



wwPDB EM Validation Summary Report ⓘ

Nov 3, 2024 – 03:43 PM EST

PDB ID : 7N8O
EMDB ID : EMD-24239
Title : High-resolution structure of photosystem II from the mesophilic cyanobacterium, *Synechocystis* sp. PCC 6803
Authors : Gisriel, C.J.; Brudvig, G.W.
Deposited on : 2021-06-15
Resolution : 1.93 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:

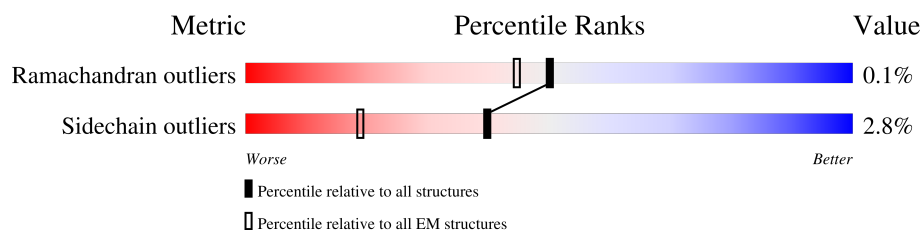
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 1.93 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



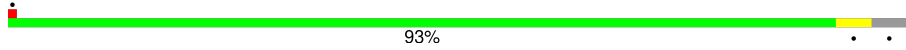


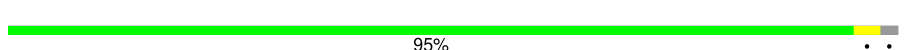
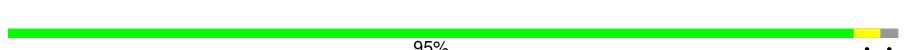
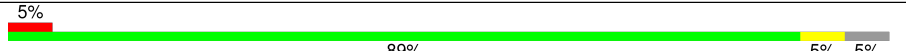
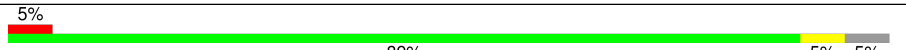
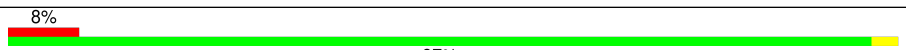
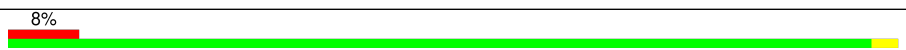
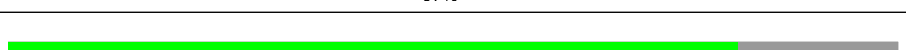
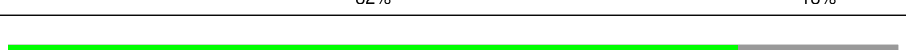
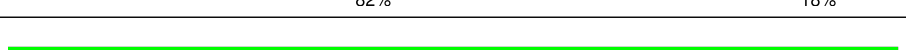
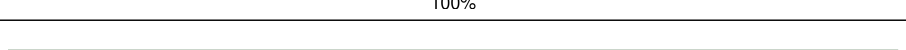
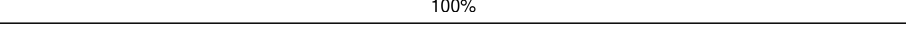
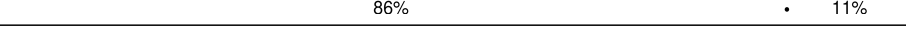
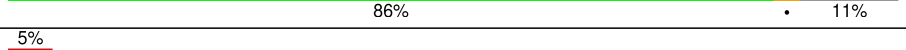
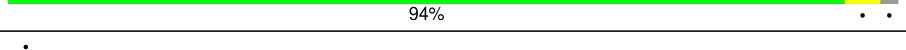
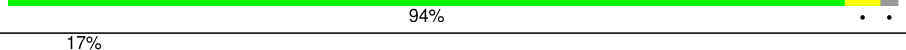



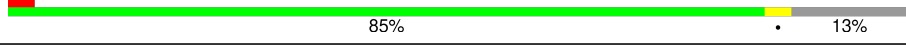
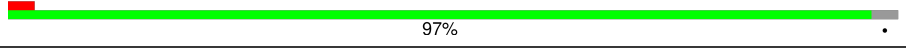
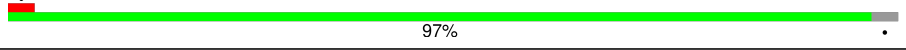

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	360	
1	a	360	
2	B	507	
2	b	507	
3	C	460	
3	c	460	
4	D	352	
4	d	352	
5	E	81	




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Mol	Chain	Length	Quality of chain
5	e	81	
6	F	44	
6	f	44	
7	H	64	
7	h	64	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	45	
10	k	45	
11	L	39	
11	l	39	
12	M	35	
12	m	35	
13	O	247	
13	o	247	
14	Q	149	
14	q	149	
15	R	39	
15	r	39	
16	T	31	
16	t	31	
17	U	131	
17	u	131	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	A	405	X	-	-	-
25	CLA	A	406	X	-	-	-
25	CLA	A	408	X	-	-	-
25	CLA	B	601	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	609	X	-	-	-
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	508	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	511	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	C	514	X	-	-	-
25	CLA	D	401	X	-	-	-
25	CLA	D	403	X	-	-	-
25	CLA	D	404	X	-	-	-
25	CLA	a	405	X	-	-	-
25	CLA	a	406	X	-	-	-
25	CLA	a	408	X	-	-	-
25	CLA	b	601	X	-	-	-
25	CLA	b	602	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	609	X	-	-	-
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25	CLA	b	611	X	-	-	-
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25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	c	502	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-
25	CLA	c	507	X	-	-	-
25	CLA	c	508	X	-	-	-
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	c	513	X	-	-	-
25	CLA	c	514	X	-	-	-
25	CLA	d	401	X	-	-	-
25	CLA	d	403	X	-	-	-
25	CLA	d	404	X	-	-	-
32	BCT	A	417	-	X	-	-
32	BCT	a	417	-	X	-	-

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 54656 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
			2624	1718	429	462	15		
1	a	334	Total	C	N	O	S	0	0
			2624	1718	429	462	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	503	Total	C	N	O	S	0	0
			3935	2570	658	694	13		
2	b	503	Total	C	N	O	S	0	0
			3935	2570	658	694	13		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	341	Total	C	N	O	S	0	0
			2726	1807	443	464	12		
4	d	341	Total	C	N	O	S	0	0
			2726	1807	443	464	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	35	Total	C	N	O	S	0	0
			279	189	46	43	1		
6	f	35	Total	C	N	O	S	0	0
			279	189	46	43	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	36	Total	C	N	O	S	0	0
			286	192	45	48	1		
8	i	36	Total	C	N	O	S	0	0
			286	192	45	48	1		

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	243	Total	C	N	O	S	0	0
			1869	1183	304	379	3		
13	o	243	Total	C	N	O	S	0	0
			1869	1183	304	379	3		

- Molecule 14 is a protein called Sll1638 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	119	Total	C	N	O	S	0	0
			916	576	164	174	2		
14	q	119	Total	C	N	O	S	0	0
			916	576	164	174	2		

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

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

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

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

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

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

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

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

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

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

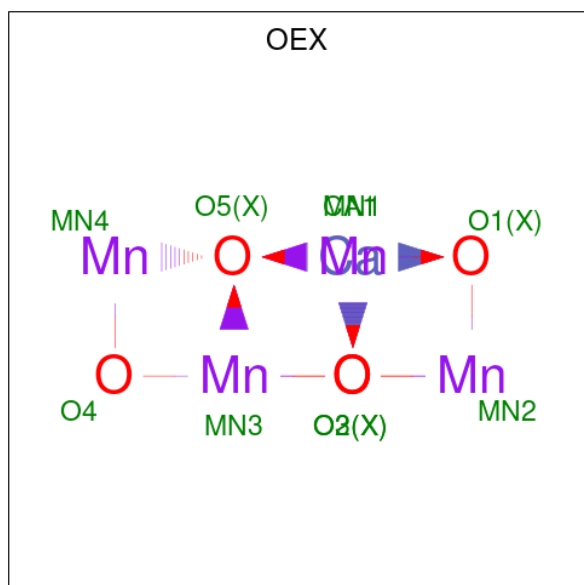
- Molecule 20 is a protein called Photosystem II reaction center protein Ycf12.

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

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

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

- Molecule 22 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: 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 (three-letter code: FE2) (formula: Fe).

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

- Molecule 24 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

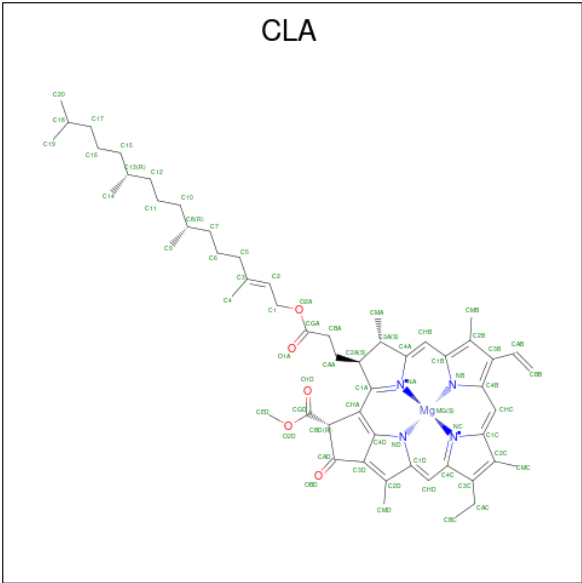
Mol	Chain	Residues	Atoms		AltConf
24	A	2	Total	Cl	0
			2	2	

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

- Molecule 25 is CHLOROPHYLL A (three-letter code: 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	

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Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 55	C 45	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 50	C 40	Mg 1	N 4	O 5	0

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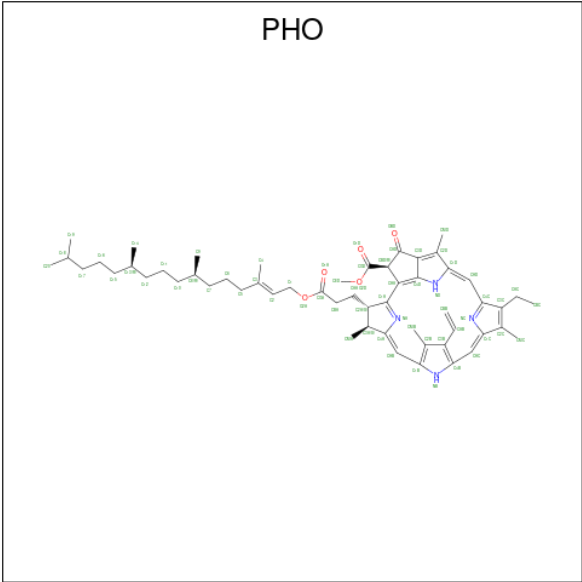
Mol	Chain	Residues	Atoms					AltConf
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	b	1	Total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

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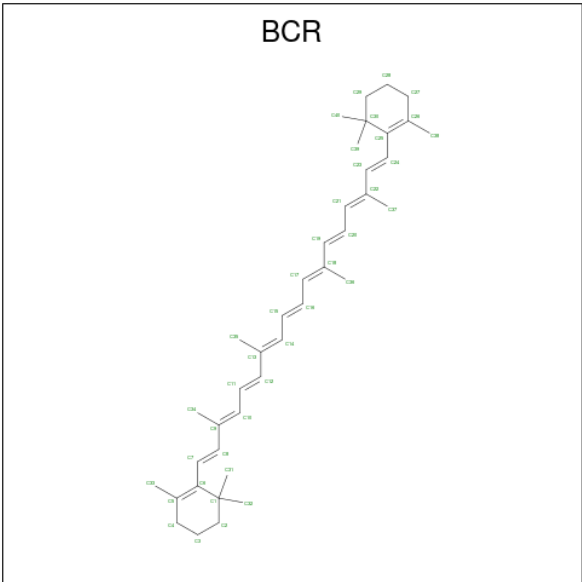
Mol	Chain	Residues	Atoms					AltConf
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 26 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



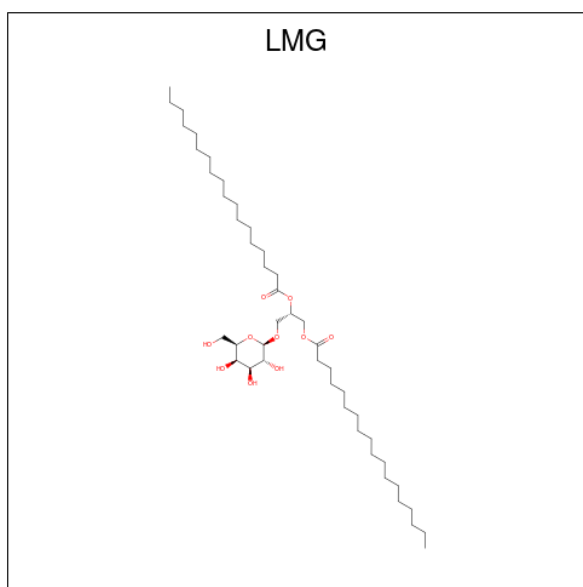
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	N	O	0
			64	55	4	5	
26	D	1	Total	C	N	O	0
			64	55	4	5	
26	a	1	Total	C	N	O	0
			64	55	4	5	
26	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 27 is BETA-CAROTENE (three-letter code: BCR) (formula: 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	k	1	Total C 40 40	0
27	z	1	Total C 40 40	0

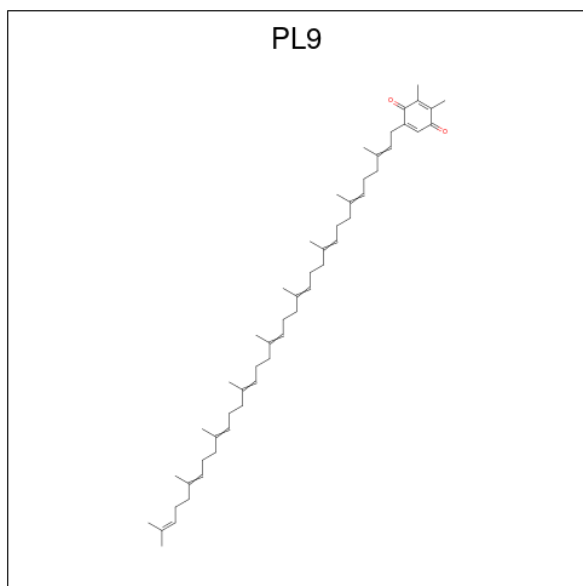
- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



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
			51	41	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
			51	41	10	

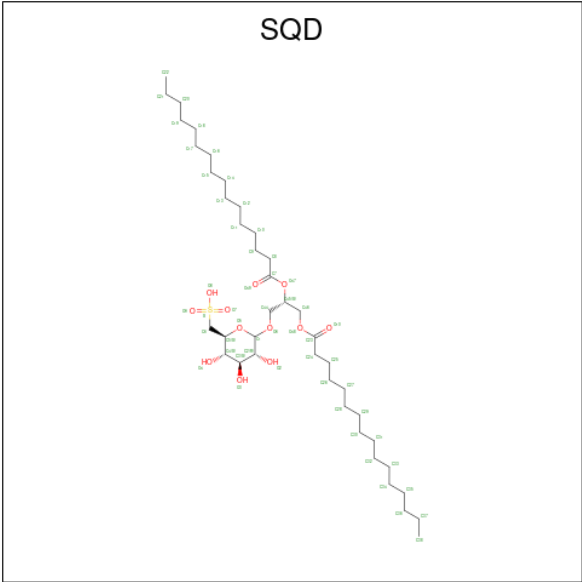
- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula:

C₅₃H₈₀O₂).



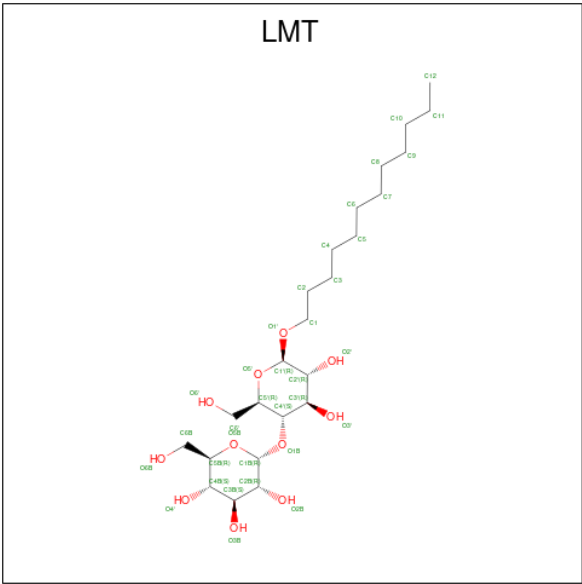
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			55	53	2	
29	D	1	Total	C	O	0
			55	53	2	
29	a	1	Total	C	O	0
			55	53	2	
29	d	1	Total	C	O	0
			55	53	2	

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



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
			48	35	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
			45	36	9		
30	a	1	Total	C	O	S	0
			54	41	12	1	
30	a	1	Total	C	O	S	0
			48	35	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
			45	36	9		

- Molecule 31 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			35	24	11	
31	A	1	Total	C	O	0
			24	18	6	
31	B	1	Total	C	O	0
			24	18	6	
31	B	1	Total	C	O	0
			24	18	6	
31	B	1	Total	C	O	0
			35	24	11	
31	B	1	Total	C	O	0
			24	18	6	
31	B	1	Total	C	O	0
			25	19	6	
31	B	1	Total	C	O	0
			35	24	11	
31	C	1	Total	C	O	0
			28	17	11	
31	C	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	

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

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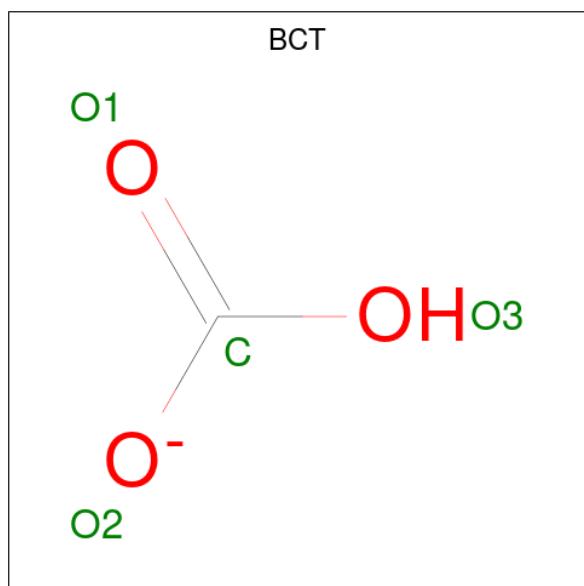
Mol	Chain	Residues	Atoms			AltConf
31	a	1	Total	C	O	0
			24	18	6	
31	b	1	Total	C	O	0
			24	18	6	
31	b	1	Total	C	O	0
			24	18	6	
31	b	1	Total	C	O	0
			35	24	11	
31	b	1	Total	C	O	0
			24	18	6	
31	b	1	Total	C	O	0
			25	19	6	
31	b	1	Total	C	O	0
			35	24	11	
31	c	1	Total	C	O	0
			28	17	11	
31	c	1	Total	C	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	d	1	Total	C	O	0
			24	18	6	
31	d	1	Total	C	O	0
			35	24	11	
31	d	1	Total	C	O	0
			35	24	11	
31	e	1	Total	C	O	0
			22	16	6	
31	e	1	Total	C	O	0
			35	24	11	
31	f	1	Total	C	O	0
			35	24	11	
31	h	1	Total	C	O	0
			24	18	6	
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	

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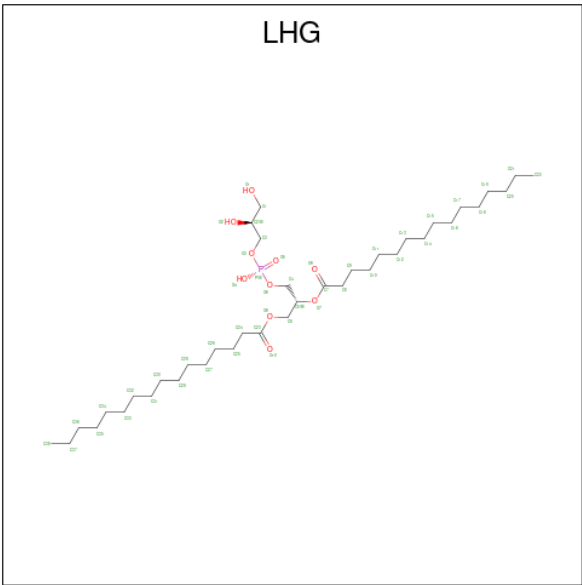
Mol	Chain	Residues	Atoms			AltConf
31	i	1	Total	C	O	0
			22	16	6	
31	j	1	Total	C	O	0
			24	18	6	
31	k	1	Total	C	O	0
			35	24	11	
31	m	1	Total	C	O	0
			24	18	6	
31	t	1	Total	C	O	0
			24	18	6	
31	x	1	Total	C	O	0
			24	18	6	
31	x	1	Total	C	O	0
			22	17	5	
31	y	1	Total	C	O	0
			21	15	6	

- Molecule 32 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



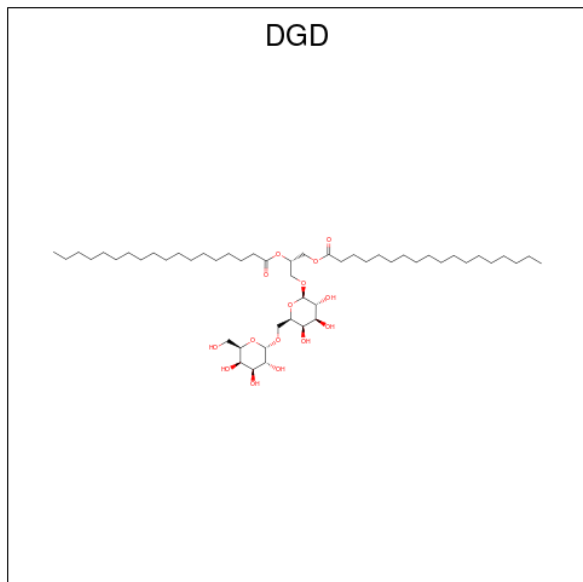
Mol	Chain	Residues	Atoms			AltConf
32	A	1	Total	C	O	0
			4	1	3	
32	a	1	Total	C	O	0
			4	1	3	

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



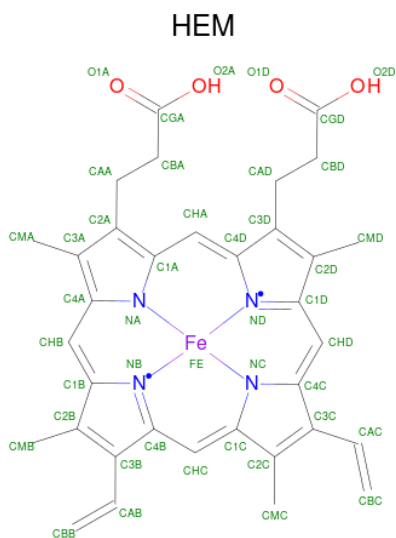
Mol	Chain	Residues	Atoms				AltConf
33	B	1	Total	C	O	P	0
			40	29	10	1	
33	B	1	Total	C	O	P	0
			49	38	10	1	
33	D	1	Total	C	O	P	0
			49	38	10	1	
33	D	1	Total	C	O	P	0
			49	38	10	1	
33	D	1	Total	C	O	P	0
			46	35	10	1	
33	E	1	Total	C	O	P	0
			40	29	10	1	
33	Z	1	Total	C	O	P	0
			36	27	8	1	
33	b	1	Total	C	O	P	0
			40	29	10	1	
33	b	1	Total	C	O	P	0
			49	38	10	1	
33	d	1	Total	C	O	P	0
			49	38	10	1	
33	d	1	Total	C	O	P	0
			49	38	10	1	
33	d	1	Total	C	O	P	0
			46	35	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) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

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

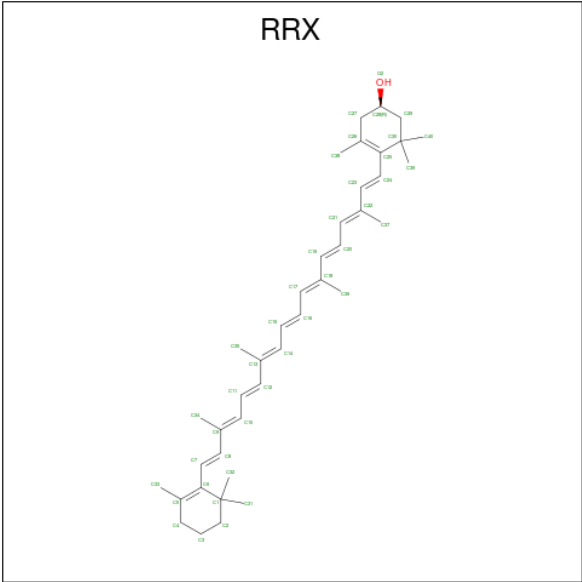


Mol	Chain	Residues	Atoms					AltConf
35	E	1	Total 43	C 34	Fe 1	N 4	O 4	0
35	V	1	Total 43	C 34	Fe 1	N 4	O 4	0
35	e	1	Total 43	C 34	Fe 1	N 4	O 4	0
35	v	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 36 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 37 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: $C_{40}H_{56}O$).



Mol	Chain	Residues	Atoms			AltConf
37	X	1	Total	C	O	0
			41	40	1	
37	x	1	Total	C	O	0
			41	40	1	

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		AltConf
38	A	119	Total	O	0
			119	119	
38	B	114	Total	O	0
			114	114	
38	C	122	Total	O	0
			122	122	
38	D	120	Total	O	0
			120	120	
38	E	13	Total	O	0
			13	13	
38	F	4	Total	O	0
			4	4	
38	H	11	Total	O	0
			11	11	
38	I	2	Total	O	0
			2	2	
38	J	3	Total	O	0
			3	3	
38	K	1	Total	O	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
38	L	9	Total 9	O 9	0
38	M	9	Total 9	O 9	0
38	O	40	Total 40	O 40	0
38	Q	2	Total 2	O 2	0
38	T	11	Total 11	O 11	0
38	U	11	Total 11	O 11	0
38	V	21	Total 21	O 21	0
38	X	7	Total 7	O 7	0
38	a	119	Total 119	O 119	0
38	b	114	Total 114	O 114	0
38	c	122	Total 122	O 122	0
38	d	120	Total 120	O 120	0
38	e	13	Total 13	O 13	0
38	f	4	Total 4	O 4	0
38	h	11	Total 11	O 11	0
38	i	2	Total 2	O 2	0
38	j	3	Total 3	O 3	0
38	k	1	Total 1	O 1	0
38	l	8	Total 8	O 8	0
38	m	8	Total 8	O 8	0
38	o	40	Total 40	O 40	0

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Mol	Chain	Residues	Atoms		AltConf
38	q	2	Total 2	O 2	0
38	t	11	Total 11	O 11	0
38	u	11	Total 11	O 11	0
38	v	21	Total 21	O 21	0
38	x	7	Total 7	O 7	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Photosystem II protein D1 2

Chain A:  92% 7%



- Molecule 1: Photosystem II protein D1 2

Chain a:  92% 7%



- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:  97% ..



- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  97% ..



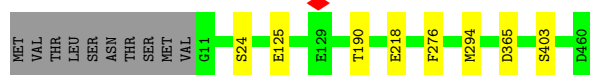
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C:  96% ..



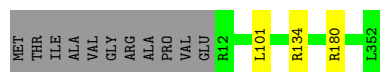
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c:  96% ..



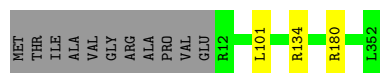
- Molecule 4: Photosystem II D2 protein

Chain D:  96% ..



- Molecule 4: Photosystem II D2 protein

Chain d:  96% ..



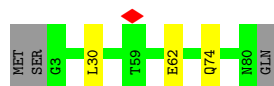
- Molecule 5: Cytochrome b559 subunit alpha

Chain E:  93% ..




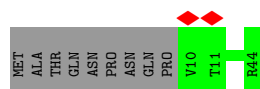
- Molecule 5: Cytochrome b559 subunit alpha

Chain e:  93% ..



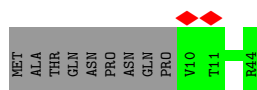
- Molecule 6: Cytochrome b559 subunit beta

Chain F:  5% 80% 20%



- Molecule 6: Cytochrome b559 subunit beta

Chain f:  5% 80% 20%



- Molecule 7: Photosystem II reaction center protein H

Chain H: 95%



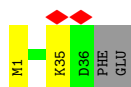
- Molecule 7: Photosystem II reaction center protein H

Chain h: 95%



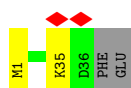
- Molecule 8: Photosystem II reaction center protein I

Chain I: 5% 89% 5% 5%



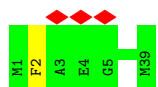
- Molecule 8: Photosystem II reaction center protein I

Chain i: 5% 89% 5% 5%



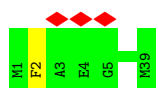
- Molecule 9: Photosystem II reaction center protein J

Chain J: 8% 97%




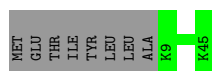
- Molecule 9: Photosystem II reaction center protein J

Chain j: 8% 97%




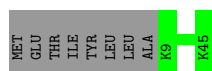
- Molecule 10: Photosystem II reaction center protein K

Chain K:  82% 18%



- Molecule 10: Photosystem II reaction center protein K

Chain k:  82% 18%



- Molecule 11: Photosystem II reaction center protein L

Chain L:  100%

There are no outlier residues recorded for this chain.

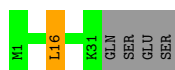
- Molecule 11: Photosystem II reaction center protein L

Chain l:  100%


There are no outlier residues recorded for this chain.

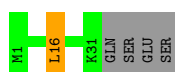
- Molecule 12: Photosystem II reaction center protein M

Chain M:  86% 11%



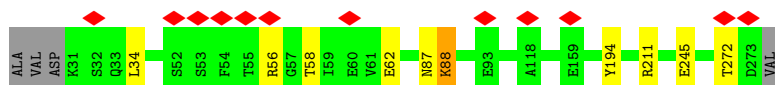
- Molecule 12: Photosystem II reaction center protein M

Chain m:  86% 11%



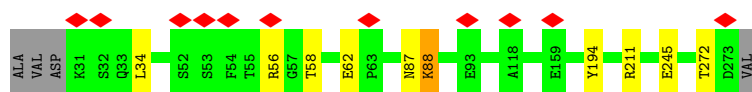
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  5% 94%

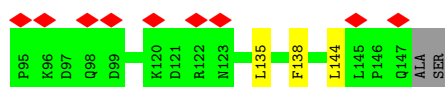
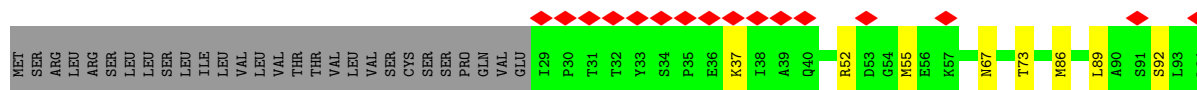
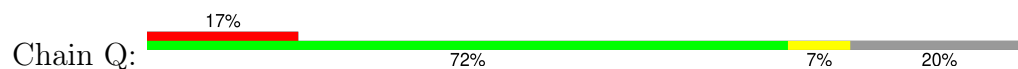


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

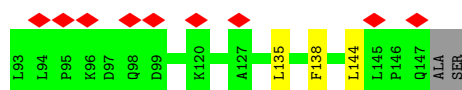
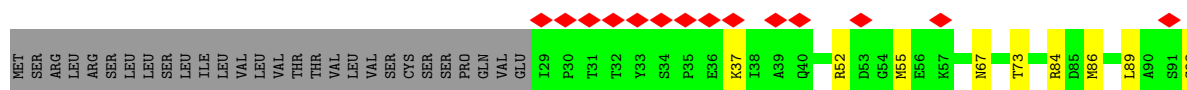
Chain o:  94%



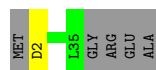
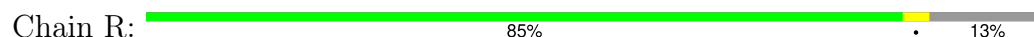
- Molecule 14: Sll1638 protein



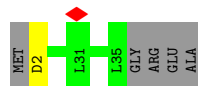
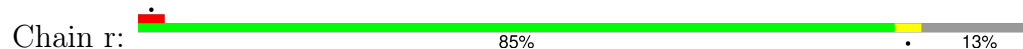
- Molecule 14: Sll1638 protein



- Molecule 15: Photosystem II protein Y



- Molecule 15: Photosystem II protein Y



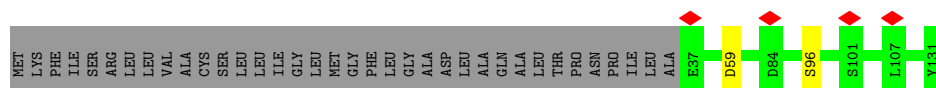
- Molecule 16: Photosystem II reaction center protein T



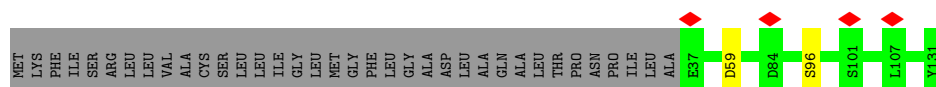
- Molecule 16: Photosystem II reaction center protein T



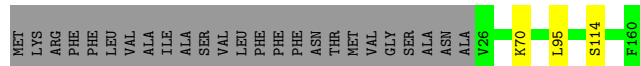
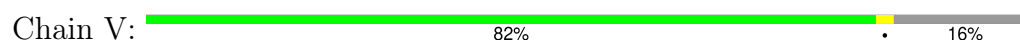
- Molecule 17: Photosystem II 12 kDa extrinsic protein



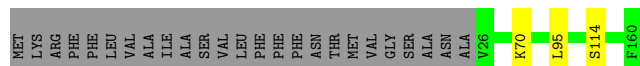
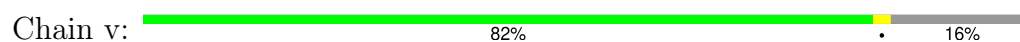
- Molecule 17: Photosystem II 12 kDa extrinsic protein



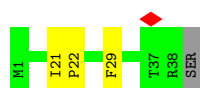
- Molecule 18: Cytochrome c-550



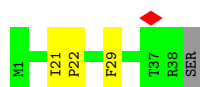
- Molecule 18: Cytochrome c-550



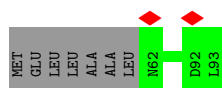
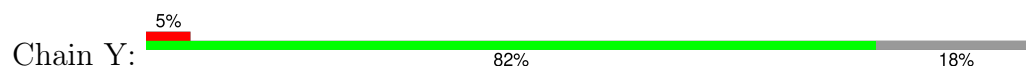
- Molecule 19: Photosystem II reaction center X protein



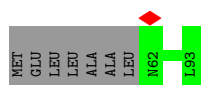
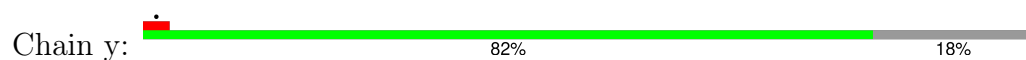
- Molecule 19: Photosystem II reaction center X protein



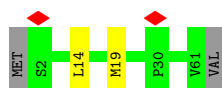
- Molecule 20: Photosystem II reaction center protein Ycf12



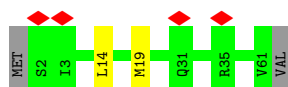
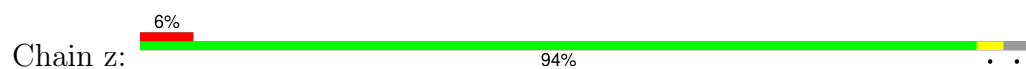
- Molecule 20: Photosystem II reaction center protein Ycf12



- Molecule 21: Photosystem II reaction center protein Z



- Molecule 21: Photosystem II reaction center protein Z



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	202844	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.135	Depositor
Minimum map value	-0.045	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.003	Depositor
Map size (\AA)	319.488, 319.488, 319.488	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.832, 0.832, 0.832	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.41	0/2709	0.51	0/3694
1	a	0.41	0/2709	0.51	0/3694
2	B	0.38	0/4068	0.51	1/5538 (0.0%)
2	b	0.38	0/4068	0.51	1/5538 (0.0%)
3	C	0.37	0/3608	0.50	0/4912
3	c	0.37	0/3608	0.50	0/4912
4	D	0.38	0/2823	0.50	0/3843
4	d	0.38	0/2823	0.50	0/3843
5	E	0.35	0/664	0.51	0/906
5	e	0.35	0/664	0.51	0/906
6	F	0.33	0/288	0.45	0/393
6	f	0.32	0/288	0.45	0/393
7	H	0.33	0/506	0.50	0/687
7	h	0.33	0/506	0.50	0/687
8	I	0.32	0/282	0.49	0/381
8	i	0.32	0/282	0.49	0/381
9	J	0.33	0/278	0.49	0/375
9	j	0.33	0/278	0.49	0/375
10	K	0.37	0/310	0.53	0/424
10	k	0.37	0/310	0.53	0/424
11	L	0.38	0/322	0.46	0/435
11	l	0.38	0/322	0.46	0/435
12	M	0.34	0/239	0.62	1/325 (0.3%)
12	m	0.34	0/239	0.62	1/325 (0.3%)
13	O	0.38	0/1907	0.59	0/2586
13	o	0.38	0/1907	0.59	0/2586
14	Q	0.28	0/930	0.44	0/1257
14	q	0.28	0/930	0.44	0/1257
15	R	0.26	0/262	0.45	0/361
15	r	0.26	0/262	0.45	0/361
16	T	0.33	0/236	0.46	0/321

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	t	0.34	0/236	0.46	0/321
17	U	0.34	0/751	0.48	0/1018
17	u	0.34	0/751	0.48	0/1018
18	V	0.31	0/1086	0.51	0/1476
18	v	0.31	0/1086	0.51	0/1476
19	X	0.31	0/293	0.53	0/399
19	x	0.31	0/293	0.53	0/399
20	Y	0.29	0/247	0.45	0/335
20	y	0.29	0/247	0.45	0/335
21	Z	0.32	0/472	0.45	0/649
21	z	0.32	0/472	0.45	0/649
All	All	0.37	0/44562	0.51	4/60630 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
13	O	0	1
13	o	0	1
19	X	0	1
19	x	0	1
All	All	0	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	121	GLU	CA-CB-CG	8.44	131.97	113.40
2	B	121	GLU	CA-CB-CG	8.43	131.95	113.40
12	M	16	LEU	CA-CB-CG	6.87	131.09	115.30
12	m	16	LEU	CA-CB-CG	6.86	131.07	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	O	88	LYS	Peptide
19	X	21	ILE	Peptide
13	o	88	LYS	Peptide

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Mol	Chain	Res	Type	Group
19	x	21	ILE	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/360 (92%)	326 (98%)	6 (2%)	0	100	100
1	a	332/360 (92%)	326 (98%)	6 (2%)	0	100	100
2	B	501/507 (99%)	492 (98%)	9 (2%)	0	100	100
2	b	501/507 (99%)	492 (98%)	9 (2%)	0	100	100
3	C	448/460 (97%)	438 (98%)	10 (2%)	0	100	100
3	c	448/460 (97%)	438 (98%)	10 (2%)	0	100	100
4	D	339/352 (96%)	332 (98%)	7 (2%)	0	100	100
4	d	339/352 (96%)	332 (98%)	7 (2%)	0	100	100
5	E	76/81 (94%)	73 (96%)	3 (4%)	0	100	100
5	e	76/81 (94%)	73 (96%)	3 (4%)	0	100	100
6	F	33/44 (75%)	30 (91%)	3 (9%)	0	100	100
6	f	33/44 (75%)	30 (91%)	3 (9%)	0	100	100
7	H	61/64 (95%)	59 (97%)	2 (3%)	0	100	100
7	h	61/64 (95%)	59 (97%)	2 (3%)	0	100	100
8	I	34/38 (90%)	34 (100%)	0	0	100	100
8	i	34/38 (90%)	34 (100%)	0	0	100	100
9	J	37/39 (95%)	37 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	j	37/39 (95%)	37 (100%)	0	0	100	100
10	K	35/45 (78%)	34 (97%)	1 (3%)	0	100	100
10	k	35/45 (78%)	34 (97%)	1 (3%)	0	100	100
11	L	37/39 (95%)	37 (100%)	0	0	100	100
11	l	37/39 (95%)	37 (100%)	0	0	100	100
12	M	29/35 (83%)	28 (97%)	1 (3%)	0	100	100
12	m	29/35 (83%)	28 (97%)	1 (3%)	0	100	100
13	O	241/247 (98%)	219 (91%)	21 (9%)	1 (0%)	30	22
13	o	241/247 (98%)	219 (91%)	21 (9%)	1 (0%)	30	22
14	Q	117/149 (78%)	114 (97%)	3 (3%)	0	100	100
14	q	117/149 (78%)	114 (97%)	3 (3%)	0	100	100
15	R	32/39 (82%)	32 (100%)	0	0	100	100
15	r	32/39 (82%)	32 (100%)	0	0	100	100
16	T	28/31 (90%)	26 (93%)	2 (7%)	0	100	100
16	t	28/31 (90%)	26 (93%)	2 (7%)	0	100	100
17	U	93/131 (71%)	88 (95%)	5 (5%)	0	100	100
17	u	93/131 (71%)	88 (95%)	5 (5%)	0	100	100
18	V	133/160 (83%)	129 (97%)	4 (3%)	0	100	100
18	v	133/160 (83%)	129 (97%)	4 (3%)	0	100	100
19	X	36/39 (92%)	34 (94%)	1 (3%)	1 (3%)	4	0
19	x	36/39 (92%)	34 (94%)	1 (3%)	1 (3%)	4	0
20	Y	30/39 (77%)	30 (100%)	0	0	100	100
20	y	30/39 (77%)	30 (100%)	0	0	100	100
21	Z	58/62 (94%)	54 (93%)	4 (7%)	0	100	100
21	z	58/62 (94%)	54 (93%)	4 (7%)	0	100	100
All	All	5460/5922 (92%)	5292 (97%)	164 (3%)	4 (0%)	50	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	87	ASN
13	o	87	ASN
19	X	22	PRO

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Mol	Chain	Res	Type
19	x	22	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	273/293 (93%)	269 (98%)	4 (2%)	60	52
1	a	273/293 (93%)	269 (98%)	4 (2%)	60	52
2	B	401/404 (99%)	391 (98%)	10 (2%)	42	30
2	b	401/404 (99%)	391 (98%)	10 (2%)	42	30
3	C	351/361 (97%)	343 (98%)	8 (2%)	45	33
3	c	351/361 (97%)	343 (98%)	8 (2%)	45	33
4	D	277/285 (97%)	274 (99%)	3 (1%)	70	64
4	d	277/285 (97%)	274 (99%)	3 (1%)	70	64
5	E	70/73 (96%)	67 (96%)	3 (4%)	25	11
5	e	70/73 (96%)	67 (96%)	3 (4%)	25	11
6	F	28/37 (76%)	28 (100%)	0	100	100
6	f	28/37 (76%)	28 (100%)	0	100	100
7	H	53/54 (98%)	51 (96%)	2 (4%)	28	14
7	h	53/54 (98%)	51 (96%)	2 (4%)	28	14
8	I	31/33 (94%)	30 (97%)	1 (3%)	34	22
8	i	31/33 (94%)	30 (97%)	1 (3%)	34	22
9	J	24/24 (100%)	23 (96%)	1 (4%)	25	12
9	j	24/24 (100%)	23 (96%)	1 (4%)	25	12
10	K	31/38 (82%)	31 (100%)	0	100	100
10	k	31/38 (82%)	31 (100%)	0	100	100
11	L	36/36 (100%)	36 (100%)	0	100	100
11	l	36/36 (100%)	36 (100%)	0	100	100
12	M	27/31 (87%)	26 (96%)	1 (4%)	29	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	m	27/31 (87%)	26 (96%)	1 (4%)	29	16
13	O	206/210 (98%)	197 (96%)	9 (4%)	24	11
13	o	206/210 (98%)	197 (96%)	9 (4%)	24	11
14	Q	93/128 (73%)	82 (88%)	11 (12%)	4	0
14	q	93/128 (73%)	81 (87%)	12 (13%)	3	0
15	R	26/29 (90%)	25 (96%)	1 (4%)	28	14
15	r	26/29 (90%)	25 (96%)	1 (4%)	28	14
16	T	24/25 (96%)	24 (100%)	0	100	100
16	t	24/25 (96%)	24 (100%)	0	100	100
17	U	83/111 (75%)	81 (98%)	2 (2%)	44	32
17	u	83/111 (75%)	81 (98%)	2 (2%)	44	32
18	V	117/137 (85%)	114 (97%)	3 (3%)	41	28
18	v	117/137 (85%)	114 (97%)	3 (3%)	41	28
19	X	32/33 (97%)	31 (97%)	1 (3%)	35	22
19	x	32/33 (97%)	31 (97%)	1 (3%)	35	22
20	Y	25/30 (83%)	25 (100%)	0	100	100
20	y	25/30 (83%)	25 (100%)	0	100	100
21	Z	49/52 (94%)	47 (96%)	2 (4%)	26	12
21	z	49/52 (94%)	47 (96%)	2 (4%)	26	12
All	All	4514/4848 (93%)	4389 (97%)	125 (3%)	40	25

5 of 125 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	V	95	LEU
14	q	86	MET
2	b	291	GLN
14	q	84	ARG
17	u	96	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 86 such sidechains are listed below:

Mol	Chain	Res	Type
3	c	309	GLN

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Mol	Chain	Res	Type
13	o	176	ASN
3	c	375	GLN
7	h	50	ASN
14	q	67	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	I	1	8	8,9,10	0.98	0	8,9,11	1.04	1 (12%)
8	FME	i	1	8	8,9,10	0.98	0	8,9,11	1.04	1 (12%)
9	FME	j	1	9	6,7,10	0.84	0	2,7,11	0.69	0
16	FME	t	1	16	8,9,10	0.97	0	8,9,11	0.93	0
9	FME	J	1	9	6,7,10	0.84	0	2,7,11	0.69	0
16	FME	T	1	16	8,9,10	0.98	0	8,9,11	0.92	0
12	FME	m	1	12	8,9,10	0.99	0	8,9,11	0.90	0
12	FME	M	1	12	8,9,10	0.99	0	8,9,11	0.90	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	I	1	8	-	0/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
9	FME	j	1	9	-	1/5/6/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	FME	t	1	16	-	1/7/9/11	-
9	FME	J	1	9	-	1/5/6/11	-
16	FME	T	1	16	-	1/7/9/11	-
12	FME	m	1	12	-	2/7/9/11	-
12	FME	M	1	12	-	2/7/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	C-CA-N	2.27	113.88	109.50
8	I	1	FME	C-CA-N	2.27	113.87	109.50

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	1	FME	N-CA-CB-CG
12	m	1	FME	N-CA-CB-CG
16	T	1	FME	N-CA-CB-CG
16	t	1	FME	N-CA-CB-CG
12	M	1	FME	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 228 ligands modelled in this entry, 12 are monoatomic - leaving 216 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	$\# Z > 2$
31	LMT	b	626	-	24,24,36	1.04	2 (8%)	29,29,47	1.14	2 (6%)
25	CLA	B	612	-	63,73,73	2.19	18 (28%)	74,113,113	2.53	23 (31%)
30	SQD	C	501	-	52,54,54	0.94	4 (7%)	62,65,65	1.58	10 (16%)
30	SQD	k	101	-	45,45,54	1.02	4 (8%)	53,53,65	1.39	7 (13%)
33	LHG	D	406	-	48,48,48	0.93	2 (4%)	51,54,54	1.11	3 (5%)
33	LHG	z	102	-	35,35,48	1.11	2 (5%)	38,40,54	1.32	6 (15%)
25	CLA	b	610	-	63,73,73	2.23	18 (28%)	74,113,113	2.52	24 (32%)
25	CLA	D	404	-	63,73,73	2.21	19 (30%)	74,113,113	2.51	23 (31%)
25	CLA	C	513	-	48,58,73	2.61	18 (37%)	56,95,113	2.74	22 (39%)
25	CLA	b	608	-	63,73,73	2.24	19 (30%)	74,113,113	2.37	22 (29%)
33	LHG	D	407	-	48,48,48	0.90	3 (6%)	51,54,54	0.99	3 (5%)
25	CLA	b	615	-	63,73,73	2.19	19 (30%)	74,113,113	2.45	25 (33%)
30	SQD	c	501	-	52,54,54	0.93	4 (7%)	62,65,65	1.58	10 (16%)
25	CLA	B	603	-	63,73,73	2.28	18 (28%)	74,113,113	2.49	23 (31%)
35	HEM	v	201	18	42,50,50	1.43	4 (9%)	46,82,82	1.43	7 (15%)
31	LMT	c	522	-	24,24,36	1.03	2 (8%)	29,29,47	1.10	1 (3%)
33	LHG	d	406	-	48,48,48	0.92	2 (4%)	51,54,54	1.11	3 (5%)
31	LMT	I	101	-	24,24,36	1.10	3 (12%)	29,29,47	1.16	2 (6%)
33	LHG	b	622	-	39,39,48	1.04	2 (5%)	42,45,54	1.10	3 (7%)
31	LMT	k	105	-	36,36,36	1.11	5 (13%)	47,47,47	0.99	2 (4%)
25	CLA	d	404	-	63,73,73	2.21	19 (30%)	74,113,113	2.50	23 (31%)
25	CLA	C	507	-	63,73,73	2.26	19 (30%)	74,113,113	2.46	24 (32%)
27	BCR	B	619	-	41,41,41	2.66	6 (14%)	56,56,56	6.62	23 (41%)
28	LMG	B	621	-	51,51,55	1.45	8 (15%)	59,59,63	1.28	5 (8%)
26	PHO	D	402	-	50,69,69	1.02	5 (10%)	48,99,99	1.24	5 (10%)
31	LMT	D	411	-	36,36,36	1.05	4 (11%)	47,47,47	1.22	4 (8%)
31	LMT	i	103	-	36,36,36	1.14	6 (16%)	47,47,47	1.11	3 (6%)
25	CLA	b	611	-	63,73,73	2.20	17 (26%)	74,113,113	2.41	23 (31%)
25	CLA	C	503	-	63,73,73	2.25	18 (28%)	74,113,113	2.47	24 (32%)
34	DGD	C	518	-	63,63,67	1.32	8 (12%)	77,77,81	1.02	3 (3%)
25	CLA	A	405	-	63,73,73	2.15	18 (28%)	74,113,113	2.61	26 (35%)
27	BCR	b	617	-	41,41,41	2.69	6 (14%)	56,56,56	6.57	25 (44%)
34	DGD	H	103	-	63,63,67	1.31	8 (12%)	77,77,81	0.97	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	OEX	a	401	1,38,3	0,15,15	-	-	-		
31	LMT	E	103	-	36,36,36	1.20	4 (11%)	47,47,47	1.14	4 (8%)
33	LHG	E	102	-	39,39,48	1.02	2 (5%)	42,45,54	1.09	3 (7%)
25	CLA	c	511	-	63,73,73	2.26	19 (30%)	74,113,113	2.47	25 (33%)
26	PHO	A	407	-	50,69,69	1.05	3 (6%)	48,99,99	1.23	5 (10%)
25	CLA	c	512	3	63,73,73	2.22	17 (26%)	74,113,113	2.56	23 (31%)
31	LMT	M	101	-	36,36,36	1.17	6 (16%)	47,47,47	0.96	0
27	BCR	Z	101	-	41,41,41	2.67	7 (17%)	56,56,56	6.48	19 (33%)
27	BCR	k	102	-	41,41,41	2.61	6 (14%)	56,56,56	6.94	24 (42%)
31	LMT	T	701	-	24,24,36	1.08	3 (12%)	29,29,47	1.27	3 (10%)
25	CLA	C	504	-	63,73,73	2.26	20 (31%)	74,113,113	2.55	26 (35%)
31	LMT	D	410	-	24,24,36	1.02	3 (12%)	29,29,47	1.34	4 (13%)
29	PL9	D	405	-	55,55,55	1.57	8 (14%)	68,69,69	1.50	13 (19%)
30	SQD	A	412	-	52,54,54	0.98	4 (7%)	62,65,65	1.59	10 (16%)
31	LMT	B	627	-	25,25,36	1.03	3 (12%)	30,30,47	1.15	2 (6%)
25	CLA	c	514	-	63,73,73	2.26	19 (30%)	74,113,113	2.50	24 (32%)
31	LMT	A	415	-	36,36,36	1.23	6 (16%)	47,47,47	1.45	4 (8%)
33	LHG	e	102	-	39,39,48	1.02	2 (5%)	42,45,54	1.09	3 (7%)
27	BCR	z	101	-	41,41,41	2.67	7 (17%)	56,56,56	6.48	21 (37%)
31	LMT	m	101	-	24,24,36	1.07	2 (8%)	29,29,47	1.08	2 (6%)
25	CLA	b	614	-	63,73,73	2.22	18 (28%)	74,113,113	2.55	23 (31%)
34	DGD	C	516	-	63,63,67	1.33	8 (12%)	77,77,81	0.99	3 (3%)
27	BCR	K	102	-	41,41,41	2.61	6 (14%)	56,56,56	6.94	24 (42%)
25	CLA	D	403	-	63,73,73	2.22	19 (30%)	74,113,113	2.57	23 (31%)
25	CLA	B	608	-	63,73,73	2.24	19 (30%)	74,113,113	2.37	22 (29%)
34	DGD	c	516	-	63,63,67	1.33	8 (12%)	77,77,81	0.99	3 (3%)
25	CLA	B	605	-	63,73,73	2.19	18 (28%)	74,113,113	2.50	23 (31%)
37	RRX	X	102	-	42,42,42	1.32	8 (19%)	56,58,58	1.46	10 (17%)
25	CLA	b	606	-	58,68,73	2.31	18 (31%)	68,107,113	2.54	24 (35%)
28	LMG	a	410	-	51,51,55	1.45	8 (15%)	59,59,63	1.24	5 (8%)
25	CLA	b	607	38	63,73,73	2.23	18 (28%)	74,113,113	2.43	24 (32%)
27	BCR	F	101	-	41,41,41	2.64	7 (17%)	56,56,56	6.65	20 (35%)
25	CLA	B	615	-	63,73,73	2.20	19 (30%)	74,113,113	2.45	25 (33%)
31	LMT	c	524	-	36,36,36	1.11	5 (13%)	47,47,47	1.08	2 (4%)
31	LMT	c	520	-	29,29,36	1.25	5 (17%)	40,40,47	0.96	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	BCR	k	103	-	41,41,41	2.64	6 (14%)	56,56,56	6.69	22 (39%)
25	CLA	B	613	-	63,73,73	2.20	19 (30%)	74,113,113	2.54	20 (27%)
25	CLA	B	606	-	58,68,73	2.31	18 (31%)	68,107,113	2.54	24 (35%)
27	BCR	a	409	-	41,41,41	2.67	6 (14%)	56,56,56	6.57	19 (33%)
29	PL9	a	411	-	55,55,55	1.09	3 (5%)	68,69,69	1.56	12 (17%)
25	CLA	C	509	-	63,73,73	2.21	20 (31%)	74,113,113	2.48	24 (32%)
25	CLA	A	406	38	63,73,73	2.19	18 (28%)	74,113,113	2.56	22 (29%)
32	BCT	a	417	23	3,3,3	1.58	1 (33%)	2,3,3	4.03	2 (100%)
25	CLA	c	505	38	63,73,73	2.26	20 (31%)	74,113,113	2.51	26 (35%)
25	CLA	a	406	38	63,73,73	2.19	18 (28%)	74,113,113	2.55	22 (29%)
31	LMT	X	101	-	24,24,36	1.05	3 (12%)	29,29,47	1.11	2 (6%)
31	LMT	I	103	-	36,36,36	1.14	5 (13%)	47,47,47	1.11	3 (6%)
31	LMT	b	625	-	36,36,36	1.22	5 (13%)	47,47,47	1.05	3 (6%)
27	BCR	B	618	-	41,41,41	2.64	6 (14%)	56,56,56	6.57	18 (32%)
25	CLA	B	610	-	63,73,73	2.23	18 (28%)	74,113,113	2.52	24 (32%)
25	CLA	B	607	38	63,73,73	2.23	18 (28%)	74,113,113	2.43	24 (32%)
27	BCR	A	409	-	41,41,41	2.67	6 (14%)	56,56,56	6.57	19 (33%)
31	LMT	C	522	-	24,24,36	1.02	2 (8%)	29,29,47	1.10	1 (3%)
25	CLA	c	513	-	48,58,73	2.61	18 (37%)	56,95,113	2.74	22 (39%)
30	SQD	a	413	-	46,48,54	1.01	4 (8%)	56,59,65	1.78	15 (26%)
31	LMT	I	102	-	24,24,36	1.07	3 (12%)	29,29,47	1.38	3 (10%)
25	CLA	C	514	-	63,73,73	2.26	19 (30%)	74,113,113	2.51	24 (32%)
25	CLA	b	604	-	63,73,73	2.21	18 (28%)	74,113,113	2.54	23 (31%)
25	CLA	d	401	38	63,73,73	2.20	18 (28%)	74,113,113	2.44	22 (29%)
31	LMT	e	103	-	36,36,36	1.20	4 (11%)	47,47,47	1.15	4 (8%)
27	BCR	c	515	-	41,41,41	2.71	6 (14%)	56,56,56	6.65	19 (33%)
31	LMT	B	626	-	24,24,36	1.03	2 (8%)	29,29,47	1.14	2 (6%)
25	CLA	B	614	-	63,73,73	2.22	18 (28%)	74,113,113	2.55	23 (31%)
25	CLA	b	605	-	63,73,73	2.19	18 (28%)	74,113,113	2.50	22 (29%)
31	LMT	D	412	-	36,36,36	1.20	6 (16%)	47,47,47	0.96	2 (4%)
31	LMT	b	627	-	25,25,36	1.03	3 (12%)	30,30,47	1.15	2 (6%)
37	RRX	x	102	-	42,42,42	1.32	8 (19%)	56,58,58	1.46	10 (17%)
25	CLA	C	502	-	63,73,73	2.31	20 (31%)	74,113,113	2.34	25 (33%)
31	LMT	H	101	-	24,24,36	1.02	2 (8%)	29,29,47	1.02	2 (6%)
27	BCR	K	103	-	41,41,41	2.64	6 (14%)	56,56,56	6.69	22 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LHG	B	628	-	48,48,48	0.92	3 (6%)	51,54,54	0.98	3 (5%)
25	CLA	d	403	-	63,73,73	2.22	19 (30%)	74,113,113	2.57	23 (31%)
31	LMT	d	412	-	36,36,36	1.20	6 (16%)	47,47,47	0.96	2 (4%)
31	LMT	C	520	-	29,29,36	1.25	5 (17%)	40,40,47	0.96	2 (5%)
31	LMT	Y	101	-	21,21,36	1.09	3 (14%)	26,26,47	1.15	2 (7%)
25	CLA	B	602	-	63,73,73	2.23	18 (28%)	74,113,113	2.52	25 (33%)
31	LMT	e	101	-	22,22,36	1.11	3 (13%)	27,27,47	1.11	1 (3%)
31	LMT	t	701	-	24,24,36	1.08	3 (12%)	29,29,47	1.26	3 (10%)
30	SQD	B	620	-	52,54,54	0.95	3 (5%)	62,65,65	1.64	11 (17%)
29	PL9	A	411	-	55,55,55	1.09	3 (5%)	68,69,69	1.56	12 (17%)
25	CLA	C	506	-	53,63,73	2.45	18 (33%)	62,101,113	2.62	22 (35%)
33	LHG	Z	102	-	35,35,48	1.11	2 (5%)	38,40,54	1.31	6 (15%)
31	LMT	I	104	-	22,22,36	1.08	3 (13%)	27,27,47	1.15	2 (7%)
28	LMG	A	414	-	36,36,55	1.11	2 (5%)	44,44,63	1.17	4 (9%)
35	HEM	V	201	18	42,50,50	1.42	4 (9%)	46,82,82	1.43	7 (15%)
25	CLA	b	609	-	63,73,73	2.23	18 (28%)	74,113,113	2.51	21 (28%)
31	LMT	E	101	-	22,22,36	1.11	3 (13%)	27,27,47	1.11	1 (3%)
25	CLA	B	601	38	43,53,73	2.54	17 (39%)	50,89,113	2.88	19 (38%)
31	LMT	y	101	-	21,21,36	1.09	3 (14%)	26,26,47	1.15	2 (7%)
35	HEM	E	104	6	42,50,50	1.57	4 (9%)	46,82,82	1.41	5 (10%)
28	LMG	a	414	-	36,36,55	1.11	2 (5%)	44,44,63	1.17	4 (9%)
25	CLA	b	603	-	63,73,73	2.28	18 (28%)	74,113,113	2.49	23 (31%)
25	CLA	b	601	38	43,53,73	2.54	17 (39%)	50,89,113	2.88	19 (38%)
31	LMT	A	416	-	24,24,36	1.03	3 (12%)	29,29,47	0.95	0
33	LHG	b	628	-	48,48,48	0.92	3 (6%)	51,54,54	0.98	3 (5%)
25	CLA	c	502	-	63,73,73	2.31	20 (31%)	74,113,113	2.35	25 (33%)
25	CLA	B	604	-	63,73,73	2.21	18 (28%)	74,113,113	2.54	23 (31%)
31	LMT	h	101	-	24,24,36	1.03	2 (8%)	29,29,47	1.02	2 (6%)
27	BCR	b	619	-	41,41,41	2.66	6 (14%)	56,56,56	6.61	23 (41%)
31	LMT	B	629	-	36,36,36	1.15	5 (13%)	47,47,47	0.94	1 (2%)
30	SQD	f	102	-	32,34,54	1.23	4 (12%)	42,45,65	1.88	10 (23%)
33	LHG	d	408	-	45,45,48	0.95	2 (4%)	48,51,54	1.00	2 (4%)
31	LMT	C	524	-	36,36,36	1.11	5 (13%)	47,47,47	1.08	2 (4%)
33	LHG	D	408	-	45,45,48	0.95	2 (4%)	48,51,54	1.00	2 (4%)
26	PHO	d	402	-	50,69,69	1.02	5 (10%)	48,99,99	1.24	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	616	-	58,68,73	2.27	18 (31%)	68,107,113	2.58	25 (36%)
25	CLA	C	505	38	63,73,73	2.26	20 (31%)	74,113,113	2.51	26 (35%)
31	LMT	C	521	-	24,24,36	1.02	3 (12%)	29,29,47	1.08	2 (6%)
30	SQD	a	412	-	52,54,54	0.98	4 (7%)	62,65,65	1.59	10 (16%)
27	BCR	b	618	-	41,41,41	2.65	6 (14%)	56,56,56	6.57	19 (33%)
31	LMT	F	103	-	36,36,36	1.14	5 (13%)	47,47,47	1.07	3 (6%)
25	CLA	b	612	-	63,73,73	2.20	18 (28%)	74,113,113	2.53	23 (31%)
30	SQD	F	102	-	32,34,54	1.23	5 (15%)	42,45,65	1.88	10 (23%)
25	CLA	C	511	-	63,73,73	2.26	19 (30%)	74,113,113	2.47	25 (33%)
31	LMT	a	415	-	36,36,36	1.22	6 (16%)	47,47,47	1.45	4 (8%)
25	CLA	C	512	3	63,73,73	2.22	17 (26%)	74,113,113	2.56	22 (29%)
25	CLA	A	408	-	58,68,73	2.31	18 (31%)	68,107,113	2.64	24 (35%)
31	LMT	B	625	-	36,36,36	1.21	6 (16%)	47,47,47	1.04	3 (6%)
25	CLA	c	503	-	63,73,73	2.25	18 (28%)	74,113,113	2.47	24 (32%)
28	LMG	C	519	-	51,51,55	1.47	8 (15%)	59,59,63	1.16	3 (5%)
34	DGD	h	103	-	63,63,67	1.32	8 (12%)	77,77,81	0.97	4 (5%)
28	LMG	d	409	-	51,51,55	1.42	8 (15%)	59,59,63	1.15	4 (6%)
28	LMG	D	409	-	51,51,55	1.42	8 (15%)	59,59,63	1.15	4 (6%)
34	DGD	c	518	-	63,63,67	1.31	8 (12%)	77,77,81	1.02	3 (3%)
31	LMT	b	624	-	24,24,36	1.04	1 (4%)	29,29,47	1.22	2 (6%)
28	LMG	C	523	-	49,49,55	0.20	0	57,57,63	0.22	0
31	LMT	i	104	-	22,22,36	1.09	3 (13%)	27,27,47	1.14	2 (7%)
30	SQD	A	413	-	46,48,54	1.01	4 (8%)	56,59,65	1.79	15 (26%)
31	LMT	L	101	-	36,36,36	1.17	6 (16%)	47,47,47	0.96	2 (4%)
31	LMT	x	101	-	24,24,36	1.05	3 (12%)	29,29,47	1.11	2 (6%)
29	PL9	d	405	-	55,55,55	1.57	8 (14%)	68,69,69	1.50	13 (19%)
28	LMG	b	621	-	51,51,55	1.45	8 (15%)	59,59,63	1.28	5 (8%)
34	DGD	c	517	-	63,63,67	1.32	8 (12%)	77,77,81	0.99	4 (5%)
30	SQD	b	620	-	52,54,54	0.94	3 (5%)	62,65,65	1.63	11 (17%)
28	LMG	A	410	-	51,51,55	1.45	8 (15%)	59,59,63	1.24	5 (8%)
31	LMT	i	101	-	24,24,36	1.10	3 (12%)	29,29,47	1.16	2 (6%)
31	LMT	b	629	-	36,36,36	1.15	5 (13%)	47,47,47	0.95	1 (2%)
31	LMT	M	102	-	24,24,36	1.07	2 (8%)	29,29,47	1.08	2 (6%)
30	SQD	h	102	-	52,54,54	0.98	5 (9%)	62,65,65	1.55	11 (17%)
31	LMT	B	624	-	24,24,36	1.04	1 (4%)	29,29,47	1.22	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LMT	c	521	-	24,24,36	1.03	3 (12%)	29,29,47	1.08	2 (6%)
25	CLA	b	613	-	63,73,73	2.20	19 (30%)	74,113,113	2.54	20 (27%)
25	CLA	C	510	-	63,73,73	2.28	18 (28%)	74,113,113	2.45	23 (31%)
26	PHO	a	407	-	50,69,69	1.06	4 (8%)	48,99,99	1.23	5 (10%)
25	CLA	c	504	-	63,73,73	2.26	20 (31%)	74,113,113	2.54	26 (35%)
27	BCR	B	617	-	41,41,41	2.69	6 (14%)	56,56,56	6.57	25 (44%)
34	DGD	C	517	-	63,63,67	1.32	8 (12%)	77,77,81	0.99	4 (5%)
30	SQD	K	101	-	45,45,54	1.02	4 (8%)	53,53,65	1.39	7 (13%)
31	LMT	a	416	-	24,24,36	1.03	3 (12%)	29,29,47	0.95	0
25	CLA	c	507	-	63,73,73	2.26	19 (30%)	74,113,113	2.46	24 (32%)
31	LMT	K	105	-	36,36,36	1.11	4 (11%)	47,47,47	0.99	2 (4%)
31	LMT	d	411	-	36,36,36	1.05	4 (11%)	47,47,47	1.22	4 (8%)
22	OEX	A	401	1,38,3	0,15,15	-	-	-	-	-
28	LMG	c	523	-	49,49,55	0.20	0	57,57,63	0.22	0
25	CLA	B	611	-	63,73,73	2.20	17 (26%)	74,113,113	2.41	23 (31%)
32	BCT	A	417	23	3,3,3	1.59	1 (33%)	2,3,3	4.03	2 (100%)
31	LMT	b	623	-	24,24,36	0.98	2 (8%)	29,29,47	1.29	3 (10%)
25	CLA	B	609	-	63,73,73	2.23	18 (28%)	74,113,113	2.51	21 (28%)
25	CLA	C	508	38	63,73,73	2.19	19 (30%)	74,113,113	2.53	26 (35%)
28	LMG	c	519	-	51,51,55	1.47	8 (15%)	59,59,63	1.16	3 (5%)
25	CLA	b	602	-	63,73,73	2.23	18 (28%)	74,113,113	2.51	25 (33%)
33	LHG	d	407	-	48,48,48	0.90	3 (6%)	51,54,54	0.99	3 (5%)
27	BCR	f	101	-	41,41,41	2.64	7 (17%)	56,56,56	6.66	20 (35%)
33	LHG	B	622	-	39,39,48	1.04	2 (5%)	42,45,54	1.10	3 (7%)
25	CLA	c	506	-	53,63,73	2.45	18 (33%)	62,101,113	2.62	22 (35%)
25	CLA	c	508	38	63,73,73	2.19	19 (30%)	74,113,113	2.54	26 (35%)
31	LMT	J	101	-	24,24,36	1.00	2 (8%)	29,29,47	1.12	3 (10%)
31	LMT	B	623	-	24,24,36	0.98	2 (8%)	29,29,47	1.29	3 (10%)
30	SQD	H	102	-	52,54,54	0.98	5 (9%)	62,65,65	1.55	11 (17%)
27	BCR	C	515	-	41,41,41	2.70	6 (14%)	56,56,56	6.65	19 (33%)
31	LMT	j	101	-	24,24,36	1.00	2 (8%)	29,29,47	1.12	3 (10%)
35	HEM	e	104	6	42,50,50	1.56	4 (9%)	46,82,82	1.41	5 (10%)
31	LMT	X	103	-	22,22,36	1.11	4 (18%)	27,27,47	1.14	1 (3%)
31	LMT	i	102	-	24,24,36	1.07	3 (12%)	29,29,47	1.37	3 (10%)
31	LMT	x	103	-	22,22,36	1.10	4 (18%)	27,27,47	1.14	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	D	401	38	63,73,73	2.20	18 (28%)	74,113,113	2.44	21 (28%)
25	CLA	a	408	-	58,68,73	2.31	18 (31%)	68,107,113	2.64	24 (35%)
25	CLA	b	616	-	58,68,73	2.28	18 (31%)	68,107,113	2.58	25 (36%)
31	LMT	d	410	-	24,24,36	1.01	3 (12%)	29,29,47	1.34	4 (13%)
31	LMT	f	103	-	36,36,36	1.14	5 (13%)	47,47,47	1.07	3 (6%)
25	CLA	c	510	-	63,73,73	2.28	18 (28%)	74,113,113	2.45	23 (31%)
25	CLA	c	509	-	63,73,73	2.21	19 (30%)	74,113,113	2.48	24 (32%)
25	CLA	a	405	-	63,73,73	2.16	18 (28%)	74,113,113	2.61	26 (35%)

