



wwPDB EM Validation Summary Report ⓘ

Jul 28, 2026 – 02:39 pm BST

PDB ID : 9HYU / pdb_00009hyu
EMDB ID : EMD-52518
Title : Cryo-EM structure of the Chromera velia PSI supercomplex at 1.84 Angstrom resolution
Authors : Yuan, X.; Qian, P.; Sobotka, R.; Naschberger, A.
Deposited on : 2025-01-10
Resolution : 1.84 Å(reported)
Based on initial model : .

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

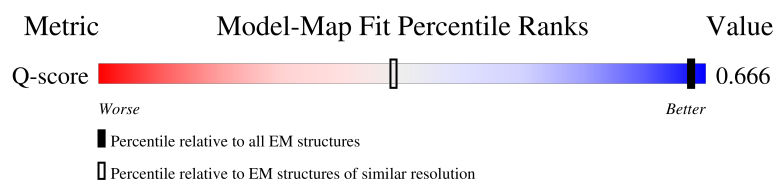
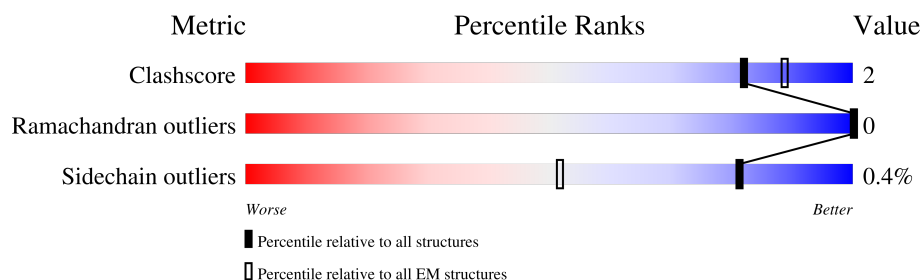
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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

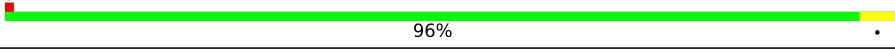
The reported resolution of this entry is 1.84 Å.

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



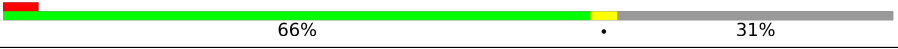
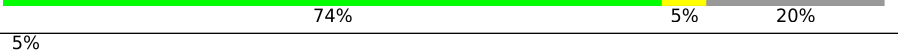
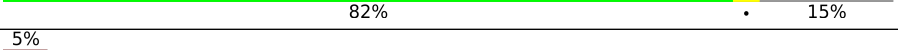
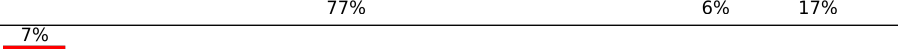
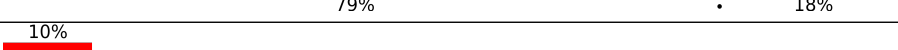
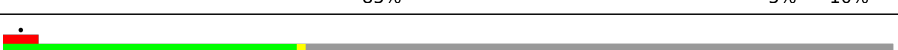
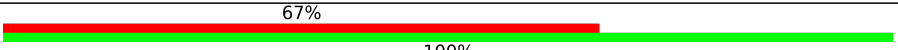
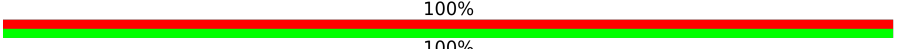
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	919 (1.34 - 2.34)

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

Mol	Chain	Length	Quality of chain
1	1	370	
2	2	267	
3	A	395	
4	C	80	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	D	269	
6	E	133	
7	F	326	
8	I	211	
9	L	277	
10	M	195	
11	R	202	
12	b	293	
13	c	237	
14	d	222	
15	e	217	
16	f	277	
17	u	424	
18	a	280	
19	B	1139	
20	G	3	
21	H	2	

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
27	XAT	f	322	X	-	-	-
35	A1I05	B	1242	X	-	-	-

2 Entry composition [i](#)

There are 36 unique types of molecules in this entry. The entry contains 92028 atoms, of which 45749 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 Superoxide dismutase [Fe].

Mol	Chain	Residues	Atoms						AltConf	Trace
1	1	306	Total	C	H	N	O	S	0	0
			4916	1597	2413	428	467	11		

- Molecule 2 is a protein called Superoxide dismutase [Fe].

Mol	Chain	Residues	Atoms						AltConf	Trace
2	2	221	Total	C	H	N	O	S	0	0
			3468	1144	1696	287	332	9		

- Molecule 3 is a protein called photosystem I.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	A	395	Total	C	H	N	O	S	0	0
			6285	2120	3099	522	534	10		

- Molecule 4 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	C	80	Total	C	H	N	O	S	0	0
			1196	376	581	104	121	14		

- Molecule 5 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	D	235	Total	C	H	N	O	S	0	0
			3822	1205	1916	348	343	10		

- Molecule 6 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	E	66	Total	C	H	N	O	S	0	0
			1054	352	527	79	95	1		

- Molecule 7 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	F	225	Total	C	H	N	O	S	0	0
			3589	1174	1802	296	311	6		

- Molecule 8 is a protein called Photosystem I protein (PsaI).

Mol	Chain	Residues	Atoms						AltConf	Trace
8	I	100	Total	C	H	N	O	S	0	0
			1553	504	767	136	143	3		

- Molecule 9 is a protein called Photosystem I reaction center subunit V.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	L	223	Total	C	H	N	O	S	0	0
			3369	1119	1656	274	312	8		

- Molecule 10 is a protein called Photosystem I protein (PsaM).

Mol	Chain	Residues	Atoms						AltConf	Trace
10	M	115	Total	C	H	N	O	S	0	0
			1861	596	919	161	182	3		

- Molecule 11 is a protein called Photosystem I protein (PsaR).

Mol	Chain	Residues	Atoms						AltConf	Trace
11	R	161	Total	C	H	N	O	S	0	0
			2617	840	1327	221	224	5		

- Molecule 12 is a protein called Plastid light harvesting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	b	248	Total	C	H	N	O	S	0	0
			3885	1288	1912	316	364	5		

- Molecule 13 is a protein called Plastid light harvesting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	c	196	Total	C	H	N	O	S	0	0
			3076	994	1538	257	277	10		

- Molecule 14 is a protein called Plastid light harvesting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	d	182	Total	C	H	N	O	S	0	0
			2815	907	1396	247	254	11		

- Molecule 15 is a protein called Plastid light harvesting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	e	175	Total	C	H	N	O	S	0	0
			2809	908	1411	232	251	7		

- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	f	249	Total	C	H	N	O	S	0	0
			4059	1321	2010	355	364	9		

- Molecule 17 is a protein called Photosystem I protein (PsaV).

Mol	Chain	Residues	Atoms						AltConf	Trace
17	u	146	Total	C	H	N	O	S	0	0
			2389	765	1194	208	215	7		

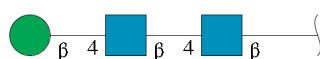
- Molecule 18 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	a	234	Total	C	H	N	O	S	0	0
			3568	1135	1817	301	310	5		

- Molecule 19 is a protein called Photosystem I protein (PsaB).

Mol	Chain	Residues	Atoms						AltConf	Trace
19	B	735	Total	C	H	N	O	S	0	0
			11726	3928	5801	965	1016	16		

- Molecule 20 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
20	G	3	Total	C	H	N	O	0	0
			73	22	34	2	15		

- Molecule 21 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

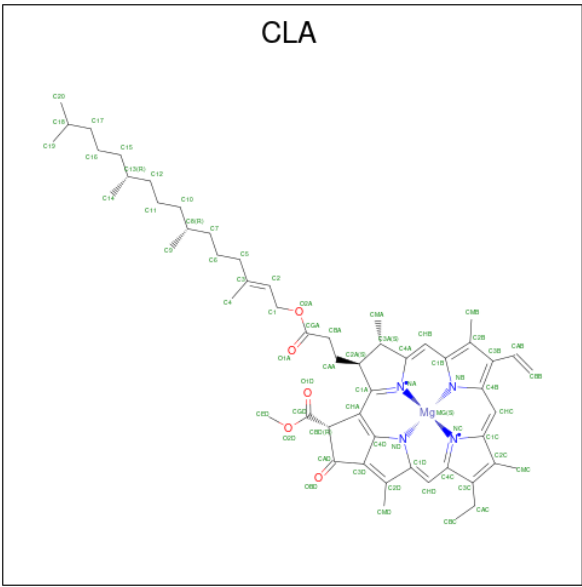


Mol	Chain	Residues	Atoms					AltConf	Trace
21	H	2	Total	C	H	N	O	0	0
			53	16	25	2	10		

- Molecule 22 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
22	2	1	Total	Fe	0
			1	1	

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
23	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf
23	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
23	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
23	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	A	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
23	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
23	F	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	F	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
23	F	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	F	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
23	L	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	L	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
23	L	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf
23	L	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
23	R	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
23	R	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	b	1	Total	C	H	Mg	N	O	0
			113	48	55	1	4	5	
23	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	b	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
23	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	b	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
23	b	1	Total	C	H	Mg	N	O	0
			102	44	48	1	4	5	
23	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	c	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
23	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	c	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
23	c	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
23	c	1	Total	C	H	Mg	N	O	0
			77	35	32	1	4	5	
23	c	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf
23	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
23	c	1	Total 78	C 35	H 33	Mg 1	N 4	O 5	0
23	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
23	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
23	c	1	Total 78	C 35	H 33	Mg 1	N 4	O 5	0
23	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
23	d	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
23	d	1	Total 107	C 46	H 51	Mg 1	N 4	O 5	0
23	d	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
23	d	1	Total 104	C 45	H 49	Mg 1	N 4	O 5	0
23	d	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
23	d	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0
23	d	1	Total 78	C 35	H 33	Mg 1	N 4	O 5	0
23	d	1	Total 78	C 35	H 33	Mg 1	N 4	O 5	0
23	e	1	Total 78	C 35	H 33	Mg 1	N 4	O 5	0
23	e	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
23	e	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
23	e	1	Total 89	C 40	H 39	Mg 1	N 4	O 5	0
23	e	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
23	e	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
23	e	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf
23	e	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	e	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	f	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
23	f	1	Total	C	H	Mg	N	O	0
			113	48	55	1	4	5	
23	f	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	f	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
23	f	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	f	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
23	f	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
23	f	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
23	f	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
23	f	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
23	f	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	a	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	a	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	a	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
23	a	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	a	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	a	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
23	a	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	

Continued on next page...

Continued from previous page...

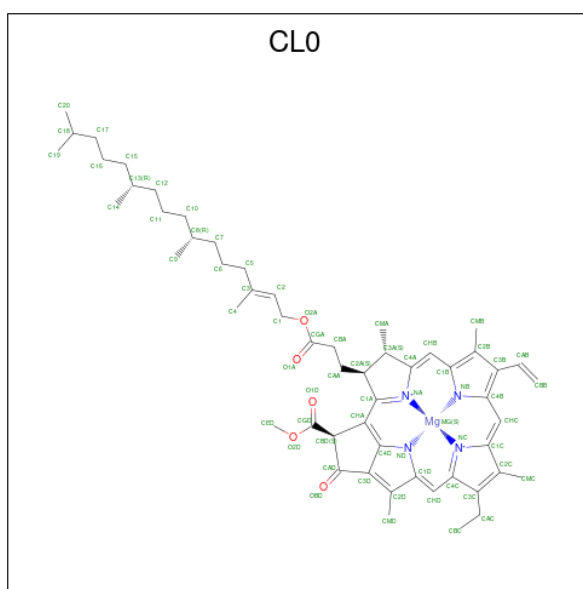
Mol	Chain	Residues	Atoms						AltConf
23	a	1	Total 98	C 43	H 45	Mg 1	N 4	O 5	0
23	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
23	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
23	B	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0
23	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
23	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
23	B	1	Total 78	C 35	H 33	Mg 1	N 4	O 5	0
23	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
23	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
23	B	1	Total 78	C 35	H 33	Mg 1	N 4	O 5	0
23	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
23	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
23	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
23	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
23	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
23	B	1	Total 98	C 43	H 45	Mg 1	N 4	O 5	0
23	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
23	B	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0
23	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
23	B	1	Total 78	C 35	H 33	Mg 1	N 4	O 5	0
23	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

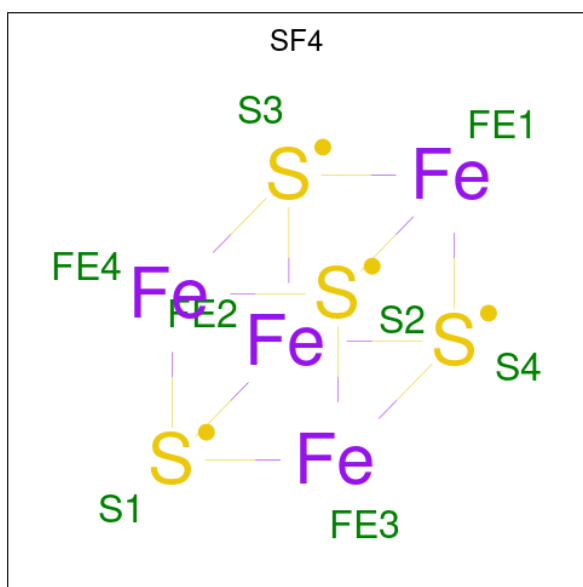
Mol	Chain	Residues	Atoms						AltConf
23	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
23	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	

- Molecule 24 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



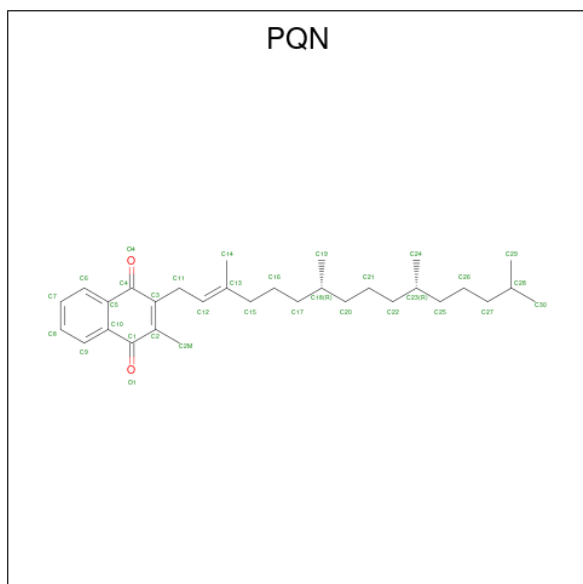
Mol	Chain	Residues	Atoms						AltConf
24	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

- Molecule 25 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



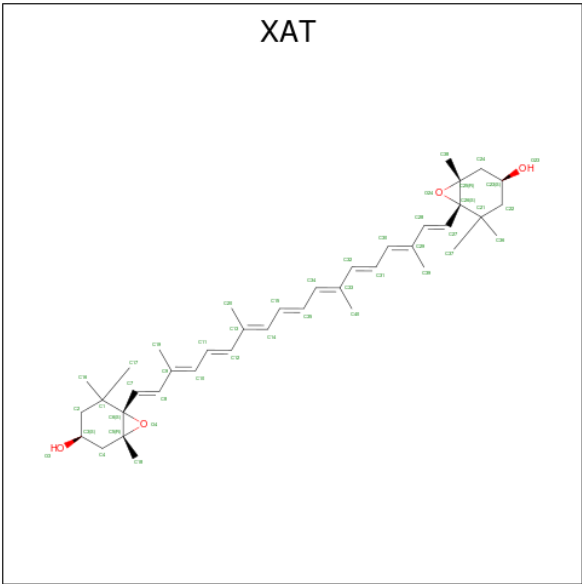
Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	Fe	S	0
			8	4	4	
25	C	1	Total	Fe	S	0
			8	4	4	
25	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 26 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	H	O	0
			79	31	46	2	
26	B	1	Total	C	H	O	0
			79	31	46	2	

- Molecule 27 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



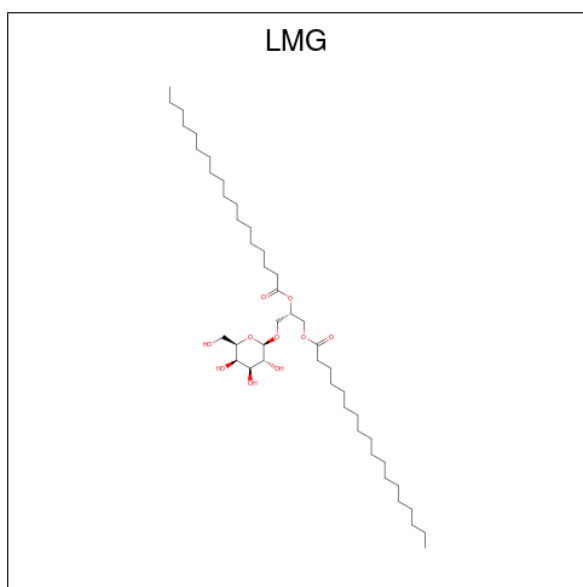
Mol	Chain	Residues	Atoms				AltConf
27	A	1	Total	C	H	O	0
			100	40	56	4	
27	R	1	Total	C	H	O	0
			100	40	56	4	
27	R	1	Total	C	H	O	0
			100	40	56	4	
27	b	1	Total	C	H	O	0
			100	40	56	4	
27	b	1	Total	C	H	O	0
			100	40	56	4	
27	b	1	Total	C	H	O	0
			100	40	56	4	
27	b	1	Total	C	H	O	0
			100	40	56	4	
27	c	1	Total	C	H	O	0
			100	40	56	4	
27	c	1	Total	C	H	O	0
			100	40	56	4	

Continued on next page...

Continued from previous page...

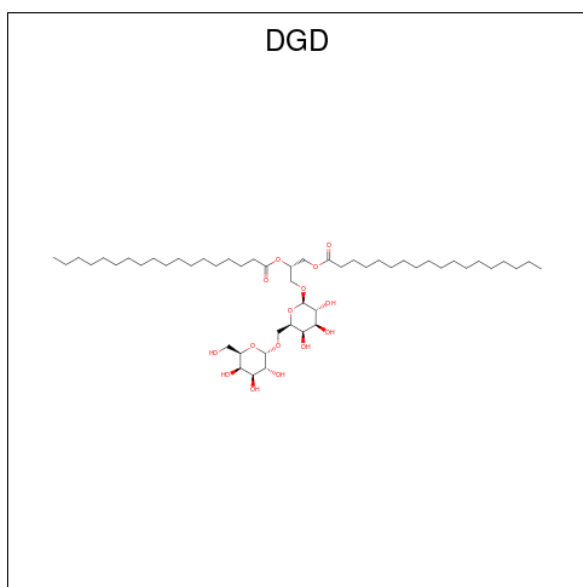
Mol	Chain	Residues	Atoms				AltConf
27	c	1	Total 100	C 40	H 56	O 4	0
27	c	1	Total 100	C 40	H 56	O 4	0
27	d	1	Total 100	C 40	H 56	O 4	0
27	d	1	Total 100	C 40	H 56	O 4	0
27	d	1	Total 100	C 40	H 56	O 4	0
27	d	1	Total 100	C 40	H 56	O 4	0
27	e	1	Total 100	C 40	H 56	O 4	0
27	e	1	Total 100	C 40	H 56	O 4	0
27	f	1	Total 100	C 40	H 56	O 4	0
27	f	1	Total 100	C 40	H 56	O 4	0
27	f	1	Total 100	C 40	H 56	O 4	0
27	f	1	Total 100	C 40	H 56	O 4	0
27	a	1	Total 100	C 40	H 56	O 4	0

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



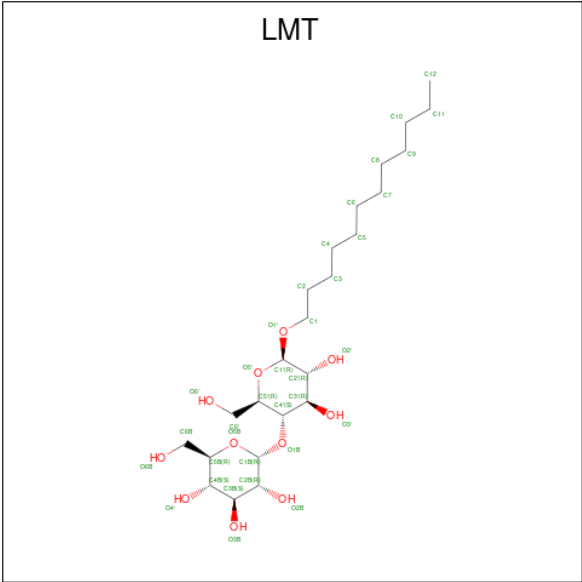
Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	H	O	0
			72	26	41	5	
28	A	1	Total	C	H	O	0
			69	23	36	10	
28	F	1	Total	C	H	O	0
			141	45	86	10	
28	F	1	Total	C	H	O	0
			105	35	60	10	
28	L	1	Total	C	H	O	0
			55	18	35	2	
28	L	1	Total	C	H	O	0
			119	39	75	5	
28	R	1	Total	C	H	O	0
			54	18	26	10	
28	b	1	Total	C	H	O	0
			81	27	44	10	
28	b	1	Total	C	H	O	0
			123	40	73	10	
28	b	1	Total	C	H	O	0
			78	26	42	10	
28	f	1	Total	C	H	O	0
			141	45	86	10	

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
29	A	1	Total	C	H	O	0
			111	35	61	15	
29	F	1	Total	C	H	O	0
			162	51	96	15	
29	b	1	Total	C	H	O	0
			99	32	52	15	
29	b	1	Total	C	H	O	0
			105	34	56	15	
29	c	1	Total	C	H	O	0
			111	36	60	15	
29	u	1	Total	C	H	O	0
			120	39	66	15	

- Molecule 30 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	H	O	0
			38	12	25	1	
30	F	1	Total	C	H	O	0
			38	12	25	1	
30	F	1	Total	C	H	O	0
			59	18	35	6	
30	F	1	Total	C	H	O	0
			38	12	25	1	
30	F	1	Total	C	H	O	0
			38	12	25	1	
30	F	1	Total	C	H	O	0
			38	12	25	1	
30	F	1	Total	C	H	O	0
			81	24	46	11	
30	L	1	Total	C	H	O	0
			38	12	25	1	
30	L	1	Total	C	H	O	0
			38	12	25	1	
30	L	1	Total	C	H	O	0
			38	12	25	1	
30	L	1	Total	C	H	O	0
			38	12	25	1	
30	R	1	Total	C	H	O	0
			38	12	25	1	
30	R	1	Total	C	H	O	0
			38	12	25	1	
30	b	1	Total	C	H	O	0
			59	18	35	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
30	b	1	Total	C	H	O	0
			38	12	25	1	
30	b	1	Total	C	H	O	0
			38	12	25	1	
30	b	1	Total	C	H		0
			23	8	15		
30	b	1	Total	C	H	O	0
			38	12	25	1	
30	b	1	Total	C	H	O	0
			47	15	26	6	
30	c	1	Total	C	H	O	0
			72	22	39	11	
30	c	1	Total	C	H	O	0
			81	24	46	11	
30	c	1	Total	C	H	O	0
			81	24	46	11	
30	c	1	Total	C	H		0
			20	7	13		
30	c	1	Total	C	H	O	0
			59	18	35	6	
30	c	1	Total	C	H	O	0
			38	12	25	1	
30	c	1	Total	C	H	O	0
			38	12	25	1	
30	c	1	Total	C	H	O	0
			38	12	25	1	
30	c	1	Total	C	H	O	0
			38	12	25	1	
30	c	1	Total	C	H	O	0
			38	12	25	1	
30	c	1	Total	C	H	O	0
			38	12	25	1	
30	c	1	Total	C	H	O	0
			81	24	46	11	
30	c	1	Total	C	H	O	0
			81	24	46	11	
30	c	1	Total	C	H	O	0
			38	12	25	1	
30	c	1	Total	C	H	O	0
			38	12	25	1	

Continued on next page...

Continued from previous page...

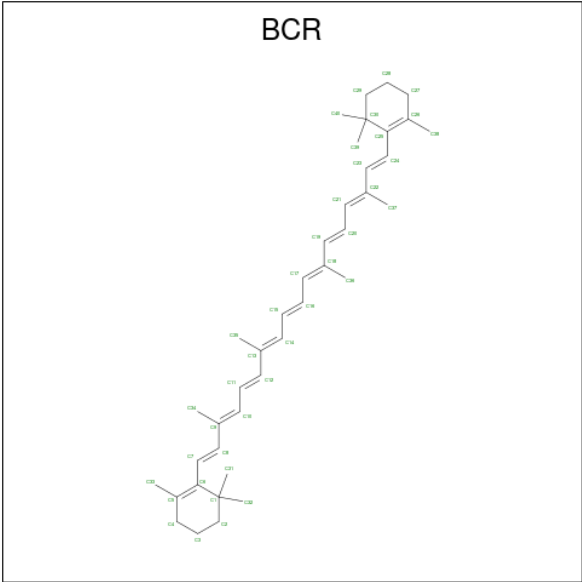
Mol	Chain	Residues	Atoms				AltConf
30	d	1	Total	C	H	O	0
			38	12	25	1	
30	d	1	Total	C	H	O	0
			38	12	25	1	
30	d	1	Total	C	H	O	0
			81	24	46	11	
30	d	1	Total	C	H	O	0
			38	12	25	1	
30	d	1	Total	C	H	O	0
			38	12	25	1	
30	d	1	Total	C	H	O	0
			38	12	25	1	
30	d	1	Total	C	H	O	0
			38	12	25	1	
30	e	1	Total	C	H	O	0
			38	12	25	1	
30	e	1	Total	C	H		0
			20	7	13		
30	e	1	Total	C	H	O	0
			38	12	25	1	
30	e	1	Total	C	H	O	0
			38	12	25	1	
30	e	1	Total	C	H		0
			26	9	17		
30	e	1	Total	C	H	O	0
			81	24	46	11	
30	f	1	Total	C	H	O	0
			38	12	25	1	
30	f	1	Total	C	H	O	0
			59	18	35	6	
30	f	1	Total	C	H	O	0
			38	12	25	1	
30	f	1	Total	C	H	O	0
			38	12	25	1	
30	f	1	Total	C	H		0
			32	11	21		
30	f	1	Total	C	H	O	0
			38	12	25	1	
30	f	1	Total	C	H	O	0
			81	24	46	11	

Continued on next page...

Continued from previous page...

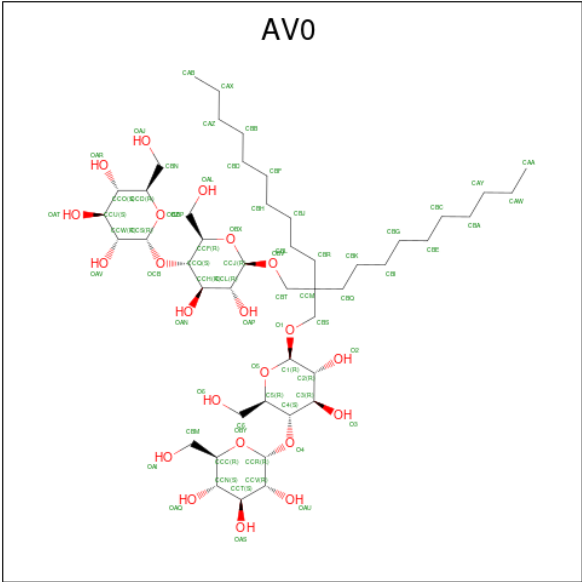
Mol	Chain	Residues	Atoms				AltConf
30	f	1	Total	C	H	O	0
			38	12	25	1	
30	f	1	Total	C	H	O	0
			59	18	35	6	
30	a	1	Total	C	H		0
			23	8	15		
30	a	1	Total	C	H	O	0
			81	24	46	11	
30	B	1	Total	C	H	O	0
			38	12	25	1	
30	B	1	Total	C	H	O	0
			54	16	27	11	
30	B	1	Total	C	H	O	0
			38	12	25	1	
30	B	1	Total	C	H	O	0
			38	12	25	1	
30	B	1	Total	C	H	O	0
			38	12	25	1	
30	B	1	Total	C	H	O	0
			38	12	25	1	
30	B	1	Total	C	H	O	0
			59	18	35	6	
30	B	1	Total	C	H	O	0
			38	12	25	1	
30	B	1	Total	C	H	O	0
			38	12	25	1	
30	B	1	Total	C	H		0
			26	9	17		
30	B	1	Total	C	H		0
			32	11	21		

- Molecule 31 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



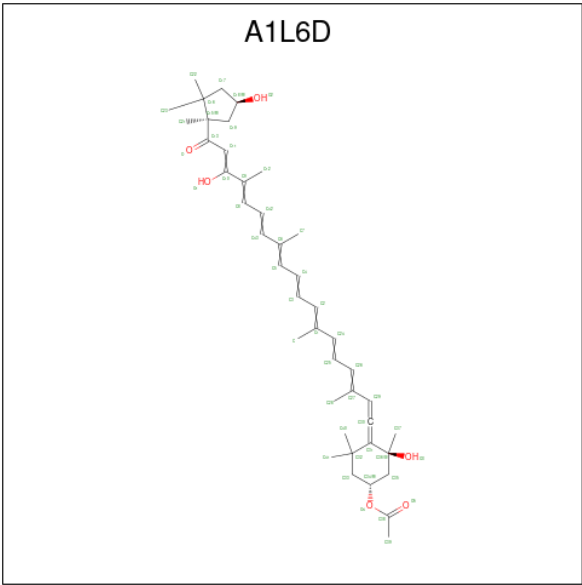
Mol	Chain	Residues	Atoms			AltConf
31	F	1	Total	C	H	0
			96	40	56	
31	L	1	Total	C	H	0
			96	40	56	
31	L	1	Total	C	H	0
			96	40	56	
31	b	1	Total	C	H	0
			96	40	56	
31	a	1	Total	C	H	0
			53	23	30	
31	B	1	Total	C	H	0
			96	40	56	
31	B	1	Total	C	H	0
			96	40	56	
31	B	1	Total	C	H	0
			96	40	56	

- Molecule 32 is Lauryl Maltose Neopentyl Glycol (CCD ID: AV0) (formula: C₄₇H₈₈O₂₂).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
32	L	1	113	35	66	12	0

- Molecule 33 is [(1 {R},5 {S})-3,3,5-trimethyl-5-oxidanyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {Z})-3,7,12,16-tetramethyl-17-oxidanyl-19-oxidanylidene-19-[(1 {R},4 {S})-1,2,2-trimethyl-4-oxidanyl-cyclopentyl]nonadeca-1,3,5,7,9,11,13,15,17-nonaenylidene]cyclohexyl] ethanoate (CCD ID: A1L6D) (formula: C₄₂H₅₈O₆) (labeled as "Ligand of Interest" by depositor).



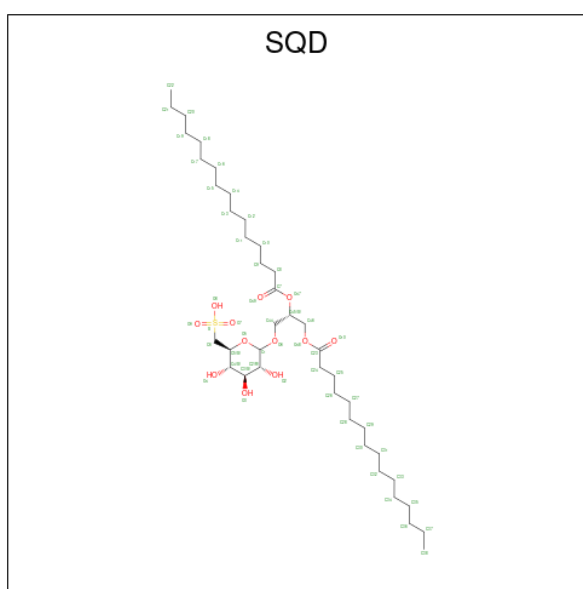
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
33	d	1	106	42	58	6	0

Continued on next page...

Continued from previous page...

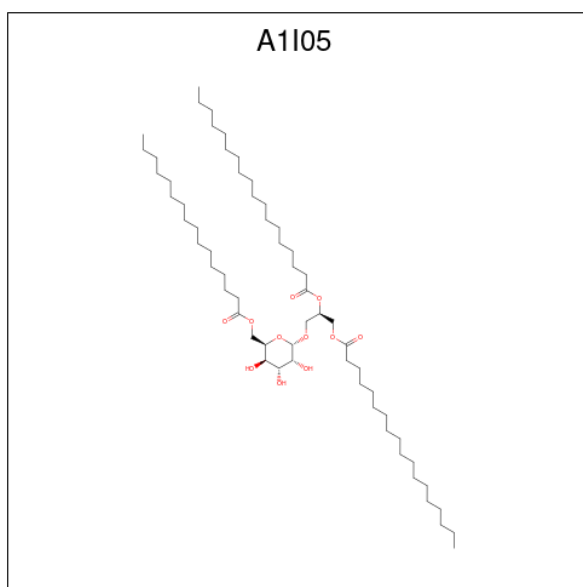
Mol	Chain	Residues	Atoms				AltConf
33	e	1	Total	C	H	O	0
			106	42	58	6	
33	f	1	Total	C	H	O	0
			106	42	58	6	
33	B	1	Total	C	H	O	0
			106	42	58	6	

- Molecule 34 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
34	d	1	Total	C	H	O	S	0
			75	24	38	12	1	

- Molecule 35 is [(2 {R})-3-[(2 {S},3 {R},4 {R},5 {R},6 {R})-6-(hexadecanoyloxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-2-octadecanoyloxy-propyl] octadecanoate (CCD ID: A1I05) (formula: C₆₁H₁₁₆O₁₁) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
35	B	1	Total	C	H	O	0
			119	41	67	11	

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		AltConf
36	1	217	Total	O	0
			217	217	
36	2	93	Total	O	0
			93	93	
36	A	143	Total	O	0
			143	143	
36	C	75	Total	O	0
			75	75	
36	D	154	Total	O	0
			154	154	
36	E	45	Total	O	0
			45	45	
36	F	77	Total	O	0
			77	77	
36	I	34	Total	O	0
			34	34	
36	L	62	Total	O	0
			62	62	
36	M	28	Total	O	0
			28	28	
36	R	40	Total	O	0
			40	40	

Continued on next page...

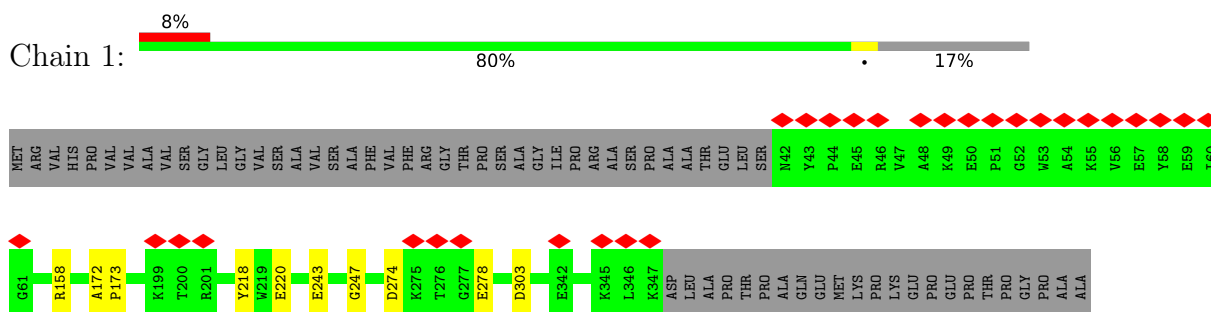
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
36	b	89	Total 89	O 89	0
36	c	34	Total 34	O 34	0
36	d	44	Total 44	O 44	0
36	e	16	Total 16	O 16	0
36	f	49	Total 49	O 49	0
36	u	39	Total 39	O 39	0
36	a	57	Total 57	O 57	0
36	B	262	Total 262	O 262	0

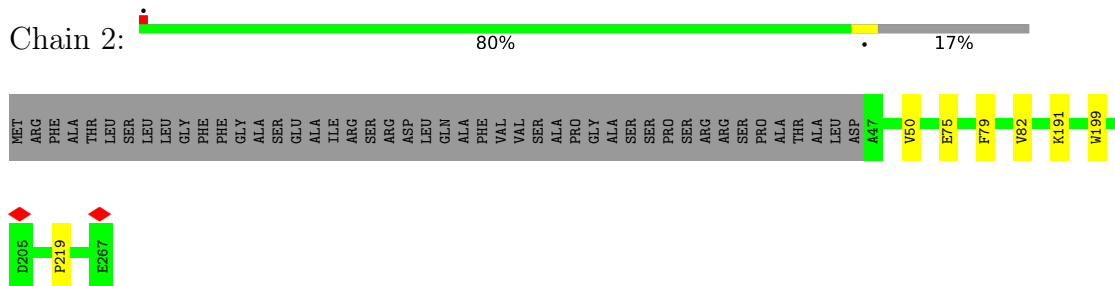
3 Residue-property plots [i](#)

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

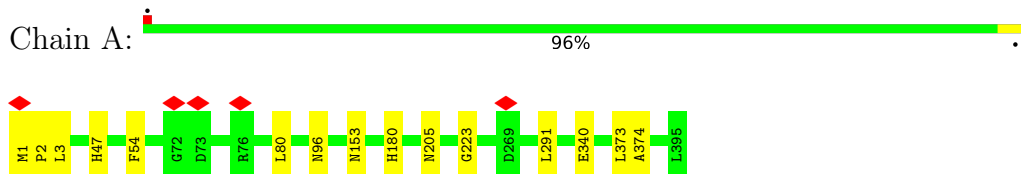
- Molecule 1: Superoxide dismutase [Fe]



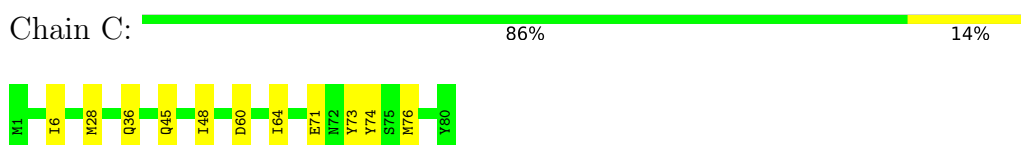
- Molecule 2: Superoxide dismutase [Fe]



- Molecule 3: photosystem I

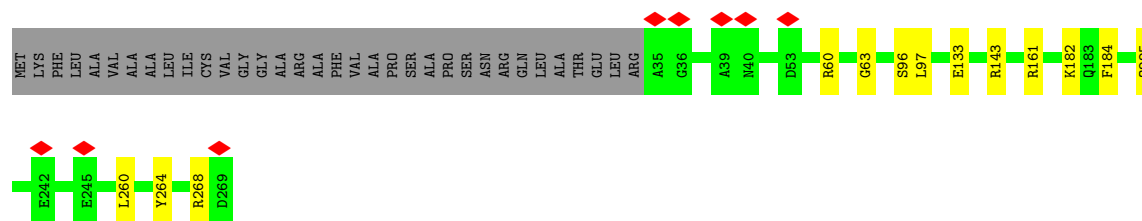


- Molecule 4: Photosystem I iron-sulfur center



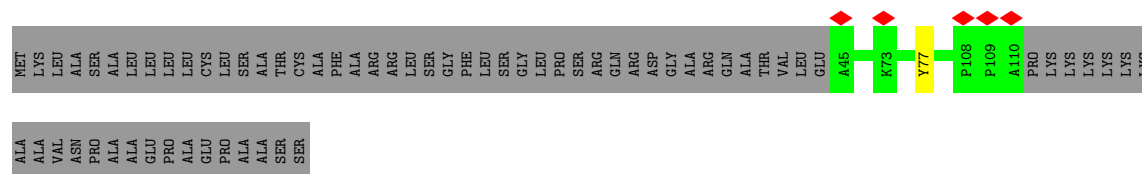
- Molecule 5: Photosystem I reaction center subunit II

Chain D:  83% 5% 13%



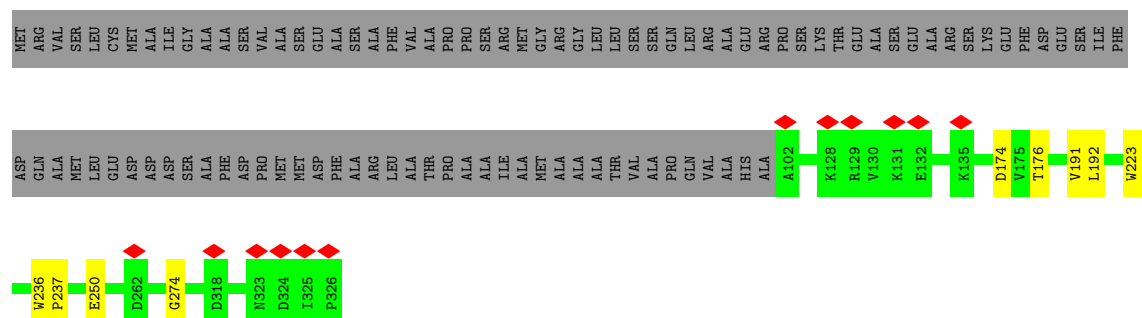
- Molecule 6: Photosystem I reaction center subunit IV

Chain E:  49% 50%



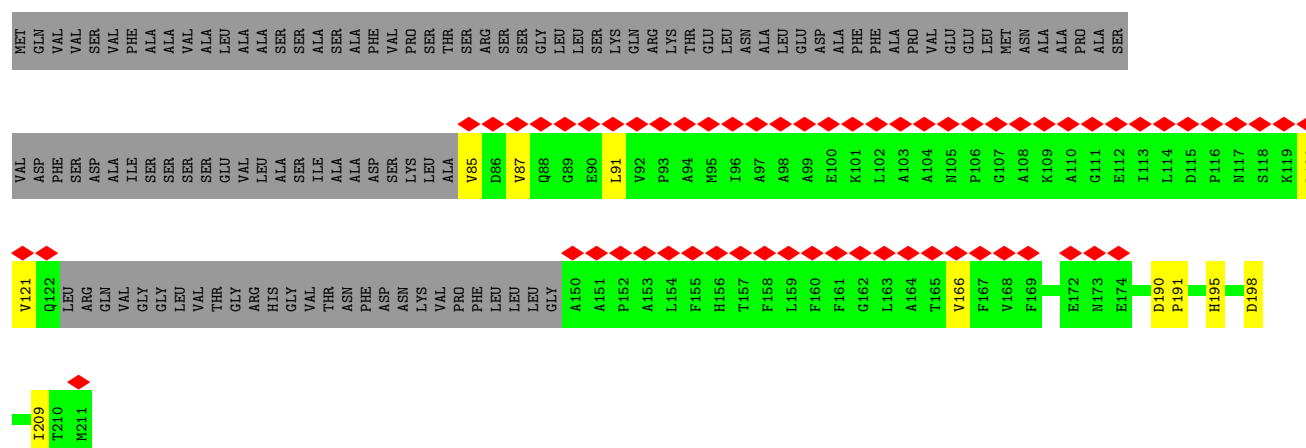
- Molecule 7: Photosystem I reaction center subunit III

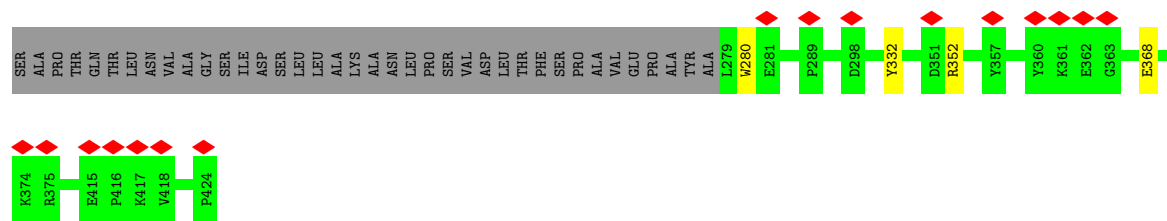
Chain F:  66% 31%



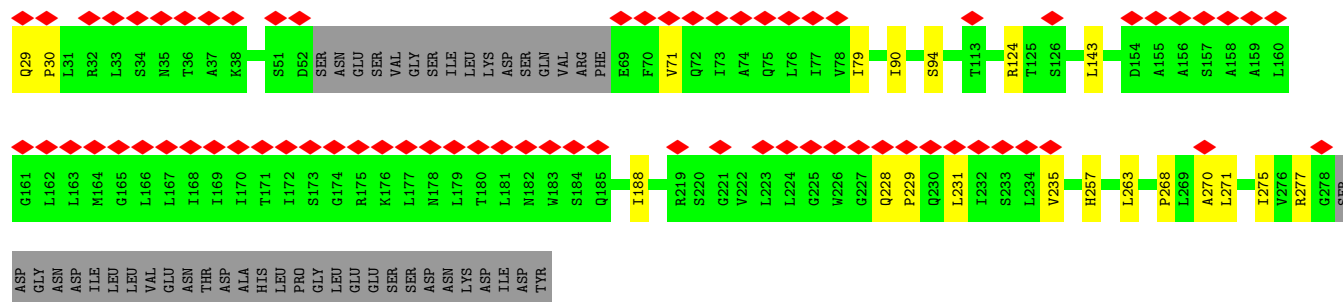
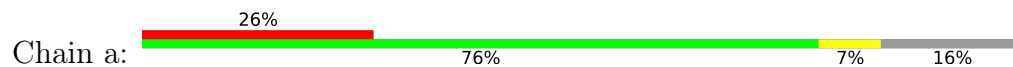
- Molecule 8: Photosystem I protein (PsaI)

Chain I:  29% 42% 5% 53%

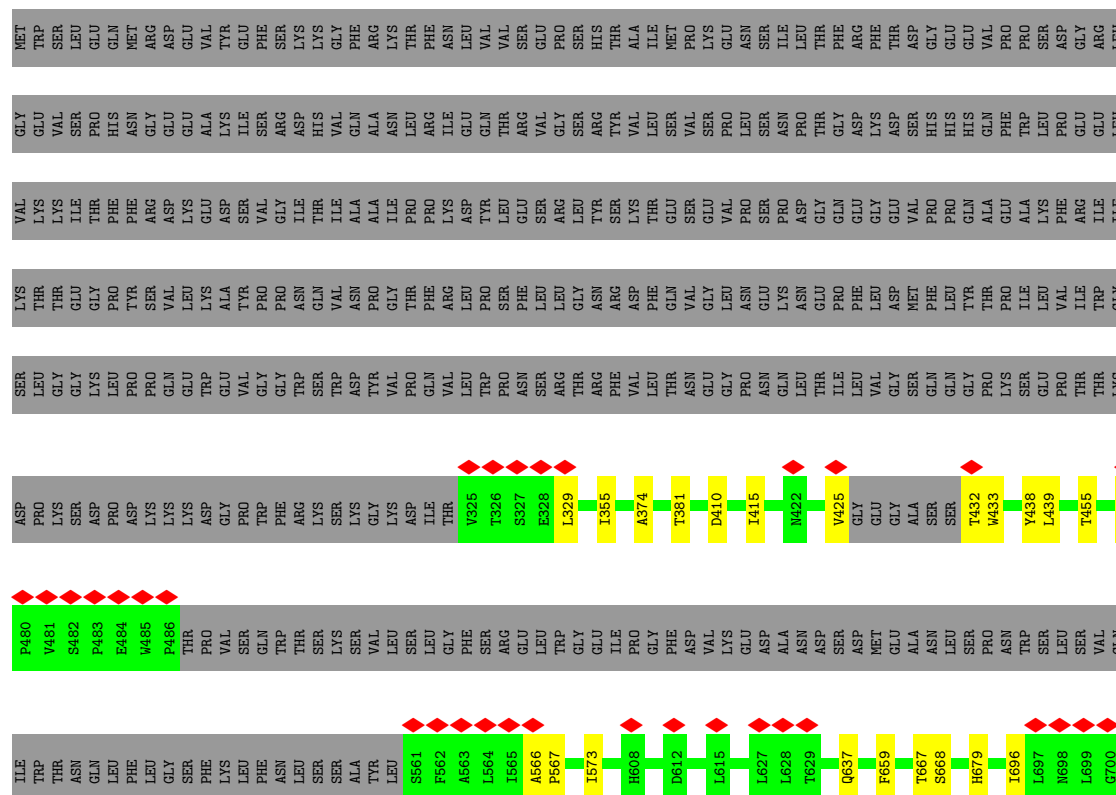


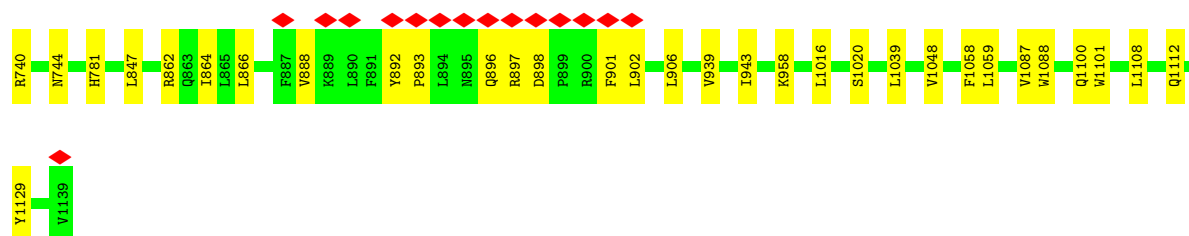


- Molecule 18: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 19: Photosystem I protein (PsaB)





- Molecule 20: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 21: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	532822	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF estimation were performed on the raw data in cryoSPARC's Live session	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	153.803	Depositor
Minimum map value	-48.503	Depositor
Average map value	0.015	Depositor
Map value standard deviation	1.246	Depositor
Recommended contour level	8	Depositor
Map size ($\text{\AA}$)	364.5, 364.5, 364.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.729, 0.729, 0.729	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCR, A1I05, PQN, LMT, SQD, AV0, NAG, A1L6D, LMG, FE, BMA, XAT, CLA, SF4, DGD, CL0

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	1	0.09	0/2574	0.25	0/3489
2	2	0.11	0/1824	0.25	0/2467
3	A	0.13	0/3297	0.29	0/4499
4	C	0.12	0/625	0.32	0/846
5	D	0.10	0/1949	0.26	0/2611
6	E	0.10	0/543	0.26	0/737
7	F	0.10	0/1839	0.24	0/2492
8	I	0.09	0/807	0.23	0/1093
9	L	0.09	0/1773	0.24	0/2418
10	M	0.08	0/961	0.20	0/1285
11	R	0.09	0/1323	0.25	0/1800
12	b	0.09	0/2027	0.23	0/2752
13	c	0.12	0/1577	0.26	0/2134
14	d	0.10	0/1452	0.24	0/1962
15	e	0.10	0/1431	0.24	0/1926
16	f	0.12	0/2104	0.25	0/2839
17	u	0.09	0/1229	0.22	0/1651
18	a	0.10	0/1785	0.26	0/2444
19	B	0.12	0/6125	0.28	0/8373
All	All	0.11	0/35245	0.26	0/47818

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 ⓘ

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	1	2503	2413	2412	6	0
2	2	1772	1696	1701	3	0
3	A	3186	3099	3099	16	0
4	C	615	581	580	8	0
5	D	1906	1916	1916	10	0
6	E	527	527	527	1	0
7	F	1787	1802	1805	9	0
8	I	786	767	767	9	0
9	L	1713	1656	1656	6	0
10	M	942	919	921	2	0
11	R	1290	1327	1327	10	0
12	b	1973	1912	1914	7	0
13	c	1538	1538	1537	14	0
14	d	1419	1396	1396	4	0
15	e	1398	1411	1411	3	0
16	f	2049	2010	2011	12	0
17	u	1195	1194	1194	3	0
18	a	1751	1817	1824	19	0
19	B	5925	5801	5809	37	0
20	G	39	34	34	0	0
21	H	28	25	25	0	0
22	2	1	0	0	0	0
23	A	906	942	942	20	0
23	B	1718	1807	1807	22	0
23	F	235	236	236	1	0
23	L	215	197	197	5	0
23	R	110	105	105	2	0
23	a	448	432	432	2	0
23	b	722	745	745	9	0
23	c	660	622	623	11	0
23	d	456	441	441	2	0
23	e	550	576	576	1	0
23	f	658	616	616	6	0
24	A	65	72	72	0	0
25	A	8	0	0	0	0
25	C	16	0	0	0	0
26	A	33	46	46	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	B	33	46	46	0	0
27	A	44	56	56	0	0
27	R	88	112	112	1	0
27	a	44	56	56	3	0
27	b	176	224	224	3	0
27	c	176	224	224	1	0
27	d	176	224	224	2	0
27	e	88	112	112	3	0
27	f	176	224	224	2	0
28	A	64	77	77	0	0
28	F	100	146	146	1	0
28	L	64	110	110	0	0
28	R	28	26	26	1	0
28	b	123	159	159	1	0
28	f	55	86	86	0	0
29	A	50	61	61	0	0
29	F	66	96	96	0	0
29	b	96	108	108	1	0
29	c	51	60	60	1	0
29	u	54	66	66	0	0
30	A	13	25	25	0	0
30	B	162	275	275	2	0
30	F	111	181	181	2	0
30	L	52	100	100	0	0
30	R	26	50	50	0	0
30	a	43	61	61	2	0
30	b	92	151	151	0	0
30	c	321	496	496	5	0
30	d	126	221	221	0	0
30	e	90	151	151	0	0
30	f	159	262	262	1	0
31	B	120	168	168	3	0
31	F	40	56	56	4	0
31	L	80	112	112	3	0
31	a	23	30	30	2	0
31	b	40	56	56	1	0
32	L	47	66	0	0	0
33	B	48	58	0	0	0
33	d	48	58	0	1	0
33	e	48	58	0	0	0
33	f	48	58	0	0	0
34	d	37	38	38	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	B	52	67	0	0	0
36	1	217	0	0	2	0
36	2	93	0	0	0	0
36	A	143	0	0	2	0
36	B	262	0	0	3	0
36	C	75	0	0	1	0
36	D	154	0	0	3	0
36	E	45	0	0	0	0
36	F	77	0	0	2	0
36	I	34	0	0	1	0
36	L	62	0	0	0	0
36	M	28	0	0	1	0
36	R	40	0	0	1	0
36	a	57	0	0	0	0
36	b	89	0	0	0	0
36	c	34	0	0	0	0
36	d	44	0	0	0	0
36	e	16	0	0	0	0
36	f	49	0	0	0	0
36	u	39	0	0	2	0
All	All	46279	45749	45410	222	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 2.

The worst 5 of 222 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)
7:F:174:ASP:OD2	7:F:176:THR:OG1	1.89	0.91
3:A:153:ASN:ND2	36:u:601:HOH:O	2.11	0.84
16:f:116:TYR:OH	16:f:127:GLU:OE2	1.98	0.79
19:B:410:ASP:OD1	36:B:1301:HOH:O	2.02	0.78
17:u:332:TYR:OH	36:u:601:HOH:O	2.02	0.77

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	1	304/370 (82%)	298 (98%)	6 (2%)	0	100	100
2	2	219/267 (82%)	214 (98%)	5 (2%)	0	100	100
3	A	393/395 (100%)	384 (98%)	9 (2%)	0	100	100
4	C	78/80 (98%)	78 (100%)	0	0	100	100
5	D	233/269 (87%)	226 (97%)	7 (3%)	0	100	100
6	E	64/133 (48%)	63 (98%)	1 (2%)	0	100	100
7	F	223/326 (68%)	219 (98%)	4 (2%)	0	100	100
8	I	96/211 (46%)	95 (99%)	1 (1%)	0	100	100
9	L	221/277 (80%)	219 (99%)	2 (1%)	0	100	100
10	M	113/195 (58%)	112 (99%)	1 (1%)	0	100	100
11	R	159/202 (79%)	159 (100%)	0	0	100	100
12	b	246/293 (84%)	245 (100%)	1 (0%)	0	100	100
13	c	194/237 (82%)	193 (100%)	1 (0%)	0	100	100
14	d	179/222 (81%)	176 (98%)	3 (2%)	0	100	100
15	e	173/217 (80%)	172 (99%)	1 (1%)	0	100	100
16	f	247/277 (89%)	246 (100%)	1 (0%)	0	100	100
17	u	144/424 (34%)	142 (99%)	2 (1%)	0	100	100
18	a	230/280 (82%)	227 (99%)	3 (1%)	0	100	100
19	B	729/1139 (64%)	712 (98%)	17 (2%)	0	100	100
All	All	4245/5814 (73%)	4180 (98%)	65 (2%)	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	1	264/312 (85%)	264 (100%)	0	100	100
2	2	189/224 (84%)	188 (100%)	1 (0%)	81	75
3	A	331/331 (100%)	331 (100%)	0	100	100
4	C	70/70 (100%)	69 (99%)	1 (1%)	59	45
5	D	197/221 (89%)	195 (99%)	2 (1%)	68	58
6	E	58/108 (54%)	58 (100%)	0	100	100
7	F	189/264 (72%)	189 (100%)	0	100	100
8	I	80/167 (48%)	80 (100%)	0	100	100
9	L	179/221 (81%)	179 (100%)	0	100	100
10	M	98/168 (58%)	98 (100%)	0	100	100
11	R	138/171 (81%)	136 (99%)	2 (1%)	59	45
12	b	204/236 (86%)	204 (100%)	0	100	100
13	c	161/194 (83%)	161 (100%)	0	100	100
14	d	146/177 (82%)	146 (100%)	0	100	100
15	e	145/176 (82%)	143 (99%)	2 (1%)	59	45
16	f	212/230 (92%)	212 (100%)	0	100	100
17	u	126/347 (36%)	126 (100%)	0	100	100
18	a	185/227 (82%)	184 (100%)	1 (0%)	81	75
19	B	632/993 (64%)	628 (99%)	4 (1%)	78	72
All	All	3604/4837 (74%)	3591 (100%)	13 (0%)	81	78

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	e	215	GLN
18	a	188	ILE
19	B	888	VAL
19	B	701	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	B	866	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
19	B	769	ASN
19	B	807	GLN
19	B	1112	GLN
5	D	183	GLN
5	D	112	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

5 monosaccharides 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	$\# Z > 2$
20	NAG	G	1	1,20	14,14,15	0.25	0	17,19,21	0.45	0
20	NAG	G	2	20	14,14,15	0.23	0	17,19,21	0.54	0
20	BMA	G	3	20	11,11,12	0.21	0	15,15,17	0.59	0
21	NAG	H	1	1,21	14,14,15	0.24	0	17,19,21	0.46	0
21	NAG	H	2	21	14,14,15	0.23	0	17,19,21	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
20	NAG	G	1	1,20	-	0/6/23/26	0/1/1/1
20	NAG	G	2	20	-	0/6/23/26	0/1/1/1
20	BMA	G	3	20	-	0/2/19/22	0/1/1/1
21	NAG	H	1	1,21	-	0/6/23/26	0/1/1/1
21	NAG	H	2	21	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

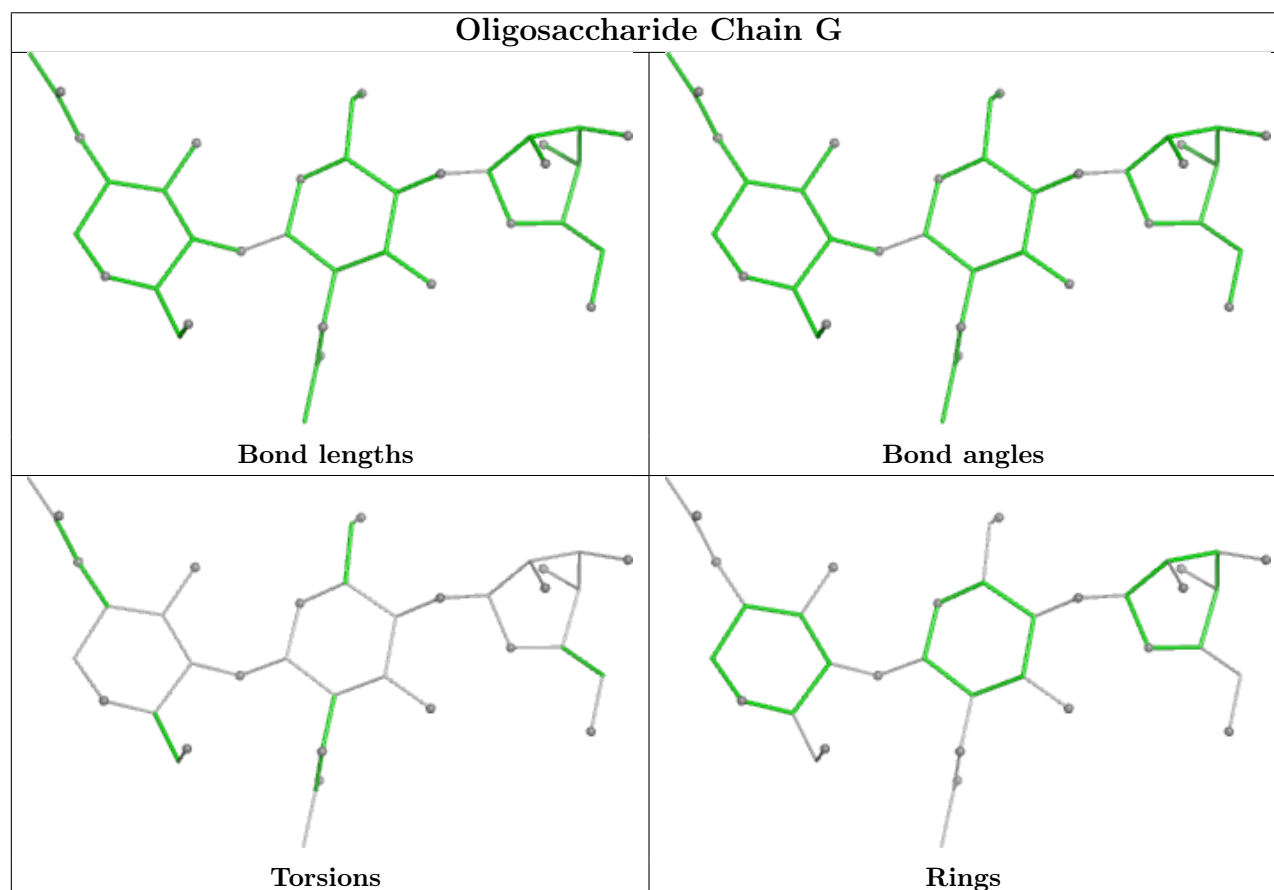
There are no chirality outliers.

