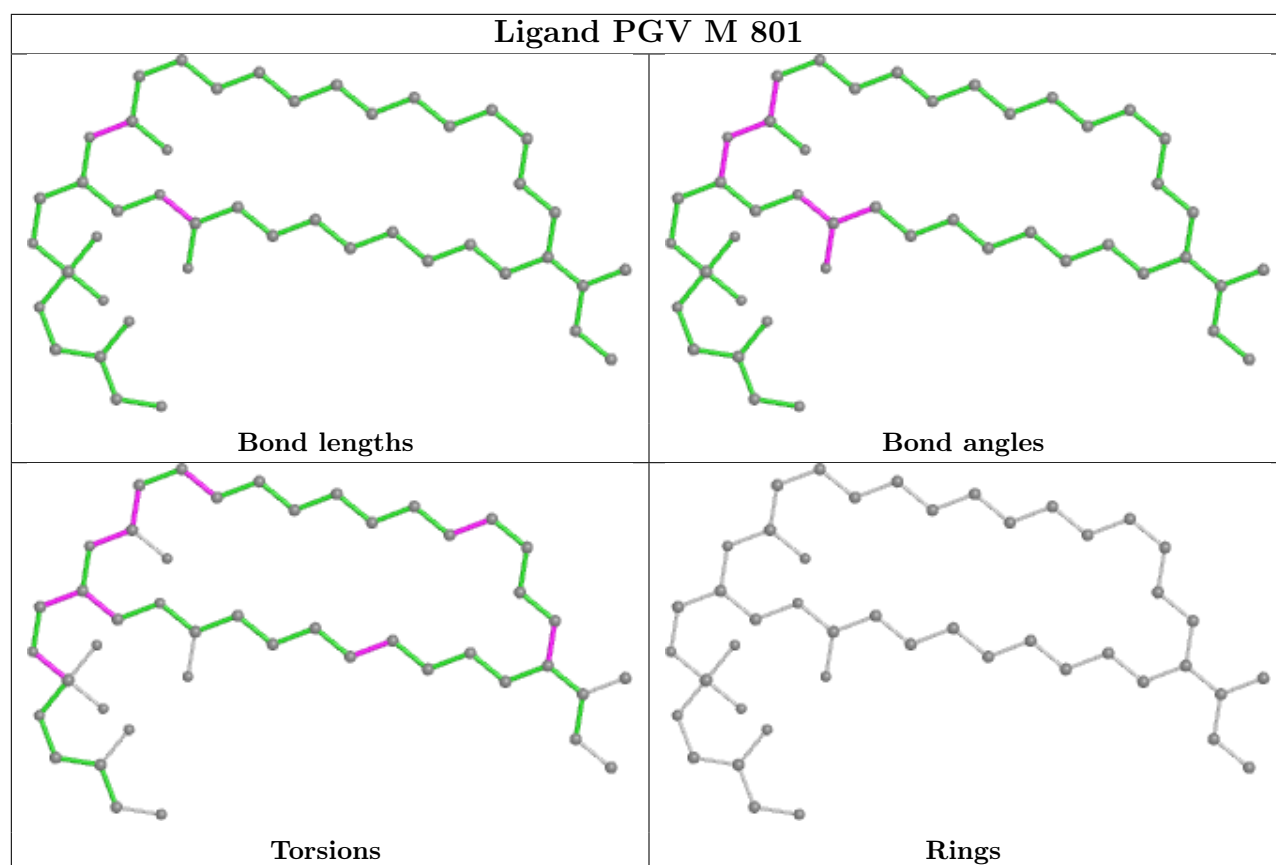


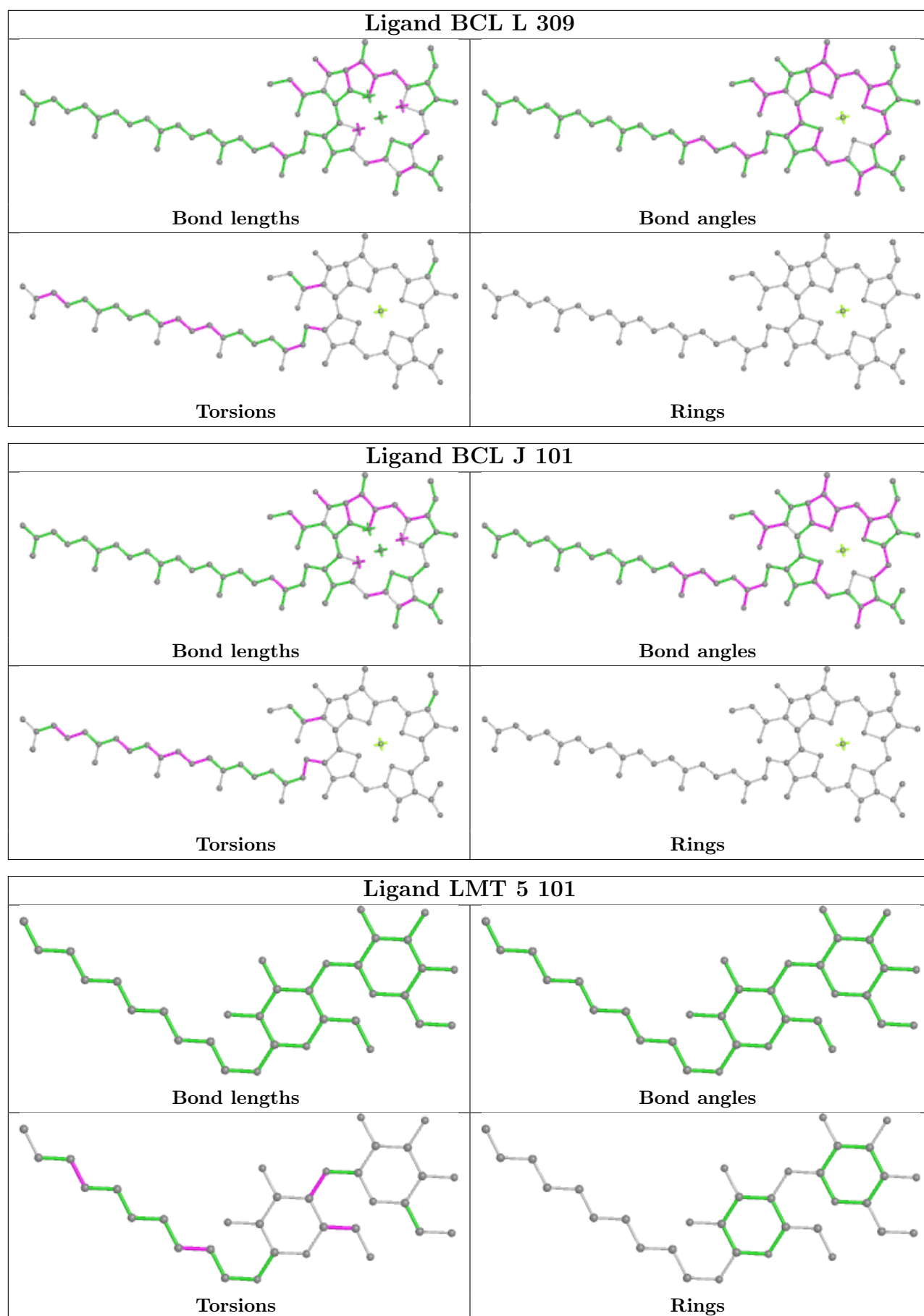


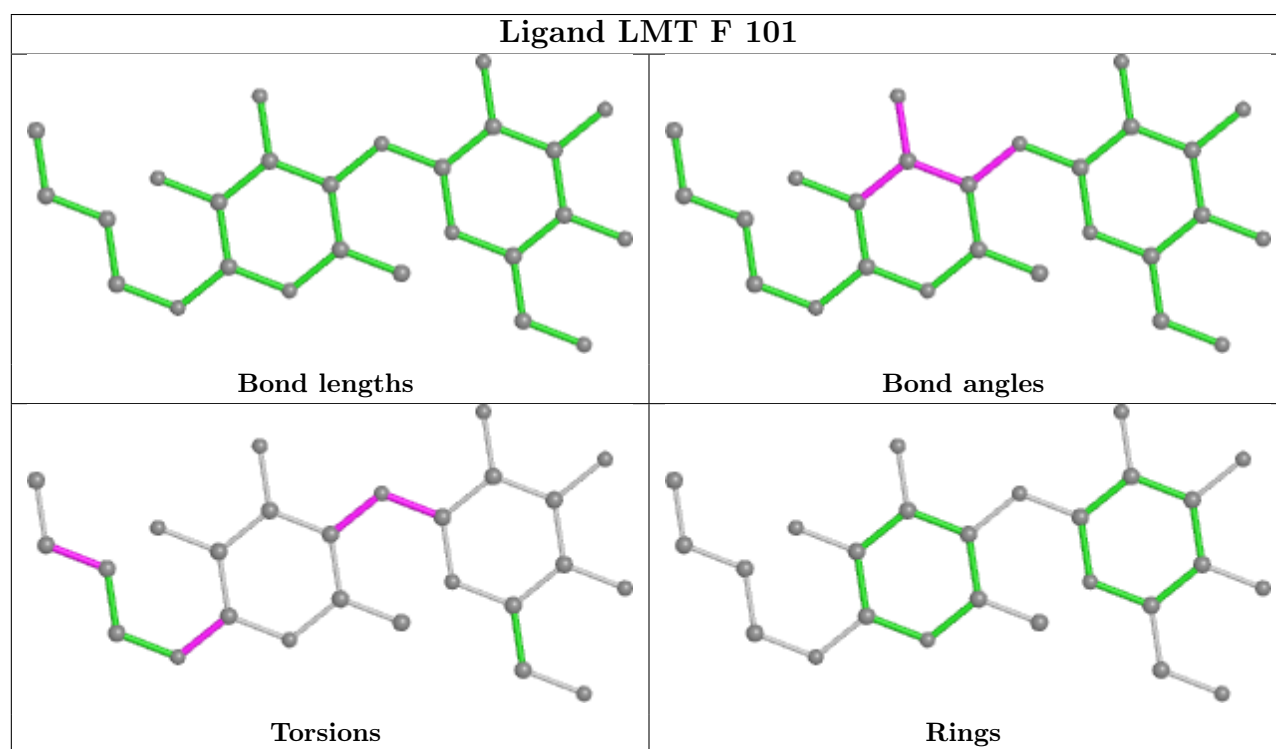