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
31	LMT	b	626	-	-	9/15/35/61	0/1/1/2
25	CLA	B	612	-	1/1/15/20	8/37/115/115	-
30	SQD	C	501	-	-	28/49/69/69	0/1/1/1
30	SQD	k	101	-	-	20/39/59/69	0/1/1/1
33	LHG	D	406	-	-	27/53/53/53	-
33	LHG	z	102	-	-	16/37/37/53	-
25	CLA	b	610	-	1/1/15/20	6/37/115/115	-
25	CLA	D	404	-	1/1/15/20	14/37/115/115	-
25	CLA	C	513	-	1/1/12/20	6/19/97/115	-
25	CLA	b	608	-	1/1/15/20	11/37/115/115	-
33	LHG	D	407	-	-	26/53/53/53	-
25	CLA	b	615	-	1/1/15/20	12/37/115/115	-
30	SQD	c	501	-	-	28/49/69/69	0/1/1/1
25	CLA	B	603	-	1/1/15/20	10/37/115/115	-
35	HEM	v	201	18	-	2/12/54/54	-
31	LMT	c	522	-	-	9/15/35/61	0/1/1/2
33	LHG	d	406	-	-	27/53/53/53	-
31	LMT	I	101	-	-	12/15/35/61	0/1/1/2
33	LHG	b	622	-	-	28/44/44/53	-
31	LMT	k	105	-	-	12/21/61/61	0/2/2/2
25	CLA	d	404	-	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	C	507	-	1/1/15/20	17/37/115/115	-
27	BCR	B	619	-	-	8/29/63/63	0/2/2/2
28	LMG	B	621	-	-	7/46/66/70	0/1/1/1
26	PHO	D	402	-	-	4/37/103/103	0/5/6/6
31	LMT	D	411	-	-	12/21/61/61	0/2/2/2
31	LMT	i	103	-	-	8/21/61/61	0/2/2/2
25	CLA	b	611	-	1/1/15/20	11/37/115/115	-
25	CLA	C	503	-	1/1/15/20	7/37/115/115	-
34	DGD	C	518	-	-	15/51/91/95	0/2/2/2
25	CLA	A	405	-	1/1/15/20	8/37/115/115	-
27	BCR	b	617	-	-	9/29/63/63	0/2/2/2
34	DGD	H	103	-	-	7/51/91/95	0/2/2/2
31	LMT	E	103	-	-	12/21/61/61	0/2/2/2
33	LHG	E	102	-	-	25/44/44/53	-
25	CLA	c	511	-	1/1/15/20	14/37/115/115	-
26	PHO	A	407	-	-	6/37/103/103	0/5/6/6
25	CLA	c	512	3	1/1/15/20	8/37/115/115	-
31	LMT	M	101	-	-	13/21/61/61	0/2/2/2
27	BCR	Z	101	-	-	8/29/63/63	0/2/2/2
27	BCR	k	102	-	-	13/29/63/63	0/2/2/2
31	LMT	T	701	-	-	5/15/35/61	0/1/1/2
25	CLA	C	504	-	1/1/15/20	10/37/115/115	-
31	LMT	D	410	-	-	12/15/35/61	0/1/1/2
29	PL9	D	405	-	-	10/53/73/73	0/1/1/1
30	SQD	A	412	-	-	25/49/69/69	0/1/1/1
31	LMT	B	627	-	-	6/17/37/61	0/1/1/2
25	CLA	c	514	-	1/1/15/20	14/37/115/115	-
31	LMT	A	415	-	-	9/21/61/61	0/2/2/2
33	LHG	e	102	-	-	25/44/44/53	-
27	BCR	z	101	-	-	8/29/63/63	0/2/2/2
31	LMT	m	101	-	-	7/15/35/61	0/1/1/2
25	CLA	b	614	-	1/1/15/20	17/37/115/115	-
34	DGD	C	516	-	-	20/51/91/95	0/2/2/2
27	BCR	K	102	-	-	13/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	D	403	-	1/1/15/20	7/37/115/115	-
25	CLA	B	608	-	1/1/15/20	11/37/115/115	-
34	DGD	c	516	-	-	20/51/91/95	0/2/2/2
25	CLA	B	605	-	1/1/15/20	13/37/115/115	-
37	RRX	X	102	-	-	21/29/65/65	0/2/2/2
25	CLA	b	606	-	1/1/14/20	9/31/109/115	-
28	LMG	a	410	-	-	17/46/66/70	0/1/1/1
25	CLA	b	607	38	1/1/15/20	9/37/115/115	-
27	BCR	F	101	-	-	10/29/63/63	0/2/2/2
25	CLA	B	615	-	1/1/15/20	12/37/115/115	-
31	LMT	c	524	-	-	9/21/61/61	0/2/2/2
31	LMT	c	520	-	-	3/14/54/61	0/2/2/2
27	BCR	k	103	-	-	6/29/63/63	0/2/2/2
25	CLA	B	613	-	1/1/15/20	12/37/115/115	-
25	CLA	B	606	-	1/1/14/20	9/31/109/115	-
27	BCR	a	409	-	-	6/29/63/63	0/2/2/2
29	PL9	a	411	-	-	27/53/73/73	0/1/1/1
25	CLA	C	509	-	1/1/15/20	7/37/115/115	-
25	CLA	A	406	38	1/1/15/20	12/37/115/115	-
25	CLA	c	505	38	1/1/15/20	11/37/115/115	-
25	CLA	a	406	38	1/1/15/20	12/37/115/115	-
31	LMT	X	101	-	-	6/15/35/61	0/1/1/2
31	LMT	I	103	-	-	8/21/61/61	0/2/2/2
31	LMT	b	625	-	-	5/21/61/61	0/2/2/2
27	BCR	B	618	-	-	6/29/63/63	0/2/2/2
25	CLA	B	610	-	1/1/15/20	5/37/115/115	-
25	CLA	B	607	38	1/1/15/20	9/37/115/115	-
27	BCR	A	409	-	-	6/29/63/63	0/2/2/2
31	LMT	C	522	-	-	9/15/35/61	0/1/1/2
25	CLA	c	513	-	1/1/12/20	6/19/97/115	-
30	SQD	a	413	-	-	21/43/63/69	0/1/1/1
31	LMT	I	102	-	-	10/15/35/61	0/1/1/2
25	CLA	C	514	-	1/1/15/20	14/37/115/115	-
25	CLA	b	604	-	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	d	401	38	1/1/15/20	9/37/115/115	-
31	LMT	e	103	-	-	12/21/61/61	0/2/2/2
27	BCR	c	515	-	-	7/29/63/63	0/2/2/2
31	LMT	B	626	-	-	9/15/35/61	0/1/1/2
25	CLA	B	614	-	1/1/15/20	17/37/115/115	-
25	CLA	b	605	-	1/1/15/20	13/37/115/115	-
31	LMT	D	412	-	-	4/21/61/61	0/2/2/2
31	LMT	b	627	-	-	6/17/37/61	0/1/1/2
37	RRX	x	102	-	-	21/29/65/65	0/2/2/2
25	CLA	C	502	-	1/1/15/20	14/37/115/115	-
31	LMT	H	101	-	-	5/15/35/61	0/1/1/2
27	BCR	K	103	-	-	6/29/63/63	0/2/2/2
33	LHG	B	628	-	-	24/53/53/53	-
25	CLA	d	403	-	1/1/15/20	7/37/115/115	-
31	LMT	d	412	-	-	4/21/61/61	0/2/2/2
31	LMT	C	520	-	-	3/14/54/61	0/2/2/2
31	LMT	Y	101	-	-	4/12/32/61	0/1/1/2
25	CLA	B	602	-	1/1/15/20	12/37/115/115	-
31	LMT	e	101	-	-	3/13/33/61	0/1/1/2
31	LMT	t	701	-	-	5/15/35/61	0/1/1/2
30	SQD	B	620	-	-	21/49/69/69	0/1/1/1
29	PL9	A	411	-	-	27/53/73/73	0/1/1/1
25	CLA	C	506	-	1/1/13/20	4/25/103/115	-
33	LHG	Z	102	-	-	16/37/37/53	-
31	LMT	I	104	-	-	3/13/33/61	0/1/1/2
28	LMG	A	414	-	-	7/31/51/70	0/1/1/1
35	HEM	V	201	18	-	2/12/54/54	-
25	CLA	b	609	-	1/1/15/20	13/37/115/115	-
31	LMT	E	101	-	-	3/13/33/61	0/1/1/2
25	CLA	B	601	38	1/1/11/20	4/13/91/115	-
31	LMT	y	101	-	-	4/12/32/61	0/1/1/2
35	HEM	E	104	6	-	2/12/54/54	-
28	LMG	a	414	-	-	7/31/51/70	0/1/1/1
25	CLA	b	603	-	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b	601	38	1/1/11/20	4/13/91/115	-
31	LMT	A	416	-	-	8/15/35/61	0/1/1/2
33	LHG	b	628	-	-	24/53/53/53	-
25	CLA	c	502	-	1/1/15/20	14/37/115/115	-
25	CLA	B	604	-	1/1/15/20	14/37/115/115	-
31	LMT	h	101	-	-	5/15/35/61	0/1/1/2
27	BCR	b	619	-	-	8/29/63/63	0/2/2/2
31	LMT	B	629	-	-	10/21/61/61	0/2/2/2
30	SQD	f	102	-	-	16/29/49/69	0/1/1/1
33	LHG	d	408	-	-	18/50/50/53	-
31	LMT	C	524	-	-	9/21/61/61	0/2/2/2
33	LHG	D	408	-	-	18/50/50/53	-
26	PHO	d	402	-	-	4/37/103/103	0/5/6/6
25	CLA	B	616	-	1/1/14/20	16/31/109/115	-
25	CLA	C	505	38	1/1/15/20	11/37/115/115	-
31	LMT	C	521	-	-	11/15/35/61	0/1/1/2
30	SQD	a	412	-	-	25/49/69/69	0/1/1/1
27	BCR	b	618	-	-	6/29/63/63	0/2/2/2
31	LMT	F	103	-	-	11/21/61/61	0/2/2/2
25	CLA	b	612	-	1/1/15/20	8/37/115/115	-
30	SQD	F	102	-	-	16/29/49/69	0/1/1/1
25	CLA	C	511	-	1/1/15/20	14/37/115/115	-
31	LMT	a	415	-	-	9/21/61/61	0/2/2/2
25	CLA	C	512	3	1/1/15/20	8/37/115/115	-
25	CLA	A	408	-	1/1/14/20	14/31/109/115	-
31	LMT	B	625	-	-	5/21/61/61	0/2/2/2
25	CLA	c	503	-	1/1/15/20	7/37/115/115	-
28	LMG	C	519	-	-	19/46/66/70	0/1/1/1
34	DGD	h	103	-	-	7/51/91/95	0/2/2/2
28	LMG	d	409	-	-	12/46/66/70	0/1/1/1
28	LMG	D	409	-	-	12/46/66/70	0/1/1/1
34	DGD	c	518	-	-	15/51/91/95	0/2/2/2
31	LMT	b	624	-	-	8/15/35/61	0/1/1/2
28	LMG	C	523	-	-	24/44/64/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	i	104	-	-	3/13/33/61	0/1/1/2
30	SQD	A	413	-	-	21/43/63/69	0/1/1/1
31	LMT	L	101	-	-	13/21/61/61	0/2/2/2
31	LMT	x	101	-	-	6/15/35/61	0/1/1/2
29	PL9	d	405	-	-	10/53/73/73	0/1/1/1
28	LMG	b	621	-	-	7/46/66/70	0/1/1/1
34	DGD	c	517	-	-	16/51/91/95	0/2/2/2
30	SQD	b	620	-	-	21/49/69/69	0/1/1/1
28	LMG	A	410	-	-	17/46/66/70	0/1/1/1
31	LMT	i	101	-	-	12/15/35/61	0/1/1/2
31	LMT	b	629	-	-	10/21/61/61	0/2/2/2
31	LMT	M	102	-	-	7/15/35/61	0/1/1/2
30	SQD	h	102	-	-	24/49/69/69	0/1/1/1
31	LMT	B	624	-	-	8/15/35/61	0/1/1/2
31	LMT	c	521	-	-	11/15/35/61	0/1/1/2
25	CLA	b	613	-	1/1/15/20	12/37/115/115	-
25	CLA	C	510	-	1/1/15/20	15/37/115/115	-
26	PHO	a	407	-	-	6/37/103/103	0/5/6/6
27	BCR	B	617	-	-	9/29/63/63	0/2/2/2
25	CLA	c	504	-	1/1/15/20	10/37/115/115	-
34	DGD	C	517	-	-	16/51/91/95	0/2/2/2
30	SQD	K	101	-	-	20/39/59/69	0/1/1/1
31	LMT	a	416	-	-	8/15/35/61	0/1/1/2
25	CLA	c	507	-	1/1/15/20	17/37/115/115	-
31	LMT	K	105	-	-	12/21/61/61	0/2/2/2
31	LMT	d	411	-	-	12/21/61/61	0/2/2/2
28	LMG	c	523	-	-	24/44/64/70	0/1/1/1
25	CLA	B	611	-	1/1/15/20	11/37/115/115	-
31	LMT	b	623	-	-	6/15/35/61	0/1/1/2
25	CLA	B	609	-	1/1/15/20	13/37/115/115	-
25	CLA	C	508	38	1/1/15/20	11/37/115/115	-
28	LMG	c	519	-	-	19/46/66/70	0/1/1/1
25	CLA	b	602	-	1/1/15/20	12/37/115/115	-
33	LHG	d	407	-	-	26/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	f	101	-	-	10/29/63/63	0/2/2/2
33	LHG	B	622	-	-	28/44/44/53	-
25	CLA	c	506	-	1/1/13/20	4/25/103/115	-
25	CLA	c	508	38	1/1/15/20	11/37/115/115	-
31	LMT	J	101	-	-	10/15/35/61	0/1/1/2
31	LMT	B	623	-	-	6/15/35/61	0/1/1/2
30	SQD	H	102	-	-	24/49/69/69	0/1/1/1
27	BCR	C	515	-	-	7/29/63/63	0/2/2/2
31	LMT	j	101	-	-	10/15/35/61	0/1/1/2
35	HEM	e	104	6	-	2/12/54/54	-
31	LMT	X	103	-	-	10/12/32/61	0/1/1/2
31	LMT	i	102	-	-	10/15/35/61	0/1/1/2
31	LMT	x	103	-	-	10/12/32/61	0/1/1/2
25	CLA	D	401	38	1/1/15/20	9/37/115/115	-
25	CLA	a	408	-	1/1/14/20	14/31/109/115	-
25	CLA	b	616	-	1/1/14/20	16/31/109/115	-
31	LMT	d	410	-	-	12/15/35/61	0/1/1/2
31	LMT	f	103	-	-	11/21/61/61	0/2/2/2
25	CLA	c	510	-	1/1/15/20	15/37/115/115	-
25	CLA	c	509	-	1/1/15/20	7/37/115/115	-
25	CLA	a	405	-	1/1/15/20	8/37/115/115	-

The worst 5 of 1916 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	z	101	BCR	C8-C9	-8.57	1.27	1.46
27	Z	101	BCR	C8-C9	-8.57	1.27	1.46
27	C	515	BCR	C8-C9	-8.45	1.27	1.46
27	c	515	BCR	C8-C9	-8.44	1.27	1.46
27	b	619	BCR	C8-C9	-8.42	1.27	1.46

The worst 5 of 2542 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	K	102	BCR	C20-C21-C22	24.77	162.02	127.28
27	k	102	BCR	C20-C21-C22	24.74	161.98	127.28
27	k	103	BCR	C20-C21-C22	22.03	158.18	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	K	103	BCR	C20-C21-C22	22.03	158.17	127.28
27	f	101	BCR	C20-C21-C22	21.95	158.06	127.28

5 of 70 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

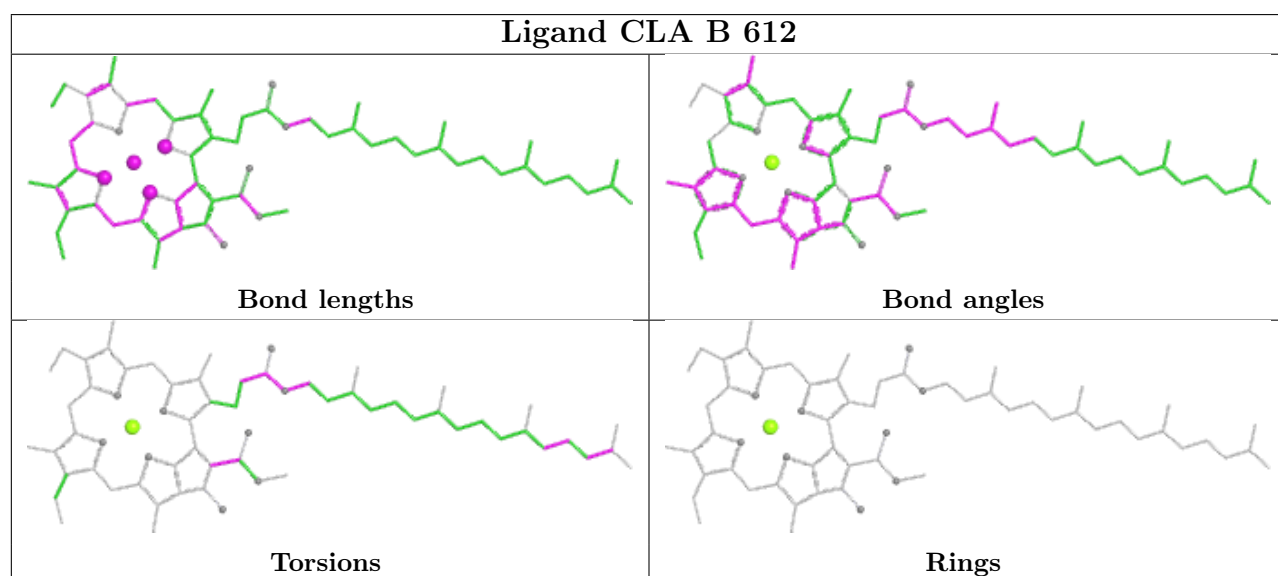
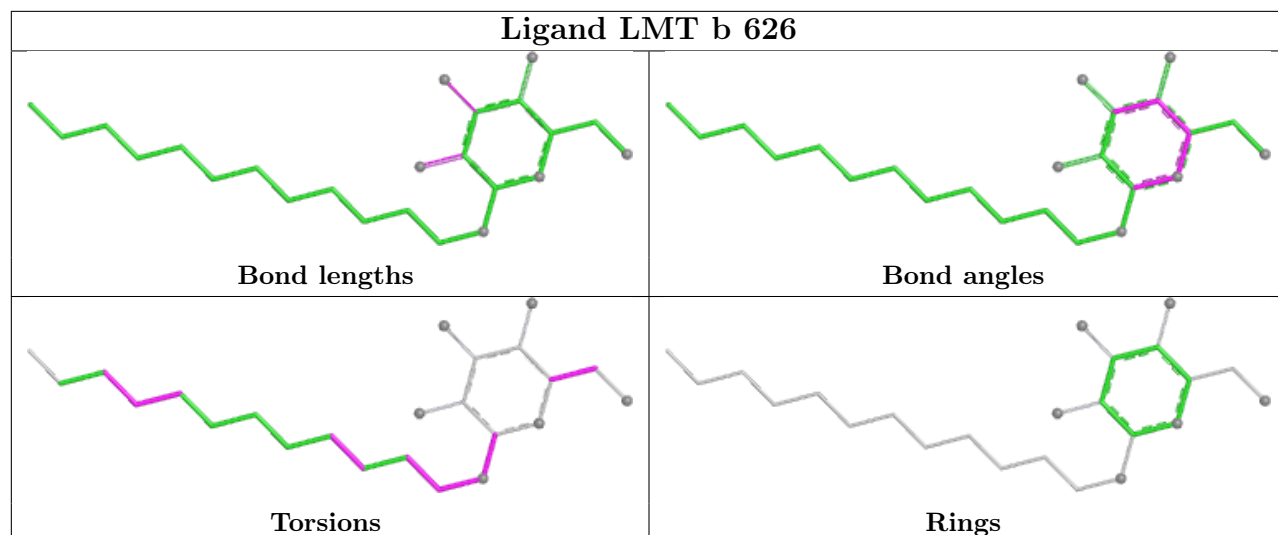
5 of 2477 torsion outliers are listed below:

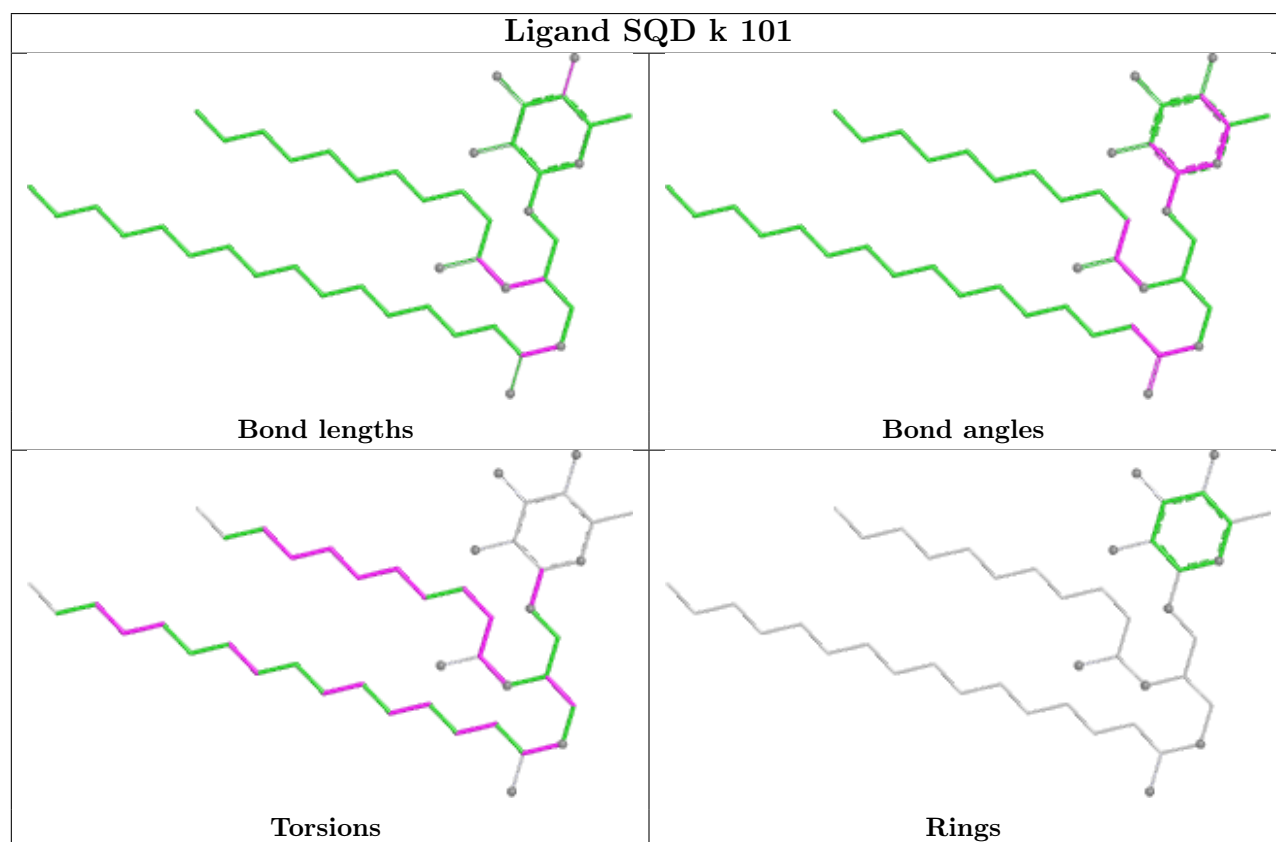
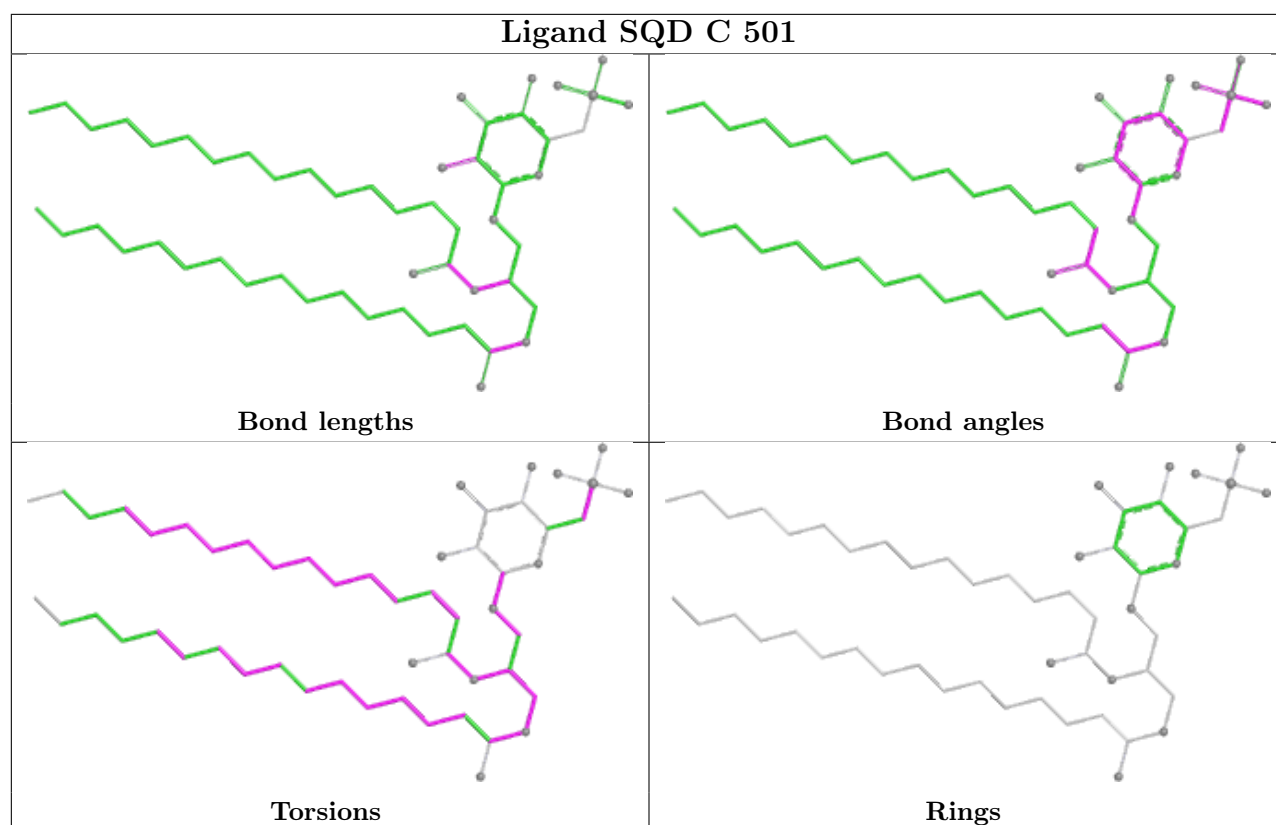
Mol	Chain	Res	Type	Atoms
25	B	601	CLA	CAD-CBD-CGD-O1D
25	B	601	CLA	CAD-CBD-CGD-O2D
25	B	607	CLA	C3A-C2A-CAA-CBA
25	B	614	CLA	CAD-CBD-CGD-O1D
25	B	614	CLA	CAD-CBD-CGD-O2D

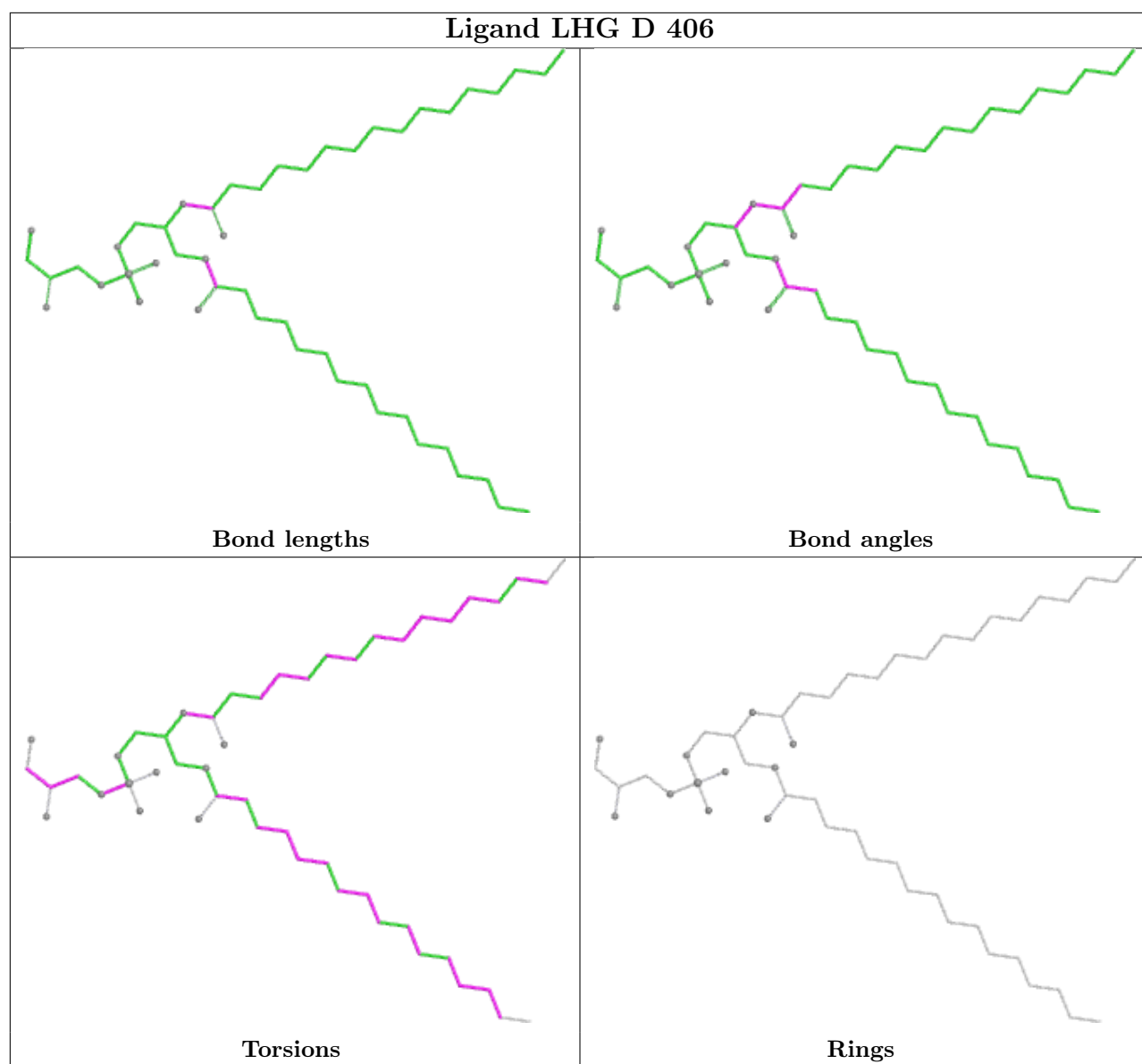
There are no ring outliers.

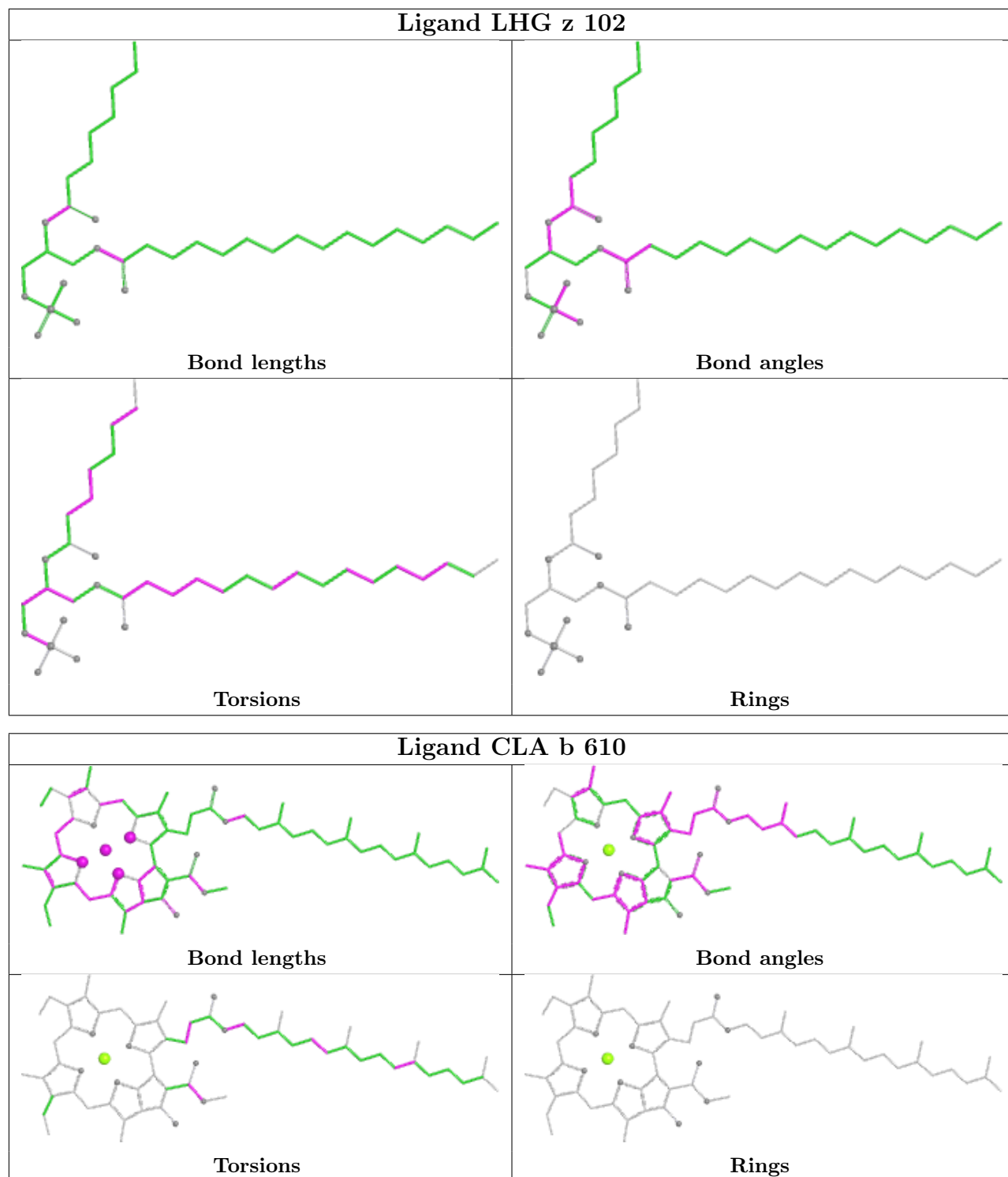
No monomer is involved in short contacts.

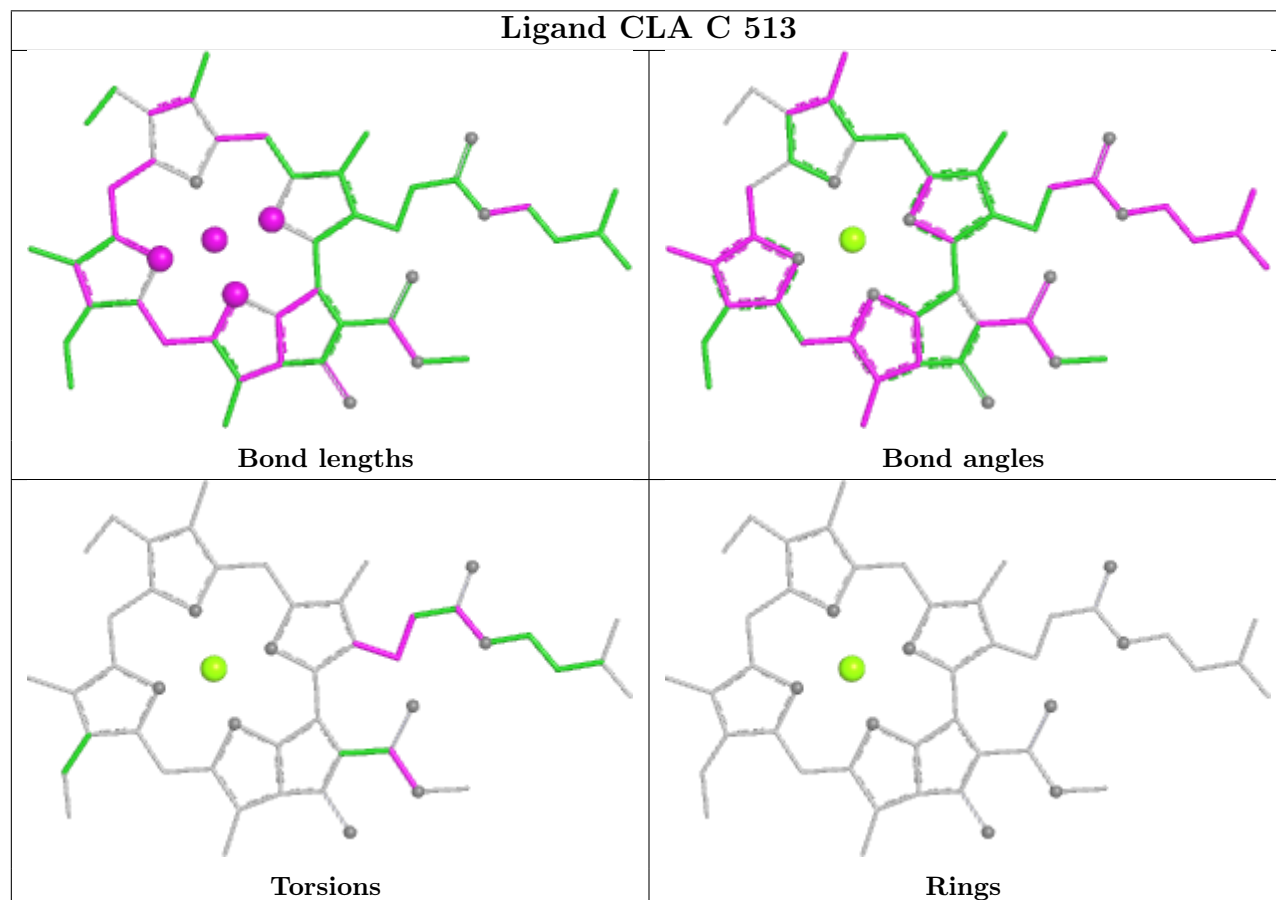
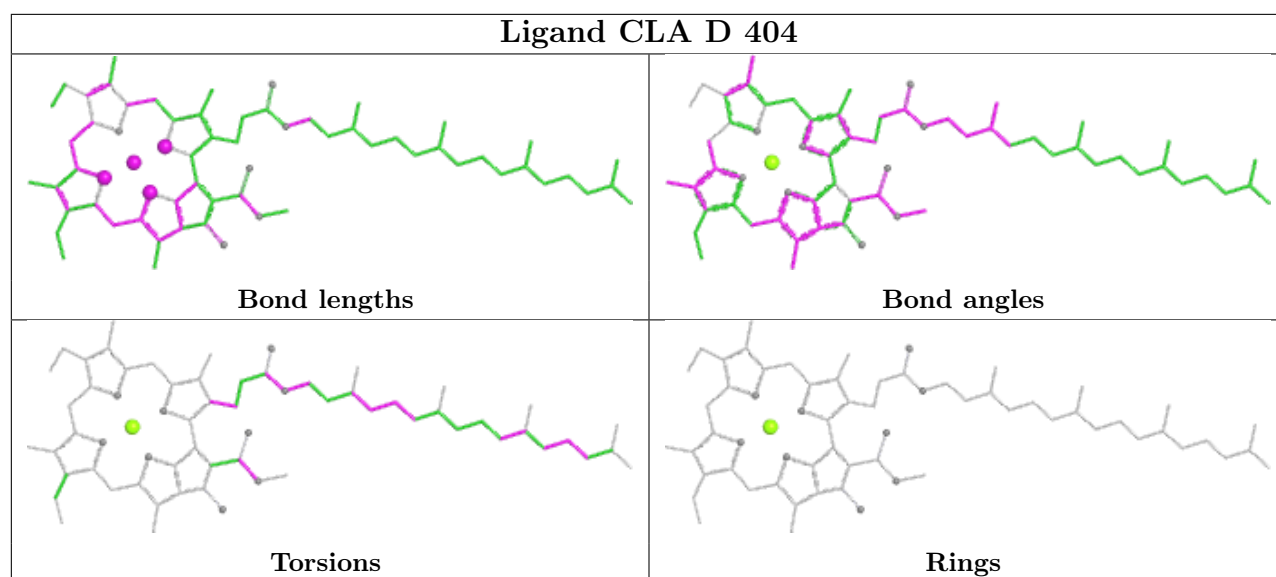
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

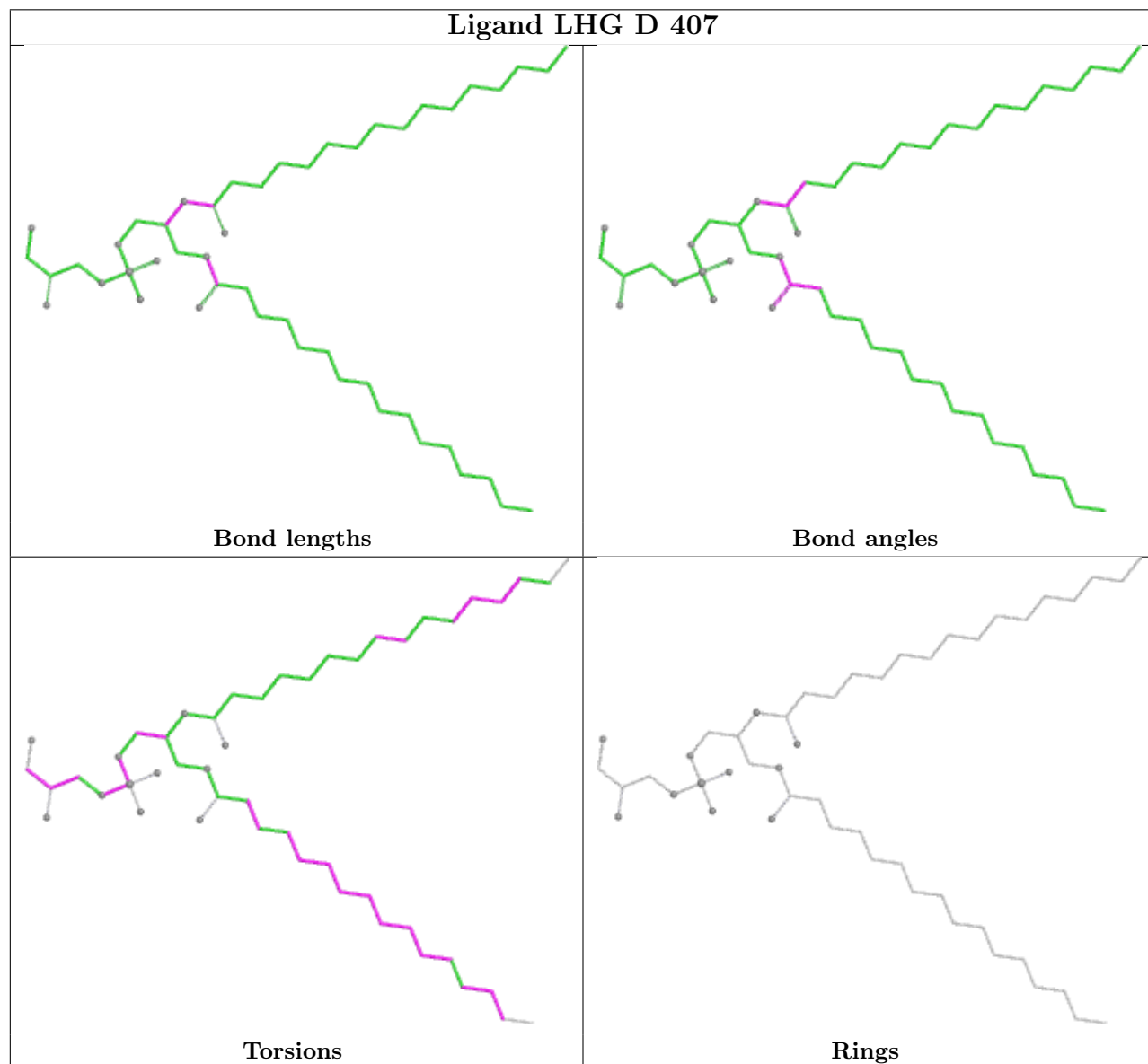
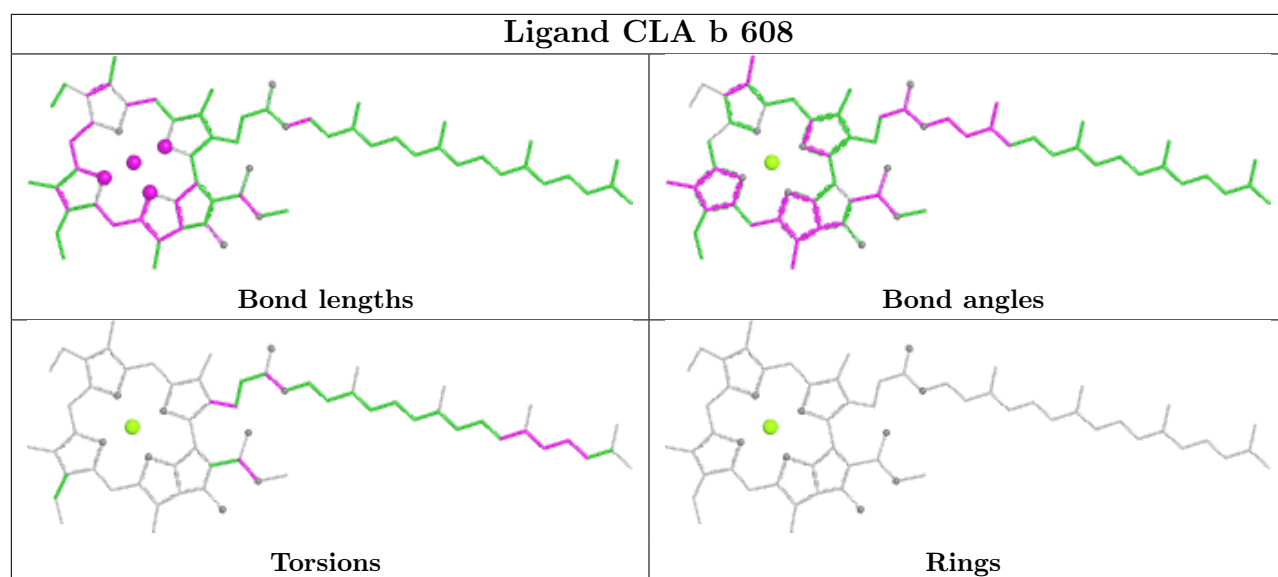


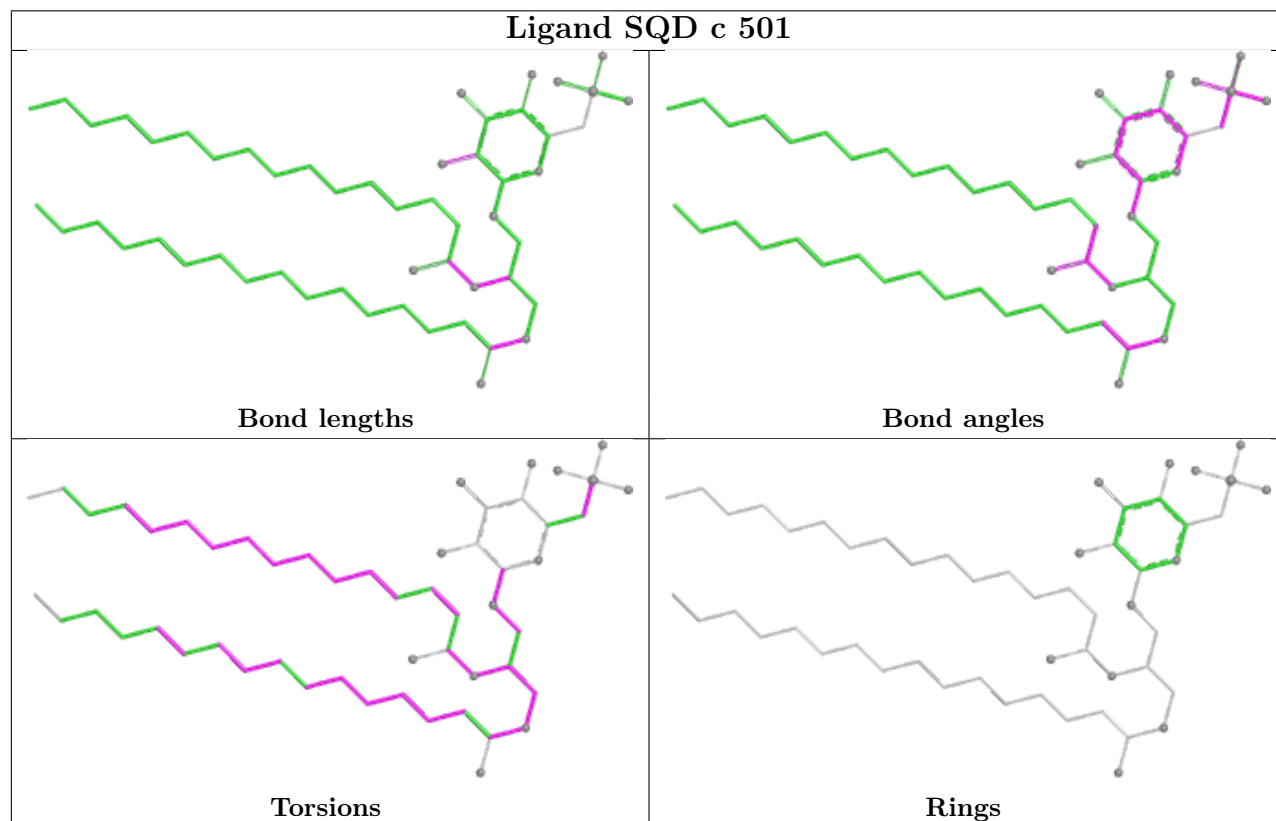
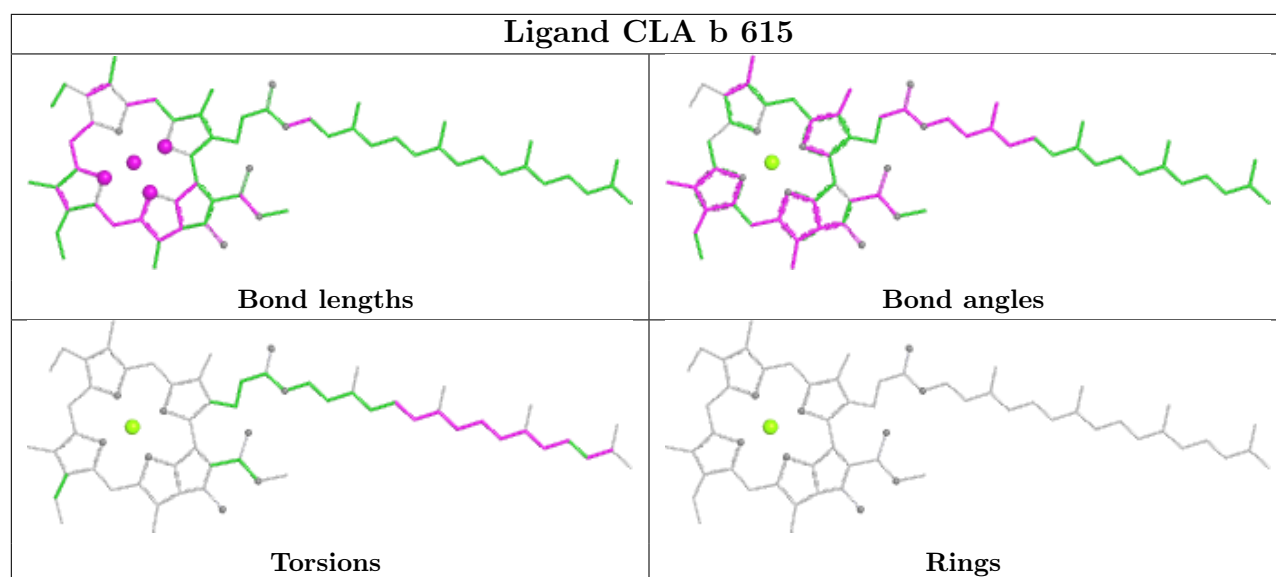


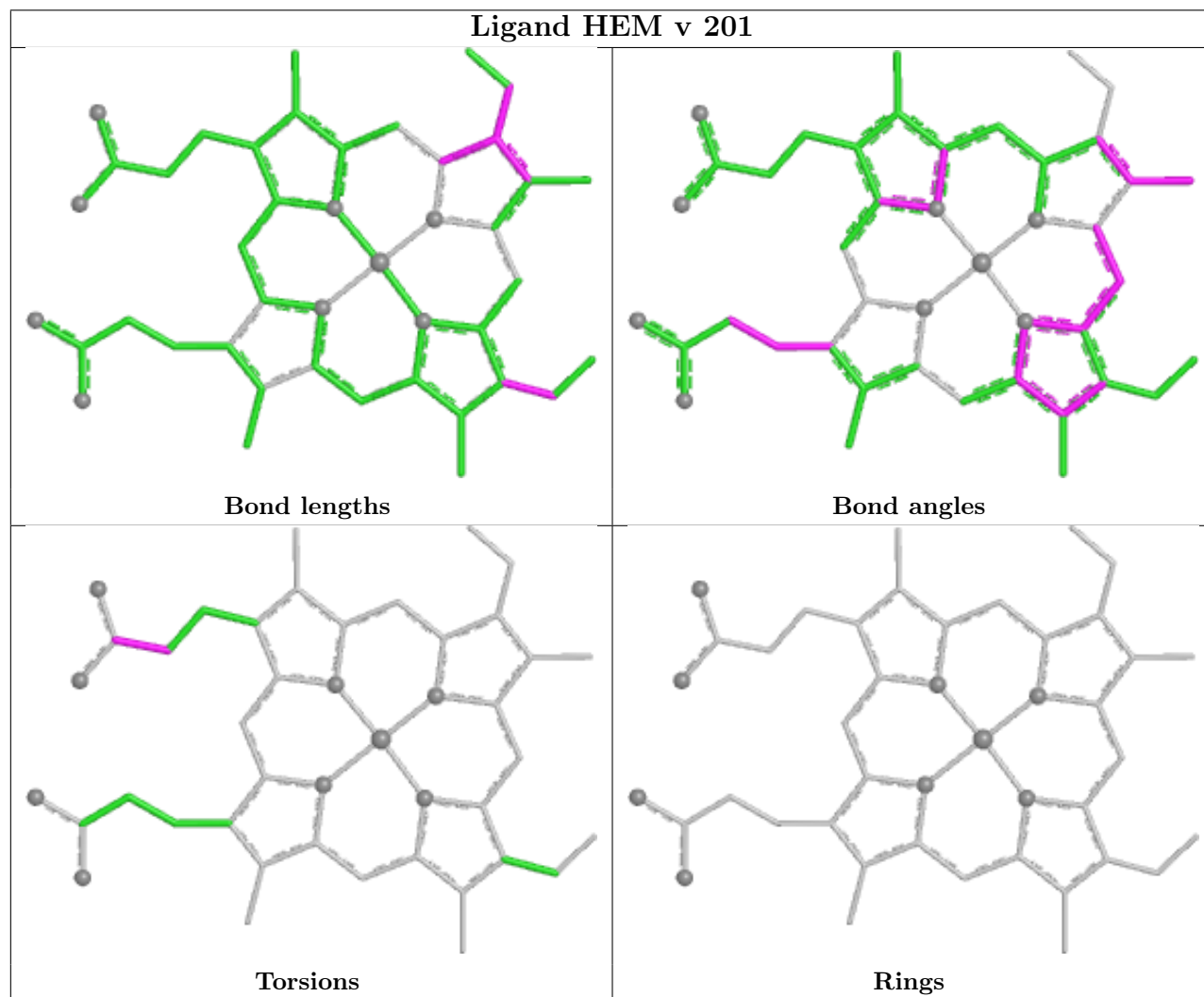
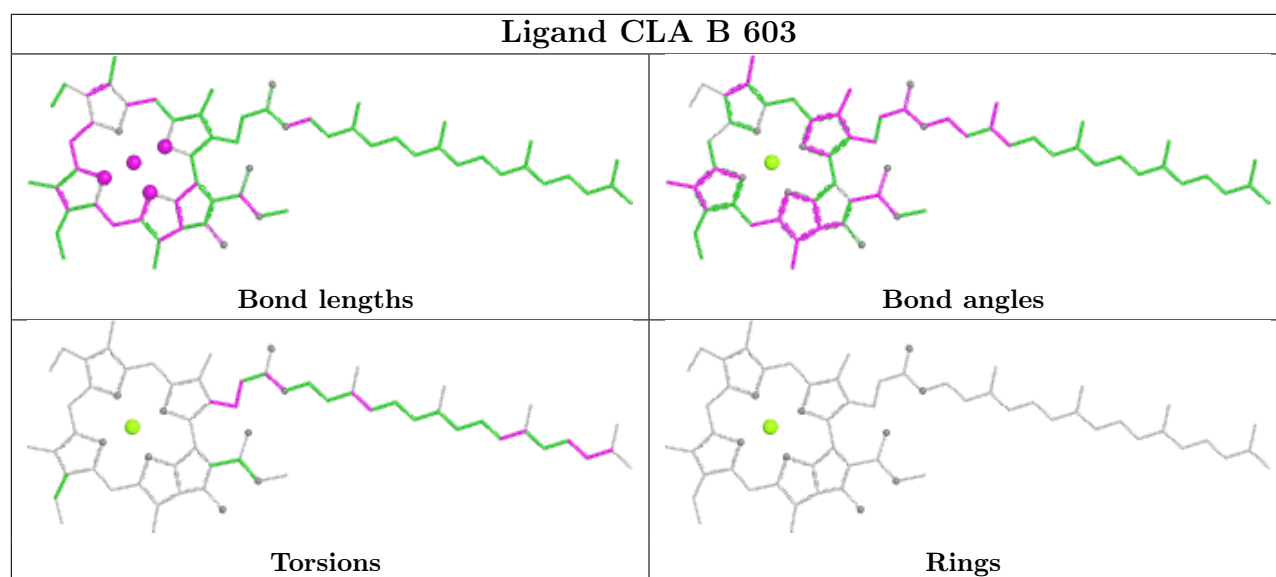


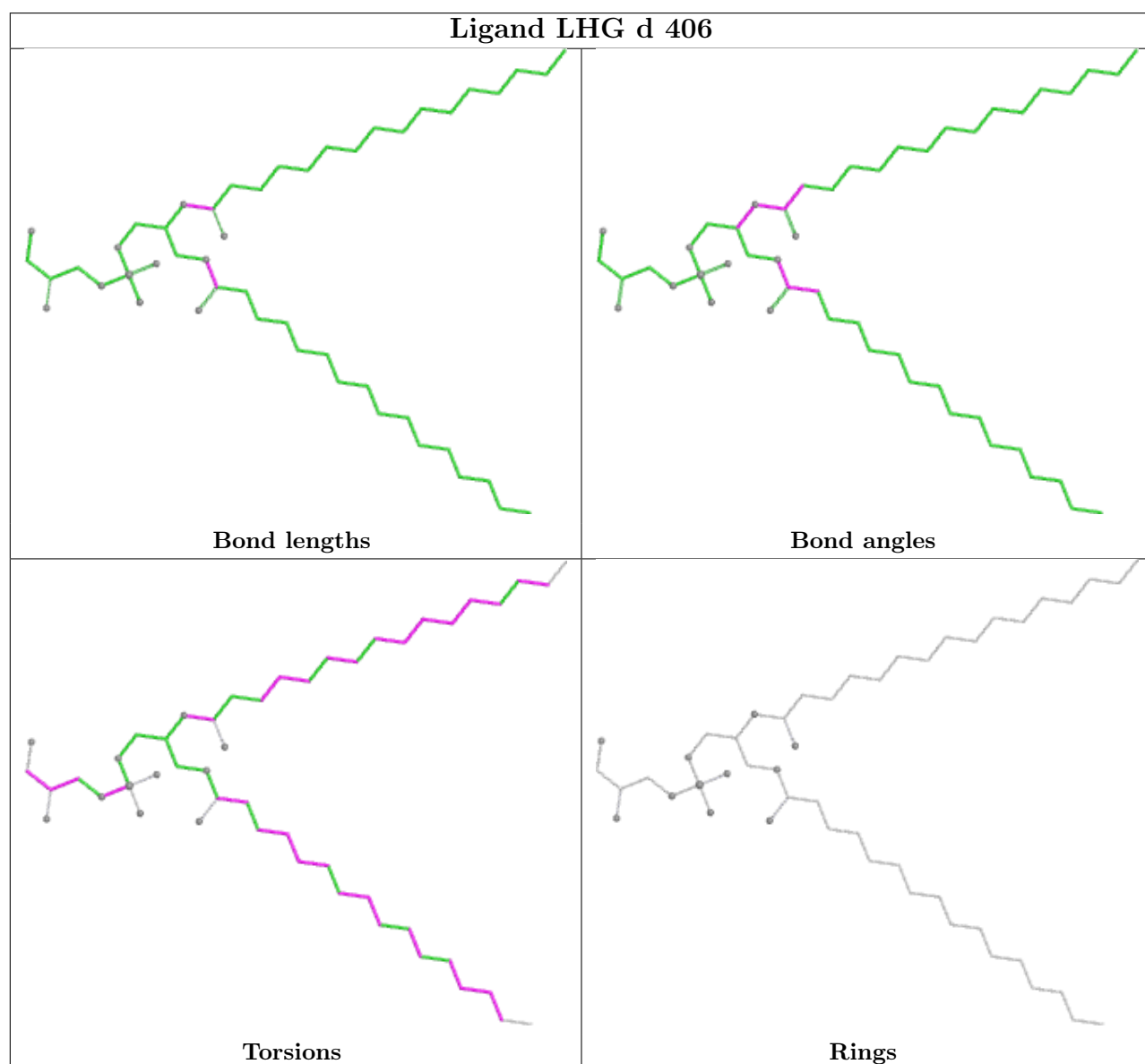
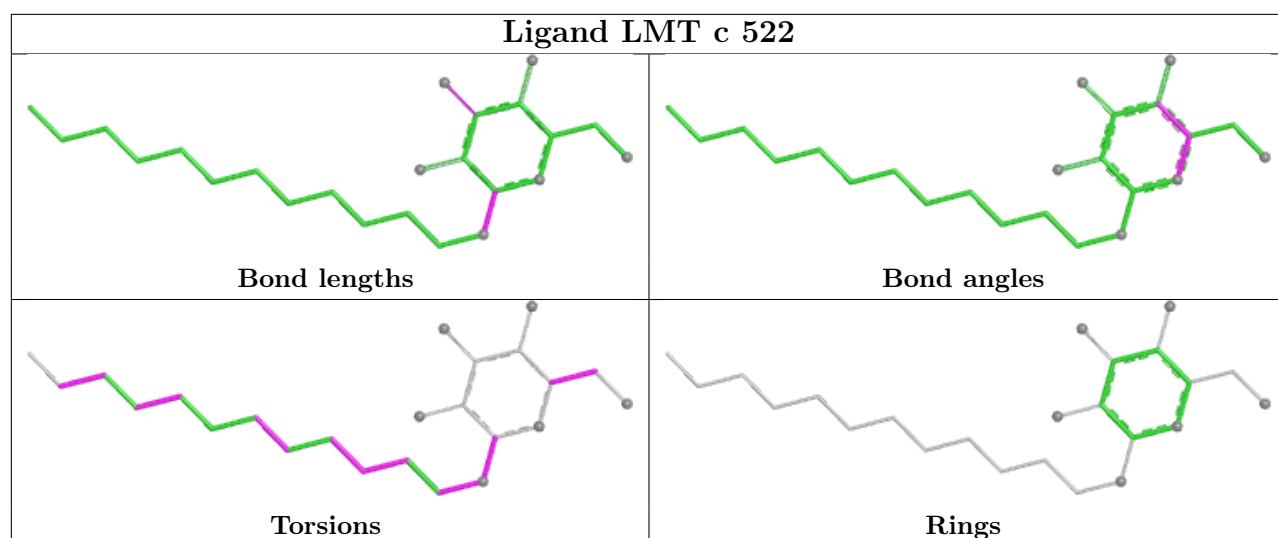


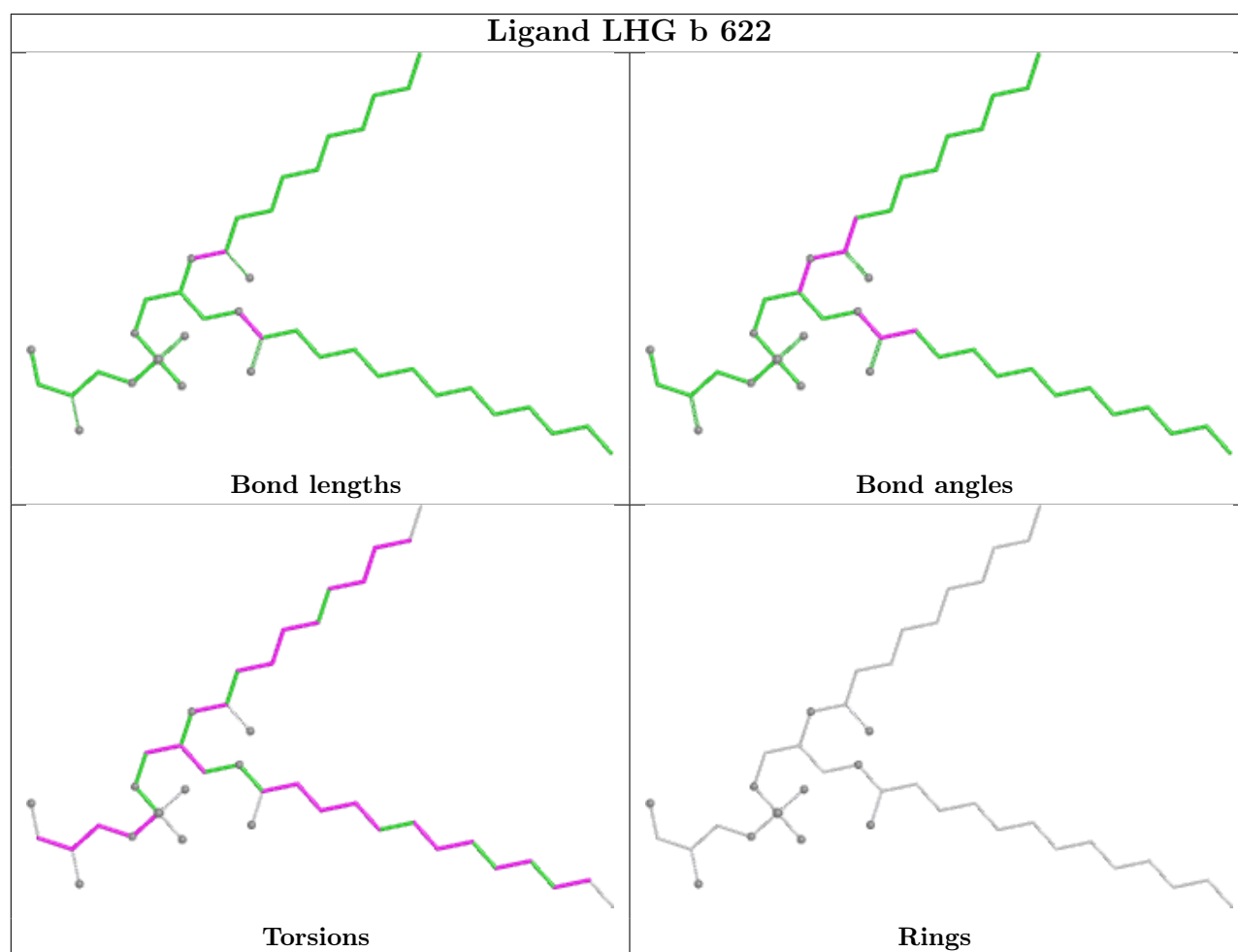
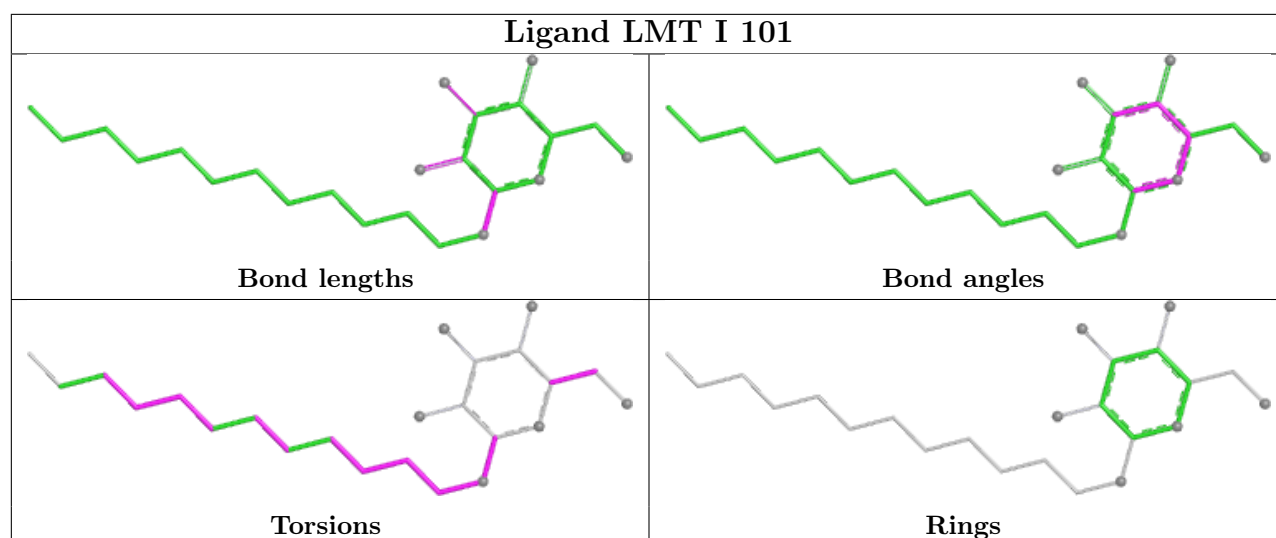


