



## wwPDB EM Validation Summary Report ⓘ

Jul 24, 2025 – 04:43 pm BST

PDB ID : 9G6H / pdb\_00009g6h  
EMDB ID : EMD-51102  
Title : active PSII dimer from native Peak4 PSII dimers  
Authors : Zhao, Z.; Vercellino, I.; Nixon, P.J.; Sazanov, L.A.  
Deposited on : 2024-07-18  
Resolution : 2.20 Å(reported)  
Based on initial model : 3KZI

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

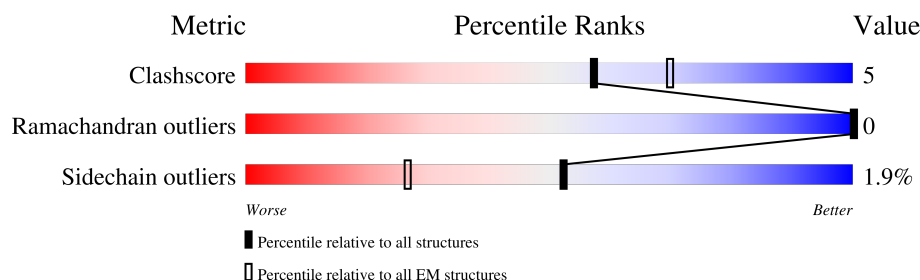
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	360	80% 12% 8%
1	a	360	81% 12% 8%
2	B	510	89% 10% .
2	b	510	89% 9% .
3	C	461	88% 9% ..
3	c	461	89% 9% .
4	D	352	87% 10% .
4	d	352	82% 14% .

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Mol	Chain	Length	Quality of chain
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	
14	t	32	
15	U	134	
15	u	134	
16	V	163	
16	v	163	
17	X	41	

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Mol	Chain	Length	Quality of chain
17	x	41	
18	Y	46	
18	y	46	
19	Z	62	
19	z	62	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	404	X	-	-	-
22	CLA	A	405	X	-	-	-
22	CLA	A	407	X	-	-	-
22	CLA	B	601	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	609	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	514	X	-	-	-
22	CLA	C	515	X	-	-	-
22	CLA	C	516	X	-	-	-
22	CLA	C	517	X	-	-	-
22	CLA	D	401	X	-	-	-
22	CLA	D	405	X	-	-	-
22	CLA	D	406	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	a	406	X	-	-	-
22	CLA	a	408	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	b	617	X	-	-	-
22	CLA	b	618	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-
22	CLA	c	514	X	-	-	-
22	CLA	c	515	X	-	-	-
22	CLA	c	516	X	-	-	-
22	CLA	c	517	X	-	-	-
22	CLA	c	518	X	-	-	-
22	CLA	d	401	X	-	-	-
22	CLA	d	403	X	-	-	-
22	CLA	d	404	X	-	-	-

## 2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 51092 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 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	333	Total	C	N	O	S	0	0
			2597	1706	429	447	15		
1	a	333	Total	C	N	O	S	0	0
			2597	1706	429	447	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	505	Total	C	N	O	S	0	0
			3935	2586	660	676	13		
2	b	505	Total	C	N	O	S	0	0
			3929	2583	657	676	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
			3458	2267	583	595	13		
3	c	450	Total	C	N	O	S	0	0
			3461	2268	583	597	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
			2710	1797	444	457	12		
4	d	341	Total	C	N	O	S	0	0
			2710	1797	444	457	12		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	81	Total	C	N	O	0	0
			650	425	106	119		
5	e	81	Total	C	N	O	0	0
			650	425	106	119		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	34	Total	C	N	O	S	0	0
			275	187	45	42	1		
6	f	34	Total	C	N	O	S	0	0
			275	187	45	42	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	62	Total	C	N	O	S	0	0
			489	327	78	82	2		
7	h	62	Total	C	N	O	S	0	0
			489	327	78	82	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	36	Total	C	N	O	S	0	0
			293	199	46	47	1		
8	i	35	Total	C	N	O	S	0	0
			288	196	45	46	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	36	Total	C	N	O	S	0	0
			257	174	40	42	1		
9	j	36	Total	C	N	O	S	0	0
			257	174	40	42	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	37	Total	C	N	O	0	0
			289	201	42	46		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	k	37	Total	C	N	O	0	0
			289	201	42	46		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	L	36	Total	C	N	O	0	0
			286	192	44	50		
11	l	36	Total	C	N	O	0	0
			286	192	44	50		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	33	Total	C	N	O	S	0	0
			254	170	38	45	1		
12	m	33	Total	C	N	O	S	0	0
			254	170	38	45	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
			1799	1131	306	358	4		
13	o	243	Total	C	N	O	S	0	0
			1794	1128	303	359	4		

- Molecule 14 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	30	Total	C	N	O	S	0	0
			256	180	36	38	2		
14	t	30	Total	C	N	O	S	0	0
			256	180	36	38	2		

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	U	97	Total	C	N	O	0	0
			758	483	129	146		
15	u	97	Total	C	N	O	0	0
			758	483	129	146		

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	V	137	Total	C	N	O	S	0	0
			1052	668	176	204	4		
16	v	137	Total	C	N	O	S	0	0
			1052	668	176	204	4		

- Molecule 17 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	X	38	Total	C	N	O	0	0
			279	187	45	47		
17	x	38	Total	C	N	O	0	0
			275	185	44	46		

- Molecule 18 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	30	Total	C	N	O	S	0	0
			214	142	35	35	2		
18	y	30	Total	C	N	O	S	0	0
			214	142	35	35	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	61	Total	C	N	O	S	0	0
			458	317	67	72	2		
19	z	61	Total	C	N	O	S	0	0
			458	317	67	72	2		

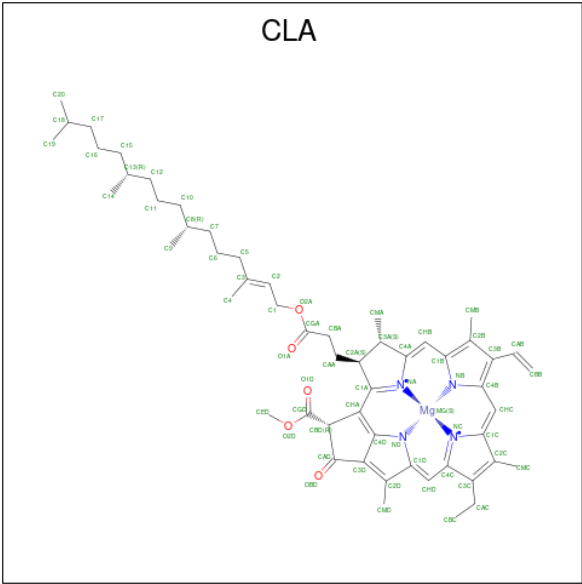
- Molecule 20 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 21 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

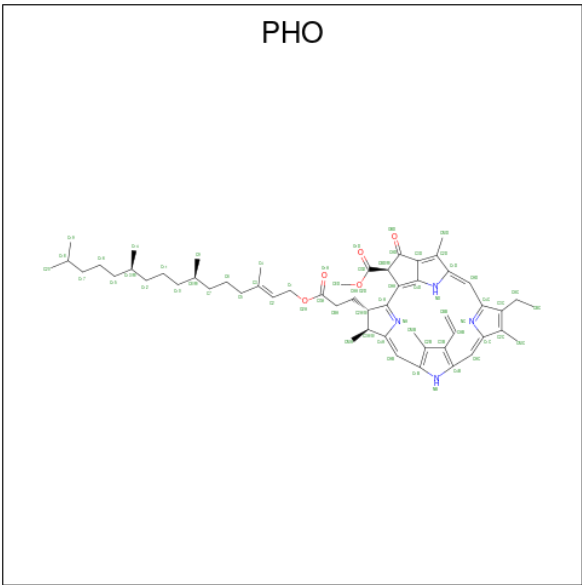
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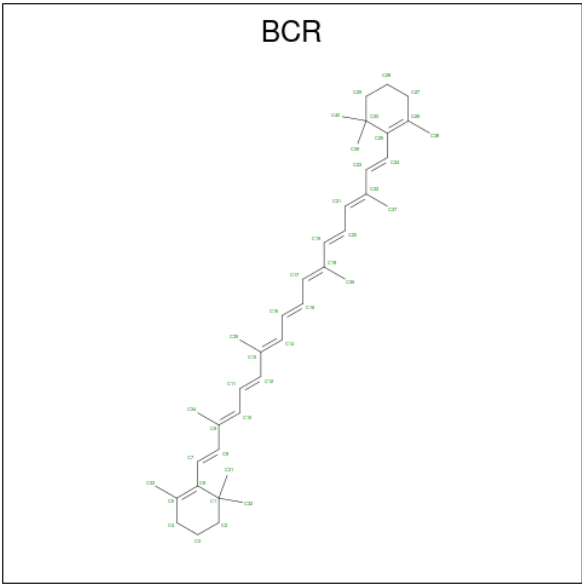
Mol	Chain	Residues	Atoms					AltConf
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 23 is PHEOPHYTIN A (CCD ID: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).



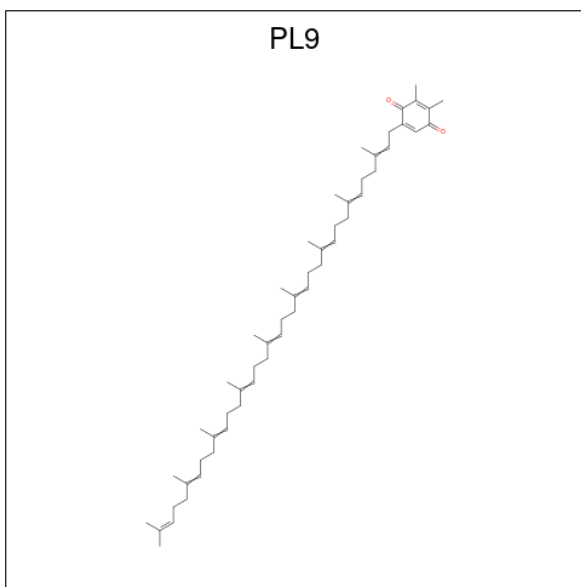
Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total	C	N	O	0
			64	55	4	5	
23	D	1	Total	C	N	O	0
			64	55	4	5	
23	a	1	Total	C	N	O	0
			64	55	4	5	
23	a	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



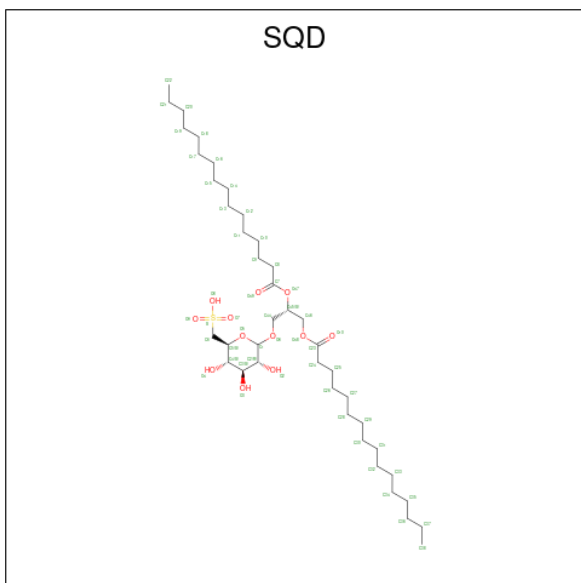
Mol	Chain	Residues	Atoms	AltConf
24	A	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	C	1	Total C 40 40	0
24	C	1	Total C 40 40	0
24	F	1	Total C 40 40	0
24	K	1	Total C 40 40	0
24	T	1	Total C 40 40	0
24	Y	1	Total C 40 40	0
24	a	1	Total C 40 40	0
24	b	1	Total C 40 40	0
24	b	1	Total C 40 40	0
24	b	1	Total C 40 40	0
24	c	1	Total C 40 40	0
24	c	1	Total C 40 40	0
24	f	1	Total C 40 40	0
24	k	1	Total C 40 40	0
24	y	1	Total C 40 40	0

- Molecule 25 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C<sub>53</sub>H<sub>80</sub>O<sub>2</sub>).



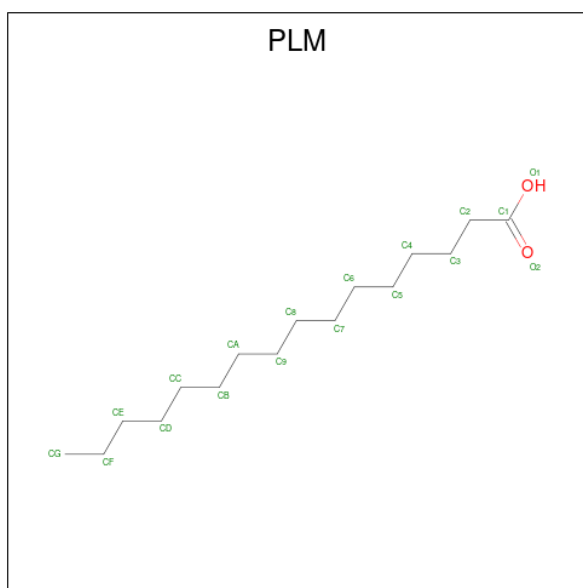
Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	C	O	0
			55	53	2	
25	D	1	Total	C	O	0
			55	53	2	
25	a	1	Total	C	O	0
			55	53	2	
25	d	1	Total	C	O	0
			55	53	2	

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	O	S	0
			54	41	12	1	
26	A	1	Total	C	O	S	0
			51	38	12	1	
26	D	1	Total	C	O	S	0
			45	32	12	1	
26	a	1	Total	C	O	S	0
			54	41	12	1	
26	a	1	Total	C	O	S	0
			51	38	12	1	
26	b	1	Total	C	O	S	0
			54	41	12	1	
26	d	1	Total	C	O	S	0
			45	32	12	1	
26	l	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 27 is PALMITIC ACID (CCD ID: PLM) (formula:  $C_{16}H_{32}O_2$ ).



Mol	Chain	Residues	Atoms			AltConf
27	A	1	Total	C	O	0
			18	16	2	
27	A	1	Total	C	O	0
			12	10	2	
27	B	1	Total	C	O	0
			18	16	2	
27	B	1	Total	C	O	0
			14	12	2	

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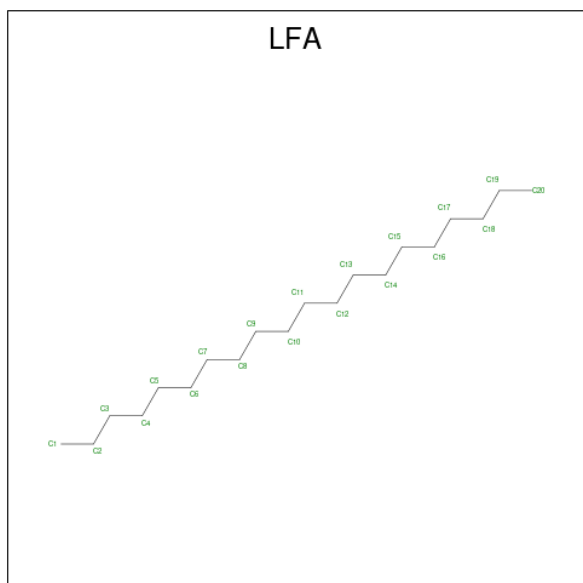
Mol	Chain	Residues	Atoms			AltConf
27	B	1	Total	C	O	0
			12	10	2	
27	B	1	Total	C	O	0
			17	15	2	
27	B	1	Total	C	O	0
			18	16	2	
27	C	1	Total	C	O	0
			15	13	2	
27	C	1	Total	C	O	0
			18	16	2	
27	C	1	Total	C	O	0
			16	14	2	
27	C	1	Total	C	O	0
			13	11	2	
27	D	1	Total	C	O	0
			13	11	2	
27	D	1	Total	C	O	0
			18	16	2	
27	E	1	Total	C	O	0
			18	16	2	
27	F	1	Total	C	O	0
			14	12	2	
27	H	1	Total	C	O	0
			12	10	2	
27	L	1	Total	C	O	0
			18	16	2	
27	M	1	Total	C	O	0
			16	14	2	
27	X	1	Total	C	O	0
			17	15	2	
27	a	1	Total	C	O	0
			18	16	2	
27	b	1	Total	C	O	0
			18	16	2	
27	b	1	Total	C	O	0
			13	11	2	
27	b	1	Total	C	O	0
			16	14	2	
27	b	1	Total	C	O	0
			18	16	2	
27	c	1	Total	C	O	0
			18	16	2	

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Mol	Chain	Residues	Atoms			AltConf
27	c	1	Total	C	O	0
			16	14	2	
27	c	1	Total	C	O	0
			18	16	2	
27	c	1	Total	C	O	0
			17	15	2	
27	d	1	Total	C	O	0
			12	10	2	
27	e	1	Total	C	O	0
			18	16	2	
27	e	1	Total	C	O	0
			18	16	2	
27	j	1	Total	C	O	0
			17	15	2	
27	j	1	Total	C	O	0
			18	16	2	
27	t	1	Total	C		0
			15	15		
27	x	1	Total	C	O	0
			18	16	2	

- Molecule 28 is EICOSANE (CCD ID: LFA) (formula:  $C_{20}H_{42}$ ).



Mol	Chain	Residues	Atoms		AltConf
28	A	1	Total	C	0
			12	12	

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Mol	Chain	Residues	Atoms	AltConf
28	B	1	Total C 8 8	0
28	B	1	Total C 7 7	0
28	B	1	Total C 8 8	0
28	B	1	Total C 5 5	0
28	C	1	Total C 9 9	0
28	E	1	Total C 20 20	0
28	H	1	Total C 10 10	0
28	I	1	Total C 20 20	0
28	I	1	Total C 11 11	0
28	I	1	Total C 8 8	0
28	J	1	Total C 20 20	0
28	J	1	Total C 11 11	0
28	T	1	Total C 17 17	0
28	a	1	Total C 7 7	0
28	a	1	Total C 11 11	0
28	a	1	Total C 7 7	0
28	b	1	Total C 8 8	0
28	b	1	Total C 4 4	0
28	d	1	Total C 13 13	0
28	d	1	Total C 14 14	0
28	i	1	Total C 20 20	0

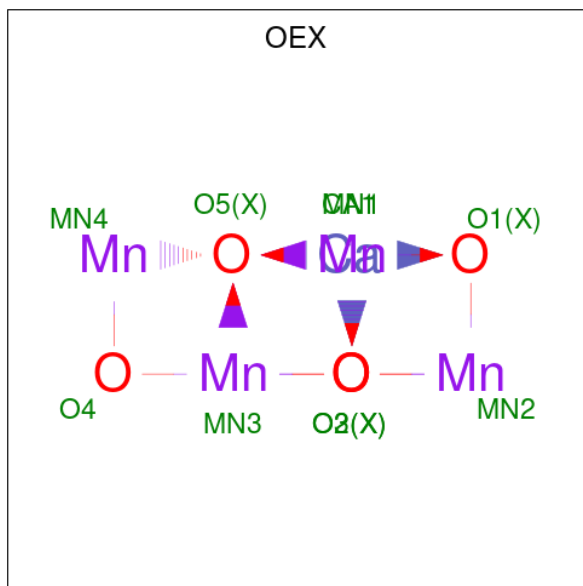
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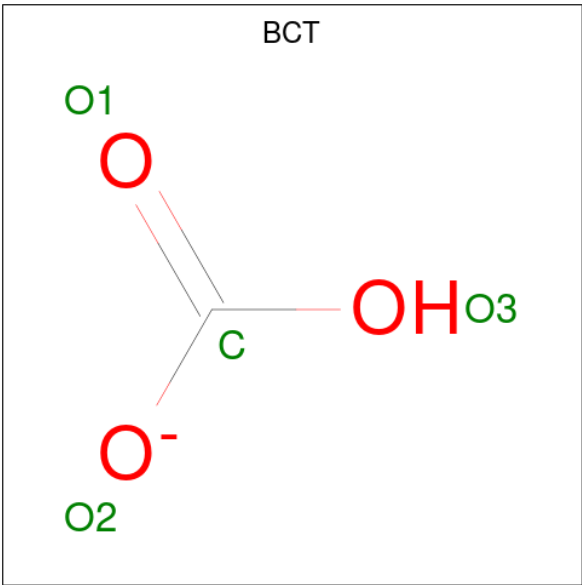
Mol	Chain	Residues	Atoms	AltConf
28	i	1	Total C 9 9	0
28	i	1	Total C 8 8	0

- Molecule 29 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ) (labeled as "Ligand of Interest" by depositor).



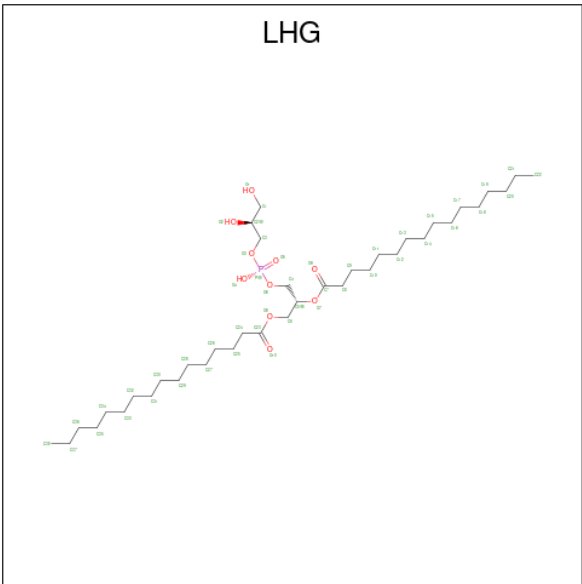
Mol	Chain	Residues	Atoms	AltConf
29	A	1	Total Ca Mn O 10 1 4 5	0
29	a	1	Total Ca Mn O 10 1 4 5	0

- Molecule 30 is BICARBONATE ION (CCD ID: BCT) (formula:  $\text{CHO}_3$ ).



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

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



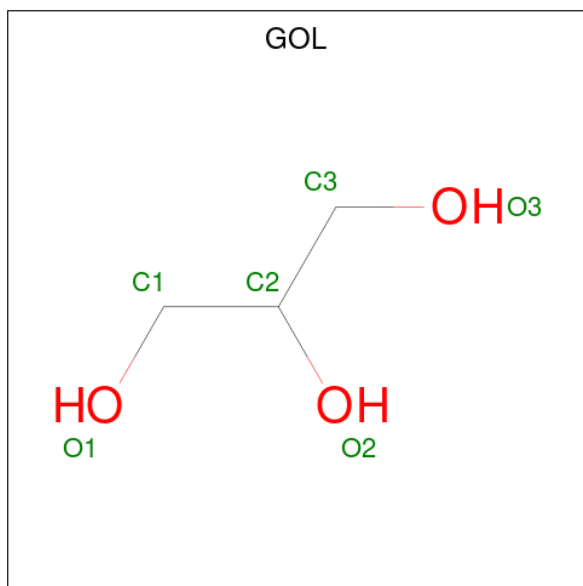
Mol	Chain	Residues	Atoms				AltConf
31	A	1	Total	C	O	P	0
			46	35	10	1	

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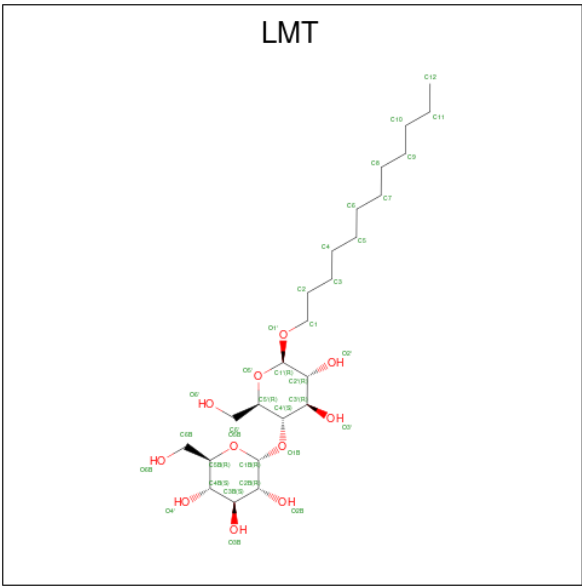
Mol	Chain	Residues	Atoms				AltConf
31	D	1	Total	C	O	P	0
			49	38	10	1	
31	D	1	Total	C	O	P	0
			49	38	10	1	
31	E	1	Total	C	O	P	0
			40	29	10	1	
31	L	1	Total	C	O	P	0
			49	38	10	1	
31	a	1	Total	C	O	P	0
			49	38	10	1	
31	a	1	Total	C	O	P	0
			46	35	10	1	
31	d	1	Total	C	O	P	0
			49	38	10	1	
31	d	1	Total	C	O	P	0
			48	37	10	1	
31	l	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 32 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			AltConf
32	A	1	Total	C	O	0
			6	3	3	
32	a	1	Total	C	O	0
			6	3	3	

- Molecule 33 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



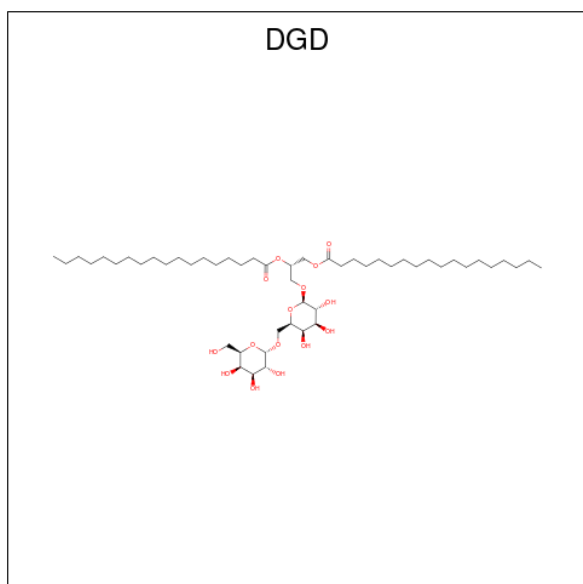
Mol	Chain	Residues	Atoms			AltConf
33	A	1	Total	C	O	0
			35	24	11	
33	B	1	Total	C	O	0
			35	24	11	
33	B	1	Total	C	O	0
			24	18	6	
33	B	1	Total	C	O	0
			35	24	11	
33	B	1	Total	C	O	0
			35	24	11	
33	C	1	Total	C	O	0
			35	24	11	
33	J	1	Total	C	O	0
			24	18	6	
33	M	1	Total	C	O	0
			35	24	11	
33	T	1	Total	C	O	0
			24	18	6	
33	T	1	Total	C	O	0
			35	24	11	
33	Z	1	Total	C	O	0
			35	24	11	
33	b	1	Total	C	O	0
			24	18	6	
33	f	1	Total	C	O	0
			35	24	11	

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Mol	Chain	Residues	Atoms			AltConf
33	i	1	Total	C	O	0
			35	24	11	
33	j	1	Total	C	O	0
			24	18	6	
33	m	1	Total	C	O	0
			35	24	11	
33	z	1	Total	C	O	0
			35	24	11	

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



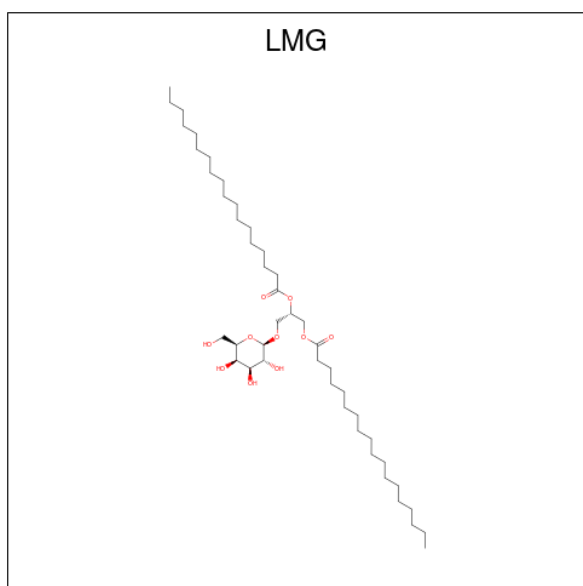
Mol	Chain	Residues	Atoms			AltConf
34	C	1	Total	C	O	0
			53	38	15	
34	C	1	Total	C	O	0
			54	39	15	
34	D	1	Total	C	O	0
			44	35	9	
34	H	1	Total	C	O	0
			58	43	15	
34	J	1	Total	C	O	0
			61	46	15	
34	c	1	Total	C	O	0
			53	38	15	
34	c	1	Total	C	O	0
			55	40	15	

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Mol	Chain	Residues	Atoms			AltConf
34	c	1	Total	C	O	0
			61	46	15	
34	d	1	Total	C	O	0
			47	36	11	
34	h	1	Total	C	O	0
			58	43	15	

- Molecule 35 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



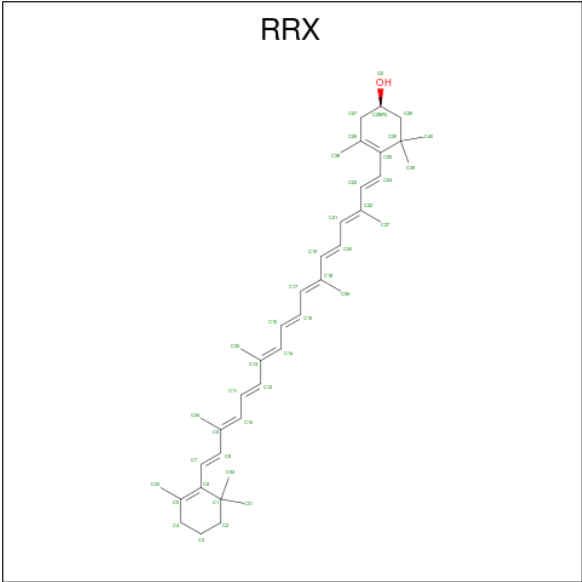
Mol	Chain	Residues	Atoms			AltConf
35	C	1	Total	C	O	0
			51	41	10	
35	C	1	Total	C	O	0
			51	41	10	
35	D	1	Total	C	O	0
			47	37	10	
35	M	1	Total	C	O	0
			51	41	10	
35	Y	1	Total	C	O	0
			51	41	10	
35	c	1	Total	C	O	0
			51	41	10	
35	c	1	Total	C	O	0
			48	38	10	
35	d	1	Total	C	O	0
			47	37	10	

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Mol	Chain	Residues	Atoms			AltConf
35	m	1	Total	C	O	0
			51	41	10	
35	y	1	Total	C	O	0
			51	41	10	

- # HEM

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



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

- Molecule 38 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
38	O	1	Total	Ca	0
			1	1	
38	o	1	Total	Ca	0
			1	1	

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		AltConf
39	A	92	Total	O	0
			92	92	
39	B	133	Total	O	0
			133	133	
39	C	101	Total	O	1
			101	101	
39	D	91	Total	O	0
			91	91	
39	E	14	Total	O	0
			14	14	

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Mol	Chain	Residues	Atoms		AltConf
39	F	3	Total 3	O 3	0
39	H	11	Total 11	O 11	0
39	I	1	Total 1	O 1	0
39	J	4	Total 4	O 4	0
39	K	1	Total 1	O 1	0
39	L	8	Total 8	O 8	0
39	M	3	Total 3	O 3	0
39	O	37	Total 37	O 37	0
39	T	4	Total 4	O 4	0
39	U	14	Total 14	O 14	0
39	V	26	Total 26	O 26	0
39	X	3	Total 3	O 3	0
39	a	94	Total 94	O 94	0
39	b	137	Total 137	O 137	0
39	c	104	Total 104	O 104	0
39	d	91	Total 91	O 91	0
39	e	15	Total 15	O 15	0
39	f	4	Total 4	O 4	0
39	h	11	Total 11	O 11	0
39	i	3	Total 3	O 3	0
39	j	4	Total 4	O 4	0

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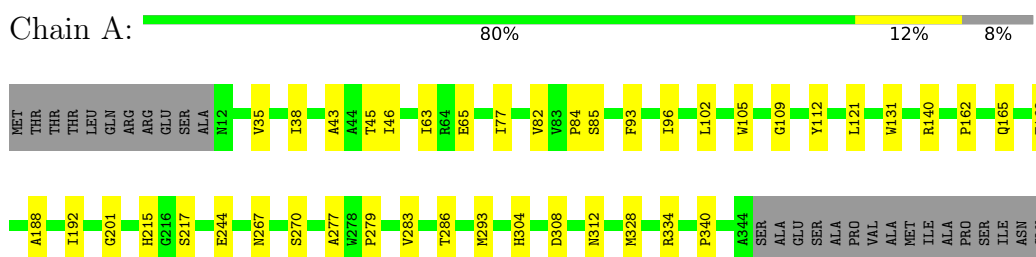
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Mol	Chain	Residues	Atoms		AltConf
39	k	1	Total 1	O 1	0
39	l	10	Total 10	O 10	0
39	m	3	Total 3	O 3	0
39	o	39	Total 39	O 39	0
39	t	4	Total 4	O 4	0
39	u	13	Total 13	O 13	0
39	v	25	Total 25	O 25	0
39	x	2	Total 2	O 2	0

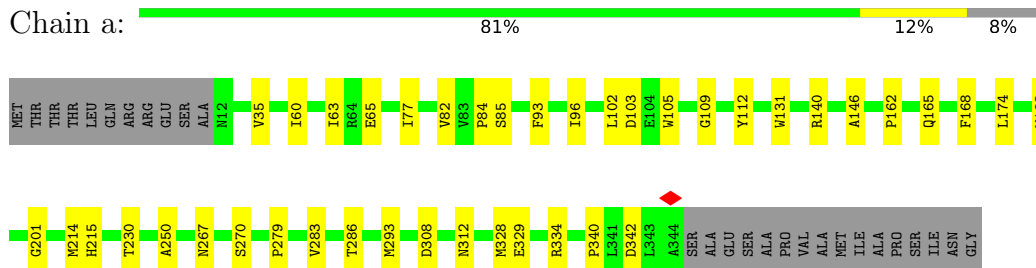
### 3 Residue-property plots

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.

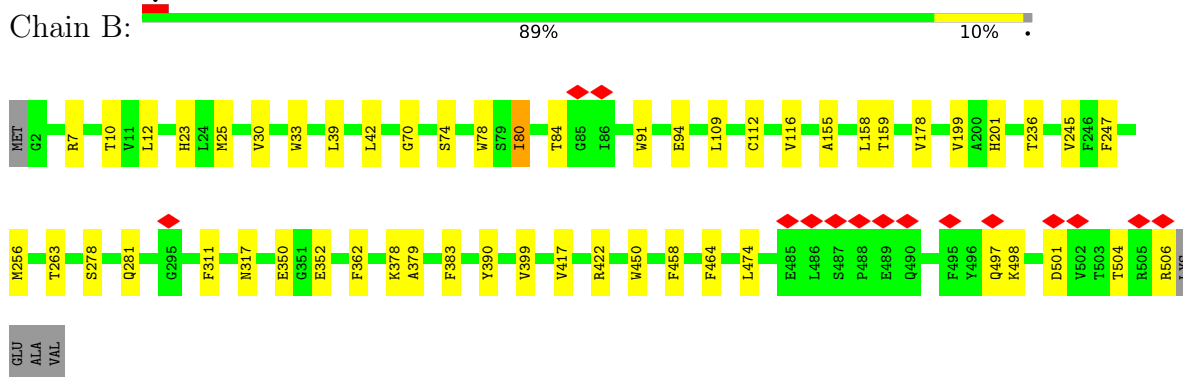
- Molecule 1: Photosystem II protein D1 1



- Molecule 1: Photosystem II protein D1 1

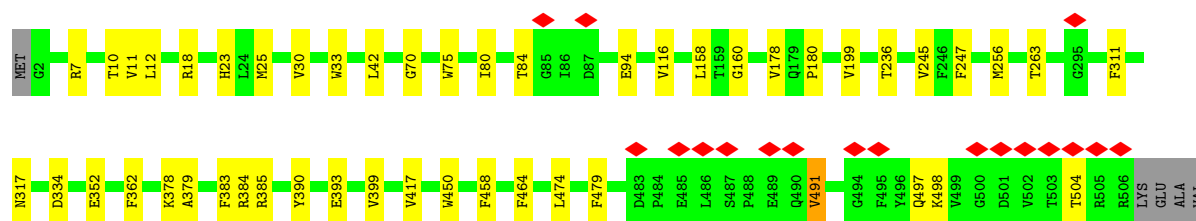


- Molecule 2: Photosystem II CP47 reaction center protein



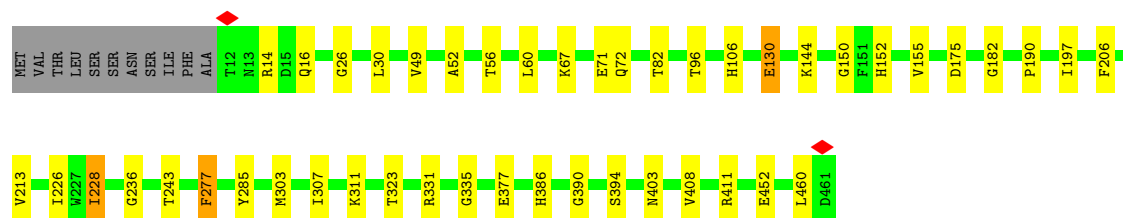
- Molecule 2: Photosystem II CP47 reaction center protein





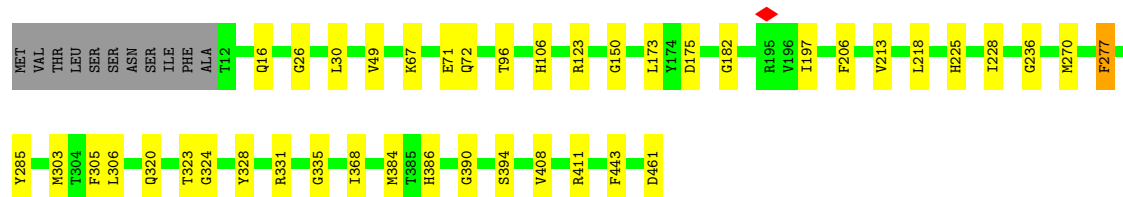
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 88% 9% ..



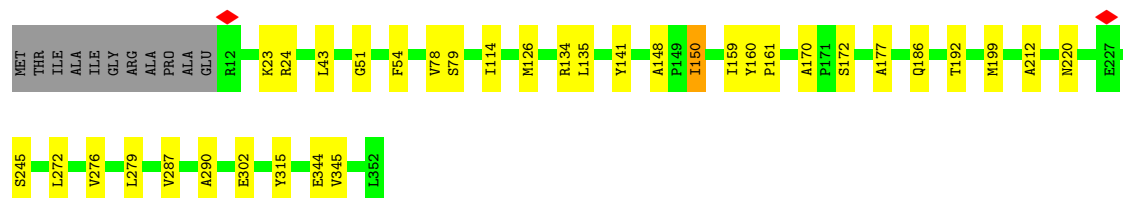
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 89% 9% .



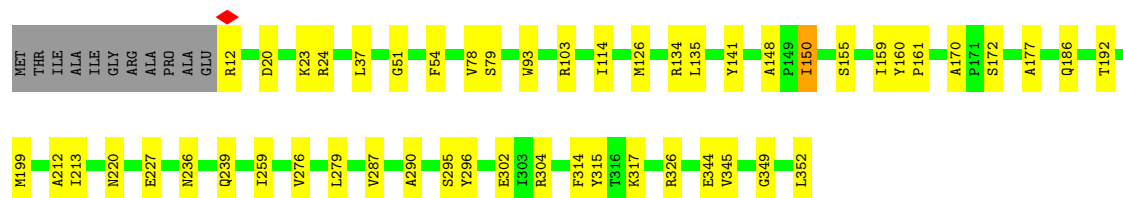
• Molecule 4: Photosystem II D2 protein

Chain D: 87% 10% .

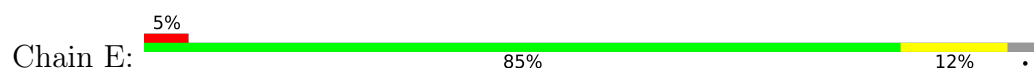


• Molecule 4: Photosystem II D2 protein

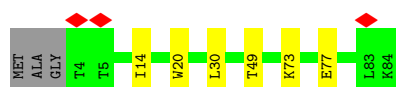
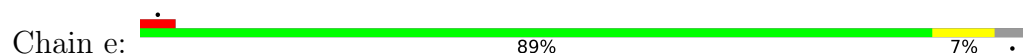
Chain d: 82% 14% .



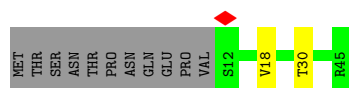
- Molecule 5: Cytochrome b559 subunit alpha



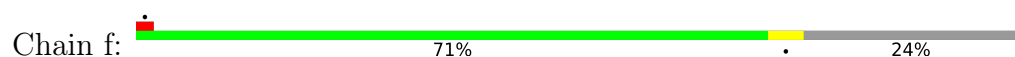
- Molecule 5: Cytochrome b559 subunit alpha



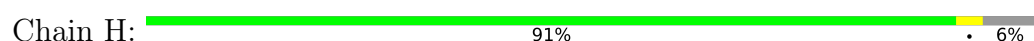
- Molecule 6: Cytochrome b559 subunit beta



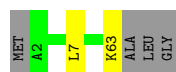
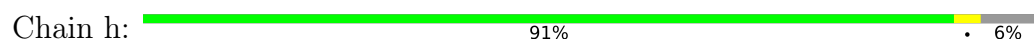
- Molecule 6: Cytochrome b559 subunit beta



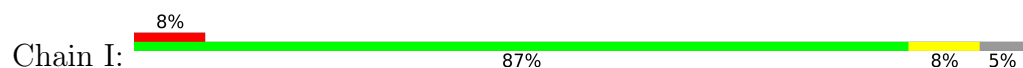
- Molecule 7: Photosystem II reaction center protein H

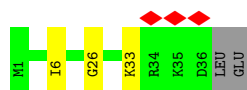


- Molecule 7: Photosystem II reaction center protein H

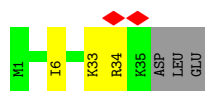
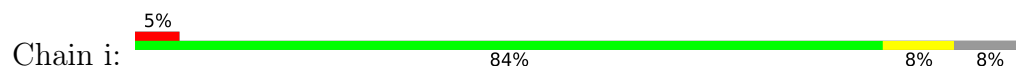


- Molecule 8: Photosystem II reaction center protein I

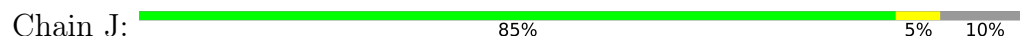




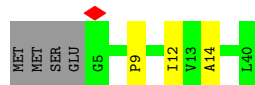
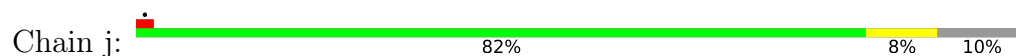
- Molecule 8: Photosystem II reaction center protein I



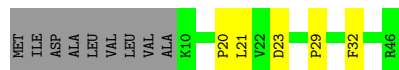
- Molecule 9: Photosystem II reaction center protein J



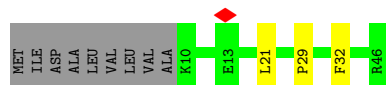
- Molecule 9: Photosystem II reaction center protein J



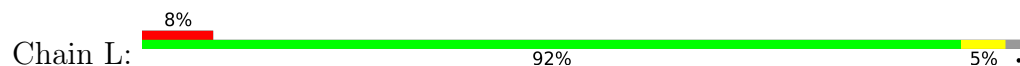
- Molecule 10: Photosystem II reaction center protein K



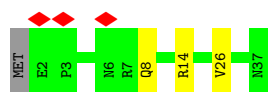
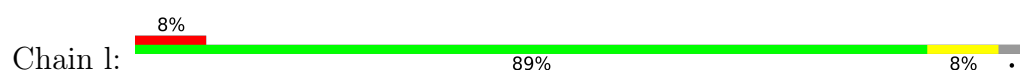
- Molecule 10: Photosystem II reaction center protein K



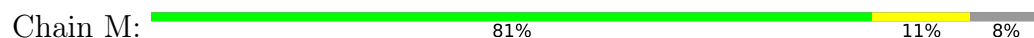
- Molecule 11: Photosystem II reaction center protein L



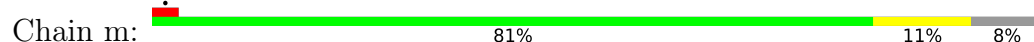
- Molecule 11: Photosystem II reaction center protein L



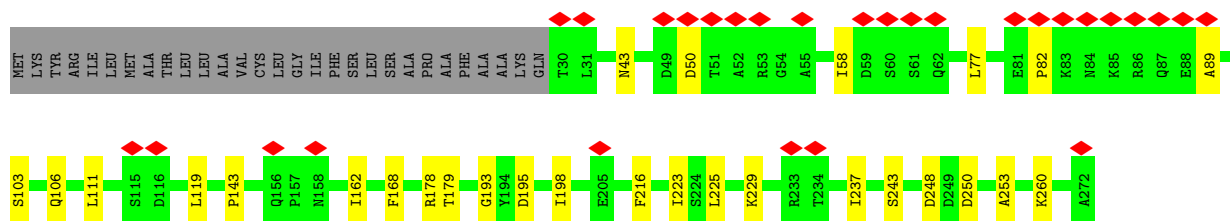
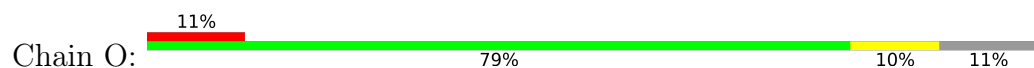
- Molecule 12: Photosystem II reaction center protein M



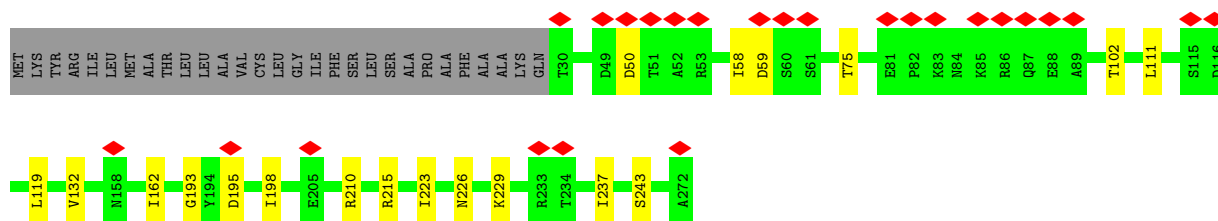
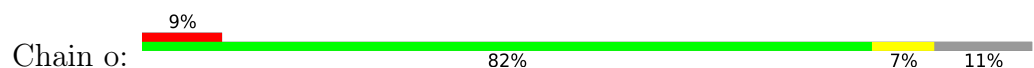
- Molecule 12: Photosystem II reaction center protein M



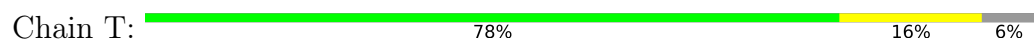
- Molecule 13: Photosystem II manganese-stabilizing polypeptide




- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 14: Photosystem II reaction center protein T



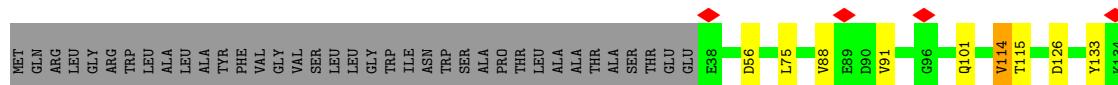
- Molecule 14: Photosystem II reaction center protein T

Chain t:  78% 16% 6%



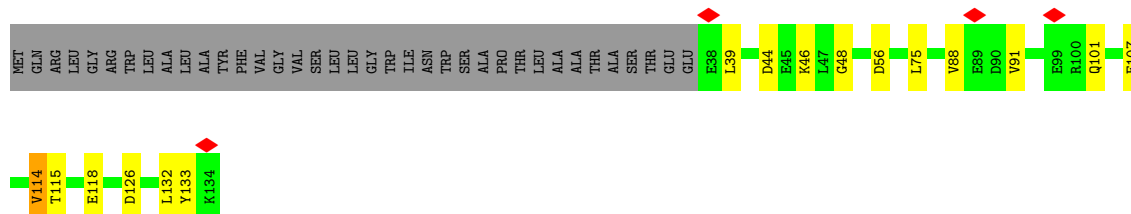
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  66% 6% 28%




- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  60% 11% 28%



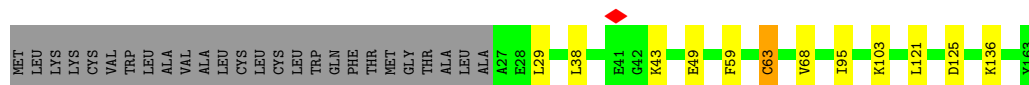
- Molecule 16: Cytochrome c-550

Chain V:  78% 6% 16%




- Molecule 16: Cytochrome c-550

Chain v:  77% 7% 16%



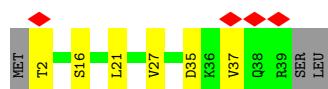
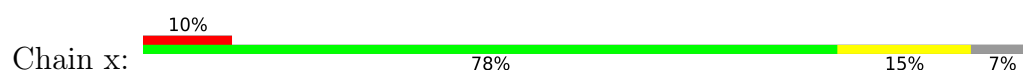
- Molecule 17: Photosystem II reaction center X protein

Chain X:  12% 83% 10% 7%

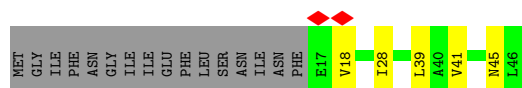


- Molecule 17: Photosystem II reaction center X protein

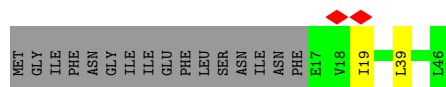




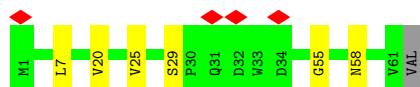
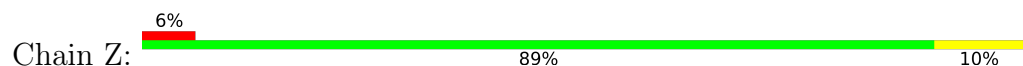
- Molecule 18: Photosystem II reaction center protein Ycf12



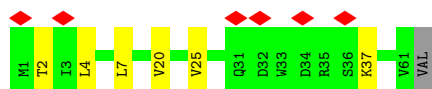
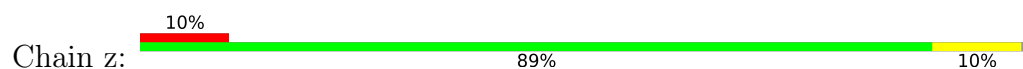
- Molecule 18: Photosystem II reaction center protein Ycf12



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	363811	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	80	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.369	Depositor
Minimum map value	-0.147	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.043	Depositor
Map size (Å)	135.5, 210.0, 118.0	wwPDB
Map dimensions	236, 420, 271	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.5, 0.5, 0.5	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0.21	0/2682	0.42	0/3661
1	a	0.21	0/2682	0.43	0/3661
2	B	0.18	0/4075	0.37	0/5558
2	b	0.18	0/4069	0.37	0/5551
3	C	0.18	0/3571	0.38	0/4864
3	c	0.19	0/3574	0.39	0/4868
4	D	0.21	0/2805	0.41	0/3823
4	d	0.21	0/2805	0.42	0/3823
5	E	0.19	0/669	0.41	0/914
5	e	0.18	0/669	0.43	0/914
6	F	0.20	0/284	0.42	0/387
6	f	0.20	0/284	0.41	0/387
7	H	0.19	0/502	0.43	0/686
7	h	0.20	0/502	0.44	0/686
8	I	0.19	0/290	0.46	0/392
8	i	0.19	0/285	0.40	0/385
9	J	0.16	0/263	0.39	0/356
9	j	0.17	0/263	0.39	0/356
10	K	0.28	0/299	0.55	0/412
10	k	0.28	0/299	0.53	0/412
11	L	0.13	0/293	0.32	0/400
11	l	0.13	0/293	0.33	0/400
12	M	0.29	0/257	0.52	0/351
12	m	0.23	0/257	0.54	0/351
13	O	0.16	0/1830	0.40	0/2492
13	o	0.16	0/1825	0.39	0/2485
14	T	0.17	0/255	0.34	0/346
14	t	0.18	0/255	0.34	0/346
15	U	0.16	0/769	0.37	0/1044
15	u	0.16	0/769	0.38	0/1044
16	V	0.14	0/1073	0.33	0/1459

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	v	0.16	0/1073	0.35	0/1459
17	X	0.14	0/282	0.27	0/381
17	x	0.14	0/278	0.30	0/376
18	Y	0.29	0/215	0.59	0/291
18	y	0.28	0/215	0.45	0/291
19	Z	0.27	0/469	0.46	0/643
19	z	0.17	0/469	0.35	0/643
All	All	0.19	0/41749	0.40	0/56898

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2597	0	2493	31	0
1	a	2597	0	2493	30	0
2	B	3935	0	3773	37	0
2	b	3929	0	3762	37	0
3	C	3458	0	3380	31	0
3	c	3461	0	3382	26	0
4	D	2710	0	2615	26	0
4	d	2710	0	2615	38	0
5	E	650	0	629	6	0
5	e	650	0	629	5	0
6	F	275	0	282	2	0
6	f	275	0	282	2	0
7	H	489	0	502	1	0
7	h	489	0	502	1	0
8	I	293	0	309	1	0
8	i	288	0	307	1	0
9	J	257	0	268	1	0
9	j	257	0	268	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	K	289	0	294	3	0
10	k	289	0	294	2	0
11	L	286	0	289	3	0
11	l	286	0	289	3	0
12	M	254	0	272	4	0
12	m	254	0	272	4	0
13	O	1799	0	1745	16	0
13	o	1794	0	1736	11	0
14	T	256	0	256	5	0
14	t	256	0	256	5	0
15	U	758	0	757	4	0
15	u	758	0	757	7	0
16	V	1052	0	1053	5	0
16	v	1052	0	1053	6	0
17	X	279	0	307	3	0
17	x	275	0	301	4	0
18	Y	214	0	234	4	0
18	y	214	0	234	1	0
19	Z	458	0	488	2	0
19	z	458	0	488	1	0
20	A	1	0	0	0	0
20	a	1	0	0	0	0
21	A	2	0	0	1	0
21	a	2	0	0	1	0
22	A	195	0	216	5	0
22	B	1020	0	1113	23	0
22	C	845	0	936	23	0
22	D	195	0	216	3	0
22	a	195	0	216	5	0
22	b	1020	0	1113	27	0
22	c	845	0	936	23	0
22	d	195	0	216	5	0
23	A	64	0	74	1	0
23	D	64	0	74	1	0
23	a	128	0	148	3	0
24	A	40	0	56	1	0
24	B	160	0	224	10	0
24	C	80	0	112	6	0
24	F	40	0	56	1	0
24	K	40	0	56	1	0
24	T	40	0	56	2	0
24	Y	40	0	56	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	40	0	56	0	0
24	b	120	0	168	10	0
24	c	80	0	112	4	0
24	f	40	0	56	0	0
24	k	40	0	56	1	0
24	y	40	0	56	1	0
25	A	55	0	80	3	0
25	D	55	0	80	4	0
25	a	55	0	80	4	0
25	d	55	0	80	4	0
26	A	105	0	147	7	0
26	D	45	0	57	2	0
26	a	105	0	147	4	0
26	b	54	0	78	2	0
26	d	45	0	57	3	0
26	l	54	0	78	3	0
27	A	30	0	47	2	0
27	B	79	0	124	5	0
27	C	62	0	95	2	0
27	D	31	0	49	1	0
27	E	18	0	31	0	0
27	F	14	0	20	0	0
27	H	12	0	16	0	0
27	L	18	0	31	1	0
27	M	16	0	24	0	0
27	X	17	0	26	0	0
27	a	18	0	31	0	0
27	b	65	0	104	1	0
27	c	69	0	112	2	0
27	d	12	0	16	0	0
27	e	36	0	62	1	0
27	j	35	0	57	1	0
27	t	15	0	26	2	0
27	x	18	0	31	2	0
28	A	12	0	20	1	0
28	B	28	0	43	3	0
28	C	9	0	14	0	0
28	E	20	0	42	2	0
28	H	10	0	16	0	0
28	I	39	0	75	2	0
28	J	31	0	60	2	0
28	T	17	0	33	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	a	25	0	38	0	0
28	b	12	0	19	2	0
28	d	27	0	49	0	0
28	i	37	0	68	1	0
29	A	10	0	0	0	0
29	a	10	0	0	0	0
30	A	4	0	0	0	0
30	a	4	0	0	0	0
31	A	46	0	65	1	0
31	D	98	0	148	5	0
31	E	40	0	53	0	0
31	L	49	0	74	4	0
31	a	95	0	139	5	0
31	d	97	0	143	5	0
31	l	49	0	74	3	0
32	A	6	0	8	0	0
32	a	6	0	8	1	0
33	A	35	0	46	0	0
33	B	129	0	173	5	0
33	C	35	0	46	1	0
33	J	24	0	35	2	0
33	M	35	0	46	1	0
33	T	59	0	81	1	0
33	Z	35	0	46	0	0
33	b	24	0	35	0	0
33	f	35	0	46	0	0
33	i	35	0	46	0	0
33	j	24	0	35	0	0
33	m	35	0	46	1	0
33	z	35	0	46	1	0
34	C	107	0	130	2	0
34	D	44	0	57	2	0
34	H	58	0	74	1	0
34	J	61	0	83	3	0
34	c	169	0	215	4	0
34	d	47	0	59	1	0
34	h	58	0	74	0	0
35	C	102	0	144	1	0
35	D	47	0	64	2	0
35	M	51	0	72	5	0
35	Y	51	0	72	2	0
35	c	99	0	138	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	d	47	0	64	2	0
35	m	51	0	72	4	0
35	y	51	0	72	1	0
36	E	43	0	30	1	0
36	V	43	0	30	1	0
36	e	43	0	30	1	0
36	v	43	0	30	1	0
37	H	41	0	56	1	0
37	h	41	0	56	1	0
38	O	1	0	0	0	0
38	o	1	0	0	0	0
39	A	92	0	0	1	0
39	B	133	0	0	0	0
39	C	101	0	0	0	0
39	D	91	0	0	1	0
39	E	14	0	0	0	0
39	F	3	0	0	0	0
39	H	11	0	0	0	0
39	I	1	0	0	0	0
39	J	4	0	0	0	0
39	K	1	0	0	0	0
39	L	8	0	0	0	0
39	M	3	0	0	0	0
39	O	37	0	0	0	0
39	T	4	0	0	0	0
39	U	14	0	0	0	0
39	V	26	0	0	0	0
39	X	3	0	0	0	0
39	a	94	0	0	1	0
39	b	137	0	0	0	0
39	c	104	0	0	0	0
39	d	91	0	0	1	0
39	e	15	0	0	0	0
39	f	4	0	0	0	0
39	h	11	0	0	0	0
39	i	3	0	0	0	0
39	j	4	0	0	0	0
39	k	1	0	0	0	0
39	l	10	0	0	0	0
39	m	3	0	0	0	0
39	o	39	0	0	1	0
39	t	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	u	13	0	0	0	0
39	v	25	0	0	0	0
39	x	2	0	0	0	0
All	All	51092	0	51568	465	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 5.

The worst 5 of 465 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)
3:C:30:LEU:HD21	22:C:515:CLA:H2A	1.69	0.74
3:c:30:LEU:HD21	22:c:516:CLA:H2A	1.71	0.72
22:c:507:CLA:H61	22:c:517:CLA:H42	1.73	0.70
5:E:8:ARG:HE	5:E:13:ILE:HG12	1.60	0.66
3:C:303:MET:HE3	3:C:307:ILE:HD11	1.78	0.65

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	331/360 (92%)	326 (98%)	5 (2%)	0	100	100
1	a	331/360 (92%)	327 (99%)	4 (1%)	0	100	100
2	B	503/510 (99%)	499 (99%)	4 (1%)	0	100	100
2	b	503/510 (99%)	498 (99%)	5 (1%)	0	100	100
3	C	448/461 (97%)	442 (99%)	6 (1%)	0	100	100
3	c	448/461 (97%)	442 (99%)	6 (1%)	0	100	100
4	D	339/352 (96%)	332 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	d	339/352 (96%)	334 (98%)	5 (2%)	0	100	100
5	E	79/84 (94%)	78 (99%)	1 (1%)	0	100	100
5	e	79/84 (94%)	78 (99%)	1 (1%)	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	60/66 (91%)	58 (97%)	2 (3%)	0	100	100
7	h	60/66 (91%)	60 (100%)	0	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
9	J	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
9	j	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	34/37 (92%)	34 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
12	m	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
13	O	241/272 (89%)	234 (97%)	7 (3%)	0	100	100
13	o	241/272 (89%)	234 (97%)	7 (3%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
15	u	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
16	V	135/163 (83%)	134 (99%)	1 (1%)	0	100	100
16	v	135/163 (83%)	133 (98%)	2 (2%)	0	100	100
17	X	36/41 (88%)	36 (100%)	0	0	100	100
17	x	36/41 (88%)	36 (100%)	0	0	100	100
18	Y	28/46 (61%)	28 (100%)	0	0	100	100
18	y	28/46 (61%)	28 (100%)	0	0	100	100
19	Z	59/62 (95%)	59 (100%)	0	0	100	100
19	z	59/62 (95%)	58 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5163/5650 (91%)	5090 (99%)	73 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	264/291 (91%)	262 (99%)	2 (1%)	79	88
1	a	264/291 (91%)	261 (99%)	3 (1%)	70	82
2	B	391/407 (96%)	385 (98%)	6 (2%)	60	75
2	b	390/407 (96%)	383 (98%)	7 (2%)	54	69
3	C	346/362 (96%)	340 (98%)	6 (2%)	56	71
3	c	347/362 (96%)	343 (99%)	4 (1%)	67	80
4	D	274/283 (97%)	271 (99%)	3 (1%)	70	82
4	d	274/283 (97%)	269 (98%)	5 (2%)	54	69
5	E	69/73 (94%)	67 (97%)	2 (3%)	37	50
5	e	69/73 (94%)	69 (100%)	0	100	100
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	28 (100%)	0	100	100
7	H	52/55 (94%)	51 (98%)	1 (2%)	52	67
7	h	52/55 (94%)	51 (98%)	1 (2%)	52	67
8	I	31/34 (91%)	29 (94%)	2 (6%)	14	16
8	i	31/34 (91%)	29 (94%)	2 (6%)	14	16
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	24 (100%)	0	100	100
10	K	29/37 (78%)	29 (100%)	0	100	100
10	k	29/37 (78%)	29 (100%)	0	100	100
11	L	32/35 (91%)	32 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	l	32/35 (91%)	32 (100%)	0	100	100
12	M	29/33 (88%)	29 (100%)	0	100	100
12	m	29/33 (88%)	29 (100%)	0	100	100
13	O	190/228 (83%)	188 (99%)	2 (1%)	70	82
13	o	189/228 (83%)	186 (98%)	3 (2%)	58	73
14	T	25/28 (89%)	25 (100%)	0	100	100
14	t	25/28 (89%)	25 (100%)	0	100	100
15	U	80/112 (71%)	77 (96%)	3 (4%)	28	37
15	u	80/112 (71%)	74 (92%)	6 (8%)	11	12
16	V	114/138 (83%)	111 (97%)	3 (3%)	41	54
16	v	114/138 (83%)	111 (97%)	3 (3%)	41	54
17	X	30/34 (88%)	29 (97%)	1 (3%)	33	44
17	x	29/34 (85%)	27 (93%)	2 (7%)	13	14
18	Y	21/37 (57%)	20 (95%)	1 (5%)	21	28
18	y	21/37 (57%)	20 (95%)	1 (5%)	21	28
19	Z	48/52 (92%)	45 (94%)	3 (6%)	15	17
19	z	48/52 (92%)	43 (90%)	5 (10%)	5	5
All	All	4152/4612 (90%)	4075 (98%)	77 (2%)	52	67

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

Mol	Chain	Res	Type
13	o	59	ASP
18	y	19	ILE
13	o	198	ILE
15	u	132	LEU
19	z	20	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
3	c	320	GLN
13	o	150	ASN
4	d	255	GLN
12	m	5	GLN

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Mol	Chain	Res	Type
13	o	202	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
8	FME	I	1	8	8,9,10	0.36	0	7,9,11	0.84	0
14	FME	T	1	14	8,9,10	0.38	0	7,9,11	0.90	0
8	FME	i	1	8	8,9,10	0.38	0	7,9,11	0.85	0
14	FME	t	1	14	8,9,10	0.39	0	7,9,11	0.98	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	I	1	8	-	0/7/9/11	-
14	FME	T	1	14	-	4/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	T	1	FME	C-CA-CB-CG
14	t	1	FME	C-CA-CB-CG
14	T	1	FME	N-CA-CB-CG
14	t	1	FME	N-CA-CB-CG
14	T	1	FME	CB-CG-SD-CE

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, 8 are monoatomic - leaving 224 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
28	LFA	H	103	-	9,9,19	0.25	0	8,8,18	0.18	0
22	CLA	a	408	-	65,73,73	1.44	6 (9%)	76,113,113	1.42	9 (11%)
22	CLA	C	508	39	65,73,73	1.45	7 (10%)	76,113,113	1.49	7 (9%)
27	PLM	j	103	-	17,17,17	0.66	0	17,17,17	0.57	0
28	LFA	J	104	-	10,10,19	0.23	0	9,9,18	0.28	0
22	CLA	c	515	-	65,73,73	1.46	6 (9%)	76,113,113	1.41	7 (9%)
22	CLA	D	401	39	65,73,73	1.42	6 (9%)	76,113,113	1.57	9 (11%)
36	HEM	v	201	16	41,50,50	1.46	3 (7%)	45,82,82	1.51	10 (22%)
24	BCR	B	617	-	41,41,41	0.34	0	56,56,56	0.73	0
36	HEM	e	103	6,5	41,50,50	1.47	4 (9%)	45,82,82	1.53	7 (15%)
27	PLM	b	622	-	12,12,17	0.79	0	12,12,17	0.69	0
27	PLM	M	103	-	15,15,17	0.67	0	15,15,17	0.68	0
35	LMG	C	519	-	51,51,55	0.51	0	59,59,63	0.65	0
24	BCR	f	101	-	41,41,41	0.35	0	56,56,56	0.93	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	a	406	39	65,73,73	1.44	6 (9%)	76,113,113	1.51	9 (11%)
33	LMT	T	101	-	24,24,36	0.50	0	29,29,47	0.73	0
22	CLA	d	403	-	65,73,73	1.45	7 (10%)	76,113,113	1.37	6 (7%)
22	CLA	C	510	-	65,73,73	1.48	7 (10%)	76,113,113	1.52	10 (13%)
23	PHO	a	407	-	51,69,69	0.65	0	47,99,99	0.90	3 (6%)
22	CLA	C	509	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	7 (9%)
24	BCR	C	502	-	41,41,41	0.35	0	56,56,56	0.82	2 (3%)
22	CLA	b	603	-	65,73,73	1.50	5 (7%)	76,113,113	1.35	7 (9%)
22	CLA	c	510	-	65,73,73	1.47	7 (10%)	76,113,113	1.41	7 (9%)
33	LMT	b	626	-	24,24,36	0.48	0	29,29,47	0.70	0
22	CLA	c	509	39	65,73,73	1.46	7 (10%)	76,113,113	1.50	7 (9%)
22	CLA	b	606	-	65,73,73	1.48	6 (9%)	76,113,113	1.57	12 (15%)
33	LMT	C	518	-	36,36,36	0.49	0	47,47,47	1.19	4 (8%)
27	PLM	c	522	-	17,17,17	0.65	0	17,17,17	0.60	0
26	SQD	l	102	-	53,54,54	1.56	9 (16%)	62,65,65	1.47	7 (11%)
22	CLA	B	610	39	65,73,73	1.49	6 (9%)	76,113,113	1.43	8 (10%)
34	DGD	d	410	-	47,47,67	0.53	0	54,55,81	0.63	0
23	PHO	A	406	-	51,69,69	0.66	0	47,99,99	0.91	3 (6%)
22	CLA	b	618	-	45,53,73	1.72	7 (15%)	52,89,113	1.77	7 (13%)
24	BCR	A	408	-	41,41,41	0.30	0	56,56,56	0.63	0
22	CLA	c	511	-	65,73,73	1.48	7 (10%)	76,113,113	1.52	10 (13%)
22	CLA	B	602	-	65,73,73	1.46	7 (10%)	76,113,113	1.44	7 (9%)
27	PLM	D	402	-	12,12,17	0.73	0	12,12,17	0.76	1 (8%)
22	CLA	D	406	-	65,73,73	1.46	6 (9%)	76,113,113	1.41	10 (13%)
34	DGD	h	101	-	59,59,67	0.57	0	73,73,81	0.76	0
22	CLA	B	615	-	65,73,73	1.46	7 (10%)	76,113,113	1.36	8 (10%)
33	LMT	B	630	-	36,36,36	0.54	0	47,47,47	0.70	0
35	LMG	d	407	-	47,47,55	0.51	0	55,55,63	0.67	0
37	RRX	h	102	-	42,42,42	0.21	0	57,58,58	0.49	0
27	PLM	B	627	-	16,16,17	0.67	0	16,16,17	0.63	0
27	PLM	d	411	-	11,11,17	0.80	0	11,11,17	0.77	0
27	PLM	E	103	-	17,17,17	0.66	0	17,17,17	0.56	0
27	PLM	c	523	-	16,16,17	0.68	0	16,16,17	0.59	0
28	LFA	A	412	-	11,11,19	0.24	0	10,10,18	0.20	0
28	LFA	T	102	-	16,16,19	0.22	0	15,15,18	0.21	0
22	CLA	C	513	-	65,73,73	1.43	6 (9%)	76,113,113	1.53	7 (9%)
35	LMG	D	409	-	47,47,55	0.52	0	55,55,63	0.68	0
33	LMT	A	419	-	36,36,36	0.55	0	47,47,47	0.87	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	PLM	B	629	-	17,17,17	0.66	0	17,17,17	0.64	0
28	LFA	b	623	-	7,7,19	0.25	0	6,6,18	0.22	0
33	LMT	f	102	-	36,36,36	0.48	0	47,47,47	0.87	2 (4%)
31	LHG	E	101	-	39,39,48	0.57	0	42,45,54	0.51	0
33	LMT	z	101	-	36,36,36	0.53	0	47,47,47	0.86	3 (6%)
24	BCR	y	102	-	41,41,41	0.35	0	56,56,56	0.93	1 (1%)
28	LFA	d	409	-	13,13,19	0.23	0	12,12,18	0.25	0
36	HEM	V	201	16	41,50,50	1.45	3 (7%)	45,82,82	1.51	9 (20%)
34	DGD	c	505	-	62,62,67	0.58	0	76,76,81	0.70	1 (1%)
31	LHG	d	405	-	48,48,48	0.50	0	51,54,54	0.56	0
25	PL9	a	410	-	55,55,55	1.10	4 (7%)	68,69,69	1.56	12 (17%)
22	CLA	c	508	-	65,73,73	1.46	6 (9%)	76,113,113	1.45	8 (10%)
27	PLM	C	523	-	15,15,17	0.69	0	15,15,17	0.64	0
24	BCR	Y	102	-	41,41,41	0.35	0	56,56,56	0.94	1 (1%)
27	PLM	e	102	-	17,17,17	0.62	0	17,17,17	0.63	0
22	CLA	B	616	-	45,53,73	1.72	7 (15%)	52,89,113	1.79	6 (11%)
22	CLA	b	609	39	65,73,73	1.46	7 (10%)	76,113,113	1.43	7 (9%)
27	PLM	B	621	-	17,17,17	0.63	0	17,17,17	0.64	0
22	CLA	b	617	-	65,73,73	1.44	6 (9%)	76,113,113	1.41	8 (10%)
33	LMT	T	104	-	36,36,36	0.51	0	47,47,47	0.72	0
28	LFA	B	620	-	7,7,19	0.23	0	6,6,18	0.22	0
24	BCR	B	619	-	41,41,41	0.32	0	56,56,56	1.04	2 (3%)
26	SQD	d	412	-	44,45,54	1.64	9 (20%)	53,56,65	1.59	10 (18%)
24	BCR	c	502	-	41,41,41	0.35	0	56,56,56	0.83	2 (3%)
22	CLA	B	606	-	65,73,73	1.47	6 (9%)	76,113,113	1.50	9 (11%)
22	CLA	b	605	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	7 (9%)
28	LFA	C	521	-	8,8,19	0.22	0	7,7,18	0.29	0
26	SQD	a	411	-	53,54,54	1.57	8 (15%)	62,65,65	1.42	9 (14%)
28	LFA	d	408	-	12,12,19	0.23	0	11,11,18	0.20	0
35	LMG	M	101	-	51,51,55	0.49	0	59,59,63	0.59	0
22	CLA	C	517	-	65,73,73	1.41	6 (9%)	76,113,113	1.55	8 (10%)
27	PLM	B	622	-	13,13,17	0.73	0	13,13,17	0.68	0
26	SQD	A	415	-	50,51,54	1.55	7 (14%)	59,62,65	1.57	10 (16%)
28	LFA	b	624	-	3,3,19	0.38	0	2,2,18	0.51	0
33	LMT	J	103	-	24,24,36	0.50	0	29,29,47	0.91	1 (3%)
22	CLA	b	613	-	65,73,73	1.44	7 (10%)	76,113,113	1.50	8 (10%)
25	PL9	d	402	-	55,55,55	1.14	3 (5%)	68,69,69	1.51	13 (19%)
24	BCR	B	618	-	41,41,41	0.33	0	56,56,56	0.80	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	B	603	-	65,73,73	1.46	6 (9%)	76,113,113	1.38	8 (10%)
22	CLA	b	614	-	65,73,73	1.42	7 (10%)	76,113,113	1.51	8 (10%)
23	PHO	D	403	-	51,69,69	0.65	0	47,99,99	0.98	3 (6%)
27	PLM	A	411	-	17,17,17	0.68	0	17,17,17	0.60	0
32	GOL	a	401	-	5,5,5	0.34	0	5,5,5	0.39	0
27	PLM	C	522	-	17,17,17	0.65	0	17,17,17	0.73	1 (5%)
22	CLA	a	405	-	65,73,73	1.44	6 (9%)	76,113,113	1.47	7 (9%)
22	CLA	b	616	-	65,73,73	1.43	7 (10%)	76,113,113	1.45	7 (9%)
34	DGD	C	504	-	55,55,67	0.59	0	69,69,81	0.92	4 (5%)
36	HEM	E	104	6,5	41,50,50	1.48	6 (14%)	45,82,82	1.54	7 (15%)
27	PLM	F	102	-	13,13,17	0.73	0	13,13,17	0.67	0
22	CLA	B	613	-	65,73,73	1.42	5 (7%)	76,113,113	1.44	8 (10%)
27	PLM	C	520	-	14,14,17	0.72	0	14,14,17	0.70	0
22	CLA	A	407	-	65,73,73	1.44	6 (9%)	76,113,113	1.42	9 (11%)
27	PLM	L	102	-	17,17,17	0.66	0	17,17,17	0.60	0
31	LHG	D	408	-	48,48,48	0.51	0	51,54,54	0.53	0
22	CLA	c	513	-	65,73,73	1.43	6 (9%)	76,113,113	1.55	9 (11%)
33	LMT	B	628	-	24,24,36	0.50	0	29,29,47	0.78	0
26	SQD	D	412	-	44,45,54	1.64	9 (20%)	53,56,65	1.58	10 (18%)
33	LMT	B	633	-	36,36,36	0.51	0	47,47,47	0.77	0
26	SQD	A	410	-	53,54,54	1.52	7 (13%)	62,65,65	1.35	6 (9%)
27	PLM	c	520	-	17,17,17	0.68	0	17,17,17	0.59	0
22	CLA	A	405	39	65,73,73	1.44	6 (9%)	76,113,113	1.51	9 (11%)
22	CLA	b	612	39	65,73,73	1.49	6 (9%)	76,113,113	1.43	8 (10%)
22	CLA	A	404	-	65,73,73	1.44	6 (9%)	76,113,113	1.48	7 (9%)
22	CLA	d	404	-	65,73,73	1.48	7 (10%)	76,113,113	1.39	9 (11%)
24	BCR	C	501	-	41,41,41	0.35	0	56,56,56	1.04	1 (1%)
27	PLM	D	410	-	17,17,17	0.65	0	17,17,17	0.66	0
37	RRX	H	102	-	42,42,42	0.22	0	57,58,58	0.48	0
30	BCT	a	419	20	2,3,3	0.88	0	2,3,3	3.27	2 (100%)
29	OEX	a	416	3,39,1	0,15,15	-	-	-	-	-
34	DGD	H	101	-	59,59,67	0.56	0	73,73,81	0.78	0
28	LFA	J	101	-	19,19,19	0.24	0	18,18,18	0.22	0
24	BCR	c	501	-	41,41,41	0.36	0	56,56,56	1.08	2 (3%)
22	CLA	b	608	-	65,73,73	1.47	7 (10%)	76,113,113	1.47	8 (10%)
22	CLA	D	405	-	65,73,73	1.45	6 (9%)	76,113,113	1.38	6 (7%)
22	CLA	B	609	-	65,73,73	1.47	5 (7%)	76,113,113	1.39	7 (9%)
27	PLM	a	412	-	17,17,17	0.67	0	17,17,17	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
35	LMG	C	525	-	51,51,55	0.50	0	59,59,63	0.87	3 (5%)
22	CLA	B	605	-	65,73,73	1.46	7 (10%)	76,113,113	1.44	7 (9%)
22	CLA	B	612	-	65,73,73	1.41	7 (10%)	76,113,113	1.51	8 (10%)
28	LFA	E	102	-	19,19,19	0.24	0	18,18,18	0.20	0
24	BCR	a	409	-	41,41,41	0.30	0	56,56,56	0.65	0
31	LHG	a	415	-	48,48,48	0.51	0	51,54,54	0.52	0
27	PLM	b	621	-	17,17,17	0.65	0	17,17,17	0.58	0
31	LHG	d	406	-	47,47,48	0.51	0	50,53,54	0.53	0
26	SQD	a	417	-	50,51,54	1.54	6 (12%)	59,62,65	1.55	9 (15%)
22	CLA	b	611	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	7 (9%)
28	LFA	i	104	-	7,7,19	0.24	0	6,6,18	0.20	0
35	LMG	m	101	-	51,51,55	0.50	0	59,59,63	0.57	0
31	LHG	D	407	-	48,48,48	0.51	0	51,54,54	0.57	0
27	PLM	b	625	-	15,15,17	0.68	0	15,15,17	0.64	0
31	LHG	l	101	-	48,48,48	0.51	0	51,54,54	0.52	0
22	CLA	C	516	-	65,73,73	1.45	6 (9%)	76,113,113	1.44	7 (9%)
28	LFA	a	413	-	6,6,19	0.25	0	5,5,18	0.18	0
34	DGD	D	411	-	44,44,67	0.54	0	52,52,81	0.74	1 (1%)
27	PLM	b	627	-	17,17,17	0.67	0	17,17,17	0.63	0
22	CLA	c	516	3	65,73,73	1.46	6 (9%)	76,113,113	1.50	8 (10%)
27	PLM	t	101	-	14,14,17	0.23	0	13,13,17	0.23	0
24	BCR	K	101	-	41,41,41	0.31	0	56,56,56	0.59	0
27	PLM	C	524	-	12,12,17	0.76	0	12,12,17	0.70	0
28	LFA	B	626	-	7,7,19	0.26	0	6,6,18	0.18	0
28	LFA	I	101	-	19,19,19	0.24	0	18,18,18	0.16	0
27	PLM	x	101	-	17,17,17	0.67	0	17,17,17	0.59	0
24	BCR	T	103	-	41,41,41	0.34	0	56,56,56	0.76	0
22	CLA	B	608	-	65,73,73	1.45	6 (9%)	76,113,113	1.50	9 (11%)
22	CLA	C	512	-	65,73,73	1.43	6 (9%)	76,113,113	1.53	9 (11%)
22	CLA	B	601	-	65,73,73	1.51	5 (7%)	76,113,113	1.35	7 (9%)
24	BCR	k	101	-	41,41,41	0.36	0	56,56,56	0.71	1 (1%)
35	LMG	c	519	-	51,51,55	0.52	0	59,59,63	0.64	0
27	PLM	X	101	-	16,16,17	0.71	0	16,16,17	0.59	0
35	LMG	c	524	-	48,48,55	0.49	0	56,56,63	0.69	0
22	CLA	b	607	-	65,73,73	1.46	6 (9%)	76,113,113	1.44	7 (9%)
28	LFA	I	103	-	7,7,19	0.25	0	6,6,18	0.21	0
22	CLA	B	607	39	65,73,73	1.46	6 (9%)	76,113,113	1.42	7 (9%)
22	CLA	B	611	-	65,73,73	1.44	7 (10%)	76,113,113	1.50	9 (11%)
27	PLM	B	625	-	11,11,17	0.82	0	11,11,17	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	LHG	L	101	-	48,48,48	0.50	0	51,54,54	0.56	0
33	LMT	j	101	-	24,24,36	0.52	0	29,29,47	0.83	0
33	LMT	i	102	-	36,36,36	0.49	0	47,47,47	1.17	5 (10%)
22	CLA	c	518	-	65,73,73	1.42	6 (9%)	76,113,113	1.55	7 (9%)
22	CLA	C	506	-	65,73,73	1.45	7 (10%)	76,113,113	1.43	6 (7%)
27	PLM	e	101	-	17,17,17	0.68	0	17,17,17	0.58	0
33	LMT	B	623	-	36,36,36	0.52	0	47,47,47	0.70	0
31	LHG	a	421	-	45,45,48	0.52	0	48,51,54	0.55	0
34	DGD	c	504	-	56,56,67	0.58	0	70,70,81	0.87	2 (2%)
22	CLA	B	604	-	65,73,73	1.48	6 (9%)	76,113,113	1.58	12 (15%)
30	BCT	A	416	20	2,3,3	0.87	0	2,3,3	3.26	2 (100%)
24	BCR	b	619	-	41,41,41	0.33	0	56,56,56	0.81	1 (1%)
27	PLM	H	104	-	11,11,17	0.80	0	11,11,17	0.73	0
22	CLA	C	511	39	65,73,73	1.46	6 (9%)	76,113,113	1.50	8 (10%)
24	BCR	B	632	-	41,41,41	0.36	0	56,56,56	1.52	7 (12%)
28	LFA	i	101	-	19,19,19	0.24	0	18,18,18	0.18	0
22	CLA	b	610	-	65,73,73	1.44	6 (9%)	76,113,113	1.49	9 (11%)
23	PHO	a	420	-	51,69,69	0.64	0	47,99,99	0.98	3 (6%)
24	BCR	F	101	-	41,41,41	0.36	0	56,56,56	0.85	2 (3%)
25	PL9	D	404	-	55,55,55	1.14	4 (7%)	68,69,69	1.50	13 (19%)
28	LFA	a	418	-	6,6,19	0.25	0	5,5,18	0.18	0
28	LFA	a	414	-	10,10,19	0.25	0	9,9,18	0.19	0
33	LMT	Z	101	-	36,36,36	0.54	0	47,47,47	0.94	3 (6%)
28	LFA	i	103	-	8,8,19	0.23	0	7,7,18	0.21	0
22	CLA	d	401	39	65,73,73	1.43	6 (9%)	76,113,113	1.57	7 (9%)
27	PLM	c	521	-	15,15,17	0.71	0	15,15,17	0.64	0
33	LMT	m	102	-	36,36,36	0.55	0	47,47,47	0.78	1 (2%)
28	LFA	I	102	-	10,10,19	0.23	0	9,9,18	0.24	0
22	CLA	C	514	-	65,73,73	1.45	6 (9%)	76,113,113	1.40	7 (9%)
22	CLA	c	514	-	65,73,73	1.43	6 (9%)	76,113,113	1.55	9 (11%)
28	LFA	B	624	-	6,6,19	0.25	0	5,5,18	0.19	0
35	LMG	Y	101	-	51,51,55	0.49	0	59,59,63	0.65	0
22	CLA	C	505	-	65,73,73	1.50	7 (10%)	76,113,113	1.34	5 (6%)
24	BCR	b	602	-	41,41,41	0.36	0	56,56,56	1.52	6 (10%)
22	CLA	c	506	-	65,73,73	1.48	6 (9%)	76,113,113	1.36	7 (9%)
27	PLM	j	102	-	16,16,17	0.69	0	16,16,17	0.69	0
35	LMG	y	101	-	51,51,55	0.51	0	59,59,63	0.97	4 (6%)
22	CLA	c	517	-	65,73,73	1.46	6 (9%)	76,113,113	1.45	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	DGD	J	102	-	62,62,67	0.57	0	76,76,81	1.29	4 (5%)
22	CLA	c	512	39	65,73,73	1.44	6 (9%)	76,113,113	1.51	8 (10%)
22	CLA	b	604	-	65,73,73	1.45	7 (10%)	76,113,113	1.44	7 (9%)
27	PLM	A	413	-	11,11,17	0.80	0	11,11,17	0.76	0
22	CLA	C	507	-	65,73,73	1.48	7 (10%)	76,113,113	1.42	8 (10%)
22	CLA	b	615	-	65,73,73	1.42	6 (9%)	76,113,113	1.44	8 (10%)
22	CLA	c	507	-	65,73,73	1.44	6 (9%)	76,113,113	1.44	6 (7%)
28	LFA	B	631	-	4,4,19	0.29	0	3,3,18	0.24	0
25	PL9	A	409	-	55,55,55	1.09	4 (7%)	68,69,69	1.57	14 (20%)
26	SQD	b	601	-	53,54,54	1.52	9 (16%)	62,65,65	1.71	10 (16%)
33	LMT	M	102	-	36,36,36	0.54	0	47,47,47	0.77	0
22	CLA	C	515	3	65,73,73	1.45	6 (9%)	76,113,113	1.51	8 (10%)
34	DGD	C	503	-	54,54,67	0.65	0	68,68,81	0.72	1 (1%)
22	CLA	B	614	-	65,73,73	1.44	7 (10%)	76,113,113	1.45	7 (9%)
29	OEX	A	414	3,39,1	0,15,15	-	-	-	-	-
34	DGD	c	503	-	54,54,67	0.64	0	68,68,81	0.73	1 (1%)
32	GOL	A	418	-	5,5,5	0.34	0	5,5,5	0.38	0
24	BCR	b	620	-	41,41,41	0.33	0	56,56,56	0.91	2 (3%)
31	LHG	A	417	-	45,45,48	0.53	0	48,51,54	0.53	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LFA	H	103	-	-	4/7/7/17	-
22	CLA	a	408	-	1/1/15/20	10/37/115/115	-
22	CLA	C	508	39	1/1/15/20	9/37/115/115	-
27	PLM	j	103	-	-	7/15/15/15	-
28	LFA	J	104	-	-	3/8/8/17	-
22	CLA	c	515	-	1/1/15/20	4/37/115/115	-
22	CLA	D	401	39	1/1/15/20	5/37/115/115	-
36	HEM	v	201	16	-	2/12/54/54	-
24	BCR	B	617	-	-	7/29/63/63	0/2/2/2
36	HEM	e	103	6,5	-	2/12/54/54	-
27	PLM	b	622	-	-	4/10/10/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PLM	M	103	-	-	11/13/13/15	-
35	LMG	C	519	-	-	25/46/66/70	0/1/1/1
24	BCR	f	101	-	-	9/29/63/63	0/2/2/2
22	CLA	a	406	39	1/1/15/20	9/37/115/115	-
33	LMT	T	101	-	-	8/15/35/61	0/1/1/2
22	CLA	d	403	-	1/1/15/20	3/37/115/115	-
22	CLA	C	510	-	1/1/15/20	16/37/115/115	-
23	PHO	a	407	-	-	2/37/103/103	0/5/6/6
22	CLA	C	509	-	1/1/15/20	8/37/115/115	-
24	BCR	C	502	-	-	11/29/63/63	0/2/2/2
22	CLA	b	603	-	1/1/15/20	12/37/115/115	-
22	CLA	c	510	-	1/1/15/20	9/37/115/115	-
33	LMT	b	626	-	-	6/15/35/61	0/1/1/2
22	CLA	c	509	39	1/1/15/20	9/37/115/115	-
22	CLA	b	606	-	1/1/15/20	14/37/115/115	-
33	LMT	C	518	-	-	10/21/61/61	0/2/2/2
27	PLM	c	522	-	-	2/15/15/15	-
26	SQD	l	102	-	-	23/49/69/69	0/1/1/1
22	CLA	B	610	39	1/1/15/20	8/37/115/115	-
34	DGD	d	410	-	-	15/41/62/95	0/1/1/2
23	PHO	A	406	-	-	3/37/103/103	0/5/6/6
22	CLA	b	618	-	1/1/11/20	1/13/91/115	-
24	BCR	A	408	-	-	2/29/63/63	0/2/2/2
22	CLA	c	511	-	1/1/15/20	15/37/115/115	-
22	CLA	B	602	-	1/1/15/20	6/37/115/115	-
27	PLM	D	402	-	-	2/10/10/15	-
22	CLA	D	406	-	1/1/15/20	9/37/115/115	-
34	DGD	h	101	-	-	7/47/87/95	0/2/2/2
22	CLA	B	615	-	1/1/15/20	6/37/115/115	-
33	LMT	B	630	-	-	3/21/61/61	0/2/2/2
35	LMG	d	407	-	-	11/42/62/70	0/1/1/1
37	RRX	h	102	-	-	3/29/65/65	0/2/2/2
27	PLM	B	627	-	-	5/14/14/15	-
27	PLM	d	411	-	-	5/9/9/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PLM	E	103	-	-	3/15/15/15	-
27	PLM	c	523	-	-	9/14/14/15	-
28	LFA	A	412	-	-	1/9/9/17	-
28	LFA	T	102	-	-	9/14/14/17	-
22	CLA	C	513	-	1/1/15/20	8/37/115/115	-
35	LMG	D	409	-	-	10/42/62/70	0/1/1/1
33	LMT	A	419	-	-	5/21/61/61	0/2/2/2
27	PLM	B	629	-	-	3/15/15/15	-
28	LFA	b	623	-	-	0/5/5/17	-
33	LMT	f	102	-	-	11/21/61/61	0/2/2/2
31	LHG	E	101	-	-	30/44/44/53	-
33	LMT	z	101	-	-	11/21/61/61	0/2/2/2
24	BCR	y	102	-	-	10/29/63/63	0/2/2/2
28	LFA	d	409	-	-	2/11/11/17	-
36	HEM	V	201	16	-	2/12/54/54	-
34	DGD	c	505	-	-	19/50/90/95	0/2/2/2
31	LHG	d	405	-	-	18/53/53/53	-
25	PL9	a	410	-	-	28/53/73/73	0/1/1/1
22	CLA	c	508	-	1/1/15/20	6/37/115/115	-
27	PLM	C	523	-	-	2/13/13/15	-
24	BCR	Y	102	-	-	10/29/63/63	0/2/2/2
27	PLM	e	102	-	-	8/15/15/15	-
22	CLA	B	616	-	1/1/11/20	1/13/91/115	-
22	CLA	b	609	39	1/1/15/20	6/37/115/115	-
27	PLM	B	621	-	-	8/15/15/15	-
22	CLA	b	617	-	1/1/15/20	6/37/115/115	-
33	LMT	T	104	-	-	8/21/61/61	0/2/2/2
28	LFA	B	620	-	-	5/5/5/17	-
24	BCR	B	619	-	-	2/29/63/63	0/2/2/2
26	SQD	d	412	-	-	11/40/60/69	0/1/1/1
24	BCR	c	502	-	-	10/29/63/63	0/2/2/2
22	CLA	B	606	-	1/1/15/20	6/37/115/115	-
22	CLA	b	605	-	1/1/15/20	12/37/115/115	-
28	LFA	C	521	-	-	5/6/6/17	-
26	SQD	a	411	-	-	25/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LFA	d	408	-	-	7/10/10/17	-
35	LMG	M	101	-	-	20/46/66/70	0/1/1/1
22	CLA	C	517	-	1/1/15/20	5/37/115/115	-
27	PLM	B	622	-	-	4/11/11/15	-
26	SQD	A	415	-	-	15/46/66/69	0/1/1/1
28	LFA	b	624	-	-	0/1/1/17	-
33	LMT	J	103	-	-	12/15/35/61	0/1/1/2
22	CLA	b	613	-	1/1/15/20	8/37/115/115	-
25	PL9	d	402	-	-	20/53/73/73	0/1/1/1
24	BCR	B	618	-	-	0/29/63/63	0/2/2/2
22	CLA	B	603	-	1/1/15/20	13/37/115/115	-
22	CLA	b	614	-	1/1/15/20	7/37/115/115	-
23	PHO	D	403	-	-	7/37/103/103	0/5/6/6
27	PLM	A	411	-	-	7/15/15/15	-
32	GOL	a	401	-	-	4/4/4/4	-
27	PLM	C	522	-	-	10/15/15/15	-
22	CLA	a	405	-	1/1/15/20	7/37/115/115	-
22	CLA	b	616	-	1/1/15/20	18/37/115/115	-
34	DGD	C	504	-	-	25/43/83/95	0/2/2/2
36	HEM	E	104	6,5	-	2/12/54/54	-
27	PLM	F	102	-	-	2/11/11/15	-
22	CLA	B	613	-	1/1/15/20	6/37/115/115	-
27	PLM	C	520	-	-	8/12/12/15	-
22	CLA	A	407	-	1/1/15/20	8/37/115/115	-
27	PLM	L	102	-	-	9/15/15/15	-
31	LHG	D	408	-	-	17/53/53/53	-
22	CLA	c	513	-	1/1/15/20	8/37/115/115	-
33	LMT	B	628	-	-	2/15/35/61	0/1/1/2
26	SQD	D	412	-	-	13/40/60/69	0/1/1/1
33	LMT	B	633	-	-	5/21/61/61	0/2/2/2
26	SQD	A	410	-	-	21/49/69/69	0/1/1/1
27	PLM	c	520	-	-	9/15/15/15	-
22	CLA	A	405	39	1/1/15/20	8/37/115/115	-
22	CLA	b	612	39	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	404	-	1/1/15/20	7/37/115/115	-
22	CLA	d	404	-	1/1/15/20	8/37/115/115	-
24	BCR	C	501	-	-	4/29/63/63	0/2/2/2
27	PLM	D	410	-	-	8/15/15/15	-
37	RRX	H	102	-	-	3/29/65/65	0/2/2/2
34	DGD	H	101	-	-	6/47/87/95	0/2/2/2
28	LFA	J	101	-	-	4/17/17/17	-
24	BCR	c	501	-	-	3/29/63/63	0/2/2/2
22	CLA	b	608	-	1/1/15/20	7/37/115/115	-
22	CLA	D	405	-	1/1/15/20	3/37/115/115	-
22	CLA	B	609	-	1/1/15/20	10/37/115/115	-
27	PLM	a	412	-	-	10/15/15/15	-
35	LMG	C	525	-	-	19/46/66/70	0/1/1/1
22	CLA	B	605	-	1/1/15/20	5/37/115/115	-
22	CLA	B	612	-	1/1/15/20	7/37/115/115	-
28	LFA	E	102	-	-	4/17/17/17	-
24	BCR	a	409	-	-	3/29/63/63	0/2/2/2
31	LHG	a	415	-	-	24/53/53/53	-
27	PLM	b	621	-	-	7/15/15/15	-
31	LHG	d	406	-	-	21/52/52/53	-
26	SQD	a	417	-	-	24/46/66/69	0/1/1/1
22	CLA	b	611	-	1/1/15/20	9/37/115/115	-
28	LFA	i	104	-	-	2/5/5/17	-
35	LMG	m	101	-	-	18/46/66/70	0/1/1/1
31	LHG	D	407	-	-	19/53/53/53	-
27	PLM	b	625	-	-	3/13/13/15	-
31	LHG	l	101	-	-	20/53/53/53	-
22	CLA	C	516	-	1/1/15/20	12/37/115/115	-
28	LFA	a	413	-	-	3/4/4/17	-
34	DGD	D	411	-	-	14/38/58/95	0/1/1/2
27	PLM	b	627	-	-	3/15/15/15	-
22	CLA	c	516	3	1/1/15/20	4/37/115/115	-
27	PLM	t	101	-	-	6/12/12/15	-
24	BCR	K	101	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PLM	C	524	-	-	2/10/10/15	-
28	LFA	B	626	-	-	0/5/5/17	-
28	LFA	I	101	-	-	7/17/17/17	-
27	PLM	x	101	-	-	10/15/15/15	-
24	BCR	T	103	-	-	5/29/63/63	0/2/2/2
22	CLA	B	608	-	1/1/15/20	5/37/115/115	-
22	CLA	C	512	-	1/1/15/20	6/37/115/115	-
22	CLA	B	601	-	1/1/15/20	12/37/115/115	-
24	BCR	k	101	-	-	8/29/63/63	0/2/2/2
35	LMG	c	519	-	-	27/46/66/70	0/1/1/1
27	PLM	X	101	-	-	8/14/14/15	-
35	LMG	c	524	-	-	16/43/63/70	0/1/1/1
22	CLA	b	607	-	1/1/15/20	5/37/115/115	-
28	LFA	I	103	-	-	2/5/5/17	-
22	CLA	B	607	39	1/1/15/20	6/37/115/115	-
22	CLA	B	611	-	1/1/15/20	8/37/115/115	-
27	PLM	B	625	-	-	1/9/9/15	-
31	LHG	L	101	-	-	17/53/53/53	-
33	LMT	j	101	-	-	14/15/35/61	0/1/1/2
33	LMT	i	102	-	-	10/21/61/61	0/2/2/2
22	CLA	c	518	-	1/1/15/20	6/37/115/115	-
22	CLA	C	506	-	1/1/15/20	12/37/115/115	-
27	PLM	e	101	-	-	7/15/15/15	-
33	LMT	B	623	-	-	3/21/61/61	0/2/2/2
31	LHG	a	421	-	-	16/50/50/53	-
34	DGD	c	504	-	-	26/44/84/95	0/2/2/2
22	CLA	B	604	-	1/1/15/20	14/37/115/115	-
24	BCR	b	619	-	-	0/29/63/63	0/2/2/2
27	PLM	H	104	-	-	1/9/9/15	-
22	CLA	C	511	39	1/1/15/20	6/37/115/115	-
24	BCR	B	632	-	-	10/29/63/63	0/2/2/2
28	LFA	i	101	-	-	12/17/17/17	-
22	CLA	b	610	-	1/1/15/20	5/37/115/115	-
23	PHO	a	420	-	-	5/37/103/103	0/5/6/6
24	BCR	F	101	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PL9	D	404	-	-	19/53/73/73	0/1/1/1
28	LFA	a	418	-	-	2/4/4/17	-
28	LFA	a	414	-	-	5/8/8/17	-
33	LMT	Z	101	-	-	11/21/61/61	0/2/2/2
28	LFA	i	103	-	-	4/6/6/17	-
22	CLA	d	401	39	1/1/15/20	5/37/115/115	-
27	PLM	c	521	-	-	4/13/13/15	-
33	LMT	m	102	-	-	4/21/61/61	0/2/2/2
28	LFA	I	102	-	-	5/8/8/17	-
22	CLA	C	514	-	1/1/15/20	5/37/115/115	-
22	CLA	c	514	-	1/1/15/20	5/37/115/115	-
28	LFA	B	624	-	-	1/4/4/17	-
35	LMG	Y	101	-	-	10/46/66/70	0/1/1/1
22	CLA	C	505	-	1/1/15/20	8/37/115/115	-
24	BCR	b	602	-	-	9/29/63/63	0/2/2/2
22	CLA	c	506	-	1/1/15/20	4/37/115/115	-
27	PLM	j	102	-	-	6/14/14/15	-
35	LMG	y	101	-	-	14/46/66/70	0/1/1/1
22	CLA	c	517	-	1/1/15/20	16/37/115/115	-
34	DGD	J	102	-	-	17/50/90/95	0/2/2/2
22	CLA	c	512	39	1/1/15/20	6/37/115/115	-
22	CLA	b	604	-	1/1/15/20	5/37/115/115	-
27	PLM	A	413	-	-	7/9/9/15	-
22	CLA	C	507	-	1/1/15/20	3/37/115/115	-
22	CLA	b	615	-	1/1/15/20	6/37/115/115	-
22	CLA	c	507	-	1/1/15/20	10/37/115/115	-
28	LFA	B	631	-	-	0/2/2/17	-
25	PL9	A	409	-	-	28/53/73/73	0/1/1/1
26	SQD	b	601	-	-	28/49/69/69	0/1/1/1
33	LMT	M	102	-	-	4/21/61/61	0/2/2/2
22	CLA	C	515	3	1/1/15/20	6/37/115/115	-
34	DGD	C	503	-	-	21/42/82/95	0/2/2/2
22	CLA	B	614	-	1/1/15/20	17/37/115/115	-
34	DGD	c	503	-	-	22/42/82/95	0/2/2/2
32	GOL	A	418	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	b	620	-	-	3/29/63/63	0/2/2/2
31	LHG	A	417	-	-	15/50/50/53	-