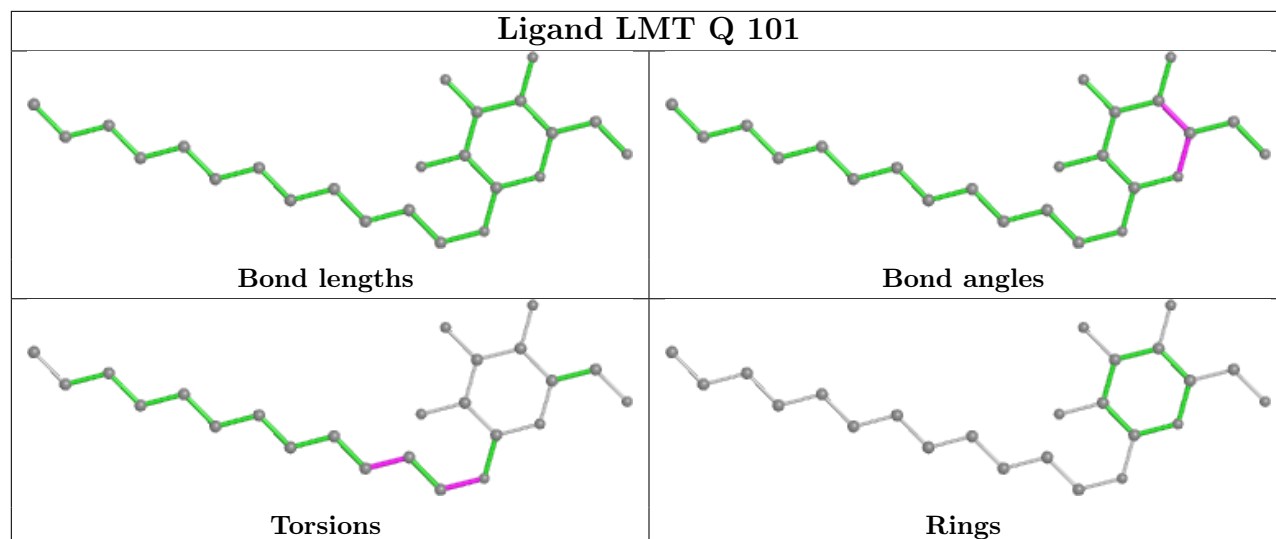


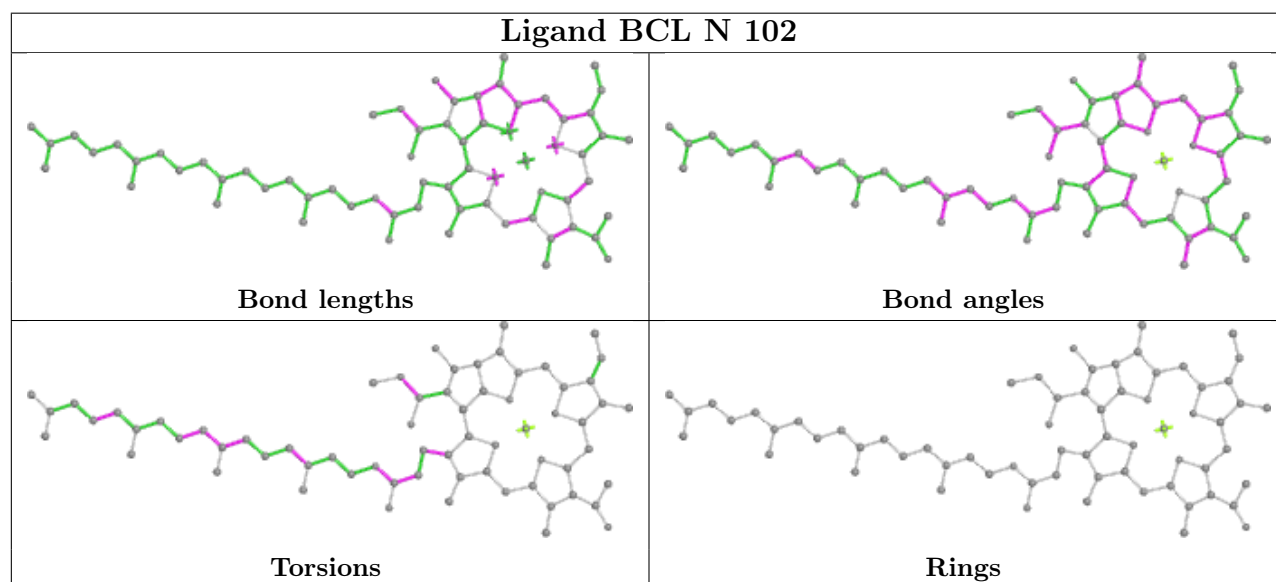
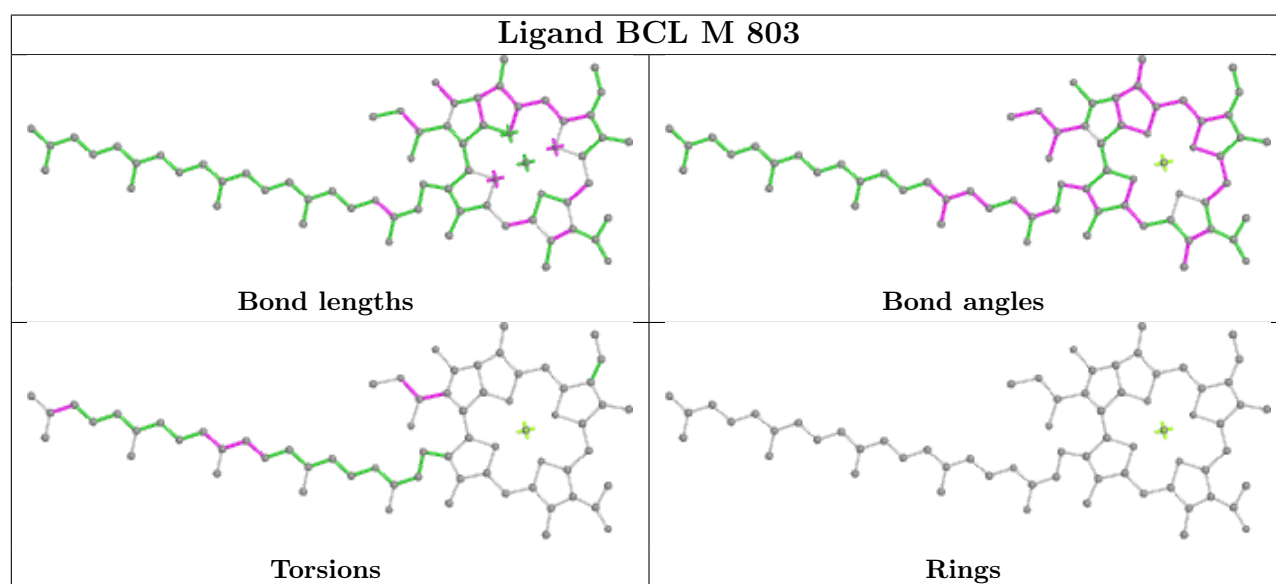