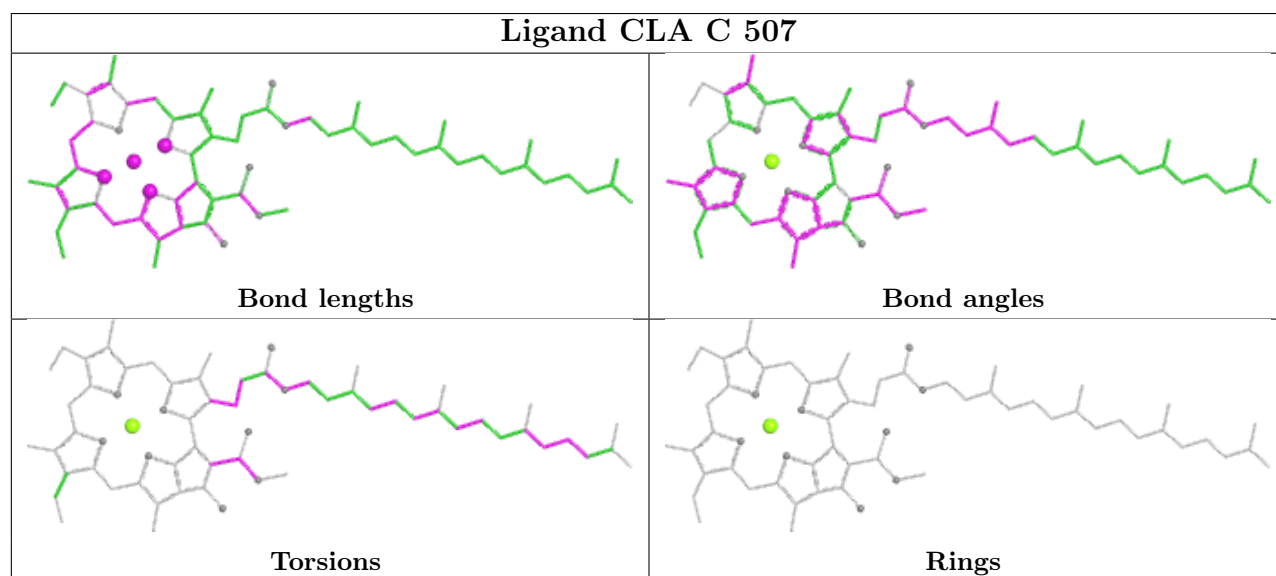
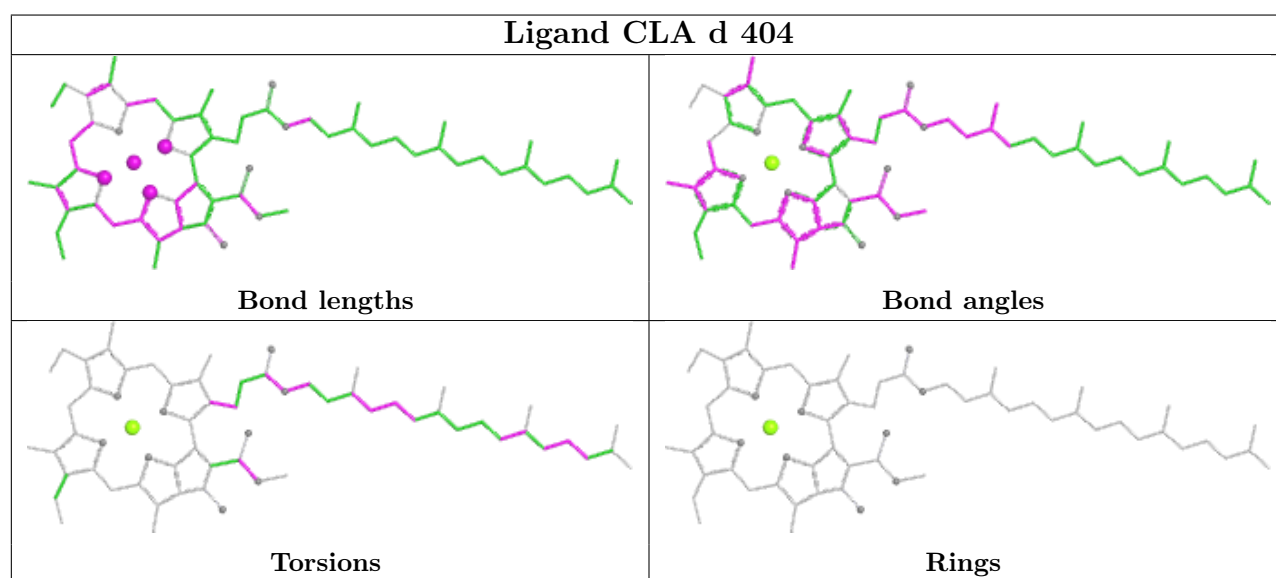
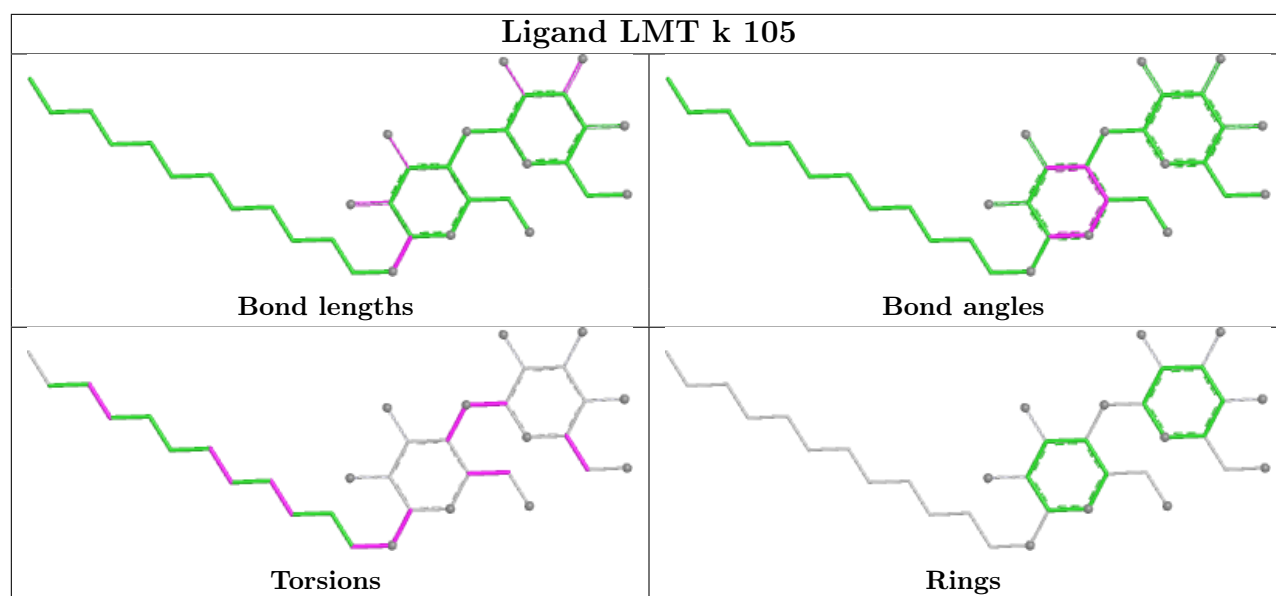


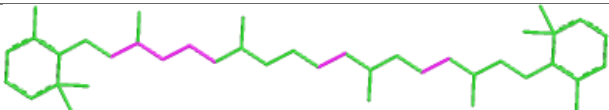
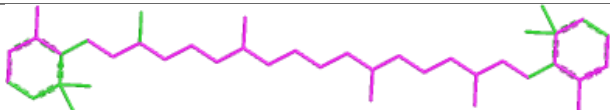
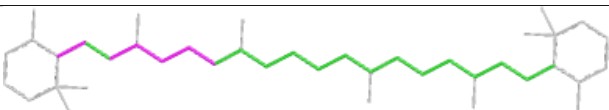
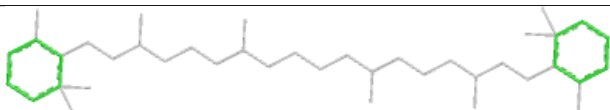


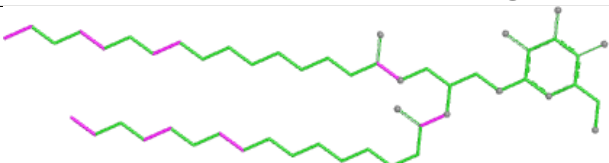
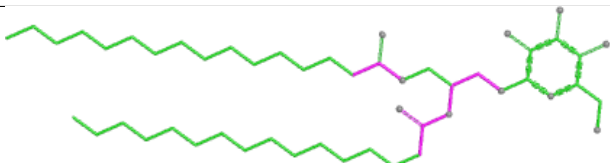
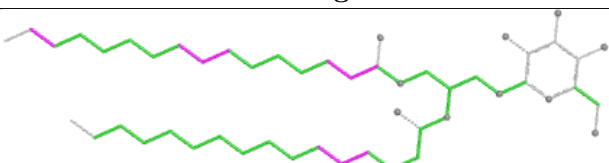
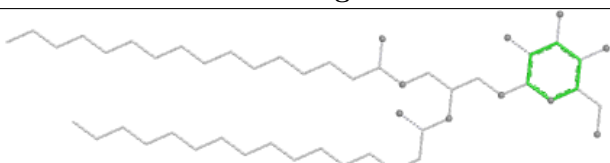


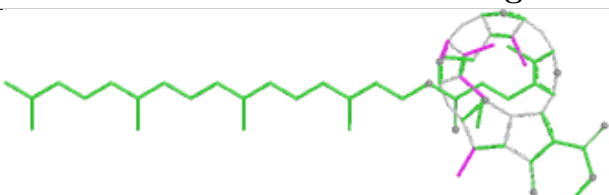
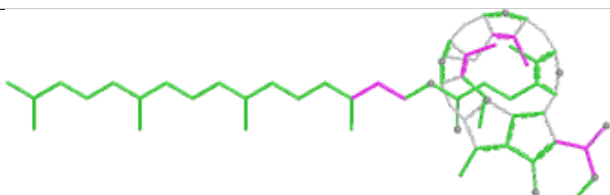
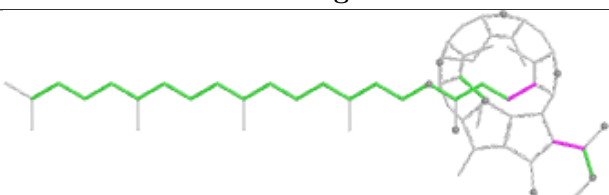
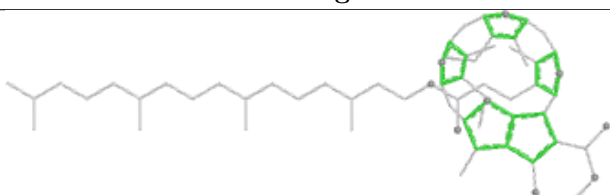


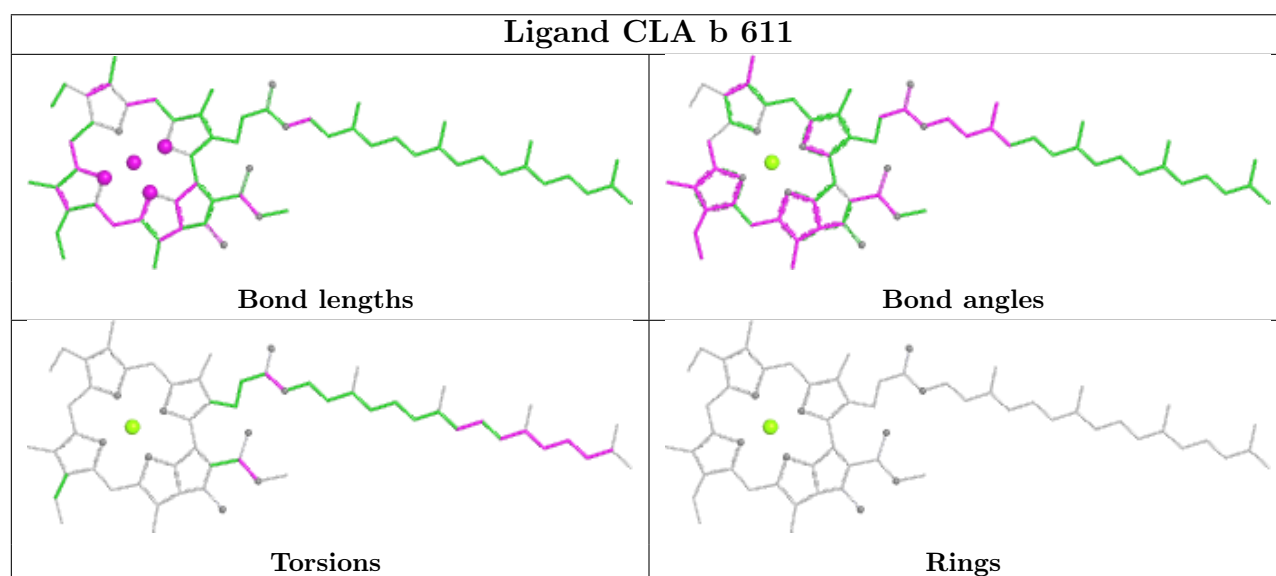
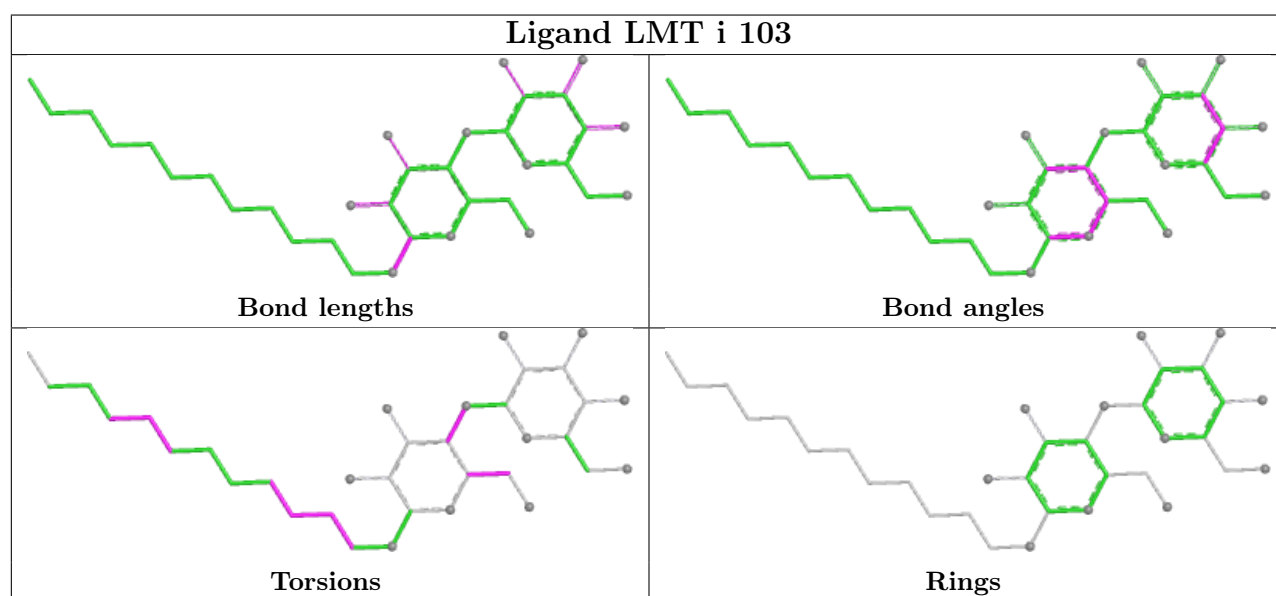
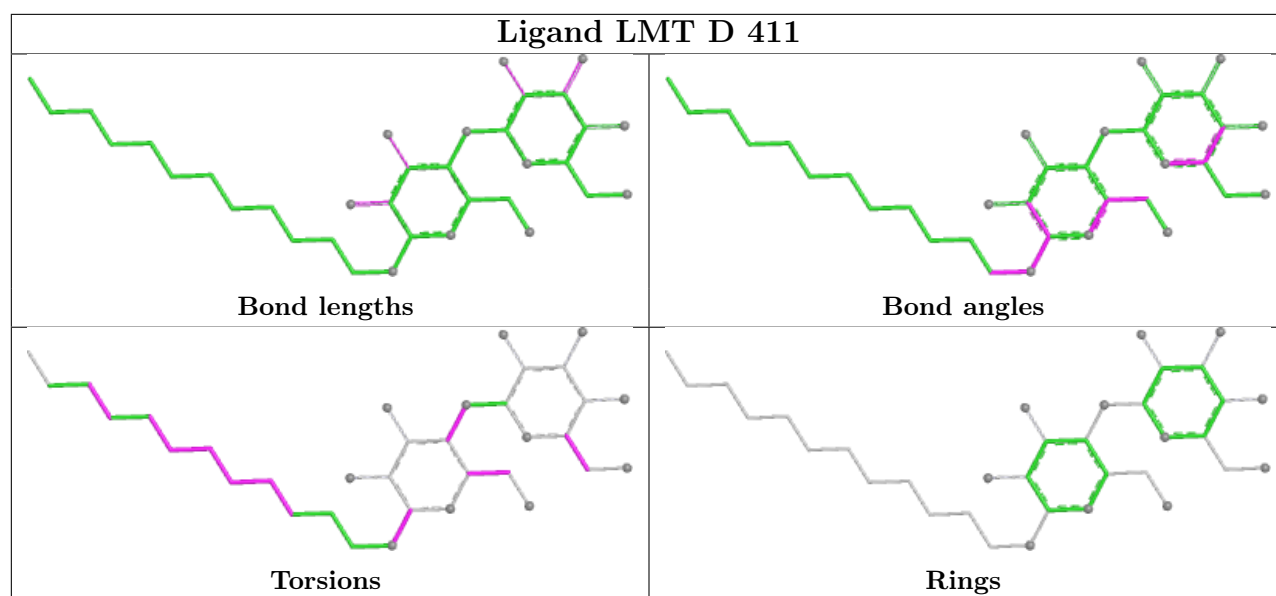


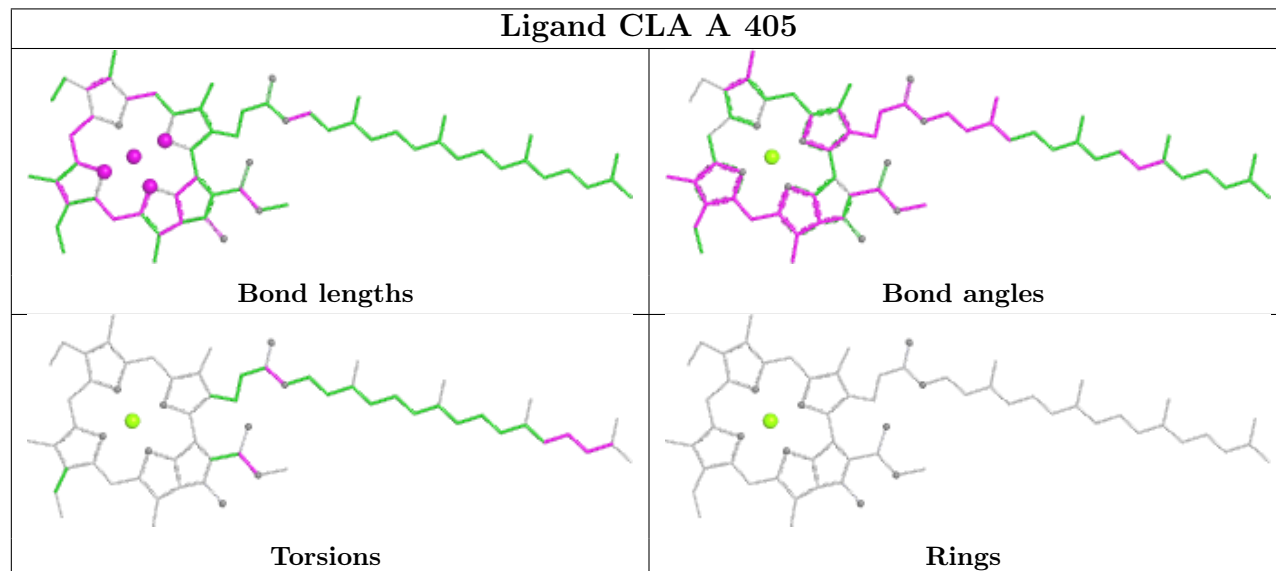
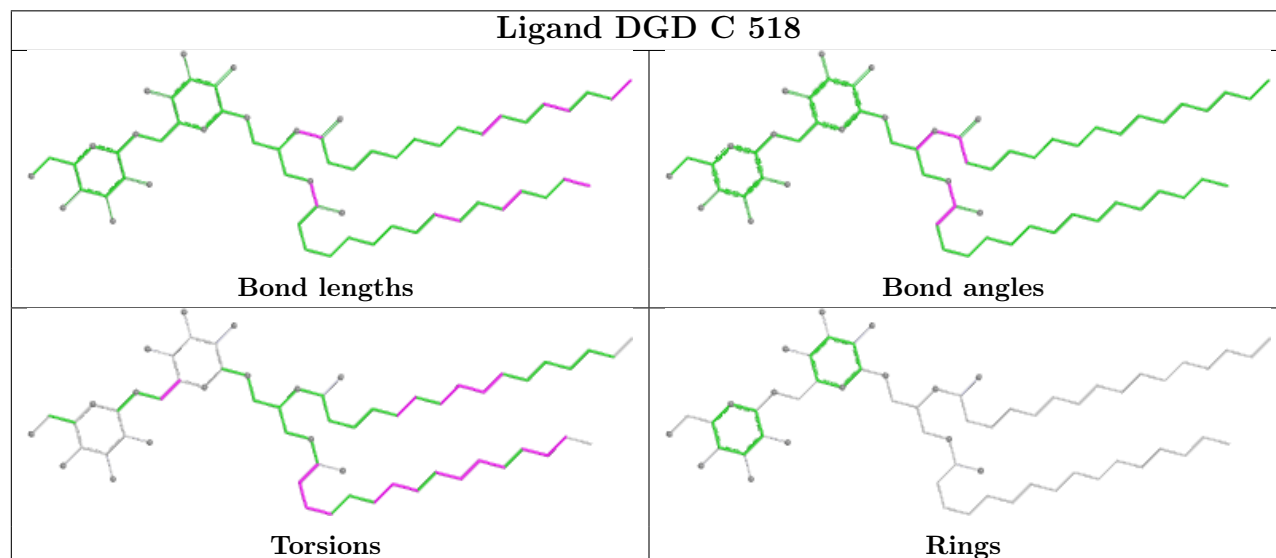
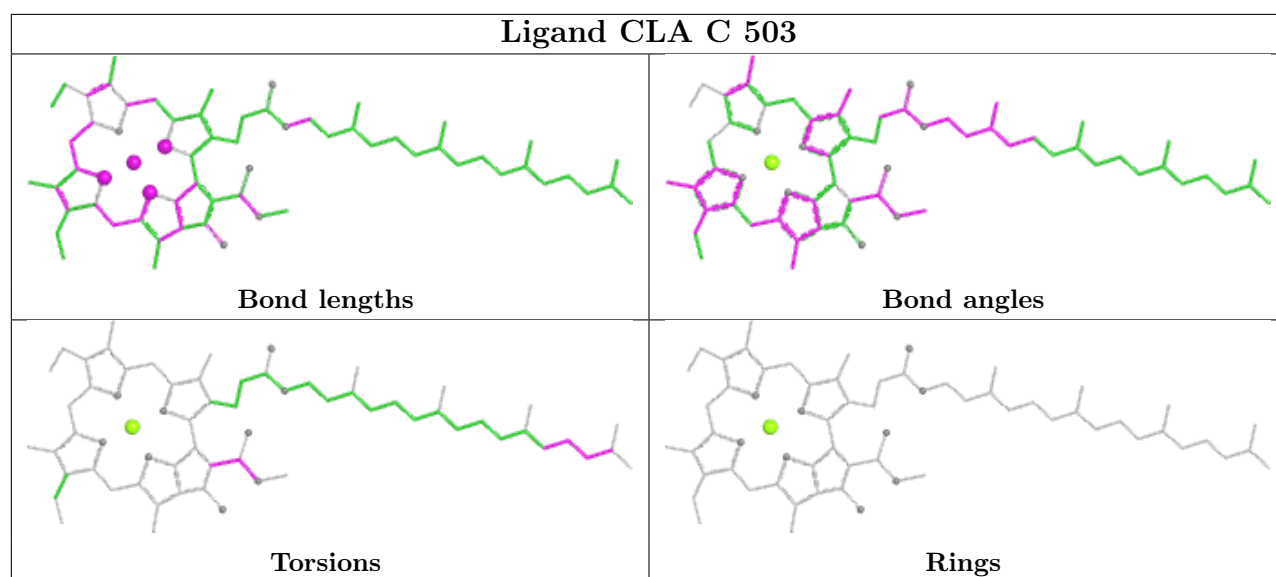


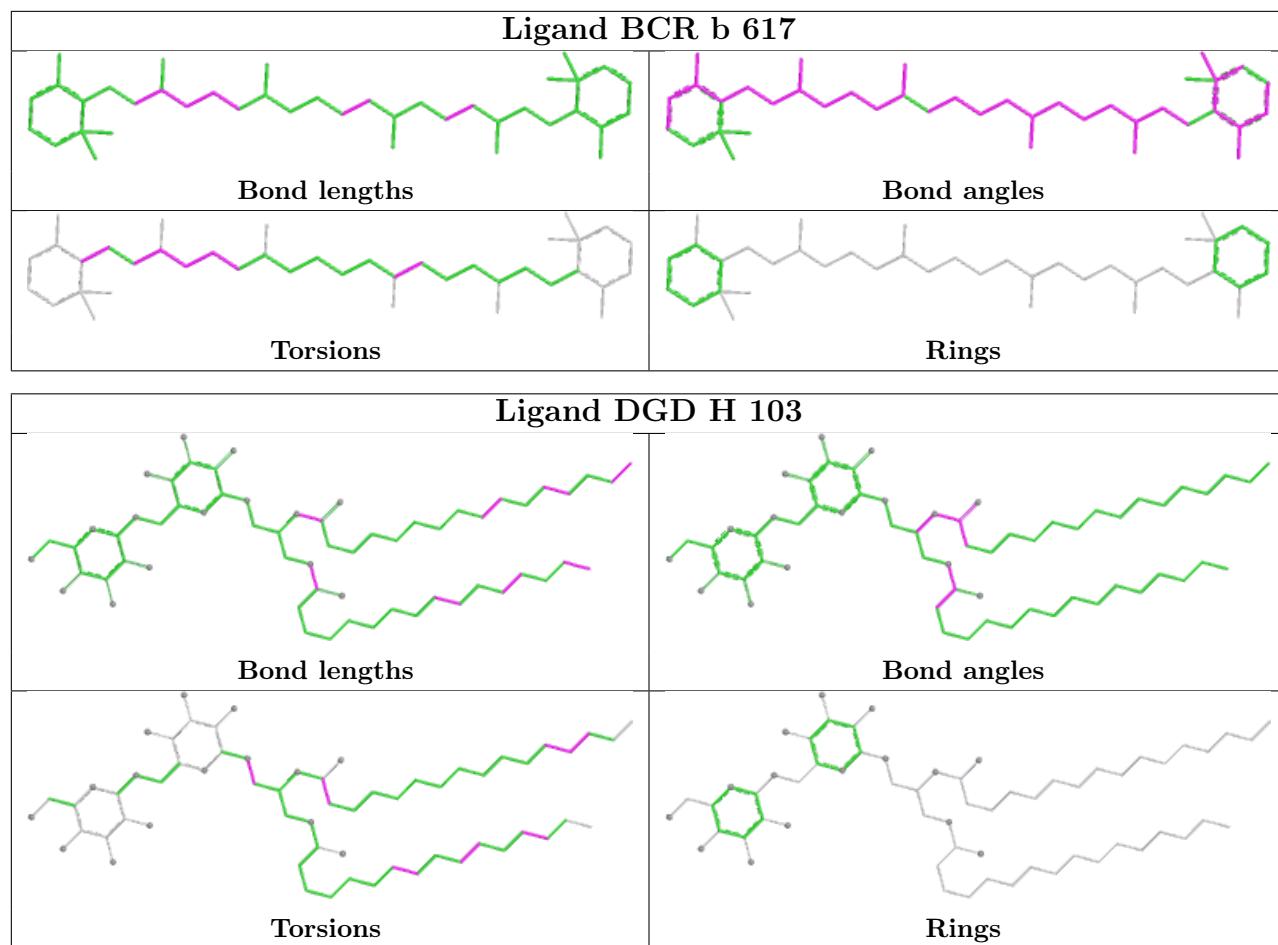
Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

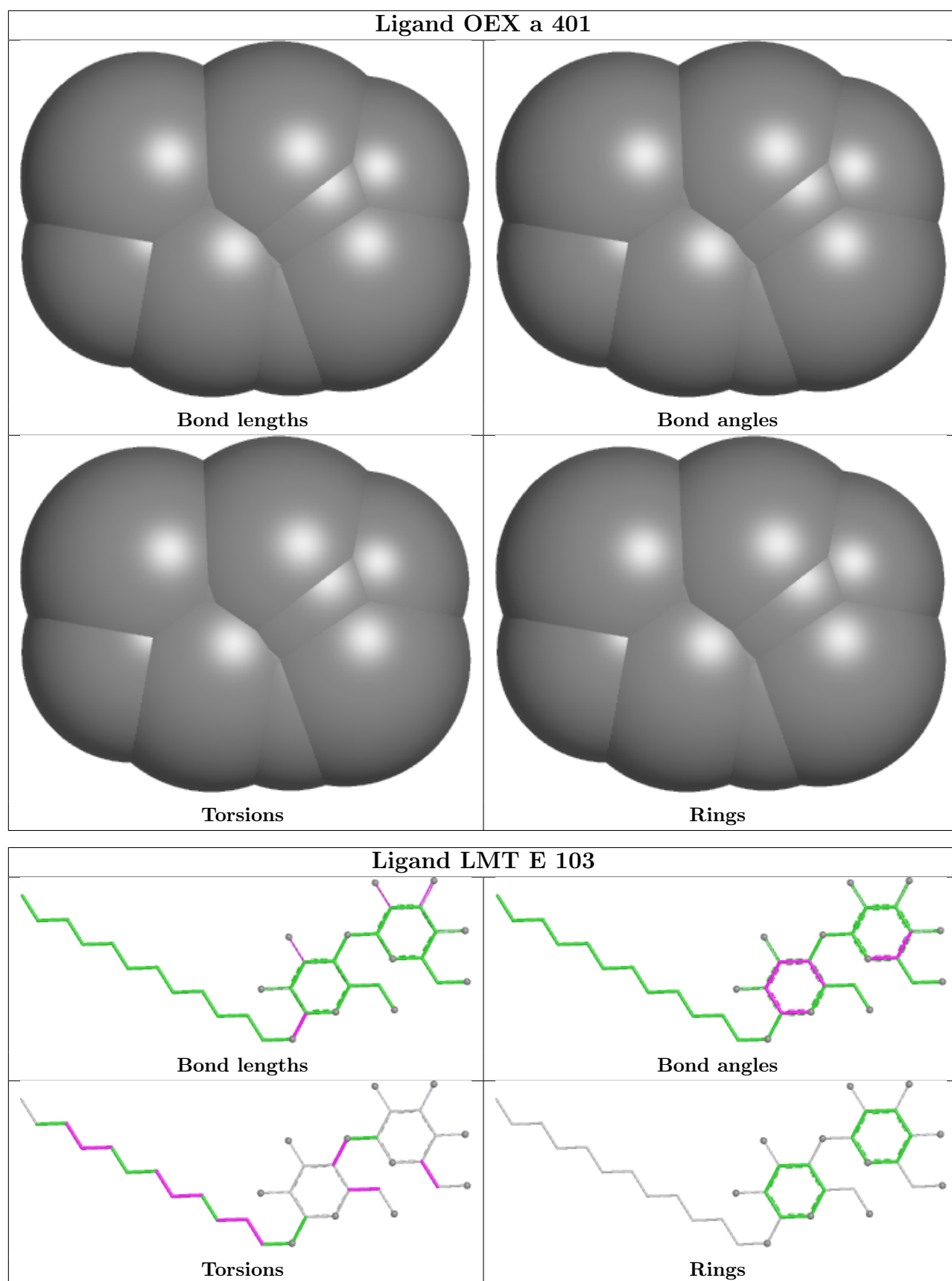
Ligand LMG B 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

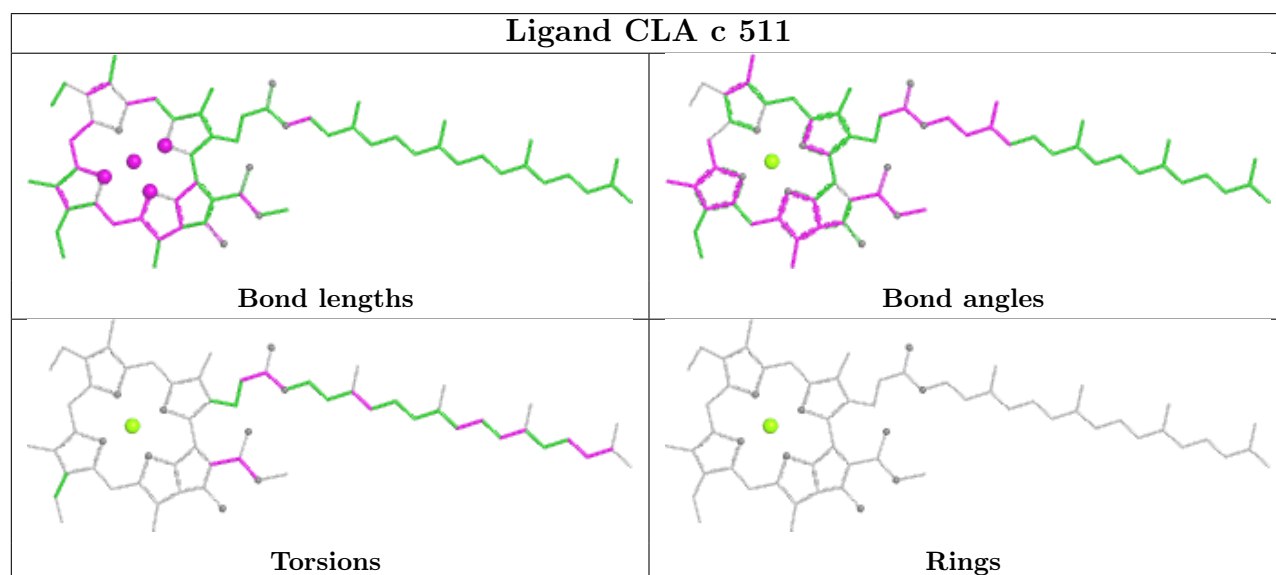
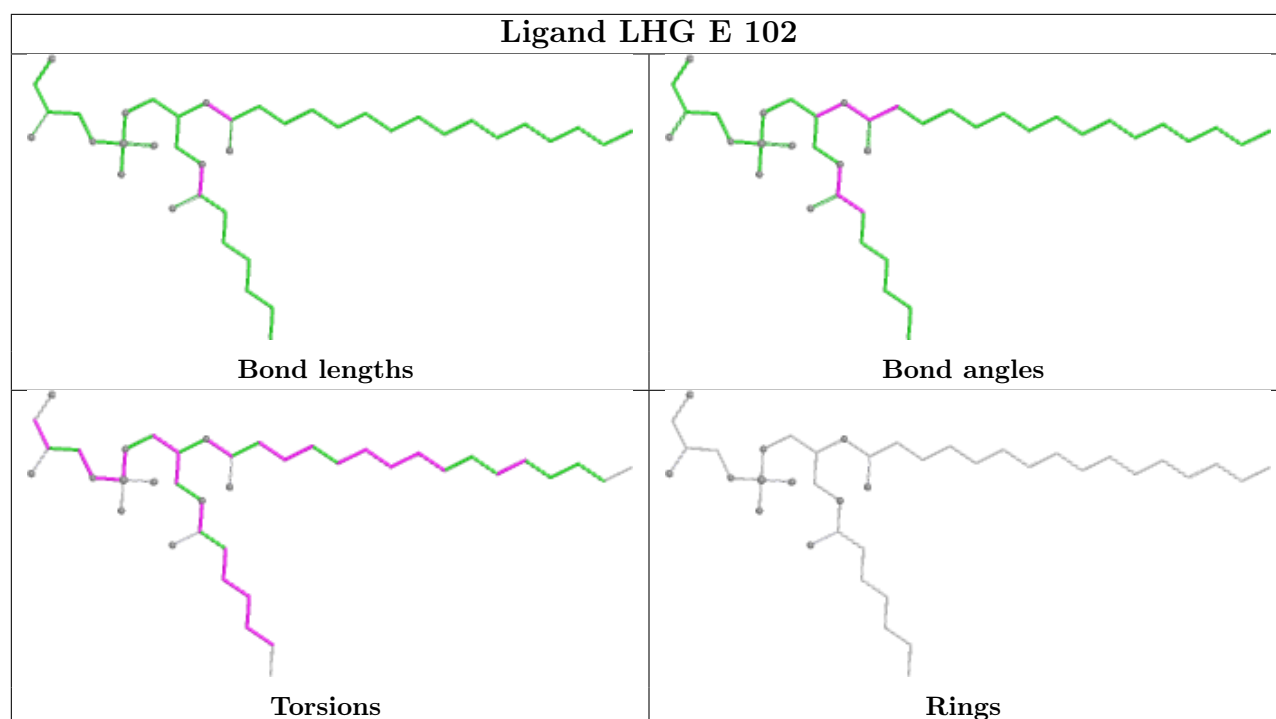
Ligand PHO D 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

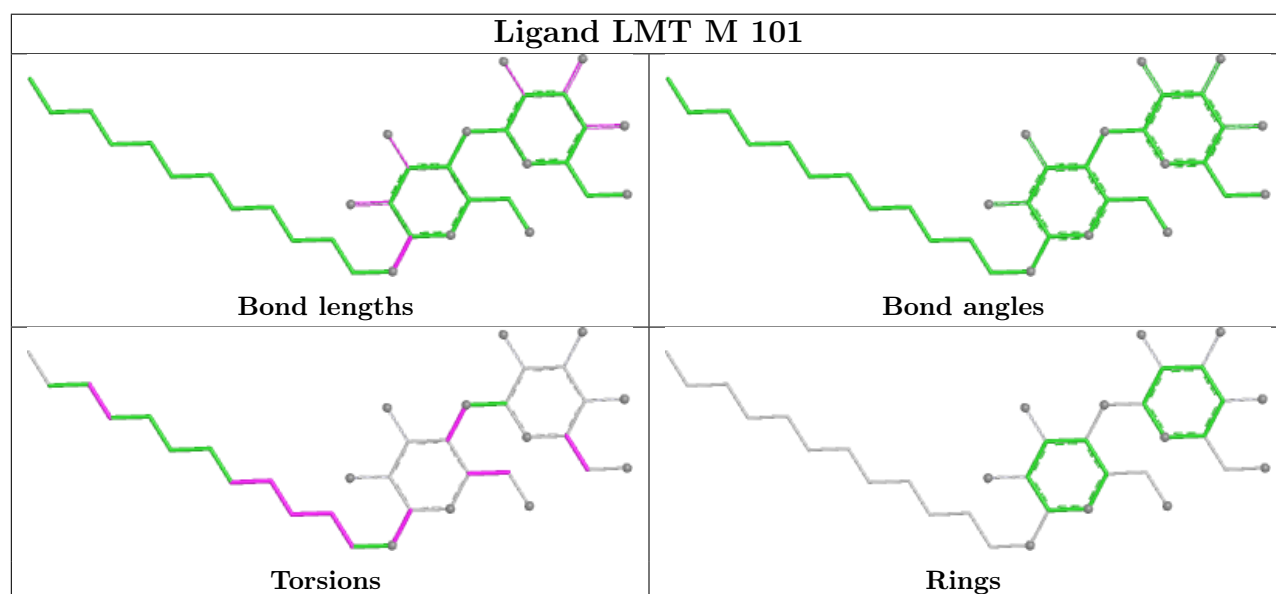
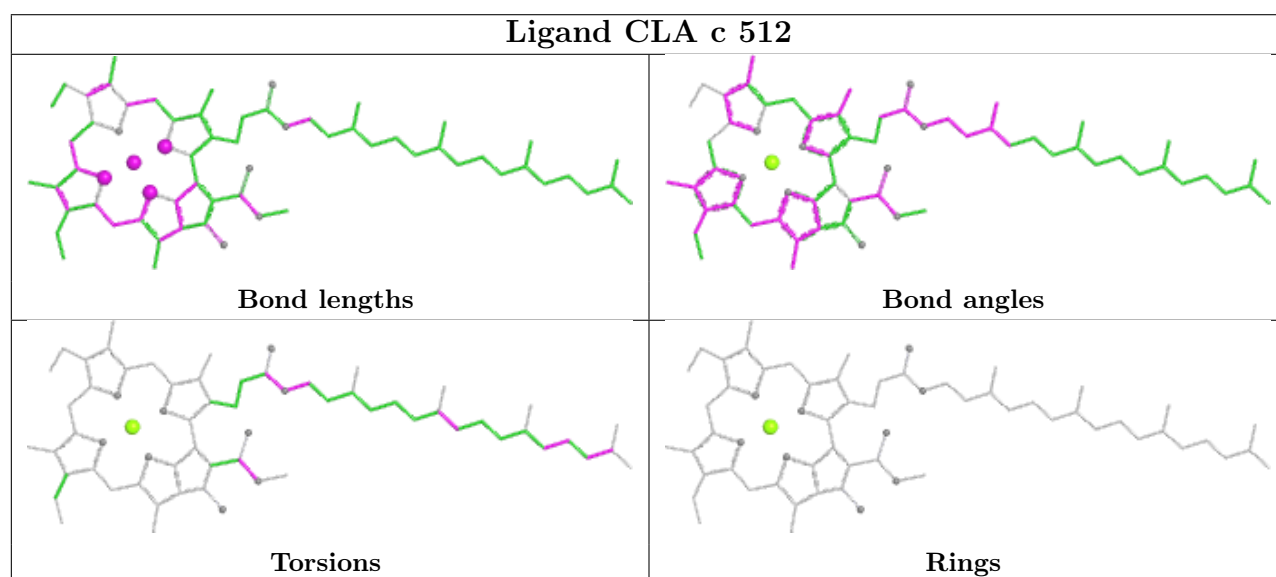
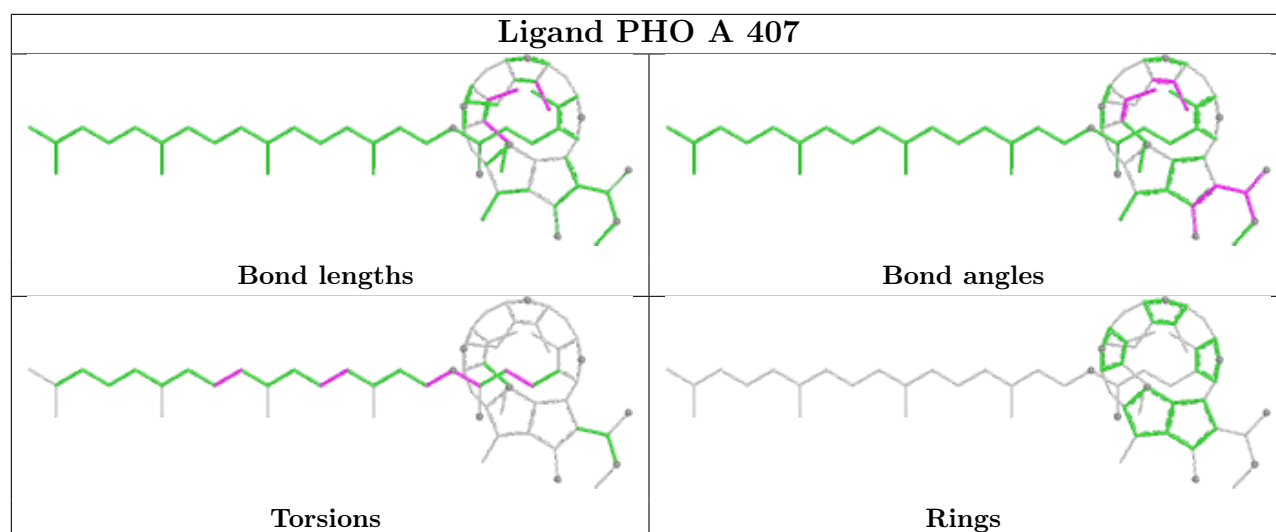


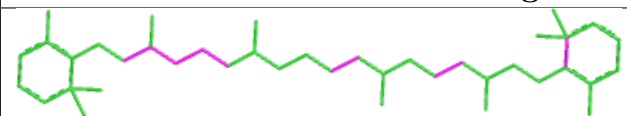
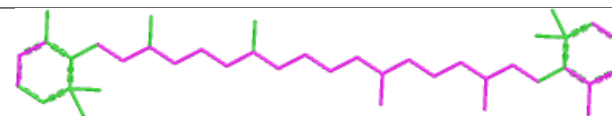
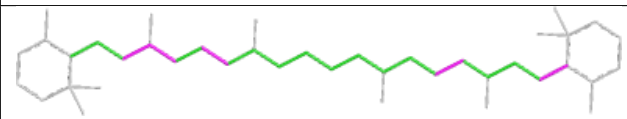
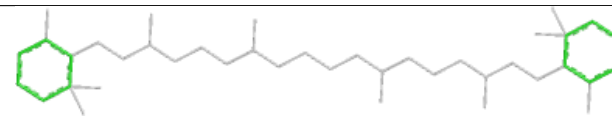


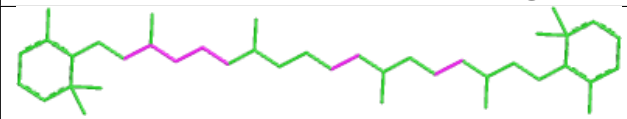
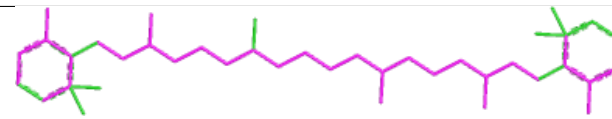
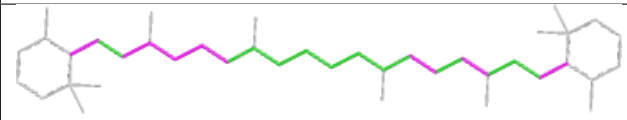
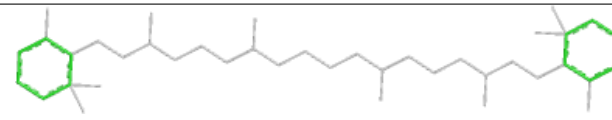


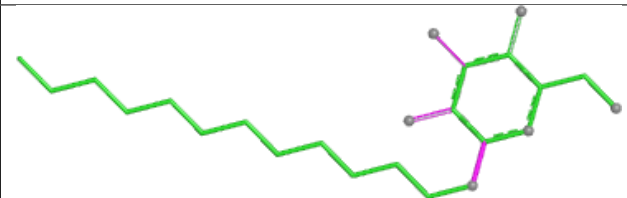
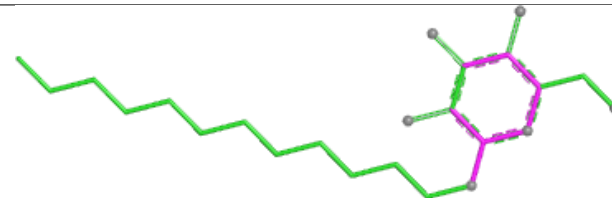
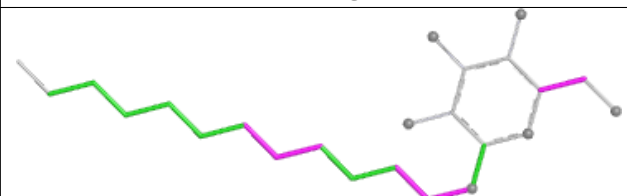
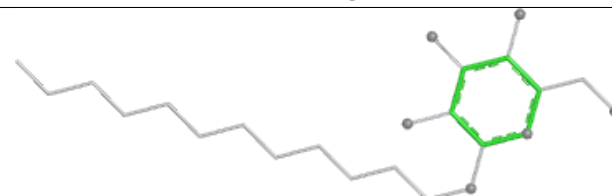


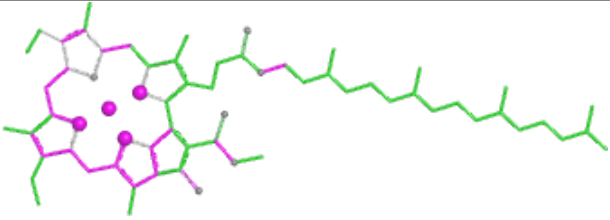
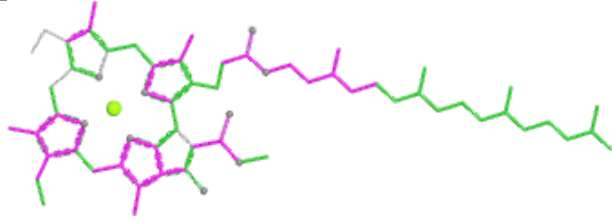
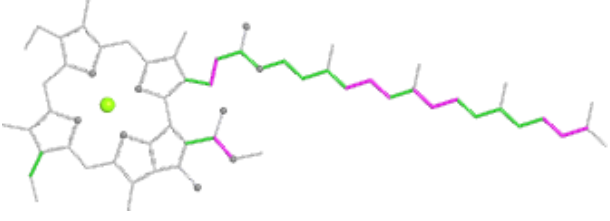
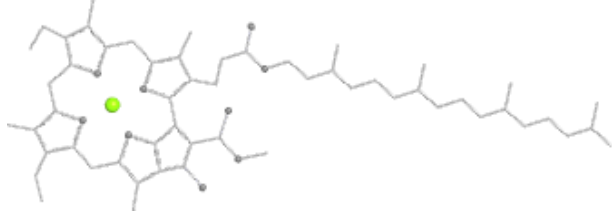


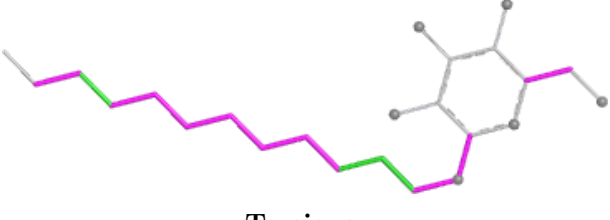
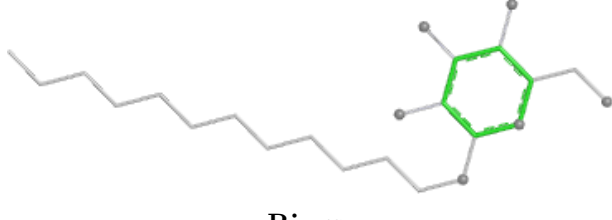
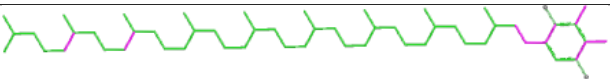
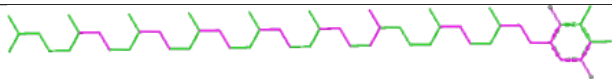
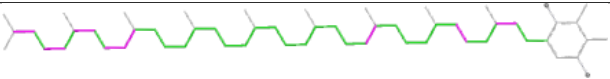
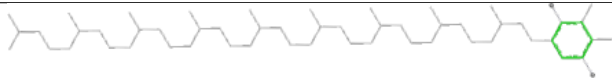


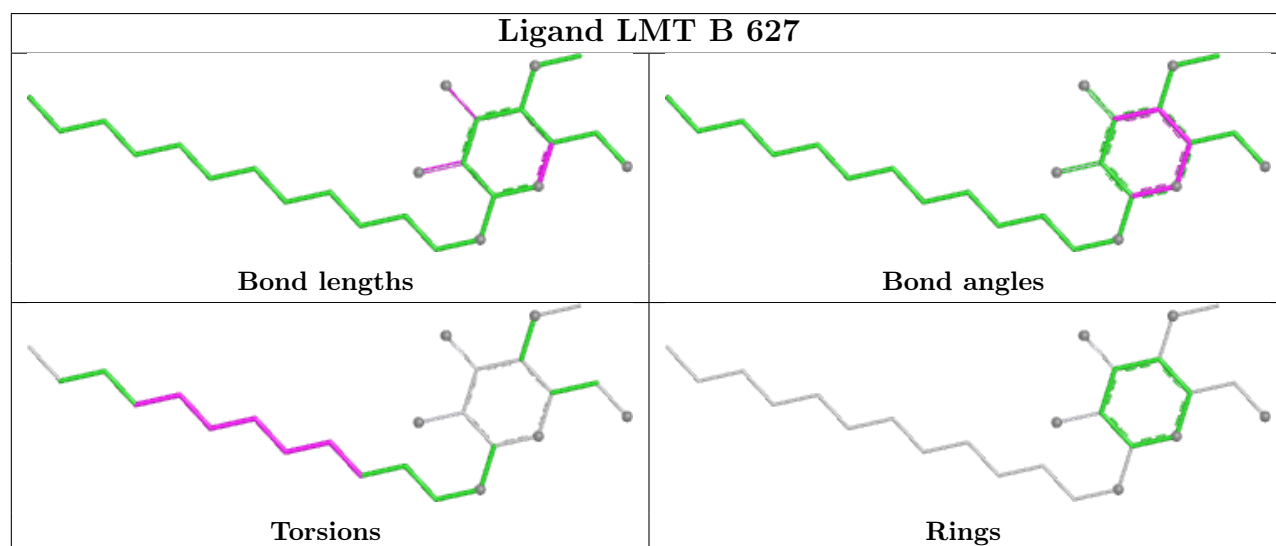
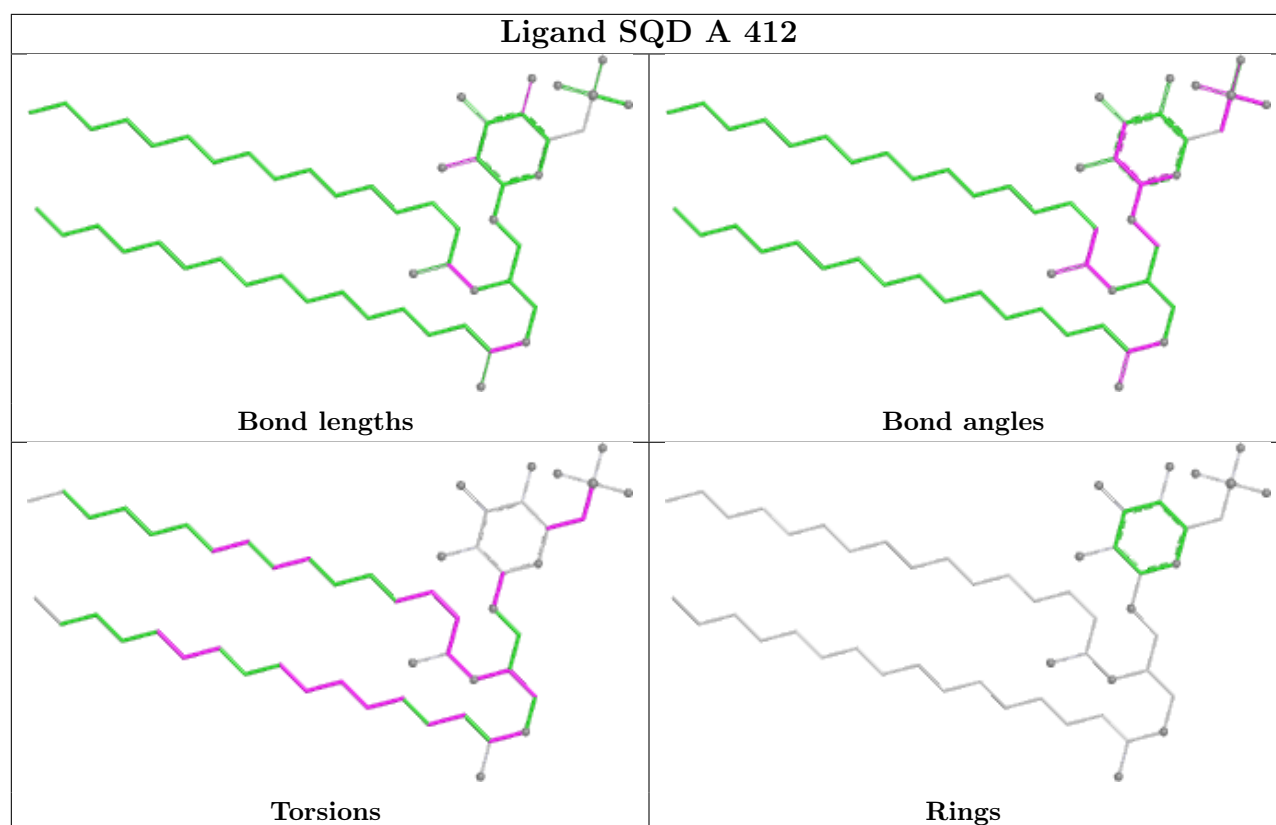


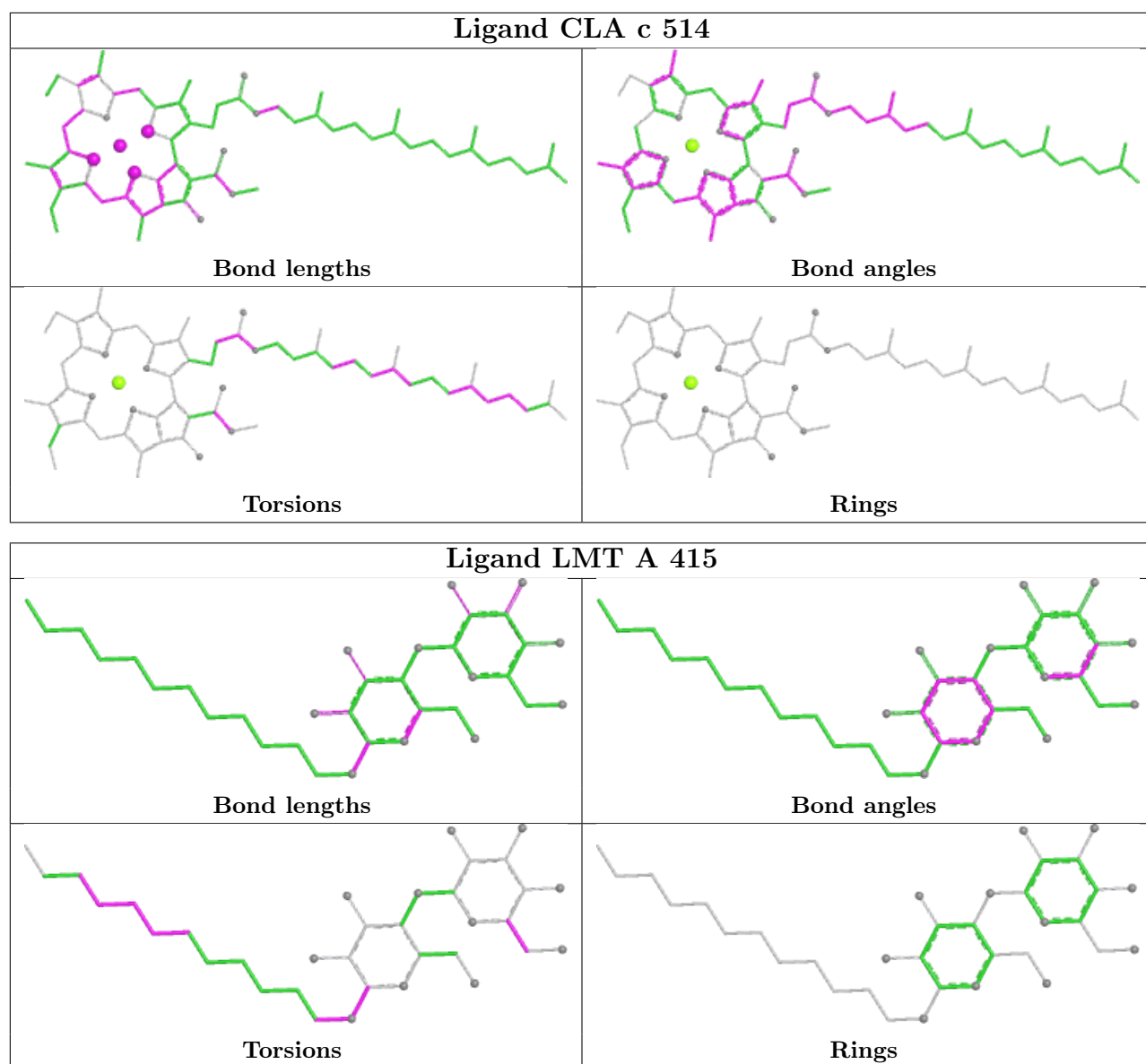
Ligand BCR Z 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

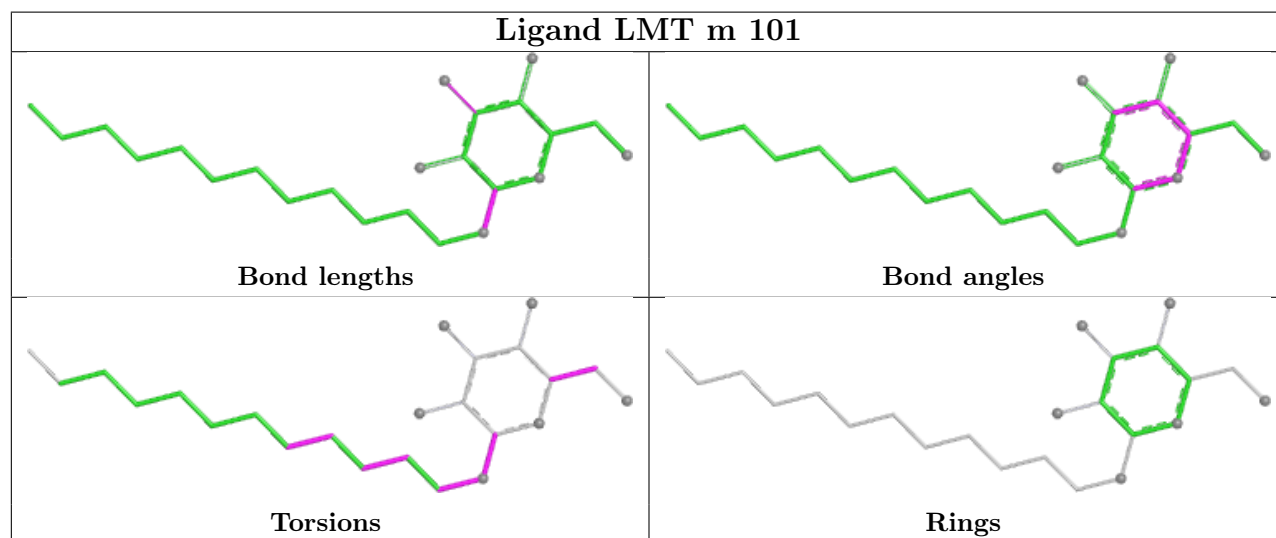
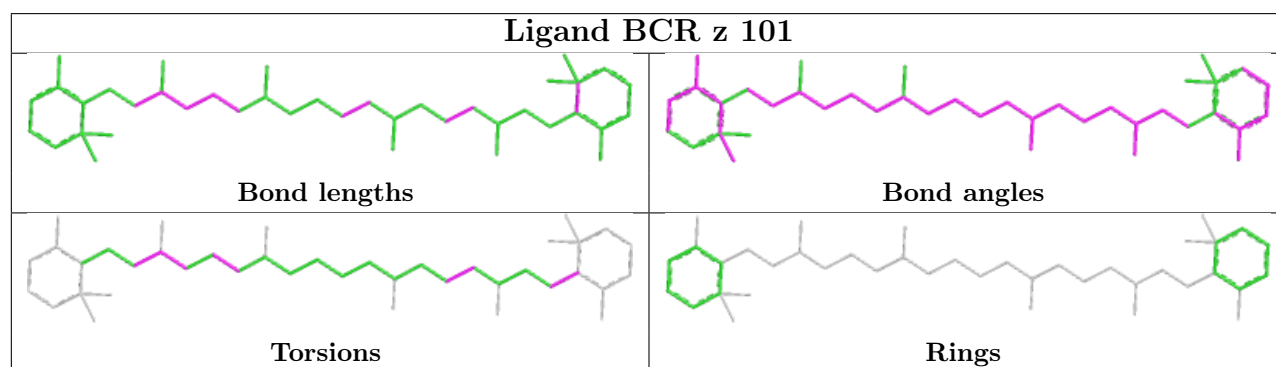
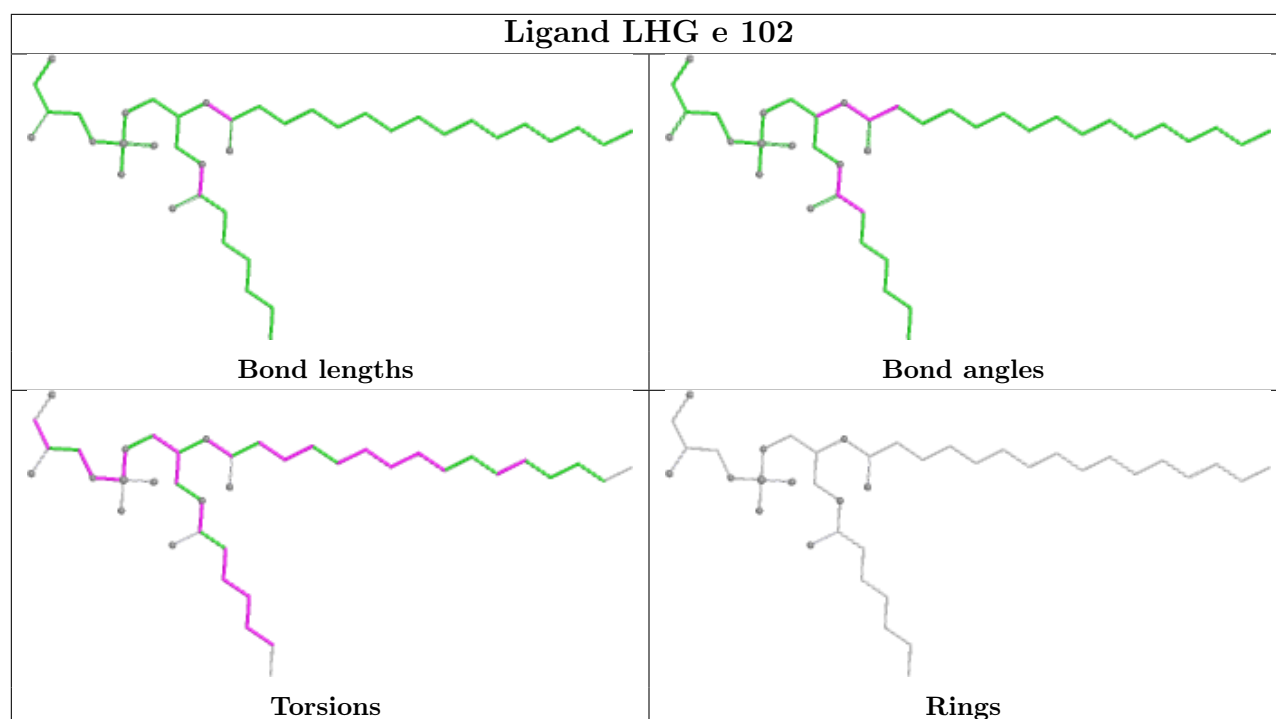
Ligand BCR k 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

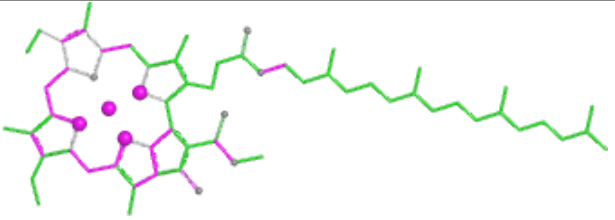
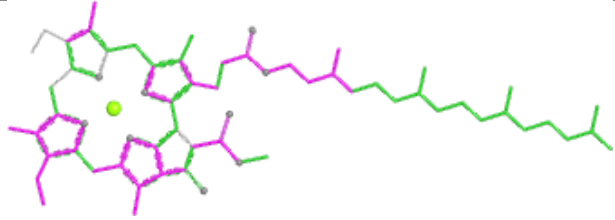
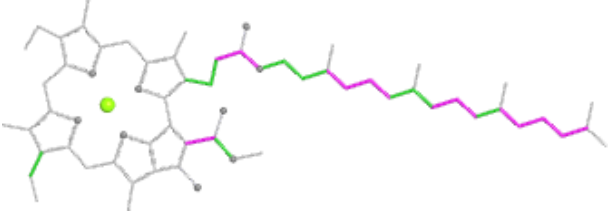
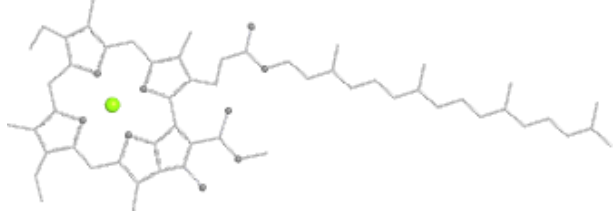
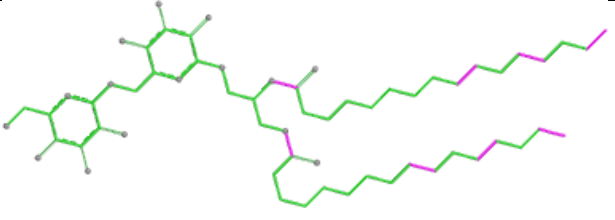
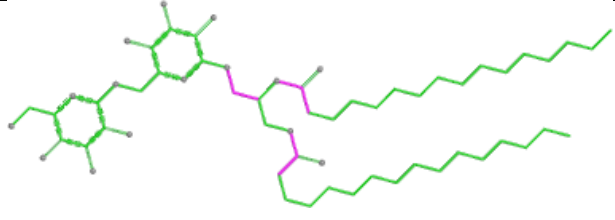
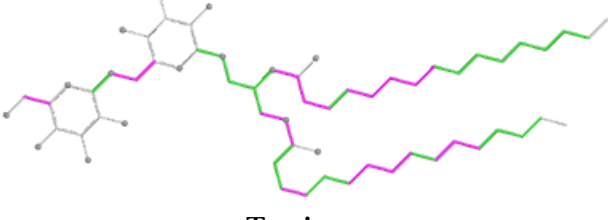
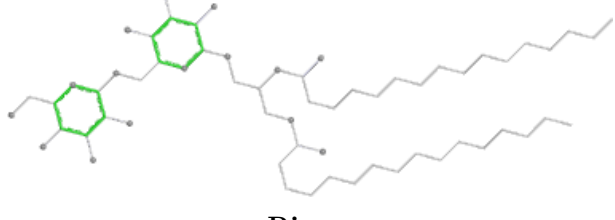
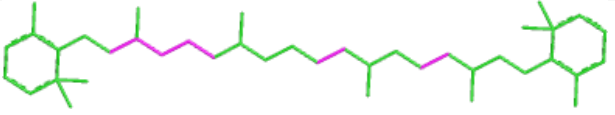
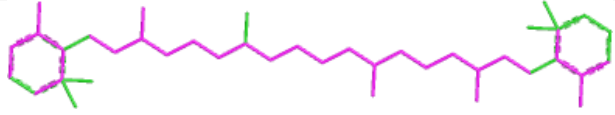
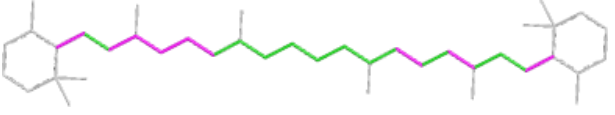
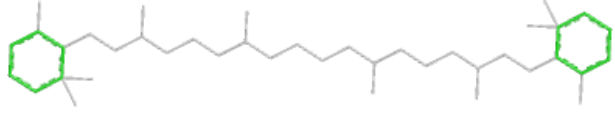
Ligand LMT T 701	
	
