



## wwPDB EM Validation Summary Report ⓘ

Mar 8, 2025 – 12:50 PM EST

PDB ID : 9EH5  
EMDB ID : EMD-48046  
Title : Structure of a mutated photosystem II complex reveals changes to the hydrogen-bonding network that affect proton egress during O-O bond formation  
Authors : Flesher, D.A.; Shin, J.; Debus, R.J.; Brudvig, G.W.  
Deposited on : 2024-11-22  
Resolution : 1.97 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

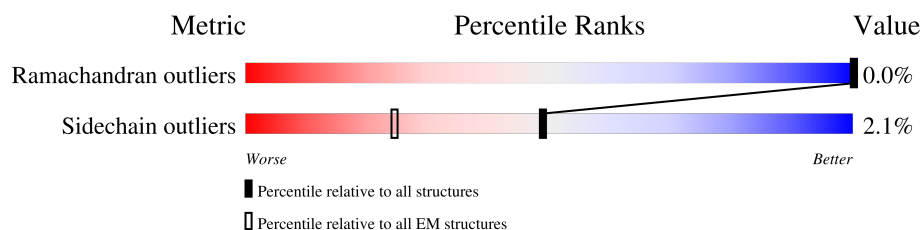
EMDB validation analysis : 0.0.1.dev117  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41.4

# 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 1.97 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.



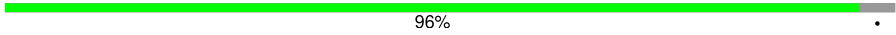


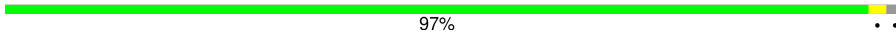
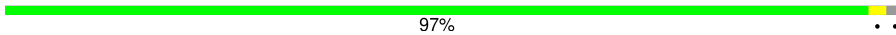
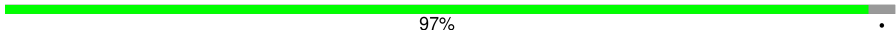
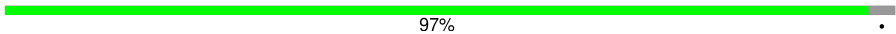


















Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	97% ..
1	a	344	97% ..
2	B	507	98% .
2	b	507	98% .
3	C	460	96% ..
3	c	460	96% ..
4	D	352	96% ..
4	d	352	96% ..
5	E	81	96% .

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Mol	Chain	Length	Quality of chain
5	e	81	 96%
6	F	44	 80% 20%
6	f	44	 80% 20%
7	H	64	 97% . .
7	h	64	 97% . .
8	I	38	 97% .
8	i	38	 97% .
9	J	39	 92% 8%
9	j	39	 92% 8%
10	K	45	 82% 18%
10	k	45	 82% 18%
11	L	39	 100%
11	l	39	 100%
12	M	35	 89% 11%
12	m	35	 89% 11%
13	O	274	 87% . 11%
13	o	274	 87% . 11%
14	Q	149	 75% . 23%
14	q	149	 75% . 23%
15	R	39	 82% 5% 13%
15	r	39	 82% 5% 13%
16	T	31	 90% 6% .
16	t	31	 90% 6% .
17	U	131	 69% . 27%
17	u	131	 69% . 27%

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Mol	Chain	Length	Quality of chain
18	V	160	
18	v	160	
19	X	39	
19	x	39	
20	Y	39	
20	y	39	
21	Z	62	
21	z	62	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	A	405	X	-	-	-
25	CLA	A	406	X	-	-	-
25	CLA	B	601	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-
25	CLA	C	501	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	509	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	C	510	X	-	-	-
25	CLA	C	511	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	D	401	X	-	-	-
25	CLA	D	403	X	-	-	-
25	CLA	a	405	X	-	-	-
25	CLA	a	406	X	-	-	-
25	CLA	b	602	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	b	617	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-
25	CLA	c	507	X	-	-	-
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-
25	CLA	d	401	X	-	-	-
25	CLA	d	403	X	-	-	-

## 2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 55154 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 Photosystem II protein D1 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	334	Total	C	N	O	S	0	0
			2625	1718	429	463	15		
1	a	334	Total	C	N	O	S	0	0
			2625	1718	429	463	15		

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	506	Total	C	N	O	S	0	0
			3958	2584	662	699	13		
2	b	506	Total	C	N	O	S	0	0
			3958	2584	662	699	13		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	450	Total	C	N	O	S	0	0
			3493	2293	584	603	13		
3	c	450	Total	C	N	O	S	0	0
			3493	2293	584	603	13		

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	341	Total	C	N	O	S	0	0
			2722	1804	442	464	12		
4	d	341	Total	C	N	O	S	0	0
			2722	1804	442	464	12		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	317	ALA	LYS	conflict	UNP P09192

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Chain	Residue	Modelled	Actual	Comment	Reference
d	317	ALA	LYS	conflict	UNP P09192

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	78	Total	C	N	O	S	0	0
			645	419	104	121	1		
5	e	78	Total	C	N	O	S	0	0
			645	419	104	121	1		

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	35	Total	C	N	O	S	0	0
			279	189	46	43	1		
6	f	35	Total	C	N	O	S	0	0
			279	189	46	43	1		

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	63	Total	C	N	O	S	0	0
			494	328	79	85	2		
7	h	63	Total	C	N	O	S	0	0
			494	328	79	85	2		

- Molecule 8 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	37	Total	C	N	O	S	0	0
			297	201	46	49	1		
8	i	37	Total	C	N	O	S	0	0
			297	201	46	49	1		

- Molecule 9 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	39	Total	C	N	O	S	0	0
			279	188	43	46	2		
9	j	39	Total	C	N	O	S	0	0
			279	188	43	46	2		

- Molecule 10 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	37	Total	C	N	O	0	0
			299	210	42	47		
10	k	37	Total	C	N	O	0	0
			299	210	42	47		

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	39	Total	C	N	O	S	0	0
			316	204	54	57	1		
11	l	39	Total	C	N	O	S	0	0
			316	204	54	57	1		

- Molecule 12 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	31	Total	C	N	O	S	0	0
			245	169	36	39	1		
12	m	31	Total	C	N	O	S	0	0
			245	169	36	39	1		

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	243	Total	C	N	O	S	0	0
			1873	1186	305	379	3		
13	o	243	Total	C	N	O	S	0	0
			1873	1186	305	379	3		

- Molecule 14 is a protein called Sll1638 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	115	Total	C	N	O	S	0	0
			896	564	160	170	2		
14	q	115	Total	C	N	O	S	0	0
			896	564	160	170	2		

- Molecule 15 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	R	34	Total	C	N	O	0	0
			258	170	45	43		
15	r	34	Total	C	N	O	0	0
			258	170	45	43		

- Molecule 16 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	30	Total	C	N	O	S	0	0
			241	163	36	40	2		
16	t	30	Total	C	N	O	S	0	0
			241	163	36	40	2		

- Molecule 17 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	U	95	Total	C	N	O	0	0
			740	461	123	156		
17	u	95	Total	C	N	O	0	0
			740	461	123	156		

- Molecule 18 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	135	Total	C	N	O	S	0	0
			1065	665	179	218	3		
18	v	135	Total	C	N	O	S	0	0
			1065	665	179	218	3		

- Molecule 19 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	38	Total	C	N	O	S	0	0
			288	193	46	48	1		
19	x	38	Total	C	N	O	S	0	0
			288	193	46	48	1		

- Molecule 20 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	Y	32	Total	C	N	O	0	0
			242	165	37	40		

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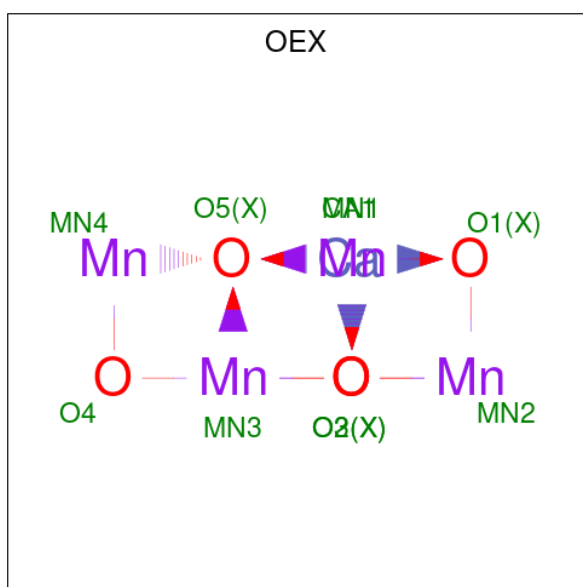
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Mol	Chain	Residues	Atoms				AltConf	Trace
20	y	32	Total	C	N	O	0	0
			242	165	37	40		

- Molecule 21 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Z	60	Total	C	N	O	S	0	0
			460	317	70	72	1		
21	z	60	Total	C	N	O	S	0	0
			460	317	70	72	1		

- Molecule 22 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



Mol	Chain	Residues	Atoms				AltConf
22	A	1	Total	Ca	Mn	O	0
			10	1	4	5	
22	a	1	Total	Ca	Mn	O	0
			10	1	4	5	

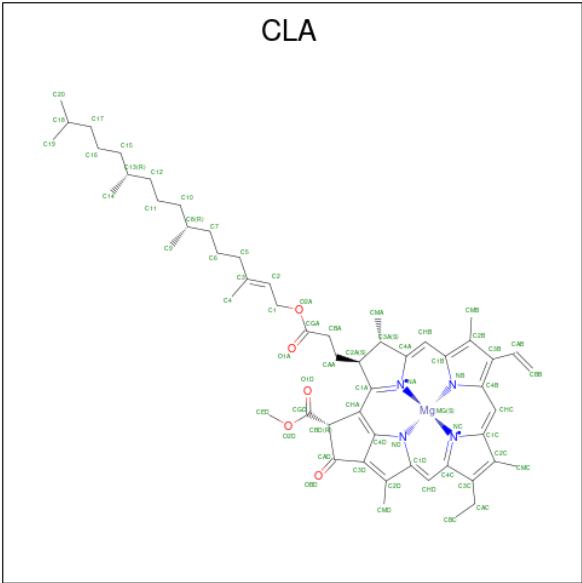
- Molecule 23 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
23	A	1	Total	Fe	0
			1	1	
23	a	1	Total	Fe	0
			1	1	

- Molecule 24 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
24	A	2	Total	Cl	0
			2	2	
24	a	2	Total	Cl	0
			2	2	

- Molecule 25 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
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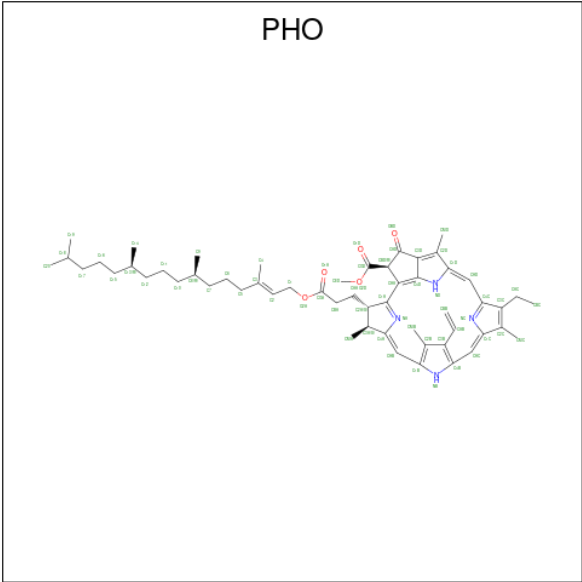
Mol	Chain	Residues	Atoms					AltConf
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25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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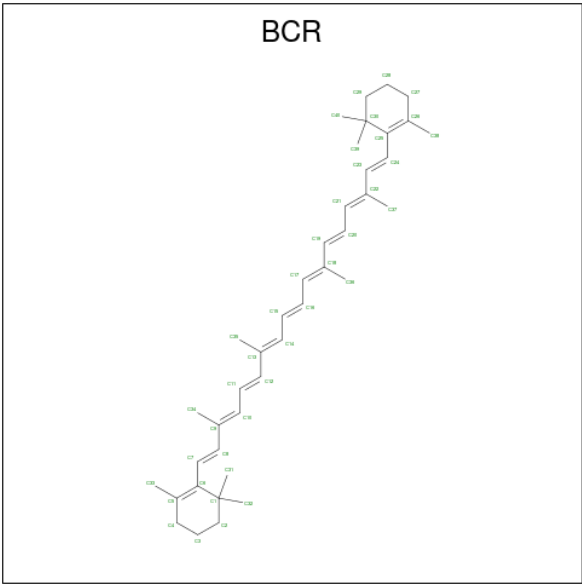
Mol	Chain	Residues	Atoms					AltConf
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	d	1	Total 65	C 55	Mg 1	N 4	O 5	0

- Molecule 26 is PHEOPHYTIN A (three-letter code: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).



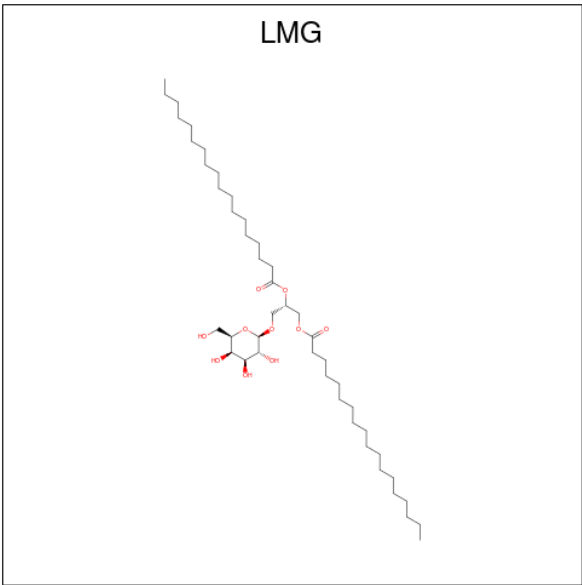
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	N	O	0
			64	55	4	5	
26	D	1	Total	C	N	O	0
			64	55	4	5	
26	a	1	Total	C	N	O	0
			64	55	4	5	
26	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 27 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



Mol	Chain	Residues	Atoms	AltConf
27	A	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	C	1	Total C 40 40	0
27	C	1	Total C 40 40	0
27	C	1	Total C 40 40	0
27	C	1	Total C 40 40	0
27	D	1	Total C 40 40	0
27	a	1	Total C 40 40	0
27	b	1	Total C 40 40	0
27	b	1	Total C 40 40	0
27	b	1	Total C 40 40	0
27	c	1	Total C 40 40	0
27	c	1	Total C 40 40	0
27	c	1	Total C 40 40	0
27	c	1	Total C 40 40	0
27	d	1	Total C 40 40	0

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



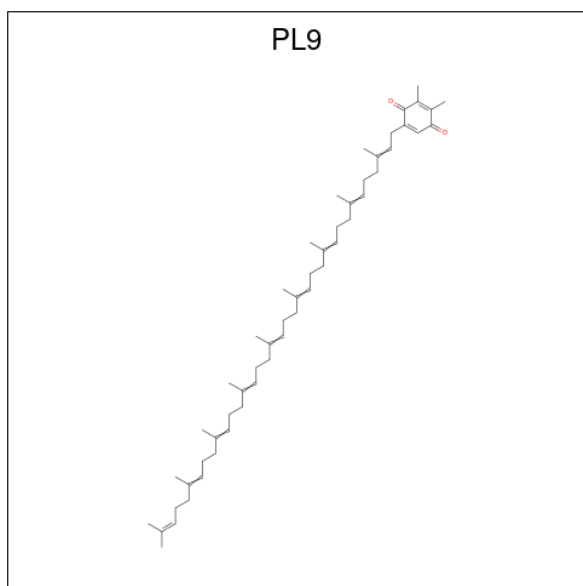
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			51	41	10	
28	A	1	Total	C	O	0
			36	26	10	
28	B	1	Total	C	O	0
			51	41	10	
28	B	1	Total	C	O	0
			47	37	10	
28	C	1	Total	C	O	0
			51	41	10	
28	C	1	Total	C	O	0
			49	39	10	
28	D	1	Total	C	O	0
			55	45	10	
28	J	1	Total	C	O	0
			55	45	10	
28	a	1	Total	C	O	0
			51	41	10	
28	a	1	Total	C	O	0
			36	26	10	
28	b	1	Total	C	O	0
			51	41	10	
28	b	1	Total	C	O	0
			47	37	10	
28	c	1	Total	C	O	0
			51	41	10	
28	c	1	Total	C	O	0
			49	39	10	

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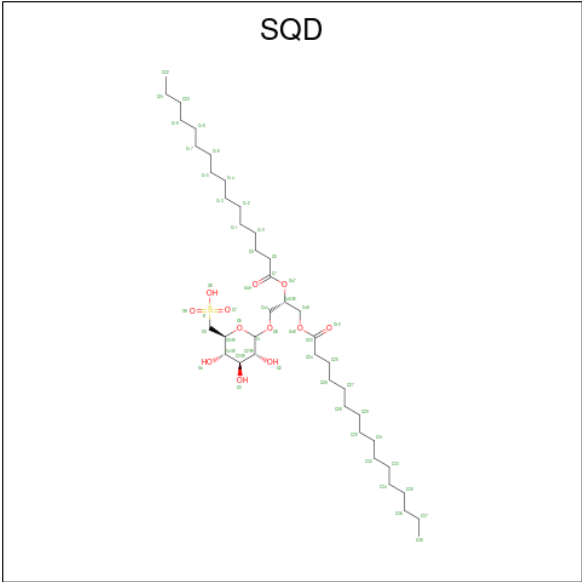
Mol	Chain	Residues	Atoms			AltConf
28	d	1	Total	C	O	0
			55	45	10	
28	j	1	Total	C	O	0
			55	45	10	

- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula:  $C_{53}H_{80}O_2$ ).



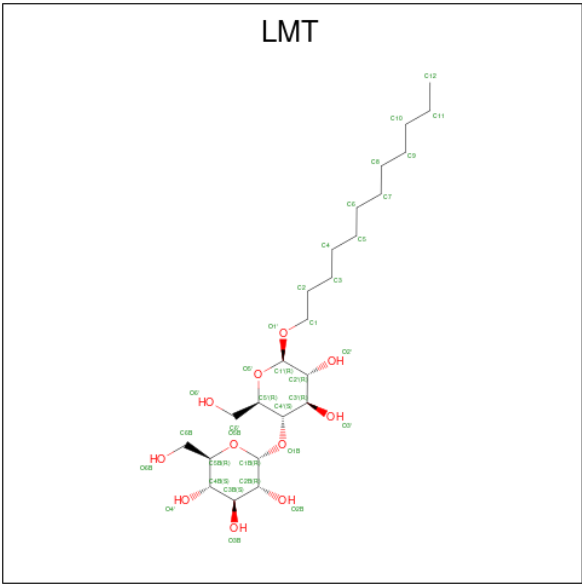
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			55	53	2	
29	D	1	Total	C	O	0
			55	53	2	
29	a	1	Total	C	O	0
			55	53	2	
29	d	1	Total	C	O	0
			55	53	2	

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O	S	0
			48	35	12	1	
30	A	1	Total	C	O	S	0
			54	41	12	1	
30	B	1	Total	C	O	S	0
			54	41	12	1	
30	B	1	Total	C	O	S	0
			54	41	12	1	
30	F	1	Total	C	O	S	0
			34	21	12	1	
30	H	1	Total	C	O	S	0
			54	41	12	1	
30	K	1	Total	C	O		0
			41	32	9		
30	a	1	Total	C	O	S	0
			48	35	12	1	
30	a	1	Total	C	O	S	0
			54	41	12	1	
30	b	1	Total	C	O	S	0
			54	41	12	1	
30	b	1	Total	C	O	S	0
			54	41	12	1	
30	f	1	Total	C	O	S	0
			34	21	12	1	
30	h	1	Total	C	O	S	0
			54	41	12	1	
30	k	1	Total	C	O		0
			41	32	9		

- Molecule 31 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			35	24	11	
31	A	1	Total	C	O	0
			24	18	6	
31	B	1	Total	C	O	0
			35	24	11	
31	B	1	Total	C	O	0
			24	18	6	
31	B	1	Total	C	O	0
			35	24	11	
31	B	1	Total	C	O	0
			24	18	6	
31	B	1	Total	C	O	0
			24	18	6	
31	B	1	Total	C	O	0
			35	24	11	
31	B	1	Total	C	O	0
			24	18	6	
31	C	1	Total	C	O	0
			24	18	6	
31	C	1	Total	C	O	0
			35	24	11	
31	C	1	Total	C	O	0
			21	15	6	
31	C	1	Total	C	O	0
			24	18	6	

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Mol	Chain	Residues	Atoms			AltConf
31	C	1	Total	C	O	0
			35	24	11	
31	D	1	Total	C	O	0
			24	18	6	
31	D	1	Total	C	O	0
			35	24	11	
31	D	1	Total	C	O	0
			35	24	11	
31	D	1	Total	C	O	0
			24	18	6	
31	E	1	Total	C	O	0
			22	16	6	
31	E	1	Total	C	O	0
			35	24	11	
31	F	1	Total	C	O	0
			35	24	11	
31	H	1	Total	C	O	0
			19	13	6	
31	I	1	Total	C	O	0
			24	18	6	
31	I	1	Total	C	O	0
			35	24	11	
31	I	1	Total	C	O	0
			22	16	6	
31	I	1	Total	C	O	0
			24	18	6	
31	J	1	Total	C	O	0
			35	24	11	
31	J	1	Total	C	O	0
			21	15	6	
31	M	1	Total	C	O	0
			35	24	11	
31	M	1	Total	C	O	0
			24	18	6	
31	T	1	Total	C	O	0
			24	18	6	
31	X	1	Total	C	O	0
			22	17	5	
31	X	1	Total	C	O	0
			22	16	6	
31	X	1	Total	C	O	0
			35	24	11	

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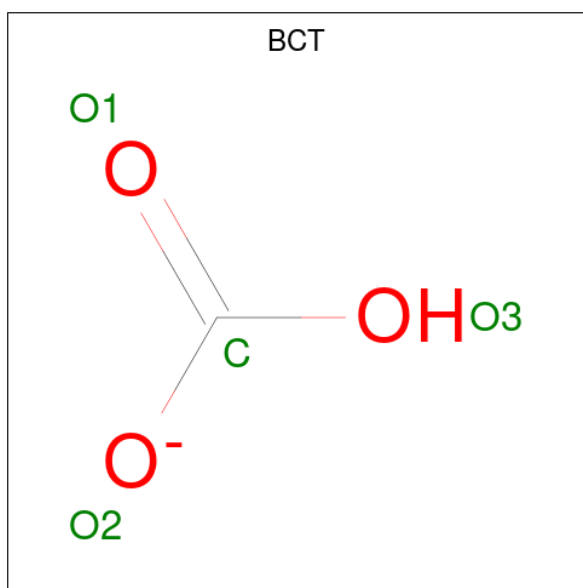
Mol	Chain	Residues	Atoms			AltConf
31	a	1	Total	C	O	0
			35	24	11	
31	a	1	Total	C	O	0
			24	18	6	
31	b	1	Total	C	O	0
			35	24	11	
31	b	1	Total	C	O	0
			24	18	6	
31	b	1	Total	C	O	0
			35	24	11	
31	b	1	Total	C	O	0
			24	18	6	
31	b	1	Total	C	O	0
			35	24	11	
31	b	1	Total	C	O	0
			24	18	6	
31	c	1	Total	C	O	0
			24	18	6	
31	c	1	Total	C	O	0
			35	24	11	
31	c	1	Total	C	O	0
			21	15	6	
31	c	1	Total	C	O	0
			24	18	6	
31	c	1	Total	C	O	0
			35	24	11	
31	d	1	Total	C	O	0
			24	18	6	
31	d	1	Total	C	O	0
			35	24	11	
31	d	1	Total	C	O	0
			35	24	11	
31	d	1	Total	C	O	0
			24	18	6	
31	e	1	Total	C	O	0
			22	16	6	
31	e	1	Total	C	O	0
			35	24	11	
31	f	1	Total	C	O	0
			35	24	11	
31	h	1	Total	C	O	0
			19	13	6	

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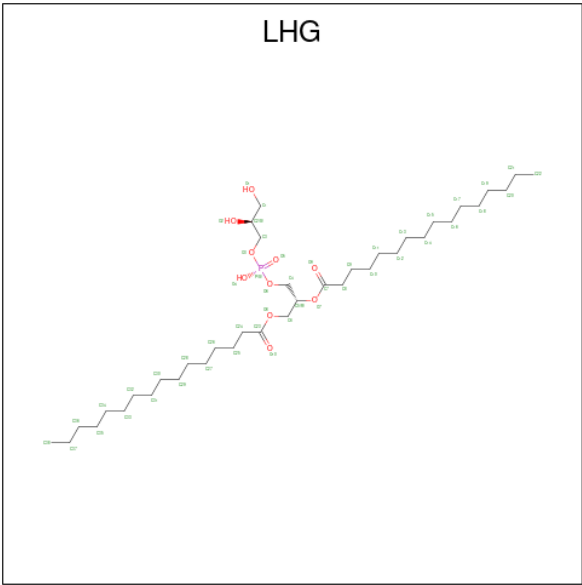
Mol	Chain	Residues	Atoms			AltConf
31	i	1	Total	C	O	0
			24	18	6	
31	i	1	Total	C	O	0
			35	24	11	
31	i	1	Total	C	O	0
			22	16	6	
31	i	1	Total	C	O	0
			24	18	6	
31	j	1	Total	C	O	0
			35	24	11	
31	j	1	Total	C	O	0
			21	15	6	
31	m	1	Total	C	O	0
			35	24	11	
31	m	1	Total	C	O	0
			24	18	6	
31	t	1	Total	C	O	0
			24	18	6	
31	x	1	Total	C	O	0
			22	17	5	
31	x	1	Total	C	O	0
			22	16	6	
31	x	1	Total	C	O	0
			35	24	11	

- Molecule 32 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3^-$ ).



Mol	Chain	Residues	Atoms			AltConf
32	A	1	Total	C	O	0
			4	1	3	
32	a	1	Total	C	O	0
			4	1	3	

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



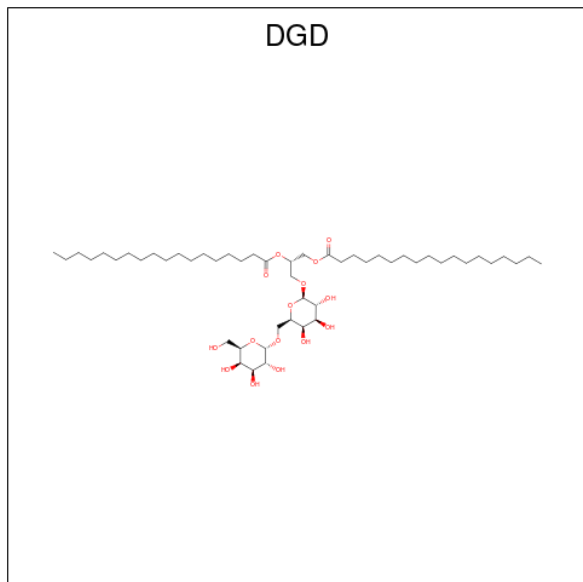
Mol	Chain	Residues	Atoms				AltConf
33	A	1	Total	C	O	P	0
			49	38	10	1	
33	A	1	Total	C	O	P	0
			49	38	10	1	
33	B	1	Total	C	O	P	0
			49	38	10	1	
33	D	1	Total	C	O	P	0
			49	38	10	1	
33	E	1	Total	C	O	P	0
			40	29	10	1	
33	L	1	Total	C	O	P	0
			49	38	10	1	
33	Z	1	Total	C	O	P	0
			36	27	8	1	
33	a	1	Total	C	O	P	0
			49	38	10	1	
33	a	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
33	b	1	Total	C	O	P	0
			49	38	10	1	
33	d	1	Total	C	O	P	0
			49	38	10	1	
33	e	1	Total	C	O	P	0
			40	29	10	1	
33	l	1	Total	C	O	P	0
			49	38	10	1	
33	z	1	Total	C	O	P	0
			36	27	8	1	

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



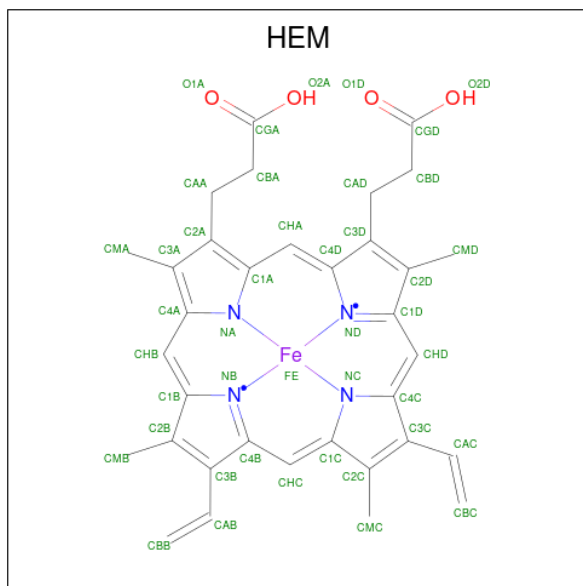
Mol	Chain	Residues	Atoms			AltConf
34	C	1	Total	C	O	0
			62	47	15	
34	C	1	Total	C	O	0
			62	47	15	
34	C	1	Total	C	O	0
			62	47	15	
34	H	1	Total	C	O	0
			62	47	15	
34	c	1	Total	C	O	0
			62	47	15	
34	c	1	Total	C	O	0
			62	47	15	

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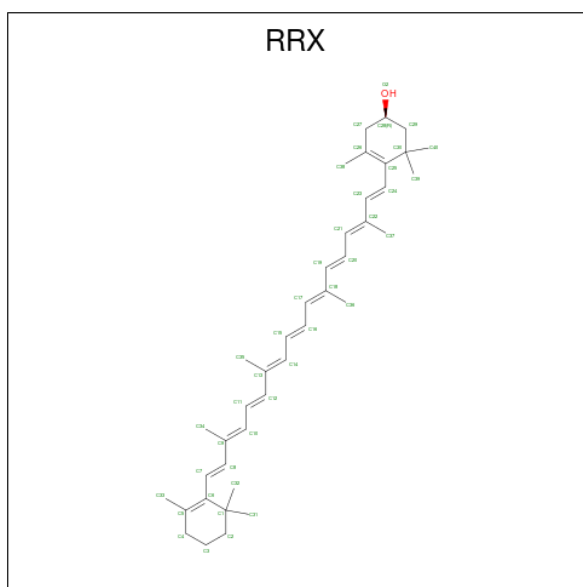
Mol	Chain	Residues	Atoms			AltConf
34	c	1	Total	C	O	0
			62	47	15	
34	h	1	Total	C	O	0
			62	47	15	

- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms					AltConf
35	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
35	V	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
35	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
35	v	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 36 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula:  $C_{40}H_{56}O$ ).



Mol	Chain	Residues	Atoms			AltConf
36	H	1	Total	C	O	0
			41	40	1	
36	h	1	Total	C	O	0
			41	40	1	

- Molecule 37 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
37	K	1	Total	Ca	0
			1	1	
37	U	1	Total	Ca	0
			1	1	
37	V	1	Total	Ca	0
			1	1	
37	k	1	Total	Ca	0
			1	1	
37	u	1	Total	Ca	0
			1	1	
37	v	1	Total	Ca	0
			1	1	

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		AltConf
38	A	131	Total	O	0
			131	131	

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Mol	Chain	Residues	Atoms		AltConf
38	B	147	Total 147	O 147	0
38	C	112	Total 112	O 112	0
38	D	110	Total 110	O 110	0
38	E	15	Total 15	O 15	0
38	F	5	Total 5	O 5	0
38	H	13	Total 13	O 13	0
38	I	5	Total 5	O 5	0
38	J	2	Total 2	O 2	0
38	K	2	Total 2	O 2	0
38	L	10	Total 10	O 10	0
38	M	7	Total 7	O 7	0
38	O	35	Total 35	O 35	0
38	T	11	Total 11	O 11	0
38	U	10	Total 10	O 10	0
38	V	28	Total 28	O 28	0
38	X	4	Total 4	O 4	0
38	a	132	Total 132	O 132	0
38	b	147	Total 147	O 147	0
38	c	112	Total 112	O 112	0
38	d	109	Total 109	O 109	0
38	e	15	Total 15	O 15	0

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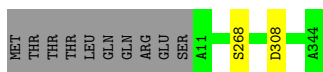
Mol	Chain	Residues	Atoms		AltConf
38	f	5	Total 5	O 5	0
38	h	13	Total 13	O 13	0
38	i	5	Total 5	O 5	0
38	j	2	Total 2	O 2	0
38	k	2	Total 2	O 2	0
38	l	10	Total 10	O 10	0
38	m	7	Total 7	O 7	0
38	o	35	Total 35	O 35	0
38	t	11	Total 11	O 11	0
38	u	10	Total 10	O 10	0
38	v	28	Total 28	O 28	0
38	x	4	Total 4	O 4	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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

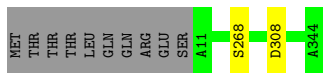
- Molecule 1: Photosystem II protein D1 2

Chain A:  97%



- Molecule 1: Photosystem II protein D1 2

Chain a:  97%



- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:  98%



- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  98%



- Molecule 3: Photosystem II CP43 reaction center protein

Chain C:  96%



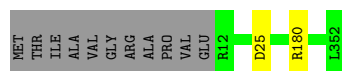
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c:  96% ..



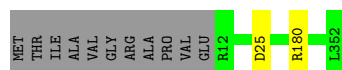
- Molecule 4: Photosystem II D2 protein

Chain D:  96% ..



- Molecule 4: Photosystem II D2 protein

Chain d:  96% ..



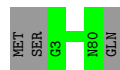
- Molecule 5: Cytochrome b559 subunit alpha

Chain E:  96% .




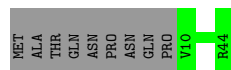
- Molecule 5: Cytochrome b559 subunit alpha

Chain e:  96% .




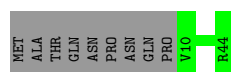
- Molecule 6: Cytochrome b559 subunit beta

Chain F:  80% 20%

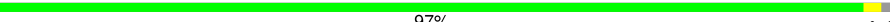


- Molecule 6: Cytochrome b559 subunit beta

Chain f:  80% 20%



- Molecule 7: Photosystem II reaction center protein H

Chain H:  97% ..



- Molecule 7: Photosystem II reaction center protein H

Chain h:  97% ..



- Molecule 8: Photosystem II reaction center protein I

Chain I:  97% .



- Molecule 8: Photosystem II reaction center protein I

Chain i:  97% .



- Molecule 9: Photosystem II reaction center protein J

Chain J:  92% 8%



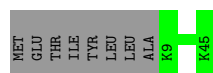
- Molecule 9: Photosystem II reaction center protein J

Chain j:  92% 8%




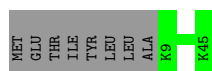
- Molecule 10: Photosystem II reaction center protein K

Chain K:  82% 18%



- Molecule 10: Photosystem II reaction center protein K

Chain k:  82% 18%



- Molecule 11: Photosystem II reaction center protein L

Chain L:  100%

There are no outlier residues recorded for this chain.

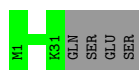
- Molecule 11: Photosystem II reaction center protein L

Chain l:  100%

There are no outlier residues recorded for this chain.

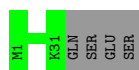
- Molecule 12: Photosystem II reaction center protein M

Chain M:  89% 11%



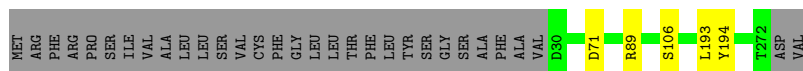
- Molecule 12: Photosystem II reaction center protein M

Chain m:  89% 11%




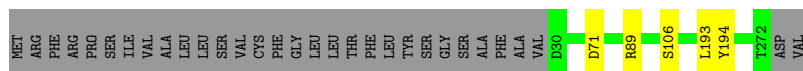
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  87% 11%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

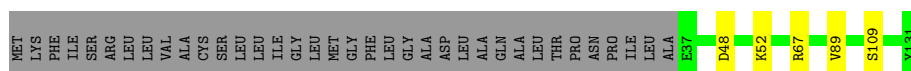
Chain o:  87% 11%



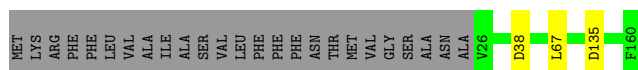
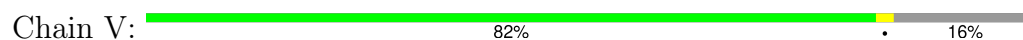
- Molecule 14: Sll1638 protein

Chain Q:  75% 23%

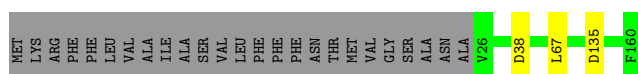




- Molecule 18: Cytochrome c-550



- Molecule 18: Cytochrome c-550



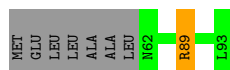
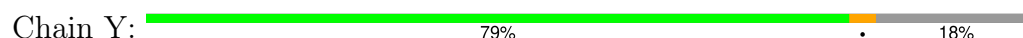
- Molecule 19: Photosystem II reaction center X protein



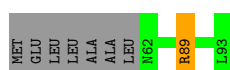
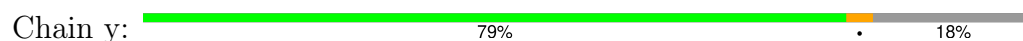
- Molecule 19: Photosystem II reaction center X protein



- Molecule 20: Photosystem II reaction center protein Ycf12



- Molecule 20: Photosystem II reaction center protein Ycf12



- Molecule 21: Photosystem II reaction center protein Z





- Molecule 21: Photosystem II reaction center protein Z

Chain z:  94% . .





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	518876	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	38	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.059	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	346.112, 346.112, 346.112	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, LMG, BCR, SQD, CLA, FME, PHO, OEX, HEM, BCT, LMT, CL, LHG, DGD, PL9, CA, RRX

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	A	0.42	0/2710	0.60	0/3694
1	a	0.42	0/2710	0.60	0/3694
2	B	0.41	0/4091	0.59	0/5568
2	b	0.41	0/4091	0.59	0/5568
3	C	0.40	0/3608	0.58	0/4912
3	c	0.40	0/3608	0.58	0/4912
4	D	0.39	0/2819	0.59	0/3839
4	d	0.39	0/2819	0.59	0/3839
5	E	0.38	0/664	0.61	0/906
5	e	0.38	0/664	0.61	0/906
6	F	0.42	0/288	0.67	0/393
6	f	0.42	0/288	0.67	0/393
7	H	0.33	0/506	0.59	0/687
7	h	0.33	0/506	0.59	0/687
8	I	0.38	0/294	0.57	0/397
8	i	0.38	0/294	0.57	0/397
9	J	0.35	0/278	0.54	0/375
9	j	0.35	0/278	0.54	0/375
10	K	0.40	0/310	0.58	0/424
10	k	0.40	0/310	0.58	0/424
11	L	0.35	0/322	0.53	0/435
11	l	0.35	0/322	0.53	0/435
12	M	0.32	0/239	0.49	0/325
12	m	0.32	0/239	0.49	0/325
13	O	0.39	0/1911	0.64	0/2590
13	o	0.39	0/1911	0.64	0/2590
14	Q	0.37	0/910	0.61	0/1229
14	q	0.37	0/910	0.61	0/1229
15	R	0.30	0/262	0.60	0/361
15	r	0.30	0/262	0.60	0/361
16	T	0.32	0/236	0.49	0/321

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	t	0.32	0/236	0.50	0/321
17	U	0.33	0/751	0.61	0/1018
17	u	0.33	0/751	0.61	0/1018
18	V	0.34	0/1086	0.58	0/1476
18	v	0.34	0/1086	0.58	0/1476
19	X	0.28	0/293	0.55	0/399
19	x	0.28	0/293	0.55	0/399
20	Y	0.39	0/247	0.70	1/335 (0.3%)
20	y	0.39	0/247	0.70	1/335 (0.3%)
21	Z	0.30	0/472	0.48	0/649
21	z	0.30	0/472	0.48	0/649
All	All	0.39	0/44594	0.59	2/60666 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	y	89	ARG	CG-CD-NE	5.23	122.78	111.80
20	Y	89	ARG	CG-CD-NE	5.21	122.75	111.80

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	A	332/344 (96%)	326 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	332/344 (96%)	326 (98%)	6 (2%)	0	100	100
2	B	504/507 (99%)	492 (98%)	11 (2%)	1 (0%)	44	35
2	b	504/507 (99%)	492 (98%)	11 (2%)	1 (0%)	44	35
3	C	448/460 (97%)	442 (99%)	6 (1%)	0	100	100
3	c	448/460 (97%)	442 (99%)	6 (1%)	0	100	100
4	D	339/352 (96%)	331 (98%)	8 (2%)	0	100	100
4	d	339/352 (96%)	331 (98%)	8 (2%)	0	100	100
5	E	76/81 (94%)	76 (100%)	0	0	100	100
5	e	76/81 (94%)	76 (100%)	0	0	100	100
6	F	33/44 (75%)	31 (94%)	2 (6%)	0	100	100
6	f	33/44 (75%)	31 (94%)	2 (6%)	0	100	100
7	H	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
7	h	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
8	I	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
8	i	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
9	J	37/39 (95%)	37 (100%)	0	0	100	100
9	j	37/39 (95%)	37 (100%)	0	0	100	100
10	K	35/45 (78%)	35 (100%)	0	0	100	100
10	k	35/45 (78%)	35 (100%)	0	0	100	100
11	L	37/39 (95%)	37 (100%)	0	0	100	100
11	l	37/39 (95%)	37 (100%)	0	0	100	100
12	M	29/35 (83%)	28 (97%)	1 (3%)	0	100	100
12	m	29/35 (83%)	28 (97%)	1 (3%)	0	100	100
13	O	241/274 (88%)	223 (92%)	18 (8%)	0	100	100
13	o	241/274 (88%)	223 (92%)	18 (8%)	0	100	100
14	Q	113/149 (76%)	109 (96%)	4 (4%)	0	100	100
14	q	113/149 (76%)	109 (96%)	4 (4%)	0	100	100
15	R	32/39 (82%)	32 (100%)	0	0	100	100
15	r	32/39 (82%)	32 (100%)	0	0	100	100
16	T	28/31 (90%)	28 (100%)	0	0	100	100
16	t	28/31 (90%)	28 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	U	93/131 (71%)	90 (97%)	3 (3%)	0	100	100
17	u	93/131 (71%)	90 (97%)	3 (3%)	0	100	100
18	V	133/160 (83%)	130 (98%)	3 (2%)	0	100	100
18	v	133/160 (83%)	130 (98%)	3 (2%)	0	100	100
19	X	36/39 (92%)	36 (100%)	0	0	100	100
19	x	36/39 (92%)	36 (100%)	0	0	100	100
20	Y	30/39 (77%)	30 (100%)	0	0	100	100
20	y	30/39 (77%)	30 (100%)	0	0	100	100
21	Z	58/62 (94%)	58 (100%)	0	0	100	100
21	z	58/62 (94%)	58 (100%)	0	0	100	100
All	All	5460/5944 (92%)	5330 (98%)	128 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	76	ASN
2	b	76	ASN

### 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	A	273/283 (96%)	271 (99%)	2 (1%)	81	82
1	a	273/283 (96%)	271 (99%)	2 (1%)	81	82
2	B	403/404 (100%)	395 (98%)	8 (2%)	50	43
2	b	403/404 (100%)	395 (98%)	8 (2%)	50	43
3	C	351/361 (97%)	341 (97%)	10 (3%)	38	28
3	c	351/361 (97%)	341 (97%)	10 (3%)	38	28
4	D	276/284 (97%)	274 (99%)	2 (1%)	81	82
4	d	276/284 (97%)	274 (99%)	2 (1%)	81	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	70/73 (96%)	70 (100%)	0	100	100
5	e	70/73 (96%)	70 (100%)	0	100	100
6	F	28/37 (76%)	28 (100%)	0	100	100
6	f	28/37 (76%)	28 (100%)	0	100	100
7	H	53/54 (98%)	52 (98%)	1 (2%)	52	46
7	h	53/54 (98%)	52 (98%)	1 (2%)	52	46
8	I	32/33 (97%)	32 (100%)	0	100	100
8	i	32/33 (97%)	32 (100%)	0	100	100
9	J	24/24 (100%)	21 (88%)	3 (12%)	3	1
9	j	24/24 (100%)	21 (88%)	3 (12%)	3	1
10	K	31/38 (82%)	31 (100%)	0	100	100
10	k	31/38 (82%)	31 (100%)	0	100	100
11	L	36/36 (100%)	36 (100%)	0	100	100
11	l	36/36 (100%)	36 (100%)	0	100	100
12	M	27/31 (87%)	27 (100%)	0	100	100
12	m	27/31 (87%)	27 (100%)	0	100	100
13	O	207/233 (89%)	202 (98%)	5 (2%)	44	36
13	o	207/233 (89%)	202 (98%)	5 (2%)	44	36
14	Q	93/128 (73%)	90 (97%)	3 (3%)	34	24
14	q	93/128 (73%)	90 (97%)	3 (3%)	34	24
15	R	26/29 (90%)	24 (92%)	2 (8%)	10	3
15	r	26/29 (90%)	24 (92%)	2 (8%)	10	3
16	T	24/25 (96%)	23 (96%)	1 (4%)	25	14
16	t	24/25 (96%)	23 (96%)	1 (4%)	25	14
17	U	83/111 (75%)	78 (94%)	5 (6%)	16	6
17	u	83/111 (75%)	78 (94%)	5 (6%)	16	6
18	V	117/137 (85%)	114 (97%)	3 (3%)	41	32
18	v	117/137 (85%)	114 (97%)	3 (3%)	41	32
19	X	32/33 (97%)	32 (100%)	0	100	100
19	x	32/33 (97%)	32 (100%)	0	100	100
20	Y	25/30 (83%)	24 (96%)	1 (4%)	27	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	y	25/30 (83%)	24 (96%)	1 (4%)	27	16
21	Z	49/52 (94%)	47 (96%)	2 (4%)	26	15
21	z	49/52 (94%)	47 (96%)	2 (4%)	26	15
All	All	4520/4872 (93%)	4424 (98%)	96 (2%)	49	42

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	491	GLU
9	j	2	PHE
3	c	114	LEU
3	c	369	ASN
13	o	89	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
3	c	314	ASN
13	o	64	ASN
4	d	301	GLN
7	h	3	GLN
13	o	153	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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
8	FME	I	1	8	8,9,10	0.39	0	8,9,11	0.97	0
12	FME	M	1	12	8,9,10	0.36	0	8,9,11	0.99	0
16	FME	t	1	16	8,9,10	0.38	0	8,9,11	1.26	1 (12%)
16	FME	T	1	16	8,9,10	0.38	0	8,9,11	1.25	1 (12%)
12	FME	m	1	12	8,9,10	0.36	0	8,9,11	0.99	0
8	FME	i	1	8	8,9,10	0.39	0	8,9,11	0.97	0
9	FME	j	1	9	6,7,10	0.66	0	2,7,11	0.17	0
9	FME	J	1	9	6,7,10	0.66	0	2,7,11	0.17	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	I	1	8	-	0/7/9/11	-
12	FME	M	1	12	-	0/7/9/11	-
16	FME	t	1	16	-	3/7/9/11	-
16	FME	T	1	16	-	3/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
9	FME	j	1	9	-	3/5/6/11	-
9	FME	J	1	9	-	3/5/6/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	T	1	FME	CA-N-CN	2.52	126.70	122.82
16	t	1	FME	CA-N-CN	2.52	126.70	122.82

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	J	1	FME	N-CA-CB-CG
9	J	1	FME	C-CA-CB-CG
16	T	1	FME	N-CA-CB-CG
9	j	1	FME	N-CA-CB-CG
9	j	1	FME	C-CA-CB-CG



There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 236 ligands modelled in this entry, 12 are monoatomic - leaving 224 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
25	CLA	C	504	38	63,73,73	1.33	9 (14%)	74,113,113	1.30	6 (8%)
31	LMT	D	410	-	36,36,36	0.22	0	47,47,47	0.34	0
25	CLA	d	401	38	63,73,73	1.50	9 (14%)	74,113,113	1.47	10 (13%)
31	LMT	E	101	-	22,22,36	0.17	0	27,27,47	0.36	0
27	BCR	c	527	-	41,41,41	2.65	6 (14%)	56,56,56	6.56	22 (39%)
31	LMT	B	623	-	24,24,36	0.19	0	29,29,47	0.31	0
33	LHG	a	418	-	48,48,48	0.92	3 (6%)	51,54,54	1.04	4 (7%)
30	SQD	A	412	-	46,48,54	1.08	5 (10%)	56,59,65	1.02	4 (7%)
25	CLA	c	503	3	63,73,73	1.34	8 (12%)	74,113,113	1.44	7 (9%)
26	PHO	a	407	-	50,69,69	0.56	1 (2%)	48,99,99	0.68	0
27	BCR	c	526	-	41,41,41	2.71	7 (17%)	56,56,56	6.57	18 (32%)
25	CLA	c	512	3	63,73,73	1.27	8 (12%)	74,113,113	1.45	8 (10%)
25	CLA	C	508	3	63,73,73	1.38	9 (14%)	74,113,113	1.57	7 (9%)
34	DGD	C	515	-	63,63,67	1.30	9 (14%)	77,77,81	1.01	2 (2%)
28	LMG	b	622	-	51,51,55	1.44	9 (17%)	59,59,63	1.18	5 (8%)
31	LMT	b	623	-	36,36,36	0.21	0	47,47,47	0.37	0
35	HEM	v	201	18	42,50,50	1.40	6 (14%)	46,82,82	1.92	11 (23%)
31	LMT	C	524	-	36,36,36	0.30	0	47,47,47	0.56	1 (2%)
25	CLA	C	512	3	63,73,73	1.27	8 (12%)	74,113,113	1.45	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	LMT	i	104	-	24,24,36	0.19	0	29,29,47	0.32	0
25	CLA	a	406	38	63,73,73	1.36	8 (12%)	74,113,113	1.37	9 (12%)
31	LMT	c	520	-	24,24,36	0.18	0	29,29,47	0.29	0
33	LHG	e	102	-	39,39,48	0.99	3 (7%)	42,45,54	1.23	4 (9%)
31	LMT	d	410	-	36,36,36	0.22	0	47,47,47	0.34	0
25	CLA	B	612	2	63,73,73	1.35	7 (11%)	74,113,113	1.59	8 (10%)
31	LMT	a	415	-	24,24,36	0.19	0	29,29,47	0.35	0
31	LMT	i	101	-	24,24,36	0.17	0	29,29,47	0.33	0
22	OEX	A	401	38,3,1	0,15,15	-	-	-	-	-
25	CLA	b	606	2	63,73,73	1.60	9 (14%)	74,113,113	1.48	8 (10%)
30	SQD	B	630	-	52,54,54	1.73	6 (11%)	62,65,65	0.89	1 (1%)
35	HEM	F	101	6,5	42,50,50	1.43	7 (16%)	46,82,82	2.09	13 (28%)
25	CLA	B	615	2	63,73,73	1.45	7 (11%)	74,113,113	1.68	12 (16%)
28	LMG	J	101	-	55,55,55	1.52	8 (14%)	63,63,63	1.14	3 (4%)
30	SQD	k	102	-	41,41,54	0.25	0	49,49,65	0.22	0
31	LMT	D	409	-	36,36,36	0.22	0	47,47,47	0.45	0
27	BCR	C	514	-	41,41,41	2.72	6 (14%)	56,56,56	6.64	22 (39%)
31	LMT	c	521	-	36,36,36	0.23	0	47,47,47	0.39	0
25	CLA	c	504	38	63,73,73	1.34	9 (14%)	74,113,113	1.30	6 (8%)
34	DGD	C	516	-	63,63,67	1.32	8 (12%)	77,77,81	1.11	5 (6%)
25	CLA	B	604	2	63,73,73	1.47	9 (14%)	74,113,113	1.79	12 (16%)
26	PHO	d	402	-	50,69,69	0.70	2 (4%)	48,99,99	0.98	2 (4%)
25	CLA	c	509	3	63,73,73	1.40	8 (12%)	74,113,113	1.65	7 (9%)
31	LMT	d	412	-	24,24,36	0.18	0	29,29,47	0.31	0
31	LMT	c	524	-	36,36,36	0.30	0	47,47,47	0.56	1 (2%)
25	CLA	C	513	3	63,73,73	1.28	6 (9%)	74,113,113	1.48	7 (9%)
31	LMT	D	408	-	24,24,36	0.24	0	29,29,47	0.38	0
25	CLA	c	507	38	63,73,73	1.36	10 (15%)	74,113,113	1.44	9 (12%)
33	LHG	E	102	-	39,39,48	0.99	3 (7%)	42,45,54	1.23	4 (9%)
28	LMG	b	630	-	47,47,55	1.39	6 (12%)	55,55,63	1.16	3 (5%)
36	RRX	H	101	-	42,42,42	1.42	4 (9%)	56,58,58	1.29	8 (14%)
25	CLA	c	502	3	63,73,73	1.21	7 (11%)	74,113,113	1.58	8 (10%)
25	CLA	C	501	3	63,73,73	1.39	8 (12%)	74,113,113	1.64	8 (10%)
25	CLA	b	616	2	63,73,73	1.45	7 (11%)	74,113,113	1.68	12 (16%)
30	SQD	a	412	-	46,48,54	1.08	5 (10%)	56,59,65	1.02	4 (7%)
29	PL9	d	405	-	55,55,55	0.81	1 (1%)	68,69,69	0.63	2 (2%)
34	DGD	c	516	-	63,63,67	1.32	8 (12%)	77,77,81	1.11	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	b	607	2	58,68,73	1.51	7 (12%)	68,107,113	1.70	8 (11%)
31	LMT	B	625	-	24,24,36	0.16	0	29,29,47	0.30	0
31	LMT	J	103	-	21,21,36	0.31	0	26,26,47	0.62	0
25	CLA	D	401	38	63,73,73	1.51	9 (14%)	74,113,113	1.48	10 (13%)
28	LMG	c	519	-	49,49,55	1.45	6 (12%)	57,57,63	1.21	4 (7%)
25	CLA	b	615	2	63,73,73	1.41	7 (11%)	74,113,113	1.66	8 (10%)
27	BCR	b	620	-	41,41,41	2.67	7 (17%)	56,56,56	6.51	22 (39%)
31	LMT	I	102	-	36,36,36	0.15	0	47,47,47	0.28	0
31	LMT	F	103	-	36,36,36	0.52	0	47,47,47	0.86	1 (2%)
25	CLA	B	602	2	63,73,73	1.46	8 (12%)	74,113,113	1.69	13 (17%)
31	LMT	I	101	-	24,24,36	0.17	0	29,29,47	0.33	0
28	LMG	a	413	-	36,36,55	1.93	8 (22%)	44,44,63	1.46	7 (15%)
25	CLA	B	611	2	63,73,73	1.38	8 (12%)	74,113,113	1.70	9 (12%)
25	CLA	a	405	1	63,73,73	1.43	7 (11%)	74,113,113	1.81	7 (9%)
25	CLA	B	610	38	63,73,73	1.42	7 (11%)	74,113,113	1.66	9 (12%)
31	LMT	C	522	-	21,21,36	0.28	0	26,26,47	0.55	0
27	BCR	C	525	-	41,41,41	2.67	6 (14%)	56,56,56	6.89	21 (37%)
25	CLA	b	602	38	43,53,73	1.50	7 (16%)	50,89,113	1.52	8 (16%)
31	LMT	m	102	-	24,24,36	0.20	0	29,29,47	0.30	0
28	LMG	a	410	-	51,51,55	2.25	14 (27%)	59,59,63	1.69	10 (16%)
31	LMT	J	102	-	36,36,36	0.17	0	47,47,47	0.40	0
35	HEM	f	101	6,5	42,50,50	1.43	7 (16%)	46,82,82	2.09	13 (28%)
27	BCR	C	526	-	41,41,41	2.71	7 (17%)	56,56,56	6.57	18 (32%)
28	LMG	B	629	-	47,47,55	1.39	6 (12%)	55,55,63	1.16	3 (5%)
28	LMG	D	407	-	55,55,55	1.54	9 (16%)	63,63,63	1.72	7 (11%)
25	CLA	b	603	2	63,73,73	1.47	8 (12%)	74,113,113	1.69	13 (17%)
30	SQD	A	417	-	52,54,54	0.46	0	62,65,65	0.44	0
33	LHG	b	627	-	48,48,48	0.93	2 (4%)	51,54,54	1.15	3 (5%)
30	SQD	F	102	-	32,34,54	1.87	9 (28%)	42,45,65	1.66	10 (23%)
36	RRX	h	101	-	42,42,42	1.43	5 (11%)	56,58,58	1.29	9 (16%)
25	CLA	B	607	38	63,73,73	1.36	8 (12%)	74,113,113	1.22	6 (8%)
25	CLA	A	408	1	58,68,73	1.39	6 (10%)	68,107,113	1.75	10 (14%)
28	LMG	A	410	-	51,51,55	2.25	14 (27%)	59,59,63	1.69	10 (16%)
31	LMT	e	101	-	22,22,36	0.18	0	27,27,47	0.36	0
25	CLA	b	614	2	63,73,73	1.54	7 (11%)	74,113,113	1.63	12 (16%)
27	BCR	B	619	-	41,41,41	2.67	7 (17%)	56,56,56	6.51	22 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	LHG	A	419	-	48,48,48	0.89	3 (6%)	51,54,54	0.96	3 (5%)
25	CLA	c	513	3	63,73,73	1.28	6 (9%)	74,113,113	1.47	7 (9%)
30	SQD	K	102	-	41,41,54	0.25	0	49,49,65	0.22	0
31	LMT	b	629	-	24,24,36	0.19	0	29,29,47	0.33	0
27	BCR	a	409	-	41,41,41	2.74	6 (14%)	56,56,56	6.34	18 (32%)
31	LMT	M	101	-	36,36,36	0.20	0	47,47,47	0.38	0
25	CLA	a	408	1	58,68,73	1.40	6 (10%)	68,107,113	1.75	10 (14%)
31	LMT	X	102	-	22,22,36	0.18	0	27,27,47	0.48	0
33	LHG	B	626	-	48,48,48	0.93	2 (4%)	51,54,54	1.15	3 (5%)
25	CLA	C	507	38	63,73,73	1.36	10 (15%)	74,113,113	1.44	9 (12%)
31	LMT	X	101	-	22,22,36	0.17	0	27,27,47	0.36	0
29	PL9	a	411	-	55,55,55	0.84	1 (1%)	68,69,69	0.55	2 (2%)
34	DGD	H	103	-	63,63,67	1.33	9 (14%)	77,77,81	1.06	3 (3%)
31	LMT	h	104	-	19,19,36	0.17	0	24,24,47	0.31	0
28	LMG	C	518	-	51,51,55	1.45	8 (15%)	59,59,63	1.21	5 (8%)
25	CLA	b	617	2	58,68,73	1.32	7 (12%)	68,107,113	1.51	9 (13%)
25	CLA	C	509	3	63,73,73	1.40	8 (12%)	74,113,113	1.65	7 (9%)
31	LMT	i	103	-	22,22,36	0.18	0	27,27,47	0.32	0
25	CLA	b	611	38	63,73,73	1.43	7 (11%)	74,113,113	1.66	9 (12%)
31	LMT	X	103	-	36,36,36	0.17	0	47,47,47	0.36	0
25	CLA	C	503	3	63,73,73	1.34	8 (12%)	74,113,113	1.44	7 (9%)
31	LMT	H	104	-	19,19,36	0.16	0	24,24,47	0.31	0
25	CLA	C	502	3	63,73,73	1.21	7 (11%)	74,113,113	1.57	8 (10%)
27	BCR	b	619	-	41,41,41	2.74	7 (17%)	56,56,56	6.53	19 (33%)
31	LMT	d	409	-	36,36,36	0.22	0	47,47,47	0.45	0
31	LMT	b	625	-	36,36,36	0.19	0	47,47,47	0.27	0
30	SQD	a	417	-	52,54,54	0.46	0	62,65,65	0.44	0
31	LMT	x	101	-	22,22,36	0.16	0	27,27,47	0.35	0
25	CLA	B	603	2	63,73,73	1.33	7 (11%)	74,113,113	1.57	8 (10%)
28	LMG	C	519	-	49,49,55	1.45	6 (12%)	57,57,63	1.21	4 (7%)
33	LHG	D	406	-	48,48,48	0.90	2 (4%)	51,54,54	1.07	4 (7%)
34	DGD	c	517	-	63,63,67	1.34	8 (12%)	77,77,81	1.00	3 (3%)
31	LMT	B	627	-	36,36,36	0.17	0	47,47,47	0.26	0
22	OEX	a	401	38,3,1	0,15,15	-	-	-	-	-
25	CLA	B	608	2	63,73,73	1.36	9 (14%)	74,113,113	1.68	11 (14%)
25	CLA	c	510	3	63,73,73	1.28	7 (11%)	74,113,113	1.61	13 (17%)
25	CLA	c	511	3	63,73,73	1.35	9 (14%)	74,113,113	1.41	9 (12%)
31	LMT	C	520	-	24,24,36	0.18	0	29,29,47	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	B	609	2	63,73,73	1.30	6 (9%)	74,113,113	1.46	9 (12%)
31	LMT	c	522	-	21,21,36	0.28	0	26,26,47	0.55	0
31	LMT	m	101	-	36,36,36	0.20	0	47,47,47	0.39	0
35	HEM	V	201	18	42,50,50	1.39	6 (14%)	46,82,82	1.92	11 (23%)
25	CLA	b	608	38	63,73,73	1.37	8 (12%)	74,113,113	1.22	6 (8%)
25	CLA	b	609	2	63,73,73	1.36	9 (14%)	74,113,113	1.68	11 (14%)
25	CLA	b	613	2	63,73,73	1.35	7 (11%)	74,113,113	1.59	8 (10%)
25	CLA	c	505	3	63,73,73	1.36	8 (12%)	74,113,113	1.43	8 (10%)
31	LMT	B	624	-	36,36,36	0.19	0	47,47,47	0.27	0
33	LHG	Z	101	-	35,35,48	1.06	3 (8%)	38,40,54	1.32	6 (15%)
31	LMT	T	101	-	24,24,36	0.21	0	29,29,47	0.35	0
31	LMT	b	628	-	36,36,36	0.17	0	47,47,47	0.26	0
25	CLA	A	406	38	63,73,73	1.37	8 (12%)	74,113,113	1.36	9 (12%)
29	PL9	D	405	-	55,55,55	0.81	1 (1%)	68,69,69	0.63	2 (2%)
28	LMG	j	101	-	55,55,55	1.52	8 (14%)	63,63,63	1.14	3 (4%)
25	CLA	b	610	2	63,73,73	1.30	6 (9%)	74,113,113	1.46	9 (12%)
33	LHG	d	406	-	48,48,48	0.90	2 (4%)	51,54,54	1.07	4 (7%)
25	CLA	B	614	2	63,73,73	1.41	7 (11%)	74,113,113	1.66	8 (10%)
25	CLA	B	616	2	58,68,73	1.32	7 (12%)	68,107,113	1.51	9 (13%)
31	LMT	A	415	-	24,24,36	0.19	0	29,29,47	0.35	0
31	LMT	C	521	-	36,36,36	0.23	0	47,47,47	0.39	0
31	LMT	E	103	-	36,36,36	0.30	0	47,47,47	0.66	0
30	SQD	H	102	-	52,54,54	0.42	0	62,65,65	0.44	0
34	DGD	h	103	-	63,63,67	1.33	9 (14%)	77,77,81	1.06	3 (3%)
30	SQD	b	601	-	52,54,54	1.73	6 (11%)	62,65,65	0.89	1 (1%)
31	LMT	c	523	-	24,24,36	0.17	0	29,29,47	0.32	0
33	LHG	L	101	-	48,48,48	0.89	2 (4%)	51,54,54	1.11	3 (5%)
25	CLA	C	506	3	63,73,73	1.33	9 (14%)	74,113,113	1.53	8 (10%)
31	LMT	I	103	-	22,22,36	0.18	0	27,27,47	0.32	0
25	CLA	d	404	4	63,73,73	1.25	4 (6%)	74,113,113	1.68	12 (16%)
25	CLA	c	501	3	63,73,73	1.39	8 (12%)	74,113,113	1.64	8 (10%)
25	CLA	B	601	38	43,53,73	1.50	7 (16%)	50,89,113	1.52	8 (16%)
25	CLA	B	613	2	63,73,73	1.53	7 (11%)	74,113,113	1.63	12 (16%)
31	LMT	B	622	-	36,36,36	0.21	0	47,47,47	0.37	0
30	SQD	b	621	-	52,54,54	0.43	0	62,65,65	0.56	1 (1%)
32	BCT	a	416	23	3,3,3	0.97	0	2,3,3	0.56	0
25	CLA	c	508	3	63,73,73	1.38	9 (14%)	74,113,113	1.57	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	B	605	2	63,73,73	1.60	9 (14%)	74,113,113	1.48	8 (10%)
25	CLA	d	403	4	63,73,73	1.33	7 (11%)	74,113,113	1.48	7 (9%)
25	CLA	b	612	2	63,73,73	1.39	8 (12%)	74,113,113	1.70	8 (10%)
34	DGD	C	517	-	63,63,67	1.34	8 (12%)	77,77,81	1.00	3 (3%)
25	CLA	A	405	1	63,73,73	1.43	7 (11%)	74,113,113	1.81	7 (9%)
26	PHO	A	407	-	50,69,69	0.56	1 (2%)	48,99,99	0.67	0
31	LMT	f	103	-	36,36,36	0.53	0	47,47,47	0.86	1 (2%)
25	CLA	b	605	2	63,73,73	1.47	9 (14%)	74,113,113	1.79	12 (16%)
25	CLA	C	511	3	63,73,73	1.35	9 (14%)	74,113,113	1.41	9 (12%)
31	LMT	I	104	-	24,24,36	0.19	0	29,29,47	0.33	0
28	LMG	c	518	-	51,51,55	1.45	8 (15%)	59,59,63	1.21	5 (8%)
31	LMT	x	103	-	36,36,36	0.17	0	47,47,47	0.36	0
27	BCR	C	527	-	41,41,41	2.65	6 (14%)	56,56,56	6.55	22 (39%)
32	BCT	A	416	23	3,3,3	0.97	0	2,3,3	0.56	0
31	LMT	A	414	-	36,36,36	0.19	0	47,47,47	0.40	0
26	PHO	D	402	-	50,69,69	0.70	2 (4%)	48,99,99	0.99	2 (4%)
31	LMT	D	412	-	24,24,36	0.18	0	29,29,47	0.31	0
27	BCR	d	411	-	41,41,41	2.61	6 (14%)	56,56,56	6.62	20 (35%)
30	SQD	f	102	-	32,34,54	1.87	9 (28%)	42,45,65	1.66	10 (23%)
27	BCR	D	411	-	41,41,41	2.61	6 (14%)	56,56,56	6.62	20 (35%)
31	LMT	b	626	-	24,24,36	0.16	0	29,29,47	0.30	0
28	LMG	B	621	-	51,51,55	1.44	9 (17%)	59,59,63	1.18	5 (8%)
31	LMT	j	102	-	36,36,36	0.17	0	47,47,47	0.40	0
33	LHG	A	418	-	48,48,48	0.92	3 (6%)	51,54,54	1.04	4 (7%)
34	DGD	c	515	-	63,63,67	1.31	9 (14%)	77,77,81	1.01	2 (2%)
31	LMT	C	523	-	24,24,36	0.17	0	29,29,47	0.32	0
31	LMT	e	103	-	36,36,36	0.30	0	47,47,47	0.66	0
27	BCR	c	514	-	41,41,41	2.72	6 (14%)	56,56,56	6.65	22 (39%)
25	CLA	D	403	4	63,73,73	1.34	7 (11%)	74,113,113	1.48	8 (10%)
31	LMT	x	102	-	22,22,36	0.19	0	27,27,47	0.48	0
31	LMT	j	103	-	21,21,36	0.31	0	26,26,47	0.62	0
31	LMT	t	101	-	24,24,36	0.22	0	29,29,47	0.35	0
31	LMT	M	102	-	24,24,36	0.20	0	29,29,47	0.30	0
25	CLA	C	510	3	63,73,73	1.28	7 (11%)	74,113,113	1.62	13 (17%)
25	CLA	D	404	4	63,73,73	1.24	4 (6%)	74,113,113	1.68	12 (16%)
30	SQD	B	620	-	52,54,54	0.44	0	62,65,65	0.56	1 (1%)
27	BCR	B	617	-	41,41,41	2.74	8 (19%)	56,56,56	6.56	19 (33%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	LMT	b	624	-	24,24,36	0.19	0	29,29,47	0.31	0
33	LHG	z	101	-	35,35,48	1.06	3 (8%)	38,40,54	1.32	6 (15%)
27	BCR	A	409	-	41,41,41	2.74	6 (14%)	56,56,56	6.33	18 (32%)
25	CLA	C	505	3	63,73,73	1.36	8 (12%)	74,113,113	1.43	8 (10%)
31	LMT	a	414	-	36,36,36	0.19	0	47,47,47	0.40	0
33	LHG	l	101	-	48,48,48	0.89	2 (4%)	51,54,54	1.11	3 (5%)
27	BCR	B	618	-	41,41,41	2.74	7 (17%)	56,56,56	6.53	19 (33%)
28	LMG	A	413	-	36,36,55	1.92	8 (22%)	44,44,63	1.46	7 (15%)
33	LHG	a	419	-	48,48,48	0.89	3 (6%)	51,54,54	0.96	3 (5%)
27	BCR	b	618	-	41,41,41	2.74	7 (17%)	56,56,56	6.56	20 (35%)
25	CLA	c	506	3	63,73,73	1.33	9 (14%)	74,113,113	1.53	8 (10%)
31	LMT	d	408	-	24,24,36	0.24	0	29,29,47	0.38	0
28	LMG	d	407	-	55,55,55	1.54	9 (16%)	63,63,63	1.72	7 (11%)
25	CLA	b	604	2	63,73,73	1.33	7 (11%)	74,113,113	1.56	8 (10%)
31	LMT	i	102	-	36,36,36	0.15	0	47,47,47	0.28	0
25	CLA	B	606	2	58,68,73	1.51	7 (12%)	68,107,113	1.69	8 (11%)
30	SQD	h	102	-	52,54,54	0.41	0	62,65,65	0.44	0
31	LMT	B	628	-	24,24,36	0.20	0	29,29,47	0.33	0
27	BCR	c	525	-	41,41,41	2.67	6 (14%)	56,56,56	6.89	21 (37%)
29	PL9	A	411	-	55,55,55	0.84	1 (1%)	68,69,69	0.55	2 (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
25	CLA	C	504	38	1/1/15/20	7/37/115/115	-
31	LMT	D	410	-	-	7/21/61/61	0/2/2/2
25	CLA	d	401	38	1/1/15/20	4/37/115/115	-
31	LMT	E	101	-	-	9/13/33/61	0/1/1/2
27	BCR	c	527	-	-	4/29/63/63	0/2/2/2
31	LMT	B	623	-	-	9/15/35/61	0/1/1/2
33	LHG	a	418	-	-	18/53/53/53	-
30	SQD	A	412	-	-	25/43/63/69	0/1/1/1
25	CLA	c	503	3	1/1/15/20	9/37/115/115	-
26	PHO	a	407	-	-	2/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	c	526	-	-	6/29/63/63	0/2/2/2
25	CLA	c	512	3	1/1/15/20	17/37/115/115	-
25	CLA	C	508	3	-	10/37/115/115	-
34	DGD	C	515	-	-	22/51/91/95	0/2/2/2
28	LMG	b	622	-	-	12/46/66/70	0/1/1/1
31	LMT	b	623	-	-	10/21/61/61	0/2/2/2
35	HEM	v	201	18	-	2/12/54/54	-
31	LMT	C	524	-	-	16/21/61/61	0/2/2/2
25	CLA	C	512	3	1/1/15/20	17/37/115/115	-
31	LMT	i	104	-	-	11/15/35/61	0/1/1/2
25	CLA	a	406	38	1/1/15/20	5/37/115/115	-
31	LMT	c	520	-	-	9/15/35/61	0/1/1/2
33	LHG	e	102	-	-	20/44/44/53	-
31	LMT	d	410	-	-	7/21/61/61	0/2/2/2
25	CLA	B	612	2	1/1/15/20	8/37/115/115	-
31	LMT	a	415	-	-	12/15/35/61	0/1/1/2
31	LMT	i	101	-	-	7/15/35/61	0/1/1/2
25	CLA	b	606	2	1/1/15/20	11/37/115/115	-
30	SQD	B	630	-	-	30/49/69/69	0/1/1/1
35	HEM	F	101	6,5	-	3/12/54/54	-
25	CLA	B	615	2	1/1/15/20	7/37/115/115	-
28	LMG	J	101	-	-	34/50/70/70	0/1/1/1
30	SQD	k	102	-	-	21/35/55/69	0/1/1/1
31	LMT	D	409	-	-	12/21/61/61	0/2/2/2
27	BCR	C	514	-	-	10/29/63/63	0/2/2/2
31	LMT	c	521	-	-	7/21/61/61	0/2/2/2
25	CLA	c	504	38	1/1/15/20	7/37/115/115	-
34	DGD	C	516	-	-	19/51/91/95	0/2/2/2
25	CLA	B	604	2	1/1/15/20	15/37/115/115	-
26	PHO	d	402	-	-	4/37/103/103	0/5/6/6
25	CLA	c	509	3	1/1/15/20	10/37/115/115	-
31	LMT	d	412	-	-	10/15/35/61	0/1/1/2
31	LMT	c	524	-	-	16/21/61/61	0/2/2/2
25	CLA	C	513	3	-	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	D	408	-	-	13/15/35/61	0/1/1/2
25	CLA	c	507	38	1/1/15/20	9/37/115/115	-
33	LHG	E	102	-	-	20/44/44/53	-
28	LMG	b	630	-	-	19/42/62/70	0/1/1/1
36	RRX	H	101	-	-	15/29/65/65	0/2/2/2
25	CLA	c	502	3	-	9/37/115/115	-
25	CLA	C	501	3	1/1/15/20	4/37/115/115	-
25	CLA	b	616	2	1/1/15/20	7/37/115/115	-
30	SQD	a	412	-	-	24/43/63/69	0/1/1/1
29	PL9	d	405	-	-	14/53/73/73	0/1/1/1
34	DGD	c	516	-	-	19/51/91/95	0/2/2/2
25	CLA	b	607	2	1/1/14/20	2/31/109/115	-
31	LMT	B	625	-	-	11/15/35/61	0/1/1/2
31	LMT	J	103	-	-	5/12/32/61	0/1/1/2
25	CLA	D	401	38	1/1/15/20	4/37/115/115	-
28	LMG	c	519	-	-	27/44/64/70	0/1/1/1
25	CLA	b	615	2	1/1/15/20	15/37/115/115	-
27	BCR	b	620	-	-	8/29/63/63	0/2/2/2
31	LMT	I	102	-	-	12/21/61/61	0/2/2/2
31	LMT	F	103	-	-	13/21/61/61	0/2/2/2
25	CLA	B	602	2	-	6/37/115/115	-
31	LMT	I	101	-	-	7/15/35/61	0/1/1/2
28	LMG	a	413	-	-	15/31/51/70	0/1/1/1
25	CLA	B	611	2	1/1/15/20	11/37/115/115	-
25	CLA	a	405	1	1/1/15/20	6/37/115/115	-
25	CLA	B	610	38	1/1/15/20	5/37/115/115	-
31	LMT	C	522	-	-	6/12/32/61	0/1/1/2
27	BCR	C	525	-	-	11/29/63/63	0/2/2/2
25	CLA	b	602	38	1/1/11/20	3/13/91/115	-
31	LMT	m	102	-	-	8/15/35/61	0/1/1/2
28	LMG	a	410	-	-	23/46/66/70	0/1/1/1
31	LMT	J	102	-	-	8/21/61/61	0/2/2/2
35	HEM	f	101	6,5	-	3/12/54/54	-
27	BCR	C	526	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMG	B	629	-	-	19/42/62/70	0/1/1/1
28	LMG	D	407	-	-	22/50/70/70	0/1/1/1
25	CLA	b	603	2	-	6/37/115/115	-
30	SQD	A	417	-	-	23/49/69/69	0/1/1/1
33	LHG	b	627	-	-	39/53/53/53	-
30	SQD	F	102	-	-	17/29/49/69	0/1/1/1
36	RRX	h	101	-	-	15/29/65/65	0/2/2/2
25	CLA	B	607	38	1/1/15/20	7/37/115/115	-
25	CLA	A	408	1	-	7/31/109/115	-
28	LMG	A	410	-	-	23/46/66/70	0/1/1/1
31	LMT	e	101	-	-	9/13/33/61	0/1/1/2
25	CLA	b	614	2	1/1/15/20	9/37/115/115	-
27	BCR	B	619	-	-	8/29/63/63	0/2/2/2
33	LHG	A	419	-	-	20/53/53/53	-
25	CLA	c	513	3	-	9/37/115/115	-
30	SQD	K	102	-	-	21/35/55/69	0/1/1/1
31	LMT	b	629	-	-	5/15/35/61	0/1/1/2
27	BCR	a	409	-	-	9/29/63/63	0/2/2/2
31	LMT	M	101	-	-	13/21/61/61	0/2/2/2
25	CLA	a	408	1	-	7/31/109/115	-
31	LMT	X	102	-	-	7/13/33/61	0/1/1/2
33	LHG	B	626	-	-	39/53/53/53	-
25	CLA	C	507	38	1/1/15/20	9/37/115/115	-
31	LMT	X	101	-	-	8/12/32/61	0/1/1/2
29	PL9	a	411	-	-	23/53/73/73	0/1/1/1
34	DGD	H	103	-	-	15/51/91/95	0/2/2/2
31	LMT	h	104	-	-	7/10/30/61	0/1/1/2
28	LMG	C	518	-	-	21/46/66/70	0/1/1/1
25	CLA	b	617	2	1/1/14/20	10/31/109/115	-
25	CLA	C	509	3	1/1/15/20	10/37/115/115	-
31	LMT	i	103	-	-	9/13/33/61	0/1/1/2
25	CLA	b	611	38	1/1/15/20	5/37/115/115	-
31	LMT	X	103	-	-	14/21/61/61	0/2/2/2
25	CLA	C	503	3	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	H	104	-	-	7/10/30/61	0/1/1/2
25	CLA	C	502	3	-	9/37/115/115	-
27	BCR	b	619	-	-	8/29/63/63	0/2/2/2
31	LMT	d	409	-	-	12/21/61/61	0/2/2/2
31	LMT	b	625	-	-	16/21/61/61	0/2/2/2
30	SQD	a	417	-	-	23/49/69/69	0/1/1/1
31	LMT	x	101	-	-	8/12/32/61	0/1/1/2
25	CLA	B	603	2	1/1/15/20	13/37/115/115	-
28	LMG	C	519	-	-	27/44/64/70	0/1/1/1
33	LHG	D	406	-	-	22/53/53/53	-
34	DGD	c	517	-	-	22/51/91/95	0/2/2/2
31	LMT	B	627	-	-	9/21/61/61	0/2/2/2
25	CLA	B	608	2	1/1/15/20	6/37/115/115	-
25	CLA	c	510	3	1/1/15/20	8/37/115/115	-
25	CLA	c	511	3	1/1/15/20	3/37/115/115	-
31	LMT	C	520	-	-	9/15/35/61	0/1/1/2
25	CLA	B	609	2	-	3/37/115/115	-
31	LMT	c	522	-	-	6/12/32/61	0/1/1/2
31	LMT	m	101	-	-	13/21/61/61	0/2/2/2
35	HEM	V	201	18	-	2/12/54/54	-
25	CLA	b	608	38	1/1/15/20	6/37/115/115	-
25	CLA	b	609	2	1/1/15/20	6/37/115/115	-
25	CLA	b	613	2	1/1/15/20	8/37/115/115	-
25	CLA	c	505	3	1/1/15/20	9/37/115/115	-
31	LMT	B	624	-	-	16/21/61/61	0/2/2/2
33	LHG	Z	101	-	-	14/37/37/53	-
31	LMT	T	101	-	-	10/15/35/61	0/1/1/2
31	LMT	b	628	-	-	9/21/61/61	0/2/2/2
25	CLA	A	406	38	1/1/15/20	5/37/115/115	-
29	PL9	D	405	-	-	14/53/73/73	0/1/1/1
28	LMG	j	101	-	-	34/50/70/70	0/1/1/1
25	CLA	b	610	2	-	3/37/115/115	-
33	LHG	d	406	-	-	22/53/53/53	-
25	CLA	B	614	2	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	616	2	1/1/14/20	10/31/109/115	-
31	LMT	A	415	-	-	12/15/35/61	0/1/1/2
31	LMT	C	521	-	-	7/21/61/61	0/2/2/2
31	LMT	E	103	-	-	11/21/61/61	0/2/2/2
30	SQD	H	102	-	-	22/49/69/69	0/1/1/1
34	DGD	h	103	-	-	15/51/91/95	0/2/2/2
30	SQD	b	601	-	-	30/49/69/69	0/1/1/1
31	LMT	c	523	-	-	11/15/35/61	0/1/1/2
33	LHG	L	101	-	-	30/53/53/53	-
25	CLA	C	506	3	1/1/15/20	12/37/115/115	-
31	LMT	I	103	-	-	9/13/33/61	0/1/1/2
25	CLA	d	404	4	-	8/37/115/115	-
25	CLA	c	501	3	1/1/15/20	4/37/115/115	-
25	CLA	B	601	38	1/1/11/20	3/13/91/115	-
25	CLA	B	613	2	1/1/15/20	9/37/115/115	-
31	LMT	B	622	-	-	10/21/61/61	0/2/2/2
30	SQD	b	621	-	-	25/49/69/69	0/1/1/1
25	CLA	c	508	3	-	10/37/115/115	-
25	CLA	B	605	2	1/1/15/20	11/37/115/115	-
25	CLA	d	403	4	1/1/15/20	4/37/115/115	-
25	CLA	b	612	2	1/1/15/20	11/37/115/115	-
34	DGD	C	517	-	-	22/51/91/95	0/2/2/2
25	CLA	A	405	1	1/1/15/20	6/37/115/115	-
26	PHO	A	407	-	-	2/37/103/103	0/5/6/6
31	LMT	f	103	-	-	13/21/61/61	0/2/2/2
25	CLA	b	605	2	1/1/15/20	15/37/115/115	-
25	CLA	C	511	3	1/1/15/20	3/37/115/115	-
31	LMT	I	104	-	-	11/15/35/61	0/1/1/2
28	LMG	c	518	-	-	21/46/66/70	0/1/1/1
31	LMT	x	103	-	-	14/21/61/61	0/2/2/2
27	BCR	C	527	-	-	4/29/63/63	0/2/2/2
31	LMT	A	414	-	-	10/21/61/61	0/2/2/2
26	PHO	D	402	-	-	4/37/103/103	0/5/6/6
31	LMT	D	412	-	-	10/15/35/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	d	411	-	-	10/29/63/63	0/2/2/2
30	SQD	f	102	-	-	17/29/49/69	0/1/1/1
27	BCR	D	411	-	-	10/29/63/63	0/2/2/2
31	LMT	b	626	-	-	11/15/35/61	0/1/1/2
28	LMG	B	621	-	-	12/46/66/70	0/1/1/1
31	LMT	j	102	-	-	8/21/61/61	0/2/2/2
33	LHG	A	418	-	-	18/53/53/53	-
34	DGD	c	515	-	-	22/51/91/95	0/2/2/2
31	LMT	C	523	-	-	11/15/35/61	0/1/1/2
31	LMT	e	103	-	-	11/21/61/61	0/2/2/2
27	BCR	c	514	-	-	10/29/63/63	0/2/2/2
25	CLA	D	403	4	1/1/15/20	4/37/115/115	-
31	LMT	x	102	-	-	7/13/33/61	0/1/1/2
31	LMT	j	103	-	-	5/12/32/61	0/1/1/2
31	LMT	t	101	-	-	10/15/35/61	0/1/1/2
31	LMT	M	102	-	-	8/15/35/61	0/1/1/2
25	CLA	C	510	3	1/1/15/20	8/37/115/115	-
25	CLA	D	404	4	-	8/37/115/115	-
30	SQD	B	620	-	-	25/49/69/69	0/1/1/1
27	BCR	B	617	-	-	10/29/63/63	0/2/2/2
31	LMT	b	624	-	-	9/15/35/61	0/1/1/2
33	LHG	z	101	-	-	14/37/37/53	-
27	BCR	A	409	-	-	9/29/63/63	0/2/2/2
25	CLA	C	505	3	1/1/15/20	9/37/115/115	-
31	LMT	a	414	-	-	10/21/61/61	0/2/2/2
33	LHG	l	101	-	-	30/53/53/53	-
27	BCR	B	618	-	-	8/29/63/63	0/2/2/2
28	LMG	A	413	-	-	15/31/51/70	0/1/1/1
33	LHG	a	419	-	-	20/53/53/53	-
27	BCR	b	618	-	-	10/29/63/63	0/2/2/2
25	CLA	c	506	3	1/1/15/20	12/37/115/115	-
31	LMT	d	408	-	-	13/15/35/61	0/1/1/2
28	LMG	d	407	-	-	22/50/70/70	0/1/1/1
25	CLA	b	604	2	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	i	102	-	-	12/21/61/61	0/2/2/2
25	CLA	B	606	2	1/1/14/20	2/31/109/115	-
30	SQD	h	102	-	-	22/49/69/69	0/1/1/1
31	LMT	B	628	-	-	5/15/35/61	0/1/1/2
27	BCR	c	525	-	-	11/29/63/63	0/2/2/2
29	PL9	A	411	-	-	23/53/73/73	0/1/1/1