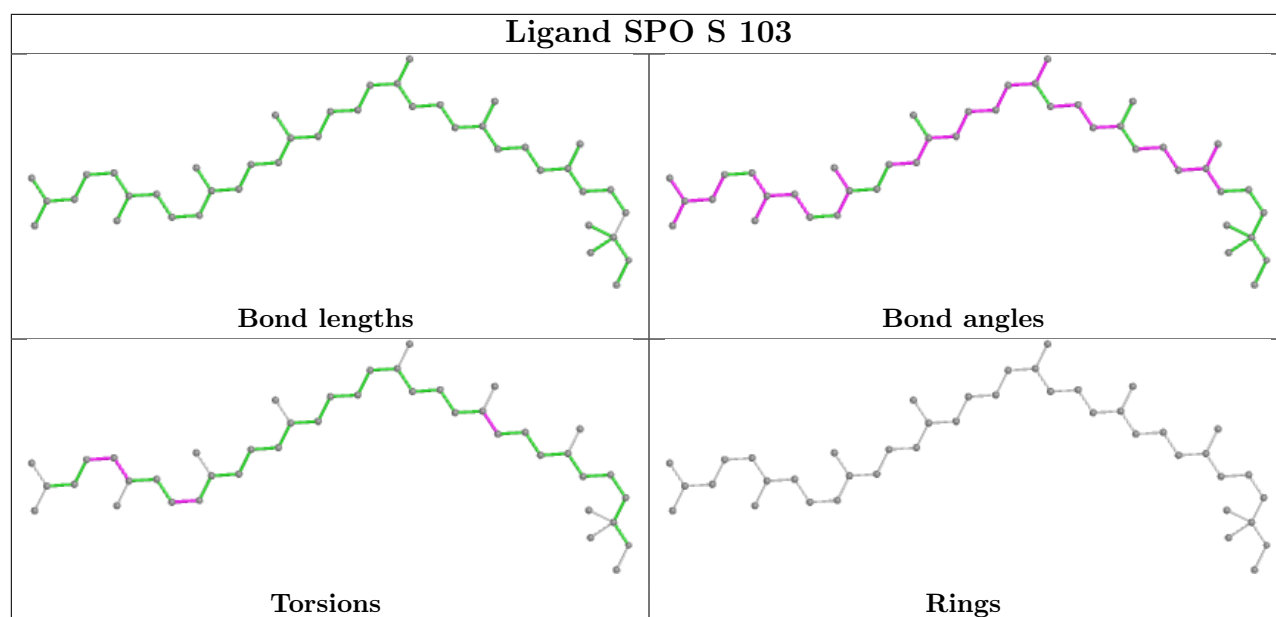


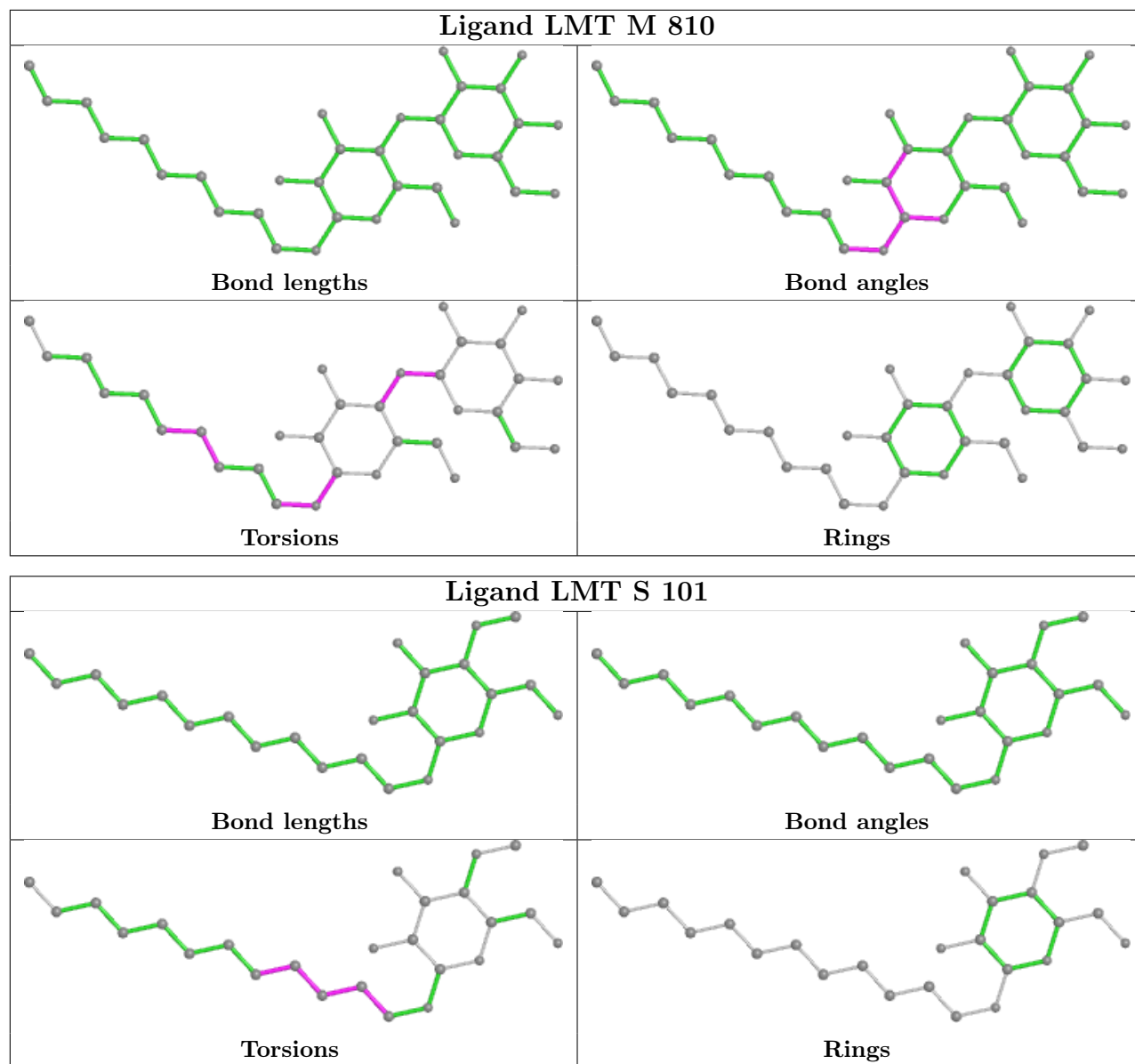


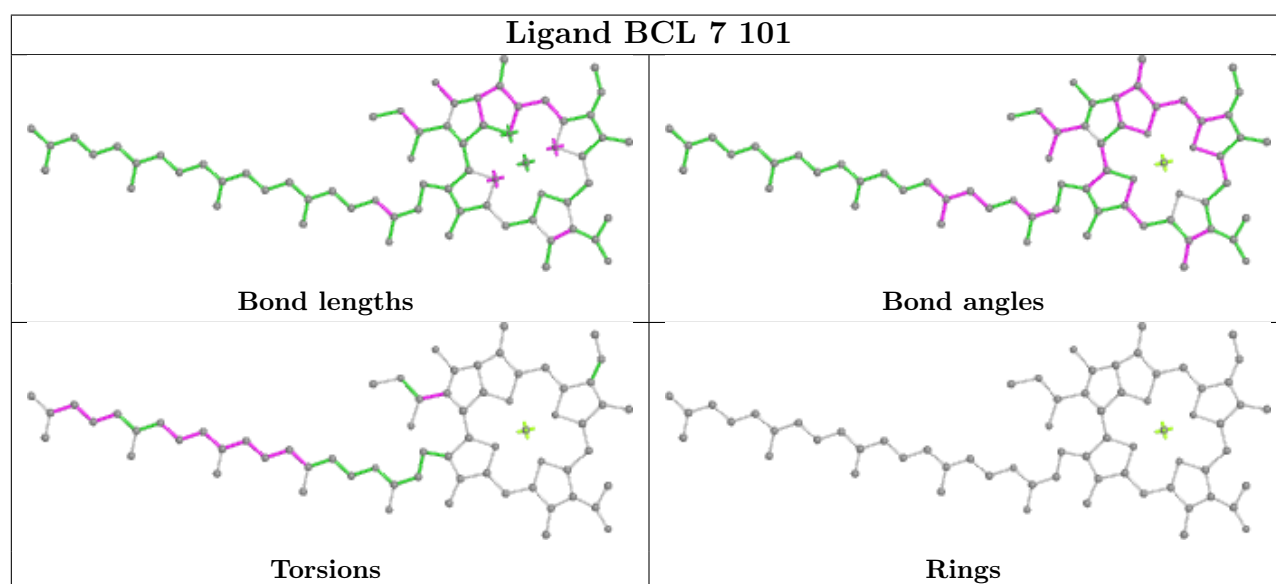
