



wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 05:37 AM UTC

PDB ID : 9PHW / pdb_00009phw
EMDB ID : EMD-71652
Title : Structure of the D1-Val185Asn mutated photosystem II complex with slow O-O bond formation reveals changes in the Cl1 water channel
Authors : Flesher, D.A.; Debus, R.J.; Brudvig, G.W.
Deposited on : 2025-07-09
Resolution : 1.99 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : **FAILED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

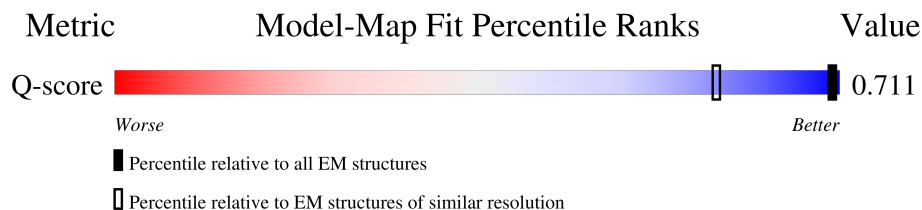
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 1.99 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	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Q-score	25397	1416 (1.50 - 2.49)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 54592 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
			2626	1717	430	464	15		
1	a	334	Total	C	N	O	S	0	0
			2626	1717	430	464	15		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	185	ASN	VAL	engineered mutation	UNP P16033
a	185	ASN	VAL	engineered mutation	UNP P16033

- 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		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	508	HIS	-	expression tag	UNP P05429
B	509	HIS	-	expression tag	UNP P05429
B	510	HIS	-	expression tag	UNP P05429
B	511	HIS	-	expression tag	UNP P05429
B	512	HIS	-	expression tag	UNP P05429
B	513	HIS	-	expression tag	UNP P05429
b	508	HIS	-	expression tag	UNP P05429
b	509	HIS	-	expression tag	UNP P05429
b	510	HIS	-	expression tag	UNP P05429
b	511	HIS	-	expression tag	UNP P05429
b	512	HIS	-	expression tag	UNP P05429

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
b	513	HIS	-	expression tag	UNP P05429

- 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	1	0
			2735	1813	445	465	12		
4	d	341	Total	C	N	O	S	1	0
			2735	1813	445	465	12		

- 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	34	Total	C	N	O	S	0	0
			274	186	45	42	1		
6	f	34	Total	C	N	O	S	0	0
			274	186	45	42	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	35	Total	C	N	O	S	0	0
			246	166	39	40	1		
9	j	35	Total	C	N	O	S	0	0
			246	166	39	40	1		

- 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	S	0	0
			299	210	42	47			
10	k	37	Total	C	N	O	S	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	242	Total	C	N	O	S	0	0
			1865	1182	304	376	3		
13	o	242	Total	C	N	O	S	0	0
			1865	1182	304	376	3		

- Molecule 14 is a protein called Sll1638 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	114	Total	C	N	O	S	0	0
			891	561	159	169	2		
14	q	114	Total	C	N	O	S	0	0
			891	561	159	169	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		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
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		

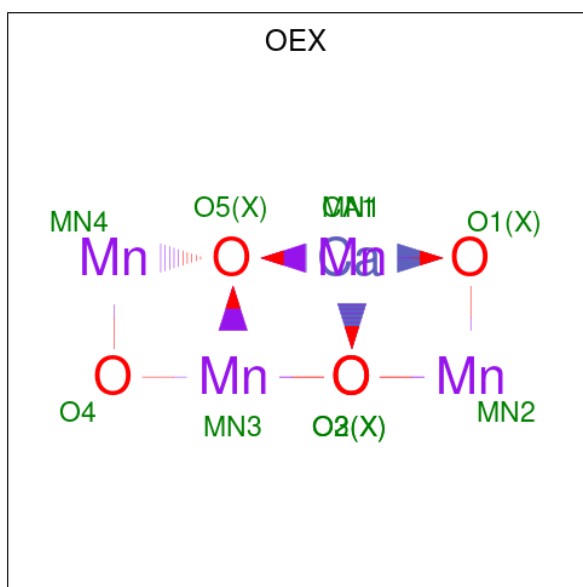
- Molecule 20 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	Y	32	Total	C	N	O	0	0
			242	165	37	40		
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 (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



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	

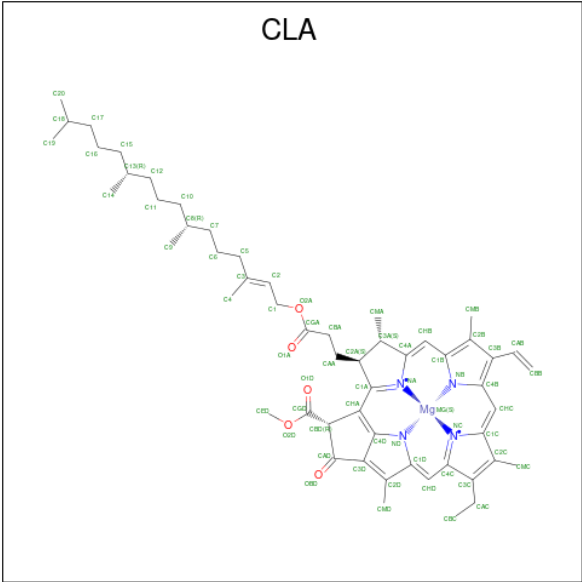
- Molecule 23 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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 (CCD ID: CL) (formula: Cl).

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 (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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	
25	B	1	Total	C	Mg	N	O	0
			60	50	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	

Continued on next page...

Continued from previous page...

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 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

Continued on next page...

Continued from previous page...

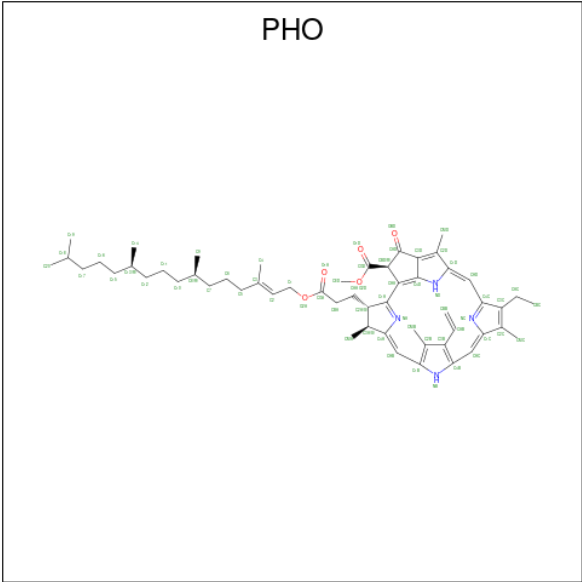
Mol	Chain	Residues	Atoms					AltConf
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total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

Continued on next page...

Continued from previous page...

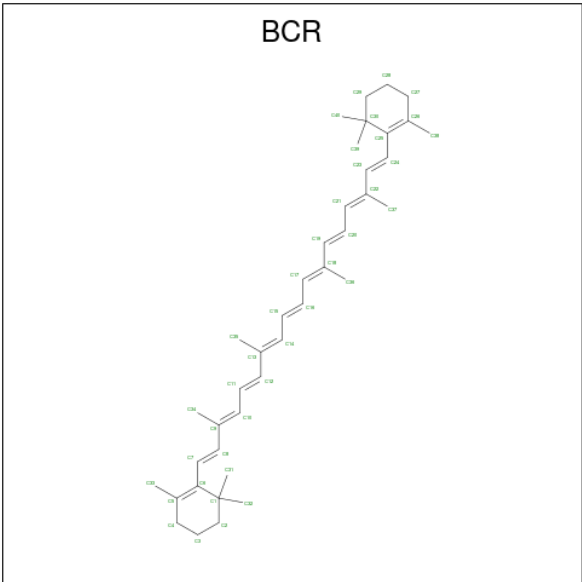
Mol	Chain	Residues	Atoms					AltConf
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 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 (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



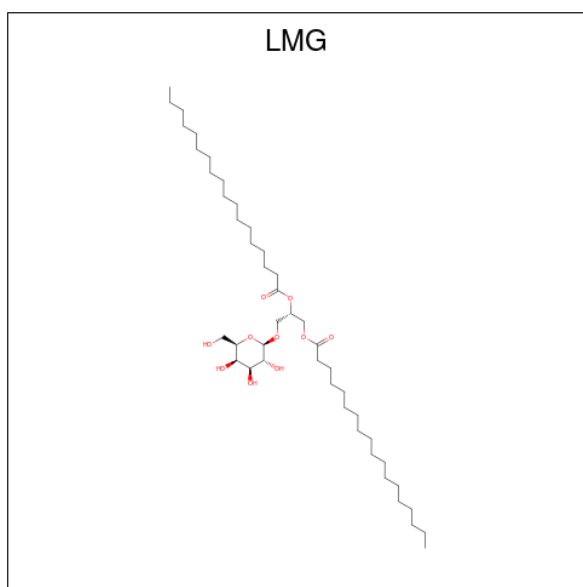
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	N	O	0
			64	55	4	5	
26	D	1	Total	C	N	O	0
			64	55	4	5	
26	a	1	Total	C	N	O	0
			64	55	4	5	
26	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 27 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



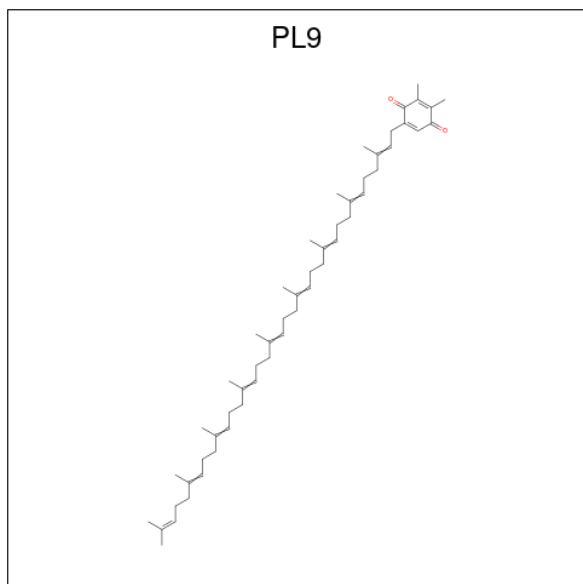
Mol	Chain	Residues	Atoms	AltConf
27	A	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	C	1	Total C 40 40	0
27	F	1	Total C 40 40	0
27	K	1	Total C 40 40	0
27	K	1	Total C 40 40	0
27	Z	1	Total C 40 40	0
27	a	1	Total C 40 40	0
27	b	1	Total C 40 40	0
27	b	1	Total C 40 40	0
27	b	1	Total C 40 40	0
27	c	1	Total C 40 40	0
27	f	1	Total C 40 40	0
27	k	1	Total C 40 40	0
27	z	1	Total C 40 40	0
27	z	1	Total C 40 40	0

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



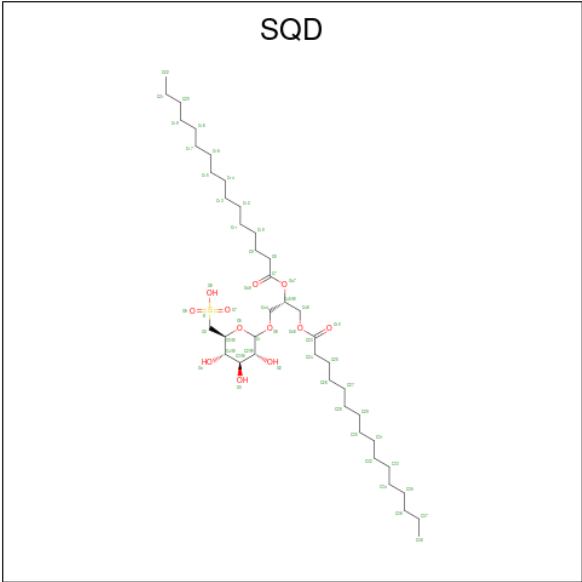
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			51	41	10	
28	A	1	Total	C	O	0
			36	26	10	
28	B	1	Total	C	O	0
			51	41	10	
28	C	1	Total	C	O	0
			51	41	10	
28	C	1	Total	C	O	0
			49	39	10	
28	D	1	Total	C	O	0
			55	45	10	
28	J	1	Total	C	O	0
			55	45	10	
28	a	1	Total	C	O	0
			51	41	10	
28	a	1	Total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

- 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 (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



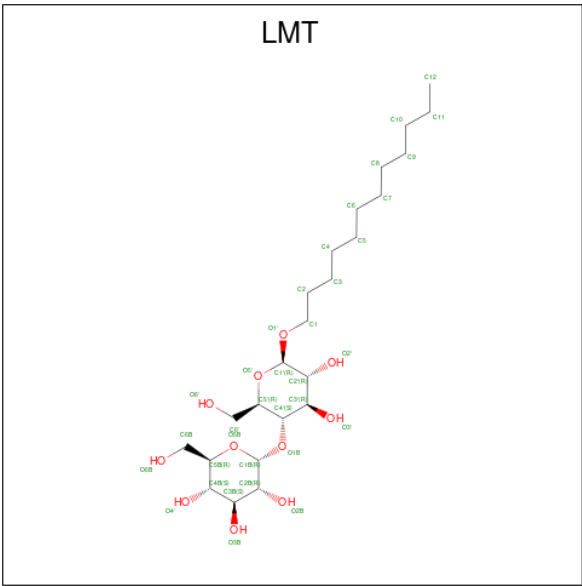
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			55	53	2	
29	D	1	Total	C	O	0
			55	53	2	
29	a	1	Total	C	O	0
			55	53	2	
29	d	1	Total	C	O	0
			55	53	2	

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



Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O	S	0
			54	41	12	1	
30	A	1	Total	C	O	S	0
			44	31	12	1	
30	B	1	Total	C	O	S	0
			54	41	12	1	
30	C	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
			54	41	12	1	
30	a	1	Total	C	O	S	0
			44	31	12	1	
30	b	1	Total	C	O	S	0
			54	41	12	1	
30	c	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 (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			35	24	11	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
31	D	1	Total	C	O	0
			35	24	11	
31	D	1	Total	C	O	0
			35	24	11	
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	I	1	Total	C	O	0
			24	18	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	K	1	Total	C	O	0
			35	24	11	
31	L	1	Total	C	O	0
			35	24	11	
31	M	1	Total	C	O	0
			24	18	6	
31	M	1	Total	C	O	0
			35	24	11	
31	T	1	Total	C	O	0
			24	18	6	
31	X	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	Y	1	Total	C	O	0
			21	15	6	
31	a	1	Total	C	O	0
			35	24	11	
31	b	1	Total	C	O	0
			35	24	11	

Continued on next page...

Continued from previous page...

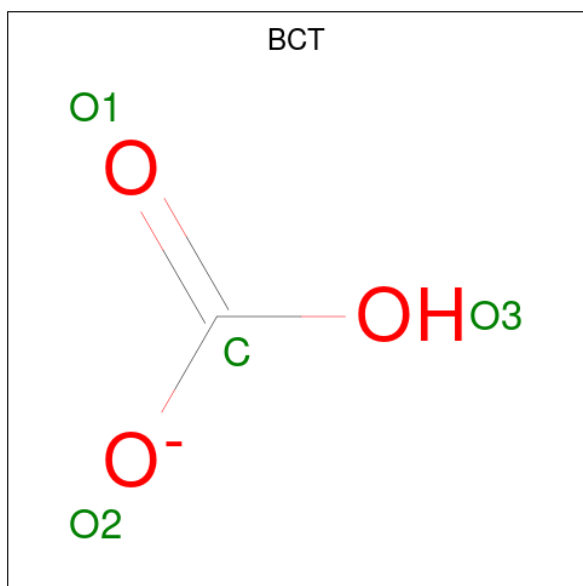
Mol	Chain	Residues	Atoms			AltConf
31	b	1	Total	C	O	0
			24	18	6	
31	b	1	Total	C	O	0
			35	24	11	
31	b	1	Total	C	O	0
			24	18	6	
31	b	1	Total	C	O	0
			35	24	11	
31	b	1	Total	C	O	0
			24	18	6	
31	c	1	Total	C	O	0
			24	18	6	
31	c	1	Total	C	O	0
			35	24	11	
31	c	1	Total	C	O	0
			21	15	6	
31	c	1	Total	C	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	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	i	1	Total	C	O	0
			24	18	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	k	1	Total	C	O	0
			35	24	11	

Continued on next page...

Continued from previous page...

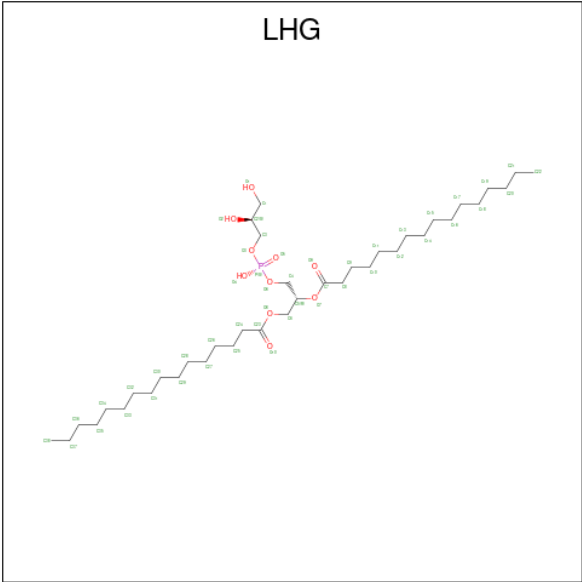
Mol	Chain	Residues	Atoms			AltConf
31	m	1	Total	C	O	0
			24	18	6	
31	t	1	Total	C	O	0
			24	18	6	
31	x	1	Total	C	O	0
			24	18	6	
31	x	1	Total	C	O	0
			35	24	11	
31	x	1	Total	C	O	0
			22	17	5	
31	x	1	Total	C	O	0
			22	16	6	
31	y	1	Total	C	O	0
			21	15	6	

- Molecule 32 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



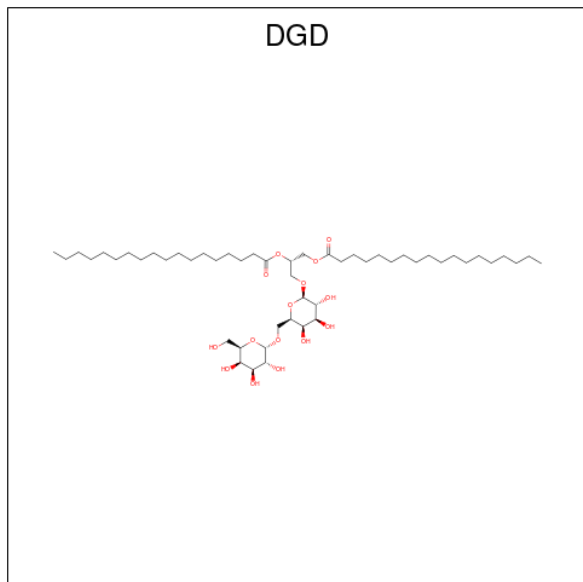
Mol	Chain	Residues	Atoms			AltConf
32	A	1	Total	C	O	0
			4	1	3	
32	a	1	Total	C	O	0
			4	1	3	

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $\text{C}_{38}\text{H}_{75}\text{O}_{10}\text{P}$).



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	D	1	Total	C	O	P	0
			49	38	10	1	
33	D	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	Z	1	Total	C	O	P	0
			36	27	8	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	d	1	Total	C	O	P	0
			49	38	10	1	
33	d	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	z	1	Total	C	O	P	0
			36	27	8	1	

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



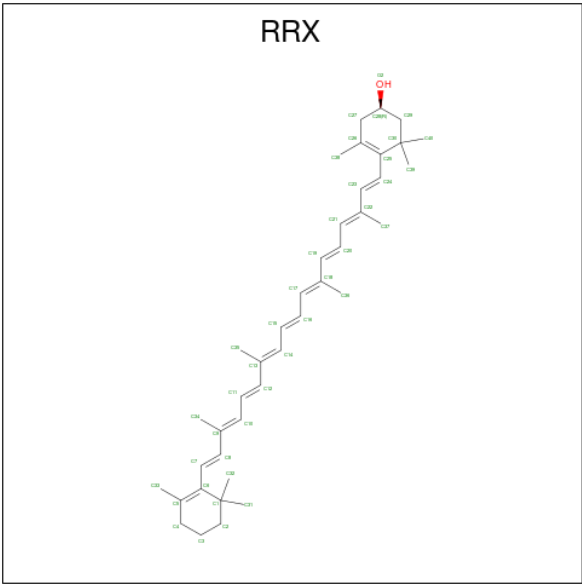
Mol	Chain	Residues	Atoms			AltConf
34	C	1	Total	C	O	0
			62	47	15	
34	C	1	Total	C	O	0
			62	47	15	
34	C	1	Total	C	O	0
			62	47	15	
34	H	1	Total	C	O	0
			62	47	15	
34	c	1	Total	C	O	0
			62	47	15	
34	c	1	Total	C	O	0
			62	47	15	
34	c	1	Total	C	O	0
			62	47	15	
34	h	1	Total	C	O	0
			62	47	15	

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



Mol	Chain	Residues	Atoms					AltConf
35	E	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	e	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 (CCD ID: RRX) (formula: C₄₀H₅₆O).



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 (CCD ID: 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	114	Total	O	0
			114	114	
38	B	106	Total	O	0
			106	106	
38	C	91	Total	O	0
			91	91	
38	D	93	Total	O	0
			93	93	
38	E	8	Total	O	0
			8	8	
38	F	5	Total	O	0
			5	5	
38	H	9	Total	O	0
			9	9	
38	I	2	Total	O	0
			2	2	
38	J	6	Total	O	0
			6	6	
38	L	8	Total	O	0
			8	8	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
38	M	2	Total 2	O 2	0
38	O	25	Total 25	O 25	0
38	T	5	Total 5	O 5	0
38	U	6	Total 6	O 6	0
38	V	26	Total 26	O 26	0
38	X	2	Total 2	O 2	0
38	a	114	Total 114	O 114	0
38	b	106	Total 106	O 106	0
38	c	91	Total 91	O 91	0
38	d	93	Total 93	O 93	0
38	e	8	Total 8	O 8	0
38	f	5	Total 5	O 5	0
38	h	9	Total 9	O 9	0
38	i	2	Total 2	O 2	0
38	j	6	Total 6	O 6	0
38	l	8	Total 8	O 8	0
38	m	2	Total 2	O 2	0
38	o	25	Total 25	O 25	0
38	t	5	Total 5	O 5	0
38	u	6	Total 6	O 6	0
38	v	26	Total 26	O 26	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
38	x	2	Total	O	0
			2	2	

MolProbity failed to run properly - this section is therefore empty.

3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	72628	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 ($e^-/\text{\AA}^2$)	49.6	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.032	Depositor
Minimum map value	-0.008	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0022	Depositor
Map size (Å)	389.4, 389.4, 389.4	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.649, 0.649, 0.649	Depositor

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

6 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	$\# Z > 2$
16	FME	t	1	16	8,9,10	0.46	0	8,9,11	1.48	2 (25%)
12	FME	m	1	12	8,9,10	0.34	0	8,9,11	0.75	0
16	FME	T	1	16	8,9,10	0.45	0	8,9,11	1.48	2 (25%)
12	FME	M	1	12	8,9,10	0.34	0	8,9,11	0.75	0

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	0.40	0	8,9,11	0.62	0
8	FME	I	1	8	8,9,10	0.40	0	8,9,11	0.62	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
16	FME	t	1	16	-	5/7/9/11	-
12	FME	m	1	12	-	3/7/9/11	-
16	FME	T	1	16	-	5/7/9/11	-
12	FME	M	1	12	-	3/7/9/11	-
8	FME	i	1	8	-	2/7/9/11	-
8	FME	I	1	8	-	2/7/9/11	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	t	1	FME	O-C-CA	-2.89	117.34	124.77
16	T	1	FME	O-C-CA	-2.89	117.34	124.77
16	T	1	FME	CA-N-CN	2.24	126.27	122.82
16	t	1	FME	CA-N-CN	2.24	126.27	122.82

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	O-C-CA-CB
16	T	1	FME	O1-CN-N-CA
16	T	1	FME	C-CA-CB-CG
8	i	1	FME	O-C-CA-CB
16	t	1	FME	O1-CN-N-CA

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 230 ligands modelled in this entry, 12 are monoatomic - leaving 218 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$
30	SQD	h	103	-	52,54,54	0.43	0	62,65,65	0.52	0
31	LMT	I	103	-	22,22,36	0.39	0	27,27,47	0.73	0
31	LMT	D	410	-	24,24,36	0.38	0	29,29,47	0.73	0
31	LMT	a	415	-	36,36,36	0.19	0	47,47,47	0.39	0
27	BCR	z	101	-	41,41,41	1.42	8 (19%)	56,56,56	1.41	9 (16%)
29	PL9	D	405	-	55,55,55	0.90	1 (1%)	68,69,69	0.60	1 (1%)
33	LHG	D	413	-	48,48,48	0.32	0	51,54,54	0.32	0
34	DGD	c	517	-	63,63,67	0.83	3 (4%)	77,77,81	1.07	5 (6%)
25	CLA	B	611	2	69,73,73	1.17	8 (11%)	82,113,113	1.40	9 (10%)
31	LMT	I	101	-	24,24,36	0.33	0	29,29,47	0.70	0
25	CLA	C	503	3	69,73,73	1.22	8 (11%)	82,113,113	1.23	9 (10%)
28	LMG	c	519	-	49,49,55	0.29	0	57,57,63	0.50	0
25	CLA	B	605	2	69,73,73	1.11	6 (8%)	82,113,113	1.30	7 (8%)
33	LHG	B	628	-	48,48,48	0.36	0	51,54,54	0.46	0
25	CLA	C	513	3	69,73,73	1.18	9 (13%)	82,113,113	1.34	8 (9%)
25	CLA	b	605	2	69,73,73	1.11	6 (8%)	82,113,113	1.30	7 (8%)
34	DGD	c	516	-	63,63,67	0.83	2 (3%)	77,77,81	1.04	4 (5%)
25	CLA	B	614	2	69,73,73	1.17	9 (13%)	82,113,113	1.40	9 (10%)
25	CLA	a	405	1	69,73,73	1.16	7 (10%)	82,113,113	1.25	4 (4%)
25	CLA	C	509	3	69,73,73	1.38	9 (13%)	82,113,113	1.48	13 (15%)
31	LMT	x	103	-	22,22,36	0.44	0	27,27,47	0.98	4 (14%)
31	LMT	e	103	-	36,36,36	0.46	1 (2%)	47,47,47	1.23	4 (8%)
35	HEM	V	201	18	50,50,50	1.42	7 (14%)	67,82,82	1.16	6 (8%)
25	CLA	B	608	2	69,73,73	1.26	9 (13%)	82,113,113	1.29	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LMT	B	623	-	36,36,36	0.40	0	47,47,47	0.79	1 (2%)
28	LMG	j	101	-	55,55,55	0.24	0	63,63,63	0.30	0
31	LMT	i	104	-	24,24,36	0.42	0	29,29,47	0.92	1 (3%)
31	LMT	x	102	-	22,22,36	0.49	0	27,27,47	0.90	0
31	LMT	C	523	-	24,24,36	0.40	0	29,29,47	0.88	0
25	CLA	C	510	3	69,73,73	1.30	9 (13%)	82,113,113	1.29	8 (9%)
31	LMT	X	101	-	24,24,36	0.33	0	29,29,47	0.81	0
31	LMT	c	522	-	21,21,36	0.46	0	26,26,47	1.30	5 (19%)
33	LHG	d	408	-	48,48,48	0.36	0	51,54,54	0.39	0
30	SQD	f	102	-	32,34,54	1.83	8 (25%)	42,45,65	1.80	11 (26%)
25	CLA	d	403	4	69,73,73	1.16	7 (10%)	82,113,113	1.21	5 (6%)
25	CLA	D	404	4	69,73,73	1.11	7 (10%)	82,113,113	1.39	7 (8%)
31	LMT	M	102	-	24,24,36	0.38	0	29,29,47	0.84	1 (3%)
31	LMT	x	104	-	36,36,36	0.32	0	47,47,47	0.80	0
29	PL9	A	411	-	55,55,55	0.78	1 (1%)	68,69,69	0.61	3 (4%)
25	CLA	c	511	3	69,73,73	1.12	8 (11%)	82,113,113	1.38	6 (7%)
34	DGD	c	515	-	63,63,67	0.84	3 (4%)	77,77,81	0.95	3 (3%)
35	HEM	v	201	18	50,50,50	1.42	7 (14%)	67,82,82	1.16	6 (8%)
27	BCR	B	618	-	41,41,41	1.47	6 (14%)	56,56,56	1.30	10 (17%)
31	LMT	B	629	-	36,36,36	0.33	0	47,47,47	0.79	1 (2%)
22	OEX	a	401	38,3,1	0,15,15	-	-	-	-	-
31	LMT	I	105	-	24,24,36	0.22	0	29,29,47	0.41	0
31	LMT	C	522	-	21,21,36	0.46	0	26,26,47	1.30	5 (19%)
34	DGD	C	516	-	63,63,67	0.83	2 (3%)	77,77,81	1.04	4 (5%)
25	CLA	b	611	2	69,73,73	1.17	8 (11%)	82,113,113	1.40	9 (10%)
27	BCR	C	514	-	41,41,41	1.44	4 (9%)	56,56,56	1.45	11 (19%)
28	LMG	D	409	-	55,55,55	0.29	0	63,63,63	0.43	1 (1%)
28	LMG	C	518	-	51,51,55	0.33	0	59,59,63	0.48	1 (1%)
27	BCR	b	619	-	41,41,41	1.43	4 (9%)	56,56,56	1.34	10 (17%)
30	SQD	k	102	-	41,41,54	0.28	0	49,49,65	0.30	0
27	BCR	B	617	-	41,41,41	1.47	6 (14%)	56,56,56	1.32	10 (17%)
25	CLA	c	513	3	69,73,73	1.18	8 (11%)	82,113,113	1.34	8 (9%)
31	LMT	B	626	-	24,24,36	0.36	0	29,29,47	0.77	0
31	LMT	F	103	-	36,36,36	0.54	0	47,47,47	0.82	1 (2%)
31	LMT	i	102	-	36,36,36	0.35	0	47,47,47	0.85	1 (2%)
31	LMT	d	410	-	24,24,36	0.38	0	29,29,47	0.73	0
33	LHG	d	412	-	48,48,48	0.32	0	51,54,54	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	BCR	c	514	-	41,41,41	1.44	4 (9%)	56,56,56	1.44	11 (19%)
30	SQD	A	413	-	42,44,54	0.45	1 (2%)	52,55,65	0.53	1 (1%)
25	CLA	B	616	2	64,68,73	1.35	9 (14%)	76,107,113	1.29	5 (6%)
25	CLA	B	603	2	69,73,73	1.19	9 (13%)	82,113,113	1.31	7 (8%)
30	SQD	C	525	-	52,54,54	0.44	0	62,65,65	0.44	0
31	LMT	B	625	-	36,36,36	0.32	0	47,47,47	0.88	1 (2%)
25	CLA	b	616	2	64,68,73	1.35	9 (14%)	76,107,113	1.29	5 (6%)
27	BCR	F	101	-	41,41,41	1.44	5 (12%)	56,56,56	1.39	10 (17%)
31	LMT	m	102	-	24,24,36	0.38	0	29,29,47	0.84	1 (3%)
25	CLA	c	501	3	69,73,73	1.23	9 (13%)	82,113,113	1.29	9 (10%)
31	LMT	b	624	-	24,24,36	0.47	0	29,29,47	0.71	0
31	LMT	T	101	-	24,24,36	0.36	0	29,29,47	0.90	1 (3%)
25	CLA	a	408	1	64,68,73	1.14	7 (10%)	76,107,113	1.34	8 (10%)
31	LMT	y	101	-	21,21,36	0.35	0	26,26,47	0.73	0
28	LMG	a	410	-	51,51,55	0.27	0	59,59,63	0.33	0
28	LMG	c	518	-	51,51,55	0.33	0	59,59,63	0.48	1 (1%)
25	CLA	b	601	38	49,53,73	1.35	8 (16%)	58,89,113	1.42	5 (8%)
25	CLA	c	509	3	69,73,73	1.38	9 (13%)	82,113,113	1.47	13 (15%)
27	BCR	K	103	-	41,41,41	1.41	5 (12%)	56,56,56	1.47	11 (19%)
31	LMT	L	105	-	36,36,36	0.43	0	47,47,47	1.27	4 (8%)
35	HEM	e	104	5,6	50,50,50	1.77	10 (20%)	67,82,82	1.79	12 (17%)
25	CLA	b	614	2	69,73,73	1.17	9 (13%)	82,113,113	1.40	9 (10%)
25	CLA	C	508	3	69,73,73	1.22	8 (11%)	82,113,113	1.30	7 (8%)
34	DGD	C	515	-	63,63,67	0.84	3 (4%)	77,77,81	0.95	3 (3%)
32	BCT	a	416	23	3,3,3	1.22	0	2,3,3	0.35	0
25	CLA	b	610	38	69,73,73	1.13	8 (11%)	82,113,113	1.31	8 (9%)
25	CLA	A	406	38	69,73,73	1.10	7 (10%)	82,113,113	1.33	7 (8%)
26	PHO	a	407	-	58,69,69	0.83	4 (6%)	55,99,99	0.94	2 (3%)
31	LMT	D	411	-	36,36,36	0.50	0	47,47,47	1.27	5 (10%)
25	CLA	C	512	3	69,73,73	1.17	8 (11%)	82,113,113	1.25	6 (7%)
30	SQD	A	412	-	52,54,54	0.44	1 (1%)	62,65,65	0.42	0
25	CLA	B	610	38	69,73,73	1.13	8 (11%)	82,113,113	1.31	8 (9%)
25	CLA	b	602	2	69,73,73	1.15	7 (10%)	82,113,113	1.27	9 (10%)
27	BCR	K	104	-	41,41,41	1.45	6 (14%)	56,56,56	1.35	10 (17%)
25	CLA	C	506	3	69,73,73	1.14	8 (11%)	82,113,113	1.34	6 (7%)
27	BCR	Z	101	-	41,41,41	1.42	8 (19%)	56,56,56	1.41	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LMT	C	521	-	36,36,36	0.35	0	47,47,47	0.90	2 (4%)
25	CLA	C	507	38	69,73,73	1.15	7 (10%)	82,113,113	1.50	7 (8%)
29	PL9	a	411	-	55,55,55	0.78	1 (1%)	68,69,69	0.61	3 (4%)
29	PL9	d	405	-	55,55,55	0.90	1 (1%)	68,69,69	0.60	1 (1%)
30	SQD	c	525	-	52,54,54	0.44	0	62,65,65	0.44	0
31	LMT	i	101	-	24,24,36	0.33	0	29,29,47	0.70	0
25	CLA	c	504	38	69,73,73	1.10	7 (10%)	82,113,113	1.25	6 (7%)
33	LHG	b	628	-	48,48,48	0.36	0	51,54,54	0.46	0
25	CLA	c	506	3	69,73,73	1.14	8 (11%)	82,113,113	1.34	6 (7%)
31	LMT	c	521	-	36,36,36	0.35	0	47,47,47	0.90	2 (4%)
33	LHG	D	406	-	48,48,48	0.35	0	51,54,54	0.37	0
25	CLA	b	604	2	69,73,73	1.32	10 (14%)	82,113,113	1.47	10 (12%)
25	CLA	c	507	38	69,73,73	1.15	7 (10%)	82,113,113	1.51	7 (8%)
25	CLA	B	615	2	69,73,73	1.18	10 (14%)	82,113,113	1.30	8 (9%)
31	LMT	C	520	-	24,24,36	0.37	0	29,29,47	0.99	2 (6%)
28	LMG	a	414	-	36,36,55	0.30	0	44,44,63	0.51	1 (2%)
31	LMT	B	627	-	24,24,36	0.44	0	29,29,47	1.11	3 (10%)
31	LMT	b	623	-	36,36,36	0.40	0	47,47,47	0.79	1 (2%)
31	LMT	x	101	-	24,24,36	0.33	0	29,29,47	0.81	0
25	CLA	b	608	2	69,73,73	1.26	9 (13%)	82,113,113	1.29	10 (12%)
31	LMT	t	101	-	24,24,36	0.36	0	29,29,47	0.90	1 (3%)
25	CLA	A	408	1	64,68,73	1.14	6 (9%)	76,107,113	1.34	8 (10%)
30	SQD	b	620	-	52,54,54	0.41	0	62,65,65	0.52	0
25	CLA	C	501	3	69,73,73	1.23	9 (13%)	82,113,113	1.30	9 (10%)
31	LMT	B	624	-	24,24,36	0.47	0	29,29,47	0.71	0
31	LMT	b	630	-	24,24,36	0.44	0	29,29,47	1.11	3 (10%)
25	CLA	C	511	3	69,73,73	1.12	8 (11%)	82,113,113	1.38	6 (7%)
25	CLA	C	505	3	69,73,73	1.19	9 (13%)	82,113,113	1.23	4 (4%)
27	BCR	k	103	-	41,41,41	1.41	5 (12%)	56,56,56	1.47	11 (19%)
25	CLA	C	504	38	69,73,73	1.10	7 (10%)	82,113,113	1.25	6 (7%)
30	SQD	B	620	-	52,54,54	0.42	0	62,65,65	0.52	0
25	CLA	c	503	3	69,73,73	1.22	8 (11%)	82,113,113	1.23	9 (10%)
27	BCR	b	617	-	41,41,41	1.47	6 (14%)	56,56,56	1.32	10 (17%)
28	LMG	A	410	-	51,51,55	0.27	0	59,59,63	0.33	0
31	LMT	i	103	-	22,22,36	0.38	0	27,27,47	0.72	0
33	LHG	E	102	-	39,39,48	0.33	0	42,45,54	0.41	0
25	CLA	d	401	38	69,73,73	1.19	10 (14%)	82,113,113	1.40	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	BCR	z	103	-	41,41,41	1.45	6 (14%)	56,56,56	1.35	10 (17%)
31	LMT	X	103	-	22,22,36	0.44	0	27,27,47	0.98	4 (14%)
27	BCR	b	618	-	41,41,41	1.46	6 (14%)	56,56,56	1.30	10 (17%)
27	BCR	A	409	-	41,41,41	1.46	4 (9%)	56,56,56	1.30	8 (14%)
31	LMT	f	103	-	36,36,36	0.55	0	47,47,47	0.82	1 (2%)
33	LHG	d	406	-	48,48,48	0.34	0	51,54,54	0.37	0
33	LHG	D	407	-	48,48,48	0.37	0	51,54,54	0.35	0
34	DGD	h	104	-	63,63,67	0.85	3 (4%)	77,77,81	0.98	3 (3%)
25	CLA	b	603	2	69,73,73	1.19	9 (13%)	82,113,113	1.31	7 (8%)
27	BCR	a	409	-	41,41,41	1.46	4 (9%)	56,56,56	1.30	8 (14%)
31	LMT	E	101	-	22,22,36	0.35	0	27,27,47	0.69	0
25	CLA	c	502	3	69,73,73	1.17	9 (13%)	82,113,113	1.38	7 (8%)
28	LMG	d	409	-	55,55,55	0.29	0	63,63,63	0.43	1 (1%)
31	LMT	I	102	-	36,36,36	0.35	0	47,47,47	0.85	1 (2%)
25	CLA	c	508	3	69,73,73	1.22	8 (11%)	82,113,113	1.30	7 (8%)
34	DGD	H	104	-	63,63,67	0.85	3 (4%)	77,77,81	0.98	3 (3%)
35	HEM	E	104	5,6	50,50,50	1.77	10 (20%)	67,82,82	1.79	12 (17%)
25	CLA	B	604	2	69,73,73	1.32	10 (14%)	82,113,113	1.47	10 (12%)
31	LMT	c	523	-	24,24,36	0.40	0	29,29,47	0.88	0
25	CLA	c	505	3	69,73,73	1.20	9 (13%)	82,113,113	1.23	4 (4%)
28	LMG	A	414	-	36,36,55	0.30	0	44,44,63	0.51	1 (2%)
28	LMG	J	101	-	55,55,55	0.24	0	63,63,63	0.30	0
28	LMG	C	519	-	49,49,55	0.29	0	57,57,63	0.50	0
31	LMT	I	104	-	24,24,36	0.42	0	29,29,47	0.92	1 (3%)
31	LMT	E	103	-	36,36,36	0.46	0	47,47,47	1.23	4 (8%)
25	CLA	B	602	2	69,73,73	1.15	7 (10%)	82,113,113	1.27	9 (10%)
25	CLA	B	606	2	64,68,73	1.23	10 (15%)	76,107,113	1.30	8 (10%)
31	LMT	b	625	-	36,36,36	0.32	0	47,47,47	0.88	1 (2%)
30	SQD	K	102	-	41,41,54	0.28	0	49,49,65	0.30	0
25	CLA	b	606	2	64,68,73	1.23	10 (15%)	76,107,113	1.30	8 (10%)
25	CLA	b	609	2	69,73,73	1.20	10 (14%)	82,113,113	1.26	8 (9%)
33	LHG	D	408	-	48,48,48	0.36	0	51,54,54	0.39	0
30	SQD	a	412	-	52,54,54	0.44	1 (1%)	62,65,65	0.42	0
31	LMT	D	412	-	36,36,36	0.32	0	47,47,47	0.80	0
25	CLA	c	512	3	69,73,73	1.17	8 (11%)	82,113,113	1.25	6 (7%)
31	LMT	b	629	-	36,36,36	0.33	0	47,47,47	0.79	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	b	615	2	69,73,73	1.18	10 (14%)	82,113,113	1.31	8 (9%)
36	RRX	h	101	-	42,42,42	1.43	7 (16%)	56,58,58	1.35	11 (19%)
25	CLA	d	404	4	69,73,73	1.11	7 (10%)	82,113,113	1.39	7 (8%)
31	LMT	K	105	-	36,36,36	0.38	0	47,47,47	1.38	6 (12%)
25	CLA	a	406	38	69,73,73	1.10	7 (10%)	82,113,113	1.33	8 (9%)
30	SQD	F	102	-	32,34,54	1.83	8 (25%)	42,45,65	1.80	11 (26%)
26	PHO	D	402	-	58,69,69	0.83	3 (5%)	55,99,99	0.99	3 (5%)
34	DGD	C	517	-	63,63,67	0.82	3 (4%)	77,77,81	1.08	5 (6%)
33	LHG	e	102	-	39,39,48	0.33	0	42,45,54	0.41	0
31	LMT	Y	101	-	21,21,36	0.35	0	26,26,47	0.73	0
30	SQD	H	103	-	52,54,54	0.43	0	62,65,65	0.52	0
25	CLA	b	612	2	69,73,73	1.25	8 (11%)	82,113,113	1.30	8 (9%)
31	LMT	e	101	-	22,22,36	0.36	0	27,27,47	0.69	0
28	LMG	b	621	-	51,51,55	0.32	0	59,59,63	0.47	1 (1%)
27	BCR	B	619	-	41,41,41	1.43	4 (9%)	56,56,56	1.34	10 (17%)
25	CLA	B	612	2	69,73,73	1.24	8 (11%)	82,113,113	1.30	8 (9%)
27	BCR	f	101	-	41,41,41	1.44	5 (12%)	56,56,56	1.39	10 (17%)
25	CLA	B	607	38	69,73,73	1.19	10 (14%)	82,113,113	1.45	7 (8%)
25	CLA	c	510	3	69,73,73	1.31	9 (13%)	82,113,113	1.29	8 (9%)
26	PHO	d	402	-	58,69,69	0.83	3 (5%)	55,99,99	0.99	3 (5%)
26	PHO	A	407	-	58,69,69	0.83	4 (6%)	55,99,99	0.94	2 (3%)
25	CLA	b	607	38	69,73,73	1.19	10 (14%)	82,113,113	1.45	7 (8%)
22	OEX	A	401	38,3,1	0,15,15	-	-	-	-	-
32	BCT	A	417	23	3,3,3	1.22	0	2,3,3	0.35	0
31	LMT	A	415	-	36,36,36	0.19	0	47,47,47	0.39	0
28	LMG	B	621	-	51,51,55	0.32	0	59,59,63	0.47	1 (1%)
31	LMT	k	105	-	36,36,36	0.38	0	47,47,47	1.38	6 (12%)
25	CLA	B	613	2	69,73,73	1.30	9 (13%)	82,113,113	1.28	8 (9%)
25	CLA	C	502	3	69,73,73	1.17	9 (13%)	82,113,113	1.38	7 (8%)
30	SQD	a	413	-	42,44,54	0.45	1 (2%)	52,55,65	0.54	1 (1%)
31	LMT	C	524	-	36,36,36	0.41	0	47,47,47	1.05	3 (6%)
25	CLA	b	613	2	69,73,73	1.30	9 (13%)	82,113,113	1.28	8 (9%)
31	LMT	X	102	-	22,22,36	0.49	0	27,27,47	0.89	0
33	LHG	z	102	-	35,35,48	0.47	0	38,40,54	0.52	1 (2%)
31	LMT	c	524	-	36,36,36	0.41	0	47,47,47	1.05	3 (6%)
25	CLA	B	601	38	49,53,73	1.35	8 (16%)	58,89,113	1.43	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	A	405	1	69,73,73	1.16	7 (10%)	82,113,113	1.25	4 (4%)
25	CLA	D	403	4	69,73,73	1.15	7 (10%)	82,113,113	1.21	5 (6%)
31	LMT	M	101	-	36,36,36	0.43	0	47,47,47	1.27	4 (8%)
31	LMT	c	520	-	24,24,36	0.37	0	29,29,47	0.99	2 (6%)
31	LMT	i	105	-	24,24,36	0.22	0	29,29,47	0.41	0
25	CLA	B	609	2	69,73,73	1.20	10 (14%)	82,113,113	1.26	8 (9%)
31	LMT	b	626	-	24,24,36	0.36	0	29,29,47	0.77	0
25	CLA	D	401	38	69,73,73	1.19	10 (14%)	82,113,113	1.40	7 (8%)
33	LHG	d	407	-	48,48,48	0.37	0	51,54,54	0.35	0
31	LMT	d	411	-	36,36,36	0.49	0	47,47,47	1.27	5 (10%)
33	LHG	Z	102	-	35,35,48	0.47	0	38,40,54	0.52	1 (2%)
36	RRX	H	101	-	42,42,42	1.44	6 (14%)	56,58,58	1.36	11 (19%)

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
30	SQD	h	103	-	-	28/49/69/69	0/1/1/1
31	LMT	I	103	-	-	8/13/33/61	0/1/1/2
31	LMT	D	410	-	-	9/15/35/61	0/1/1/2
31	LMT	a	415	-	-	15/21/61/61	0/2/2/2
27	BCR	z	101	-	-	21/29/63/63	0/2/2/2
29	PL9	D	405	-	-	7/53/73/73	0/1/1/1
33	LHG	D	413	-	-	44/53/53/53	-
34	DGD	c	517	-	-	16/51/91/95	0/2/2/2
25	CLA	B	611	2	1/1/15/20	9/39/115/115	-
31	LMT	I	101	-	-	9/15/35/61	0/1/1/2
25	CLA	C	503	3	1/1/15/20	6/39/115/115	-
28	LMG	c	519	-	-	26/44/64/70	0/1/1/1
25	CLA	B	605	2	1/1/15/20	14/39/115/115	-
33	LHG	B	628	-	-	30/53/53/53	-
25	CLA	C	513	3	1/1/15/20	19/39/115/115	-
25	CLA	b	605	2	1/1/15/20	14/39/115/115	-
34	DGD	c	516	-	-	20/51/91/95	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	614	2	1/1/15/20	16/39/115/115	-
25	CLA	a	405	1	1/1/15/20	7/39/115/115	-
25	CLA	C	509	3	1/1/15/20	9/39/115/115	-
31	LMT	x	103	-	-	5/13/33/61	0/1/1/2
31	LMT	e	103	-	-	12/21/61/61	0/2/2/2
35	HEM	V	201	18	-	0/14/54/54	-
25	CLA	B	608	2	1/1/15/20	2/39/115/115	-
31	LMT	B	623	-	-	8/21/61/61	0/2/2/2
28	LMG	j	101	-	-	34/50/70/70	0/1/1/1
31	LMT	i	104	-	-	7/15/35/61	0/1/1/2
31	LMT	x	102	-	-	8/12/32/61	0/1/1/2
31	LMT	C	523	-	-	10/15/35/61	0/1/1/2
25	CLA	C	510	3	1/1/15/20	10/39/115/115	-
31	LMT	X	101	-	-	7/15/35/61	0/1/1/2
31	LMT	c	522	-	-	8/12/32/61	0/1/1/2
33	LHG	d	408	-	-	24/53/53/53	-
30	SQD	f	102	-	-	14/29/49/69	0/1/1/1
25	CLA	d	403	4	1/1/15/20	5/39/115/115	-
25	CLA	D	404	4	-	11/39/115/115	-
31	LMT	M	102	-	-	10/15/35/61	0/1/1/2
31	LMT	x	104	-	-	7/21/61/61	0/2/2/2
29	PL9	A	411	-	-	23/53/73/73	0/1/1/1
25	CLA	c	511	3	1/1/15/20	5/39/115/115	-
34	DGD	c	515	-	-	24/51/91/95	0/2/2/2
35	HEM	v	201	18	-	0/14/54/54	-
27	BCR	B	618	-	-	11/29/63/63	0/2/2/2
31	LMT	B	629	-	-	9/21/61/61	0/2/2/2
31	LMT	I	105	-	-	10/15/35/61	0/1/1/2
31	LMT	C	522	-	-	8/12/32/61	0/1/1/2
34	DGD	C	516	-	-	20/51/91/95	0/2/2/2
25	CLA	b	611	2	1/1/15/20	9/39/115/115	-
27	BCR	C	514	-	-	11/29/63/63	0/2/2/2
28	LMG	D	409	-	-	28/50/70/70	0/1/1/1
28	LMG	C	518	-	-	19/46/66/70	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	b	619	-	-	9/29/63/63	0/2/2/2
30	SQD	k	102	-	-	27/35/55/69	0/1/1/1
27	BCR	B	617	-	-	13/29/63/63	0/2/2/2
25	CLA	c	513	3	1/1/15/20	19/39/115/115	-
31	LMT	B	626	-	-	11/15/35/61	0/1/1/2
31	LMT	F	103	-	-	11/21/61/61	0/2/2/2
31	LMT	i	102	-	-	12/21/61/61	0/2/2/2
31	LMT	d	410	-	-	9/15/35/61	0/1/1/2
33	LHG	d	412	-	-	44/53/53/53	-
27	BCR	c	514	-	-	11/29/63/63	0/2/2/2
30	SQD	A	413	-	-	21/39/59/69	0/1/1/1
25	CLA	B	616	2	1/1/14/20	11/33/109/115	-
25	CLA	B	603	2	1/1/15/20	13/39/115/115	-
30	SQD	C	525	-	-	22/49/69/69	0/1/1/1
31	LMT	B	625	-	-	16/21/61/61	0/2/2/2
25	CLA	b	616	2	1/1/14/20	11/33/109/115	-
27	BCR	F	101	-	-	11/29/63/63	0/2/2/2
31	LMT	m	102	-	-	10/15/35/61	0/1/1/2
25	CLA	c	501	3	1/1/15/20	5/39/115/115	-
31	LMT	b	624	-	-	11/15/35/61	0/1/1/2
31	LMT	T	101	-	-	9/15/35/61	0/1/1/2
25	CLA	a	408	1	-	13/33/109/115	-
31	LMT	y	101	-	-	8/12/32/61	0/1/1/2
28	LMG	a	410	-	-	23/46/66/70	0/1/1/1
28	LMG	c	518	-	-	19/46/66/70	0/1/1/1
25	CLA	b	601	38	1/1/11/20	5/15/91/115	-
25	CLA	c	509	3	1/1/15/20	9/39/115/115	-
27	BCR	K	103	-	-	19/29/63/63	0/2/2/2
31	LMT	L	105	-	-	13/21/61/61	0/2/2/2
35	HEM	e	104	5,6	-	4/14/54/54	-
25	CLA	b	614	2	1/1/15/20	16/39/115/115	-
25	CLA	C	508	3	1/1/15/20	10/39/115/115	-
34	DGD	C	515	-	-	24/51/91/95	0/2/2/2
25	CLA	b	610	38	1/1/15/20	12/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	A	406	38	1/1/15/20	11/39/115/115	-
26	PHO	a	407	-	-	13/37/103/103	0/5/6/6
31	LMT	D	411	-	-	14/21/61/61	0/2/2/2
25	CLA	C	512	3	1/1/15/20	18/39/115/115	-
30	SQD	A	412	-	-	31/49/69/69	0/1/1/1
25	CLA	B	610	38	1/1/15/20	12/39/115/115	-
25	CLA	b	602	2	1/1/15/20	9/39/115/115	-
27	BCR	K	104	-	-	12/29/63/63	0/2/2/2
25	CLA	C	506	3	1/1/15/20	11/39/115/115	-
27	BCR	Z	101	-	-	21/29/63/63	0/2/2/2
31	LMT	C	521	-	-	10/21/61/61	0/2/2/2
25	CLA	C	507	38	1/1/15/20	15/39/115/115	-
29	PL9	a	411	-	-	23/53/73/73	0/1/1/1
29	PL9	d	405	-	-	7/53/73/73	0/1/1/1
30	SQD	c	525	-	-	22/49/69/69	0/1/1/1
31	LMT	i	101	-	-	9/15/35/61	0/1/1/2
25	CLA	c	504	38	1/1/15/20	9/39/115/115	-
33	LHG	b	628	-	-	30/53/53/53	-
25	CLA	c	506	3	1/1/15/20	11/39/115/115	-
31	LMT	c	521	-	-	10/21/61/61	0/2/2/2
33	LHG	D	406	-	-	20/53/53/53	-
25	CLA	b	604	2	1/1/15/20	10/39/115/115	-
25	CLA	c	507	38	1/1/15/20	15/39/115/115	-
25	CLA	B	615	2	1/1/15/20	11/39/115/115	-
31	LMT	C	520	-	-	9/15/35/61	0/1/1/2
28	LMG	a	414	-	-	14/31/51/70	0/1/1/1
31	LMT	B	627	-	-	7/15/35/61	0/1/1/2
31	LMT	b	623	-	-	8/21/61/61	0/2/2/2
31	LMT	x	101	-	-	7/15/35/61	0/1/1/2
25	CLA	b	608	2	1/1/15/20	2/39/115/115	-
31	LMT	t	101	-	-	9/15/35/61	0/1/1/2
25	CLA	A	408	1	1/1/14/20	13/33/109/115	-
30	SQD	b	620	-	-	24/49/69/69	0/1/1/1
25	CLA	C	501	3	1/1/15/20	5/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	B	624	-	-	11/15/35/61	0/1/1/2
31	LMT	b	630	-	-	7/15/35/61	0/1/1/2
25	CLA	C	511	3	1/1/15/20	5/39/115/115	-
25	CLA	C	505	3	1/1/15/20	11/39/115/115	-
27	BCR	k	103	-	-	19/29/63/63	0/2/2/2
25	CLA	C	504	38	1/1/15/20	9/39/115/115	-
30	SQD	B	620	-	-	24/49/69/69	0/1/1/1
25	CLA	c	503	3	1/1/15/20	6/39/115/115	-
27	BCR	b	617	-	-	13/29/63/63	0/2/2/2
28	LMG	A	410	-	-	23/46/66/70	0/1/1/1
31	LMT	i	103	-	-	8/13/33/61	0/1/1/2
33	LHG	E	102	-	-	21/44/44/53	-
25	CLA	d	401	38	1/1/15/20	7/39/115/115	-
27	BCR	z	103	-	-	12/29/63/63	0/2/2/2
31	LMT	X	103	-	-	5/13/33/61	0/1/1/2
27	BCR	b	618	-	-	11/29/63/63	0/2/2/2
27	BCR	A	409	-	-	10/29/63/63	0/2/2/2
31	LMT	f	103	-	-	11/21/61/61	0/2/2/2
33	LHG	d	406	-	-	20/53/53/53	-
33	LHG	D	407	-	-	19/53/53/53	-
34	DGD	h	104	-	-	16/51/91/95	0/2/2/2
25	CLA	b	603	2	1/1/15/20	13/39/115/115	-
27	BCR	a	409	-	-	10/29/63/63	0/2/2/2
31	LMT	E	101	-	-	7/13/33/61	0/1/1/2
25	CLA	c	502	3	-	9/39/115/115	-
28	LMG	d	409	-	-	28/50/70/70	0/1/1/1
31	LMT	I	102	-	-	12/21/61/61	0/2/2/2
25	CLA	c	508	3	1/1/15/20	10/39/115/115	-
34	DGD	H	104	-	-	16/51/91/95	0/2/2/2
35	HEM	E	104	5,6	-	4/14/54/54	-
25	CLA	B	604	2	1/1/15/20	10/39/115/115	-
31	LMT	c	523	-	-	10/15/35/61	0/1/1/2
25	CLA	c	505	3	1/1/15/20	11/39/115/115	-
28	LMG	A	414	-	-	14/31/51/70	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMG	J	101	-	-	33/50/70/70	0/1/1/1
28	LMG	C	519	-	-	26/44/64/70	0/1/1/1
31	LMT	I	104	-	-	7/15/35/61	0/1/1/2
31	LMT	E	103	-	-	12/21/61/61	0/2/2/2
25	CLA	B	602	2	1/1/15/20	9/39/115/115	-
25	CLA	B	606	2	1/1/14/20	5/33/109/115	-
31	LMT	b	625	-	-	16/21/61/61	0/2/2/2
30	SQD	K	102	-	-	27/35/55/69	0/1/1/1
25	CLA	b	606	2	1/1/14/20	5/33/109/115	-
25	CLA	b	609	2	1/1/15/20	7/39/115/115	-
33	LHG	D	408	-	-	24/53/53/53	-
30	SQD	a	412	-	-	31/49/69/69	0/1/1/1
31	LMT	D	412	-	-	7/21/61/61	0/2/2/2
25	CLA	c	512	3	1/1/15/20	18/39/115/115	-
31	LMT	b	629	-	-	9/21/61/61	0/2/2/2
25	CLA	b	615	2	1/1/15/20	11/39/115/115	-
36	RRX	h	101	-	-	13/29/65/65	0/2/2/2
25	CLA	d	404	4	-	11/39/115/115	-
31	LMT	K	105	-	-	15/21/61/61	0/2/2/2
25	CLA	a	406	38	1/1/15/20	11/39/115/115	-
30	SQD	F	102	-	-	14/29/49/69	0/1/1/1
26	PHO	D	402	-	-	2/37/103/103	0/5/6/6
34	DGD	C	517	-	-	16/51/91/95	0/2/2/2
33	LHG	e	102	-	-	21/44/44/53	-
31	LMT	Y	101	-	-	8/12/32/61	0/1/1/2
30	SQD	H	103	-	-	28/49/69/69	0/1/1/1
25	CLA	b	612	2	1/1/15/20	9/39/115/115	-
31	LMT	e	101	-	-	7/13/33/61	0/1/1/2
28	LMG	b	621	-	-	20/46/66/70	0/1/1/1
27	BCR	B	619	-	-	9/29/63/63	0/2/2/2
25	CLA	B	612	2	1/1/15/20	9/39/115/115	-
27	BCR	f	101	-	-	11/29/63/63	0/2/2/2
25	CLA	B	607	38	1/1/15/20	7/39/115/115	-
25	CLA	c	510	3	1/1/15/20	10/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PHO	d	402	-	-	2/37/103/103	0/5/6/6
26	PHO	A	407	-	-	13/37/103/103	0/5/6/6
25	CLA	b	607	38	1/1/15/20	7/39/115/115	-
31	LMT	A	415	-	-	15/21/61/61	0/2/2/2
28	LMG	B	621	-	-	20/46/66/70	0/1/1/1
31	LMT	k	105	-	-	15/21/61/61	0/2/2/2
25	CLA	B	613	2	1/1/15/20	9/39/115/115	-
25	CLA	C	502	3	-	9/39/115/115	-
30	SQD	a	413	-	-	21/39/59/69	0/1/1/1
31	LMT	C	524	-	-	12/21/61/61	0/2/2/2
25	CLA	b	613	2	1/1/15/20	9/39/115/115	-
31	LMT	X	102	-	-	8/12/32/61	0/1/1/2
33	LHG	z	102	-	-	18/37/37/53	-
31	LMT	c	524	-	-	12/21/61/61	0/2/2/2
25	CLA	B	601	38	1/1/11/20	5/15/91/115	-
25	CLA	A	405	1	1/1/15/20	7/39/115/115	-
25	CLA	D	403	4	1/1/15/20	5/39/115/115	-
31	LMT	M	101	-	-	13/21/61/61	0/2/2/2
31	LMT	c	520	-	-	9/15/35/61	0/1/1/2
31	LMT	i	105	-	-	10/15/35/61	0/1/1/2
25	CLA	B	609	2	1/1/15/20	7/39/115/115	-
31	LMT	b	626	-	-	11/15/35/61	0/1/1/2
25	CLA	D	401	38	1/1/15/20	7/39/115/115	-
33	LHG	d	407	-	-	19/53/53/53	-
31	LMT	d	411	-	-	14/21/61/61	0/2/2/2
33	LHG	Z	102	-	-	18/37/37/53	-
36	RRX	H	101	-	-	13/29/65/65	0/2/2/2

The worst 5 of 788 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	D	405	PL9	C3-C4	-5.69	1.40	1.49
29	d	405	PL9	C3-C4	-5.69	1.40	1.49
35	e	104	HEM	FE-NB	5.21	2.10	1.94
35	E	104	HEM	FE-NB	5.19	2.10	1.94
25	C	510	CLA	MG-ND	-5.13	1.95	2.05

The worst 5 of 931 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	507	CLA	C4A-NA-C1A	8.74	110.67	106.68
25	C	507	CLA	C4A-NA-C1A	8.66	110.63	106.68
25	B	607	CLA	C4A-NA-C1A	8.26	110.45	106.68
25	b	607	CLA	C4A-NA-C1A	8.26	110.45	106.68
25	C	506	CLA	C4A-NA-C1A	7.12	109.93	106.68

5 of 65 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	405	CLA	ND
25	A	406	CLA	ND
25	A	408	CLA	ND
25	B	601	CLA	ND
25	B	602	CLA	ND

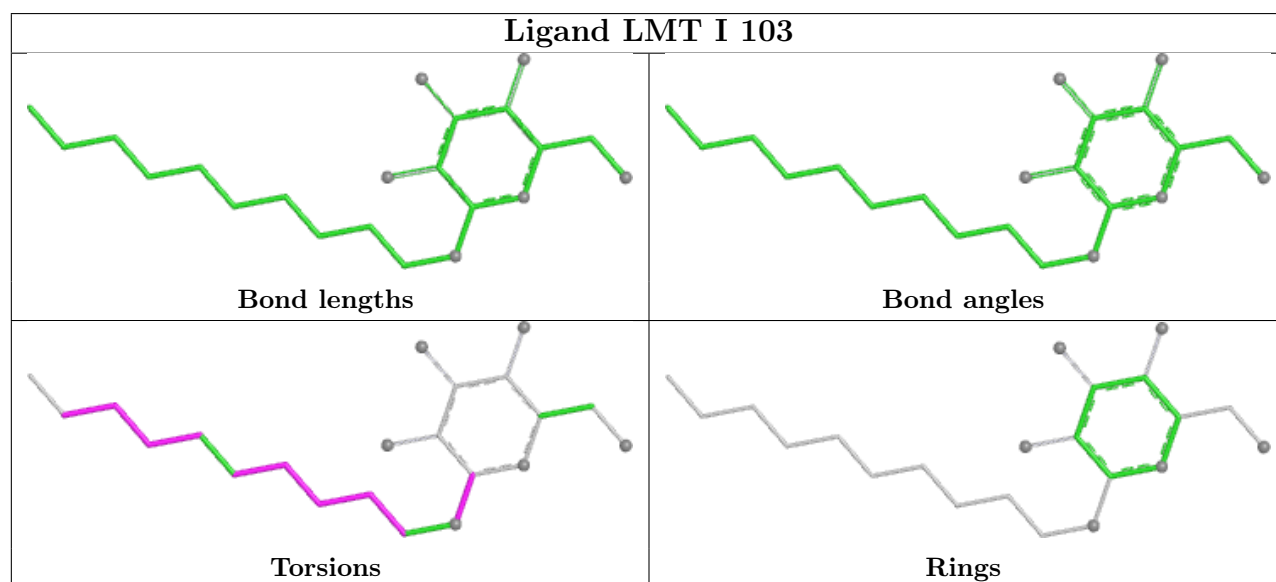
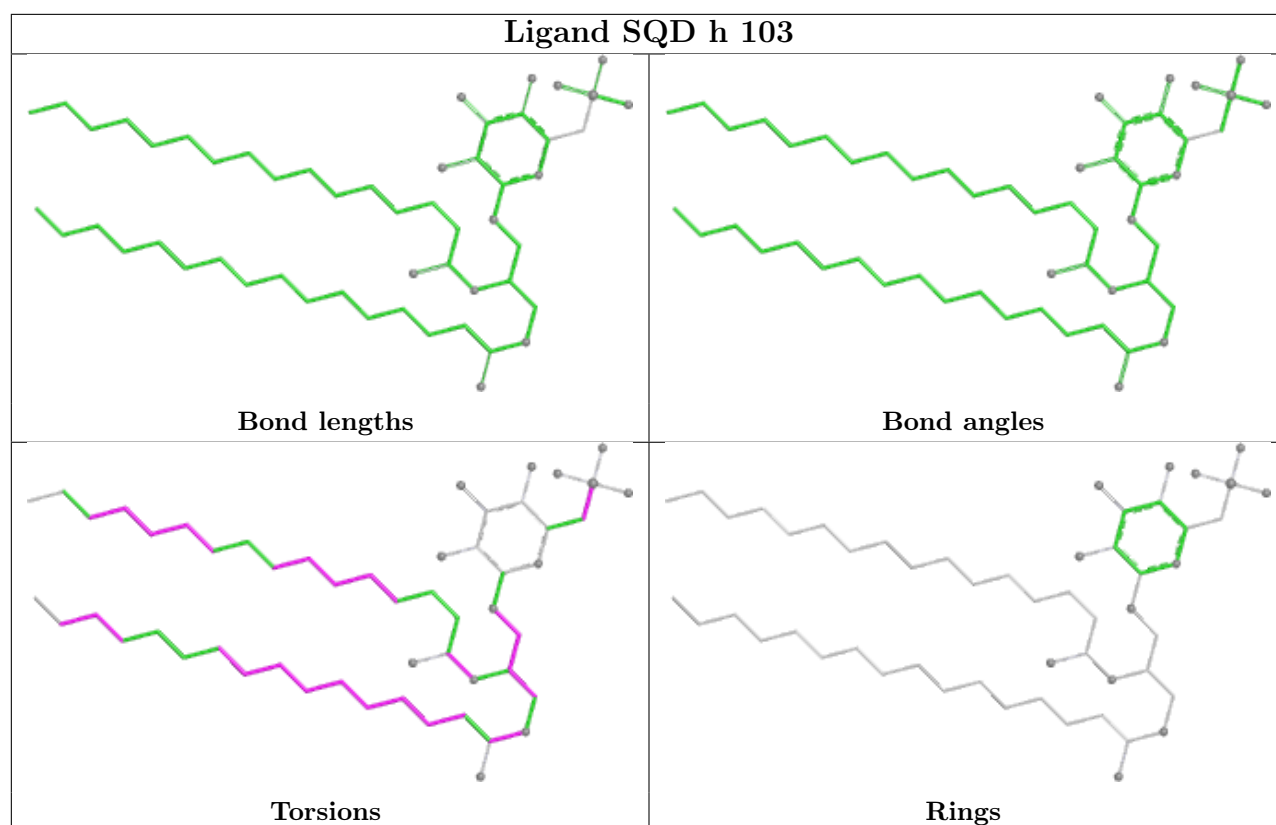
5 of 2817 torsion outliers are listed below:

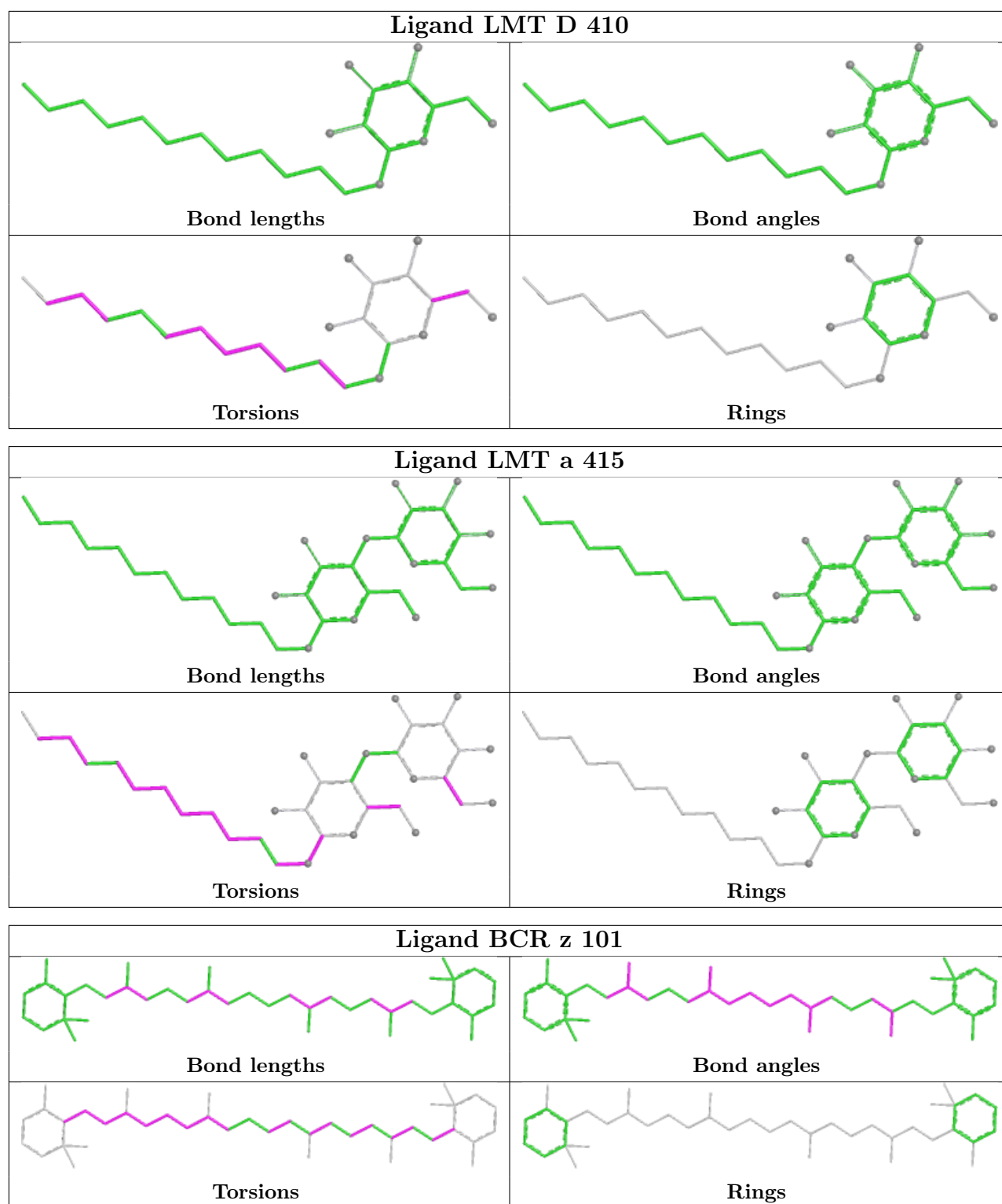
Mol	Chain	Res	Type	Atoms
25	B	613	CLA	C12-C13-C15-C16
25	B	614	CLA	CAD-CBD-CGD-O1D
25	B	614	CLA	CAD-CBD-CGD-O2D
25	C	506	CLA	C11-C12-C13-C14
25	C	507	CLA	C2B-C3B-CAB-CBB

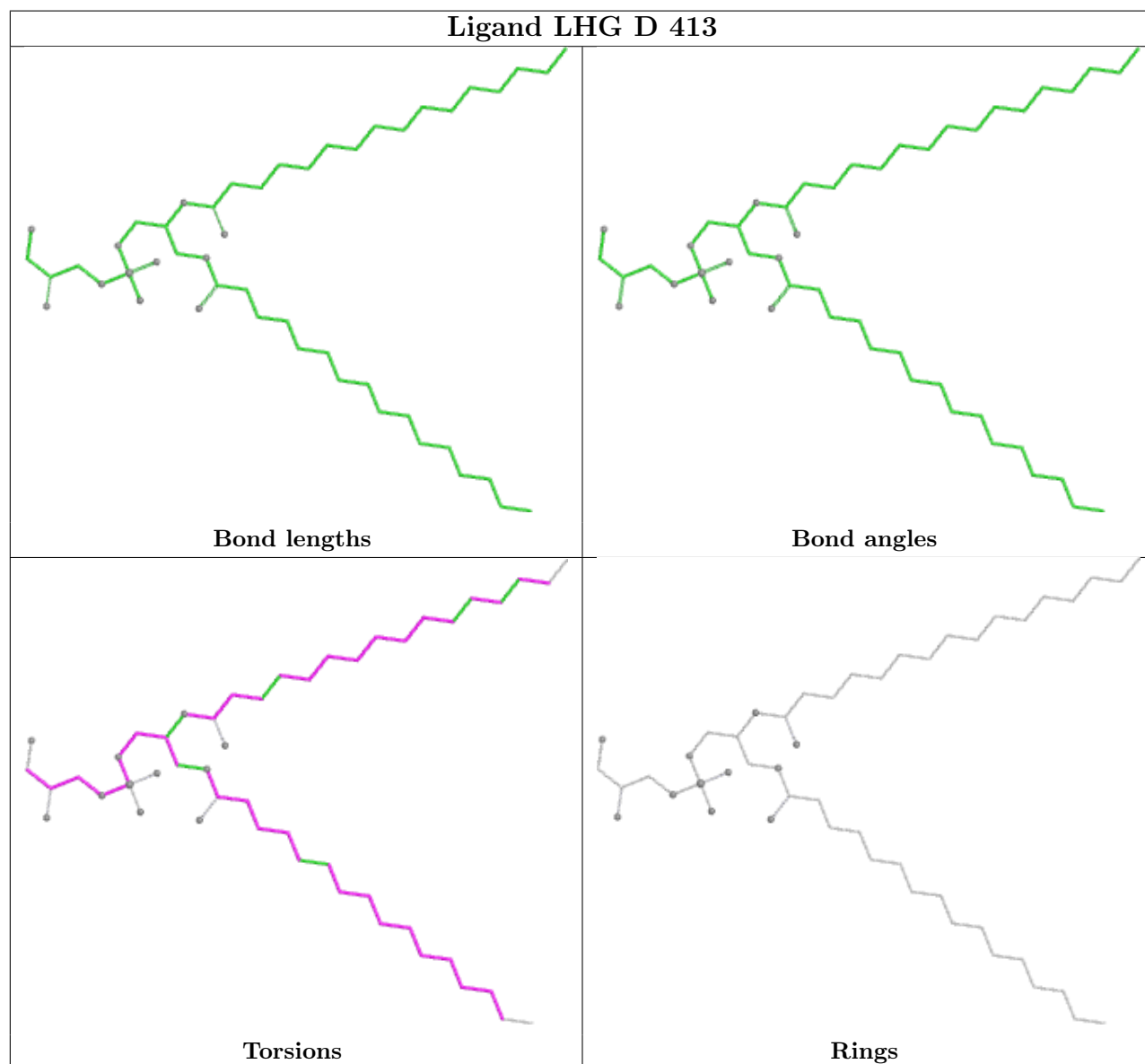
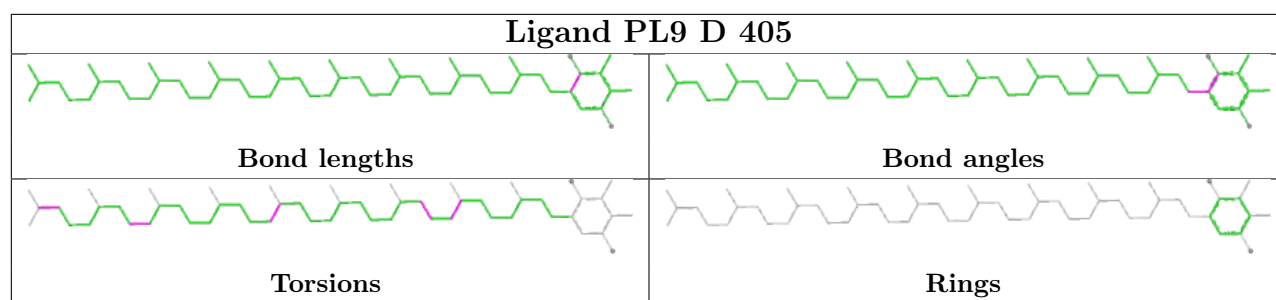
There are no ring outliers.