The worst 5 of 534 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	601	CLA	C4B-NB	7.68	1.42	1.35
22	C	505	CLA	C4B-NB	7.53	1.41	1.35
22	b	603	CLA	C4B-NB	7.52	1.41	1.35
22	B	610	CLA	C4B-NB	7.42	1.41	1.35
22	C	507	CLA	C4B-NB	7.37	1.41	1.35

The worst 5 of 795 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	606	CLA	C4A-NA-C1A	7.94	110.28	106.71
22	C	516	CLA	C4A-NA-C1A	7.92	110.27	106.71
22	B	604	CLA	C4A-NA-C1A	7.80	110.21	106.71
22	C	511	CLA	C4A-NA-C1A	7.58	110.11	106.71
22	c	517	CLA	C4A-NA-C1A	7.51	110.08	106.71

5 of 70 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	404	CLA	ND
22	A	405	CLA	ND
22	A	407	CLA	ND
22	B	601	CLA	ND
22	B	602	CLA	ND

5 of 1911 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	404	CLA	CBD-CGD-O2D-CED
22	A	405	CLA	CHA-CBD-CGD-O1D
22	B	601	CLA	CHA-CBD-CGD-O1D
22	B	601	CLA	CHA-CBD-CGD-O2D
22	B	602	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

163 monomers are involved in 253 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	a	408	CLA	2	0
22	C	508	CLA	1	0
27	j	103	PLM	1	0
28	J	104	LFA	1	0
22	c	515	CLA	4	0
22	D	401	CLA	1	0
36	v	201	HEM	1	0
24	B	617	BCR	4	0
36	e	103	HEM	1	0
27	b	622	PLM	1	0
35	C	519	LMG	1	0
22	a	406	CLA	1	0
33	T	101	LMT	1	0
22	d	403	CLA	2	0
22	C	510	CLA	2	0
23	a	407	PHO	1	0
22	C	509	CLA	3	0
24	C	502	BCR	4	0
22	c	510	CLA	2	0
22	c	509	CLA	1	0
22	b	606	CLA	4	0
33	C	518	LMT	1	0
26	l	102	SQD	3	0
22	B	610	CLA	1	0
34	d	410	DGD	1	0
23	A	406	PHO	1	0
22	b	618	CLA	2	0
24	A	408	BCR	1	0
22	c	511	CLA	2	0
22	B	602	CLA	2	0
27	D	402	PLM	1	0
22	B	615	CLA	6	0
33	B	630	LMT	3	0
35	d	407	LMG	2	0
37	h	102	RRX	1	0
28	A	412	LFA	1	0
28	T	102	LFA	2	0
22	C	513	CLA	1	0
35	D	409	LMG	2	0
27	B	629	PLM	1	0
28	b	623	LFA	2	0
33	z	101	LMT	1	0
24	y	102	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	V	201	HEM	1	0
34	c	505	DGD	2	0
31	d	405	LHG	3	0
25	a	410	PL9	4	0
22	c	508	CLA	3	0
24	Y	102	BCR	2	0
27	e	102	PLM	1	0
22	B	616	CLA	2	0
22	b	609	CLA	3	0
27	B	621	PLM	1	0
22	b	617	CLA	6	0
28	B	620	LFA	1	0
24	B	619	BCR	1	0
26	d	412	SQD	3	0
24	c	502	BCR	3	0
22	B	606	CLA	1	0
22	b	605	CLA	1	0
26	a	411	SQD	2	0
35	M	101	LMG	5	0
27	B	622	PLM	1	0
26	A	415	SQD	4	0
33	J	103	LMT	2	0
22	b	613	CLA	1	0
25	d	402	PL9	4	0
24	B	618	BCR	1	0
22	b	614	CLA	2	0
23	D	403	PHO	1	0
32	a	401	GOL	1	0
22	a	405	CLA	2	0
22	b	616	CLA	1	0
34	C	504	DGD	2	0
36	E	104	HEM	1	0
22	B	613	CLA	2	0
22	A	407	CLA	2	0
27	L	102	PLM	1	0
31	D	408	LHG	2	0
22	c	513	CLA	4	0
33	B	628	LMT	1	0
26	D	412	SQD	2	0
33	B	633	LMT	1	0
26	A	410	SQD	3	0
27	c	520	PLM	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	405	CLA	1	0
22	b	612	CLA	1	0
22	A	404	CLA	2	0
22	d	404	CLA	2	0
24	C	501	BCR	2	0
27	D	410	PLM	1	0
37	H	102	RRX	1	0
34	H	101	DGD	1	0
28	J	101	LFA	1	0
24	c	501	BCR	1	0
22	b	608	CLA	1	0
22	D	405	CLA	2	0
22	B	609	CLA	1	0
22	B	605	CLA	3	0
22	B	612	CLA	2	0
28	E	102	LFA	2	0
31	a	415	LHG	3	0
31	d	406	LHG	2	0
26	a	417	SQD	2	0
22	b	611	CLA	1	0
28	i	104	LFA	1	0
35	m	101	LMG	4	0
31	D	407	LHG	3	0
31	l	101	LHG	3	0
22	C	516	CLA	3	0
34	D	411	DGD	2	0
22	c	516	CLA	2	0
27	t	101	PLM	2	0
24	K	101	BCR	1	0
27	C	524	PLM	2	0
28	B	626	LFA	2	0
27	x	101	PLM	2	0
24	T	103	BCR	2	0
22	B	608	CLA	1	0
22	C	512	CLA	1	0
24	k	101	BCR	1	0
35	c	519	LMG	1	0
35	c	524	LMG	2	0
22	b	607	CLA	4	0
28	I	103	LFA	2	0
22	B	607	CLA	3	0
22	B	611	CLA	2	0

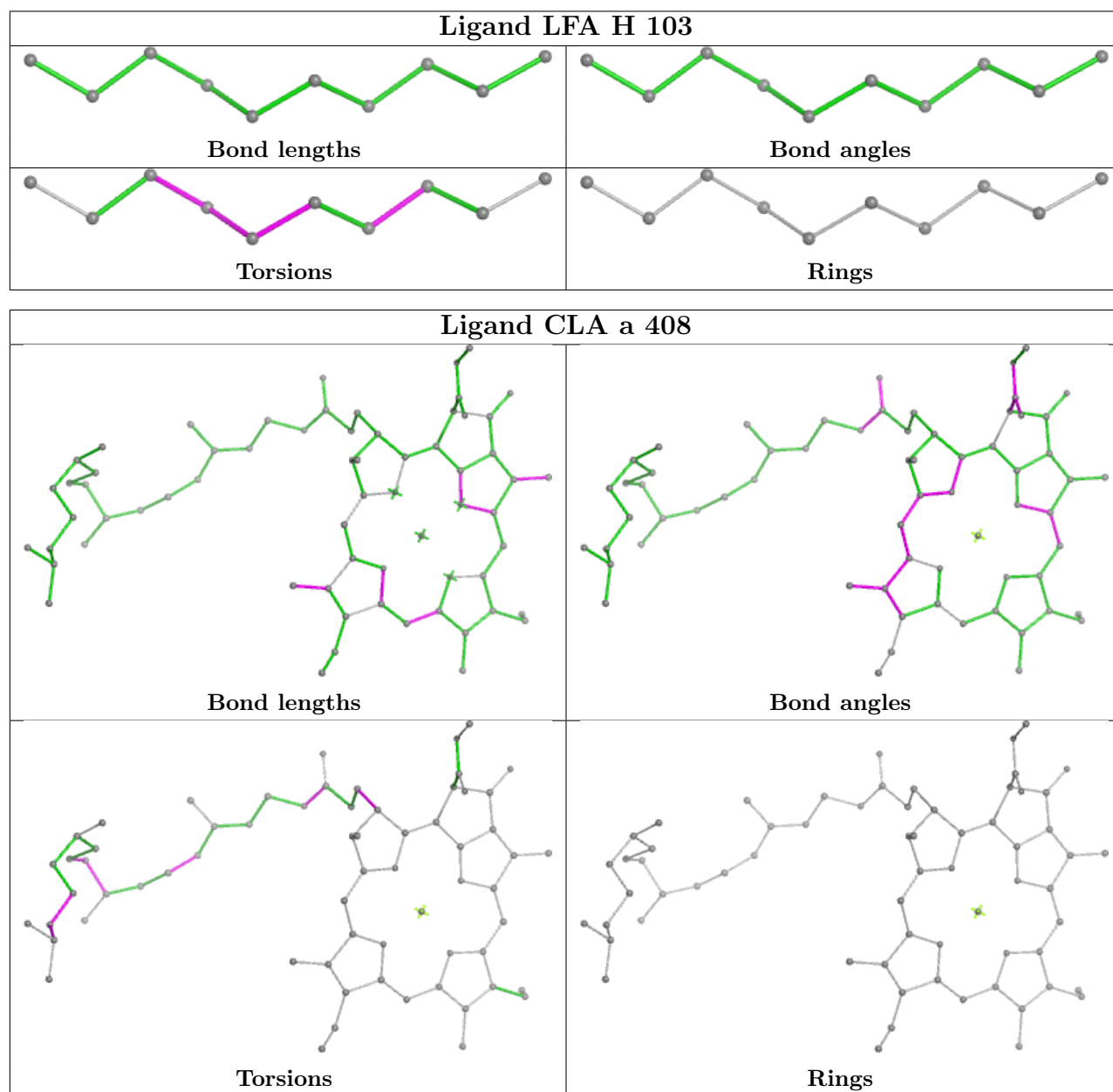
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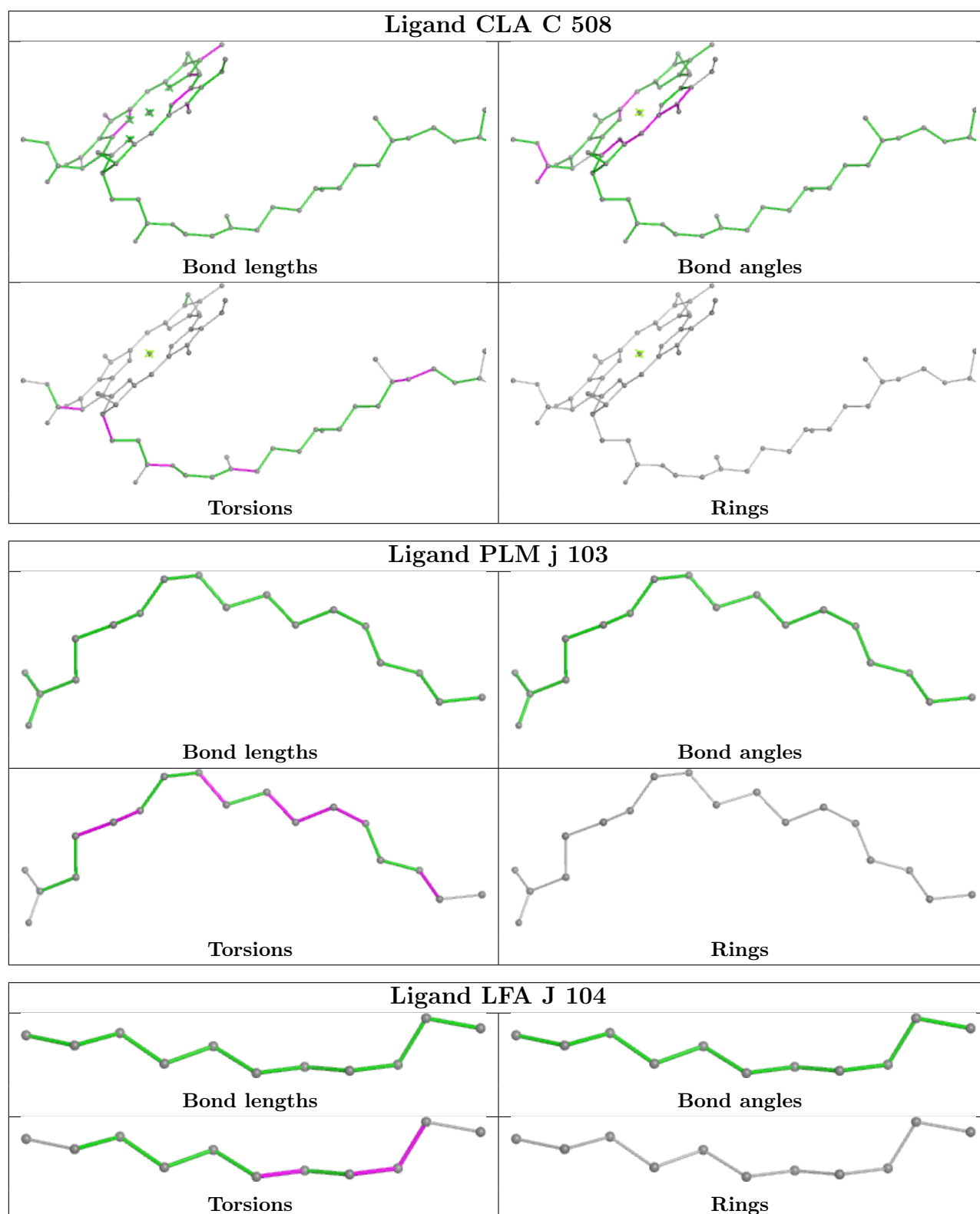
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B	625	PLM	2	0
31	L	101	LHG	4	0
22	c	518	CLA	2	0
22	C	506	CLA	1	0
31	a	421	LHG	2	0
34	c	504	DGD	2	0
22	B	604	CLA	4	0
24	b	619	BCR	3	0
22	C	511	CLA	4	0
24	B	632	BCR	5	0
22	b	610	CLA	3	0
23	a	420	PHO	2	0
24	F	101	BCR	1	0
25	D	404	PL9	4	0
22	d	401	CLA	1	0
33	m	102	LMT	1	0
22	C	514	CLA	4	0
35	Y	101	LMG	2	0
22	C	505	CLA	6	0
24	b	602	BCR	5	0
22	c	506	CLA	5	0
35	y	101	LMG	1	0
22	c	517	CLA	1	0
34	J	102	DGD	3	0
22	c	512	CLA	2	0
22	b	604	CLA	1	0
27	A	413	PLM	2	0
22	C	507	CLA	3	0
22	b	615	CLA	3	0
22	c	507	CLA	2	0
25	A	409	PL9	3	0
26	b	601	SQD	2	0
33	M	102	LMT	1	0
22	C	515	CLA	2	0
24	b	620	BCR	2	0
31	A	417	LHG	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

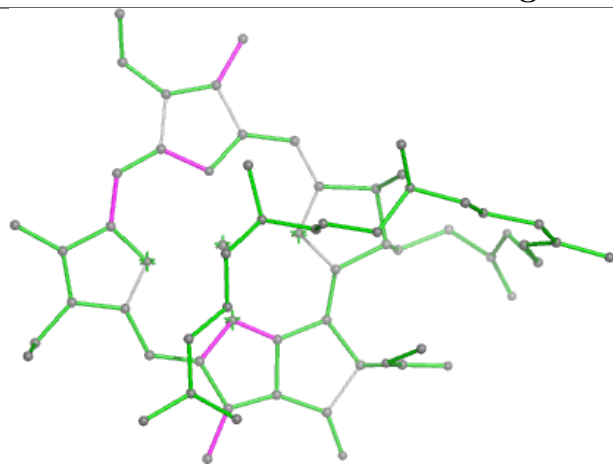
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.



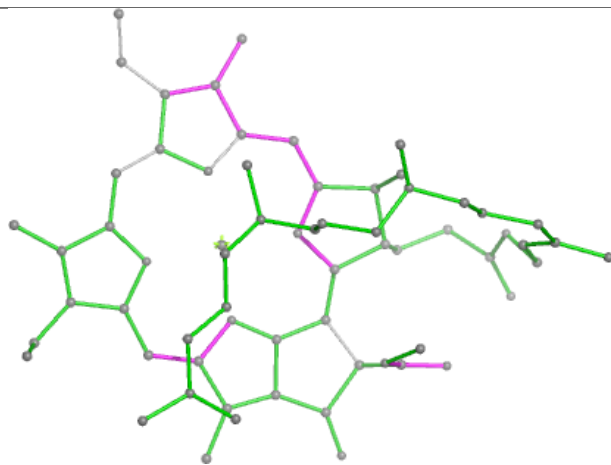




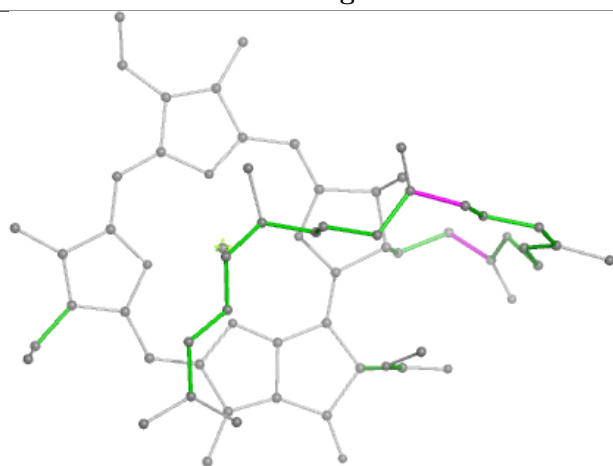
## Ligand CLA c 515



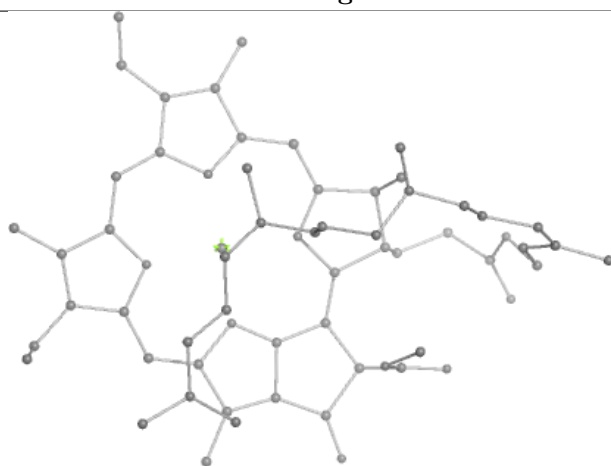
Bond lengths



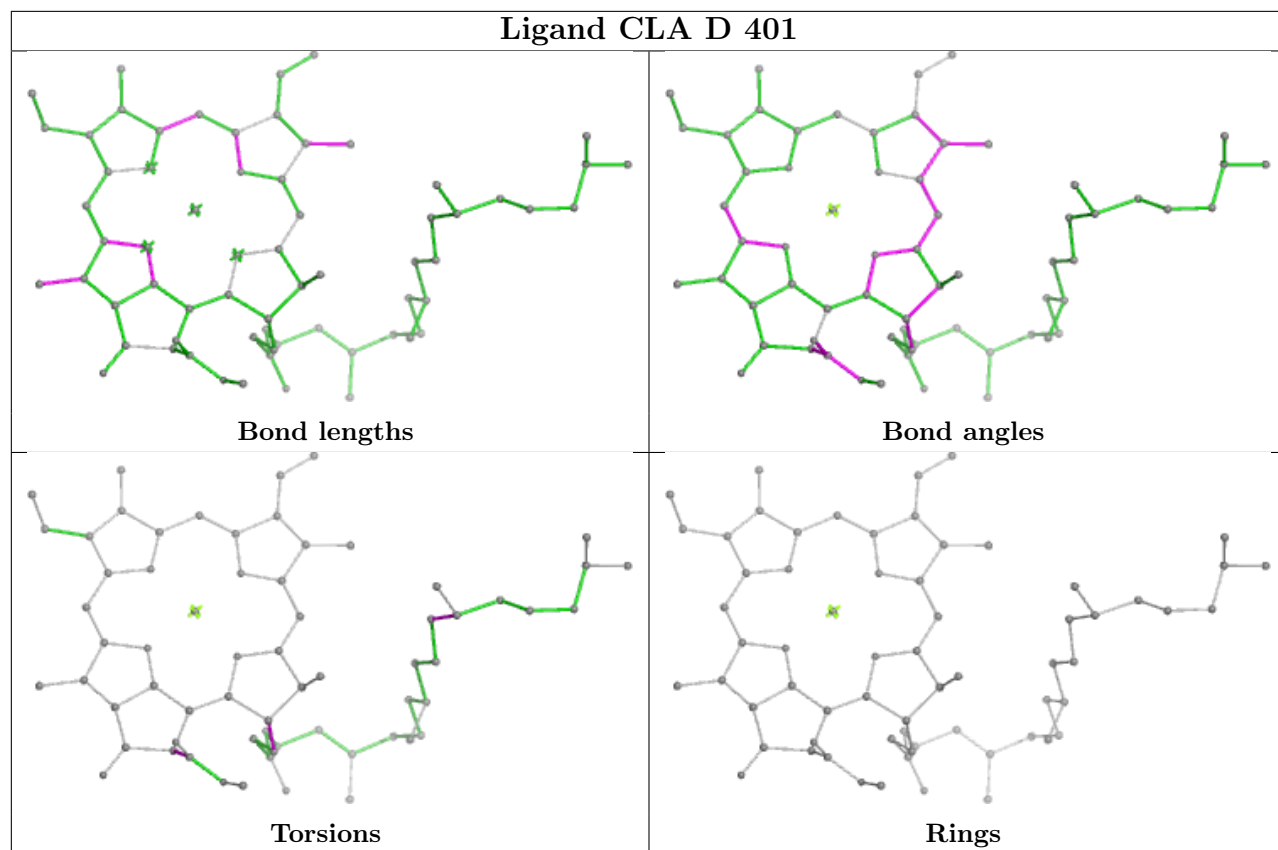
Bond angles

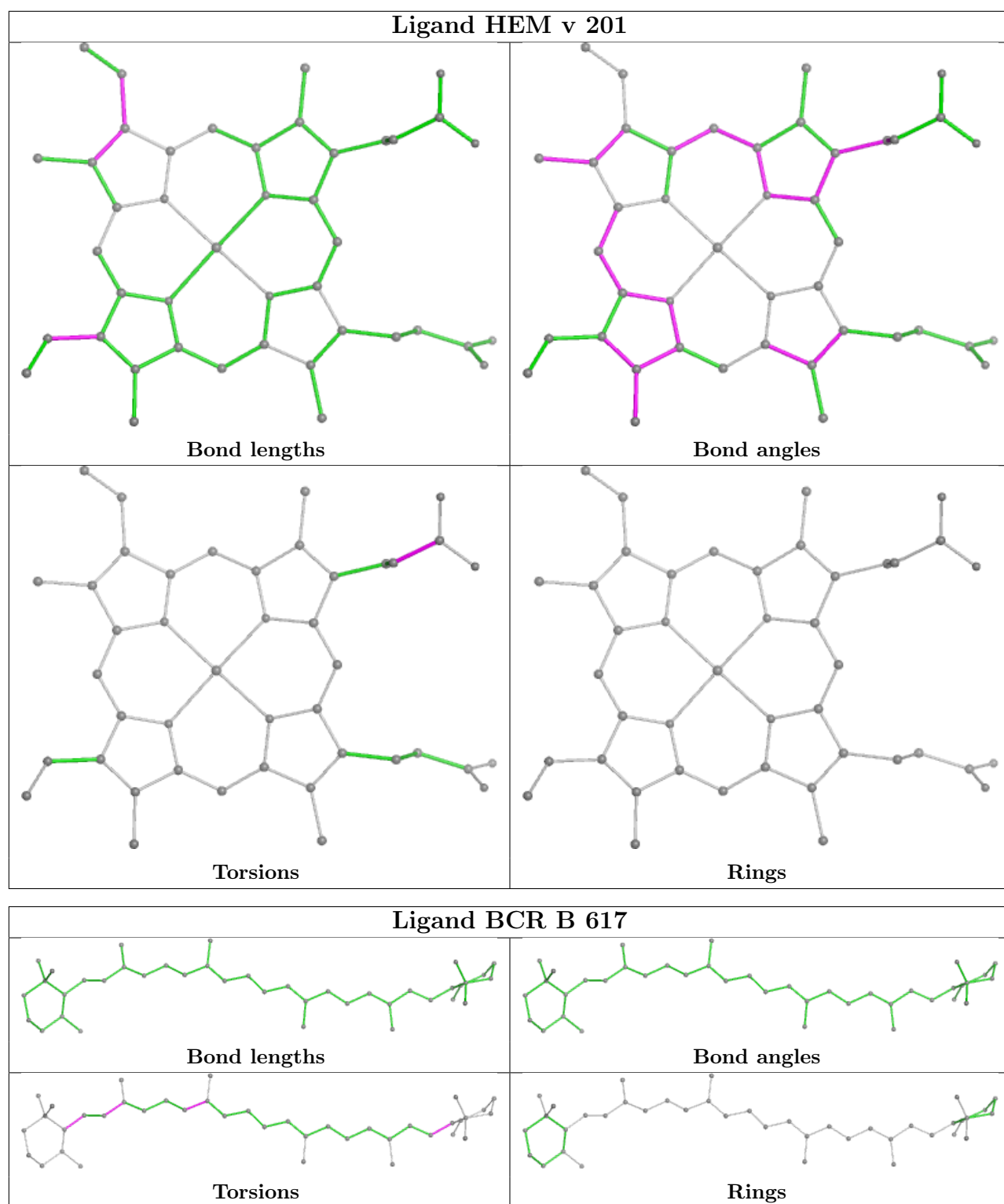


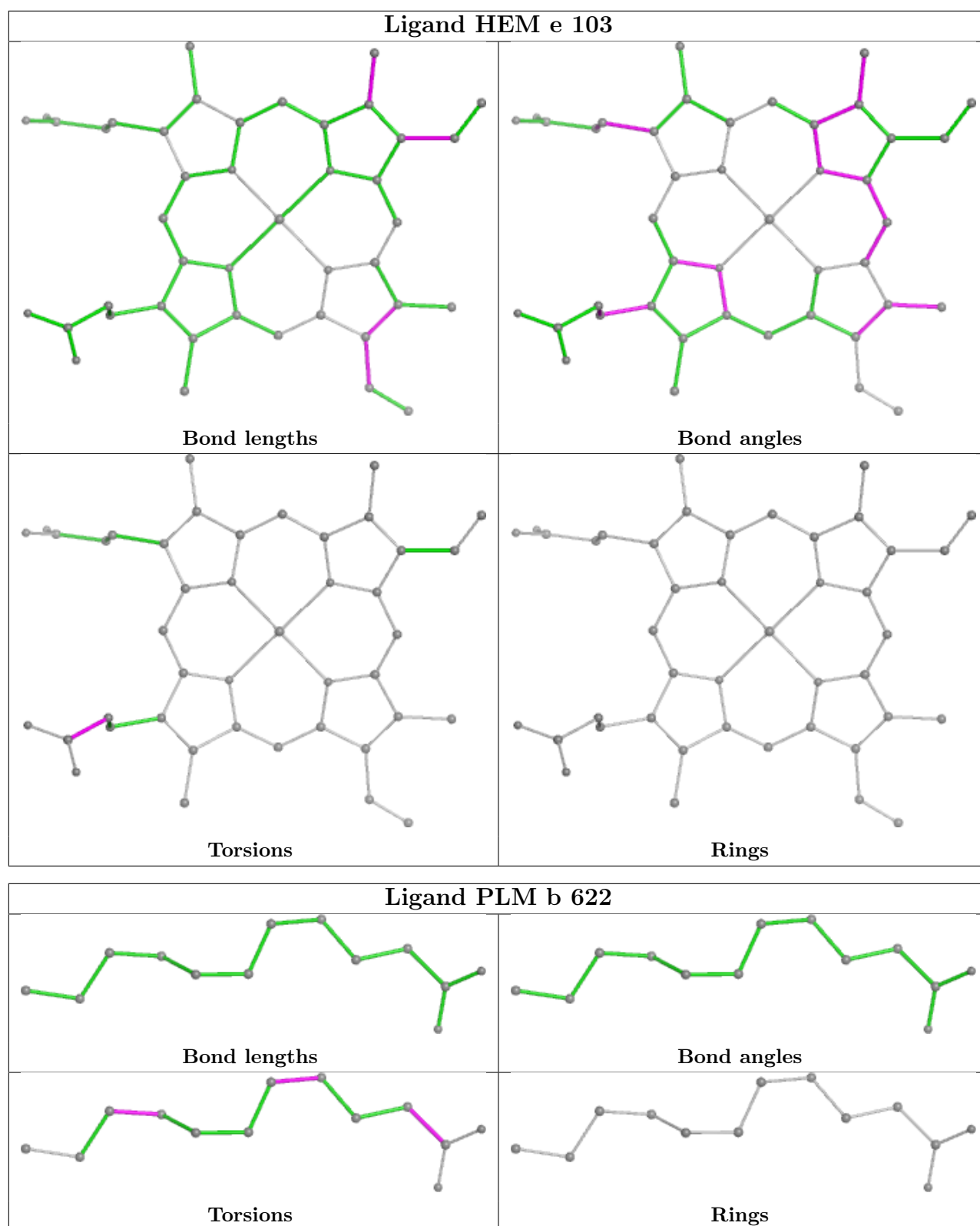
Torsions

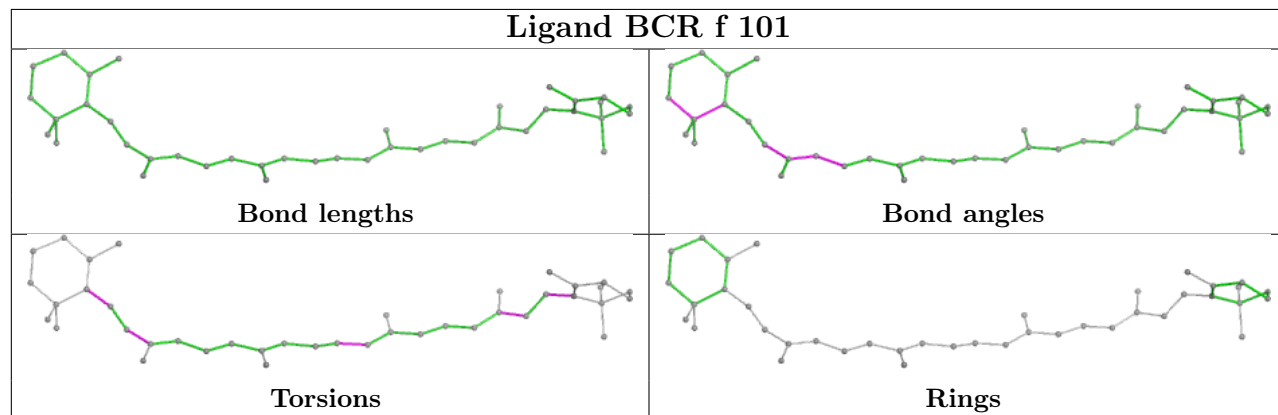
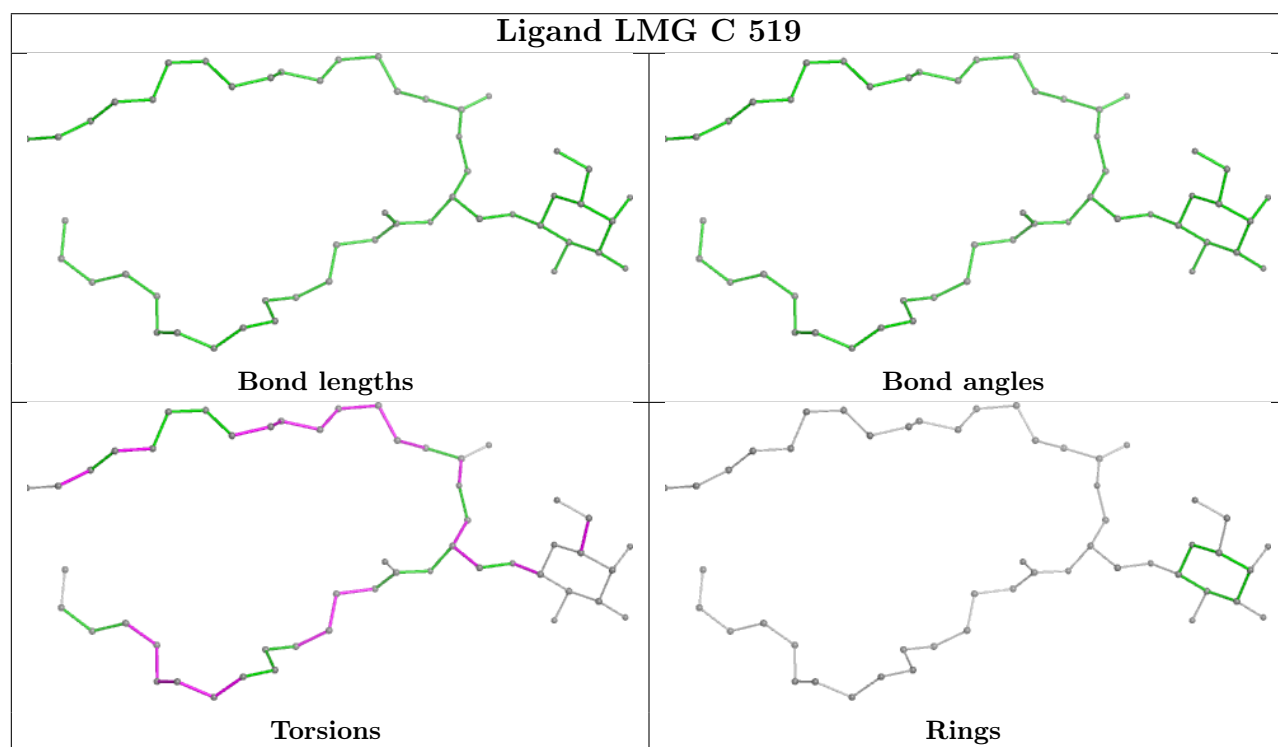
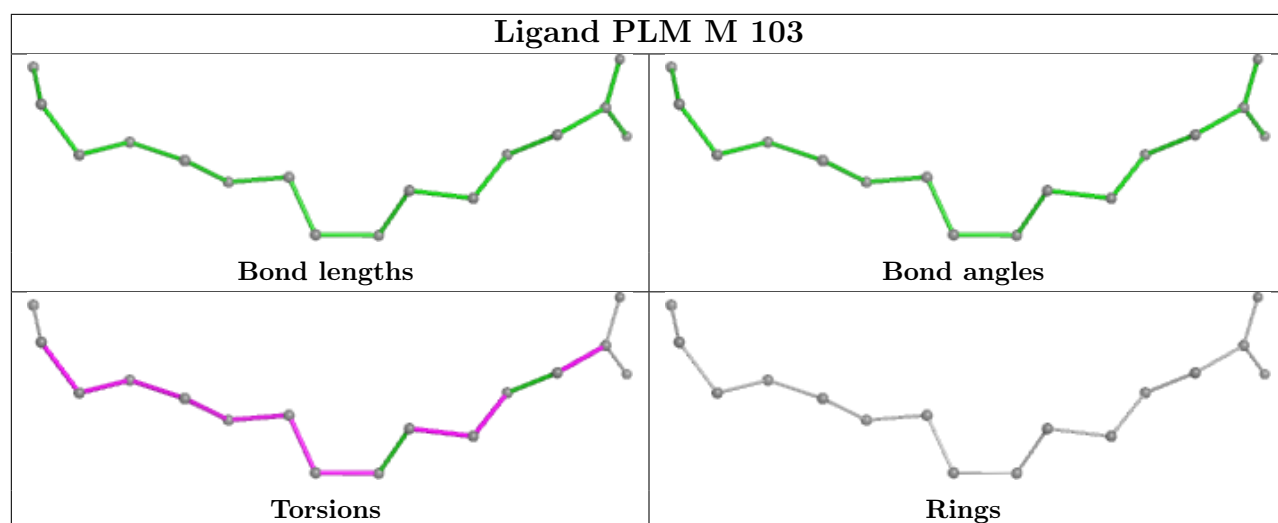


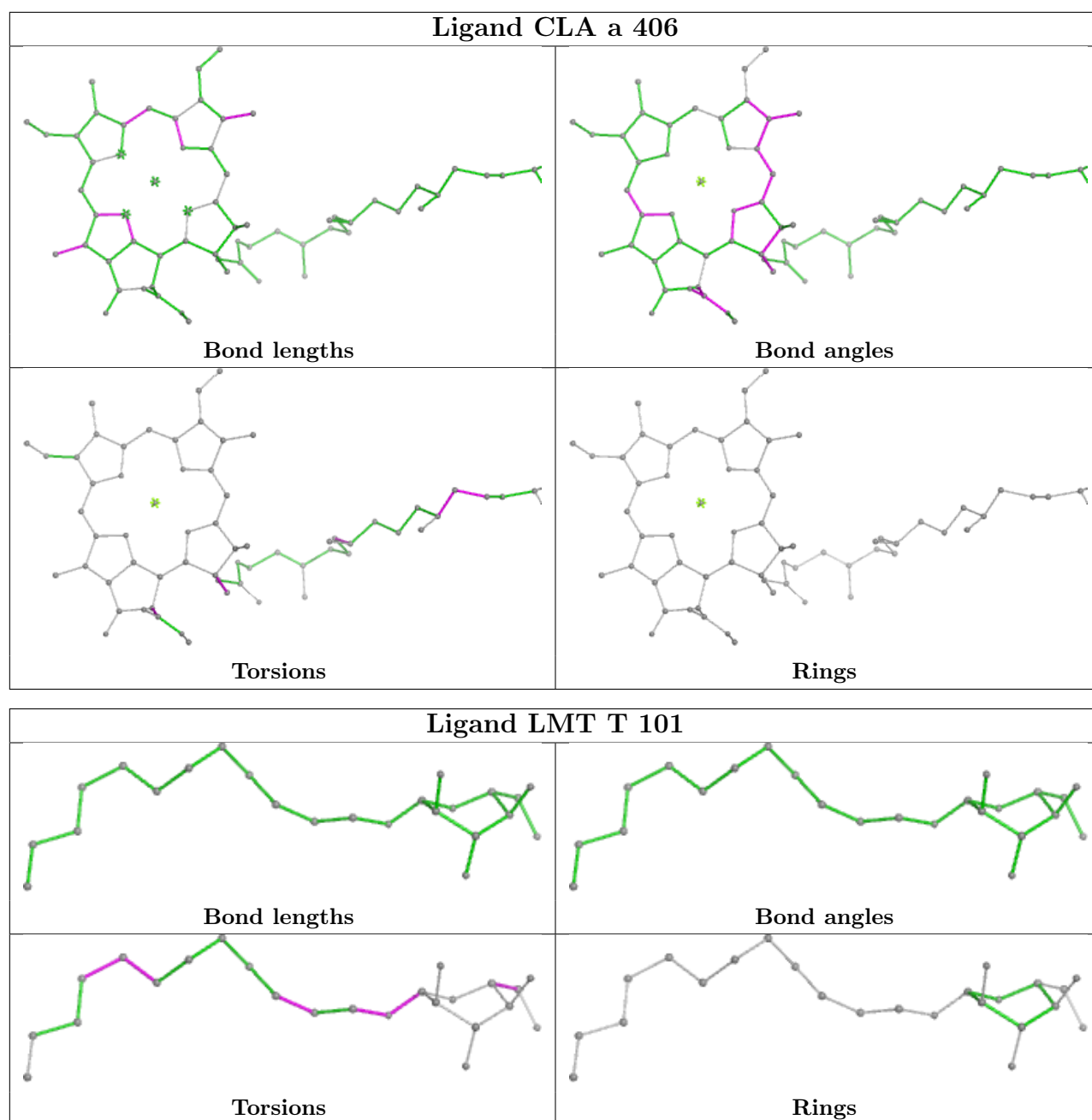
Rings

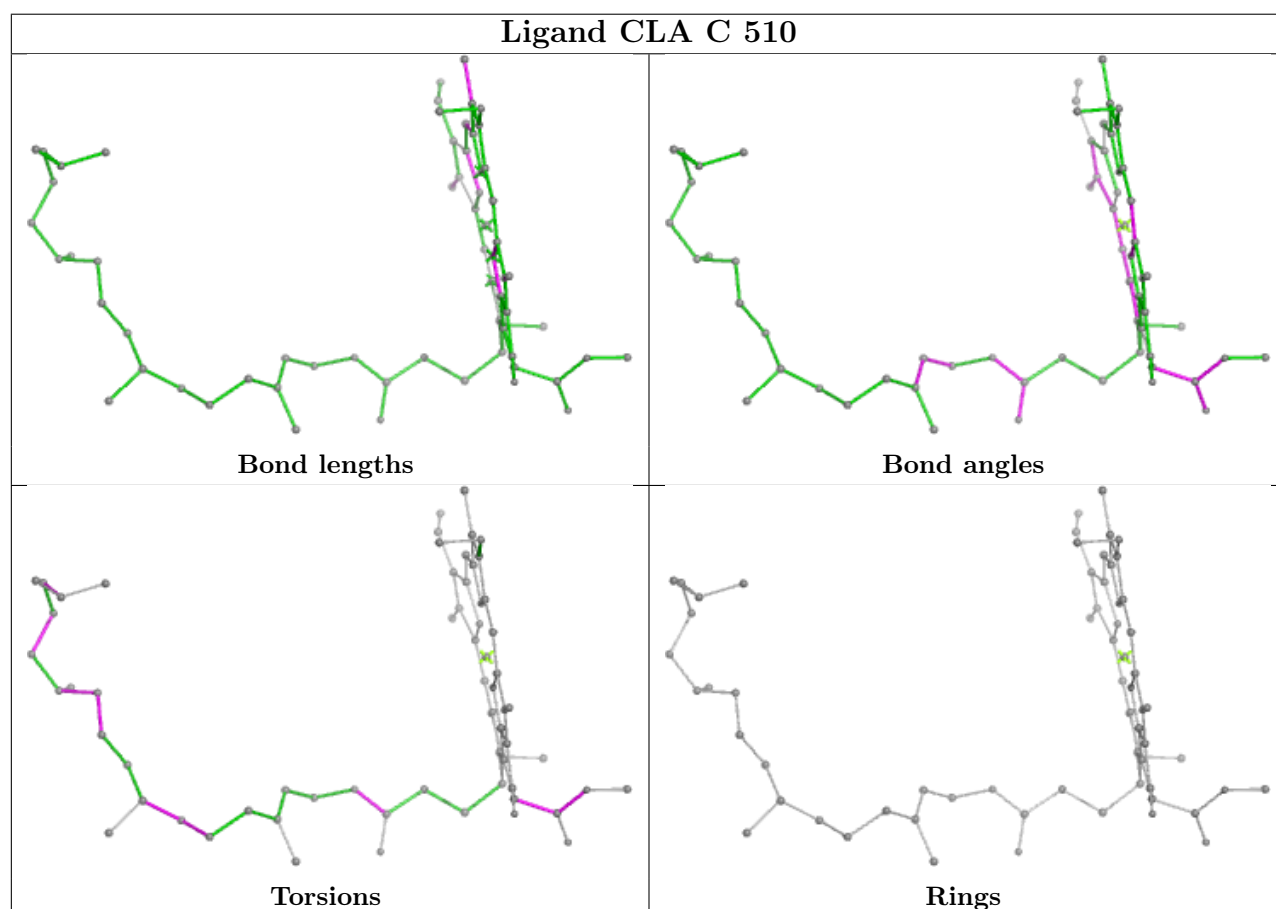
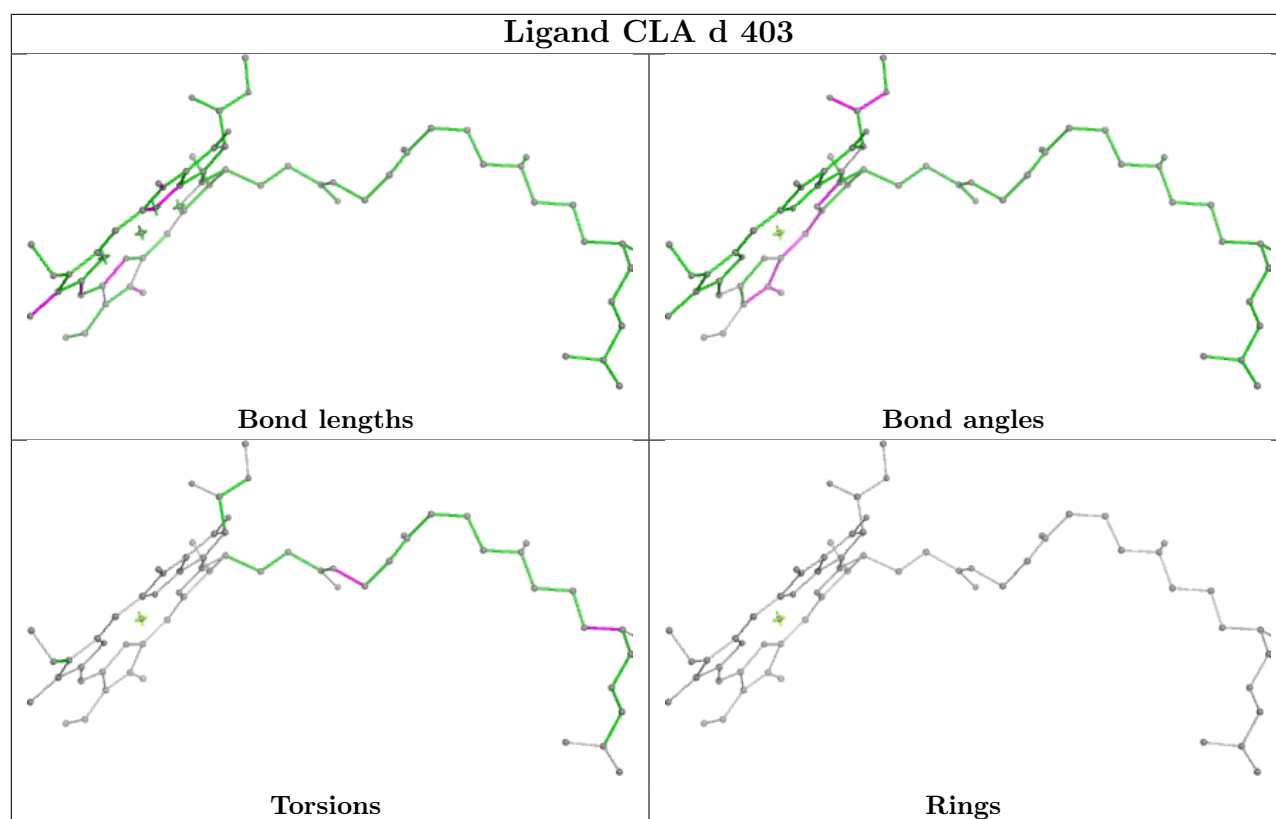




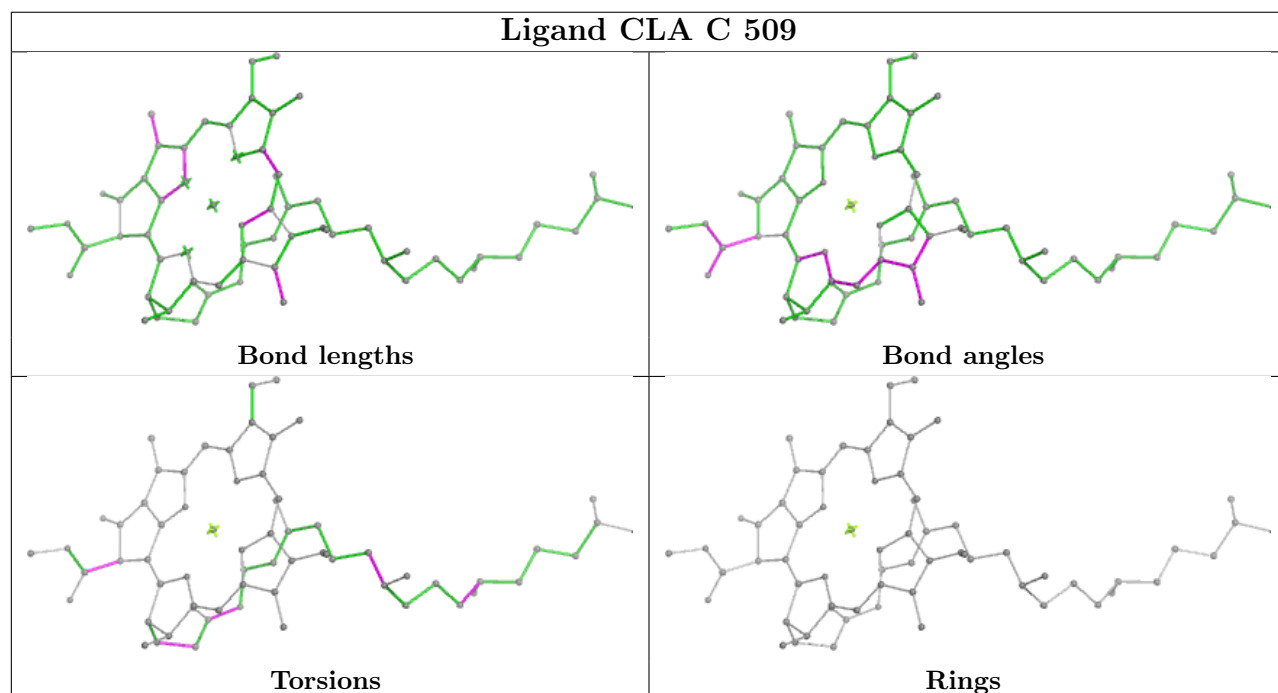
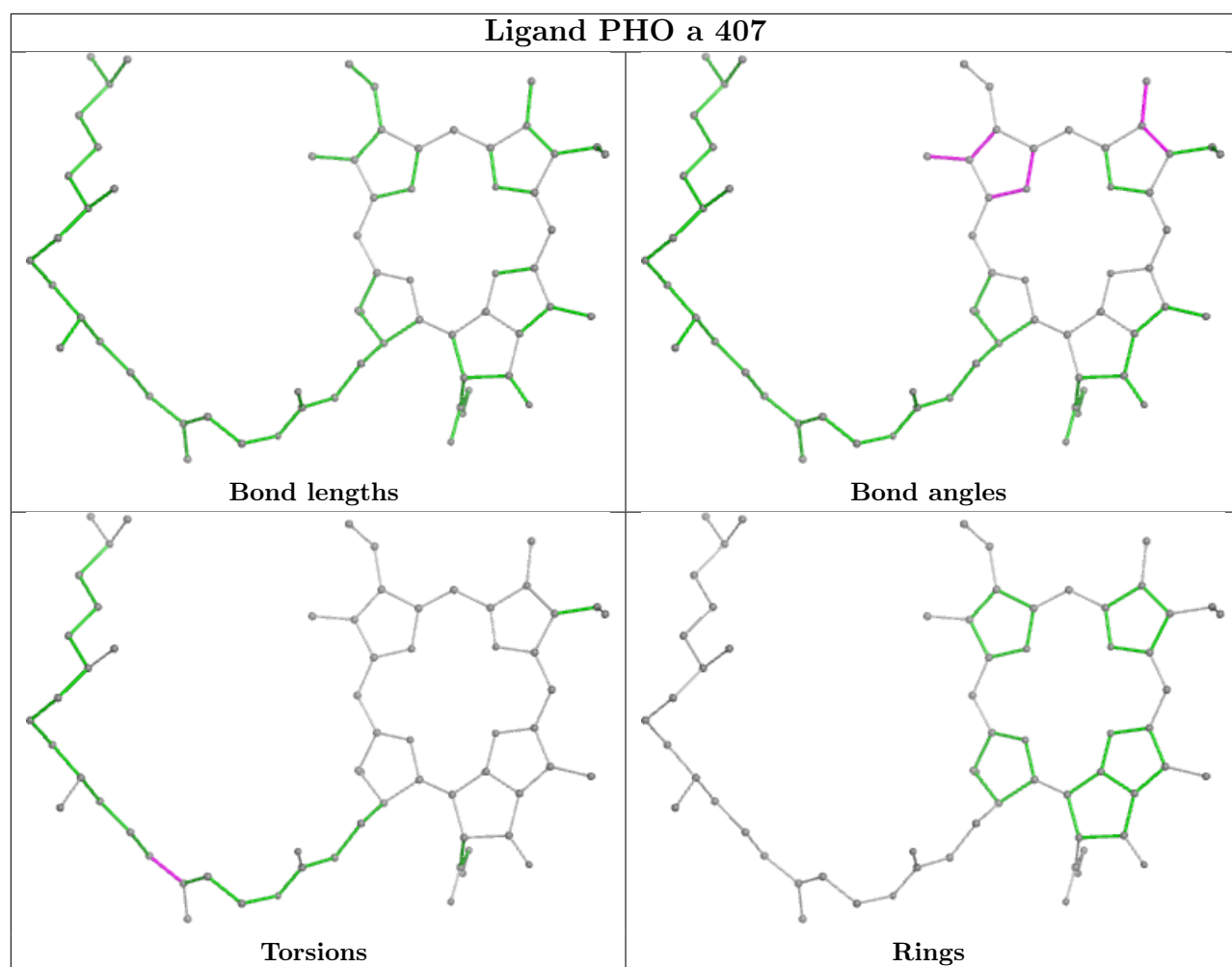


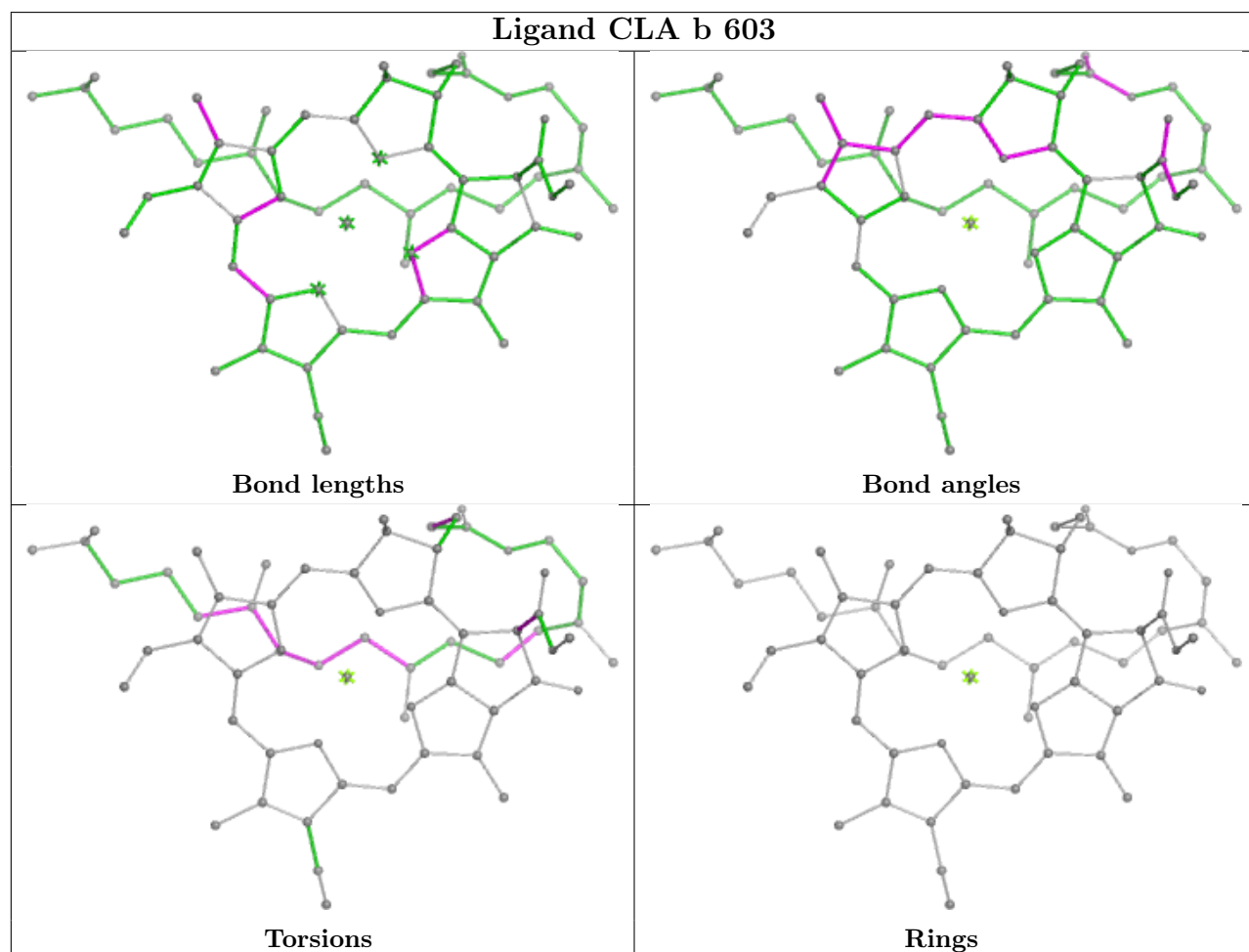
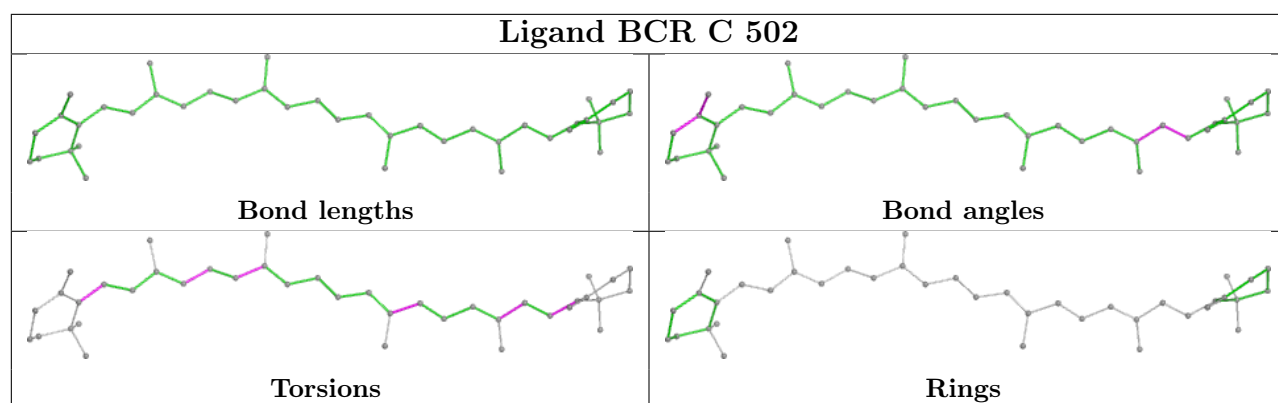


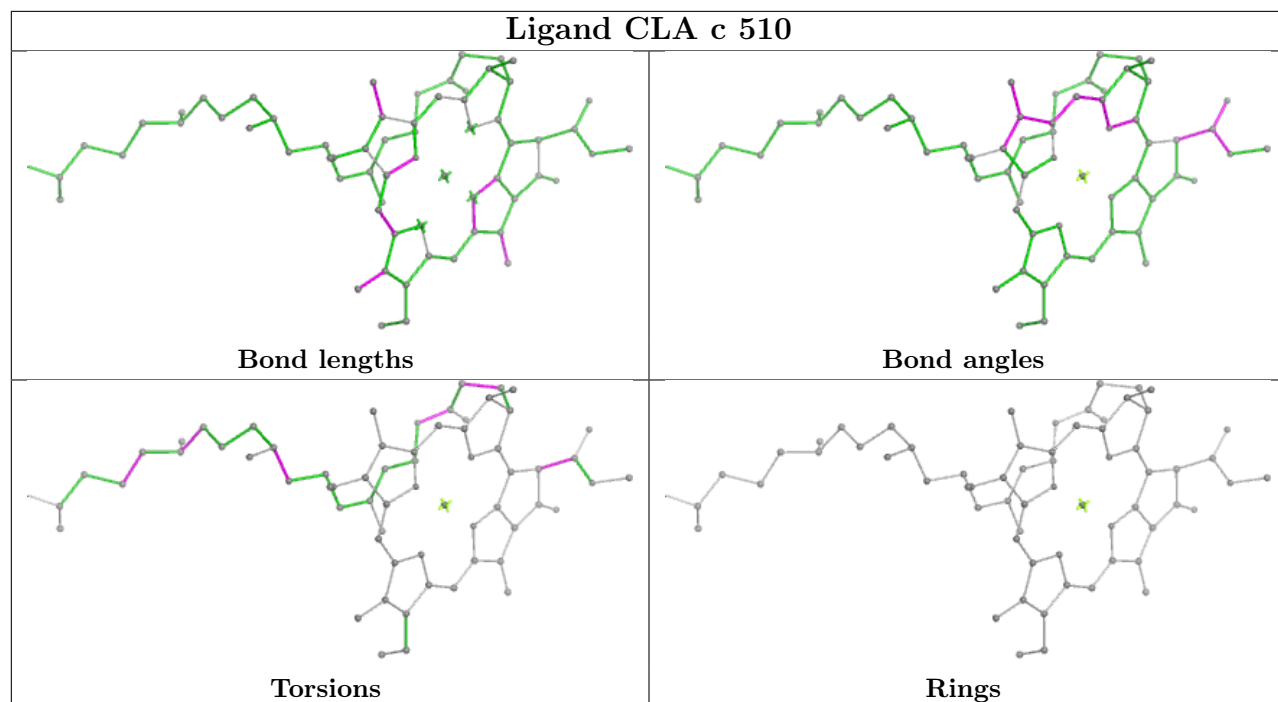
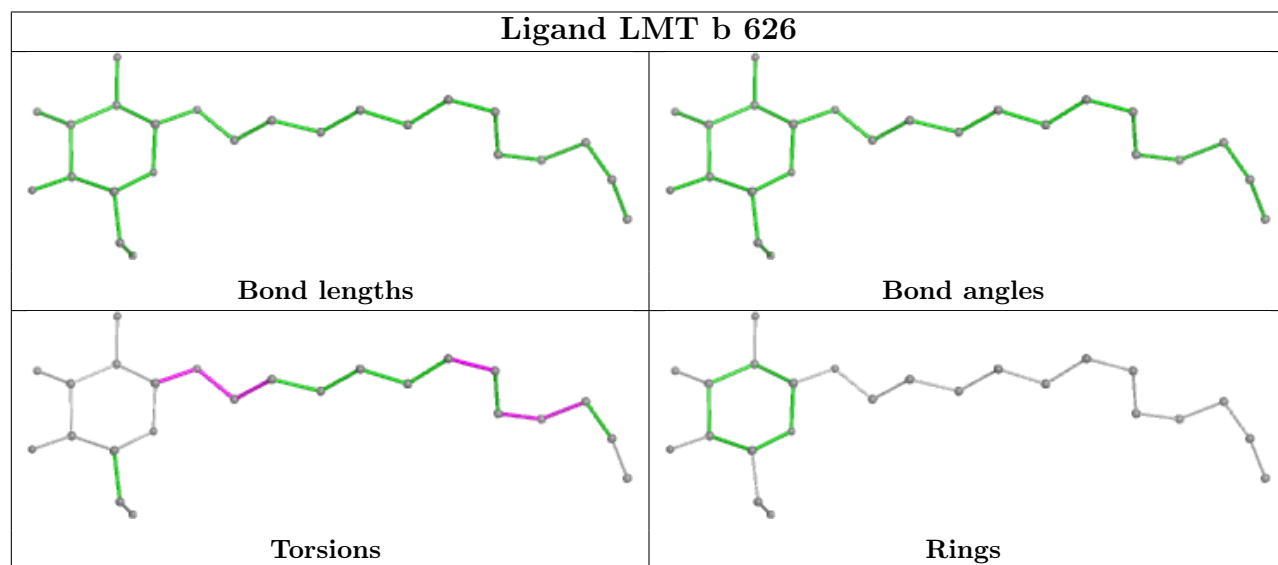


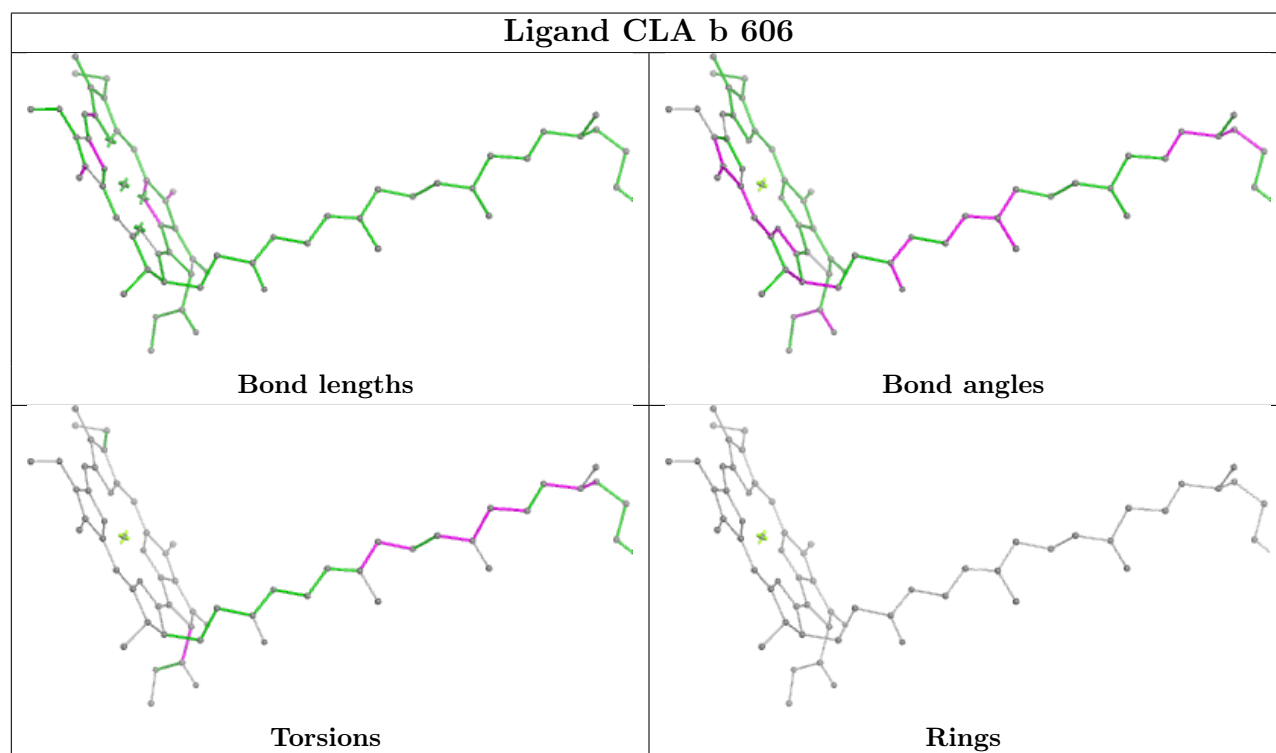
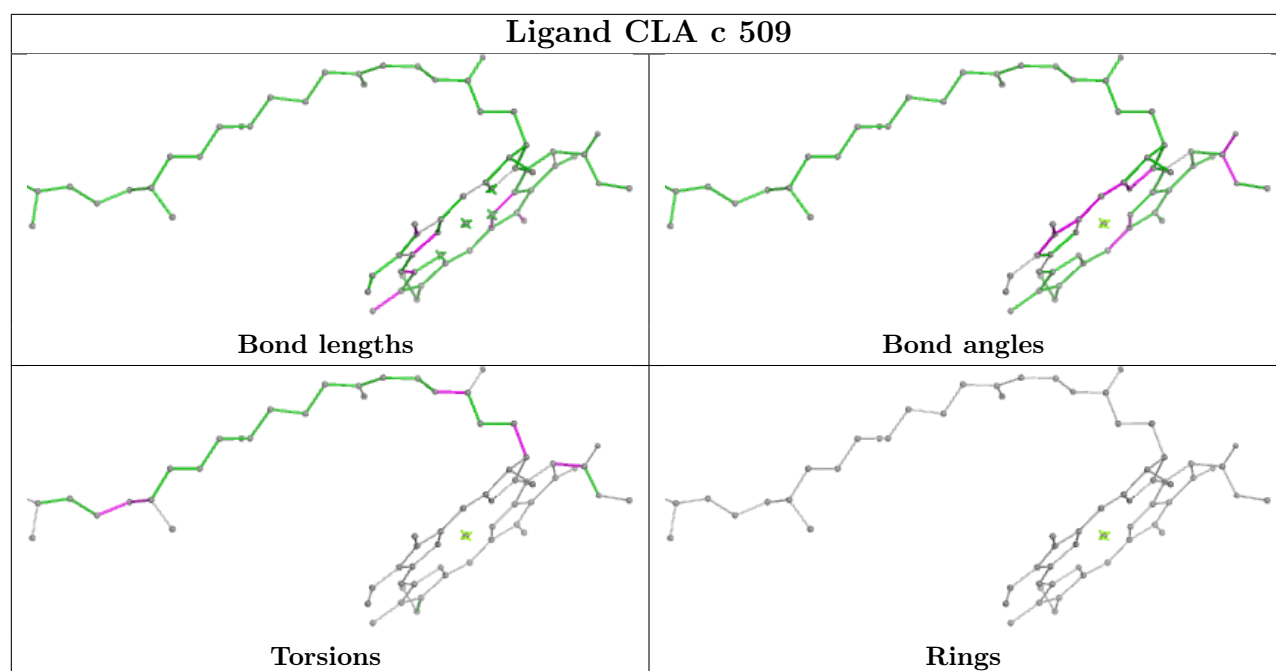