The worst 5 of 976 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	410	LMG	O1-C1	-9.19	1.24	1.40
28	a	410	LMG	O1-C1	-9.19	1.24	1.40
27	A	409	BCR	C8-C9	-8.65	1.27	1.46
27	a	409	BCR	C8-C9	-8.65	1.27	1.46
27	B	617	BCR	C8-C9	-8.56	1.27	1.46

The worst 5 of 1264 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	525	BCR	C20-C21-C22	24.79	162.05	127.28
27	c	525	BCR	C20-C21-C22	24.79	162.05	127.28
27	C	514	BCR	C20-C21-C22	22.93	159.43	127.28
27	c	514	BCR	C20-C21-C22	22.93	159.43	127.28
27	D	411	BCR	C20-C21-C22	21.21	157.02	127.28

5 of 56 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	405	CLA	ND
25	A	406	CLA	ND
25	B	601	CLA	ND
25	B	603	CLA	ND
25	B	604	CLA	ND

5 of 2642 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	B	601	CLA	CAD-CBD-CGD-O2D
25	B	614	CLA	CAD-CBD-CGD-O1D
25	B	614	CLA	CAD-CBD-CGD-O2D

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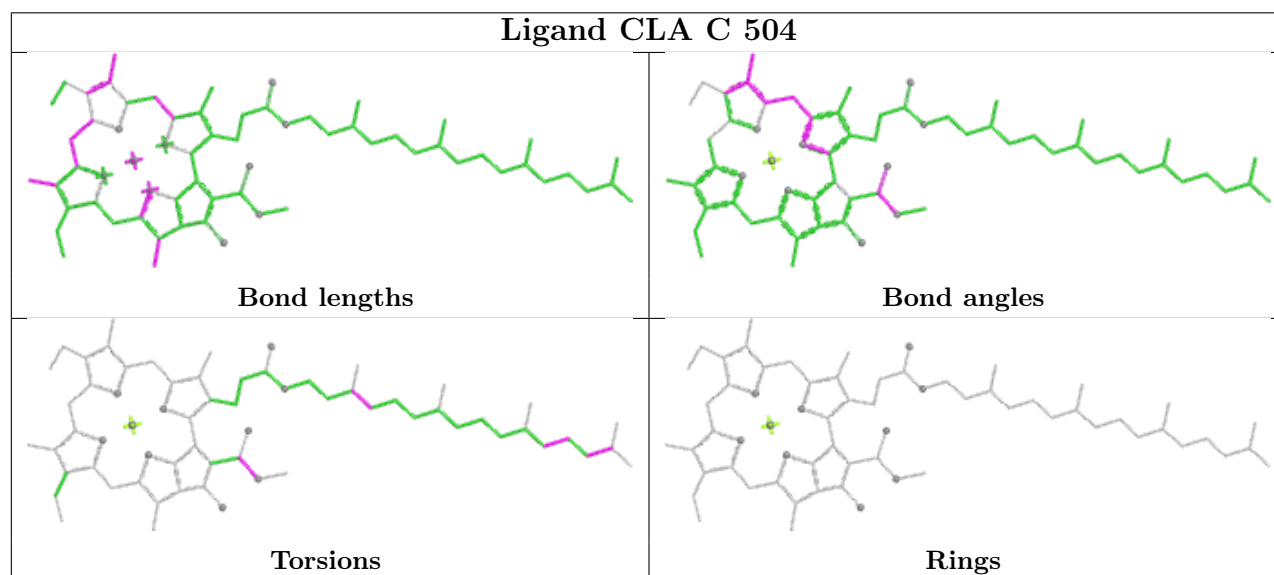
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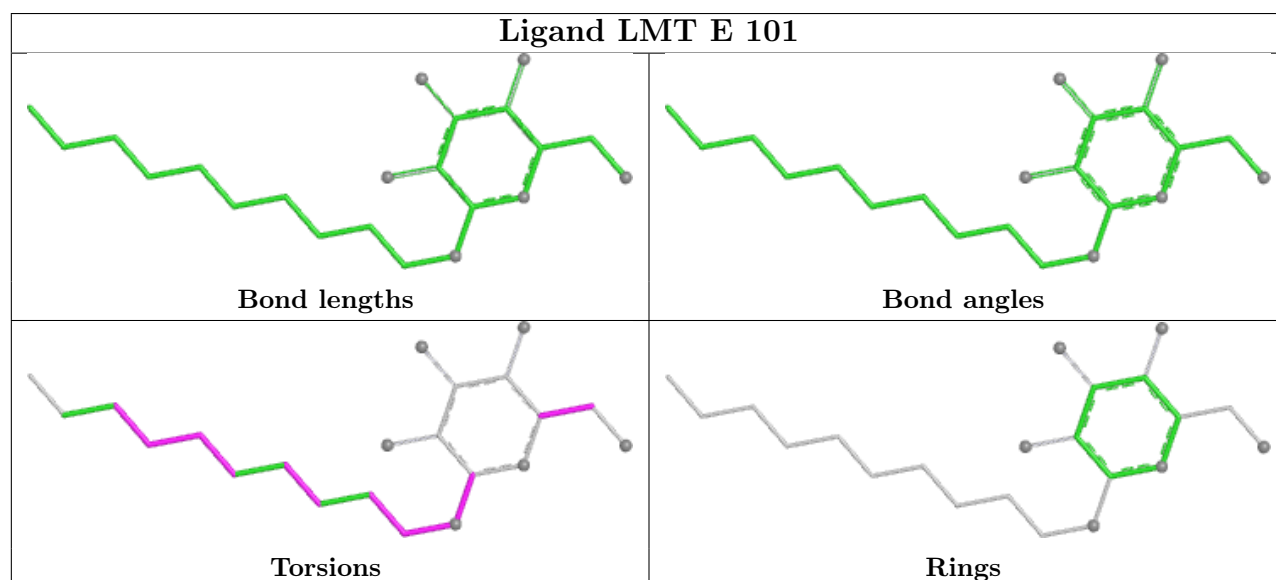
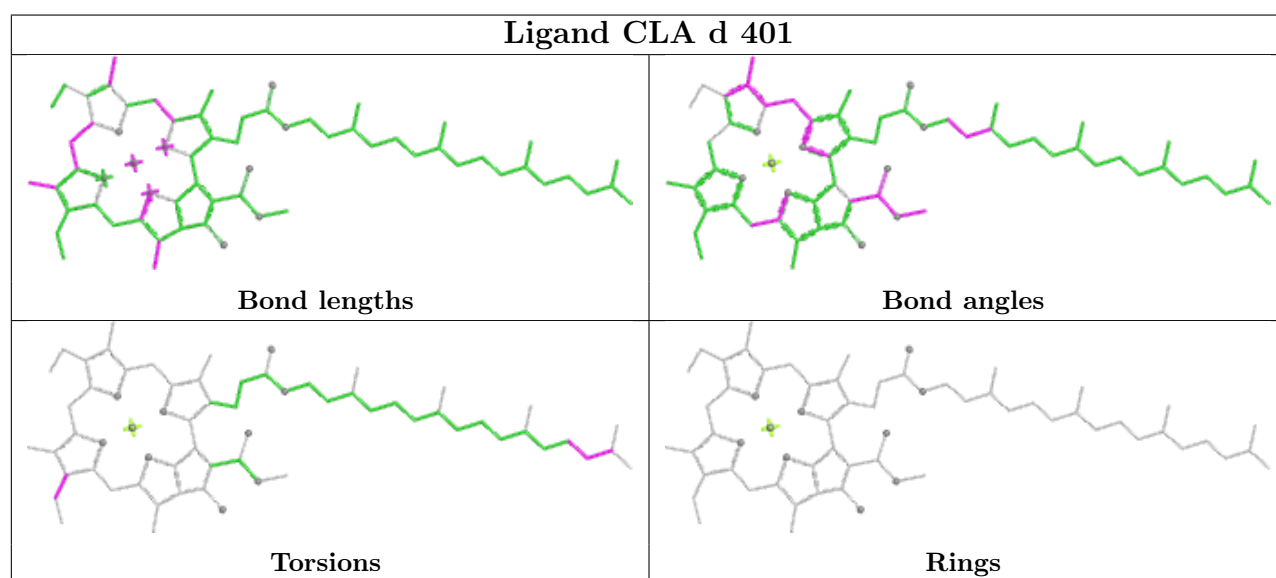
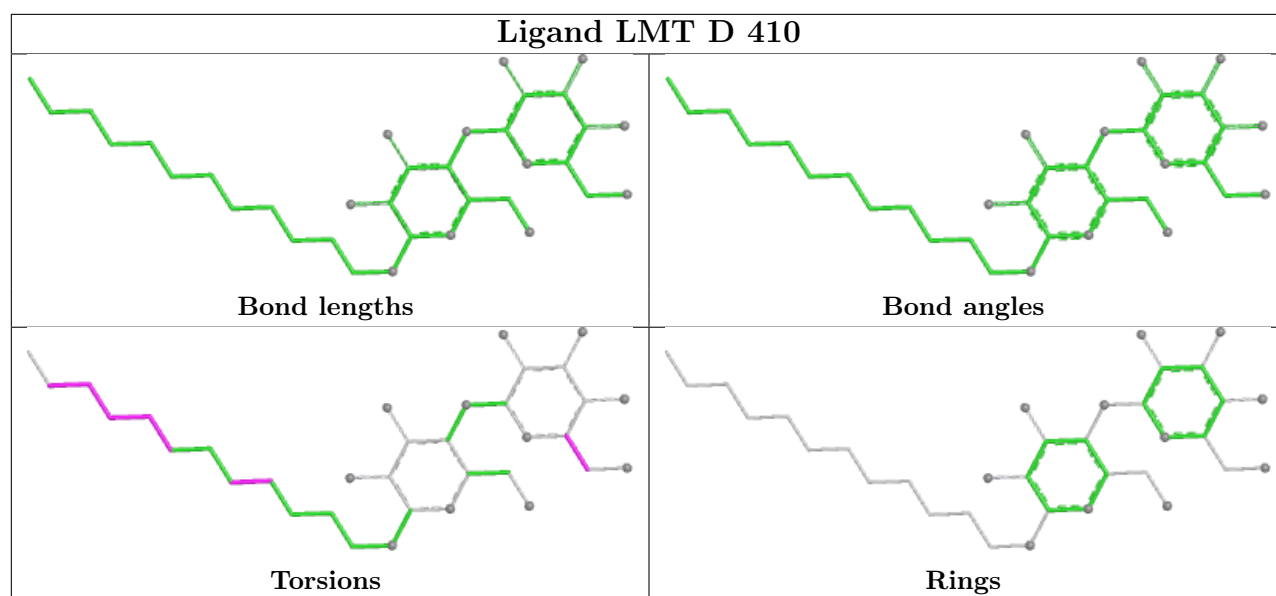
Mol	Chain	Res	Type	Atoms
25	B	614	CLA	C11-C12-C13-C15
25	C	506	CLA	C6-C7-C8-C9

There are no ring outliers.

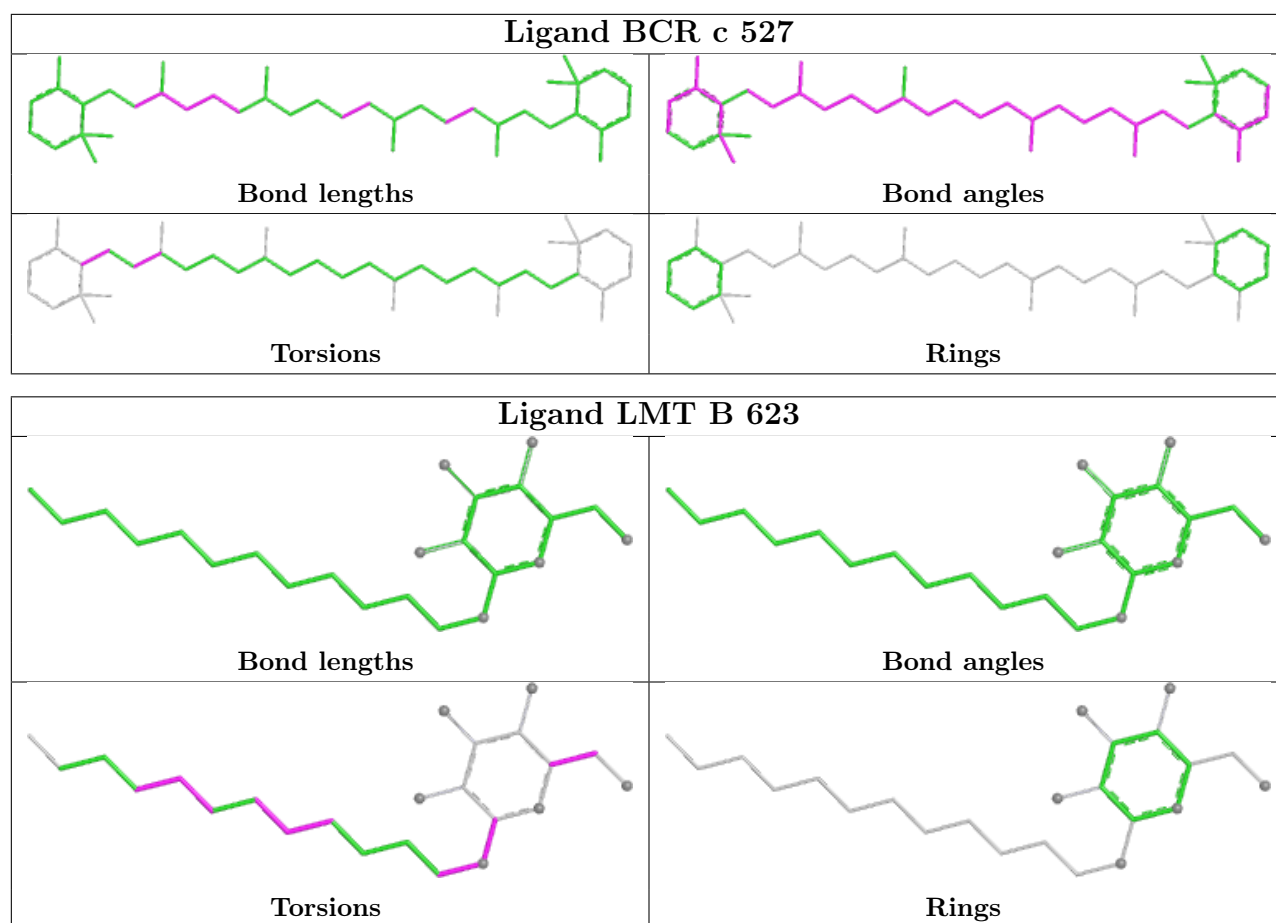
No monomer is involved in short contacts.

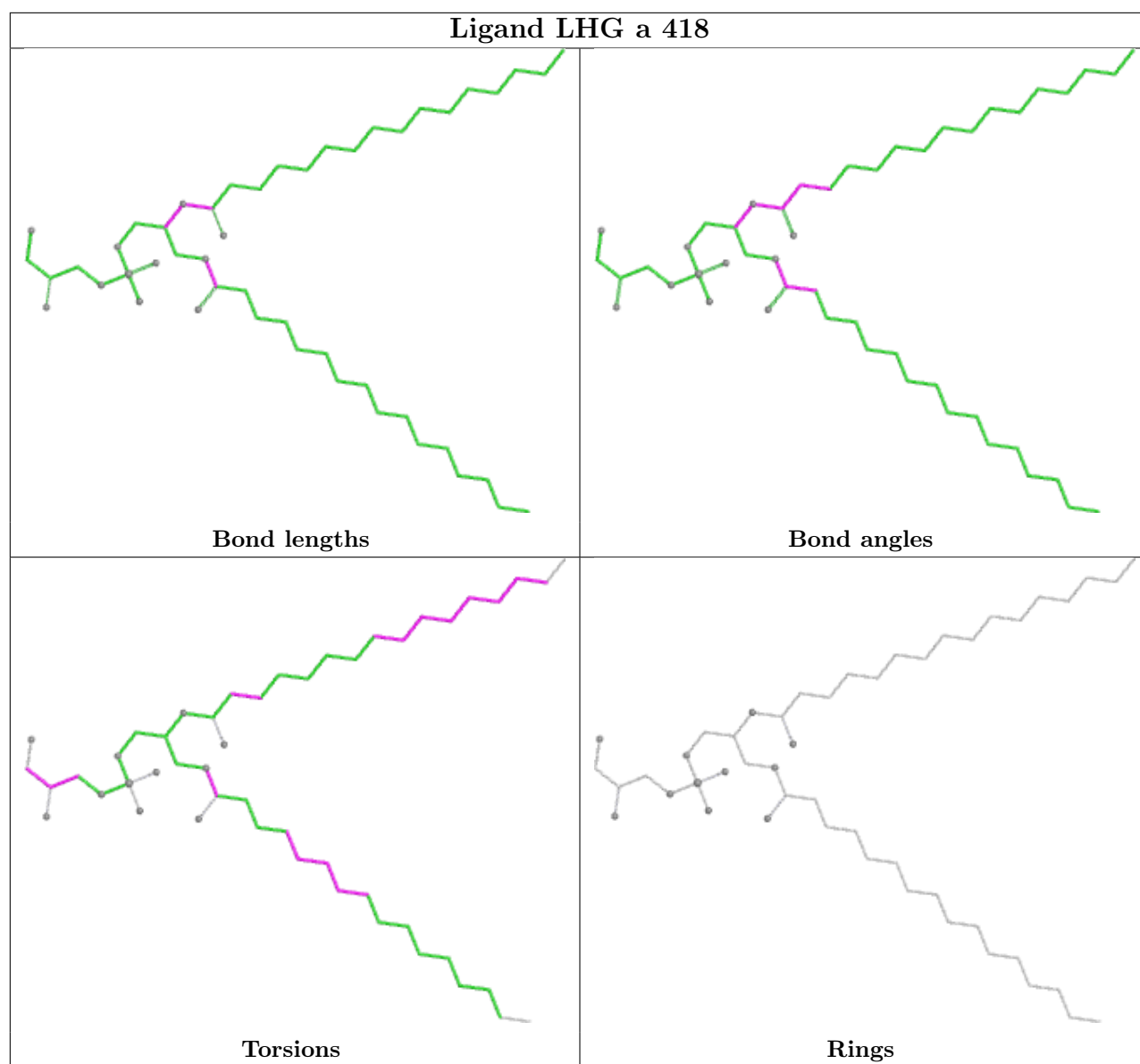
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

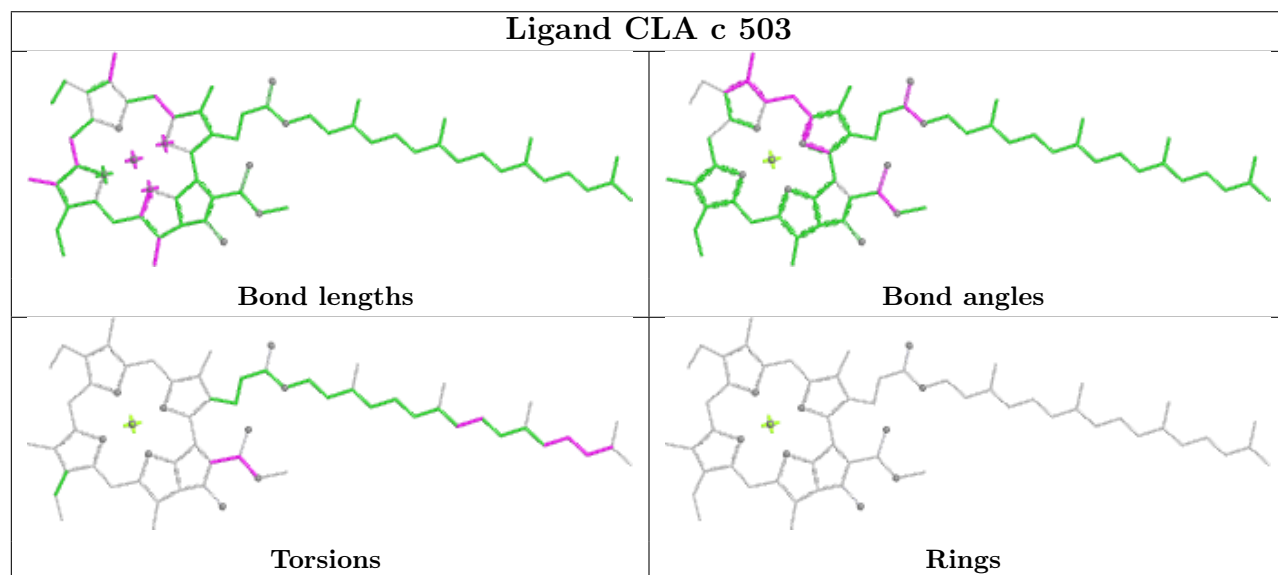
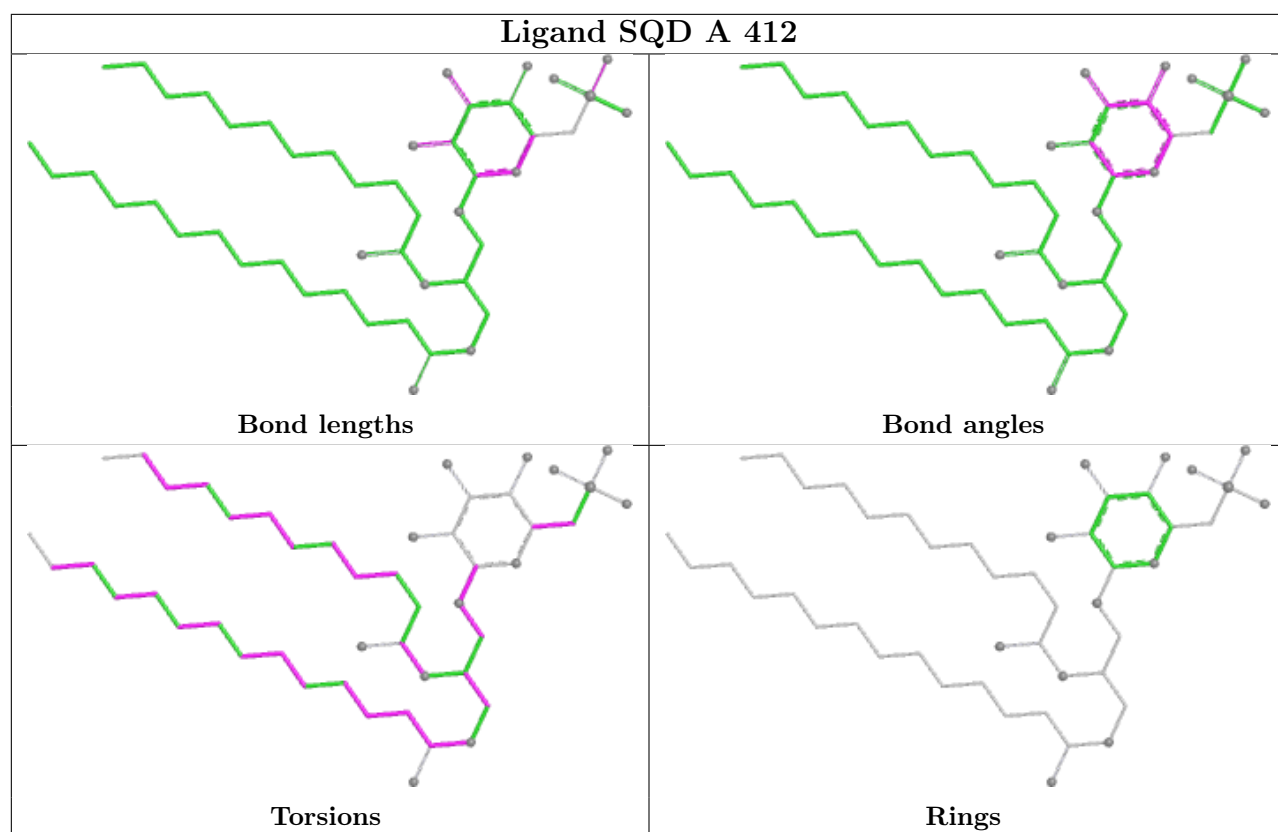


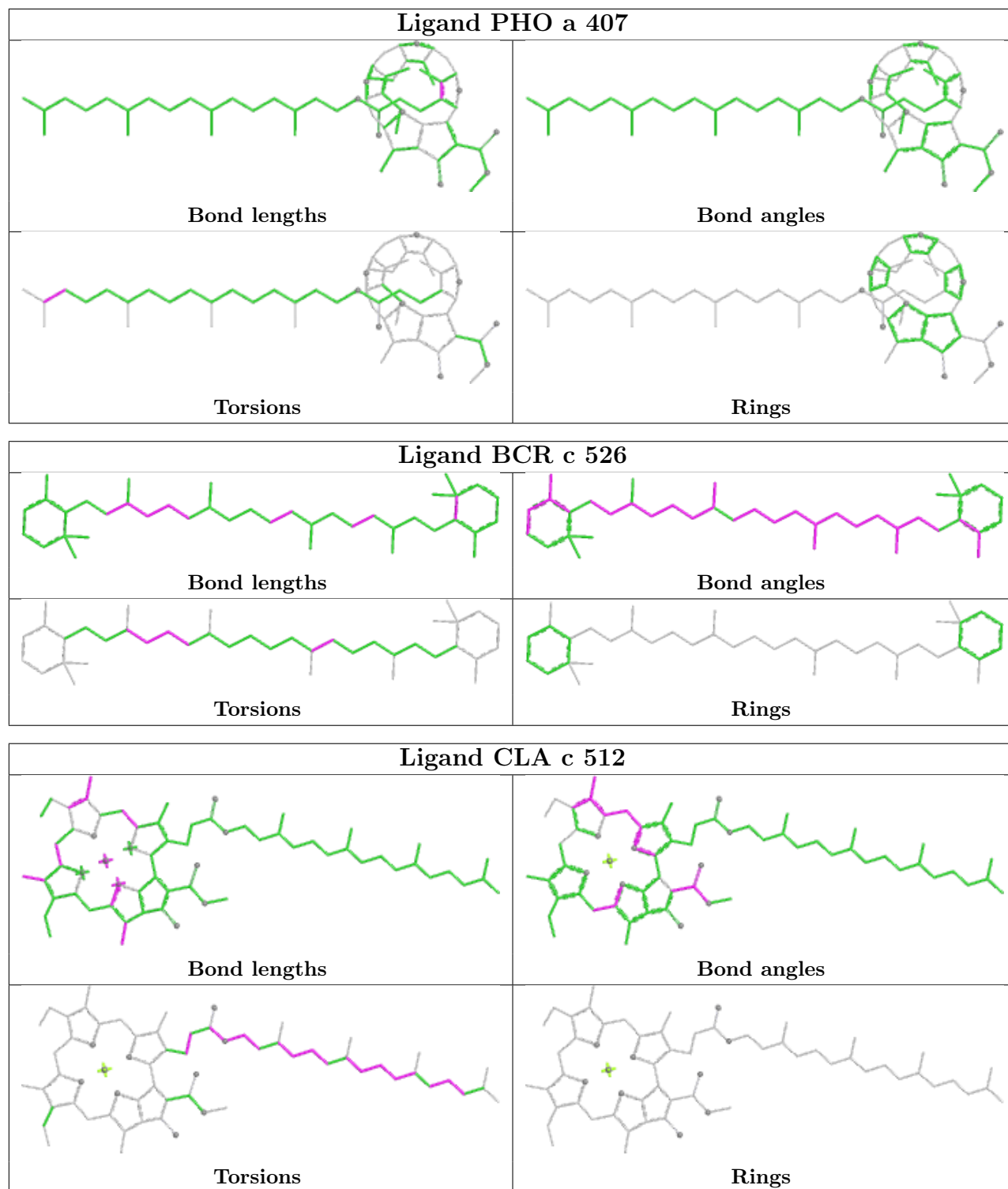


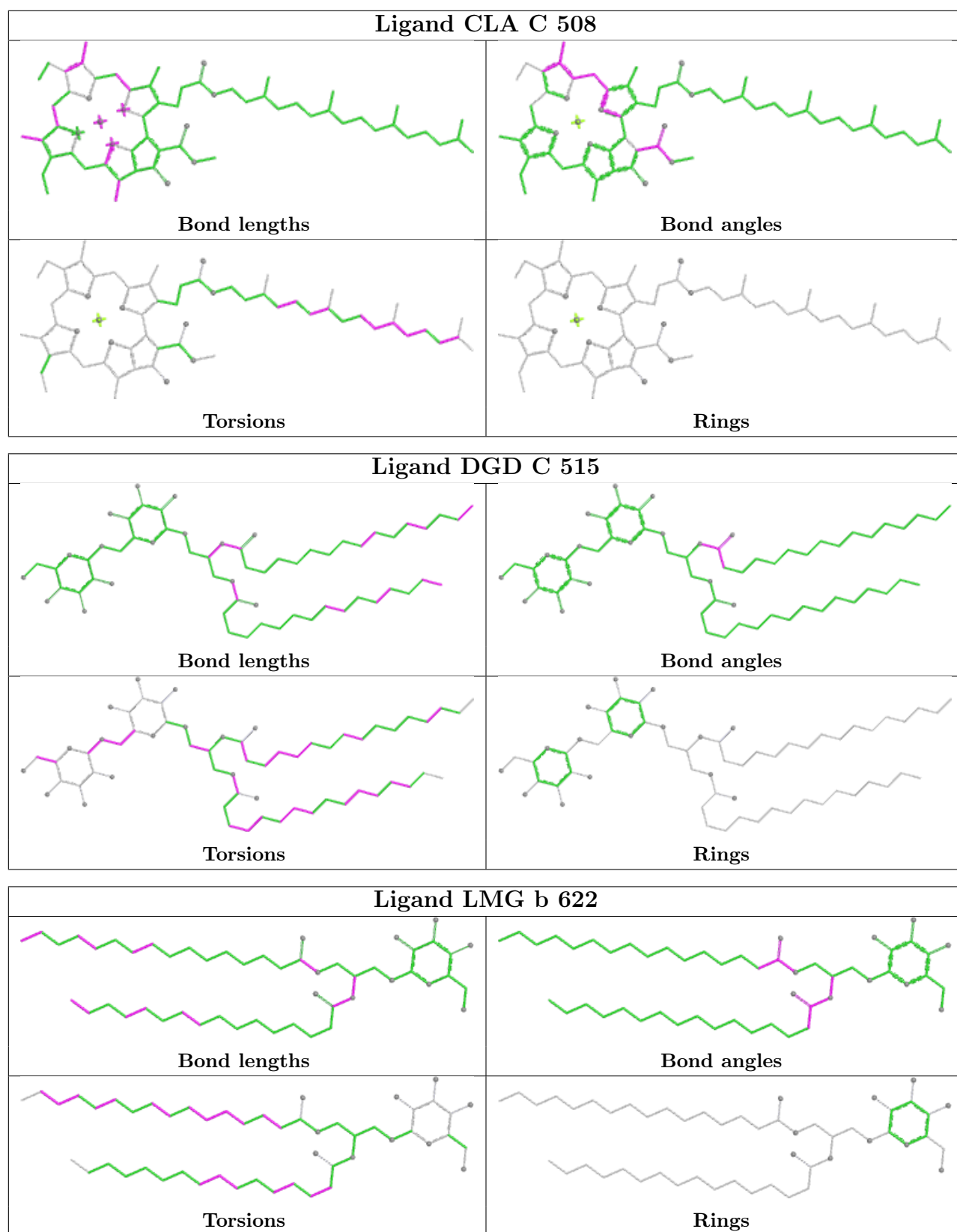


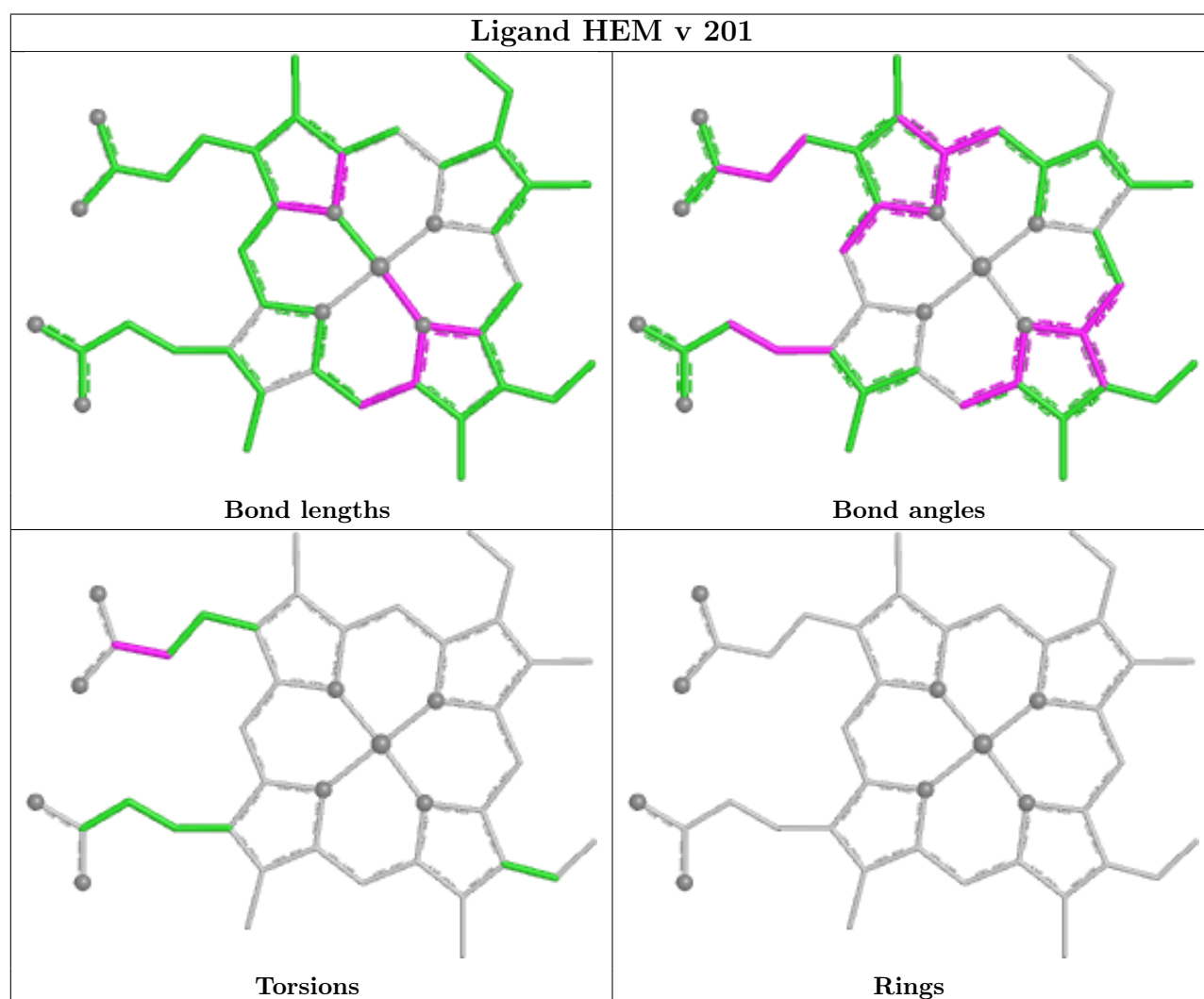
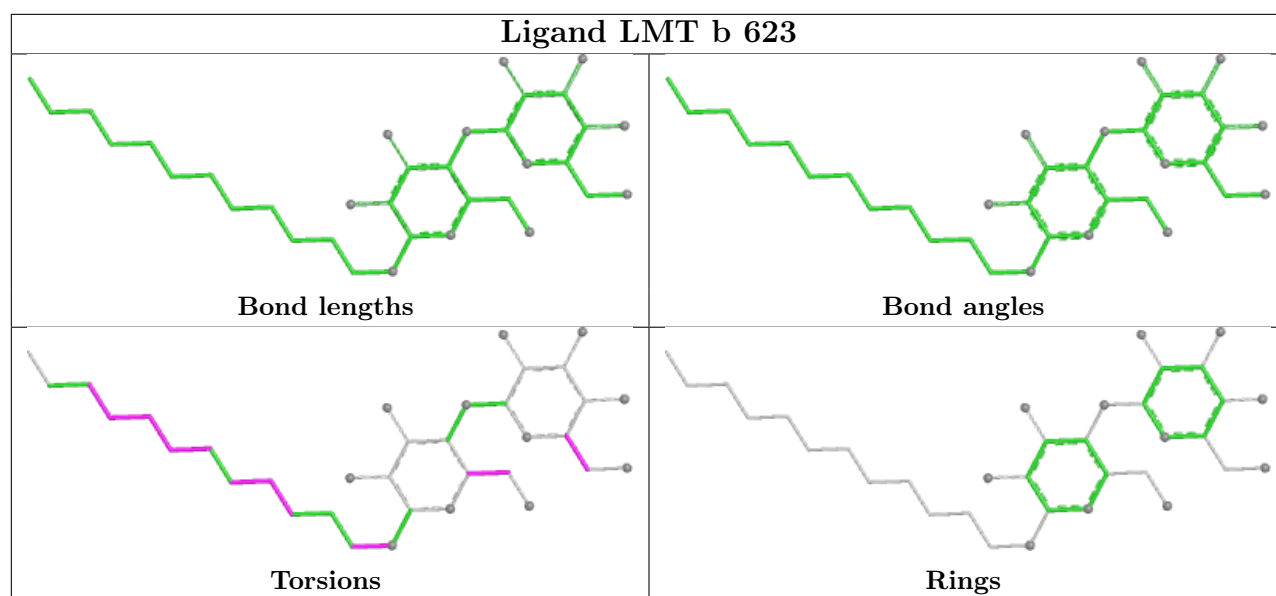


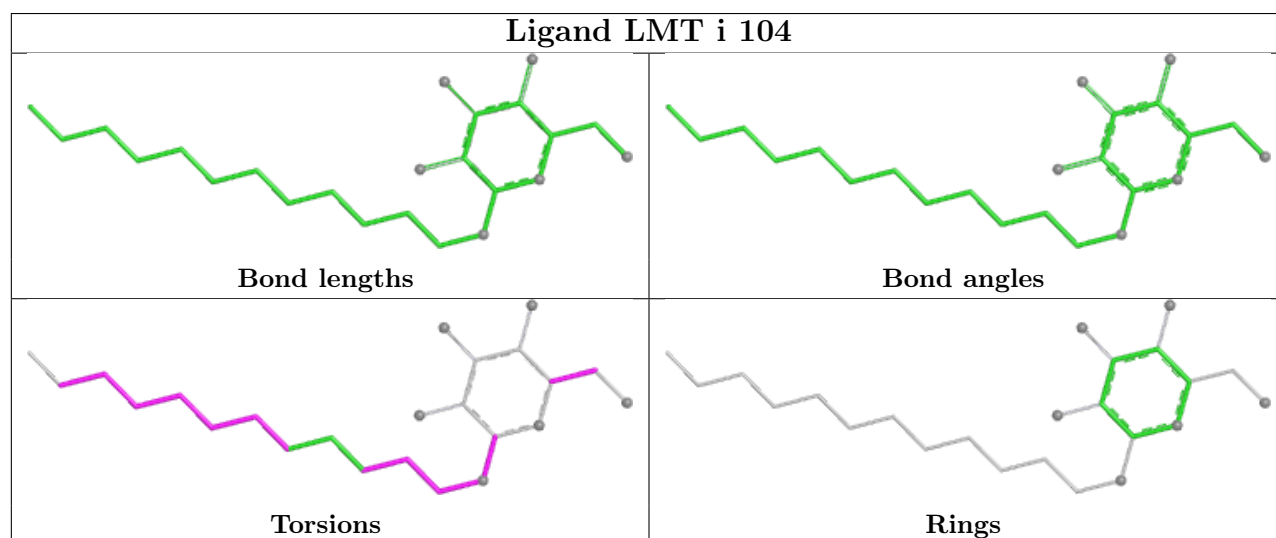
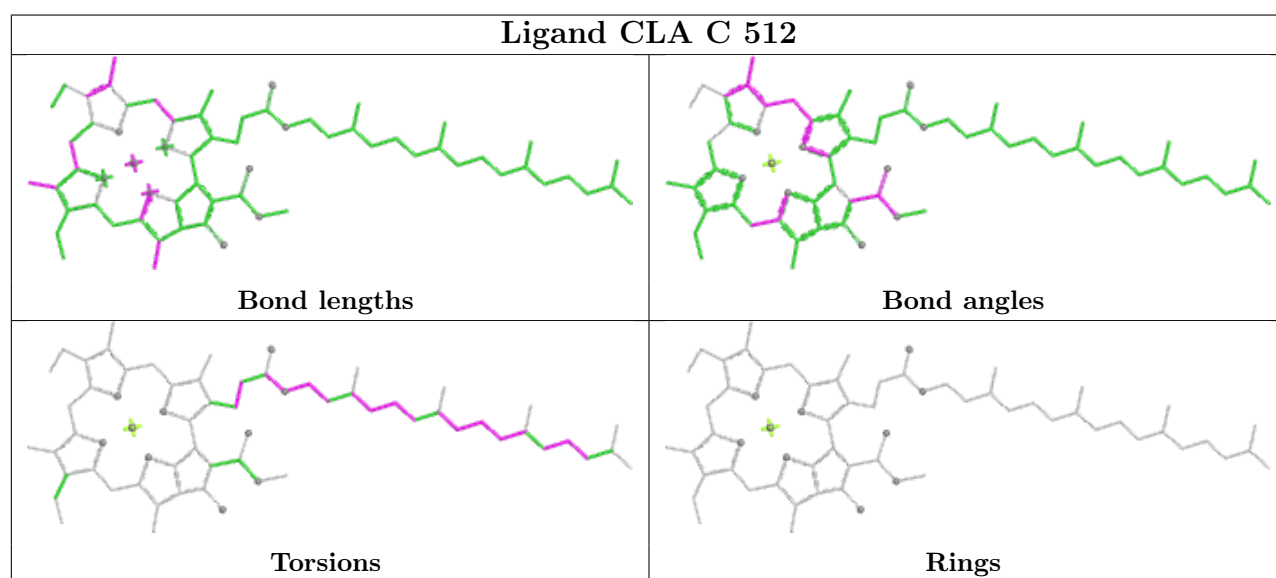
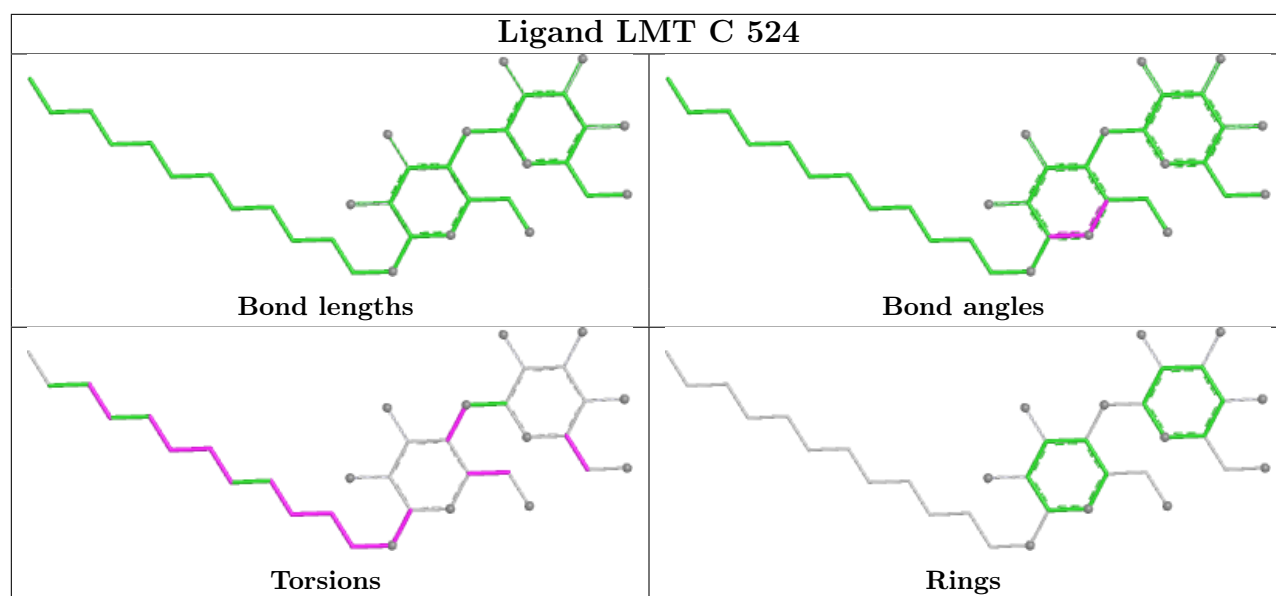


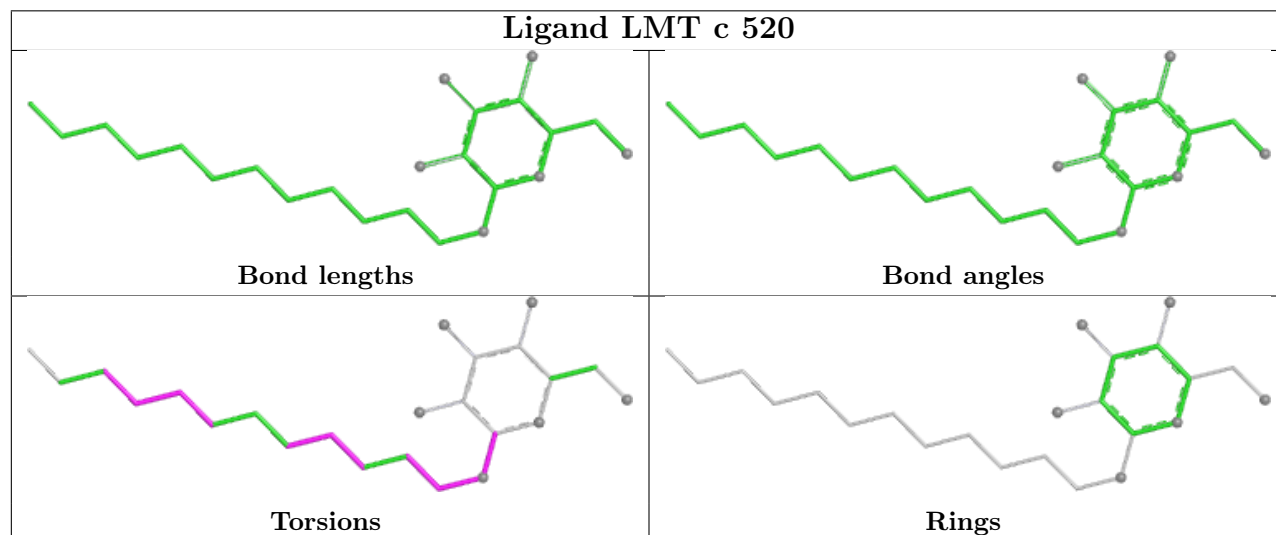
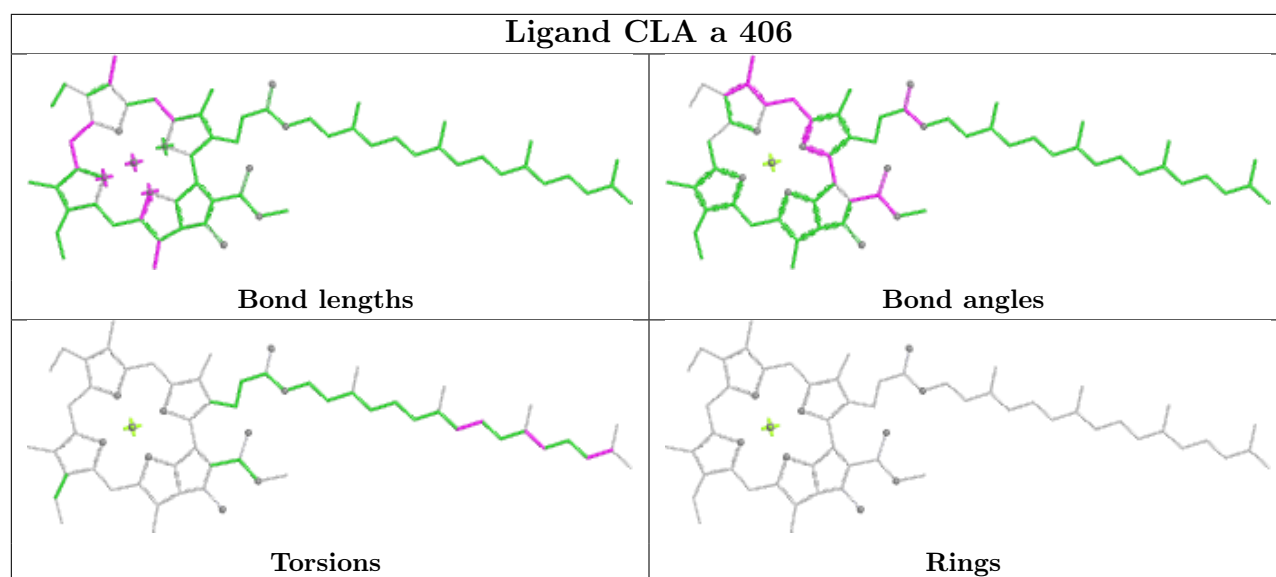




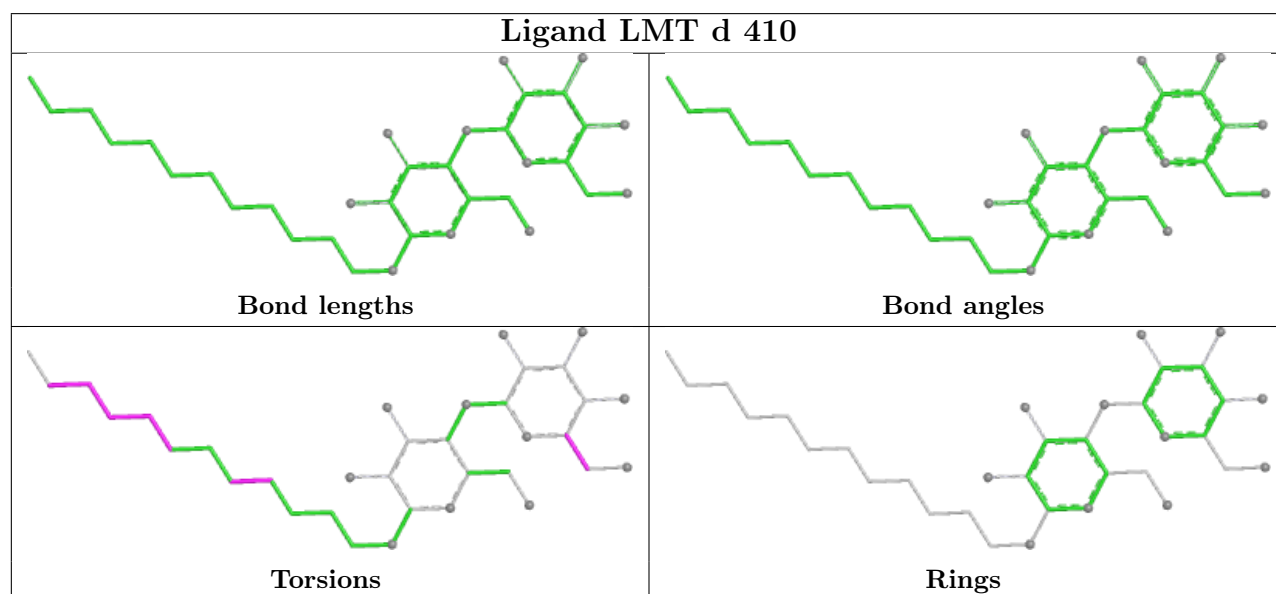
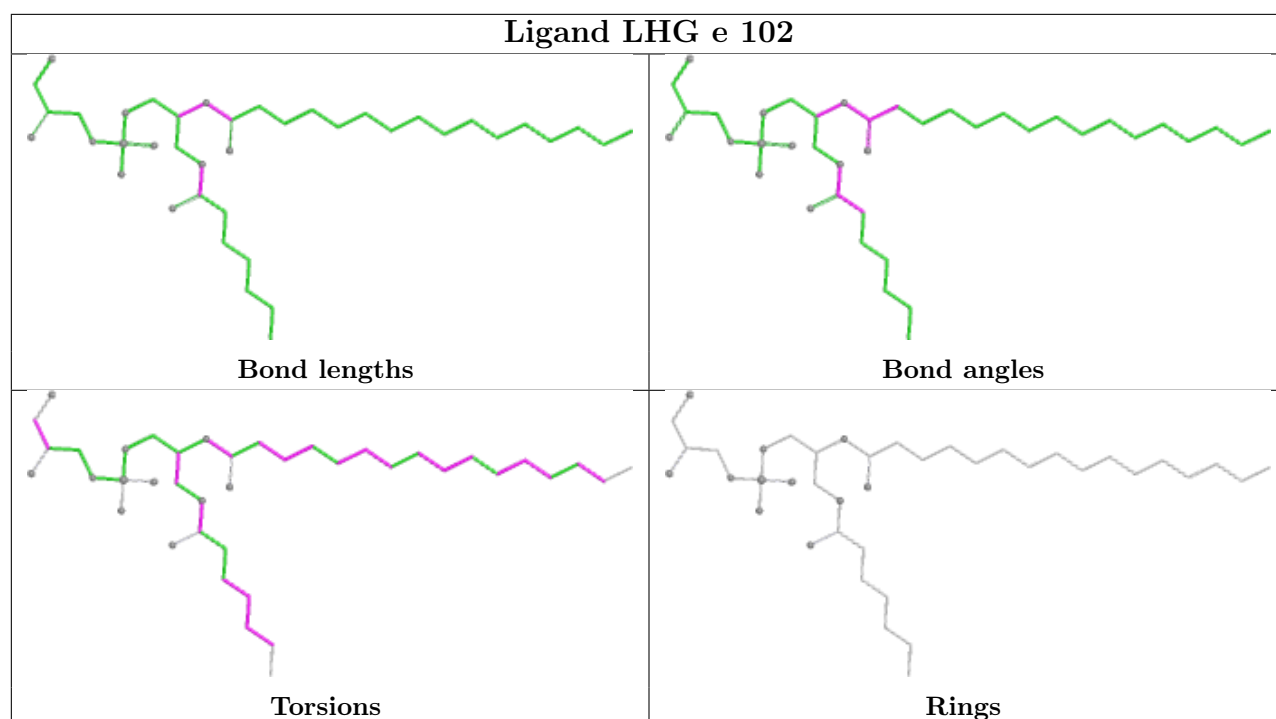


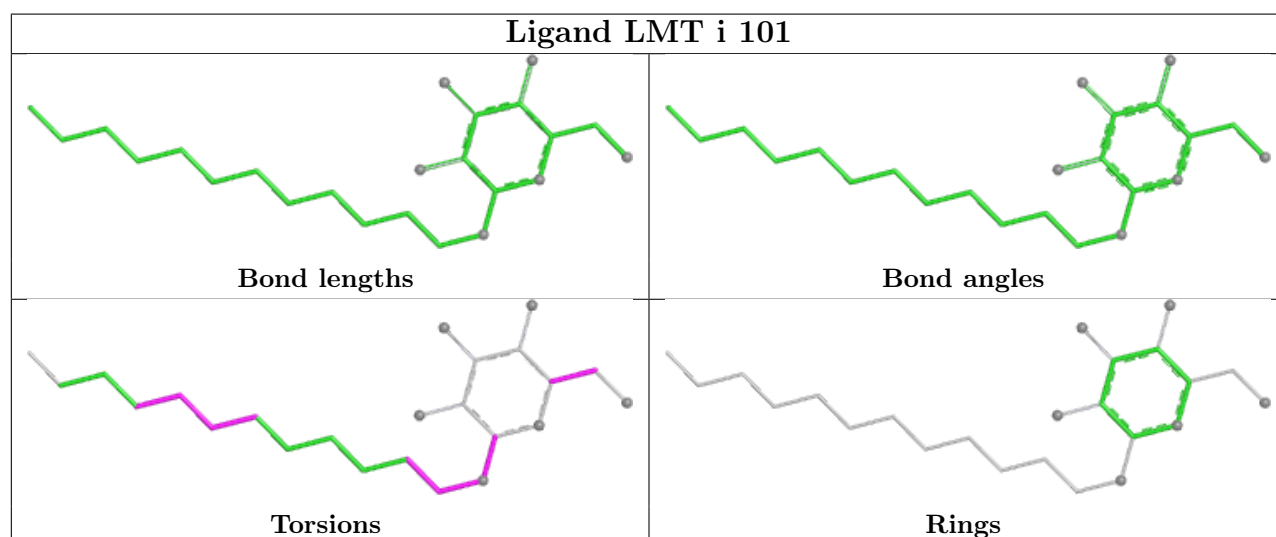
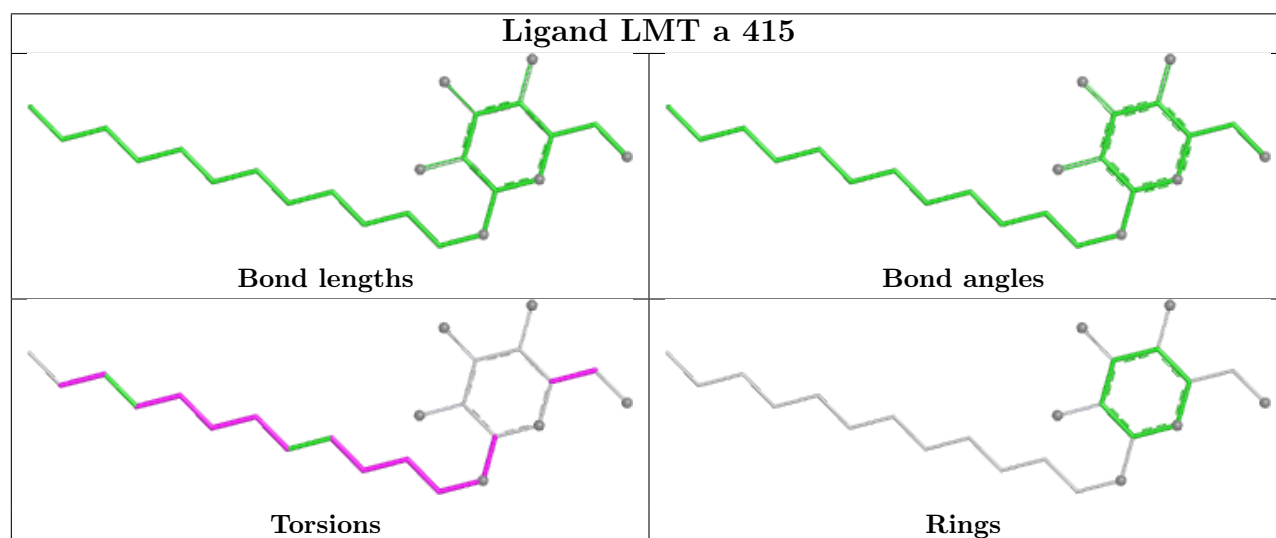
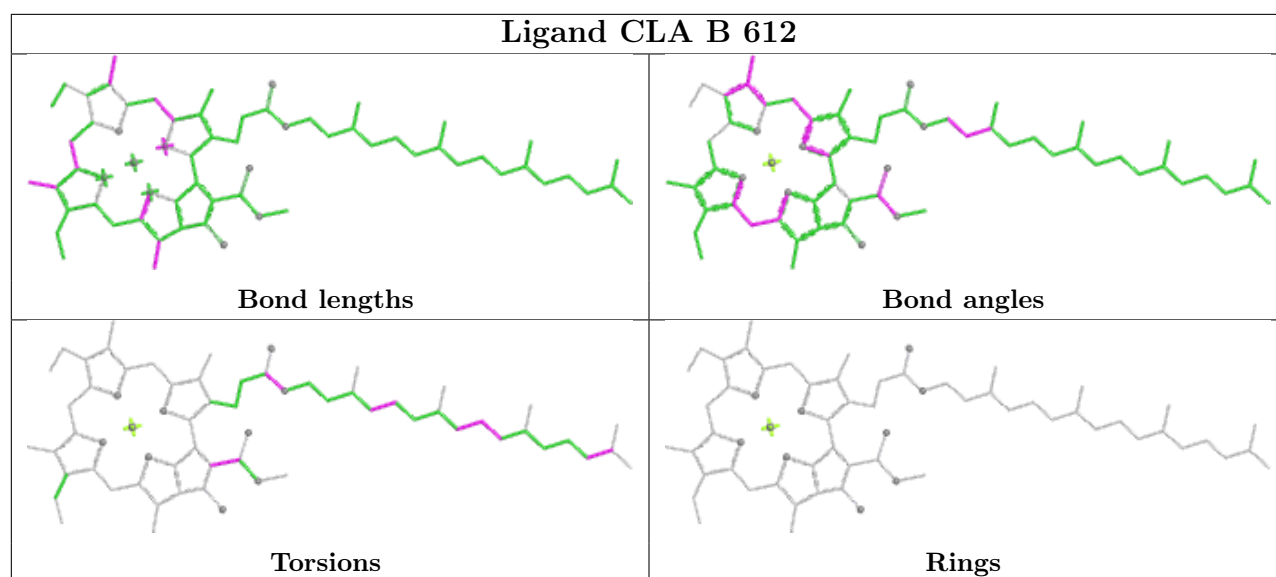


