



wwPDB EM Validation Summary Report ⓘ

Aug 5, 2026 – 09:20 AM EDT

PDB ID : 8TOW / pdb_00008tow
EMDB ID : EMD-41460
Title : Structure of a mutated photosystem II complex reveals perturbation of the oxygen-evolving complex
Authors : Flesher, D.A.; Liu, J.; Wang, J.; Gisriel, C.J.; Yang, K.R.; Batista, V.S.; Debus, R.J.; Brudvig, G.W.
Deposited on : 2023-08-04
Resolution : 2.14 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:

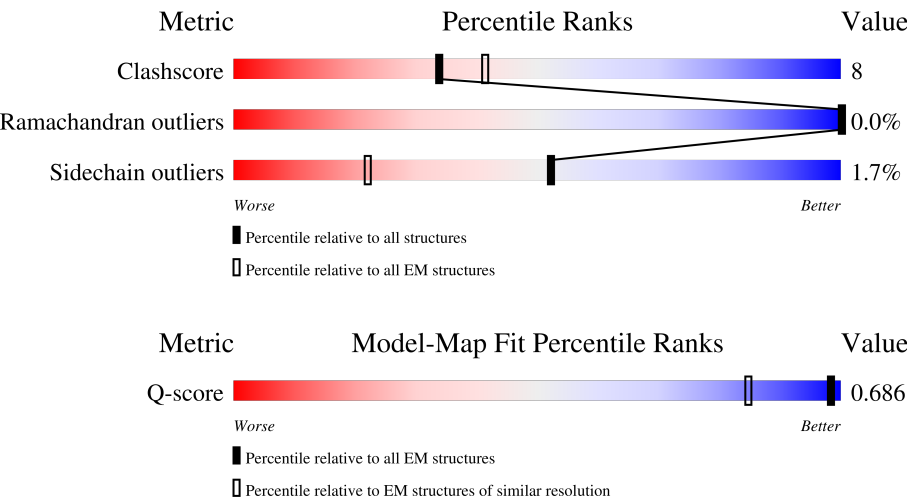
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.14 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2493 (1.66 - 2.64)

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	78%14%7%
1	a	360	78%14%7%
2	B	507	86%13%
2	b	507	86%14%

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Mol	Chain	Length	Quality of chain
3	C	460	
3	c	460	
4	D	352	
4	d	352	
5	E	81	
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	274	
13	o	274	
14	Q	149	
14	q	149	
15	R	39	

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Mol	Chain	Length	Quality of chain
15	r	39	
16	T	31	
16	t	31	
17	U	131	
17	u	131	
18	V	160	
18	v	160	
19	X	39	
19	x	39	
20	Y	39	
20	y	39	
21	Z	62	
21	z	62	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 54914 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	2	0
			2640	1728	431	466	15		
1	a	334	Total	C	N	O	S	2	0
			2640	1728	431	466	15		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	170	GLU	ASP	conflict	UNP P16033
a	170	GLU	ASP	conflict	UNP P16033

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

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

- 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		

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

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

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

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

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

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

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

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

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

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

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

- Molecule 14 is a protein called Sll1638 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	118	Total	C	N	O	S	0	0
			911	573	163	173	2		
14	q	118	Total	C	N	O	S	0	0
			911	573	163	173	2		

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

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

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

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

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

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

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

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

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

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

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

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

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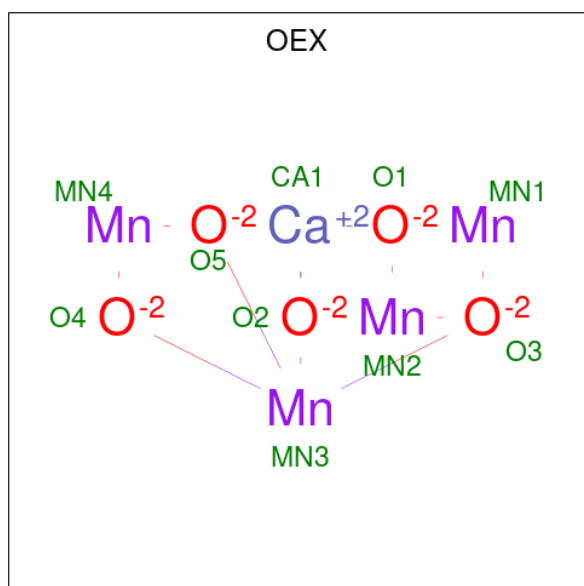
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Mol	Chain	Residues	Atoms				AltConf	Trace
20	y	32	Total	C	N	O	0	0
			242	165	37	40		

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

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

- Molecule 22 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



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

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

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

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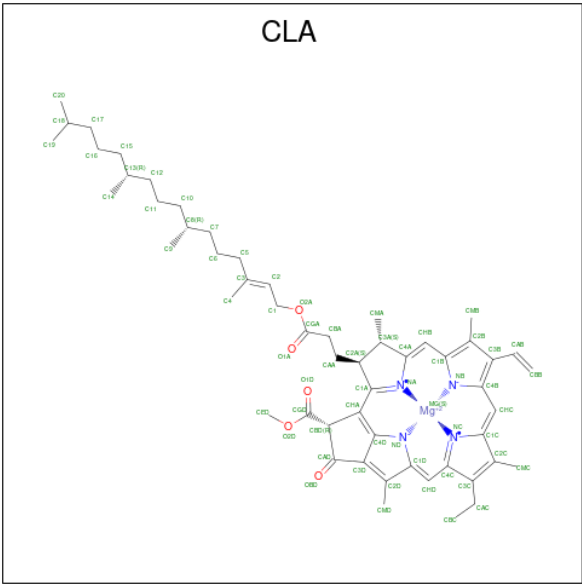
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Mol	Chain	Residues	Atoms		AltConf
23	a	1	Total	Fe	0
			1	1	

- Molecule 24 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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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 60	C 50	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 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

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Mol	Chain	Residues	Atoms					AltConf
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 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

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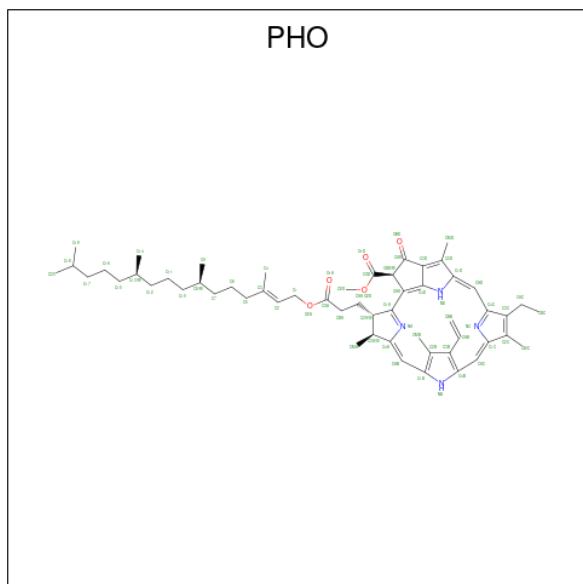
Mol	Chain	Residues	Atoms					AltConf
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total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

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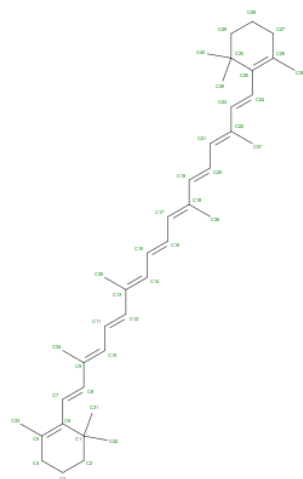
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	d	1	65	55	1	4	5	0

- Molecule 26 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 27 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).

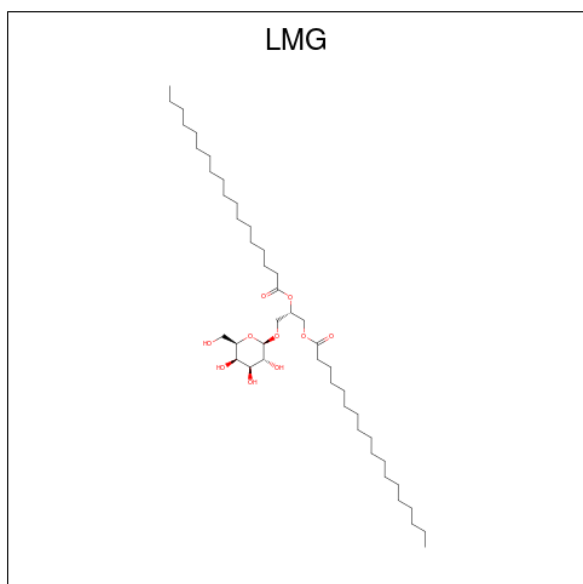


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Mol	Chain	Residues	Atoms		AltConf
27	f	1	Total	C	0
			40	40	
27	k	1	Total	C	0
			40	40	
27	k	1	Total	C	0
			40	40	
27	z	1	Total	C	0
			40	40	

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



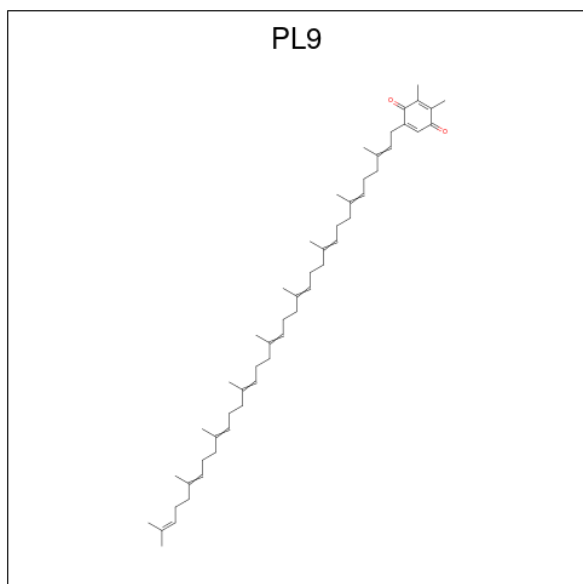
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			51	41	10	
28	A	1	Total	C	O	0
			36	26	10	
28	B	1	Total	C	O	0
			51	41	10	
28	C	1	Total	C	O	0
			51	41	10	
28	C	1	Total	C	O	0
			49	39	10	
28	D	1	Total	C	O	0
			44	34	10	
28	H	1	Total	C	O	0
			47	37	10	

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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
			44	34	10	
28	h	1	Total	C	O	0
			47	37	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-HEXATRIACONTANAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



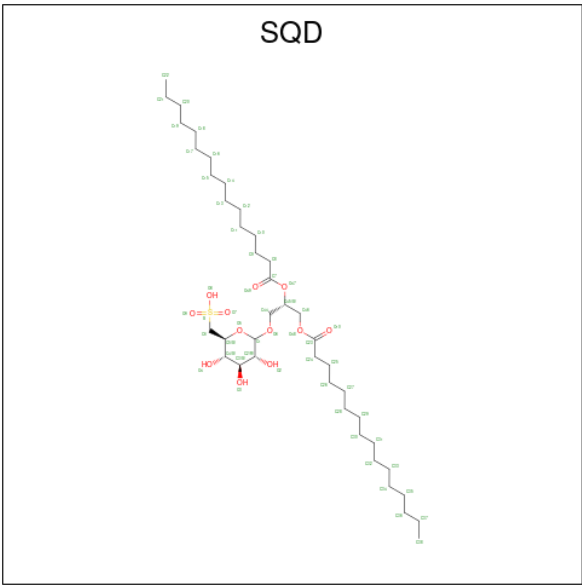
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			55	53	2	
29	D	1	Total	C	O	0
			55	53	2	
29	a	1	Total	C	O	0
			55	53	2	

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

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



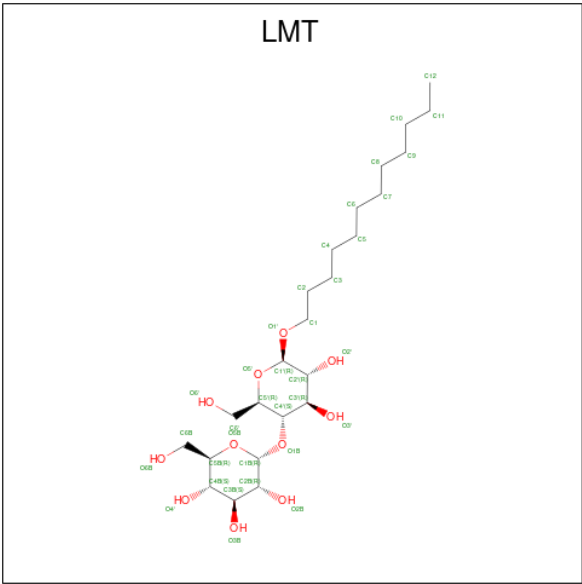
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
30	A	1	54	41	12	1	0
30	A	1	48	35	12	1	0
30	B	1	54	41	12	1	0
30	C	1	54	41	12	1	0
30	F	1	34	21	12	1	0
30	H	1	54	41	12	1	0
30	K	1	41	32	9		0
30	a	1	54	41	12	1	0
30	a	1	48	35	12	1	0
30	b	1	54	41	12	1	0

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Mol	Chain	Residues	Atoms				AltConf
30	c	1	Total	C	O	S	0
			54	41	12	1	
30	f	1	Total	C	O	S	0
			34	21	12	1	
30	h	1	Total	C	O	S	0
			54	41	12	1	
30	k	1	Total	C	O		0
			41	32	9		

- Molecule 31 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



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

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

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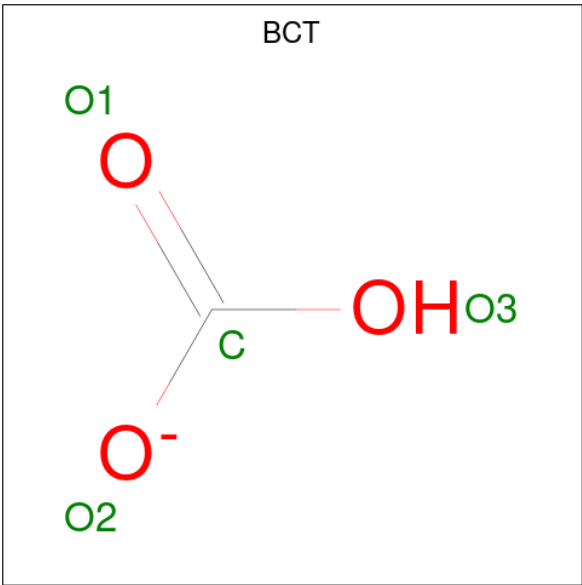
Mol	Chain	Residues	Atoms			AltConf
31	X	1	Total	C	O	0
			22	16	6	
31	X	1	Total	C	O	0
			19	13	6	
31	X	1	Total	C	O	0
			19	13	6	
31	Y	1	Total	C	O	0
			21	15	6	
31	a	1	Total	C	O	0
			35	24	11	
31	a	1	Total	C	O	0
			24	18	6	
31	b	1	Total	C	O	0
			35	24	11	
31	b	1	Total	C	O	0
			24	18	6	
31	b	1	Total	C	O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

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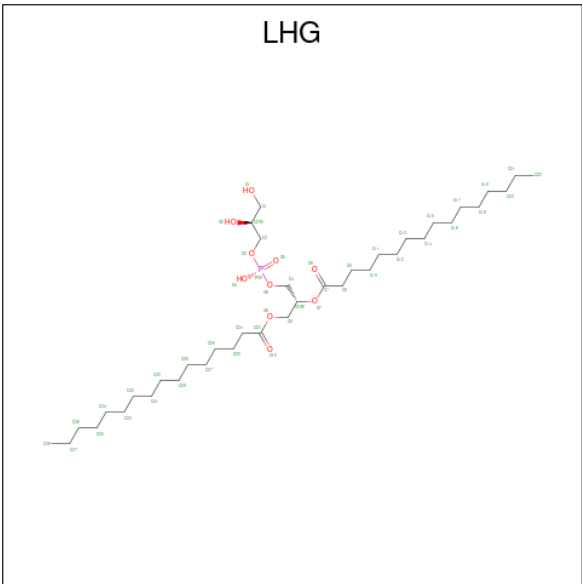
Mol	Chain	Residues	Atoms			AltConf
31	i	1	Total	C	O	0
			24	18	6	
31	i	1	Total	C	O	0
			24	18	6	
31	i	1	Total	C	O	0
			35	24	11	
31	i	1	Total	C	O	0
			22	16	6	
31	j	1	Total	C	O	0
			24	18	6	
31	k	1	Total	C	O	0
			35	24	11	
31	m	1	Total	C	O	0
			35	24	11	
31	m	1	Total	C	O	0
			24	18	6	
31	t	1	Total	C	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	x	1	Total	C	O	0
			22	16	6	
31	x	1	Total	C	O	0
			19	13	6	
31	x	1	Total	C	O	0
			19	13	6	
31	y	1	Total	C	O	0
			21	15	6	

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



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

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



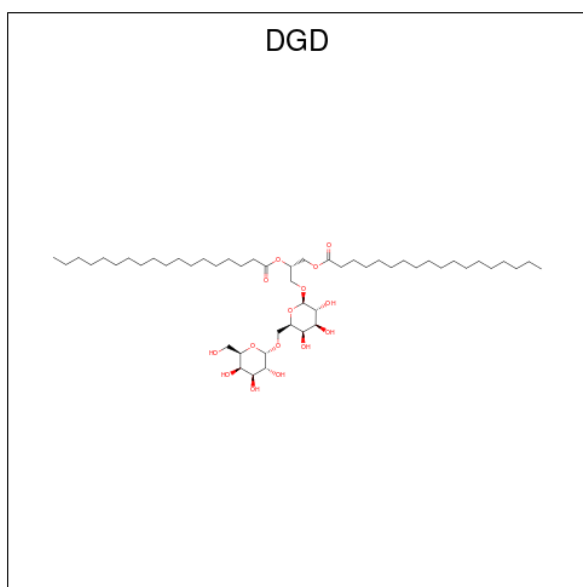
Mol	Chain	Residues	Atoms				AltConf
33	B	1	Total	C	O	P	0
			49	38	10	1	

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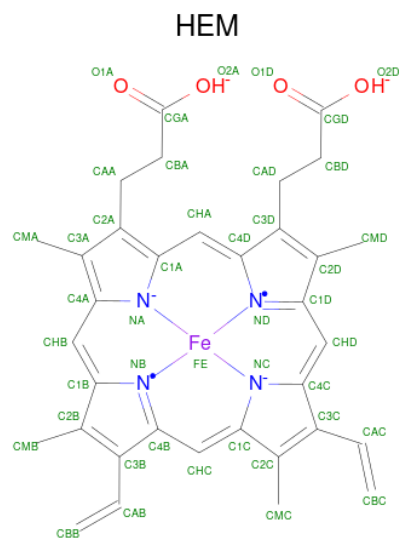
Mol	Chain	Residues	Atoms				AltConf
33	B	1	Total	C	O	P	0
			49	38	10	1	
33	D	1	Total	C	O	P	0
			49	38	10	1	
33	D	1	Total	C	O	P	0
			49	38	10	1	
33	D	1	Total	C	O	P	0
			49	38	10	1	
33	E	1	Total	C	O	P	0
			40	29	10	1	
33	Z	1	Total	C	O	P	0
			36	27	8	1	
33	b	1	Total	C	O	P	0
			49	38	10	1	
33	b	1	Total	C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

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



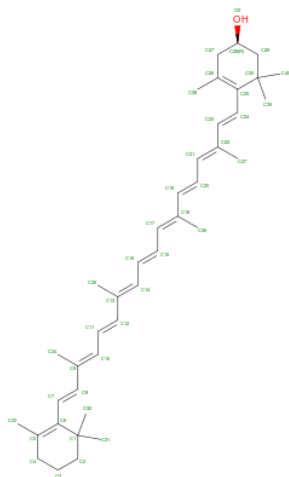
Mol	Chain	Residues	Atoms			AltConf
34	C	1	Total	C	O	0
			62	47	15	
34	C	1	Total	C	O	0
			62	47	15	
34	C	1	Total	C	O	0
			62	47	15	
34	H	1	Total	C	O	0
			62	47	15	
34	c	1	Total	C	O	0
			62	47	15	
34	c	1	Total	C	O	0
			62	47	15	
34	c	1	Total	C	O	0
			62	47	15	
34	h	1	Total	C	O	0
			62	47	15	

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



Mol	Chain	Residues	Atoms					AltConf
35	E	1	Total 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 (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: $C_{40}H_{56}O$).



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

- Molecule 37 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		AltConf
38	A	127	Total	O	0
			127	127	
38	B	127	Total	O	0
			127	127	
38	C	107	Total	O	0
			107	107	
38	D	132	Total	O	0
			132	132	
38	E	8	Total	O	0
			8	8	
38	F	4	Total	O	0
			4	4	
38	H	17	Total	O	0
			17	17	
38	I	1	Total	O	0
			1	1	
38	J	2	Total	O	0
			2	2	
38	L	14	Total	O	0
			14	14	

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Mol	Chain	Residues	Atoms		AltConf
38	M	6	Total 6	O 6	0
38	O	37	Total 37	O 37	0
38	T	12	Total 12	O 12	0
38	U	21	Total 21	O 21	0
38	V	17	Total 17	O 17	0
38	X	3	Total 3	O 3	0
38	a	127	Total 127	O 127	0
38	b	127	Total 127	O 127	0
38	c	107	Total 107	O 107	0
38	d	132	Total 132	O 132	0
38	e	8	Total 8	O 8	0
38	f	4	Total 4	O 4	0
38	h	17	Total 17	O 17	0
38	i	1	Total 1	O 1	0
38	j	2	Total 2	O 2	0
38	l	14	Total 14	O 14	0
38	m	6	Total 6	O 6	0
38	o	37	Total 37	O 37	0
38	t	12	Total 12	O 12	0
38	u	21	Total 21	O 21	0
38	v	17	Total 17	O 17	0

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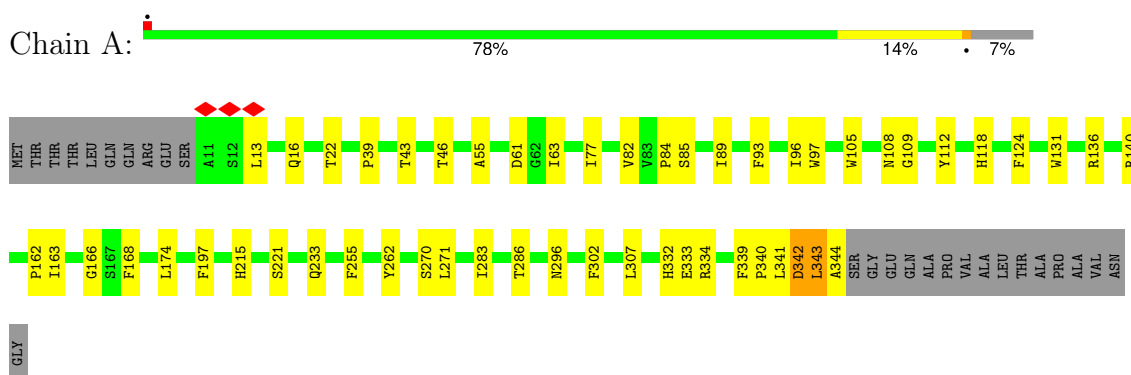
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Mol	Chain	Residues	Atoms		AltConf
38	x	3	Total	O	0
			3	3	

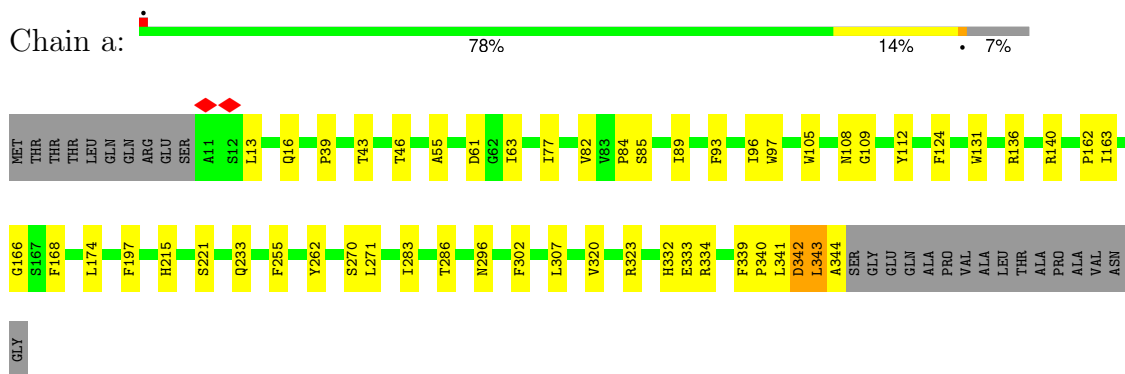
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

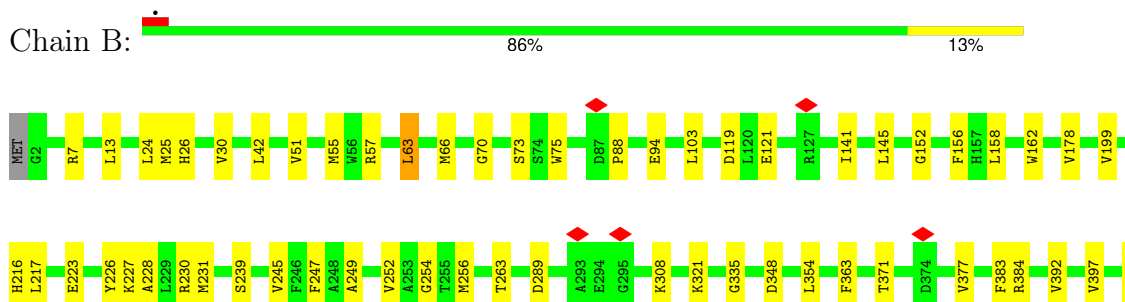
- Molecule 1: Photosystem II protein D1 2

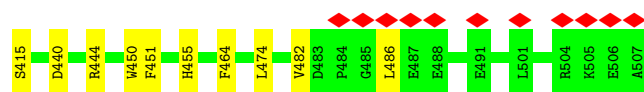


- Molecule 1: Photosystem II protein D1 2



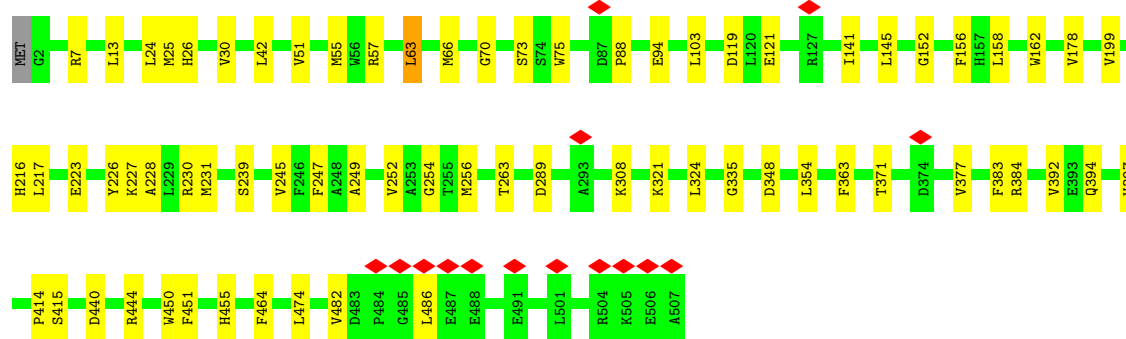
- Molecule 2: Photosystem II CP47 reaction center protein





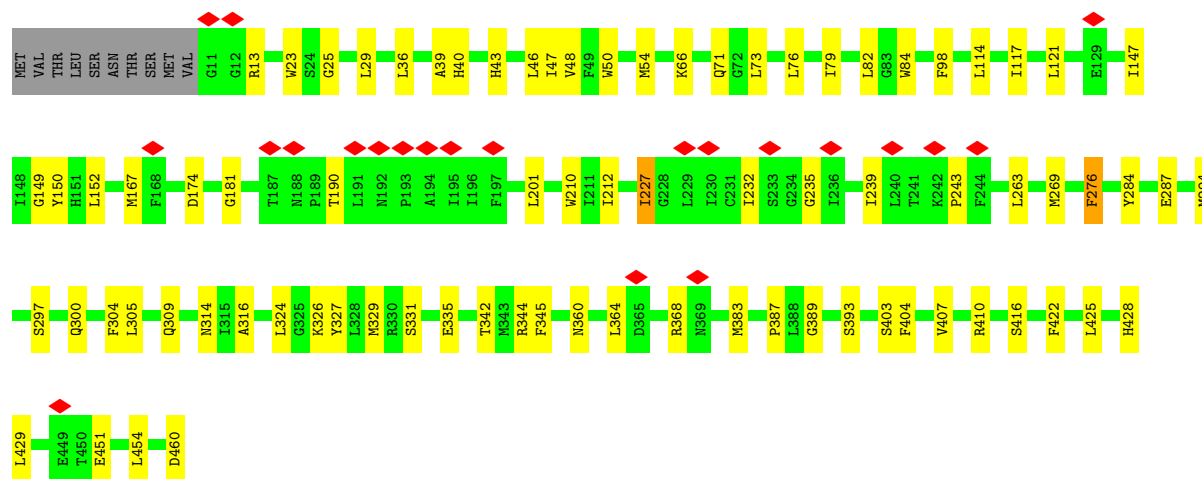
• Molecule 2: Photosystem II CP47 reaction center protein

Chain b: 86% 14%



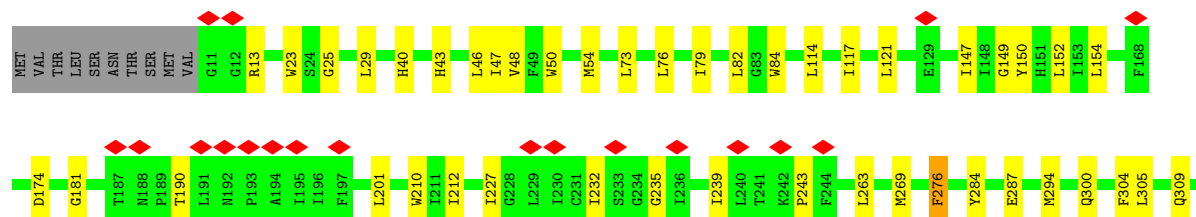
• Molecule 3: Photosystem II CP43 reaction center protein

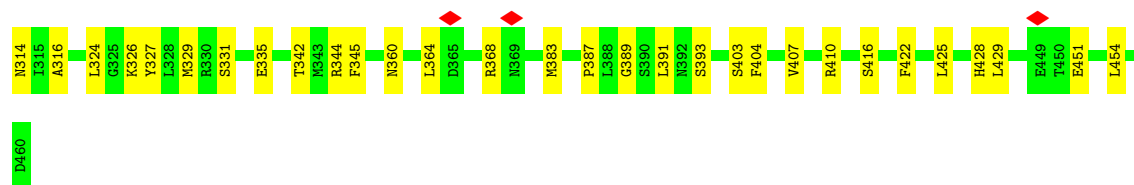
Chain C: 5% 80% 17%



• Molecule 3: Photosystem II CP43 reaction center protein

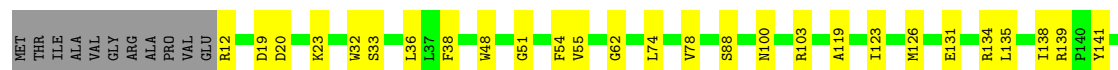
Chain c: 5% 82% 16%





- Molecule 4: Photosystem II D2 protein

Chain D: 83% 13% .



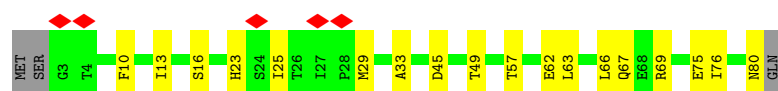
- Molecule 4: Photosystem II D2 protein

Chain d: 84% 12% .



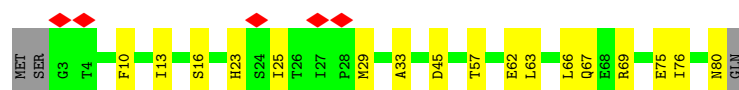
- Molecule 5: Cytochrome b559 subunit alpha

Chain E: 6% 74% 22% .



- Molecule 5: Cytochrome b559 subunit alpha

Chain e: 6% 75% 21% .

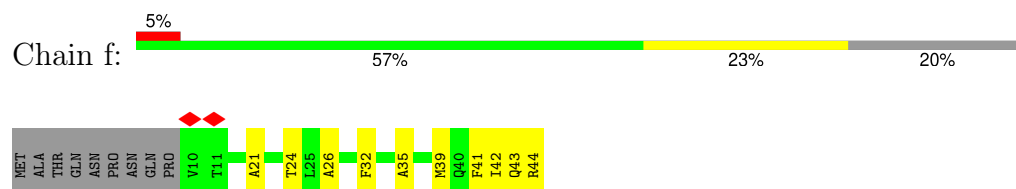


- Molecule 6: Cytochrome b559 subunit beta

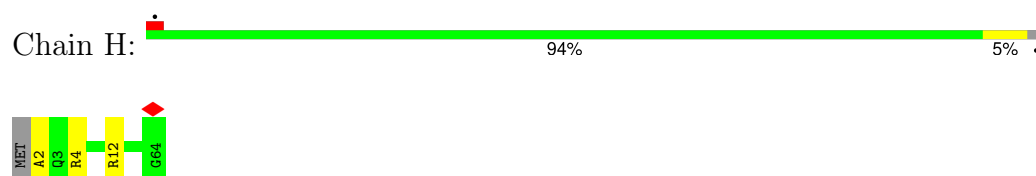
Chain F: 5% 57% 23% 20% .



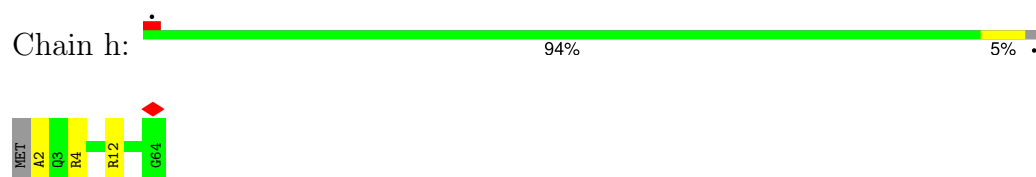
- Molecule 6: Cytochrome b559 subunit beta



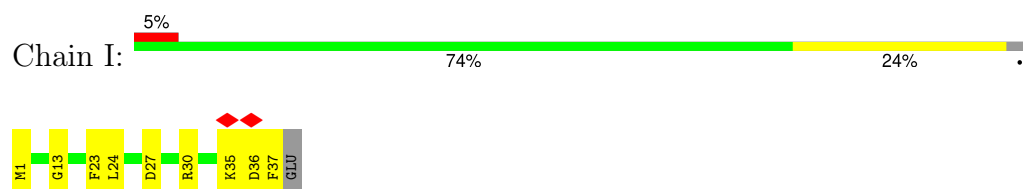
- Molecule 7: Photosystem II reaction center protein H



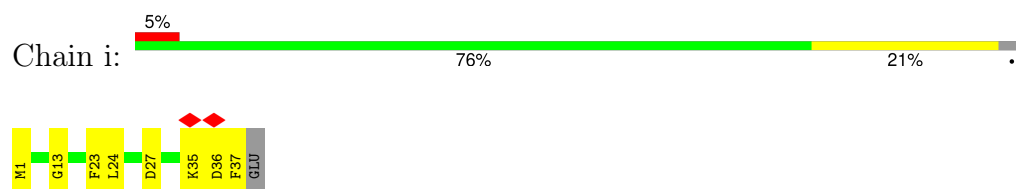
- Molecule 7: Photosystem II reaction center protein H



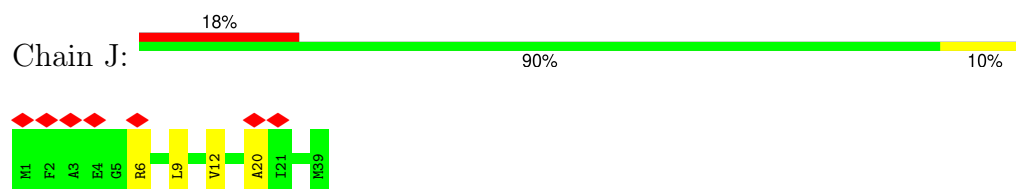
- Molecule 8: Photosystem II reaction center protein I



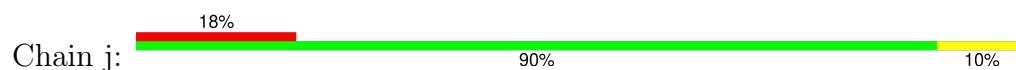
- Molecule 8: Photosystem II reaction center protein I

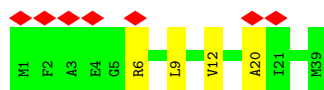


- Molecule 9: Photosystem II reaction center protein J

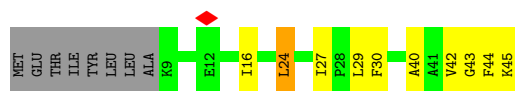


- Molecule 9: Photosystem II reaction center protein J

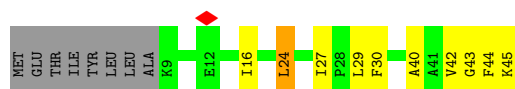




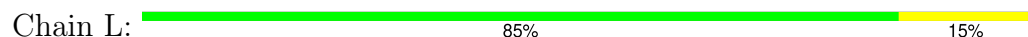
- Molecule 10: Photosystem II reaction center protein K



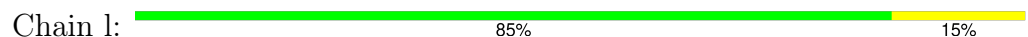
- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



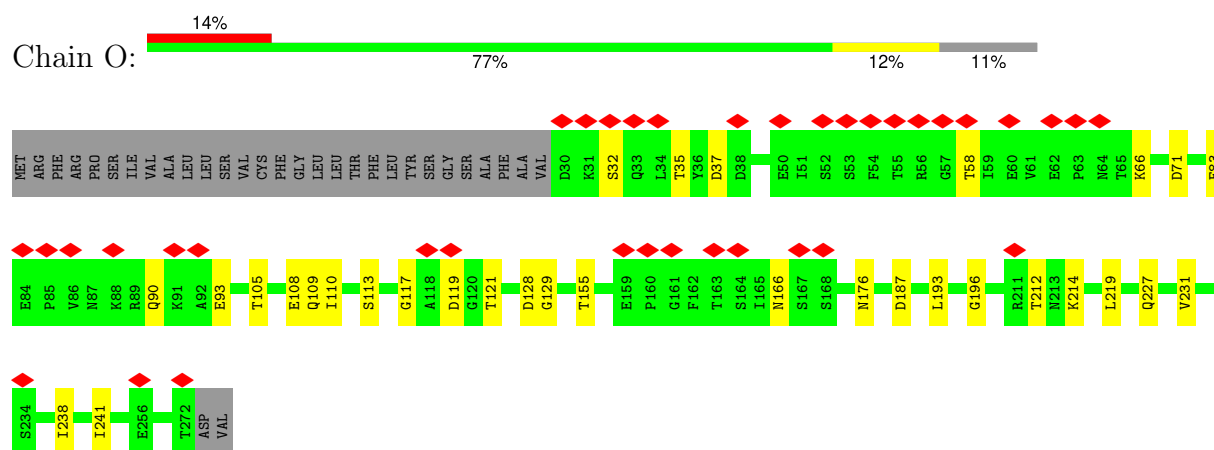
- Molecule 12: Photosystem II reaction center protein M



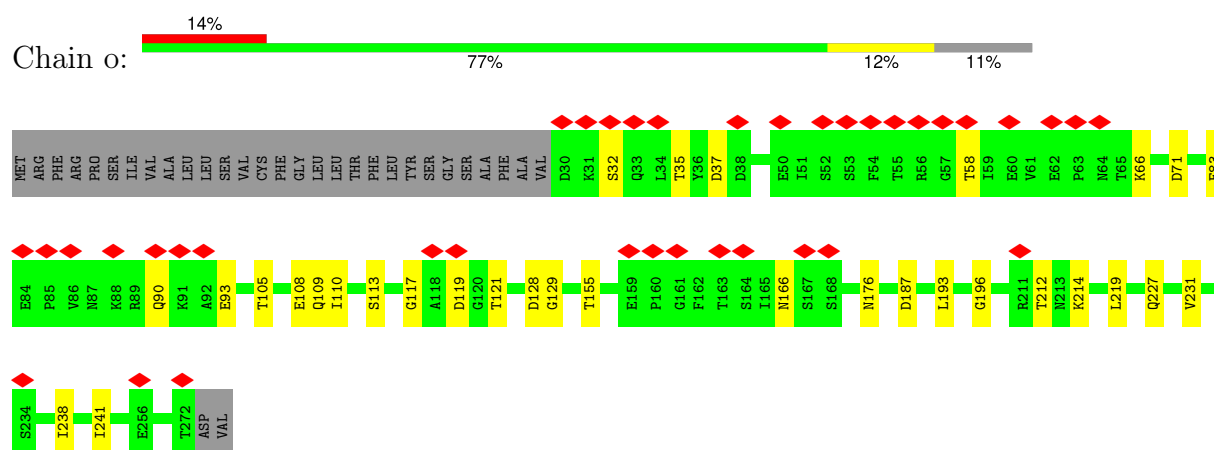
- Molecule 12: Photosystem II reaction center protein M



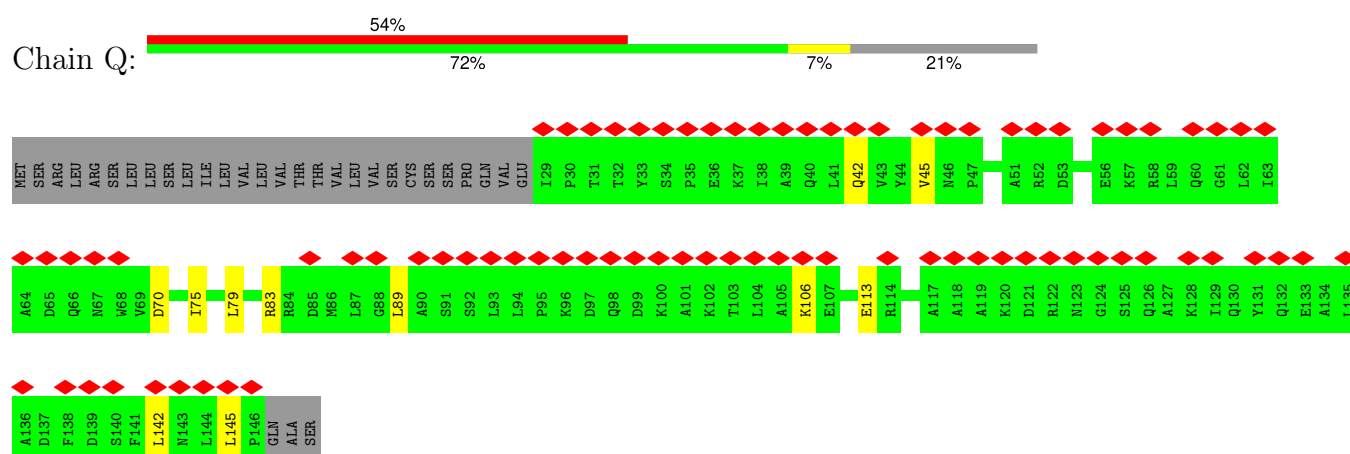
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



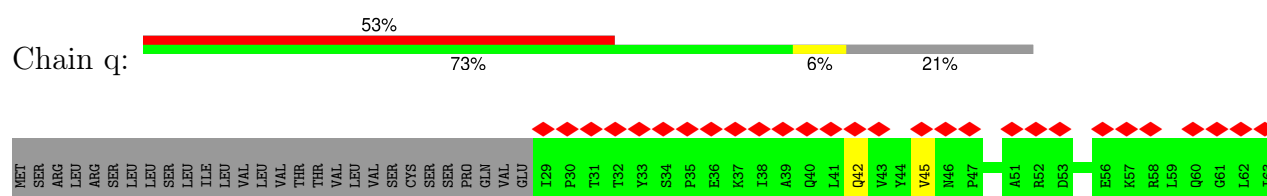
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

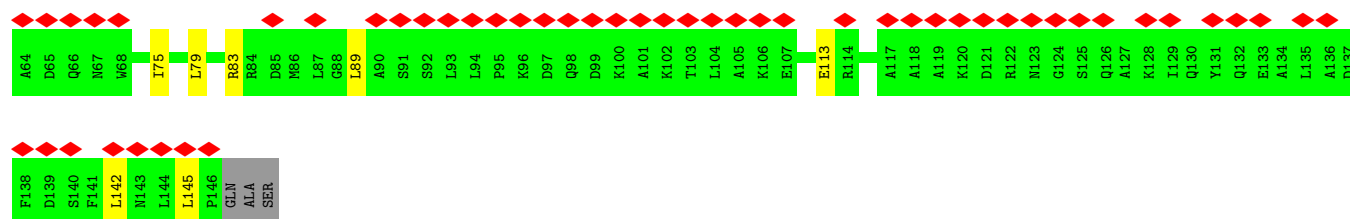


- Molecule 14: Sll1638 protein

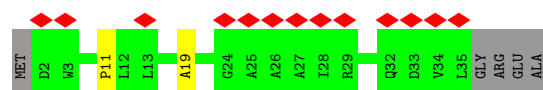
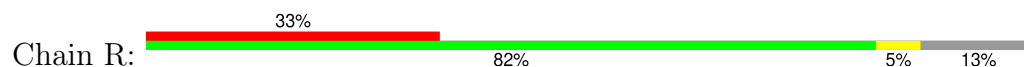


- Molecule 14: Sll1638 protein

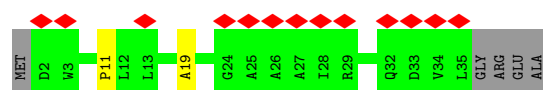
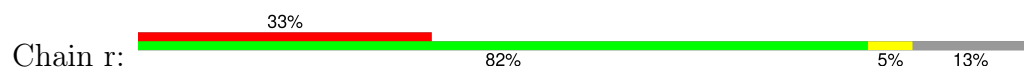




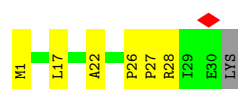
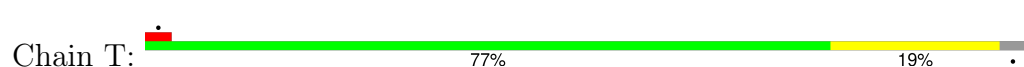
• Molecule 15: Photosystem II protein Y



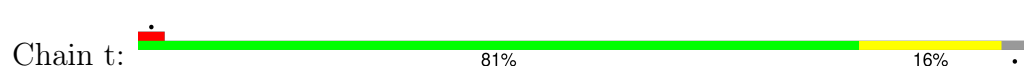
• Molecule 15: Photosystem II protein Y



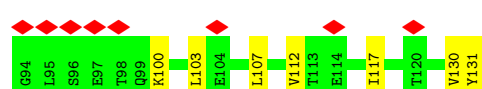
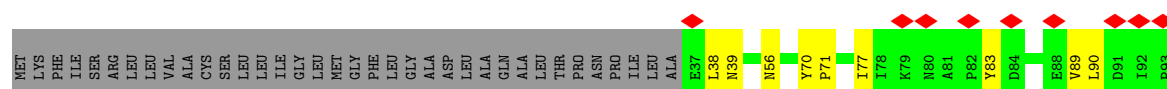
• Molecule 16: Photosystem II reaction center protein T



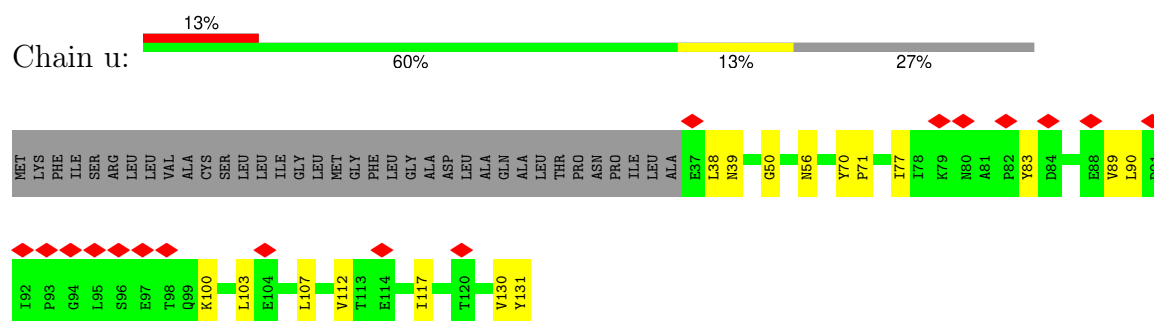
• Molecule 16: Photosystem II reaction center protein T



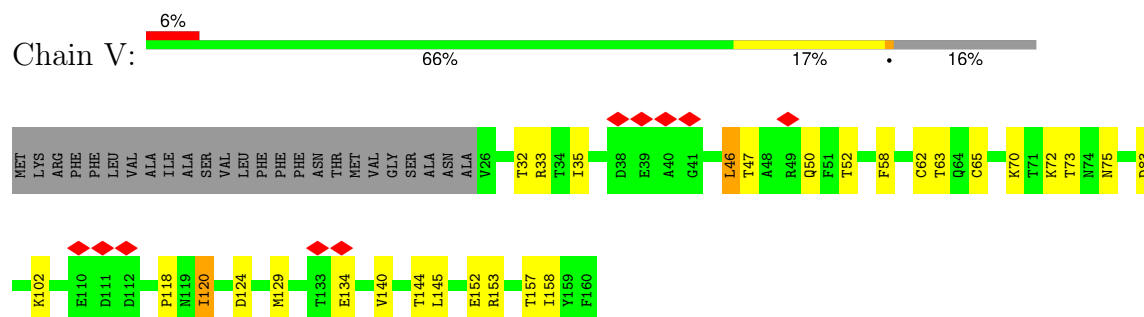
• Molecule 17: Photosystem II 12 kDa extrinsic protein



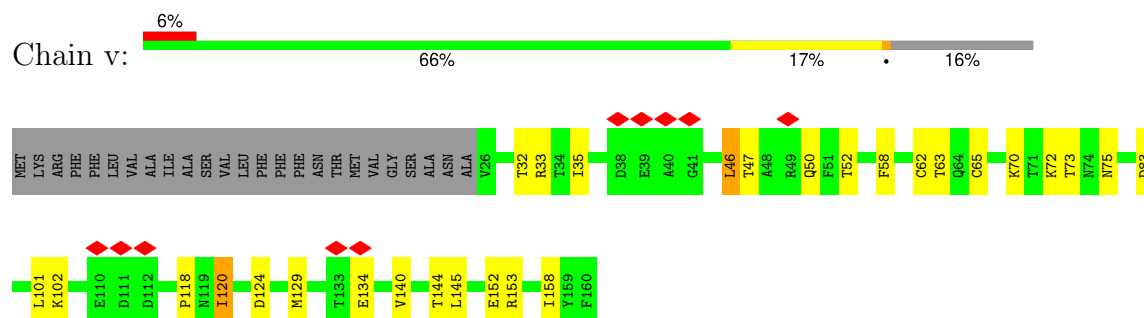
• Molecule 17: Photosystem II 12 kDa extrinsic protein



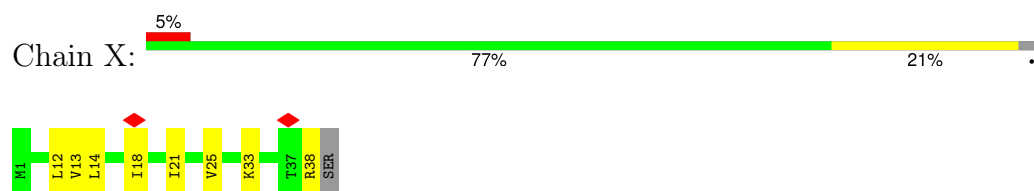
- Molecule 18: Cytochrome c-550



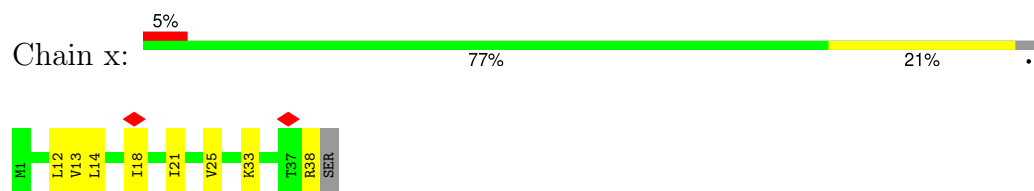
- Molecule 18: Cytochrome c-550



- Molecule 19: Photosystem II reaction center X protein



- Molecule 19: Photosystem II reaction center X protein



- Molecule 20: Photosystem II reaction center protein Ycf12

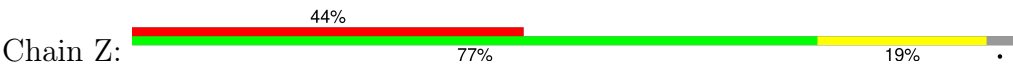




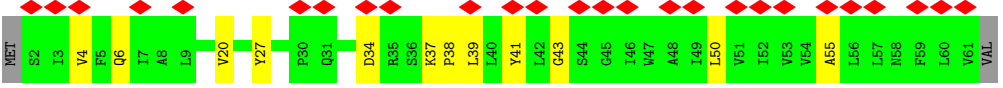
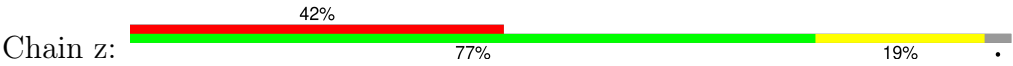
● Molecule 20: Photosystem II reaction center protein Ycf12



● 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	129229	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 ($e^-/\text{\AA}^2$)	38	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.070	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00432	Depositor
Map size (Å)	297.0, 297.0, 297.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.45	0/2724	0.69	1/3710 (0.0%)
1	a	0.45	0/2724	0.69	1/3710 (0.0%)
2	B	0.36	0/4091	0.58	0/5568
2	b	0.36	0/4091	0.58	0/5568
3	C	0.40	0/3608	0.66	0/4912
3	c	0.40	0/3608	0.66	0/4912
4	D	0.36	0/2823	0.60	1/3843 (0.0%)
4	d	0.36	0/2823	0.60	1/3843 (0.0%)
5	E	0.40	0/664	0.73	2/906 (0.2%)
5	e	0.40	0/664	0.73	2/906 (0.2%)
6	F	0.41	0/288	0.70	0/393
6	f	0.41	0/288	0.70	0/393
7	H	0.29	0/506	0.52	0/687
7	h	0.29	0/506	0.52	0/687
8	I	0.31	0/294	0.64	0/397
8	i	0.31	0/294	0.64	0/397
9	J	0.22	0/278	0.46	0/375
9	j	0.22	0/278	0.46	0/375
10	K	0.40	0/310	0.84	1/424 (0.2%)
10	k	0.40	0/310	0.84	1/424 (0.2%)
11	L	0.31	0/322	0.53	0/435
11	l	0.31	0/322	0.53	0/435
12	M	0.33	0/239	0.67	0/325
12	m	0.33	0/239	0.67	0/325
13	O	0.27	0/1911	0.59	0/2590
13	o	0.27	0/1911	0.59	0/2590
14	Q	0.25	0/925	0.65	0/1250
14	q	0.25	0/925	0.65	0/1250
15	R	0.27	0/262	0.61	0/361
15	r	0.27	0/262	0.61	0/361
16	T	0.30	0/236	0.55	0/321

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	t	0.30	0/236	0.55	0/321
17	U	0.26	0/751	0.54	0/1018
17	u	0.26	0/751	0.54	0/1018
18	V	0.32	0/1086	0.58	0/1476
18	v	0.32	0/1086	0.58	0/1476
19	X	0.28	0/293	0.60	0/399
19	x	0.28	0/293	0.60	0/399
20	Y	0.30	0/247	0.56	0/335
20	y	0.30	0/247	0.56	0/335
21	Z	0.32	0/472	0.62	0/649
21	z	0.32	0/472	0.62	0/649
All	All	0.36	0/44660	0.62	10/60748 (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
1	A	0	2
1	a	0	2
All	All	0	4

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	K	24	LEU	N-CA-C	6.18	122.10	113.57
10	k	24	LEU	N-CA-C	6.16	122.08	113.57
4	D	214	HIS	CA-CB-CG	-5.74	108.06	113.80
4	d	214	HIS	CA-CB-CG	-5.74	108.06	113.80
5	e	29	MET	CB-CG-SD	5.49	129.16	112.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	342	ASP	Mainchain
1	a	342	ASP	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2640	0	2535	49	0
1	a	2640	0	2535	47	0
2	B	3958	0	3799	54	0
2	b	3958	0	3799	55	0
3	C	3493	0	3417	65	0
3	c	3493	0	3417	58	0
4	D	2726	0	2617	38	0
4	d	2726	0	2617	36	0
5	E	645	0	616	15	0
5	e	645	0	616	14	0
6	F	279	0	282	12	0
6	f	279	0	282	12	0
7	H	494	0	508	3	0
7	h	494	0	508	3	0
8	I	297	0	313	6	0
8	i	297	0	313	5	0
9	J	279	0	282	4	0
9	j	279	0	282	4	0
10	K	299	0	308	10	0
10	k	299	0	308	9	0
11	L	316	0	321	8	0
11	l	316	0	321	8	0
12	M	245	0	270	7	0
12	m	245	0	270	7	0
13	O	1873	0	1829	17	0
13	o	1873	0	1829	17	0
14	Q	911	0	903	7	0
14	q	911	0	903	5	0
15	R	258	0	276	2	0
15	r	258	0	276	2	0
16	T	241	0	254	5	0
16	t	241	0	254	4	0
17	U	740	0	718	10	0
17	u	740	0	718	11	0
18	V	1065	0	1021	21	0
18	v	1065	0	1021	22	0
19	X	288	0	320	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	x	288	0	320	8	0
20	Y	242	0	255	6	0
20	y	242	0	255	6	0
21	Z	460	0	491	9	0
21	z	460	0	491	9	0
22	A	10	0	0	0	0
22	a	10	0	0	0	0
23	A	1	0	0	0	0
23	a	1	0	0	0	0
24	A	2	0	0	1	0
24	a	2	0	0	1	0
25	A	190	0	203	13	0
25	B	1010	0	1084	51	0
25	C	820	0	878	46	0
25	D	195	0	216	13	0
25	a	190	0	203	10	0
25	b	1010	0	1084	48	0
25	c	820	0	878	45	0
25	d	195	0	216	15	0
26	A	64	0	74	5	0
26	D	64	0	74	1	0
26	a	64	0	74	6	0
26	d	64	0	74	1	0
27	A	40	0	49	4	0
27	B	120	0	147	7	0
27	C	40	0	49	4	0
27	F	40	0	49	3	0
27	K	80	0	98	9	0
27	Z	40	0	49	2	0
27	a	40	0	49	4	0
27	b	120	0	147	6	0
27	c	40	0	49	4	0
27	f	40	0	49	4	0
27	k	80	0	98	9	0
27	z	40	0	49	3	0
28	A	87	0	114	5	0
28	B	51	0	72	1	0
28	C	100	0	140	7	0
28	D	44	0	56	1	0
28	H	47	0	64	0	0
28	a	87	0	114	6	0
28	b	51	0	72	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	c	100	0	140	6	0
28	d	44	0	56	0	0
28	h	47	0	64	0	0
29	A	55	0	80	8	0
29	D	55	0	80	2	0
29	a	55	0	80	8	0
29	d	55	0	80	2	0
30	A	102	0	136	5	0
30	B	54	0	78	2	0
30	C	54	0	77	4	0
30	F	34	0	31	0	0
30	H	54	0	77	3	0
30	K	41	0	51	4	0
30	a	102	0	136	4	0
30	b	54	0	78	2	0
30	c	54	0	77	4	0
30	f	34	0	31	0	0
30	h	54	0	77	2	0
30	k	41	0	51	4	0
31	A	59	0	78	0	0
31	B	153	0	203	5	0
31	C	80	0	106	1	0
31	D	94	0	123	4	0
31	E	57	0	74	4	0
31	F	35	0	44	2	0
31	H	24	0	34	1	0
31	I	105	0	140	5	0
31	J	24	0	34	0	0
31	K	35	0	45	8	0
31	M	59	0	80	8	0
31	T	24	0	34	1	0
31	X	106	0	129	5	0
31	Y	21	0	26	2	0
31	a	59	0	78	0	0
31	b	153	0	203	4	0
31	c	80	0	106	1	0
31	d	94	0	123	4	0
31	e	57	0	74	4	0
31	f	35	0	44	2	0
31	h	24	0	34	2	0
31	i	105	0	140	3	0
31	j	24	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	k	35	0	45	8	0
31	m	59	0	80	9	0
31	t	24	0	34	1	0
31	x	106	0	129	5	0
31	y	21	0	25	2	0
32	A	4	0	1	0	0
32	a	4	0	1	0	0
33	B	98	0	148	12	0
33	D	147	0	222	14	0
33	E	40	0	53	2	0
33	Z	36	0	48	1	0
33	b	98	0	148	11	0
33	d	147	0	222	15	0
33	e	40	0	53	2	0
33	z	36	0	48	1	0
34	C	186	0	246	18	0
34	H	62	0	82	4	0
34	c	186	0	246	15	0
34	h	62	0	82	4	0
35	E	43	0	30	7	0
35	V	43	0	30	3	0
35	e	43	0	30	7	0
35	v	43	0	30	3	0
36	H	41	0	56	2	0
36	h	41	0	56	2	0
37	K	1	0	0	0	0
37	U	1	0	0	0	0
37	V	1	0	0	0	0
37	k	1	0	0	0	0
37	u	1	0	0	0	0
37	v	1	0	0	0	0
38	A	127	0	0	1	0
38	B	127	0	0	0	0
38	C	107	0	0	2	0
38	D	132	0	0	9	0
38	E	8	0	0	0	0
38	F	4	0	0	1	0
38	H	17	0	0	0	0
38	I	1	0	0	0	0
38	J	2	0	0	0	0
38	L	14	0	0	0	0
38	M	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	O	37	0	0	0	0
38	T	12	0	0	0	0
38	U	21	0	0	2	0
38	V	17	0	0	3	0
38	X	3	0	0	0	0
38	a	127	0	0	0	0
38	b	127	0	0	0	0
38	c	107	0	0	2	0
38	d	132	0	0	8	0
38	e	8	0	0	0	0
38	f	4	0	0	1	0
38	h	17	0	0	0	0
38	i	1	0	0	0	0
38	j	2	0	0	0	0
38	l	14	0	0	0	0
38	m	6	0	0	0	0
38	o	37	0	0	0	0
38	t	12	0	0	0	0
38	u	21	0	0	2	0
38	v	17	0	0	3	0
38	x	3	0	0	0	0
All	All	54914	0	54853	889	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 889 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:V:102:LYS:HG2	18:V:120:ILE:HD11	1.52	0.91
18:v:102:LYS:HG2	18:v:120:ILE:HD11	1.52	0.89
27:B:617:BCR:H383	30:B:620:SQD:H101	1.61	0.81
27:b:617:BCR:H383	30:b:620:SQD:H101	1.61	0.81
3:C:263:LEU:HD21	25:C:509:CLA:HAB	1.65	0.78

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/360 (92%)	327 (98%)	6 (2%)	0	100	100
1	a	333/360 (92%)	327 (98%)	6 (2%)	0	100	100
2	B	504/507 (99%)	497 (99%)	7 (1%)	0	100	100
2	b	504/507 (99%)	497 (99%)	7 (1%)	0	100	100
3	C	448/460 (97%)	439 (98%)	9 (2%)	0	100	100
3	c	448/460 (97%)	439 (98%)	9 (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%)	74 (97%)	2 (3%)	0	100	100
5	e	76/81 (94%)	74 (97%)	2 (3%)	0	100	100
6	F	33/44 (75%)	33 (100%)	0	0	100	100
6	f	33/44 (75%)	33 (100%)	0	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	35/38 (92%)	33 (94%)	2 (6%)	0	100	100
8	i	35/38 (92%)	33 (94%)	2 (6%)	0	100	100
9	J	37/39 (95%)	37 (100%)	0	0	100	100
9	j	37/39 (95%)	37 (100%)	0	0	100	100
10	K	35/45 (78%)	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	241/274 (88%)	225 (93%)	15 (6%)	1 (0%)	30	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	241/274 (88%)	225 (93%)	15 (6%)	1 (0%)	30	26
14	Q	116/149 (78%)	112 (97%)	4 (3%)	0	100	100
14	q	116/149 (78%)	112 (97%)	4 (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%)	28 (100%)	0	0	100	100
16	t	28/31 (90%)	28 (100%)	0	0	100	100
17	U	93/131 (71%)	91 (98%)	2 (2%)	0	100	100
17	u	93/131 (71%)	91 (98%)	2 (2%)	0	100	100
18	V	133/160 (83%)	128 (96%)	5 (4%)	0	100	100
18	v	133/160 (83%)	128 (96%)	5 (4%)	0	100	100
19	X	36/39 (92%)	36 (100%)	0	0	100	100
19	x	36/39 (92%)	36 (100%)	0	0	100	100
20	Y	30/39 (77%)	30 (100%)	0	0	100	100
20	y	30/39 (77%)	30 (100%)	0	0	100	100
21	Z	58/62 (94%)	58 (100%)	0	0	100	100
21	z	58/62 (94%)	58 (100%)	0	0	100	100
All	All	5468/5976 (92%)	5340 (98%)	126 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	32	SER
13	o	32	SER

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	274/293 (94%)	271 (99%)	3 (1%)	65	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	274/293 (94%)	271 (99%)	3 (1%)	65	71
2	B	403/404 (100%)	398 (99%)	5 (1%)	63	69
2	b	403/404 (100%)	398 (99%)	5 (1%)	63	69
3	C	351/361 (97%)	342 (97%)	9 (3%)	40	42
3	c	351/361 (97%)	342 (97%)	9 (3%)	40	42
4	D	277/285 (97%)	276 (100%)	1 (0%)	84	88
4	d	277/285 (97%)	275 (99%)	2 (1%)	76	81
5	E	70/73 (96%)	69 (99%)	1 (1%)	59	65
5	e	70/73 (96%)	69 (99%)	1 (1%)	59	65
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%)	53 (100%)	0	100	100
7	h	53/54 (98%)	53 (100%)	0	100	100
8	I	32/33 (97%)	31 (97%)	1 (3%)	35	35
8	i	32/33 (97%)	31 (97%)	1 (3%)	35	35
9	J	24/24 (100%)	24 (100%)	0	100	100
9	j	24/24 (100%)	24 (100%)	0	100	100
10	K	31/38 (82%)	30 (97%)	1 (3%)	34	35
10	k	31/38 (82%)	30 (97%)	1 (3%)	34	35
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%)	30	29
12	m	27/31 (87%)	26 (96%)	1 (4%)	30	29
13	O	207/233 (89%)	202 (98%)	5 (2%)	43	45
13	o	207/233 (89%)	202 (98%)	5 (2%)	43	45
14	Q	93/128 (73%)	93 (100%)	0	100	100
14	q	93/128 (73%)	93 (100%)	0	100	100
15	R	26/29 (90%)	26 (100%)	0	100	100
15	r	26/29 (90%)	26 (100%)	0	100	100
16	T	24/25 (96%)	24 (100%)	0	100	100
16	t	24/25 (96%)	24 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	U	83/111 (75%)	80 (96%)	3 (4%)	31	30
17	u	83/111 (75%)	80 (96%)	3 (4%)	31	30
18	V	117/137 (85%)	111 (95%)	6 (5%)	21	17
18	v	117/137 (85%)	111 (95%)	6 (5%)	21	17
19	X	32/33 (97%)	32 (100%)	0	100	100
19	x	32/33 (97%)	32 (100%)	0	100	100
20	Y	25/30 (83%)	24 (96%)	1 (4%)	28	25
20	y	25/30 (83%)	24 (96%)	1 (4%)	28	25
21	Z	49/52 (94%)	48 (98%)	1 (2%)	48	53
21	z	49/52 (94%)	48 (98%)	1 (2%)	48	53
All	All	4524/4894 (92%)	4447 (98%)	77 (2%)	52	58

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	e	62	GLU
18	v	52	THR
10	k	24	LEU
13	o	212	THR
20	y	64	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
3	c	309	GLN
12	m	2	GLN
3	c	314	ASN
5	e	74	GLN
13	o	153	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	FME	M	1	12	8,9,10	0.99	0	8,9,11	0.93	0
8	FME	I	1	8	8,9,10	0.99	0	8,9,11	1.13	1 (12%)
9	FME	J	1	9	6,7,10	0.82	0	2,7,11	0.67	0
16	FME	T	1	16	8,9,10	0.88	0	8,9,11	1.04	1 (12%)
9	FME	j	1	9	6,7,10	0.83	0	2,7,11	0.67	0
12	FME	m	1	12	8,9,10	0.98	0	8,9,11	0.93	0
16	FME	t	1	16	8,9,10	0.88	0	8,9,11	1.04	1 (12%)
8	FME	i	1	8	8,9,10	0.98	0	8,9,11	1.13	1 (12%)

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
12	FME	M	1	12	-	0/7/9/11	-
8	FME	I	1	8	-	2/7/9/11	-
9	FME	J	1	9	-	3/5/6/11	-
16	FME	T	1	16	-	4/7/9/11	-
9	FME	j	1	9	-	3/5/6/11	-
12	FME	m	1	12	-	0/7/9/11	-
16	FME	t	1	16	-	4/7/9/11	-
8	FME	i	1	8	-	2/7/9/11	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	C-CA-N	2.50	114.31	109.50
8	I	1	FME	C-CA-N	2.48	114.28	109.50
16	T	1	FME	C-CA-N	2.10	113.55	109.50
16	t	1	FME	C-CA-N	2.10	113.55	109.50