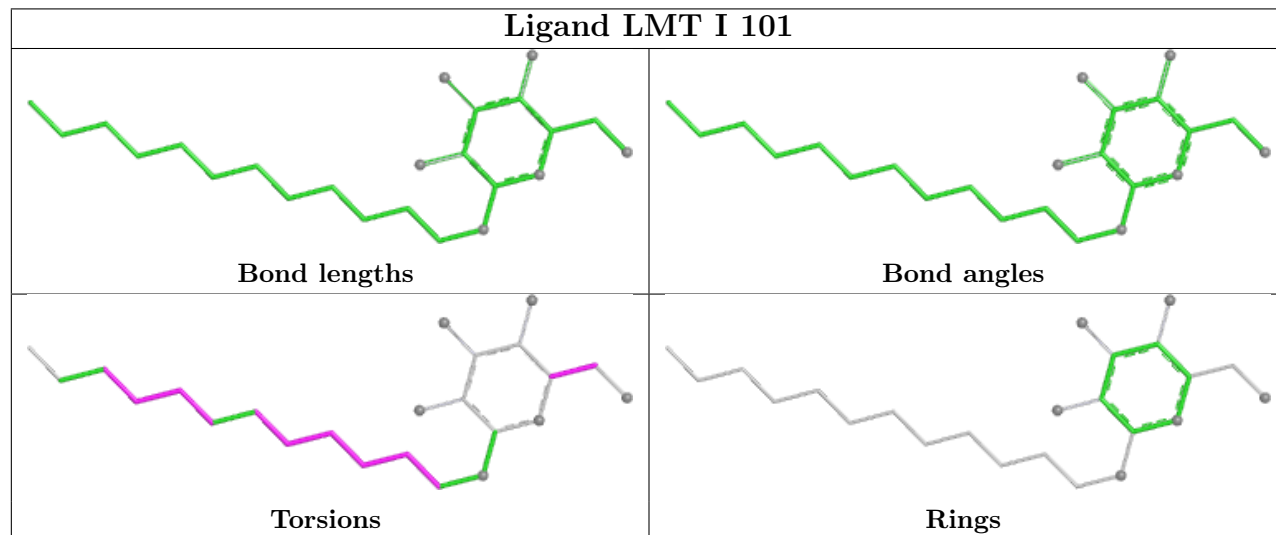
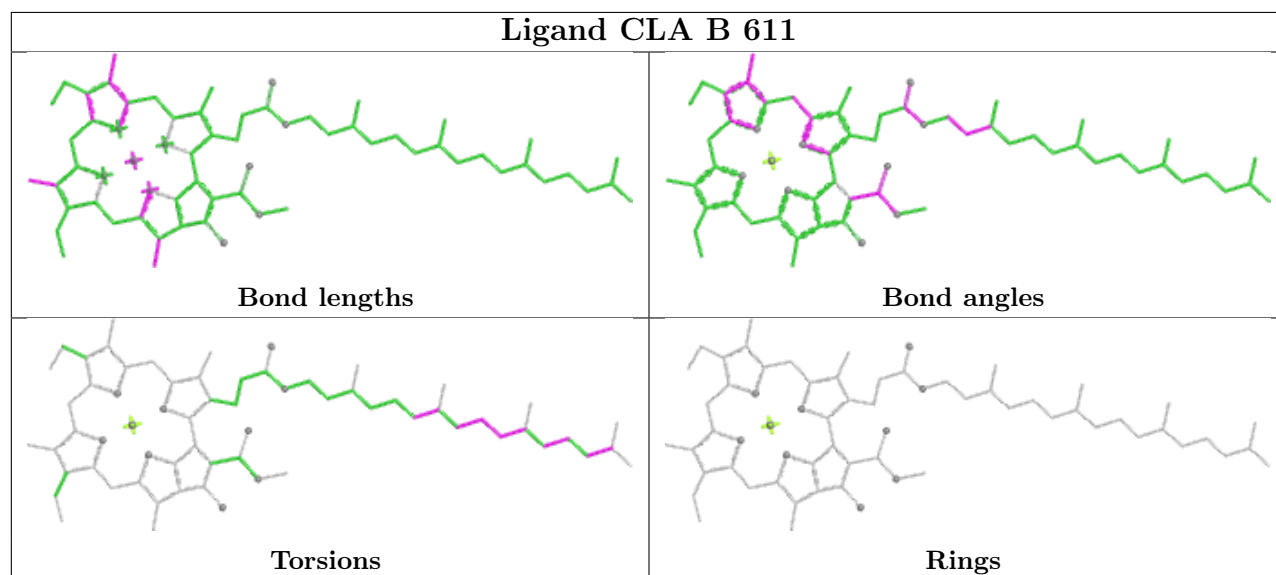
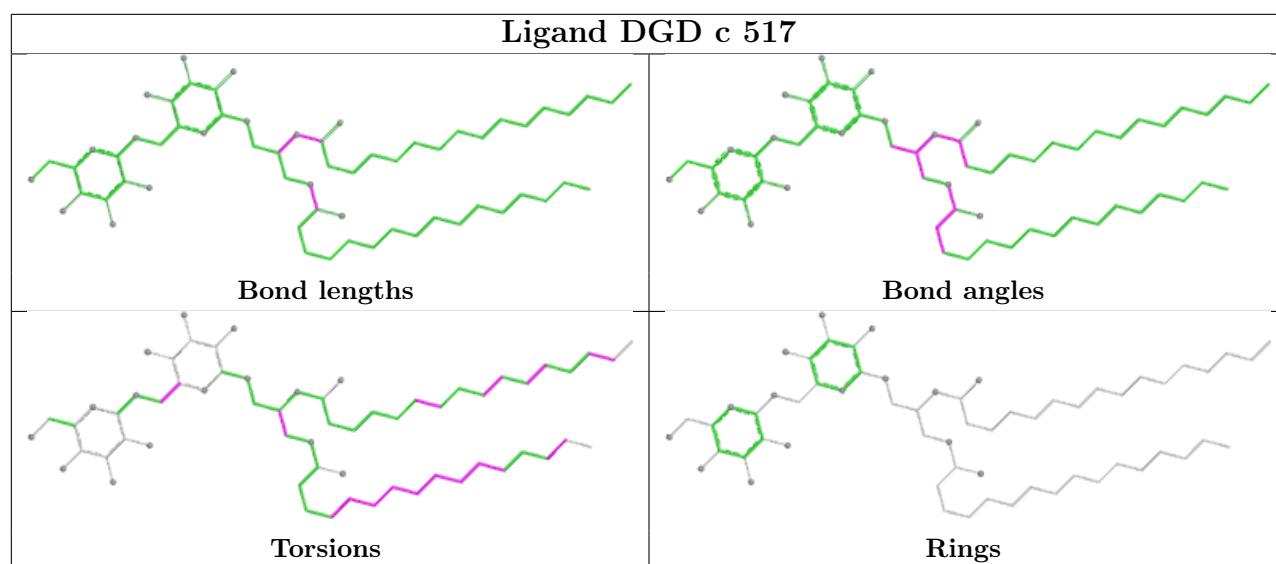
No monomer is involved in short contacts.

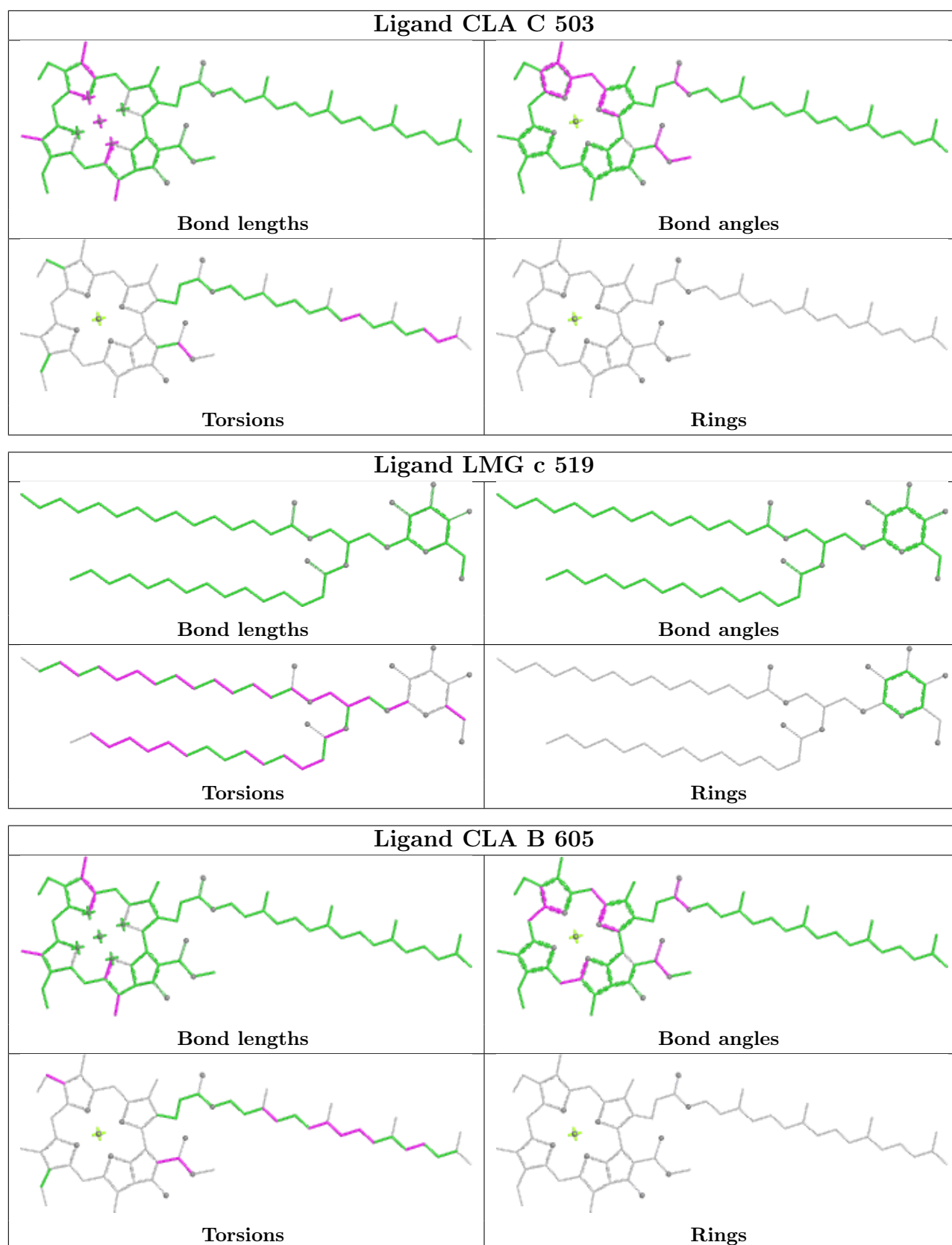
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

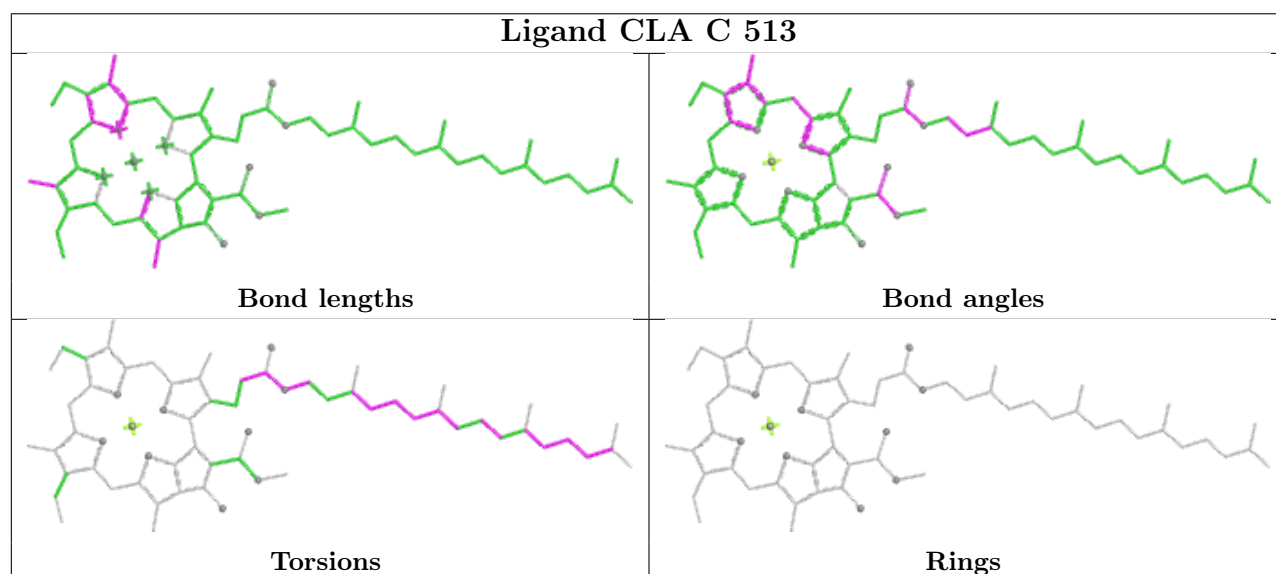
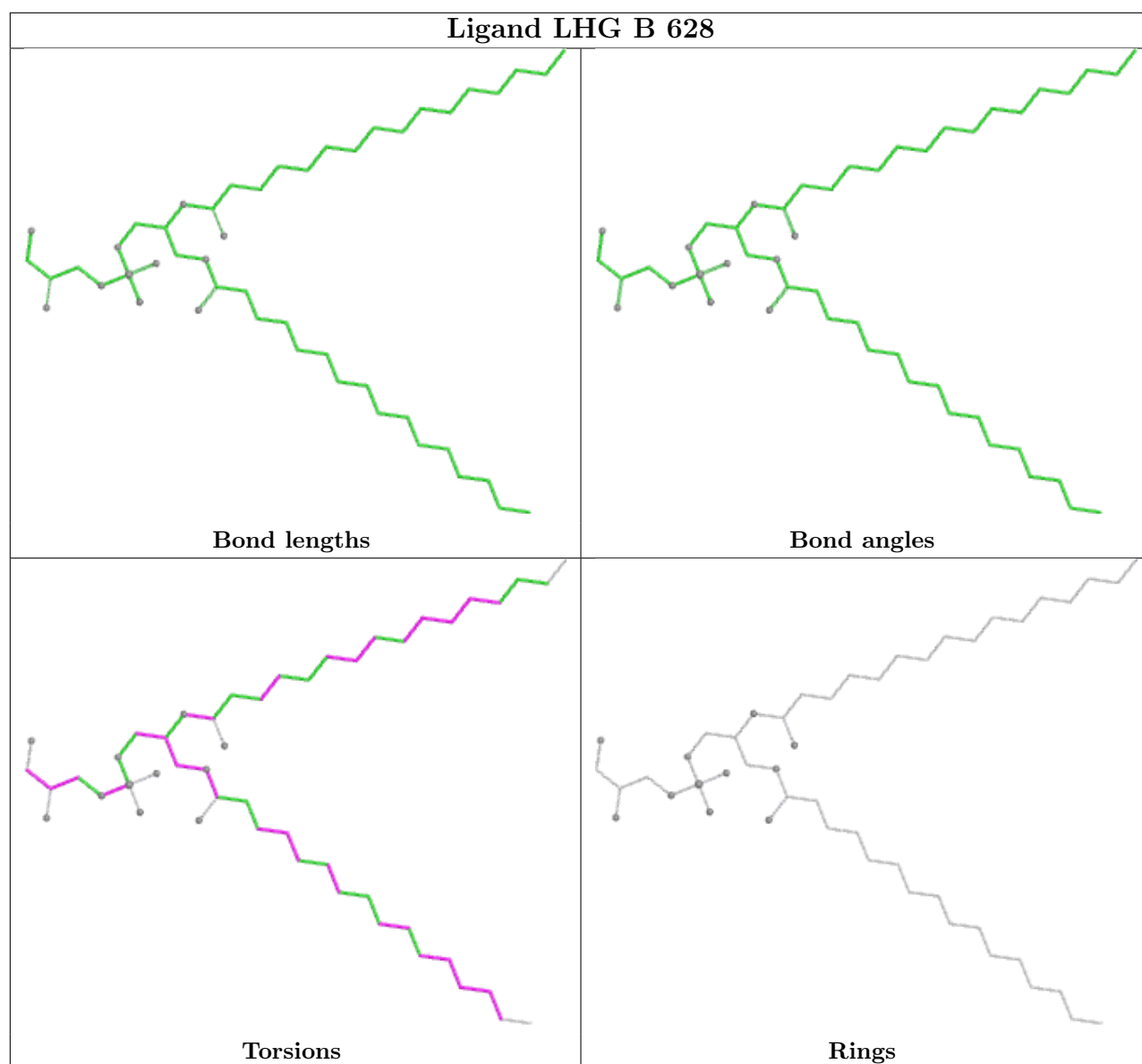


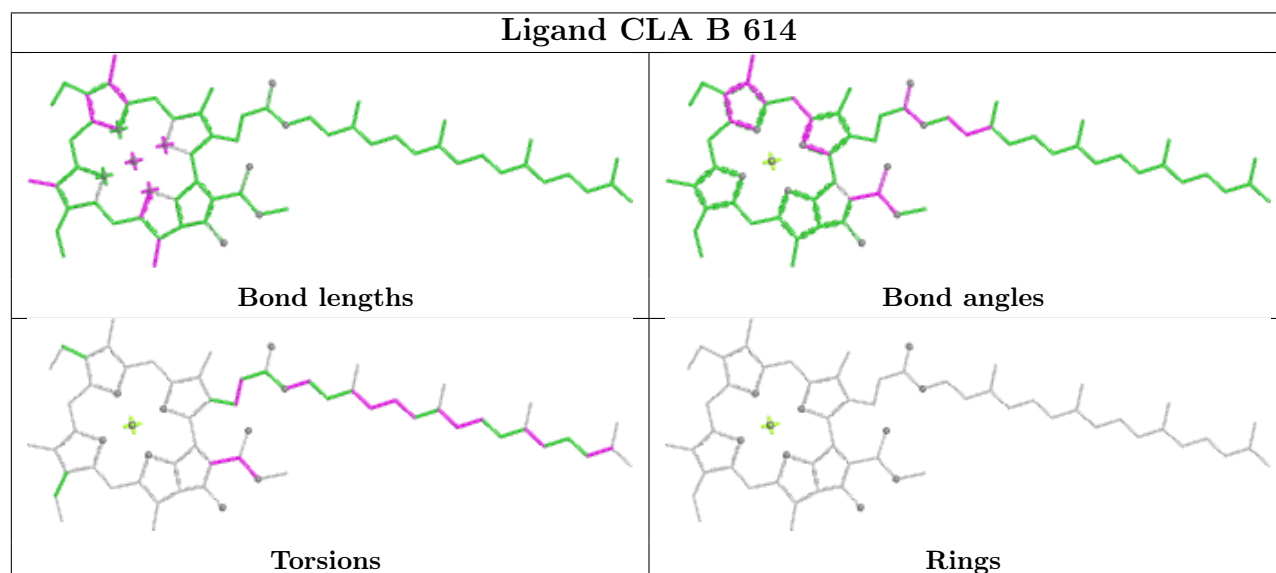
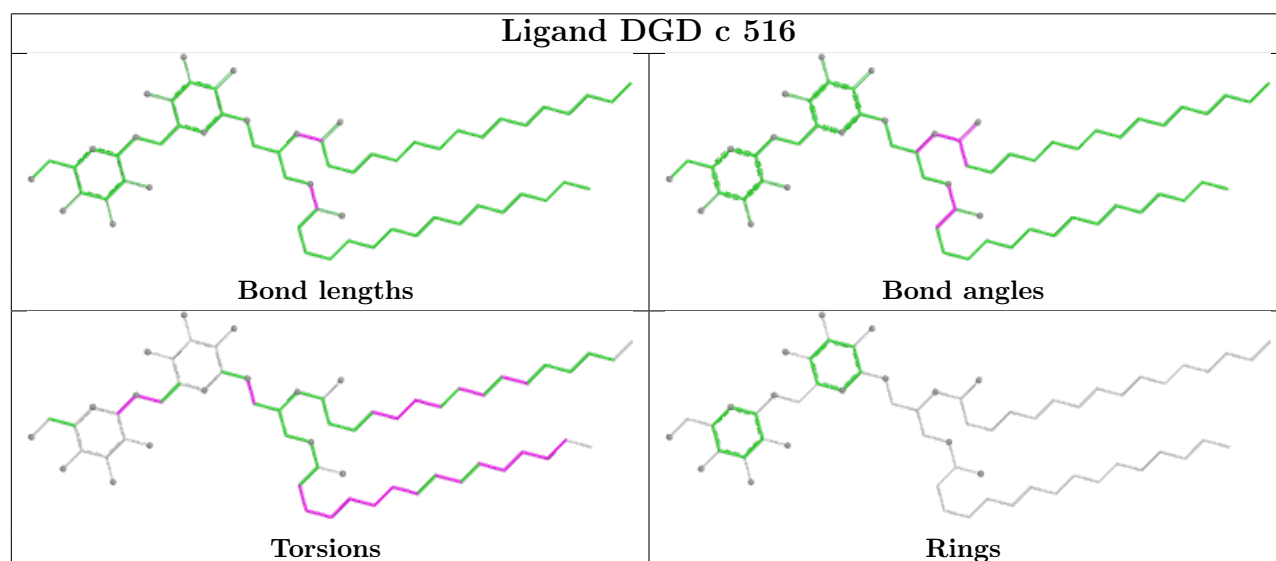
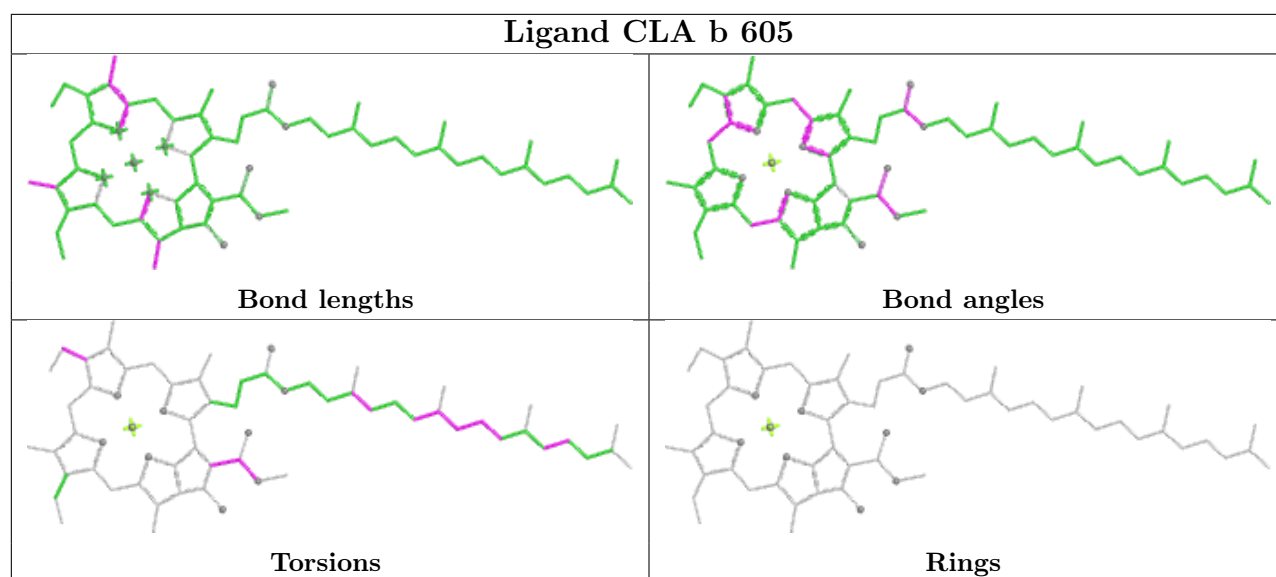


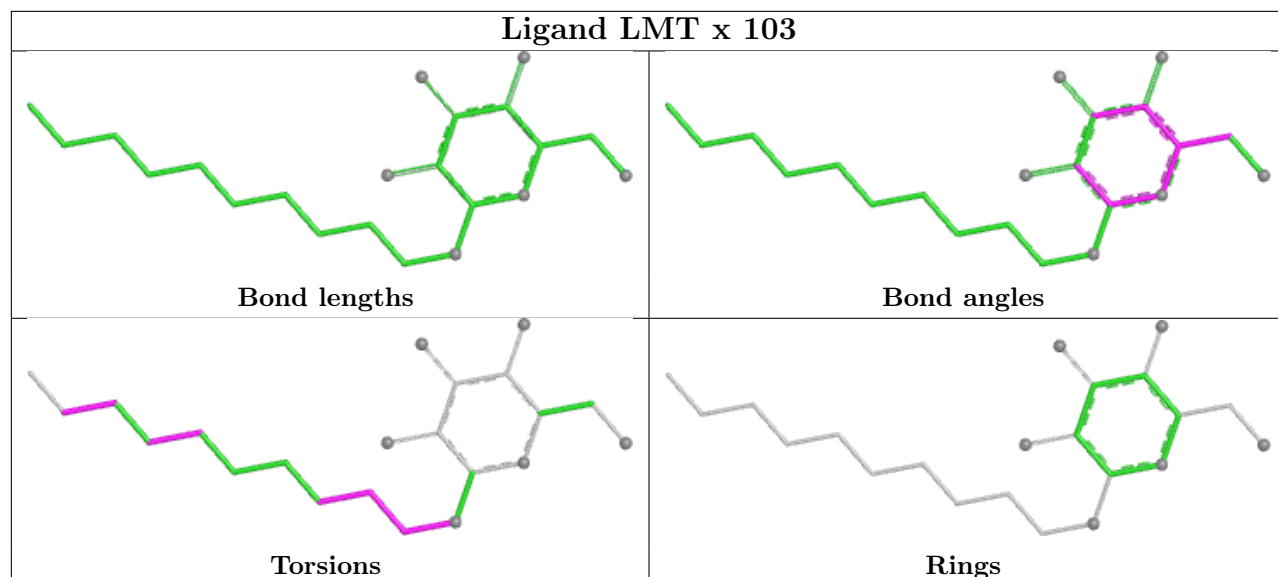
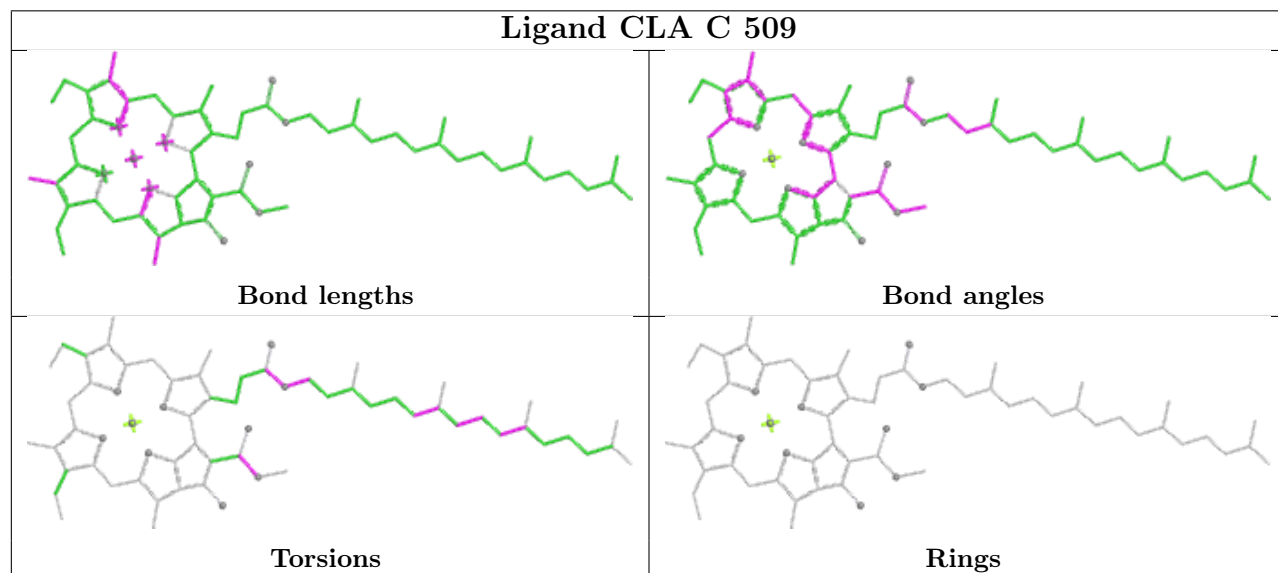
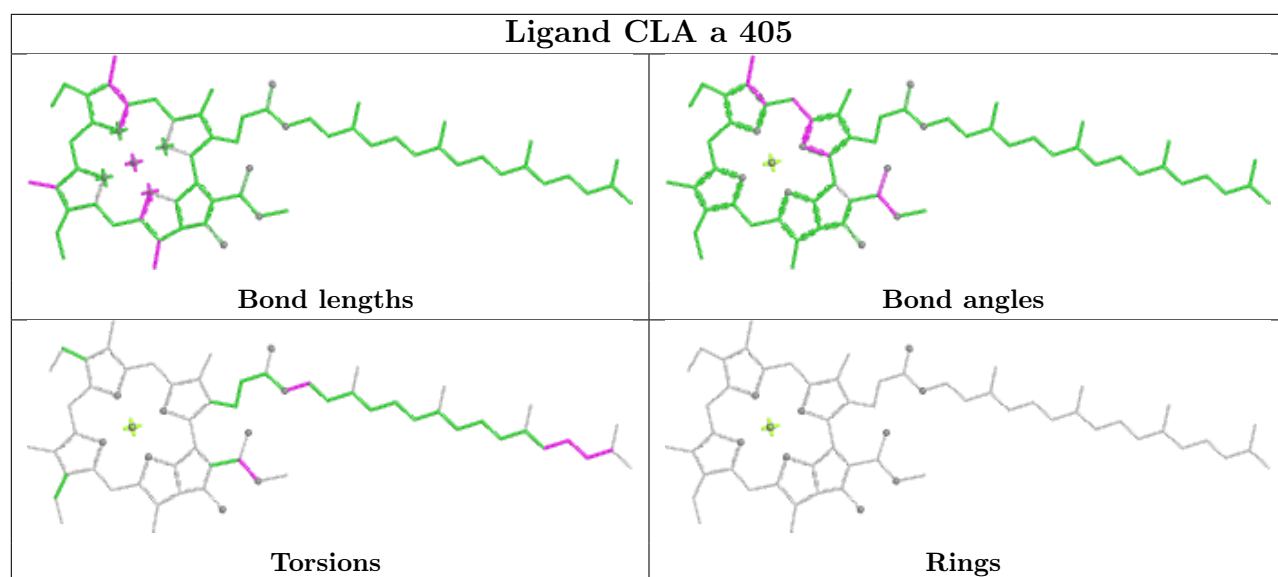


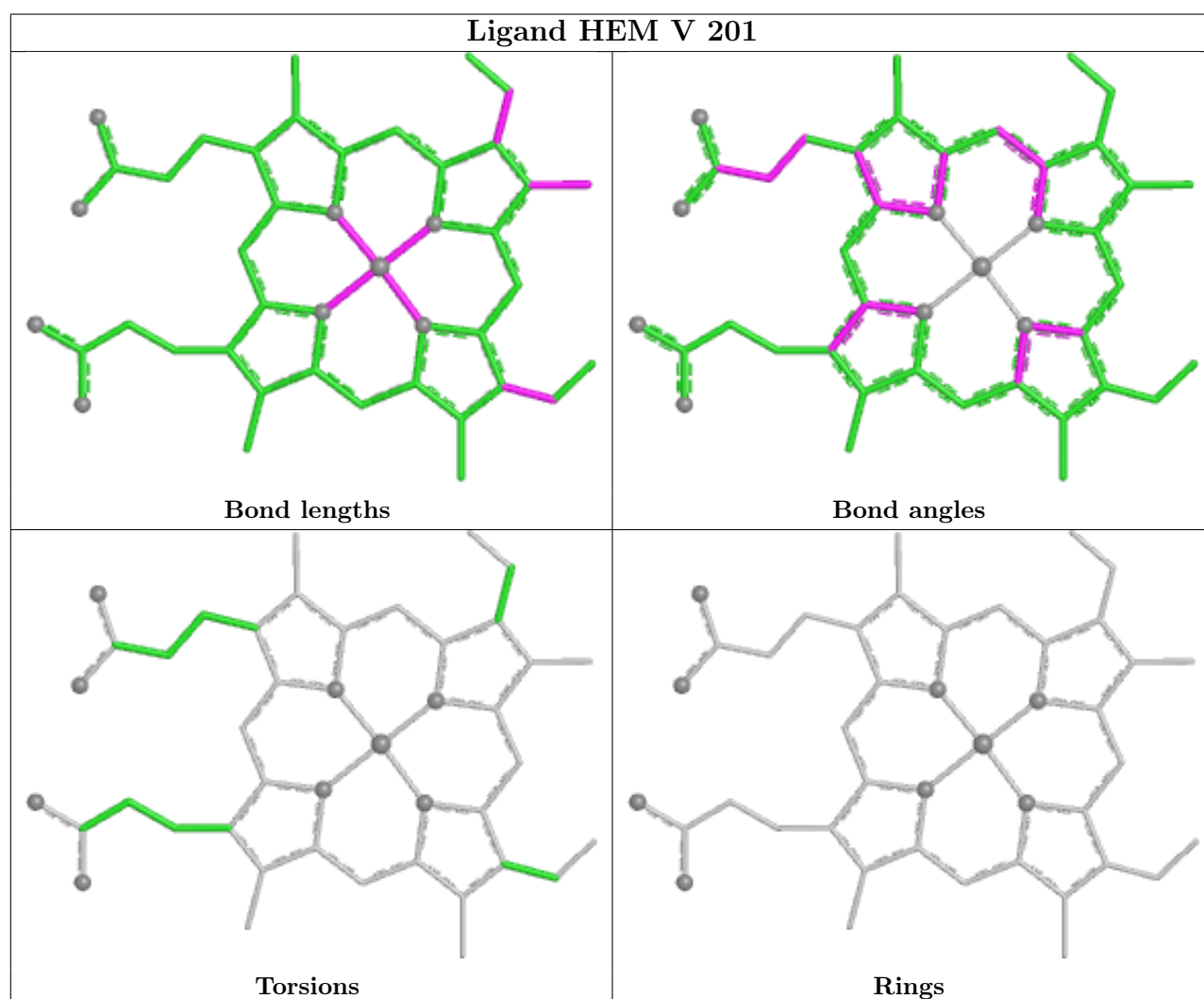
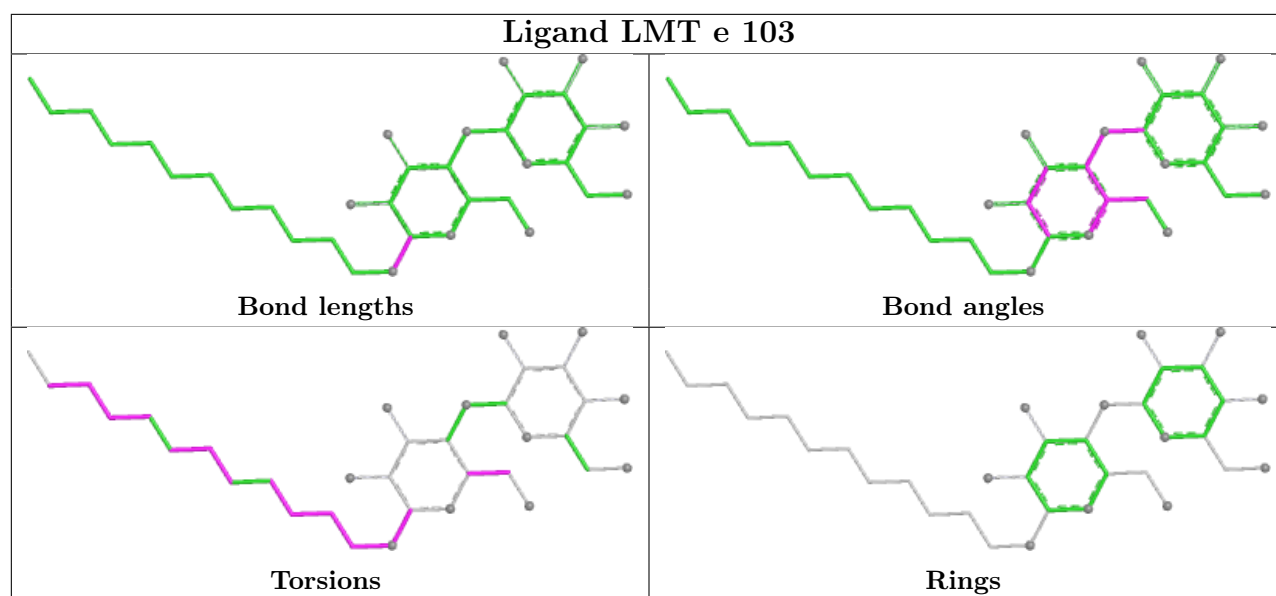


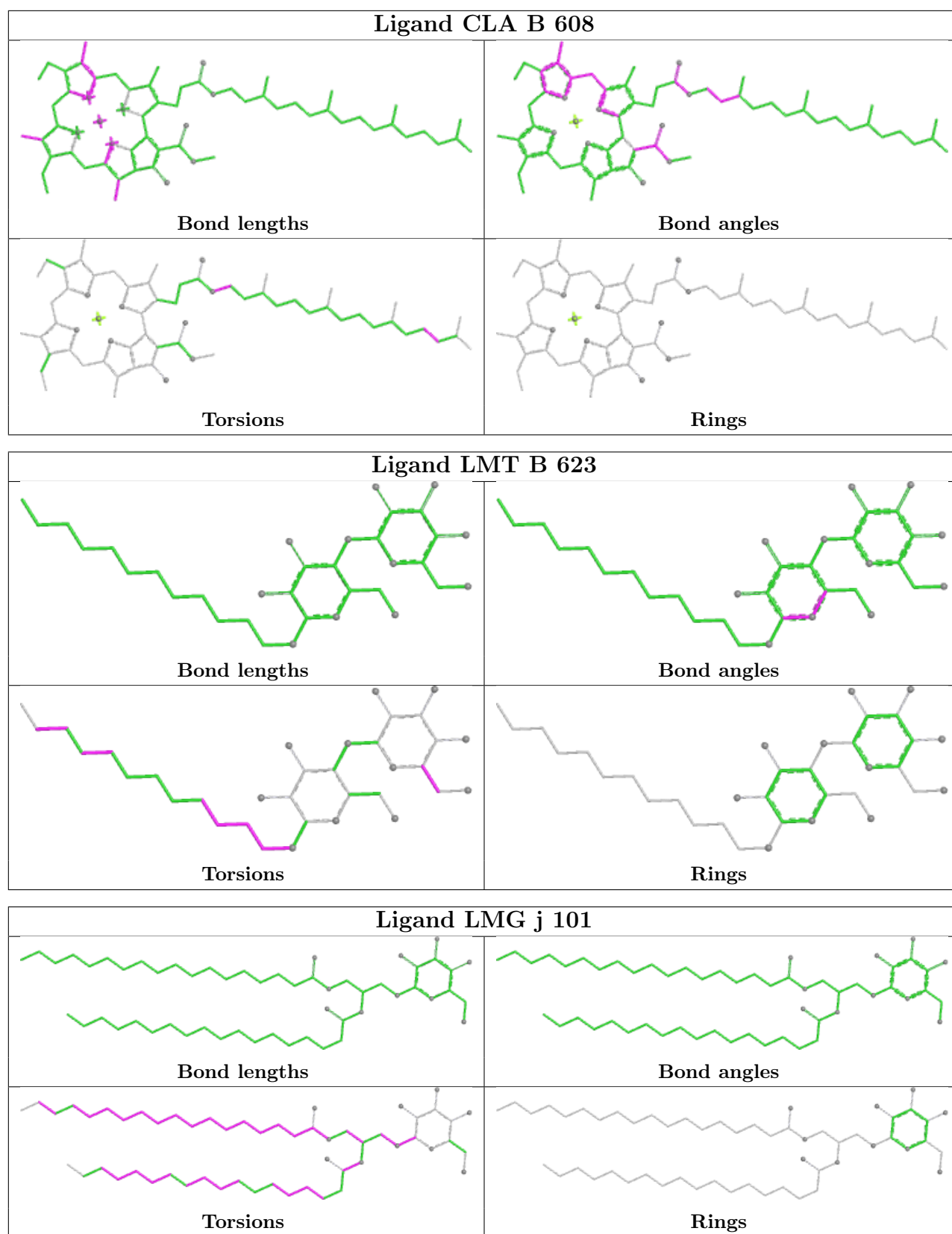


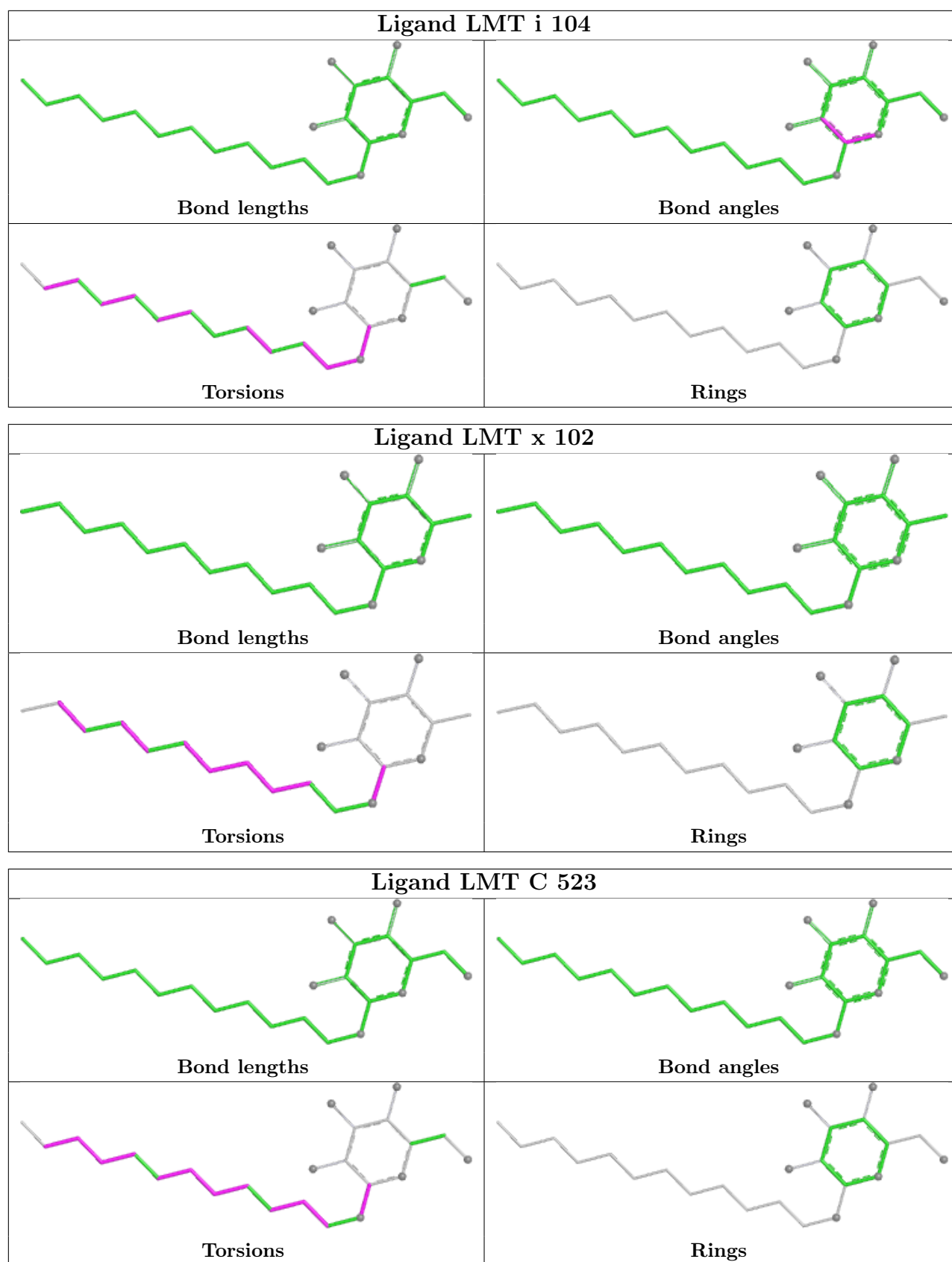


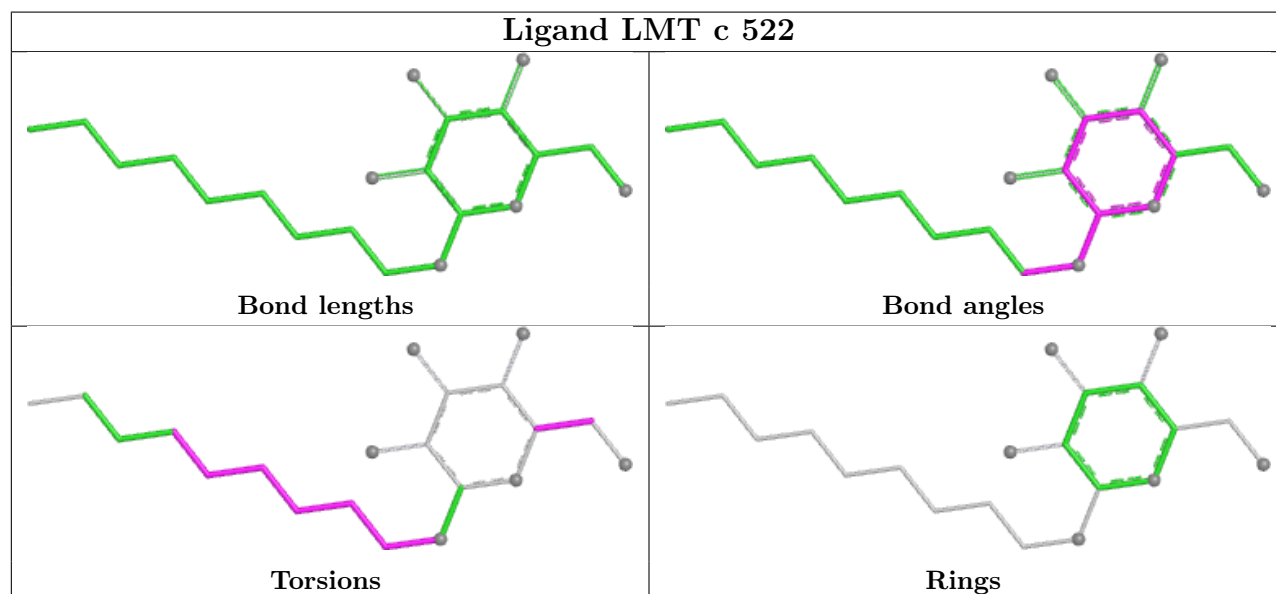
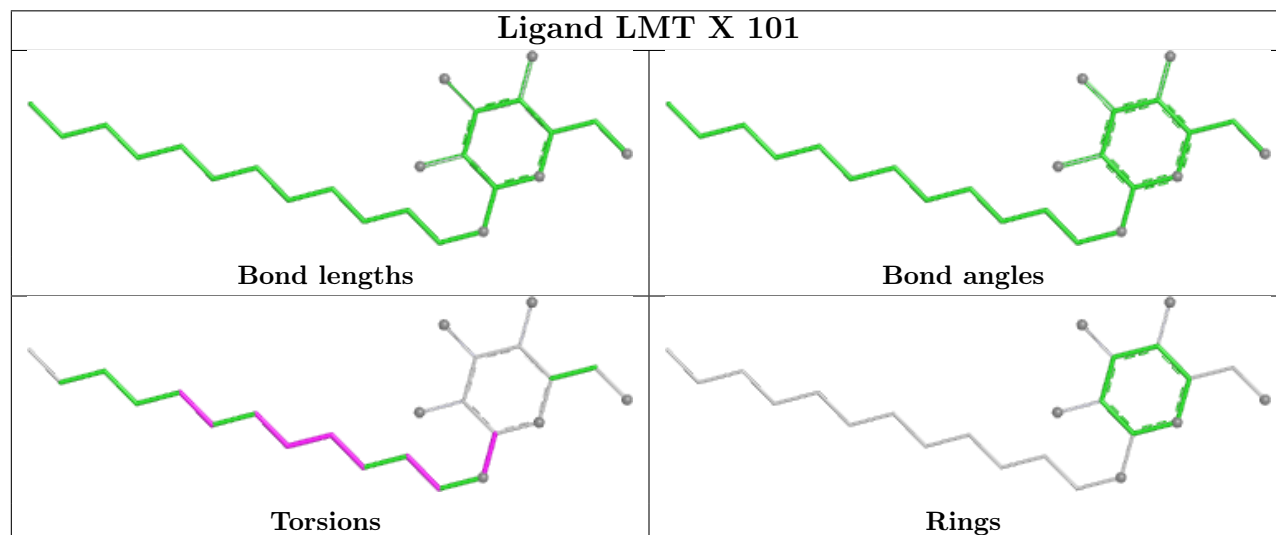
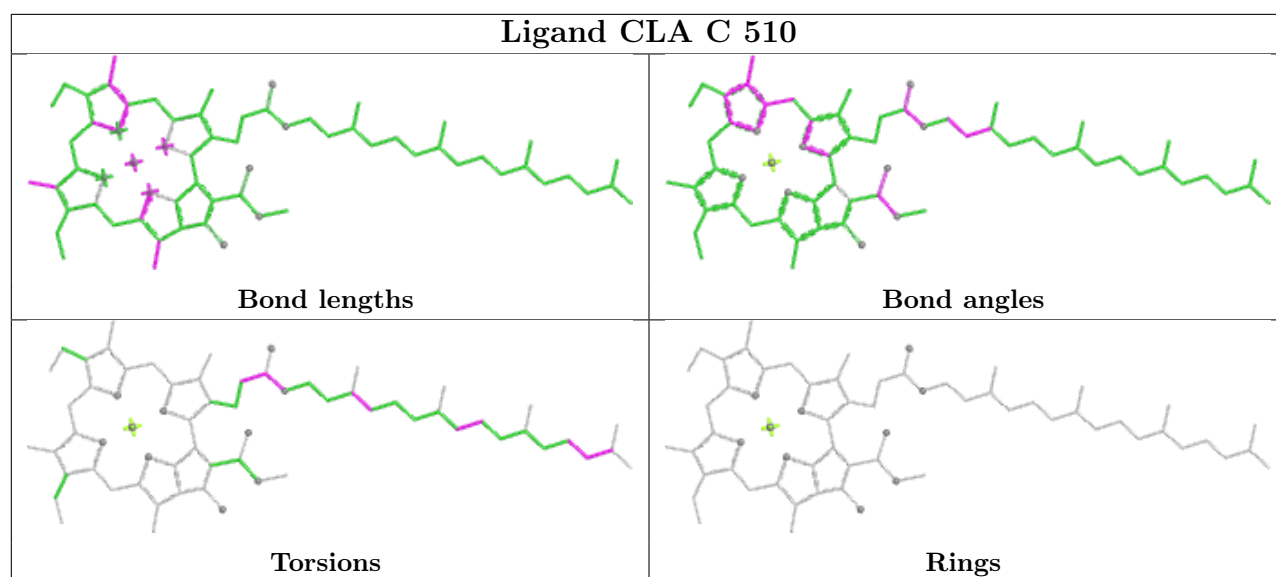


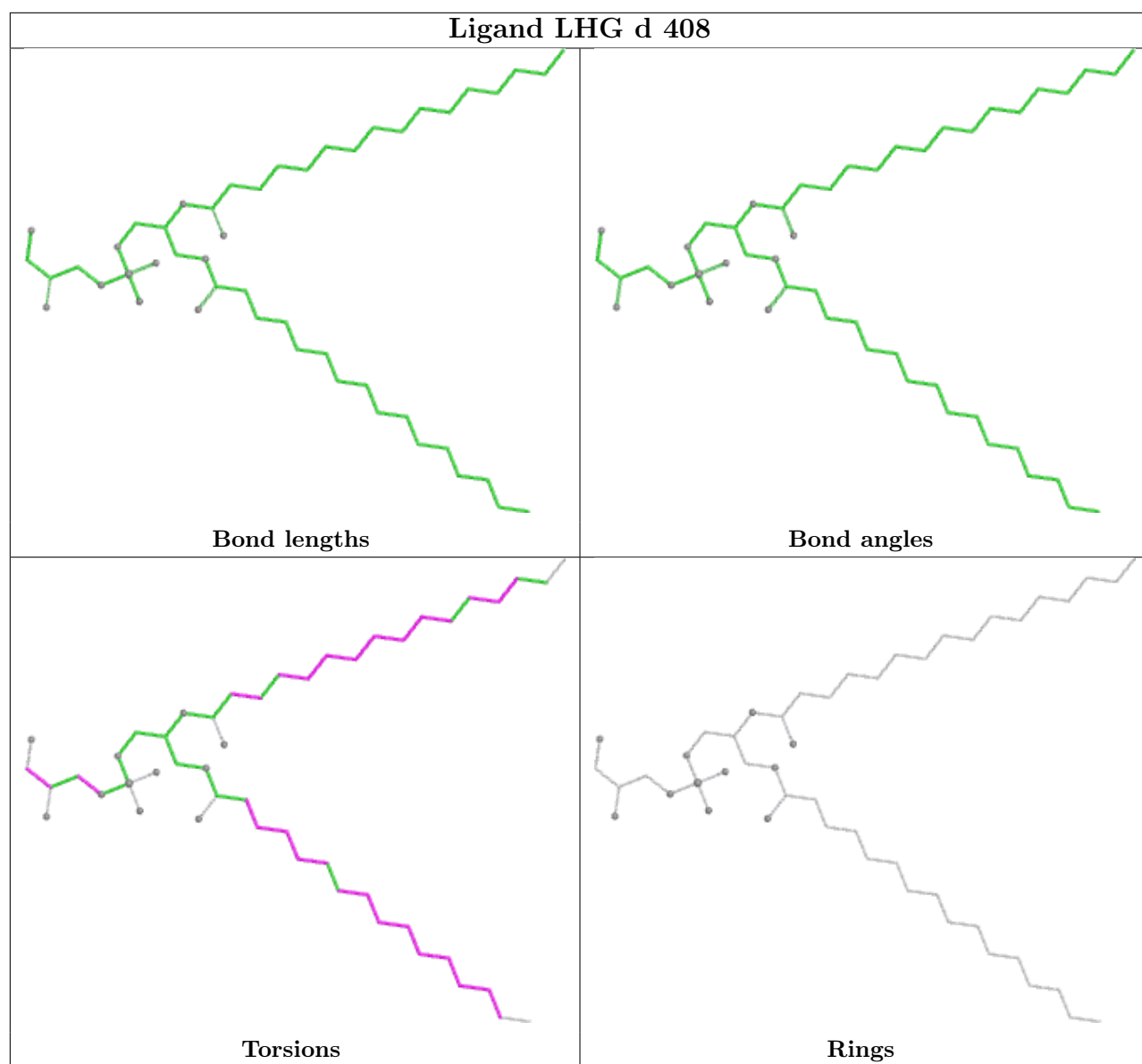




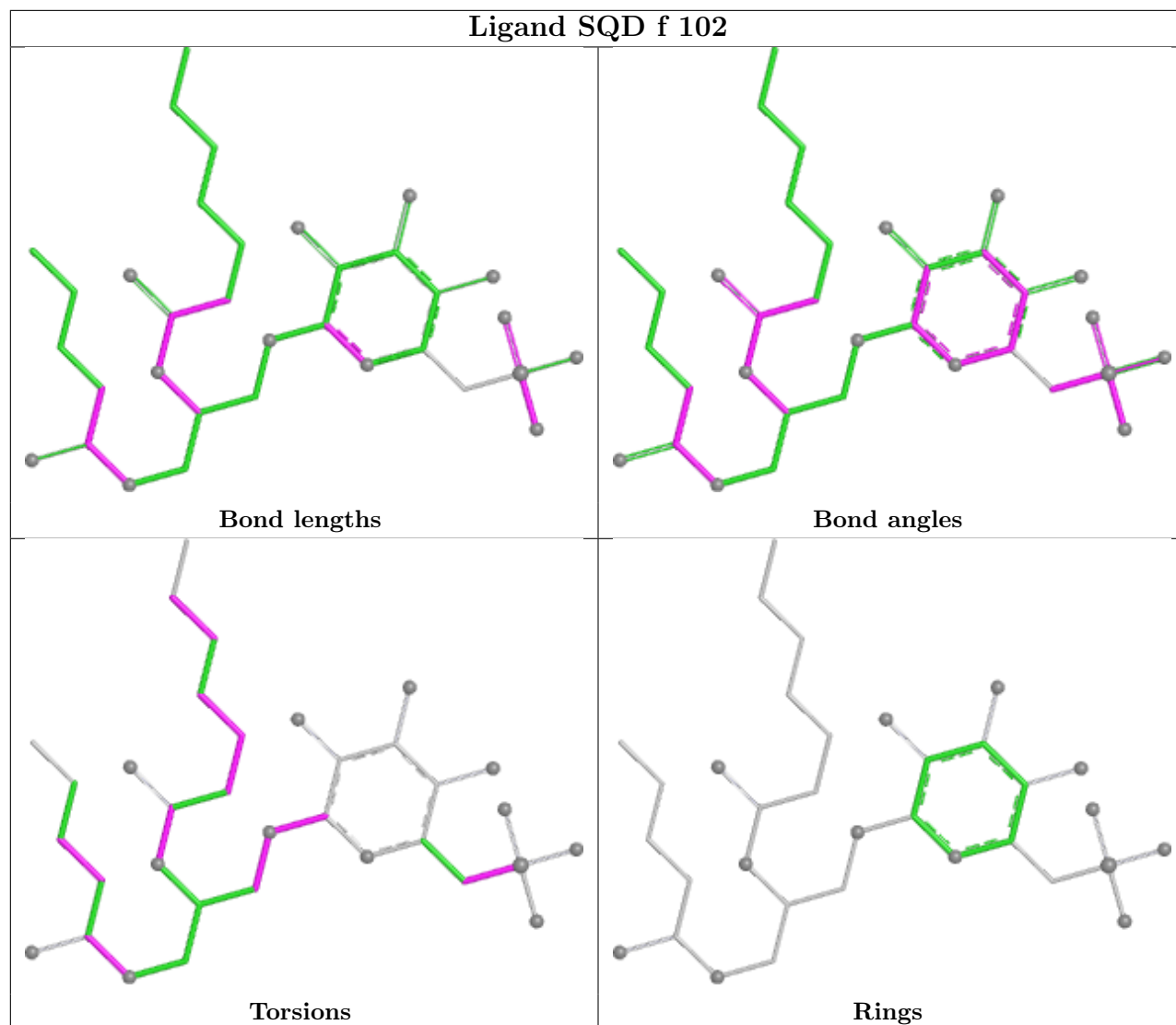




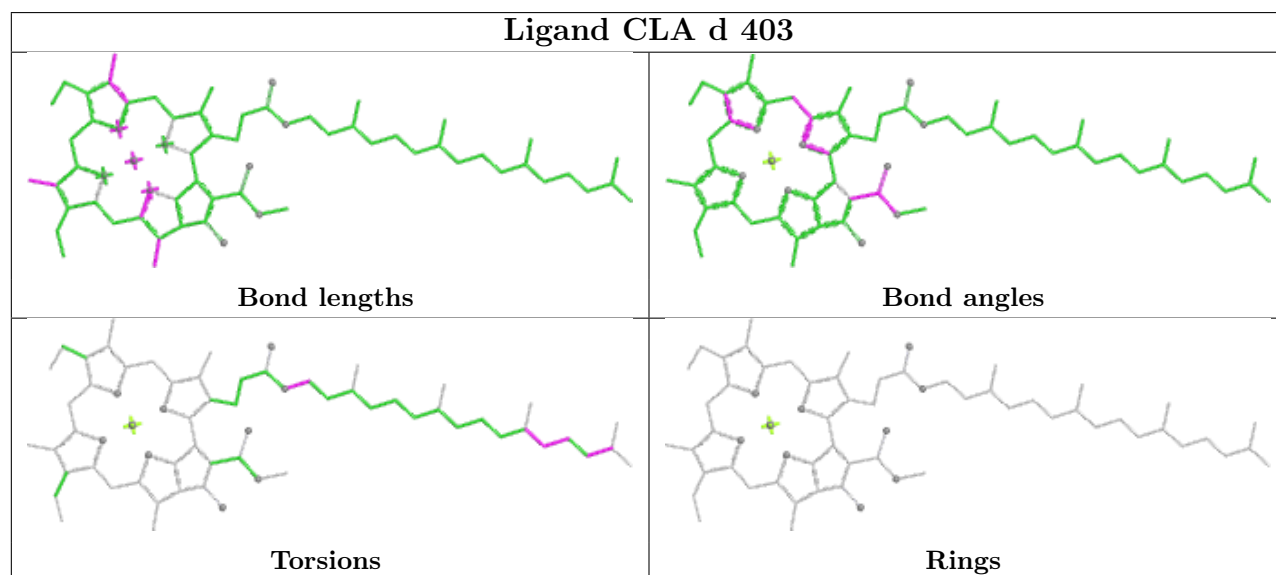


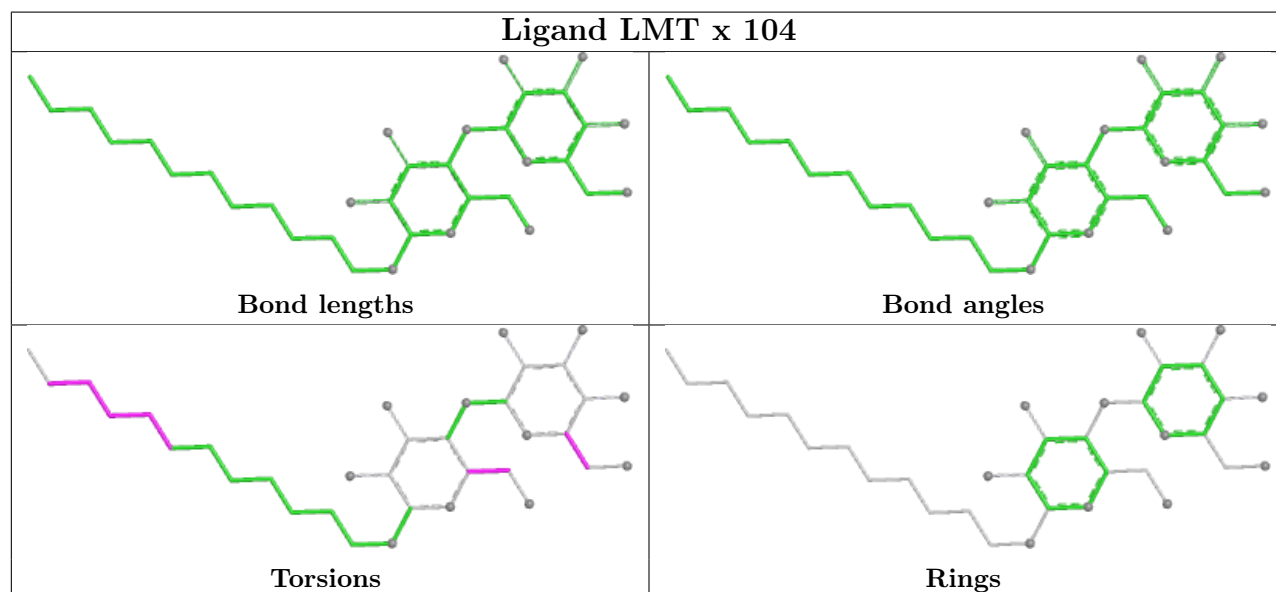
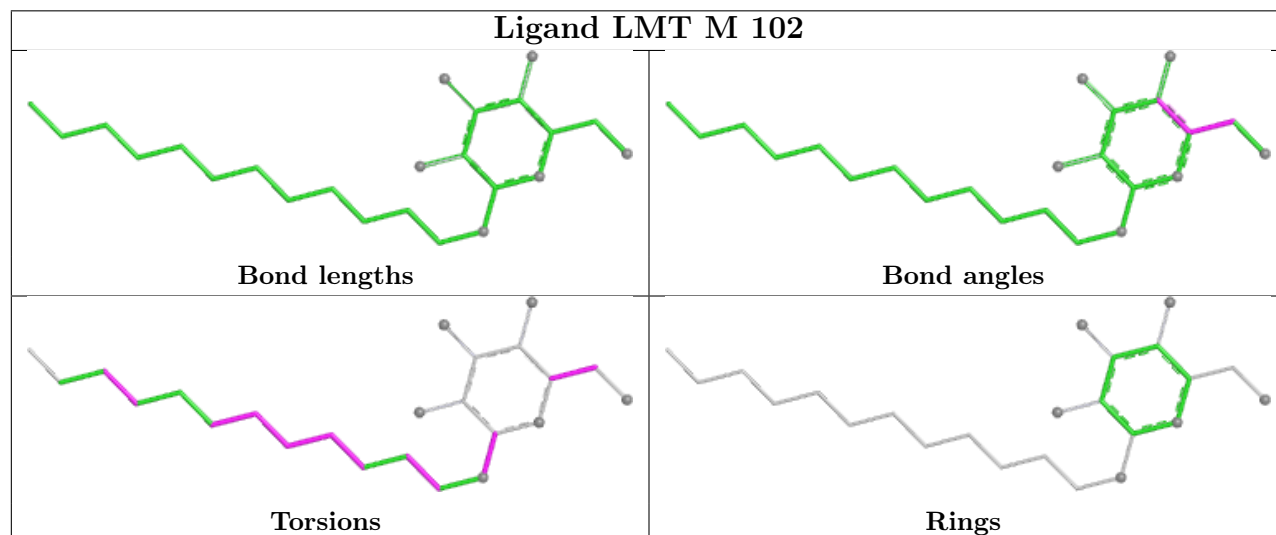
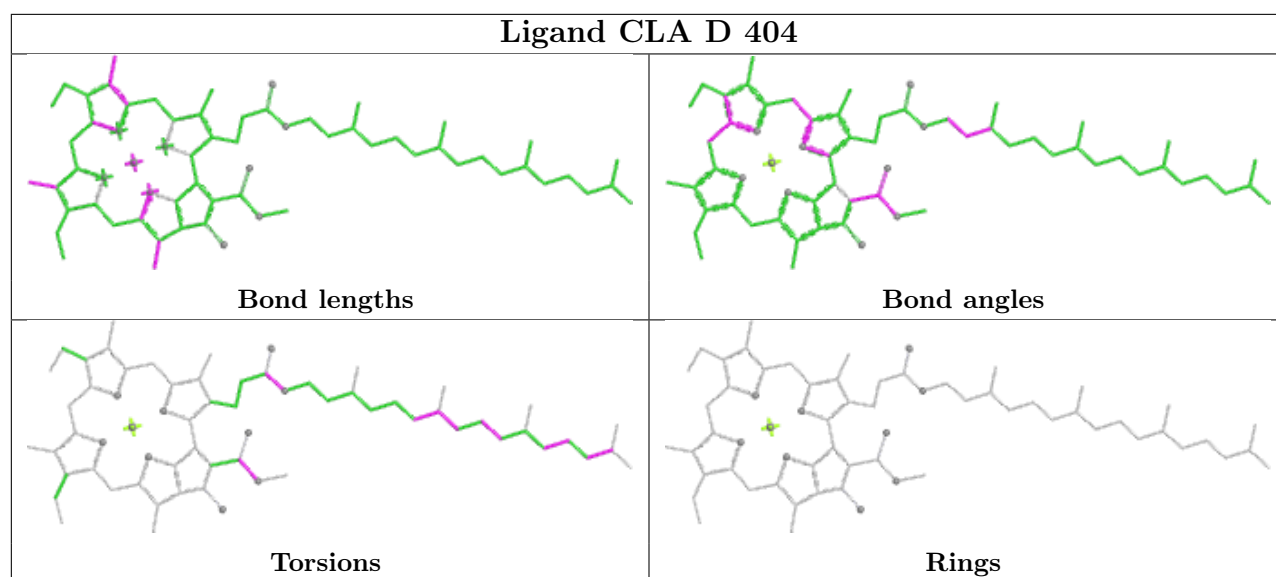