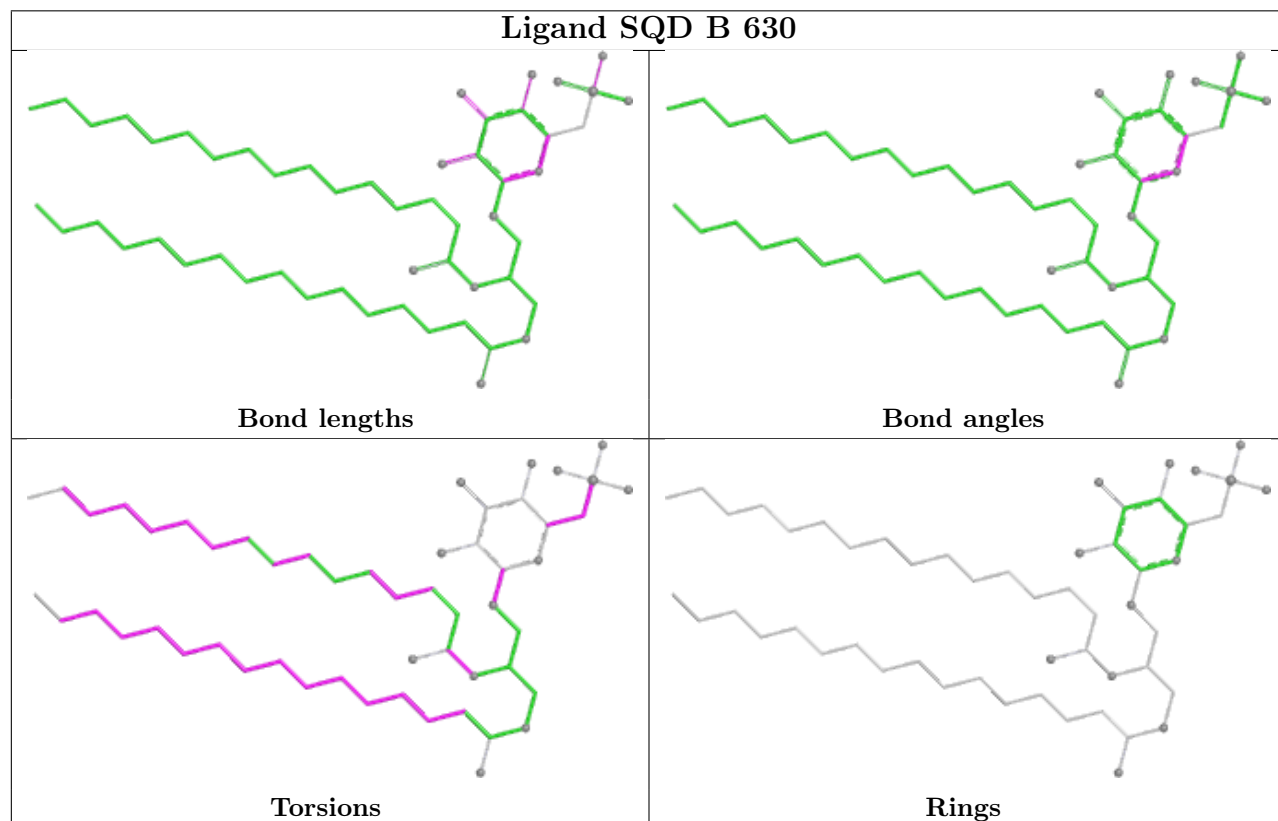
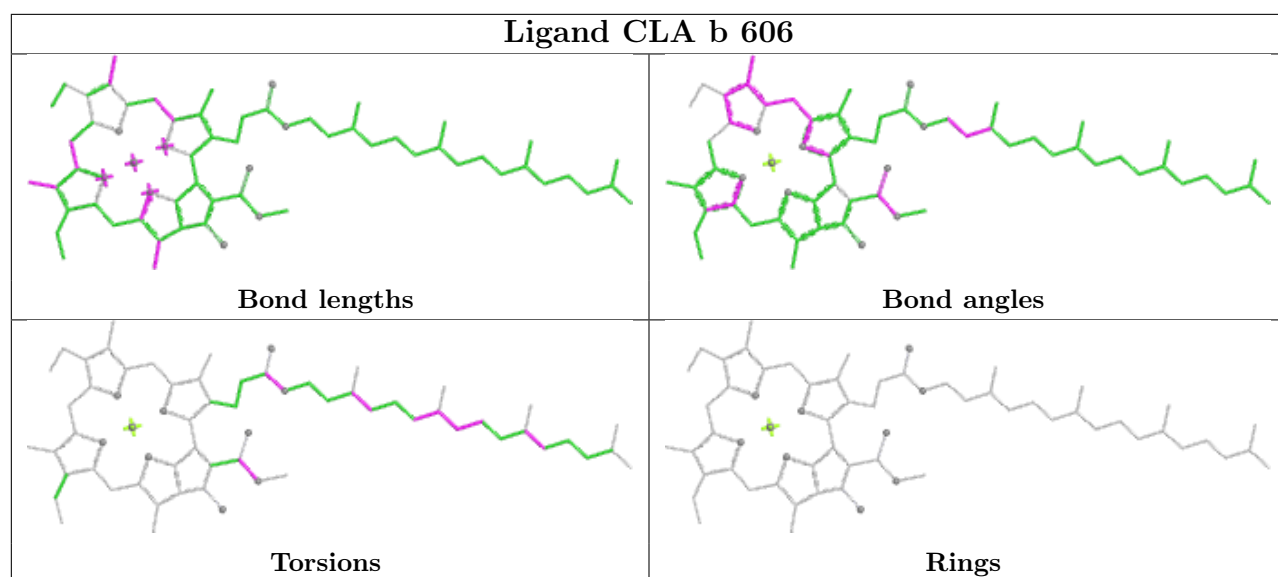


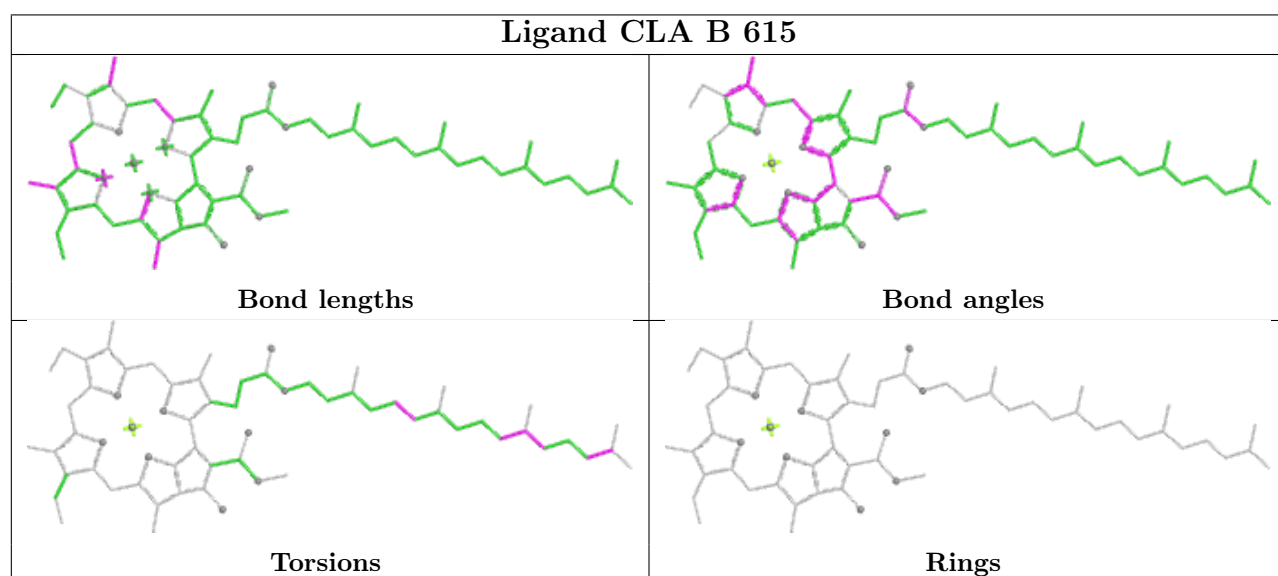
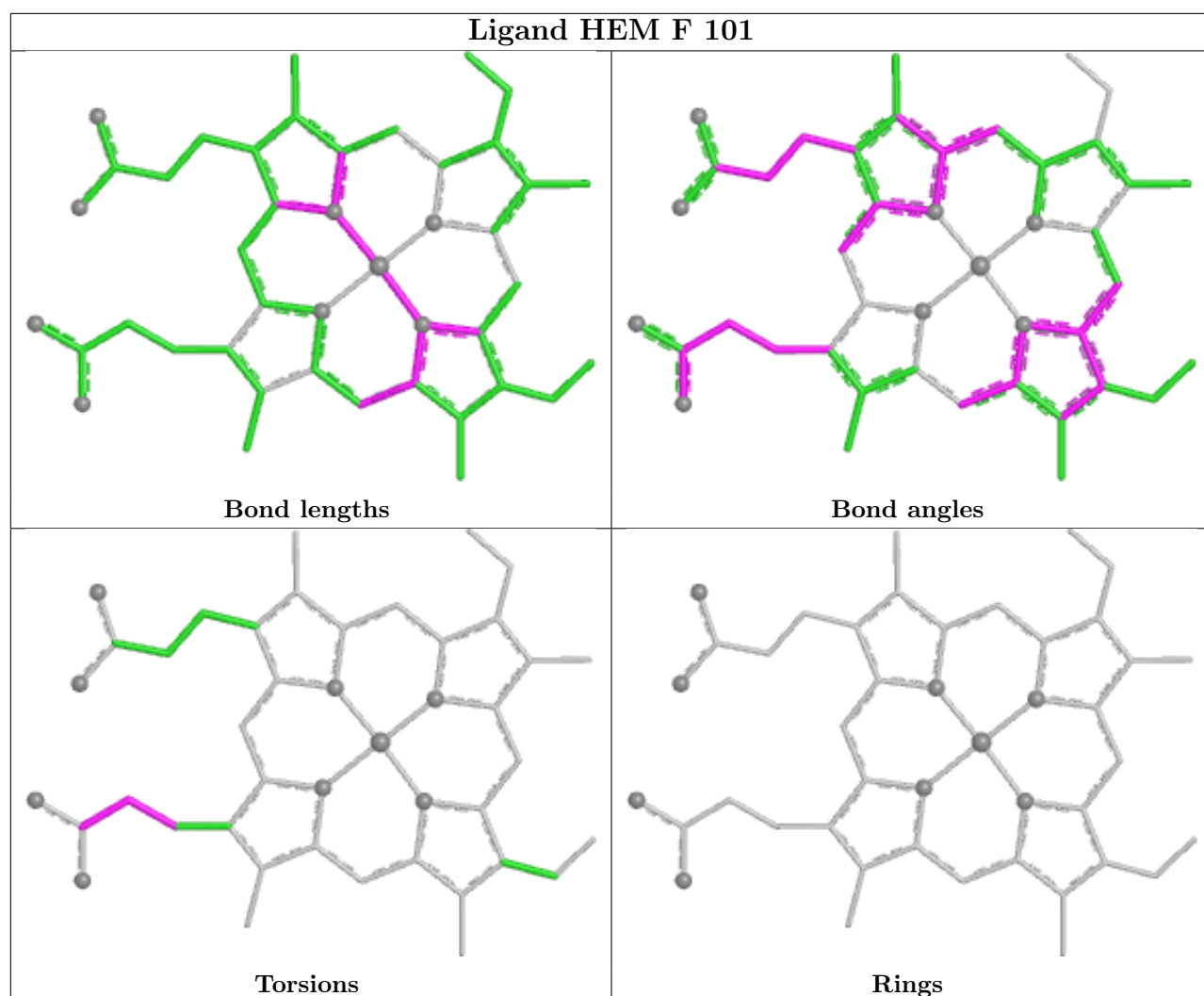


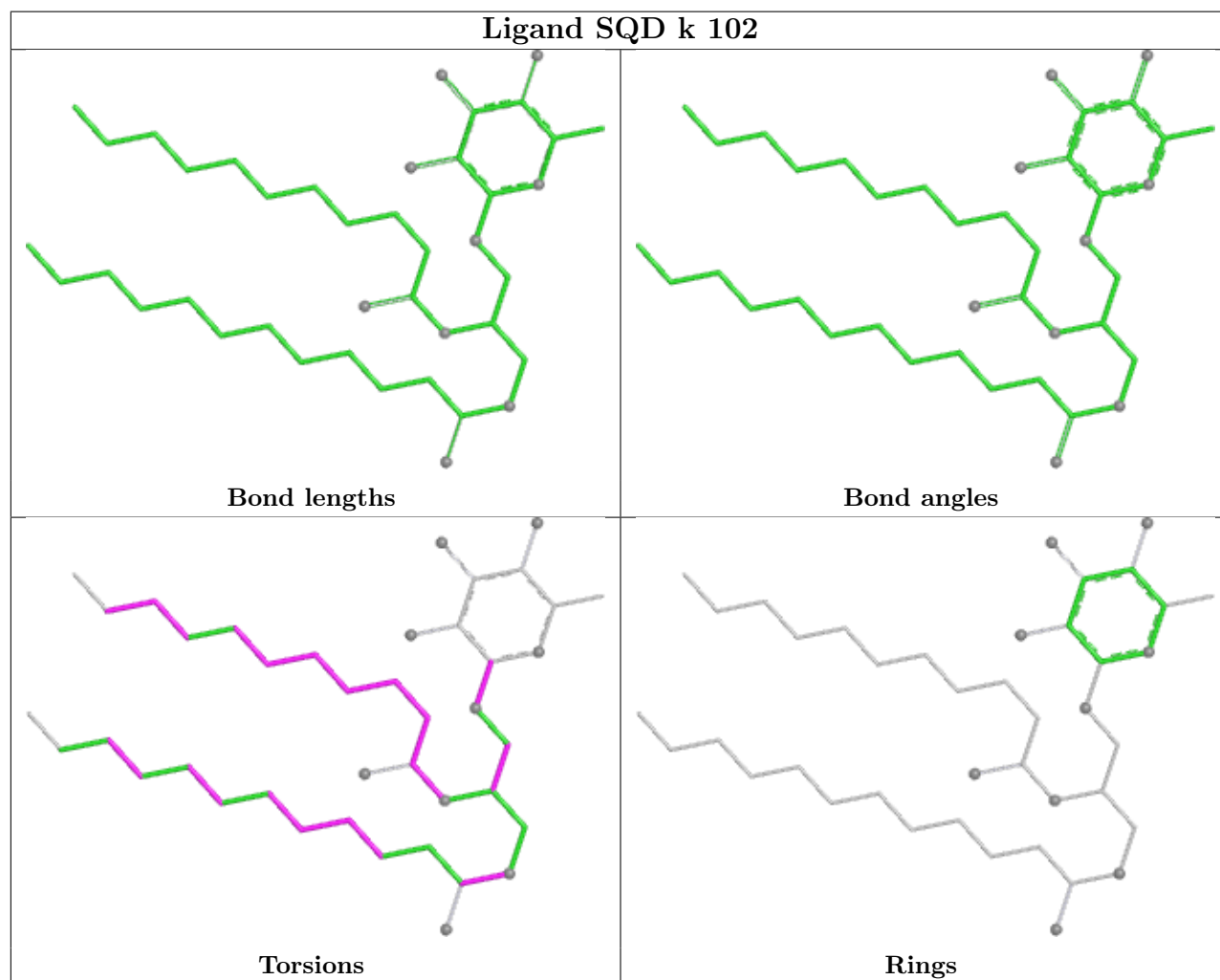
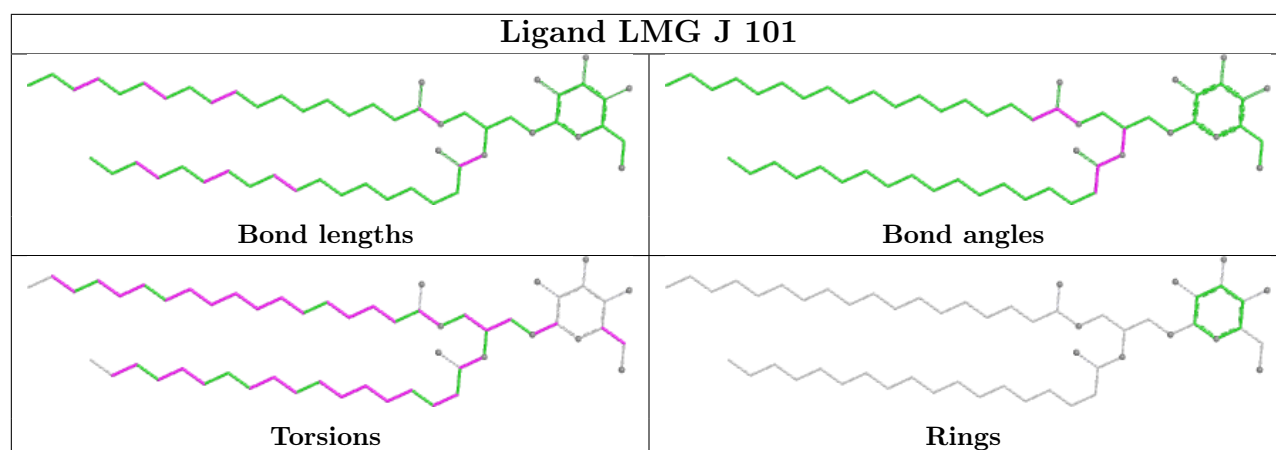


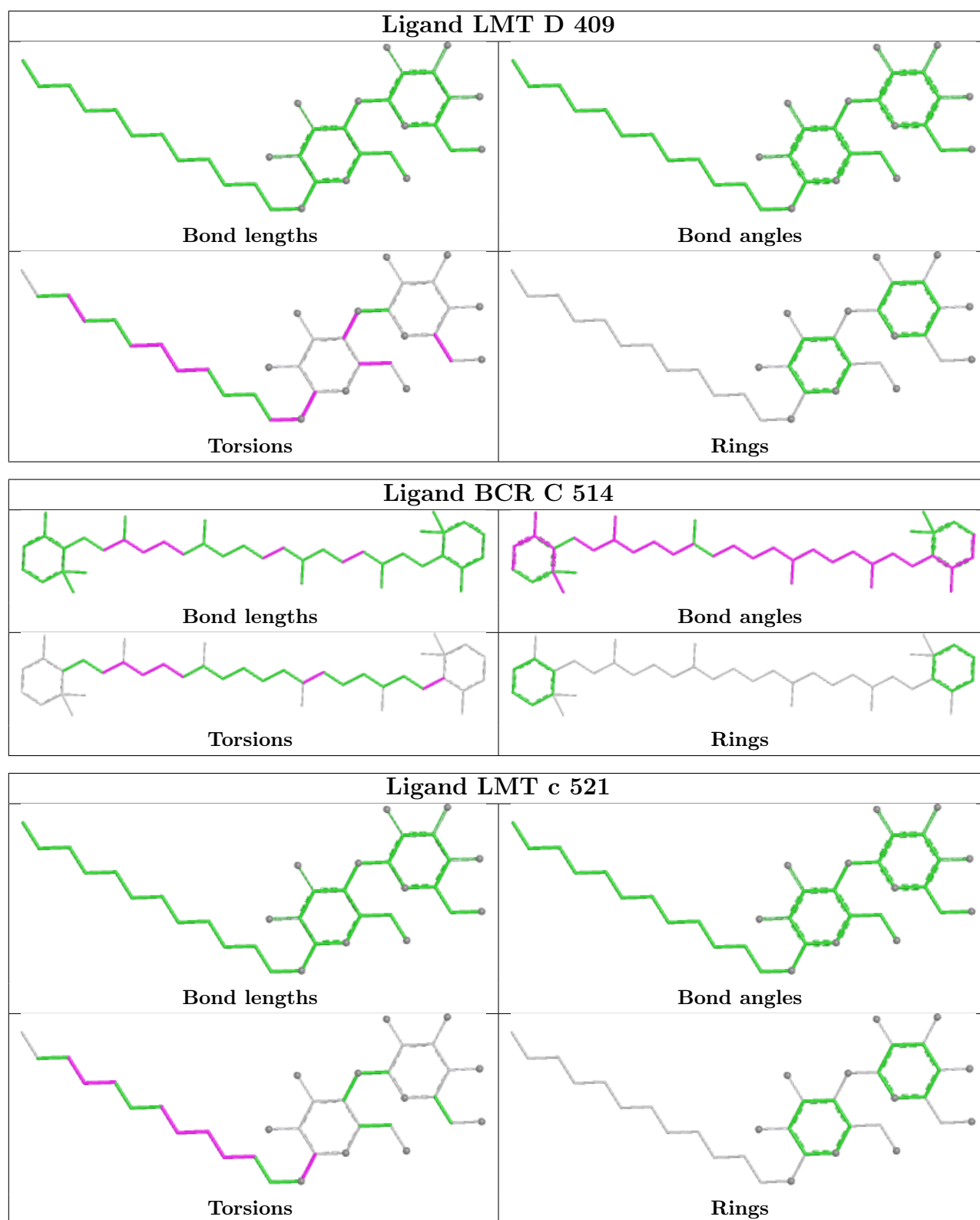


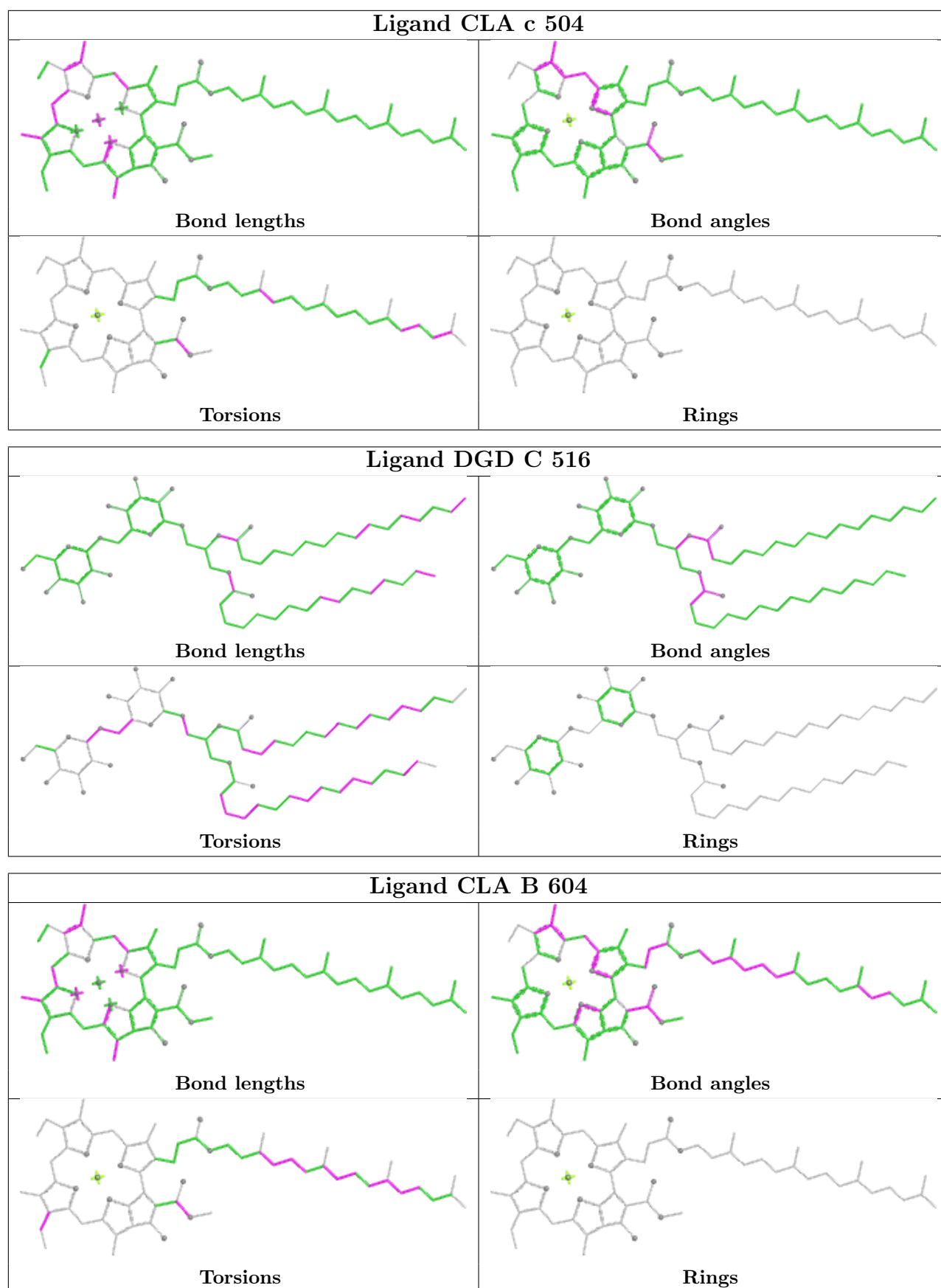


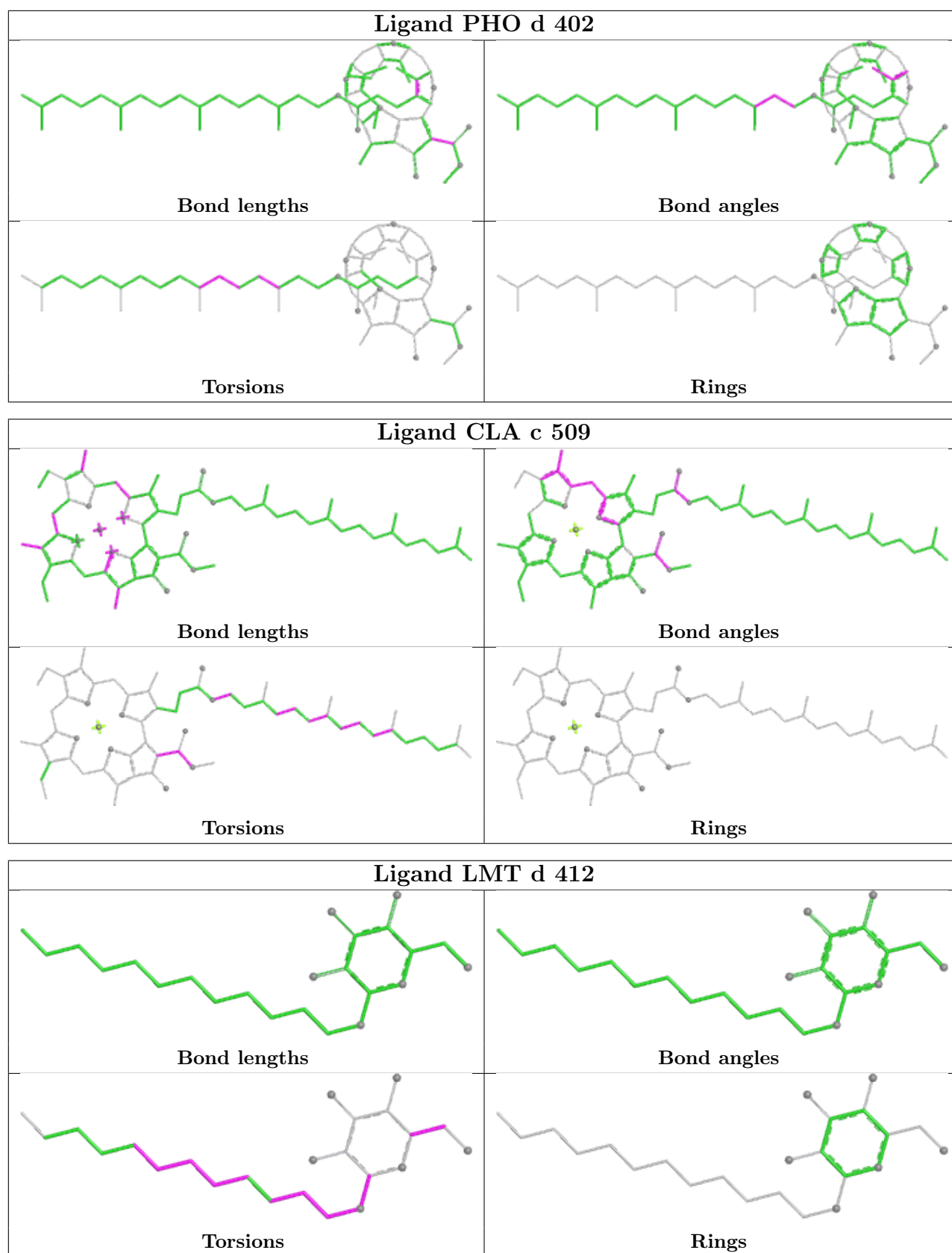




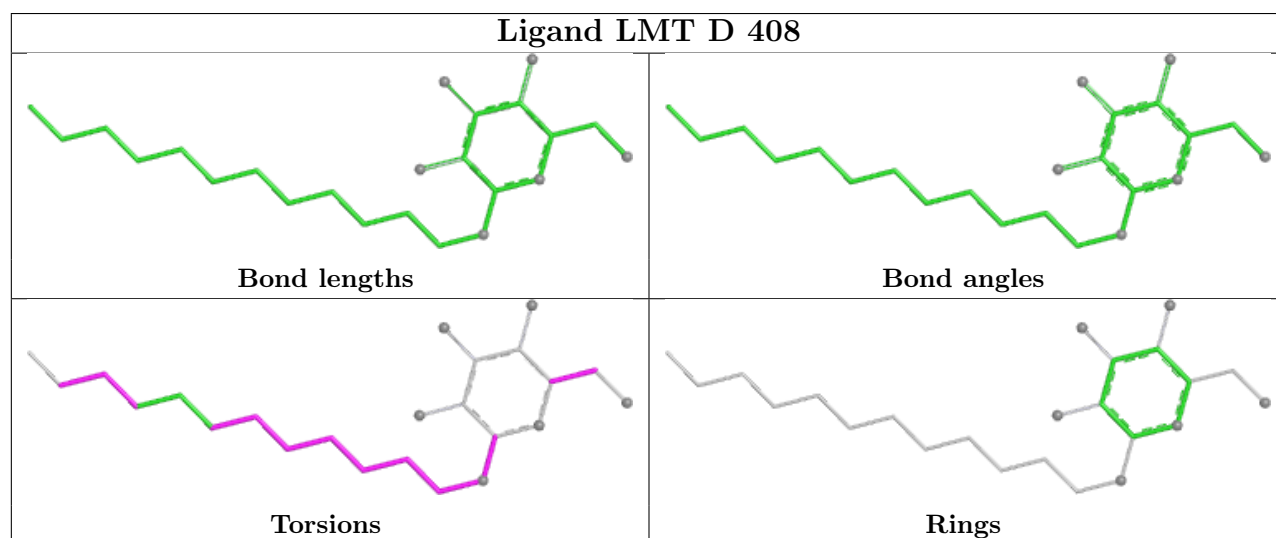
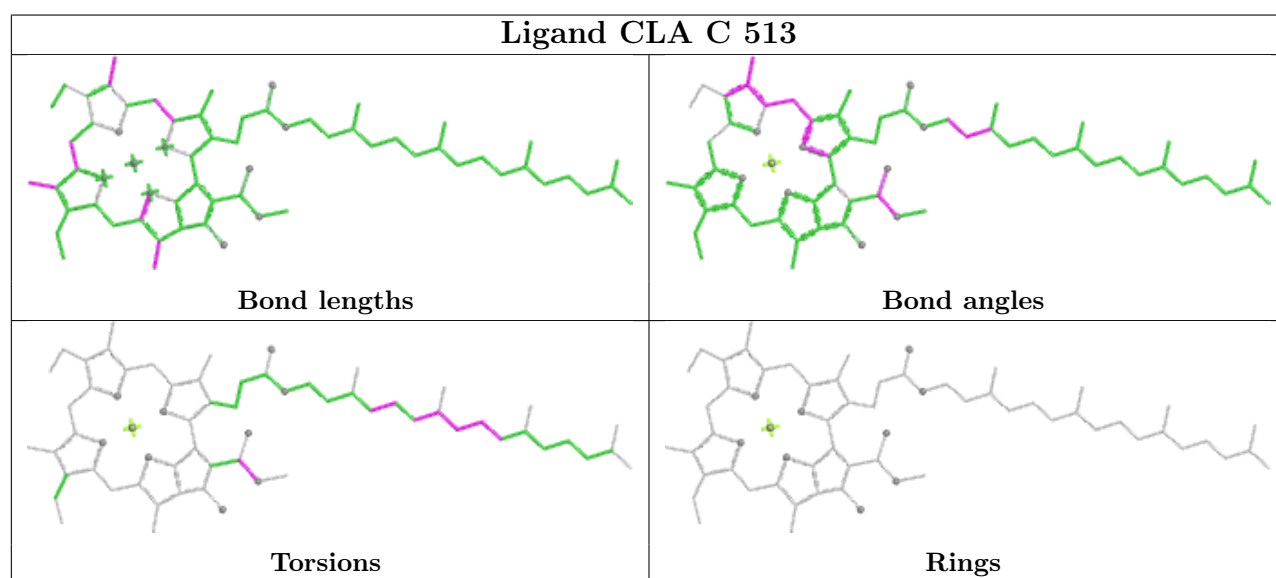
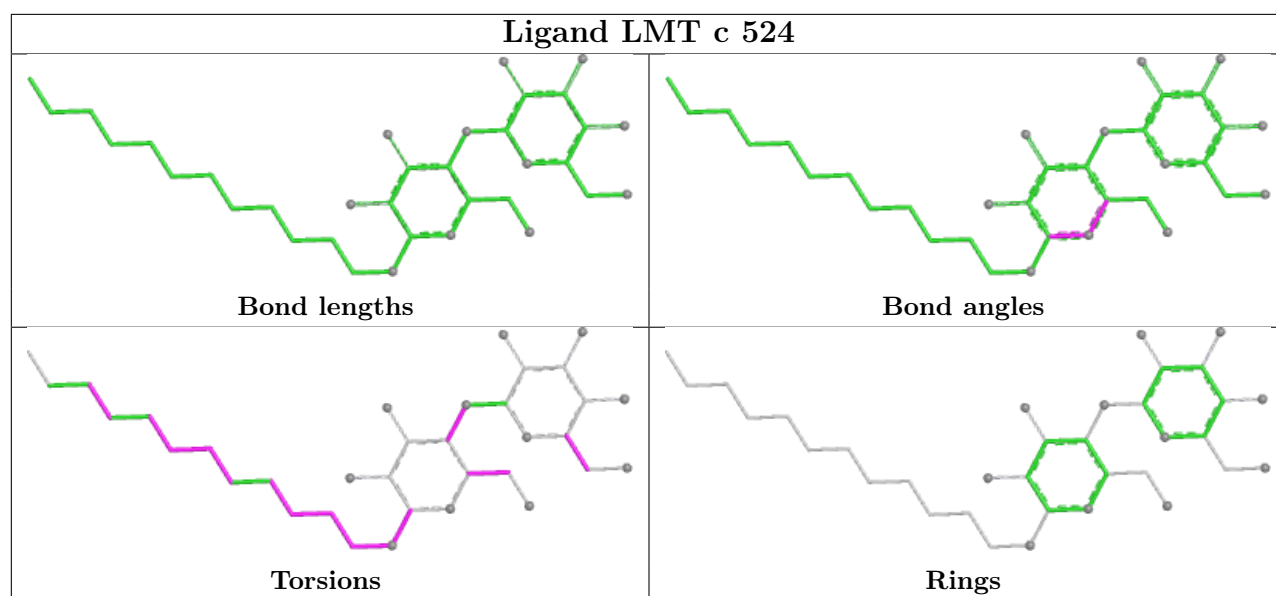


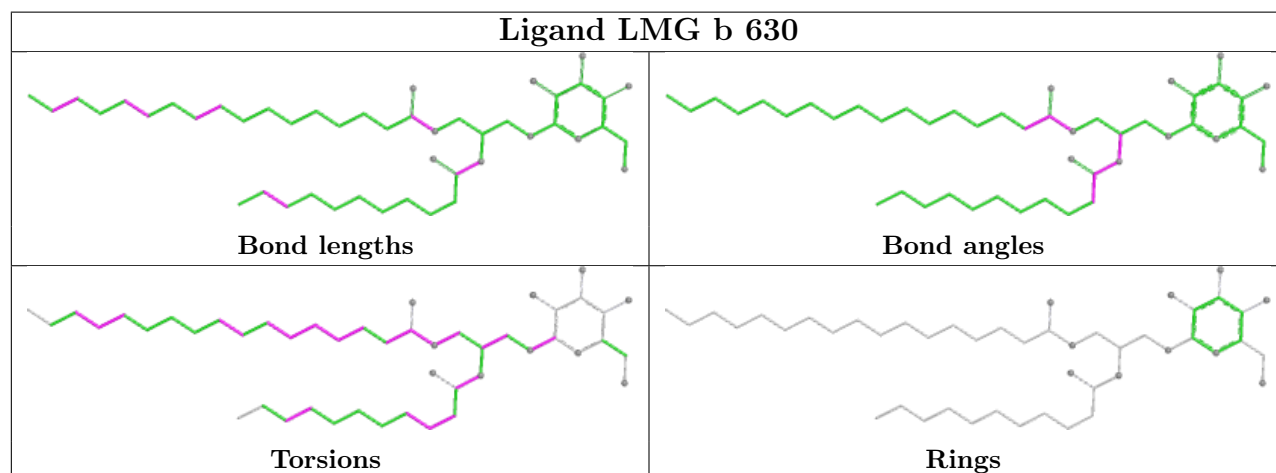
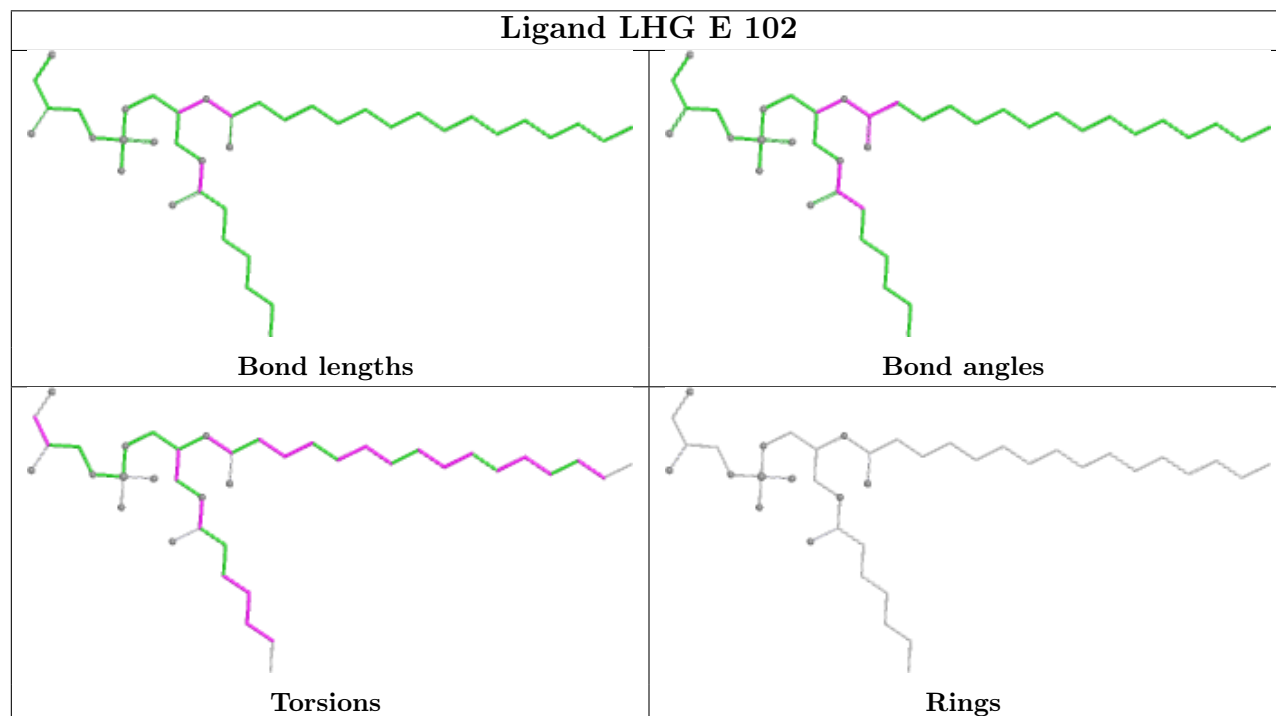
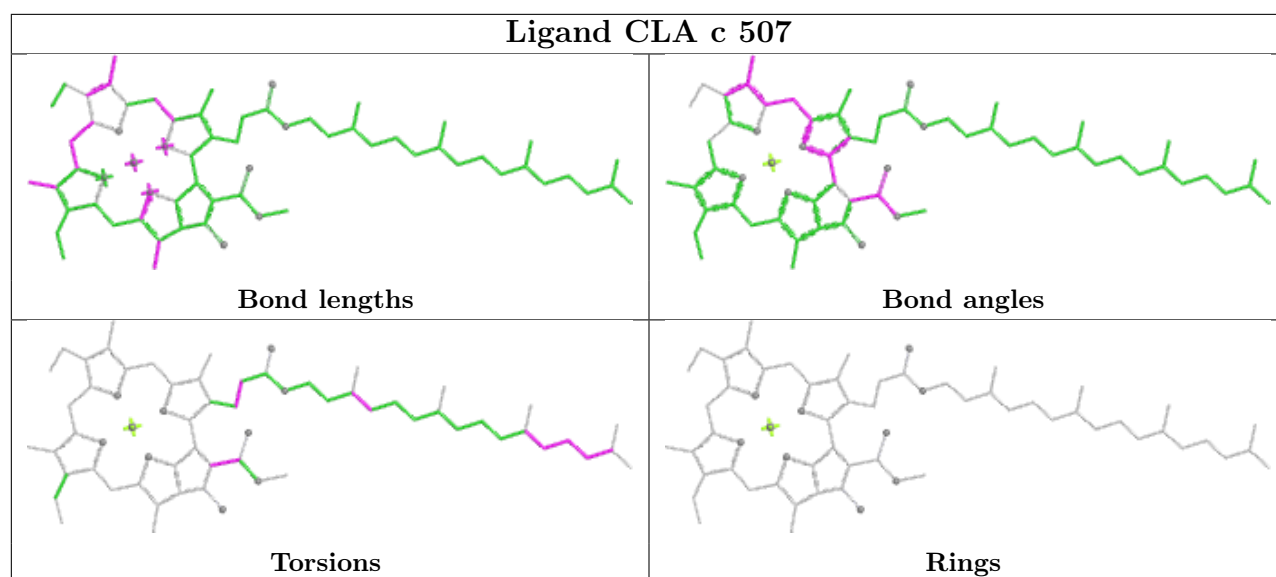


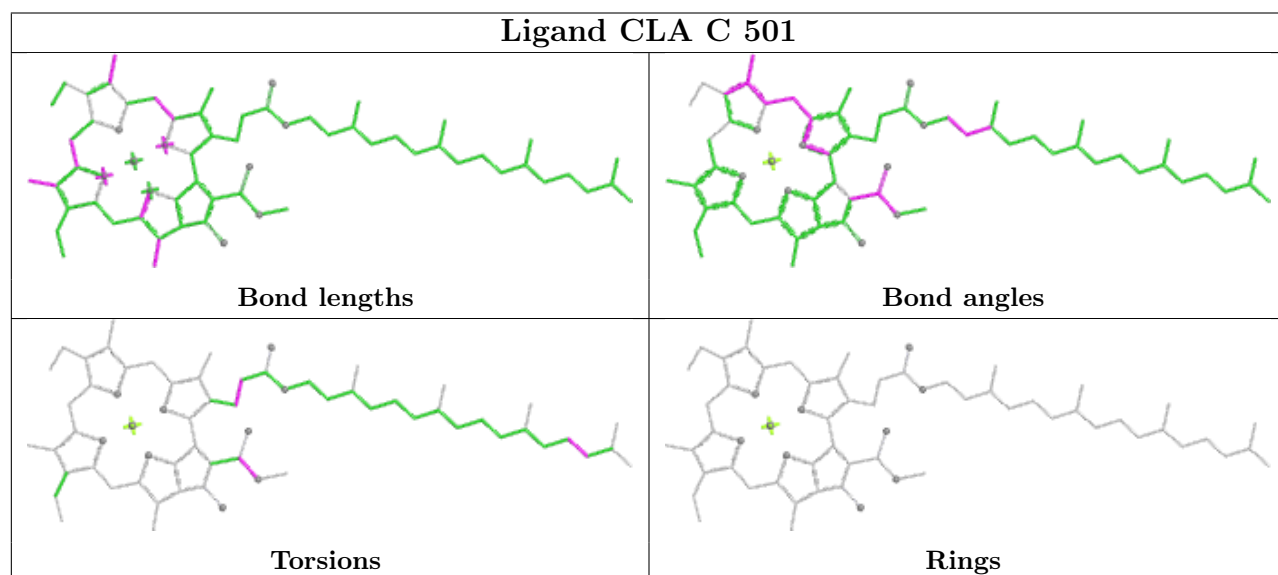
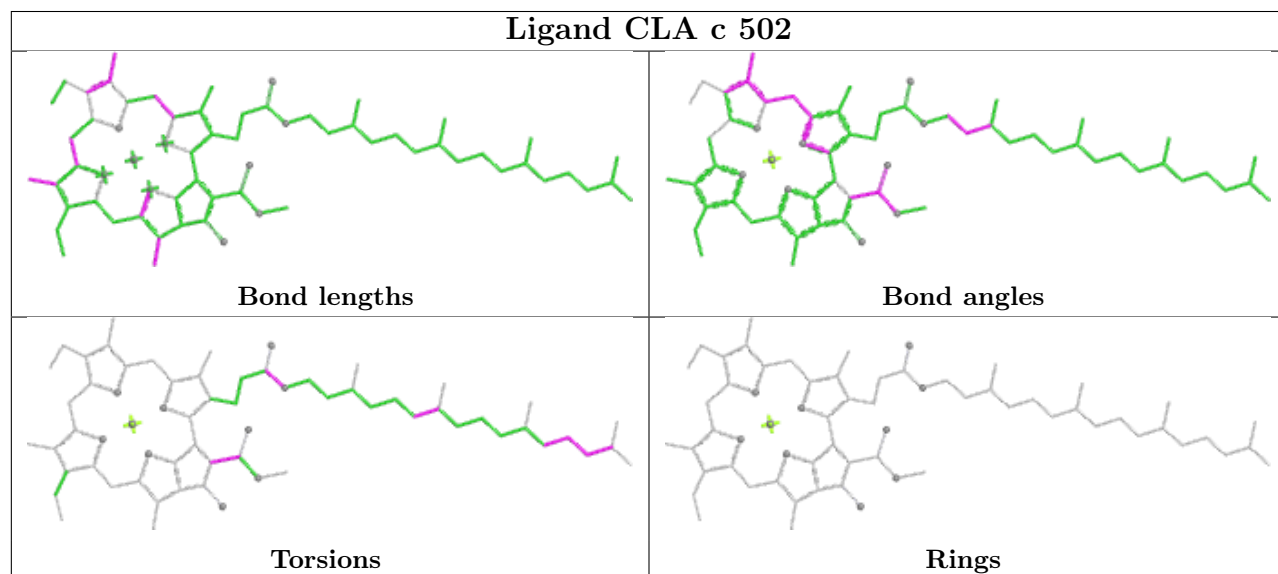
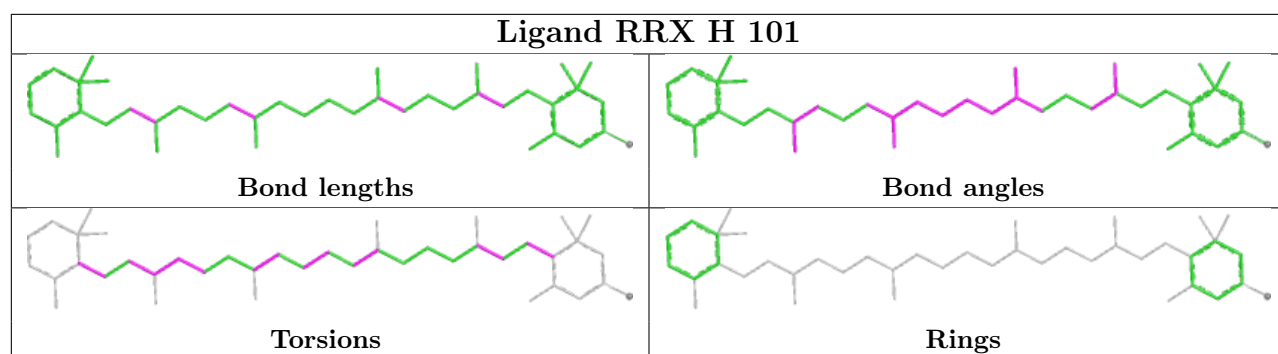


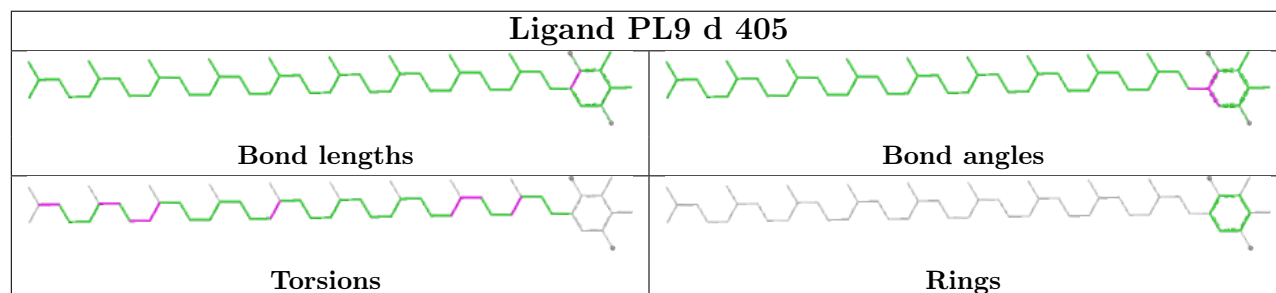
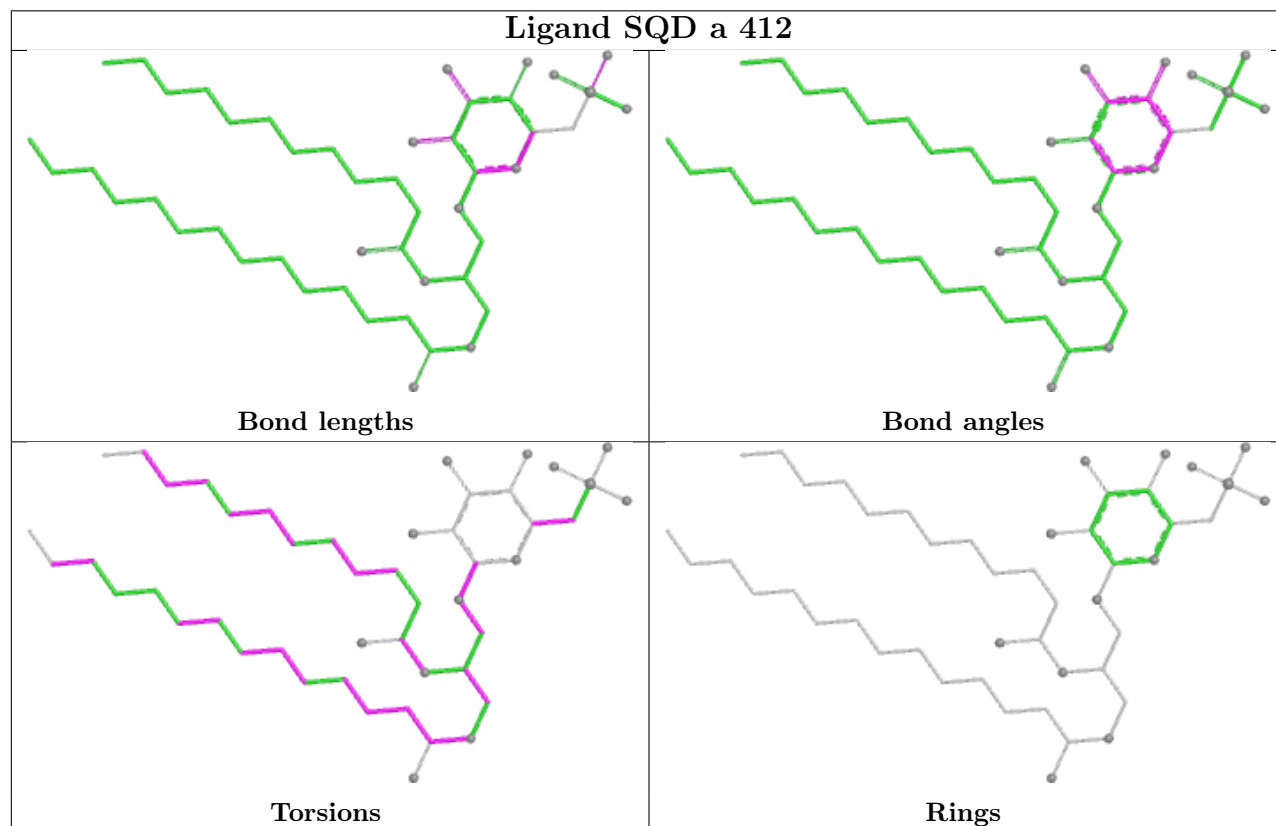
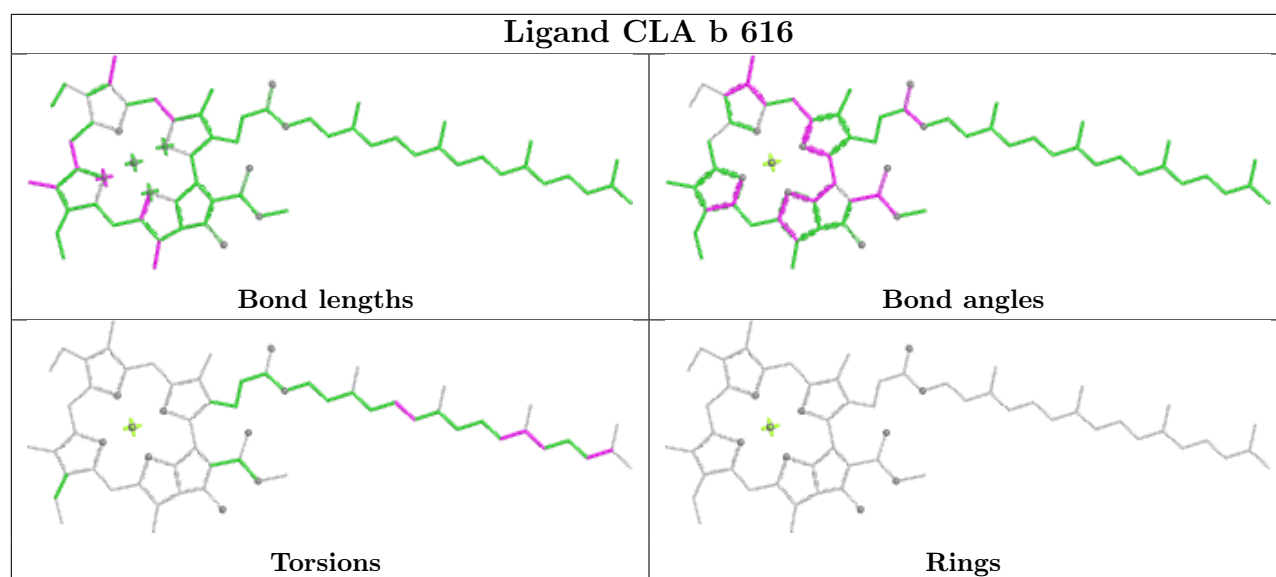


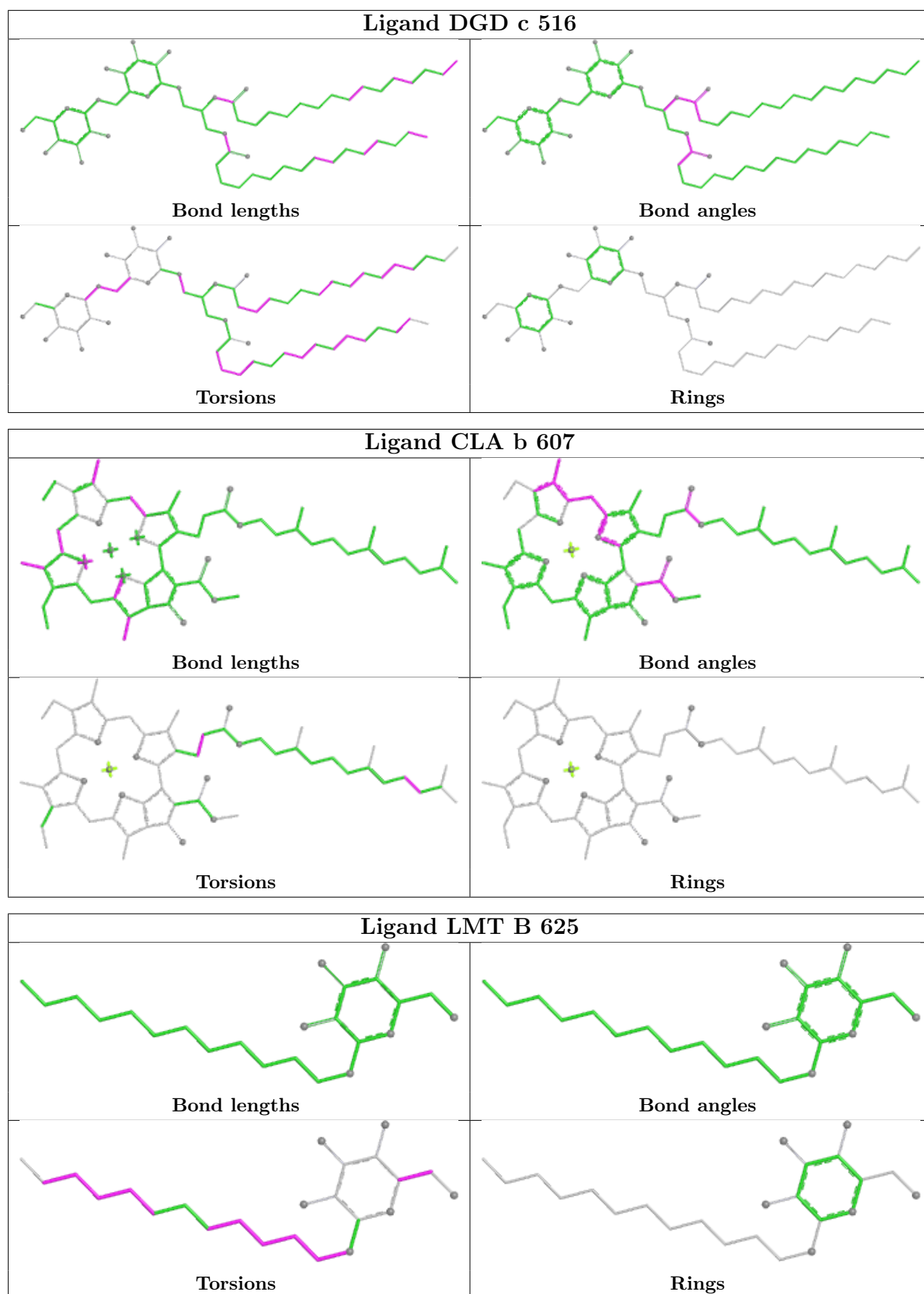


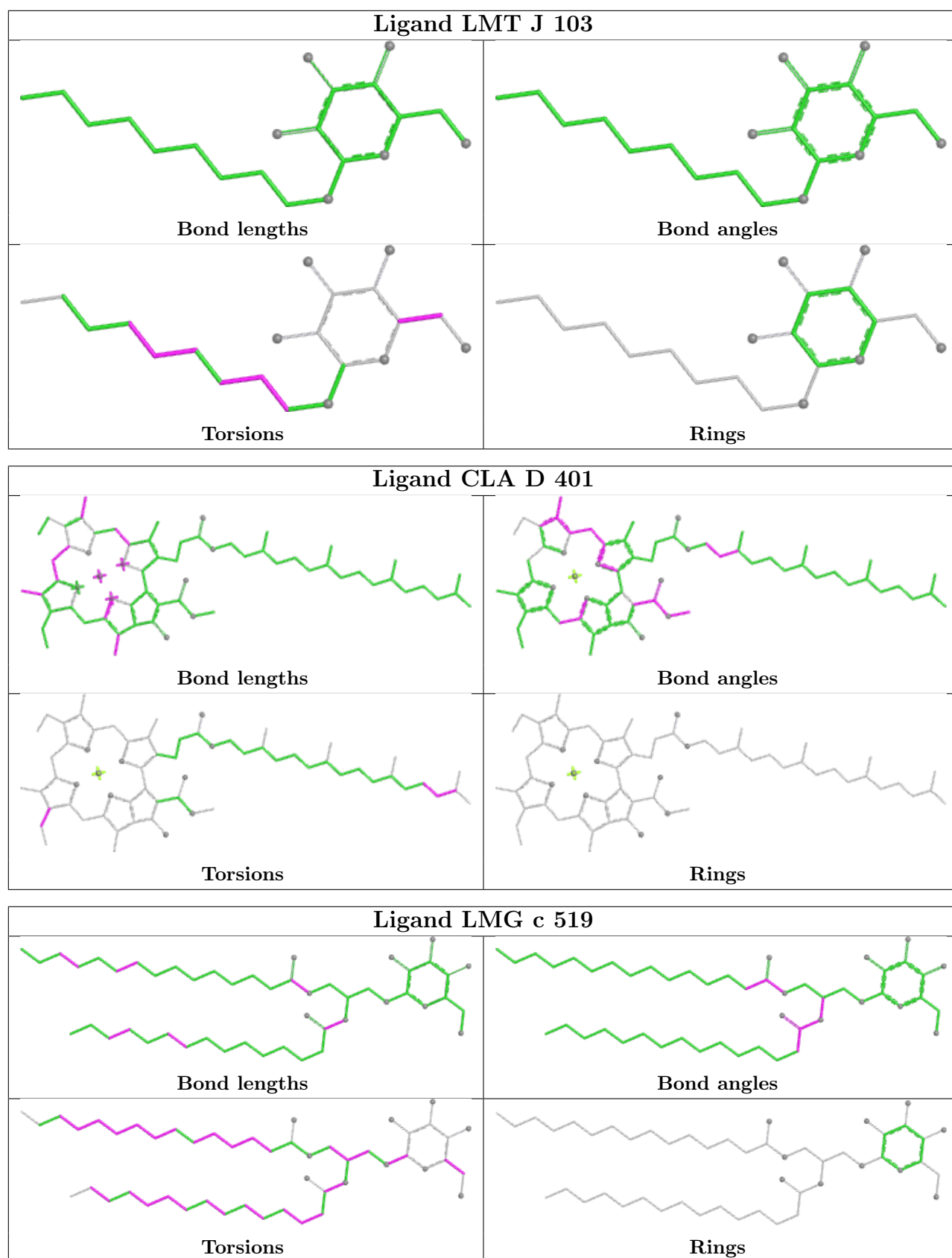


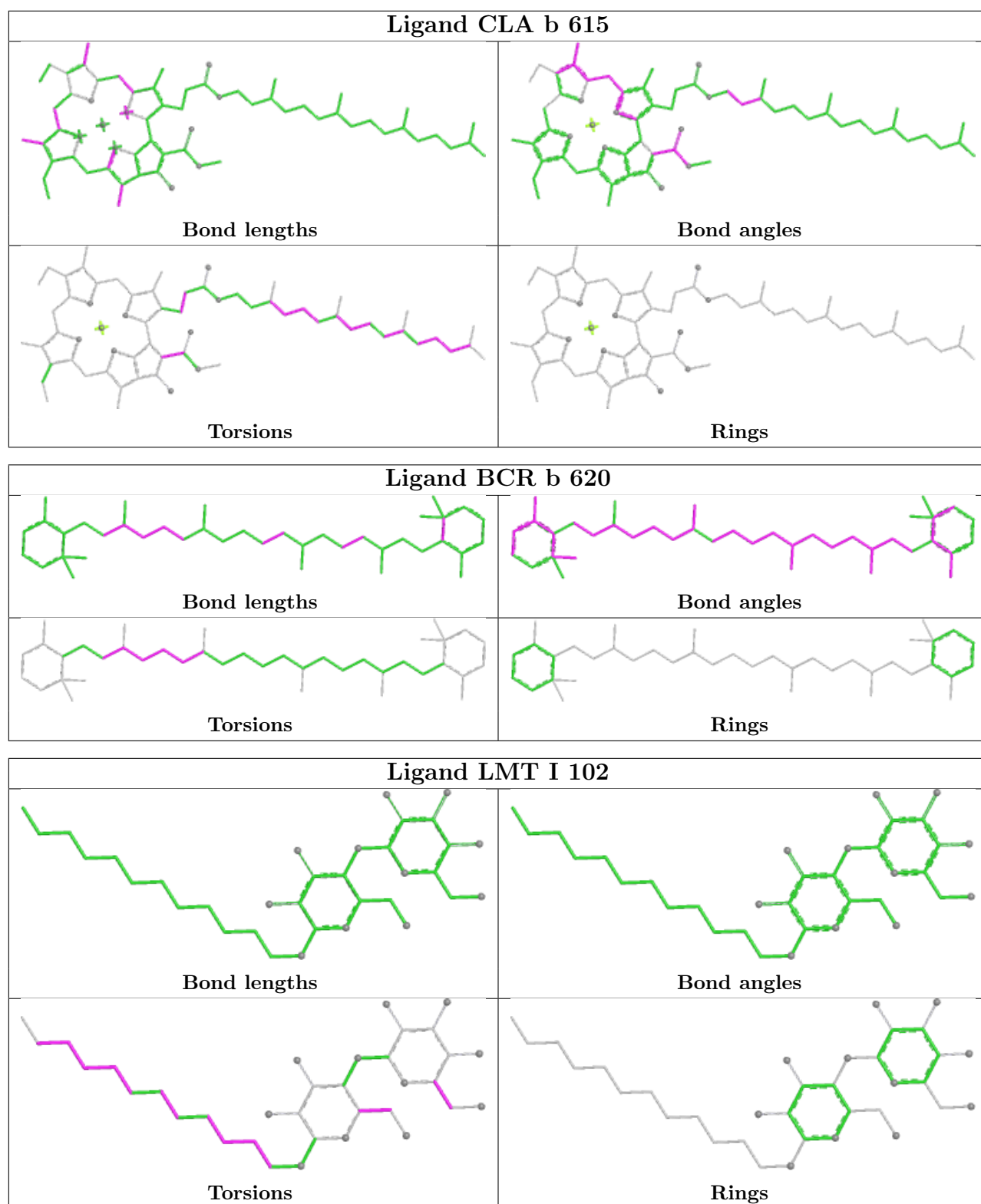


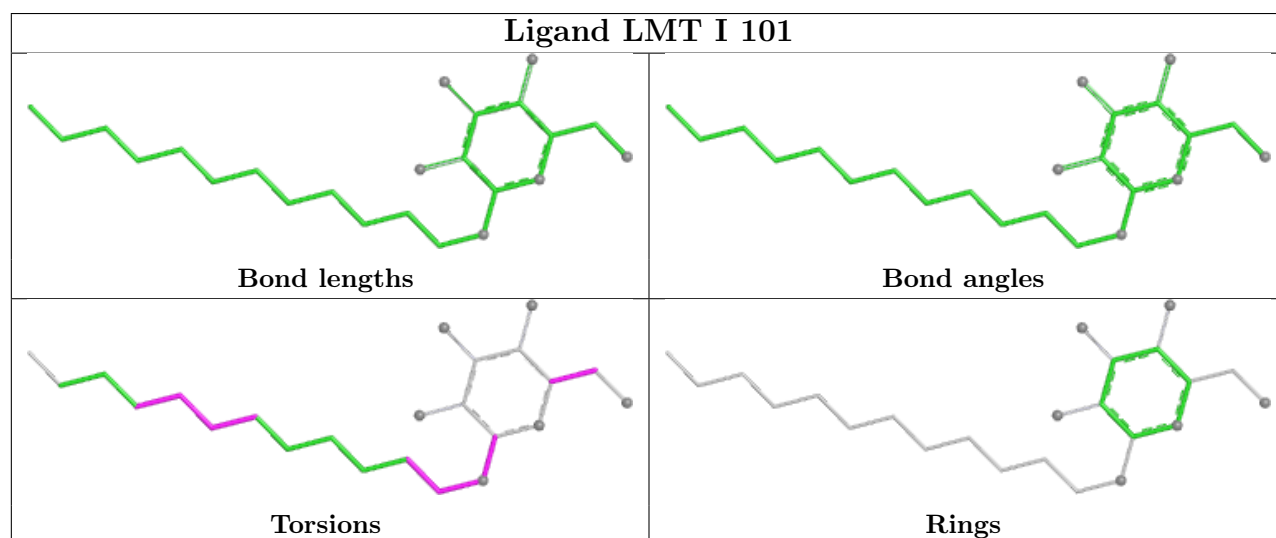
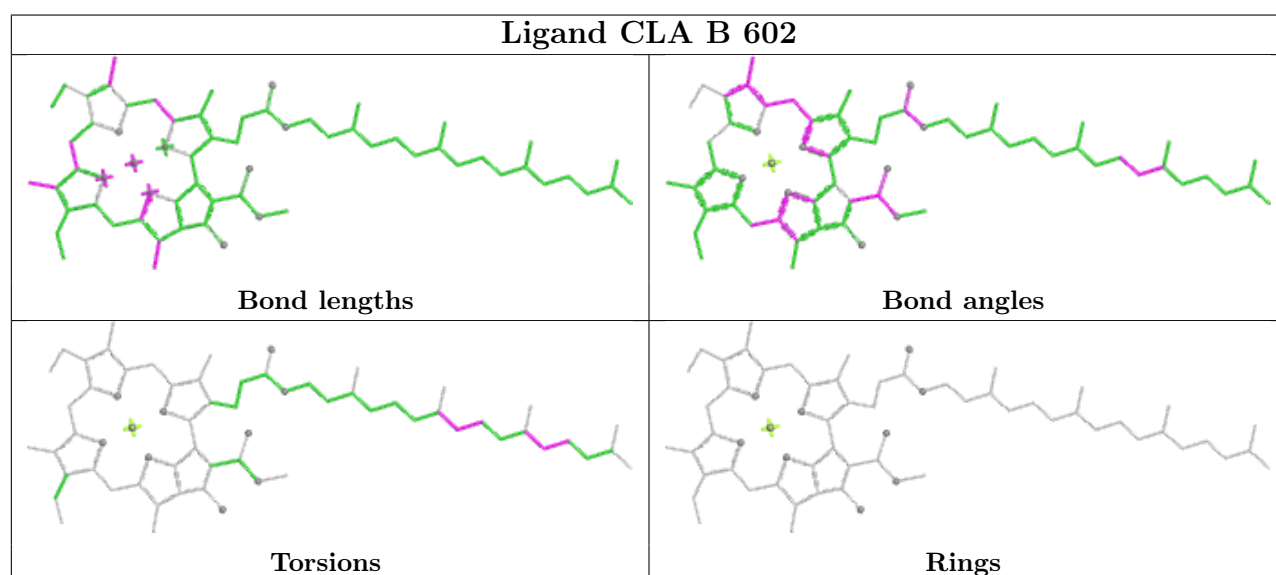
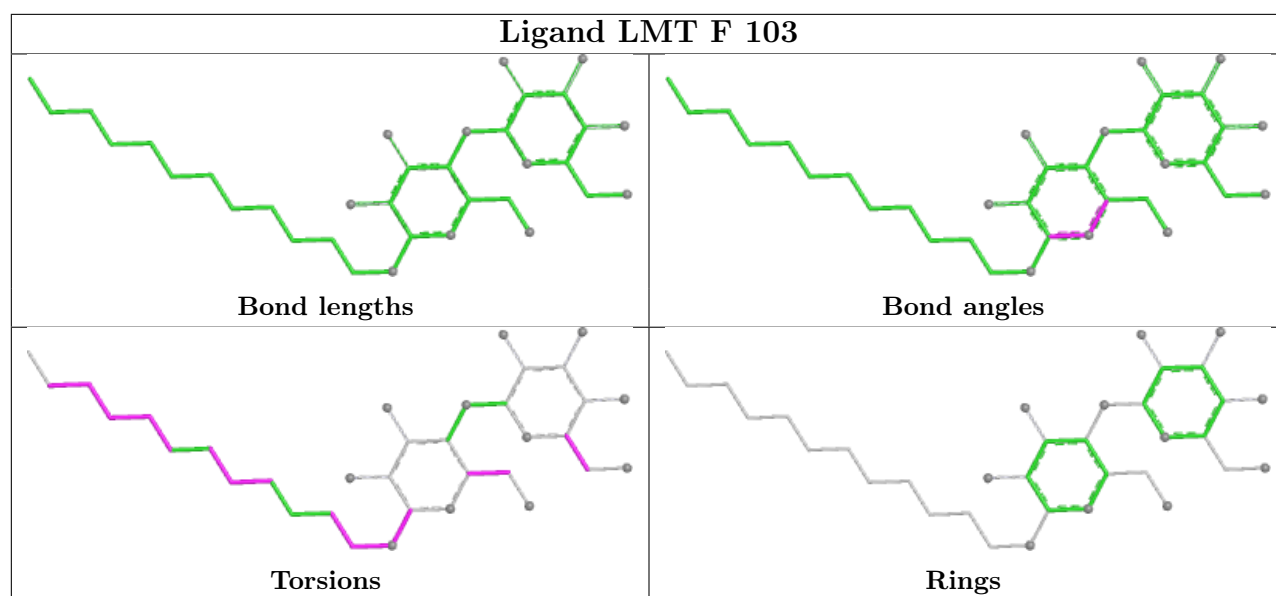