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 232 ligands modelled in this entry, 12 are monoatomic - leaving 220 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
28	LMG	d	409	-	43,43,55	1.30	5 (11%)	51,51,63	1.11	3 (5%)
33	LHG	d	408	-	48,48,48	0.91	2 (4%)	51,54,54	0.96	2 (3%)
30	SQD	b	620	-	52,54,54	0.41	0	62,65,65	0.44	0
25	CLA	b	614	2	69,73,73	2.23	21 (30%)	82,113,113	2.50	26 (31%)
29	PL9	D	405	-	55,55,55	1.20	5 (9%)	68,69,69	1.41	11 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	c	514	3	69,73,73	2.25	22 (31%)	82,113,113	2.41	26 (31%)
31	LMT	c	524	-	36,36,36	1.18	4 (11%)	47,47,47	1.18	3 (6%)
25	CLA	c	504	3	69,73,73	2.25	23 (33%)	82,113,113	2.51	28 (34%)
27	BCR	b	618	-	41,41,41	2.68	6 (14%)	56,56,56	6.46	20 (35%)
25	CLA	b	608	2	69,73,73	2.24	21 (30%)	82,113,113	2.39	27 (32%)
31	LMT	e	101	-	22,22,36	1.09	2 (9%)	27,27,47	1.16	3 (11%)
25	CLA	c	502	3	69,73,73	2.22	22 (31%)	82,113,113	2.50	28 (34%)
31	LMT	X	103	-	22,22,36	1.01	2 (9%)	27,27,47	1.28	3 (11%)
31	LMT	x	105	-	19,19,36	1.12	2 (10%)	24,24,47	1.00	0
33	LHG	z	102	-	35,35,48	1.15	2 (5%)	38,40,54	1.16	3 (7%)
31	LMT	M	102	-	24,24,36	1.06	2 (8%)	29,29,47	1.08	1 (3%)
25	CLA	d	401	38	69,73,73	2.19	22 (31%)	82,113,113	2.50	26 (31%)
25	CLA	b	616	2	64,68,73	2.26	21 (32%)	76,107,113	2.62	27 (35%)
25	CLA	c	506	3	59,63,73	2.40	22 (37%)	70,101,113	2.74	28 (40%)
27	BCR	C	515	-	41,41,41	2.66	6 (14%)	56,56,56	6.60	16 (28%)
31	LMT	E	103	-	36,36,36	1.23	6 (16%)	47,47,47	1.57	6 (12%)
25	CLA	c	512	3	69,73,73	2.24	23 (33%)	82,113,113	2.60	28 (34%)
31	LMT	C	522	-	24,24,36	1.15	5 (20%)	29,29,47	1.32	5 (17%)
33	LHG	B	627	-	48,48,48	0.95	2 (4%)	51,54,54	1.06	2 (3%)
31	LMT	i	104	-	22,22,36	1.05	2 (9%)	27,27,47	1.05	0
25	CLA	C	506	3	59,63,73	2.40	22 (37%)	70,101,113	2.74	28 (40%)
27	BCR	B	618	-	41,41,41	2.68	6 (14%)	56,56,56	6.46	20 (35%)
25	CLA	B	613	2	69,73,73	2.16	22 (31%)	82,113,113	2.52	26 (31%)
25	CLA	b	607	38	69,73,73	2.18	22 (31%)	82,113,113	2.49	28 (34%)
28	LMG	D	409	-	43,43,55	1.30	5 (11%)	51,51,63	1.11	3 (5%)
32	BCT	a	417	-	3,3,3	1.15	0	2,3,3	4.17	2 (100%)
25	CLA	C	512	3	69,73,73	2.24	23 (33%)	82,113,113	2.60	28 (34%)
31	LMT	y	101	-	21,21,36	1.10	2 (9%)	26,26,47	1.05	1 (3%)
30	SQD	A	413	-	46,48,54	1.00	3 (6%)	56,59,65	1.86	12 (21%)
25	CLA	C	508	38	69,73,73	2.21	22 (31%)	82,113,113	2.55	29 (35%)
25	CLA	C	505	38	69,73,73	2.18	21 (30%)	82,113,113	2.54	29 (35%)
33	LHG	B	628	-	48,48,48	0.93	2 (4%)	51,54,54	1.01	3 (5%)
30	SQD	B	620	-	52,54,54	0.41	0	62,65,65	0.44	0
31	LMT	E	101	-	22,22,36	1.08	2 (9%)	27,27,47	1.16	3 (11%)
31	LMT	X	105	-	19,19,36	1.12	2 (10%)	24,24,47	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	604	2	69,73,73	2.19	20 (28%)	82,113,113	2.49	30 (36%)
31	LMT	i	102	-	24,24,36	1.04	3 (12%)	29,29,47	1.07	1 (3%)
31	LMT	x	101	-	24,24,36	1.04	2 (8%)	29,29,47	1.06	1 (3%)
33	LHG	Z	102	-	35,35,48	1.15	2 (5%)	38,40,54	1.16	3 (7%)
27	BCR	F	101	-	41,41,41	2.60	6 (14%)	56,56,56	6.63	22 (39%)
28	LMG	C	523	-	49,49,55	1.44	6 (12%)	57,57,63	1.22	4 (7%)
25	CLA	b	612	2	69,73,73	2.23	21 (30%)	82,113,113	2.44	27 (32%)
31	LMT	x	104	-	19,19,36	1.20	3 (15%)	24,24,47	1.06	1 (4%)
28	LMG	A	414	-	36,36,55	1.11	2 (5%)	44,44,63	1.19	3 (6%)
31	LMT	A	416	-	24,24,36	1.07	3 (12%)	29,29,47	1.00	1 (3%)
31	LMT	h	102	-	24,24,36	1.07	2 (8%)	29,29,47	1.11	2 (6%)
25	CLA	B	605	2	69,73,73	2.18	21 (30%)	82,113,113	2.58	26 (31%)
31	LMT	B	624	-	24,24,36	1.04	3 (12%)	29,29,47	0.90	0
25	CLA	B	614	2	69,73,73	2.22	21 (30%)	82,113,113	2.50	26 (31%)
25	CLA	A	408	1	64,68,73	2.31	22 (34%)	76,107,113	2.61	25 (32%)
25	CLA	b	605	2	69,73,73	2.18	21 (30%)	82,113,113	2.58	25 (30%)
25	CLA	b	601	38	49,53,73	2.53	23 (46%)	58,89,113	2.86	24 (41%)
33	LHG	D	406	-	48,48,48	0.91	3 (6%)	51,54,54	0.99	3 (5%)
31	LMT	X	102	-	22,22,36	1.09	2 (9%)	27,27,47	1.05	1 (3%)
26	PHO	a	407	-	58,69,69	2.16	10 (17%)	55,99,99	1.62	7 (12%)
31	LMT	H	102	-	24,24,36	1.07	2 (8%)	29,29,47	1.12	2 (6%)
27	BCR	k	103	-	41,41,41	2.64	6 (14%)	56,56,56	6.56	26 (46%)
31	LMT	e	103	-	36,36,36	1.22	6 (16%)	47,47,47	1.57	6 (12%)
25	CLA	C	513	3	54,58,73	2.52	21 (38%)	64,95,113	2.75	21 (32%)
30	SQD	k	101	-	41,41,54	1.04	3 (7%)	49,49,65	1.77	9 (18%)
31	LMT	I	101	-	24,24,36	1.06	2 (8%)	29,29,47	1.06	2 (6%)
31	LMT	x	103	-	22,22,36	1.01	2 (9%)	27,27,47	1.28	3 (11%)
30	SQD	a	413	-	46,48,54	1.00	3 (6%)	56,59,65	1.86	12 (21%)
31	LMT	b	625	-	36,36,36	1.23	6 (16%)	47,47,47	1.06	1 (2%)
31	LMT	t	101	-	24,24,36	1.09	2 (8%)	29,29,47	1.16	2 (6%)
27	BCR	b	619	-	41,41,41	2.70	6 (14%)	56,56,56	6.55	22 (39%)
27	BCR	B	617	-	41,41,41	2.69	6 (14%)	56,56,56	6.53	16 (28%)
31	LMT	C	524	-	36,36,36	1.18	4 (11%)	47,47,47	1.18	3 (6%)
35	HEM	v	201	18	50,50,50	1.78	14 (28%)	67,82,82	1.90	12 (17%)
31	LMT	d	410	-	24,24,36	0.99	2 (8%)	29,29,47	1.21	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	BCR	K	102	-	41,41,41	2.61	6 (14%)	56,56,56	6.89	21 (37%)
25	CLA	c	510	3	69,73,73	2.24	23 (33%)	82,113,113	2.50	26 (31%)
25	CLA	c	507	3	69,73,73	2.23	22 (31%)	82,113,113	2.43	26 (31%)
31	LMT	I	102	-	24,24,36	1.03	3 (12%)	29,29,47	1.06	1 (3%)
36	RRX	H	101	-	42,42,42	1.33	8 (19%)	56,58,58	1.39	9 (16%)
28	LMG	A	410	-	51,51,55	1.48	8 (15%)	59,59,63	1.11	3 (5%)
31	LMT	M	101	-	36,36,36	1.17	6 (16%)	47,47,47	1.04	2 (4%)
27	BCR	c	515	-	41,41,41	2.66	6 (14%)	56,56,56	6.60	16 (28%)
31	LMT	m	102	-	24,24,36	1.07	2 (8%)	29,29,47	1.08	1 (3%)
25	CLA	d	403	4	69,73,73	2.19	21 (30%)	82,113,113	2.55	25 (30%)
25	CLA	C	510	3	69,73,73	2.24	23 (33%)	82,113,113	2.50	26 (31%)
25	CLA	c	508	38	69,73,73	2.21	21 (30%)	82,113,113	2.55	29 (35%)
28	LMG	a	410	-	51,51,55	1.48	8 (15%)	59,59,63	1.11	3 (5%)
31	LMT	c	522	-	24,24,36	1.14	4 (16%)	29,29,47	1.33	5 (17%)
31	LMT	I	103	-	36,36,36	1.18	5 (13%)	47,47,47	0.93	1 (2%)
28	LMG	B	621	-	51,51,55	1.46	8 (15%)	59,59,63	1.03	2 (3%)
25	CLA	B	610	38	69,73,73	2.25	23 (33%)	82,113,113	2.47	32 (39%)
33	LHG	d	407	-	48,48,48	0.91	2 (4%)	51,54,54	1.07	4 (7%)
25	CLA	d	404	4	69,73,73	2.22	23 (33%)	82,113,113	2.49	26 (31%)
31	LMT	Y	101	-	21,21,36	1.10	2 (9%)	26,26,47	1.05	1 (3%)
27	BCR	z	101	-	41,41,41	2.64	6 (14%)	56,56,56	6.49	20 (35%)
31	LMT	d	412	-	36,36,36	1.17	5 (13%)	47,47,47	0.95	1 (2%)
31	LMT	x	102	-	22,22,36	1.10	2 (9%)	27,27,47	1.05	1 (3%)
25	CLA	B	608	2	69,73,73	2.24	21 (30%)	82,113,113	2.39	27 (32%)
25	CLA	c	511	3	69,73,73	2.21	22 (31%)	82,113,113	2.52	30 (36%)
30	SQD	K	101	-	41,41,54	1.04	3 (7%)	49,49,65	1.77	9 (18%)
31	LMT	j	101	-	24,24,36	1.04	3 (12%)	29,29,47	1.19	4 (13%)
25	CLA	b	609	2	69,73,73	2.25	21 (30%)	82,113,113	2.41	24 (29%)
34	DGD	H	104	-	63,63,67	1.34	8 (12%)	77,77,81	0.97	3 (3%)
34	DGD	c	516	-	63,63,67	1.33	8 (12%)	77,77,81	0.93	2 (2%)
34	DGD	c	518	-	63,63,67	1.33	8 (12%)	77,77,81	1.05	3 (3%)
30	SQD	C	501	-	52,54,54	0.93	4 (7%)	62,65,65	1.62	9 (14%)
28	LMG	h	105	-	47,47,55	1.41	6 (12%)	55,55,63	1.39	7 (12%)
26	PHO	A	407	-	58,69,69	2.15	10 (17%)	55,99,99	1.63	7 (12%)
31	LMT	J	101	-	24,24,36	1.04	3 (12%)	29,29,47	1.19	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LMT	i	101	-	24,24,36	1.06	2 (8%)	29,29,47	1.06	2 (6%)
30	SQD	F	102	-	32,34,54	1.20	4 (12%)	42,45,65	1.97	11 (26%)
30	SQD	f	102	-	32,34,54	1.20	4 (12%)	42,45,65	1.97	11 (26%)
34	DGD	c	517	-	63,63,67	1.33	8 (12%)	77,77,81	1.08	5 (6%)
27	BCR	a	409	-	41,41,41	2.64	6 (14%)	56,56,56	6.48	20 (35%)
31	LMT	B	629	-	36,36,36	1.18	5 (13%)	47,47,47	1.00	1 (2%)
25	CLA	B	615	2	69,73,73	2.17	21 (30%)	82,113,113	2.55	28 (34%)
31	LMT	b	629	-	36,36,36	1.18	5 (13%)	47,47,47	1.00	1 (2%)
25	CLA	b	602	2	69,73,73	2.21	21 (30%)	82,113,113	2.45	26 (31%)
27	BCR	b	617	-	41,41,41	2.69	6 (14%)	56,56,56	6.53	16 (28%)
31	LMT	X	104	-	19,19,36	1.20	3 (15%)	24,24,47	1.06	1 (4%)
31	LMT	b	623	-	36,36,36	1.18	4 (11%)	47,47,47	1.10	4 (8%)
31	LMT	K	105	-	36,36,36	1.20	6 (16%)	47,47,47	1.22	5 (10%)
33	LHG	e	102	-	39,39,48	1.03	2 (5%)	42,45,54	1.12	3 (7%)
34	DGD	C	516	-	63,63,67	1.33	8 (12%)	77,77,81	0.93	2 (2%)
30	SQD	h	103	-	52,54,54	0.94	3 (5%)	62,65,65	1.53	8 (12%)
25	CLA	b	606	2	64,68,73	2.34	23 (35%)	76,107,113	2.49	28 (36%)
31	LMT	C	525	-	21,21,36	1.01	1 (4%)	26,26,47	1.28	2 (7%)
31	LMT	f	103	-	36,36,36	1.20	6 (16%)	47,47,47	1.02	2 (4%)
25	CLA	c	503	3	69,73,73	2.19	20 (28%)	82,113,113	2.42	28 (34%)
33	LHG	b	628	-	48,48,48	0.93	2 (4%)	51,54,54	1.00	3 (5%)
26	PHO	d	402	-	58,69,69	2.18	10 (17%)	55,99,99	1.71	10 (18%)
25	CLA	b	604	2	69,73,73	2.19	20 (28%)	82,113,113	2.49	30 (36%)
27	BCR	B	619	-	41,41,41	2.70	6 (14%)	56,56,56	6.55	22 (39%)
25	CLA	a	406	38	69,73,73	2.24	23 (33%)	82,113,113	2.53	26 (31%)
32	BCT	A	417	-	3,3,3	1.15	0	2,3,3	4.18	2 (100%)
33	LHG	E	102	-	39,39,48	1.03	2 (5%)	42,45,54	1.12	3 (7%)
30	SQD	c	501	-	52,54,54	0.94	4 (7%)	62,65,65	1.63	9 (14%)
25	CLA	B	609	2	69,73,73	2.25	21 (30%)	82,113,113	2.42	24 (29%)
31	LMT	d	411	-	36,36,36	1.17	5 (13%)	47,47,47	0.92	0
25	CLA	C	507	3	69,73,73	2.23	22 (31%)	82,113,113	2.44	26 (31%)
31	LMT	A	415	-	36,36,36	1.19	5 (13%)	47,47,47	1.01	3 (6%)
25	CLA	B	612	2	69,73,73	2.23	21 (30%)	82,113,113	2.44	27 (32%)
31	LMT	B	625	-	36,36,36	1.23	6 (16%)	47,47,47	1.06	1 (2%)
25	CLA	b	603	2	69,73,73	2.24	20 (28%)	82,113,113	2.41	27 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	b	613	2	69,73,73	2.15	22 (31%)	82,113,113	2.53	26 (31%)
31	LMT	b	624	-	24,24,36	1.04	3 (12%)	29,29,47	0.90	0
27	BCR	Z	101	-	41,41,41	2.64	6 (14%)	56,56,56	6.49	20 (35%)
25	CLA	B	607	38	69,73,73	2.18	22 (31%)	82,113,113	2.50	28 (34%)
25	CLA	B	603	2	69,73,73	2.24	20 (28%)	82,113,113	2.41	27 (32%)
31	LMT	B	626	-	24,24,36	1.01	2 (8%)	29,29,47	0.91	0
28	LMG	C	519	-	51,51,55	1.47	8 (15%)	59,59,63	1.12	3 (5%)
27	BCR	f	101	-	41,41,41	2.60	6 (14%)	56,56,56	6.63	22 (39%)
31	LMT	m	101	-	36,36,36	1.17	6 (16%)	47,47,47	1.04	2 (4%)
31	LMT	X	101	-	24,24,36	1.05	2 (8%)	29,29,47	1.06	1 (3%)
30	SQD	a	412	-	52,54,54	0.96	3 (5%)	62,65,65	1.69	15 (24%)
31	LMT	b	626	-	24,24,36	1.01	2 (8%)	29,29,47	0.90	0
25	CLA	b	611	2	69,73,73	2.19	20 (28%)	82,113,113	2.40	26 (31%)
25	CLA	c	505	38	69,73,73	2.18	21 (30%)	82,113,113	2.54	29 (35%)
25	CLA	c	513	3	54,58,73	2.51	21 (38%)	64,95,113	2.75	21 (32%)
29	PL9	a	411	-	55,55,55	1.10	4 (7%)	68,69,69	1.46	11 (16%)
25	CLA	B	602	2	69,73,73	2.20	21 (30%)	82,113,113	2.45	26 (31%)
31	LMT	B	623	-	36,36,36	1.18	4 (11%)	47,47,47	1.10	4 (8%)
31	LMT	k	105	-	36,36,36	1.20	6 (16%)	47,47,47	1.22	5 (10%)
35	HEM	V	201	18	50,50,50	1.78	14 (28%)	67,82,82	1.90	12 (17%)
25	CLA	C	502	3	69,73,73	2.22	22 (31%)	82,113,113	2.50	28 (34%)
31	LMT	F	103	-	36,36,36	1.20	6 (16%)	47,47,47	1.02	2 (4%)
31	LMT	a	416	-	24,24,36	1.06	3 (12%)	29,29,47	1.00	1 (3%)
25	CLA	c	509	3	69,73,73	2.22	22 (31%)	82,113,113	2.33	26 (31%)
25	CLA	A	406	38	69,73,73	2.24	22 (31%)	82,113,113	2.53	26 (31%)
29	PL9	A	411	-	55,55,55	1.10	4 (7%)	68,69,69	1.46	11 (16%)
31	LMT	c	525	-	21,21,36	1.00	1 (4%)	26,26,47	1.28	2 (7%)
27	BCR	A	409	-	41,41,41	2.64	6 (14%)	56,56,56	6.48	20 (35%)
25	CLA	C	511	3	69,73,73	2.21	21 (30%)	82,113,113	2.52	30 (36%)
33	LHG	D	407	-	48,48,48	0.91	2 (4%)	51,54,54	1.07	4 (7%)
25	CLA	B	606	2	64,68,73	2.34	23 (35%)	76,107,113	2.48	28 (36%)
28	LMG	c	523	-	49,49,55	1.44	6 (12%)	57,57,63	1.22	4 (7%)
25	CLA	C	504	3	69,73,73	2.25	23 (33%)	82,113,113	2.51	28 (34%)
27	BCR	k	102	-	41,41,41	2.61	6 (14%)	56,56,56	6.89	21 (37%)
33	LHG	d	406	-	48,48,48	0.92	3 (6%)	51,54,54	0.99	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	DGD	h	104	-	63,63,67	1.34	8 (12%)	77,77,81	0.97	3 (3%)
35	HEM	E	104	5,6	50,50,50	1.62	9 (18%)	67,82,82	1.68	13 (19%)
25	CLA	D	403	4	69,73,73	2.19	21 (30%)	82,113,113	2.55	25 (30%)
33	LHG	b	627	-	48,48,48	0.94	2 (4%)	51,54,54	1.06	2 (3%)
25	CLA	D	404	4	69,73,73	2.22	23 (33%)	82,113,113	2.49	26 (31%)
25	CLA	B	601	38	49,53,73	2.53	23 (46%)	58,89,113	2.86	23 (39%)
34	DGD	C	518	-	63,63,67	1.33	8 (12%)	77,77,81	1.05	3 (3%)
25	CLA	a	405	1	69,73,73	2.16	21 (30%)	82,113,113	2.48	27 (32%)
33	LHG	D	408	-	48,48,48	0.91	2 (4%)	51,54,54	0.96	2 (3%)
25	CLA	C	514	3	69,73,73	2.25	22 (31%)	82,113,113	2.41	26 (31%)
31	LMT	i	103	-	36,36,36	1.19	5 (13%)	47,47,47	0.93	1 (2%)
25	CLA	b	615	2	69,73,73	2.18	21 (30%)	82,113,113	2.56	28 (34%)
35	HEM	e	104	5,6	50,50,50	1.62	9 (18%)	67,82,82	1.68	13 (19%)
25	CLA	C	503	3	69,73,73	2.19	20 (28%)	82,113,113	2.42	28 (34%)
28	LMG	b	621	-	51,51,55	1.46	8 (15%)	59,59,63	1.03	2 (3%)
29	PL9	d	405	-	55,55,55	1.20	5 (9%)	68,69,69	1.42	11 (16%)
30	SQD	H	103	-	52,54,54	0.94	3 (5%)	62,65,65	1.53	8 (12%)
27	BCR	K	103	-	41,41,41	2.64	6 (14%)	56,56,56	6.56	26 (46%)
25	CLA	a	408	1	64,68,73	2.31	22 (34%)	76,107,113	2.61	25 (32%)
25	CLA	B	616	2	64,68,73	2.26	21 (32%)	76,107,113	2.62	27 (35%)
25	CLA	C	509	3	69,73,73	2.22	22 (31%)	82,113,113	2.33	26 (31%)
25	CLA	D	401	38	69,73,73	2.20	22 (31%)	82,113,113	2.50	26 (31%)
26	PHO	D	402	-	58,69,69	2.18	10 (17%)	55,99,99	1.70	10 (18%)
36	RRX	h	101	-	42,42,42	1.33	8 (19%)	56,58,58	1.39	9 (16%)
31	LMT	D	412	-	36,36,36	1.17	5 (13%)	47,47,47	0.95	1 (2%)
31	LMT	D	410	-	24,24,36	0.99	2 (8%)	29,29,47	1.21	4 (13%)
28	LMG	H	105	-	47,47,55	1.41	6 (12%)	55,55,63	1.39	7 (12%)
31	LMT	I	104	-	22,22,36	1.05	2 (9%)	27,27,47	1.05	0
22	OEX	A	401	3,1,38	0,14,14	-	-	-	-	-
25	CLA	A	405	1	69,73,73	2.16	21 (30%)	82,113,113	2.48	27 (32%)
28	LMG	c	519	-	51,51,55	1.47	8 (15%)	59,59,63	1.12	3 (5%)
30	SQD	A	412	-	52,54,54	0.96	3 (5%)	62,65,65	1.69	15 (24%)
31	LMT	D	411	-	36,36,36	1.17	5 (13%)	47,47,47	0.92	0
22	OEX	a	401	3,1,38	0,14,14	-	-	-	-	-
25	CLA	B	611	2	69,73,73	2.19	20 (28%)	82,113,113	2.40	26 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	DGD	C	517	-	63,63,67	1.33	8 (12%)	77,77,81	1.08	5 (6%)
31	LMT	T	101	-	24,24,36	1.09	2 (8%)	29,29,47	1.16	2 (6%)
31	LMT	a	415	-	36,36,36	1.19	5 (13%)	47,47,47	1.01	3 (6%)
28	LMG	a	414	-	36,36,55	1.12	2 (5%)	44,44,63	1.19	3 (6%)
25	CLA	b	610	38	69,73,73	2.26	22 (31%)	82,113,113	2.47	32 (39%)

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
28	LMG	d	409	-	-	14/38/58/70	0/1/1/1
33	LHG	d	408	-	-	24/53/53/53	-
30	SQD	b	620	-	-	24/49/69/69	0/1/1/1
25	CLA	b	614	2	-	14/39/115/115	-
29	PL9	D	405	-	-	9/53/73/73	0/1/1/1
25	CLA	c	514	3	-	17/39/115/115	-
31	LMT	c	524	-	-	10/21/61/61	0/2/2/2
25	CLA	c	504	3	-	5/39/115/115	-
27	BCR	b	618	-	-	6/29/63/63	0/2/2/2
25	CLA	b	608	2	-	8/39/115/115	-
31	LMT	e	101	-	-	5/13/33/61	0/1/1/2
25	CLA	c	502	3	-	12/39/115/115	-
31	LMT	X	103	-	-	3/13/33/61	0/1/1/2
31	LMT	x	105	-	-	6/10/30/61	0/1/1/2
33	LHG	z	102	-	-	24/37/37/53	-
31	LMT	M	102	-	-	4/15/35/61	0/1/1/2
25	CLA	d	401	38	-	10/39/115/115	-
25	CLA	b	616	2	-	16/33/109/115	-
25	CLA	c	506	3	-	11/27/103/115	-
27	BCR	C	515	-	-	9/29/63/63	0/2/2/2
31	LMT	E	103	-	-	9/21/61/61	0/2/2/2
25	CLA	c	512	3	-	19/39/115/115	-
31	LMT	C	522	-	-	7/15/35/61	0/1/1/2
33	LHG	B	627	-	-	30/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	i	104	-	-	9/13/33/61	0/1/1/2
25	CLA	C	506	3	-	11/27/103/115	-
27	BCR	B	618	-	-	6/29/63/63	0/2/2/2
25	CLA	B	613	2	-	8/39/115/115	-
25	CLA	b	607	38	-	11/39/115/115	-
28	LMG	D	409	-	-	14/38/58/70	0/1/1/1
25	CLA	C	512	3	-	19/39/115/115	-
31	LMT	y	101	-	-	7/12/32/61	0/1/1/2
30	SQD	A	413	-	-	22/43/63/69	0/1/1/1
25	CLA	C	508	38	-	12/39/115/115	-
25	CLA	C	505	38	-	13/39/115/115	-
33	LHG	B	628	-	-	24/53/53/53	-
30	SQD	B	620	-	-	24/49/69/69	0/1/1/1
31	LMT	E	101	-	-	5/13/33/61	0/1/1/2
31	LMT	X	105	-	-	6/10/30/61	0/1/1/2
25	CLA	B	604	2	-	11/39/115/115	-
31	LMT	i	102	-	-	8/15/35/61	0/1/1/2
31	LMT	x	101	-	-	6/15/35/61	0/1/1/2
33	LHG	Z	102	-	-	24/37/37/53	-
27	BCR	F	101	-	-	9/29/63/63	0/2/2/2
28	LMG	C	523	-	-	17/44/64/70	0/1/1/1
25	CLA	b	612	2	-	10/39/115/115	-
31	LMT	x	104	-	-	7/10/30/61	0/1/1/2
28	LMG	A	414	-	-	6/31/51/70	0/1/1/1
31	LMT	A	416	-	-	5/15/35/61	0/1/1/2
31	LMT	h	102	-	-	9/15/35/61	0/1/1/2
25	CLA	B	605	2	-	11/39/115/115	-
31	LMT	B	624	-	-	9/15/35/61	0/1/1/2
25	CLA	B	614	2	-	14/39/115/115	-
25	CLA	A	408	1	-	14/33/109/115	-
25	CLA	b	605	2	-	11/39/115/115	-
25	CLA	b	601	38	-	3/15/91/115	-
33	LHG	D	406	-	-	24/53/53/53	-
31	LMT	X	102	-	-	9/12/32/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PHO	a	407	-	-	7/37/103/103	0/5/6/6
31	LMT	H	102	-	-	9/15/35/61	0/1/1/2
27	BCR	k	103	-	-	8/29/63/63	0/2/2/2
31	LMT	e	103	-	-	9/21/61/61	0/2/2/2
25	CLA	C	513	3	-	7/21/97/115	-
30	SQD	k	101	-	-	21/35/55/69	0/1/1/1
31	LMT	I	101	-	-	11/15/35/61	0/1/1/2
31	LMT	x	103	-	-	3/13/33/61	0/1/1/2
30	SQD	a	413	-	-	22/43/63/69	0/1/1/1
31	LMT	b	625	-	-	11/21/61/61	0/2/2/2
31	LMT	t	101	-	-	11/15/35/61	0/1/1/2
27	BCR	b	619	-	-	11/29/63/63	0/2/2/2
27	BCR	B	617	-	-	6/29/63/63	0/2/2/2
31	LMT	C	524	-	-	10/21/61/61	0/2/2/2
35	HEM	v	201	18	-	2/14/54/54	-
31	LMT	d	410	-	-	8/15/35/61	0/1/1/2
27	BCR	K	102	-	-	15/29/63/63	0/2/2/2
25	CLA	c	510	3	-	11/39/115/115	-
25	CLA	c	507	3	-	16/39/115/115	-
31	LMT	I	102	-	-	8/15/35/61	0/1/1/2
36	RRX	H	101	-	-	15/29/65/65	0/2/2/2
28	LMG	A	410	-	-	22/46/66/70	0/1/1/1
31	LMT	M	101	-	-	10/21/61/61	0/2/2/2
27	BCR	c	515	-	-	9/29/63/63	0/2/2/2
31	LMT	m	102	-	-	4/15/35/61	0/1/1/2
25	CLA	d	403	4	-	9/39/115/115	-
25	CLA	C	510	3	-	11/39/115/115	-
25	CLA	c	508	38	-	12/39/115/115	-
28	LMG	a	410	-	-	22/46/66/70	0/1/1/1
31	LMT	c	522	-	-	7/15/35/61	0/1/1/2
31	LMT	I	103	-	-	7/21/61/61	0/2/2/2
28	LMG	B	621	-	-	7/46/66/70	0/1/1/1
25	CLA	B	610	38	-	10/39/115/115	-
33	LHG	d	407	-	-	25/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	d	404	4	-	13/39/115/115	-
31	LMT	Y	101	-	-	7/12/32/61	0/1/1/2
27	BCR	z	101	-	-	8/29/63/63	0/2/2/2
31	LMT	d	412	-	-	7/21/61/61	0/2/2/2
31	LMT	x	102	-	-	9/12/32/61	0/1/1/2
25	CLA	B	608	2	-	8/39/115/115	-
25	CLA	c	511	3	-	11/39/115/115	-
30	SQD	K	101	-	-	21/35/55/69	0/1/1/1
31	LMT	j	101	-	-	11/15/35/61	0/1/1/2
25	CLA	b	609	2	-	14/39/115/115	-
34	DGD	H	104	-	-	11/51/91/95	0/2/2/2
34	DGD	c	516	-	-	14/51/91/95	0/2/2/2
34	DGD	c	518	-	-	16/51/91/95	0/2/2/2
30	SQD	C	501	-	-	28/49/69/69	0/1/1/1
28	LMG	h	105	-	-	17/42/62/70	0/1/1/1
26	PHO	A	407	-	-	7/37/103/103	0/5/6/6
31	LMT	J	101	-	-	11/15/35/61	0/1/1/2
31	LMT	i	101	-	-	11/15/35/61	0/1/1/2
30	SQD	F	102	-	-	16/29/49/69	0/1/1/1
30	SQD	f	102	-	-	16/29/49/69	0/1/1/1
34	DGD	c	517	-	-	17/51/91/95	0/2/2/2
27	BCR	a	409	-	-	9/29/63/63	0/2/2/2
31	LMT	B	629	-	-	10/21/61/61	0/2/2/2
25	CLA	B	615	2	-	12/39/115/115	-
31	LMT	b	629	-	-	10/21/61/61	0/2/2/2
25	CLA	b	602	2	-	17/39/115/115	-
27	BCR	b	617	-	-	6/29/63/63	0/2/2/2
31	LMT	X	104	-	-	7/10/30/61	0/1/1/2
31	LMT	b	623	-	-	11/21/61/61	0/2/2/2
31	LMT	K	105	-	-	13/21/61/61	0/2/2/2
33	LHG	e	102	-	-	29/44/44/53	-
34	DGD	C	516	-	-	14/51/91/95	0/2/2/2
30	SQD	h	103	-	-	16/49/69/69	0/1/1/1
25	CLA	b	606	2	-	9/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	C	525	-	-	8/12/32/61	0/1/1/2
31	LMT	f	103	-	-	11/21/61/61	0/2/2/2
25	CLA	c	503	3	-	9/39/115/115	-
33	LHG	b	628	-	-	24/53/53/53	-
26	PHO	d	402	-	-	4/37/103/103	0/5/6/6
25	CLA	b	604	2	-	11/39/115/115	-
27	BCR	B	619	-	-	11/29/63/63	0/2/2/2
25	CLA	a	406	38	-	11/39/115/115	-
33	LHG	E	102	-	-	29/44/44/53	-
30	SQD	c	501	-	-	28/49/69/69	0/1/1/1
25	CLA	B	609	2	-	14/39/115/115	-
31	LMT	d	411	-	-	10/21/61/61	0/2/2/2
25	CLA	C	507	3	-	16/39/115/115	-
31	LMT	A	415	-	-	10/21/61/61	0/2/2/2
25	CLA	B	612	2	-	10/39/115/115	-
31	LMT	B	625	-	-	11/21/61/61	0/2/2/2
25	CLA	b	603	2	-	17/39/115/115	-
25	CLA	b	613	2	-	8/39/115/115	-
31	LMT	b	624	-	-	9/15/35/61	0/1/1/2
27	BCR	Z	101	-	-	8/29/63/63	0/2/2/2
25	CLA	B	607	38	-	11/39/115/115	-
25	CLA	B	603	2	-	17/39/115/115	-
31	LMT	B	626	-	-	5/15/35/61	0/1/1/2
28	LMG	C	519	-	-	17/46/66/70	0/1/1/1
27	BCR	f	101	-	-	9/29/63/63	0/2/2/2
31	LMT	m	101	-	-	10/21/61/61	0/2/2/2
31	LMT	X	101	-	-	6/15/35/61	0/1/1/2
30	SQD	a	412	-	-	26/49/69/69	0/1/1/1
31	LMT	b	626	-	-	5/15/35/61	0/1/1/2
25	CLA	b	611	2	-	9/39/115/115	-
25	CLA	c	505	38	-	13/39/115/115	-
25	CLA	c	513	3	-	7/21/97/115	-
29	PL9	a	411	-	-	18/53/73/73	0/1/1/1
25	CLA	B	602	2	-	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	B	623	-	-	11/21/61/61	0/2/2/2
31	LMT	k	105	-	-	13/21/61/61	0/2/2/2
35	HEM	V	201	18	-	2/14/54/54	-
25	CLA	C	502	3	-	12/39/115/115	-
31	LMT	F	103	-	-	11/21/61/61	0/2/2/2
31	LMT	a	416	-	-	5/15/35/61	0/1/1/2
25	CLA	c	509	3	-	9/39/115/115	-
25	CLA	A	406	38	-	11/39/115/115	-
29	PL9	A	411	-	-	18/53/73/73	0/1/1/1
31	LMT	c	525	-	-	8/12/32/61	0/1/1/2
27	BCR	A	409	-	-	9/29/63/63	0/2/2/2
25	CLA	C	511	3	-	11/39/115/115	-
33	LHG	D	407	-	-	25/53/53/53	-
25	CLA	B	606	2	-	9/33/109/115	-
28	LMG	c	523	-	-	17/44/64/70	0/1/1/1
25	CLA	C	504	3	-	6/39/115/115	-
27	BCR	k	102	-	-	15/29/63/63	0/2/2/2
33	LHG	d	406	-	-	24/53/53/53	-
34	DGD	h	104	-	-	11/51/91/95	0/2/2/2
35	HEM	E	104	5,6	-	7/14/54/54	-
25	CLA	D	403	4	-	9/39/115/115	-
33	LHG	b	627	-	-	30/53/53/53	-
25	CLA	D	404	4	-	13/39/115/115	-
25	CLA	B	601	38	-	3/15/91/115	-
34	DGD	C	518	-	-	16/51/91/95	0/2/2/2
25	CLA	a	405	1	-	9/39/115/115	-
33	LHG	D	408	-	-	24/53/53/53	-
25	CLA	C	514	3	-	17/39/115/115	-
31	LMT	i	103	-	-	7/21/61/61	0/2/2/2
25	CLA	b	615	2	-	12/39/115/115	-
35	HEM	e	104	5,6	-	7/14/54/54	-
25	CLA	C	503	3	-	9/39/115/115	-
28	LMG	b	621	-	-	7/46/66/70	0/1/1/1
29	PL9	d	405	-	-	9/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	SQD	H	103	-	-	16/49/69/69	0/1/1/1
27	BCR	K	103	-	-	8/29/63/63	0/2/2/2
25	CLA	a	408	1	-	14/33/109/115	-
25	CLA	B	616	2	-	16/33/109/115	-
25	CLA	C	509	3	-	9/39/115/115	-
25	CLA	D	401	38	-	9/39/115/115	-
26	PHO	D	402	-	-	4/37/103/103	0/5/6/6
36	RRX	h	101	-	-	15/29/65/65	0/2/2/2
31	LMT	D	412	-	-	7/21/61/61	0/2/2/2
31	LMT	D	410	-	-	8/15/35/61	0/1/1/2
28	LMG	H	105	-	-	17/42/62/70	0/1/1/1
31	LMT	I	104	-	-	9/13/33/61	0/1/1/2
25	CLA	A	405	1	-	9/39/115/115	-
28	LMG	c	519	-	-	17/46/66/70	0/1/1/1
30	SQD	A	412	-	-	26/49/69/69	0/1/1/1
31	LMT	D	411	-	-	10/21/61/61	0/2/2/2
25	CLA	B	611	2	-	9/39/115/115	-
34	DGD	C	517	-	-	17/51/91/95	0/2/2/2
31	LMT	T	101	-	-	11/15/35/61	0/1/1/2
31	LMT	a	415	-	-	10/21/61/61	0/2/2/2
28	LMG	a	414	-	-	6/31/51/70	0/1/1/1
25	CLA	b	610	38	-	10/39/115/115	-

The worst 5 of 2179 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D	402	PHO	C3B-C4B	9.27	1.50	1.41
26	d	402	PHO	C3B-C4B	9.27	1.50	1.41
26	D	402	PHO	C1B-C2B	9.24	1.49	1.39
26	d	402	PHO	C1B-C2B	9.24	1.49	1.39
26	A	407	PHO	C1B-C2B	9.12	1.49	1.39

The worst 5 of 2764 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	k	102	BCR	C16-C17-C18	23.42	160.12	127.28
27	K	102	BCR	C16-C17-C18	23.40	160.10	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	K	102	BCR	C20-C21-C22	23.22	159.84	127.28
27	k	102	BCR	C20-C21-C22	23.20	159.81	127.28
27	C	515	BCR	C20-C21-C22	21.80	157.85	127.28

There are no chirality outliers.

5 of 2598 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	405	CLA	CBD-CGD-O2D-CED
25	B	601	CLA	C1A-C2A-CAA-CBA
25	B	601	CLA	C3A-C2A-CAA-CBA
25	B	606	CLA	C2B-C3B-CAB-CBB
25	B	606	CLA	C4B-C3B-CAB-CBB

There are no ring outliers.

178 monomers are involved in 523 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	d	408	LHG	6	0
30	b	620	SQD	2	0
25	b	614	CLA	5	0
29	D	405	PL9	2	0
25	c	514	CLA	3	0
25	c	504	CLA	6	0
27	b	618	BCR	1	0
25	b	608	CLA	5	0
31	e	101	LMT	1	0
25	c	502	CLA	4	0
31	X	103	LMT	2	0
33	z	102	LHG	1	0
31	M	102	LMT	2	0
25	d	401	CLA	4	0
25	b	616	CLA	4	0
25	c	506	CLA	5	0
27	C	515	BCR	4	0
31	E	103	LMT	3	0
25	c	512	CLA	7	0
33	B	627	LHG	8	0
25	C	506	CLA	5	0
27	B	618	BCR	1	0
25	B	613	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	b	607	CLA	6	0
28	D	409	LMG	1	0
25	C	512	CLA	9	0
31	y	101	LMT	2	0
30	A	413	SQD	1	0
25	C	508	CLA	4	0
25	C	505	CLA	4	0
33	B	628	LHG	4	0
30	B	620	SQD	2	0
31	E	101	LMT	1	0
25	B	604	CLA	4	0
33	Z	102	LHG	1	0
27	F	101	BCR	3	0
25	b	612	CLA	4	0
28	A	414	LMG	2	0
31	h	102	LMT	2	0
25	B	605	CLA	6	0
31	B	624	LMT	1	0
25	B	614	CLA	6	0
25	A	408	CLA	7	0
25	b	605	CLA	5	0
25	b	601	CLA	2	0
33	D	406	LHG	2	0
31	X	102	LMT	3	0
26	a	407	PHO	6	0
31	H	102	LMT	1	0
27	k	103	BCR	4	0
31	e	103	LMT	3	0
25	C	513	CLA	1	0
30	k	101	SQD	4	0
31	I	101	LMT	1	0
31	x	103	LMT	2	0
30	a	413	SQD	1	0
31	t	101	LMT	1	0
27	b	619	BCR	1	0
27	B	617	BCR	4	0
35	v	201	HEM	3	0
31	d	410	LMT	3	0
27	K	102	BCR	5	0
25	c	507	CLA	3	0
31	I	102	LMT	2	0
36	H	101	RRX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	A	410	LMG	3	0
31	M	101	LMT	6	0
27	c	515	BCR	4	0
31	m	102	LMT	2	0
25	d	403	CLA	7	0
25	c	508	CLA	5	0
28	a	410	LMG	3	0
31	I	103	LMT	2	0
28	B	621	LMG	1	0
25	B	610	CLA	2	0
33	d	407	LHG	7	0
25	d	404	CLA	4	0
31	Y	101	LMT	2	0
27	z	101	BCR	3	0
31	d	412	LMT	1	0
31	x	102	LMT	3	0
25	B	608	CLA	6	0
25	c	511	CLA	6	0
30	K	101	SQD	4	0
25	b	609	CLA	7	0
34	H	104	DGD	4	0
34	c	516	DGD	6	0
34	c	518	DGD	5	0
30	C	501	SQD	4	0
26	A	407	PHO	5	0
31	i	101	LMT	1	0
34	c	517	DGD	5	0
27	a	409	BCR	4	0
25	B	615	CLA	3	0
25	b	602	CLA	2	0
27	b	617	BCR	4	0
31	b	623	LMT	3	0
31	K	105	LMT	8	0
33	e	102	LHG	2	0
34	C	516	DGD	7	0
30	h	103	SQD	2	0
25	b	606	CLA	1	0
31	C	525	LMT	1	0
31	f	103	LMT	2	0
25	c	503	CLA	4	0
33	b	628	LHG	4	0
26	d	402	PHO	1	0

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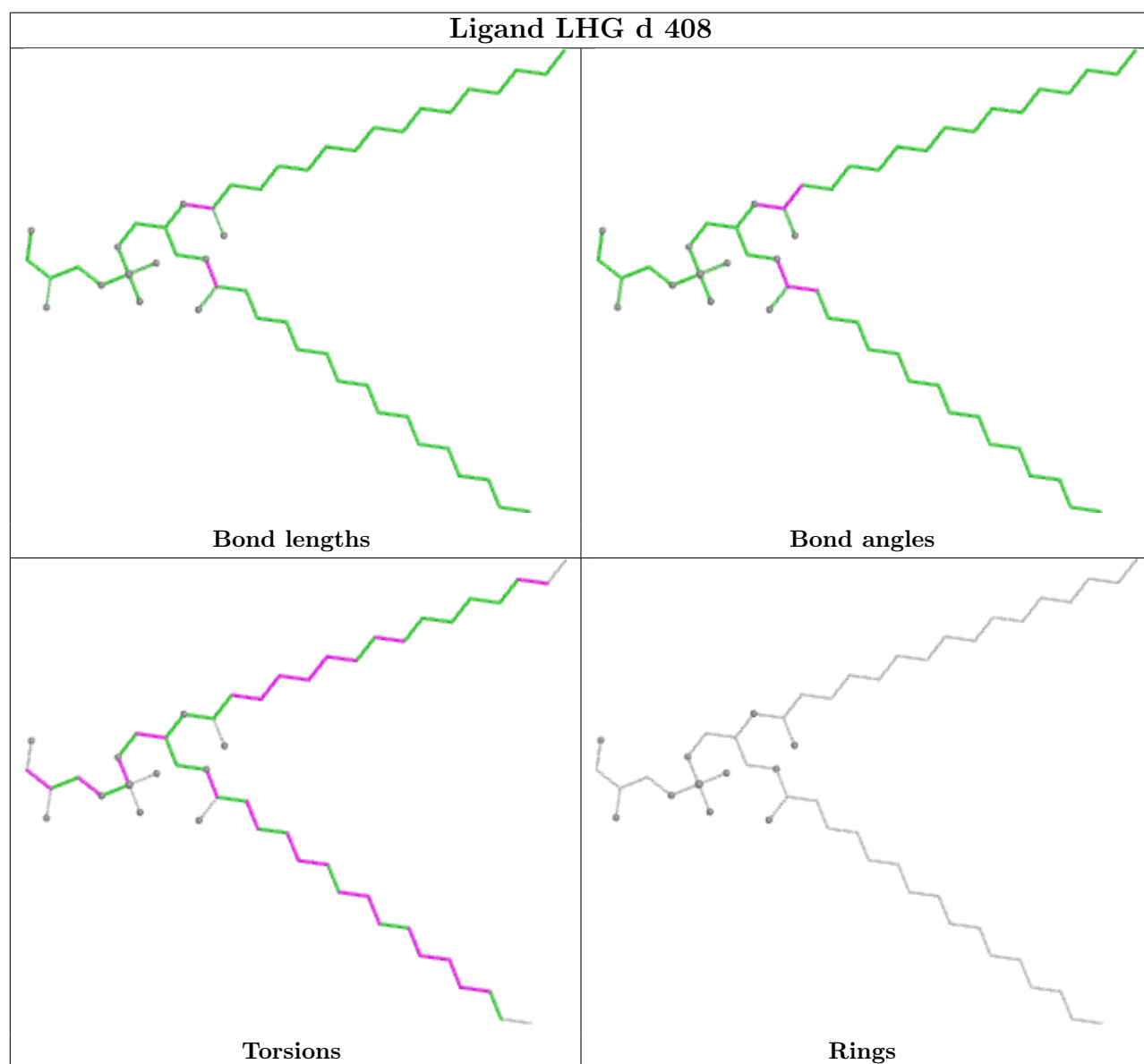
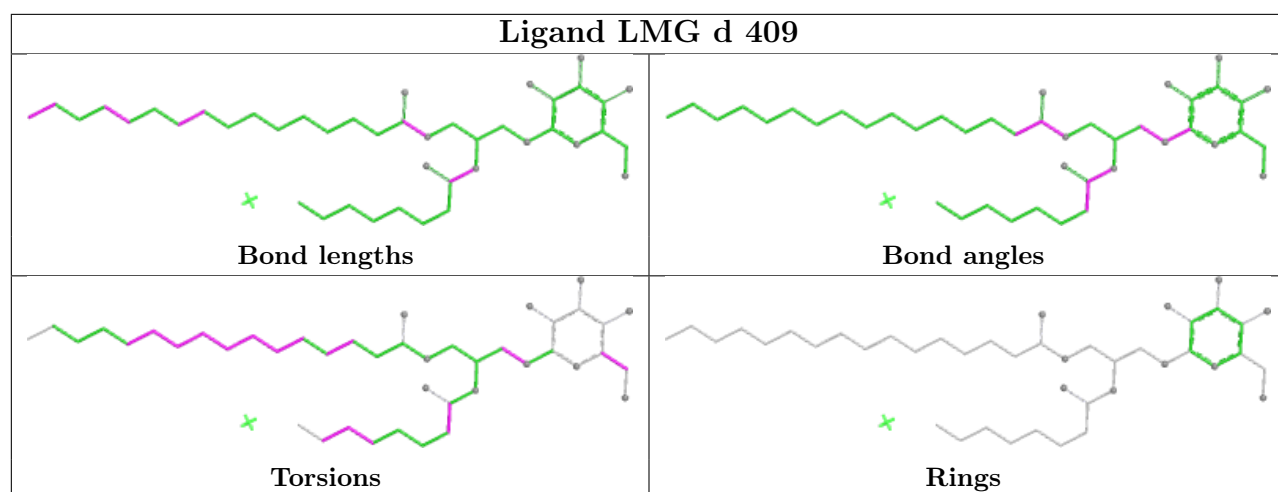
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	b	604	CLA	5	0
27	B	619	BCR	2	0
33	E	102	LHG	2	0
30	c	501	SQD	4	0
25	B	609	CLA	8	0
25	C	507	CLA	4	0
25	B	612	CLA	4	0
25	b	603	CLA	2	0
25	b	613	CLA	4	0
31	b	624	LMT	1	0
27	Z	101	BCR	2	0
25	B	607	CLA	6	0
25	B	603	CLA	2	0
28	C	519	LMG	7	0
27	f	101	BCR	4	0
31	m	101	LMT	7	0
30	a	412	SQD	3	0
25	b	611	CLA	3	0
25	c	505	CLA	3	0
25	c	513	CLA	1	0
29	a	411	PL9	8	0
25	B	602	CLA	2	0
31	B	623	LMT	4	0
31	k	105	LMT	8	0
35	V	201	HEM	3	0
25	C	502	CLA	3	0
31	F	103	LMT	2	0
25	c	509	CLA	7	0
29	A	411	PL9	8	0
31	c	525	LMT	1	0
27	A	409	BCR	4	0
25	C	511	CLA	6	0
33	D	407	LHG	7	0
25	B	606	CLA	1	0
25	C	504	CLA	7	0
27	k	102	BCR	5	0
33	d	406	LHG	2	0
34	h	104	DGD	4	0
35	E	104	HEM	7	0
25	D	403	CLA	6	0
33	b	627	LHG	7	0
25	D	404	CLA	2	0

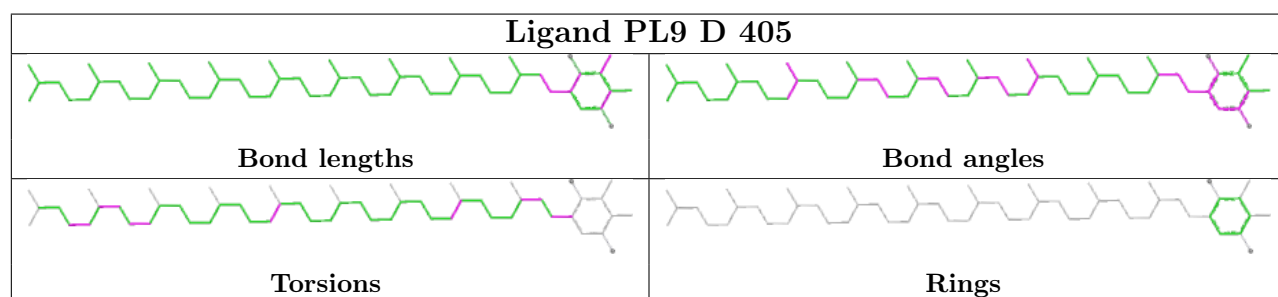
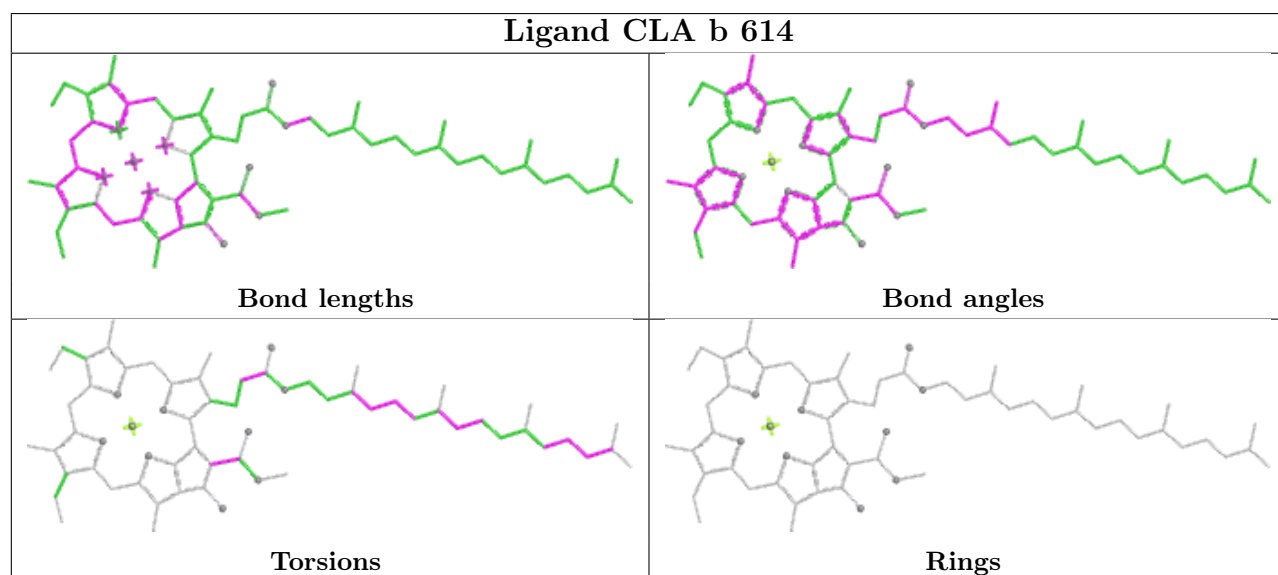
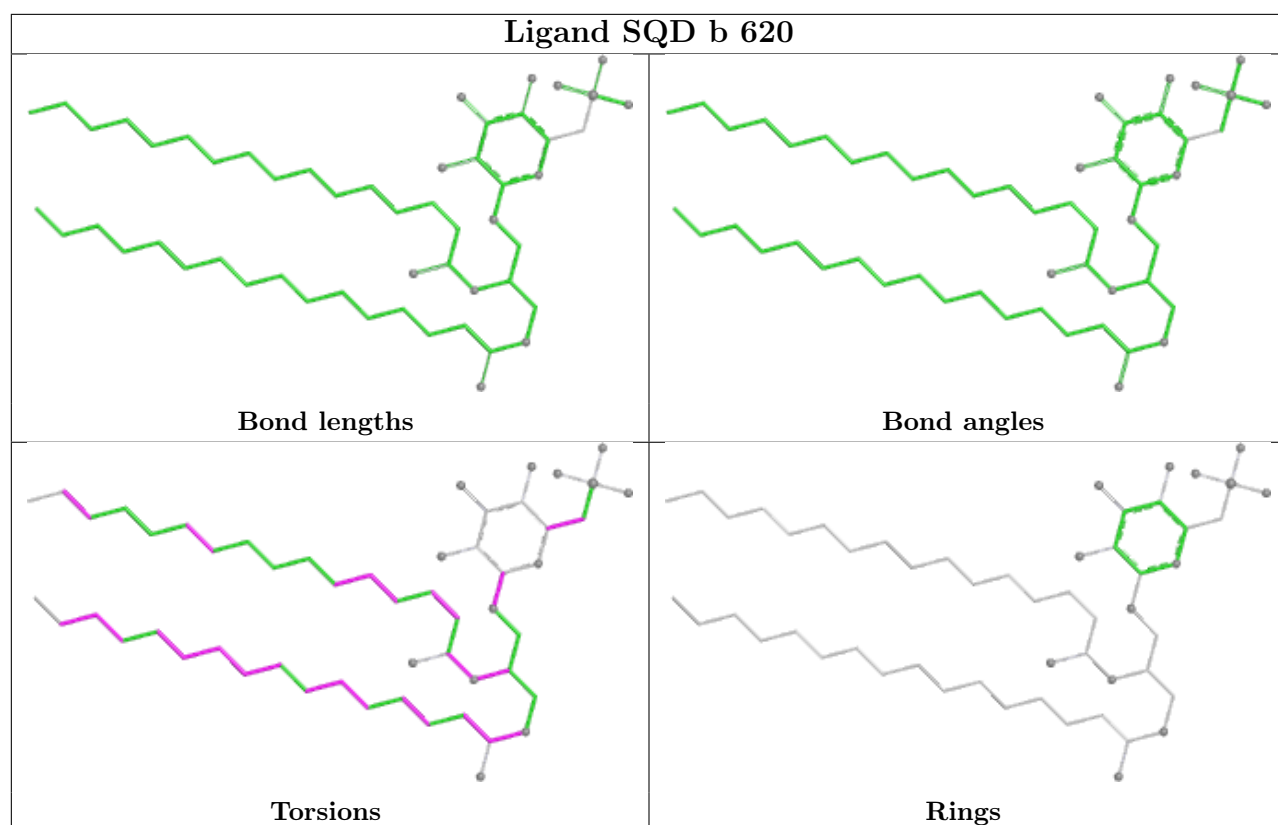
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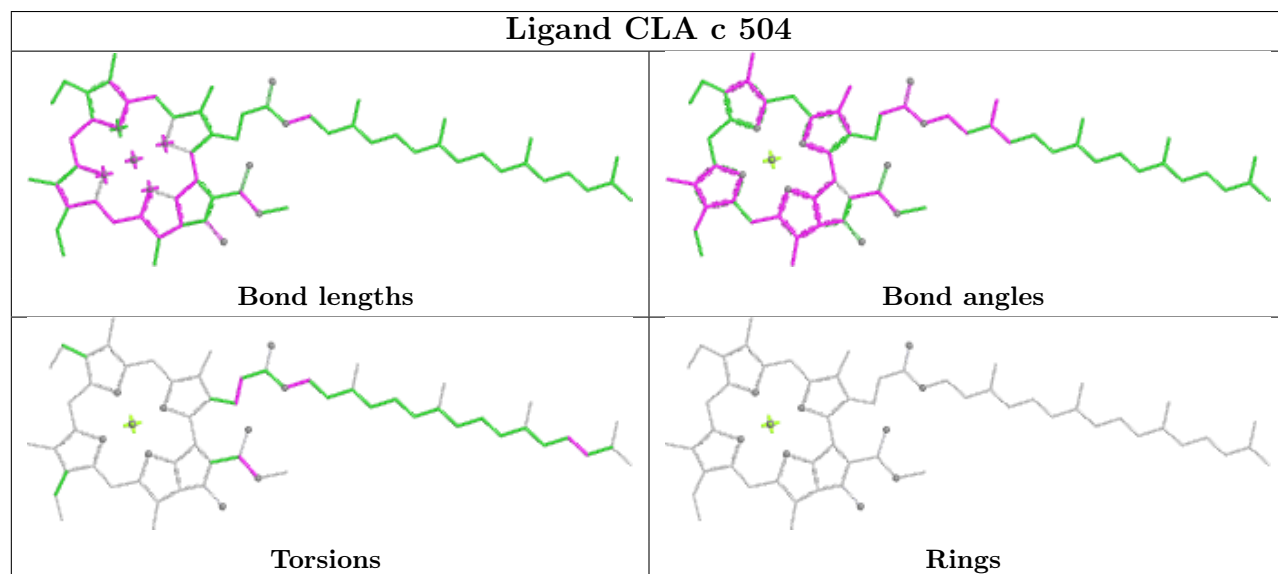
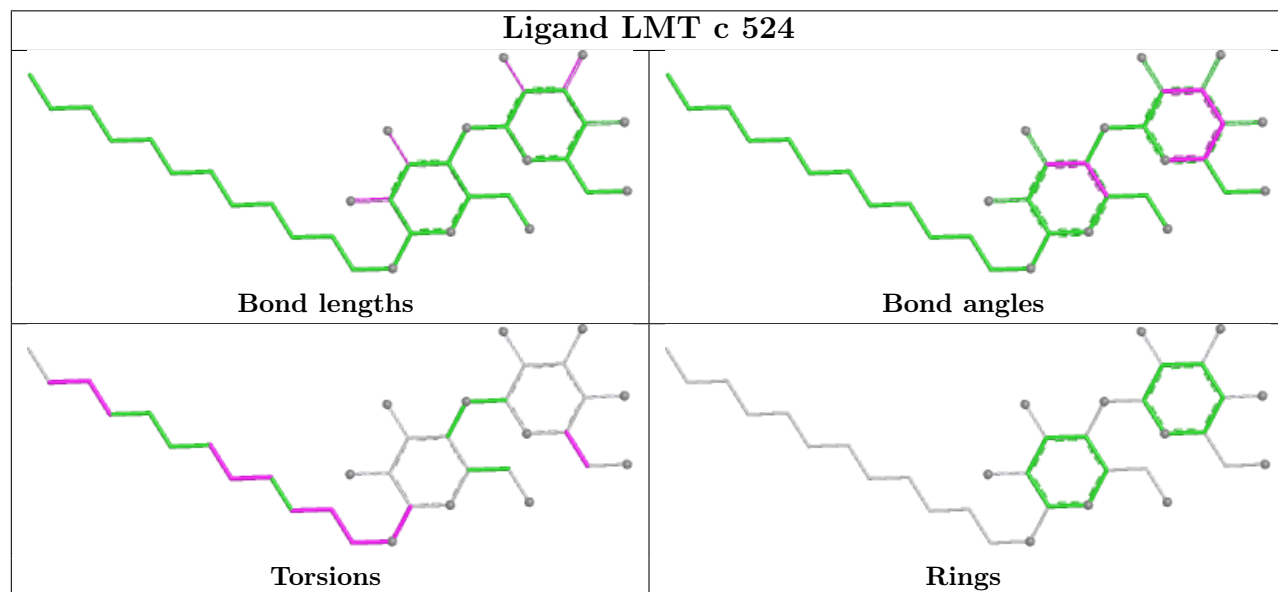
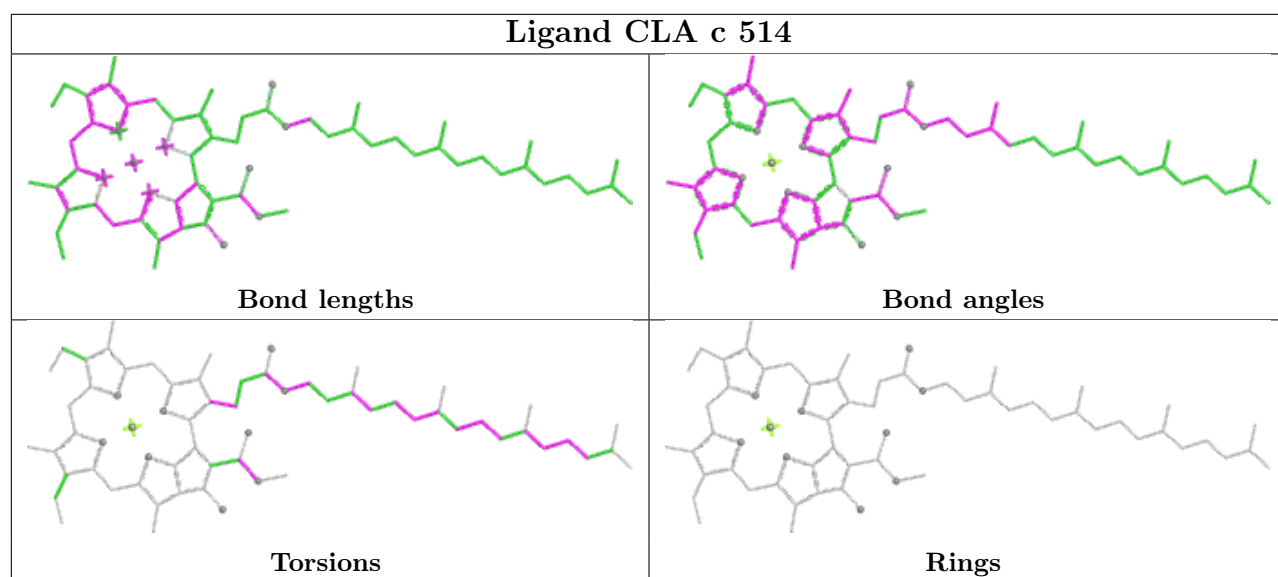
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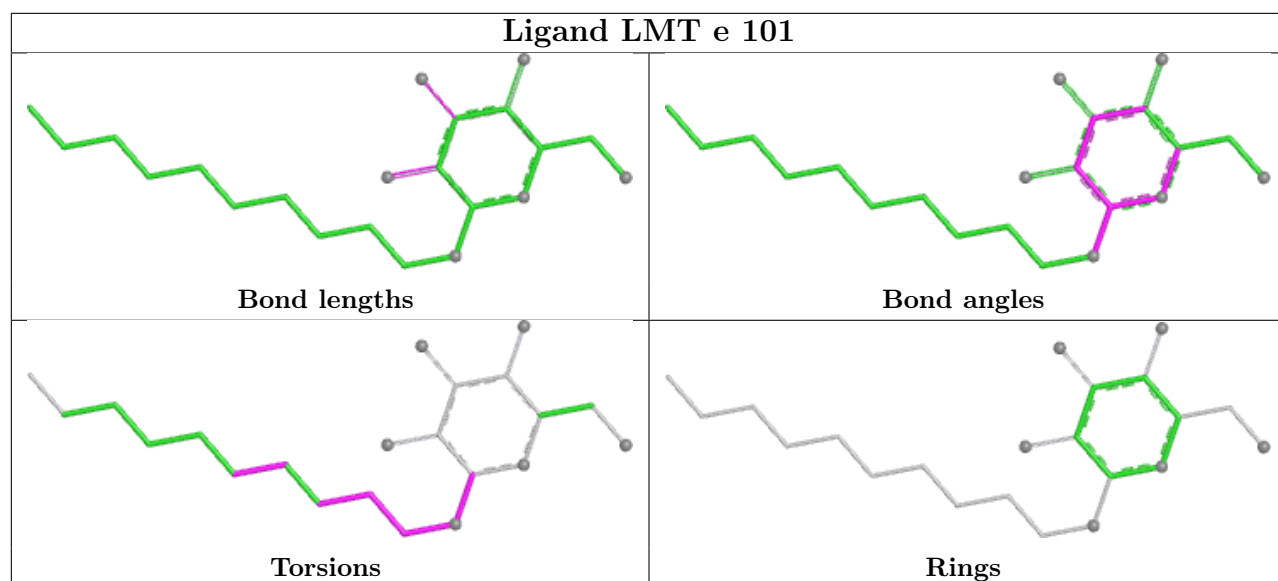
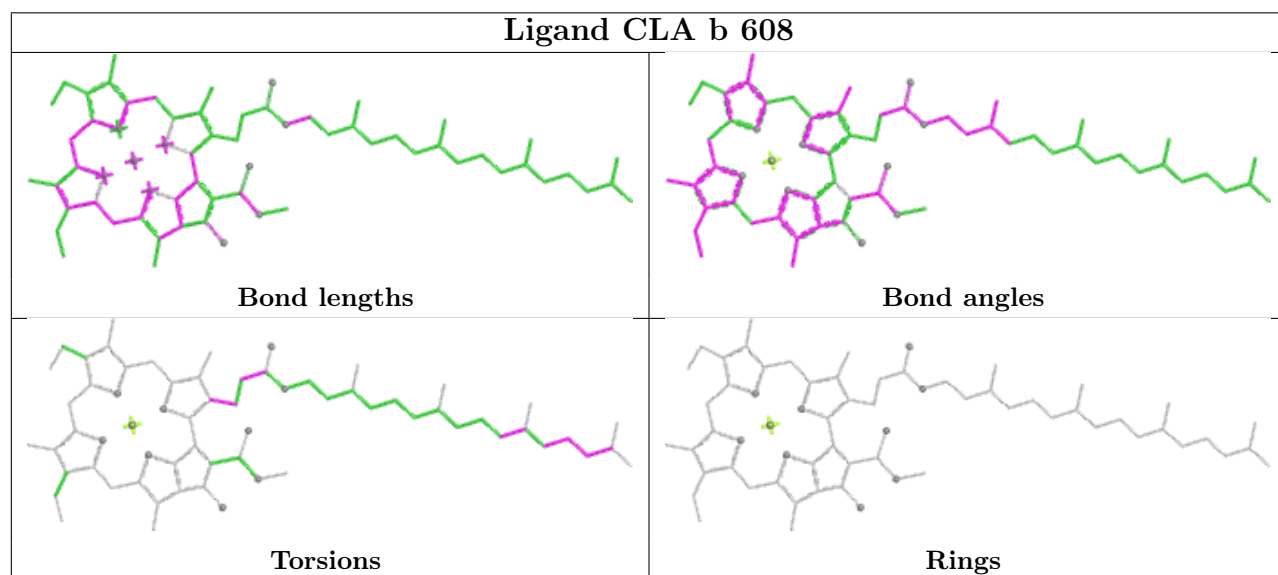
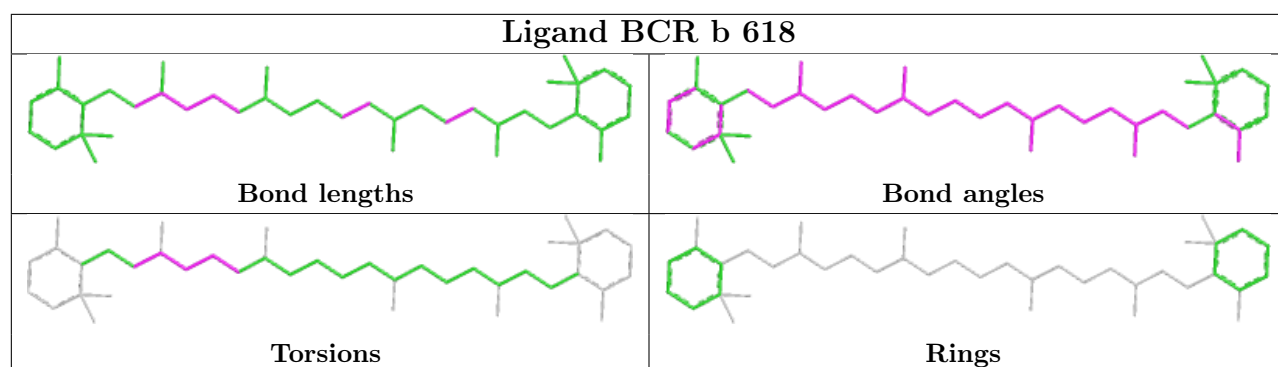
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	601	CLA	2	0
34	C	518	DGD	6	0
25	a	405	CLA	4	0
33	D	408	LHG	5	0
25	C	514	CLA	1	0
31	i	103	LMT	2	0
25	b	615	CLA	4	0
35	e	104	HEM	7	0
25	C	503	CLA	4	0
28	b	621	LMG	1	0
29	d	405	PL9	2	0
30	H	103	SQD	3	0
27	K	103	BCR	4	0
25	a	408	CLA	6	0
25	B	616	CLA	4	0
25	C	509	CLA	7	0
25	D	401	CLA	5	0
26	D	402	PHO	1	0
36	h	101	RRX	2	0
31	D	412	LMT	1	0
31	D	410	LMT	3	0
25	A	405	CLA	6	0
28	c	519	LMG	6	0
30	A	412	SQD	4	0
25	B	611	CLA	3	0
34	C	517	DGD	6	0
31	T	101	LMT	1	0
28	a	414	LMG	3	0
25	b	610	CLA	1	0

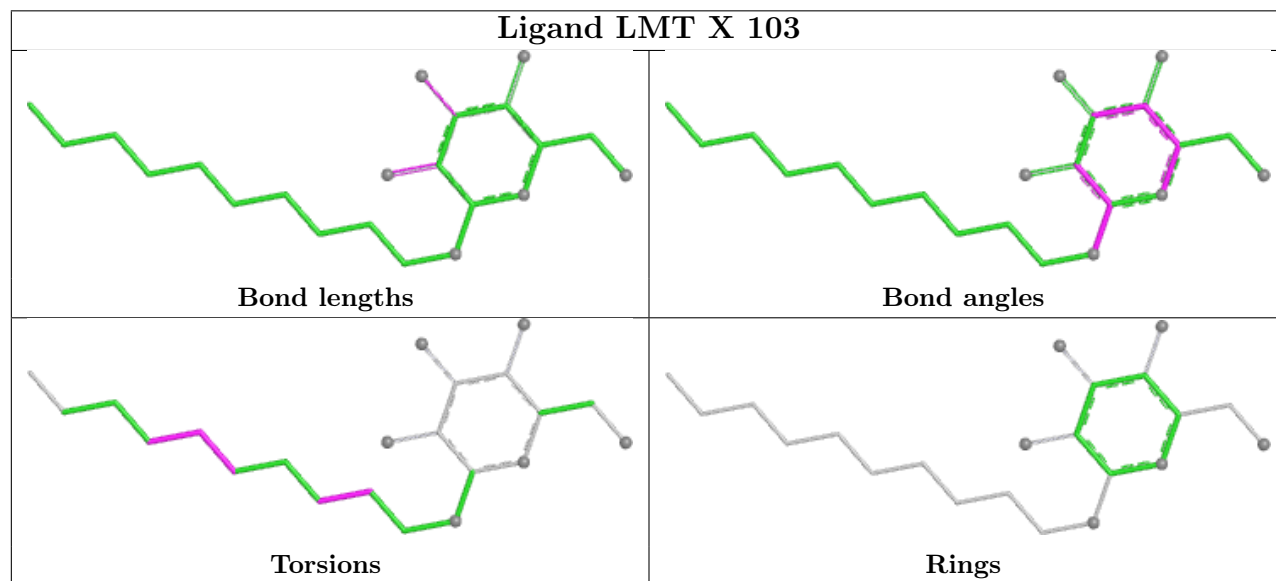
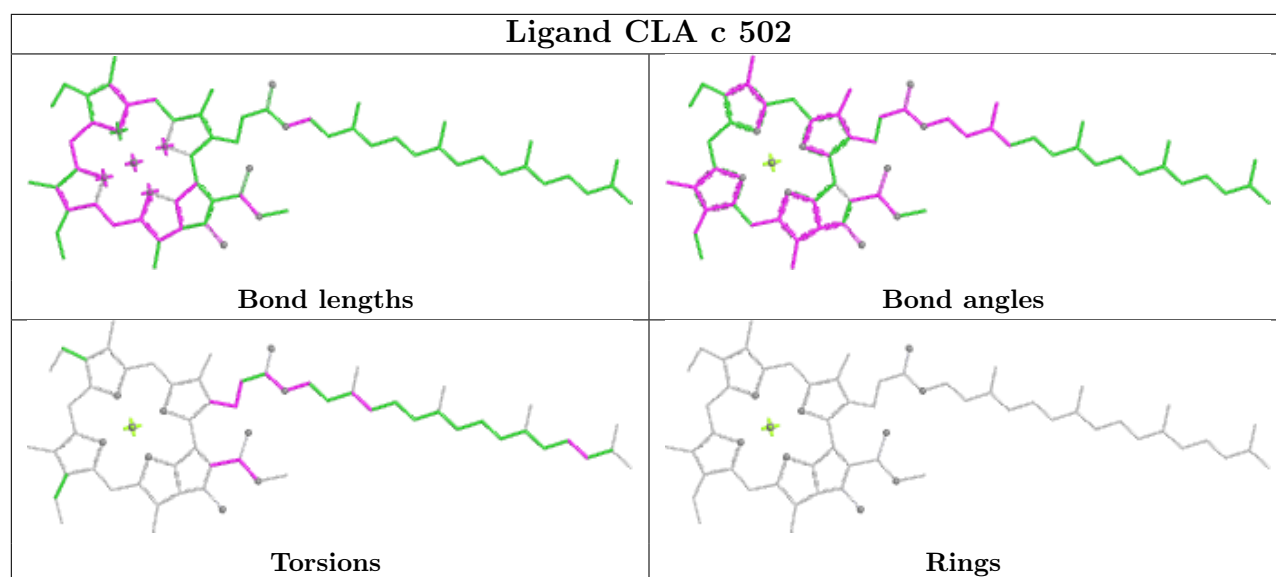
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

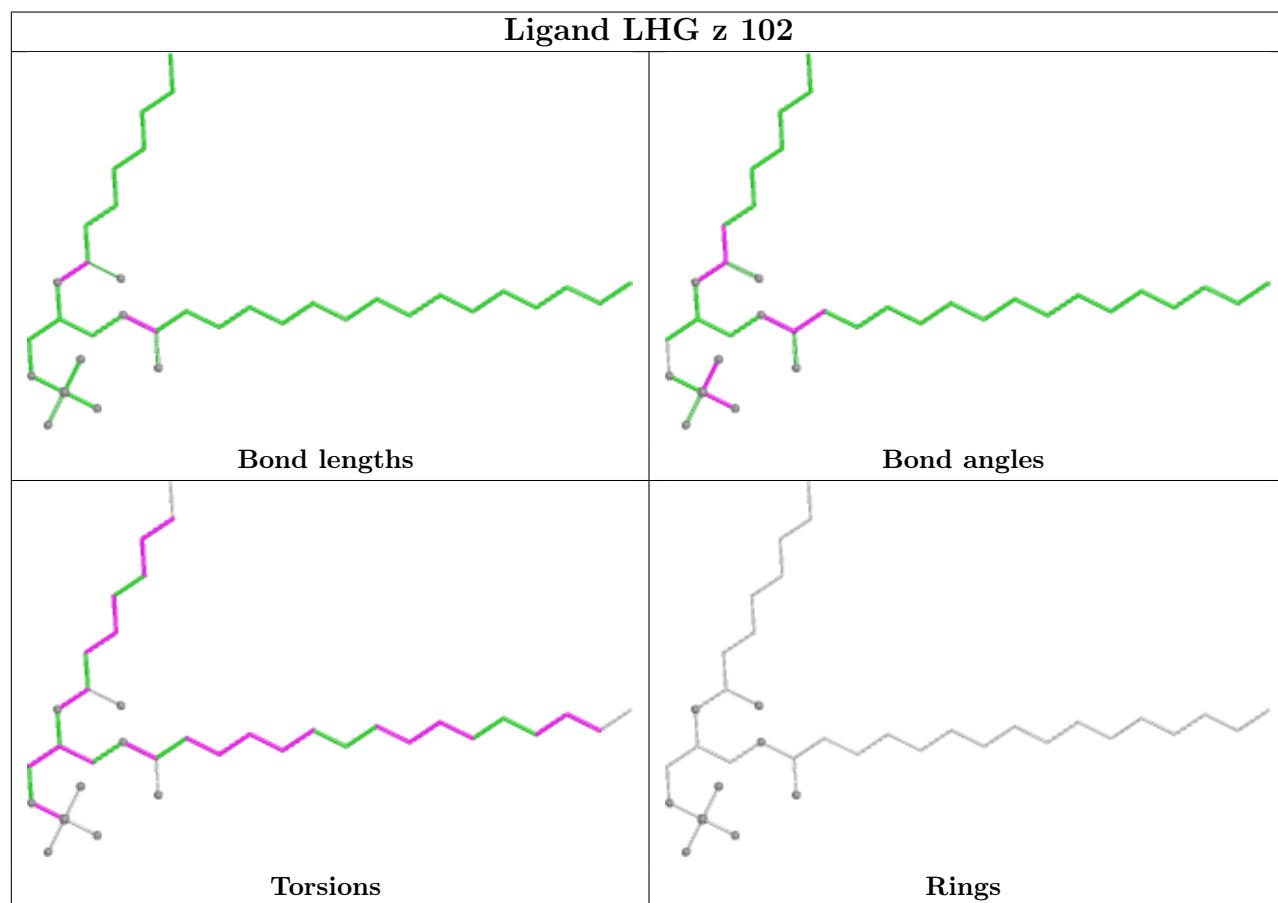
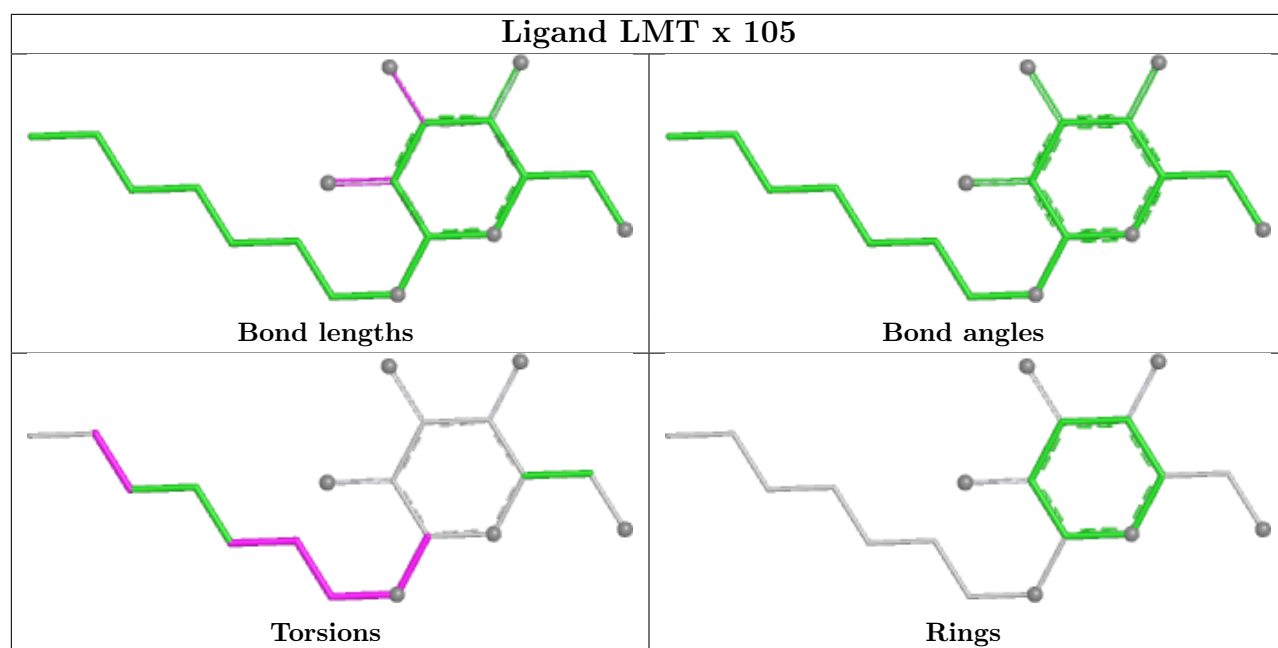


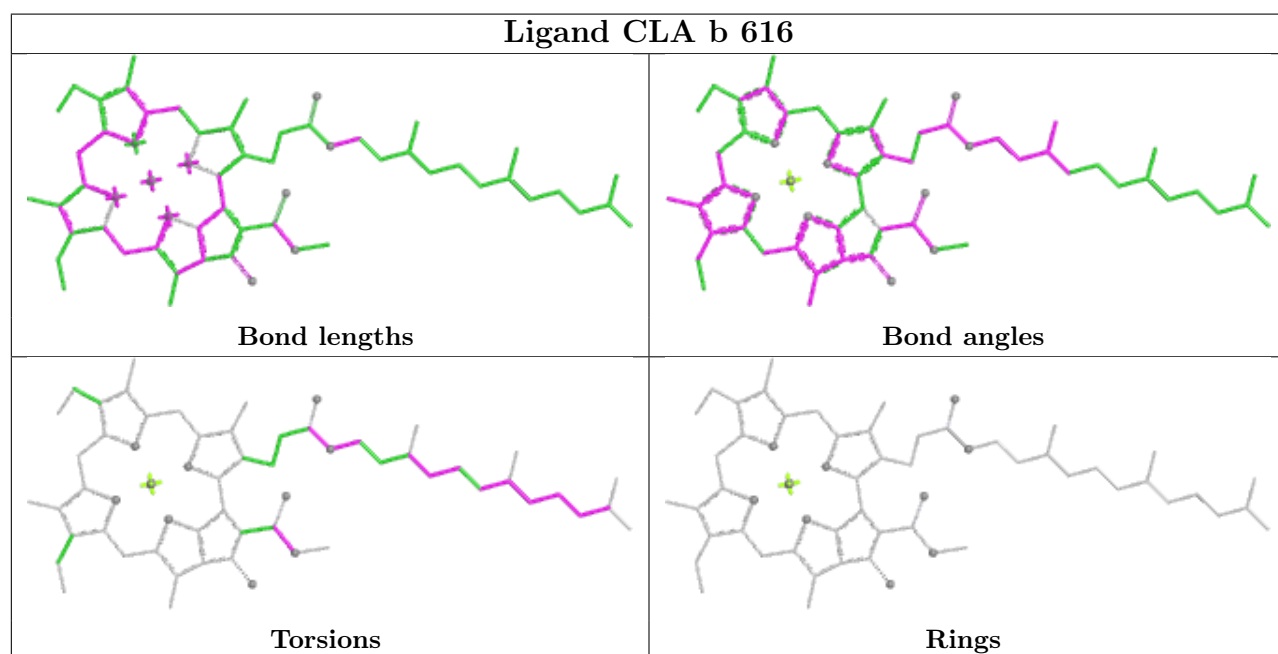
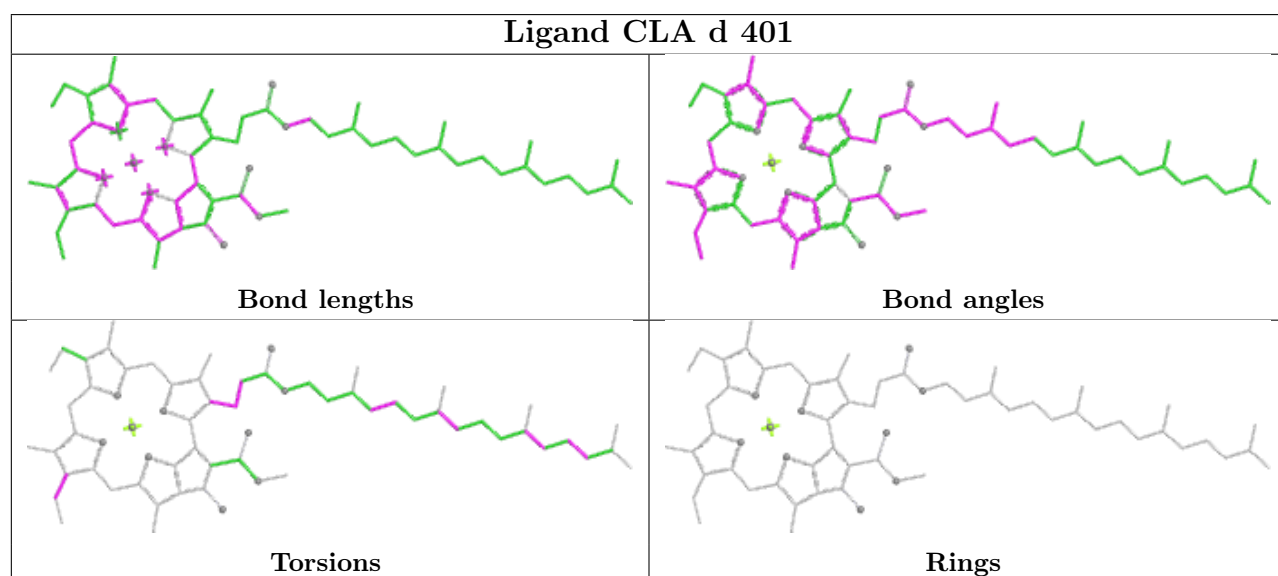
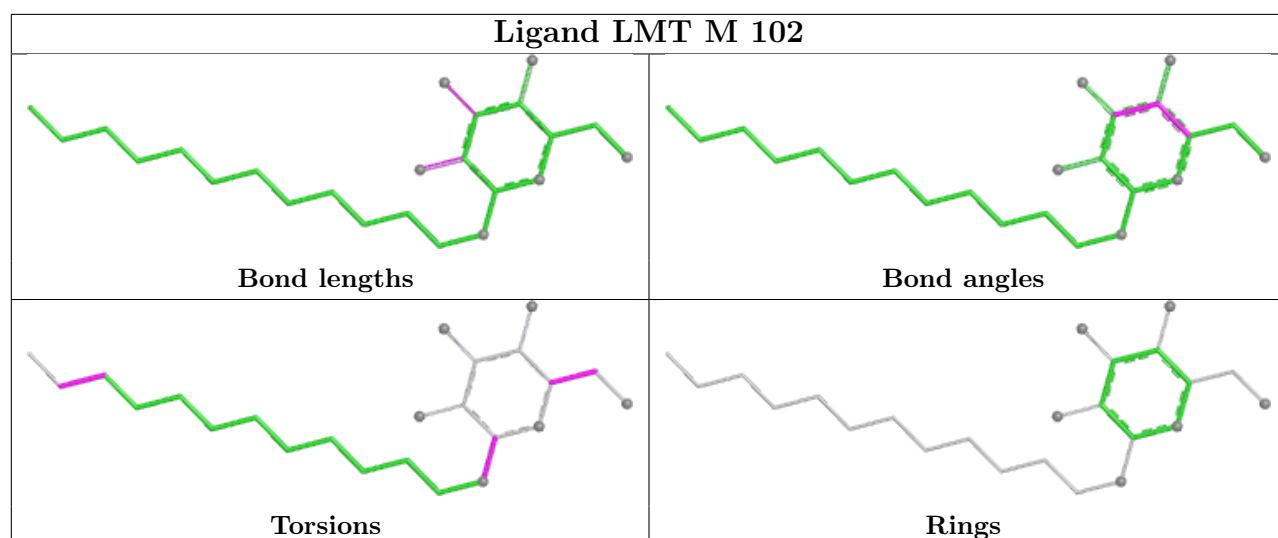