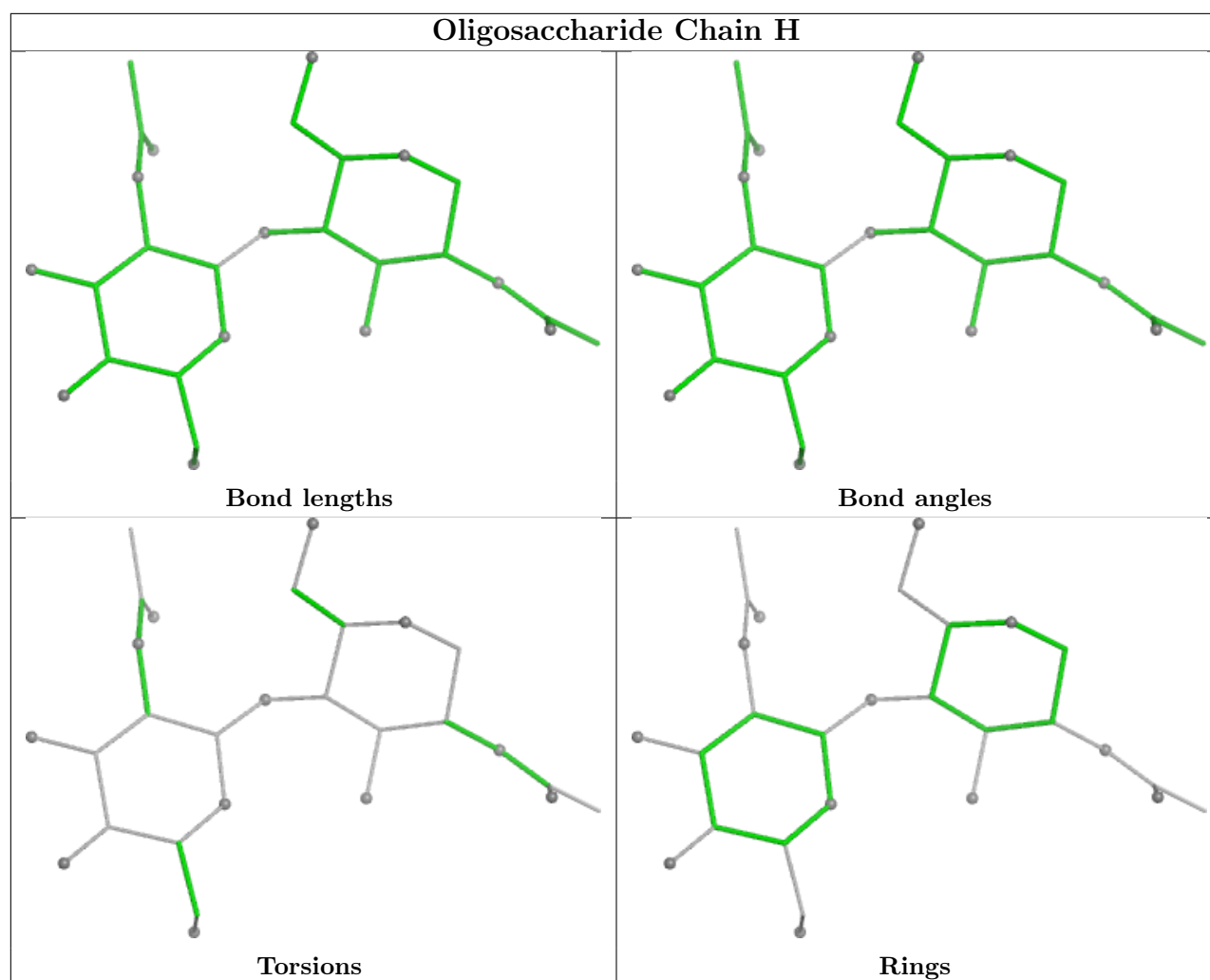
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

Of 246 ligands modelled in this entry, 1 is monoatomic - leaving 245 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
30	LMT	d	318	-	12,12,36	0.18	0	11,11,47	0.16	0
23	CLA	c	311	13	49,53,73	1.41	4 (8%)	59,89,113	1.06	3 (5%)
23	CLA	B	1231	19	49,53,73	1.28	4 (8%)	59,89,113	1.04	4 (6%)
23	CLA	b	311	36	49,53,73	1.39	4 (8%)	59,89,113	1.05	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LMT	c	326	-	12,12,36	0.17	0	11,11,47	0.19	0
23	CLA	B	1219	19	69,73,73	1.13	4 (5%)	83,113,113	0.87	3 (3%)
26	PQN	B	1232	-	34,34,34	0.31	0	42,45,45	0.36	0
31	BCR	b	317	-	41,41,41	0.13	0	56,56,56	0.28	0
23	CLA	F	404	36	69,73,73	1.15	4 (5%)	83,113,113	0.88	3 (3%)
30	LMT	e	313	-	12,12,36	0.16	0	11,11,47	0.20	0
31	BCR	L	306	-	41,41,41	0.14	0	56,56,56	0.37	0
27	XAT	d	310	-	39,47,47	0.12	0	54,74,74	0.47	0
23	CLA	f	311	16	69,73,73	1.16	5 (7%)	83,113,113	0.87	3 (3%)
23	CLA	A	414	36	69,73,73	1.15	4 (5%)	83,113,113	0.89	4 (4%)
30	LMT	d	321	-	12,12,36	0.17	0	11,11,47	0.18	0
30	LMT	a	409	-	36,36,36	0.13	0	47,47,47	0.19	0
23	CLA	B	1216	19	69,73,73	1.12	4 (5%)	83,113,113	0.86	3 (3%)
30	LMT	c	332	-	12,12,36	0.14	0	11,11,47	0.21	0
25	SF4	A	415	19,3	0,12,12	-	-	-	-	-
27	XAT	b	315	-	39,47,47	0.11	0	54,74,74	0.52	0
23	CLA	A	403	3	69,73,73	1.13	4 (5%)	83,113,113	0.85	3 (3%)
23	CLA	f	316	36	49,53,73	1.40	4 (8%)	59,89,113	1.04	3 (5%)
23	CLA	d	307	14	64,68,73	1.22	4 (6%)	77,107,113	0.95	4 (5%)
23	CLA	B	1206	36	64,68,73	1.19	4 (6%)	77,107,113	0.91	5 (6%)
30	LMT	c	331	-	36,36,36	0.12	0	47,47,47	0.17	0
23	CLA	c	310	36	69,73,73	1.18	4 (5%)	83,113,113	0.88	3 (3%)
23	CLA	B	1209	19	49,53,73	1.38	4 (8%)	59,89,113	1.03	3 (5%)
27	XAT	f	319	-	39,47,47	0.12	0	54,74,74	0.51	0
23	CLA	c	303	13	59,63,73	1.23	5 (8%)	71,101,113	0.95	3 (4%)
30	LMT	L	302	-	12,12,36	0.17	0	11,11,47	0.20	0
30	LMT	B	1204	-	28,28,36	0.11	0	39,39,47	0.35	0
28	LMG	b	320	-	37,37,55	0.21	0	45,45,63	0.22	0
23	CLA	f	309	16	49,53,73	1.37	4 (8%)	59,89,113	1.03	3 (5%)
30	LMT	b	324	-	7,7,36	0.19	0	6,6,47	0.14	0
30	LMT	d	301	-	12,12,36	0.18	0	11,11,47	0.19	0
23	CLA	B	1224	19	69,73,73	1.13	4 (5%)	83,113,113	0.90	4 (4%)
31	BCR	L	307	-	41,41,41	0.13	0	56,56,56	0.34	0
23	CLA	e	308	-	69,73,73	1.19	4 (5%)	83,113,113	0.87	3 (3%)
33	A1L6D	B	1235	-	43,49,49	0.49	1 (2%)	50,72,72	0.48	0
23	CLA	c	306	13	49,53,73	1.39	4 (8%)	59,89,113	1.04	3 (5%)
29	DGD	F	408	-	67,67,67	0.16	0	81,81,81	0.19	0
27	XAT	b	313	-	39,47,47	0.13	0	54,74,74	0.68	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	d	306	14	69,73,73	1.18	5 (7%)	83,113,113	0.91	3 (3%)
30	LMT	c	327	-	12,12,36	0.18	0	11,11,47	0.19	0
30	LMT	a	404	-	7,7,36	0.19	0	6,6,47	0.13	0
30	LMT	c	318	-	36,36,36	0.13	0	47,47,47	0.14	0
23	CLA	e	304	15	54,58,73	1.34	4 (7%)	65,95,113	0.97	2 (3%)
23	CLA	f	312	16	49,53,73	1.39	4 (8%)	59,89,113	1.07	4 (6%)
27	XAT	b	314	-	39,47,47	0.13	0	54,74,74	0.56	0
30	LMT	B	1241	-	12,12,36	0.16	0	11,11,47	0.25	0
30	LMT	f	303	-	12,12,36	0.16	0	11,11,47	0.20	0
23	CLA	B	1213	19	69,73,73	1.12	4 (5%)	83,113,113	0.89	3 (3%)
23	CLA	F	402	36	69,73,73	1.15	4 (5%)	83,113,113	0.87	3 (3%)
23	CLA	F	405	7	49,53,73	1.41	4 (8%)	59,89,113	1.06	3 (5%)
23	CLA	f	308	36	69,73,73	1.16	4 (5%)	83,113,113	0.90	4 (4%)
23	CLA	B	1201	-	69,73,73	1.12	4 (5%)	83,113,113	0.81	2 (2%)
30	LMT	F	406	-	12,12,36	0.17	0	11,11,47	0.18	0
30	LMT	d	322	-	12,12,36	0.17	0	11,11,47	0.20	0
23	CLA	c	309	13	69,73,73	1.15	4 (5%)	83,113,113	0.87	3 (3%)
23	CLA	e	305	15	69,73,73	1.14	4 (5%)	83,113,113	0.86	3 (3%)
30	LMT	c	330	-	36,36,36	0.12	0	47,47,47	0.17	0
23	CLA	f	317	36	69,73,73	1.18	5 (7%)	83,113,113	0.84	3 (3%)
23	CLA	B	1228	19	69,73,73	1.08	4 (5%)	83,113,113	0.89	3 (3%)
30	LMT	b	326	-	21,21,36	0.16	0	26,26,47	0.30	0
30	LMT	f	301	-	12,12,36	0.18	0	11,11,47	0.19	0
31	BCR	a	402	-	23,23,41	0.40	0	30,30,56	0.48	0
30	LMT	f	302	-	24,24,36	0.16	0	29,29,47	0.31	0
23	CLA	e	309	-	69,73,73	1.33	4 (5%)	83,113,113	0.96	5 (6%)
23	CLA	f	307	16	62,66,73	1.17	4 (6%)	74,104,113	0.87	3 (4%)
28	LMG	L	308	-	19,19,55	0.25	0	19,19,63	0.30	0
23	CLA	B	1225	36	69,73,73	1.20	4 (5%)	83,113,113	0.86	3 (3%)
23	CLA	b	305	36	69,73,73	1.15	4 (5%)	83,113,113	0.86	3 (3%)
27	XAT	A	417	-	39,47,47	0.12	0	54,74,74	0.53	0
23	CLA	B	1212	19	49,53,73	1.36	4 (8%)	59,89,113	1.00	3 (5%)
27	XAT	d	312	-	39,47,47	0.11	0	54,74,74	0.50	0
23	CLA	f	310	16	69,73,73	1.19	4 (5%)	83,113,113	0.87	3 (3%)
30	LMT	F	411	-	12,12,36	0.17	0	11,11,47	0.20	0
25	SF4	C	102	4	0,12,12	-	-	-	-	-
23	CLA	A	405	3	69,73,73	1.11	4 (5%)	83,113,113	0.87	3 (3%)
23	CLA	B	1208	-	69,73,73	1.10	4 (5%)	83,113,113	0.88	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	XAT	R	303	-	39,47,47	0.12	0	54,74,74	0.62	1 (1%)
30	LMT	b	301	-	24,24,36	0.17	0	29,29,47	0.32	0
23	CLA	c	304	36	59,63,73	1.26	4 (6%)	71,101,113	0.94	3 (4%)
29	DGD	u	501	-	55,55,67	0.18	0	69,69,81	0.23	0
30	LMT	c	319	-	36,36,36	0.12	0	47,47,47	0.17	0
23	CLA	A	420	-	69,73,73	1.39	4 (5%)	83,113,113	1.00	6 (7%)
27	XAT	f	322	-	39,47,47	0.12	0	54,74,74	0.58	1 (1%)
27	XAT	f	318	-	39,47,47	0.12	0	54,74,74	0.54	0
23	CLA	b	308	12	69,73,73	1.15	4 (5%)	83,113,113	0.86	2 (2%)
23	CLA	a	405	18	49,53,73	1.36	4 (8%)	59,89,113	1.02	3 (5%)
23	CLA	d	305	14	59,63,73	1.29	4 (6%)	71,101,113	0.96	4 (5%)
30	LMT	L	301	-	12,12,36	0.18	0	11,11,47	0.18	0
30	LMT	e	317	-	8,8,36	0.20	0	7,7,47	0.12	0
23	CLA	B	1214	19	69,73,73	1.10	4 (5%)	83,113,113	0.87	3 (3%)
23	CLA	A	406	3	49,53,73	1.39	4 (8%)	59,89,113	1.03	2 (3%)
30	LMT	b	322	-	12,12,36	0.16	0	11,11,47	0.20	0
23	CLA	c	308	36	49,53,73	1.36	4 (8%)	59,89,113	1.04	3 (5%)
30	LMT	e	316	-	12,12,36	0.17	0	11,11,47	0.21	0
23	CLA	b	306	12	69,73,73	1.15	4 (5%)	83,113,113	0.91	4 (4%)
23	CLA	R	301	11	49,53,73	1.36	4 (8%)	59,89,113	1.03	3 (5%)
30	LMT	c	333	-	12,12,36	0.17	0	11,11,47	0.22	0
27	XAT	c	315	-	39,47,47	0.10	0	54,74,74	0.66	1 (1%)
29	DGD	c	328	-	52,52,67	0.18	0	66,66,81	0.31	0
23	CLA	A	413	3	60,64,73	1.19	4 (6%)	72,102,113	0.93	3 (4%)
23	CLA	c	307	13	69,73,73	1.17	4 (5%)	83,113,113	0.89	2 (2%)
23	CLA	d	309	14	49,53,73	1.43	4 (8%)	59,89,113	1.04	3 (5%)
27	XAT	e	311	-	39,47,47	0.15	0	54,74,74	0.46	0
30	LMT	B	1238	-	12,12,36	0.18	0	11,11,47	0.19	0
28	LMG	F	412	-	45,45,55	0.19	0	53,53,63	0.34	0
30	LMT	R	306	-	12,12,36	0.16	0	11,11,47	0.20	0
30	LMT	e	315	-	12,12,36	0.17	0	11,11,47	0.19	0
30	LMT	c	317	-	34,34,36	0.12	0	45,45,47	0.16	0
30	LMT	e	314	-	6,6,36	0.19	0	5,5,47	0.14	0
23	CLA	A	401	36	69,73,73	1.15	4 (5%)	83,113,113	0.89	3 (3%)
23	CLA	f	313	16	49,53,73	1.40	4 (8%)	59,89,113	1.02	3 (5%)
30	LMT	B	1237	-	12,12,36	0.16	0	11,11,47	0.24	0
23	CLA	a	408	36	49,53,73	1.39	4 (8%)	59,89,113	1.04	3 (5%)
23	CLA	a	411	-	49,53,73	1.45	4 (8%)	59,89,113	1.04	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	1223	19	69,73,73	1.12	4 (5%)	83,113,113	0.93	4 (4%)
23	CLA	F	403	36	64,68,73	1.20	4 (6%)	77,107,113	0.90	3 (3%)
23	CLA	B	1230	19	69,73,73	1.10	4 (5%)	83,113,113	0.91	4 (4%)
29	DGD	b	319	-	50,50,67	0.18	0	64,64,81	0.19	0
30	LMT	c	323	-	12,12,36	0.18	0	11,11,47	0.20	0
23	CLA	a	412	18	57,61,73	1.25	4 (7%)	68,98,113	0.95	3 (4%)
30	LMT	b	323	-	12,12,36	0.17	0	11,11,47	0.19	0
30	LMT	d	319	-	12,12,36	0.18	0	11,11,47	0.17	0
23	CLA	b	304	12	49,53,73	1.42	4 (8%)	59,89,113	1.09	3 (5%)
23	CLA	e	302	15	69,73,73	1.19	4 (5%)	83,113,113	0.89	3 (3%)
27	XAT	c	314	-	39,47,47	0.13	0	54,74,74	0.56	0
30	LMT	d	320	-	12,12,36	0.18	0	11,11,47	0.18	0
28	LMG	b	321	-	50,50,55	0.18	0	58,58,63	0.20	0
23	CLA	B	1210	19	69,73,73	1.18	4 (5%)	83,113,113	0.88	3 (3%)
27	XAT	c	316	-	39,47,47	0.15	0	54,74,74	0.67	0
27	XAT	a	410	23	39,47,47	0.17	0	54,74,74	0.53	0
23	CLA	c	305	-	49,53,73	1.46	4 (8%)	59,89,113	1.03	3 (5%)
30	LMT	f	327	-	24,24,36	0.15	0	29,29,47	0.35	0
33	A1L6D	f	321	-	43,49,49	0.55	1 (2%)	50,72,72	0.62	1 (2%)
28	LMG	b	327	-	36,36,55	0.19	0	44,44,63	0.19	0
23	CLA	L	304	9	64,68,73	1.14	4 (6%)	77,107,113	0.95	4 (5%)
23	CLA	R	302	11	69,73,73	1.16	4 (5%)	83,113,113	0.88	3 (3%)
23	CLA	b	303	12	69,73,73	1.19	4 (5%)	83,113,113	0.90	3 (3%)
23	CLA	b	310	12	69,73,73	1.16	4 (5%)	83,113,113	0.85	3 (3%)
23	CLA	b	312	12	58,62,73	1.26	4 (6%)	69,99,113	0.94	3 (4%)
23	CLA	c	312	13	69,73,73	1.18	4 (5%)	83,113,113	0.93	3 (3%)
23	CLA	e	301	15	49,53,73	1.38	4 (8%)	59,89,113	1.07	3 (5%)
30	LMT	B	1203	-	12,12,36	0.18	0	11,11,47	0.19	0
33	A1L6D	e	312	-	43,49,49	0.50	1 (2%)	50,72,72	0.48	0
23	CLA	d	304	36	69,73,73	1.17	4 (5%)	83,113,113	0.89	3 (3%)
30	LMT	b	325	-	12,12,36	0.18	0	11,11,47	0.18	0
29	DGD	b	318	-	48,48,67	0.18	0	62,62,81	0.30	0
30	LMT	e	318	-	36,36,36	0.13	0	47,47,47	0.16	0
30	LMT	F	410	-	12,12,36	0.17	0	11,11,47	0.20	0
30	LMT	d	316	-	12,12,36	0.16	0	11,11,47	0.20	0
30	LMT	B	1243	-	12,12,36	0.17	0	11,11,47	0.20	0
23	CLA	A	404	3	69,73,73	1.11	4 (5%)	83,113,113	0.89	3 (3%)
28	LMG	L	310	-	43,43,55	0.20	0	45,45,63	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LMT	A	421	-	12,12,36	0.16	0	11,11,47	0.25	0
23	CLA	c	302	13	69,73,73	1.16	4 (5%)	83,113,113	0.88	3 (3%)
30	LMT	L	309	-	12,12,36	0.16	0	11,11,47	0.21	0
23	CLA	b	302	36	62,66,73	1.21	4 (6%)	74,104,113	0.94	3 (4%)
30	LMT	c	325	-	12,12,36	0.16	0	11,11,47	0.20	0
23	CLA	b	307	12	69,73,73	1.20	4 (5%)	83,113,113	0.93	3 (3%)
23	CLA	d	303	14	60,64,73	1.24	4 (6%)	72,102,113	0.91	3 (4%)
23	CLA	B	1229	36	69,73,73	1.16	4 (5%)	83,113,113	0.90	3 (3%)
23	CLA	A	409	3	69,73,73	1.10	4 (5%)	83,113,113	0.89	3 (3%)
23	CLA	L	305	9	49,53,73	1.40	4 (8%)	59,89,113	1.04	3 (5%)
24	CL0	A	407	3	63,73,73	2.34	8 (12%)	61,113,113	1.58	5 (8%)
30	LMT	B	1244	-	8,8,36	0.17	0	7,7,47	0.17	0
25	SF4	C	101	4	0,12,12	-	-	-	-	-
23	CLA	B	1220	19	64,68,73	1.21	4 (6%)	77,107,113	0.90	3 (3%)
30	LMT	c	322	-	12,12,36	0.17	0	11,11,47	0.18	0
30	LMT	L	311	-	12,12,36	0.17	0	11,11,47	0.20	0
23	CLA	A	402	36	69,73,73	1.16	4 (5%)	83,113,113	0.89	3 (3%)
23	CLA	A	408	3	69,73,73	1.11	4 (5%)	83,113,113	0.87	3 (3%)
27	XAT	d	311	-	39,47,47	0.14	0	54,74,74	0.60	0
31	BCR	F	401	-	41,41,41	0.20	0	56,56,56	0.36	0
23	CLA	A	423	-	49,53,73	1.42	4 (8%)	59,89,113	1.04	3 (5%)
27	XAT	c	313	-	39,47,47	0.17	0	54,74,74	0.60	0
30	LMT	c	320	-	6,6,36	0.20	0	5,5,47	0.14	0
27	XAT	R	307	-	39,47,47	0.10	0	54,74,74	0.57	0
30	LMT	d	317	-	36,36,36	0.13	0	47,47,47	0.18	0
23	CLA	B	1211	19	69,73,73	1.11	4 (5%)	83,113,113	0.89	3 (3%)
30	LMT	c	329	-	12,12,36	0.18	0	11,11,47	0.18	0
23	CLA	A	410	3	69,73,73	1.12	4 (5%)	83,113,113	0.90	3 (3%)
23	CLA	A	411	3	49,53,73	1.35	4 (8%)	59,89,113	1.03	3 (5%)
23	CLA	a	401	36	69,73,73	1.14	4 (5%)	83,113,113	0.90	3 (3%)
30	LMT	R	305	-	12,12,36	0.18	0	11,11,47	0.17	0
32	AV0	L	312	-	48,48,72	0.16	0	60,62,98	0.55	1 (1%)
34	SQD	d	315	-	36,37,54	0.20	0	45,48,65	0.20	0
23	CLA	B	1218	19	57,61,73	1.22	4 (7%)	68,98,113	0.94	3 (4%)
23	CLA	B	1207	19	69,73,73	1.14	4 (5%)	83,113,113	0.87	4 (4%)
28	LMG	f	323	-	55,55,55	0.17	0	63,63,63	0.21	0
27	XAT	b	316	-	39,47,47	0.10	0	54,74,74	0.44	0
23	CLA	d	308	14	49,53,73	1.43	4 (8%)	59,89,113	1.03	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	e	303	15	69,73,73	1.16	4 (5%)	83,113,113	0.88	4 (4%)
23	CLA	e	306	15	69,73,73	1.20	4 (5%)	83,113,113	0.89	3 (3%)
23	CLA	f	314	16	49,53,73	1.42	4 (8%)	59,89,113	1.04	3 (5%)
30	LMT	c	324	-	12,12,36	0.17	0	11,11,47	0.19	0
28	LMG	F	409	-	55,55,55	0.16	0	63,63,63	0.18	0
31	BCR	B	1233	-	41,41,41	0.12	0	56,56,56	0.48	0
23	CLA	f	306	16	64,68,73	1.26	4 (6%)	77,107,113	0.95	4 (5%)
33	A1L6D	d	314	-	43,49,49	0.51	1 (2%)	50,72,72	0.61	2 (4%)
23	CLA	L	313	36	49,53,73	1.36	4 (8%)	59,89,113	1.02	3 (5%)
30	LMT	B	1239	-	12,12,36	0.17	0	11,11,47	0.21	0
26	PQN	A	416	-	34,34,34	0.29	0	42,45,45	0.39	0
28	LMG	R	304	-	28,28,55	0.21	0	36,36,63	0.22	0
30	LMT	f	325	-	36,36,36	0.13	0	47,47,47	0.24	0
23	CLA	d	302	14	69,73,73	1.20	4 (5%)	83,113,113	0.88	3 (3%)
23	CLA	b	328	27	69,73,73	1.20	4 (5%)	83,113,113	0.88	3 (3%)
30	LMT	f	324	-	12,12,36	0.18	0	11,11,47	0.20	0
30	LMT	c	321	-	24,24,36	0.15	0	29,29,47	0.33	0
30	LMT	B	1240	-	24,24,36	0.16	0	29,29,47	0.32	0
23	CLA	a	403	18	69,73,73	1.19	4 (5%)	83,113,113	0.89	3 (3%)
27	XAT	d	313	-	39,47,47	0.14	0	54,74,74	0.63	1 (1%)
30	LMT	F	407	-	24,24,36	0.16	0	29,29,47	0.32	0
30	LMT	f	326	-	12,12,36	0.17	0	11,11,47	0.20	0
28	LMG	A	418	-	30,30,55	0.25	0	32,32,63	0.22	0
35	A1I05	B	1242	-	52,52,72	0.24	0	61,61,81	0.27	0
31	BCR	B	1234	-	41,41,41	0.13	0	56,56,56	0.40	0
29	DGD	A	419	-	51,51,67	0.15	0	65,65,81	0.26	0
30	LMT	F	413	-	12,12,36	0.18	0	11,11,47	0.18	0
23	CLA	c	301	13	49,53,73	1.41	5 (10%)	59,89,113	1.06	3 (5%)
23	CLA	b	309	36	69,73,73	1.14	4 (5%)	83,113,113	0.87	3 (3%)
27	XAT	f	320	-	39,47,47	0.10	0	54,74,74	0.61	0
23	CLA	B	1221	19	69,73,73	1.17	4 (5%)	83,113,113	0.89	3 (3%)
27	XAT	e	310	-	39,47,47	0.14	0	54,74,74	0.59	0
30	LMT	f	305	-	10,10,36	0.19	0	9,9,47	0.18	0
30	LMT	F	414	23	36,36,36	0.13	0	47,47,47	0.23	0
23	CLA	B	1215	19	69,73,73	1.09	4 (5%)	83,113,113	0.86	3 (3%)
30	LMT	B	1245	-	10,10,36	0.18	0	9,9,47	0.16	0
30	LMT	B	1236	-	12,12,36	0.17	0	11,11,47	0.20	0
23	CLA	a	406	18	69,73,73	1.14	4 (5%)	83,113,113	0.88	3 (3%)
31	BCR	B	1202	-	41,41,41	0.13	0	56,56,56	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	f	315	16	59,63,73	1.25	4 (6%)	71,101,113	0.96	3 (4%)
30	LMT	f	304	-	12,12,36	0.18	0	11,11,47	0.18	0
23	CLA	B	1222	36	49,53,73	1.41	4 (8%)	59,89,113	1.07	3 (5%)
23	CLA	B	1227	19,30	69,73,73	1.10	4 (5%)	83,113,113	0.86	3 (3%)
23	CLA	B	1217	19	69,73,73	1.10	4 (5%)	83,113,113	0.86	3 (3%)
23	CLA	e	307	36	69,73,73	1.20	4 (5%)	83,113,113	0.88	3 (3%)
23	CLA	L	303	36	69,73,73	1.15	4 (5%)	83,113,113	0.91	3 (3%)
23	CLA	B	1205	19	69,73,73	1.13	4 (5%)	83,113,113	0.88	3 (3%)
28	LMG	A	422	-	33,33,55	0.21	0	41,41,63	0.24	0
23	CLA	B	1226	36	69,73,73	1.10	4 (5%)	83,113,113	0.89	3 (3%)
23	CLA	a	407	18	69,73,73	1.14	4 (5%)	83,113,113	0.87	3 (3%)
23	CLA	A	412	3	69,73,73	1.13	4 (5%)	83,113,113	0.89	3 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LMT	d	318	-	-	0/10/10/61	-
23	CLA	c	311	13	-	4/15/91/115	-
23	CLA	B	1231	19	-	2/15/91/115	-
23	CLA	b	311	36	-	2/15/91/115	-
30	LMT	c	326	-	-	0/10/10/61	-
23	CLA	B	1219	19	-	6/39/115/115	-
26	PQN	B	1232	-	-	1/23/43/43	0/2/2/2
31	BCR	b	317	-	-	4/29/63/63	0/2/2/2
23	CLA	F	404	36	-	7/39/115/115	-
30	LMT	e	313	-	-	0/10/10/61	-
31	BCR	L	306	-	-	4/29/63/63	0/2/2/2
27	XAT	d	310	-	-	0/31/93/93	0/4/4/4
23	CLA	f	311	16	-	3/39/115/115	-
23	CLA	A	414	36	-	3/39/115/115	-
30	LMT	d	321	-	-	0/10/10/61	-
30	LMT	a	409	-	-	5/21/61/61	0/2/2/2
23	CLA	B	1216	19	-	4/39/115/115	-
30	LMT	c	332	-	-	1/10/10/61	-
25	SF4	A	415	19,3	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	XAT	b	315	-	-	0/31/93/93	0/4/4/4
23	CLA	A	403	3	-	4/39/115/115	-
23	CLA	f	316	36	-	0/15/91/115	-
23	CLA	d	307	14	-	6/33/109/115	-
23	CLA	B	1206	36	-	1/33/109/115	-
30	LMT	c	331	-	-	6/21/61/61	0/2/2/2
23	CLA	c	310	36	-	0/39/115/115	-
23	CLA	B	1209	19	-	3/15/91/115	-
27	XAT	f	319	-	-	0/31/93/93	0/4/4/4
23	CLA	c	303	13	-	4/27/103/115	-
30	LMT	L	302	-	-	1/10/10/61	-
30	LMT	B	1204	-	-	5/13/53/61	0/2/2/2
28	LMG	b	320	-	-	6/32/52/70	0/1/1/1
23	CLA	f	309	16	-	5/15/91/115	-
30	LMT	b	324	-	-	0/5/5/61	-
30	LMT	d	301	-	-	1/10/10/61	-
23	CLA	B	1224	19	-	4/39/115/115	-
31	BCR	L	307	-	-	2/29/63/63	0/2/2/2
23	CLA	e	308	-	-	1/39/115/115	-
33	A1L6D	B	1235	-	-	3/32/83/83	0/2/2/2
23	CLA	c	306	13	-	2/15/91/115	-
29	DGD	F	408	-	-	7/55/95/95	0/2/2/2
27	XAT	b	313	-	-	0/31/93/93	0/4/4/4
23	CLA	d	306	14	-	5/39/115/115	-
30	LMT	c	327	-	-	0/10/10/61	-
30	LMT	a	404	-	-	0/5/5/61	-
30	LMT	c	318	-	-	2/21/61/61	0/2/2/2
23	CLA	e	304	15	-	3/21/97/115	-
23	CLA	f	312	16	-	3/15/91/115	-
27	XAT	b	314	-	-	0/31/93/93	0/4/4/4
30	LMT	B	1241	-	-	1/10/10/61	-
30	LMT	f	303	-	-	0/10/10/61	-
23	CLA	B	1213	19	-	0/39/115/115	-
23	CLA	F	402	36	-	10/39/115/115	-
23	CLA	F	405	7	-	2/15/91/115	-
23	CLA	f	308	36	-	7/39/115/115	-
23	CLA	B	1201	-	-	2/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LMT	F	406	-	-	0/10/10/61	-
30	LMT	d	322	-	-	0/10/10/61	-
23	CLA	c	309	13	-	6/39/115/115	-
23	CLA	e	305	15	-	2/39/115/115	-
30	LMT	c	330	-	-	1/21/61/61	0/2/2/2
23	CLA	f	317	36	-	3/39/115/115	-
23	CLA	B	1228	19	-	7/39/115/115	-
30	LMT	b	326	-	-	2/12/32/61	0/1/1/2
30	LMT	f	301	-	-	1/10/10/61	-
31	BCR	a	402	-	-	2/16/33/63	0/1/1/2
30	LMT	f	302	-	-	2/15/35/61	0/1/1/2
23	CLA	e	309	-	-	3/39/115/115	-
23	CLA	f	307	16	-	3/31/107/115	-
28	LMG	L	308	-	-	4/17/17/70	-
23	CLA	B	1225	36	-	7/39/115/115	-
23	CLA	b	305	36	-	4/39/115/115	-
27	XAT	A	417	-	-	0/31/93/93	0/4/4/4
23	CLA	B	1212	19	-	2/15/91/115	-
27	XAT	d	312	-	-	0/31/93/93	0/4/4/4
23	CLA	f	310	16	-	4/39/115/115	-
30	LMT	F	411	-	-	0/10/10/61	-
25	SF4	C	102	4	-	-	0/6/5/5
23	CLA	A	405	3	-	4/39/115/115	-
23	CLA	B	1208	-	-	4/39/115/115	-
27	XAT	R	303	-	-	1/31/93/93	0/4/4/4
30	LMT	b	301	-	-	2/15/35/61	0/1/1/2
23	CLA	c	304	36	-	4/27/103/115	-
29	DGD	u	501	-	-	7/43/83/95	0/2/2/2
30	LMT	c	319	-	-	8/21/61/61	0/2/2/2
23	CLA	A	420	-	-	16/39/115/115	-
27	XAT	f	322	-	1/1/26/26	0/31/93/93	0/4/4/4
27	XAT	f	318	-	-	0/31/93/93	0/4/4/4
23	CLA	b	308	12	-	4/39/115/115	-
23	CLA	a	405	18	-	5/15/91/115	-
23	CLA	d	305	14	-	0/27/103/115	-
30	LMT	L	301	-	-	0/10/10/61	-
30	LMT	e	317	-	-	0/6/6/61	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	1214	19	-	2/39/115/115	-
23	CLA	A	406	3	-	4/15/91/115	-
30	LMT	b	322	-	-	0/10/10/61	-
23	CLA	c	308	36	-	4/15/91/115	-
30	LMT	e	316	-	-	0/10/10/61	-
23	CLA	b	306	12	-	6/39/115/115	-
23	CLA	R	301	11	-	2/15/91/115	-
30	LMT	c	333	-	-	1/10/10/61	-
27	XAT	c	315	-	-	0/31/93/93	0/4/4/4
29	DGD	c	328	-	-	9/40/80/95	0/2/2/2
23	CLA	A	413	3	-	0/29/105/115	-
23	CLA	c	307	13	-	8/39/115/115	-
23	CLA	d	309	14	-	7/15/91/115	-
27	XAT	e	311	-	-	0/31/93/93	0/4/4/4
30	LMT	B	1238	-	-	0/10/10/61	-
28	LMG	F	412	-	-	7/40/60/70	0/1/1/1
30	LMT	R	306	-	-	0/10/10/61	-
30	LMT	e	315	-	-	1/10/10/61	-
30	LMT	c	317	-	-	7/19/59/61	0/2/2/2
30	LMT	e	314	-	-	0/4/4/61	-
23	CLA	A	401	36	-	1/39/115/115	-
23	CLA	f	313	16	-	4/15/91/115	-
30	LMT	B	1237	-	-	0/10/10/61	-
23	CLA	a	408	36	-	2/15/91/115	-
23	CLA	a	411	-	-	6/15/91/115	-
23	CLA	B	1223	19	-	13/39/115/115	-
23	CLA	F	403	36	-	4/33/109/115	-
23	CLA	B	1230	19	-	5/39/115/115	-
29	DGD	b	319	-	-	8/38/78/95	0/2/2/2
30	LMT	c	323	-	-	1/10/10/61	-
23	CLA	a	412	18	-	0/25/101/115	-
30	LMT	b	323	-	-	0/10/10/61	-
30	LMT	d	319	-	-	1/10/10/61	-
23	CLA	b	304	12	-	5/15/91/115	-
23	CLA	e	302	15	-	2/39/115/115	-
27	XAT	c	314	-	-	0/31/93/93	0/4/4/4
30	LMT	d	320	-	-	2/10/10/61	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMG	b	321	-	-	7/45/65/70	0/1/1/1
23	CLA	B	1210	19	-	9/39/115/115	-
27	XAT	c	316	-	-	3/31/93/93	0/4/4/4
27	XAT	a	410	23	-	0/31/93/93	0/4/4/4
23	CLA	c	305	-	-	4/15/91/115	-
30	LMT	f	327	-	-	5/15/35/61	0/1/1/2
33	A1L6D	f	321	-	-	4/32/83/83	0/2/2/2
28	LMG	b	327	-	-	4/31/51/70	0/1/1/1
23	CLA	L	304	9	-	3/33/109/115	-
23	CLA	R	302	11	-	4/39/115/115	-
23	CLA	b	303	12	-	1/39/115/115	-
23	CLA	b	310	12	-	2/39/115/115	-
23	CLA	b	312	12	-	1/26/102/115	-
23	CLA	c	312	13	-	7/39/115/115	-
23	CLA	e	301	15	-	3/15/91/115	-
30	LMT	B	1203	-	-	0/10/10/61	-
33	A1L6D	e	312	-	-	0/32/83/83	0/2/2/2
23	CLA	d	304	36	-	7/39/115/115	-
30	LMT	b	325	-	-	1/10/10/61	-
29	DGD	b	318	-	-	8/36/76/95	0/2/2/2
30	LMT	e	318	-	-	8/21/61/61	0/2/2/2
30	LMT	F	410	-	-	0/10/10/61	-
30	LMT	d	316	-	-	0/10/10/61	-
30	LMT	B	1243	-	-	0/10/10/61	-
23	CLA	A	404	3	-	11/39/115/115	-
28	LMG	L	310	-	-	5/45/45/70	-
30	LMT	A	421	-	-	0/10/10/61	-
23	CLA	c	302	13	-	3/39/115/115	-
30	LMT	L	309	-	-	0/10/10/61	-
23	CLA	b	302	36	-	5/31/107/115	-
30	LMT	c	325	-	-	0/10/10/61	-
23	CLA	b	307	12	-	8/39/115/115	-
23	CLA	d	303	14	-	0/29/105/115	-
23	CLA	B	1229	36	-	7/39/115/115	-
23	CLA	A	409	3	-	6/39/115/115	-
23	CLA	L	305	9	-	7/15/91/115	-
24	CL0	A	407	3	-	5/37/135/135	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LMT	B	1244	-	-	0/6/6/61	-
25	SF4	C	101	4	-	-	0/6/5/5
23	CLA	B	1220	19	-	4/33/109/115	-
30	LMT	c	322	-	-	1/10/10/61	-
30	LMT	L	311	-	-	0/10/10/61	-
23	CLA	A	402	36	-	2/39/115/115	-
23	CLA	A	408	3	-	3/39/115/115	-
27	XAT	d	311	-	-	0/31/93/93	0/4/4/4
31	BCR	F	401	-	-	2/29/63/63	0/2/2/2
23	CLA	A	423	-	-	6/15/91/115	-
27	XAT	c	313	-	-	0/31/93/93	0/4/4/4
30	LMT	c	320	-	-	0/4/4/61	-
27	XAT	R	307	-	-	0/31/93/93	0/4/4/4
30	LMT	d	317	-	-	4/21/61/61	0/2/2/2
23	CLA	B	1211	19	-	6/39/115/115	-
30	LMT	c	329	-	-	0/10/10/61	-
23	CLA	A	410	3	-	4/39/115/115	-
23	CLA	A	411	3	-	3/15/91/115	-
23	CLA	a	401	36	-	7/39/115/115	-
30	LMT	R	305	-	-	1/10/10/61	-
32	AV0	L	312	-	-	4/38/78/130	0/2/2/4
34	SQD	d	315	-	-	5/32/52/69	0/1/1/1
23	CLA	B	1218	19	-	5/25/101/115	-
23	CLA	B	1207	19	-	3/39/115/115	-
28	LMG	f	323	-	-	11/50/70/70	0/1/1/1
27	XAT	b	316	-	-	1/31/93/93	0/4/4/4
23	CLA	d	308	14	-	1/15/91/115	-
23	CLA	e	303	15	-	11/39/115/115	-
23	CLA	e	306	15	-	5/39/115/115	-
23	CLA	f	314	16	-	5/15/91/115	-
30	LMT	c	324	-	-	0/10/10/61	-
28	LMG	F	409	-	-	5/50/70/70	0/1/1/1
31	BCR	B	1233	-	-	1/29/63/63	0/2/2/2
23	CLA	f	306	16	-	1/33/109/115	-
33	A1L6D	d	314	-	-	4/32/83/83	0/2/2/2
23	CLA	L	313	36	-	4/15/91/115	-
30	LMT	B	1239	-	-	0/10/10/61	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PQN	A	416	-	-	1/23/43/43	0/2/2/2
28	LMG	R	304	-	-	1/23/43/70	0/1/1/1
30	LMT	f	325	-	-	5/21/61/61	0/2/2/2
23	CLA	d	302	14	-	3/39/115/115	-
23	CLA	b	328	27	-	5/39/115/115	-
30	LMT	f	324	-	-	0/10/10/61	-
30	LMT	c	321	-	-	1/15/35/61	0/1/1/2
30	LMT	B	1240	-	-	5/15/35/61	0/1/1/2
23	CLA	a	403	18	-	9/39/115/115	-
27	XAT	d	313	-	-	0/31/93/93	0/4/4/4
35	A1H05	B	1242	-	2/2/9/9	7/48/68/88	0/1/1/1
30	LMT	F	407	-	-	1/15/35/61	0/1/1/2
28	LMG	A	418	-	-	5/32/32/70	-
30	LMT	f	326	-	-	0/10/10/61	-
31	BCR	B	1234	-	-	2/29/63/63	0/2/2/2
29	DGD	A	419	-	-	11/38/78/95	0/2/2/2
30	LMT	F	413	-	-	1/10/10/61	-
23	CLA	c	301	13	-	0/15/91/115	-
23	CLA	b	309	36	-	8/39/115/115	-
27	XAT	f	320	-	-	0/31/93/93	0/4/4/4
23	CLA	B	1221	19	-	11/39/115/115	-
27	XAT	e	310	-	-	0/31/93/93	0/4/4/4
30	LMT	f	305	-	-	0/8/8/61	-
30	LMT	F	414	23	-	10/21/61/61	0/2/2/2
23	CLA	B	1215	19	-	0/39/115/115	-
30	LMT	B	1245	-	-	0/8/8/61	-
30	LMT	B	1236	-	-	1/10/10/61	-
23	CLA	a	406	18	-	5/39/115/115	-
31	BCR	B	1202	-	-	2/29/63/63	0/2/2/2
23	CLA	f	315	16	-	3/27/103/115	-
30	LMT	f	304	-	-	1/10/10/61	-
23	CLA	B	1222	36	-	4/15/91/115	-
23	CLA	B	1227	19,30	-	2/39/115/115	-
23	CLA	B	1217	19	-	4/39/115/115	-
23	CLA	e	307	36	-	6/39/115/115	-
23	CLA	L	303	36	-	7/39/115/115	-
23	CLA	B	1205	19	-	1/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMG	A	422	-	-	4/28/48/70	0/1/1/1
23	CLA	B	1226	36	-	5/39/115/115	-
23	CLA	a	407	18	-	4/39/115/115	-
23	CLA	A	412	3	-	4/39/115/115	-

The worst 5 of 473 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	407	CL0	C4C-NC	15.60	1.49	1.35
23	A	420	CLA	MG-NB	-7.25	1.91	2.05
23	e	309	CLA	MG-NB	-6.76	1.92	2.05
23	B	1207	CLA	C1D-ND	6.05	1.45	1.37
23	A	420	CLA	MG-ND	-5.98	1.93	2.05

The worst 5 of 372 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	407	CL0	C1B-CHB-C4A	10.00	127.52	121.39
23	A	409	CLA	C1D-ND-C4D	-4.52	103.12	106.33
23	B	1216	CLA	C1D-ND-C4D	-4.40	103.21	106.33
23	f	312	CLA	C1D-ND-C4D	-4.36	103.24	106.33
23	B	1224	CLA	C1D-ND-C4D	-4.35	103.25	106.33

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	f	322	XAT	C6
35	B	1242	A1I05	C25
35	B	1242	A1I05	C49

5 of 748 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	404	CLA	C1A-C2A-CAA-CBA
23	A	405	CLA	CHA-CBD-CGD-O2D
23	A	410	CLA	C2B-C3B-CAB-CBB
23	A	410	CLA	C4B-C3B-CAB-CBB
23	A	411	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

87 monomers are involved in 111 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	b	311	CLA	1	0
23	B	1219	CLA	1	0
31	b	317	BCR	1	0
31	L	306	BCR	2	0
27	d	310	XAT	1	0
23	A	414	CLA	1	0
30	a	409	LMT	2	0
27	b	315	XAT	2	0
23	B	1206	CLA	2	0
30	c	331	LMT	2	0
23	c	310	CLA	1	0
23	B	1209	CLA	1	0
30	B	1204	LMT	1	0
23	B	1224	CLA	1	0
31	L	307	BCR	1	0
23	c	306	CLA	1	0
23	d	306	CLA	1	0
27	b	314	XAT	1	0
23	F	402	CLA	1	0
23	f	308	CLA	3	0
23	B	1201	CLA	1	0
31	a	402	BCR	2	0
23	B	1225	CLA	1	0
23	b	305	CLA	1	0
23	B	1208	CLA	3	0
27	R	303	XAT	1	0
23	c	304	CLA	2	0
30	c	319	LMT	2	0
23	A	420	CLA	10	0
27	f	318	XAT	1	0
23	b	308	CLA	1	0
23	B	1214	CLA	1	0
23	c	308	CLA	1	0
23	b	306	CLA	1	0
29	c	328	DGD	1	0
23	c	307	CLA	1	0
23	A	401	CLA	2	0
23	f	313	CLA	1	0
23	B	1223	CLA	1	0
23	F	403	CLA	1	0
23	B	1230	CLA	1	0
28	b	321	LMG	1	0
27	c	316	XAT	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	a	410	XAT	3	0
23	c	305	CLA	3	0
30	f	327	LMT	1	0
23	L	304	CLA	3	0
23	R	302	CLA	2	0
23	b	303	CLA	1	0
23	b	310	CLA	1	0
23	b	312	CLA	2	0
23	c	312	CLA	3	0
29	b	318	DGD	1	0
23	A	404	CLA	1	0
23	b	302	CLA	1	0
23	b	307	CLA	1	0
23	A	409	CLA	3	0
23	L	305	CLA	1	0
23	A	402	CLA	1	0
23	A	408	CLA	1	0
27	d	311	XAT	1	0
31	F	401	BCR	4	0
23	B	1211	CLA	1	0
30	c	329	LMT	1	0
23	A	410	CLA	2	0
23	B	1218	CLA	1	0
23	B	1207	CLA	2	0
23	e	306	CLA	1	0
28	F	409	LMG	1	0
31	B	1233	BCR	1	0
33	d	314	A1L6D	1	0
23	L	313	CLA	1	0
28	R	304	LMG	1	0
23	d	302	CLA	1	0
30	B	1240	LMT	1	0
23	a	403	CLA	1	0
31	B	1234	BCR	2	0
27	f	320	XAT	1	0
27	e	310	XAT	3	0
30	F	414	LMT	2	0
23	B	1215	CLA	2	0
23	a	406	CLA	1	0
23	f	315	CLA	2	0
23	B	1222	CLA	2	0
23	B	1227	CLA	1	0

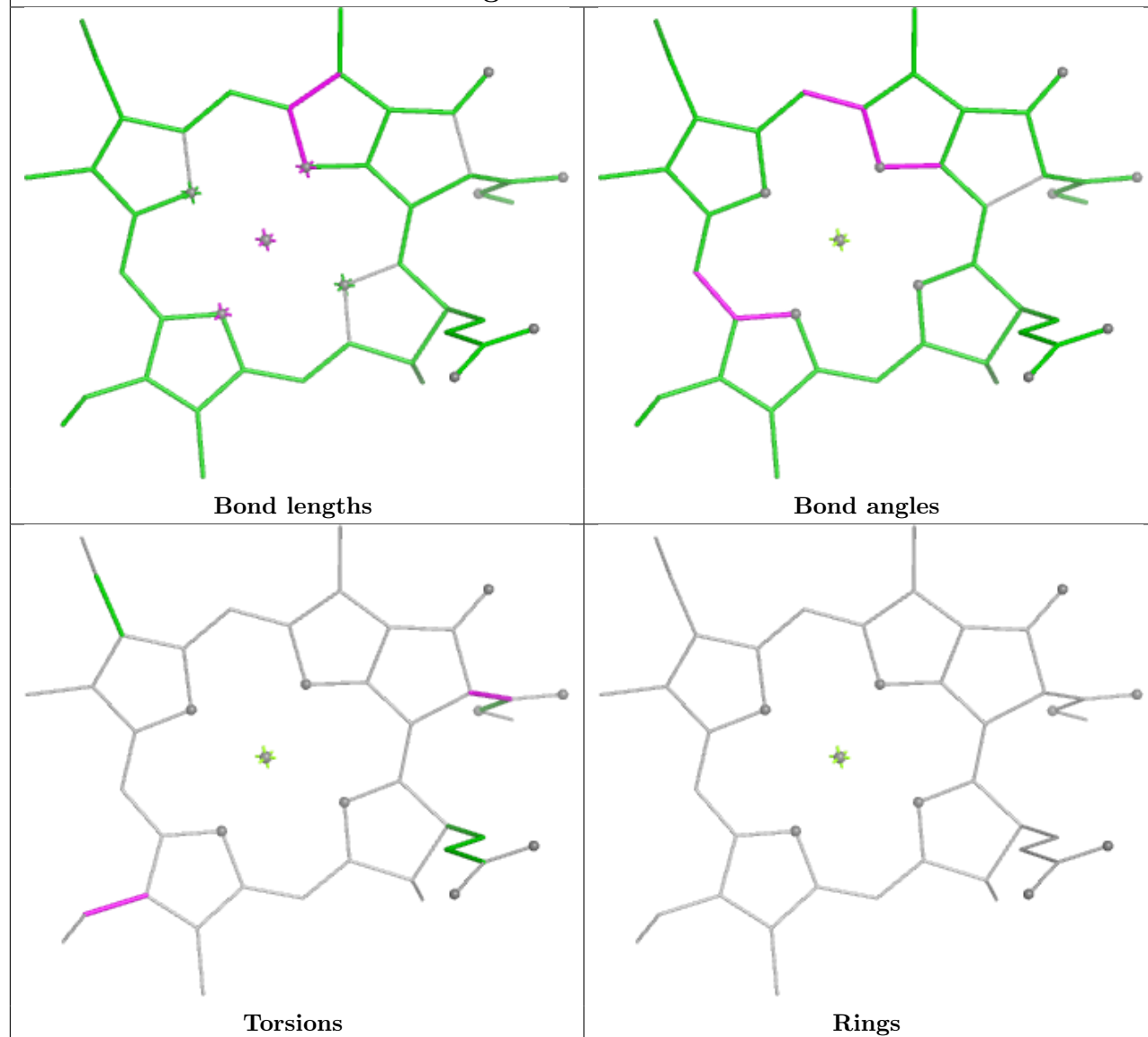
Continued on next page...

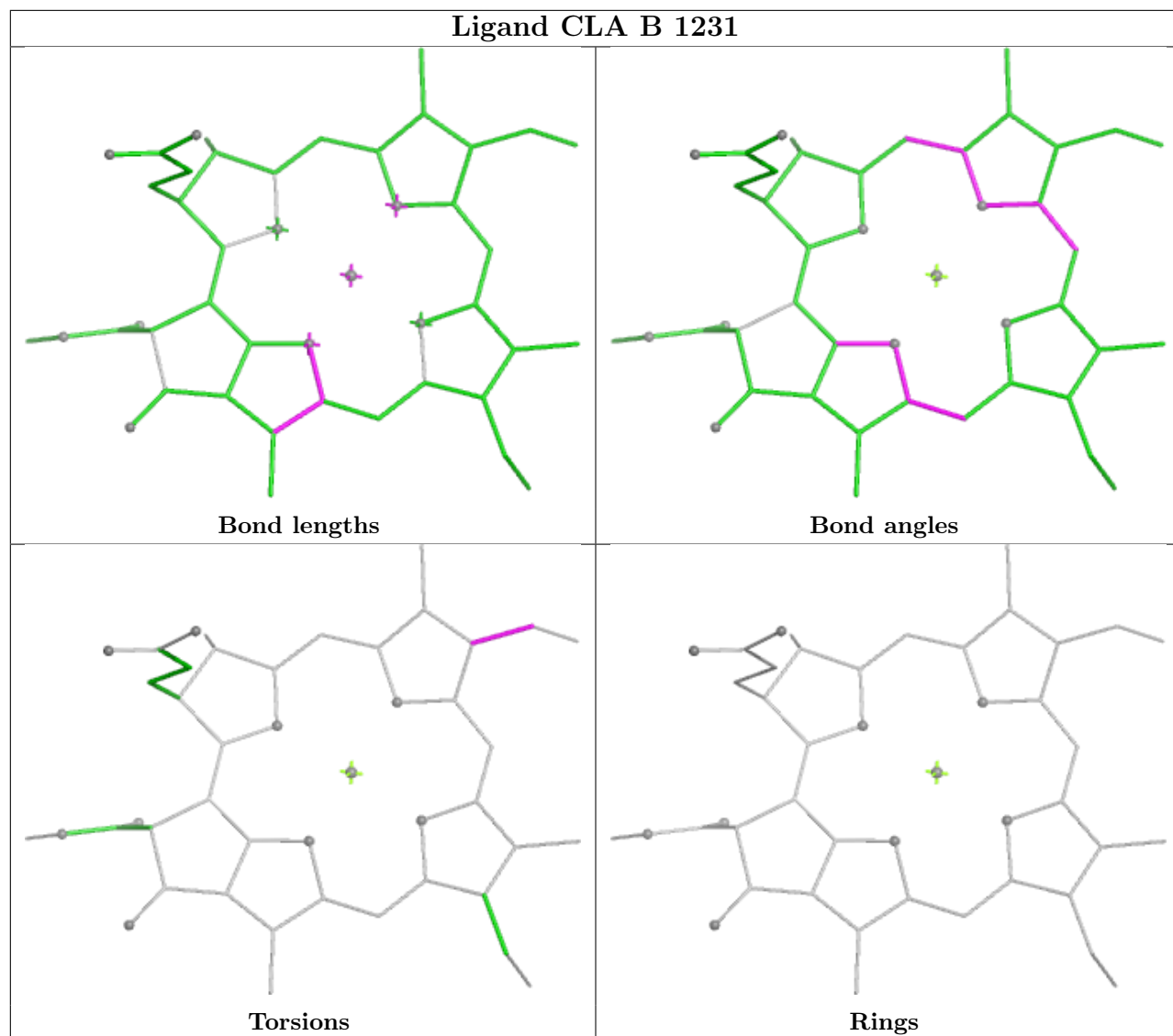
Continued from previous page...

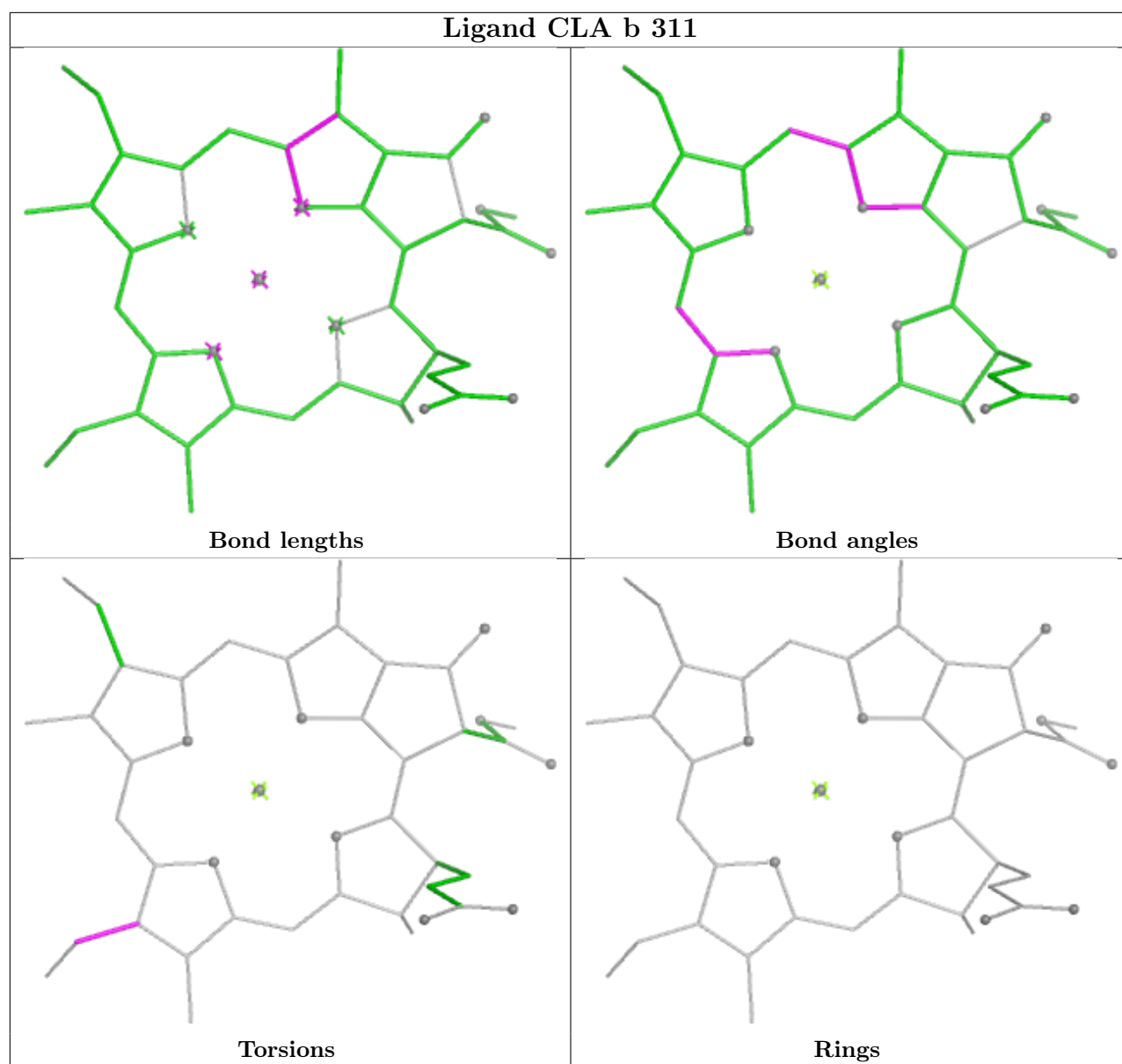
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	L	303	CLA	1	0
23	A	412	CLA	1	0

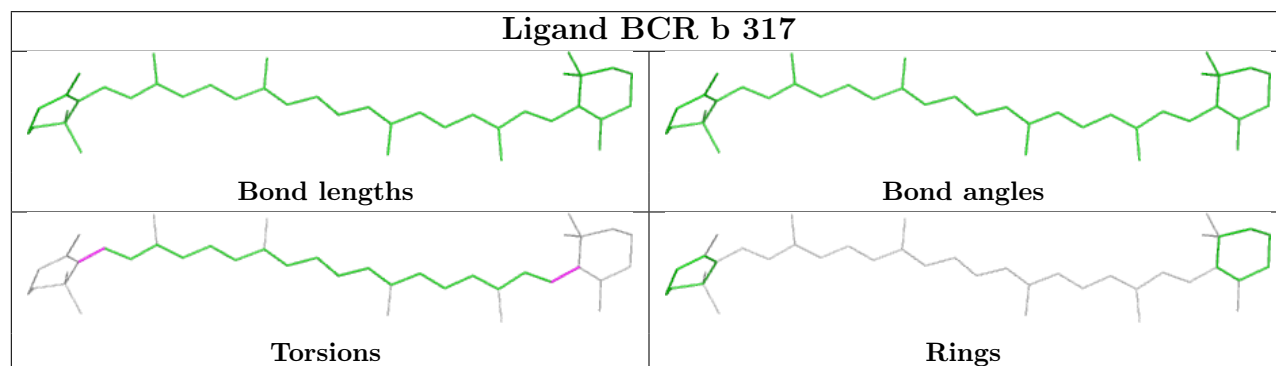
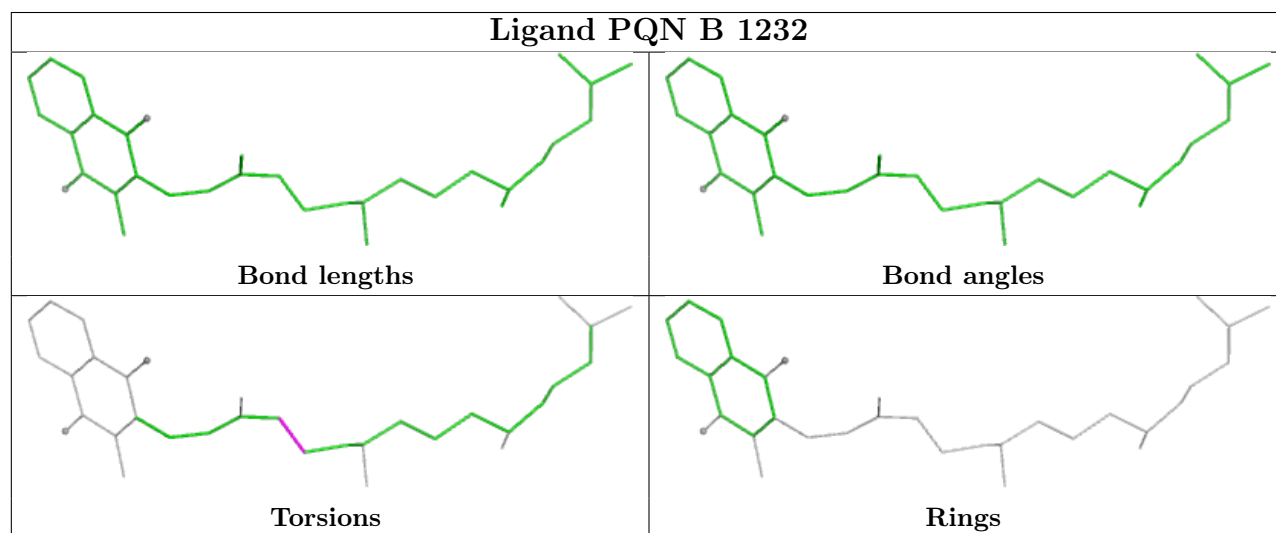
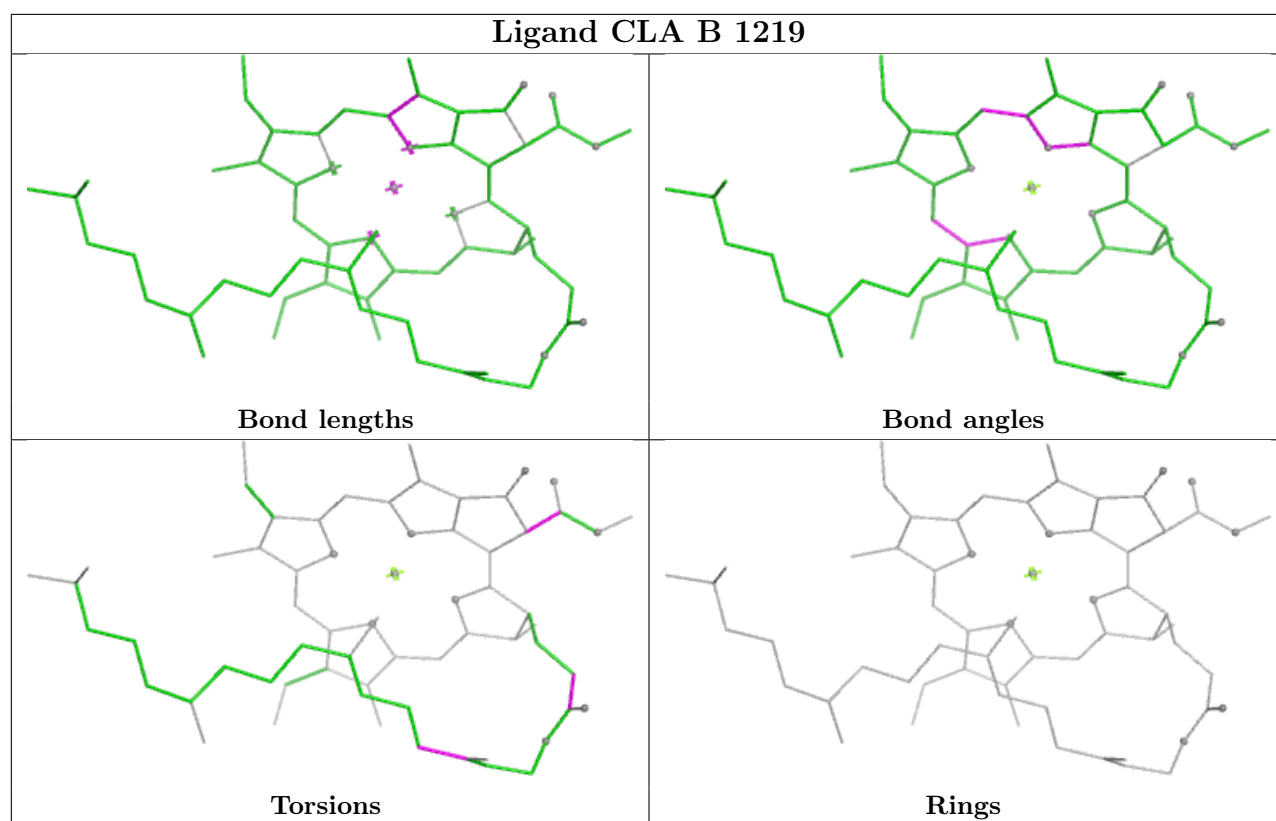
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

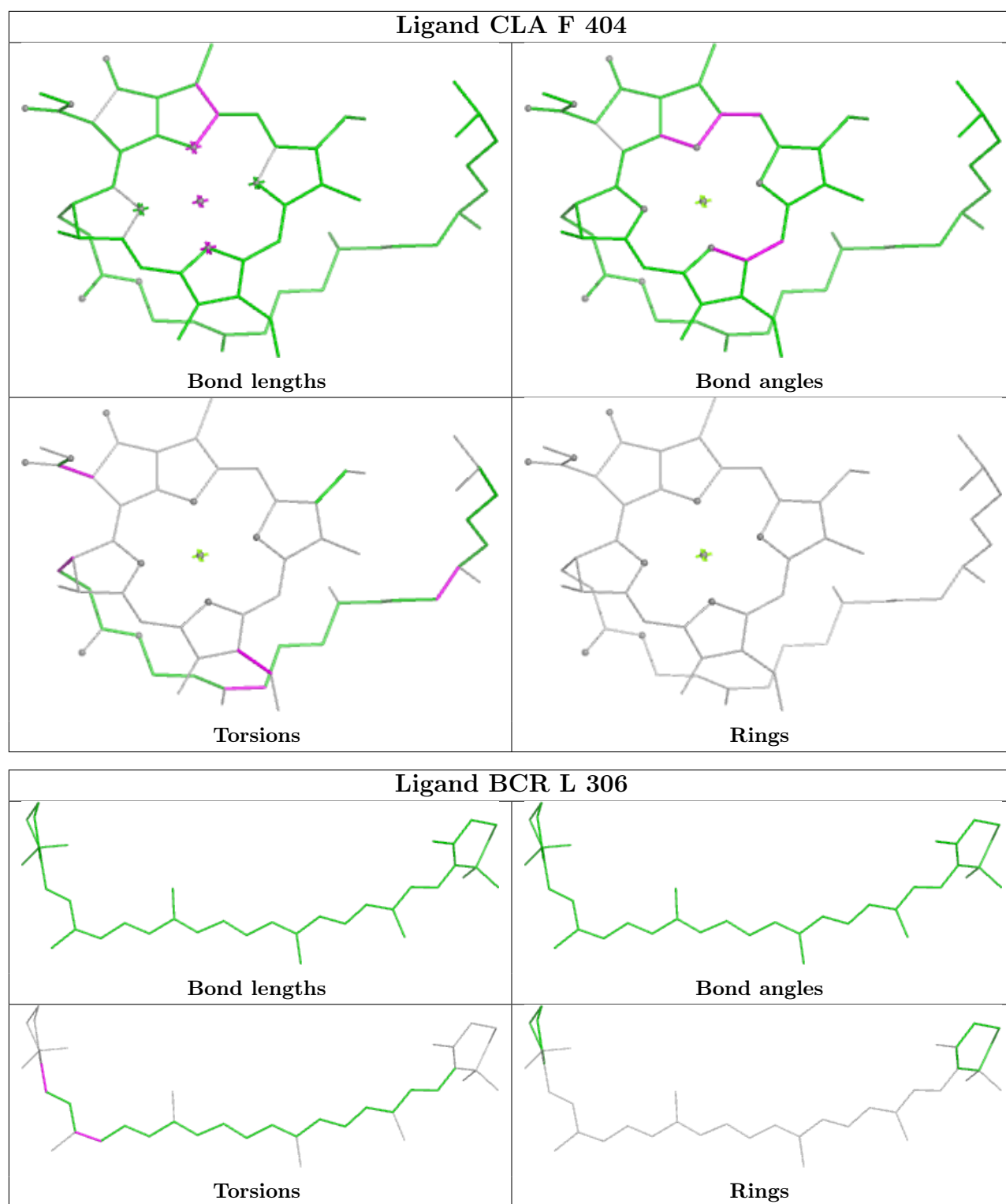
Ligand CLA c 311

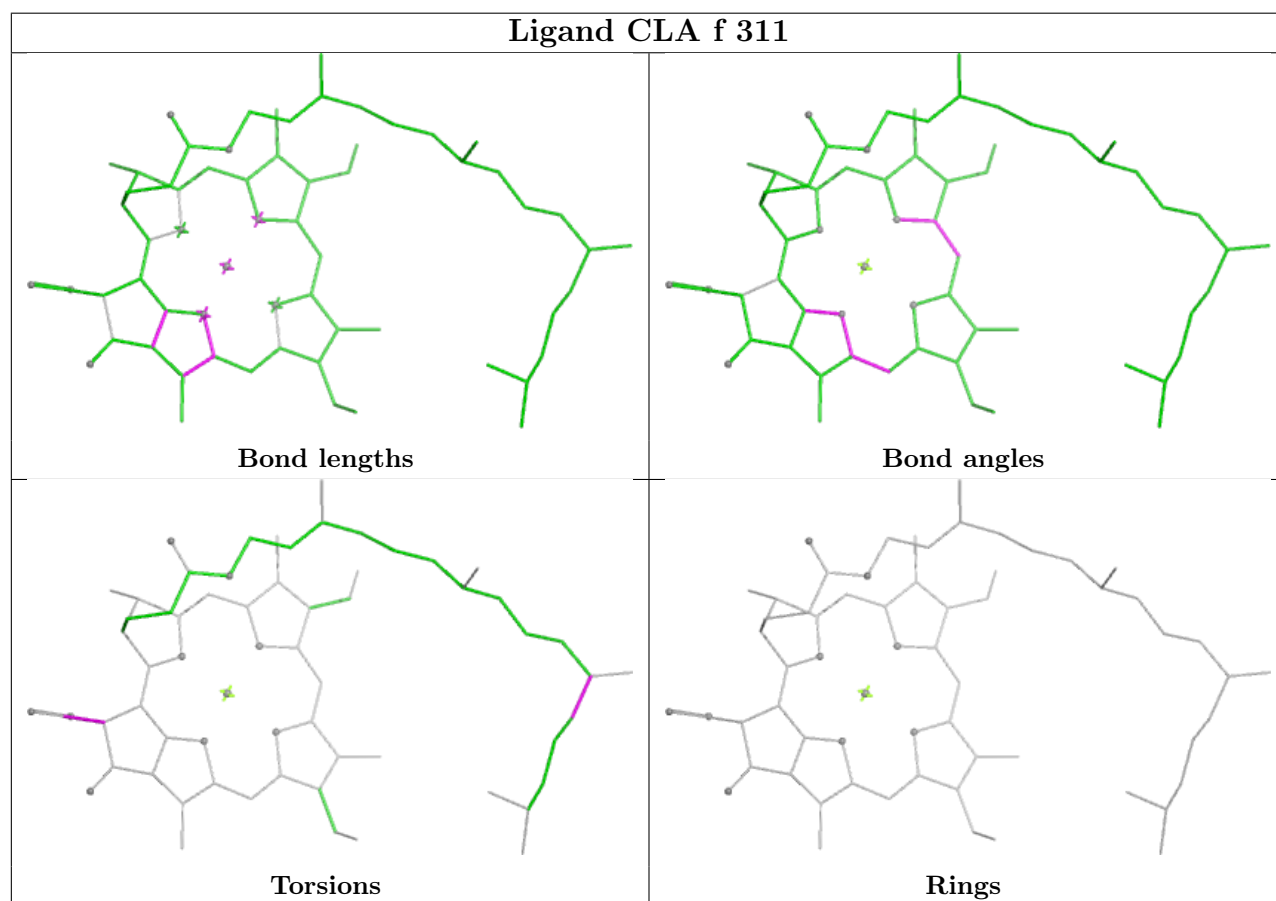
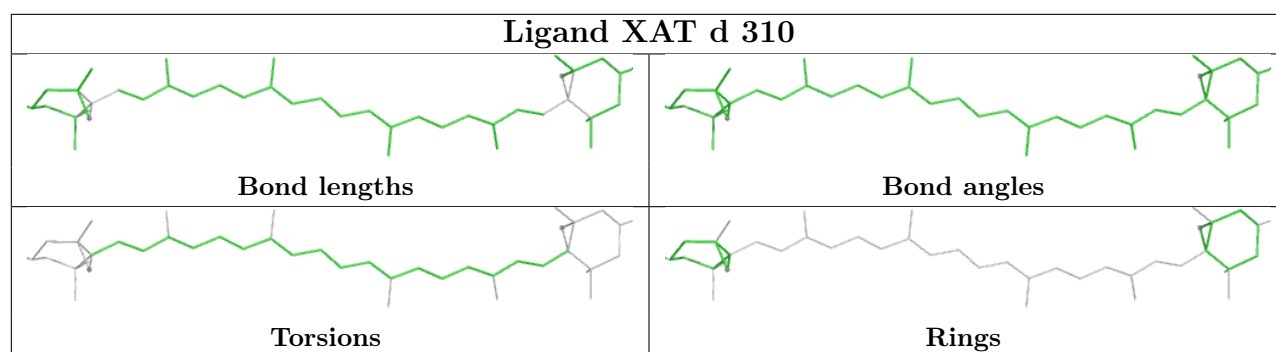