Bond lengths	Bond angles
	
Torsions	Rings

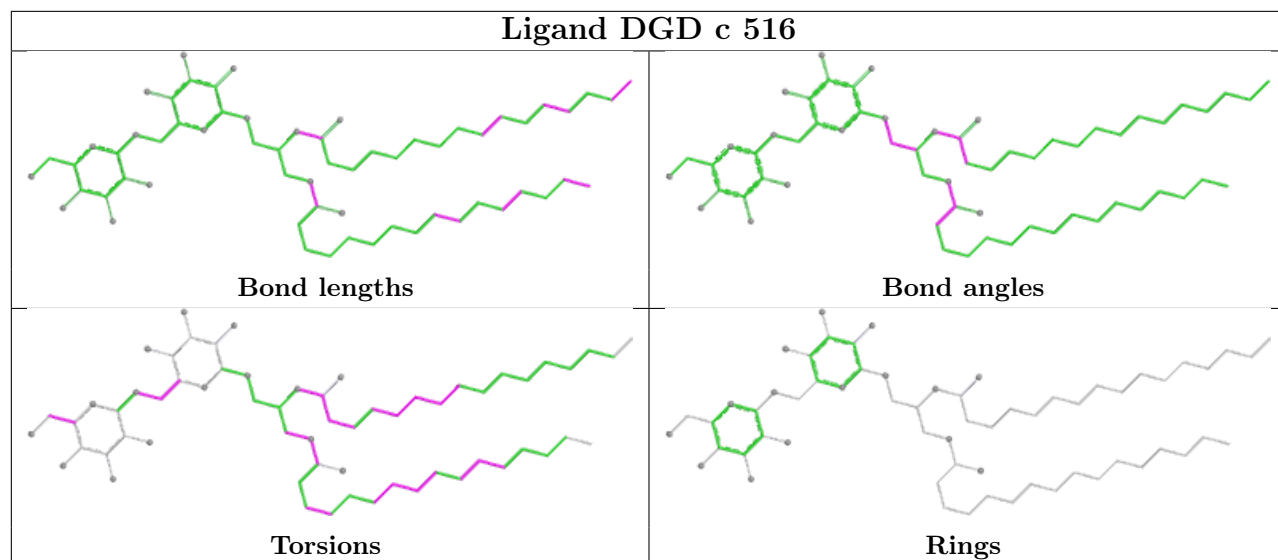
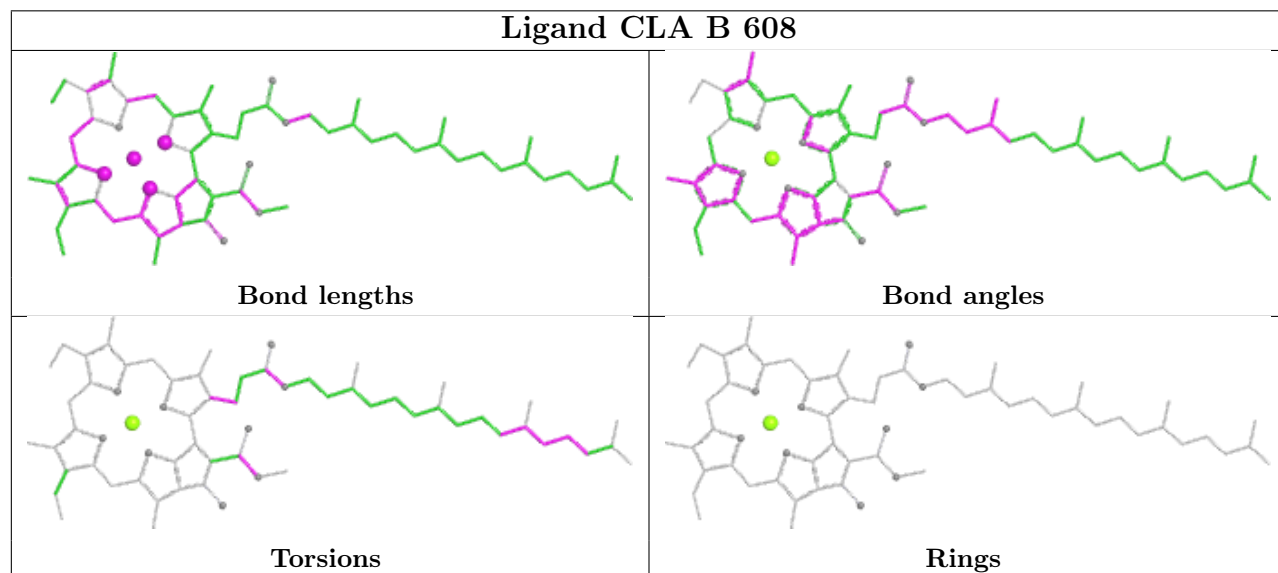
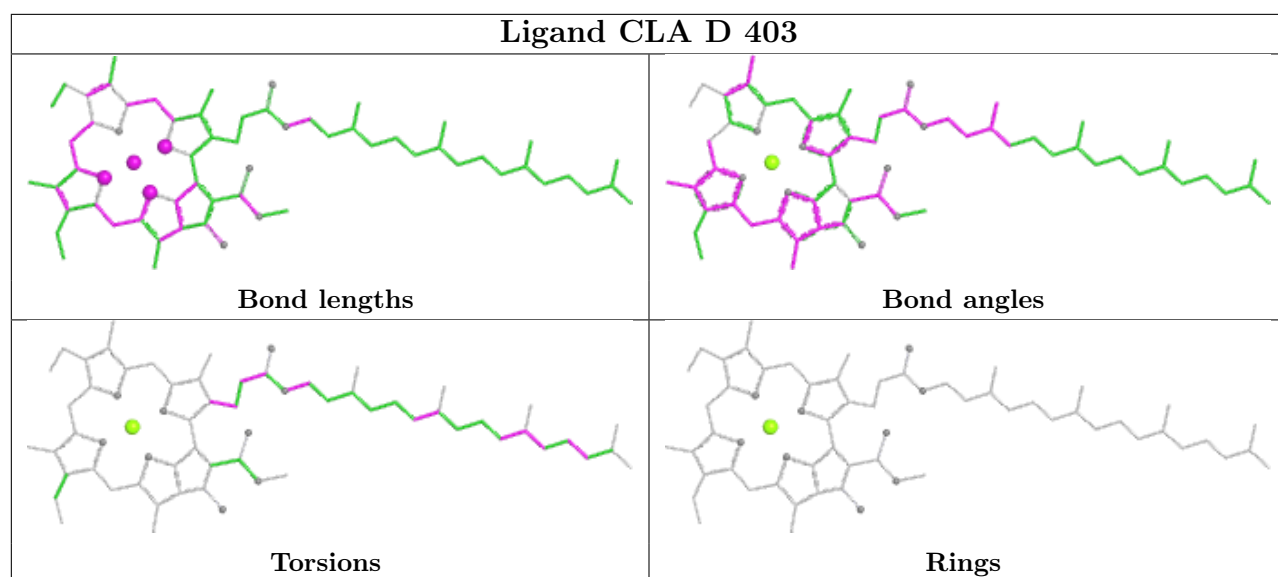
Ligand CLA C 504	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LMT D 410	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PL9 D 405	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

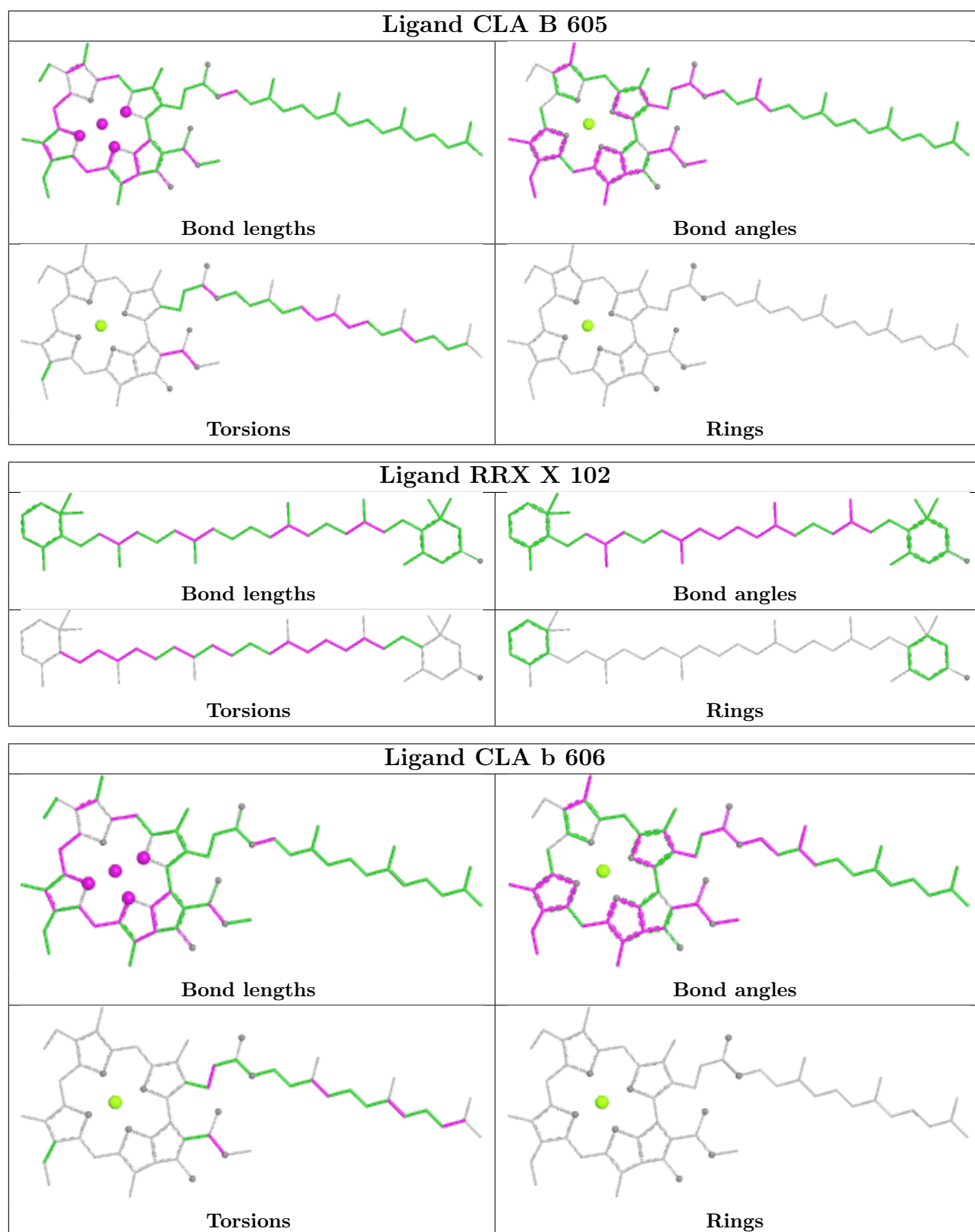


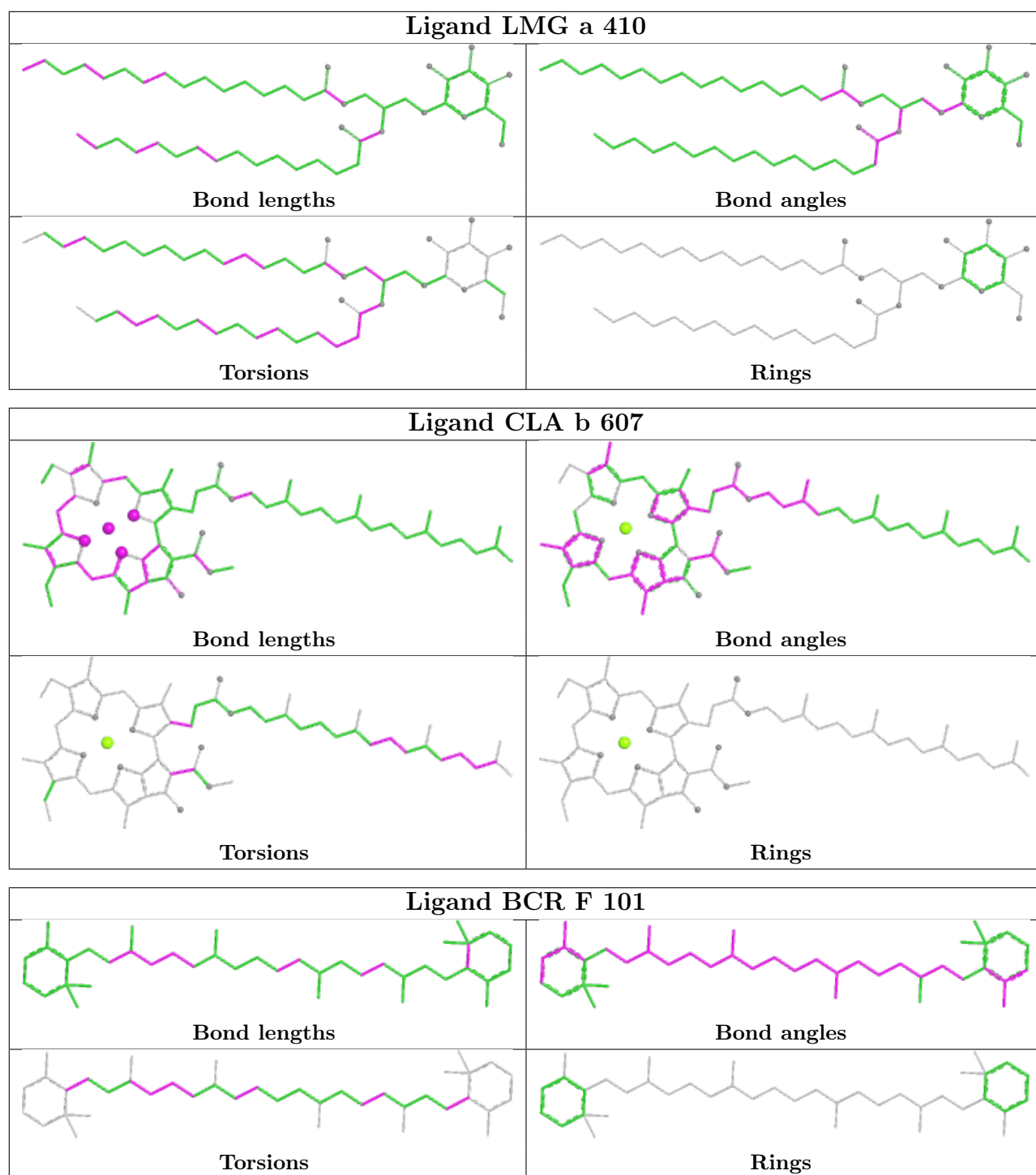


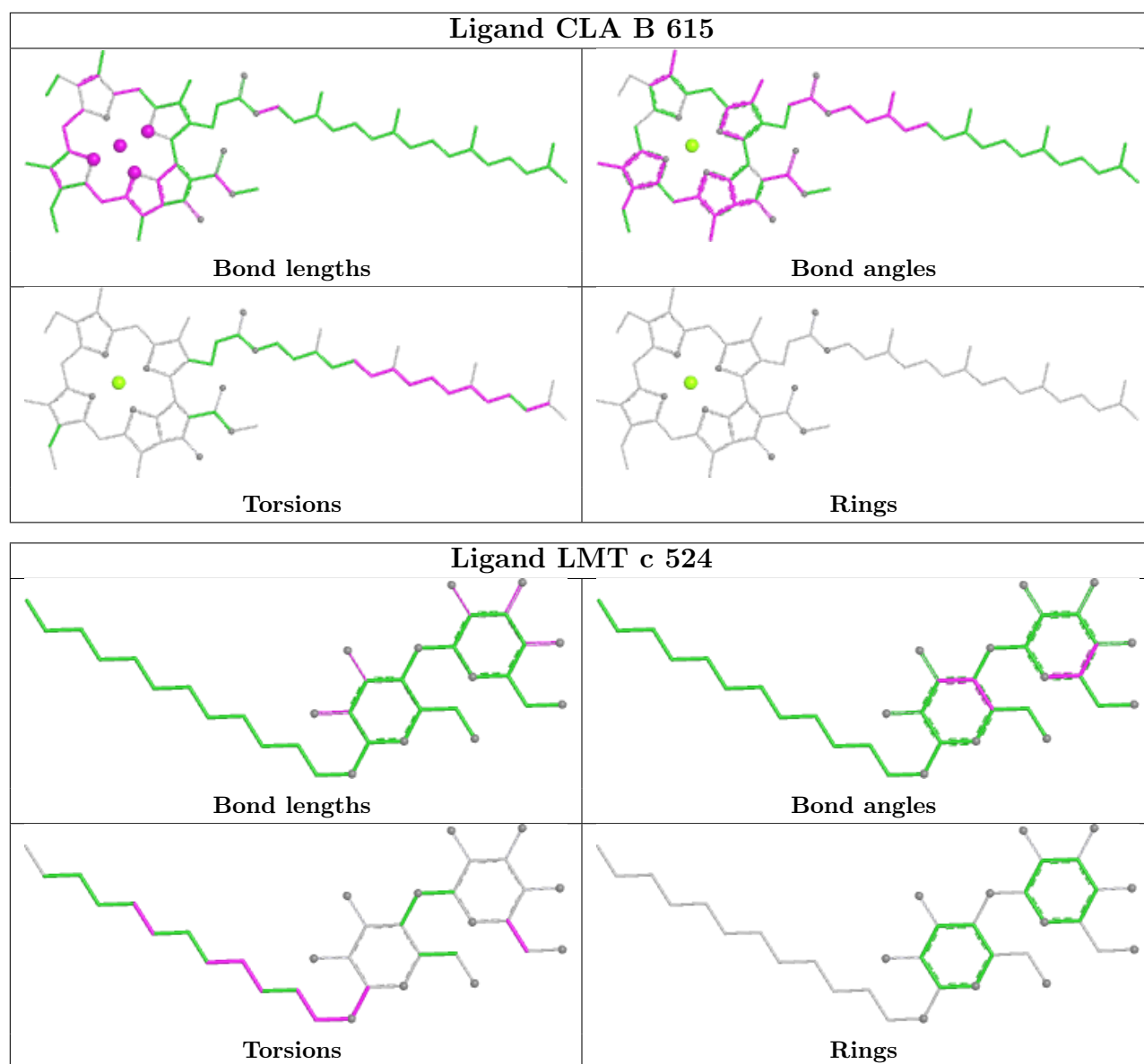


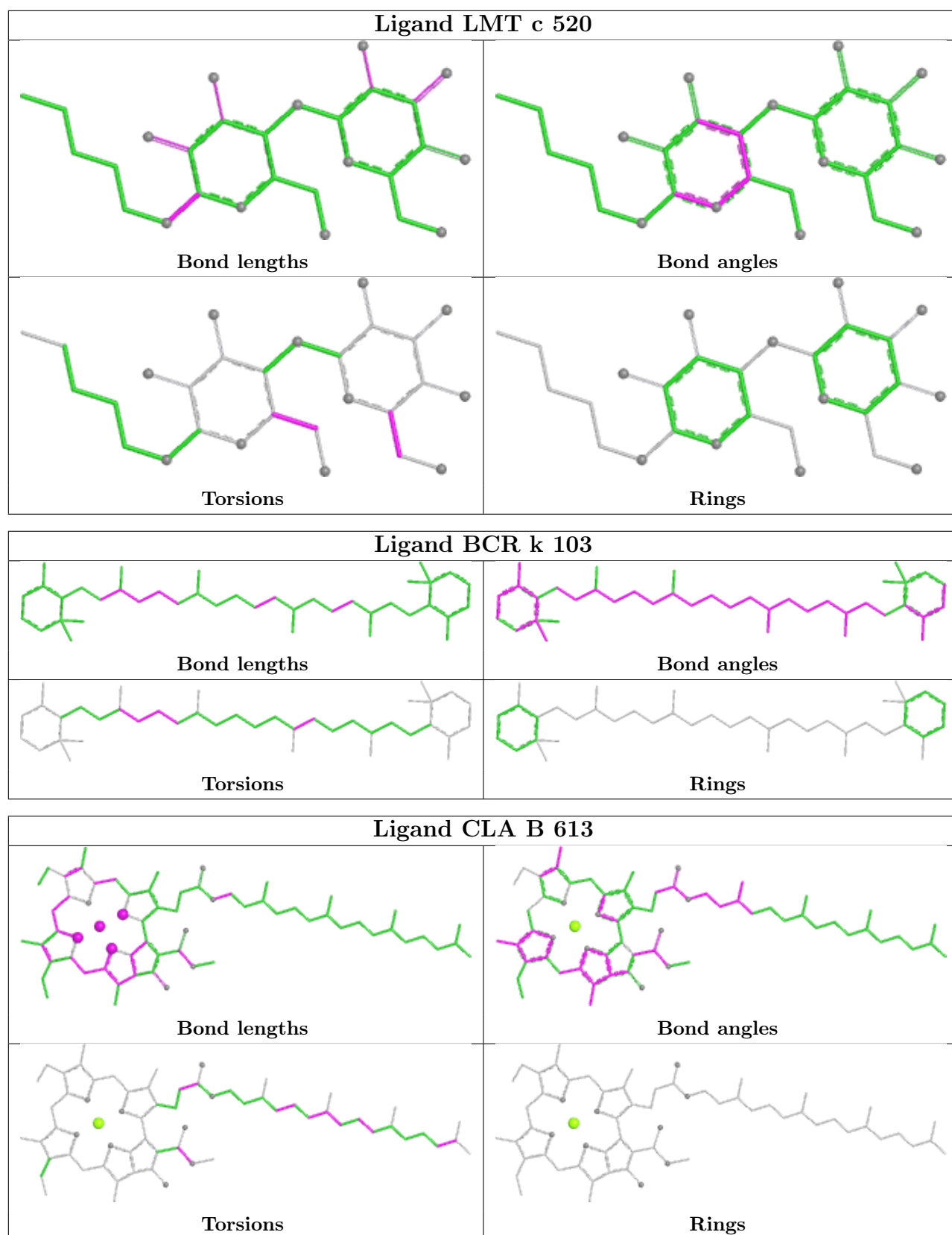
Ligand CLA b 614	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand DGD C 516	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR K 102	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

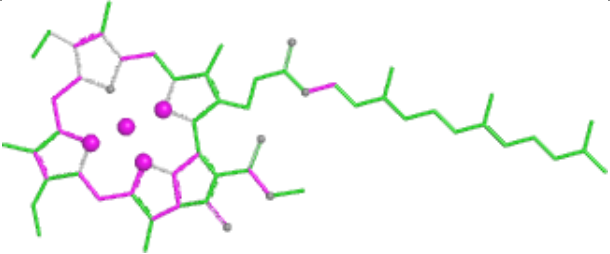
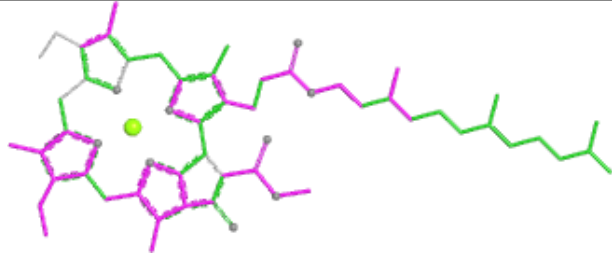
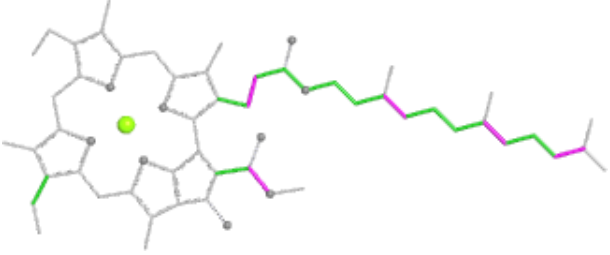
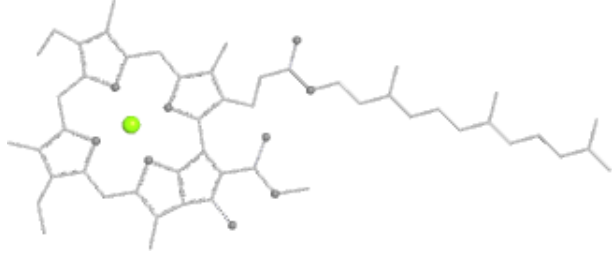
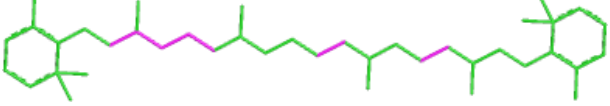
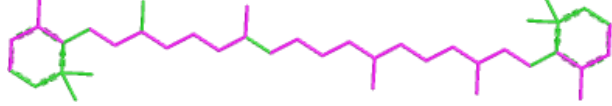
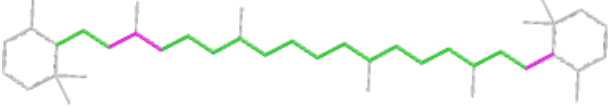
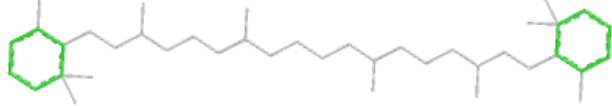
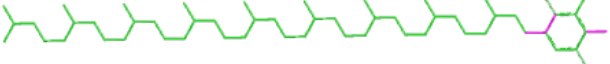

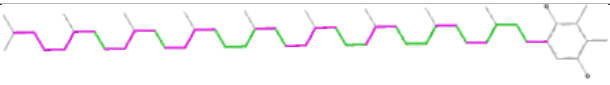
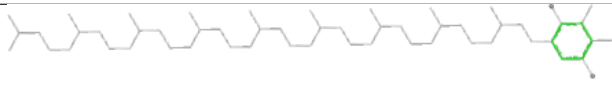


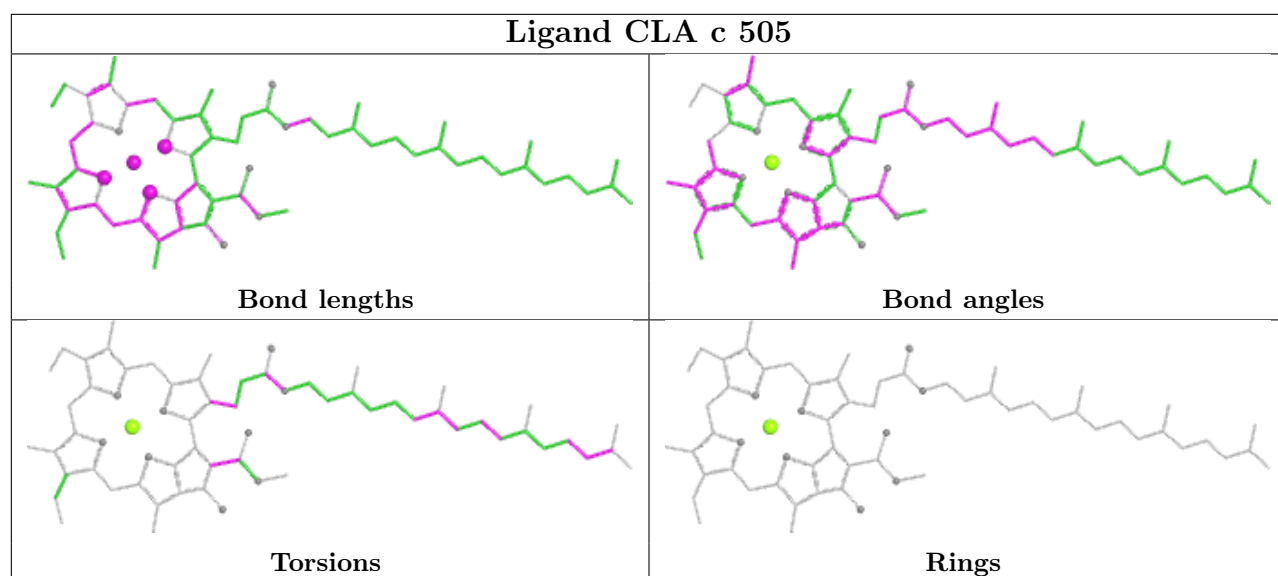
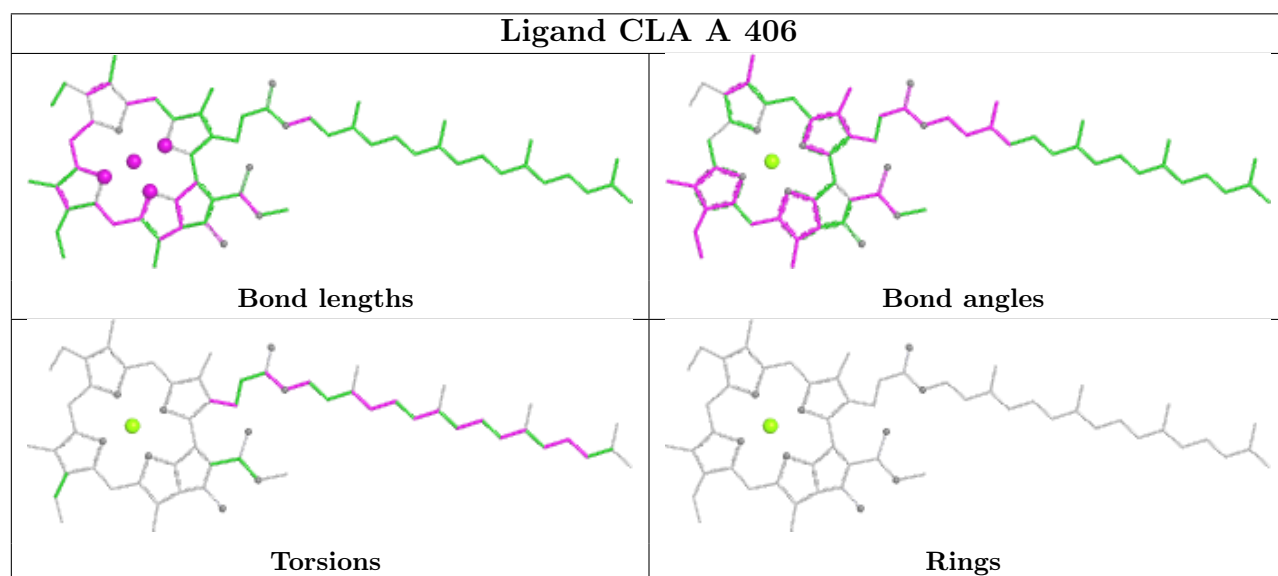
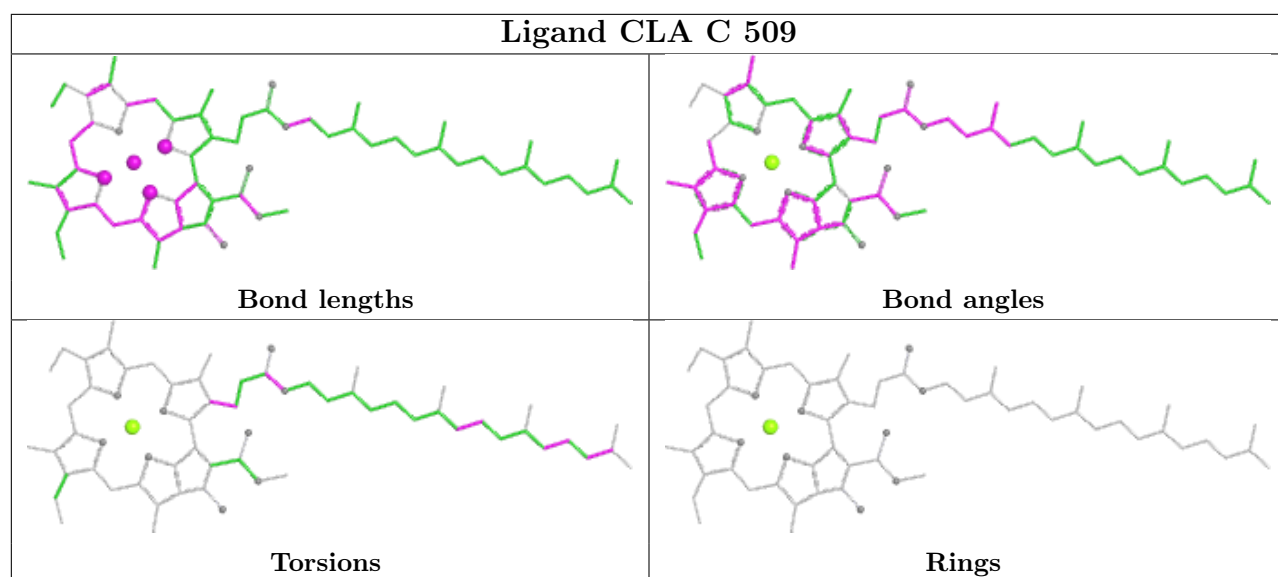


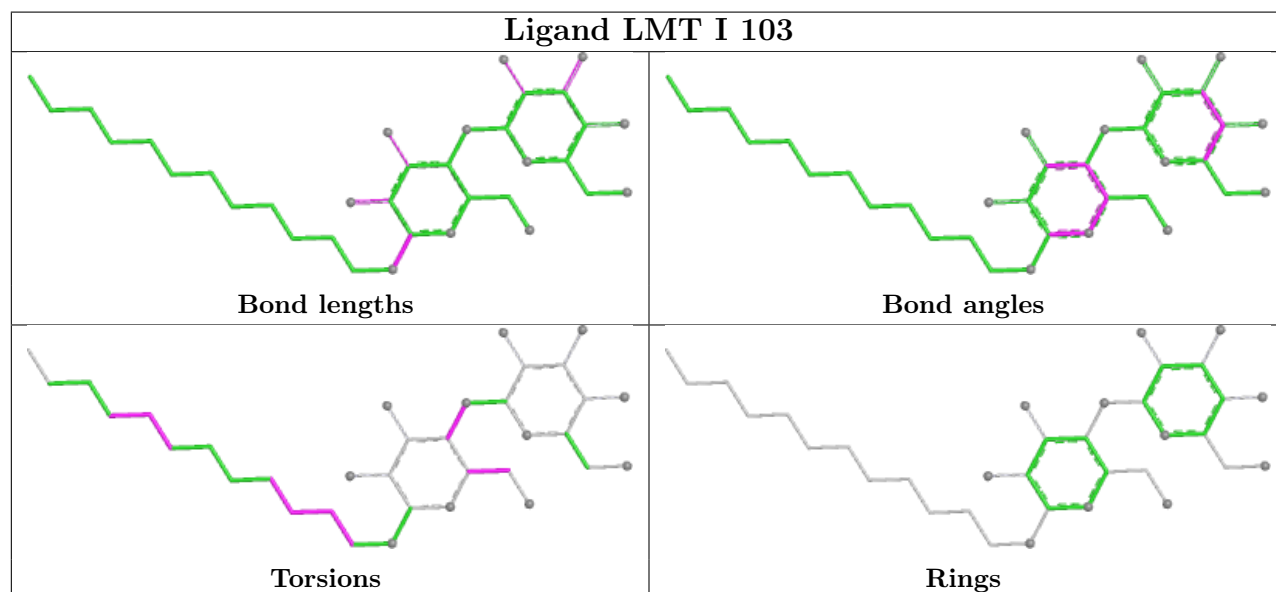
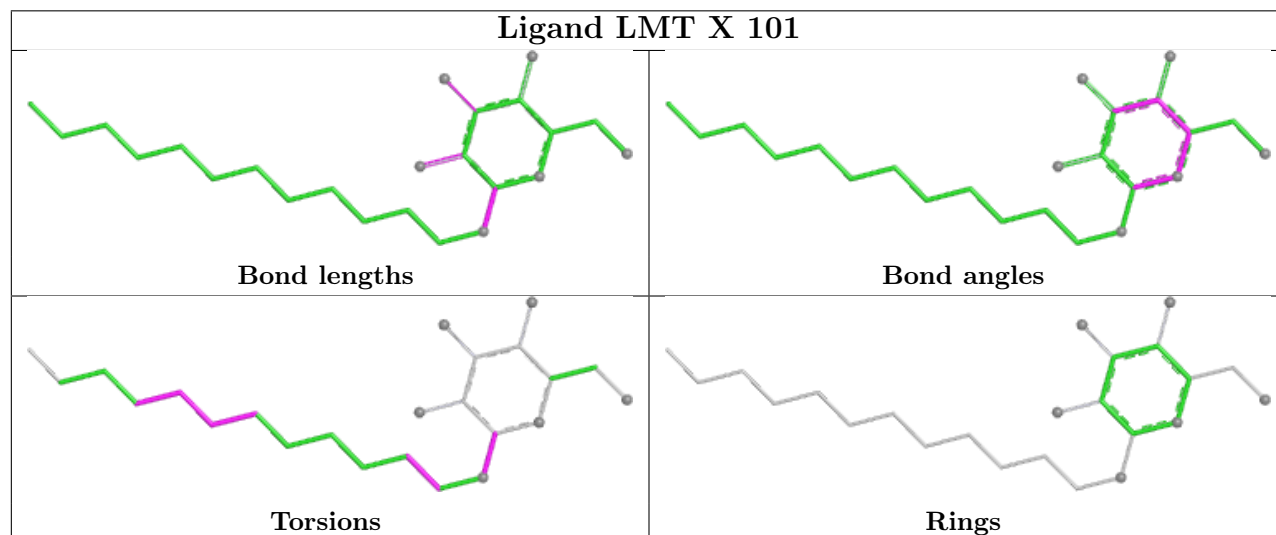
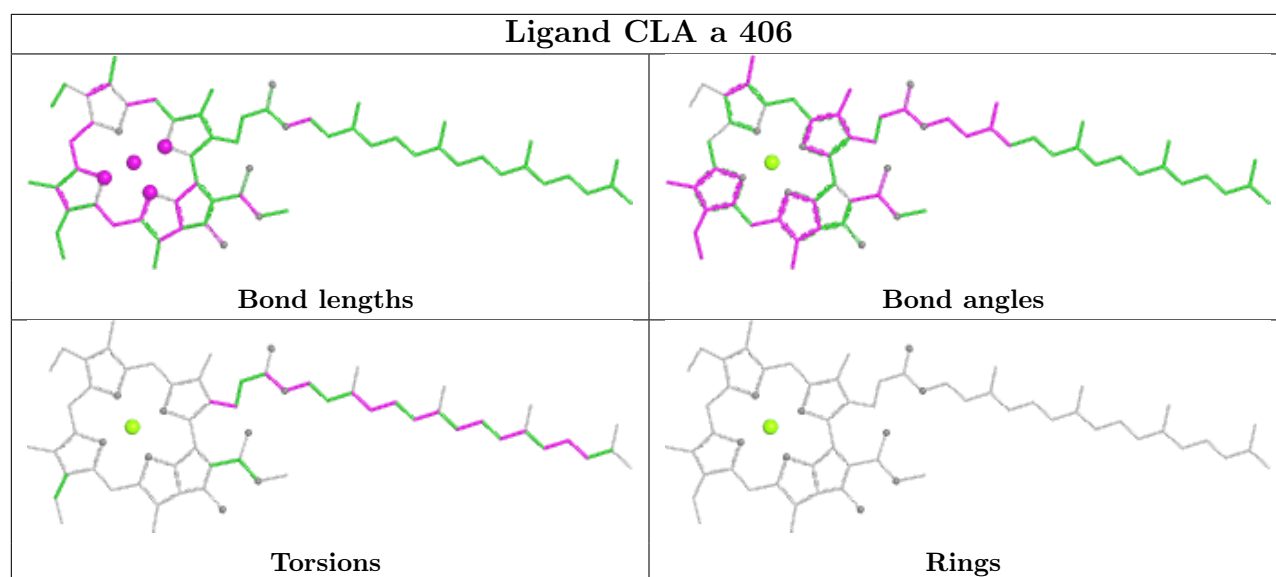


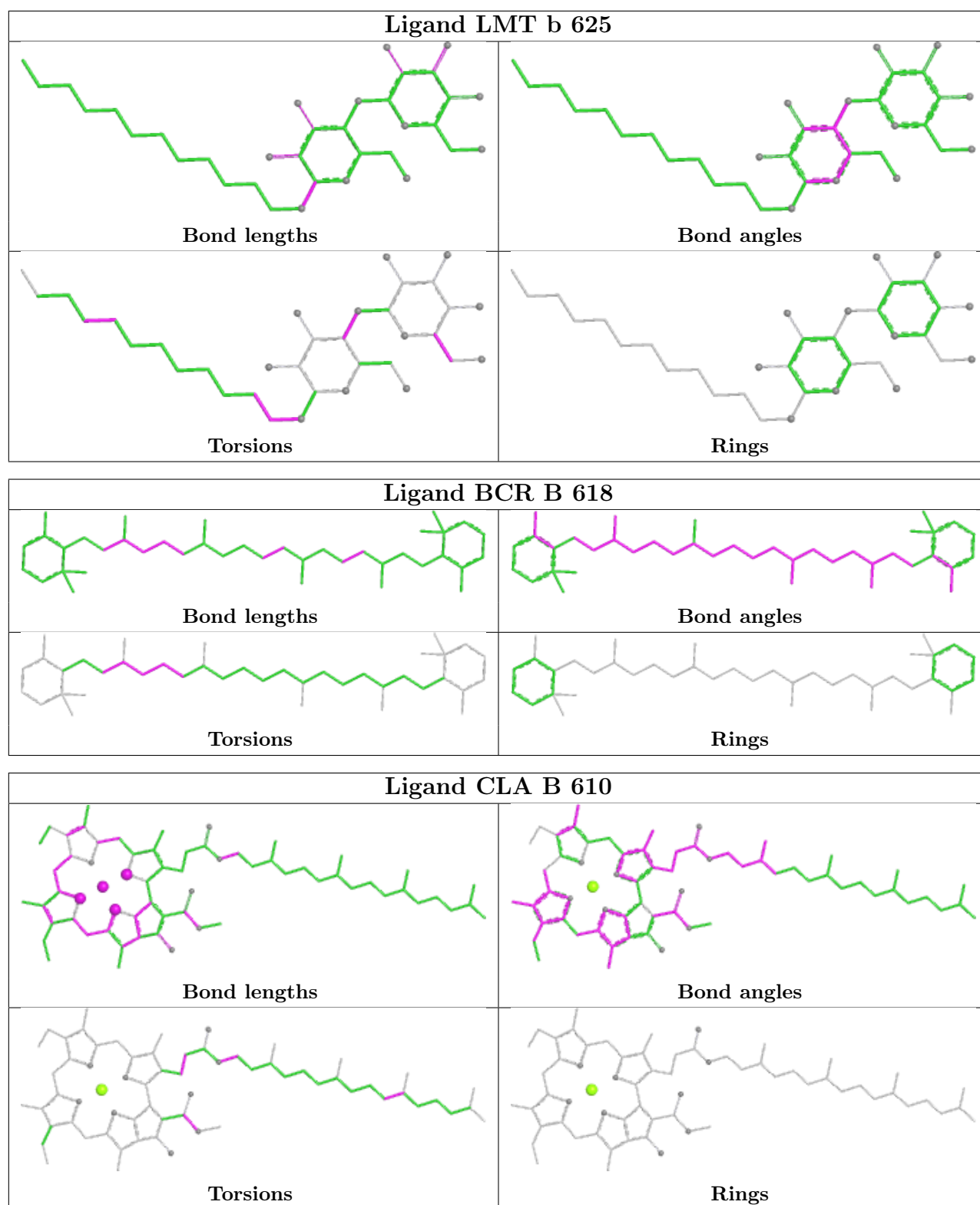


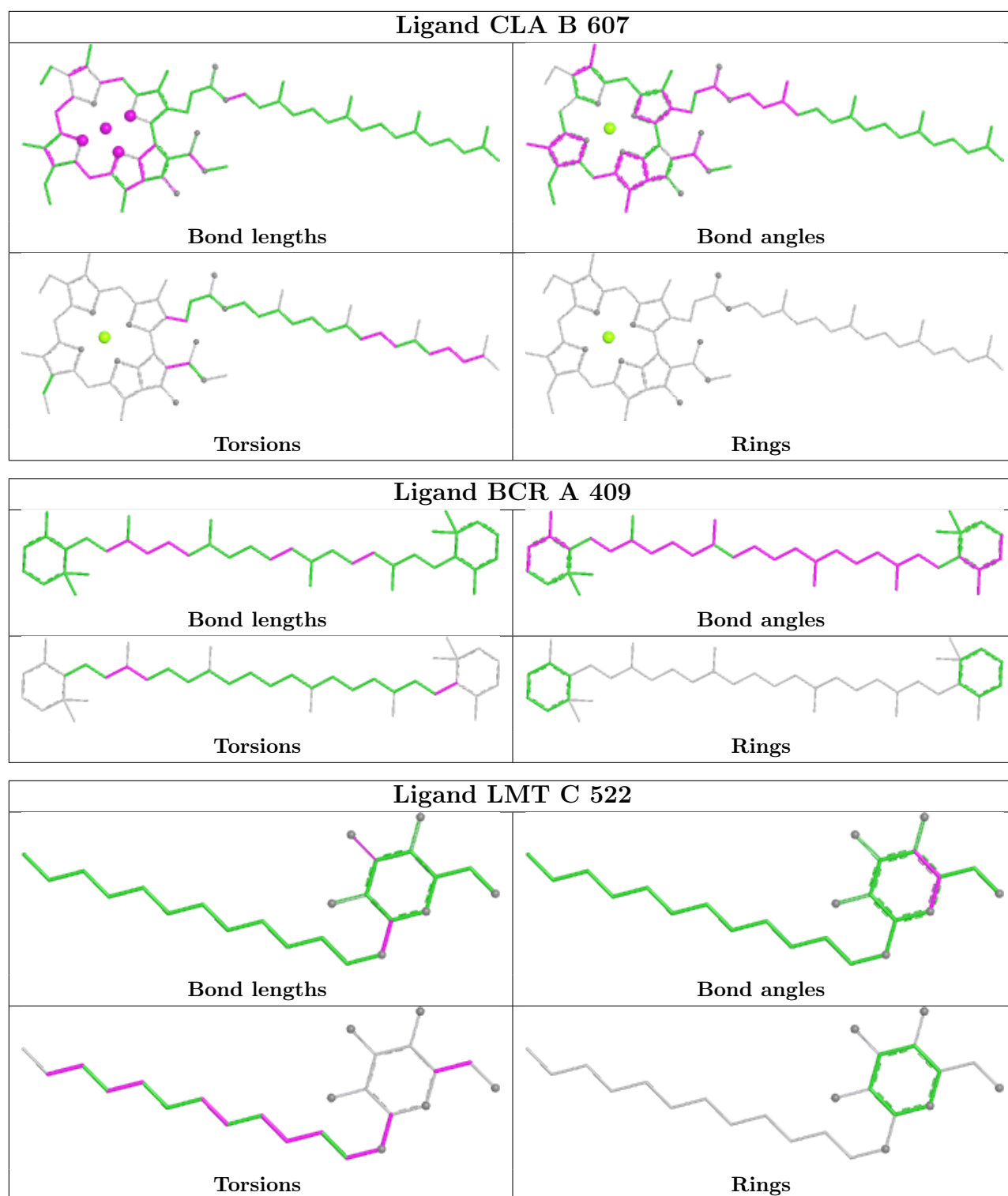


Ligand CLA B 606	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR a 409	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PL9 a 411	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

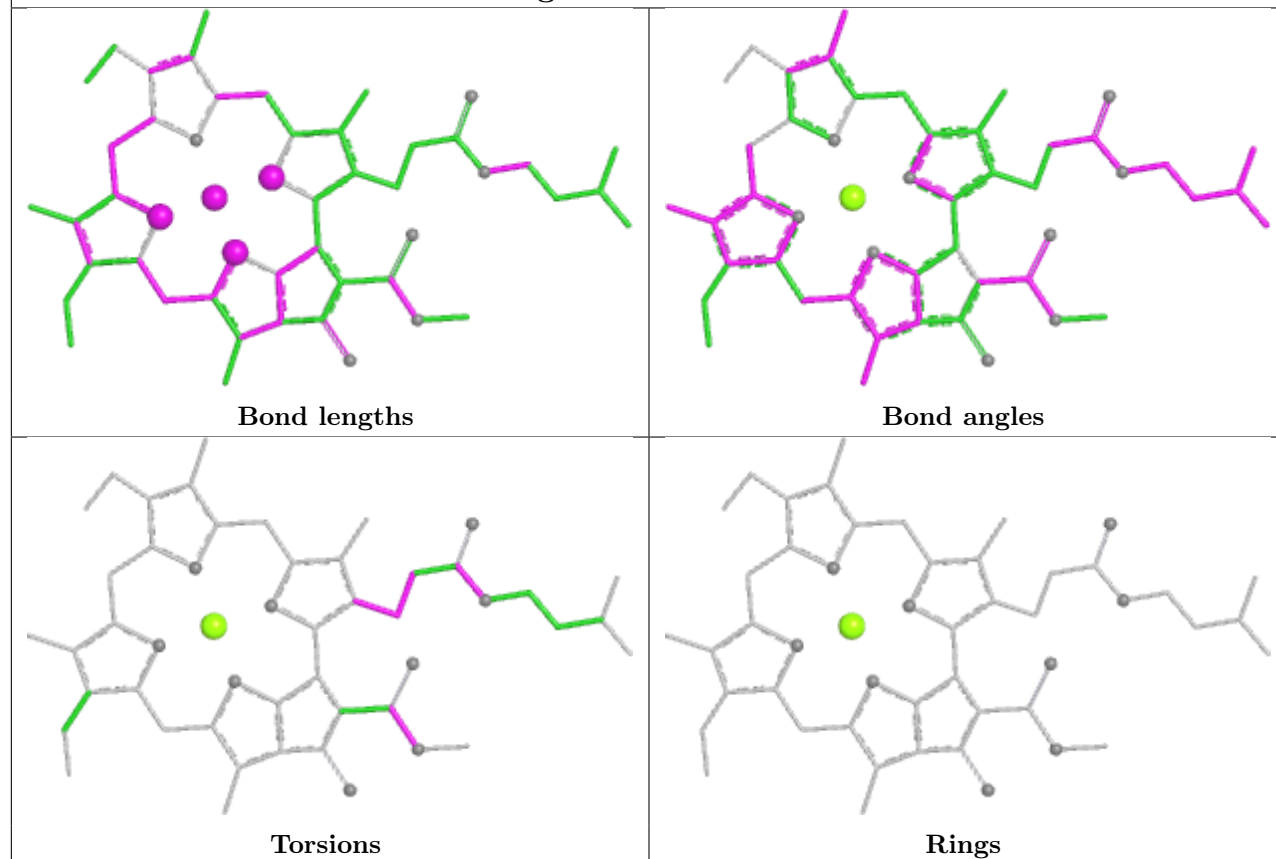




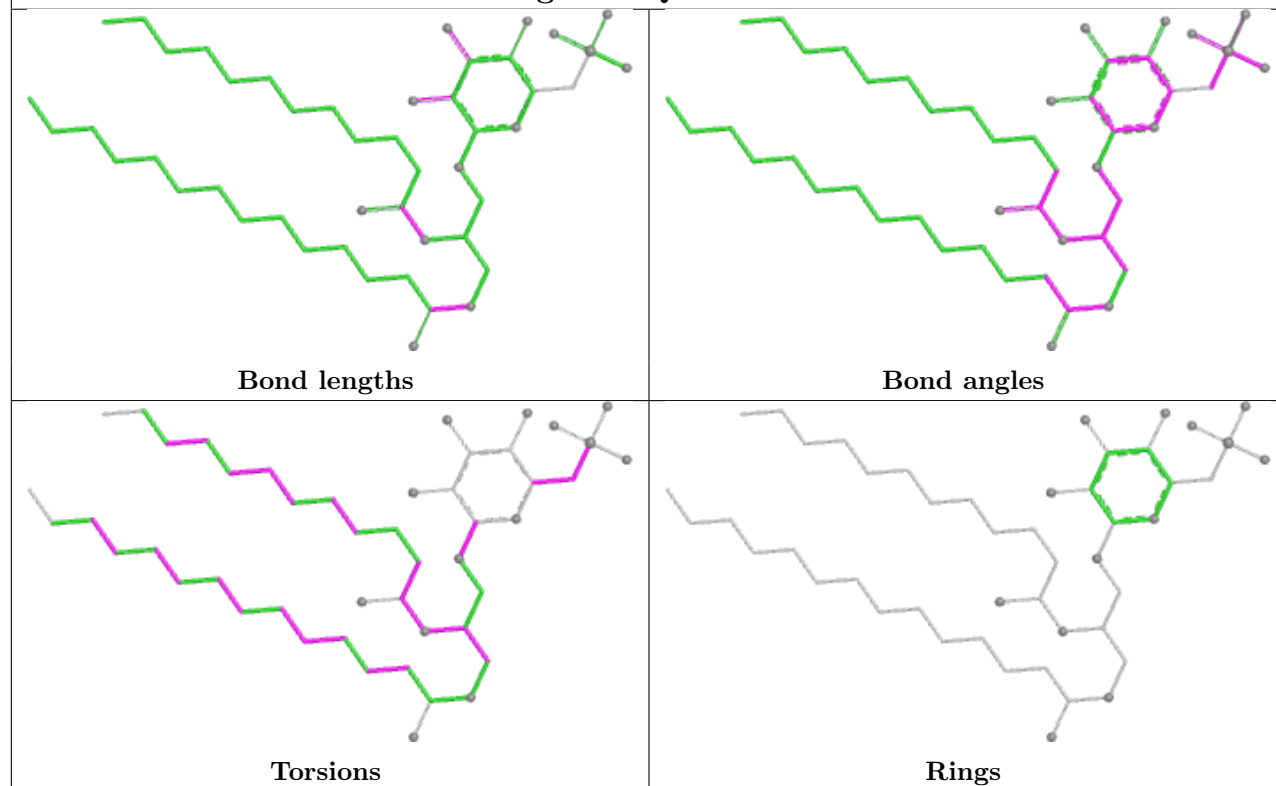


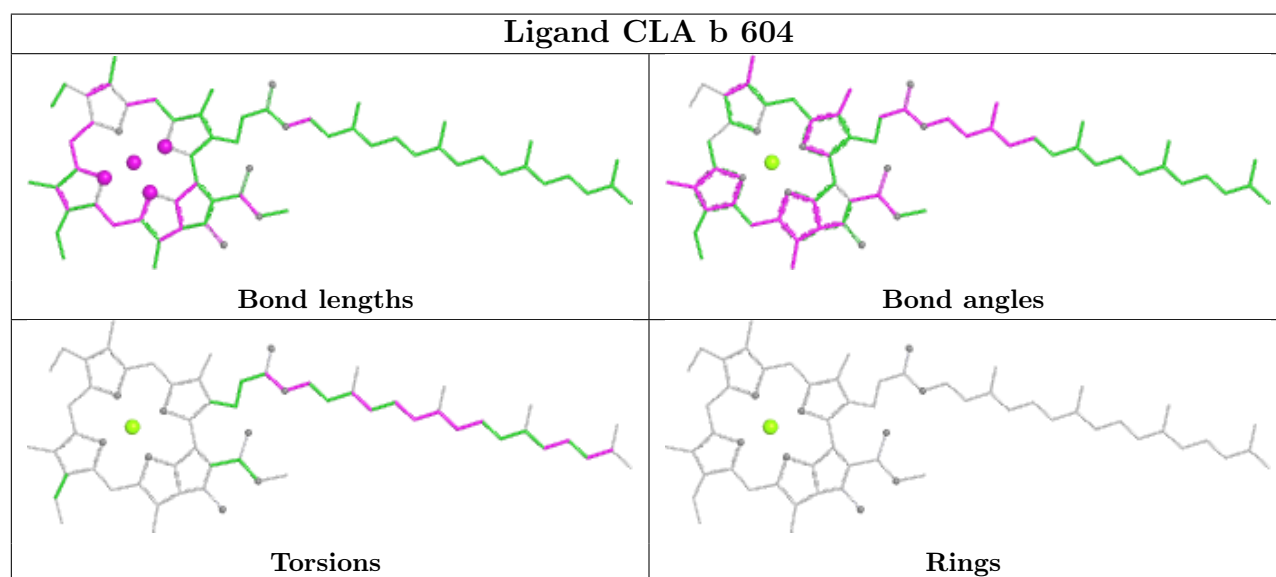
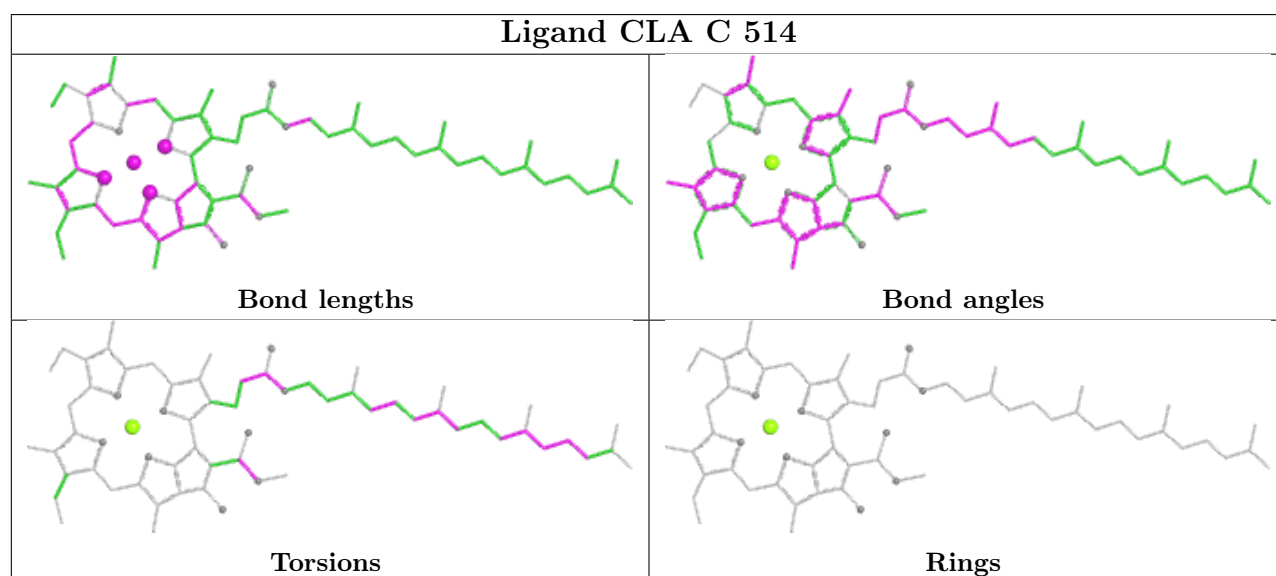
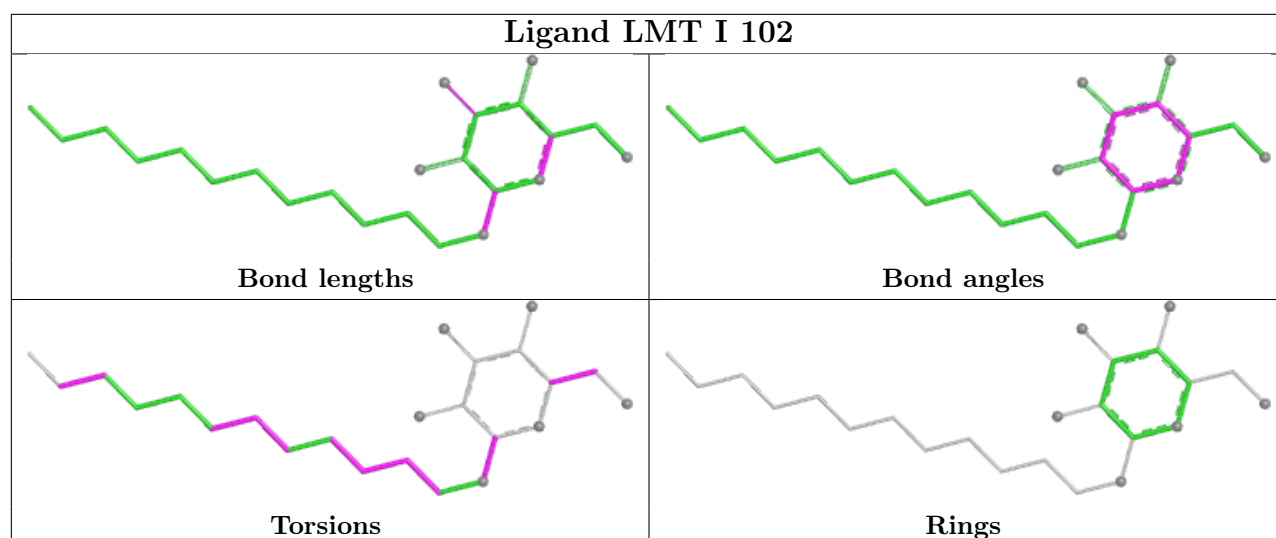


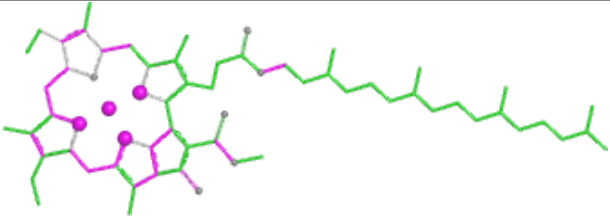
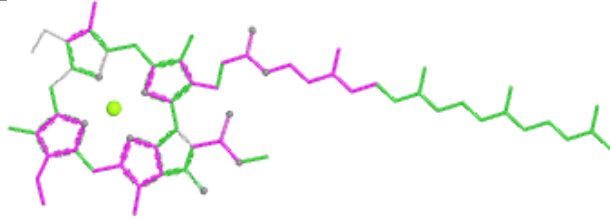
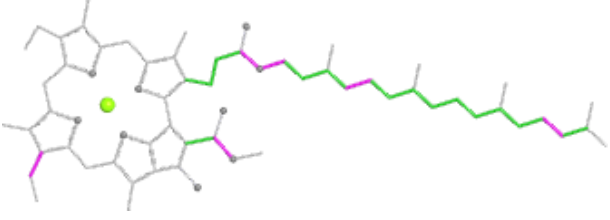
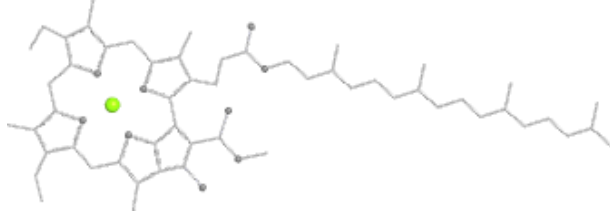
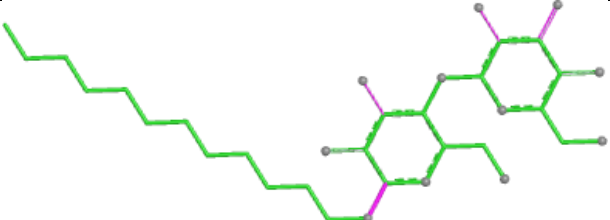
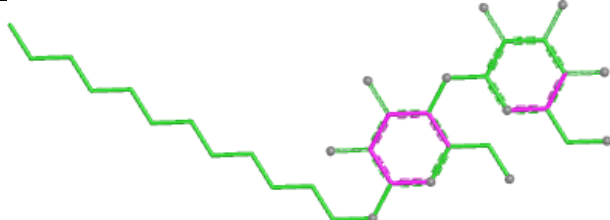
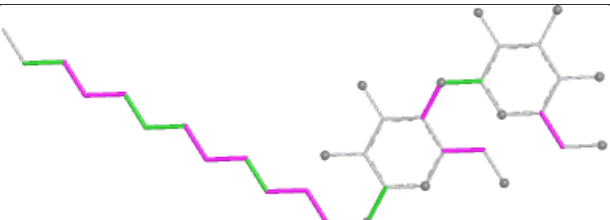
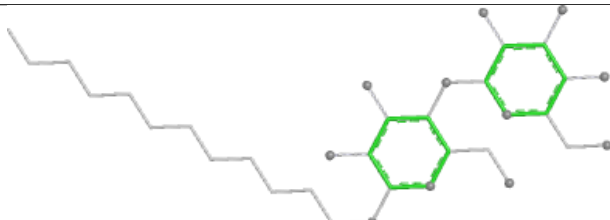
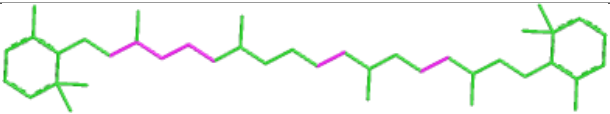
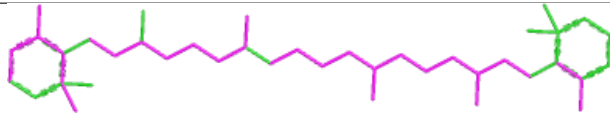
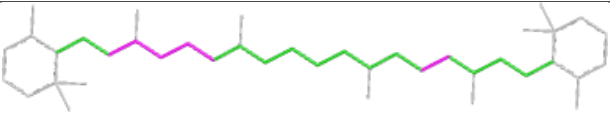
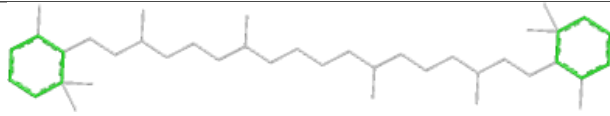
Ligand CLA c 513