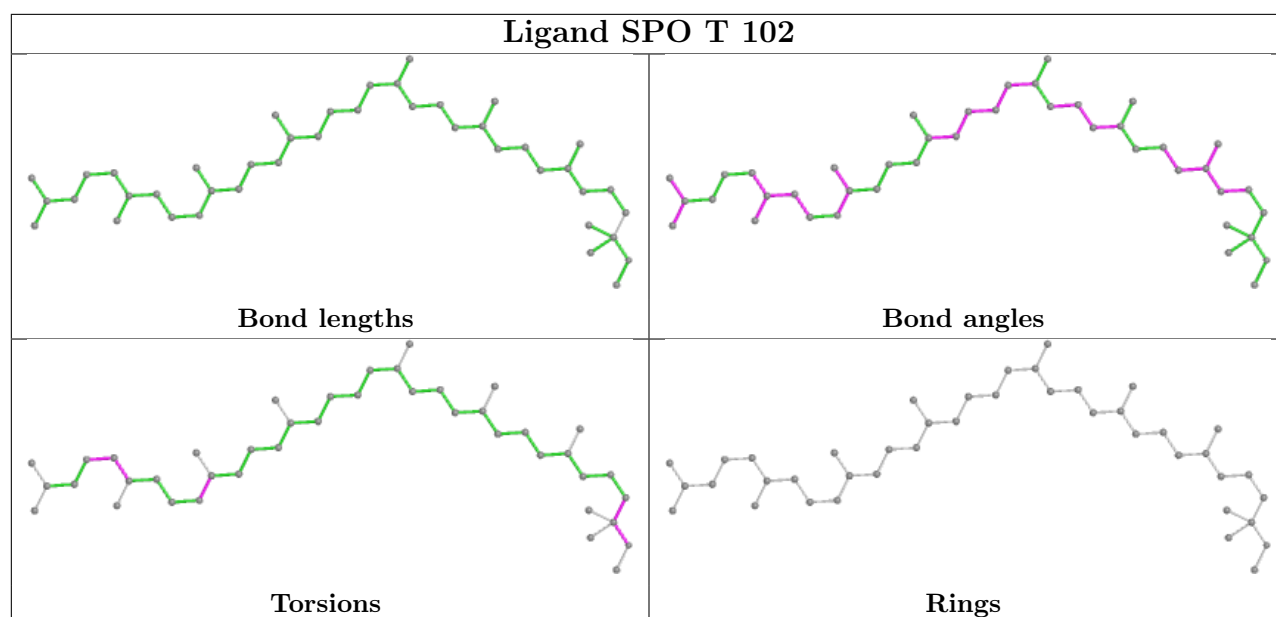


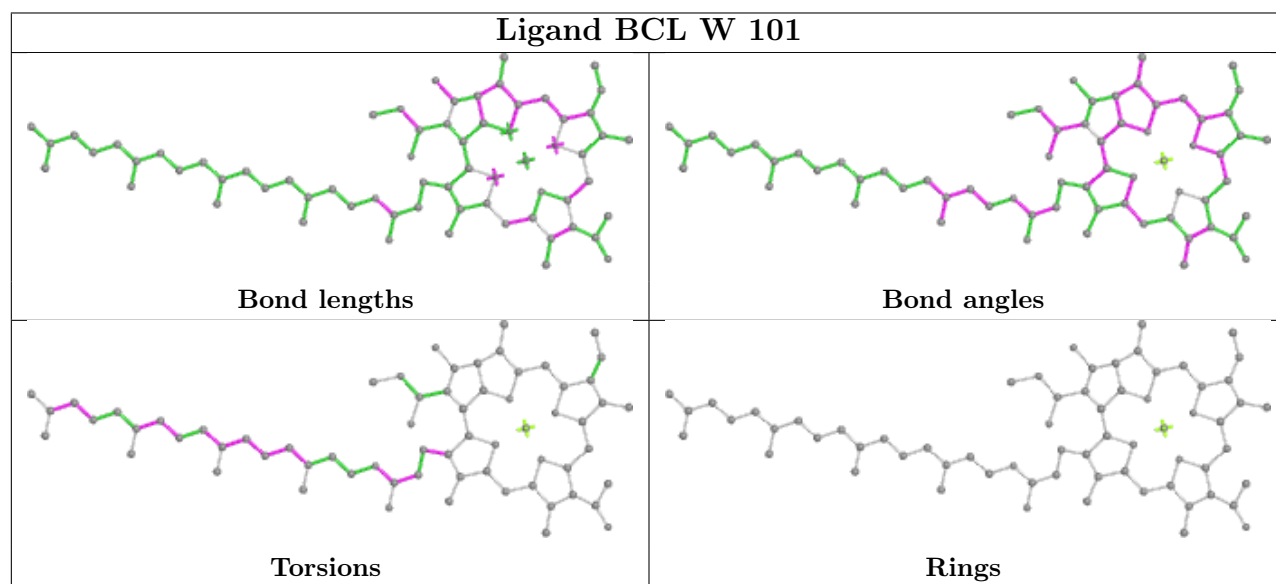
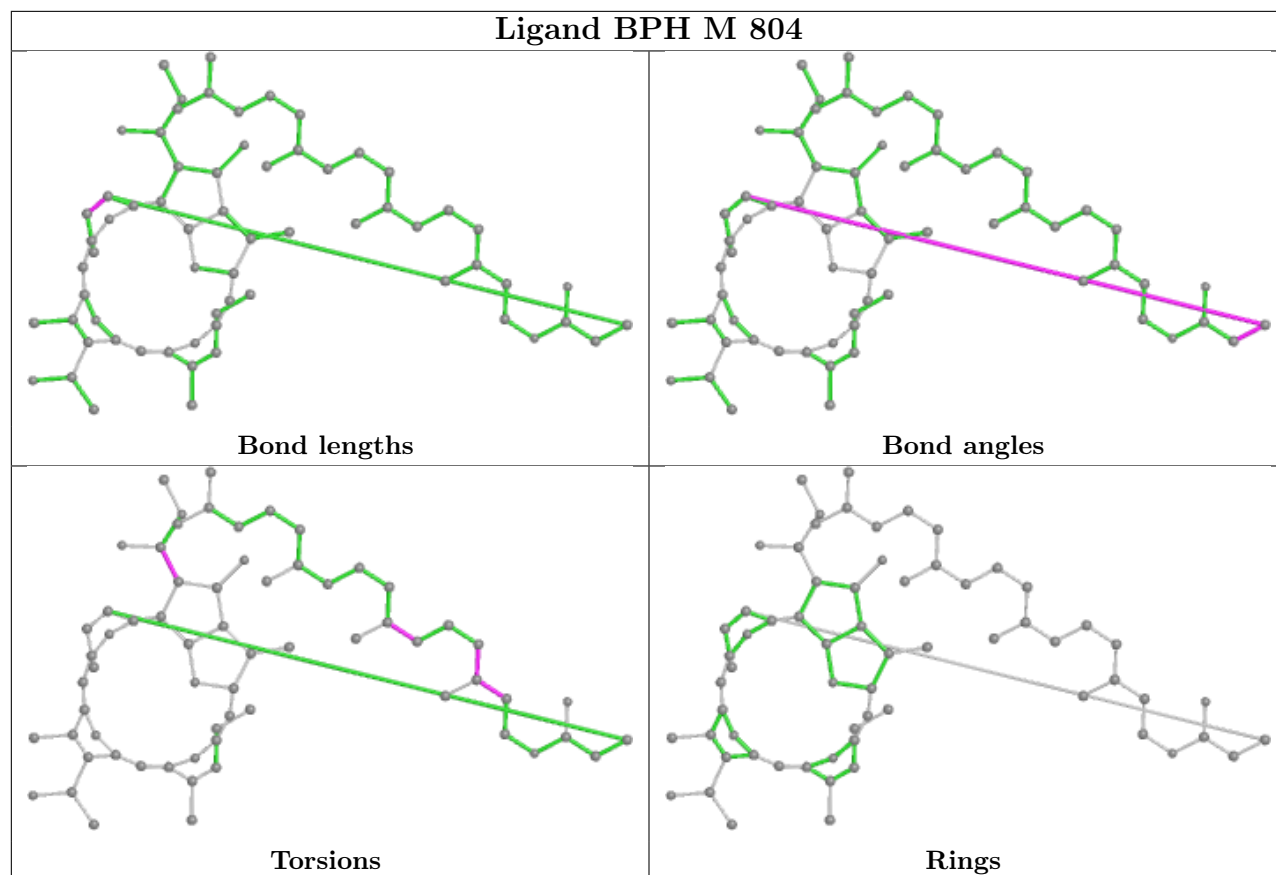