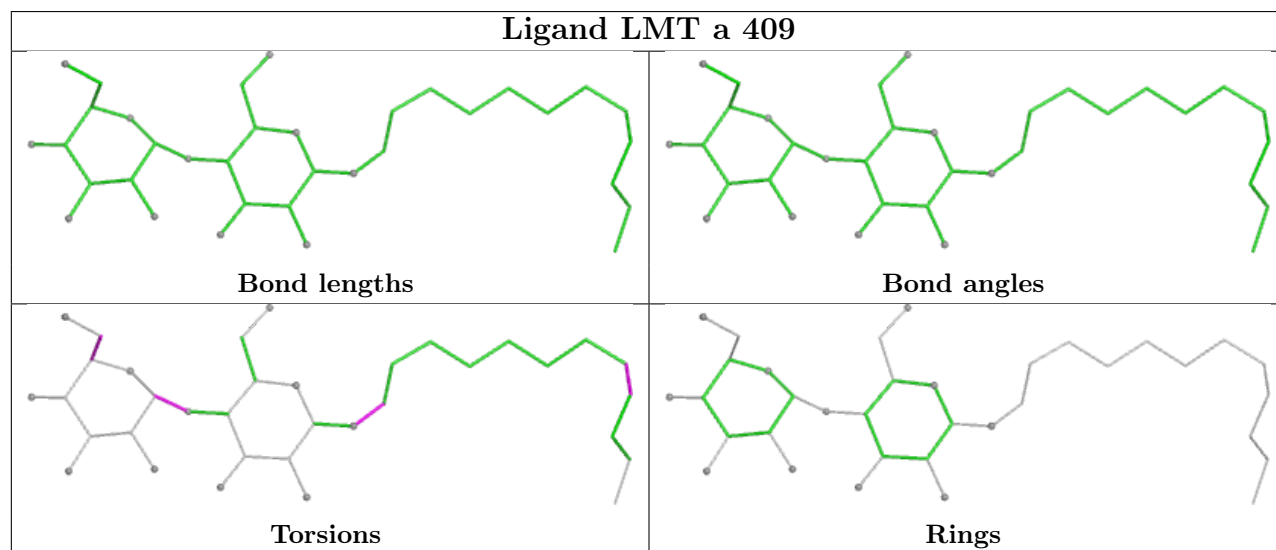
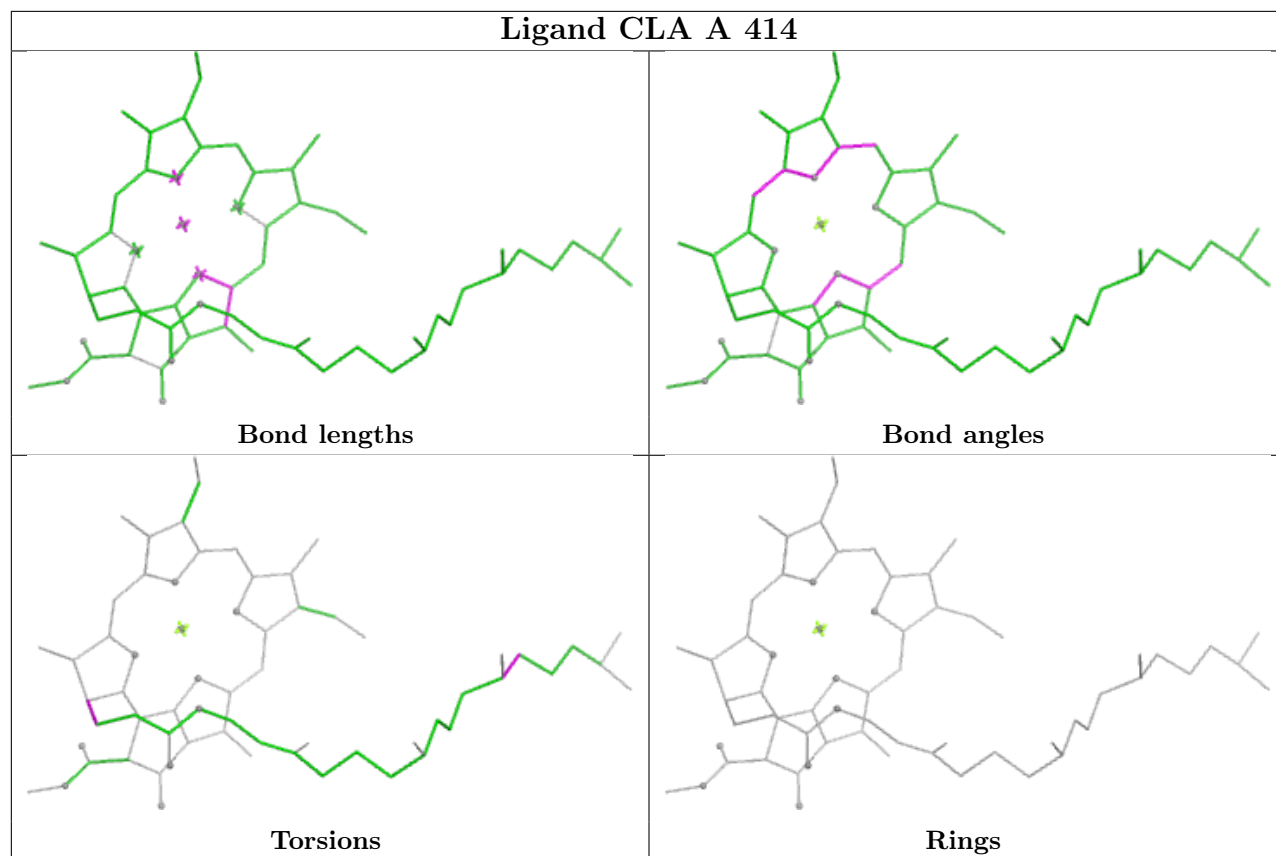


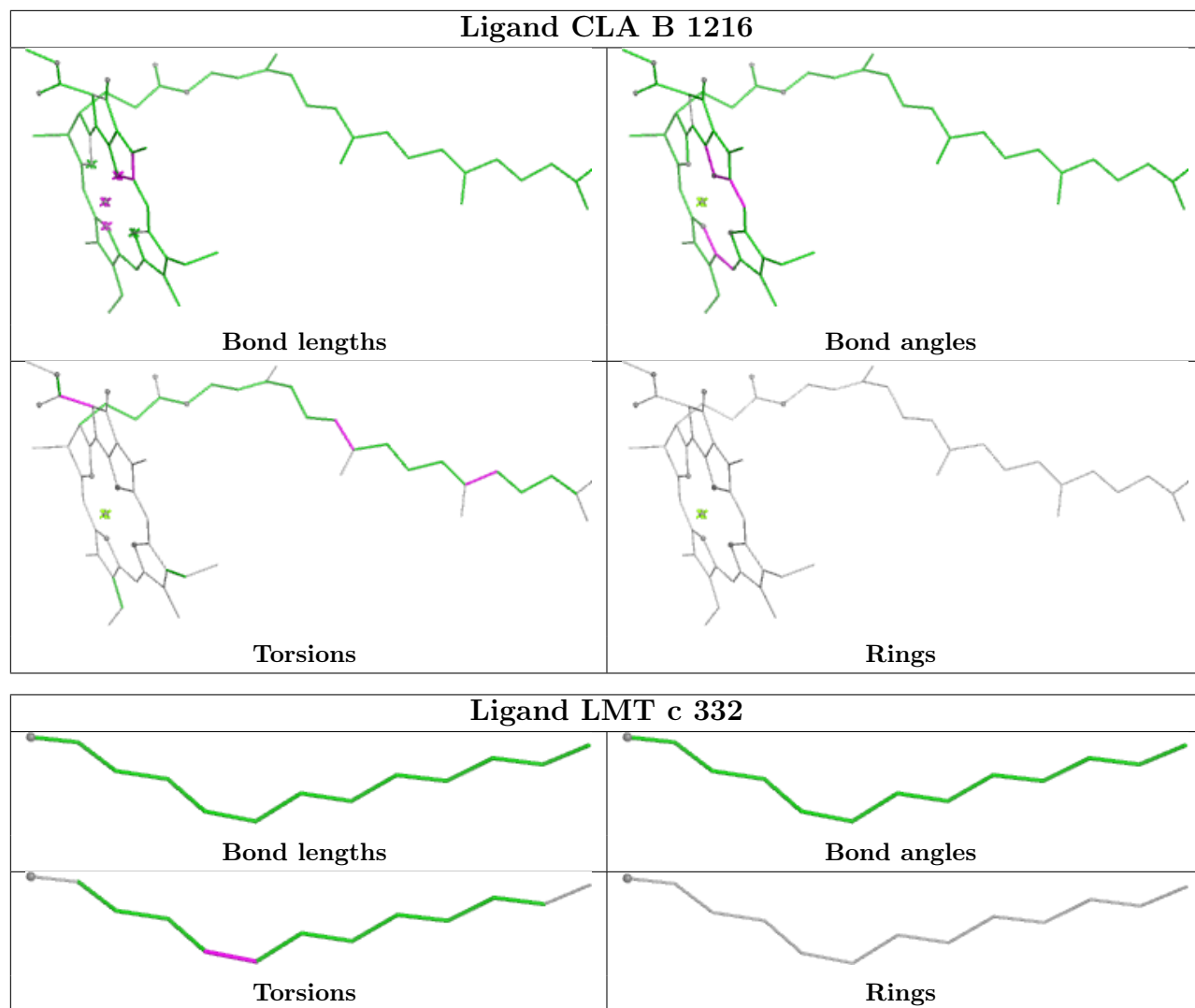


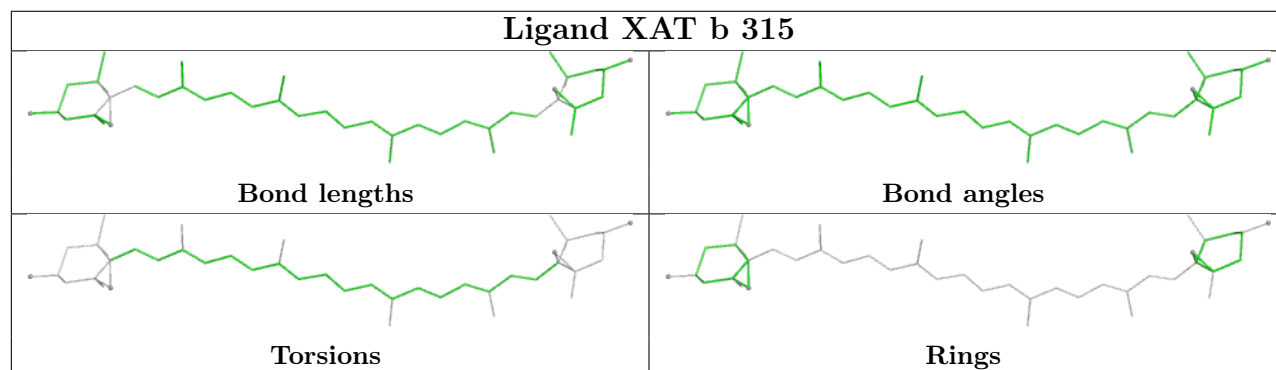
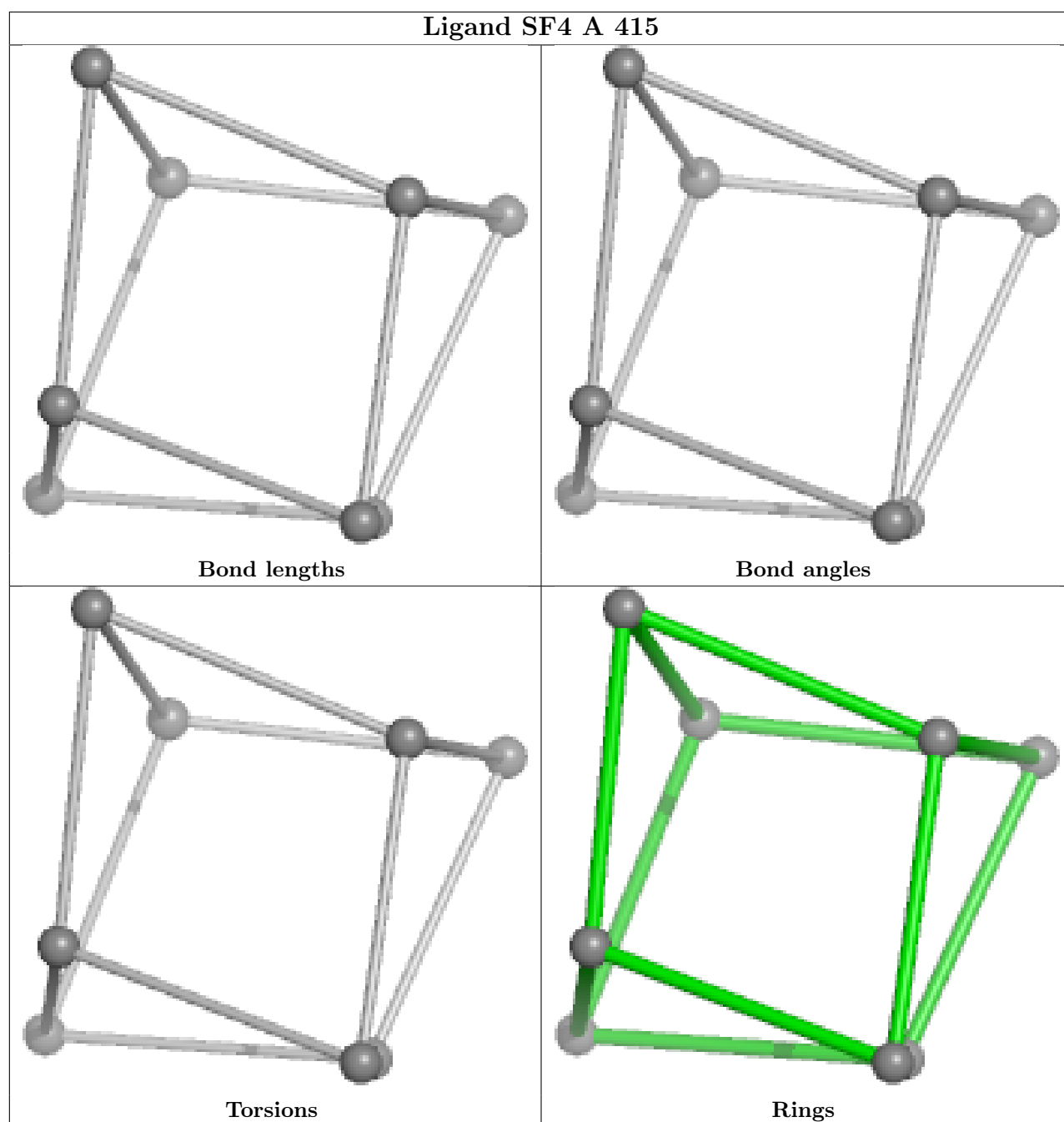


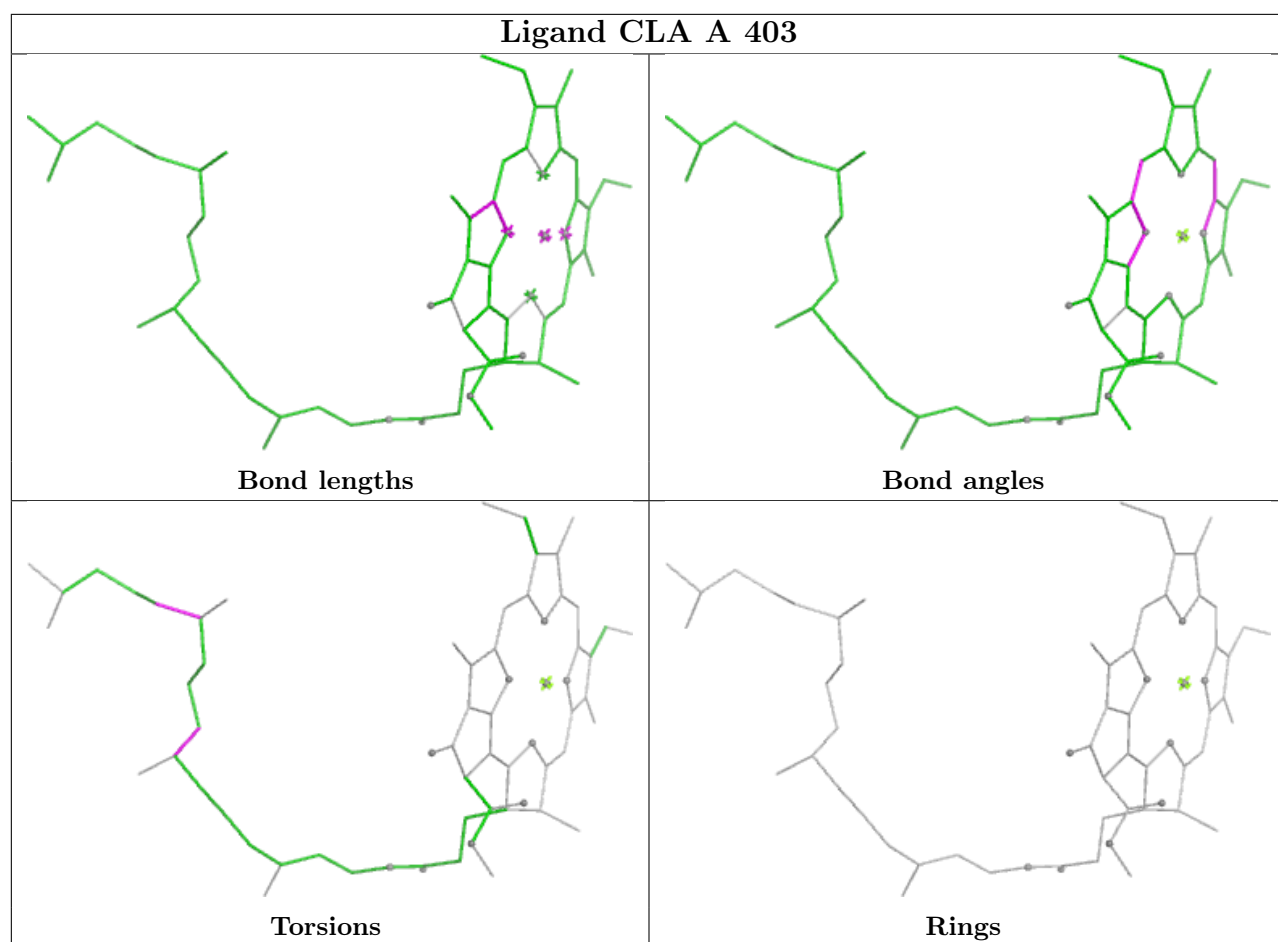




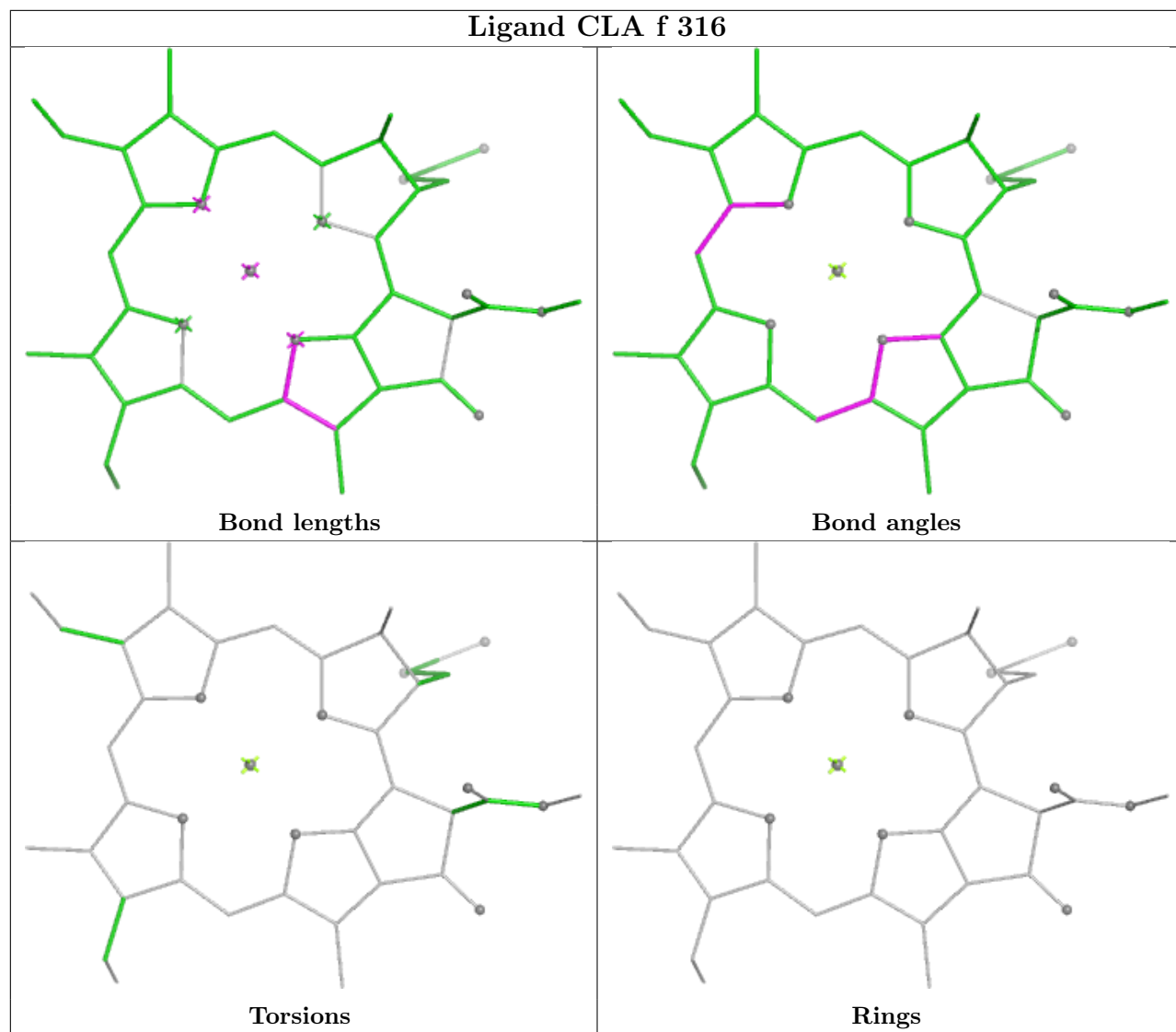


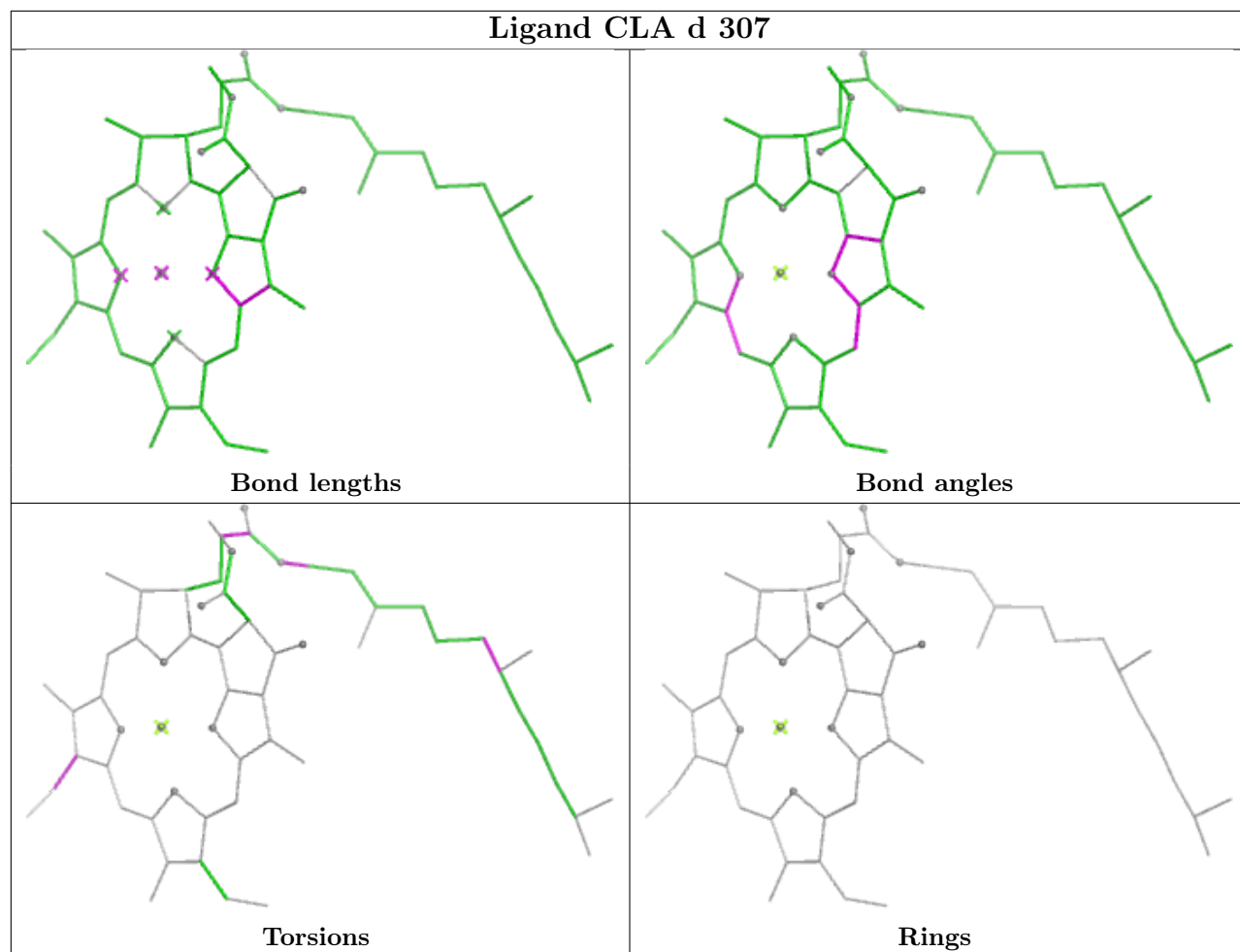


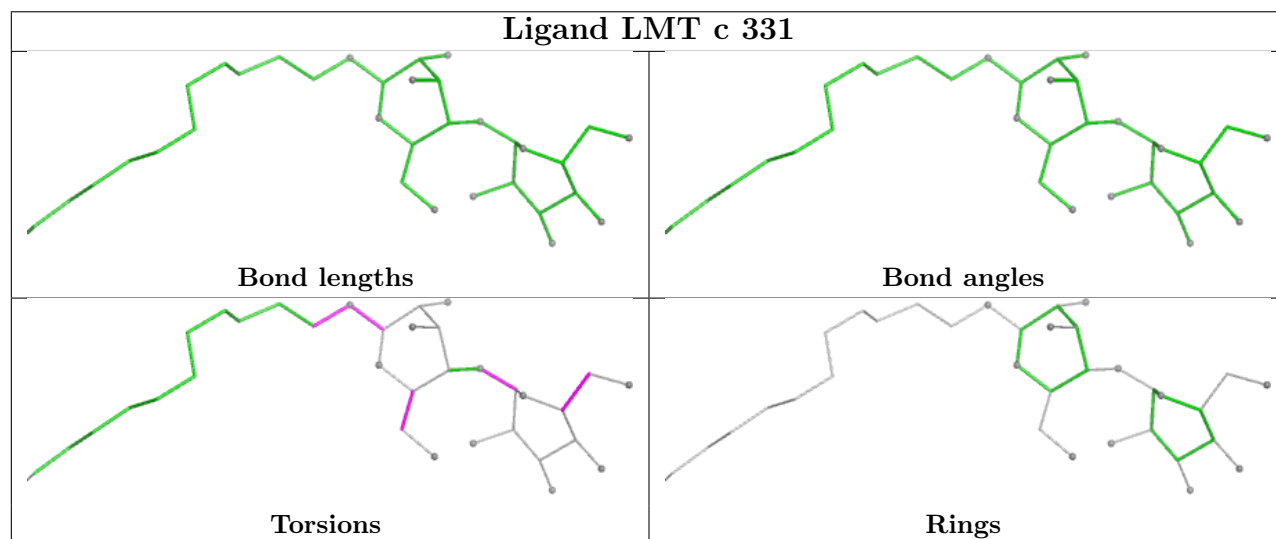
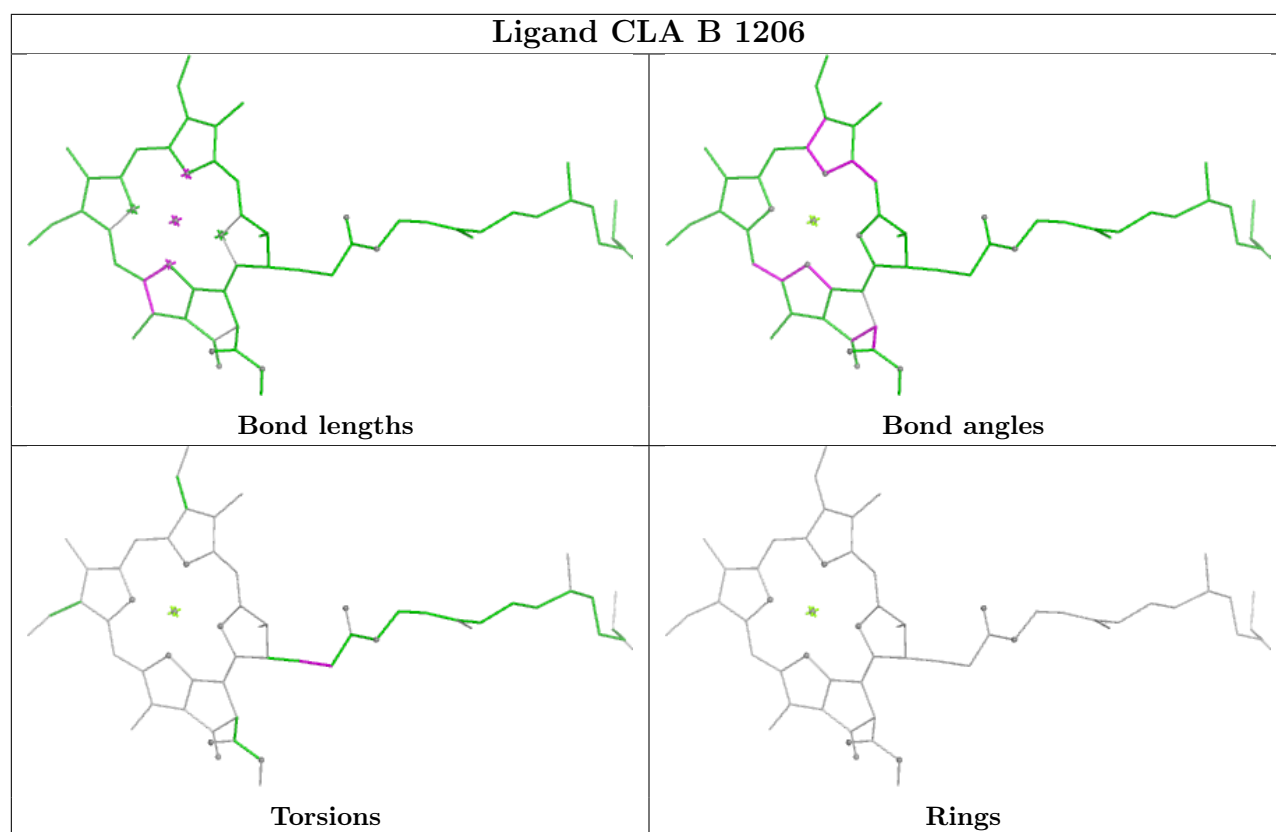


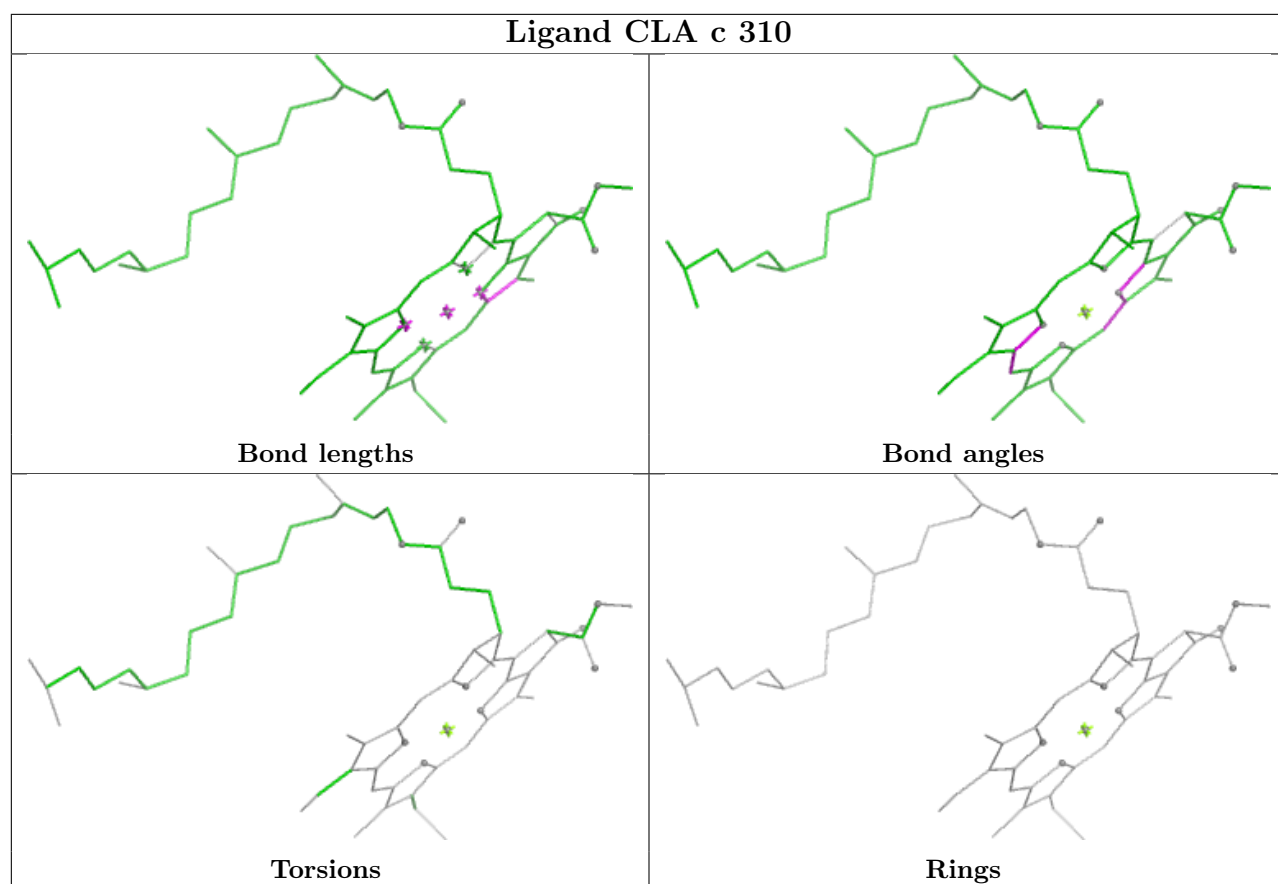


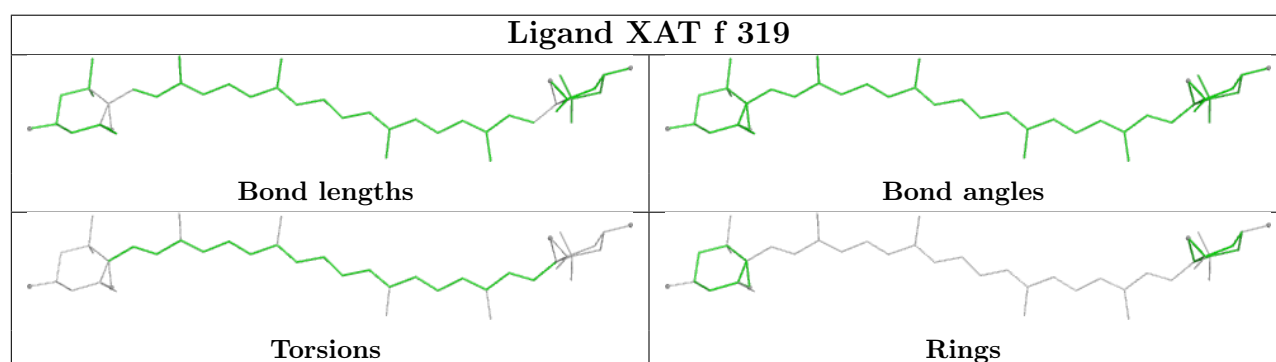
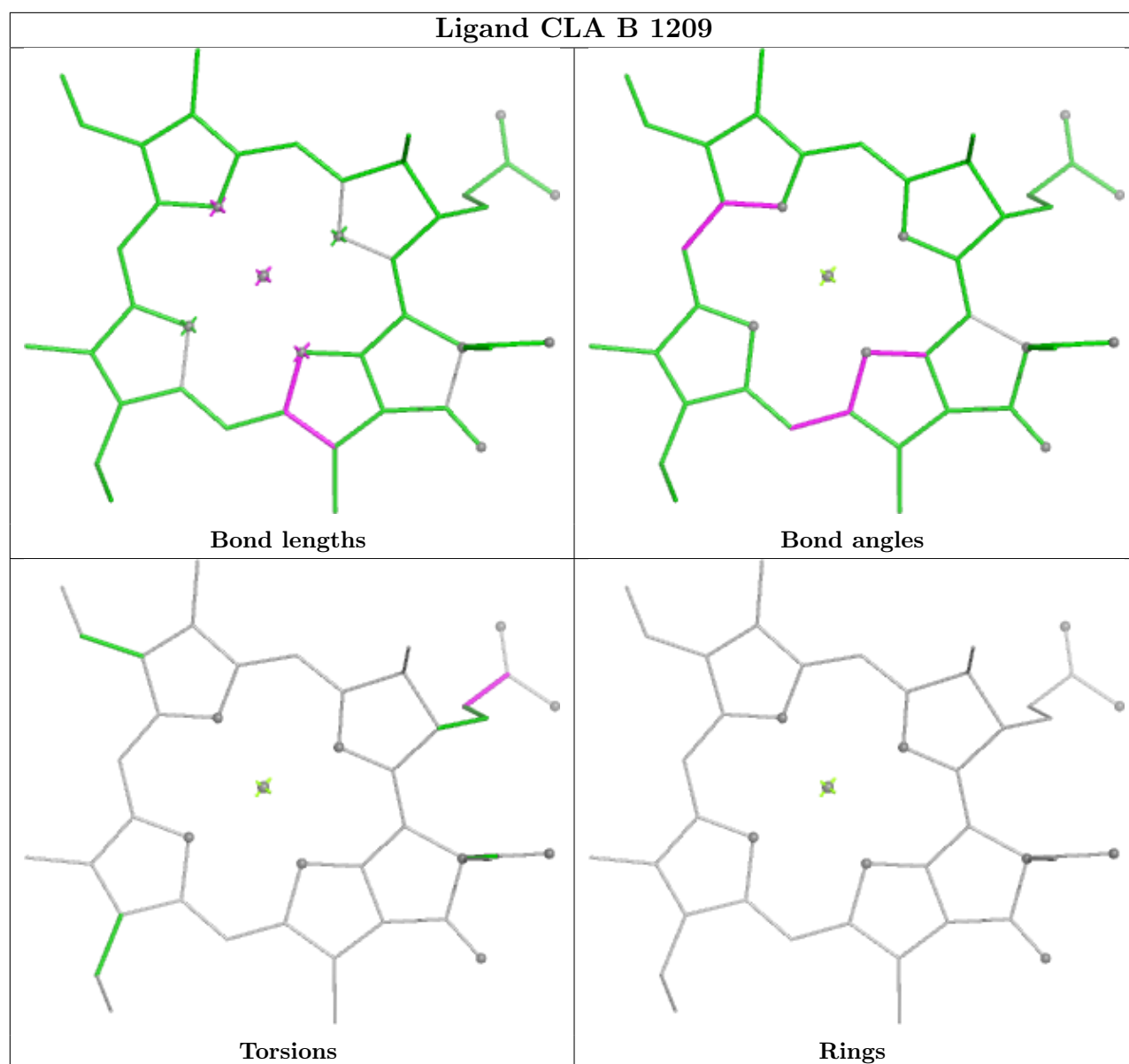
Ligand CLA f 316

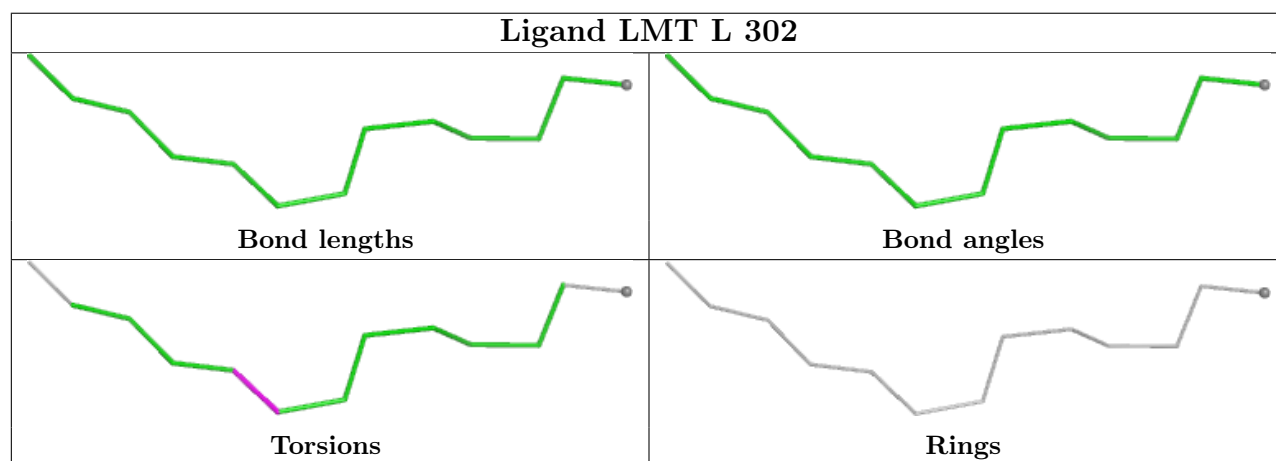
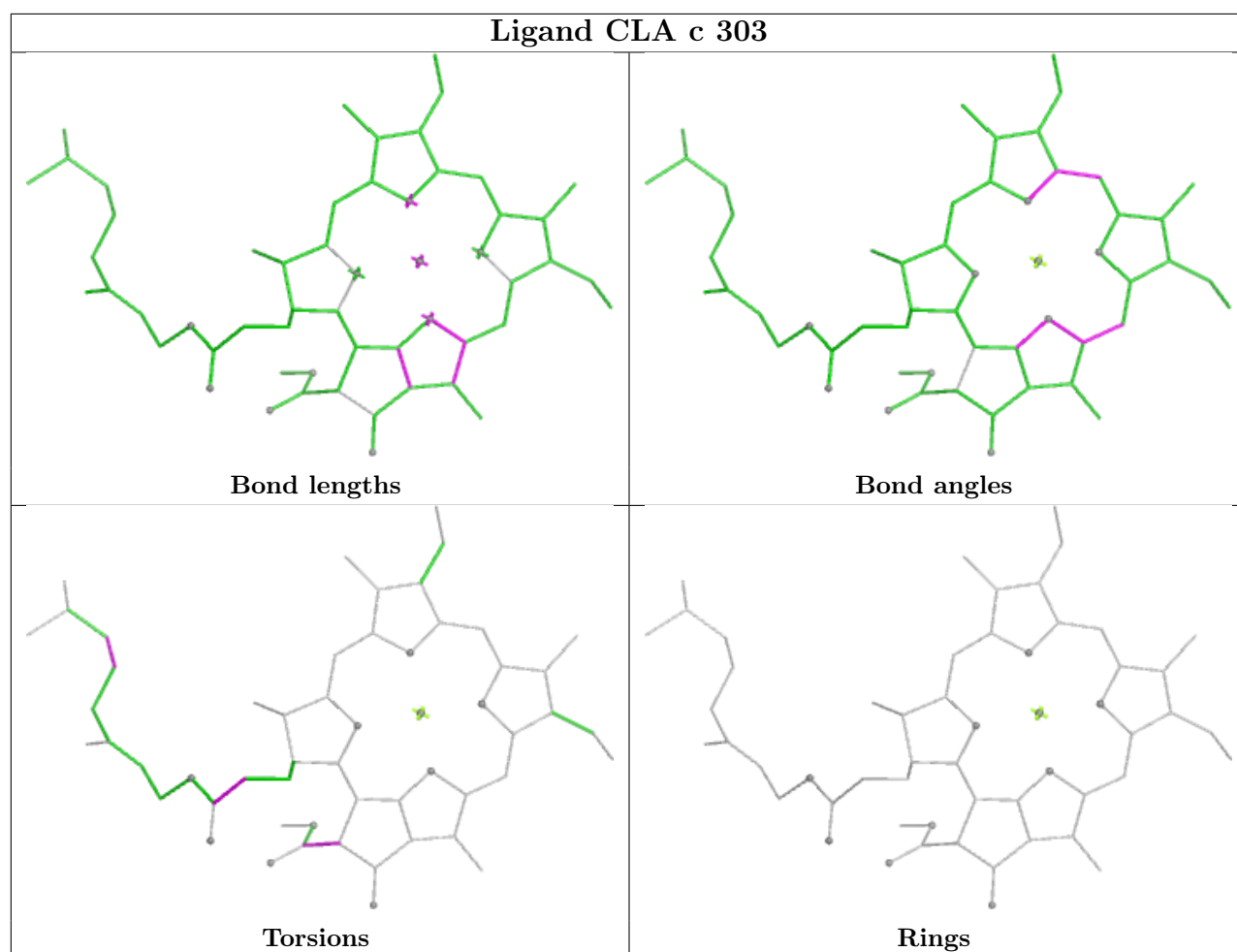


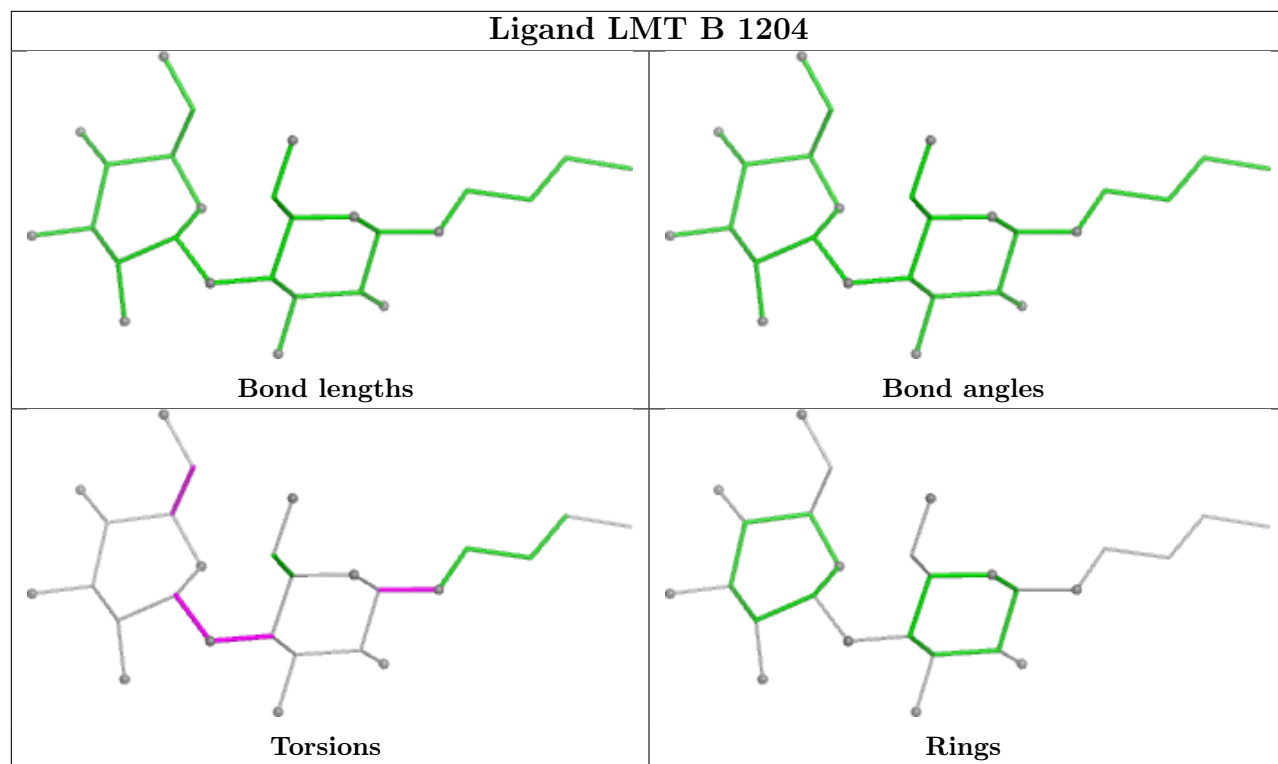


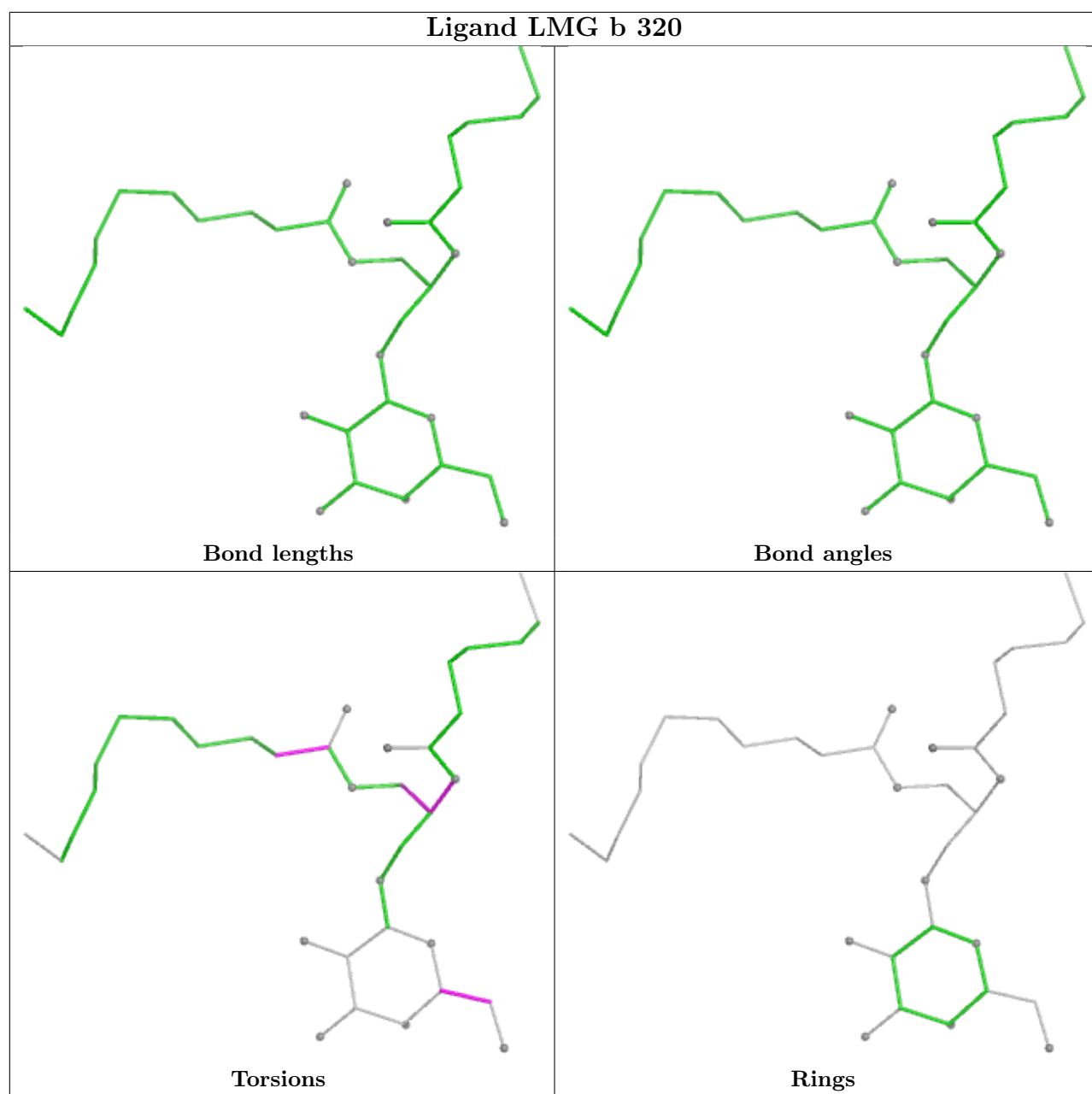


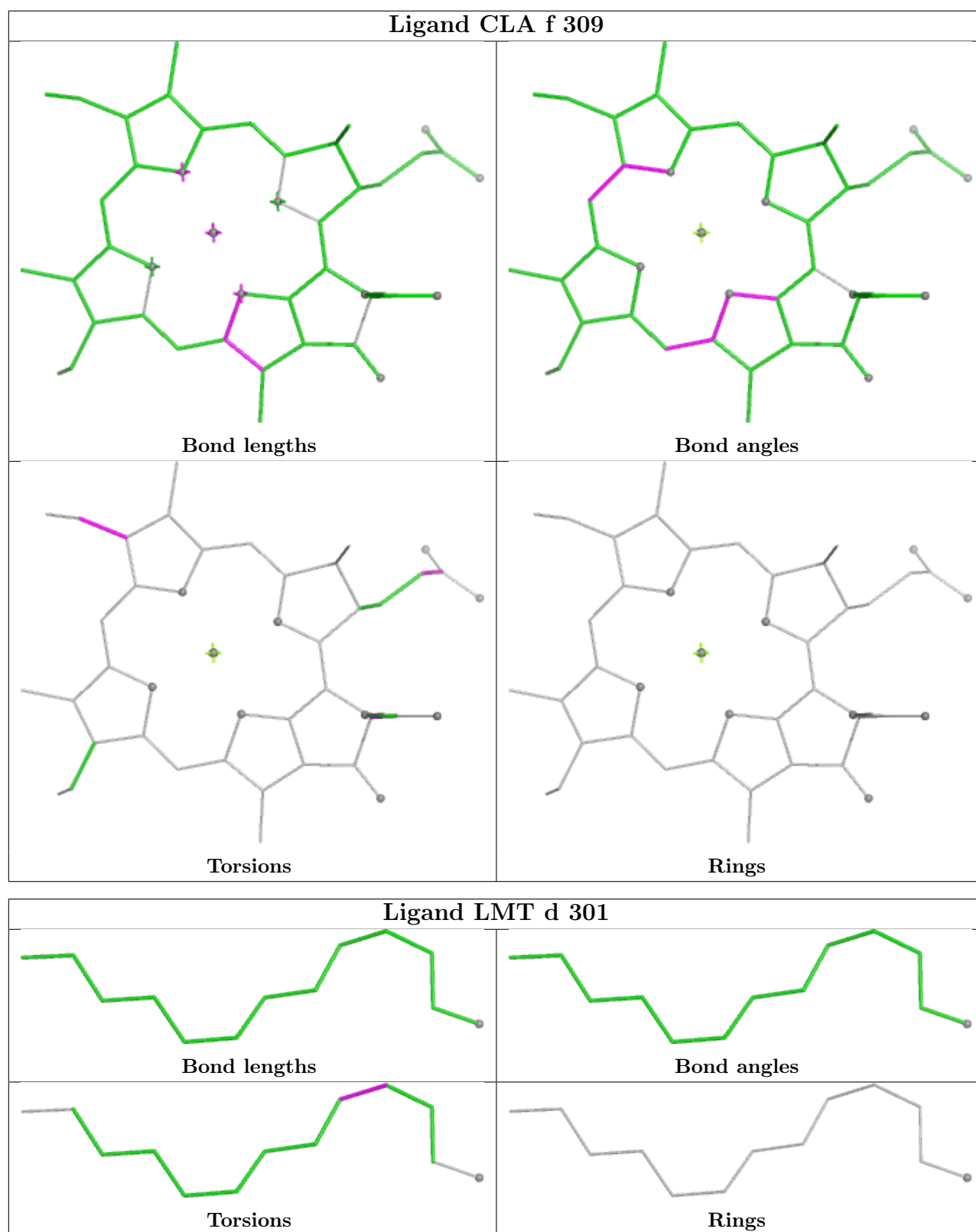




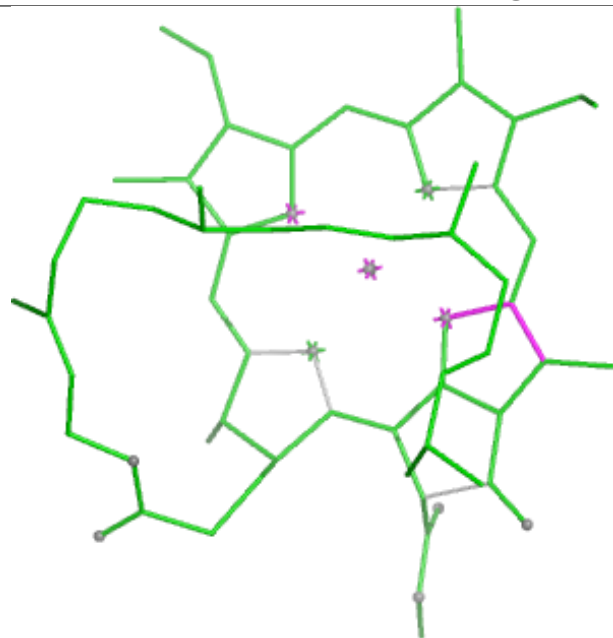




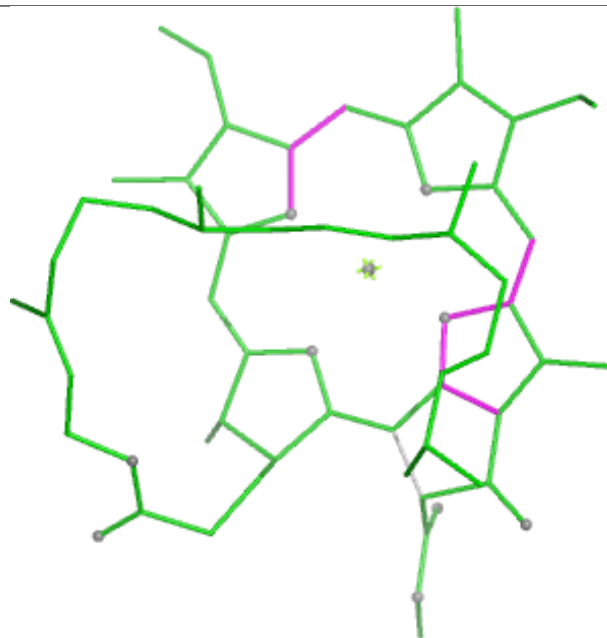




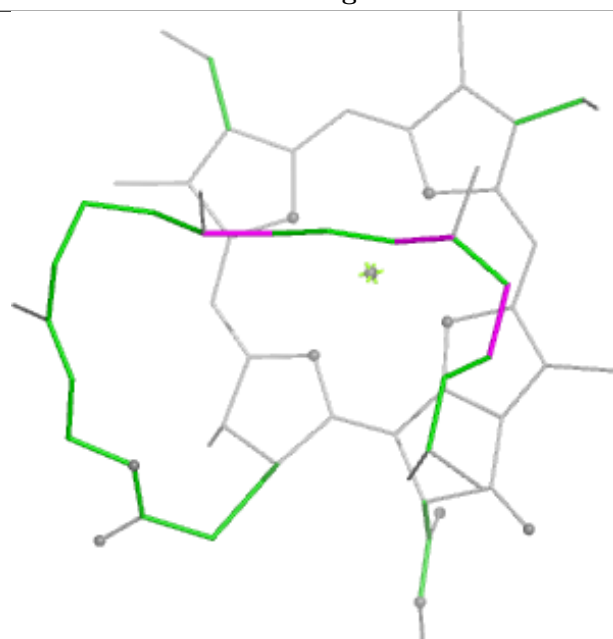
Ligand CLA B 1224



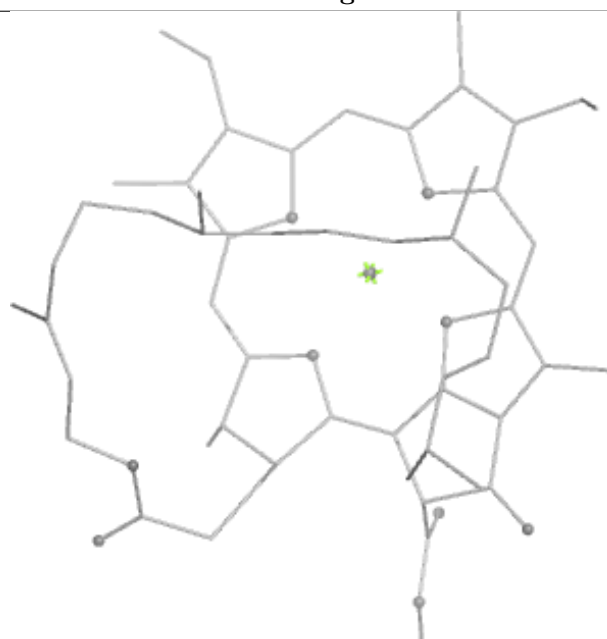
Bond lengths



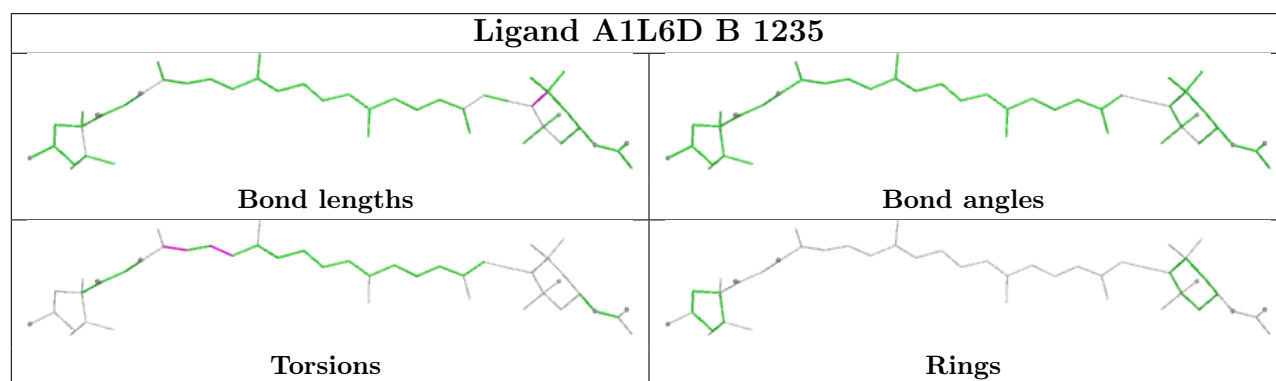
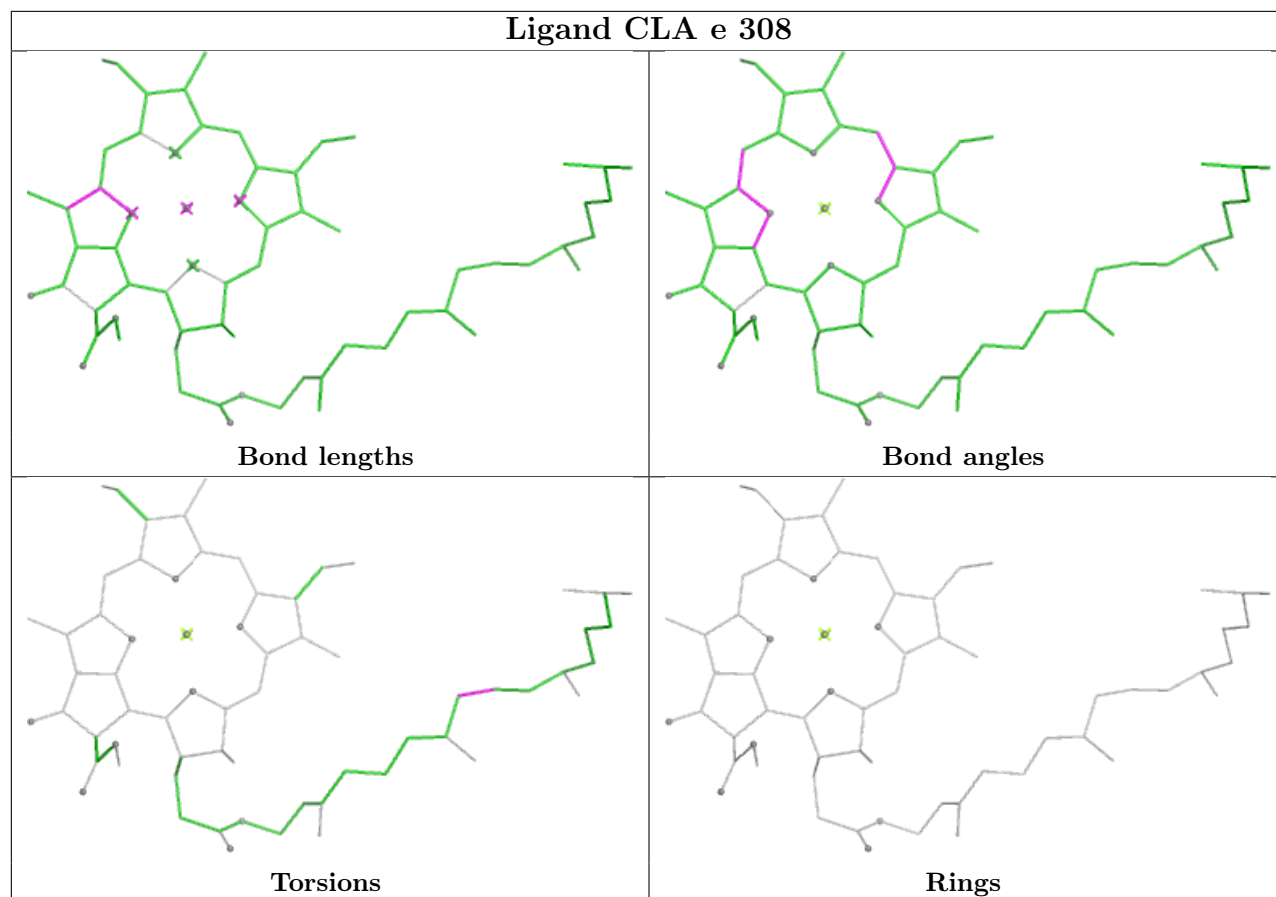
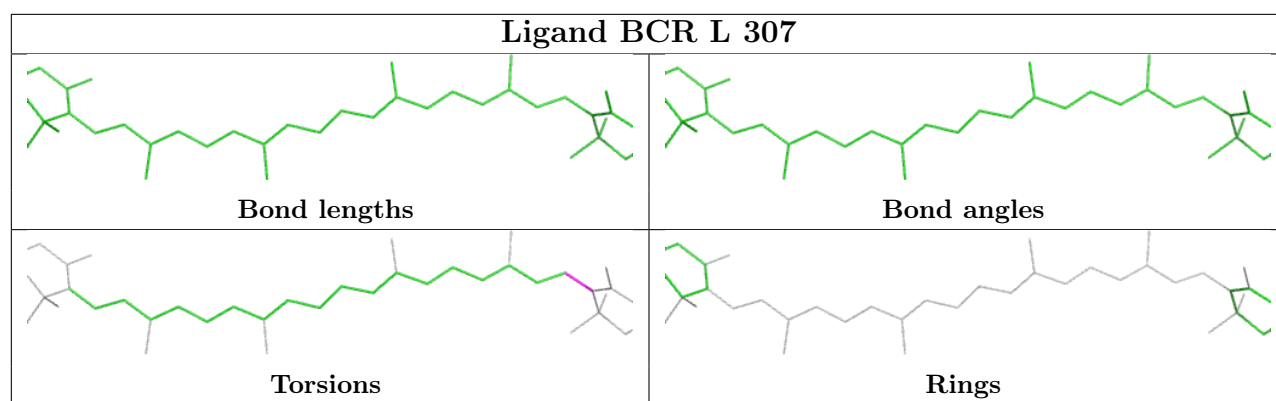
Bond angles