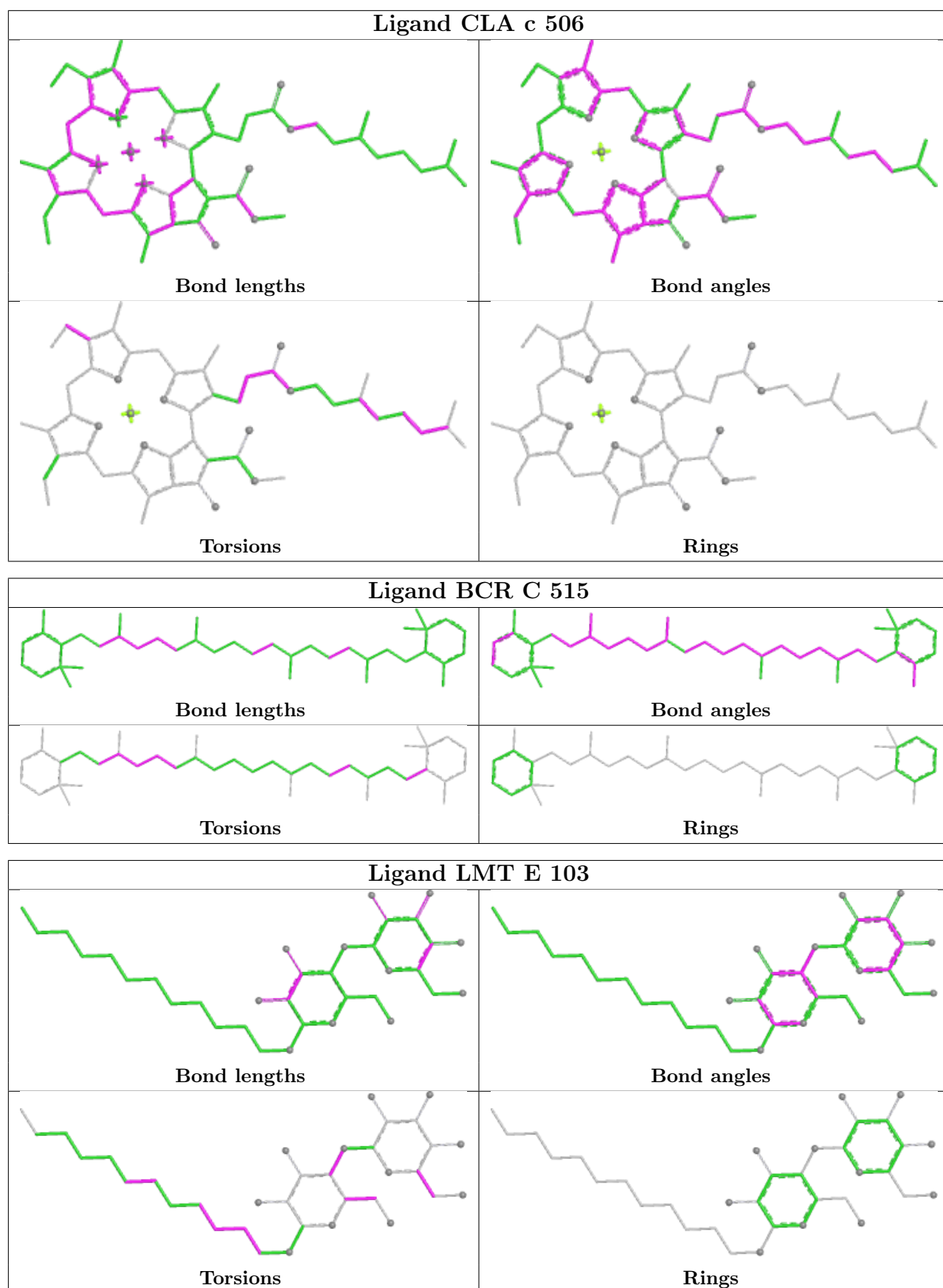


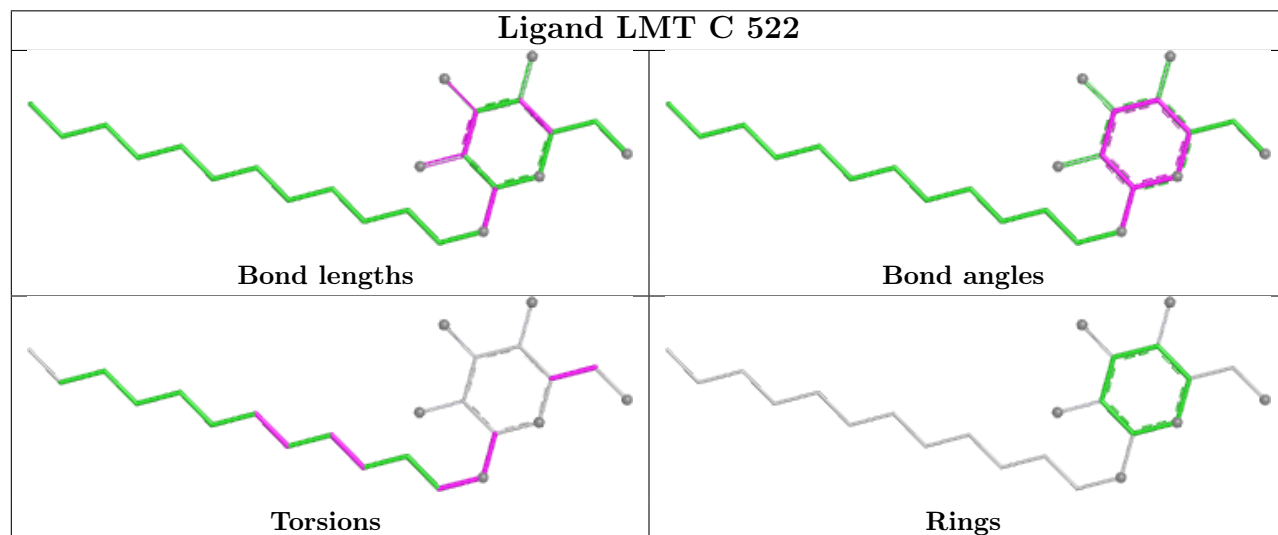
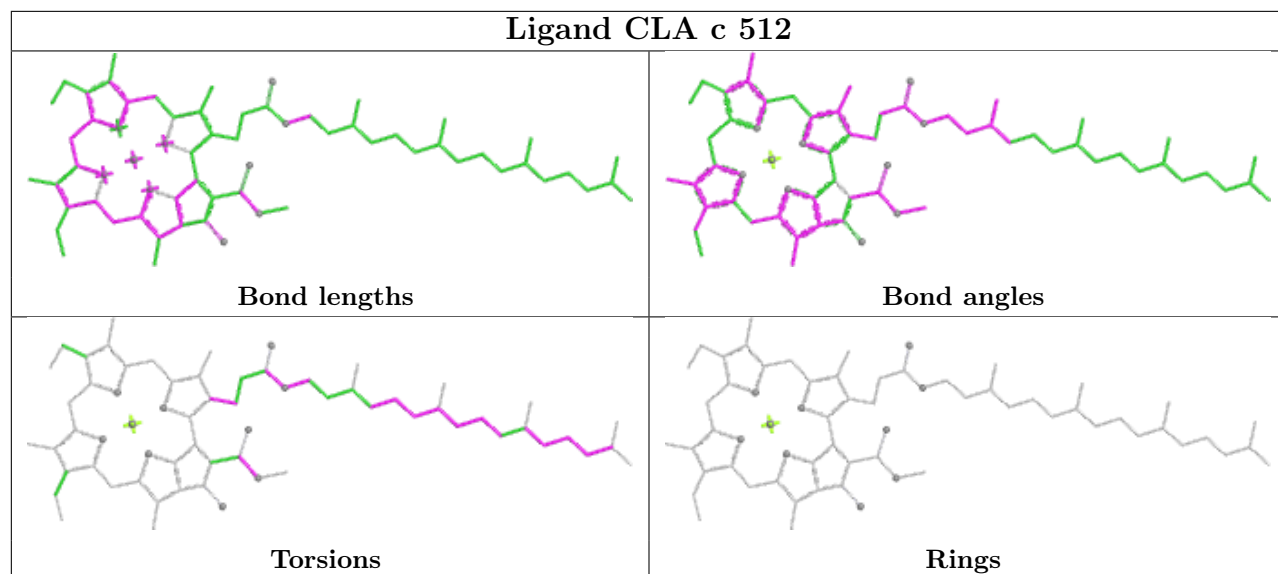


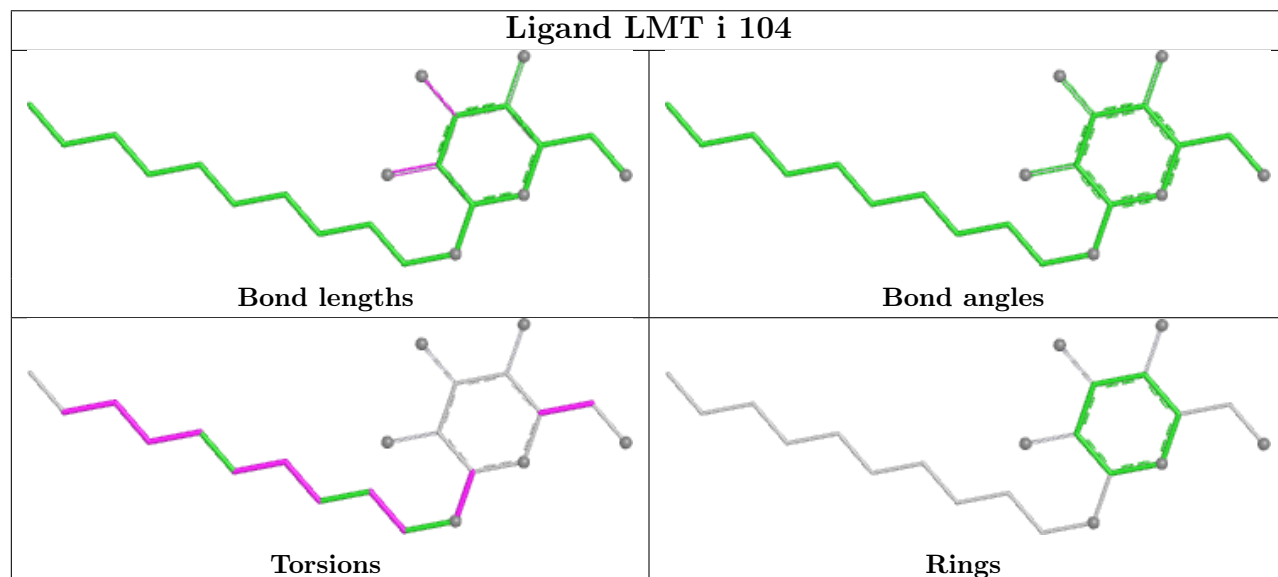
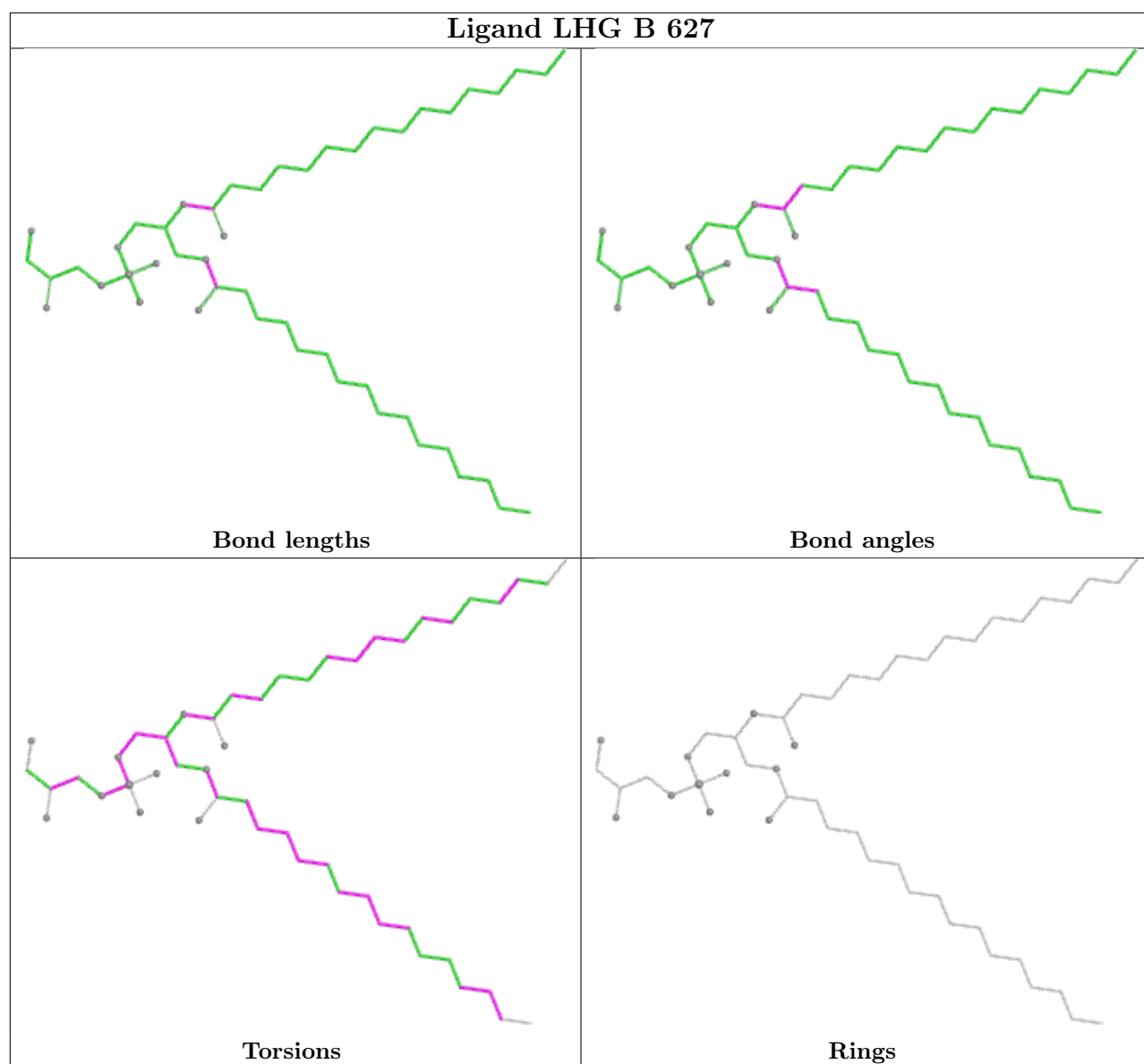


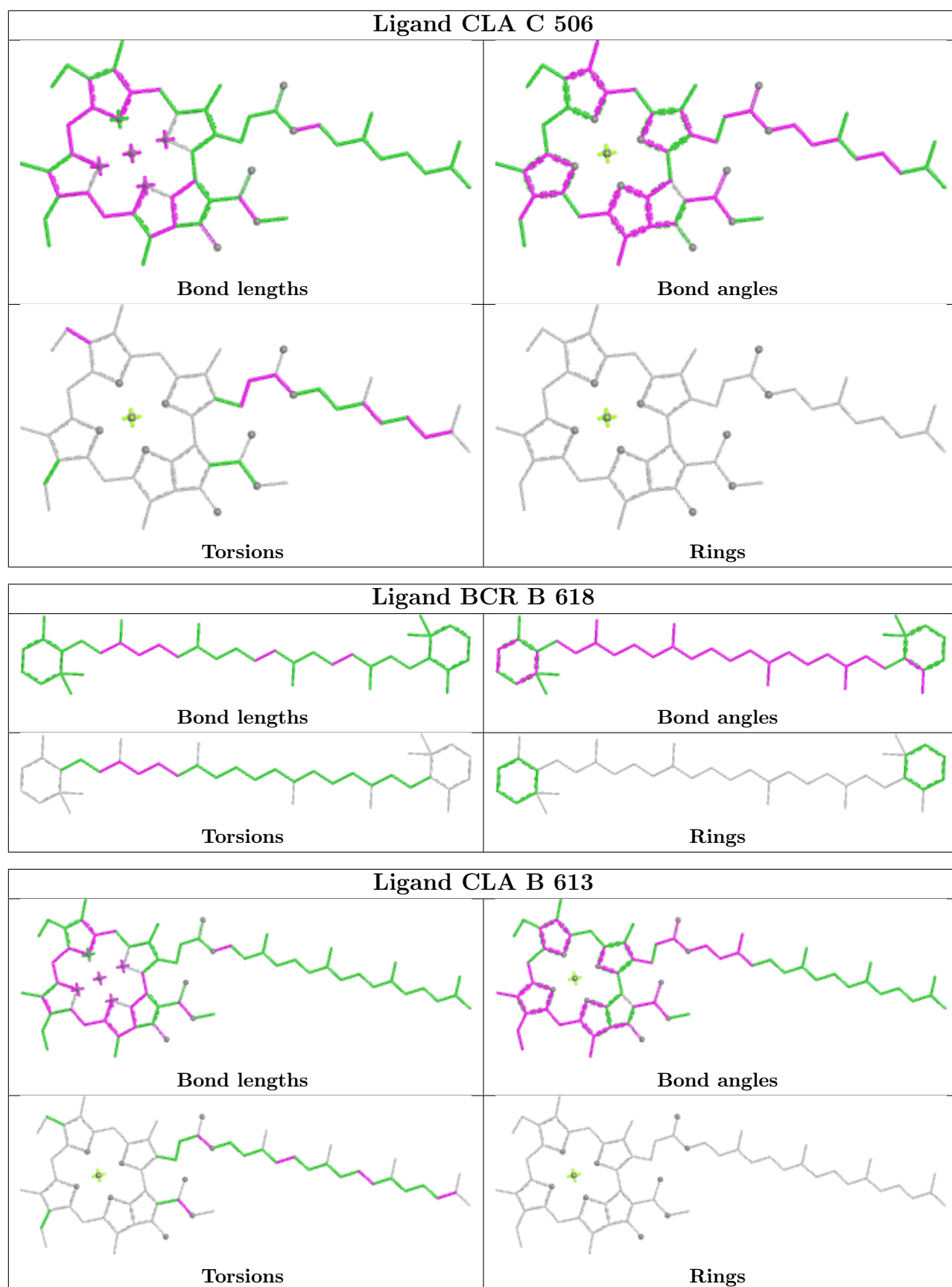


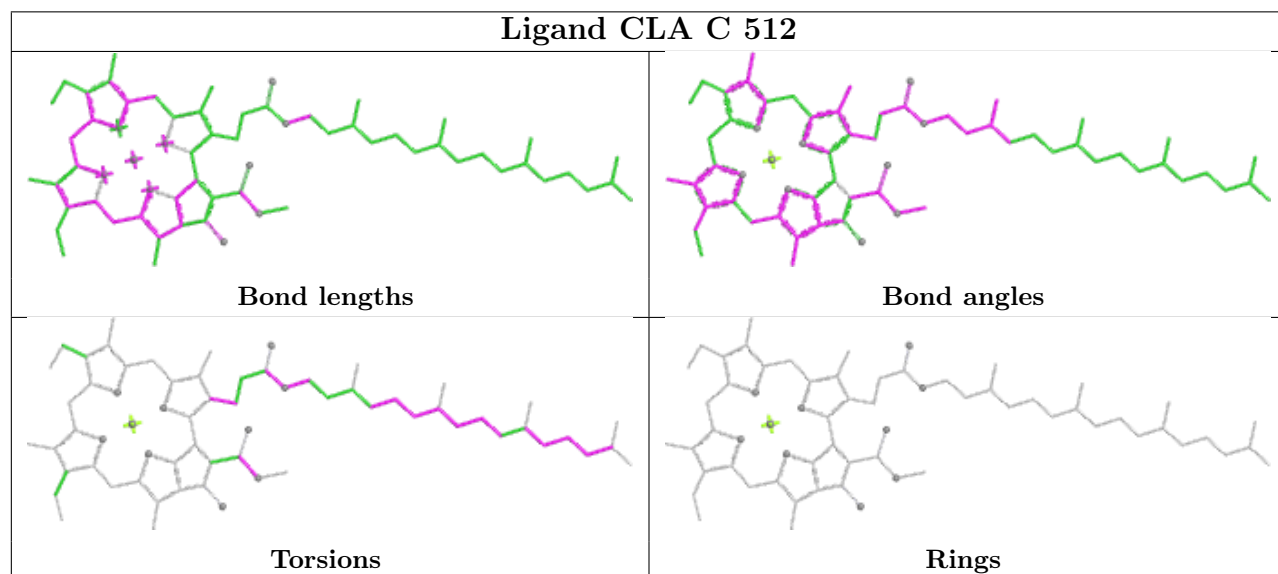
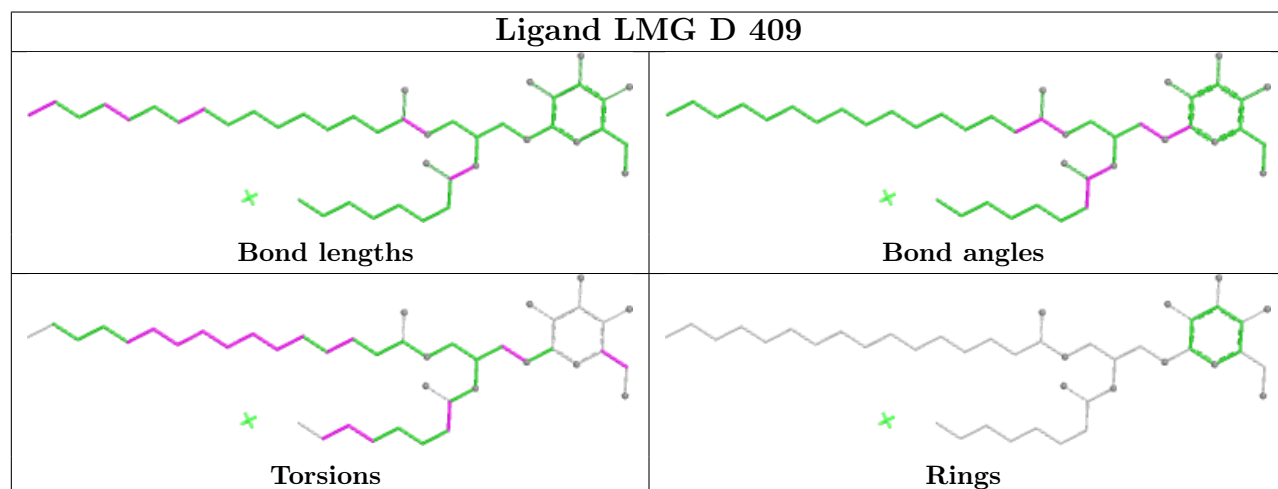
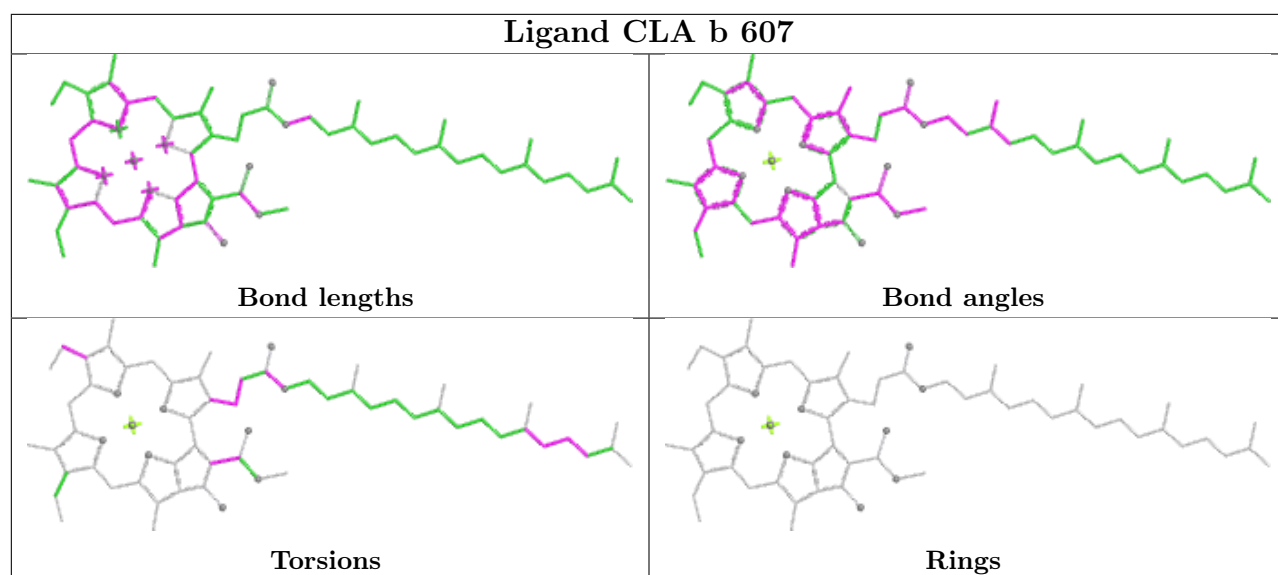


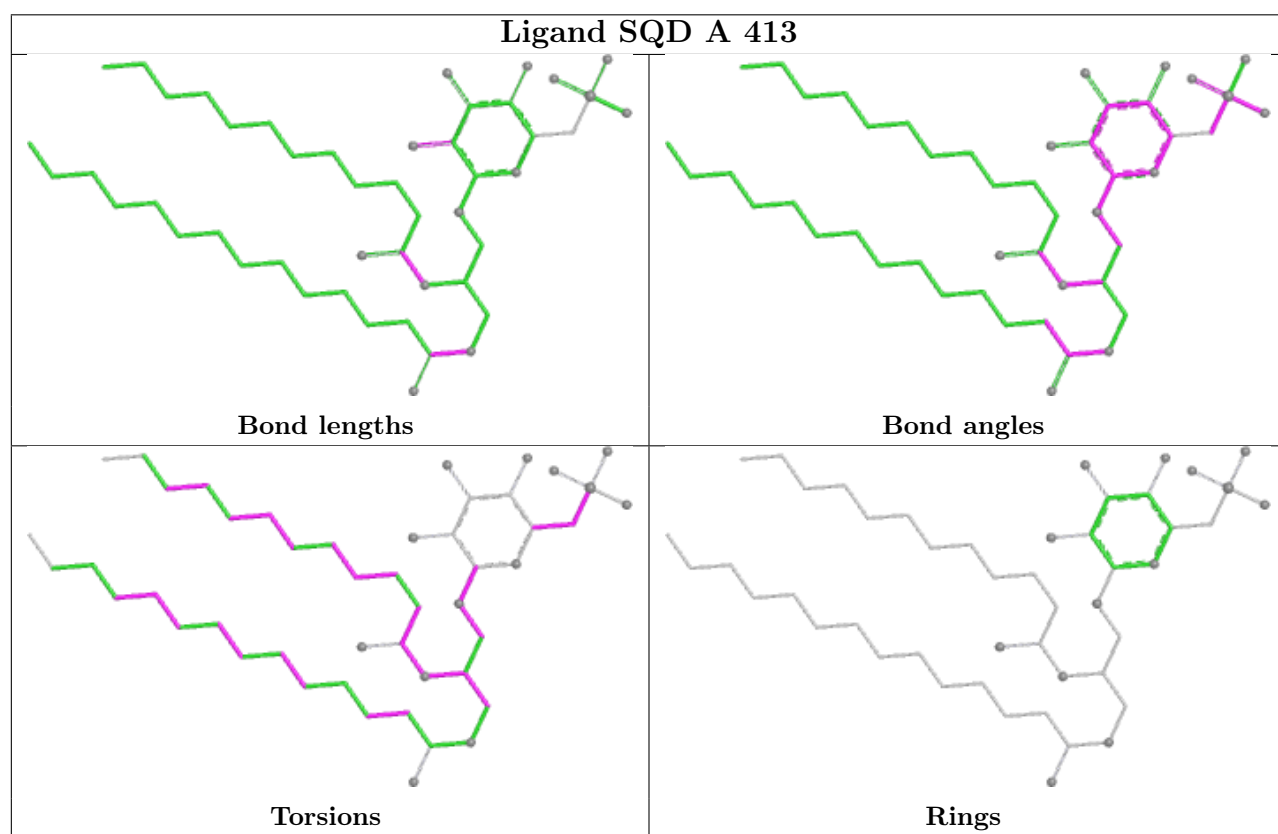
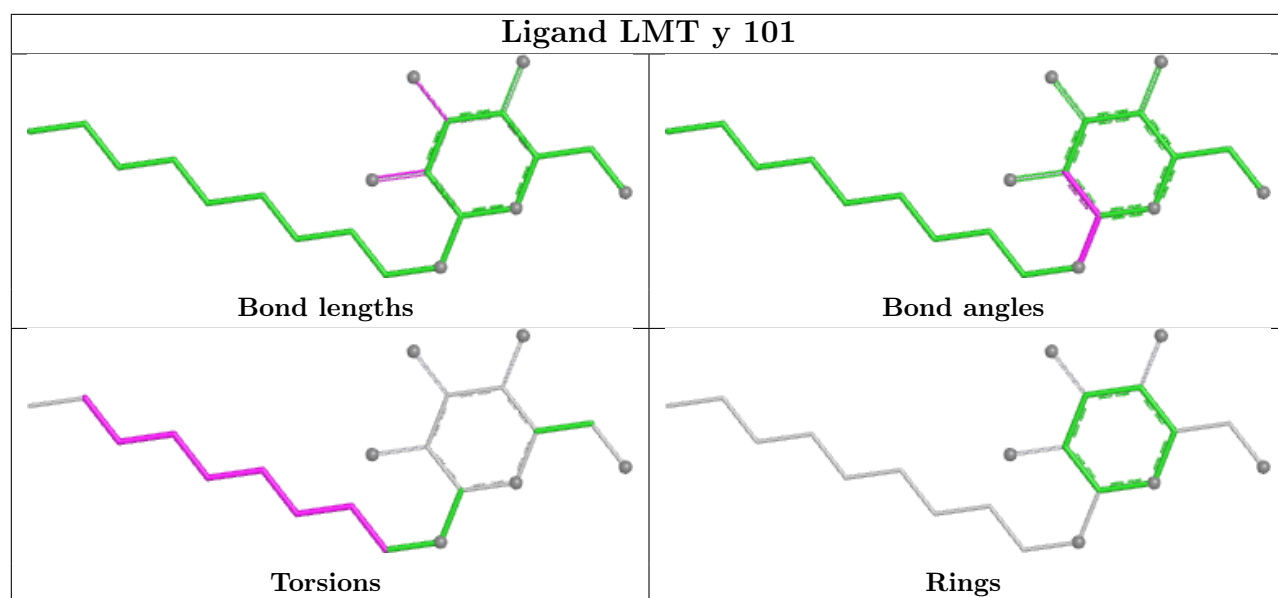


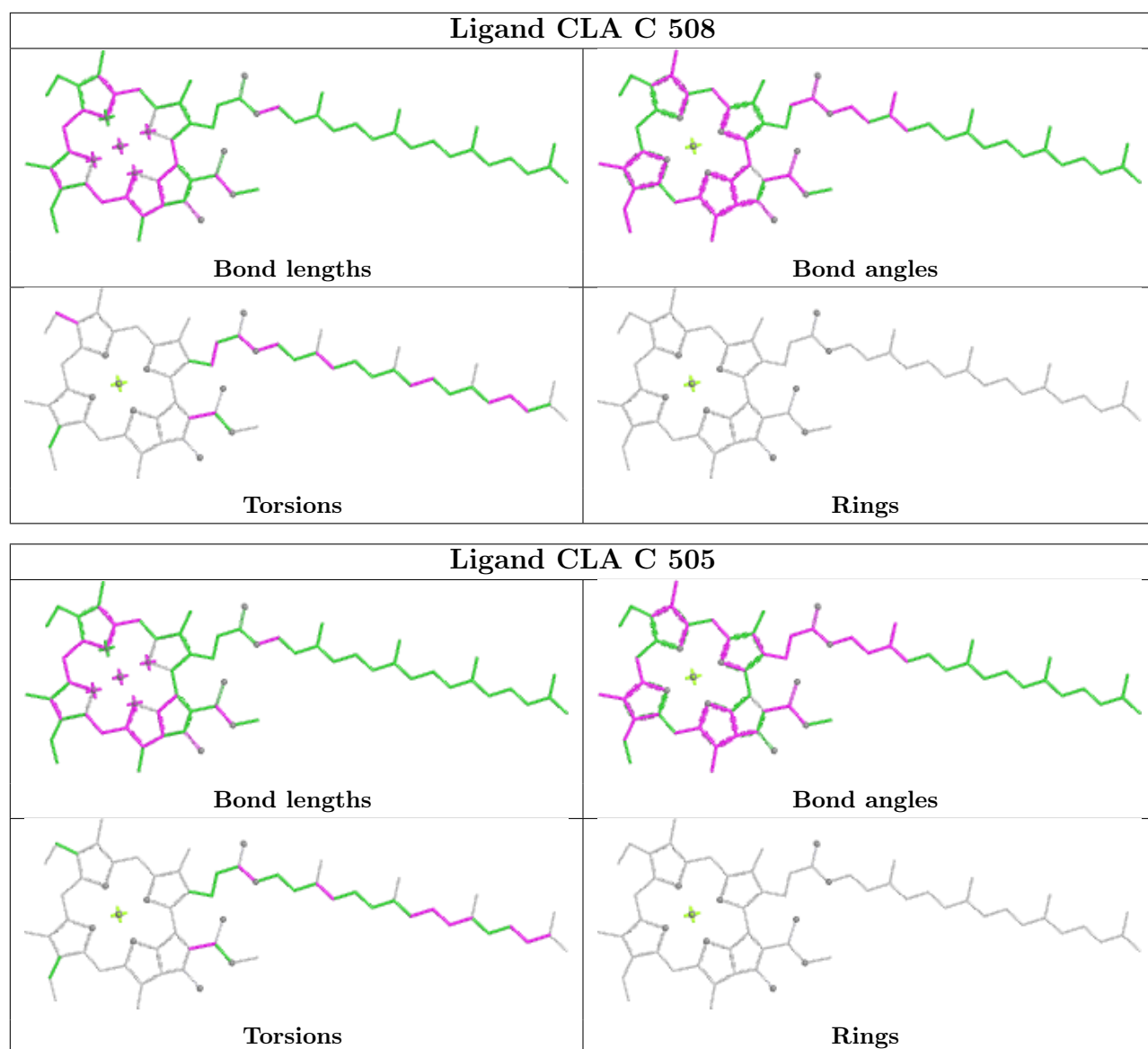


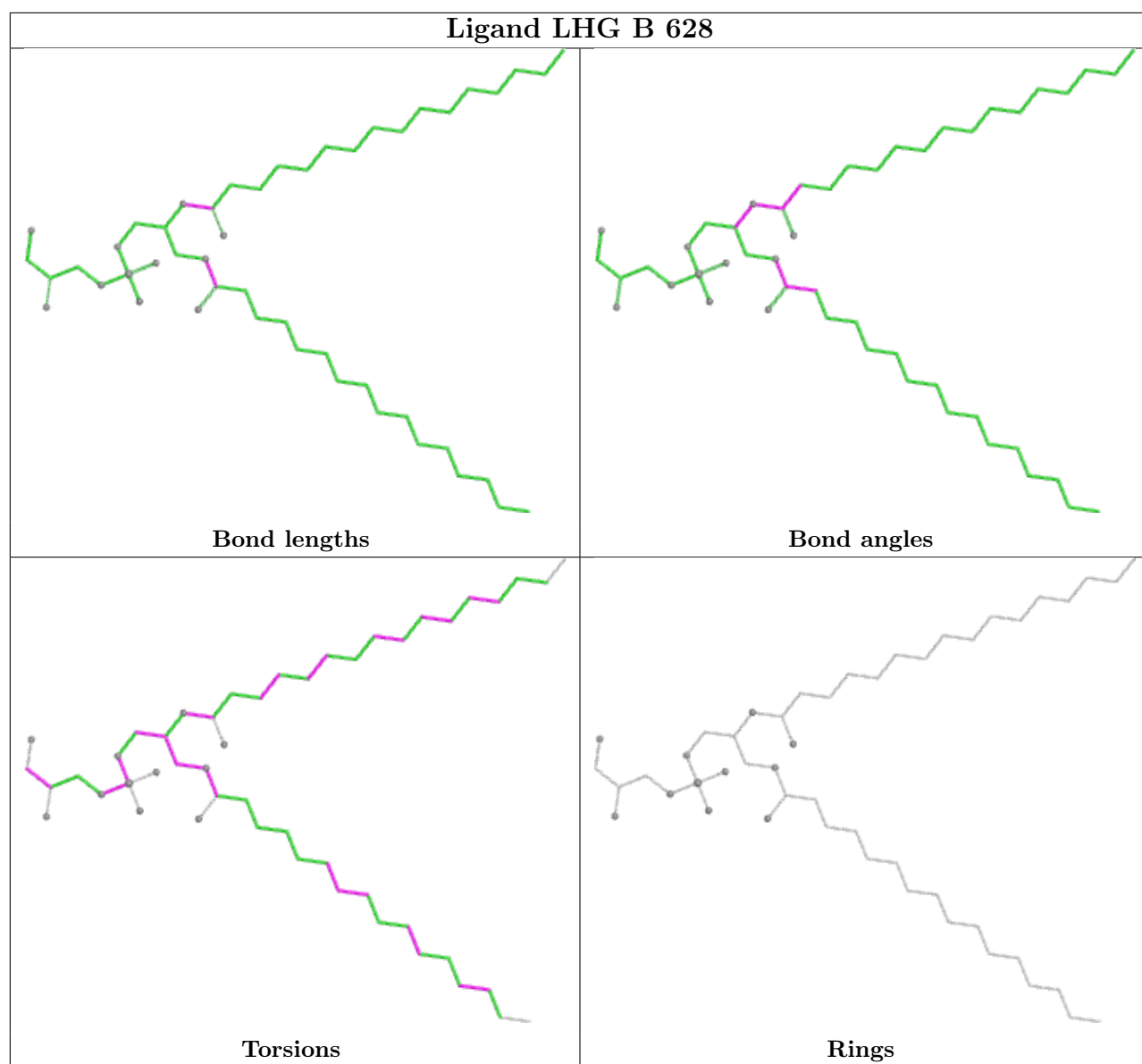


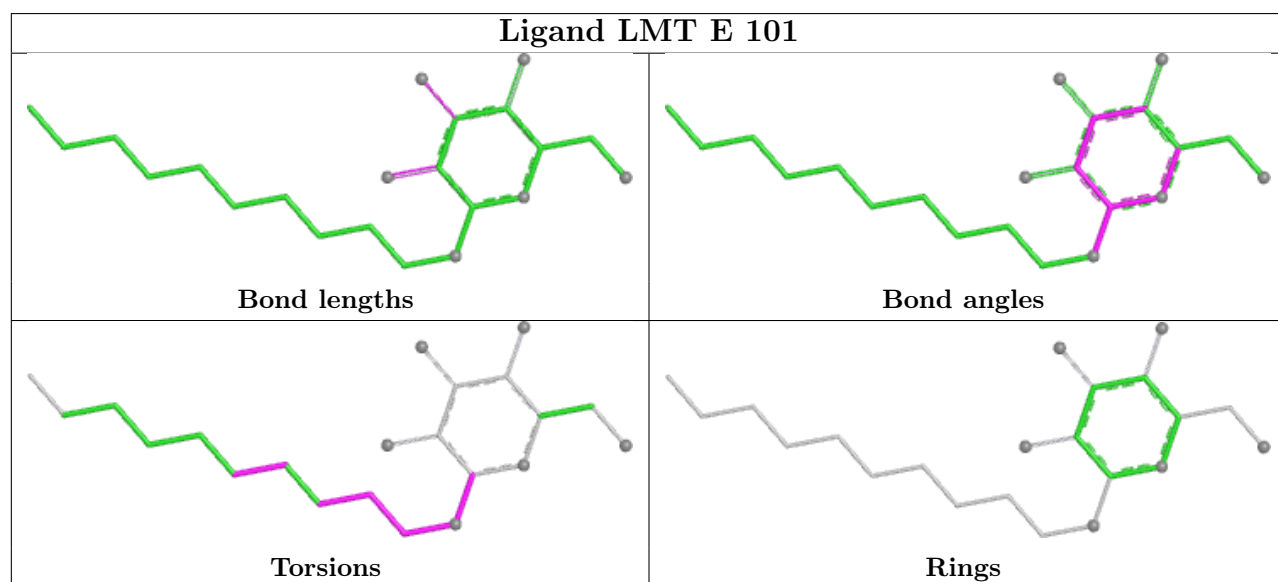
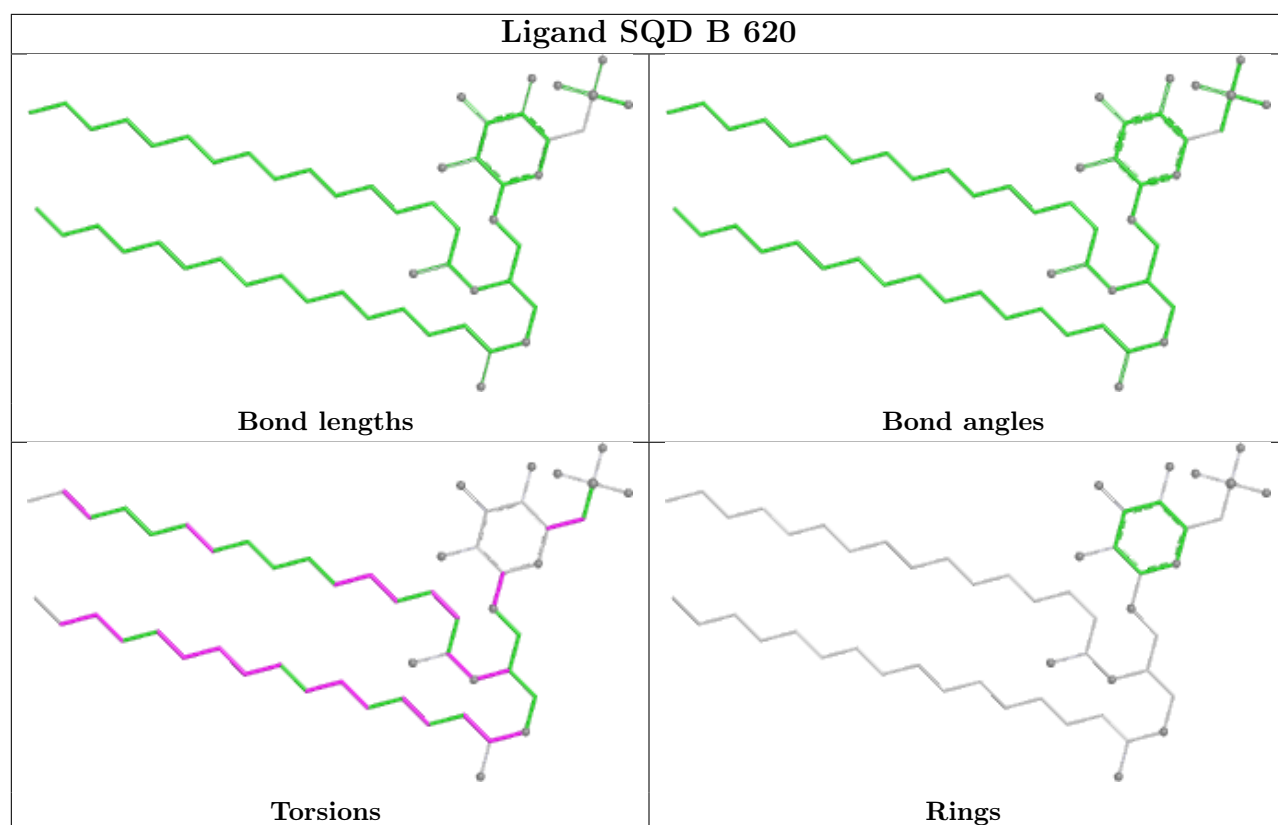


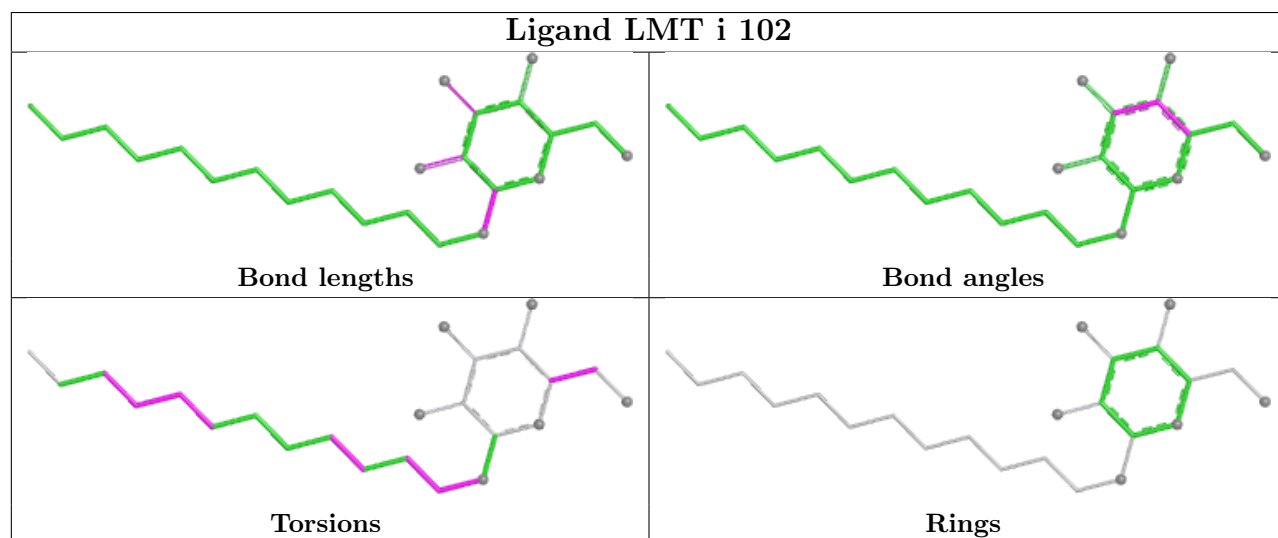
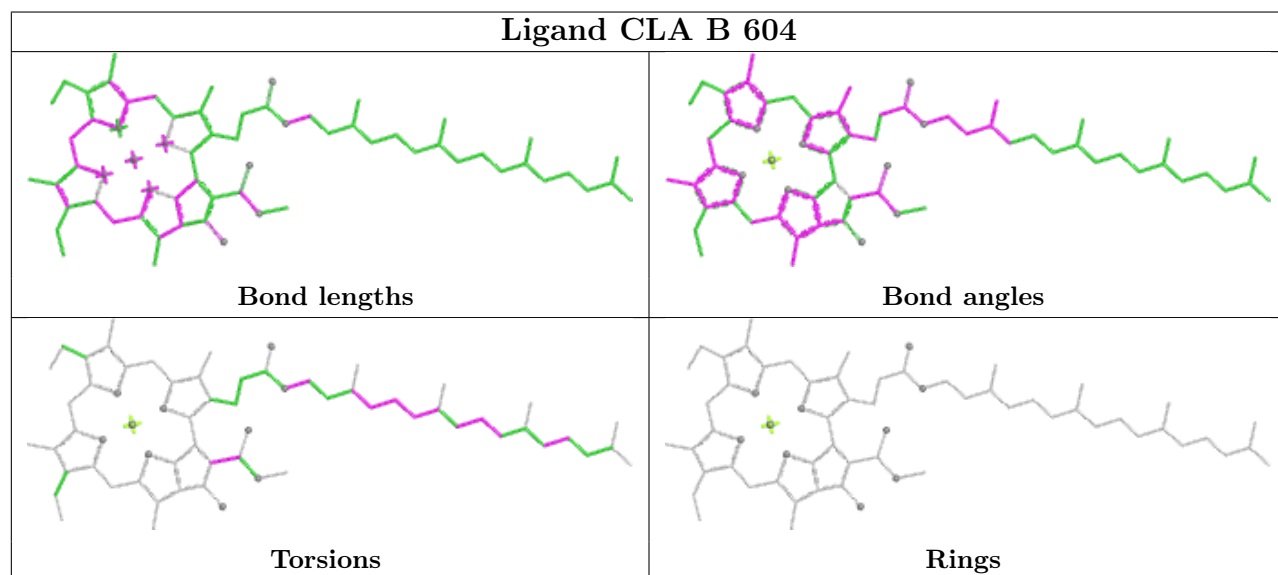
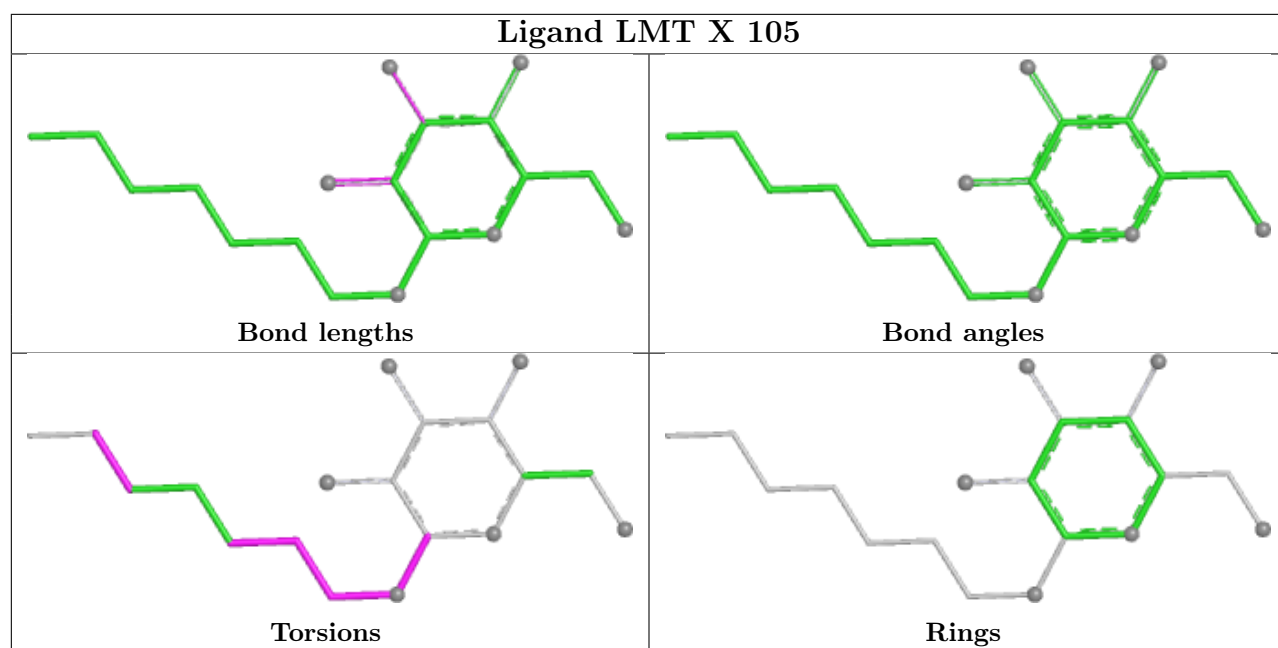


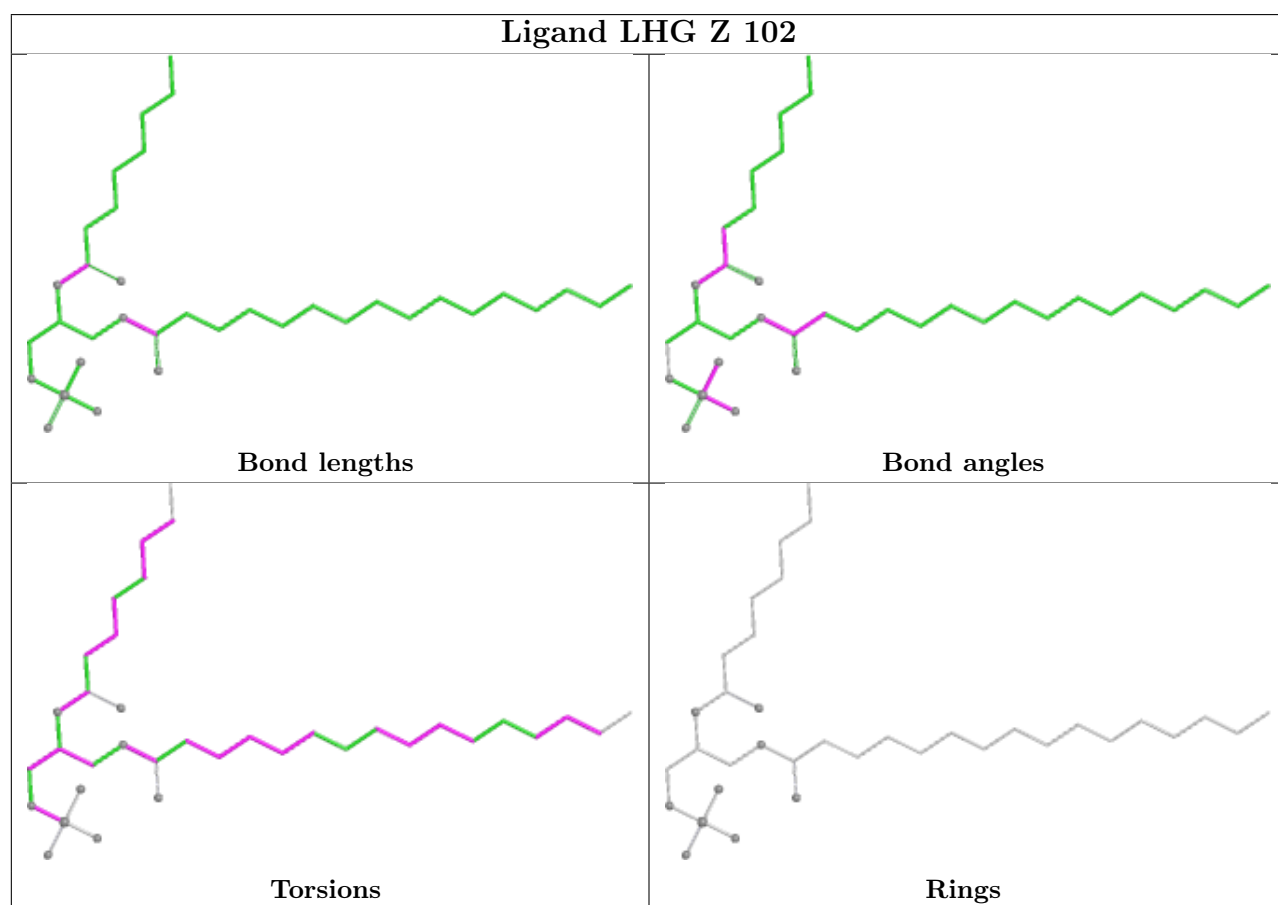
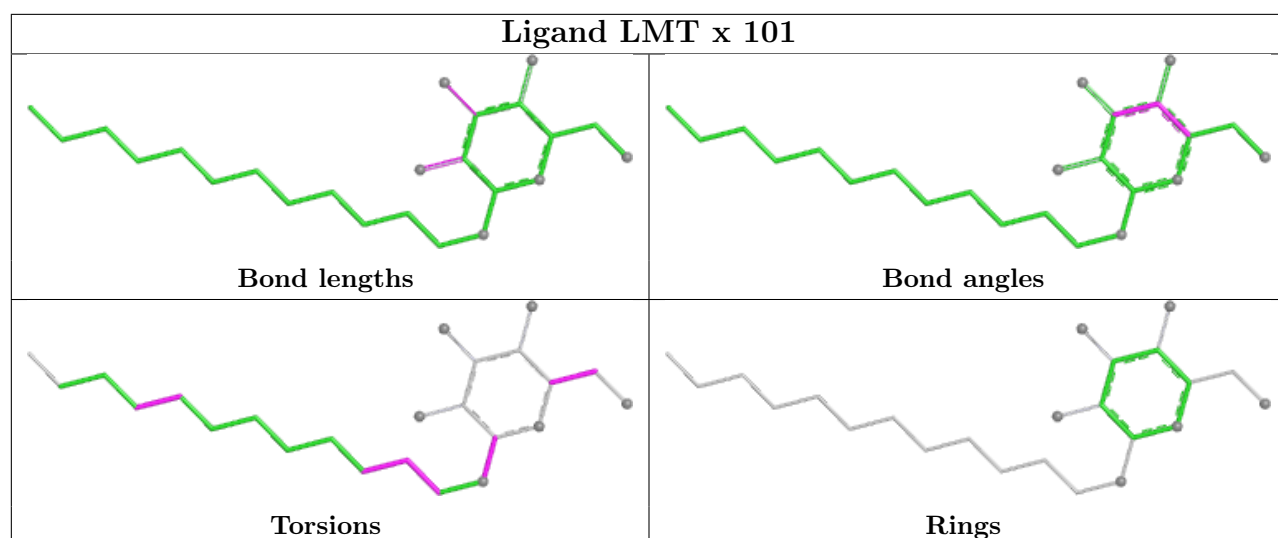


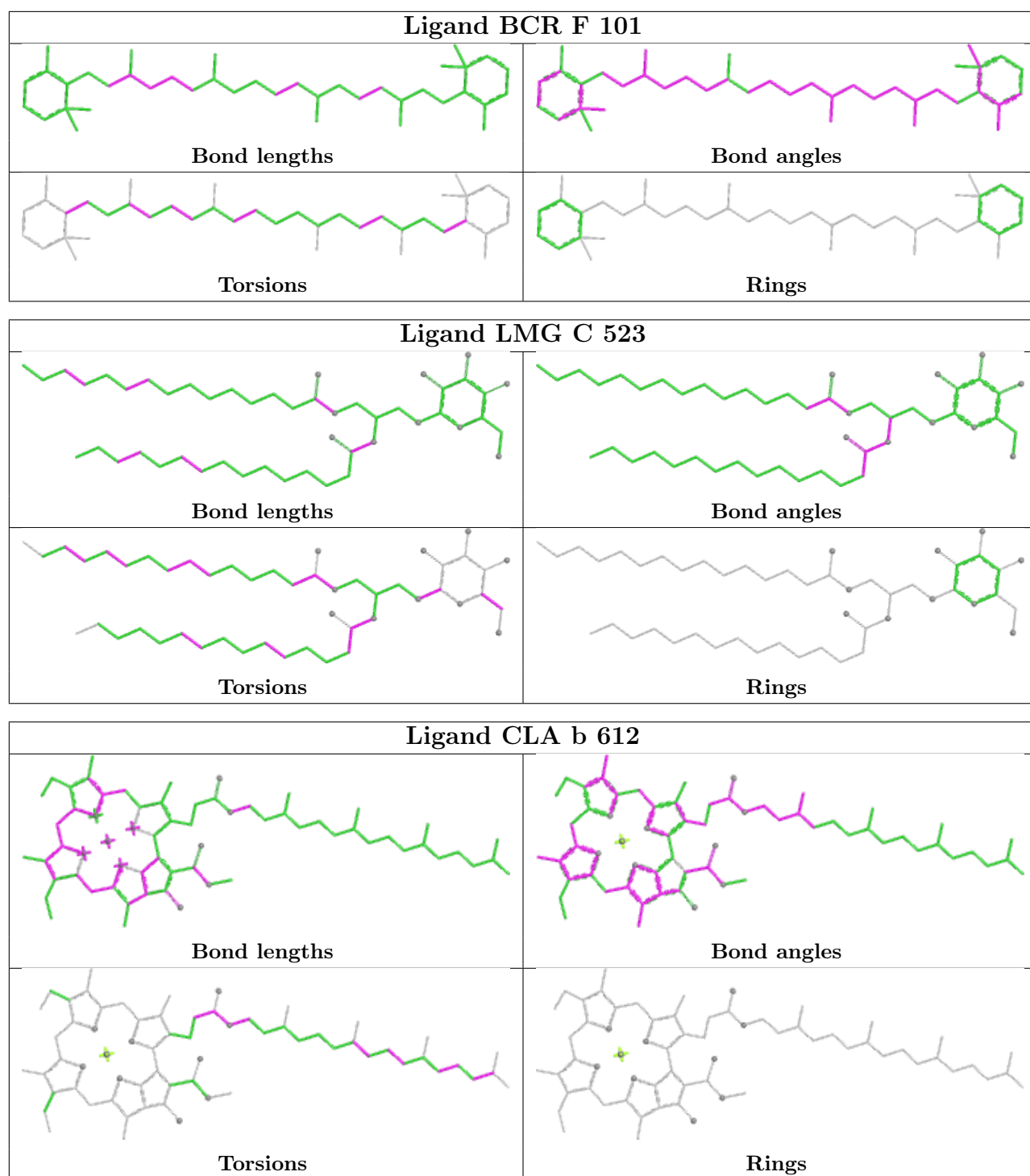


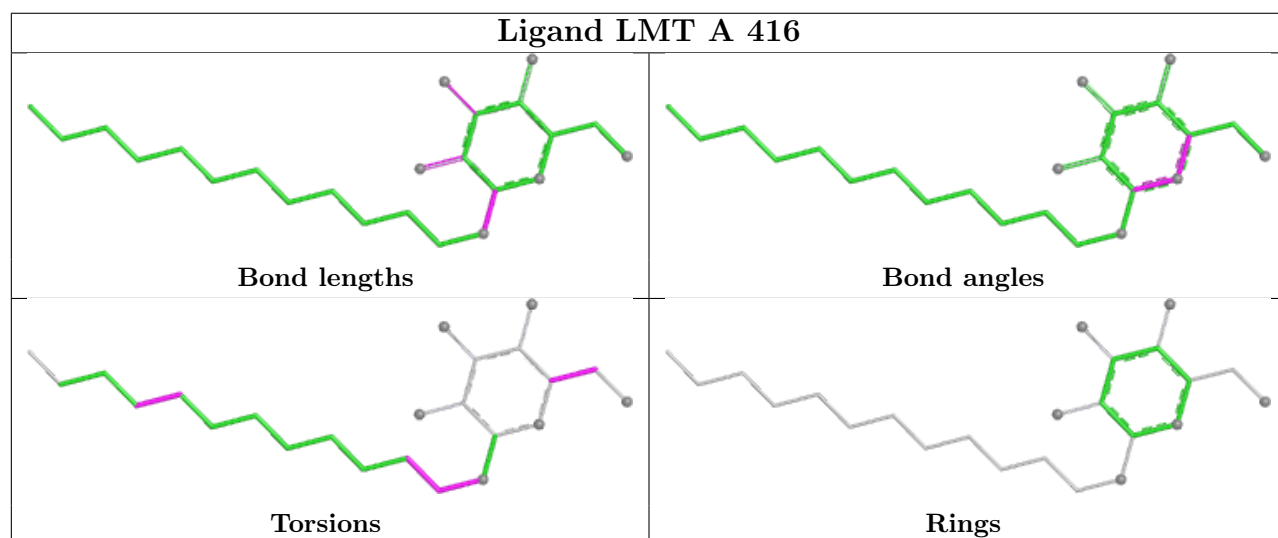
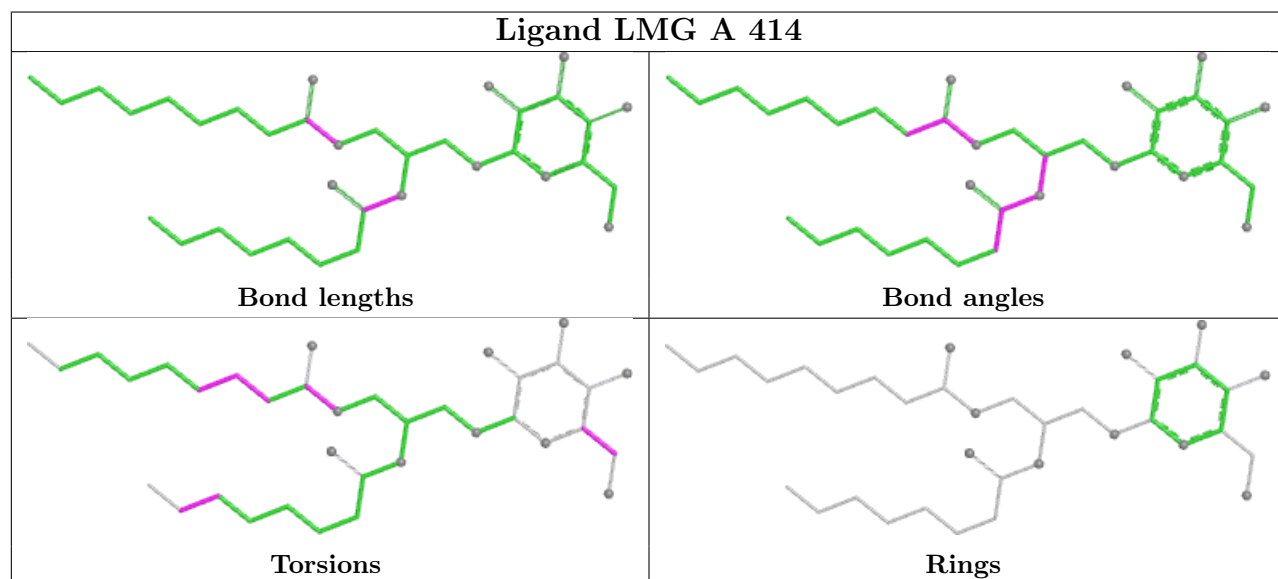
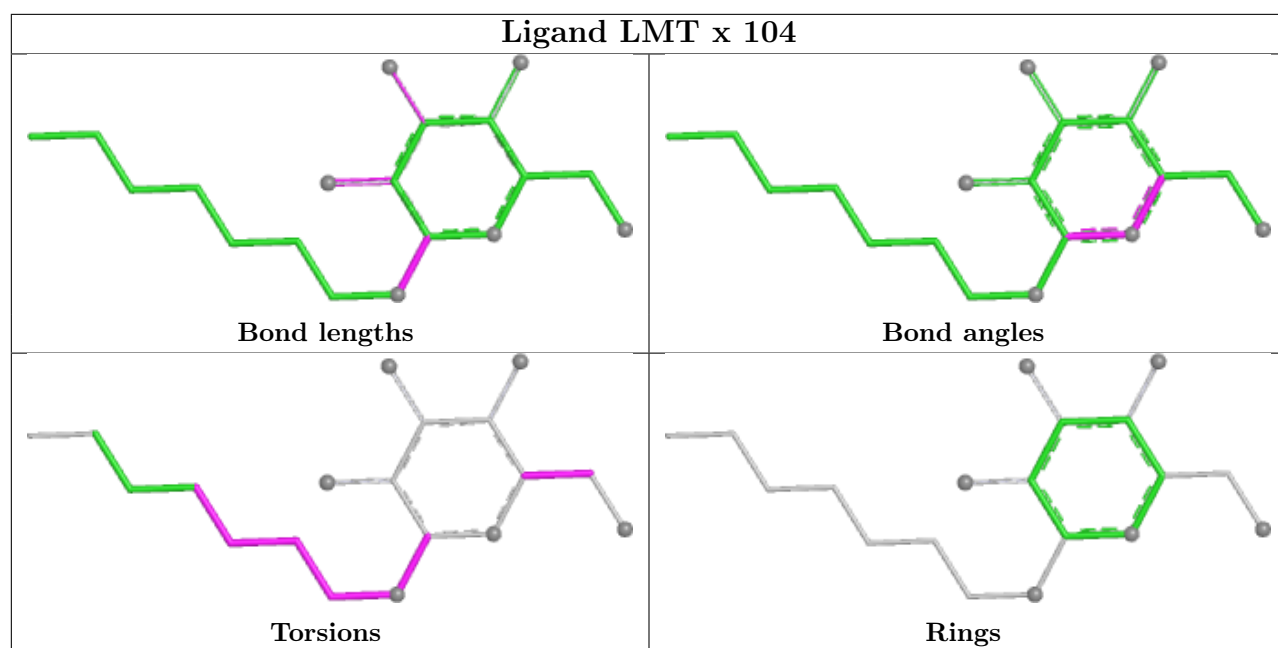


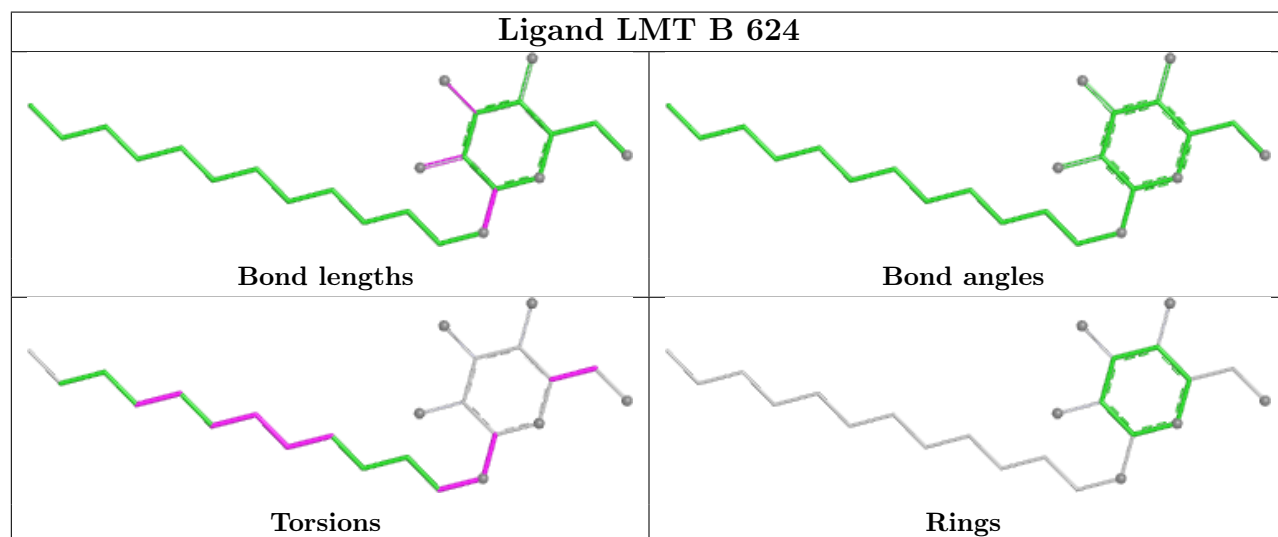
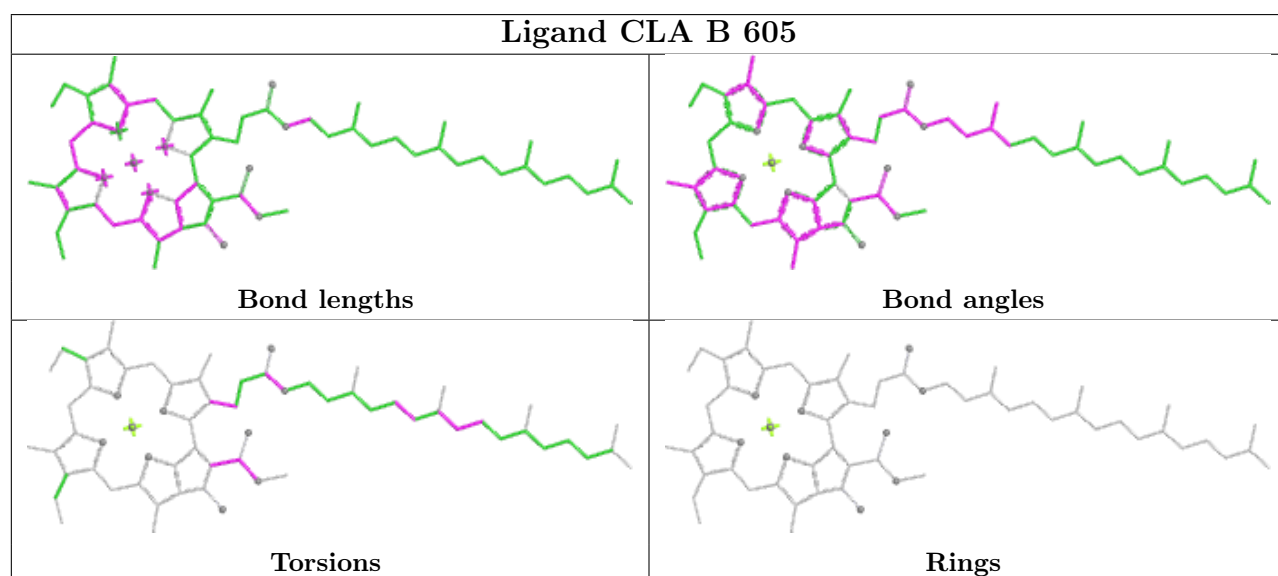
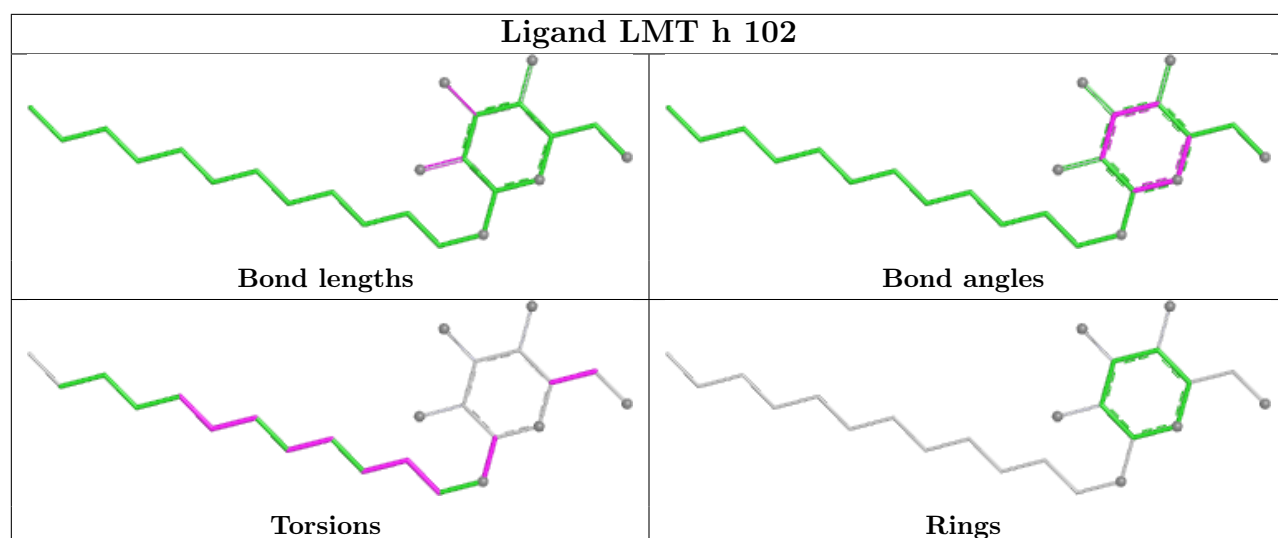


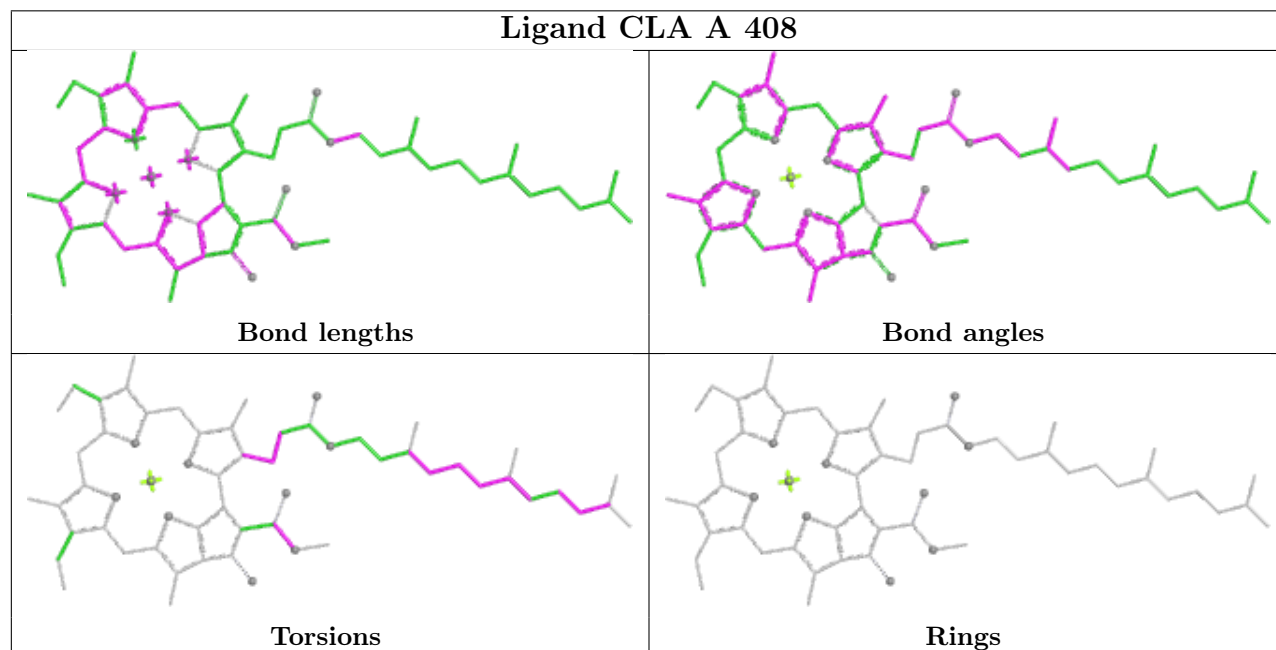
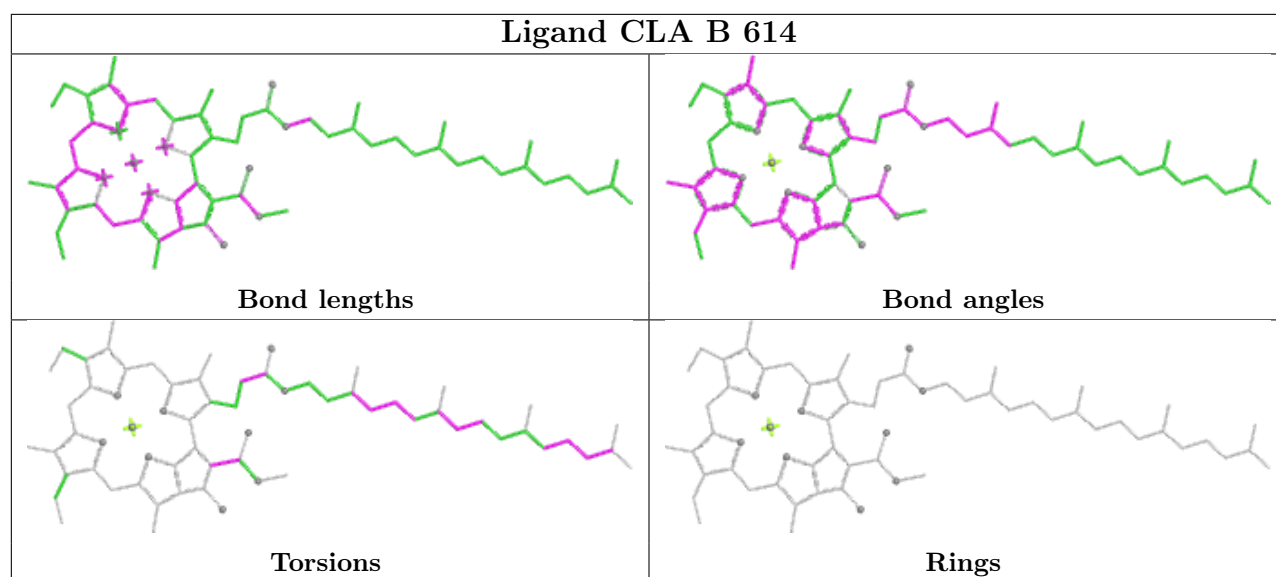


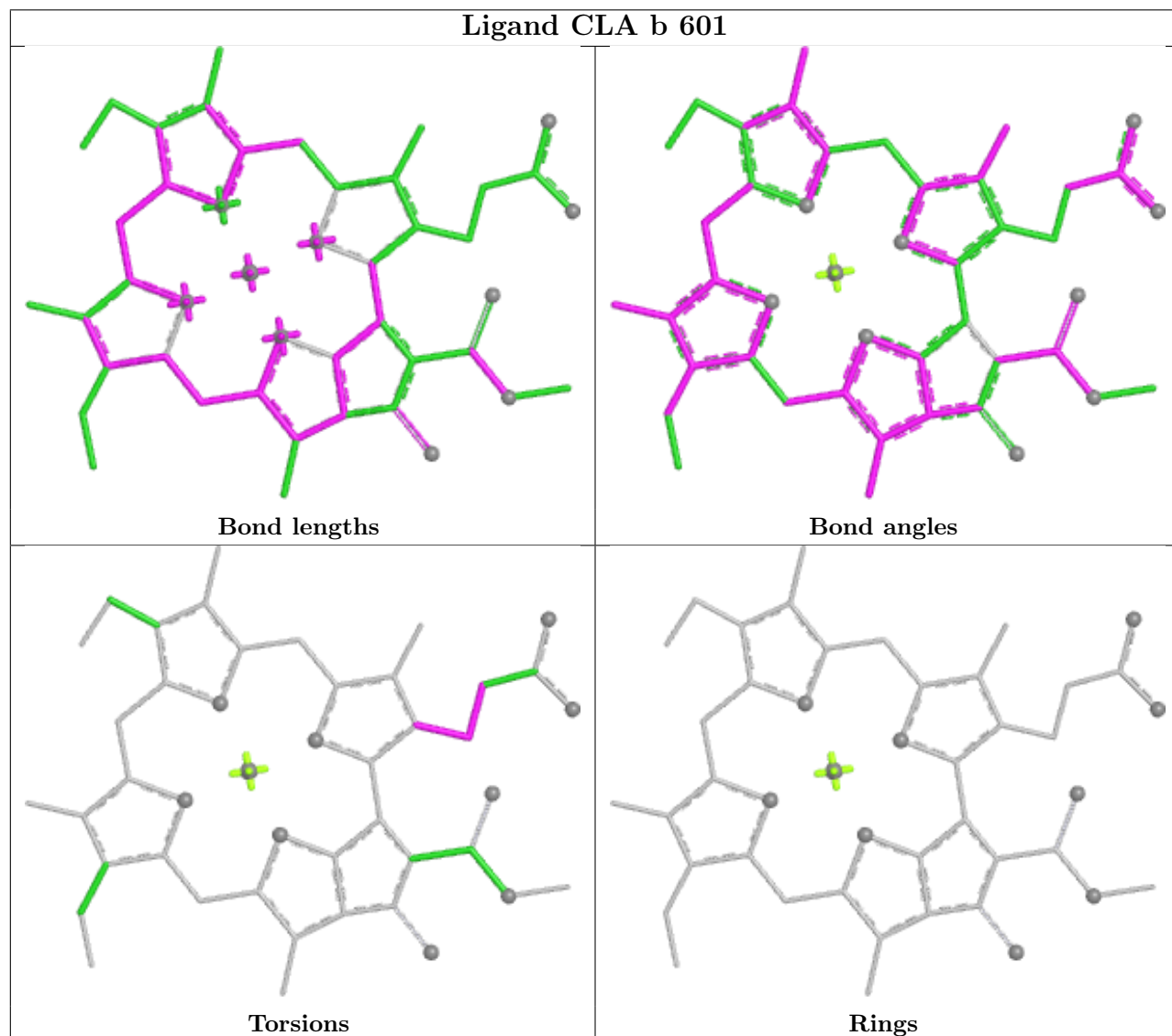
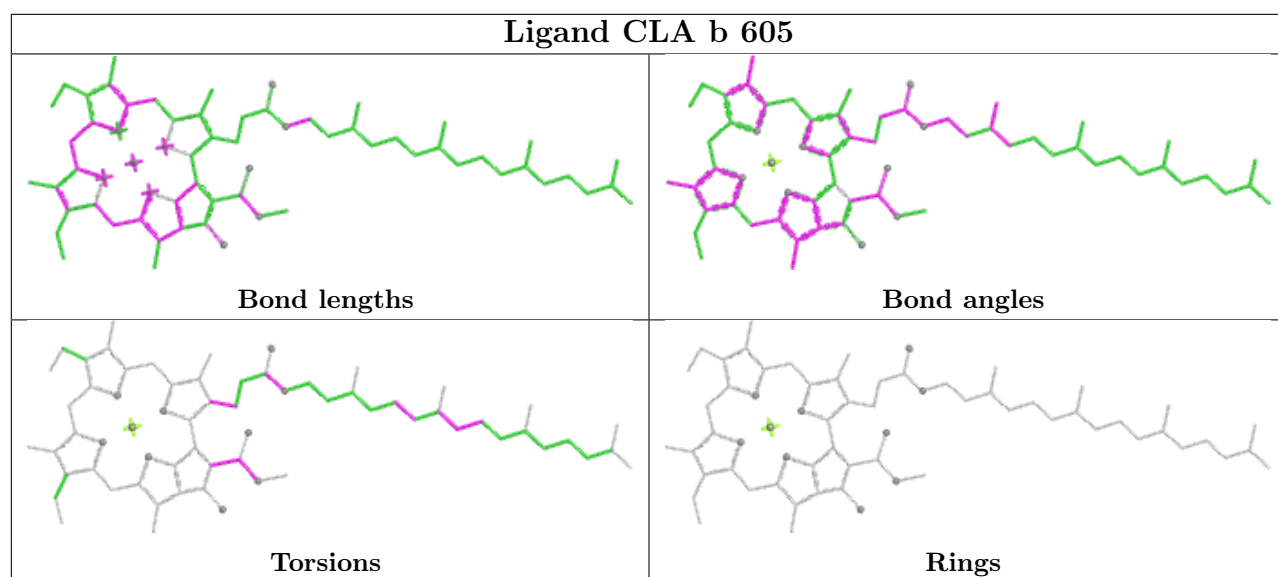