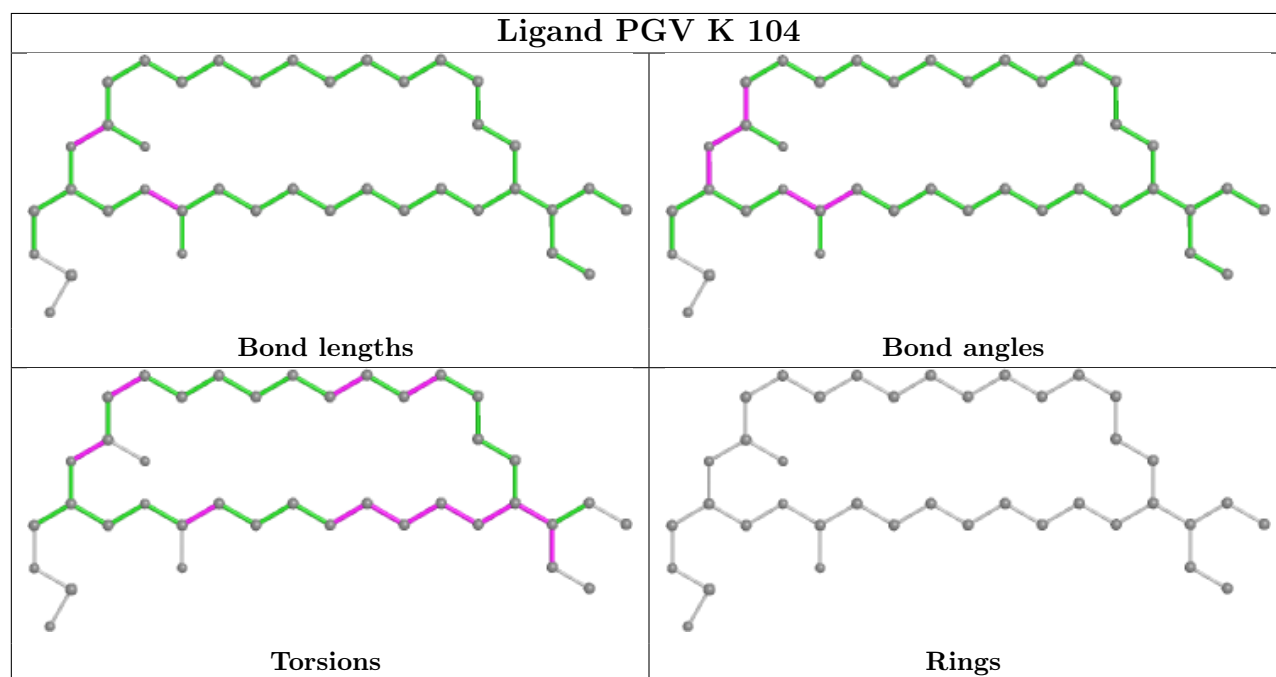
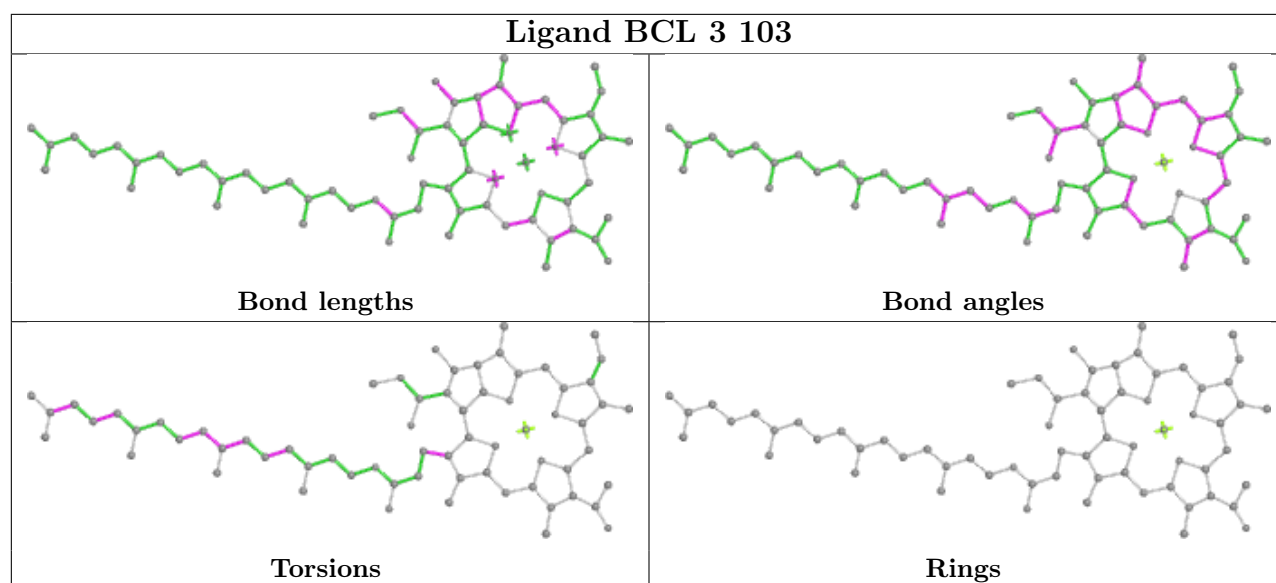


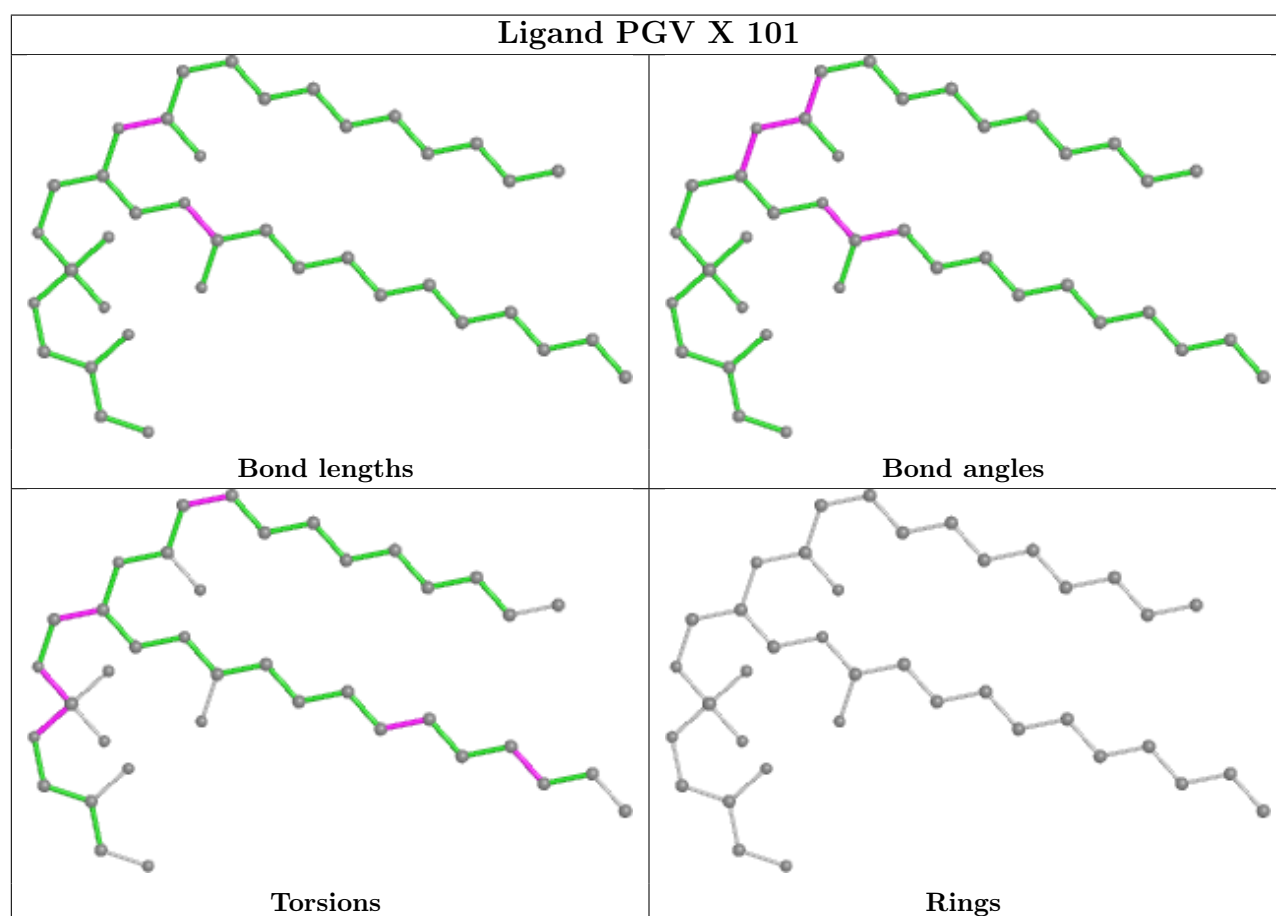
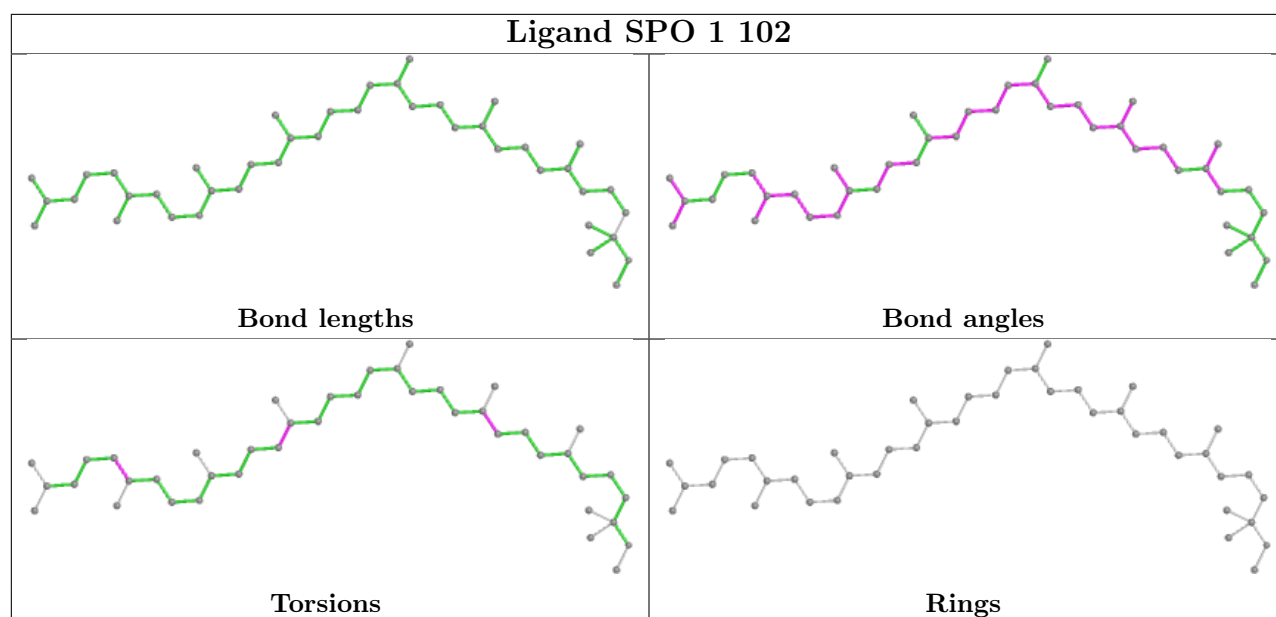