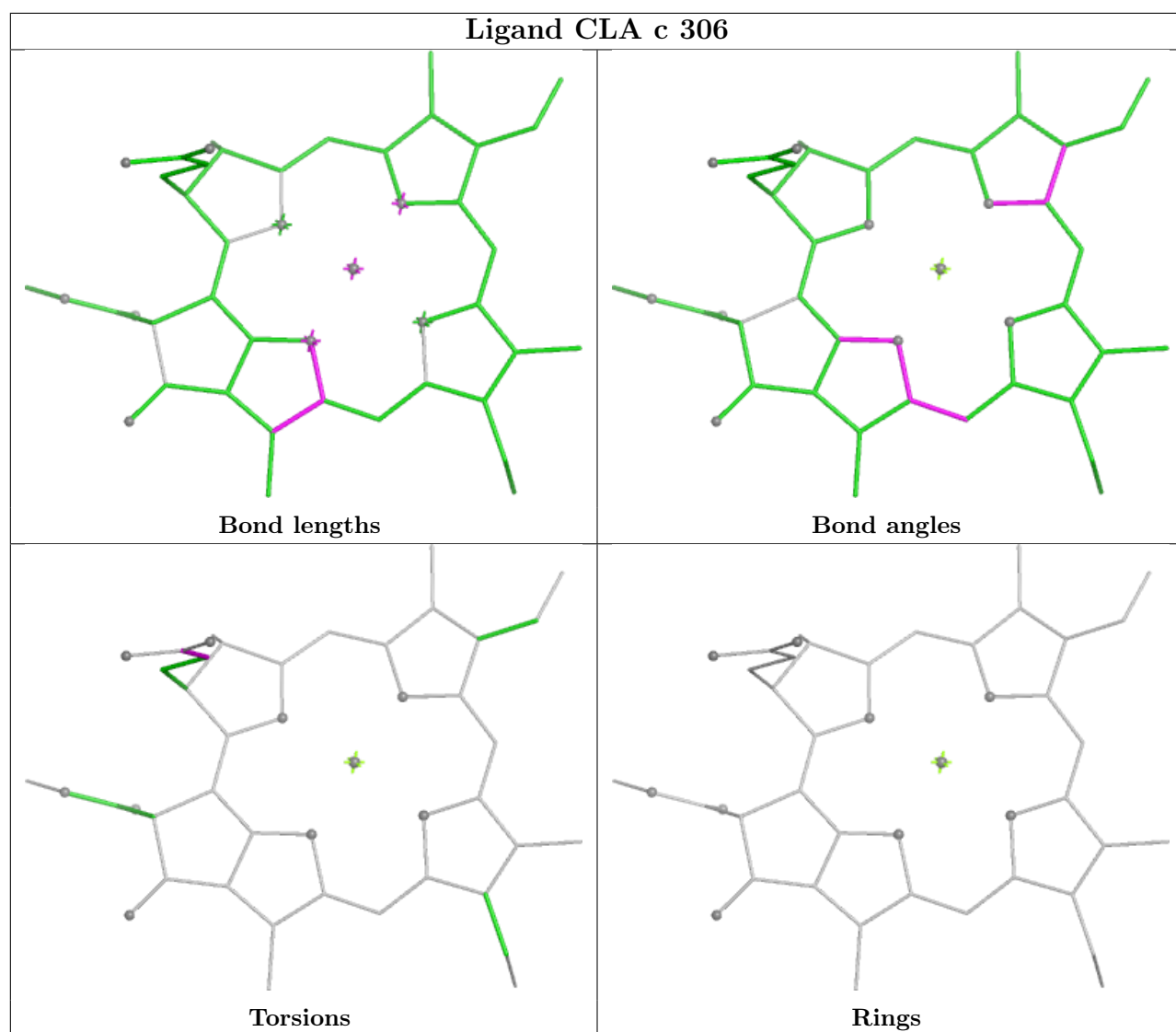


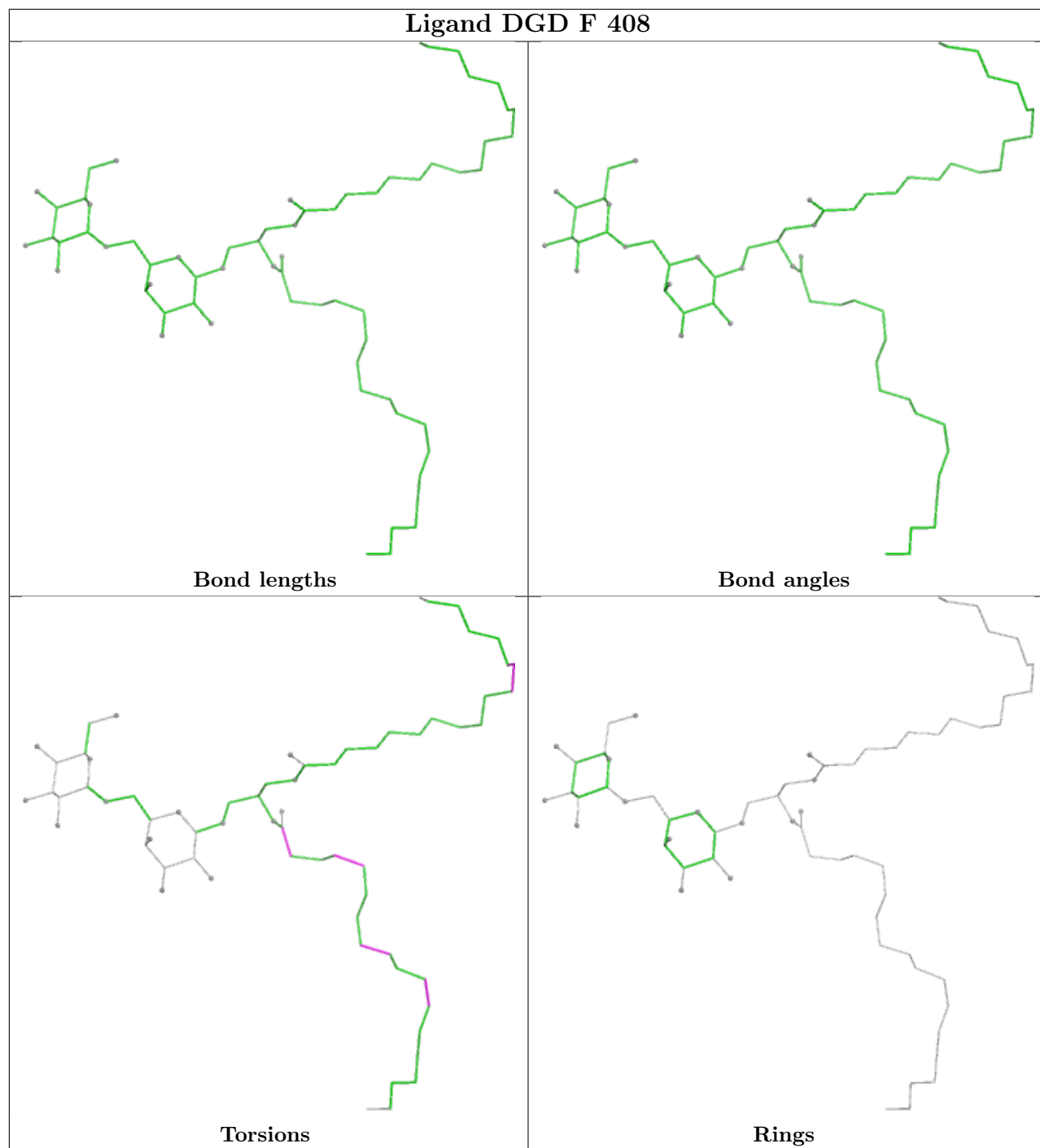
Torsions

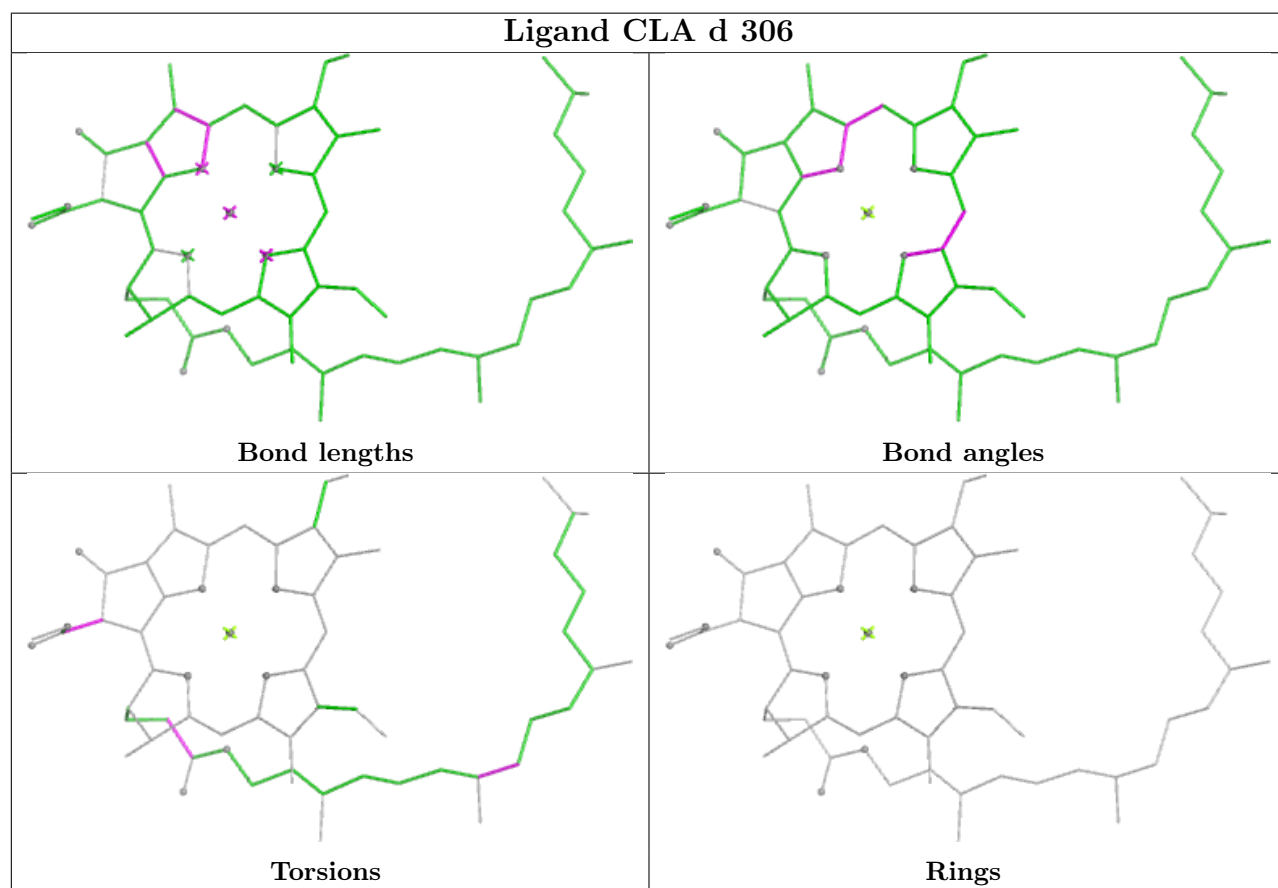
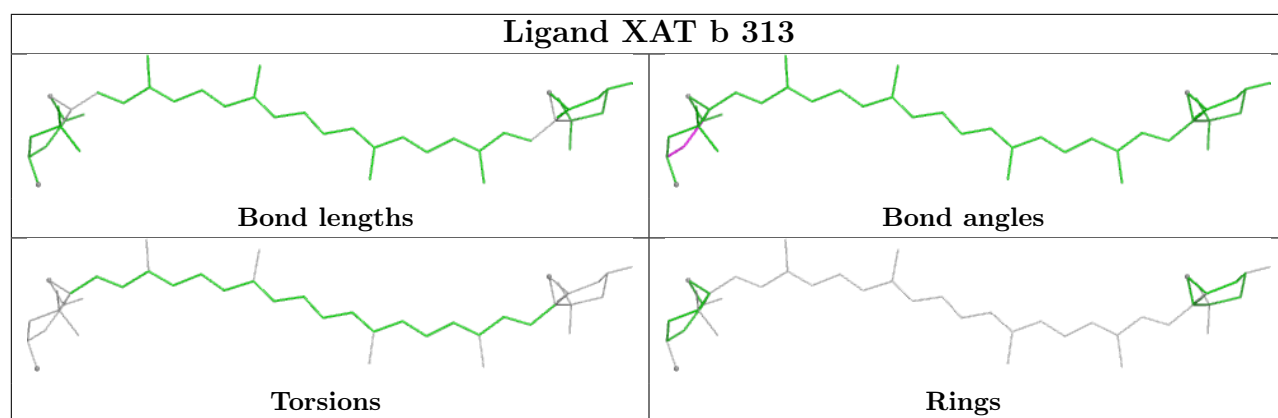


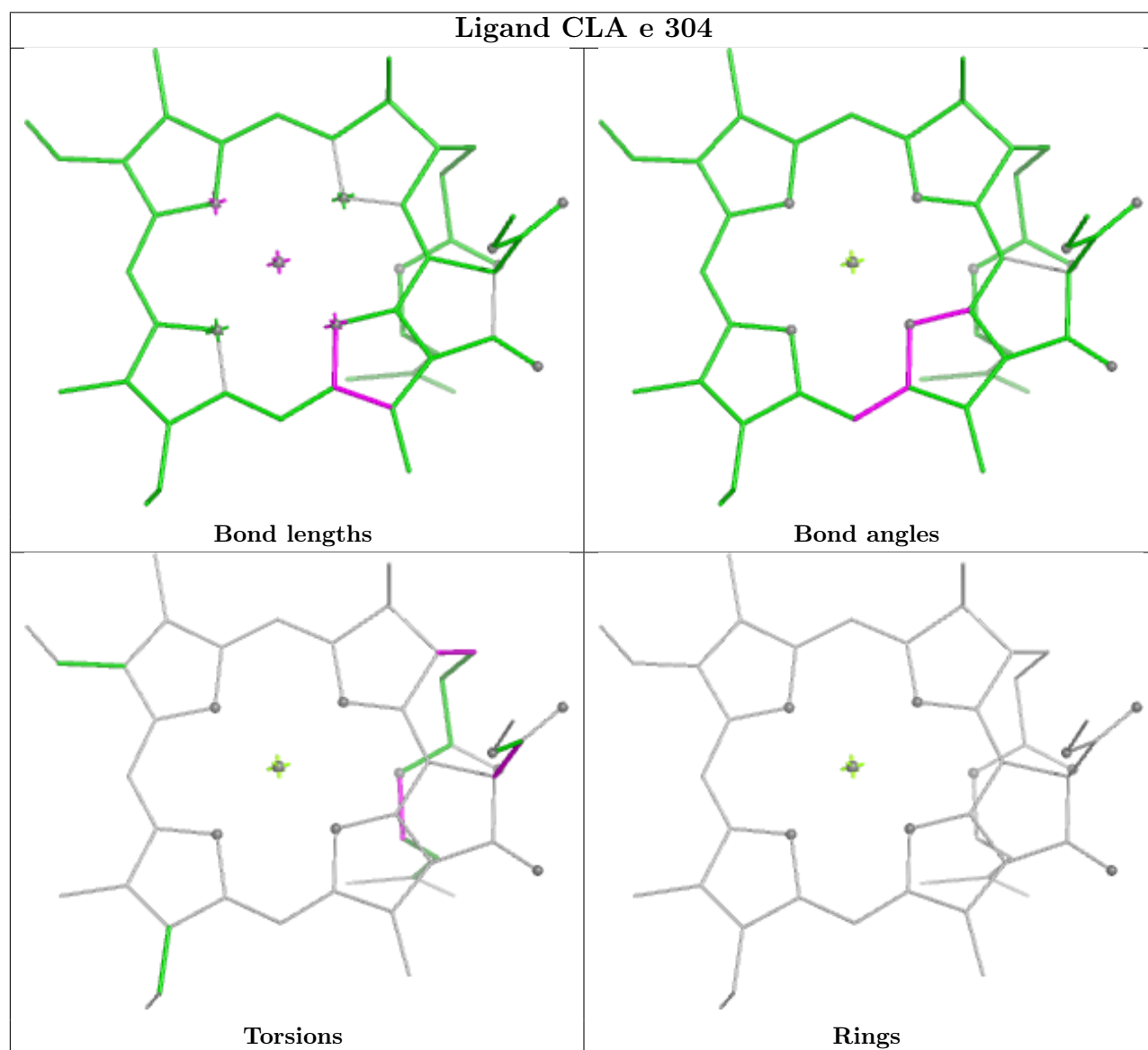
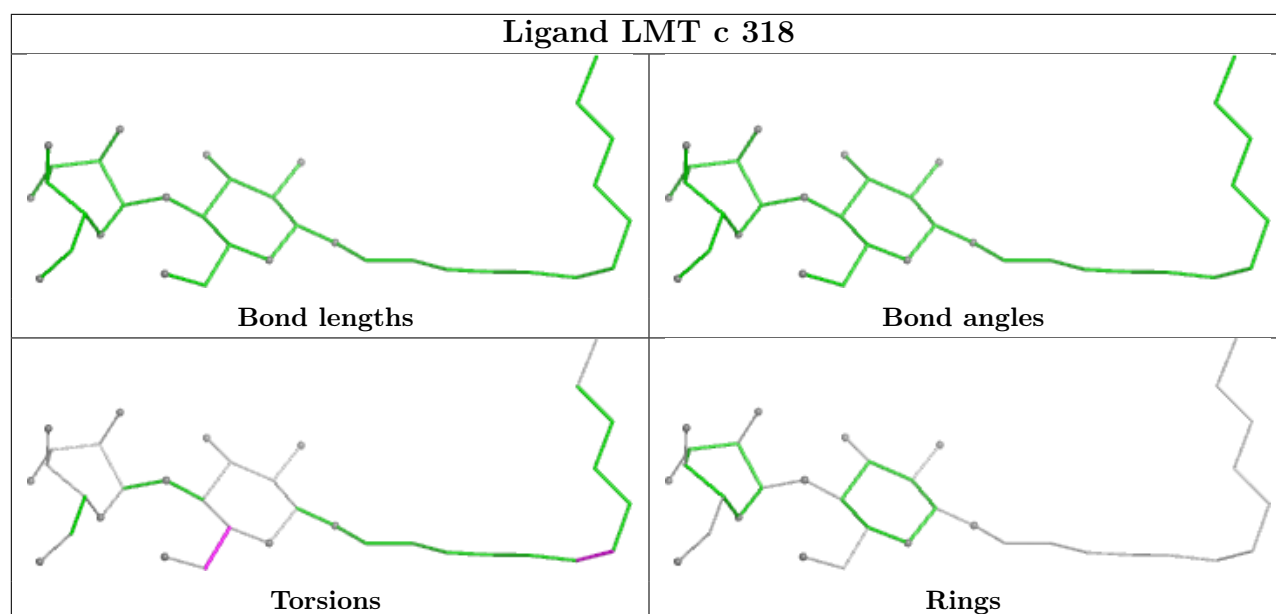
Rings

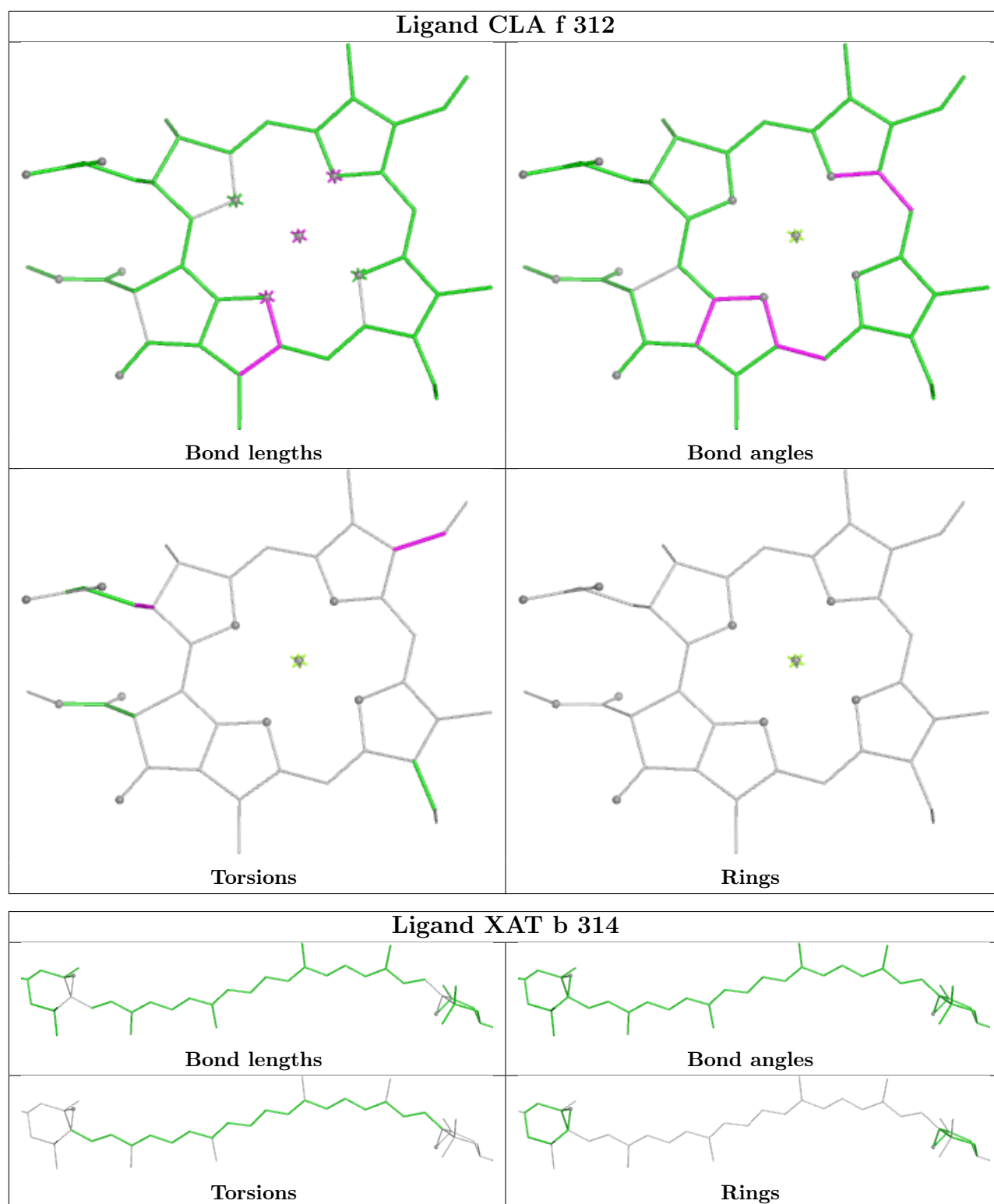


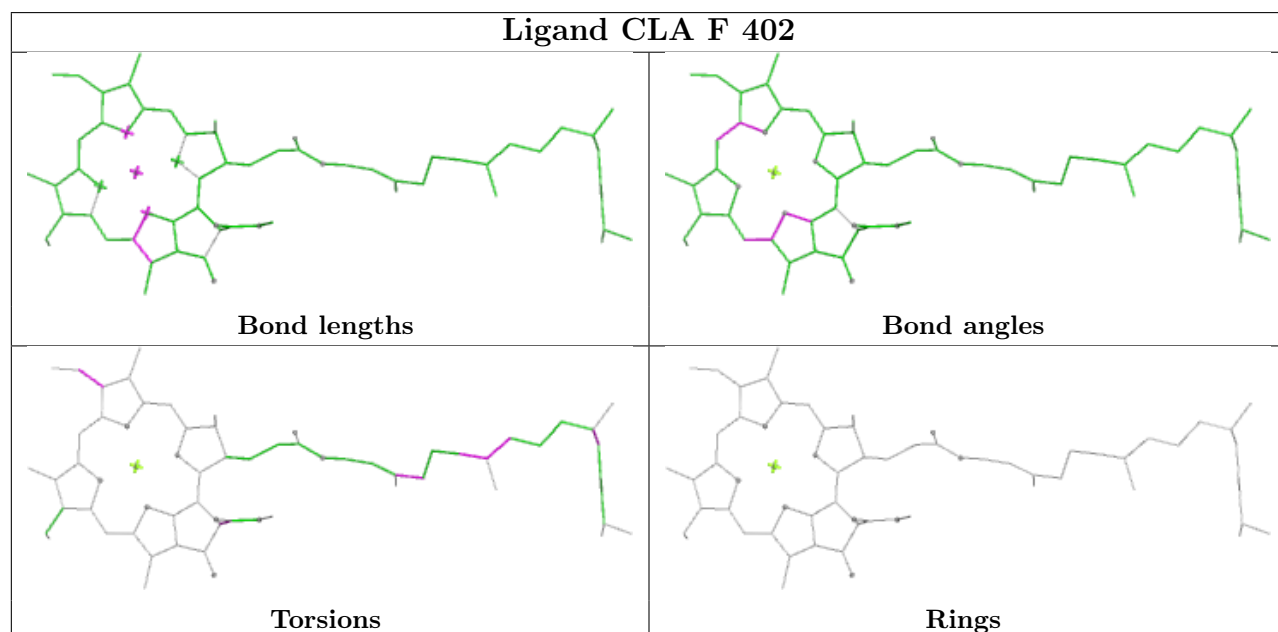
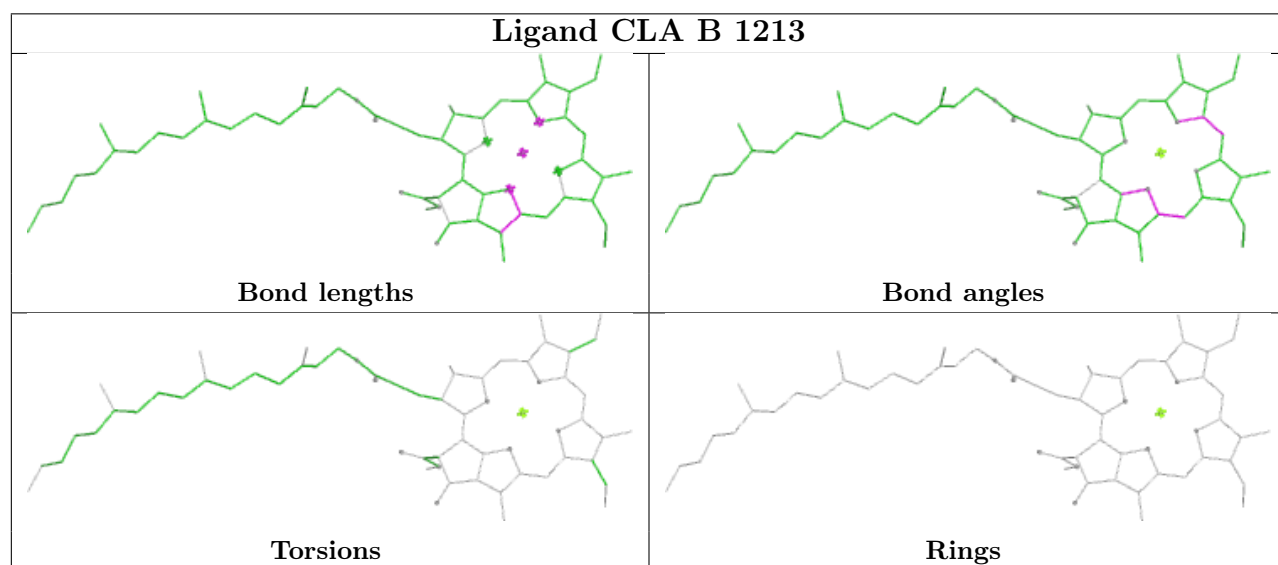
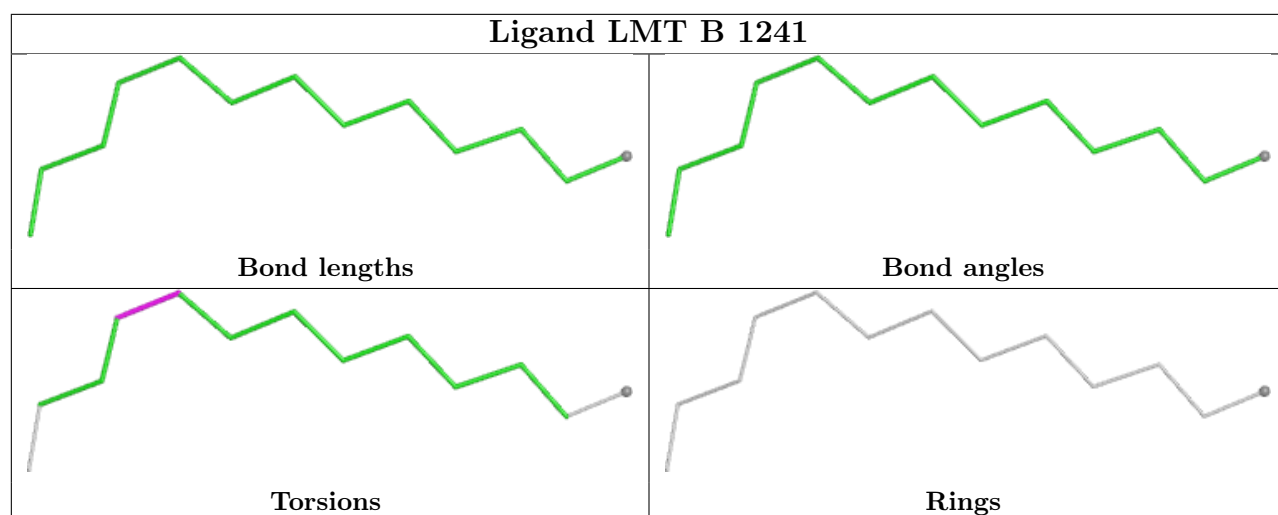




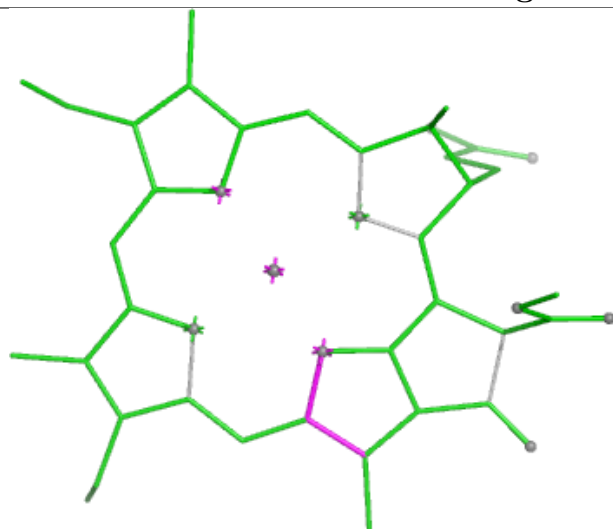




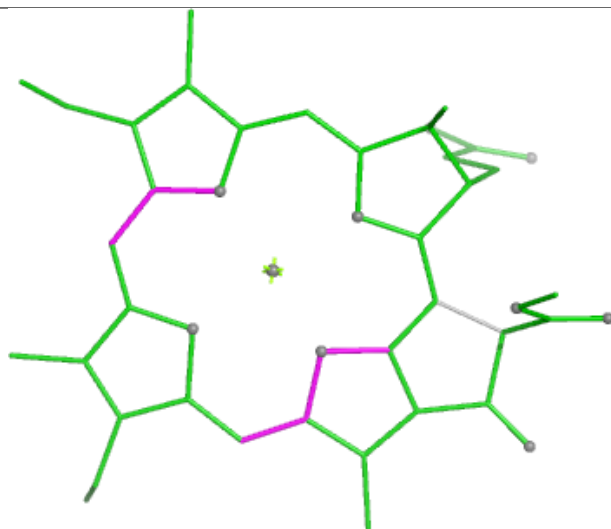




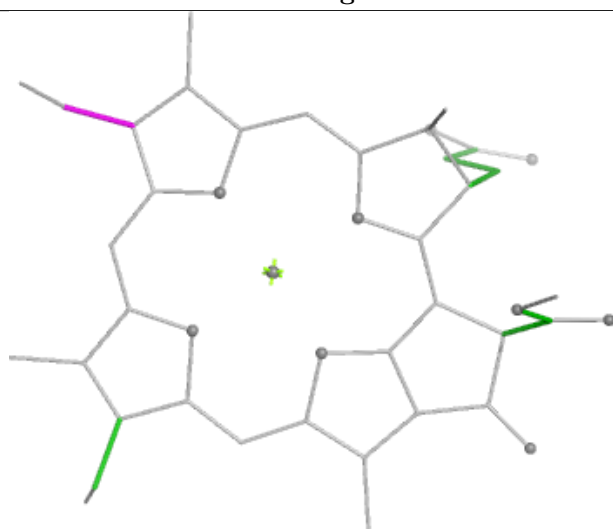
Ligand CLA F 405



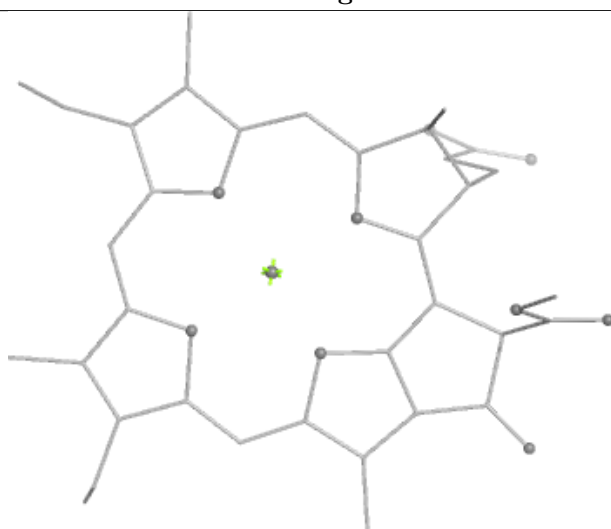
Bond lengths



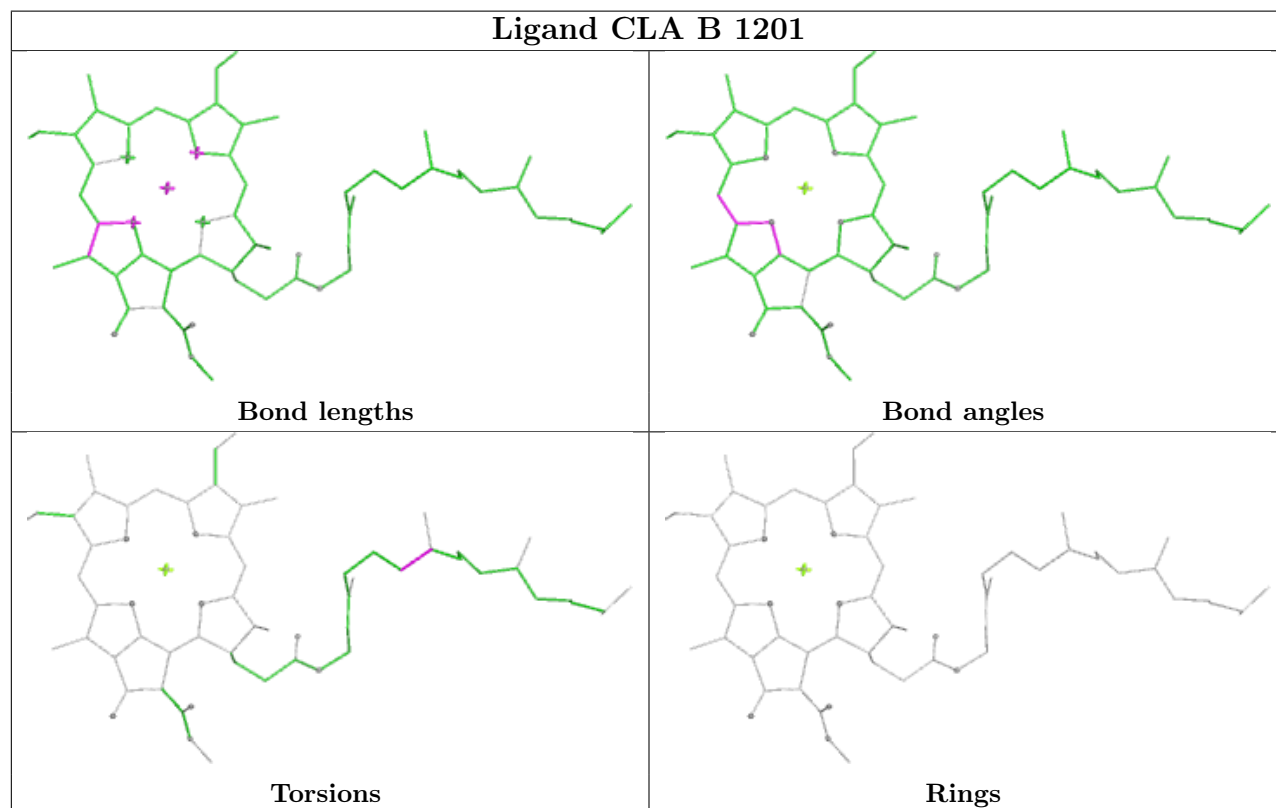
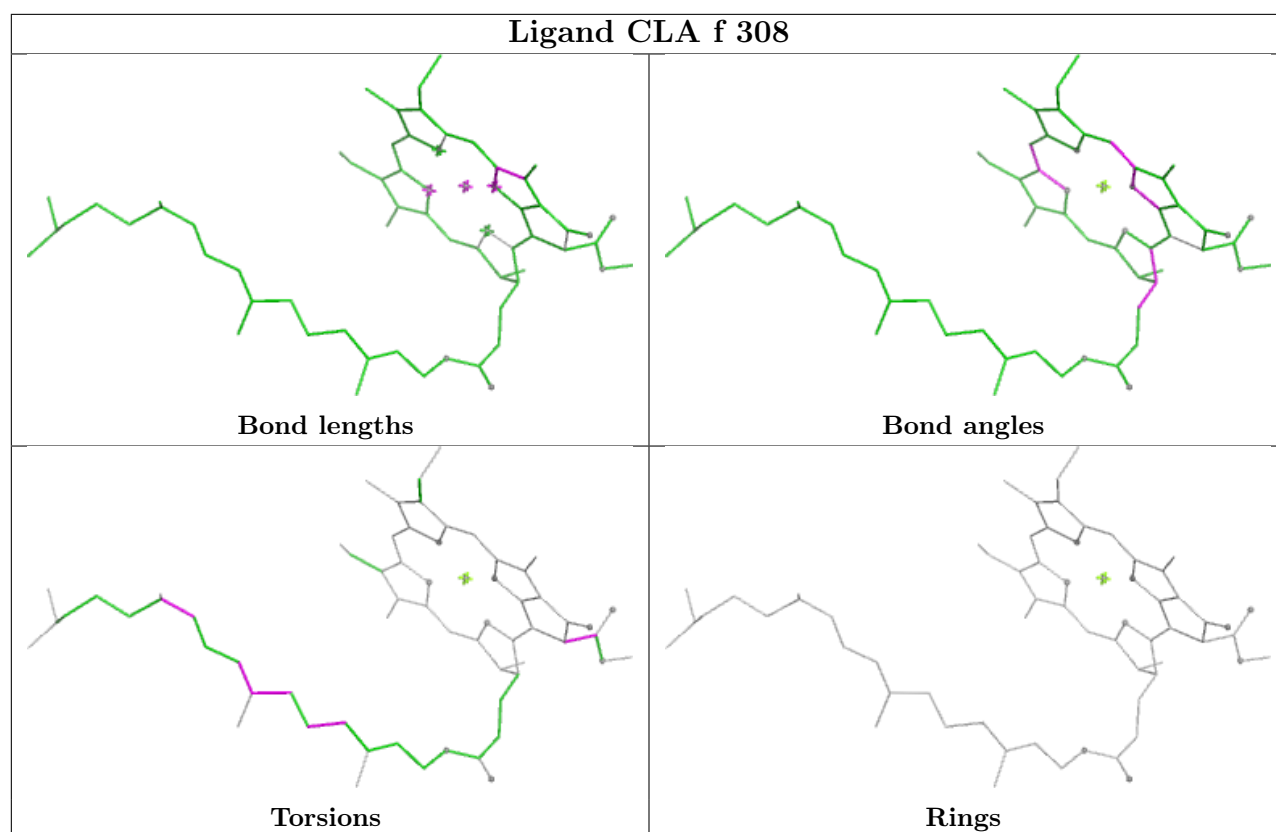
Bond angles

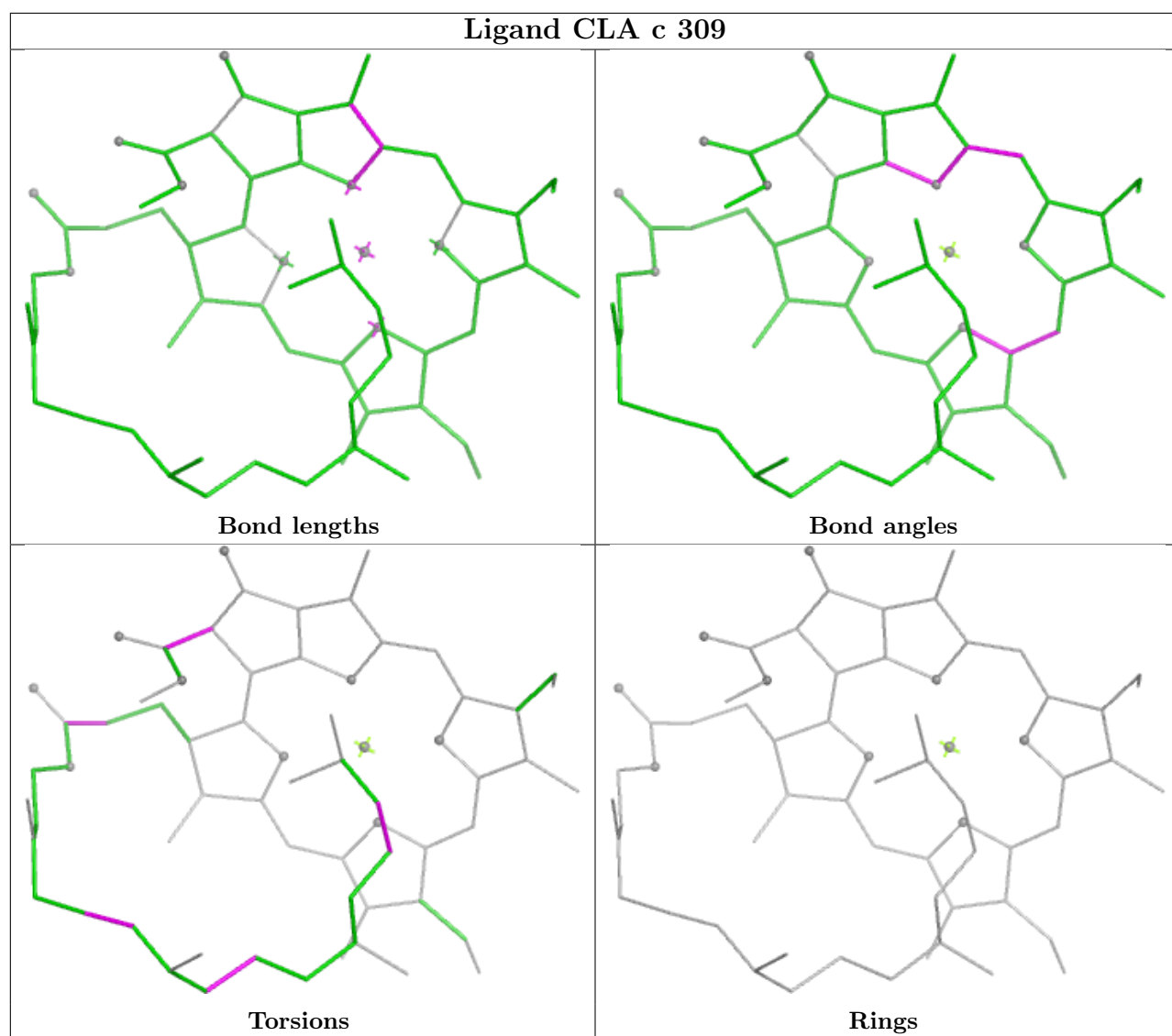


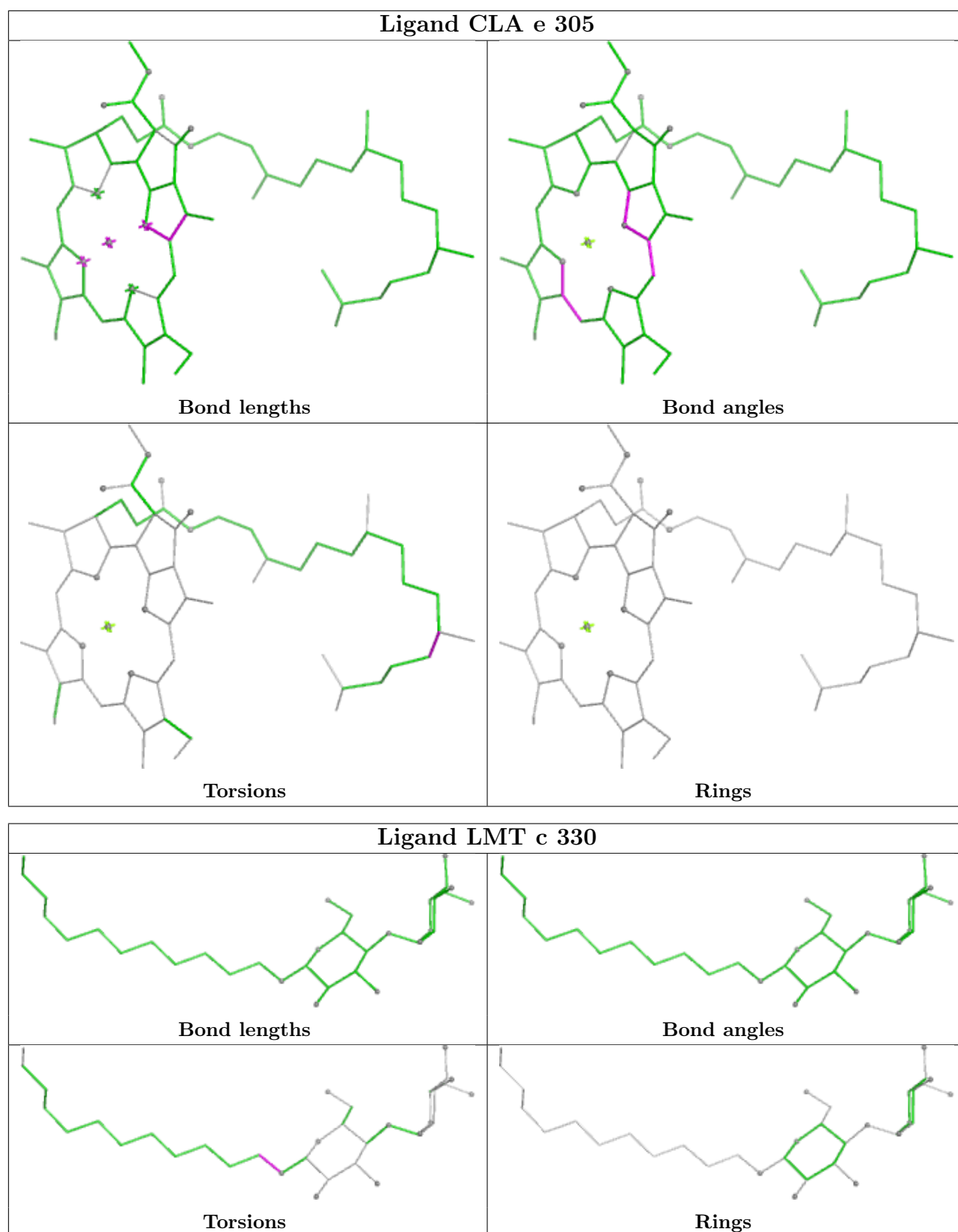
Torsions

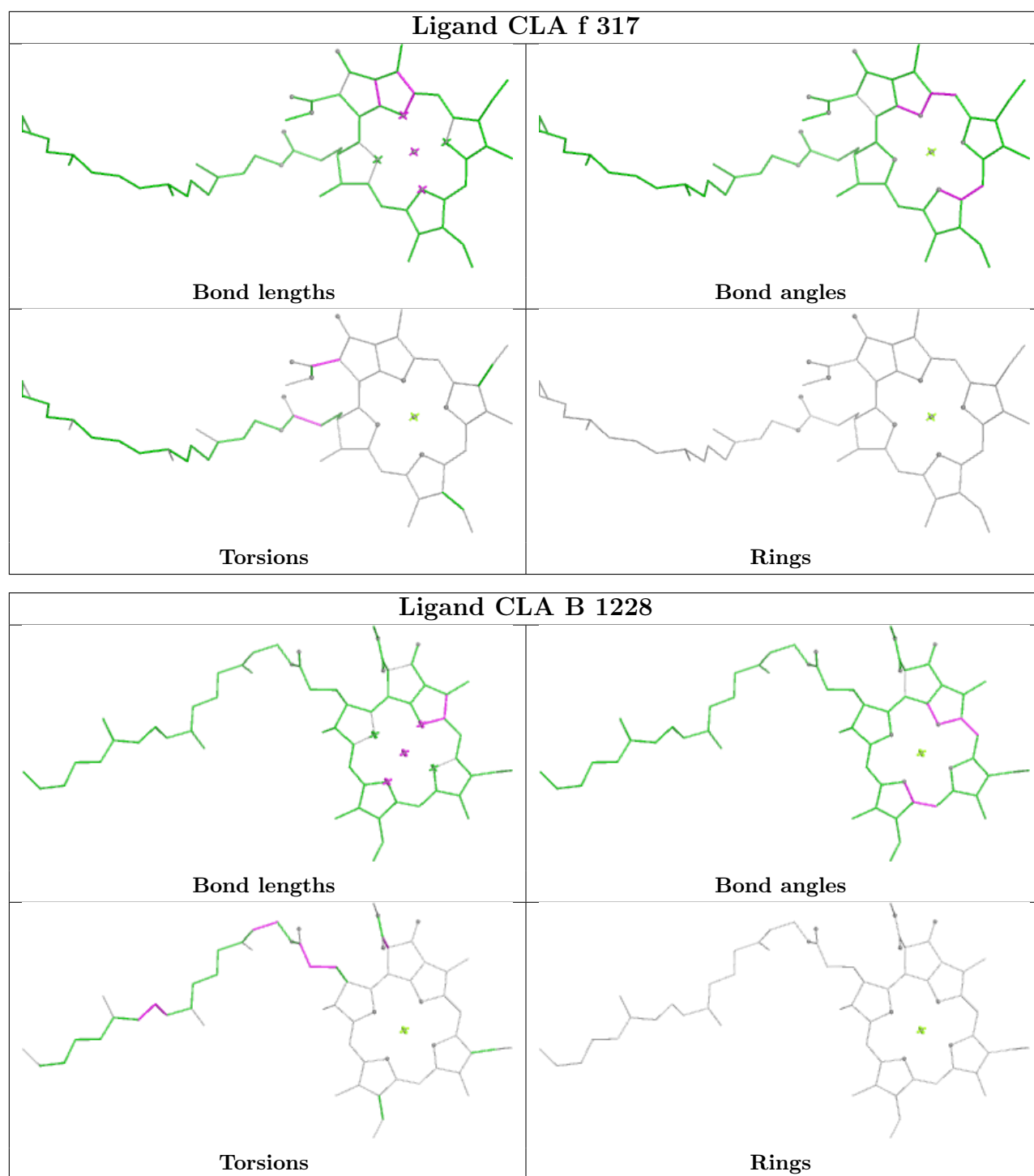


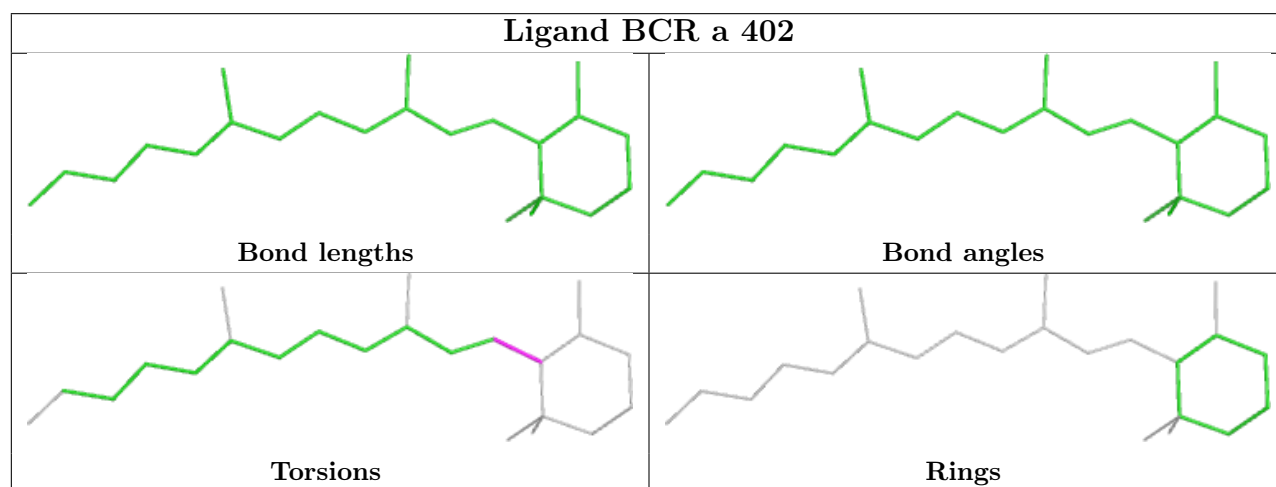
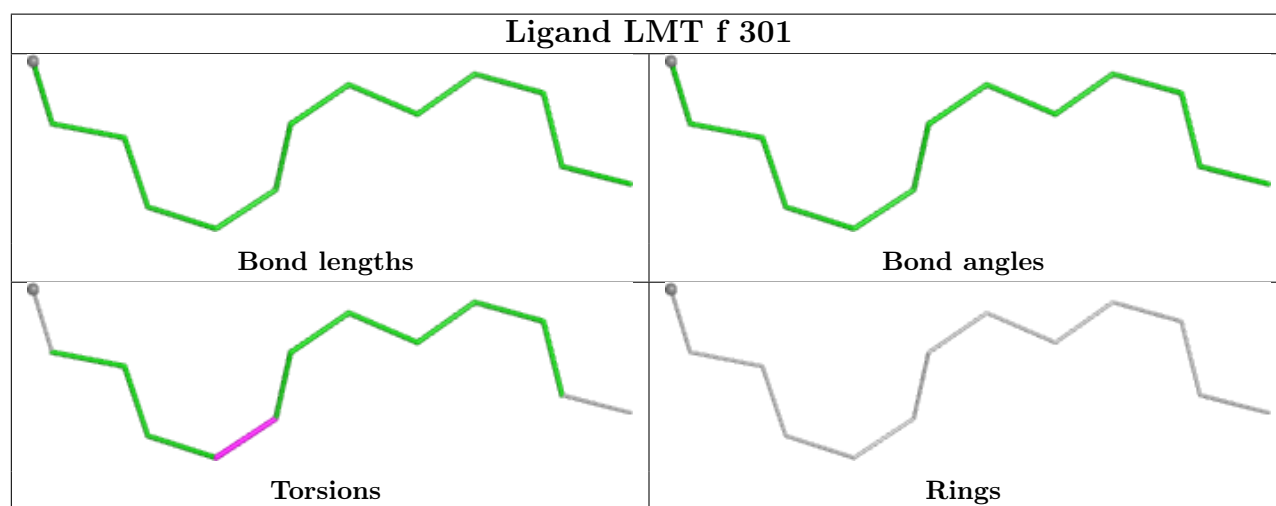
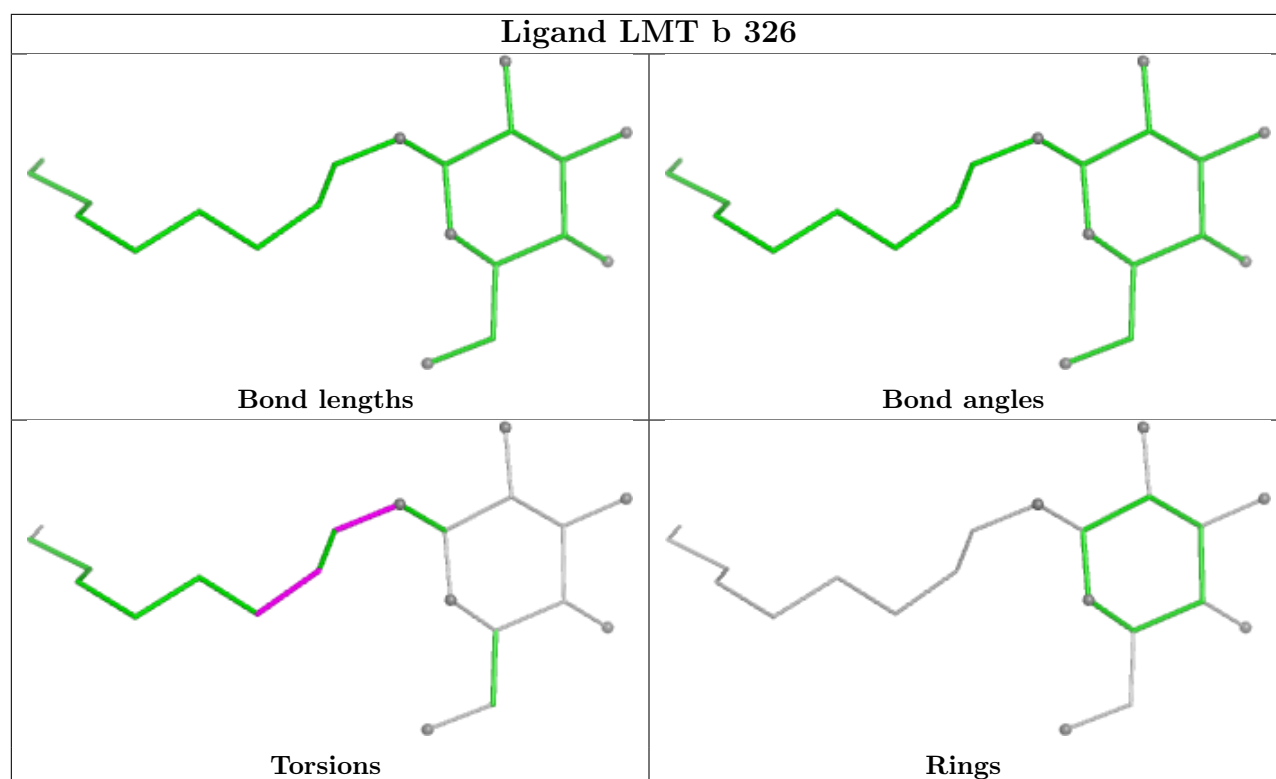
Rings

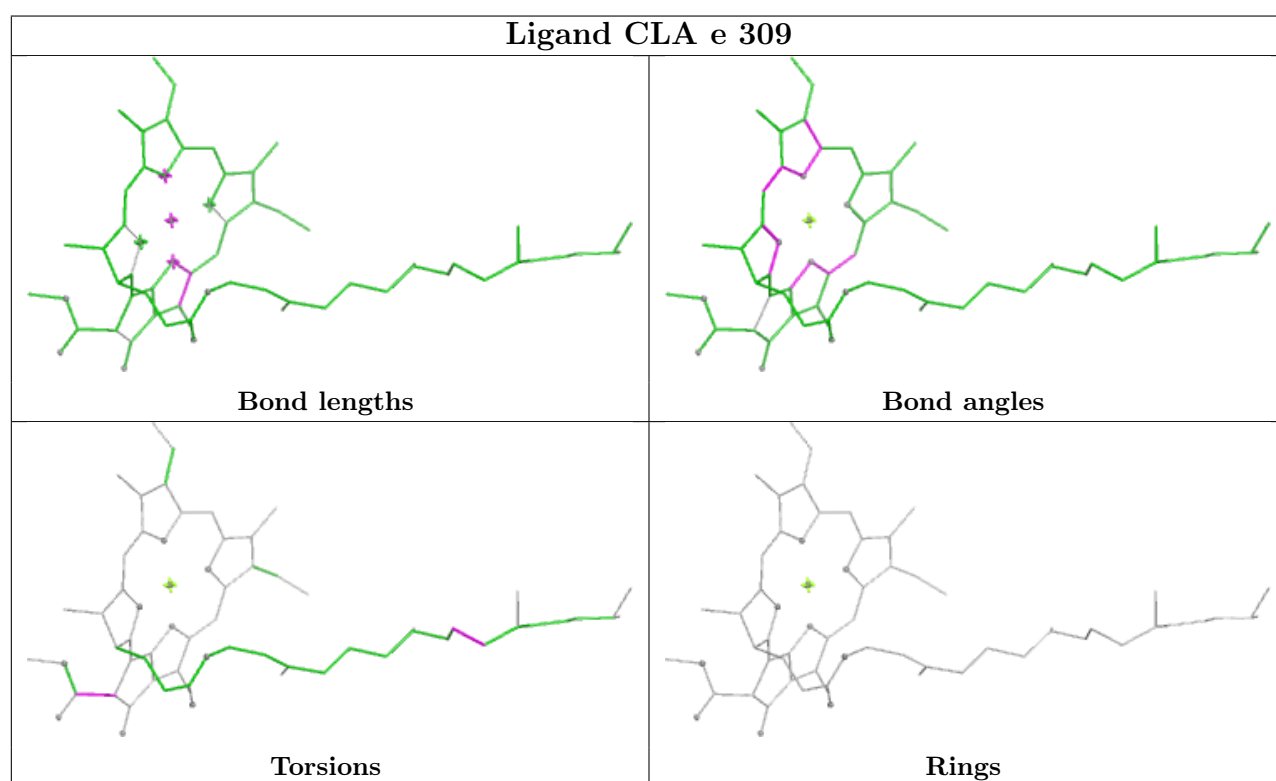
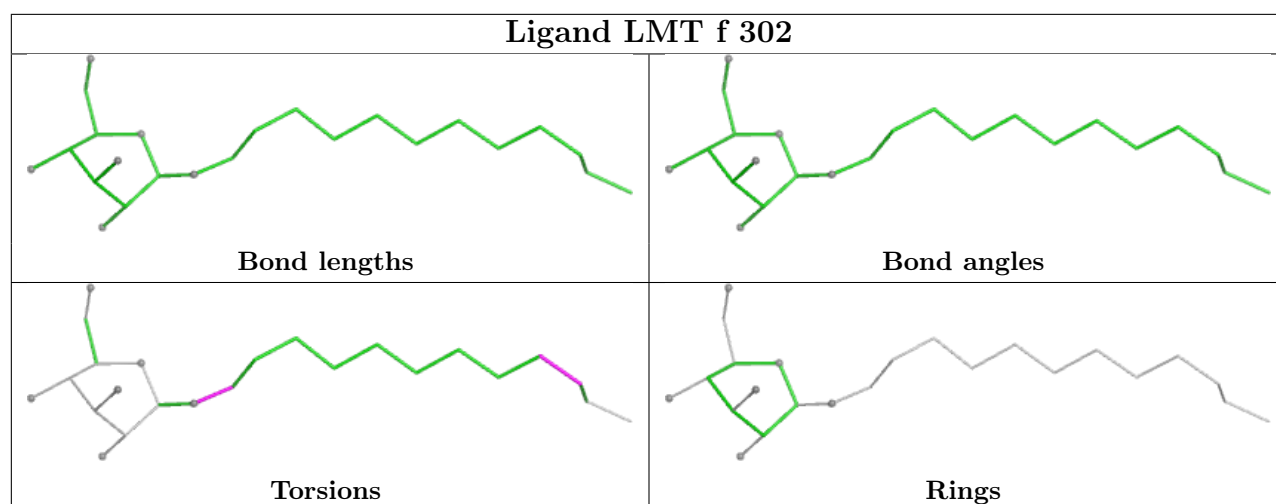


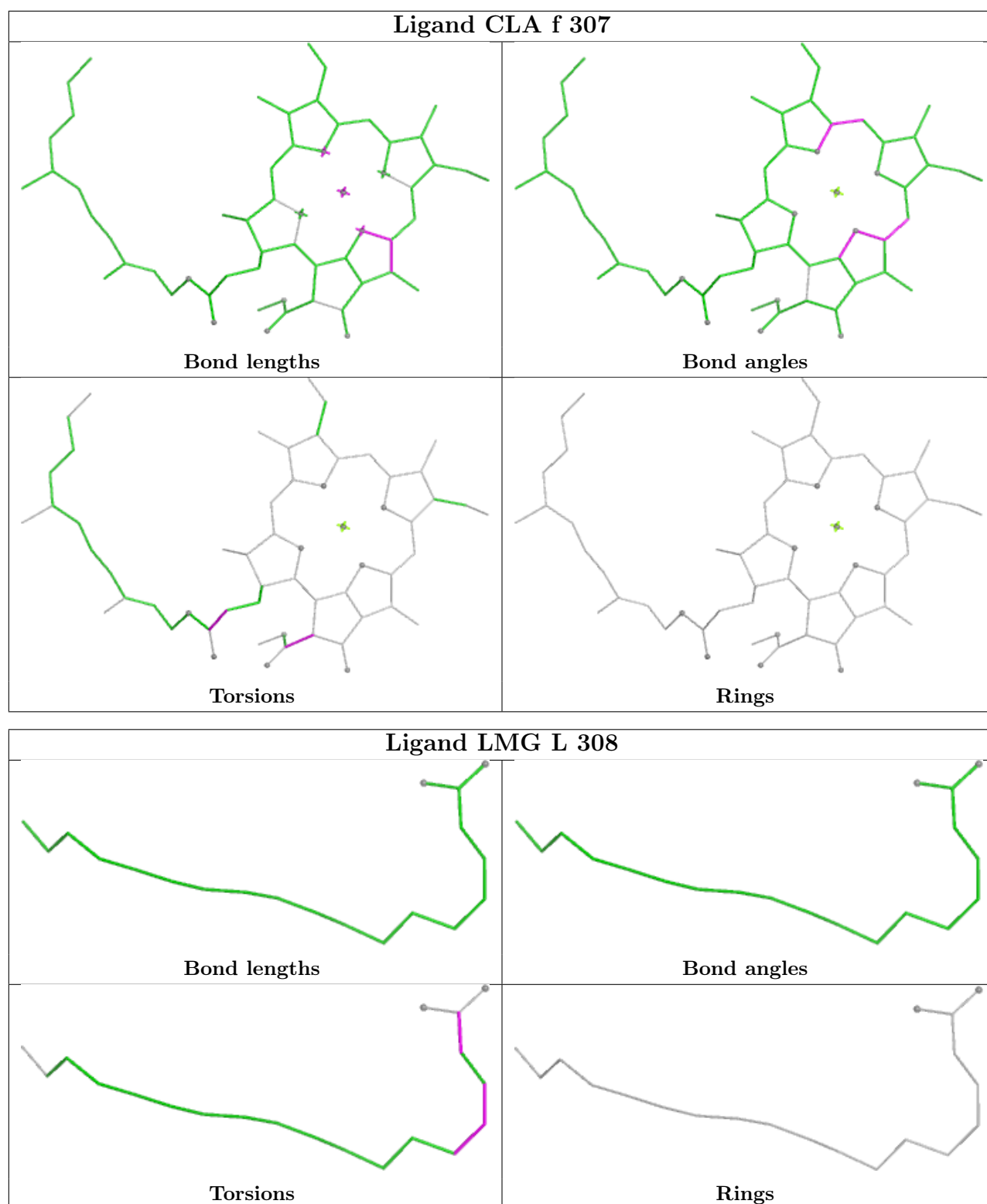




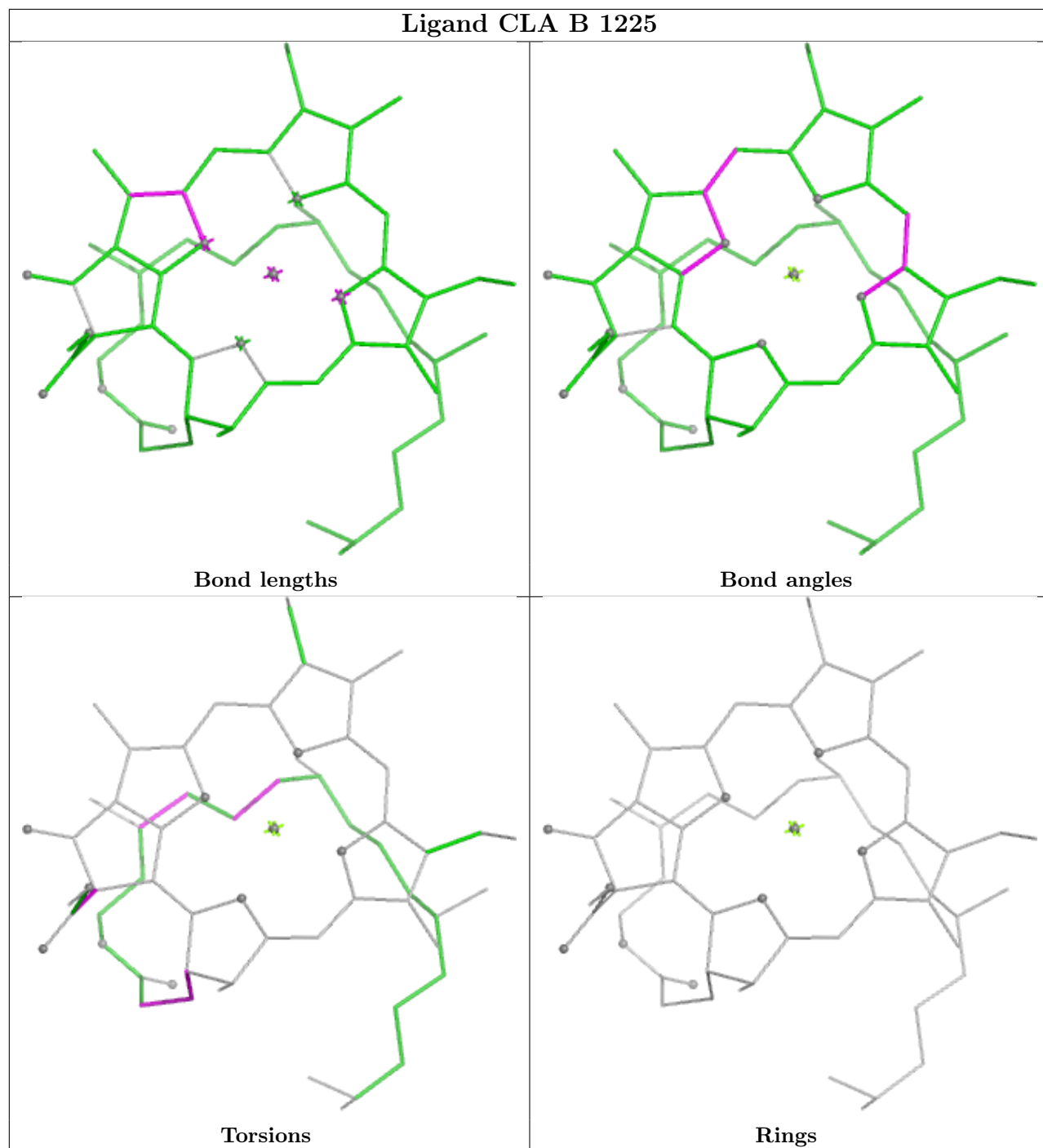


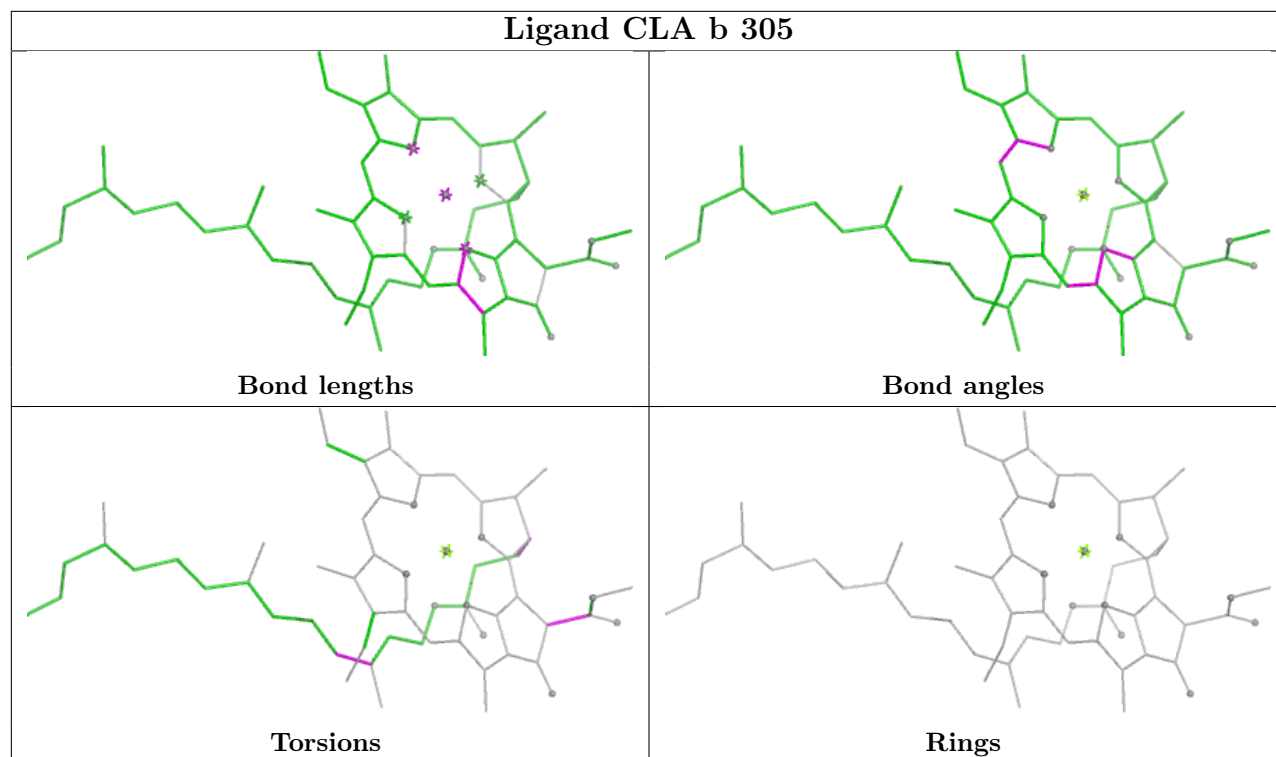
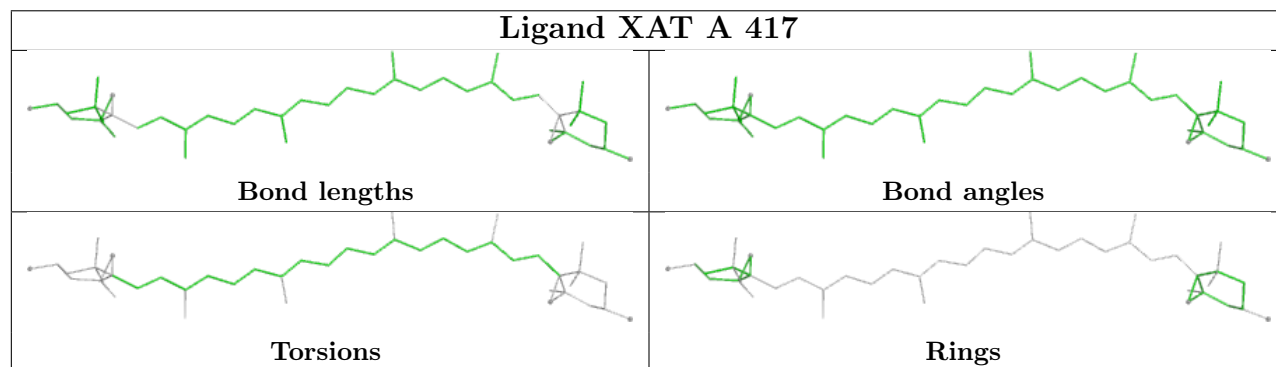