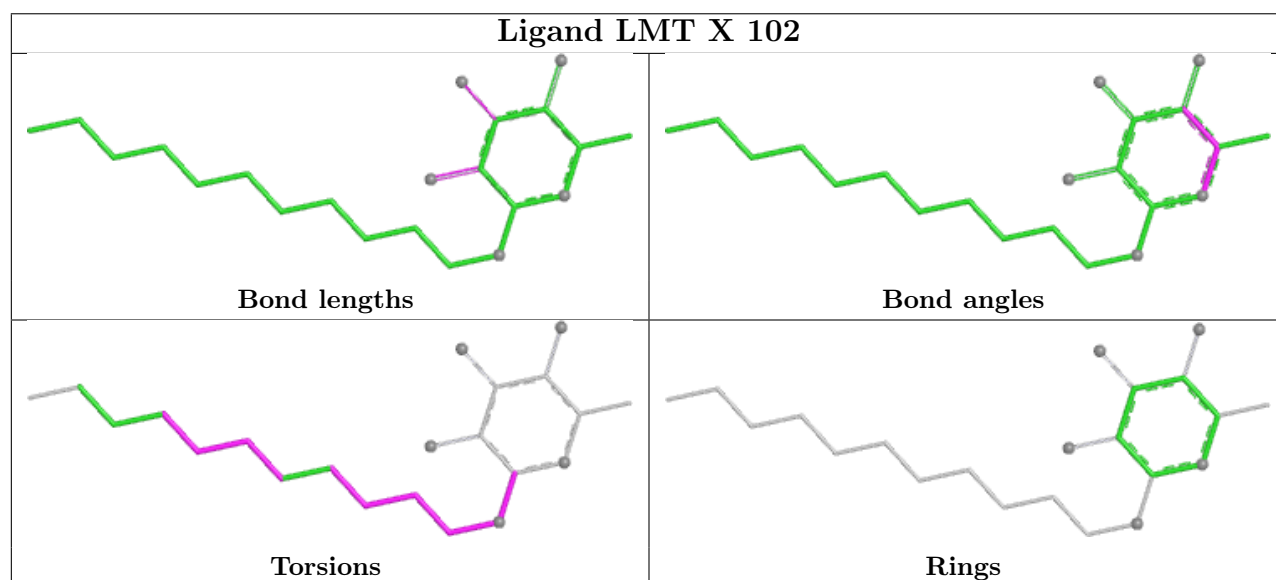
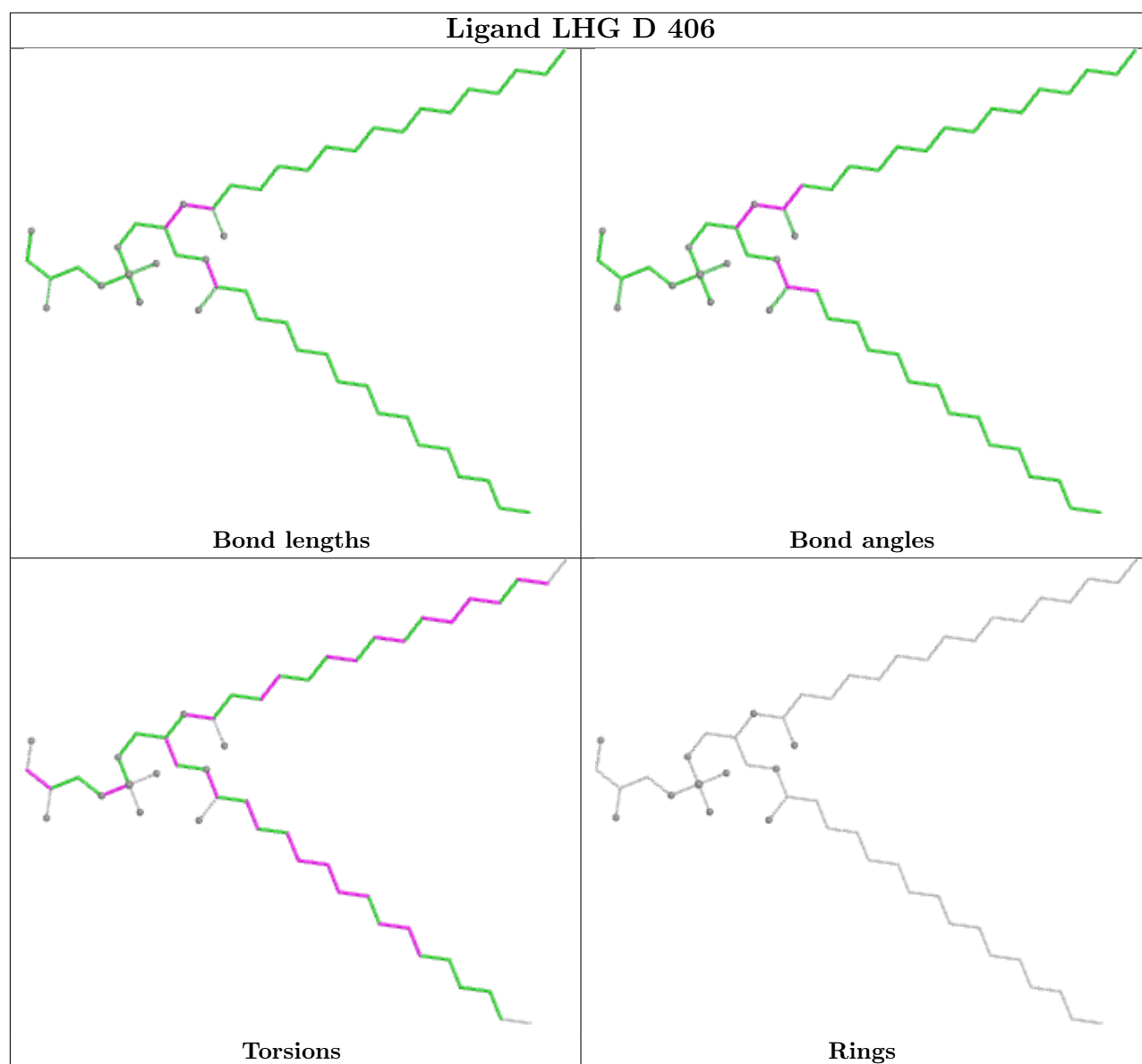


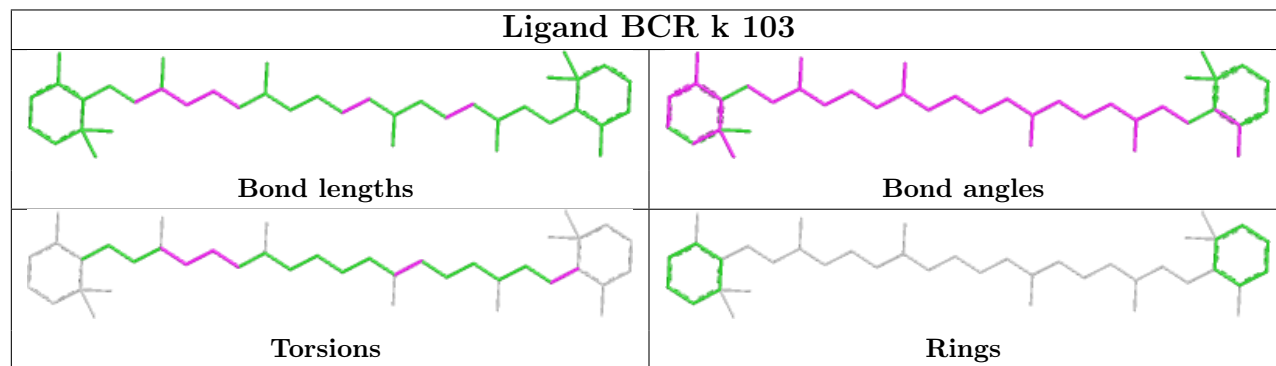
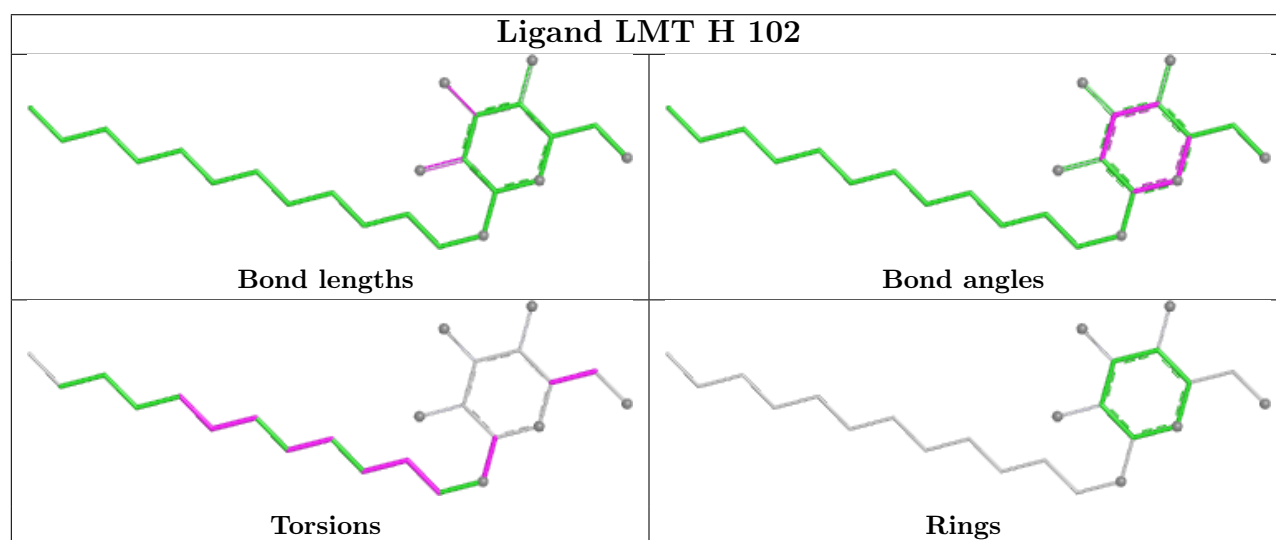
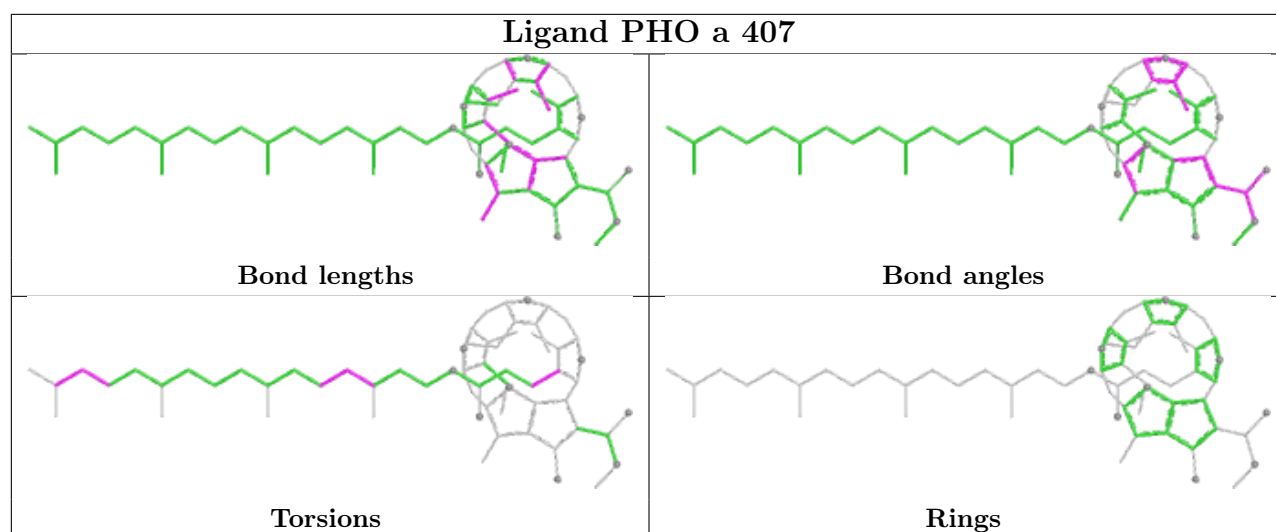


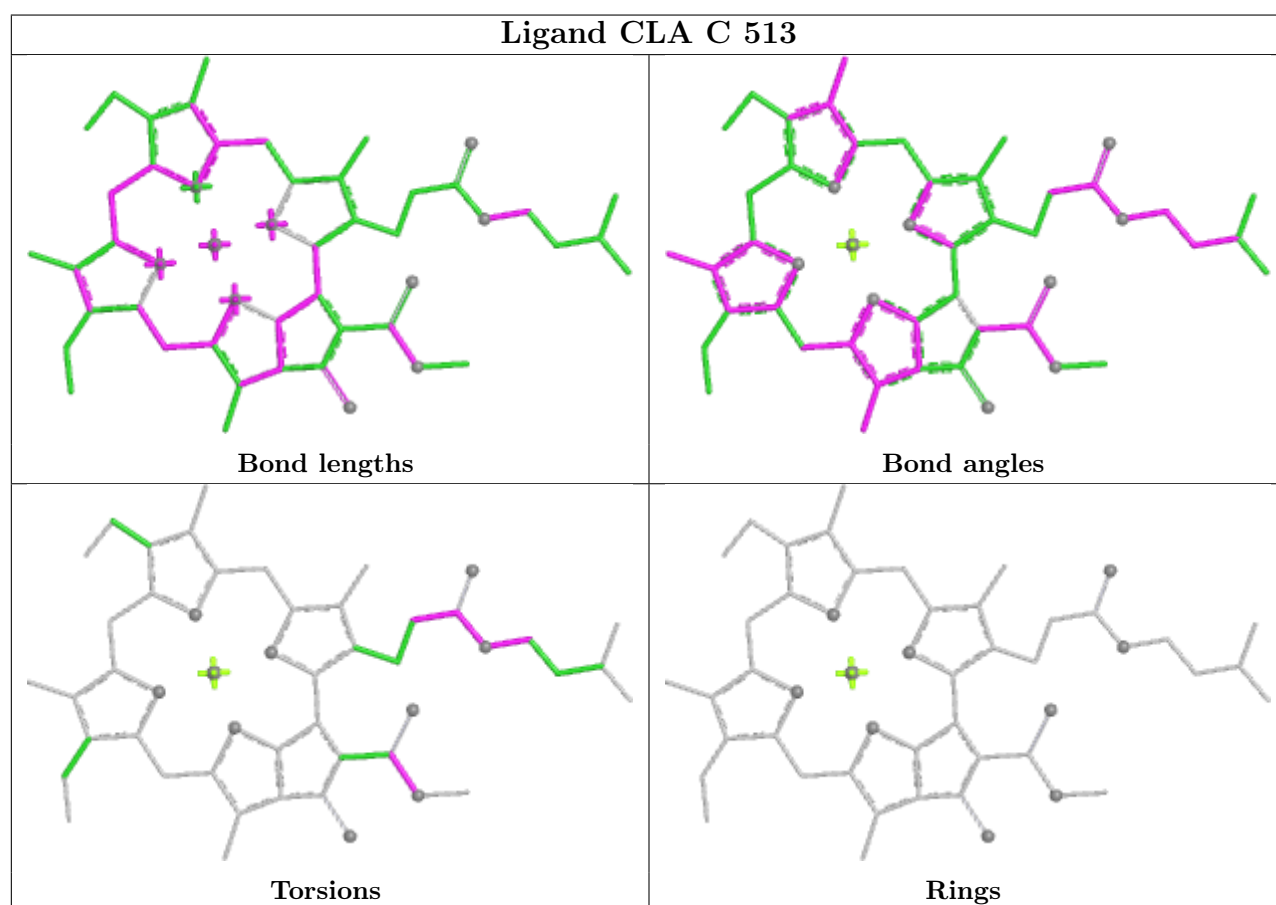
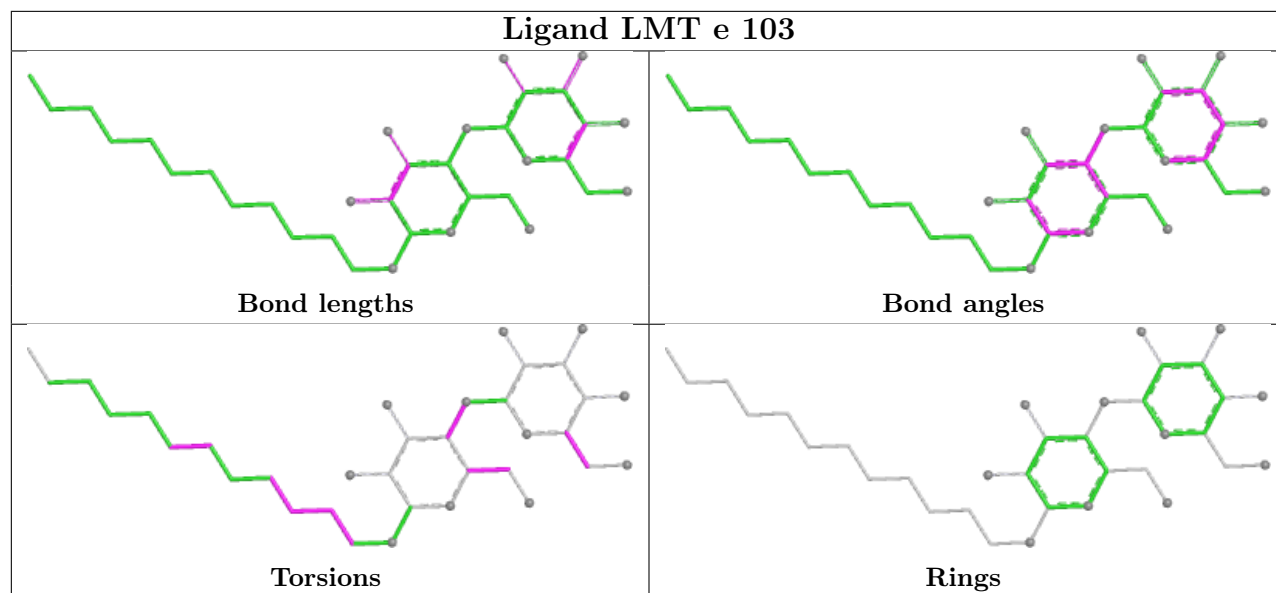


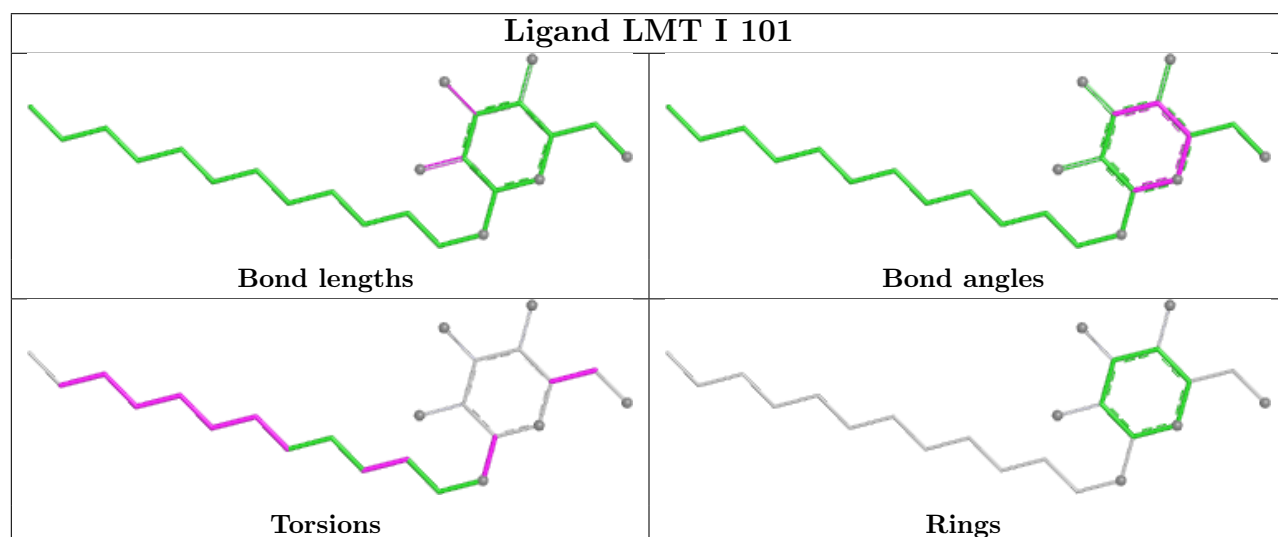
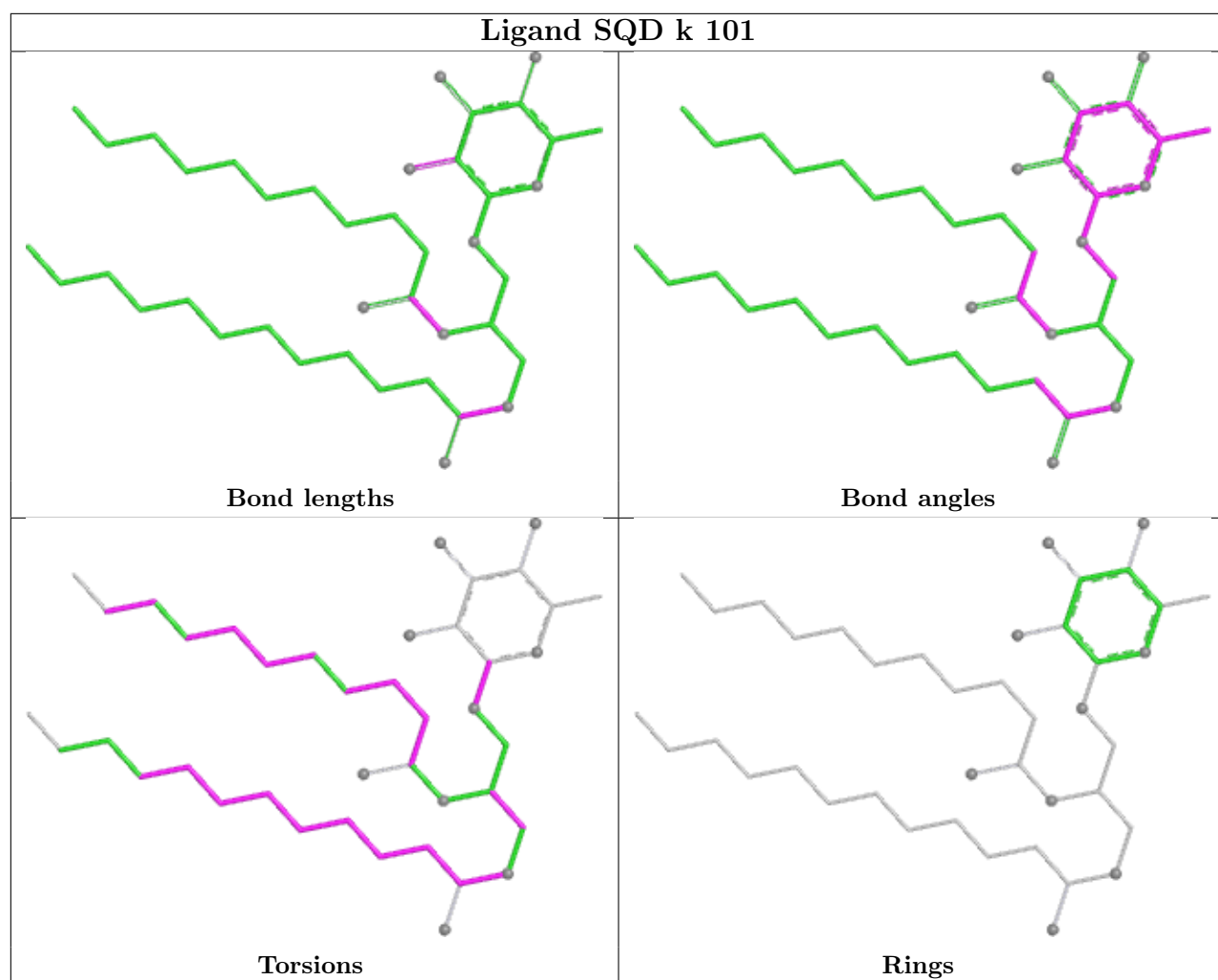


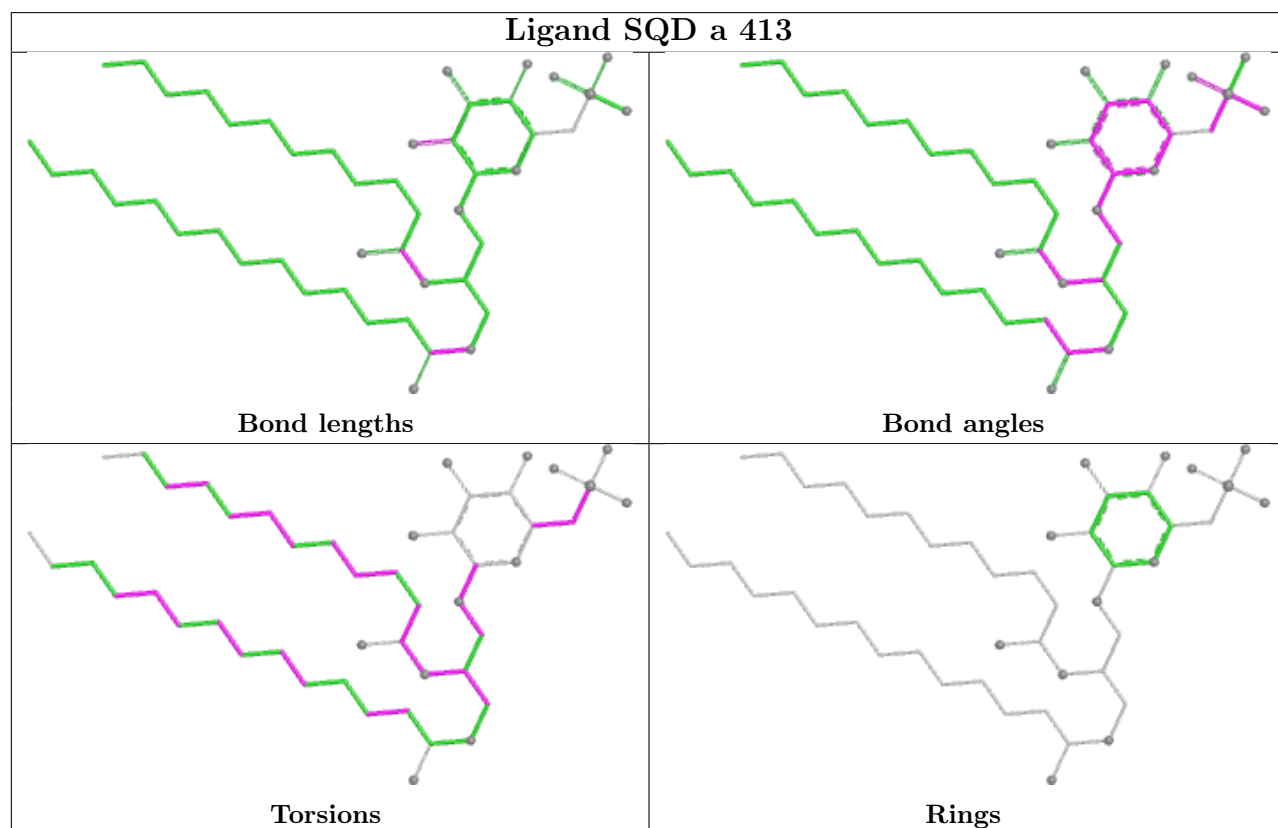
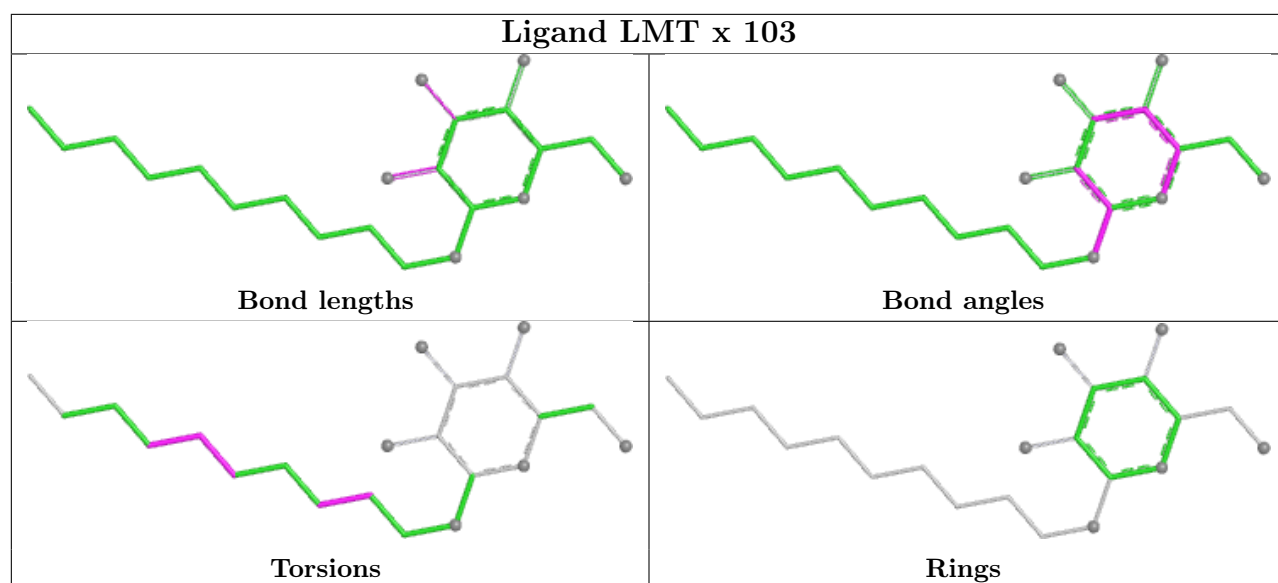


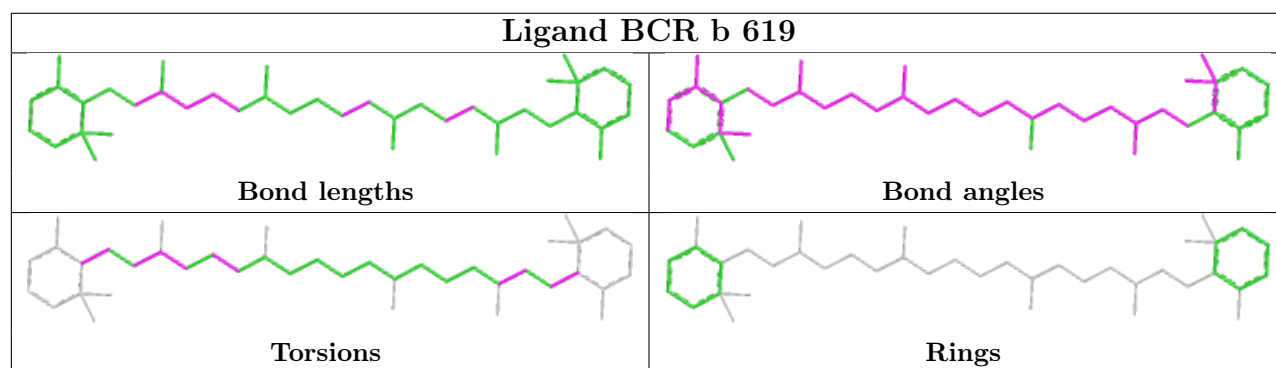
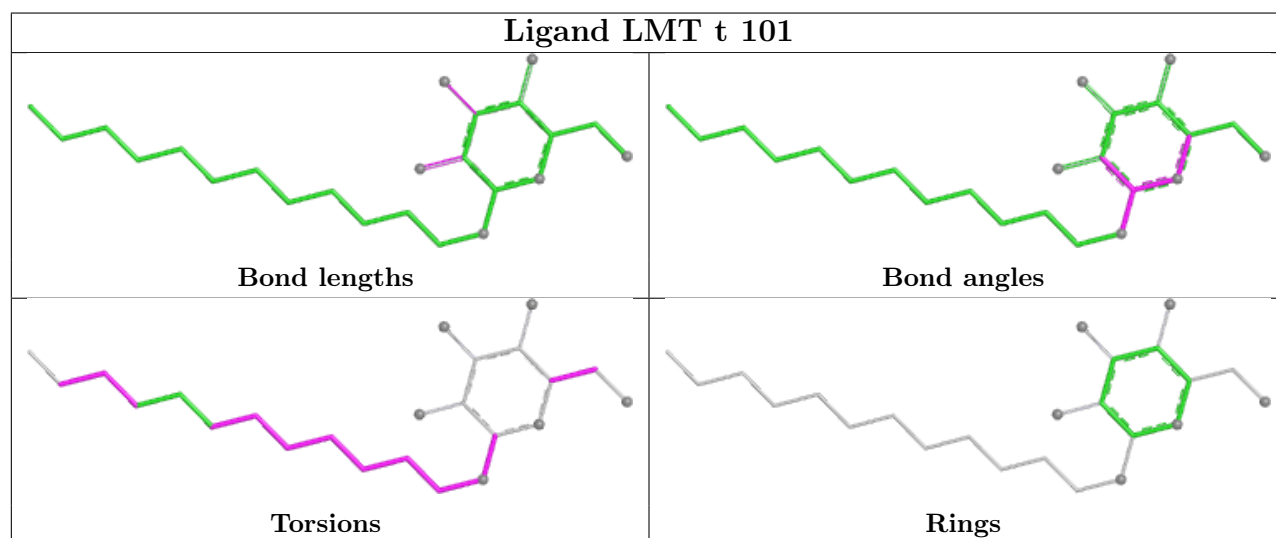
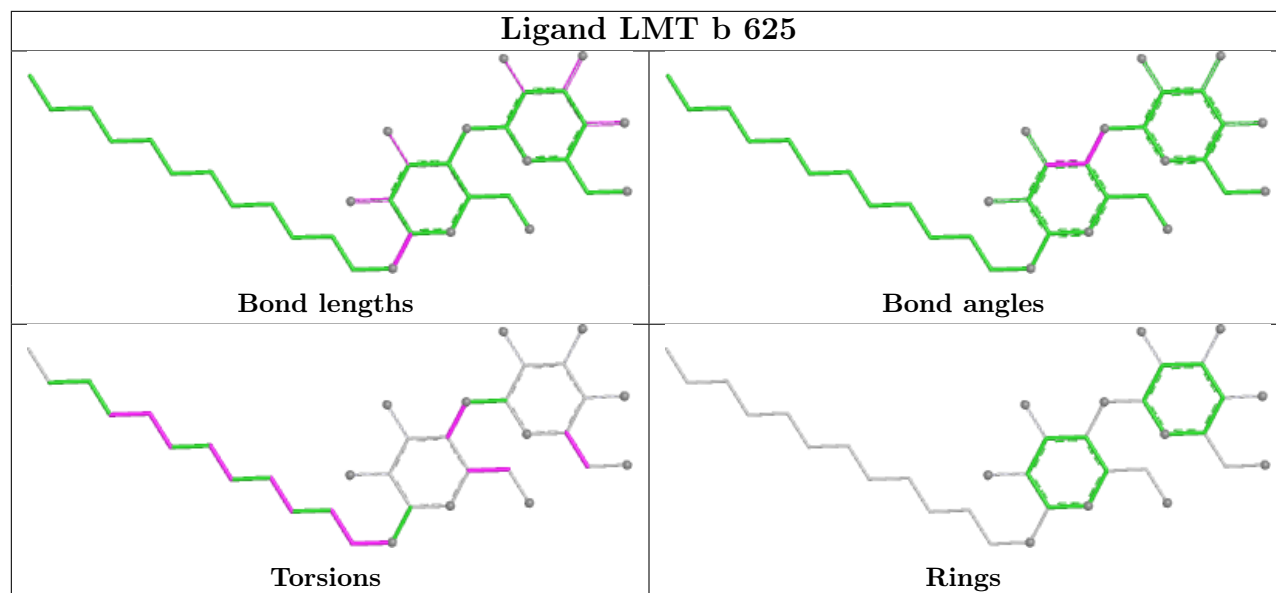


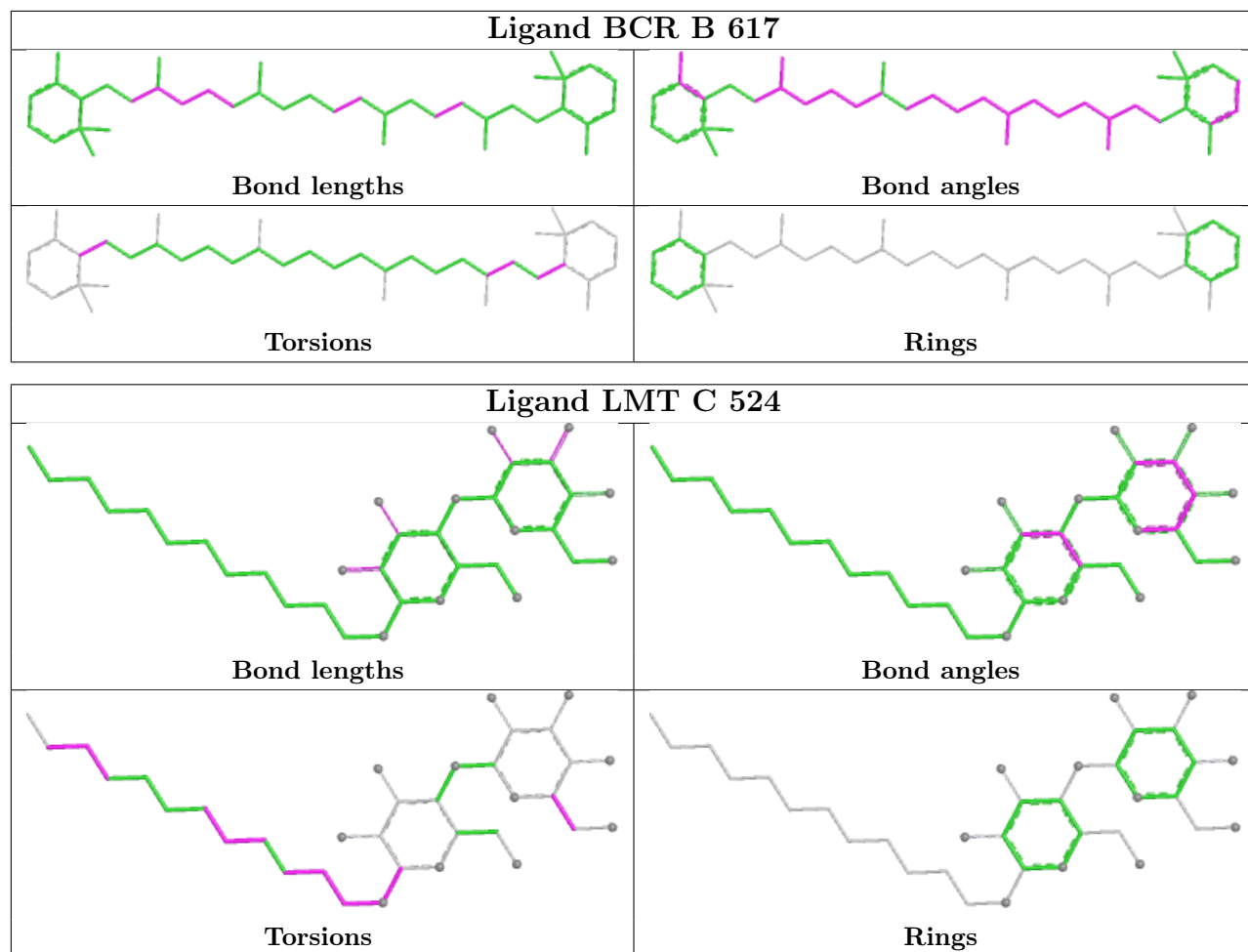


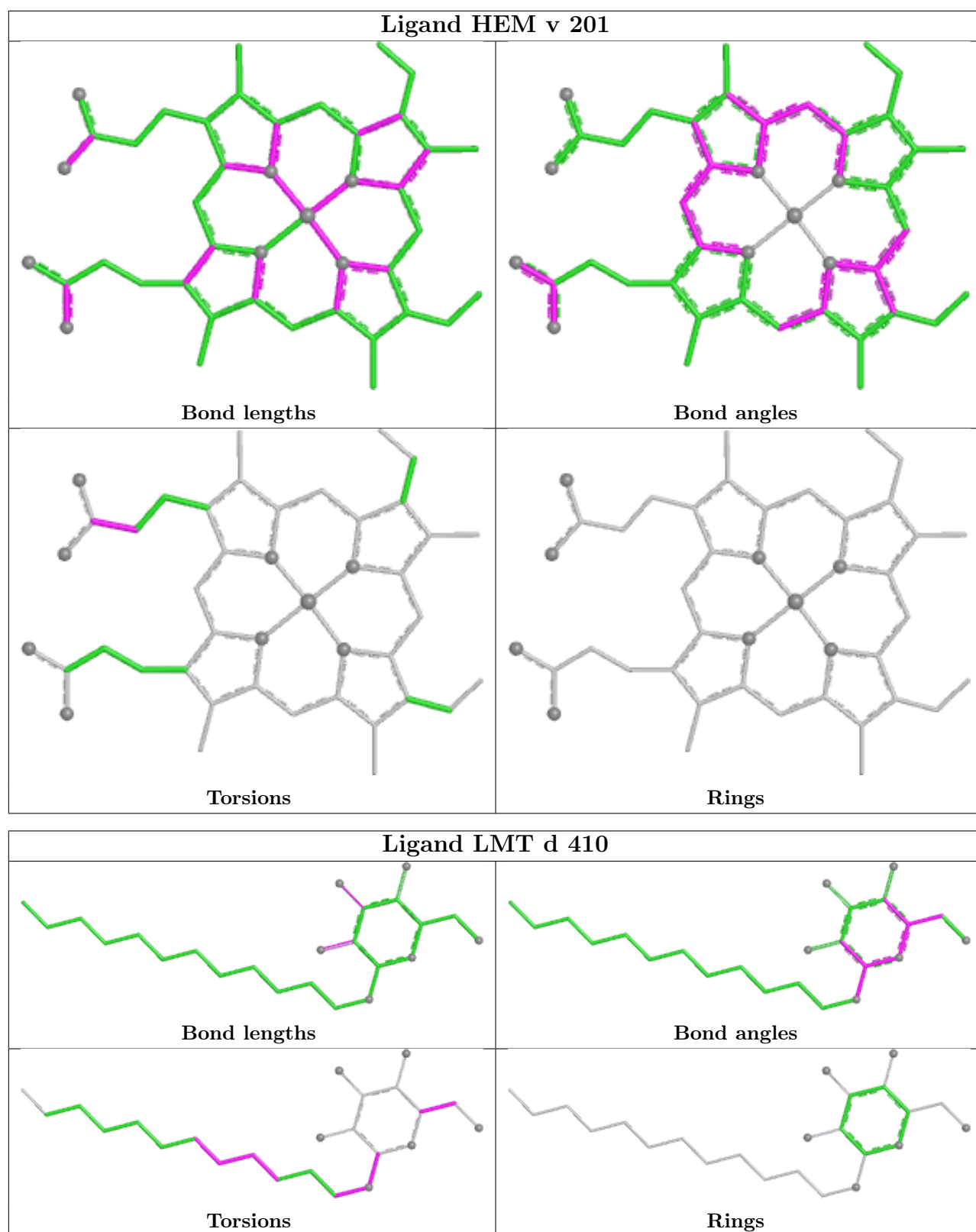


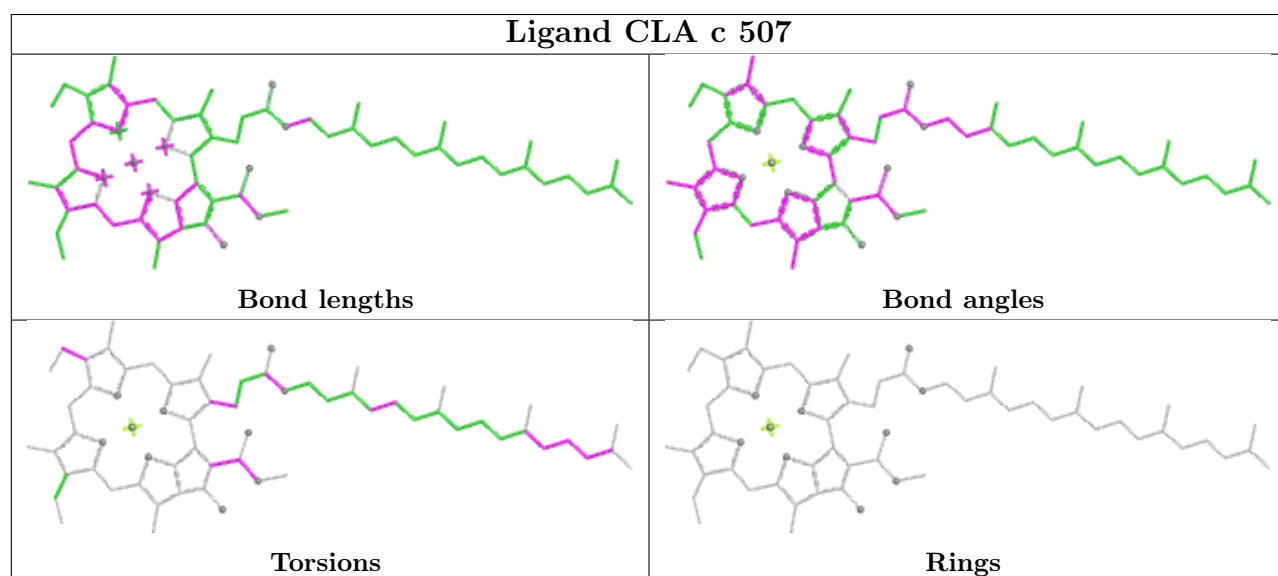
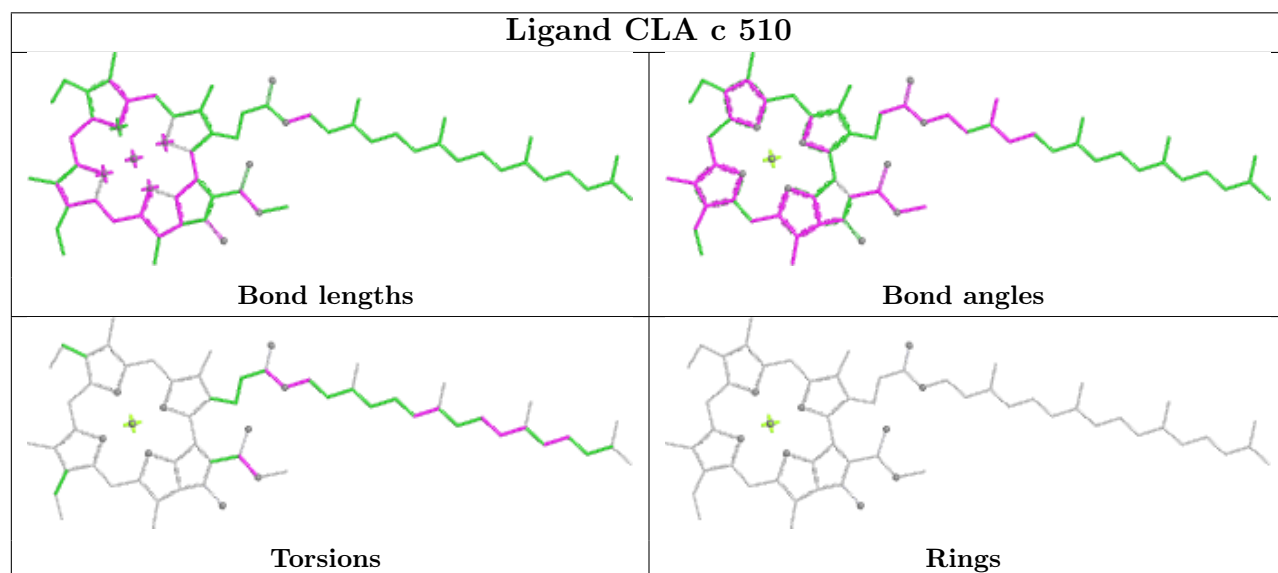
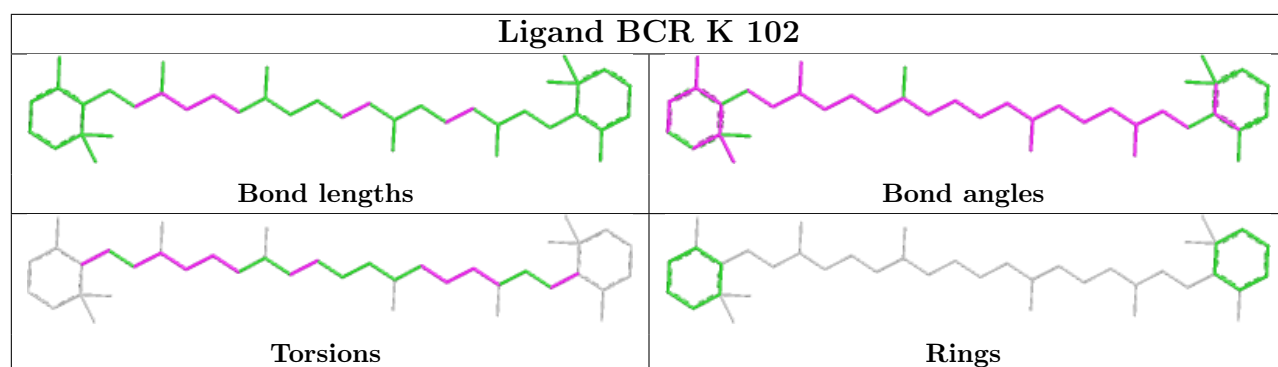


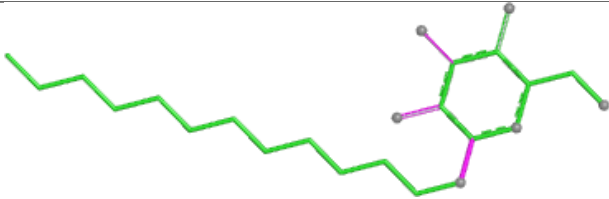
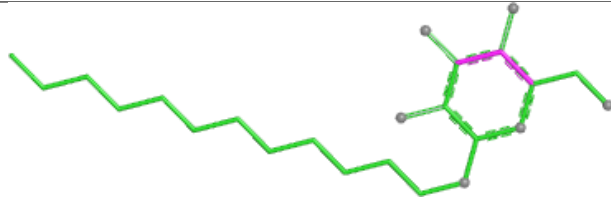
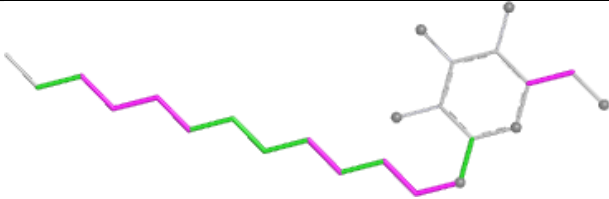


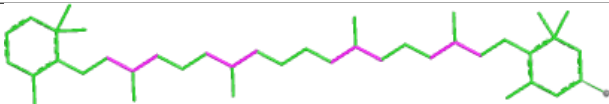
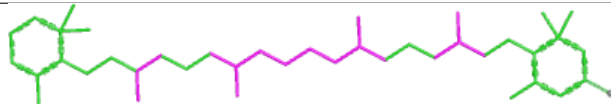
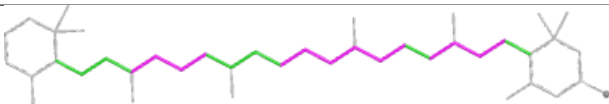
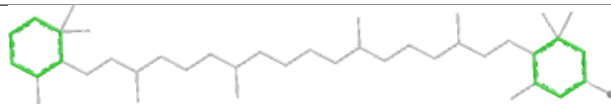


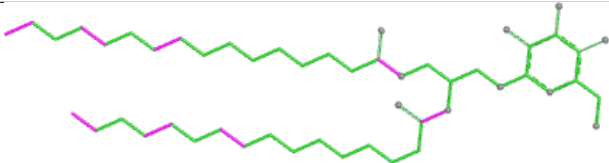
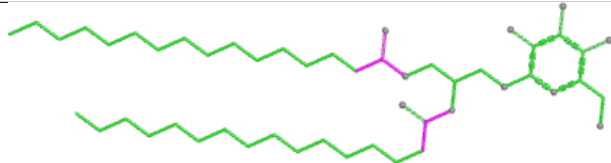
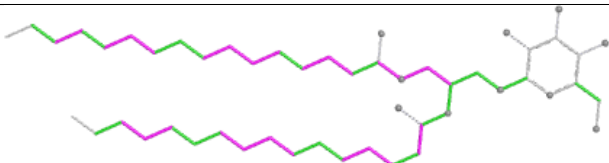
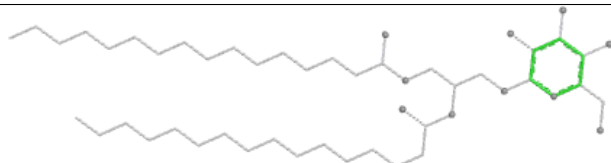


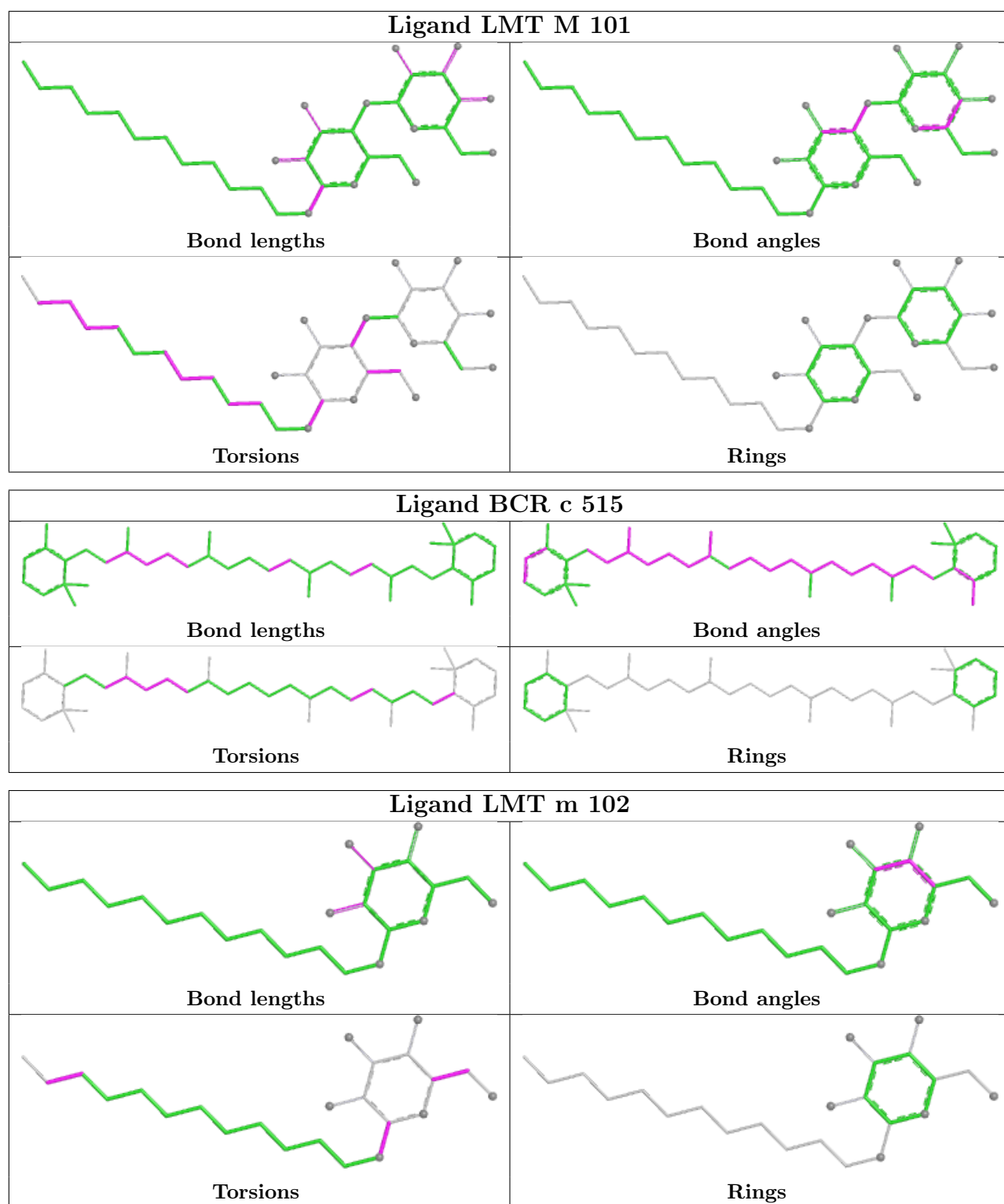


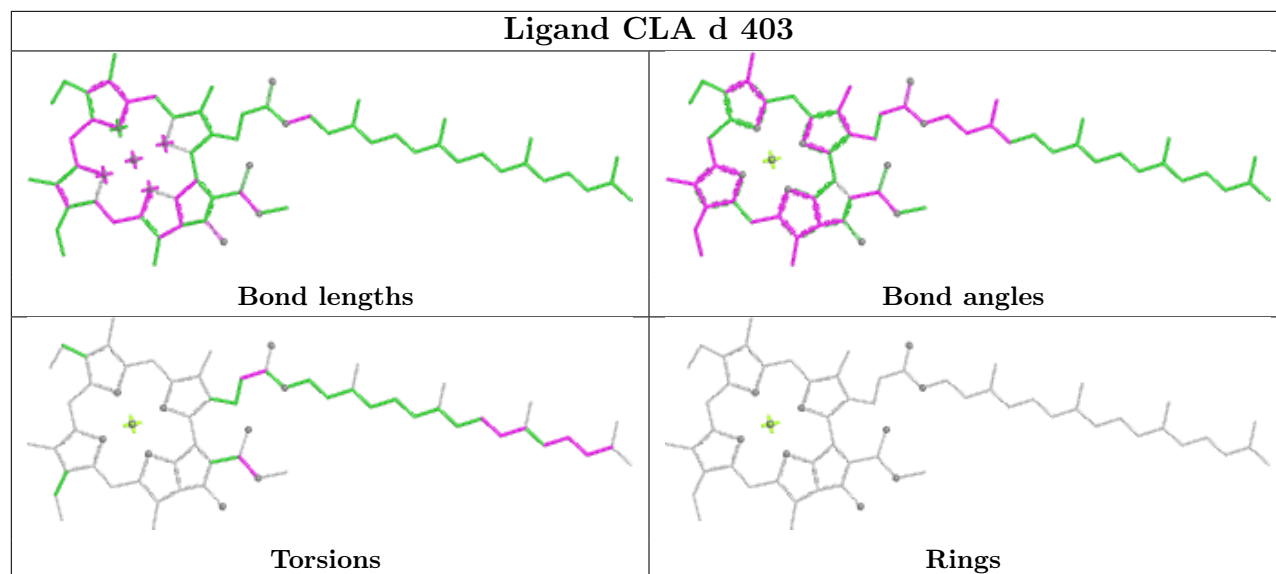
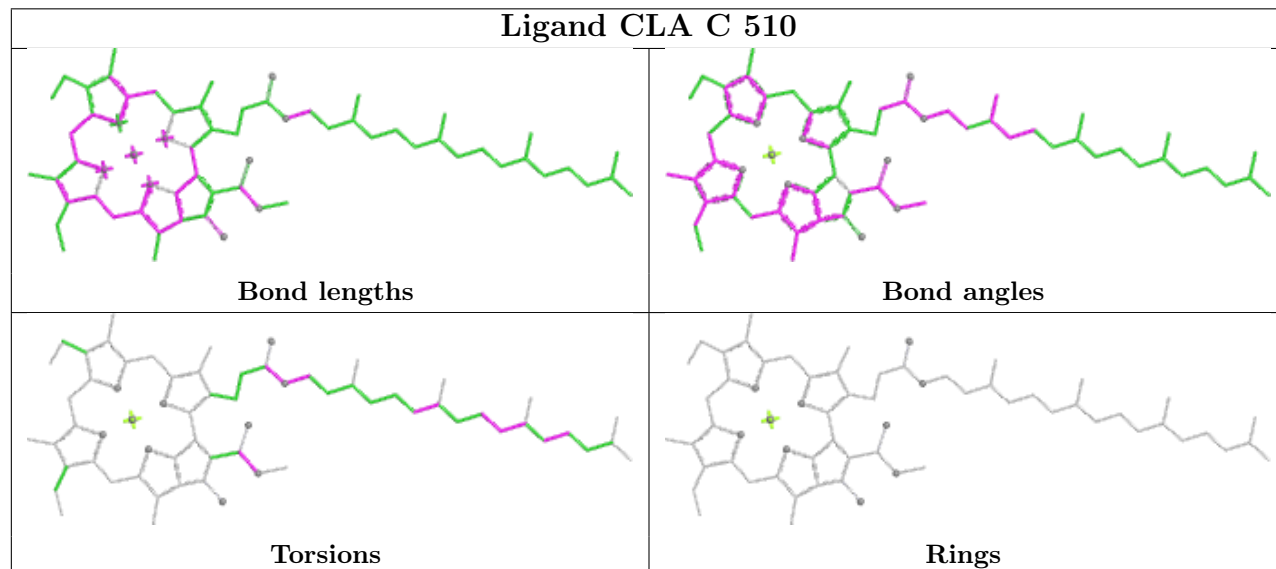
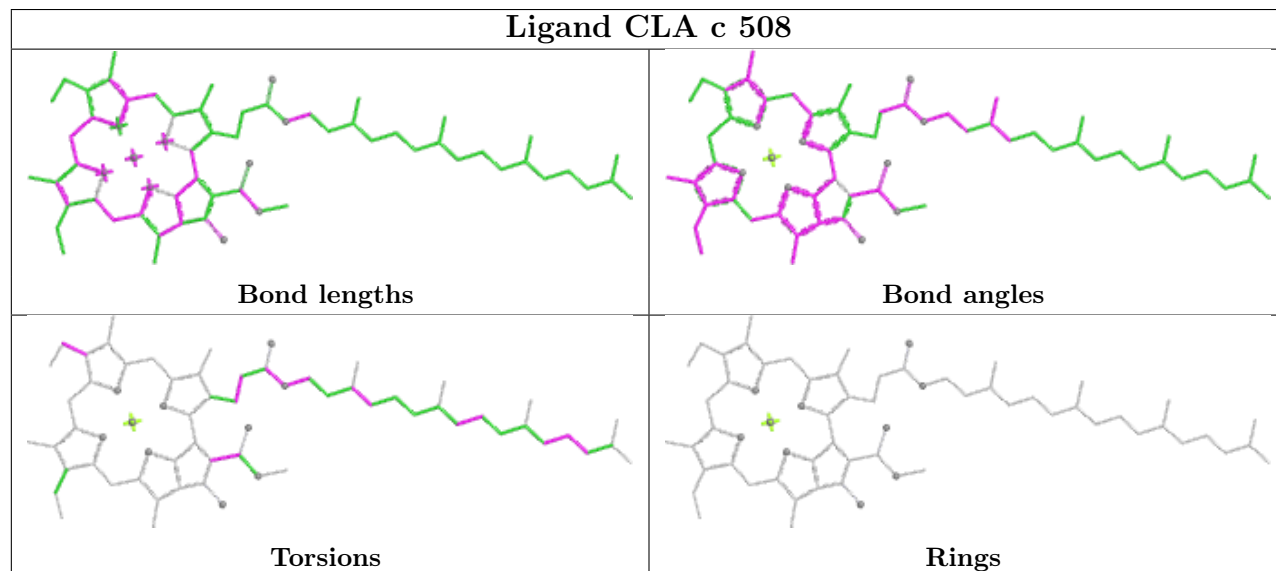


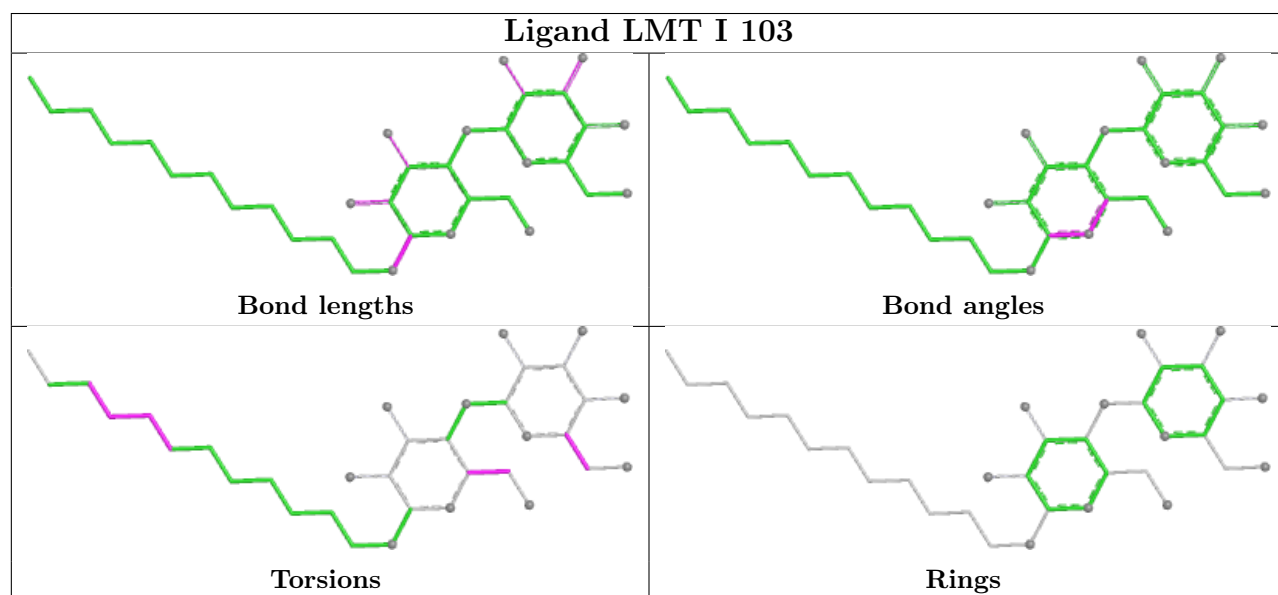
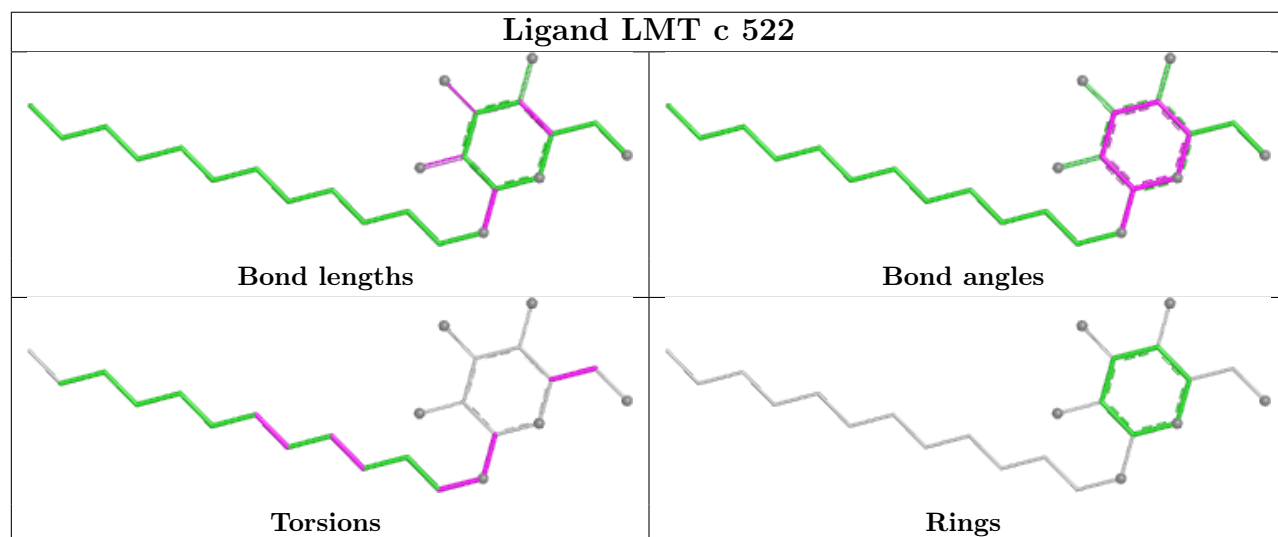
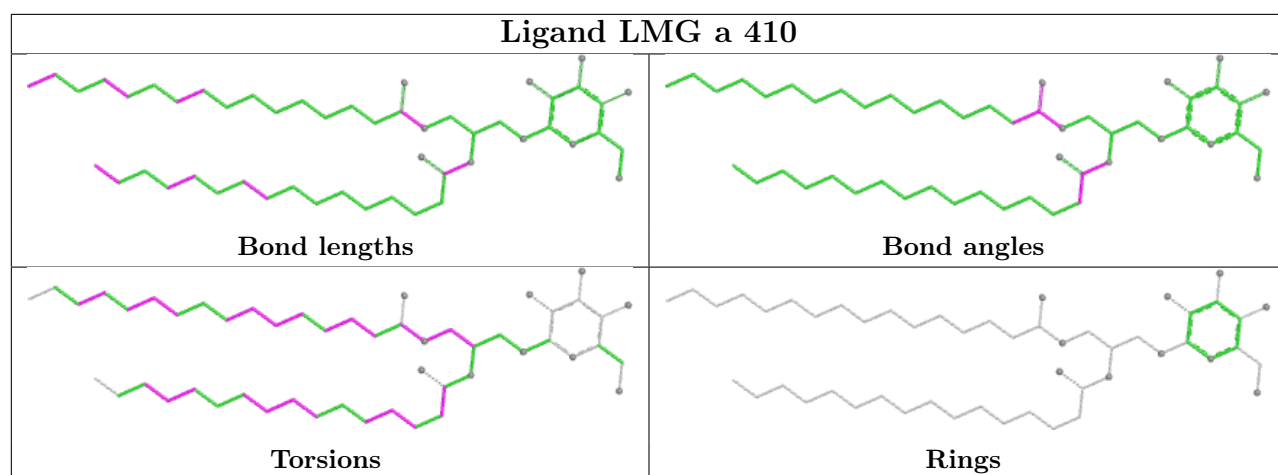
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Bond lengths	Bond angles
	
Torsions	Rings

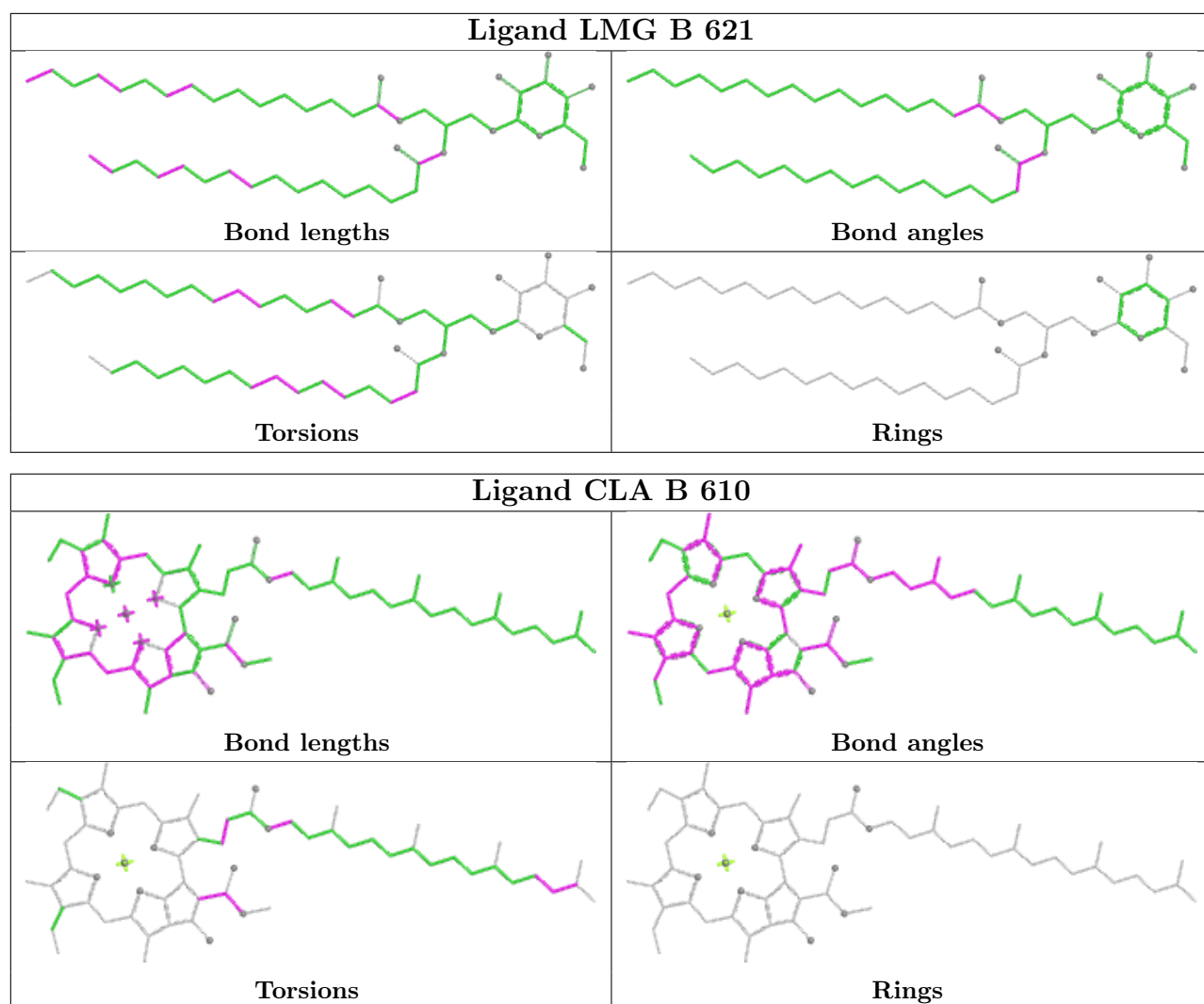
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Bond lengths	Bond angles
	
Torsions	Rings

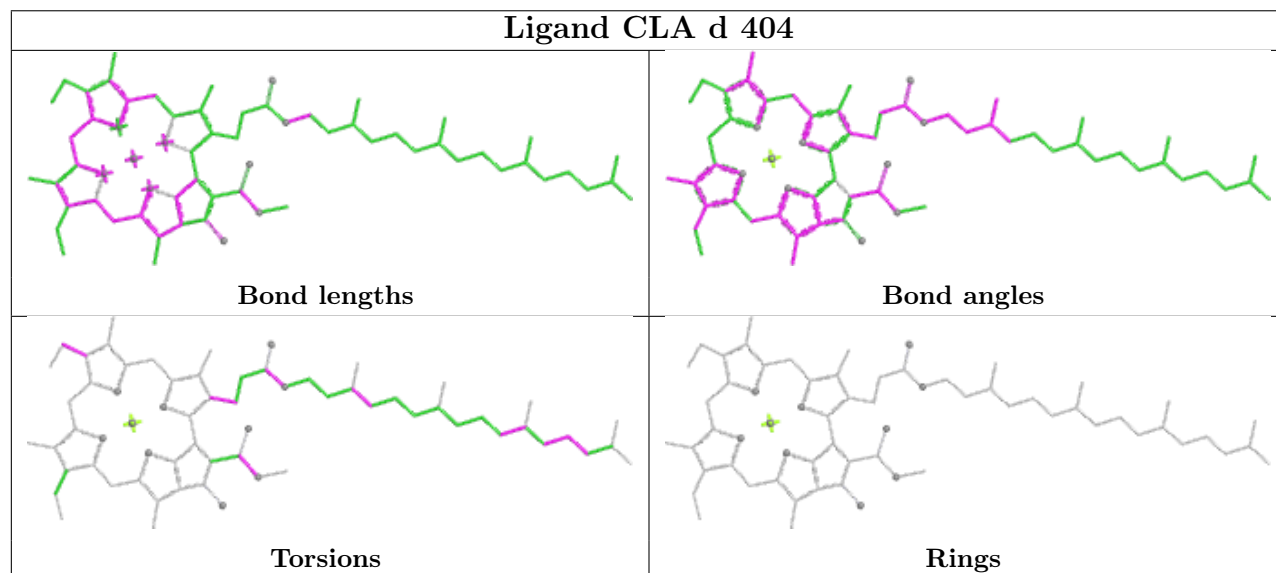
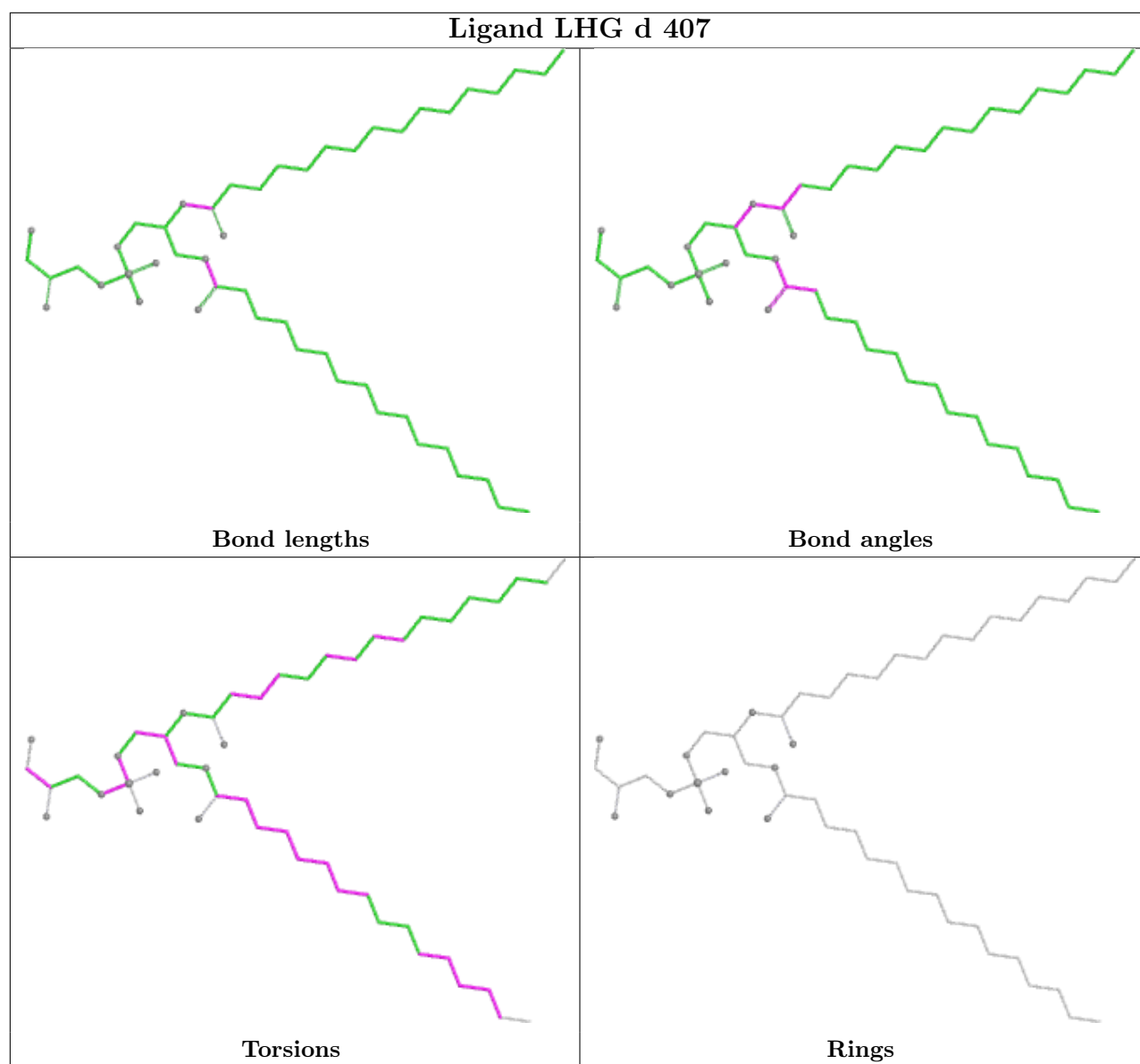
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Bond lengths	Bond angles
	