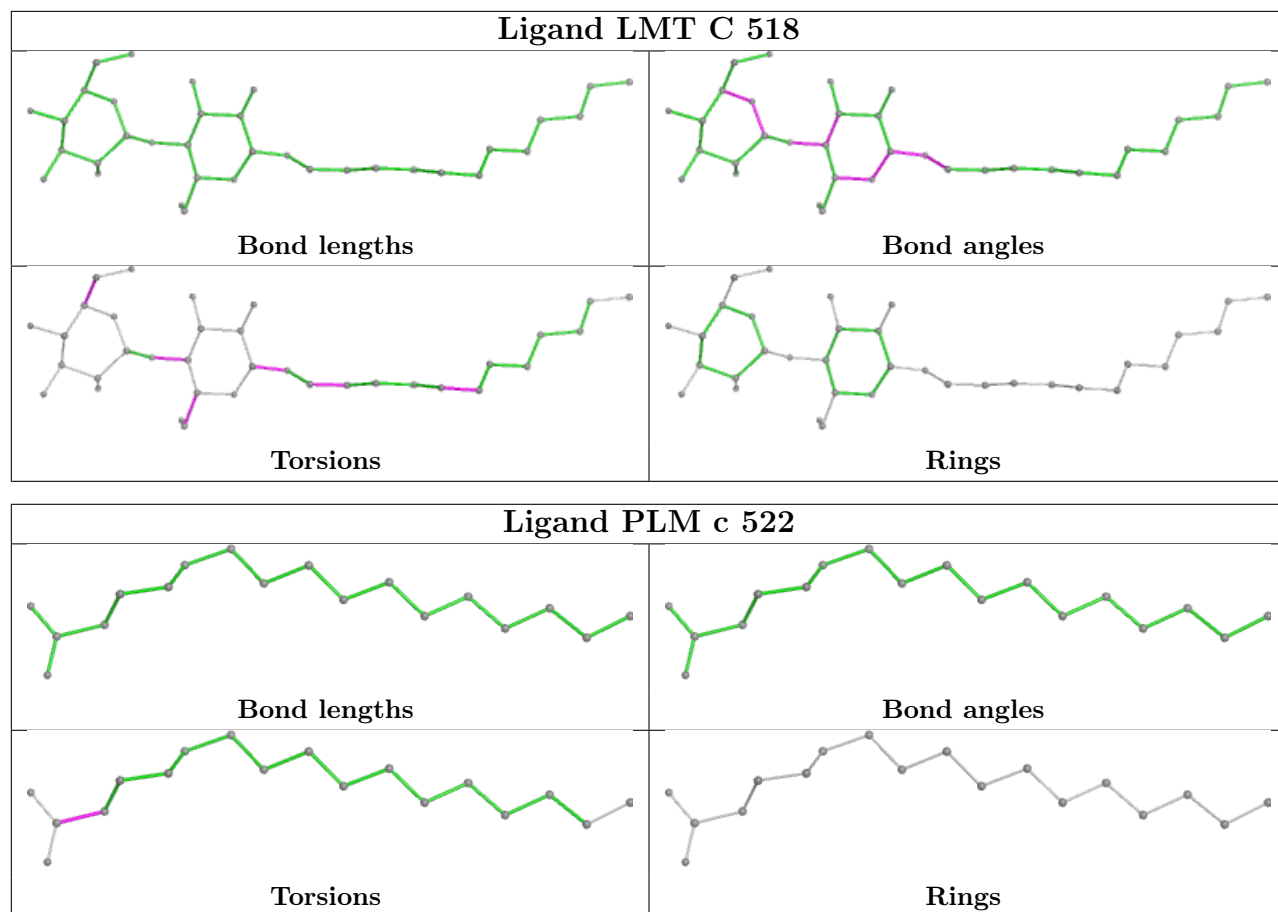


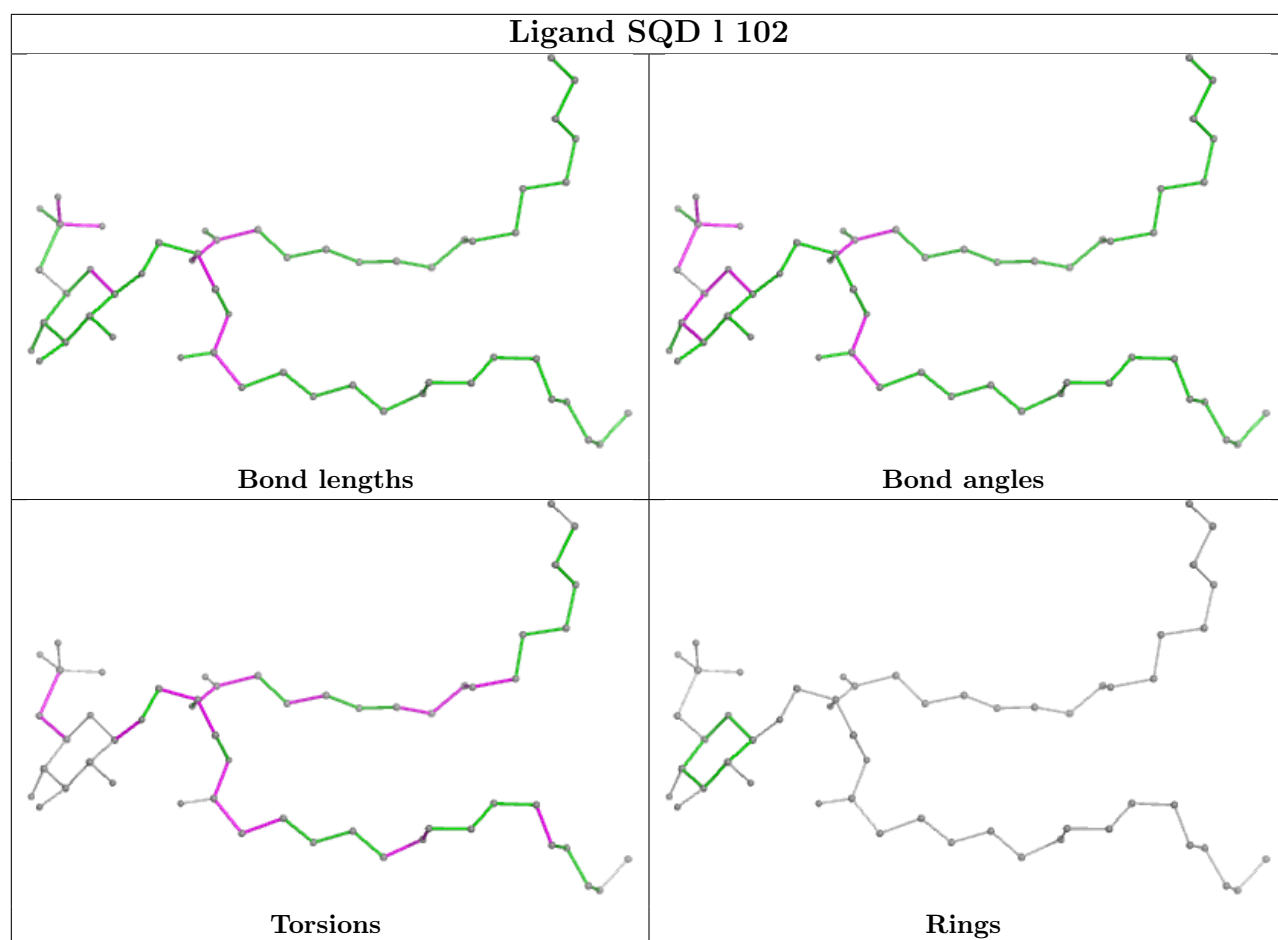




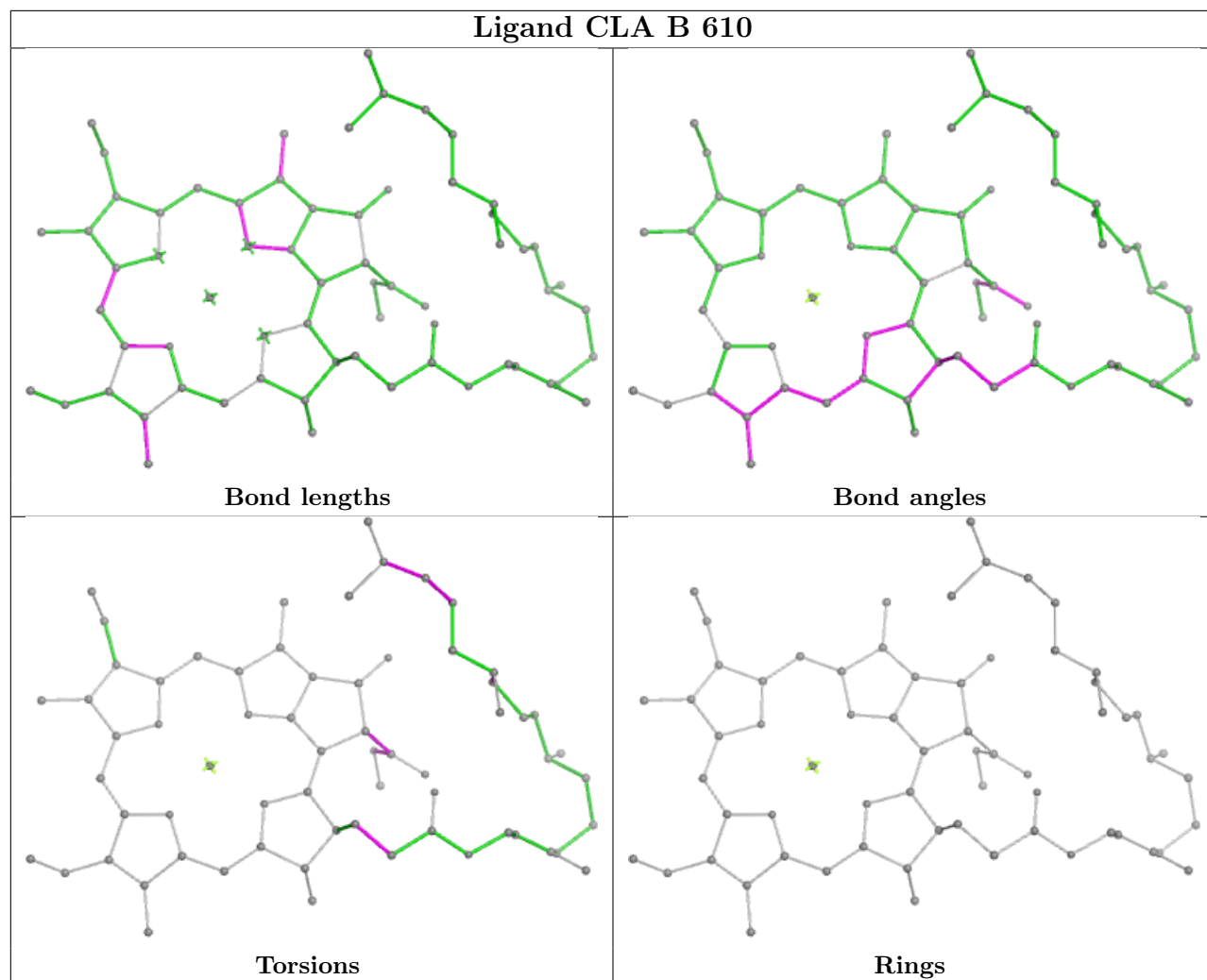
**Ligand CLA c 510****Ligand LMT b 626**

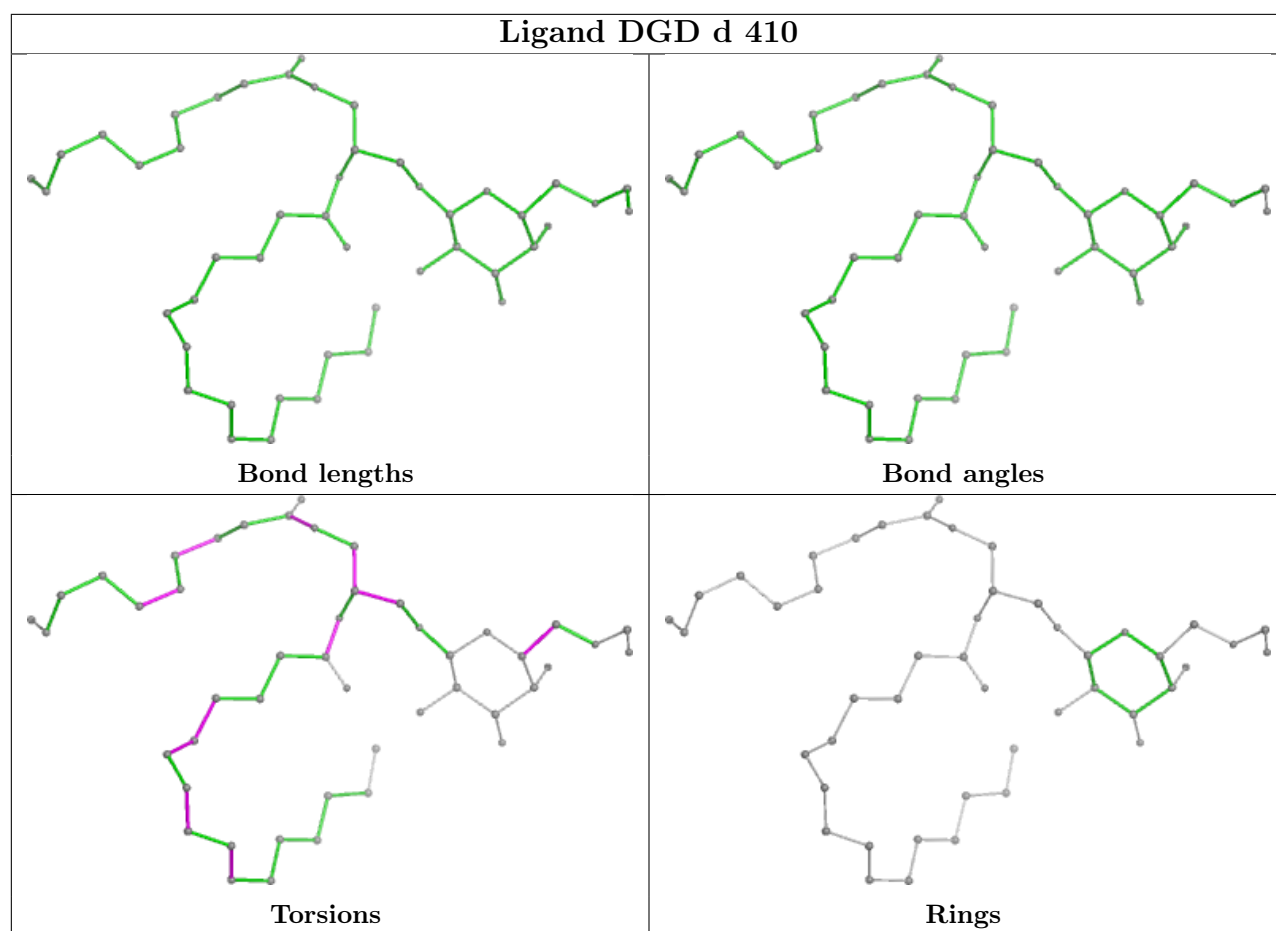




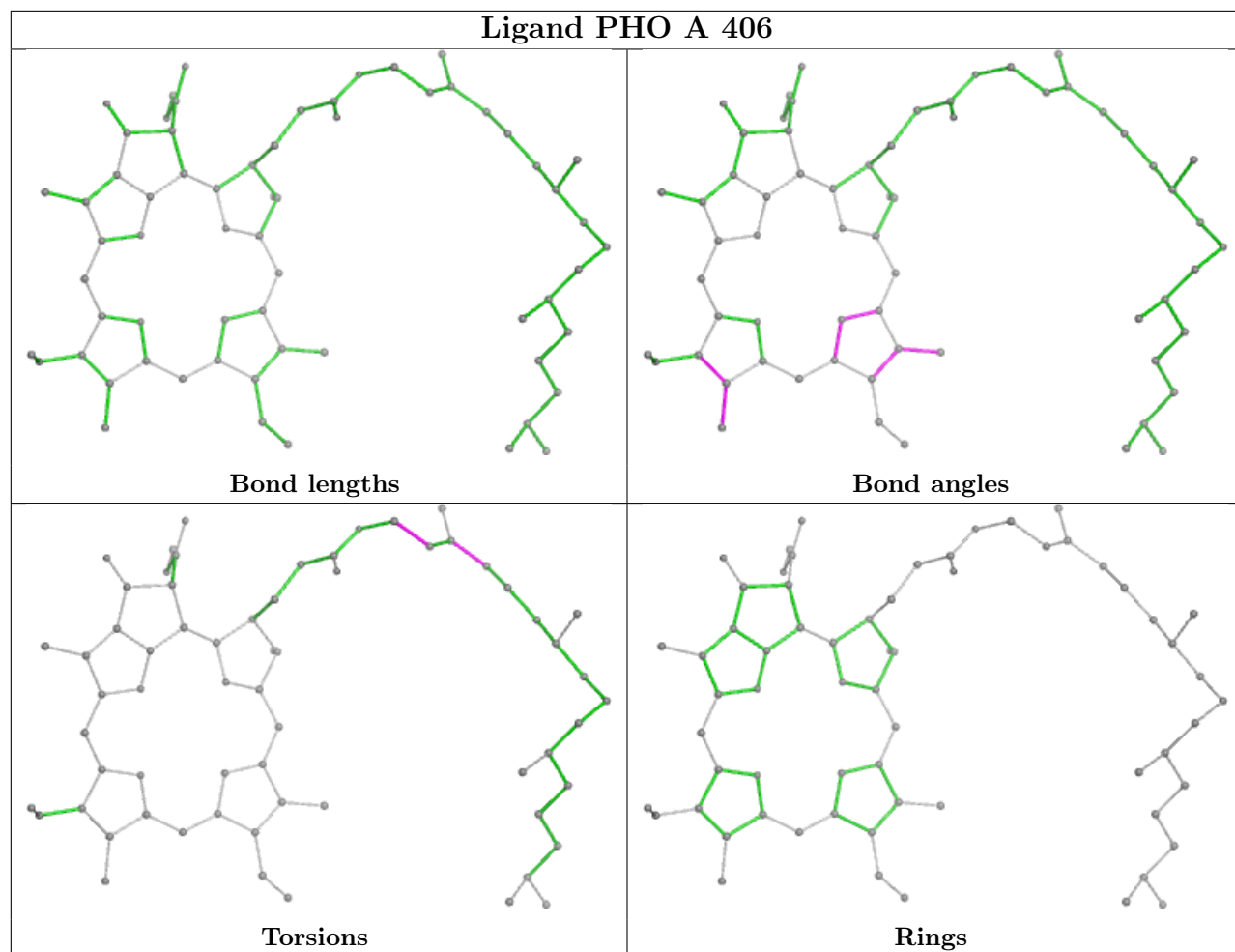


## Ligand CLA B 610

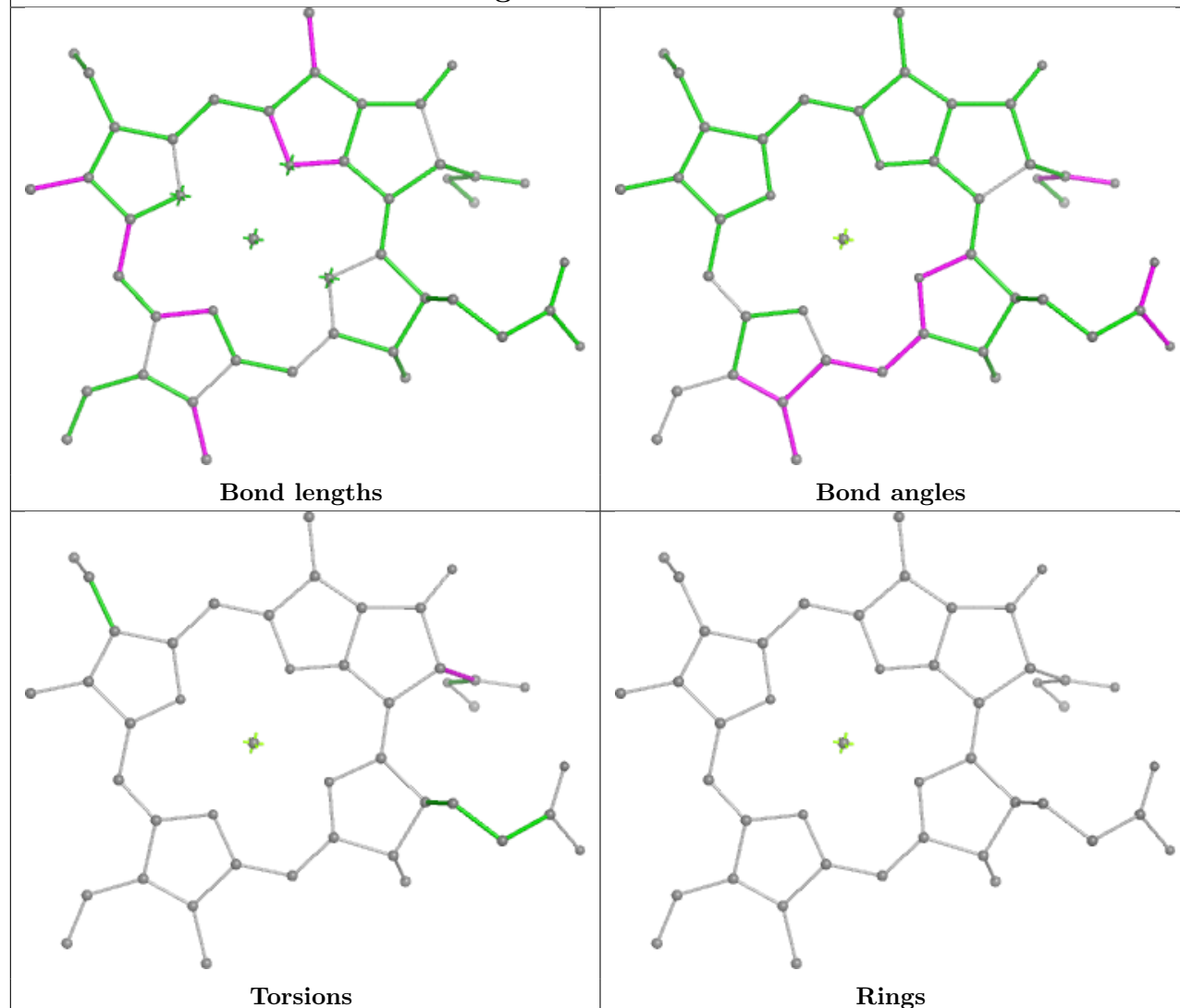




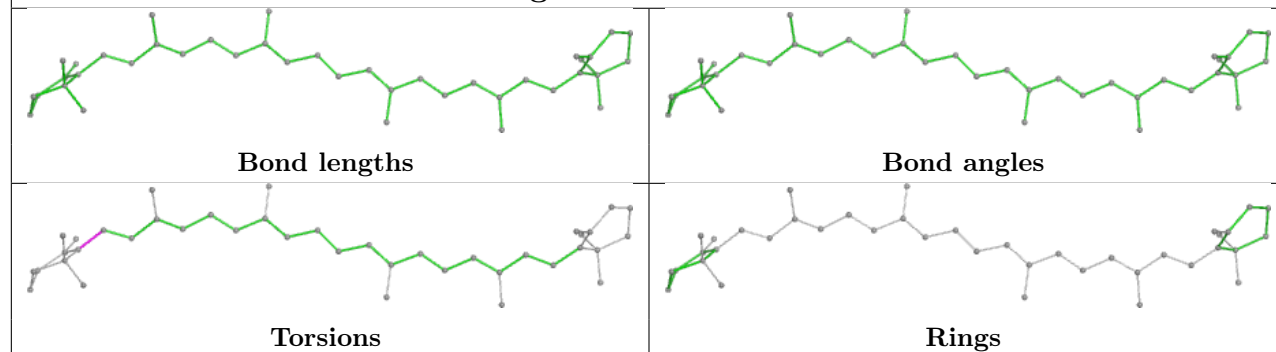


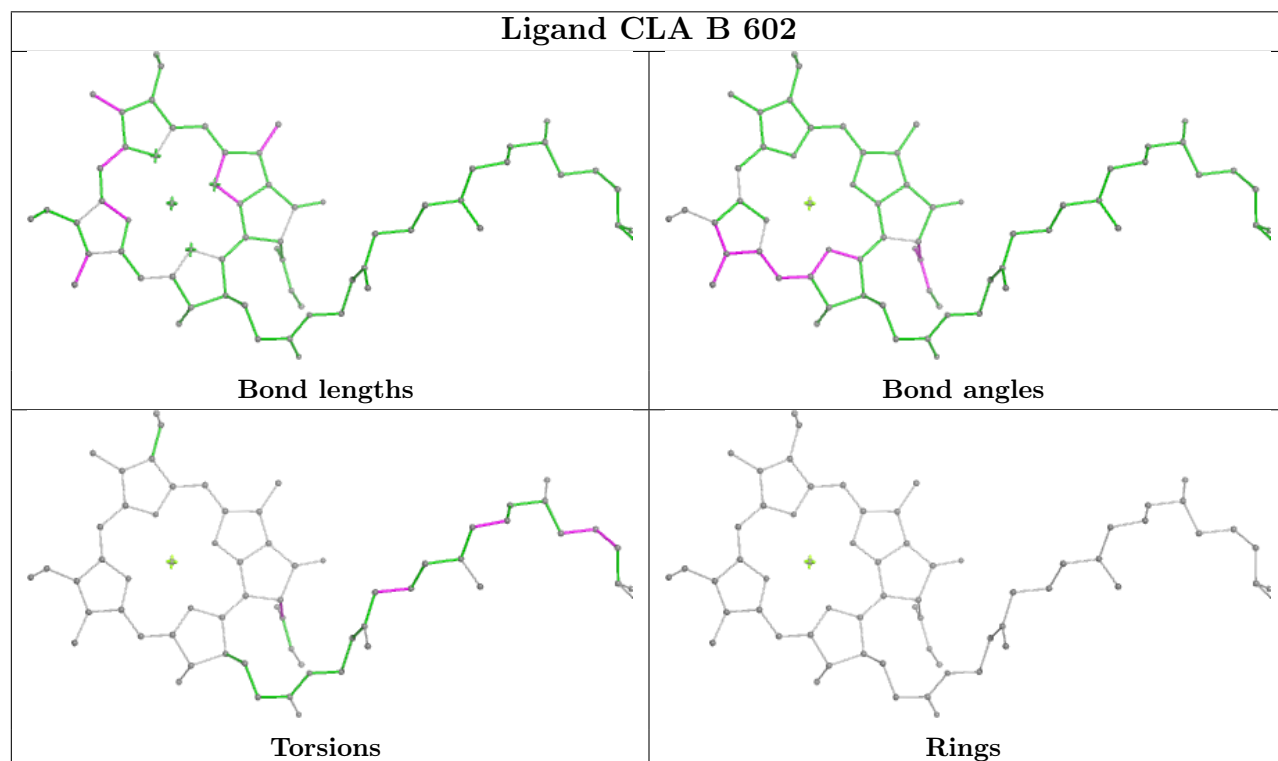
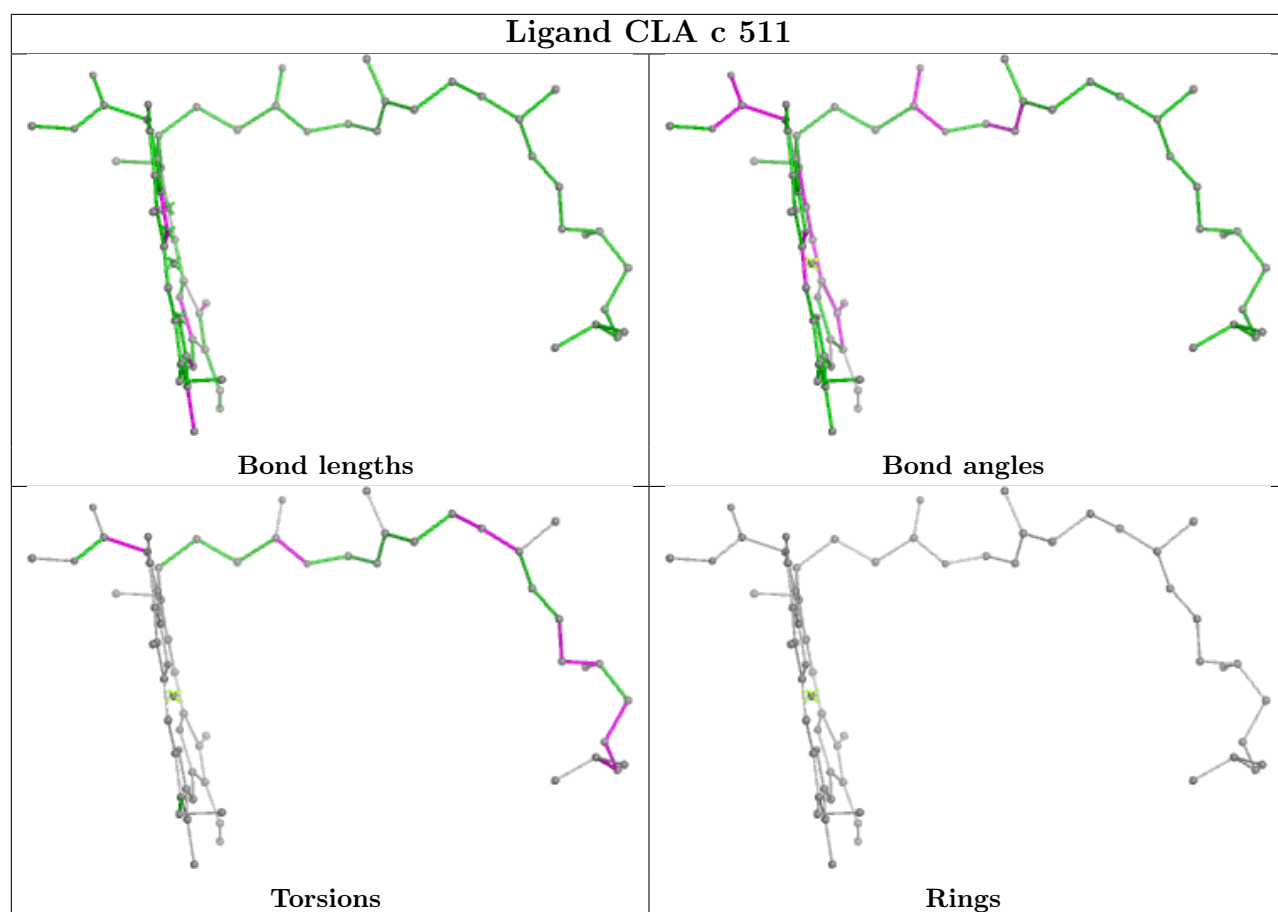


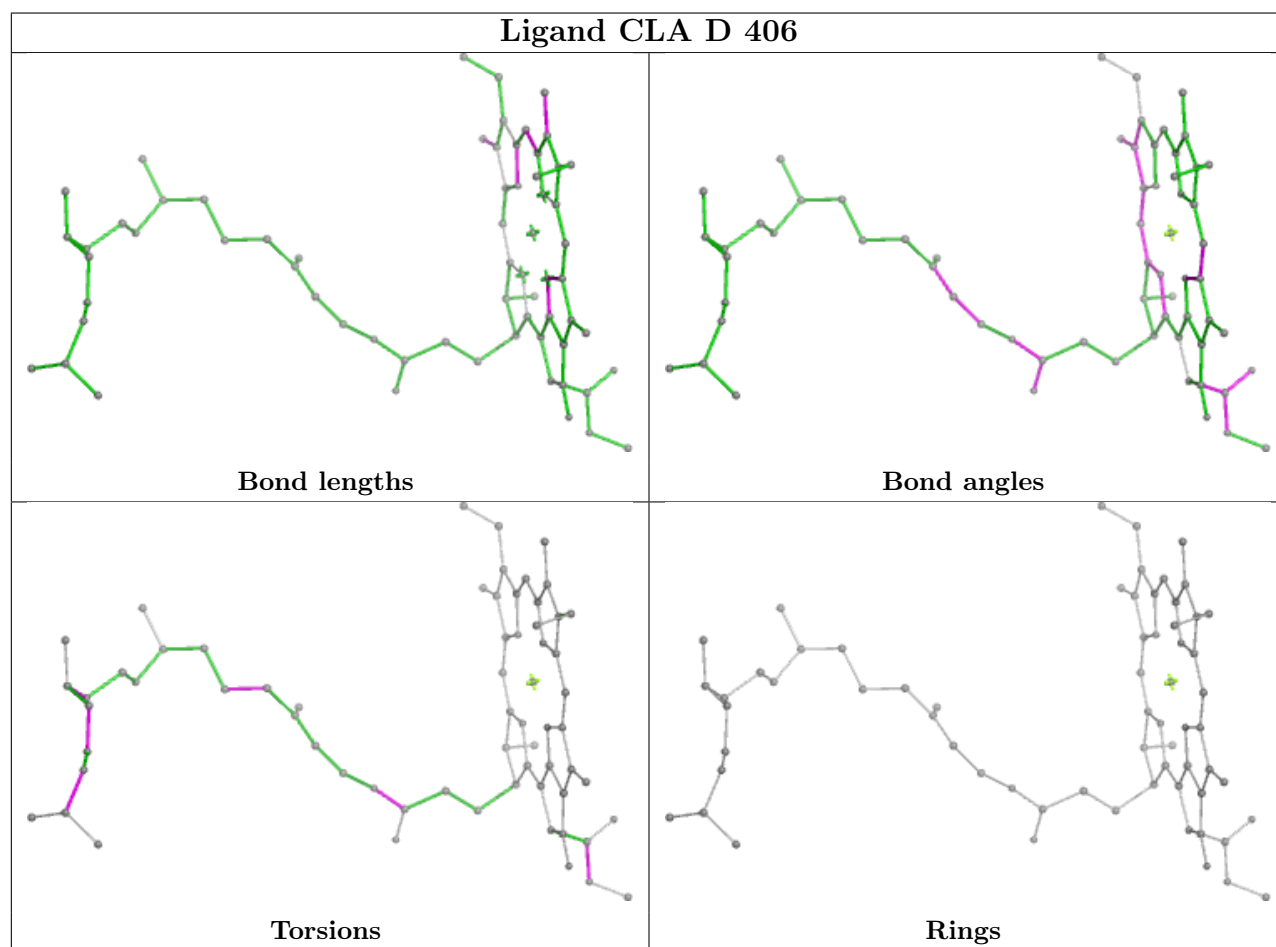
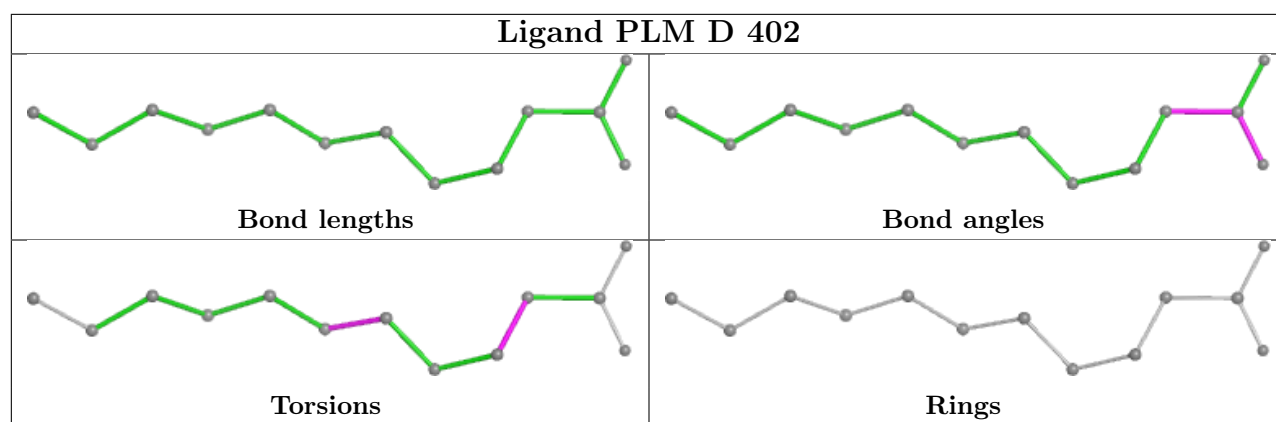
## Ligand CLA b 618

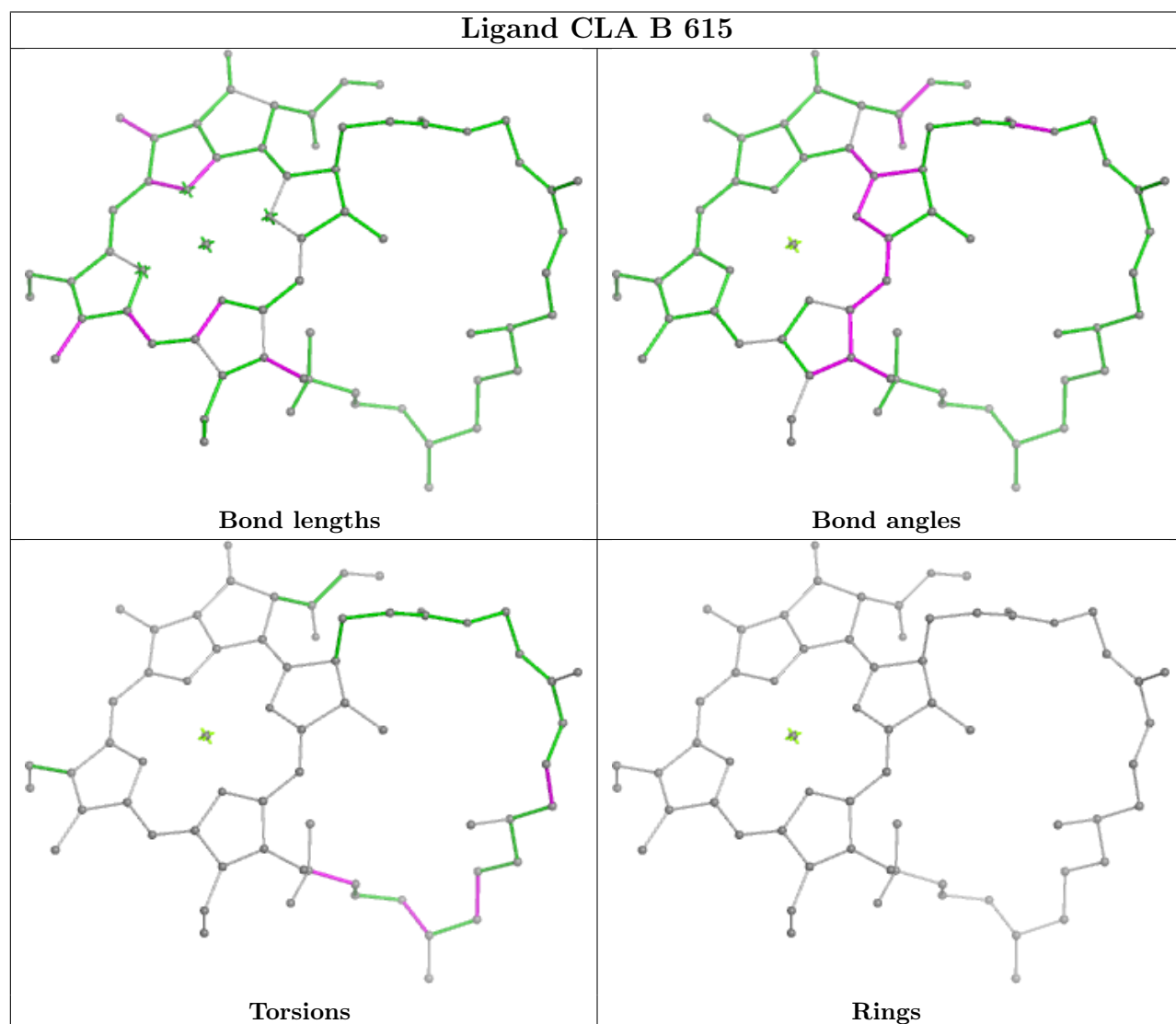
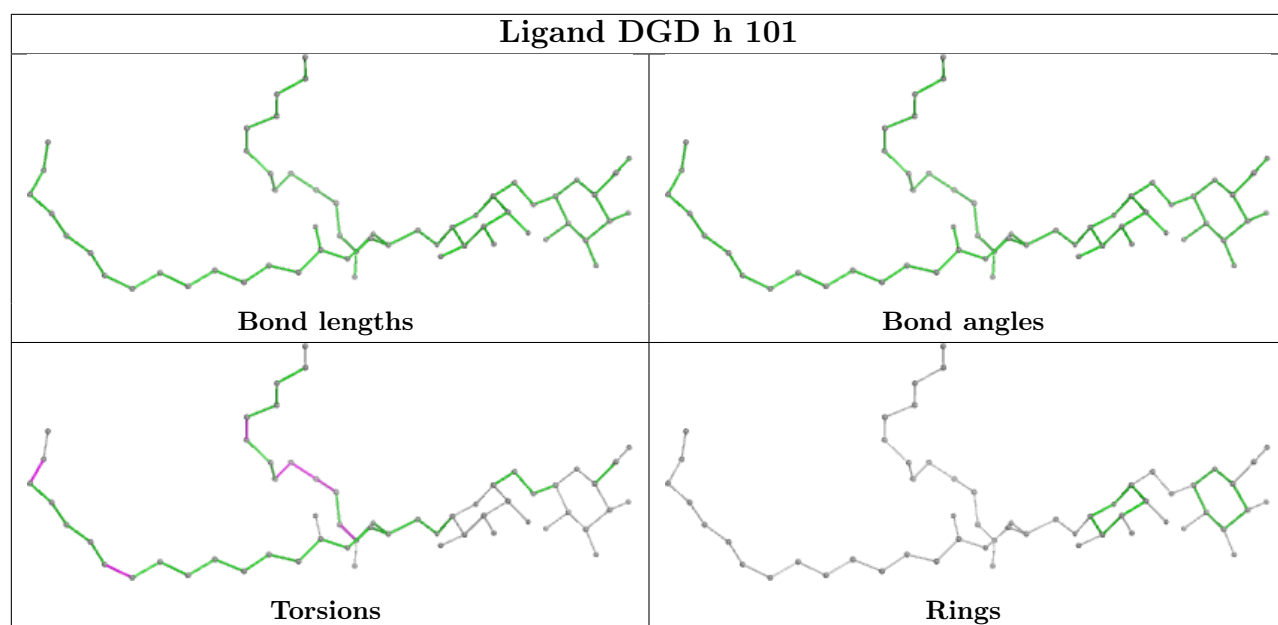


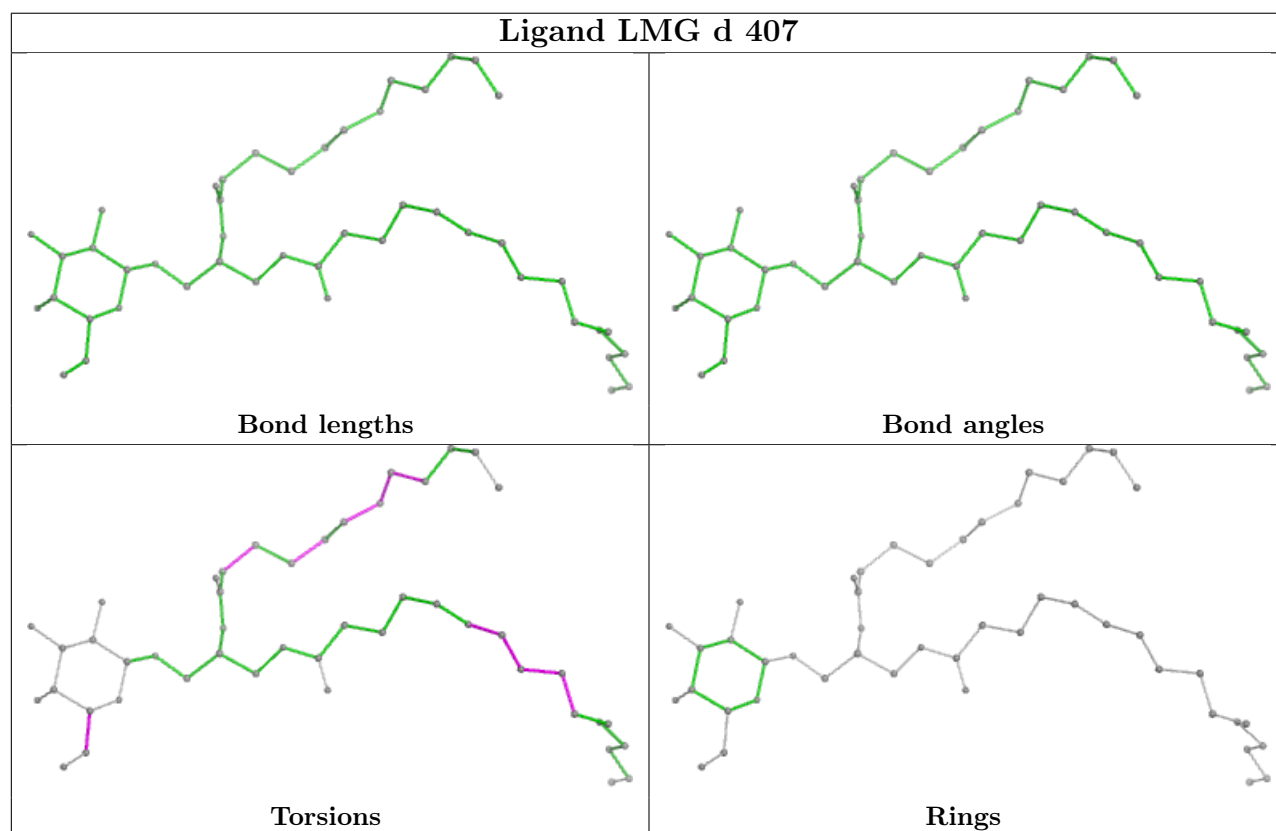
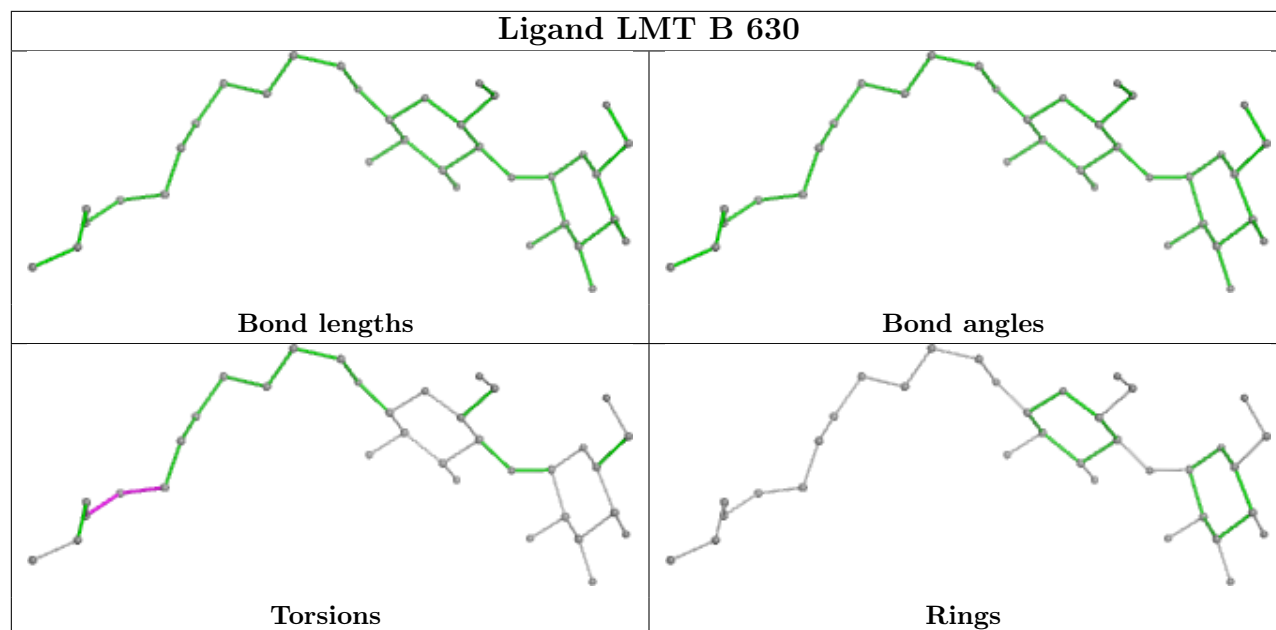
## Ligand BCR A 408

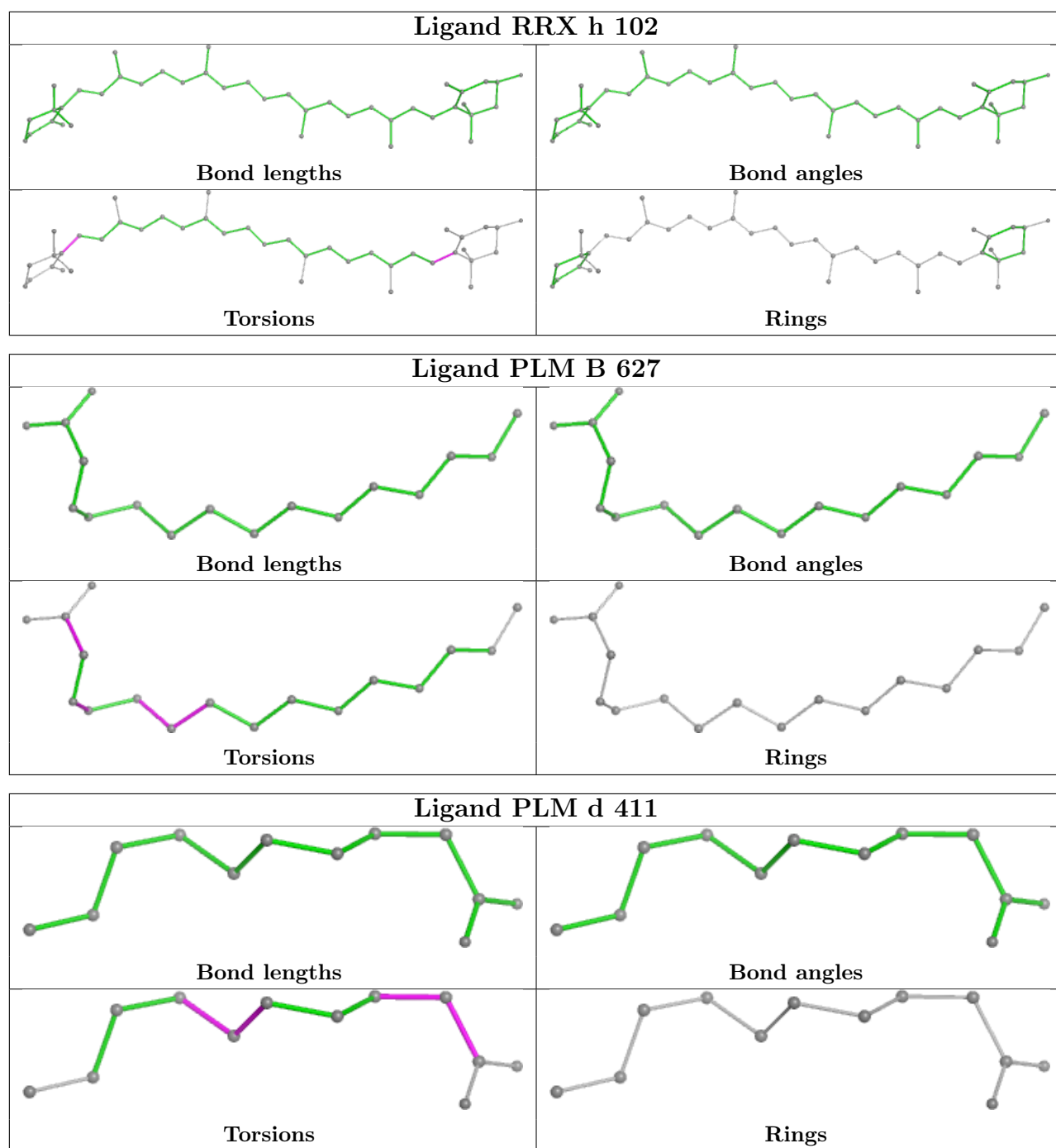


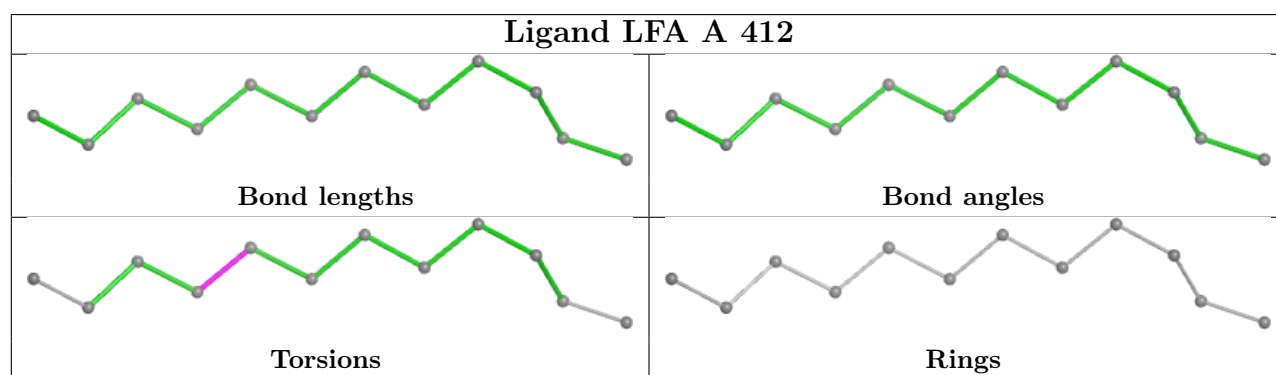
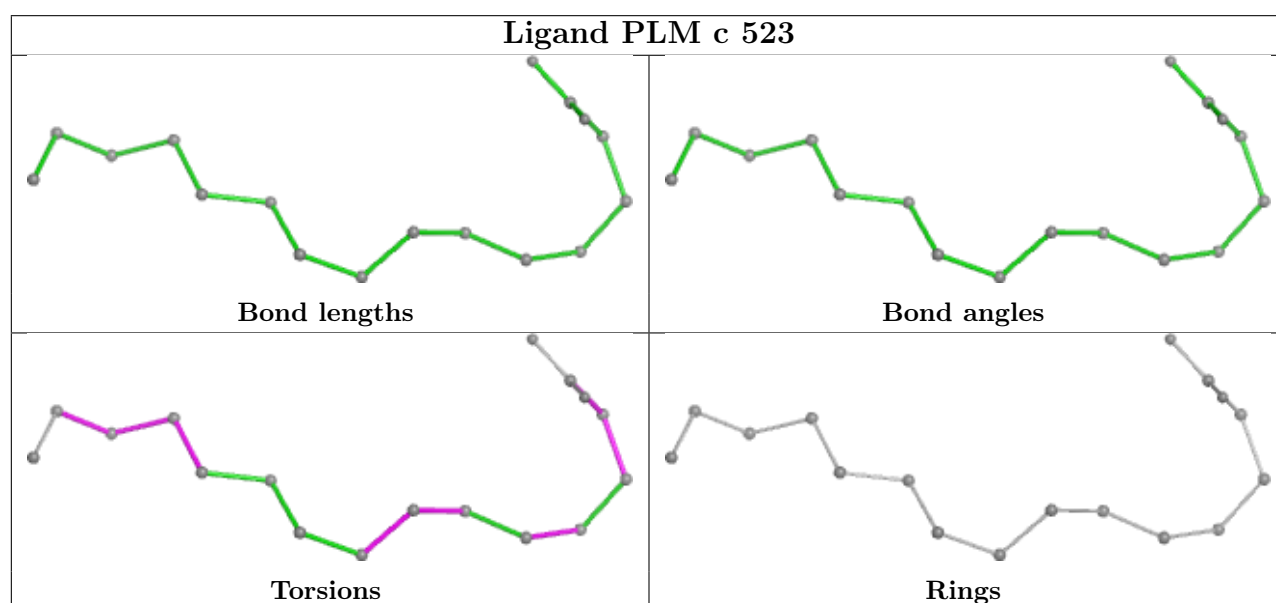
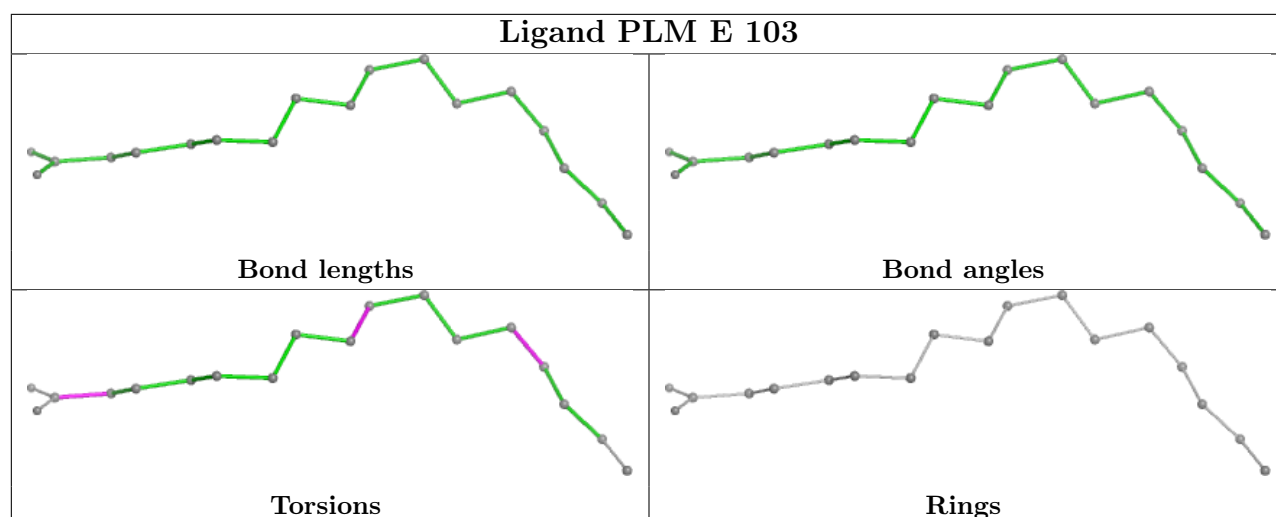




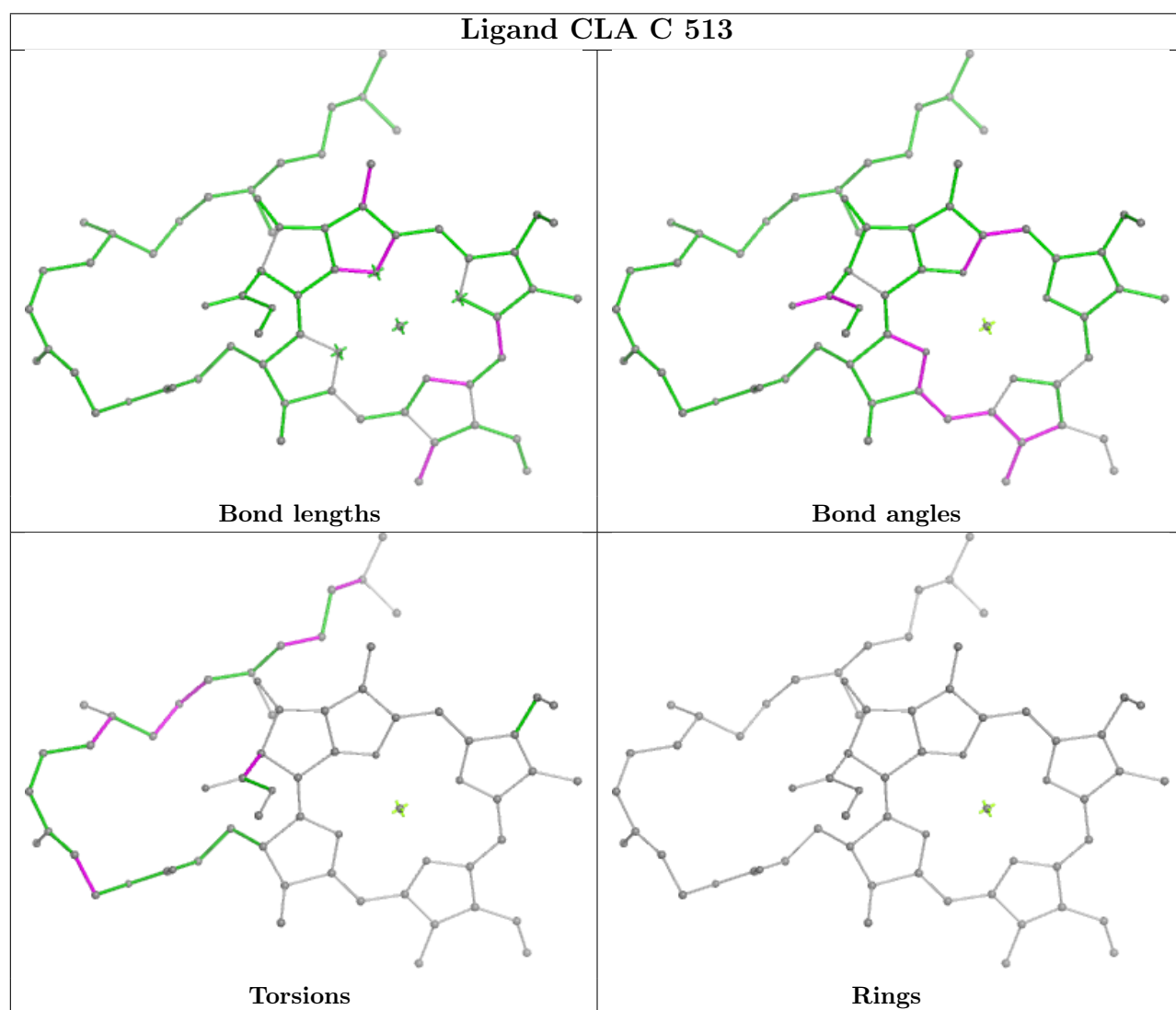
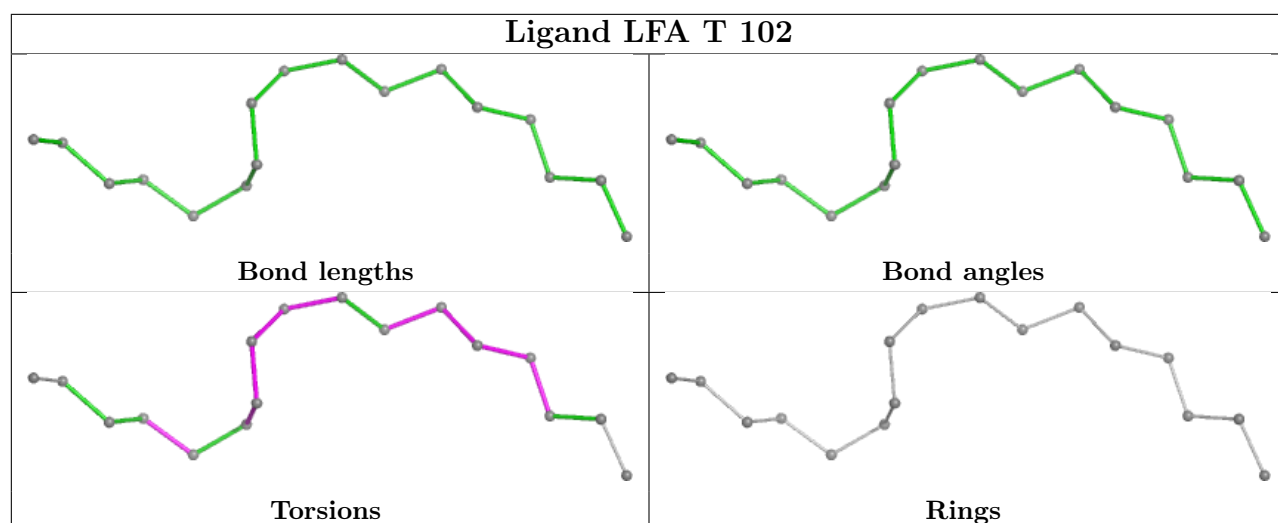


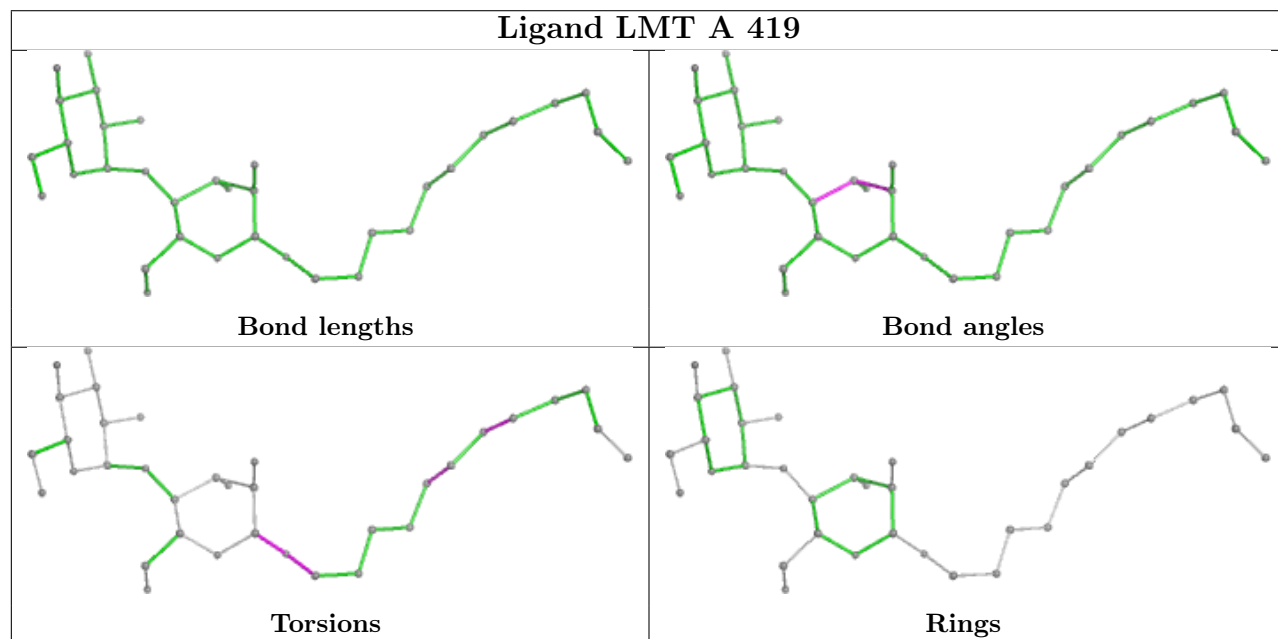
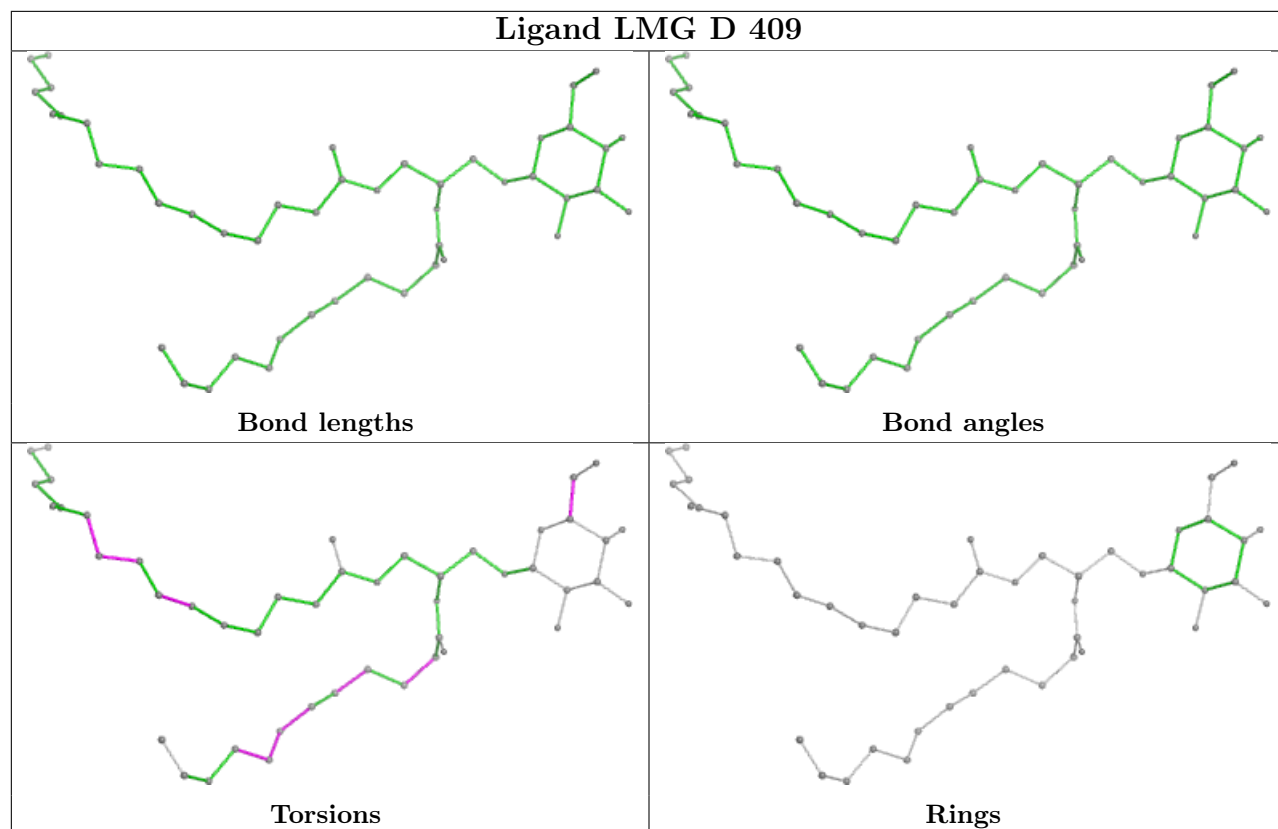


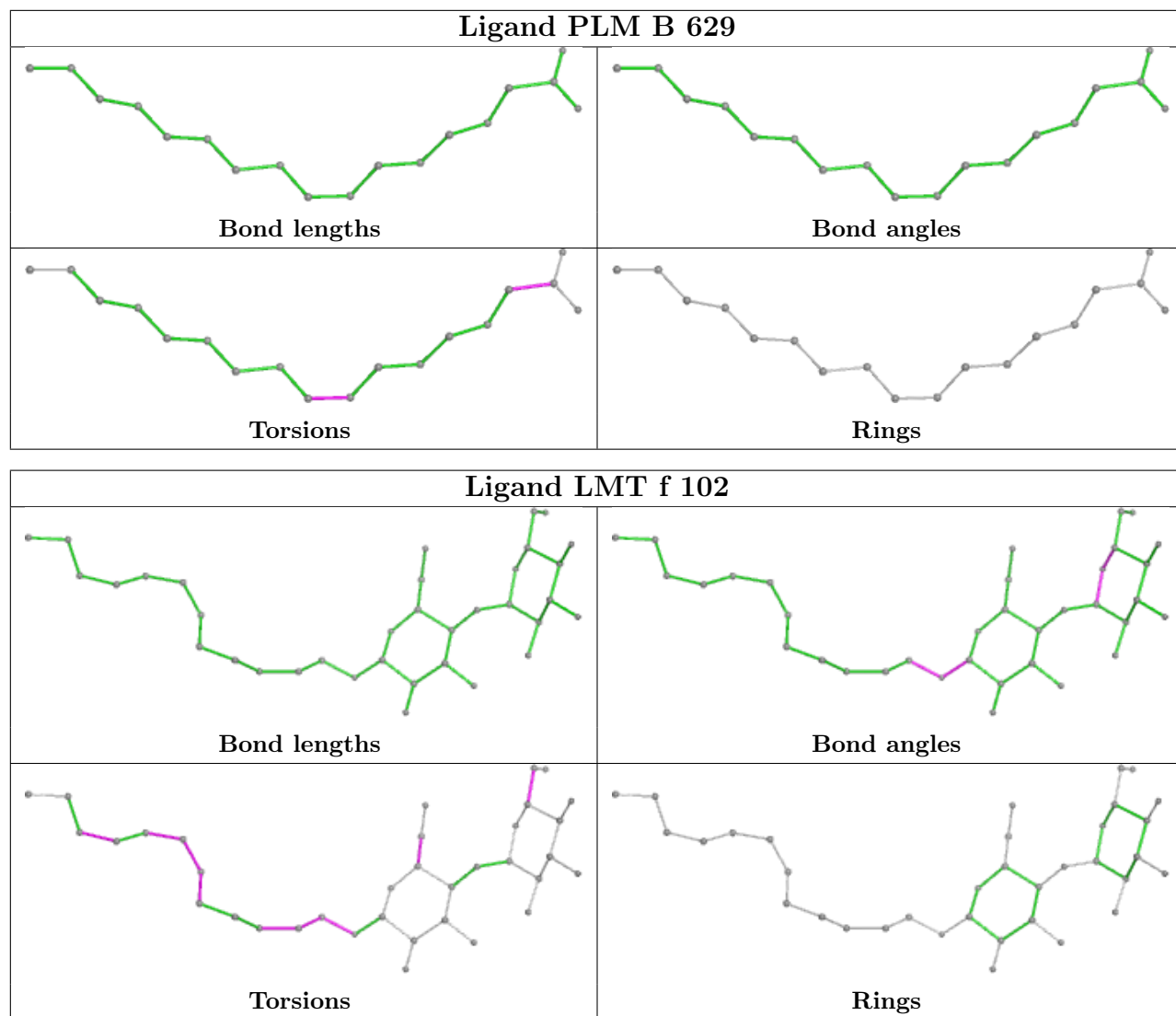


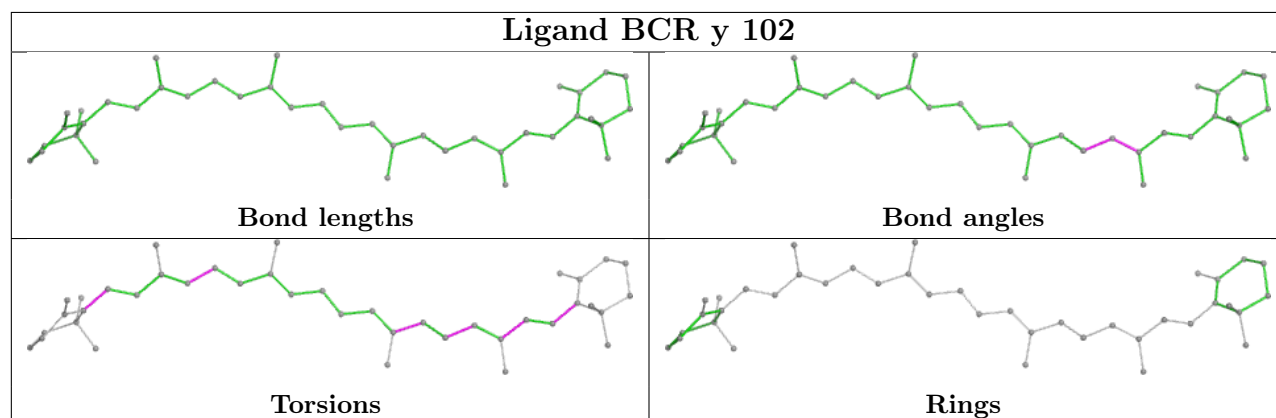
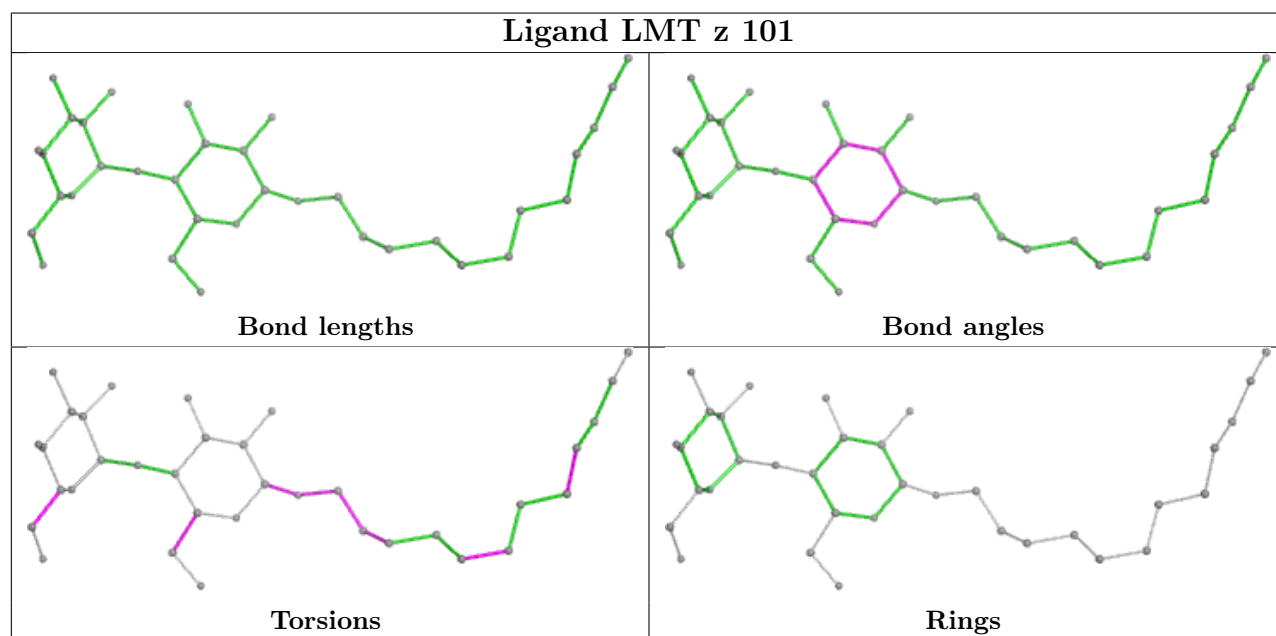
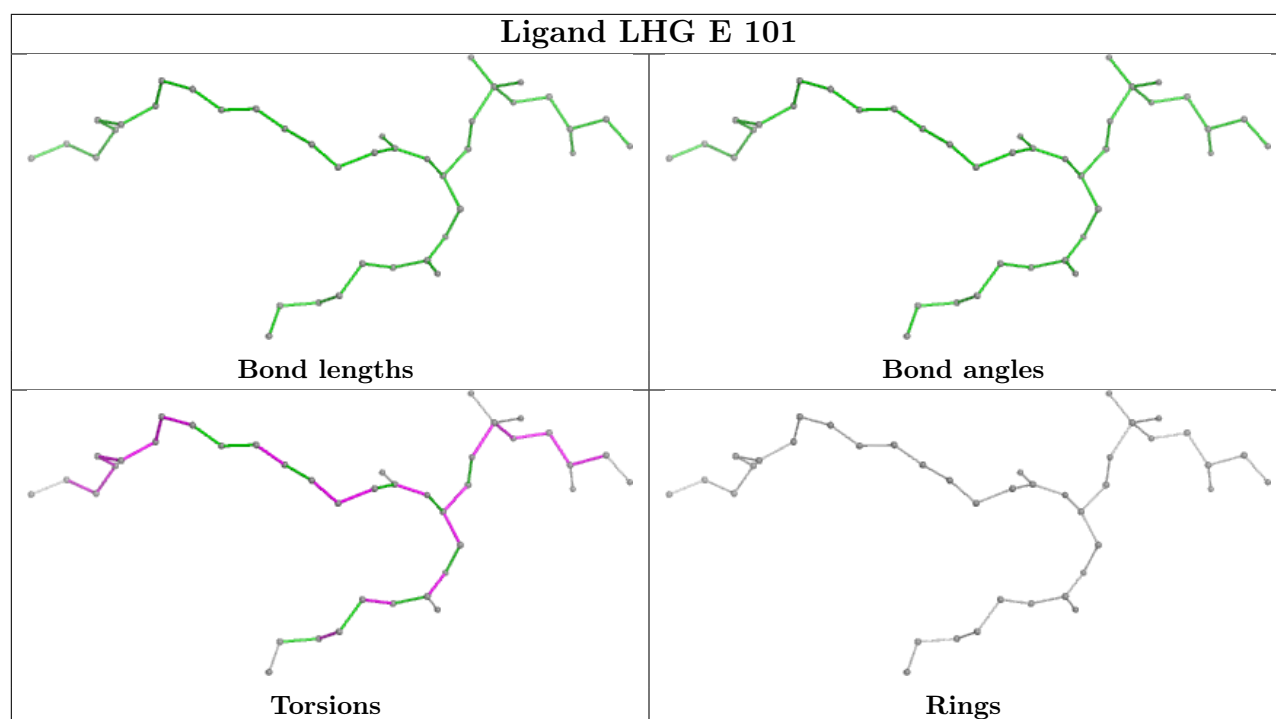


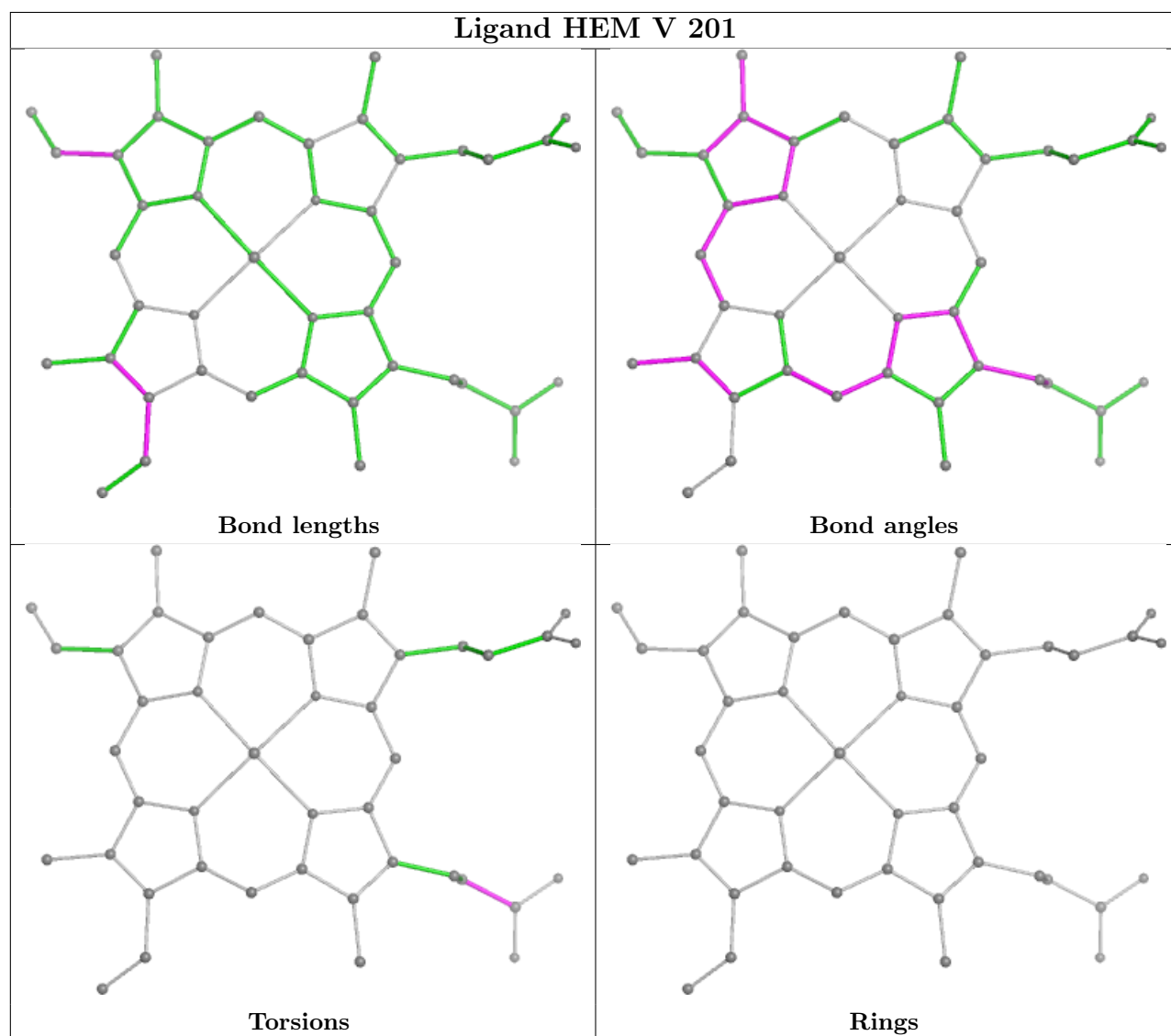
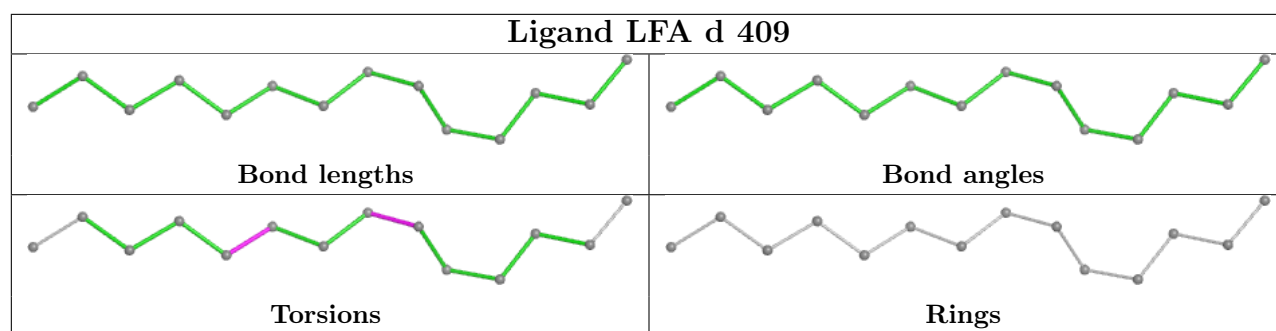