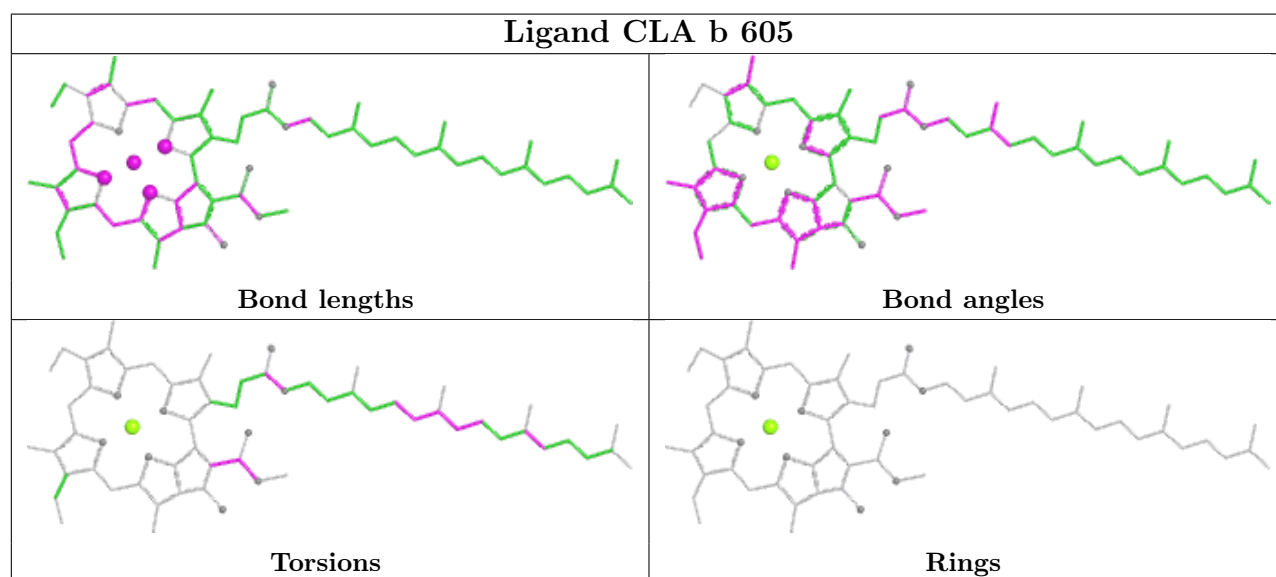
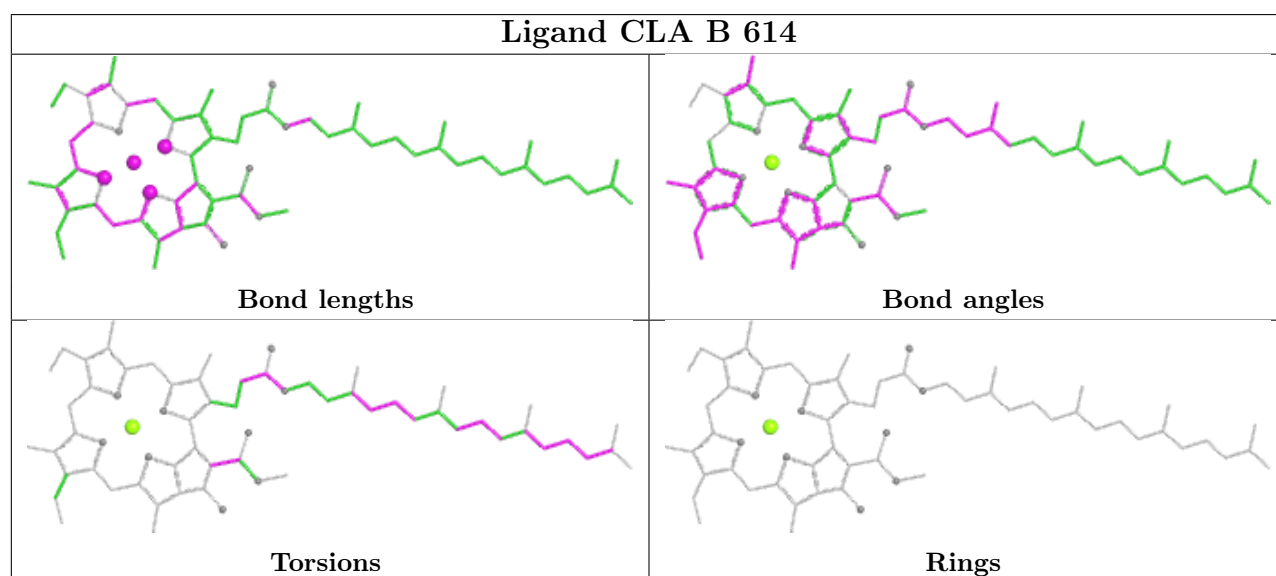
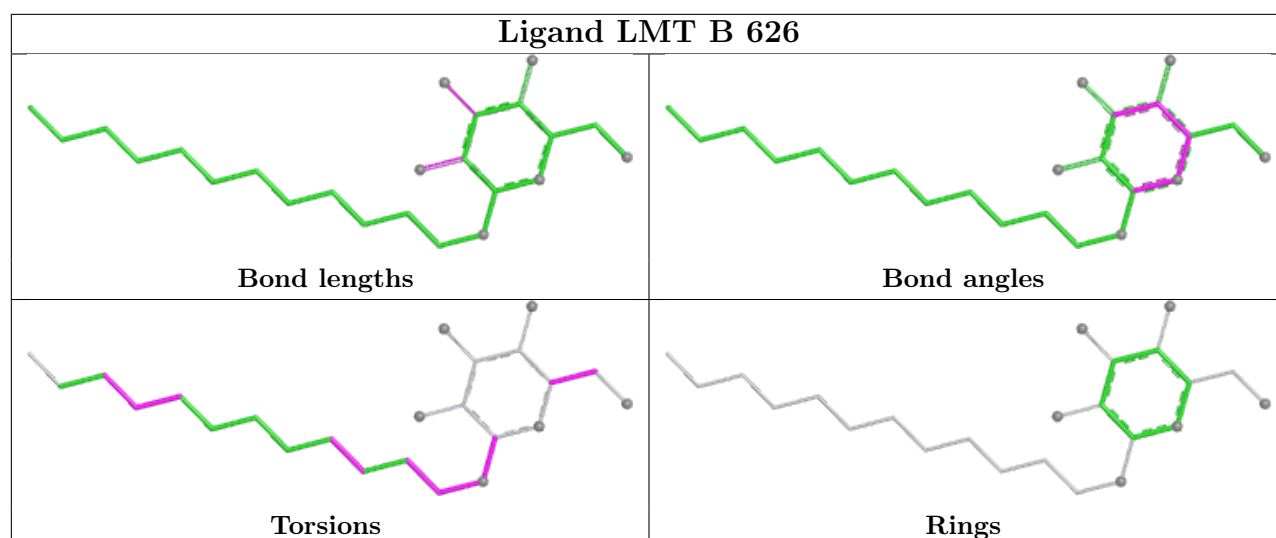


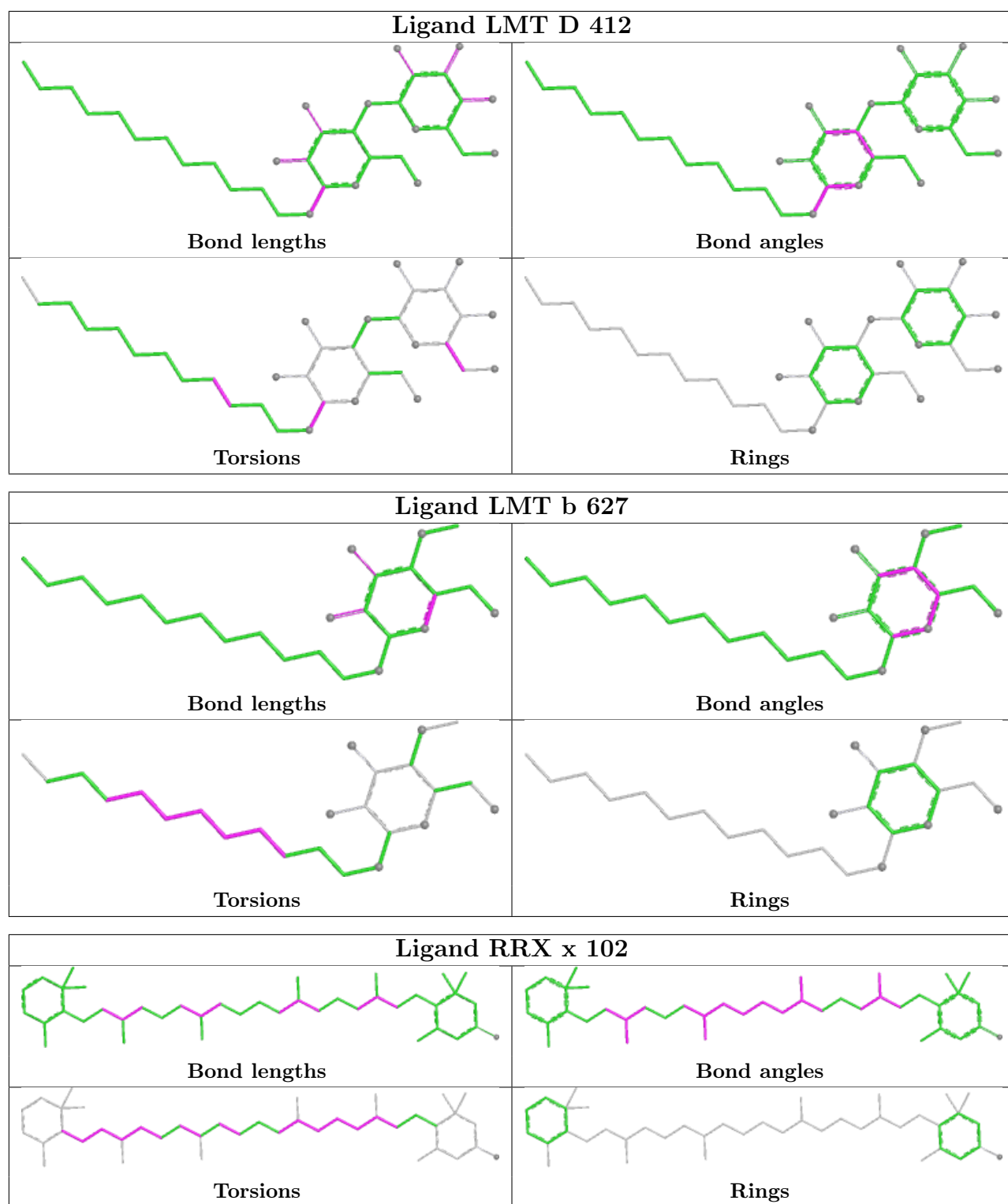
Ligand SQD a 413

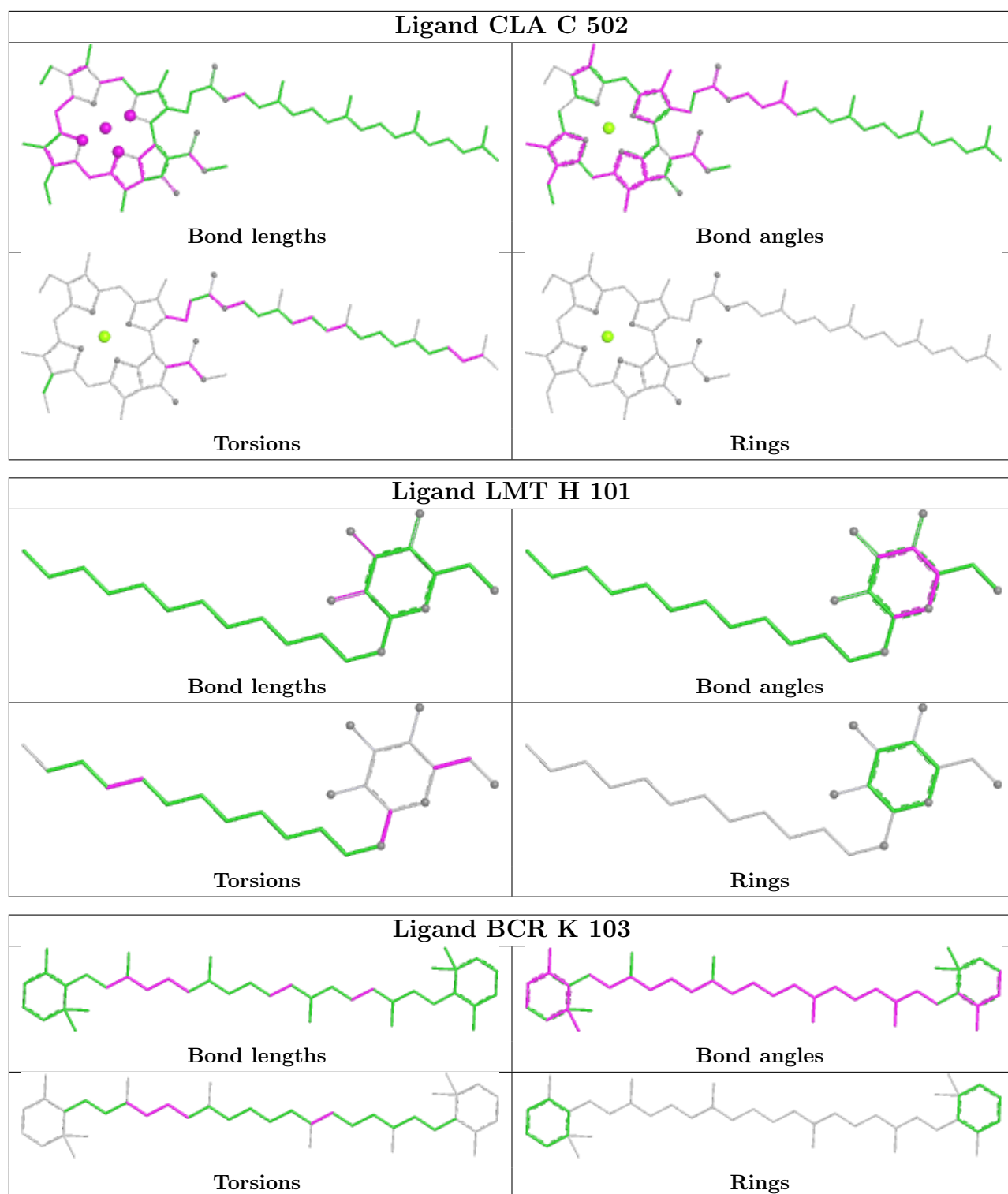


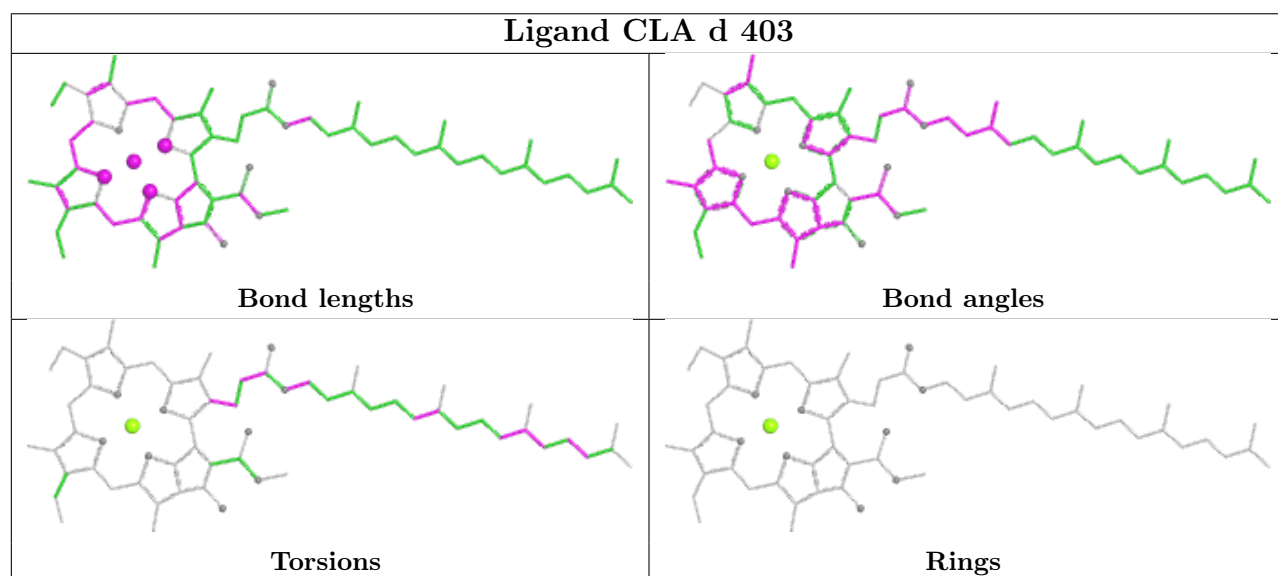
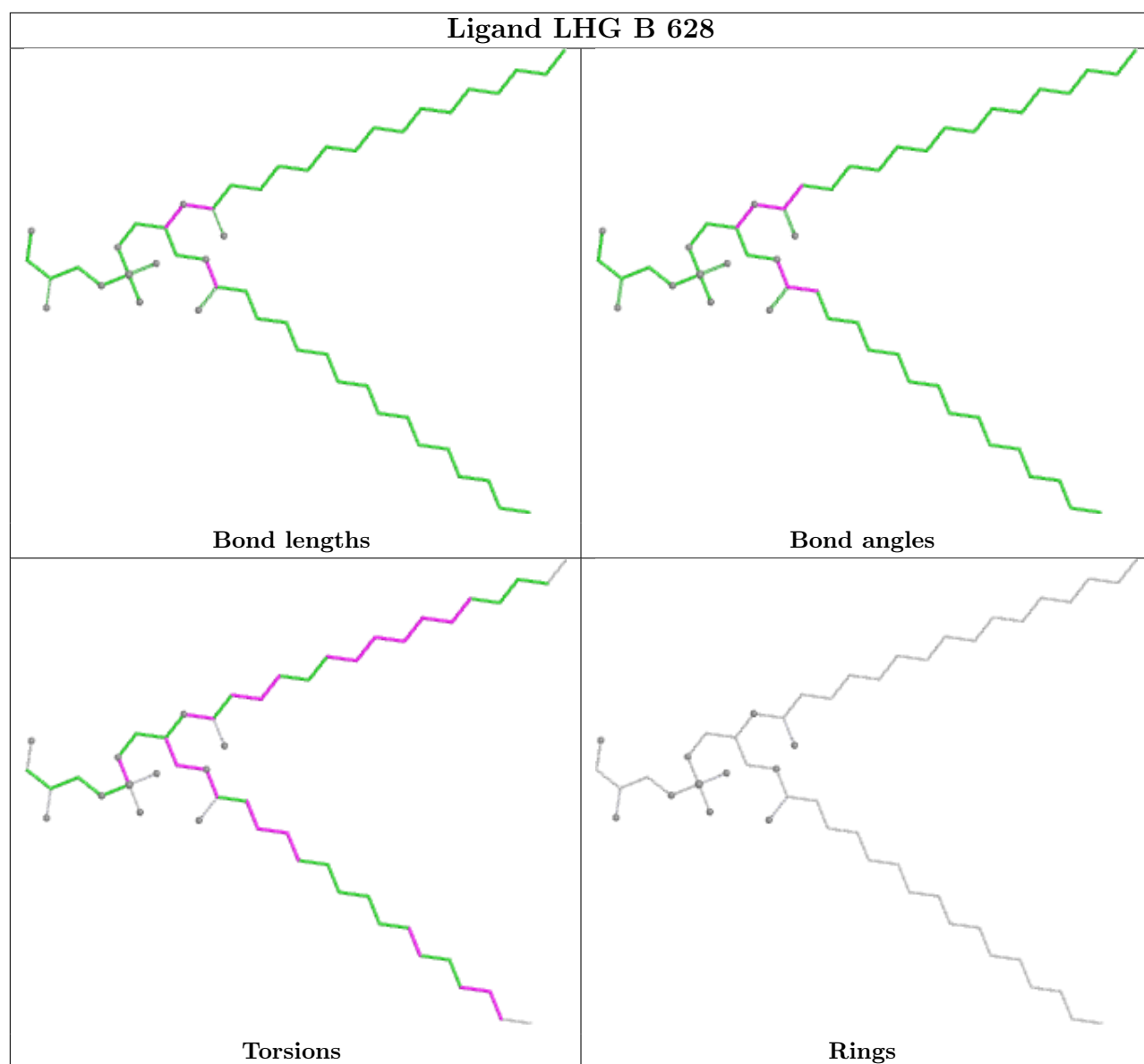


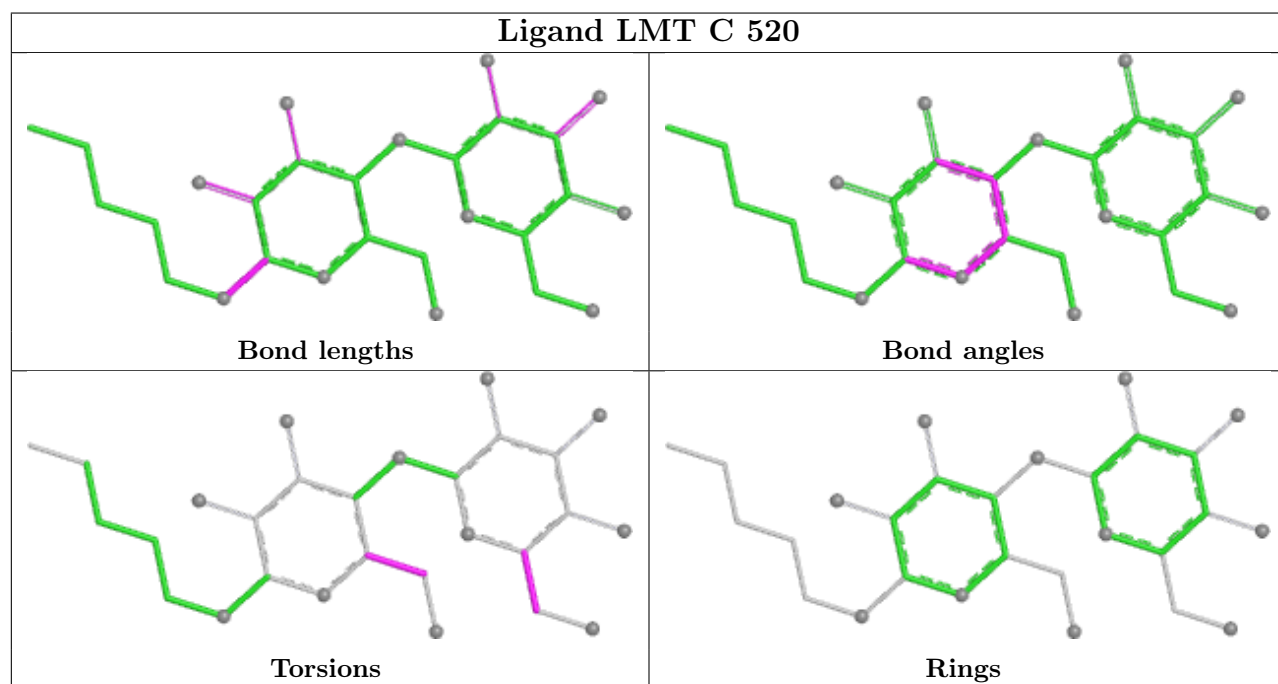
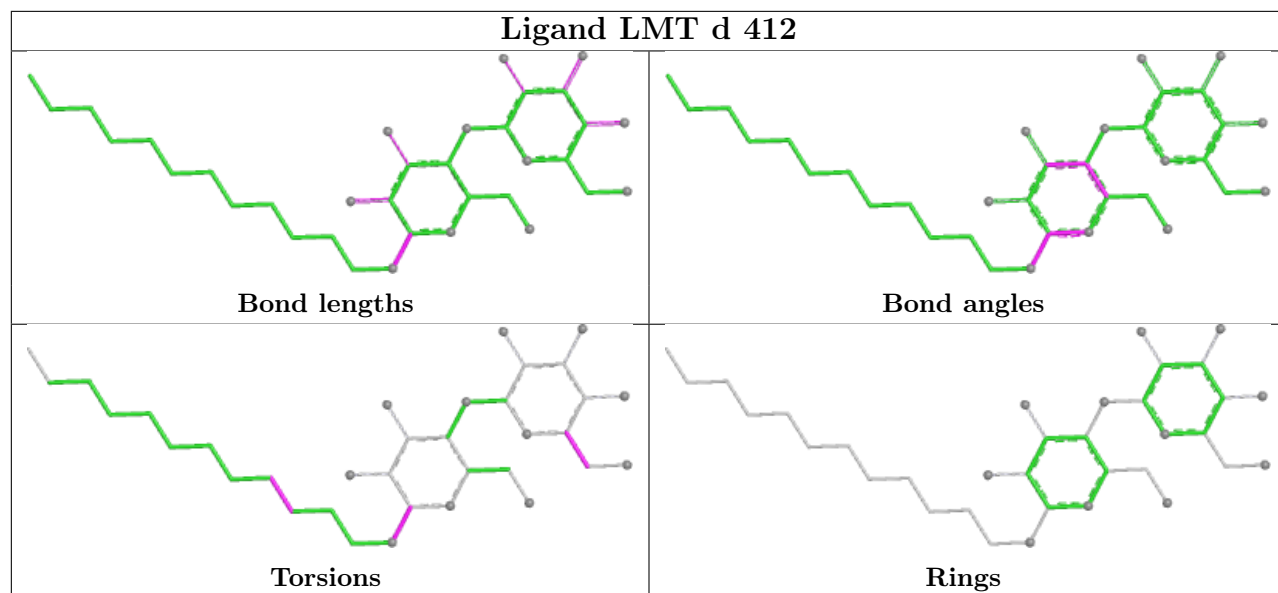
Ligand CLA d 401	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LMT e 103	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR c 515	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

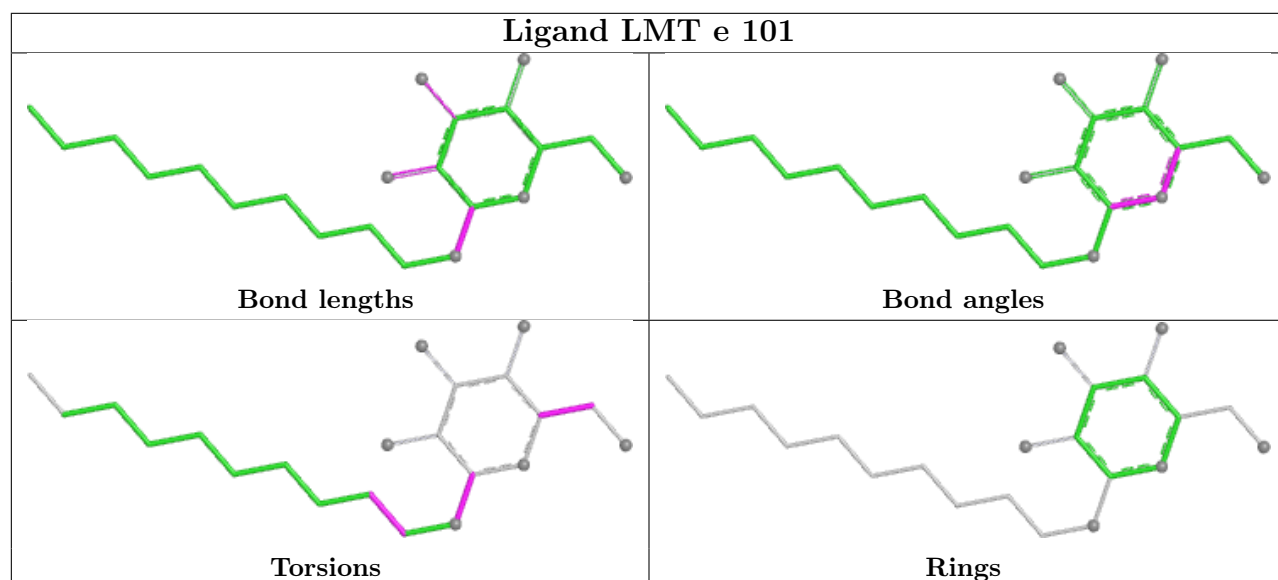
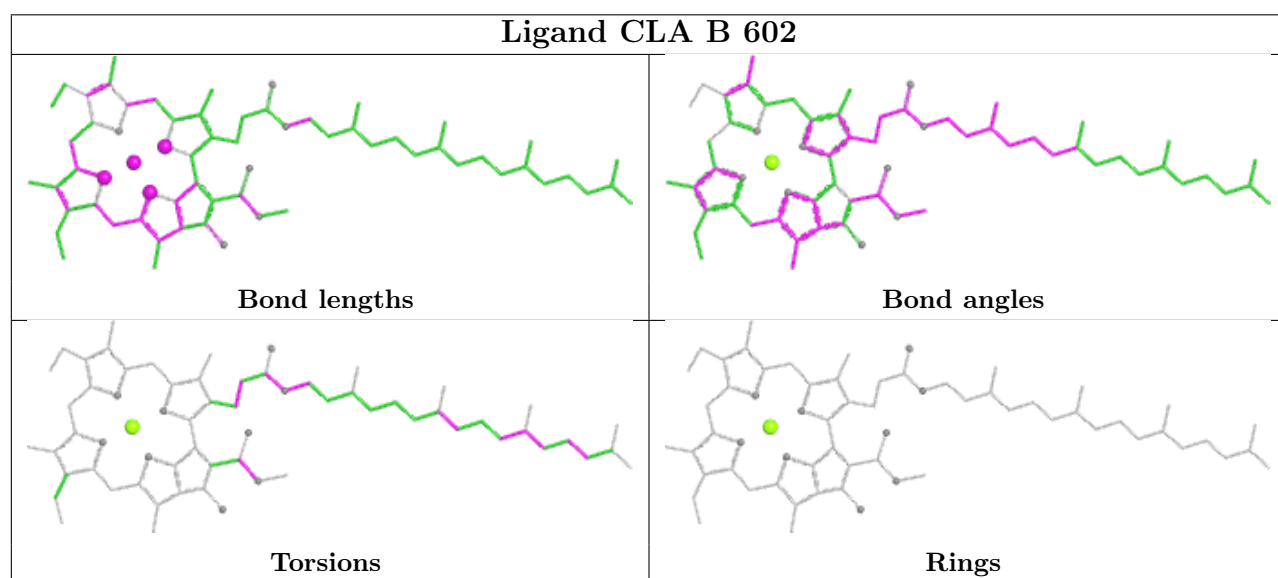
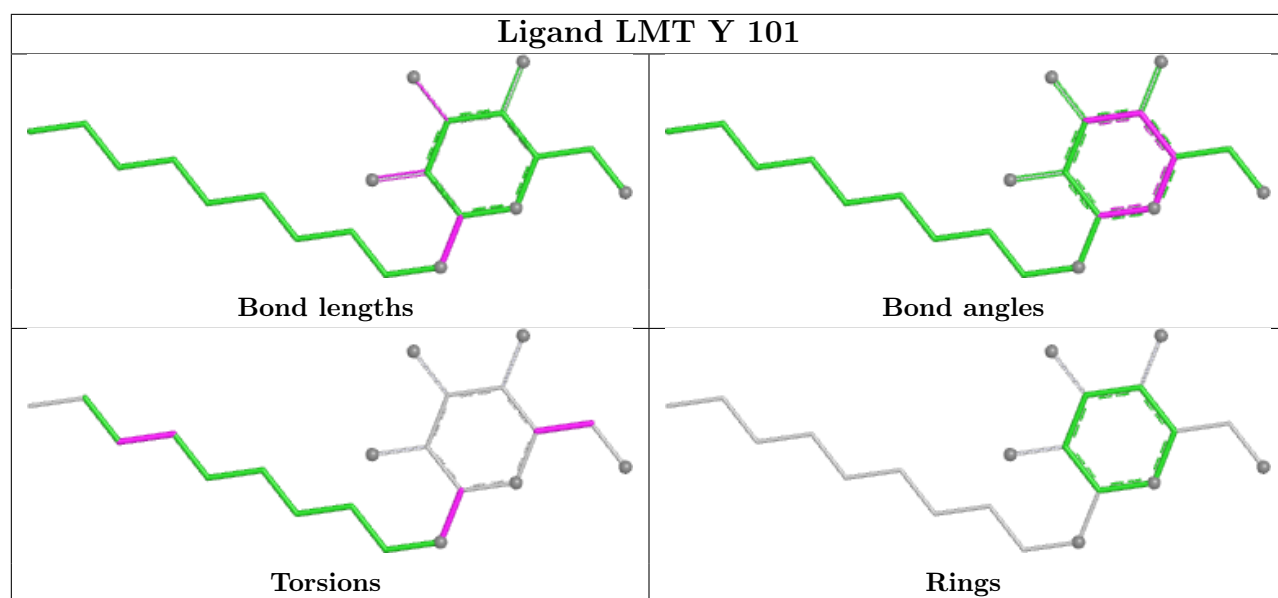


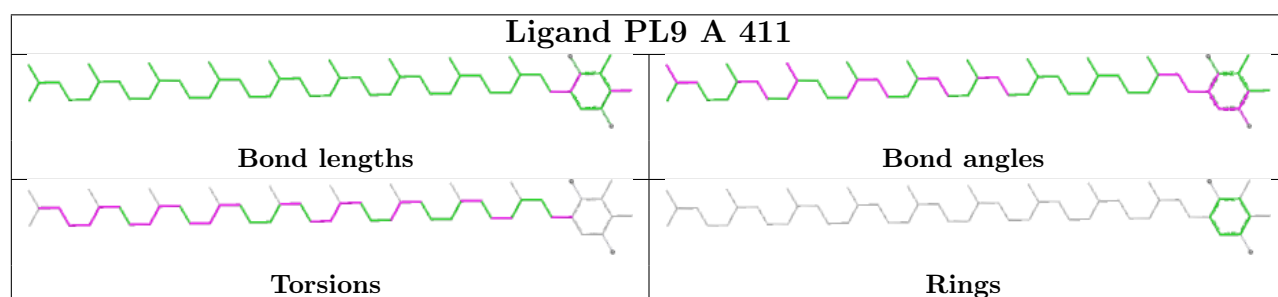
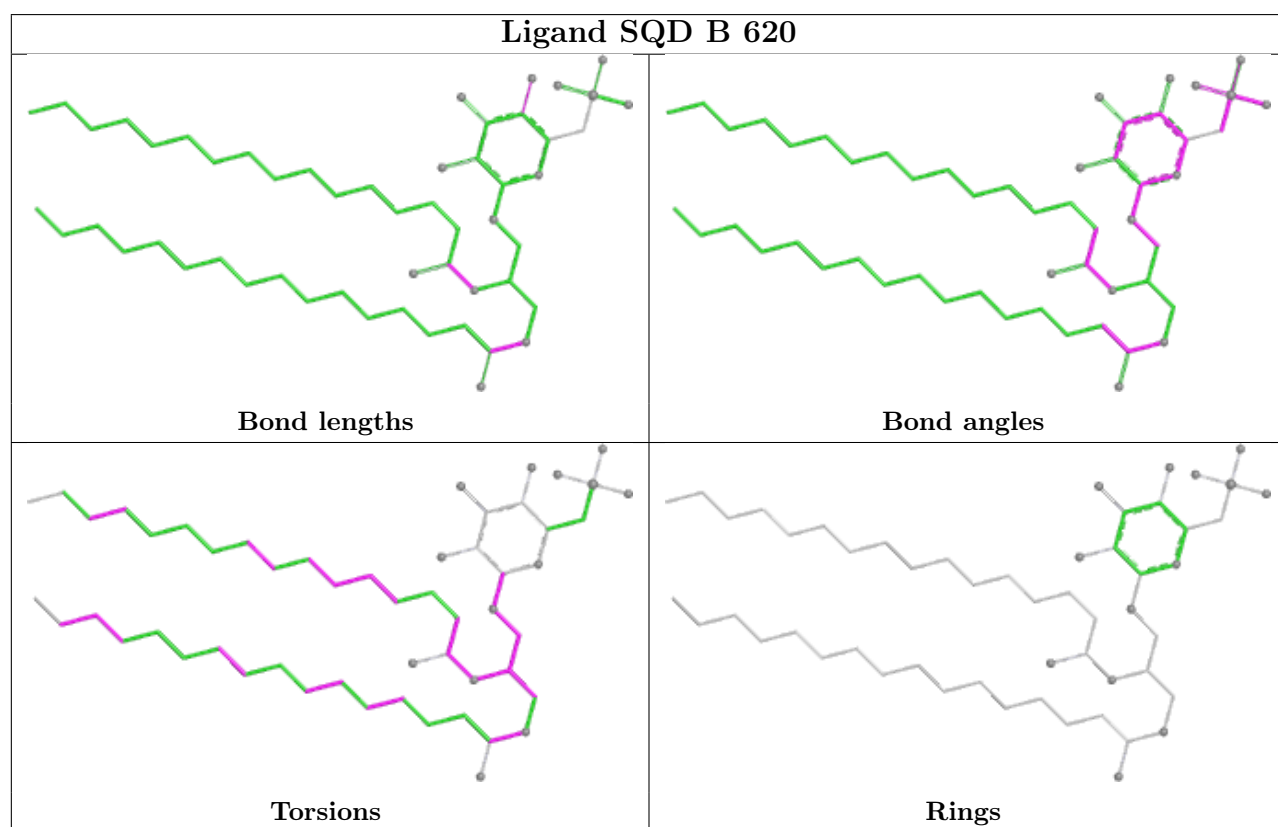
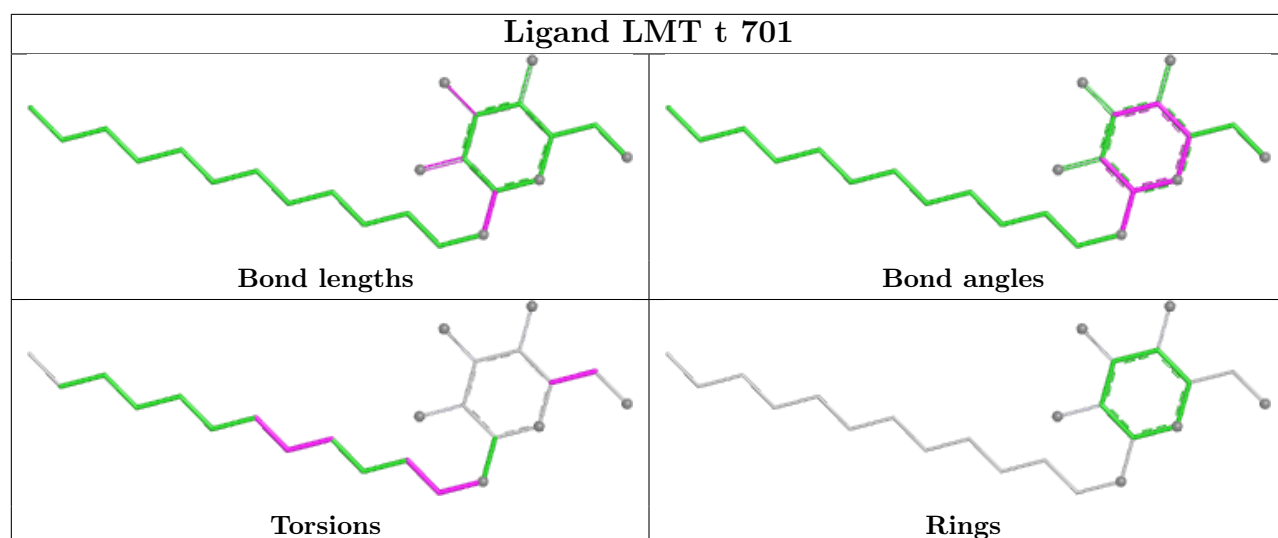




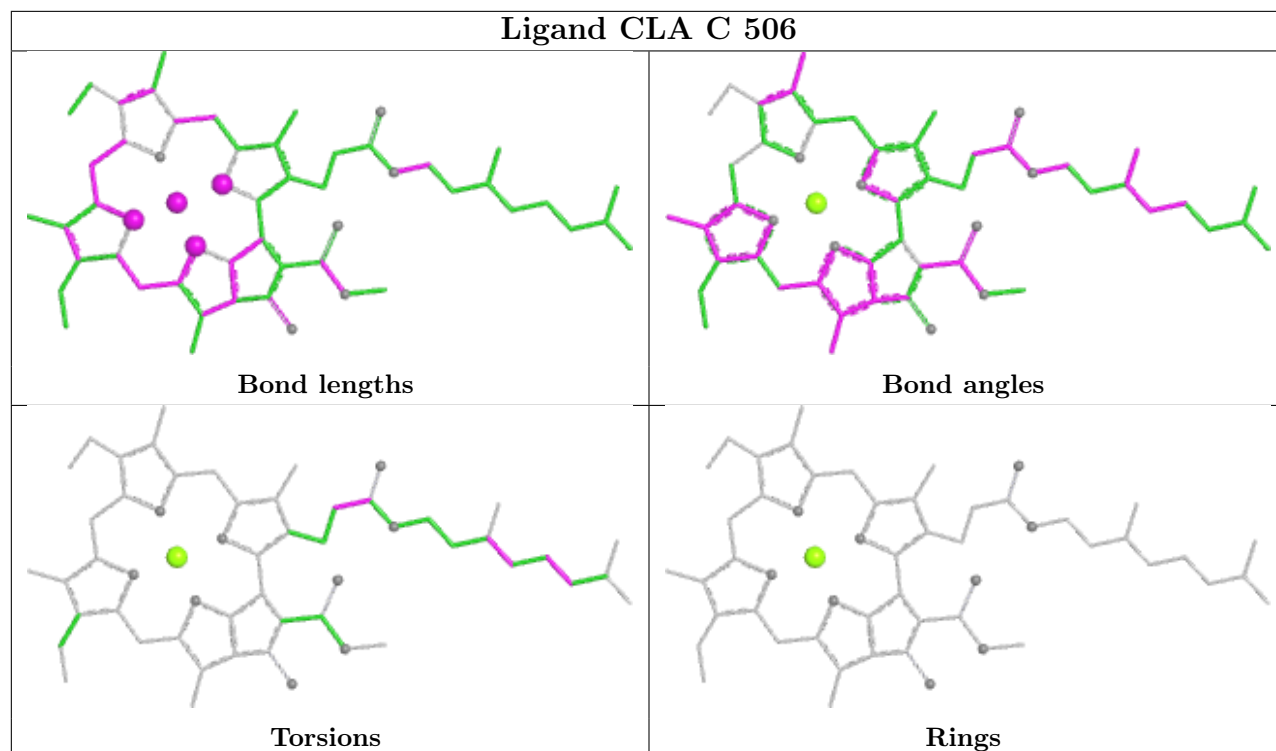




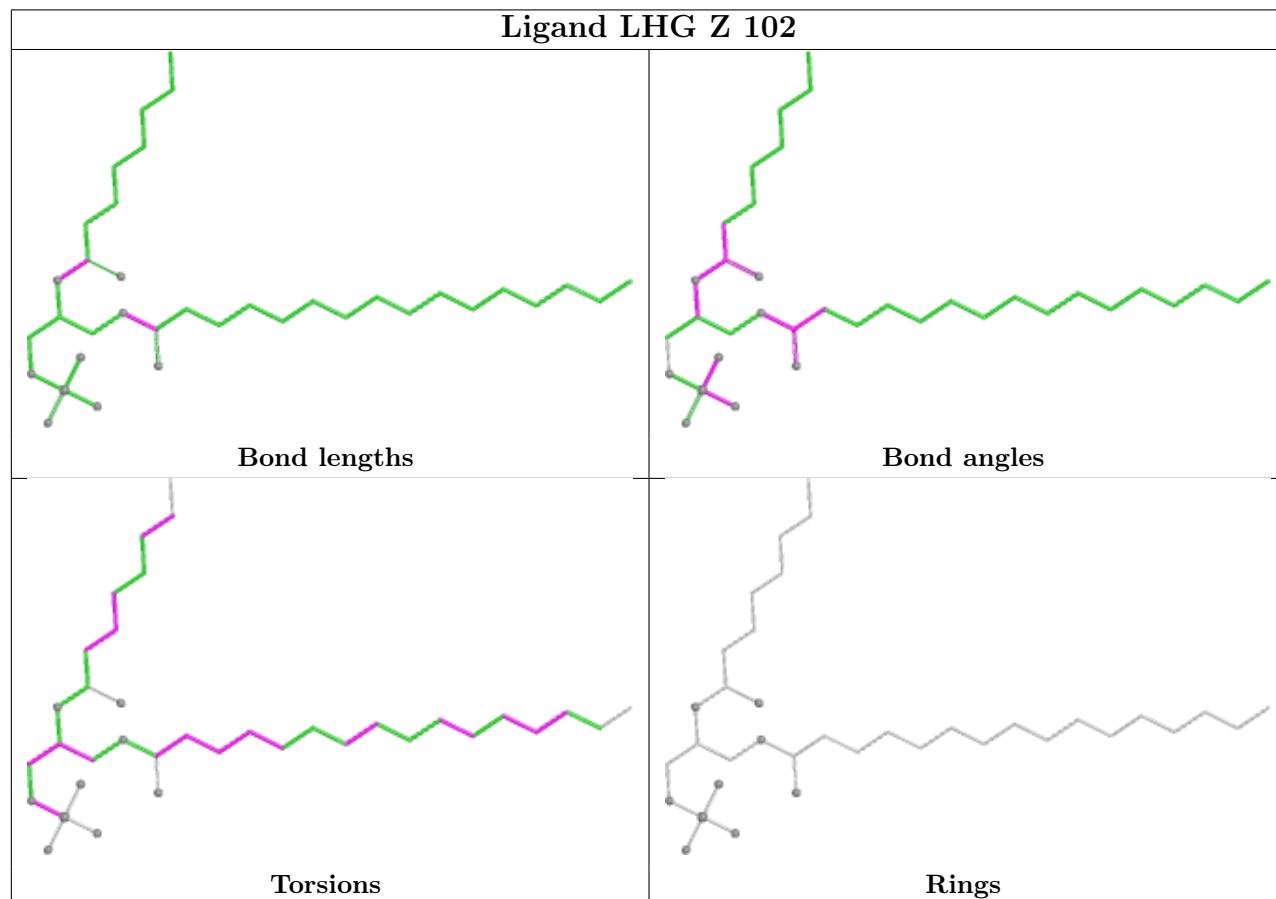


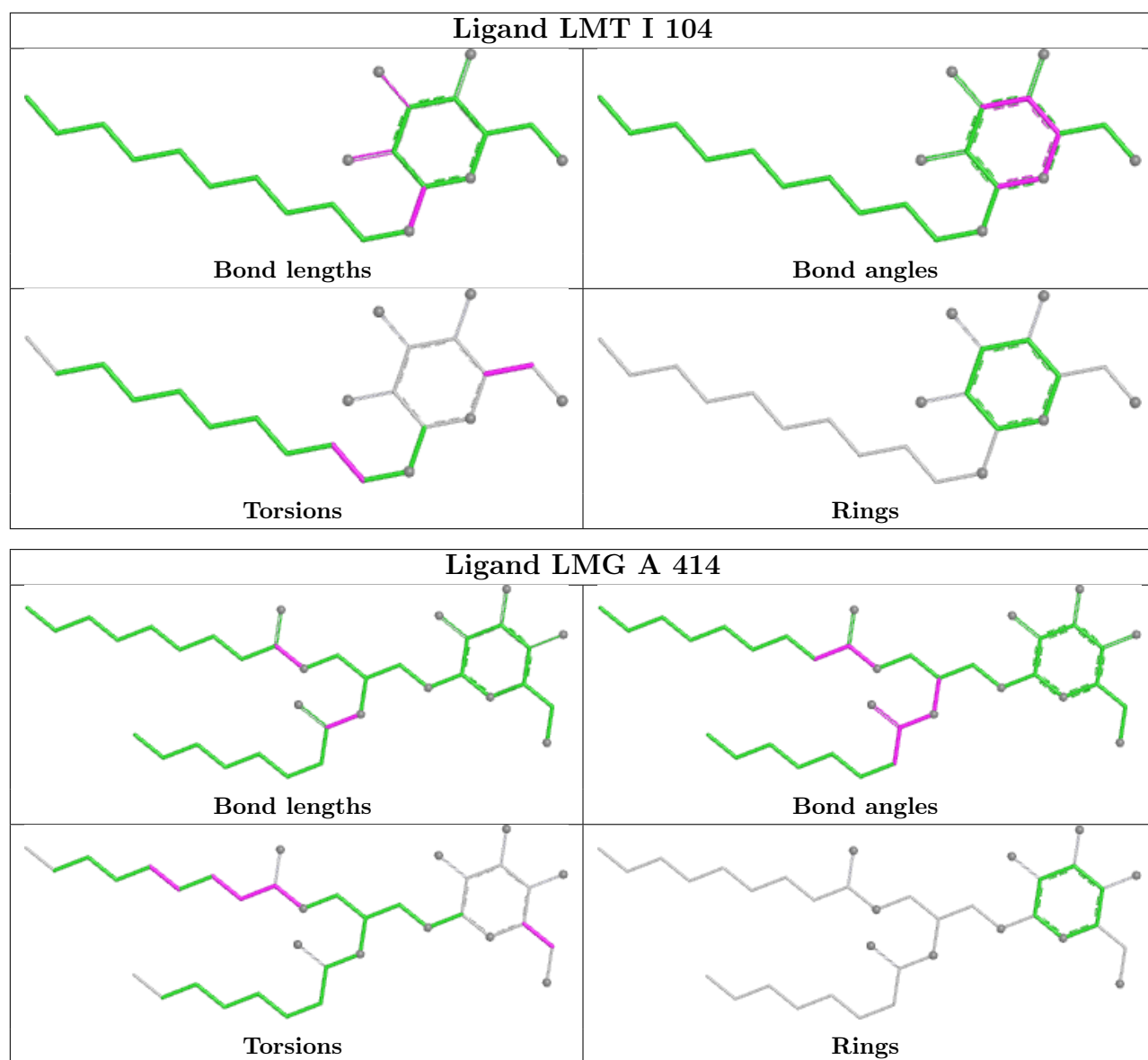


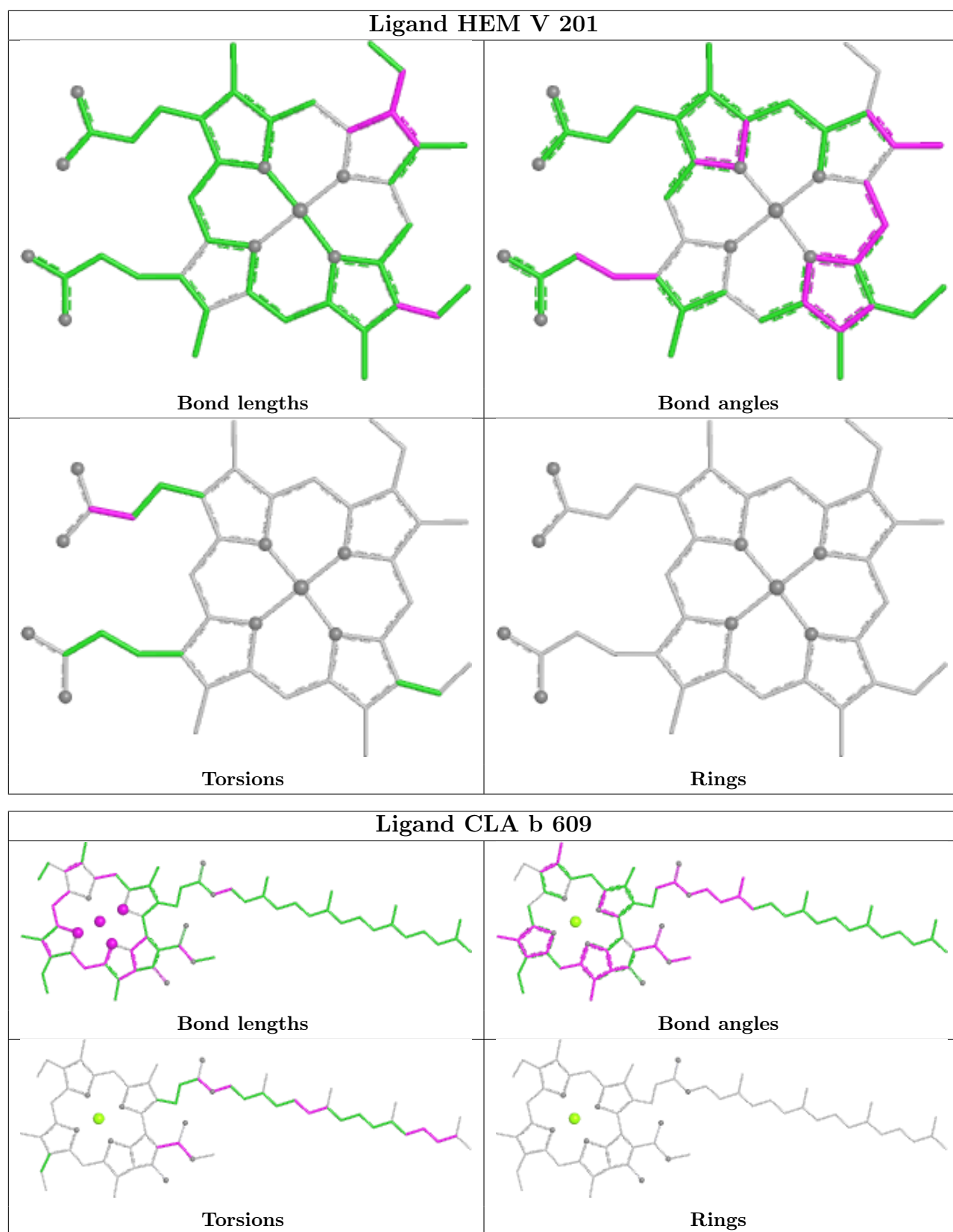
Ligand CLA C 506

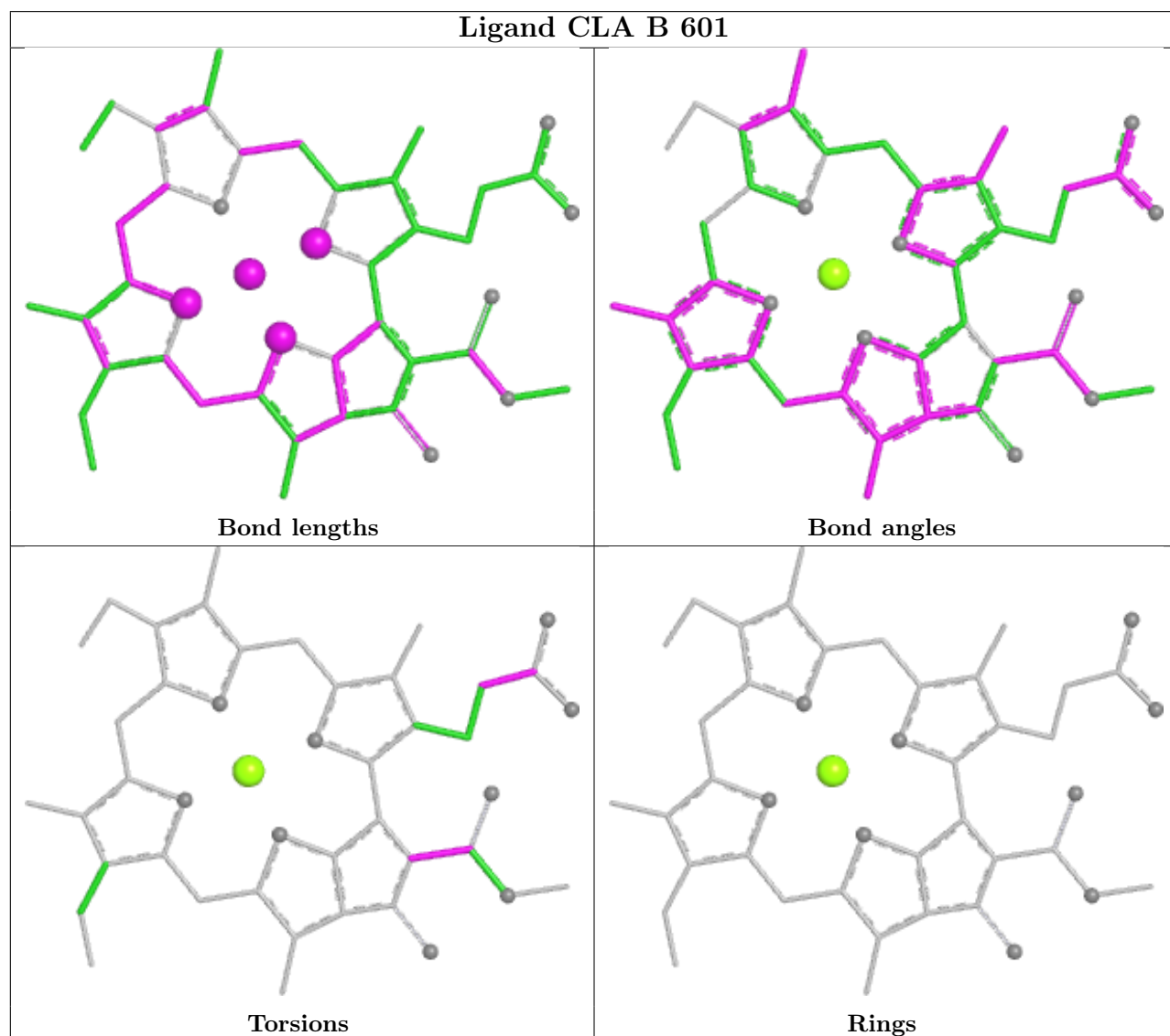
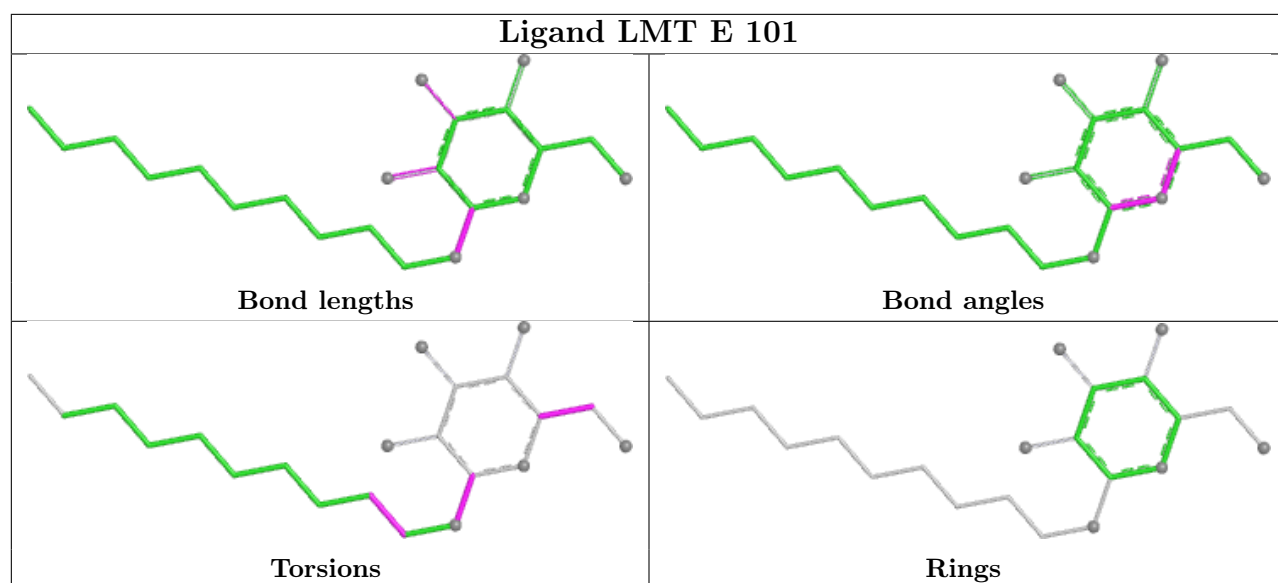


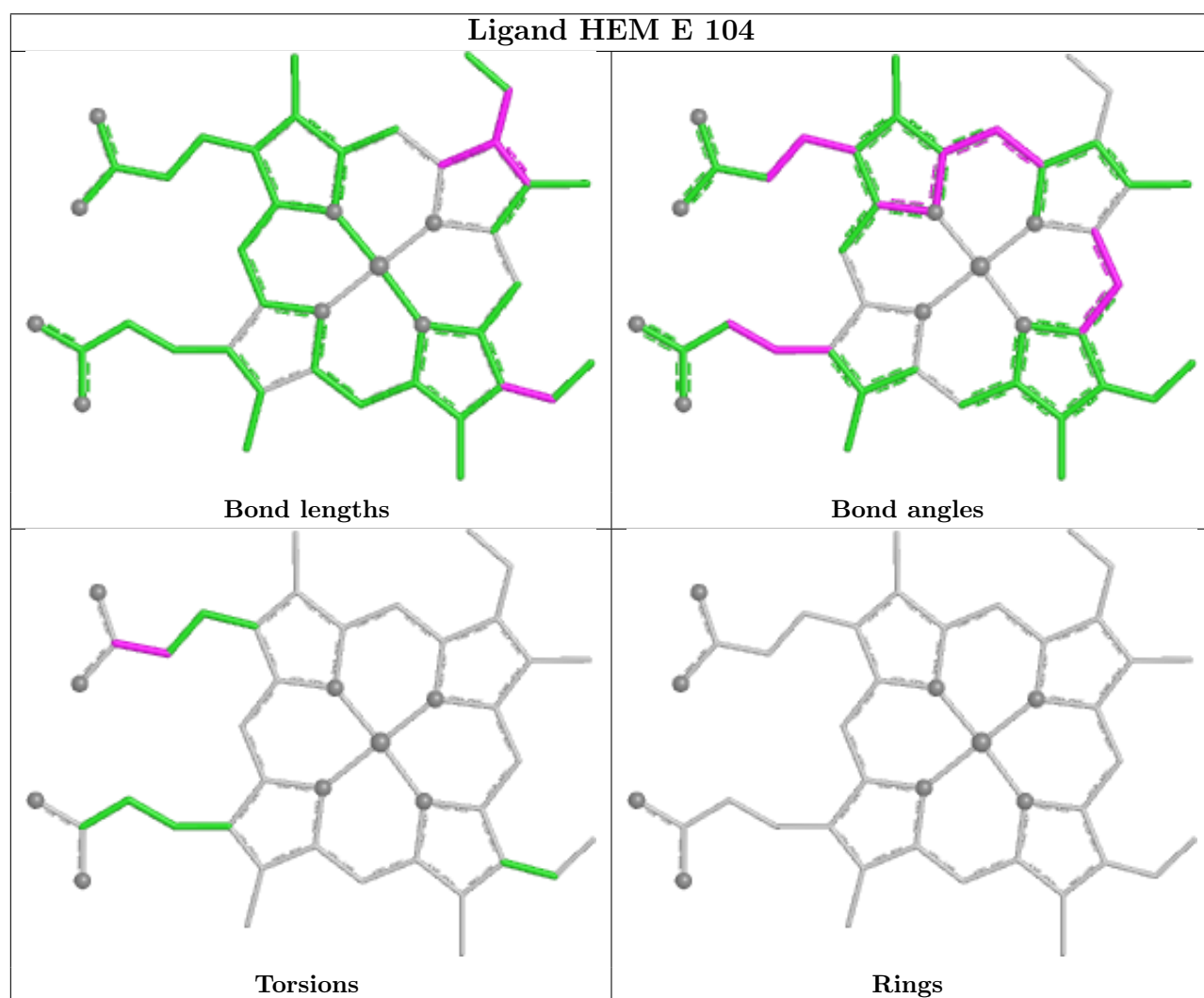
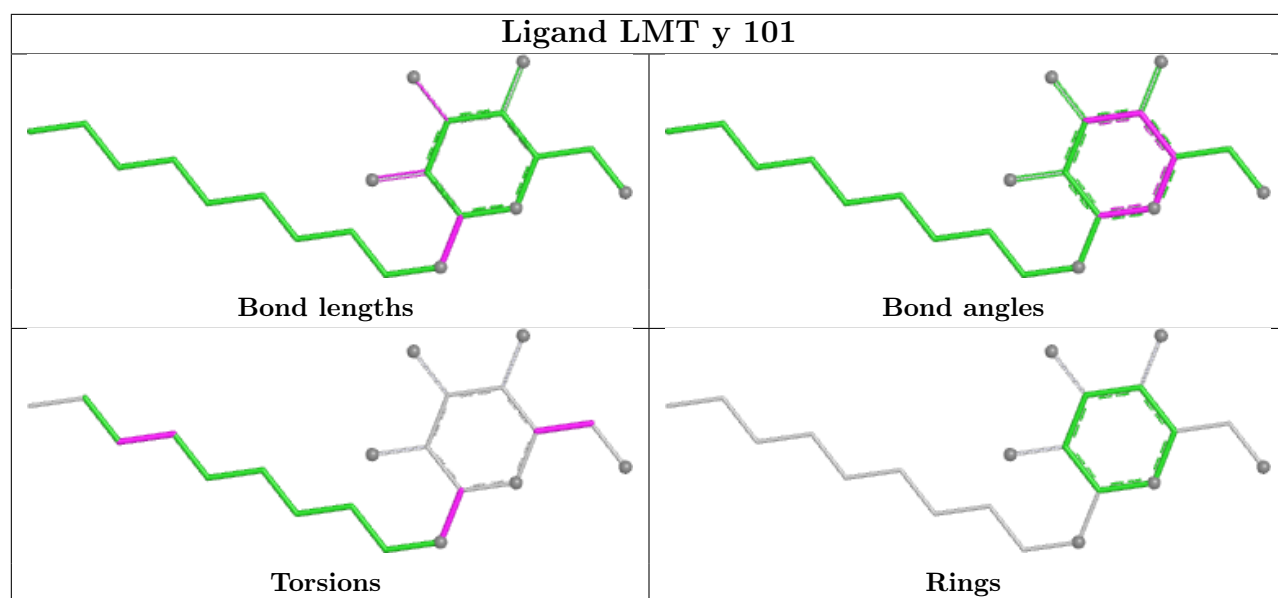
Ligand LHG Z 102

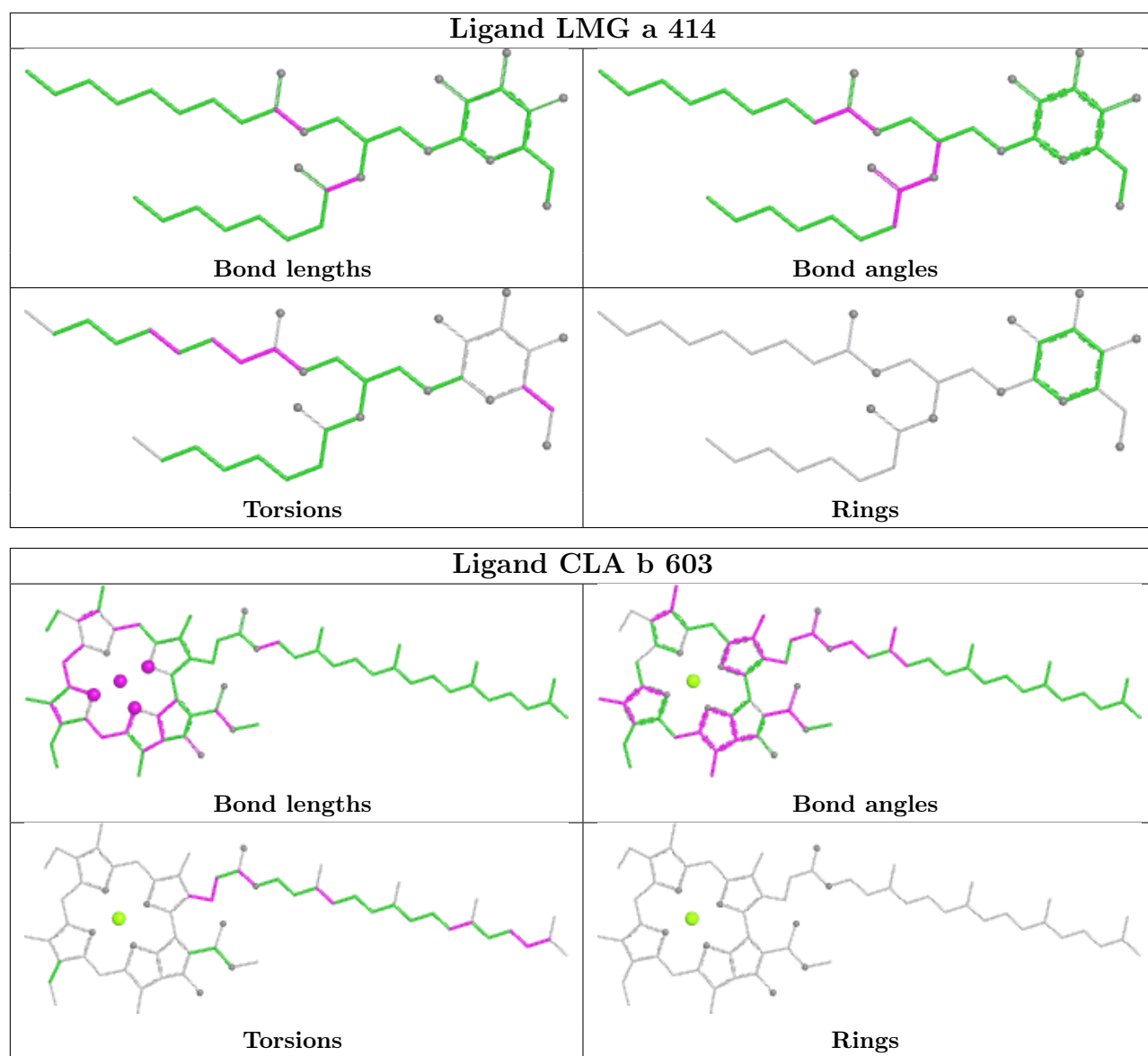


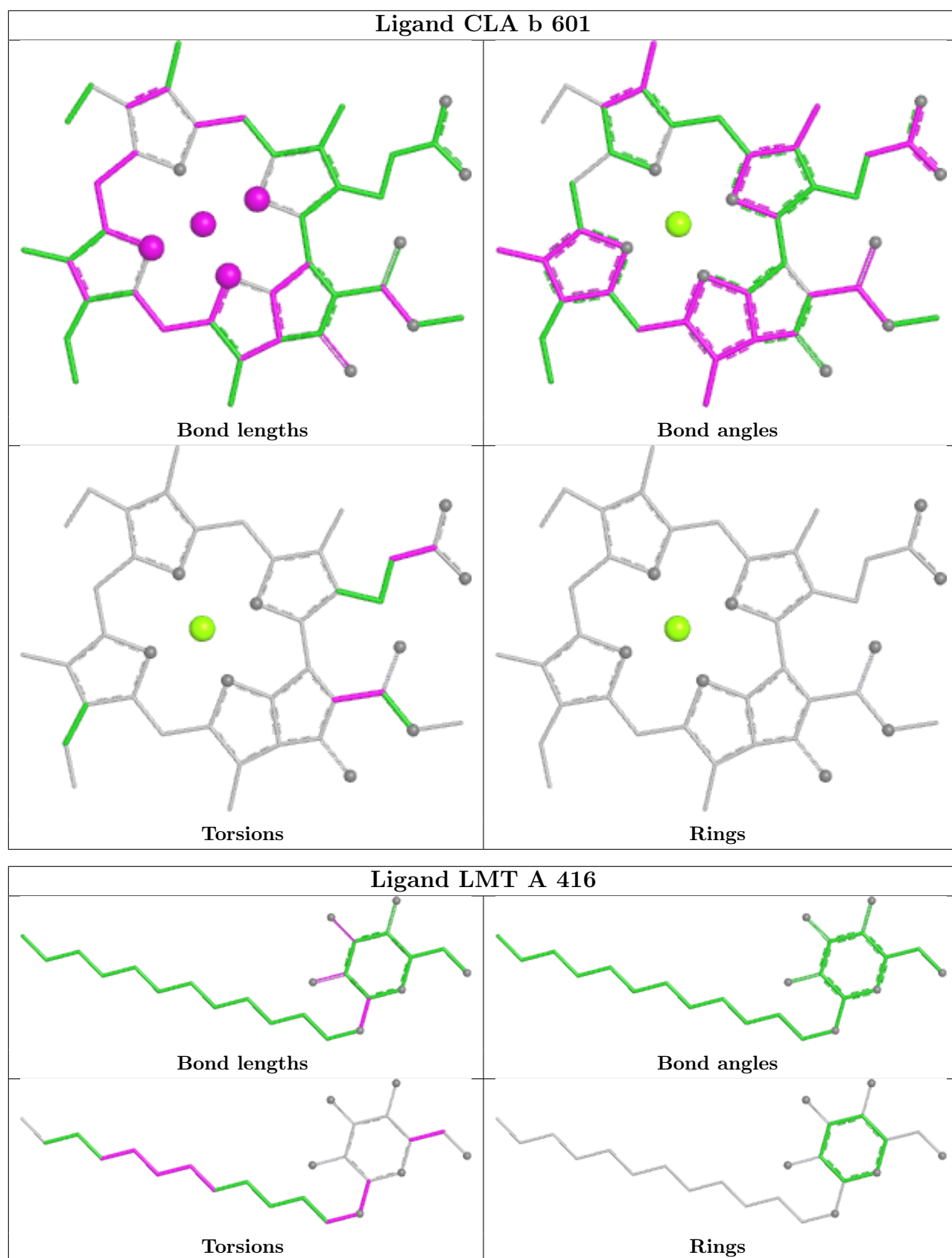


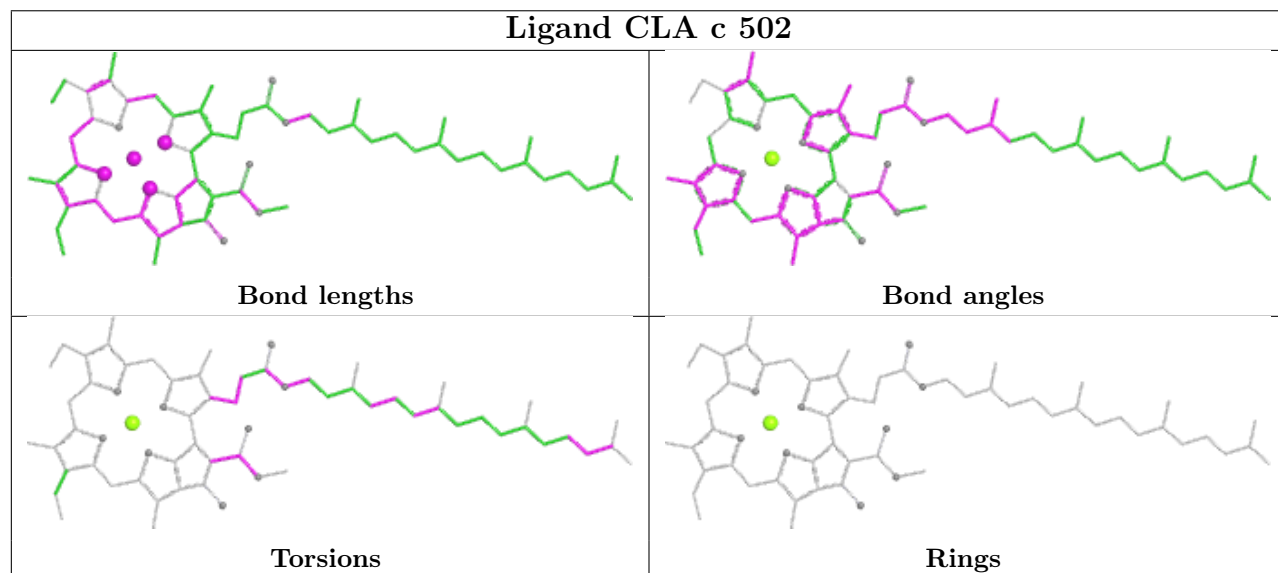
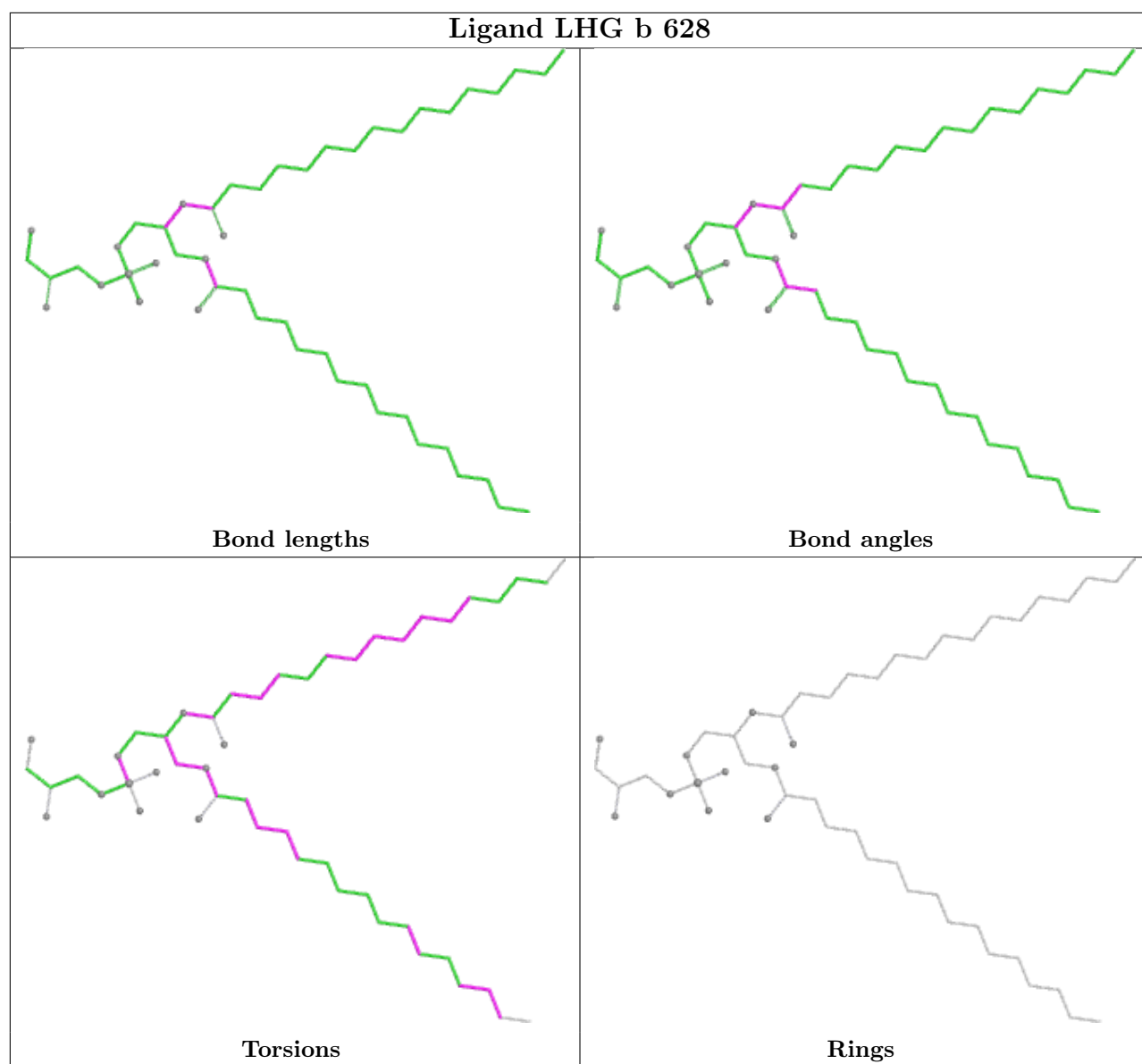