Torsions	Rings

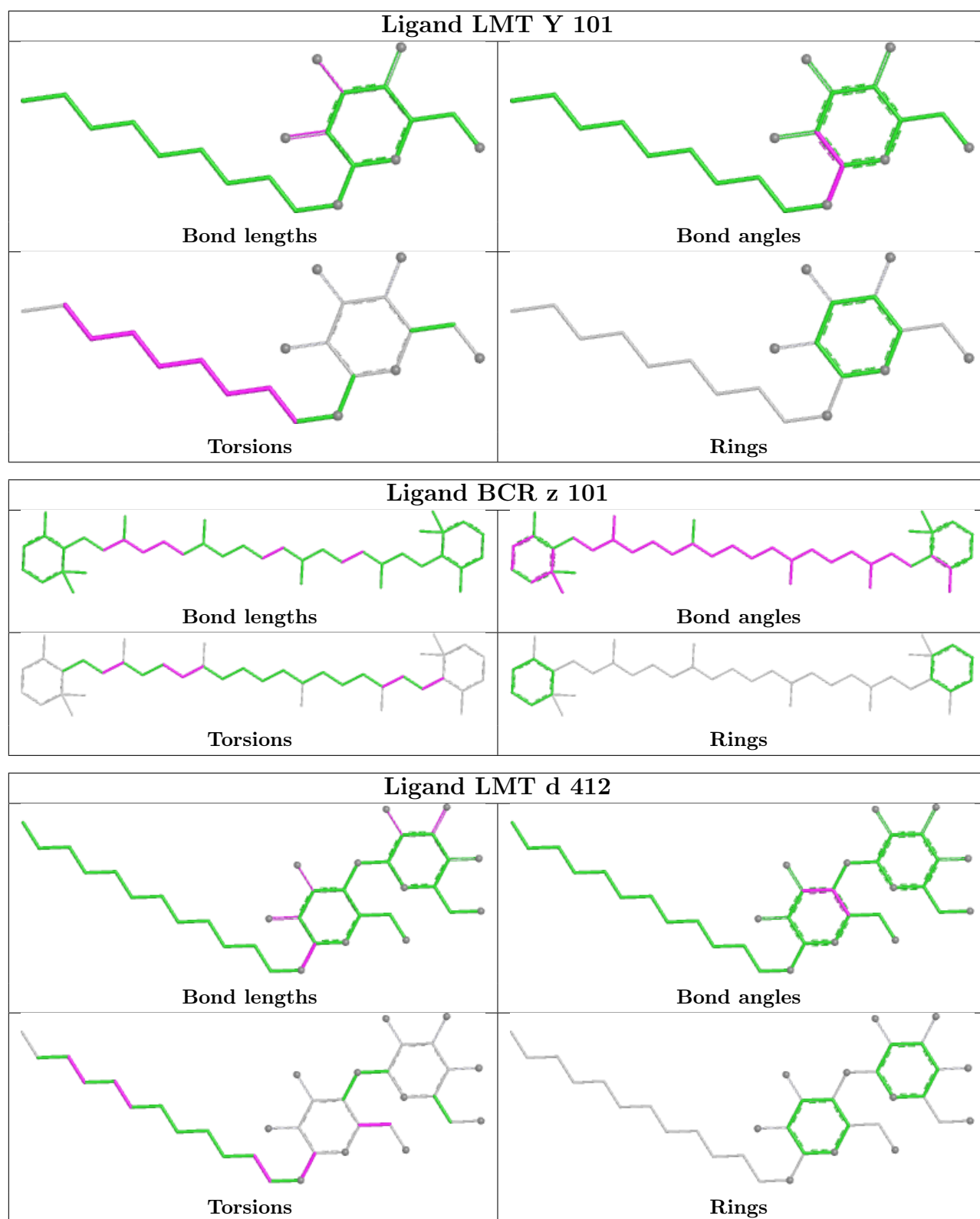


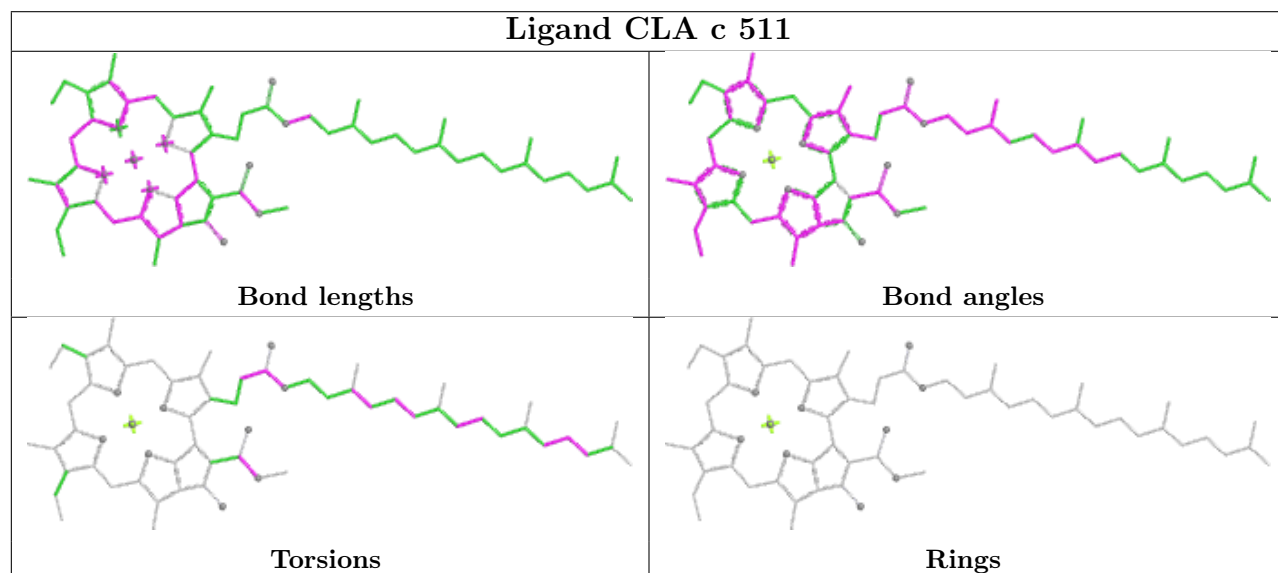
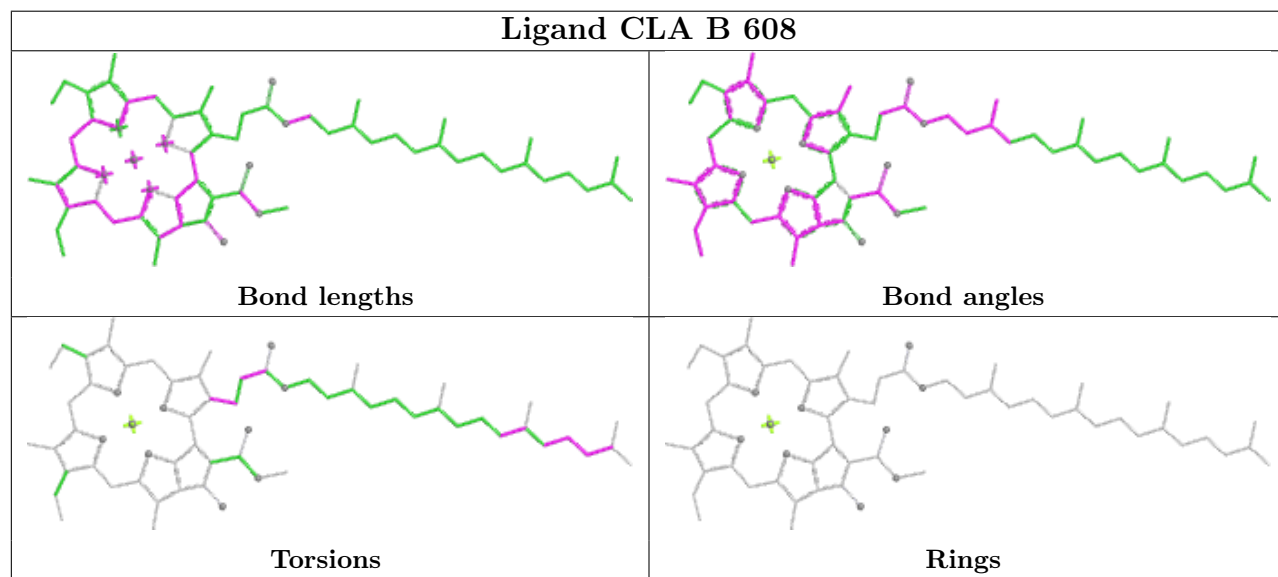
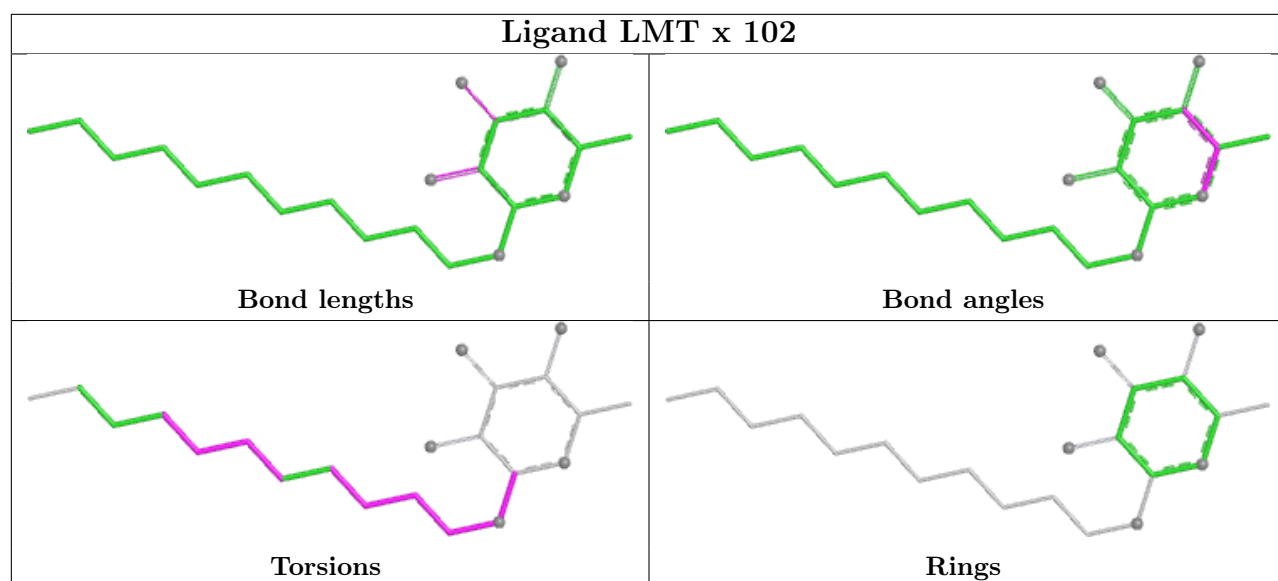
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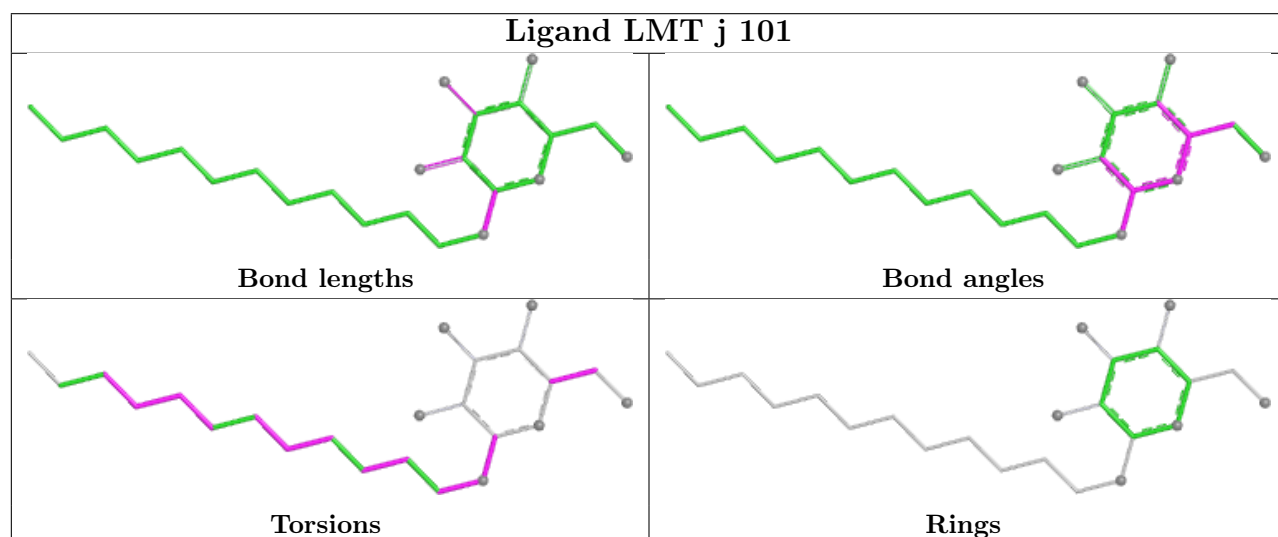
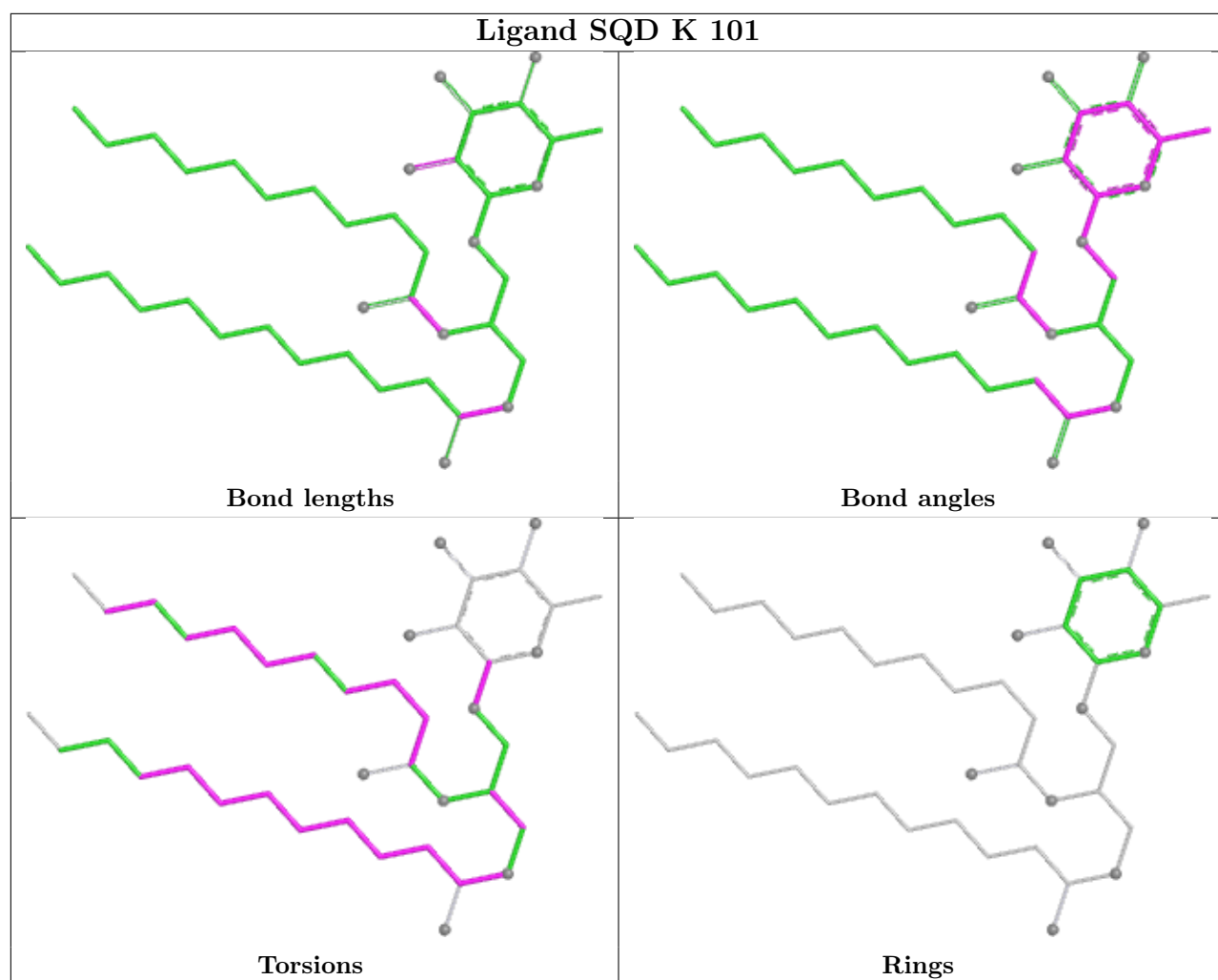


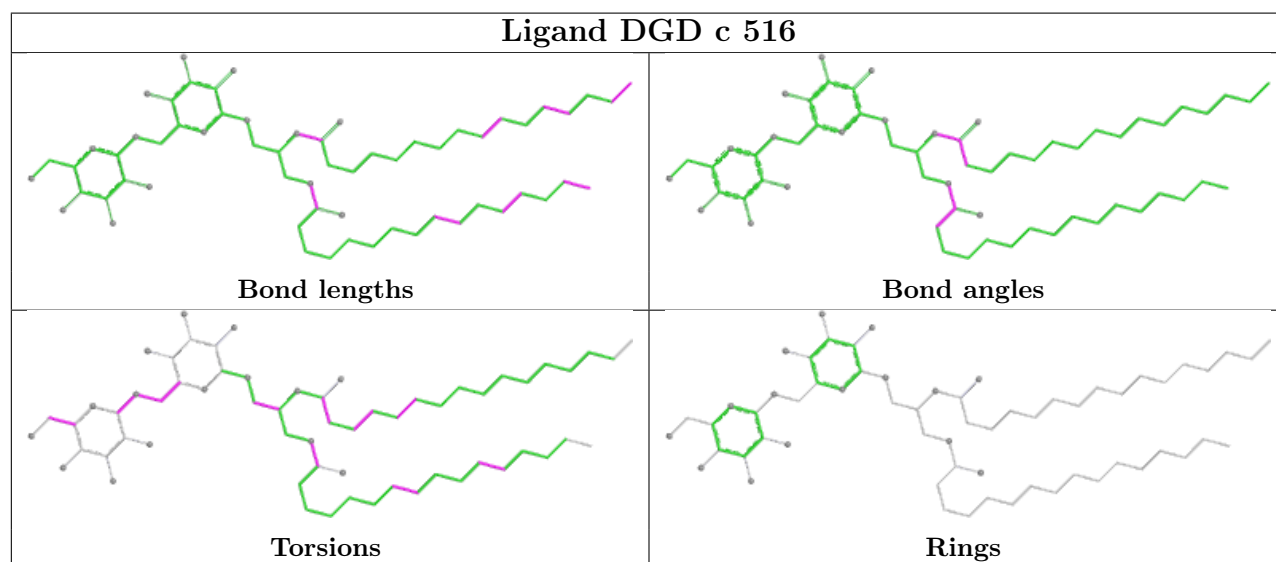
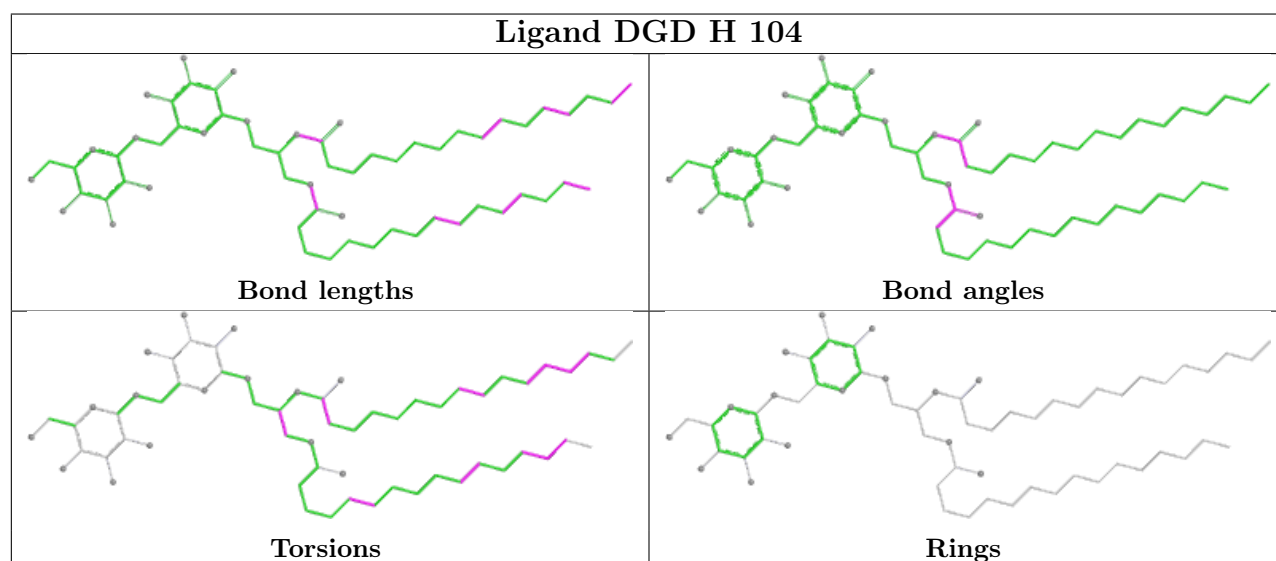
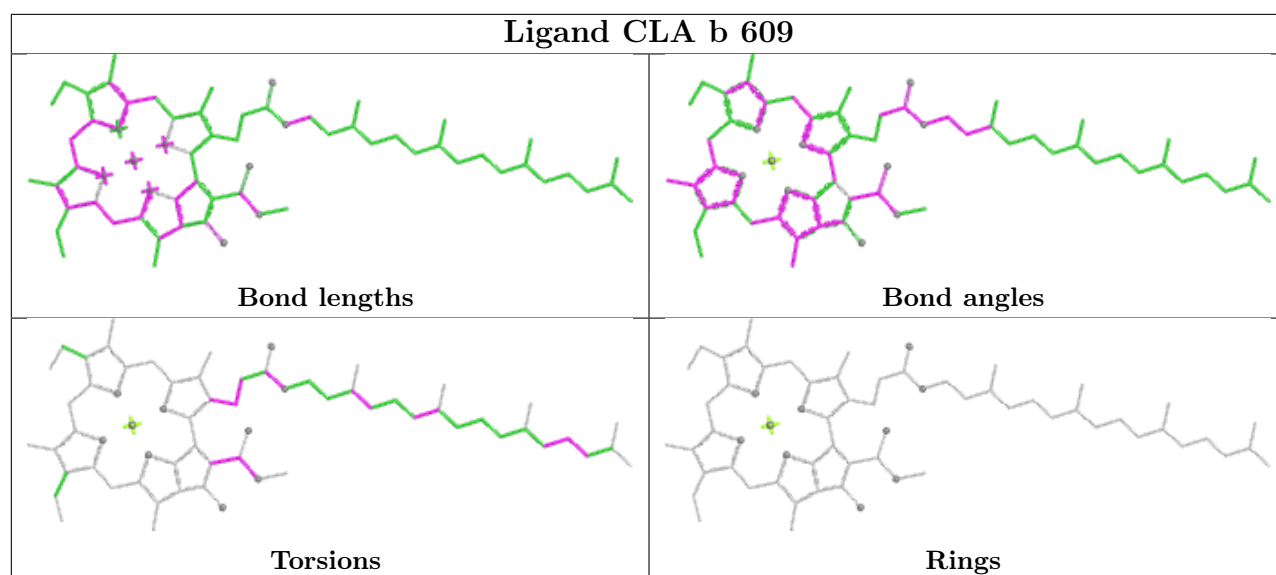


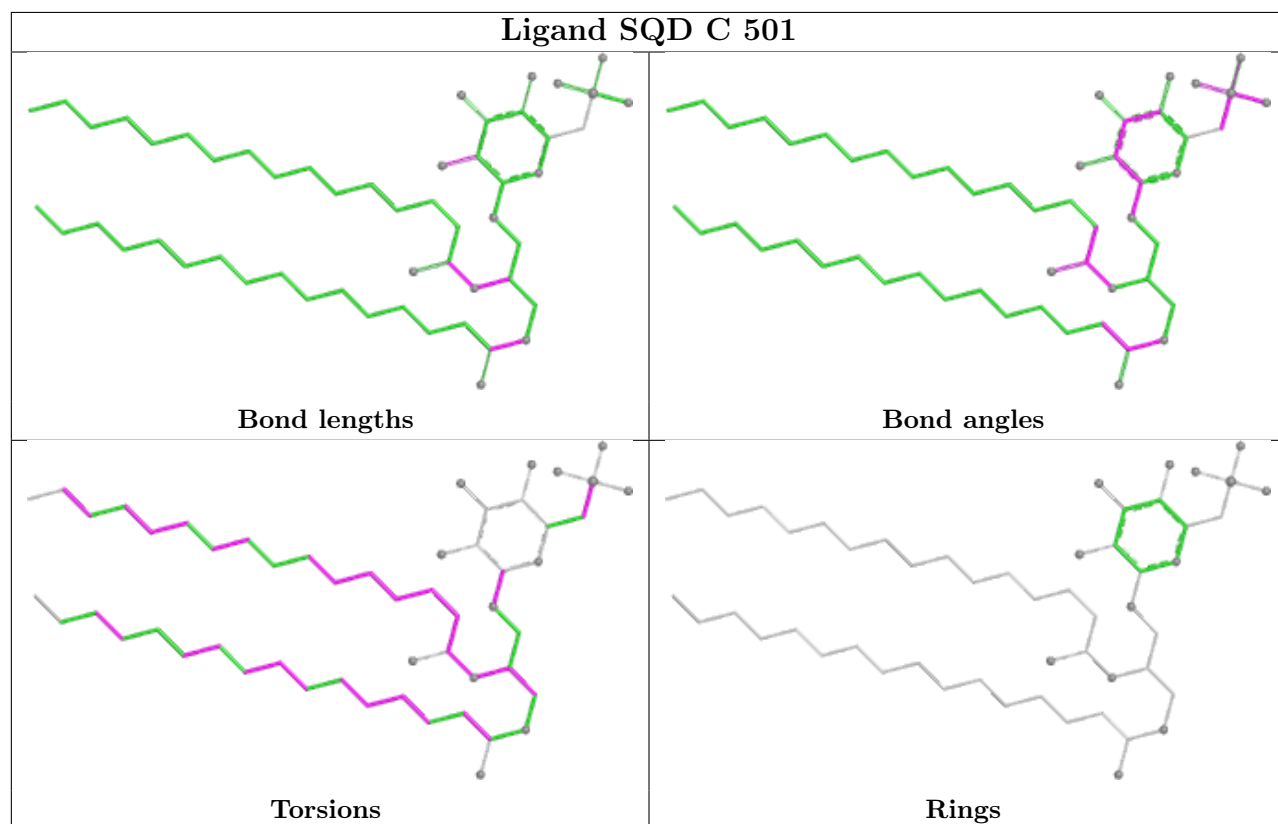
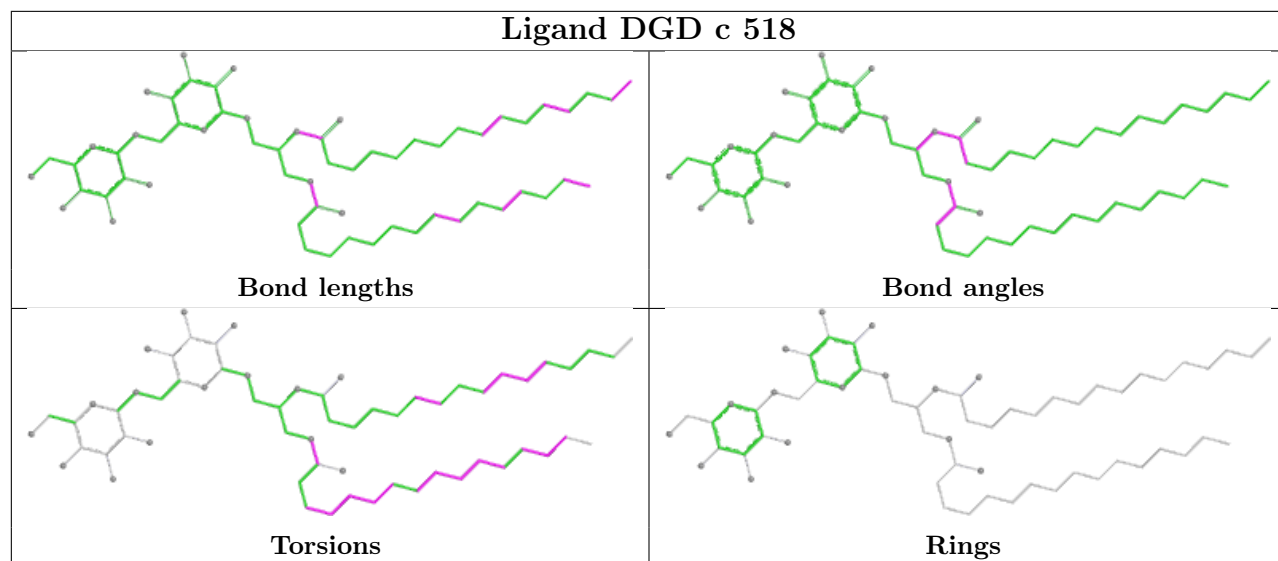


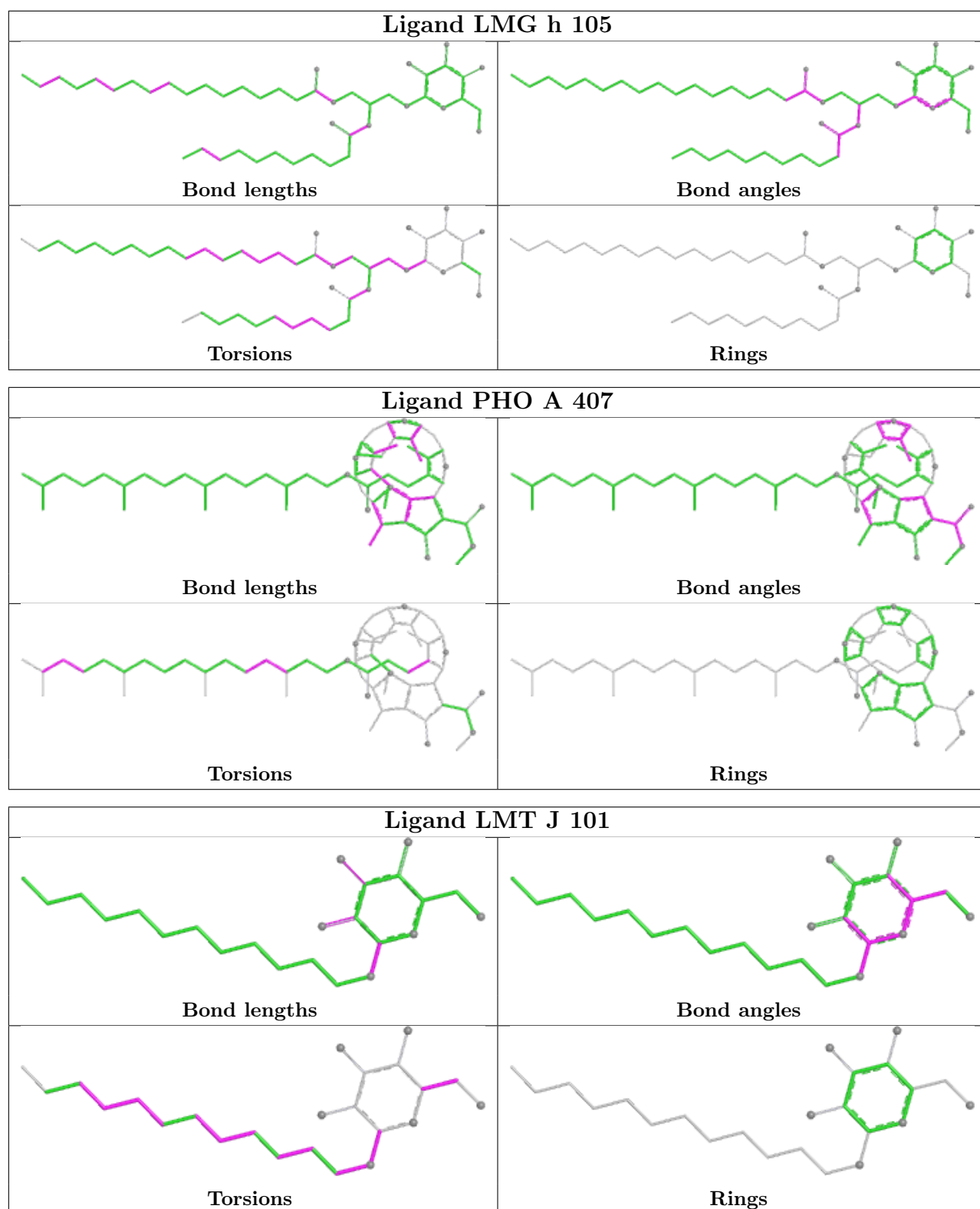


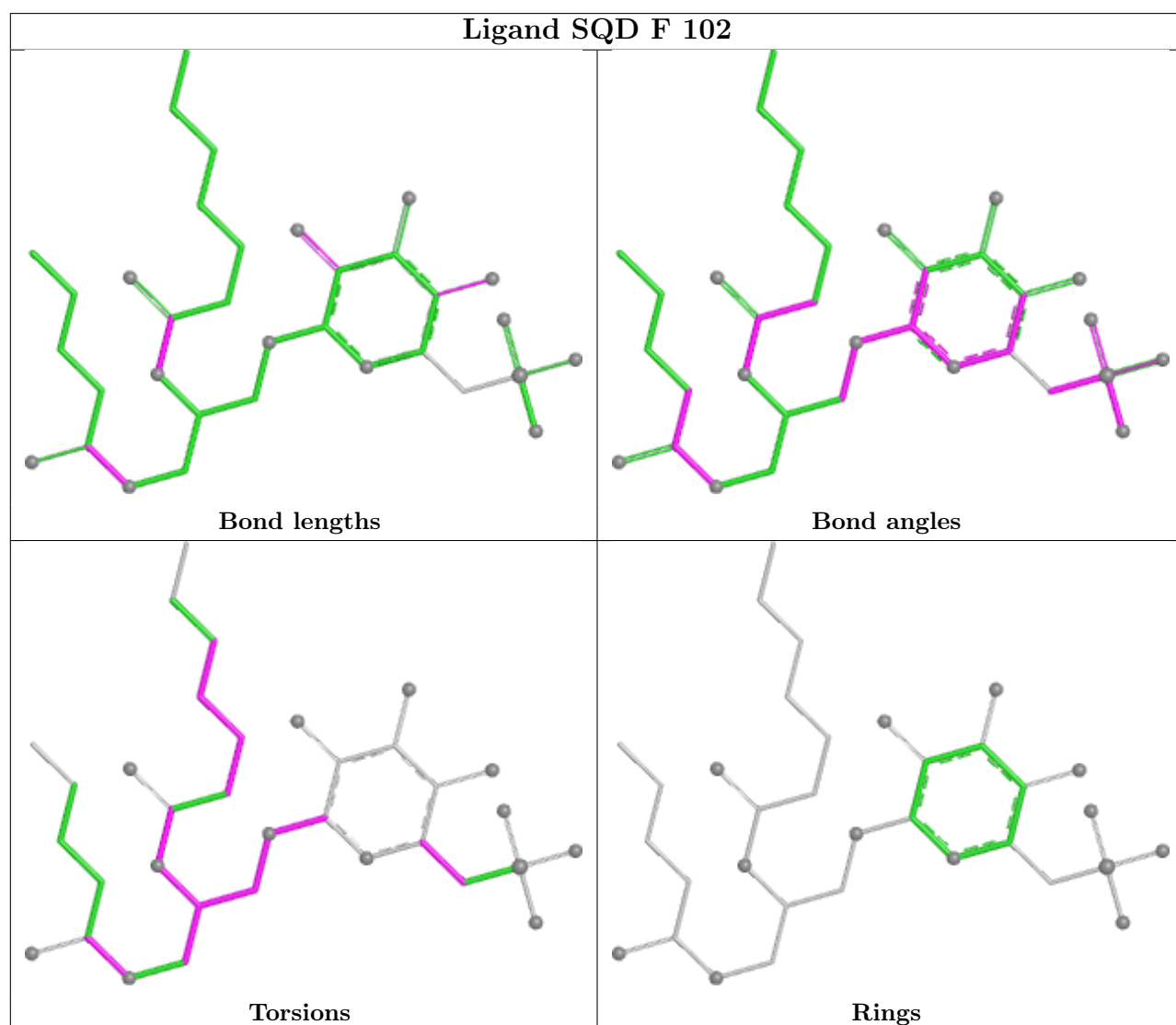
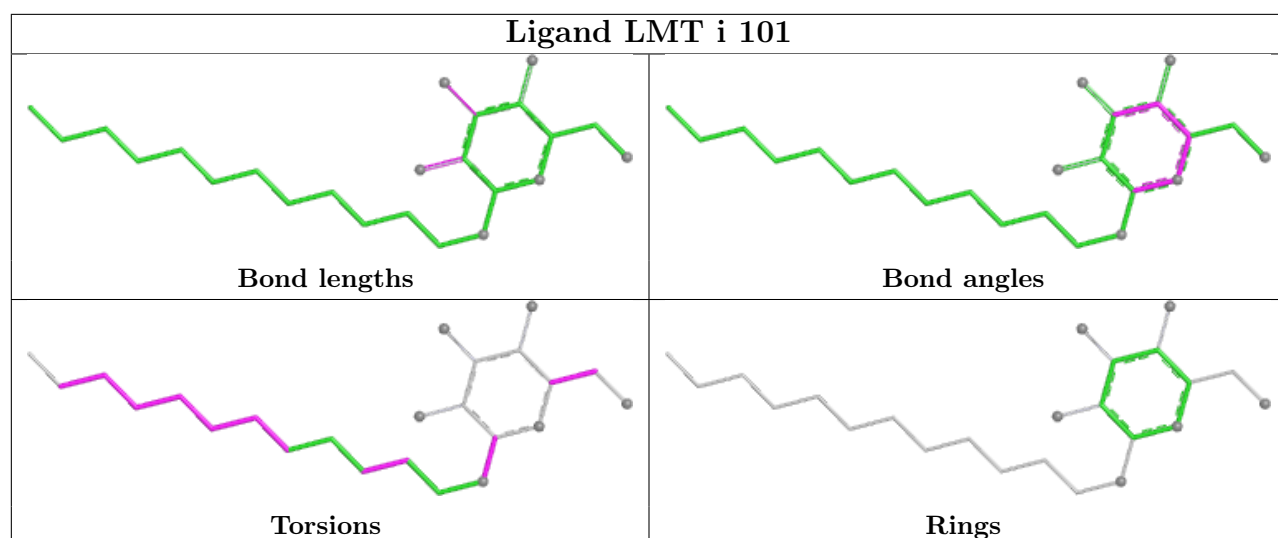




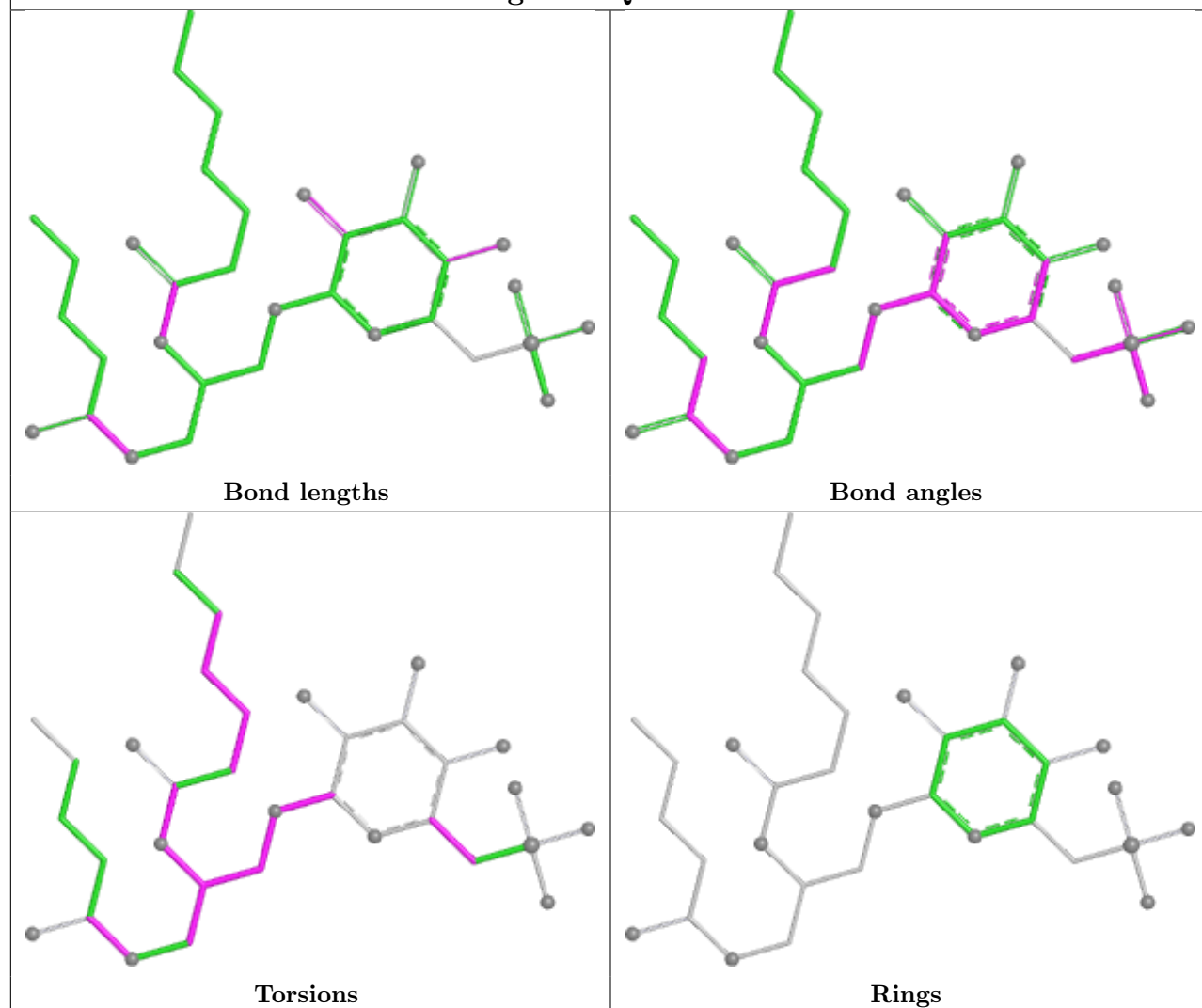




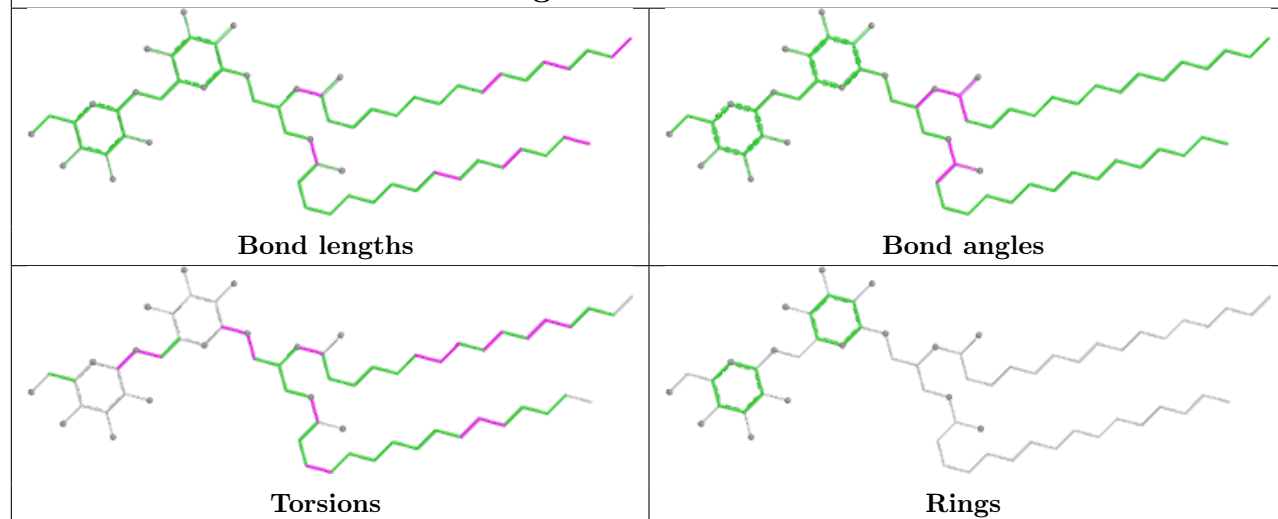


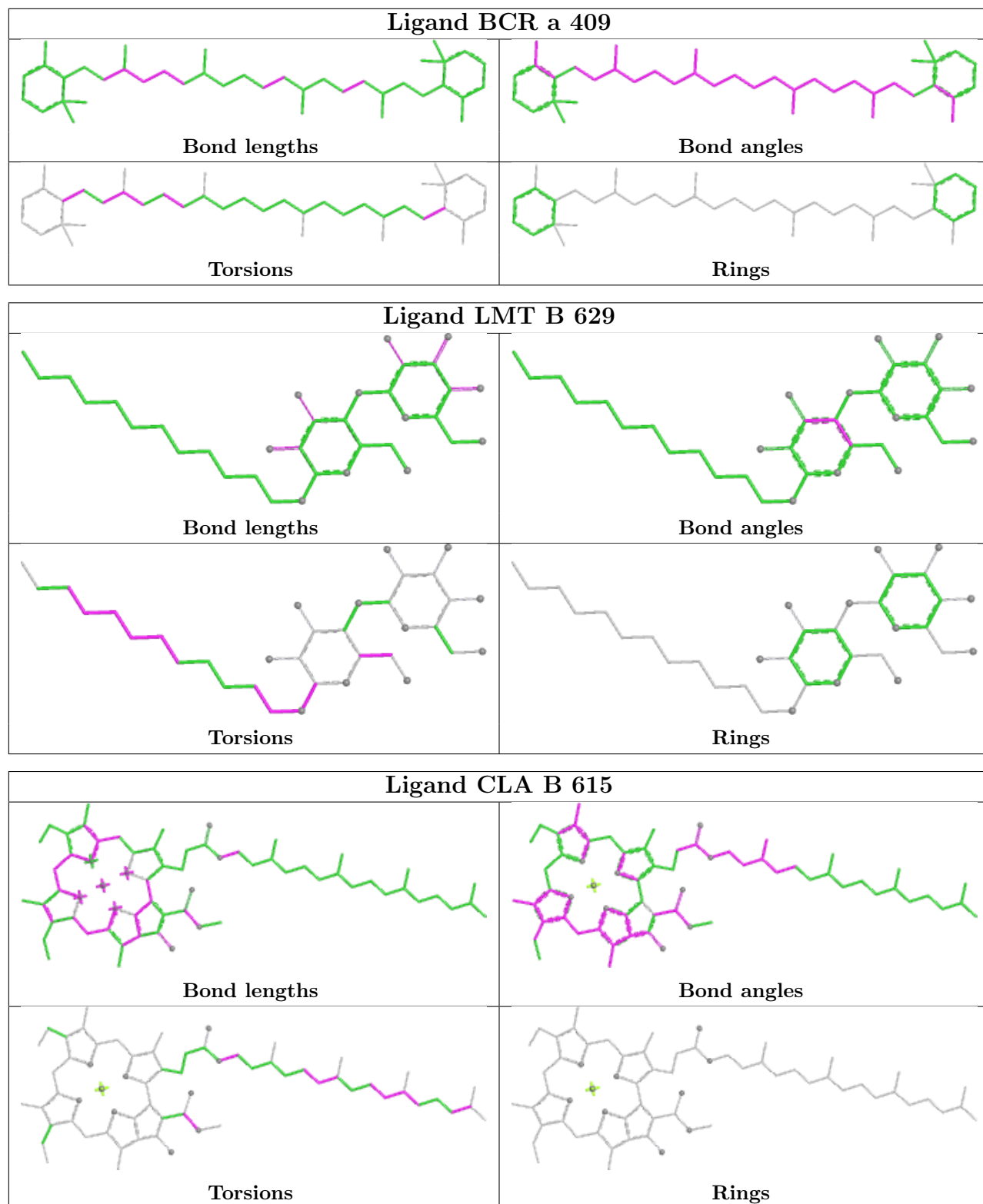


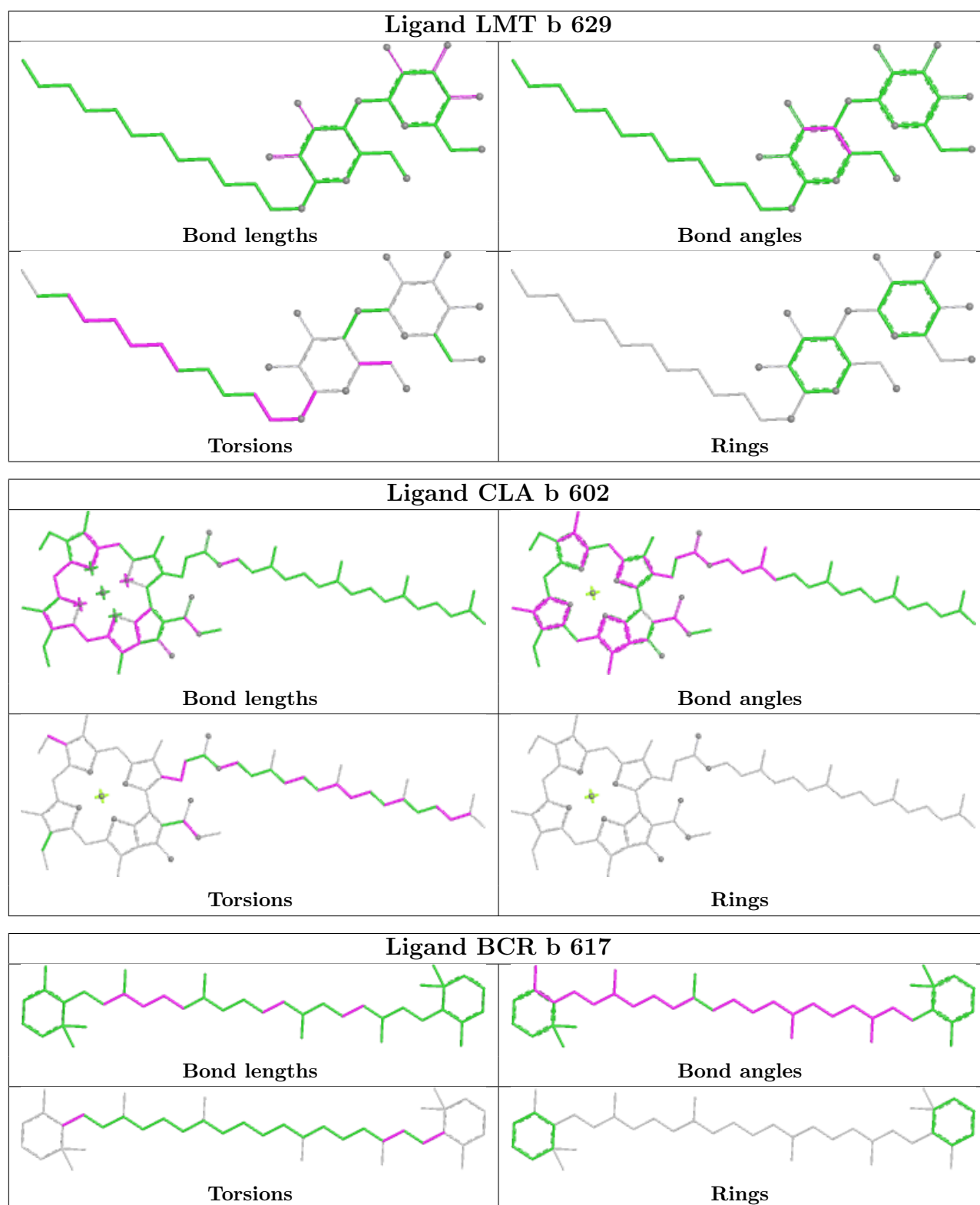
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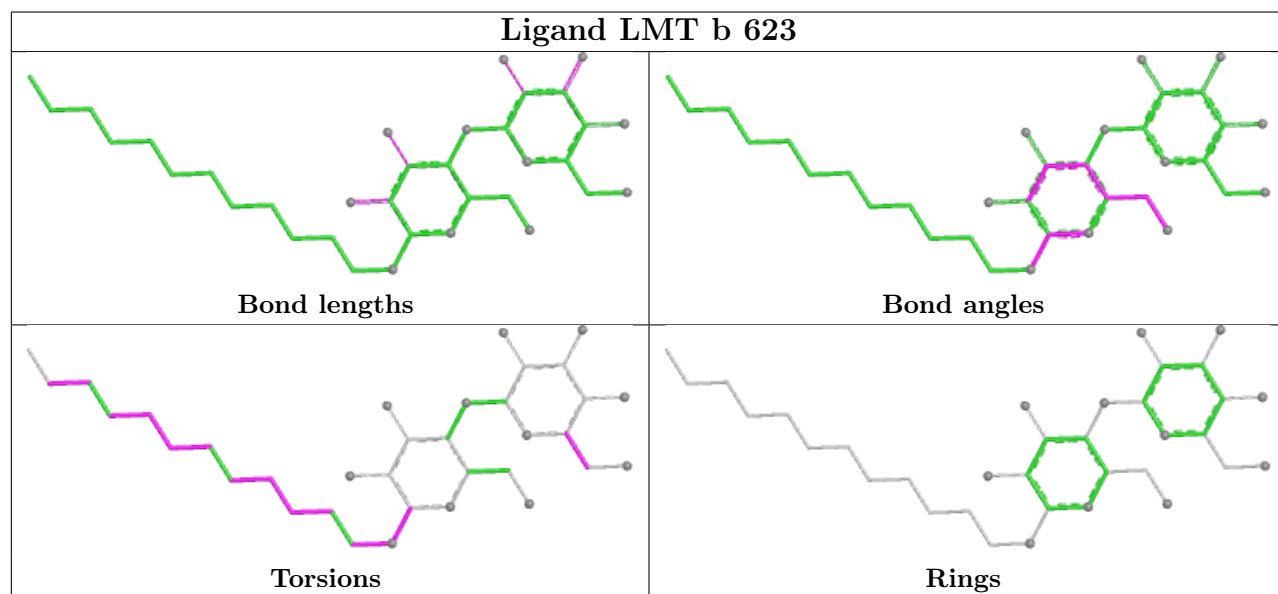
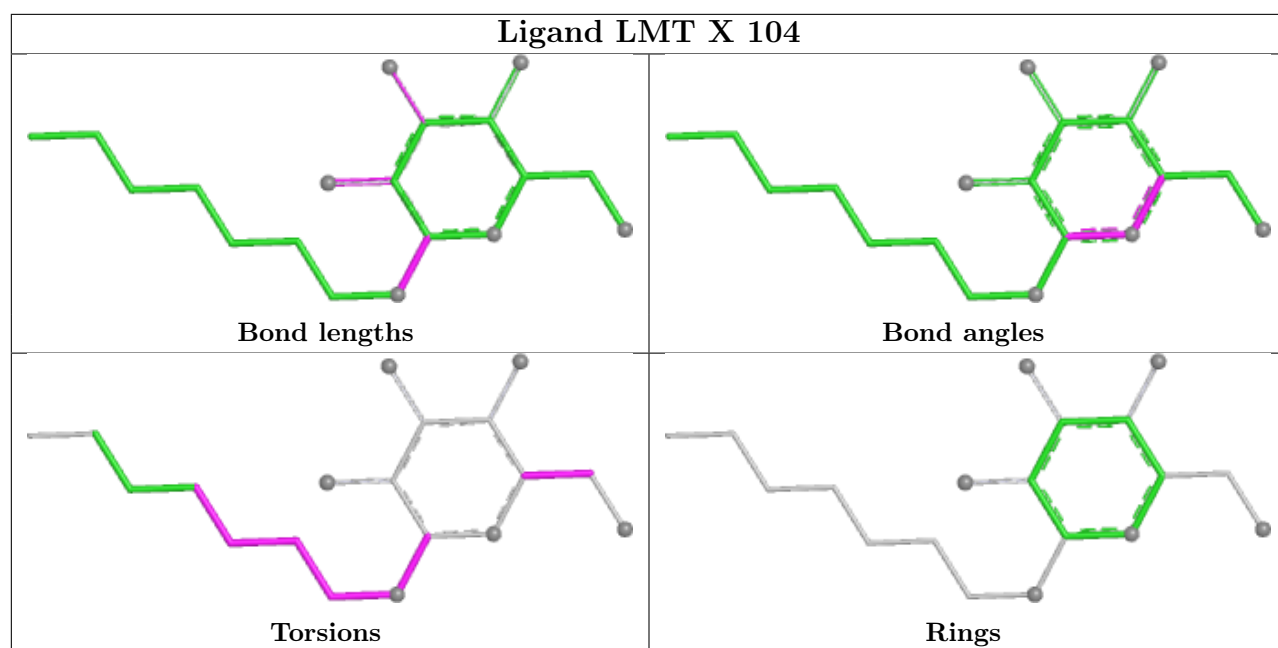


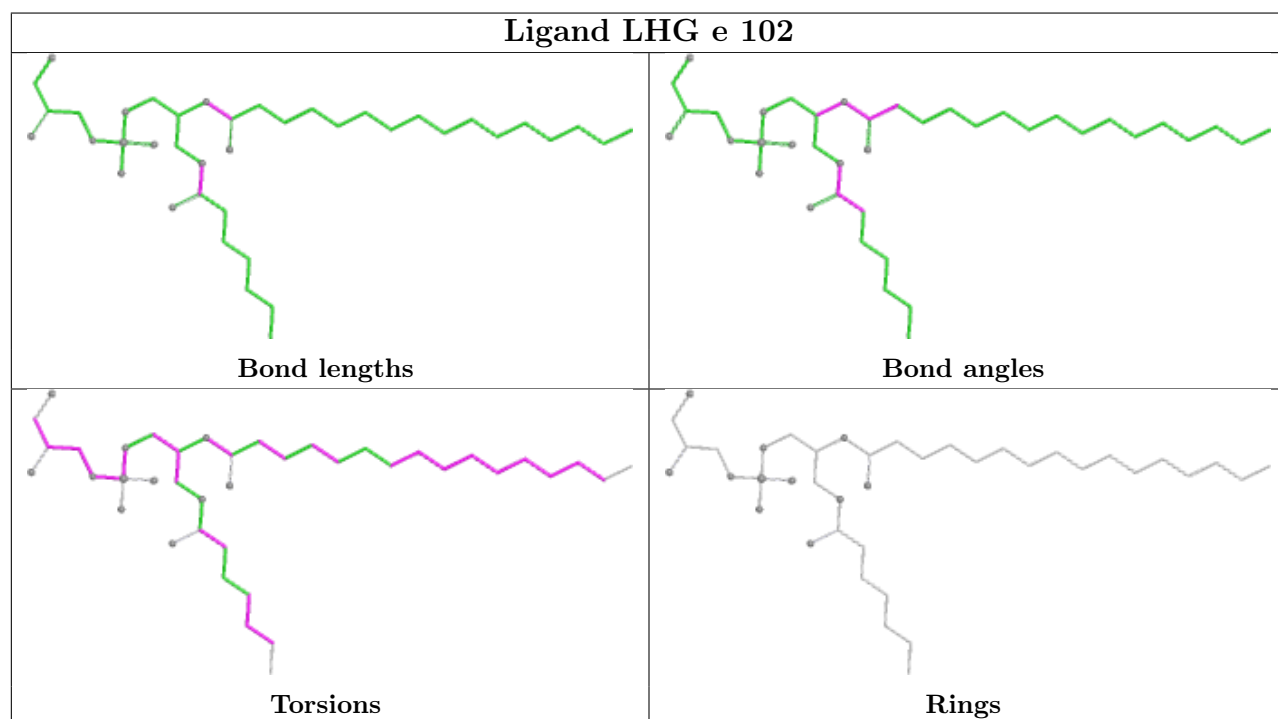
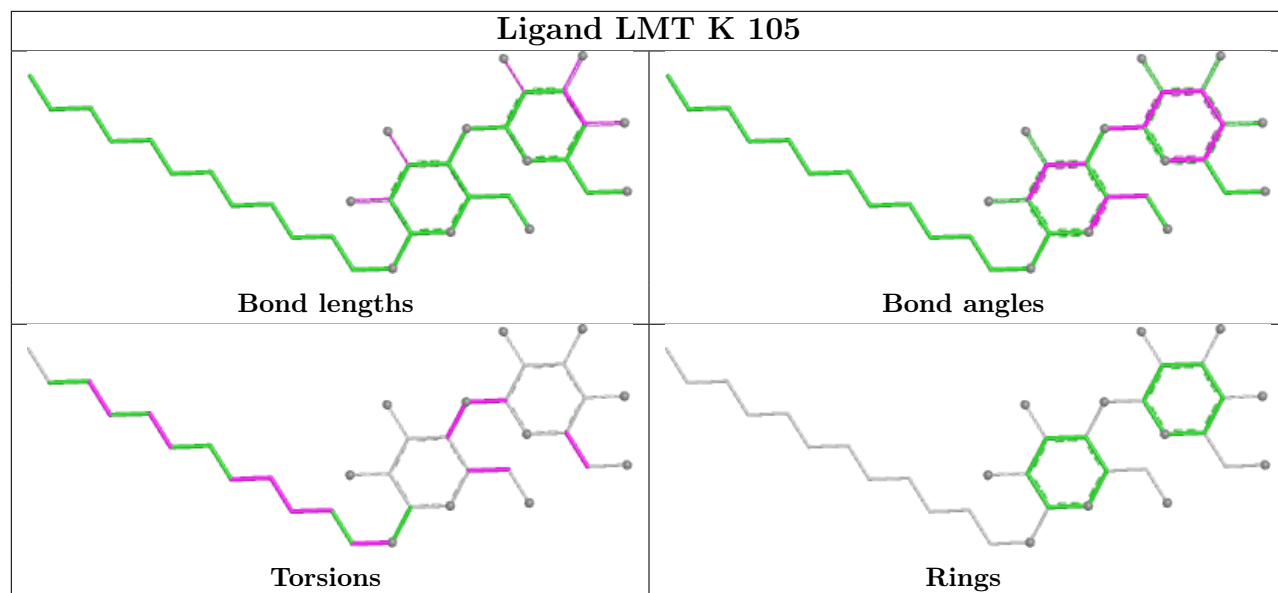
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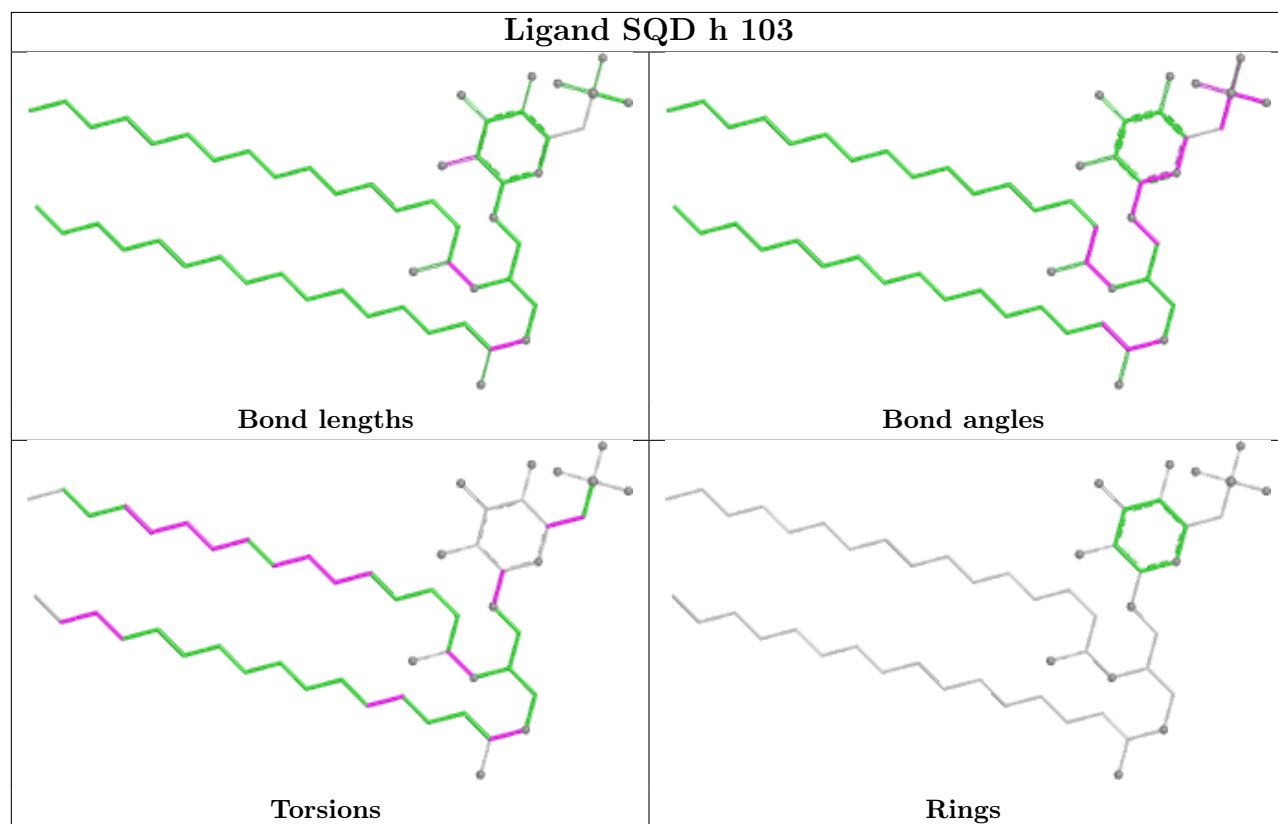
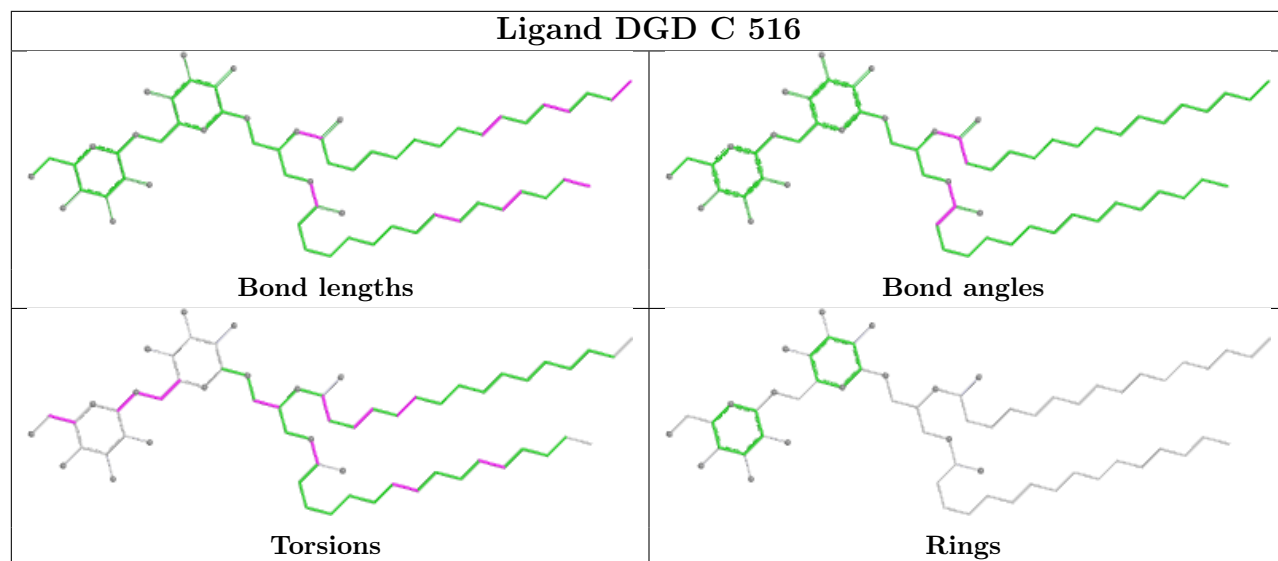


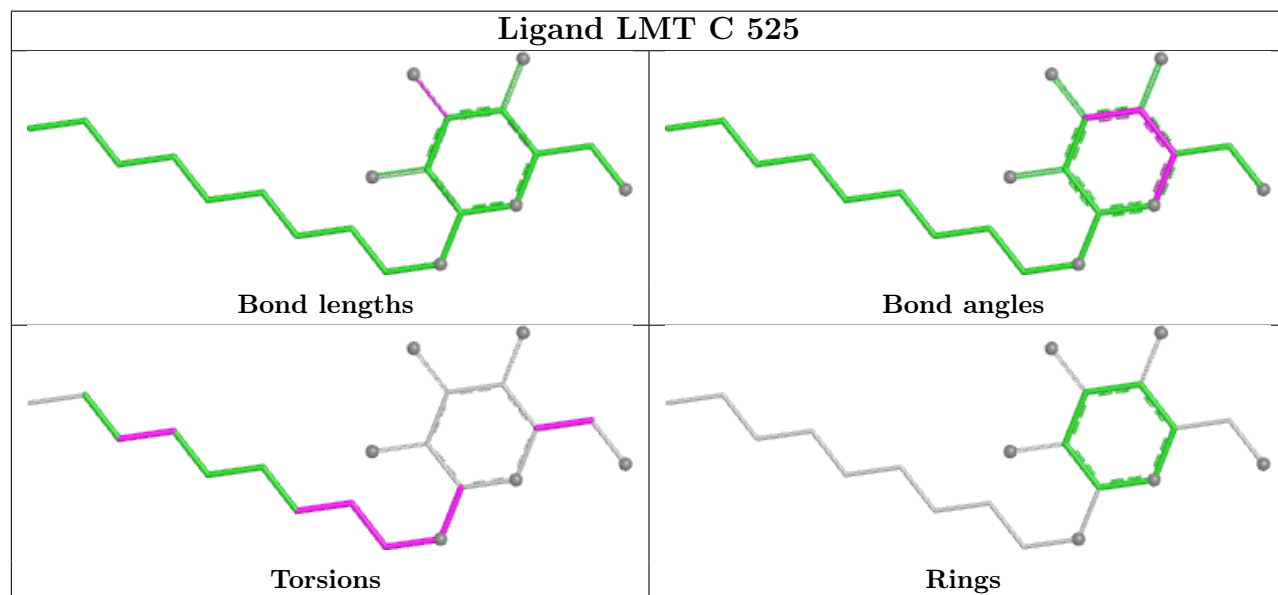
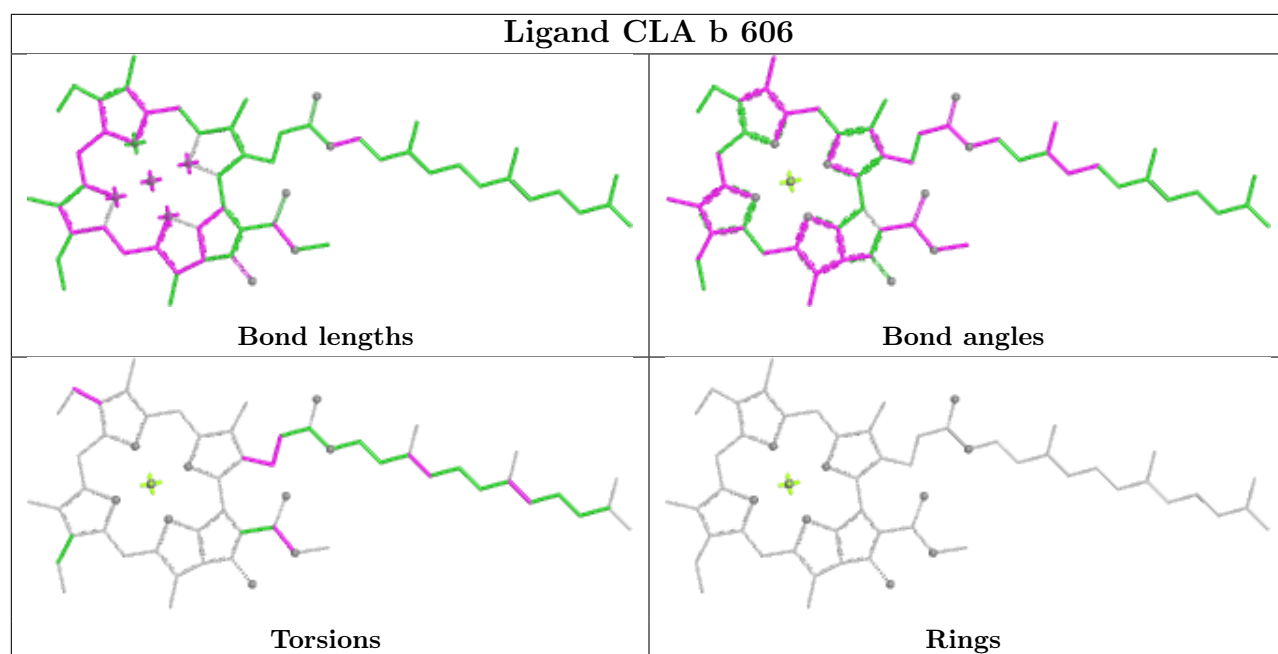


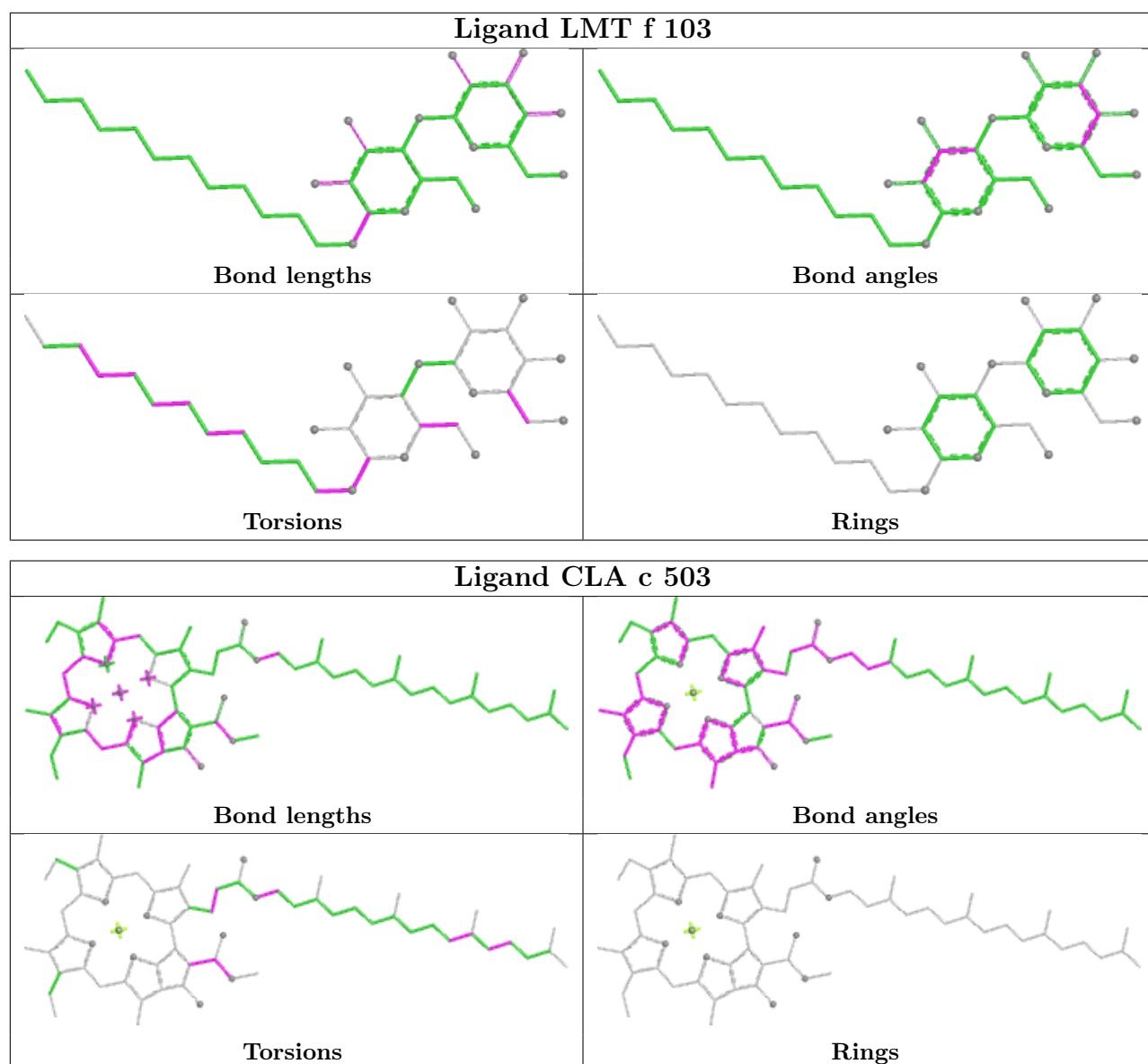


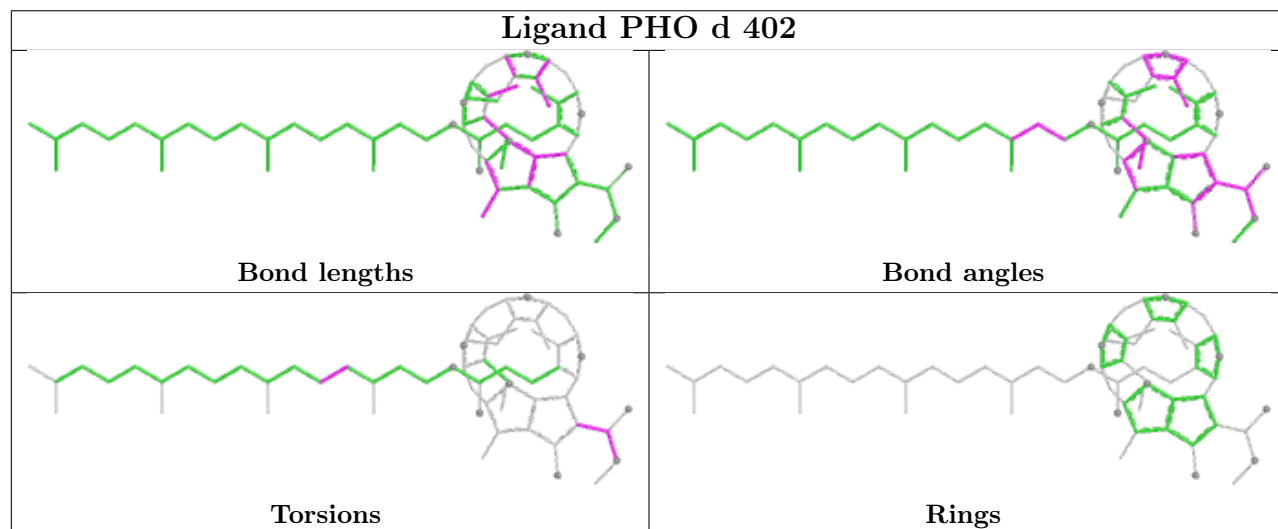
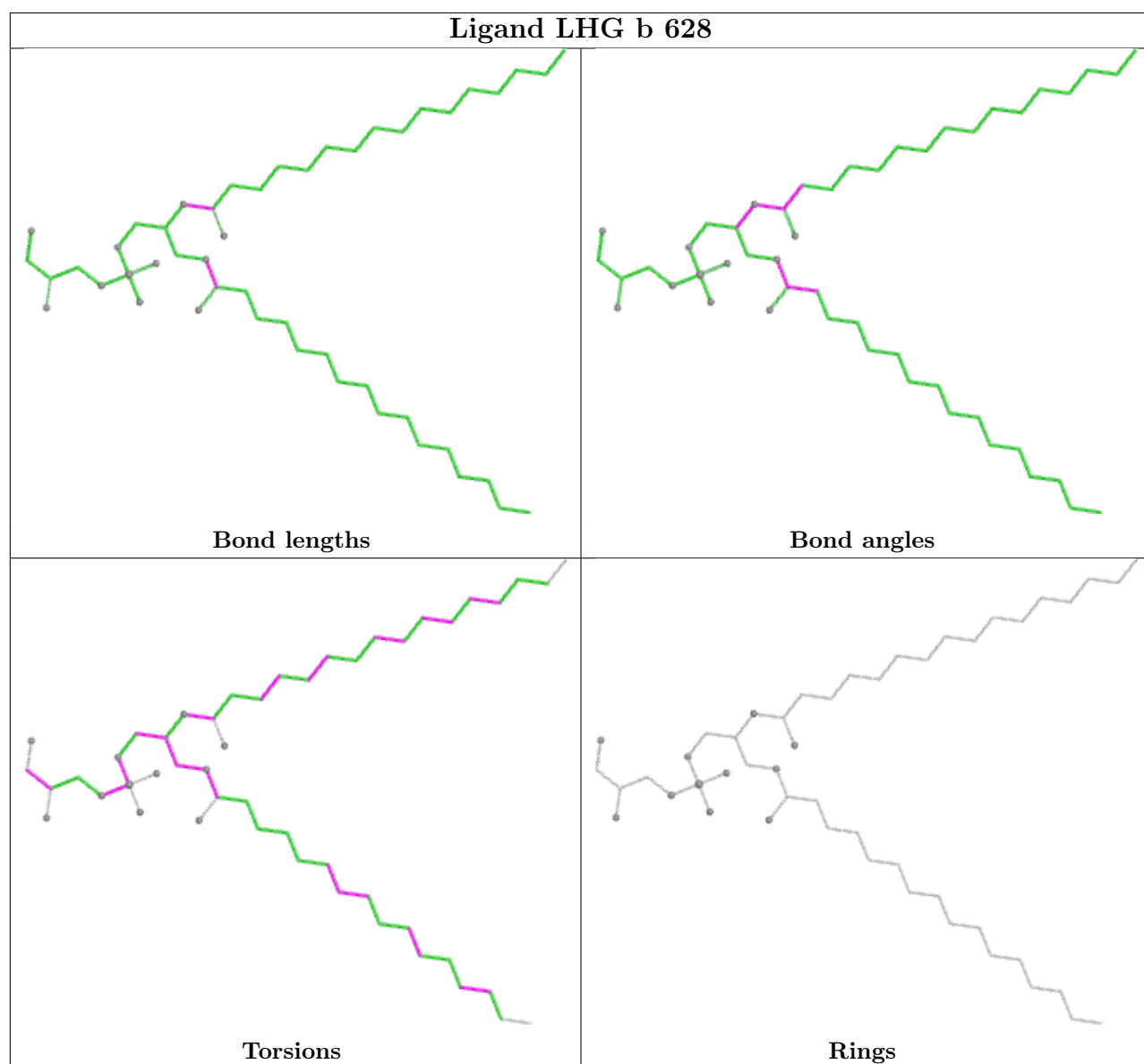