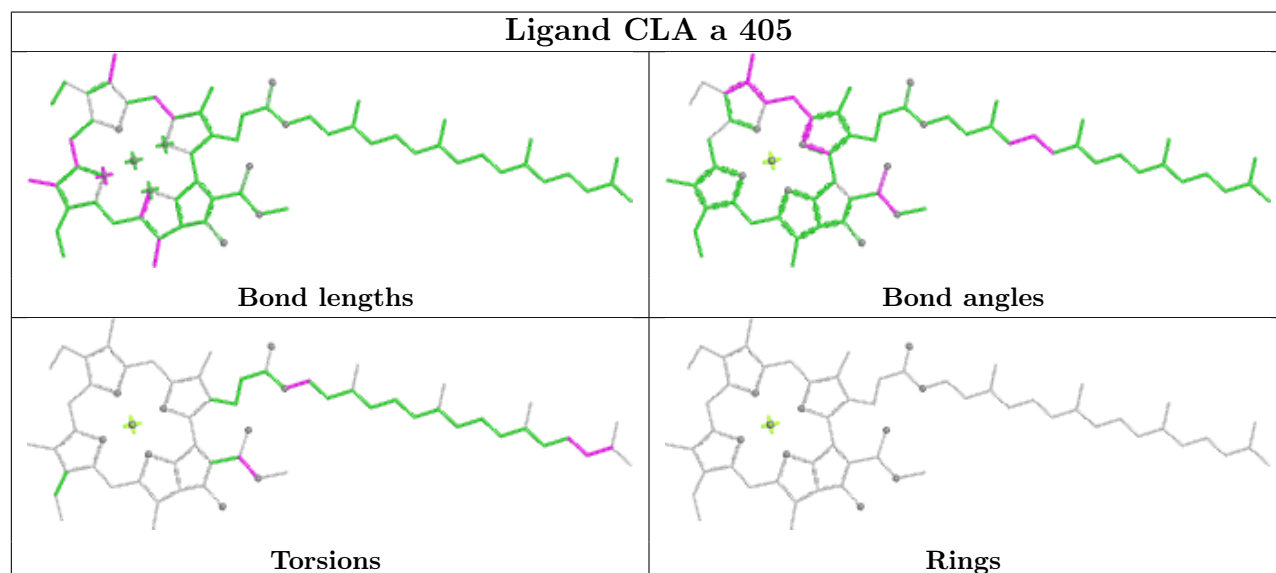
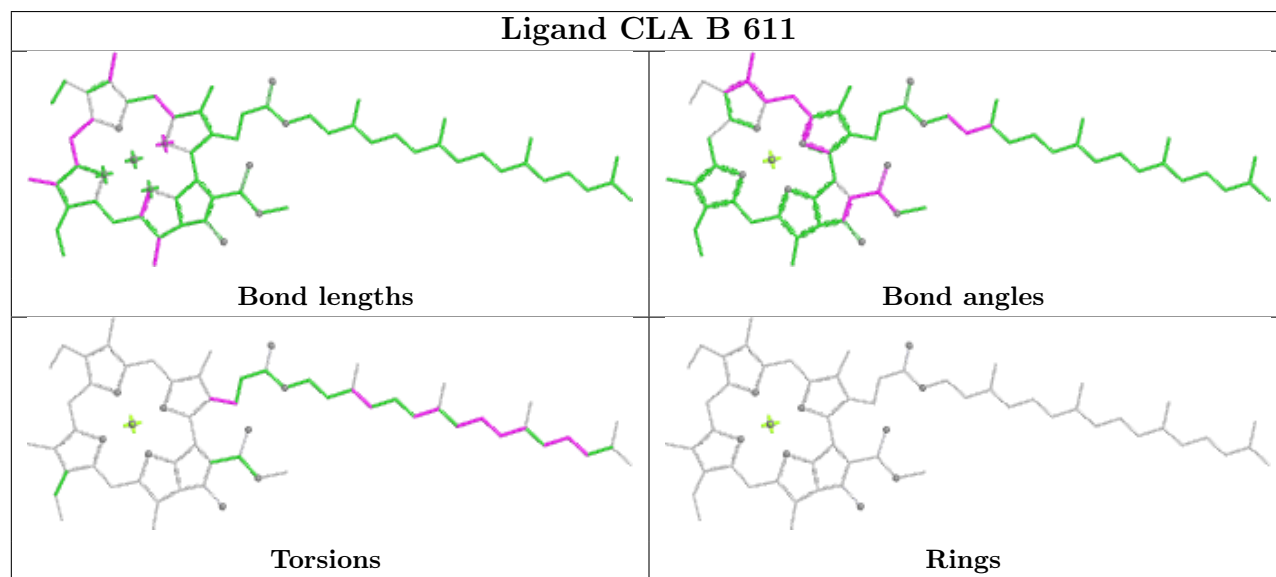
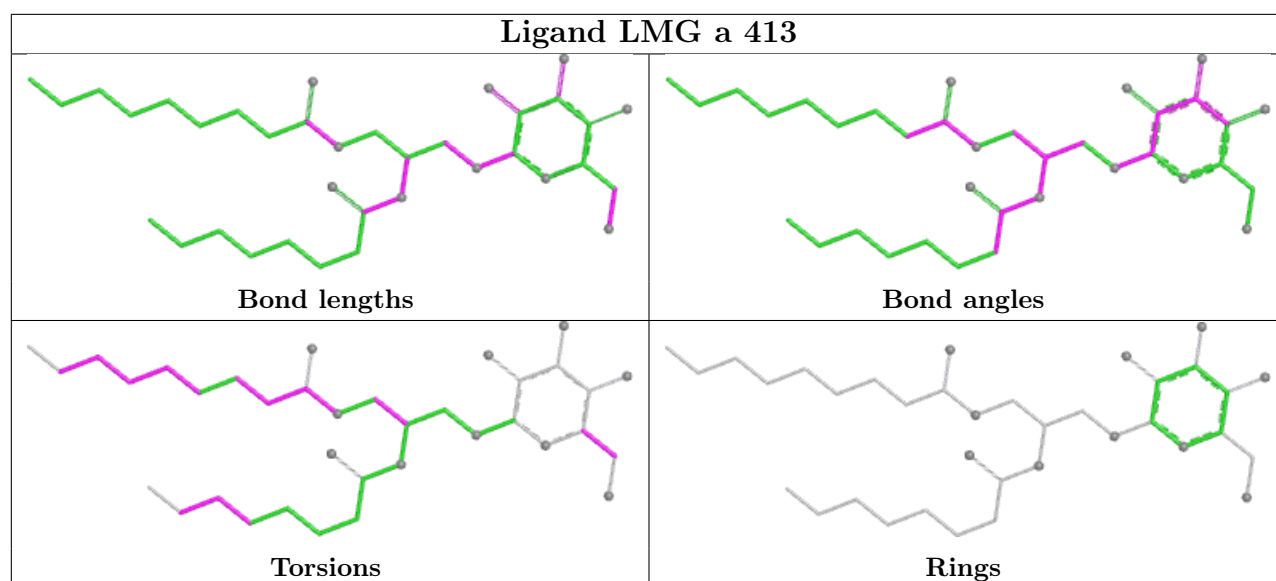


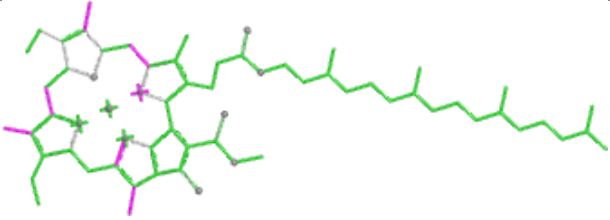
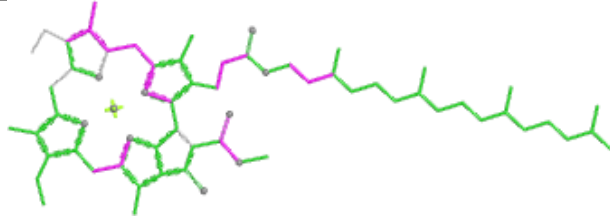
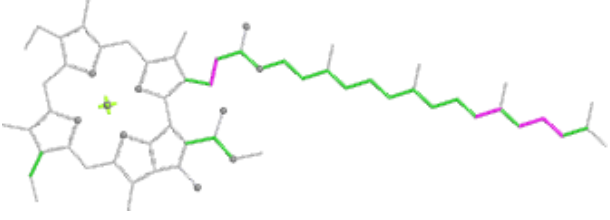
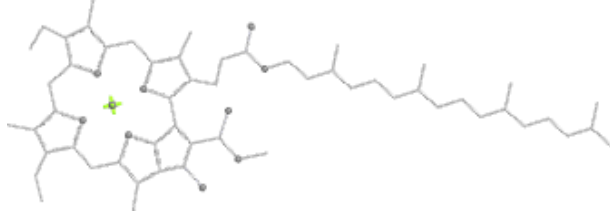
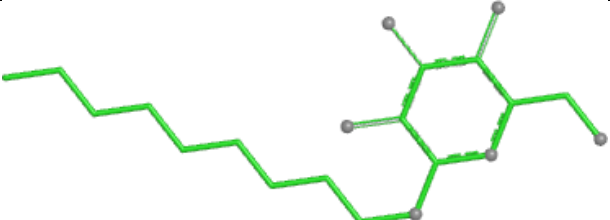
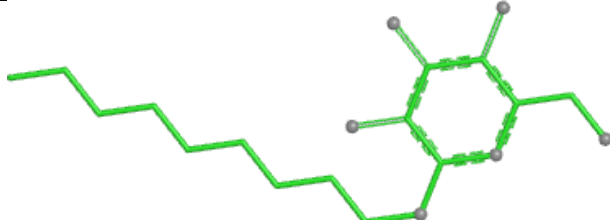
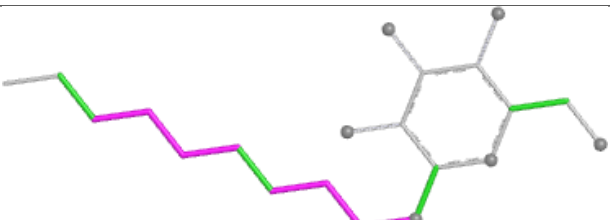
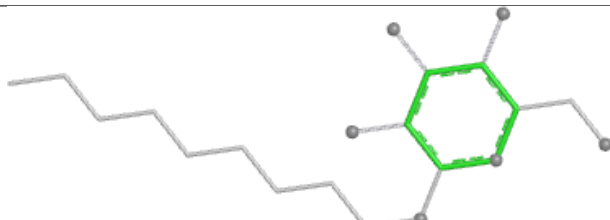
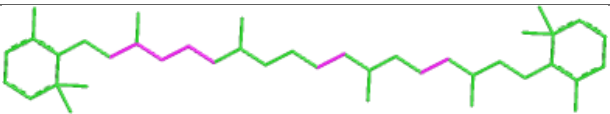
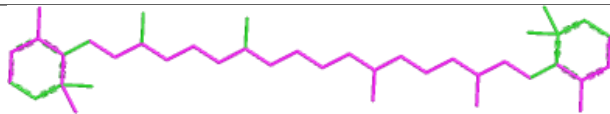
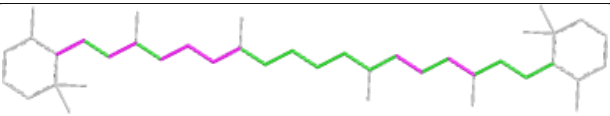
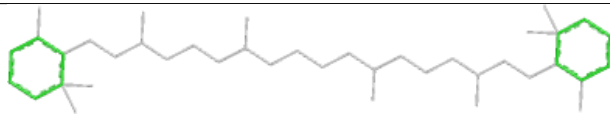




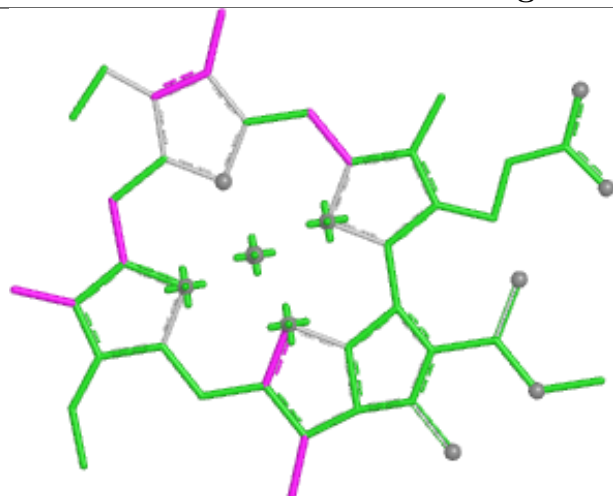




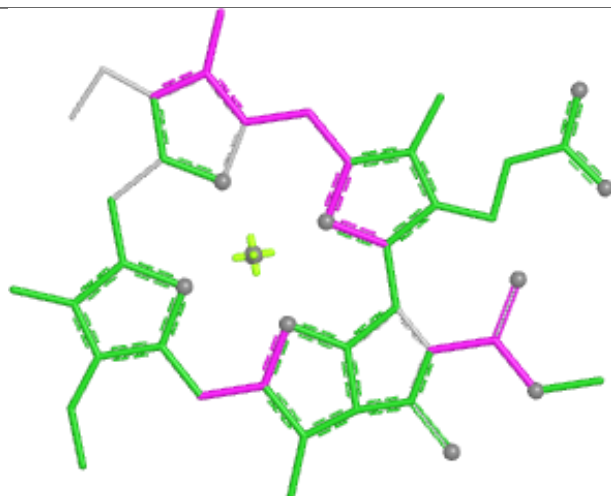


Ligand CLA B 610	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LMT C 522	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR C 525	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

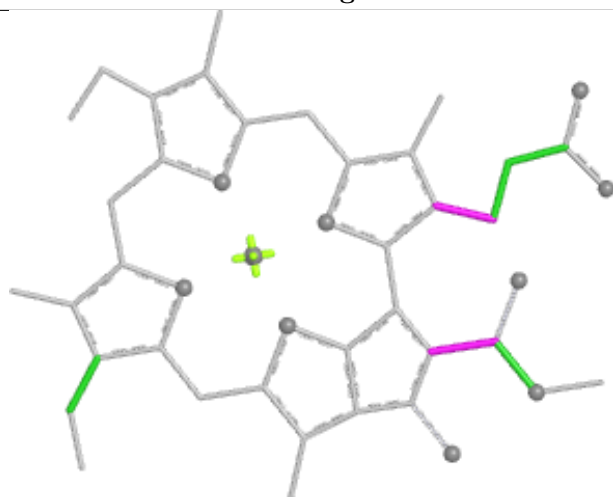
## Ligand CLA b 602



Bond lengths



Bond angles

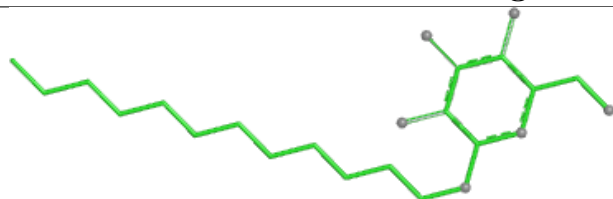


Torsions

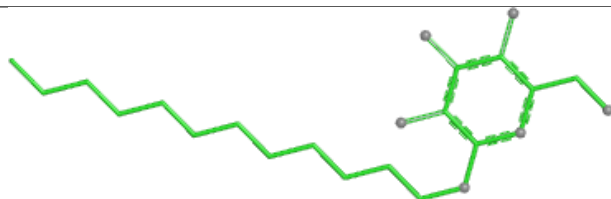


Rings

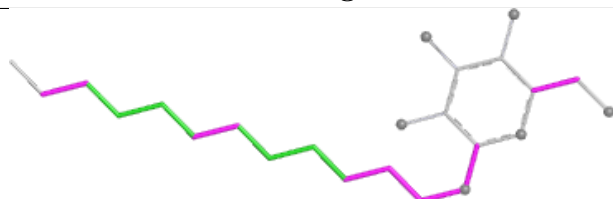
## Ligand LMT m 102



Bond lengths



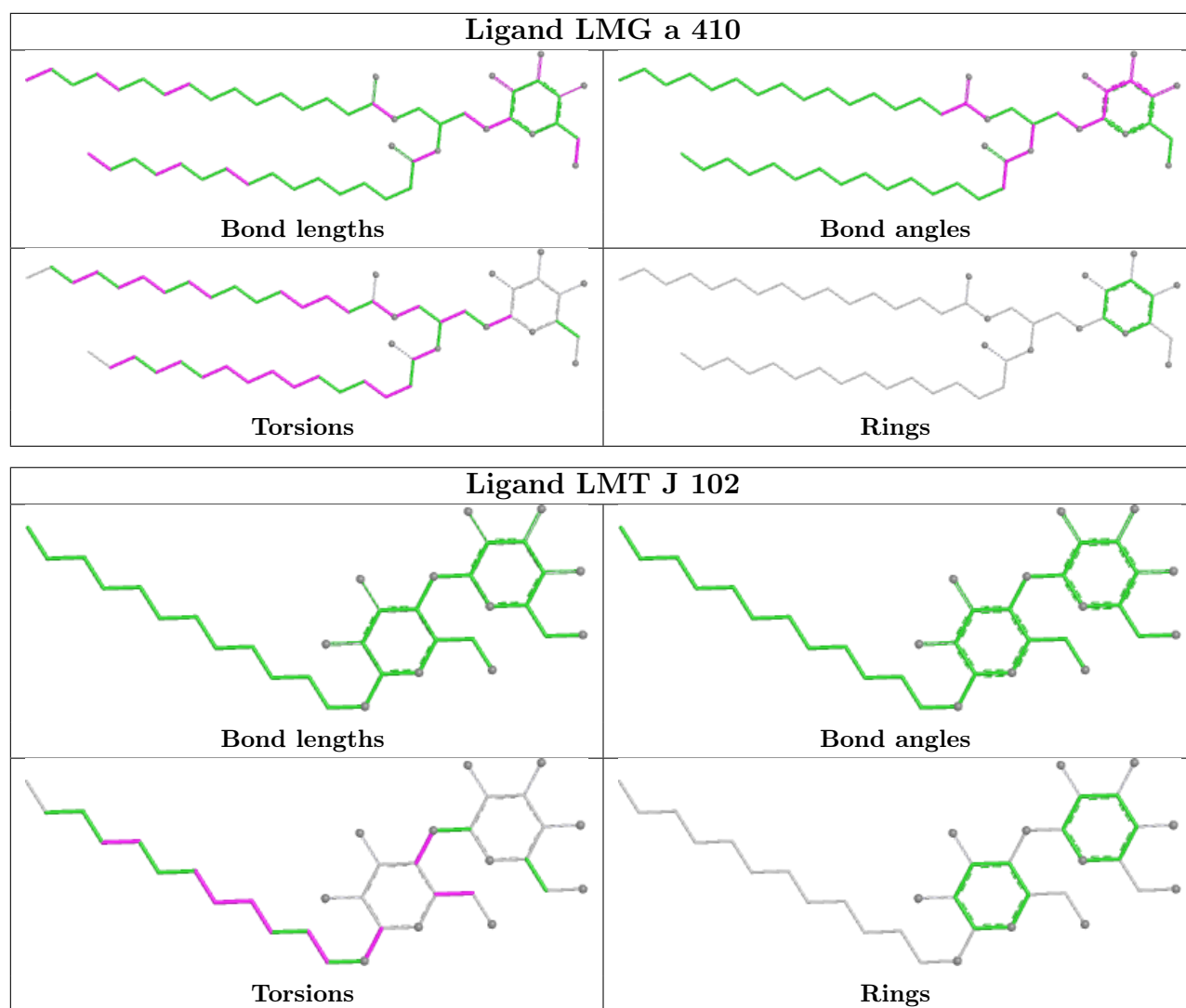
Bond angles



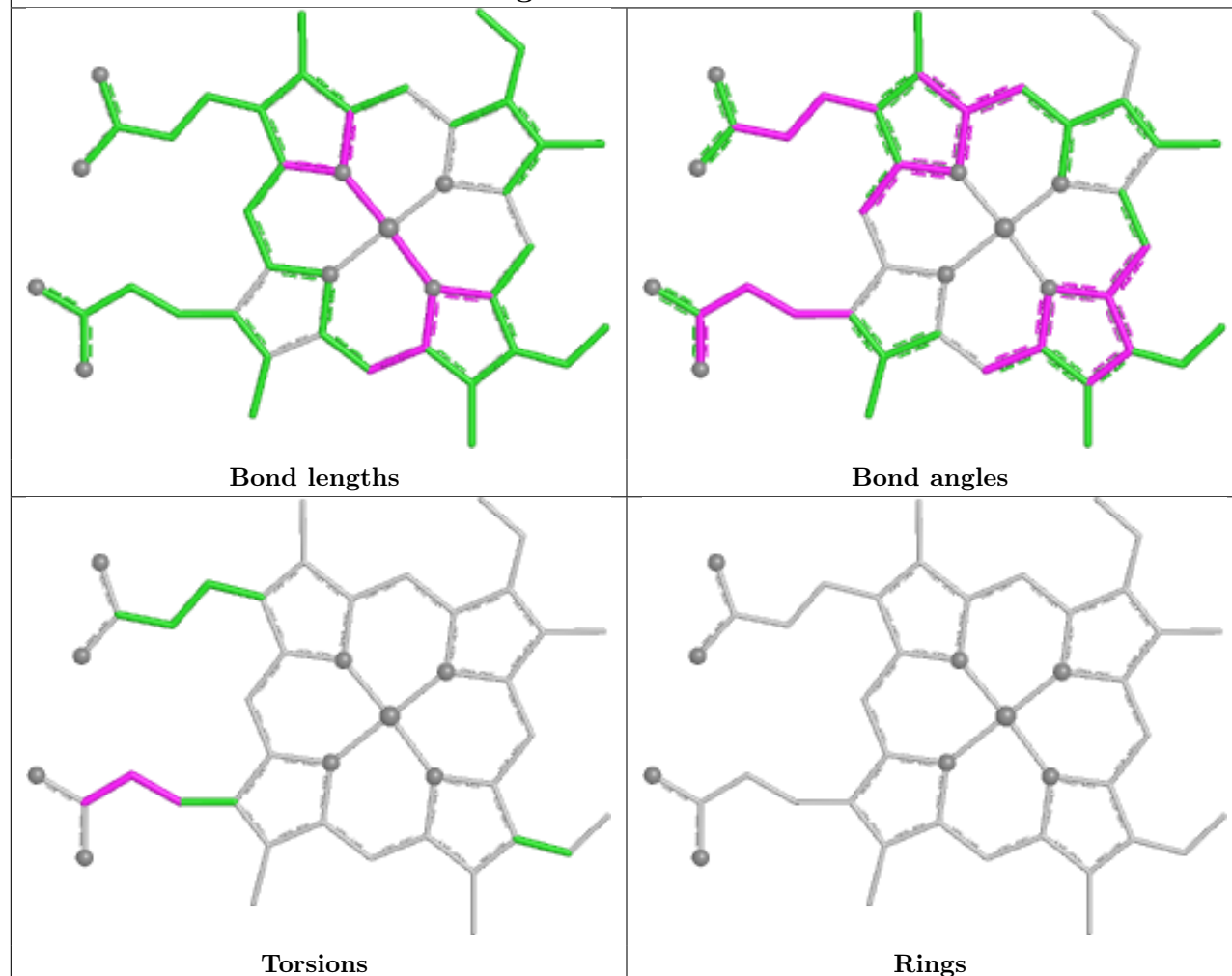
Torsions



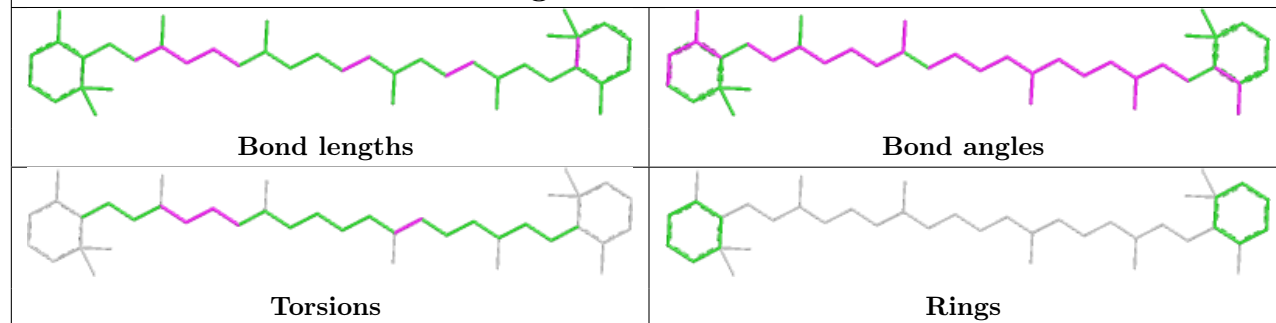
Rings

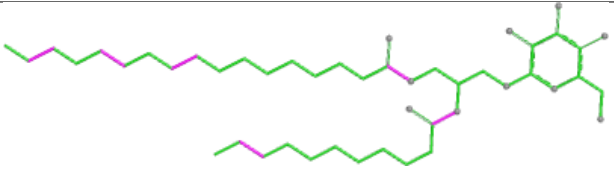
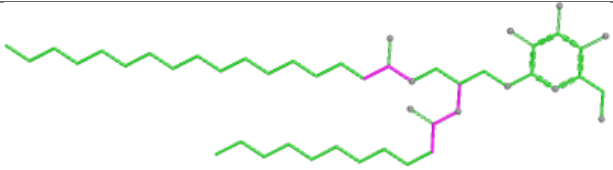
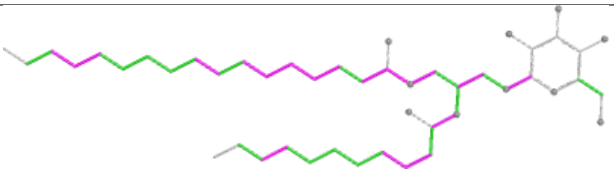
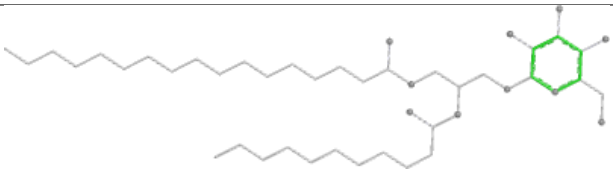


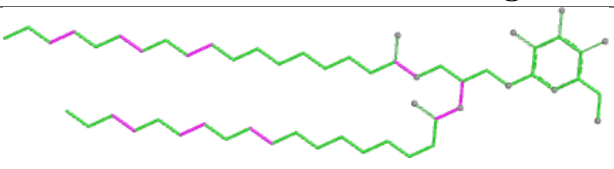
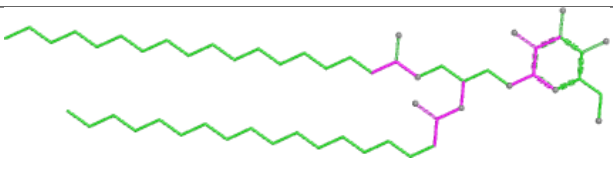
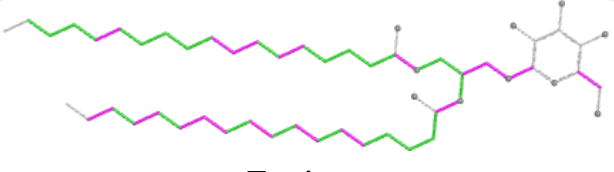
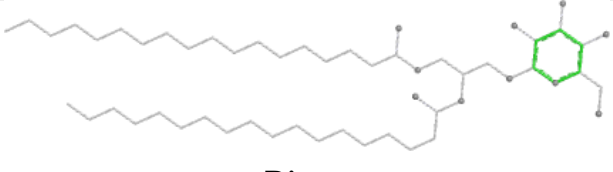
## Ligand HEM f 101

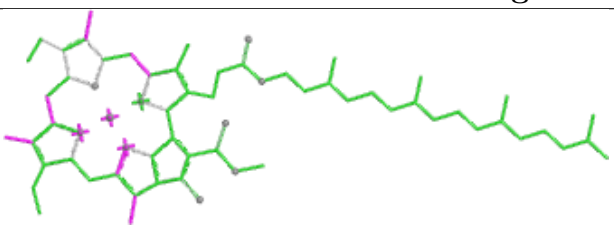
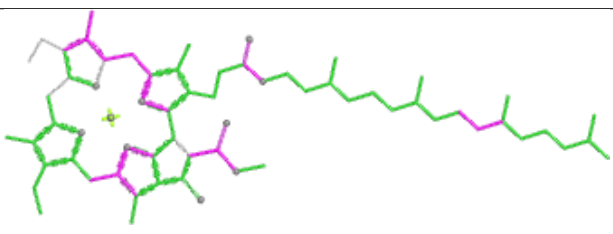
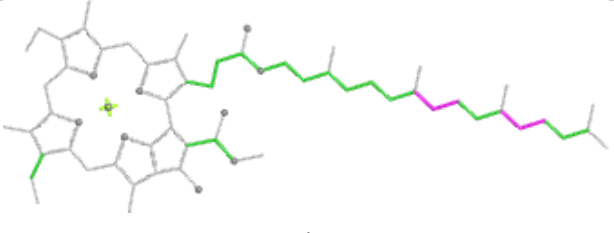
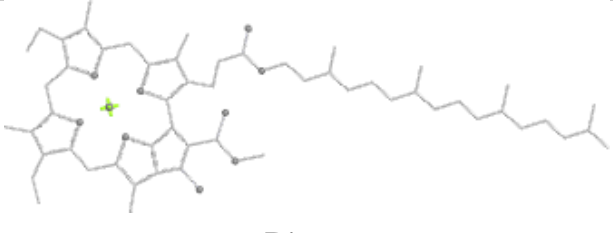


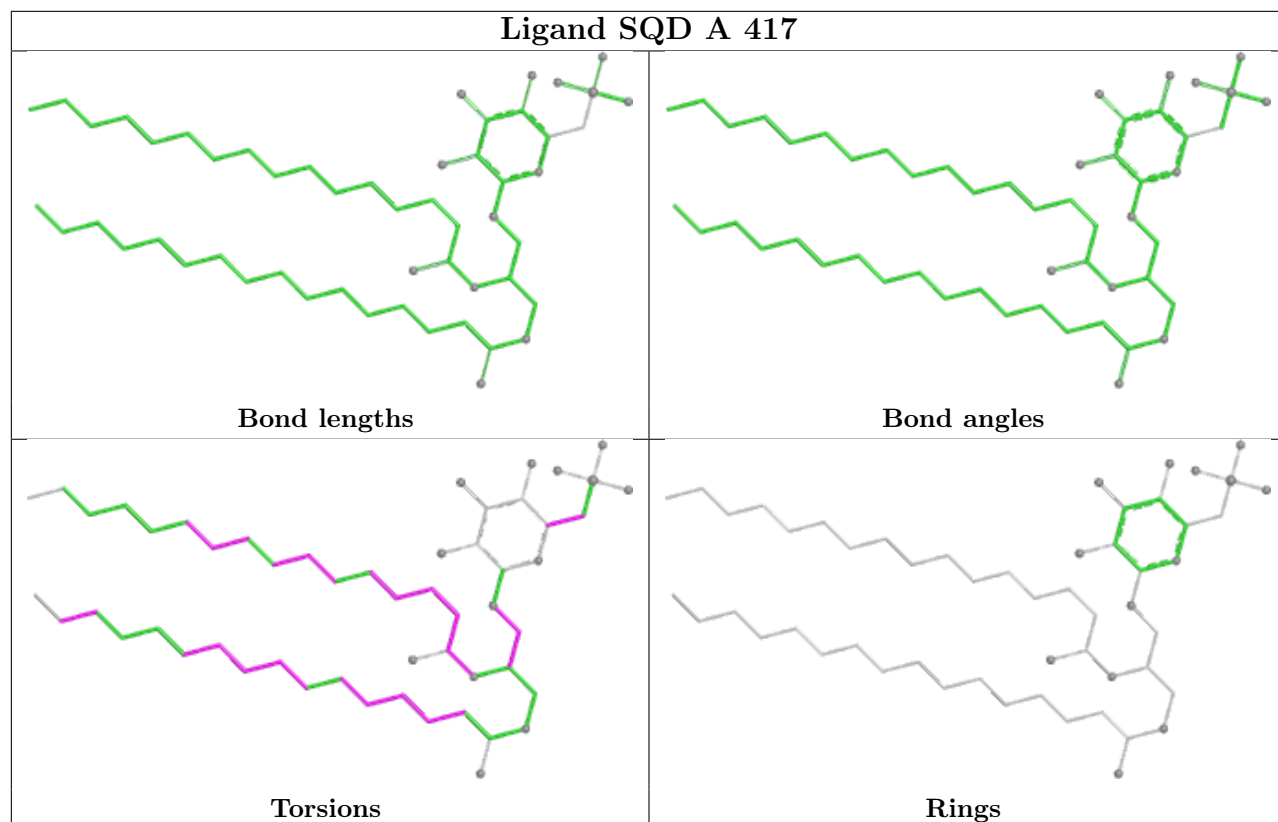
## Ligand BCR C 526

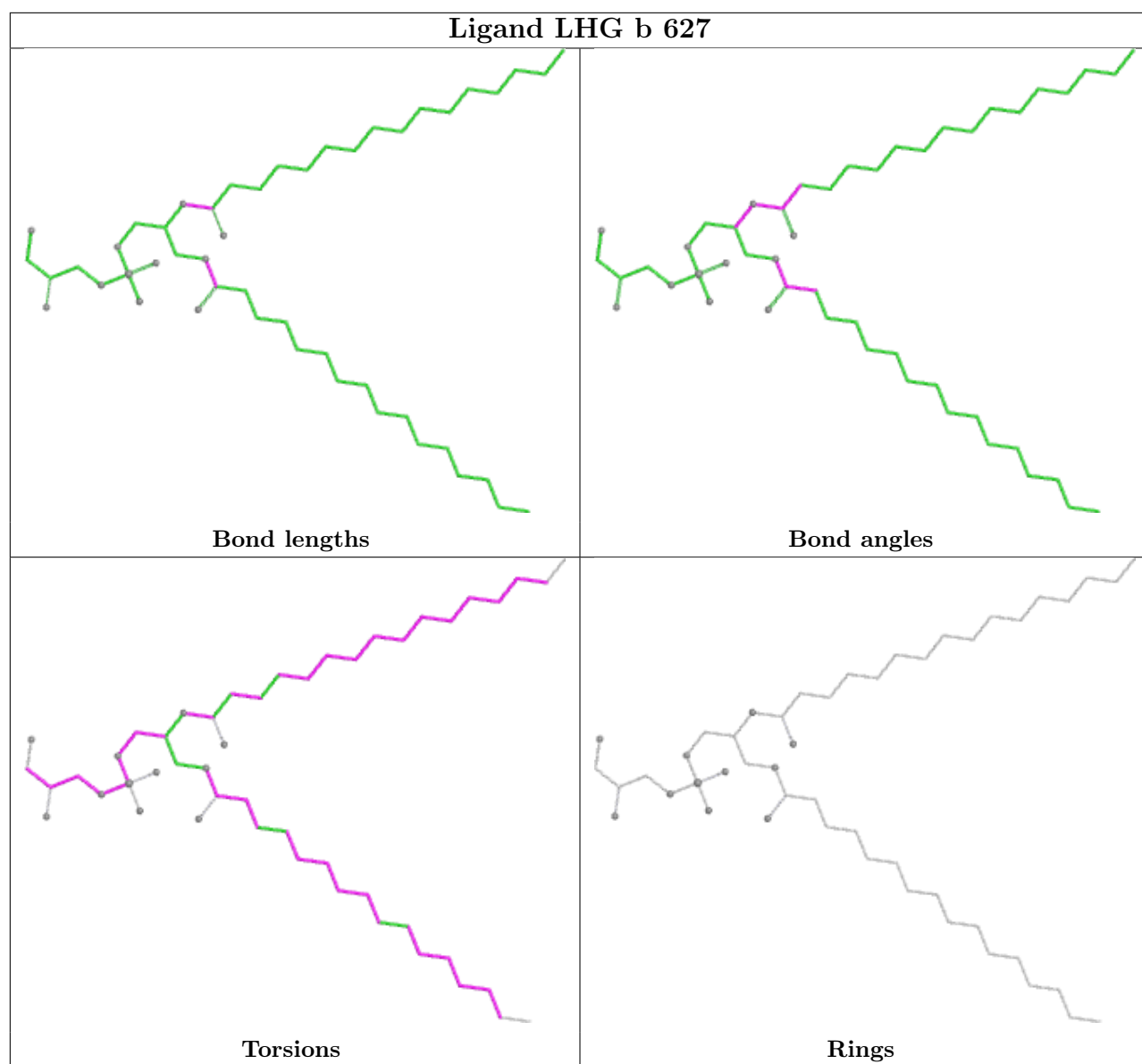


Ligand LMG B 629	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG D 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

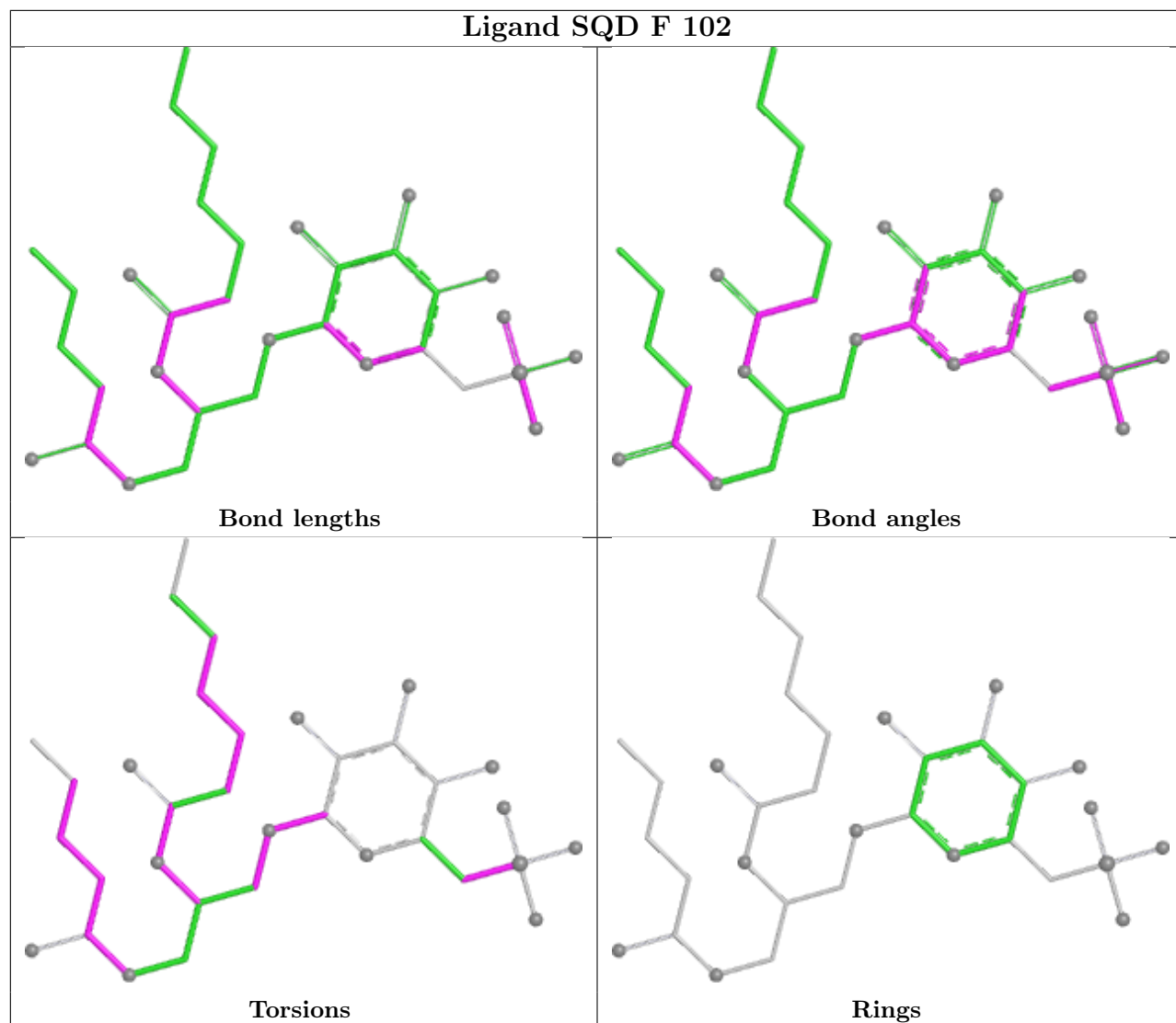
Ligand CLA b 603	
	
Bond lengths	Bond angles
	
Torsions	Rings



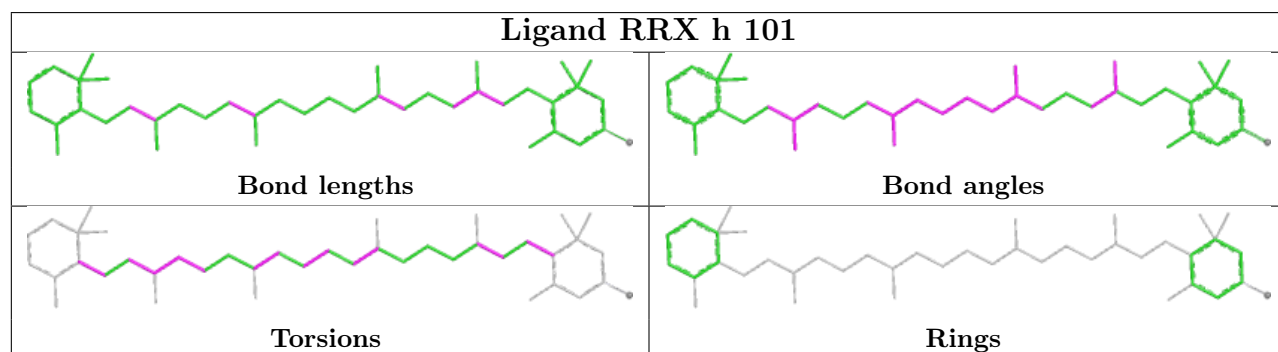


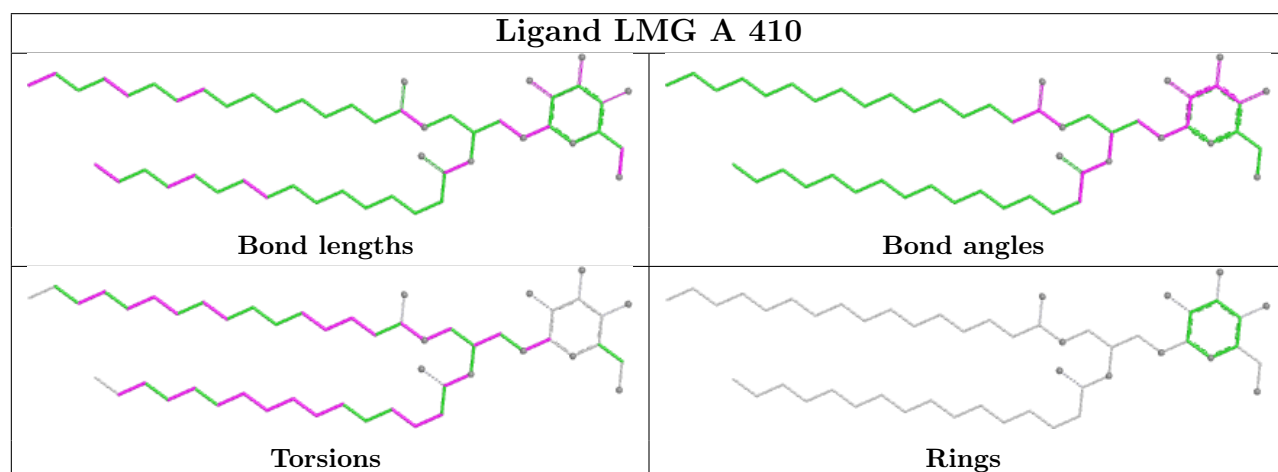
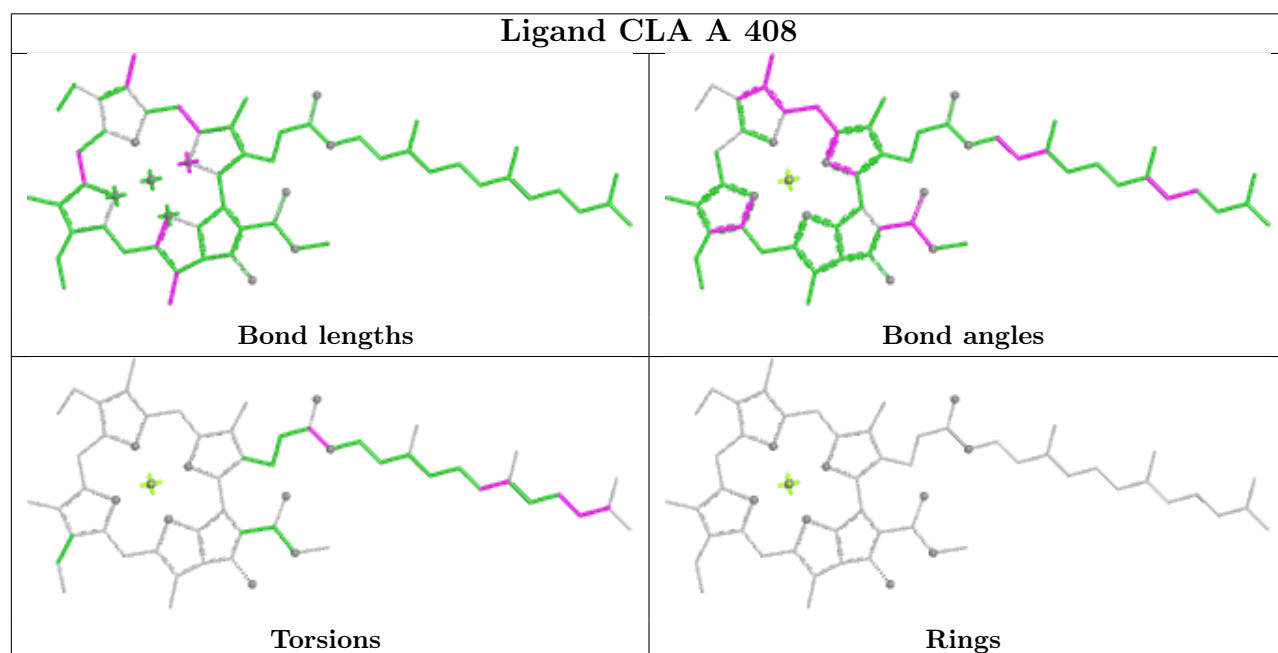
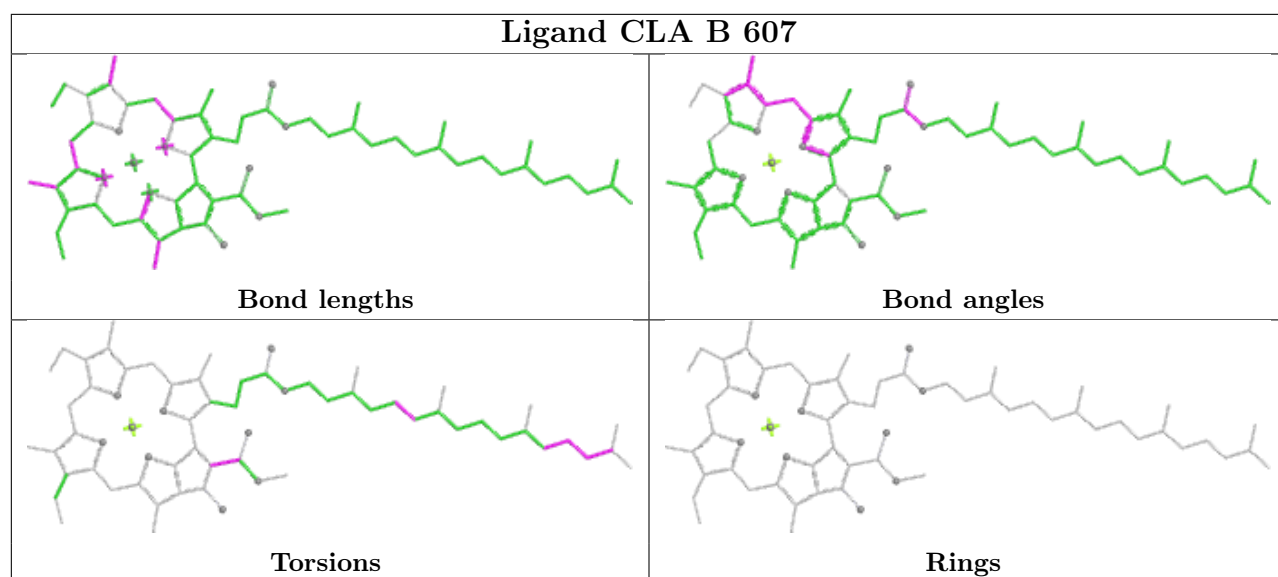


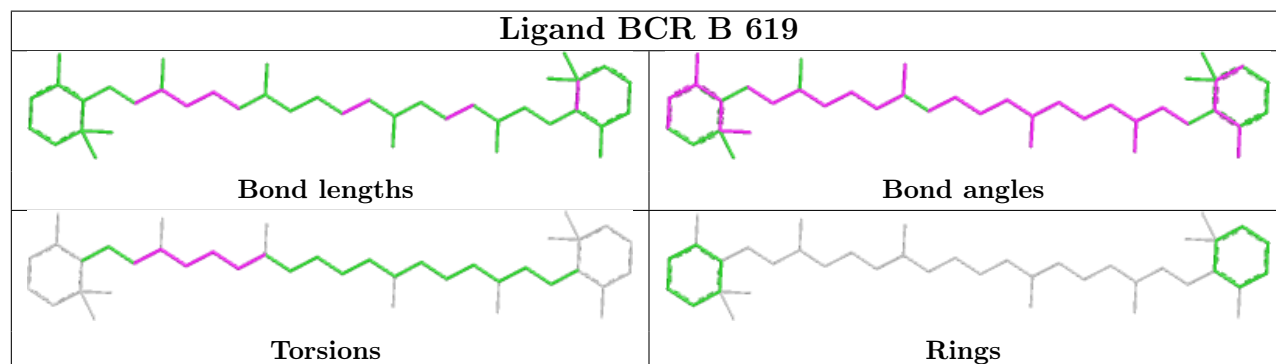
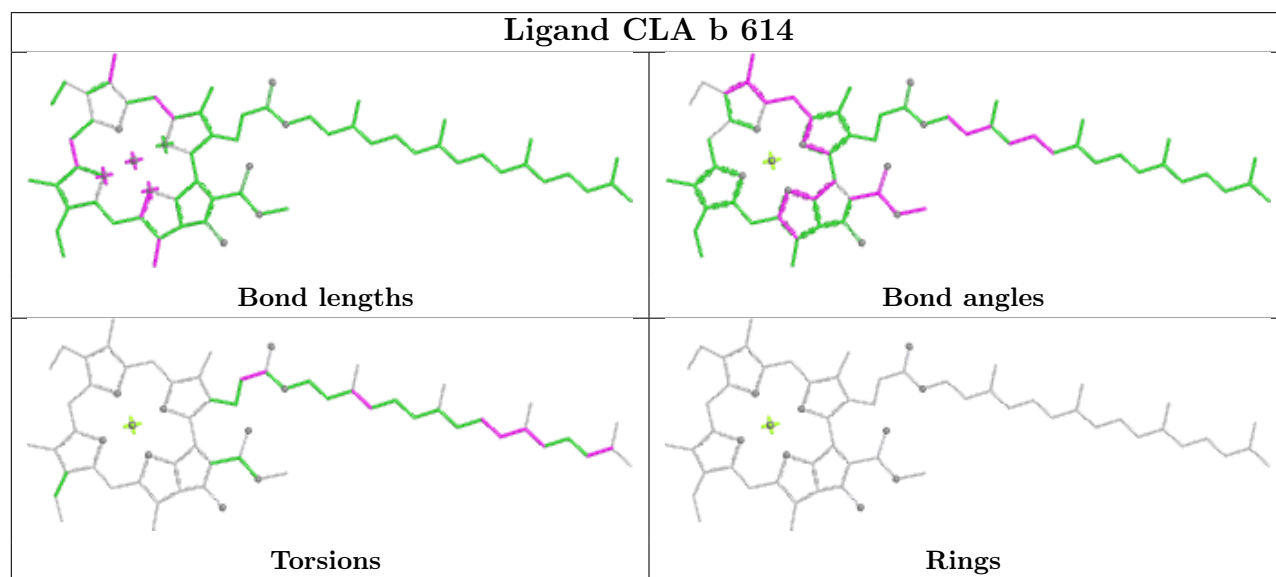
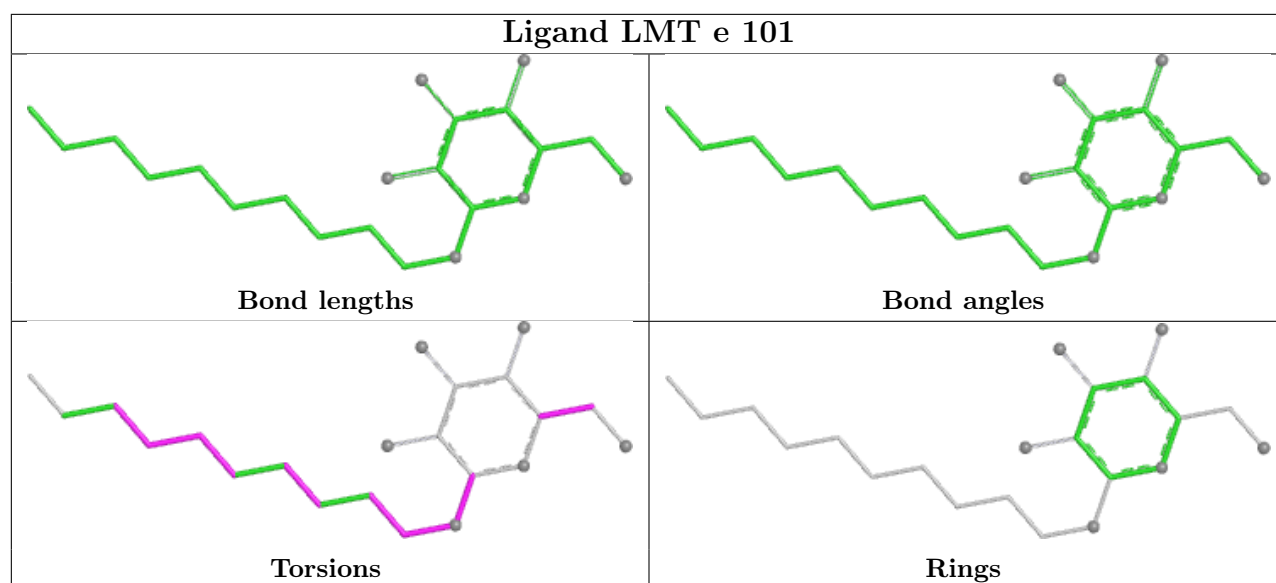
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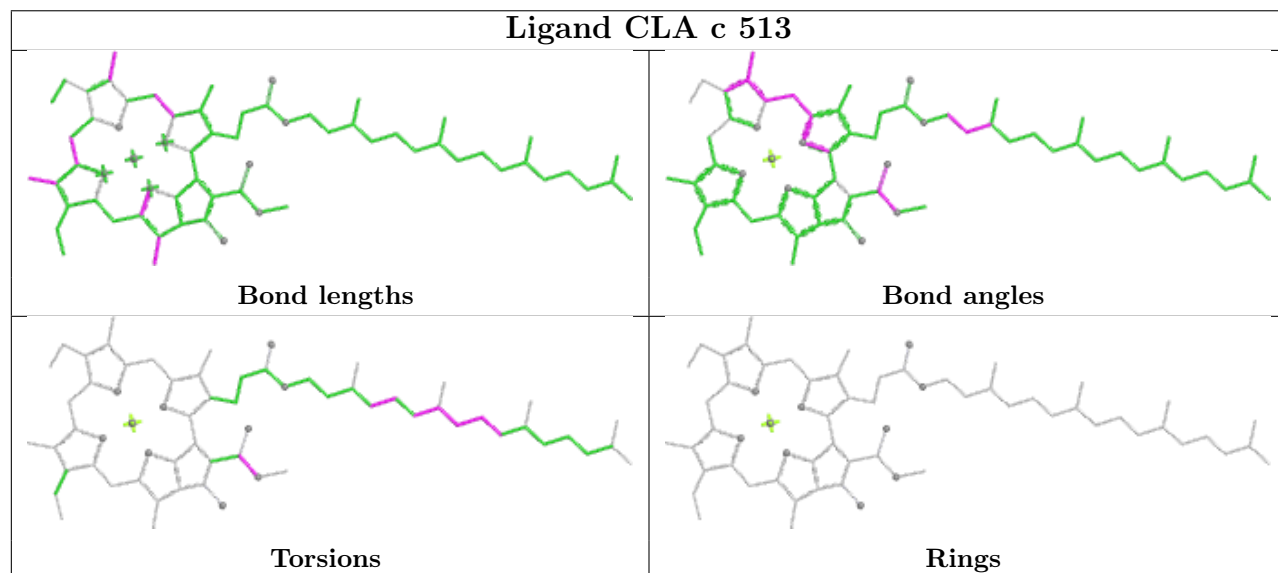
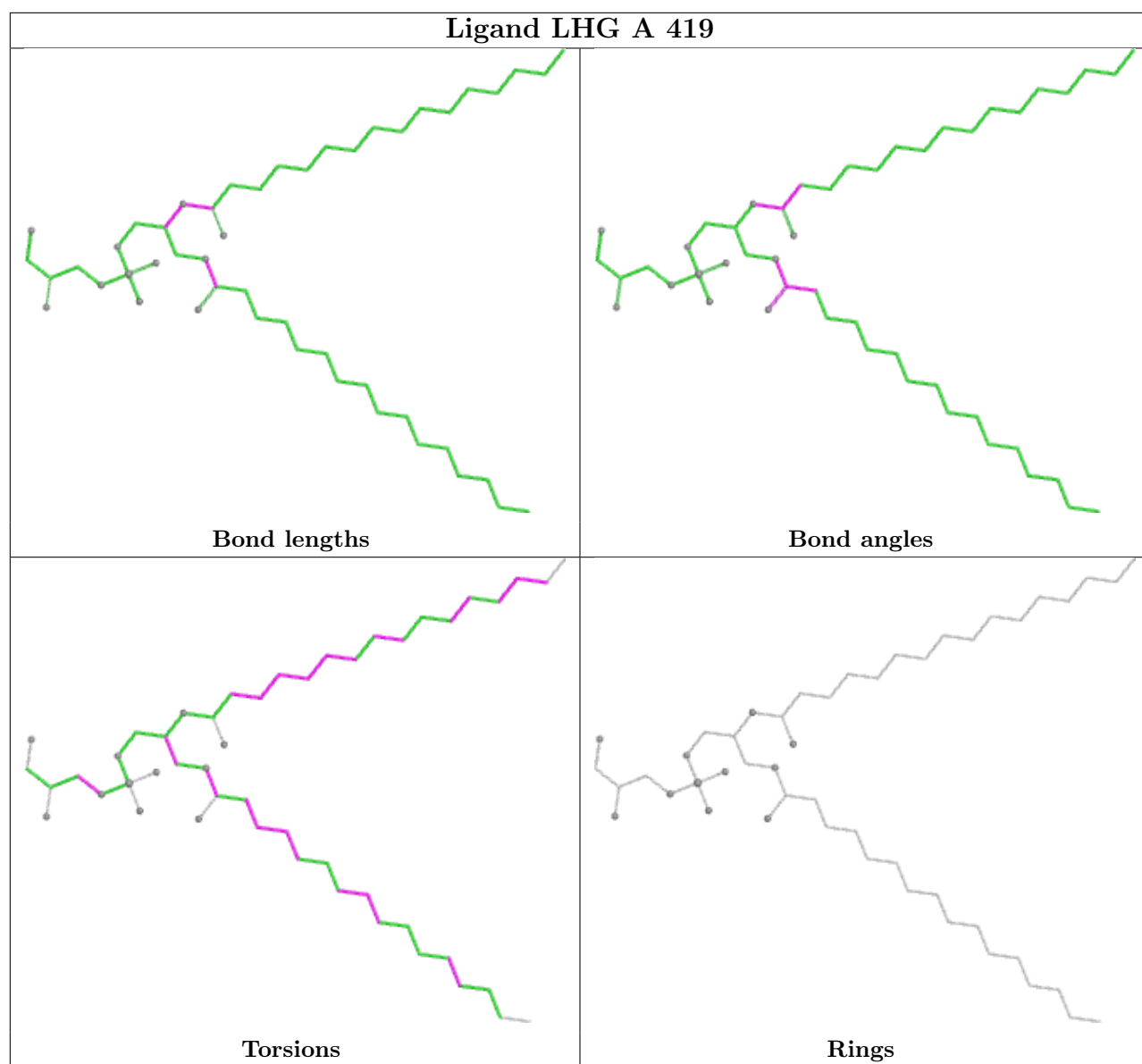


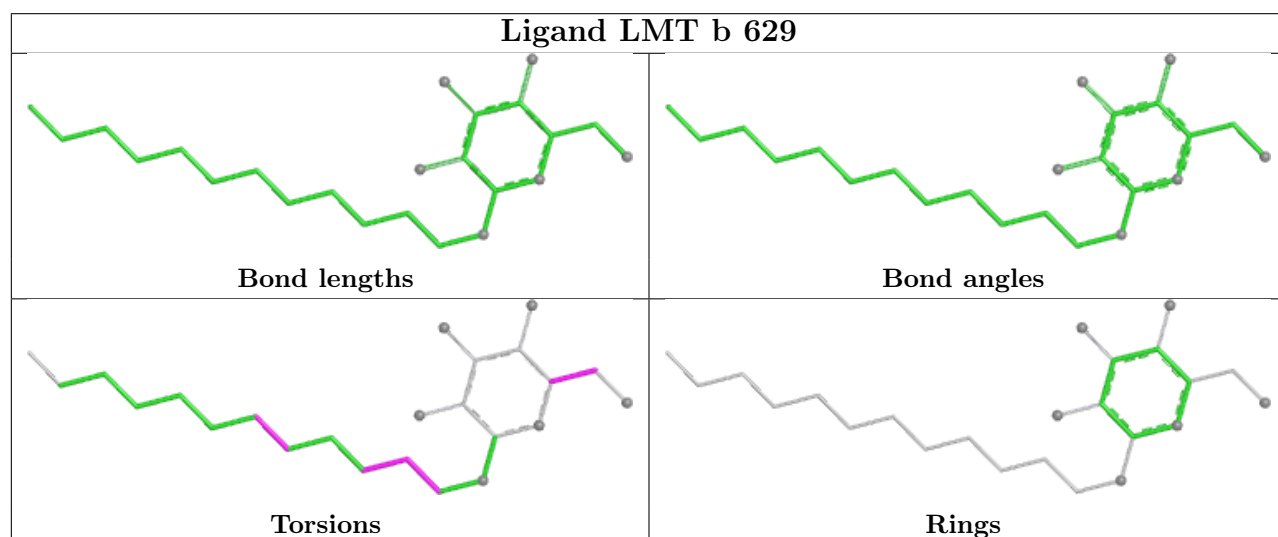
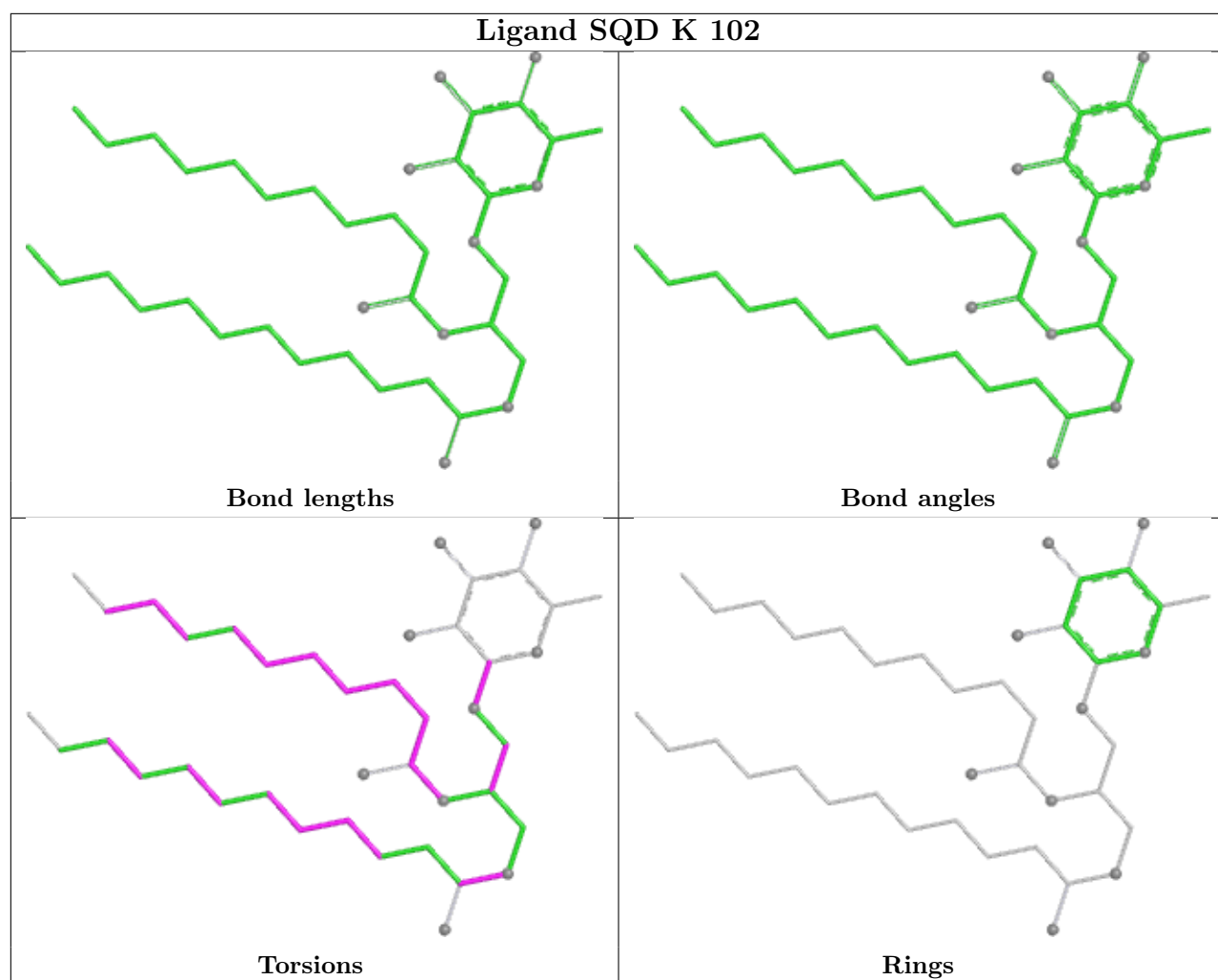
## Ligand RRX h 101

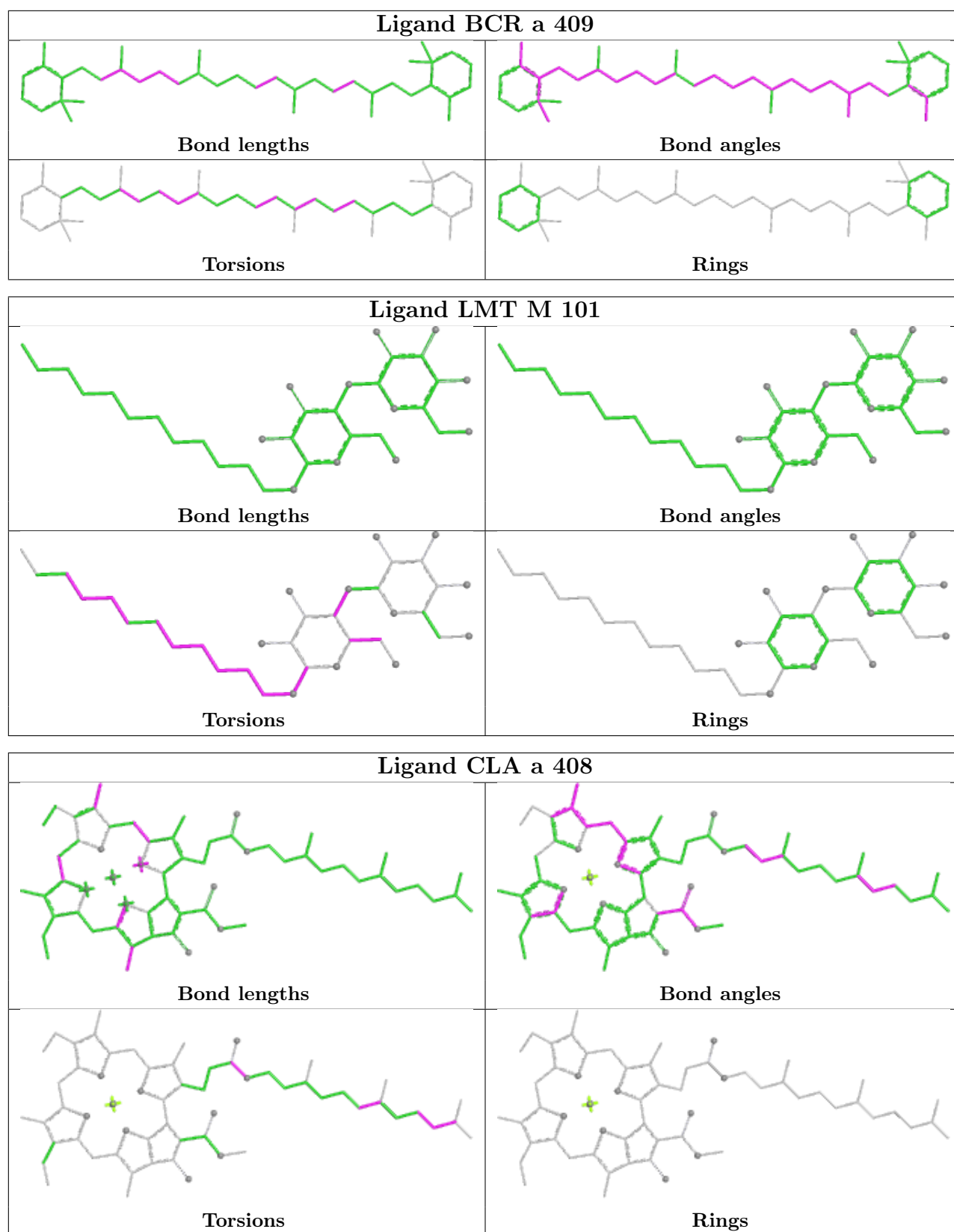


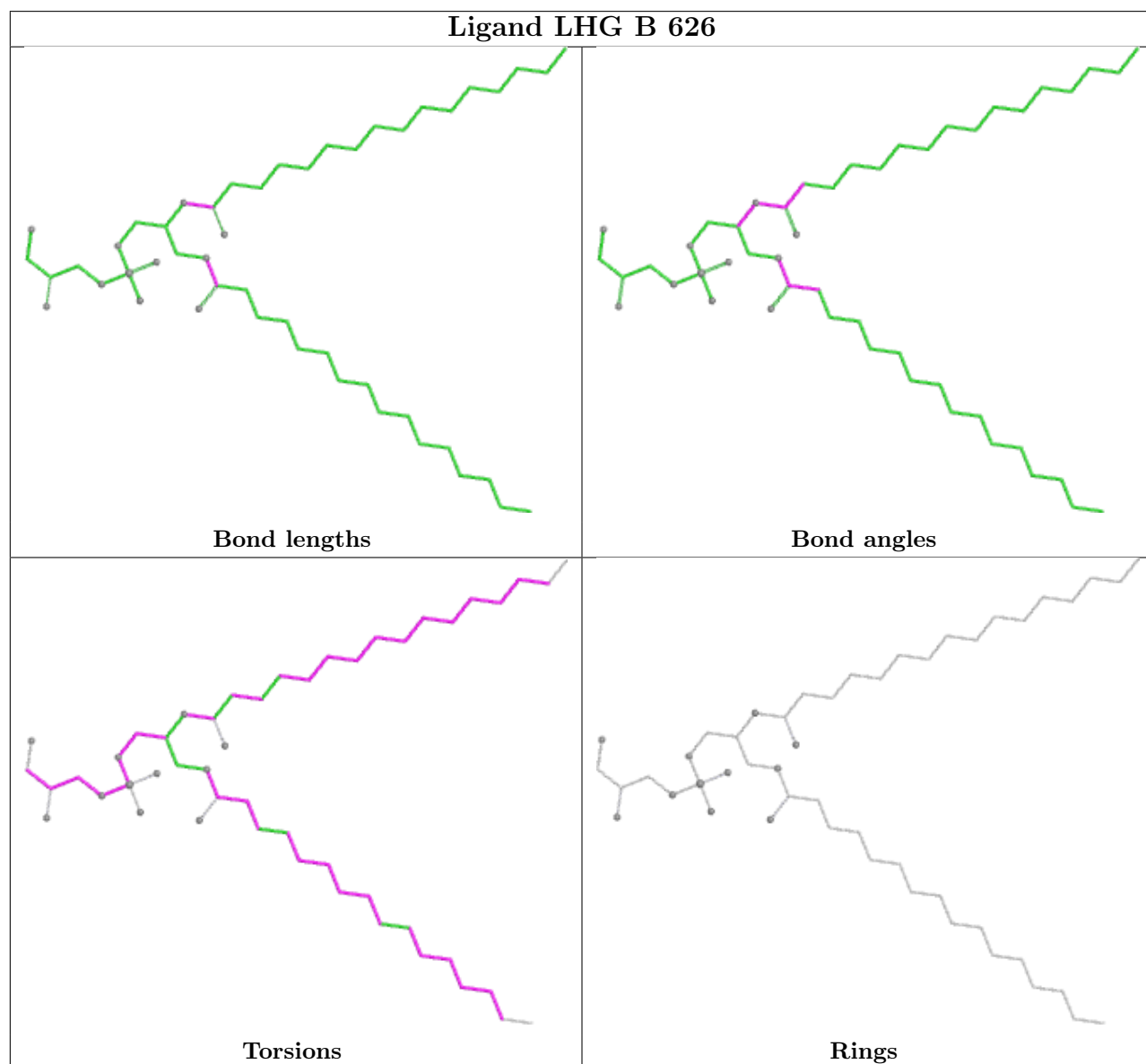
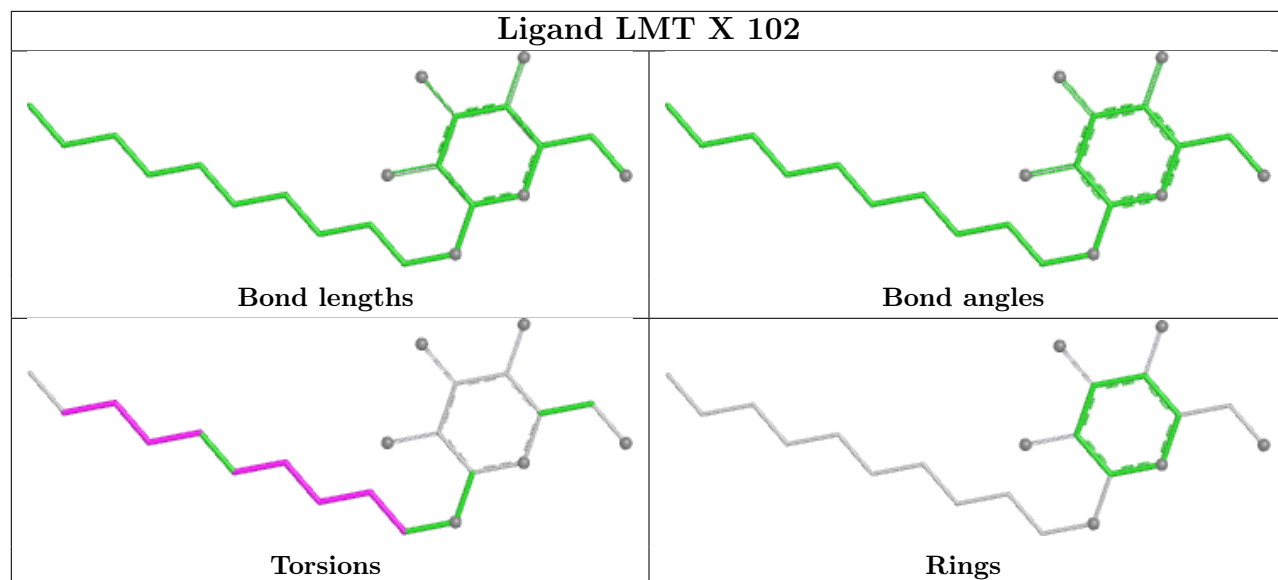