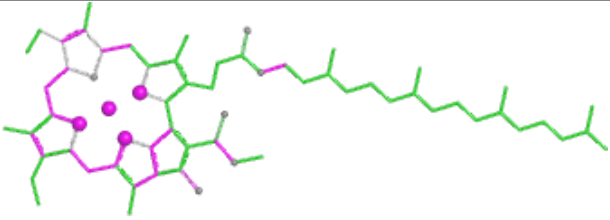
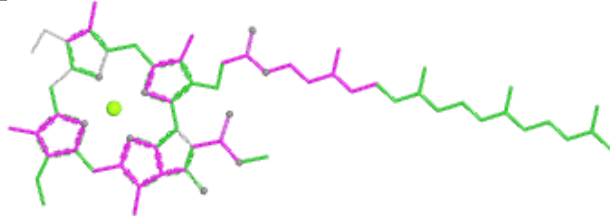
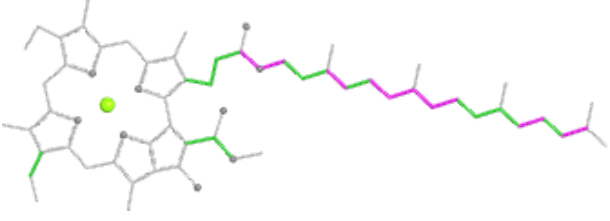
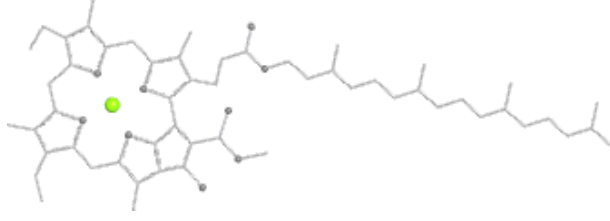

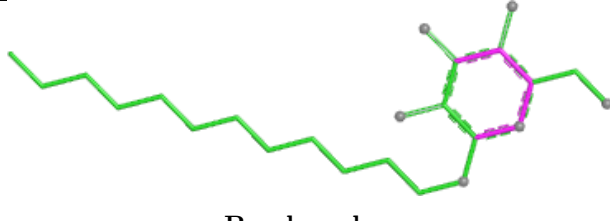
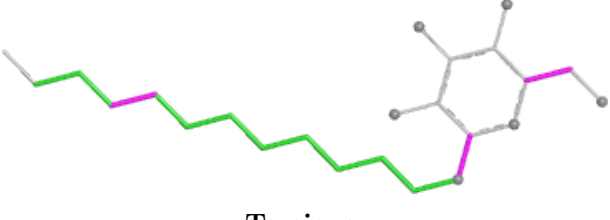
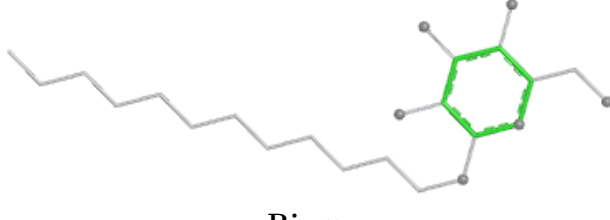
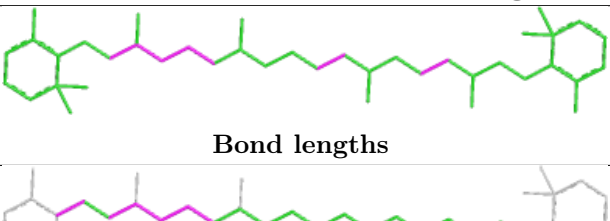
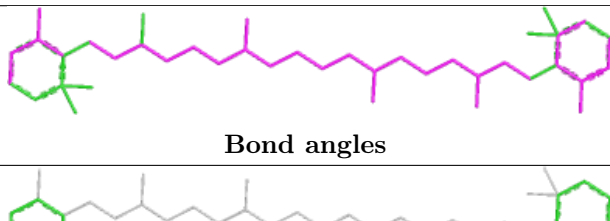
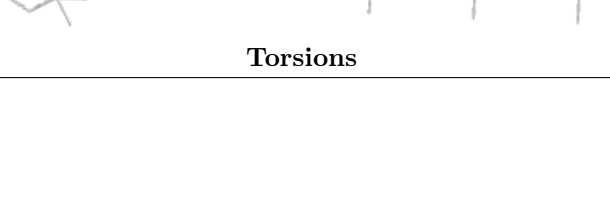
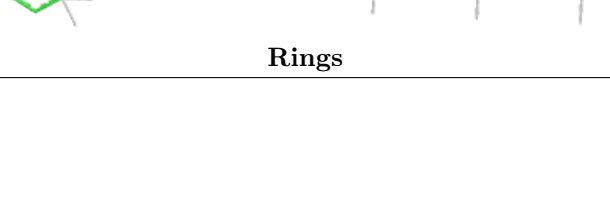


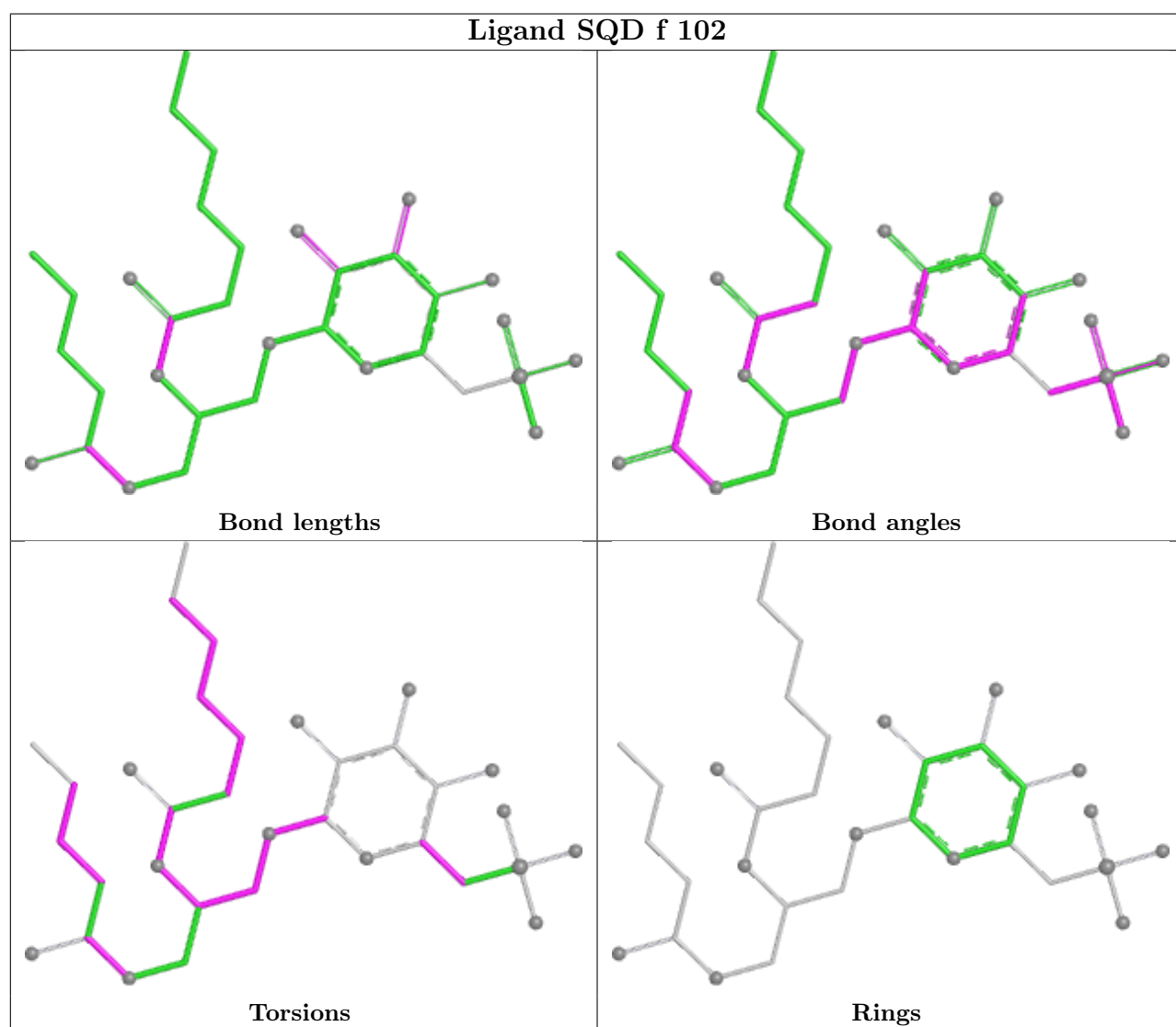
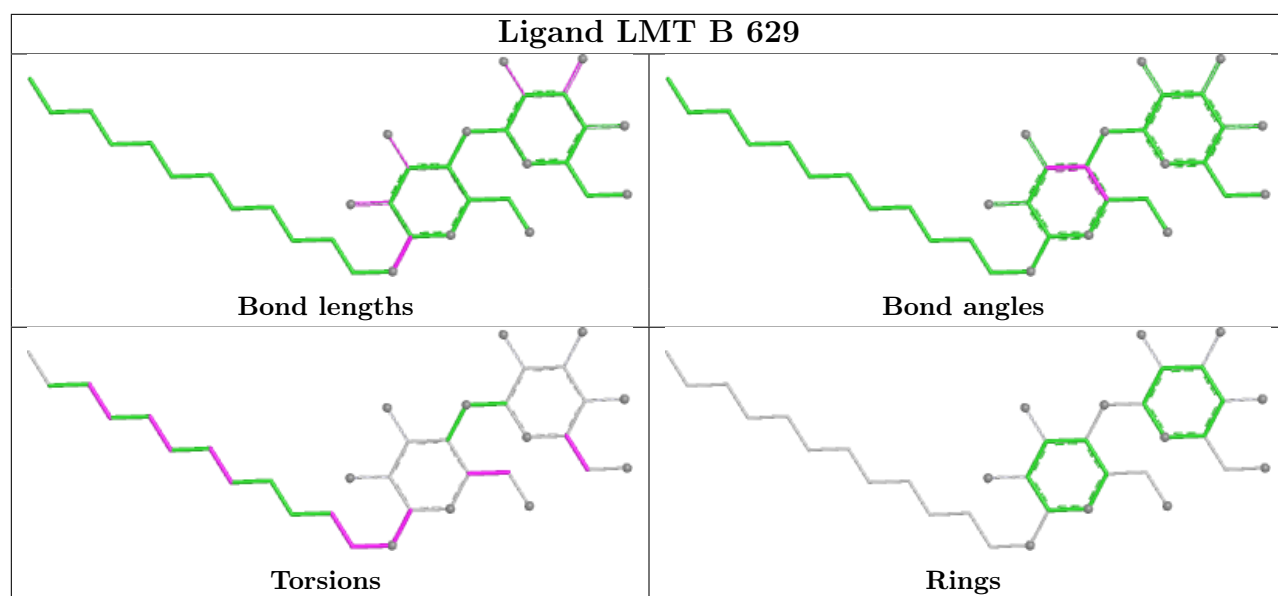


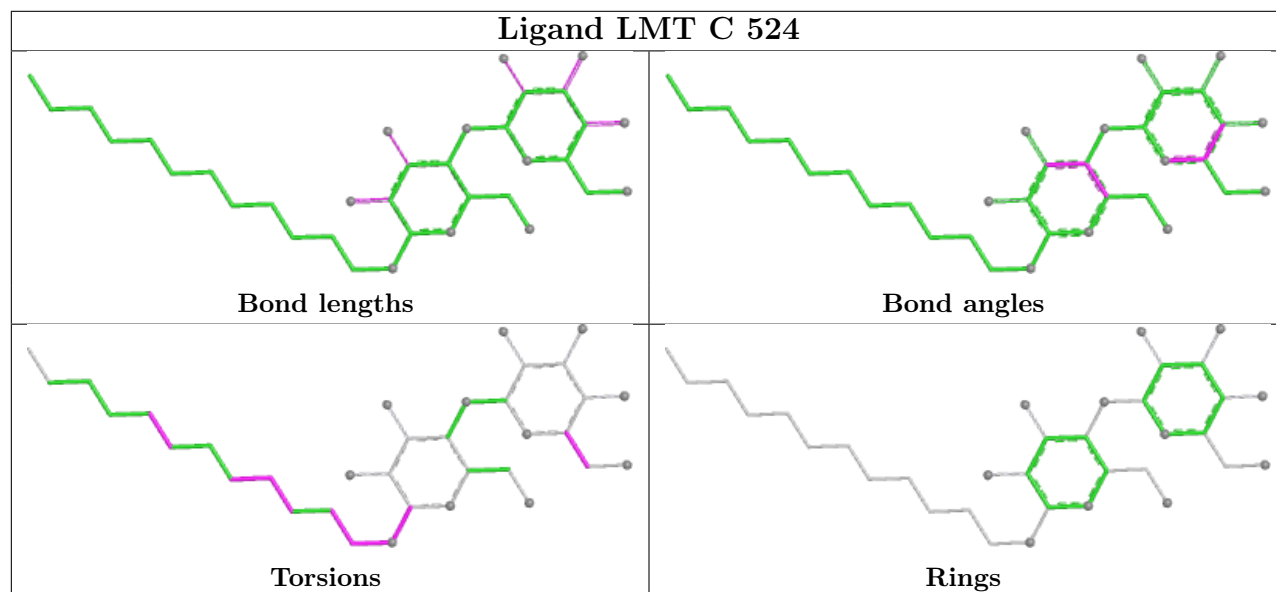
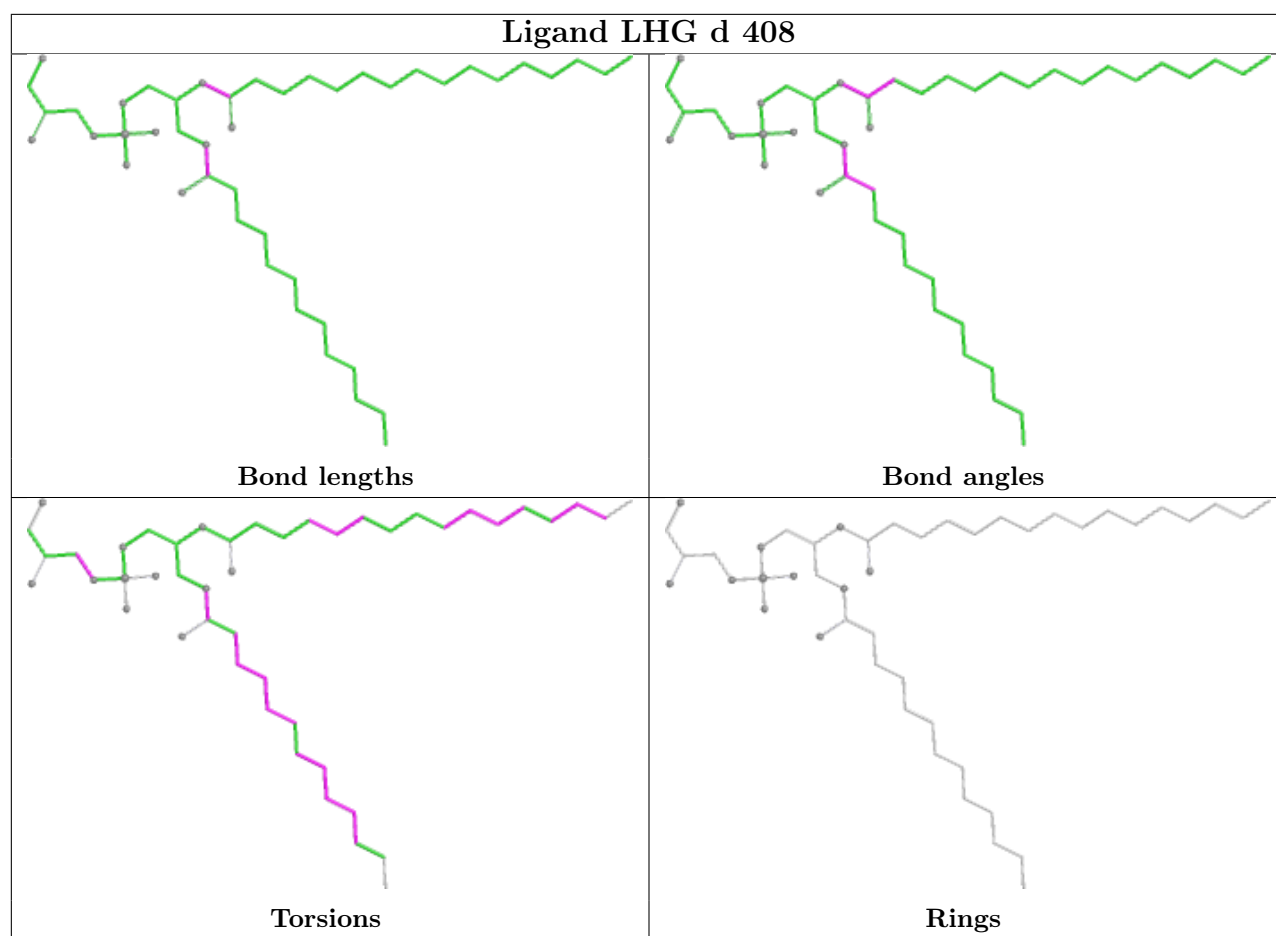


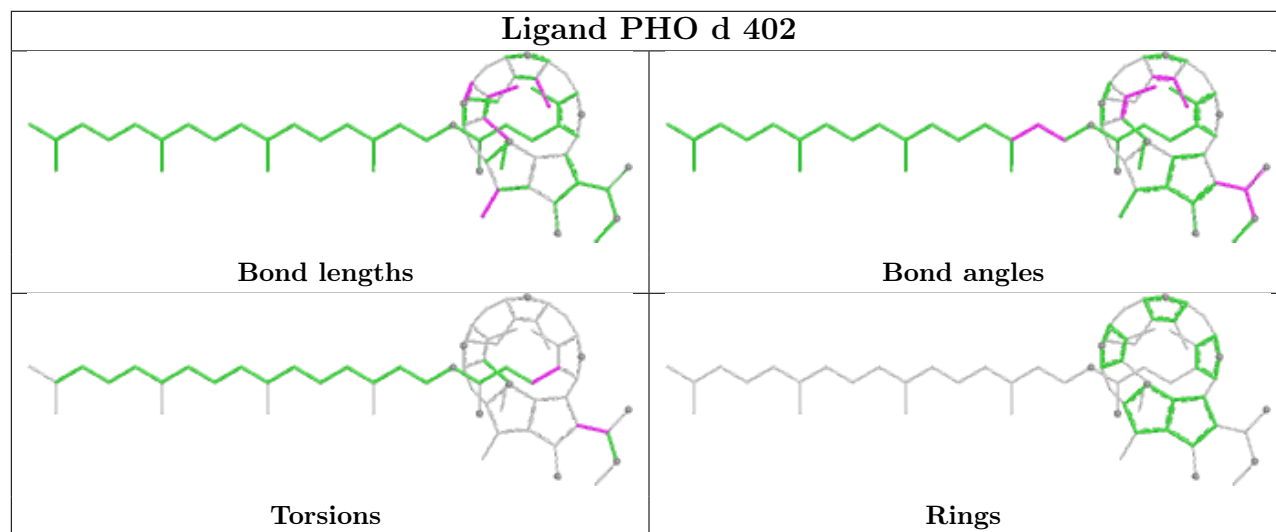
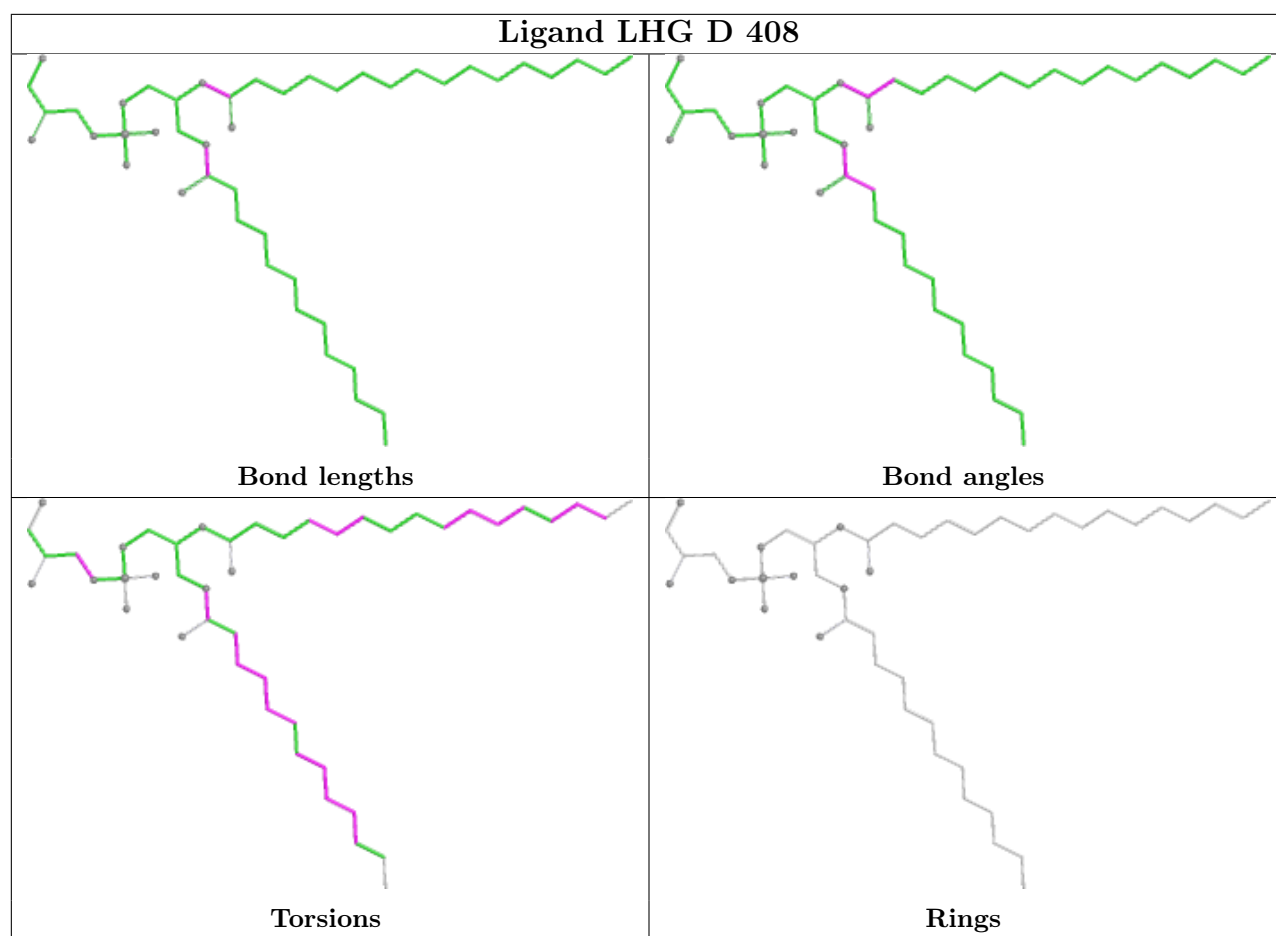


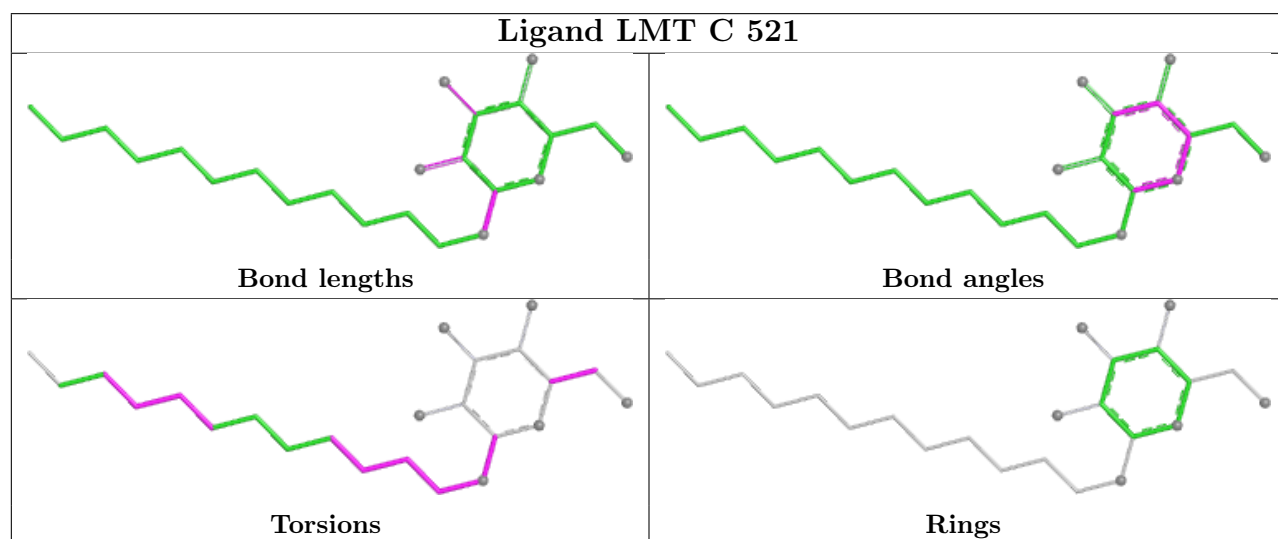
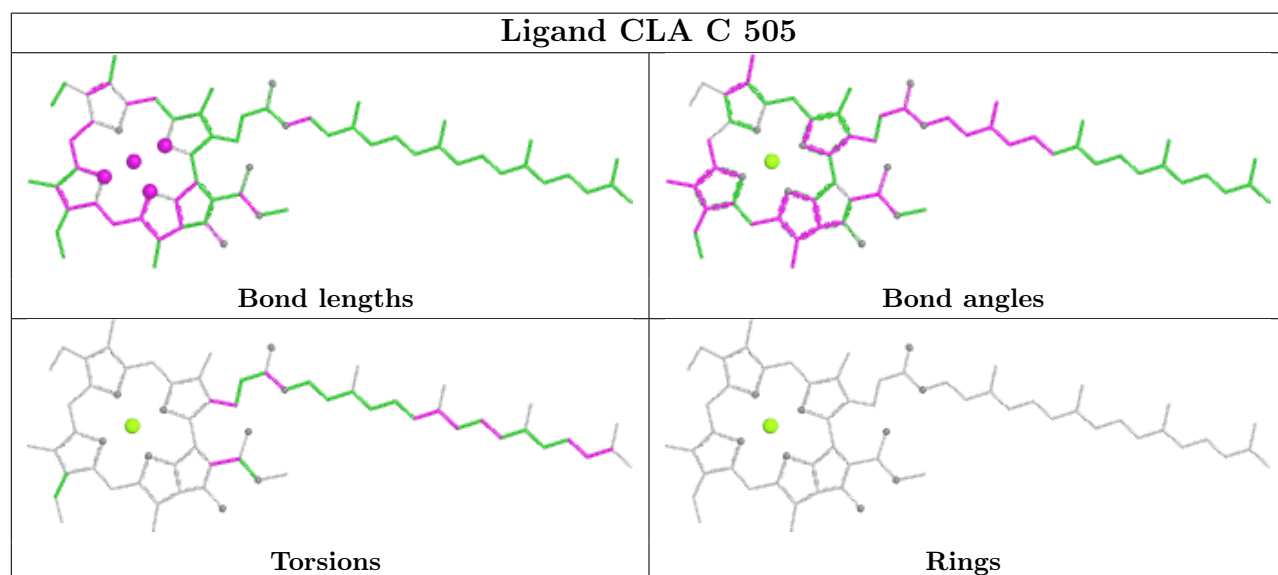
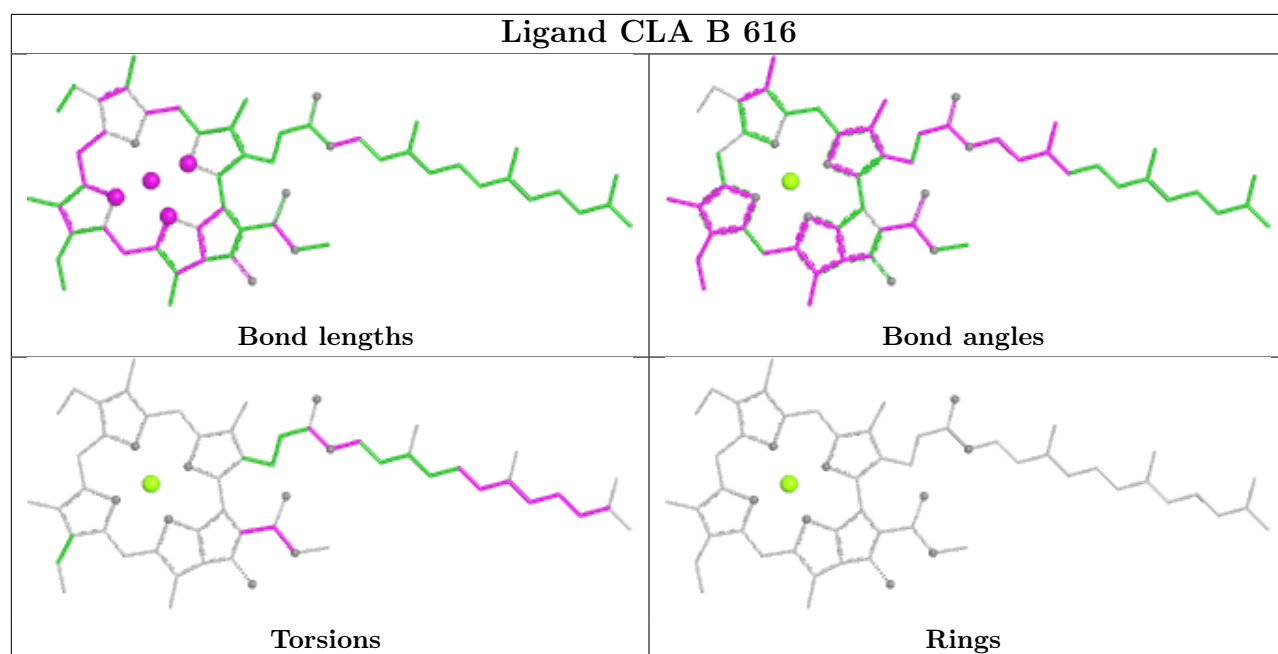


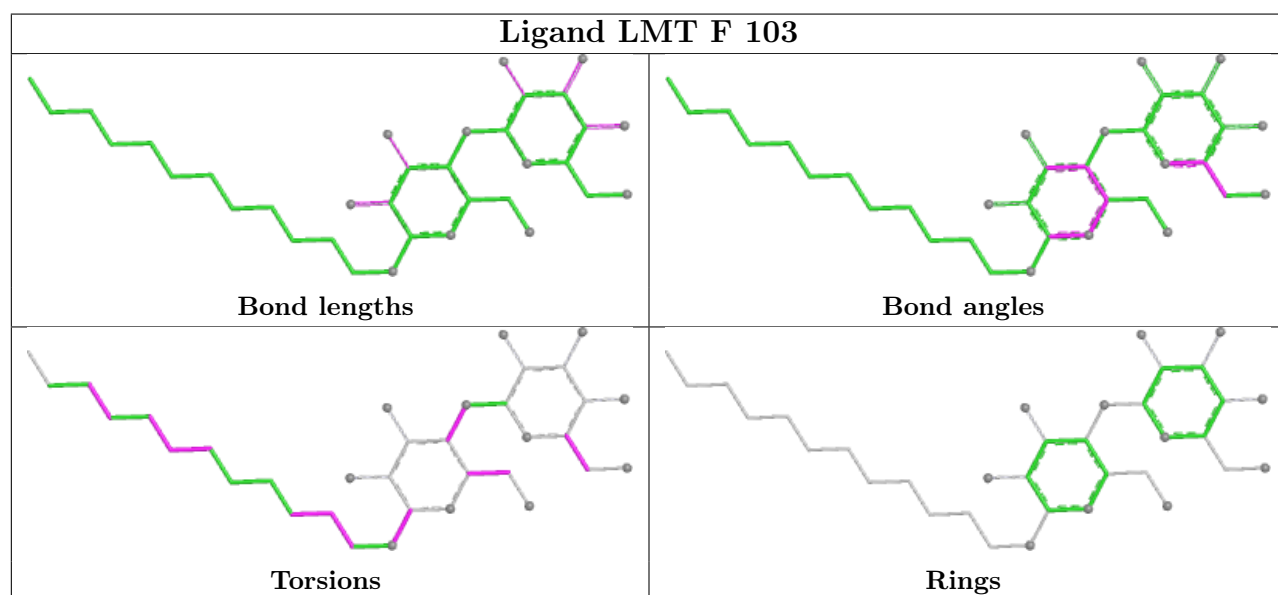
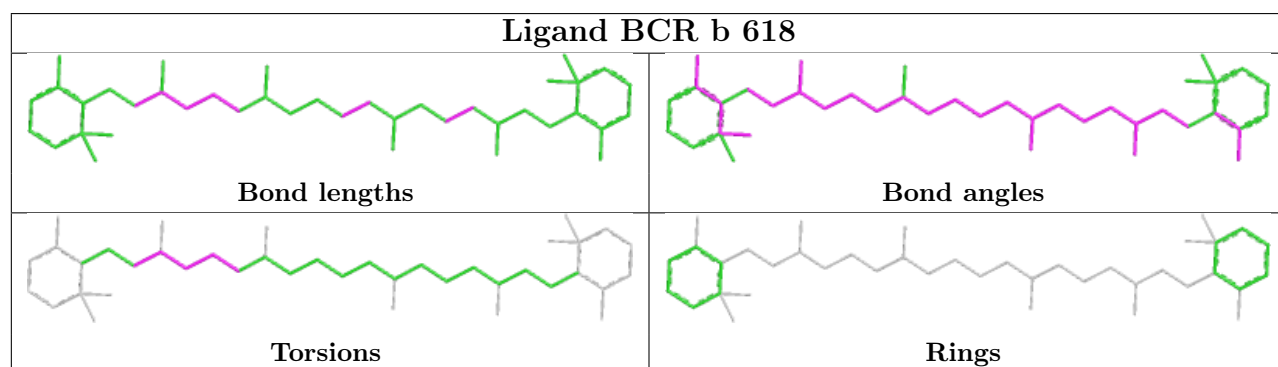
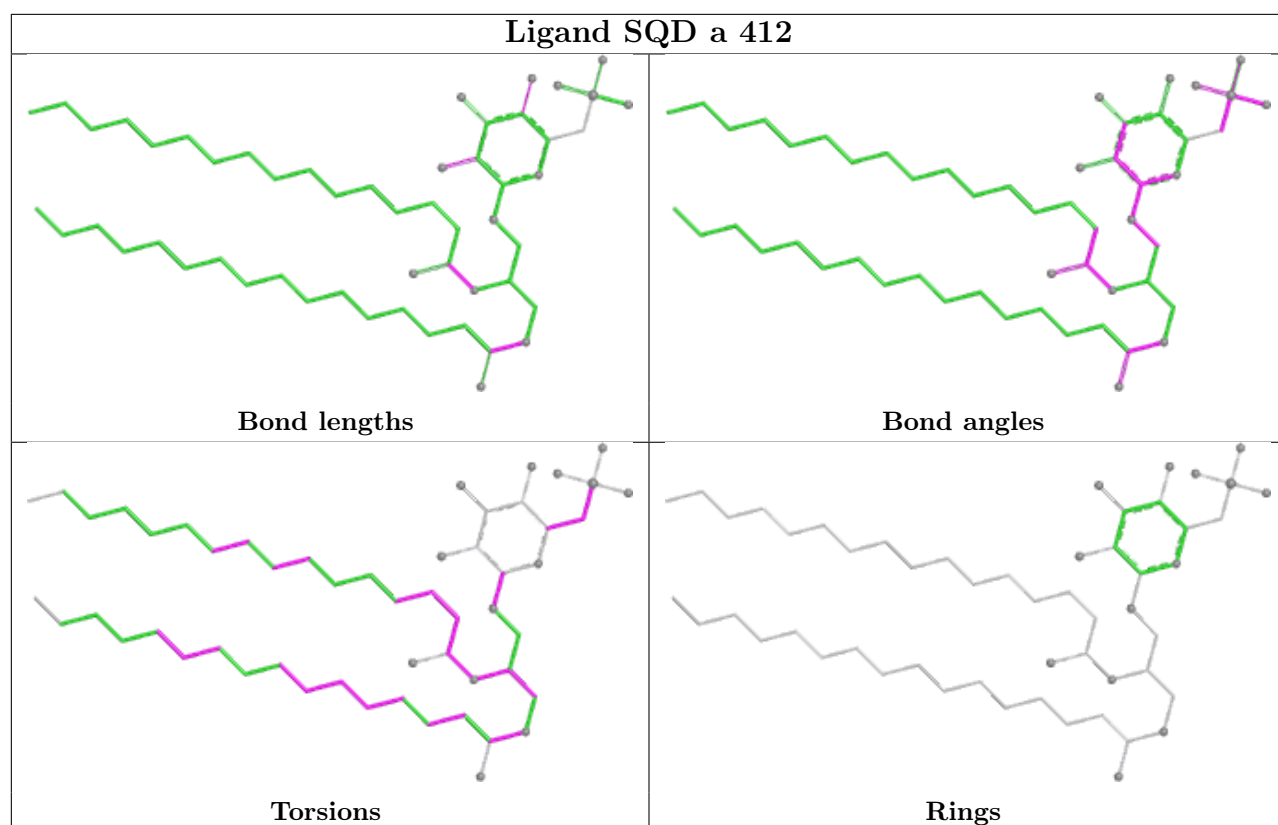
Ligand CLA B 604	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LMT h 101	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR b 619	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

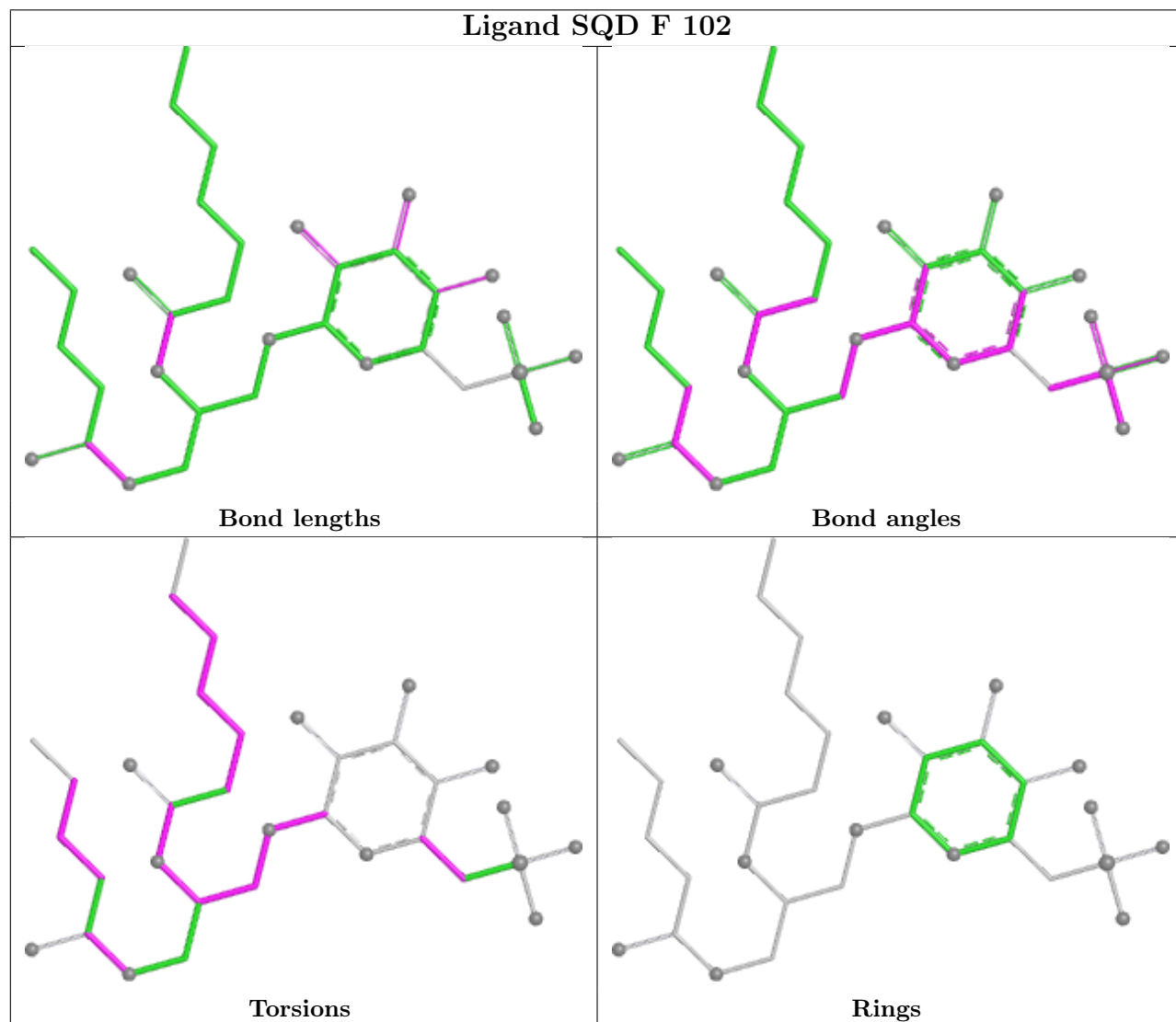
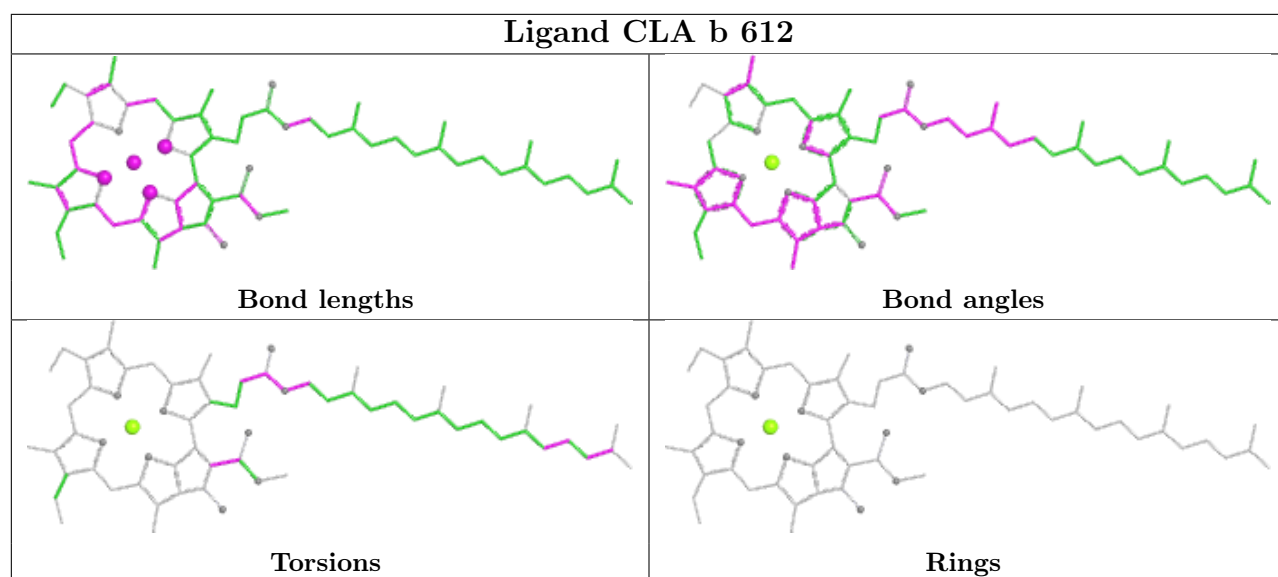


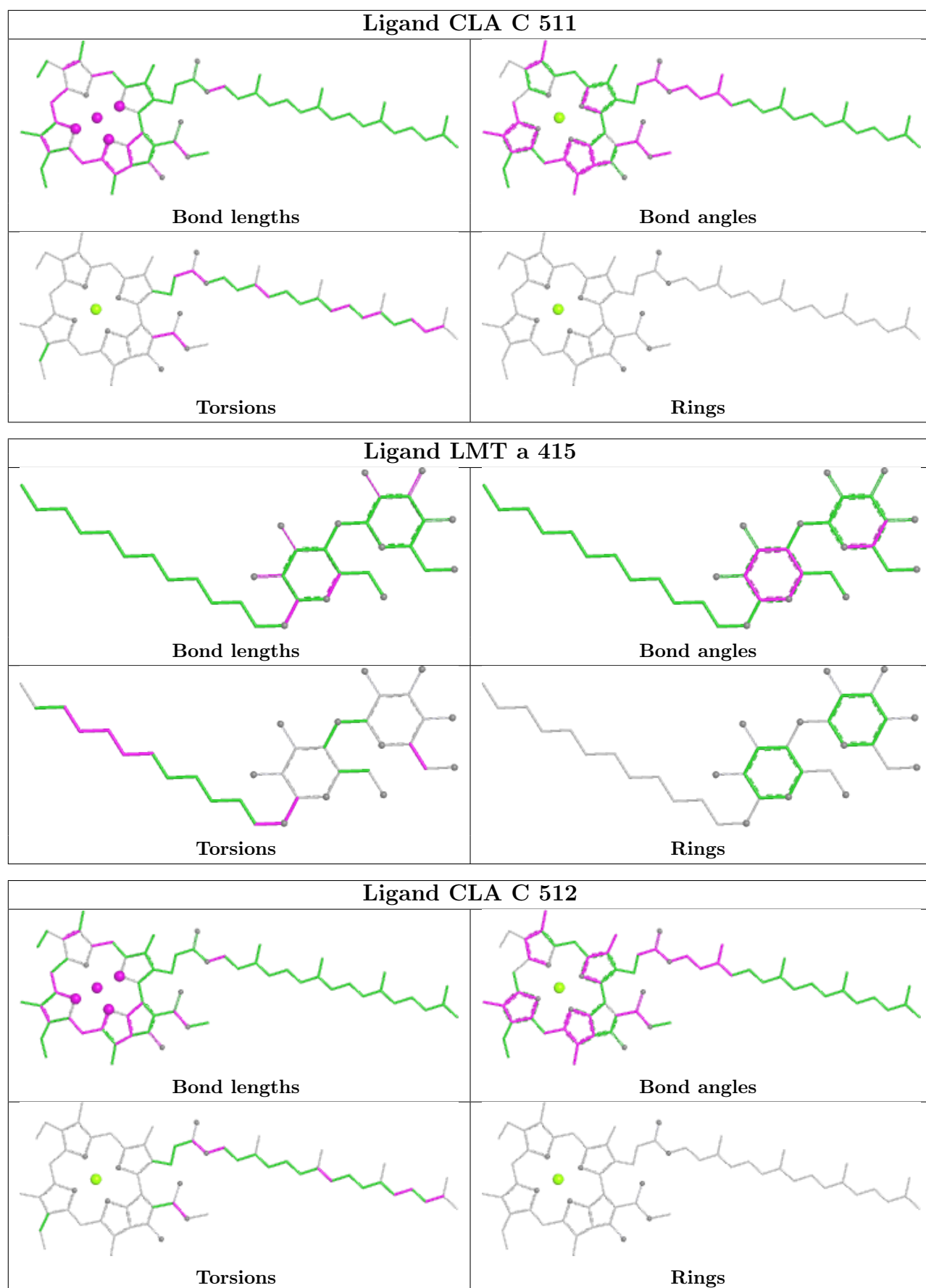


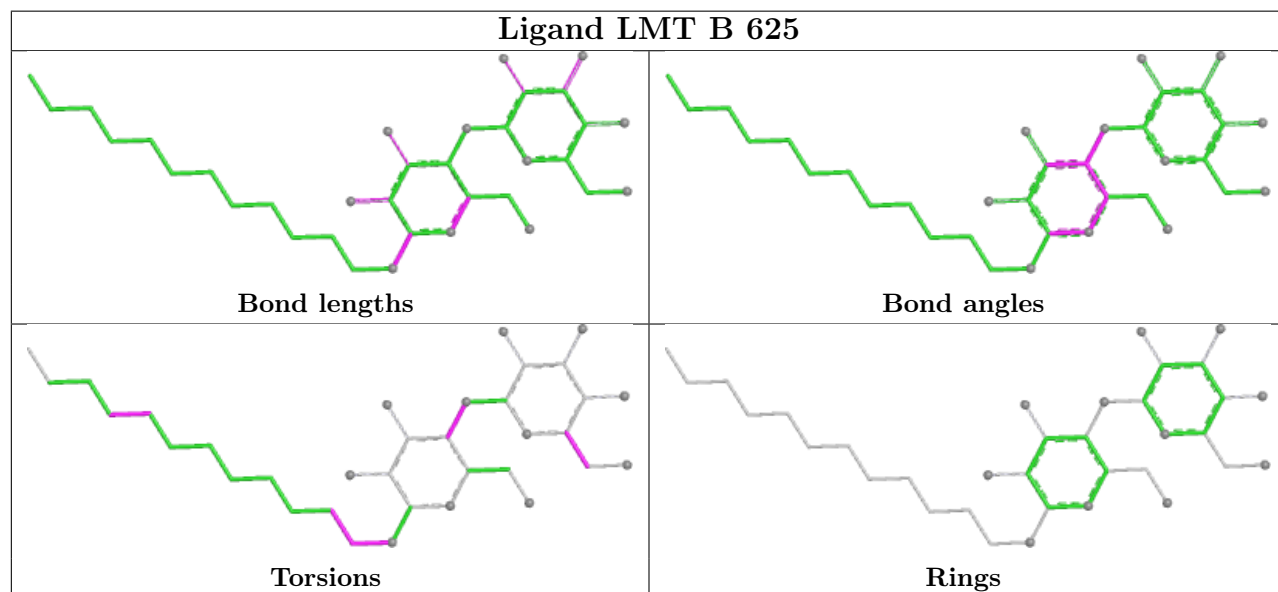
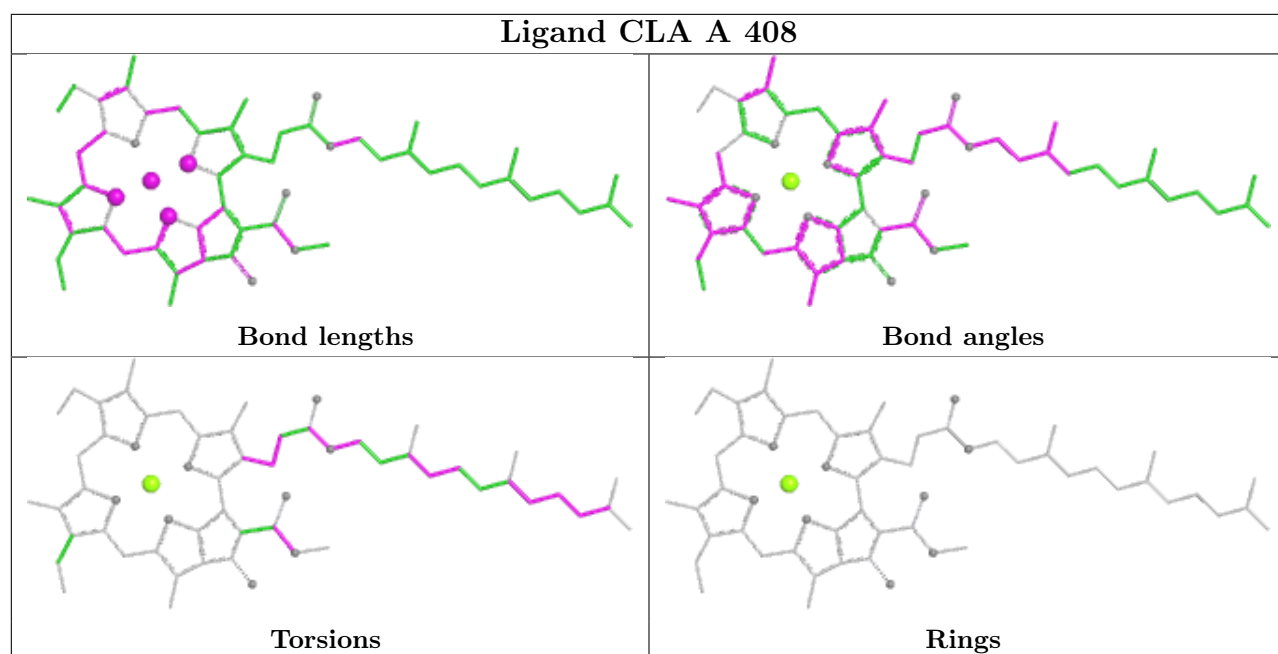


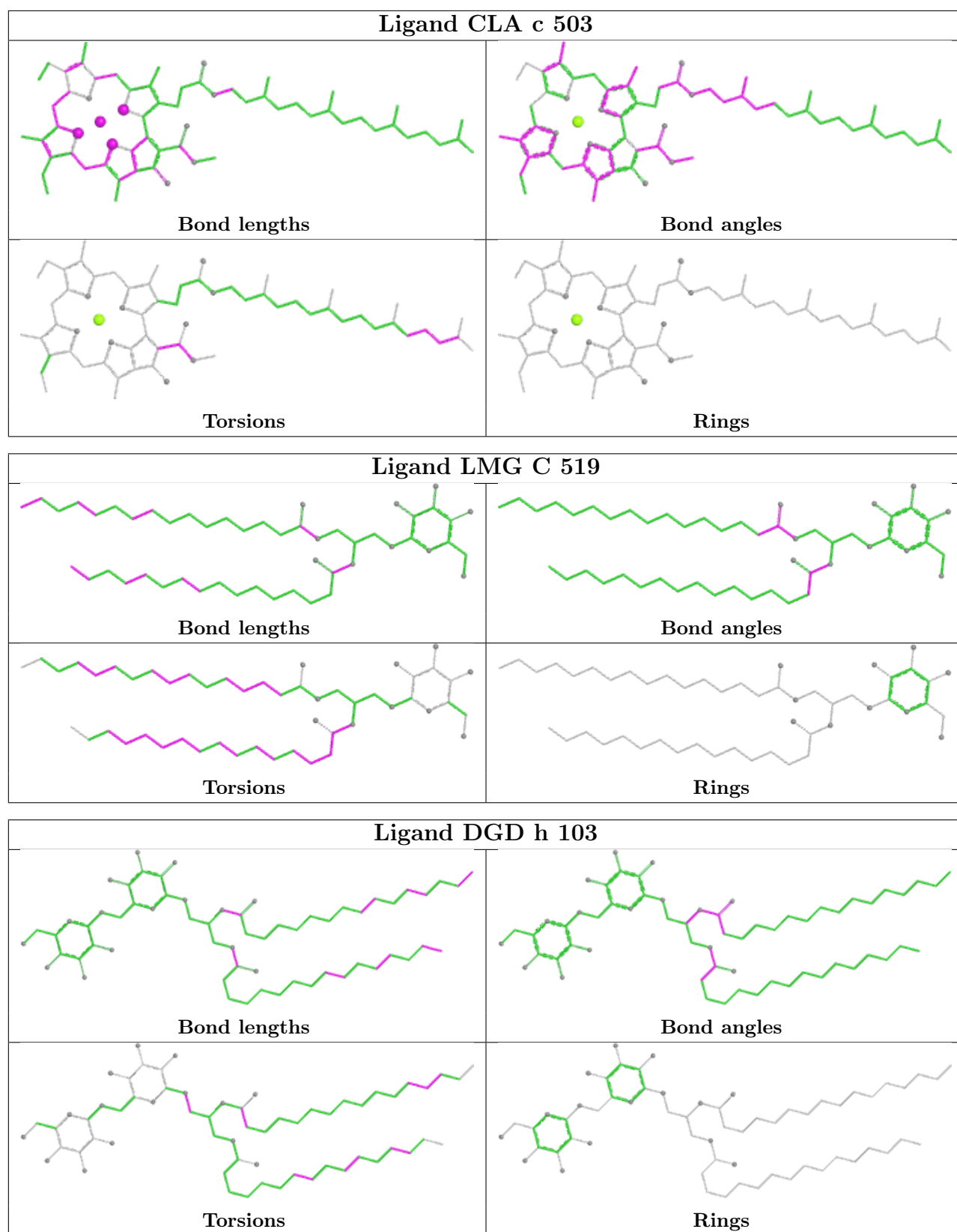


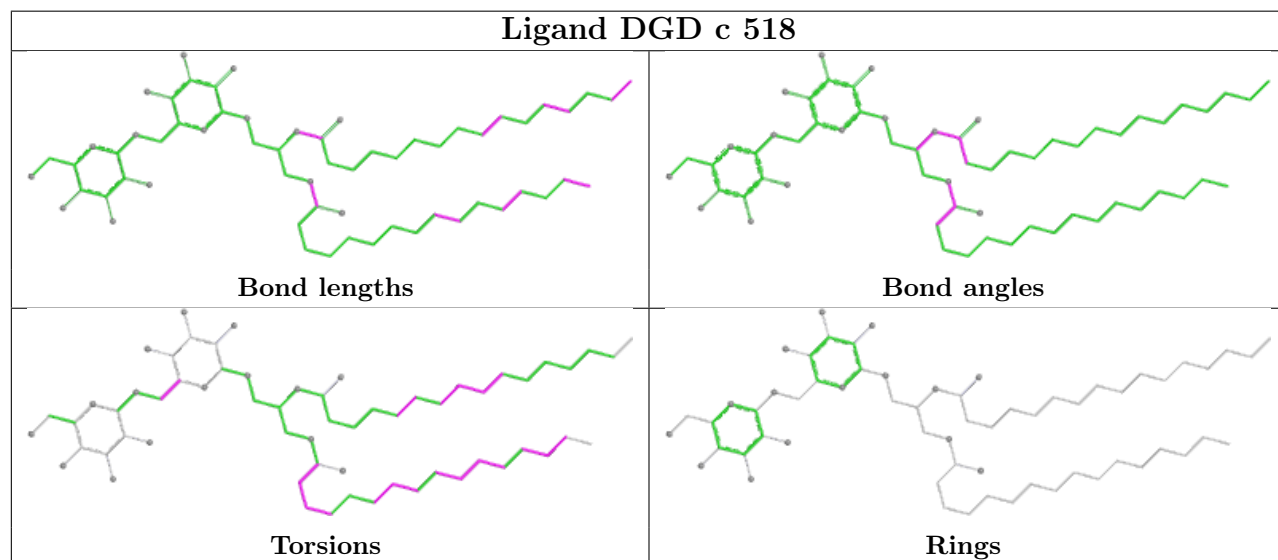
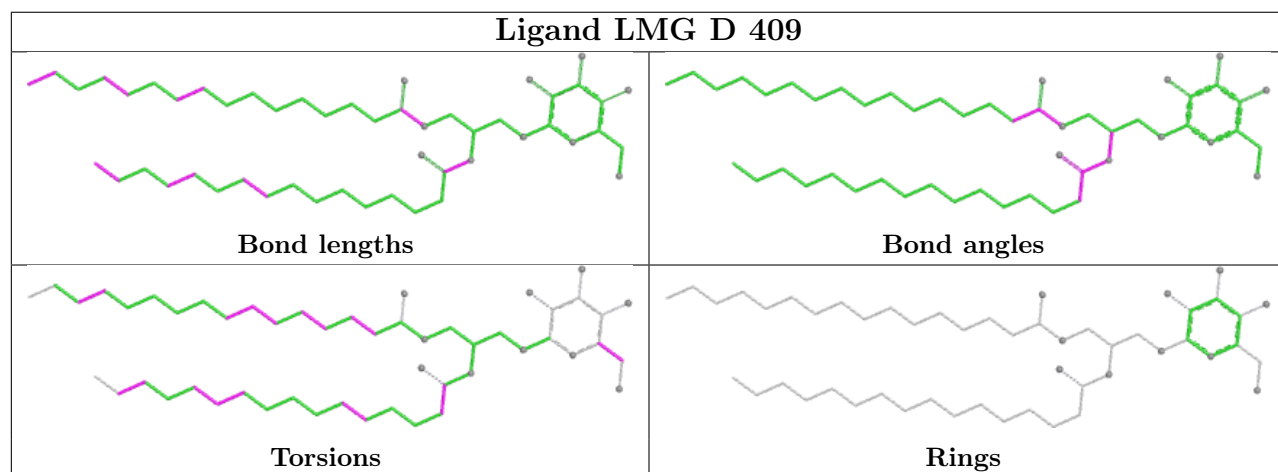
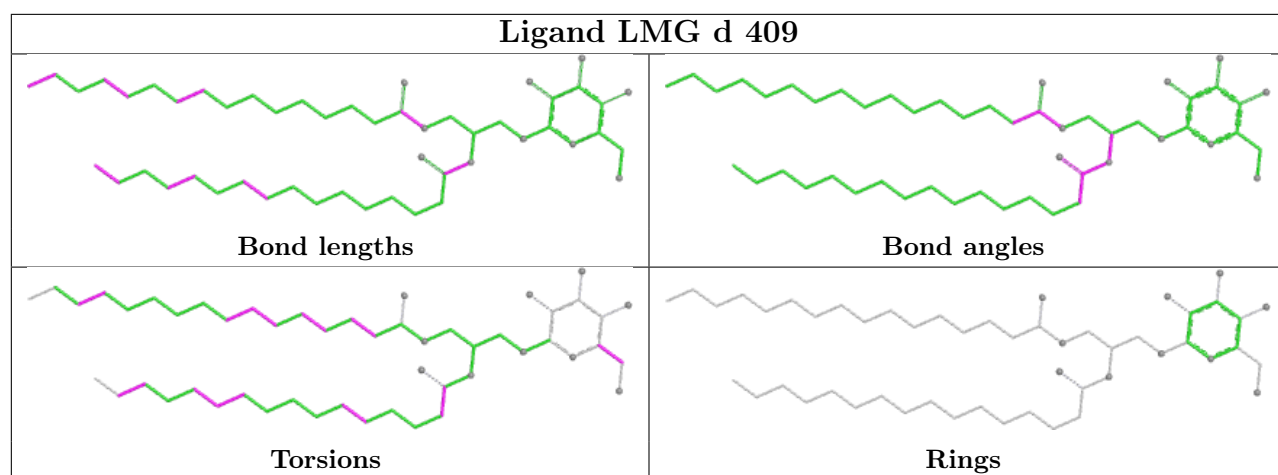