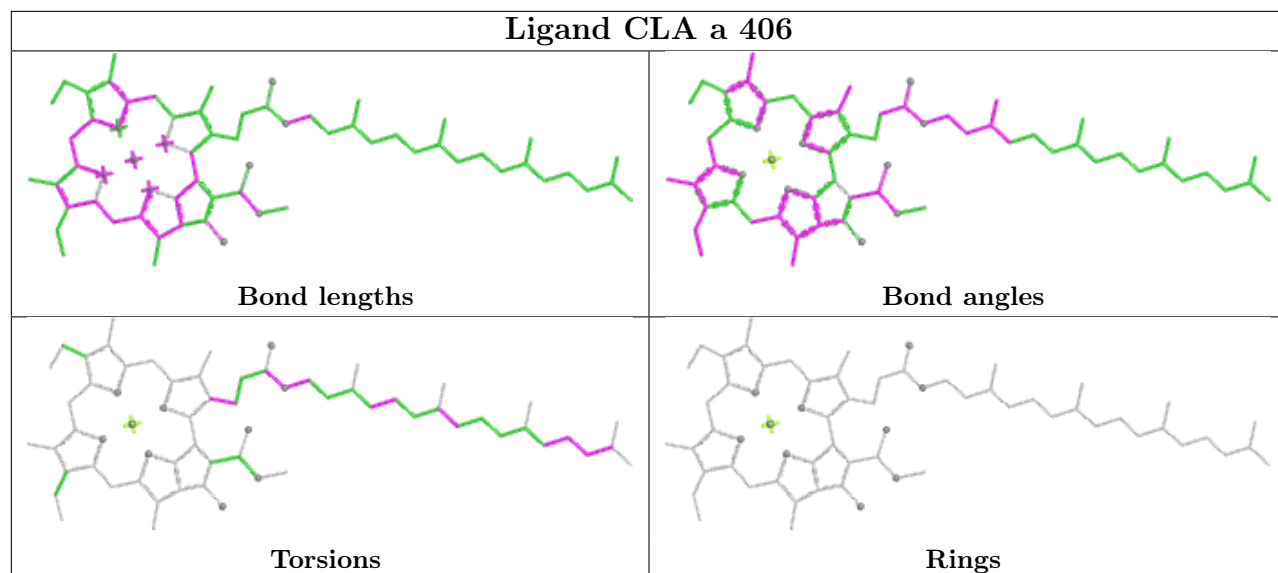
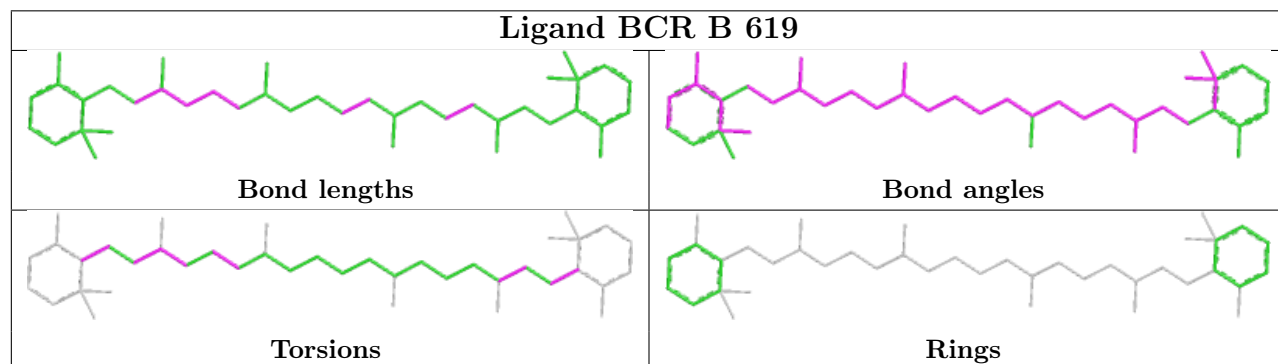
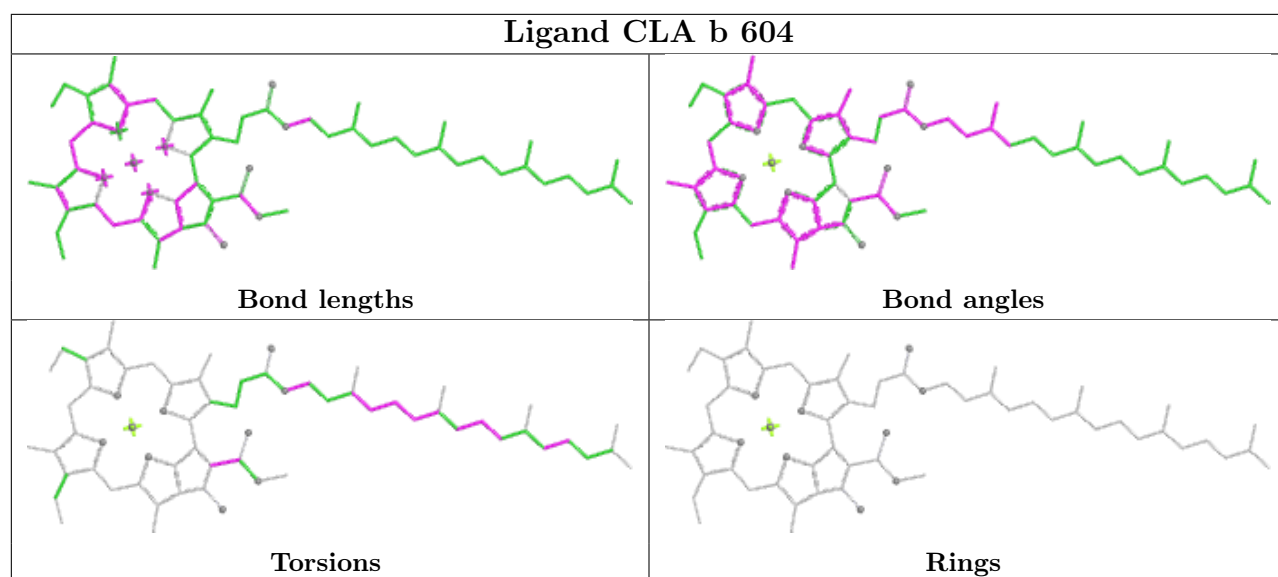


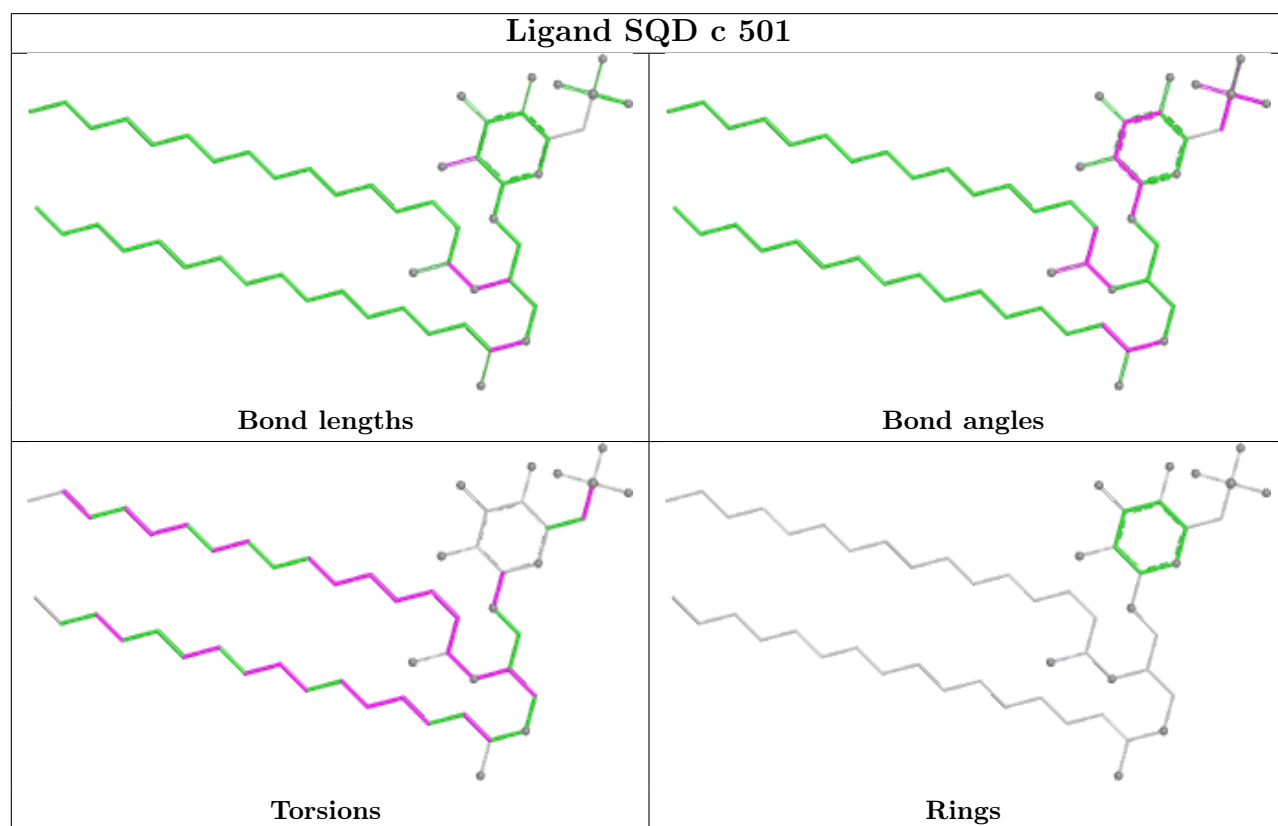
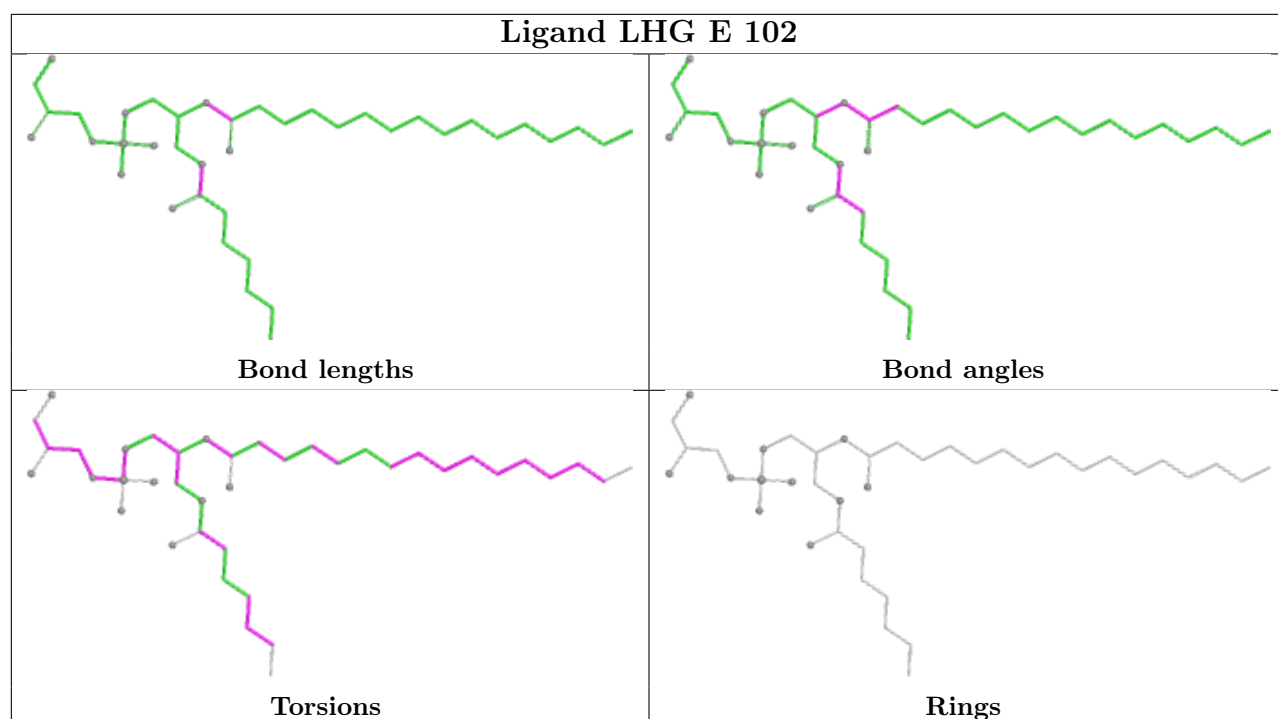


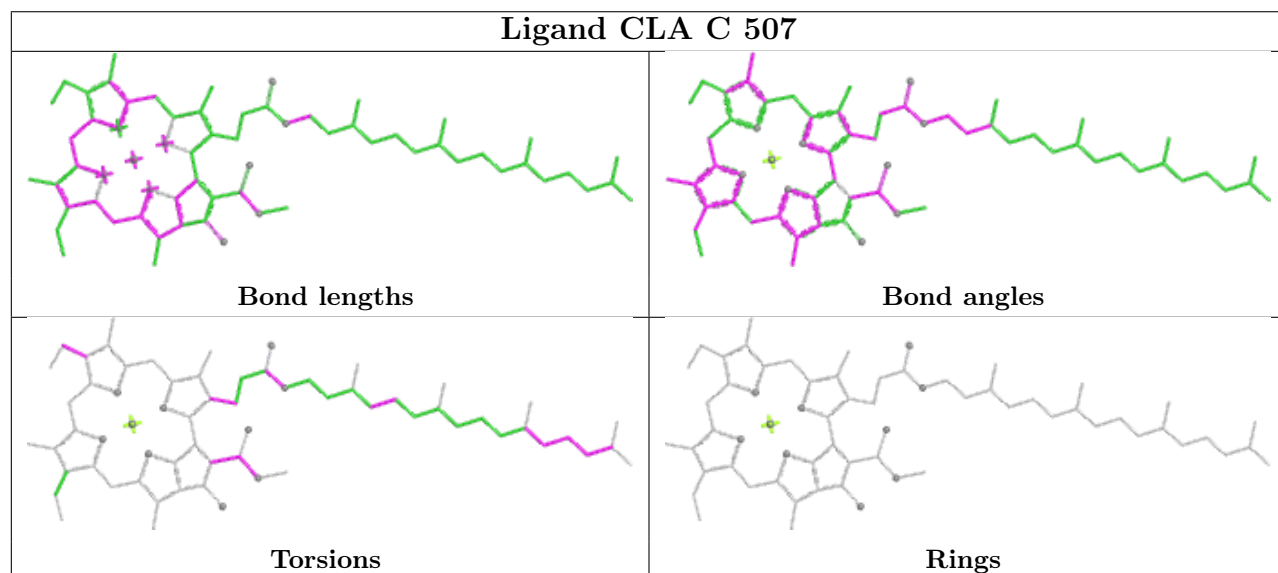
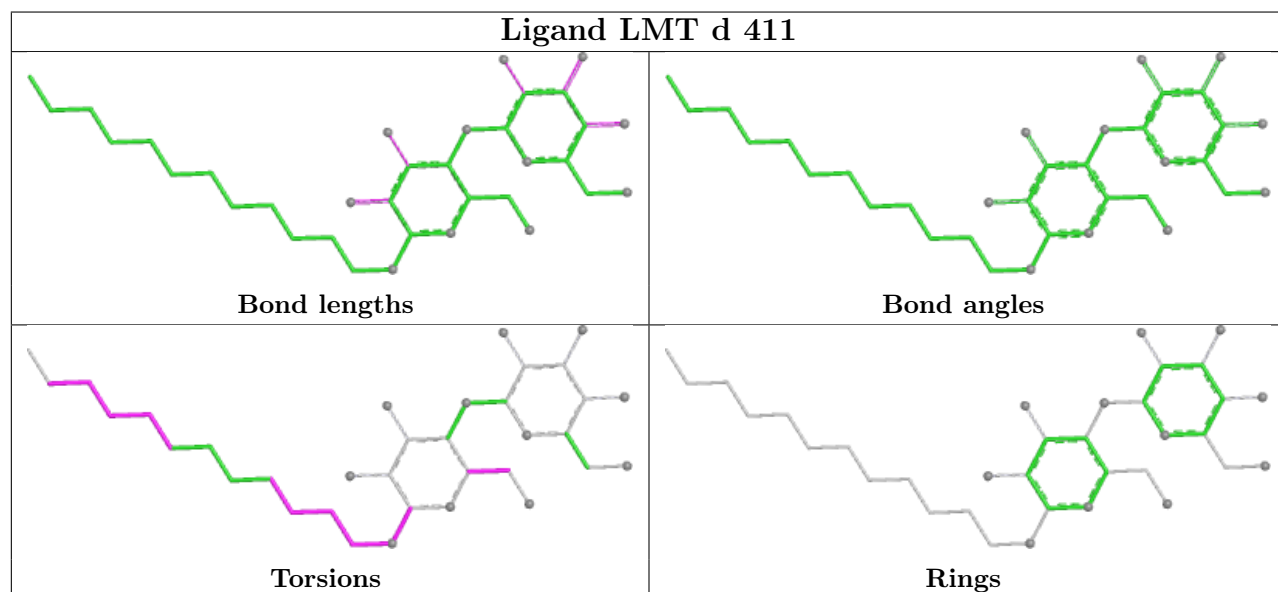
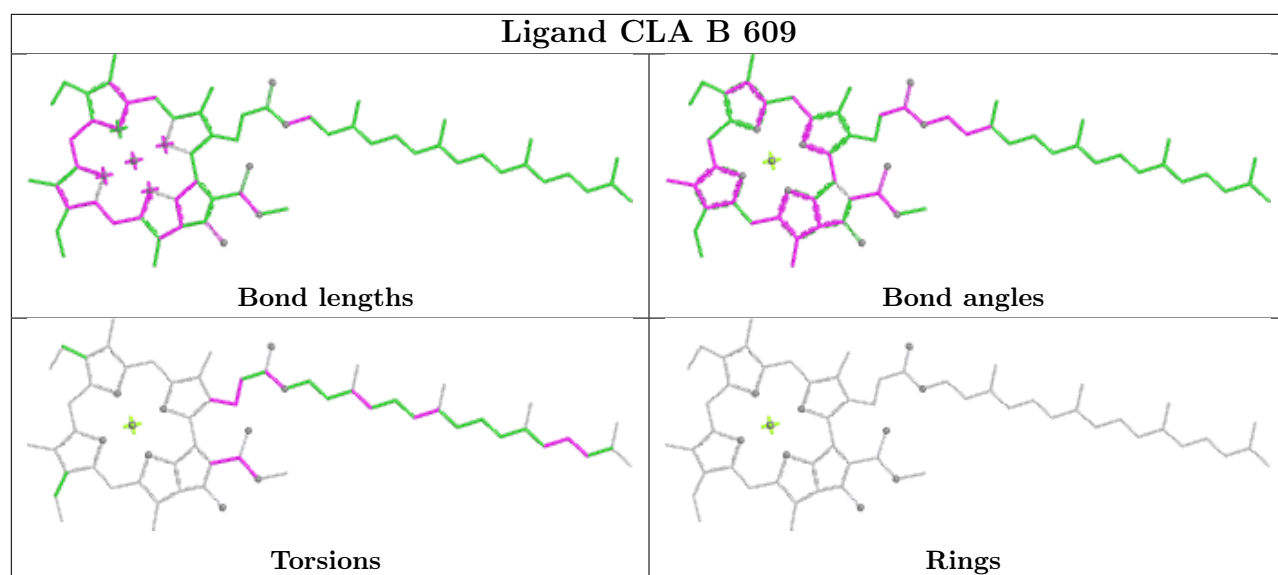


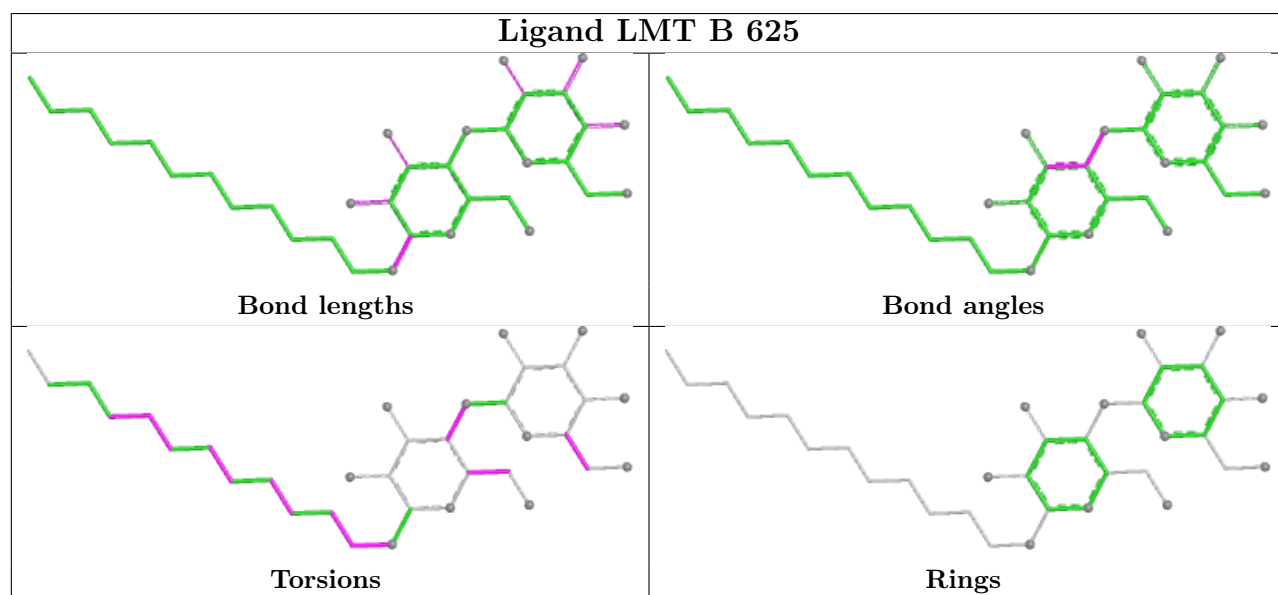
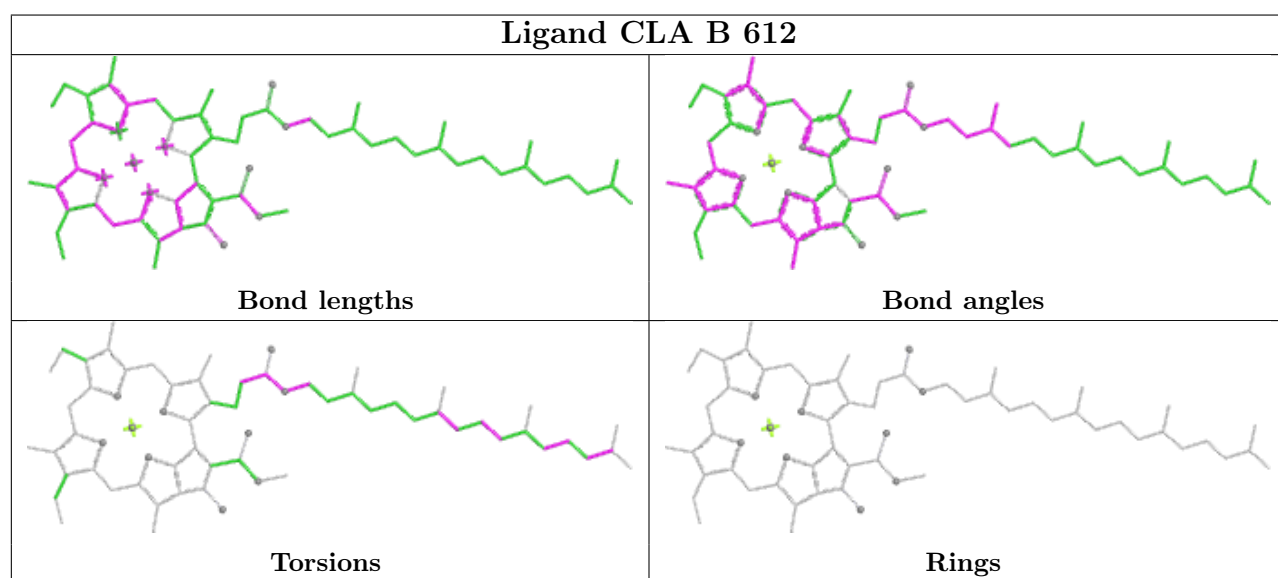
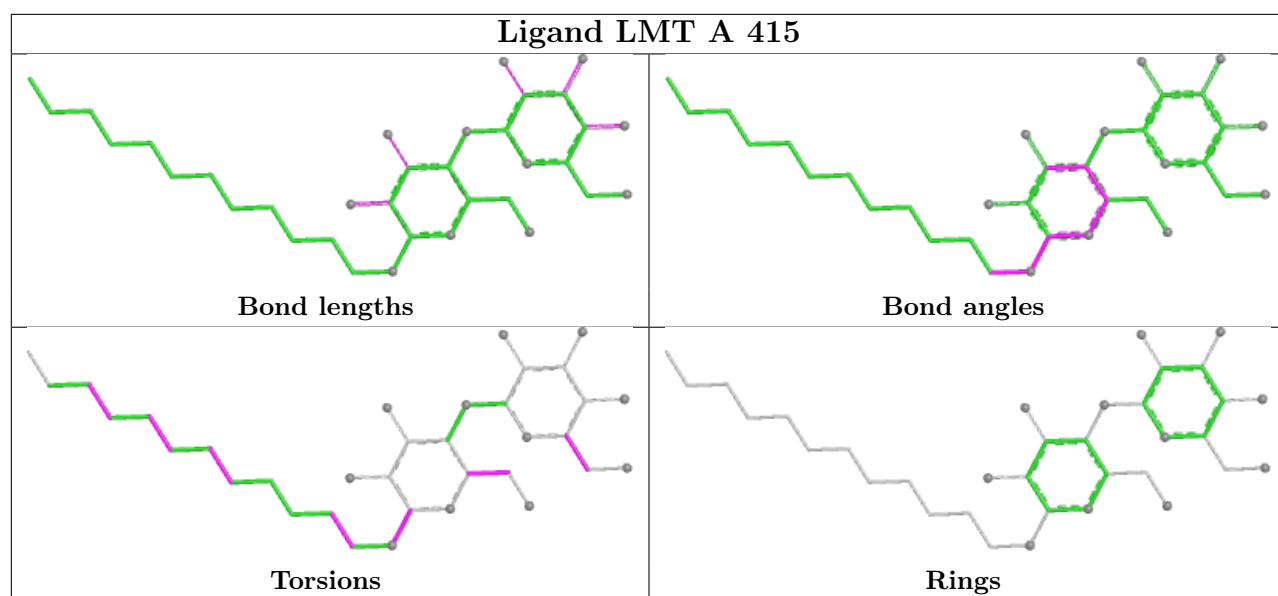


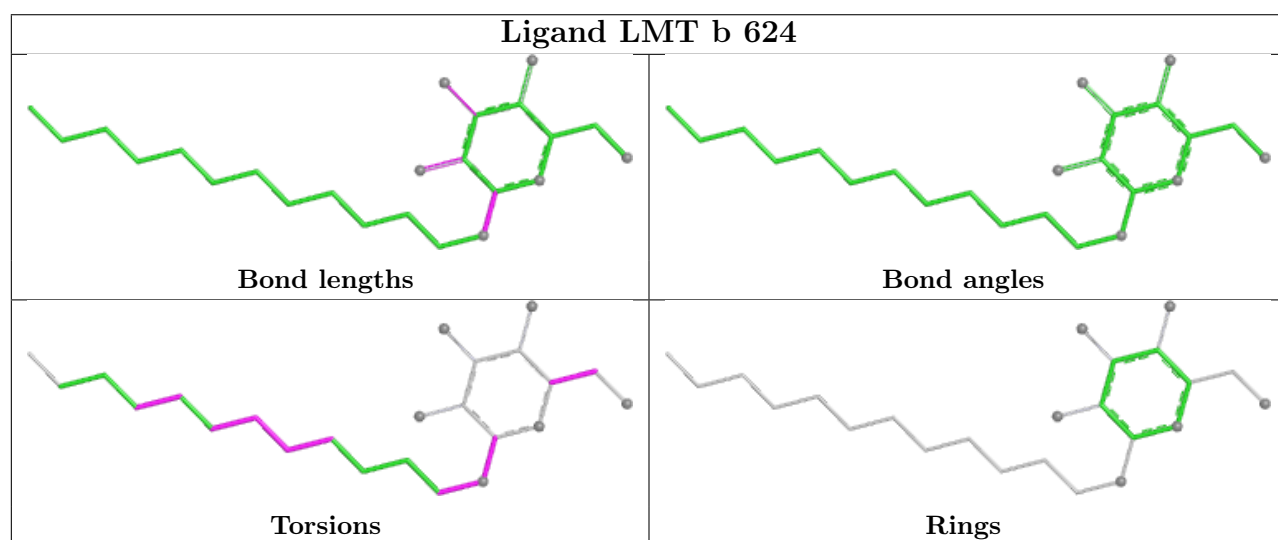
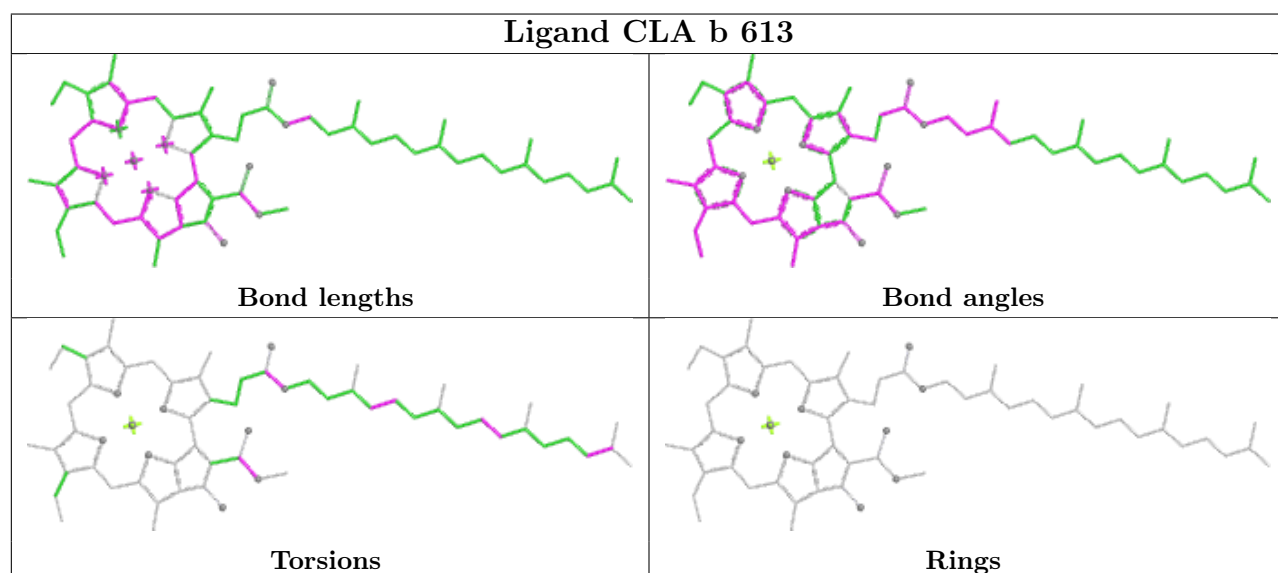
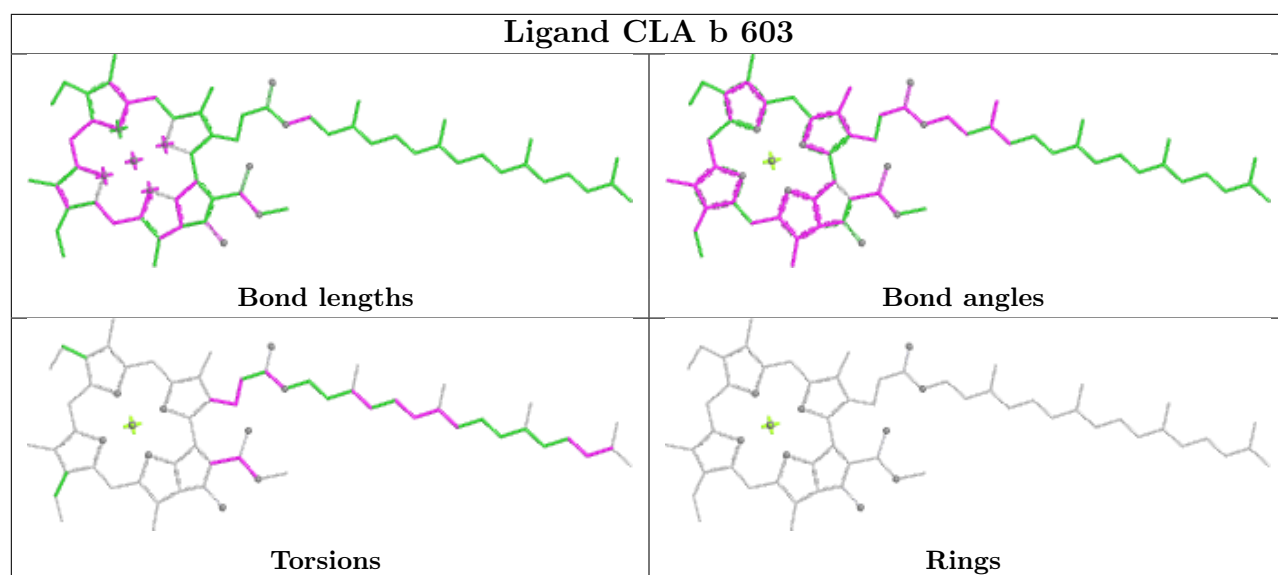


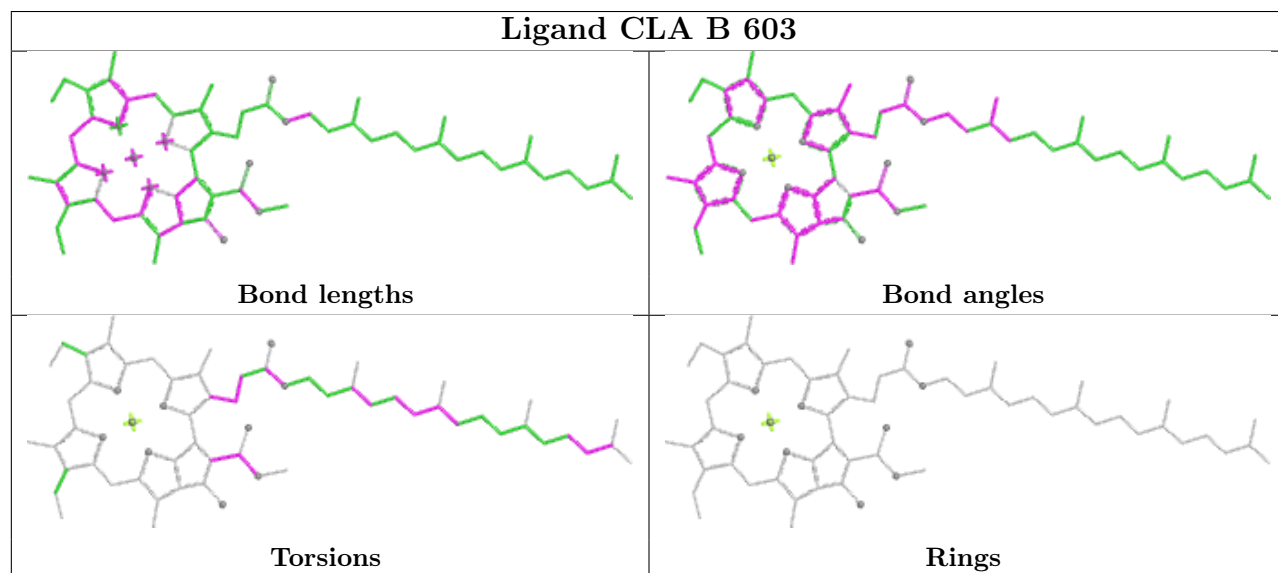
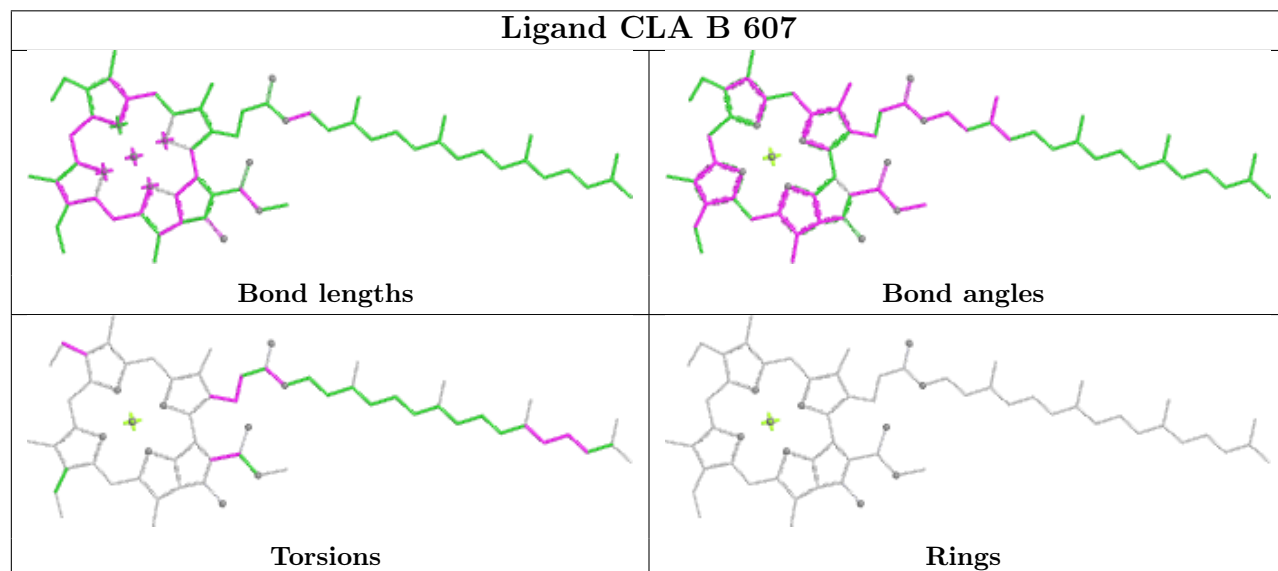
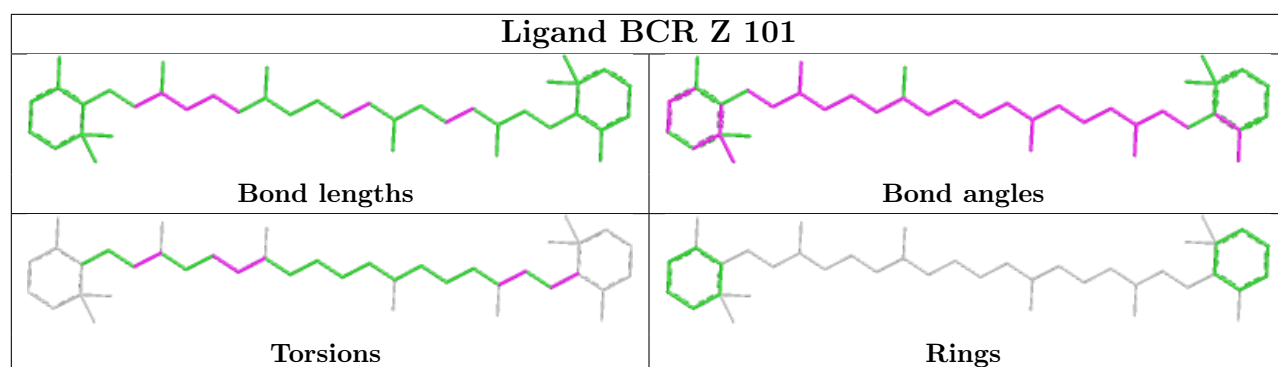


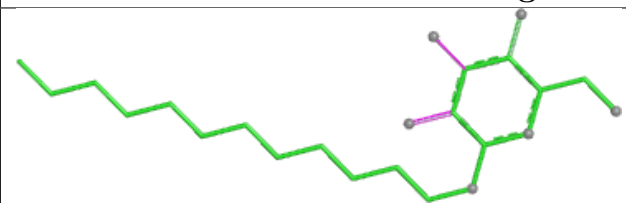
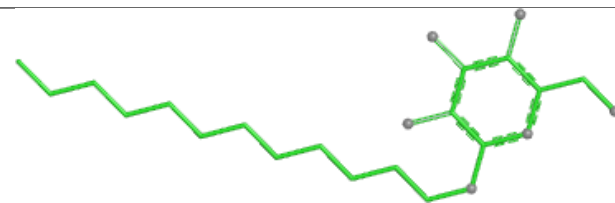
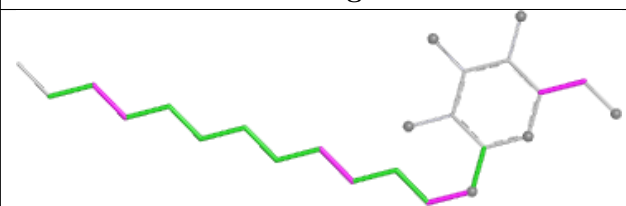
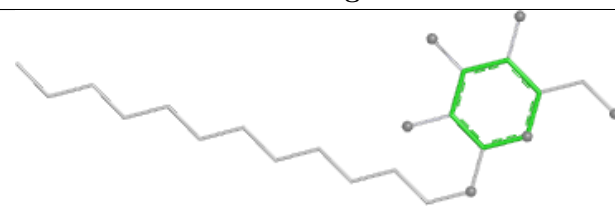


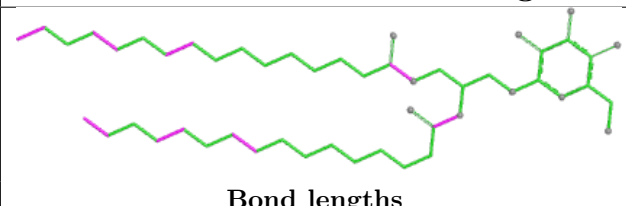
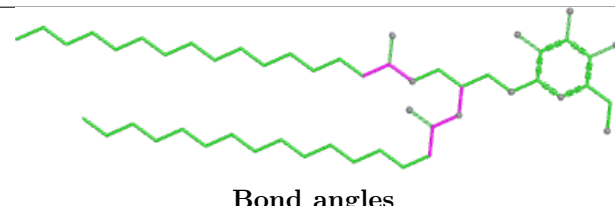
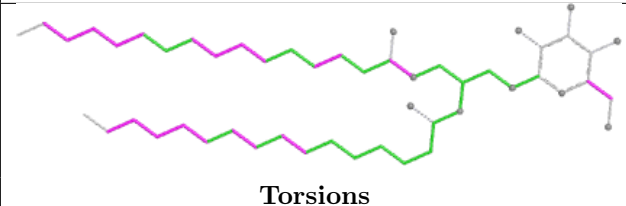
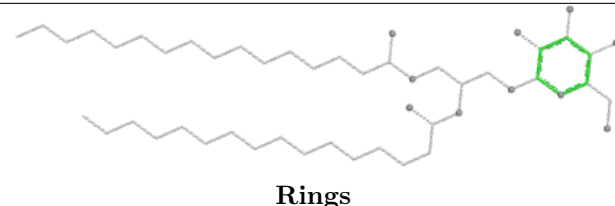


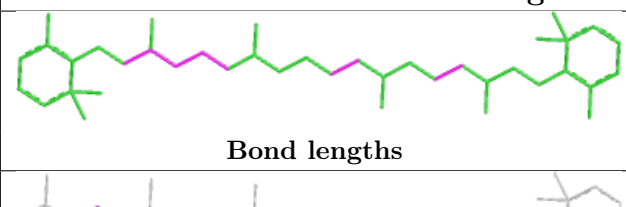
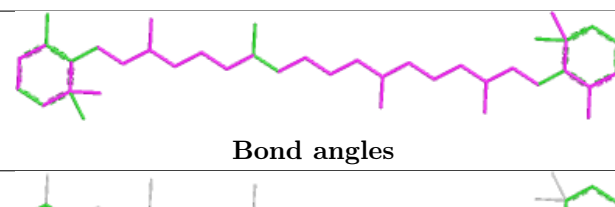
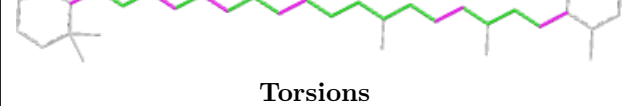


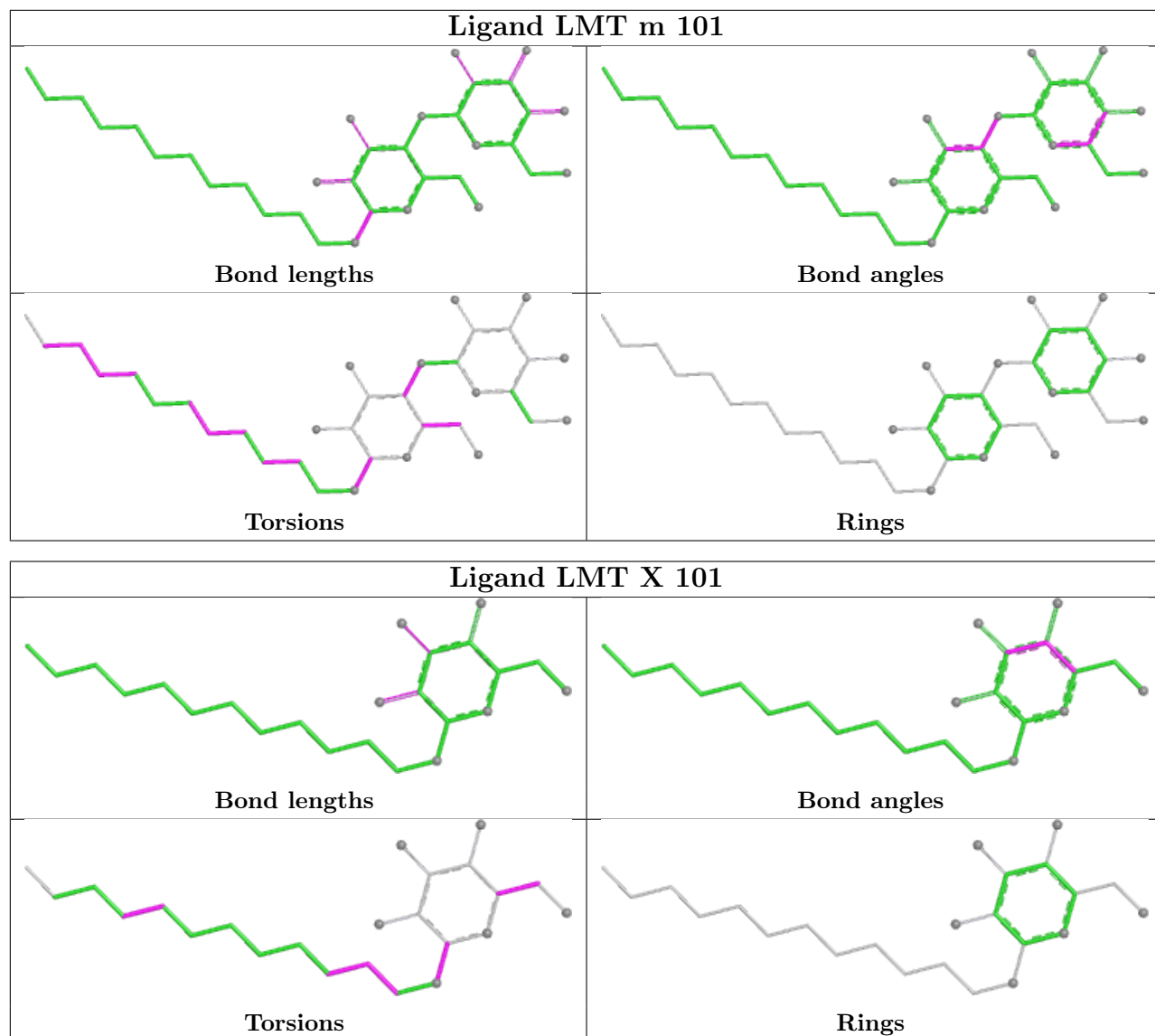


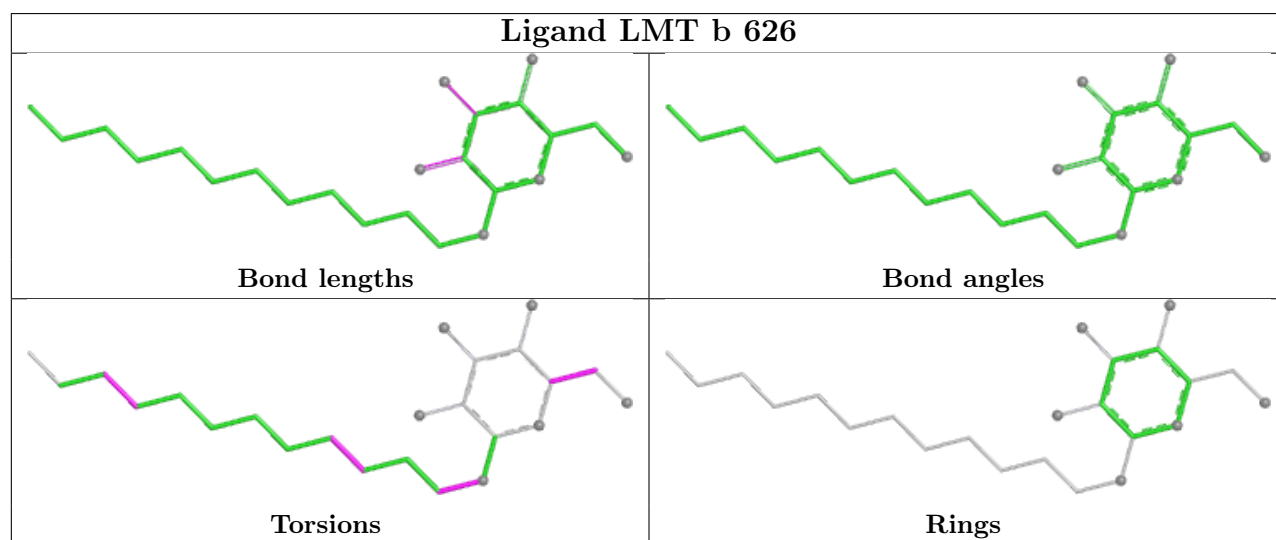
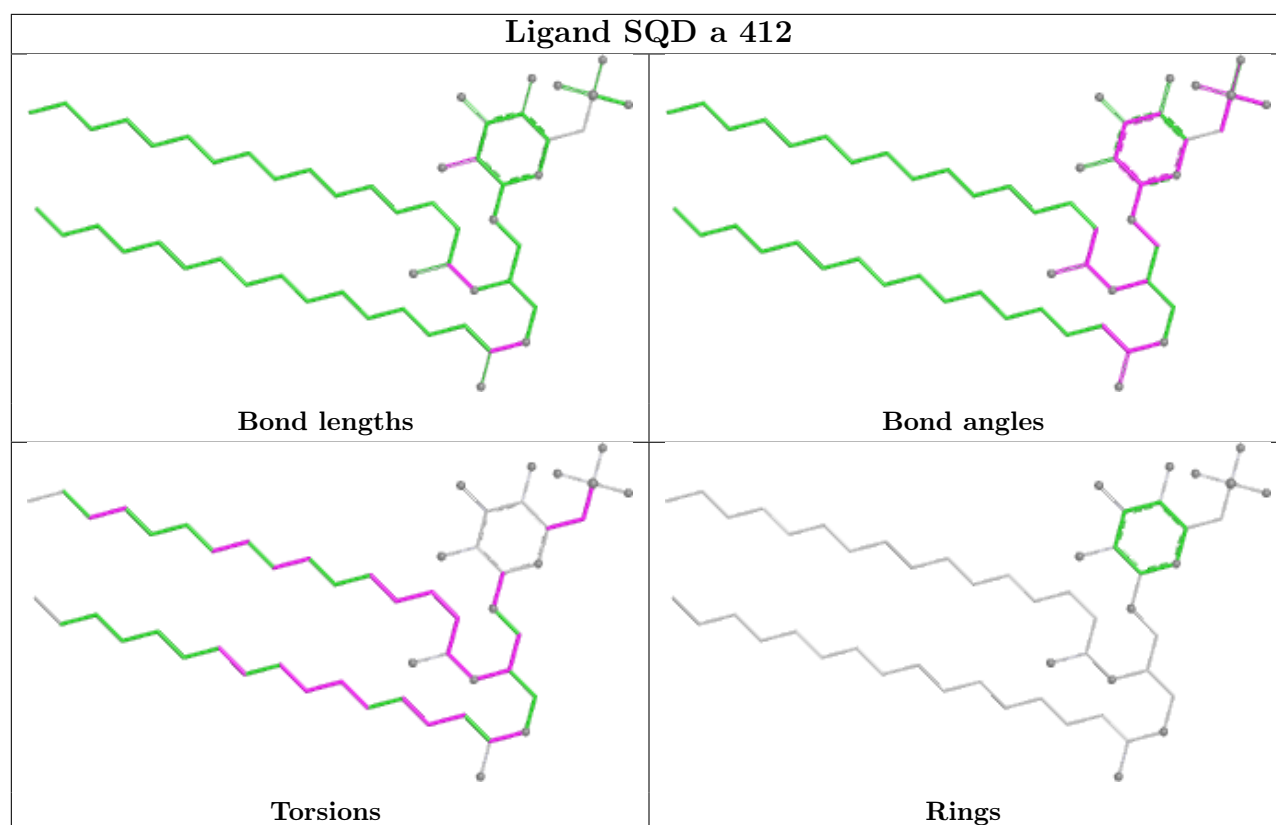


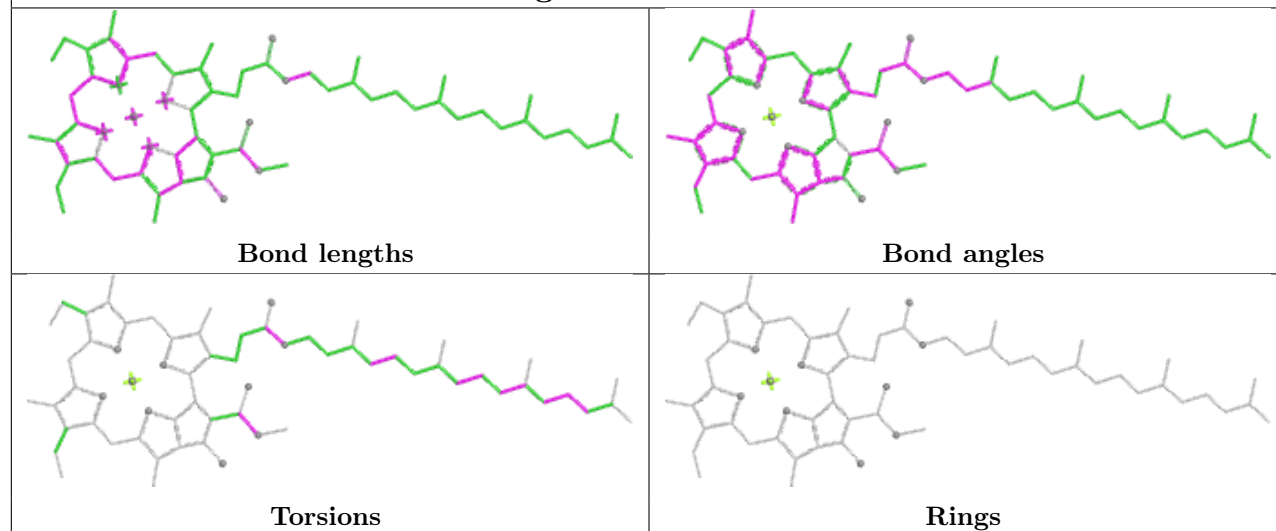
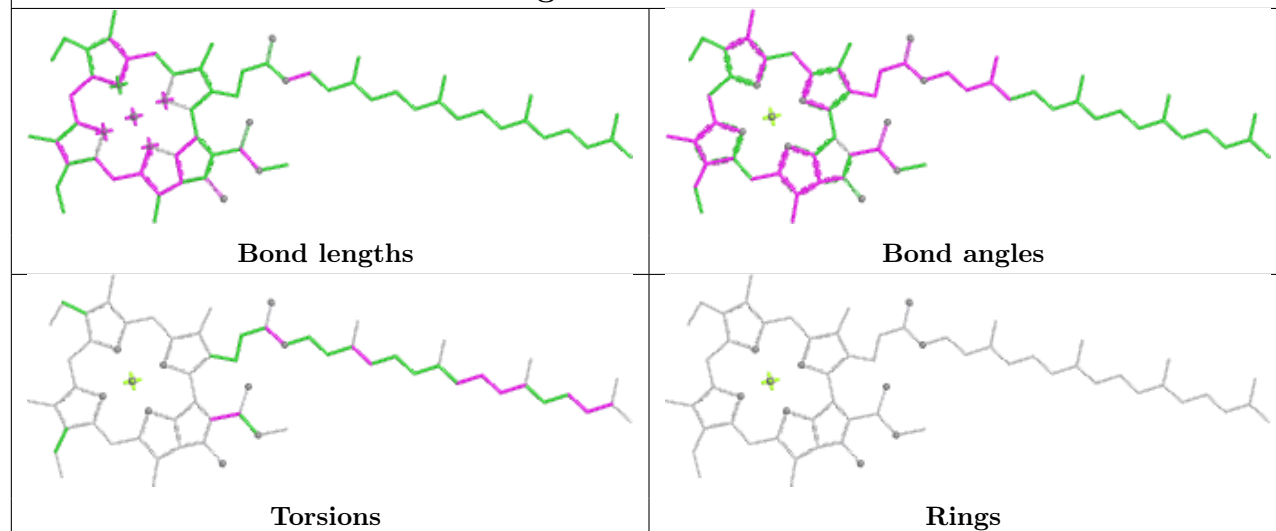
Ligand LMT B 626	
 Bond lengths	 Bond angles
 Torsions	 Rings

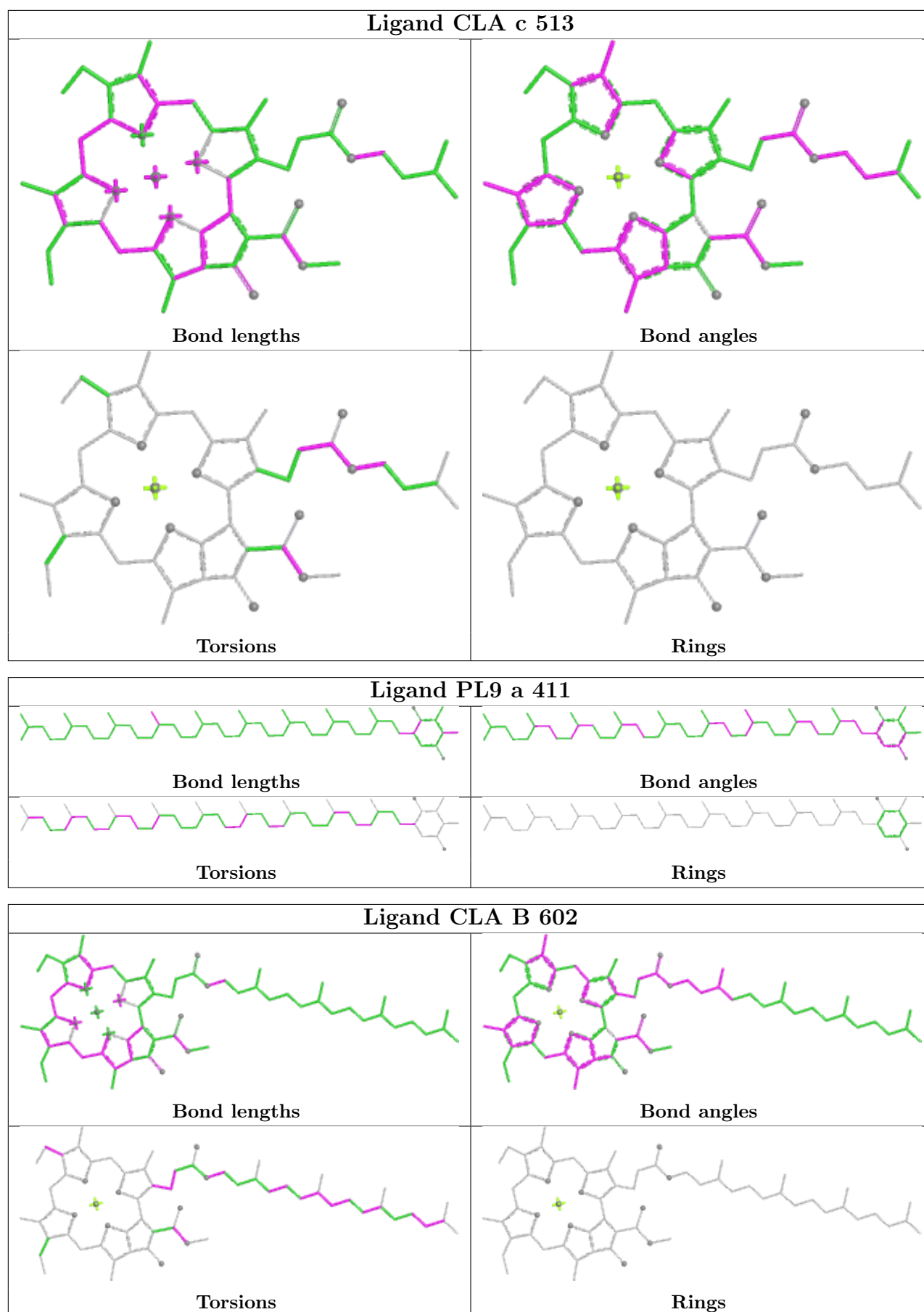
Ligand LMG C 519	
 Bond lengths	 Bond angles
 Torsions	 Rings

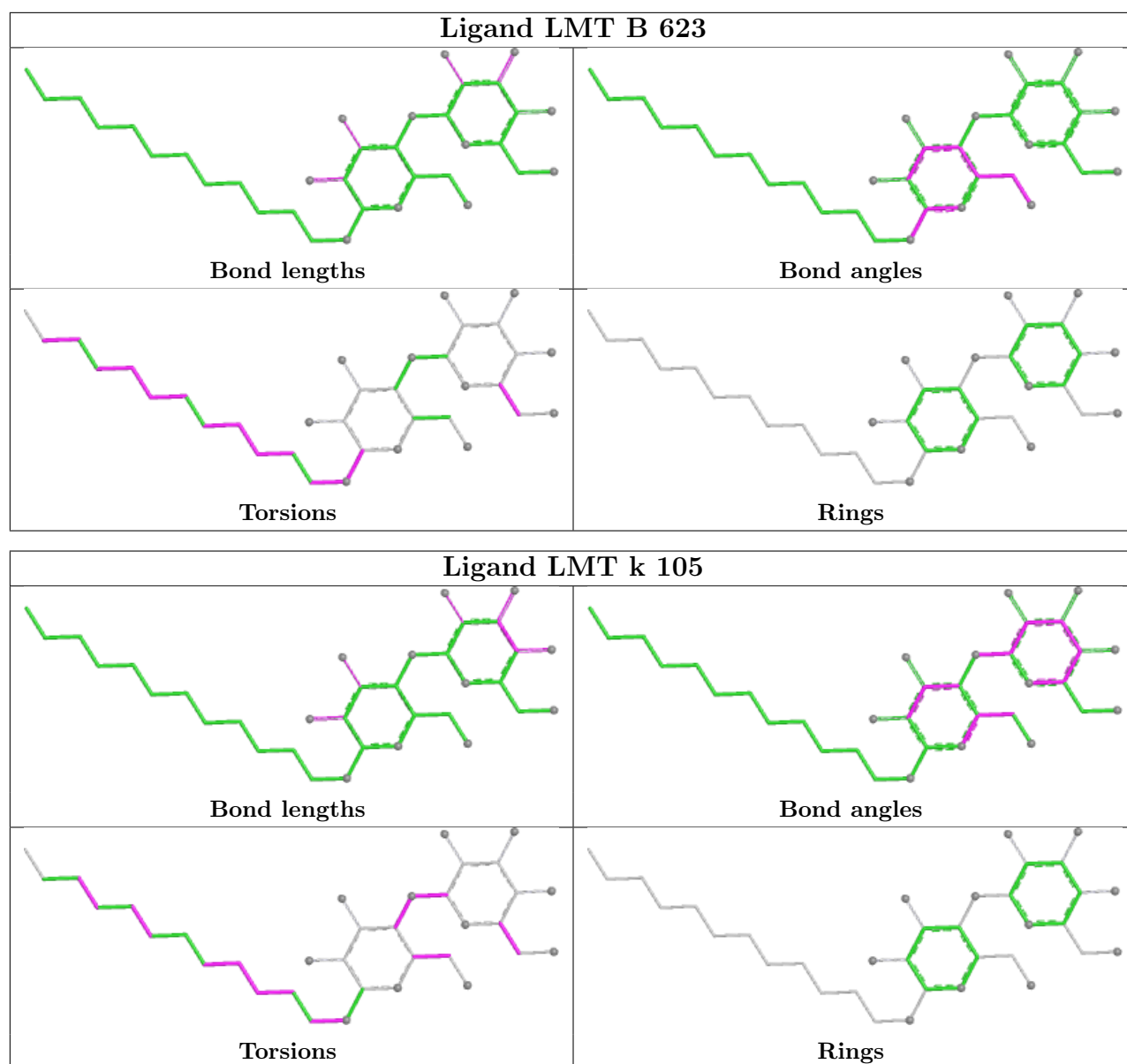
Ligand BCR f 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

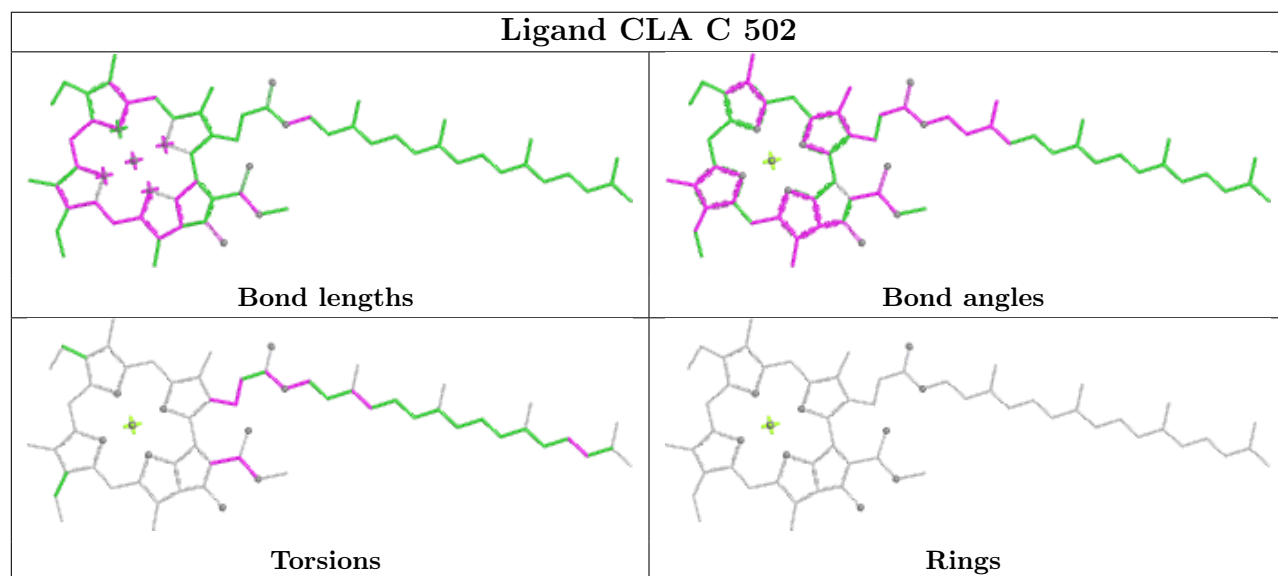
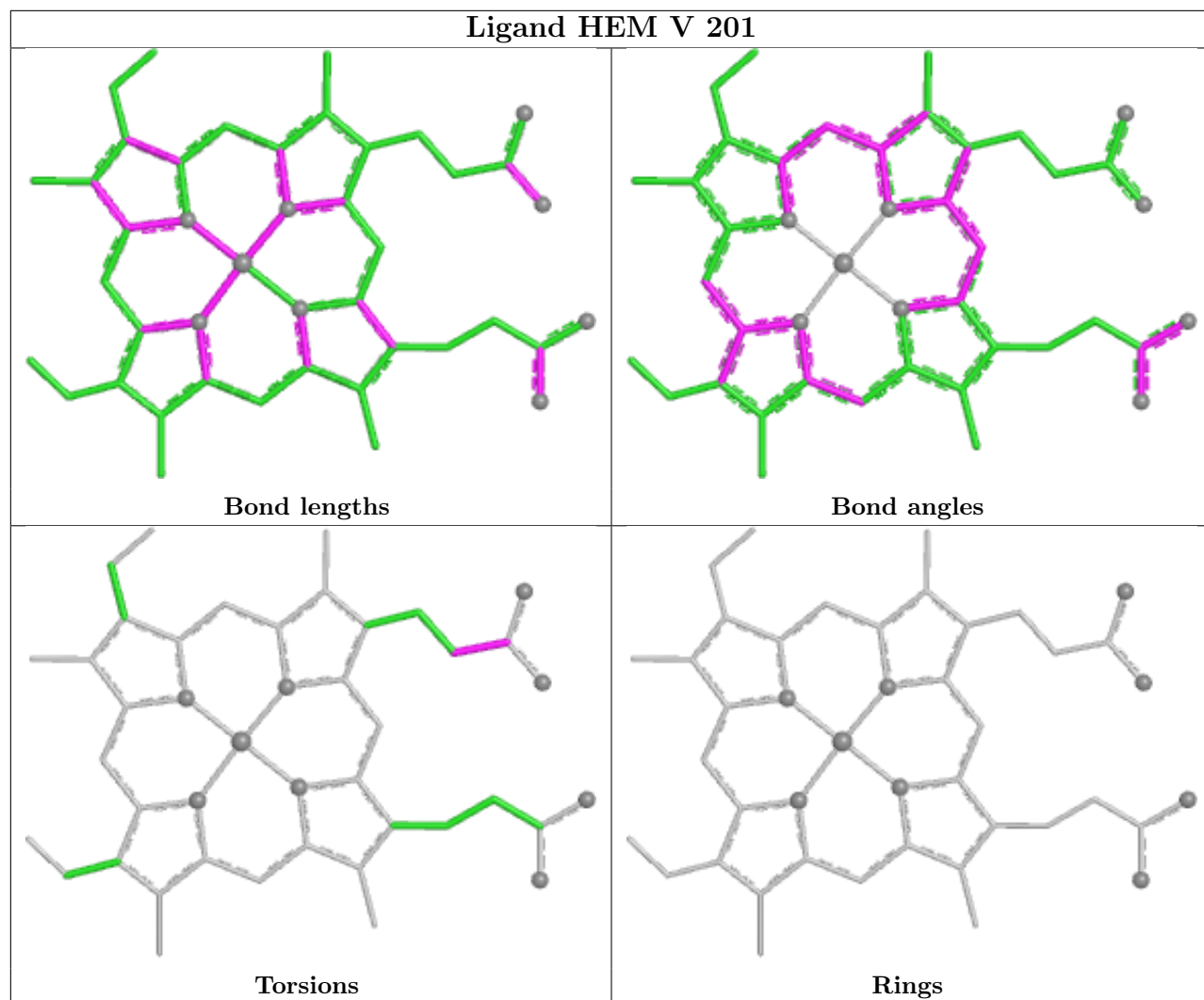


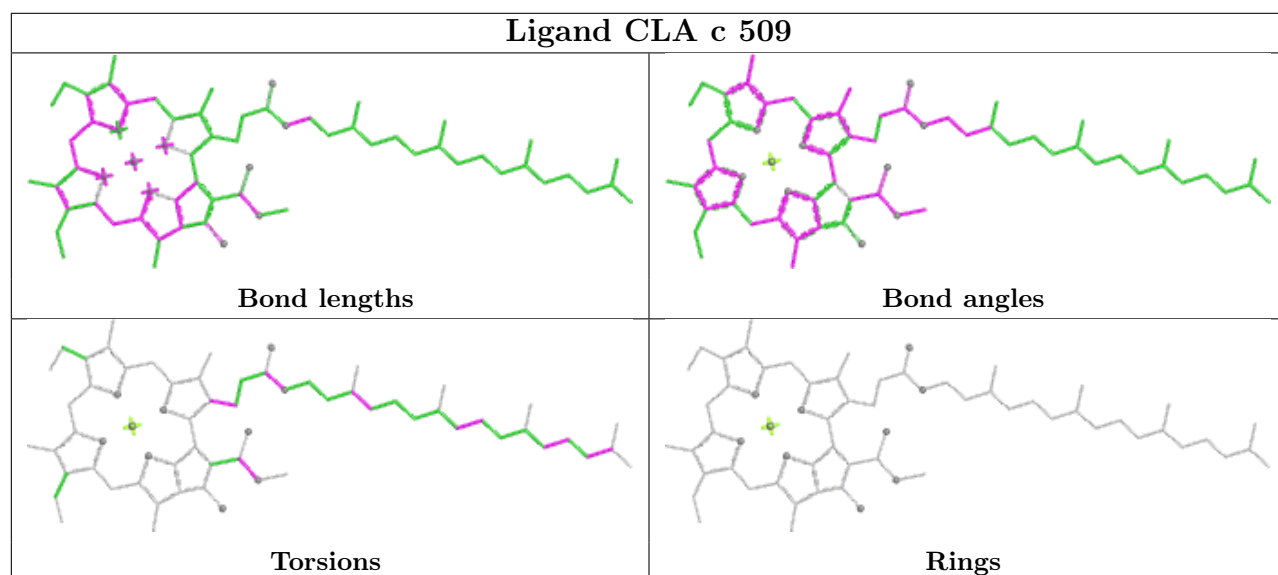
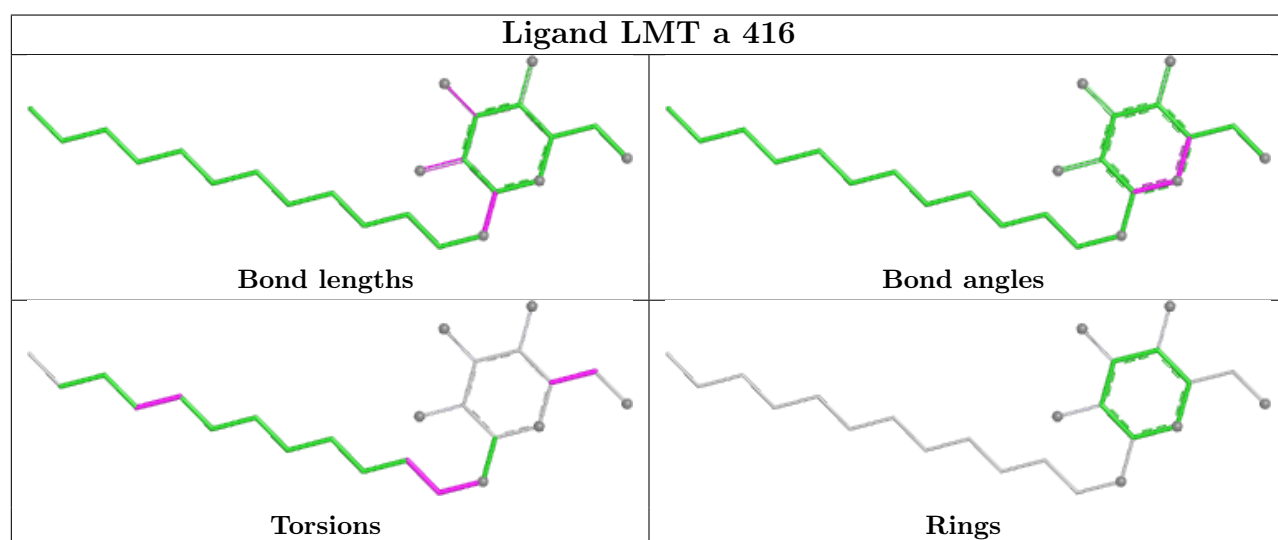
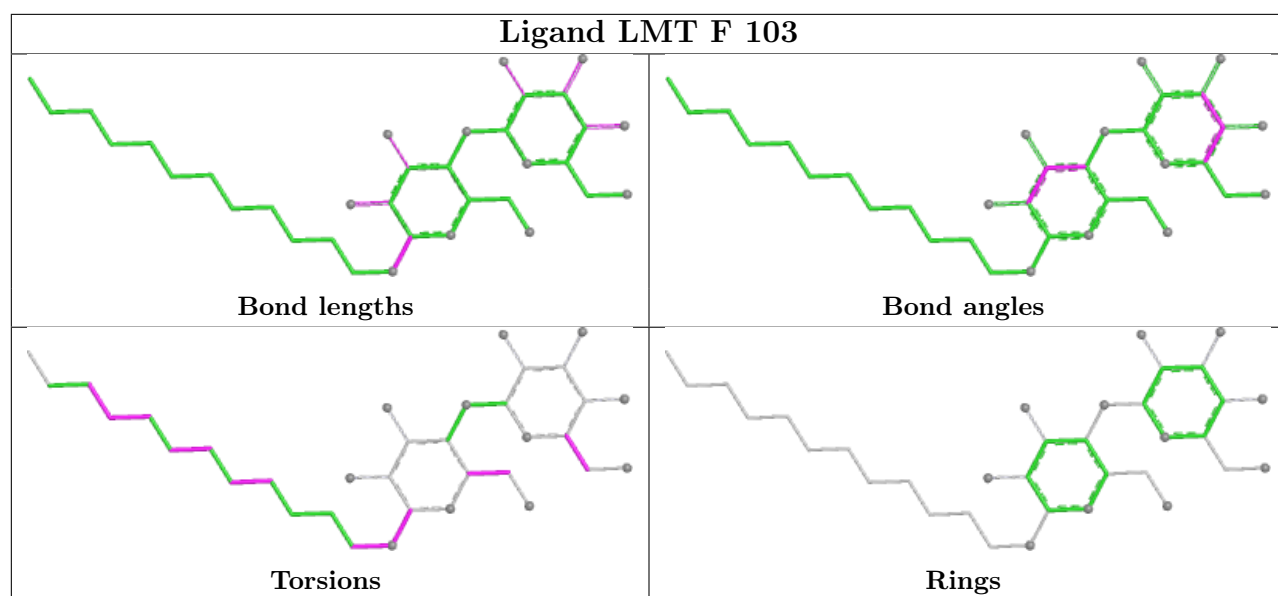