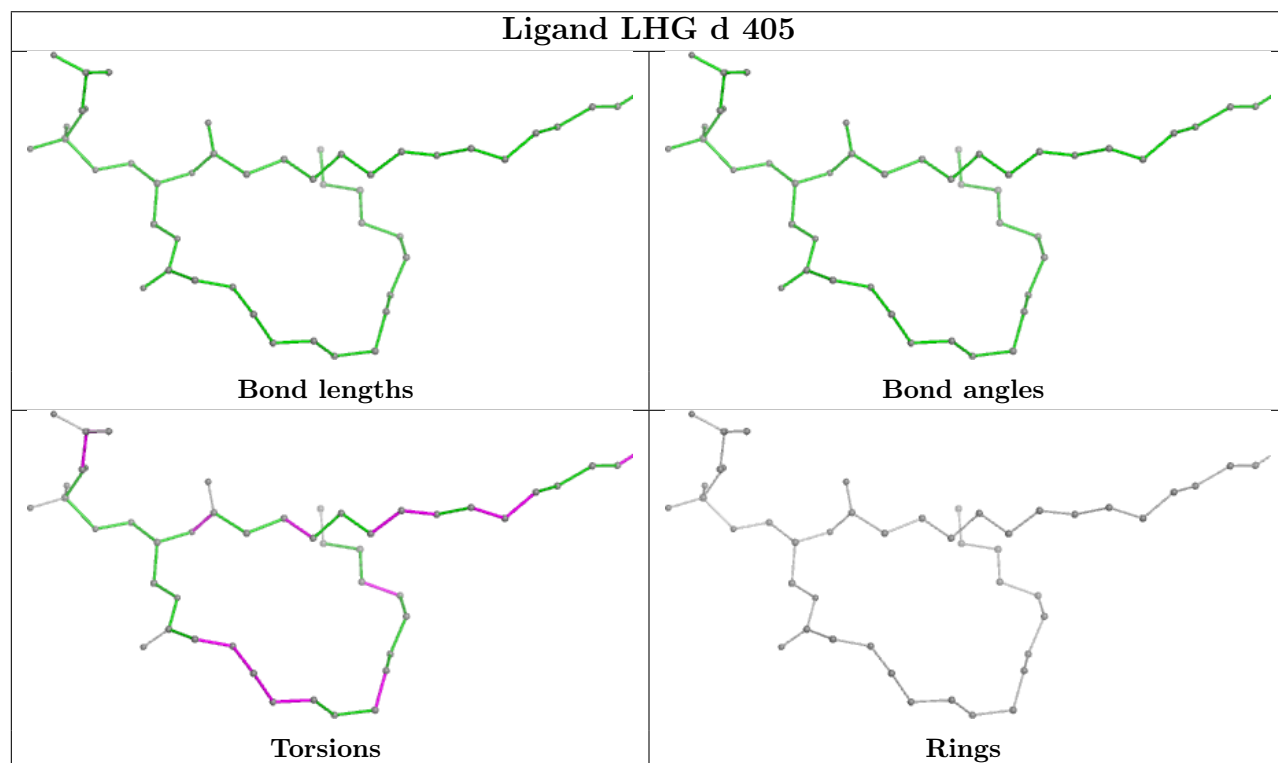
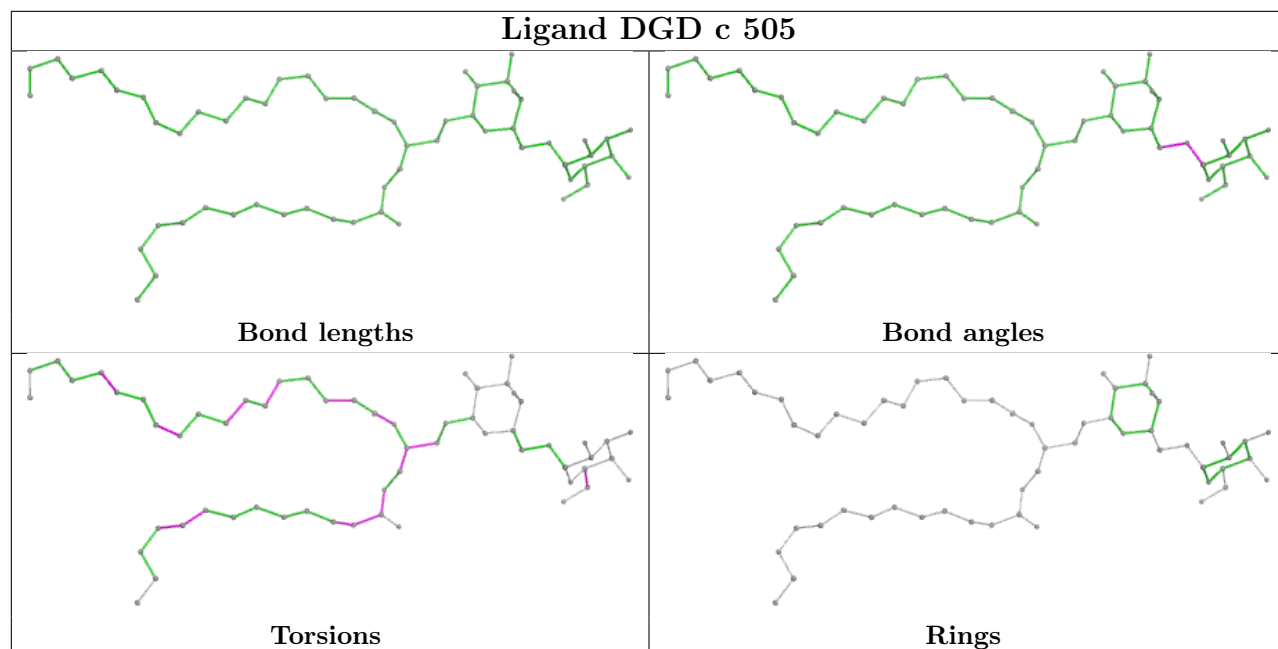


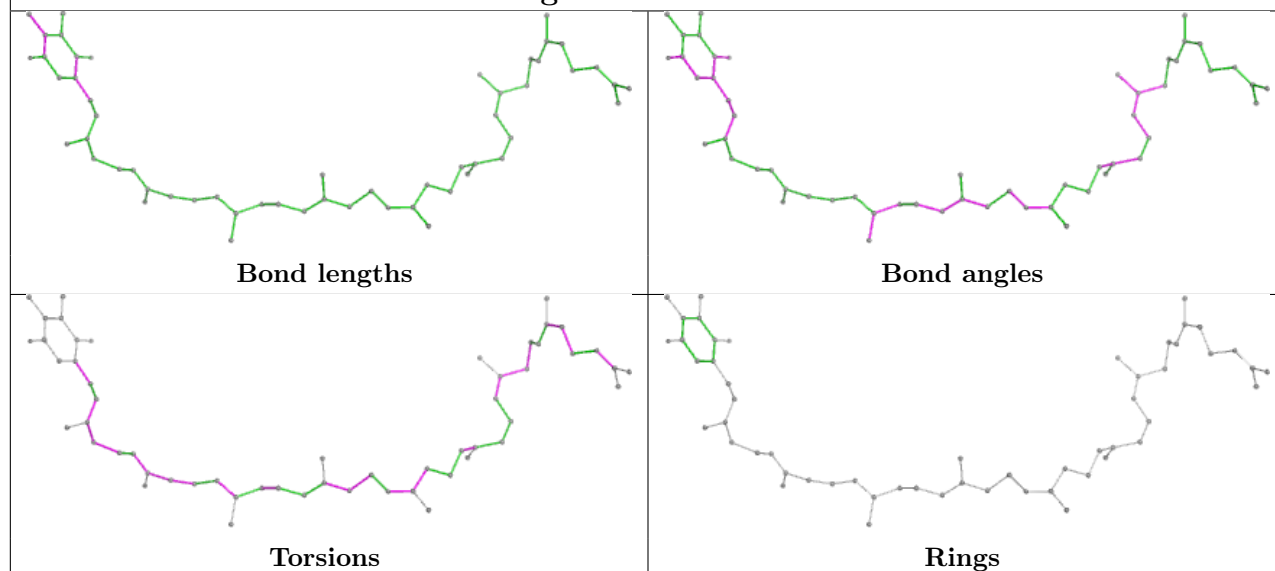
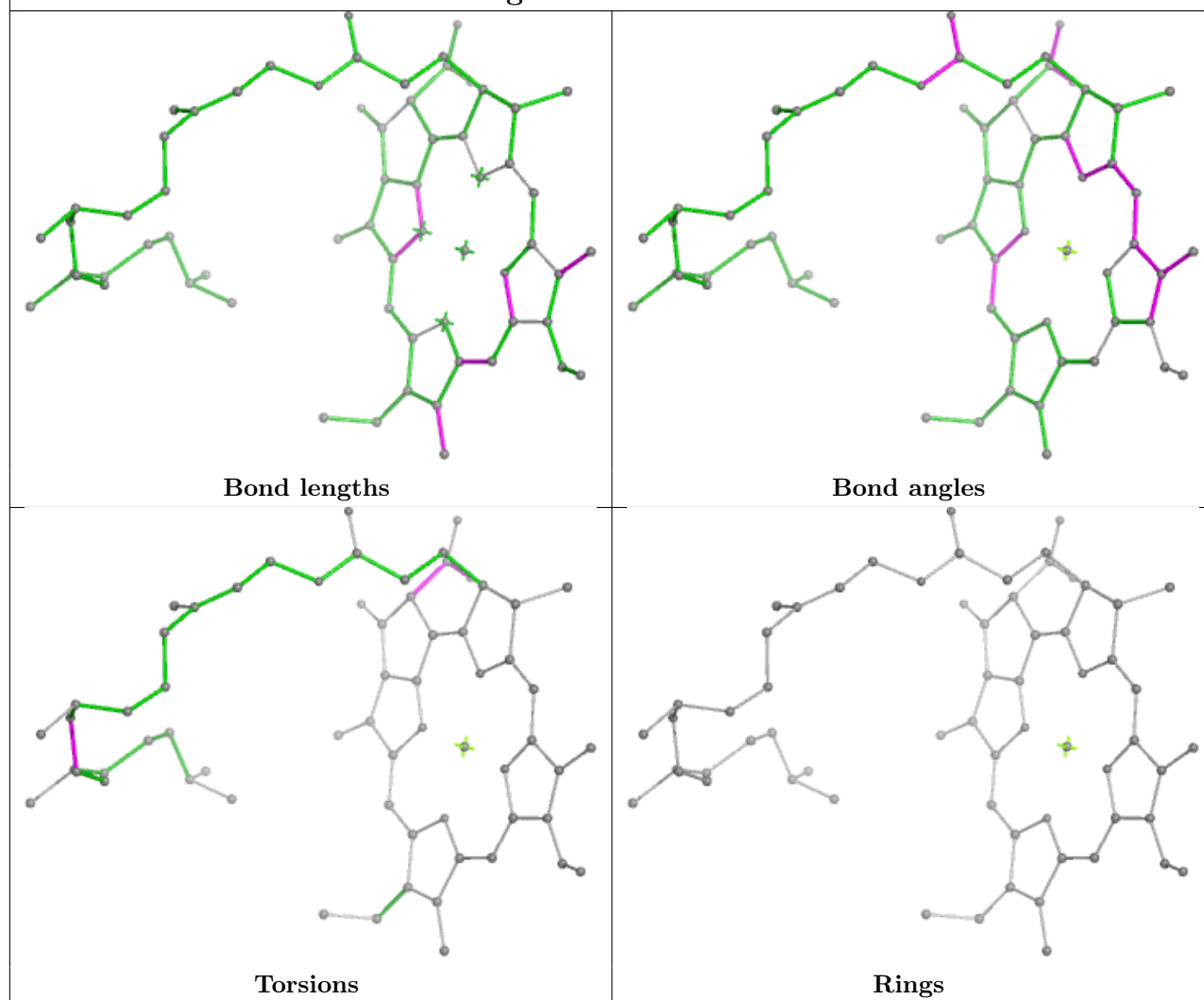


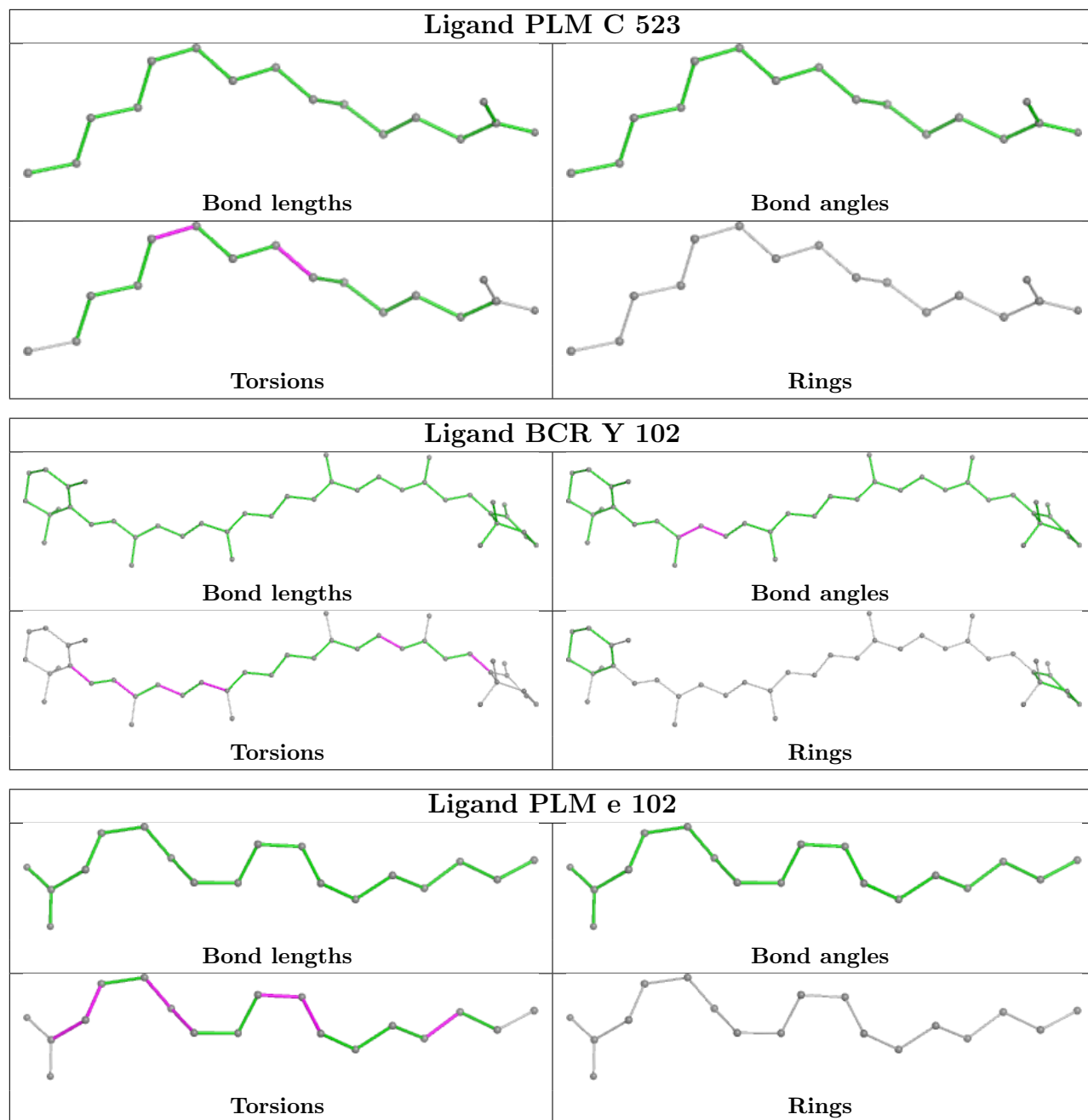






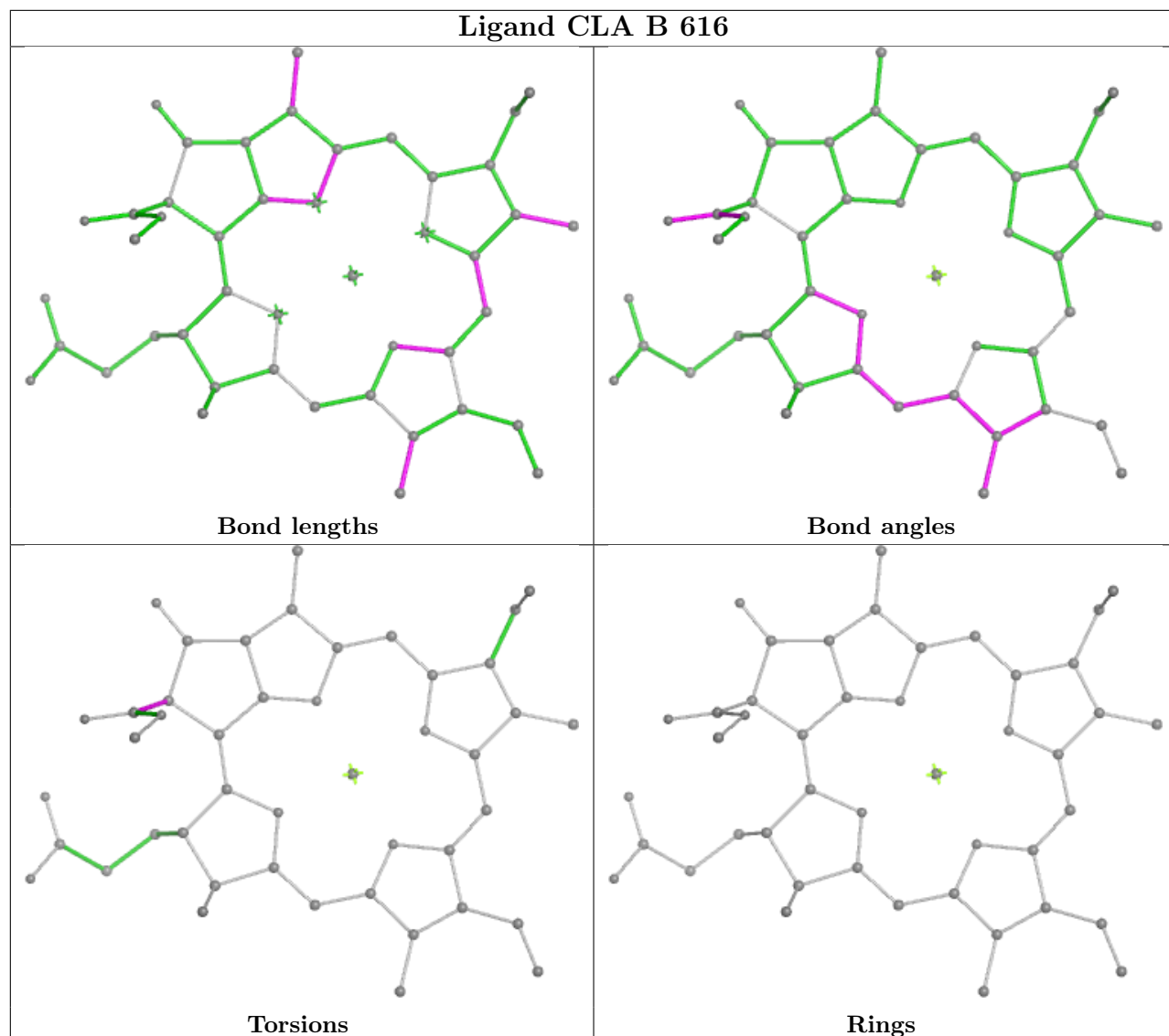


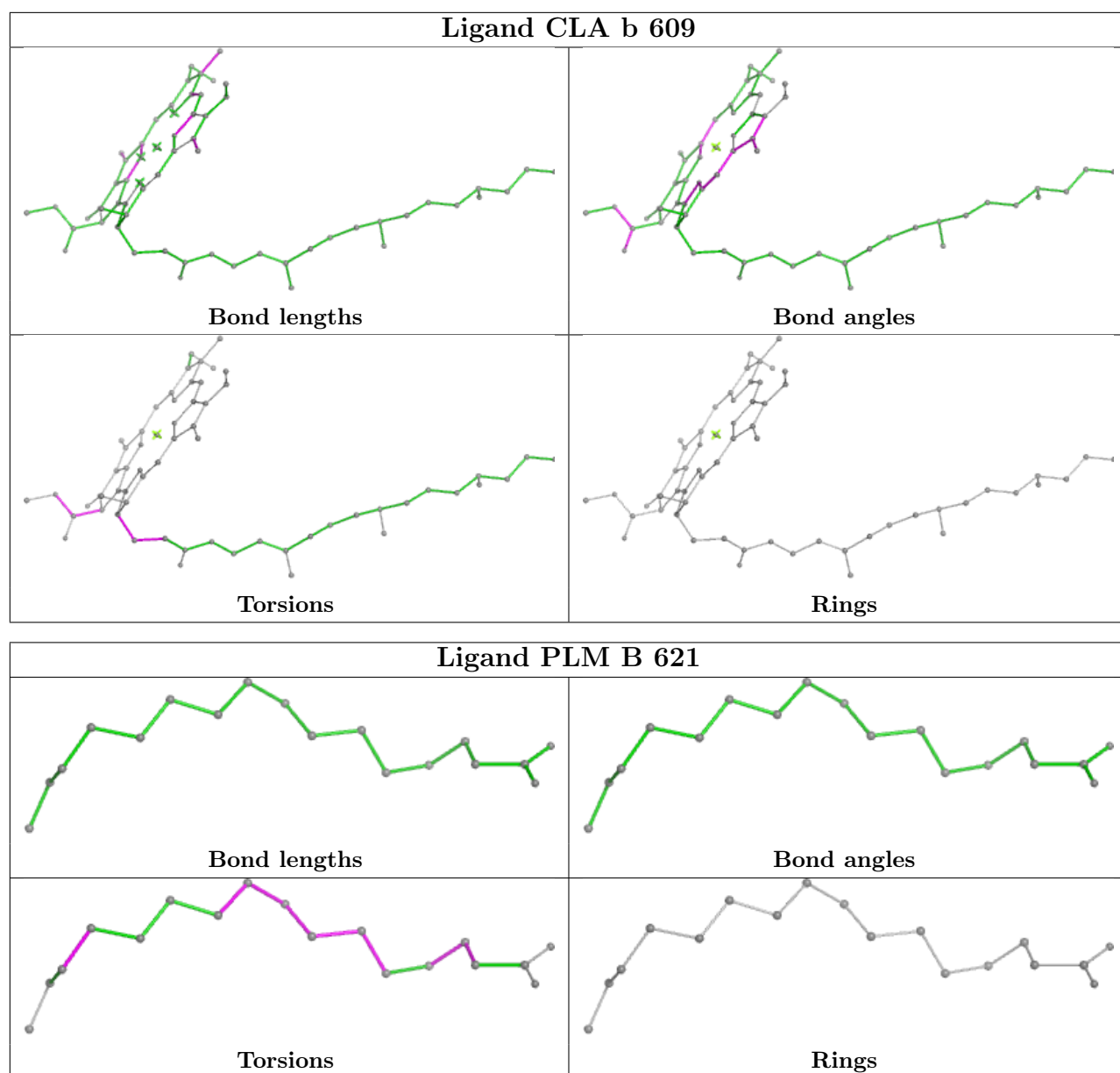
**Ligand PL9 a 410****Ligand CLA c 508**



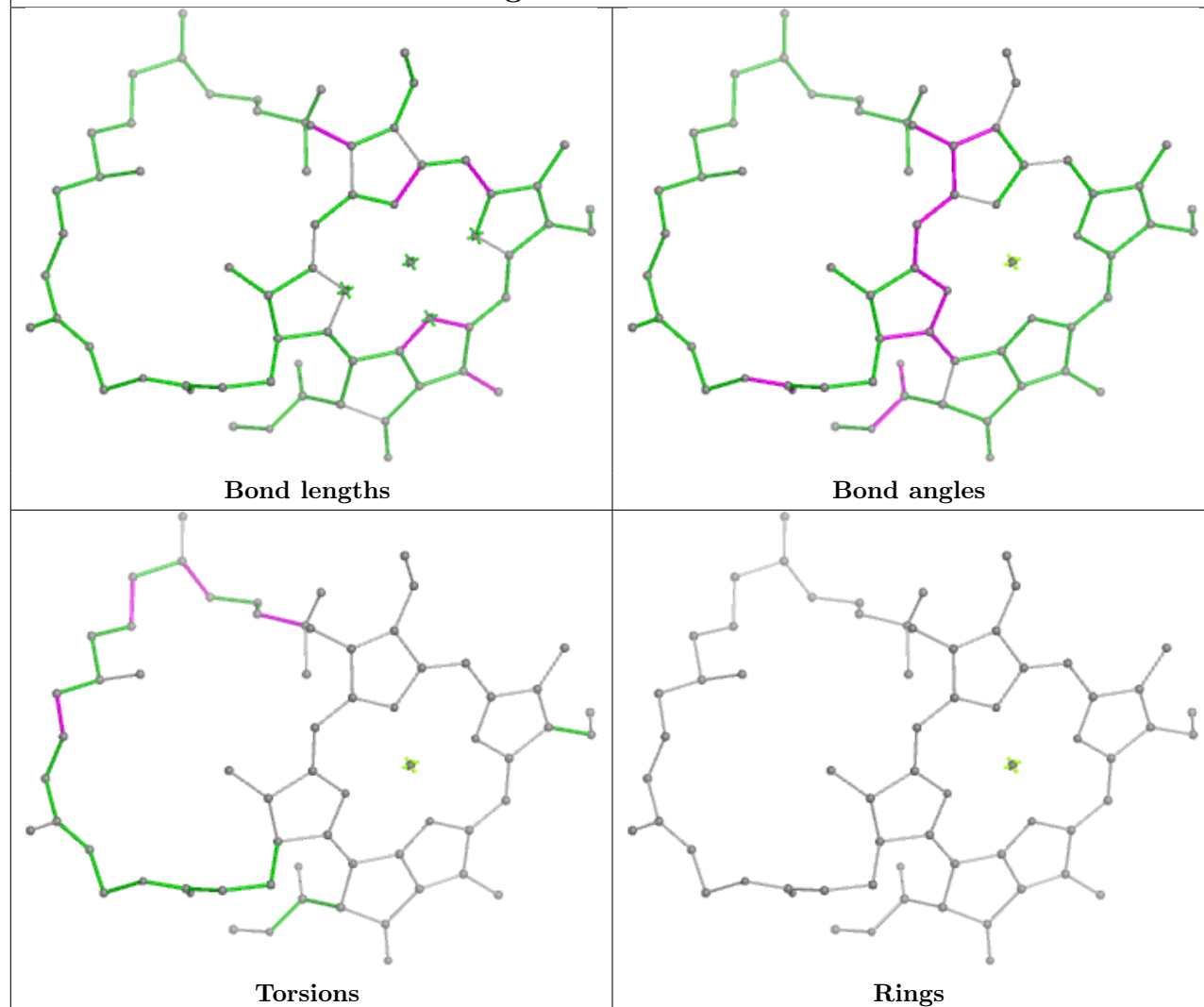


## Ligand CLA B 616

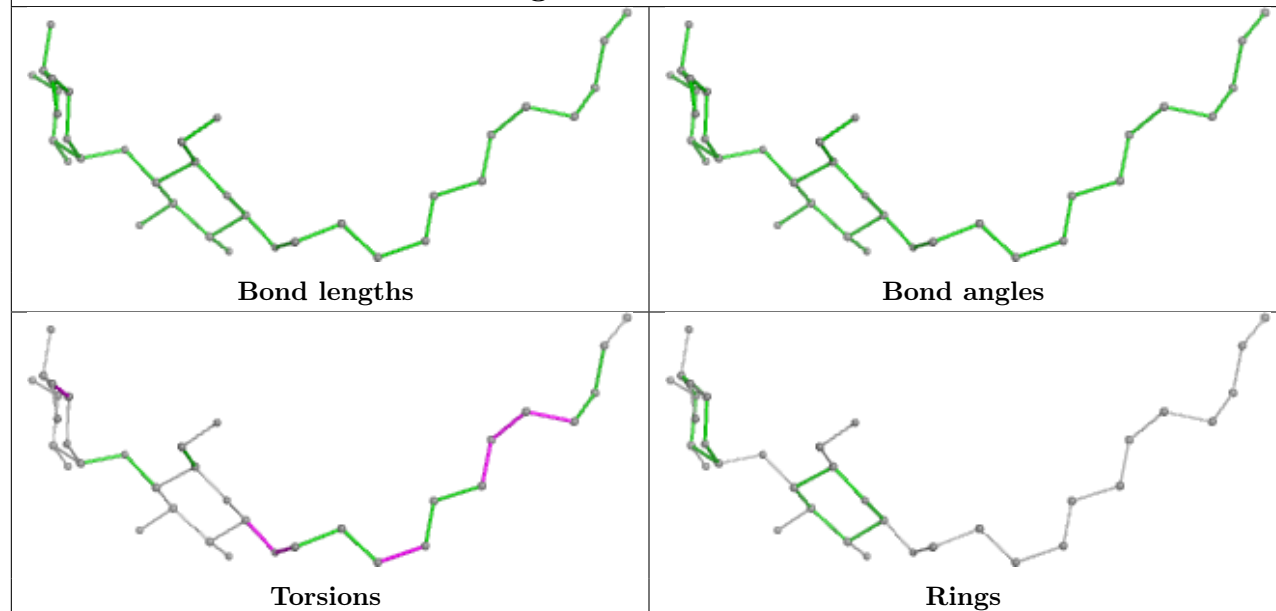


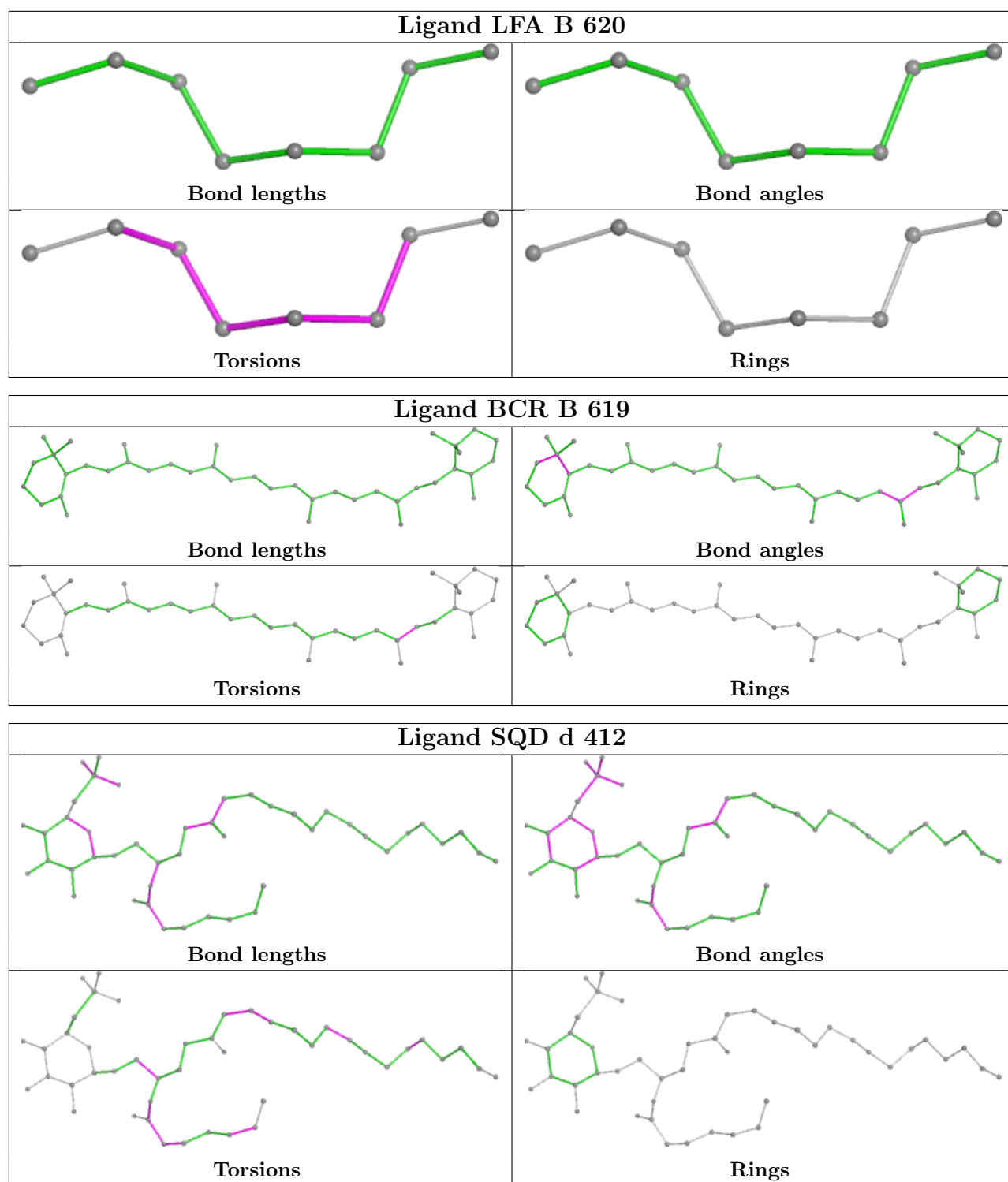


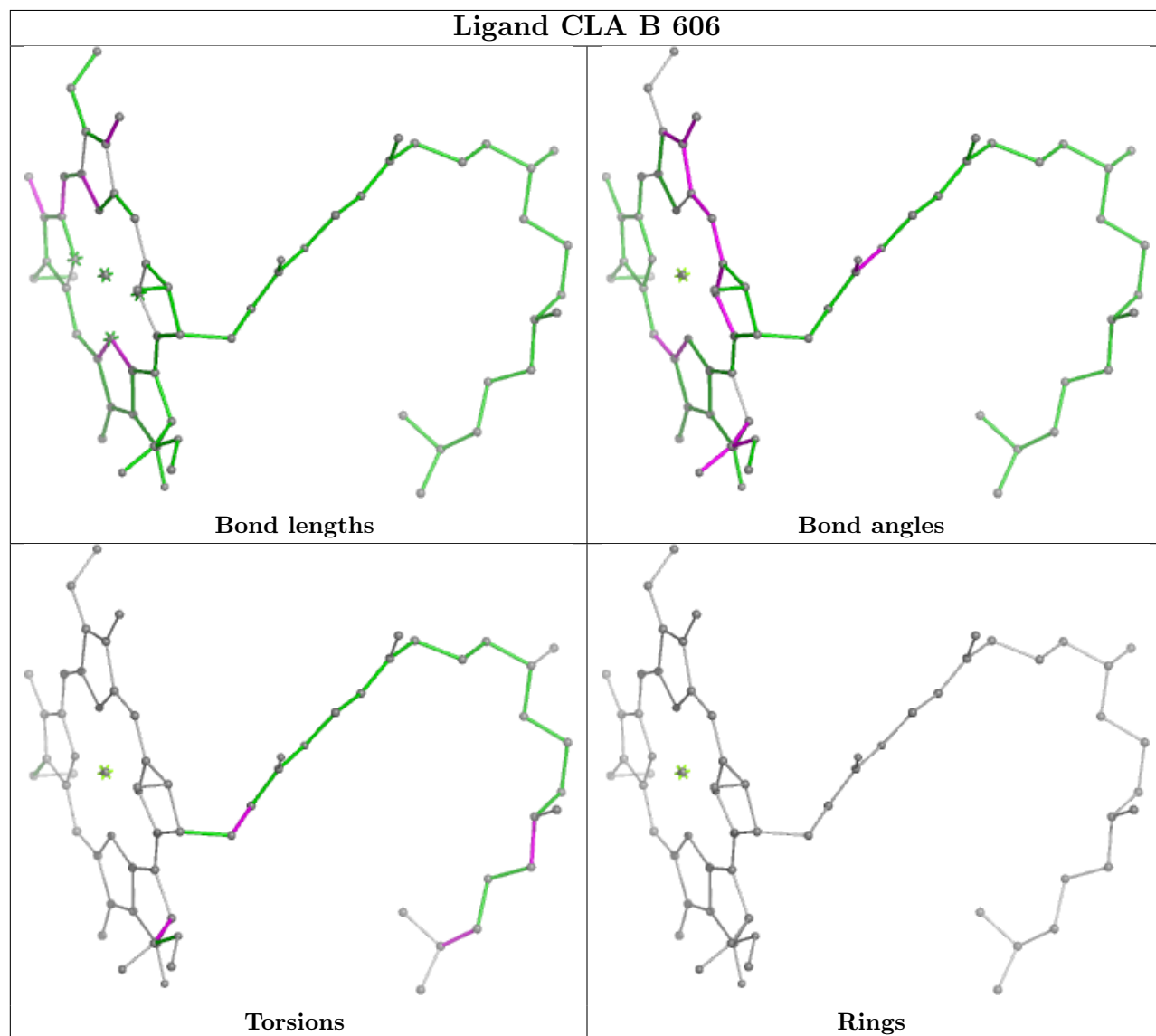
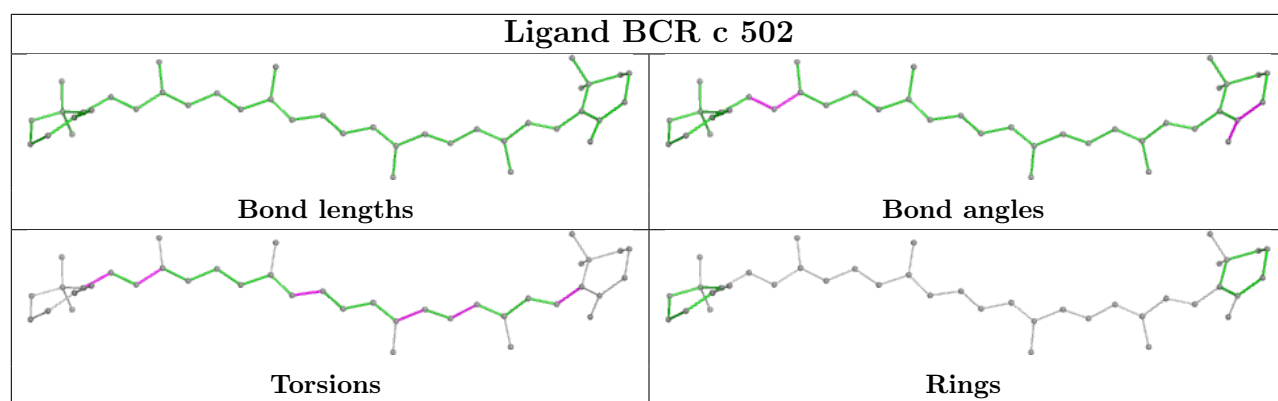
## Ligand CLA b 617

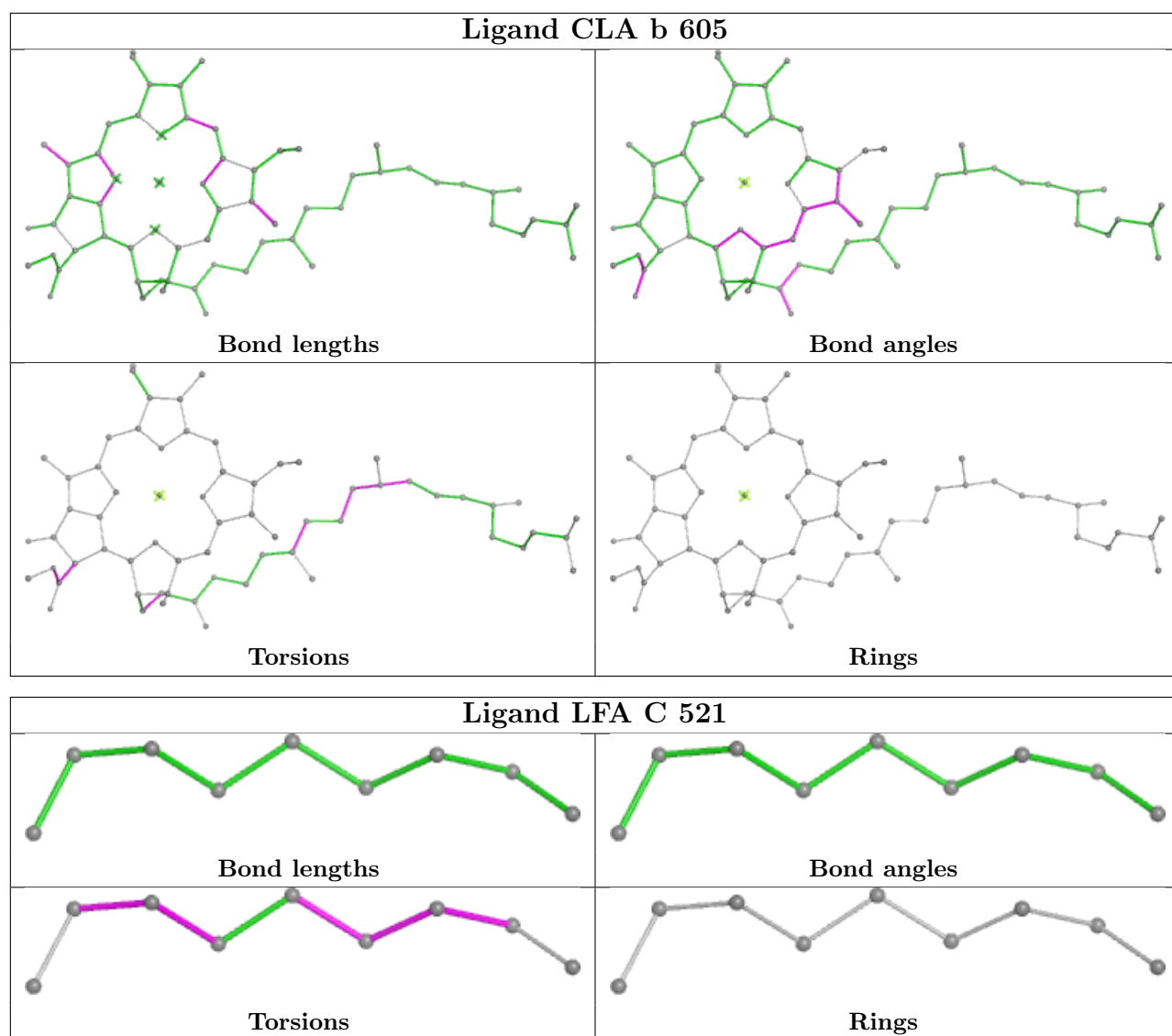


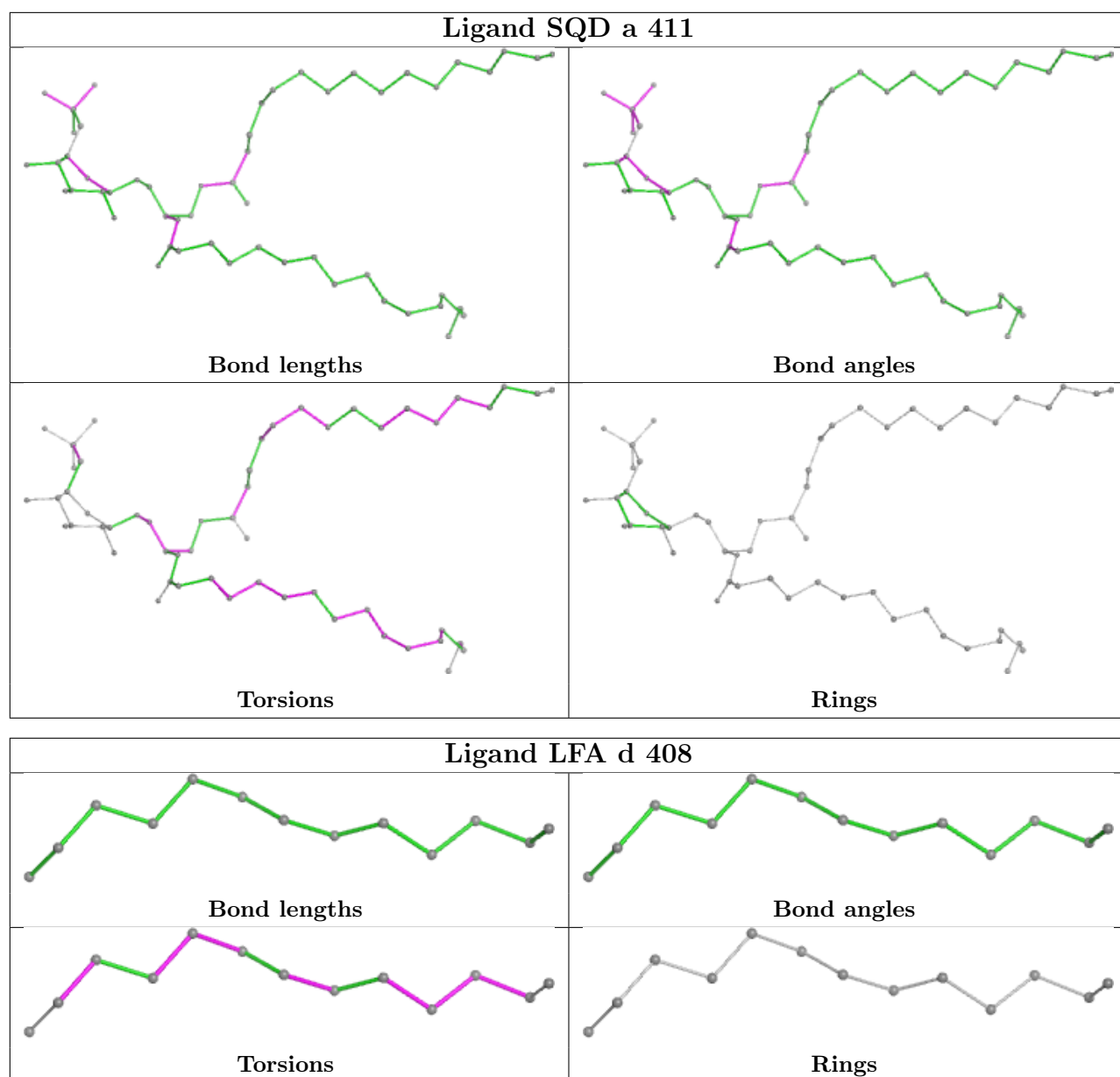
## Ligand LMT T 104

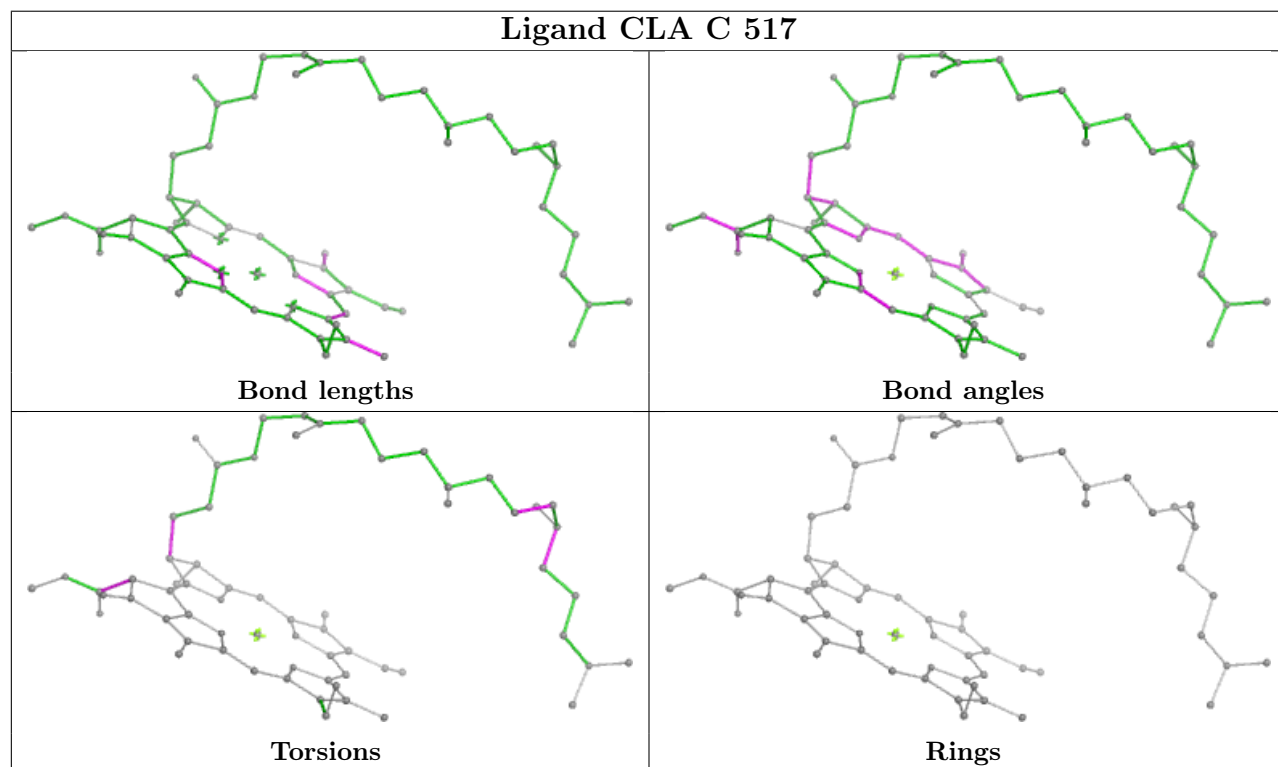
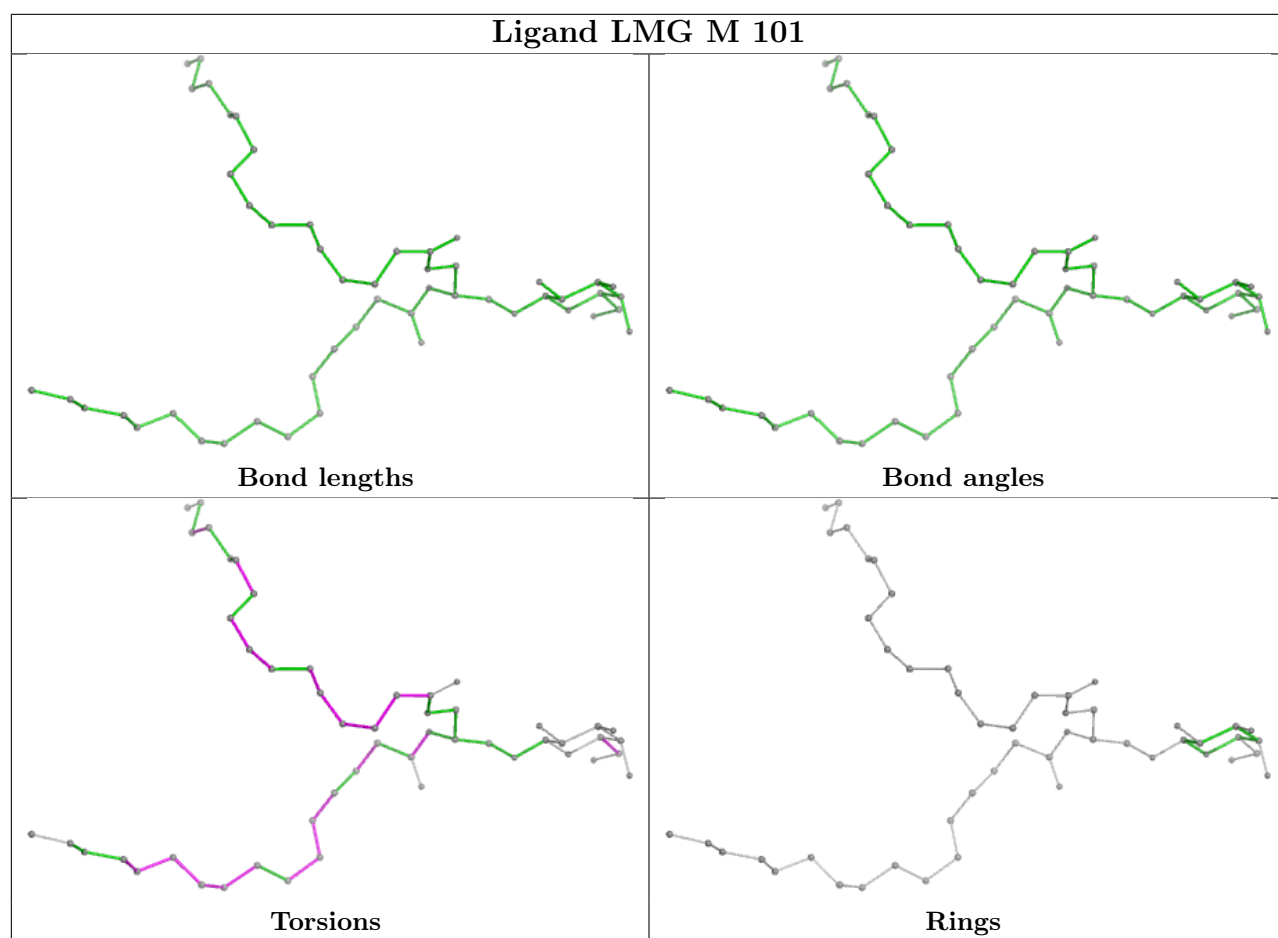




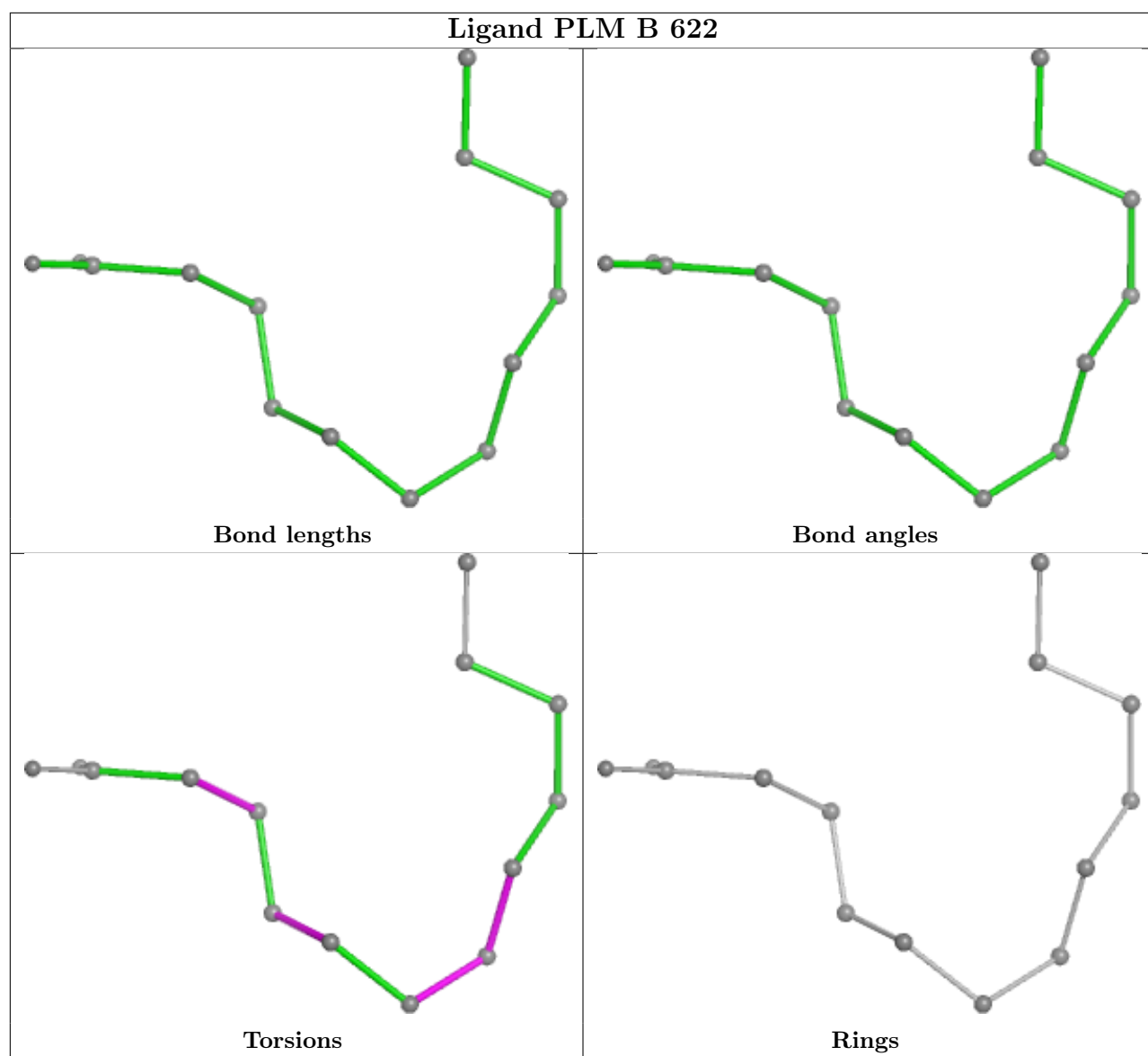


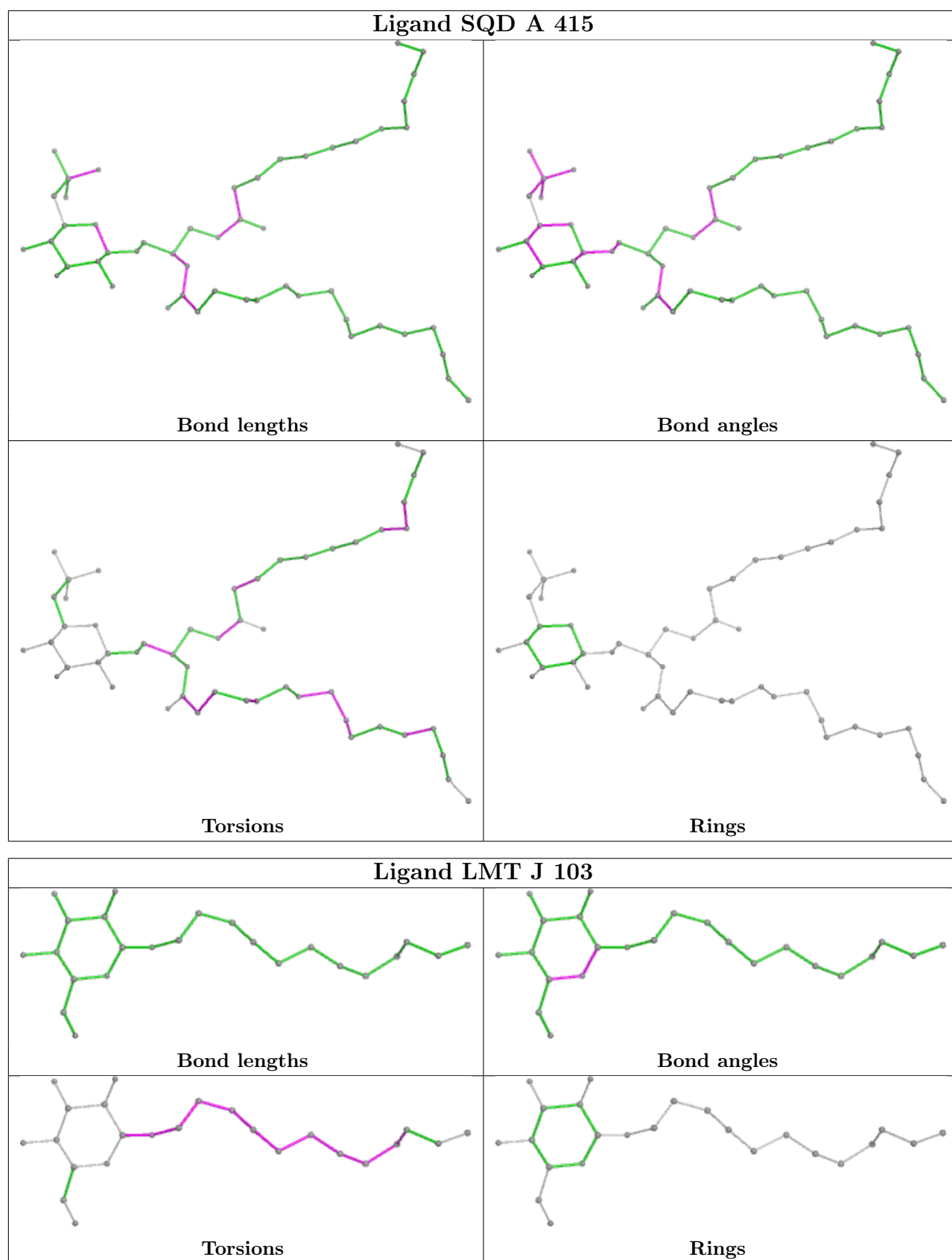




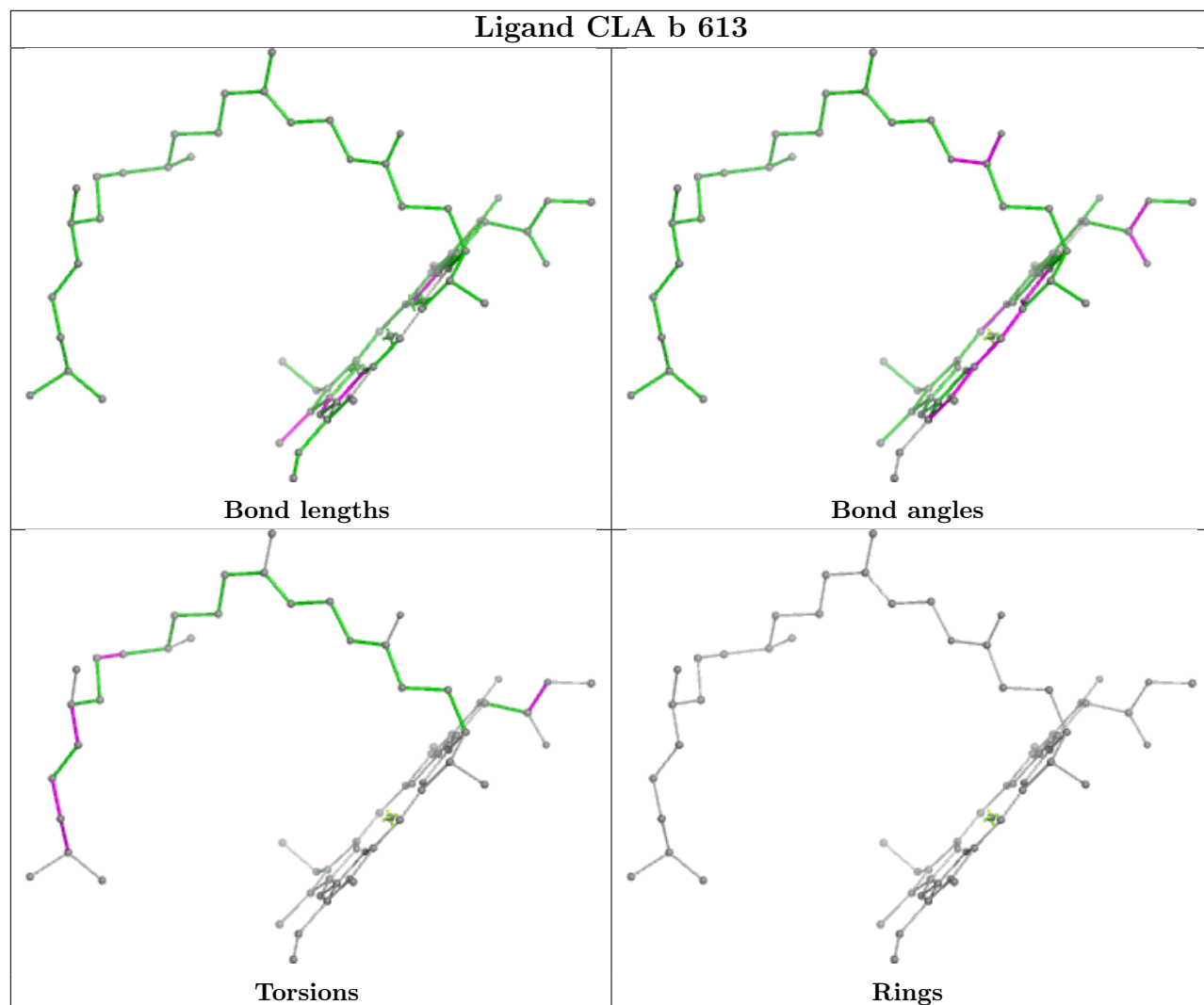


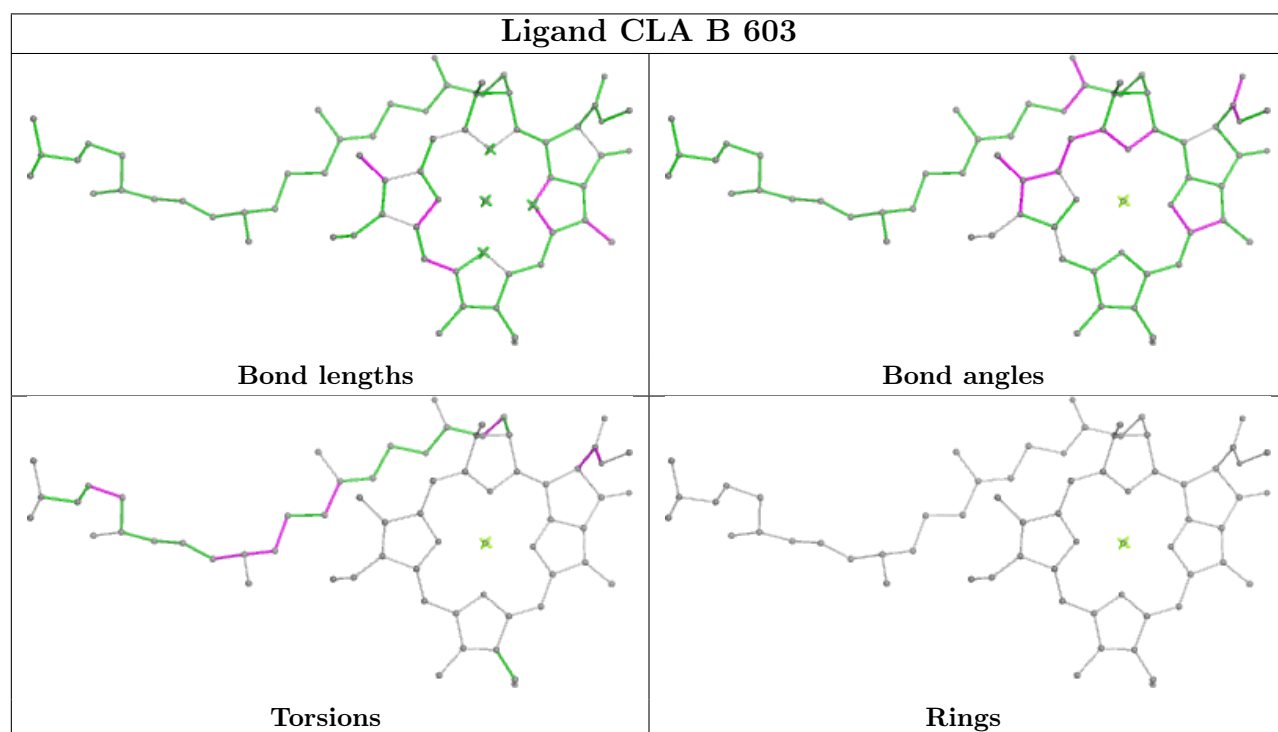
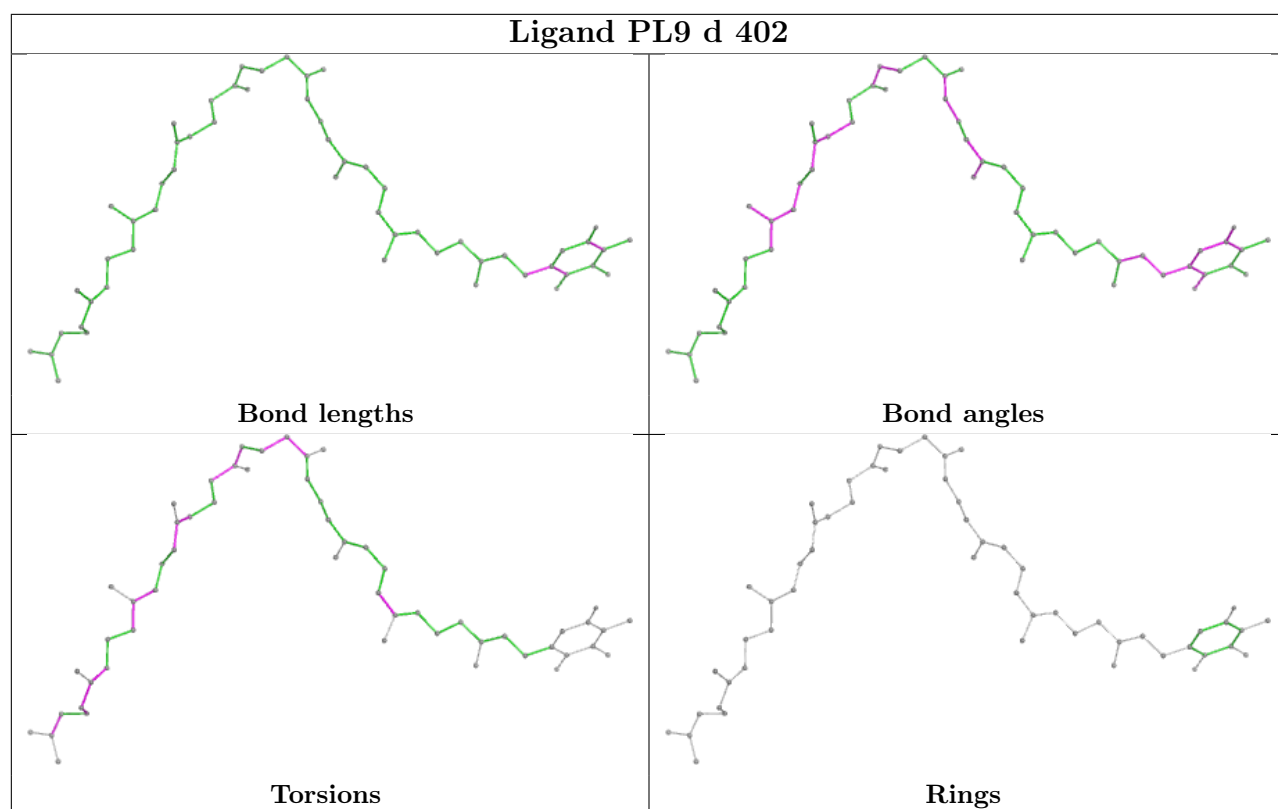


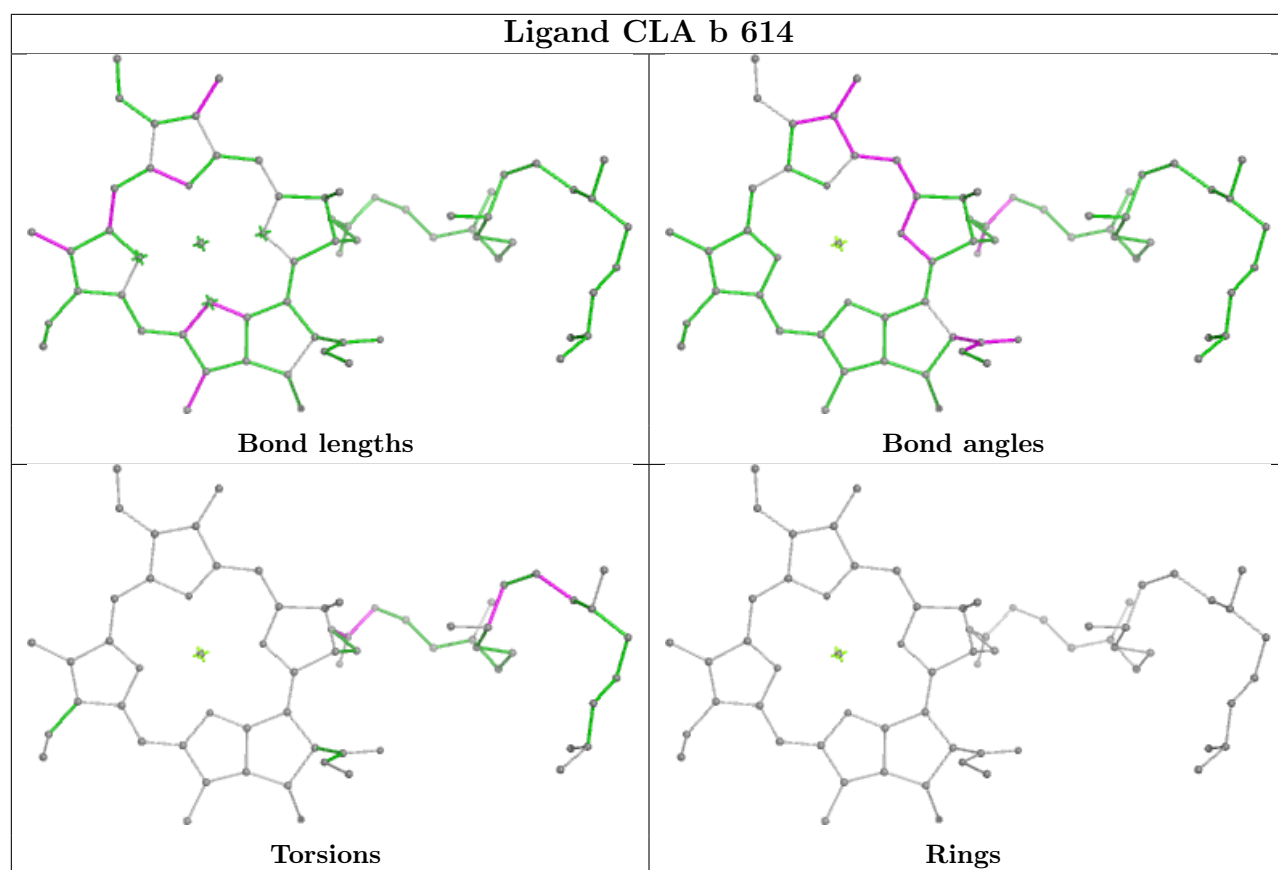


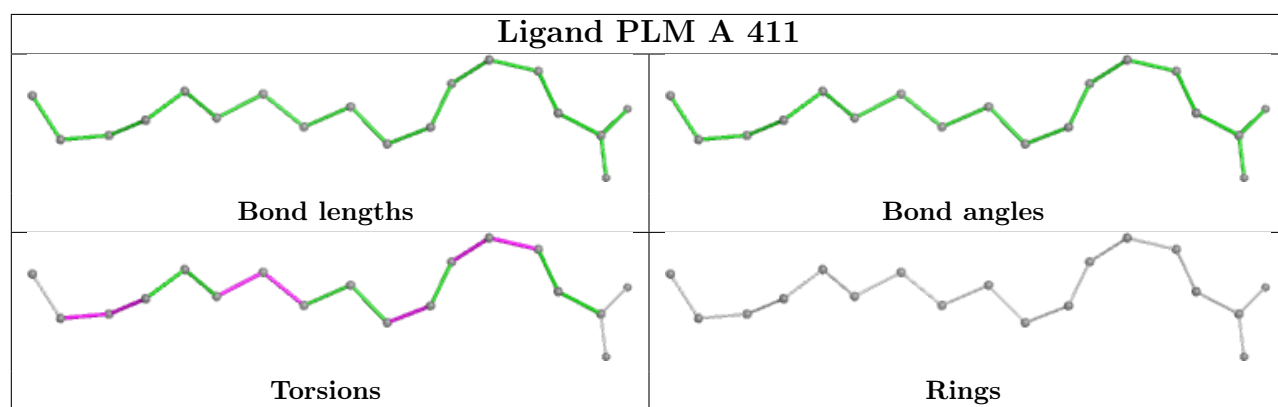
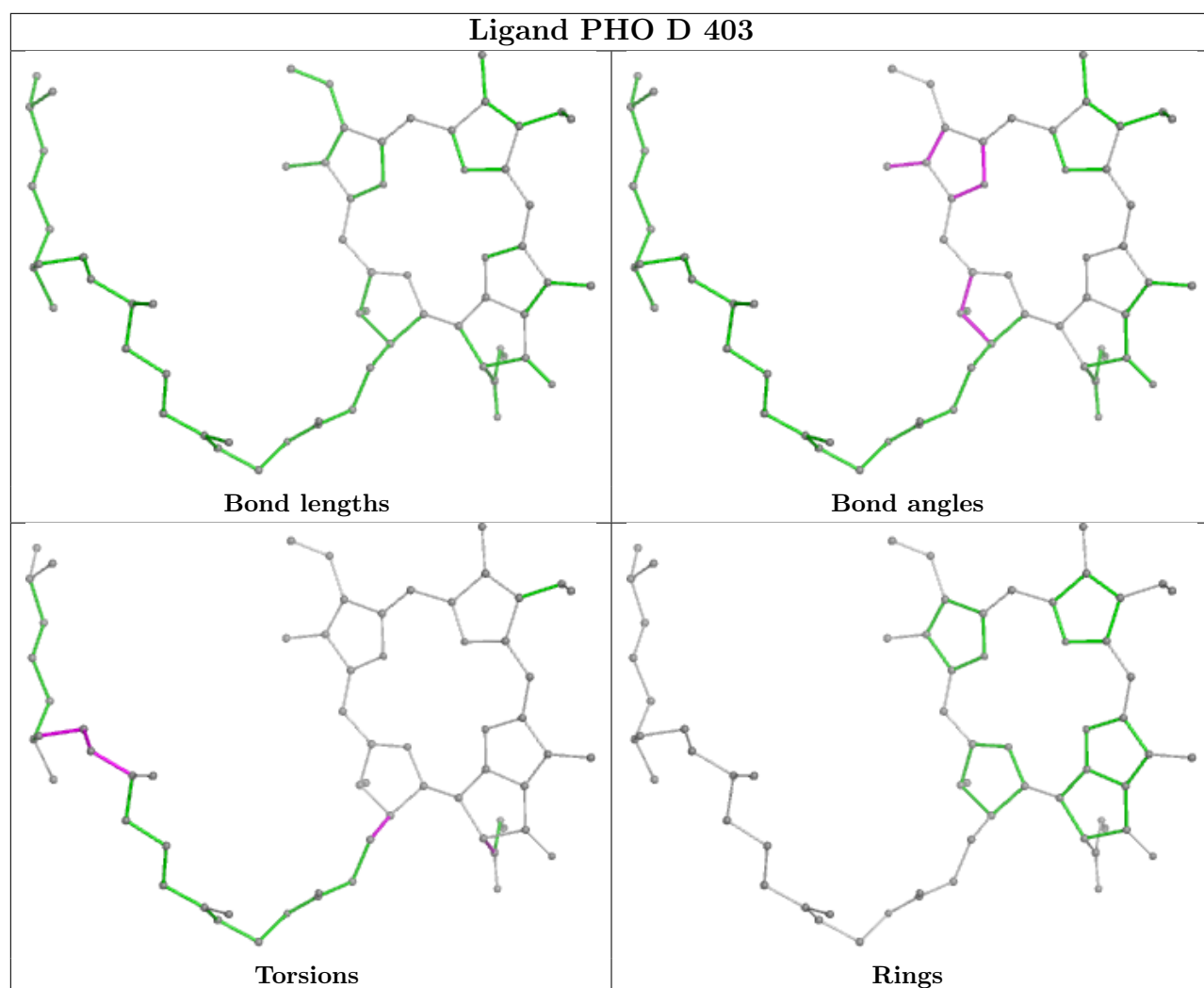


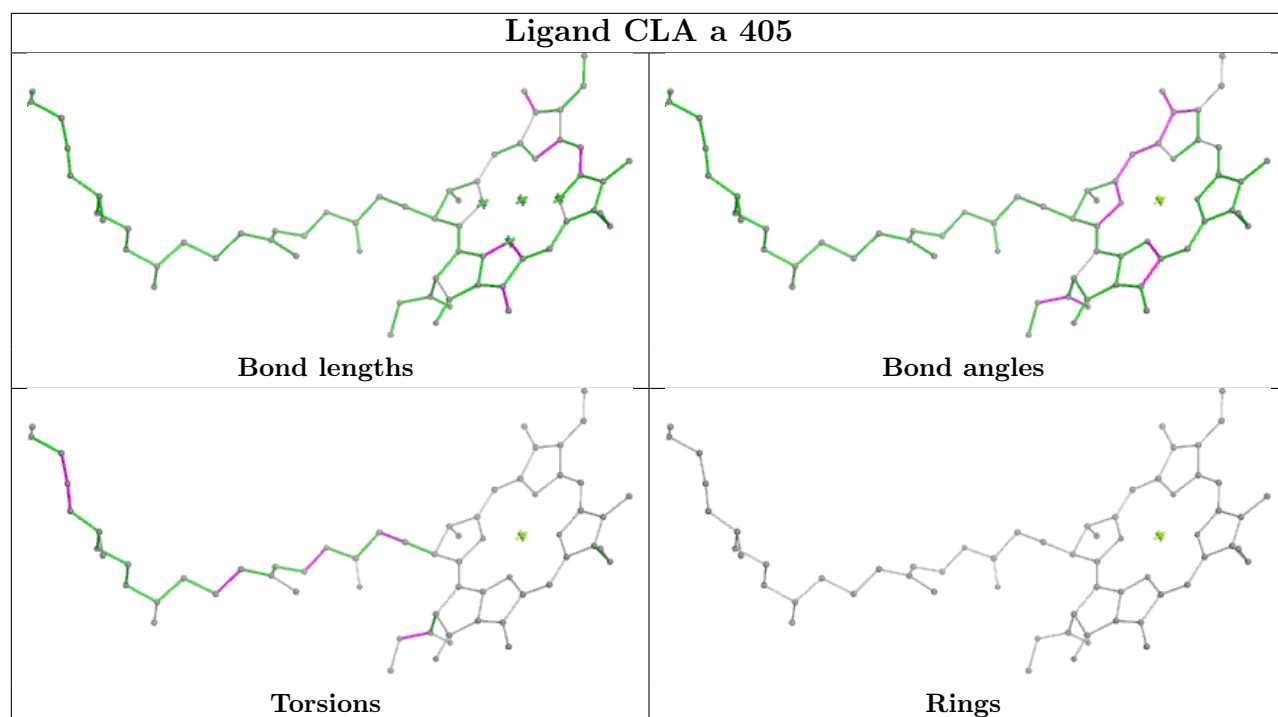
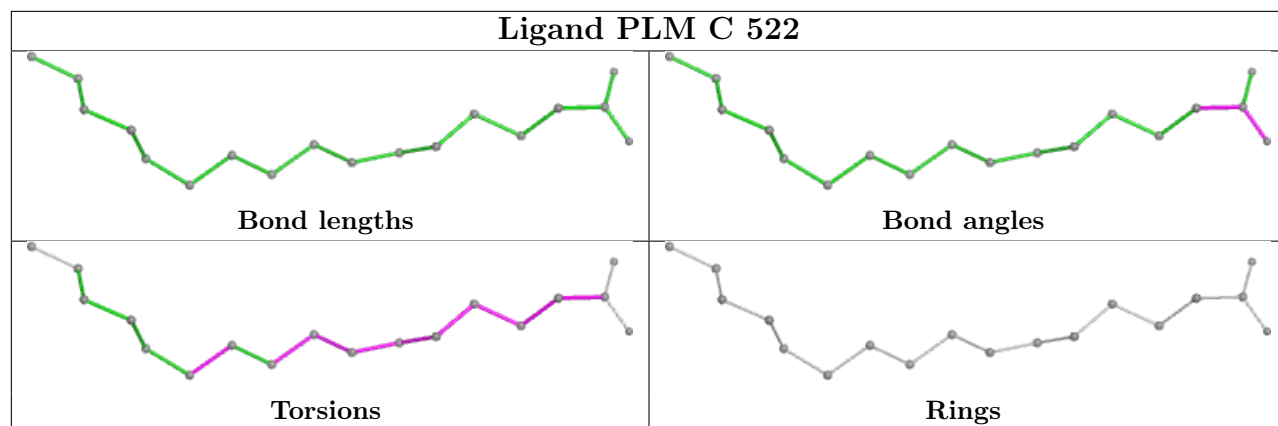
## Ligand CLA b 613