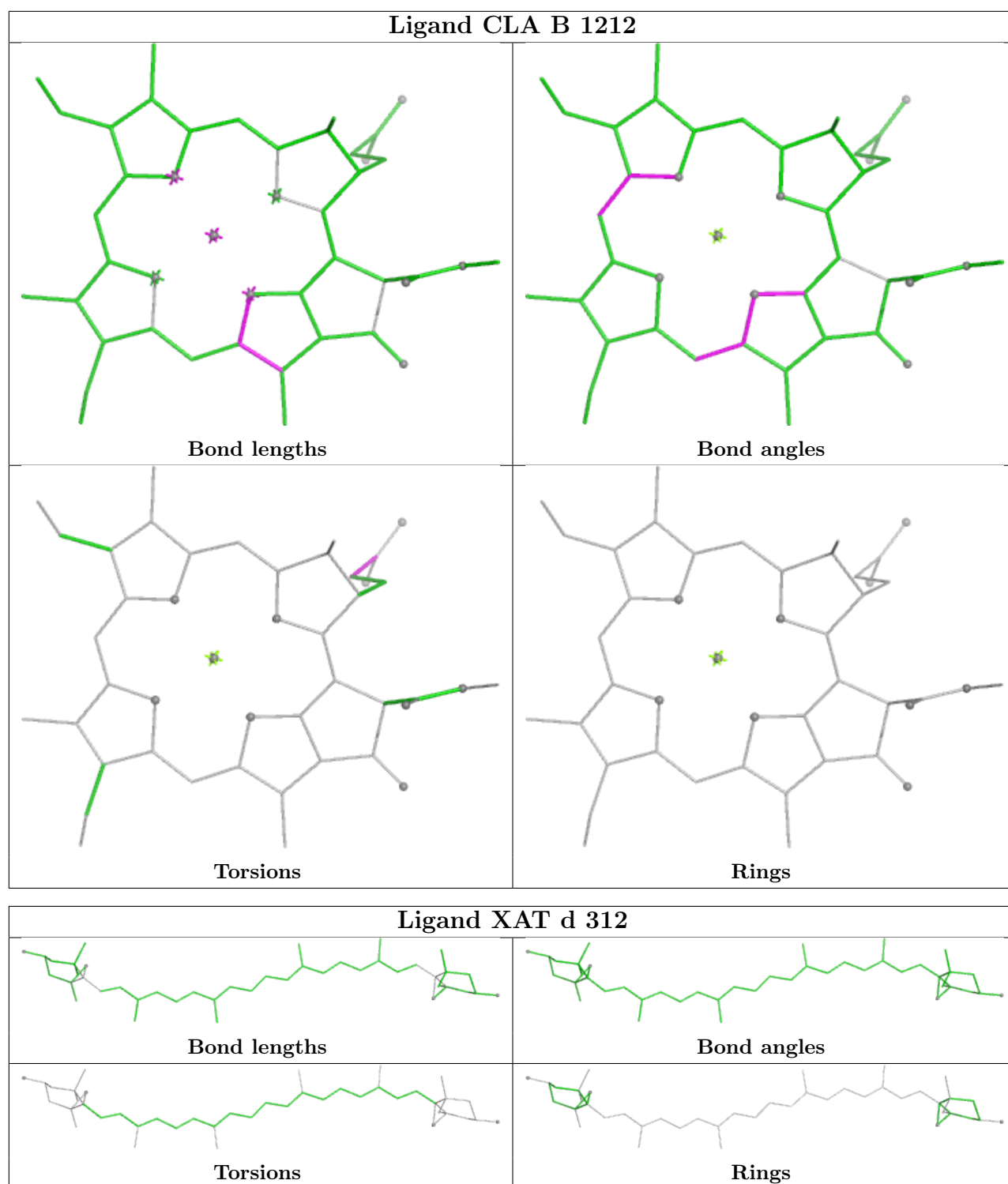


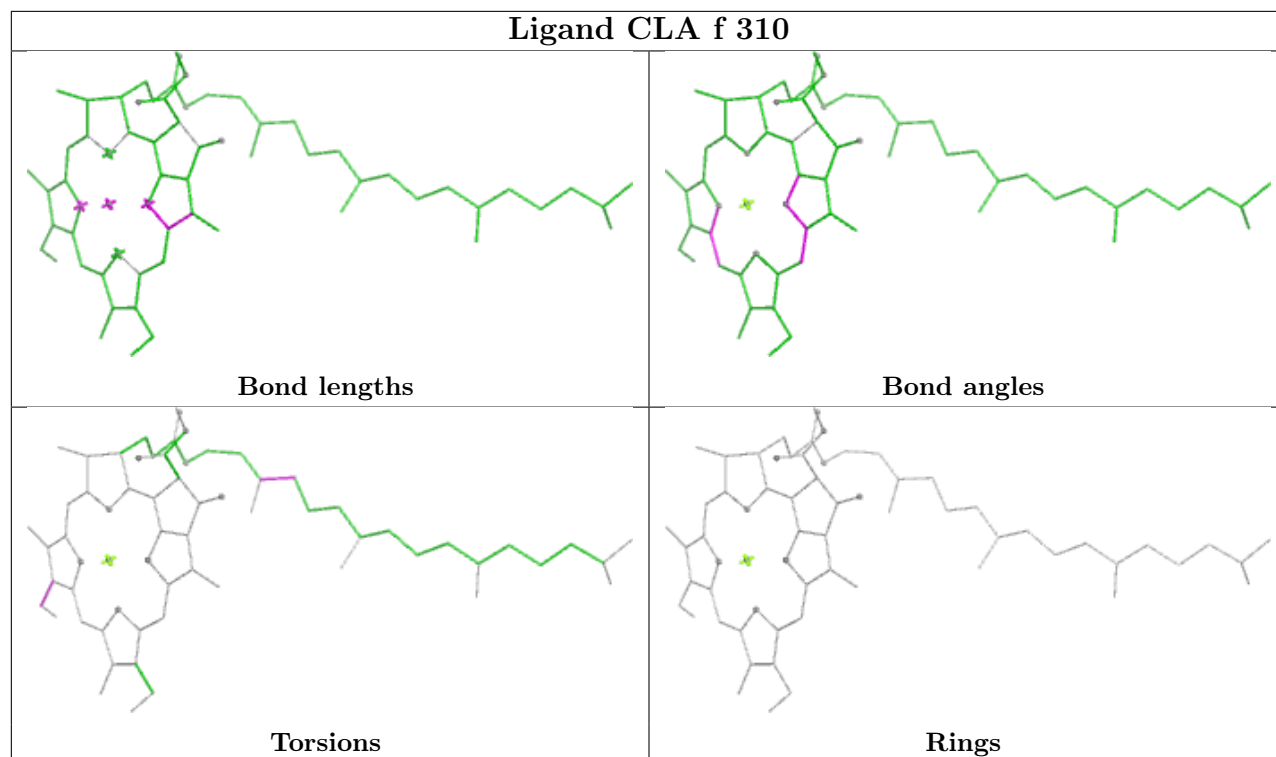


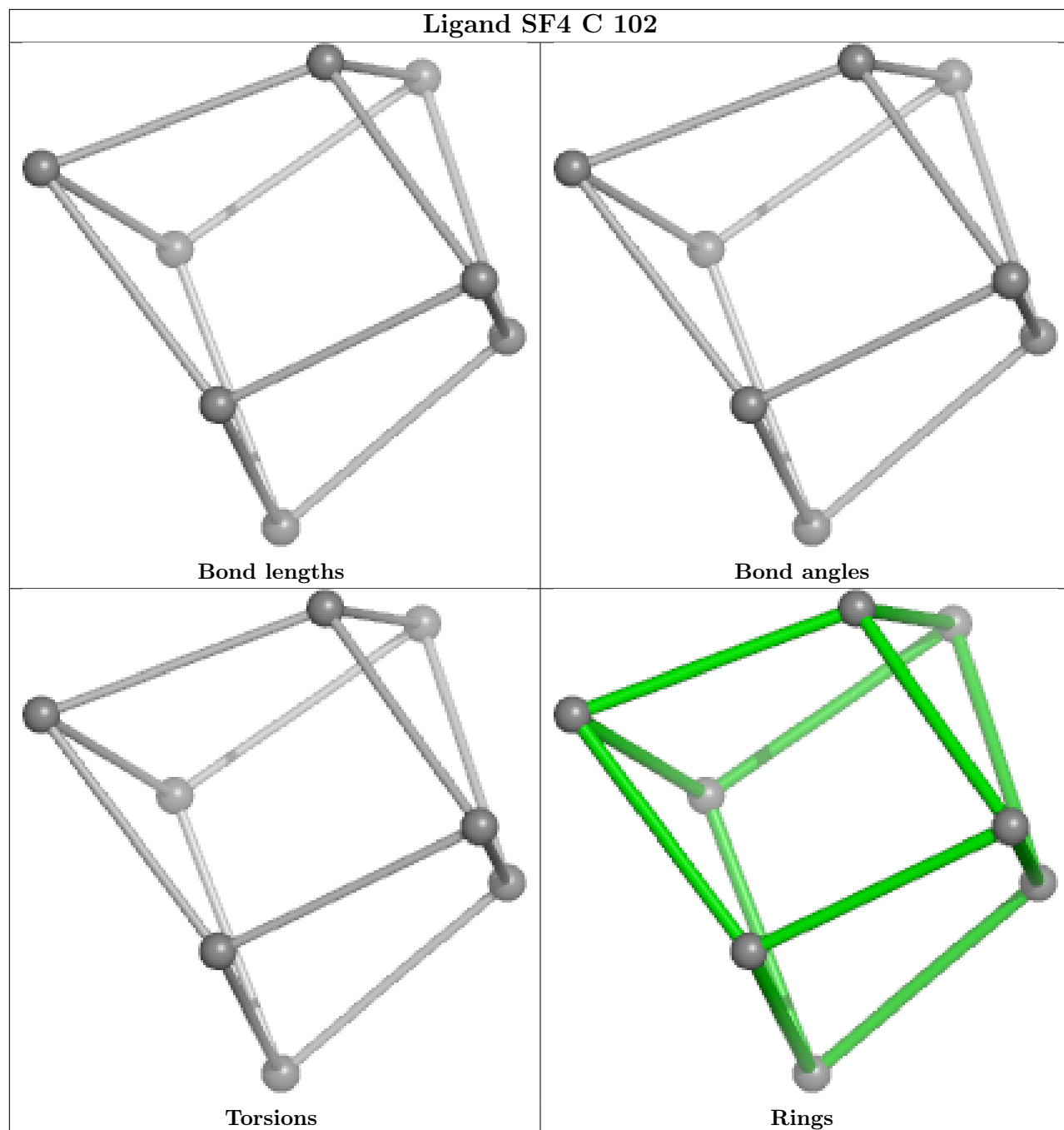
Ligand CLA B 1225

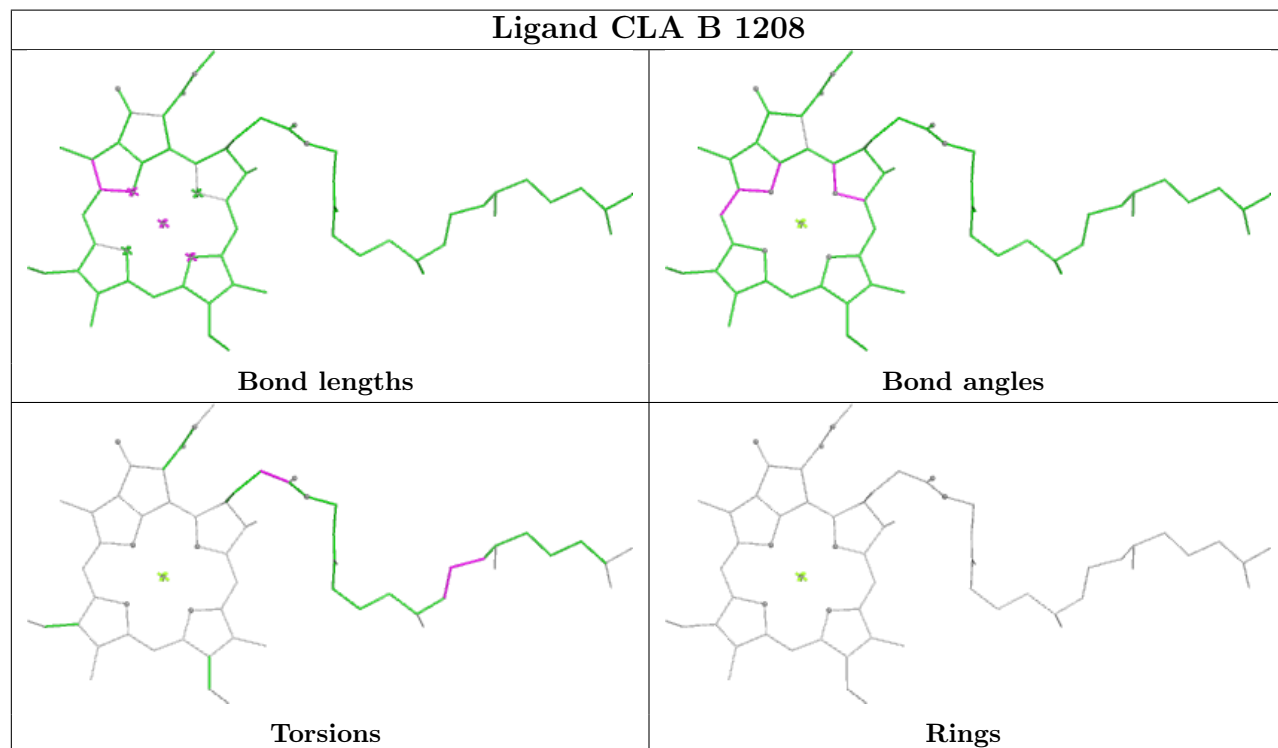
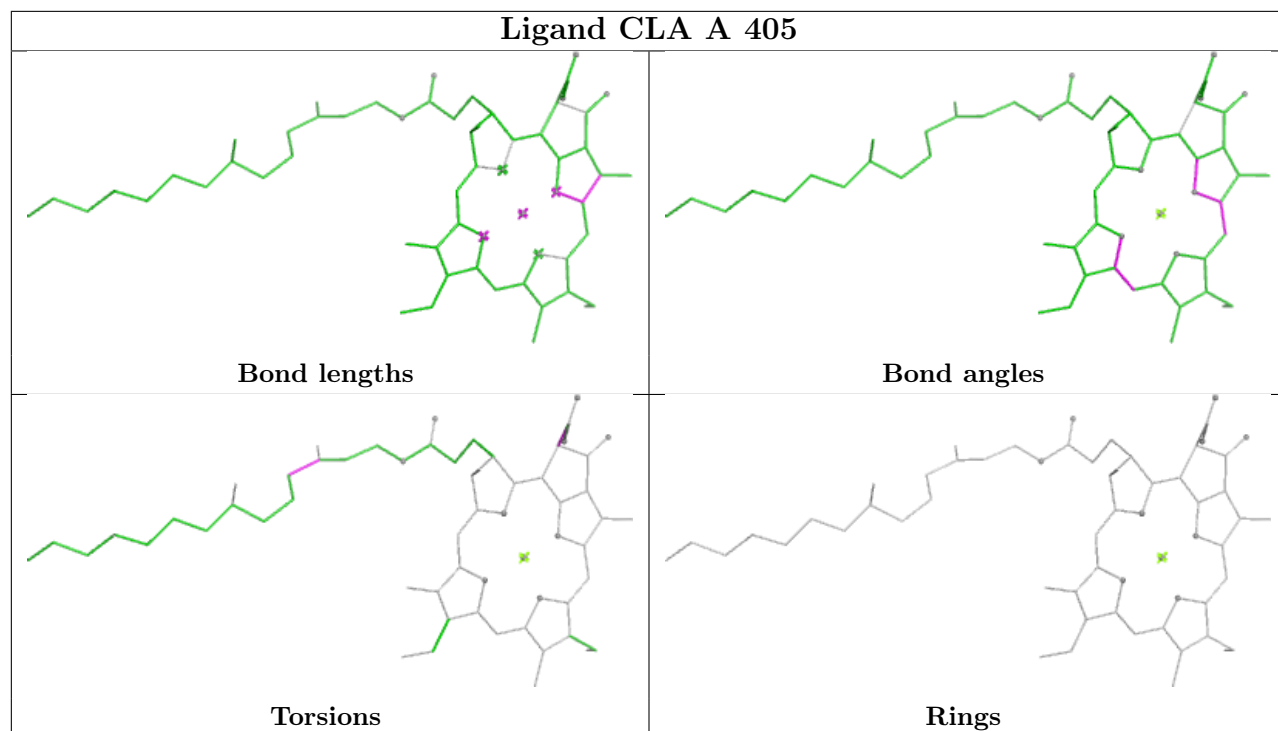


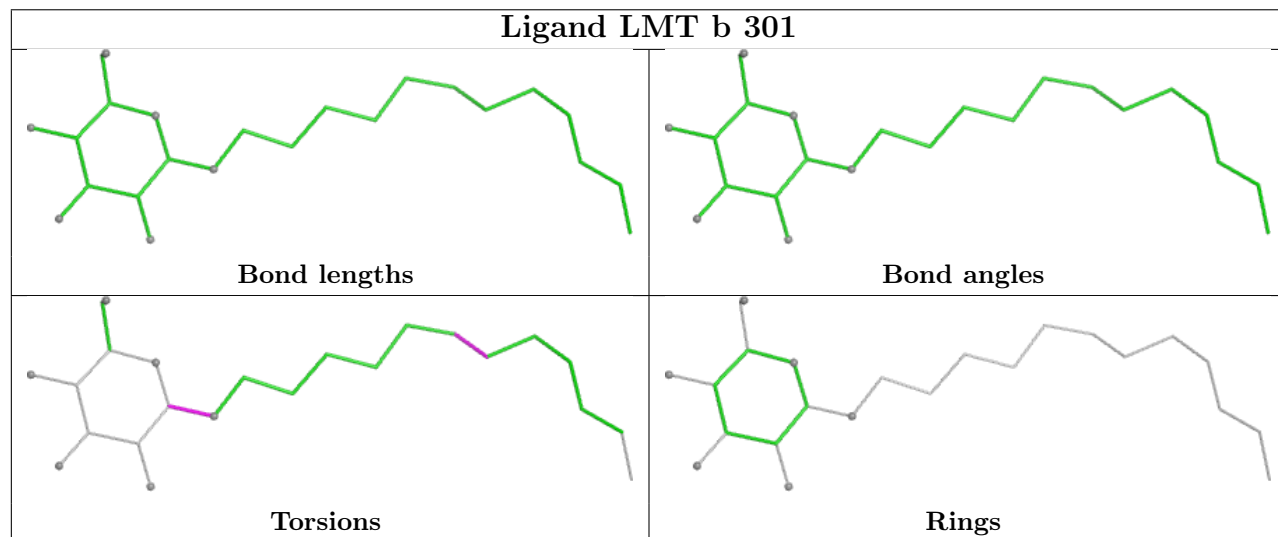
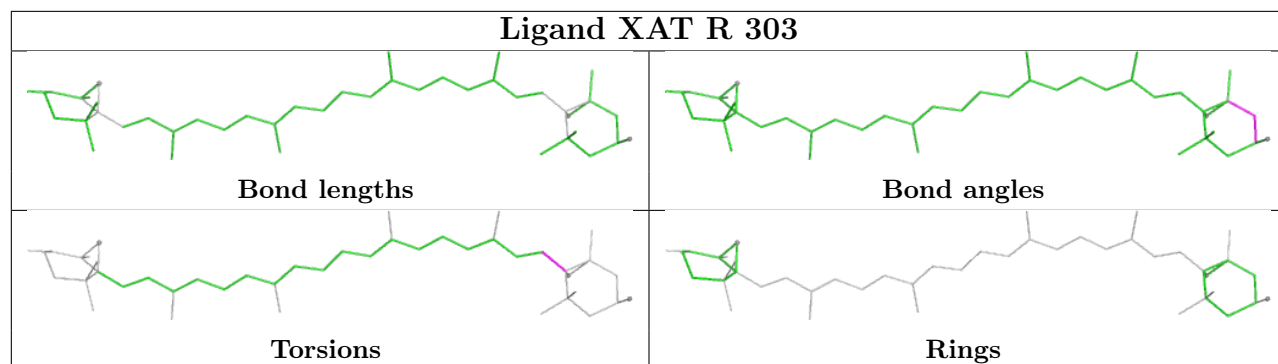
Ligand CLA b 305**Ligand XAT A 417**

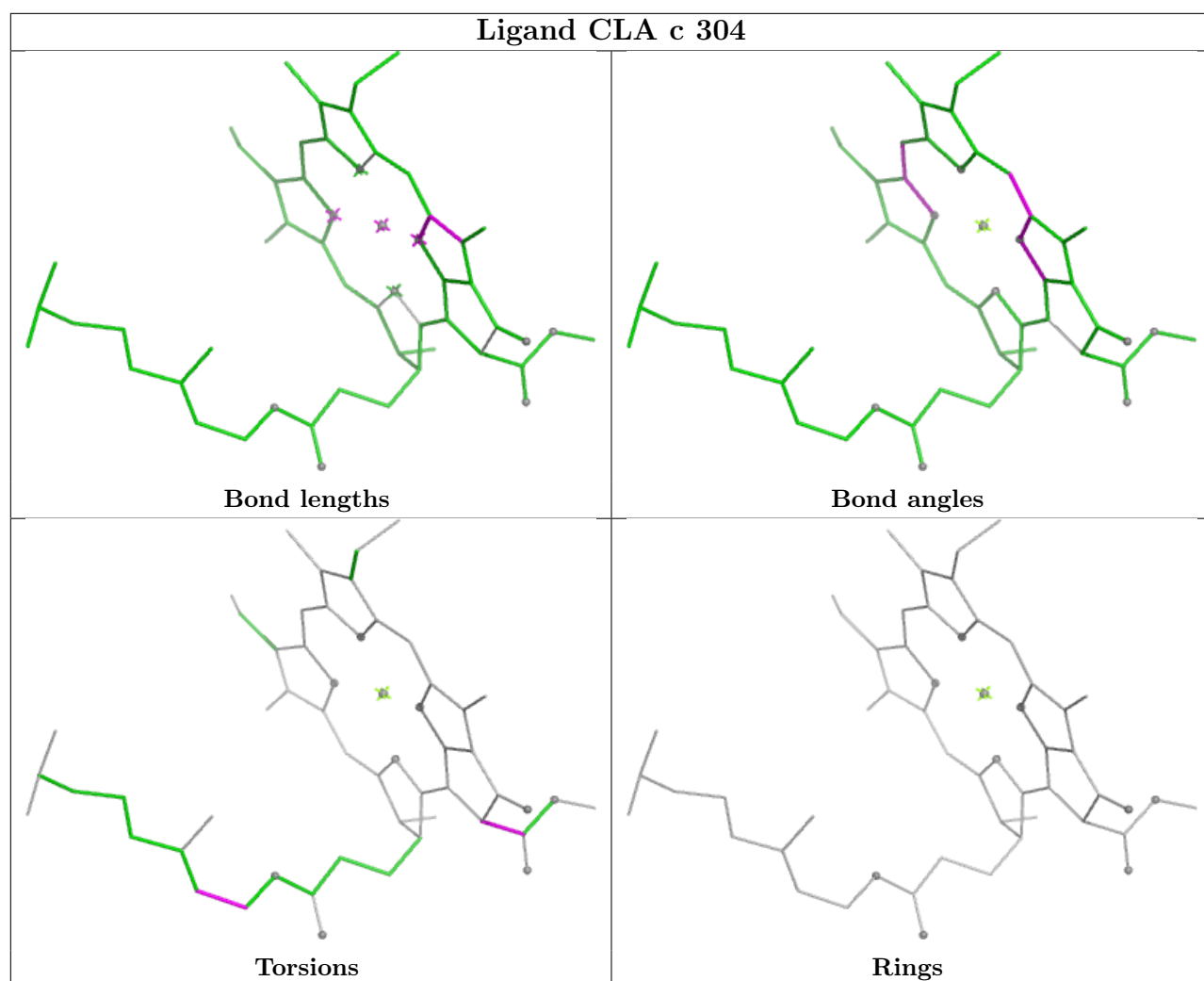


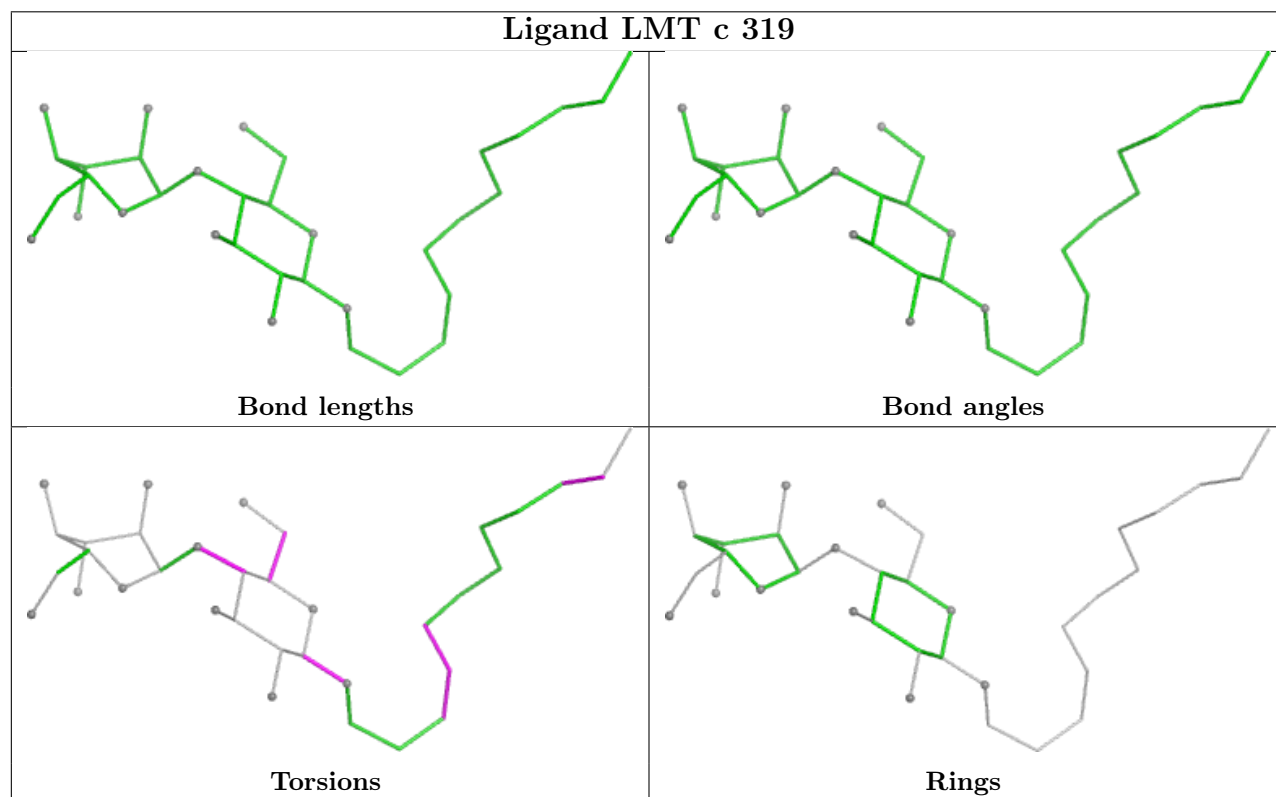
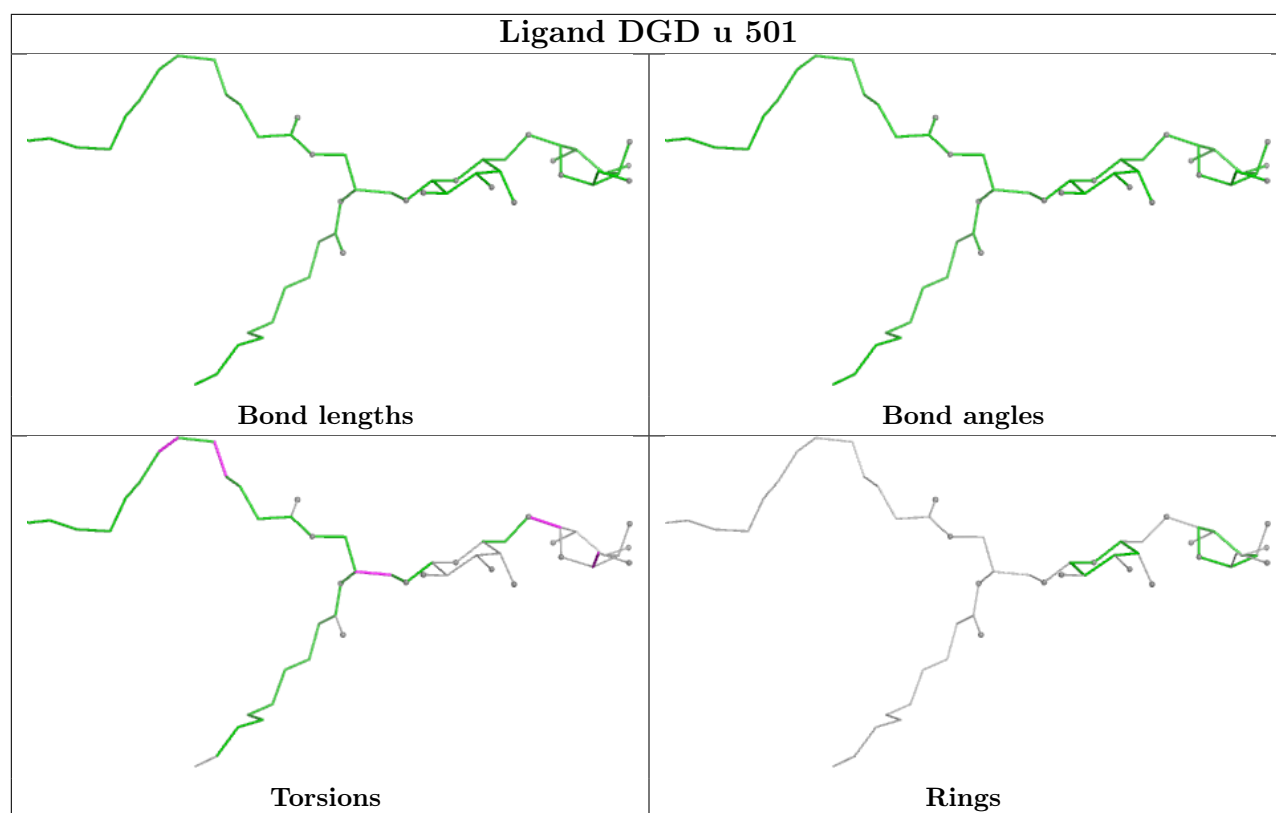


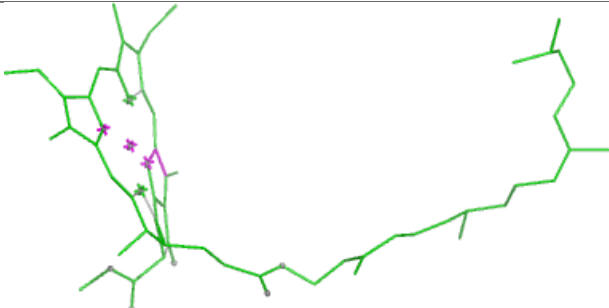
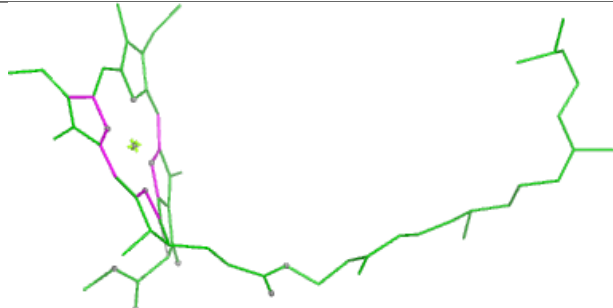
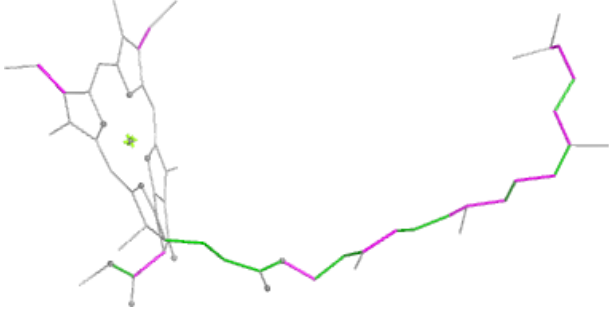


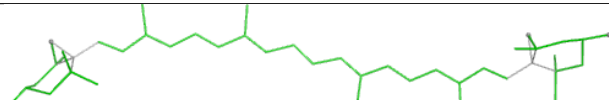
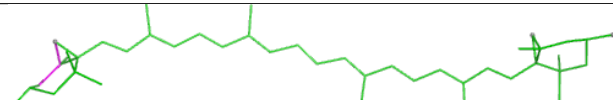




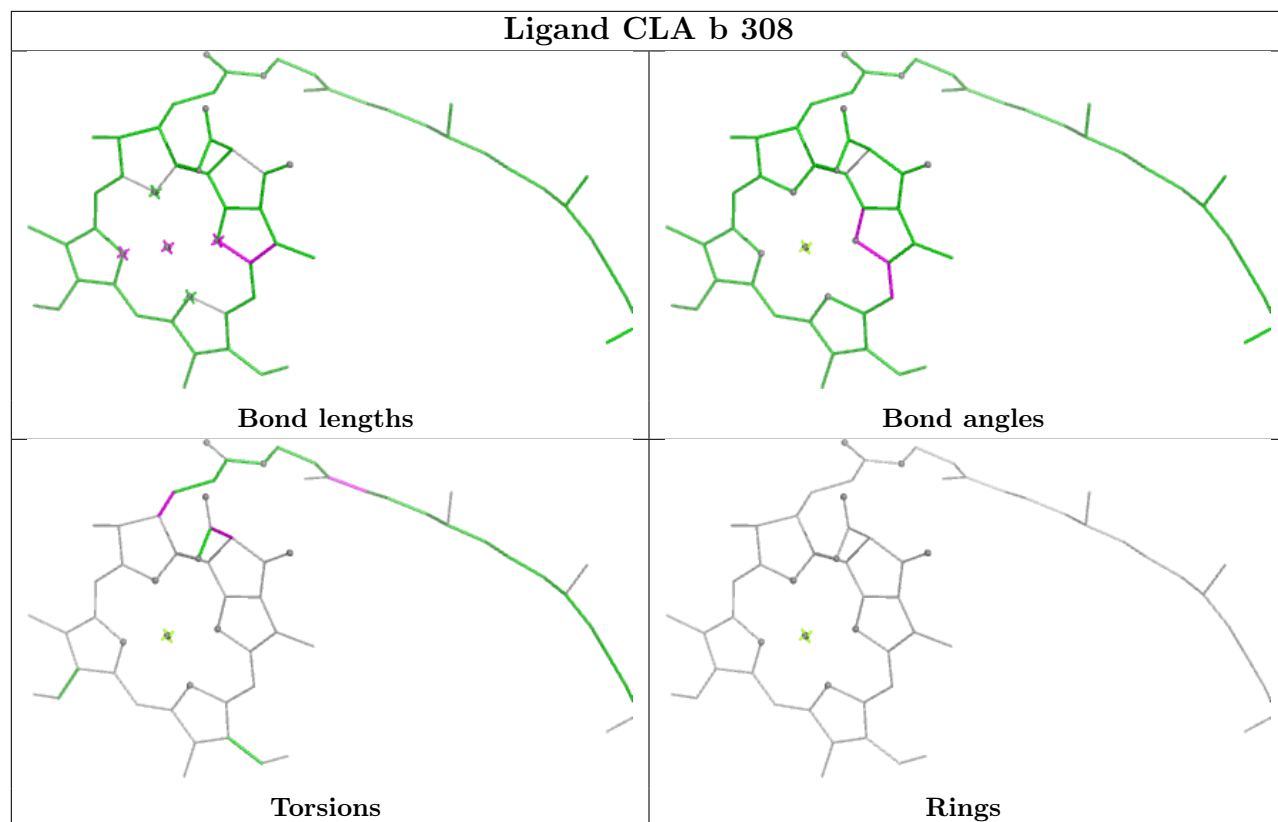


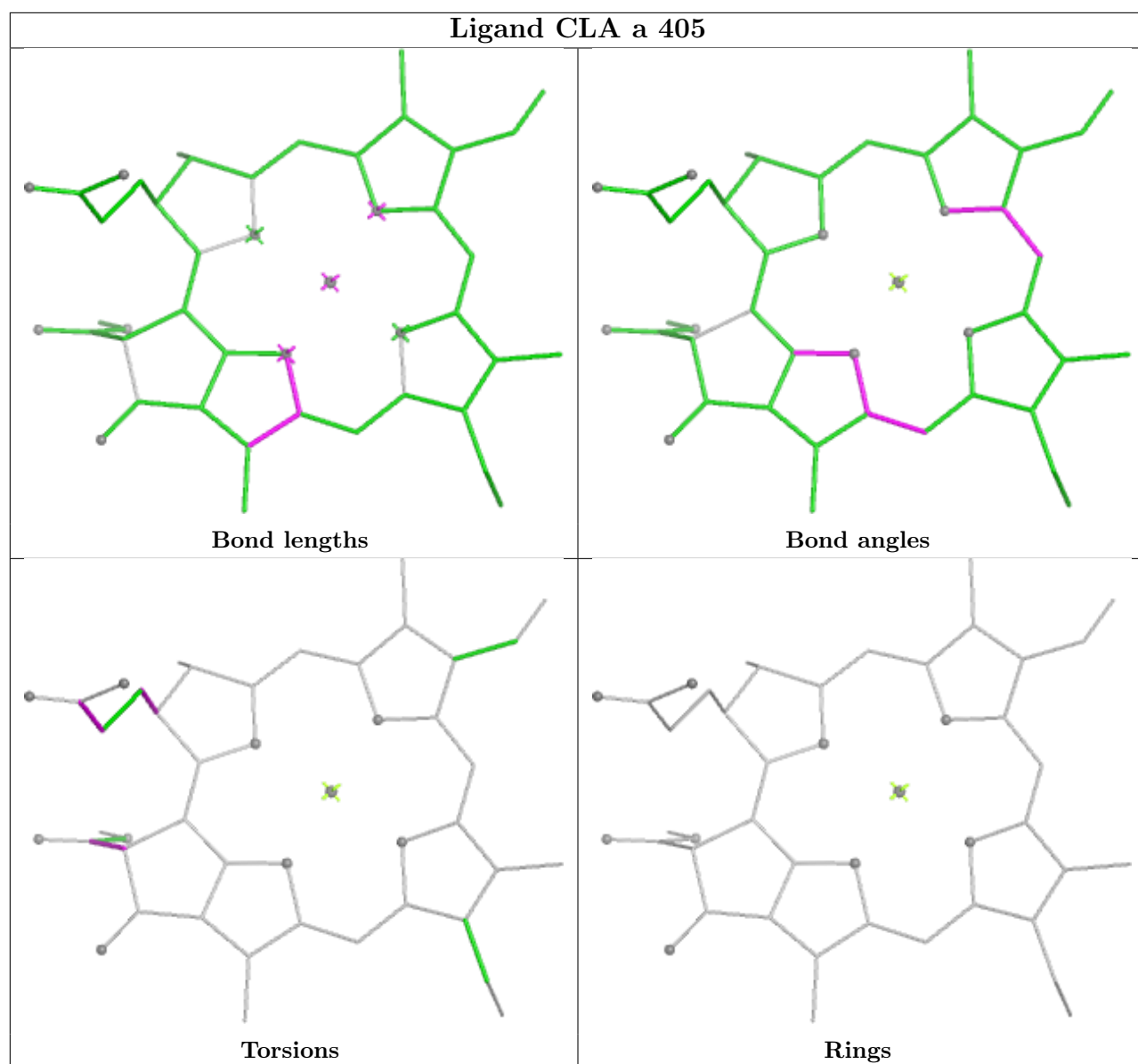


Ligand CLA A 420	
	
Bond lengths	Bond angles
	
Torsions	Rings

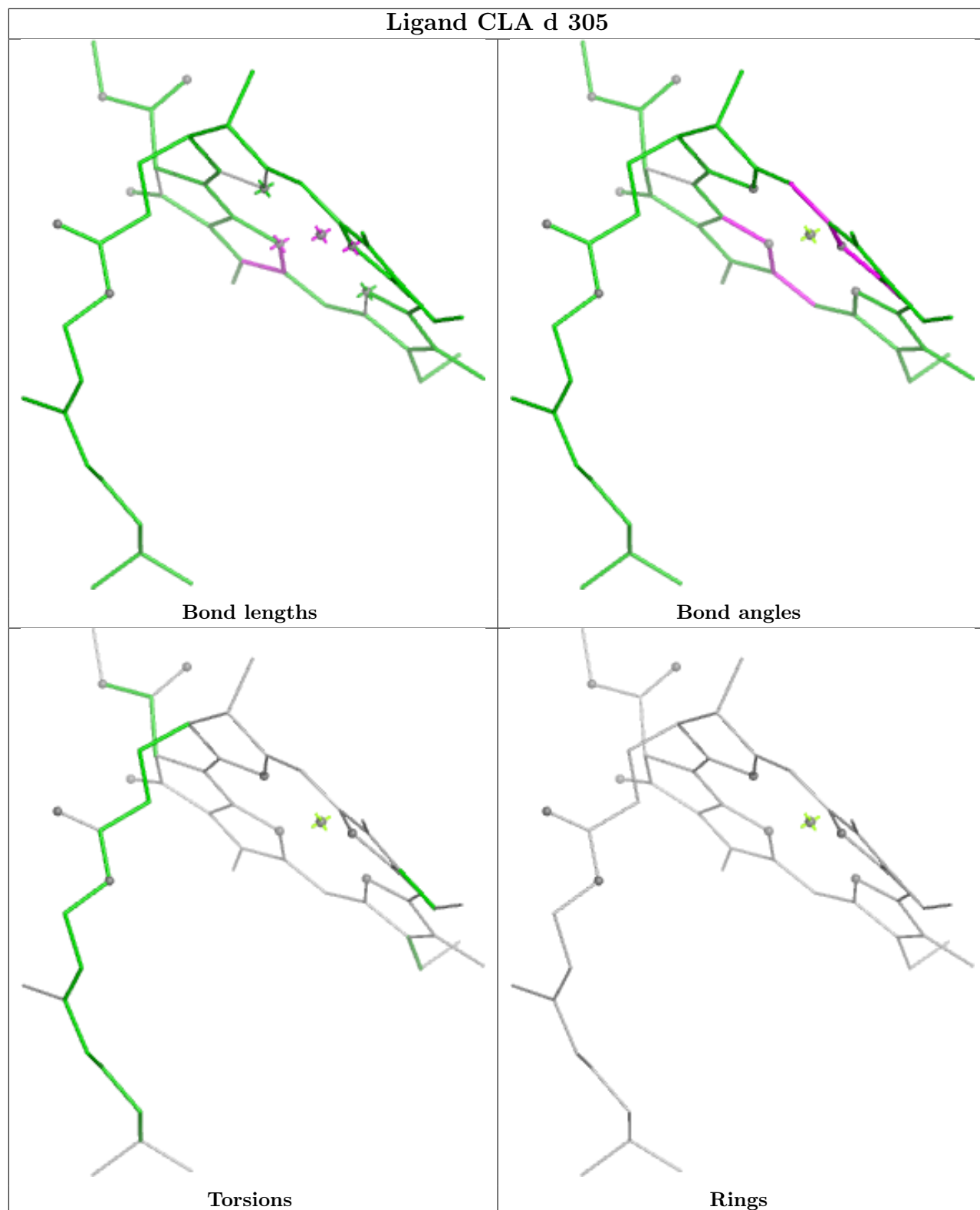
Ligand XAT f 322	
	
Bond lengths	Bond angles
	
Torsions	Rings

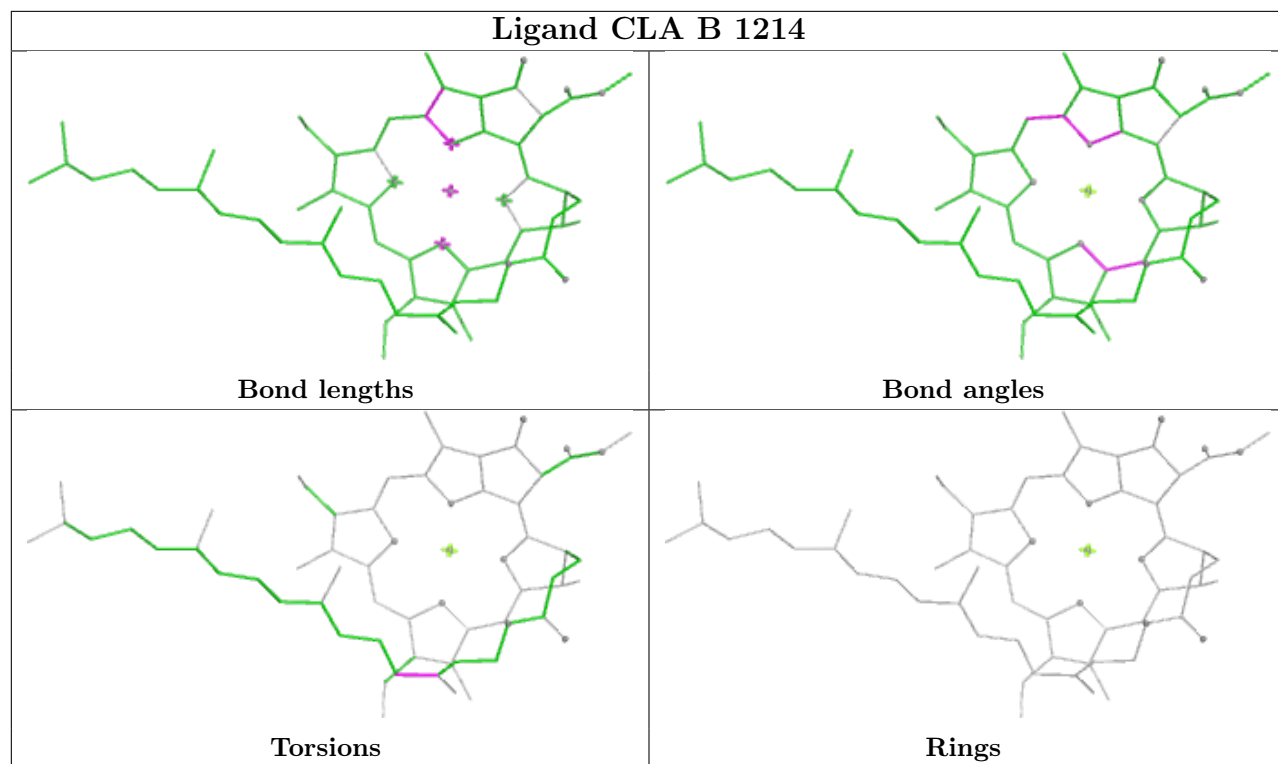
Ligand XAT f 318	
	
Bond lengths	Bond angles
	
Torsions	Rings

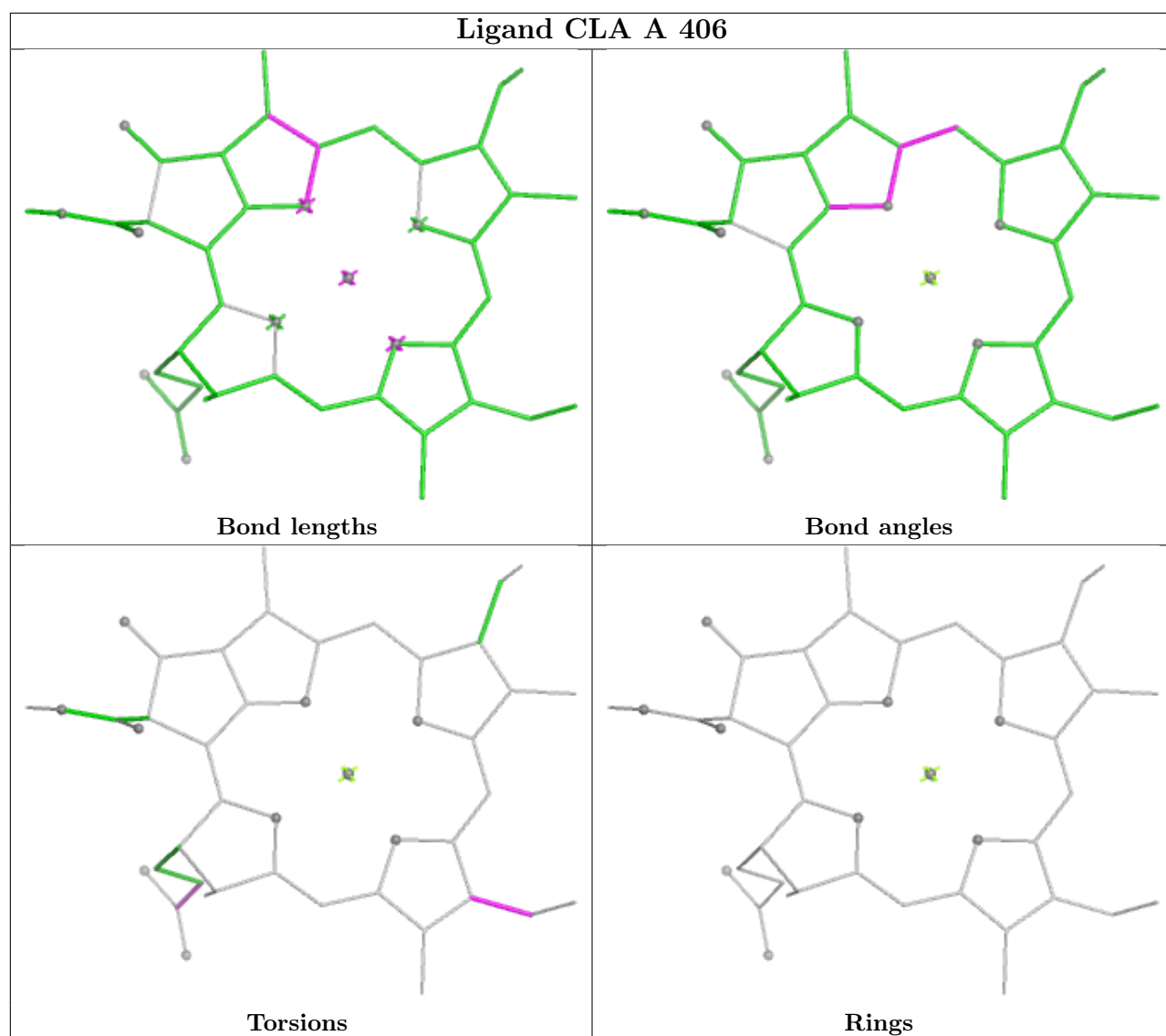




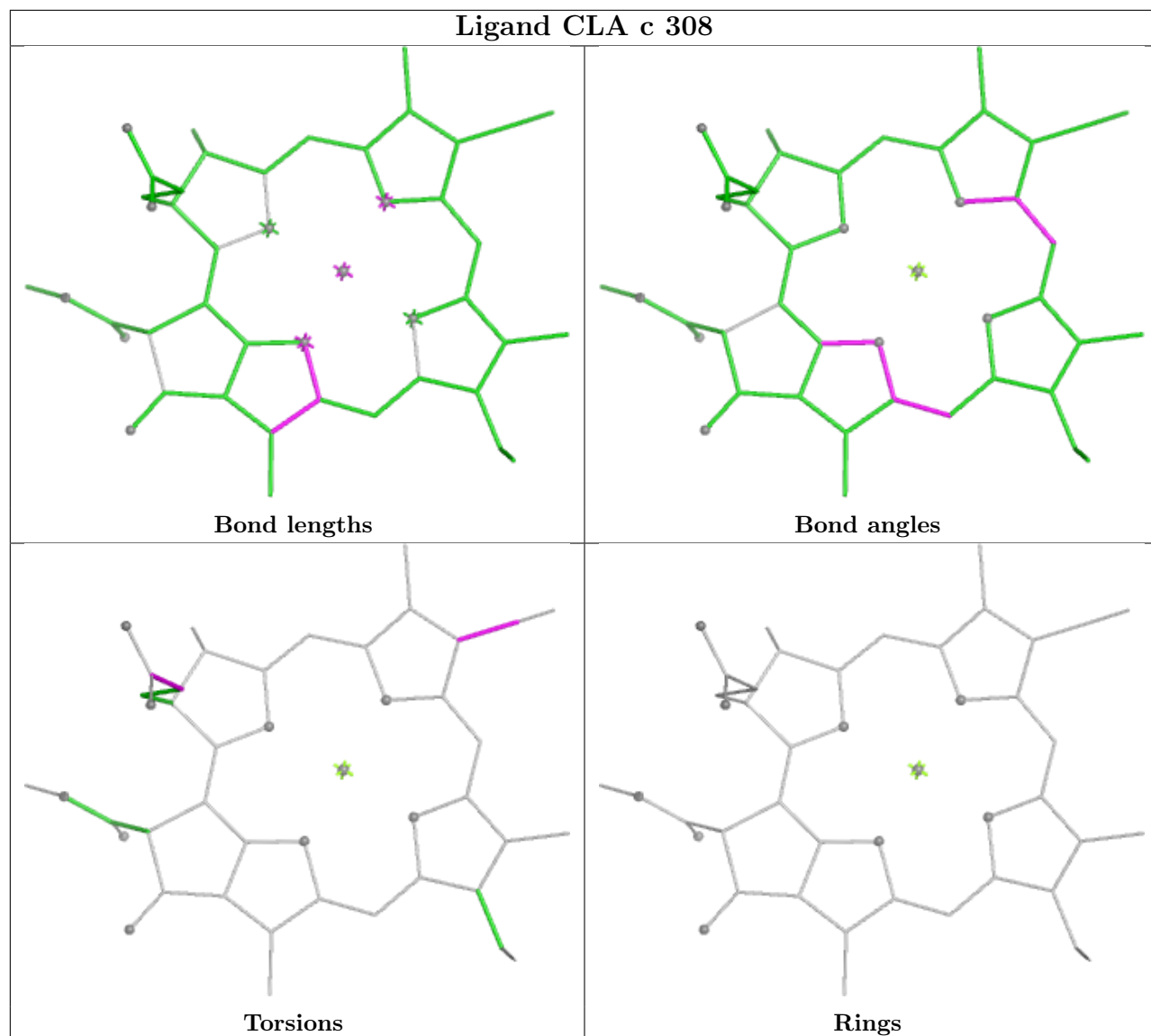
Ligand CLA d 305

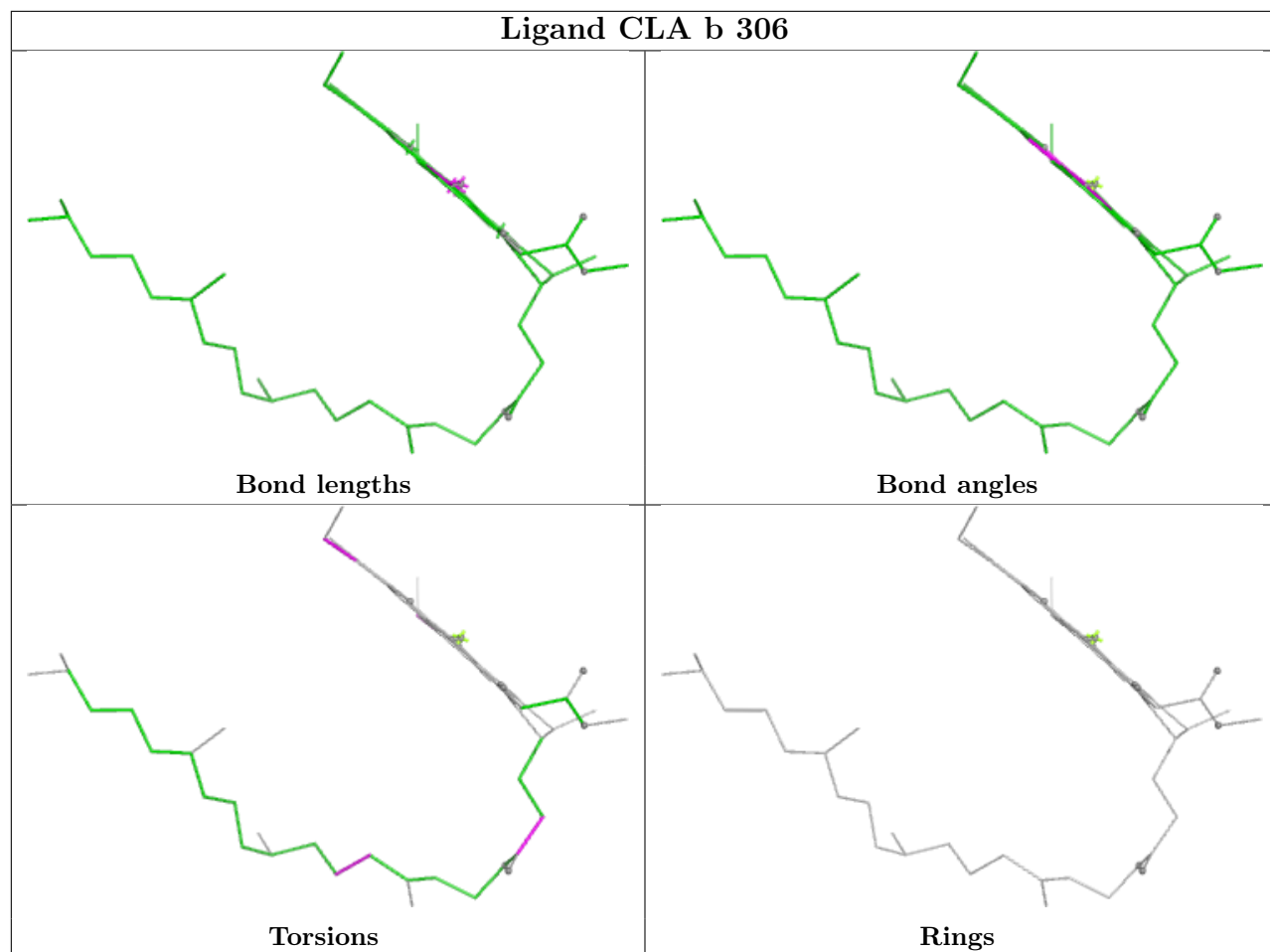




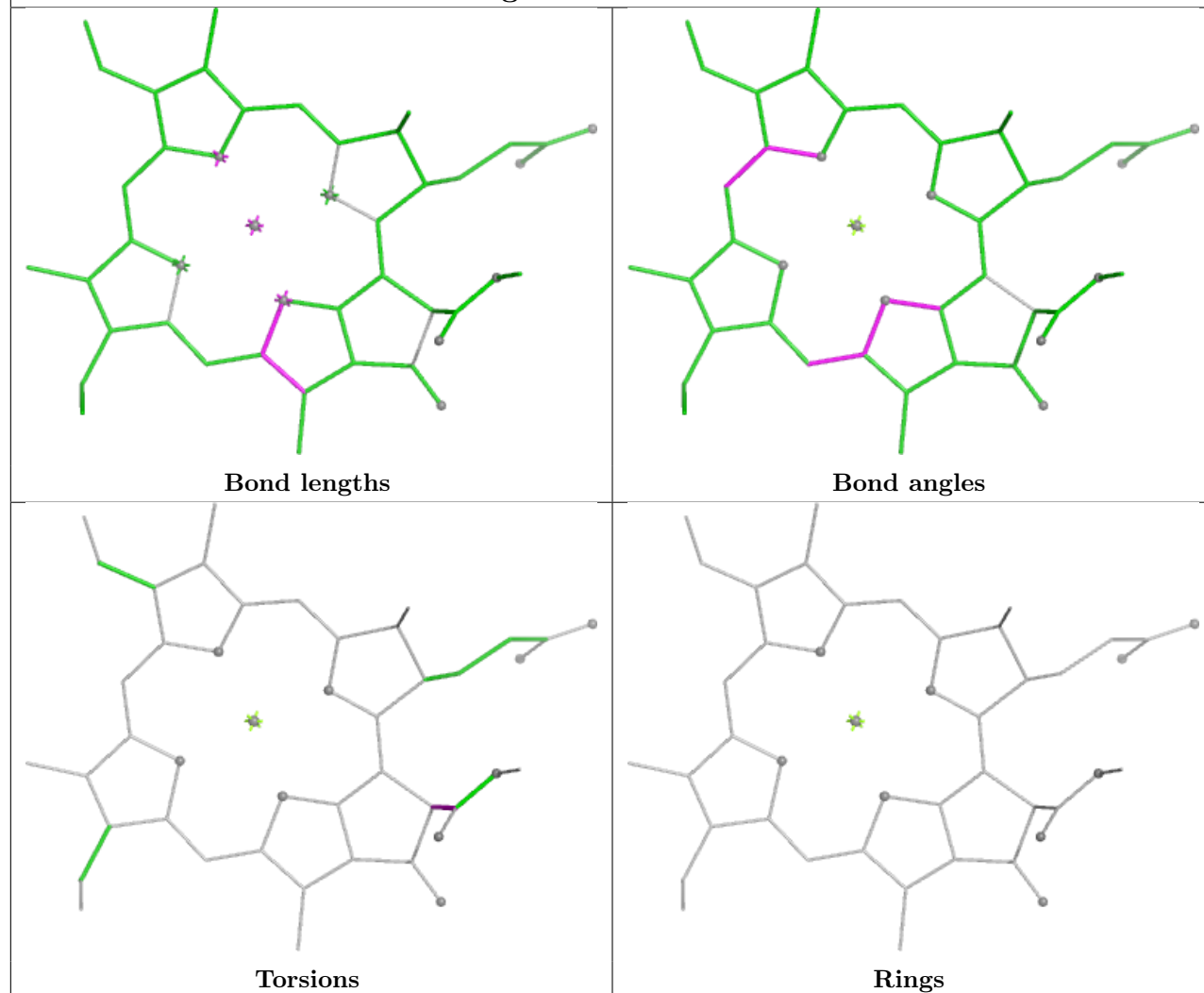


Ligand CLA c 308

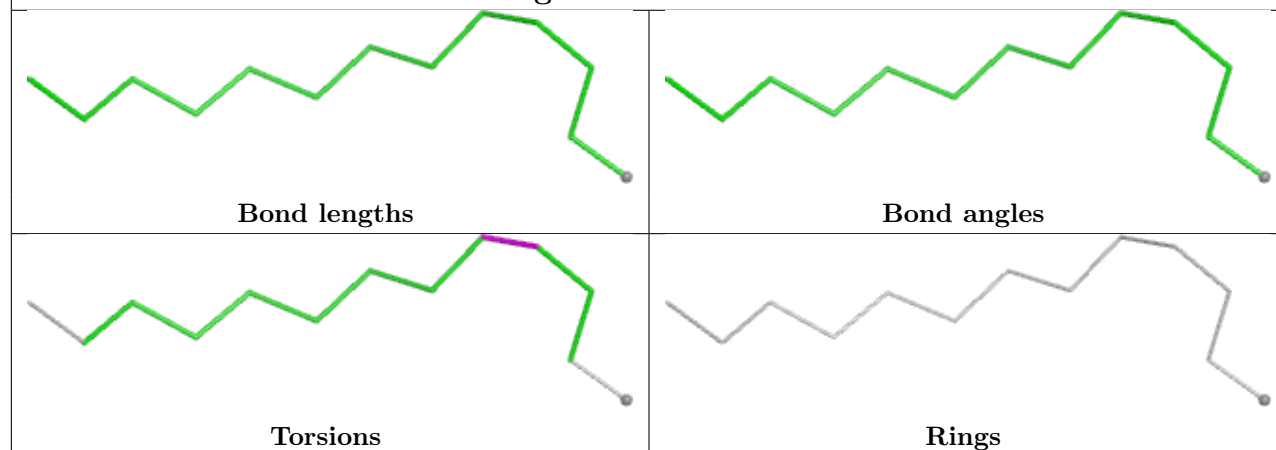


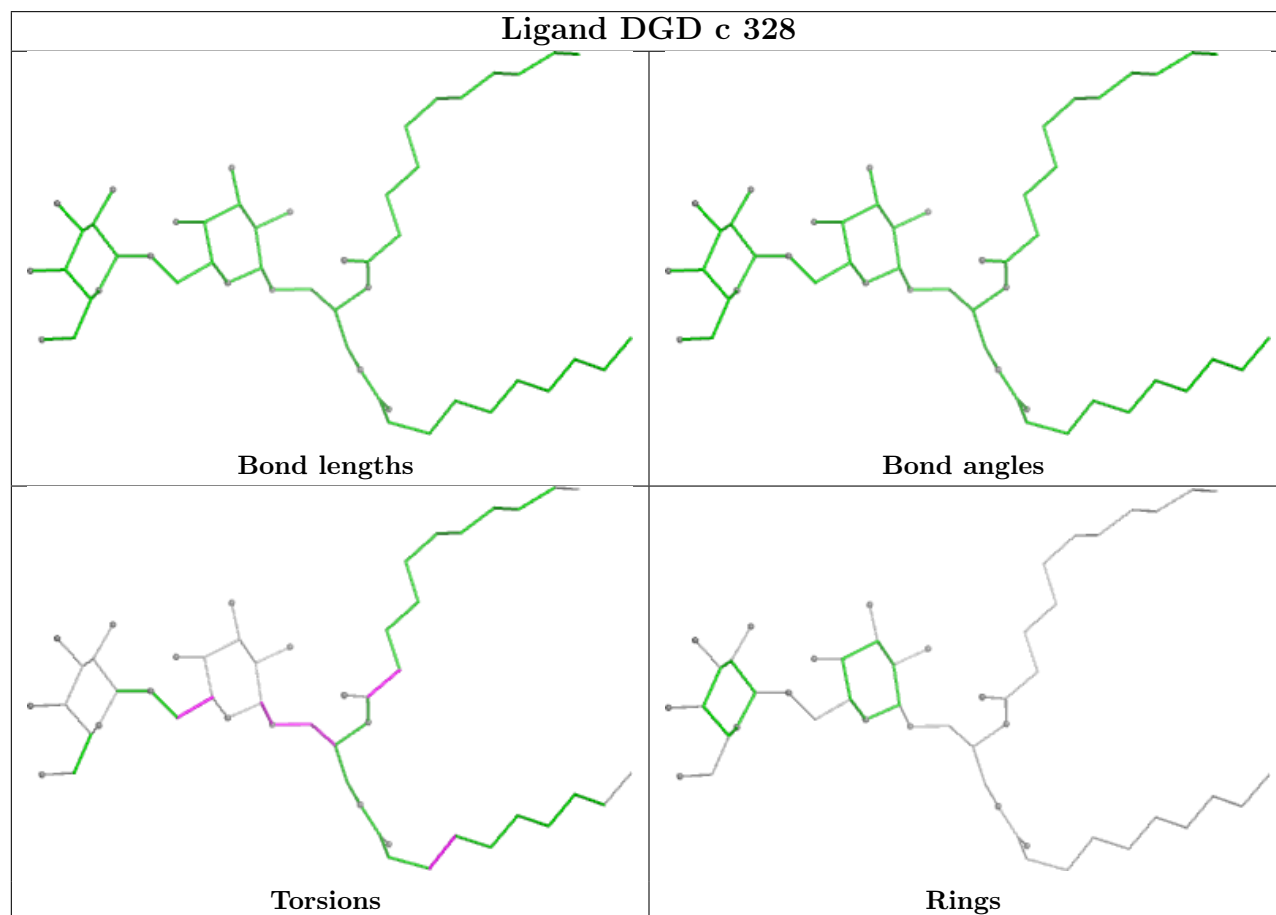
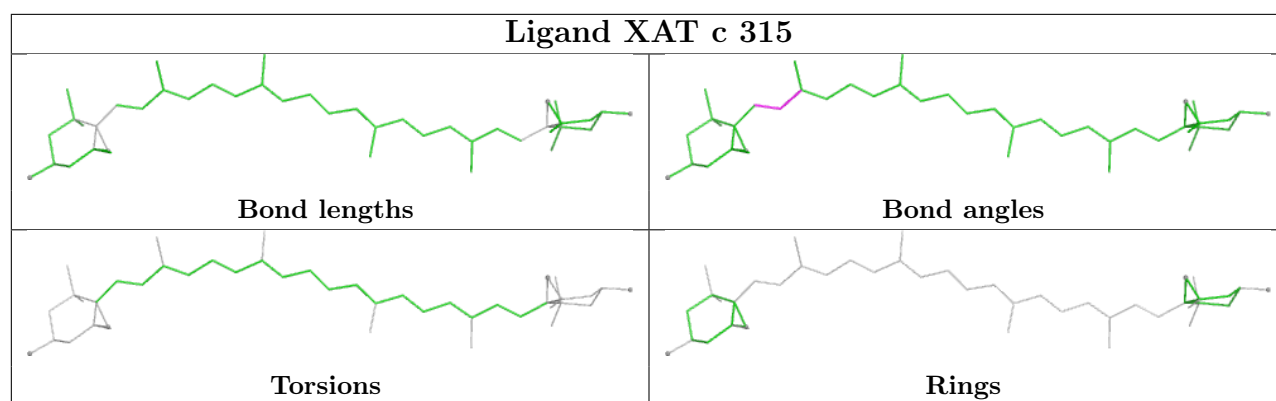