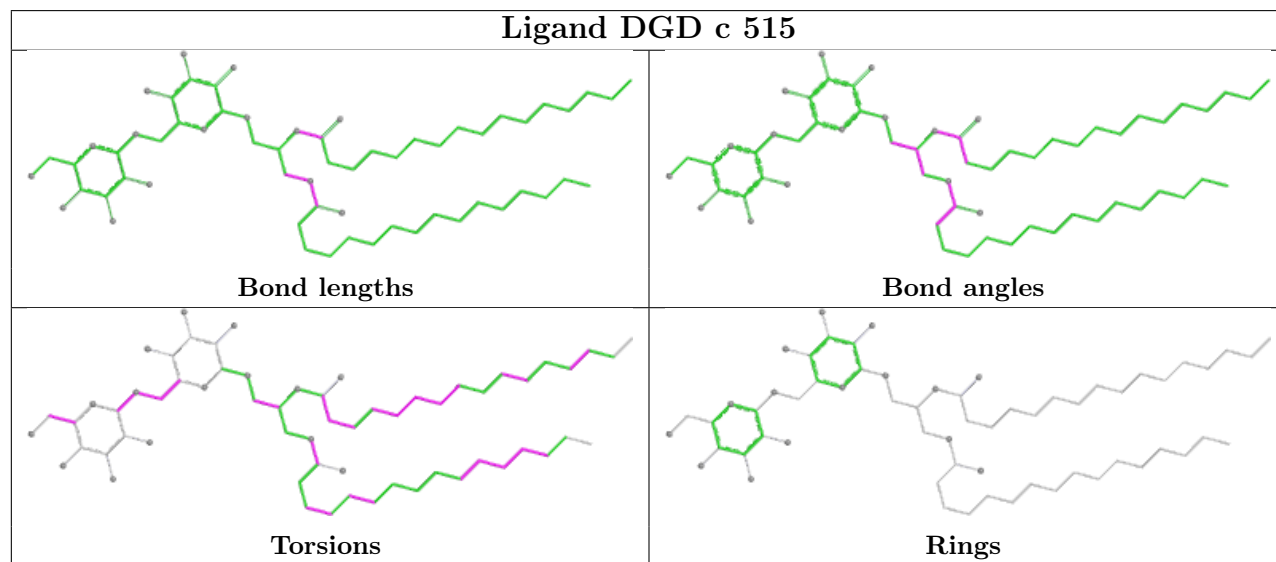
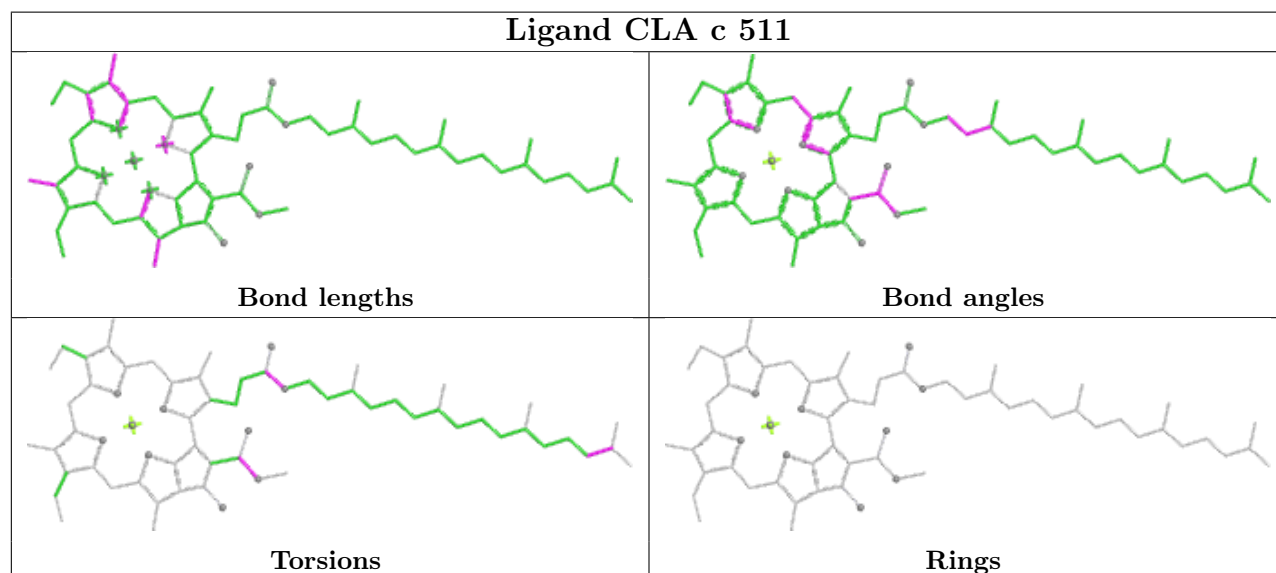
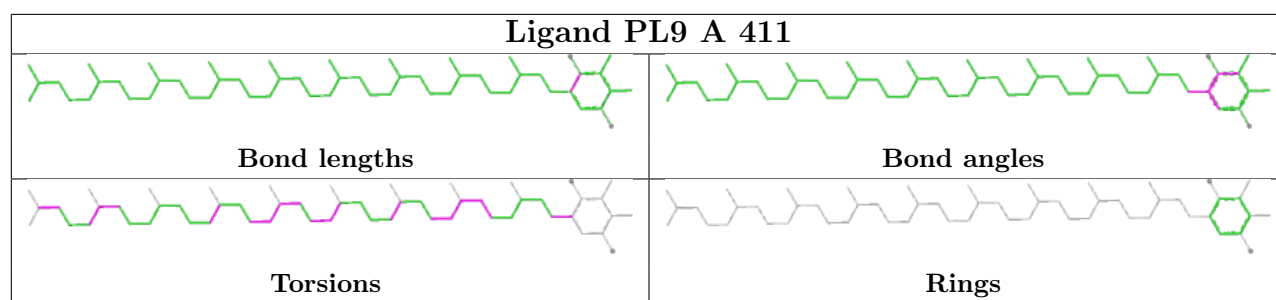
Ligand SQD f 102

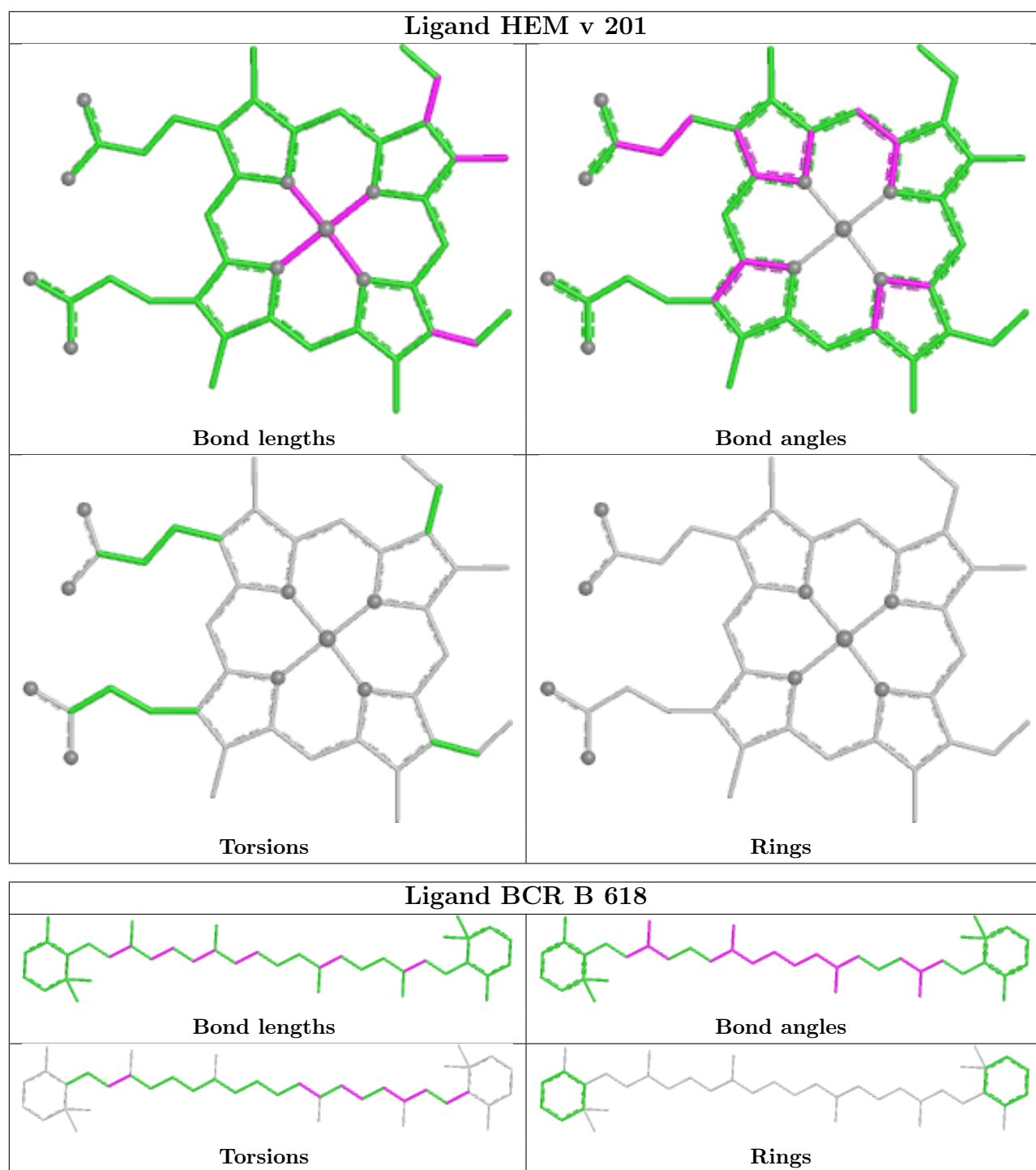


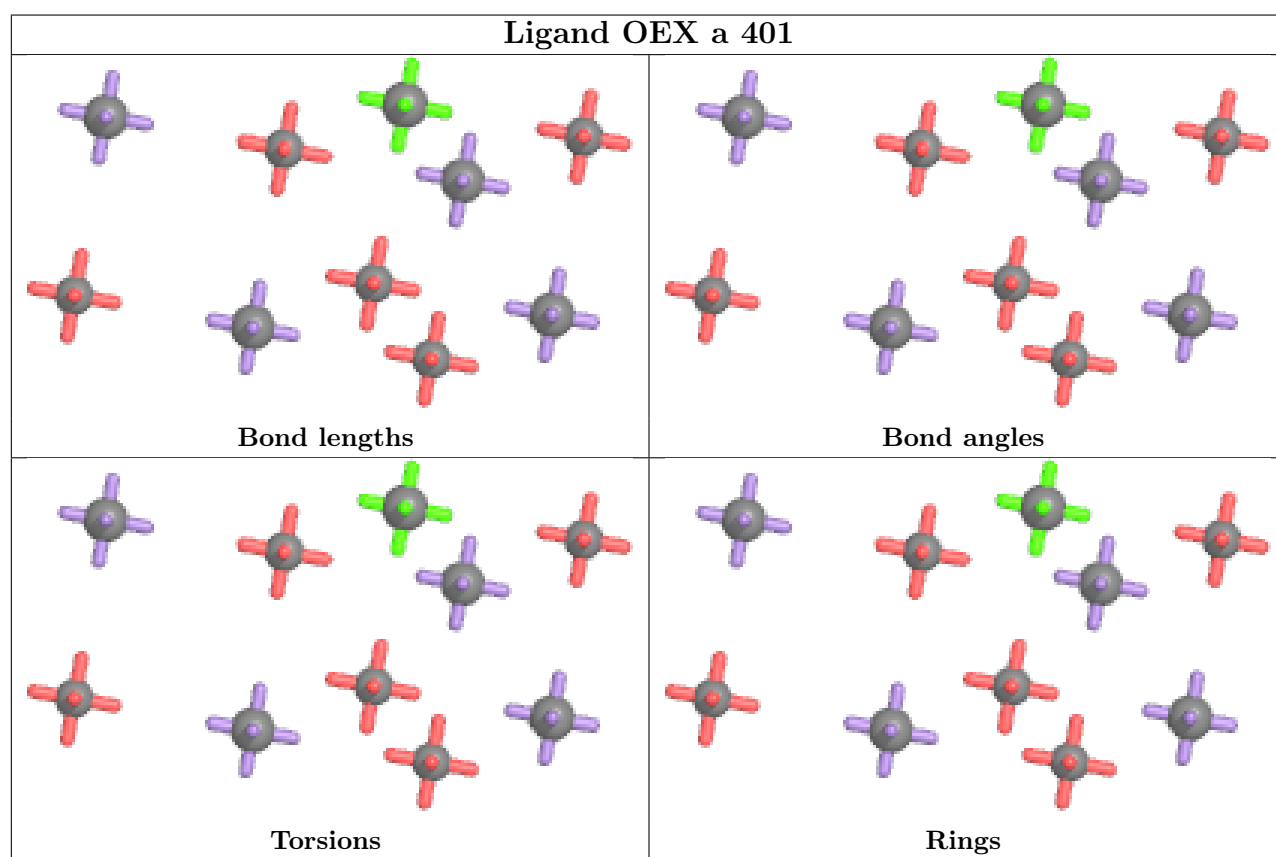
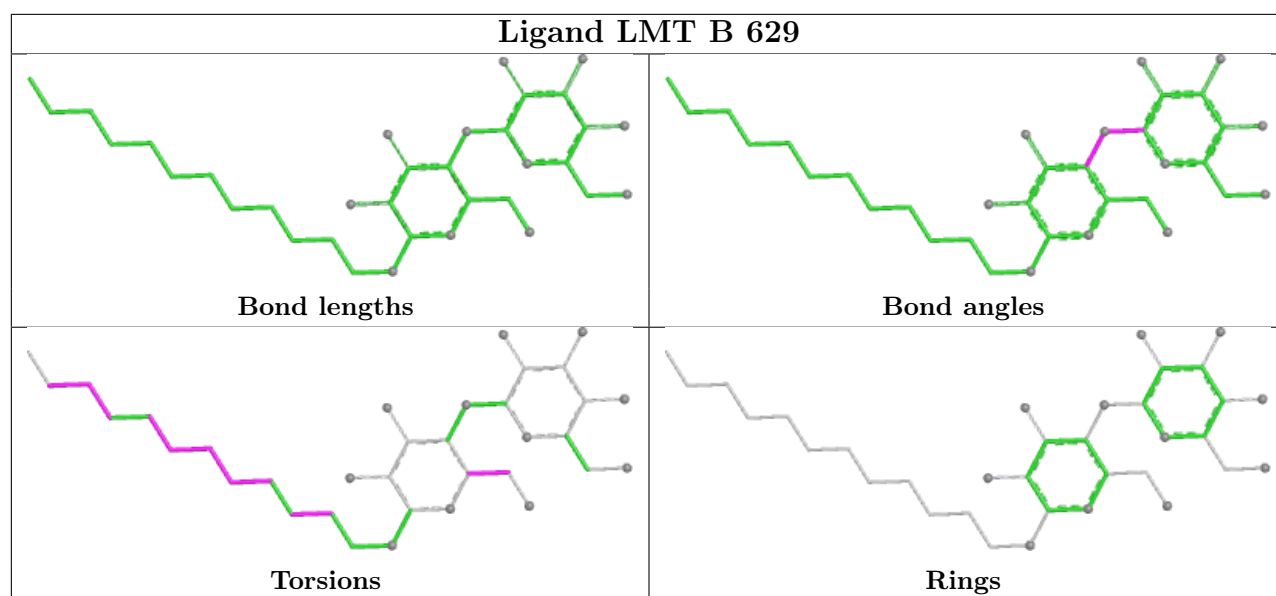
Ligand CLA d 403

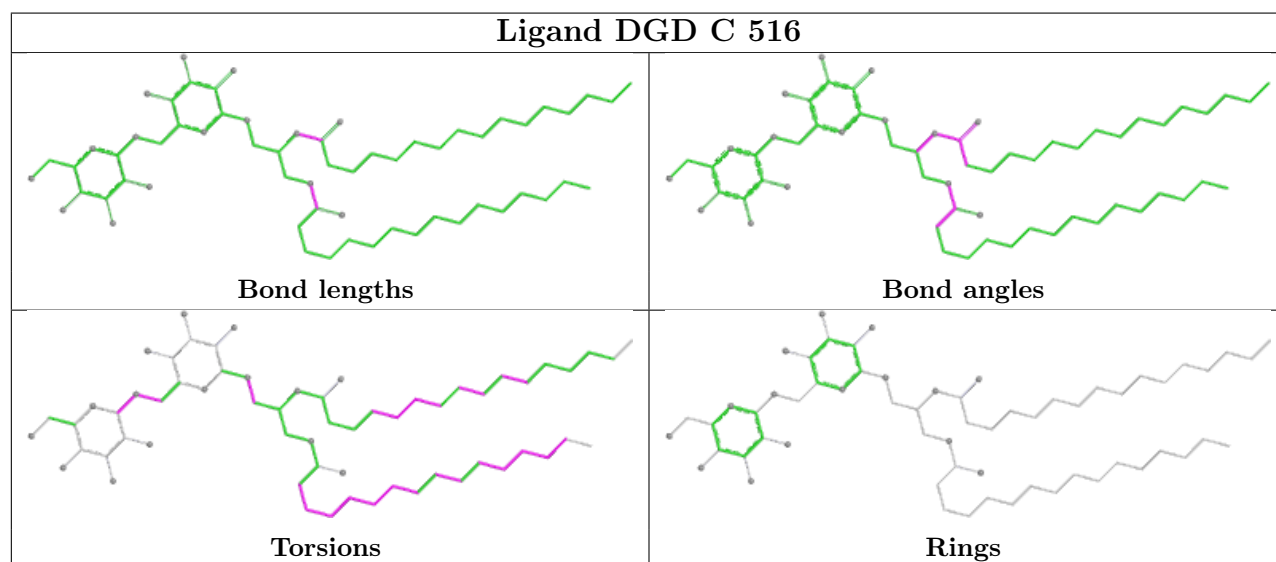
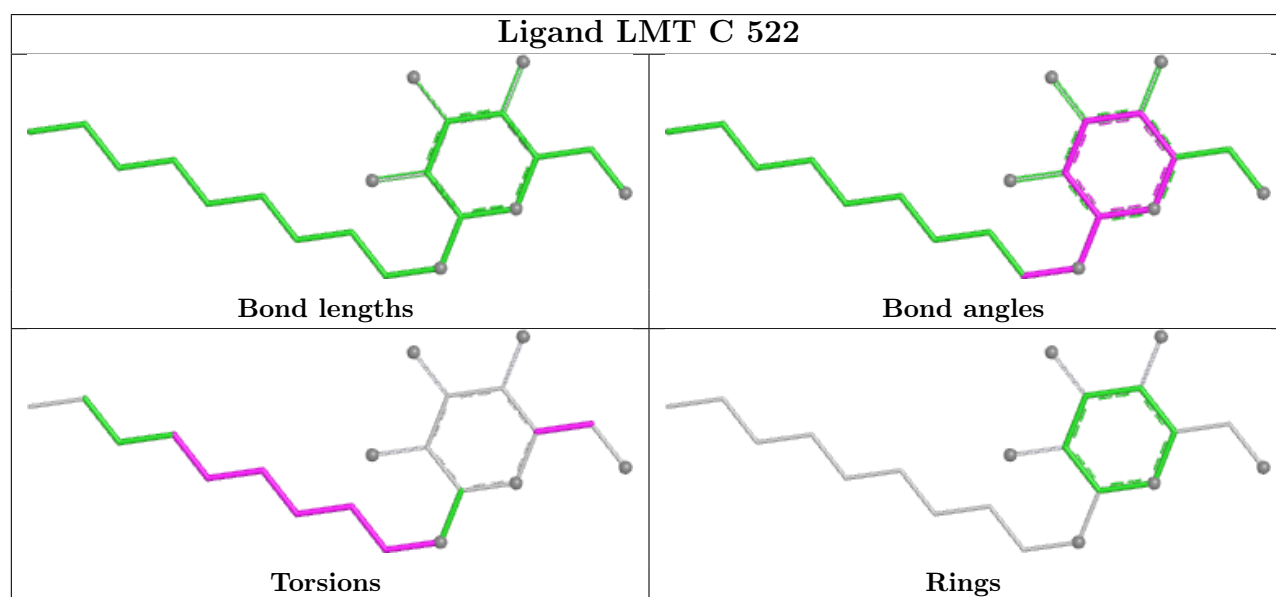
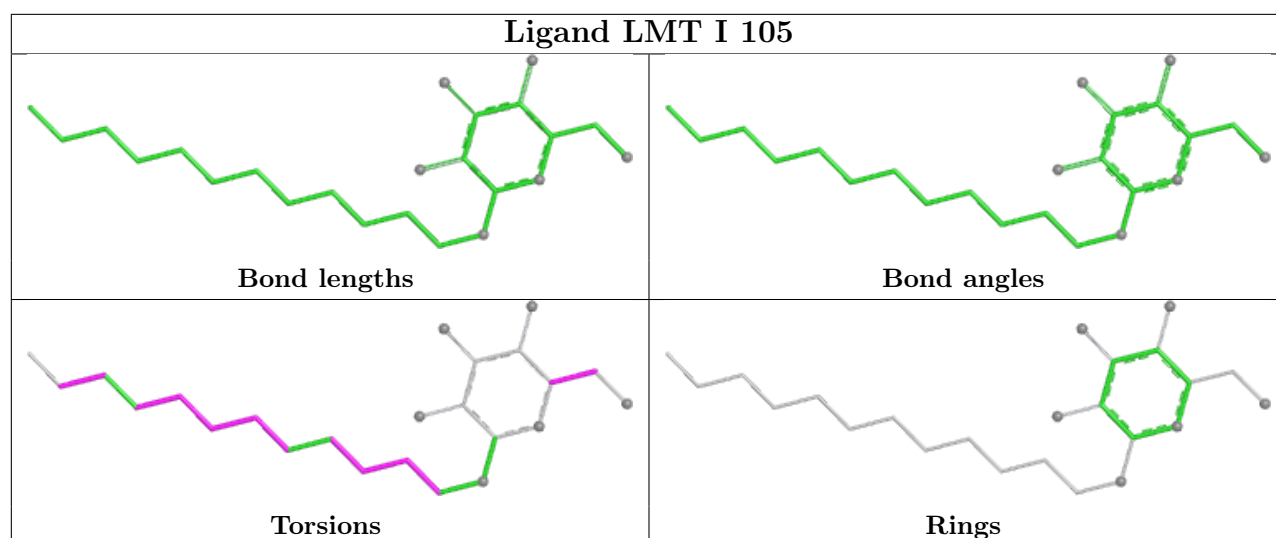


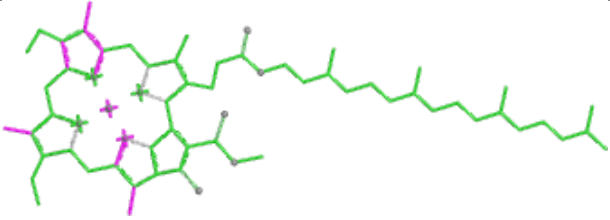
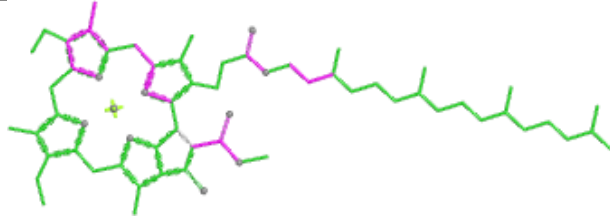
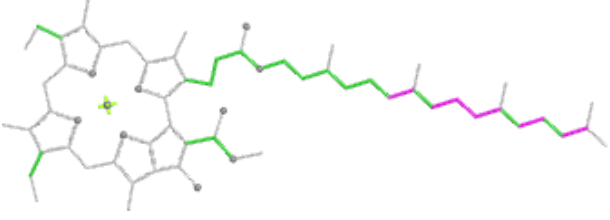
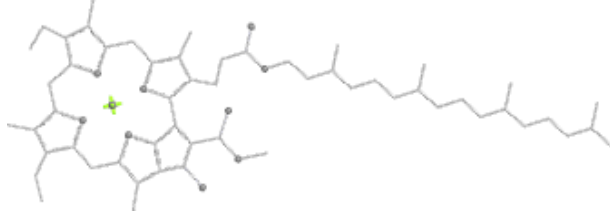
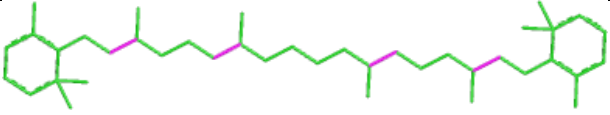
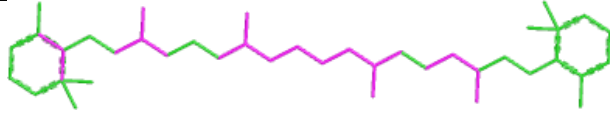

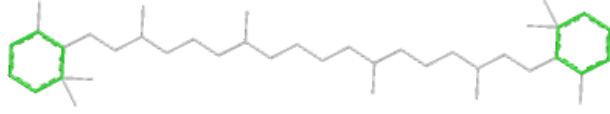
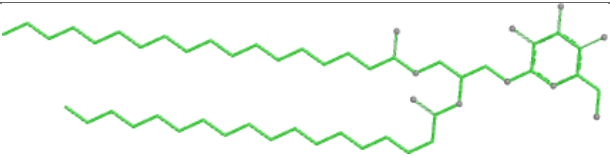
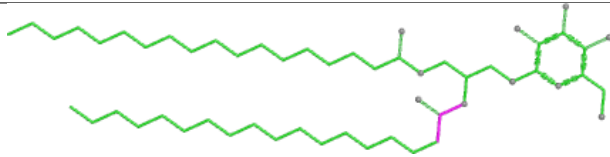
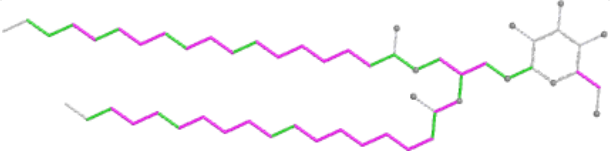
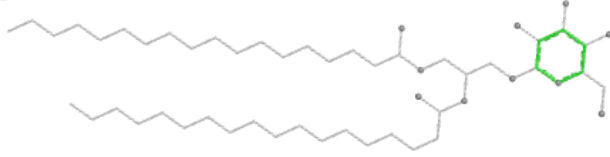


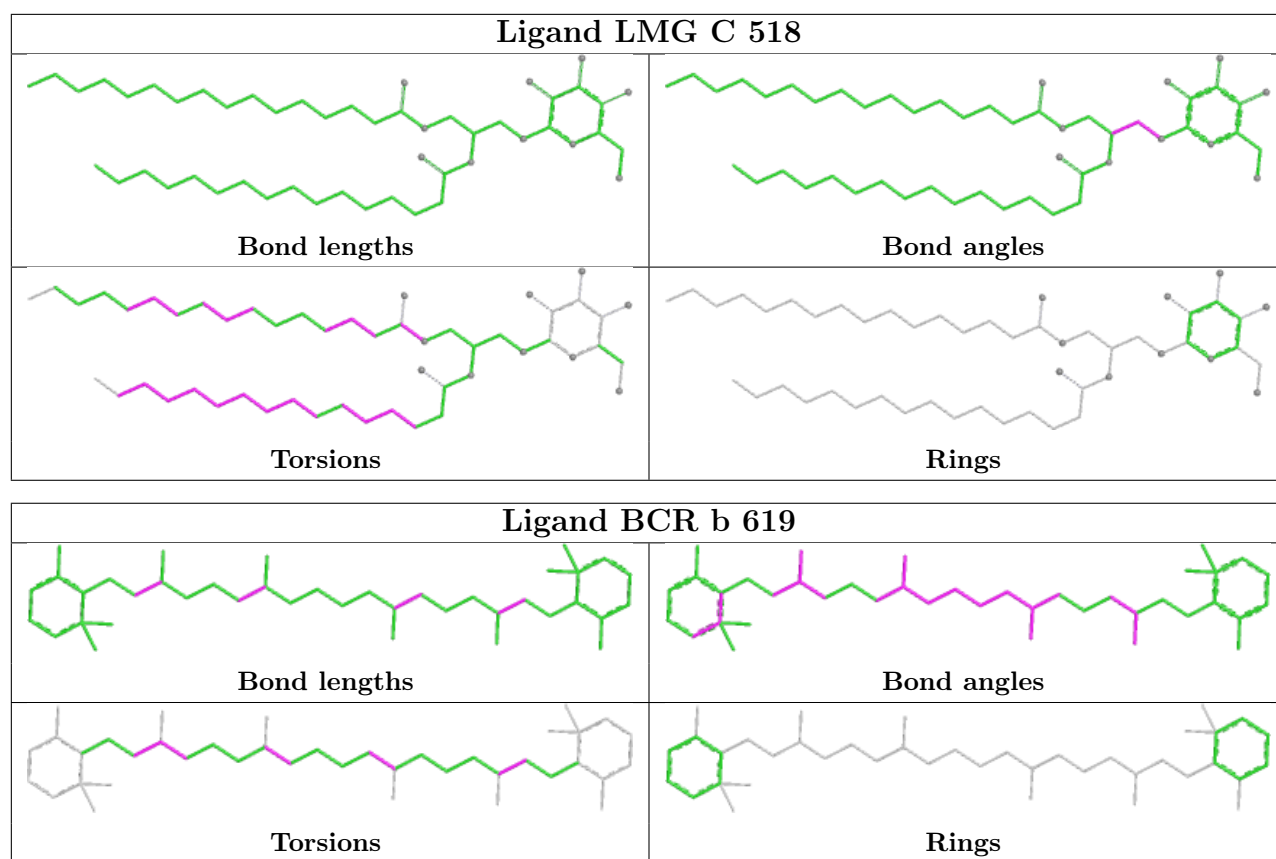


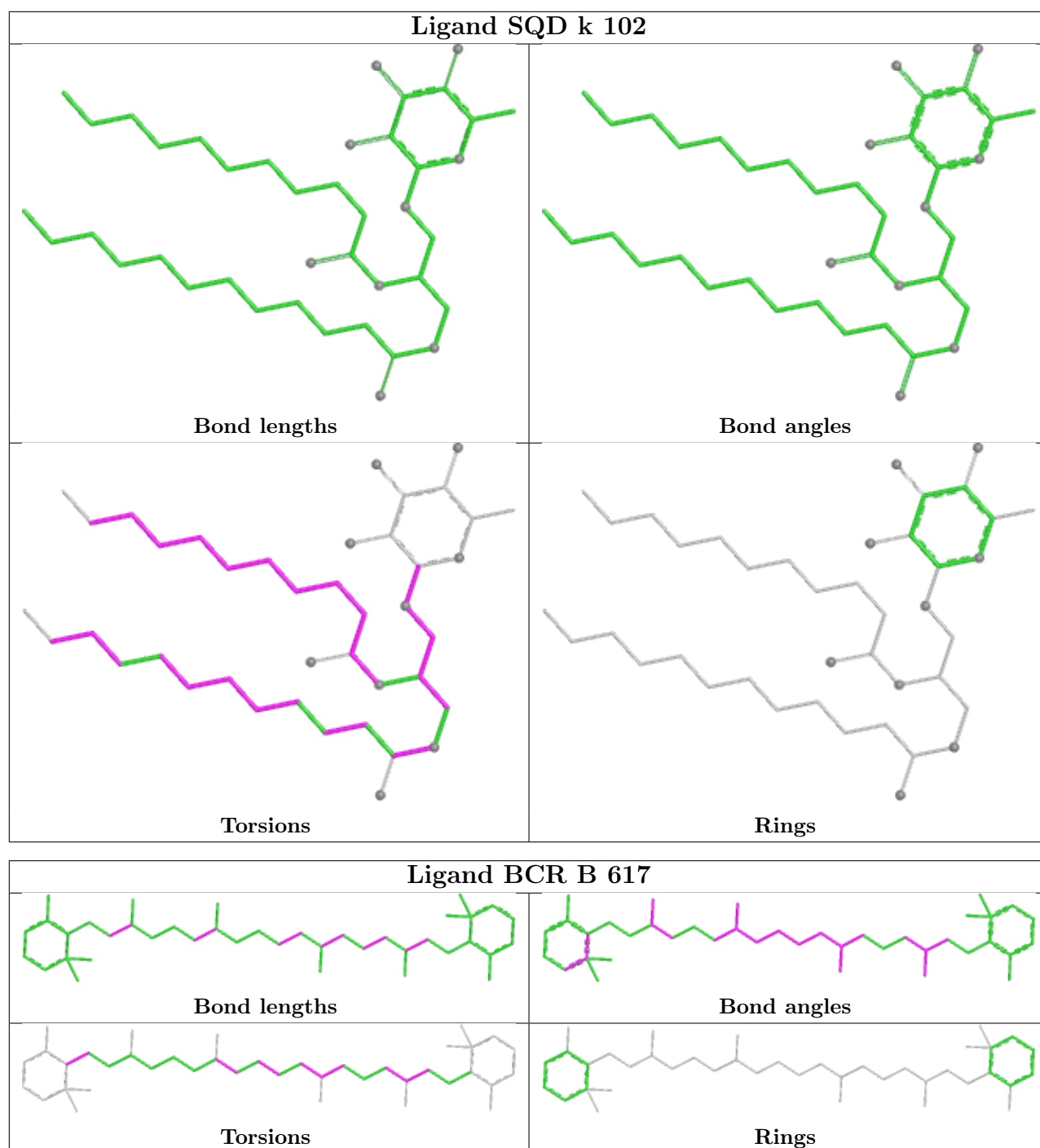


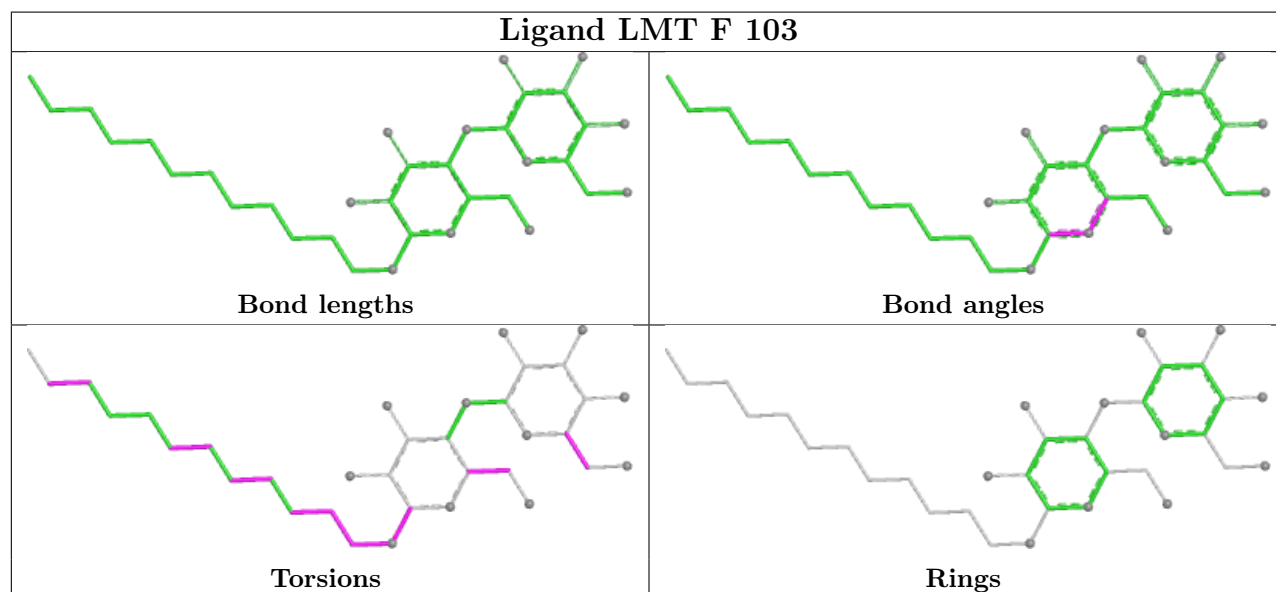
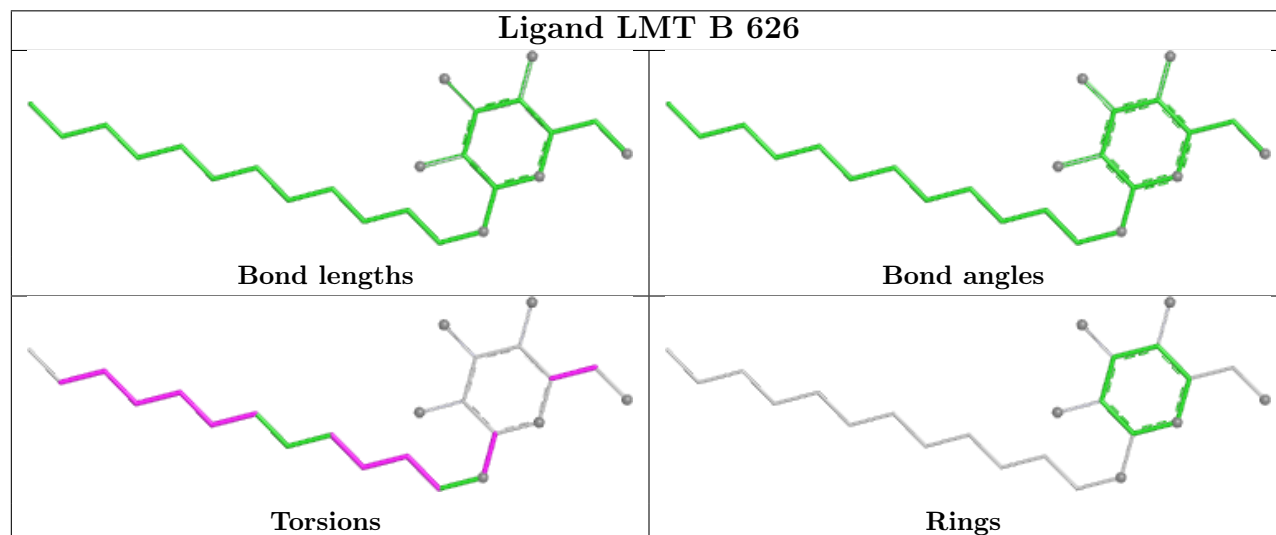
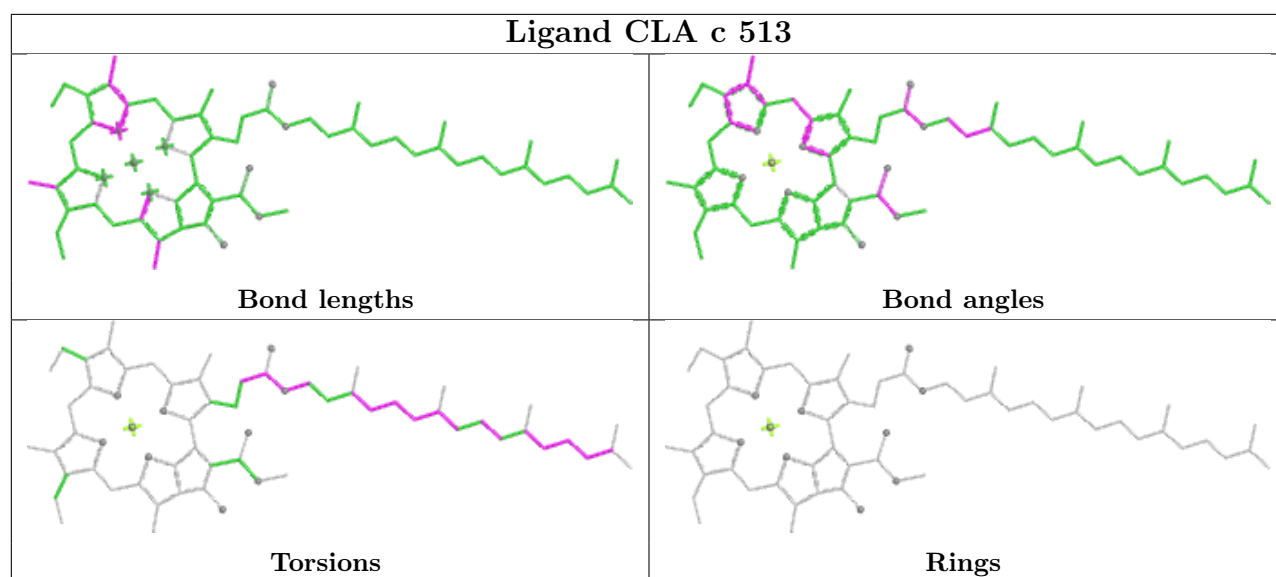


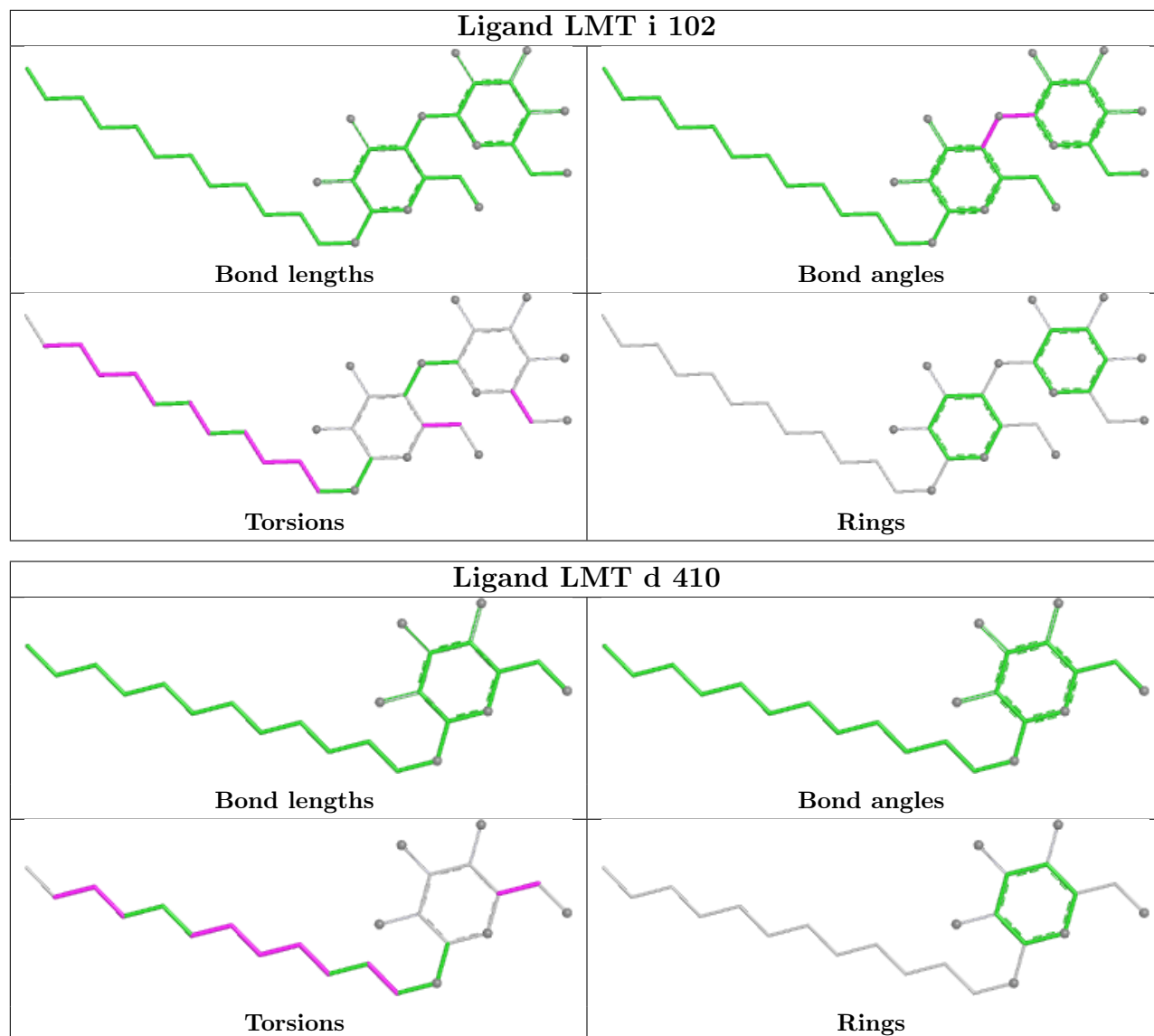


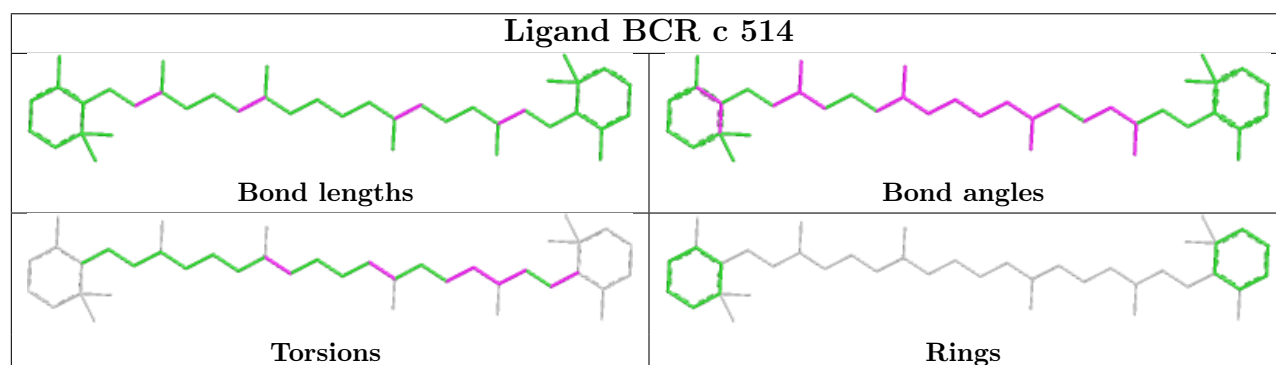
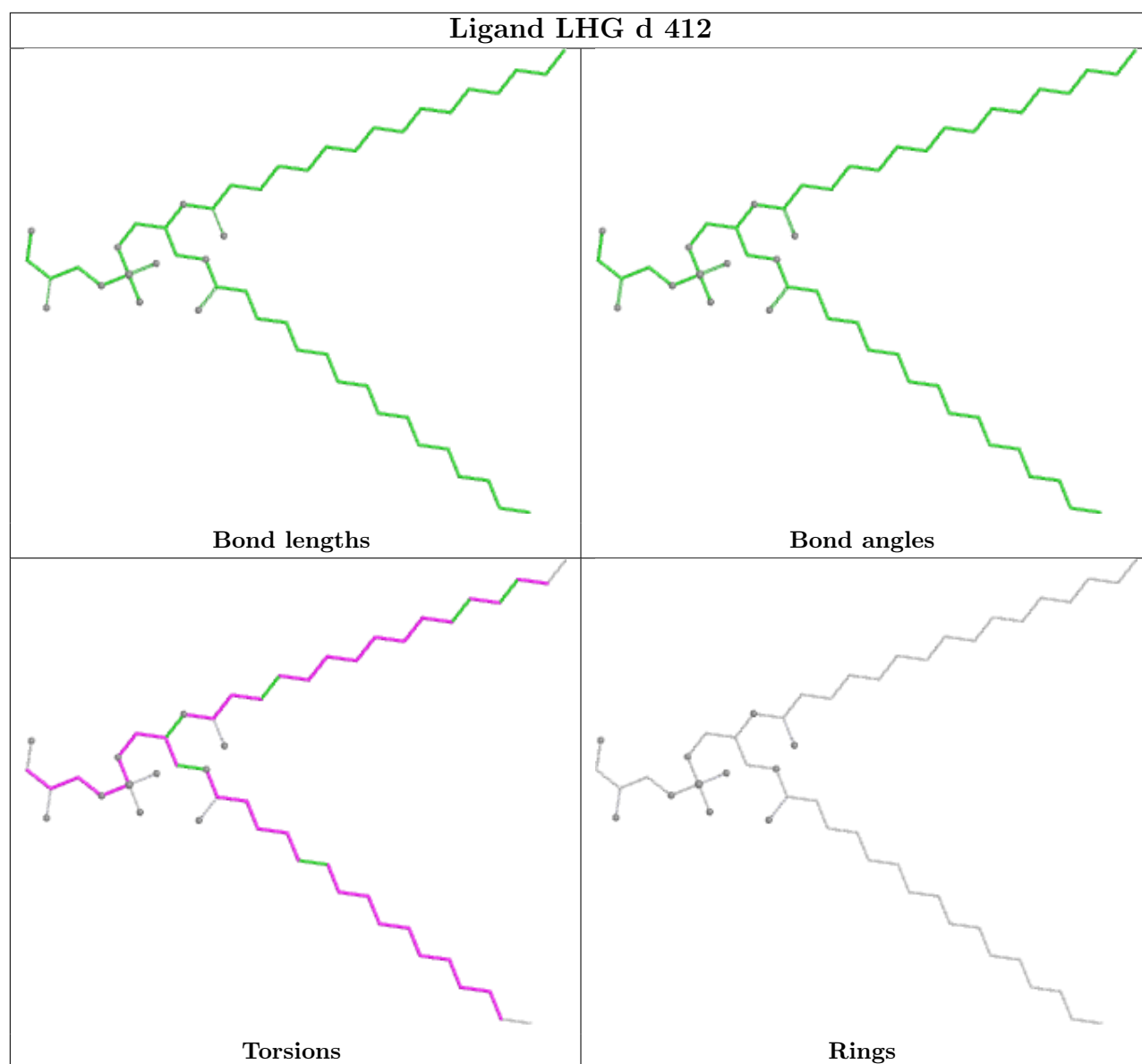
Ligand CLA b 611	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR C 514	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LMG D 409	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

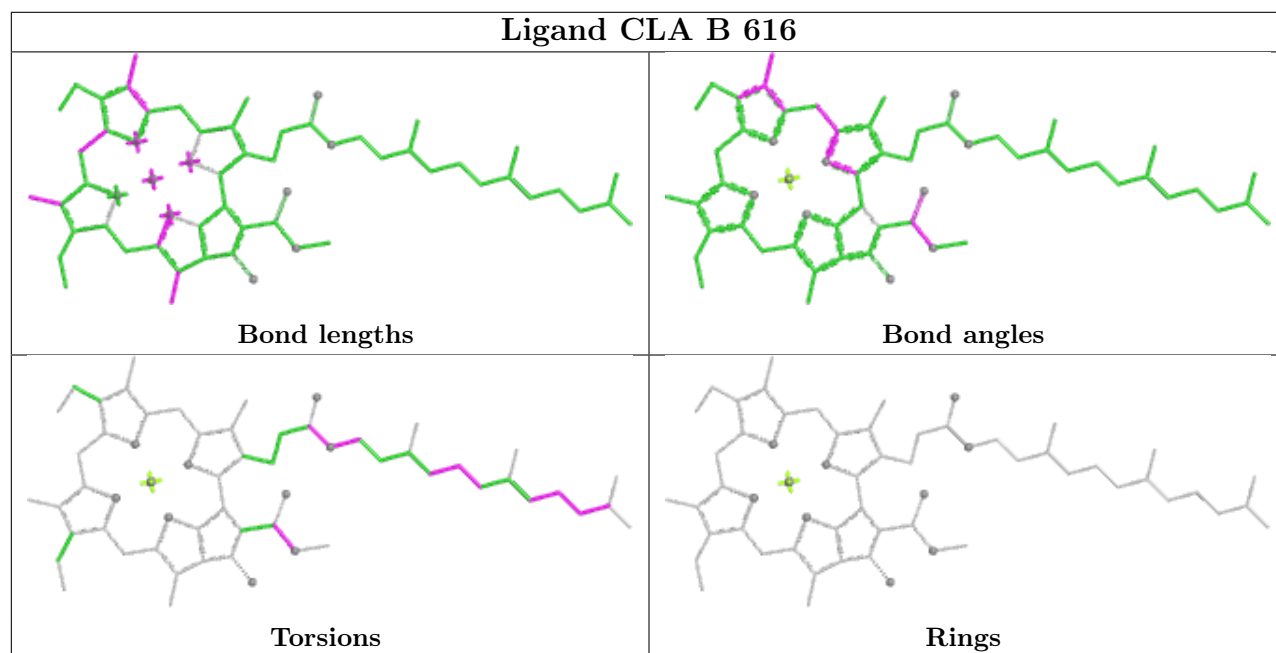
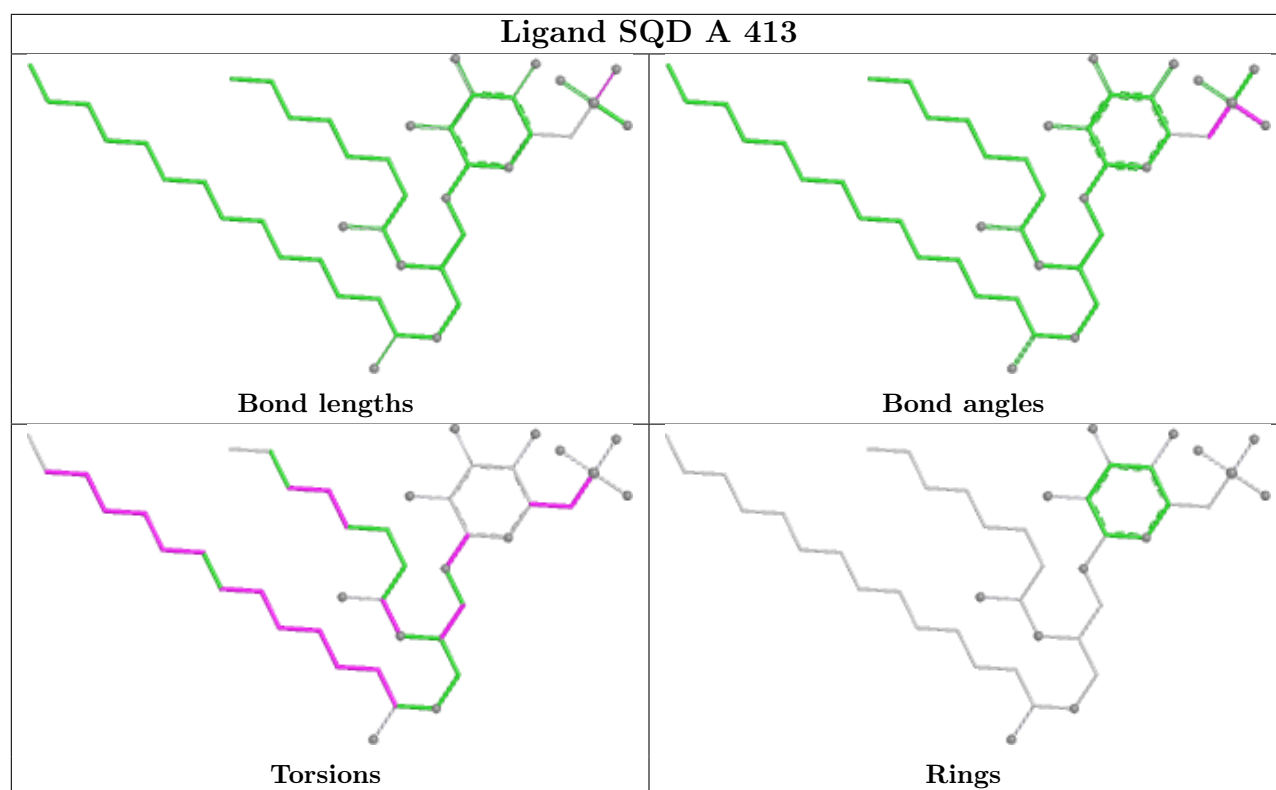


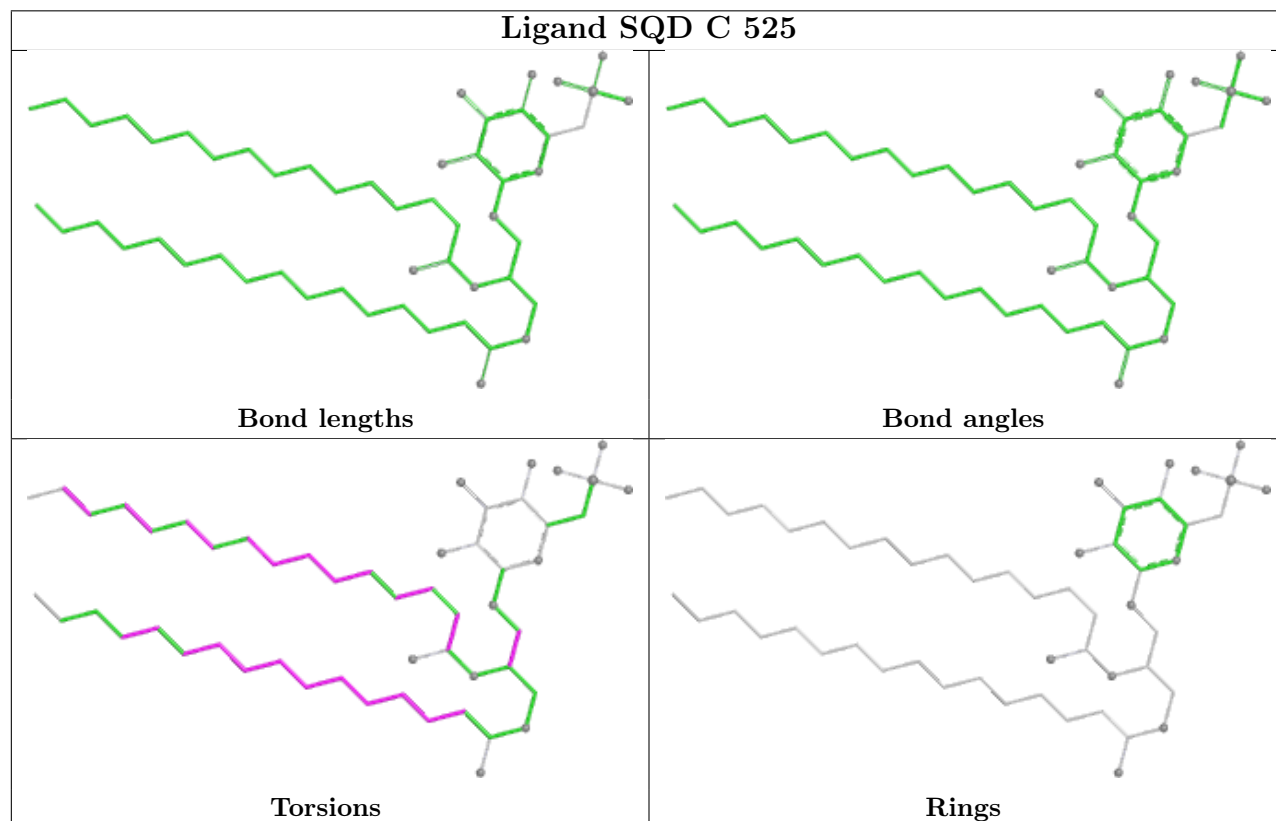
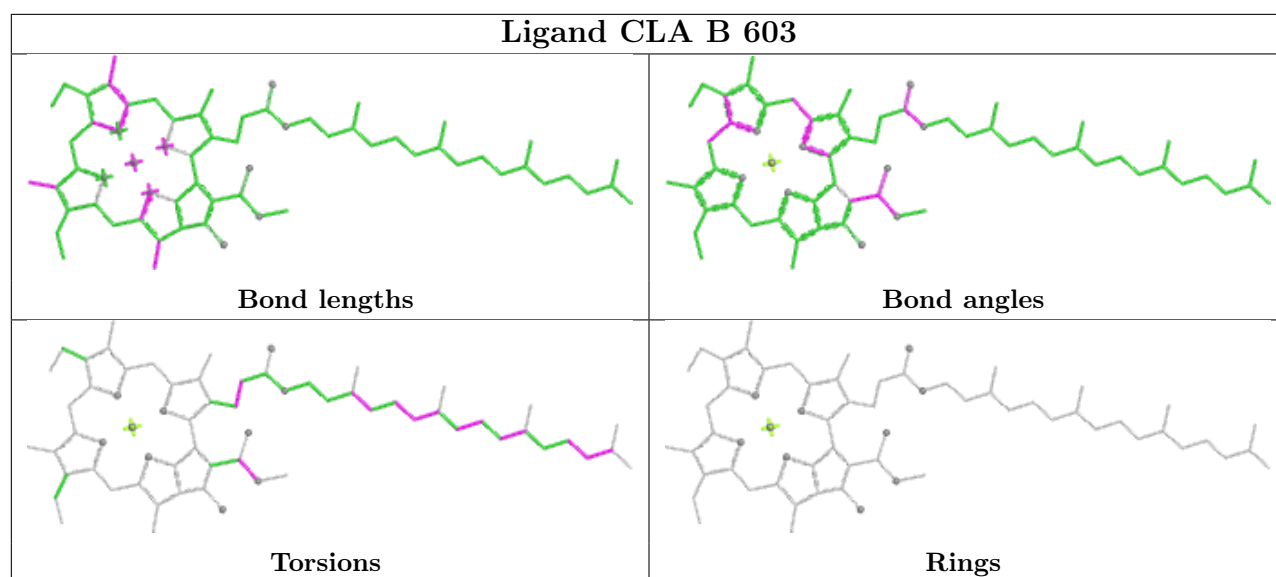


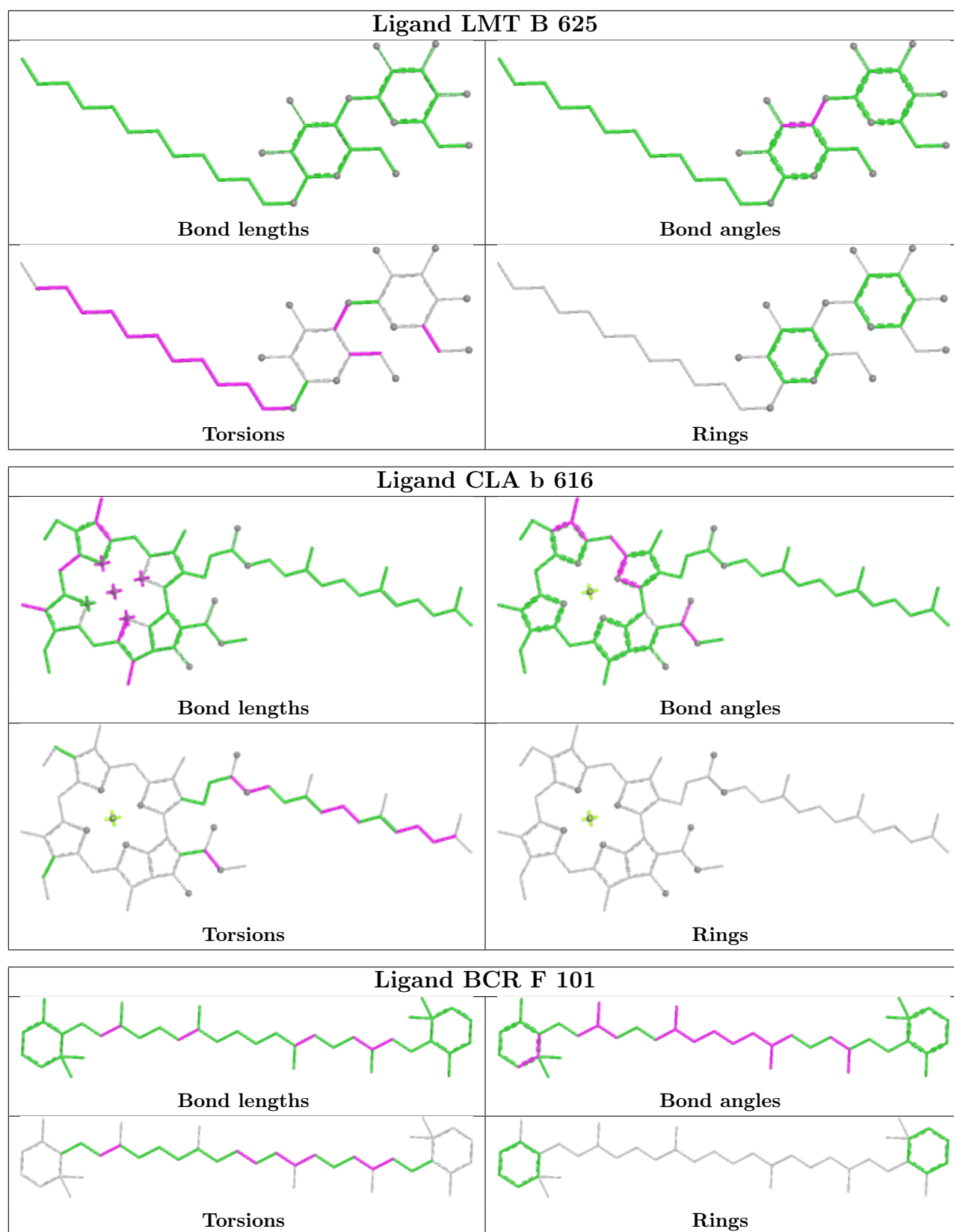


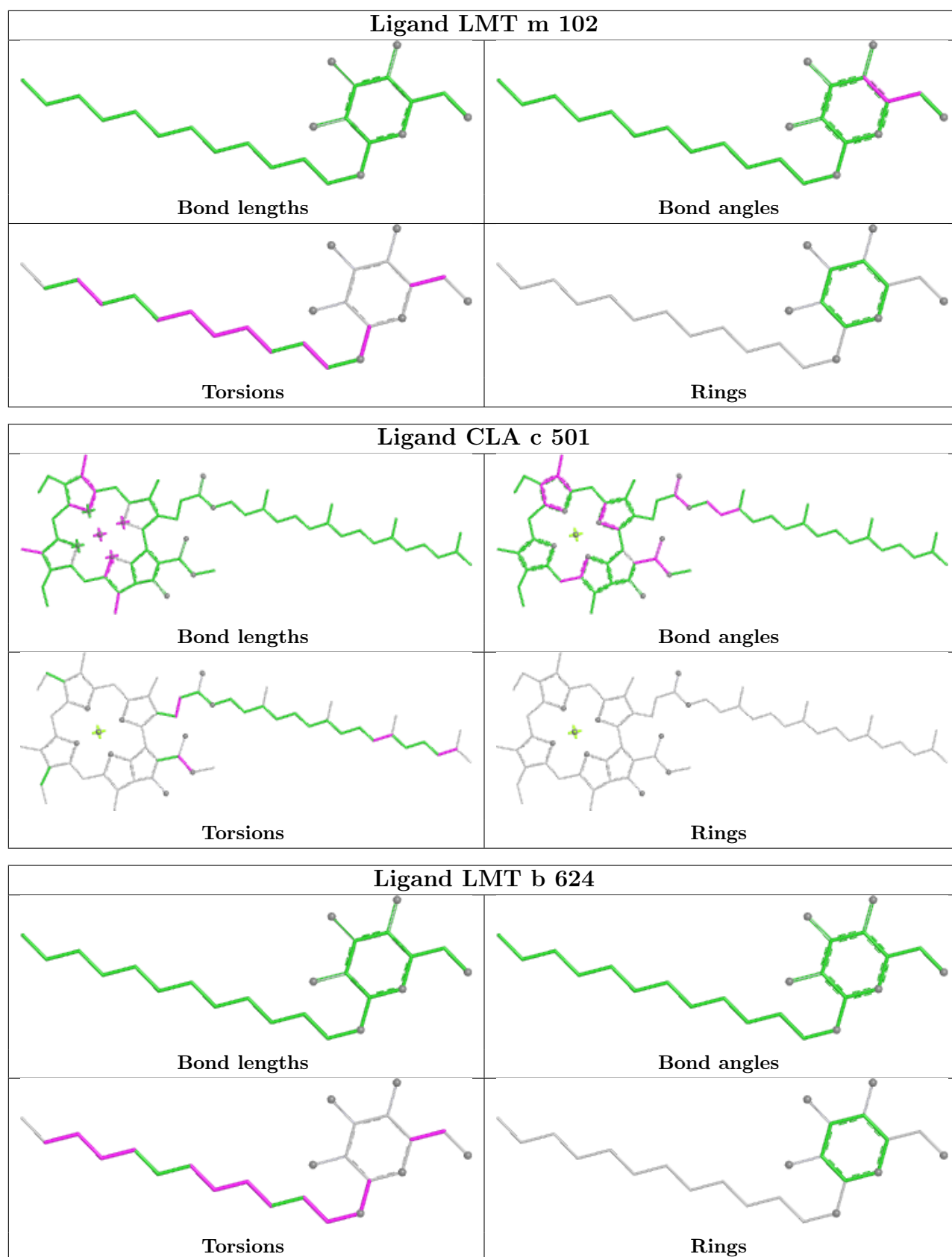


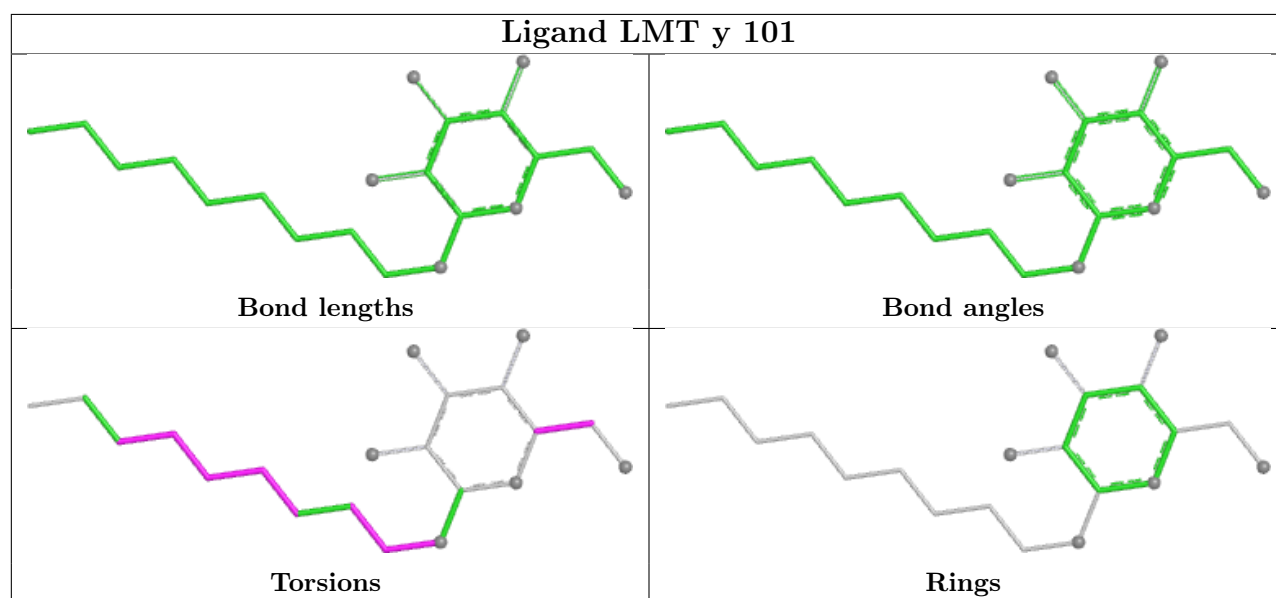
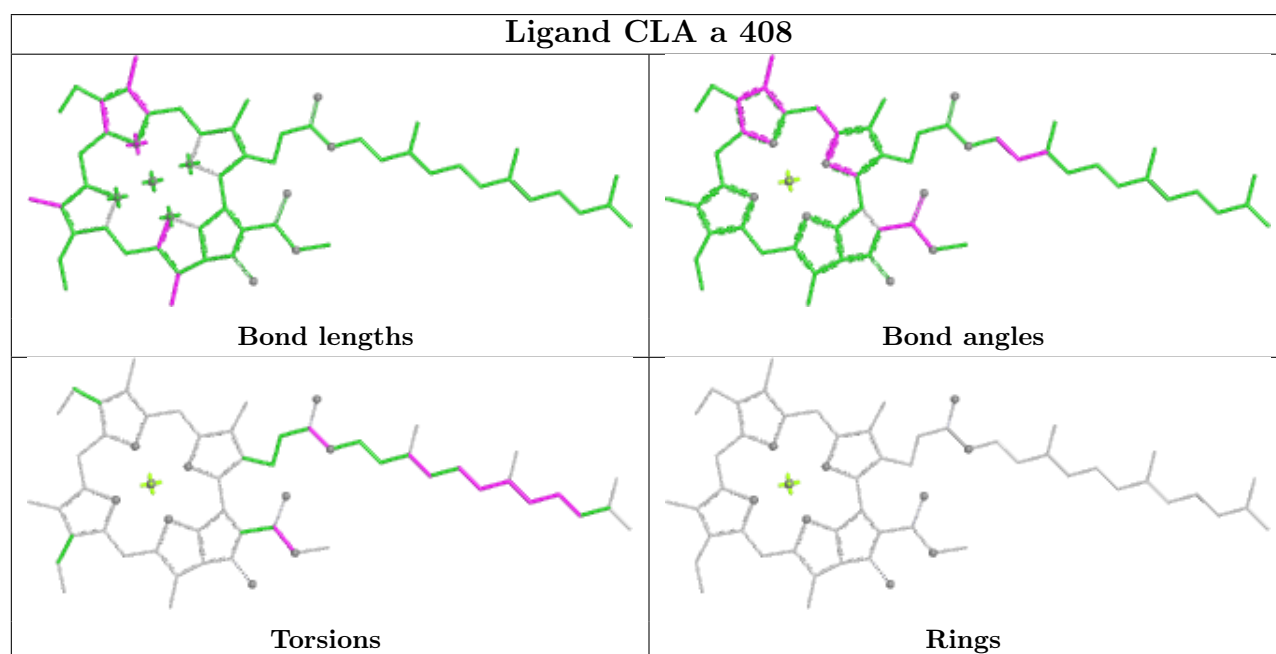
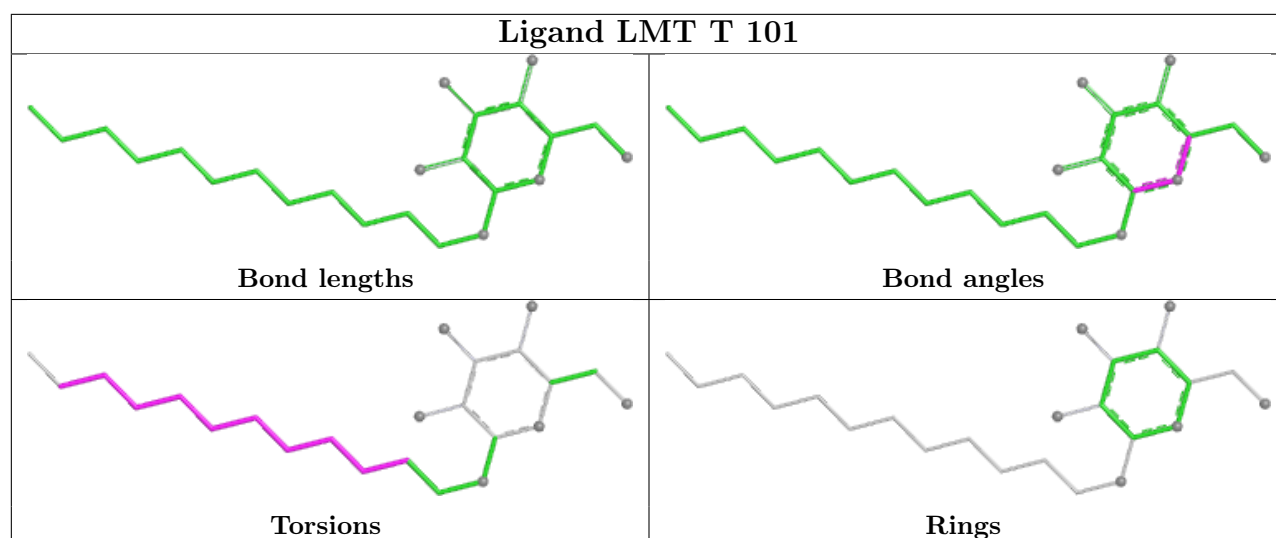