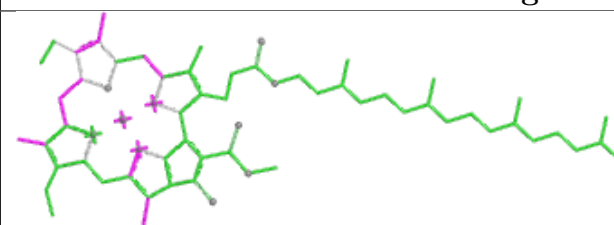
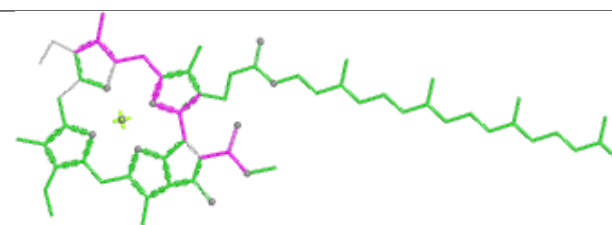
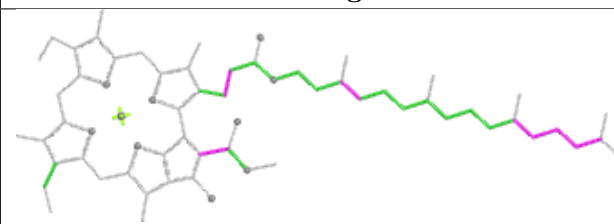
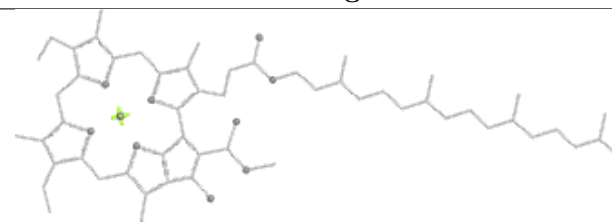




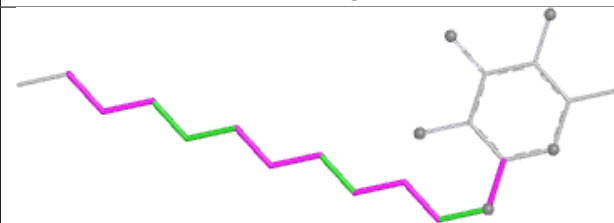
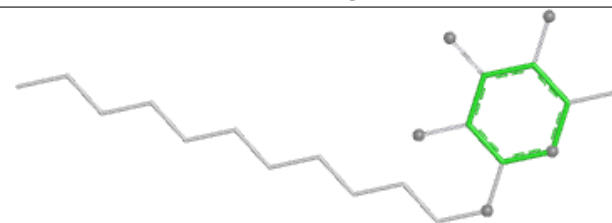


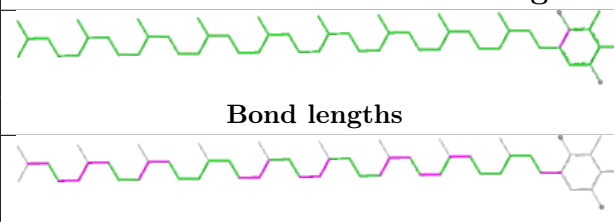
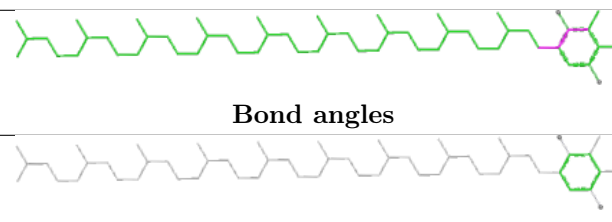
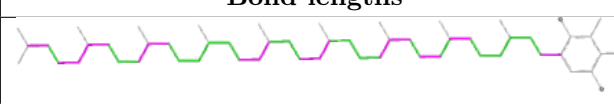
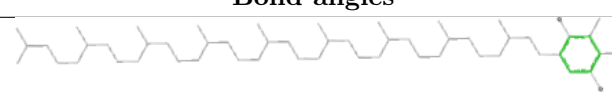




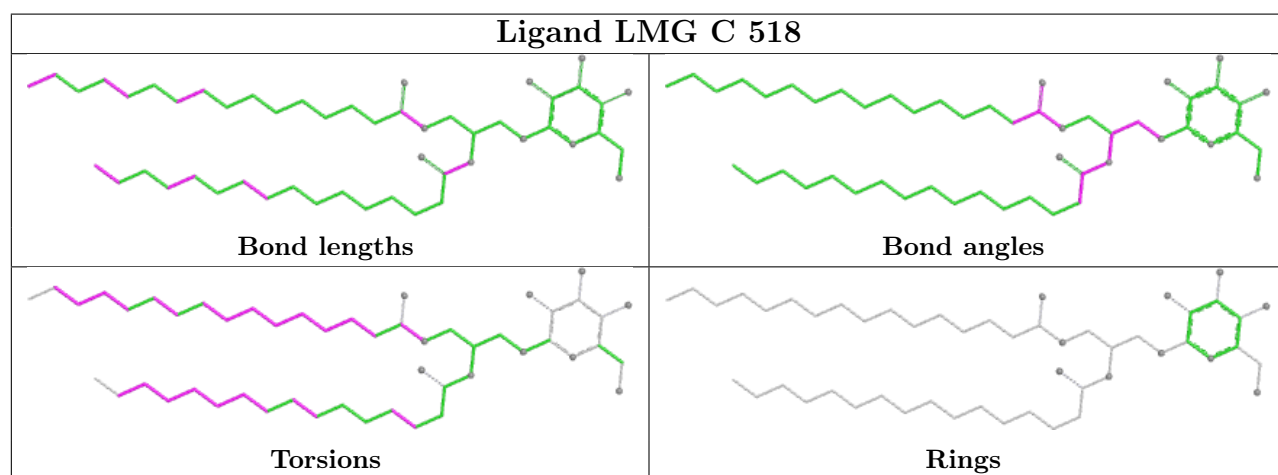
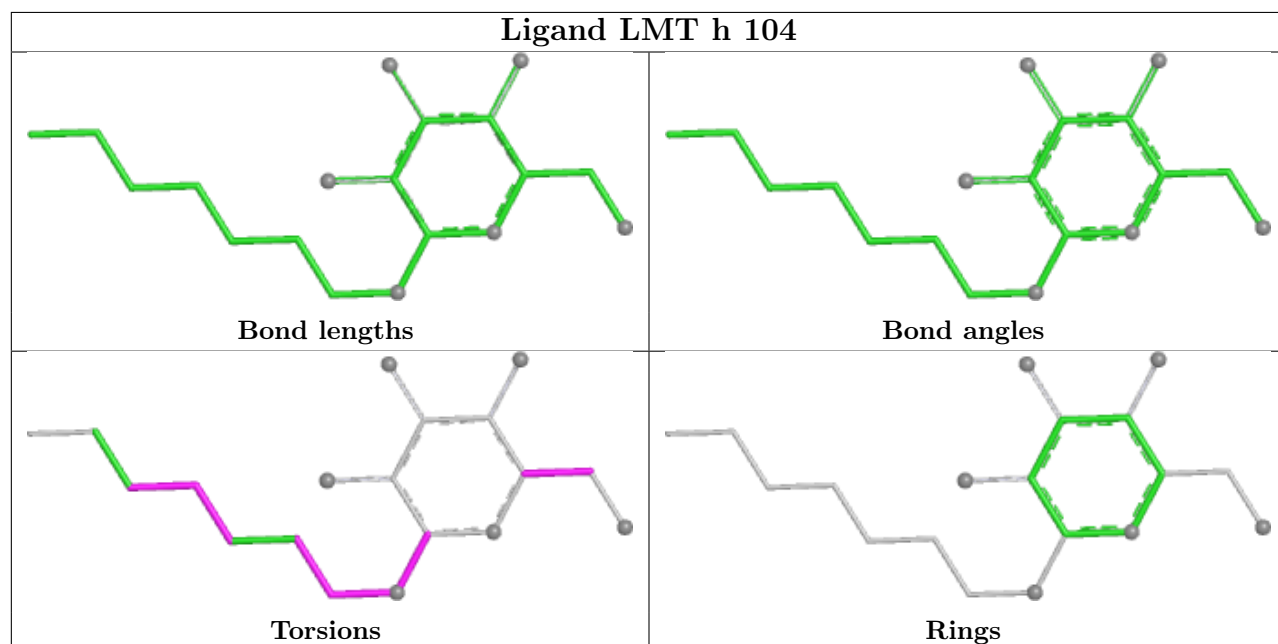
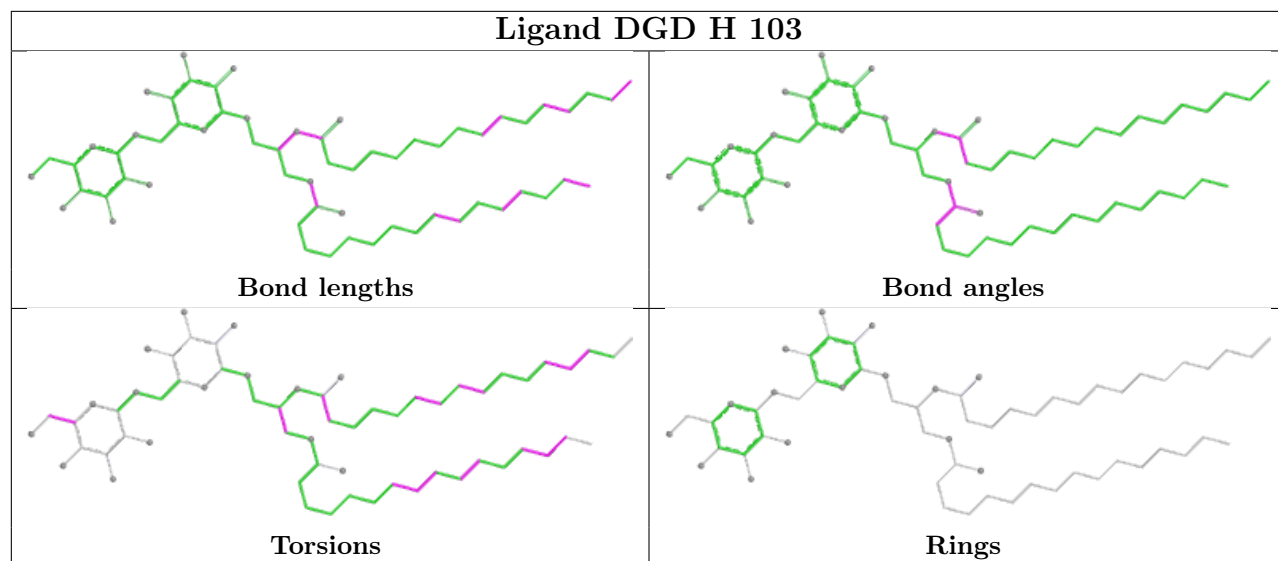


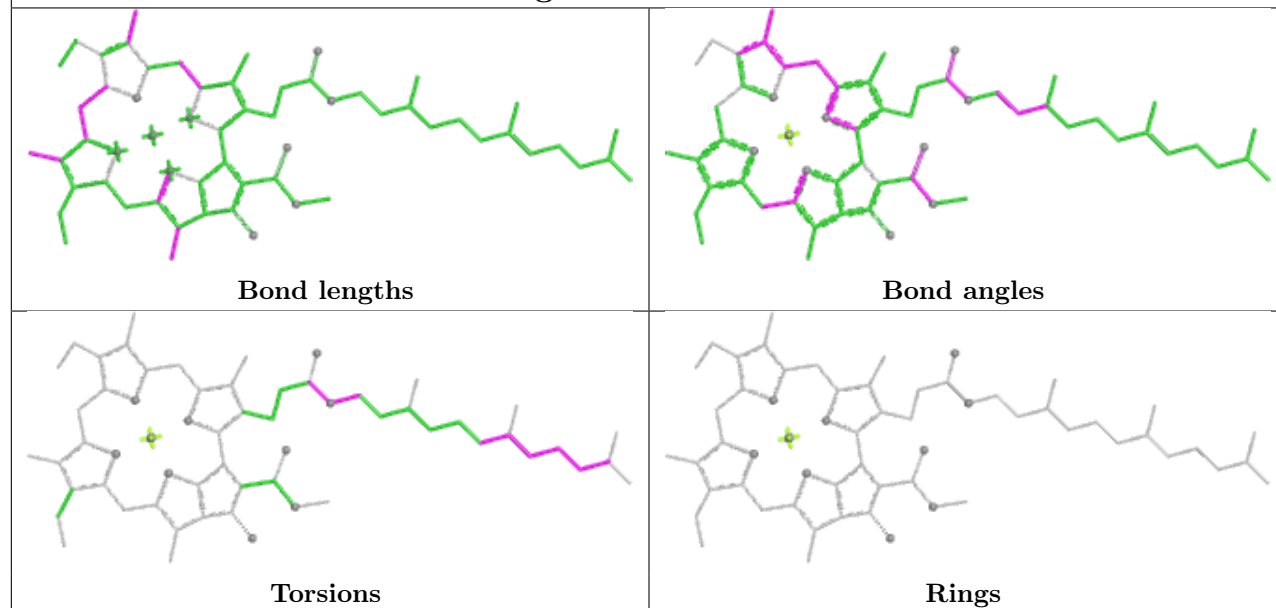
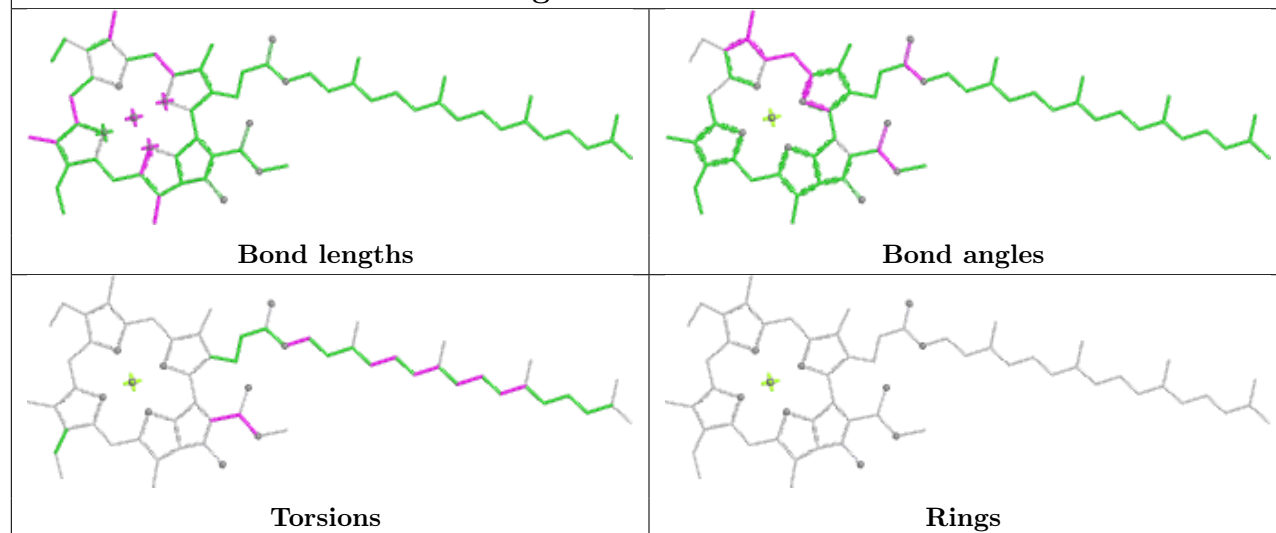
Ligand CLA C 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

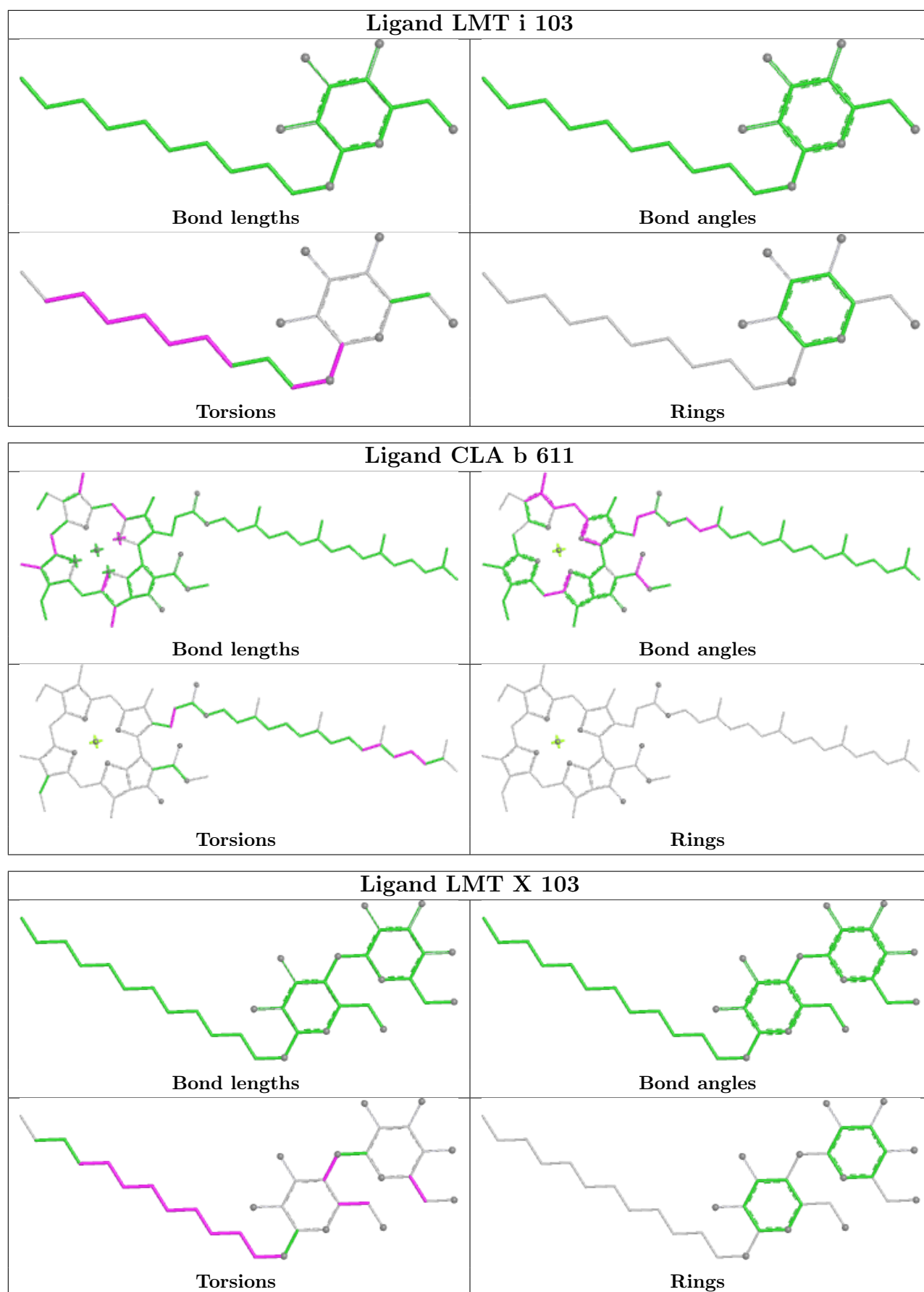
Ligand LMT X 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

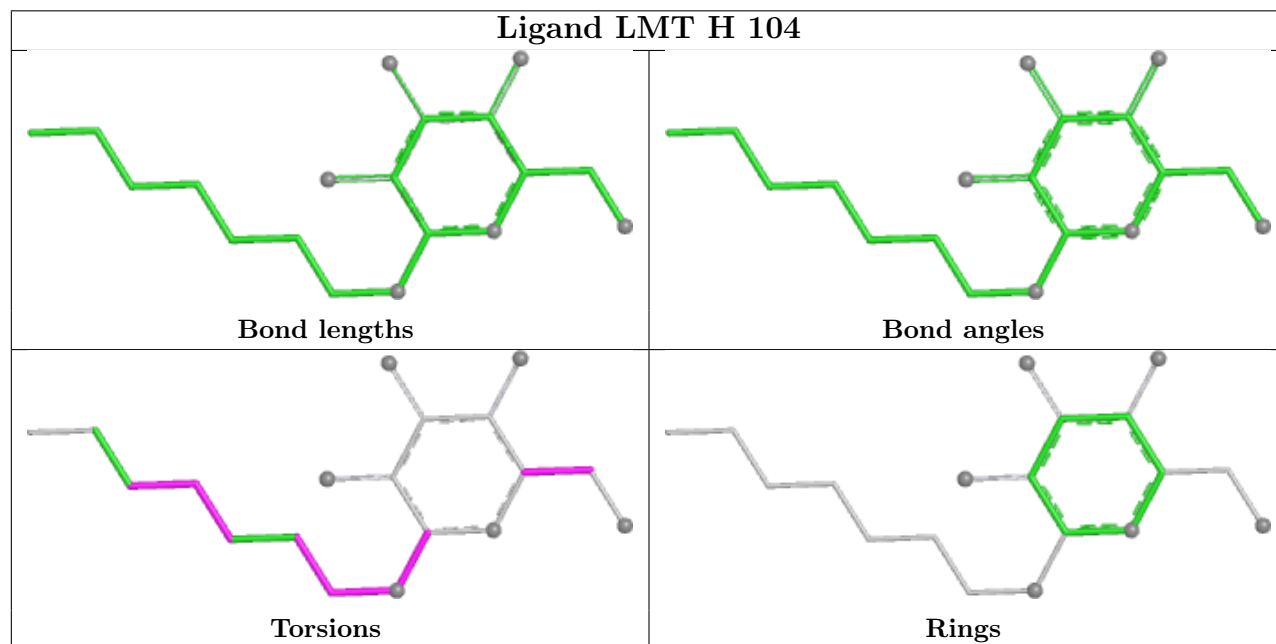
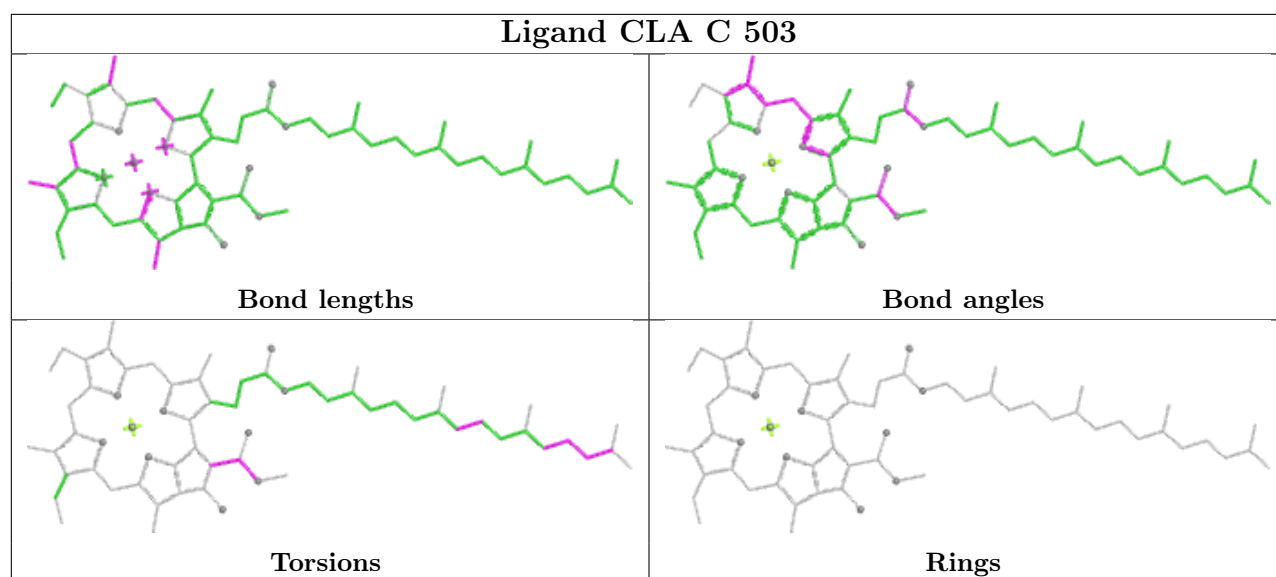
Ligand PL9 a 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

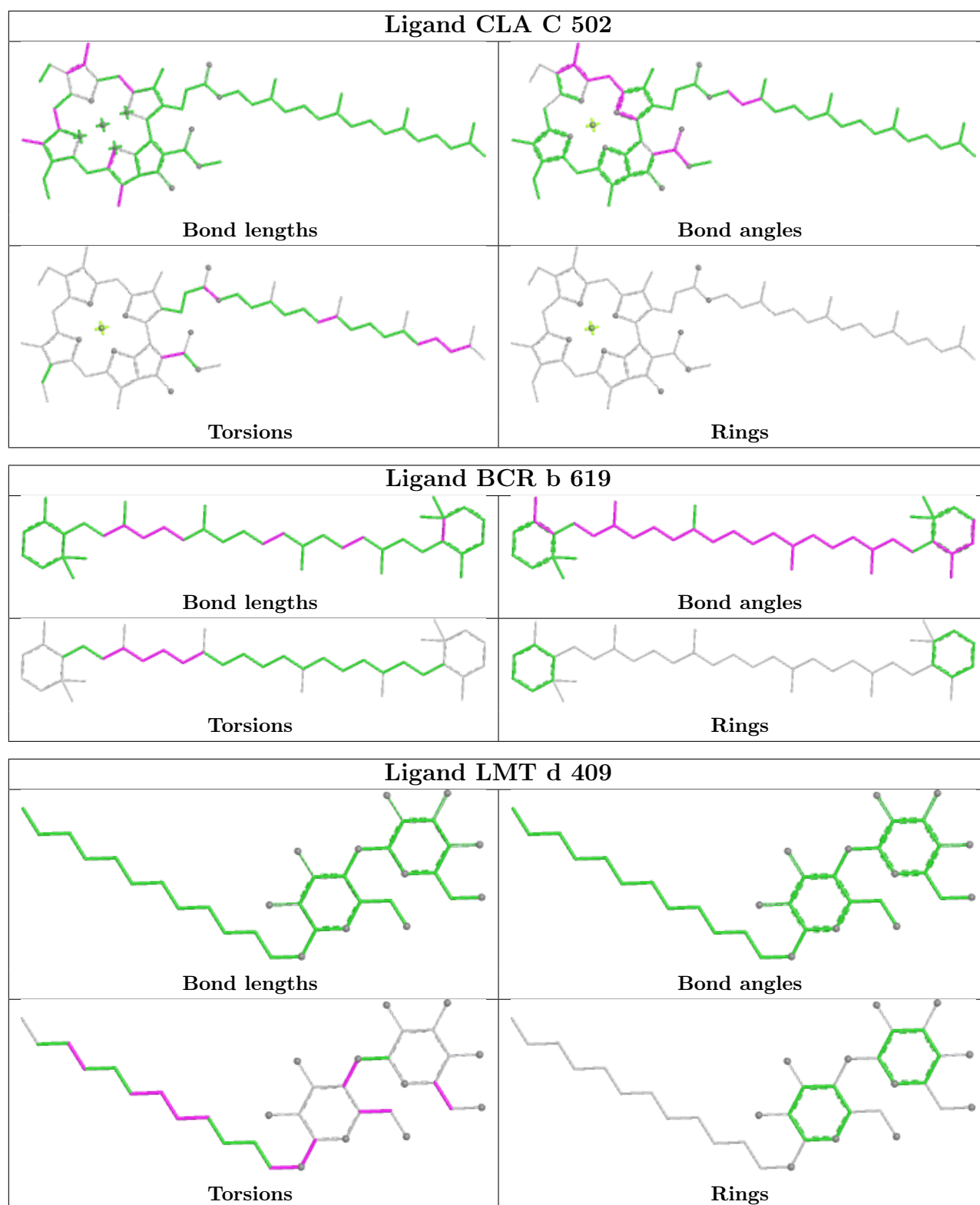


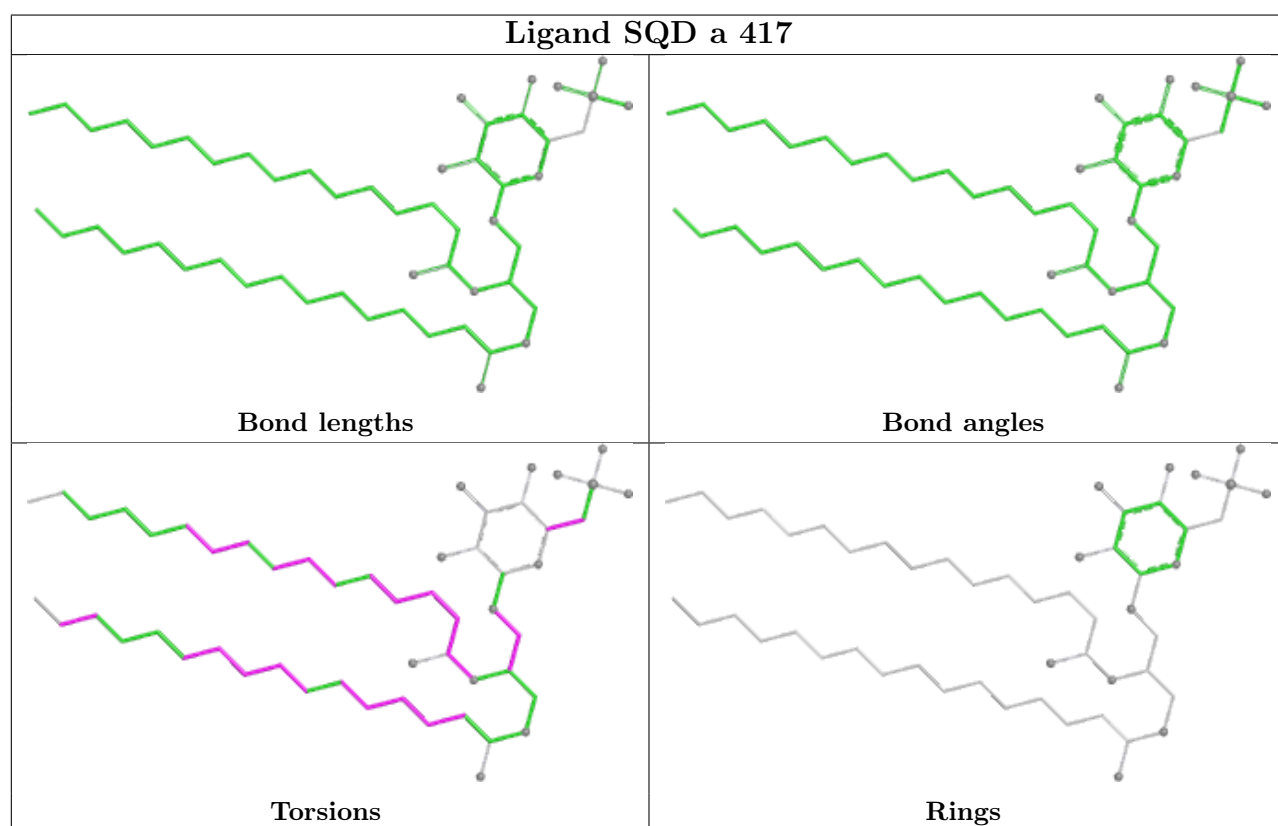
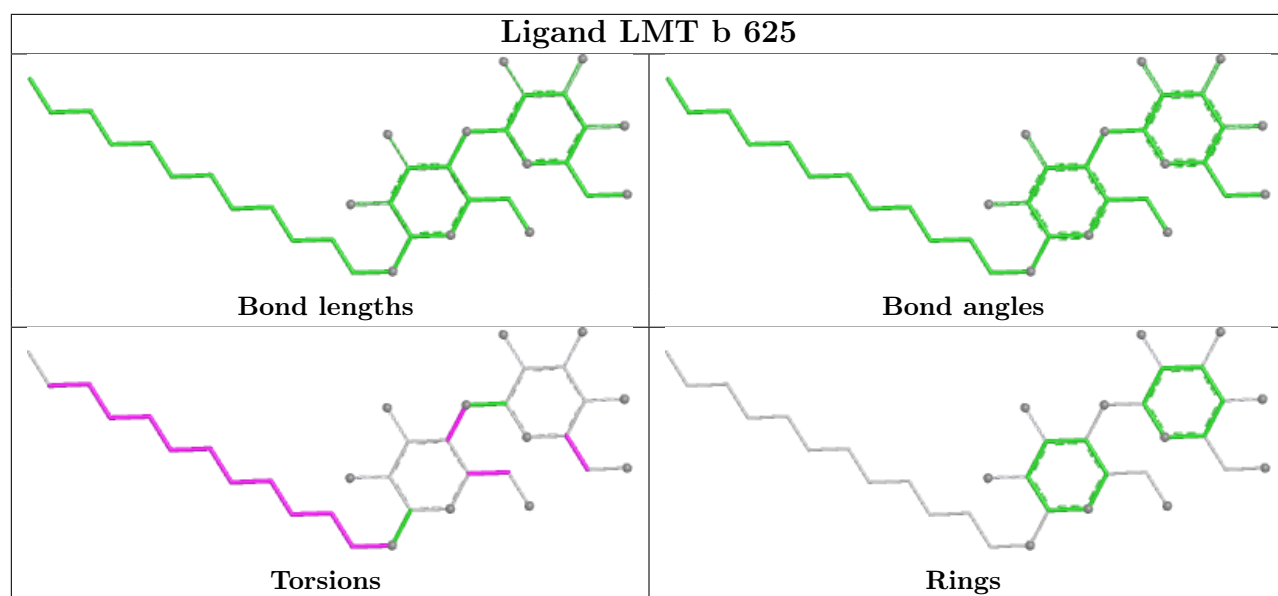


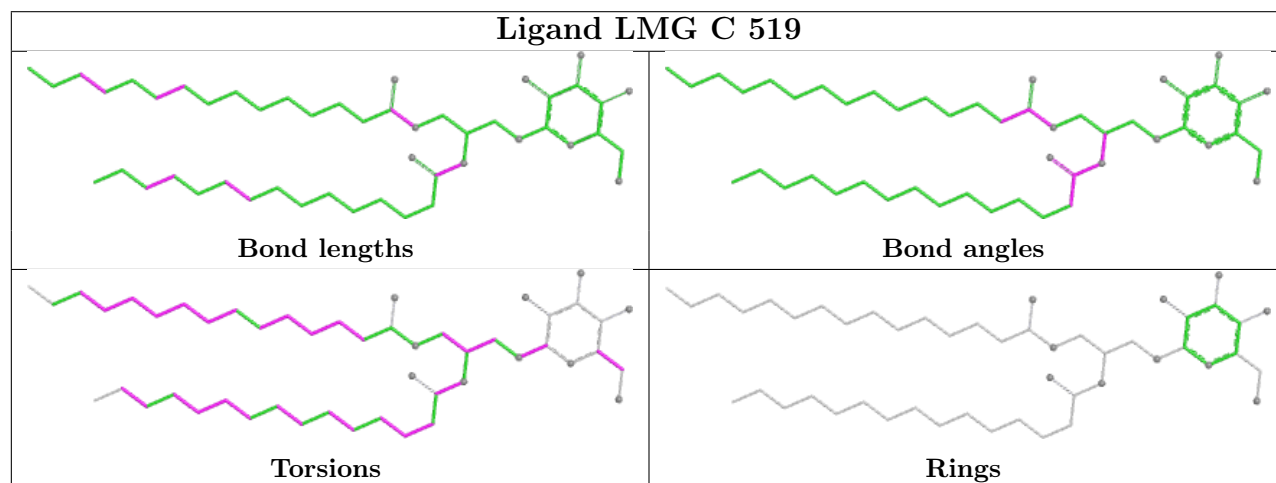
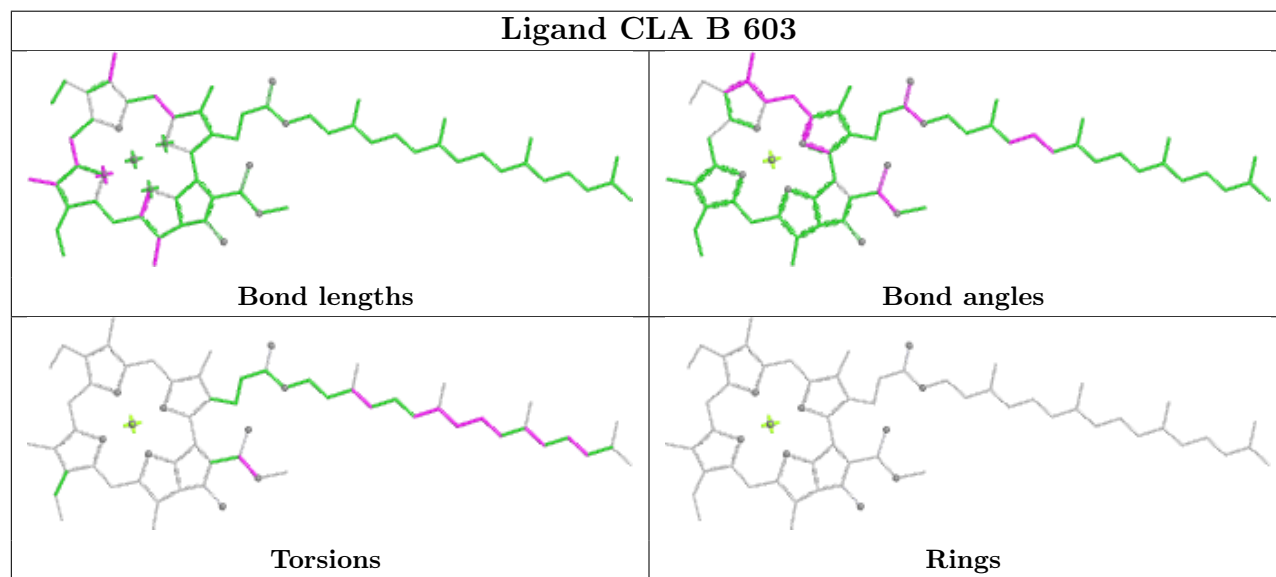
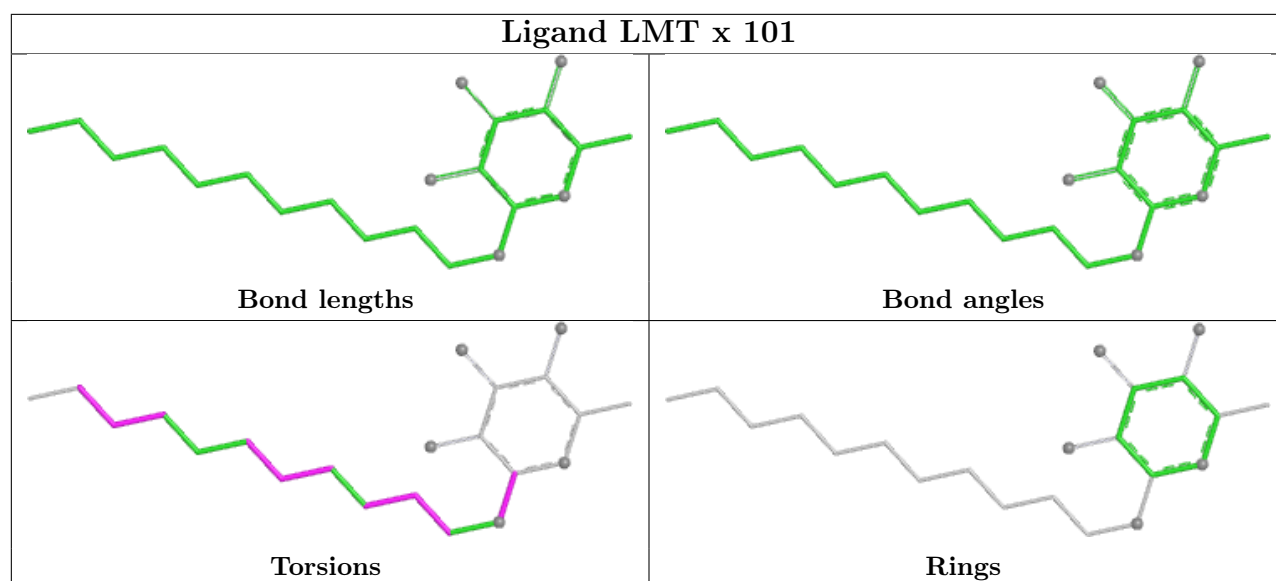
**Ligand CLA b 617****Ligand CLA C 509**

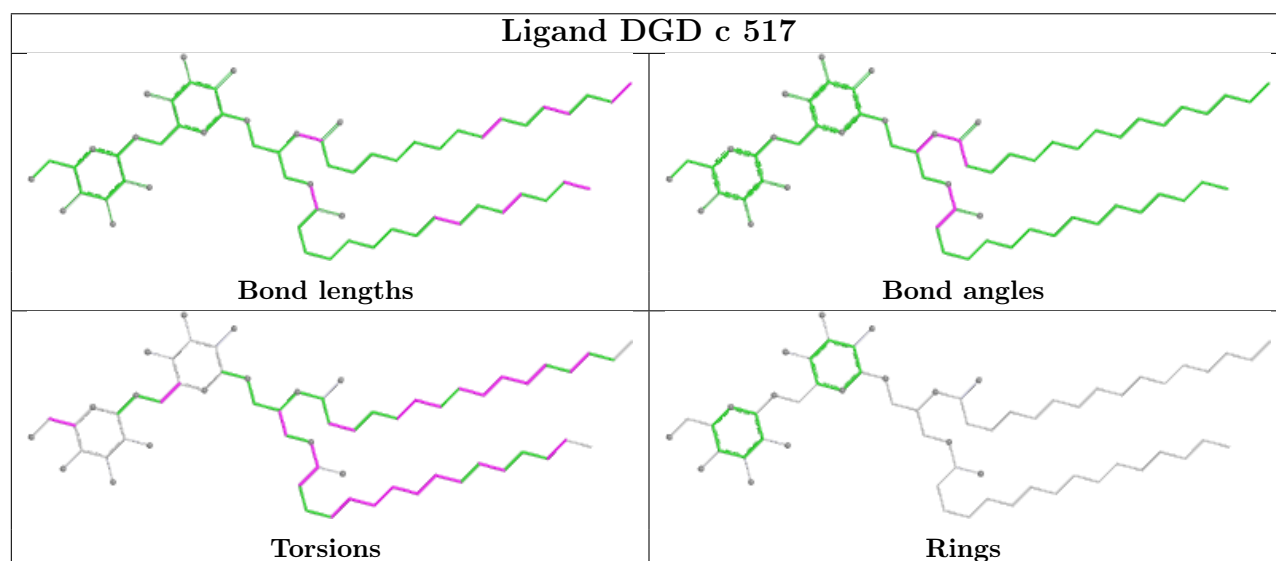
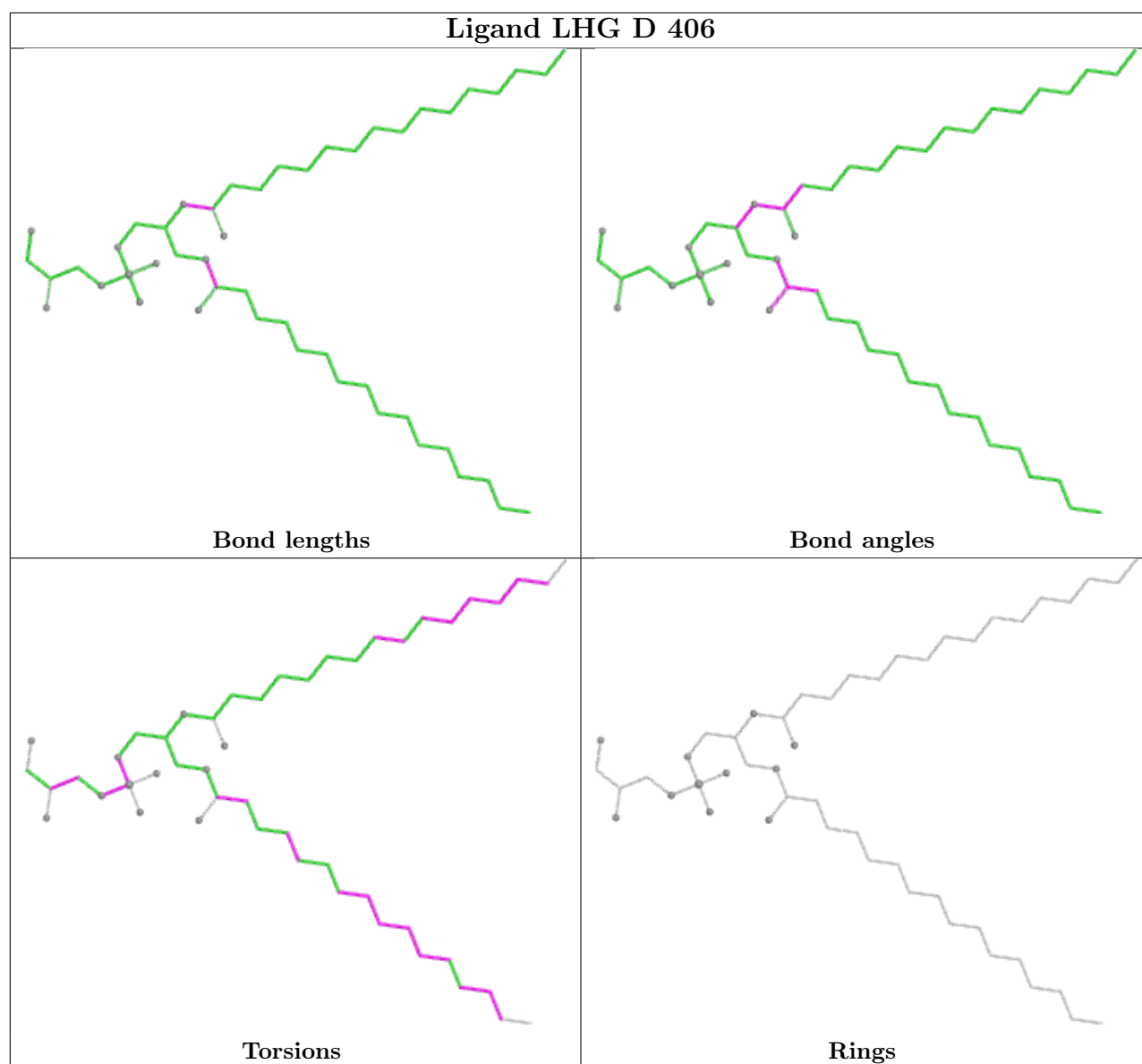




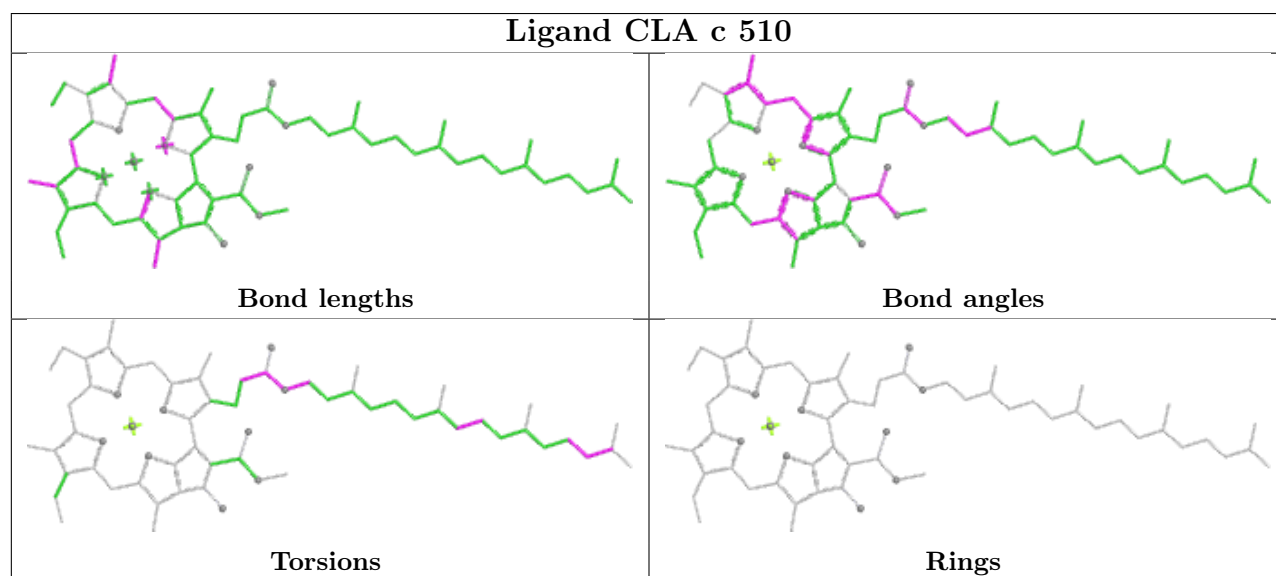
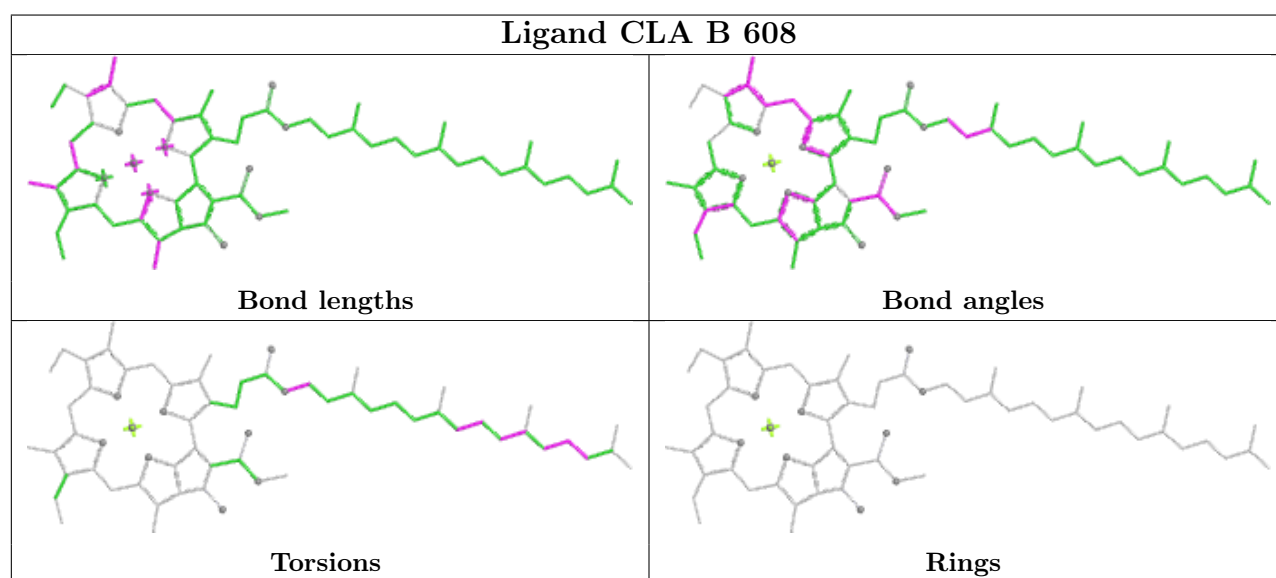
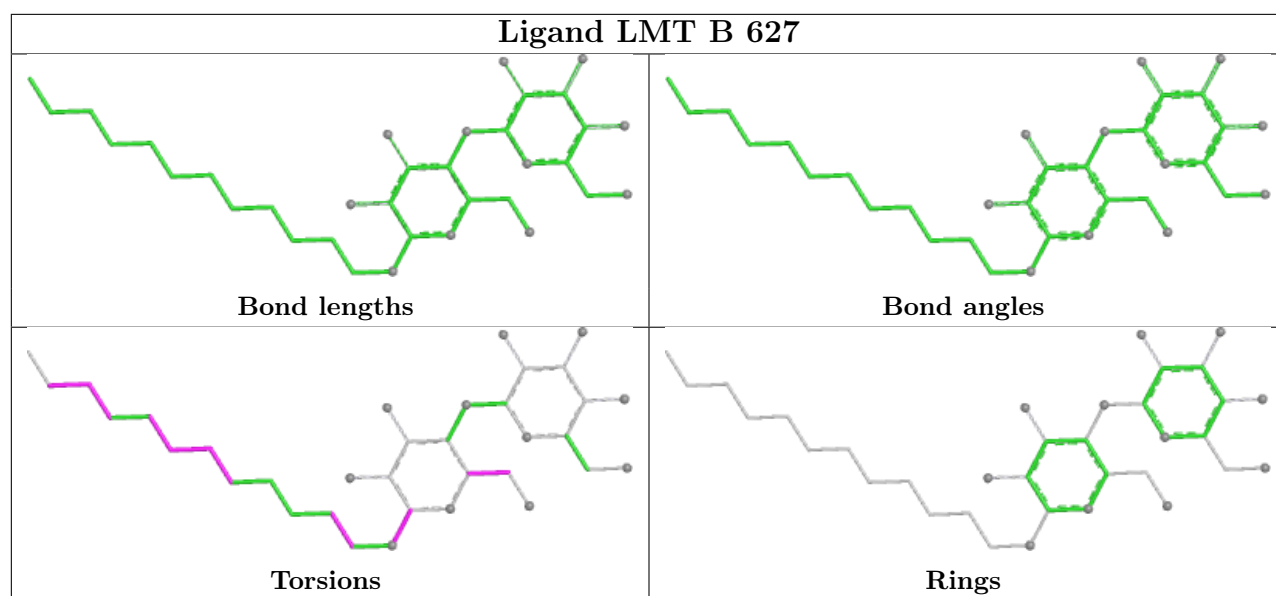




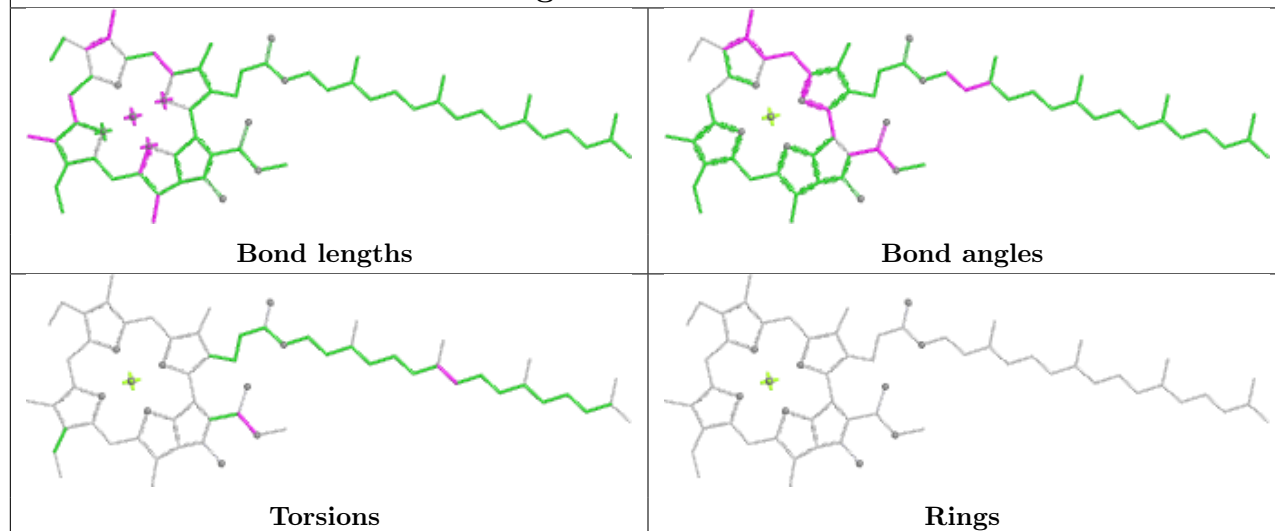




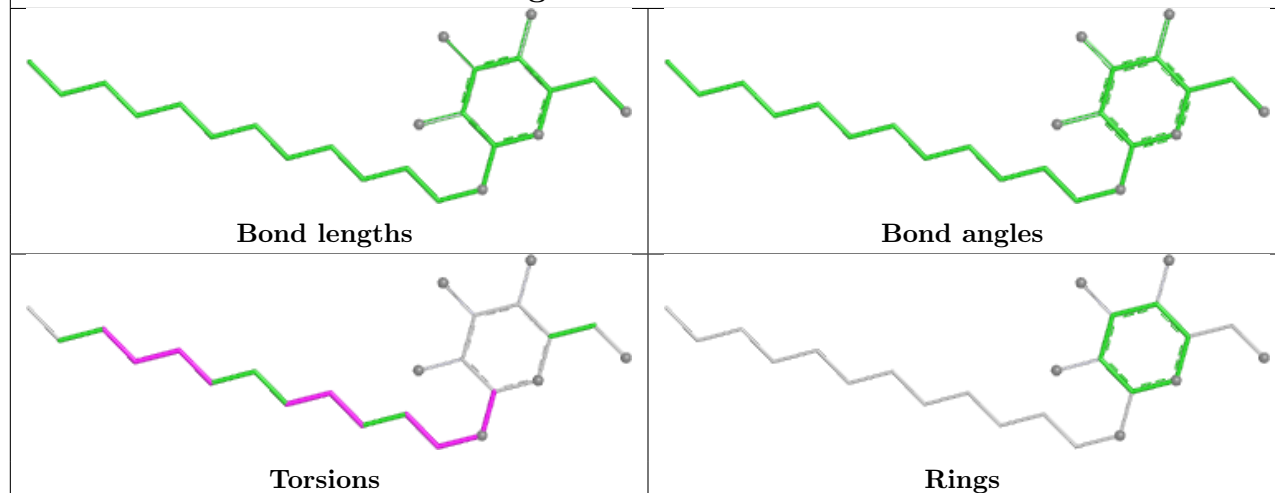




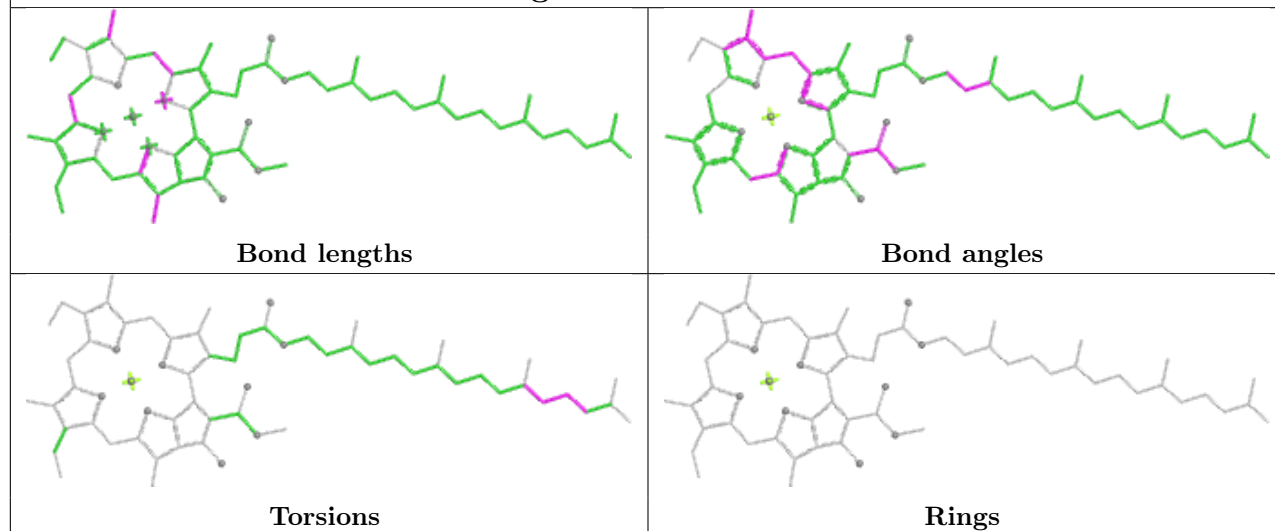
## Ligand CLA c 511

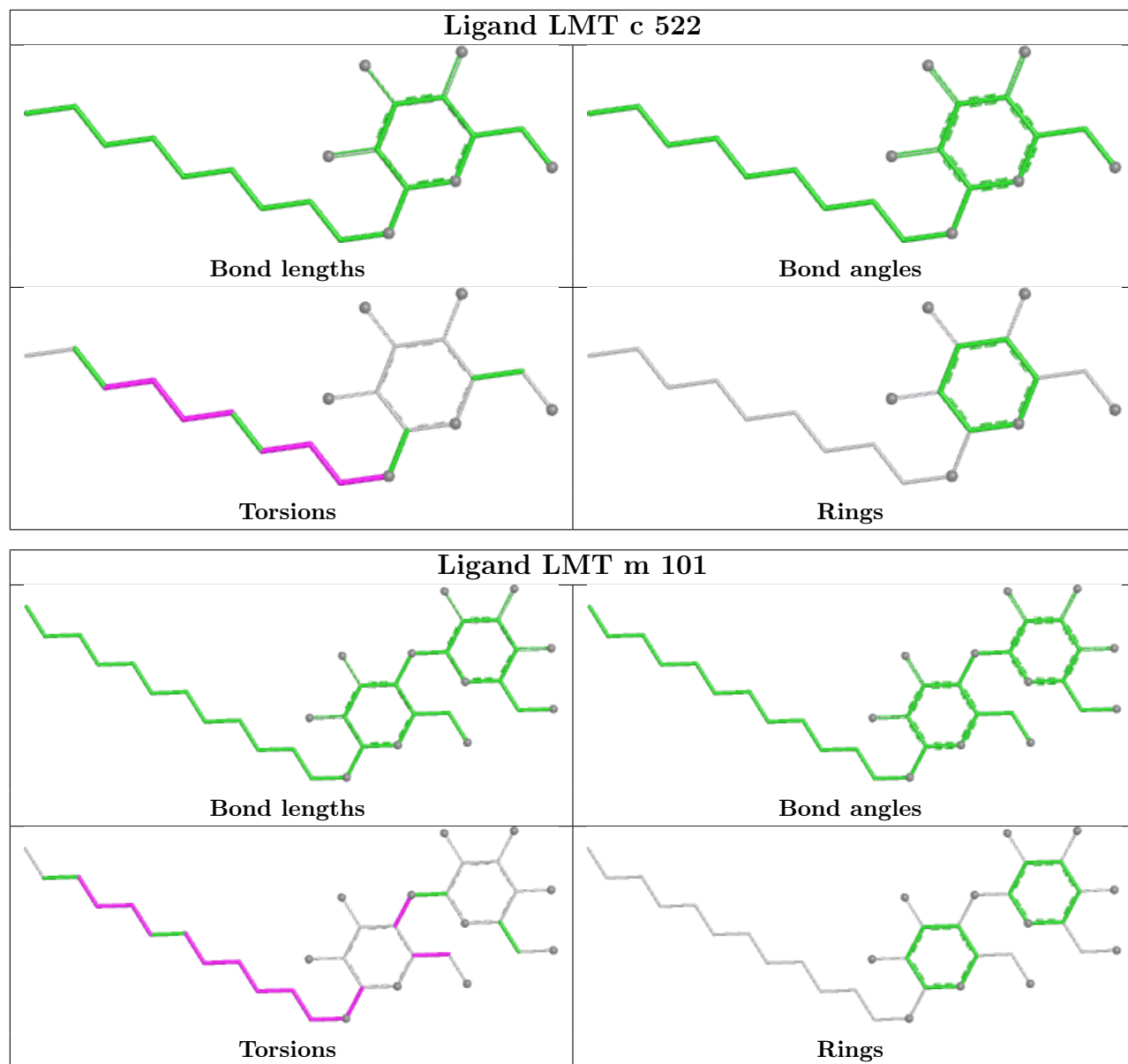


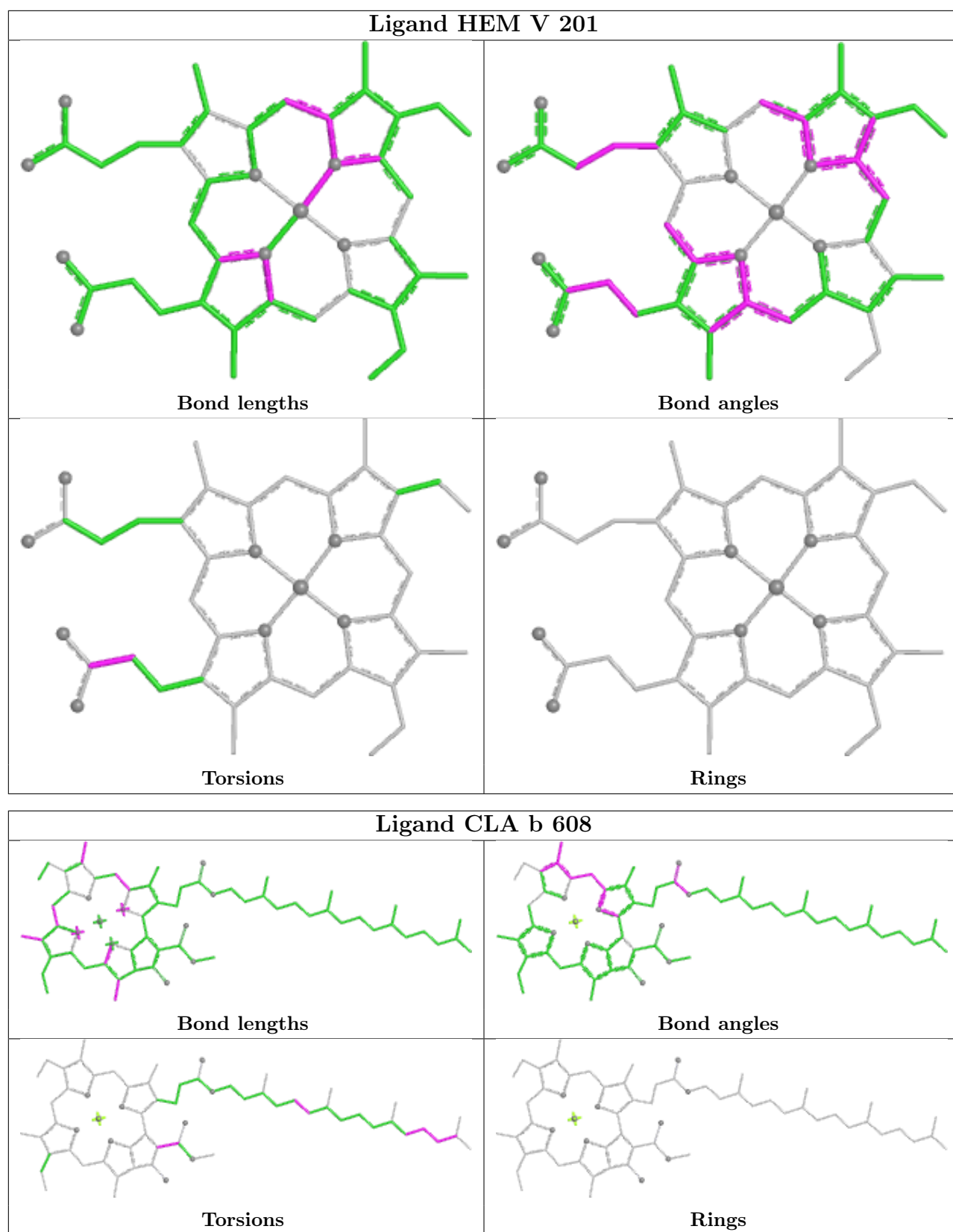
## Ligand LMT C 520

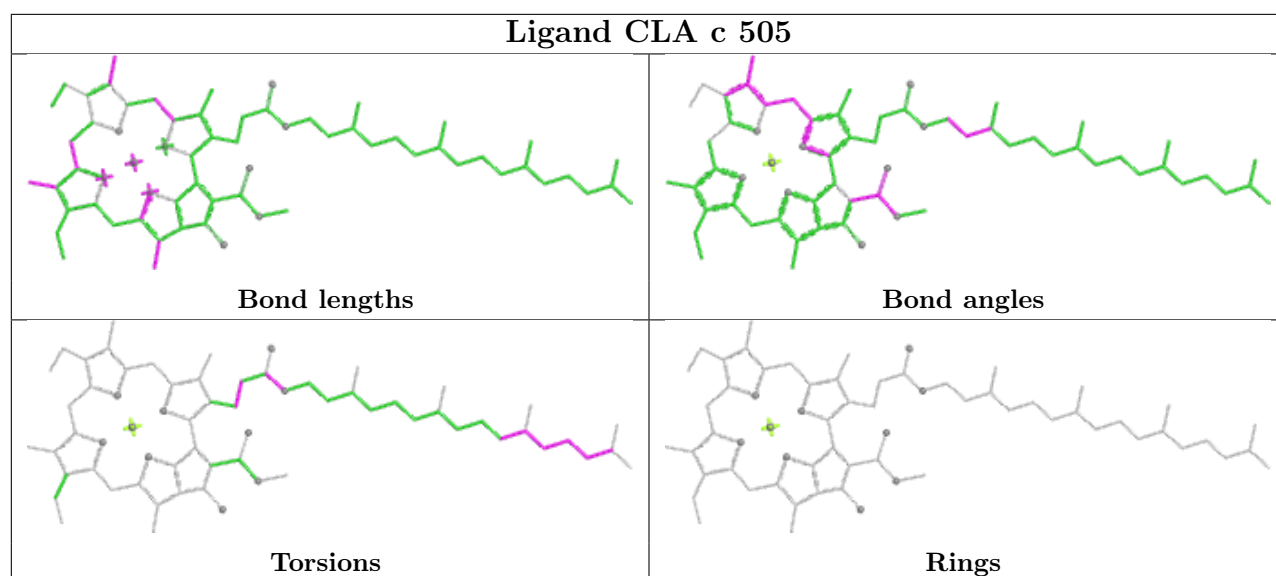
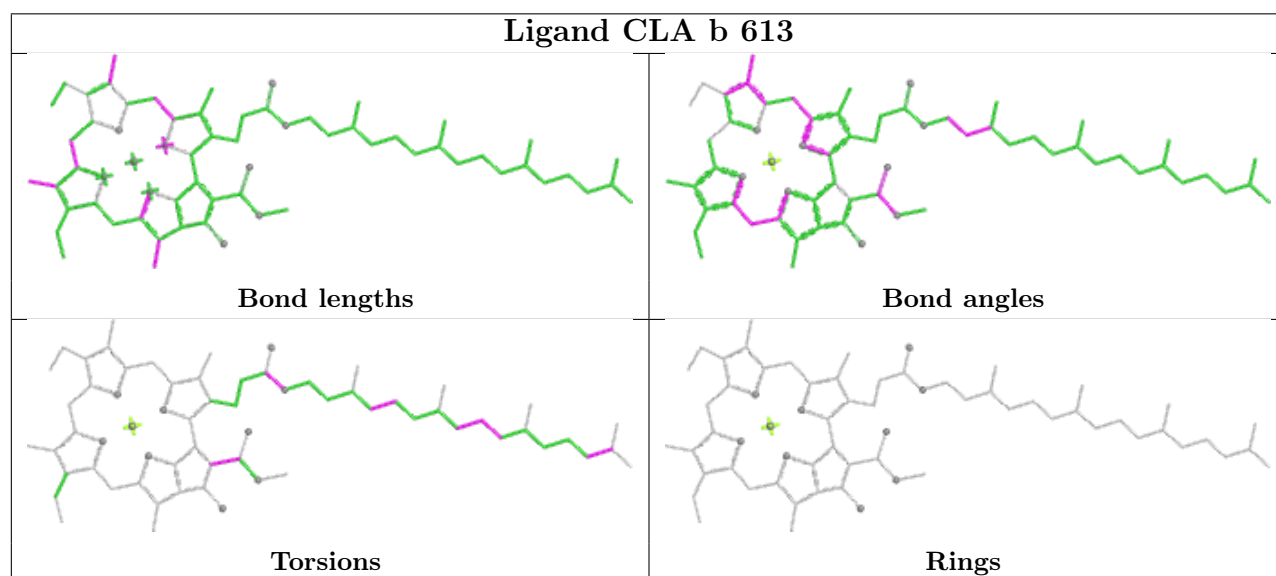
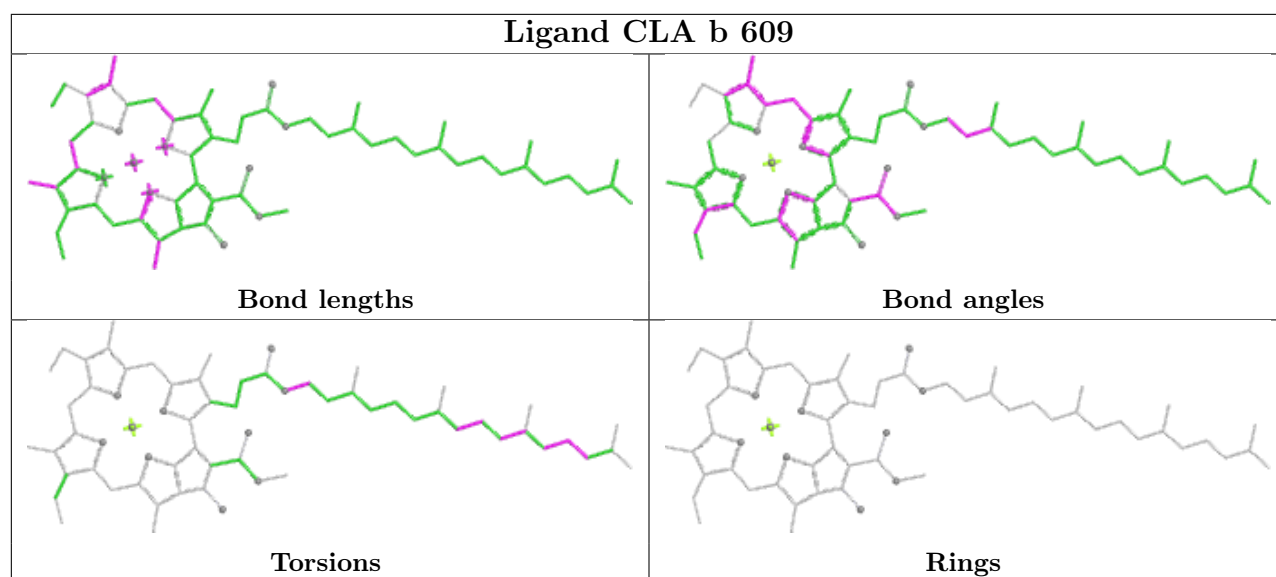