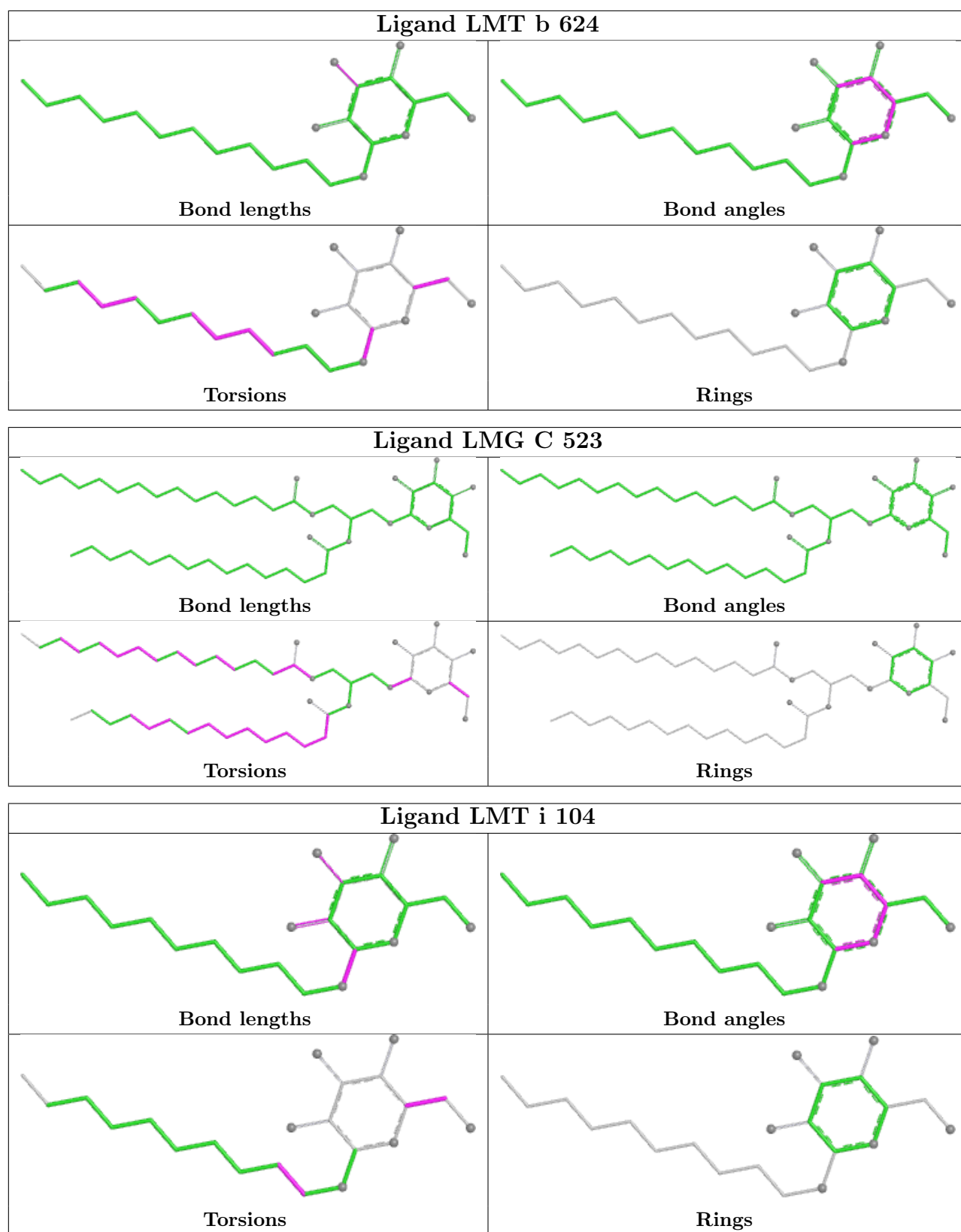


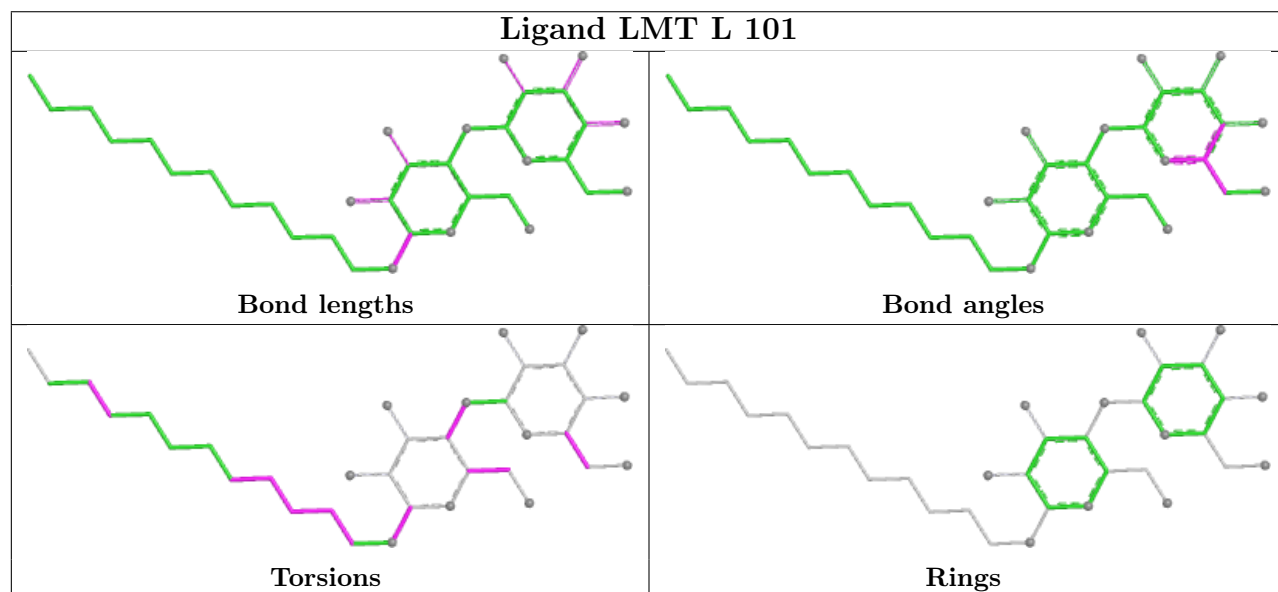
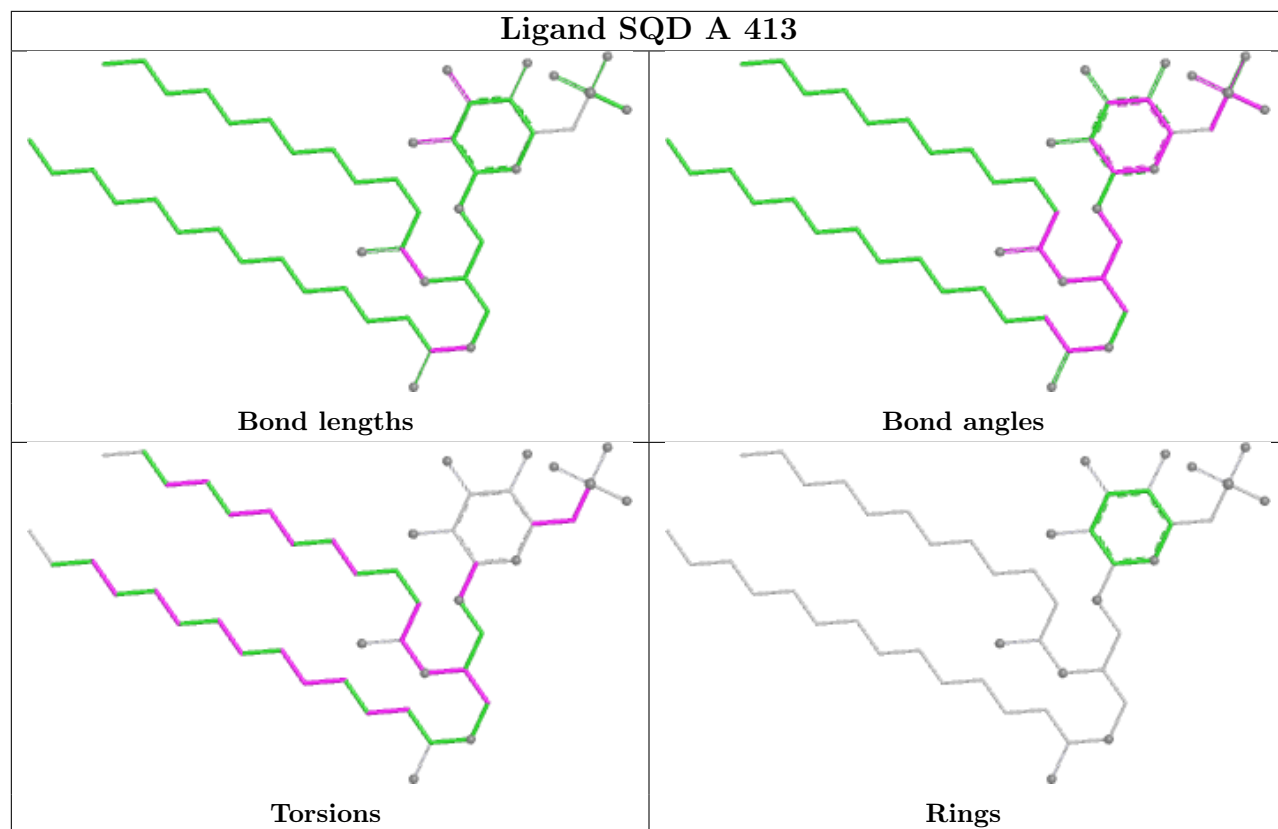


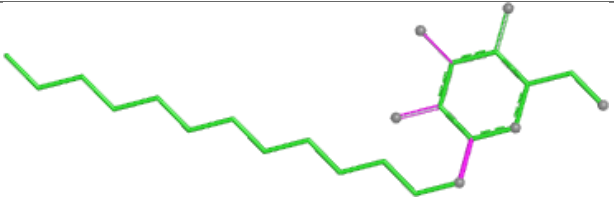




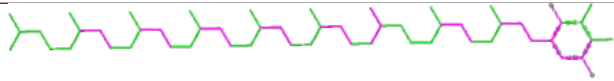
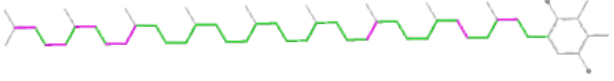
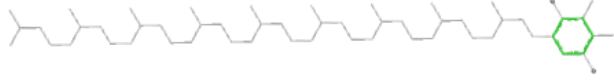
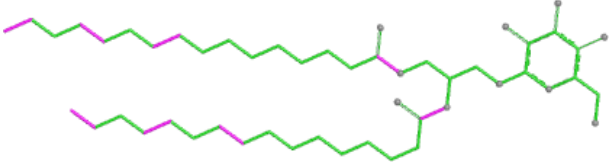
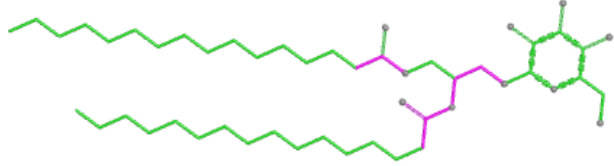
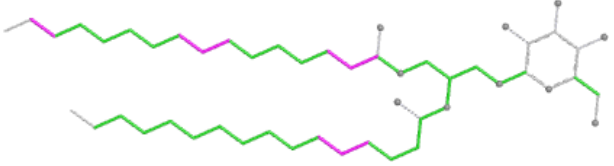
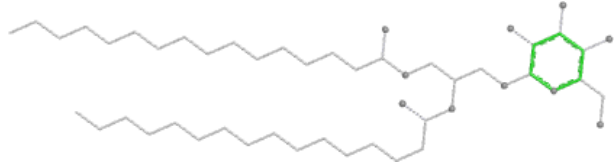


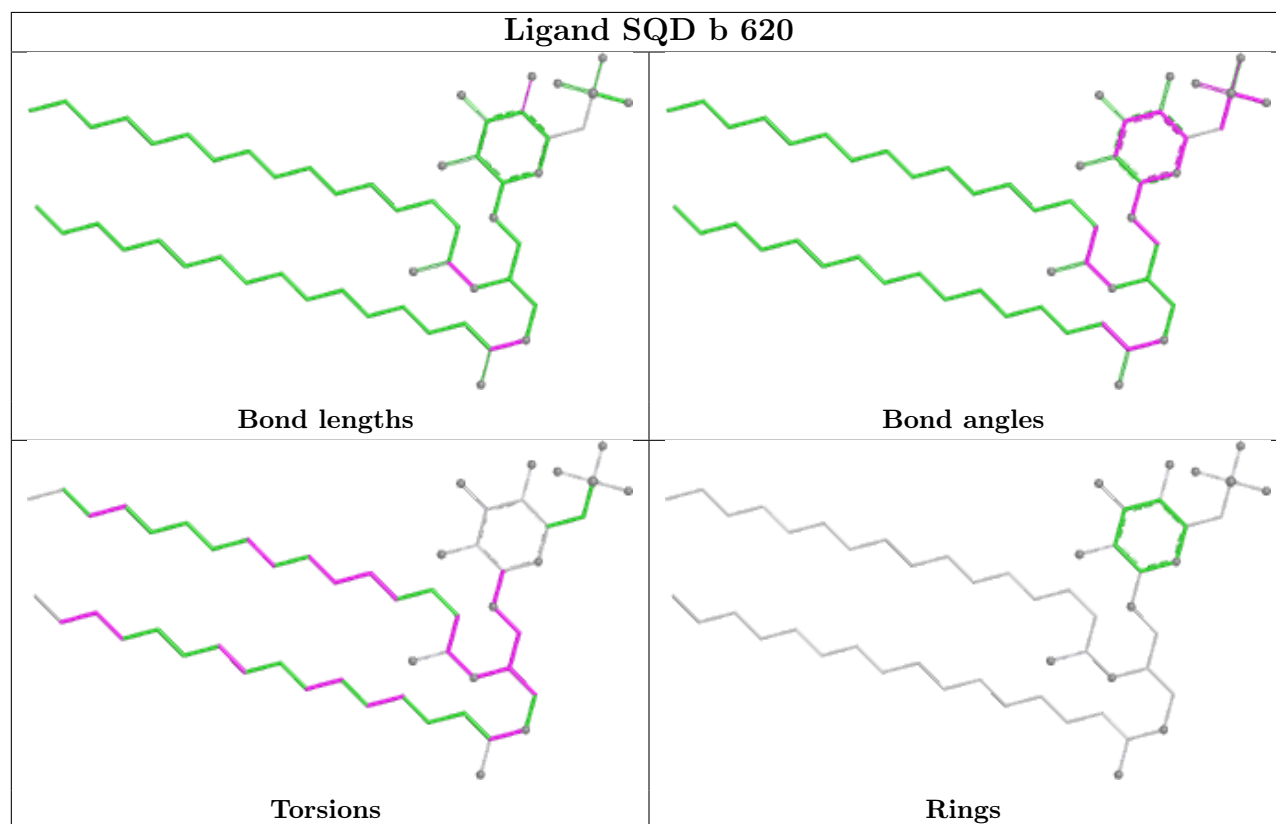
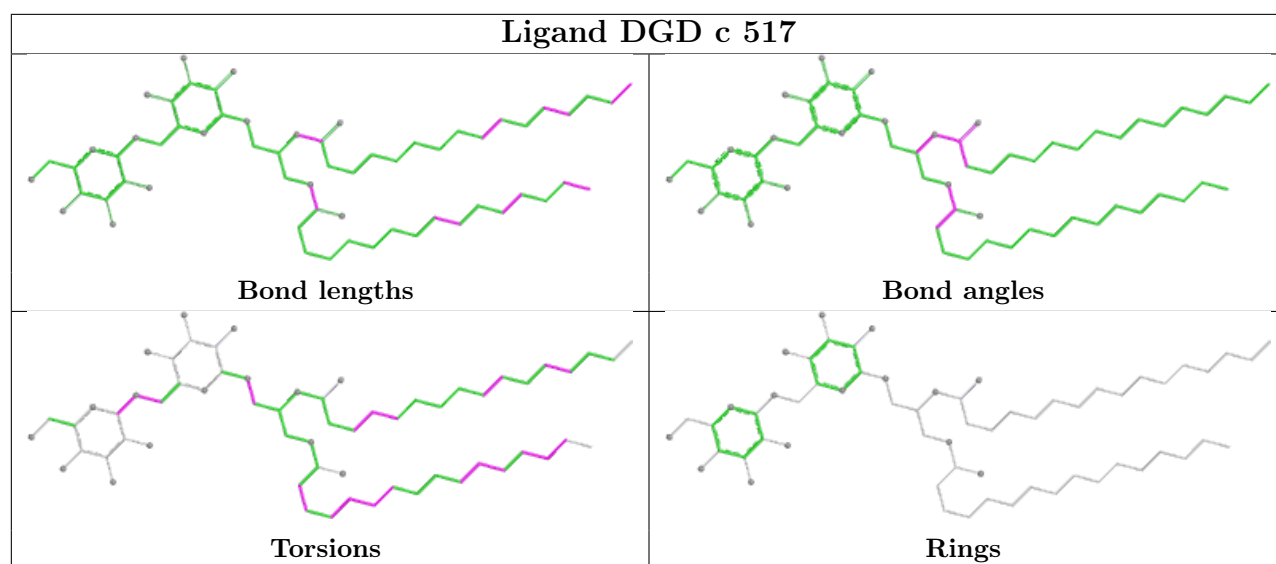


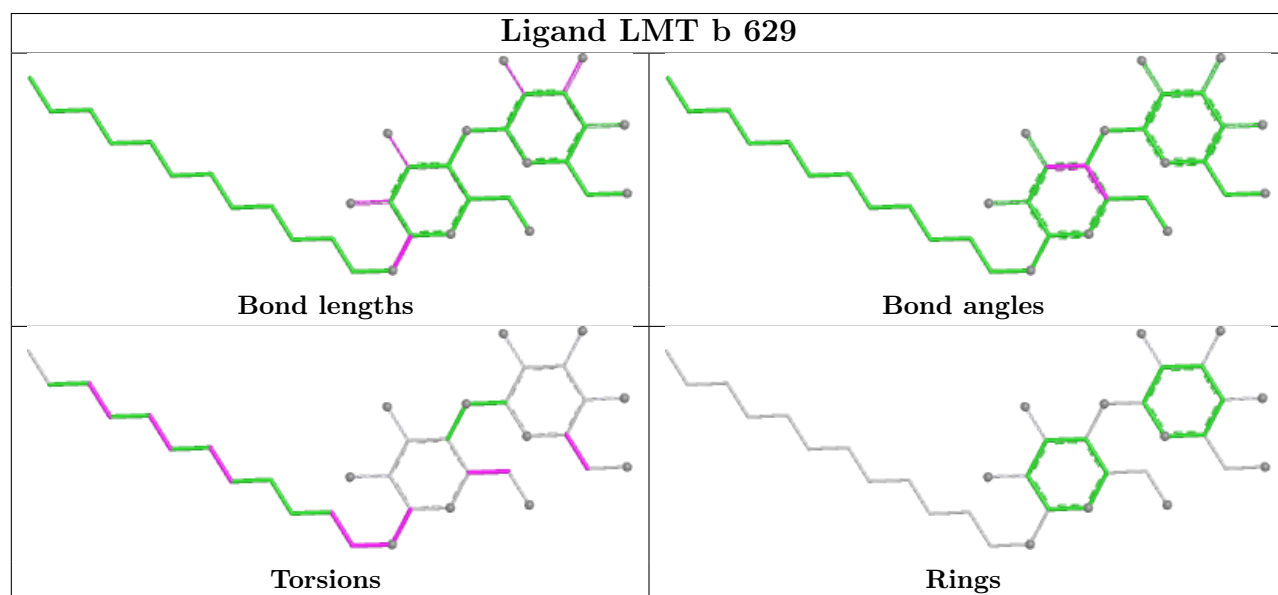
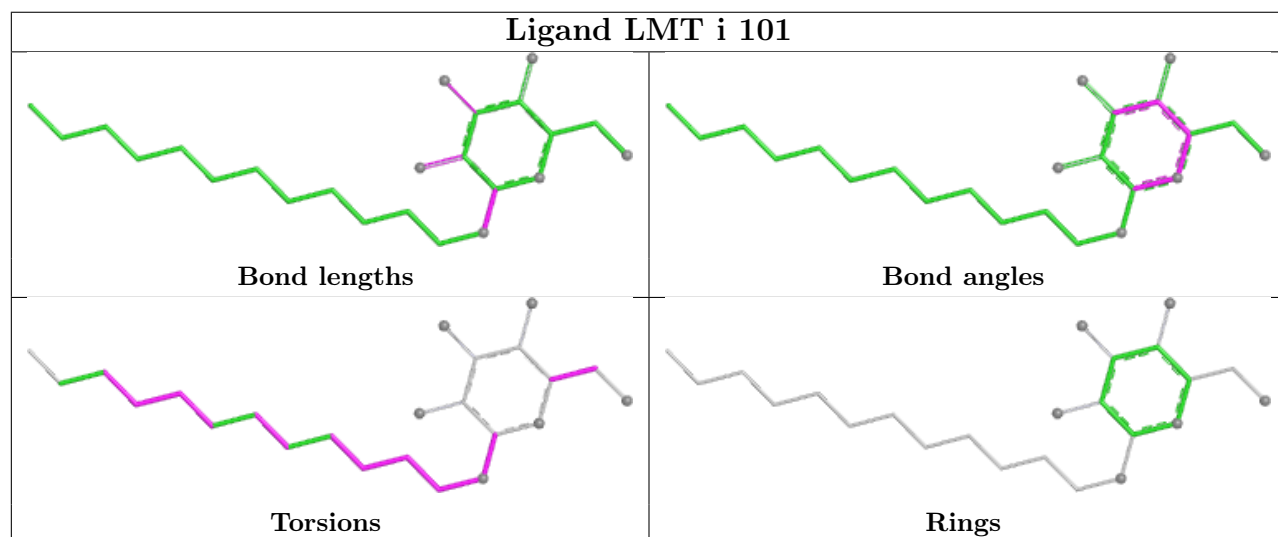
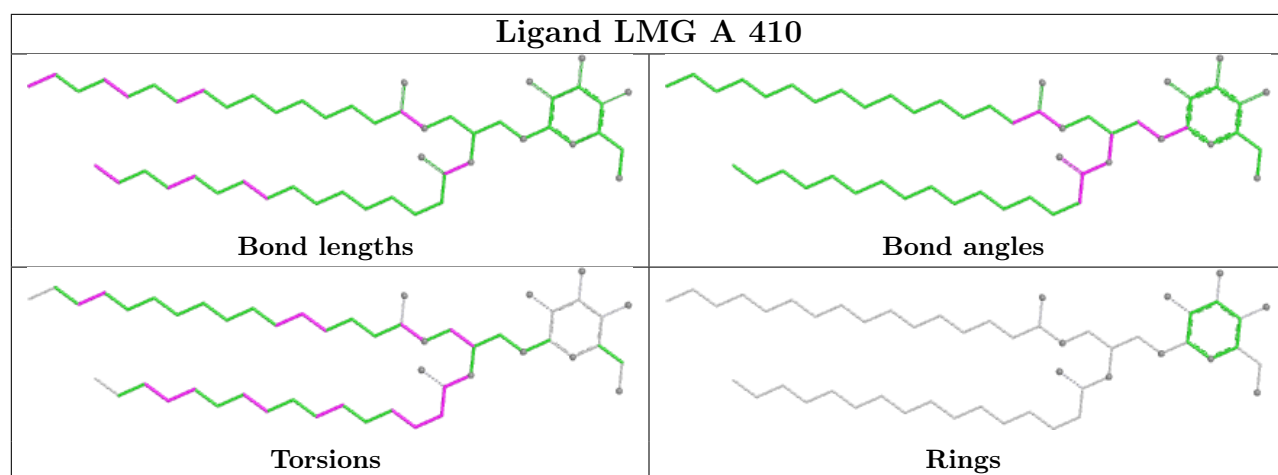


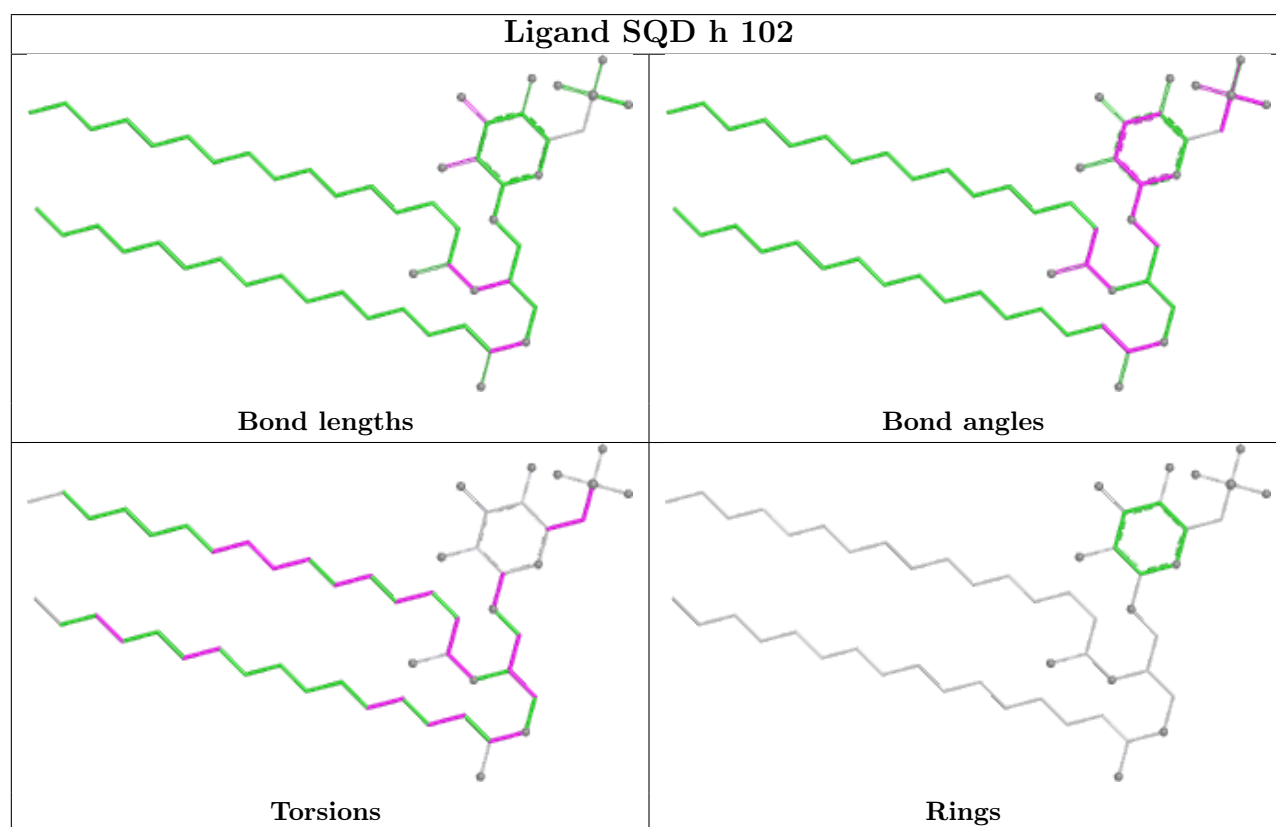
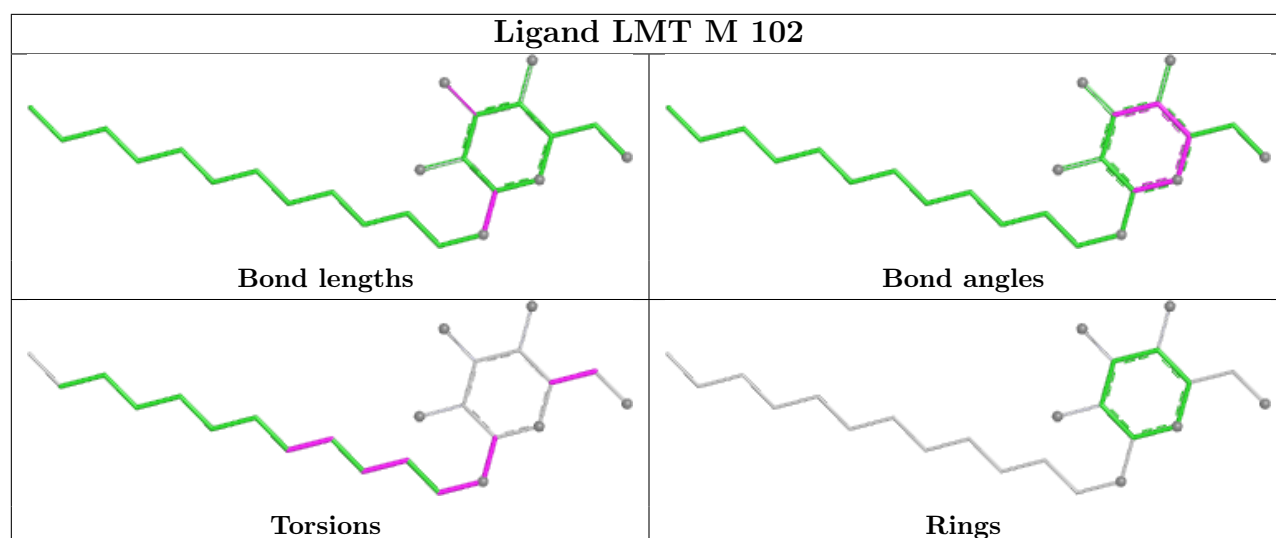


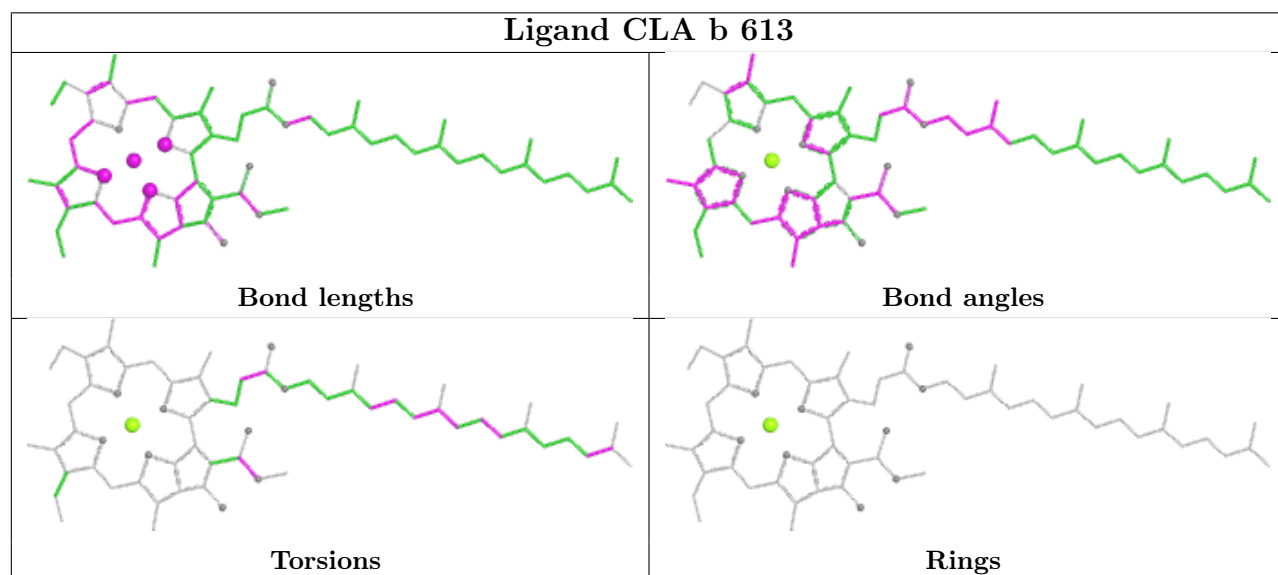
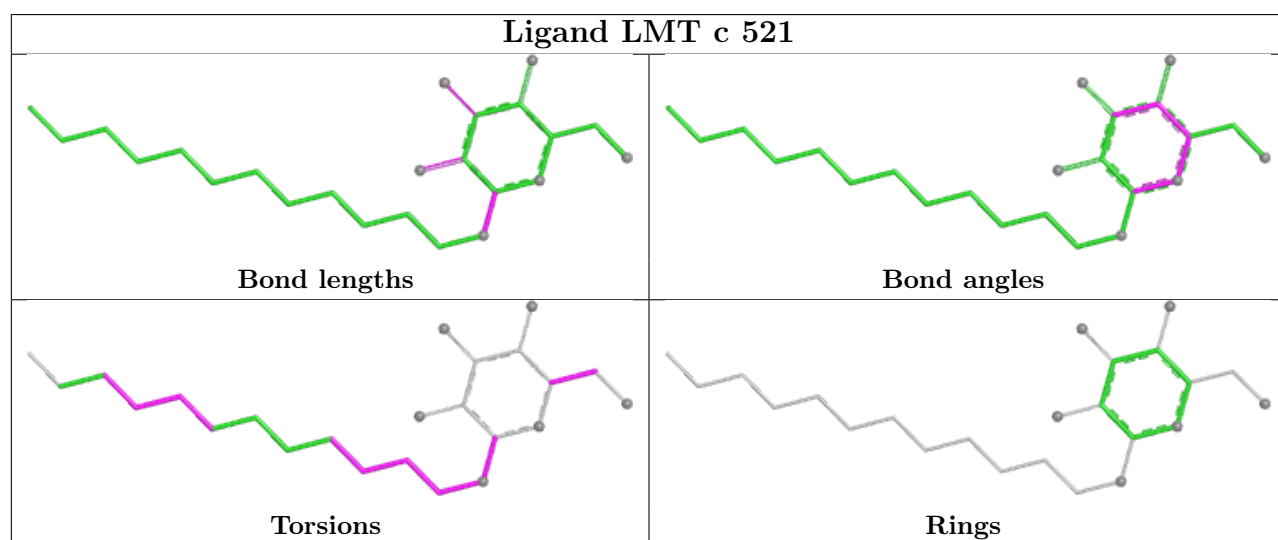
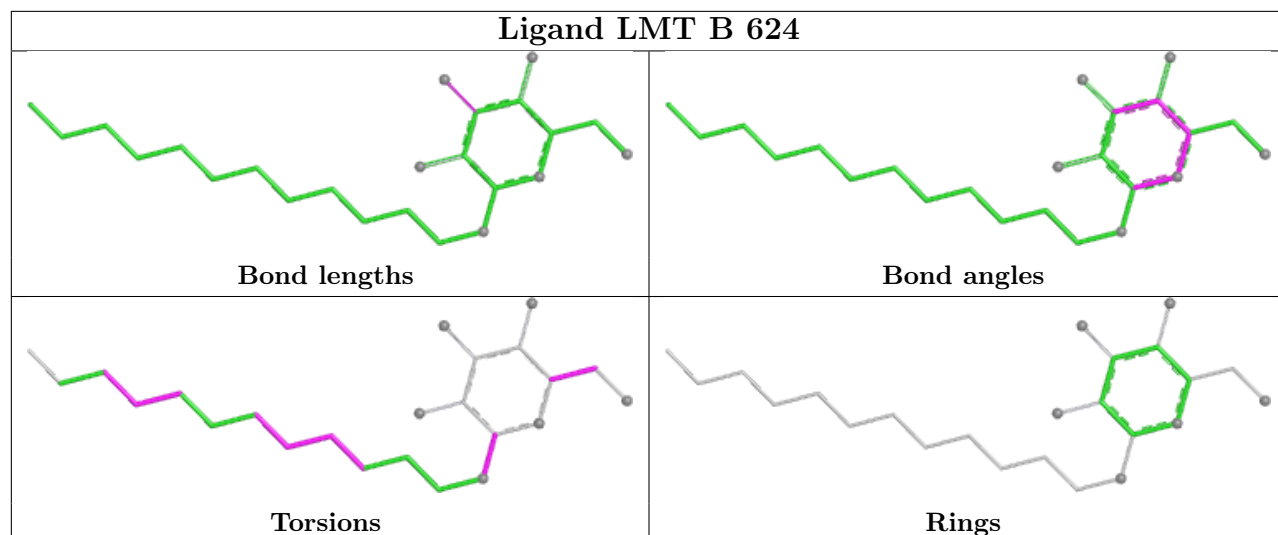


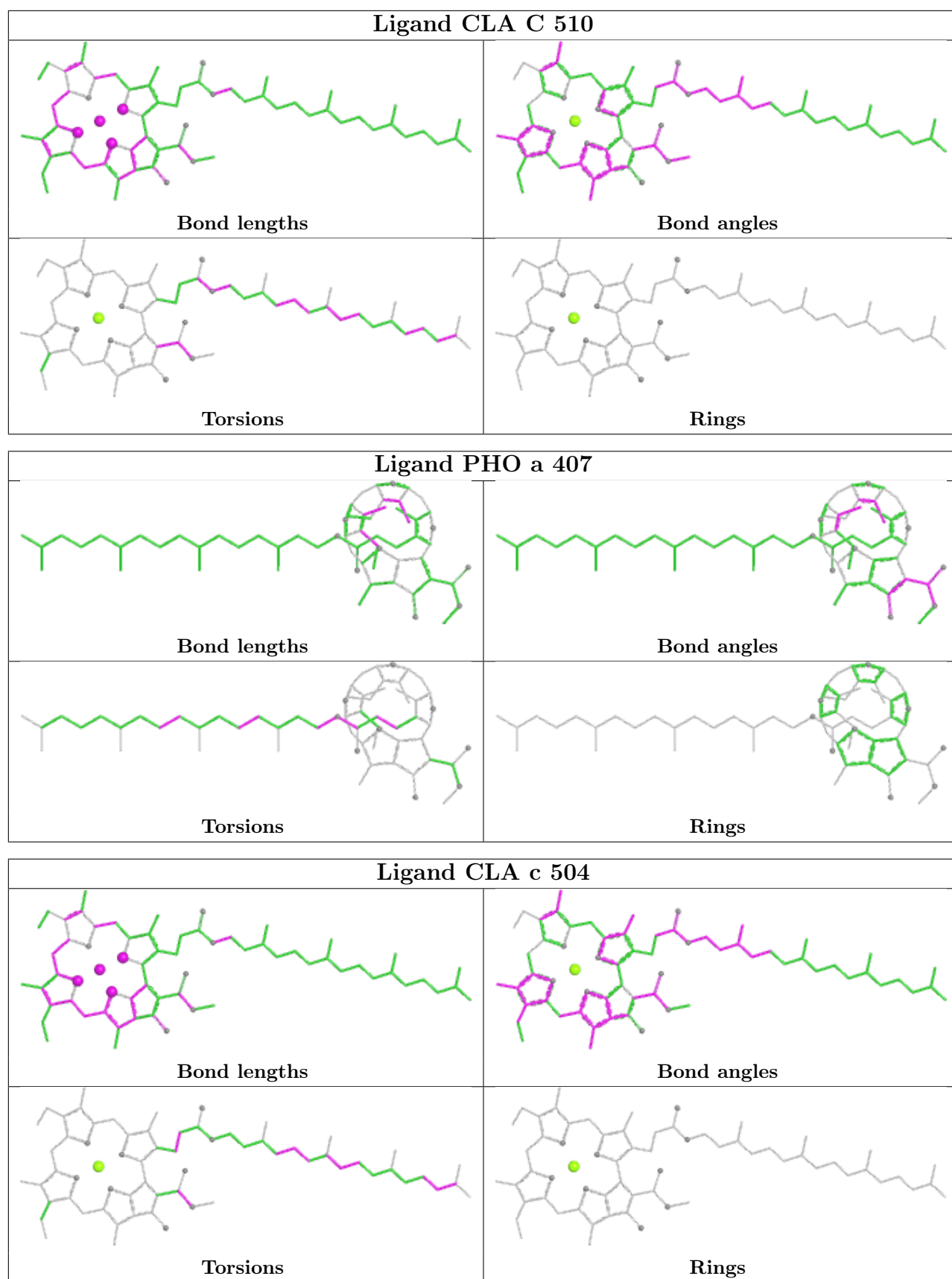
Ligand LMT x 101	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PL9 d 405	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LMG b 621	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

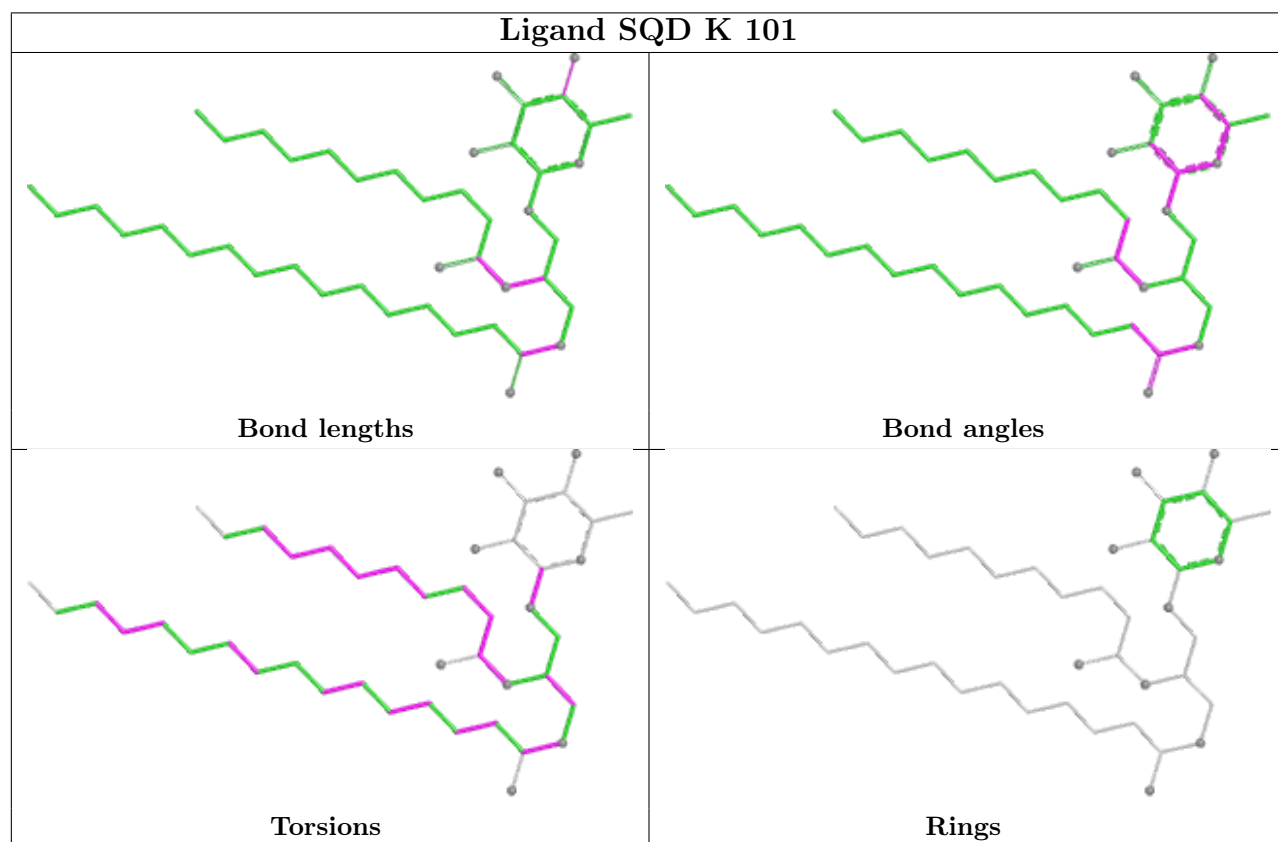
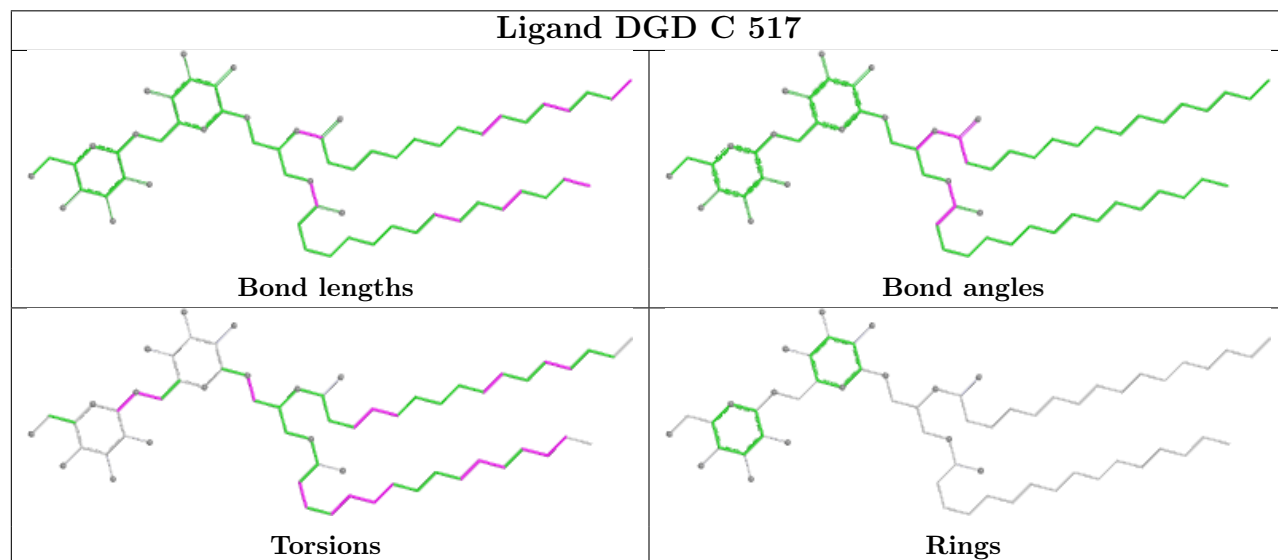
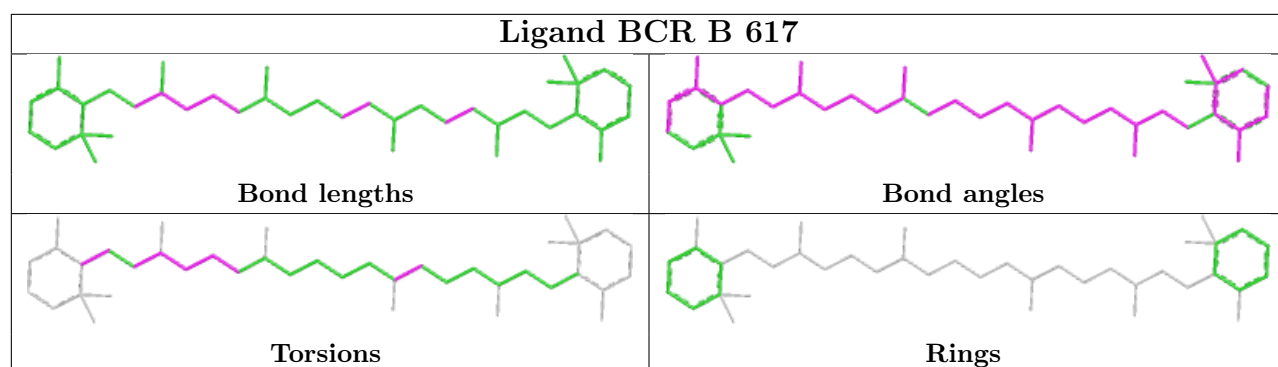


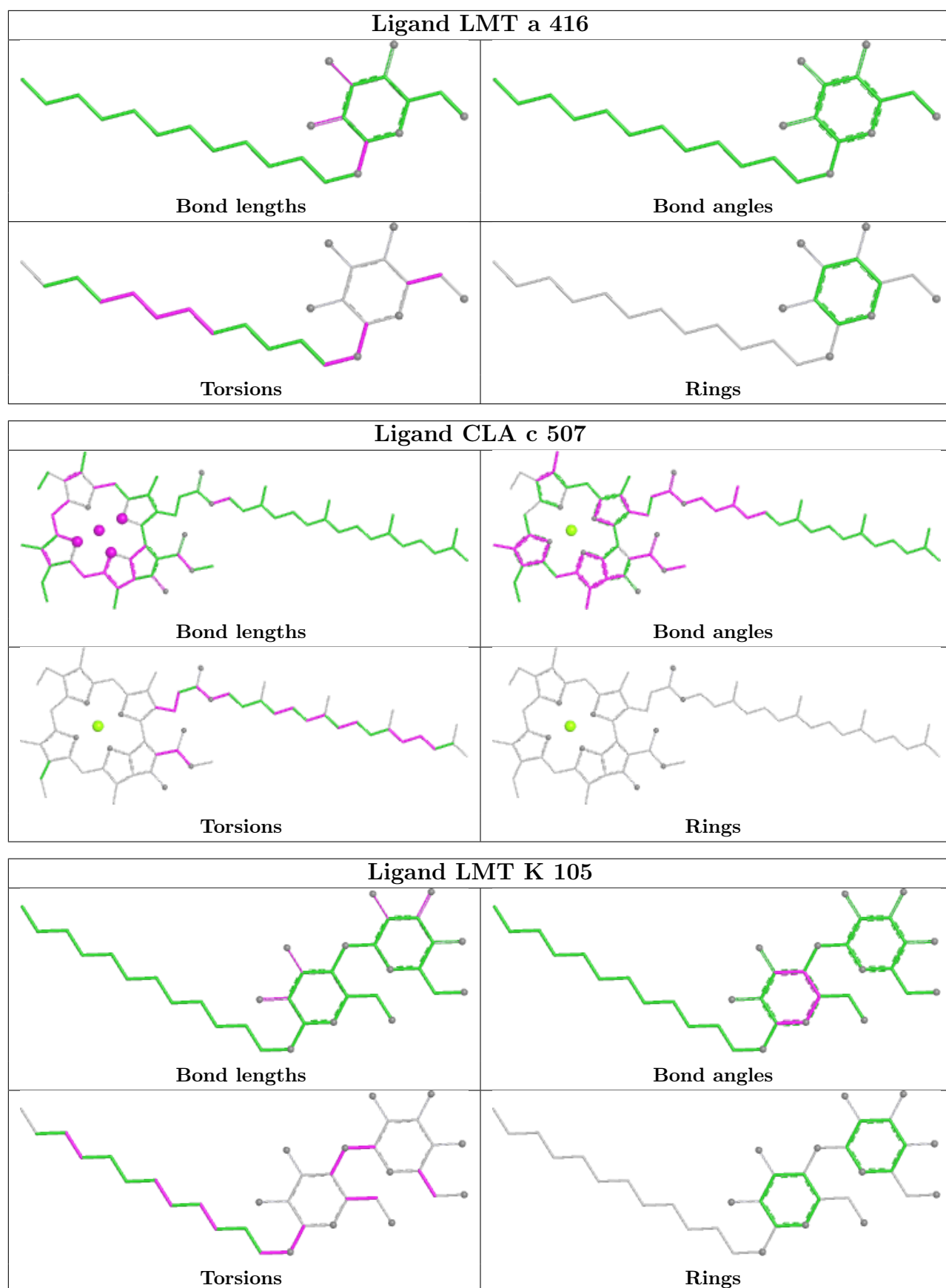


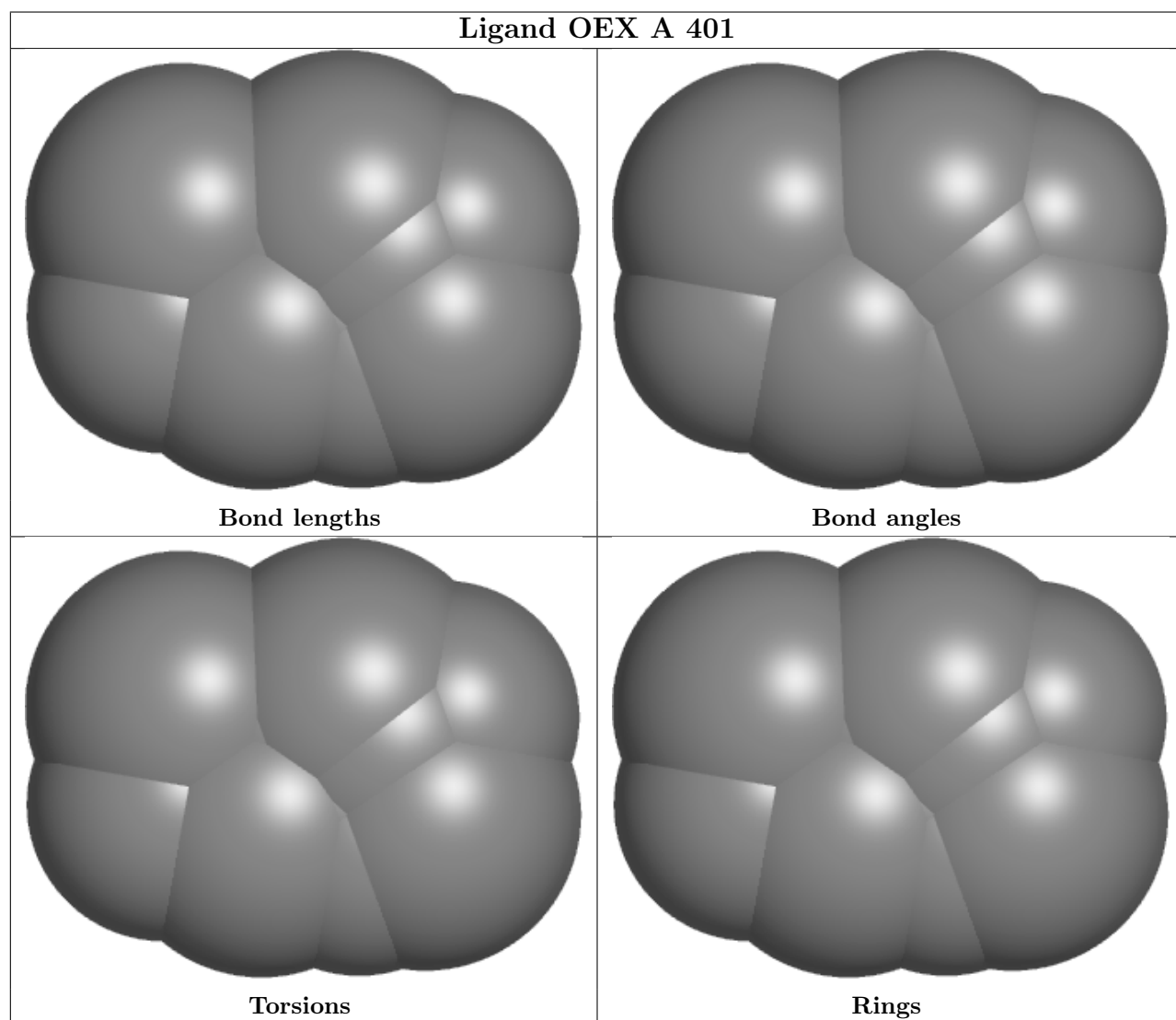
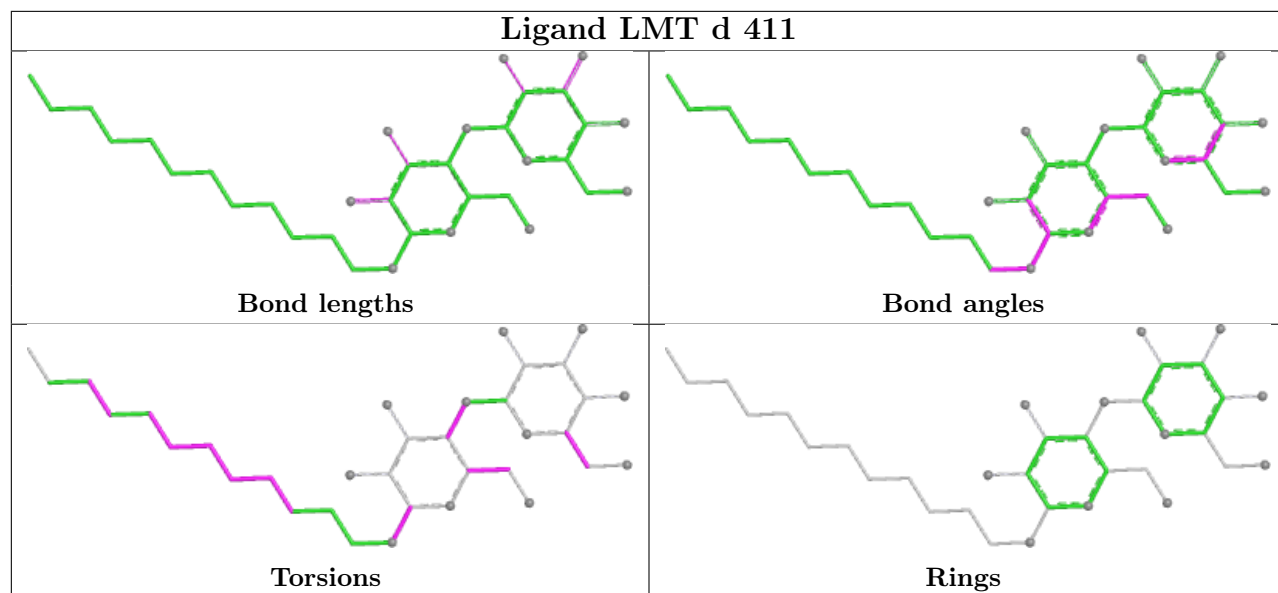


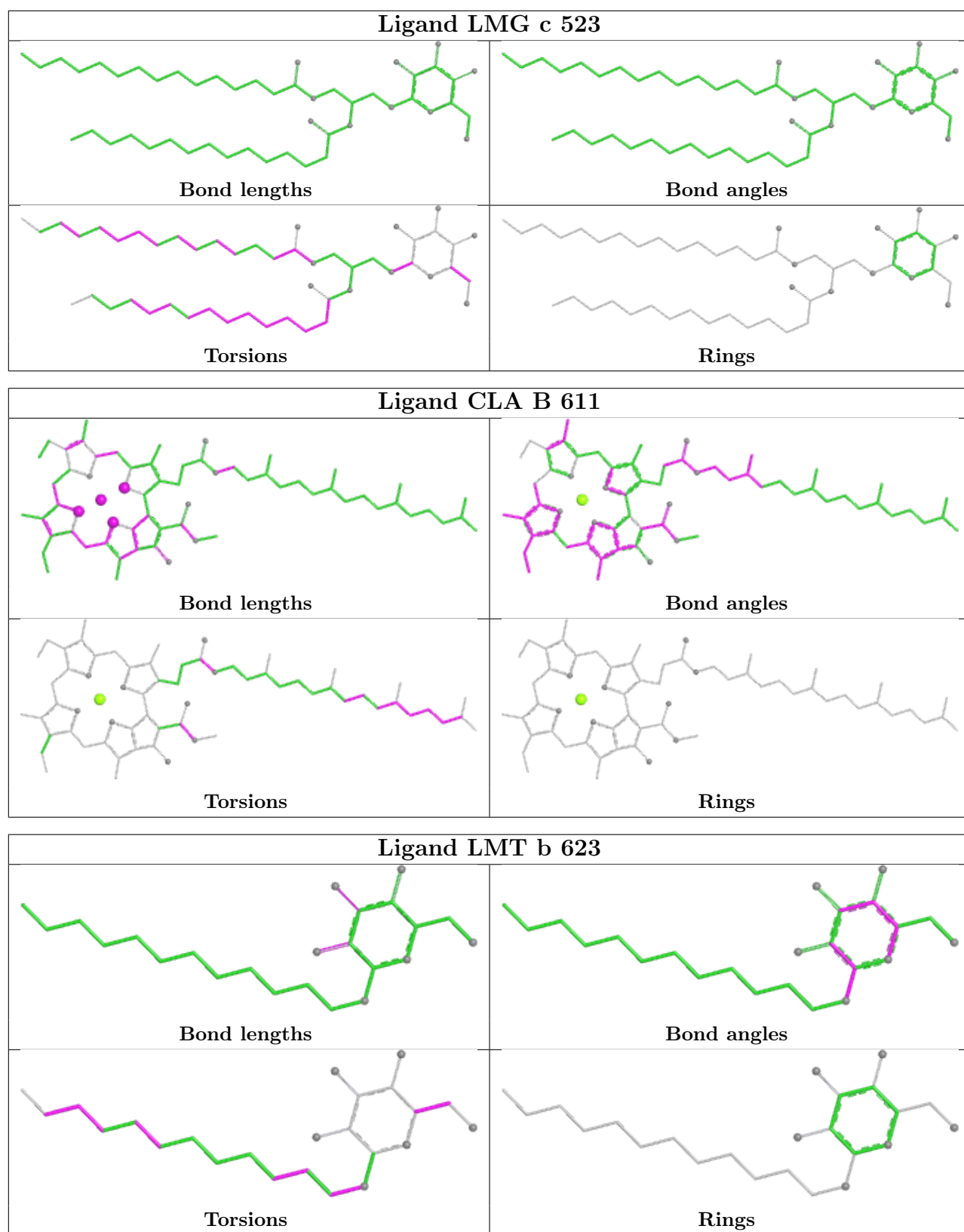


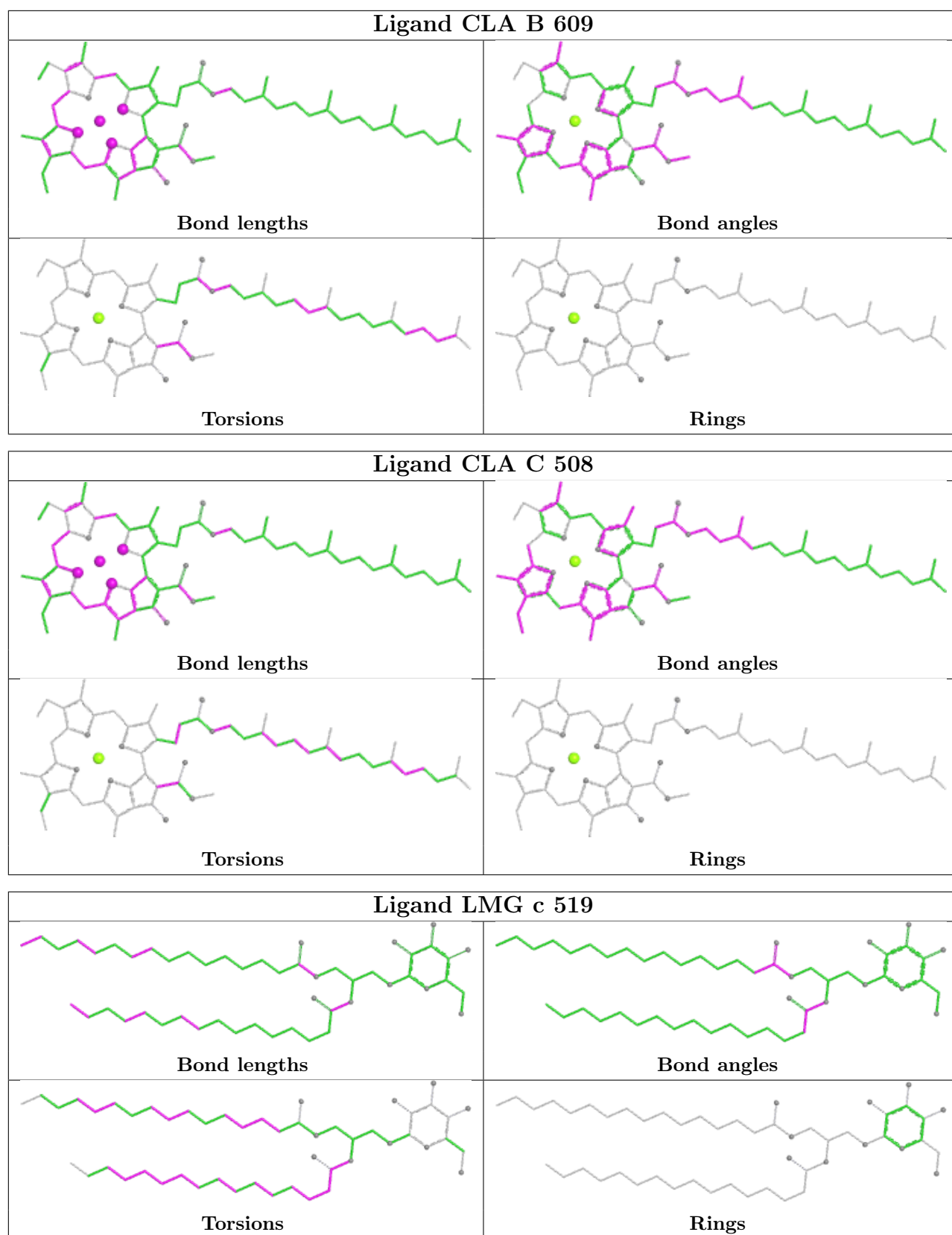


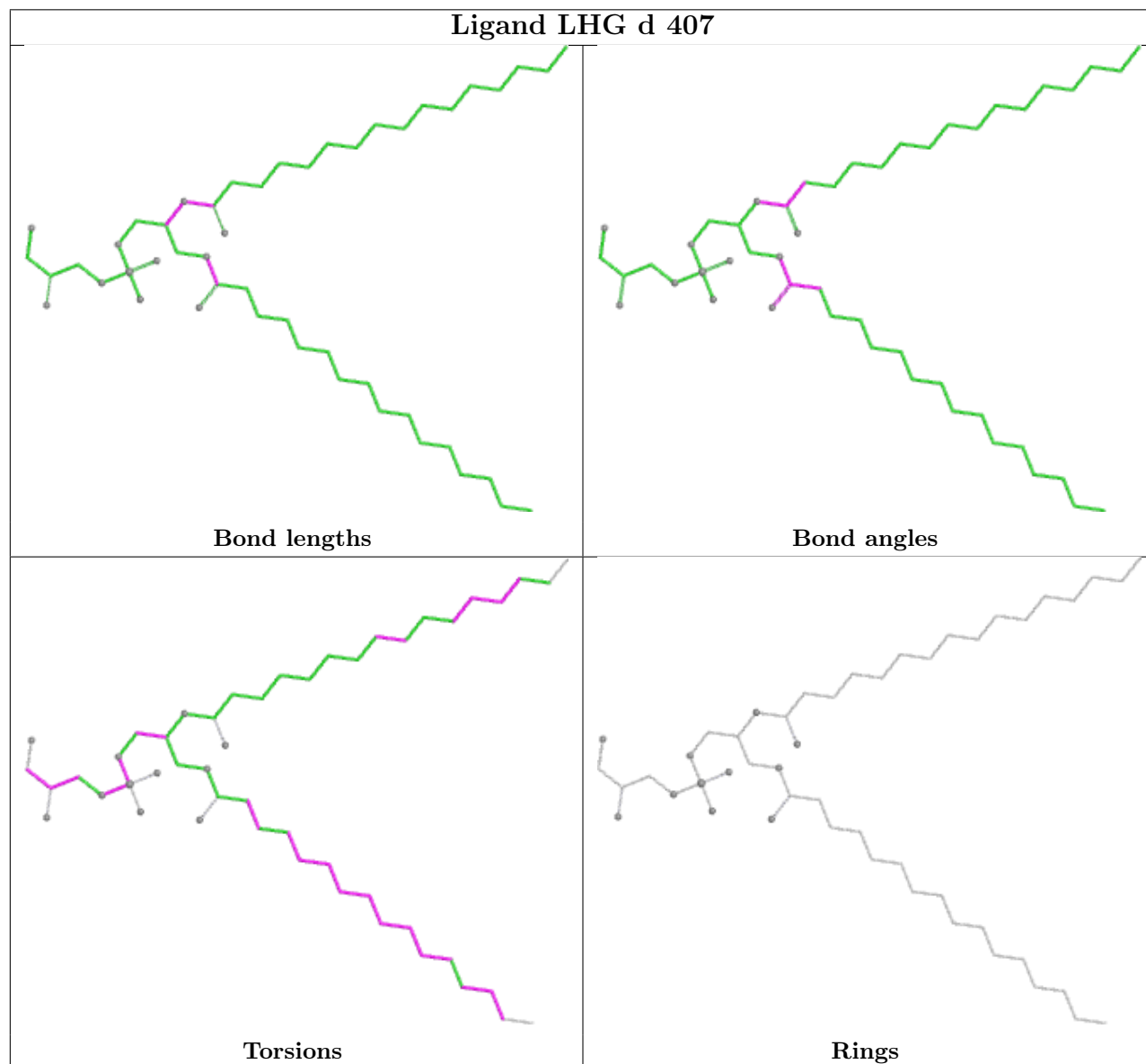
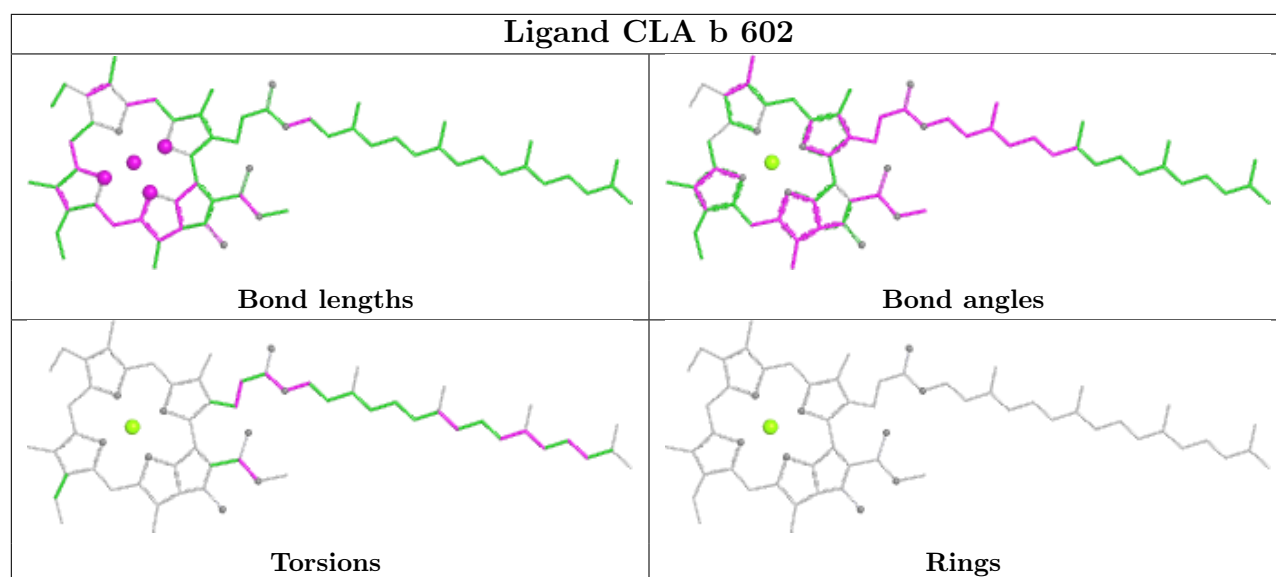