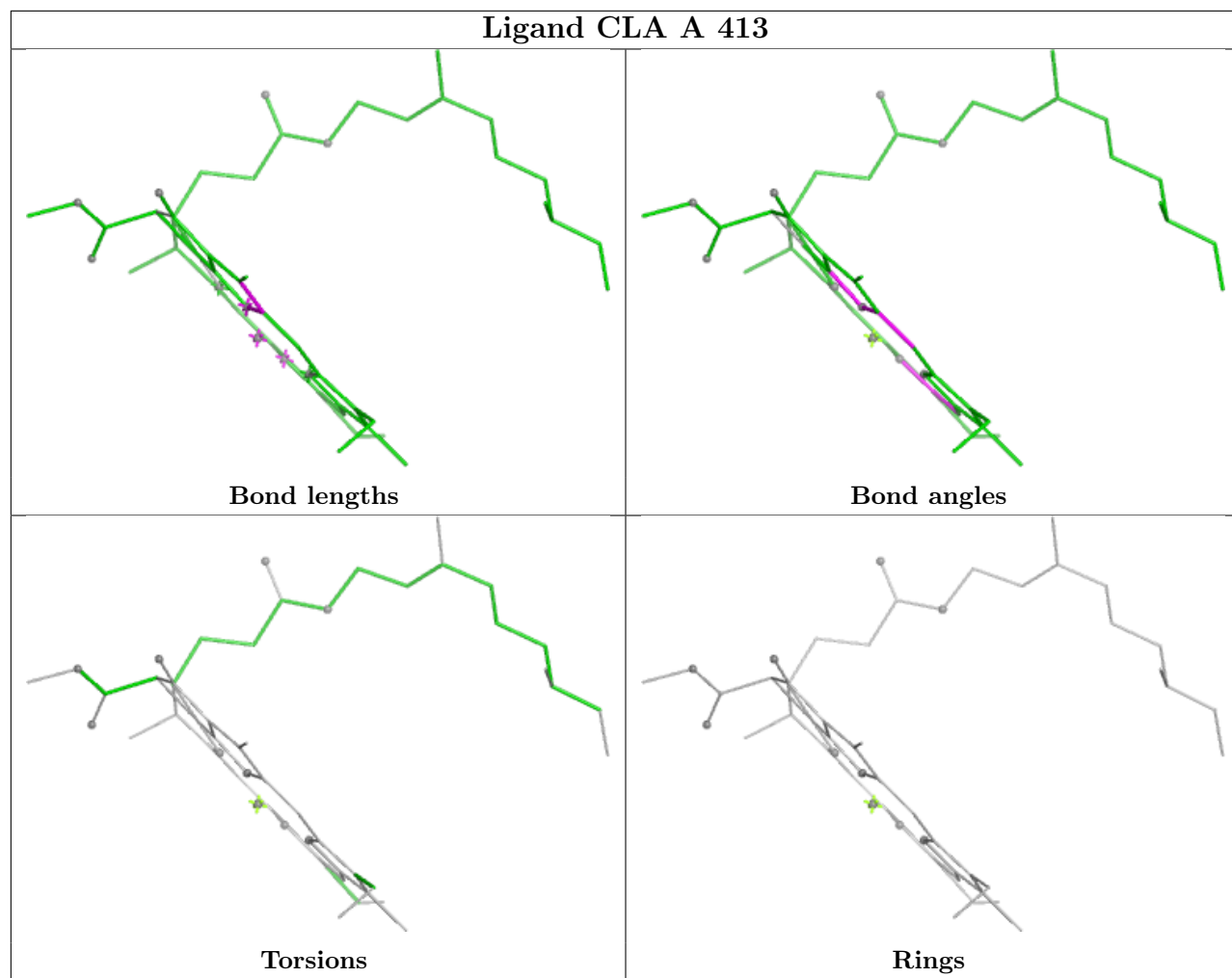
Ligand CLA R 301



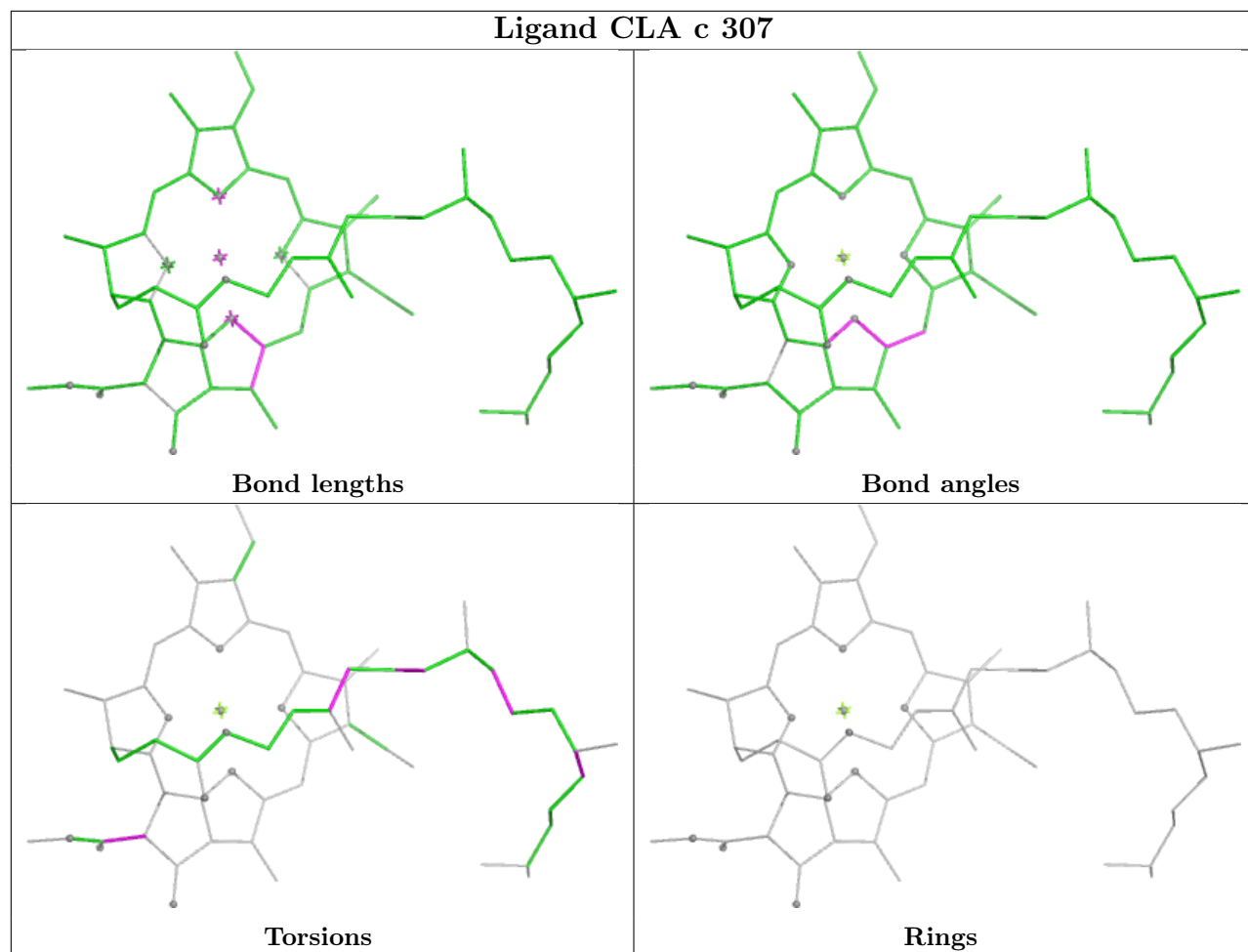
Ligand LMT c 333



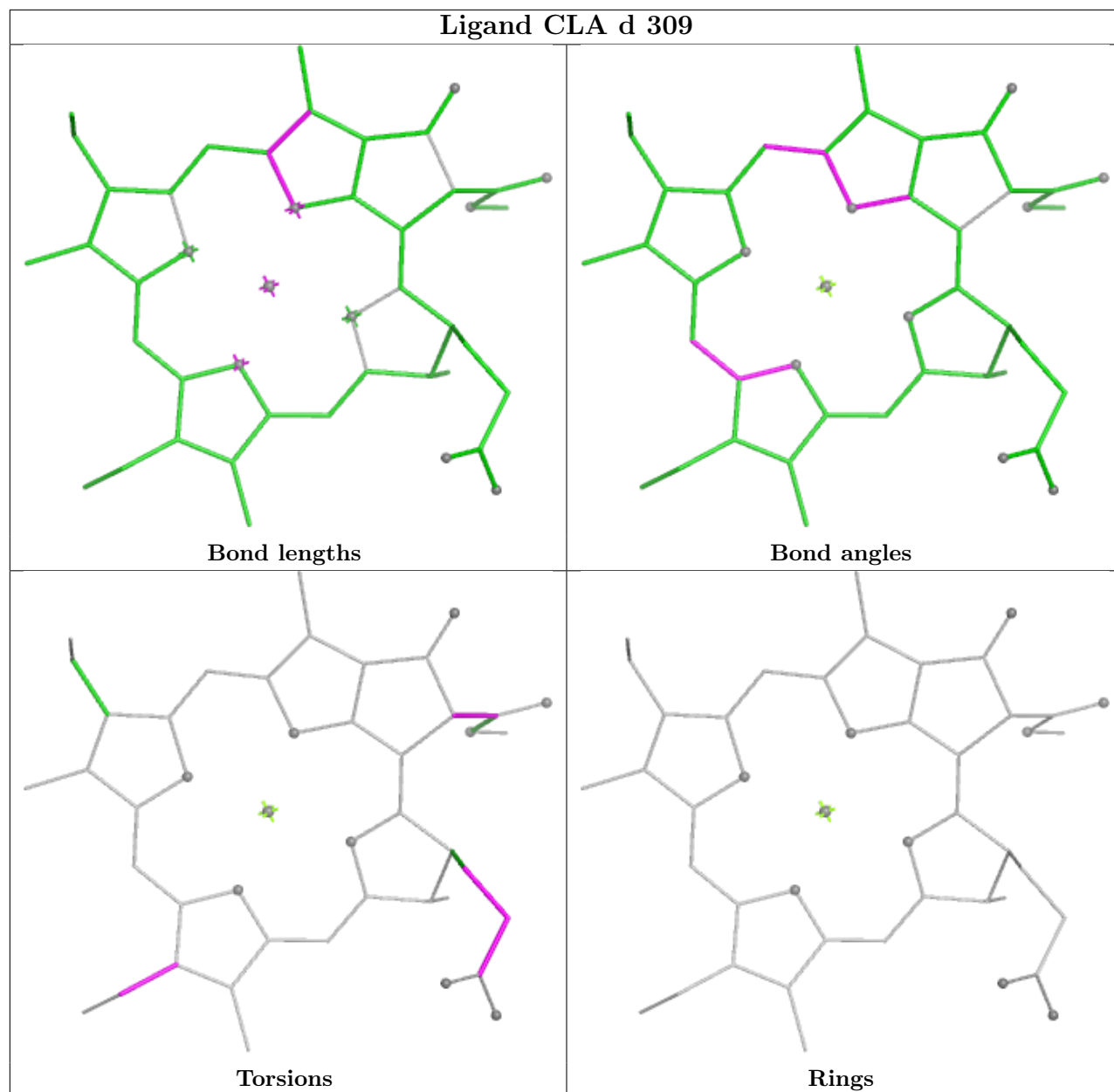




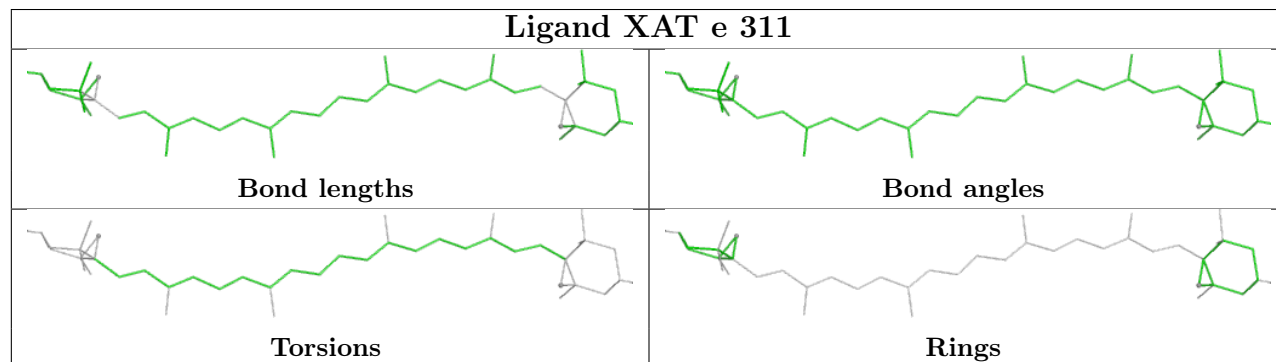
Ligand CLA c 307

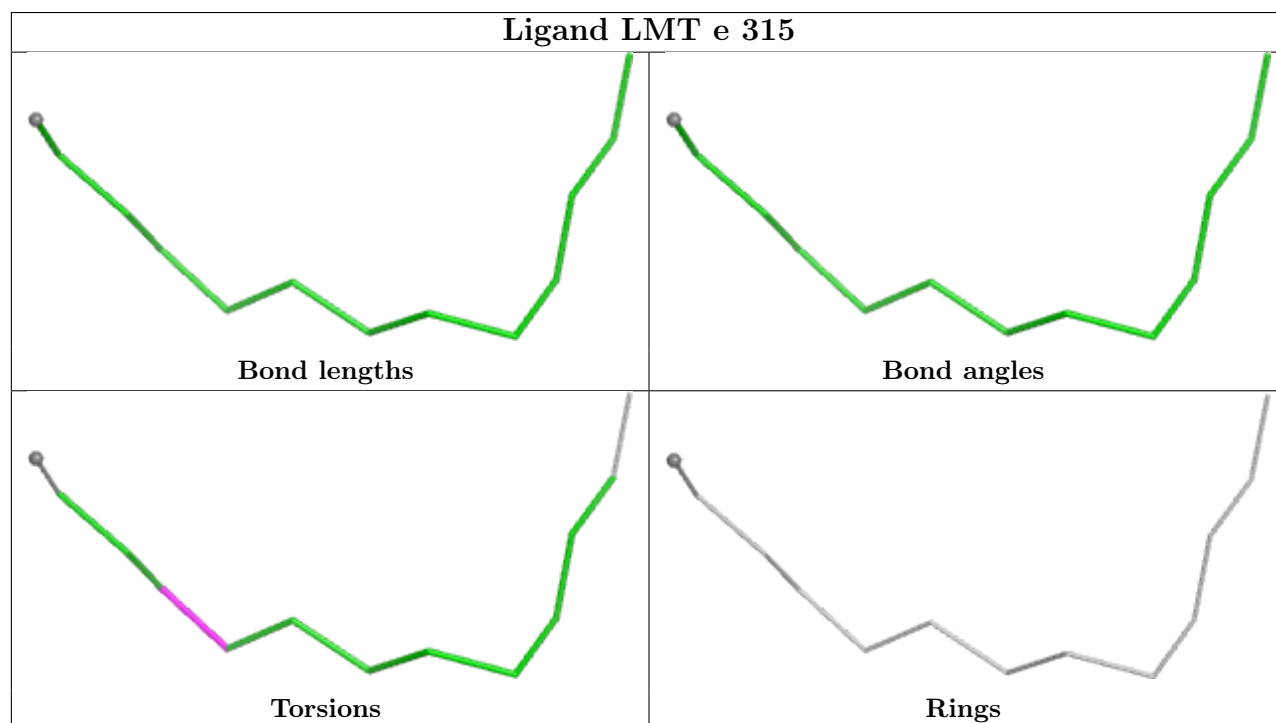
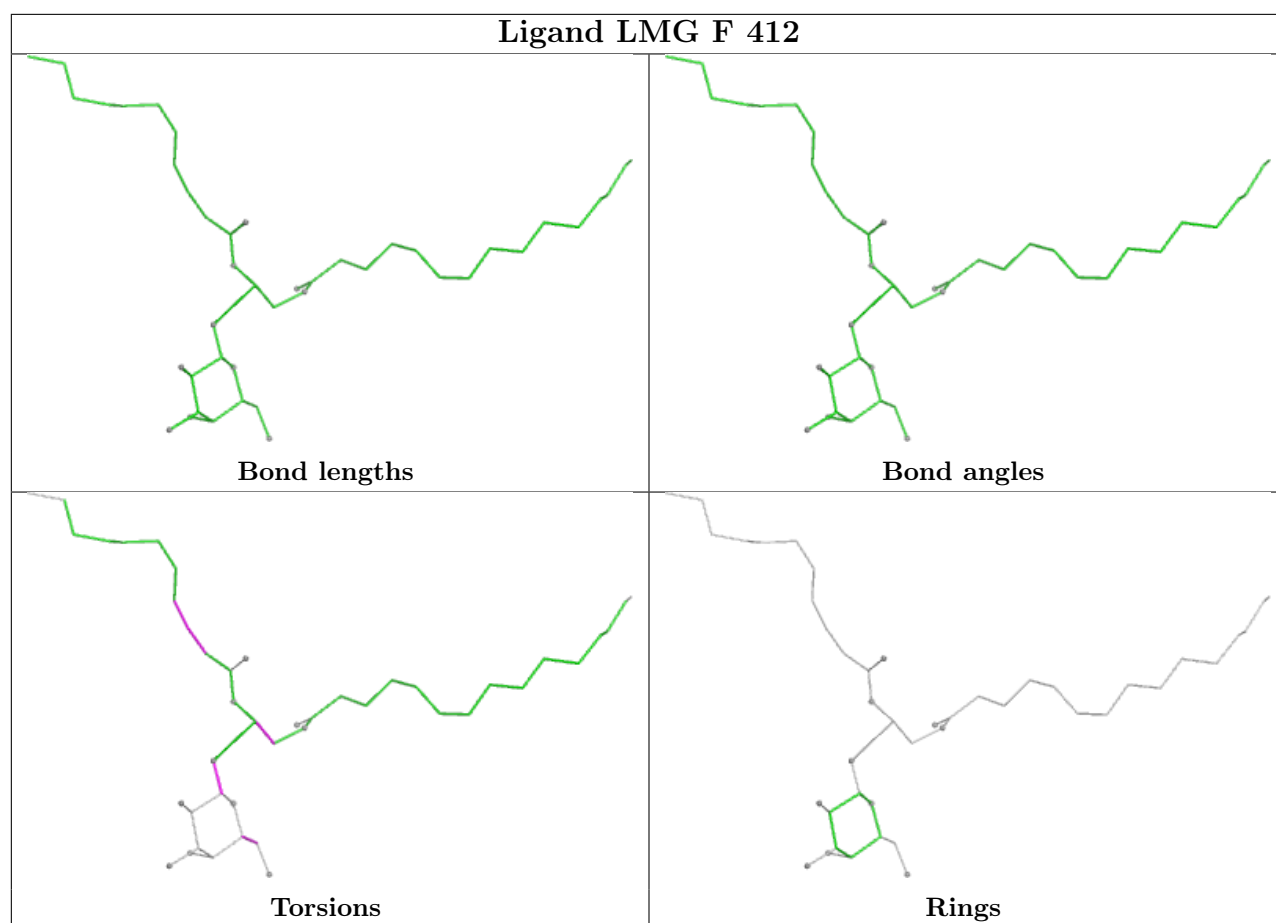


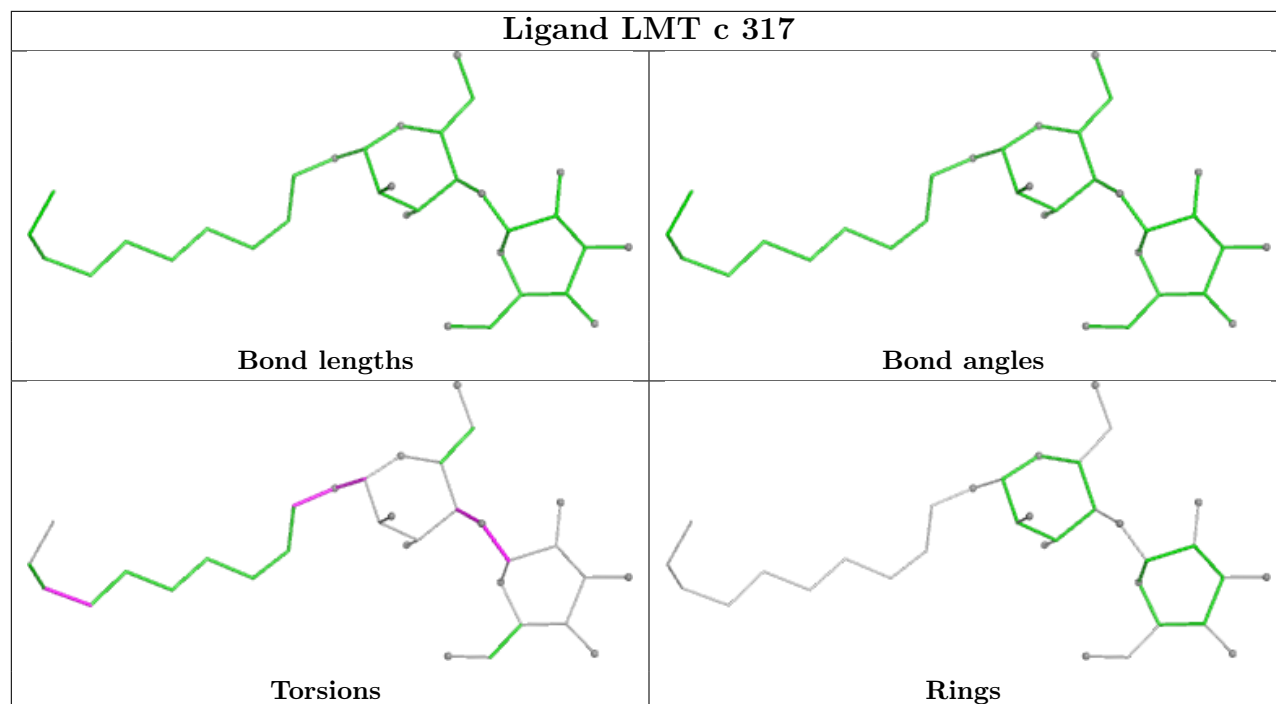
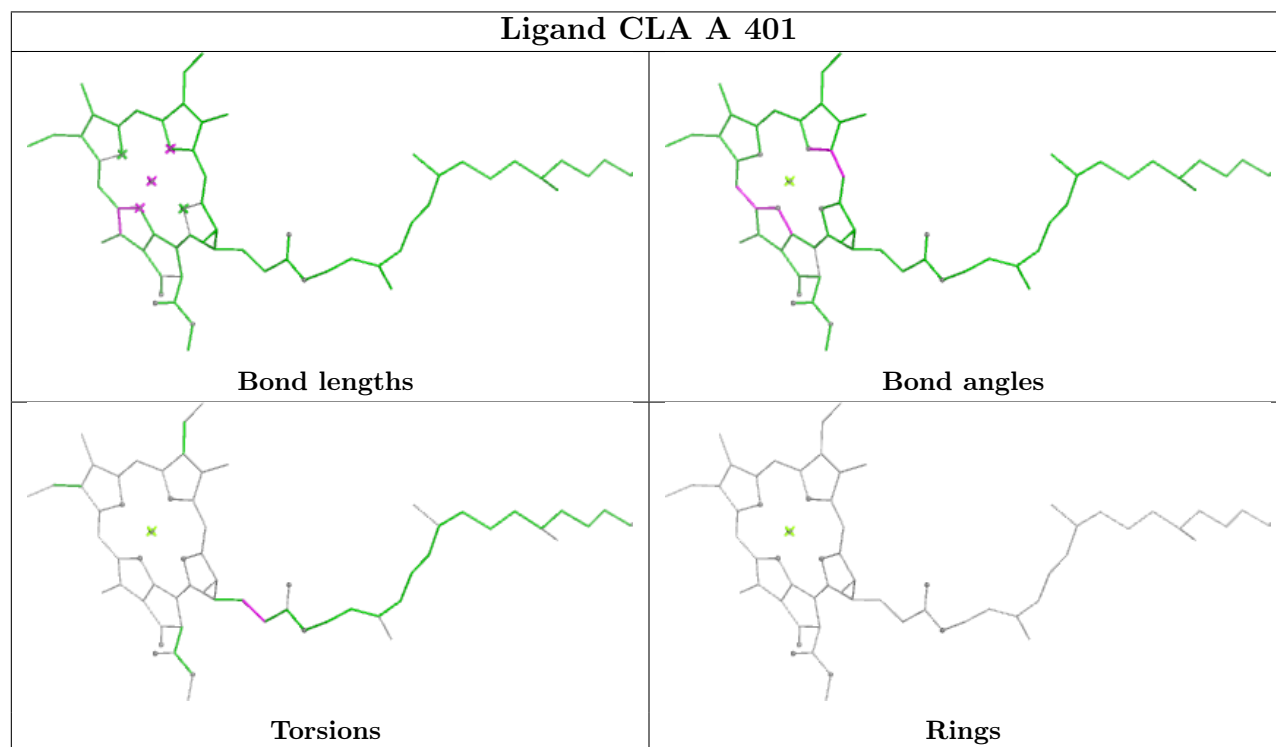
Ligand CLA d 309



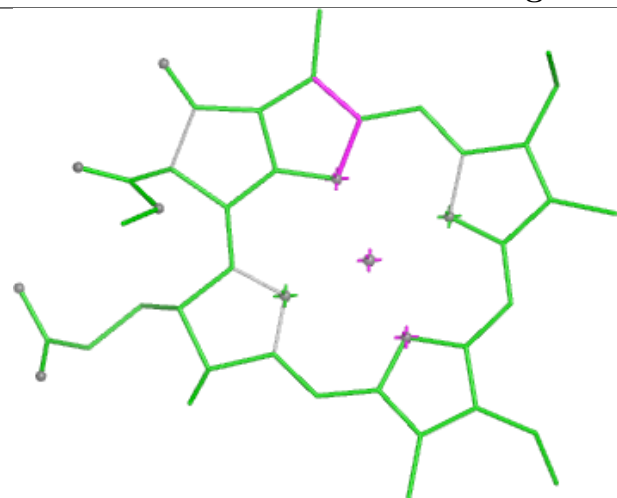
Ligand XAT e 311



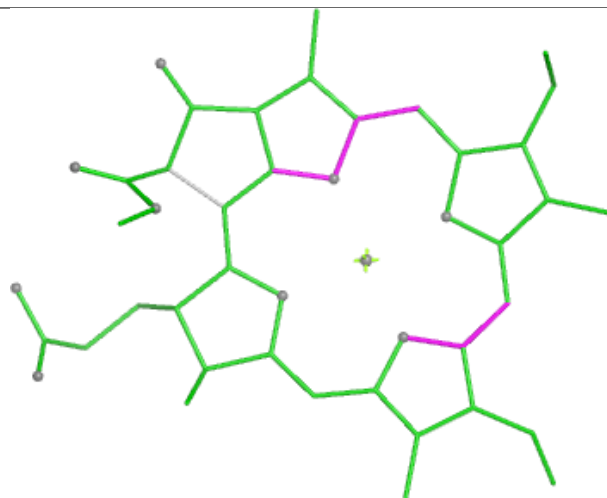


Ligand LMT c 317**Ligand CLA A 401**

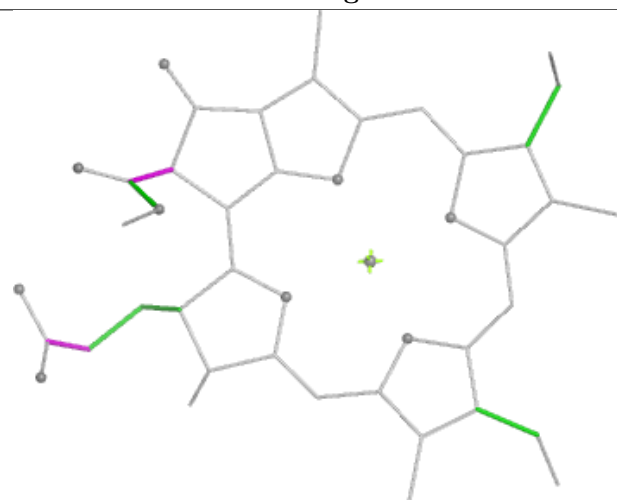
Ligand CLA f 313



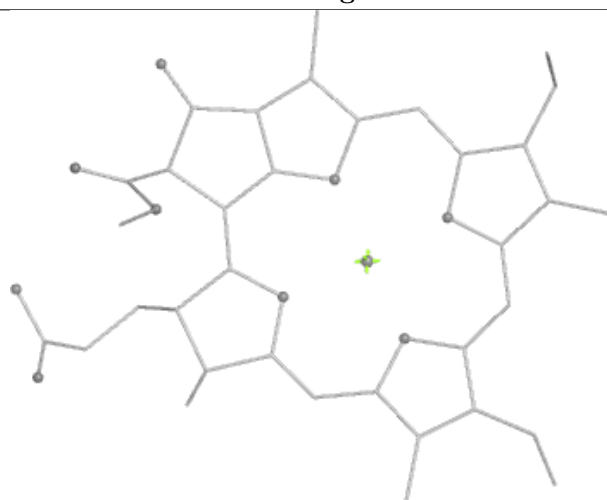
Bond lengths



Bond angles

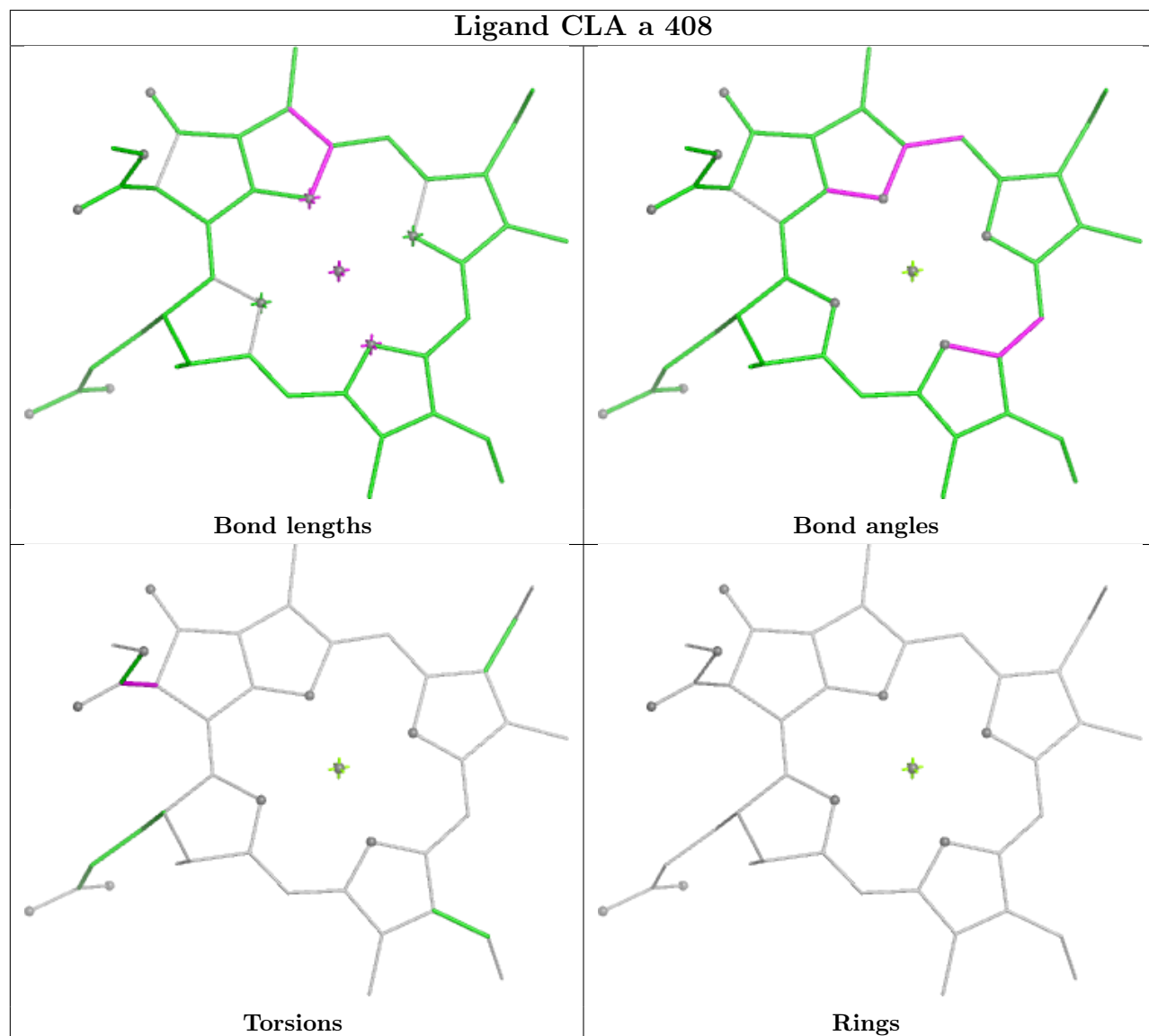


Torsions

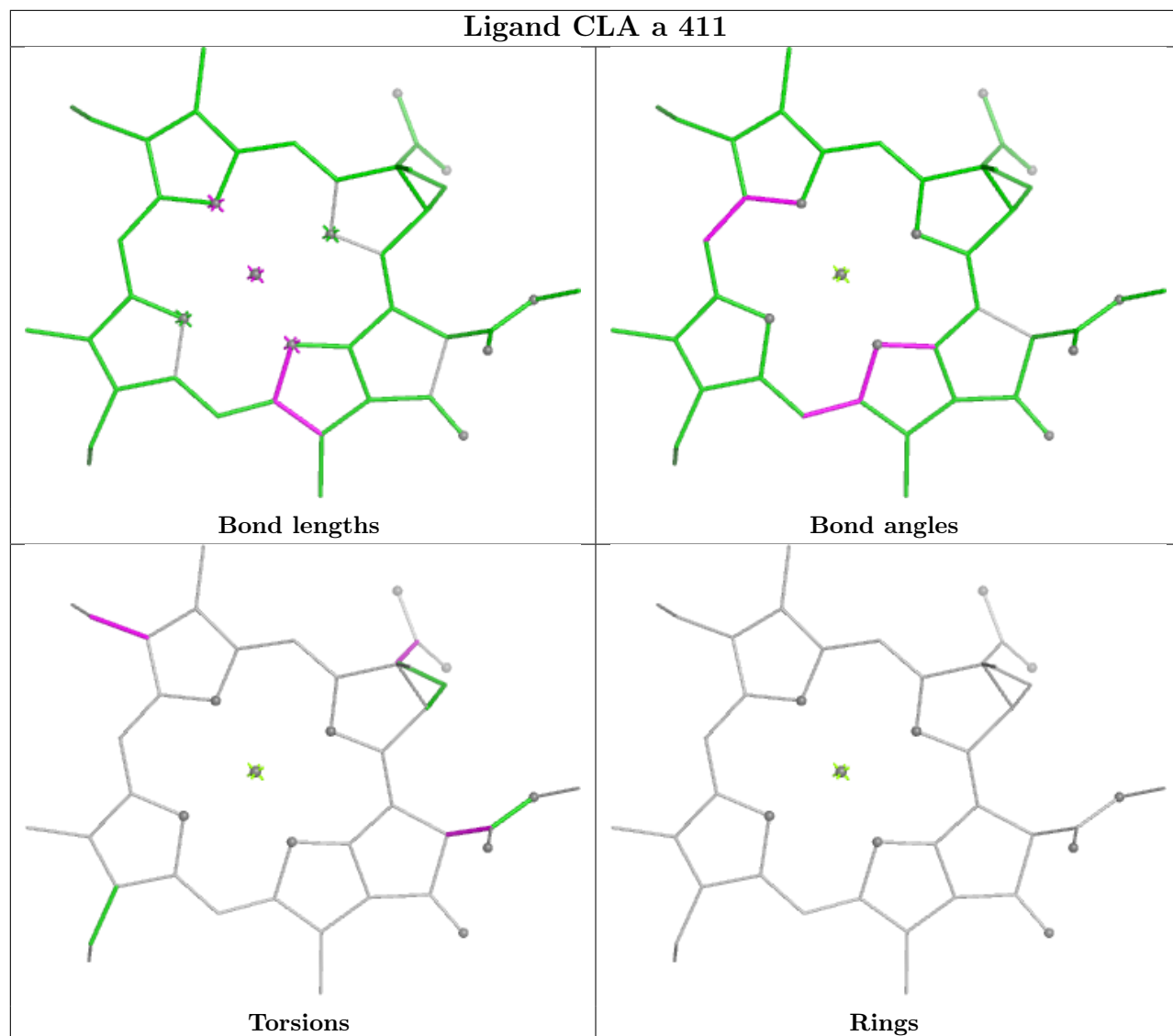


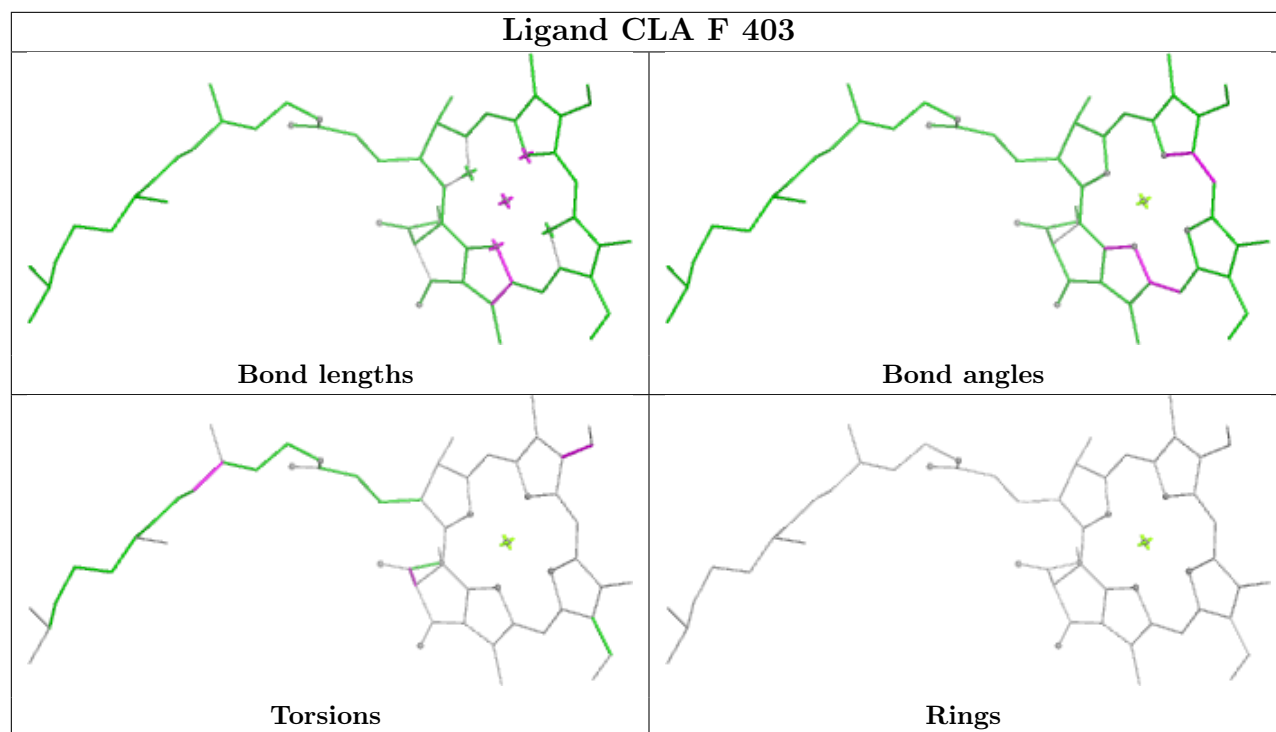
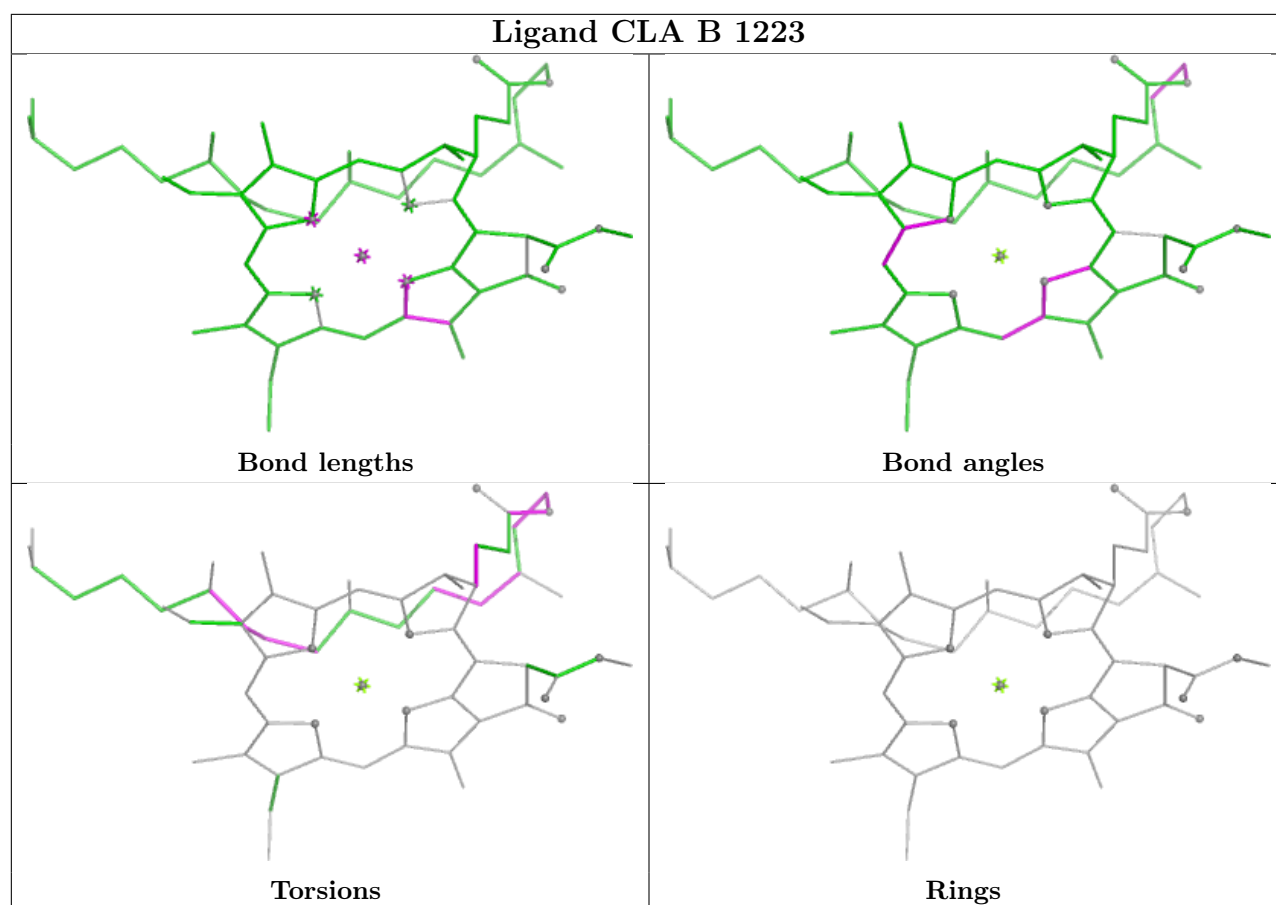
Rings

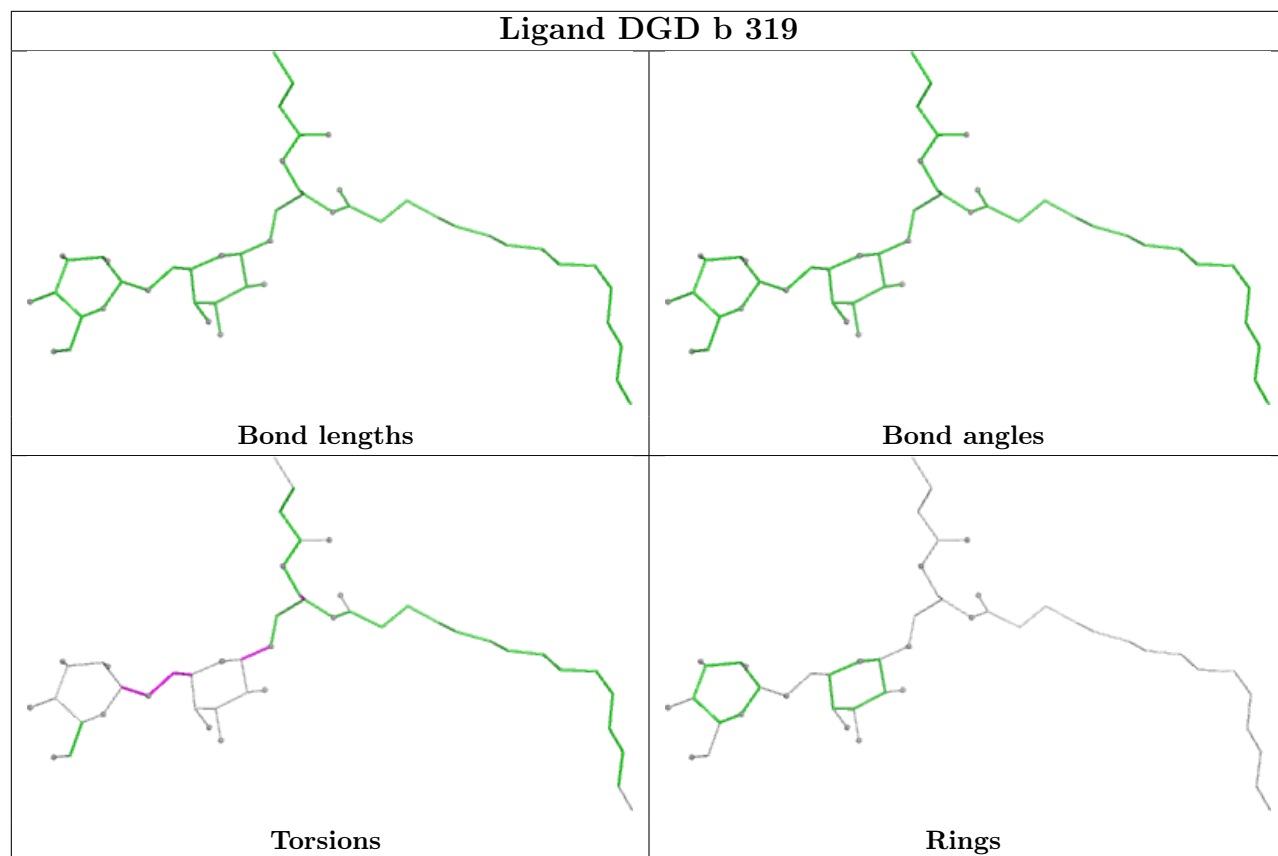
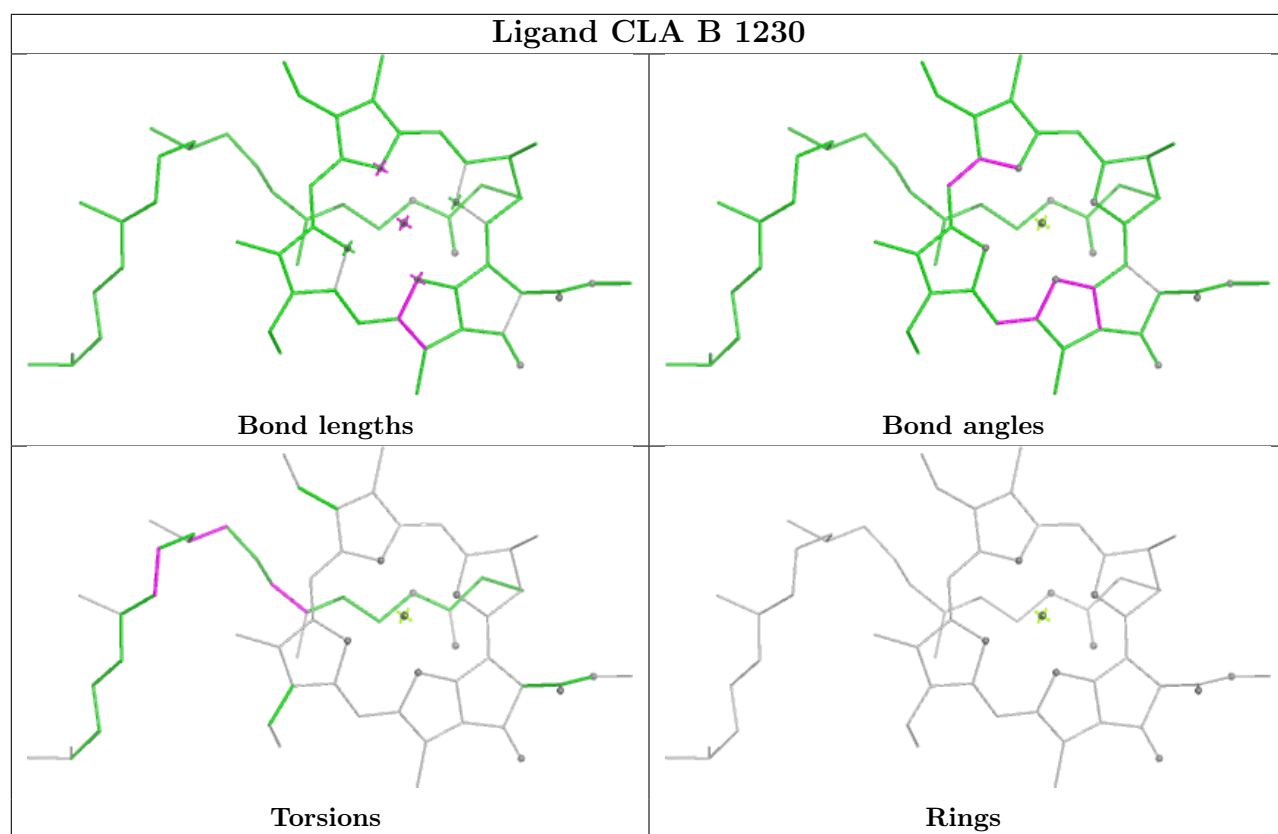
Ligand CLA a 408

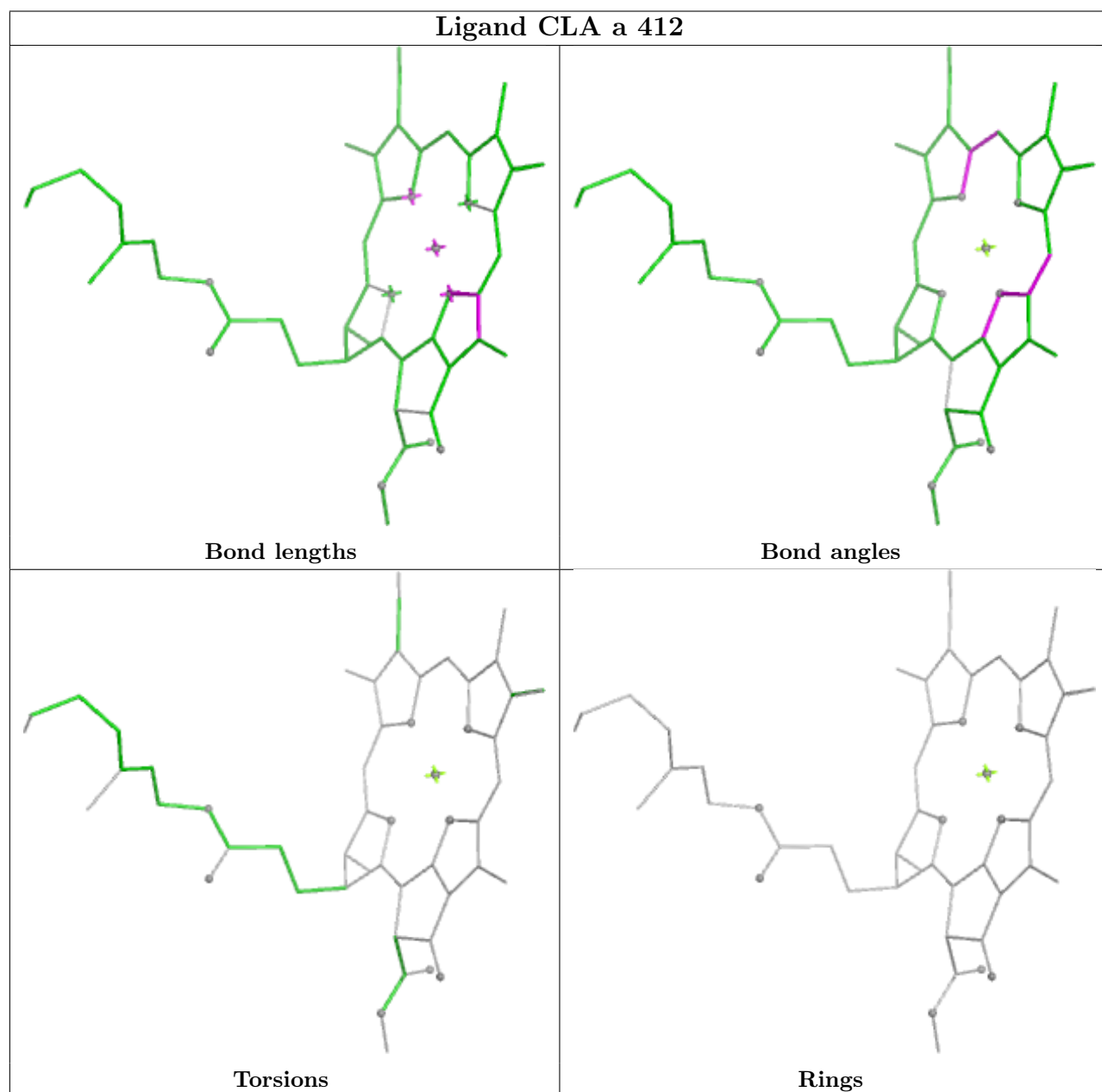
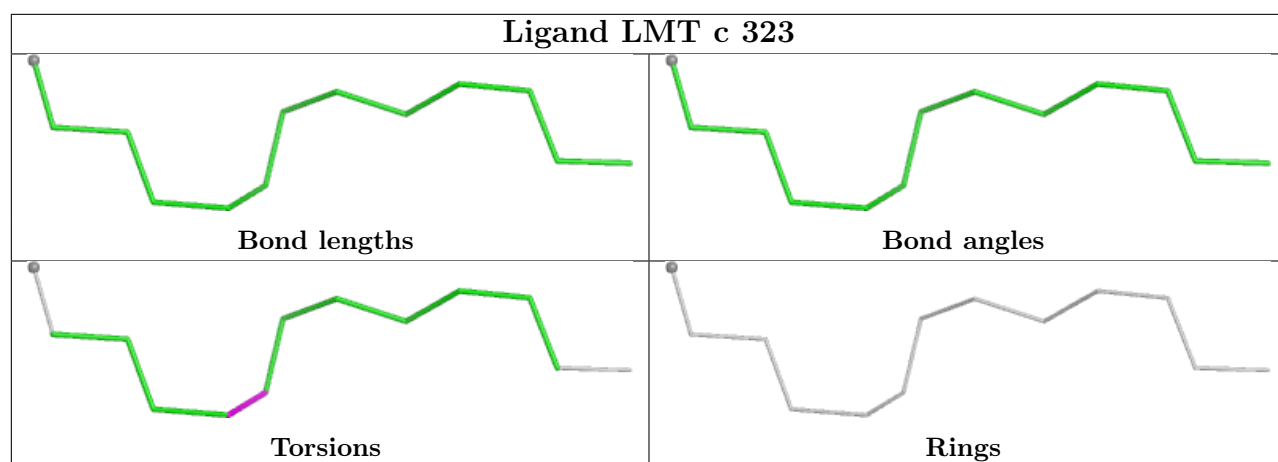


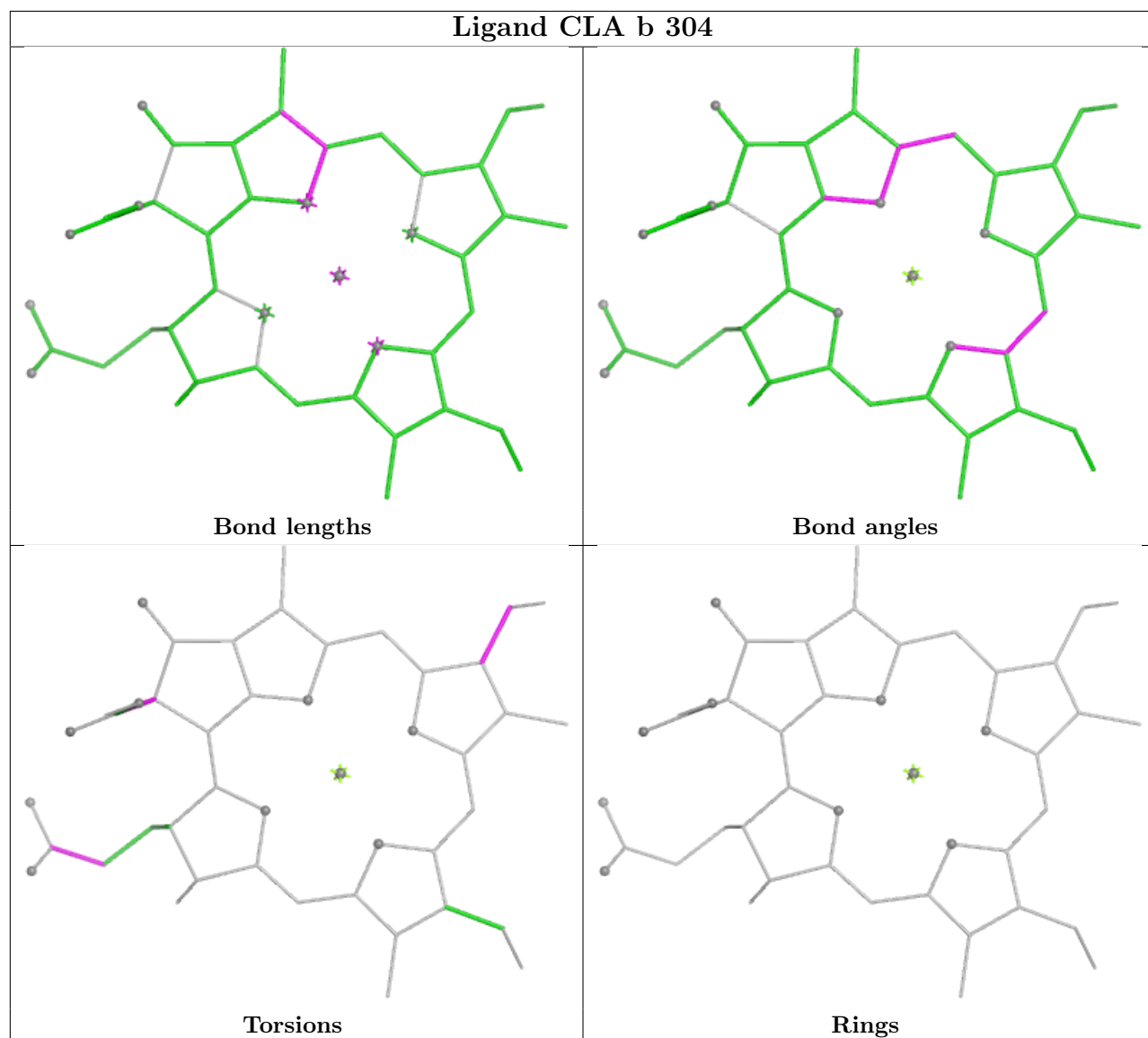
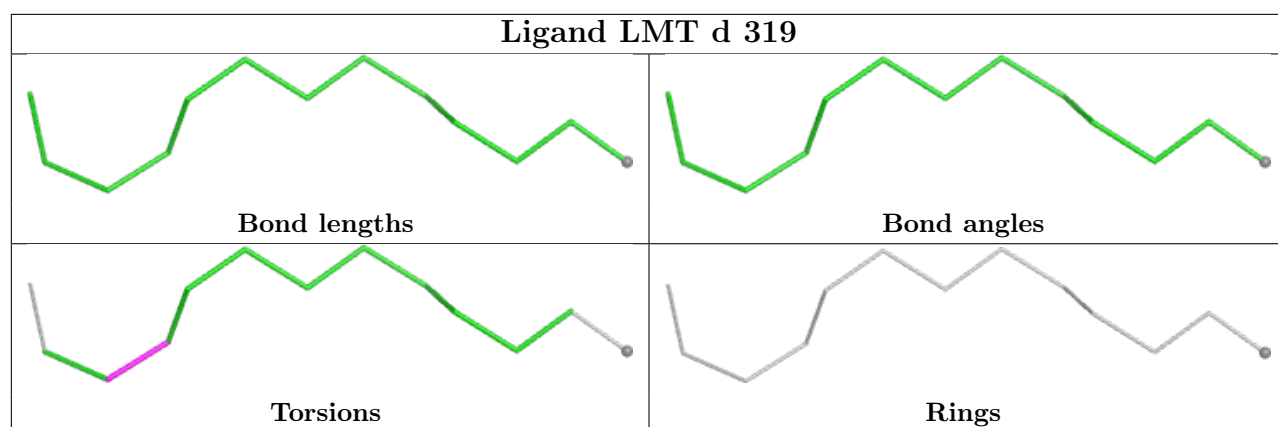
Ligand CLA a 411