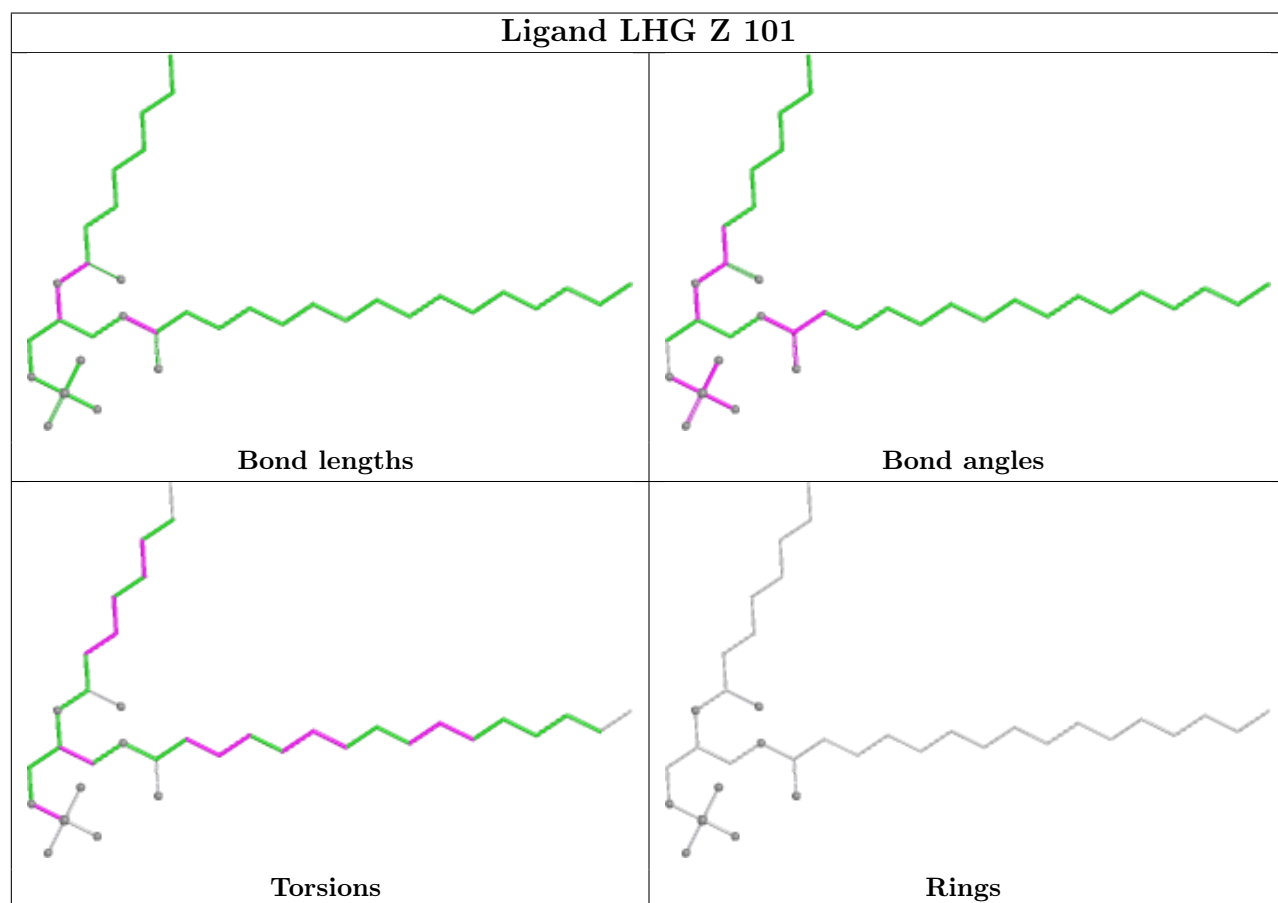
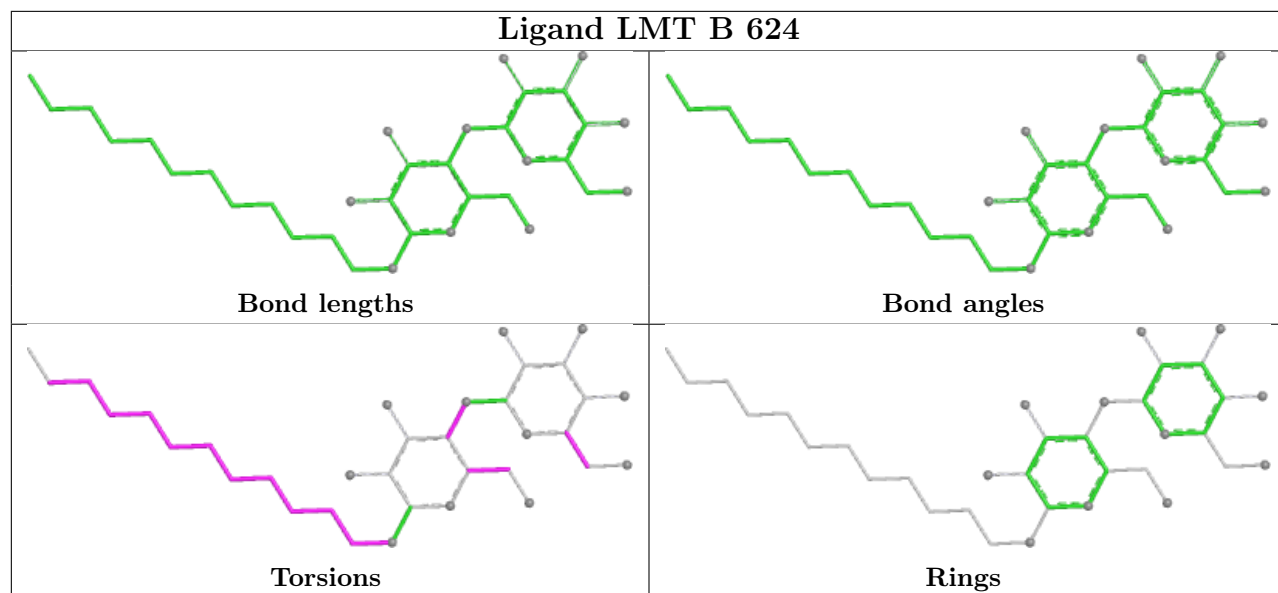
## Ligand CLA B 609

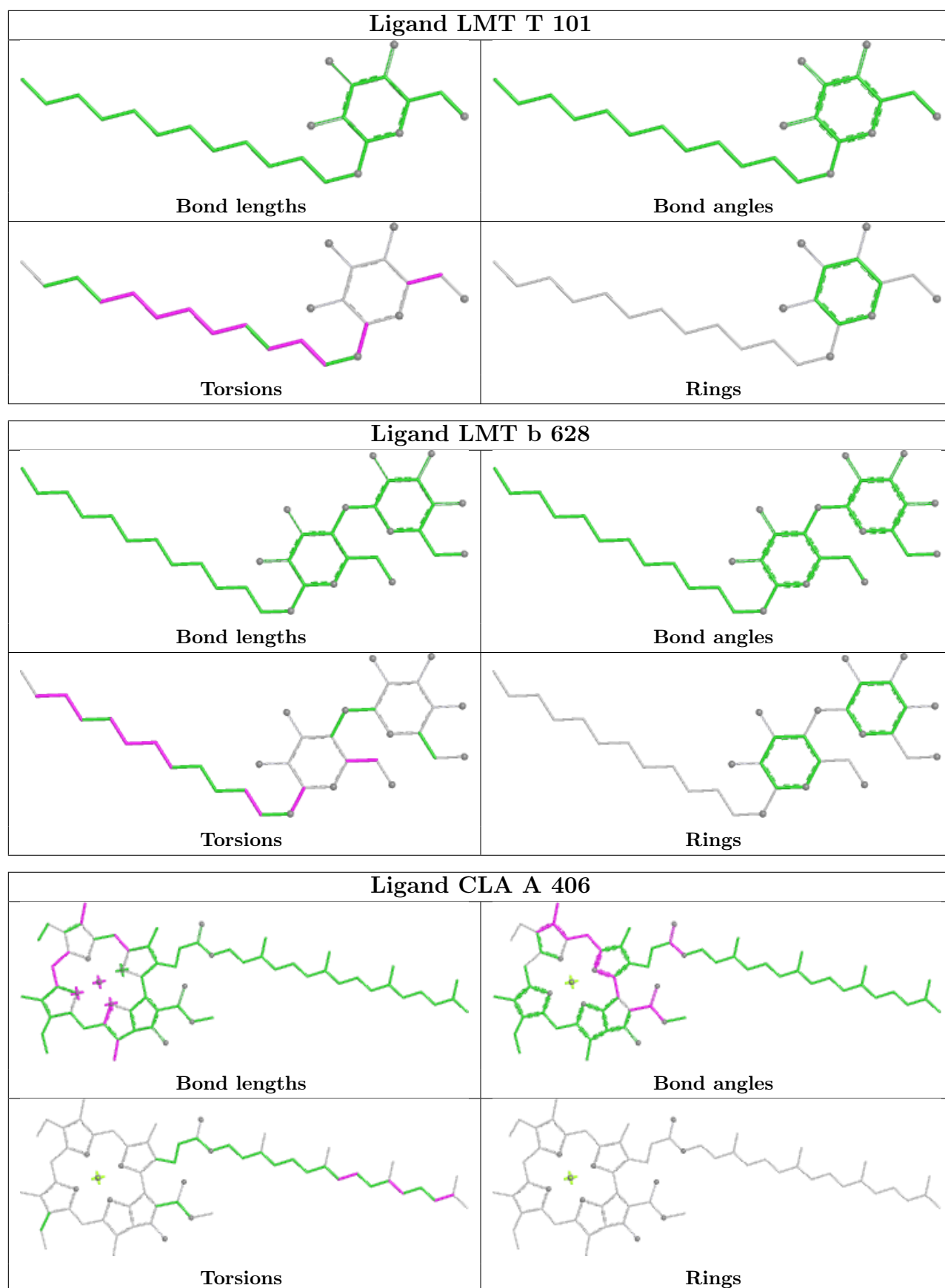


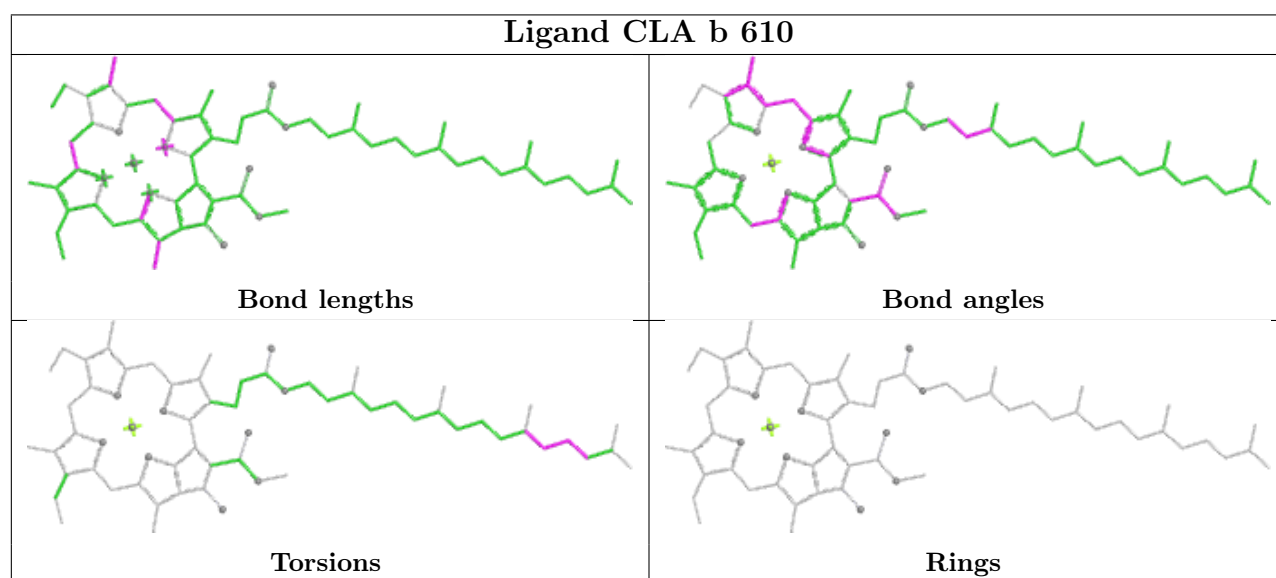
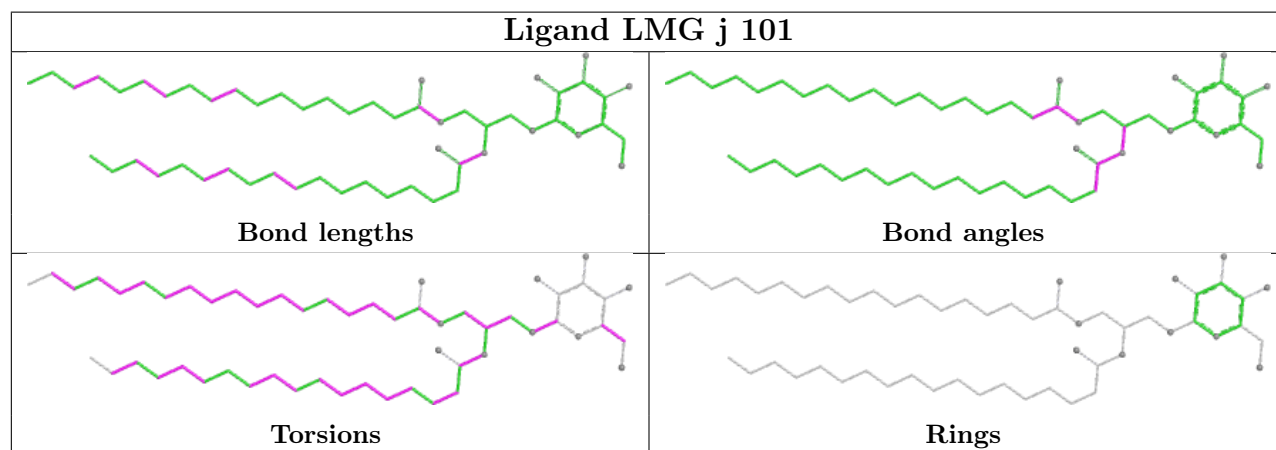
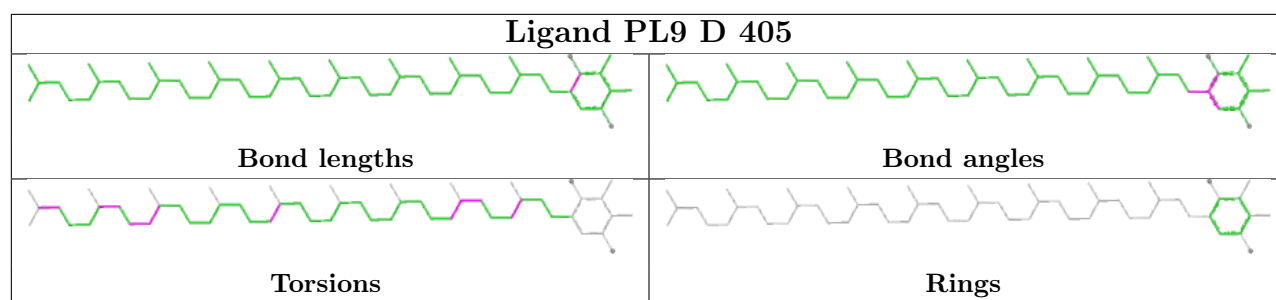




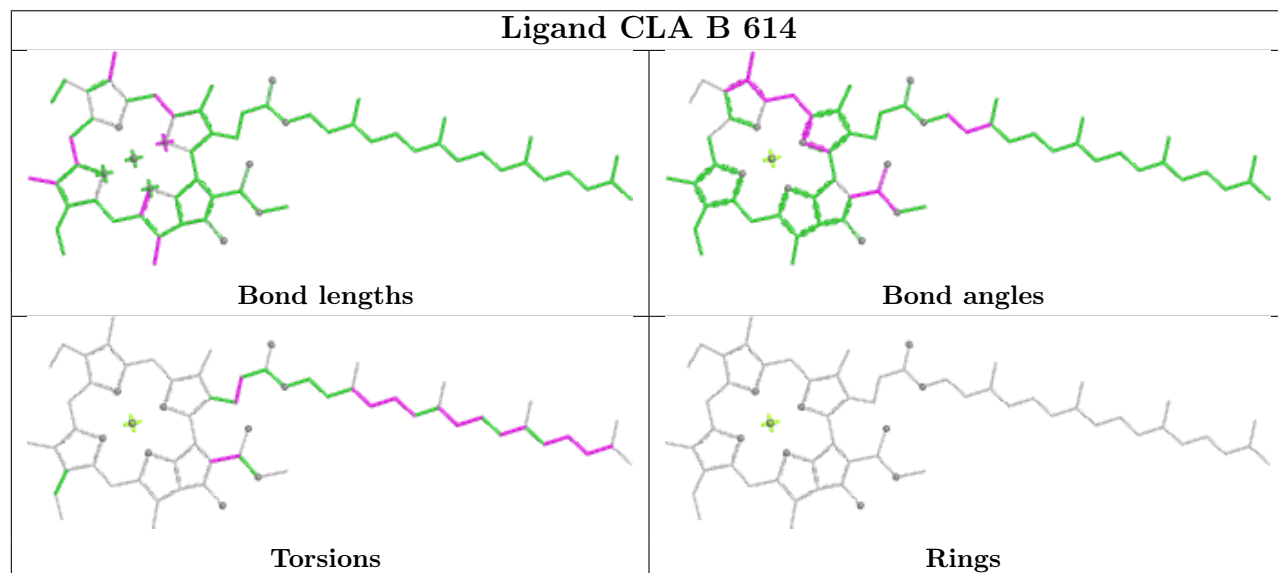
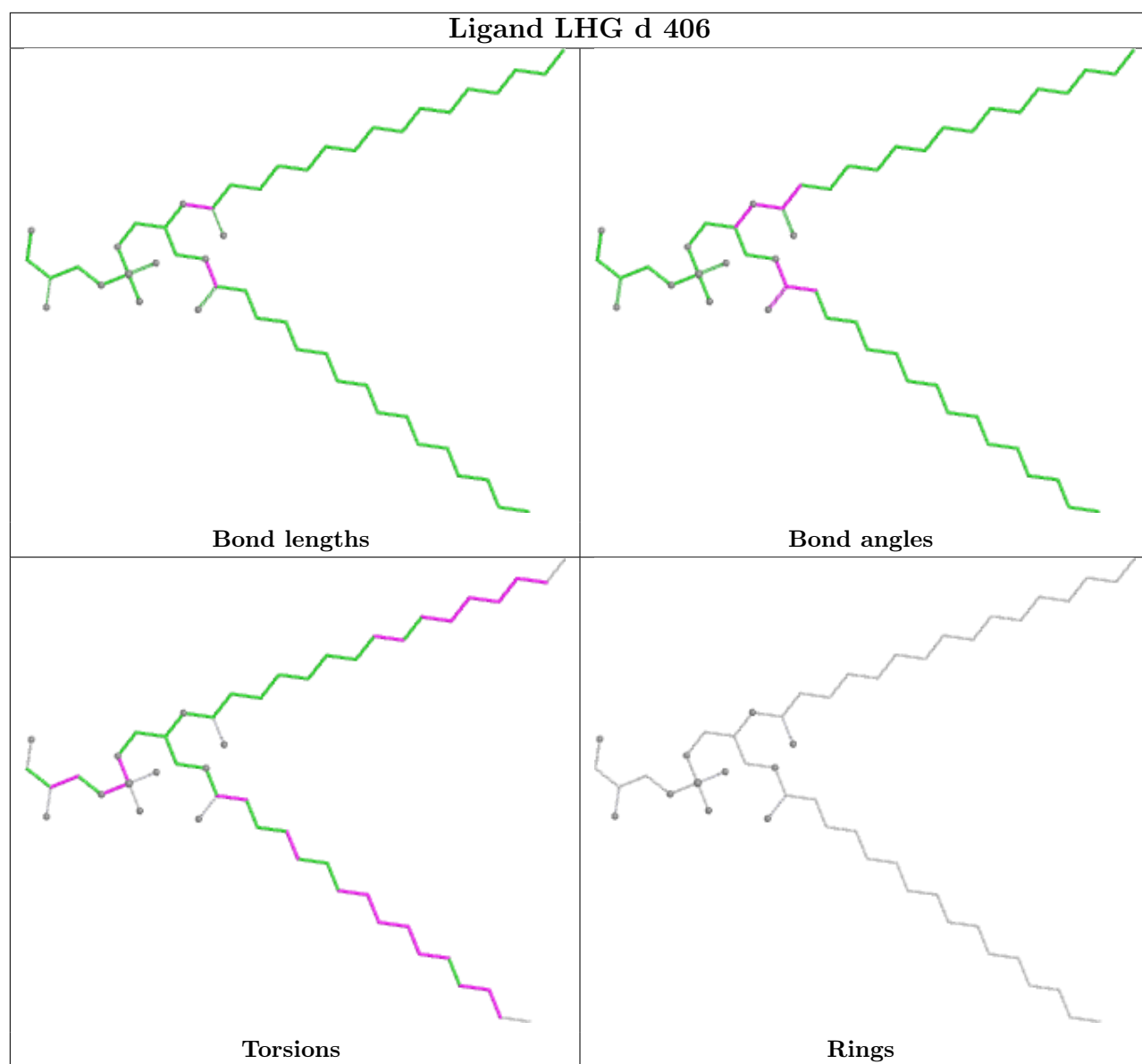


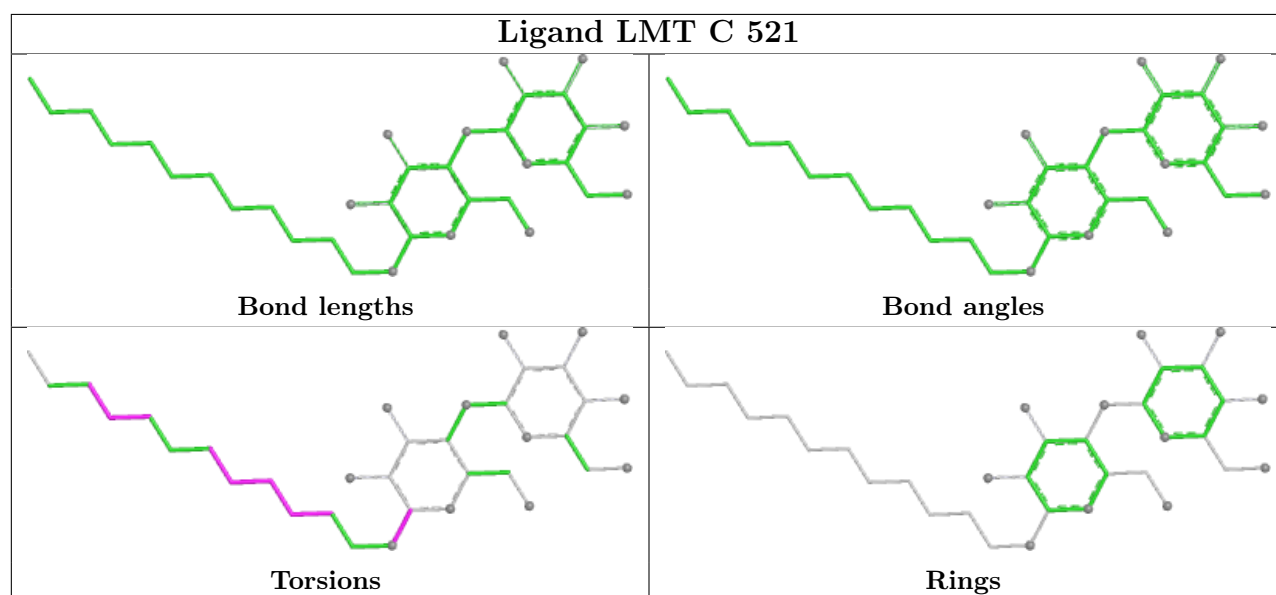
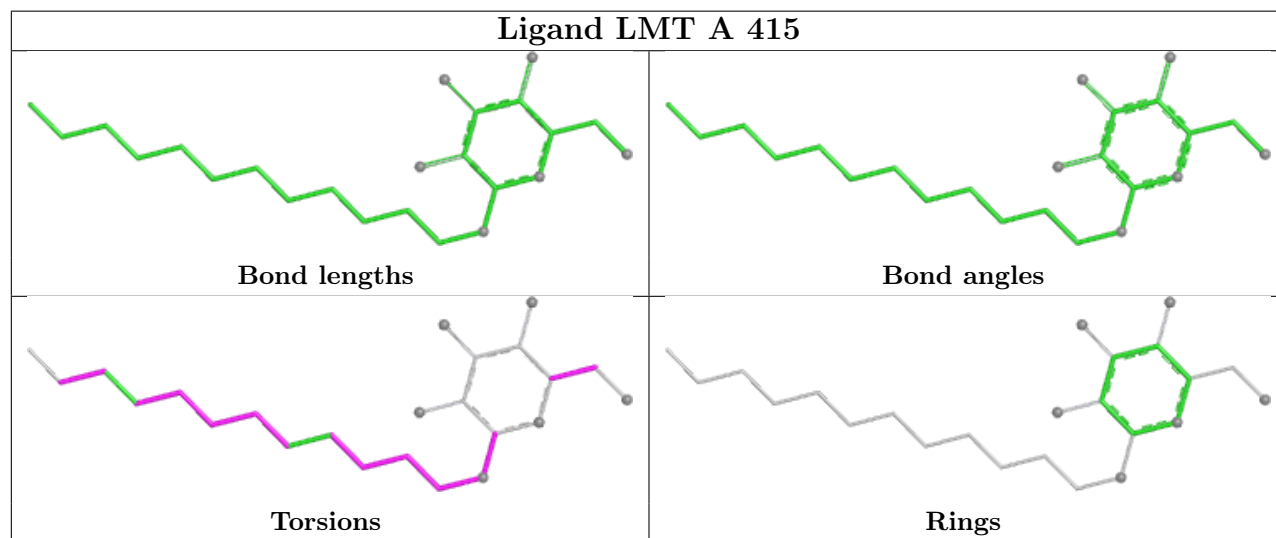
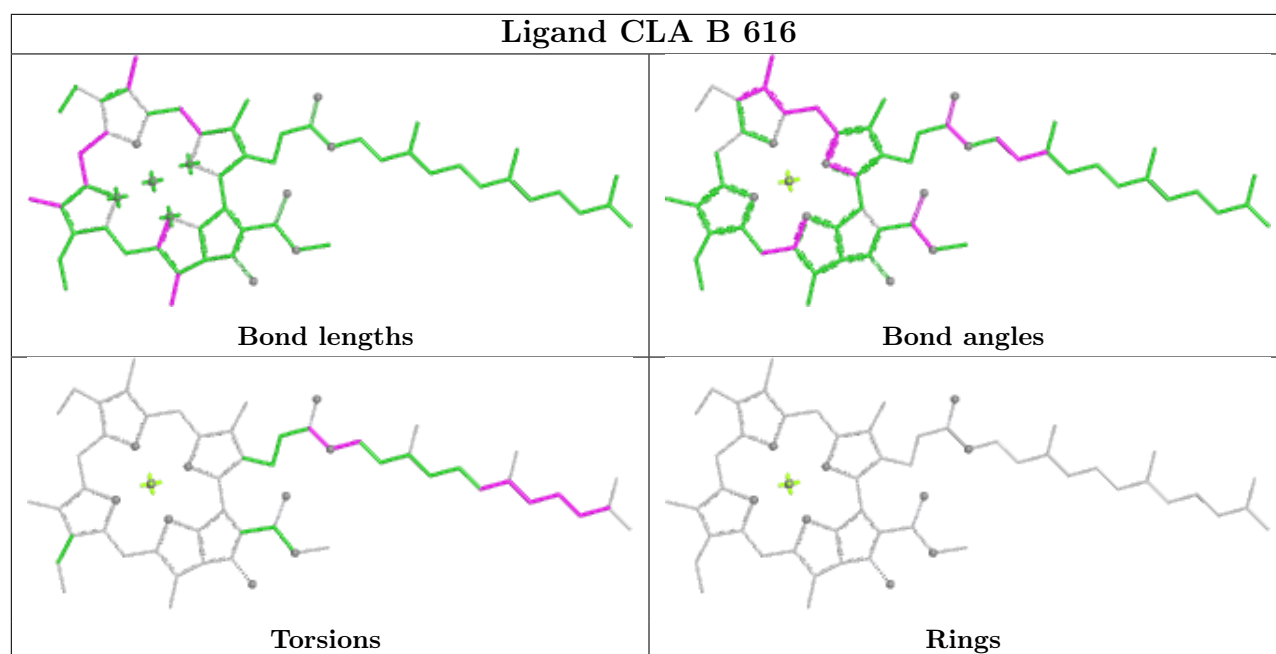


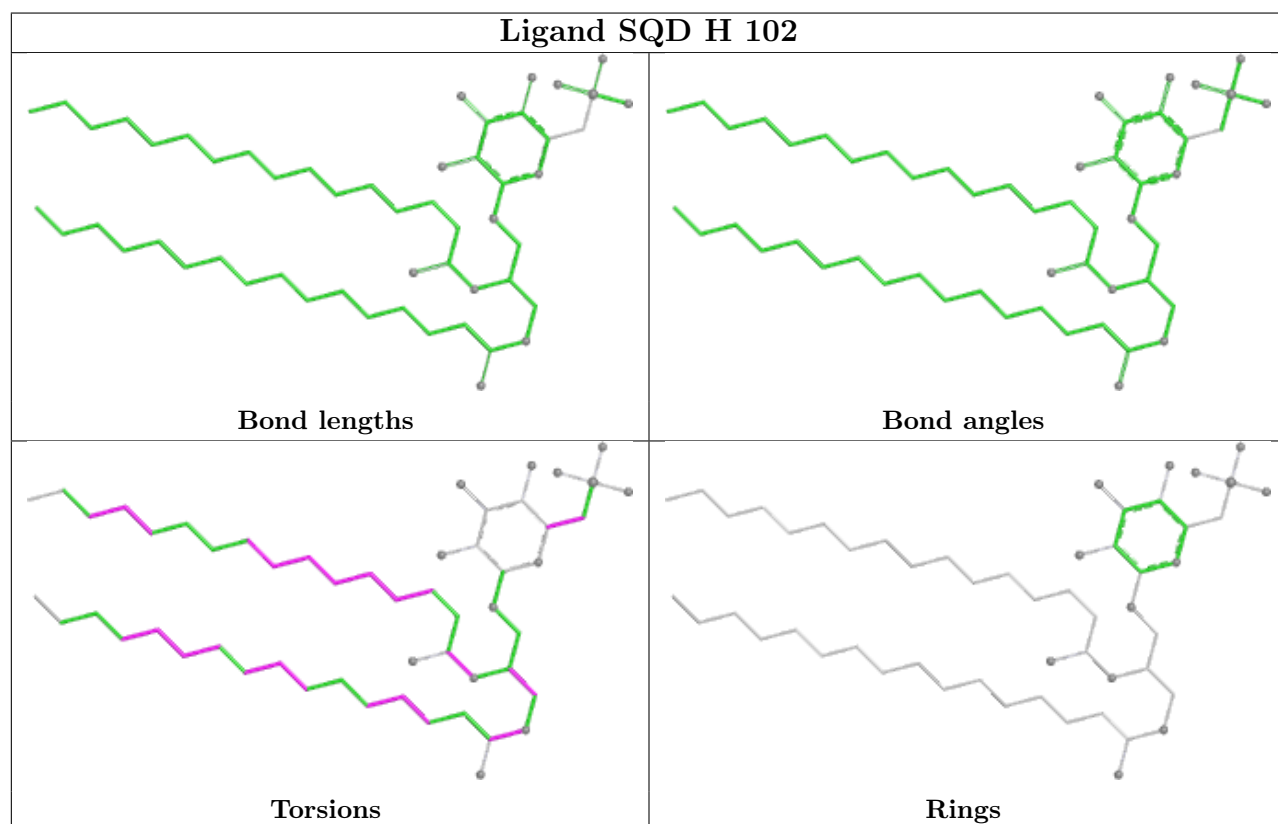
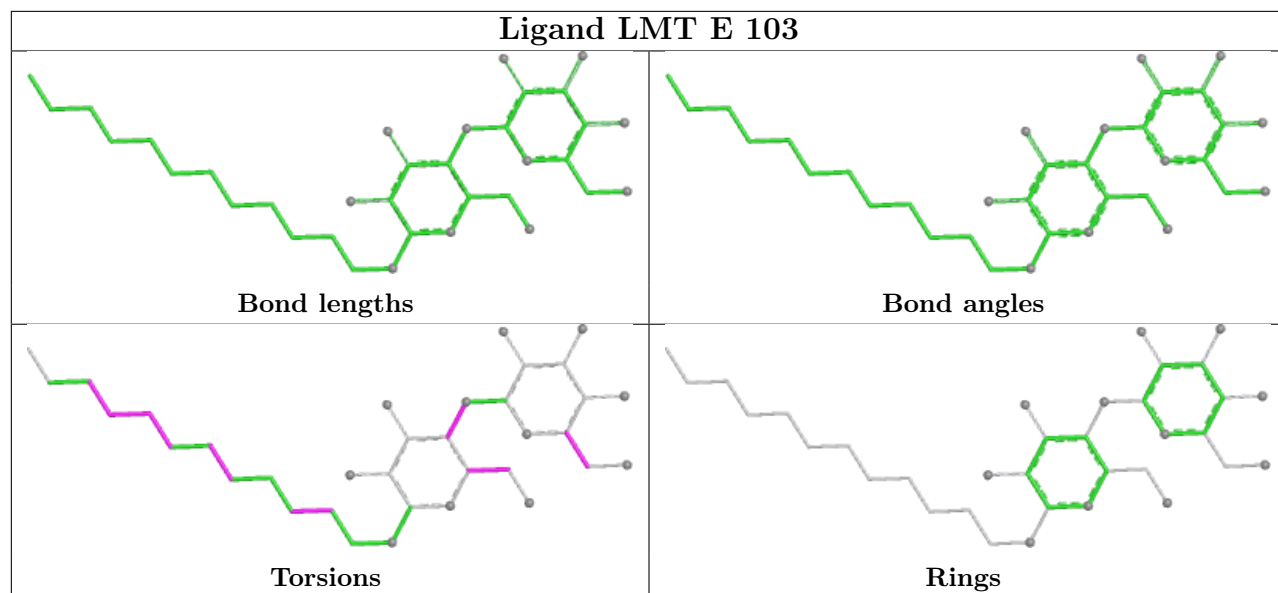


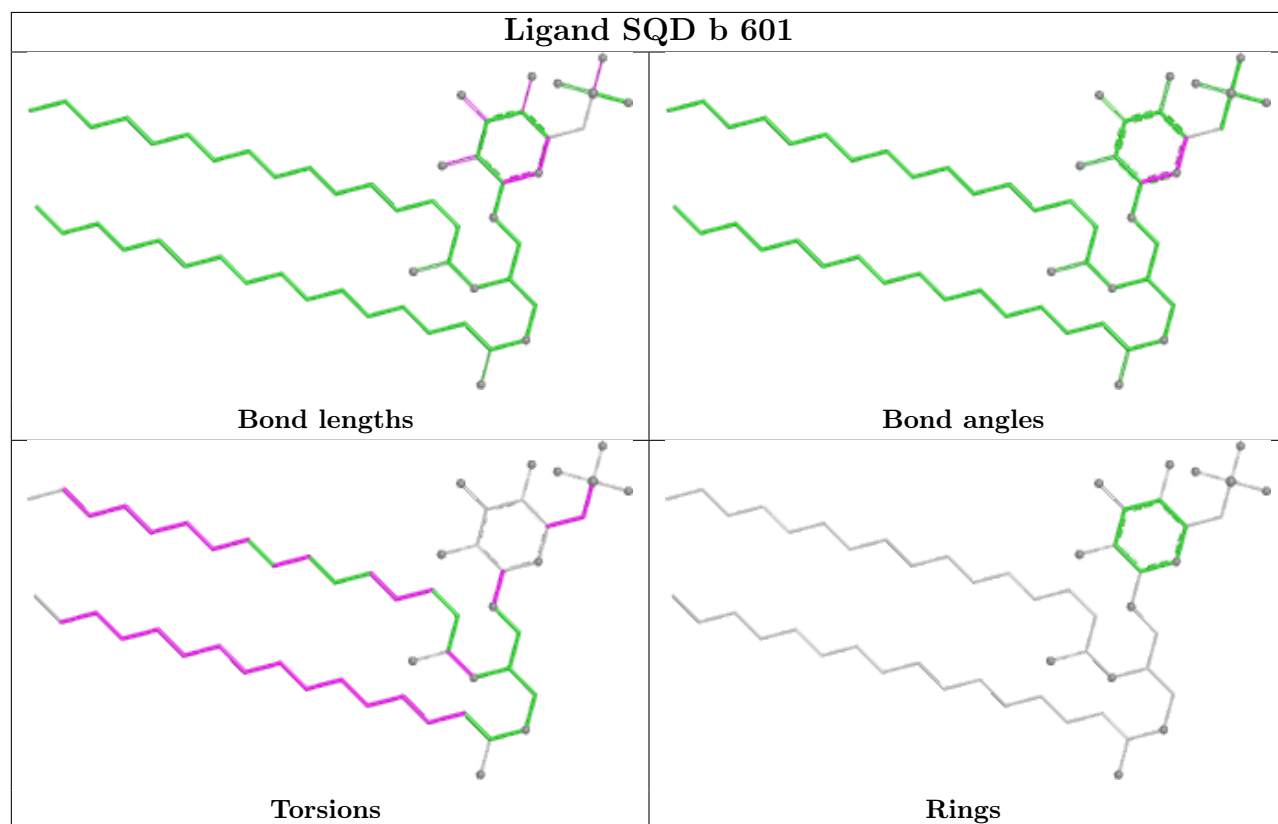
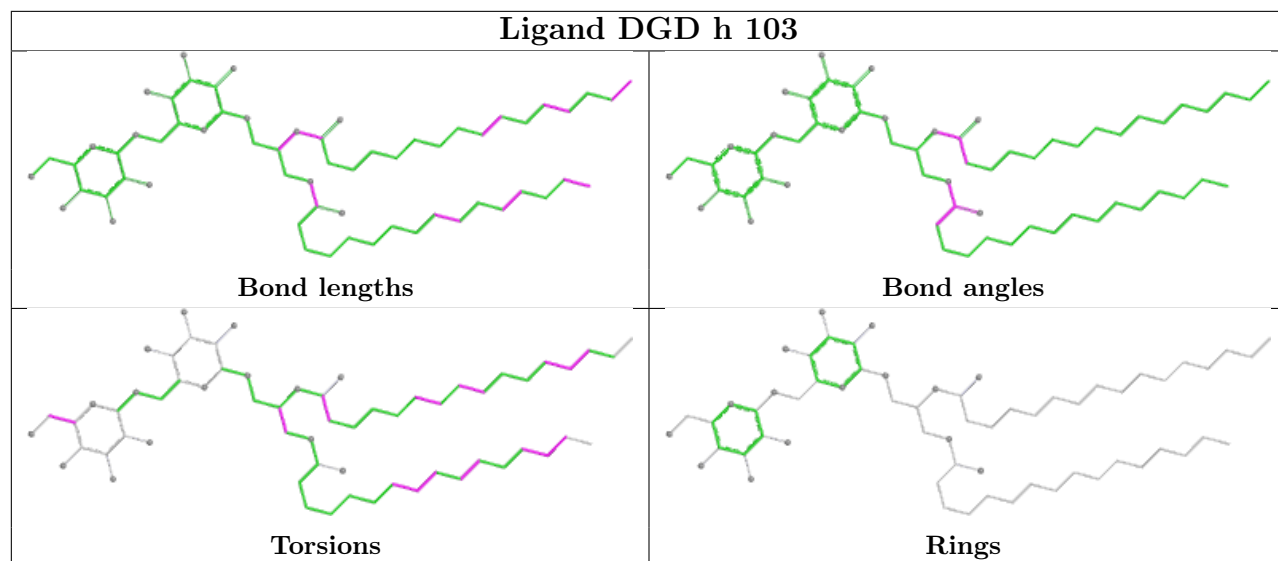


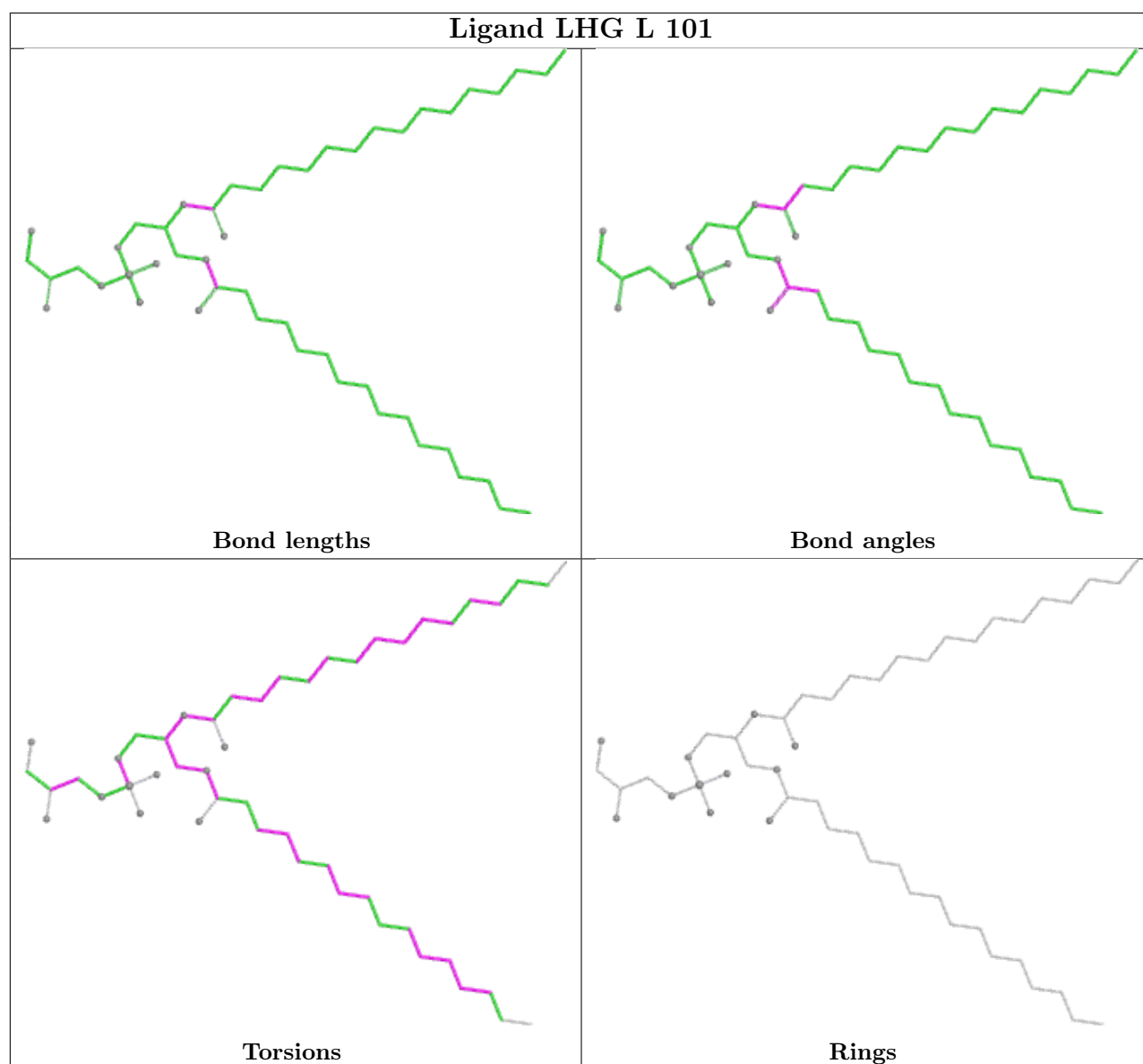
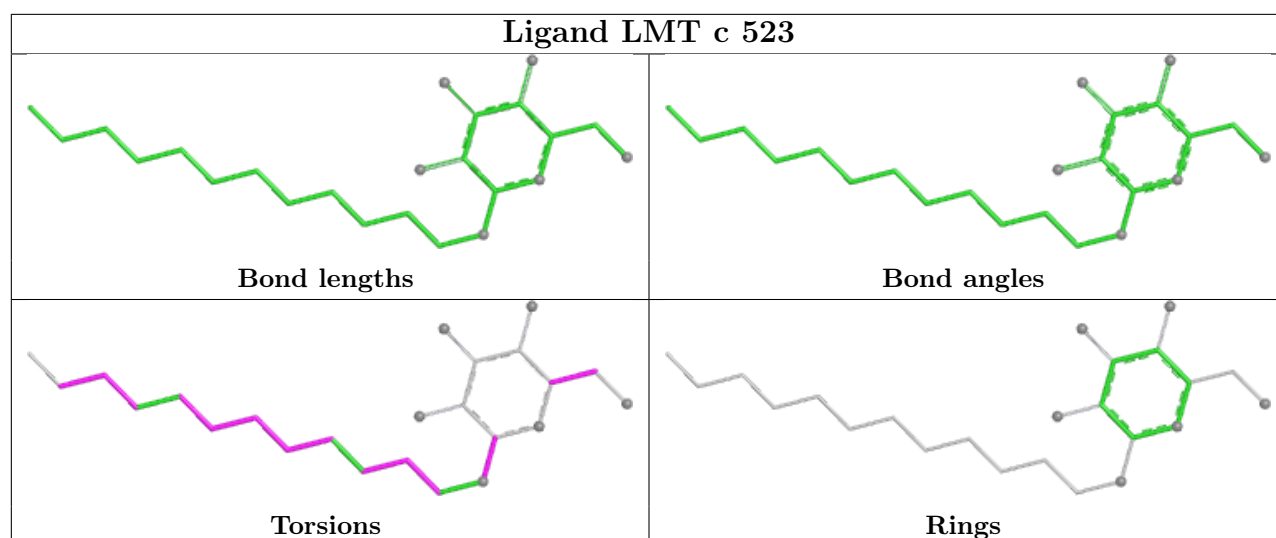


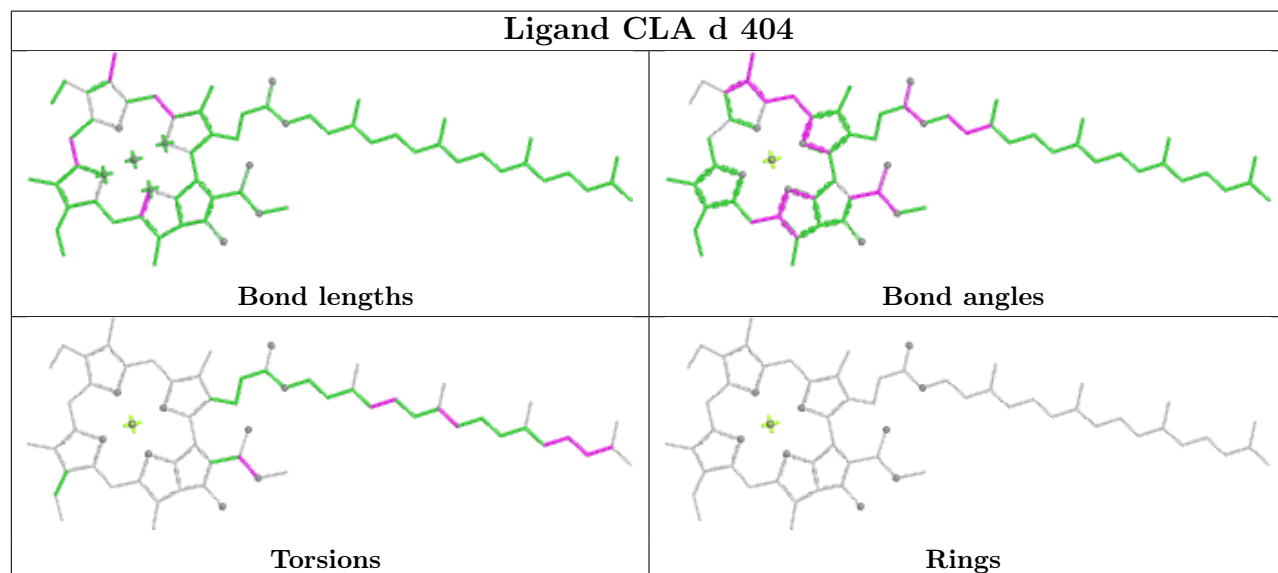
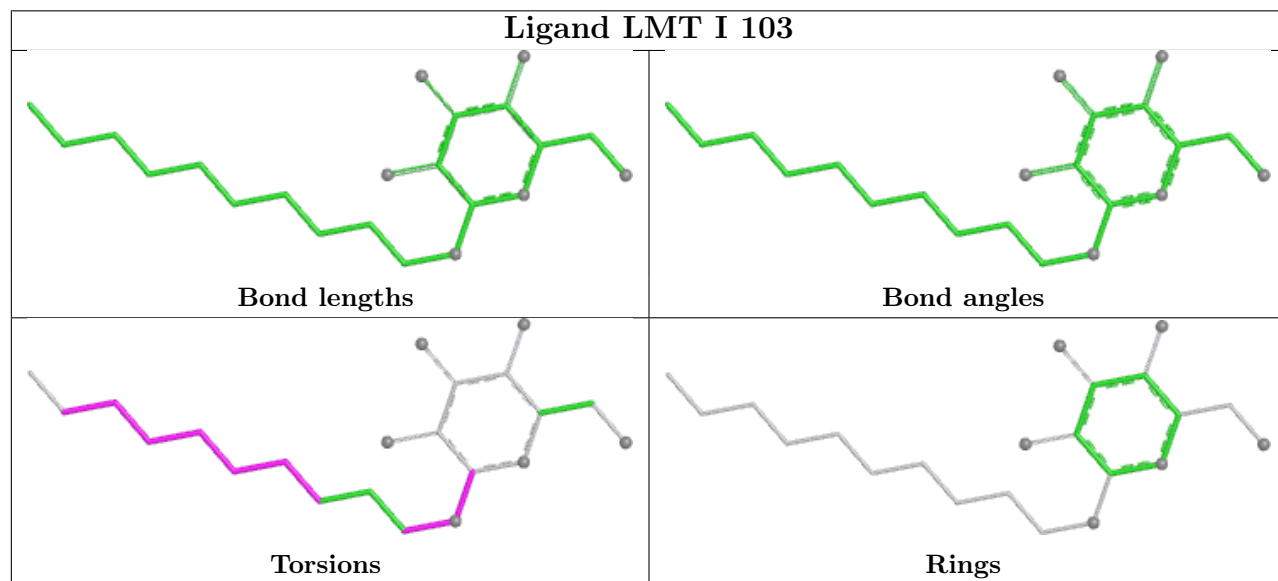
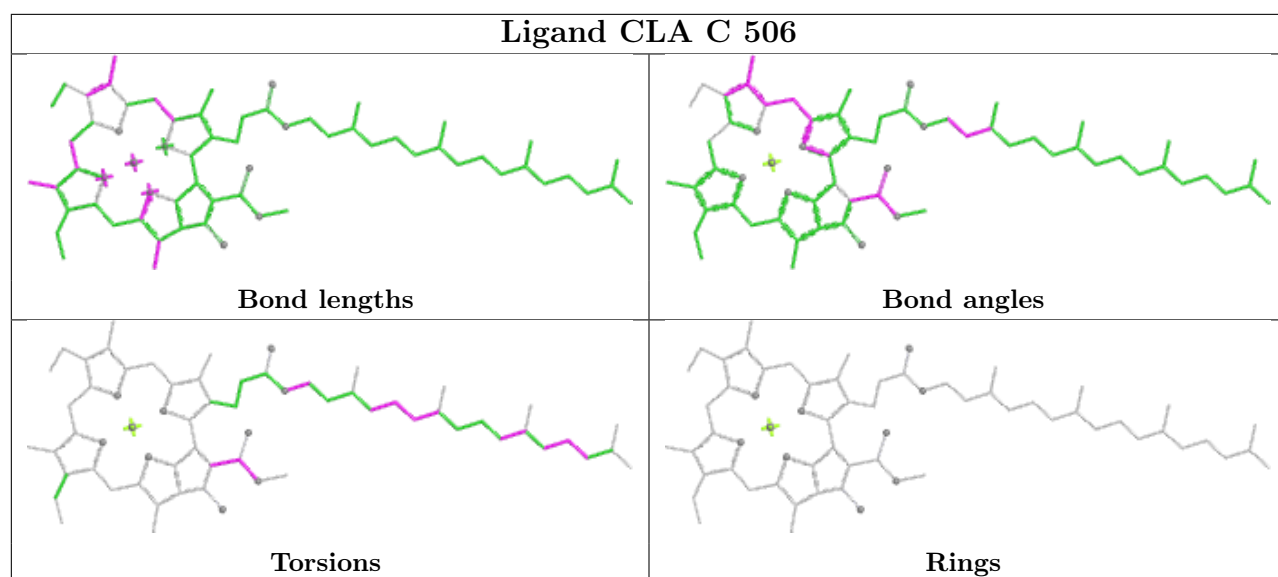




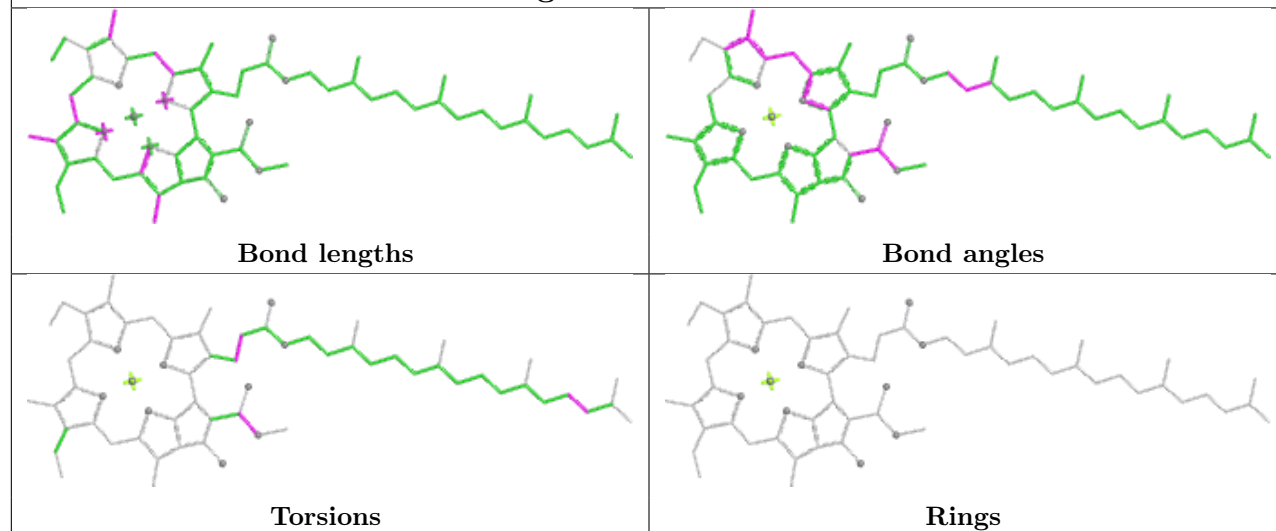




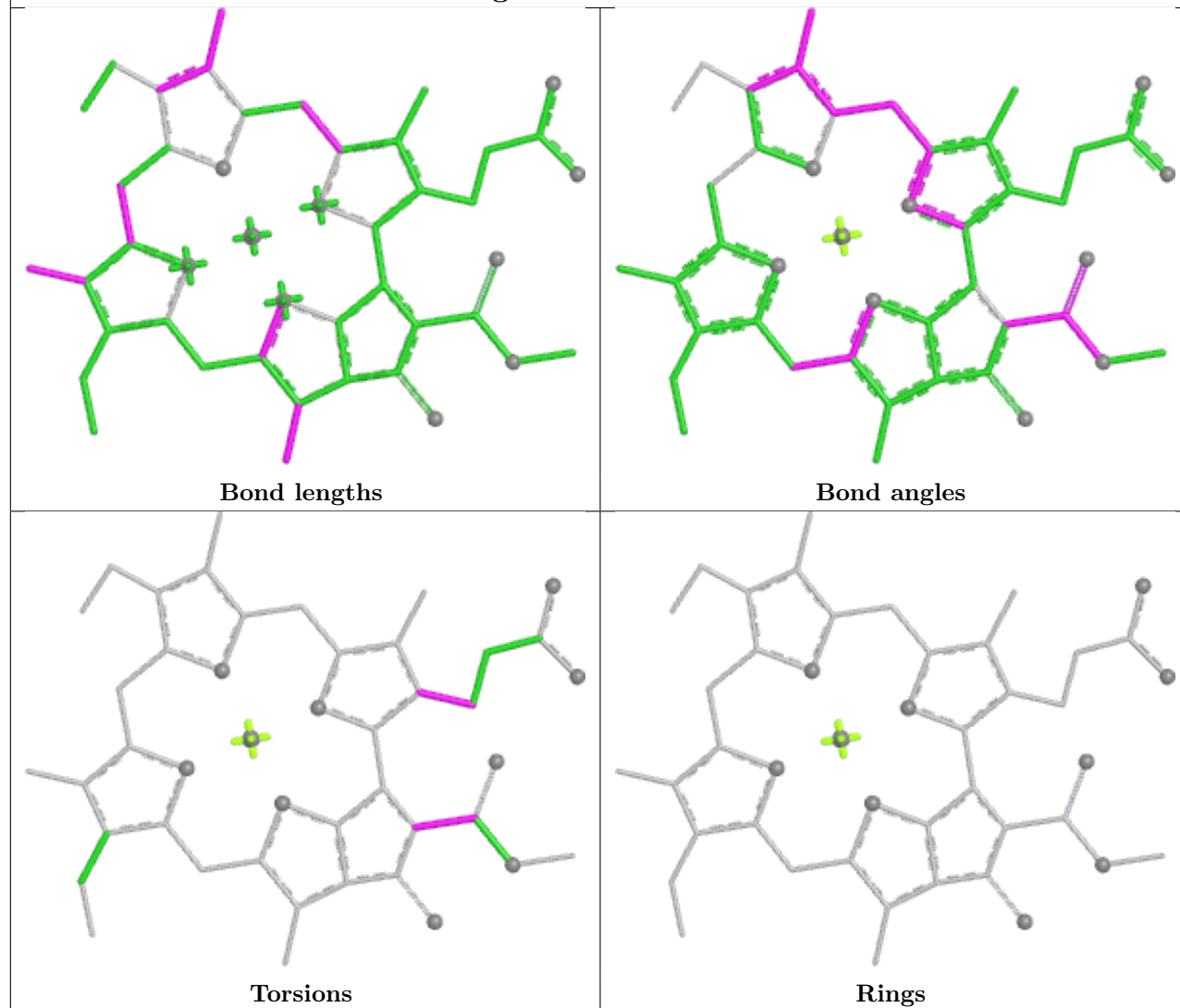


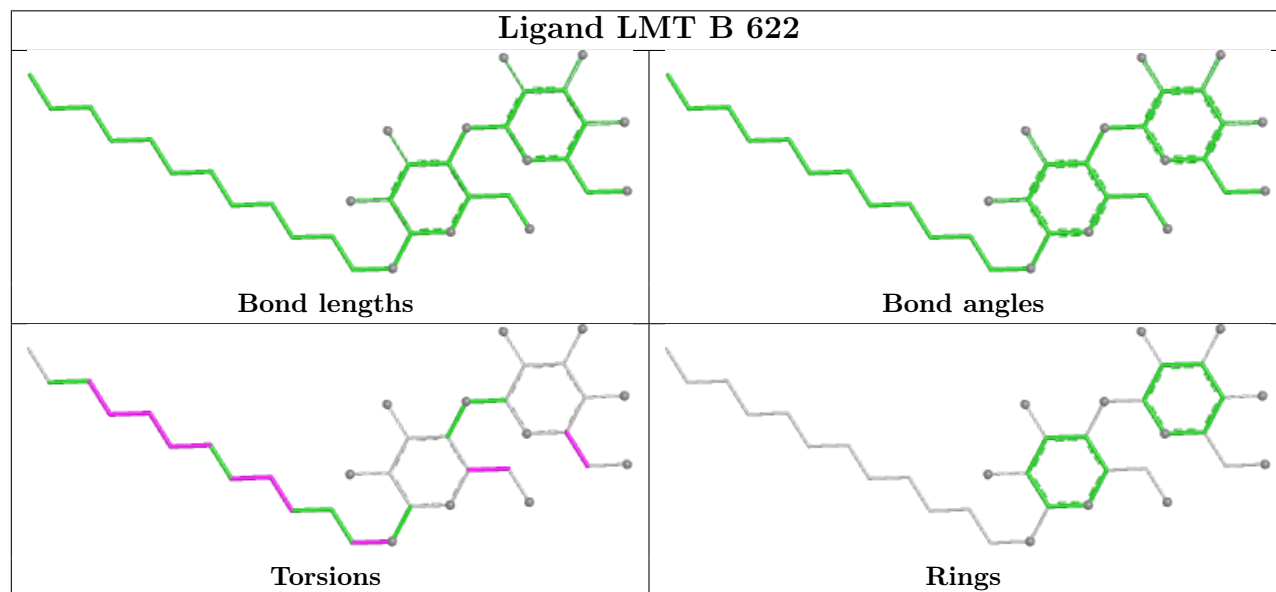
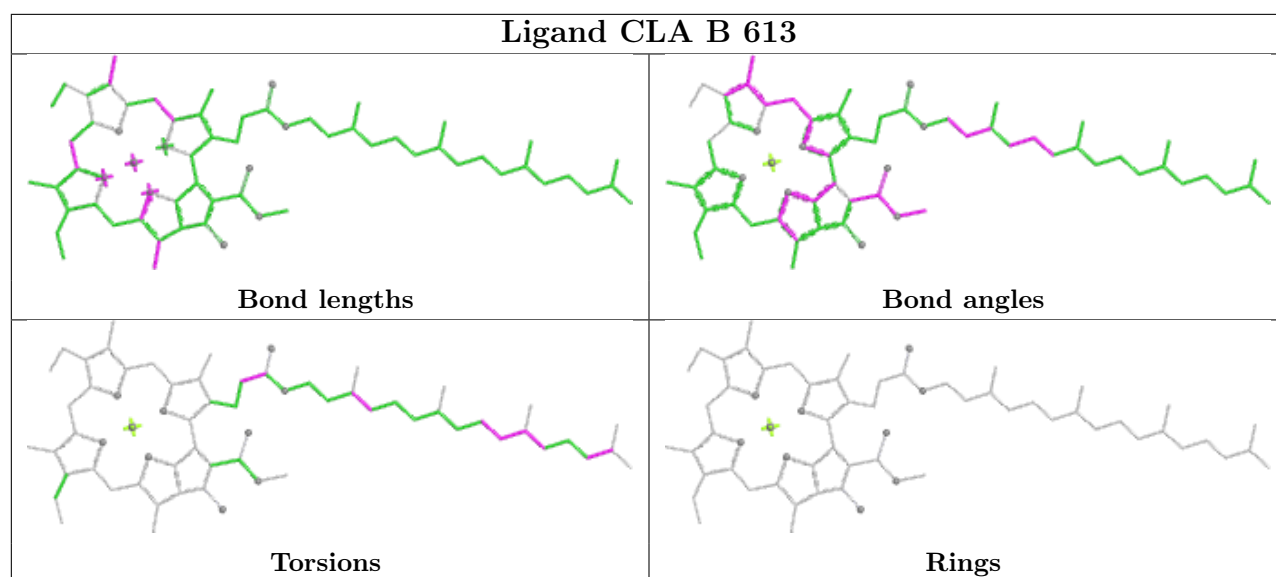


## Ligand CLA c 501

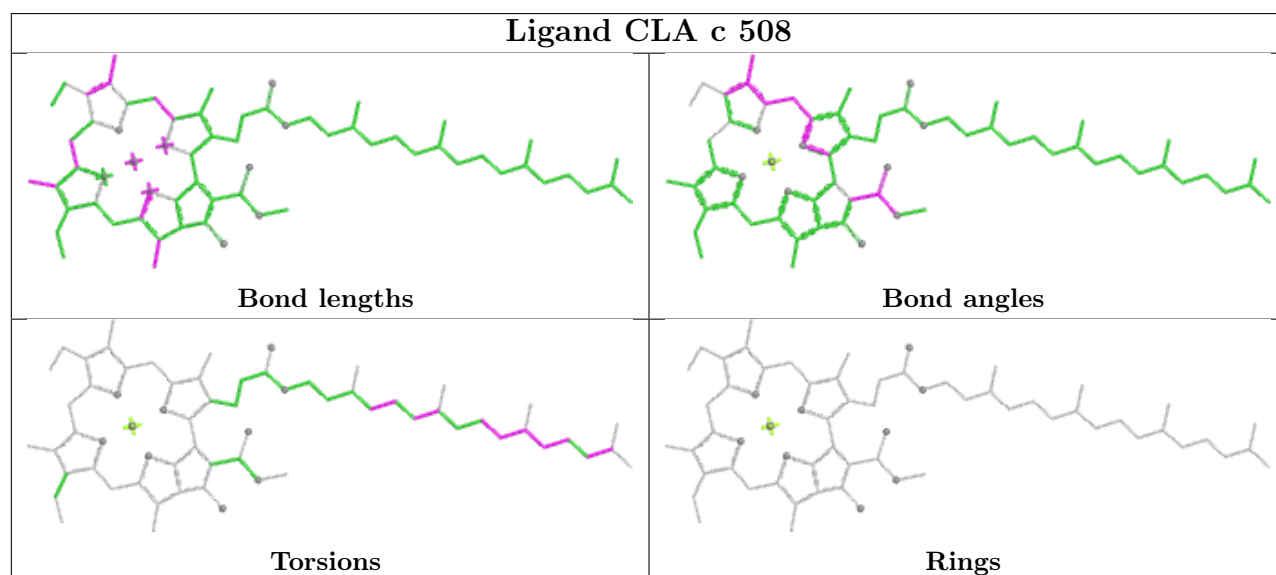
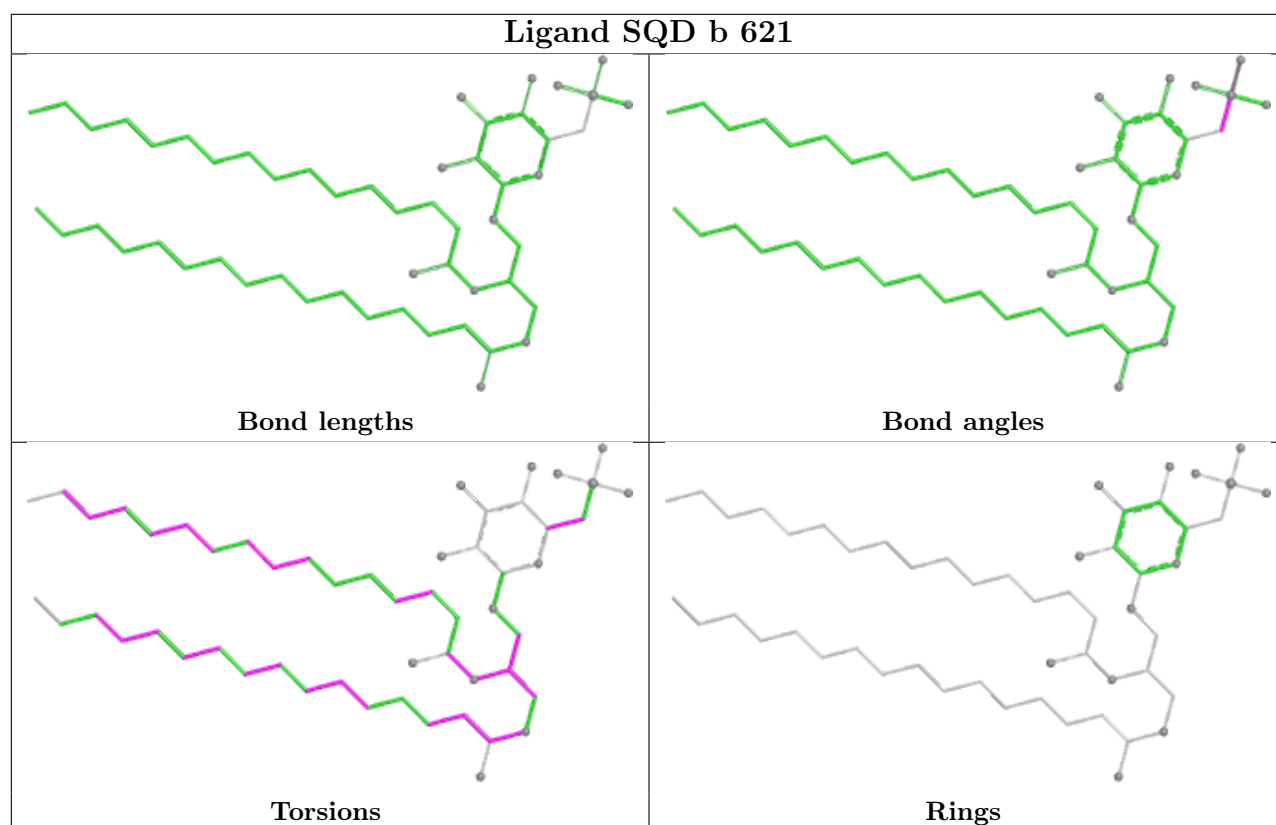


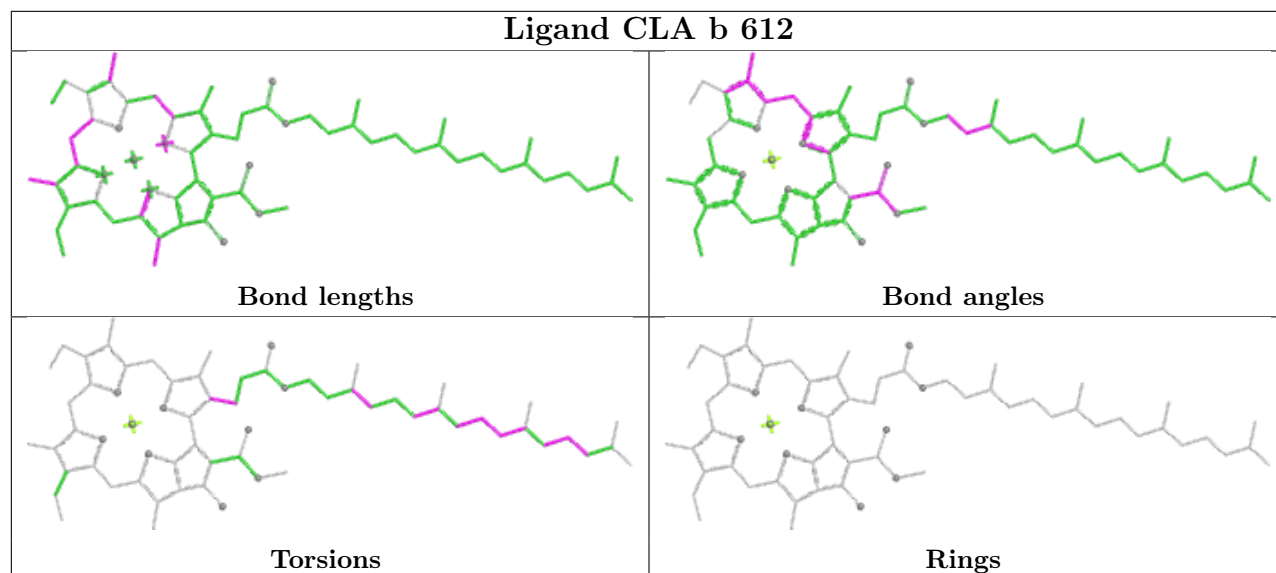
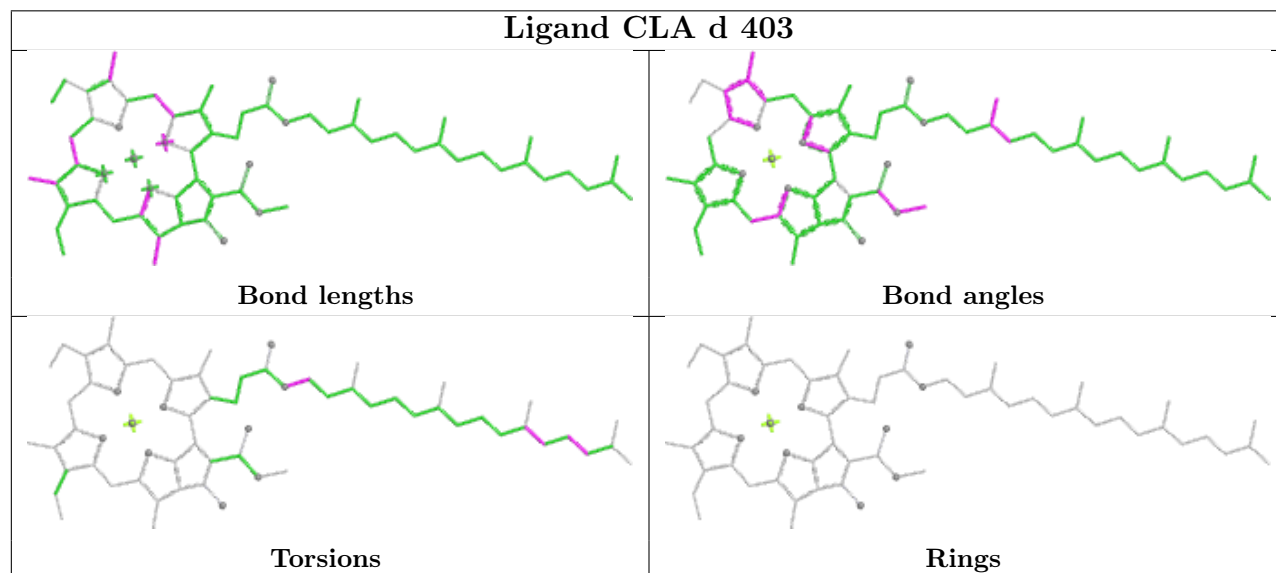
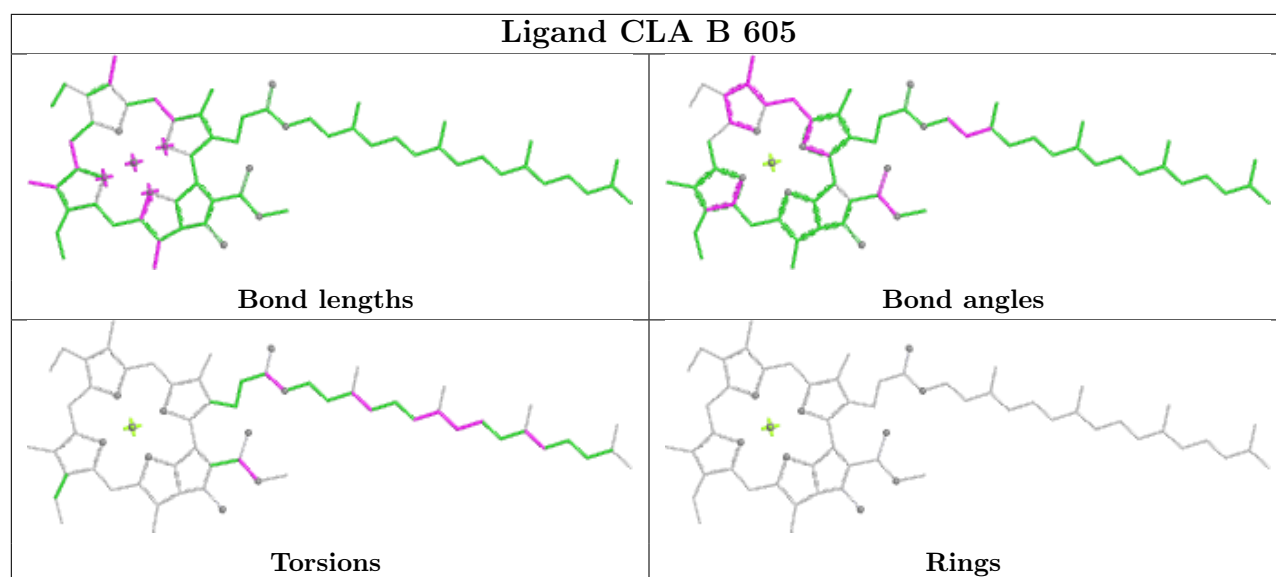
## Ligand CLA B 601