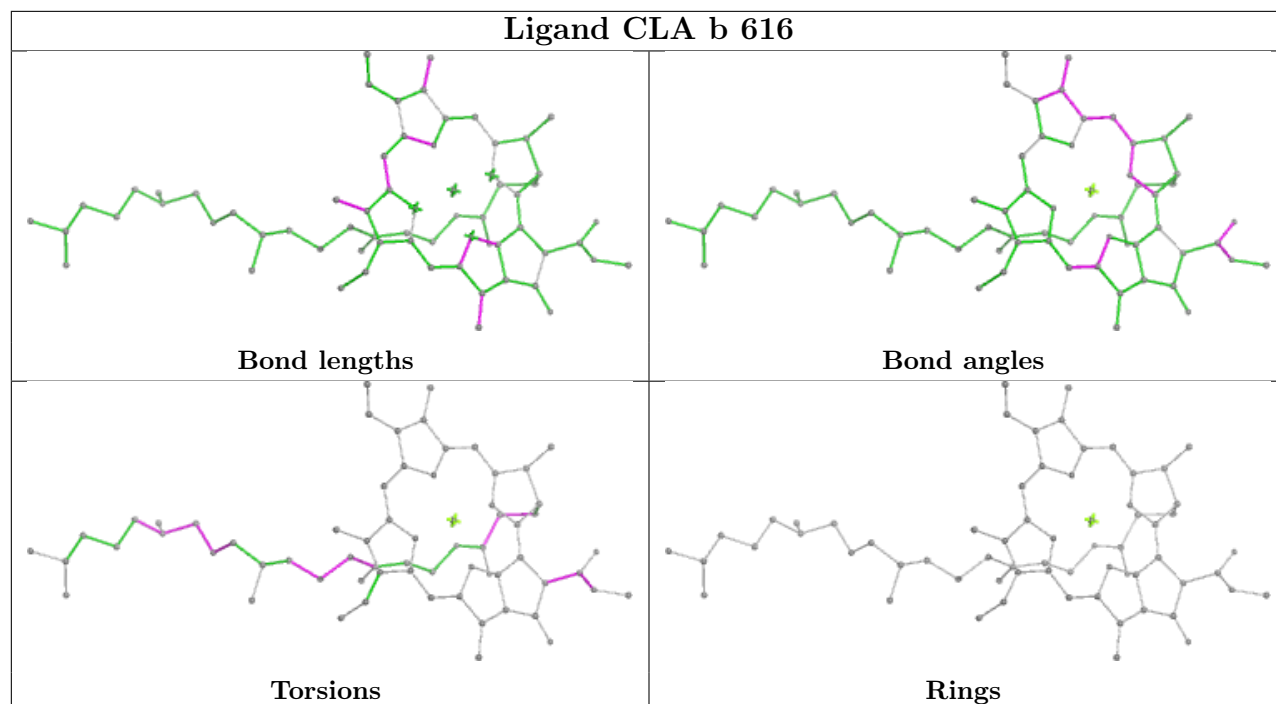
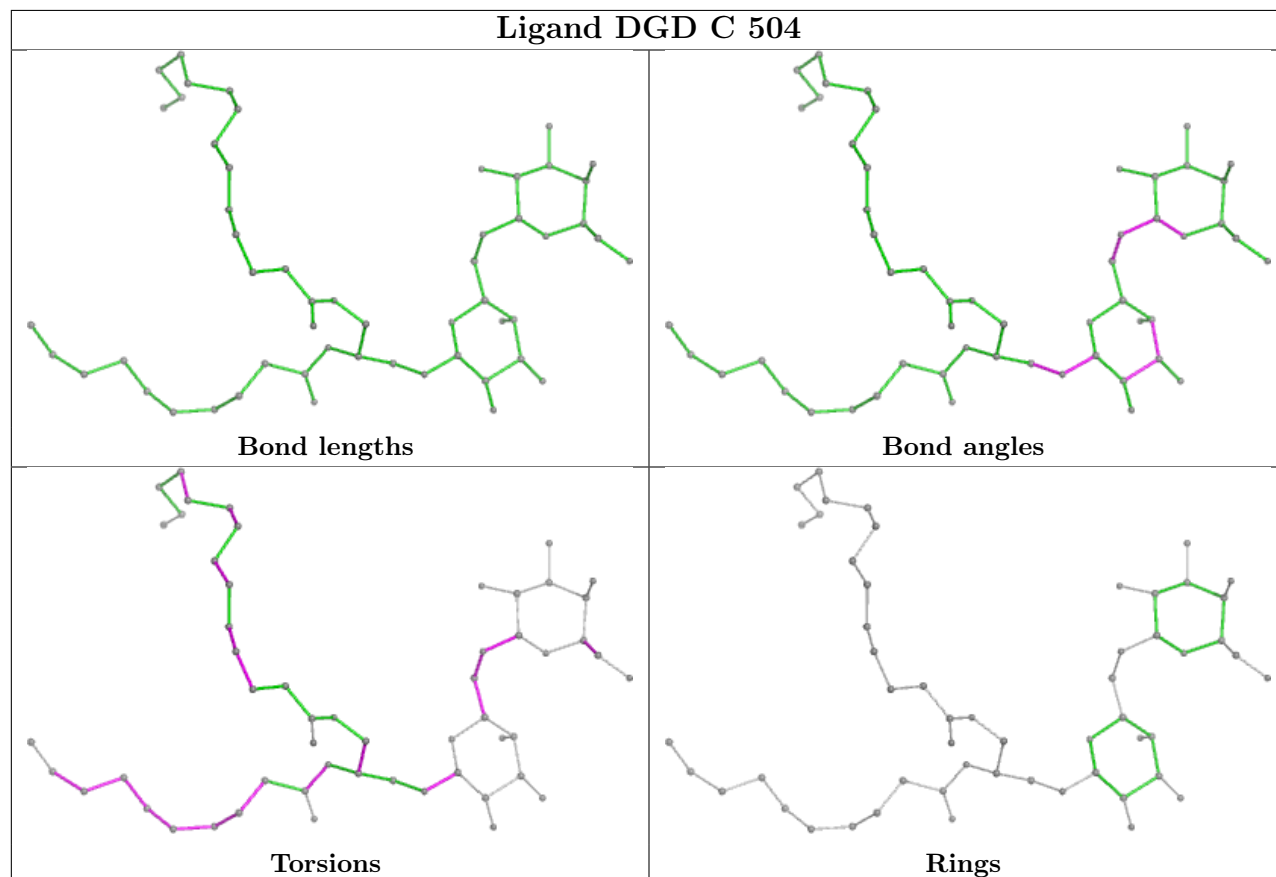




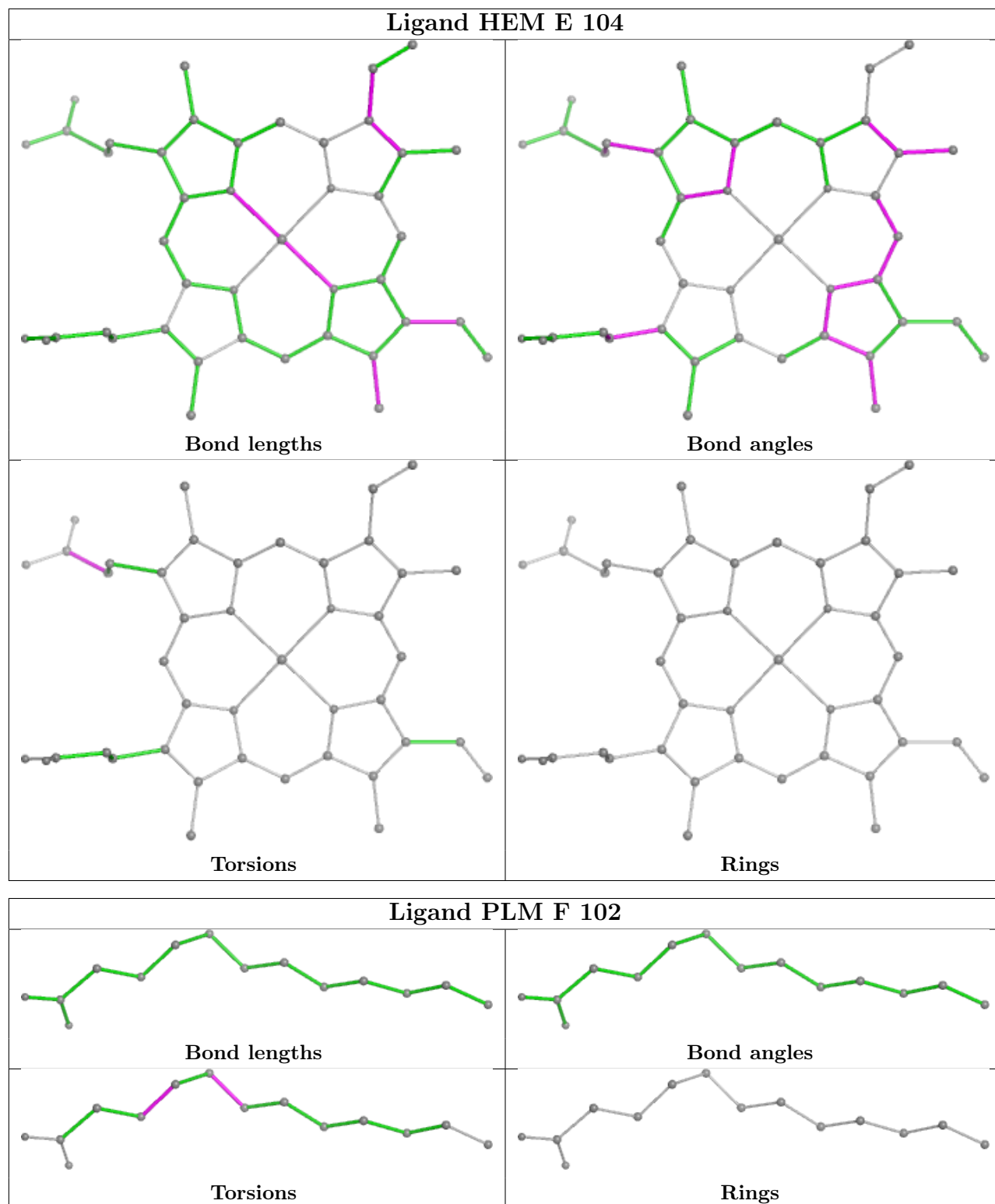




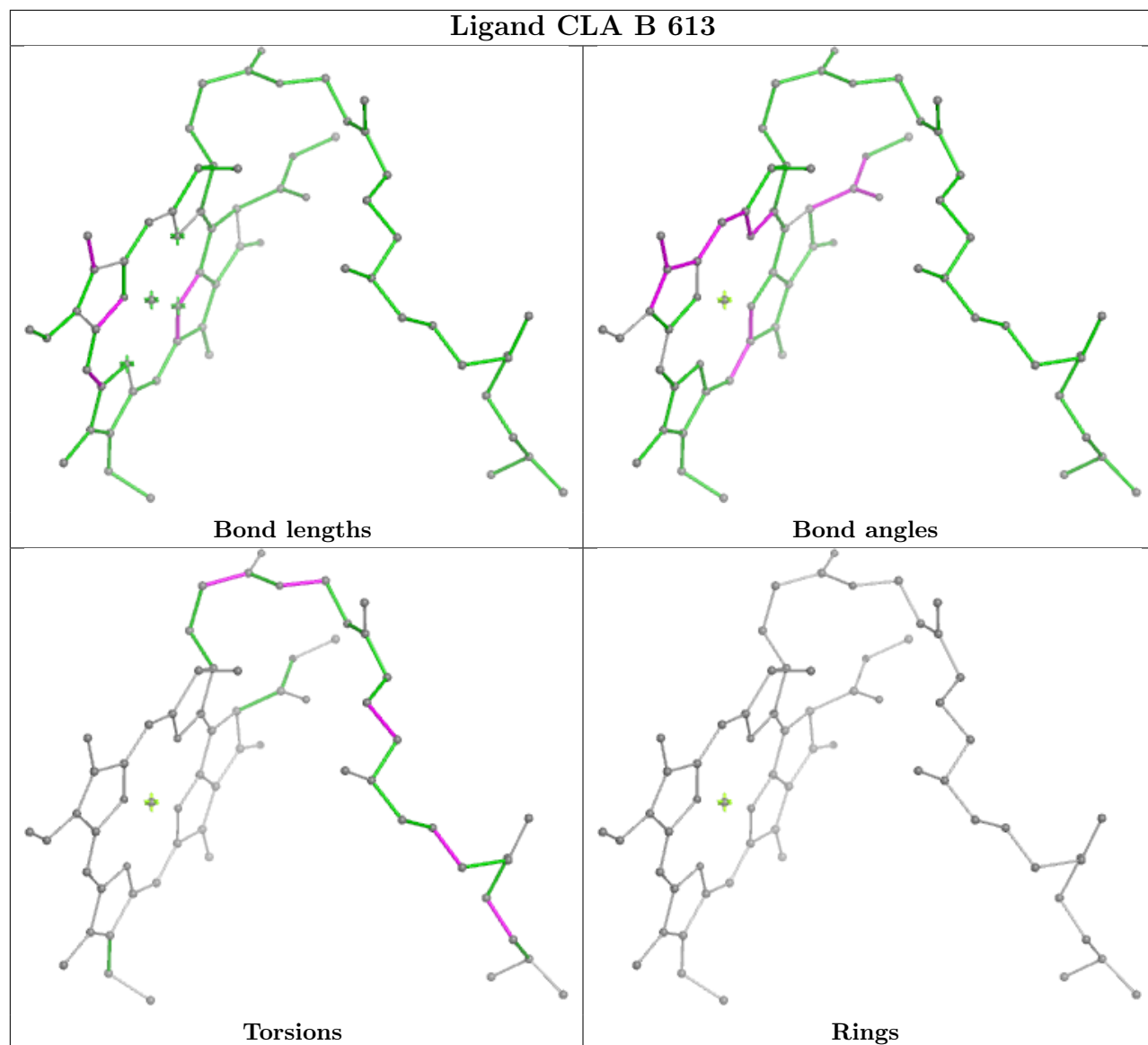


**Ligand CLA b 616****Ligand DGD C 504**

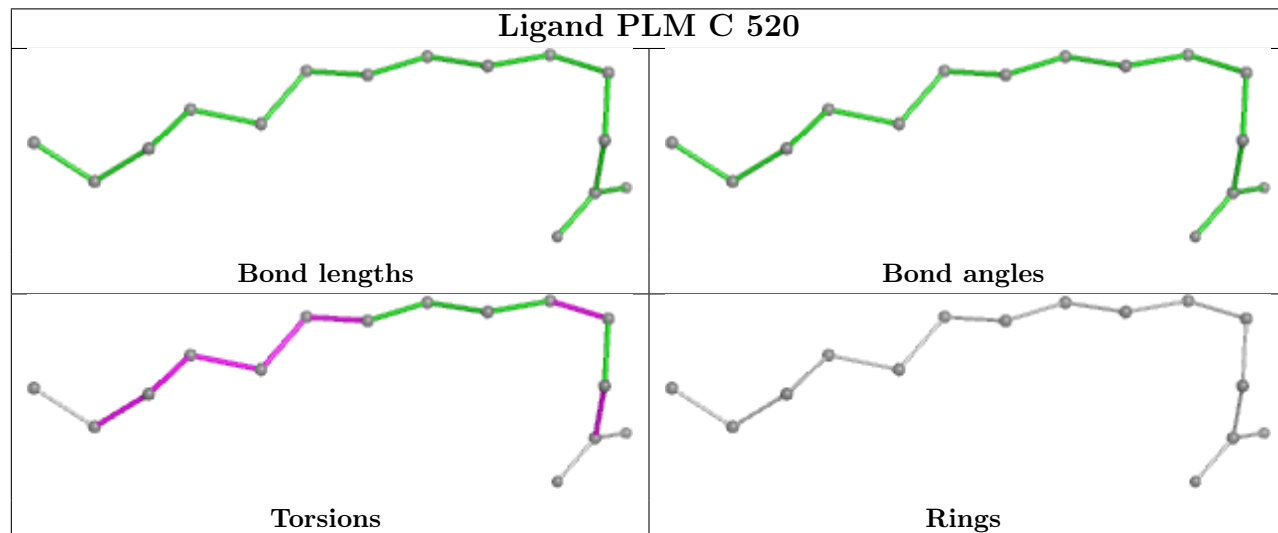


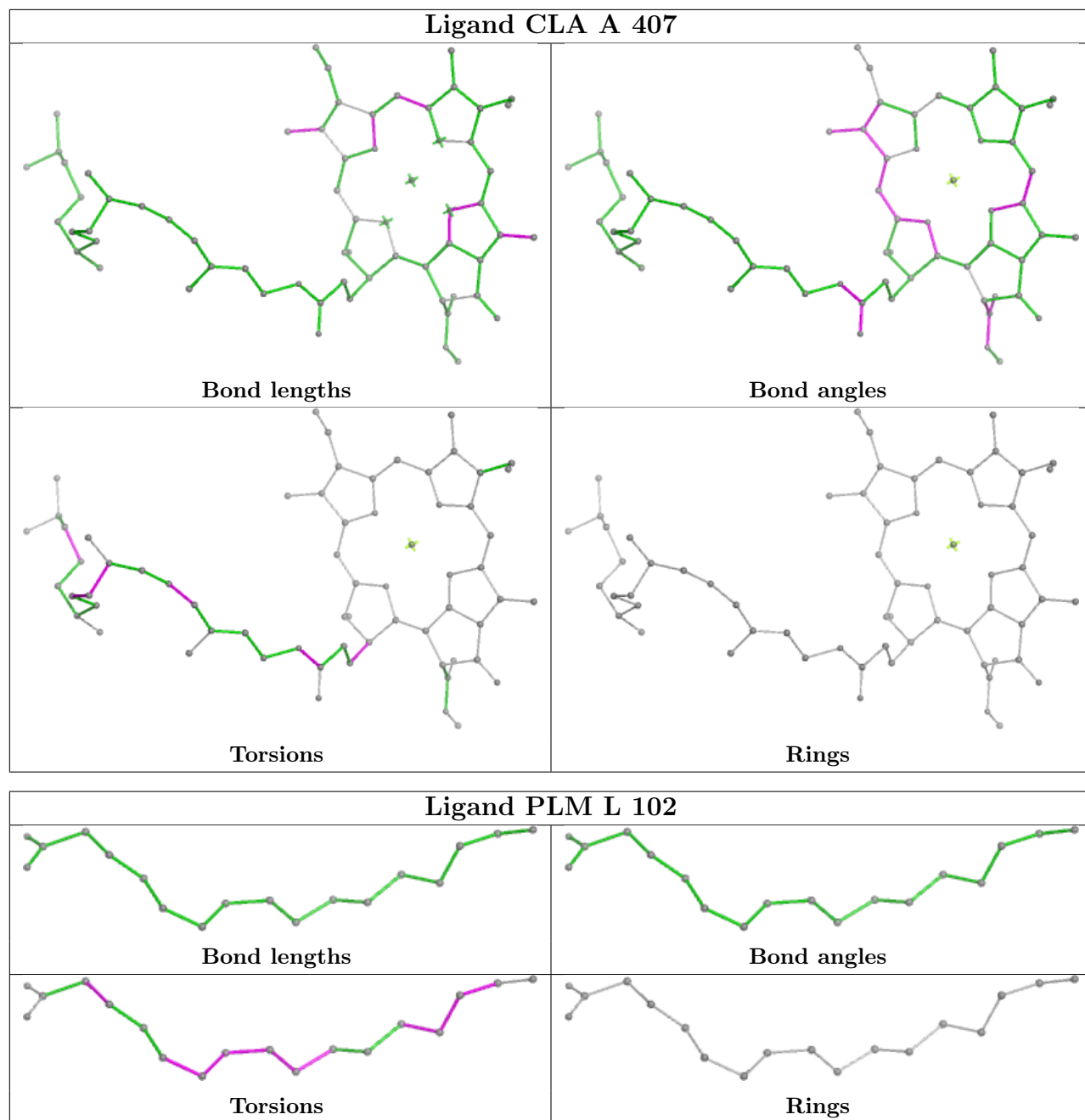


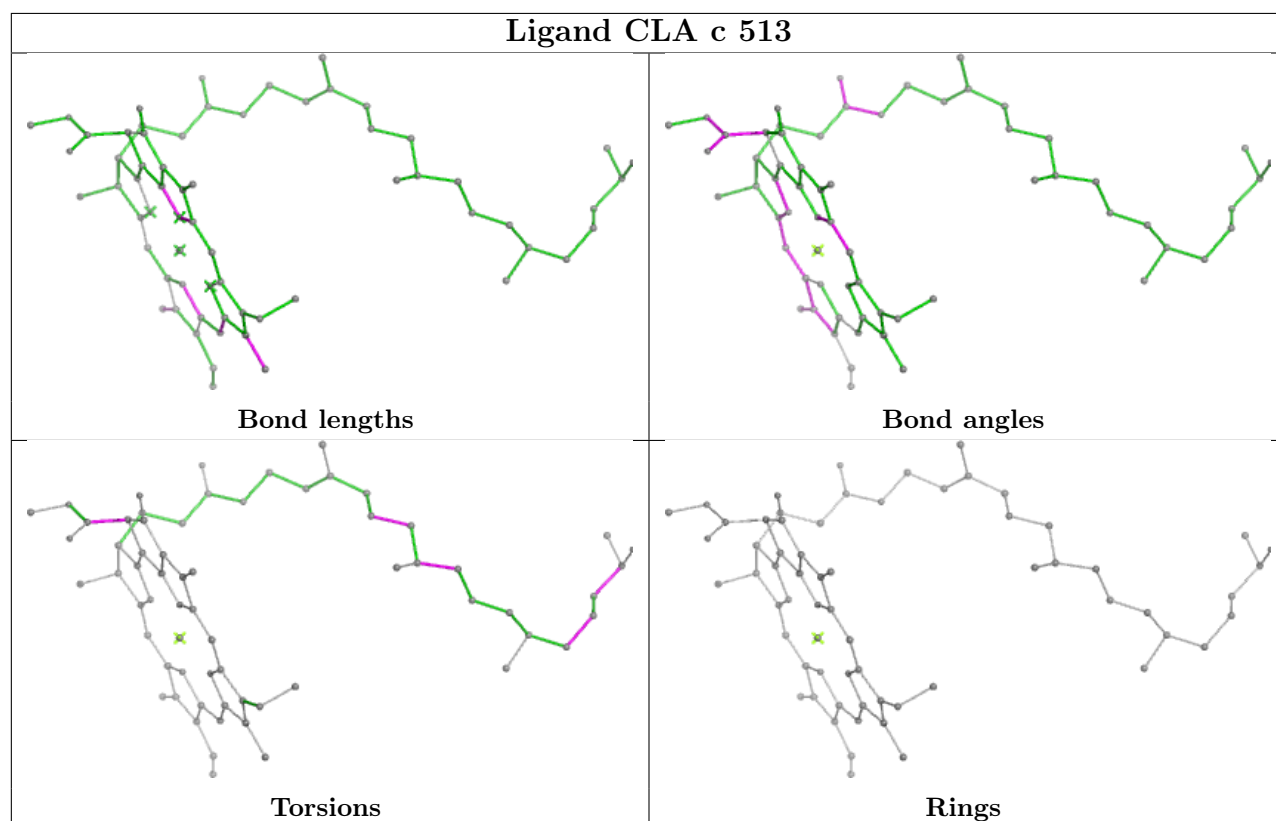
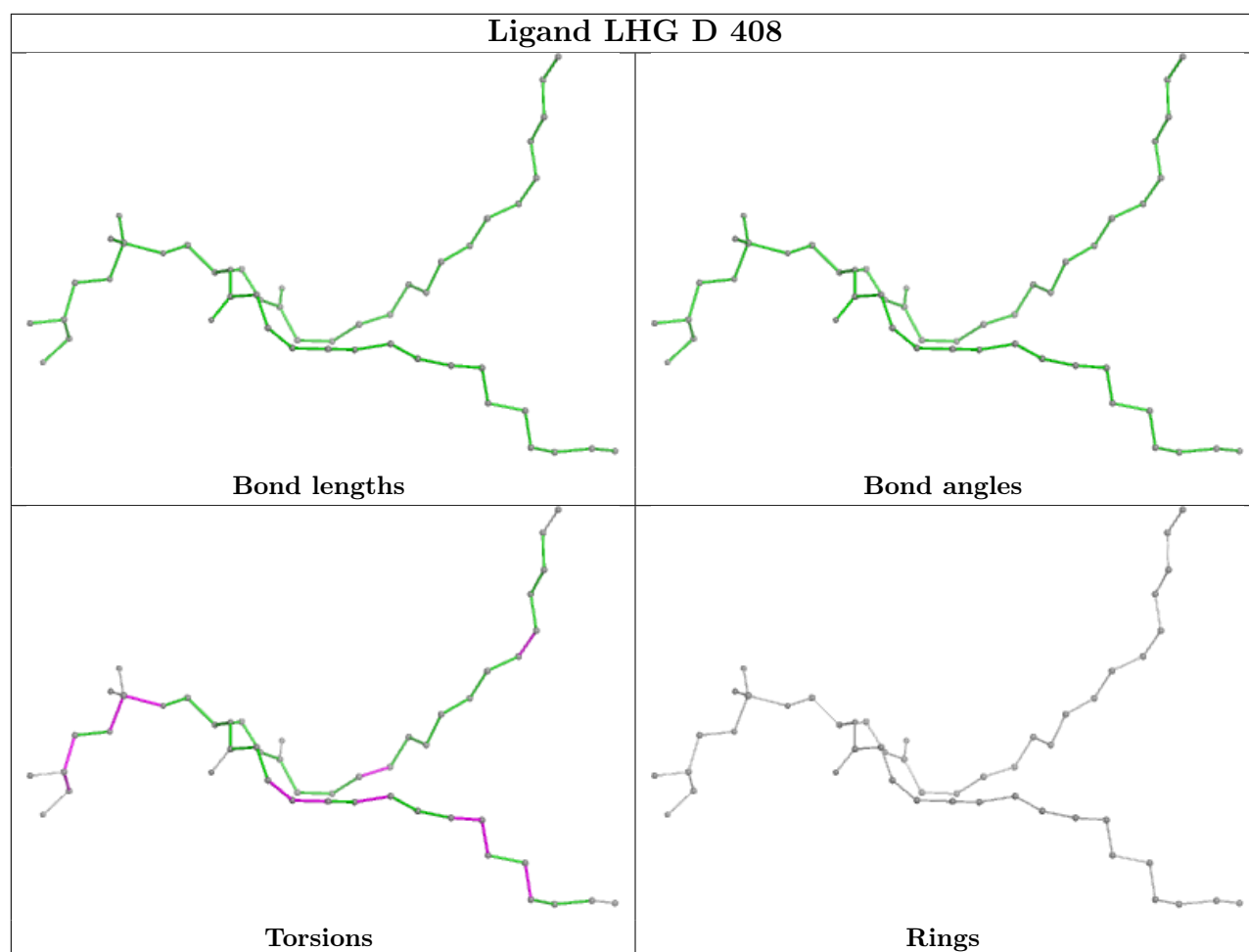
## Ligand CLA B 613

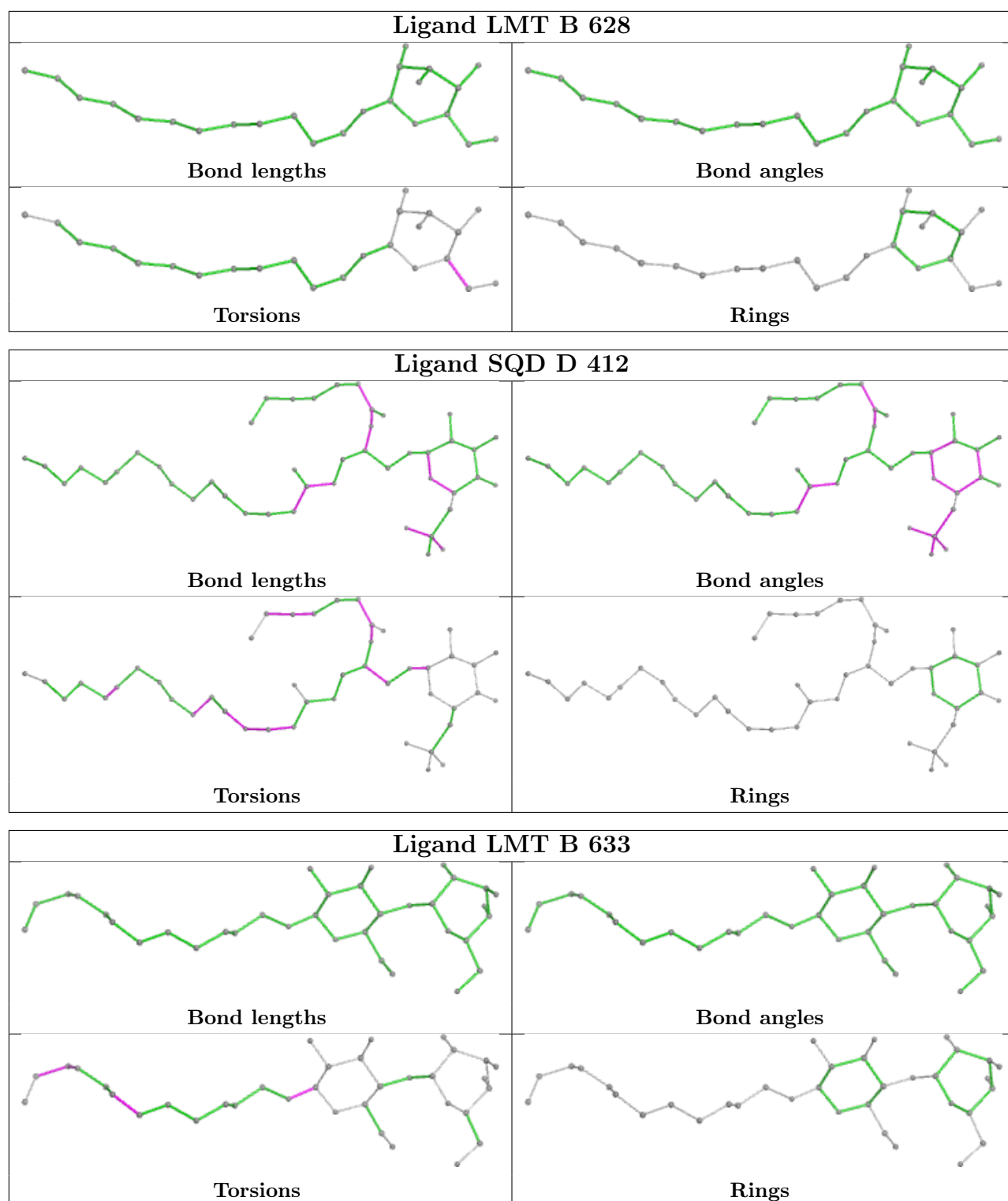


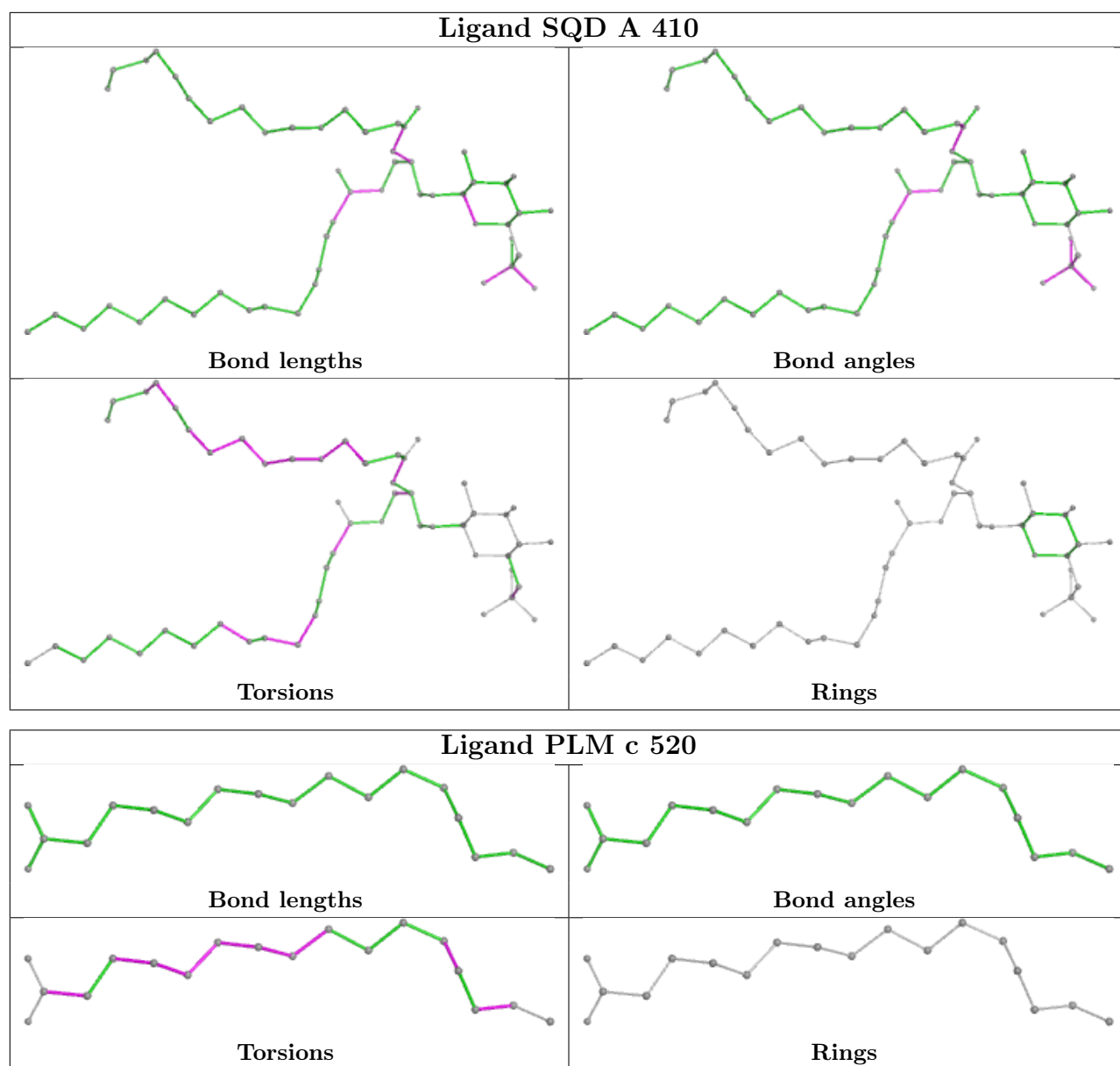
## Ligand PLM C 520

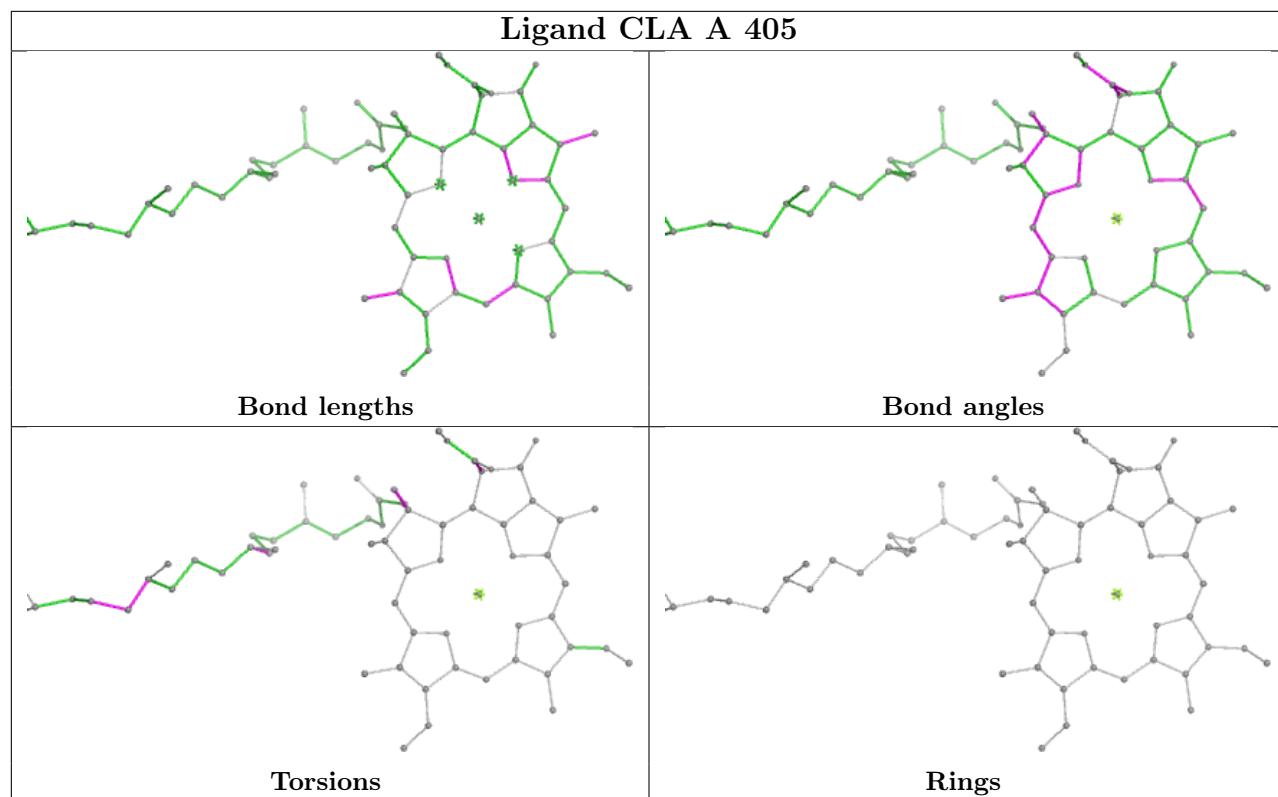




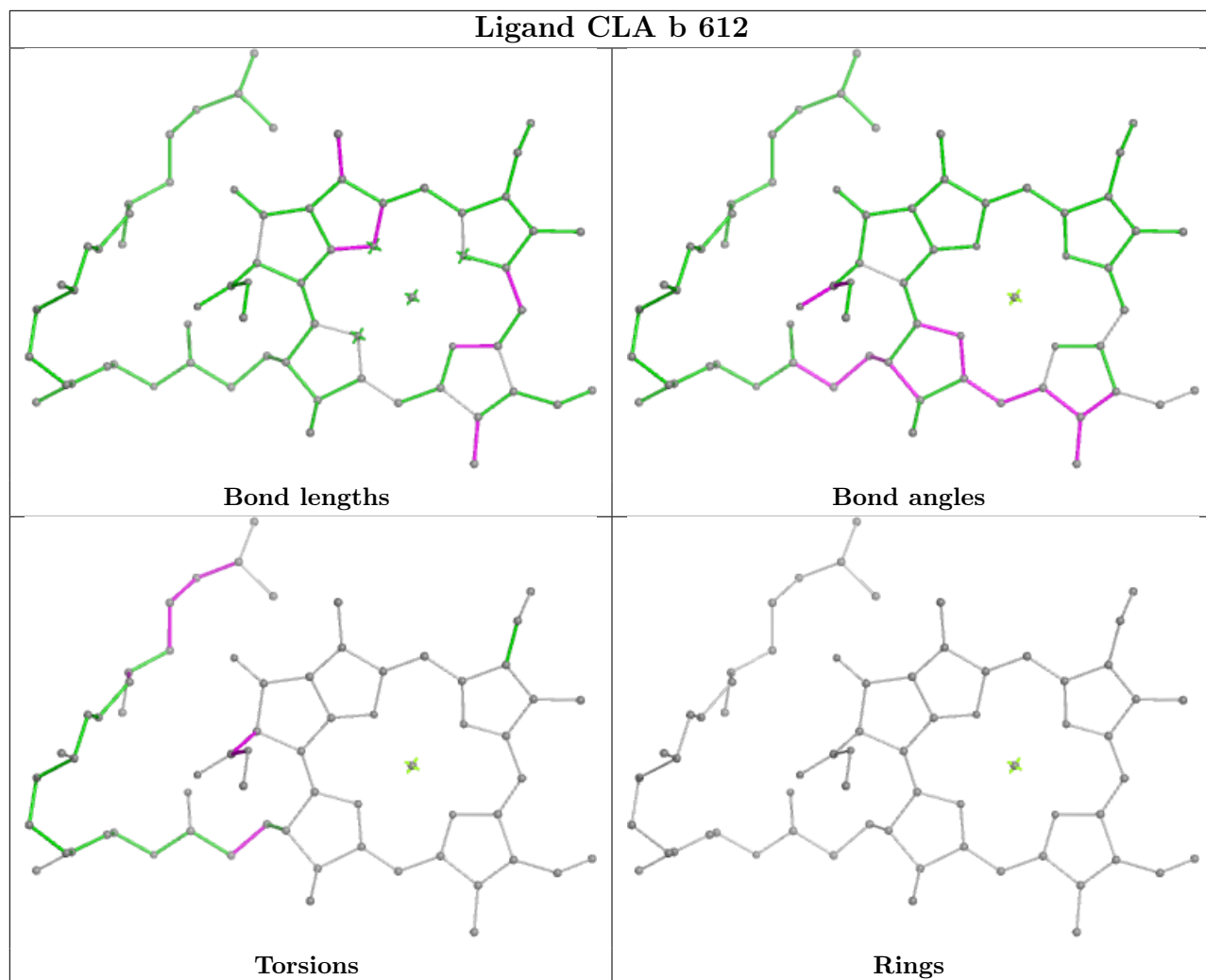




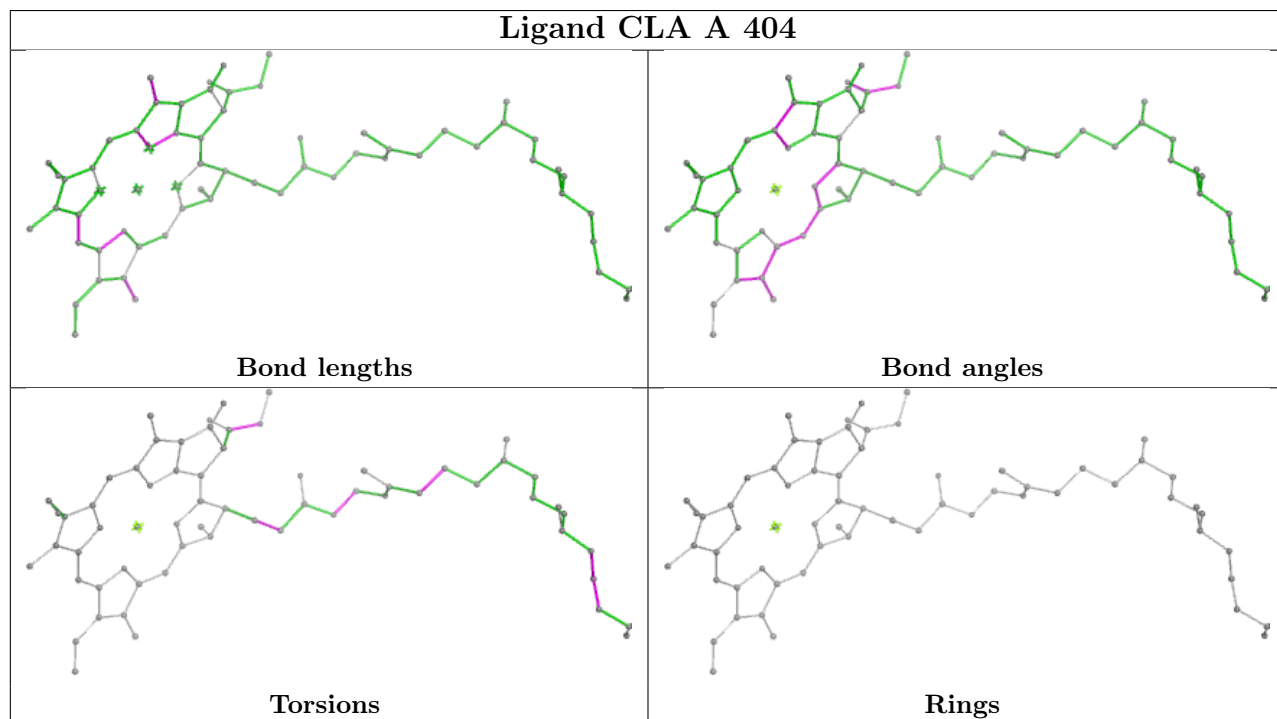




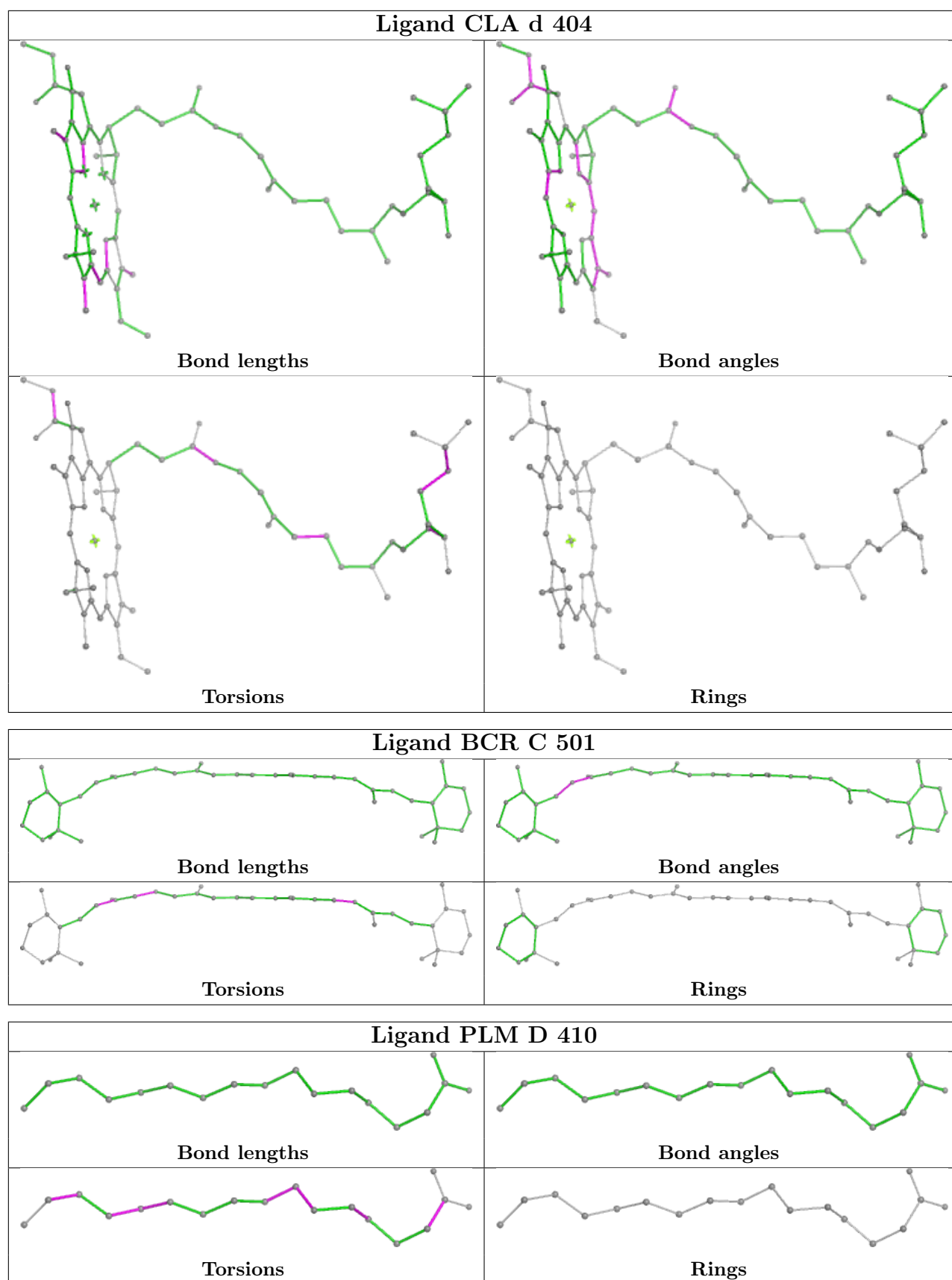
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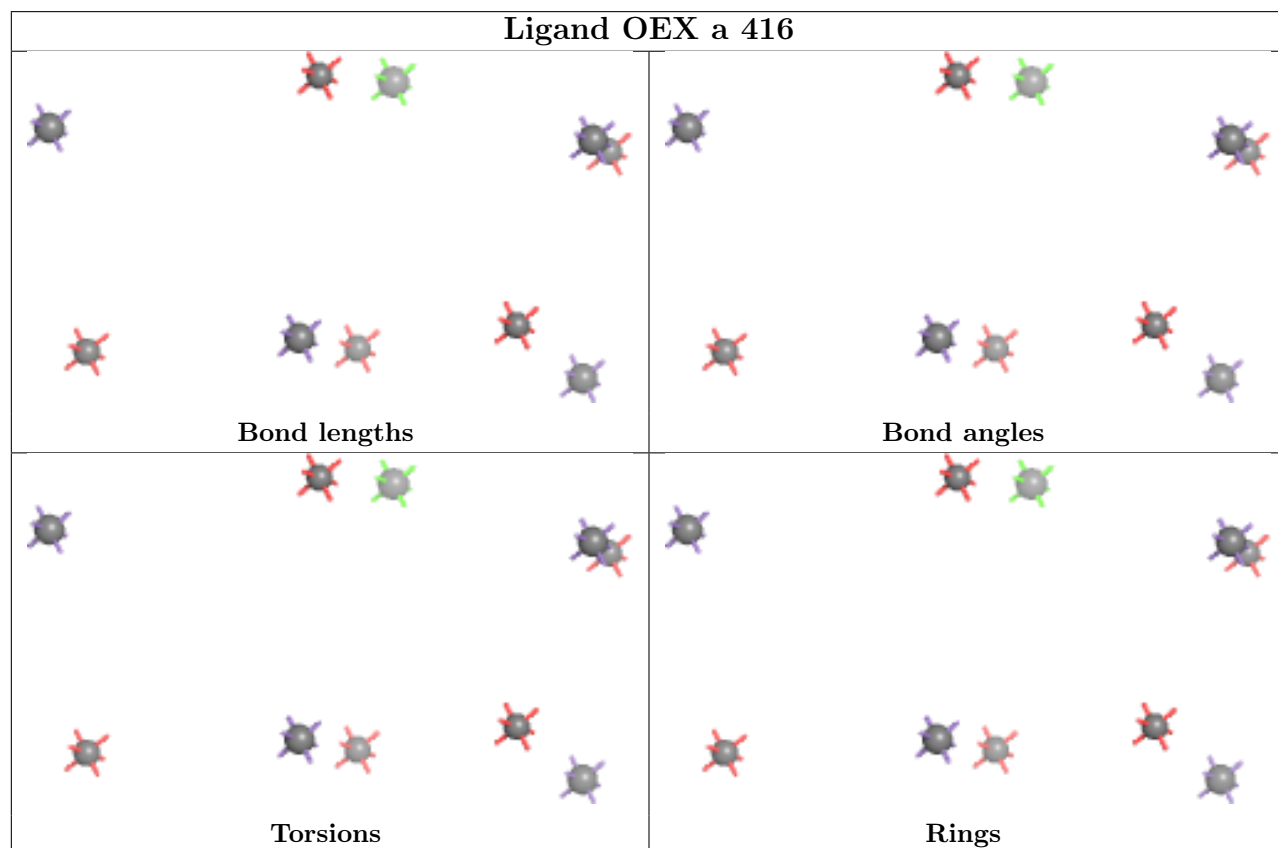
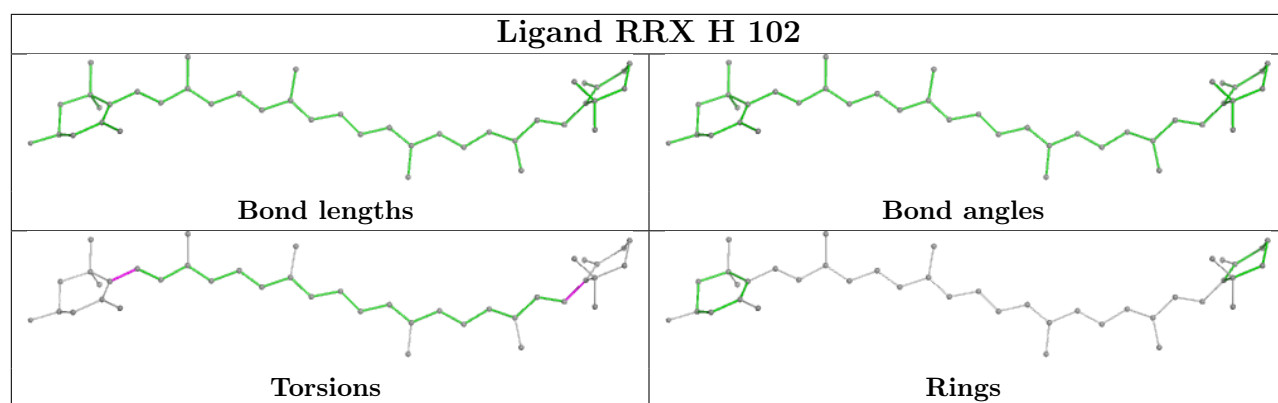


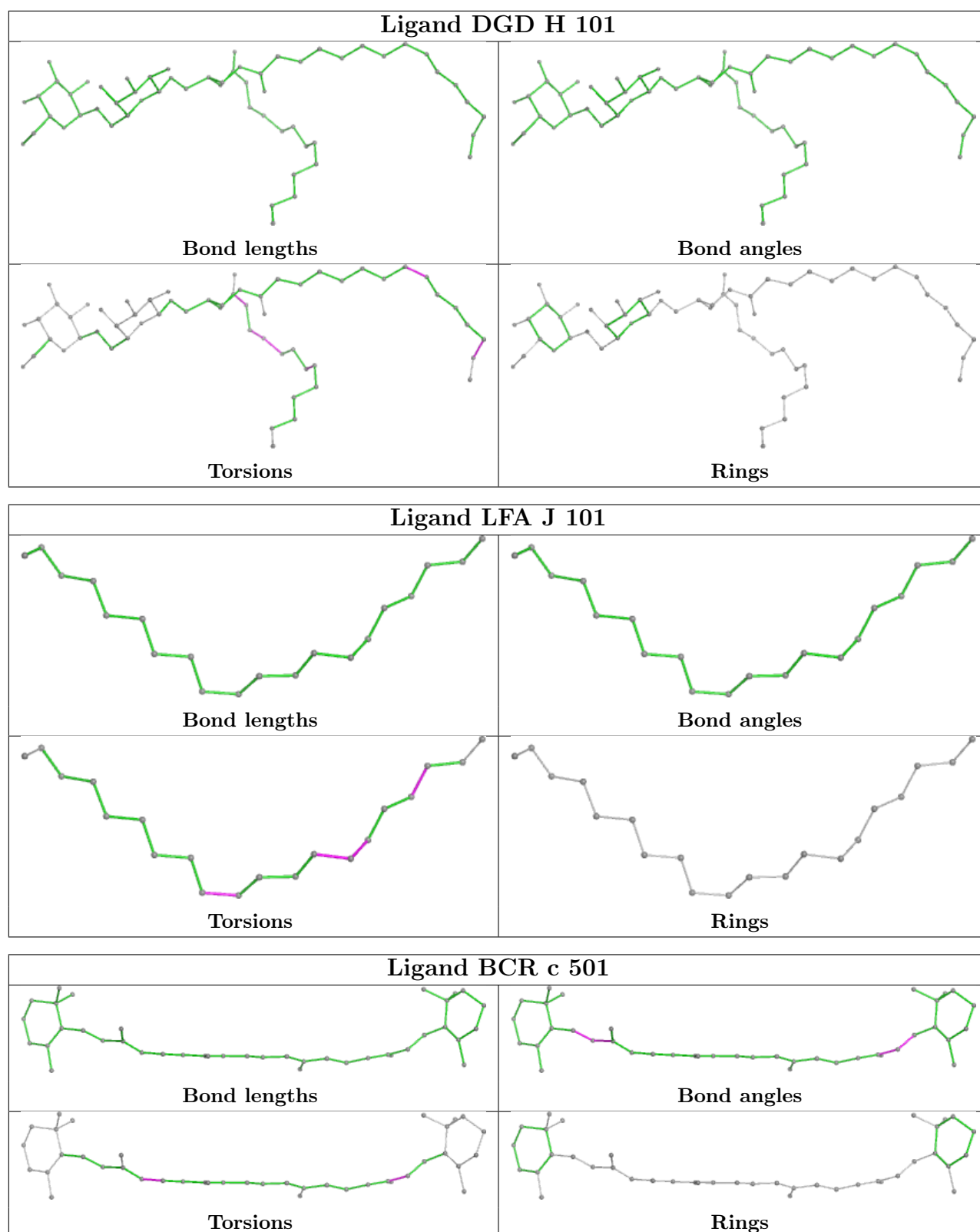
## Ligand CLA A 404

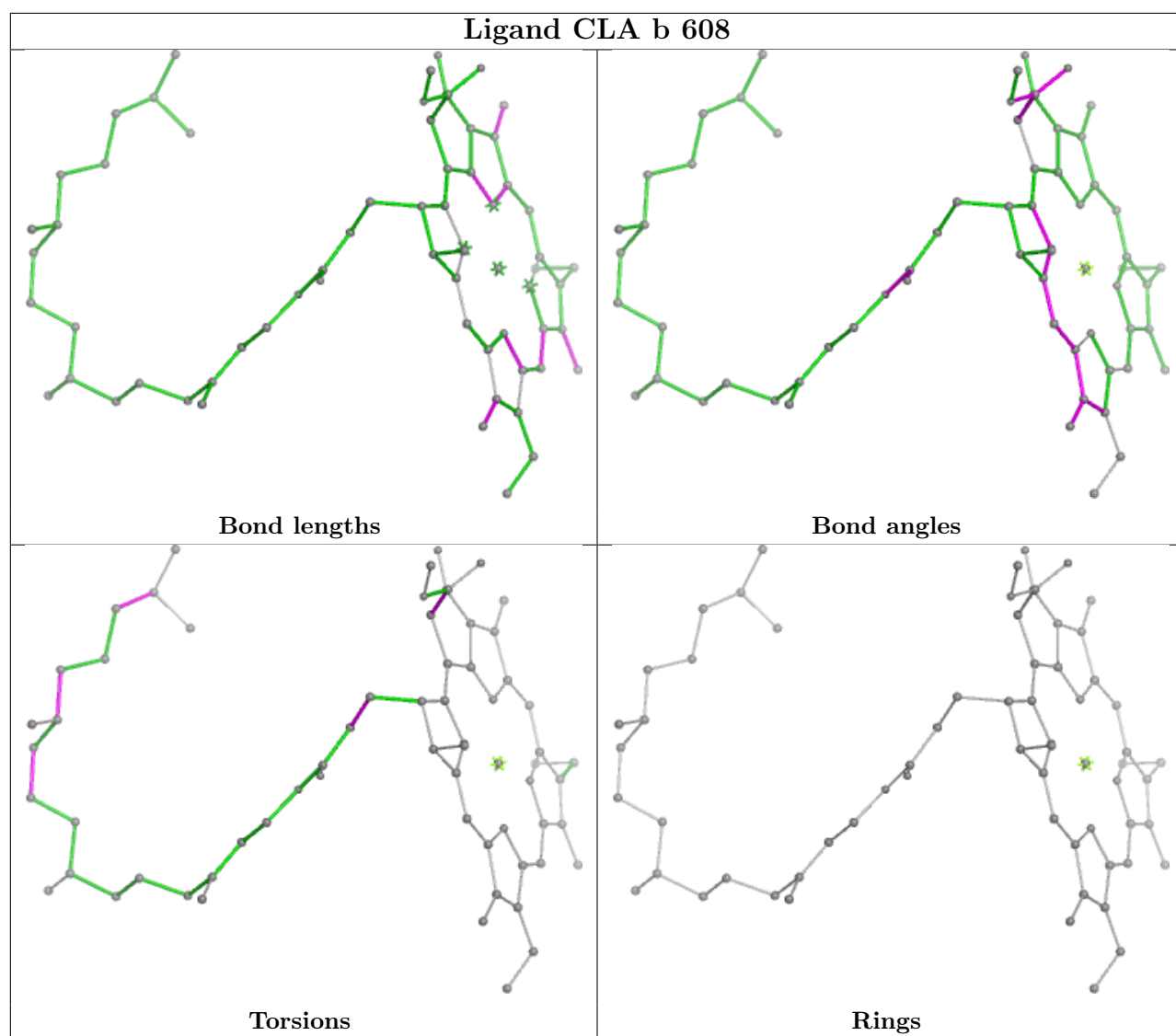


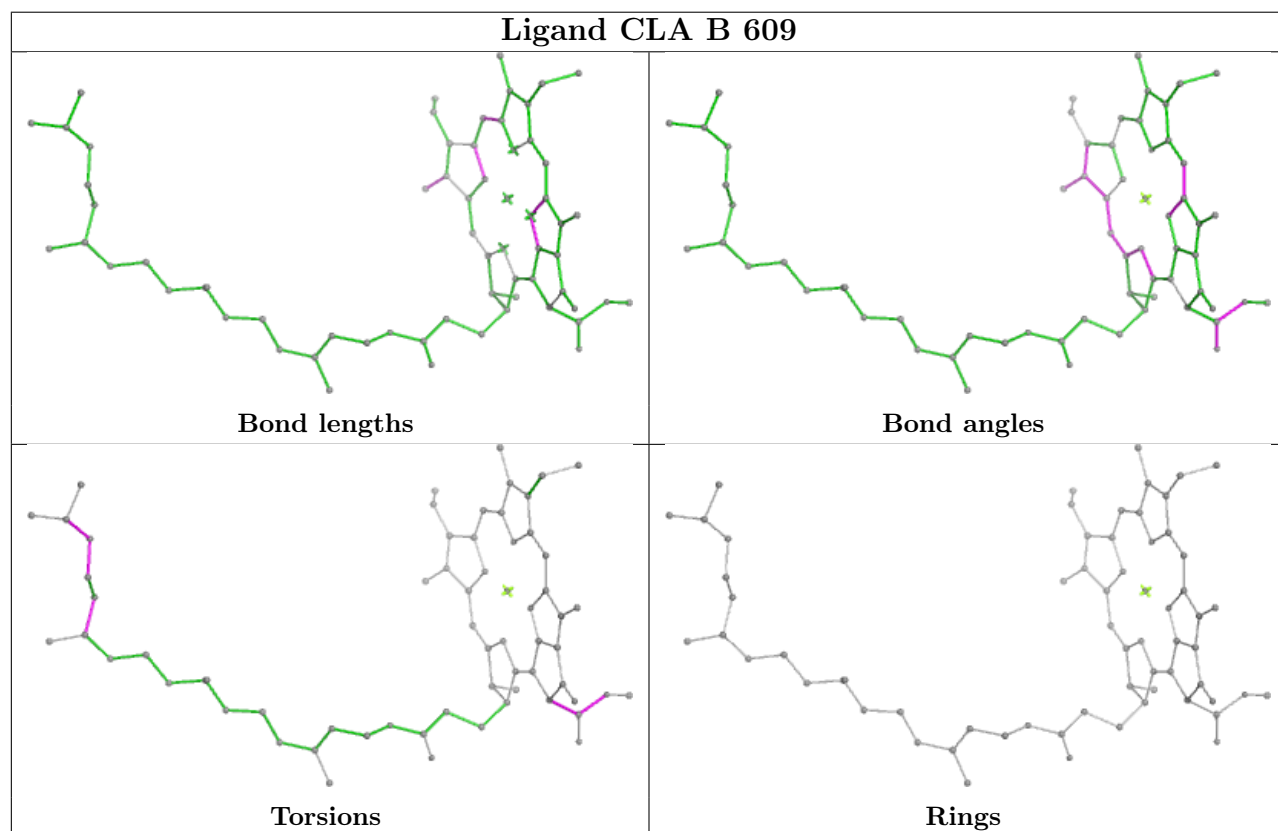
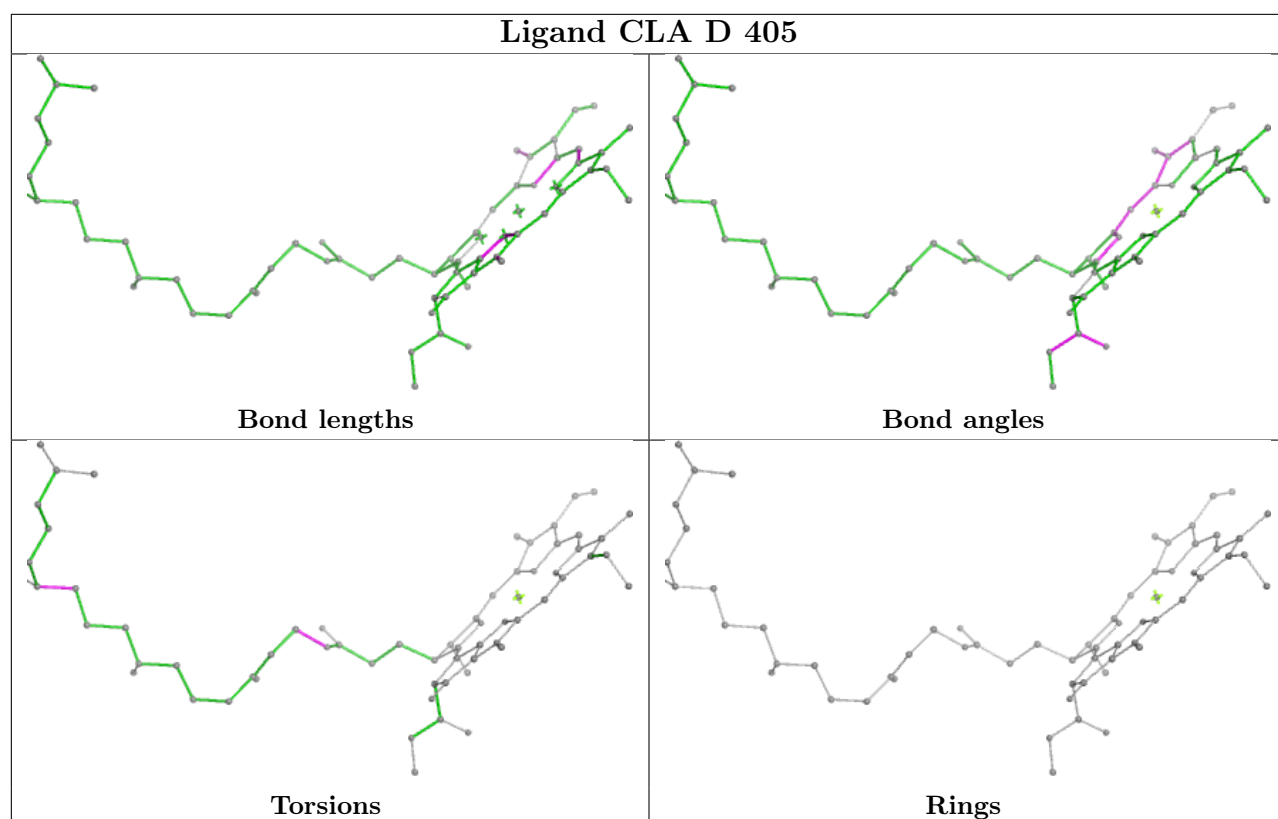


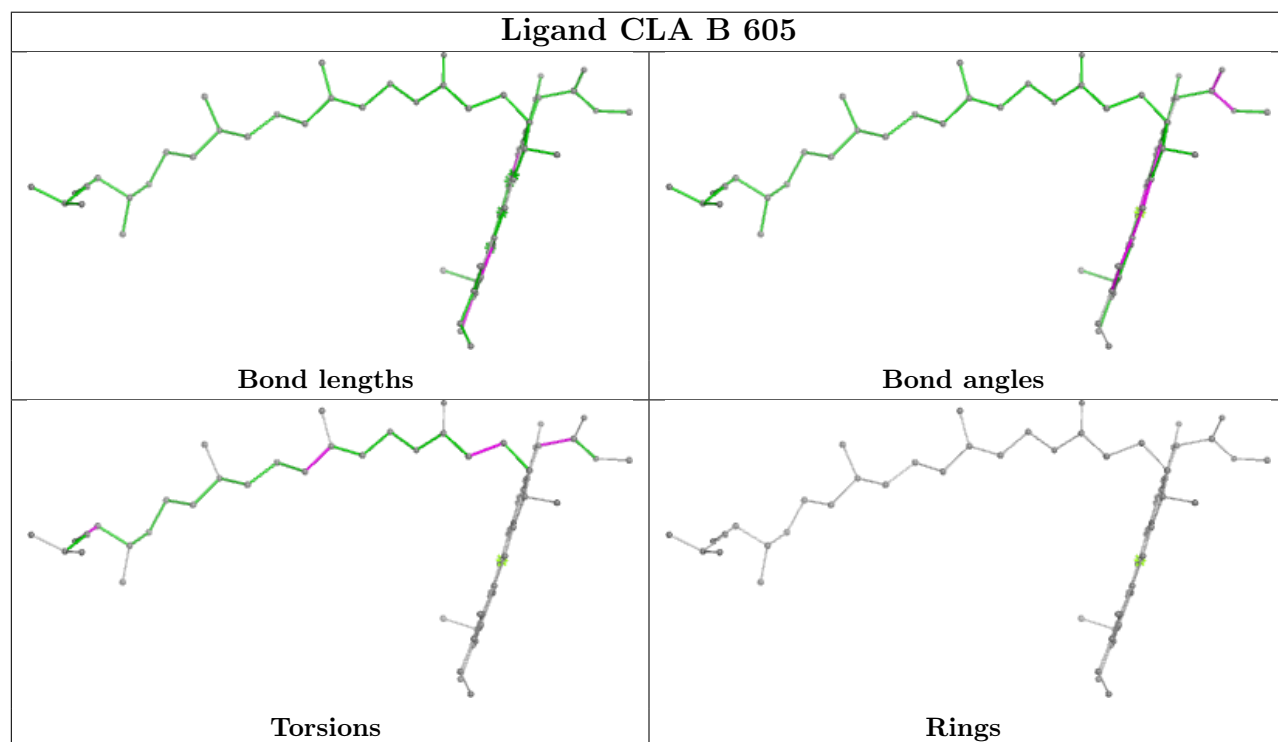
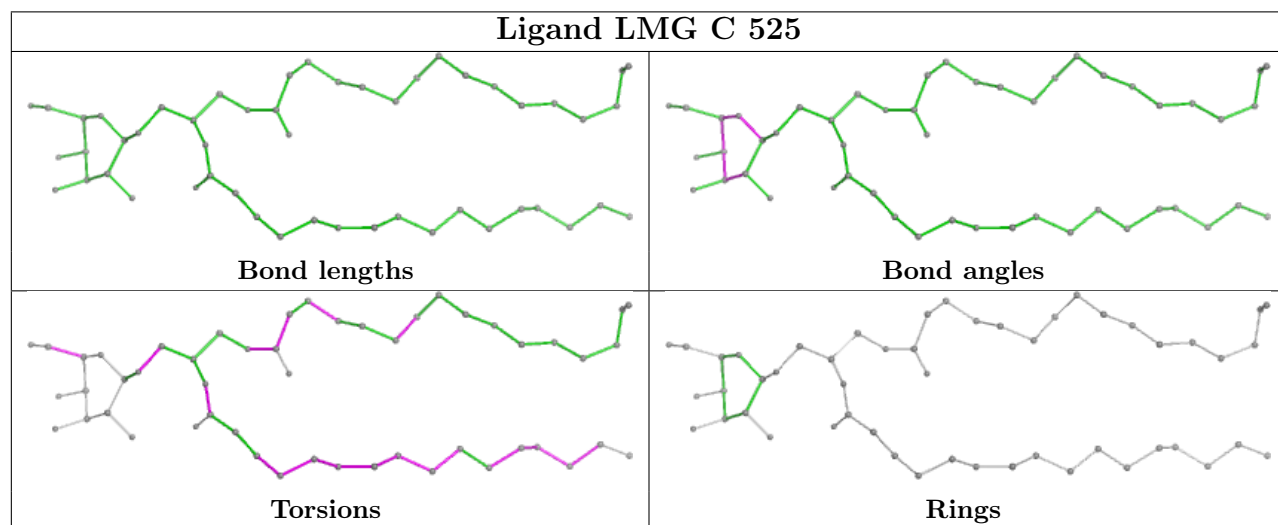
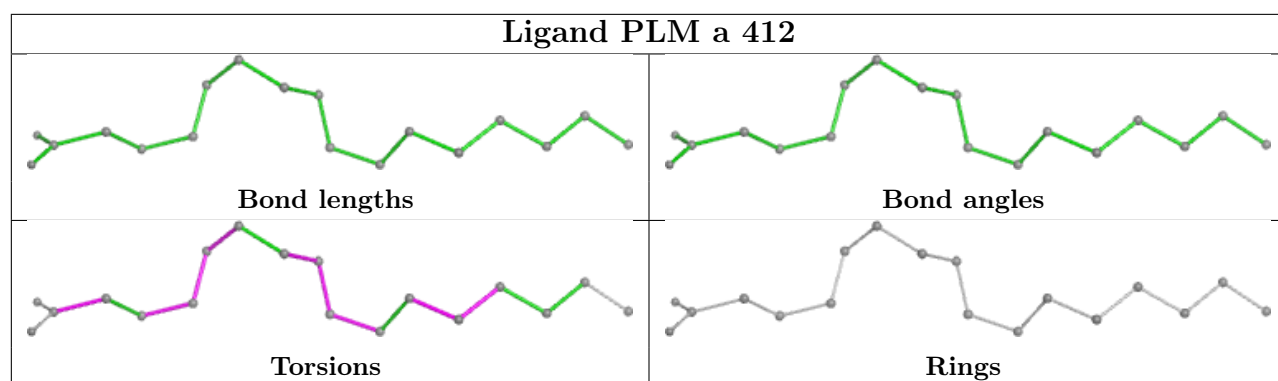


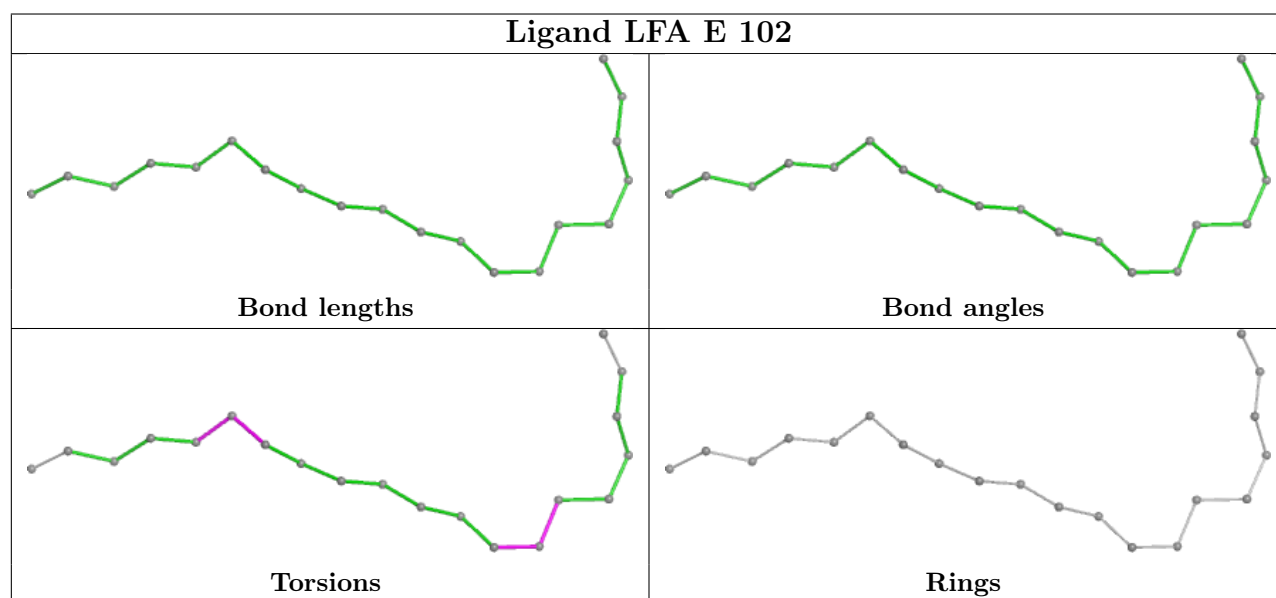
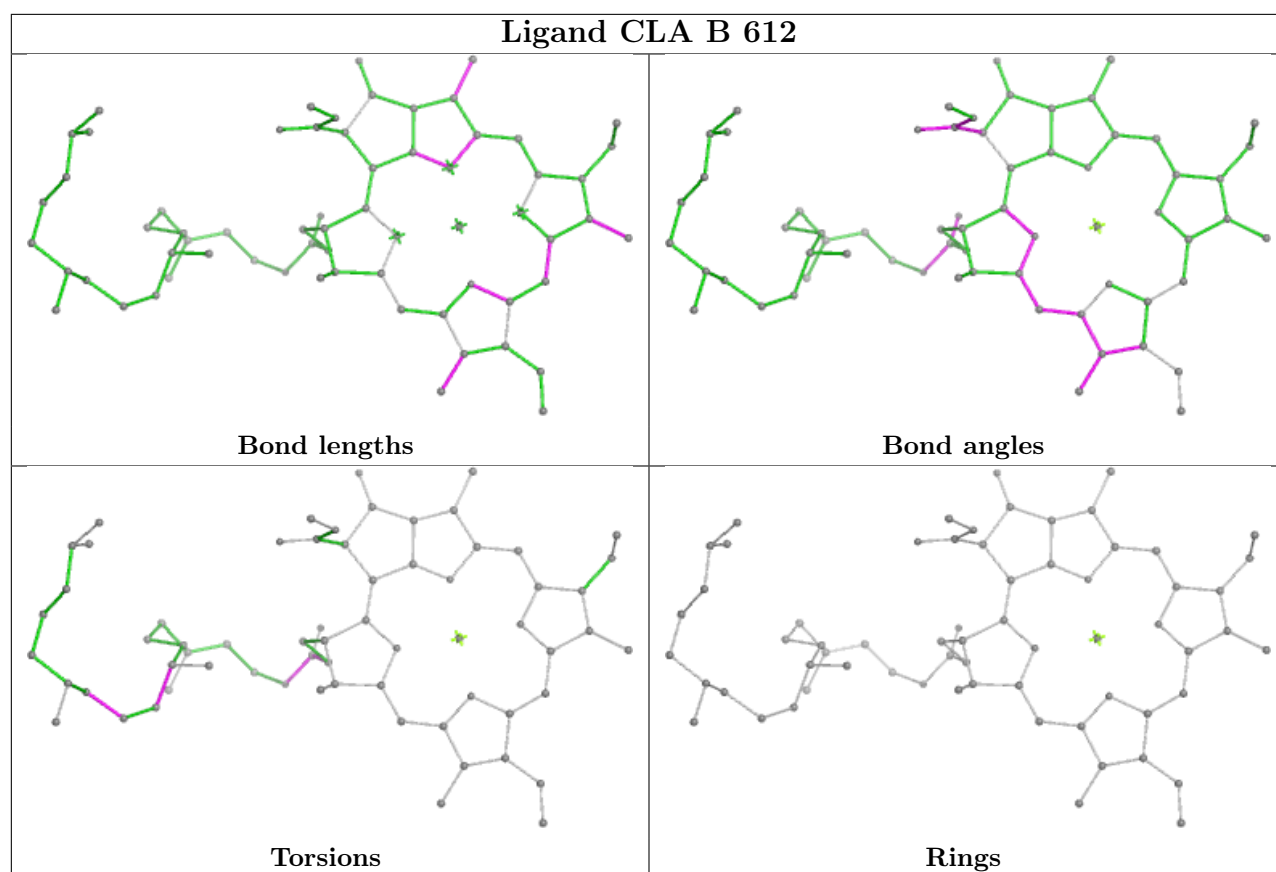


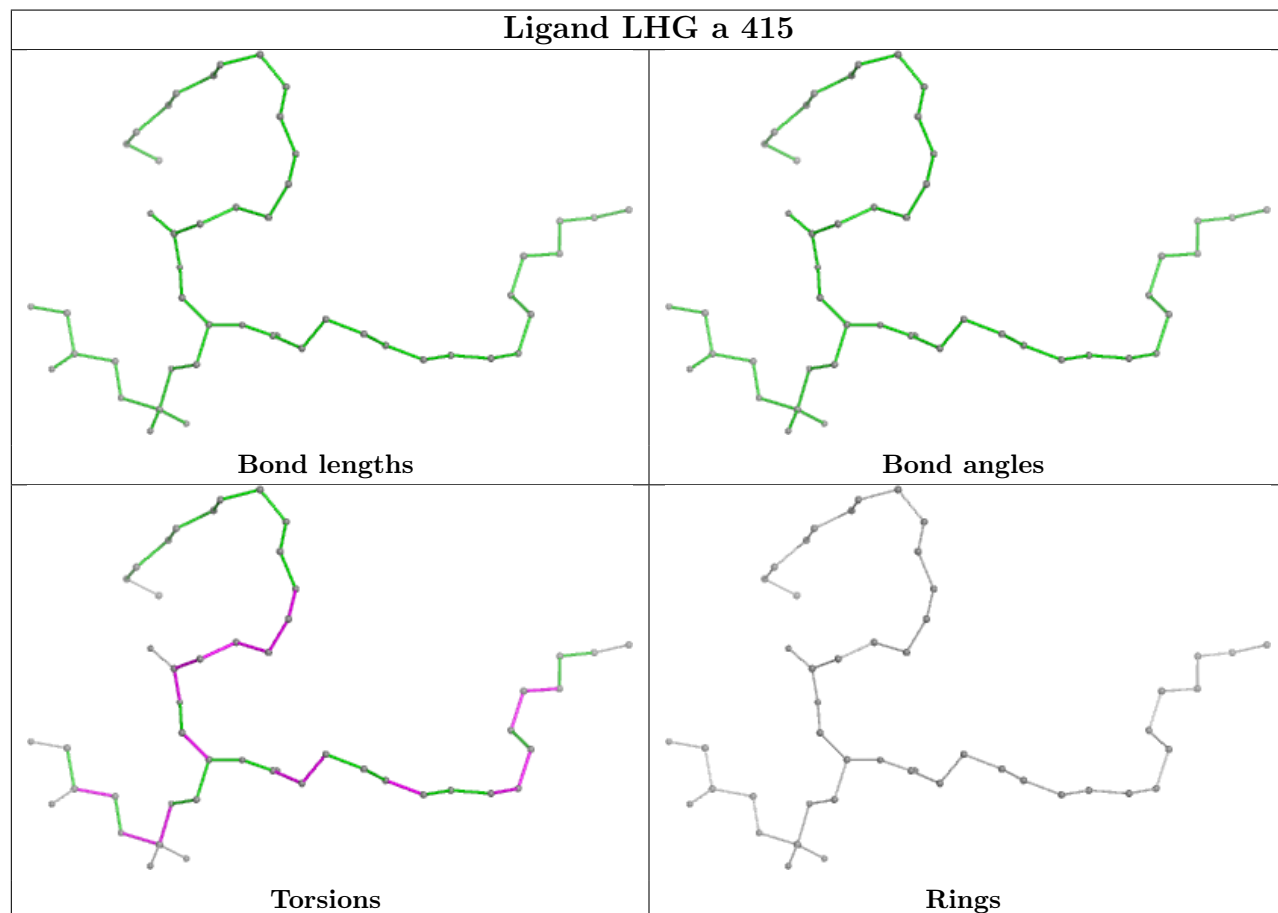
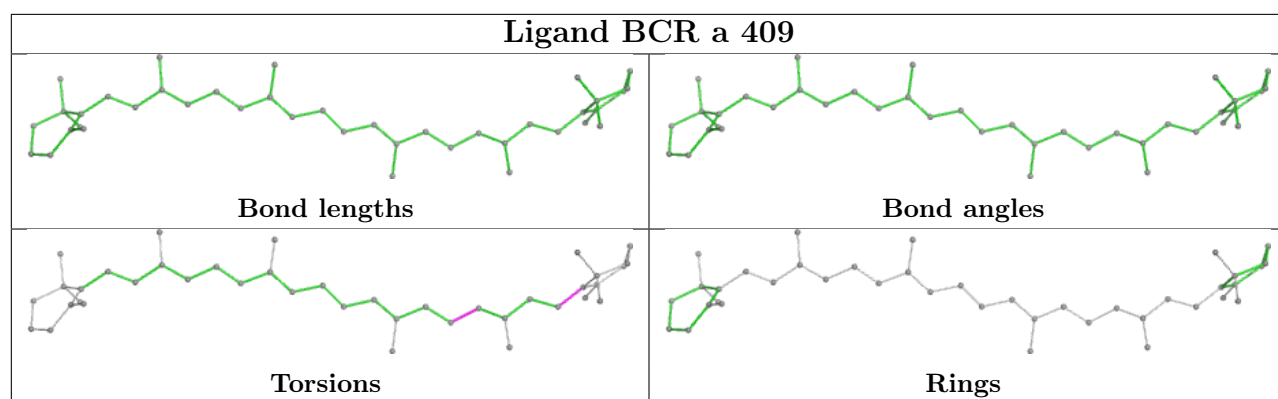