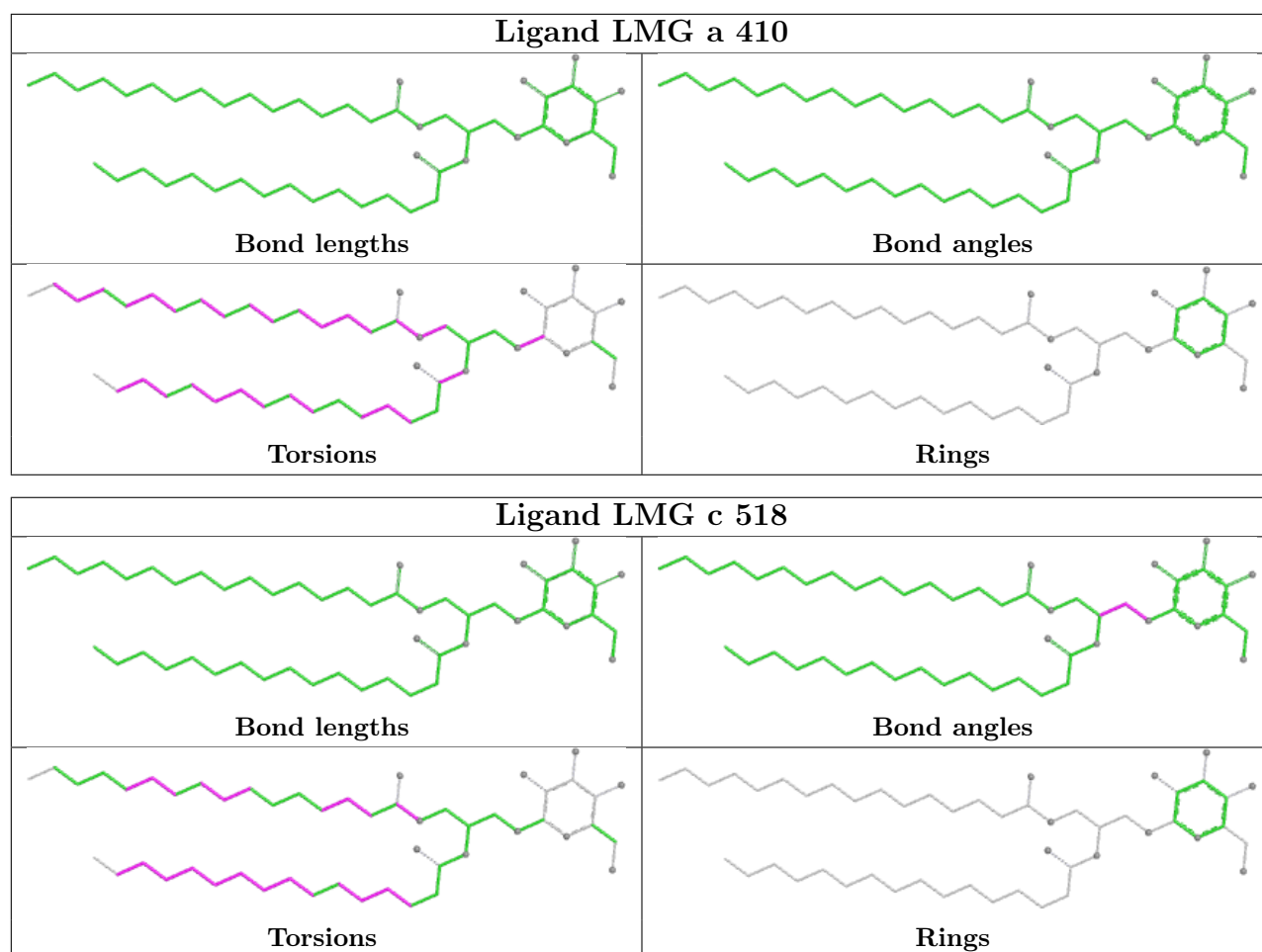




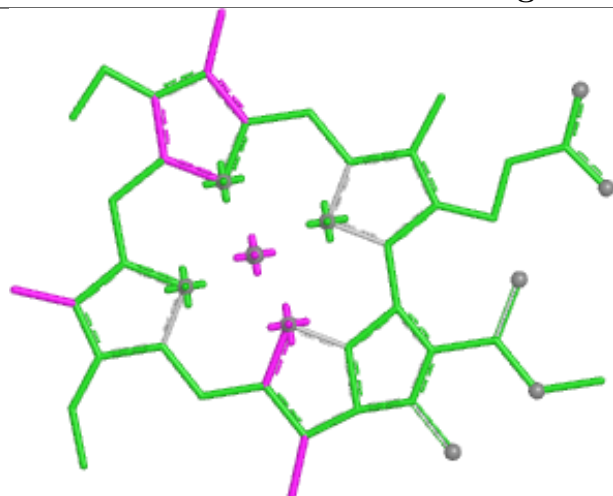




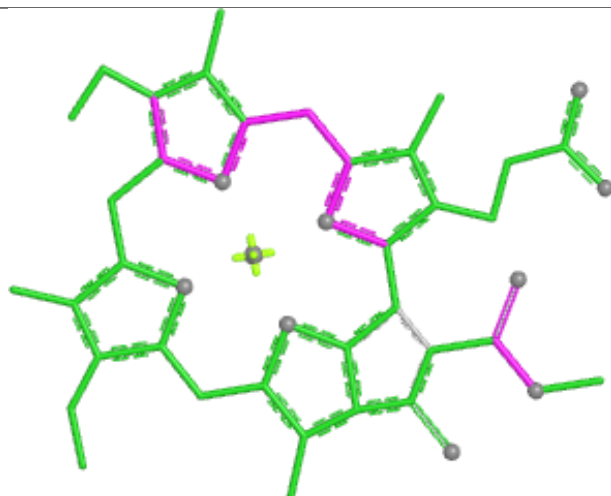




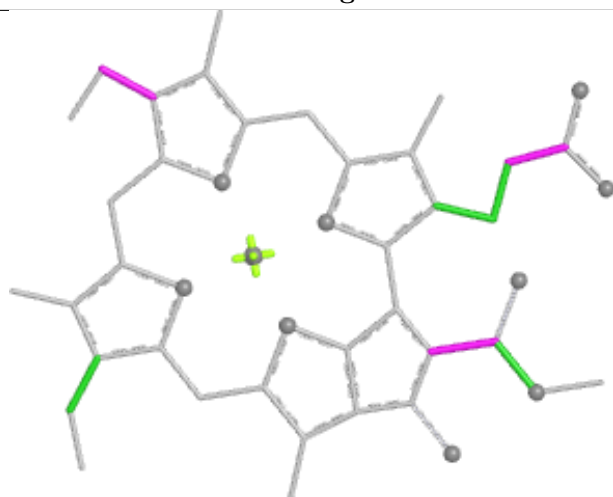
Ligand CLA b 601



Bond lengths



Bond angles

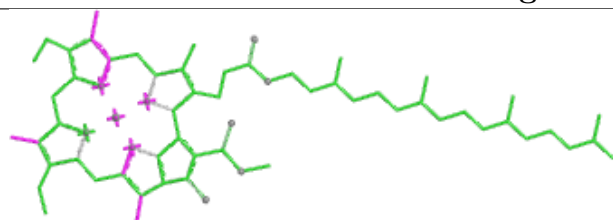


Torsions

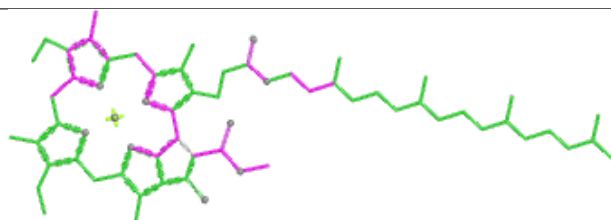


Rings

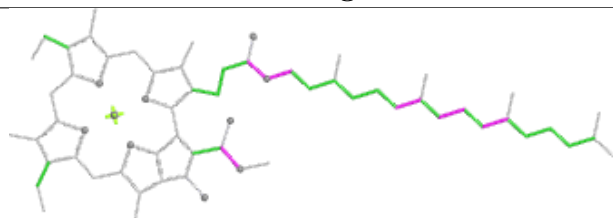
Ligand CLA c 509



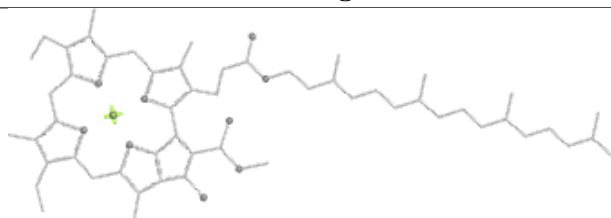
Bond lengths



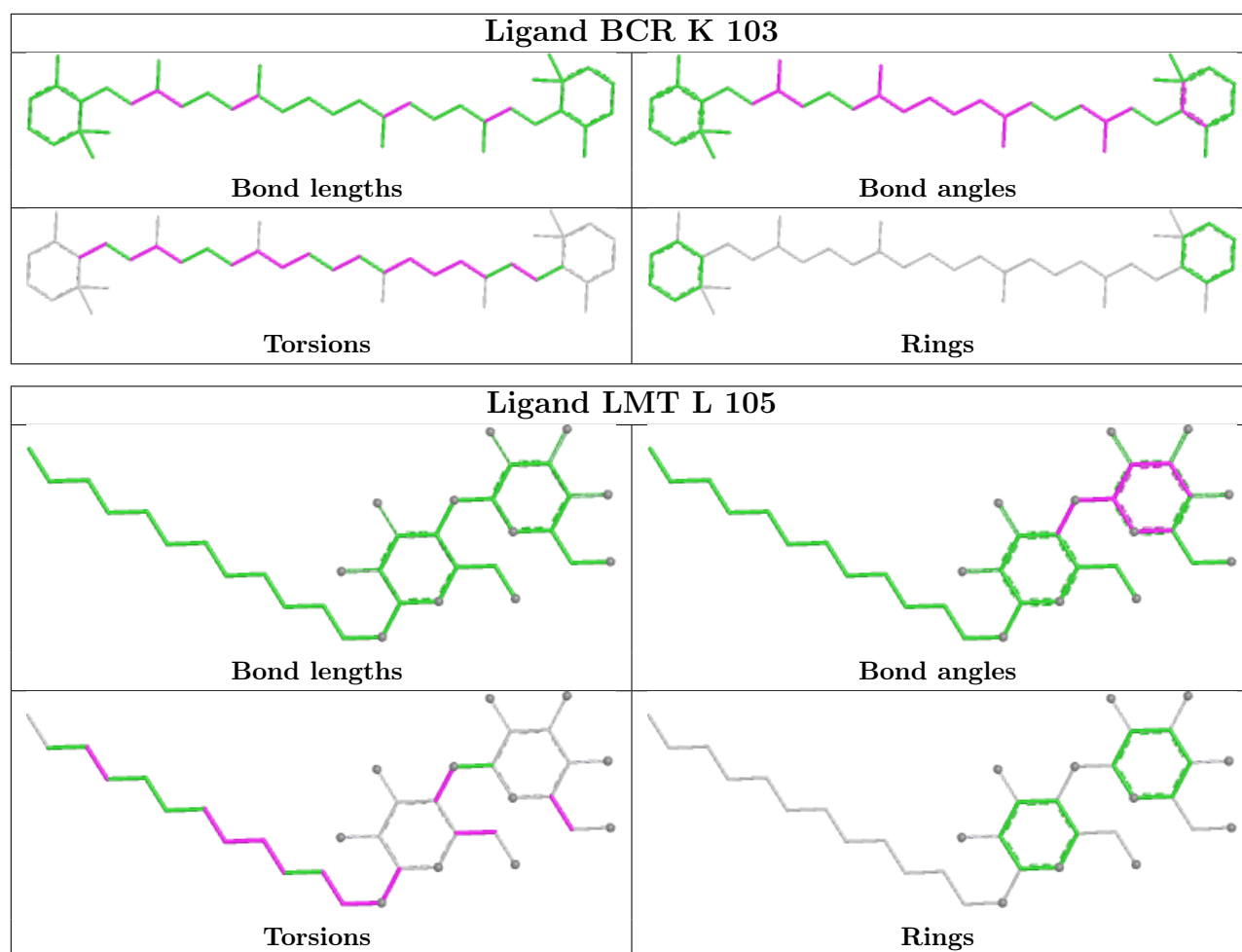
Bond angles

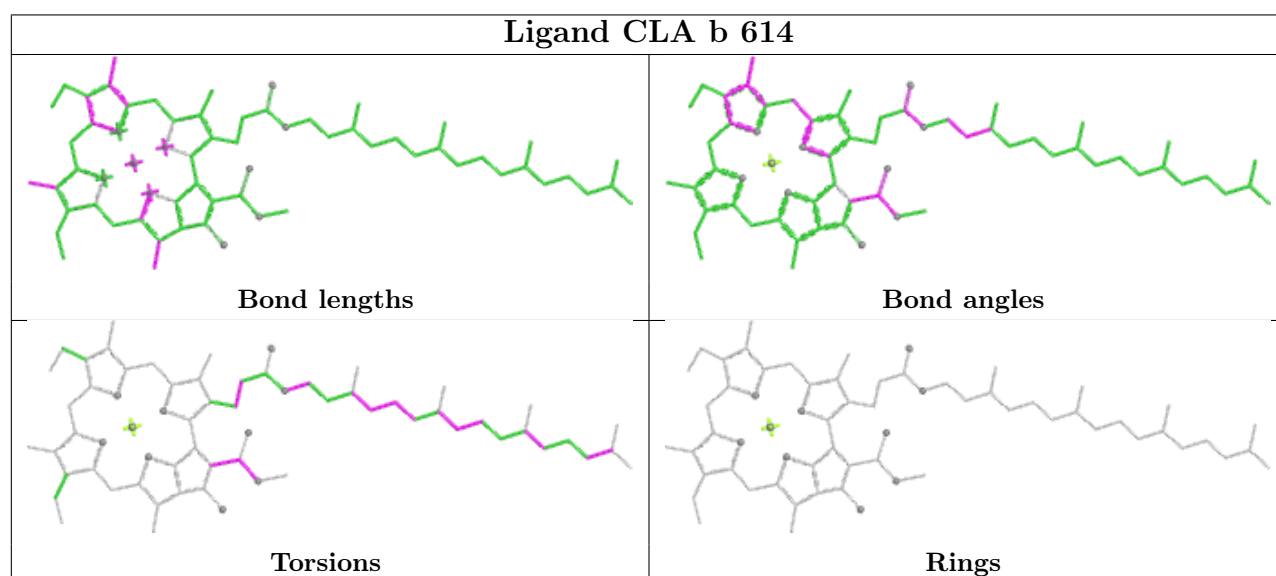
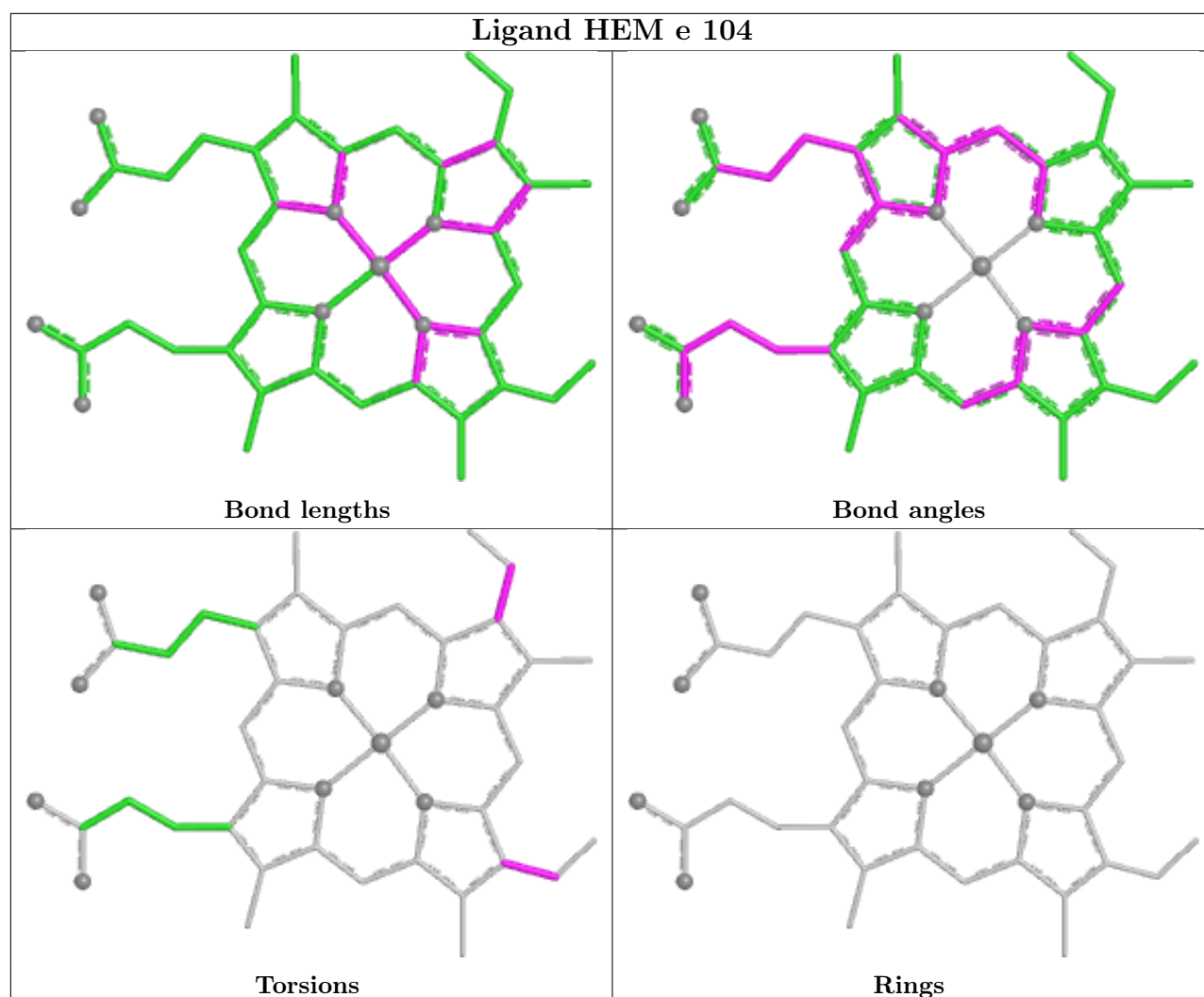


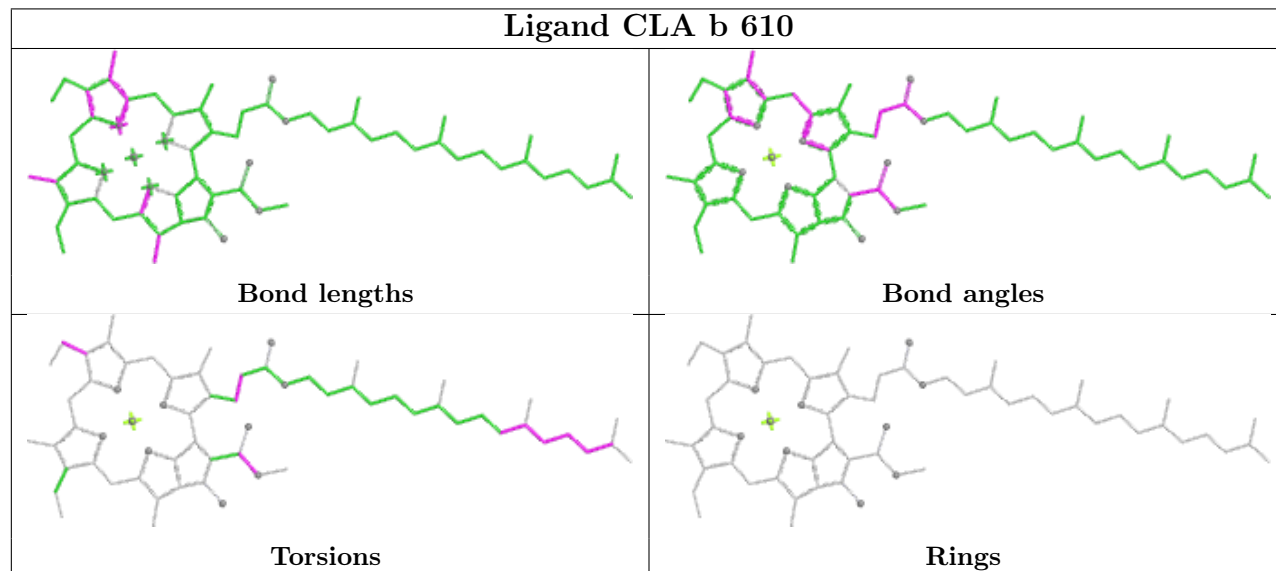
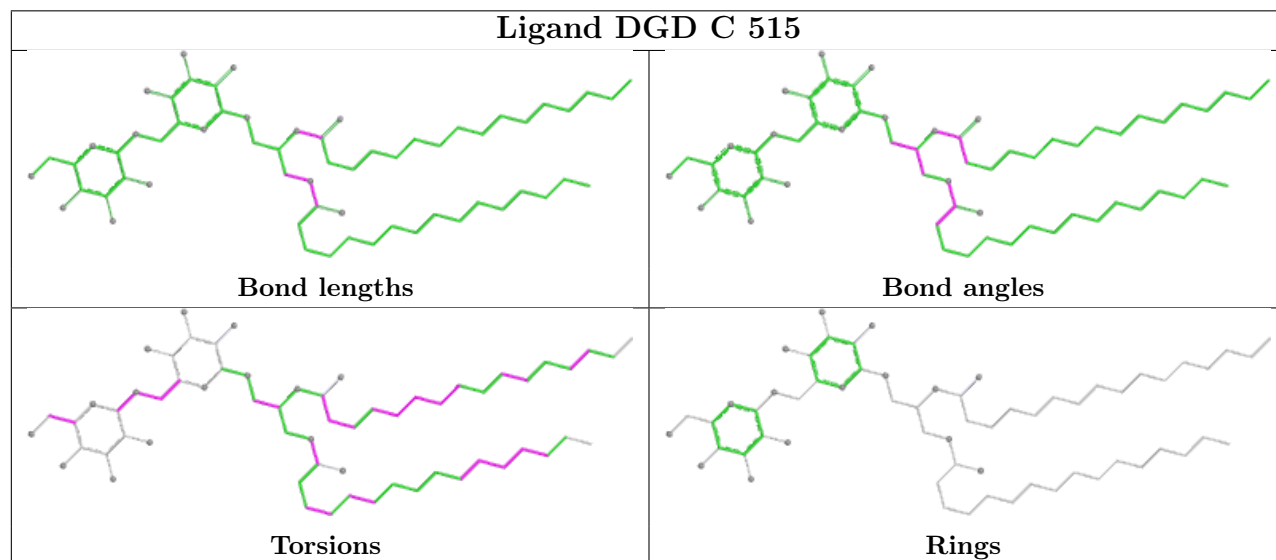
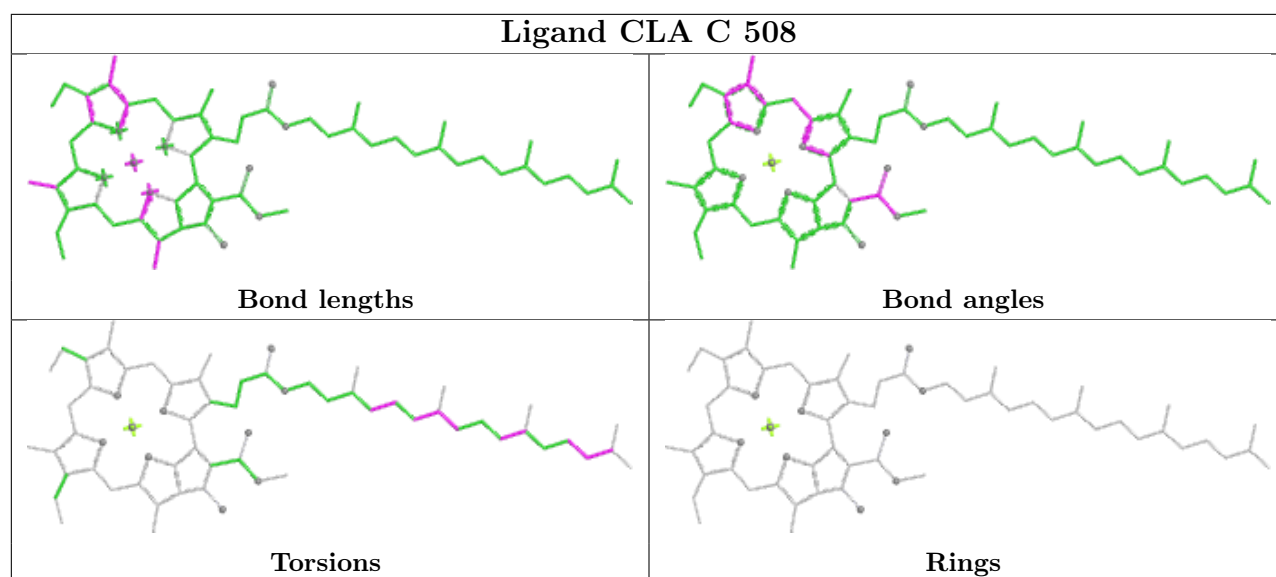
Torsions

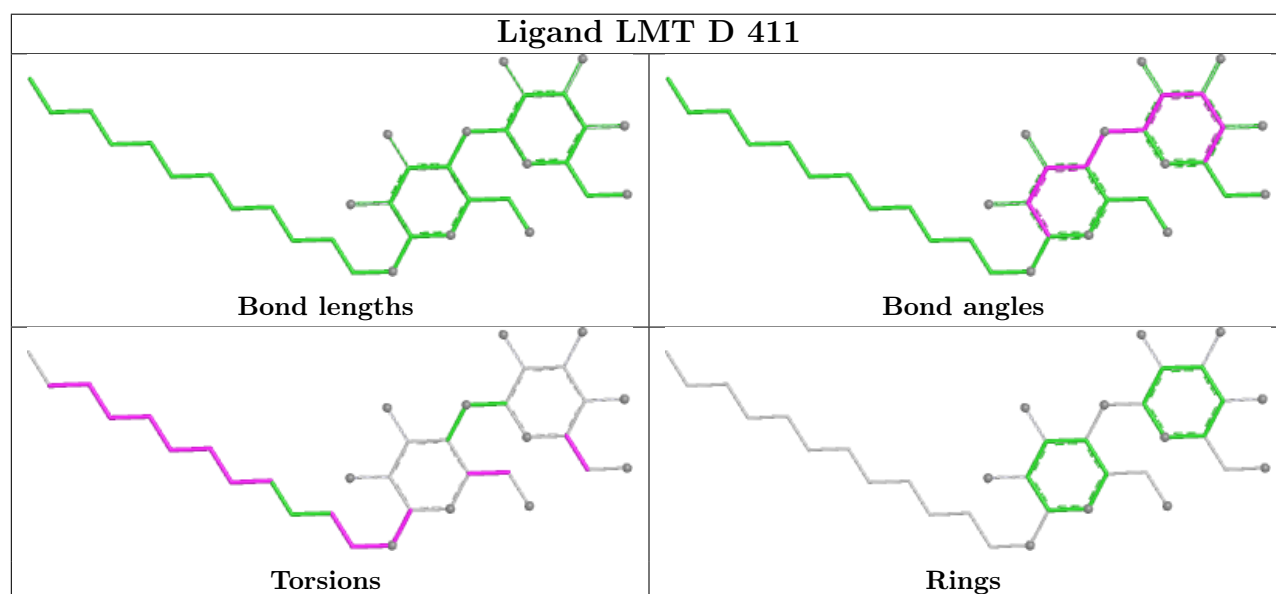
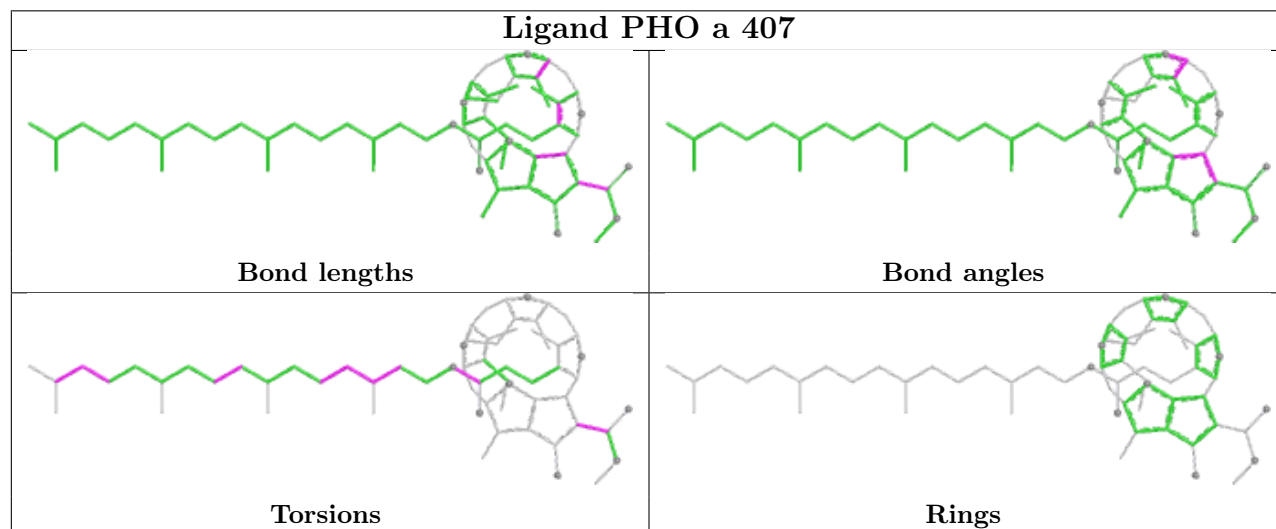
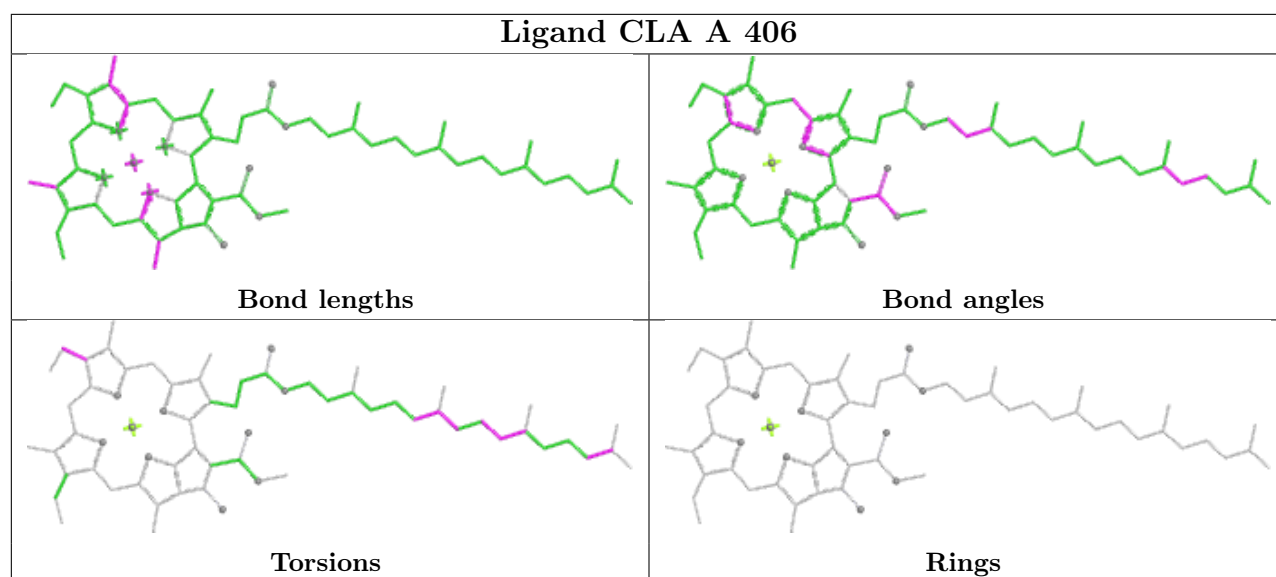


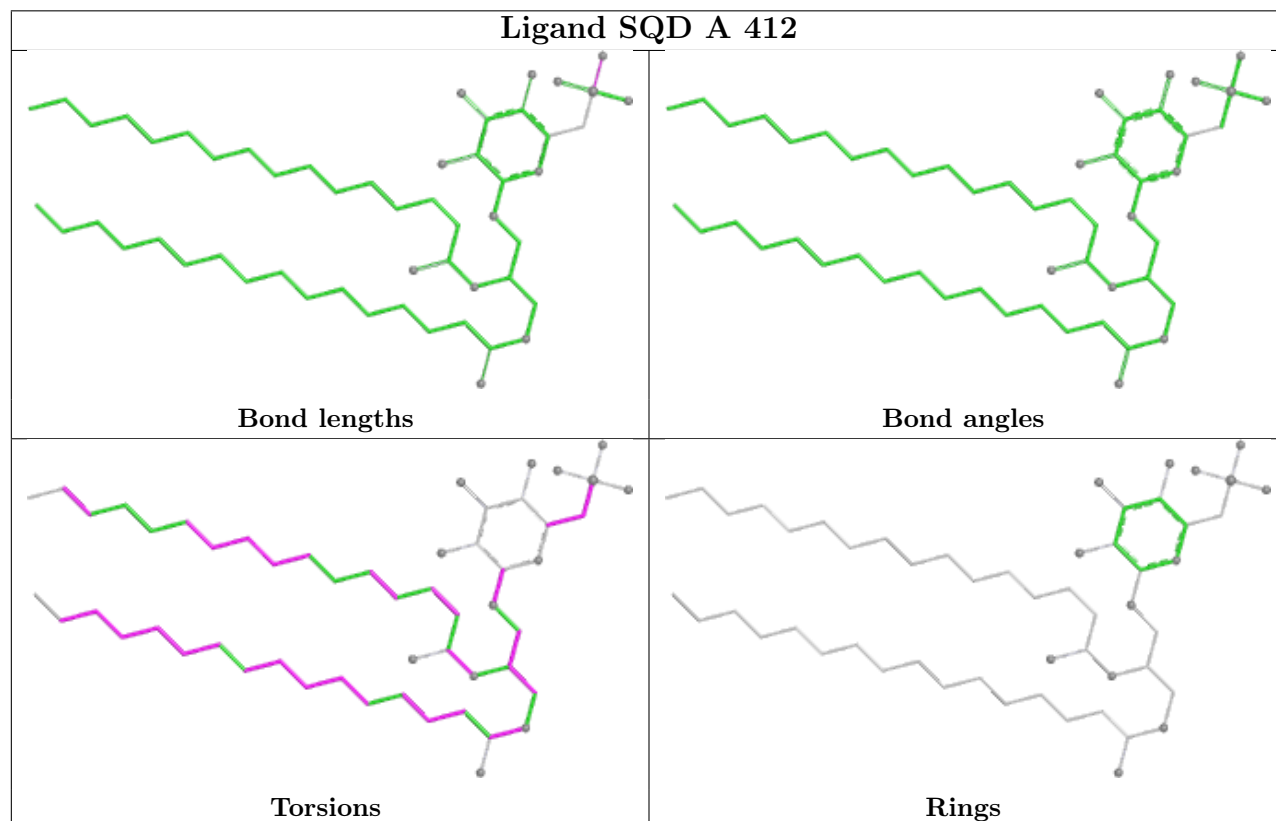
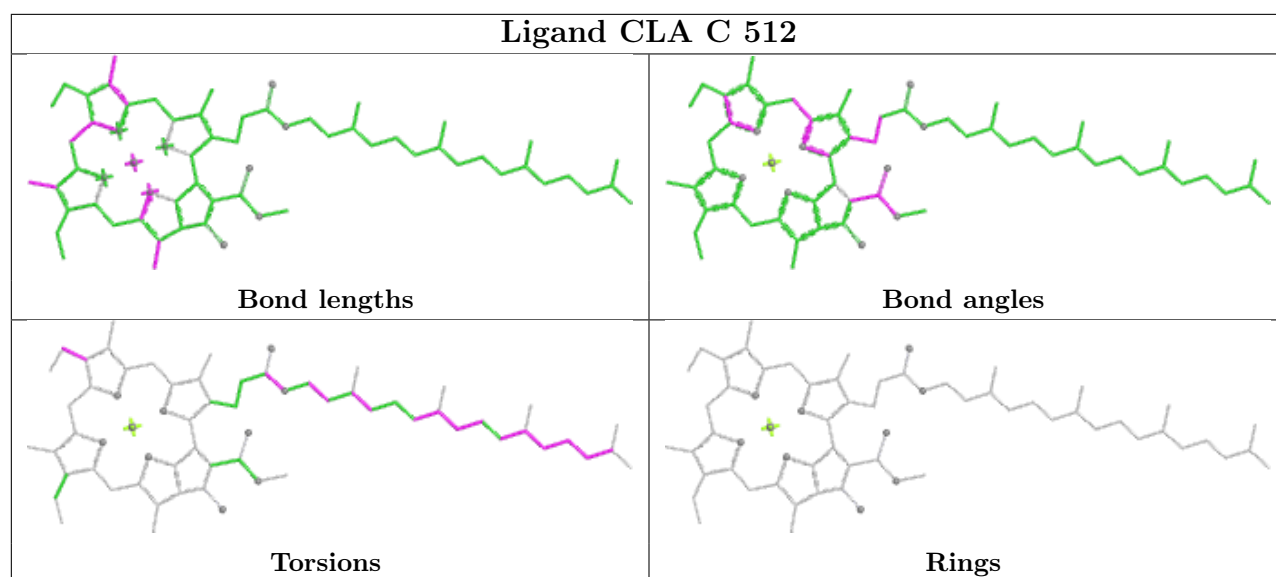
Rings

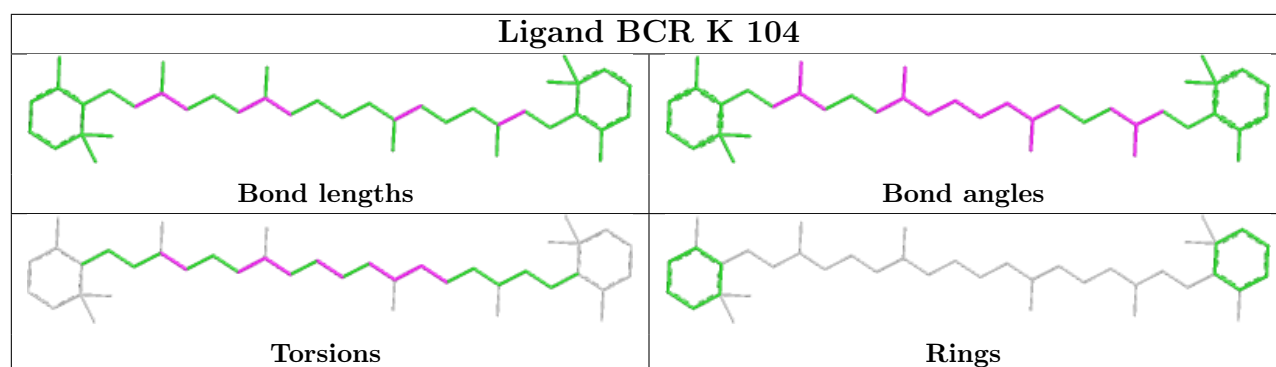
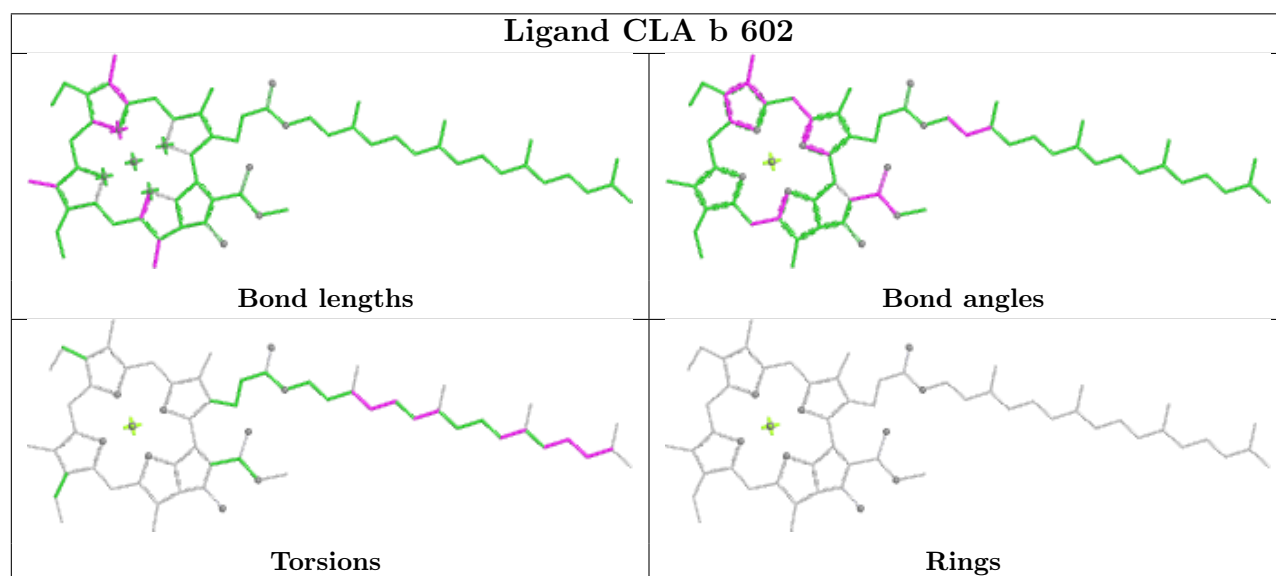
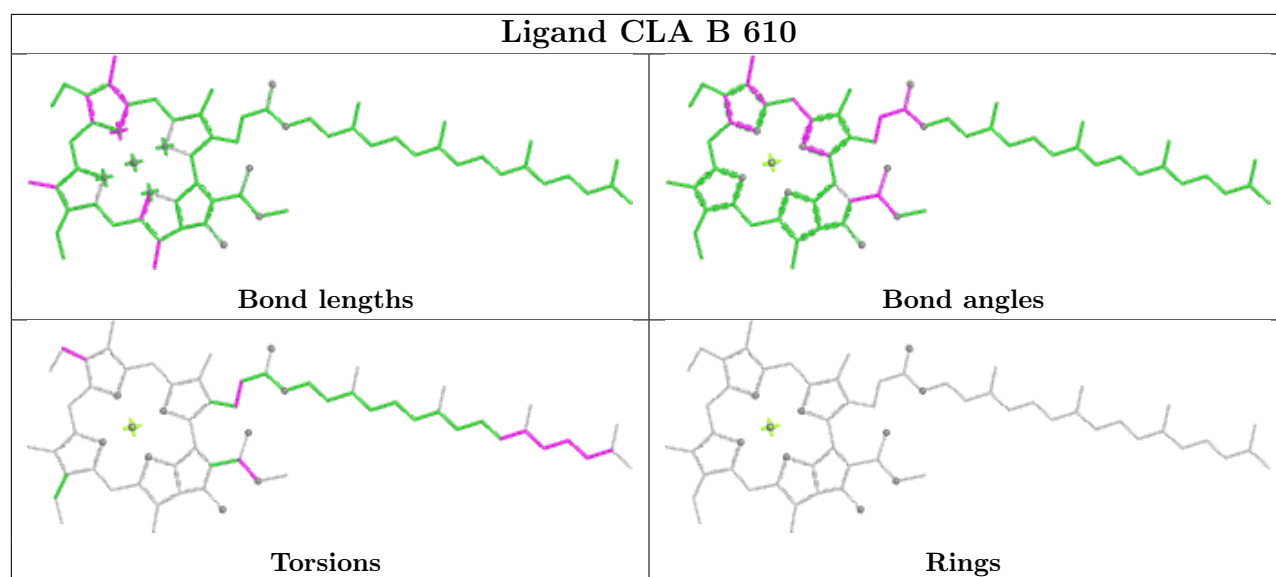


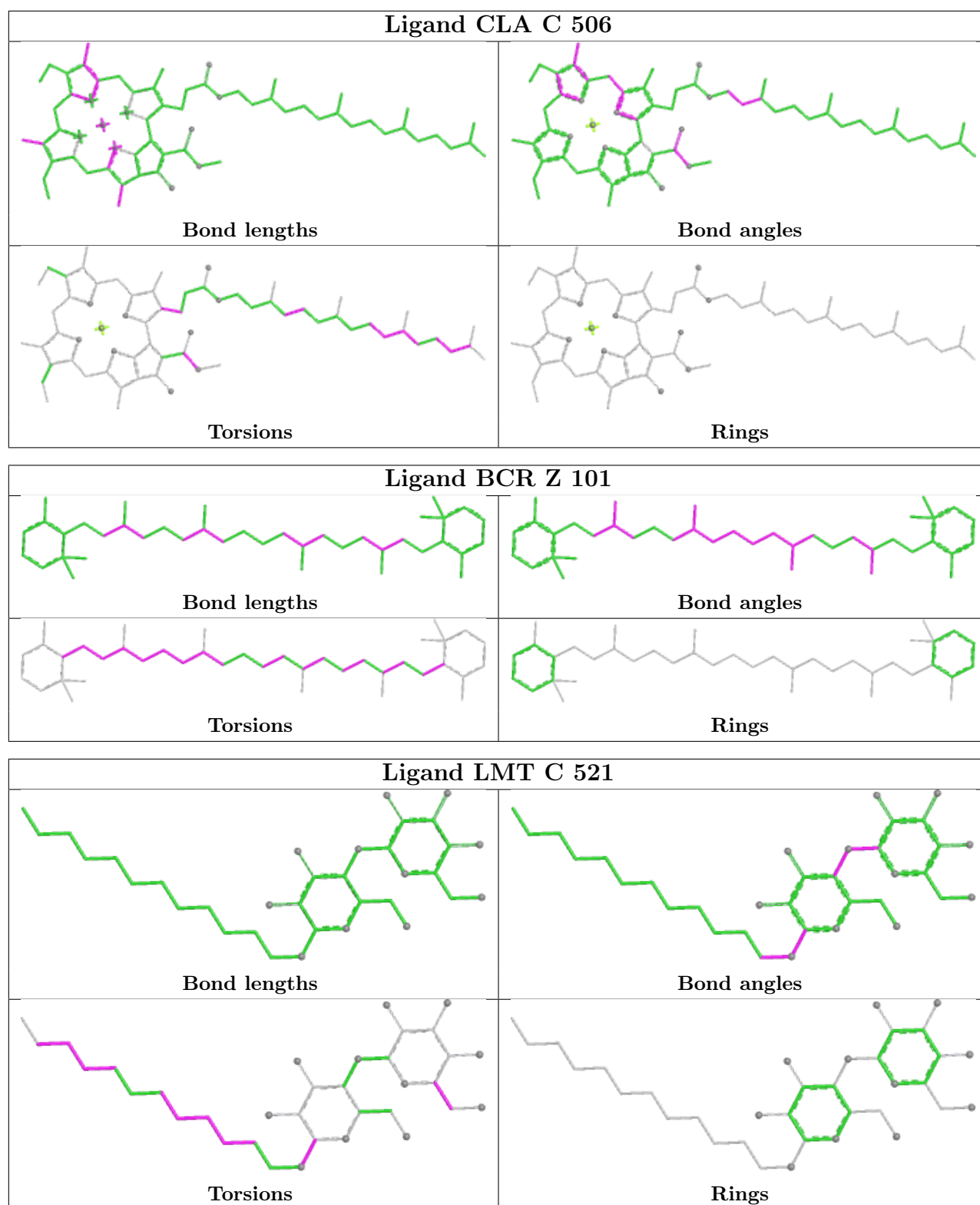


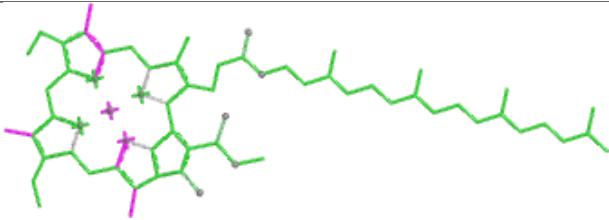
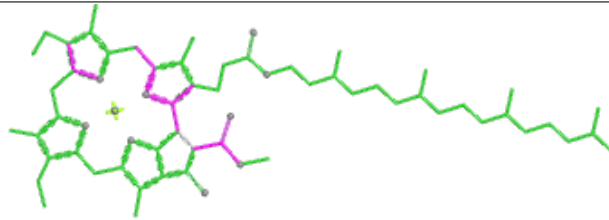
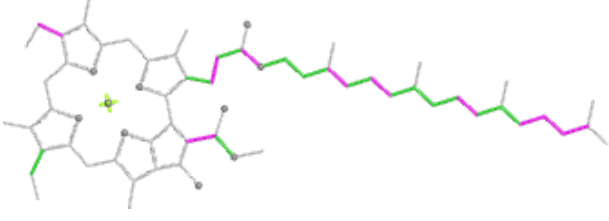
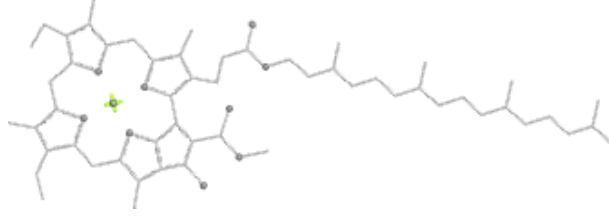




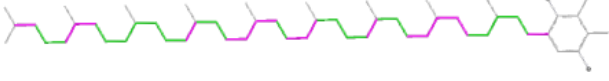
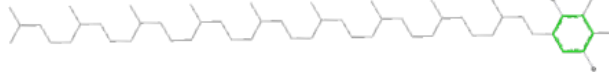


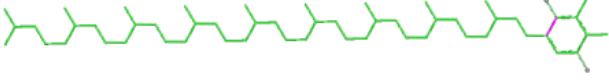
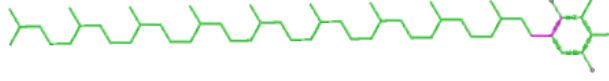

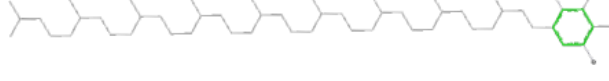


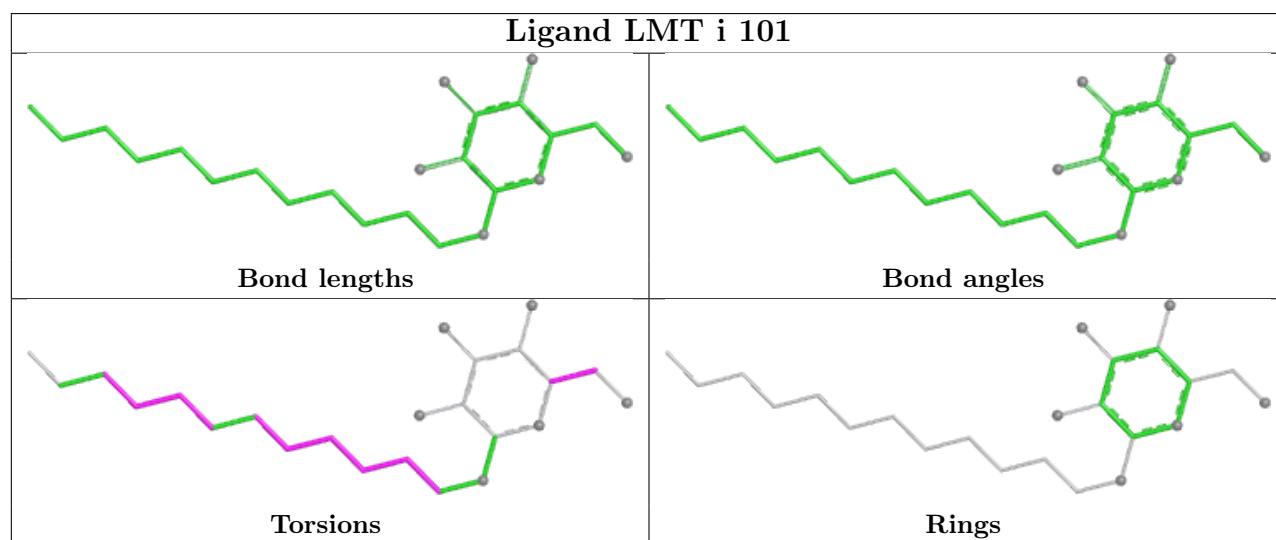
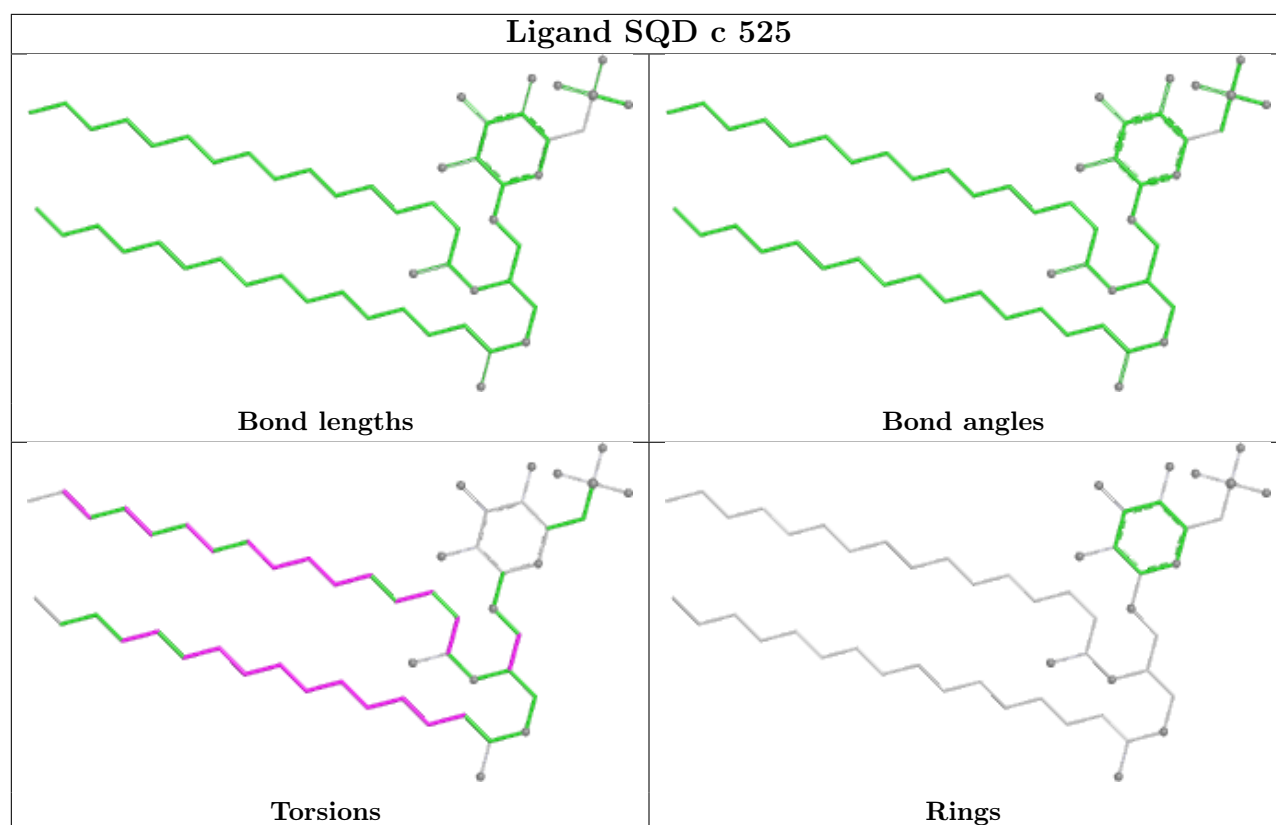


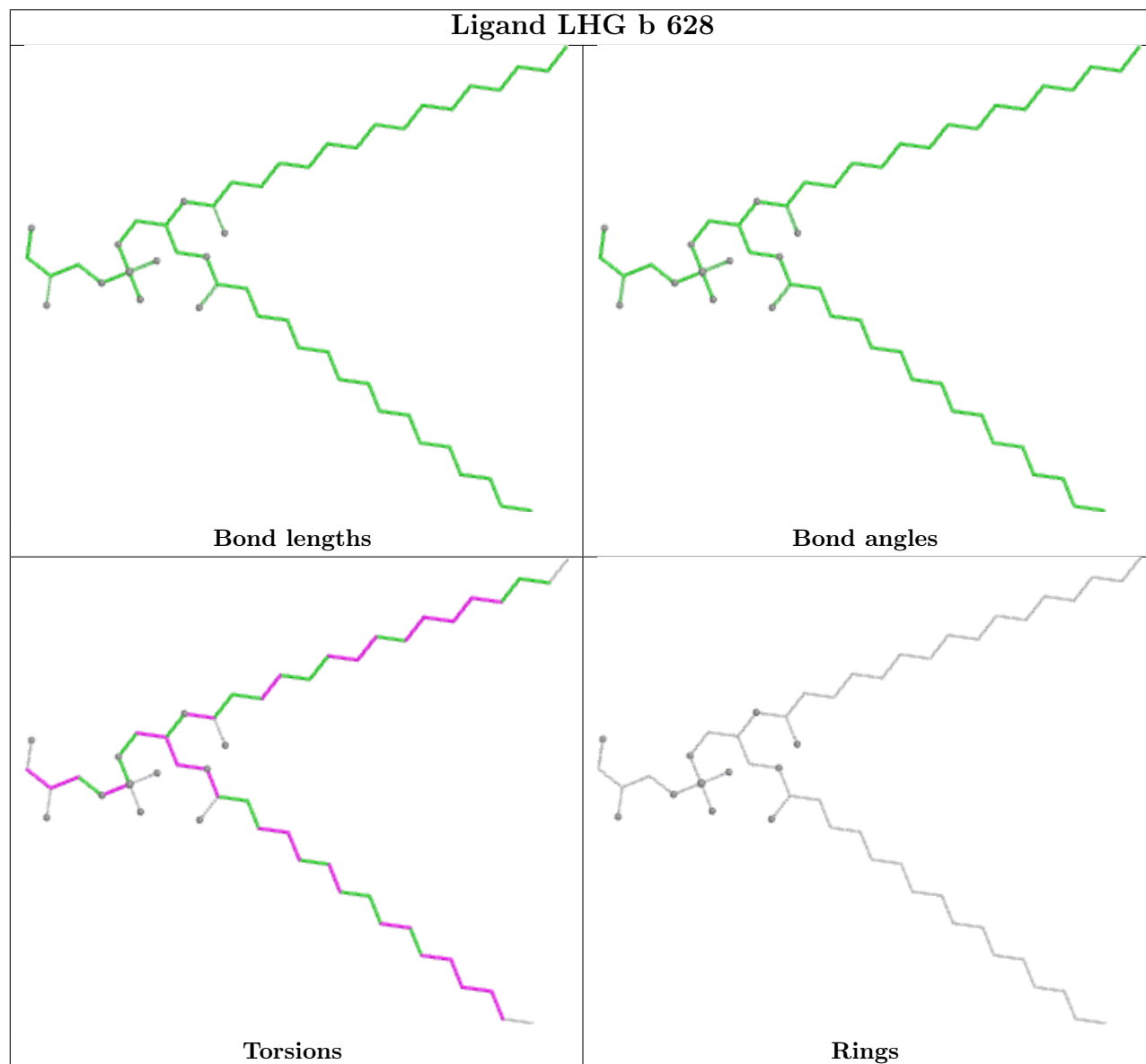
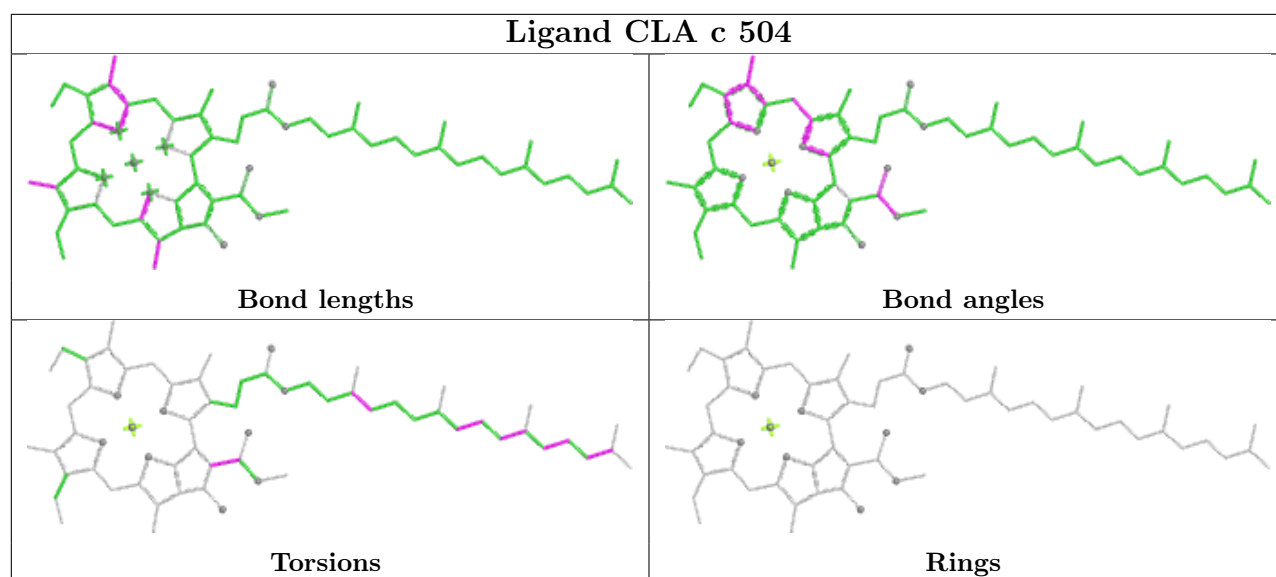


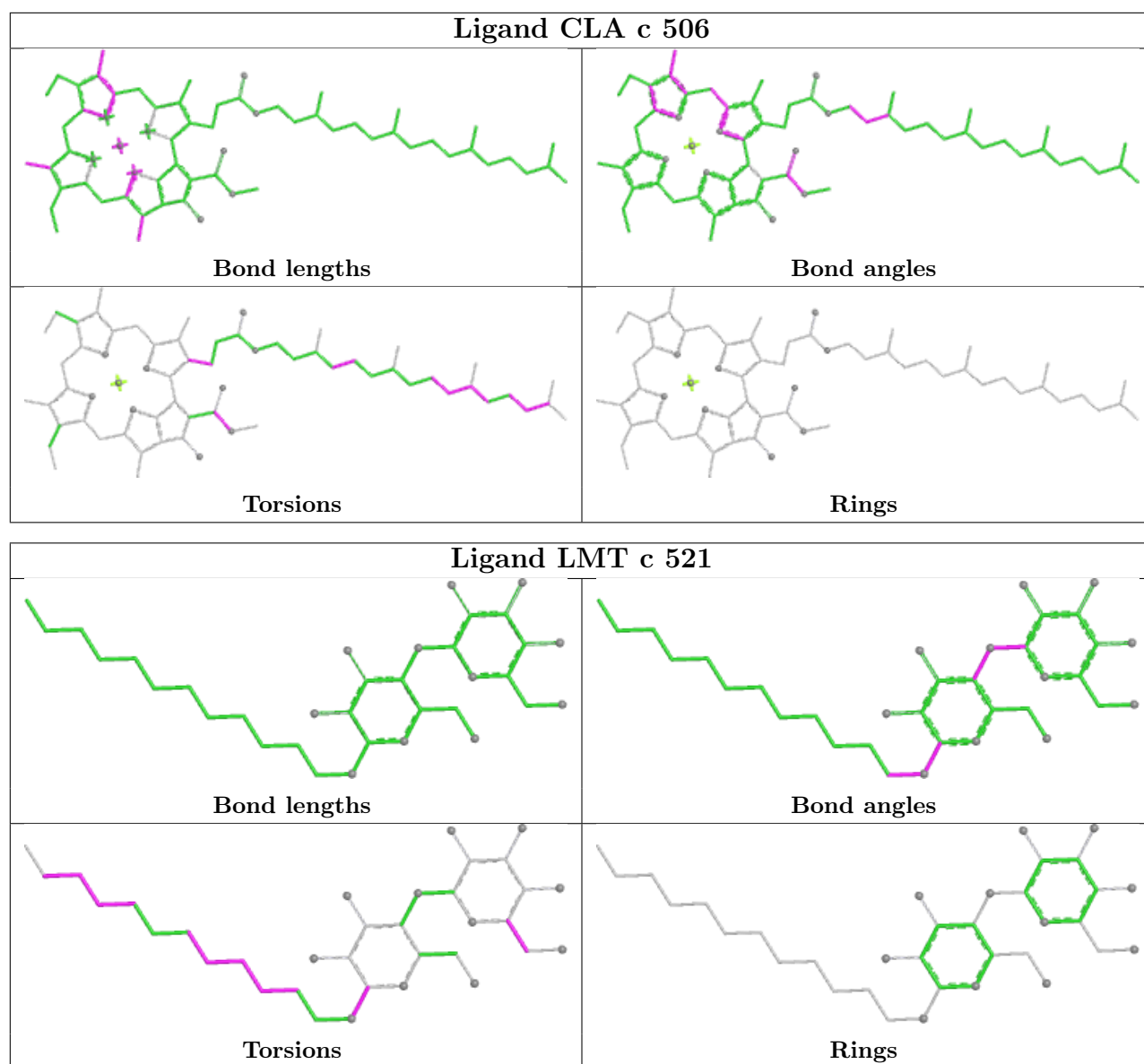
Ligand CLA C 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