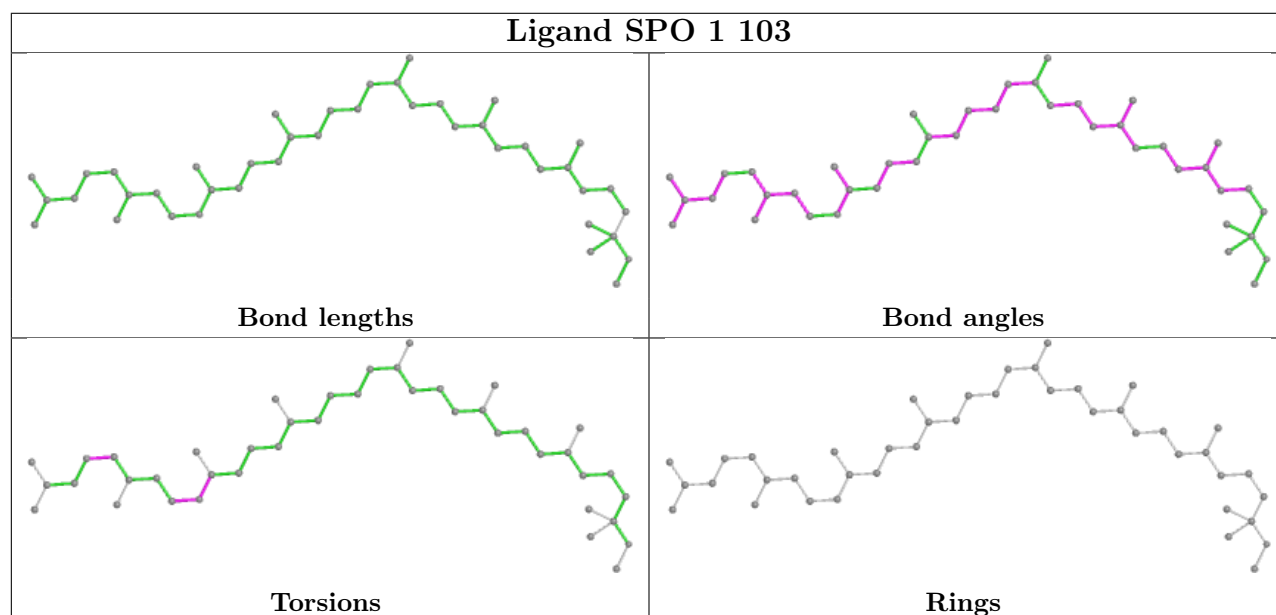
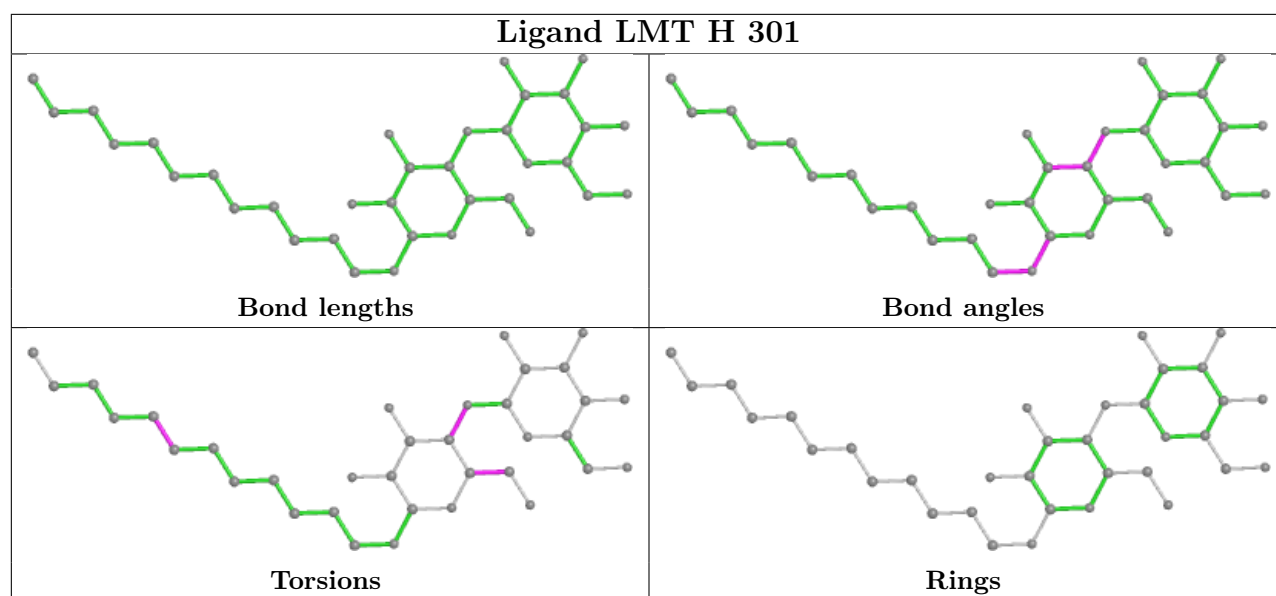


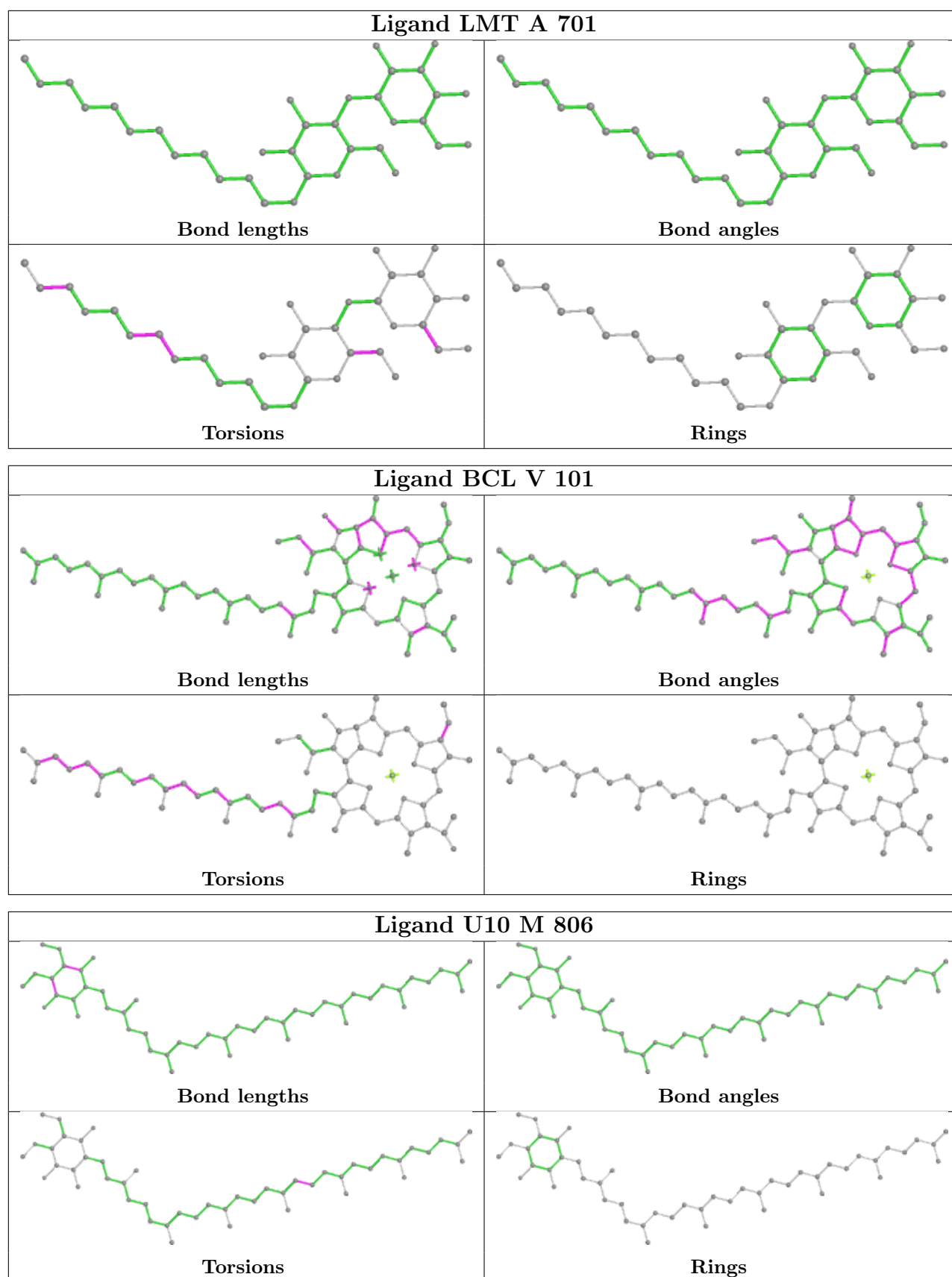