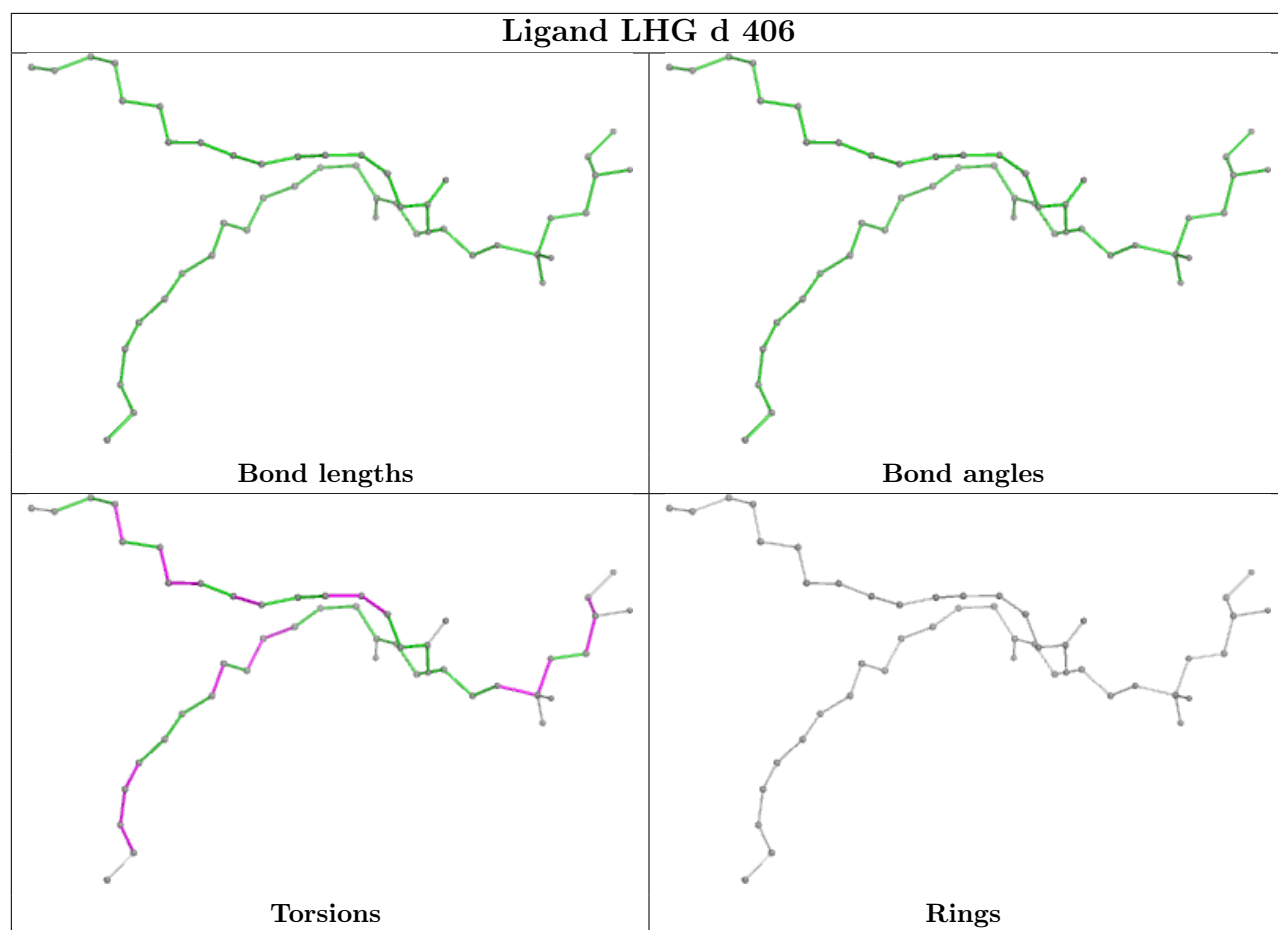
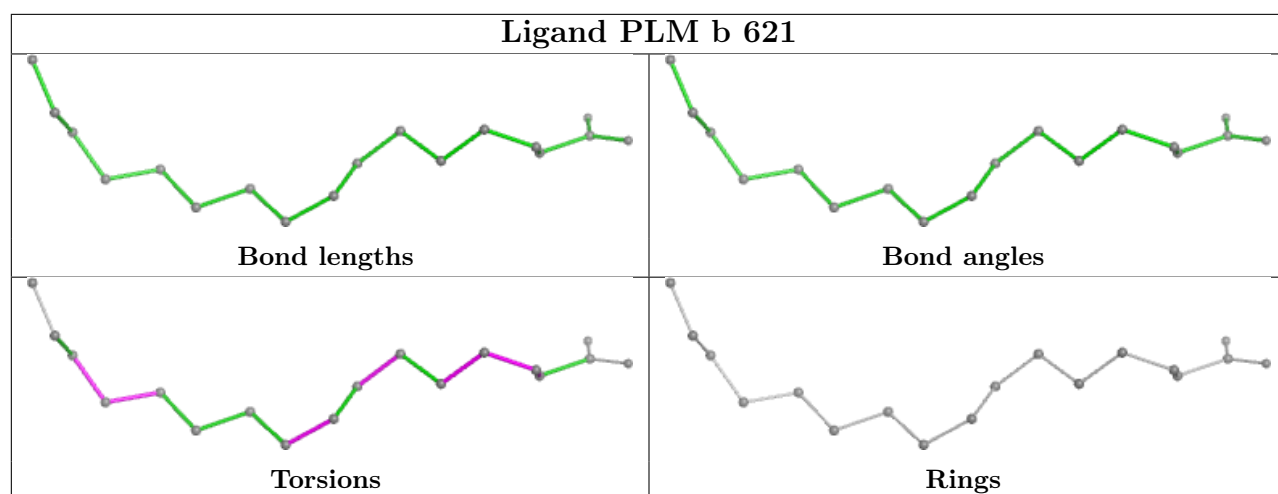


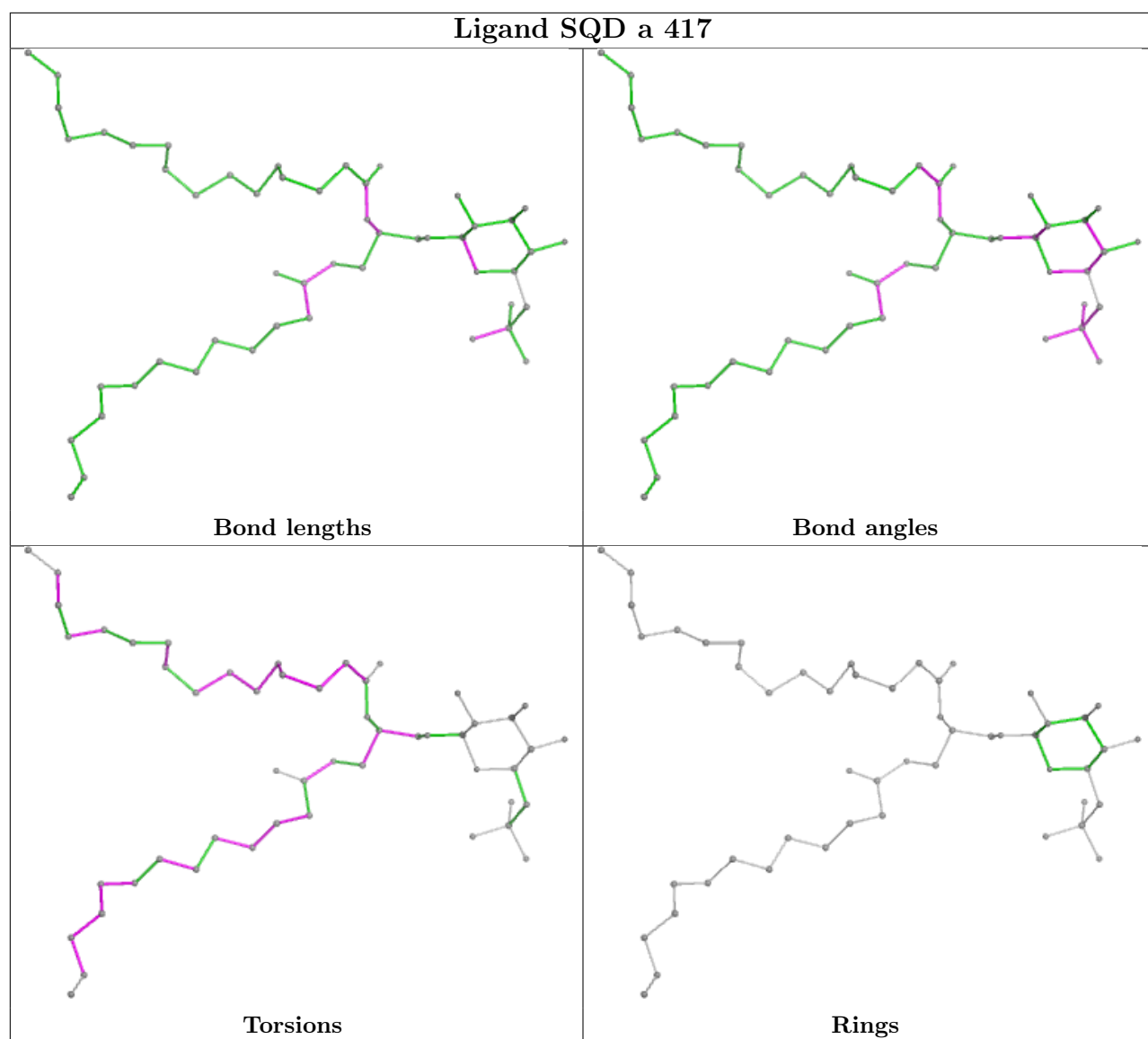


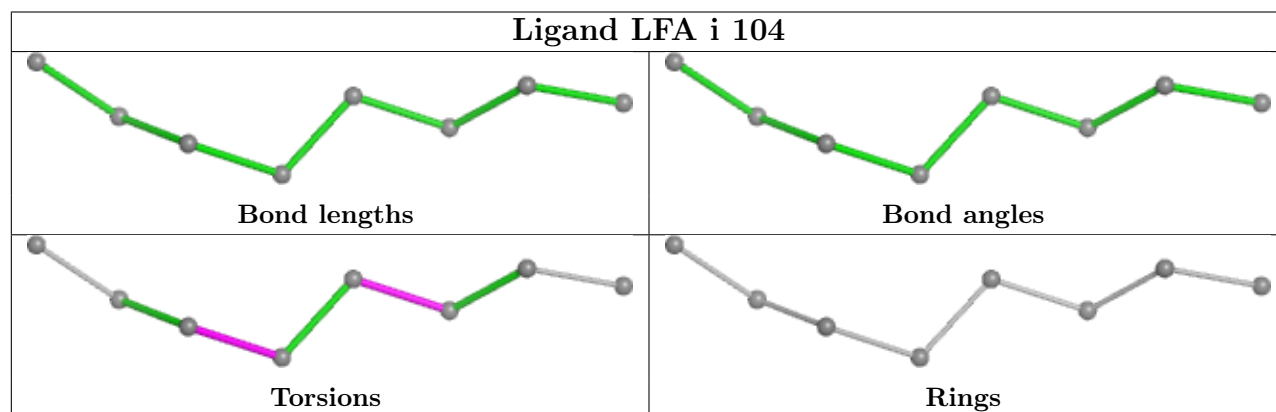
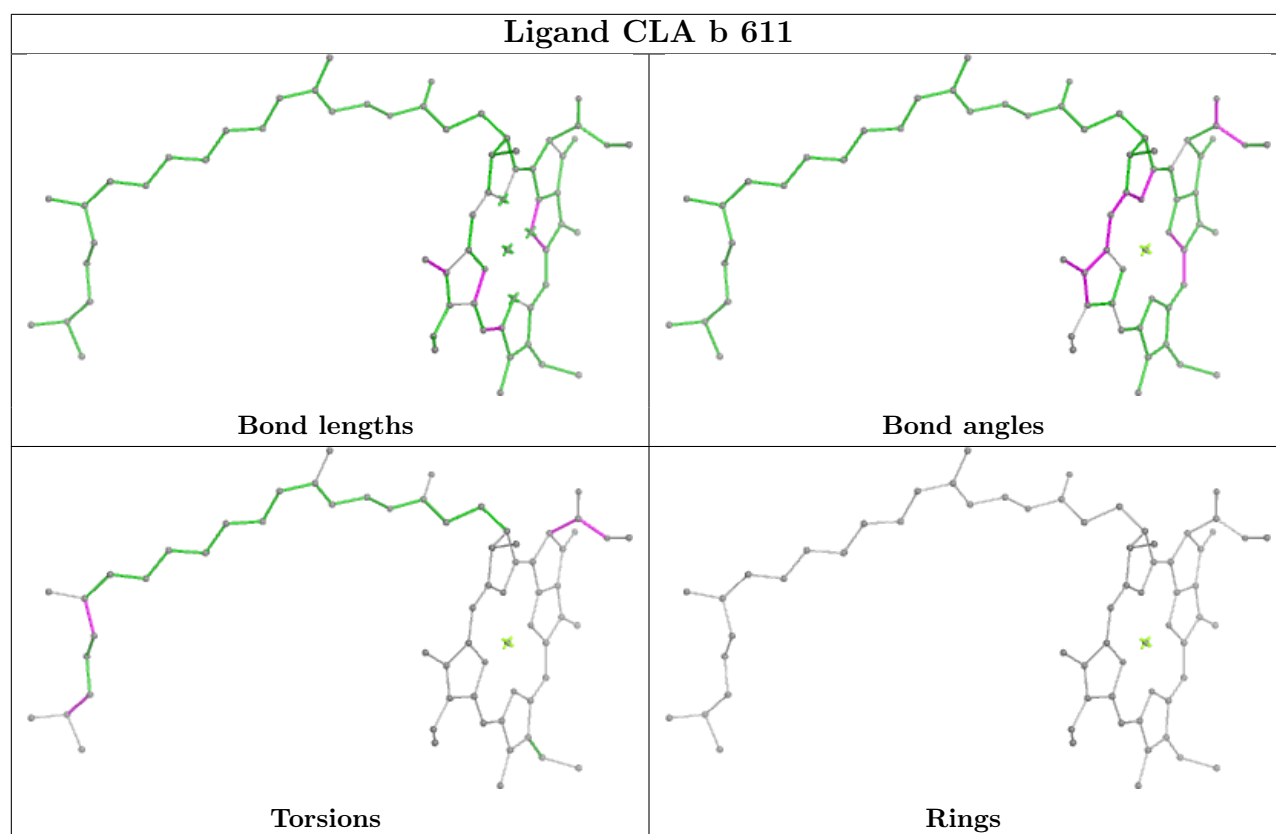


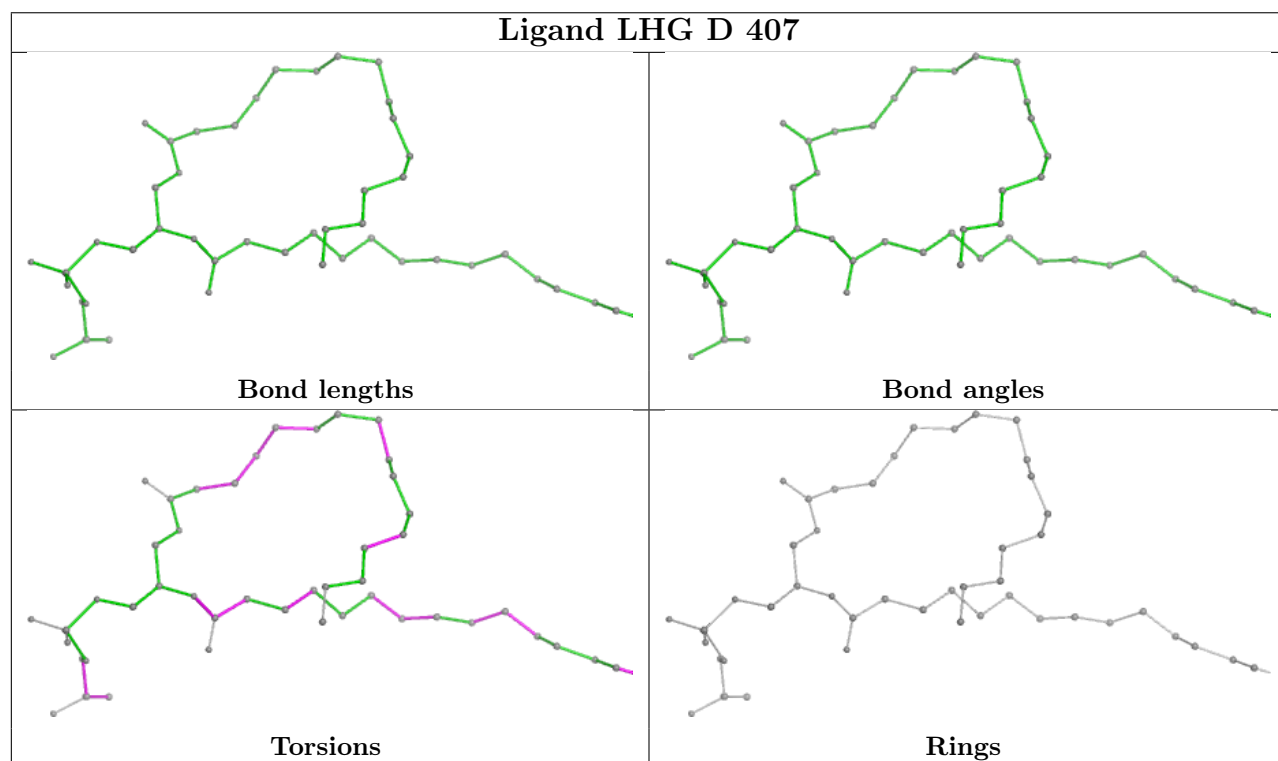
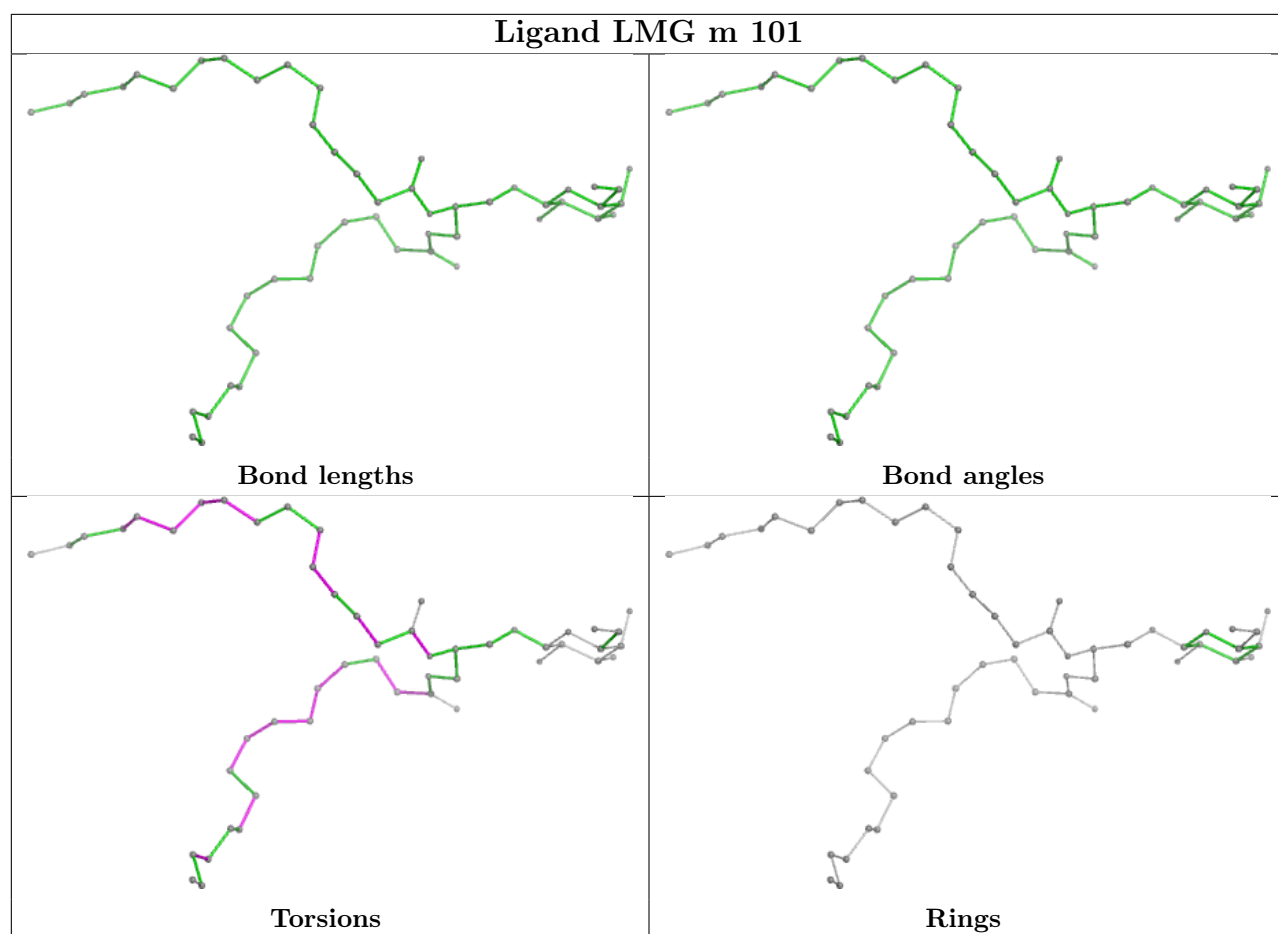


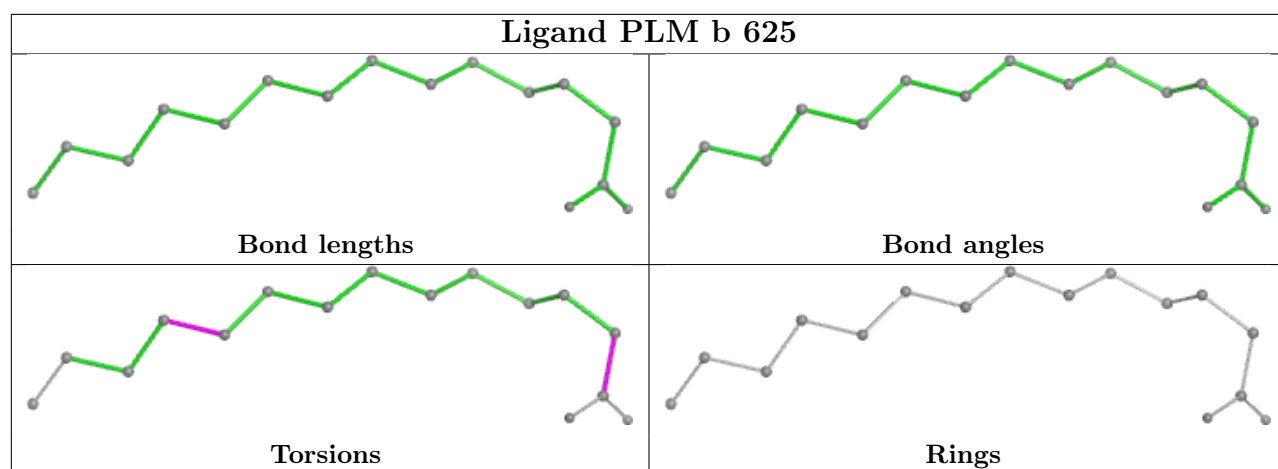


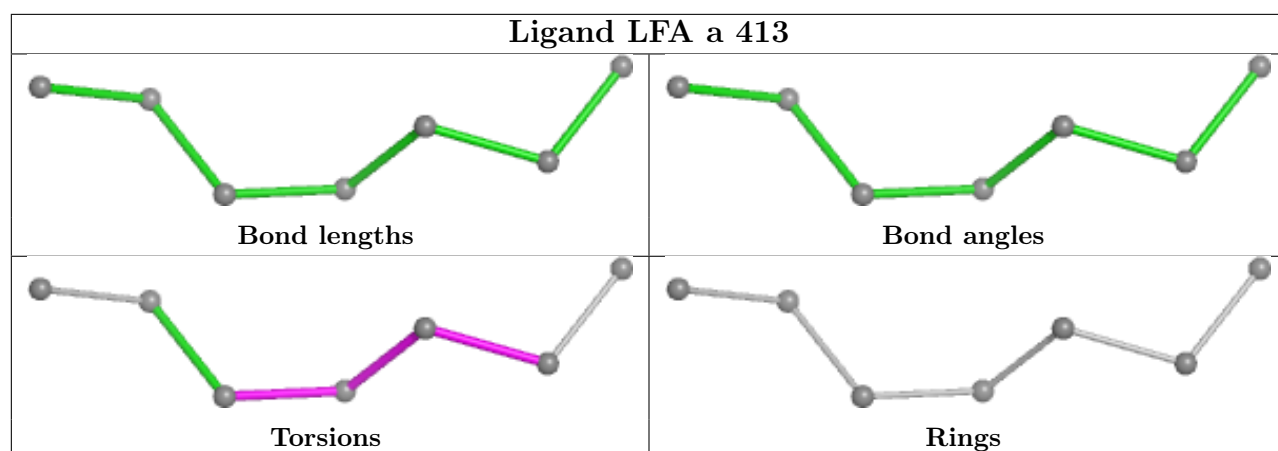
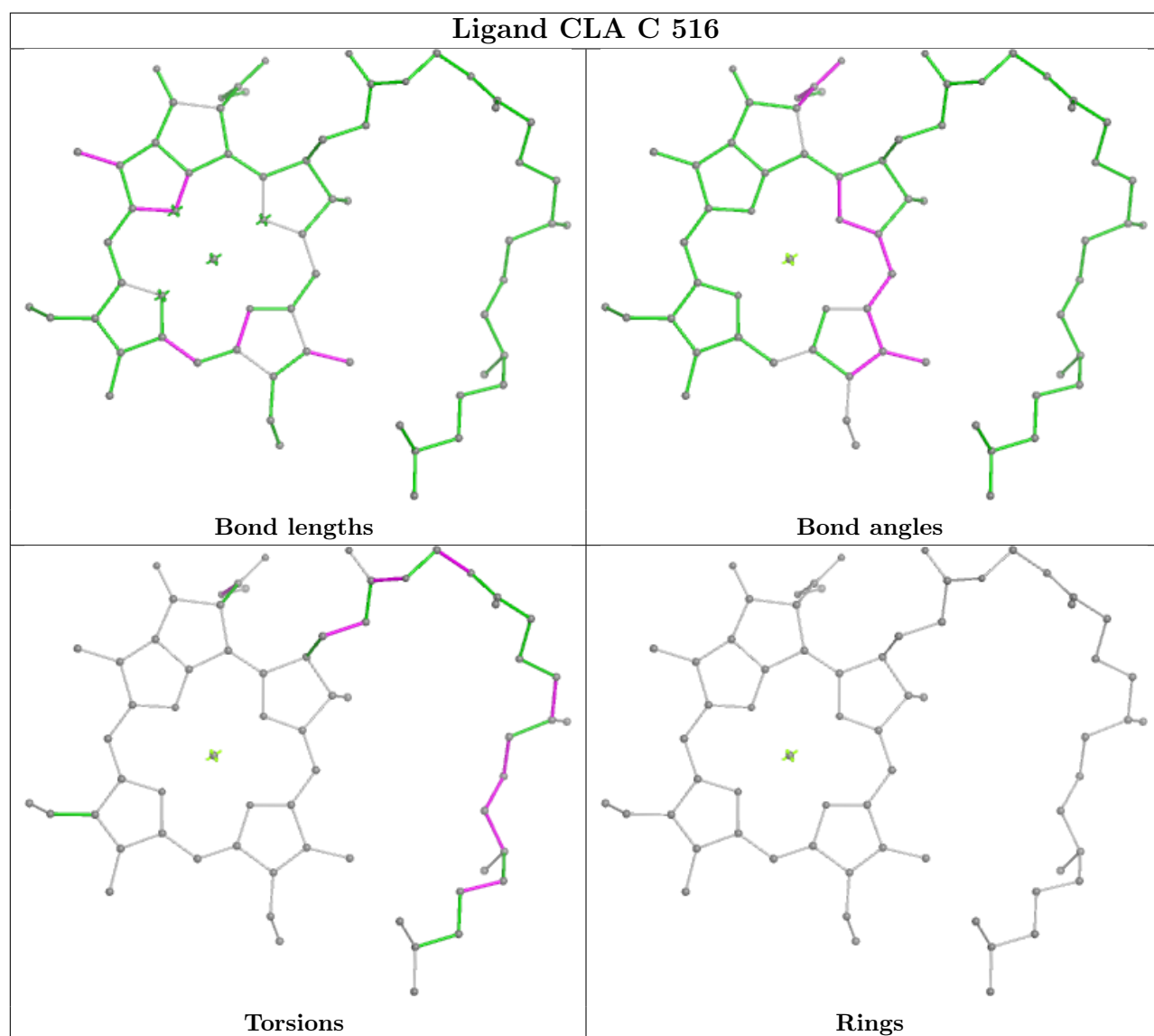


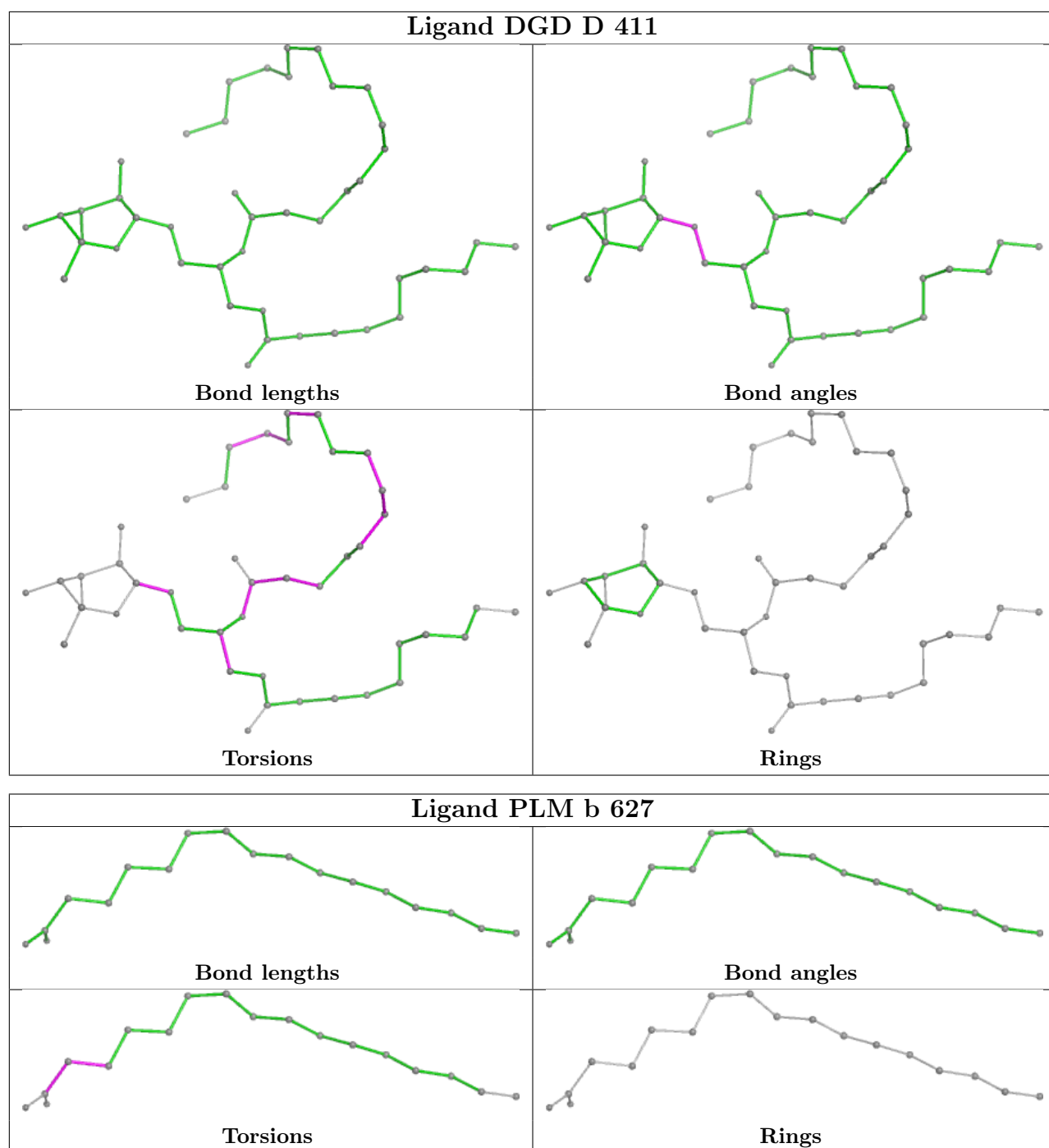


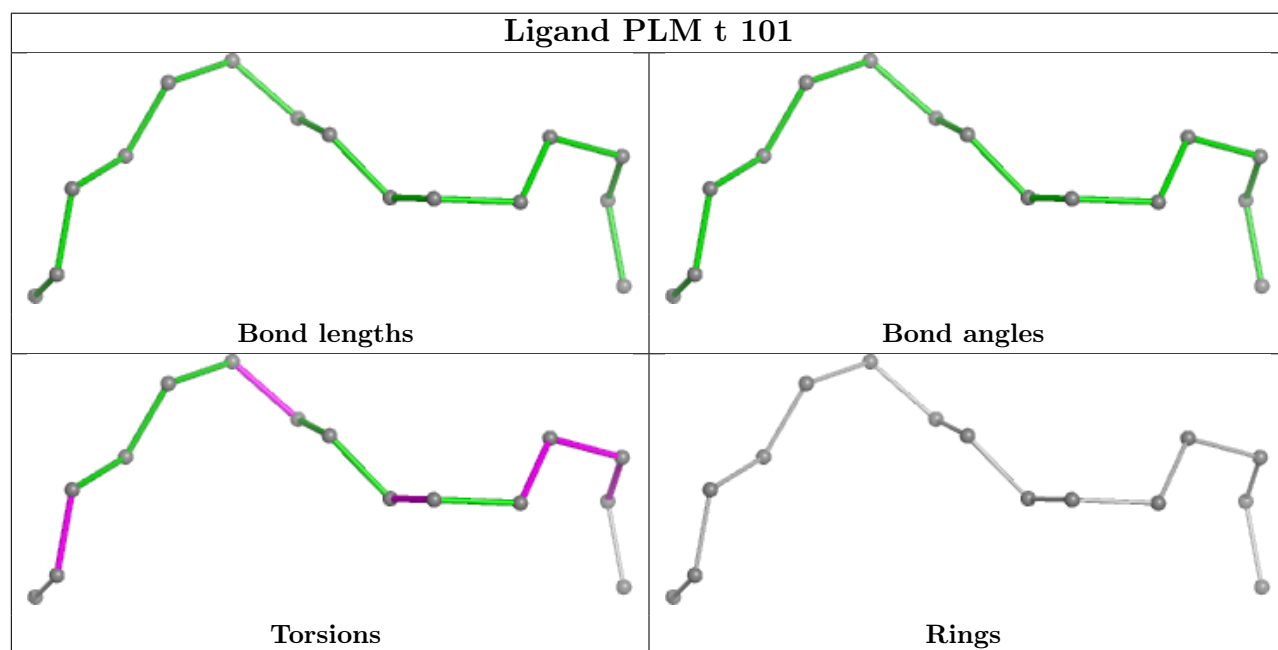
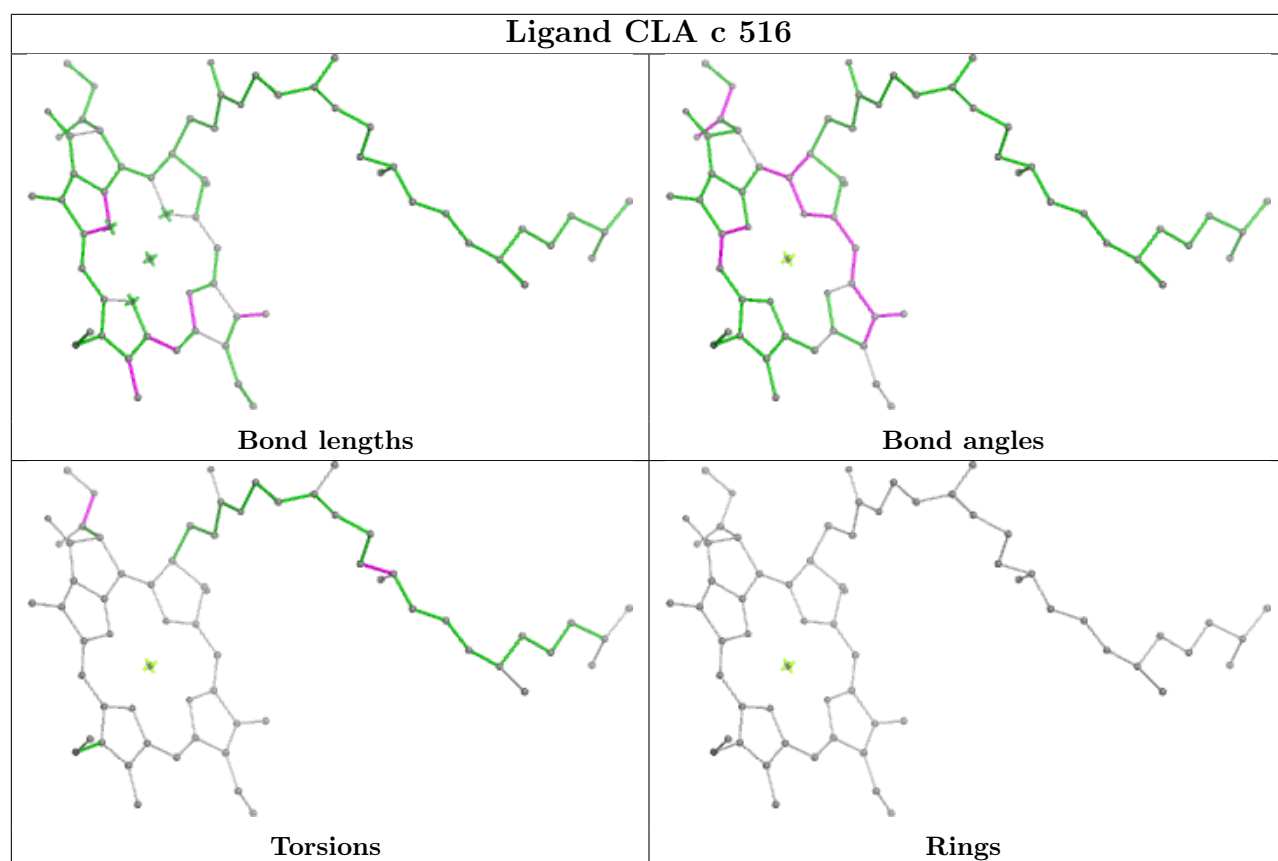




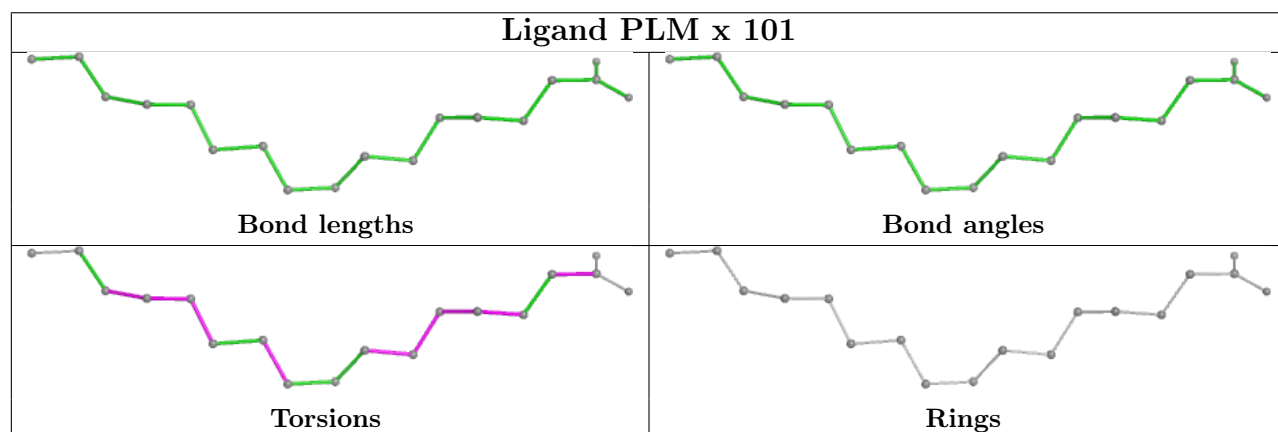
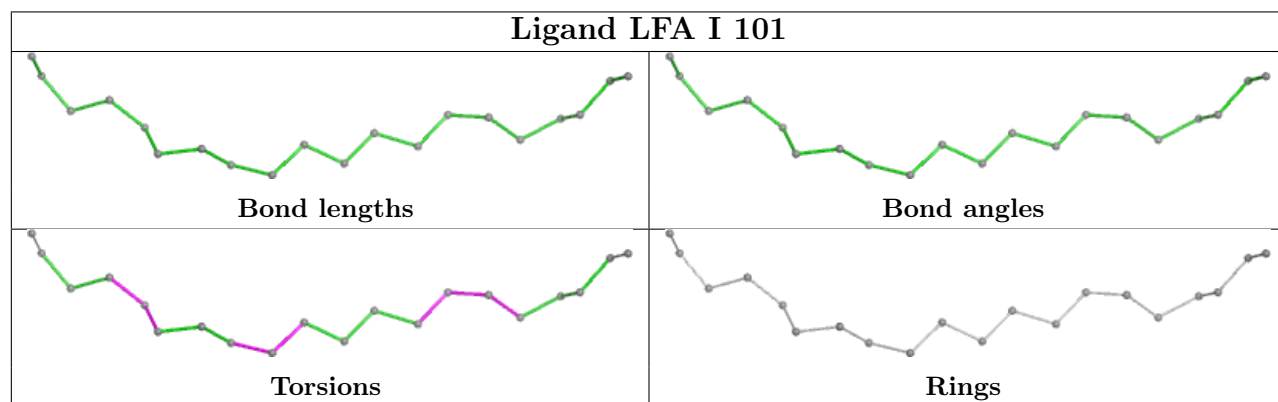
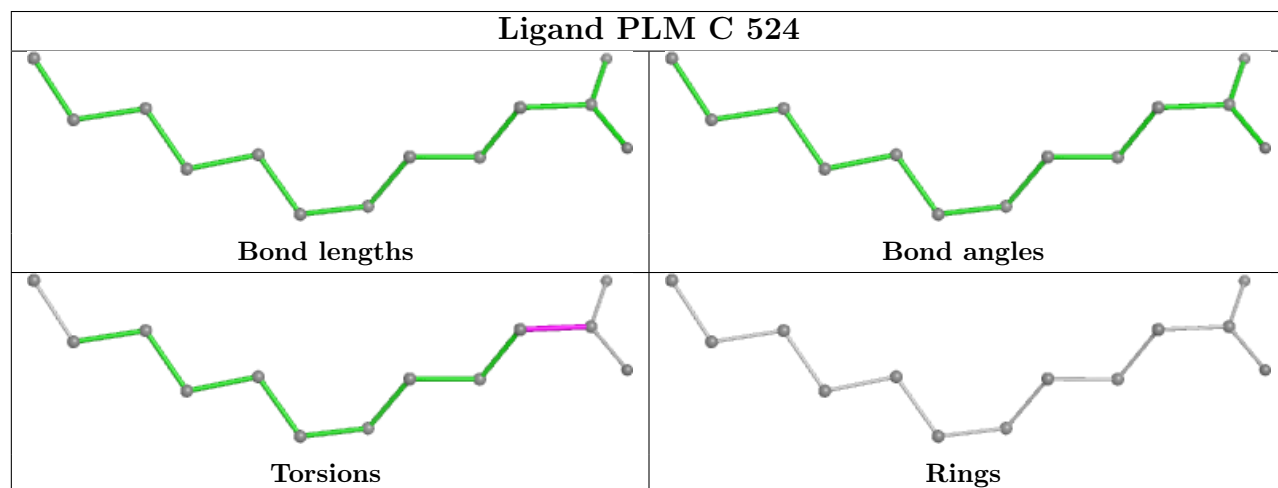
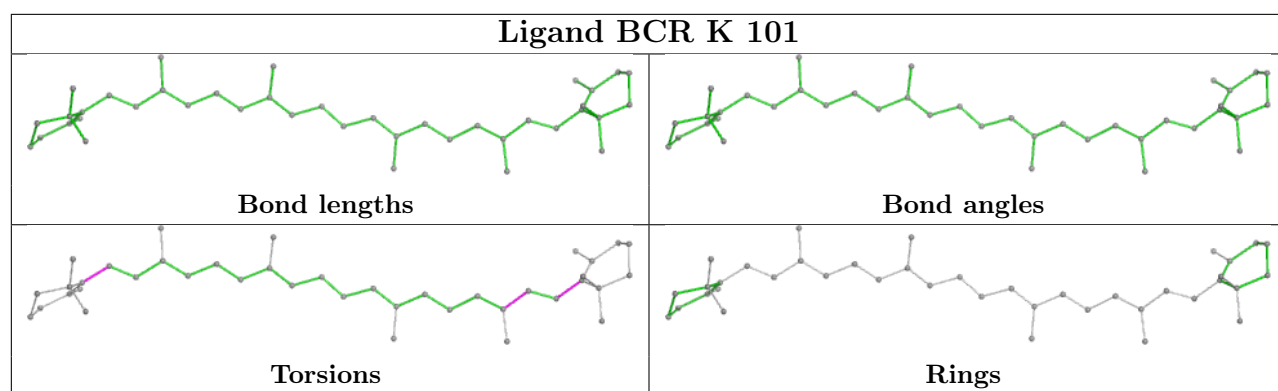


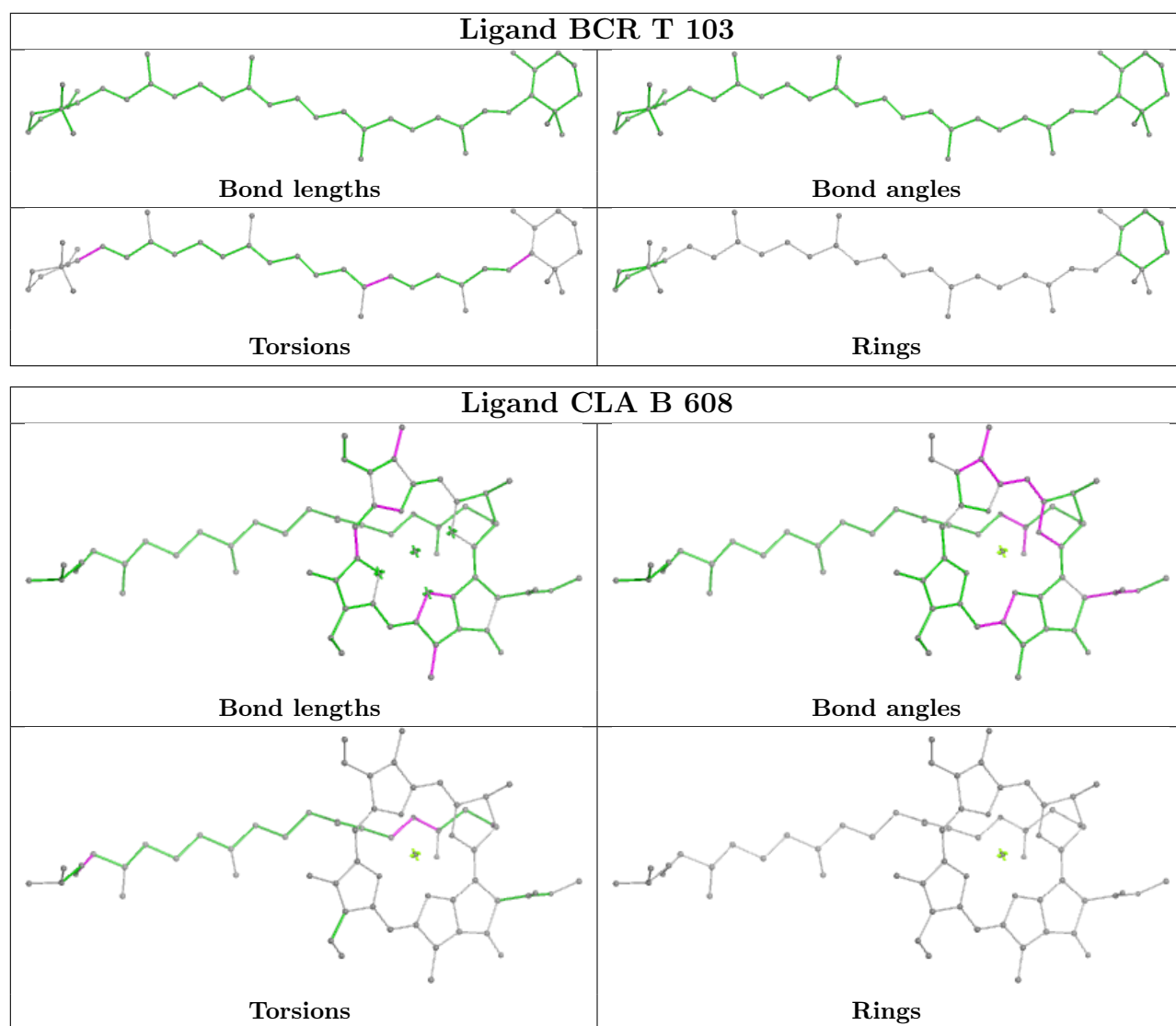




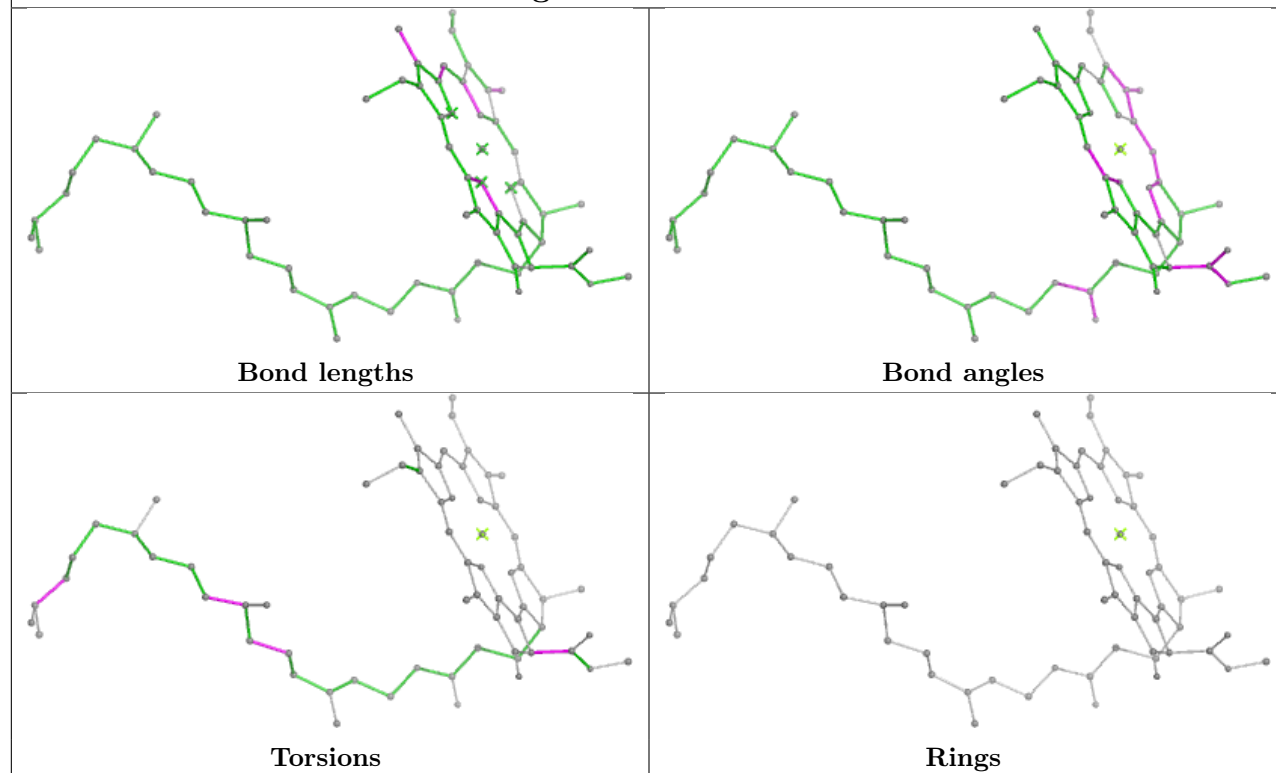




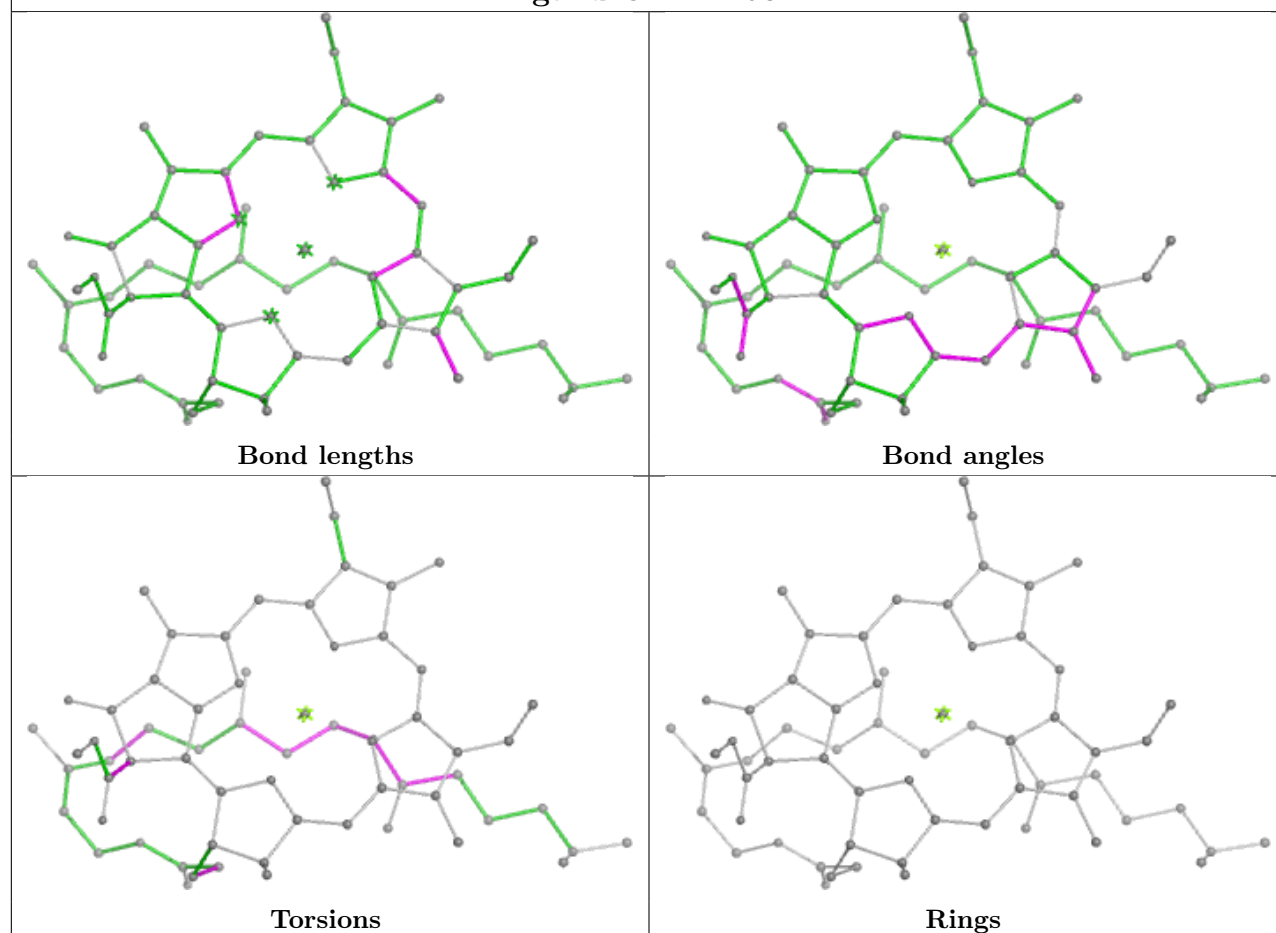


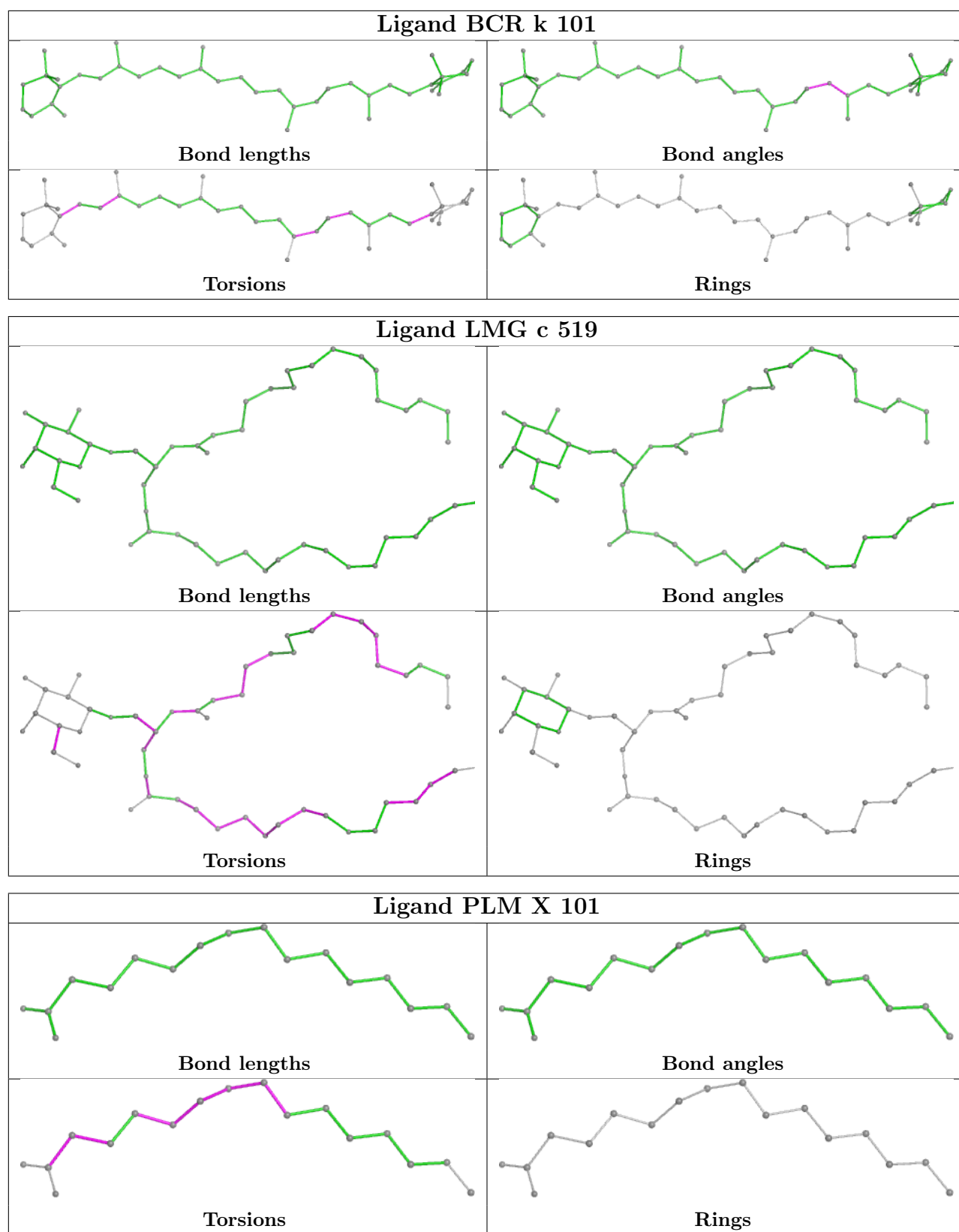


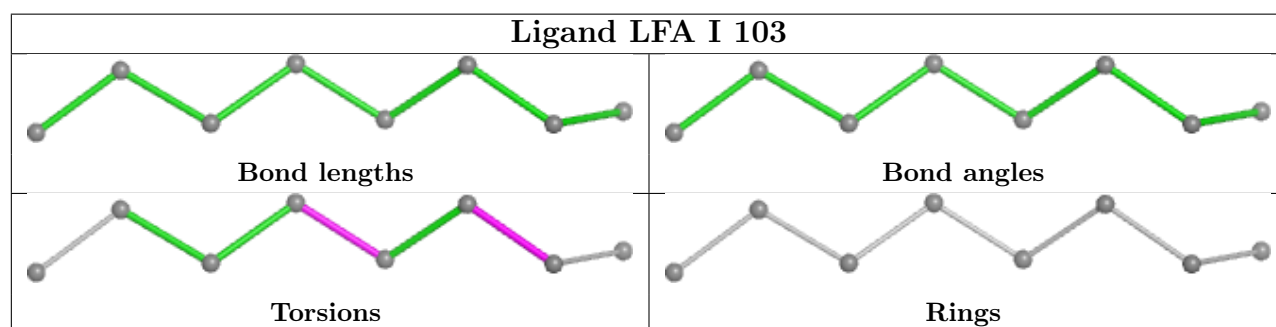
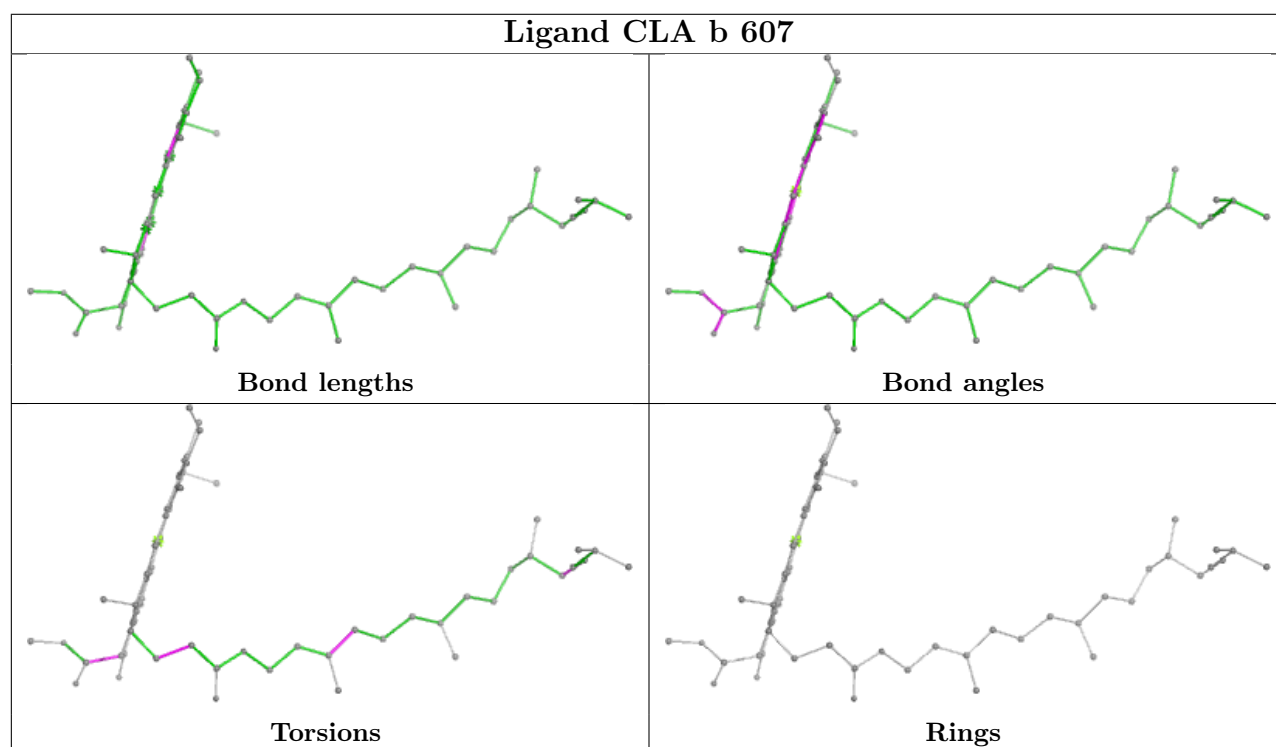
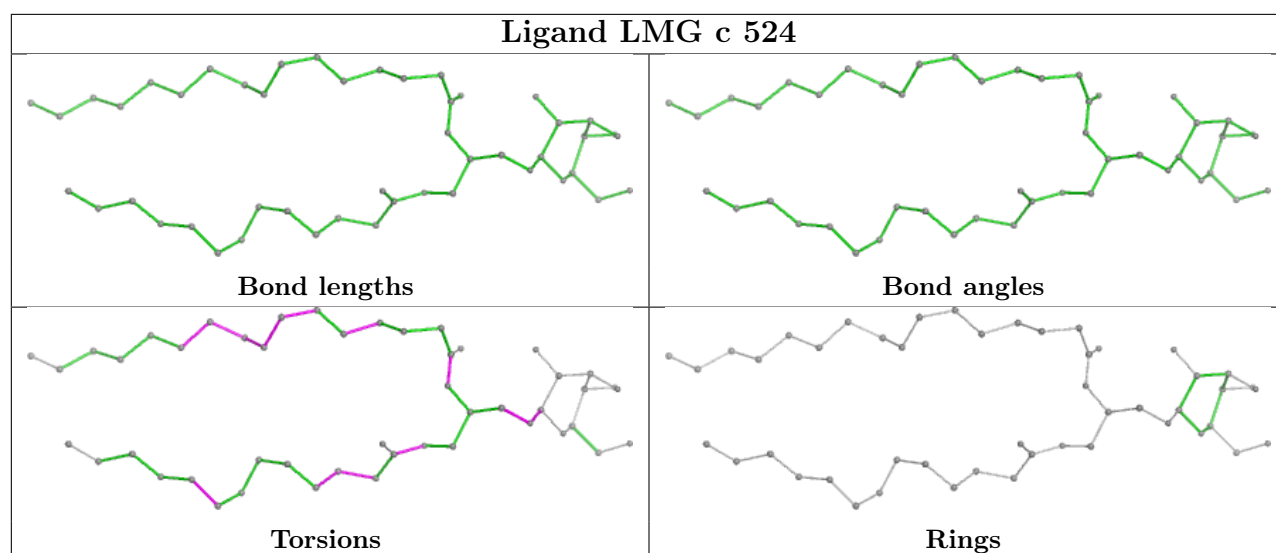
## Ligand CLA C 512

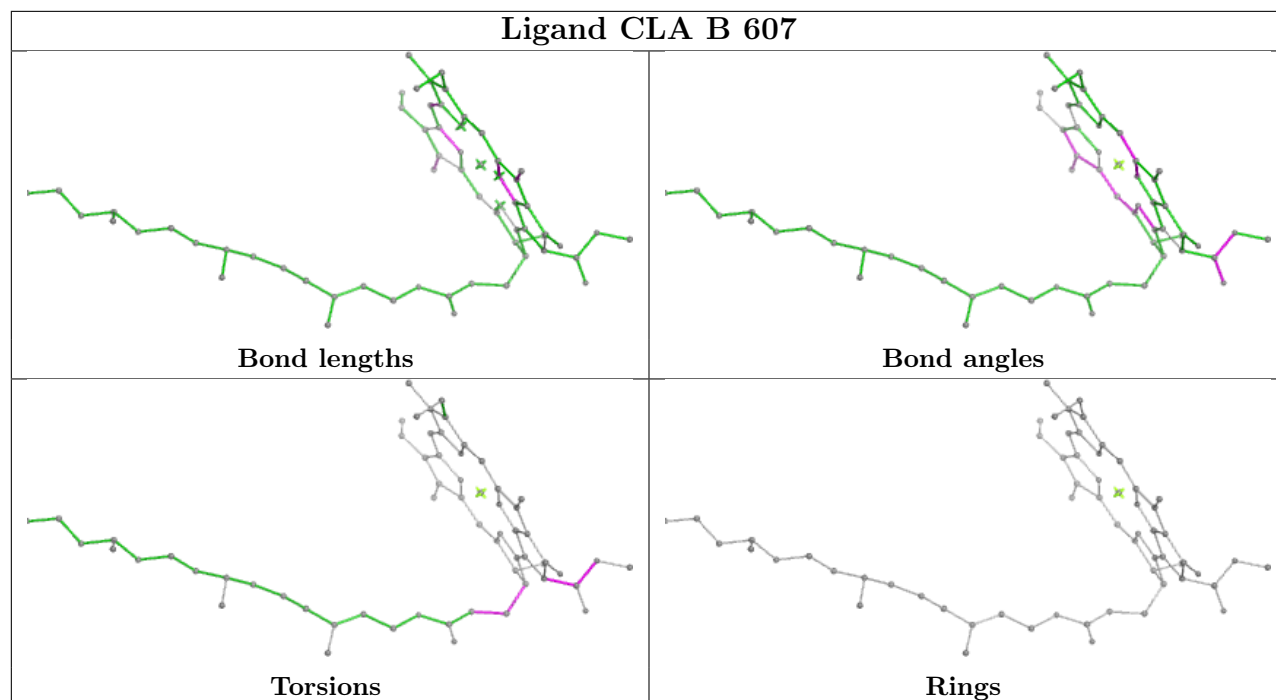
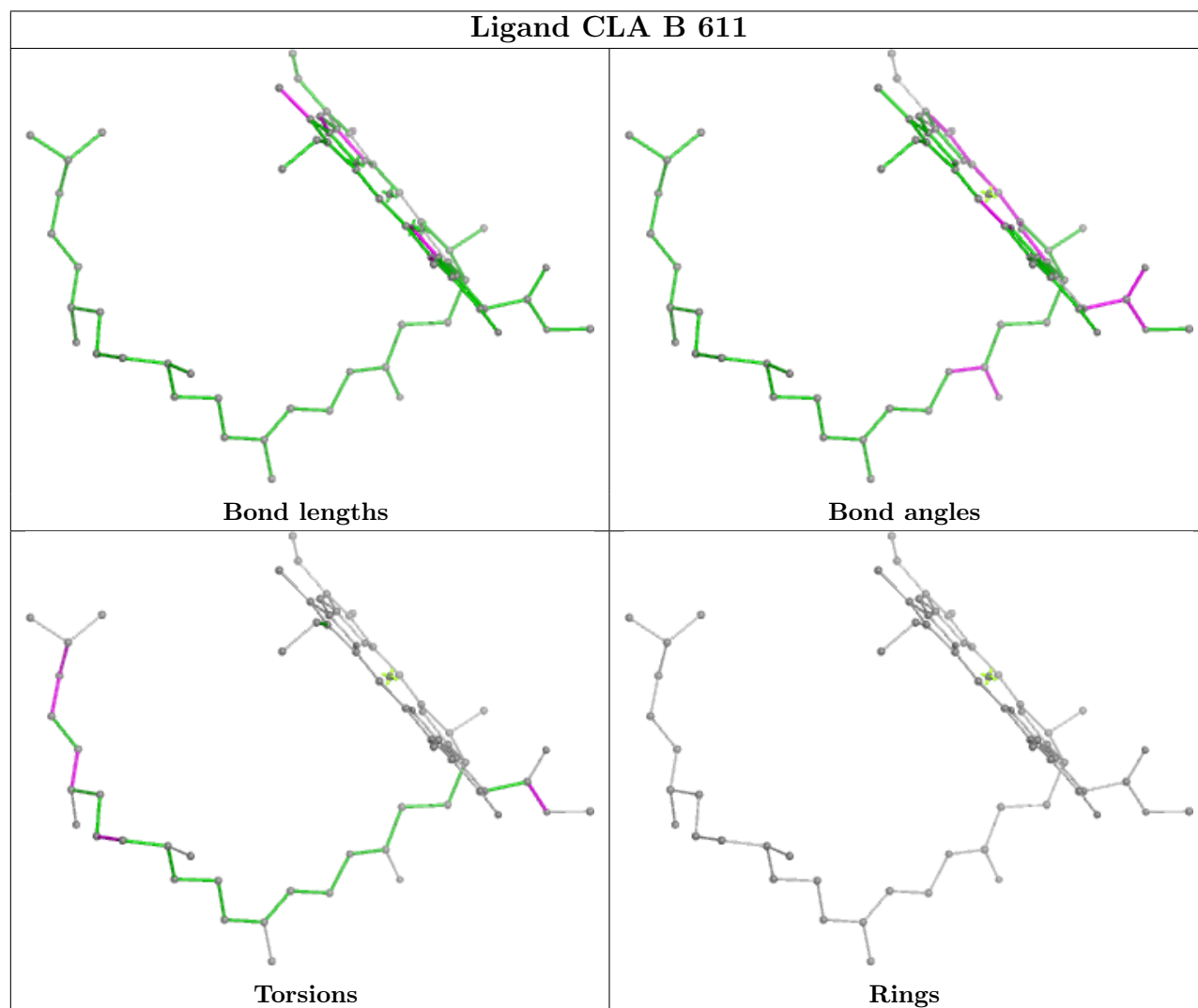


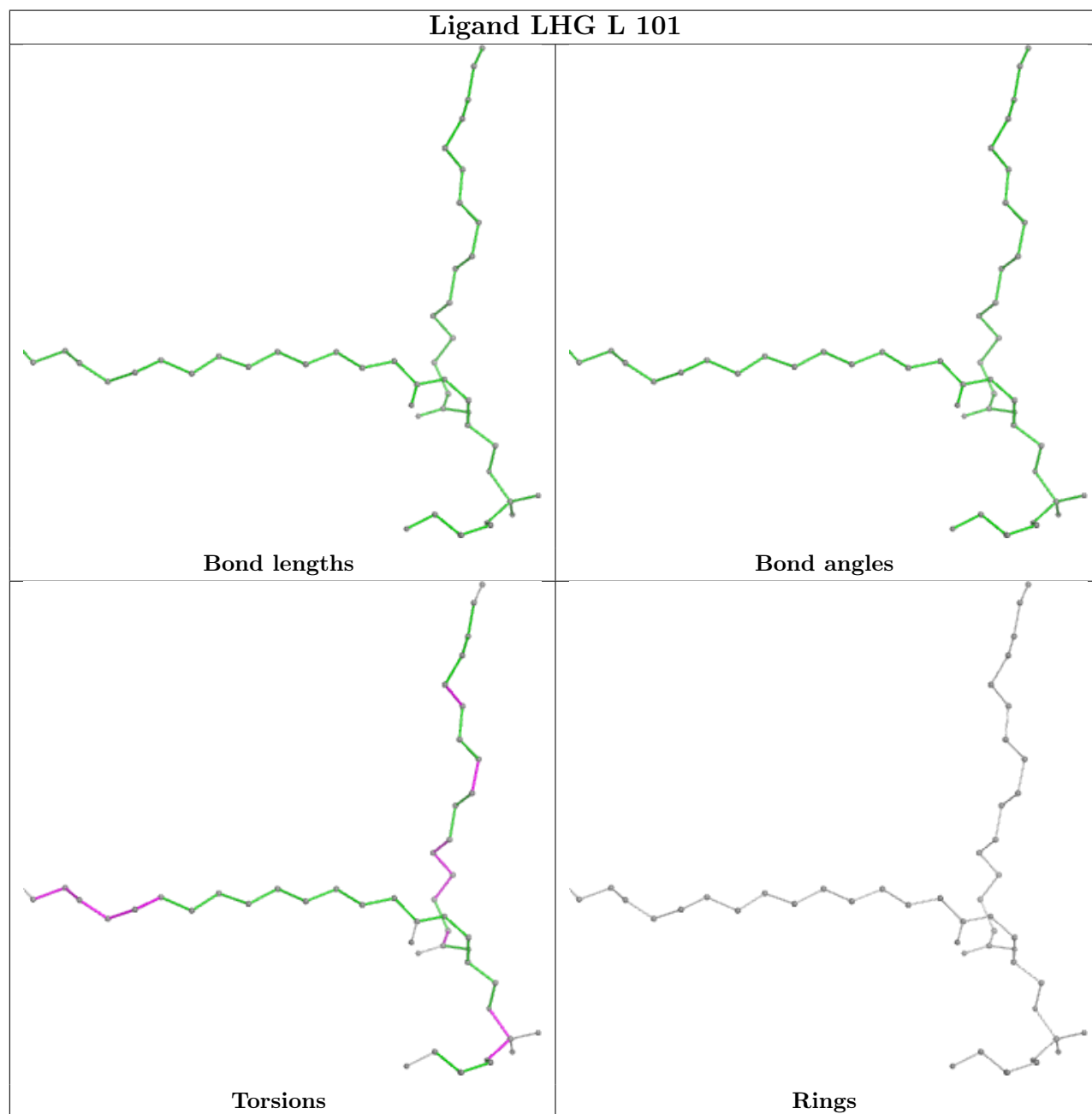
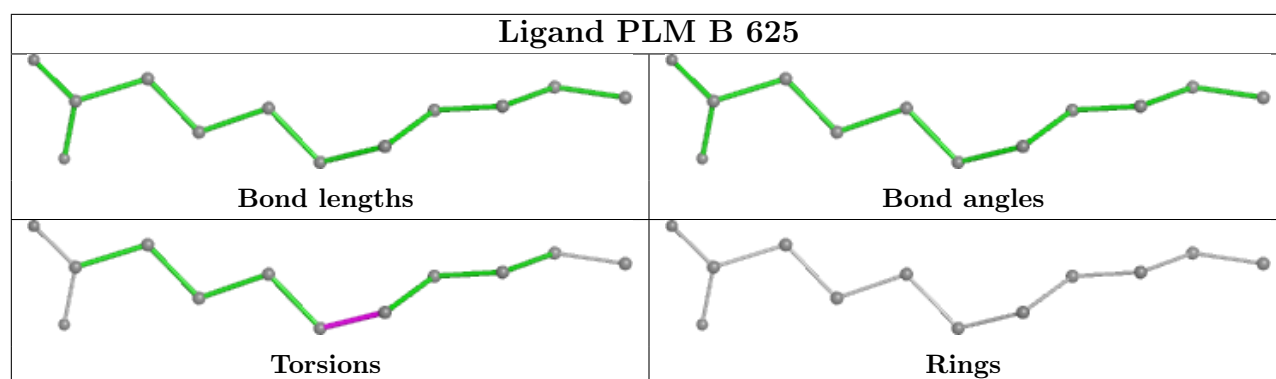
## Ligand CLA B 601

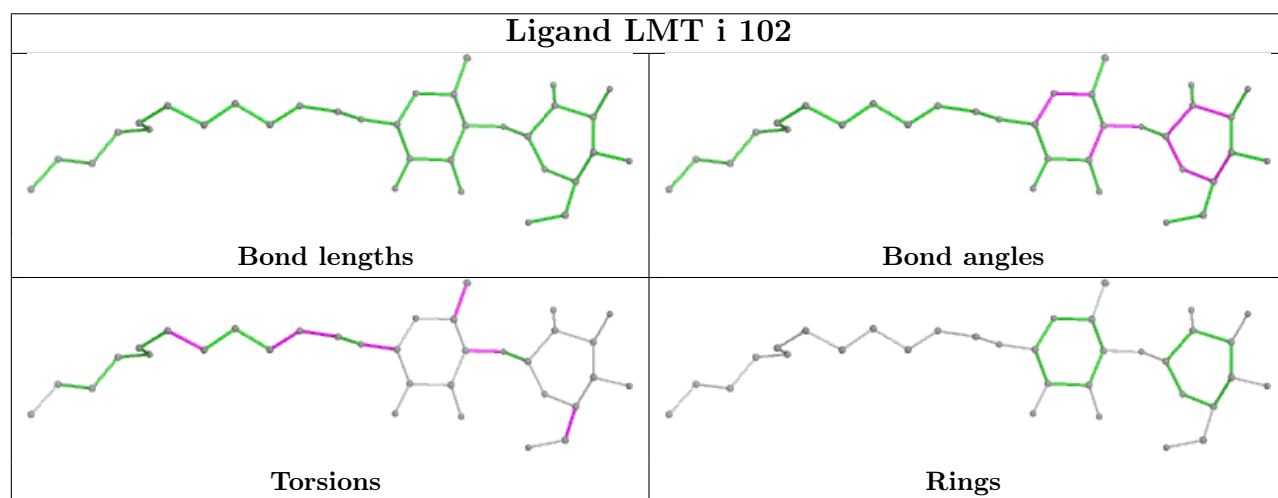
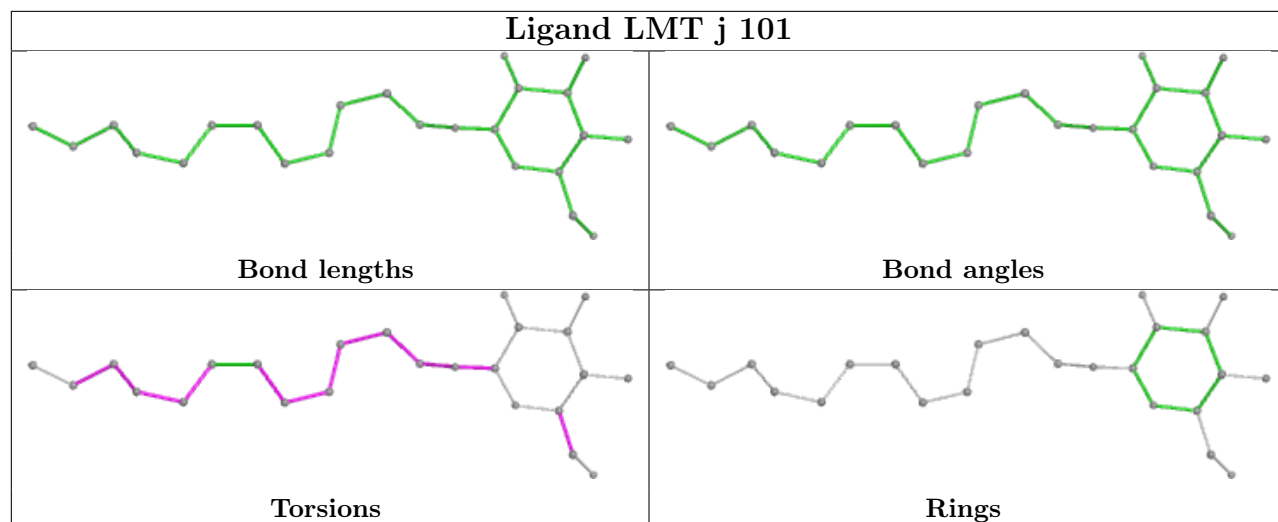