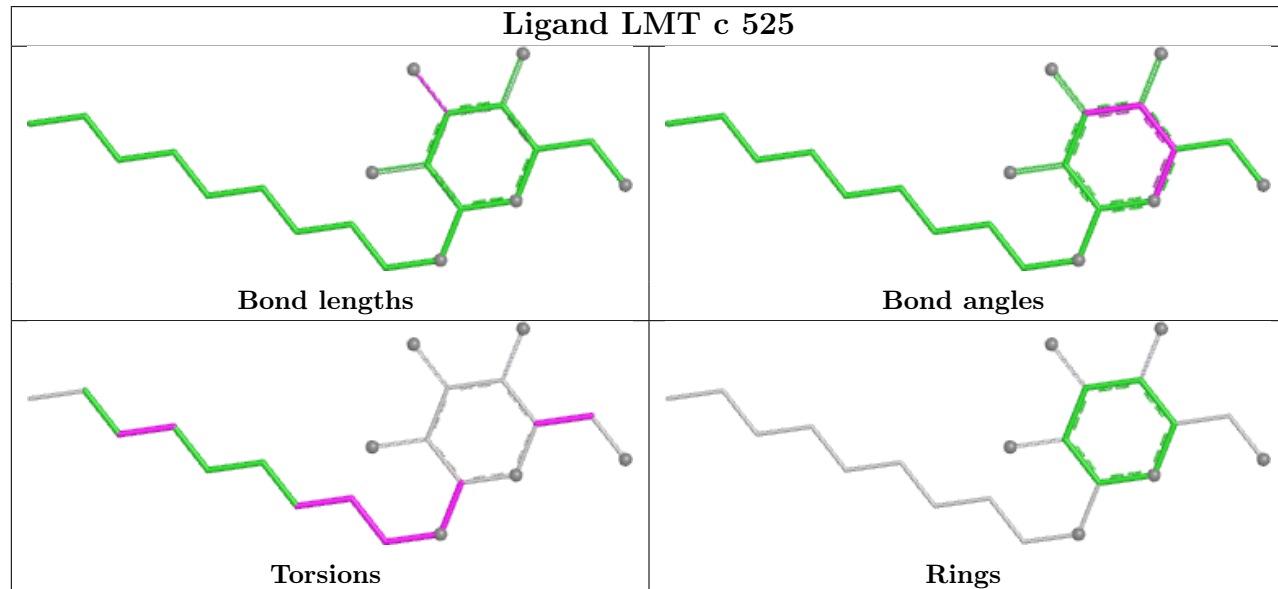
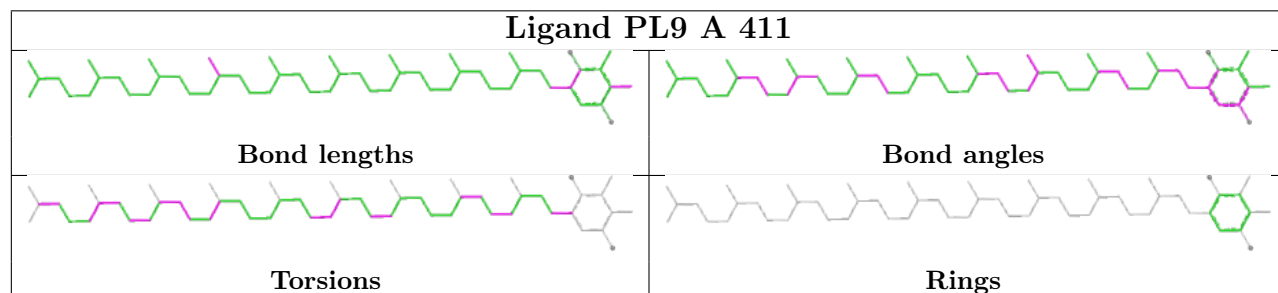
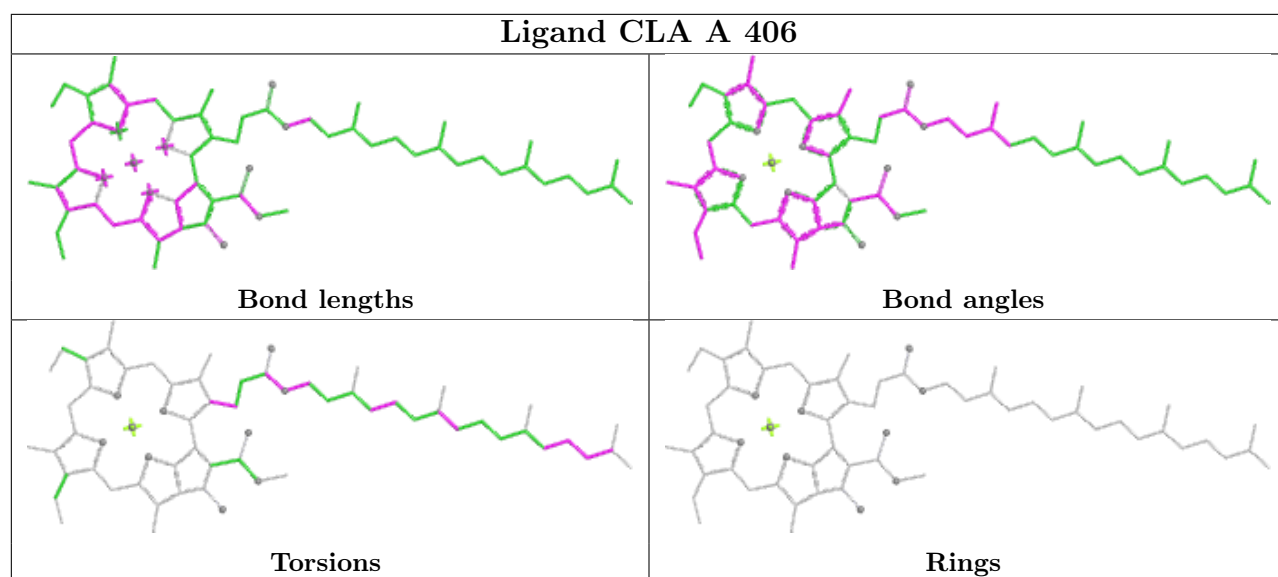
Ligand CLA b 611**Ligand CLA c 505**

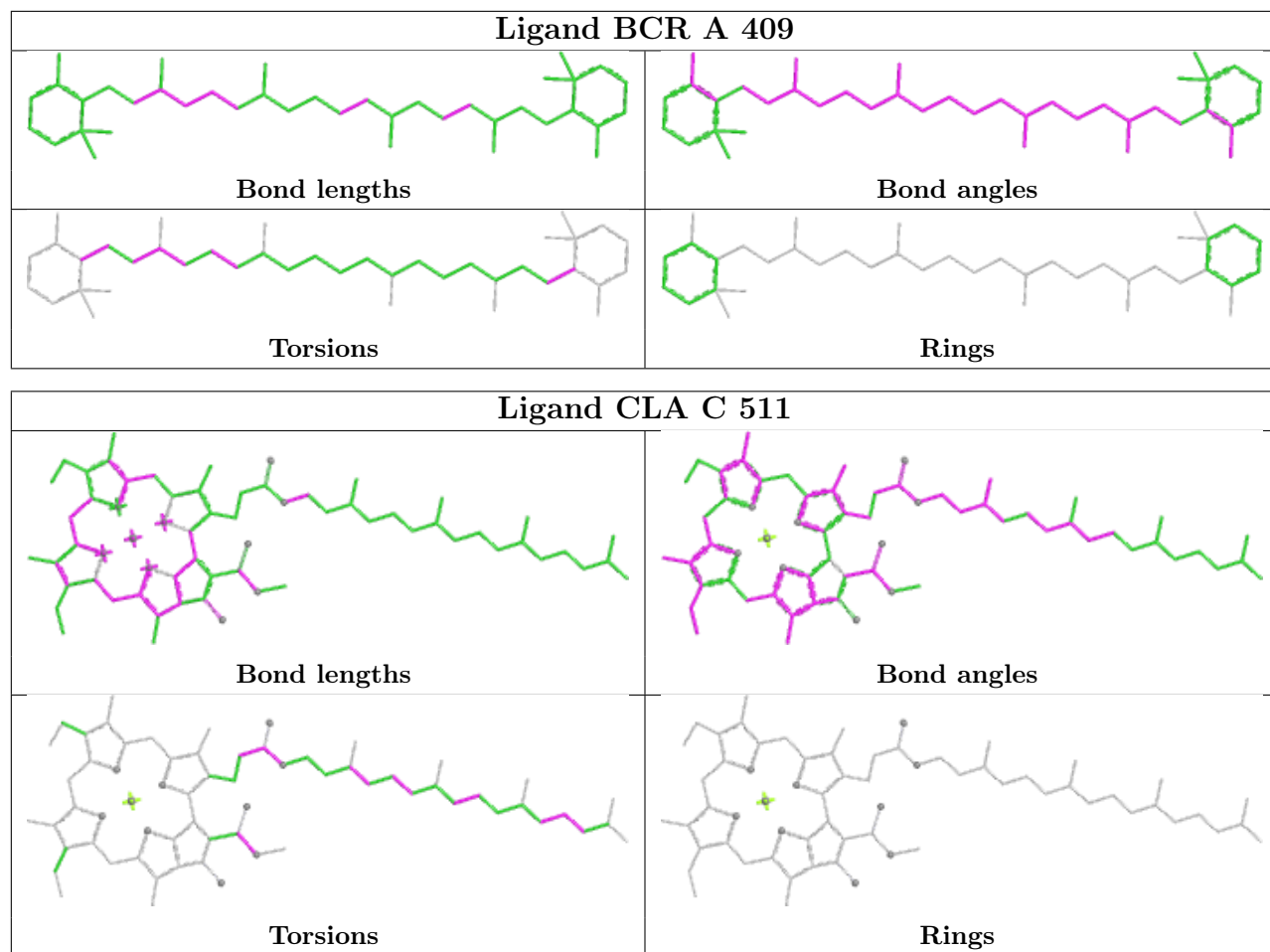


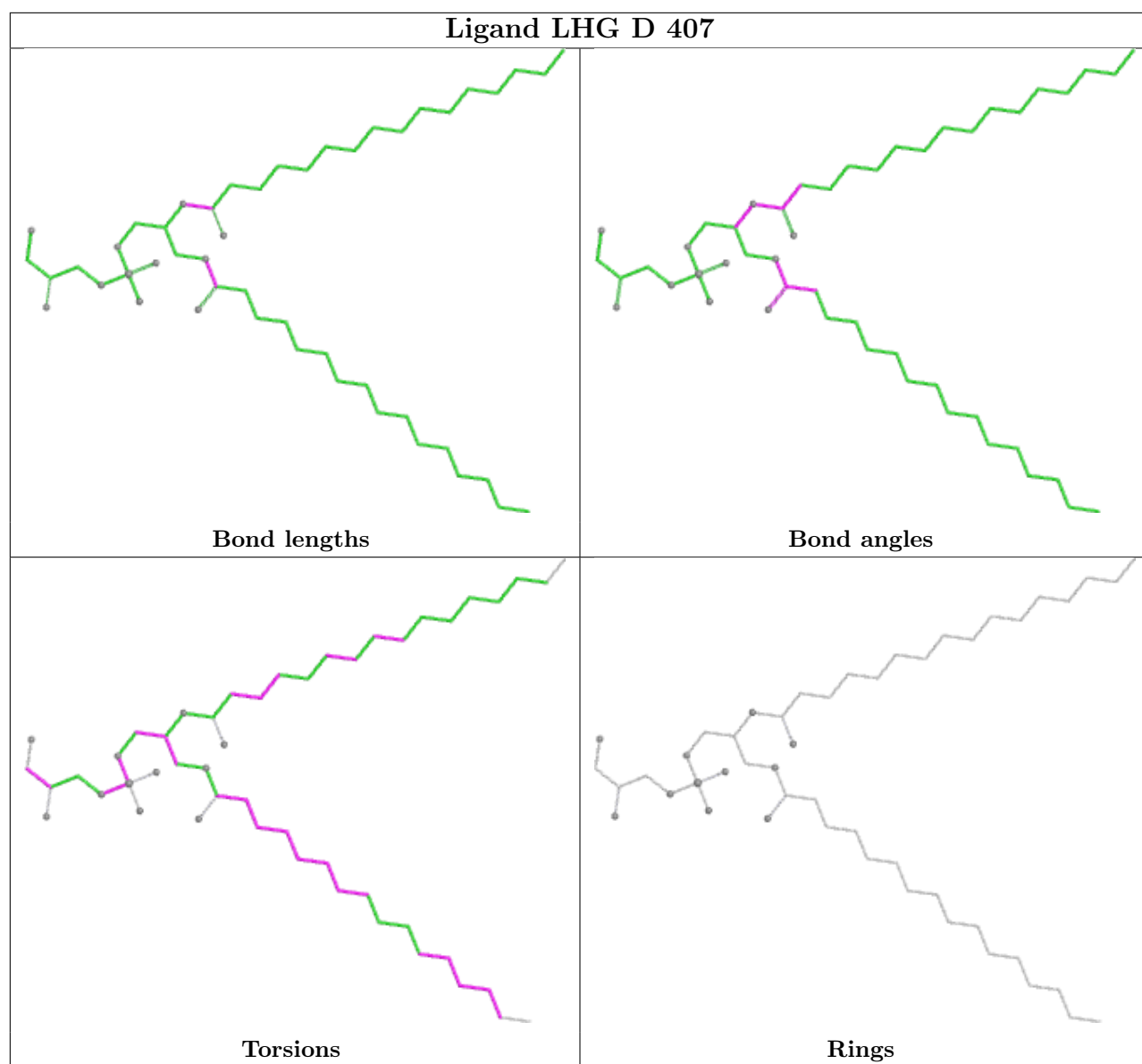


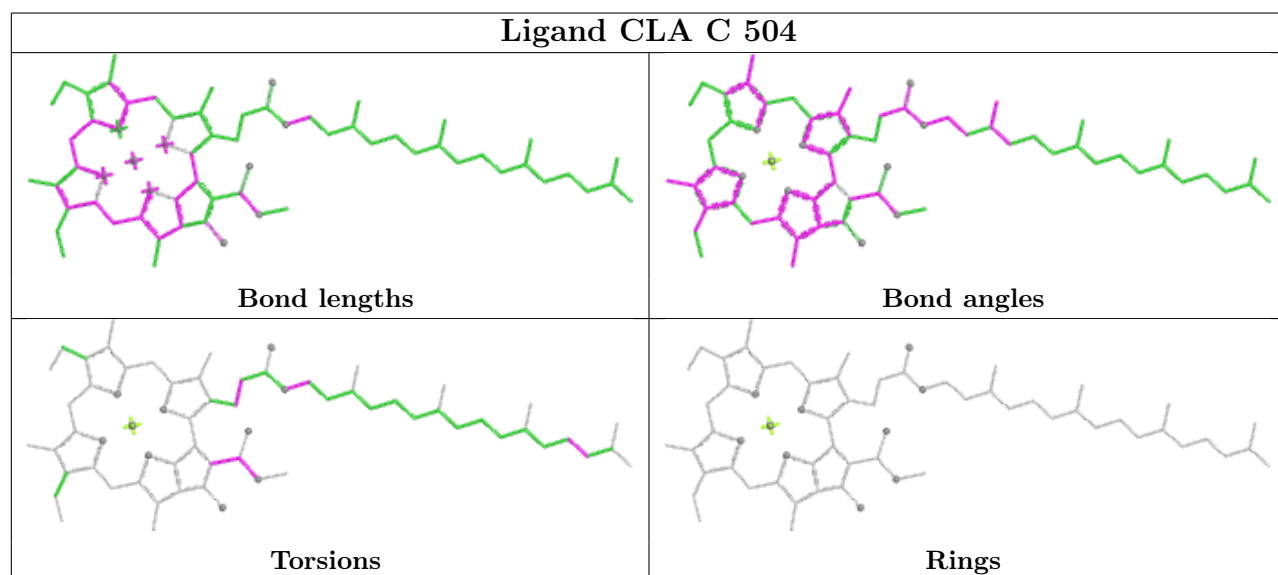
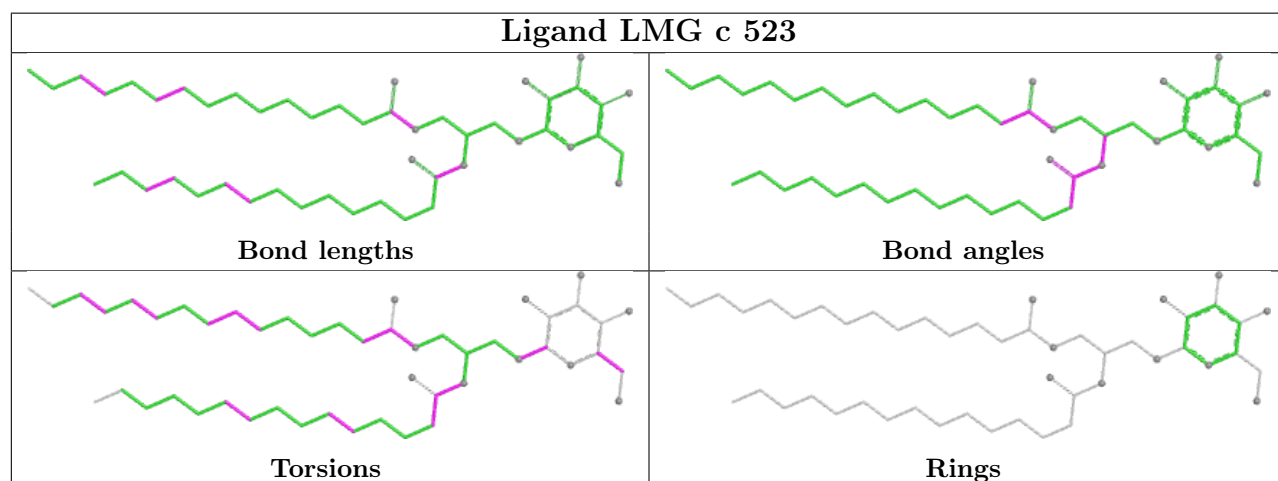
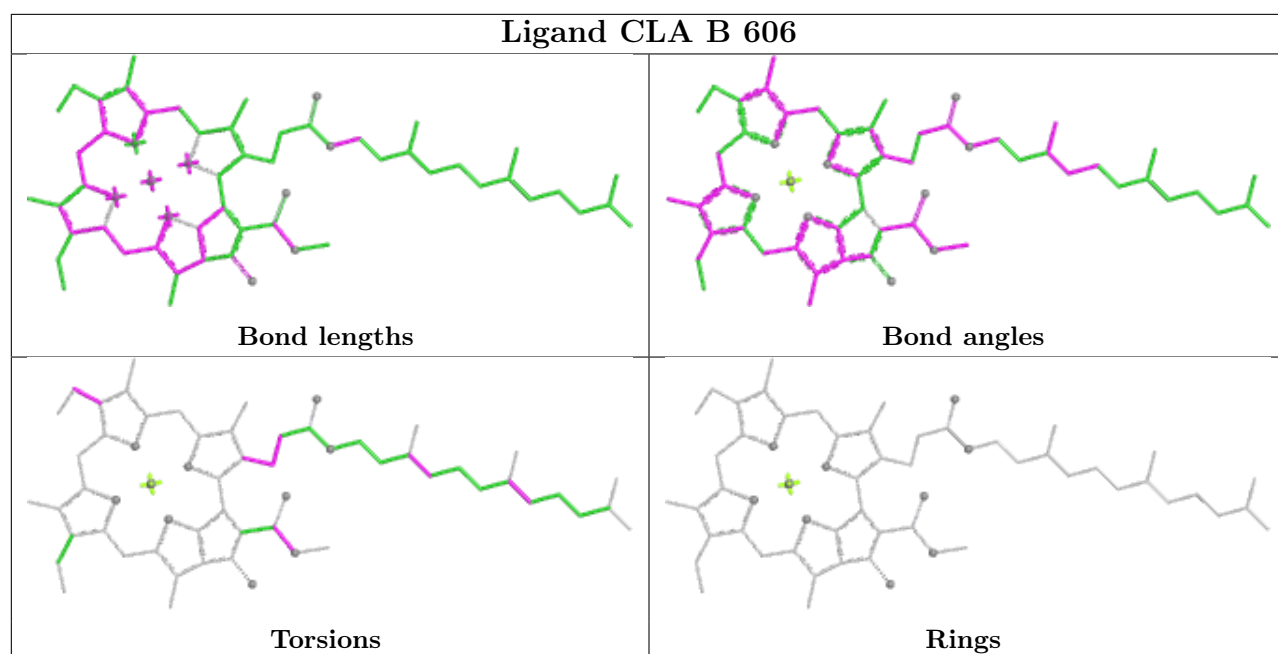


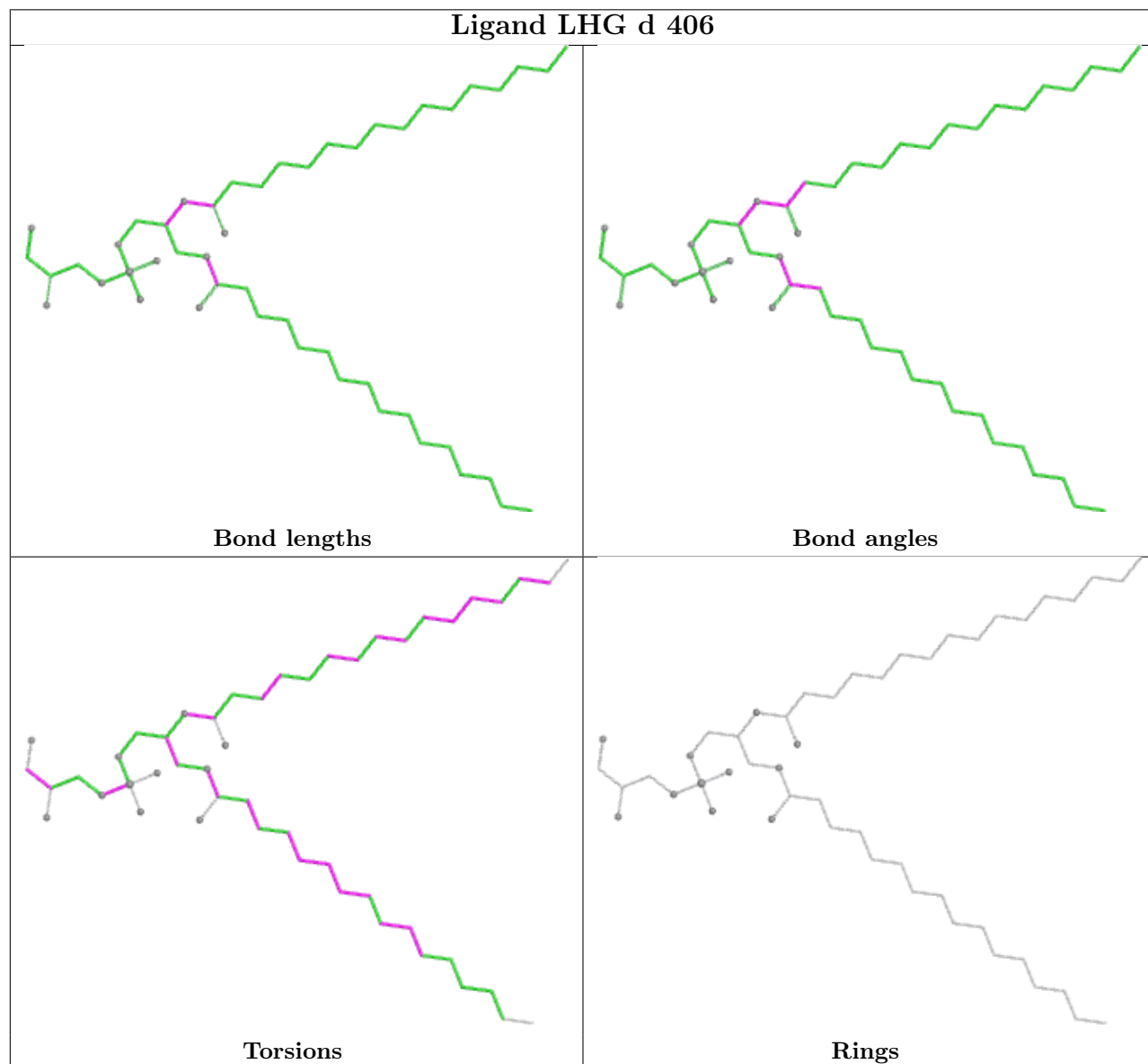
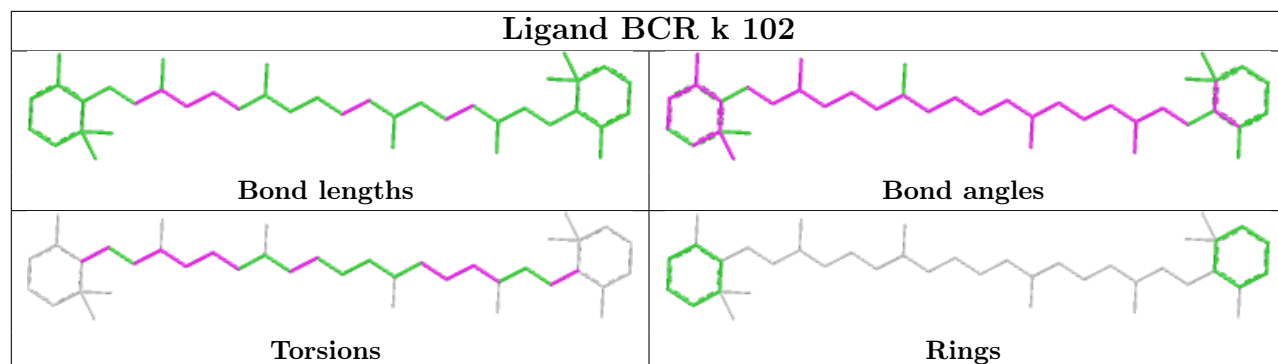


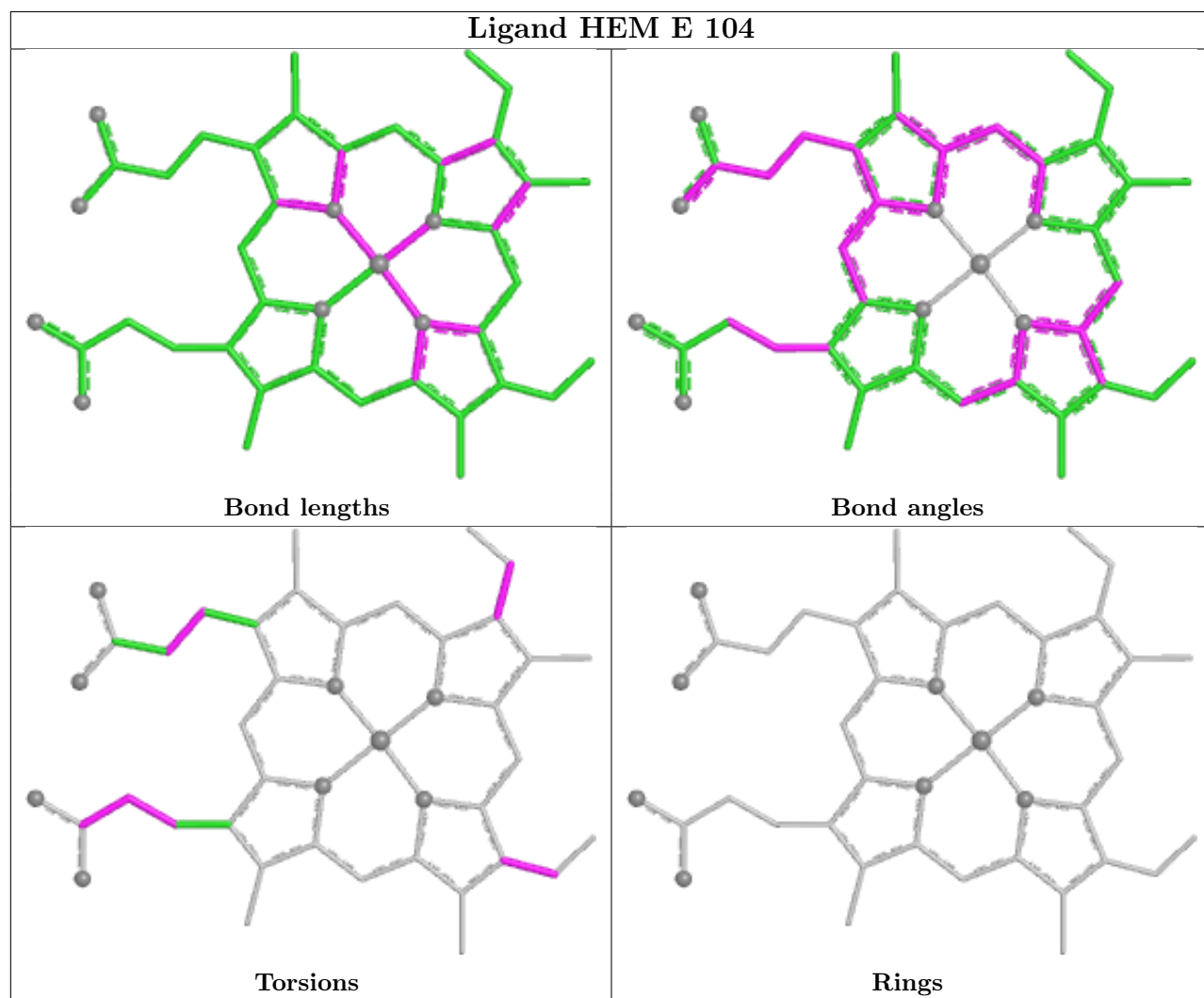
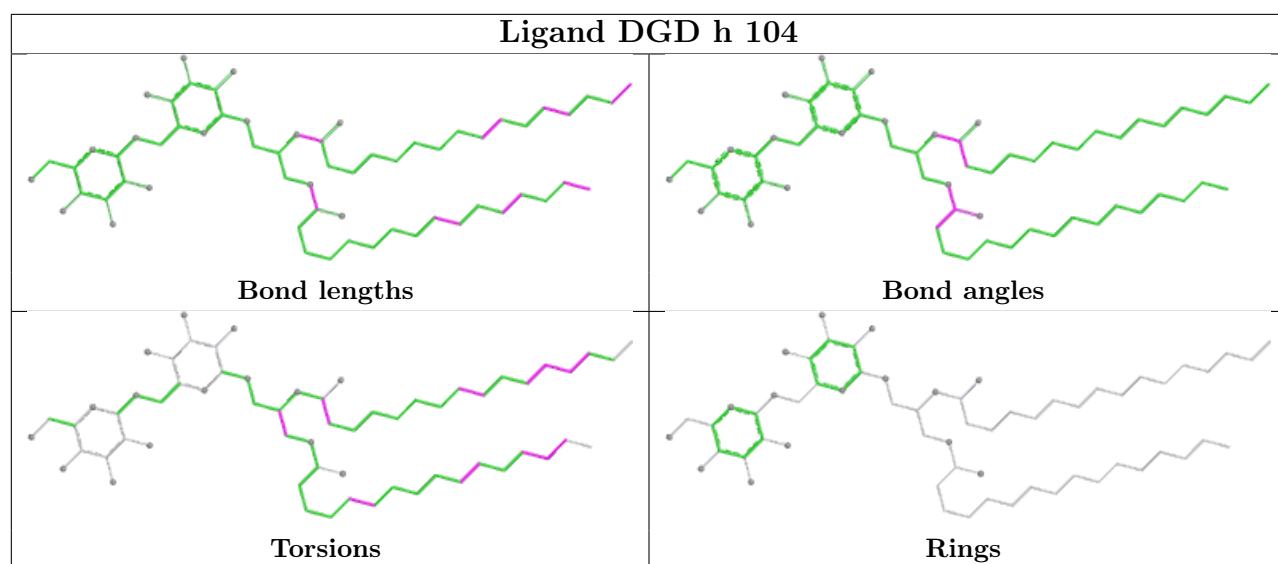


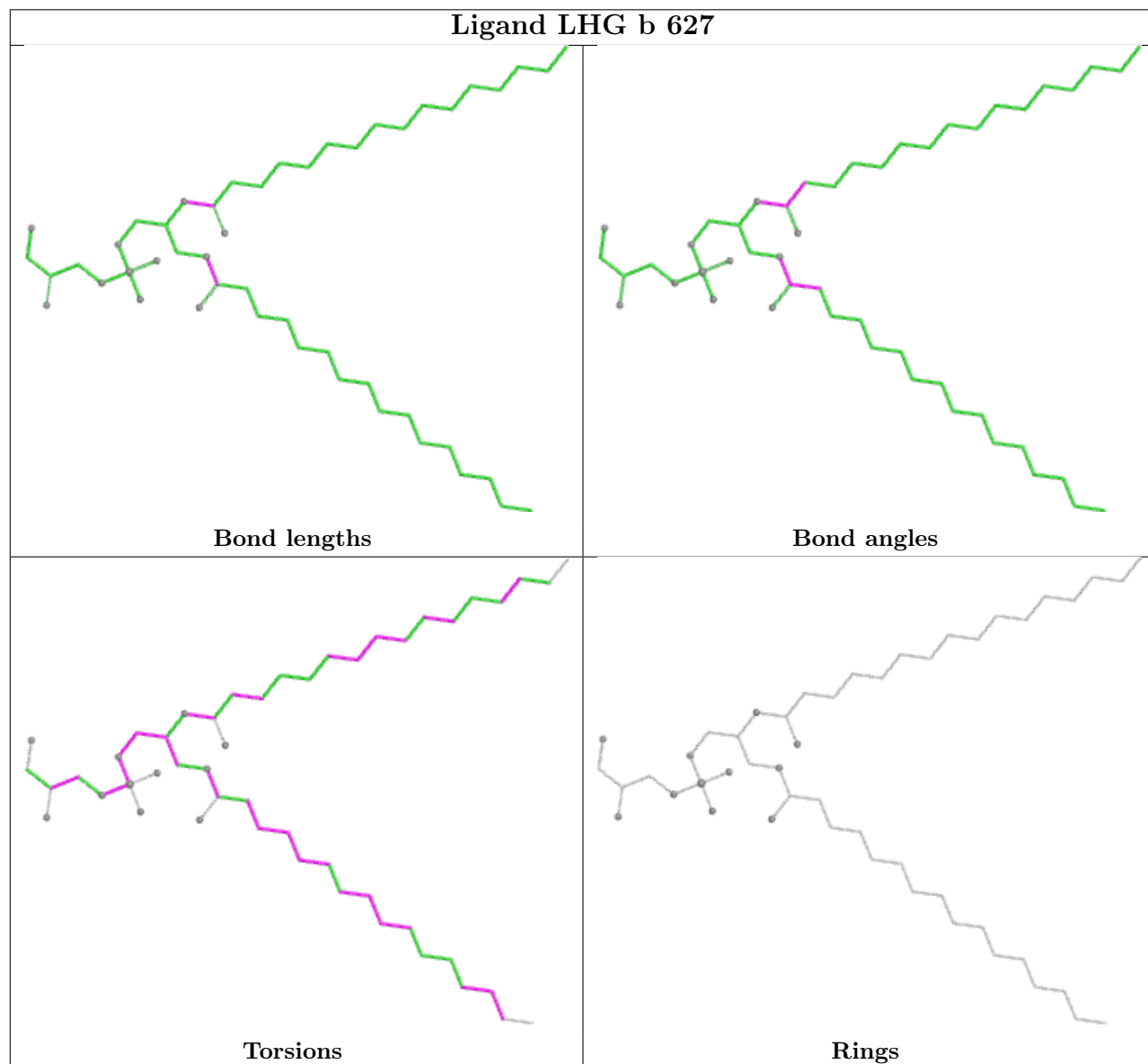
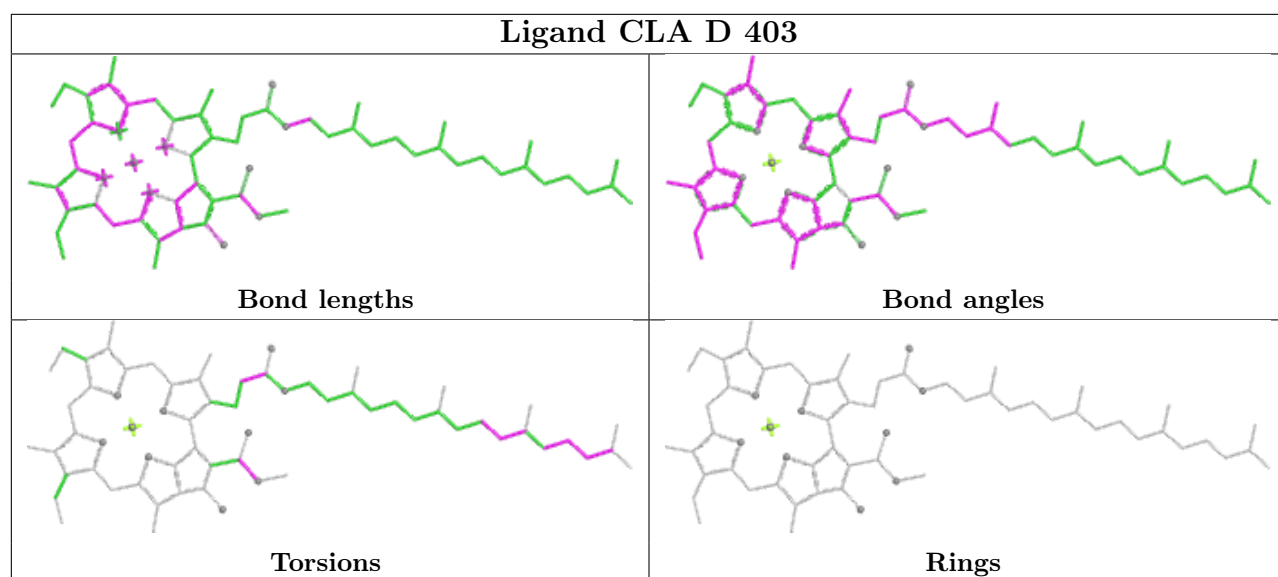


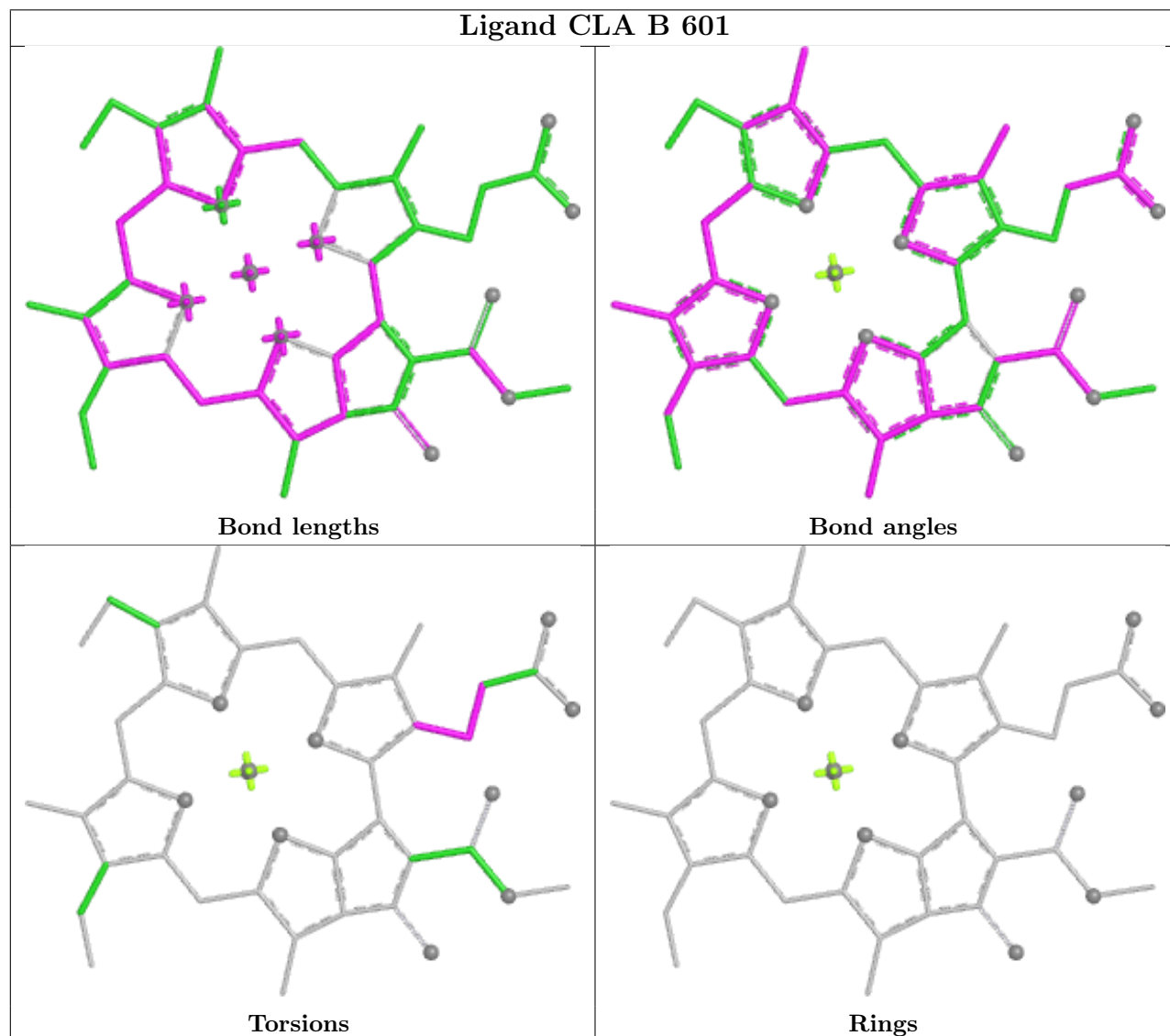
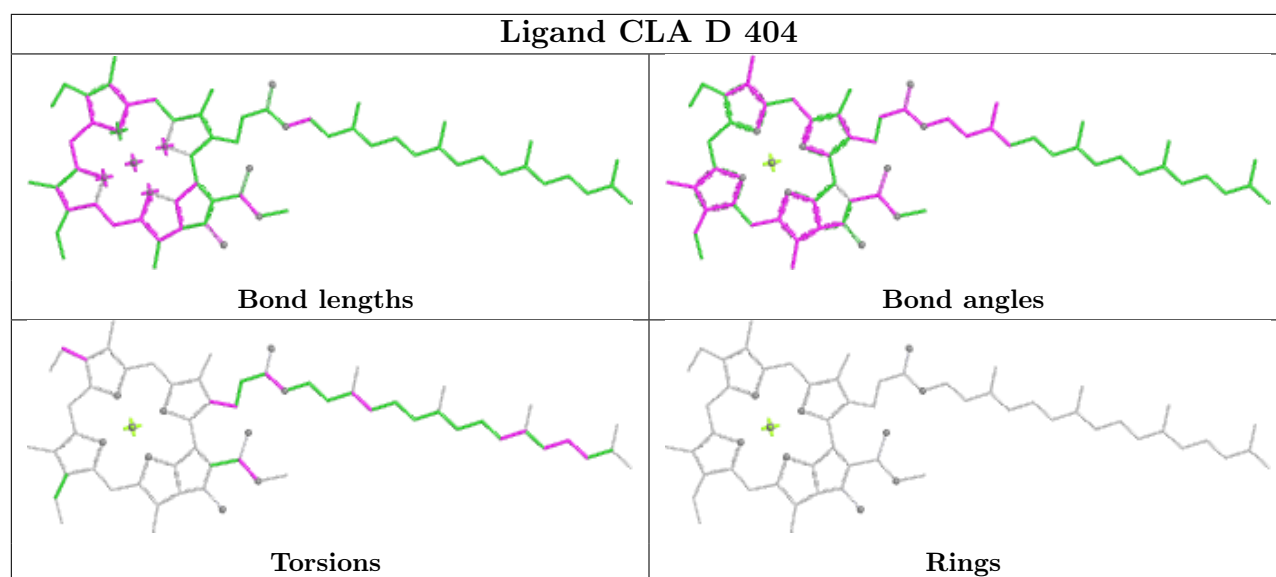


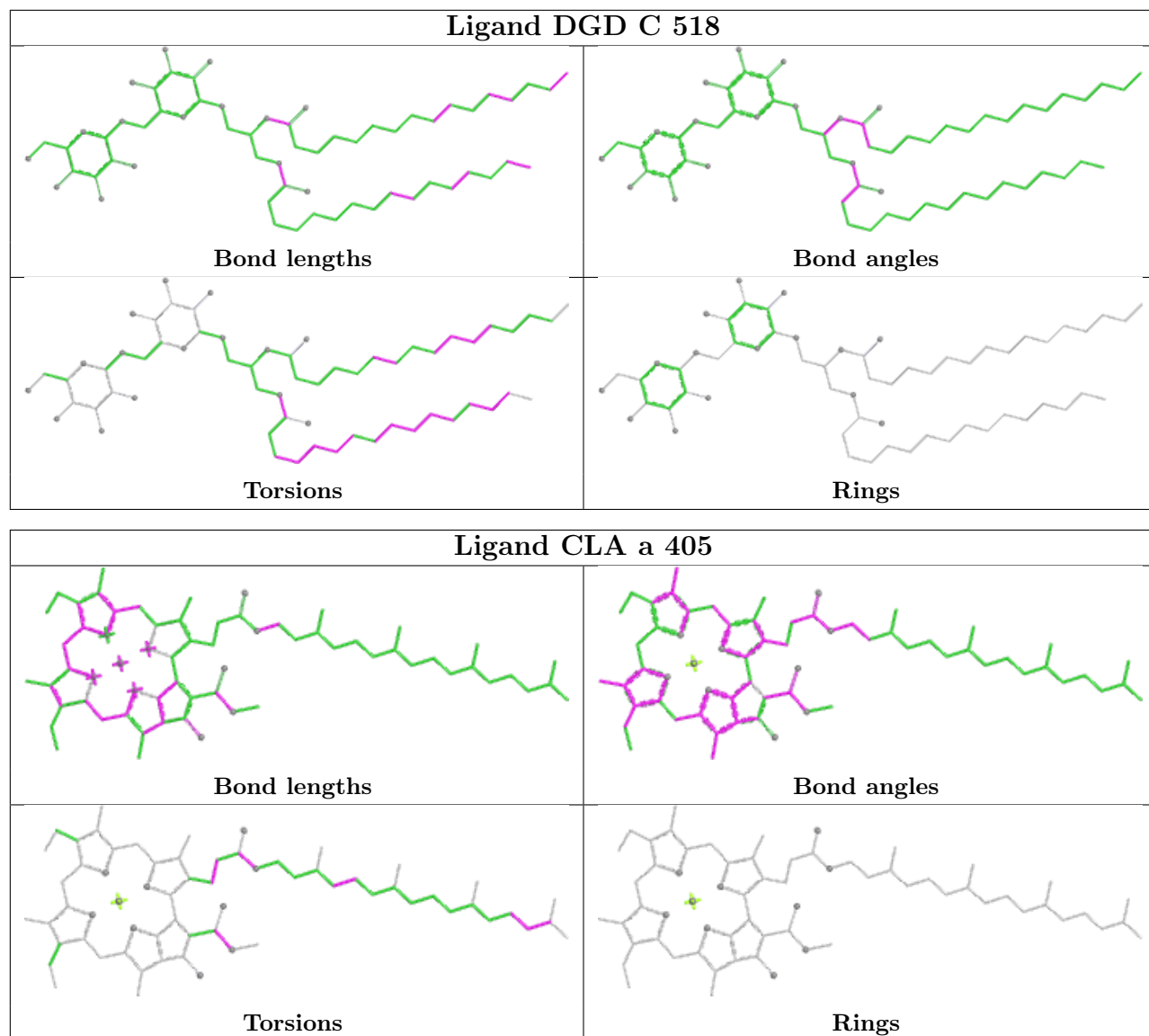


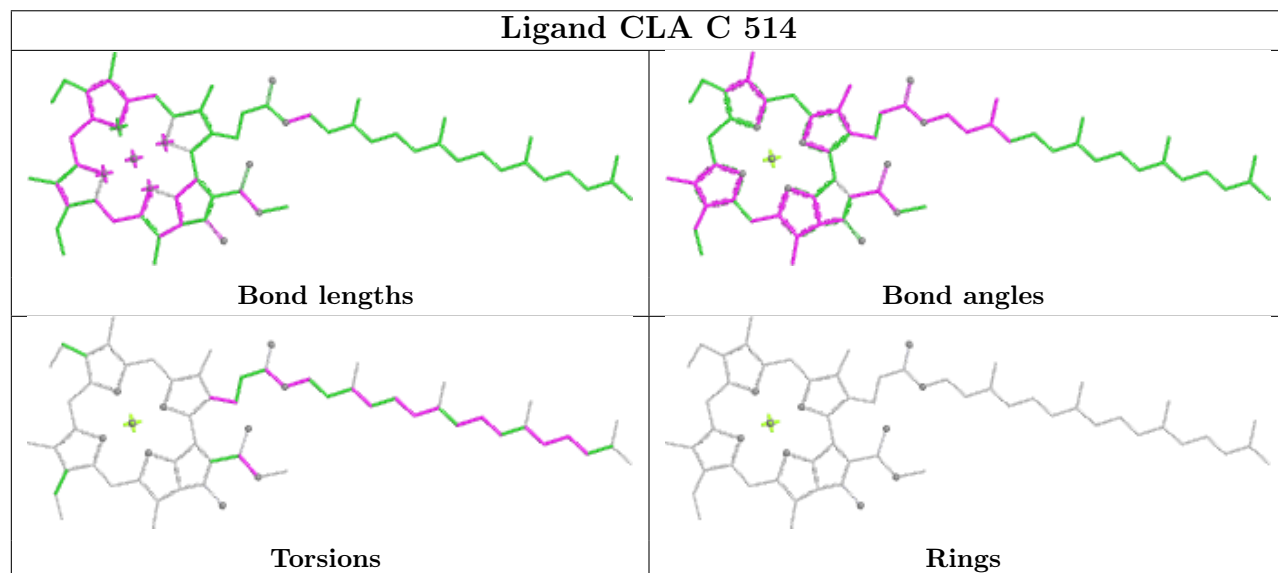
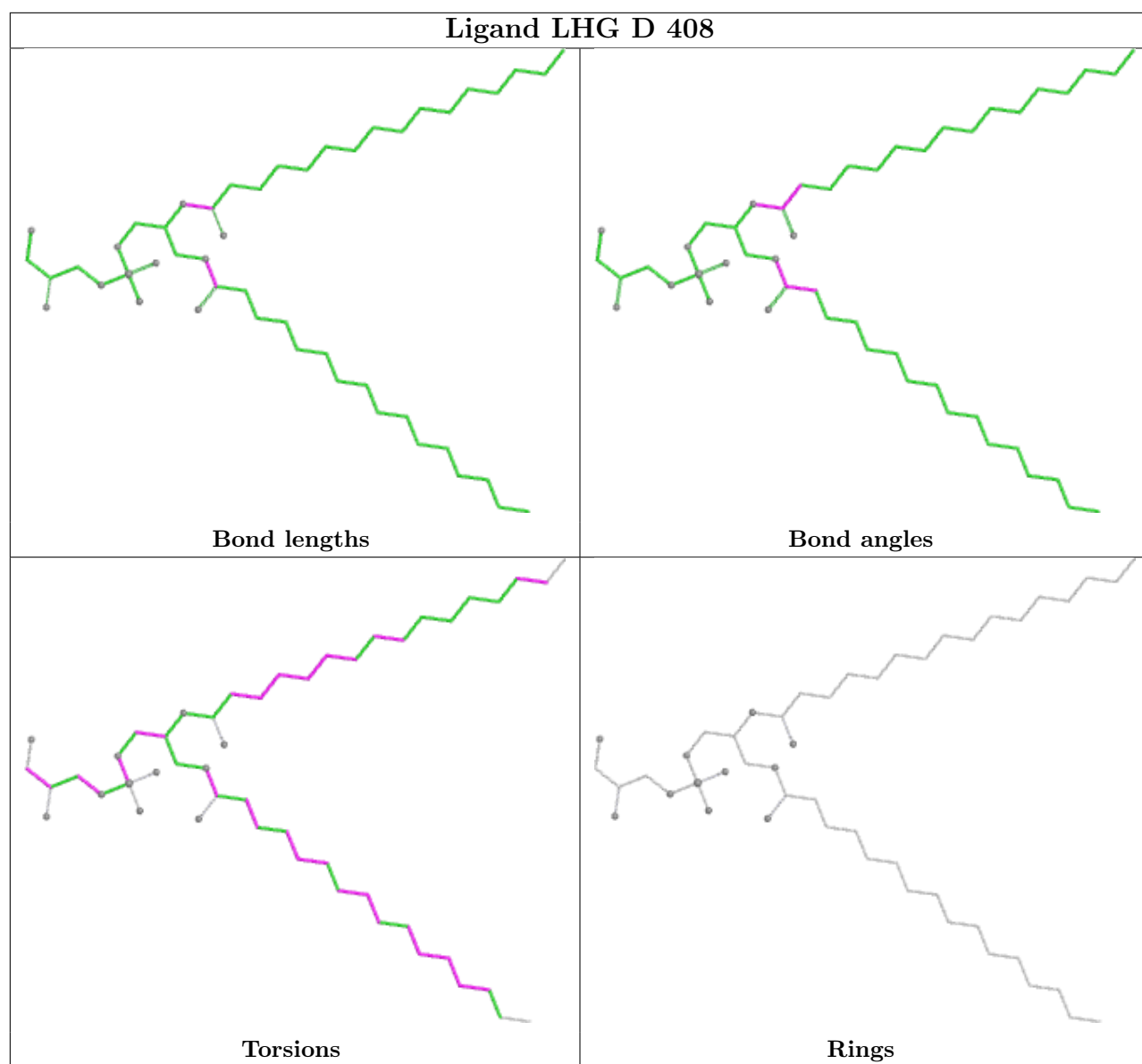


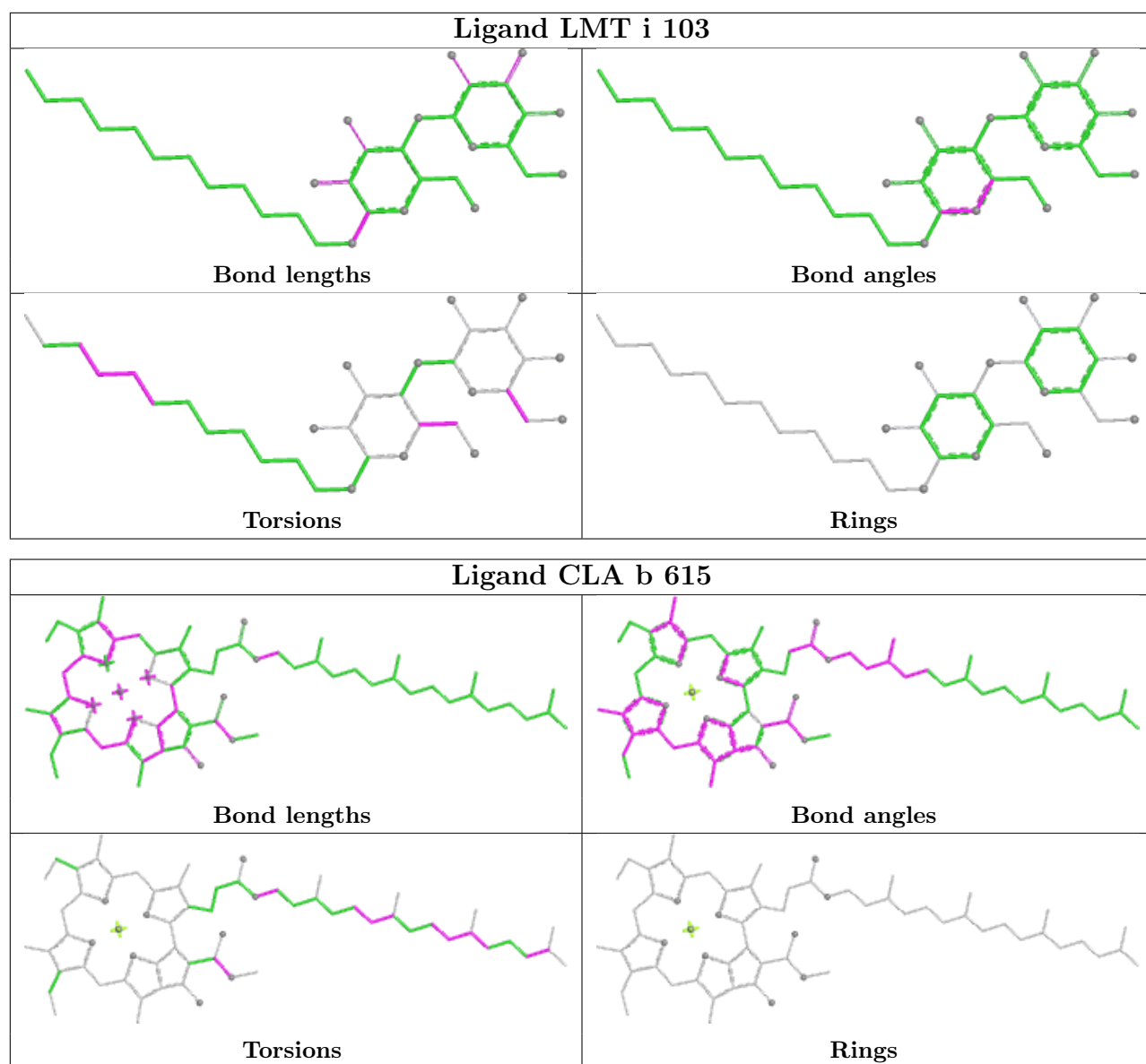




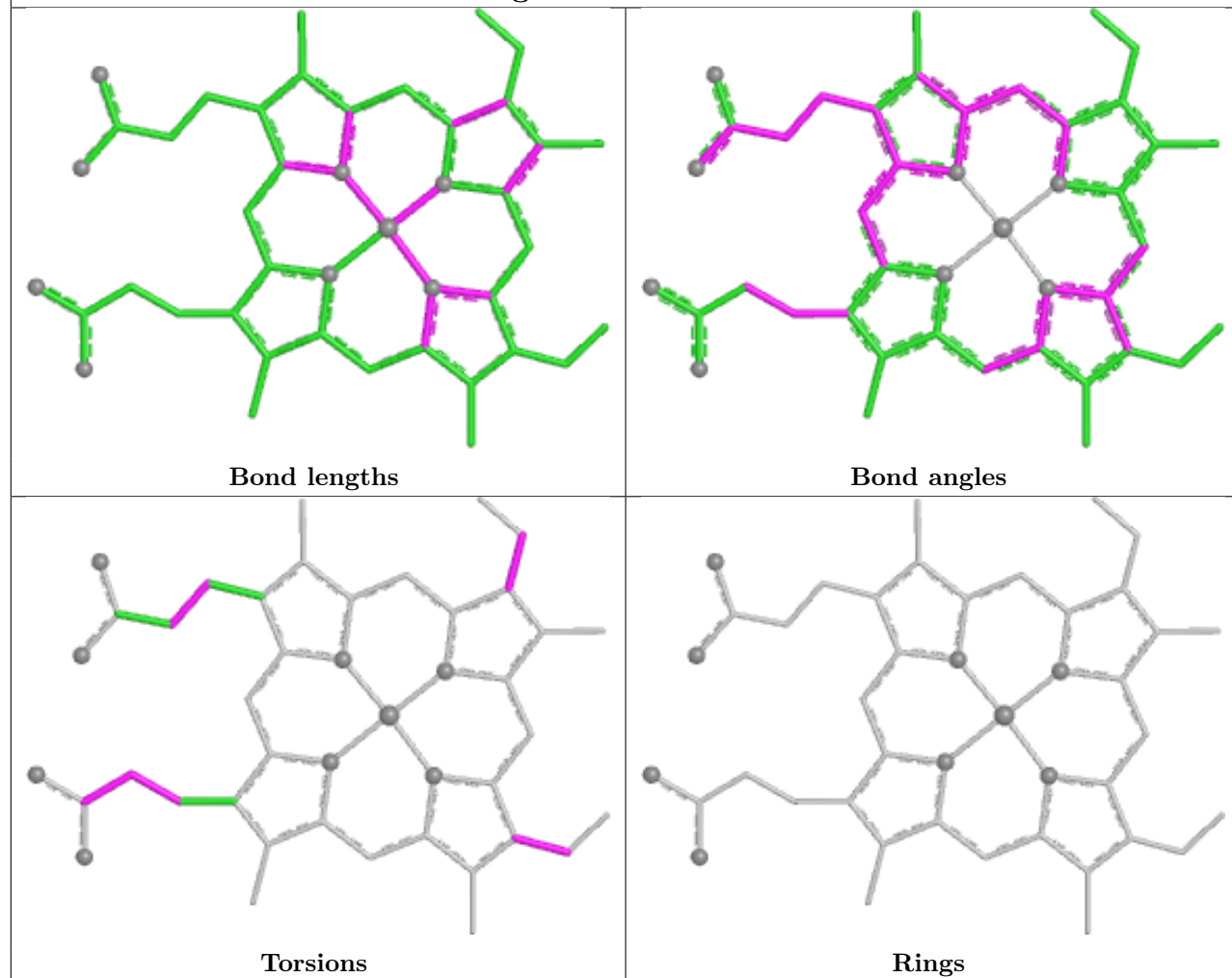




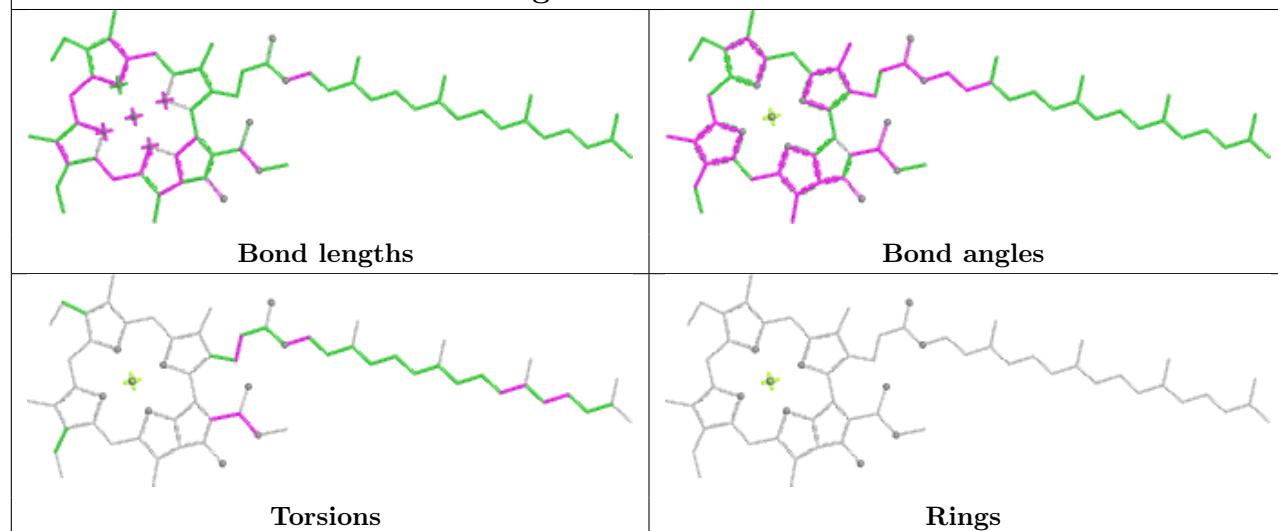


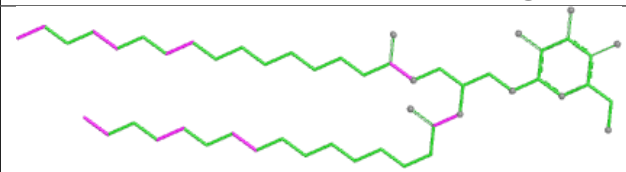
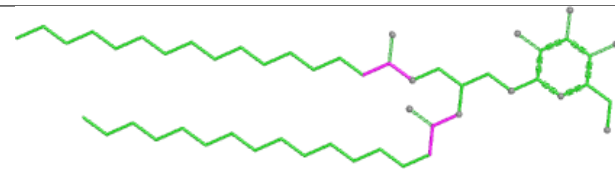
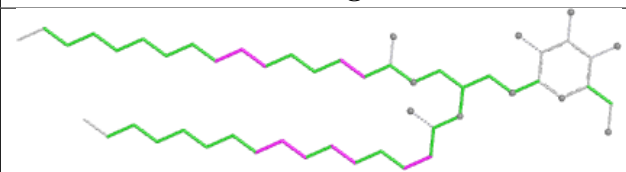
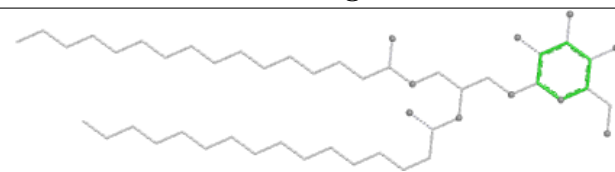


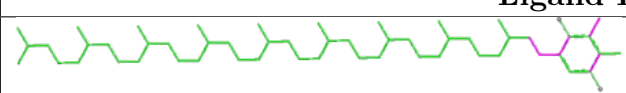
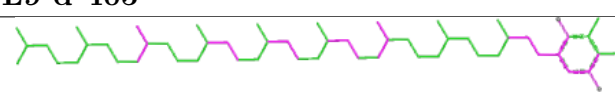
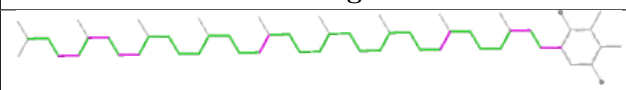
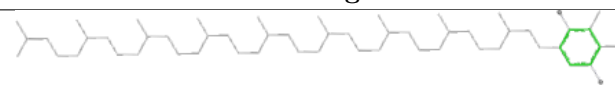
Ligand HEM e 104

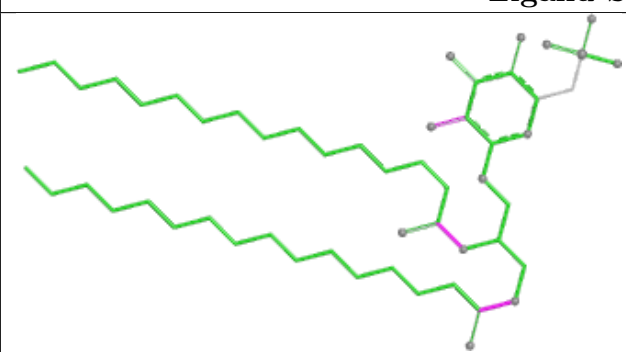
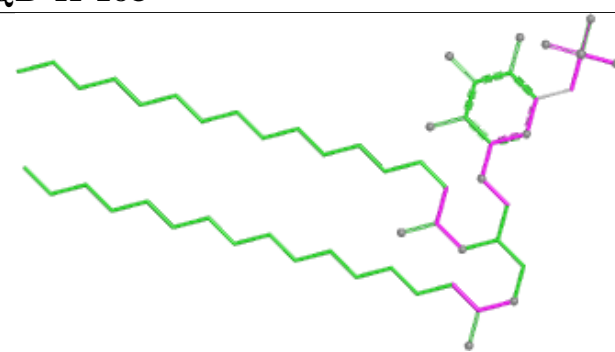
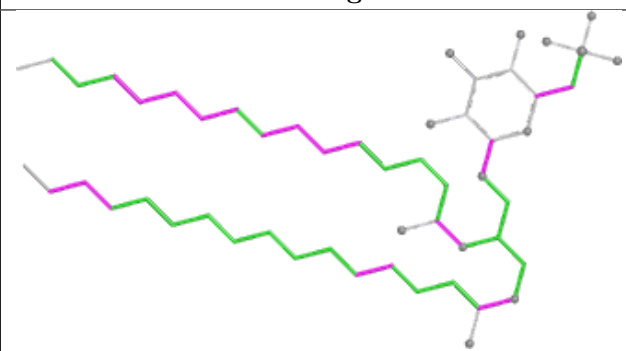
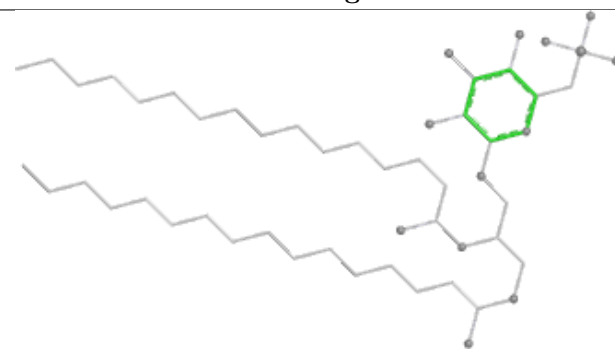


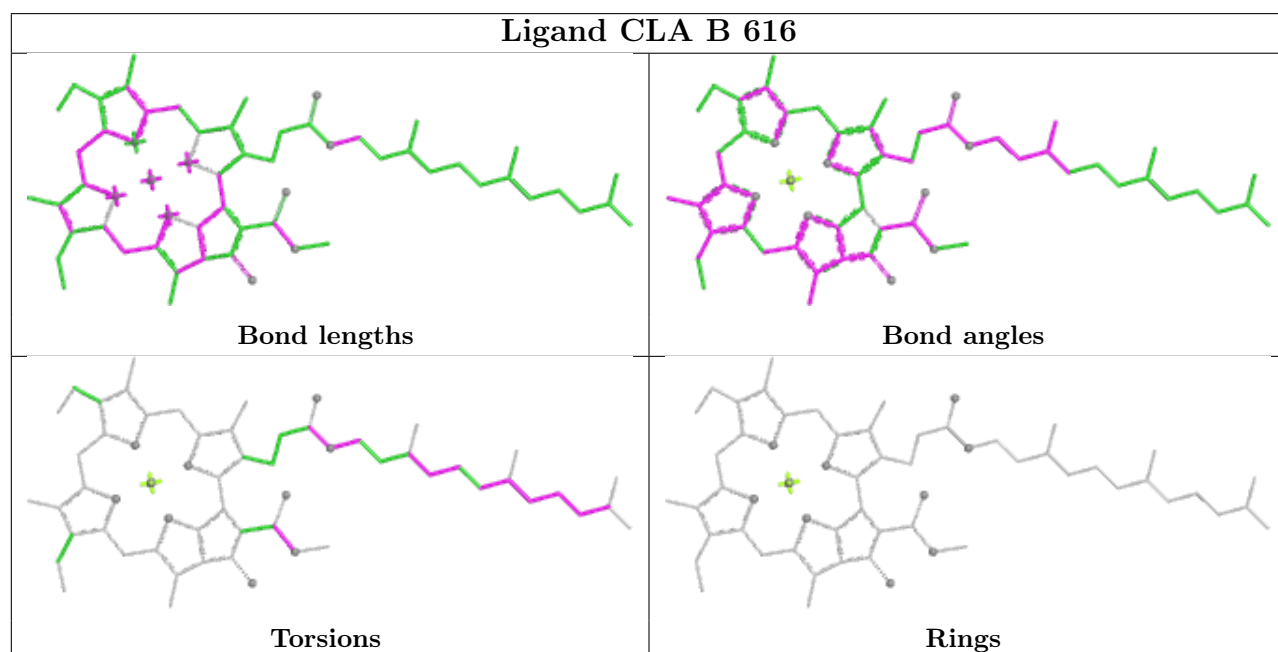
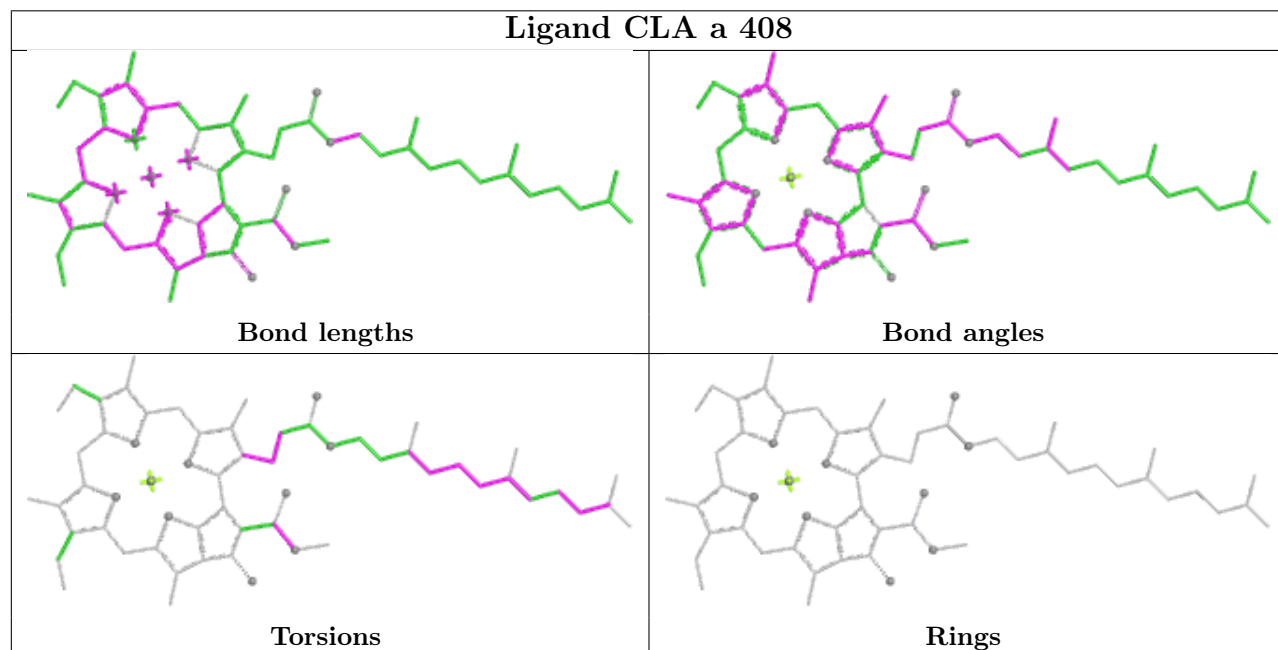
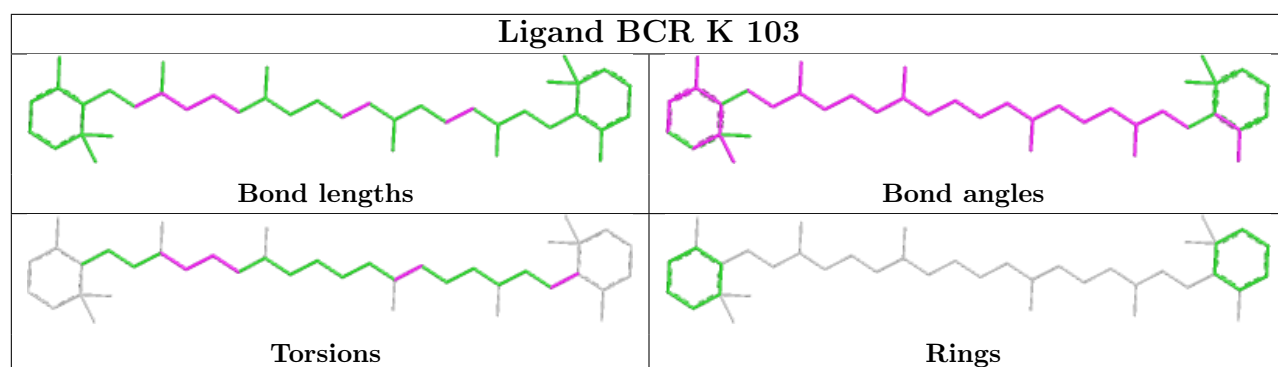
Ligand CLA C 503