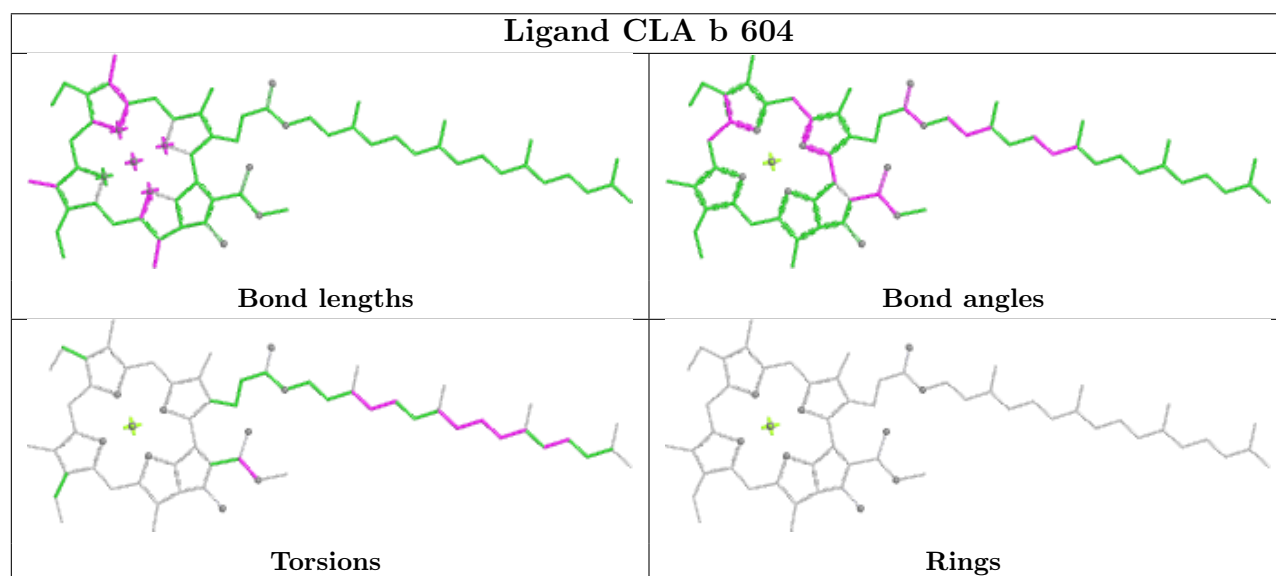
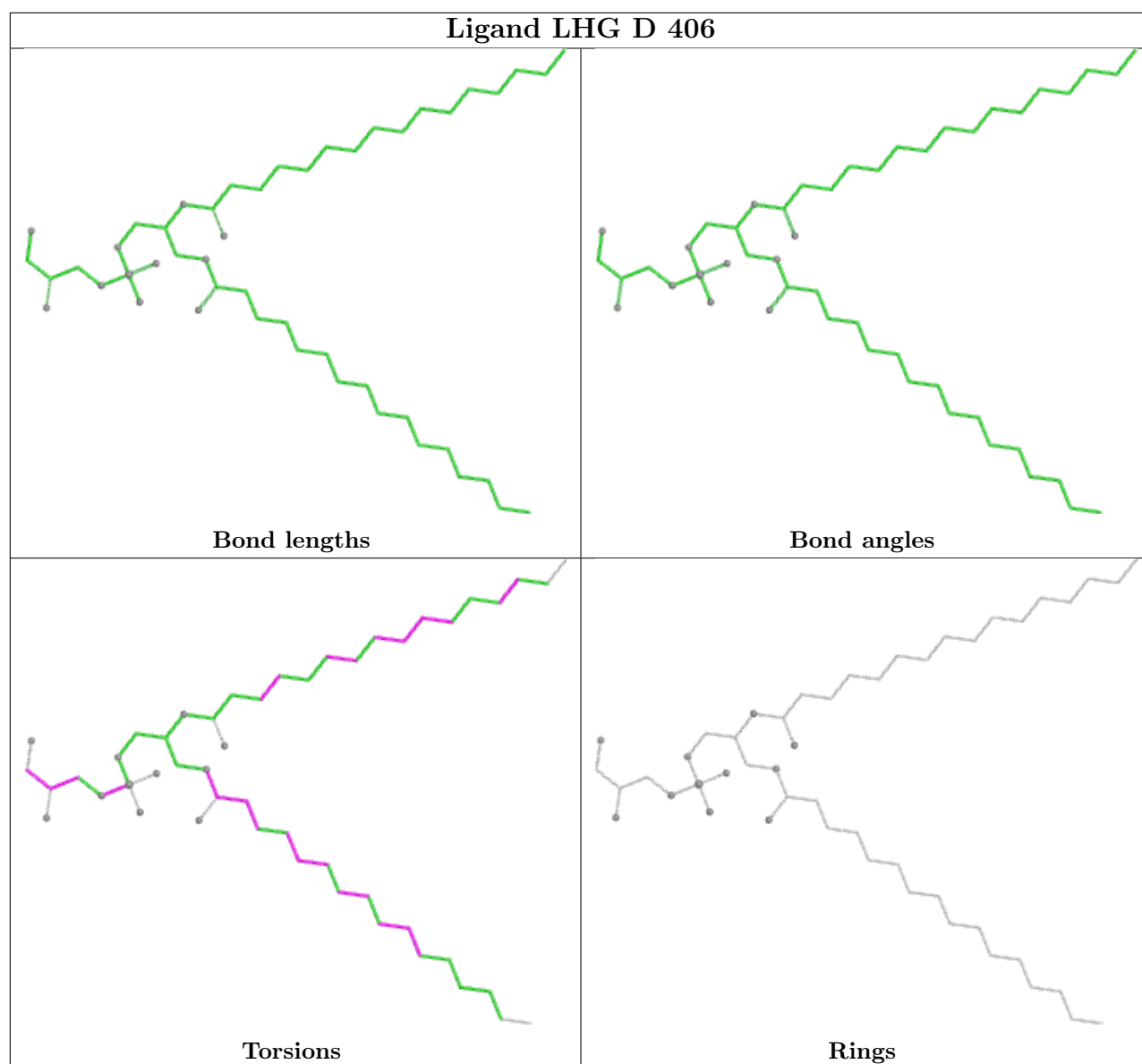
Ligand PL9 a 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

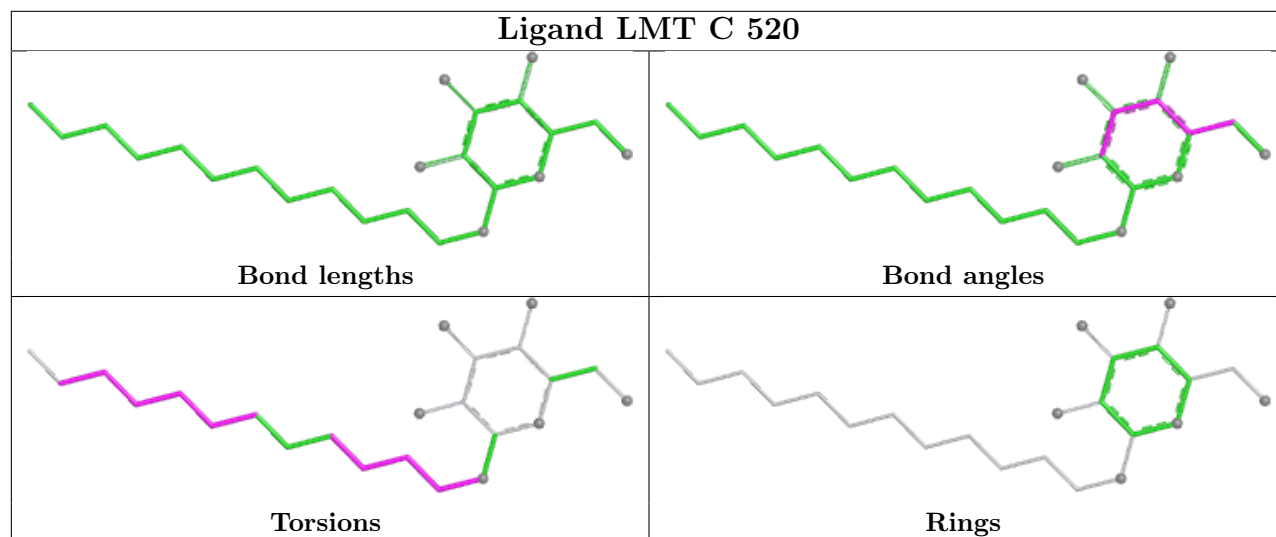
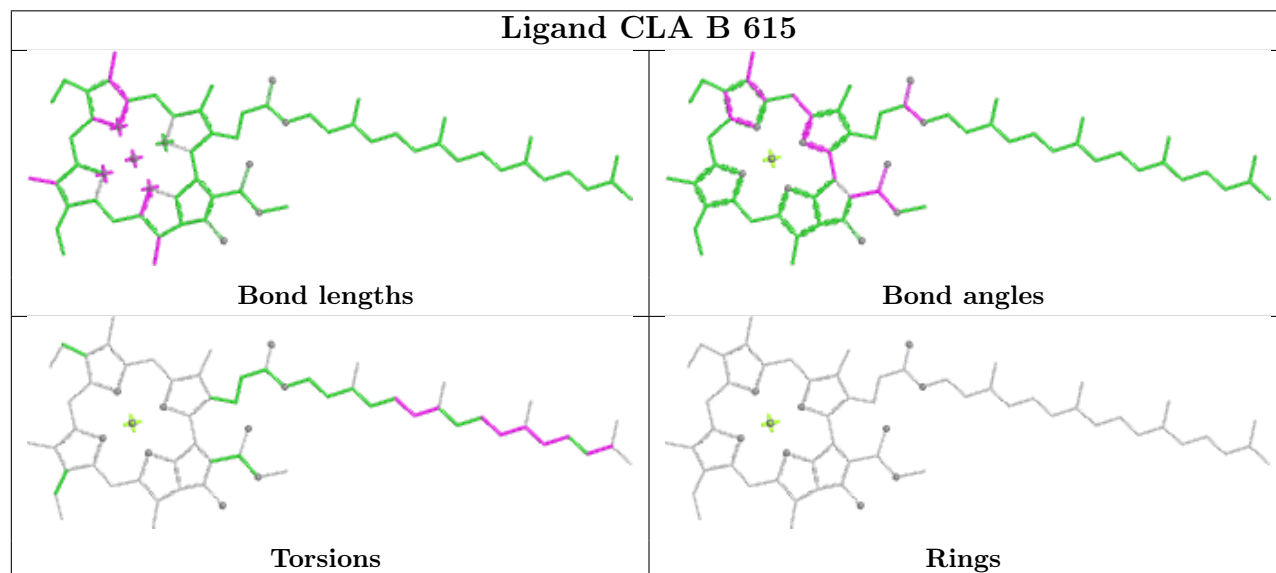
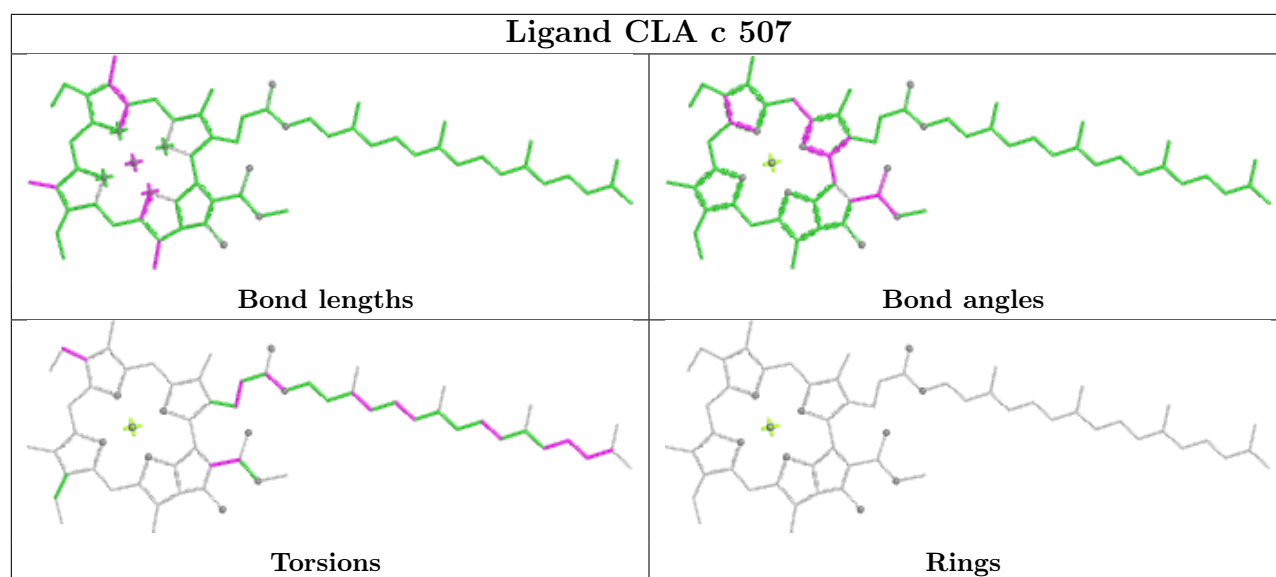
Ligand PL9 d 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

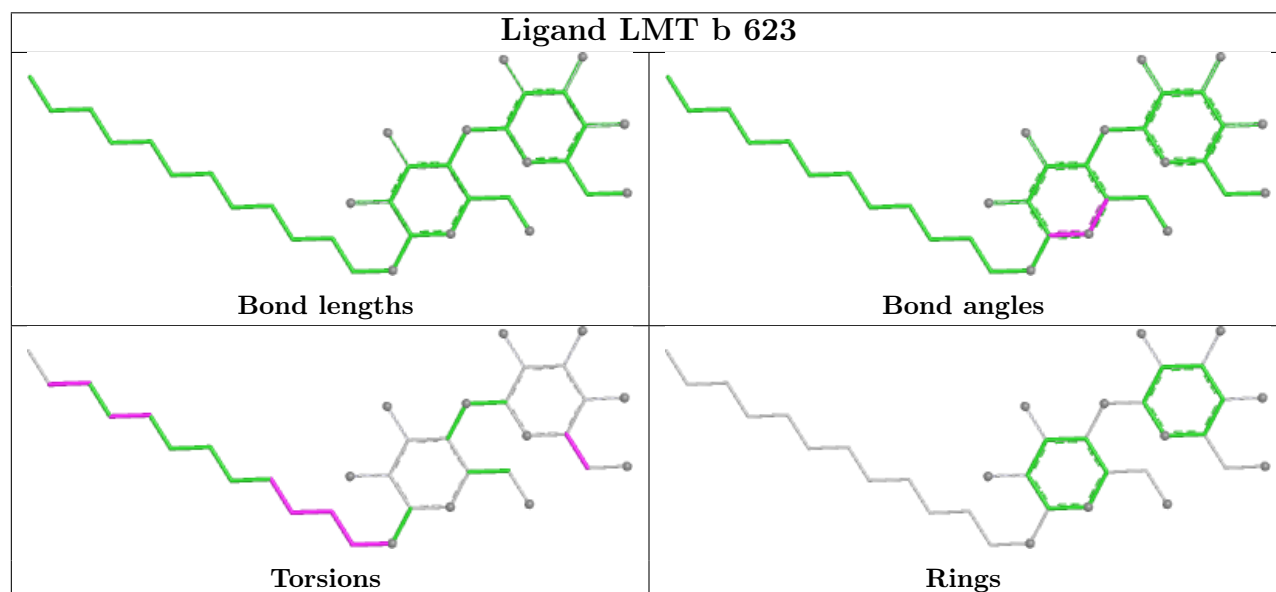
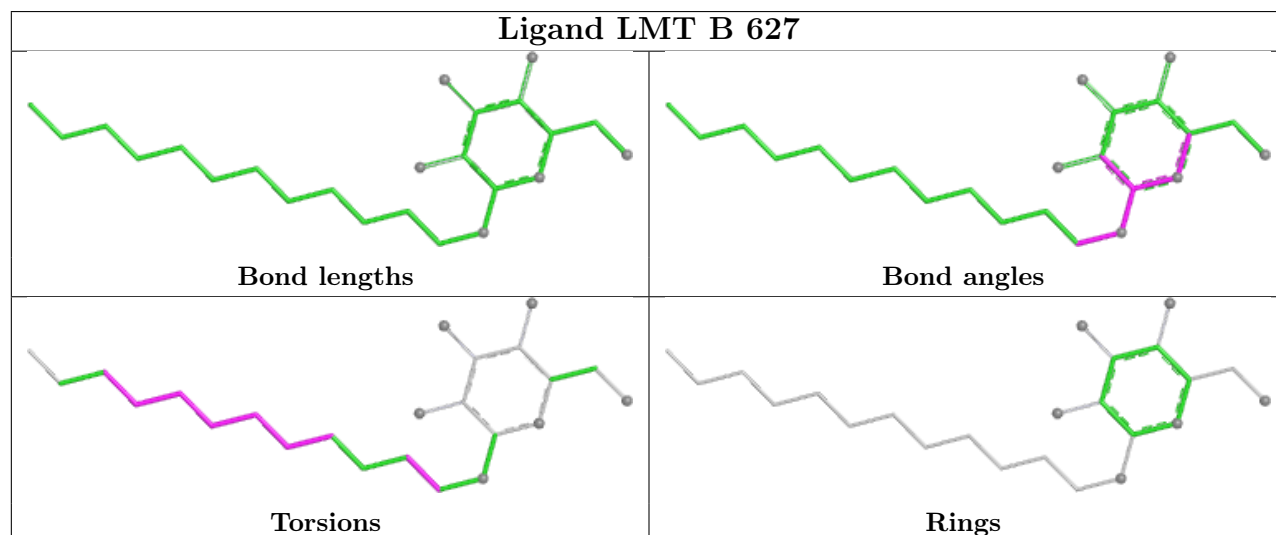
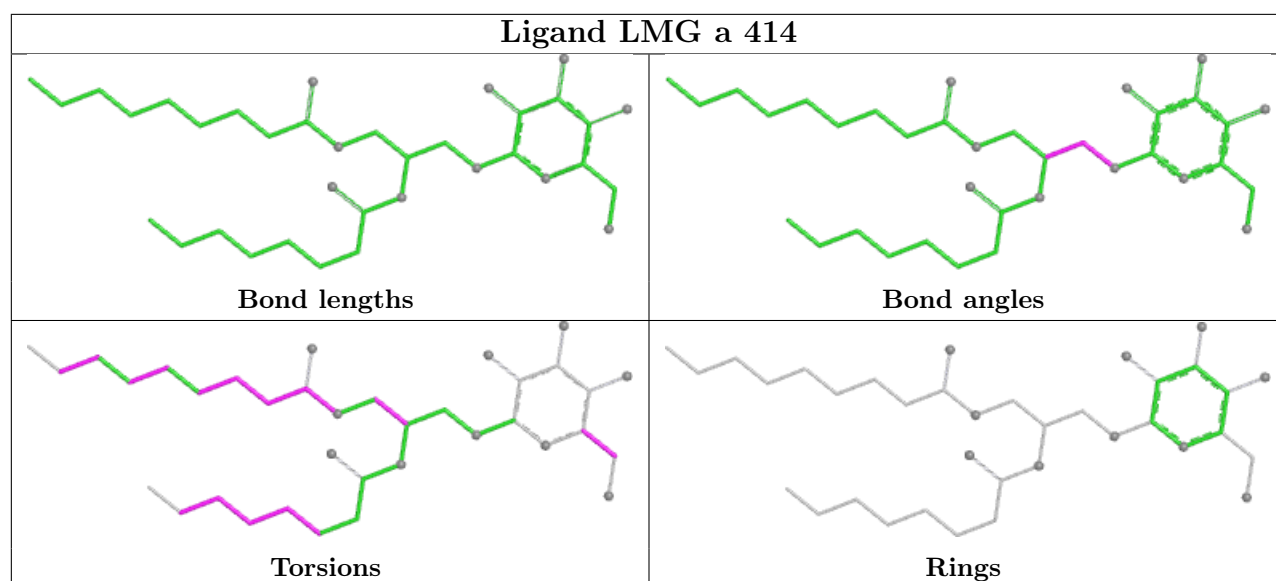


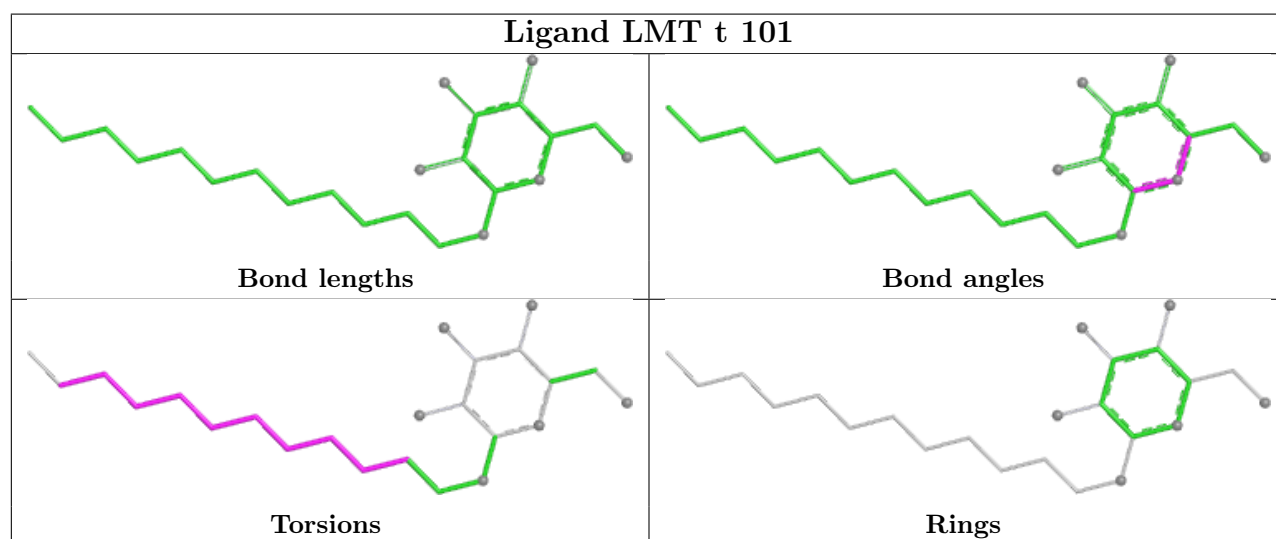
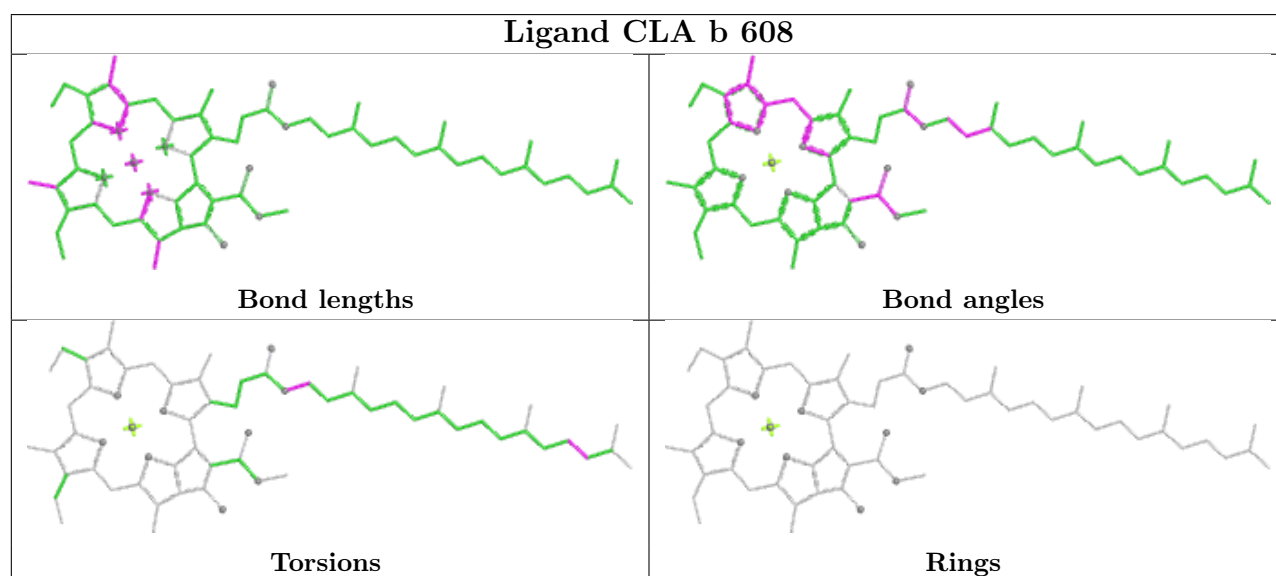
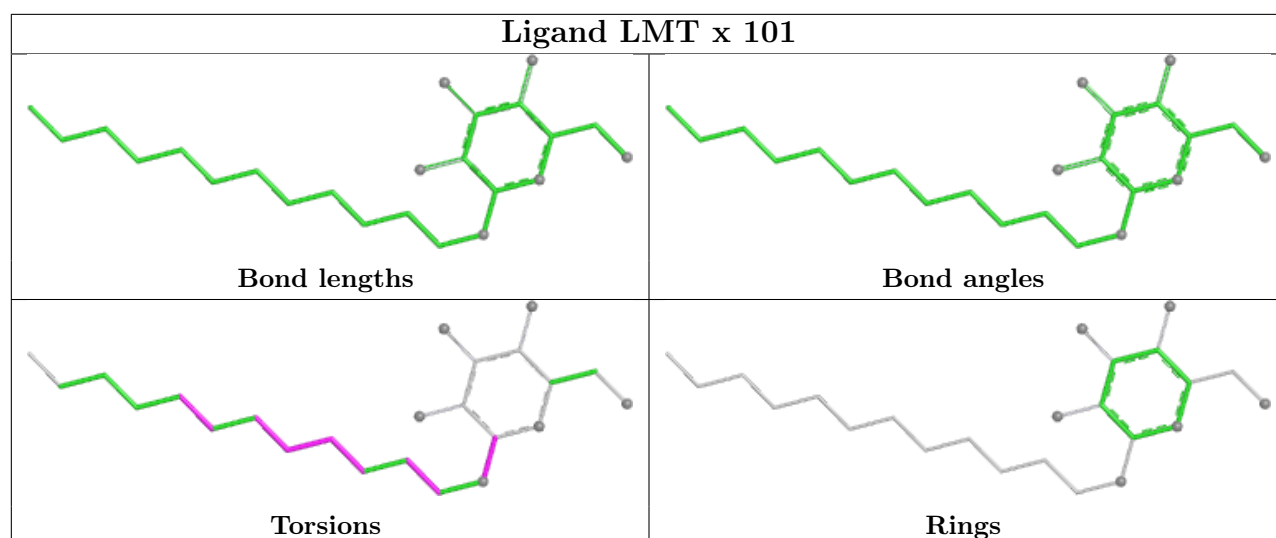


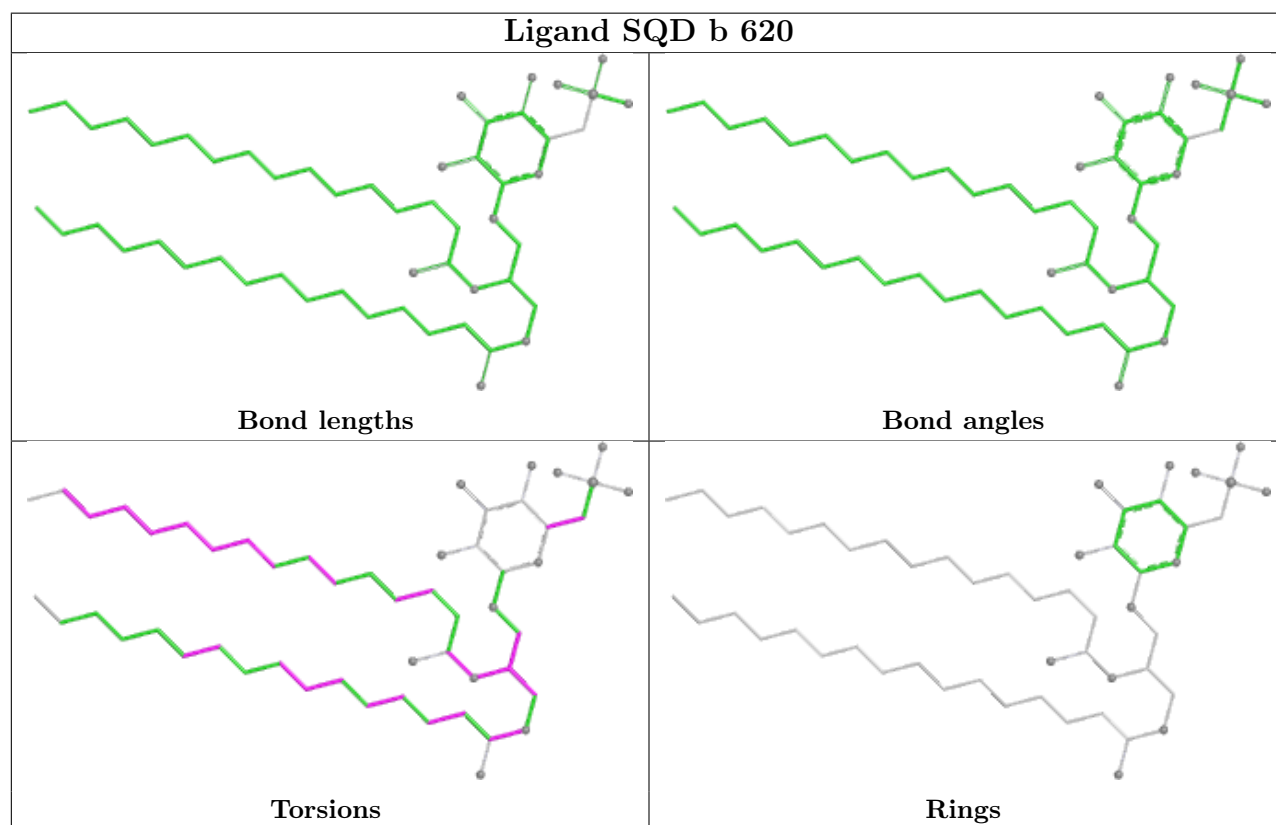
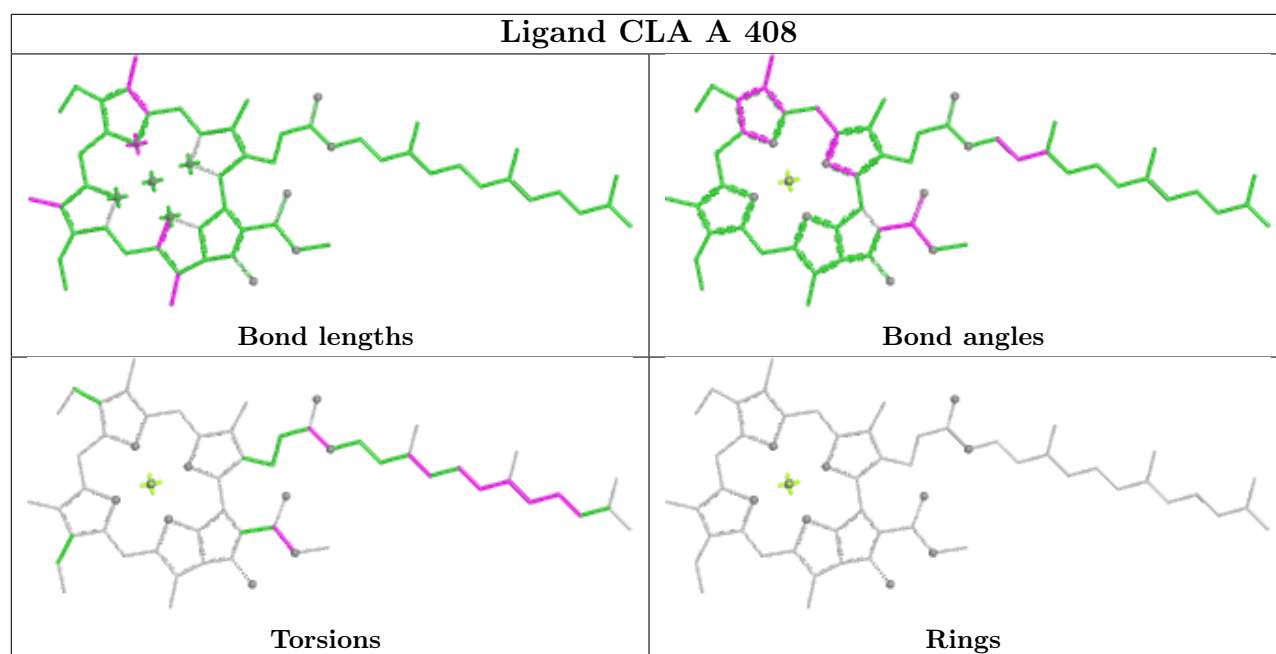


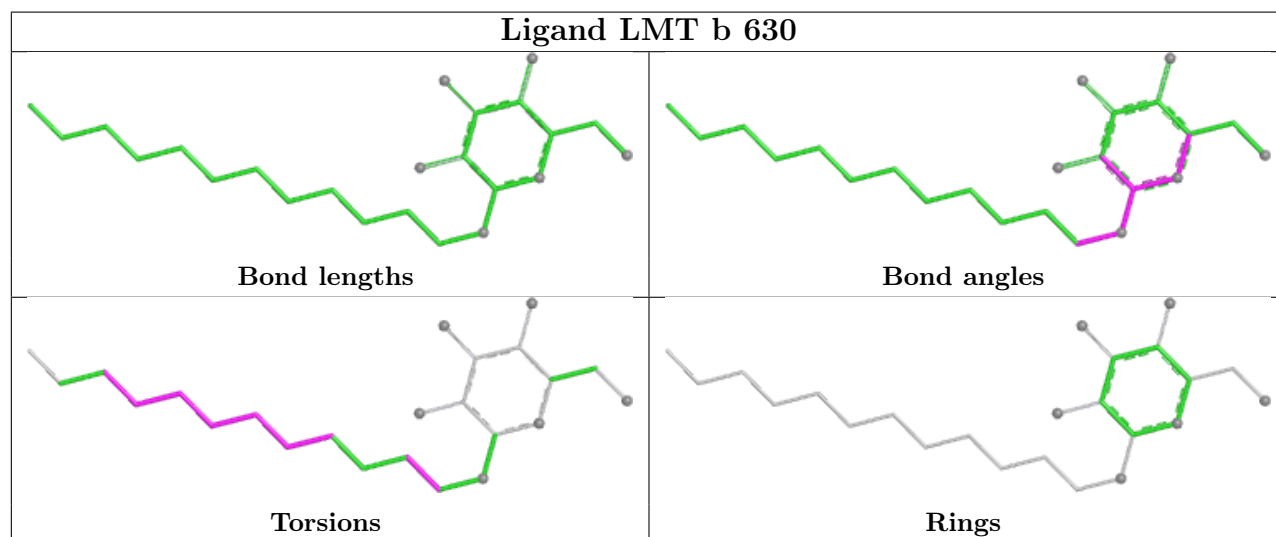
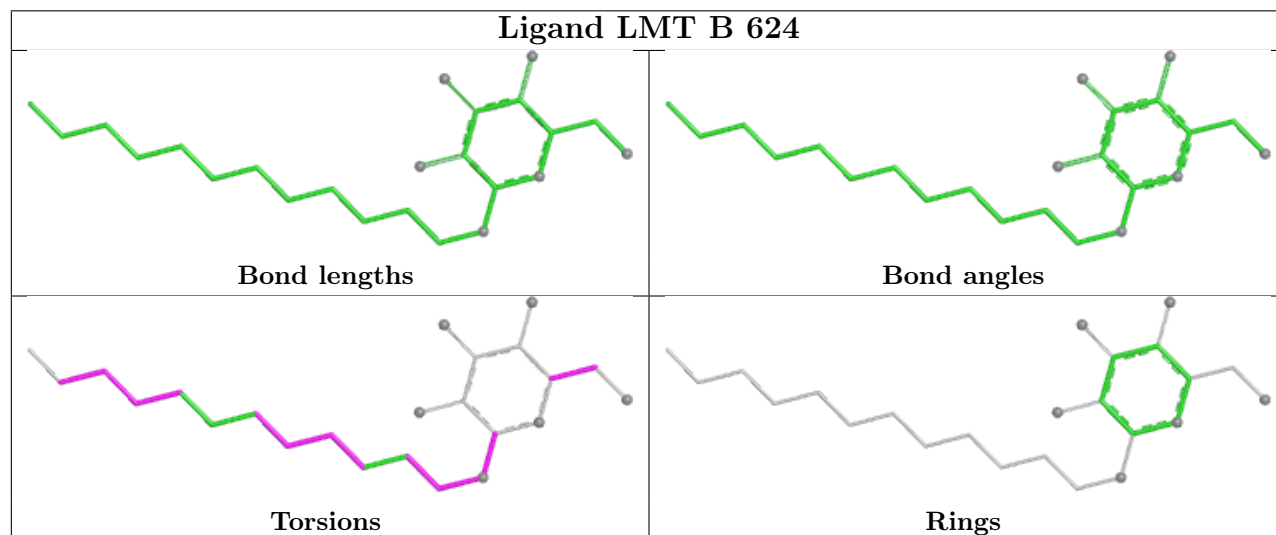
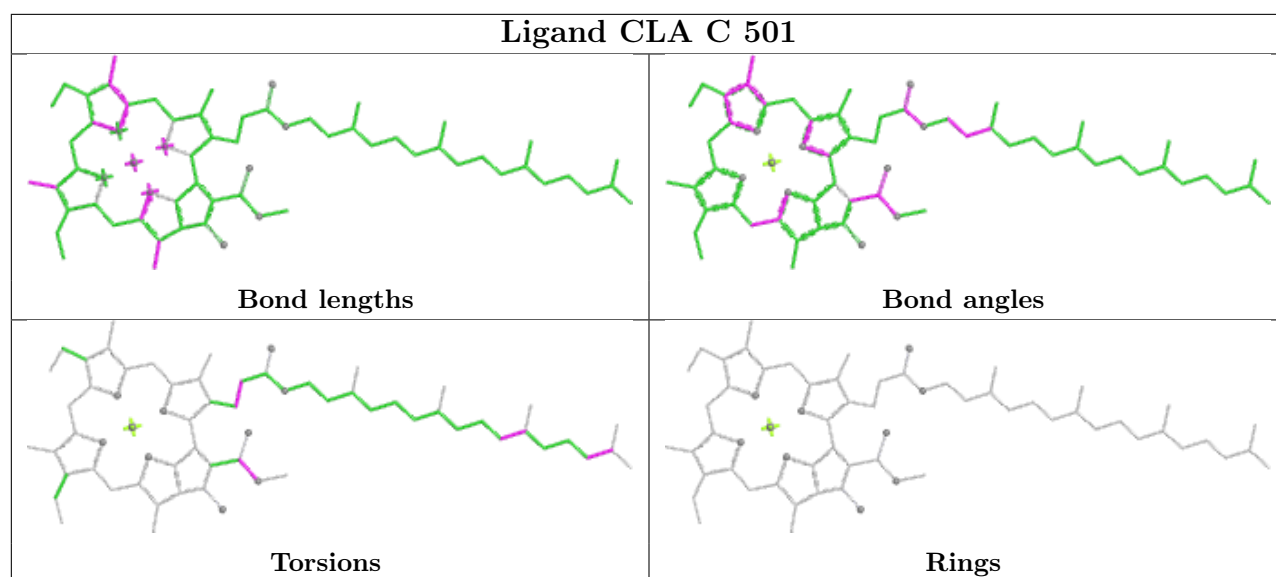


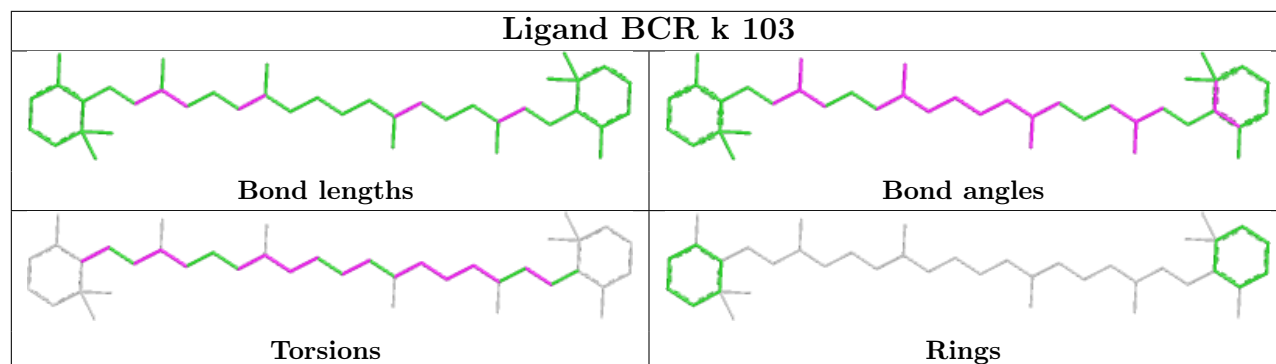
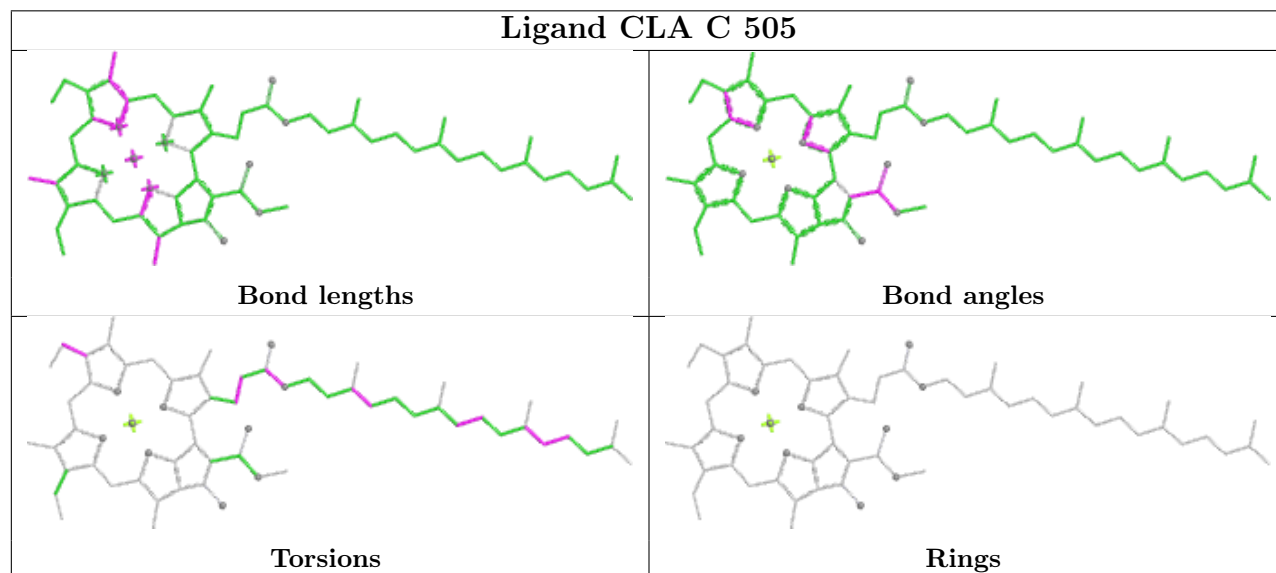
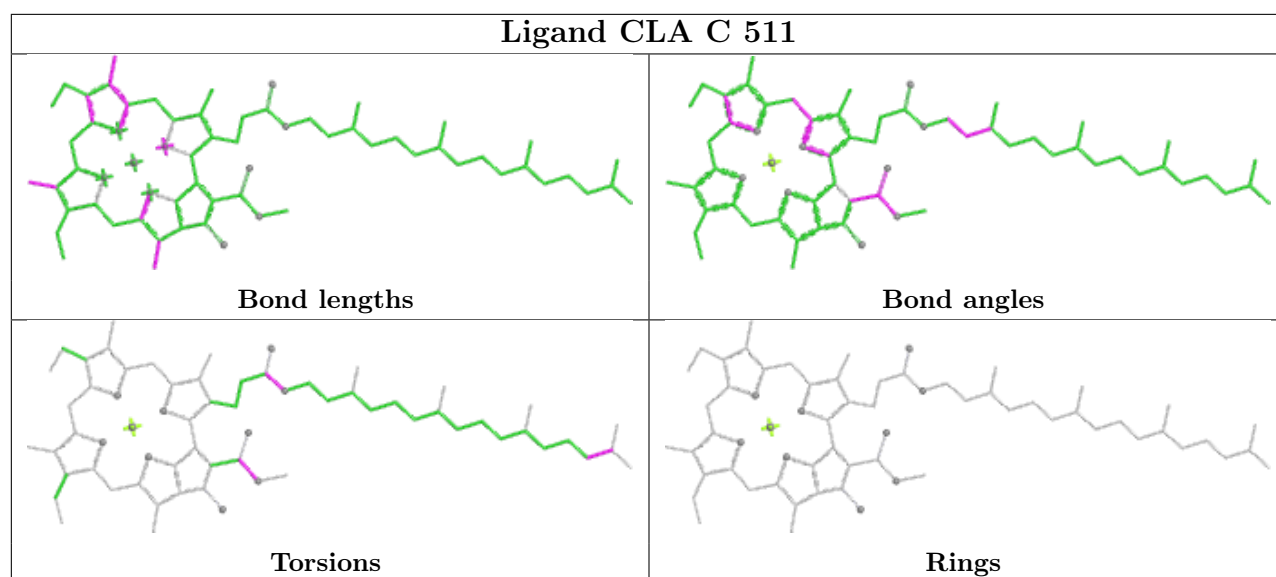


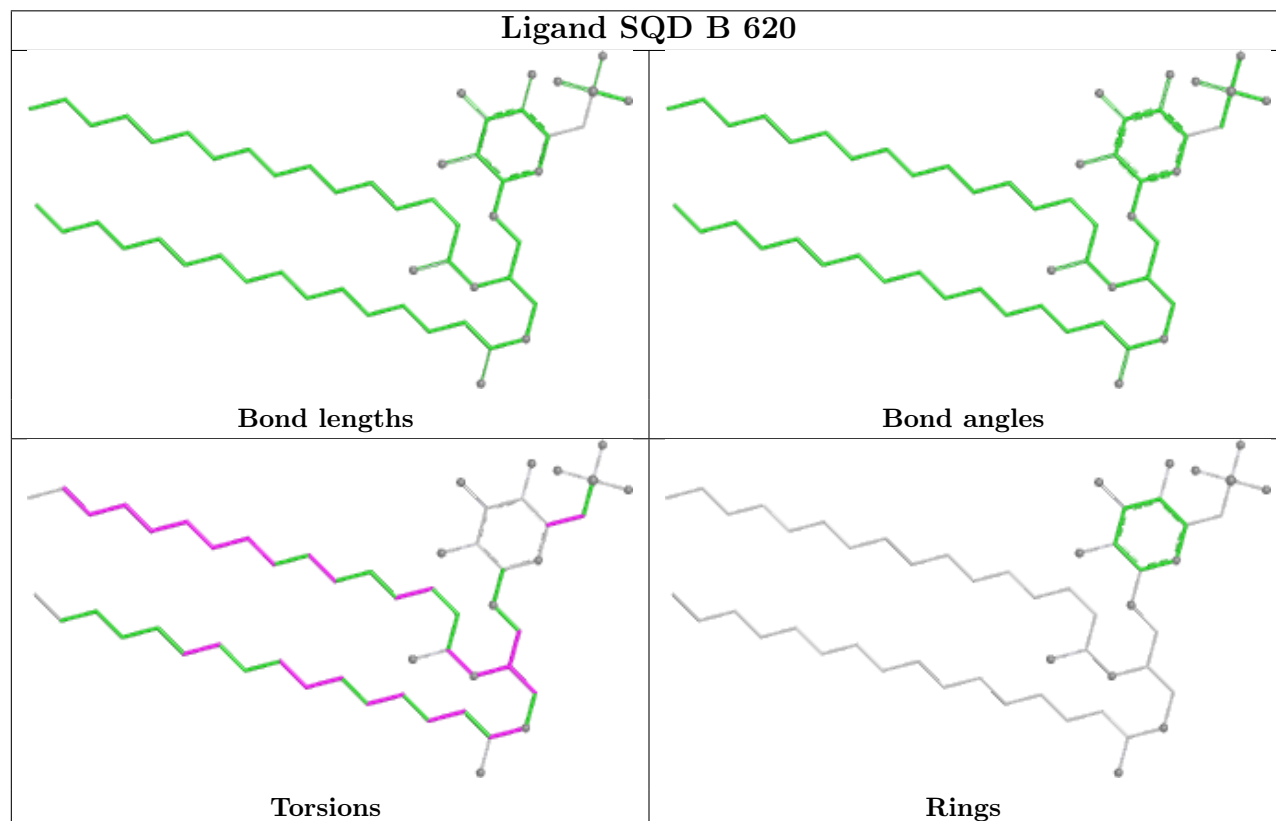
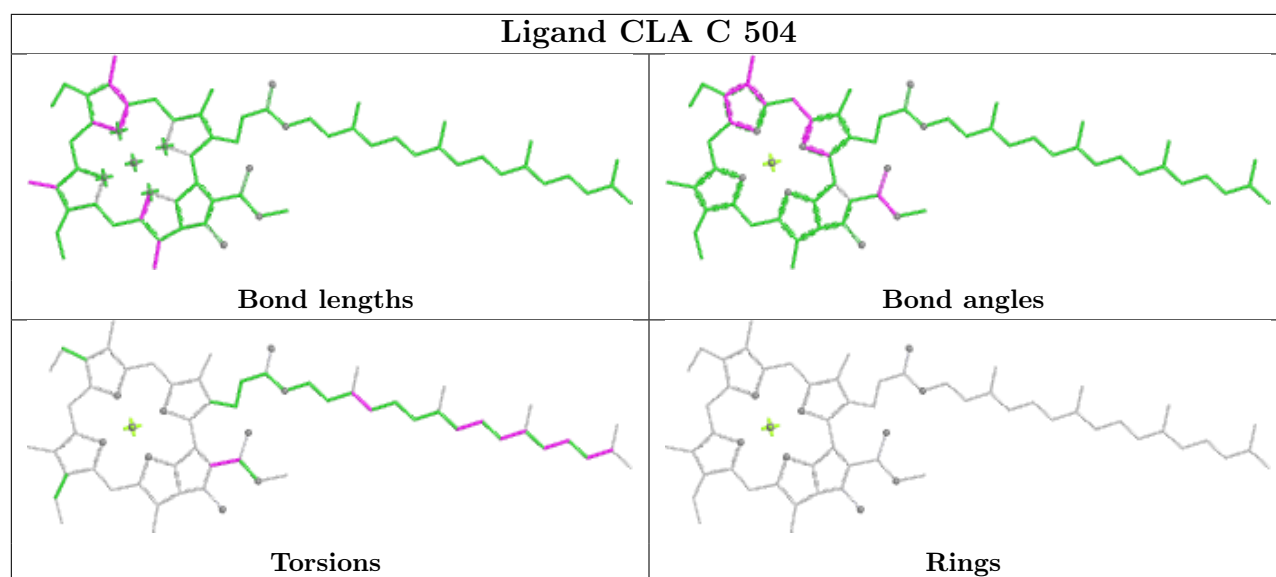


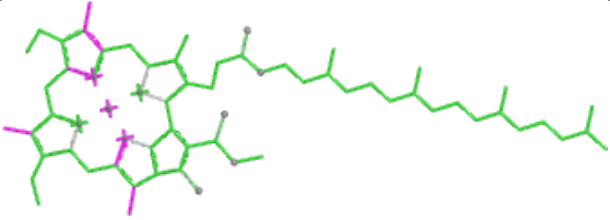
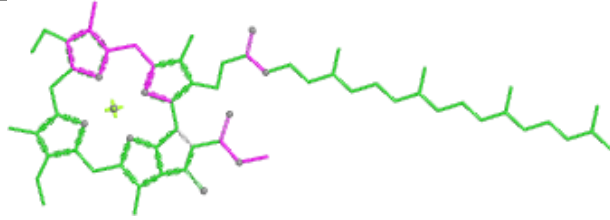
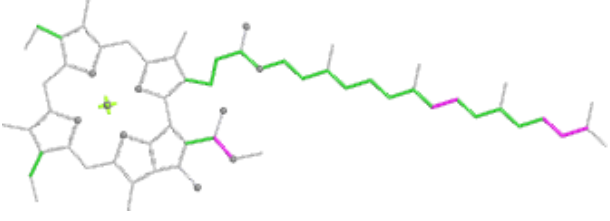
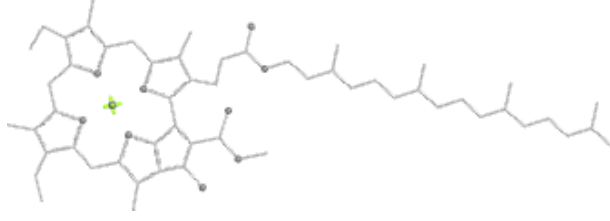
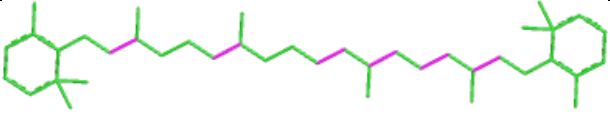
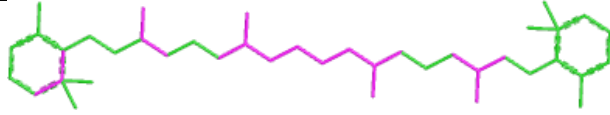
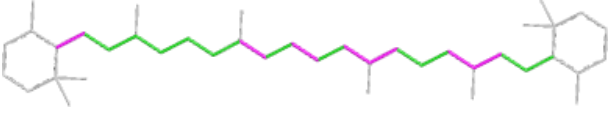
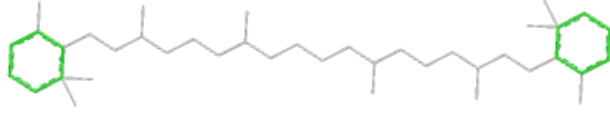
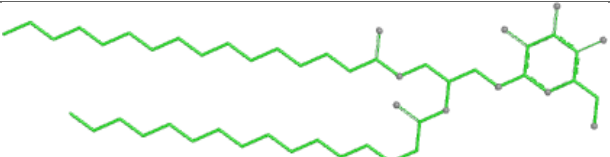
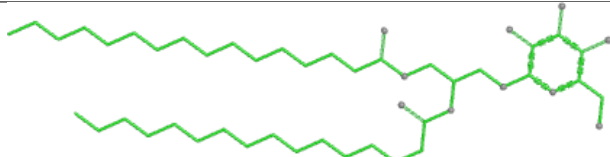
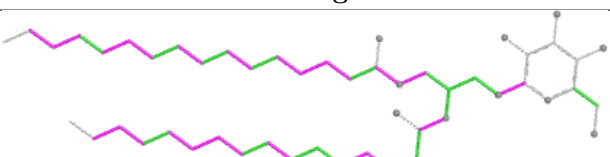
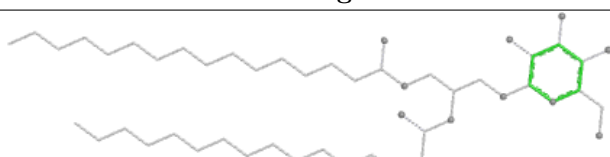


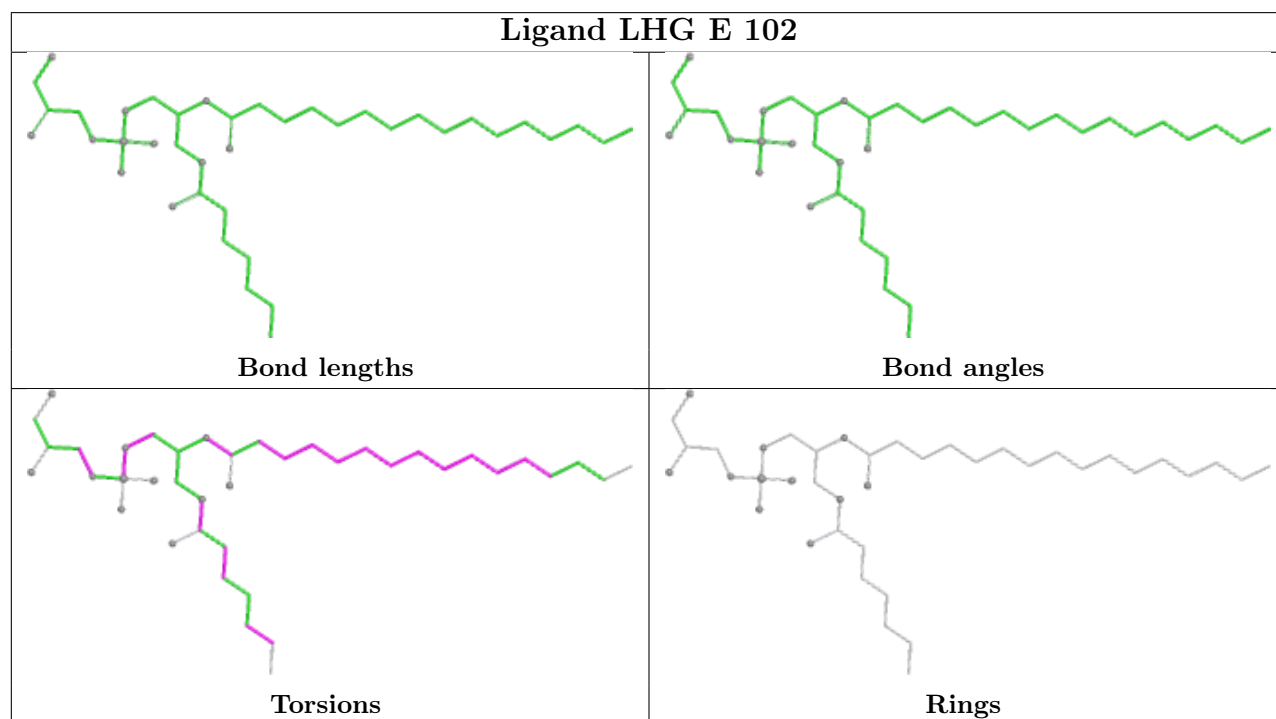
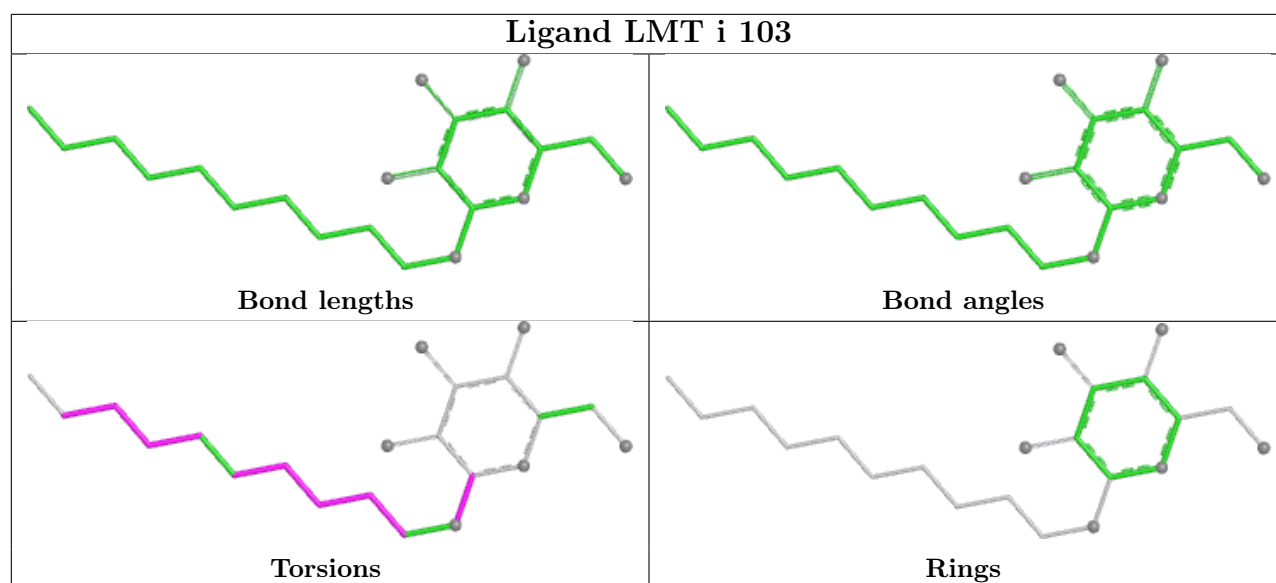


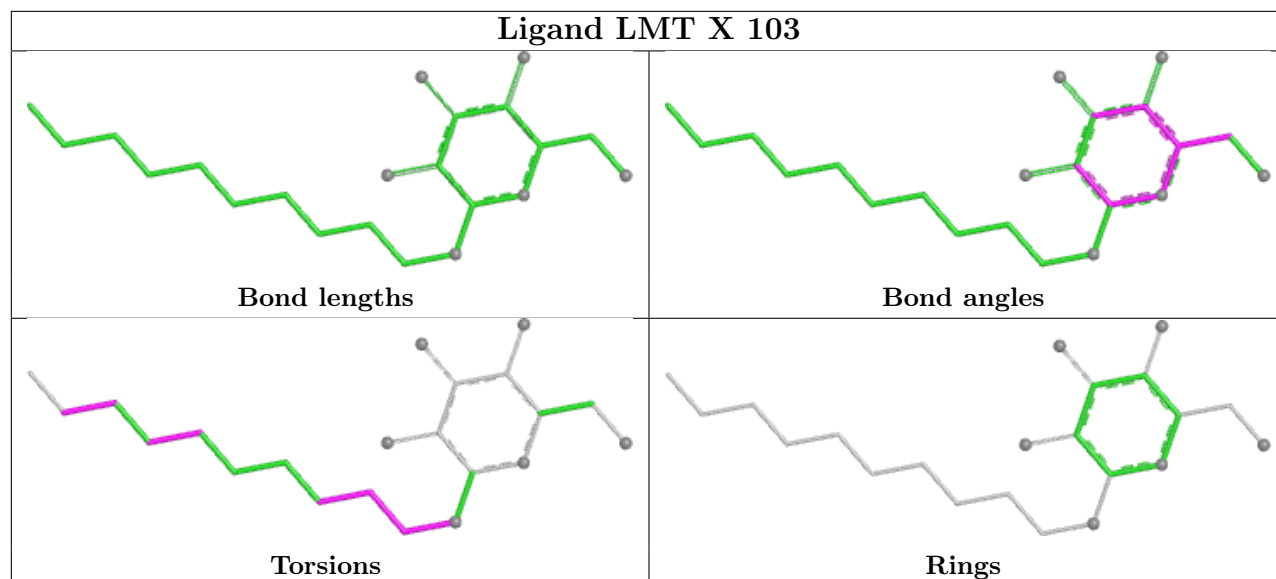
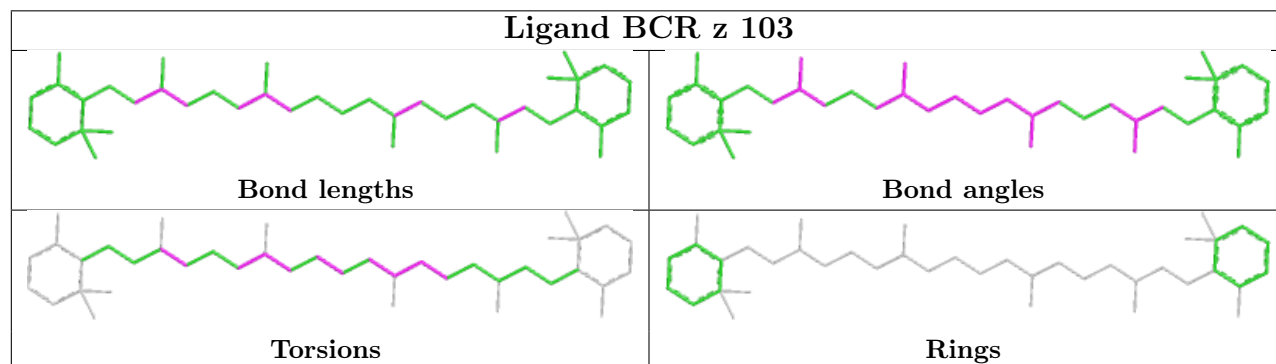
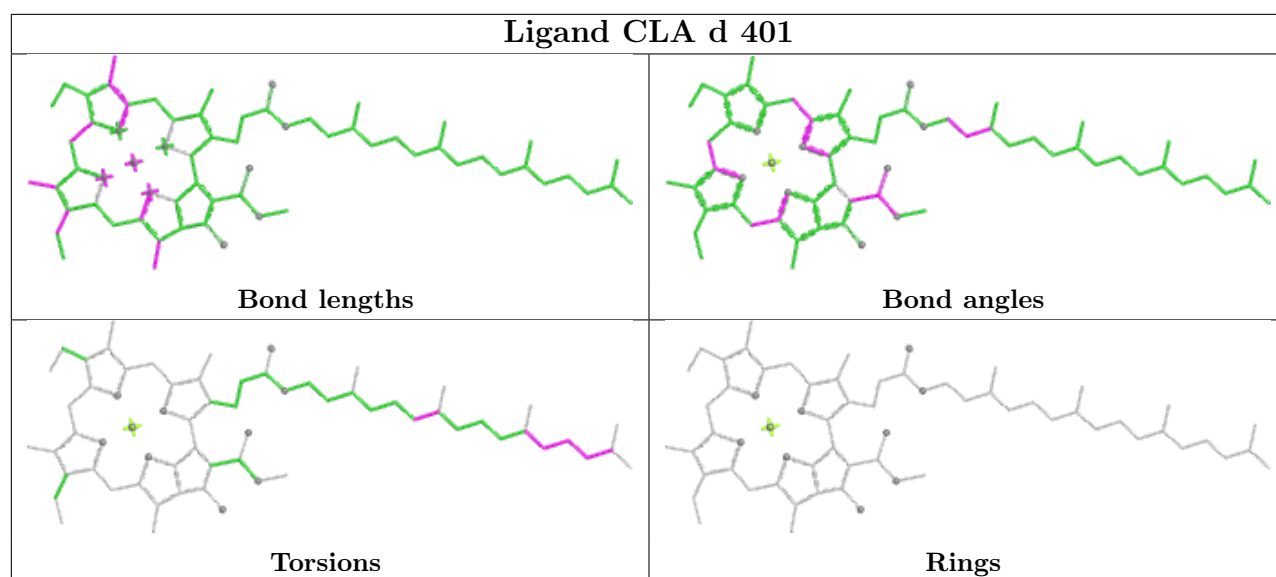


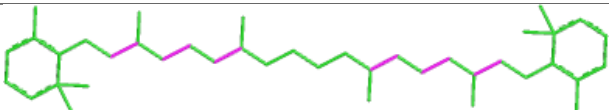
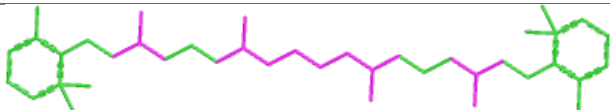
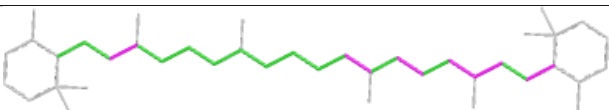
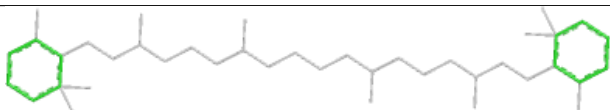




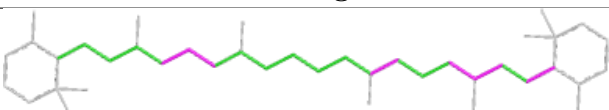
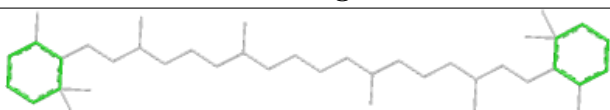


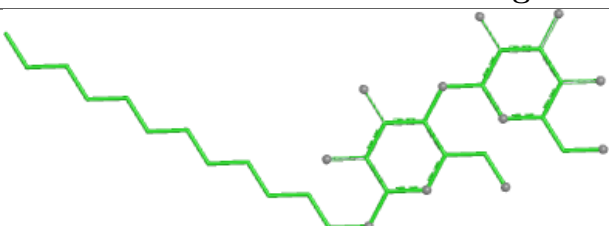
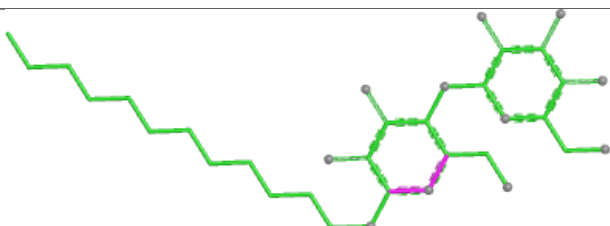
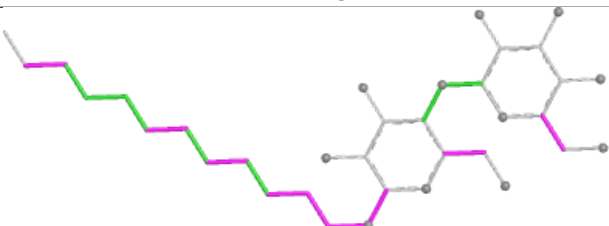
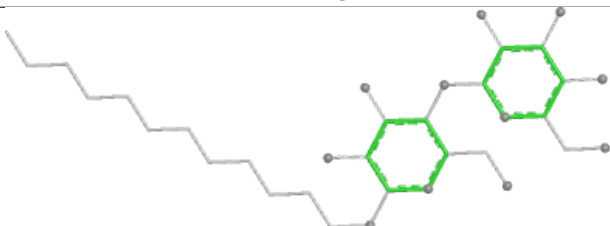
Ligand CLA c 503	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR b 617	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LMG A 410	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

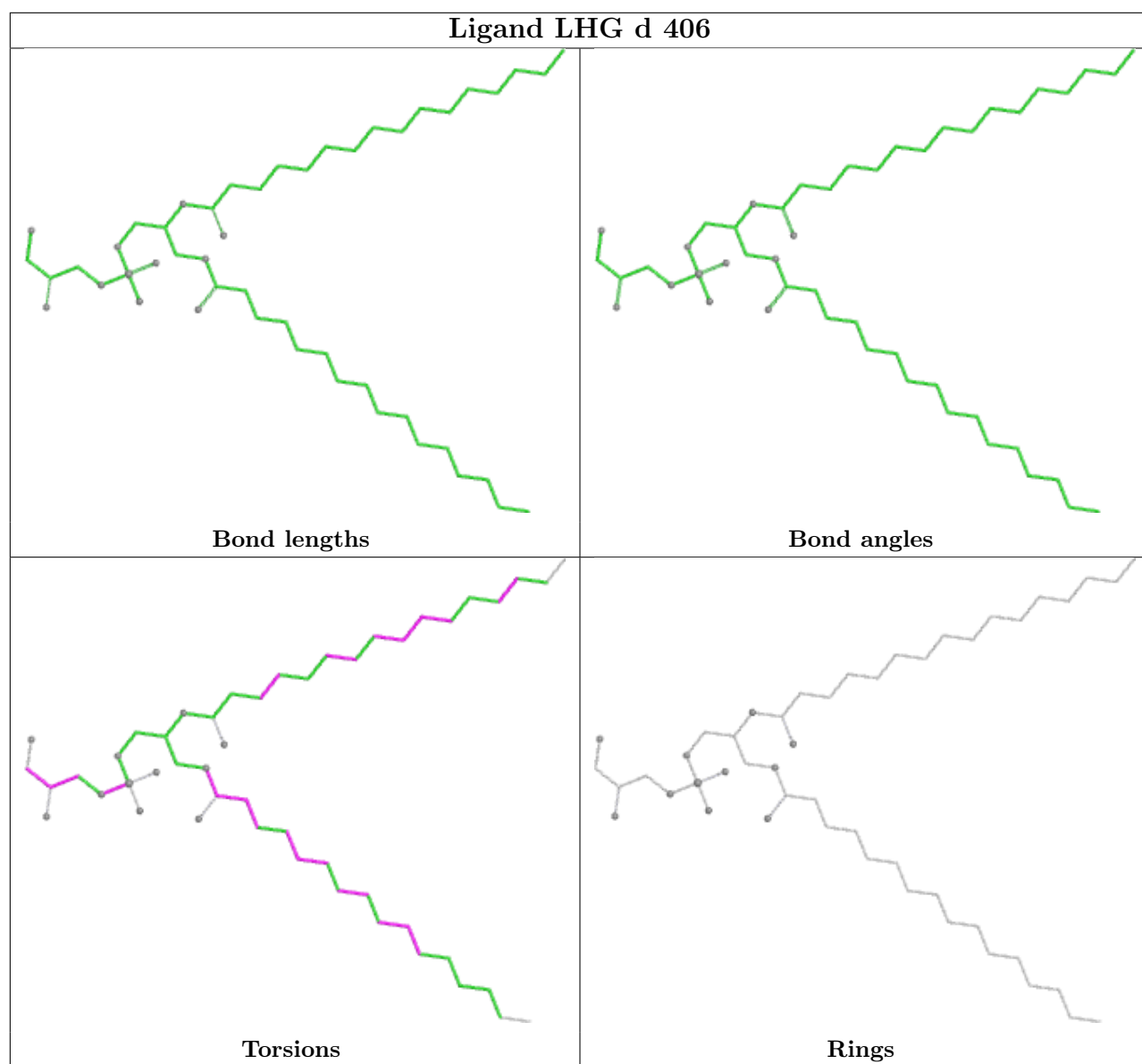


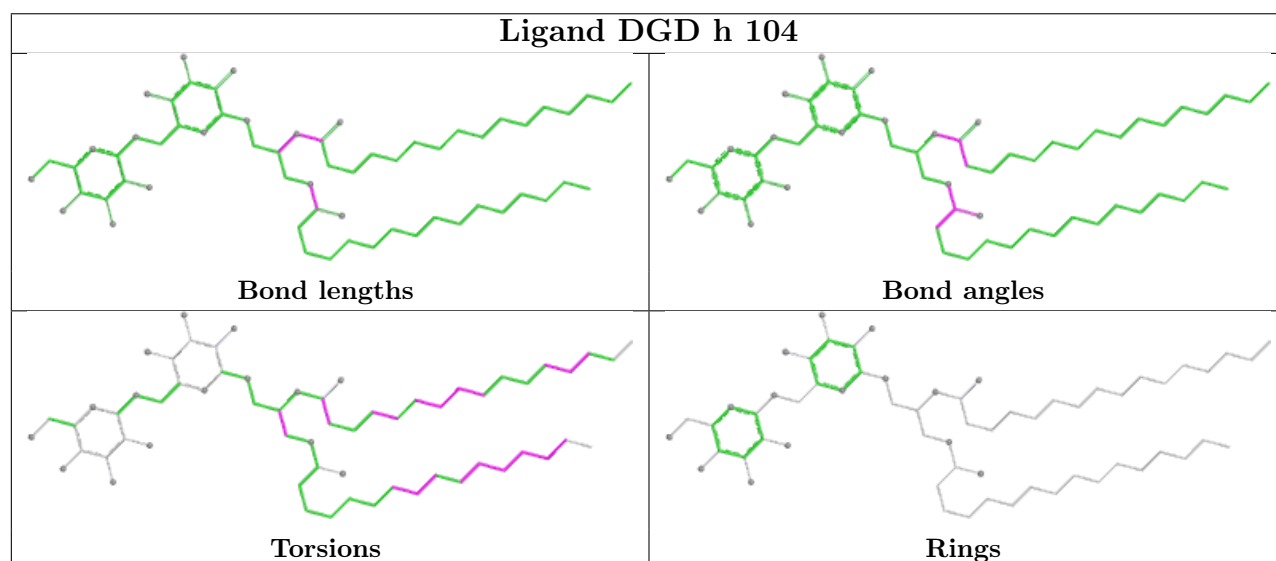
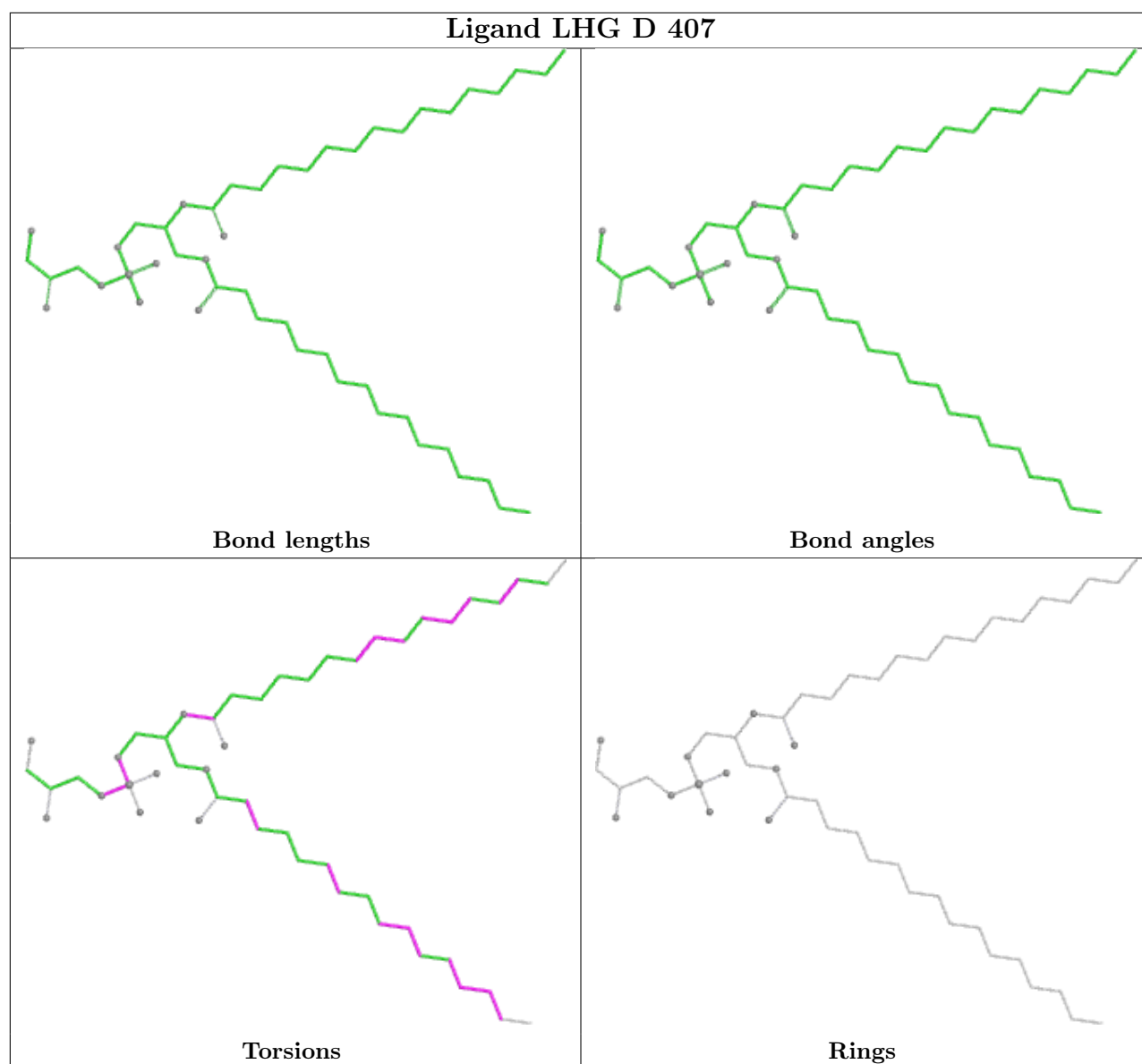