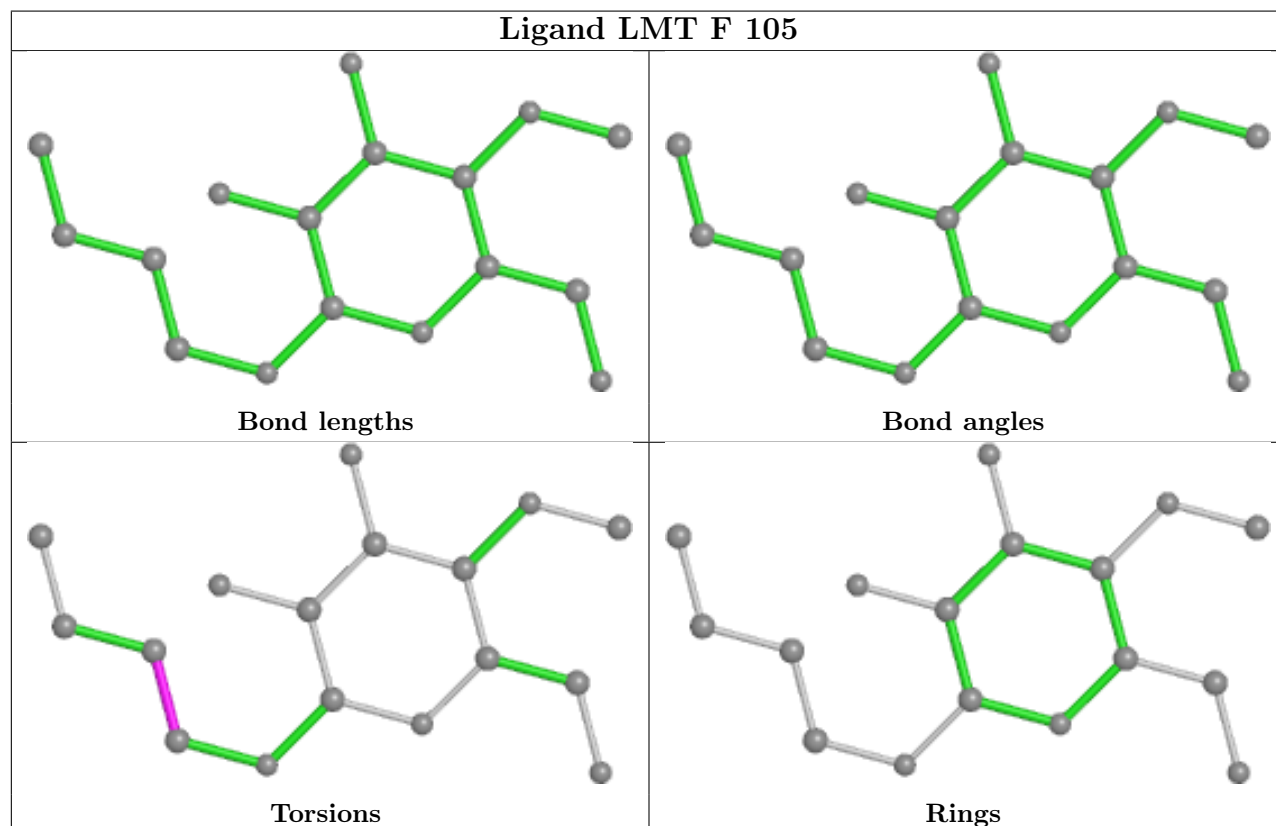
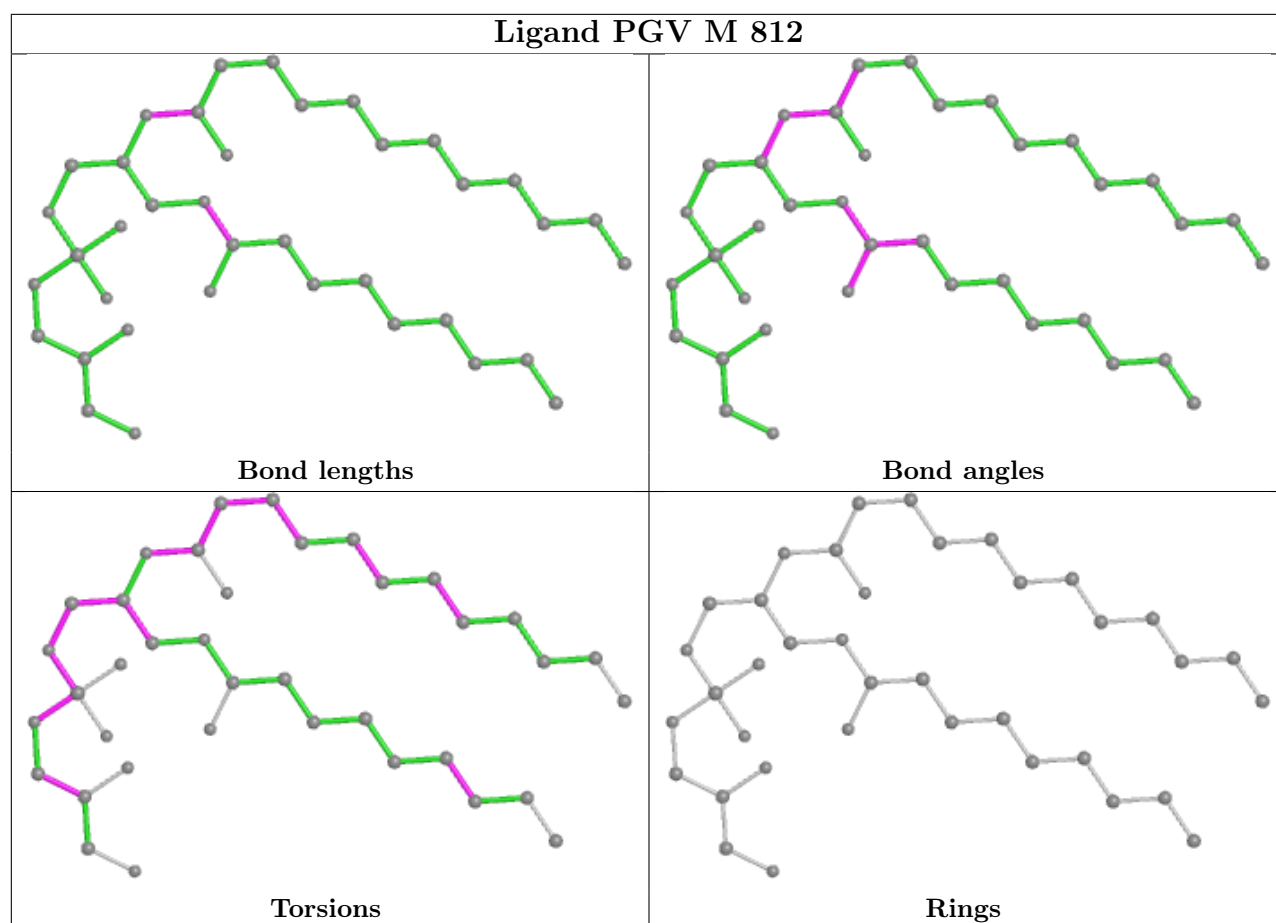


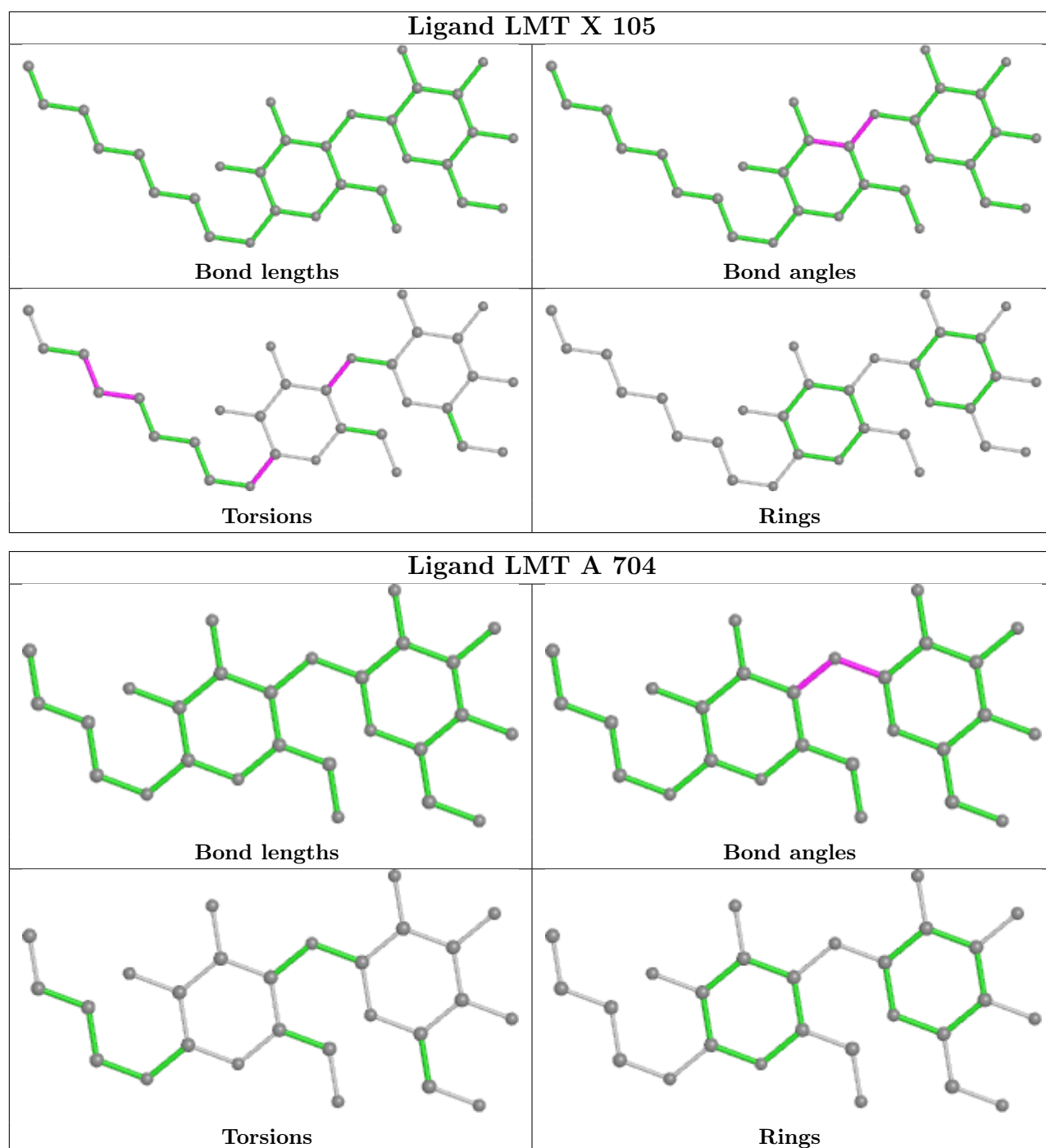












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31400. 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.