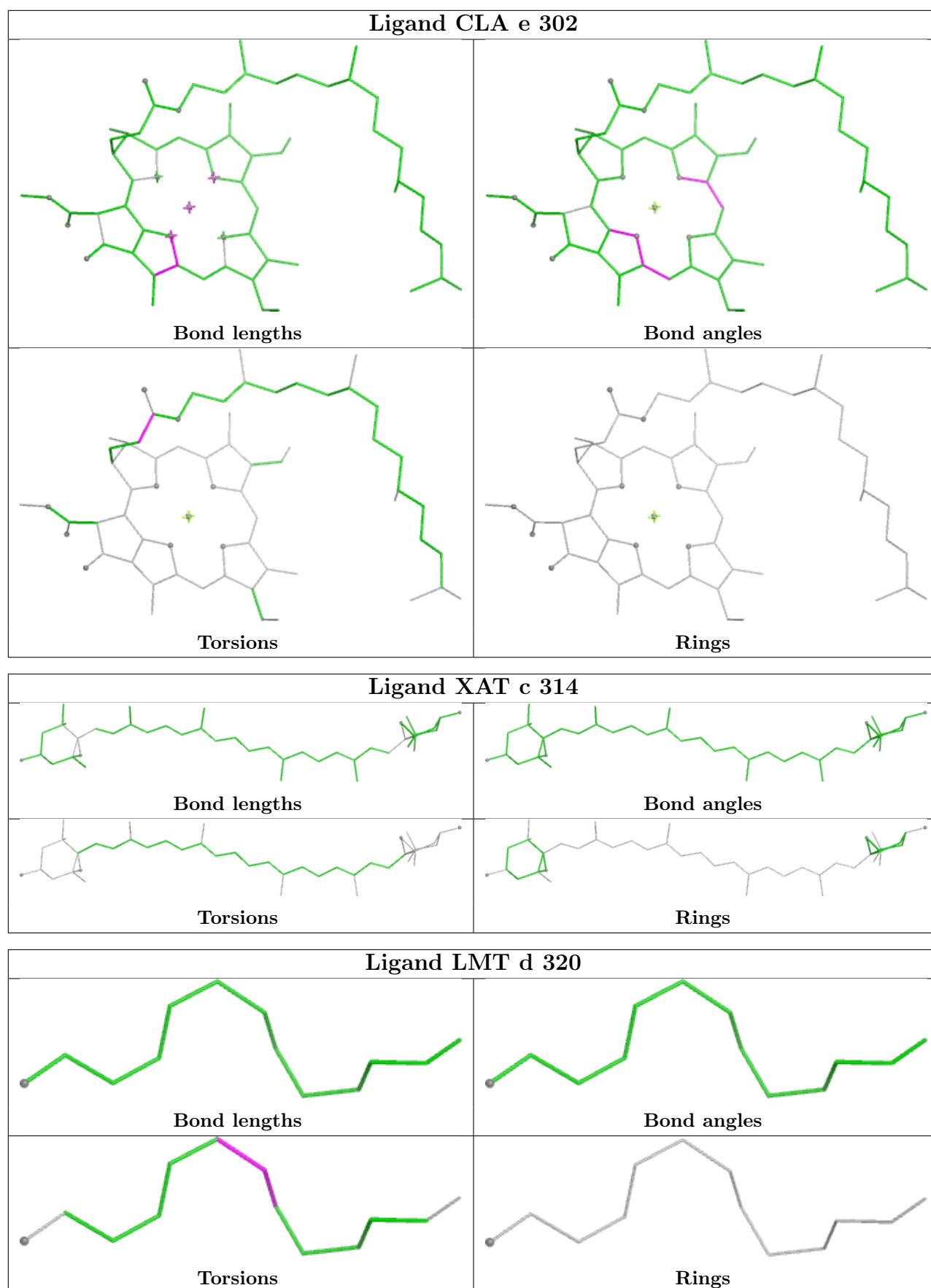


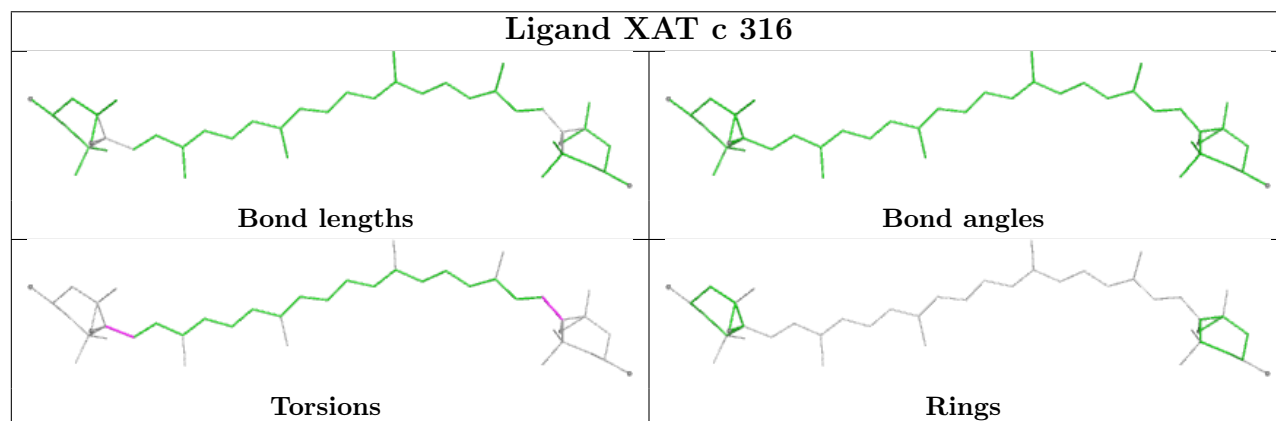
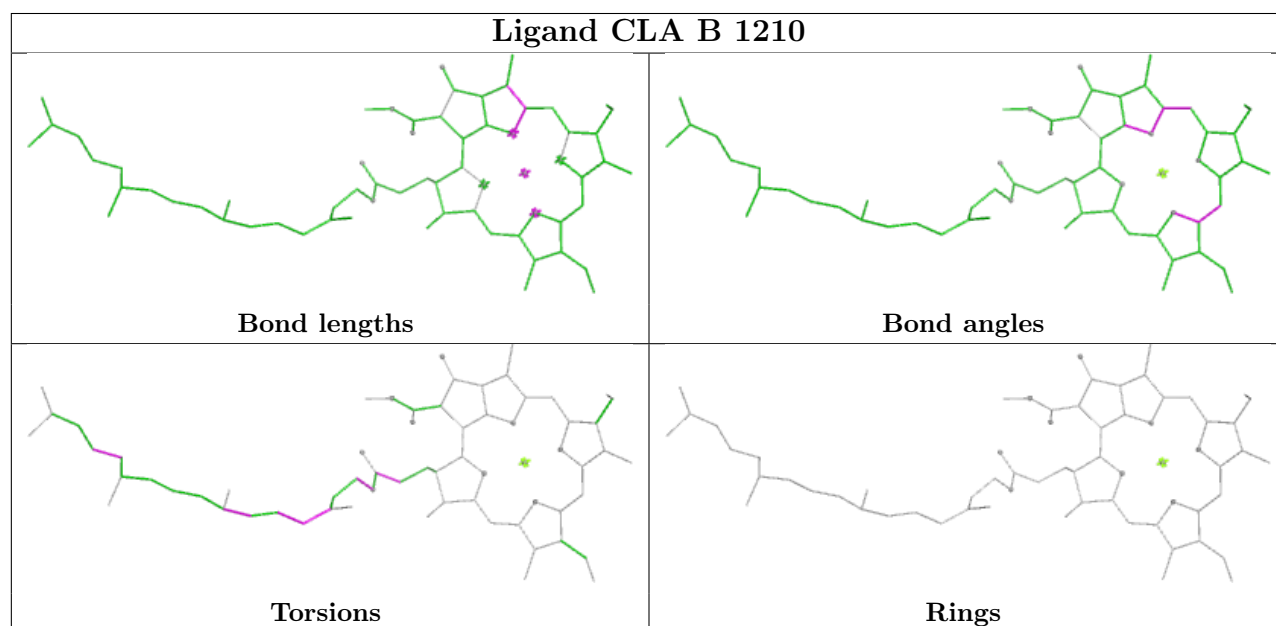
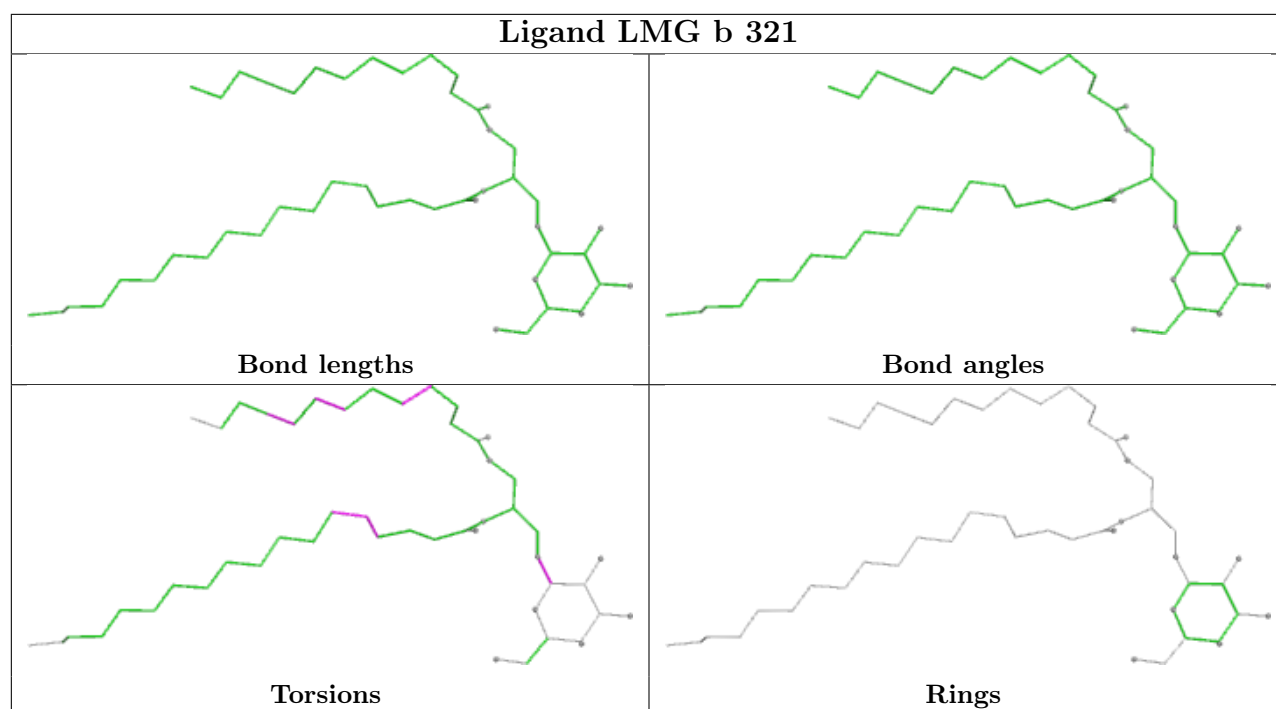


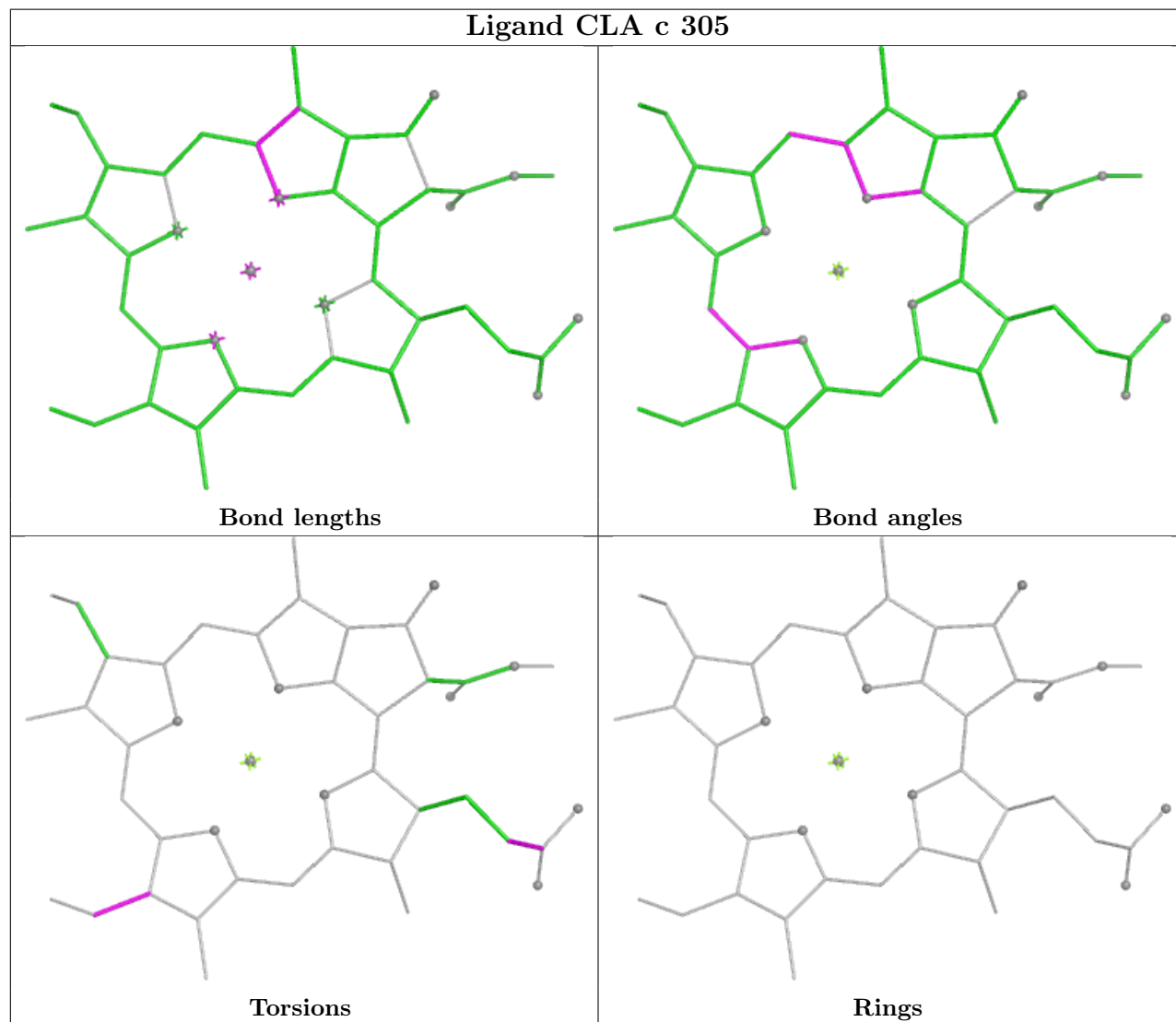
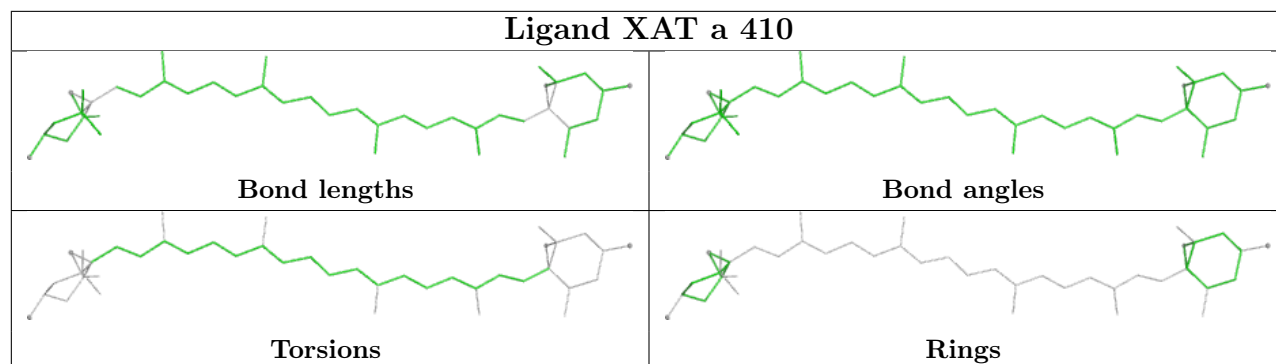


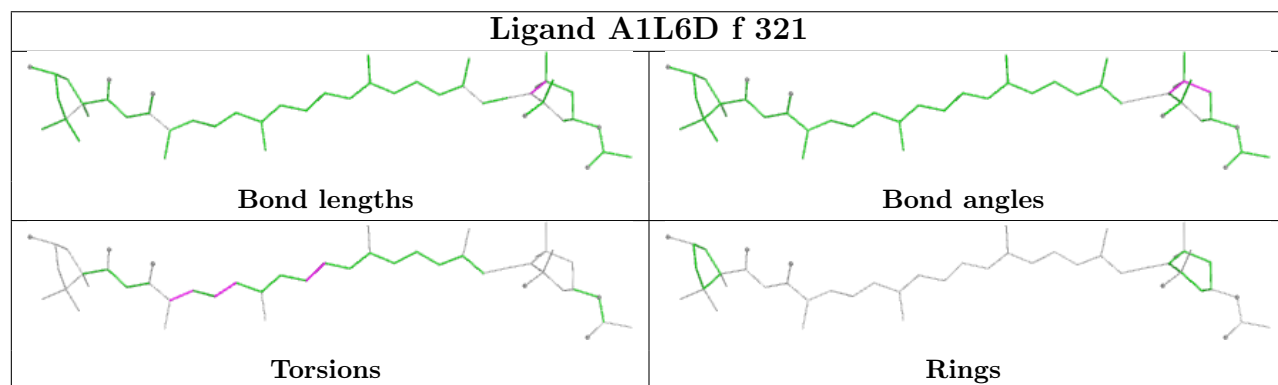
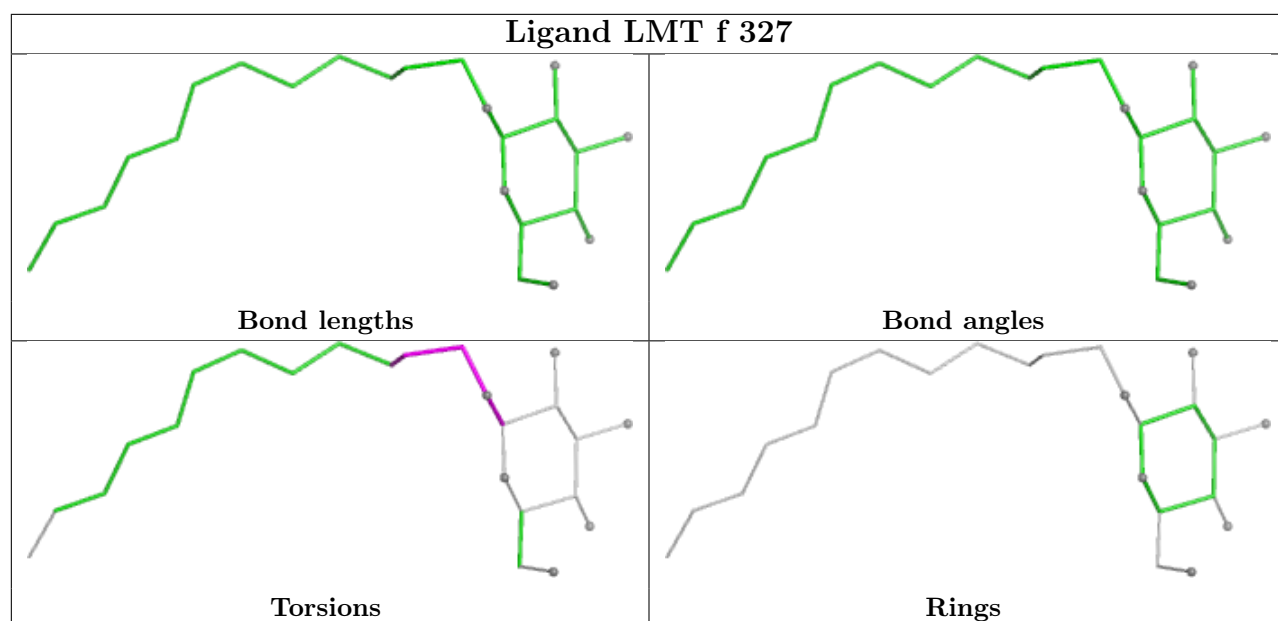


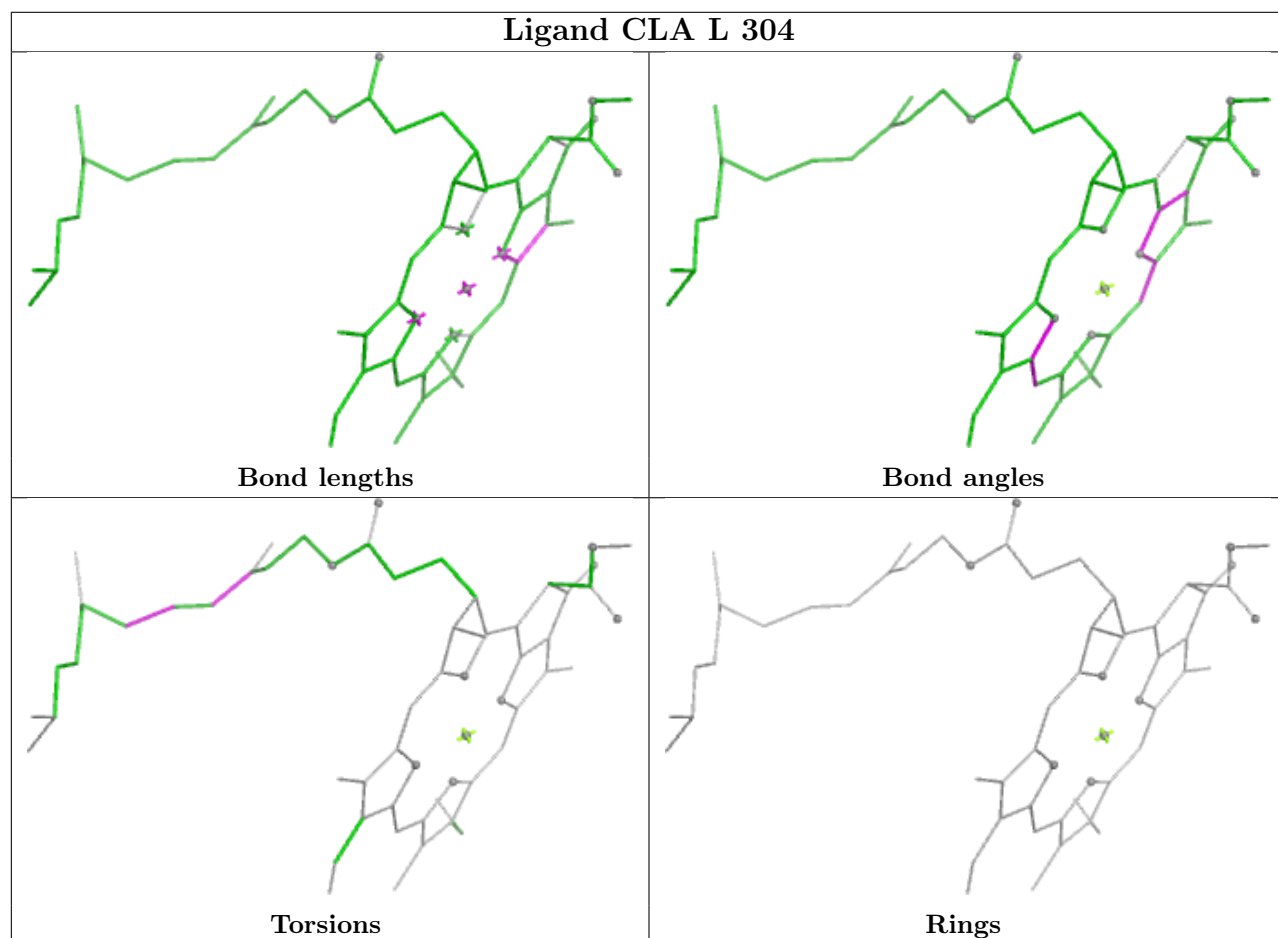
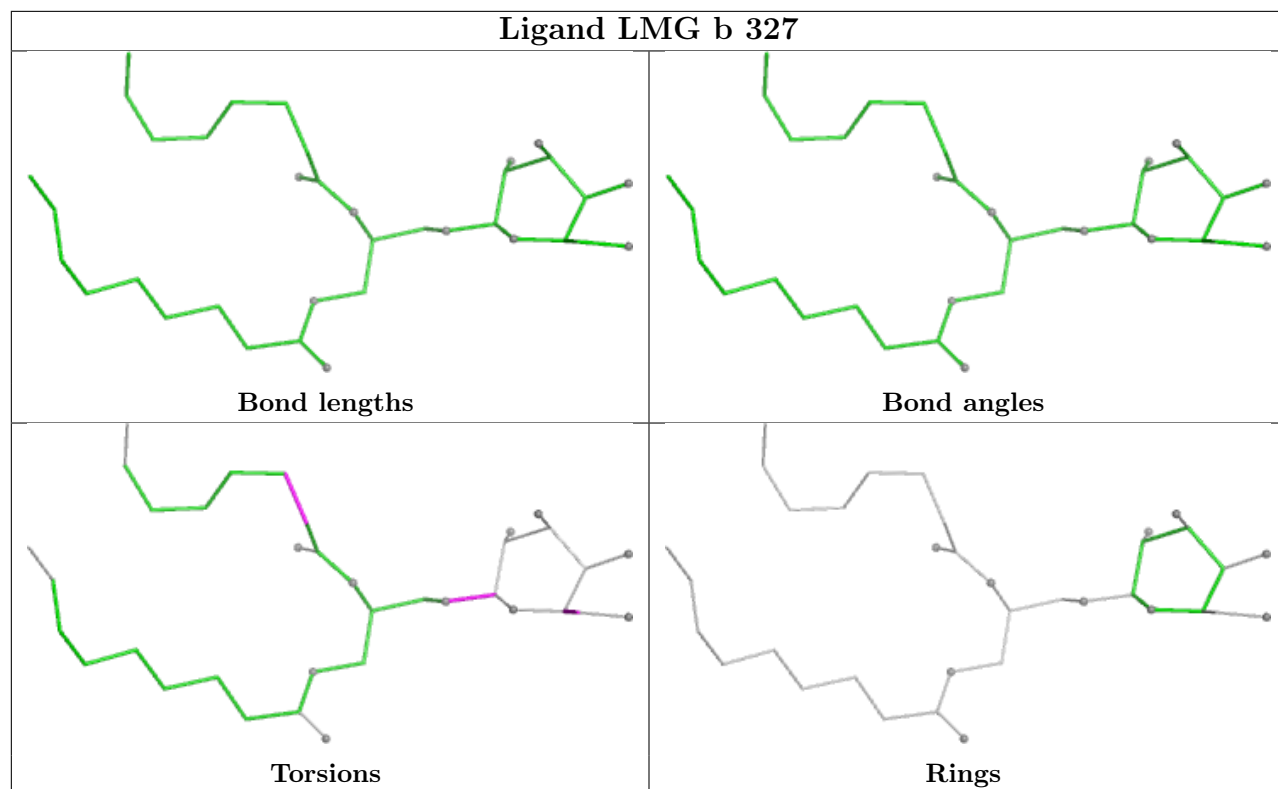




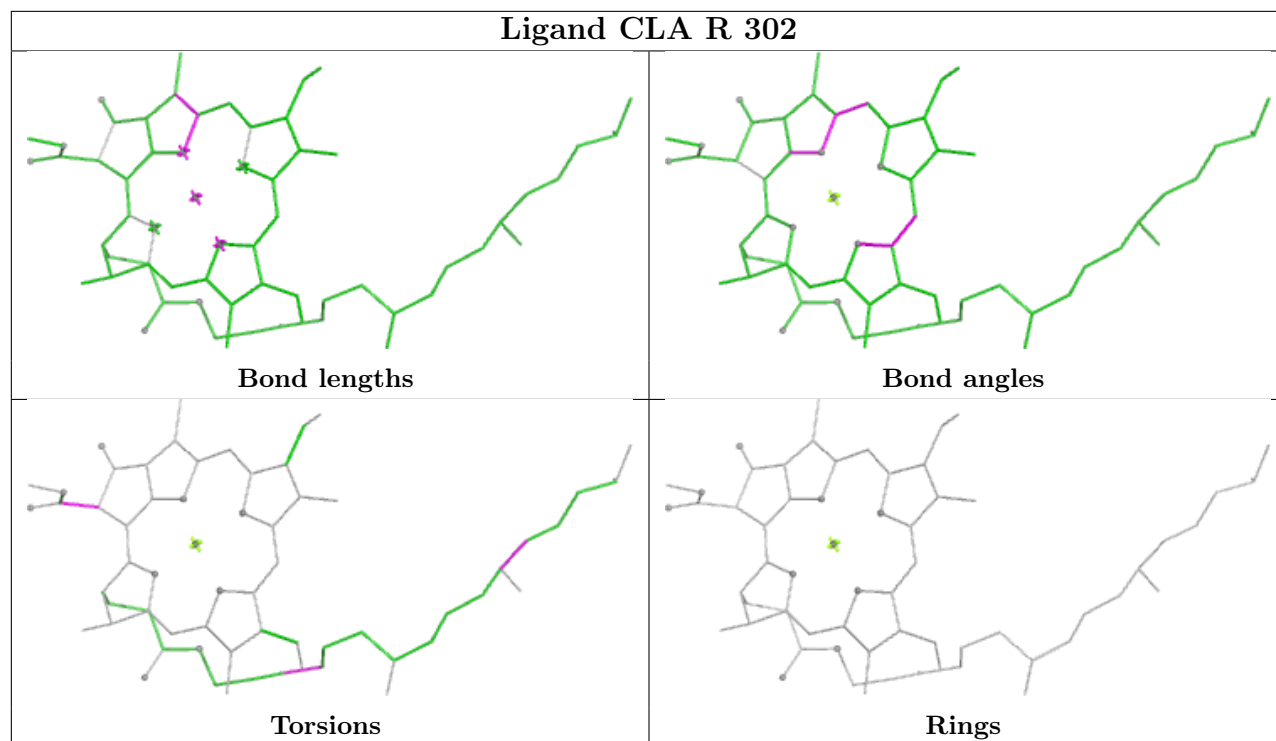




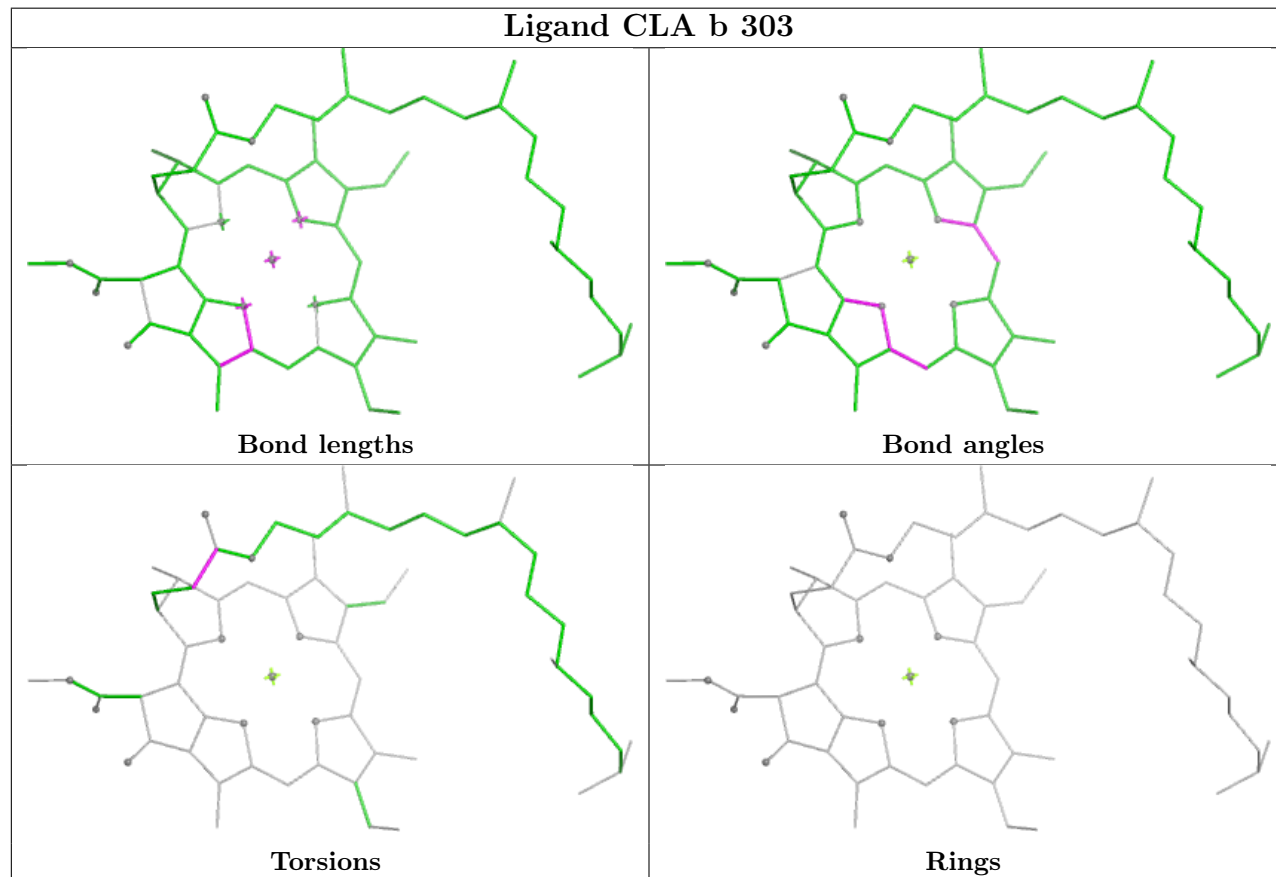


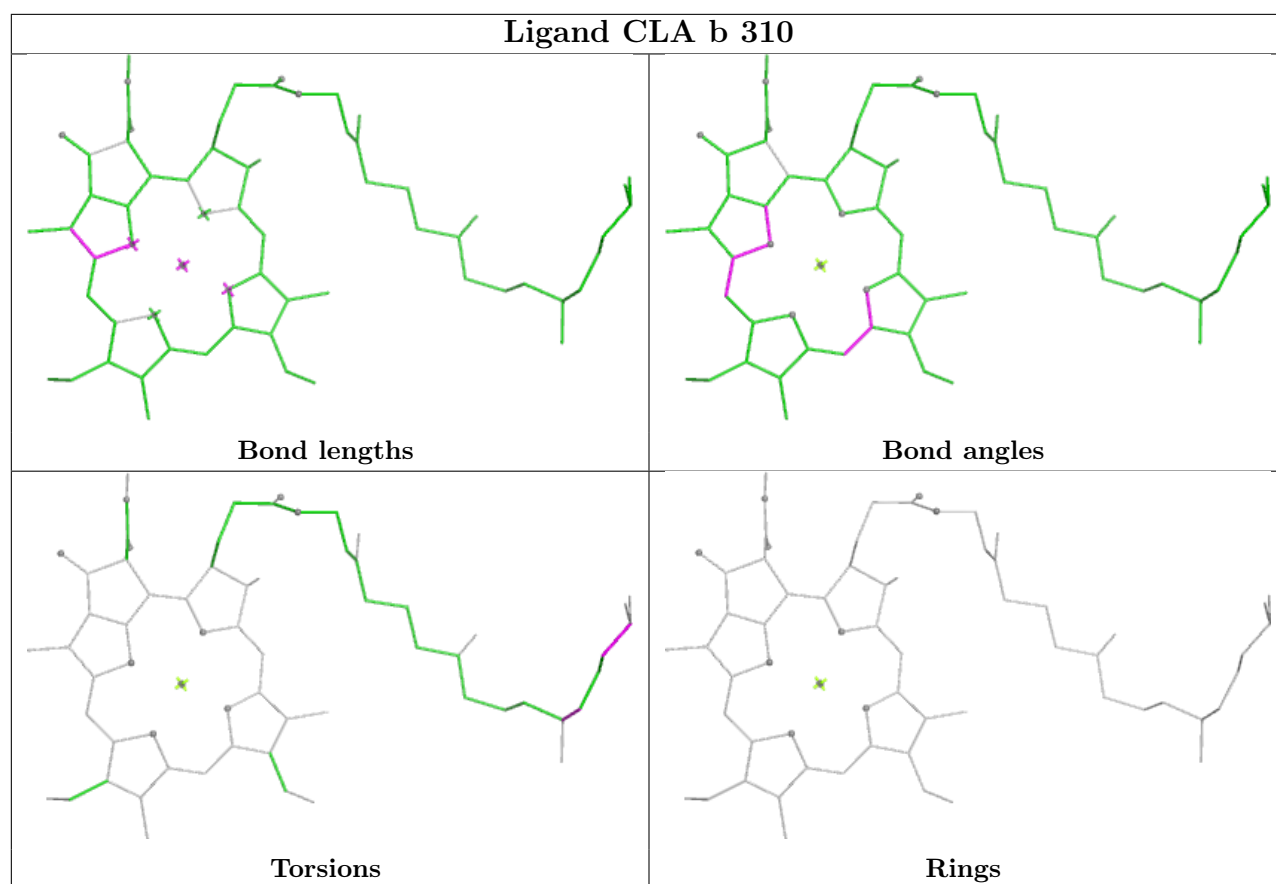


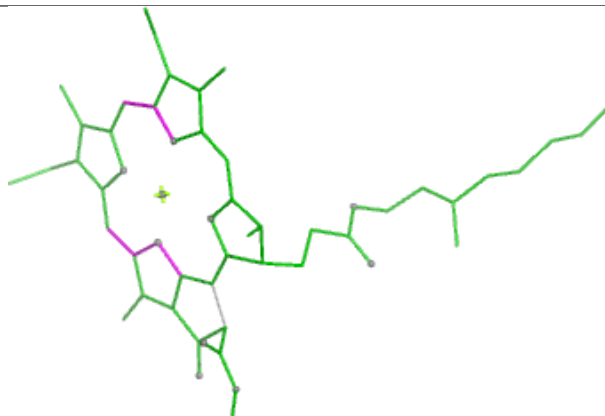
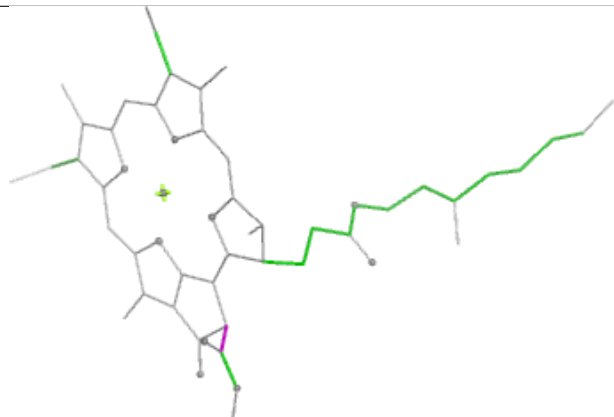
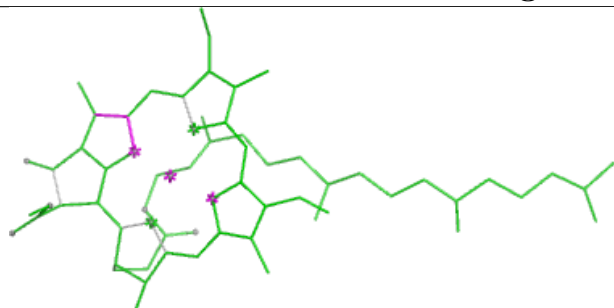
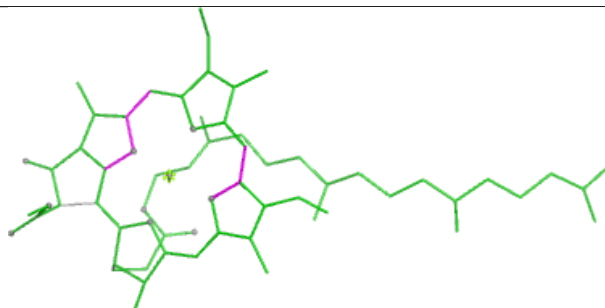
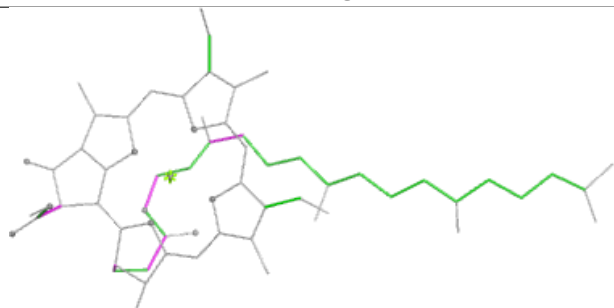
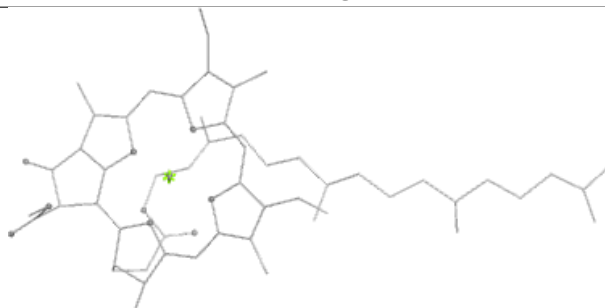
Ligand CLA R 302



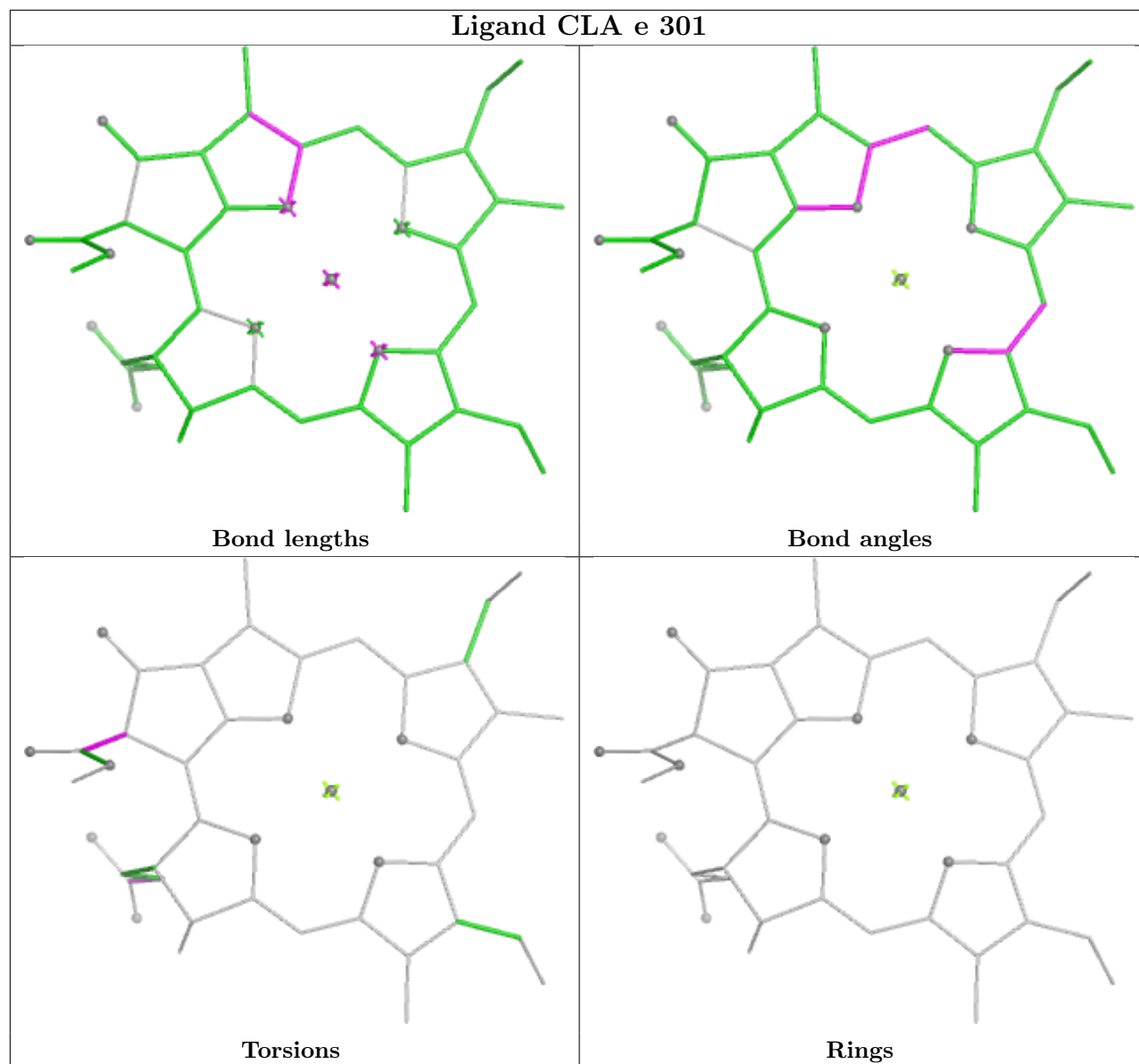
Ligand CLA b 303



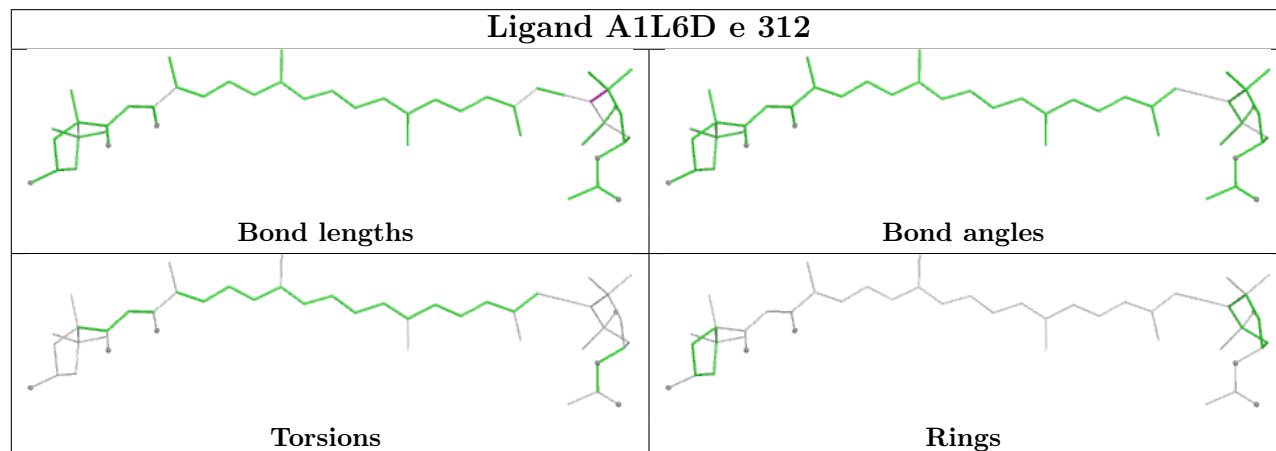


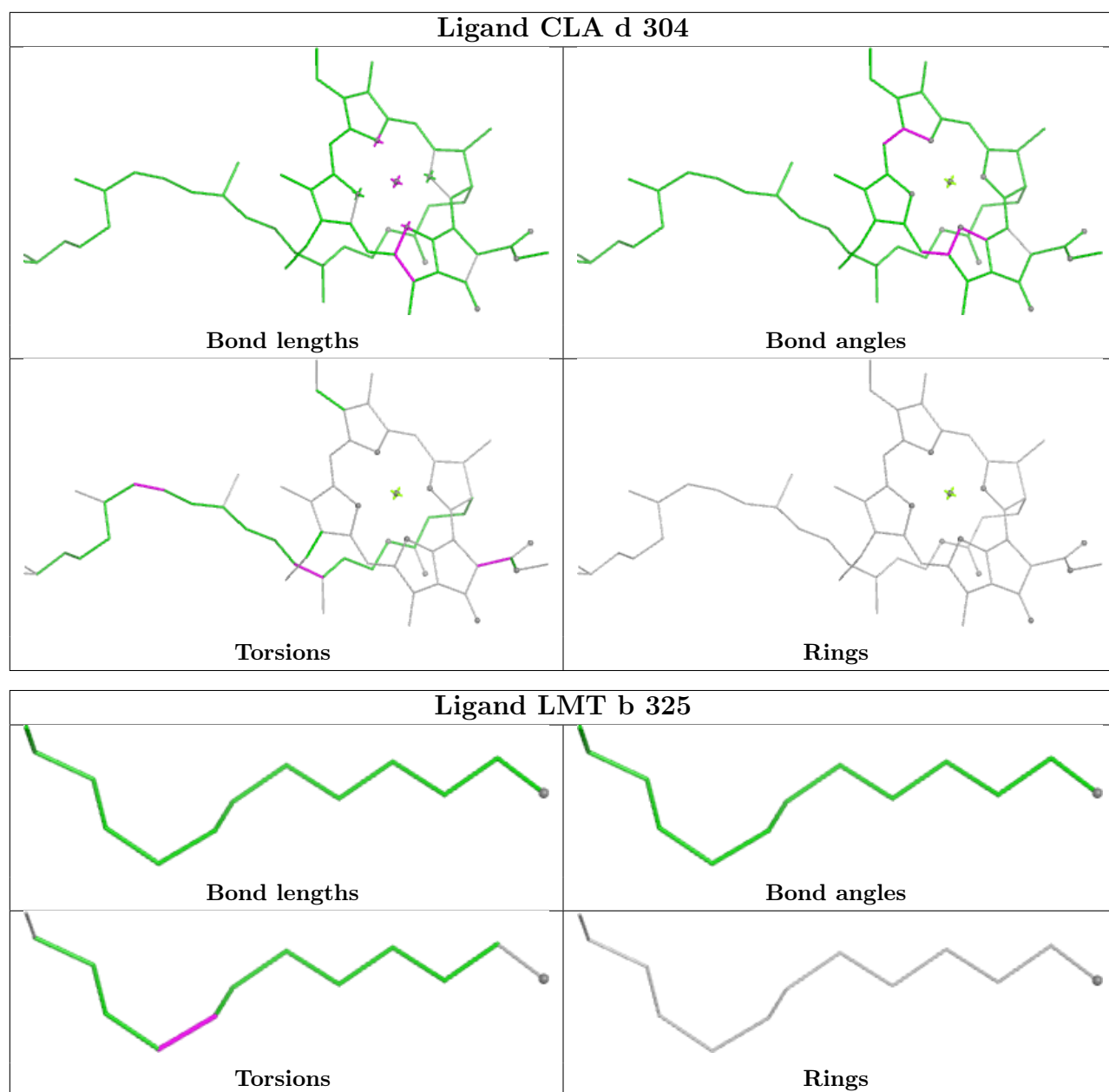
Ligand CLA b 312**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA c 312****Bond lengths****Bond angles****Torsions****Rings**

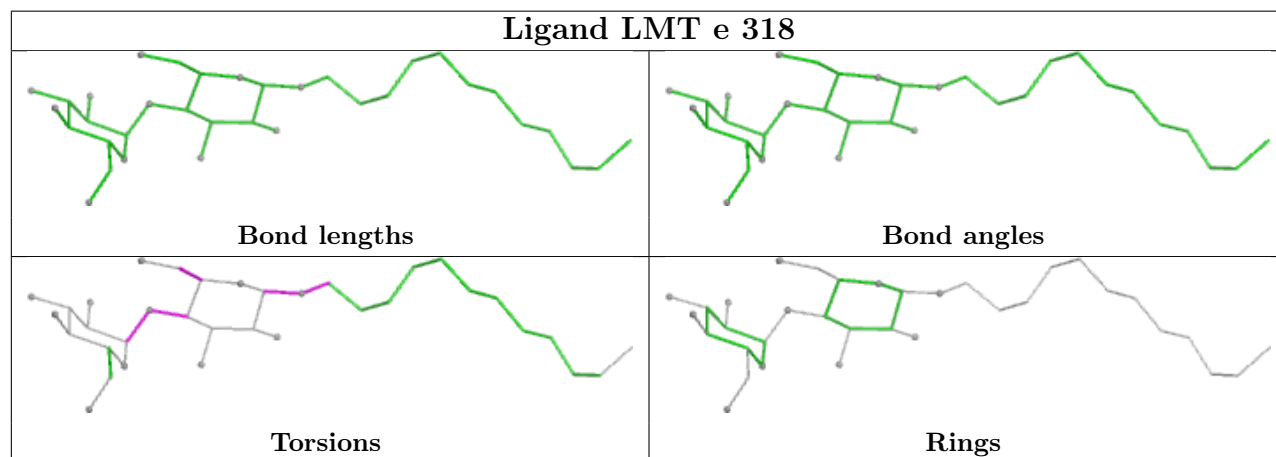
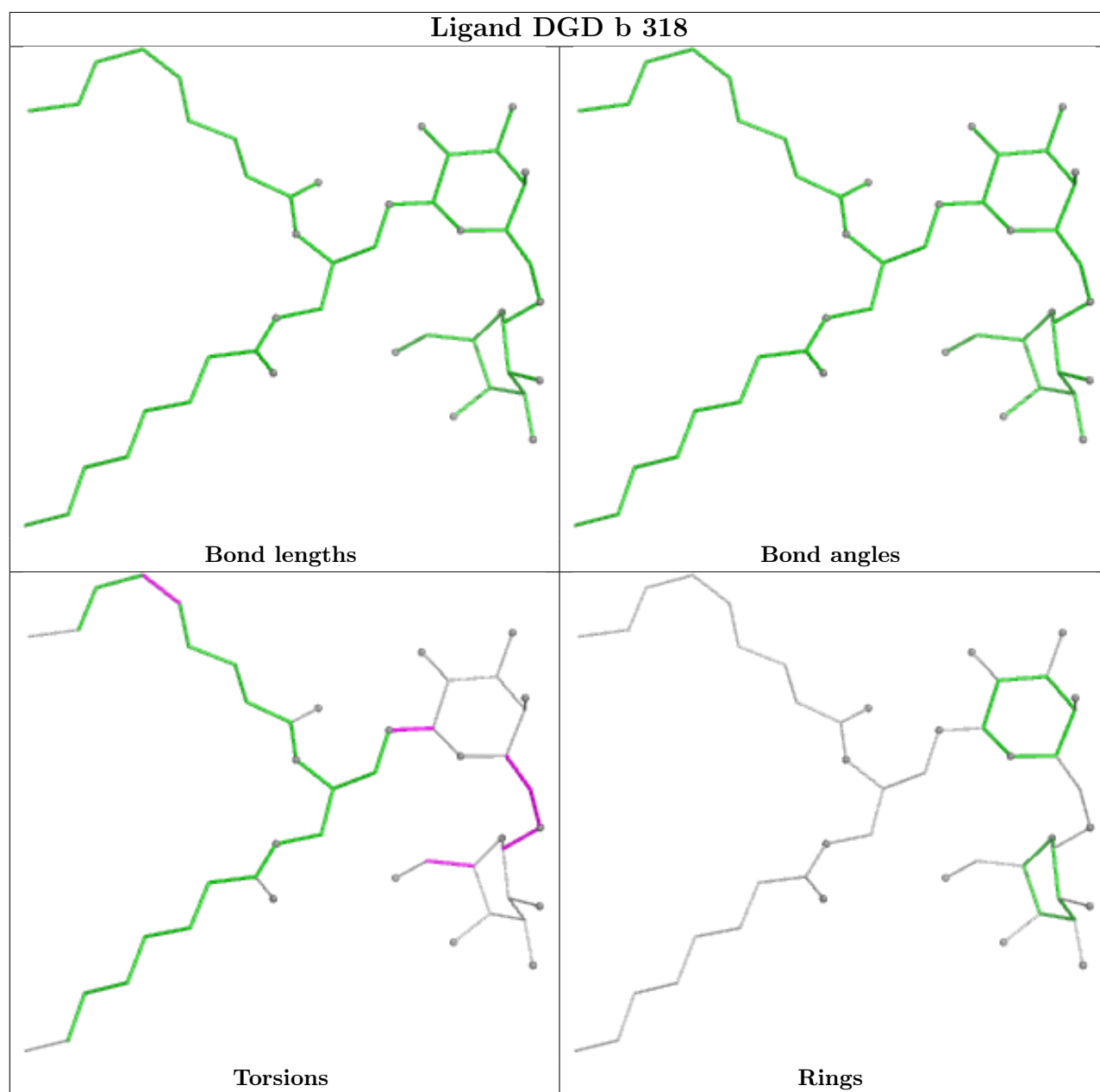
Ligand CLA e 301

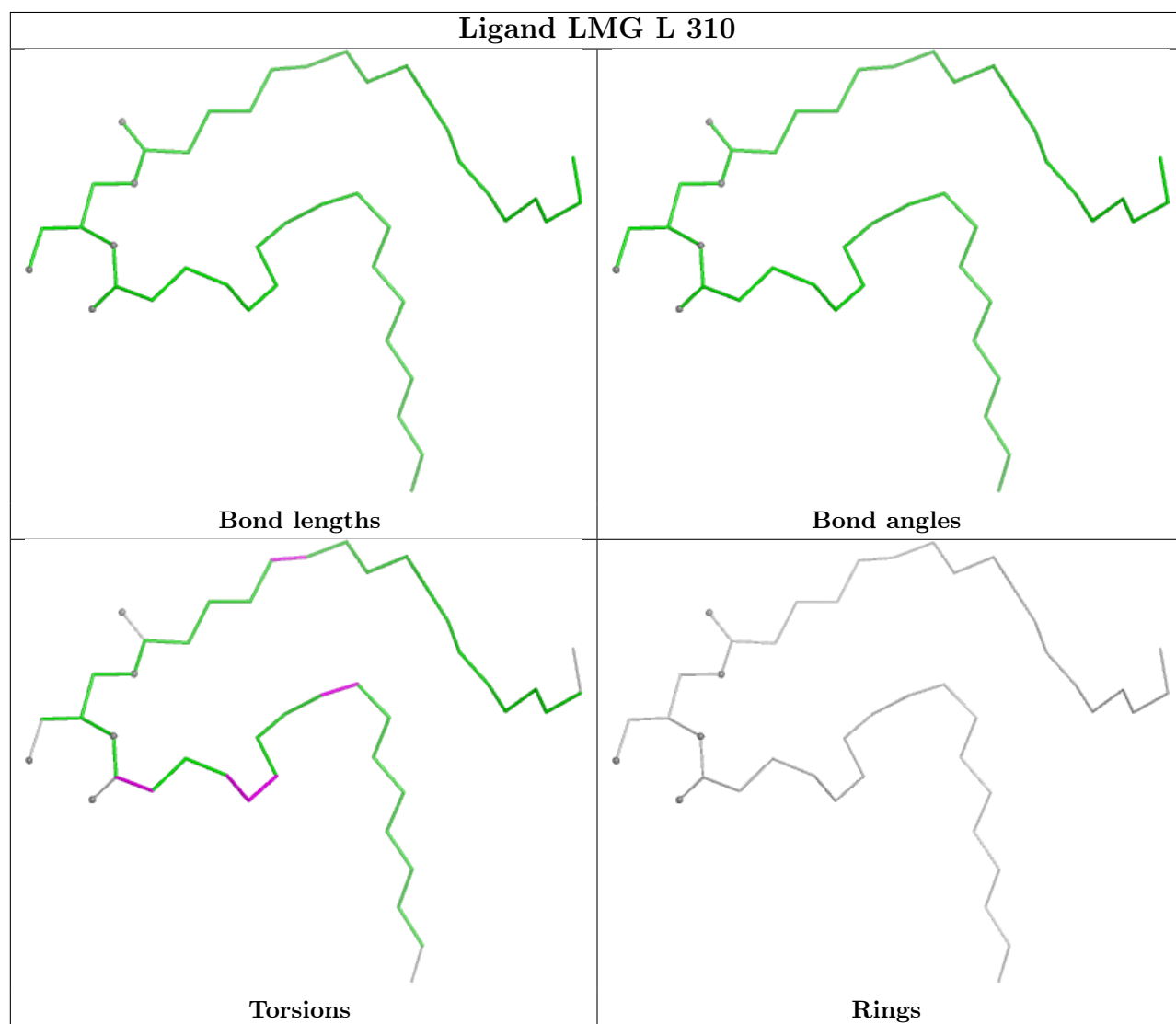
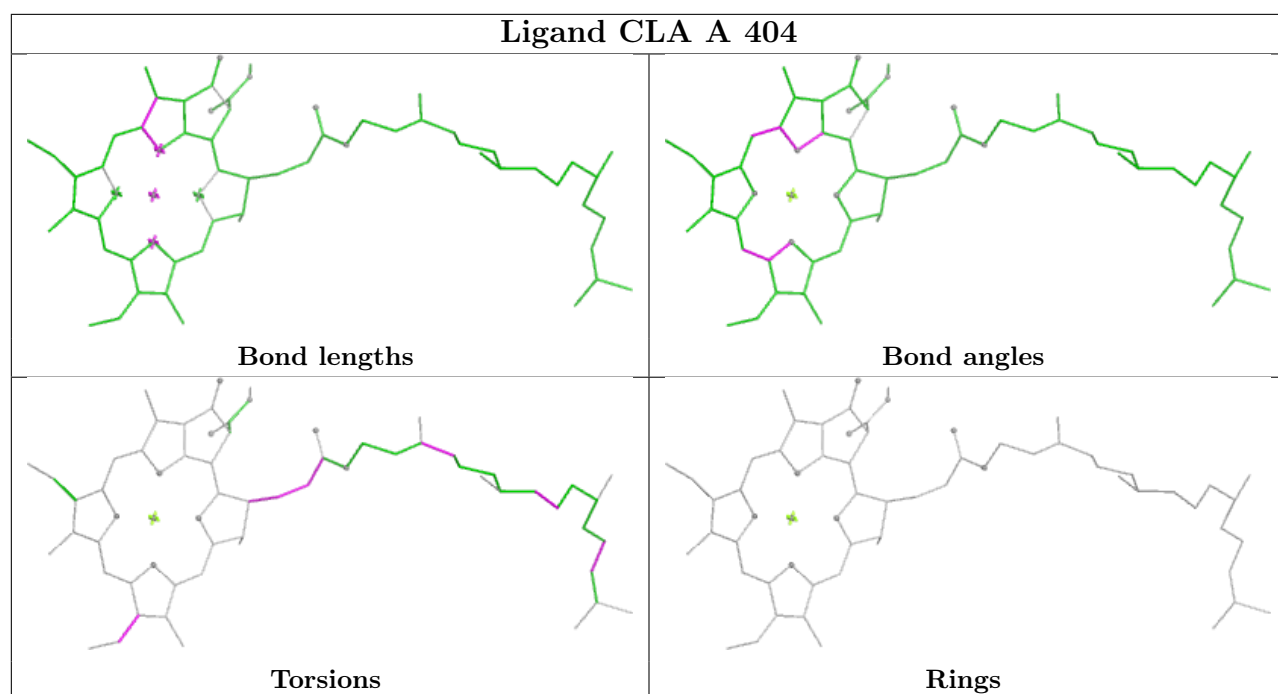