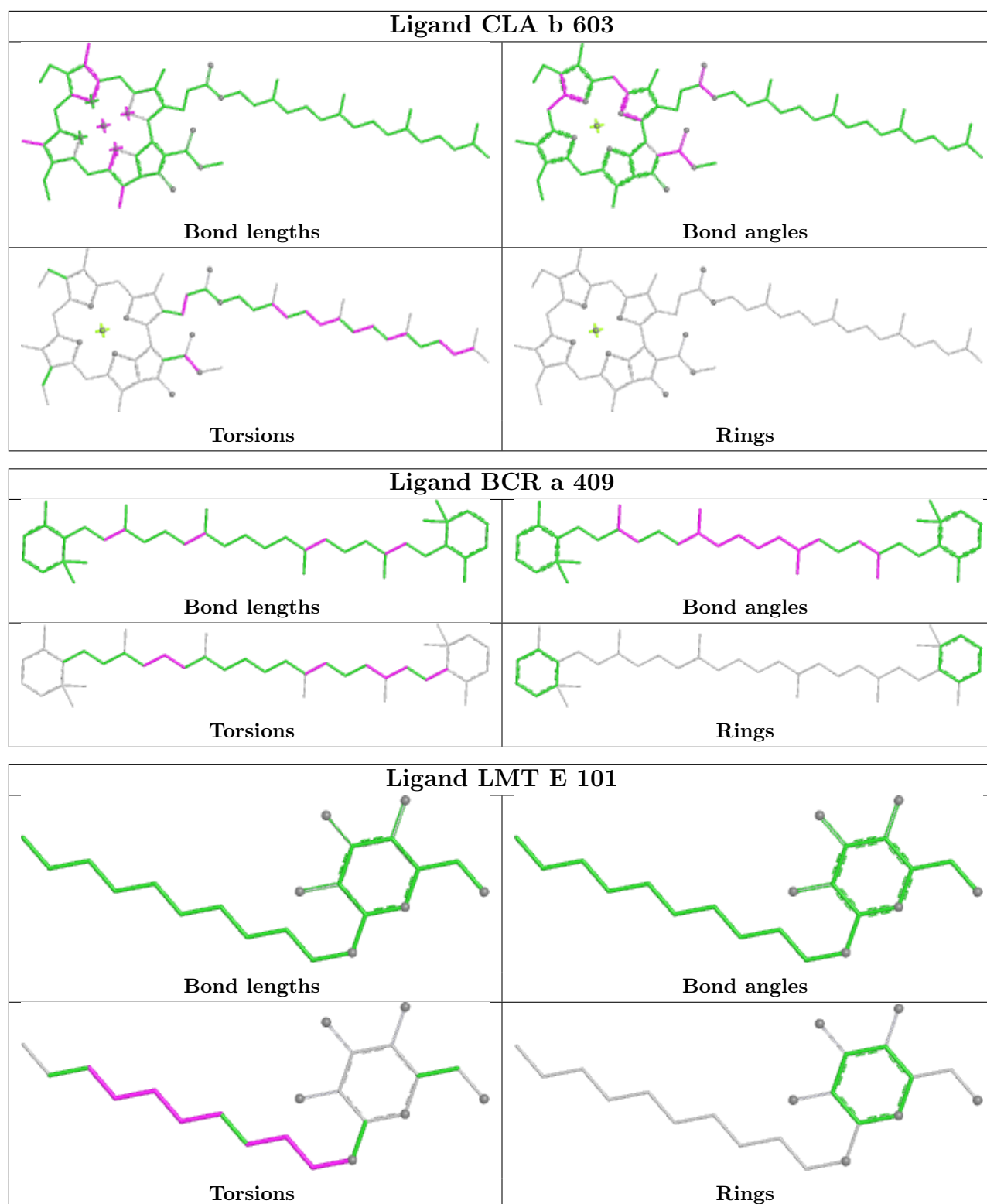
Ligand BCR b 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

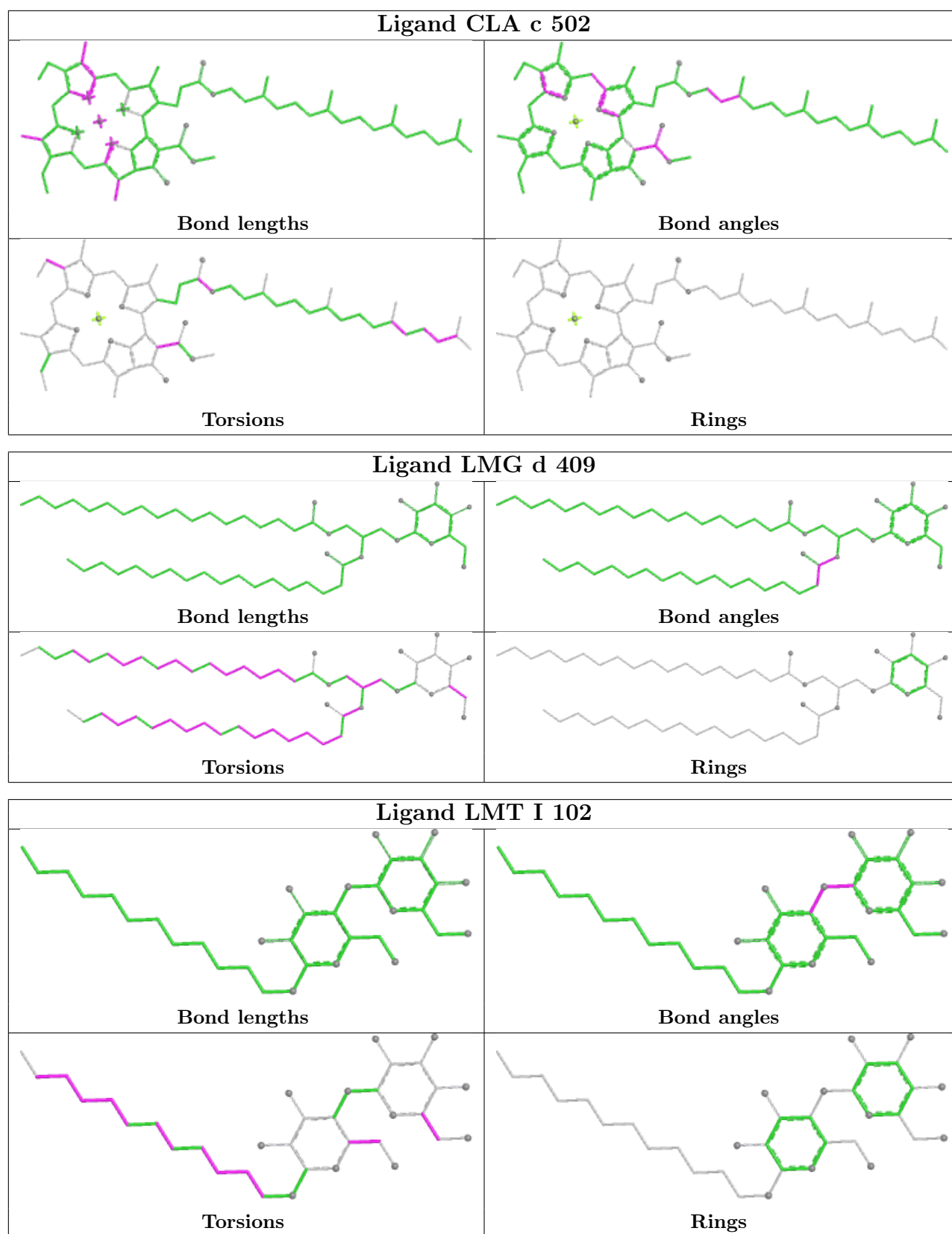
Ligand BCR A 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

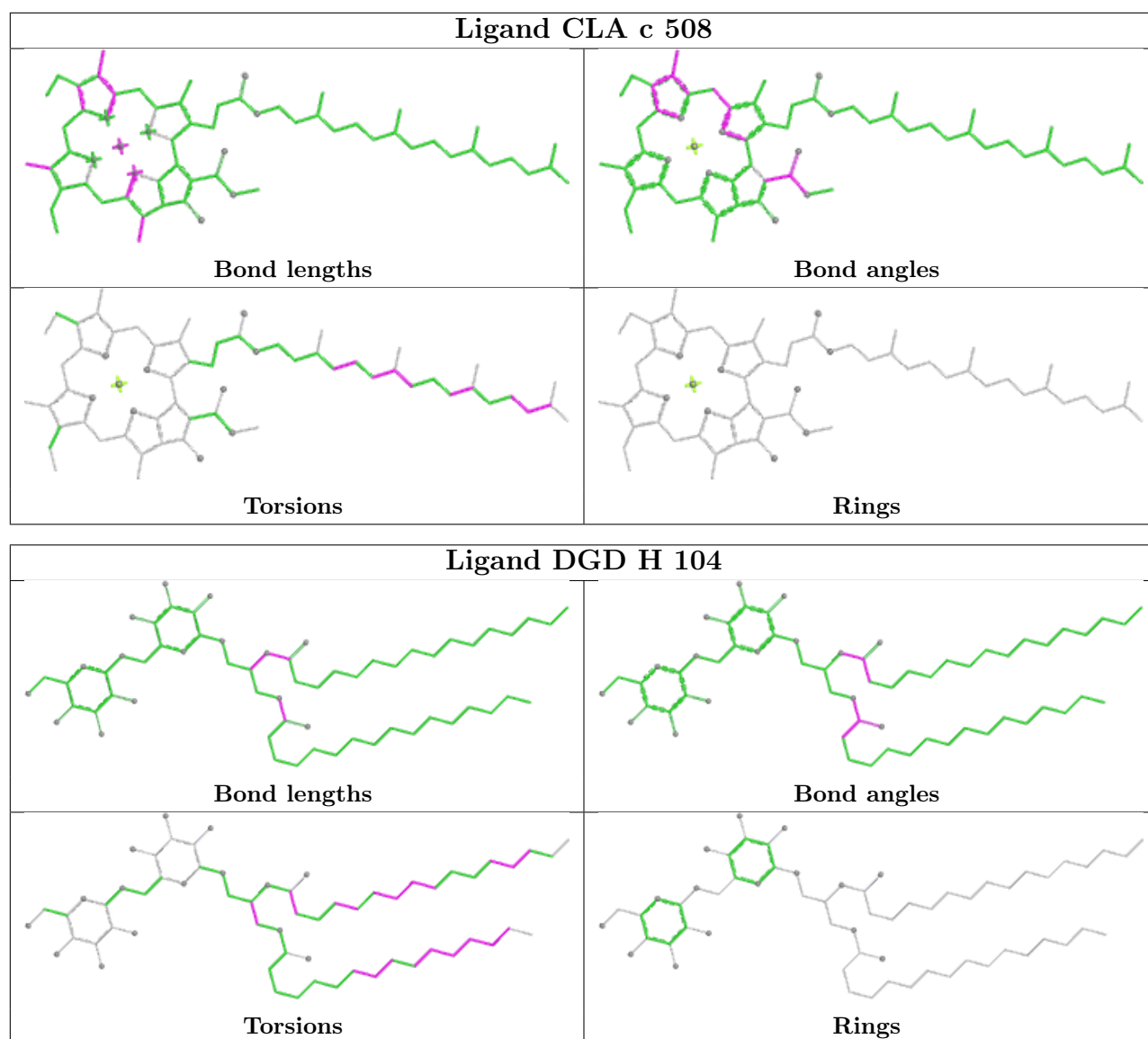
Ligand LMT f 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

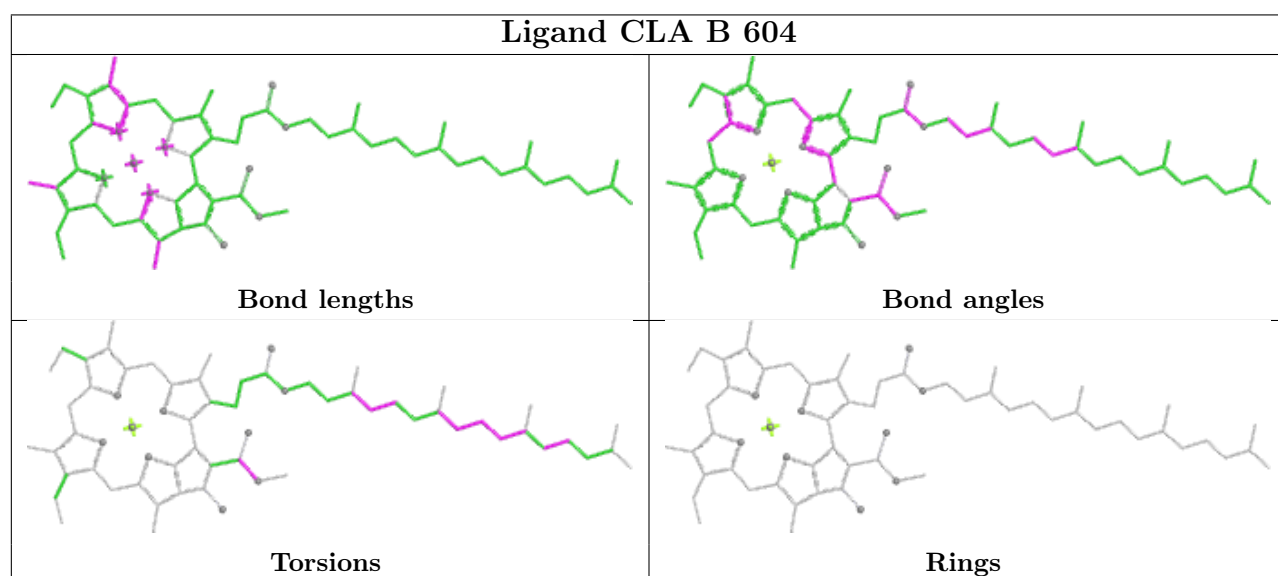
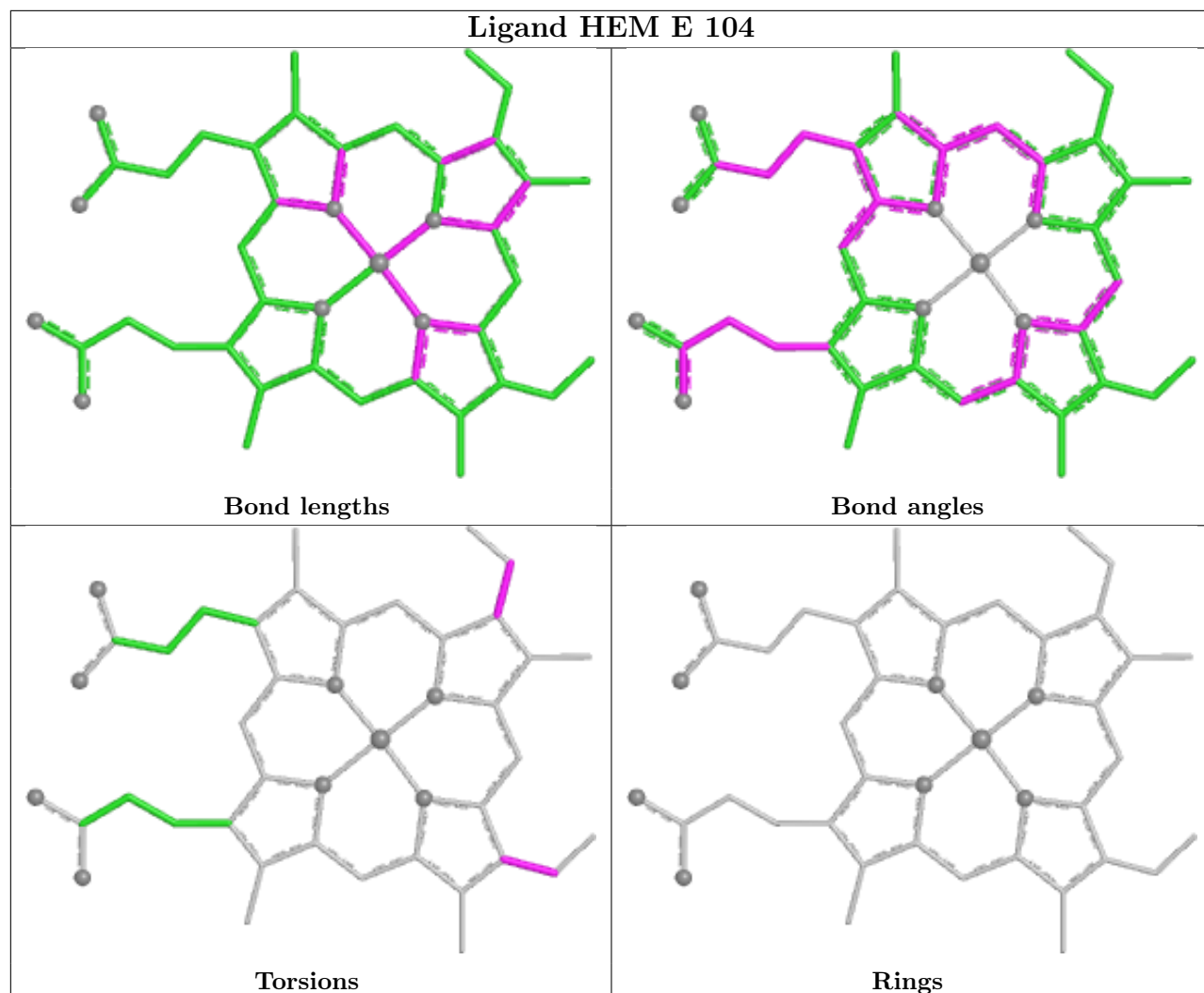


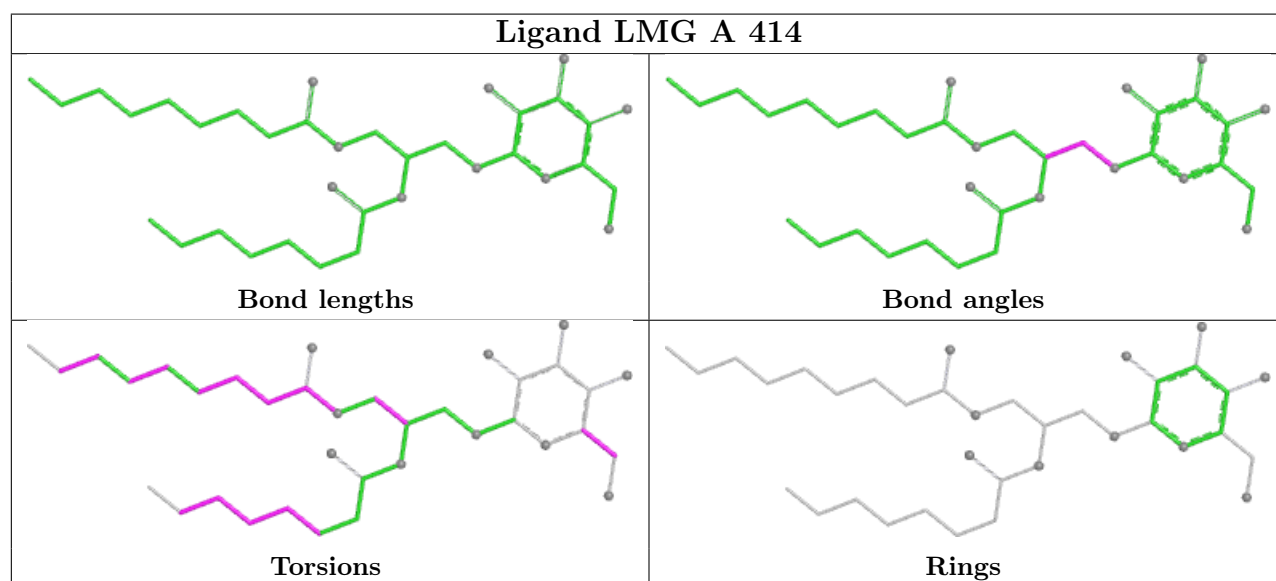
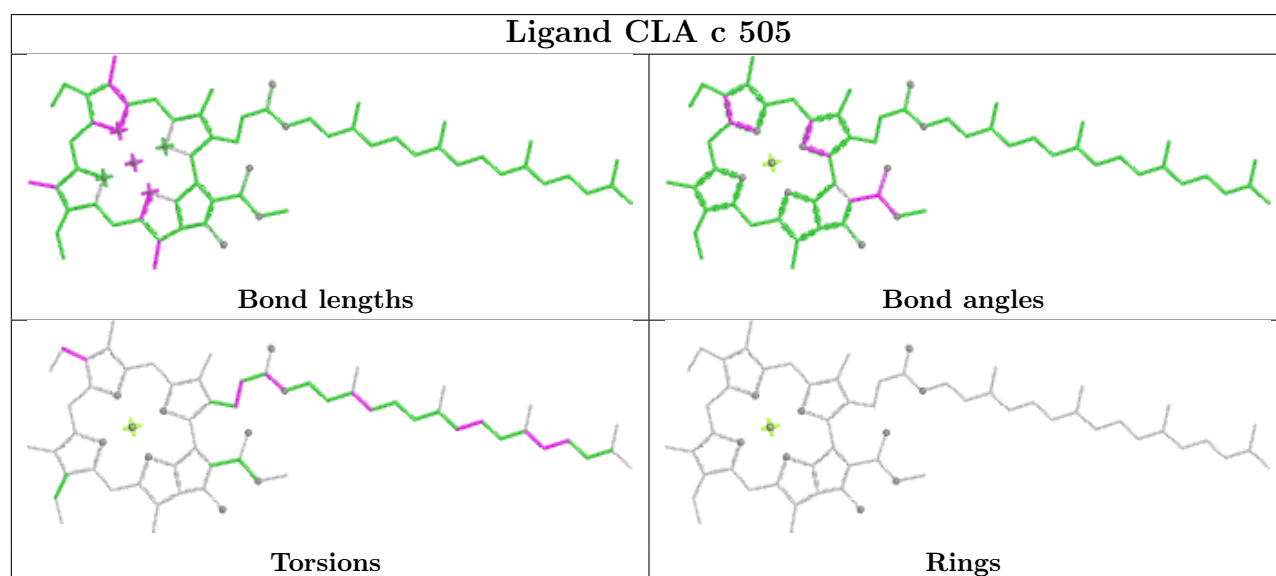
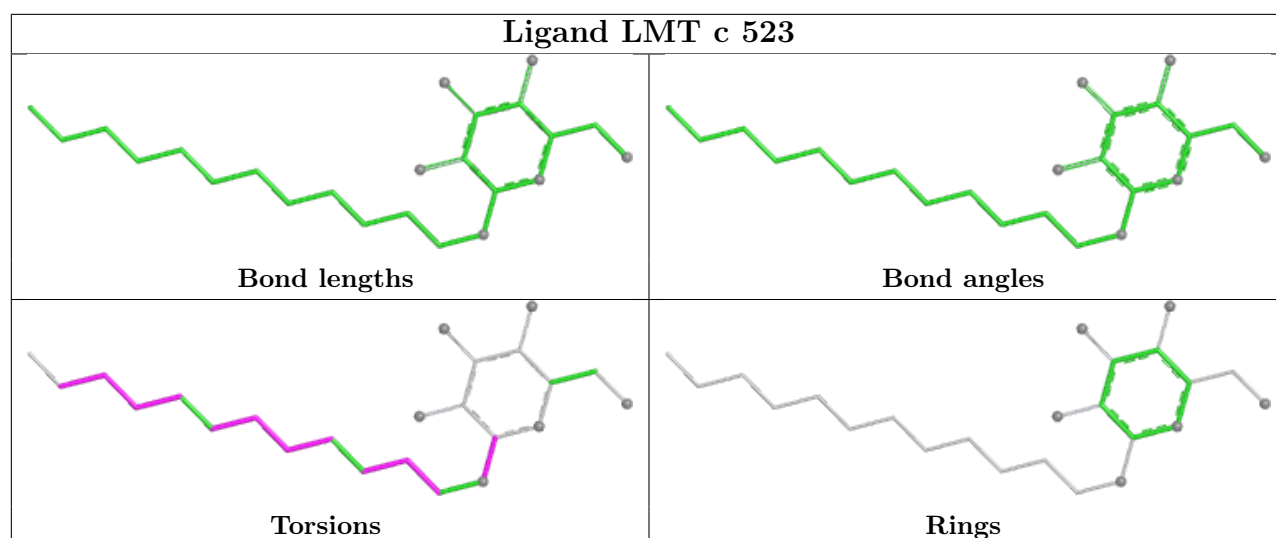


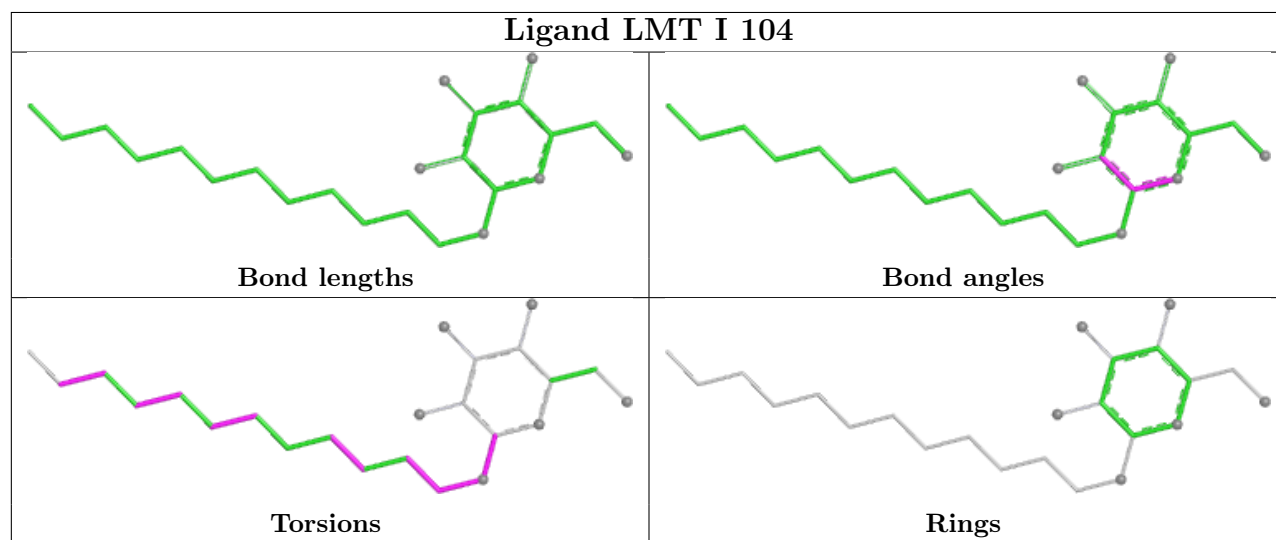
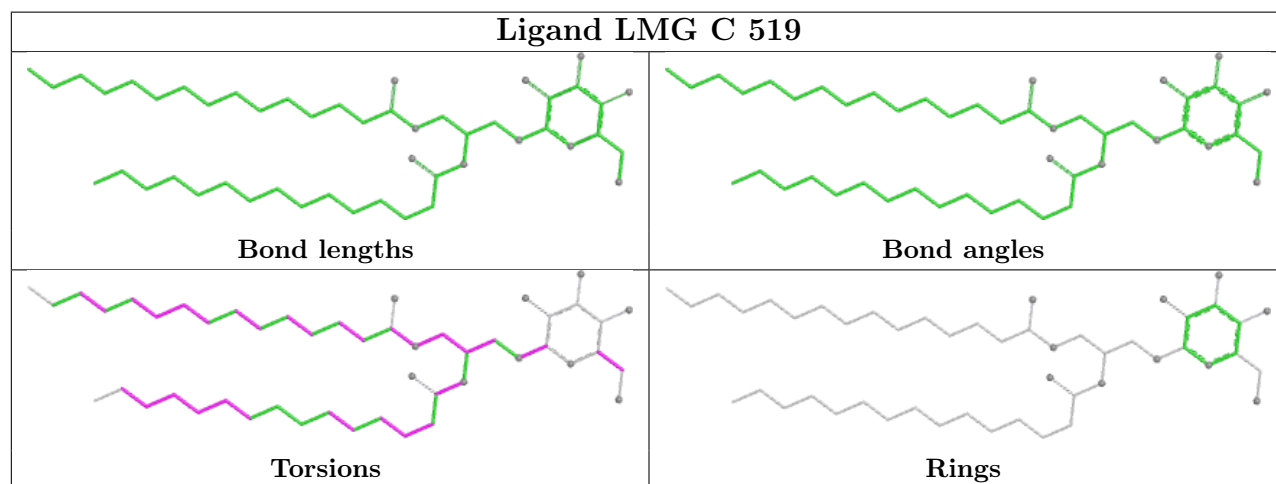
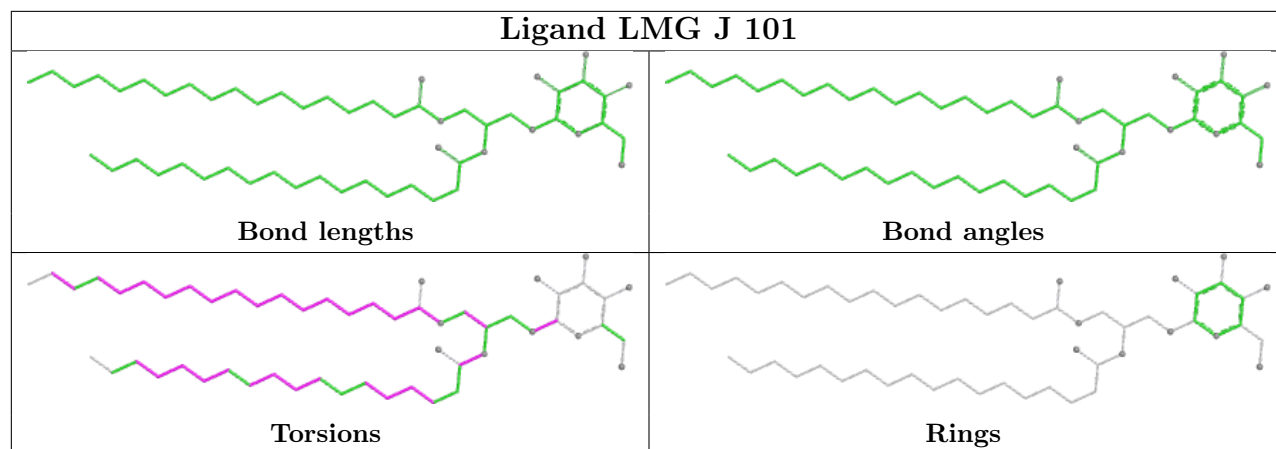


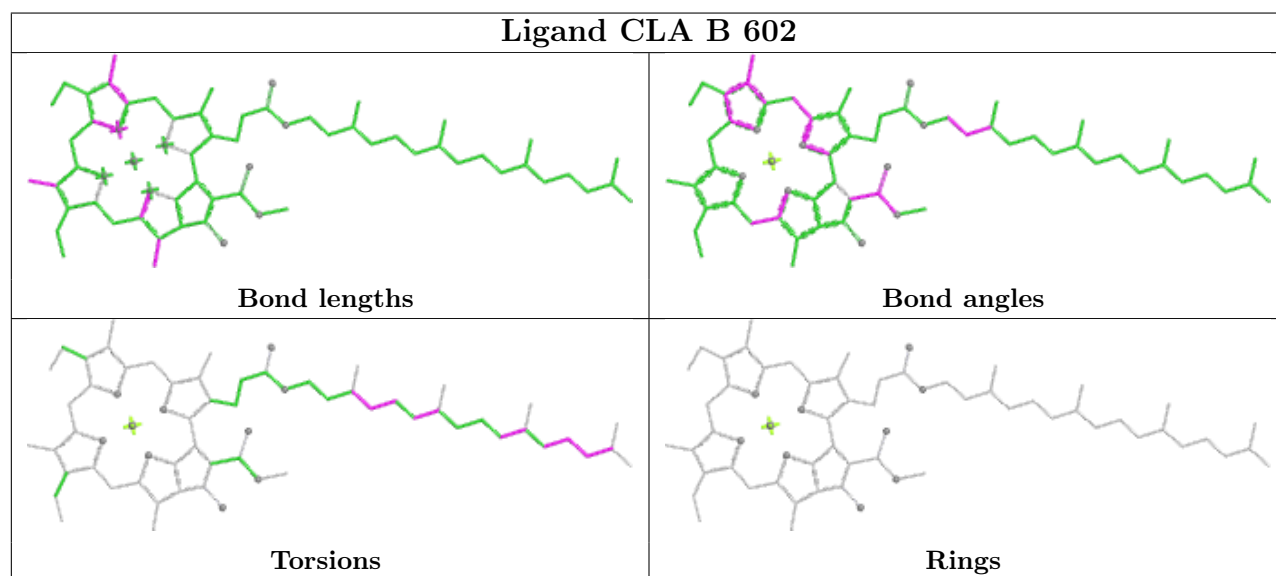
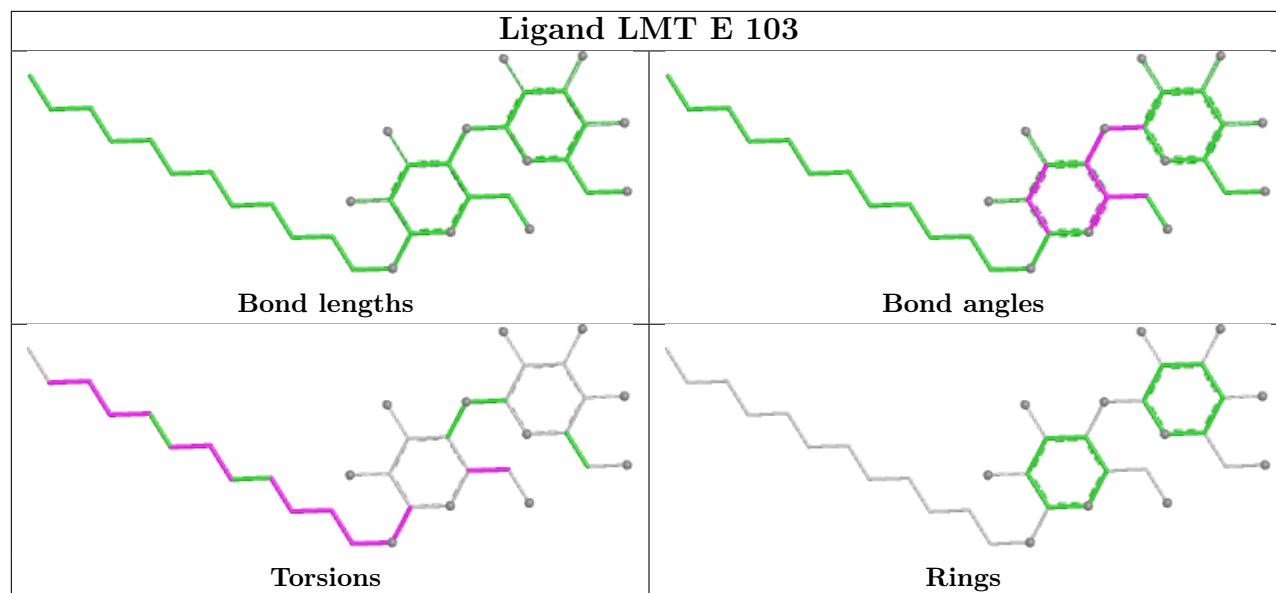


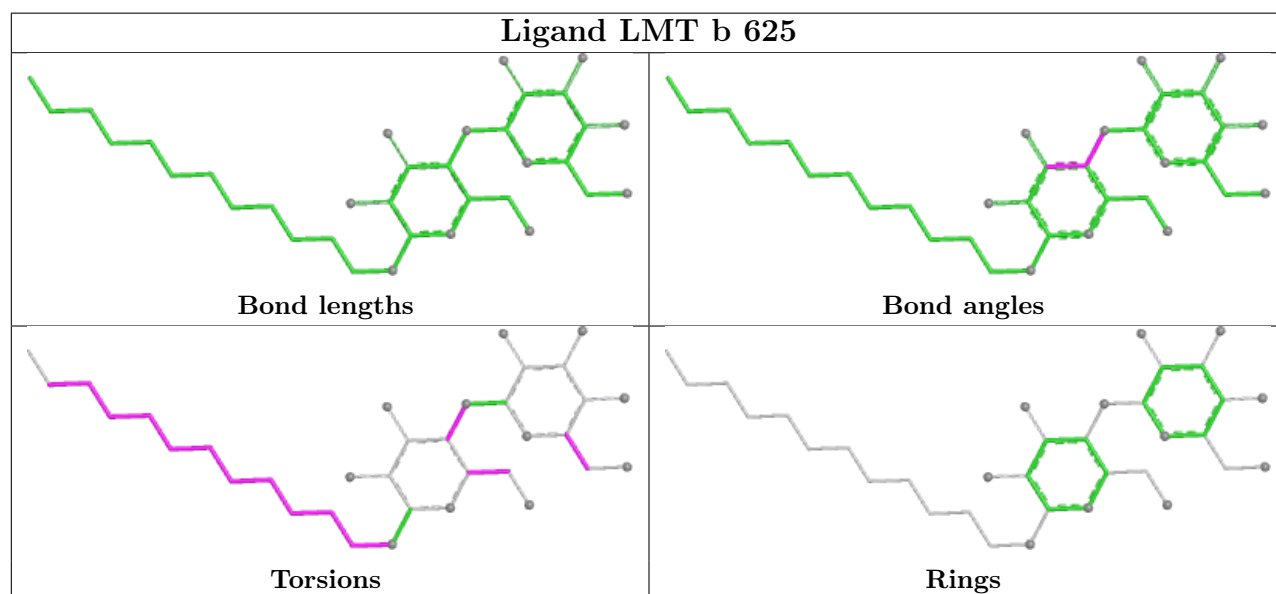
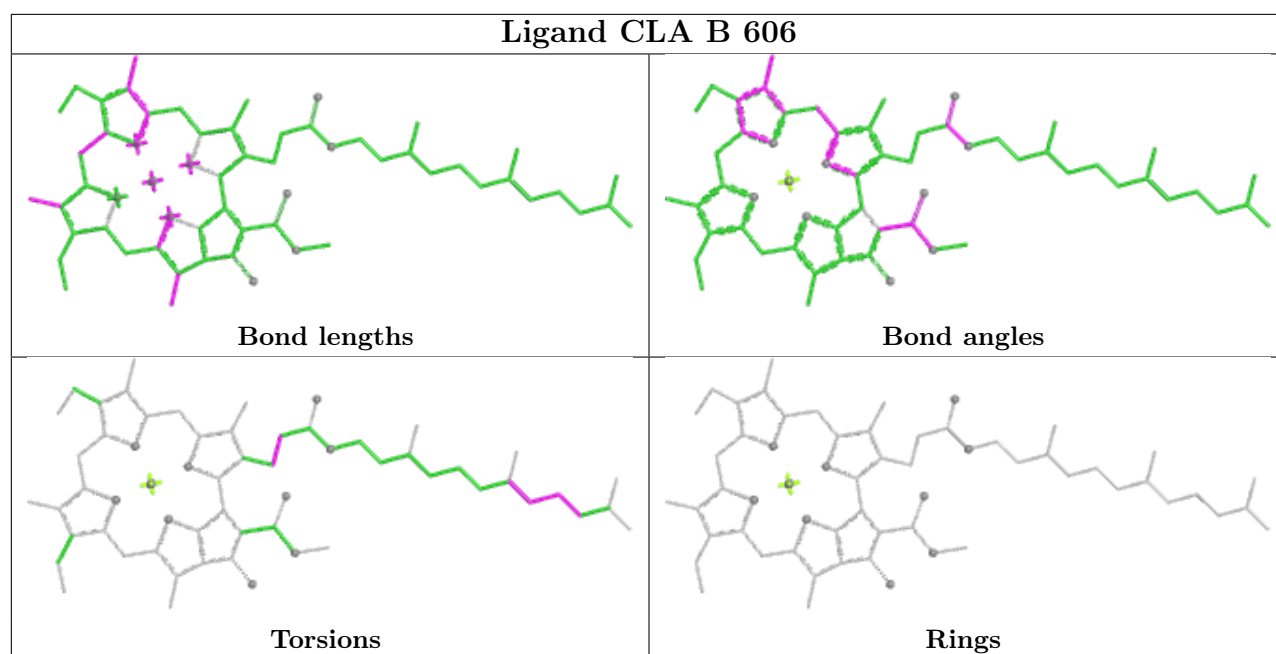


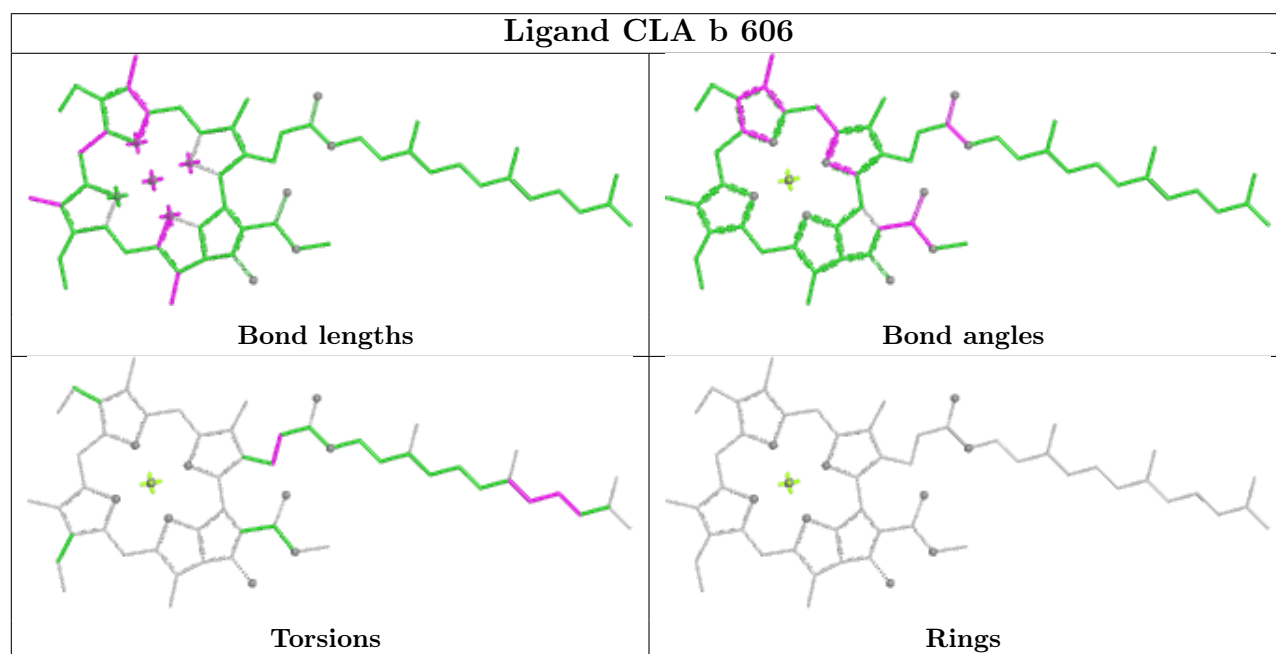
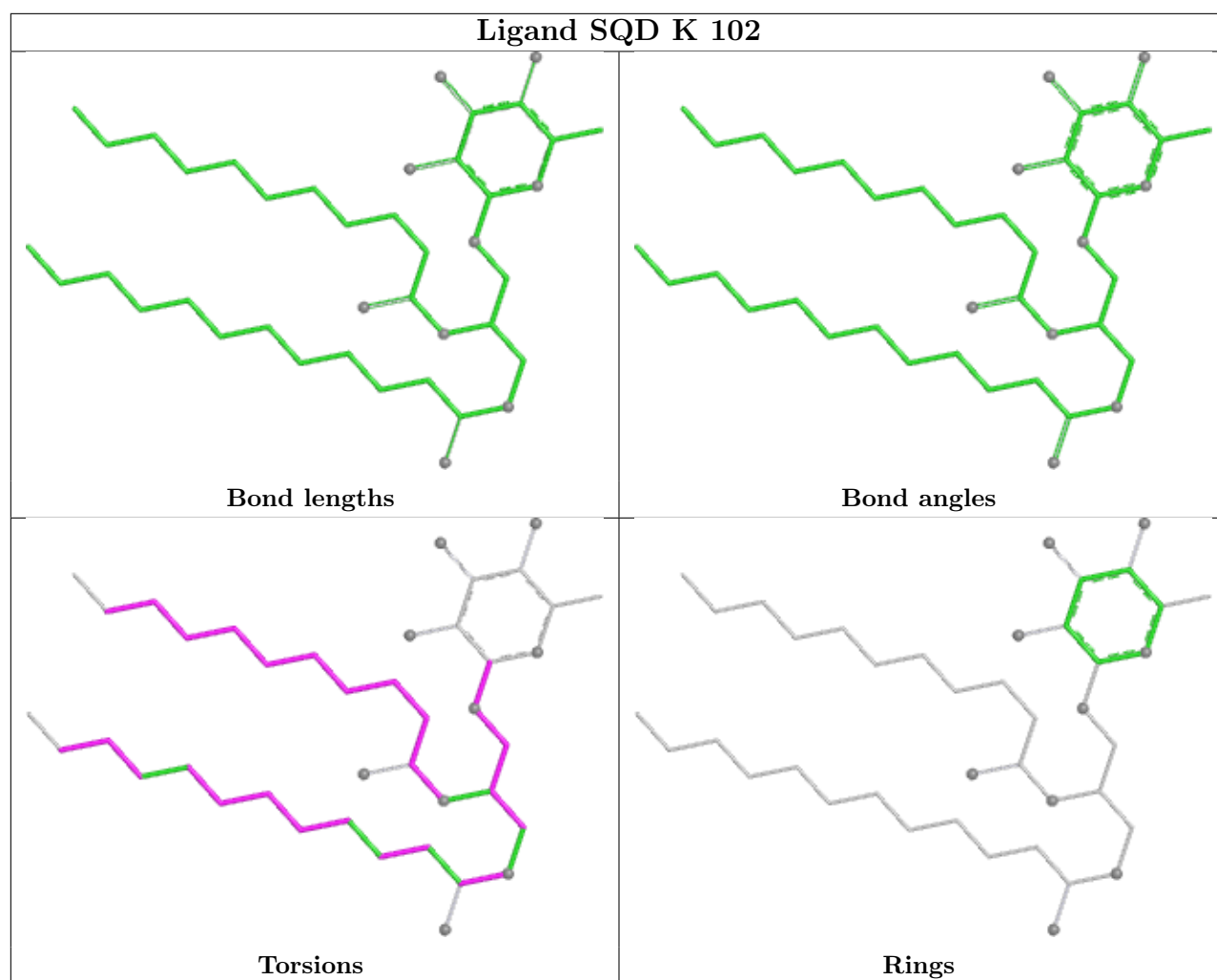


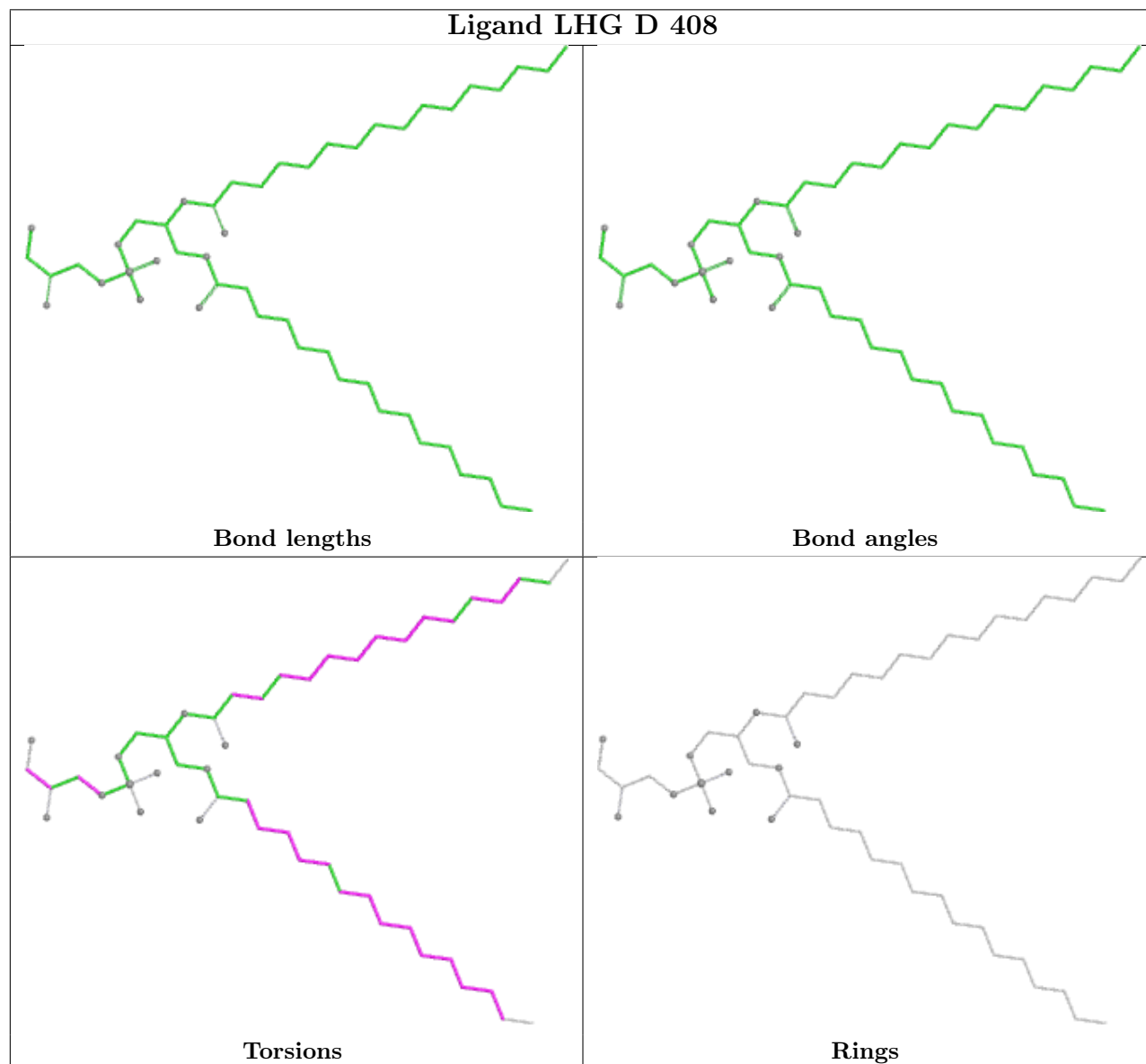
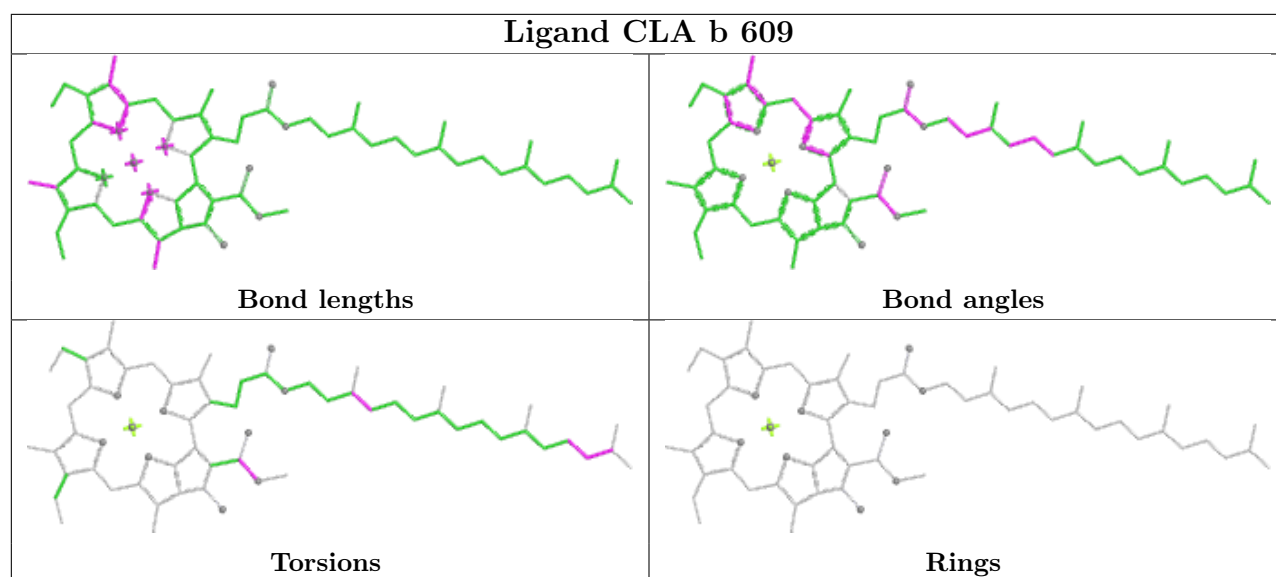


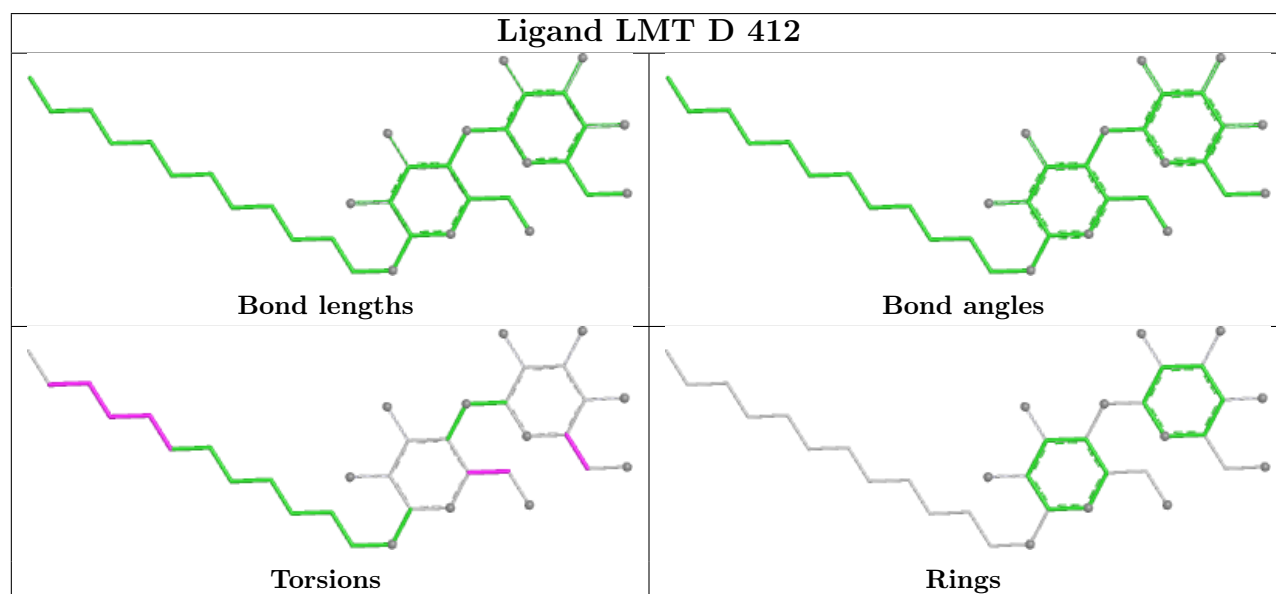
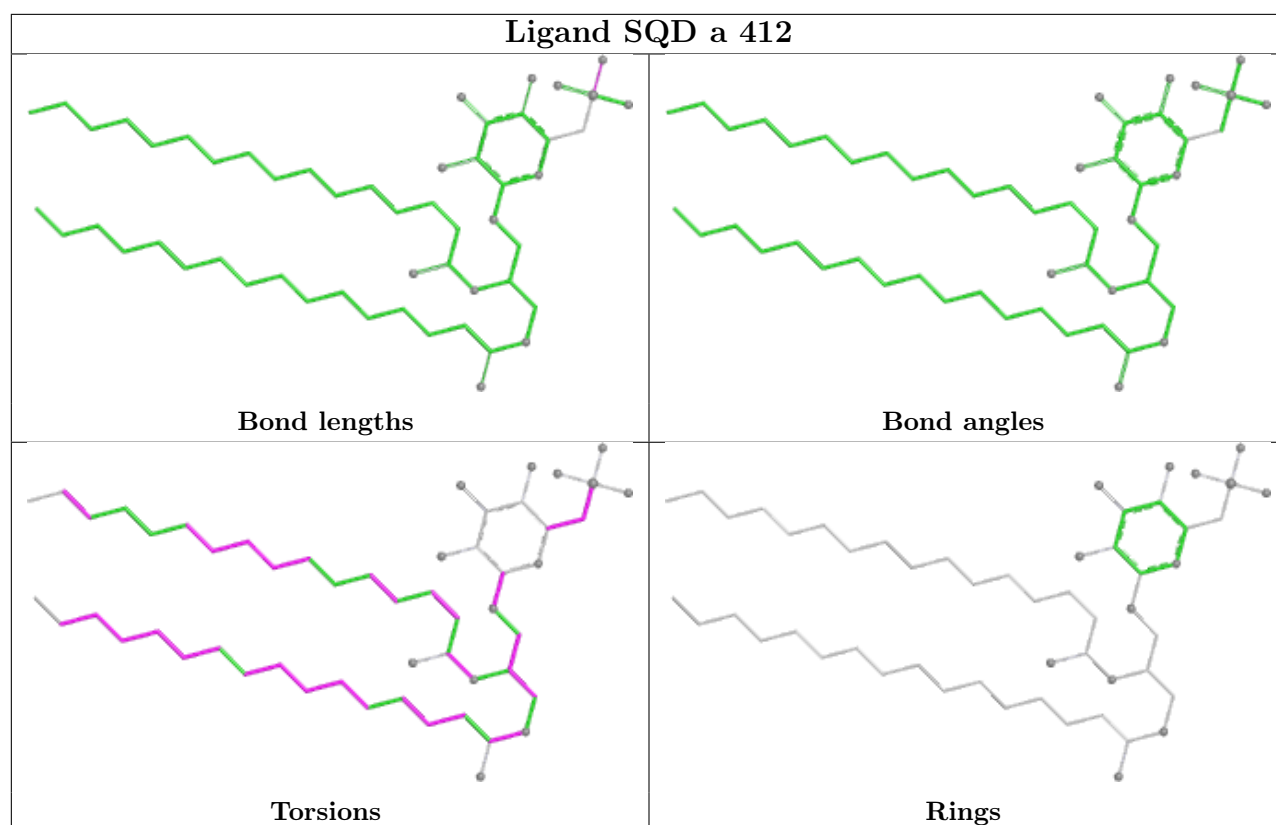


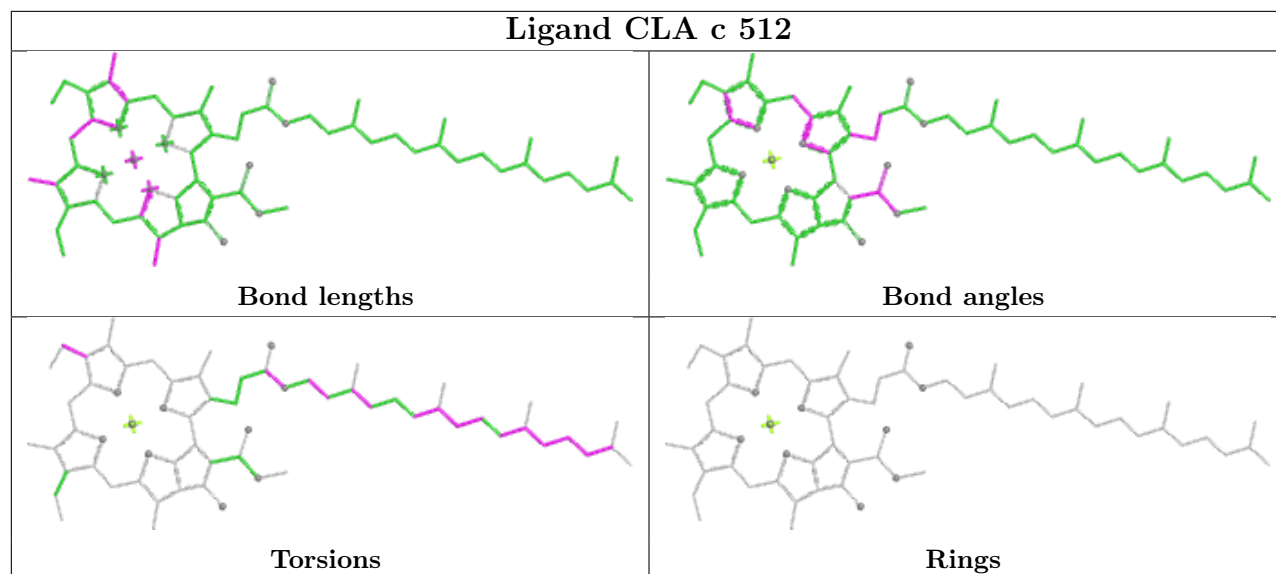
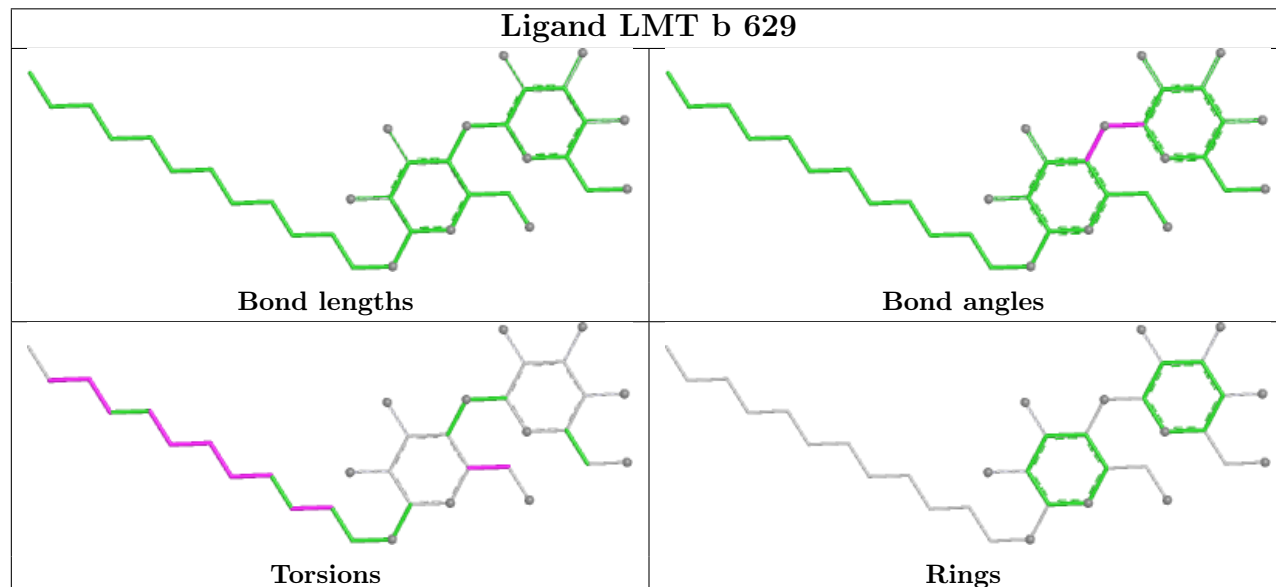
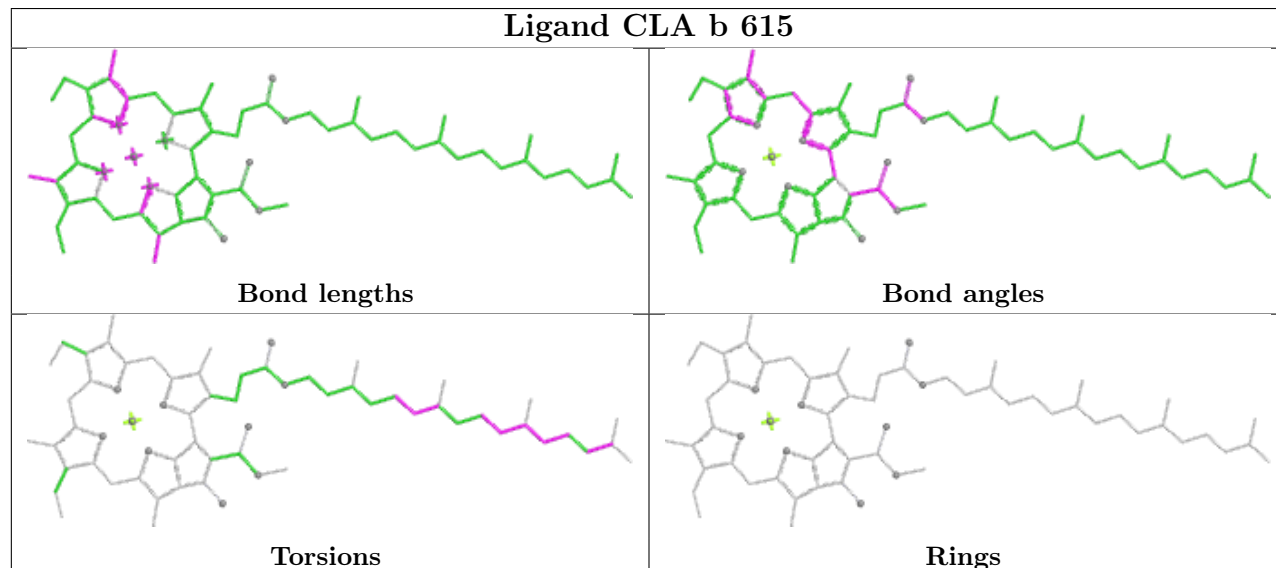


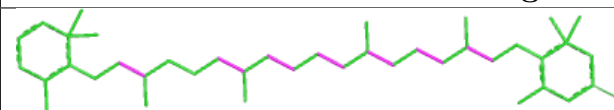
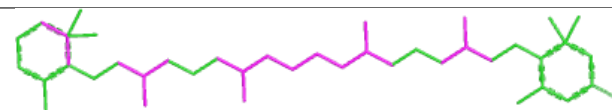
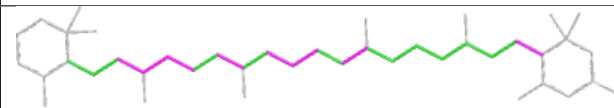
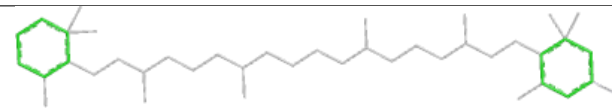


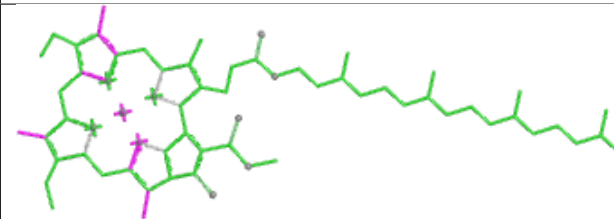
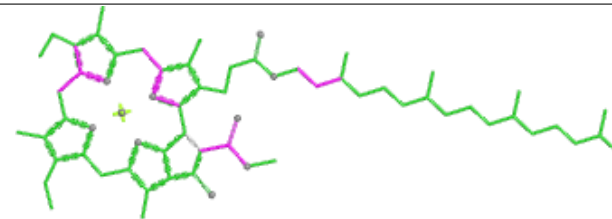
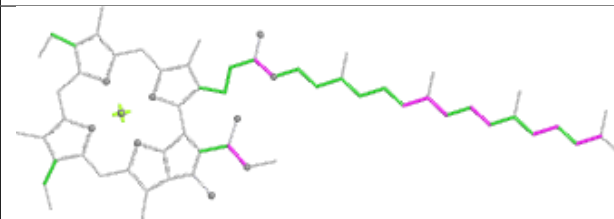
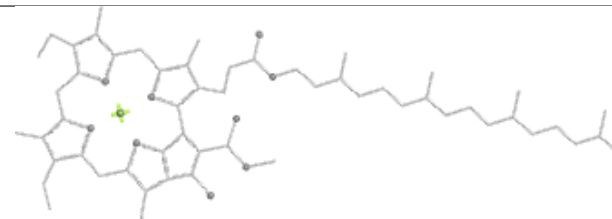