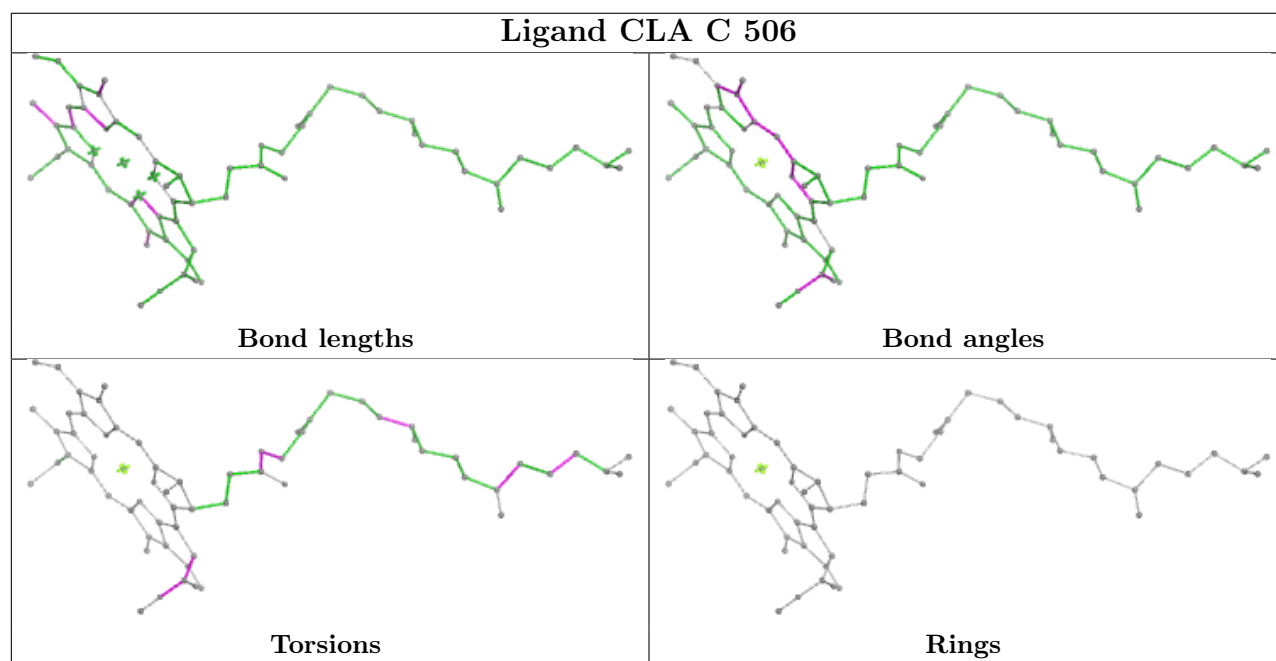
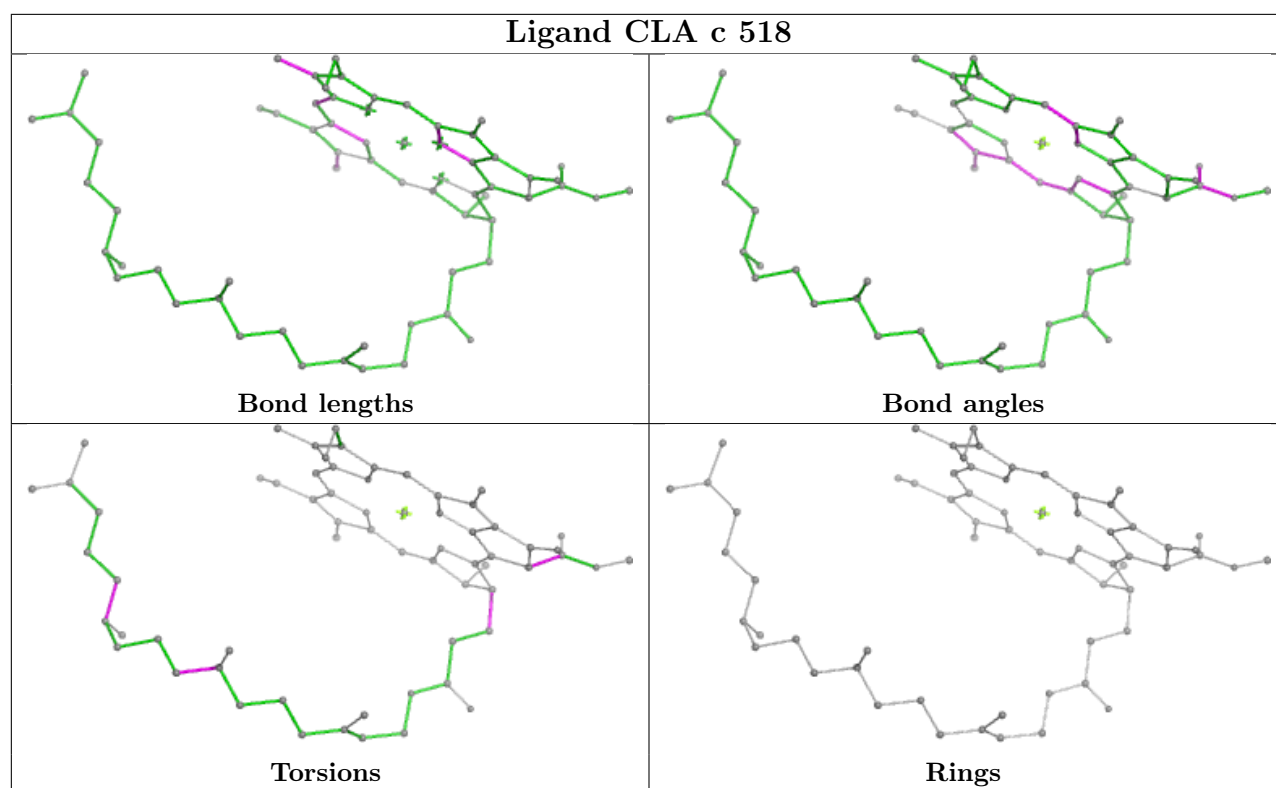


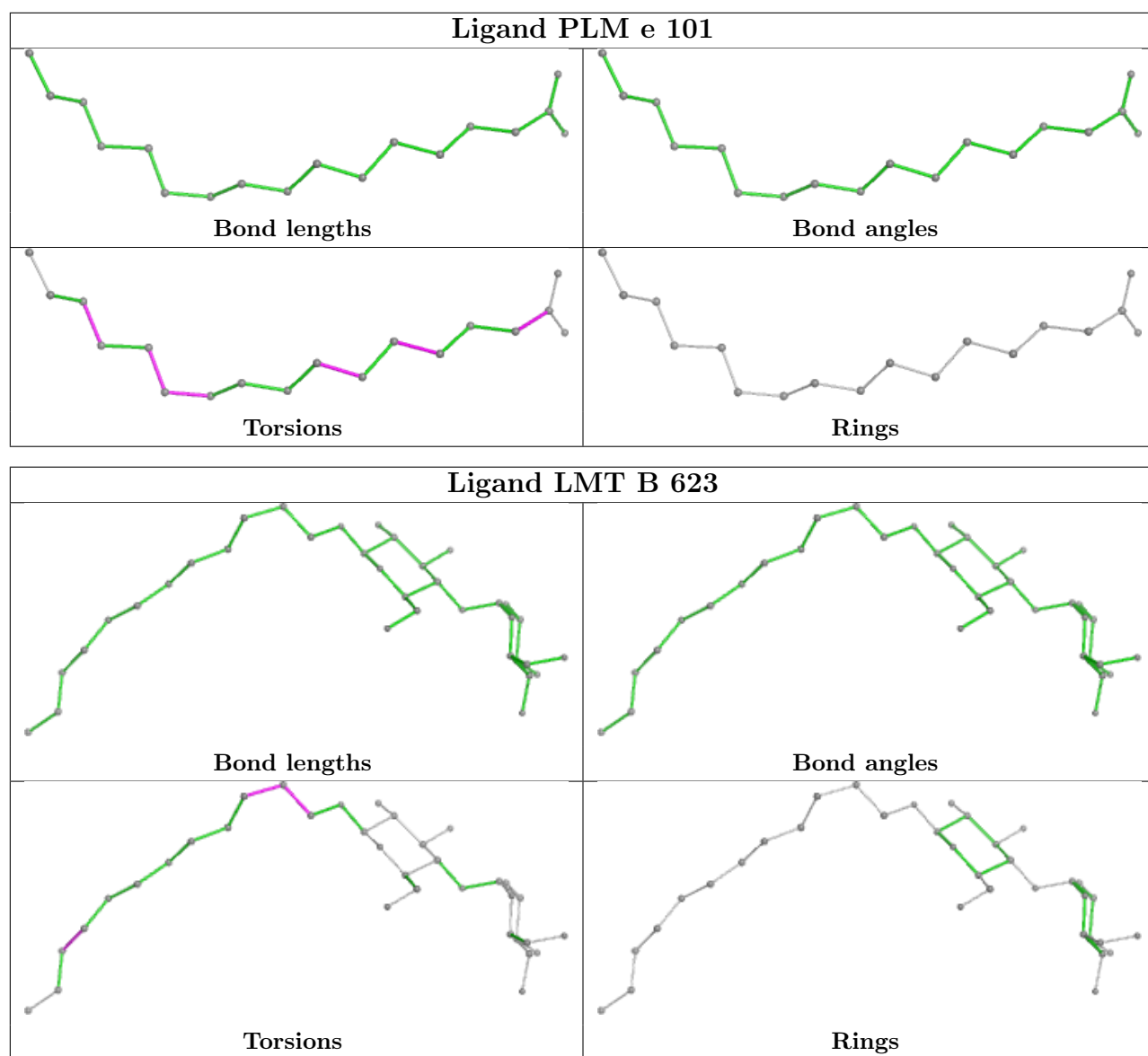
**Ligand CLA B 607****Ligand CLA B 611**

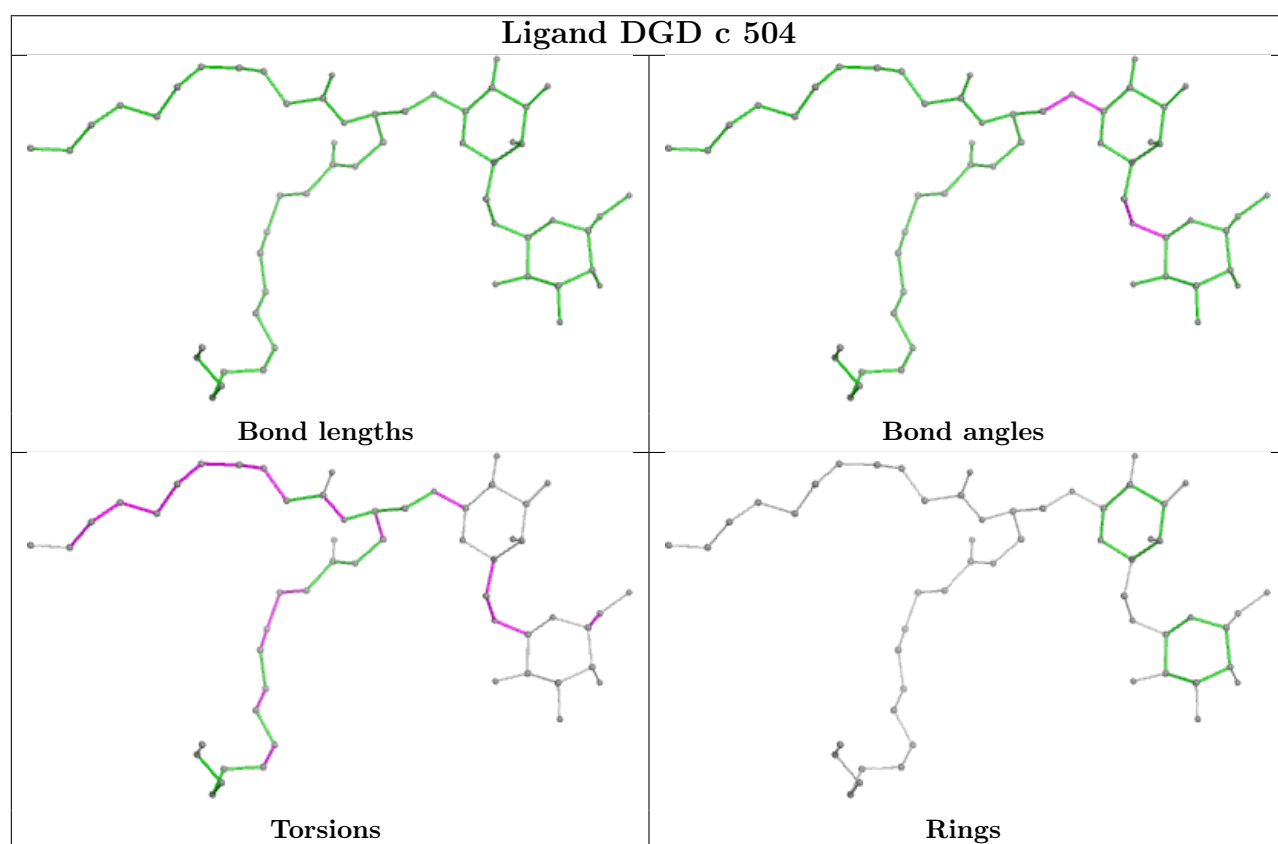
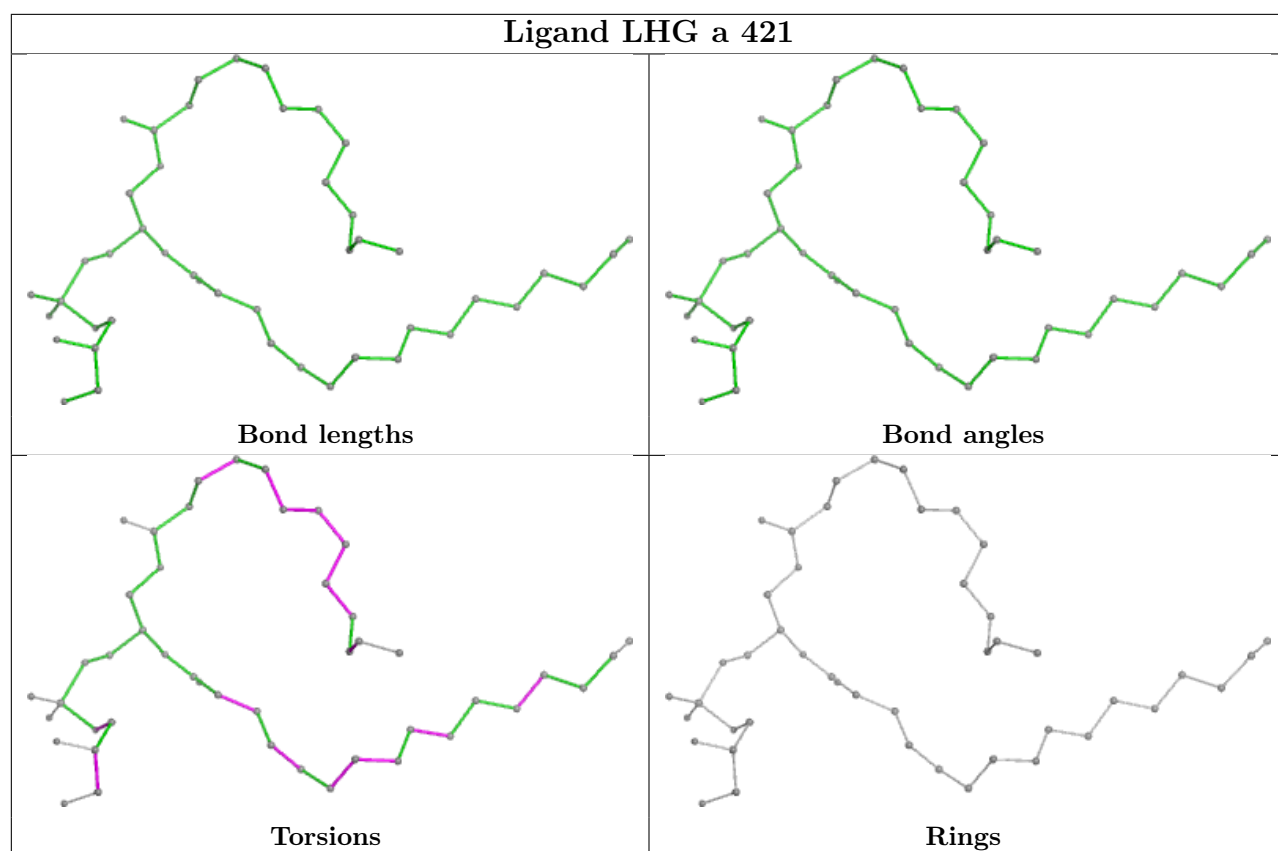


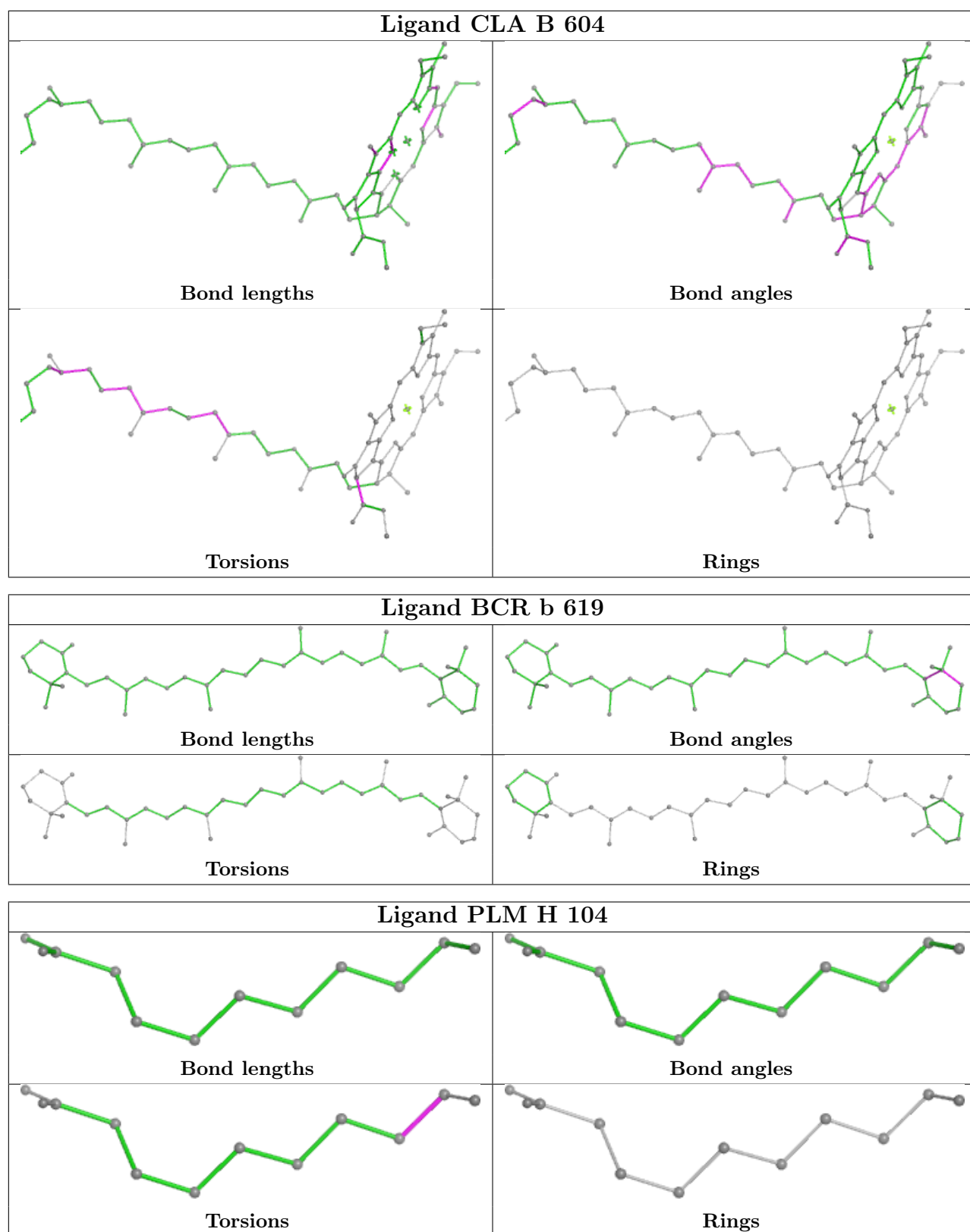




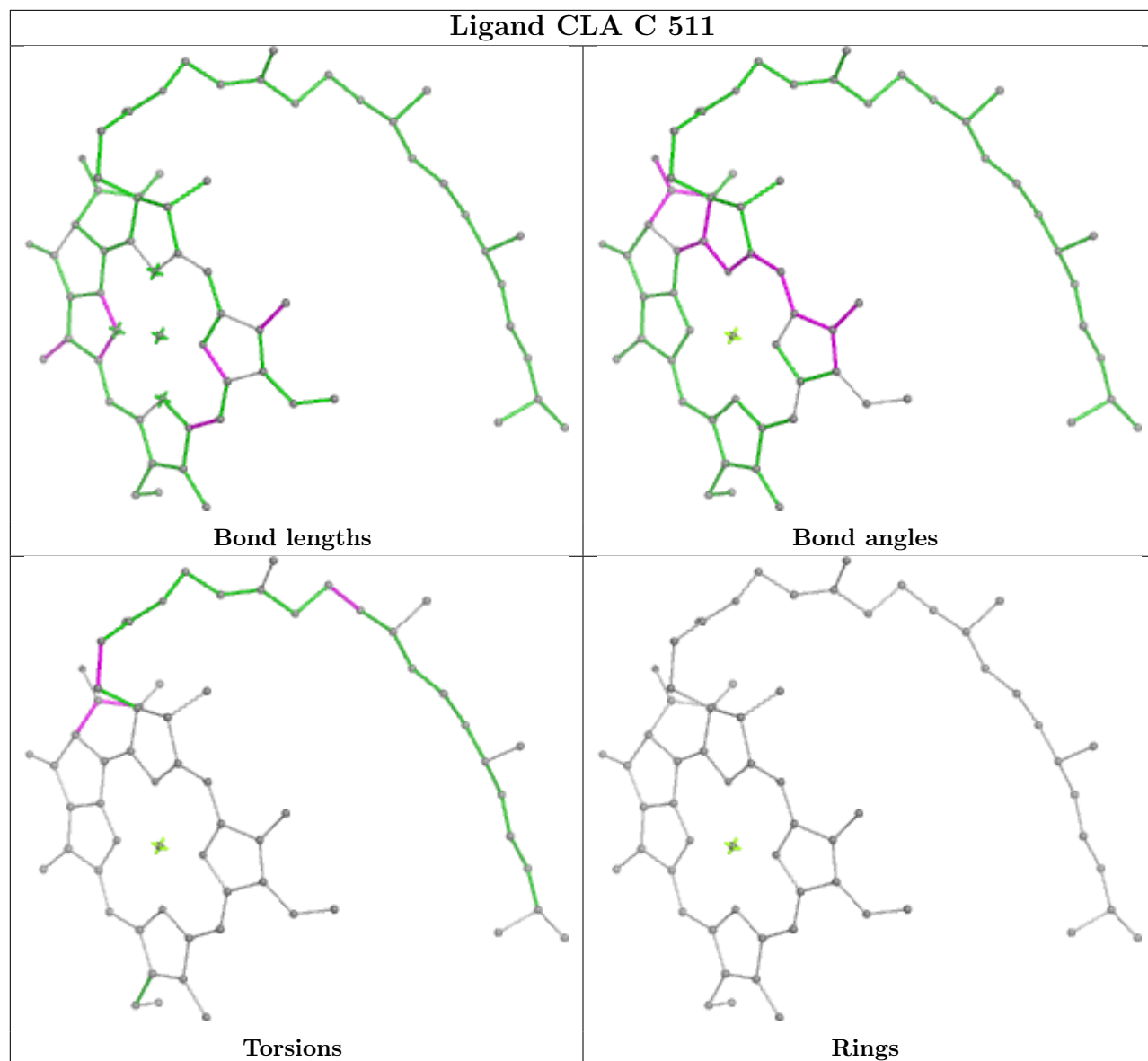




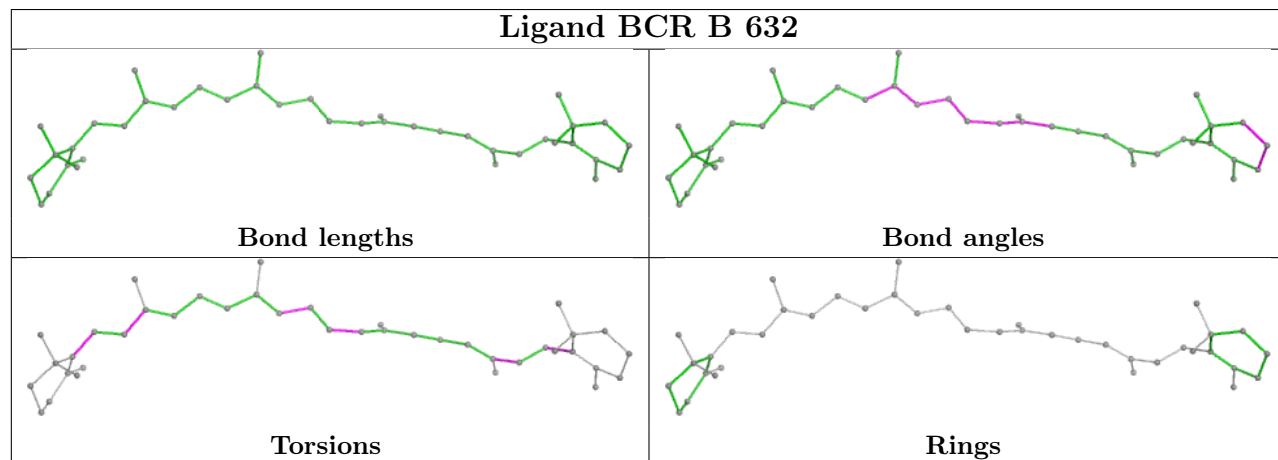


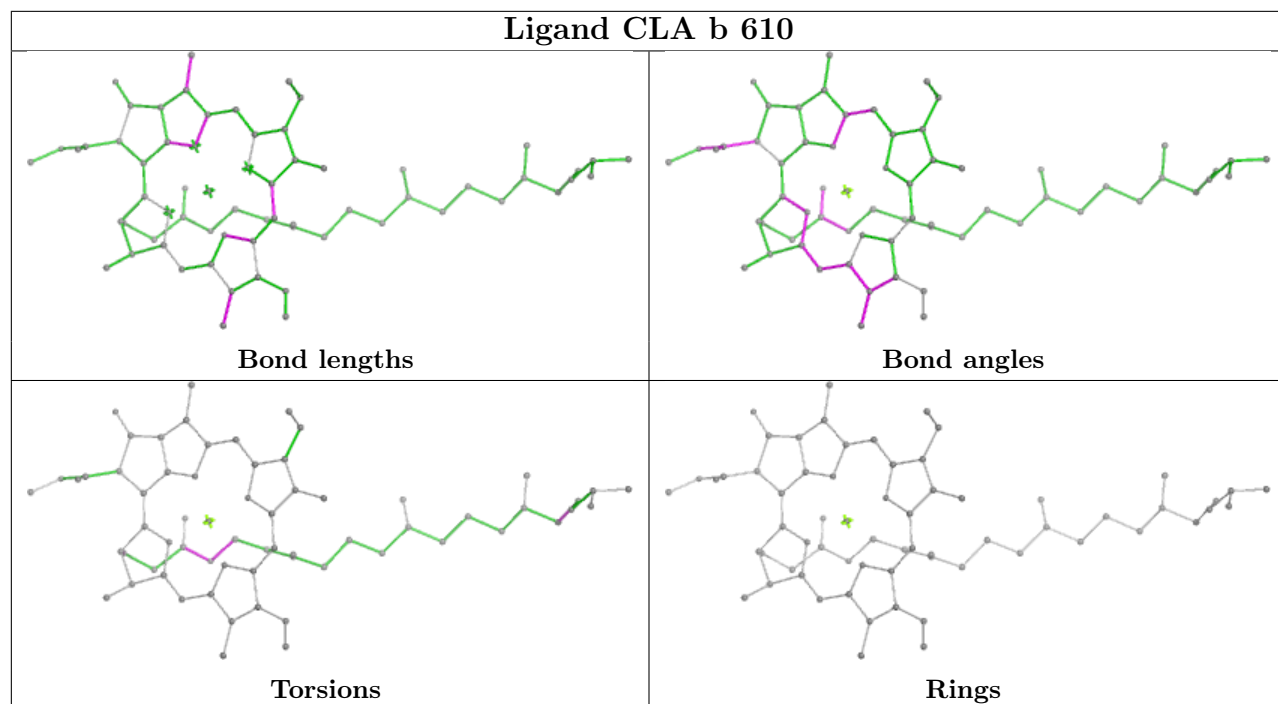
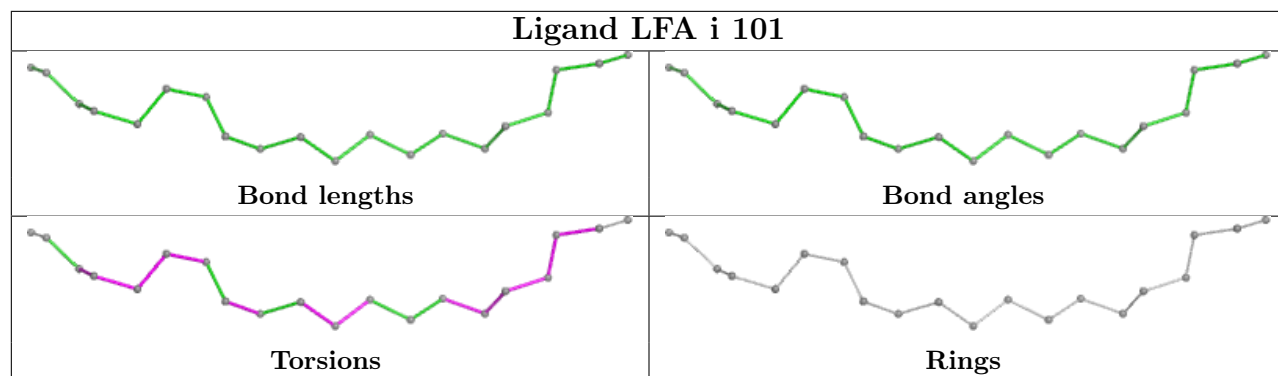


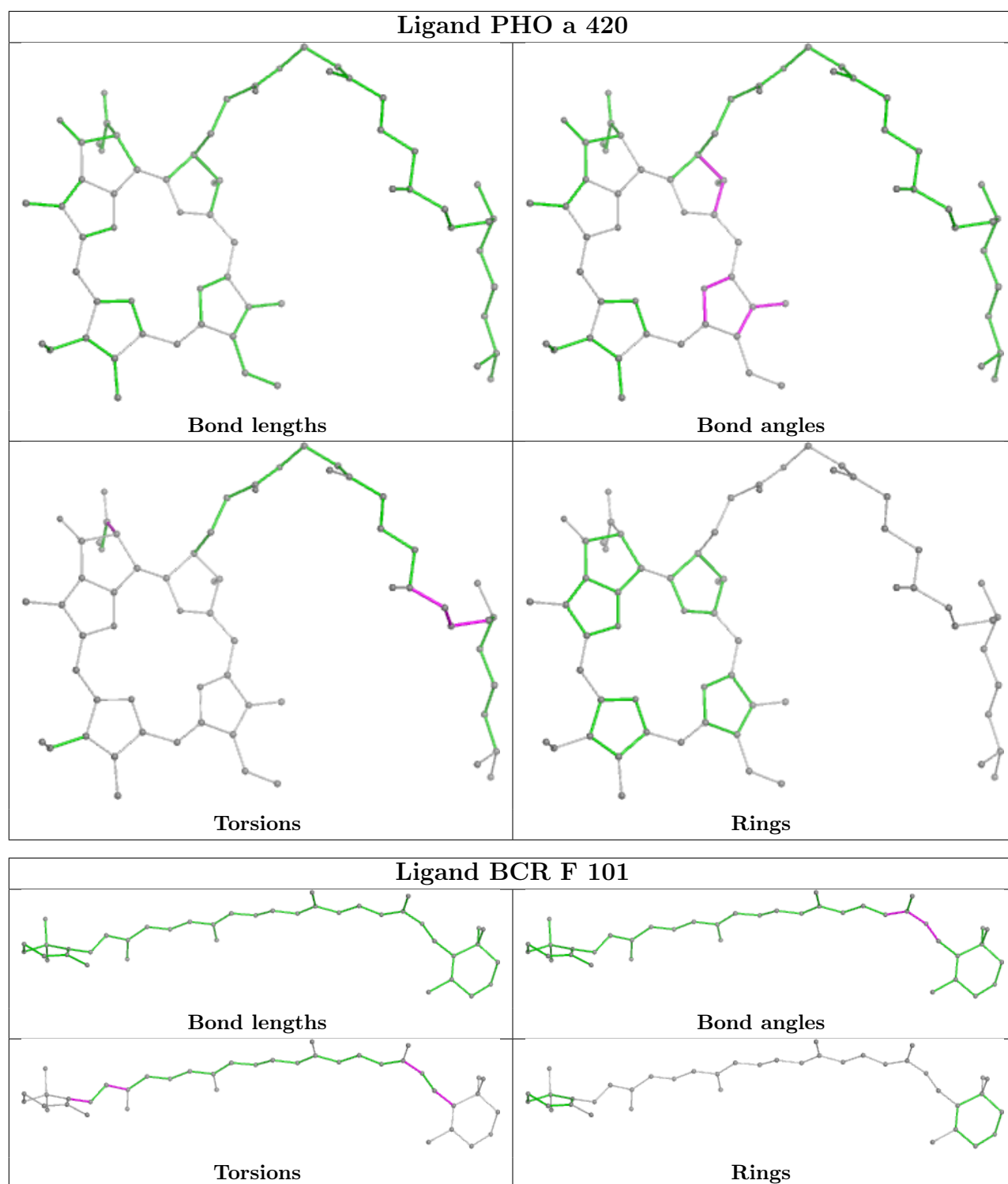
## Ligand CLA C 511

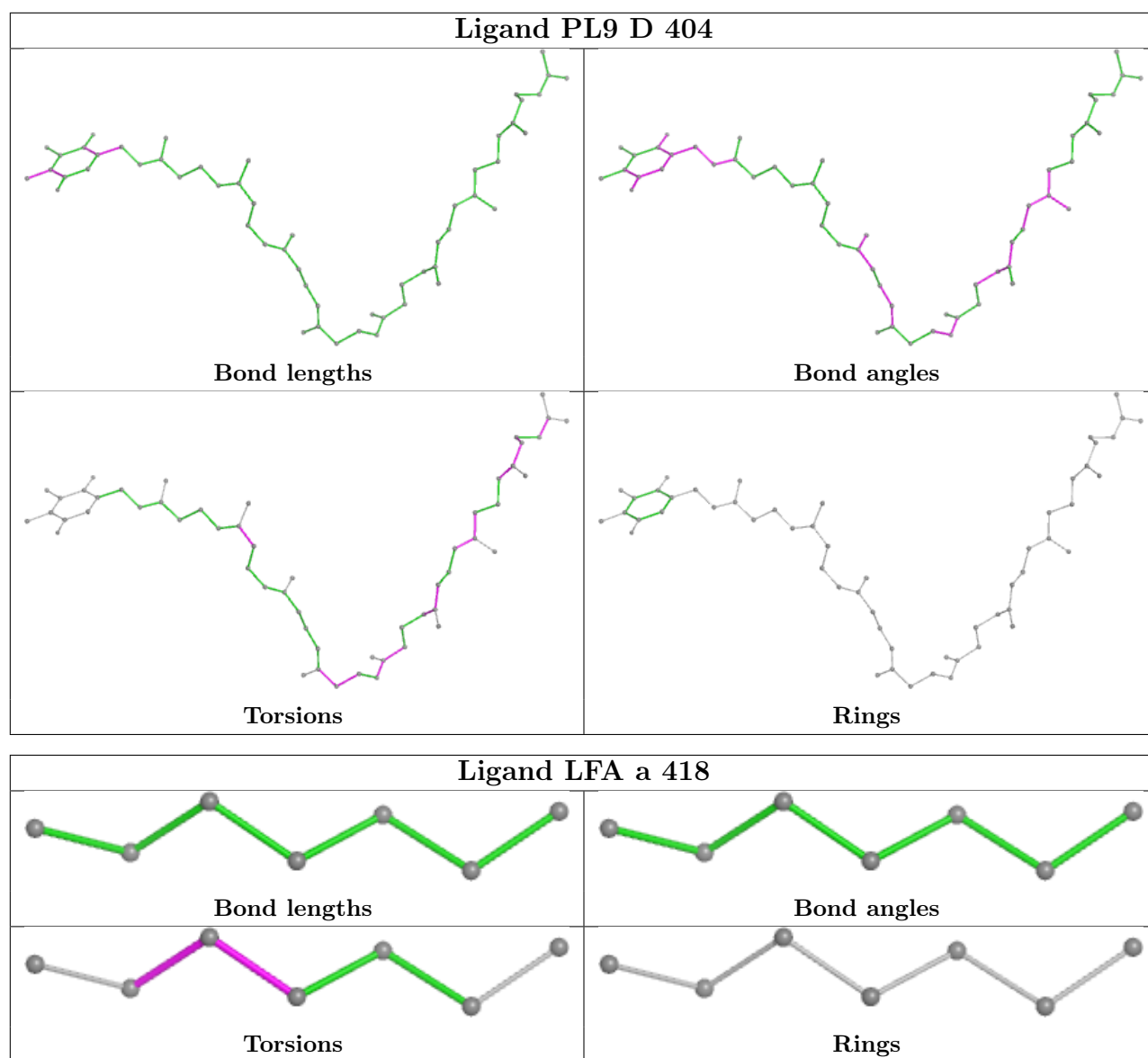


## Ligand BCR B 632

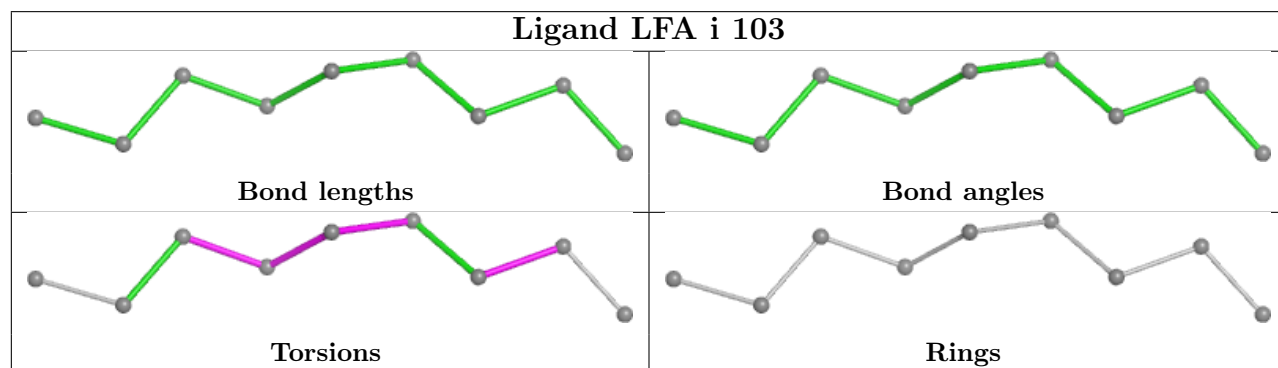
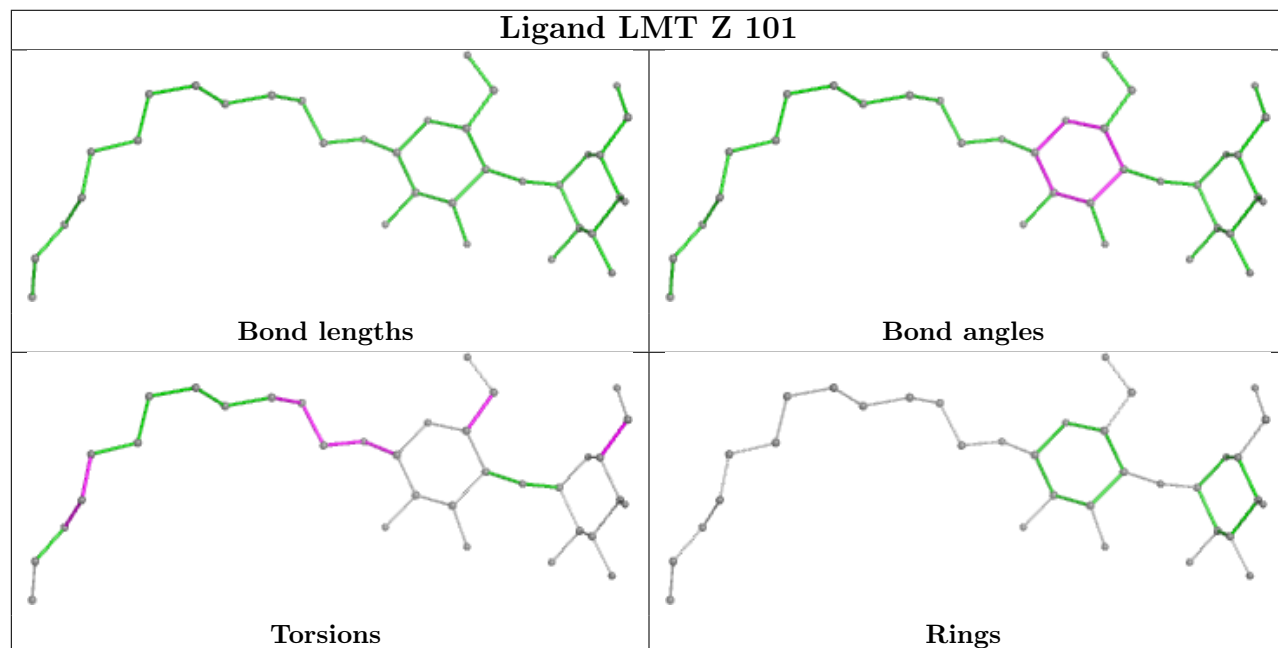
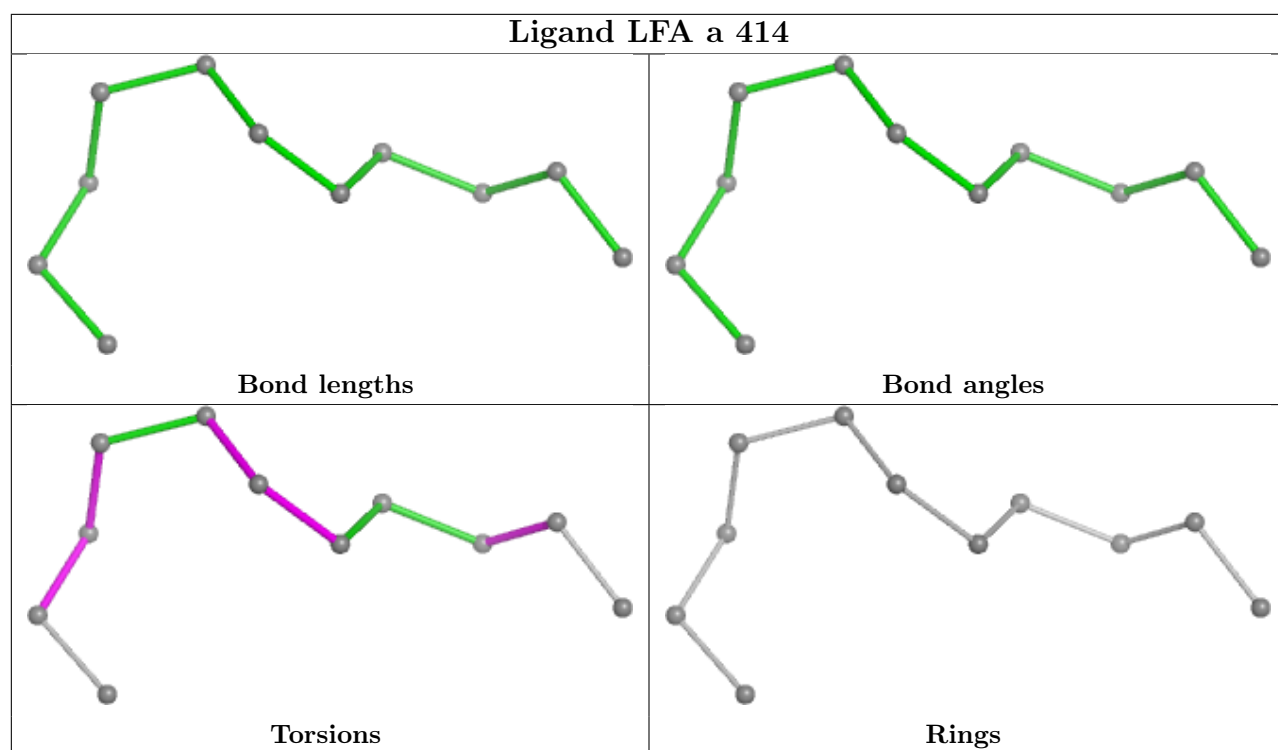


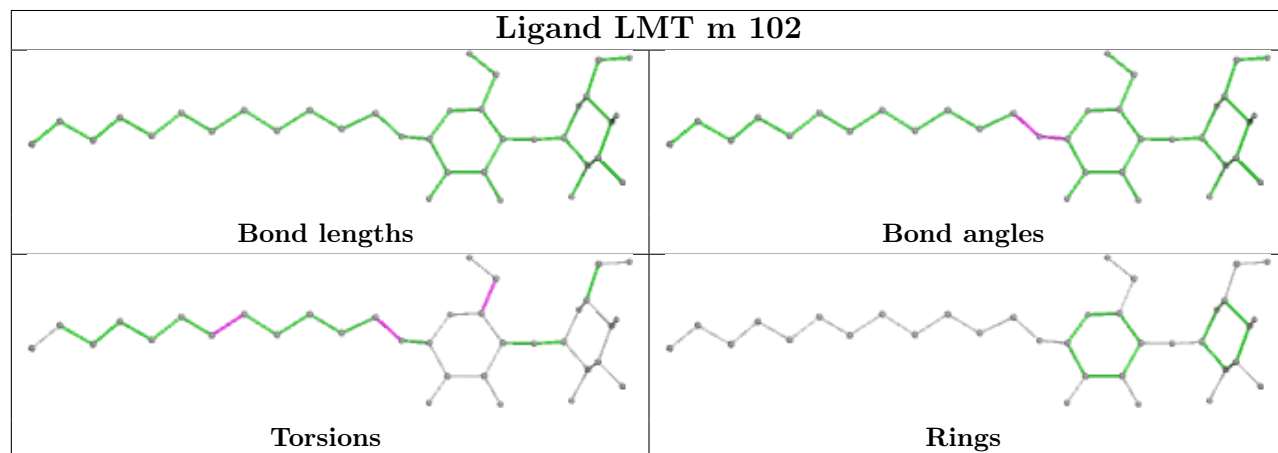
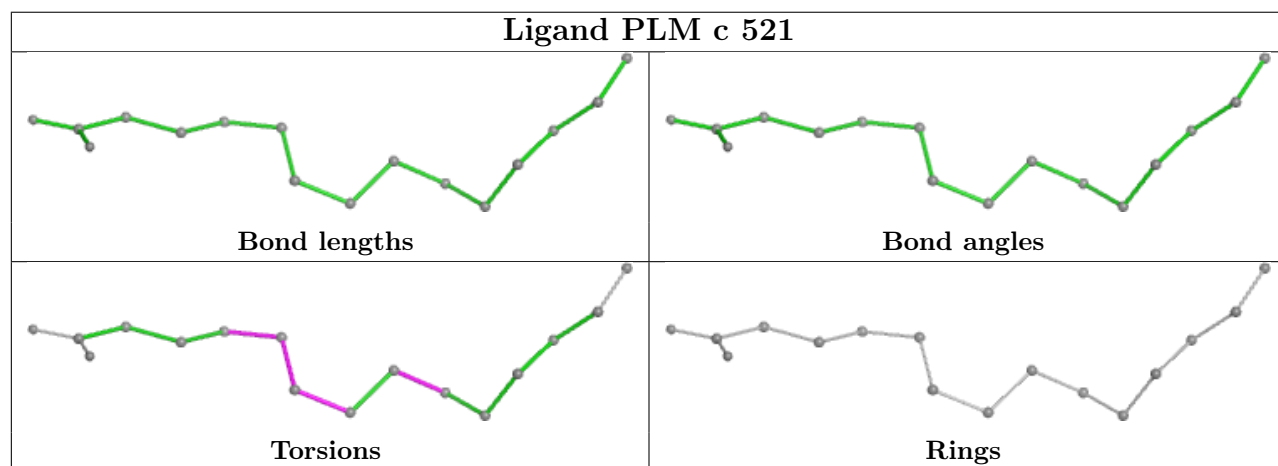
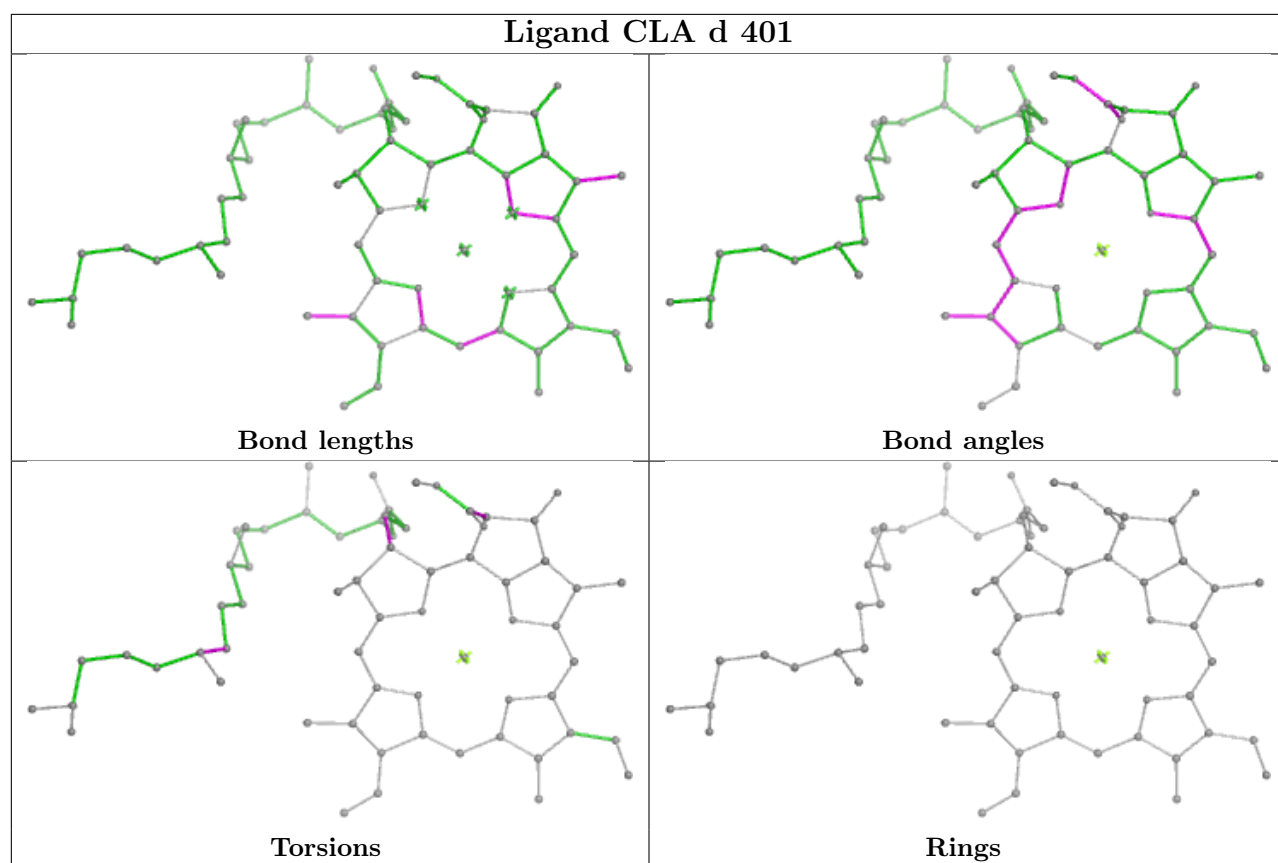


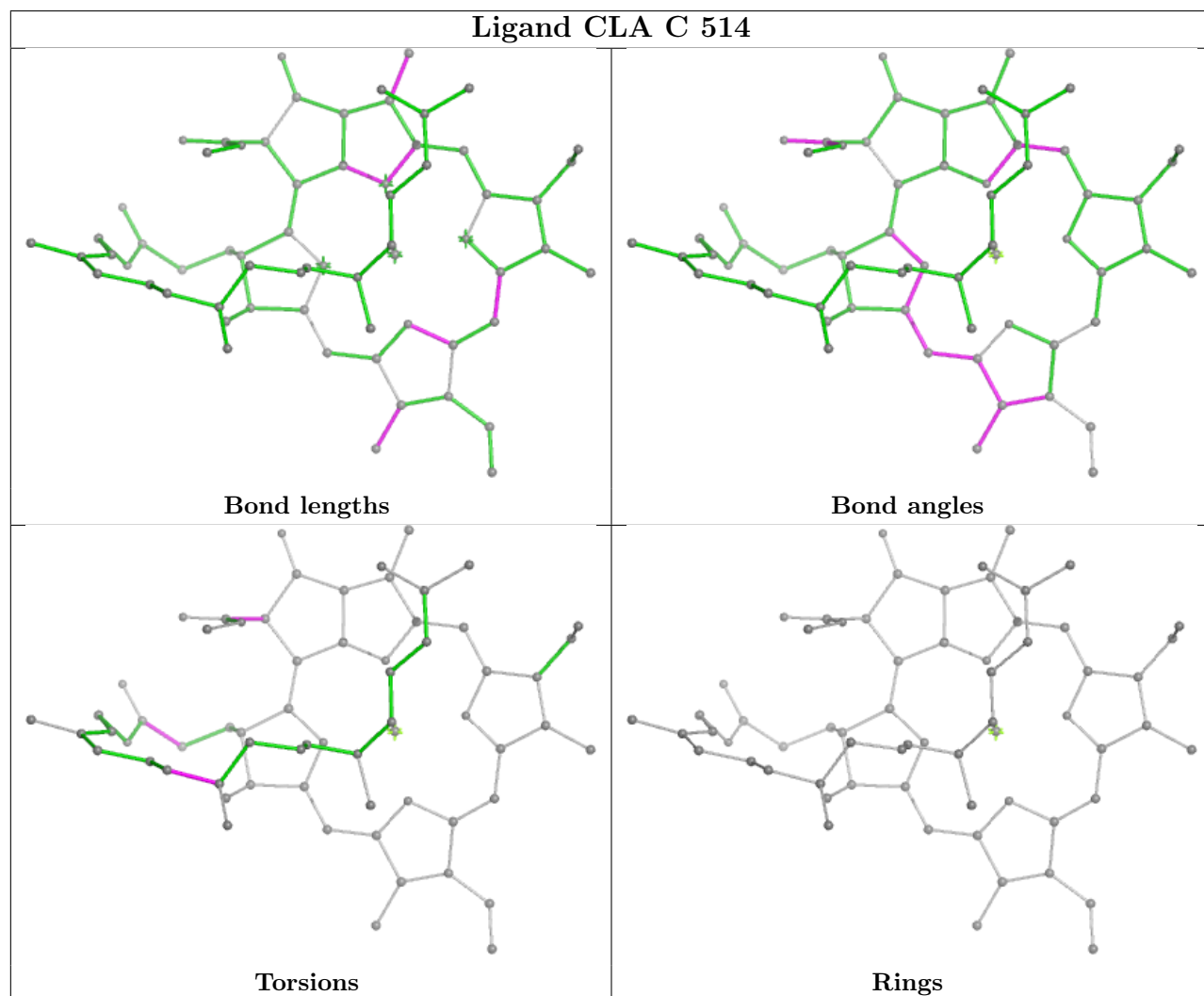
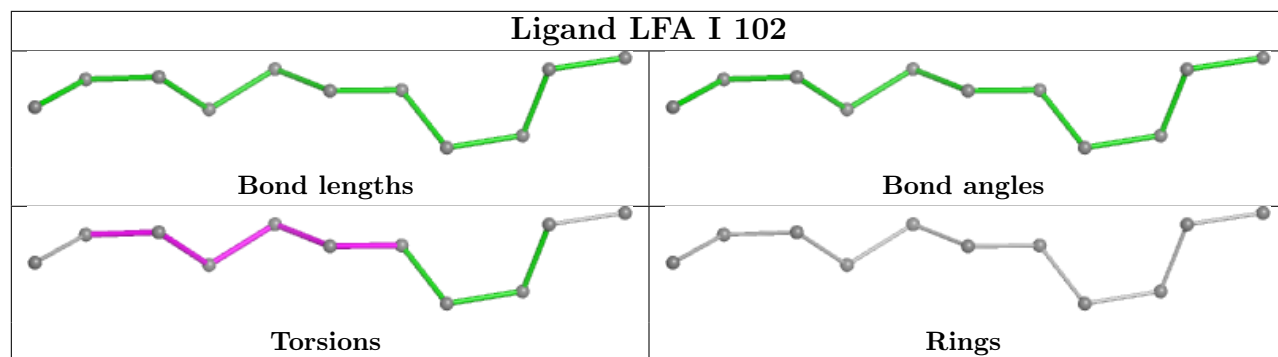




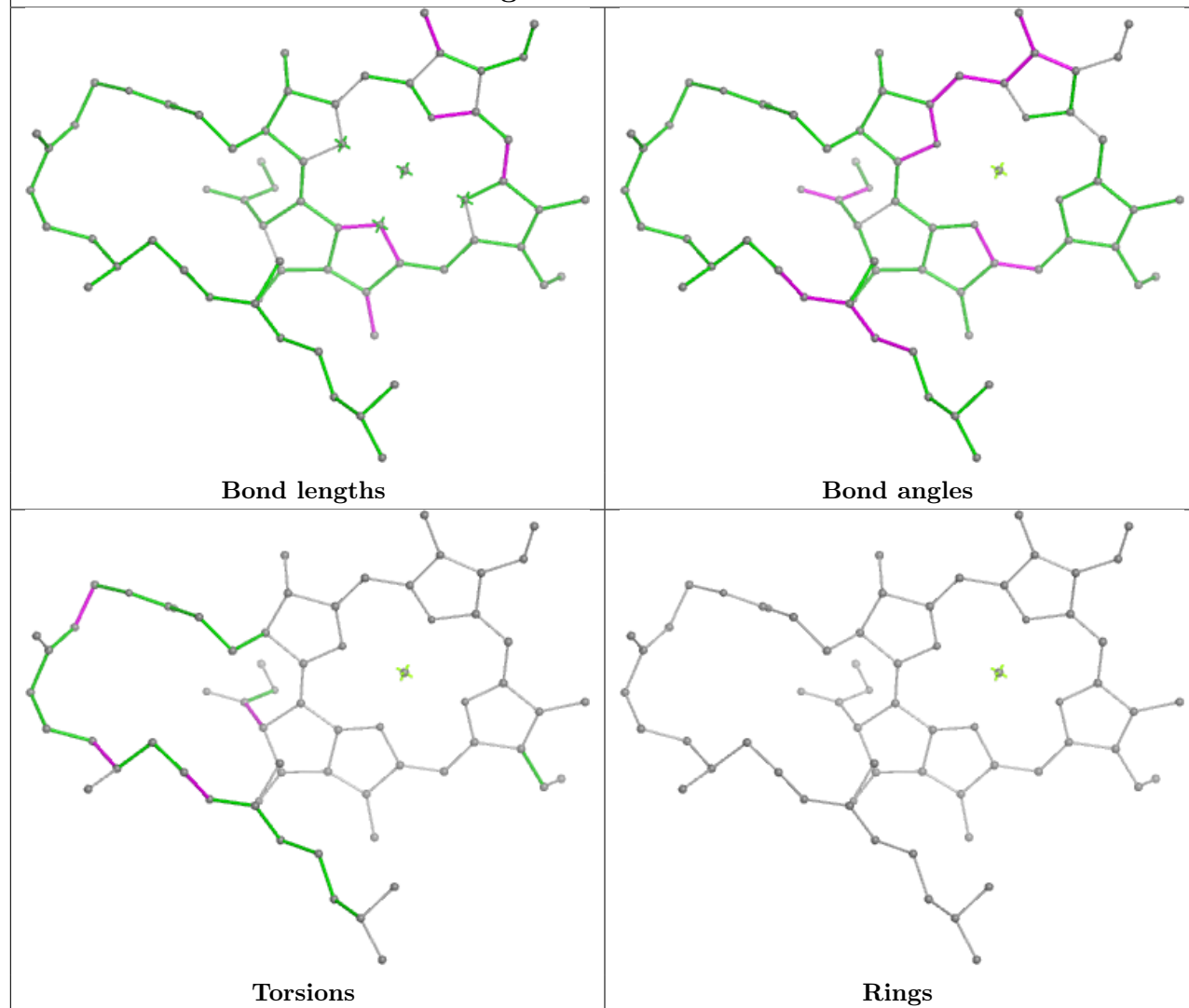




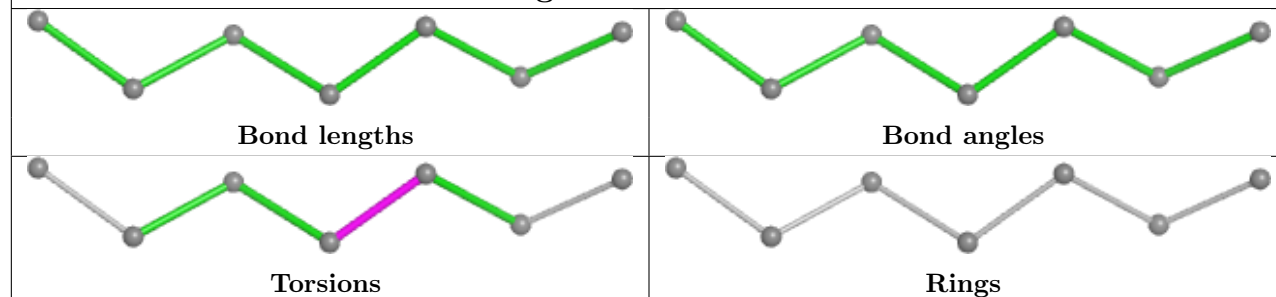


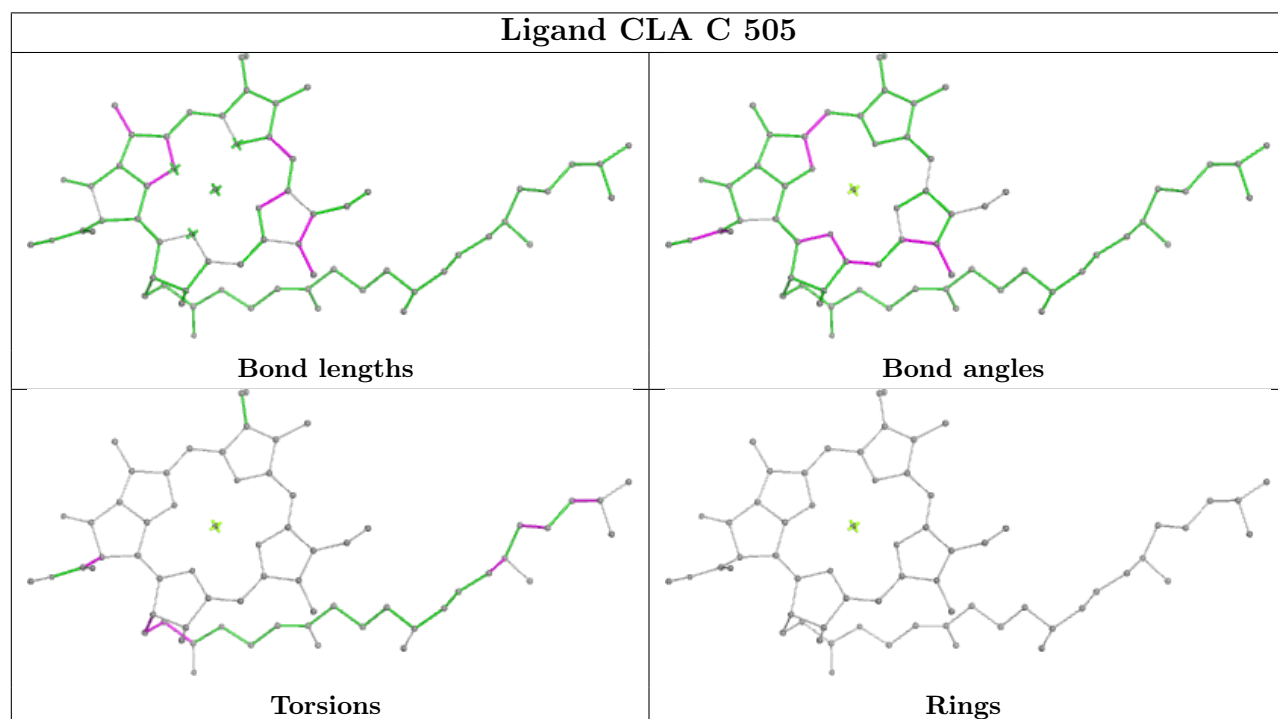
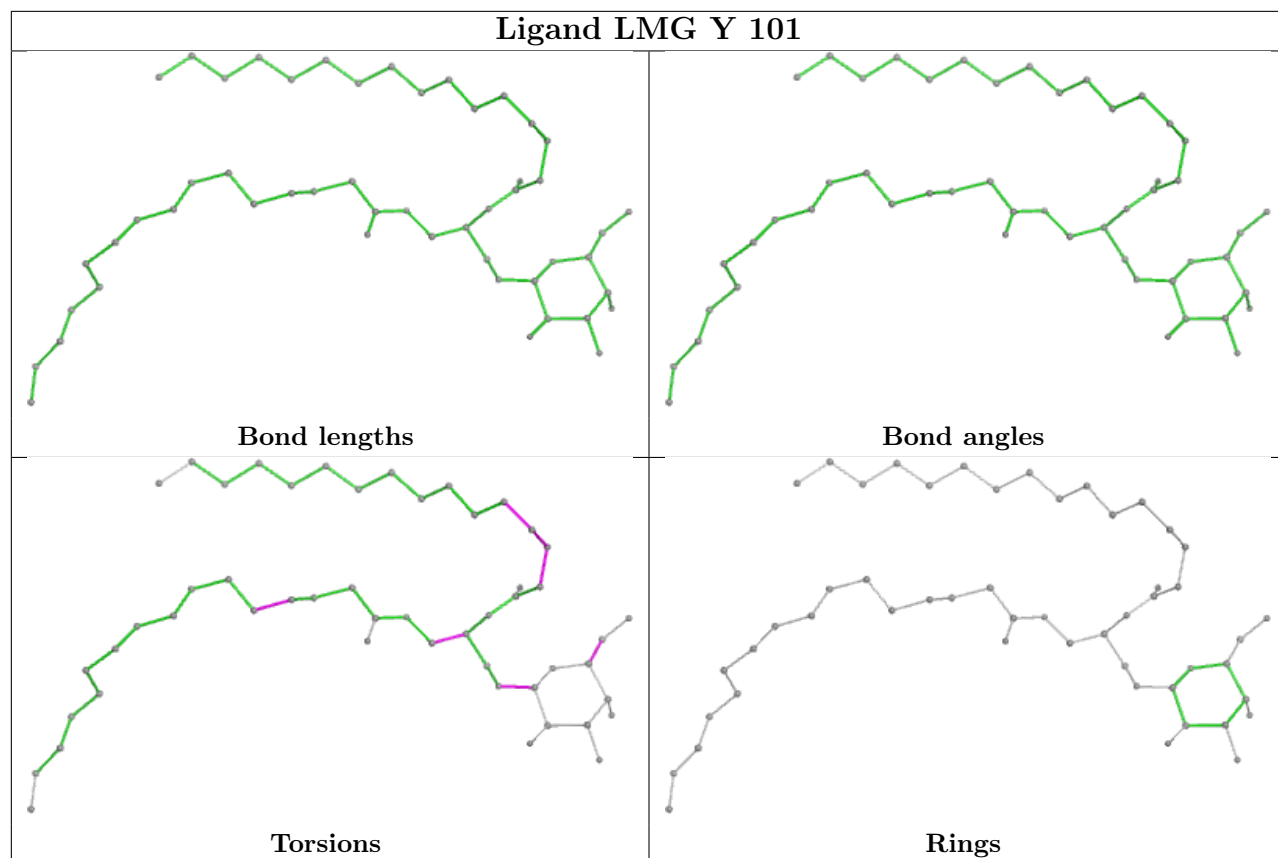


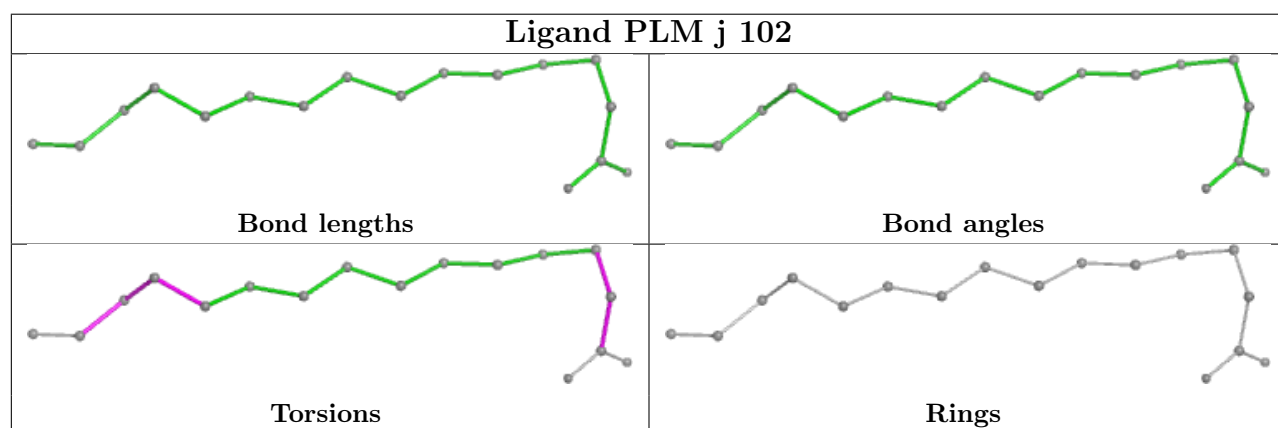
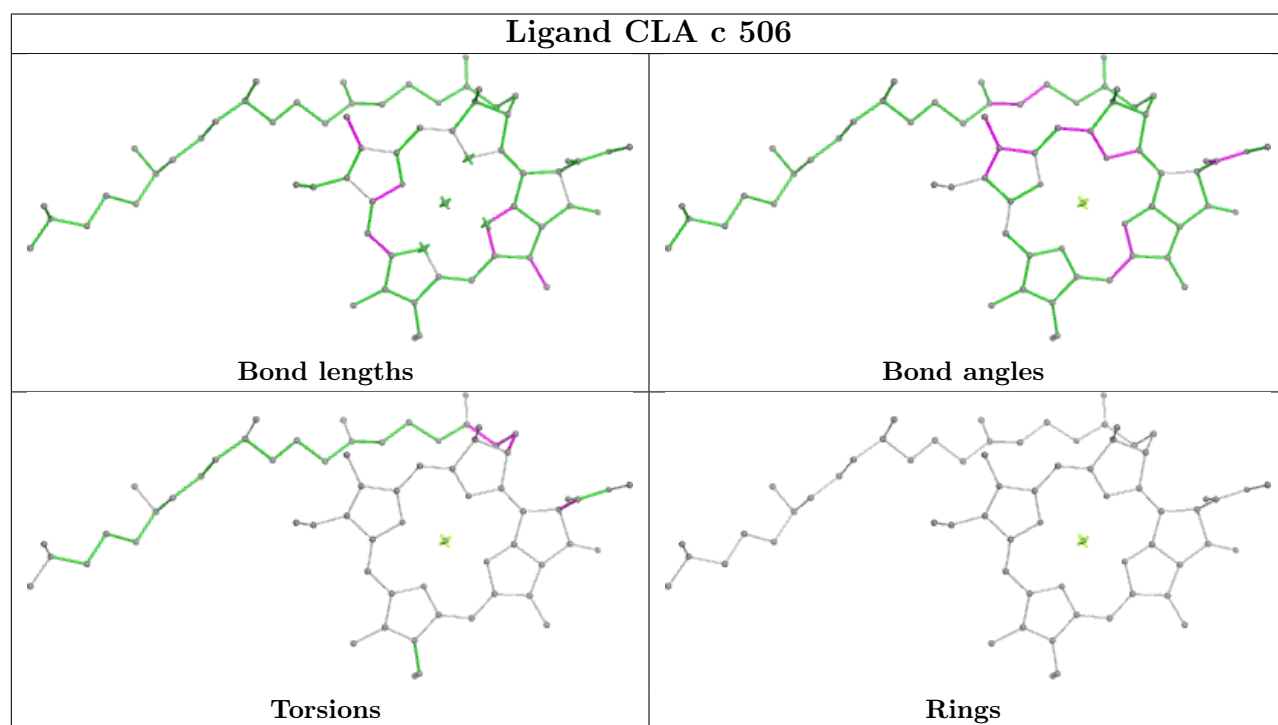
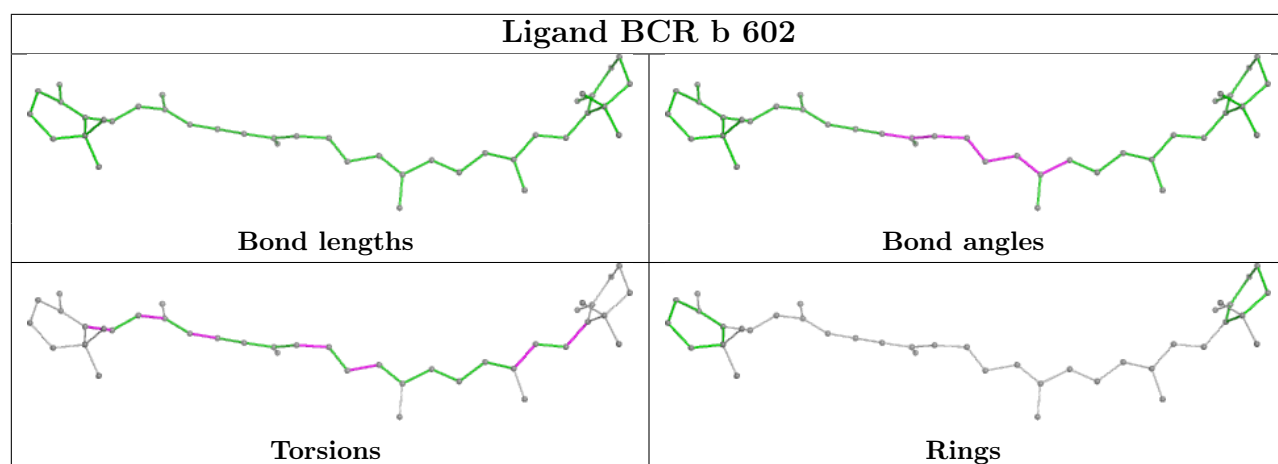
## Ligand CLA c 514