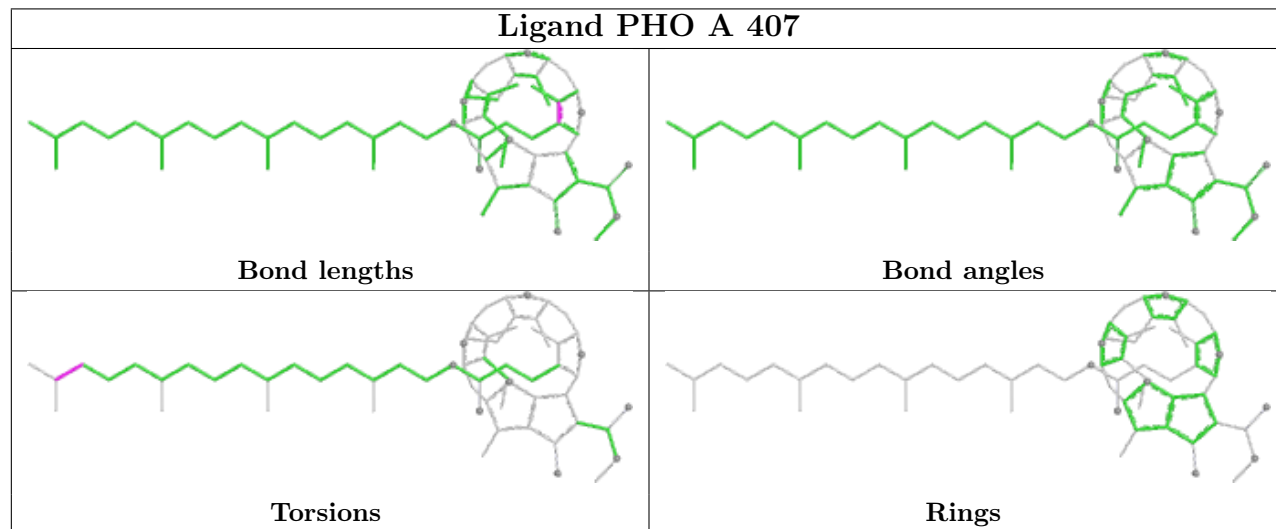
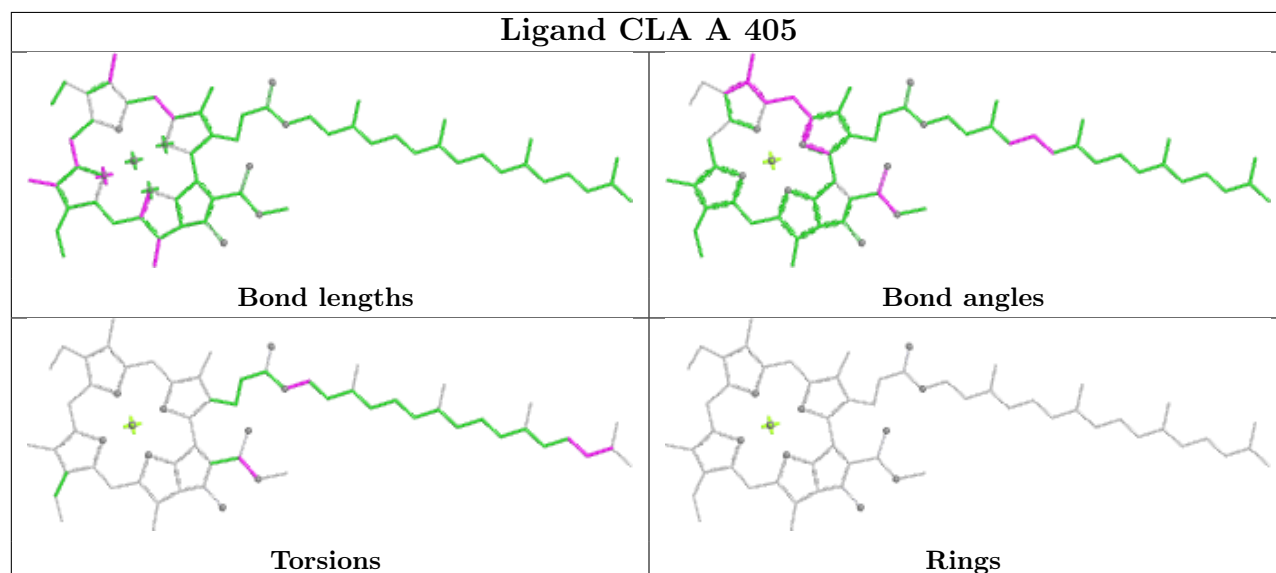
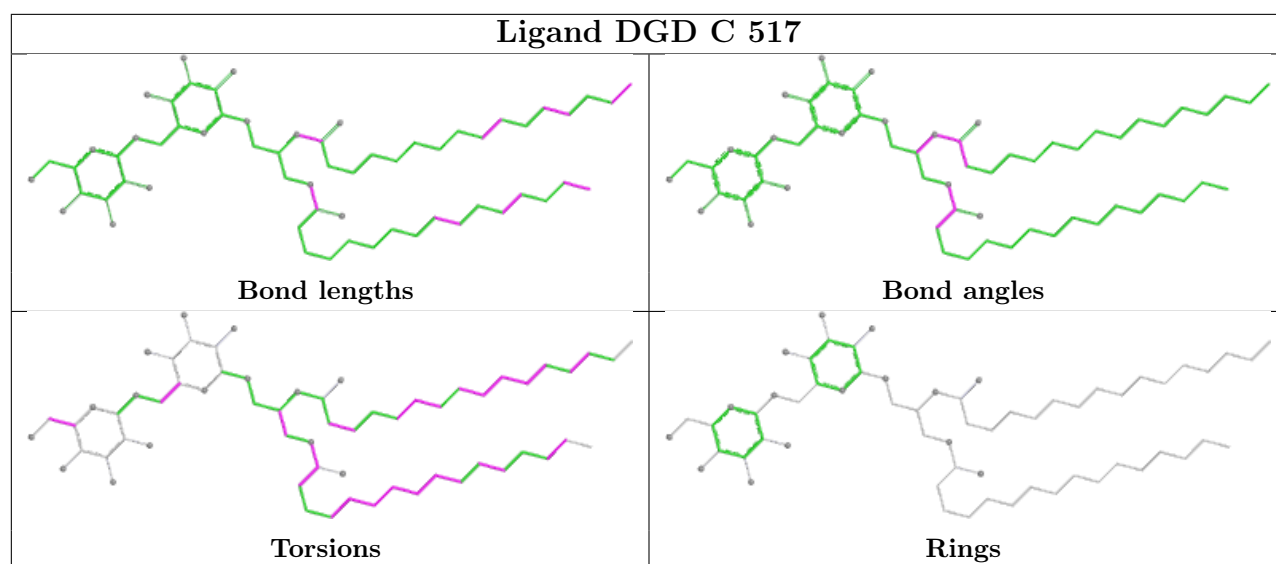


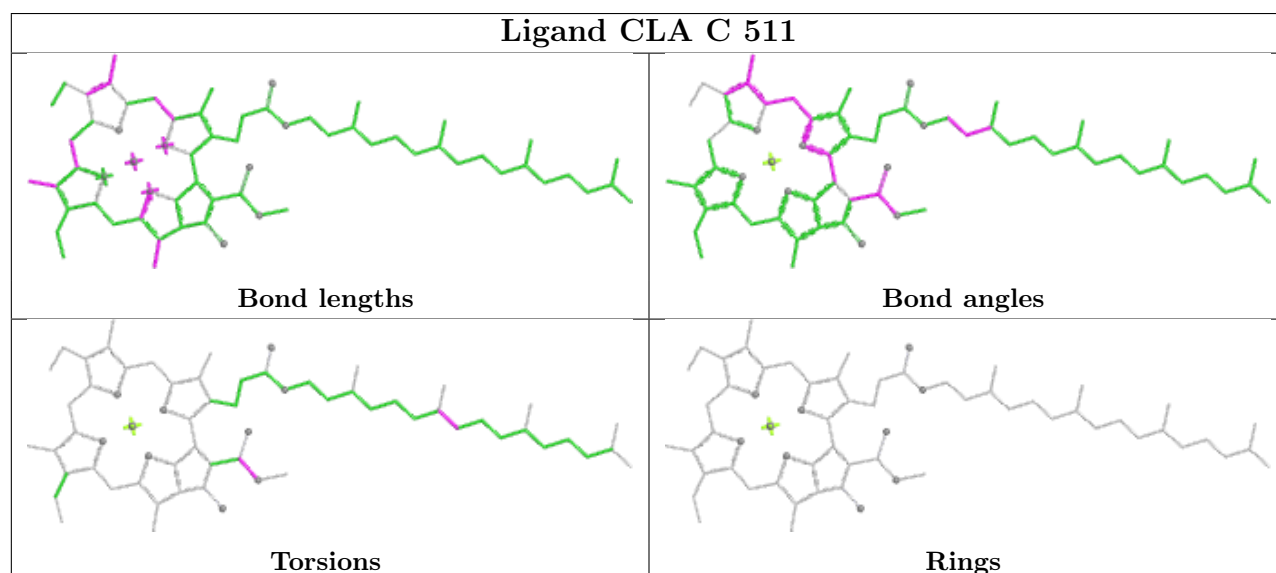
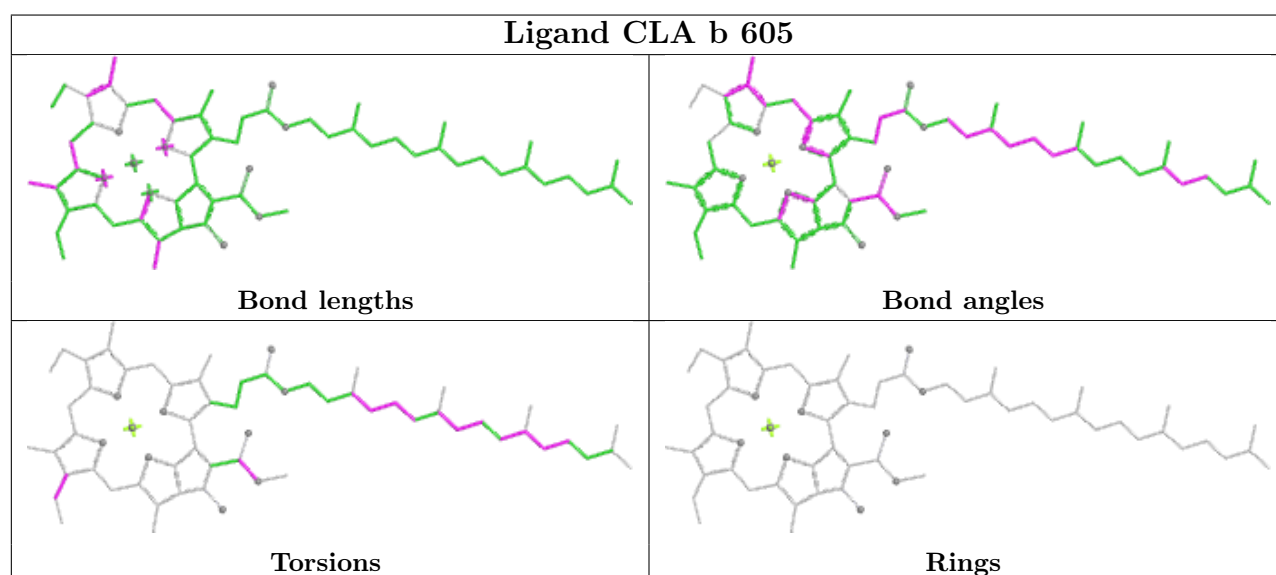
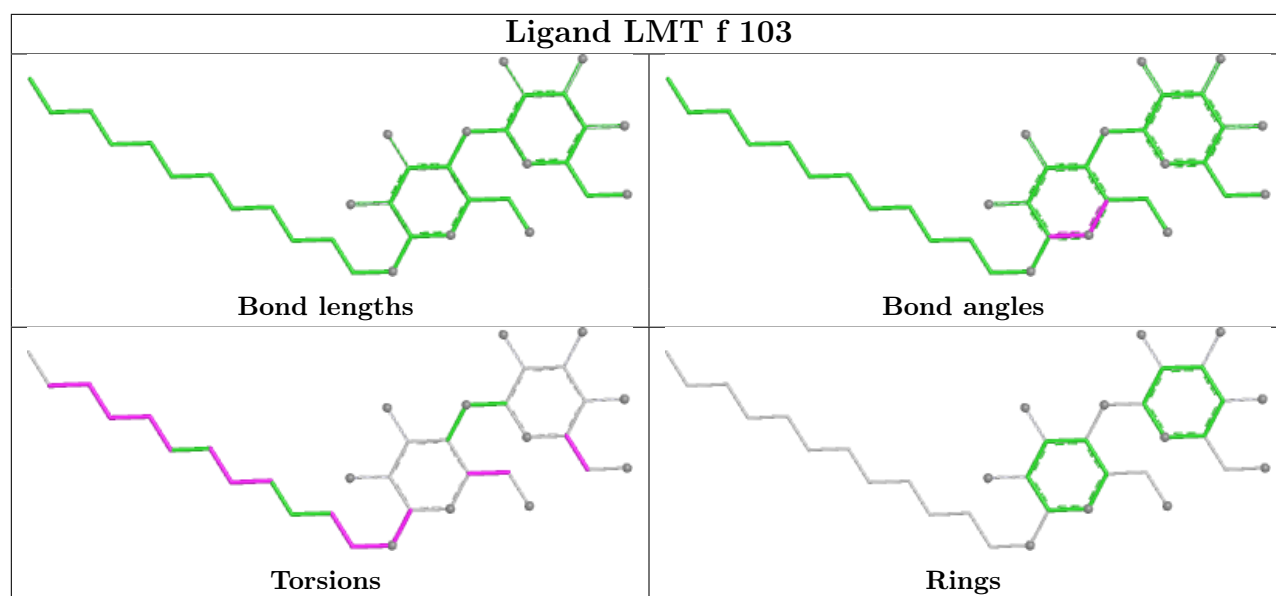


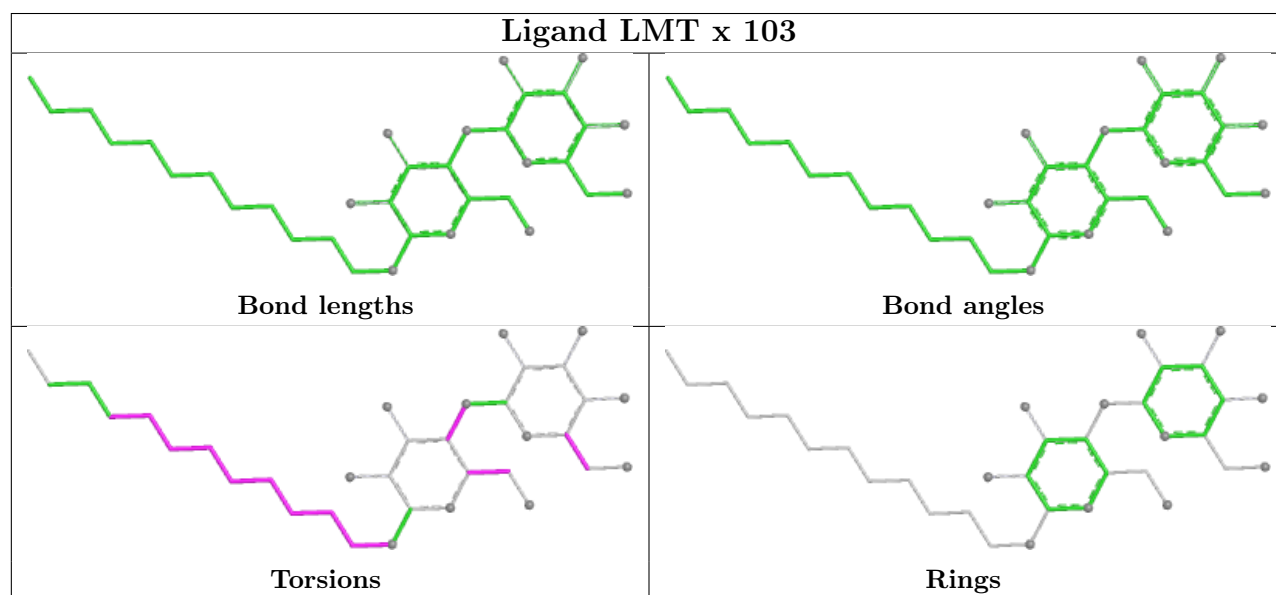
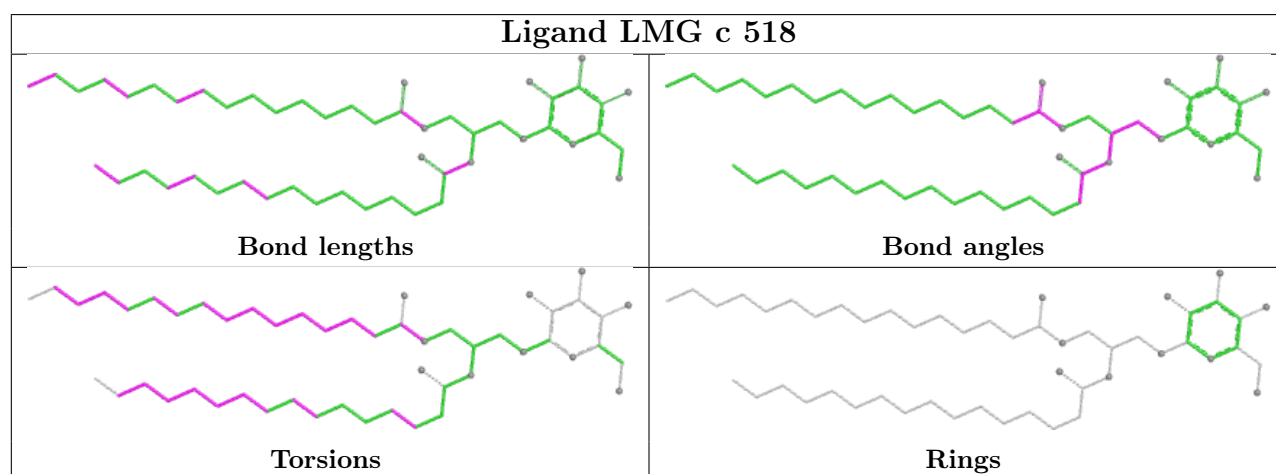
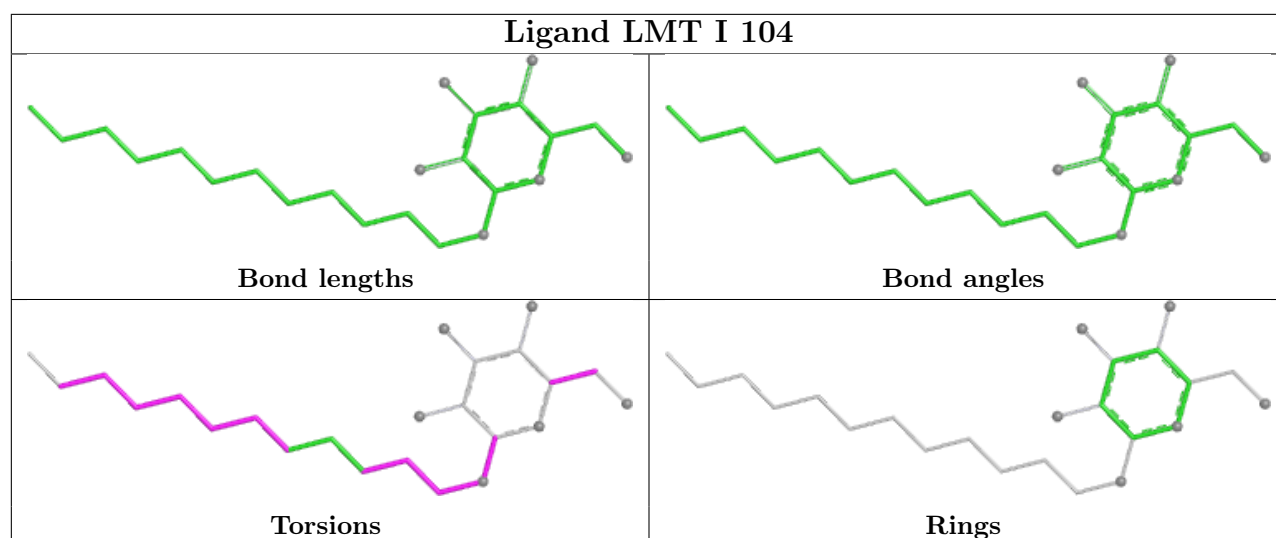


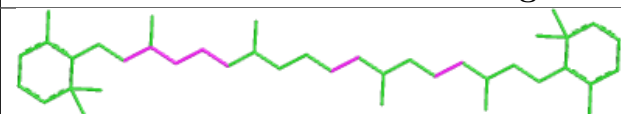
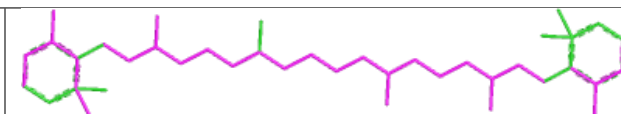
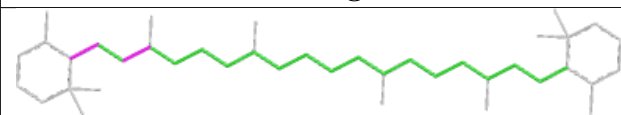
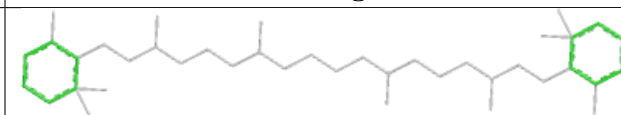

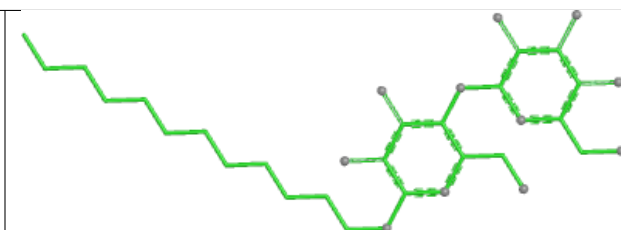
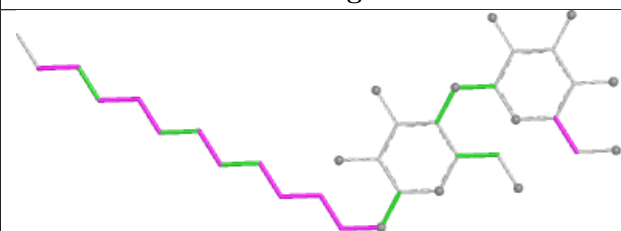
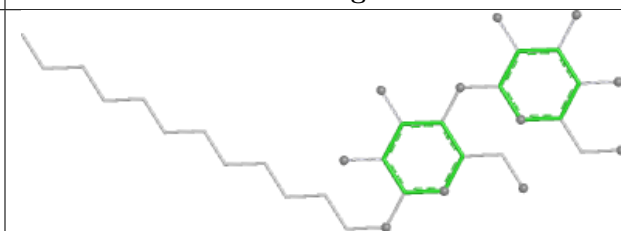
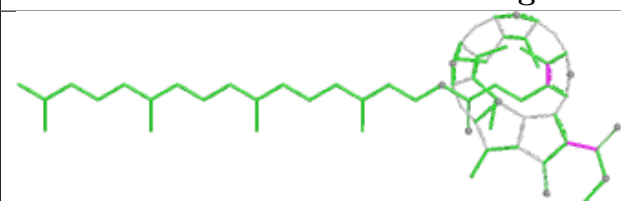
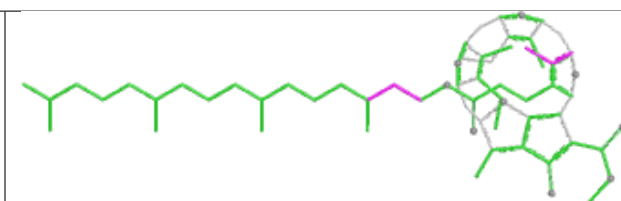
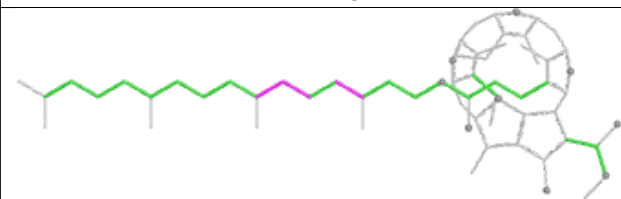
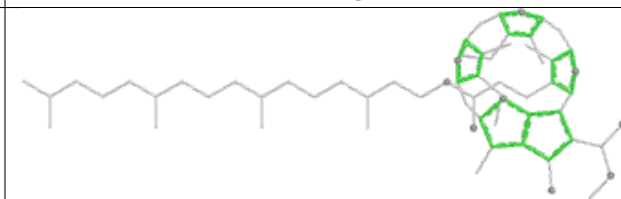


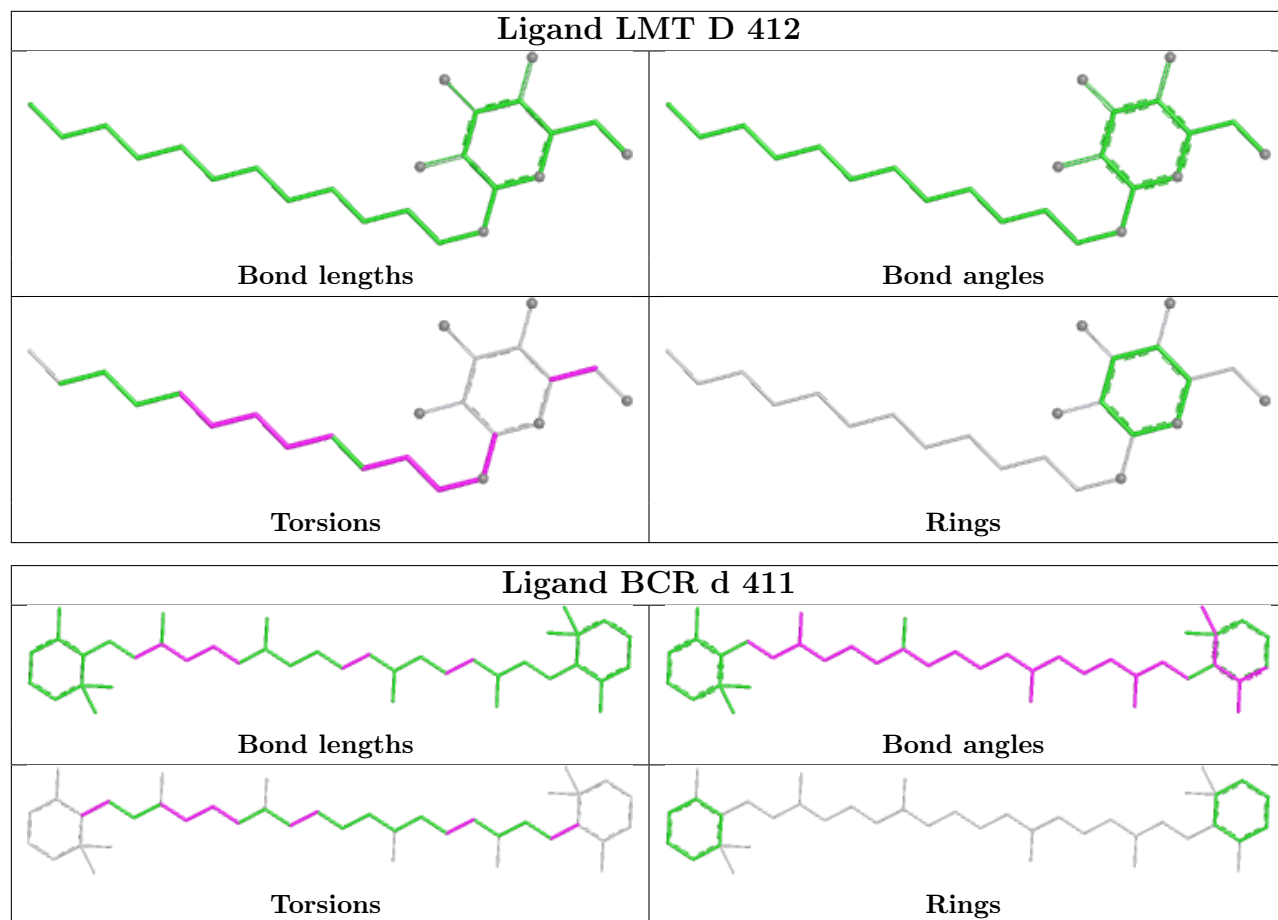




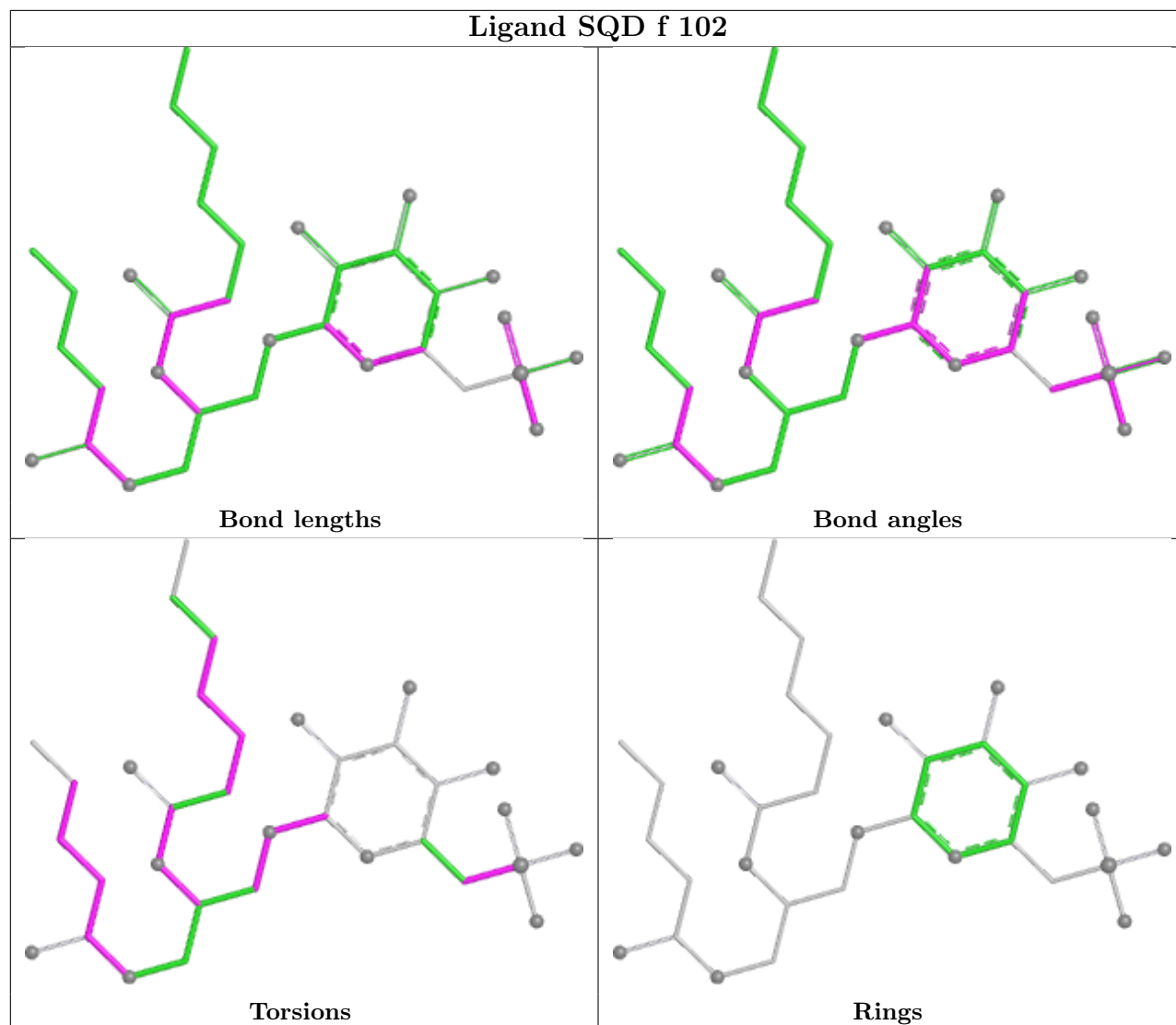




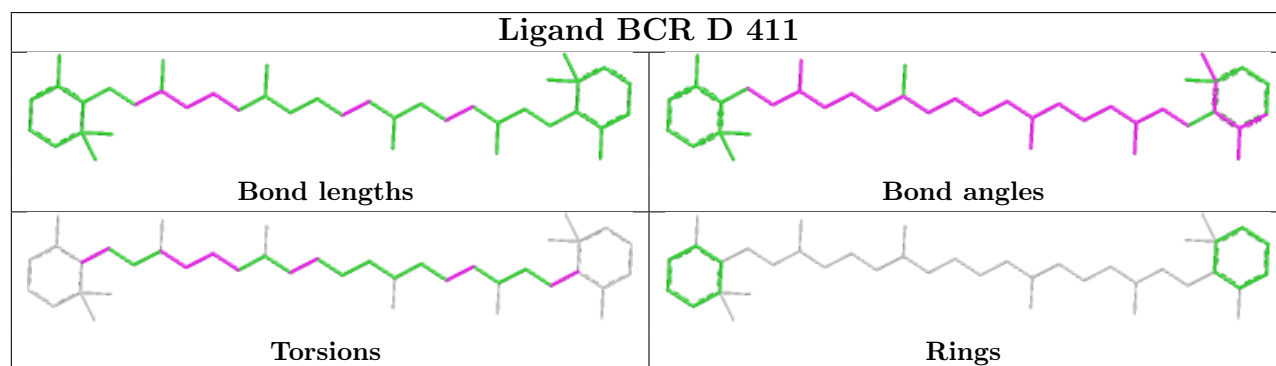
Ligand BCR C 527	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LMT A 414	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PHO D 402	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



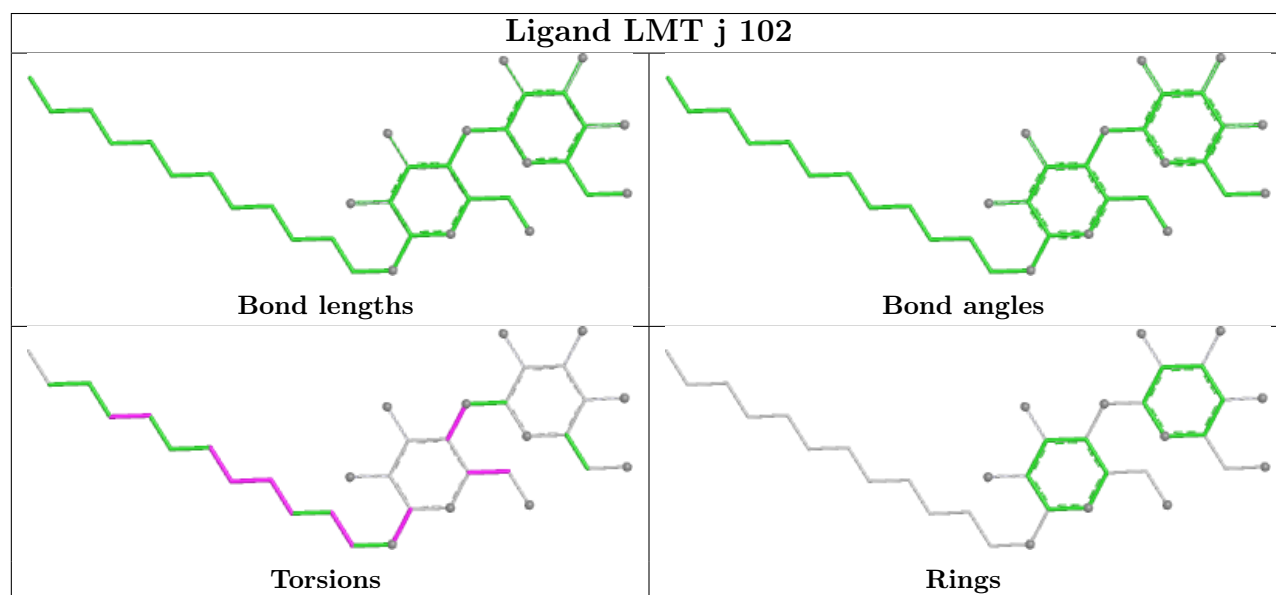
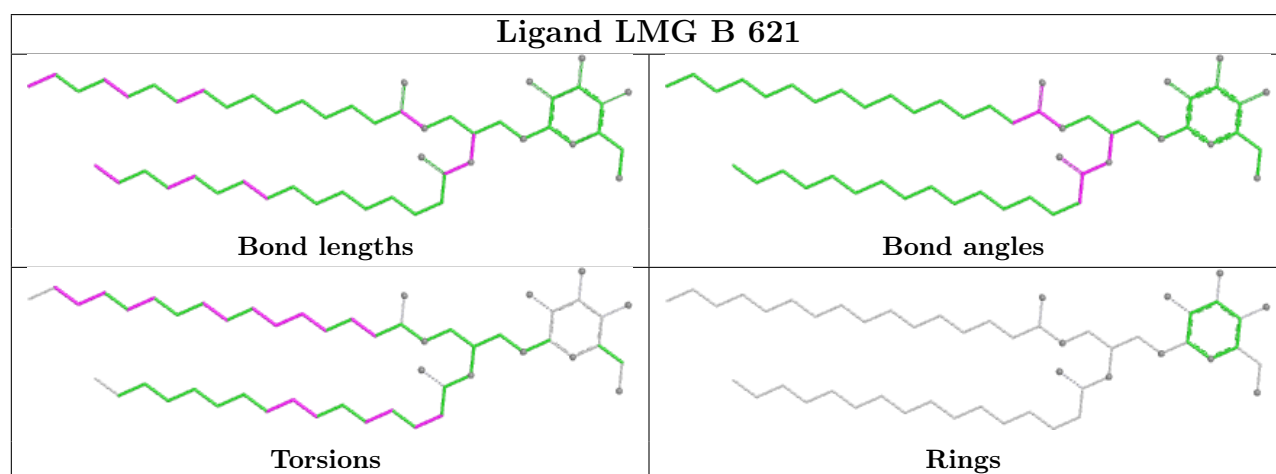
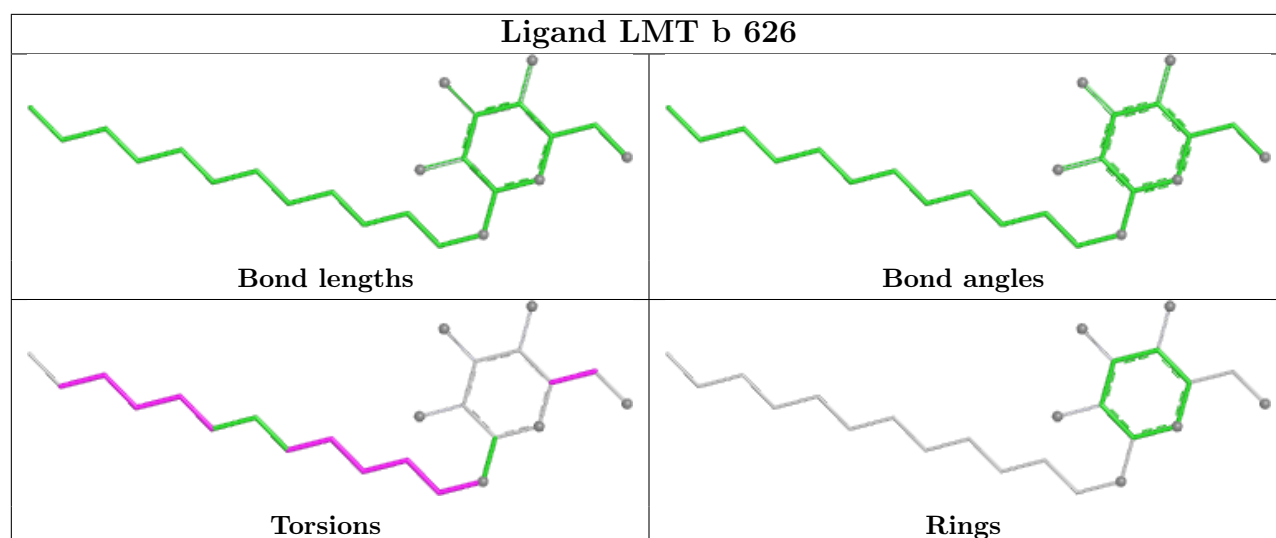
## Ligand SQD f 102

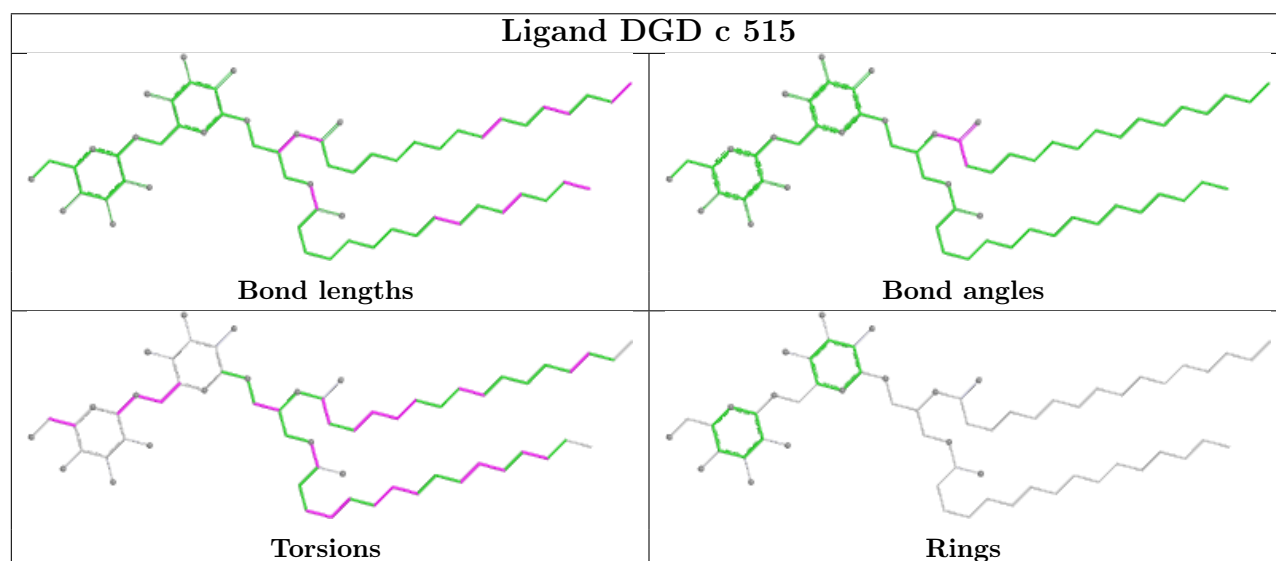
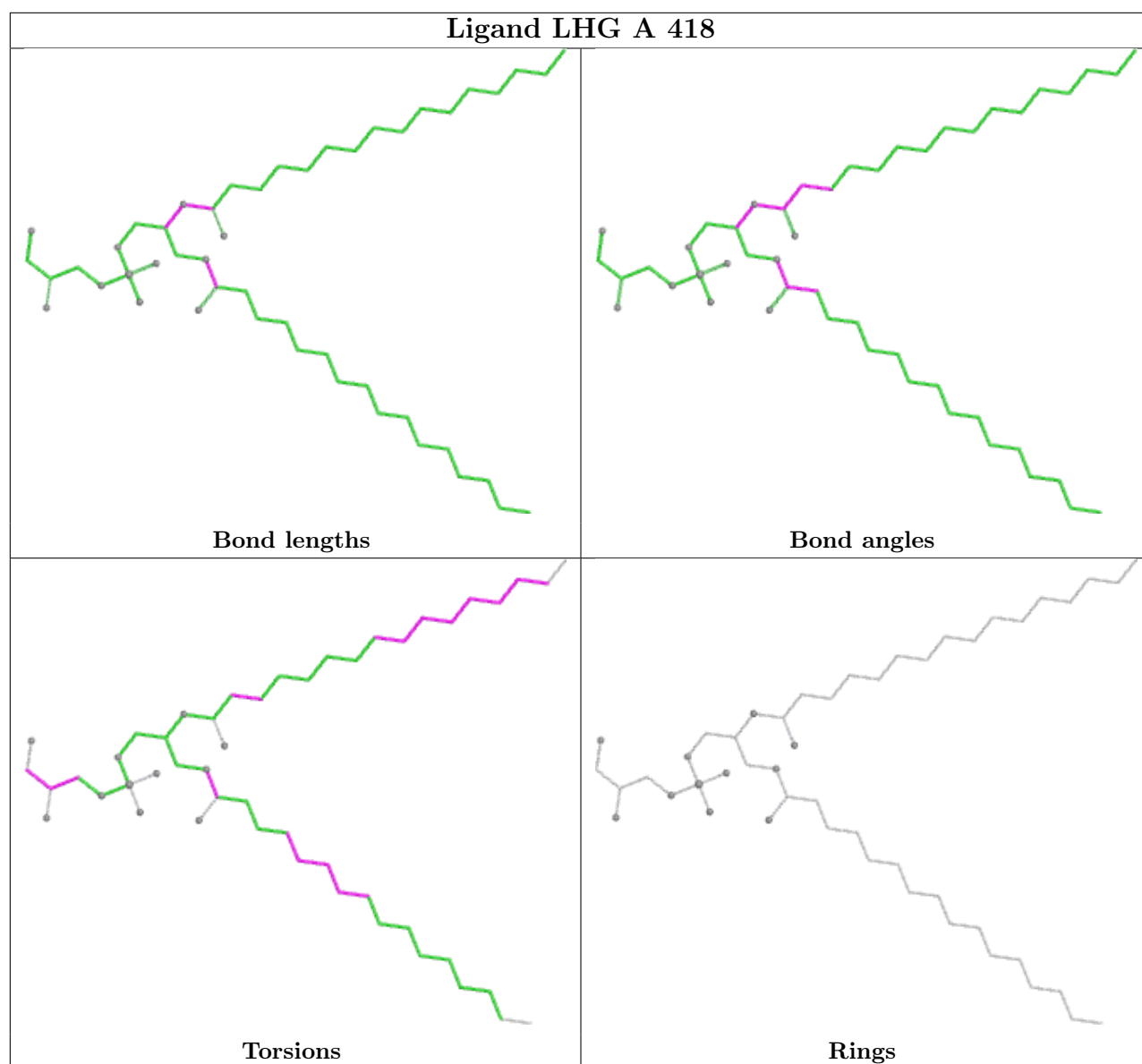



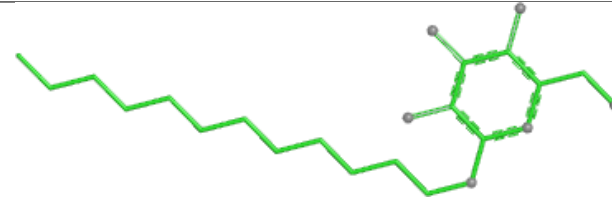
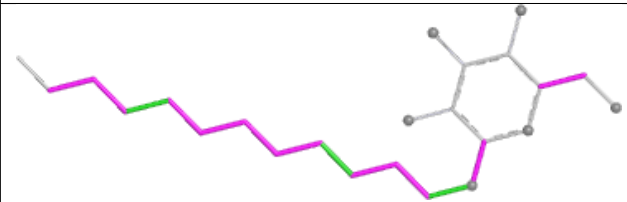
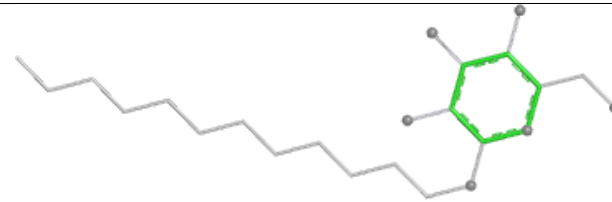
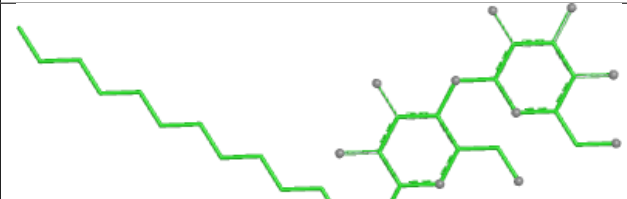
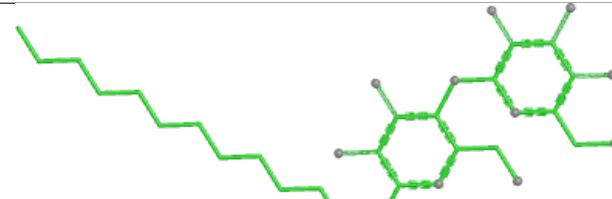
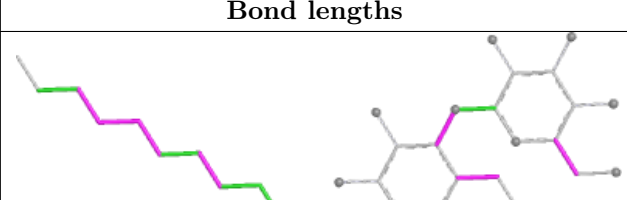
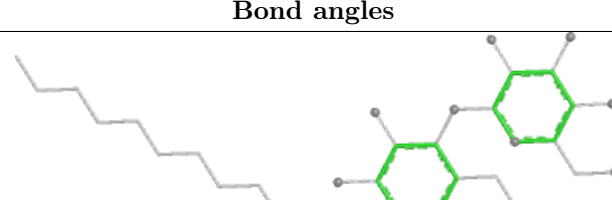
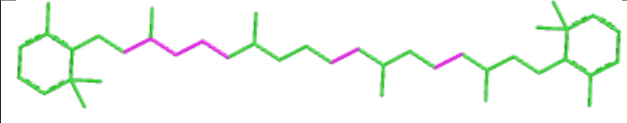
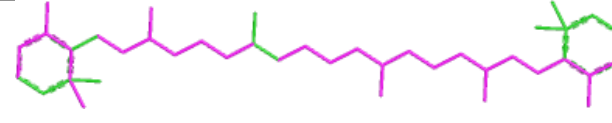
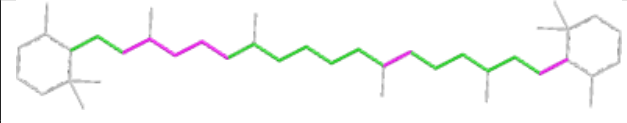
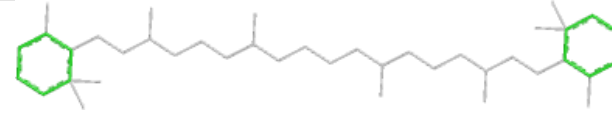
## Ligand BCR D 411

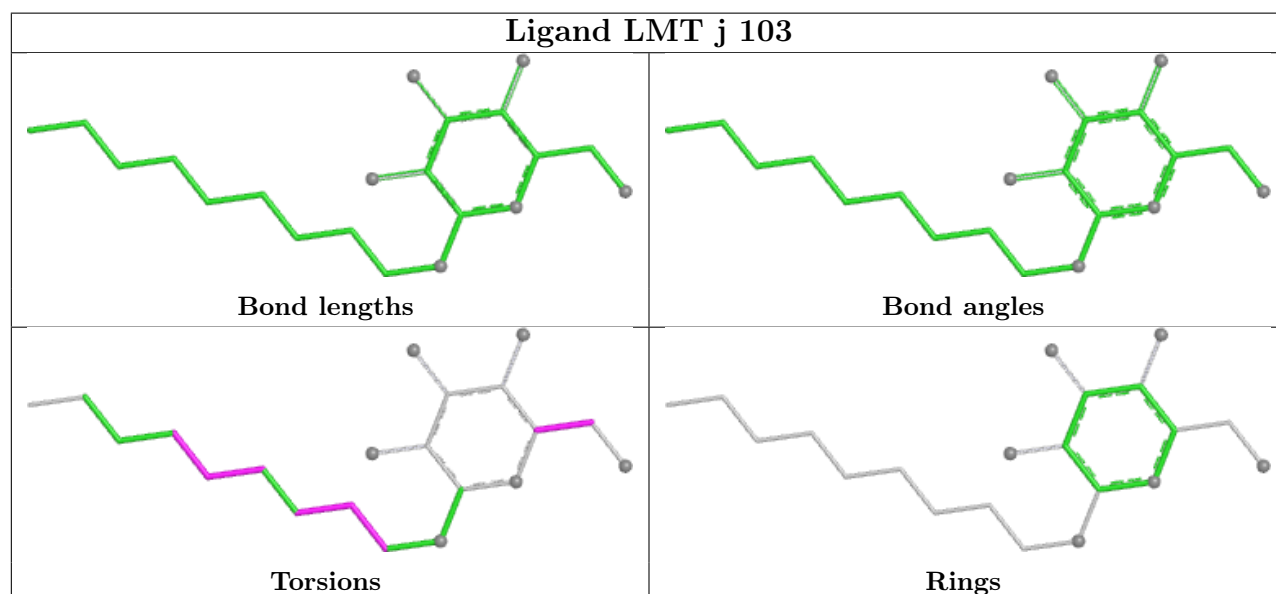
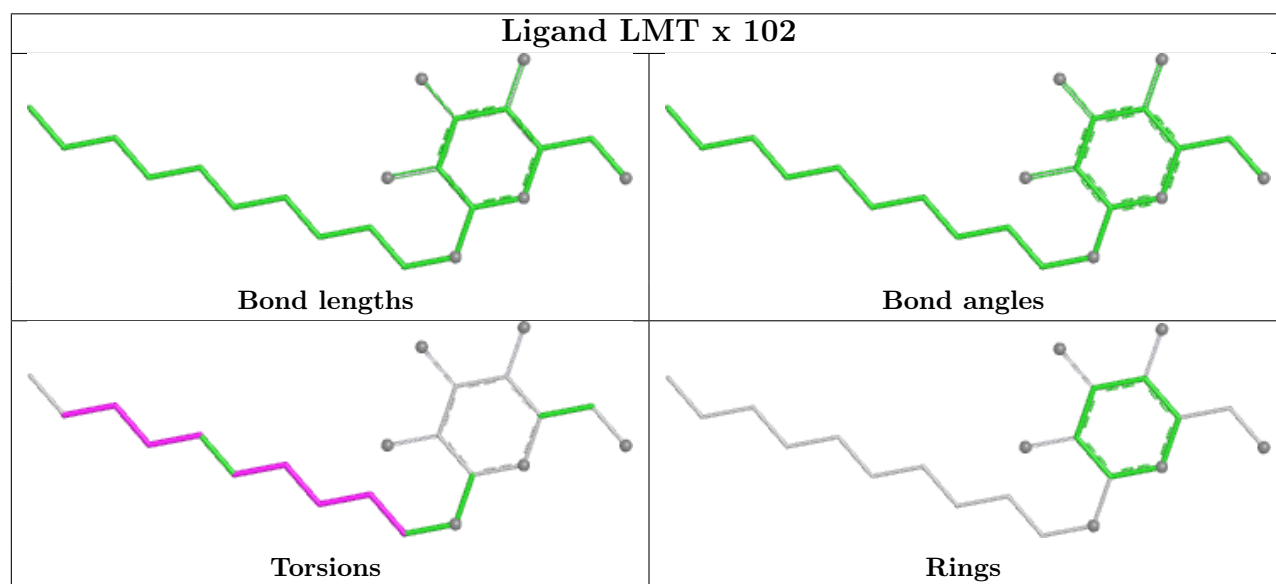
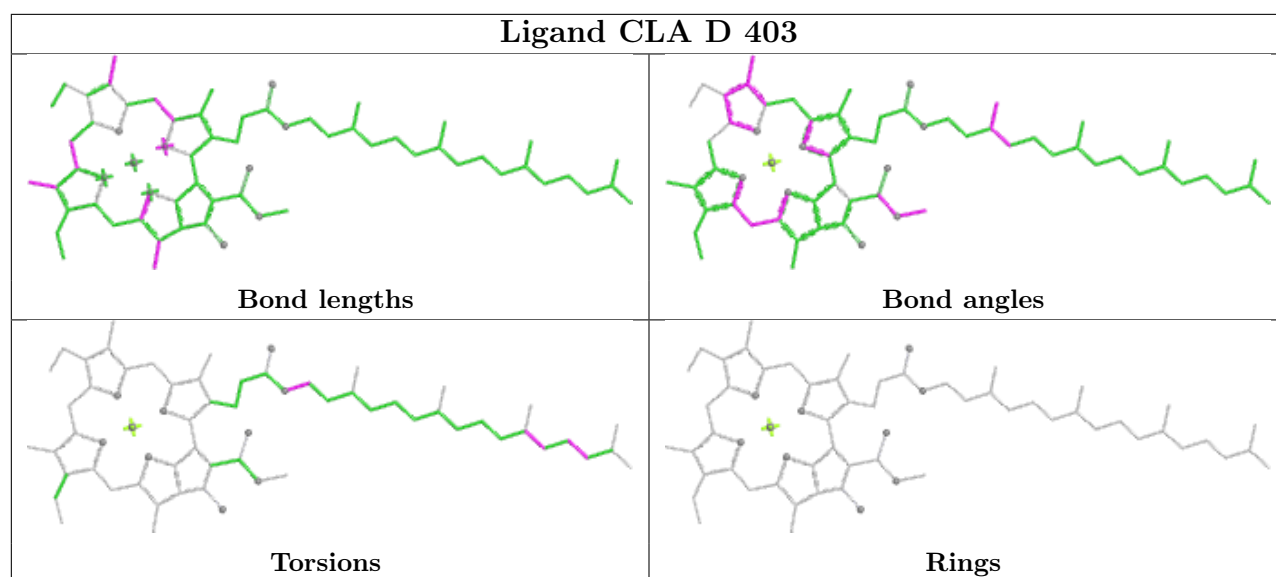


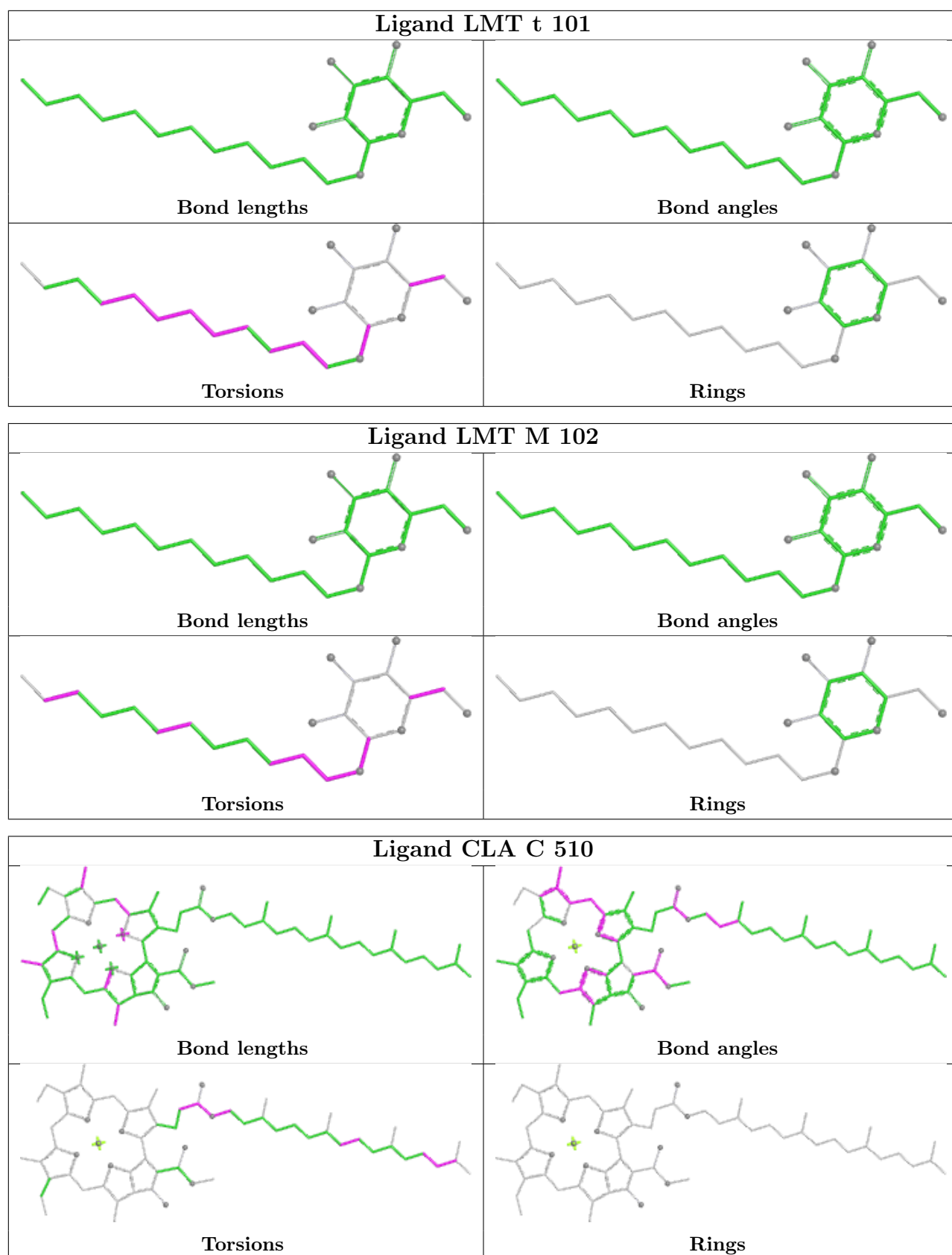


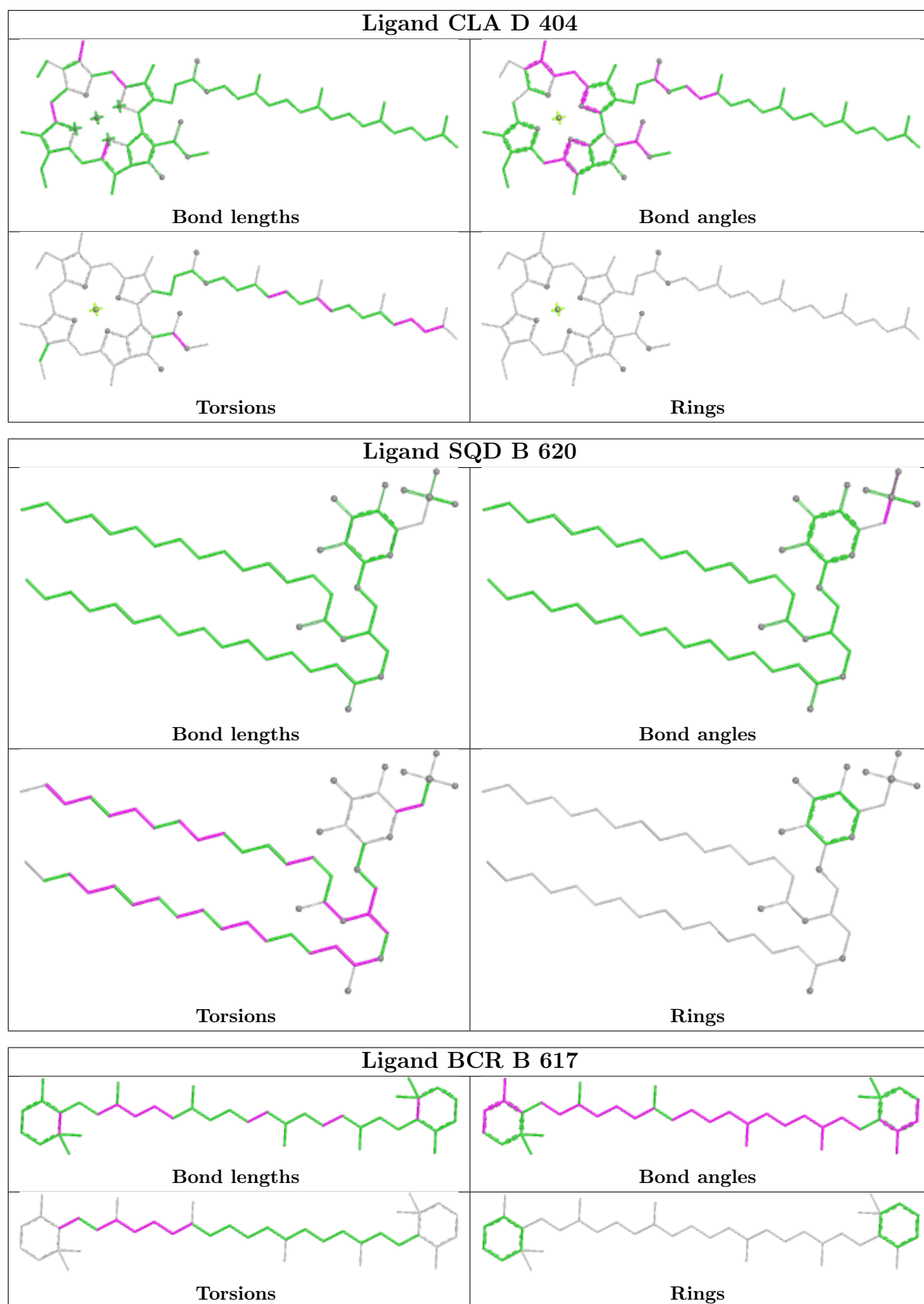


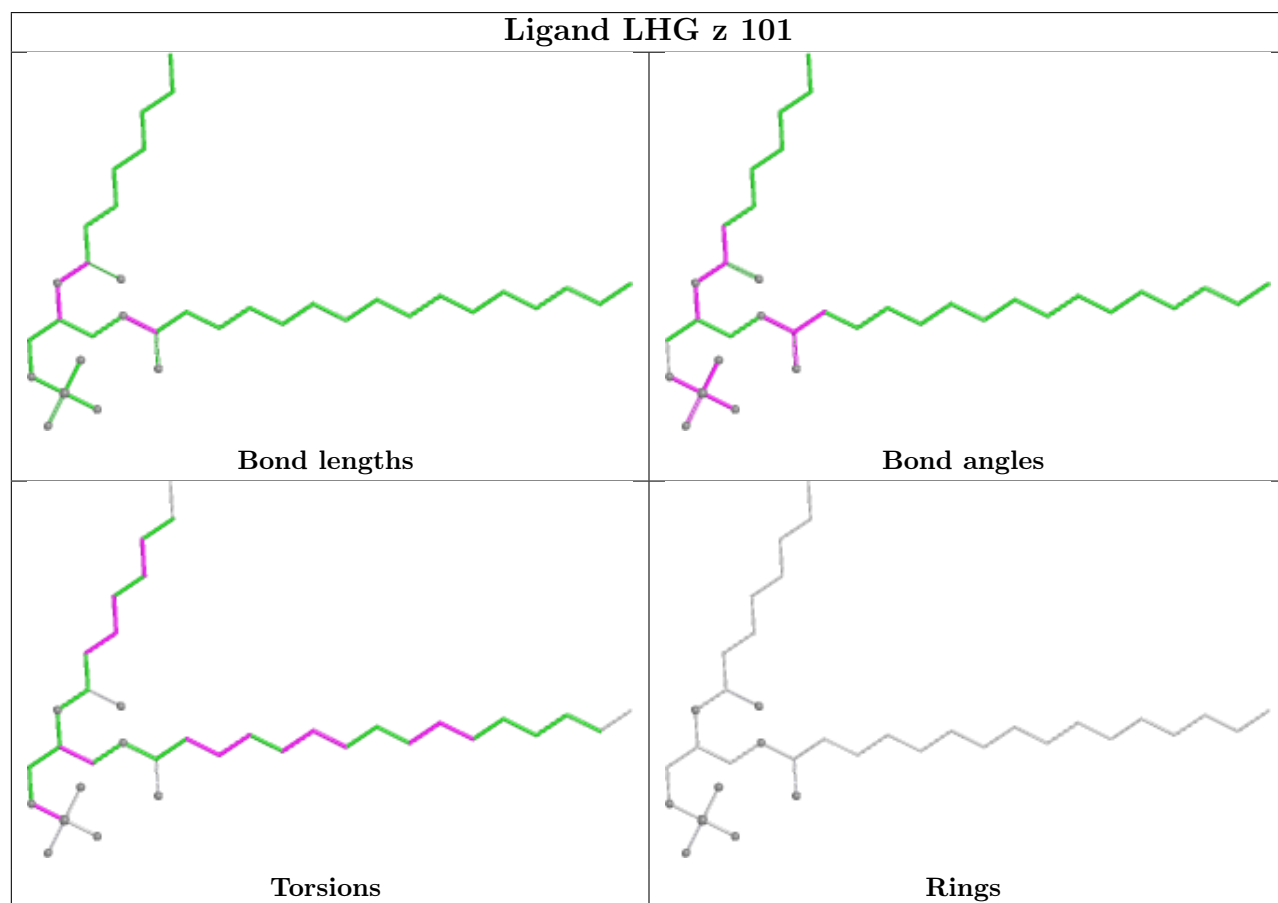
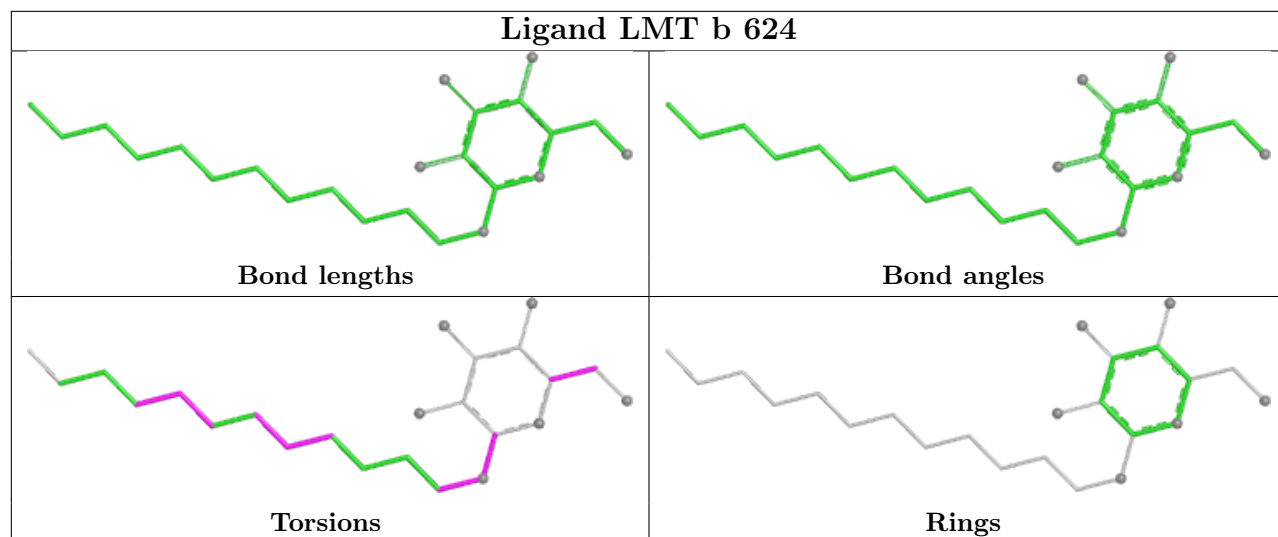