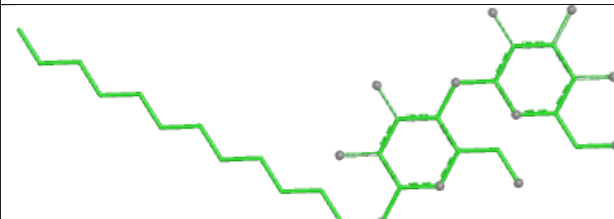
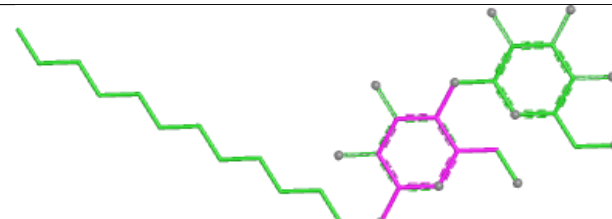
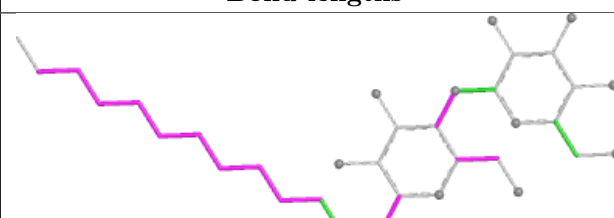
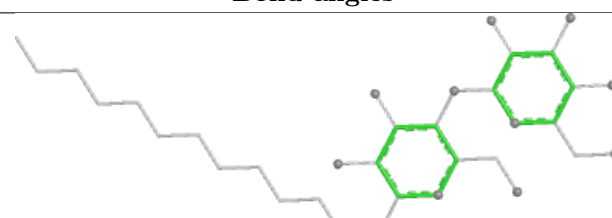




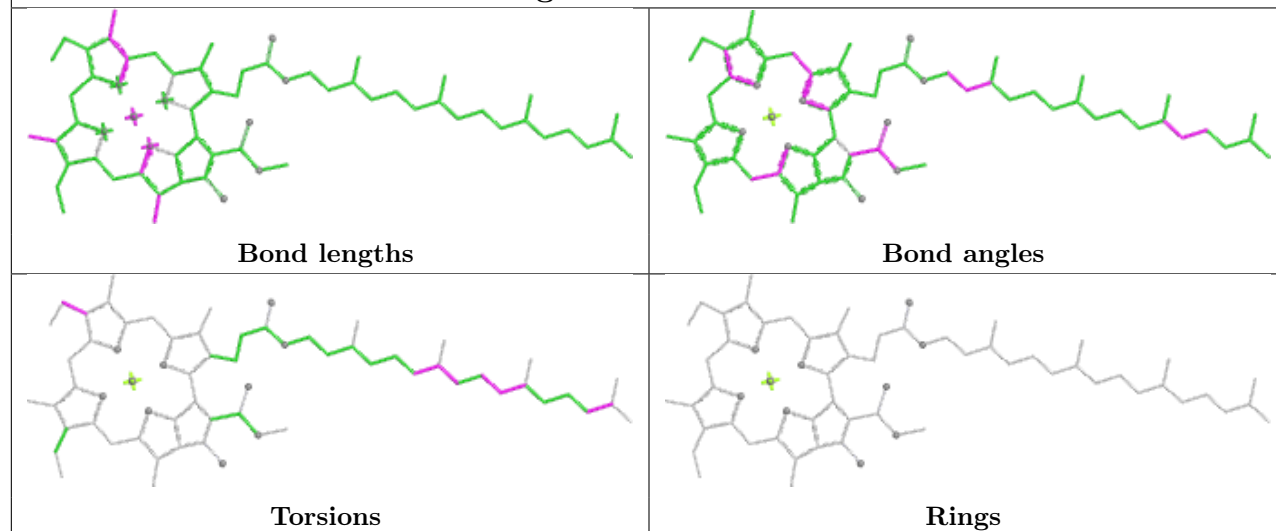
Ligand CLA c 512**Ligand LMT b 629****Ligand CLA b 615**

Ligand RRX h 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

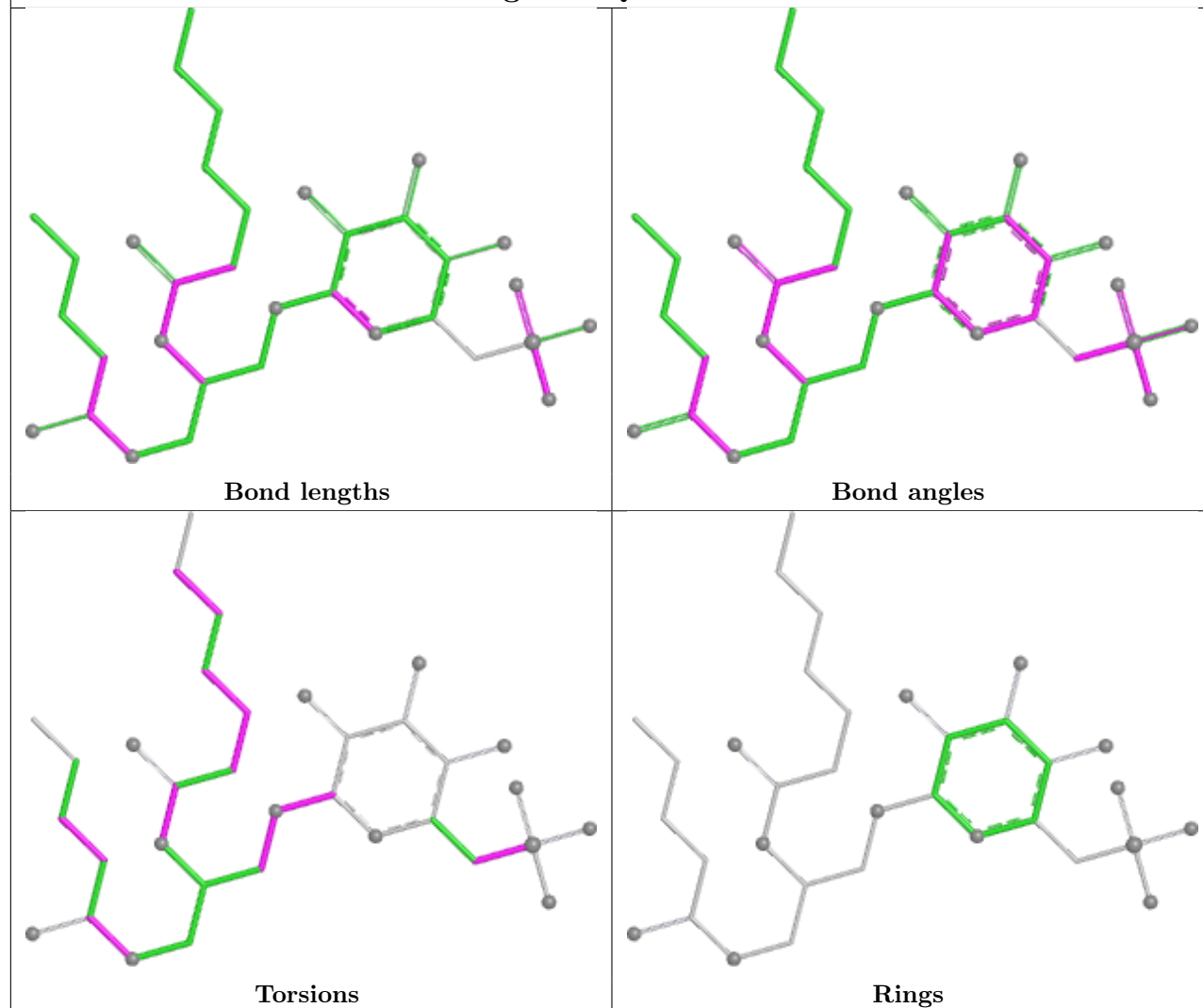
Ligand CLA d 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

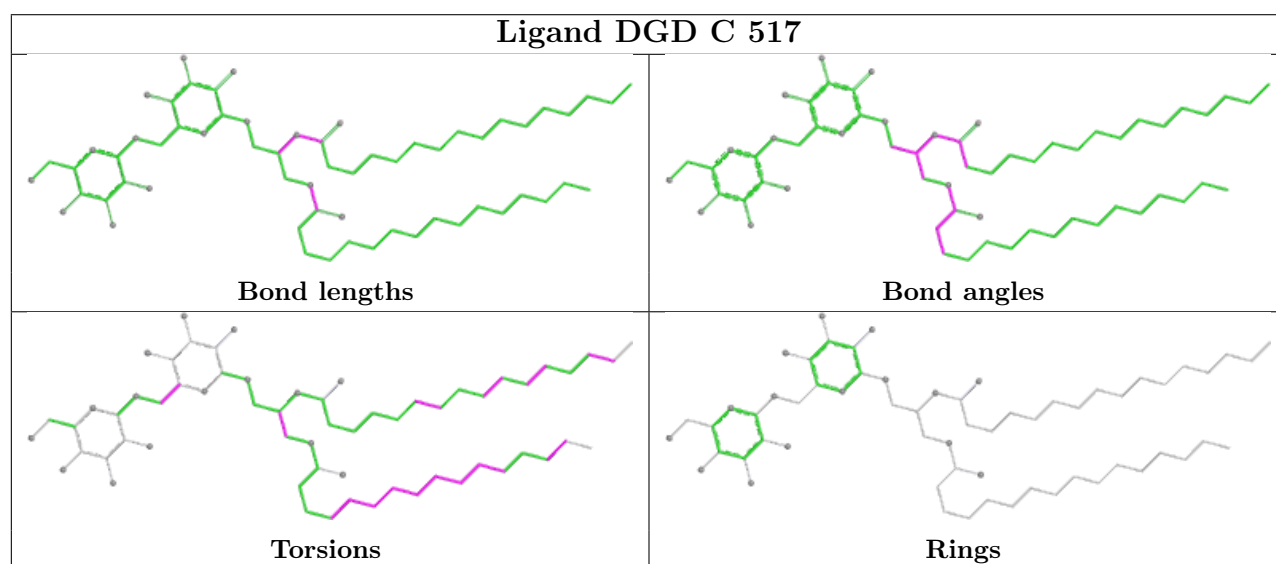
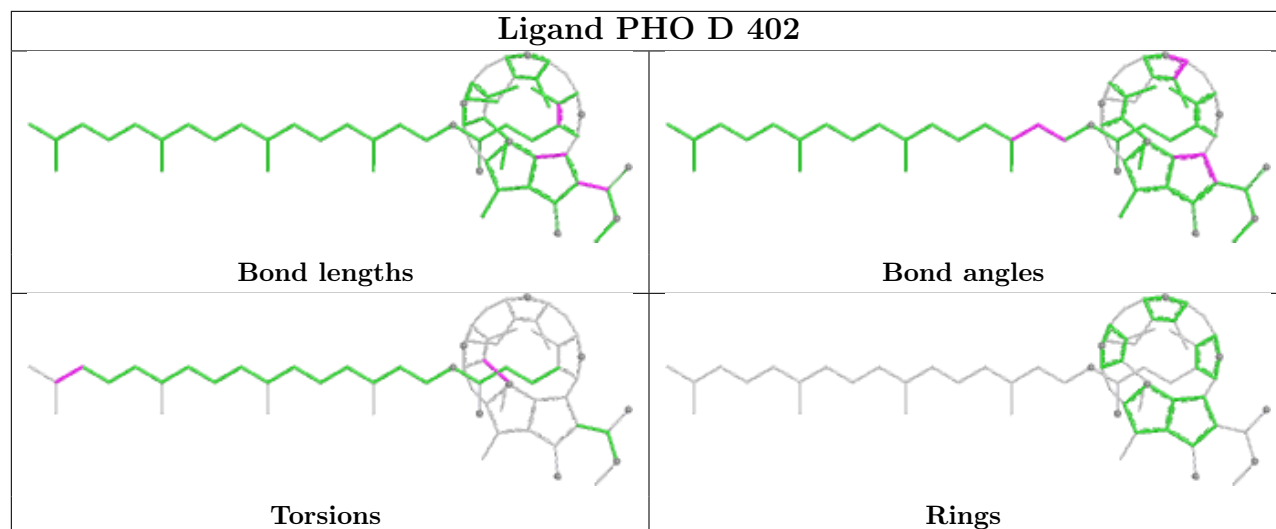
Ligand LMT K 105	
	
Bond lengths	Bond angles
	
Torsions	Rings

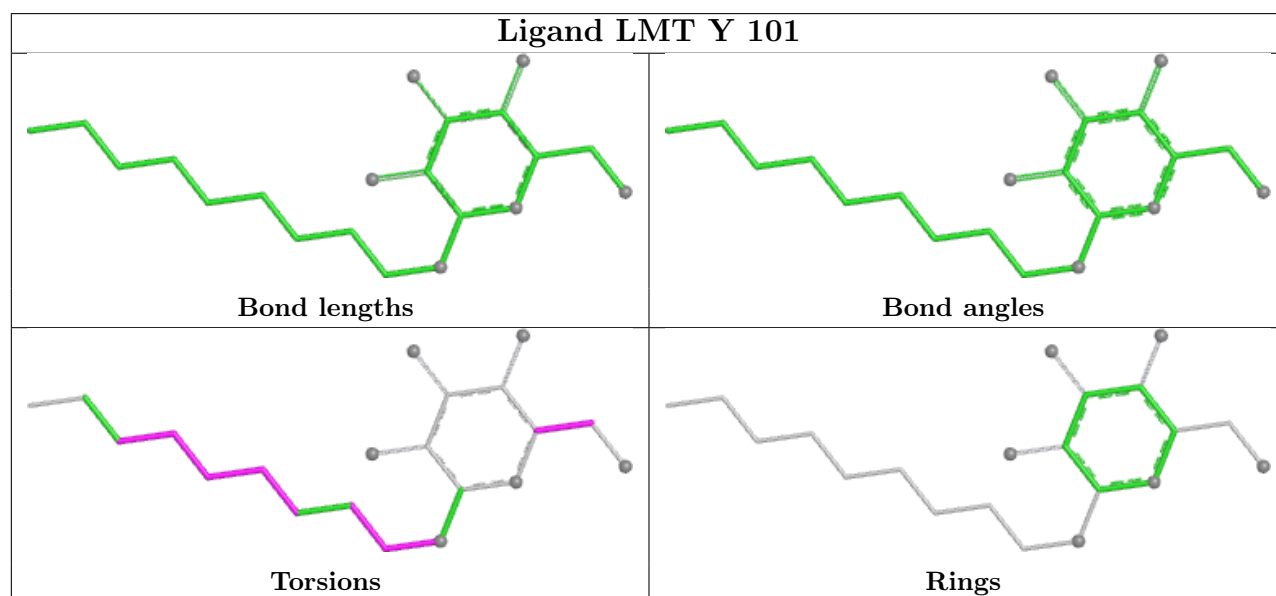
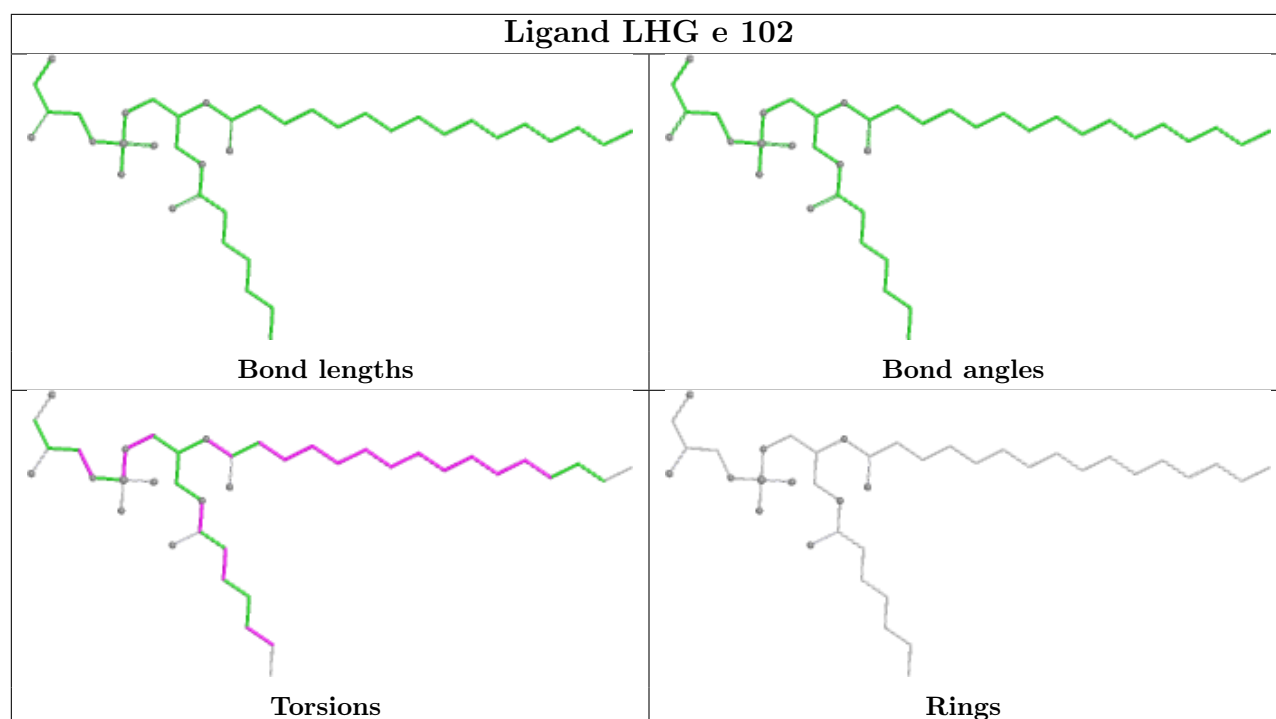
Ligand CLA a 406

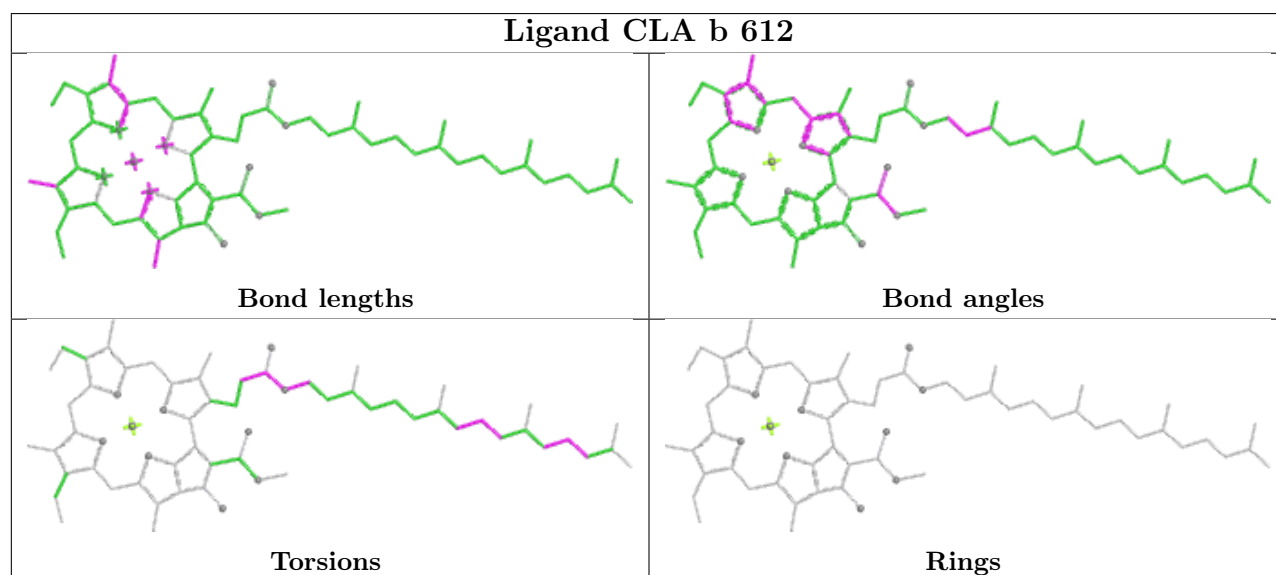
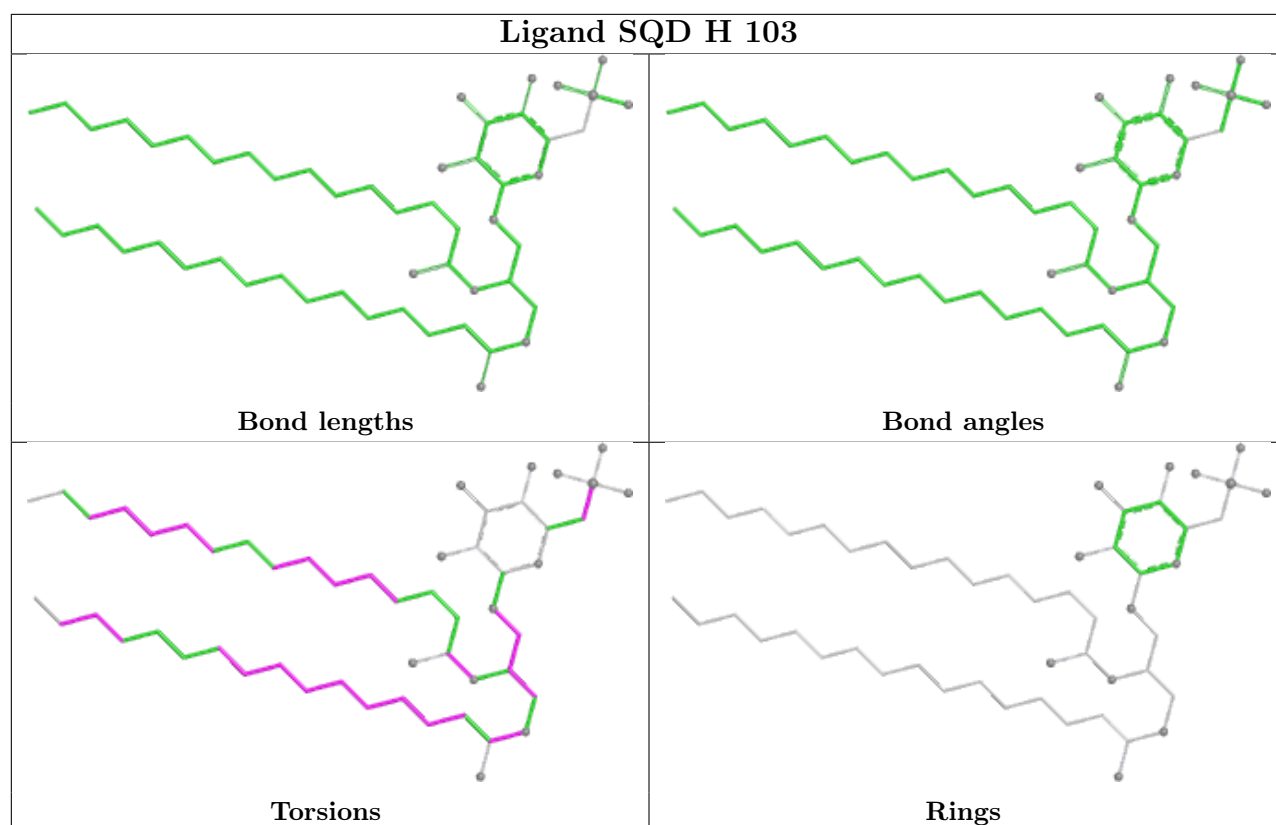


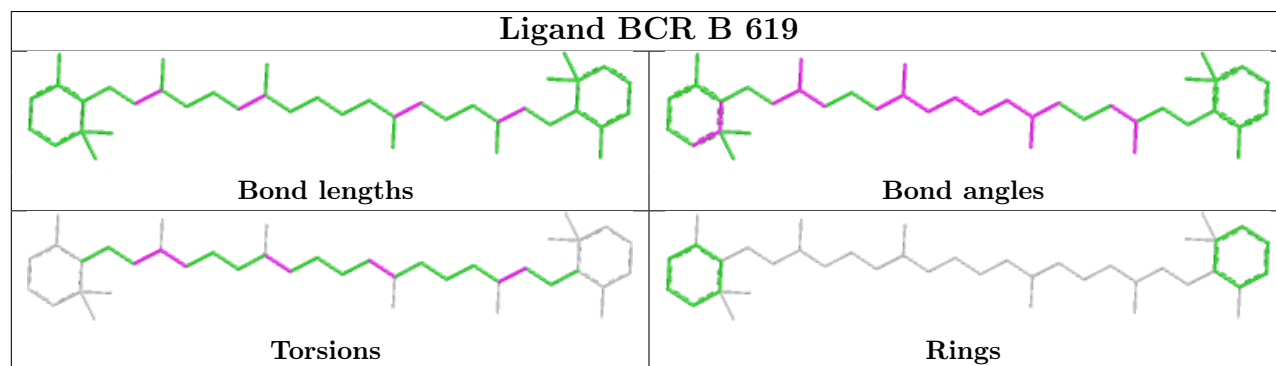
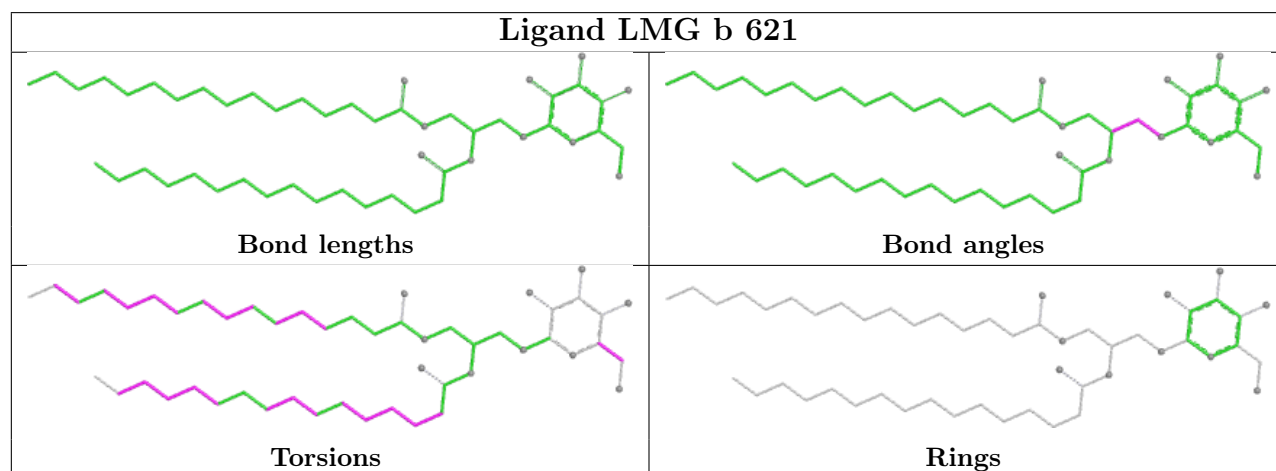
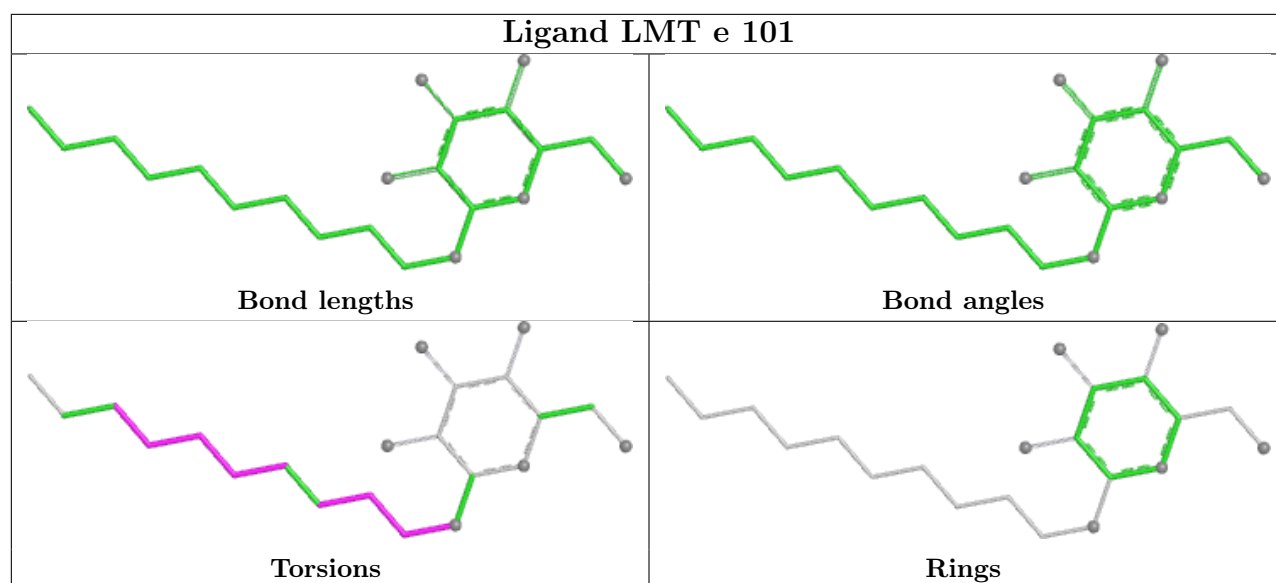
Ligand SQD F 102

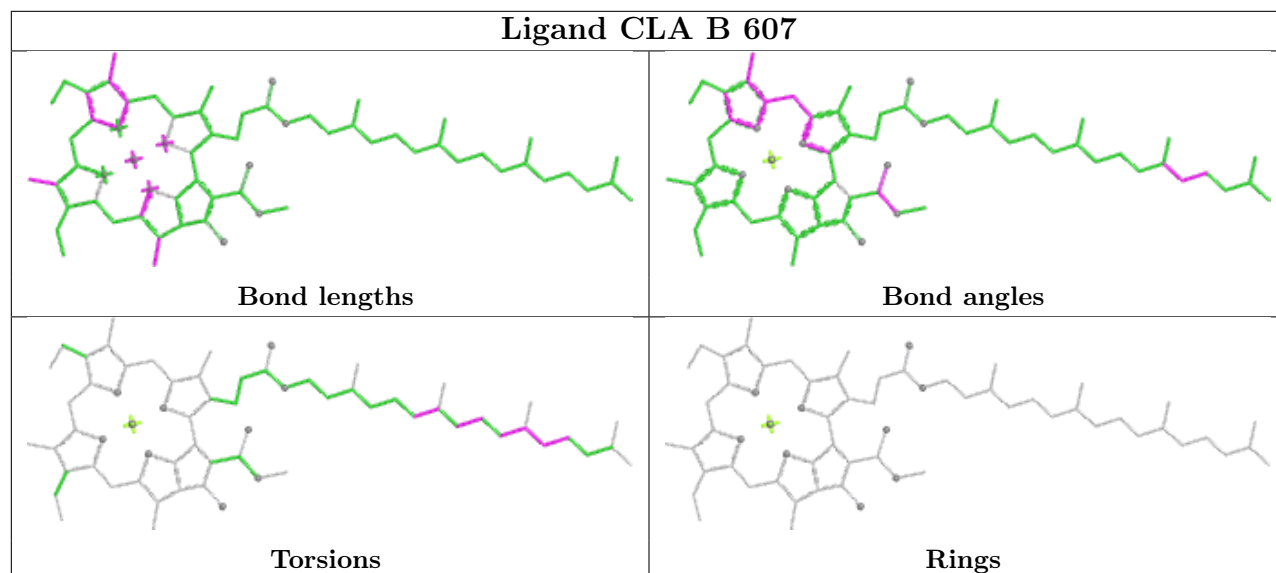
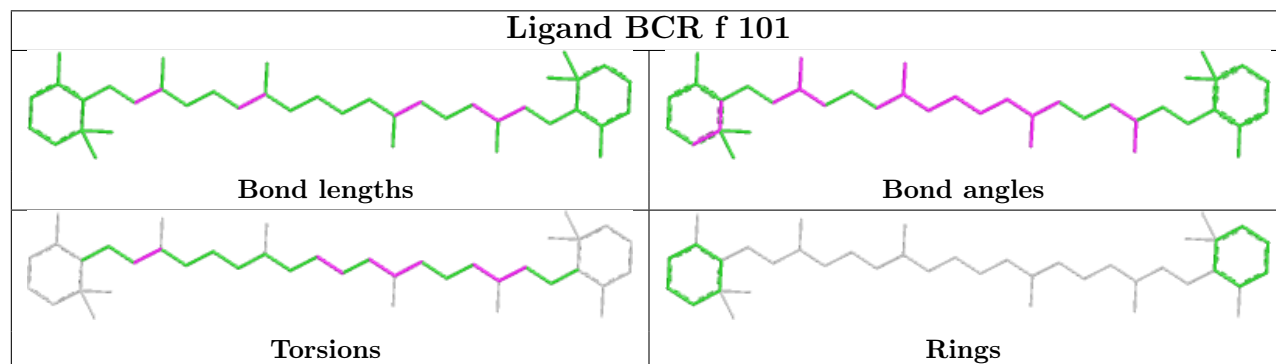
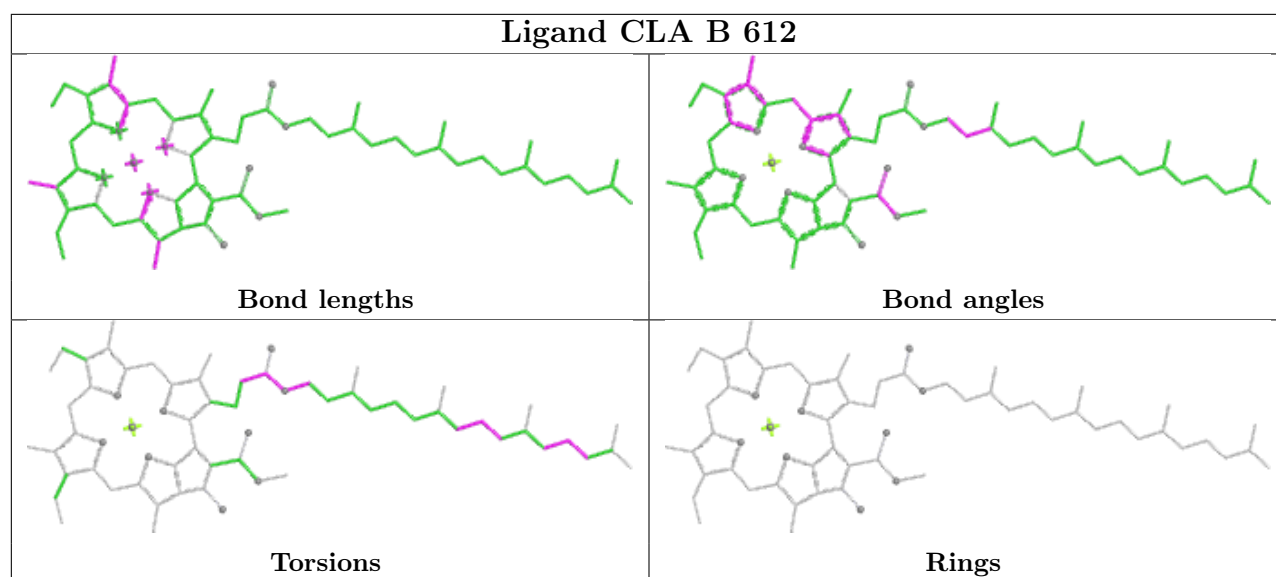


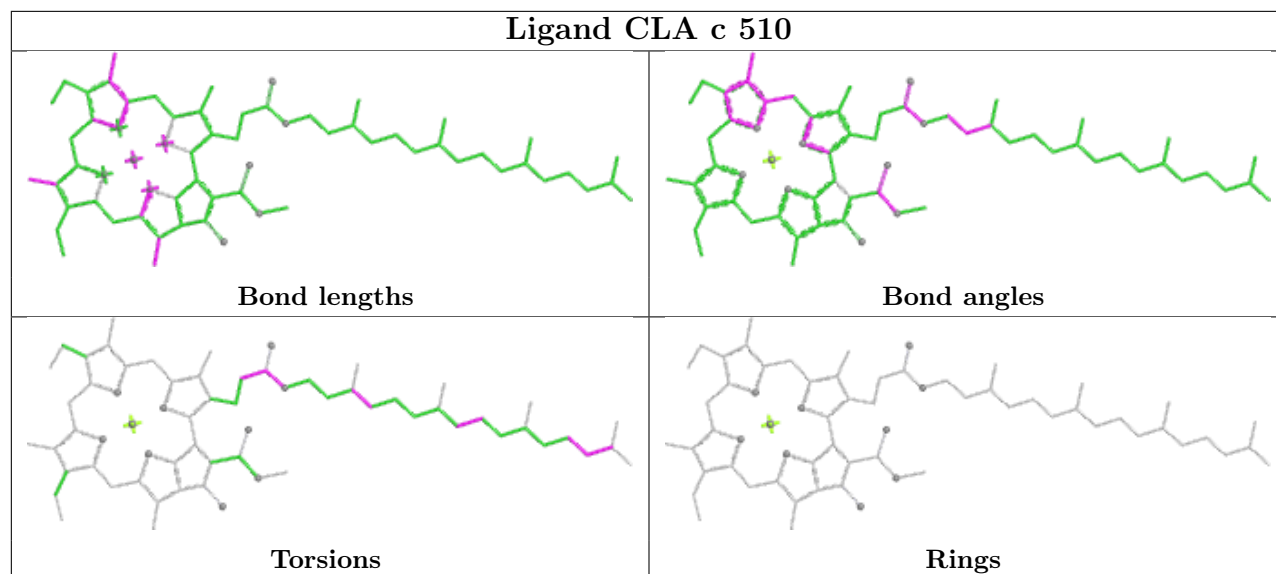
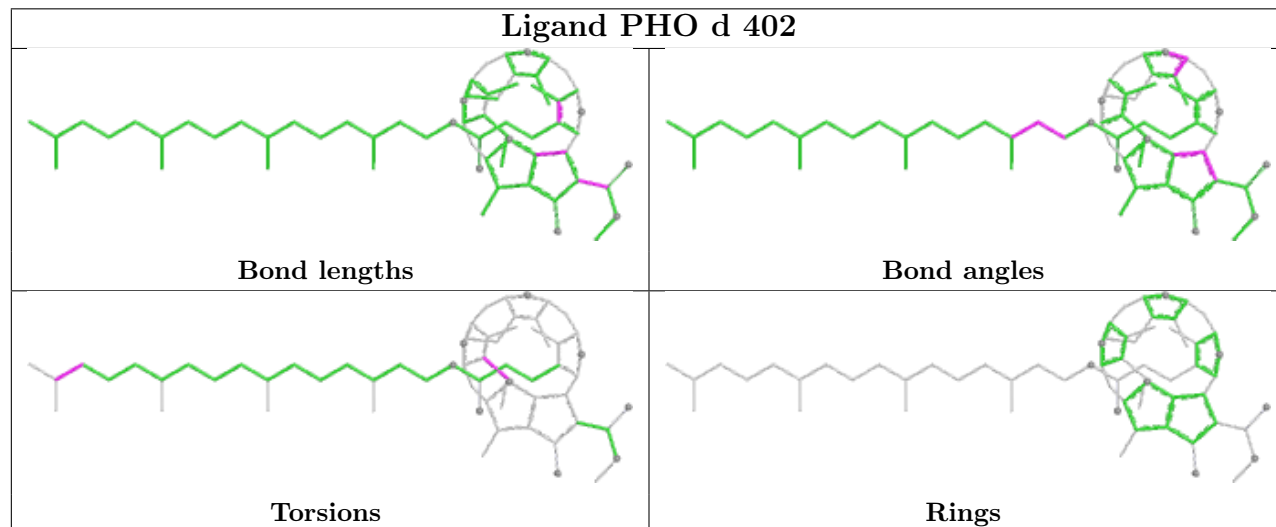
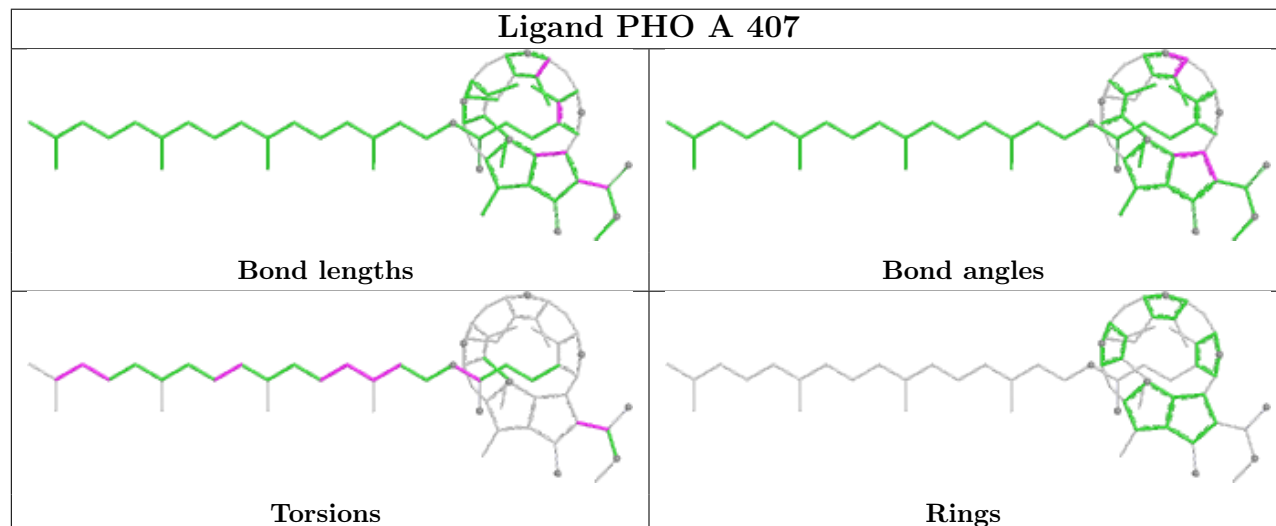


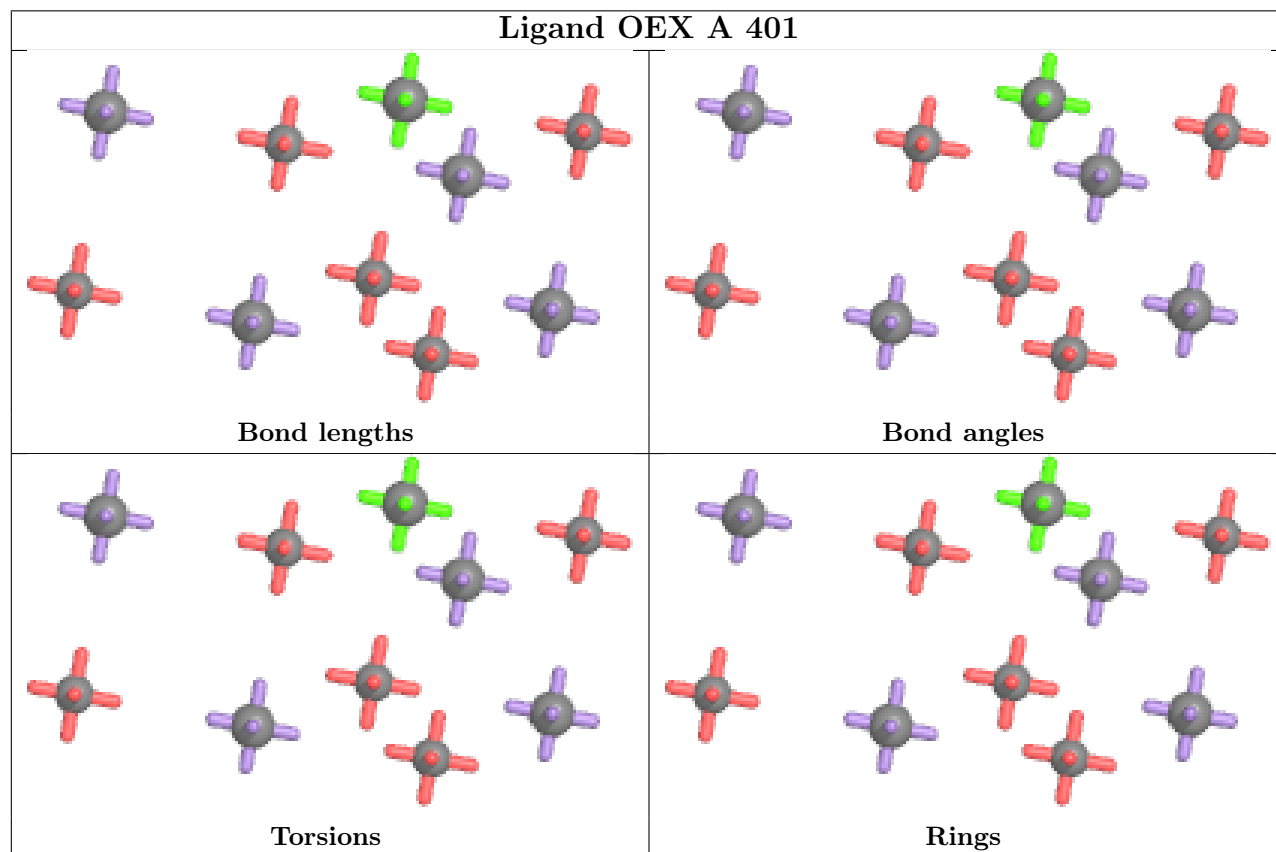
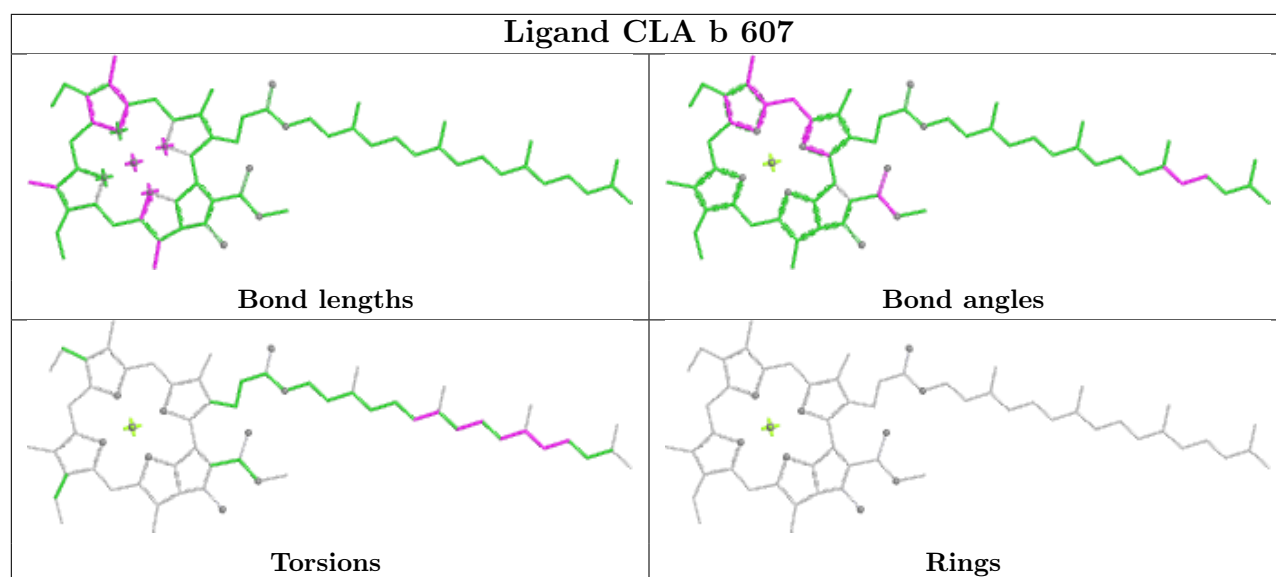


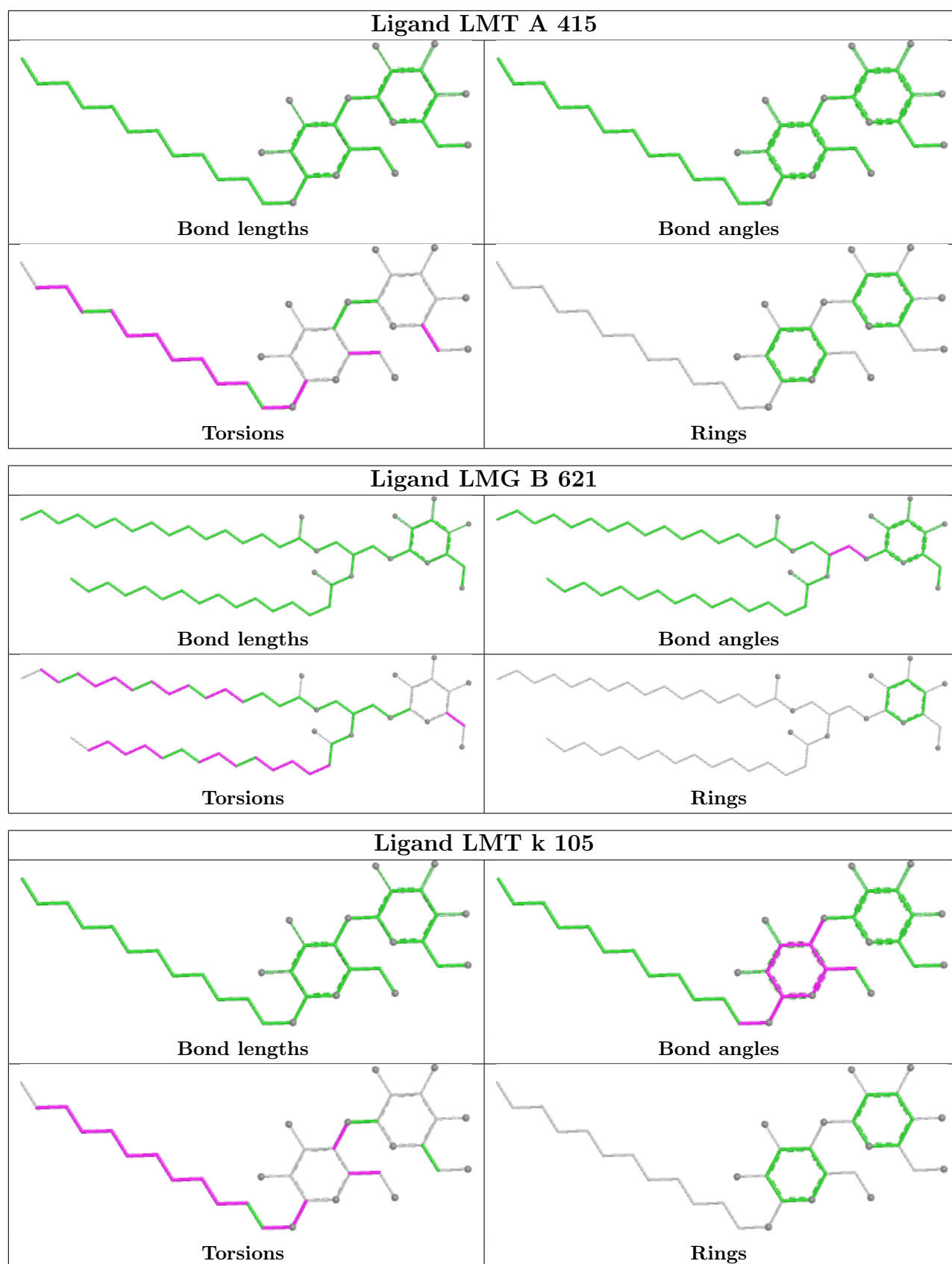


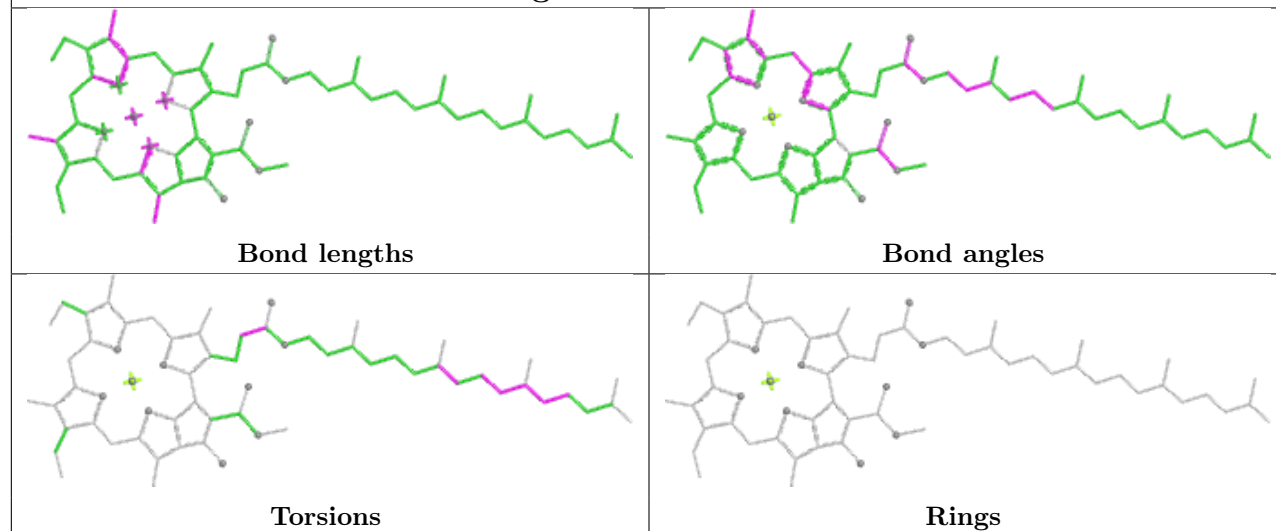
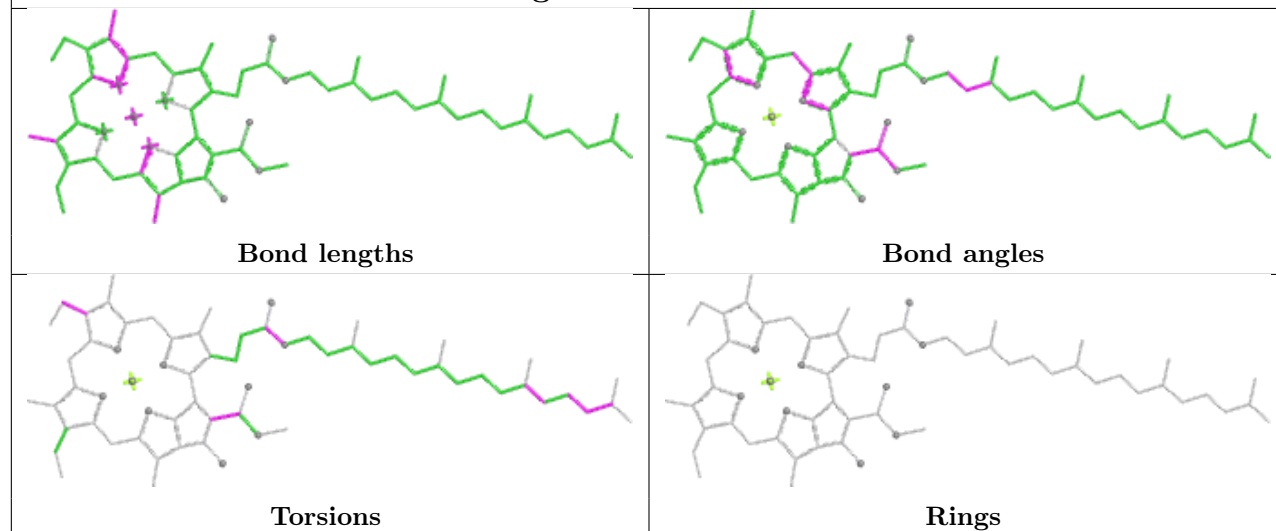


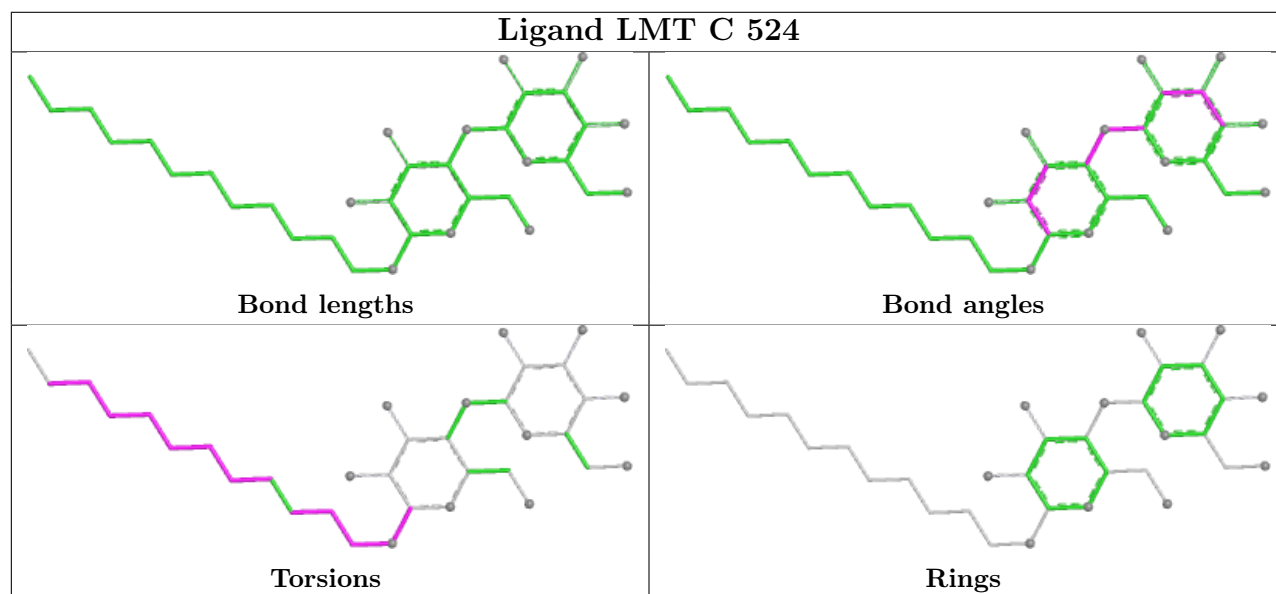
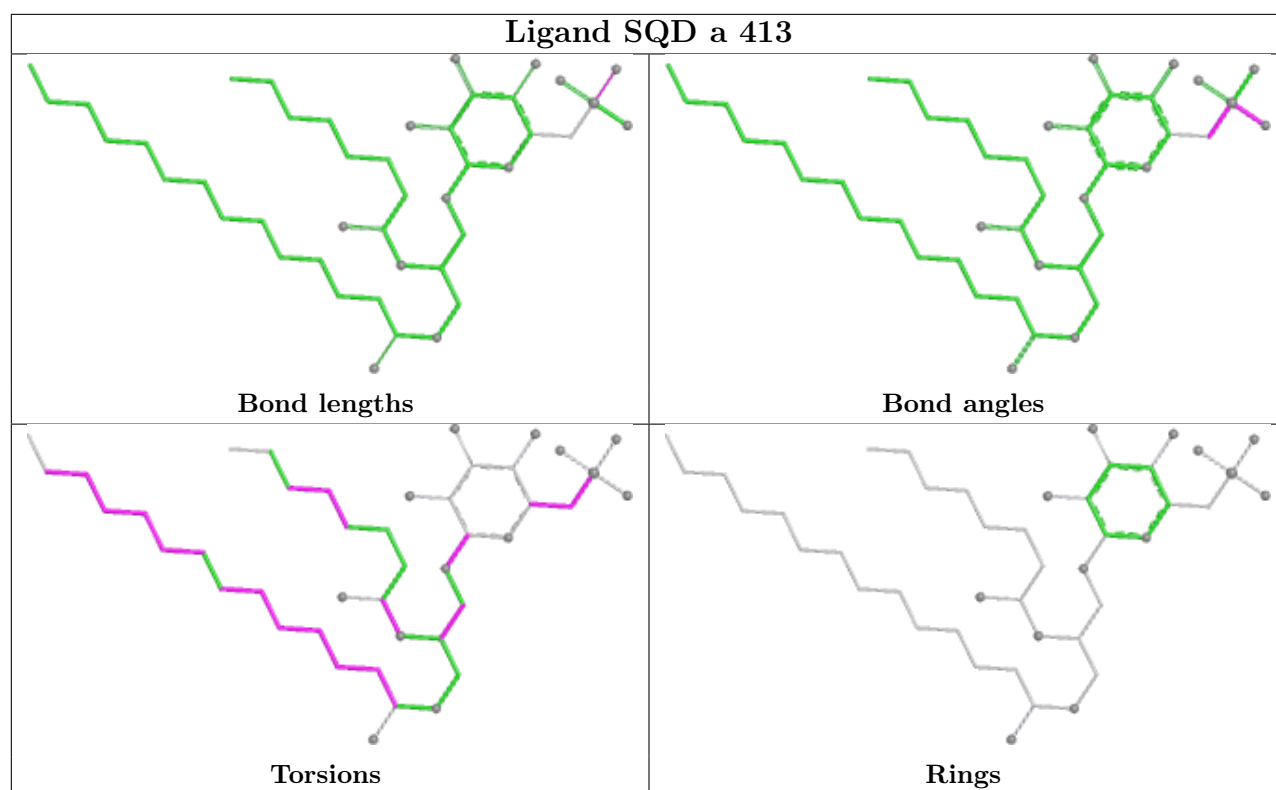


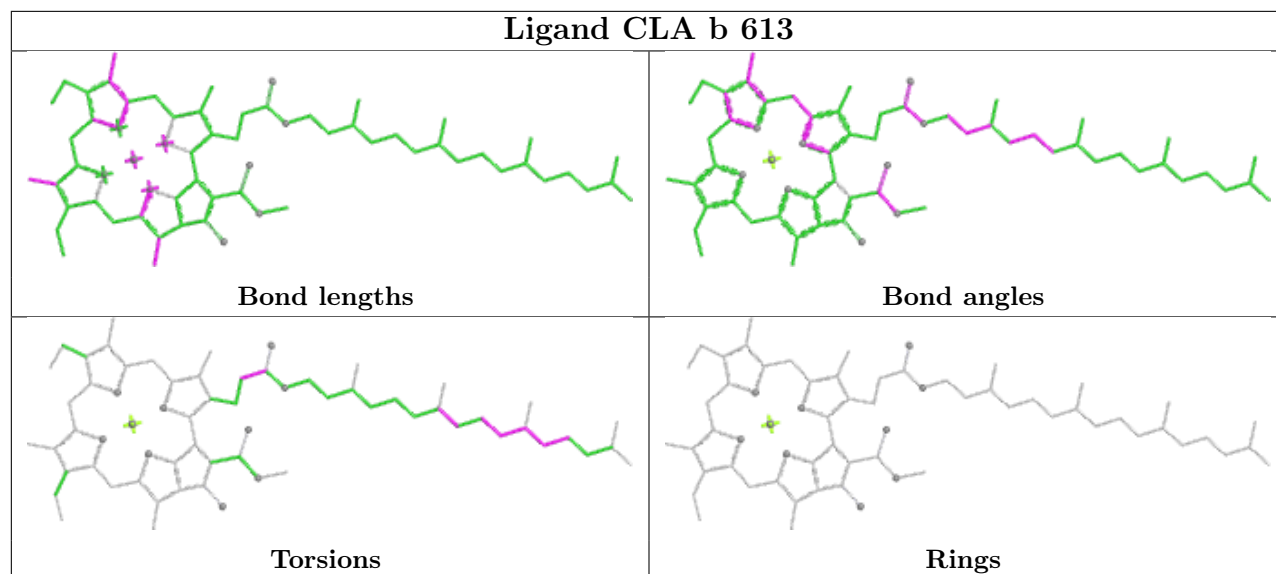
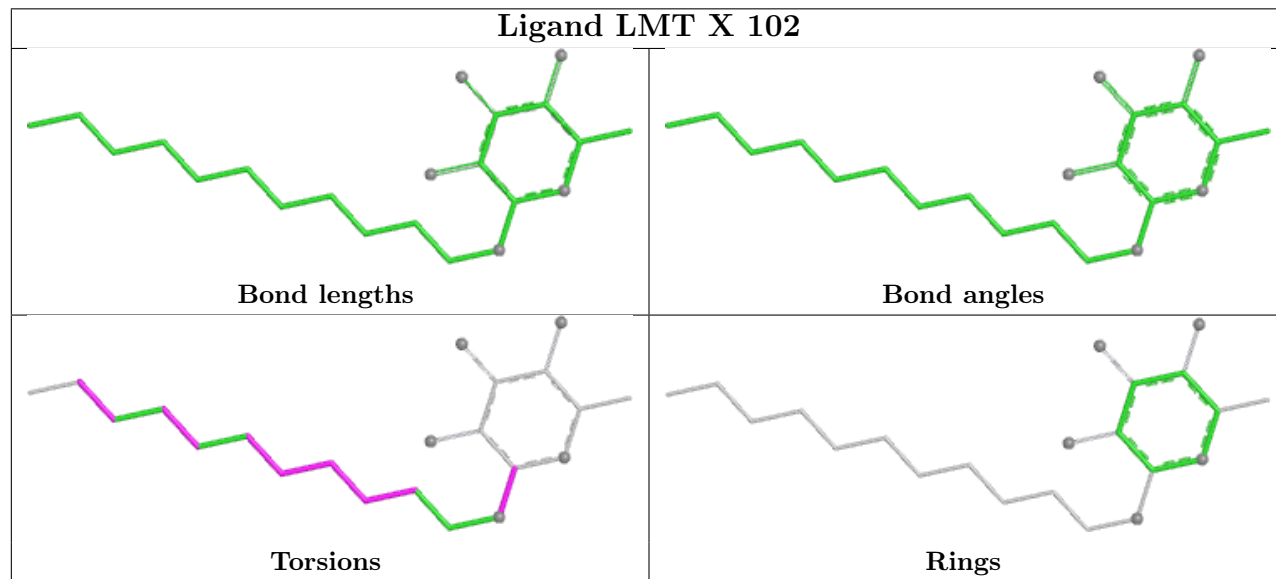
Ligand CLA c 510**Ligand PHO d 402****Ligand PHO A 407**

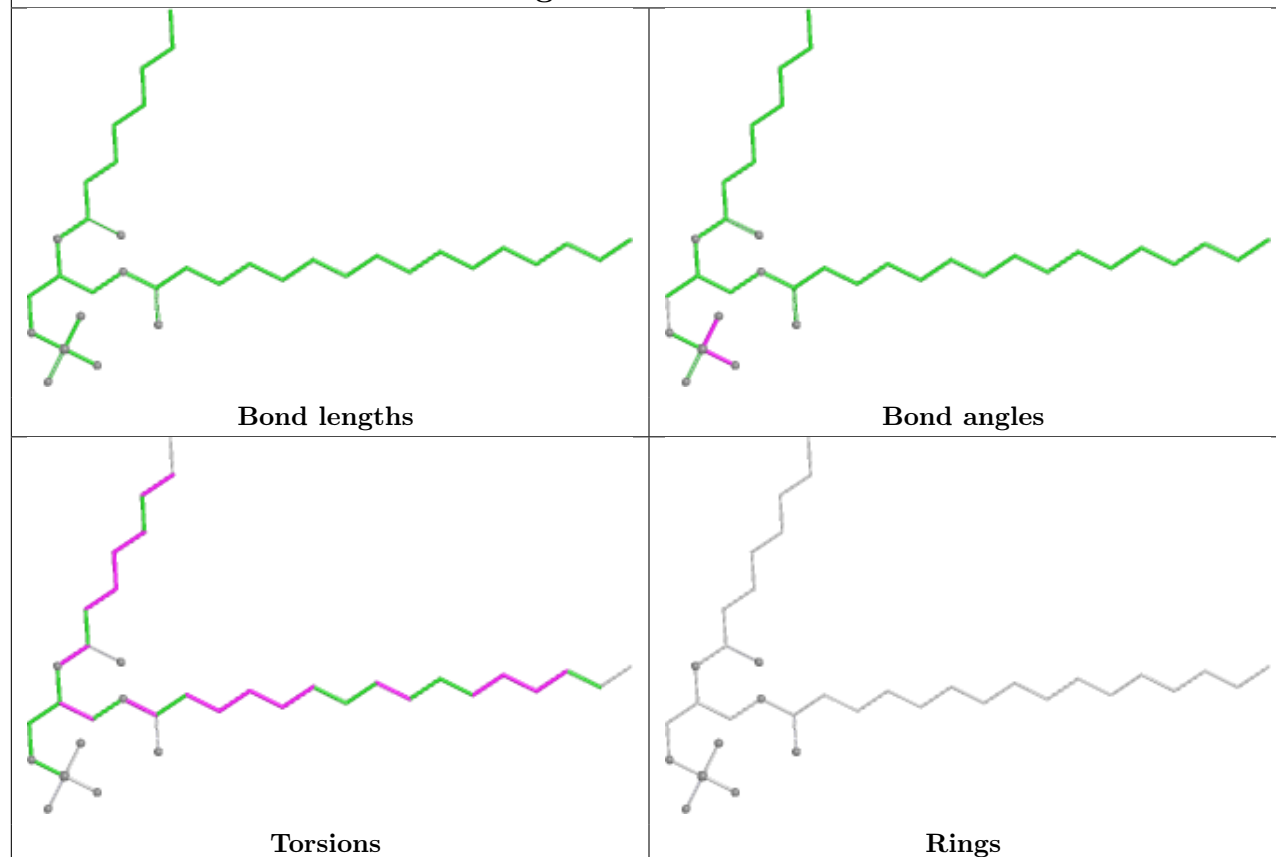
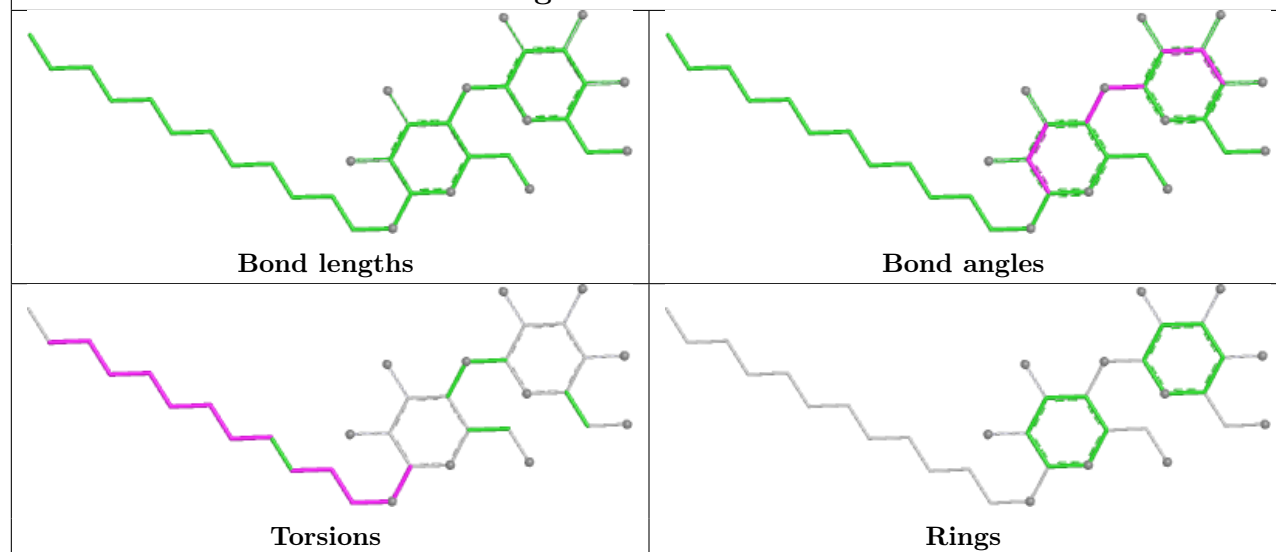