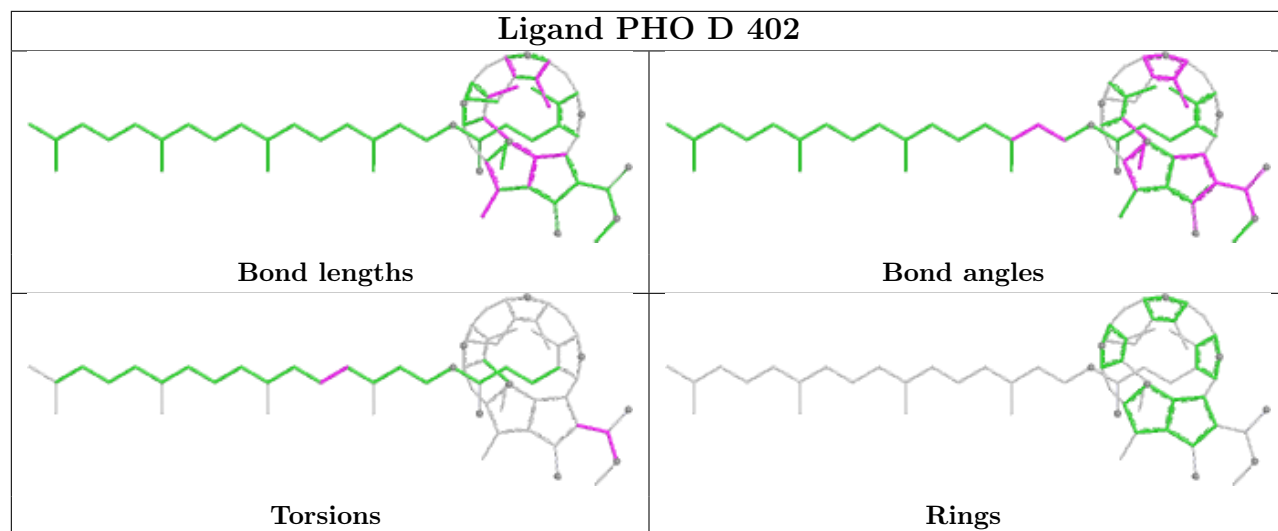
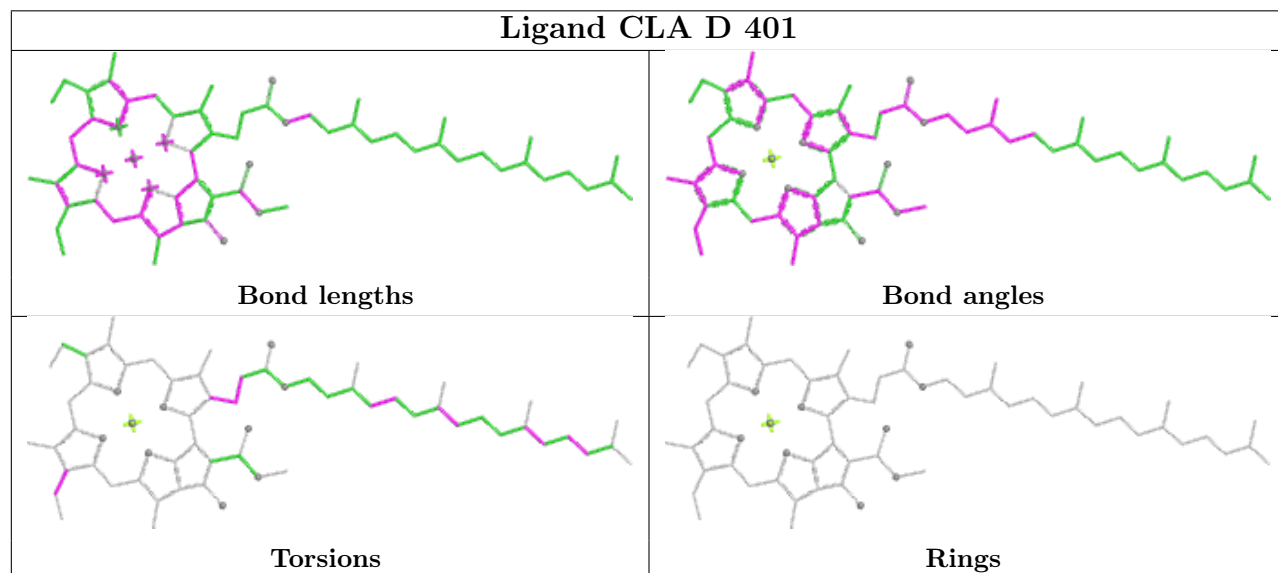
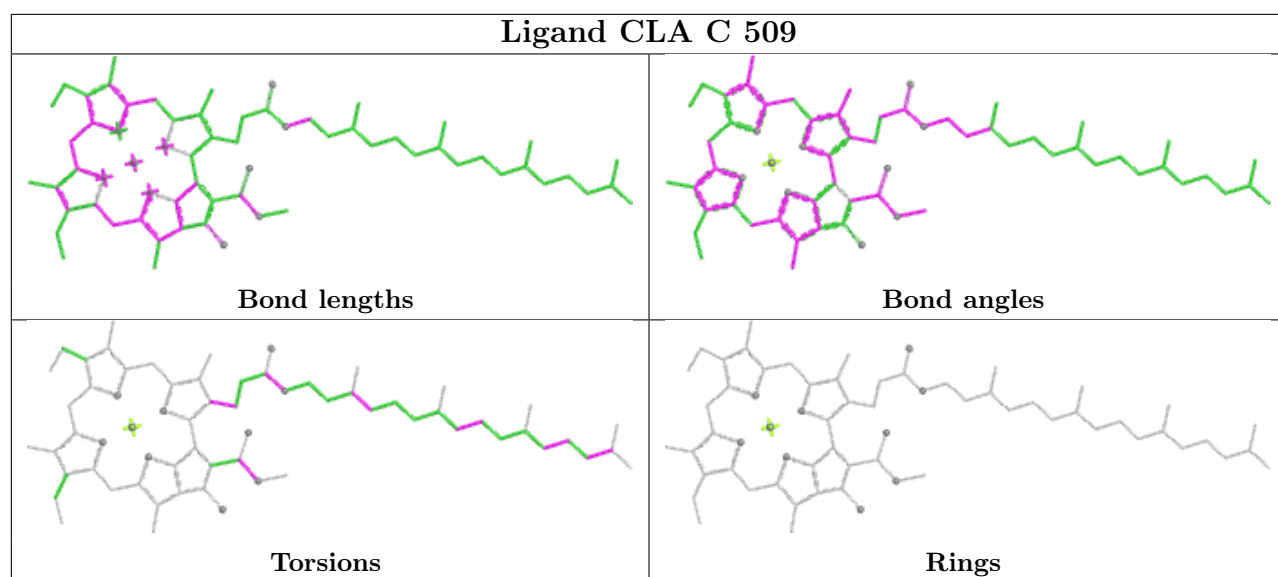


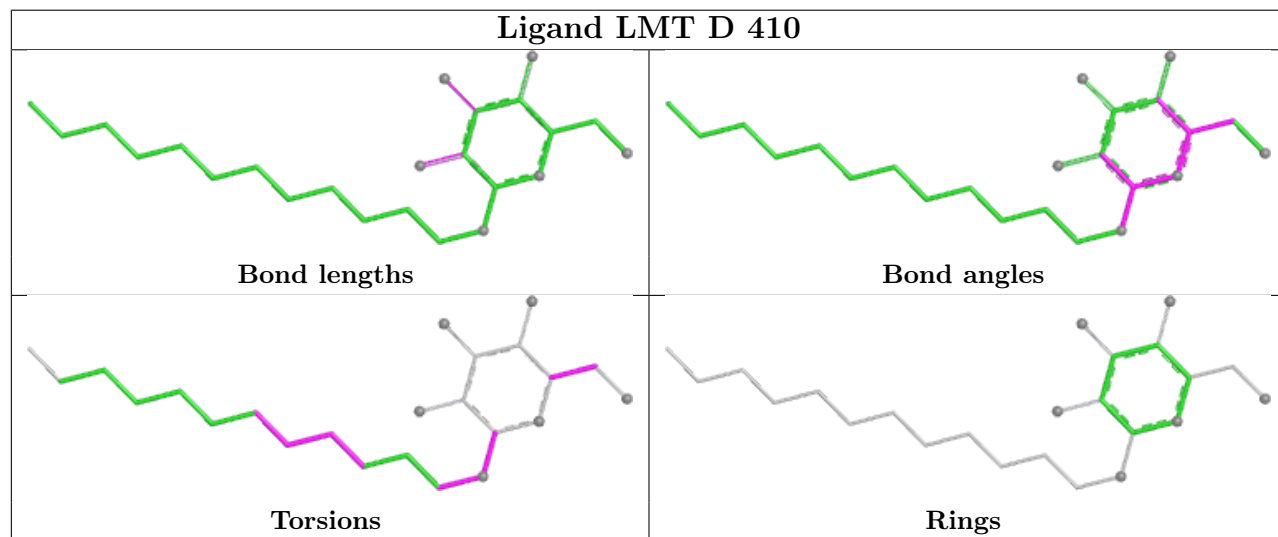
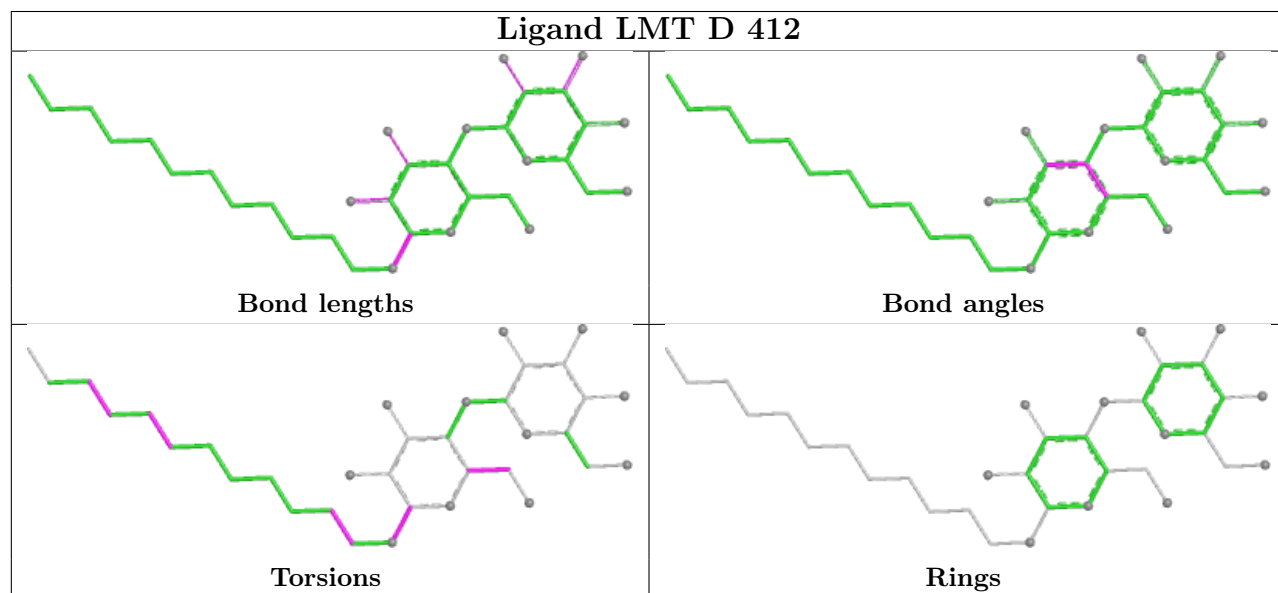
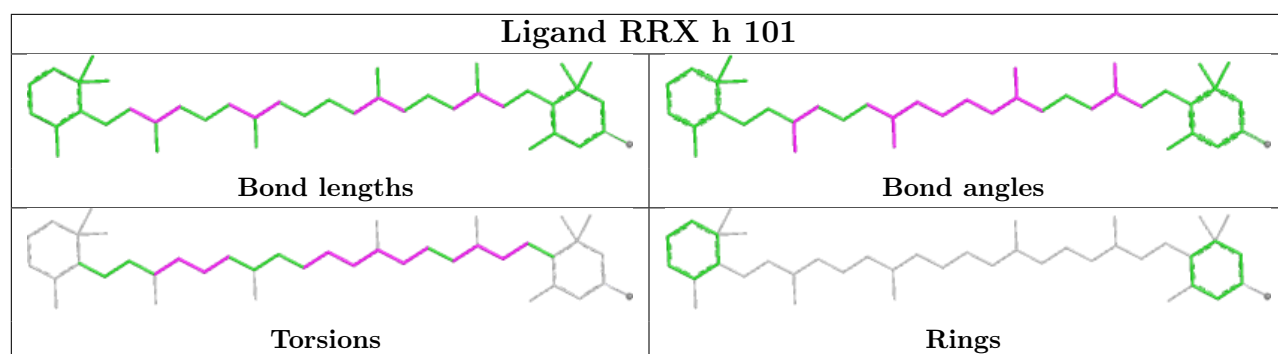
Ligand LMG b 621	
 Bond lengths	 Bond angles
 Torsions	 Rings

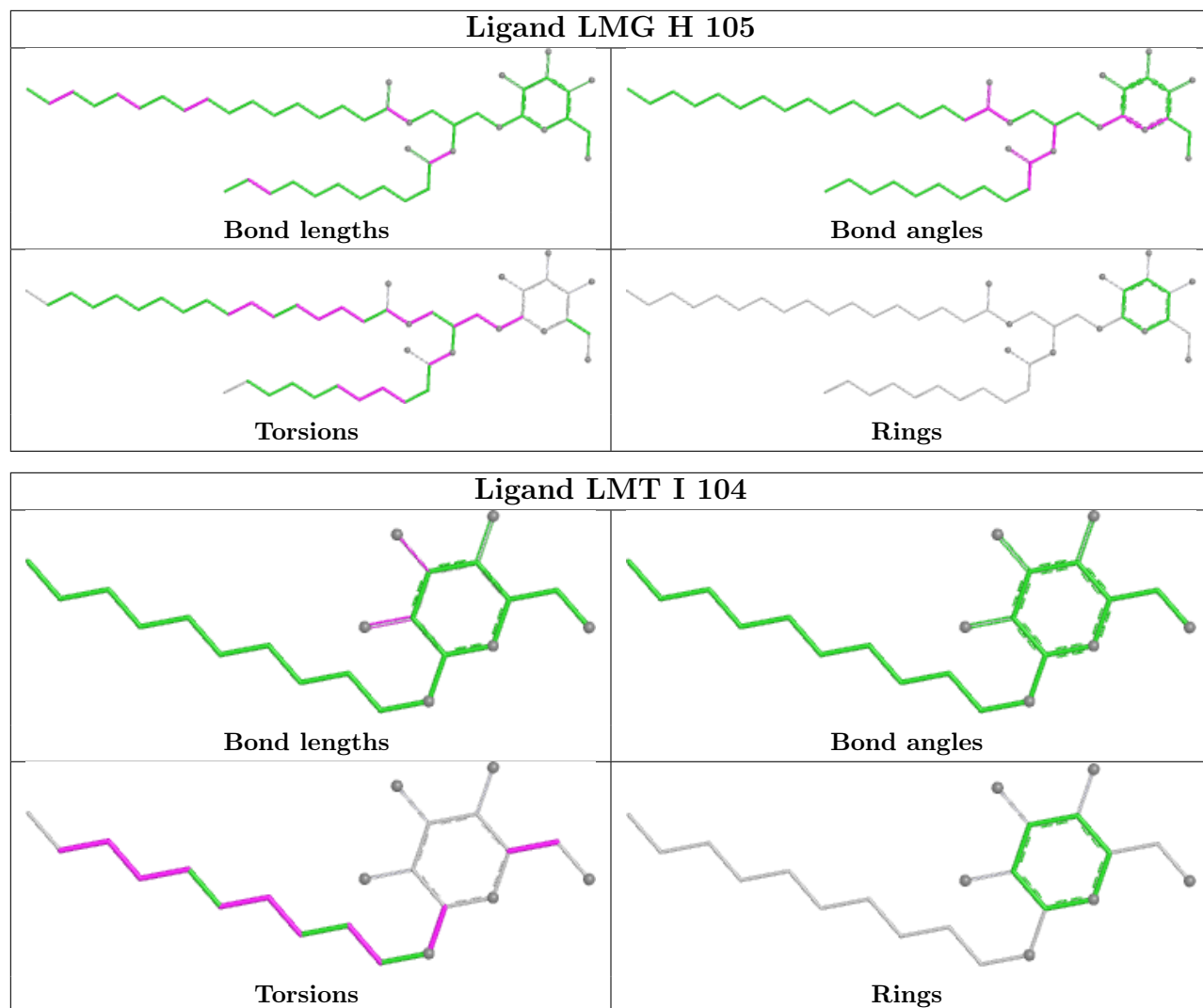
Ligand PL9 d 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

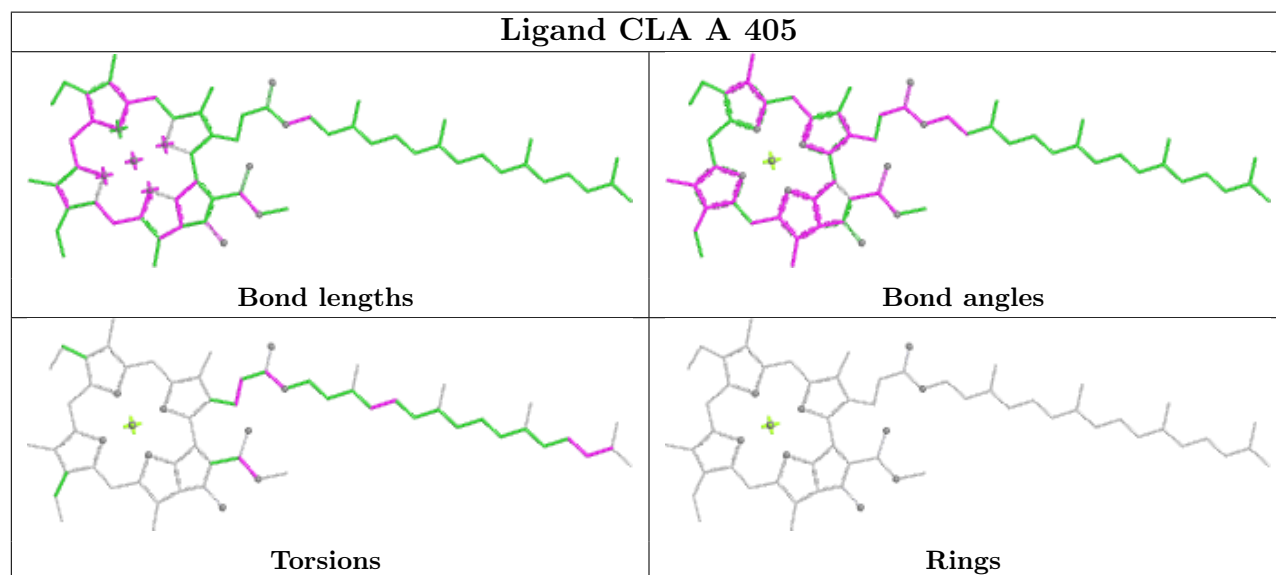
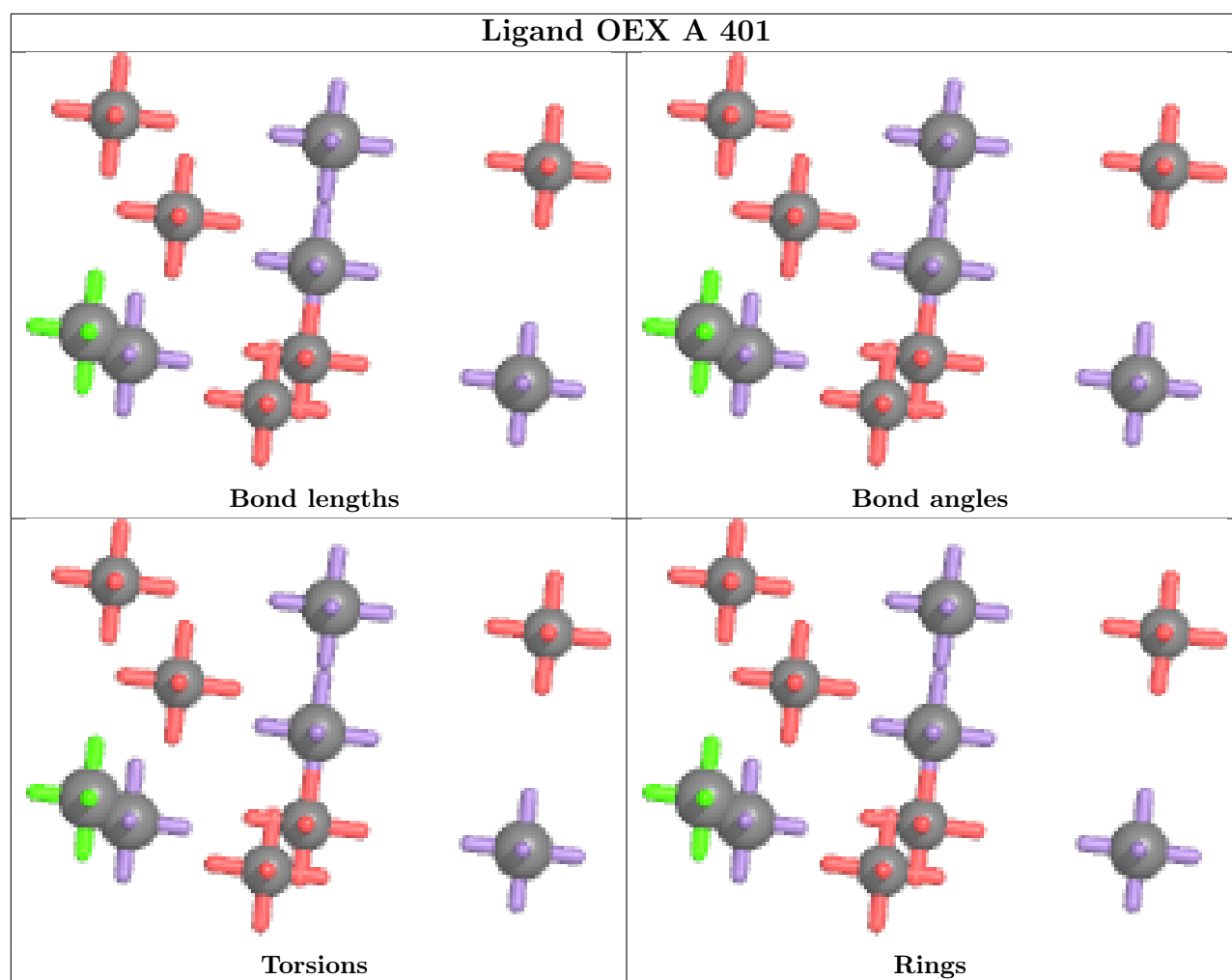
Ligand SQD H 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

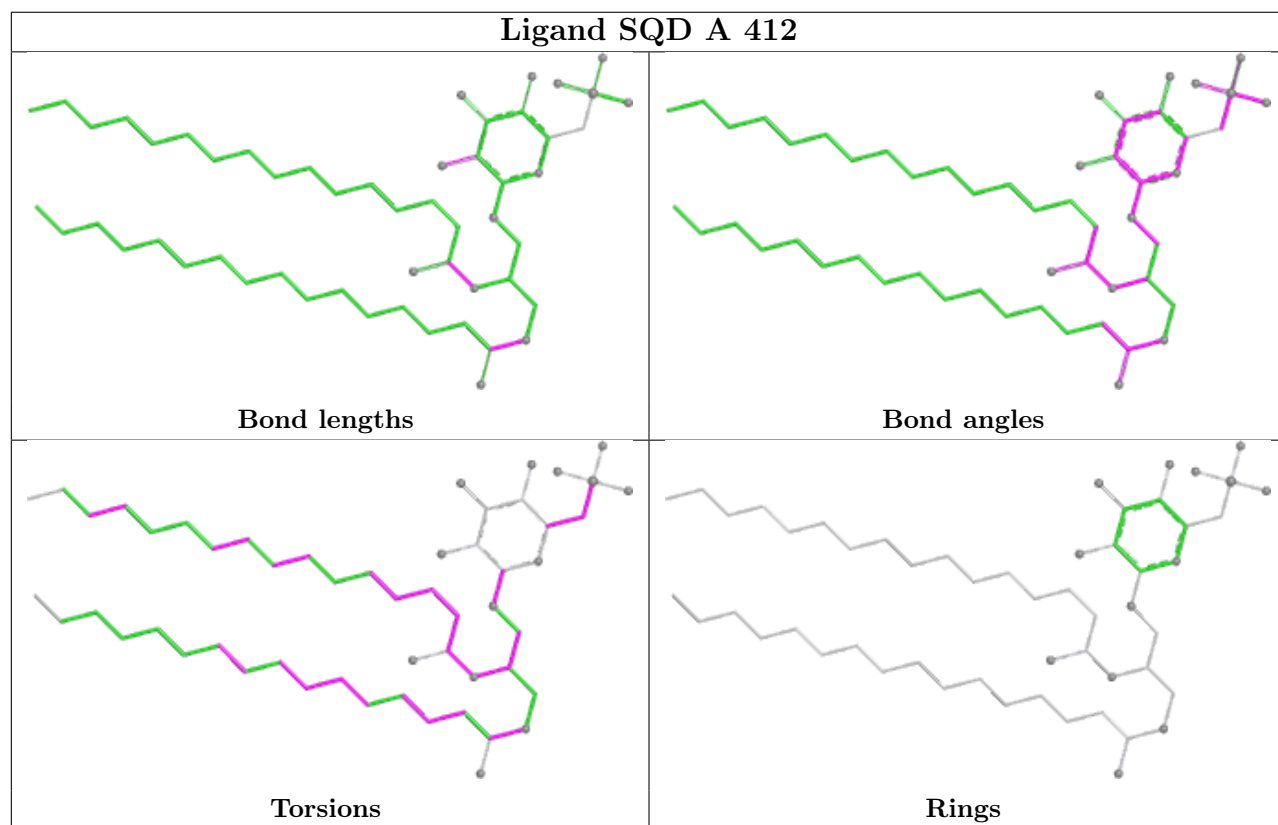
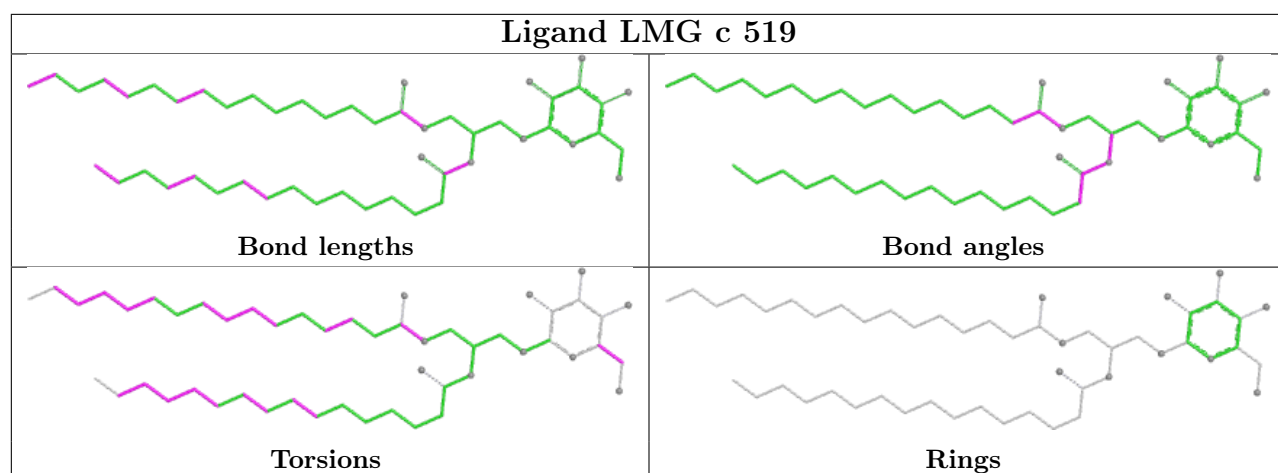


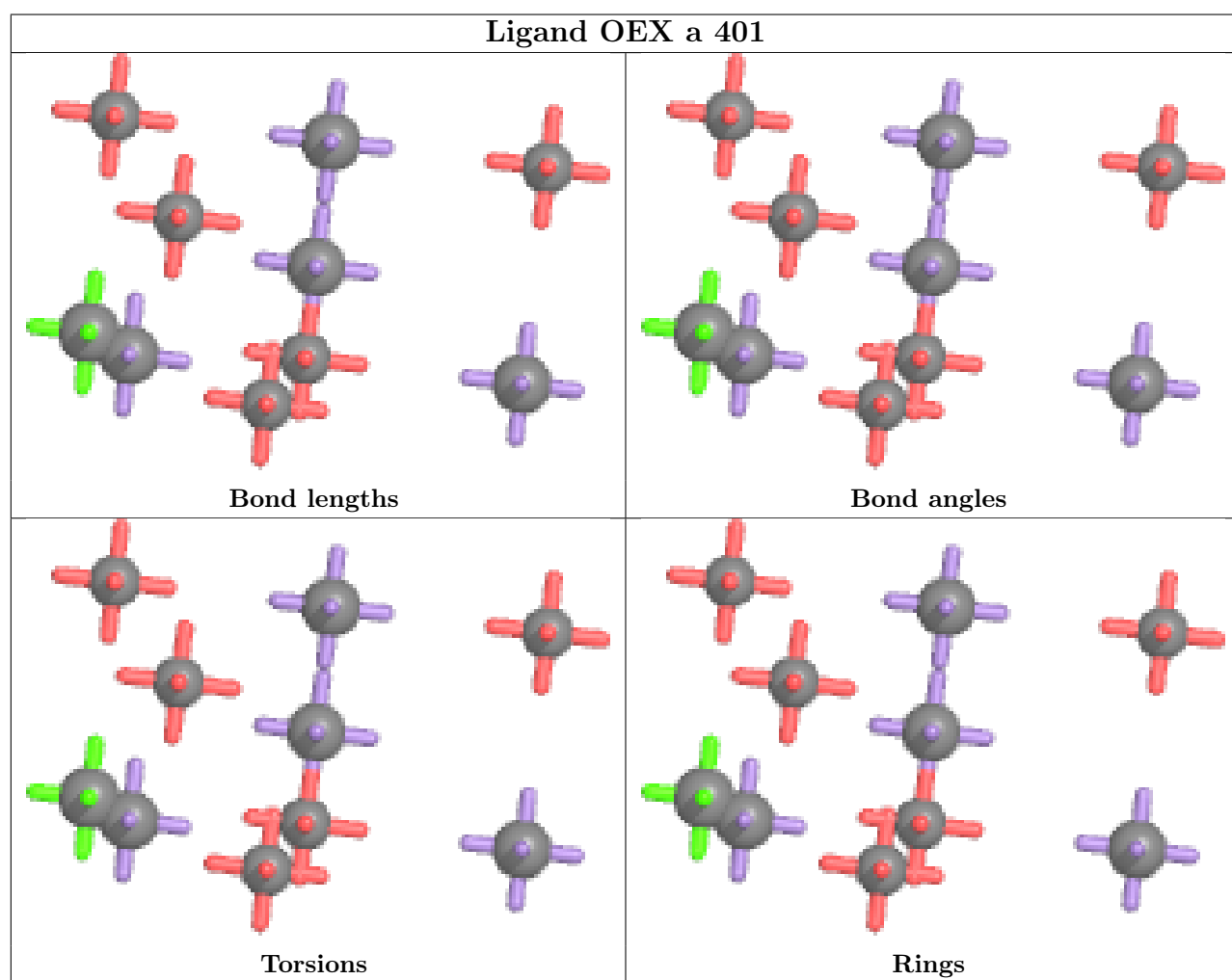
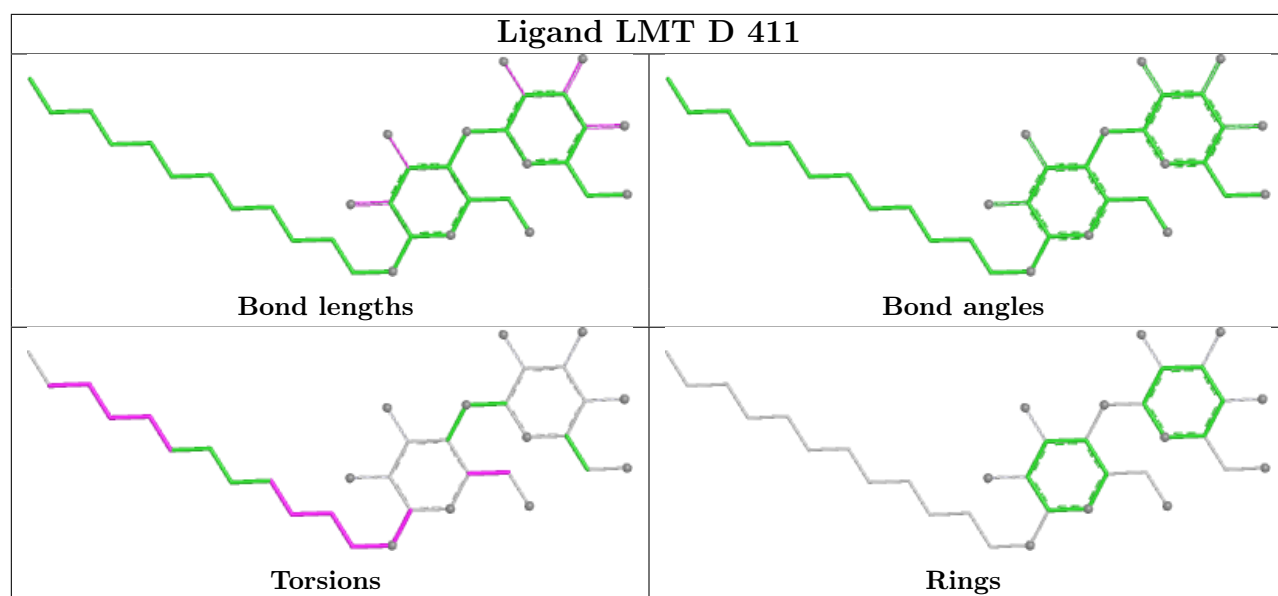


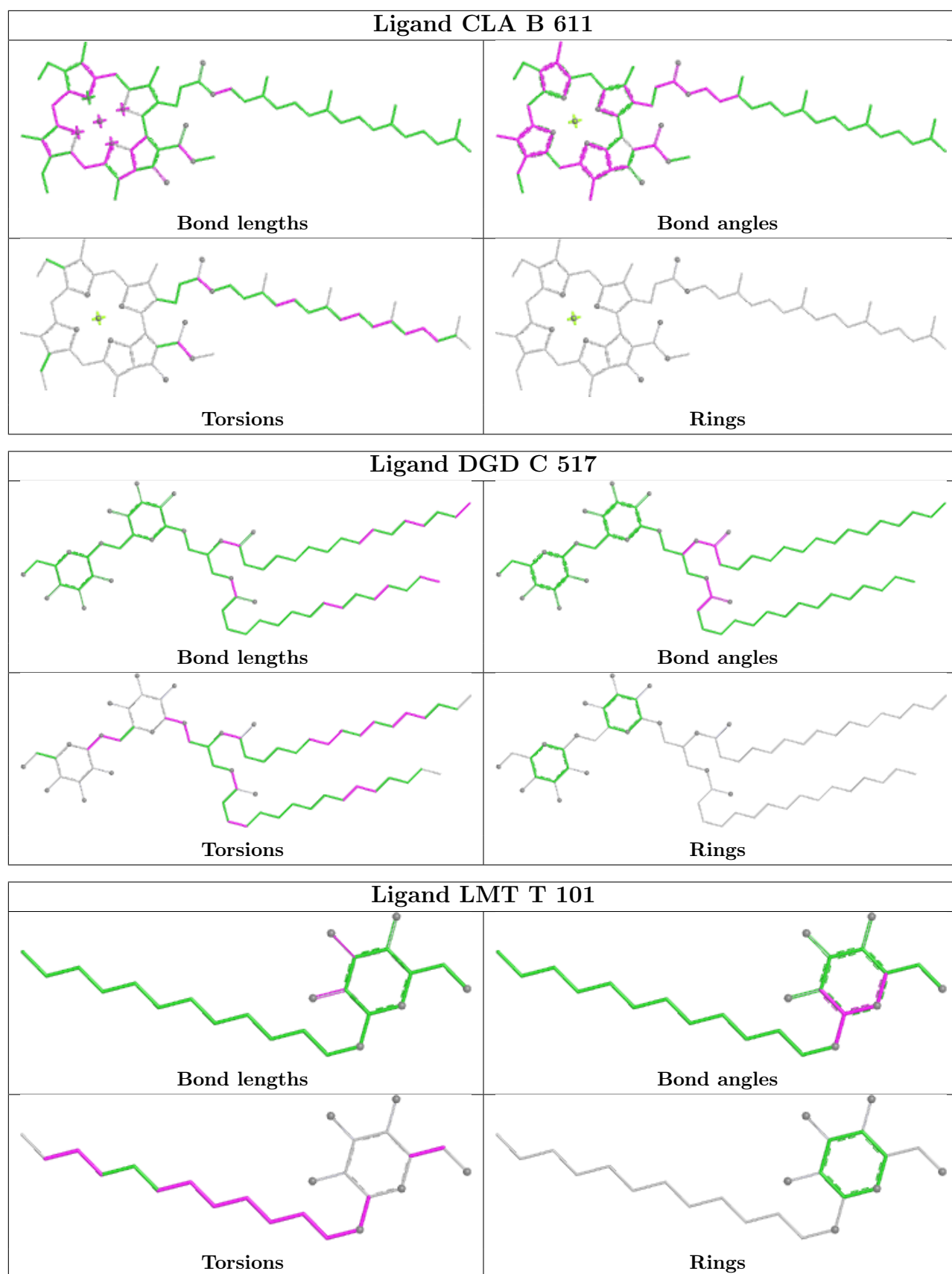


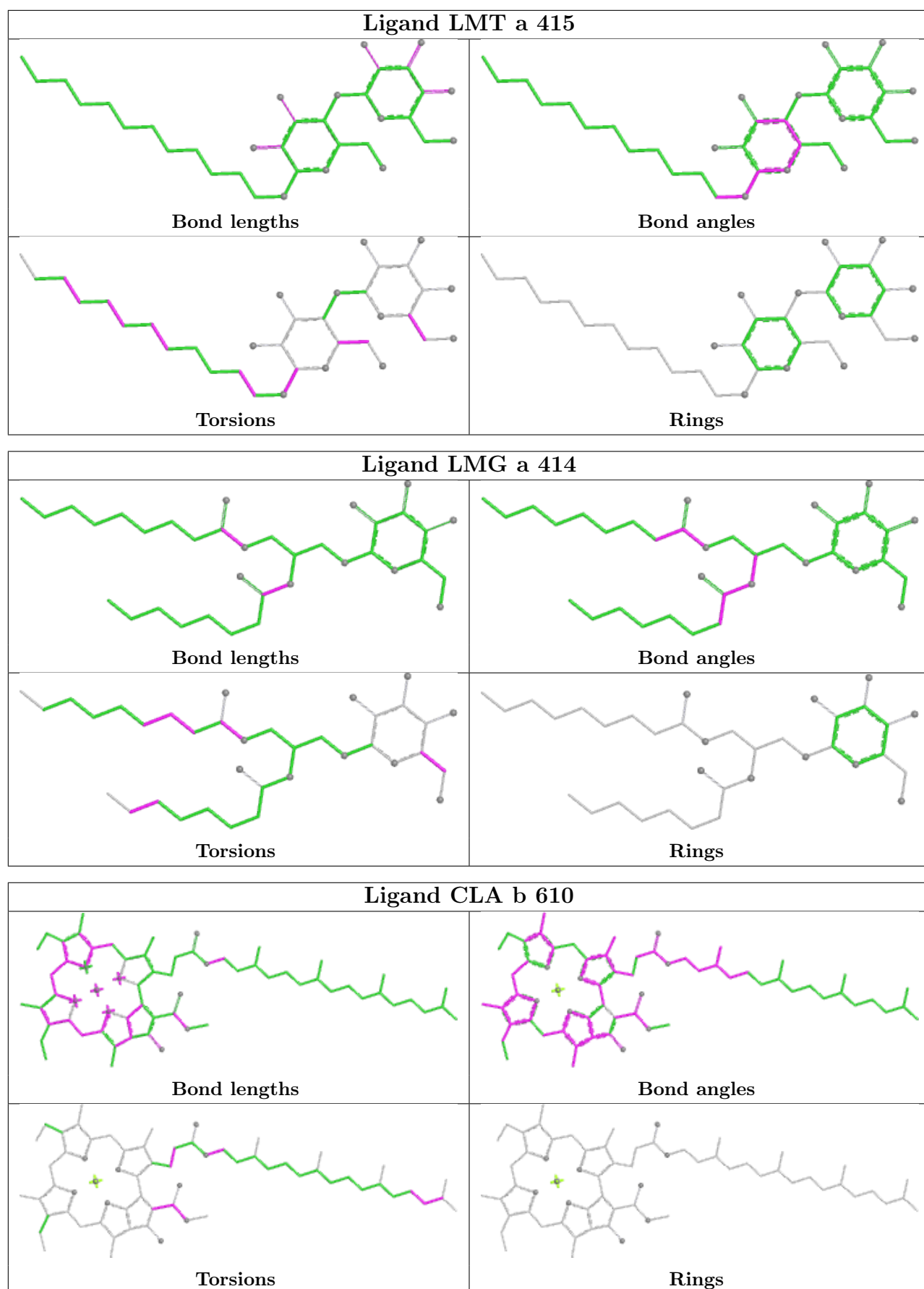












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

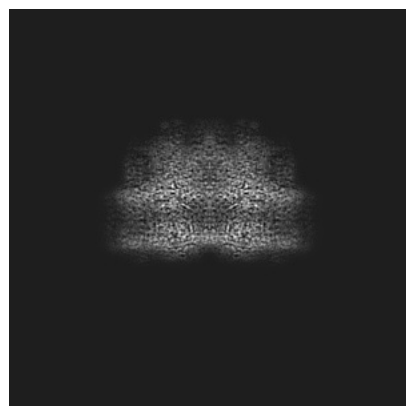
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41460. These allow visual inspection of the internal detail of the map and identification of artifacts.

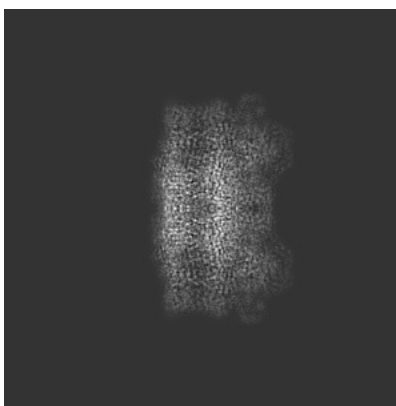
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

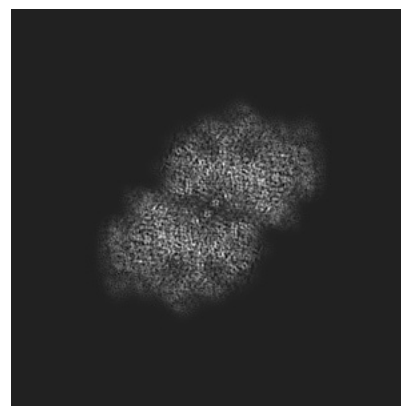
6.1.1 Primary map



X

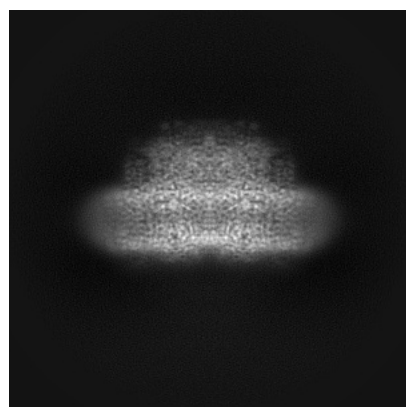


Y

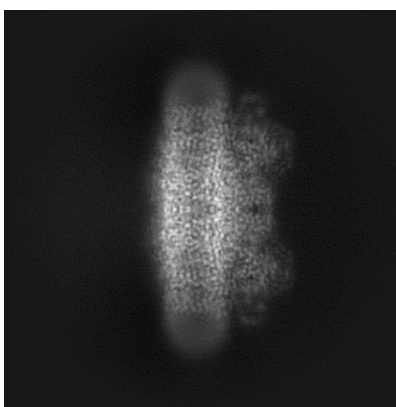


Z

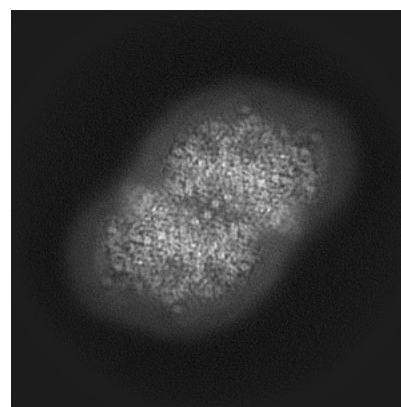
6.1.2 Raw map



X



Y



Z

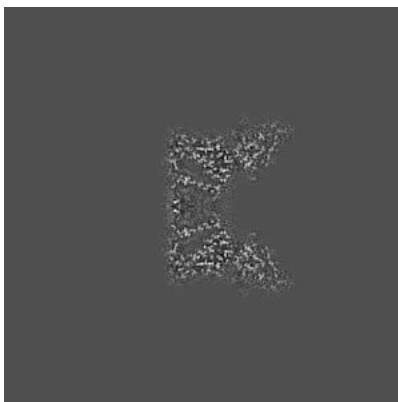
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

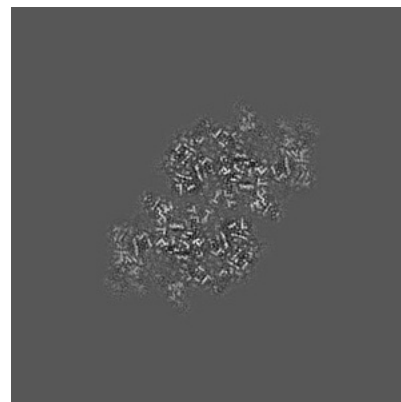
6.2.1 Primary map



X Index: 180

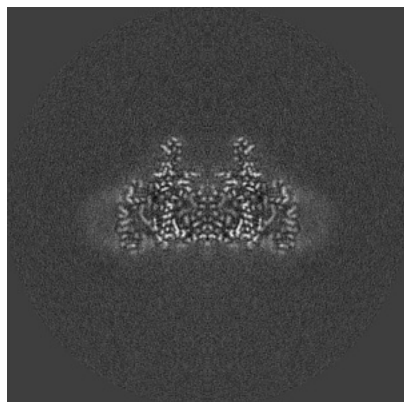


Y Index: 180

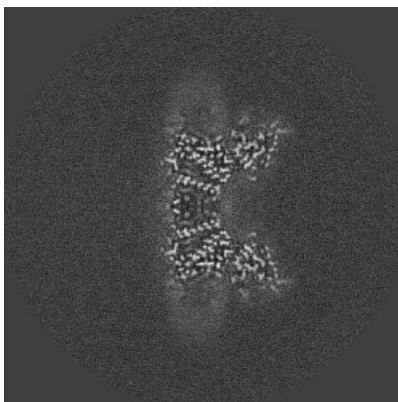


Z Index: 180

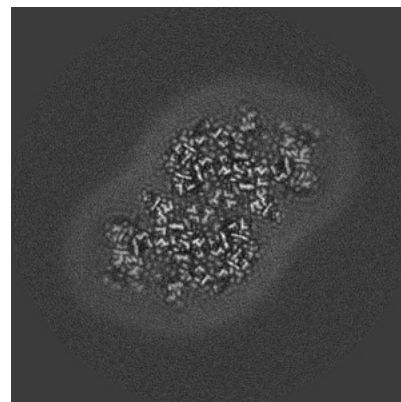
6.2.2 Raw map



X Index: 180



Y Index: 180

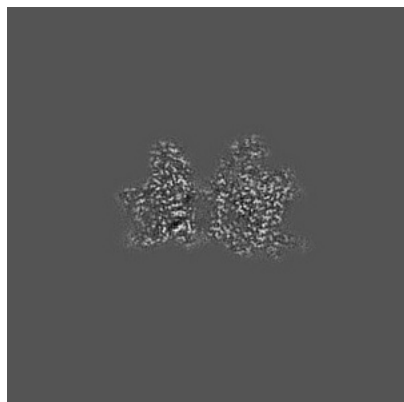


Z Index: 180

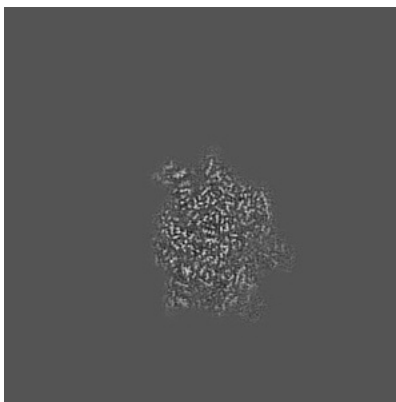
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

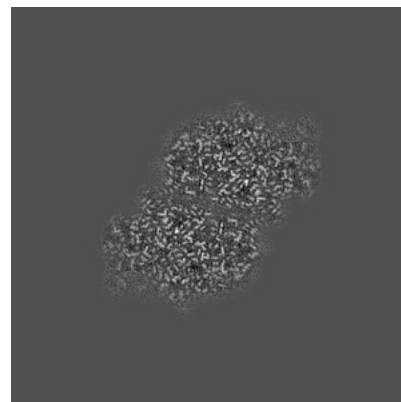
6.3.1 Primary map



X Index: 192

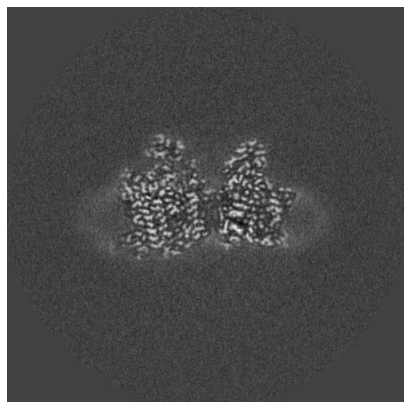


Y Index: 146

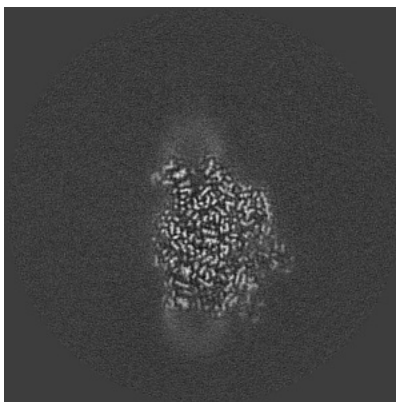


Z Index: 191

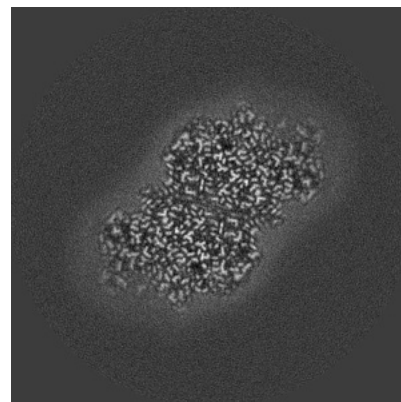
6.3.2 Raw map



X Index: 168



Y Index: 146

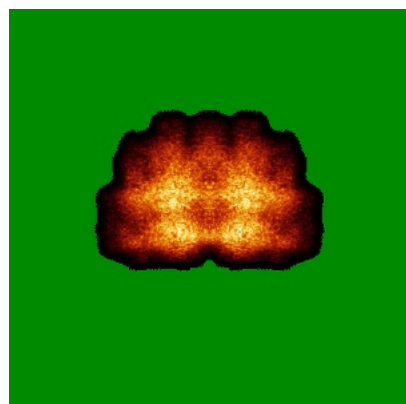


Z Index: 191

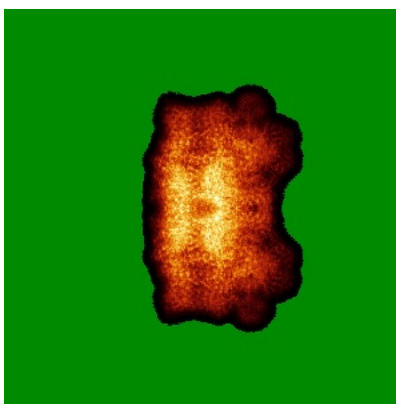
The images above show the largest variance slices of the map in three orthogonal directions.

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

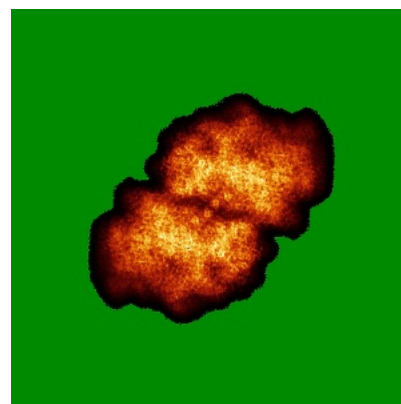
6.4.1 Primary map



X

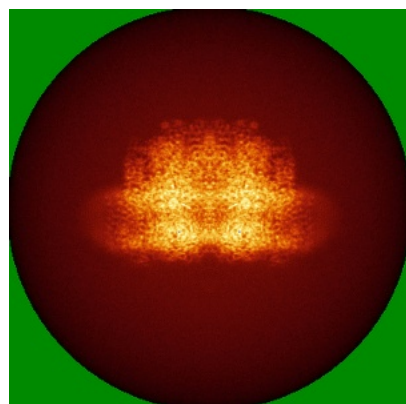


Y

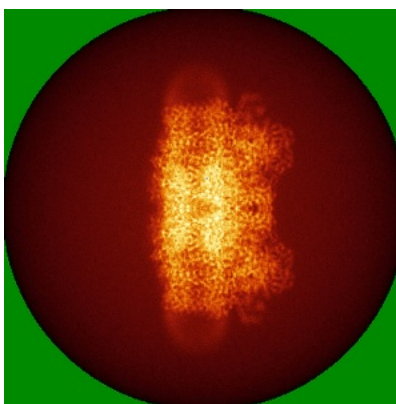


Z

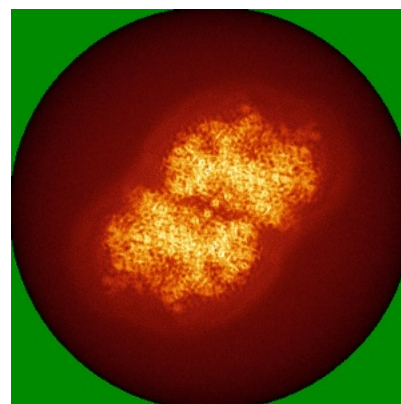
6.4.2 Raw map



X



Y

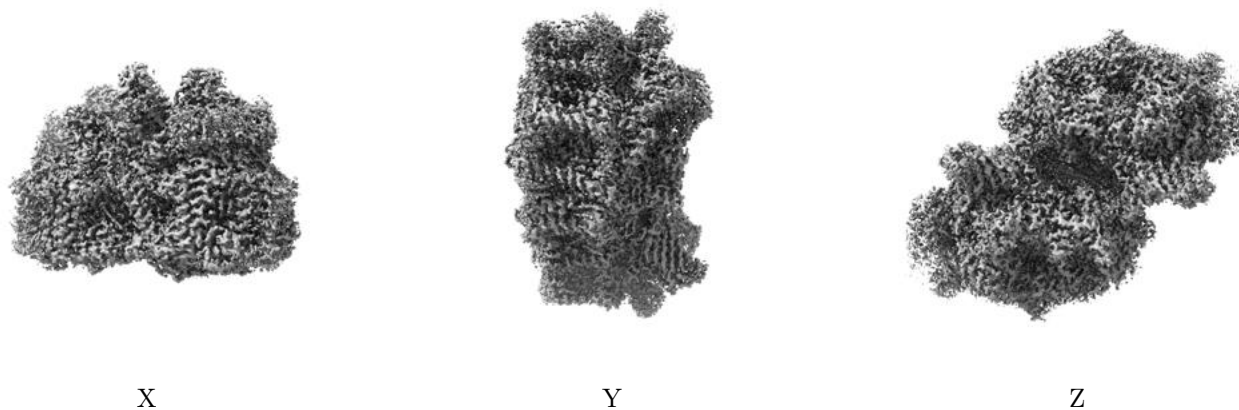


Z

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

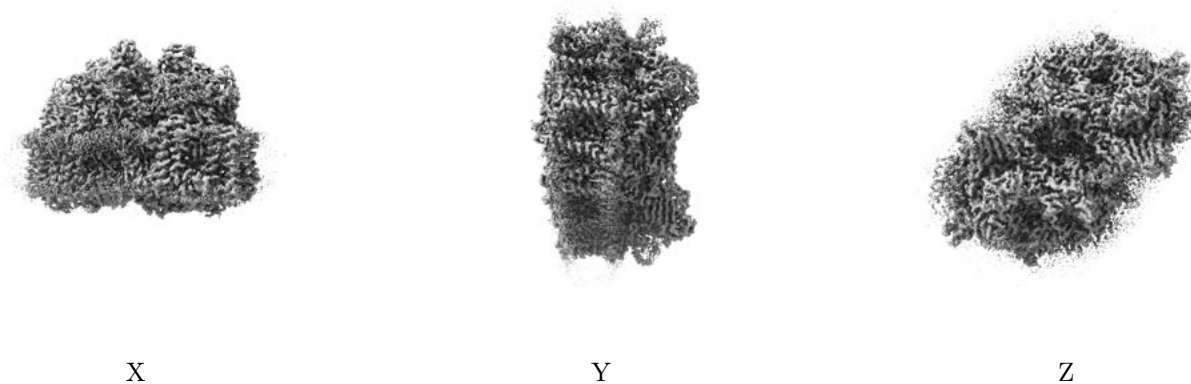
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00432. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

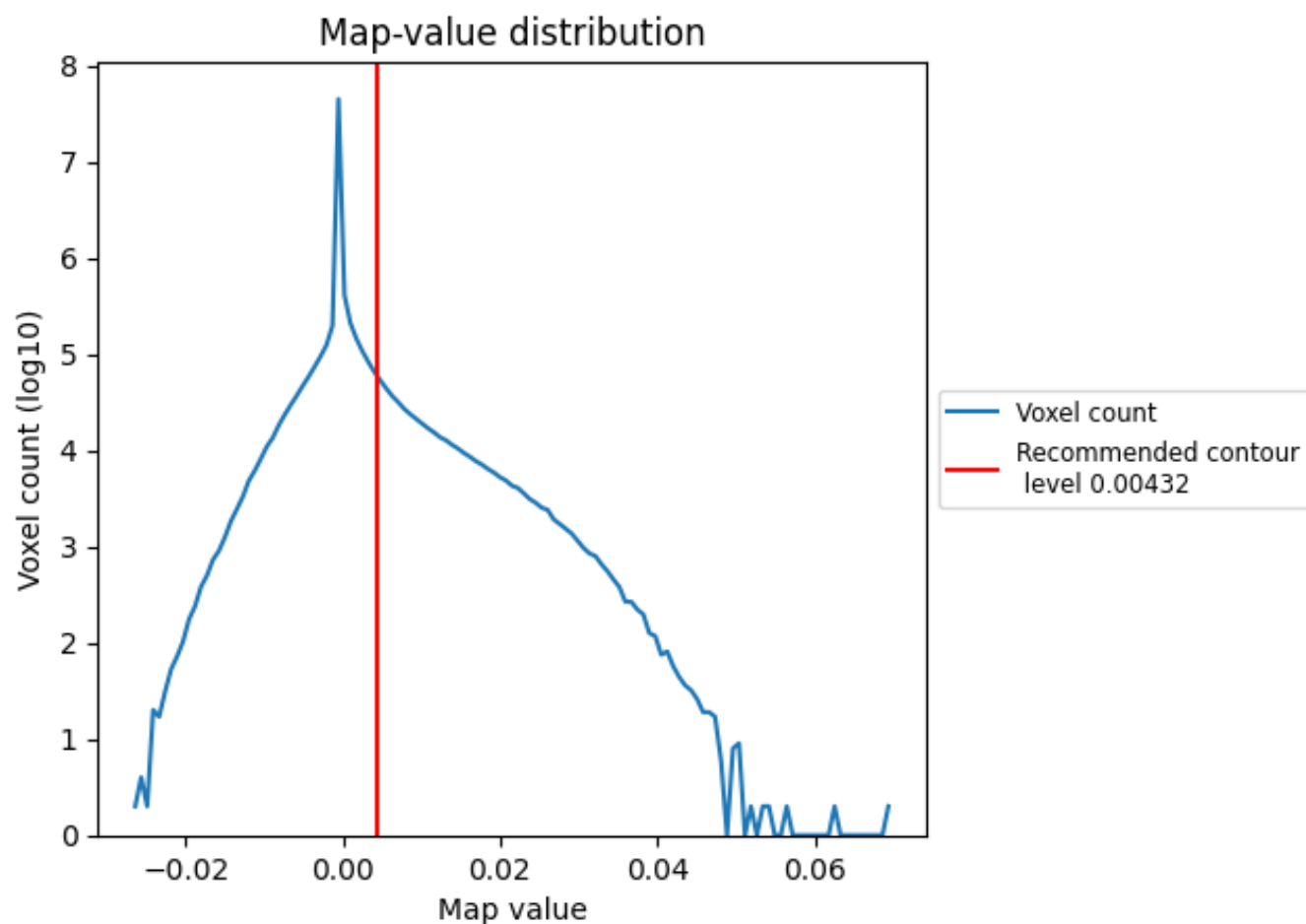
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

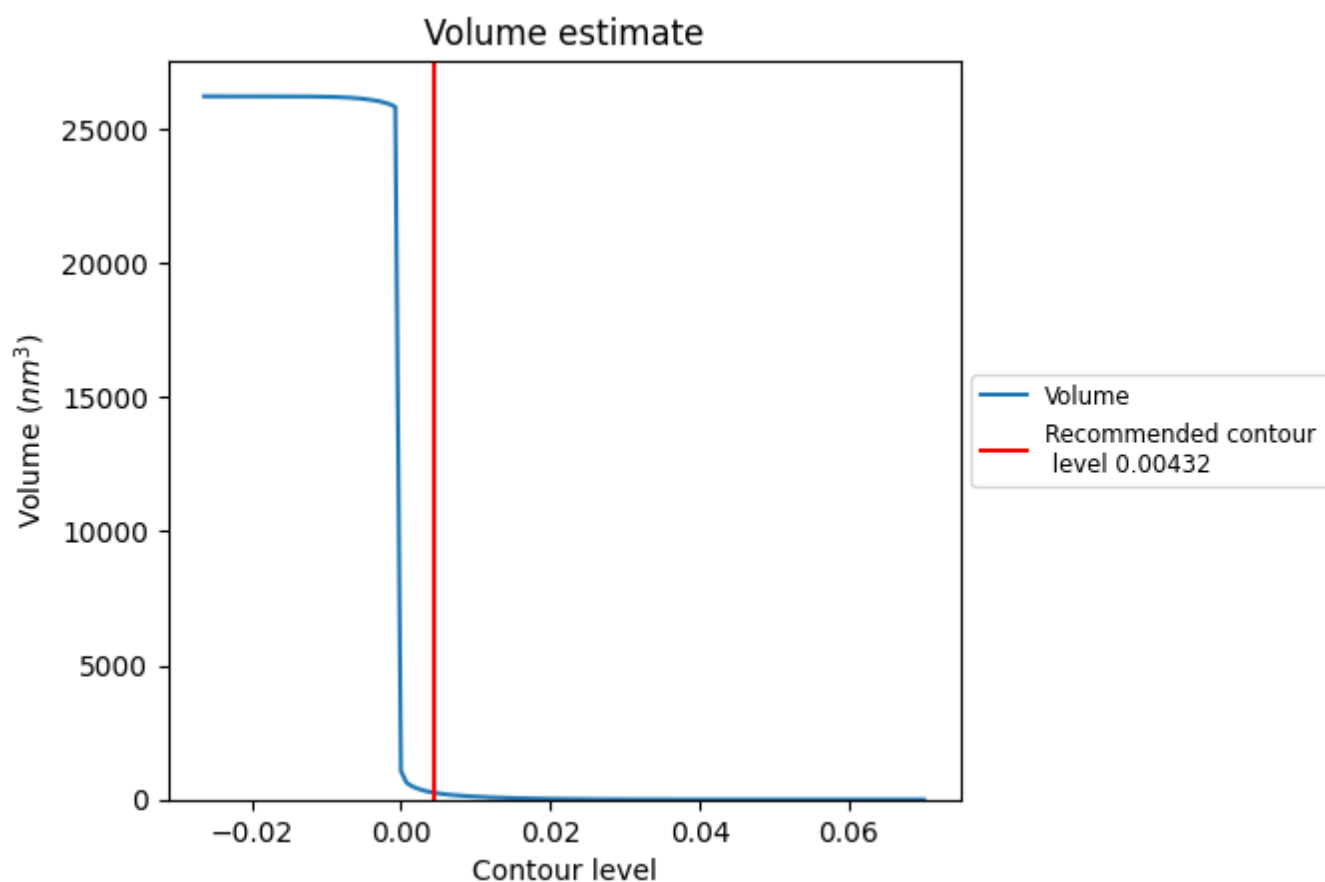
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

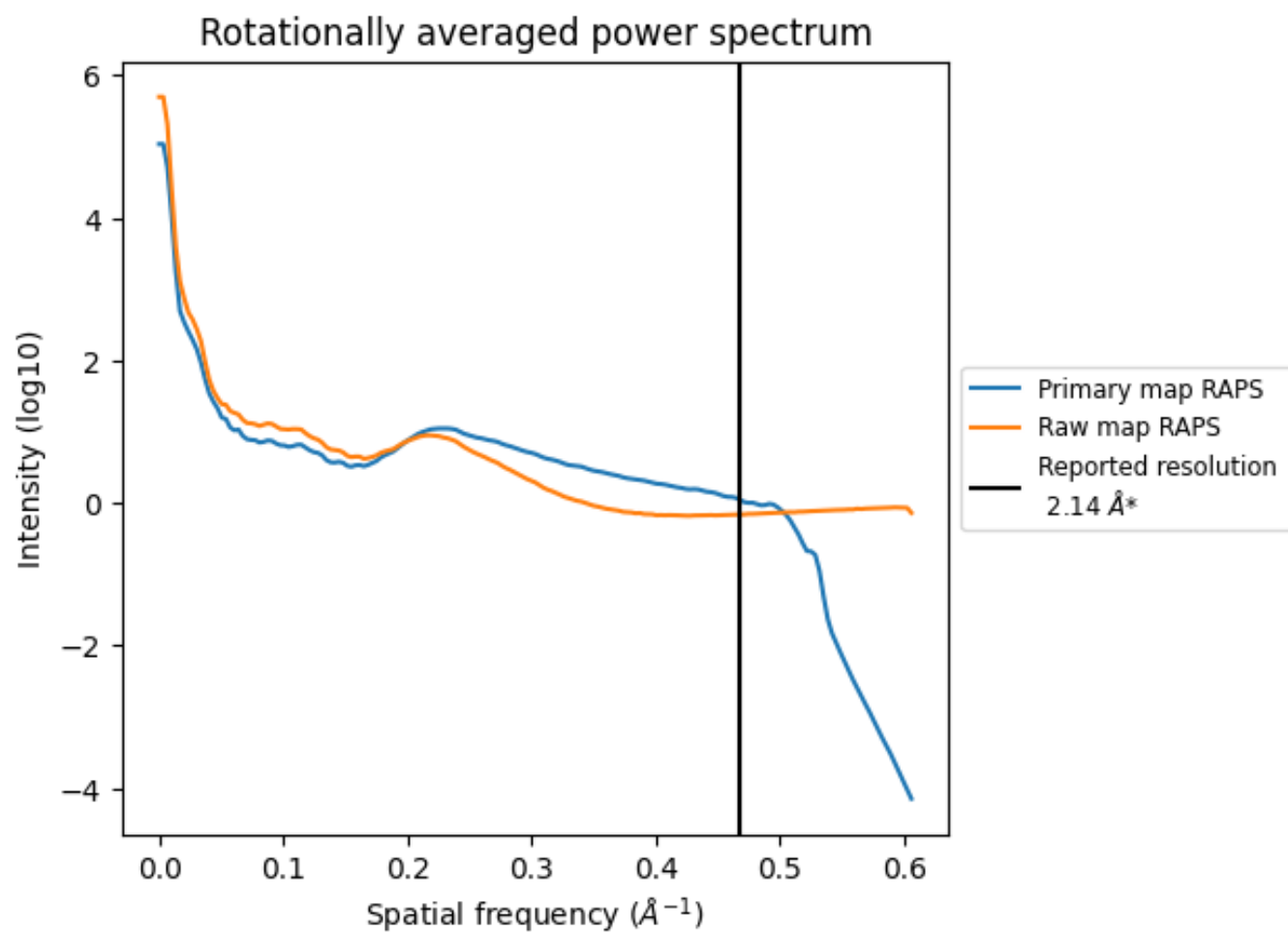
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 262 nm³; this corresponds to an approximate mass of 237 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 ⓘ

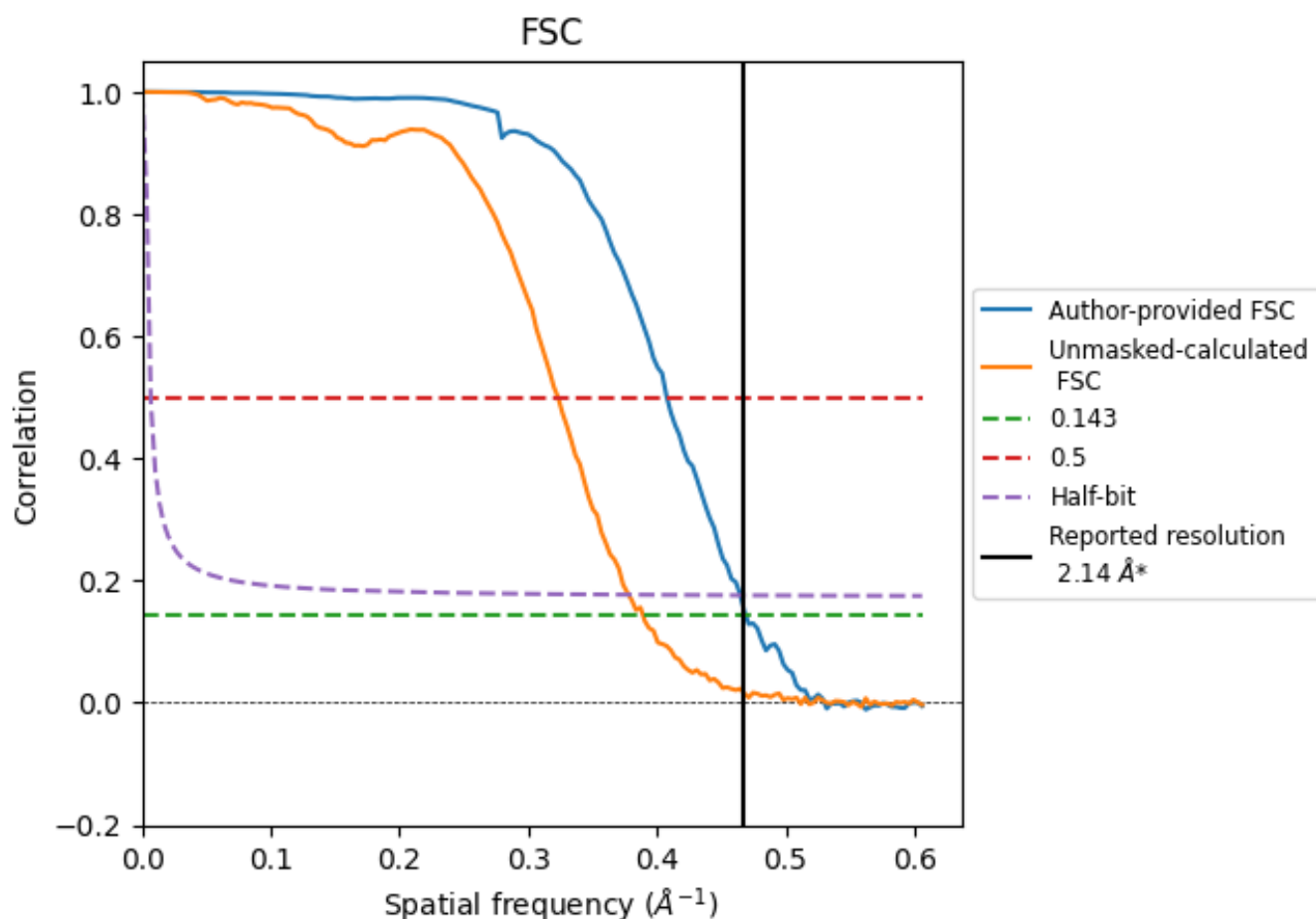


*Reported resolution corresponds to spatial frequency of 0.467 Å⁻¹

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 0.467 Å⁻¹

8.2 Resolution estimates

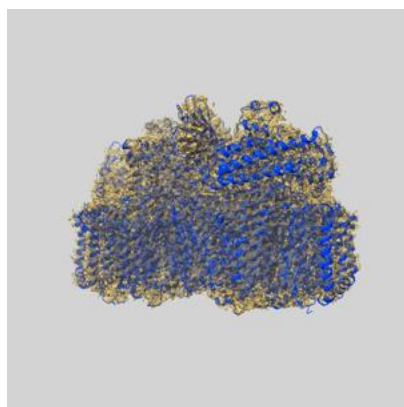
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.14	-	-
Author-provided FSC curve	2.13	2.45	2.15
Unmasked-calculated*	2.57	3.09	2.65

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.57 differs from the reported value 2.14 by more than 10 %

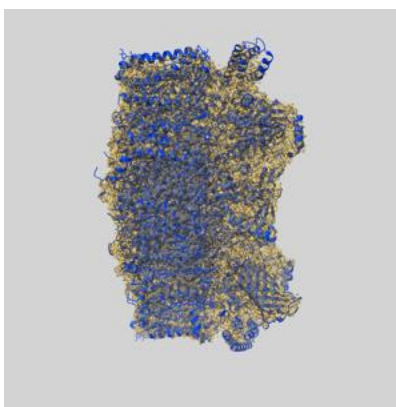
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41460 and PDB model 8TOW. Per-residue inclusion information can be found in section [3](#) on page [30](#).

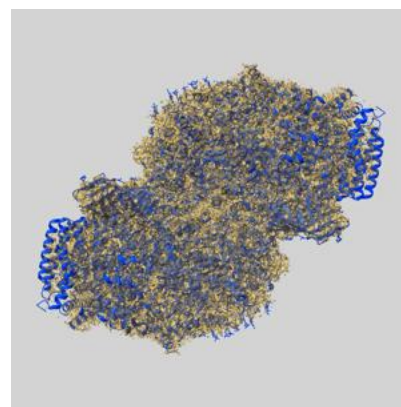
9.1 Map-model overlay [i](#)



X



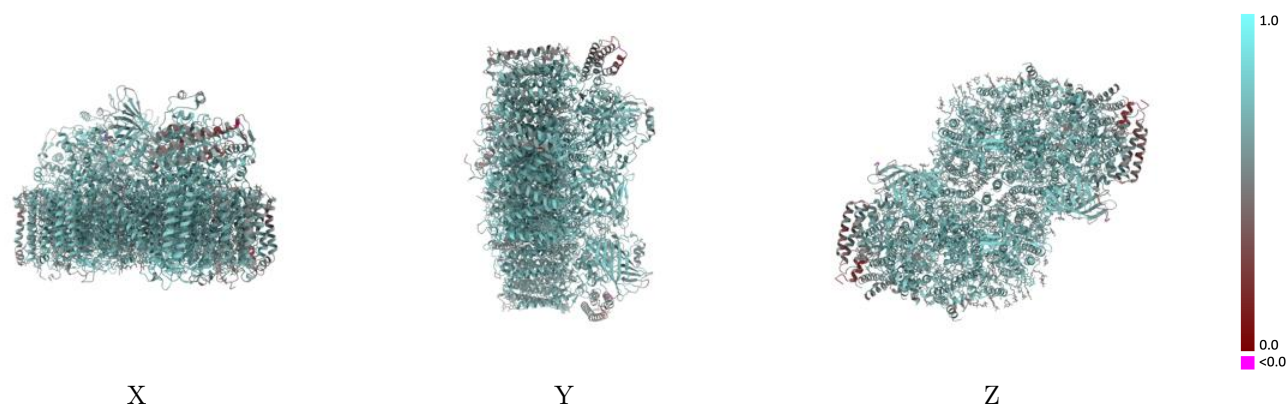
Y



Z

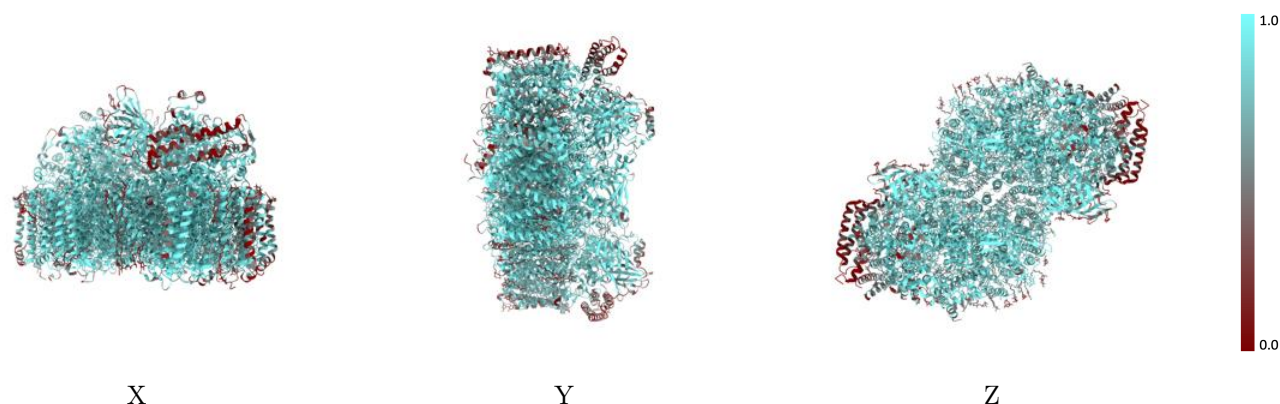
The images above show the 3D surface view of the map at the recommended contour level 0.00432 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



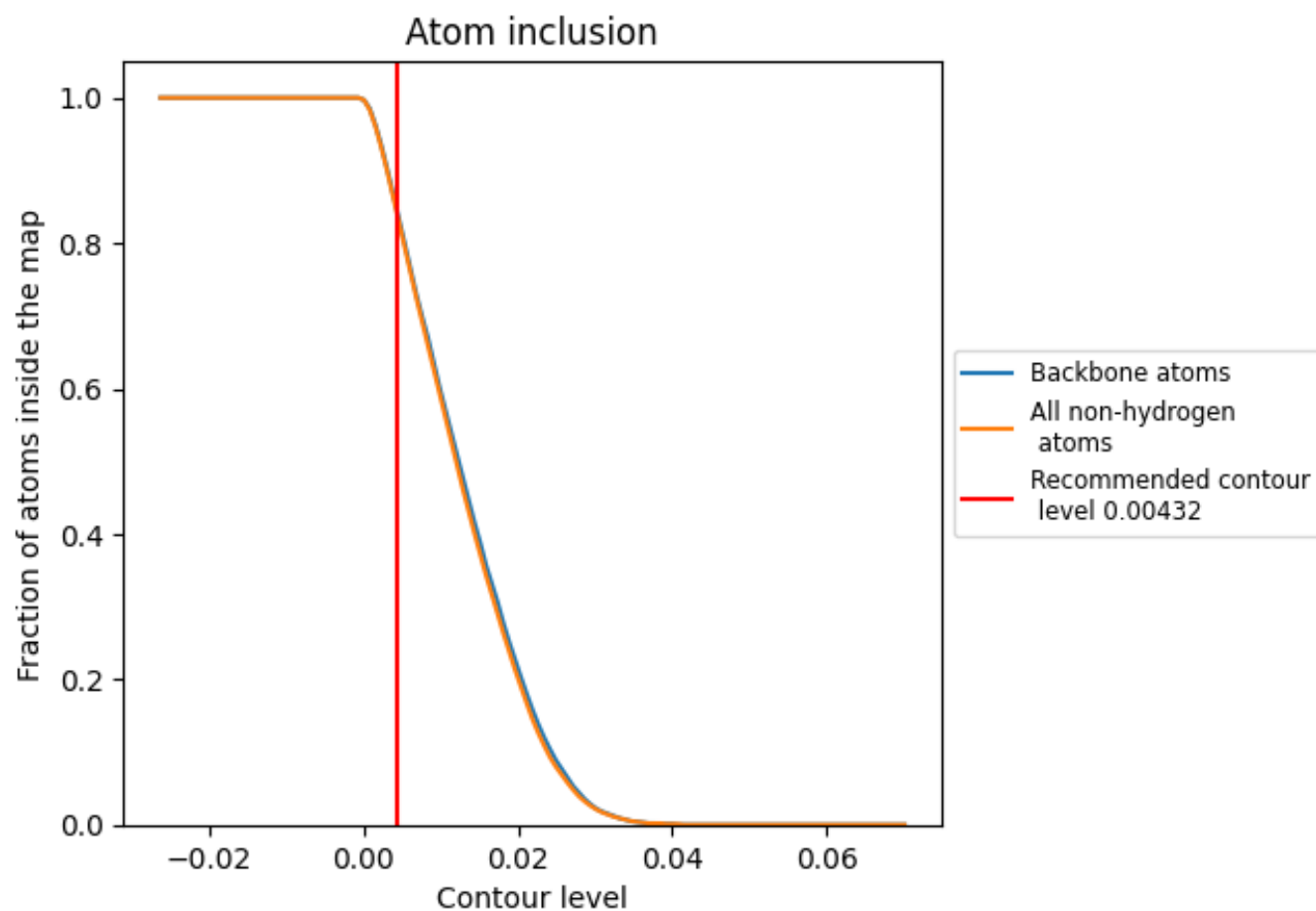
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00432).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 84% 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 (0.00432) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8390	 0.6860
A	 0.9280	 0.7330
B	 0.9220	 0.7210
C	 0.8760	 0.6950
D	 0.9540	 0.7430
E	 0.8100	 0.6680
F	 0.7770	 0.6340
H	 0.8390	 0.6850
I	 0.6350	 0.6560
J	 0.7250	 0.6350
K	 0.7770	 0.6040
L	 0.9680	 0.7420
M	 0.8880	 0.6880
O	 0.7630	 0.6520
Q	 0.3080	 0.4660
R	 0.5280	 0.5230
T	 0.9040	 0.7030
U	 0.7290	 0.6390
V	 0.8060	 0.6640
X	 0.6730	 0.6300
Y	 0.6020	 0.5660
Z	 0.4320	 0.5510
a	 0.9270	 0.7340
b	 0.9220	 0.7210
c	 0.8770	 0.6960
d	 0.9540	 0.7430
e	 0.8090	 0.6670
f	 0.7800	 0.6360
h	 0.8360	 0.6850
i	 0.6370	 0.6550
j	 0.7280	 0.6340
k	 0.7800	 0.6020
l	 0.9640	 0.7440
m	 0.8850	 0.6900
o	 0.7610	 0.6540



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Chain	Atom inclusion	Q-score
q	 0.3070	 0.4660
r	 0.5280	 0.5180
t	 0.9040	 0.7080
u	 0.7290	 0.6370
v	 0.8080	 0.6650
x	 0.6780	 0.6360
y	 0.5900	 0.5640
z	 0.4320	 0.5470