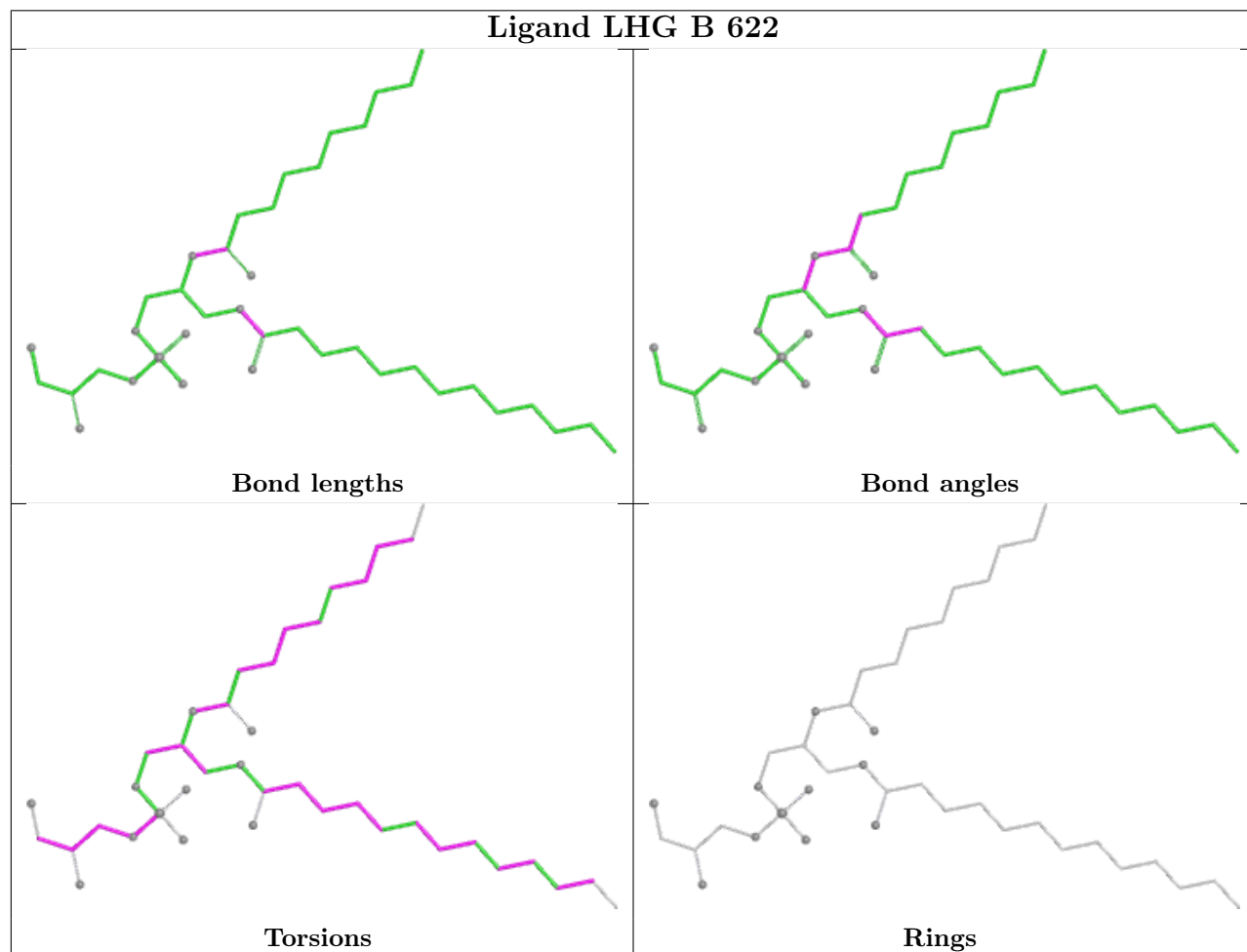
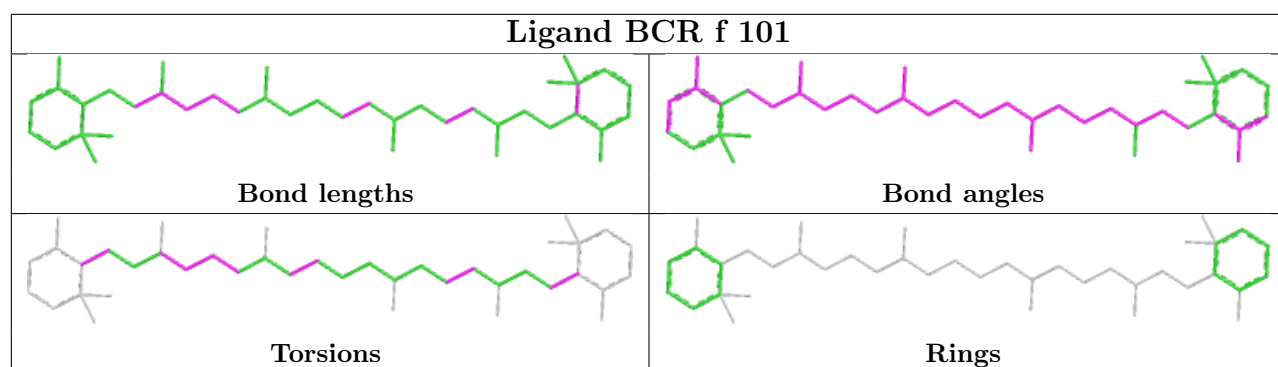


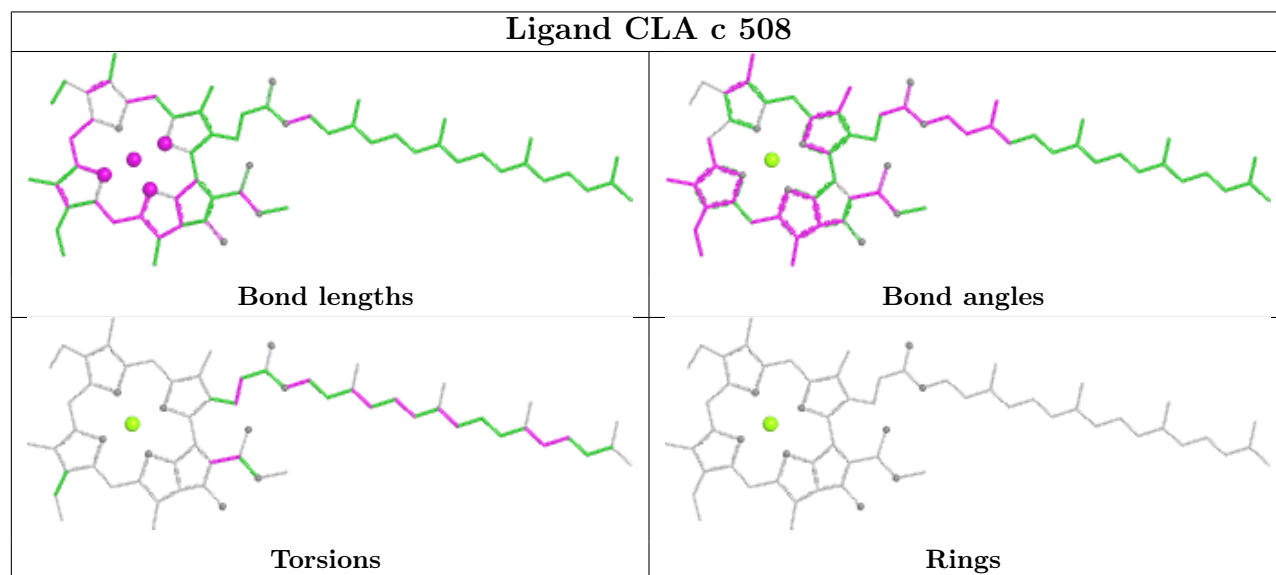
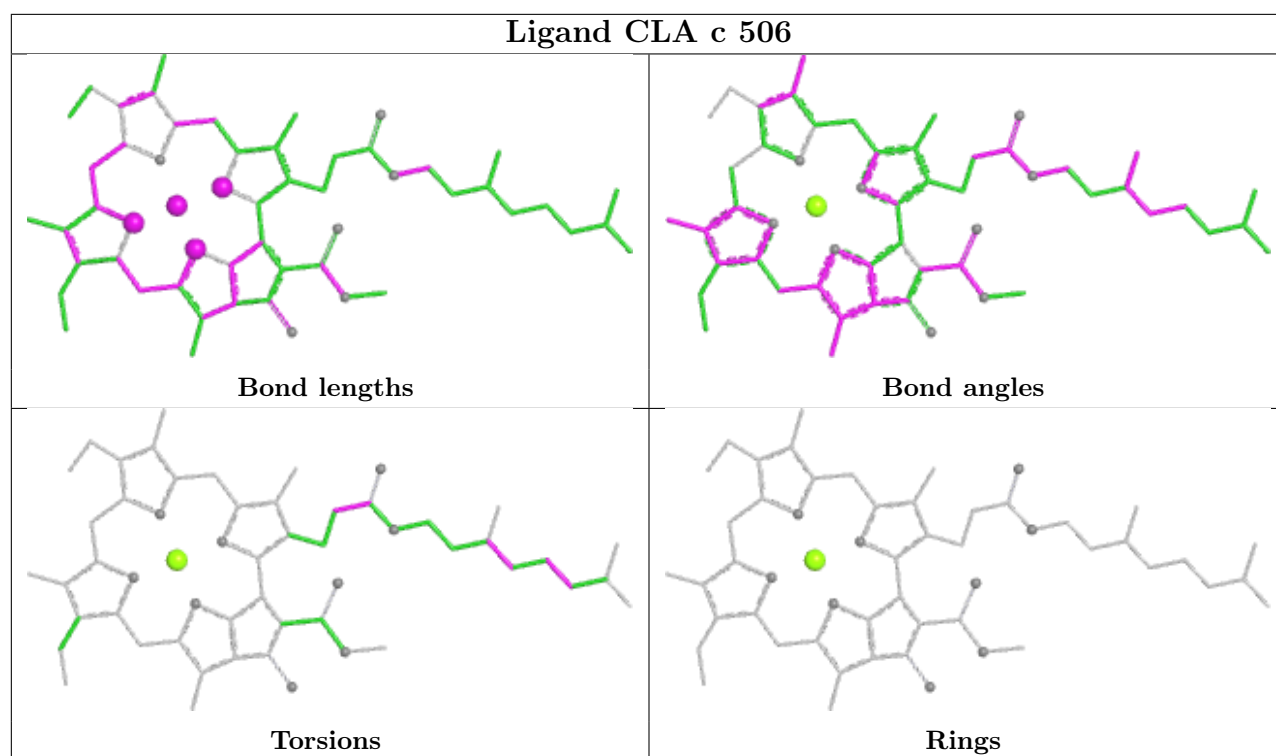


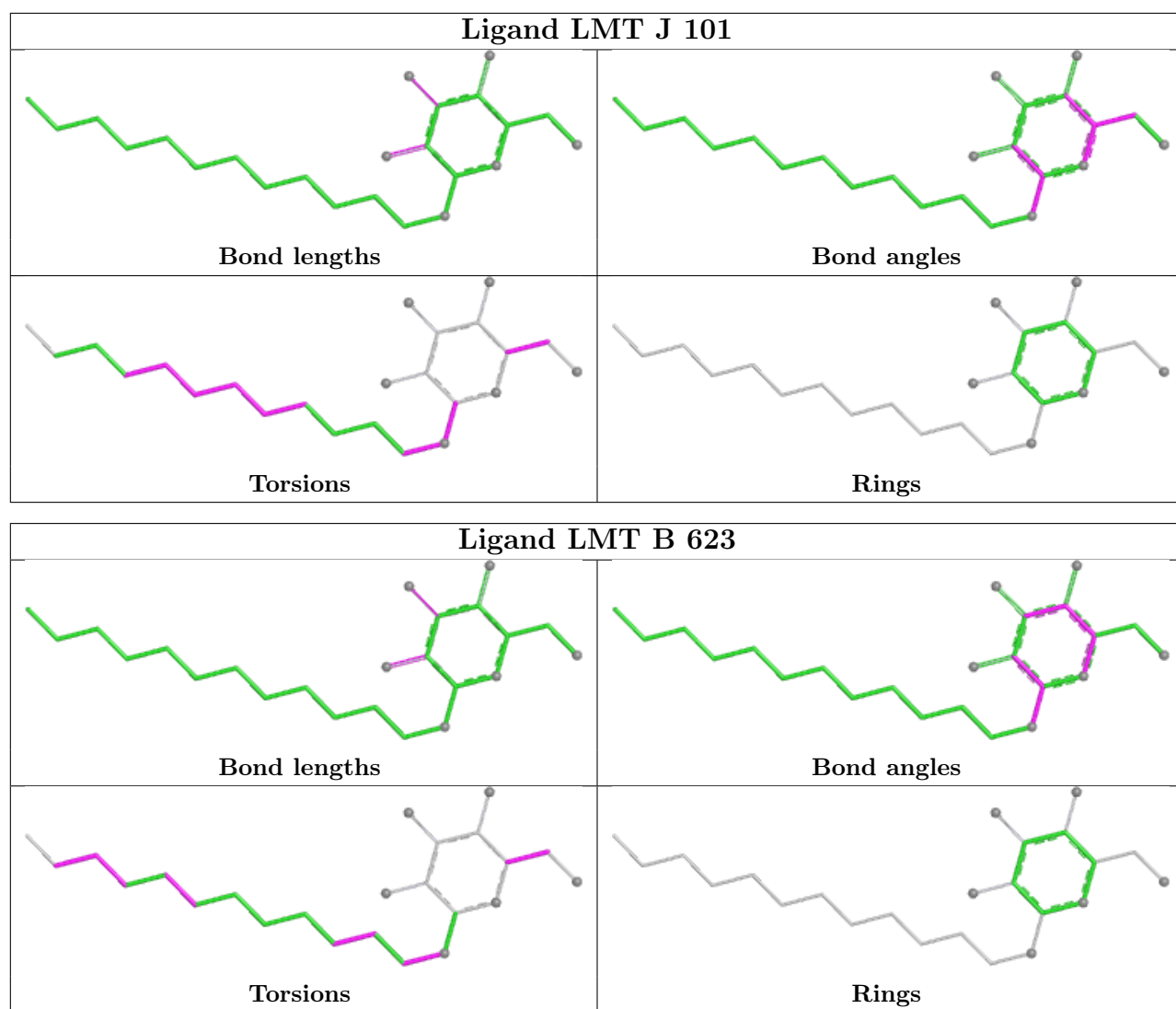


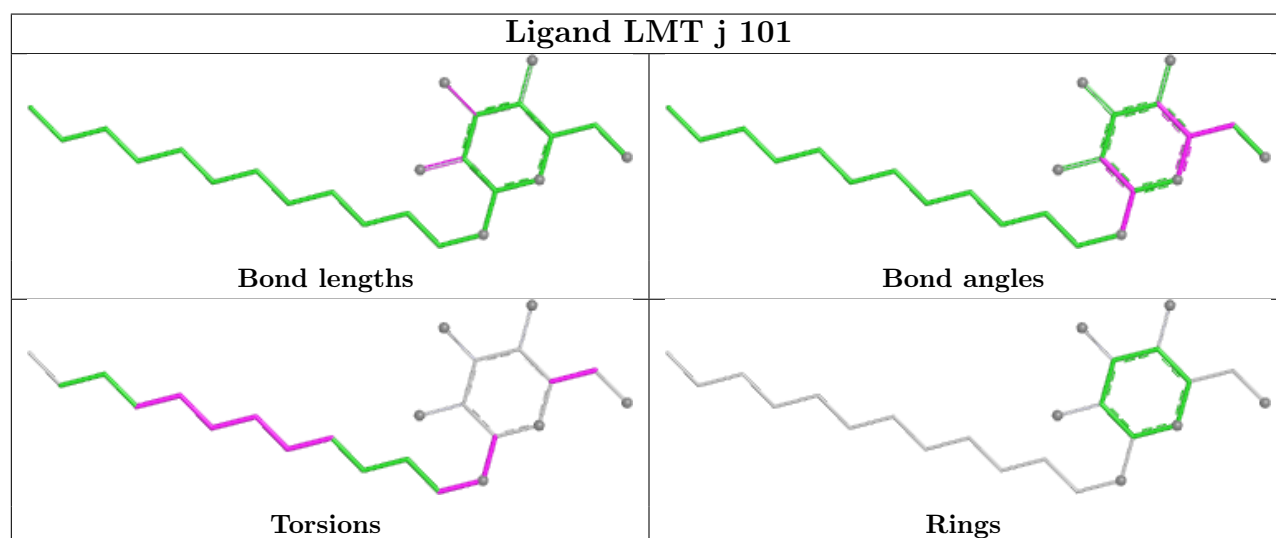
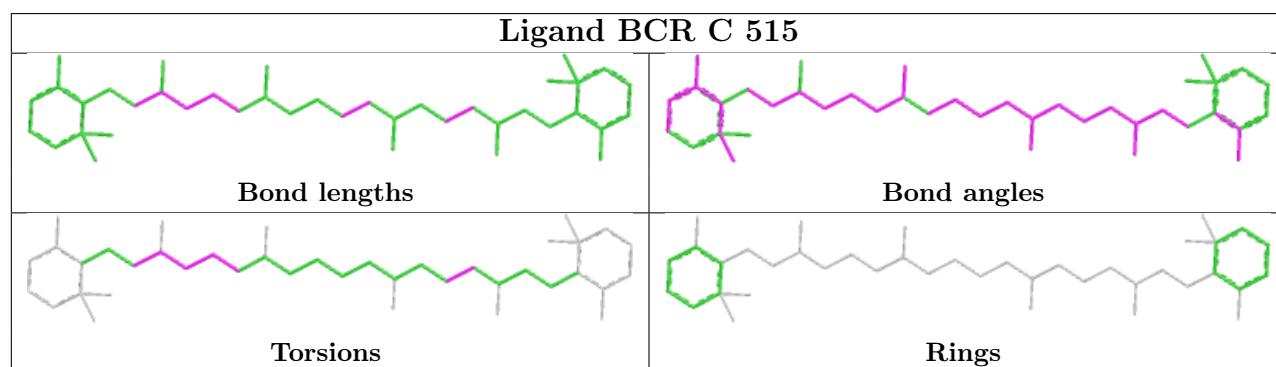
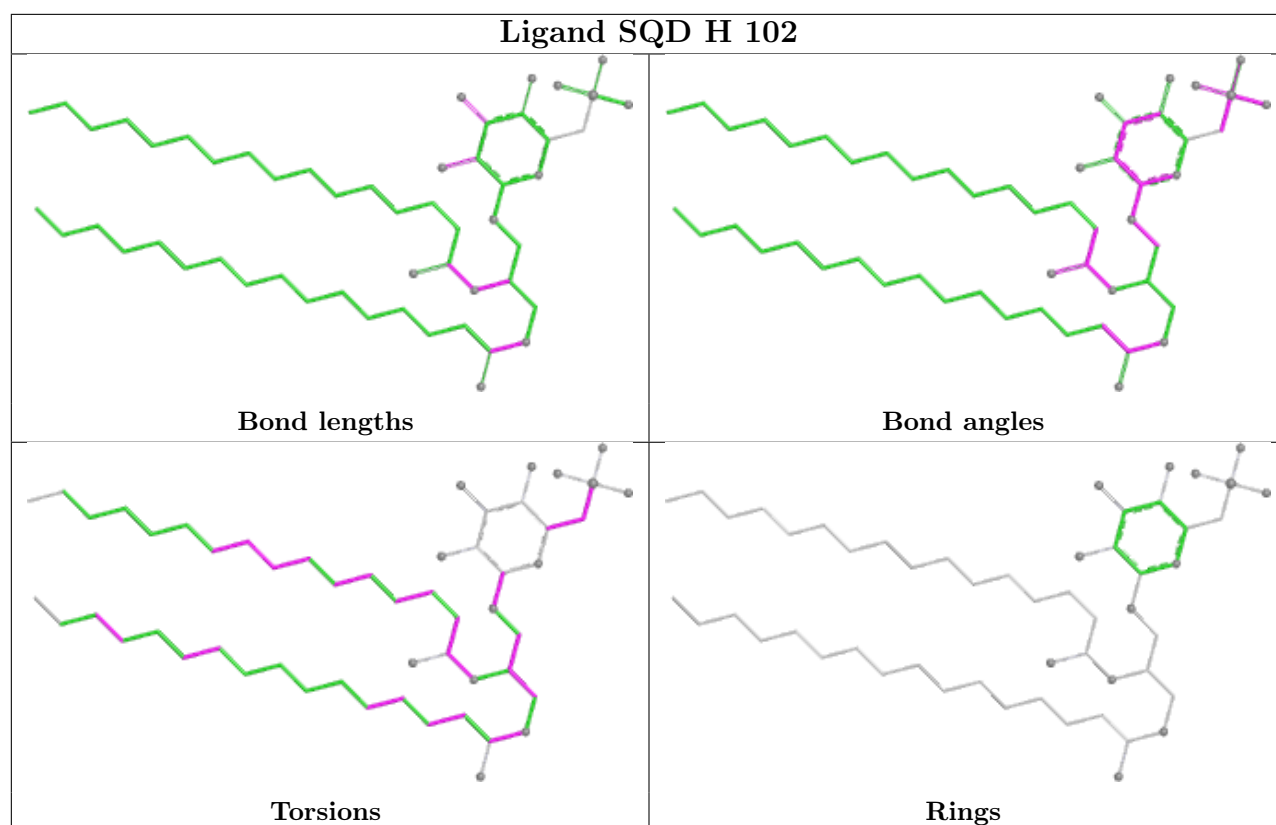


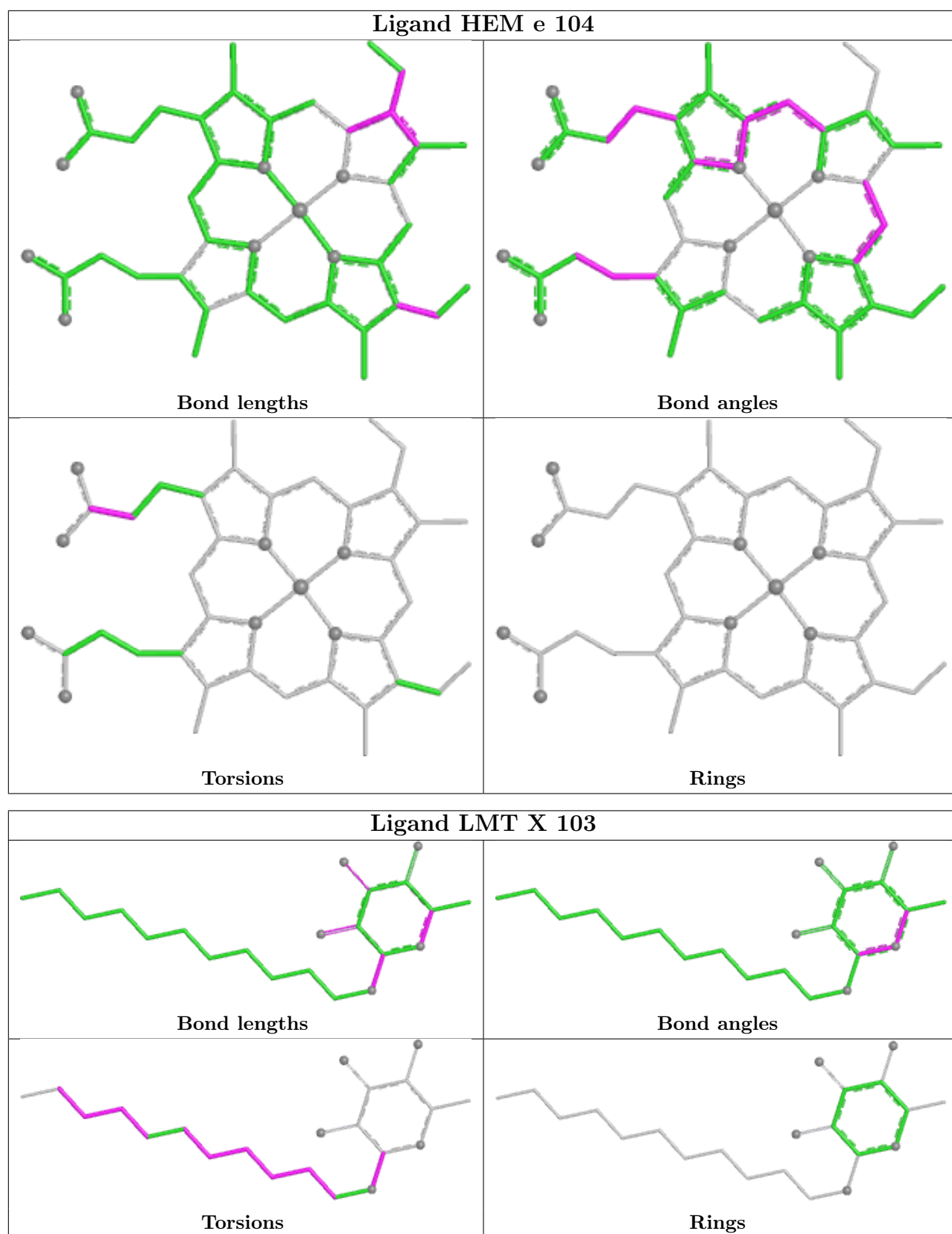


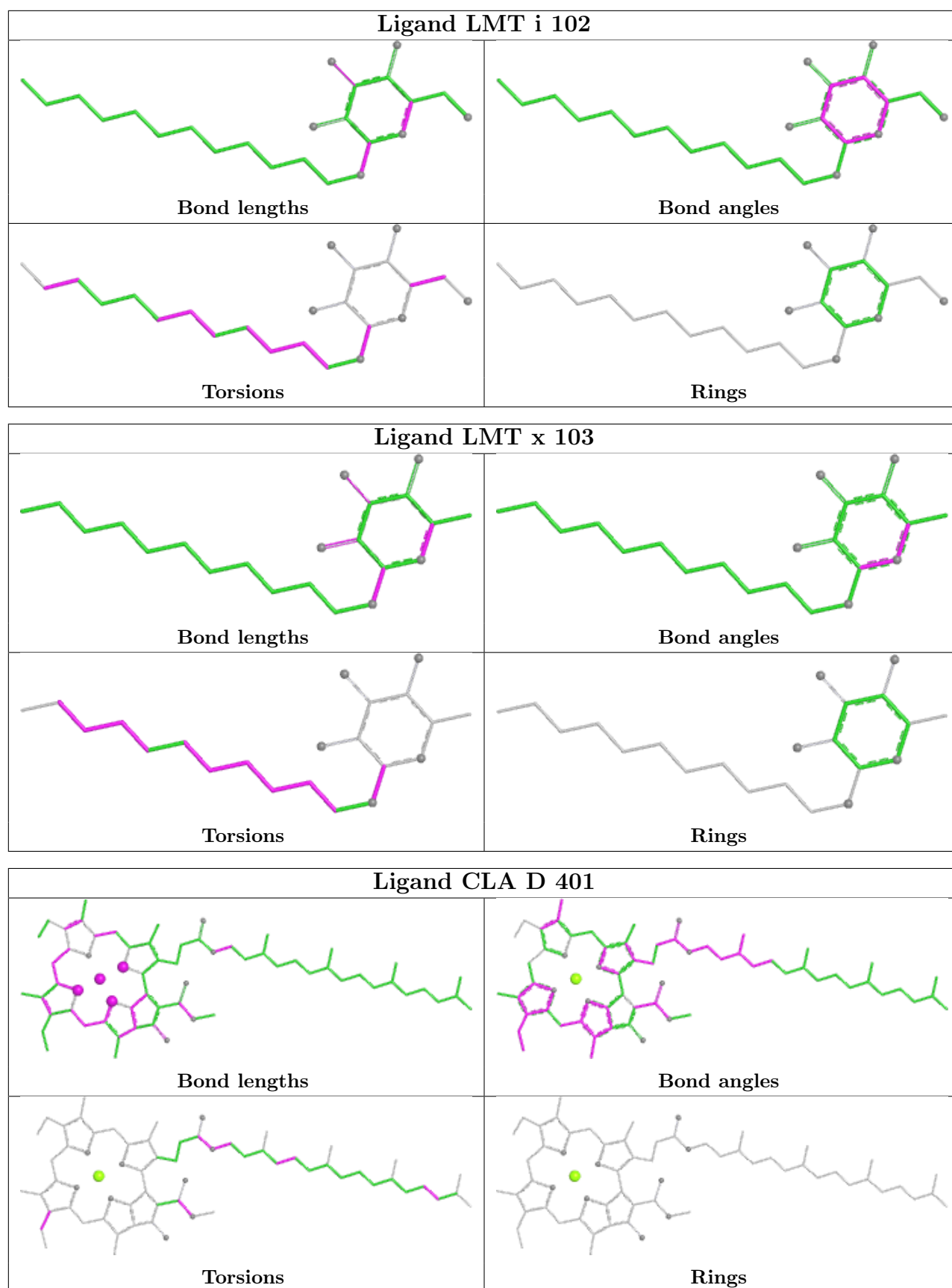


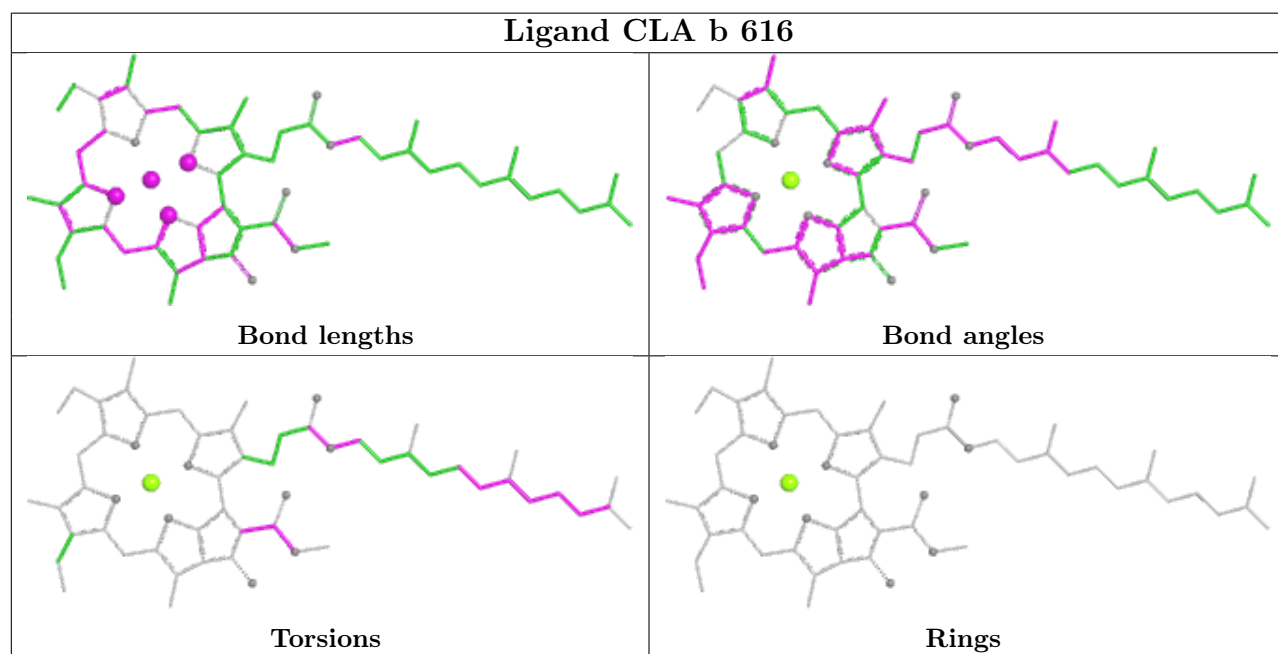
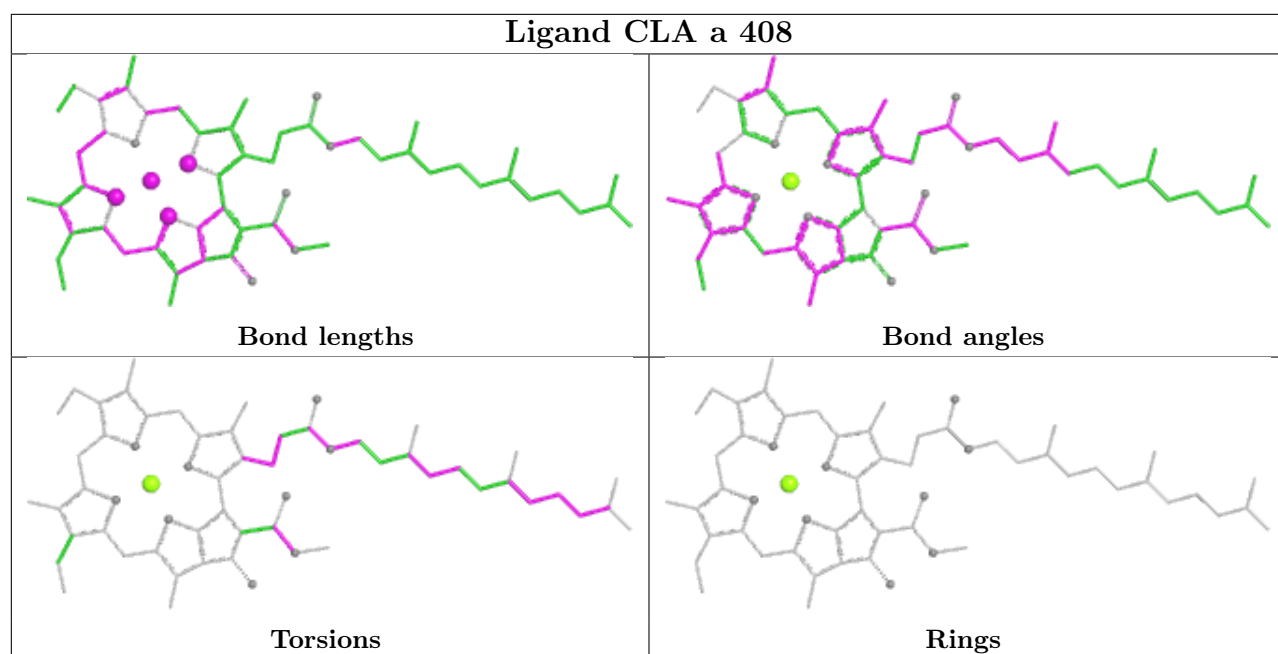


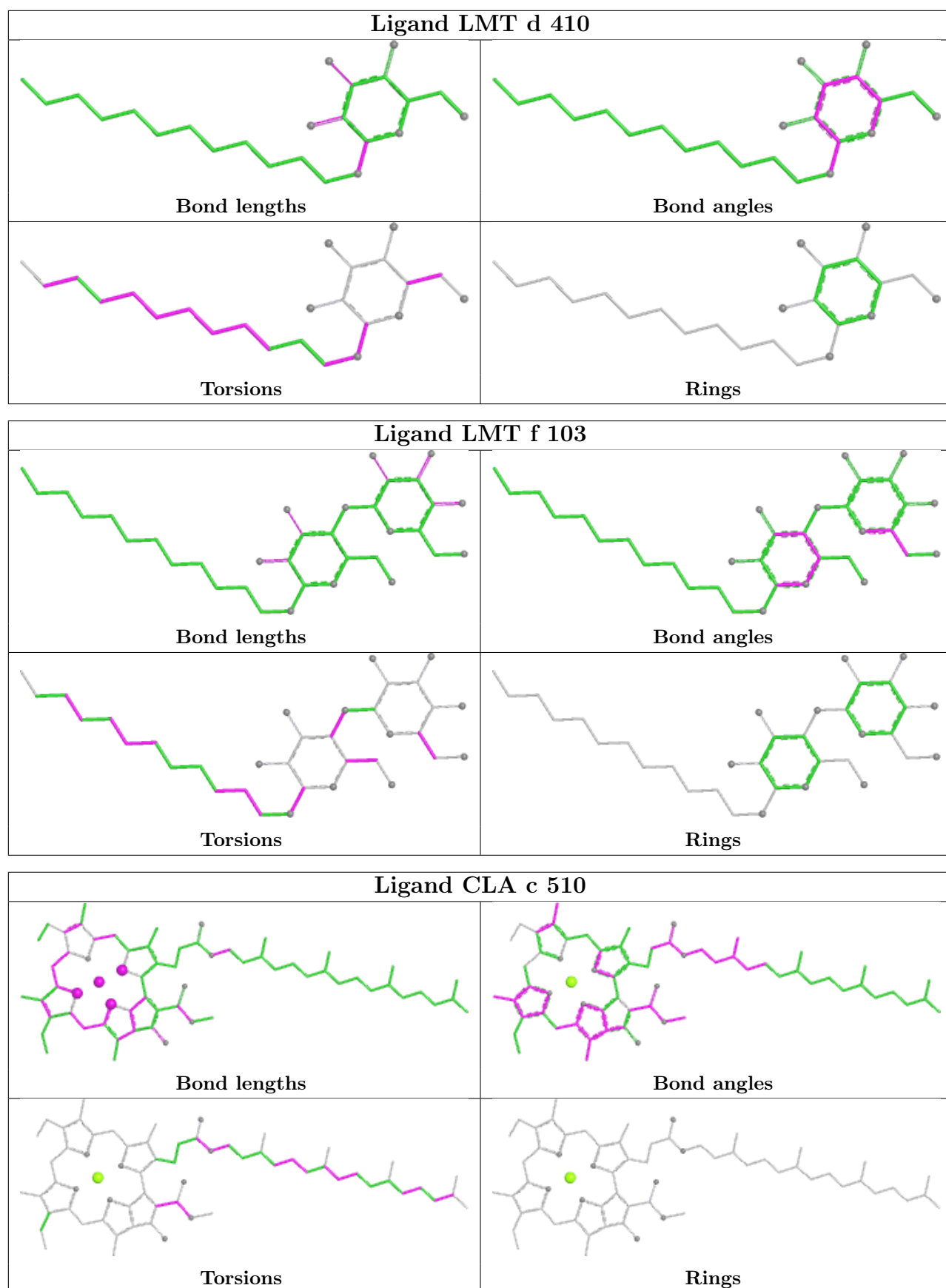


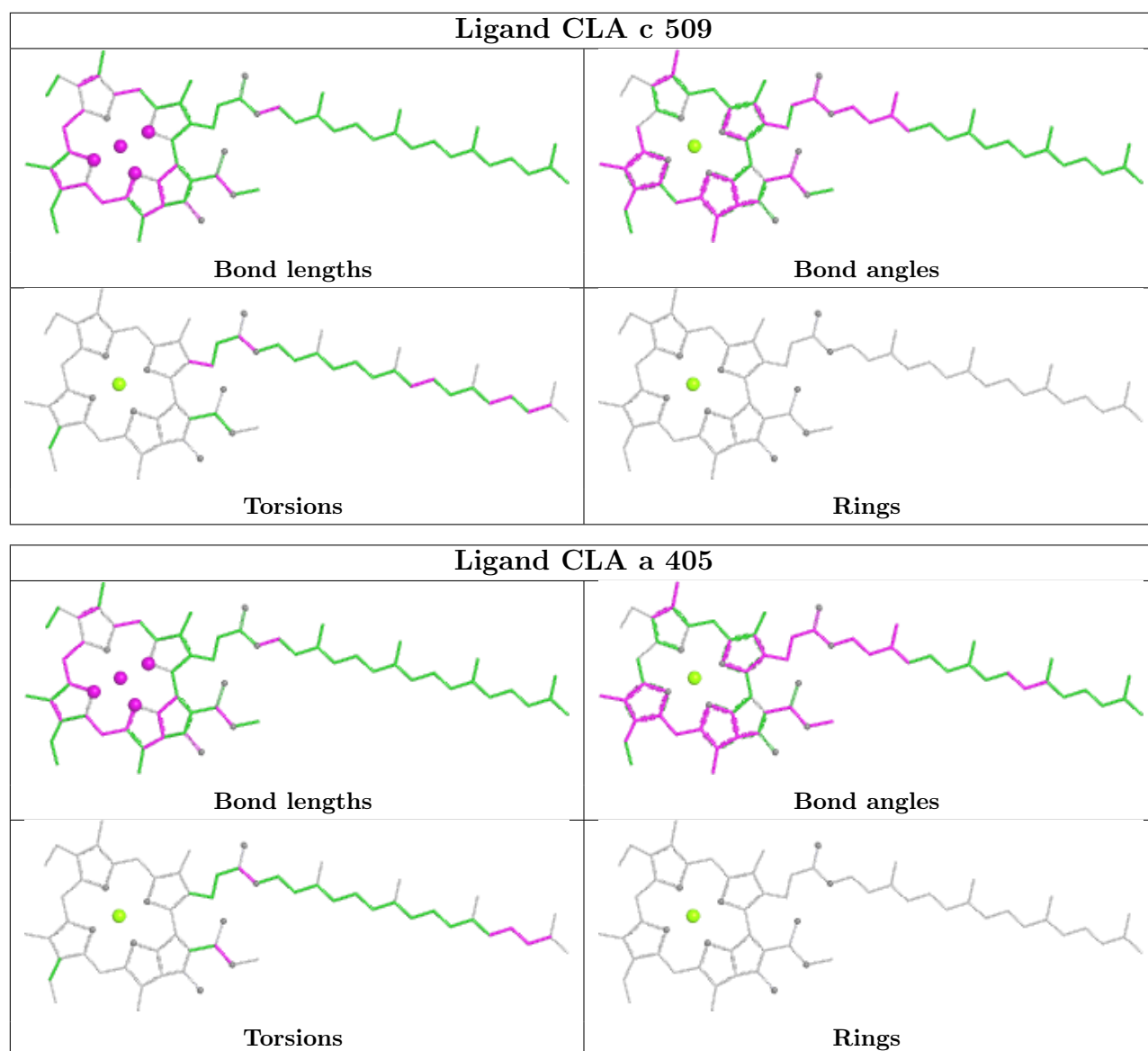












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

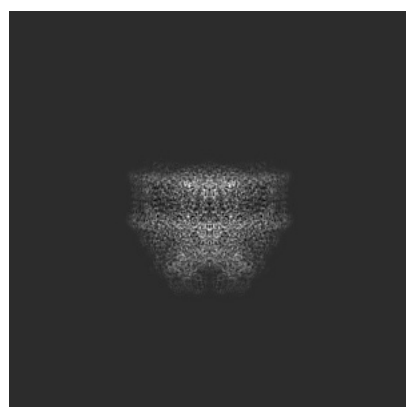
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24239. These allow visual inspection of the internal detail of the map and identification of artifacts.

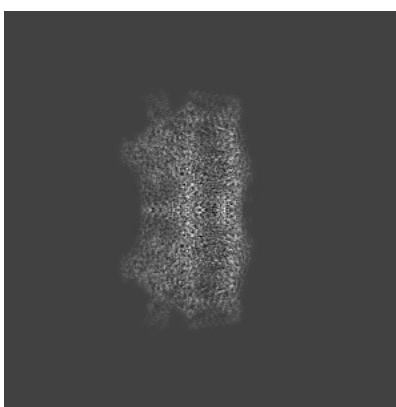
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

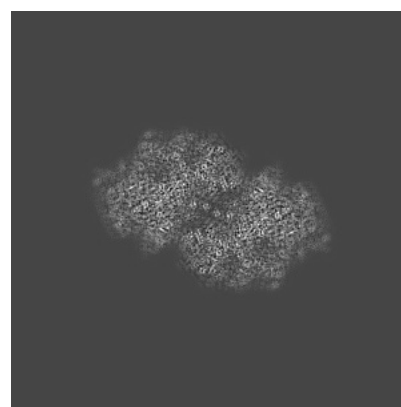
6.1.1 Primary map



X



Y



Z

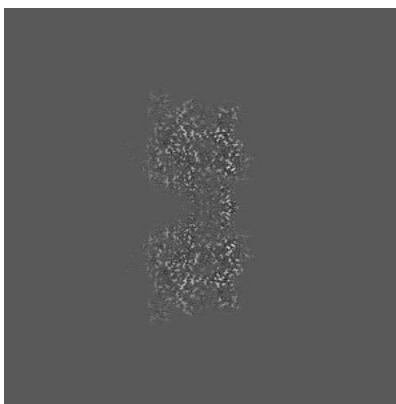
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

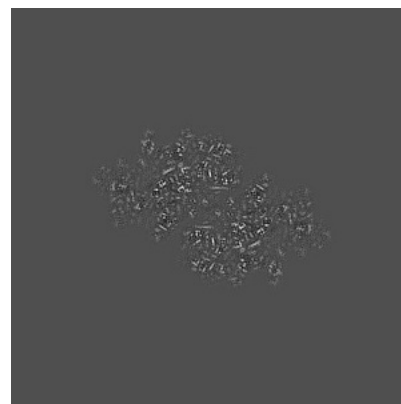
6.2.1 Primary map



X Index: 192



Y Index: 192



Z Index: 192

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

6.3 Largest variance slices [i](#)

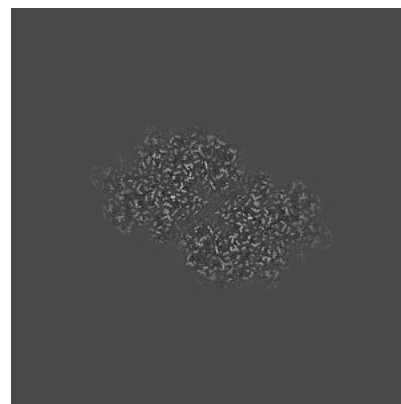
6.3.1 Primary map



X Index: 194



Y Index: 196

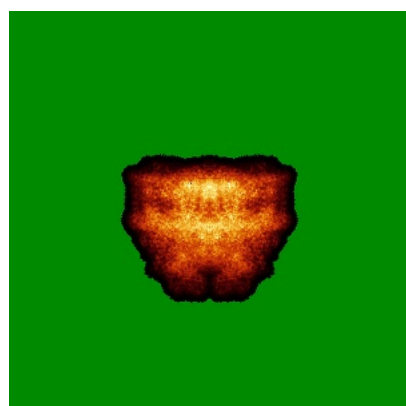


Z Index: 179

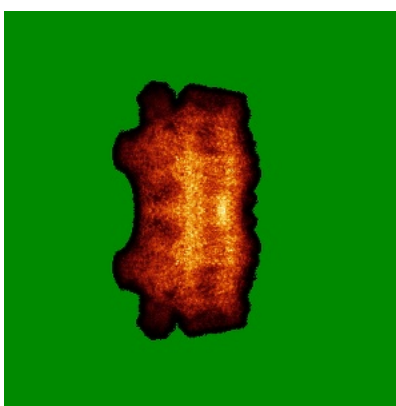
The images above show the largest variance slices of the map in three orthogonal directions.

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

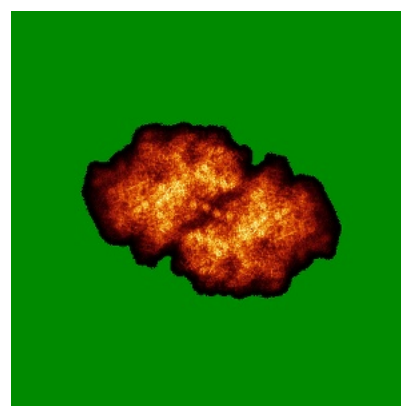
6.4.1 Primary map



X



Y

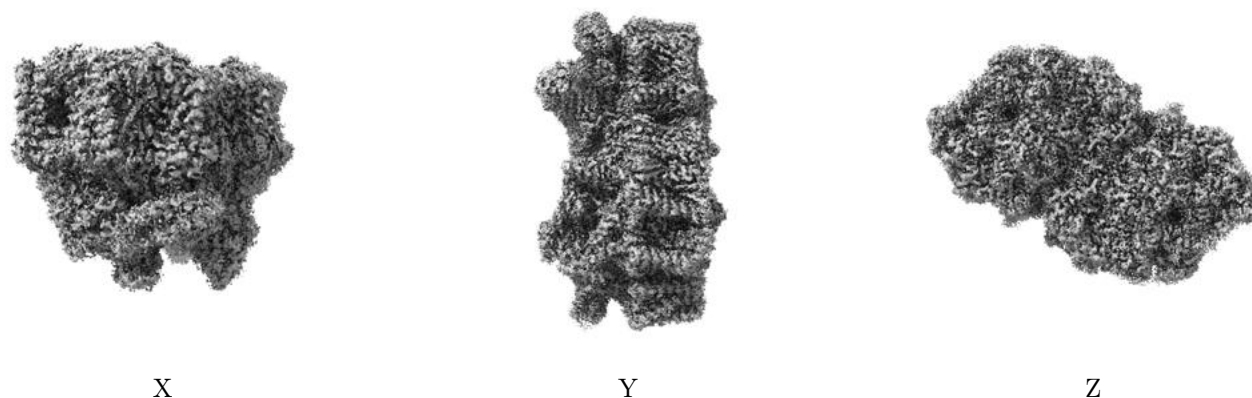


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.003. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

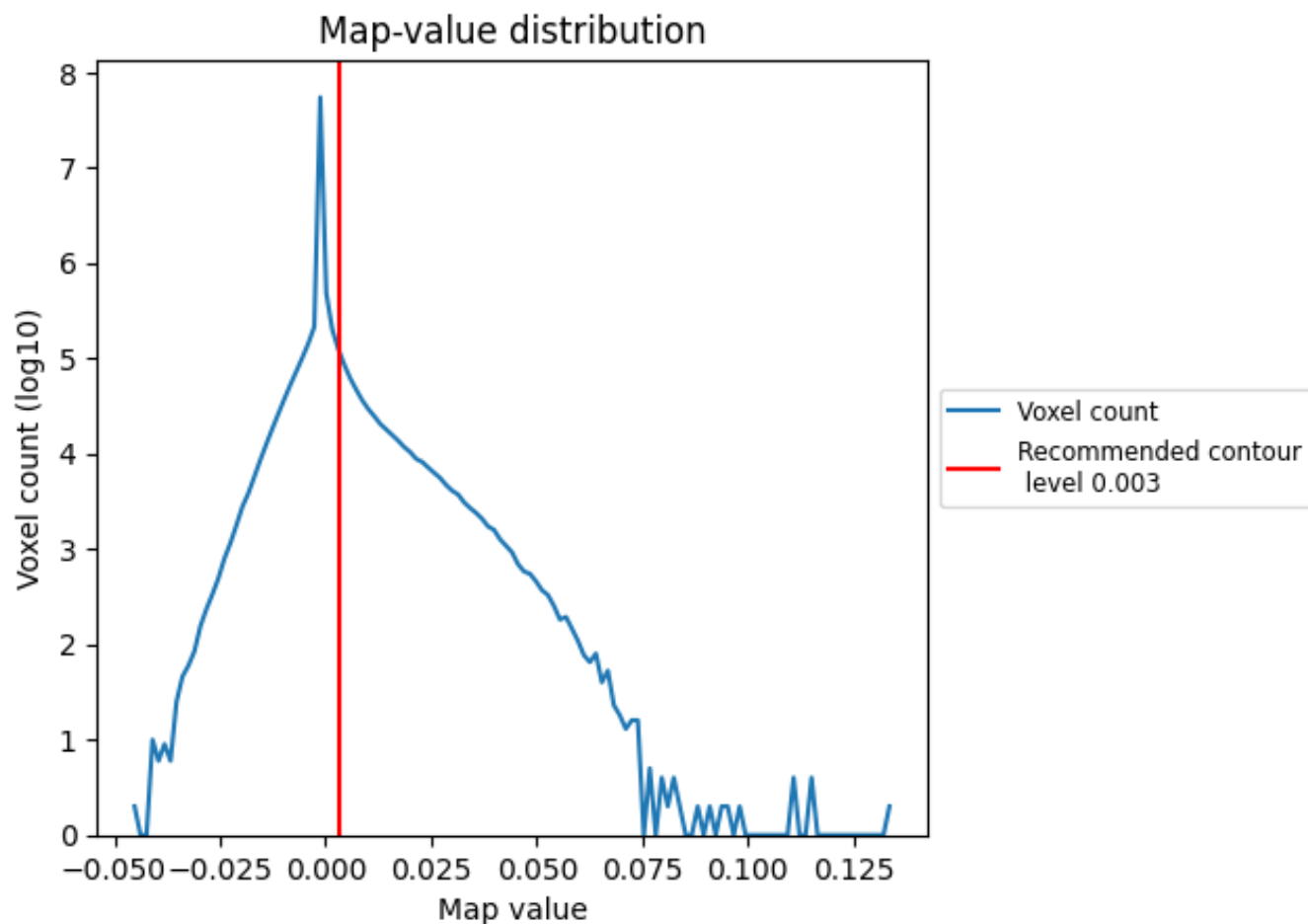
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

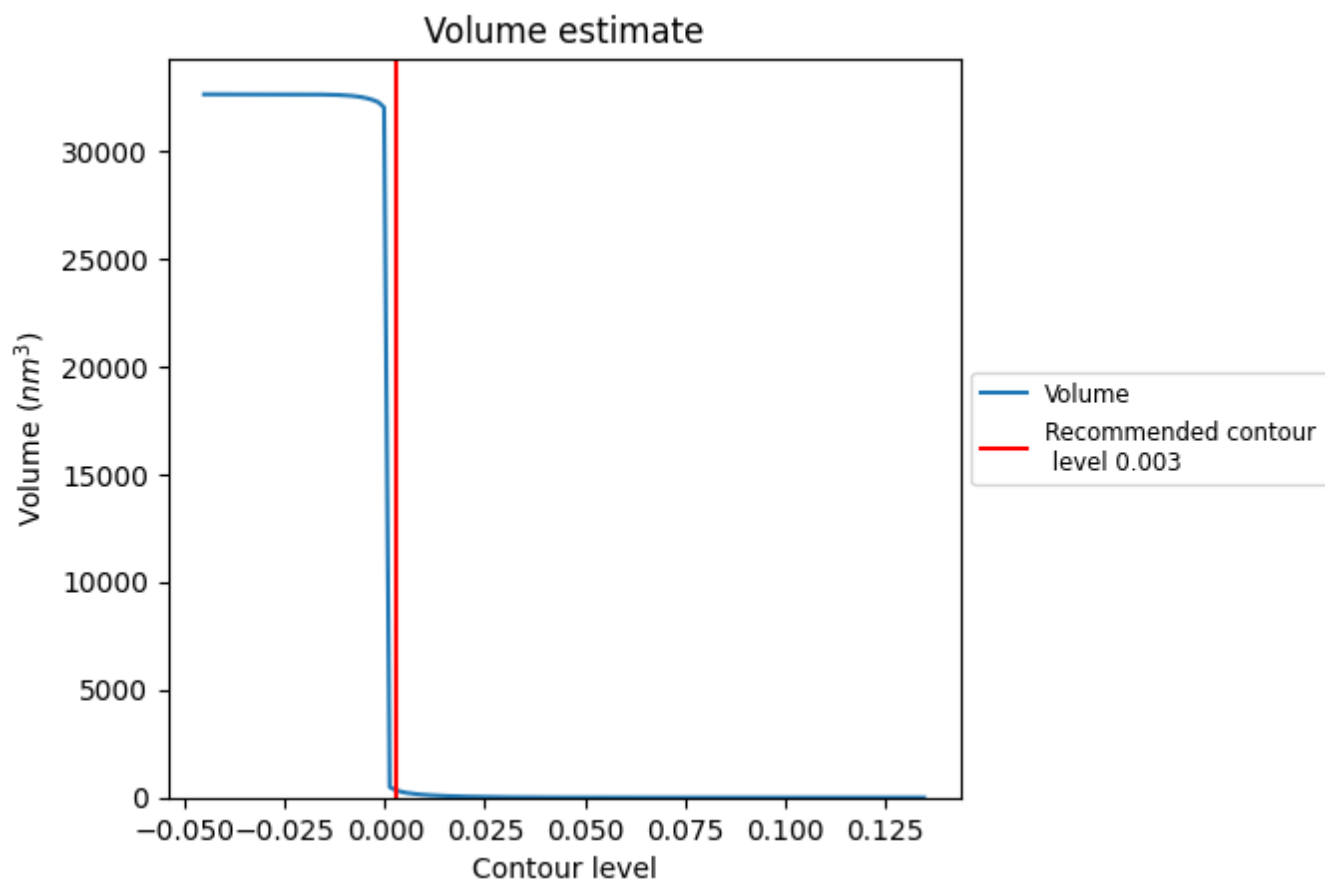
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

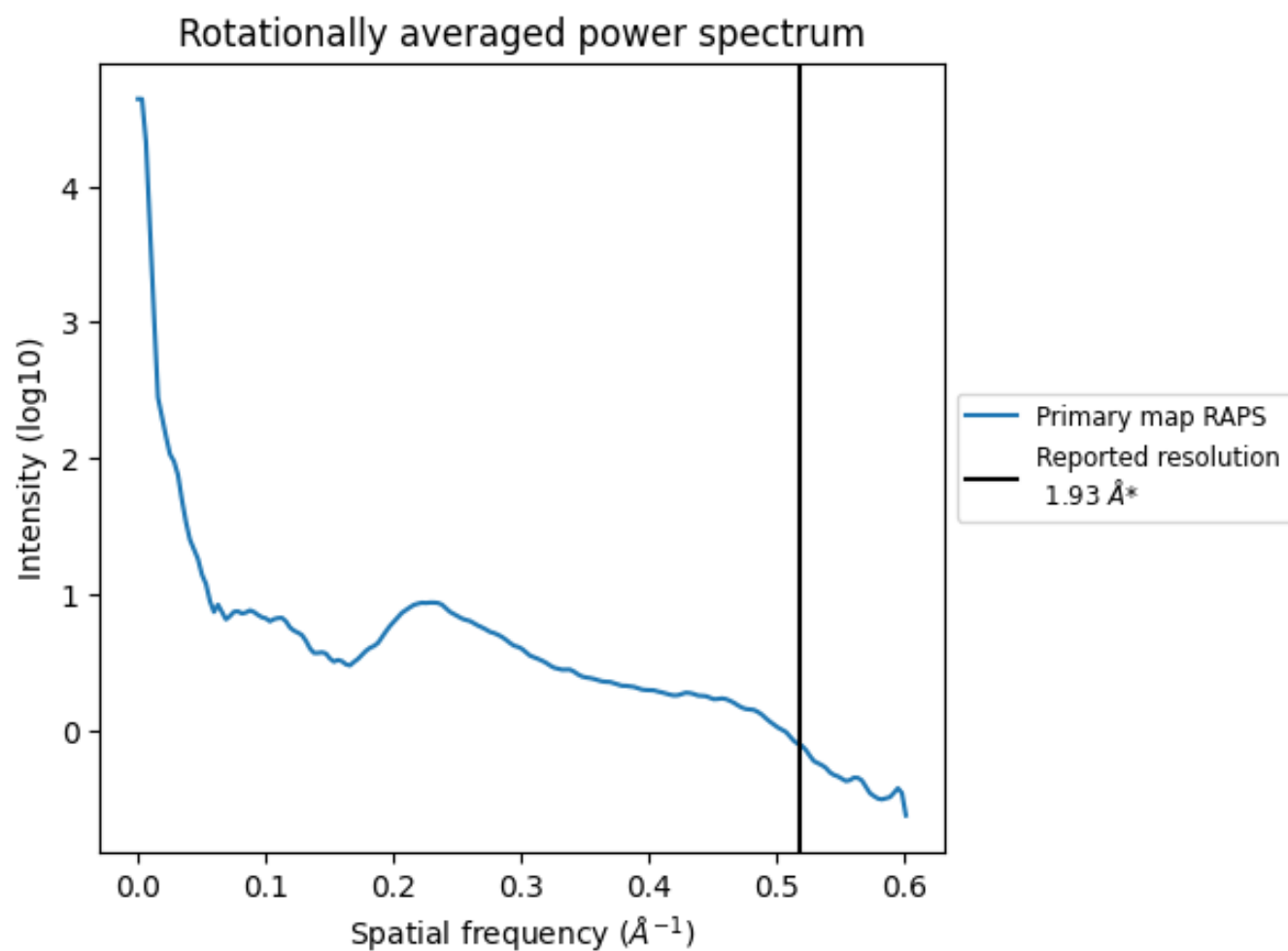
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 332 nm^3 ; this corresponds to an approximate mass of 300 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

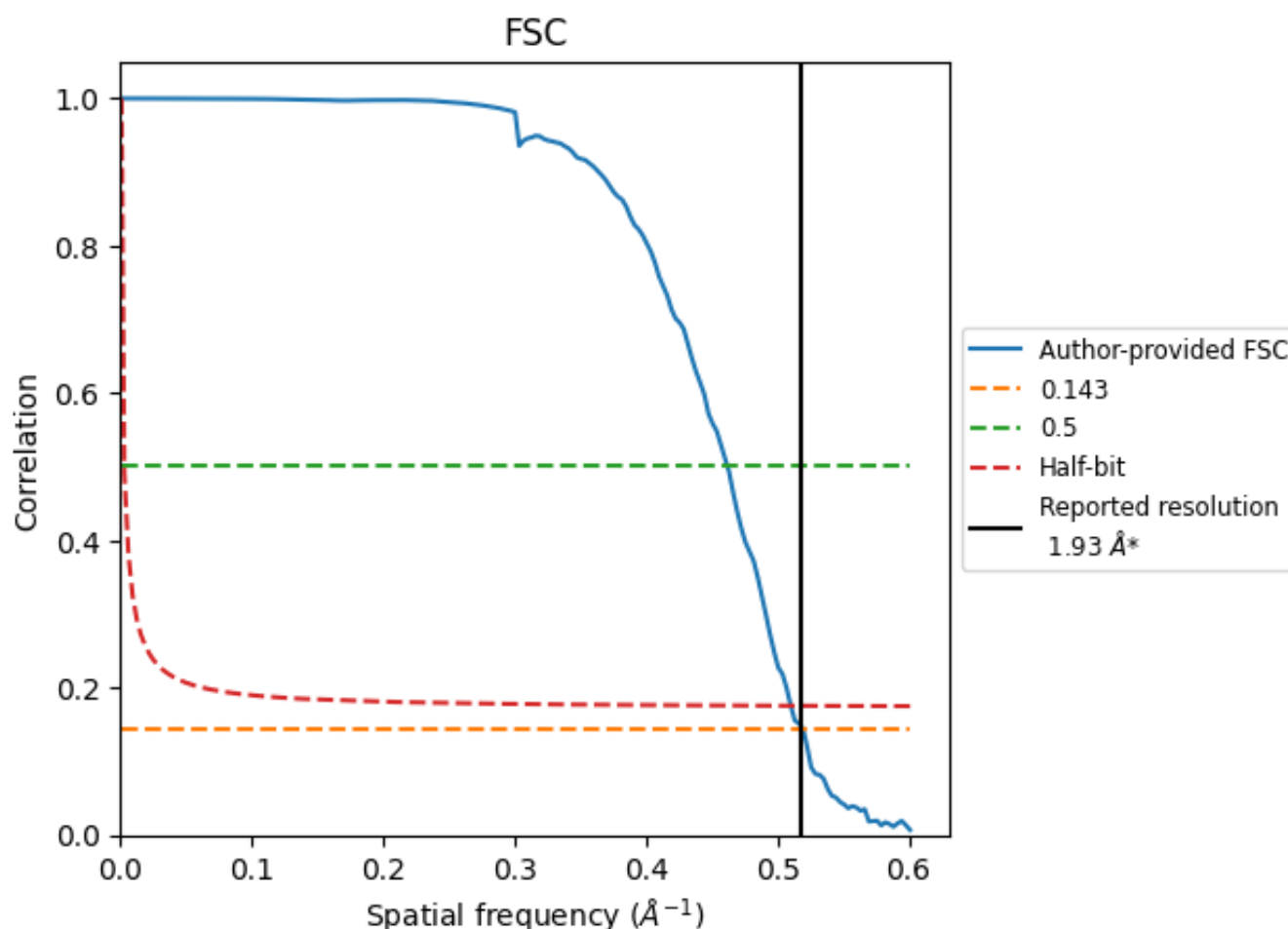


*Reported resolution corresponds to spatial frequency of 0.518 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.518 Å⁻¹

8.2 Resolution estimates [i](#)

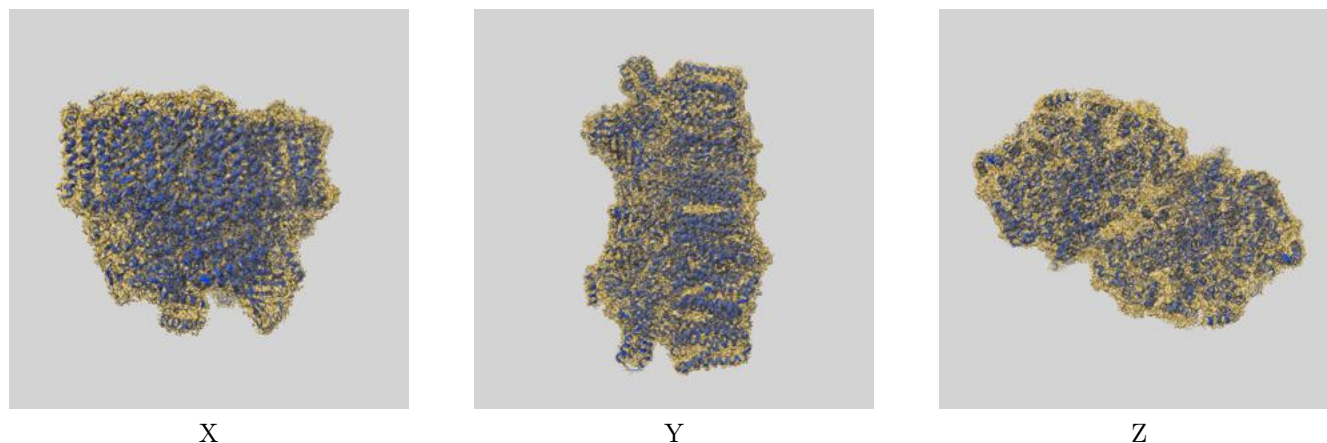
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.93	-	-
Author-provided FSC curve	1.92	2.16	1.96
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

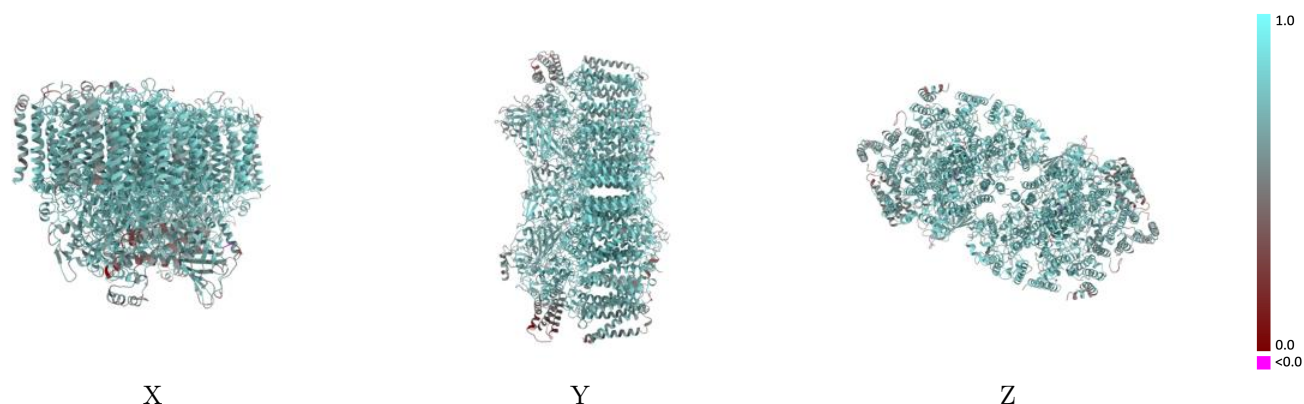
This section contains information regarding the fit between EMDB map EMD-24239 and PDB model 7N8O. Per-residue inclusion information can be found in section [3](#) on page [31](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.003 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



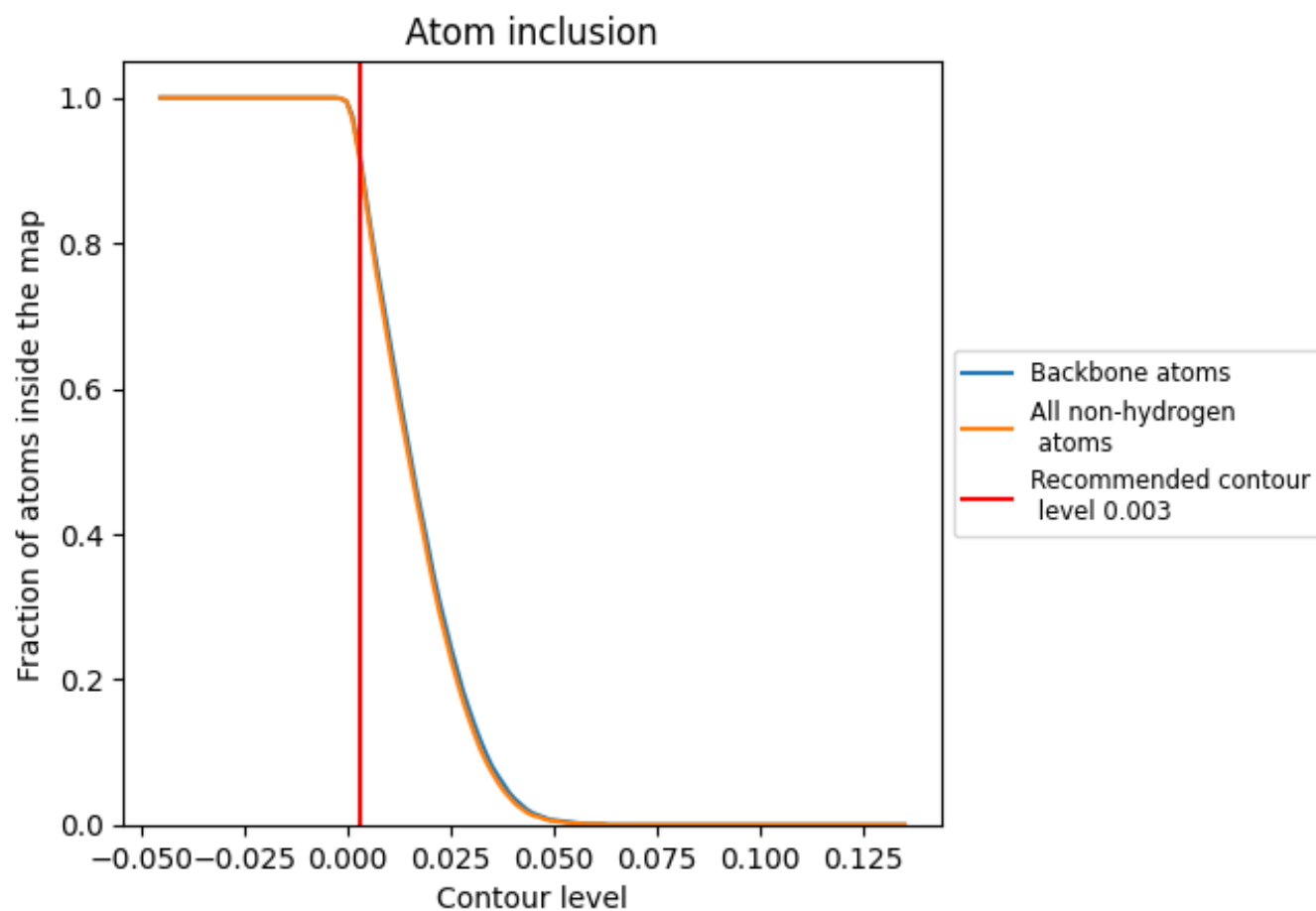
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.003).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

















The table lists the average atom inclusion at the recommended contour level (0.003) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9160	 0.7080
A	 0.9580	 0.7680
B	 0.9500	 0.7380
C	 0.9360	 0.7280
D	 0.9740	 0.7760
E	 0.9030	 0.6830
F	 0.8510	 0.6520
H	 0.9250	 0.7270
I	 0.8260	 0.6760
J	 0.8620	 0.6430
K	 0.8620	 0.6330
L	 0.9360	 0.7290
M	 0.9310	 0.7060
O	 0.8630	 0.6610
Q	 0.6410	 0.4550
R	 0.8210	 0.5670
T	 0.9390	 0.7180
U	 0.8490	 0.6340
V	 0.8960	 0.6770
X	 0.9060	 0.6630
Y	 0.7620	 0.5800
Z	 0.8320	 0.5730
a	 0.9620	 0.7710
b	 0.9470	 0.7310
c	 0.9390	 0.7240
d	 0.9720	 0.7750
e	 0.9010	 0.6780
f	 0.8590	 0.6480
h	 0.9260	 0.7220
i	 0.8290	 0.6780
j	 0.8760	 0.6510
k	 0.8540	 0.6360
l	 0.9550	 0.7510
m	 0.9480	 0.7280
o	 0.8640	 0.6580



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Chain	Atom inclusion	Q-score
q	 0.6460	 0.4600
r	 0.8330	 0.5720
t	 0.9310	 0.7170
u	 0.8480	 0.6310
v	 0.8980	 0.6760
x	 0.8950	 0.6560
y	 0.7620	 0.5840
z	 0.8280	 0.5720