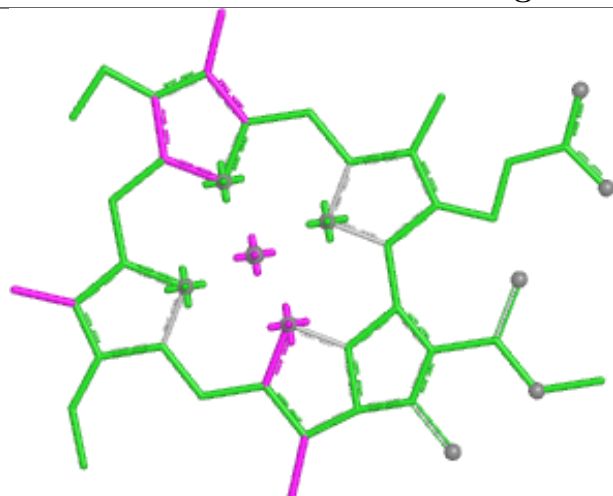
Ligand CLA B 613**Ligand CLA C 502**



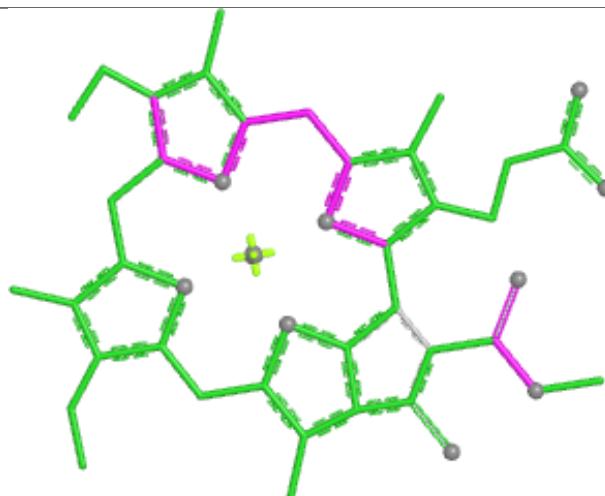
Ligand CLA b 613**Ligand LMT X 102**

Ligand LHG z 102**Ligand LMT c 524**

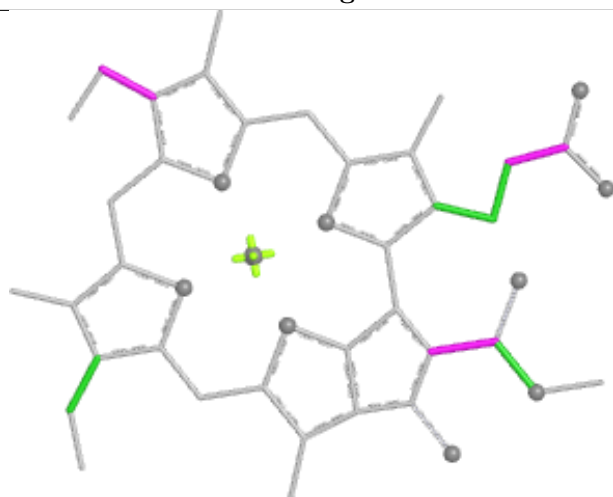
Ligand CLA B 601



Bond lengths



Bond angles

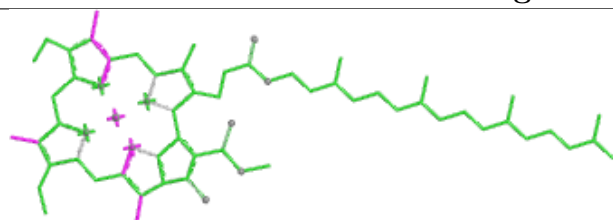


Torsions

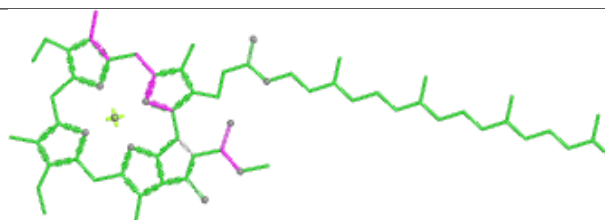


Rings

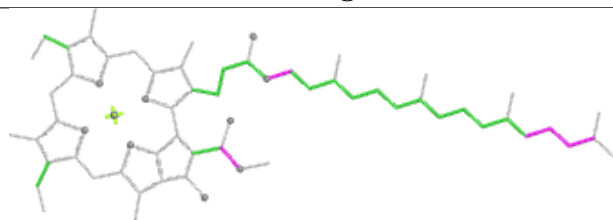
Ligand CLA A 405



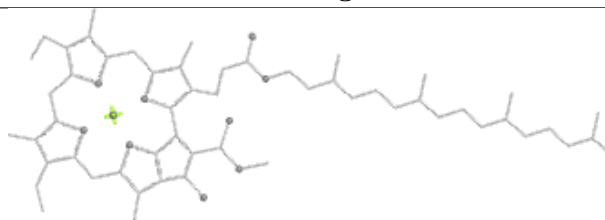
Bond lengths



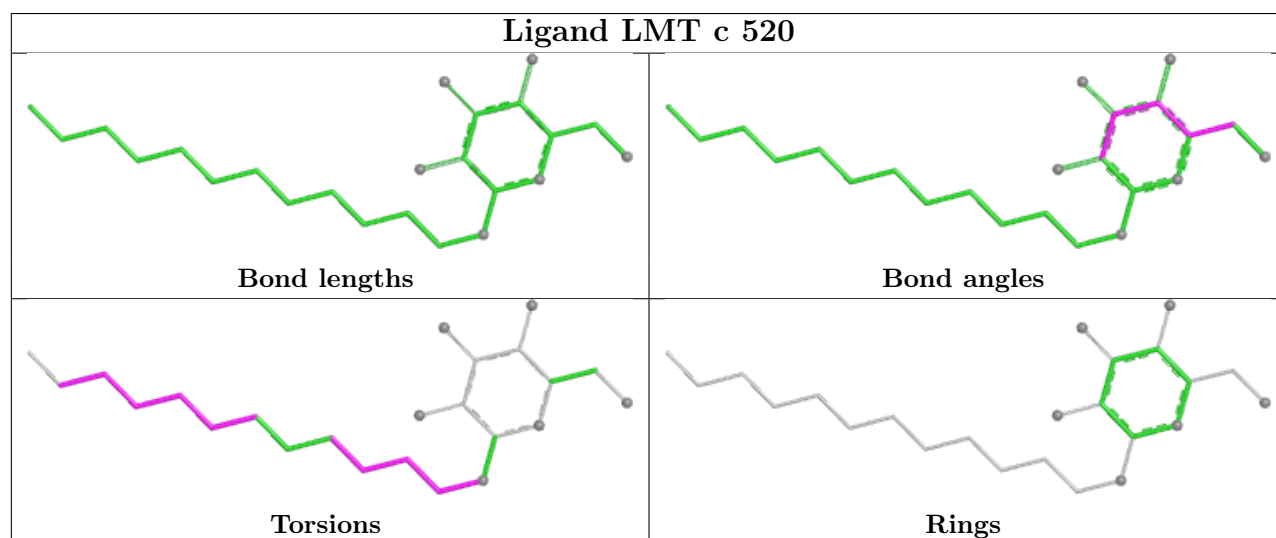
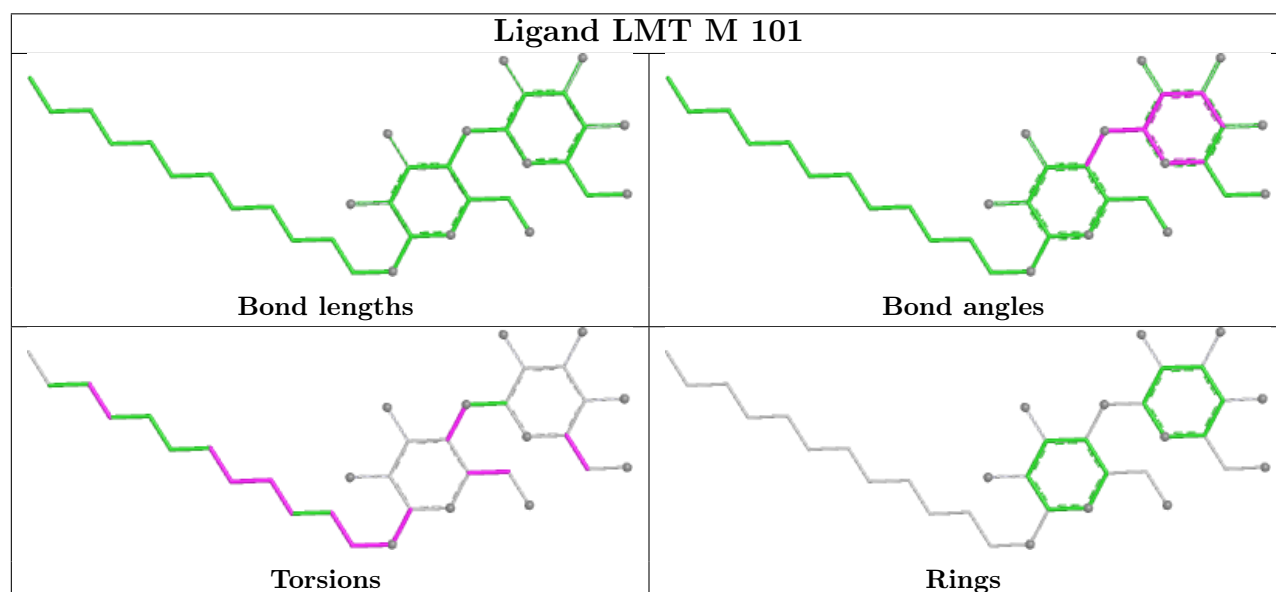
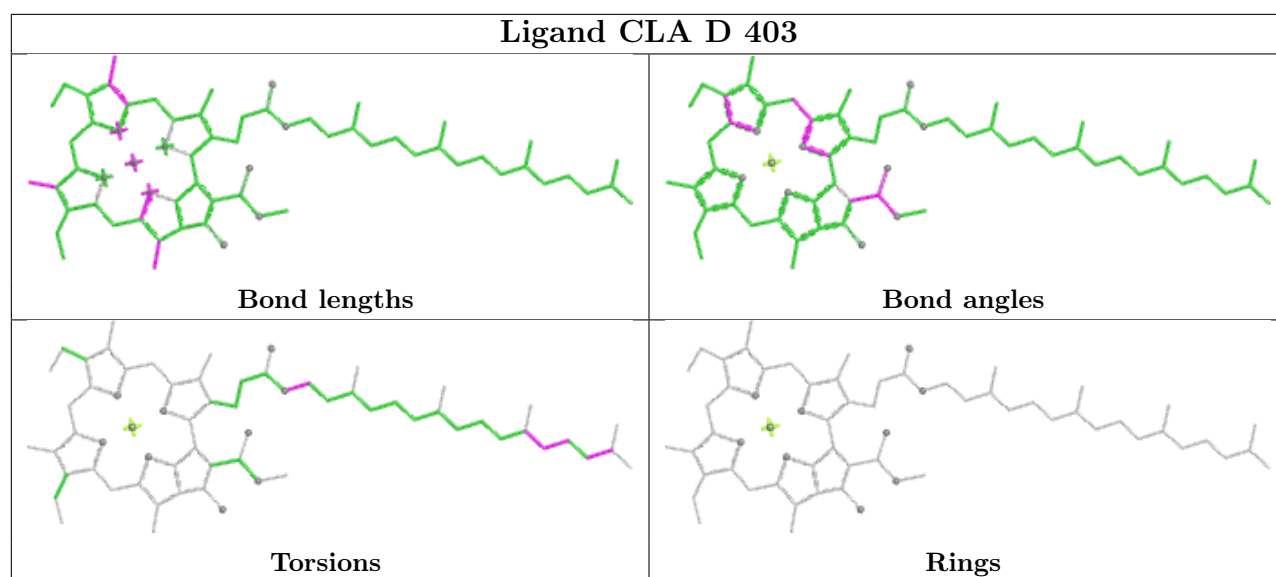
Bond angles

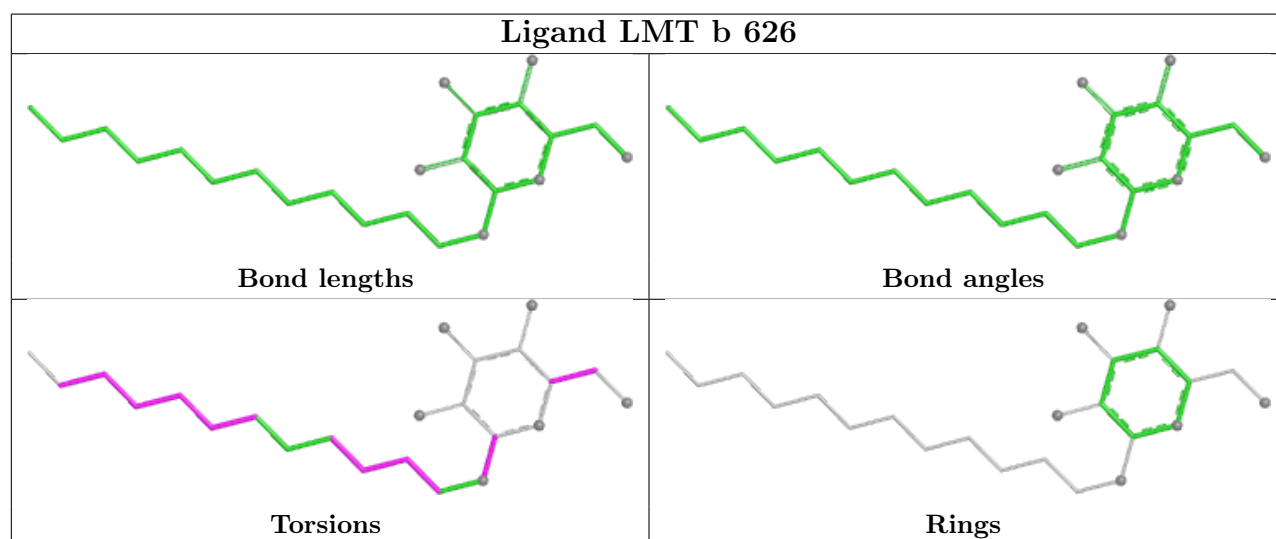
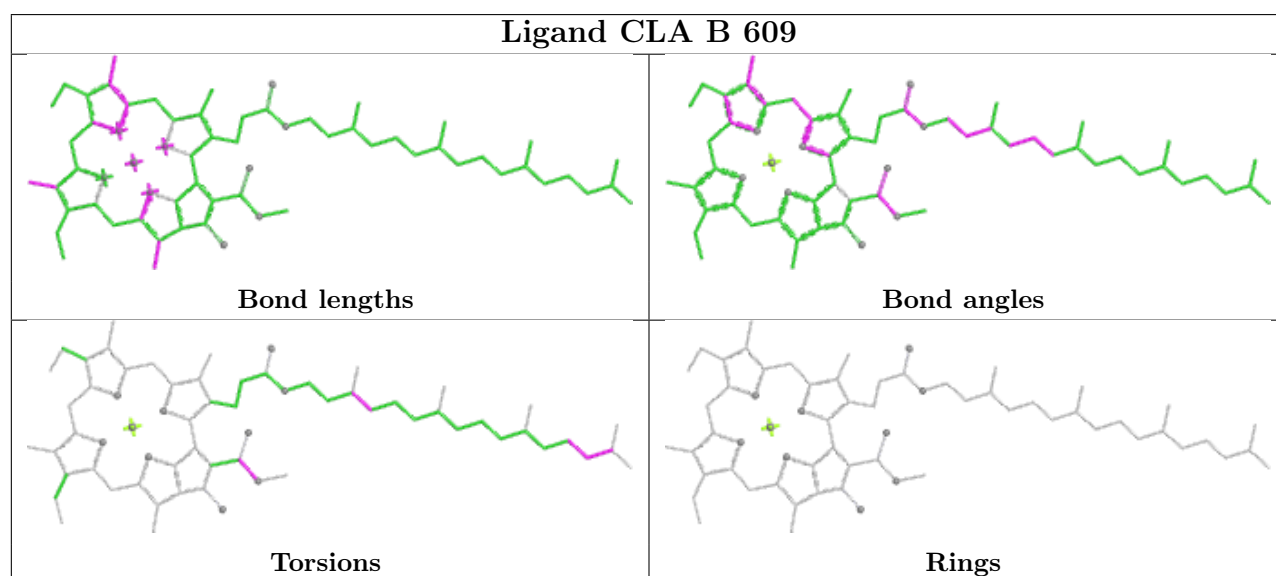
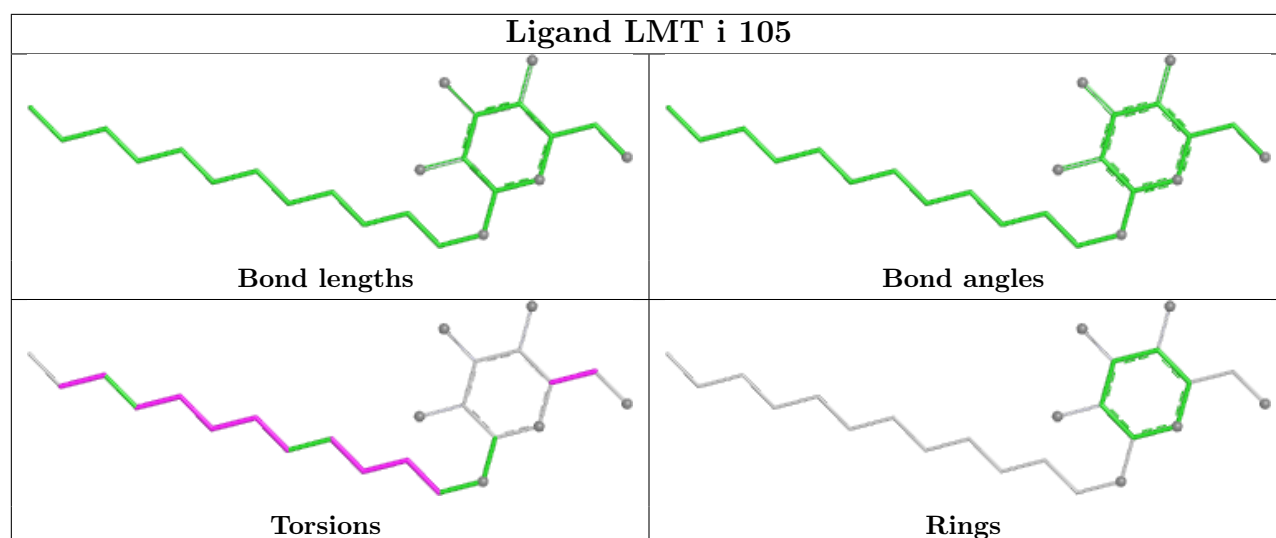


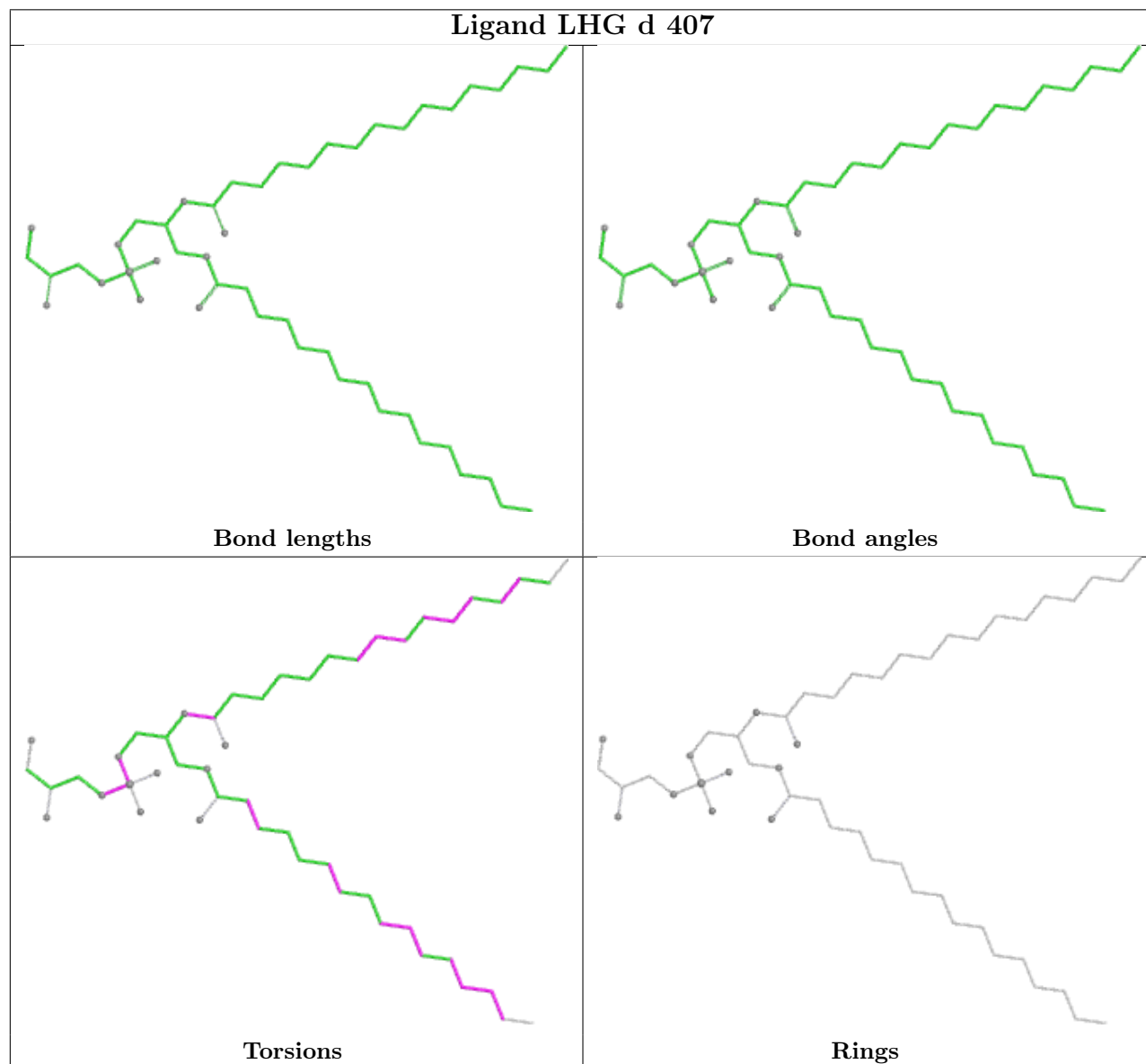
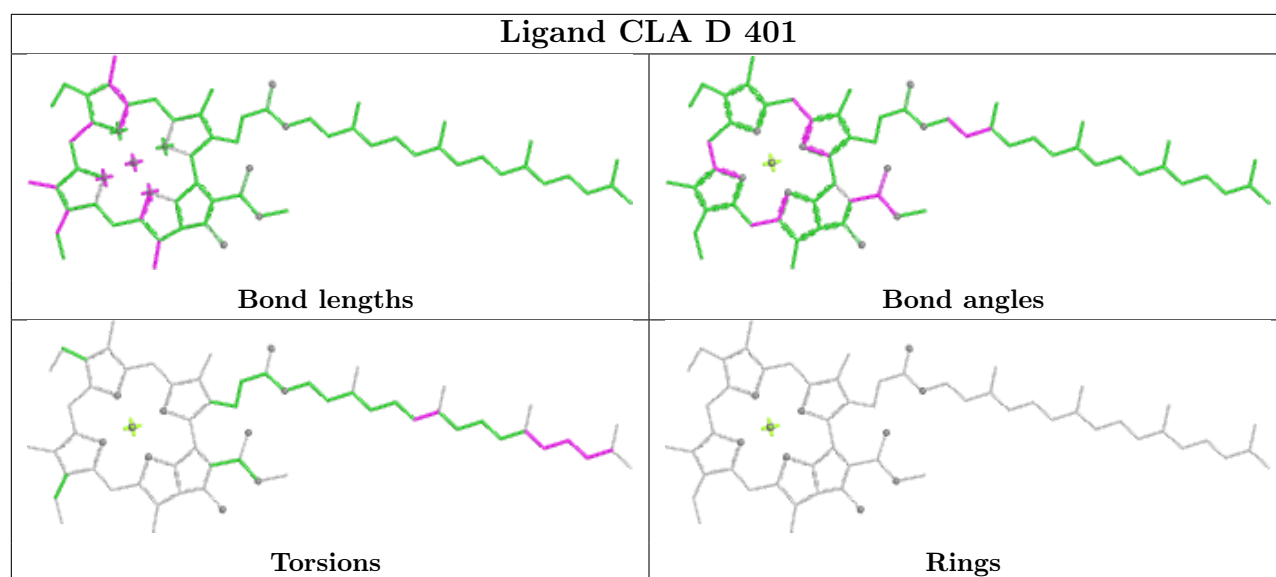
Torsions

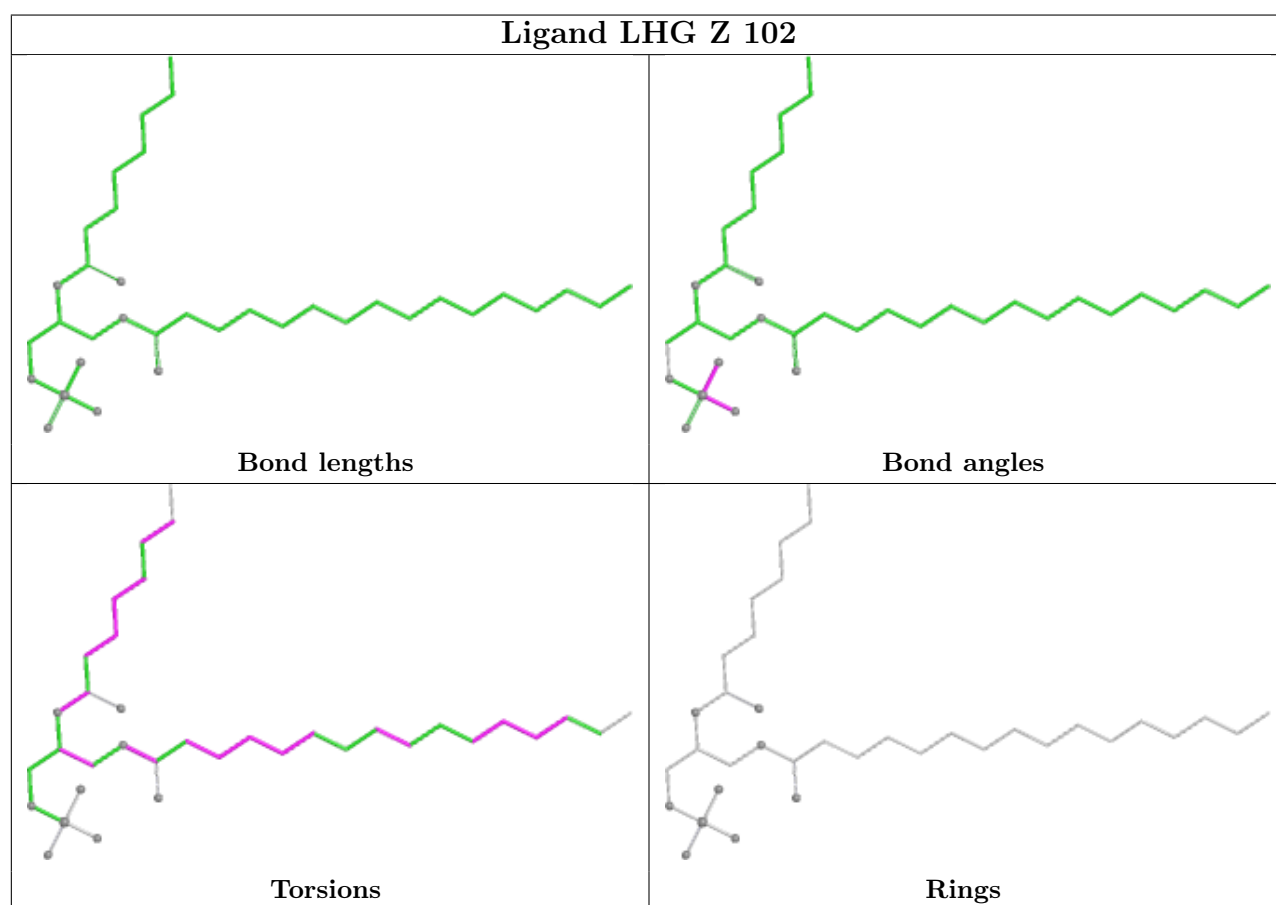
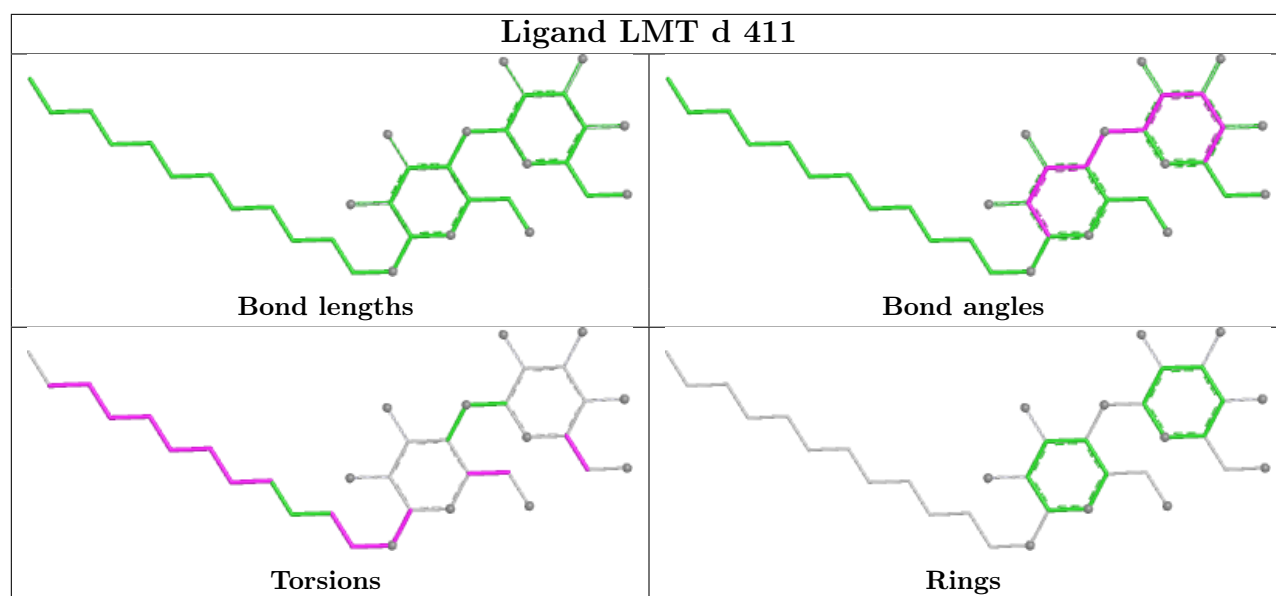


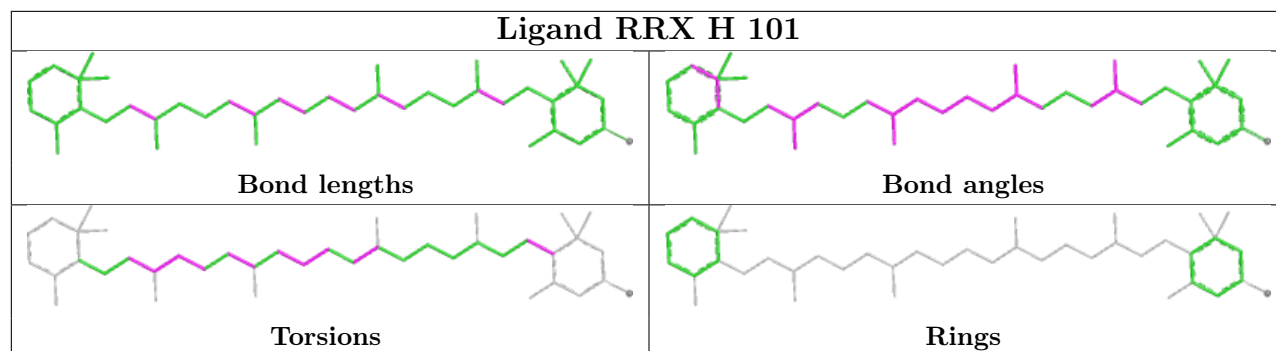
Rings











4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

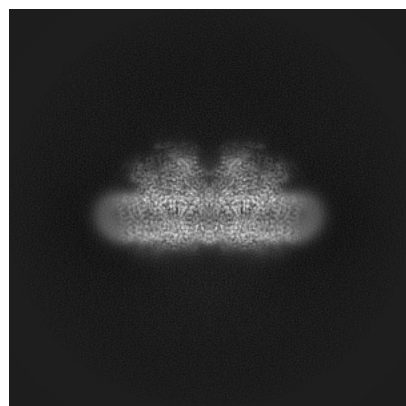
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71652. These allow visual inspection of the internal detail of the map and identification of artifacts.

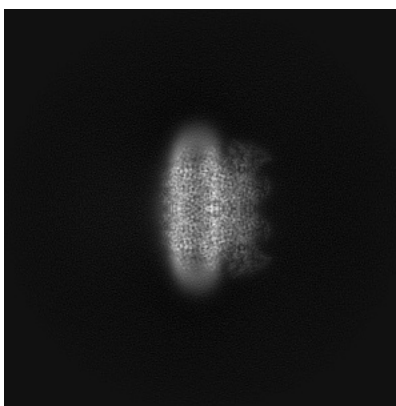
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections [i](#)

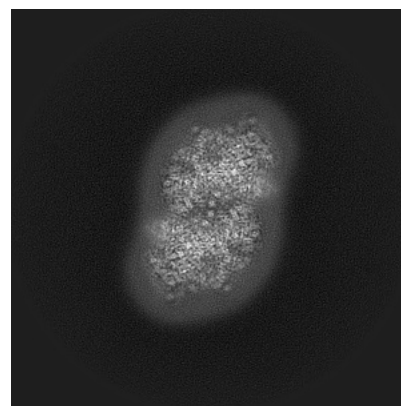
5.1.1 Primary map



X

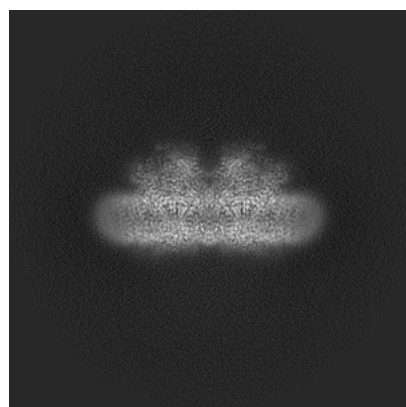


Y

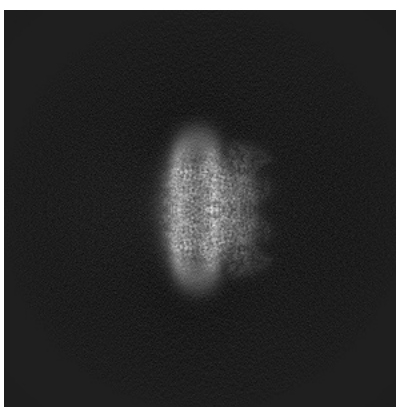


Z

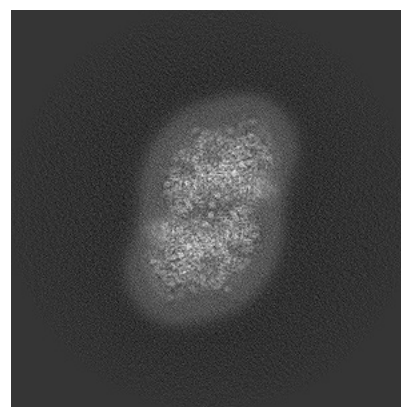
5.1.2 Raw map



X



Y

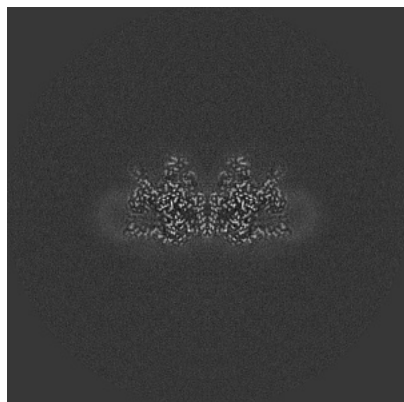


Z

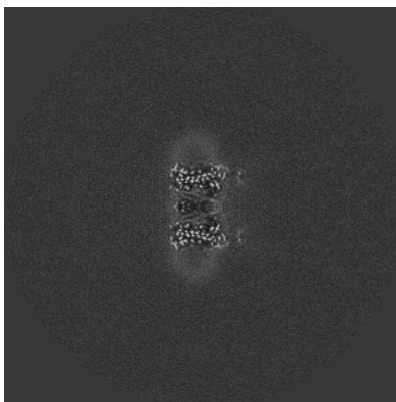
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

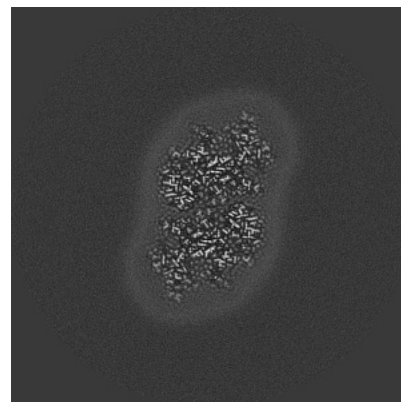
5.2.1 Primary map



X Index: 300

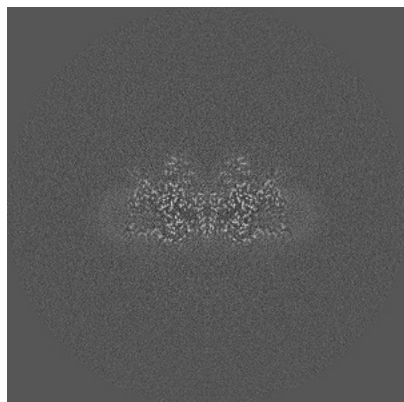


Y Index: 300

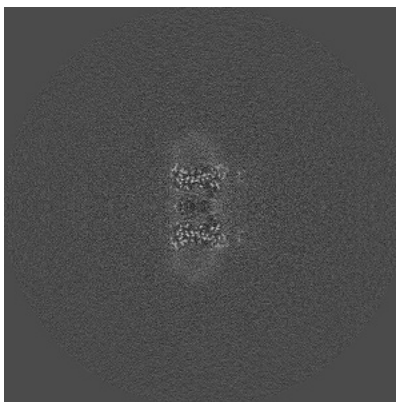


Z Index: 300

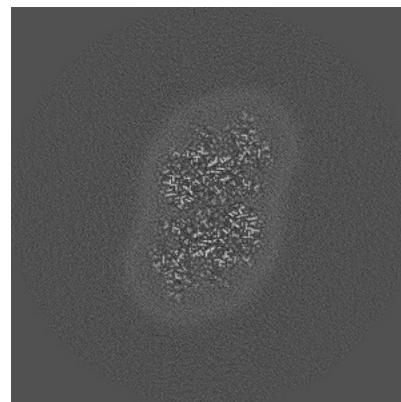
5.2.2 Raw map



X Index: 300



Y Index: 300

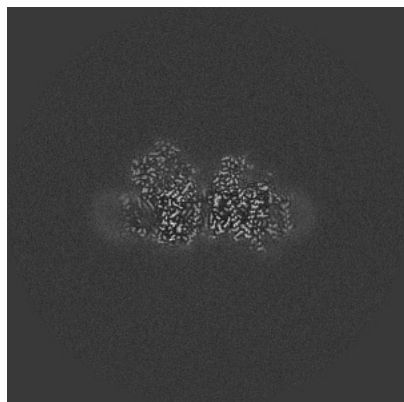


Z Index: 300

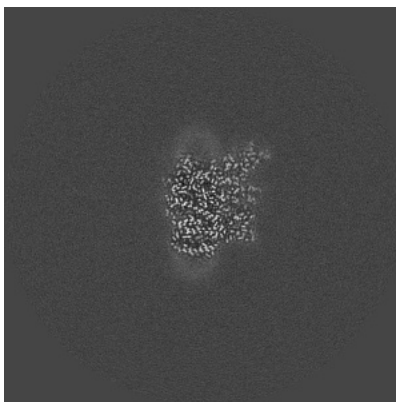
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

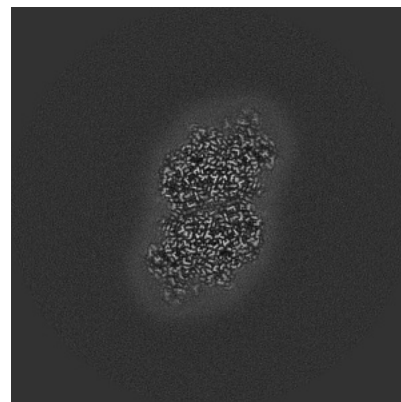
5.3.1 Primary map



X Index: 278

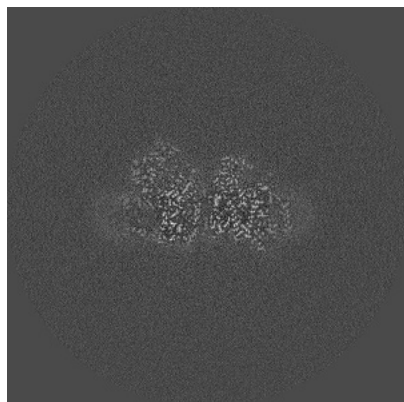


Y Index: 341

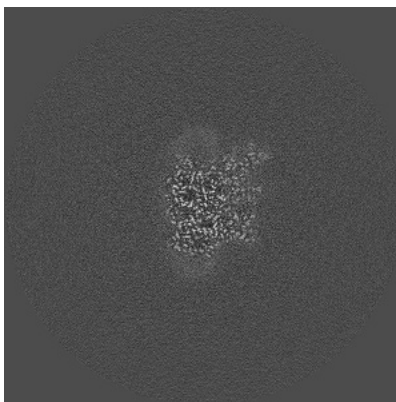


Z Index: 312

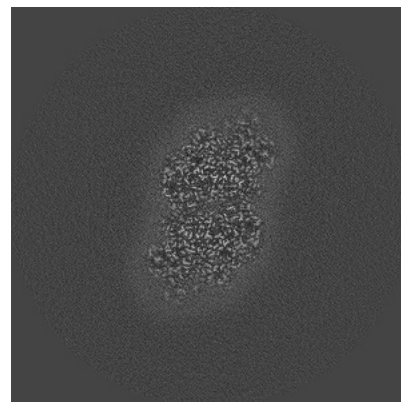
5.3.2 Raw map



X Index: 278



Y Index: 342

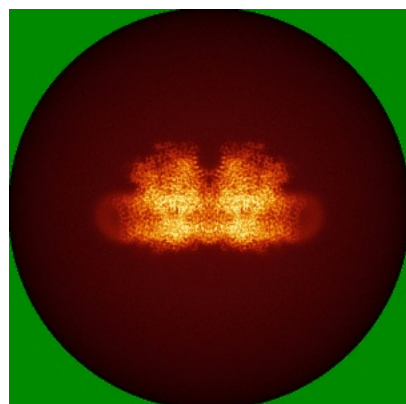


Z Index: 312

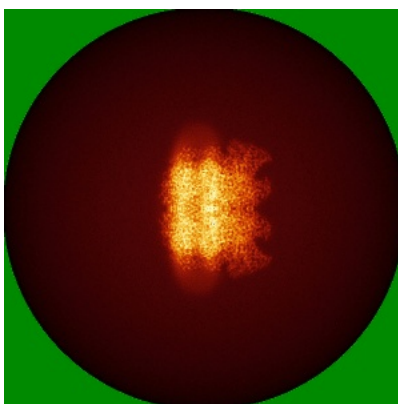
The images above show the largest variance slices of the map in three orthogonal directions.

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

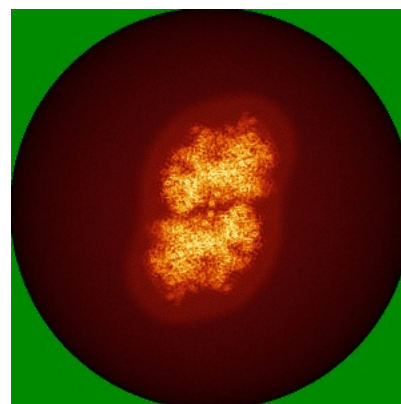
5.4.1 Primary map



X

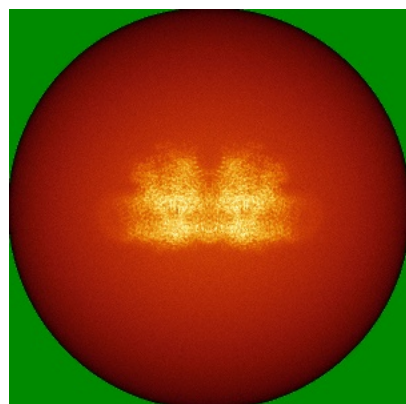


Y

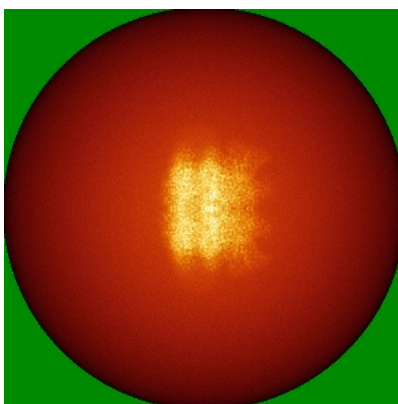


Z

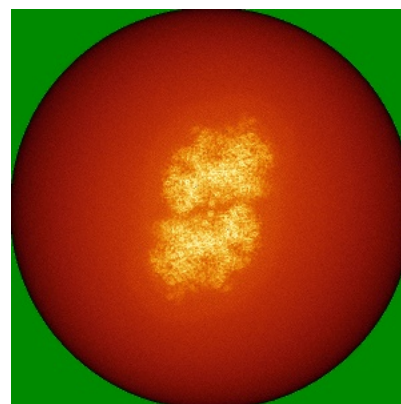
5.4.2 Raw map



X



Y

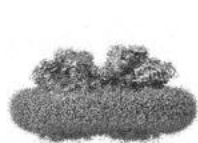


Z

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.

5.5 Orthogonal surface views [i](#)

5.5.1 Primary map



X



Y



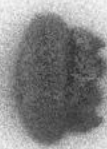
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

5.5.2 Raw map



X



Y



Z

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.

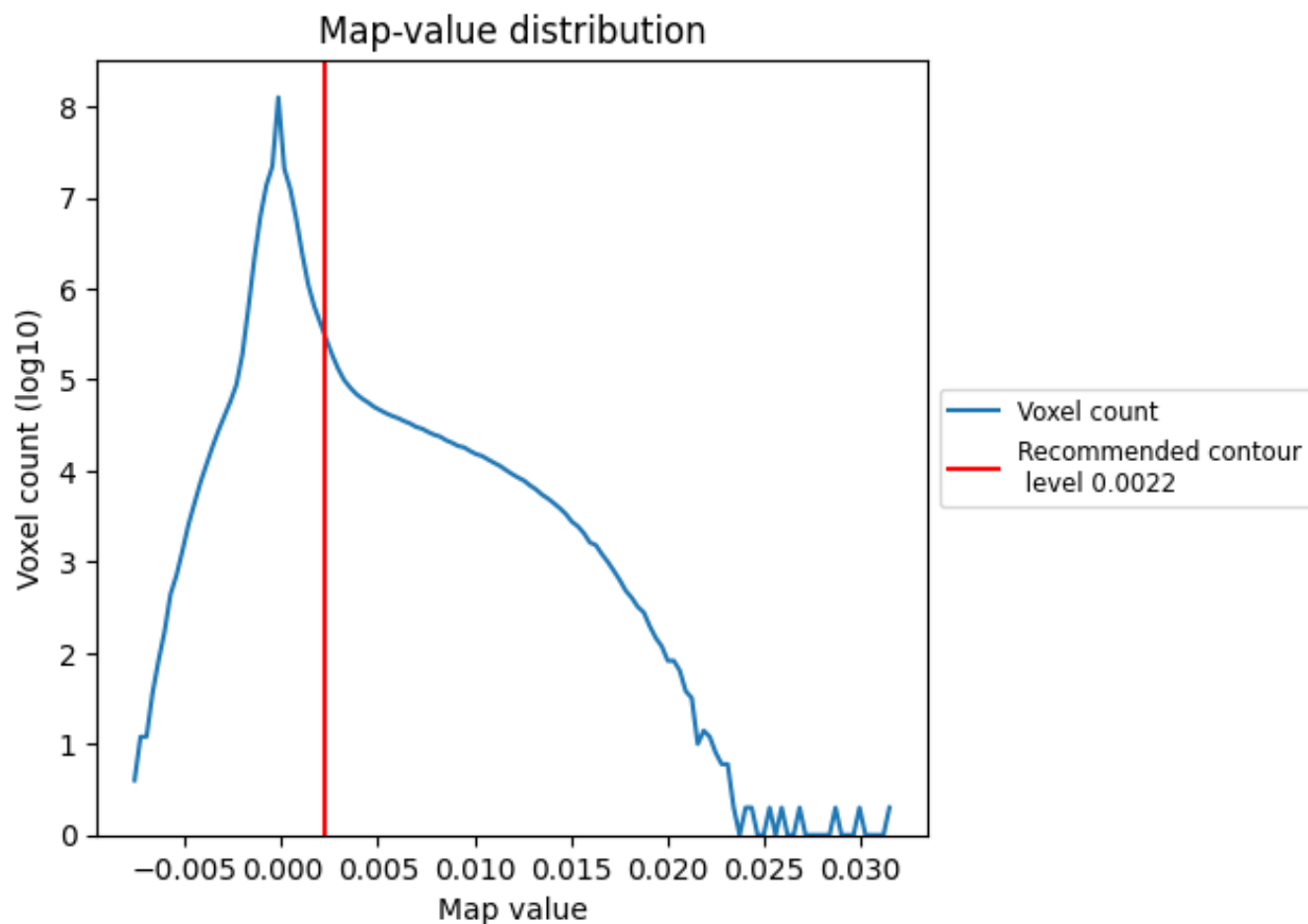
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

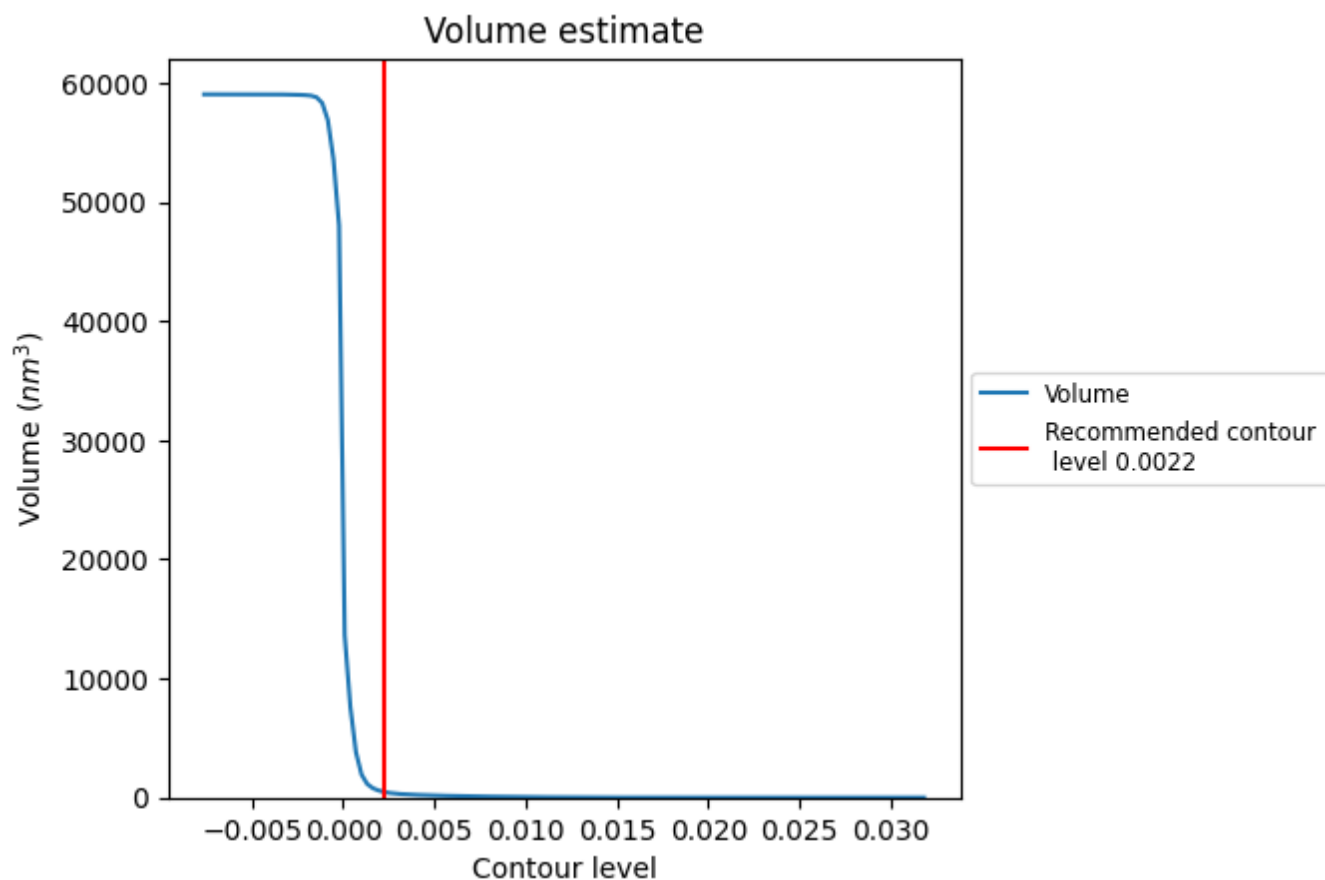
This section contains the results of statistical analysis of the map.

6.1 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.

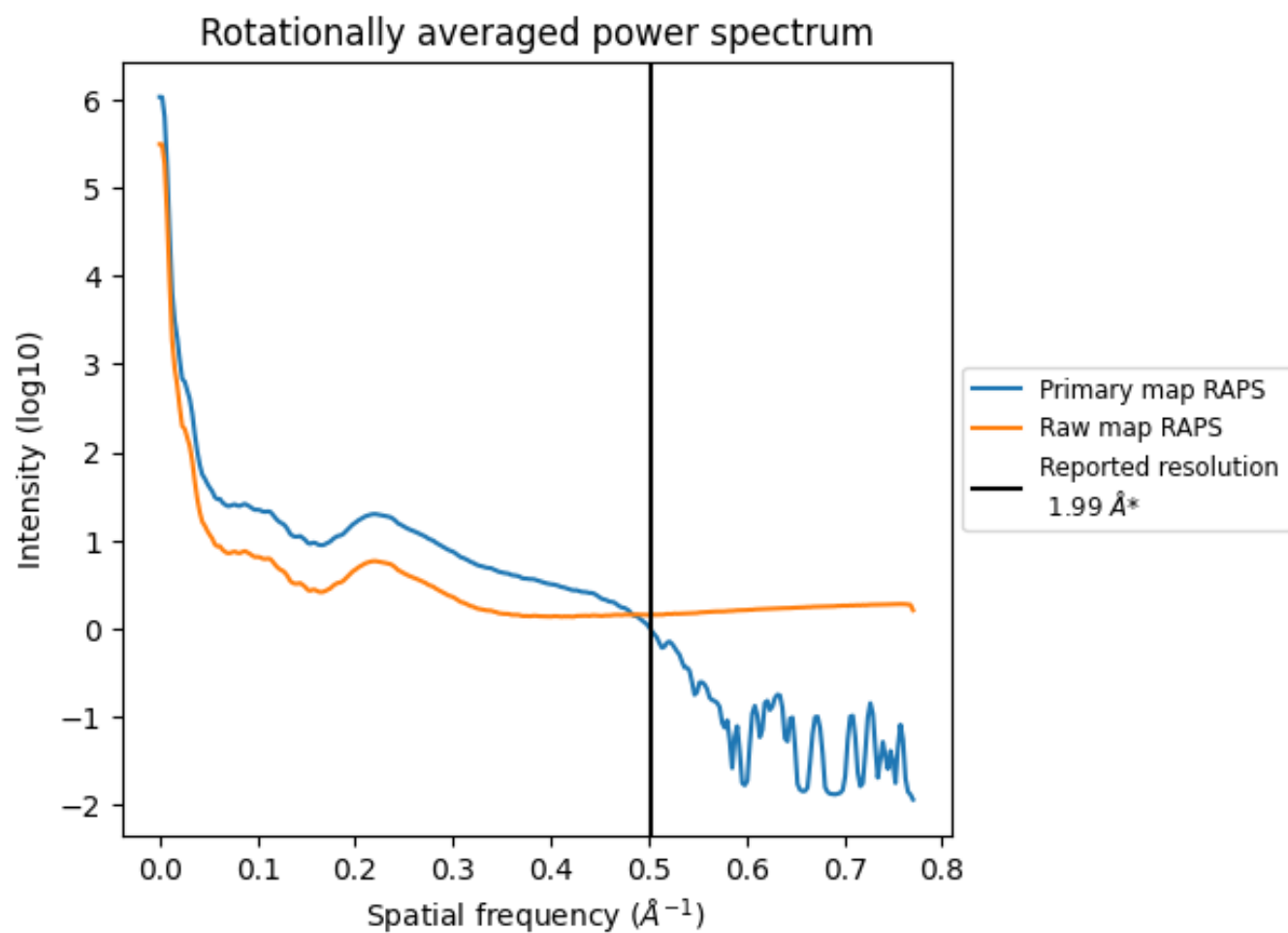
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 491 nm³; this corresponds to an approximate mass of 443 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.

6.3 Rotationally averaged power spectrum [i](#)

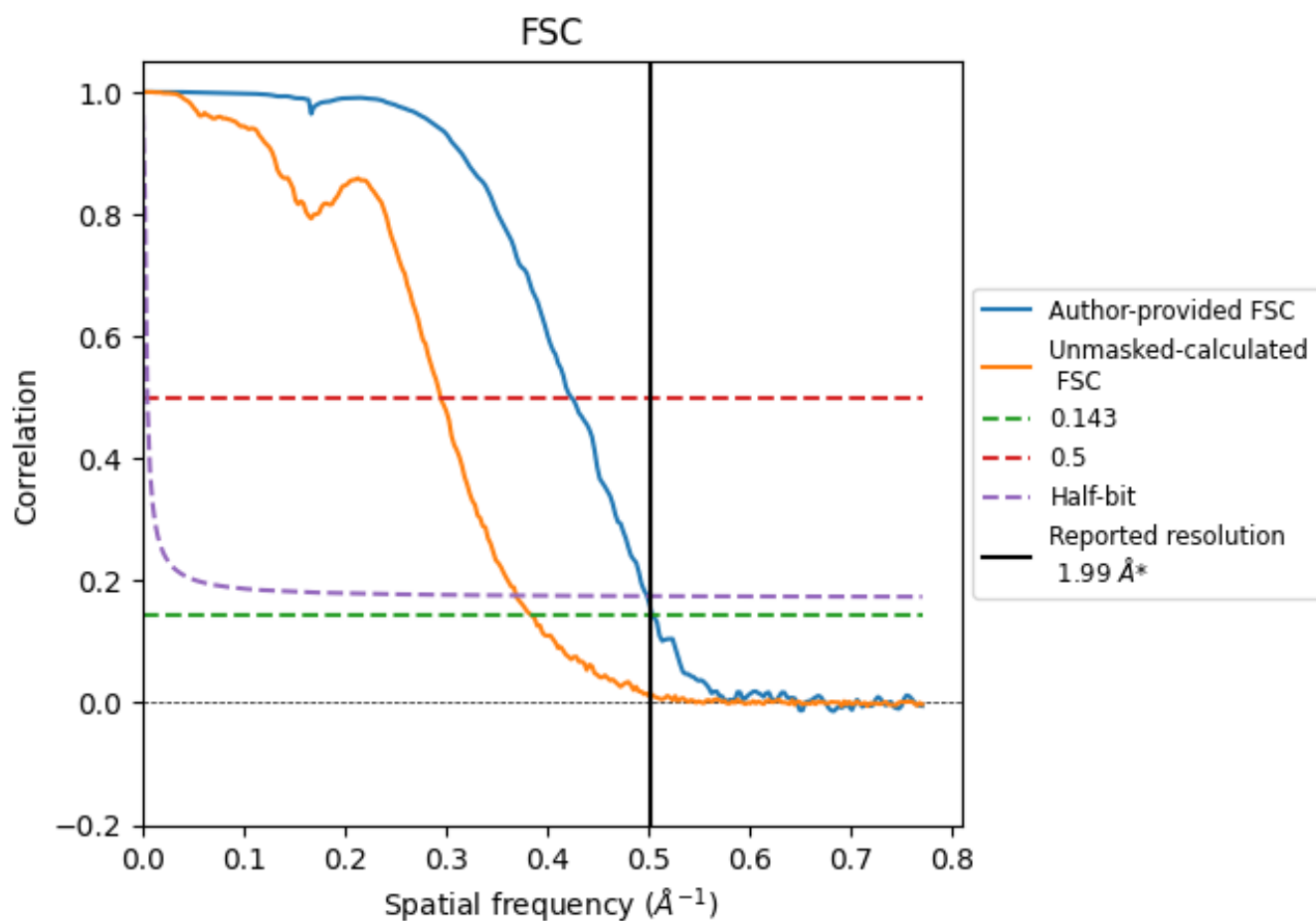


*Reported resolution corresponds to spatial frequency of 0.503 Å⁻¹

7 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.

7.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.503 \AA^{-1}

7.2 Resolution estimates [i](#)

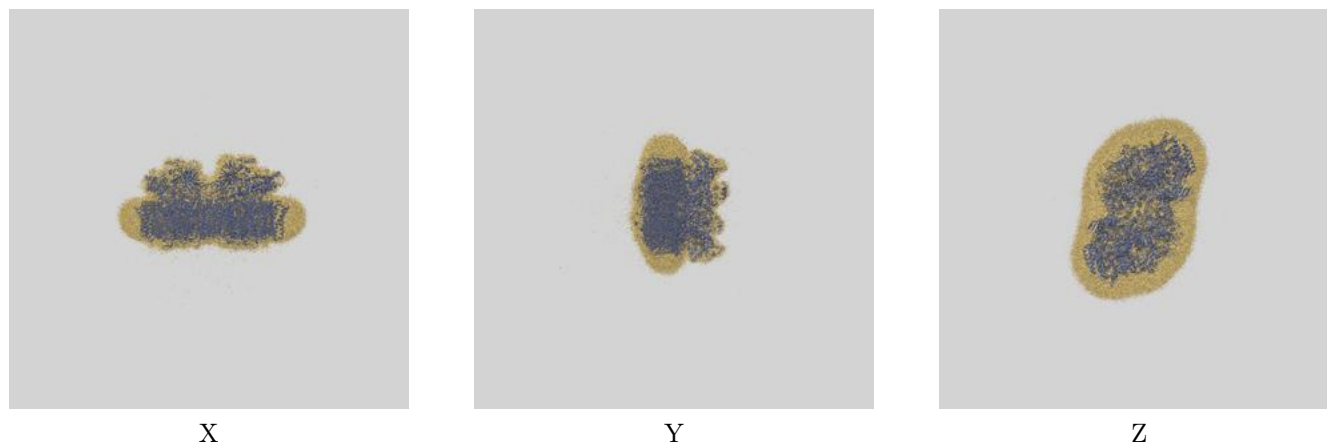
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.99	-	-
Author-provided FSC curve	1.98	2.36	2.01
Unmasked-calculated*	2.60	3.39	2.71

*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 2.60 differs from the reported value 1.99 by more than 10 %

8 Map-model fit [i](#)

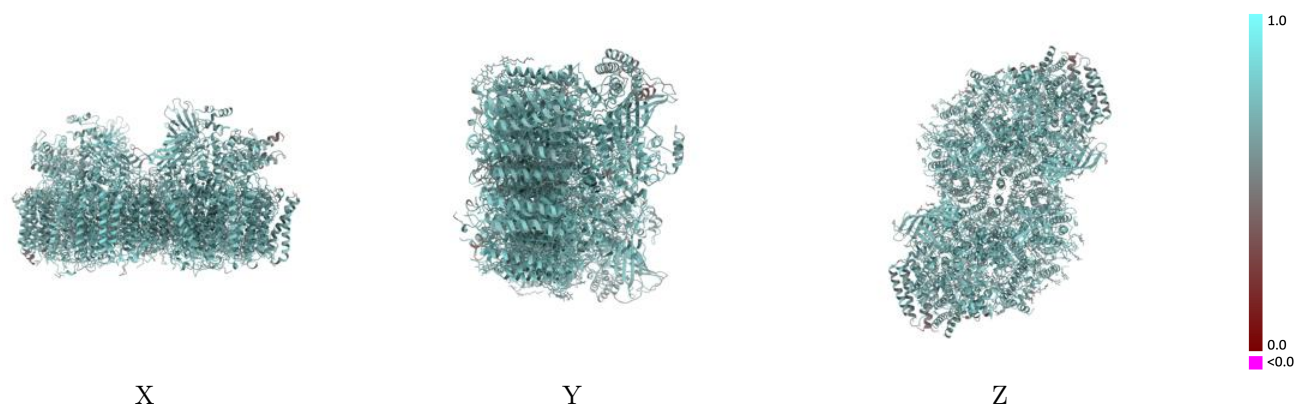
This section contains information regarding the fit between EMDB map EMD-71652 and PDB model 9PHW. Per-residue inclusion information can be found in section ?? on page ??.

8.1 Map-model overlay [i](#)



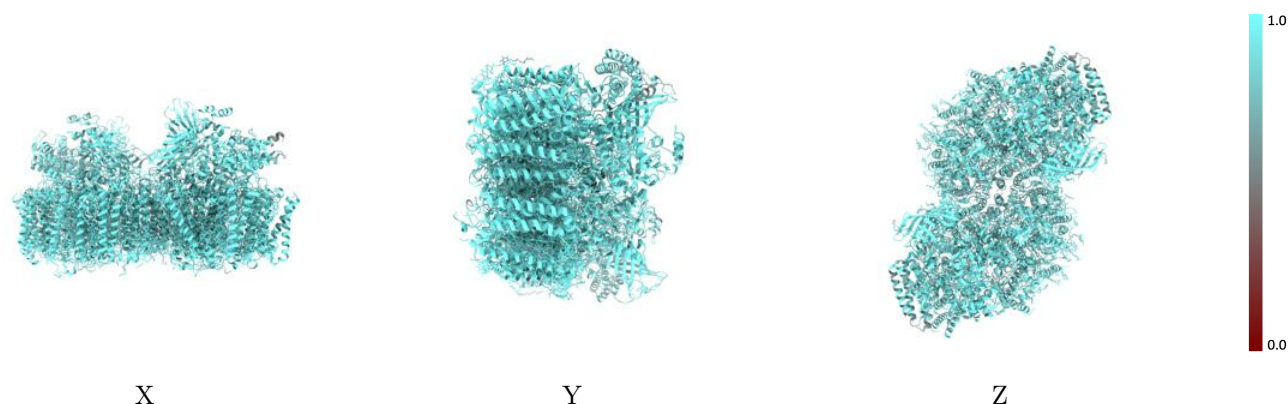
The images above show the 3D surface view of the map at the recommended contour level 0.0022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



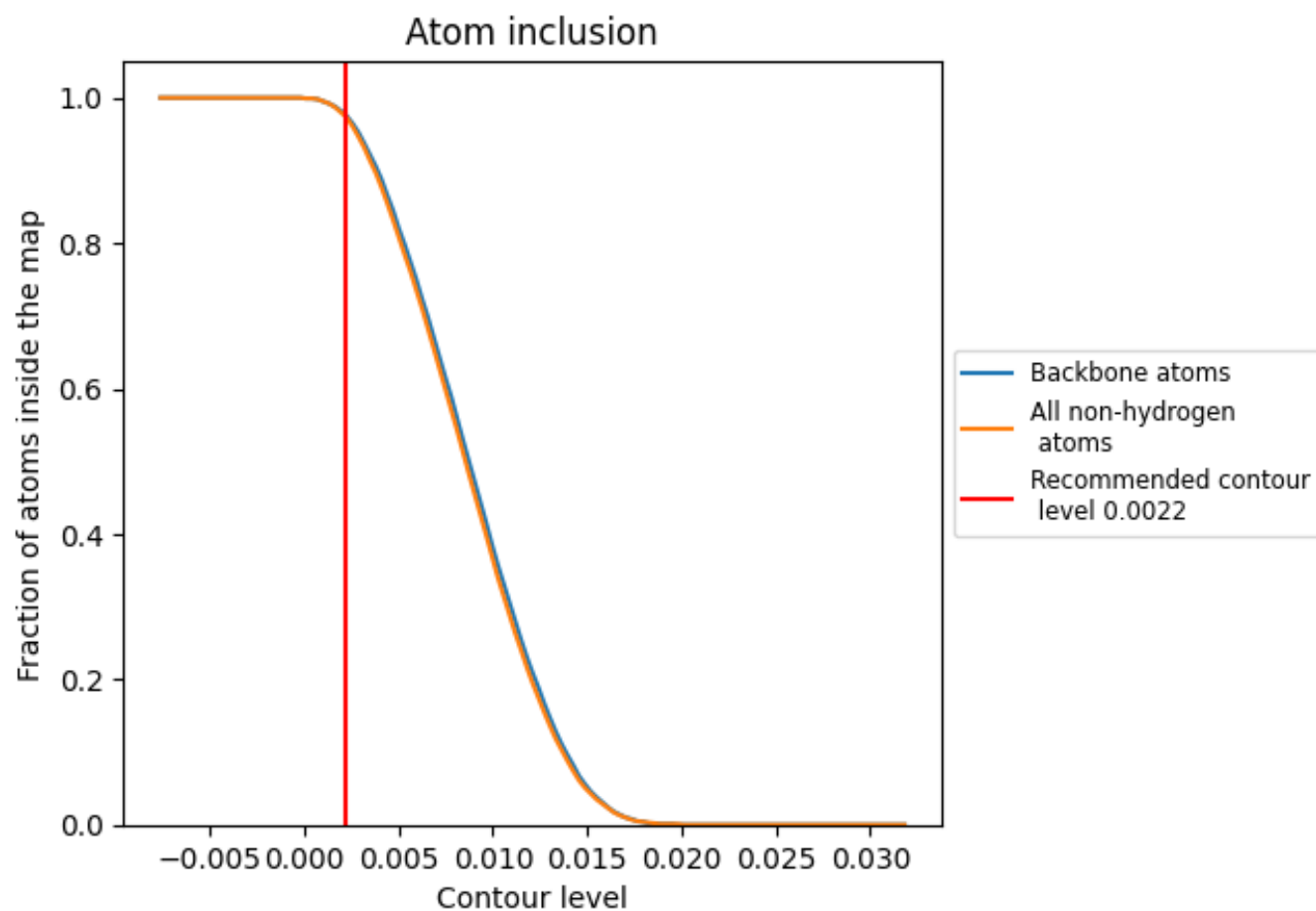
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

8.3 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 (0.0022).







































































8.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ

















The table lists the average atom inclusion at the recommended contour level (0.0022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9740	 0.7110
A	 0.9900	 0.7480
B	 0.9850	 0.7270
C	 0.9860	 0.7190
D	 0.9900	 0.7480
E	 0.9650	 0.6820
F	 0.9680	 0.6830
H	 0.9880	 0.7120
I	 0.9740	 0.6720
J	 0.9630	 0.6790
K	 0.9320	 0.6600
L	 0.9830	 0.7250
M	 0.9740	 0.7100
O	 0.9550	 0.6700
Q	 0.8460	 0.5980
R	 0.9760	 0.6260
T	 0.9690	 0.7090
U	 0.9450	 0.6700
V	 0.9630	 0.6930
X	 0.9890	 0.6870
Y	 0.9620	 0.6460
Z	 0.9720	 0.6500
a	 0.9900	 0.7490
b	 0.9850	 0.7280
c	 0.9860	 0.7190
d	 0.9900	 0.7490
e	 0.9650	 0.6820
f	 0.9680	 0.6860
h	 0.9880	 0.7130
i	 0.9740	 0.6730
j	 0.9630	 0.6810
k	 0.9250	 0.6490
l	 0.9900	 0.7430
m	 0.9810	 0.7260
o	 0.9540	 0.6710



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
q	 0.8450	 0.5980
r	 0.9760	 0.6260
t	 0.9690	 0.7110
u	 0.9460	 0.6720
v	 0.9650	 0.6920
x	 0.9850	 0.6820
y	 0.9660	 0.6470
z	 0.9770	 0.6580