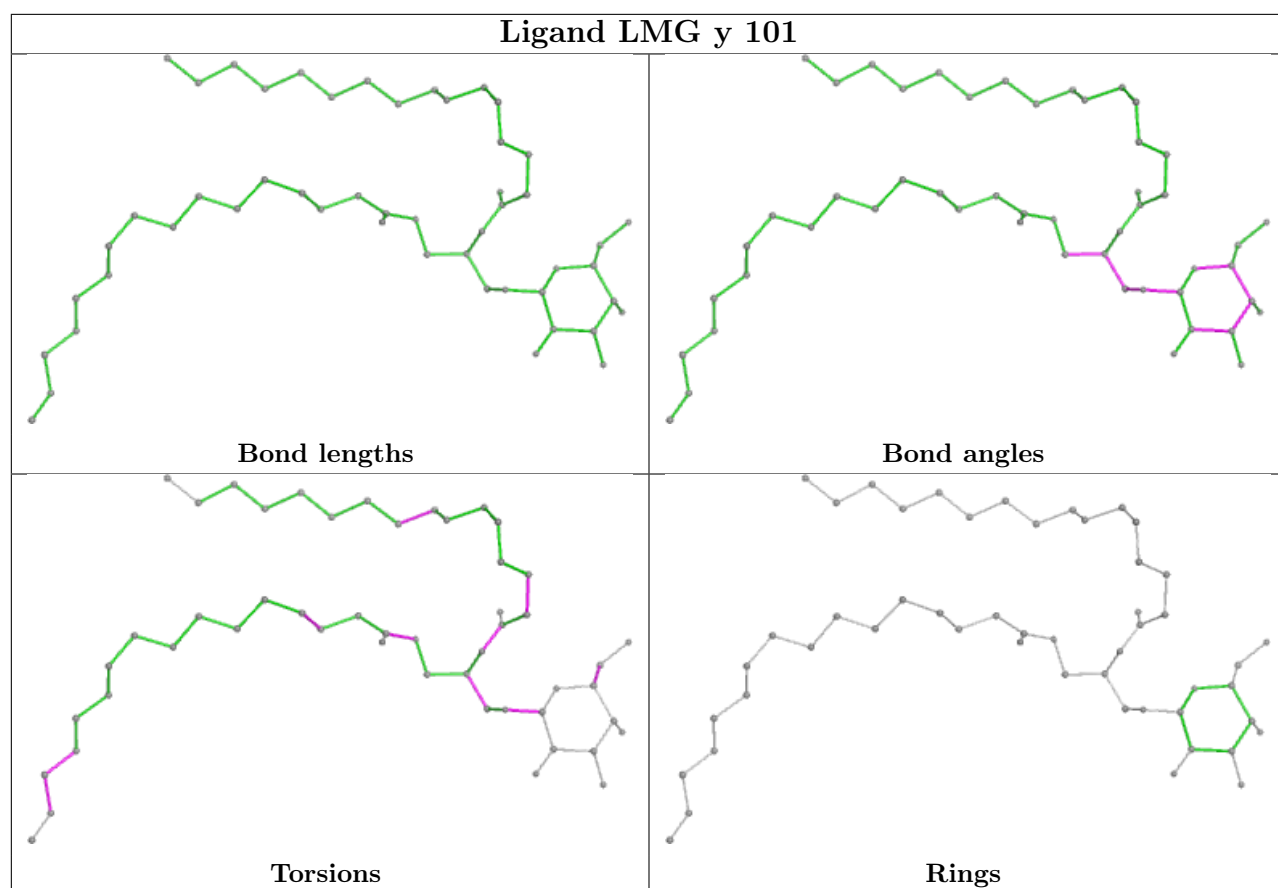


## Ligand LFA B 624

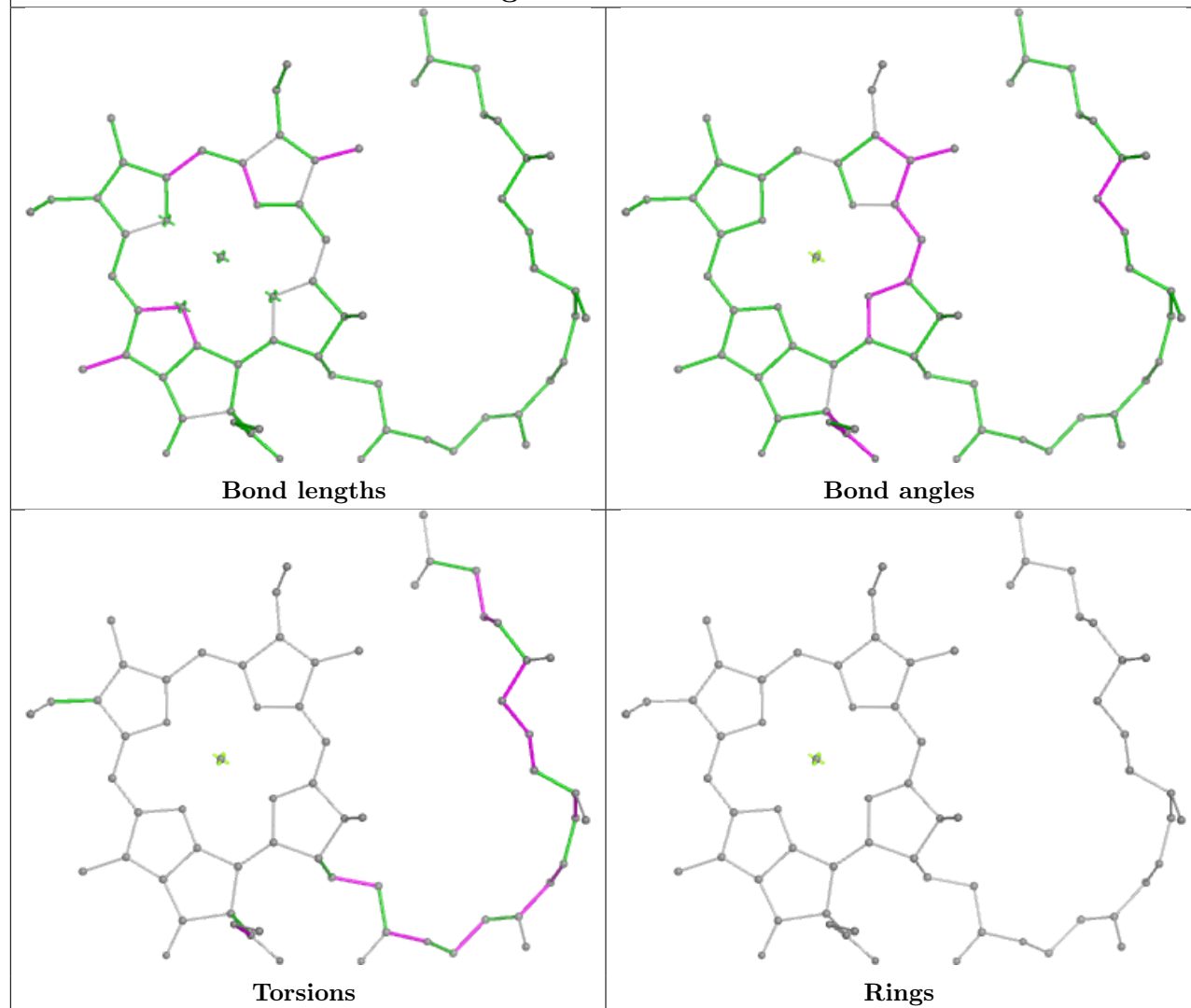




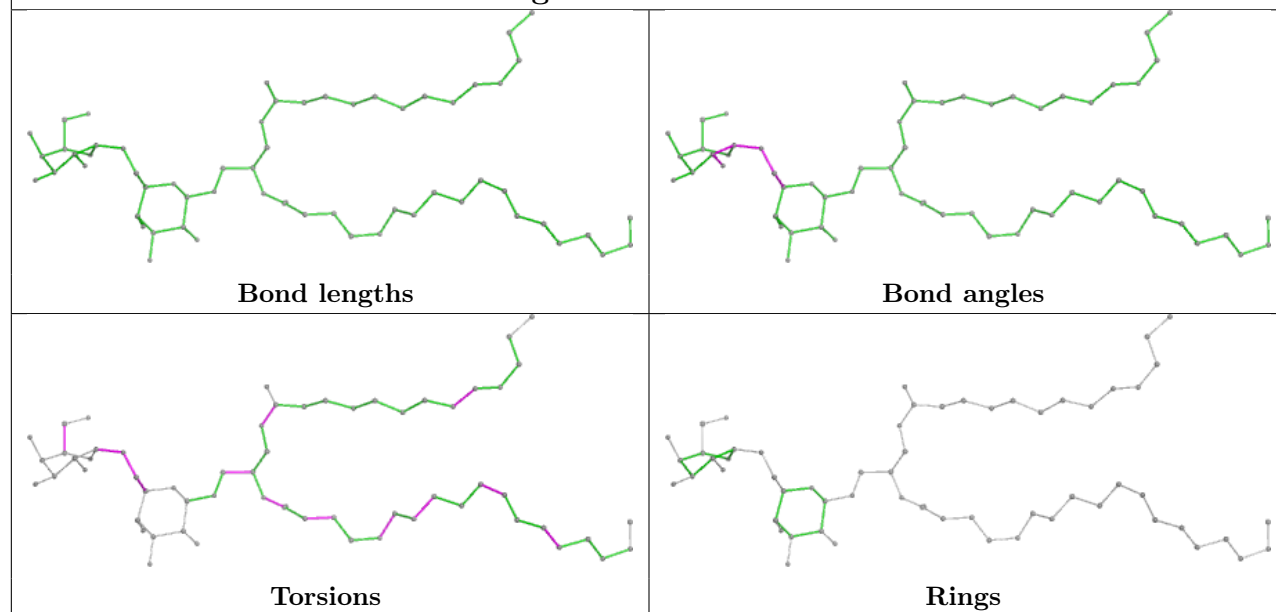




## Ligand CLA c 517

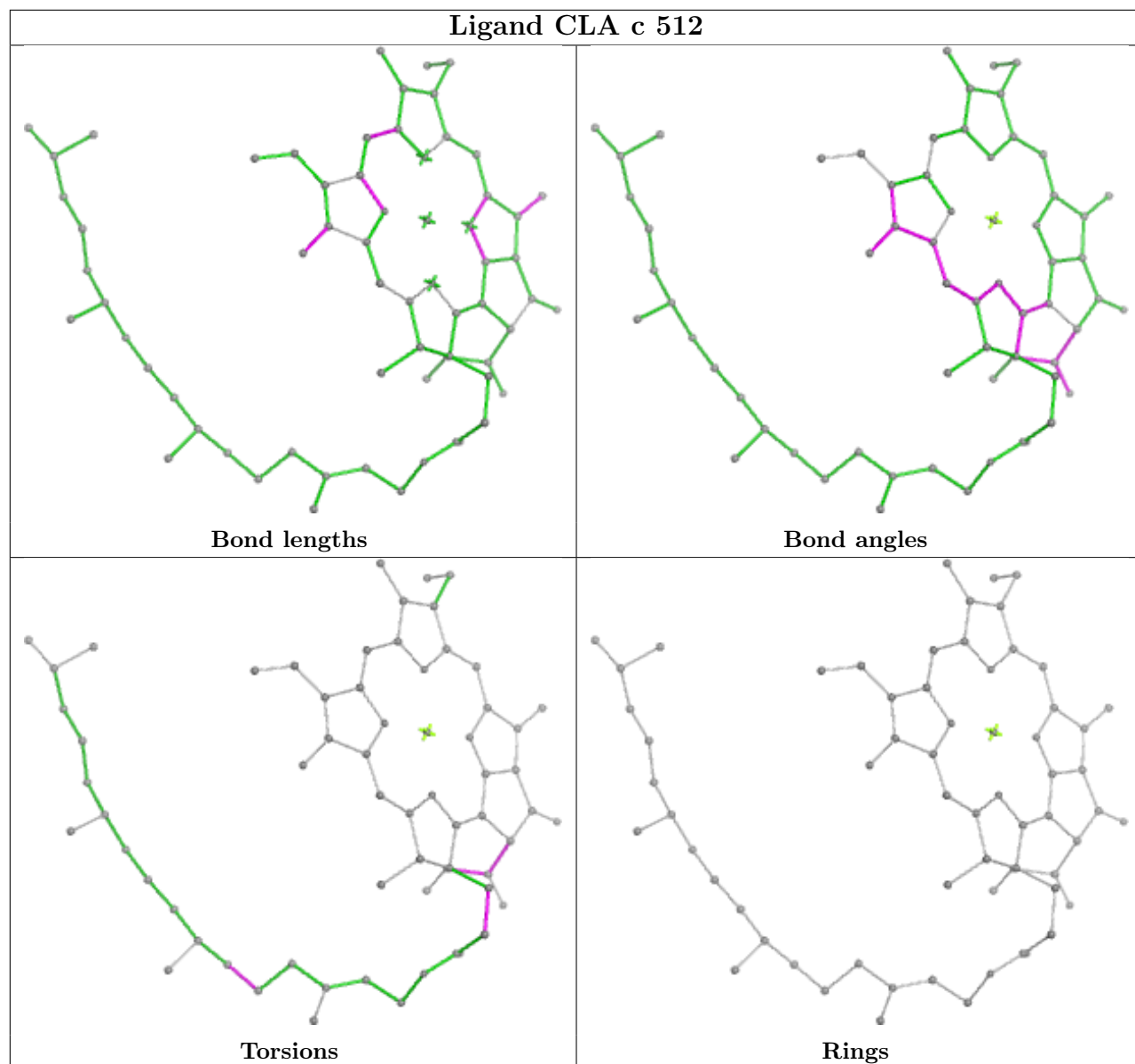


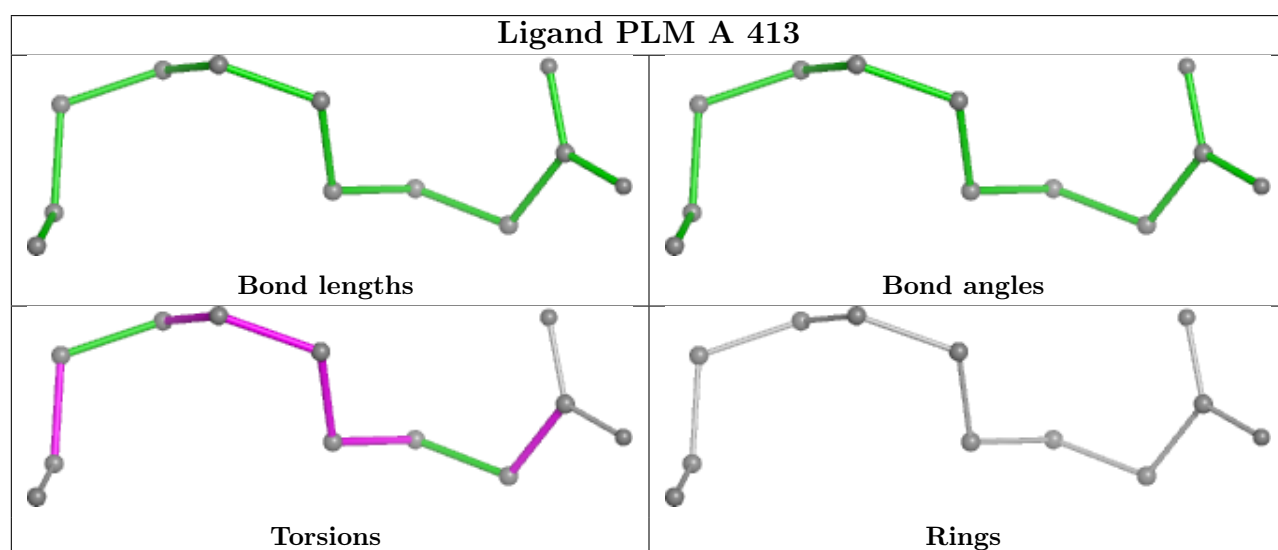
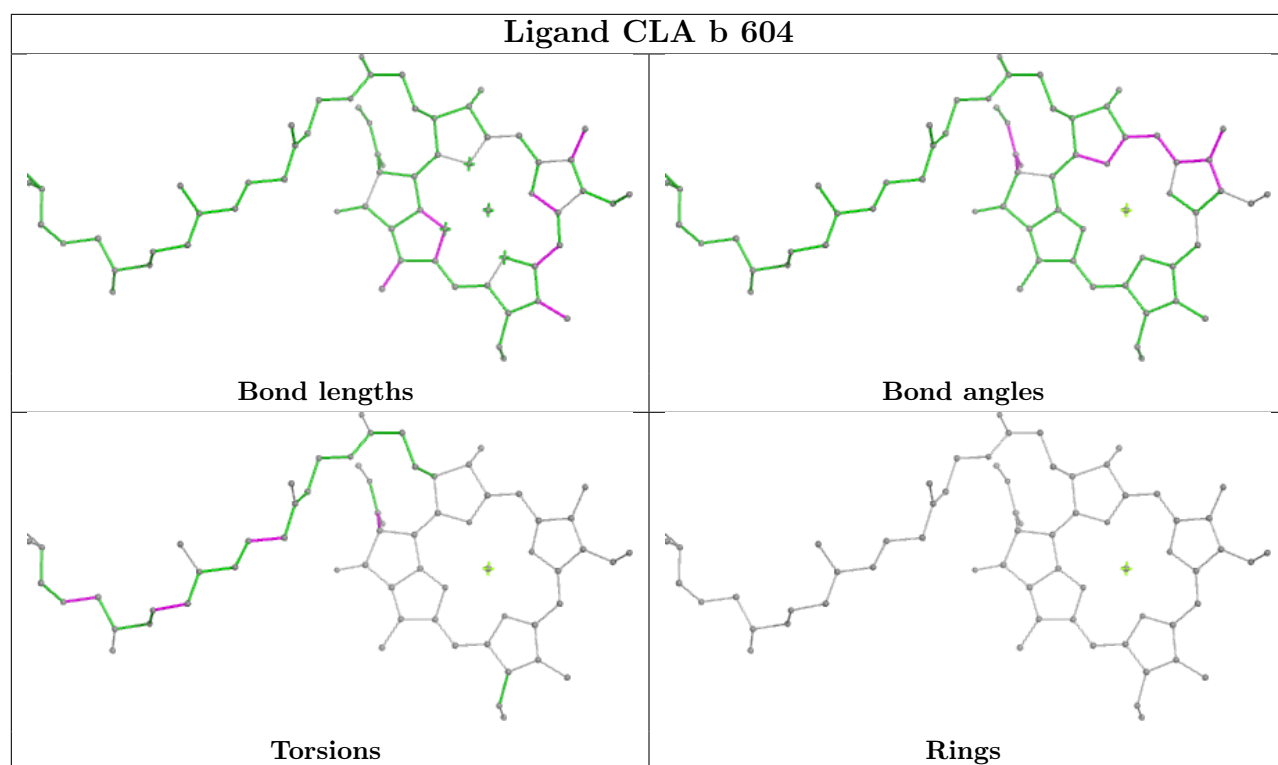
## Ligand DGD J 102



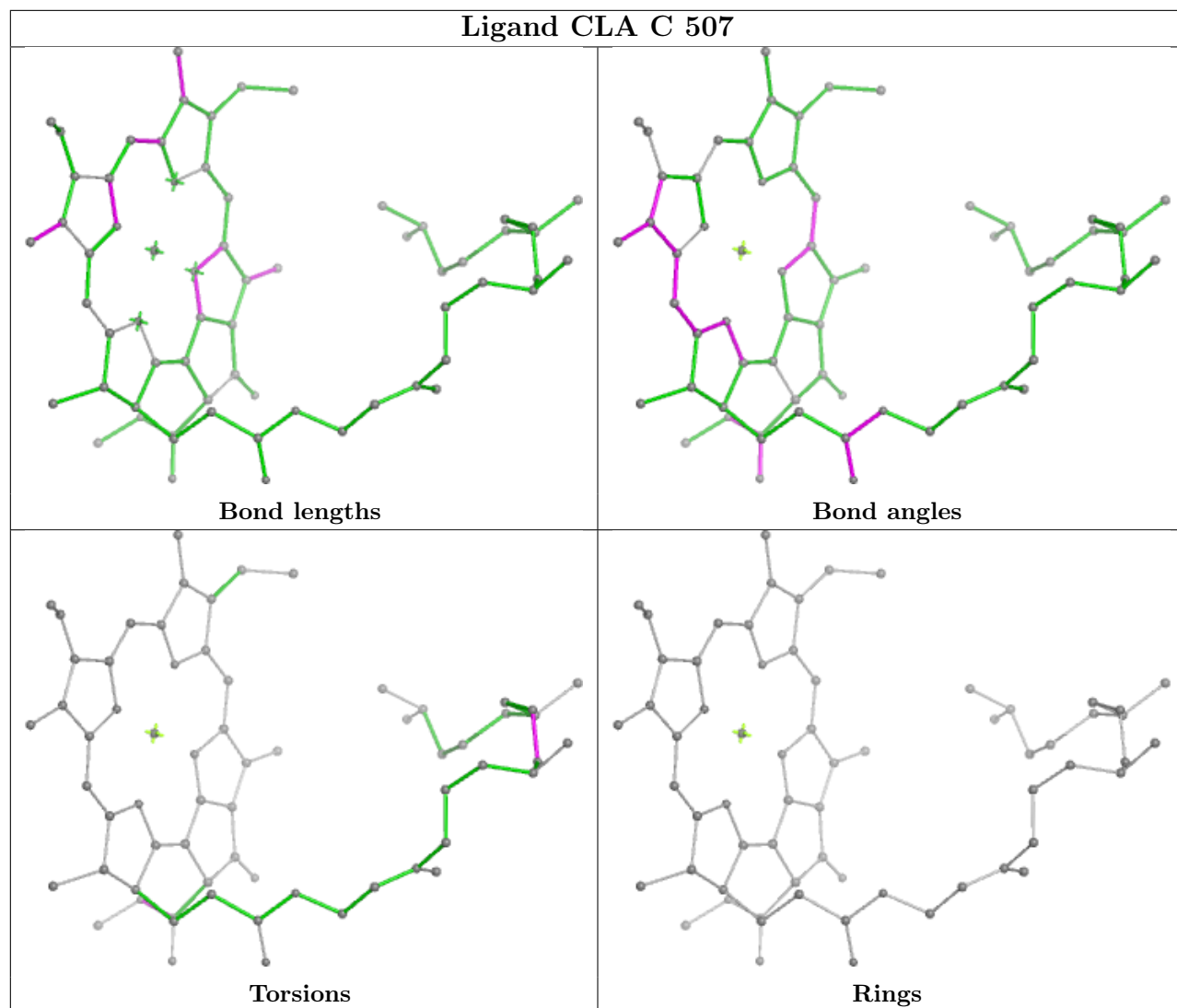


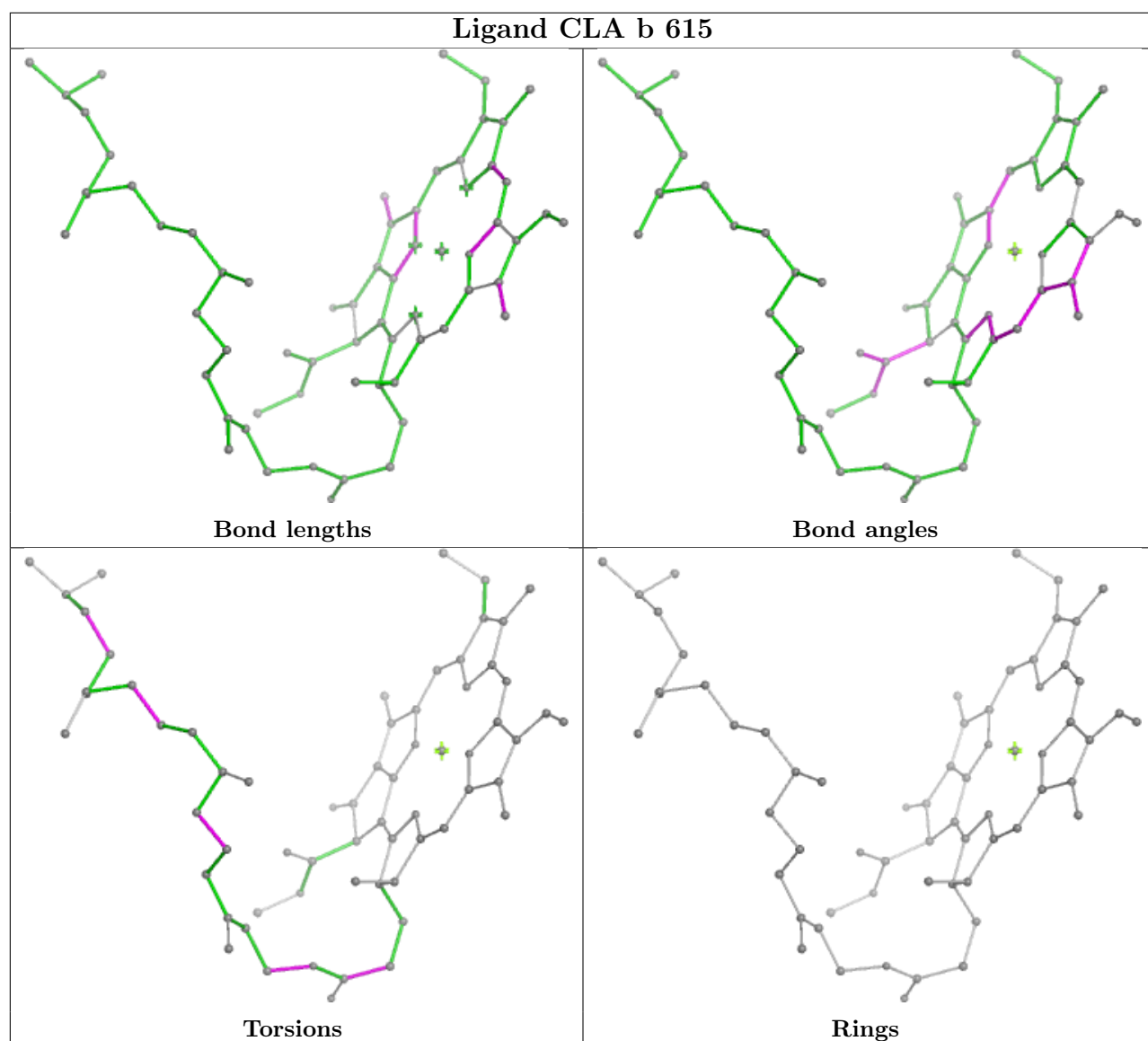
## Ligand CLA c 512

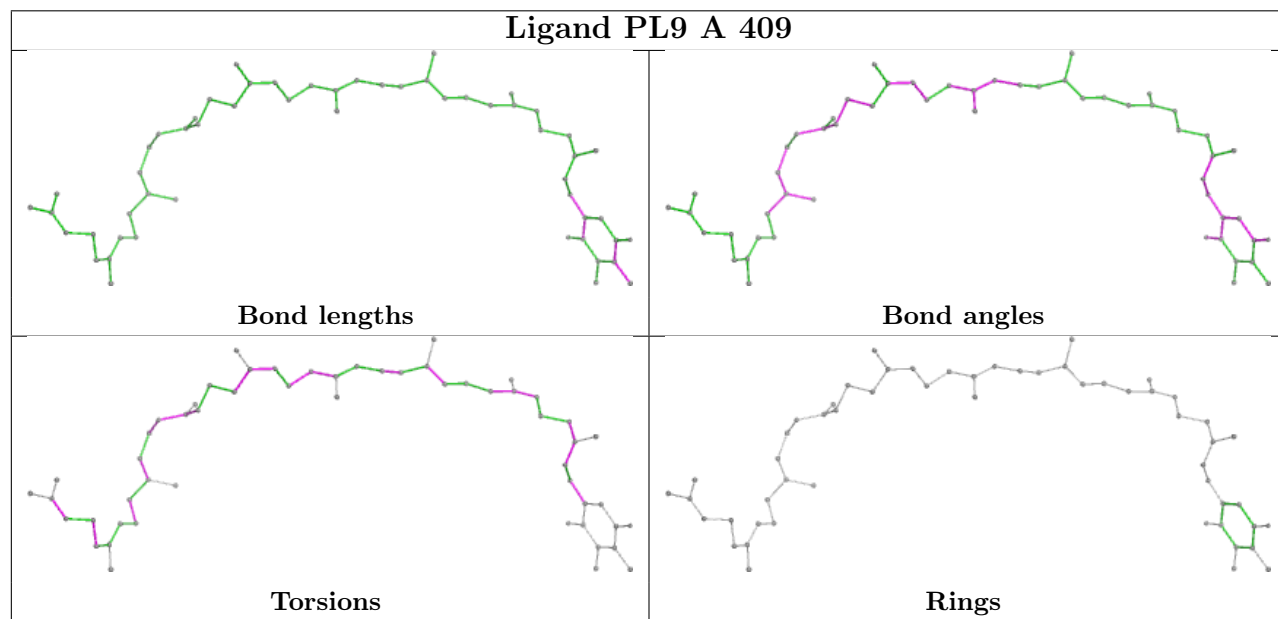
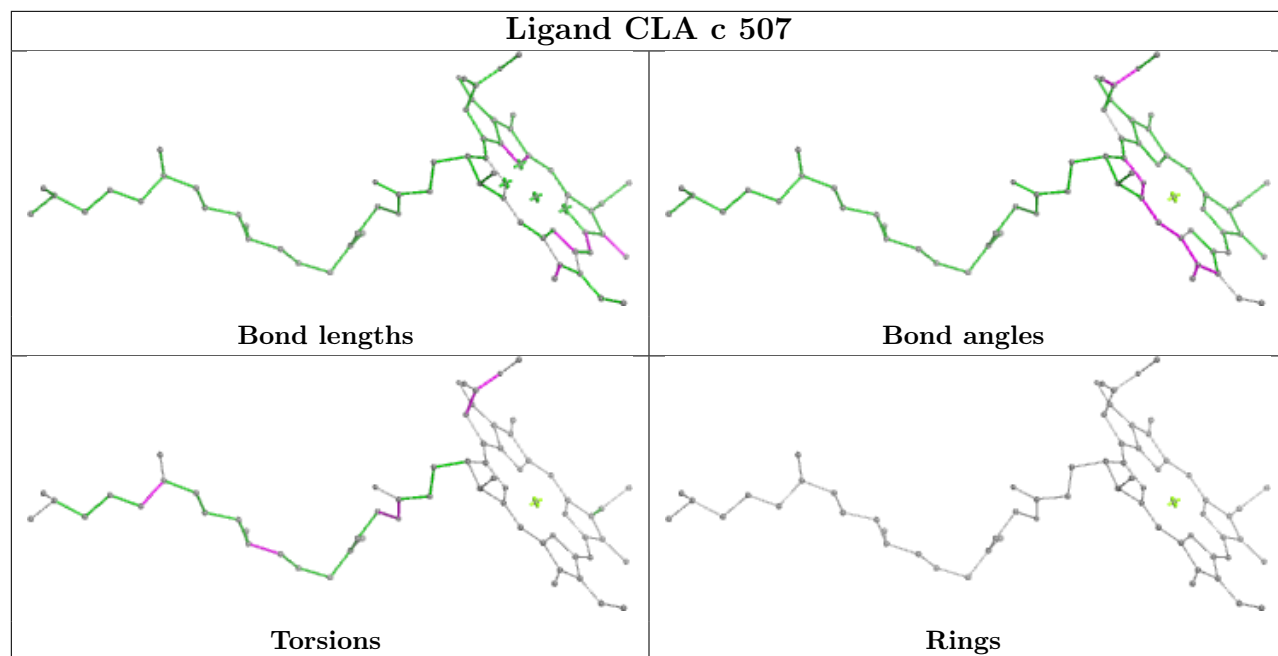


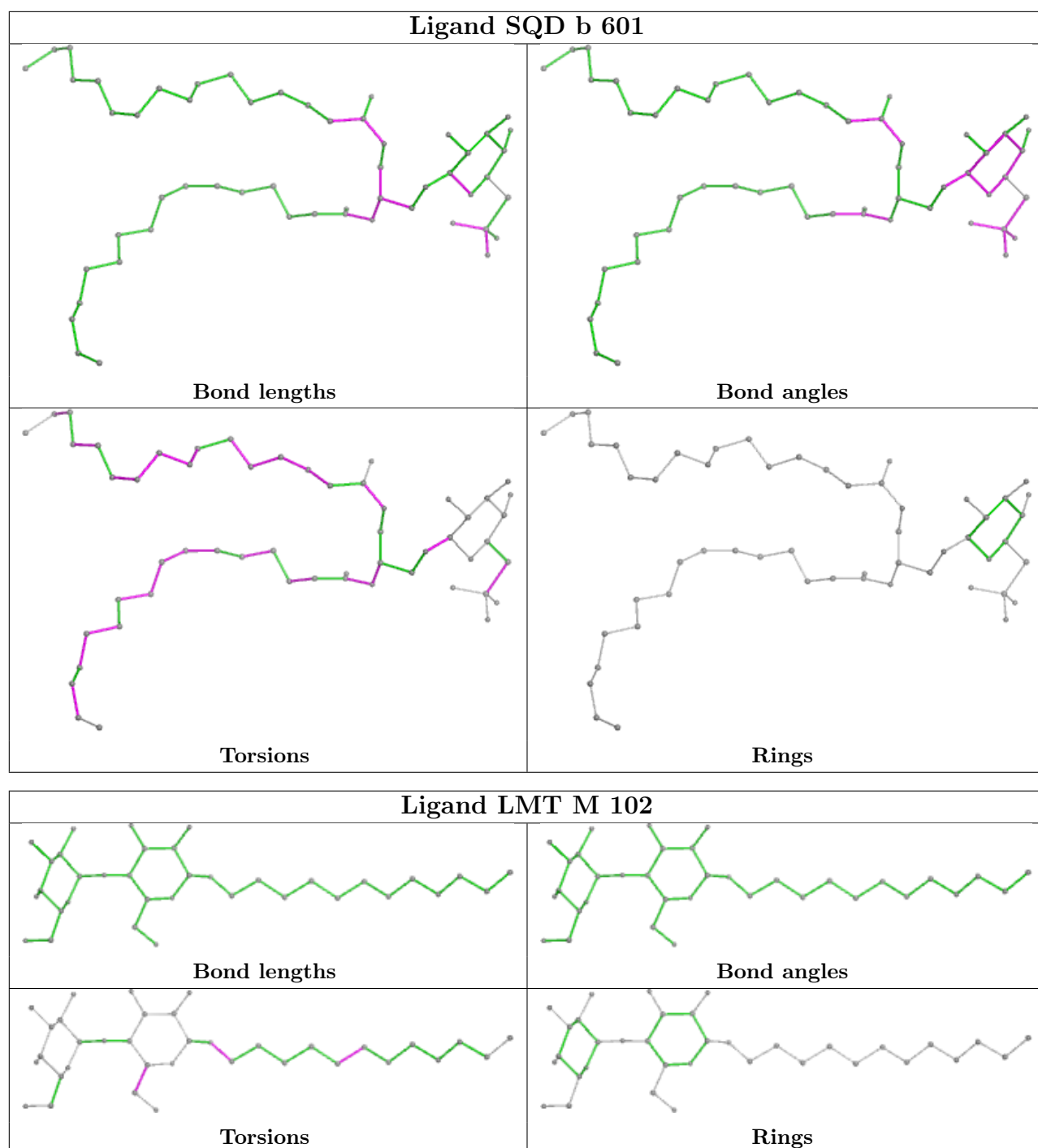


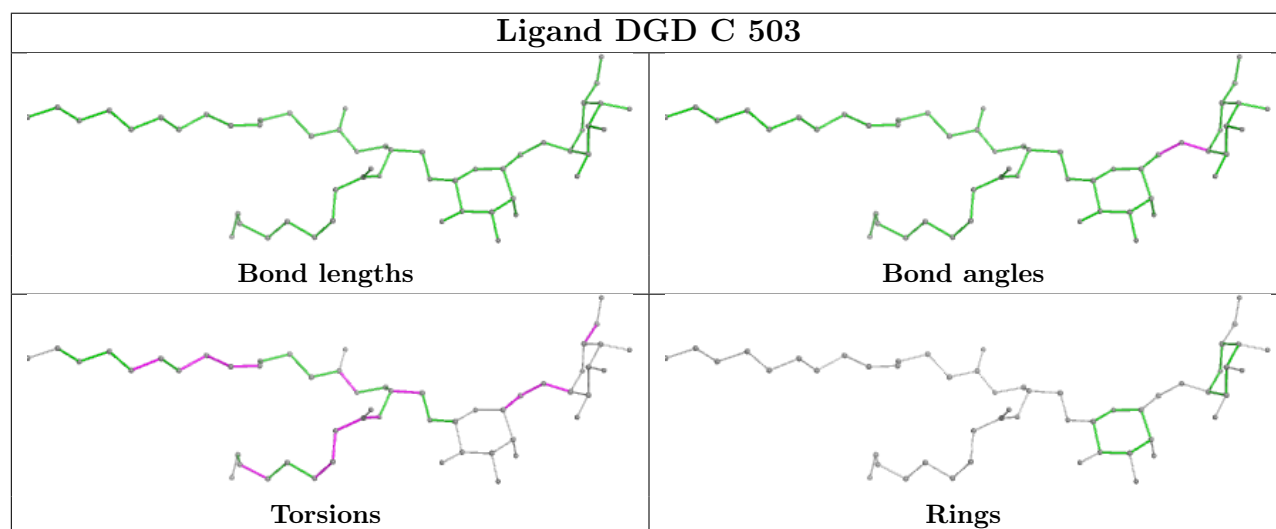
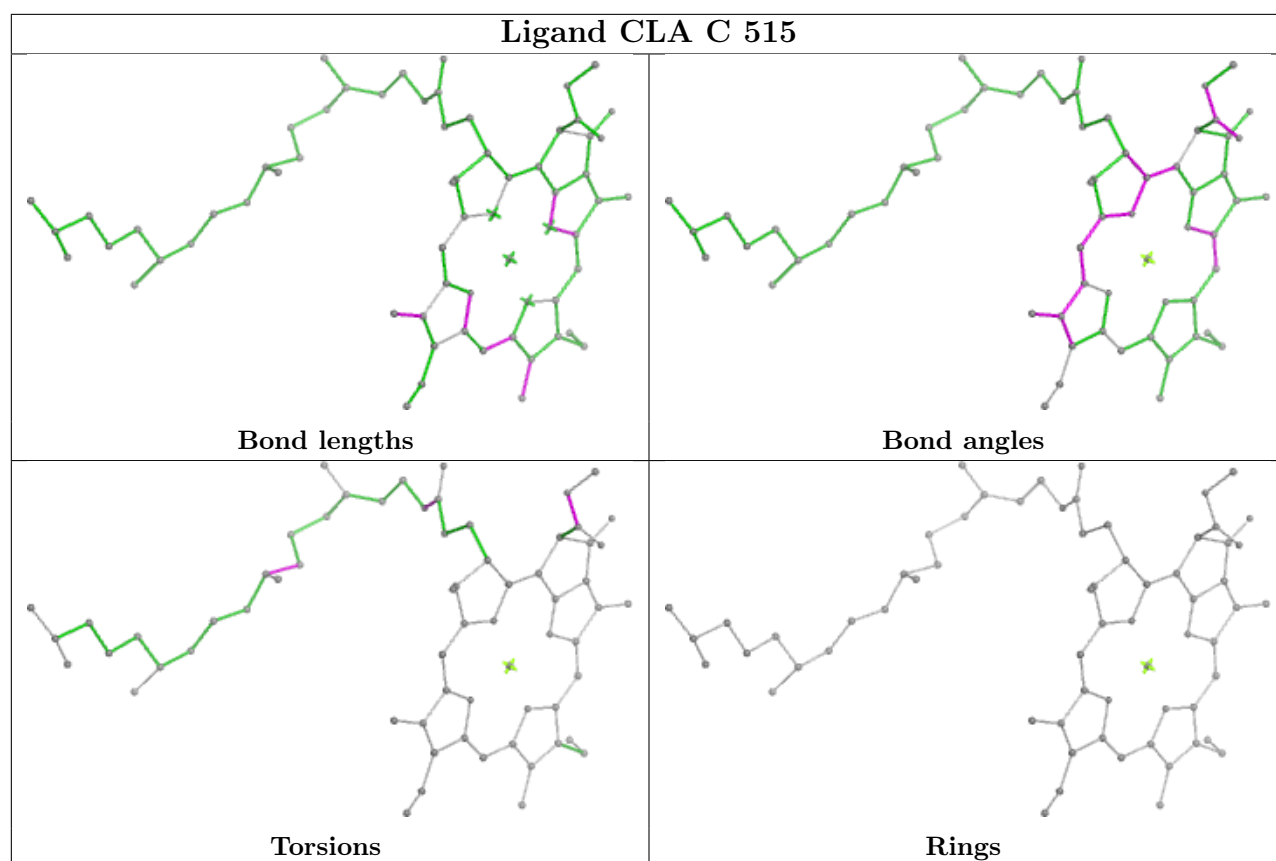
## Ligand CLA C 507

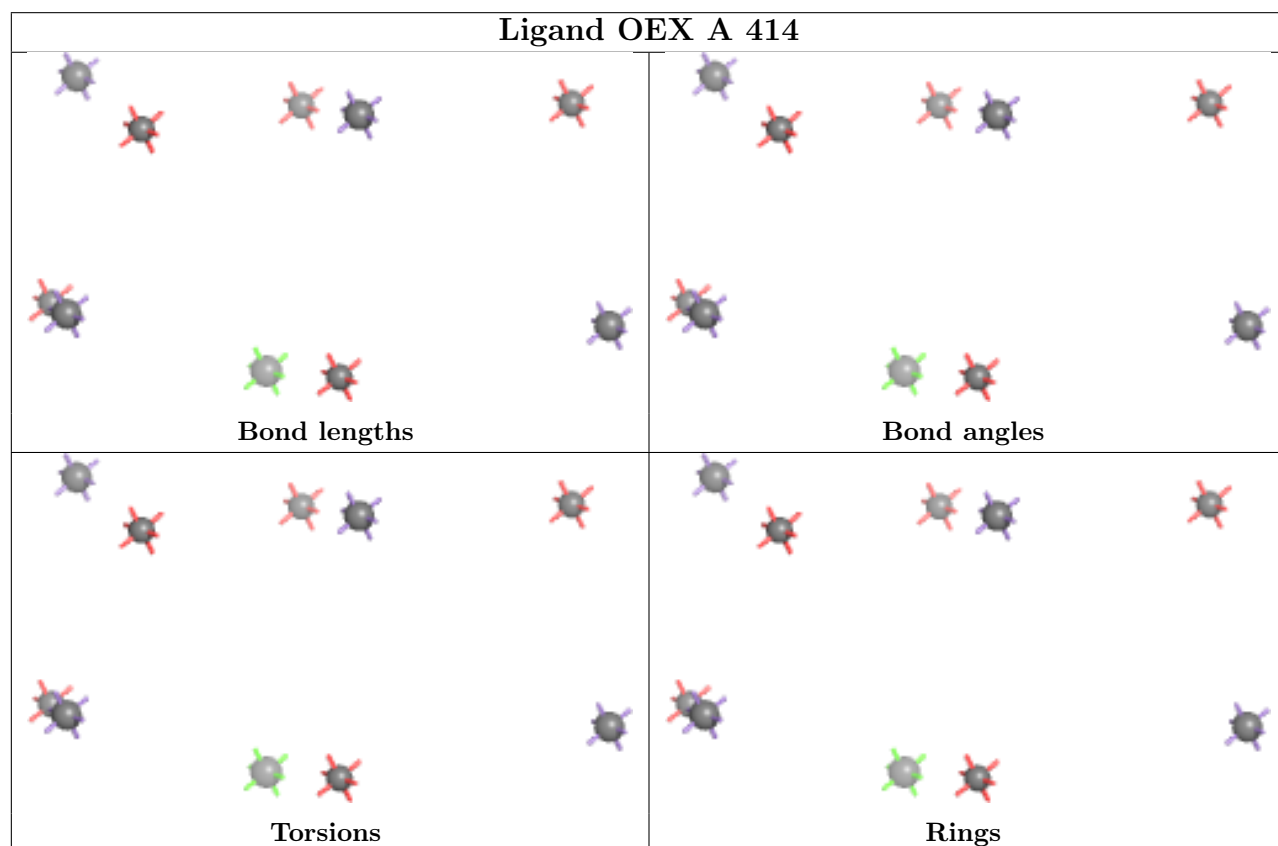
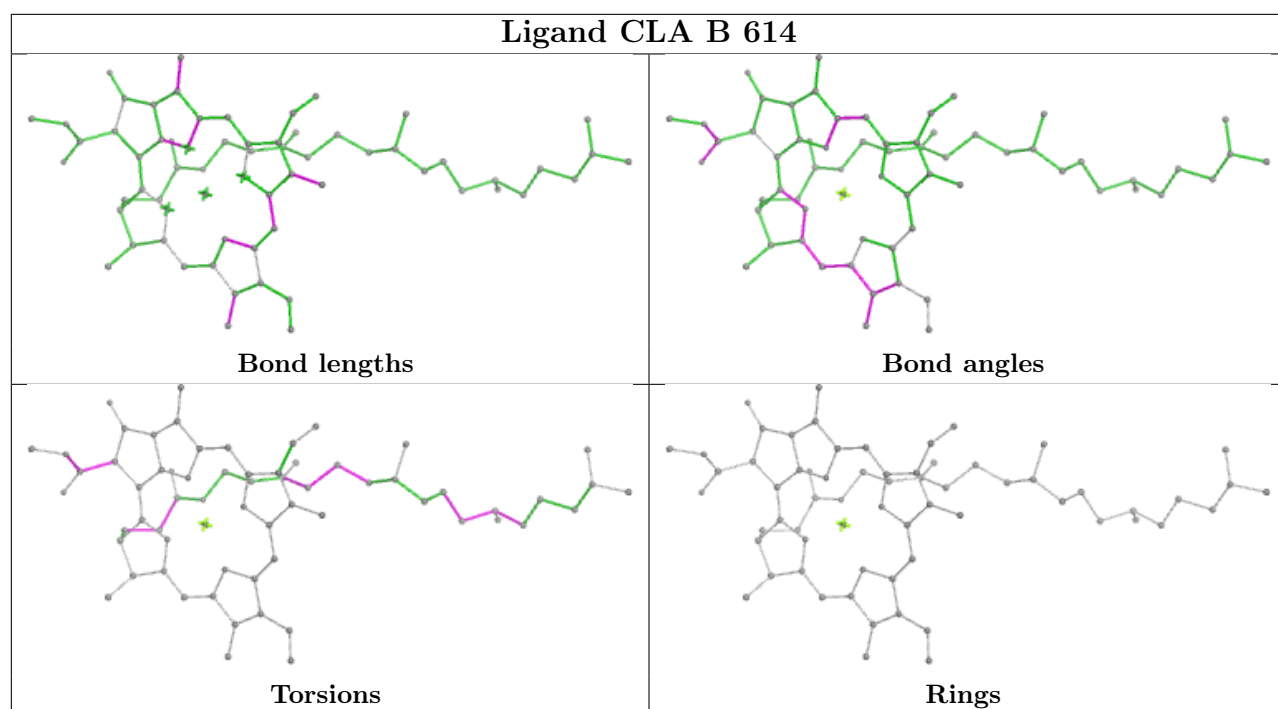




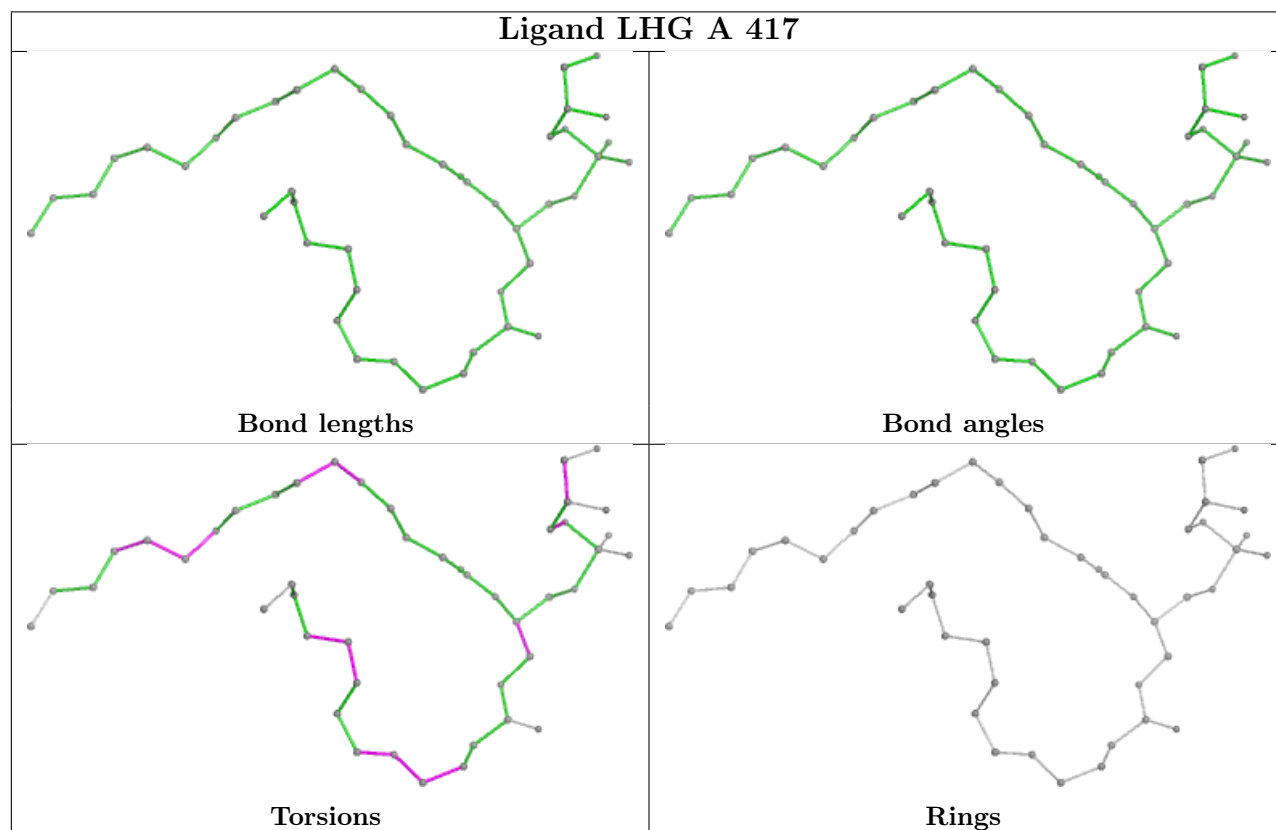
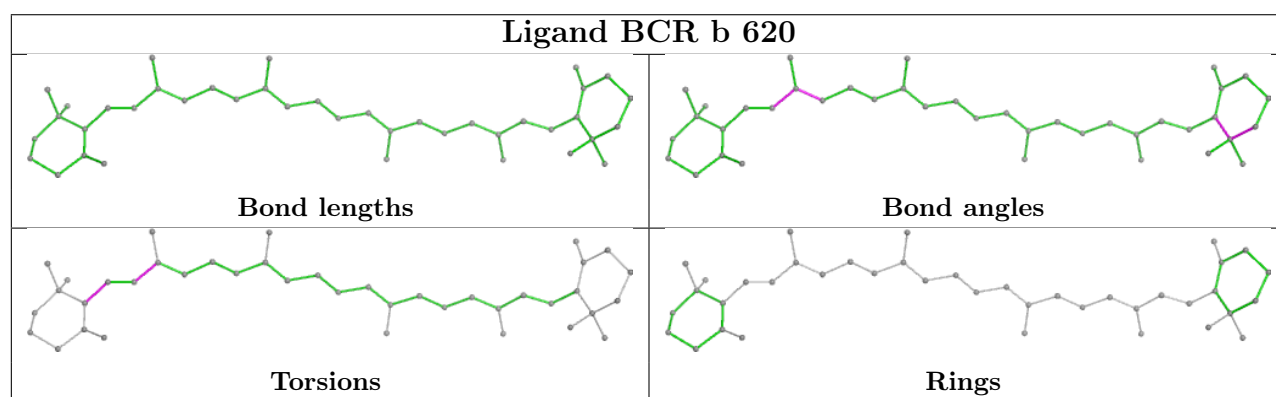
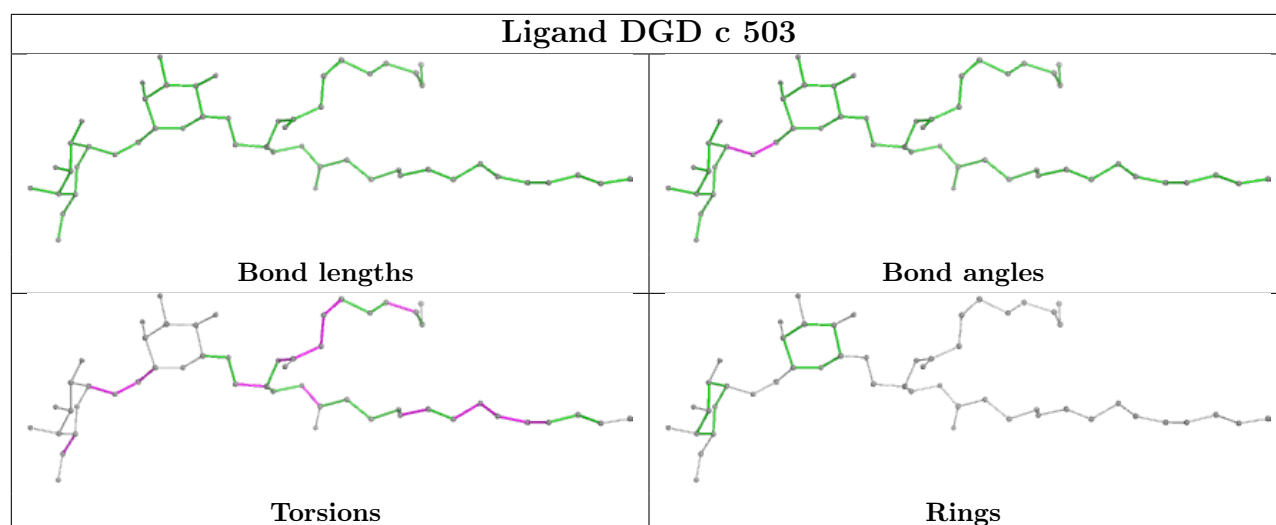












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

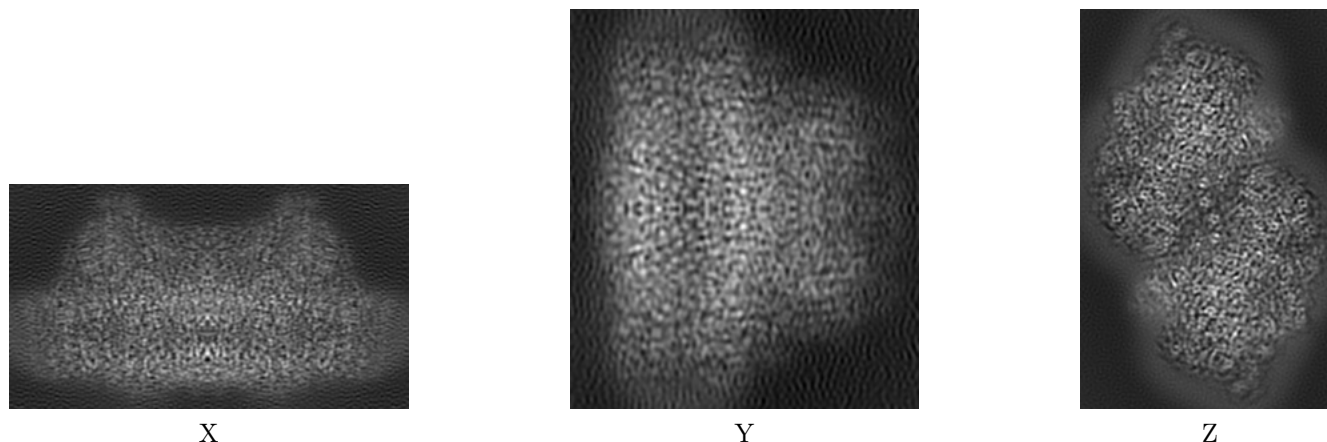
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51102. These allow visual inspection of the internal detail of the map and identification of artifacts.

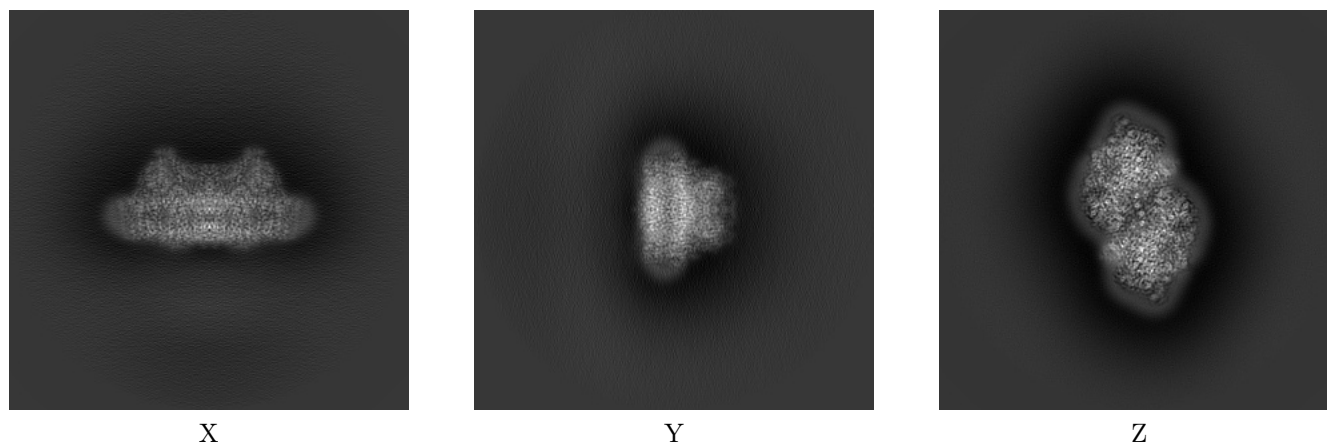
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



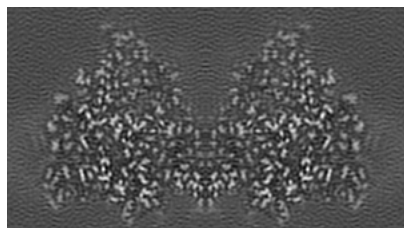
#### 6.1.2 Raw map



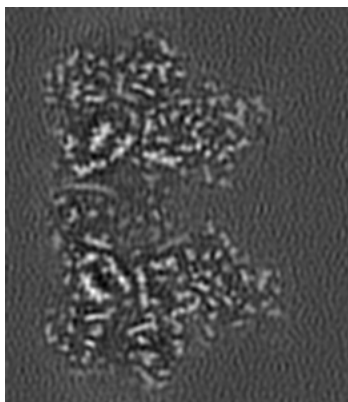
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

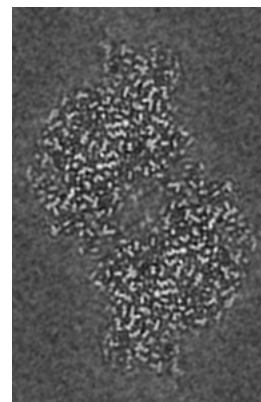
### 6.2.1 Primary map



X Index: 135

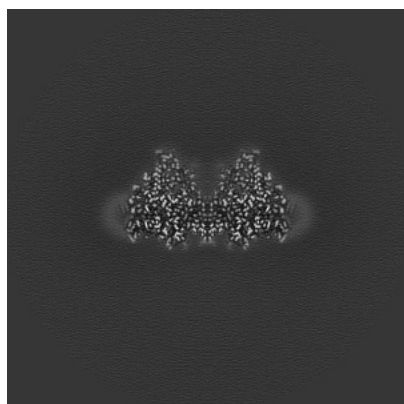


Y Index: 210

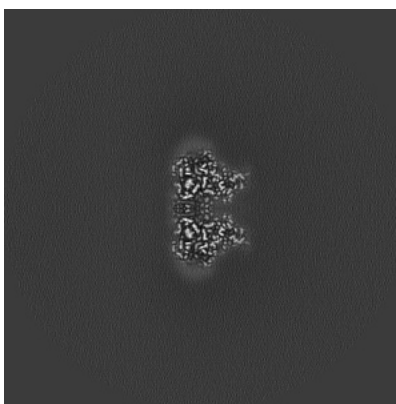


Z Index: 118

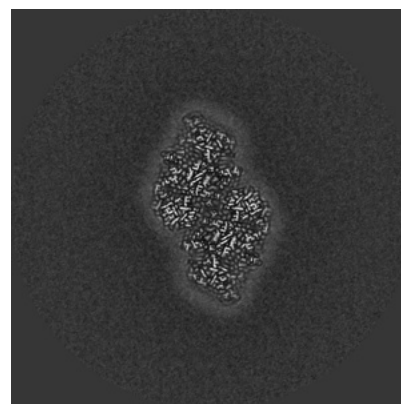
### 6.2.2 Raw map



X Index: 200



Y Index: 200

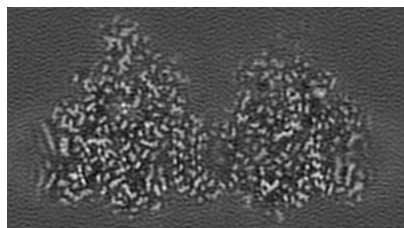


Z Index: 200

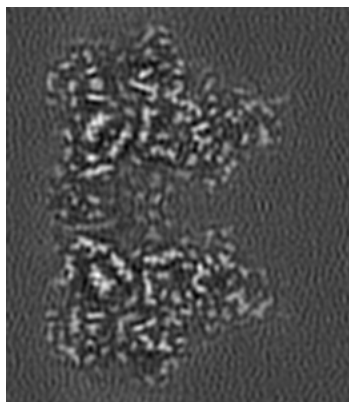
The images above show central slices of the map in three orthogonal directions.

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

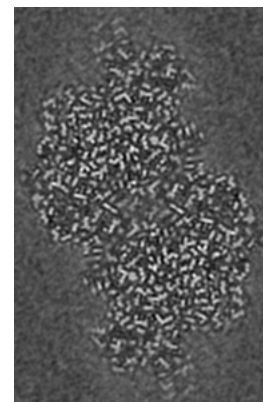
### 6.3.1 Primary map



X Index: 141

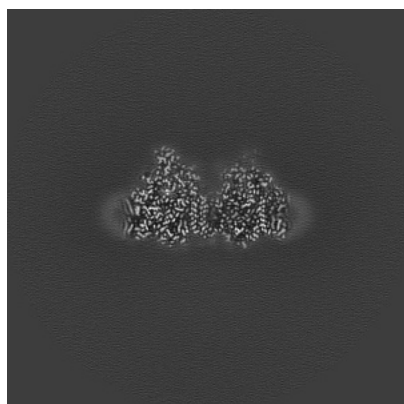


Y Index: 207

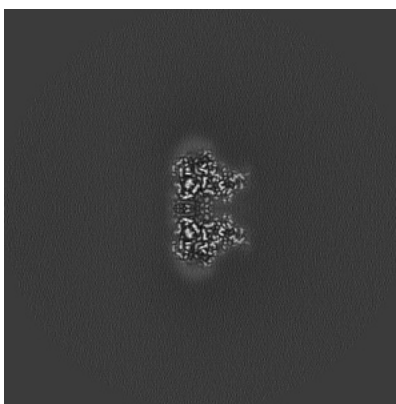


Z Index: 110

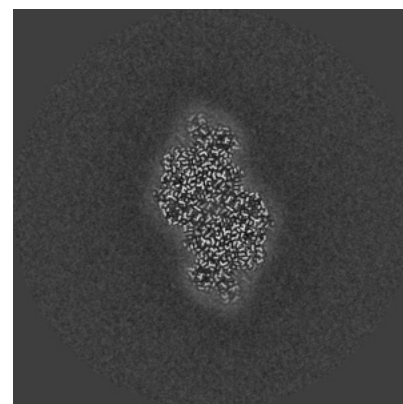
### 6.3.2 Raw map



X Index: 203



Y Index: 200

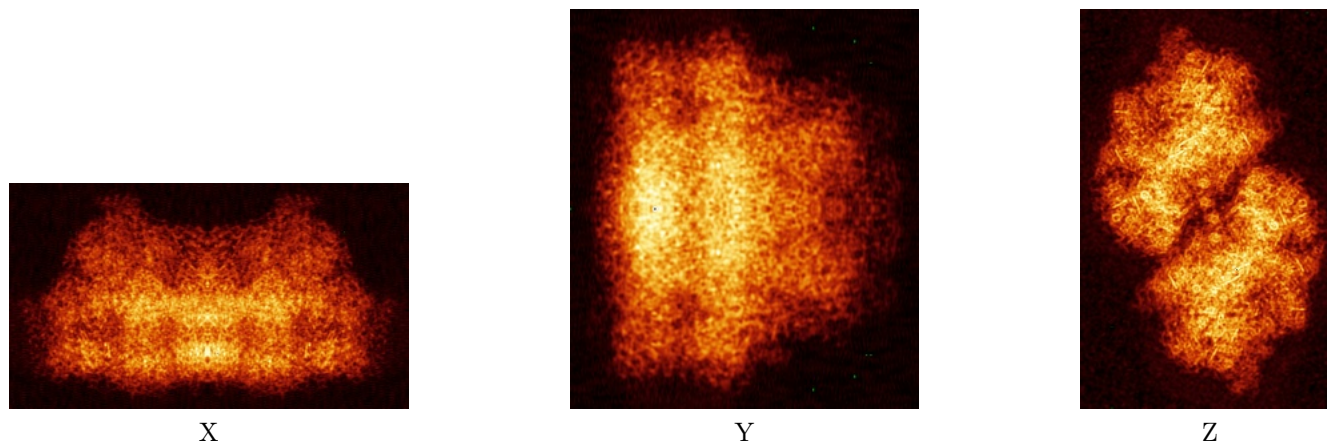


Z Index: 207

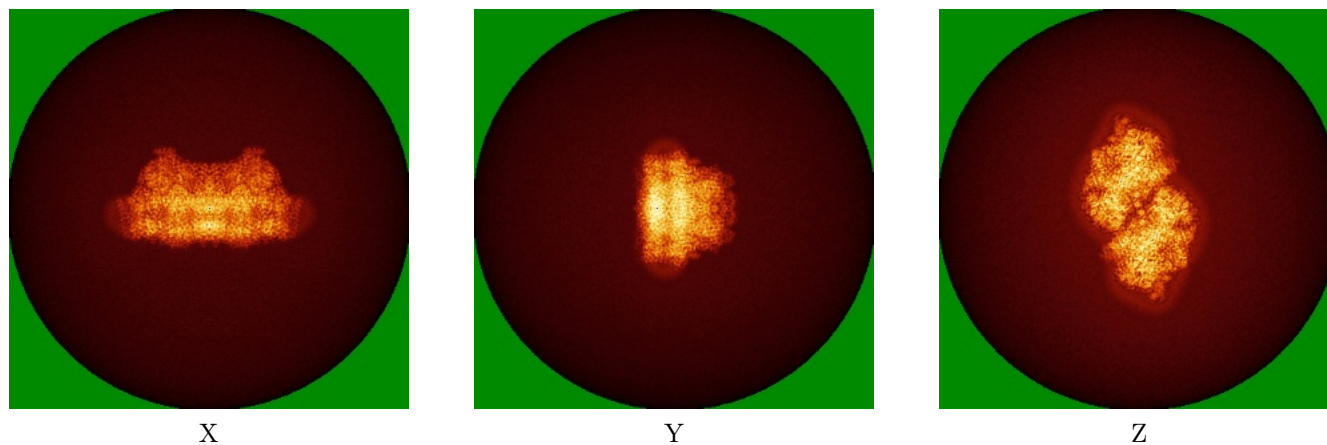
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map

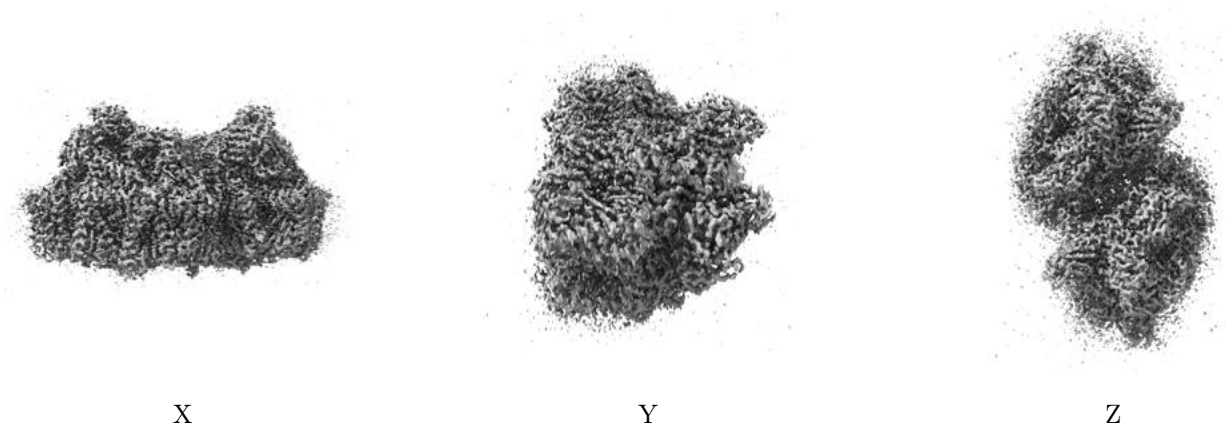


The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



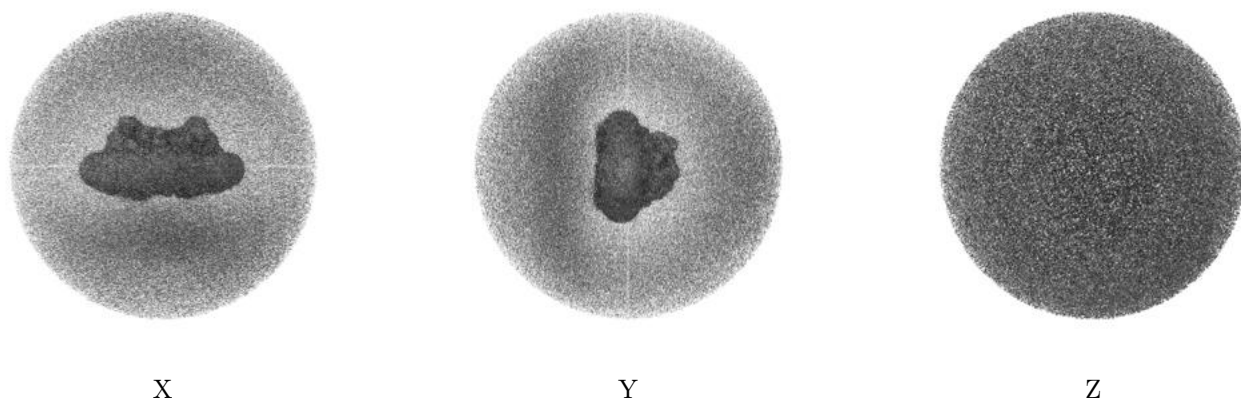
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.043. 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.

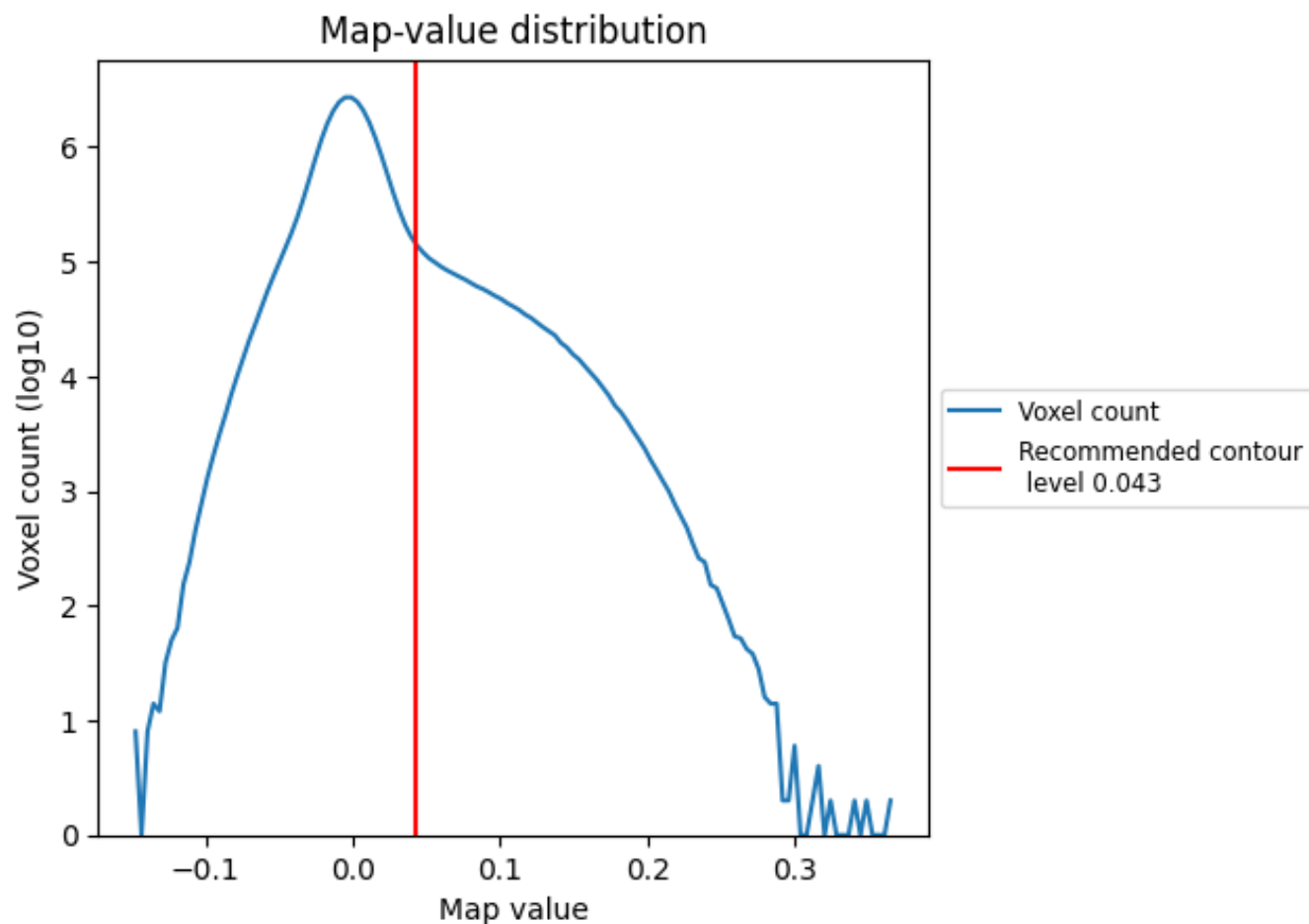
## 6.6 Mask visualisation [i](#)

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.

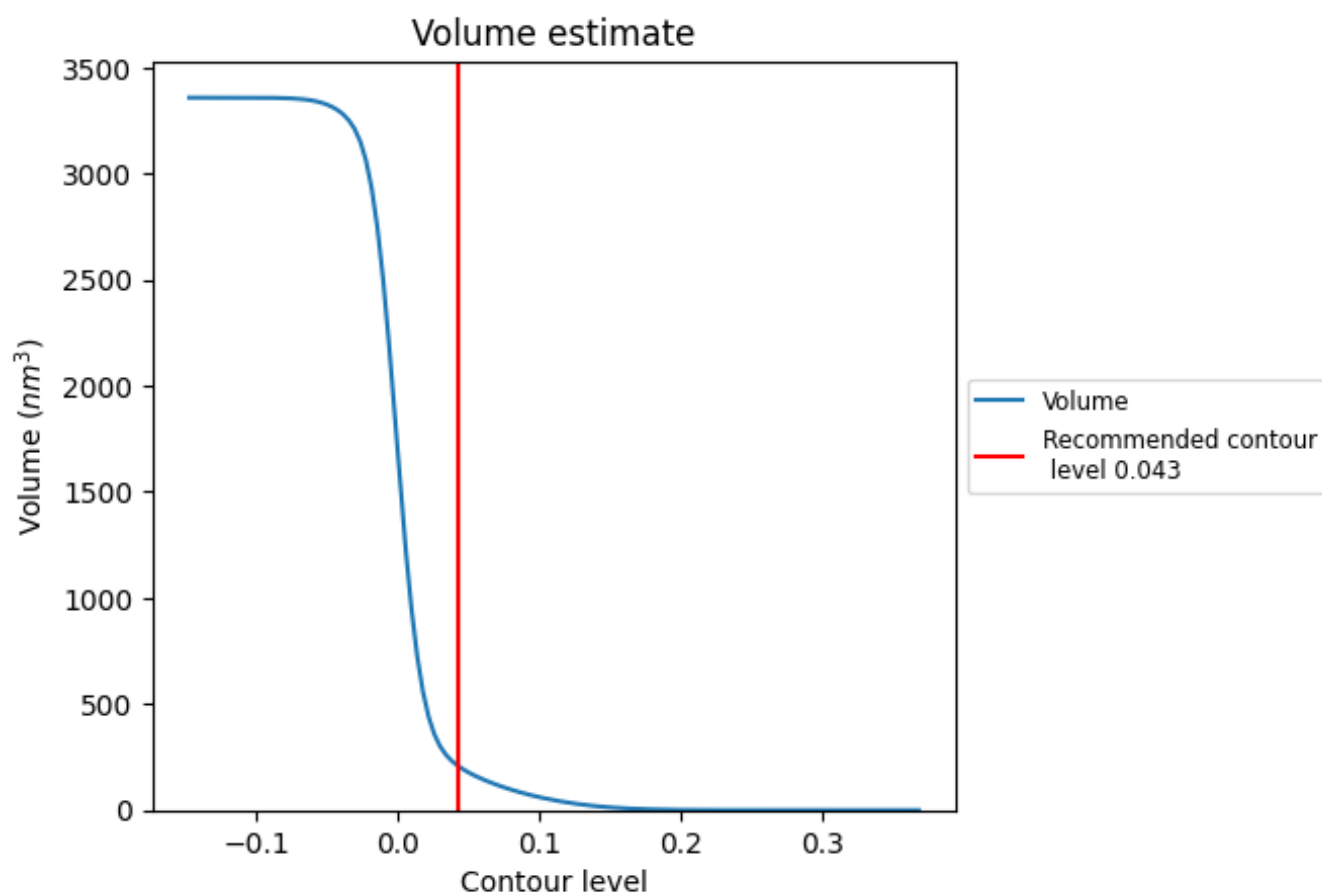
### 7.1 Map-value distribution [i](#)



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 208 nm<sup>3</sup>; this corresponds to an approximate mass of 188 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.

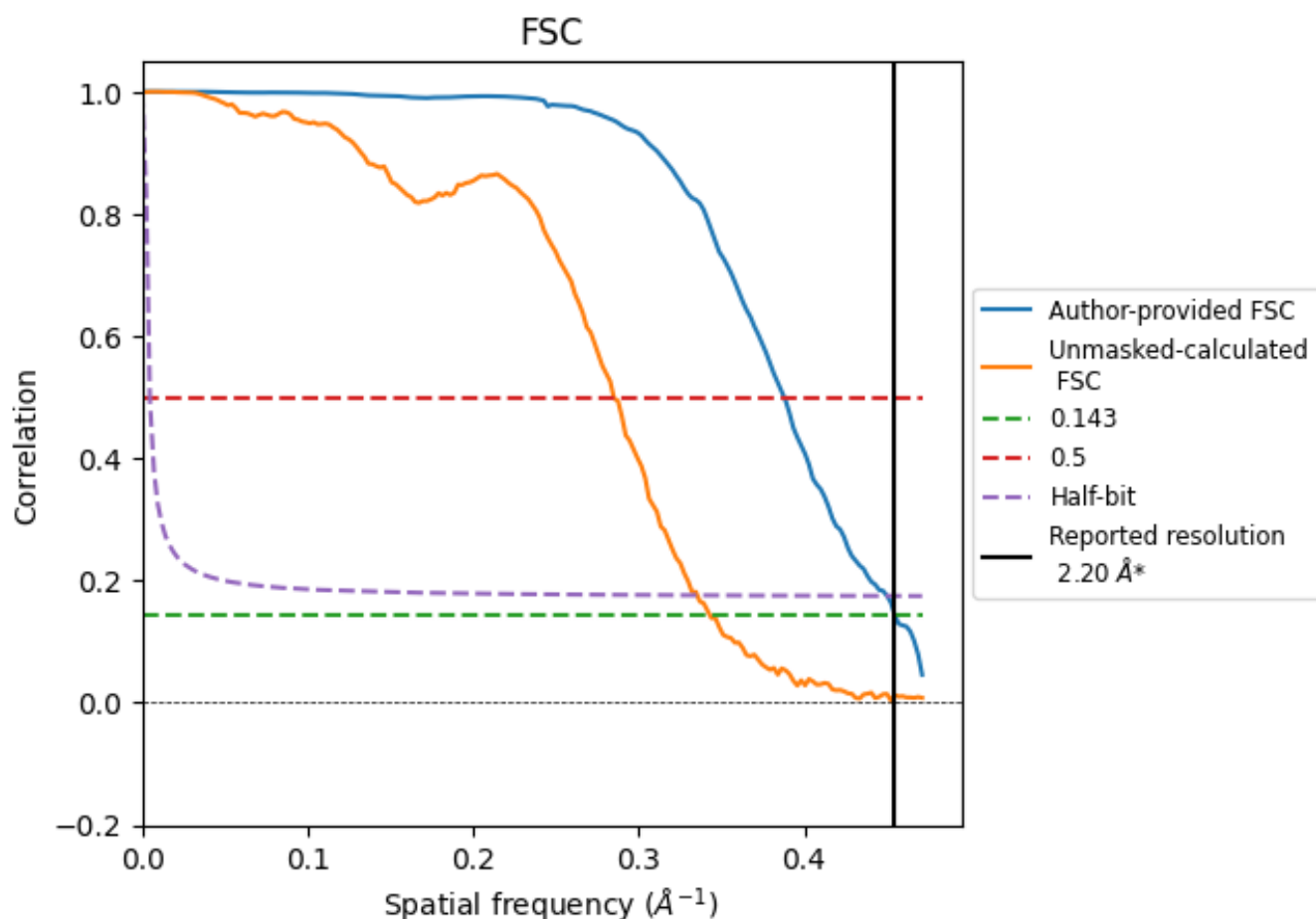
## 7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

## 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  $0.455 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

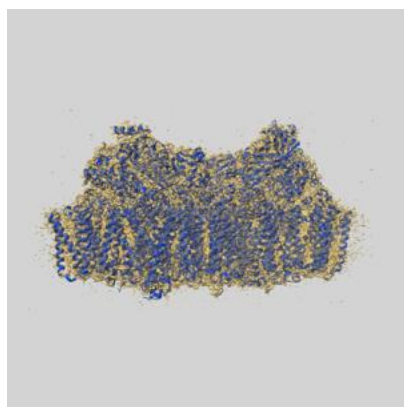
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.20	2.58	2.22
Unmasked-calculated*	2.91	3.51	2.98

\*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 2.91 differs from the reported value 2.2 by more than 10 %

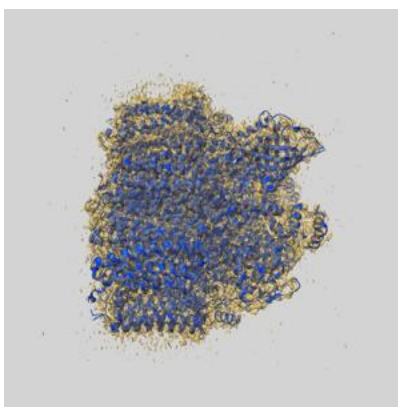
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51102 and PDB model 9G6H. Per-residue inclusion information can be found in [section 3](#) on [page 31](#).

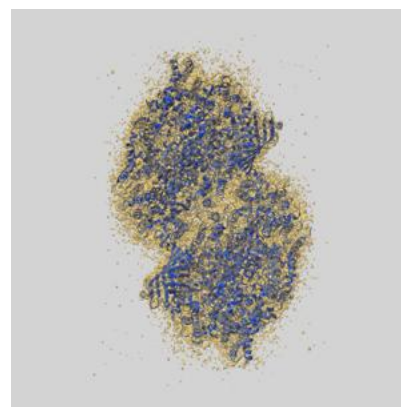
### 9.1 Map-model overlay [i](#)



X



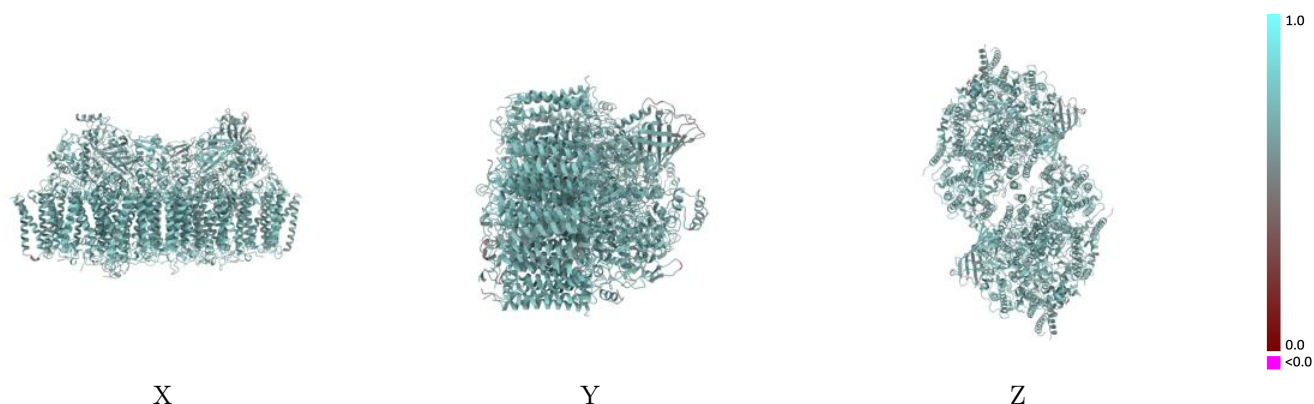
Y



Z

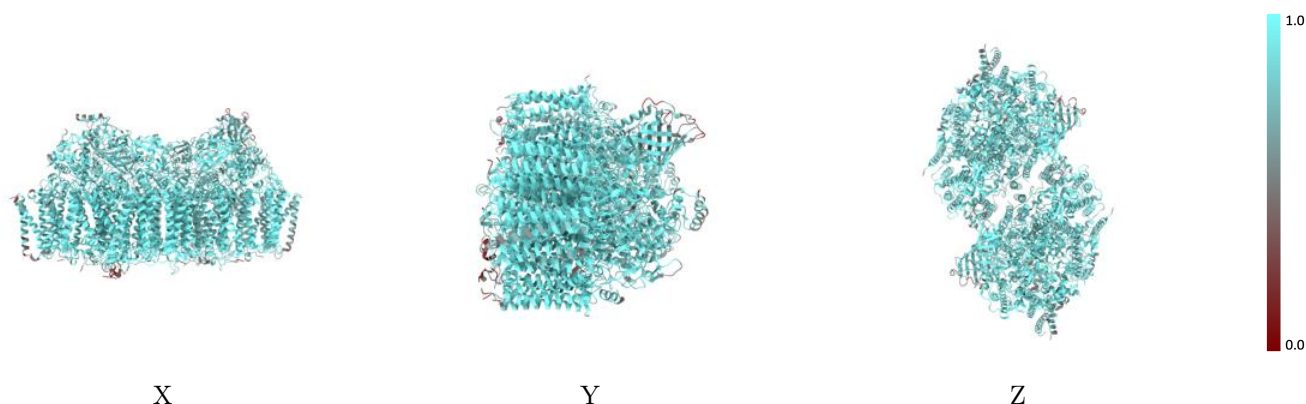
The images above show the 3D surface view of the map at the recommended contour level 0.043 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



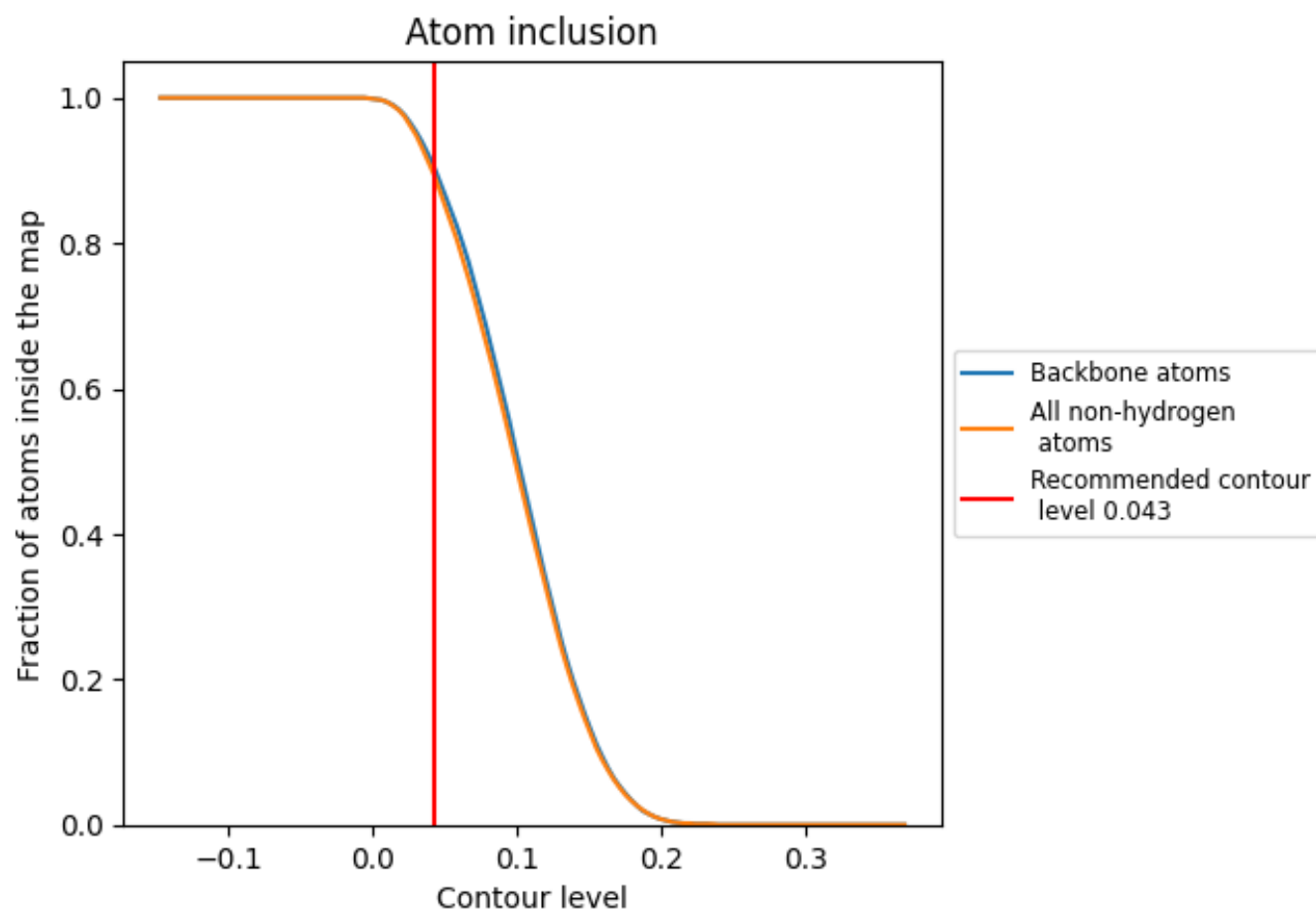
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.043).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 89% 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 (0.043) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8910	 0.6750
A	 0.9290	 0.6920
B	 0.9020	 0.6840
C	 0.9120	 0.6720
D	 0.9410	 0.7010
E	 0.8180	 0.6390
F	 0.8700	 0.6710
H	 0.9370	 0.6870
I	 0.8590	 0.6510
J	 0.8580	 0.6480
K	 0.9170	 0.6600
L	 0.8850	 0.6850
M	 0.8820	 0.6790
O	 0.7840	 0.6190
T	 0.8090	 0.6570
U	 0.8060	 0.6350
V	 0.8710	 0.6520
X	 0.8060	 0.6460
Y	 0.7430	 0.6010
Z	 0.7220	 0.6020
a	 0.9340	 0.7020
b	 0.9100	 0.6800
c	 0.9250	 0.6900
d	 0.9370	 0.6980
e	 0.8460	 0.6510
f	 0.8490	 0.6620
h	 0.9360	 0.6790
i	 0.8280	 0.6660
j	 0.8490	 0.6640
k	 0.9080	 0.6710
l	 0.8550	 0.6720
m	 0.8730	 0.6780
o	 0.7940	 0.6320
t	 0.9100	 0.6970
u	 0.8210	 0.6440



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
v	 0.8840	 0.6620
x	 0.8110	 0.6410
y	 0.7430	 0.6080
z	 0.7650	 0.6220