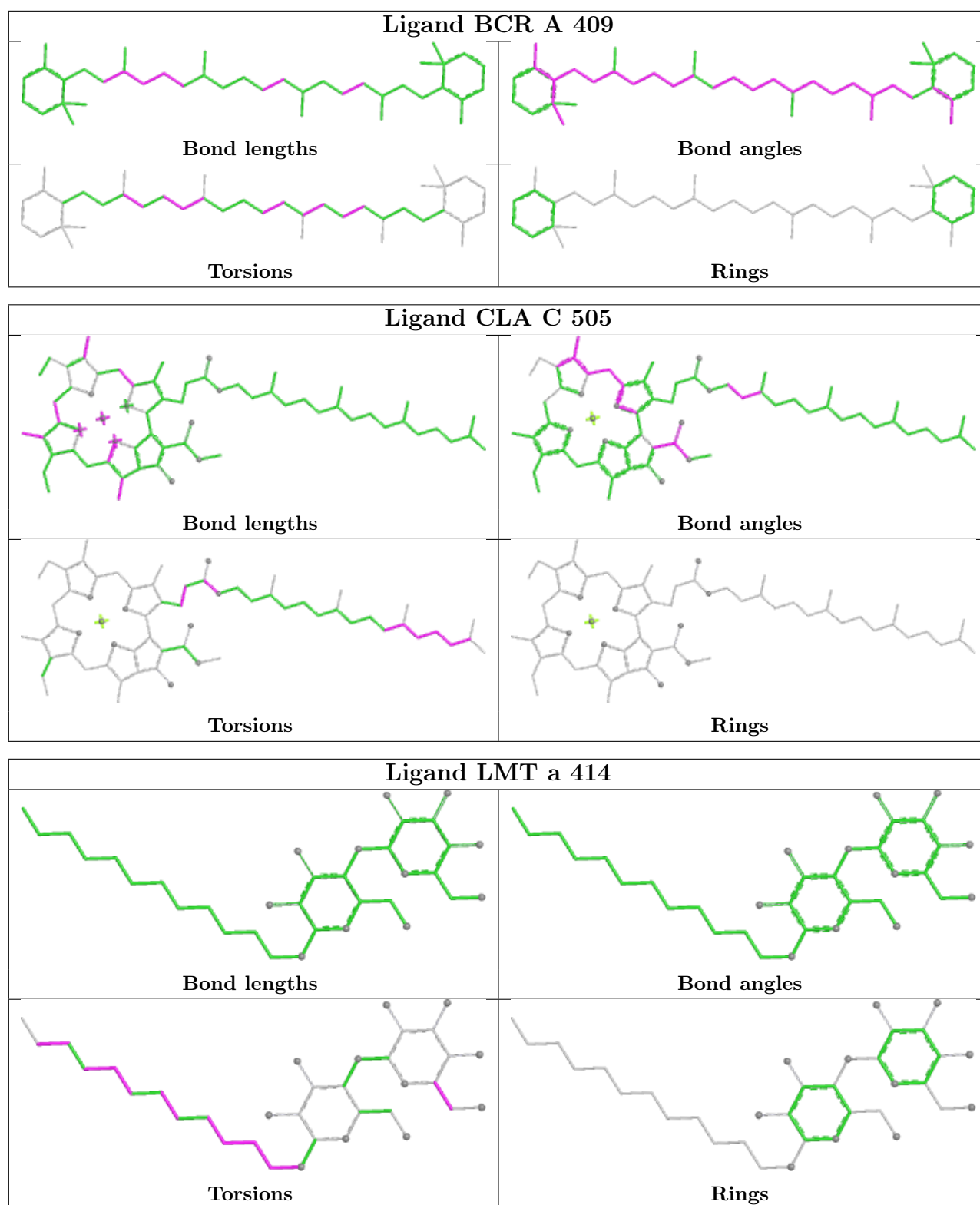
Ligand LMT C 523	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LMT e 103	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR c 514	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



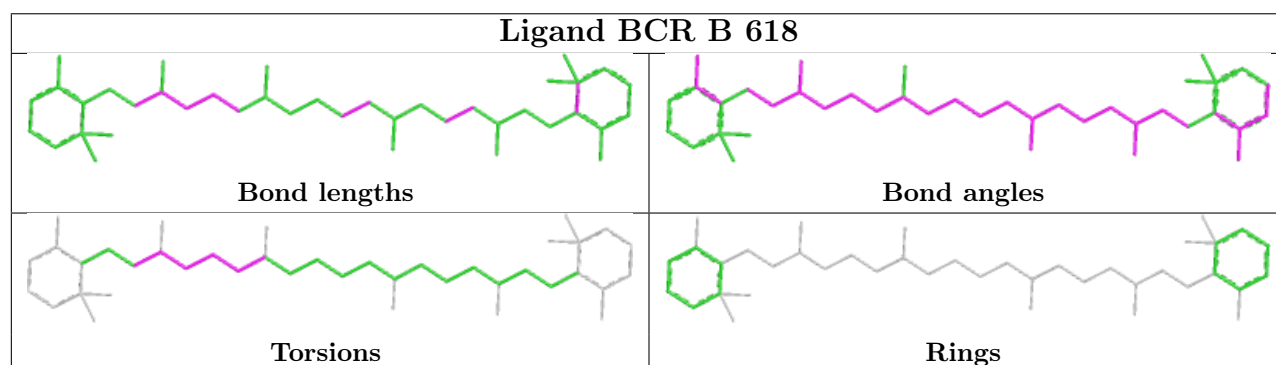
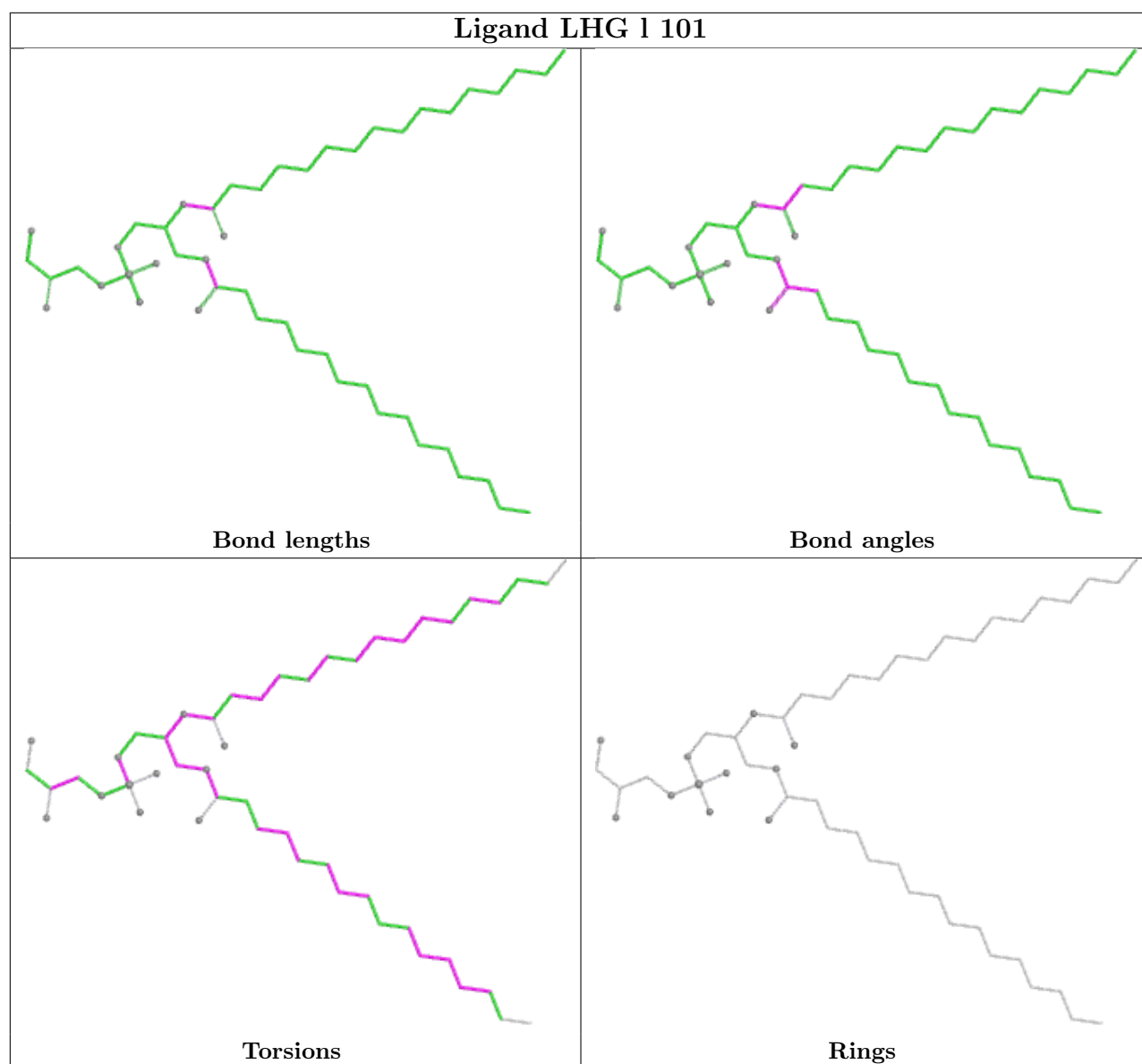


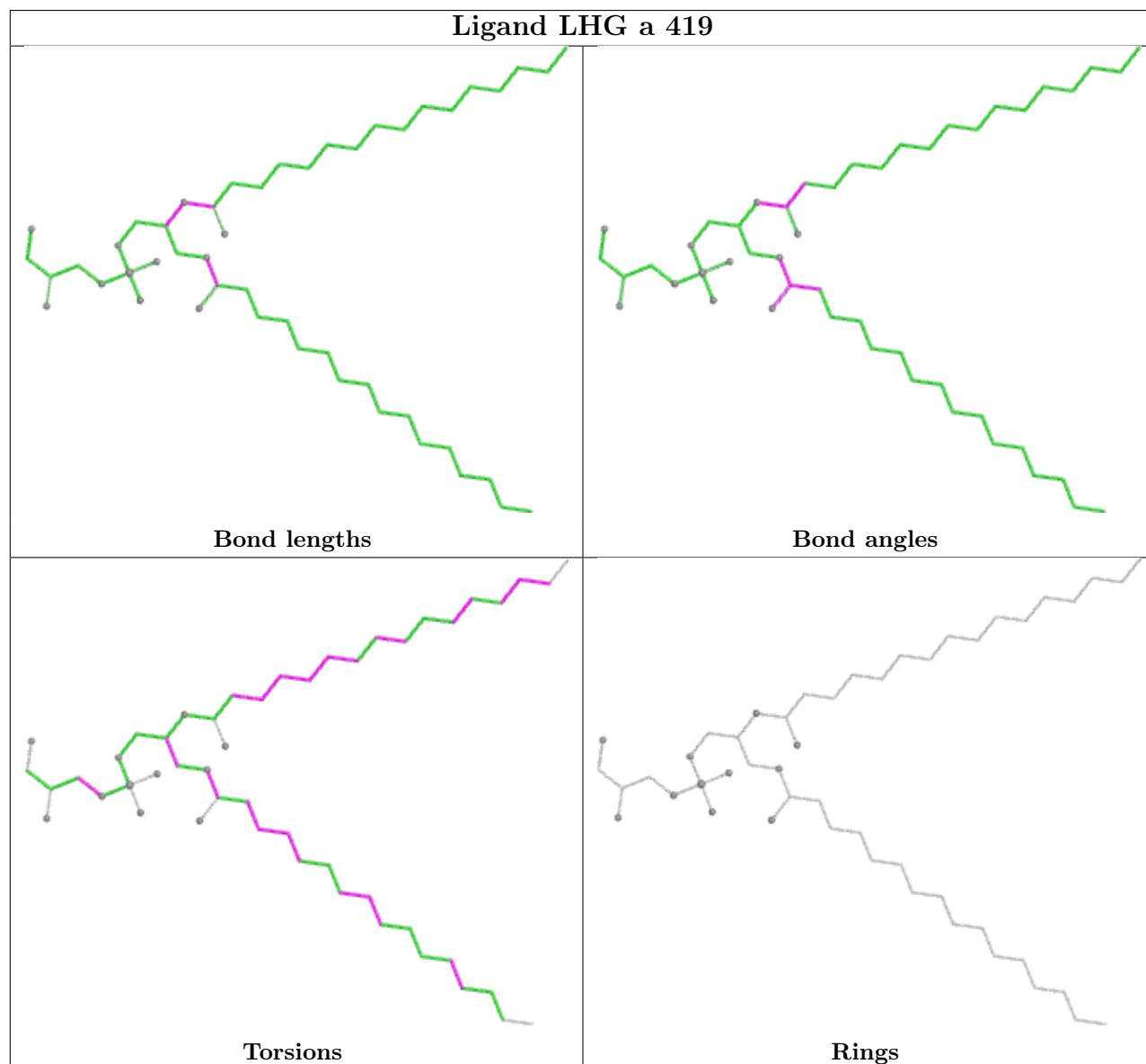
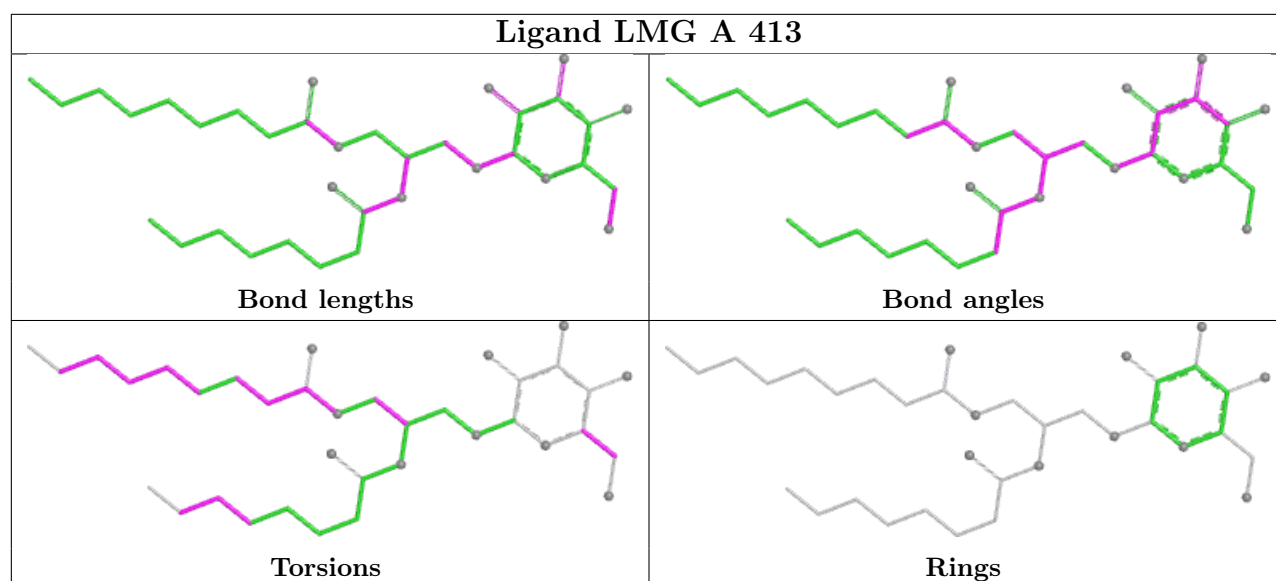


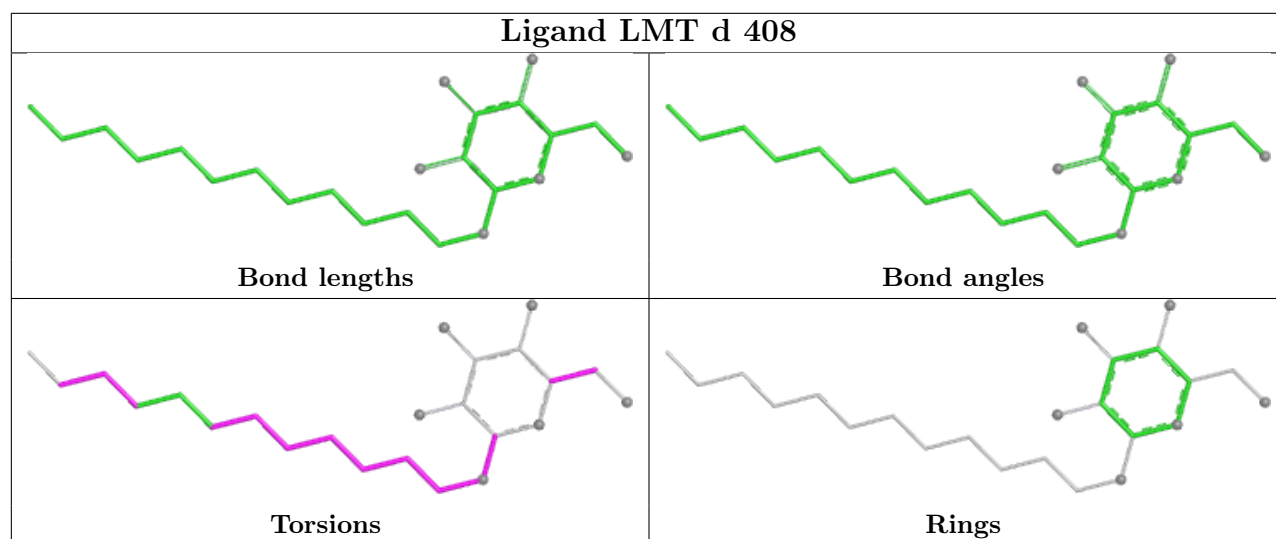
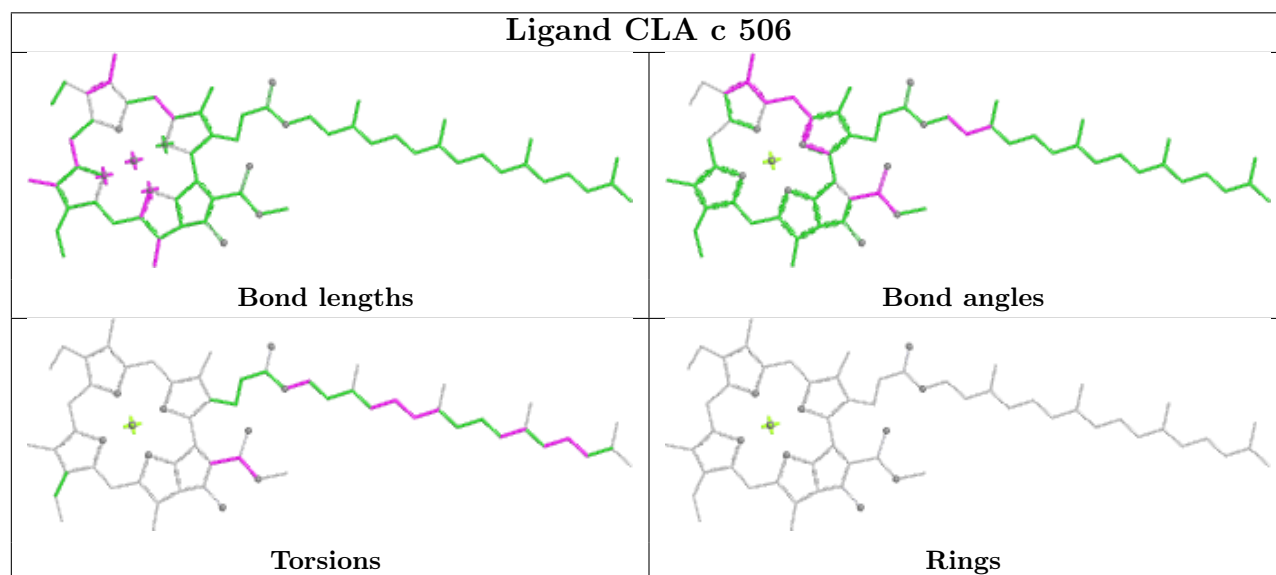
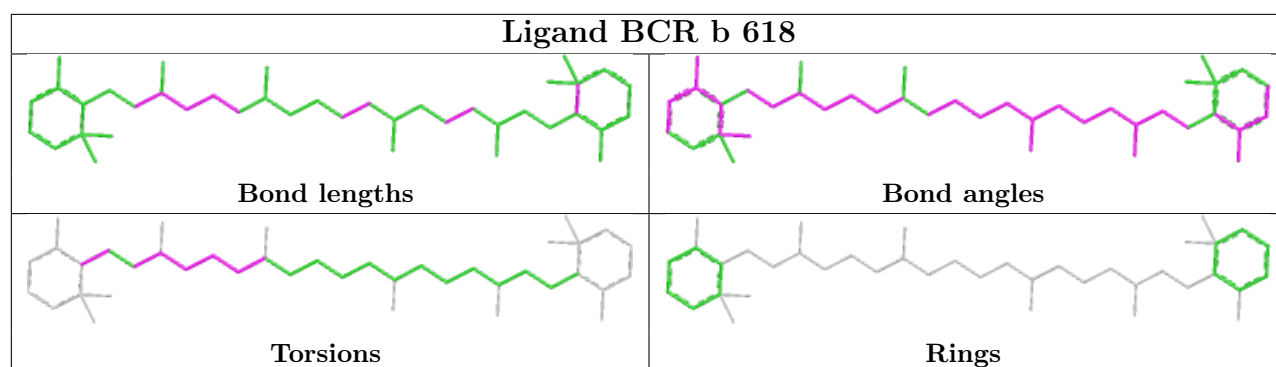


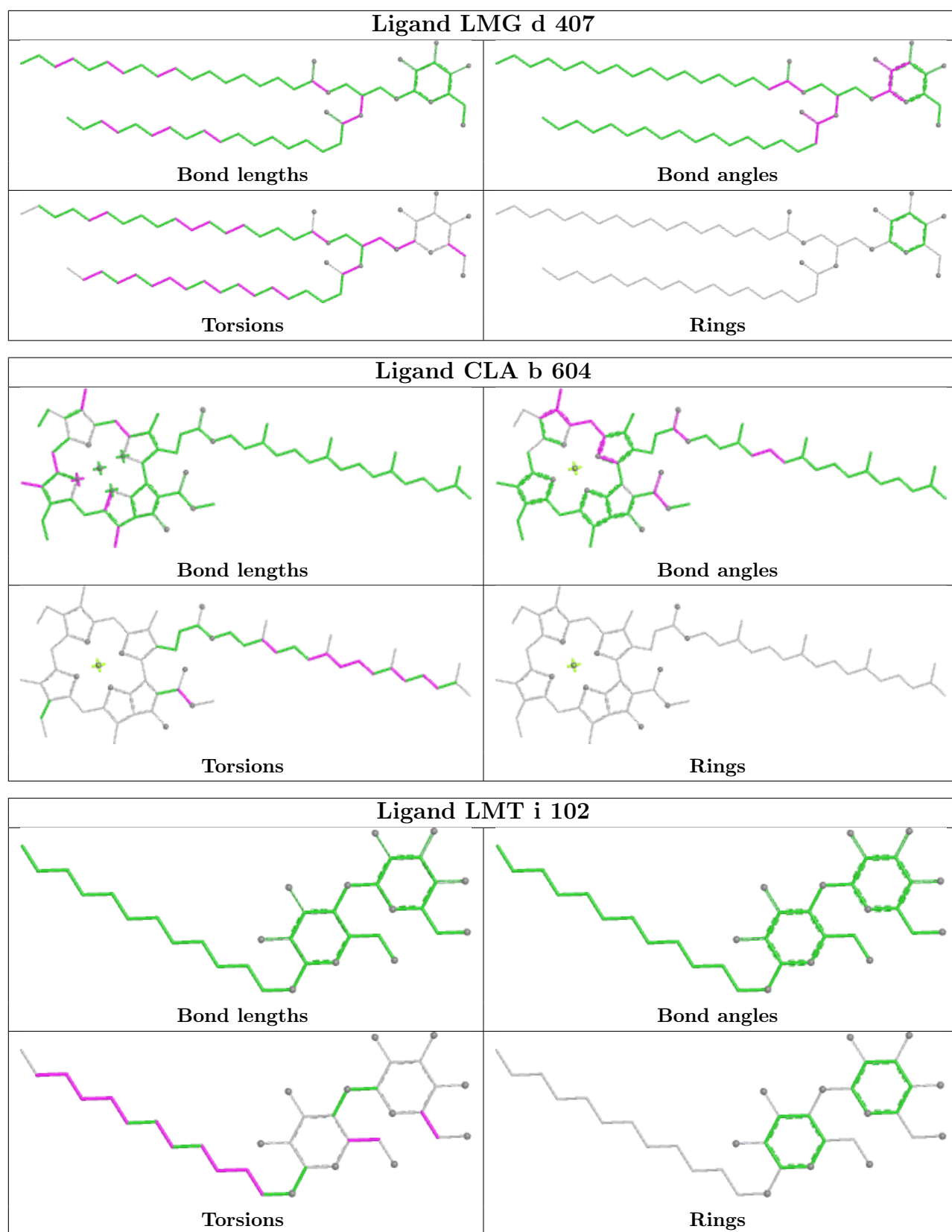


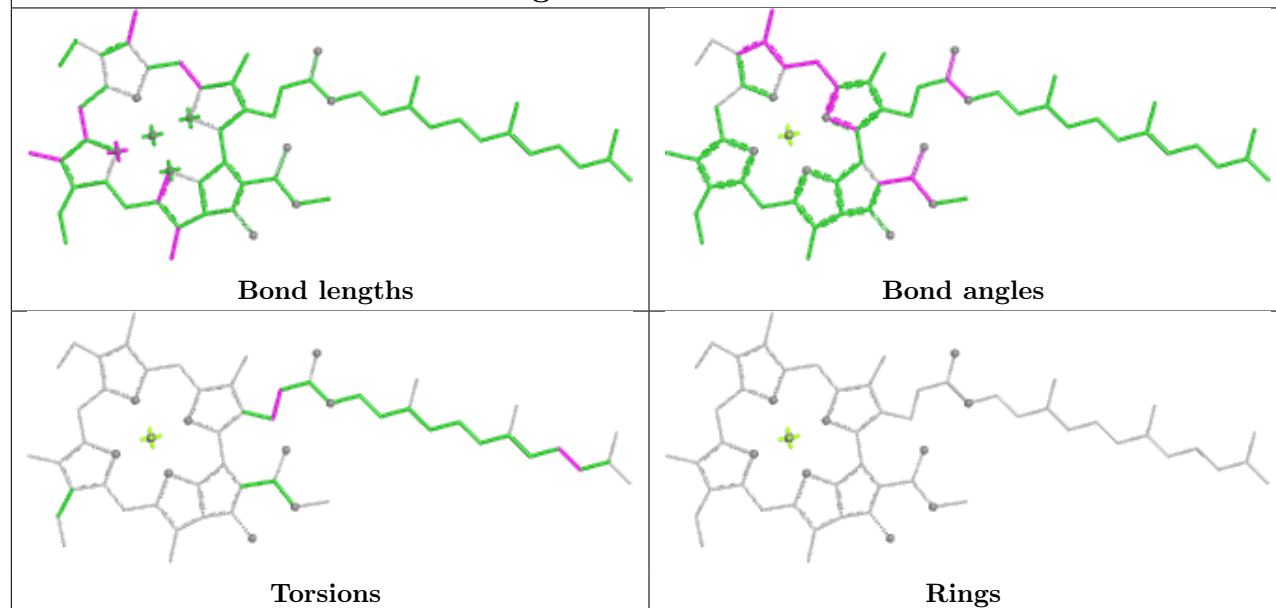
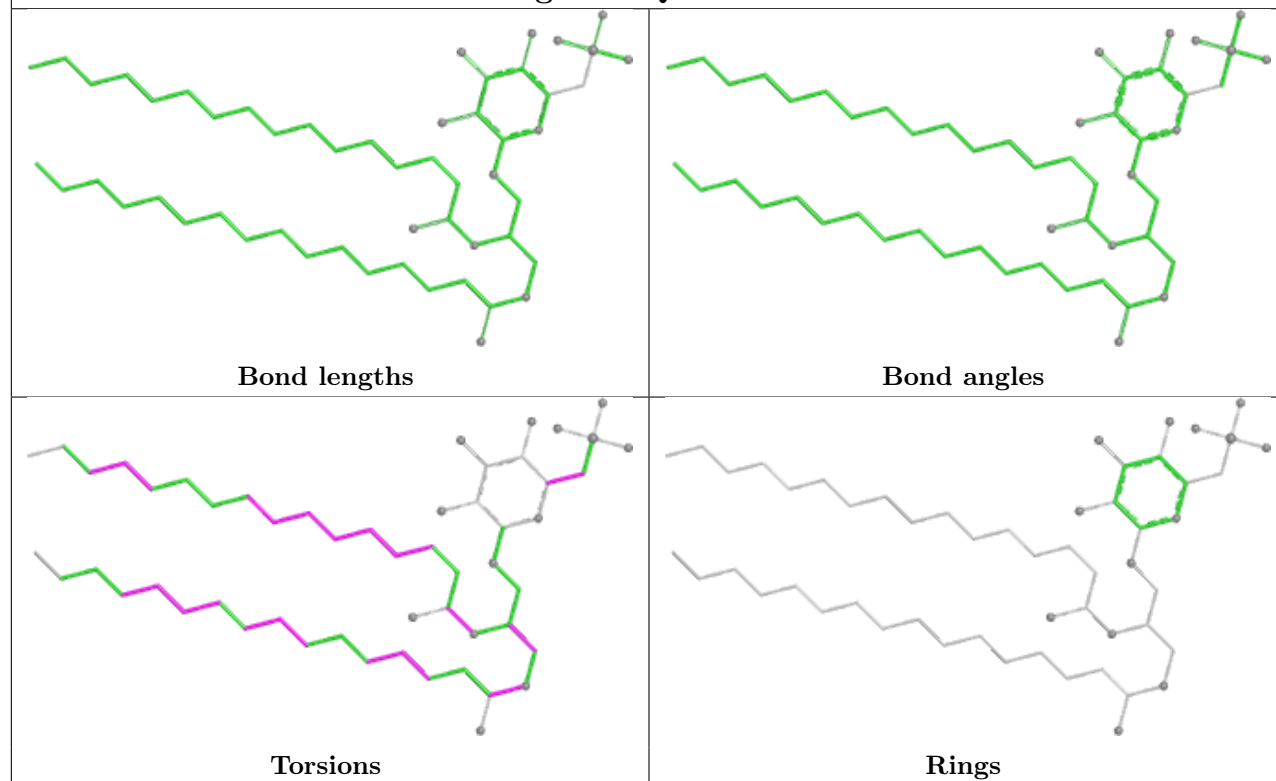


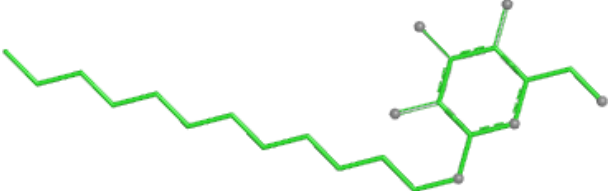
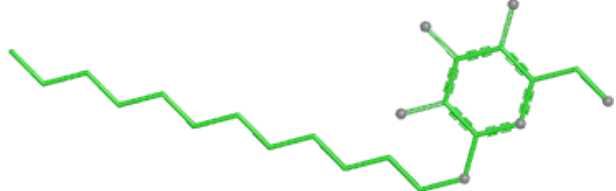


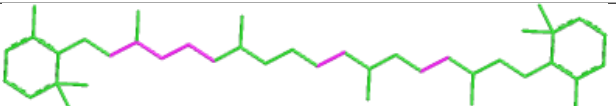
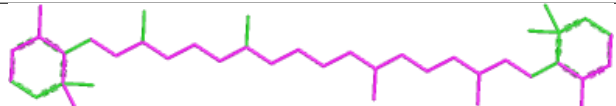
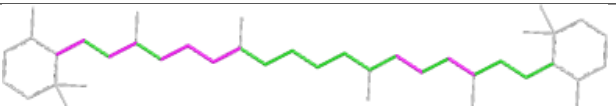
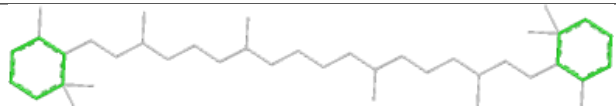
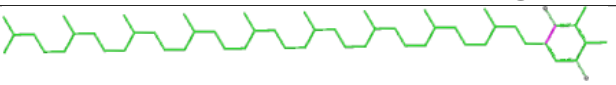
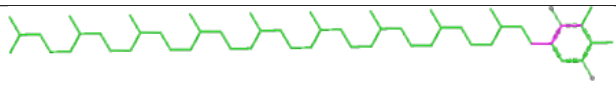
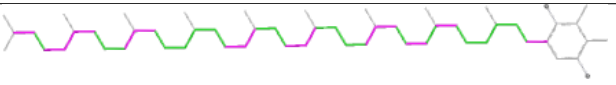
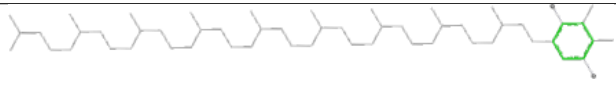








**Ligand CLA B 606****Ligand SQD h 102**

Ligand LMT B 628	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR c 525	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PL9 A 411	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

## 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.

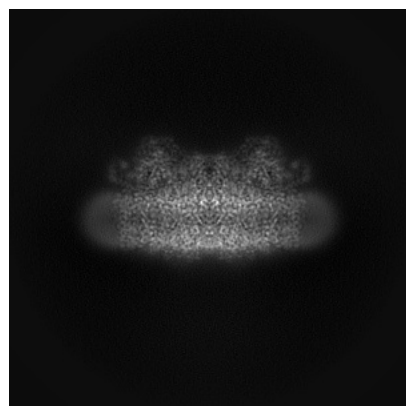
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48046. These allow visual inspection of the internal detail of the map and identification of artifacts.

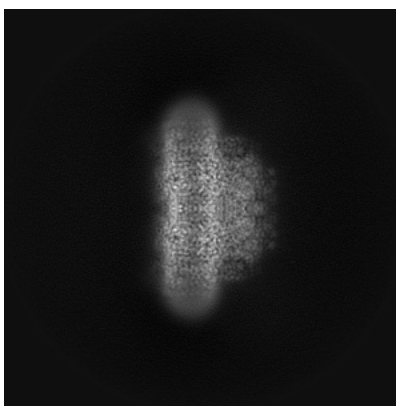
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

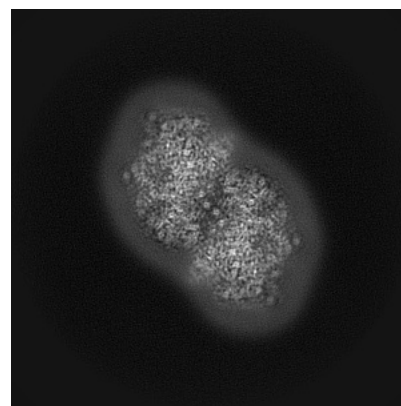
#### 6.1.1 Primary map



X

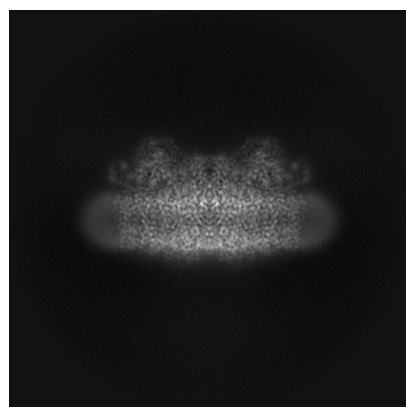


Y

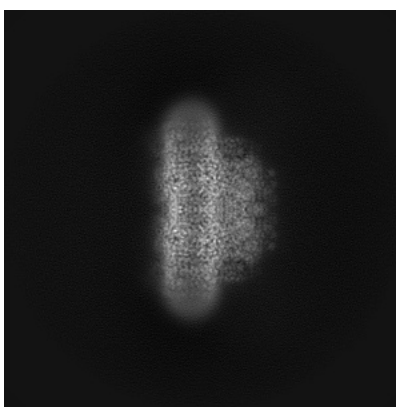


Z

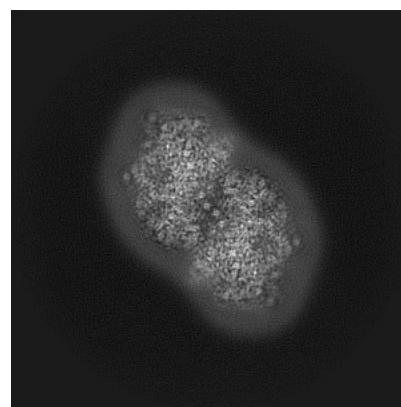
#### 6.1.2 Raw map



X



Y

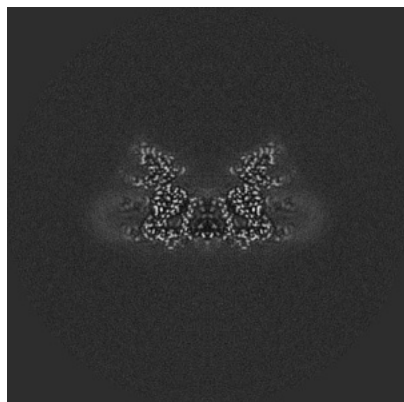


Z

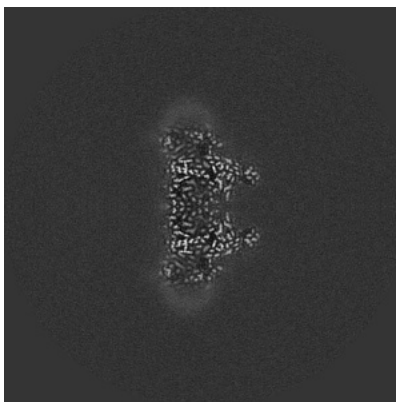
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

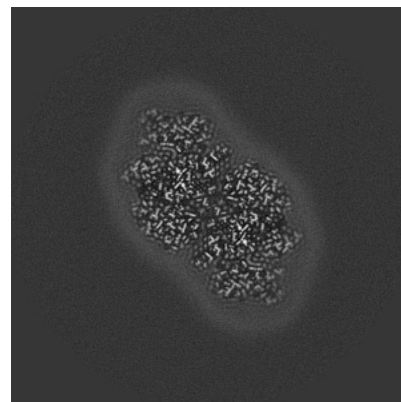
### 6.2.1 Primary map



X Index: 208

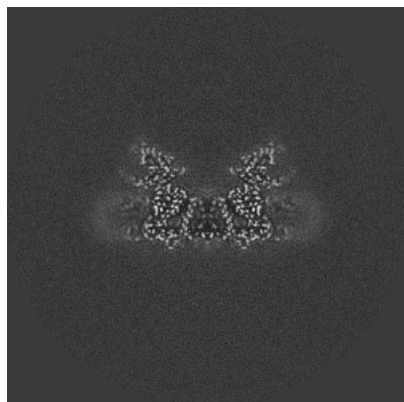


Y Index: 208

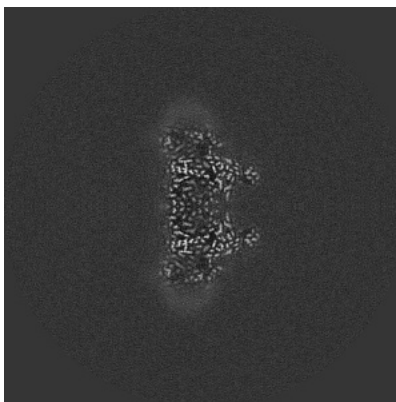


Z Index: 208

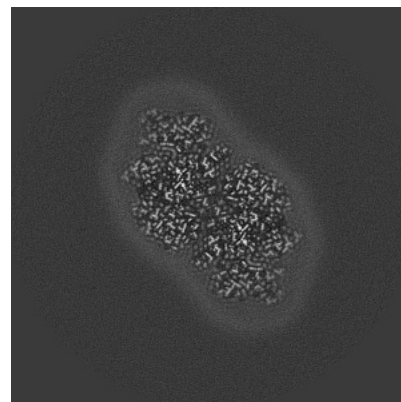
### 6.2.2 Raw map



X Index: 208



Y Index: 208



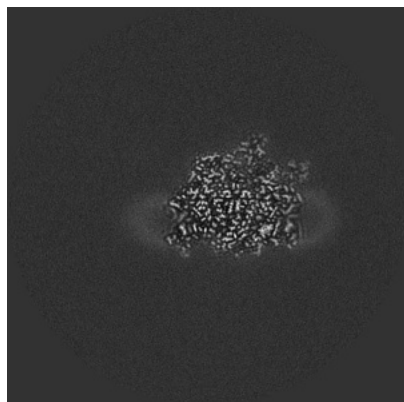
Z Index: 208

The images above show central slices of the map in three orthogonal directions.

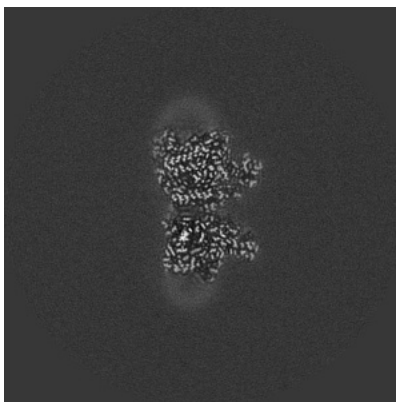


## 6.3 Largest variance slices [i](#)

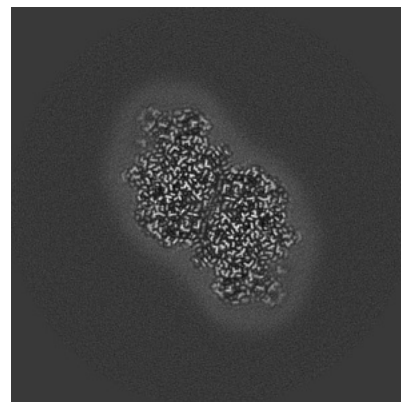
### 6.3.1 Primary map



X Index: 175

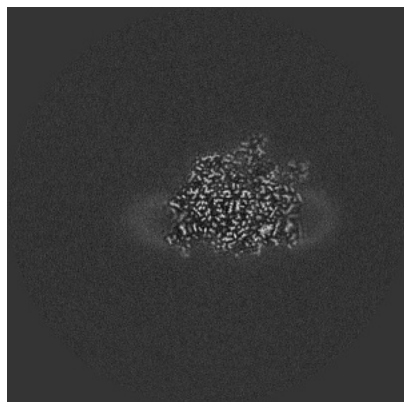


Y Index: 195

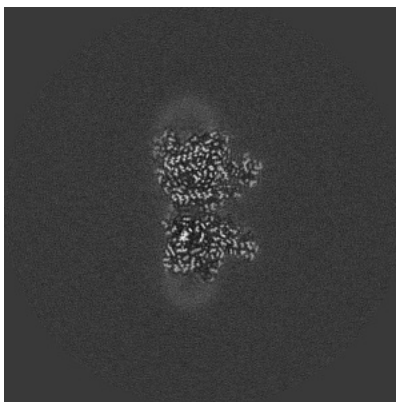


Z Index: 214

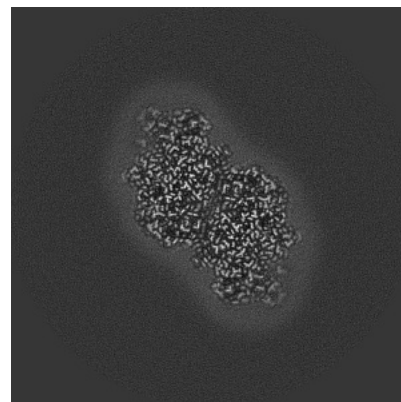
### 6.3.2 Raw map



X Index: 175



Y Index: 195

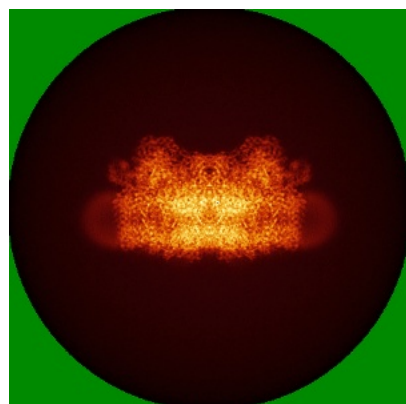


Z Index: 214

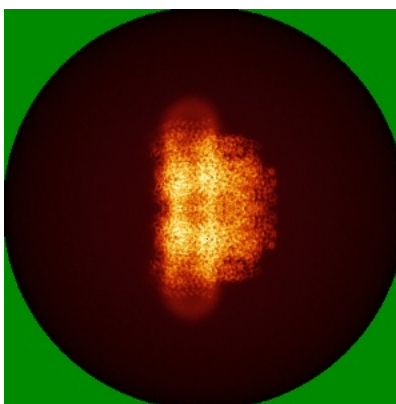
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

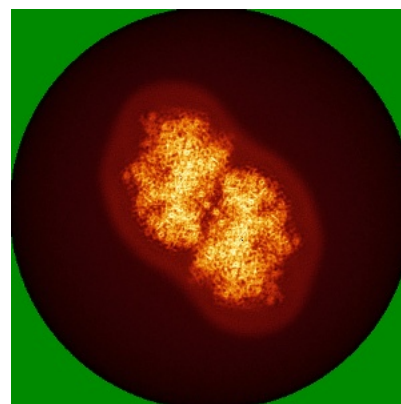
### 6.4.1 Primary map



X

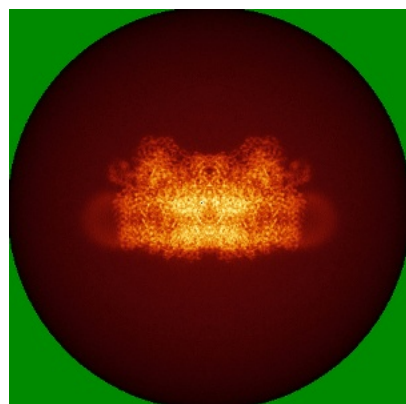


Y

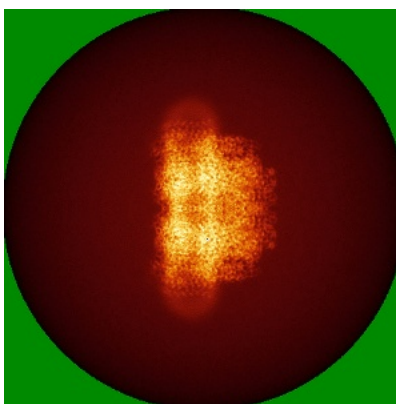


Z

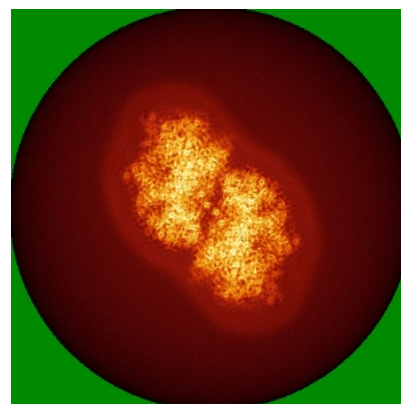
### 6.4.2 Raw map



X



Y

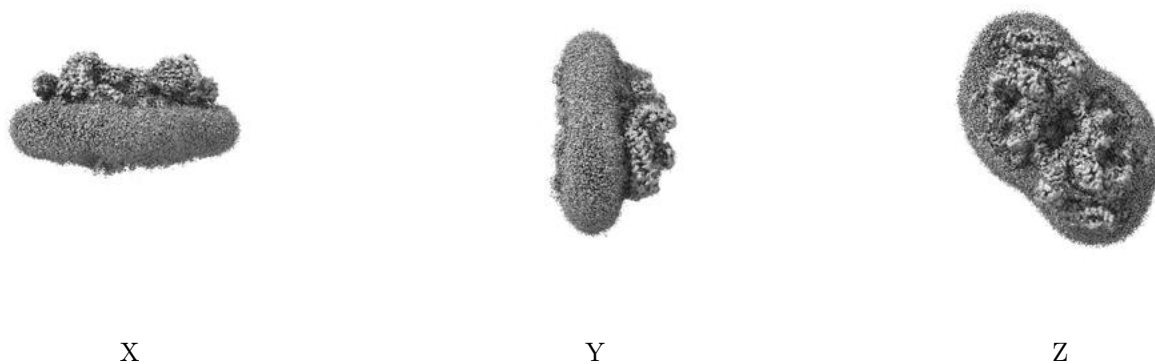


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

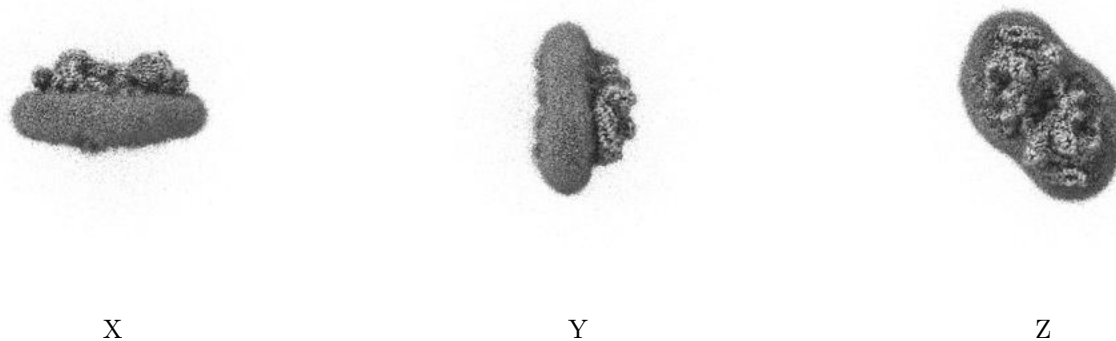
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

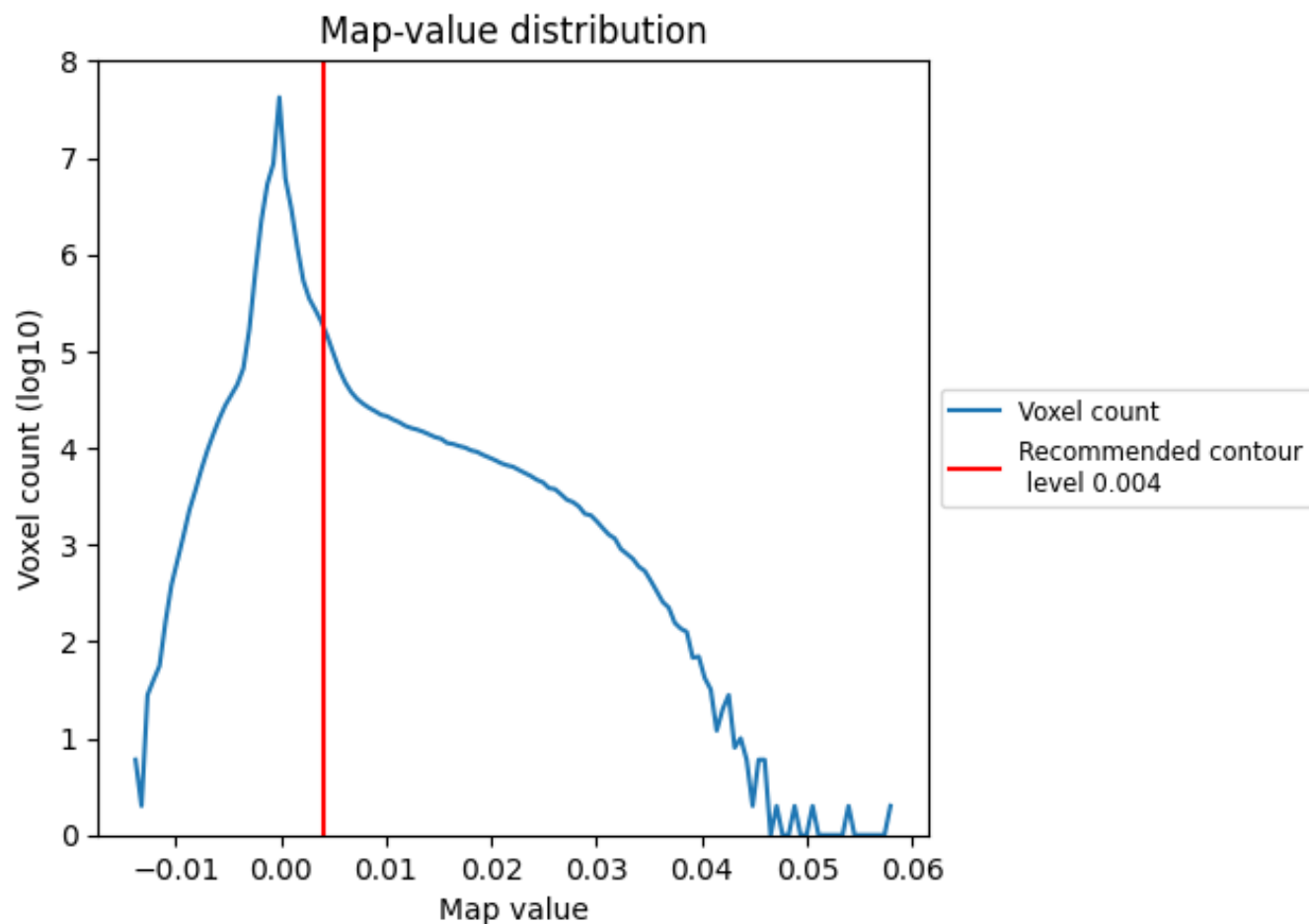
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

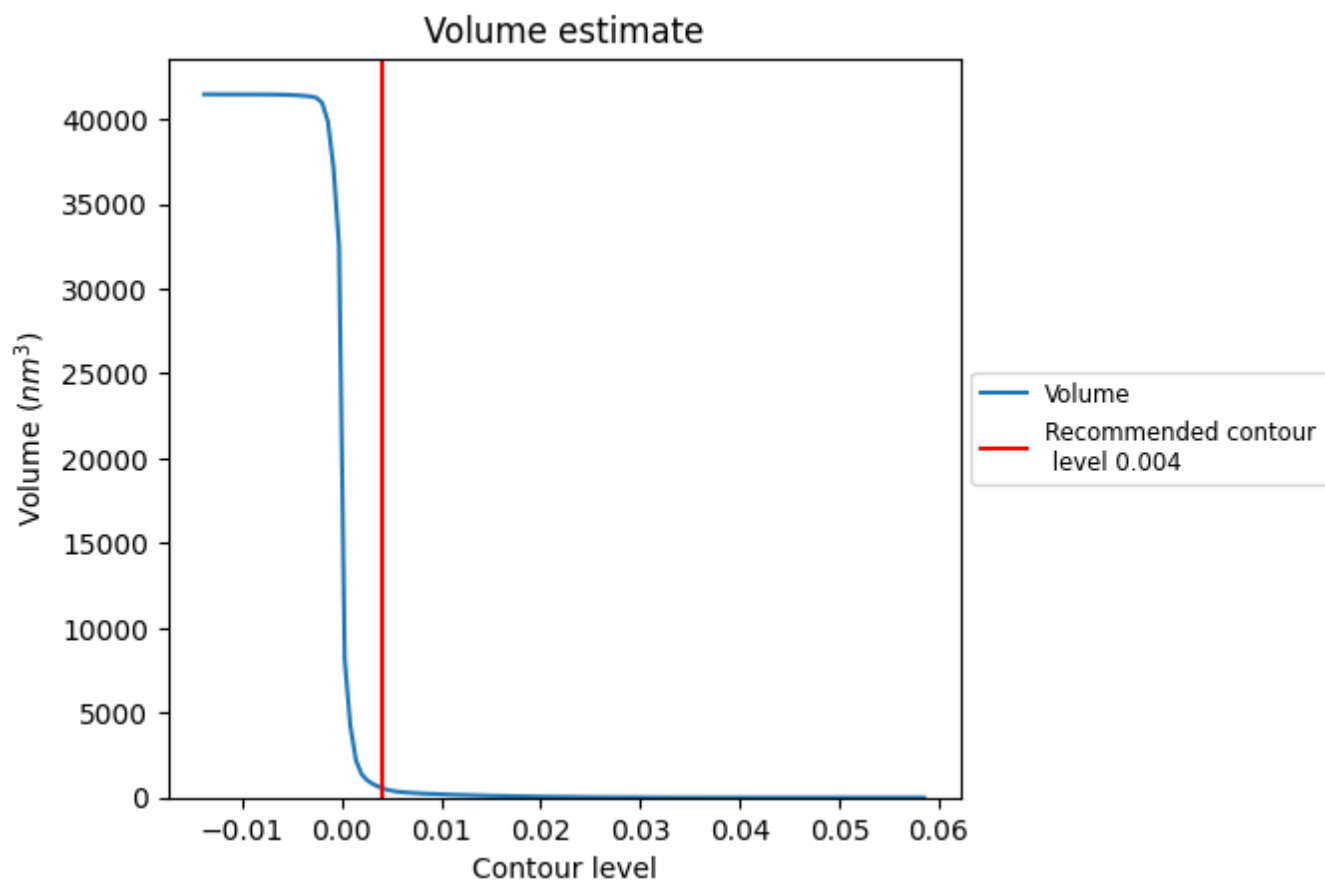
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

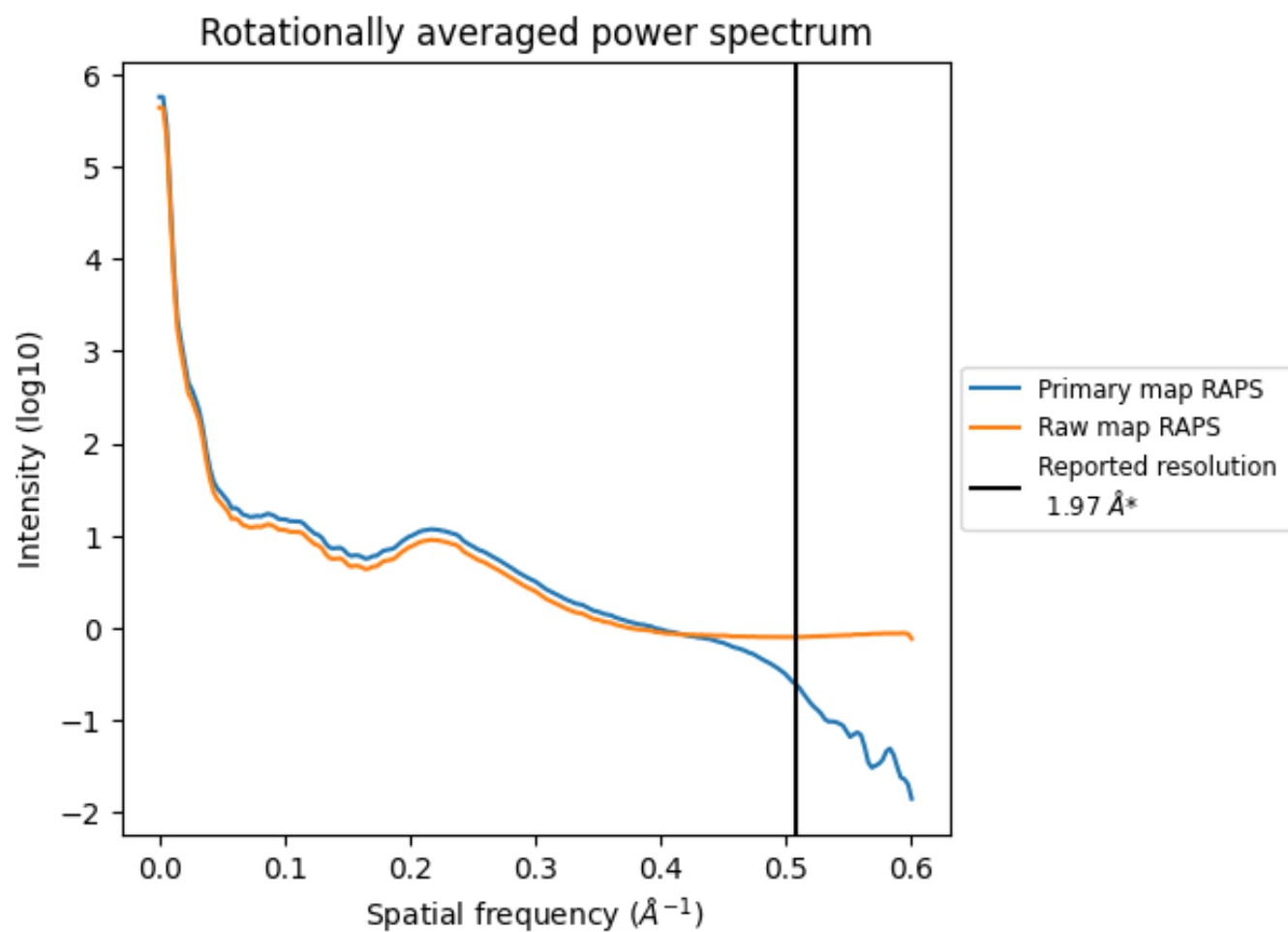
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 576  $\text{nm}^3$ ; this corresponds to an approximate mass of 520 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

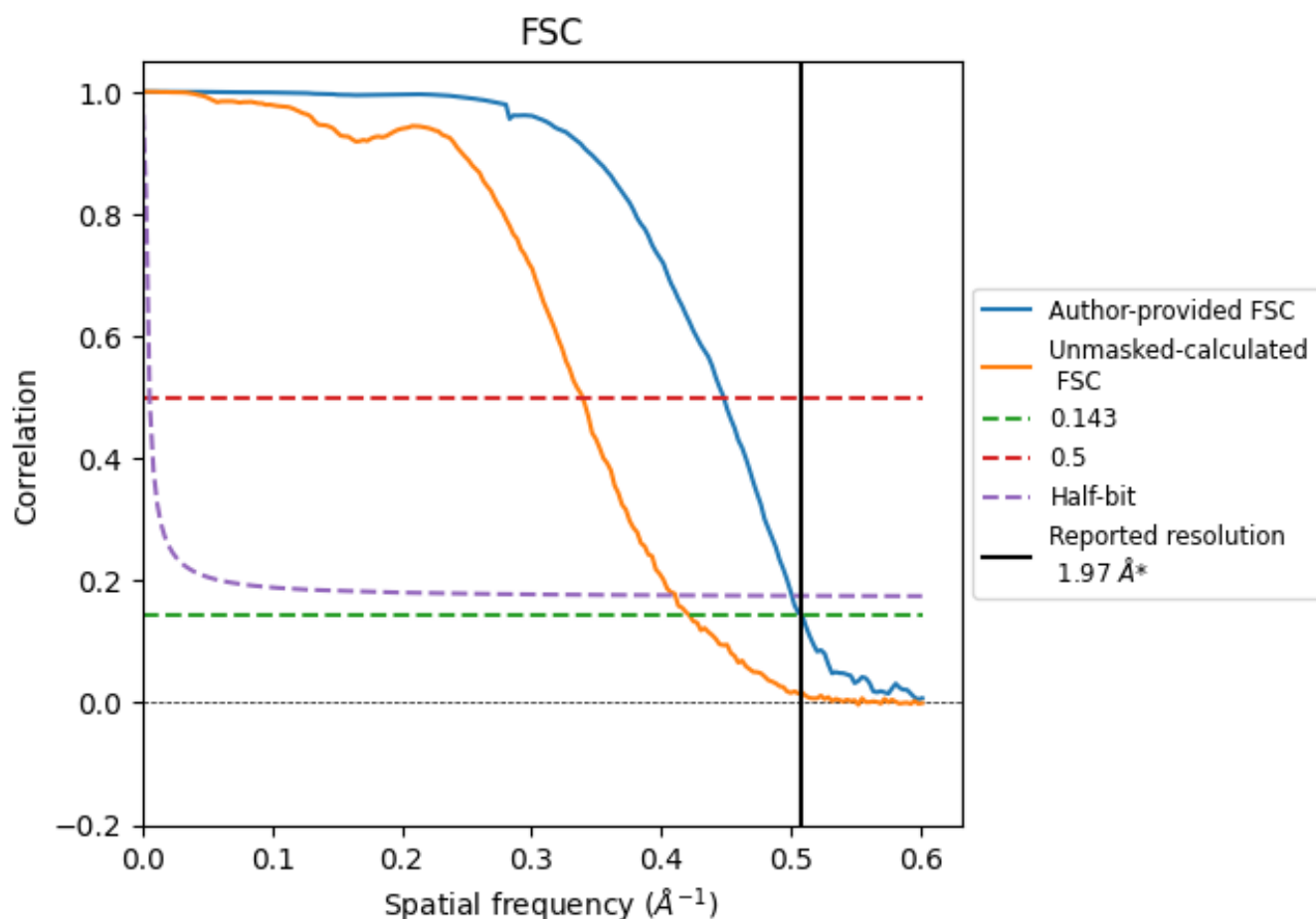


\*Reported resolution corresponds to spatial frequency of 0.508 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.508 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.97	-	-
Author-provided FSC curve	1.97	2.23	2.00
Unmasked-calculated*	2.37	2.95	2.43

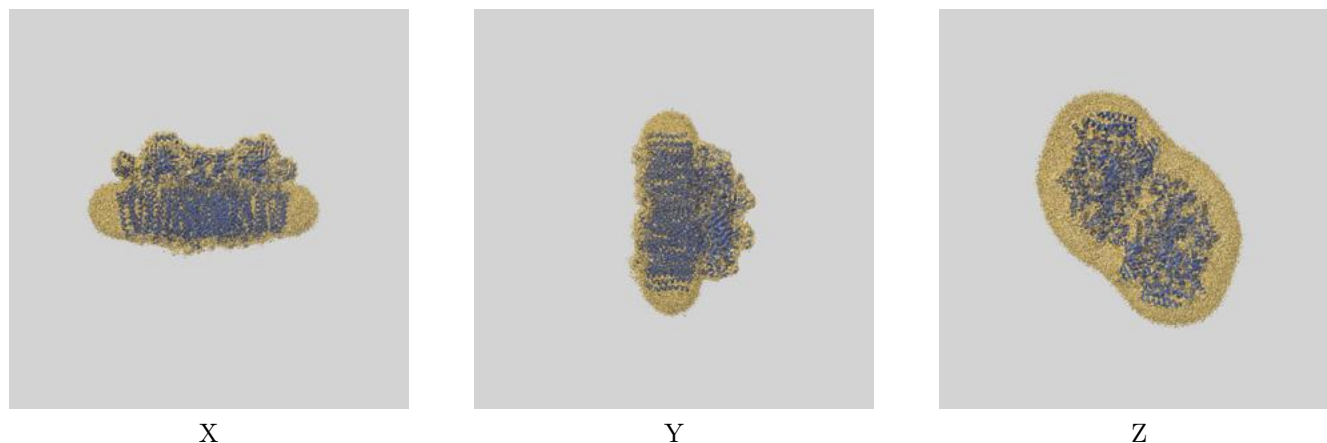
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.37 differs from the reported value 1.97 by more than 10 %



## 9 Map-model fit [i](#)

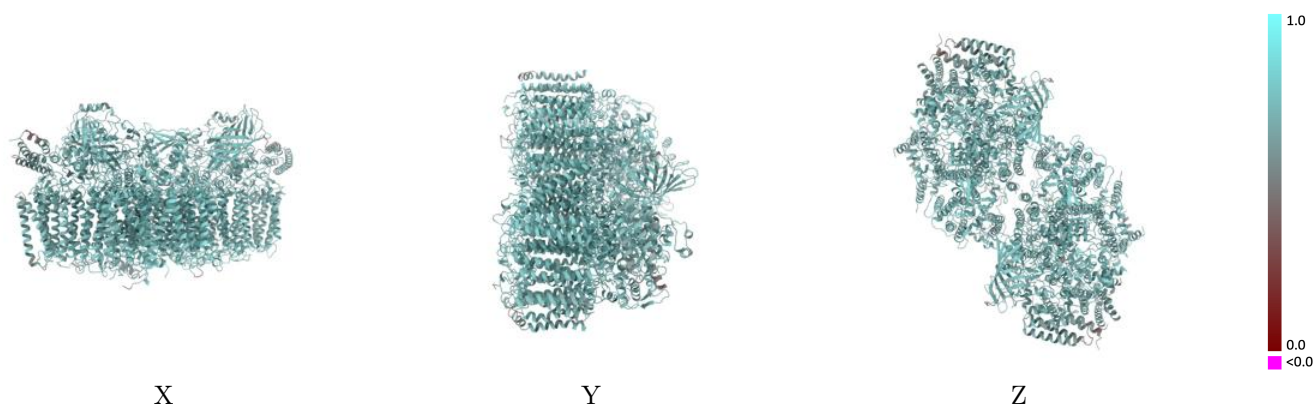
This section contains information regarding the fit between EMDB map EMD-48046 and PDB model 9EH5. Per-residue inclusion information can be found in section [3](#) on page [30](#).

### 9.1 Map-model overlay [i](#)



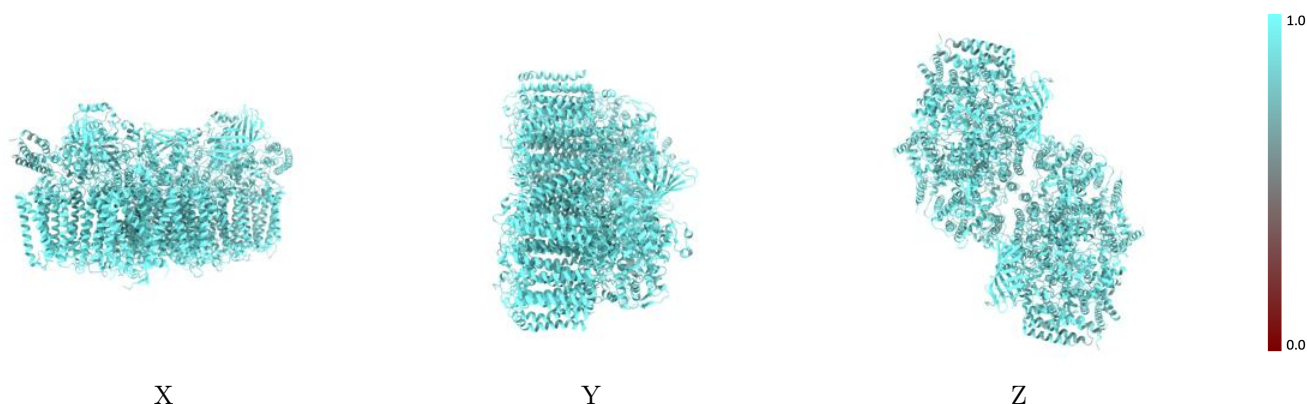
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



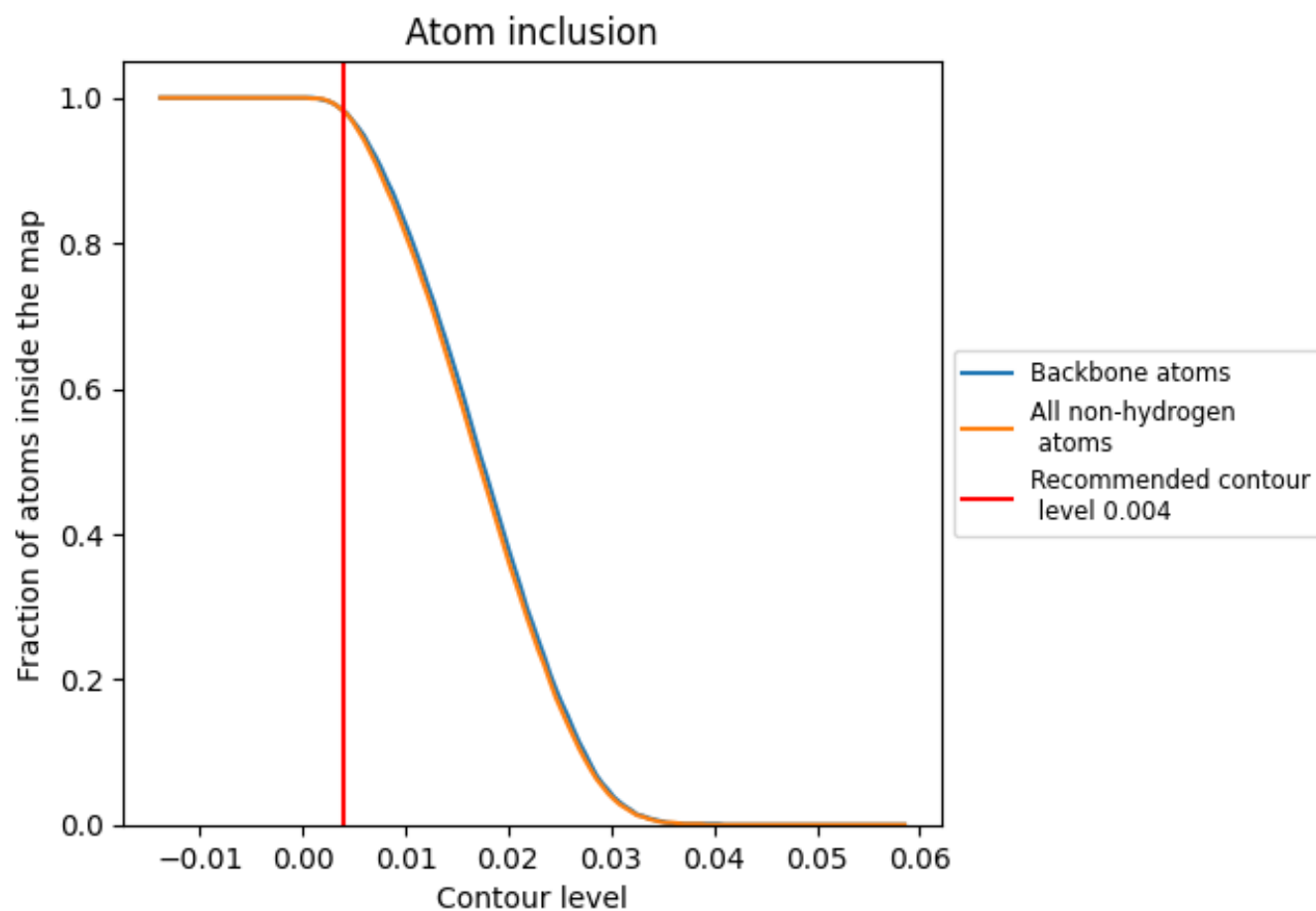
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.004).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

















The table lists the average atom inclusion at the recommended contour level (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9810	 0.7030
A	 0.9870	 0.7320
B	 0.9860	 0.7180
C	 0.9900	 0.7090
D	 0.9900	 0.7350
E	 0.9750	 0.6780
F	 0.9950	 0.6820
H	 0.9830	 0.7030
I	 0.9850	 0.6800
J	 0.9790	 0.6510
K	 0.9710	 0.6660
L	 0.9940	 0.7360
M	 0.9900	 0.6860
O	 0.9700	 0.6770
Q	 0.8780	 0.6050
R	 0.9680	 0.6240
T	 0.9850	 0.7150
U	 0.9640	 0.6820
V	 0.9820	 0.6970
X	 0.9780	 0.6510
Y	 0.9880	 0.6500
Z	 0.9800	 0.6330
a	 0.9870	 0.7310
b	 0.9860	 0.7180
c	 0.9900	 0.7090
d	 0.9900	 0.7350
e	 0.9750	 0.6760
f	 0.9950	 0.6810
h	 0.9830	 0.7010
i	 0.9850	 0.6750
j	 0.9790	 0.6550
k	 0.9740	 0.6620
l	 0.9940	 0.7330
m	 0.9900	 0.6880
o	 0.9700	 0.6770



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Chain	Atom inclusion	Q-score
q	 0.8780	 0.6020
r	 0.9680	 0.6200
t	 0.9850	 0.7170
u	 0.9640	 0.6820
v	 0.9820	 0.6960
x	 0.9780	 0.6500
y	 0.9880	 0.6530
z	 0.9800	 0.6390