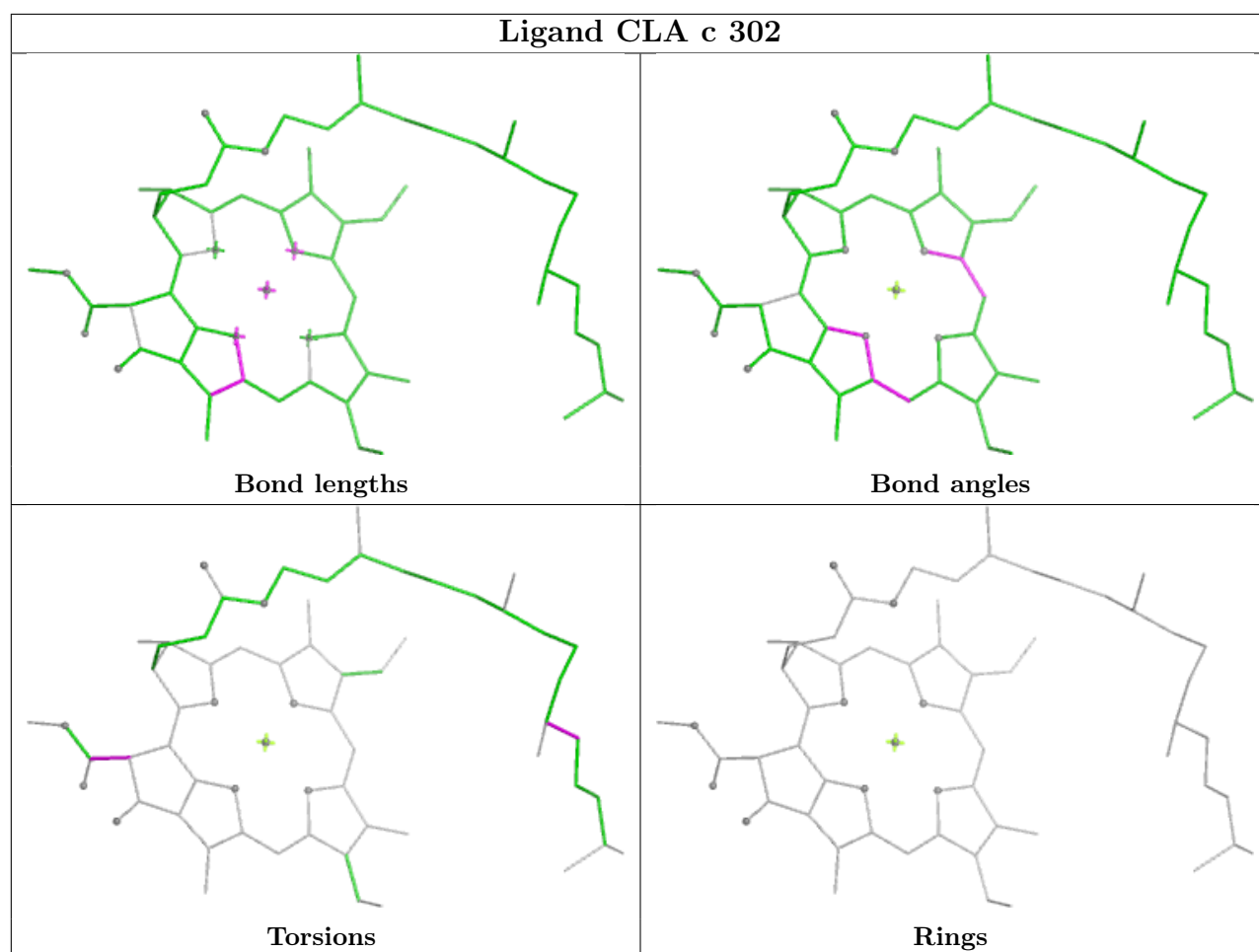
Ligand A1L6D e 312

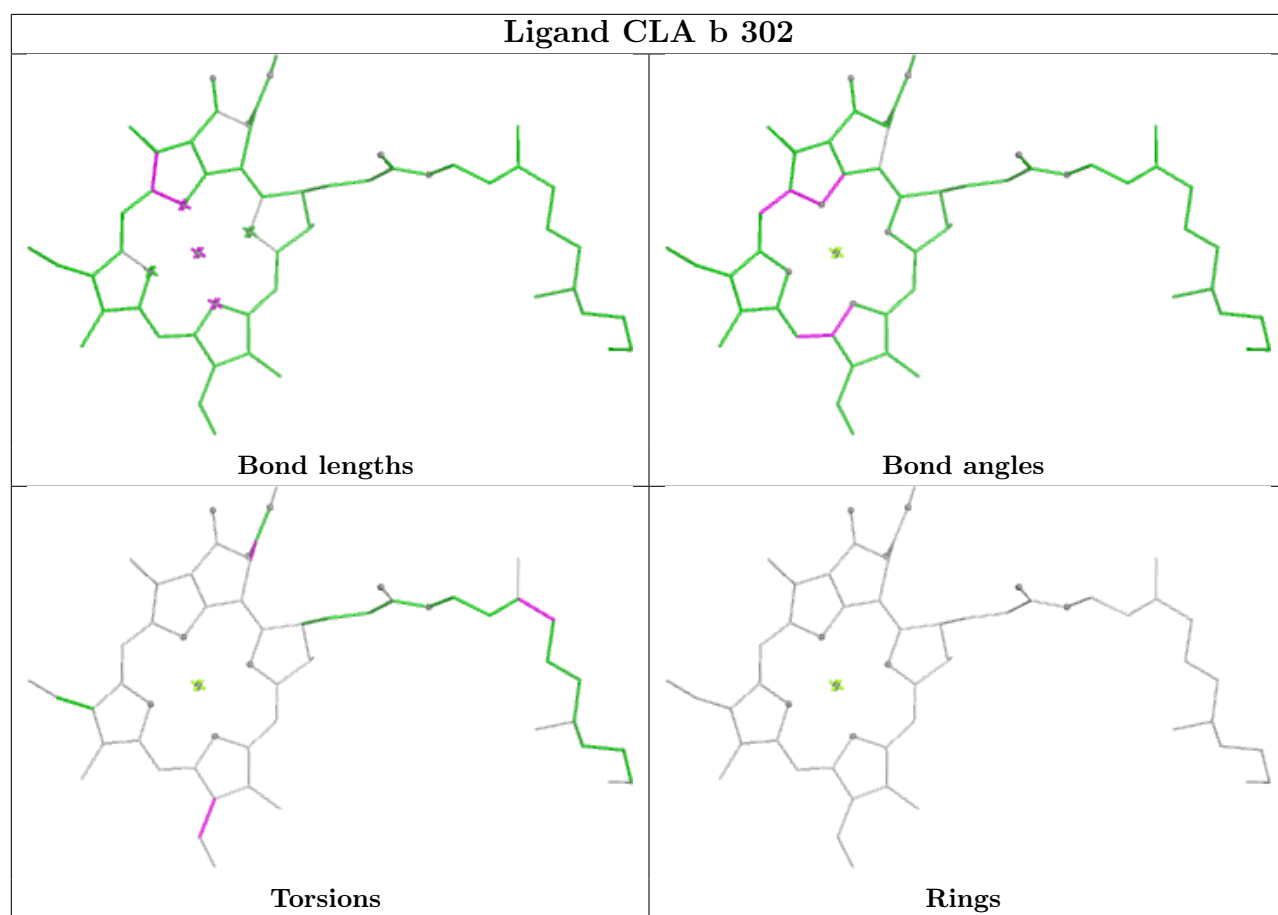




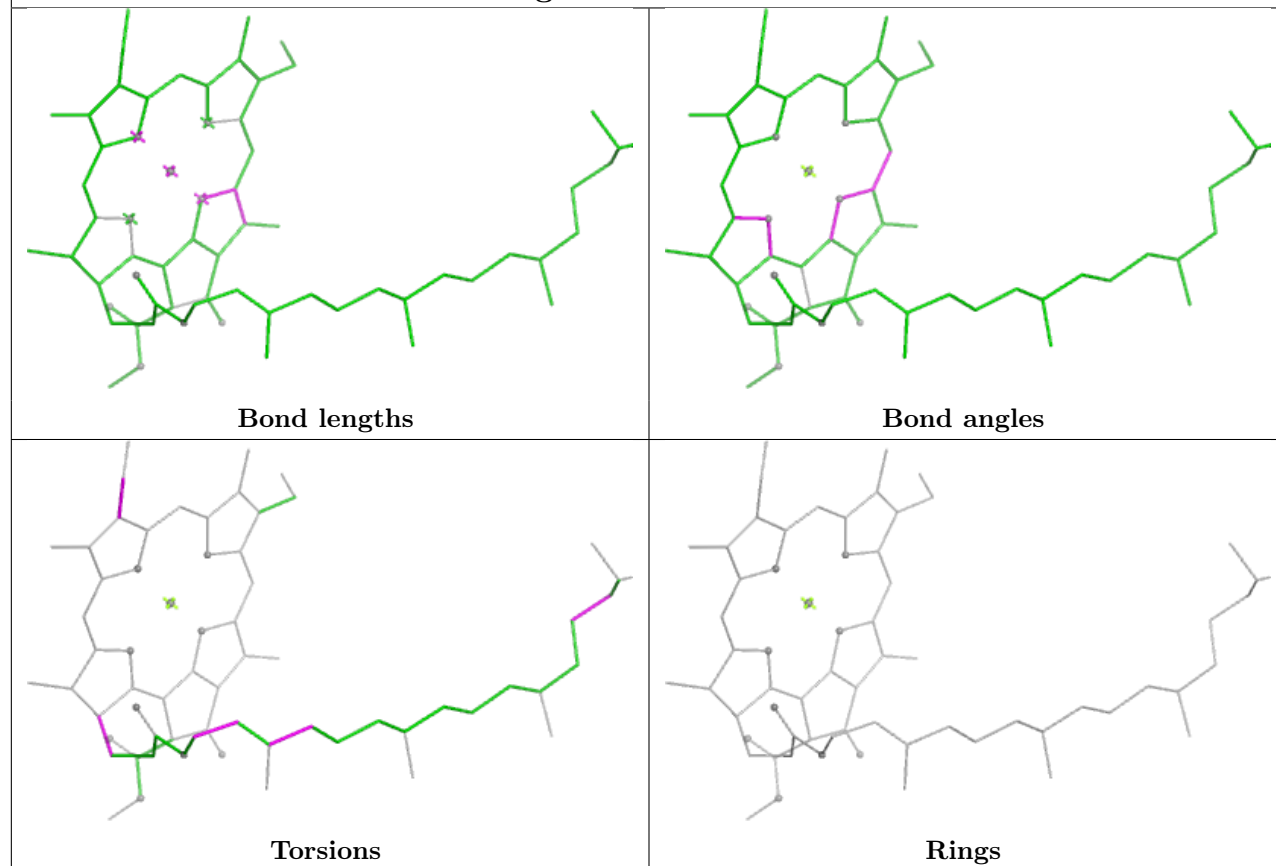




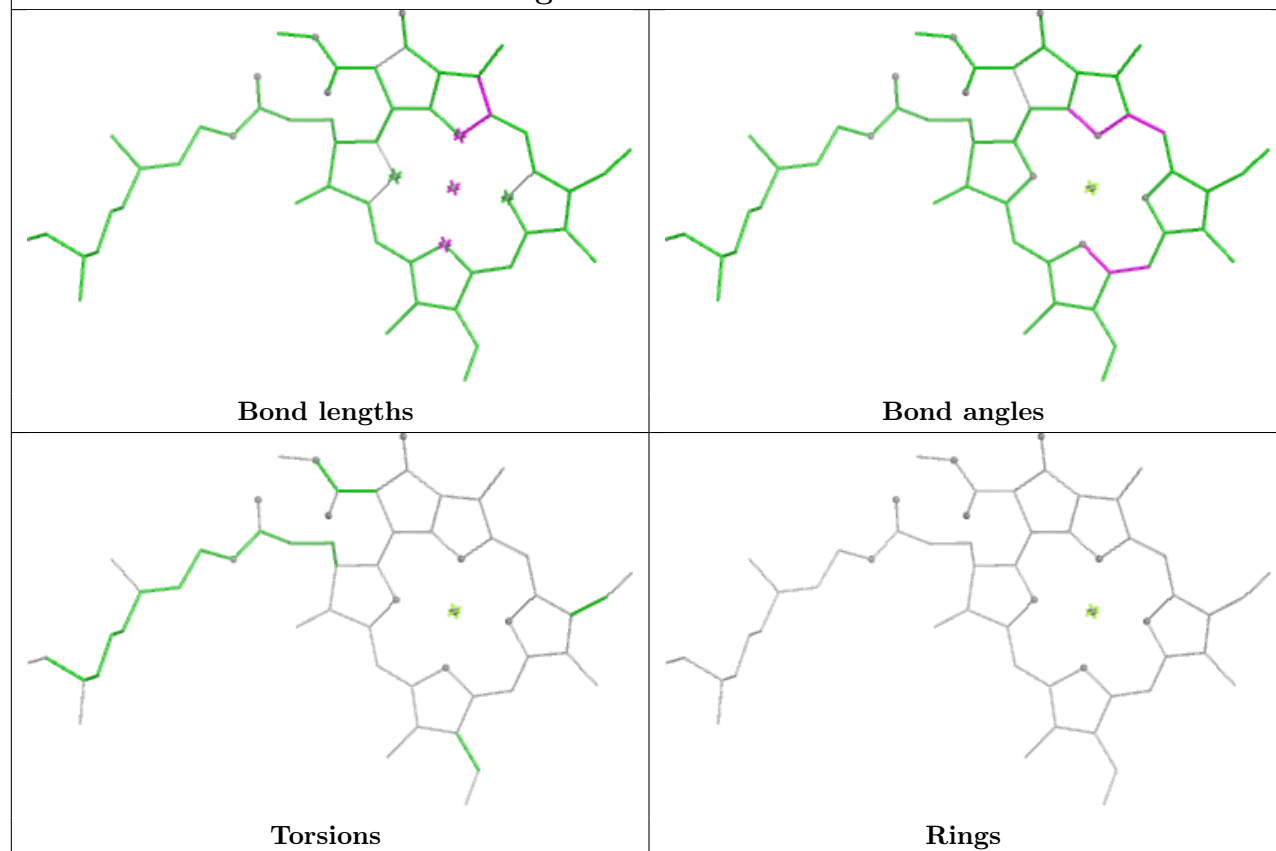


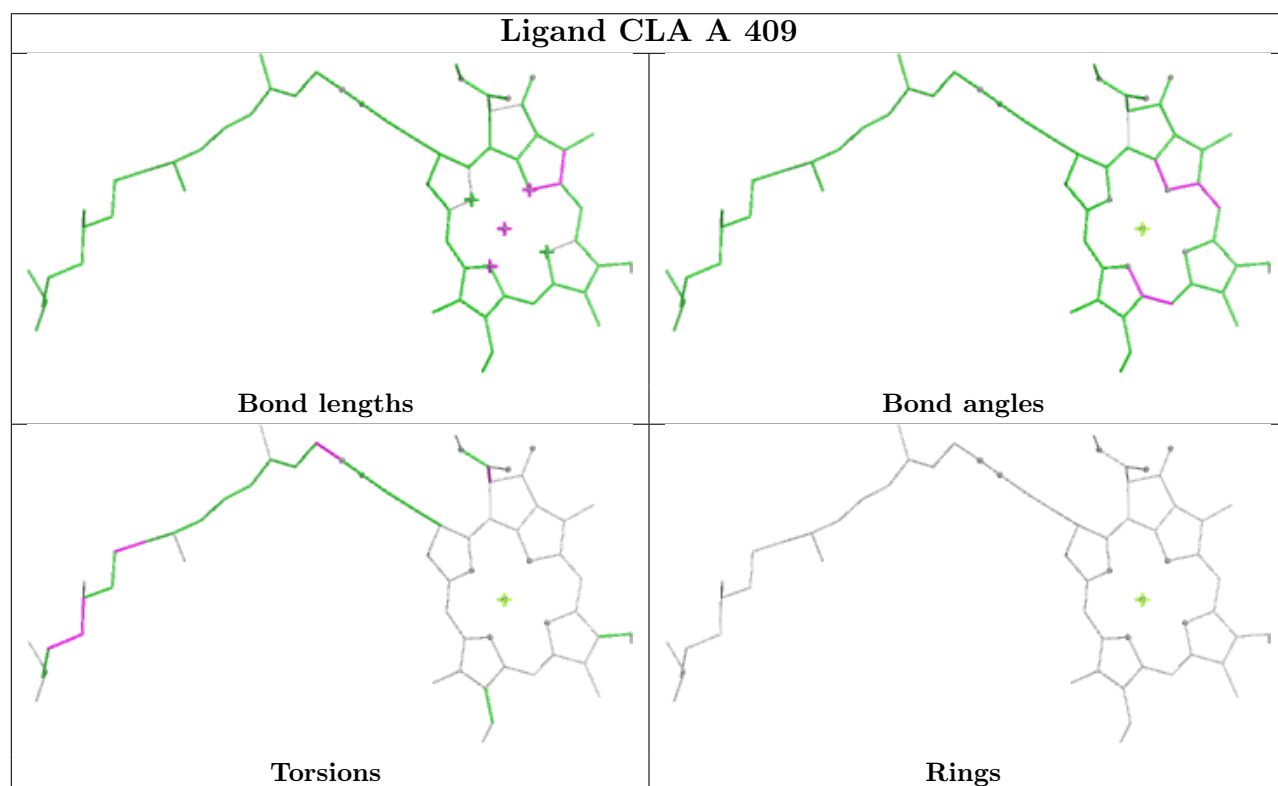
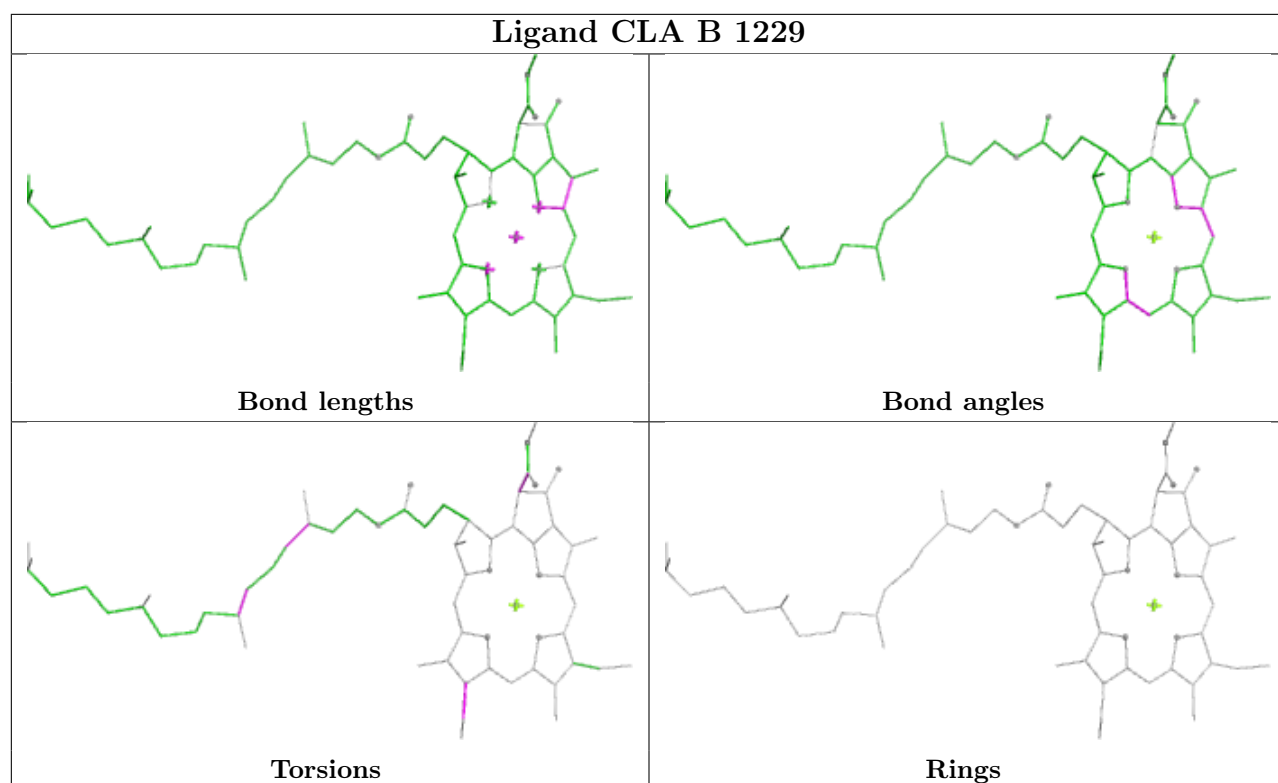


Ligand CLA b 307

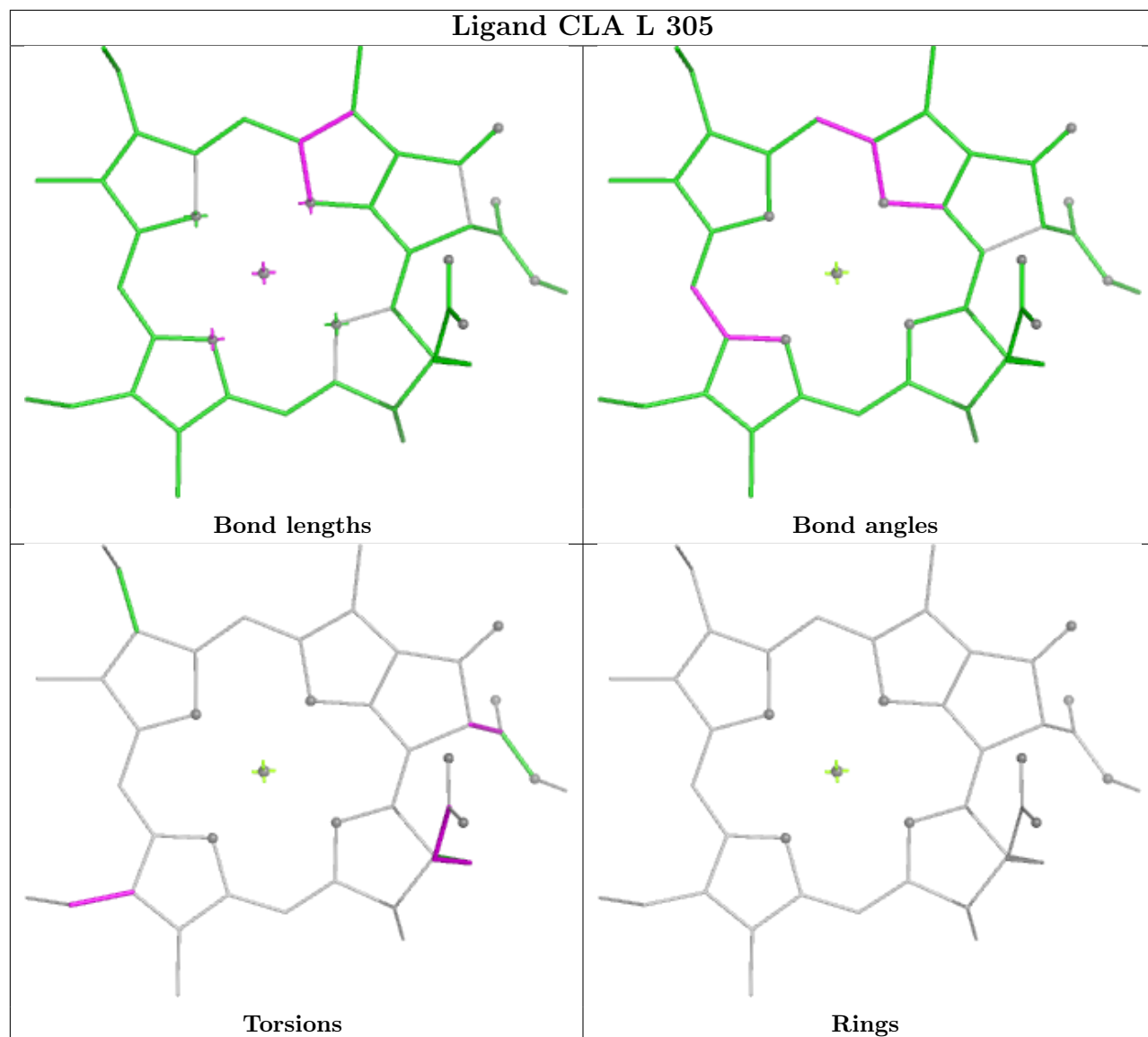


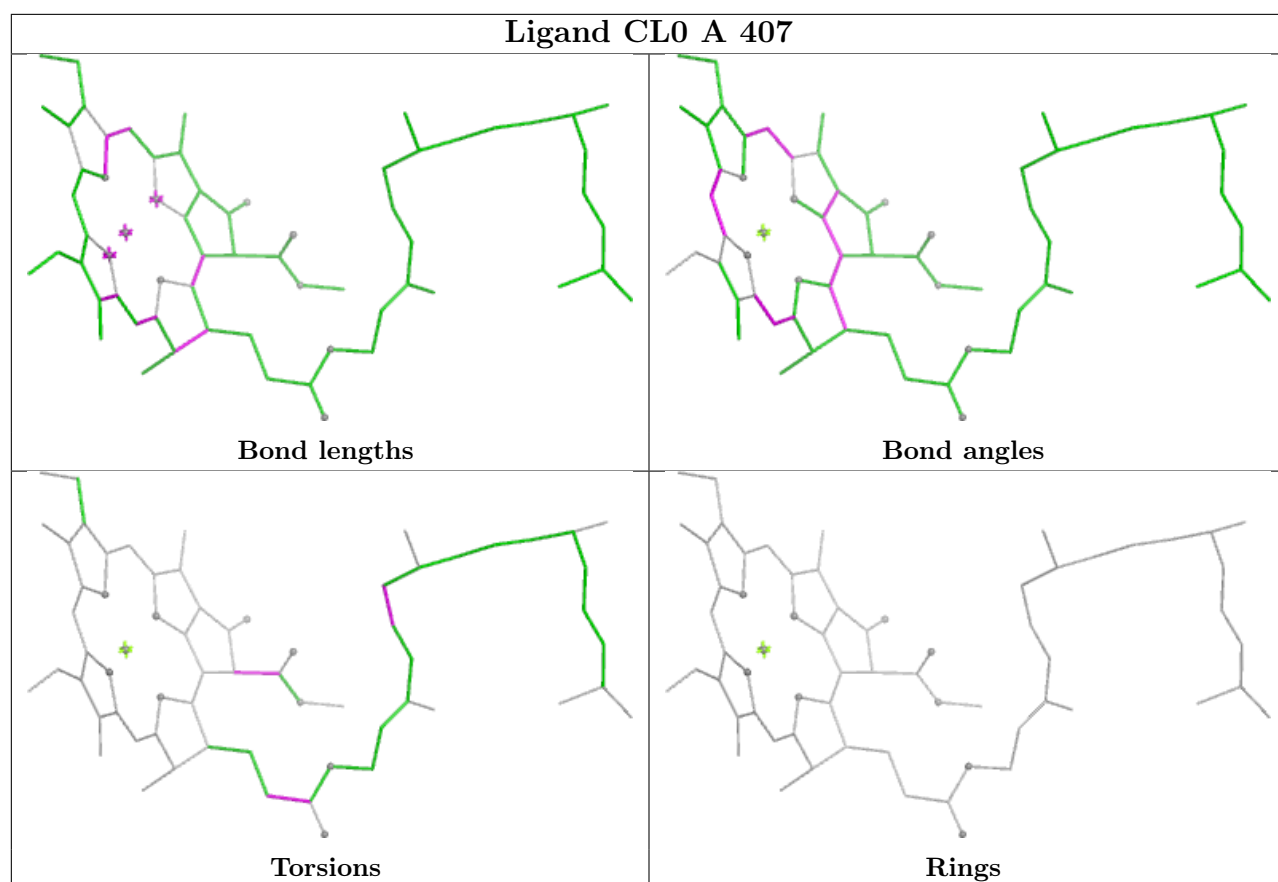
Ligand CLA d 303

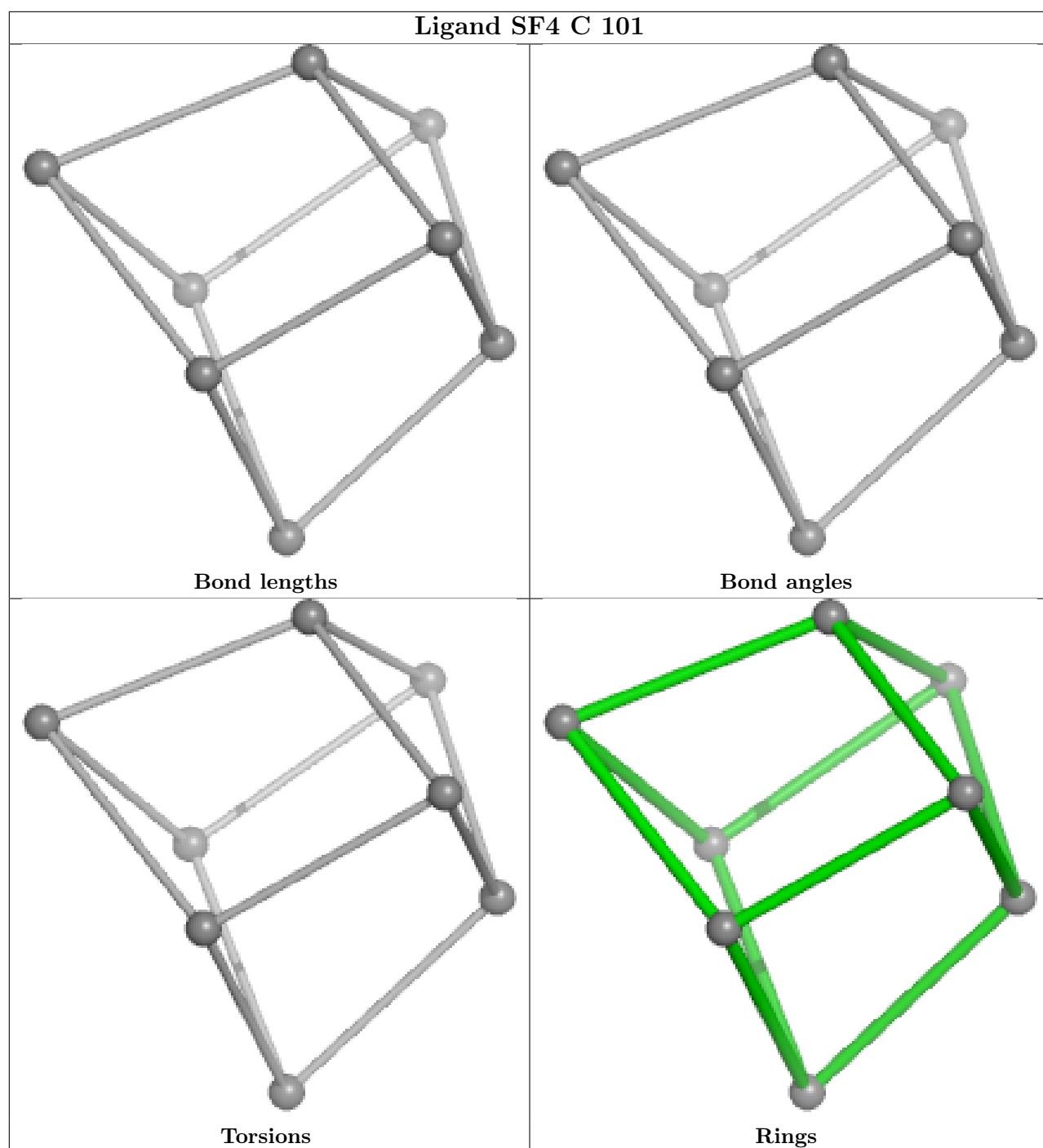


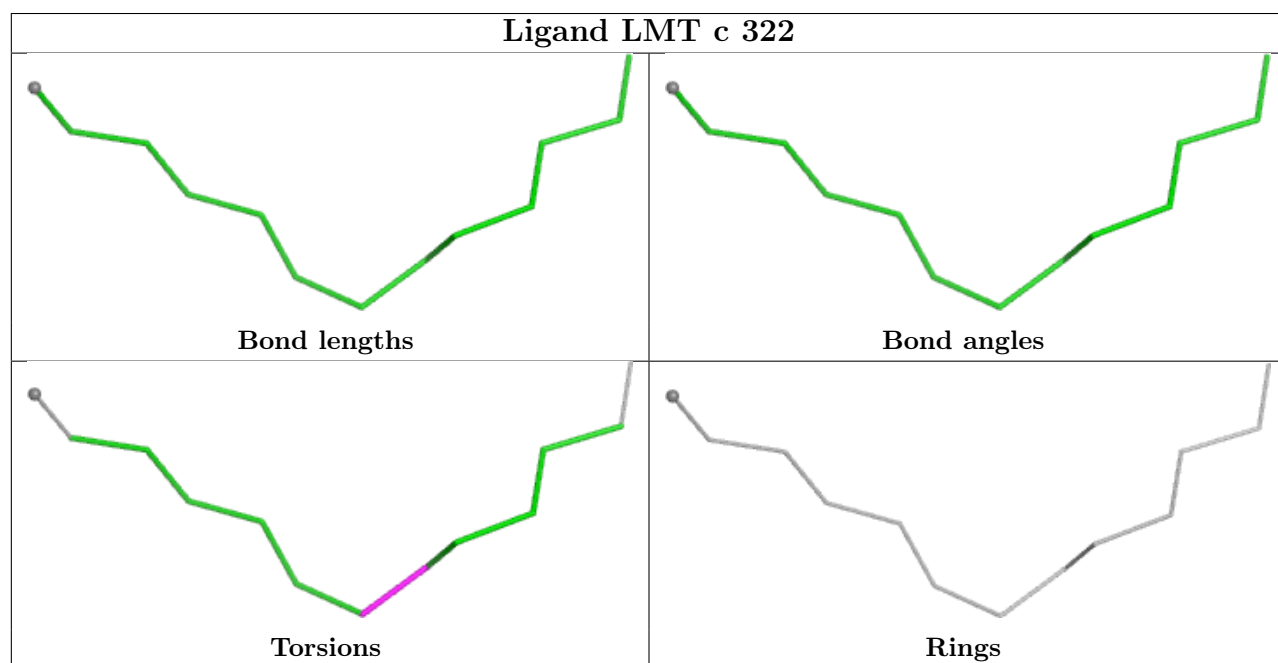
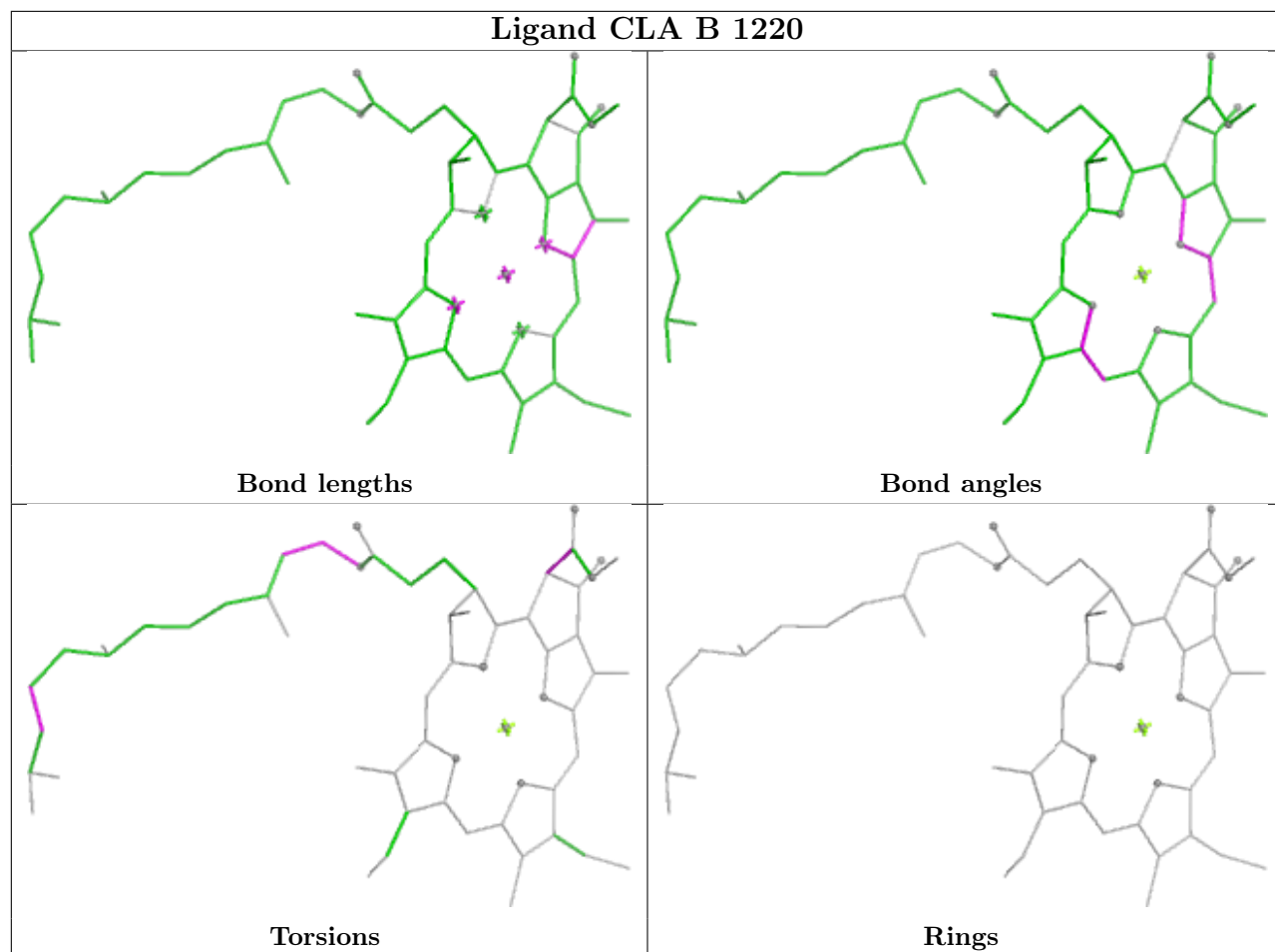


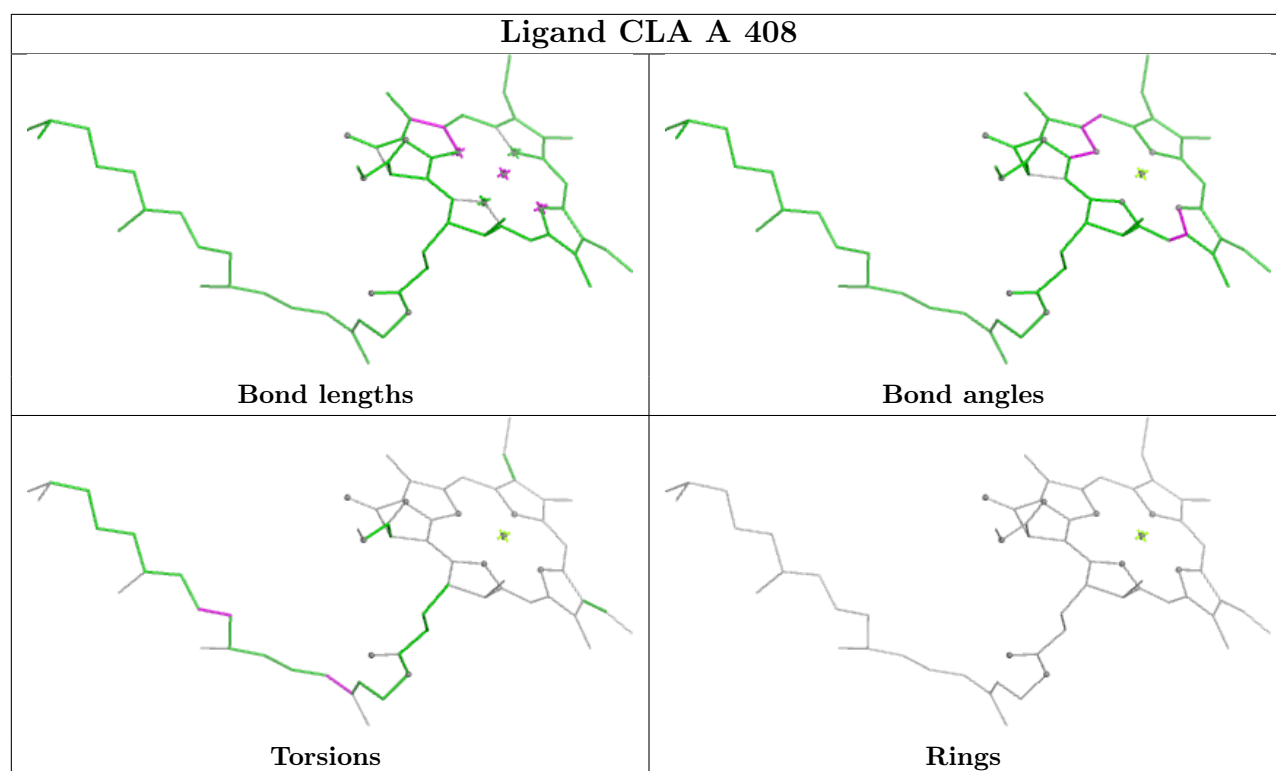
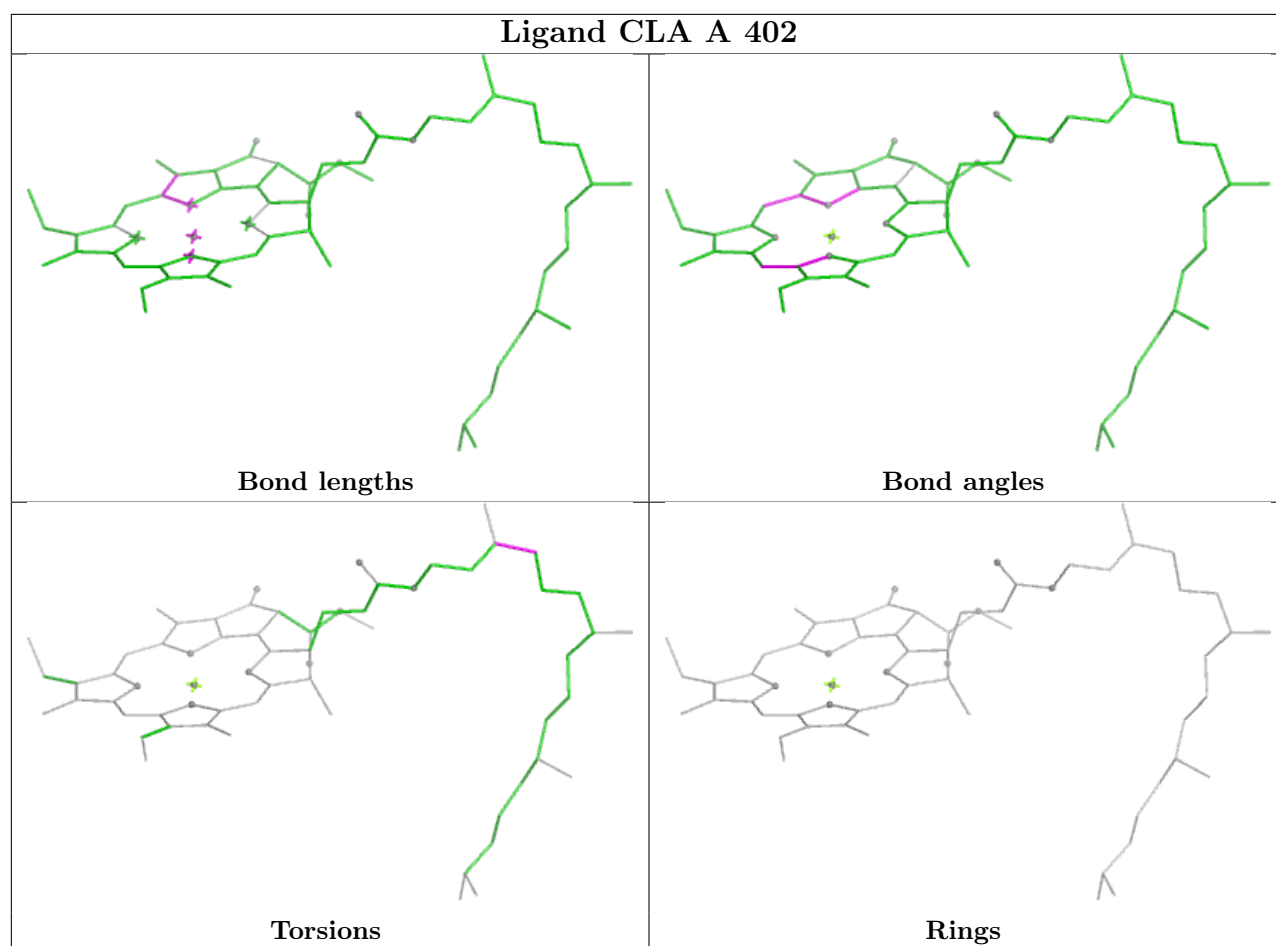
Ligand CLA L 305

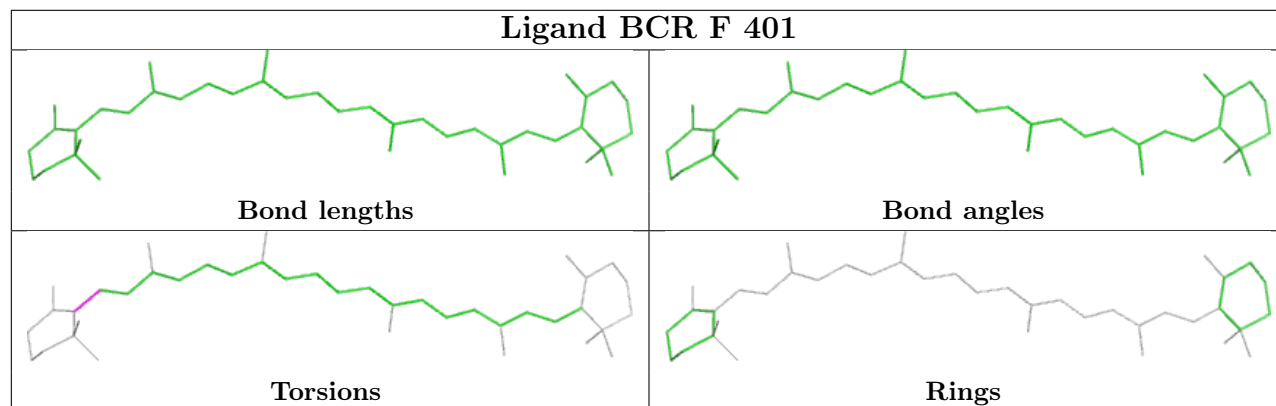
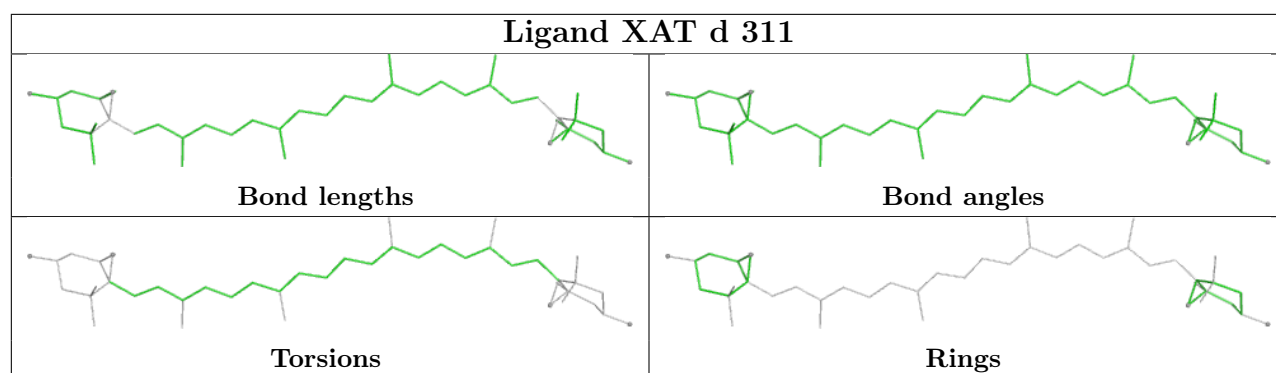


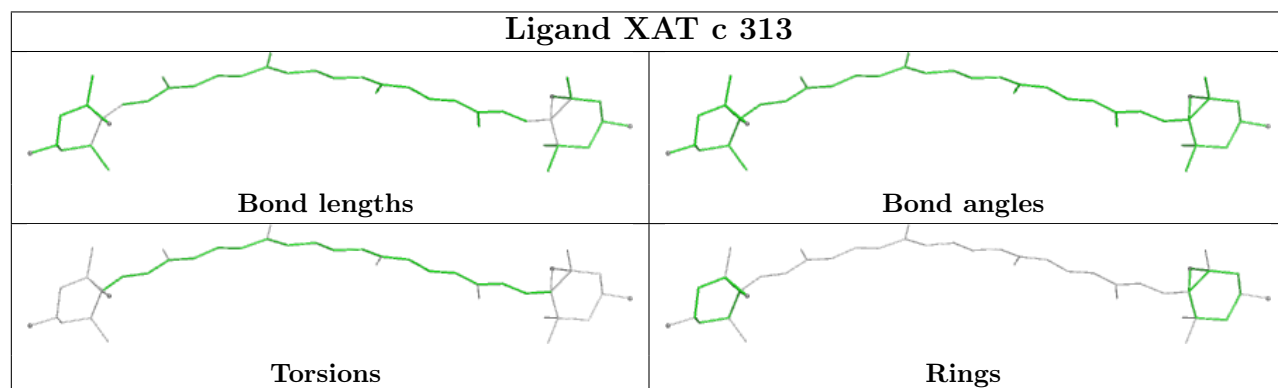
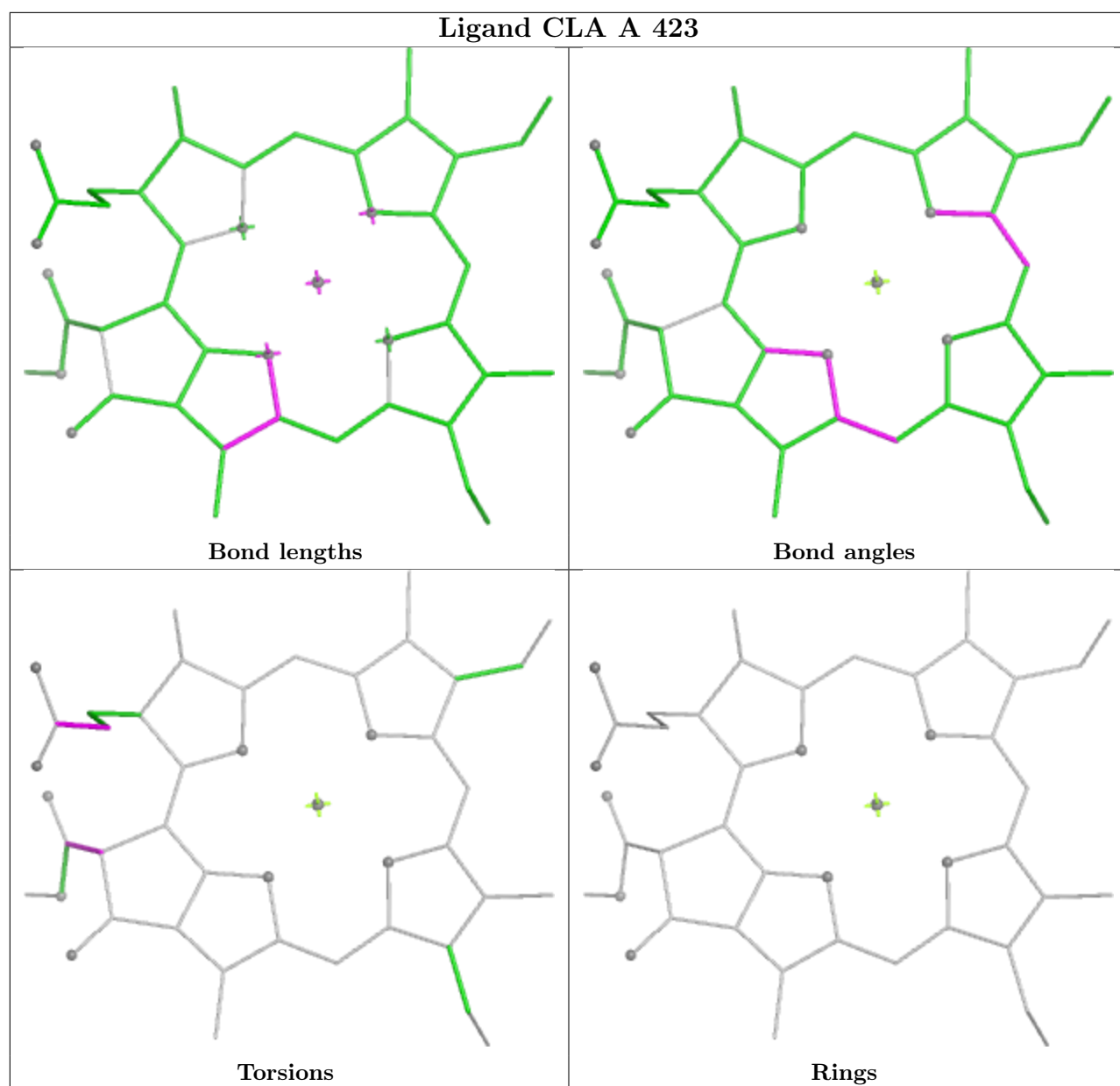


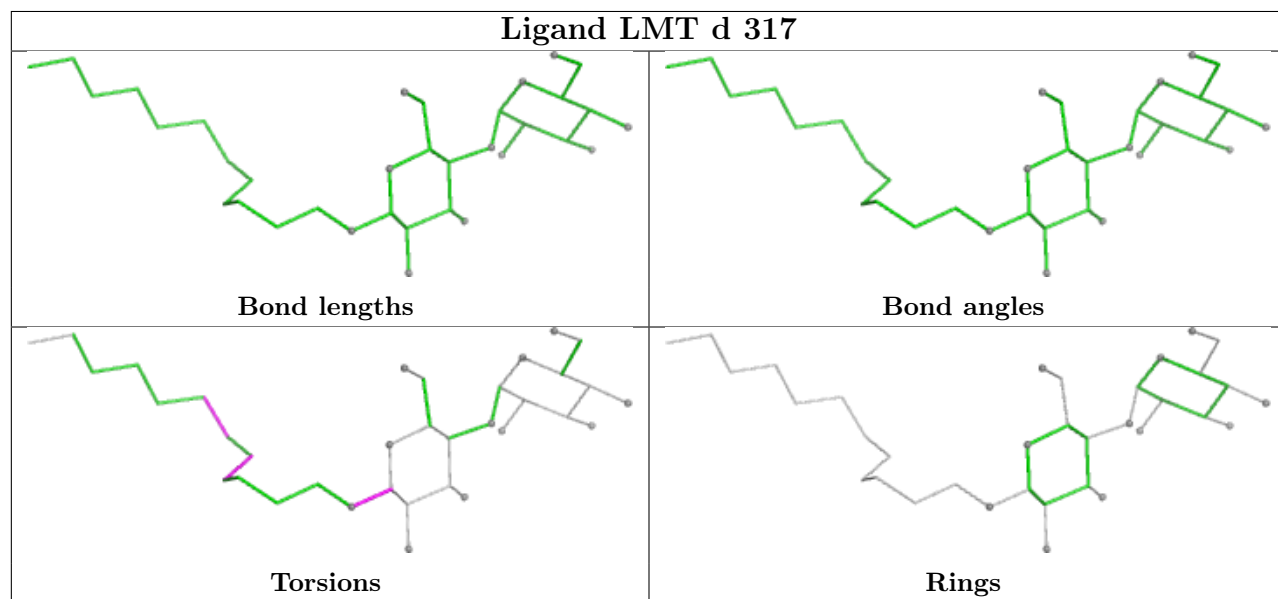
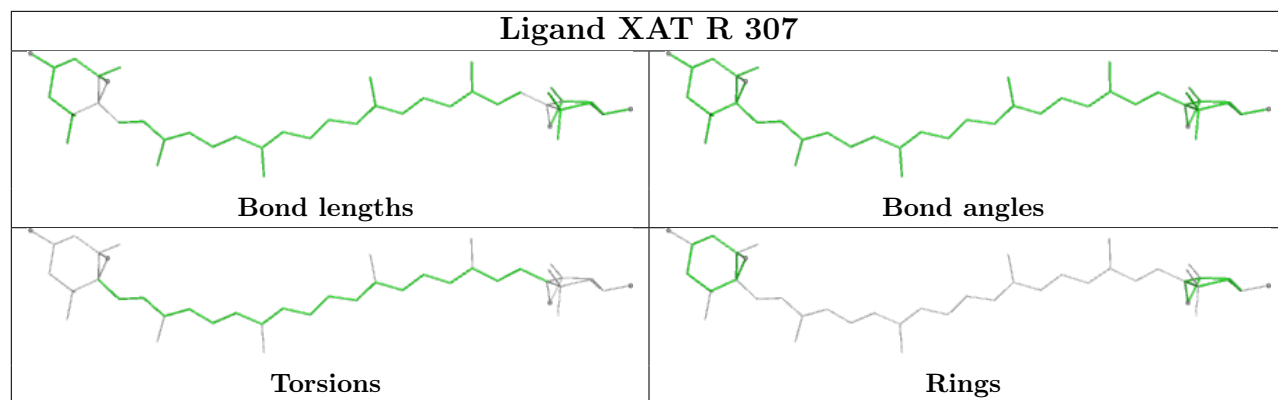


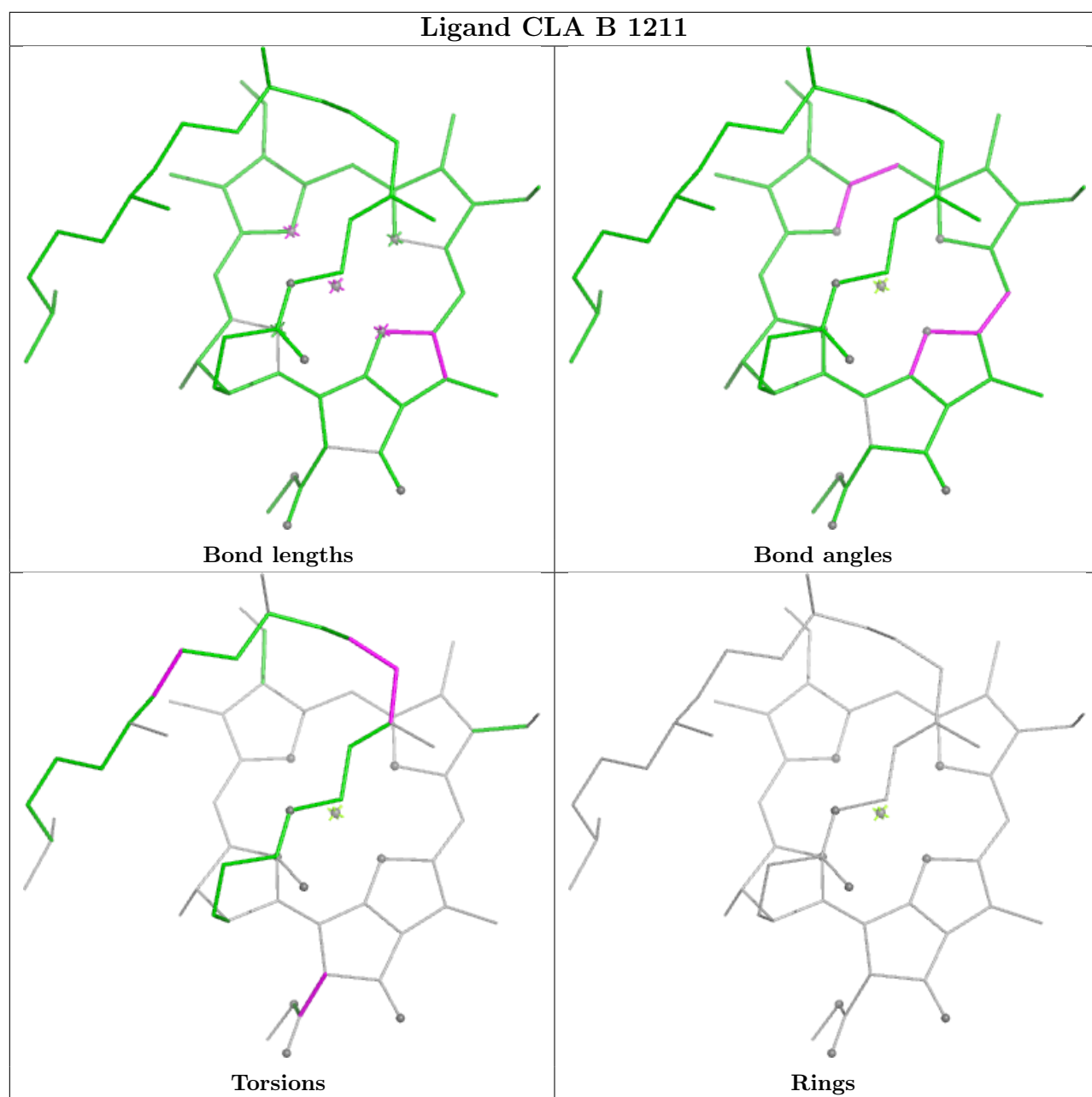


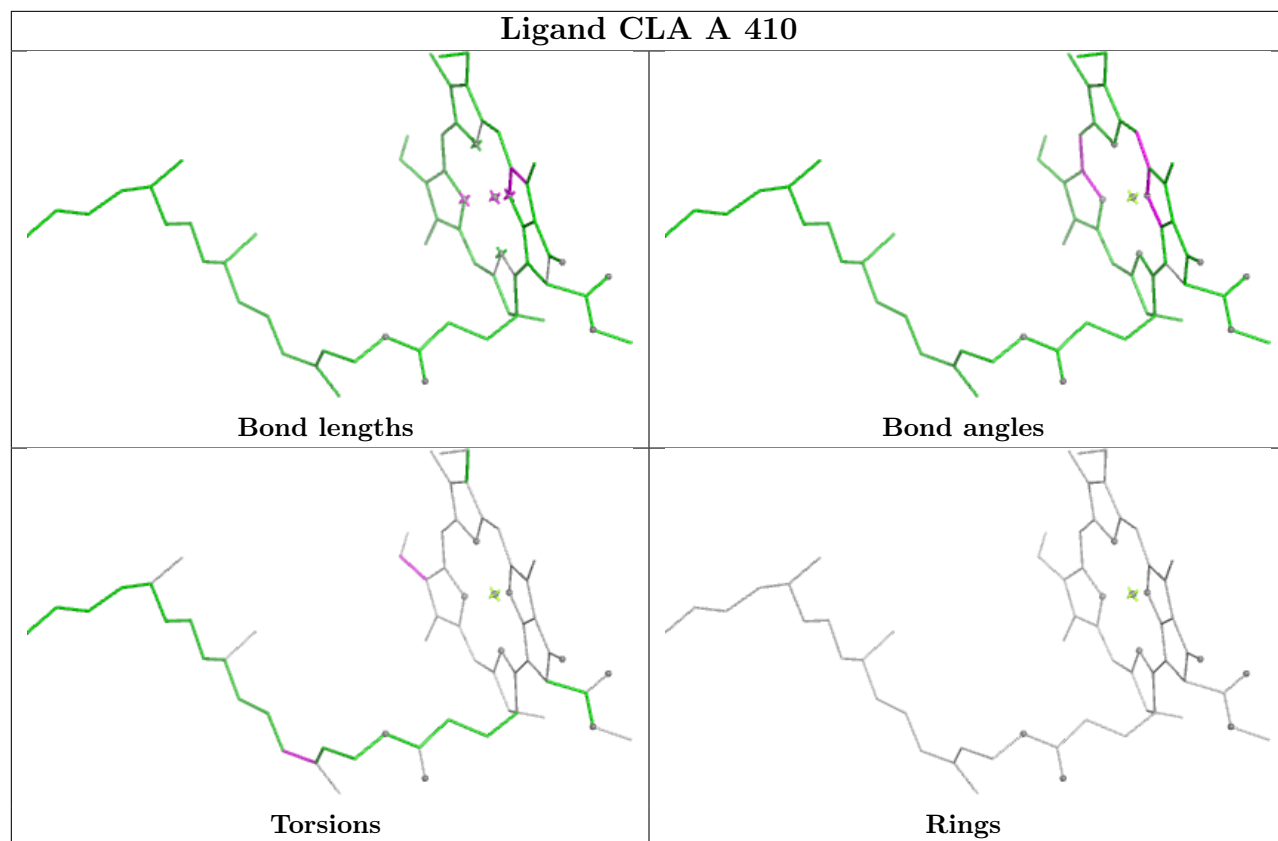


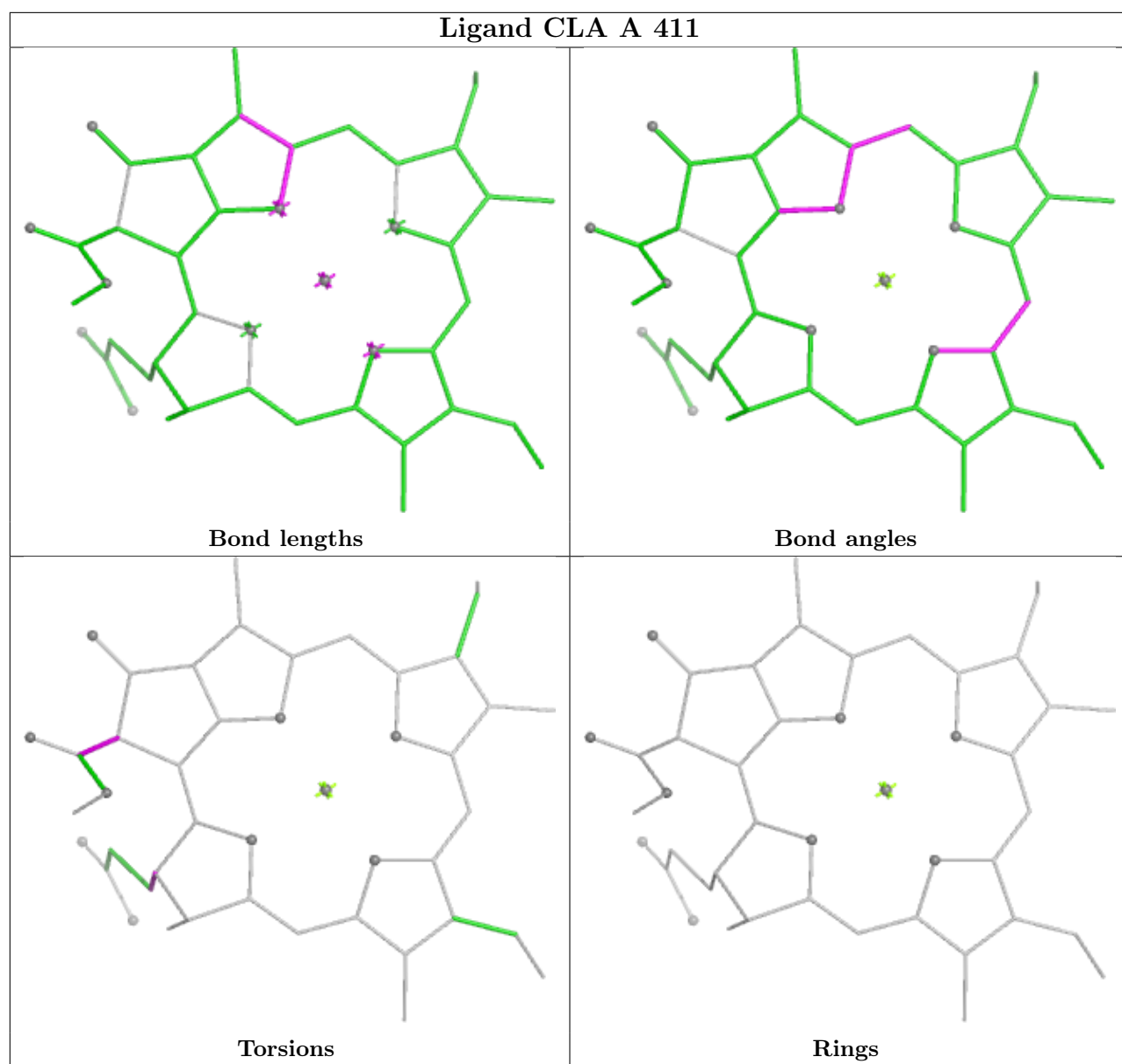


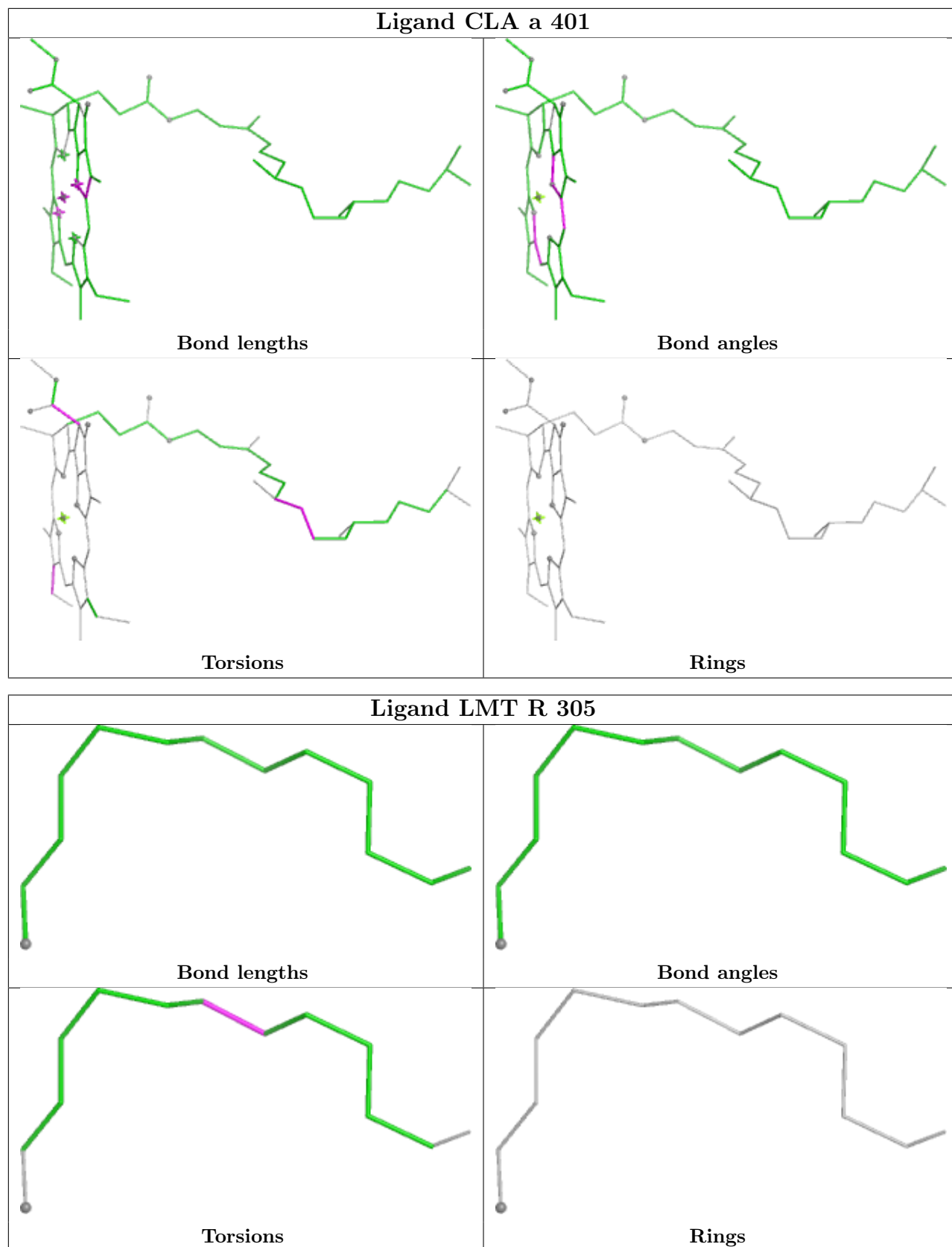


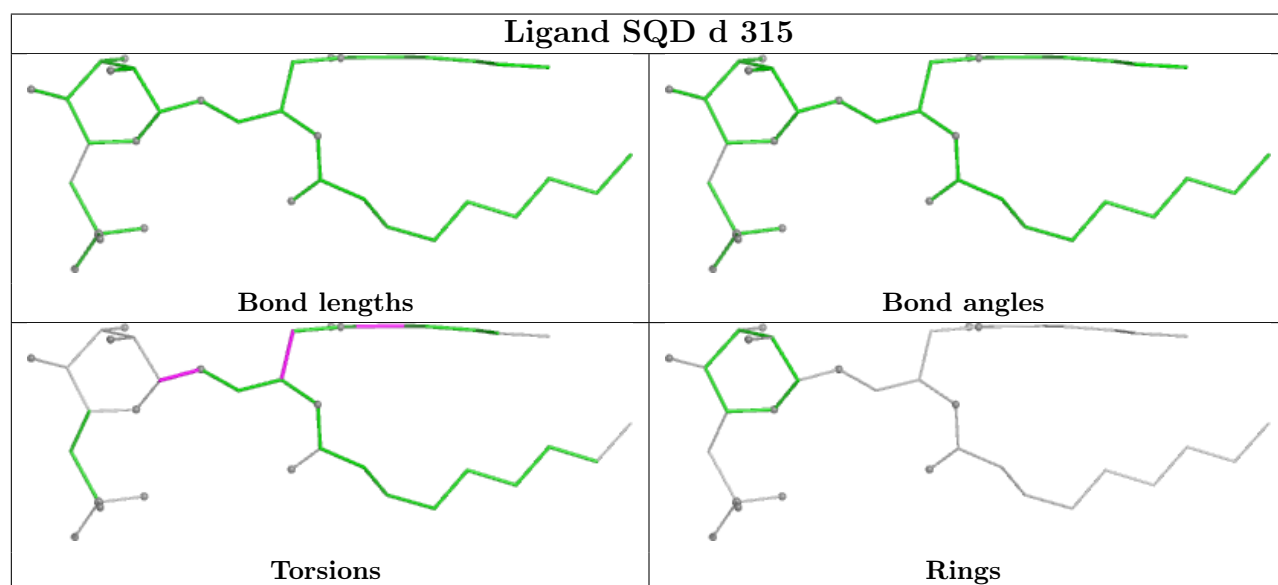
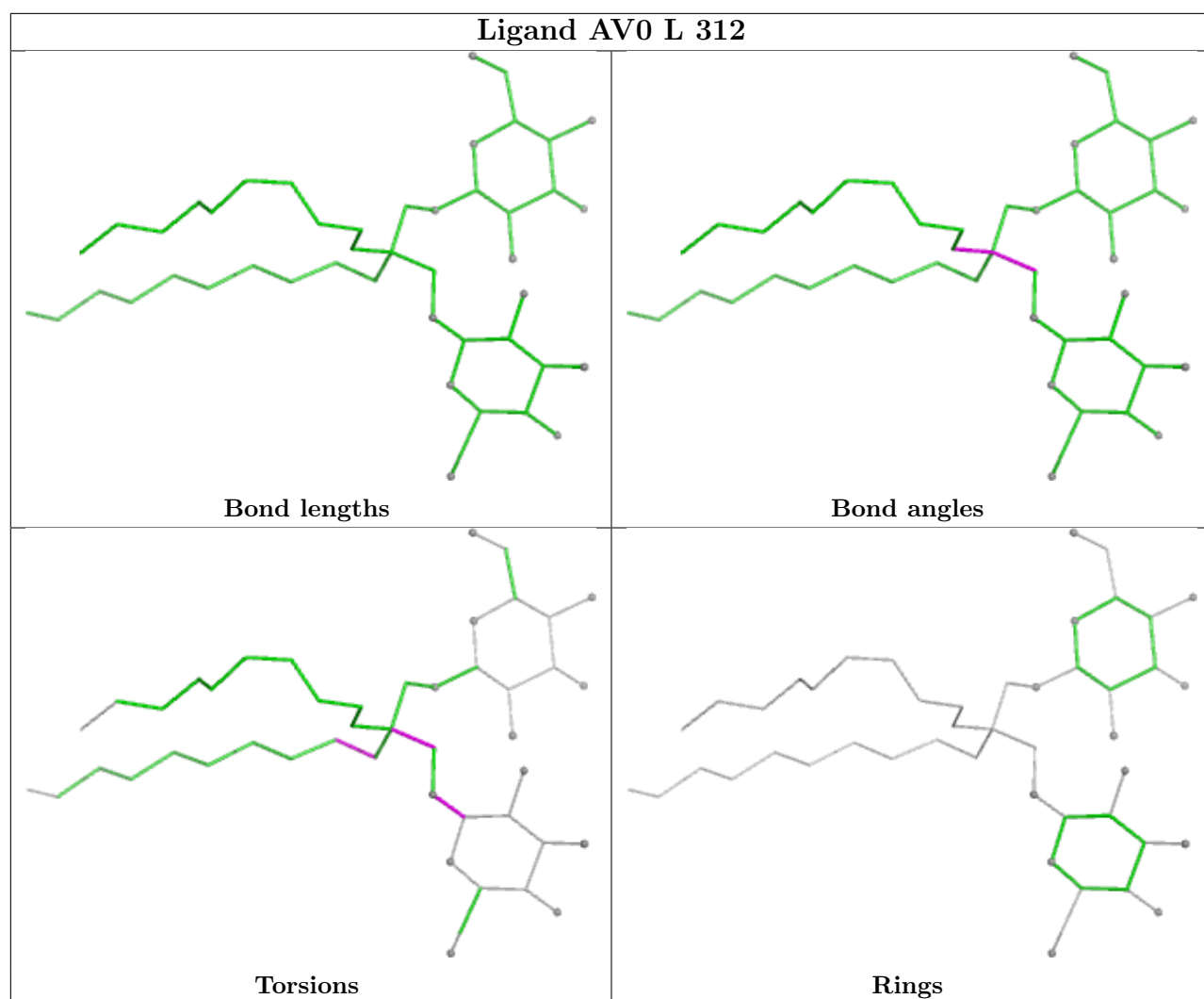


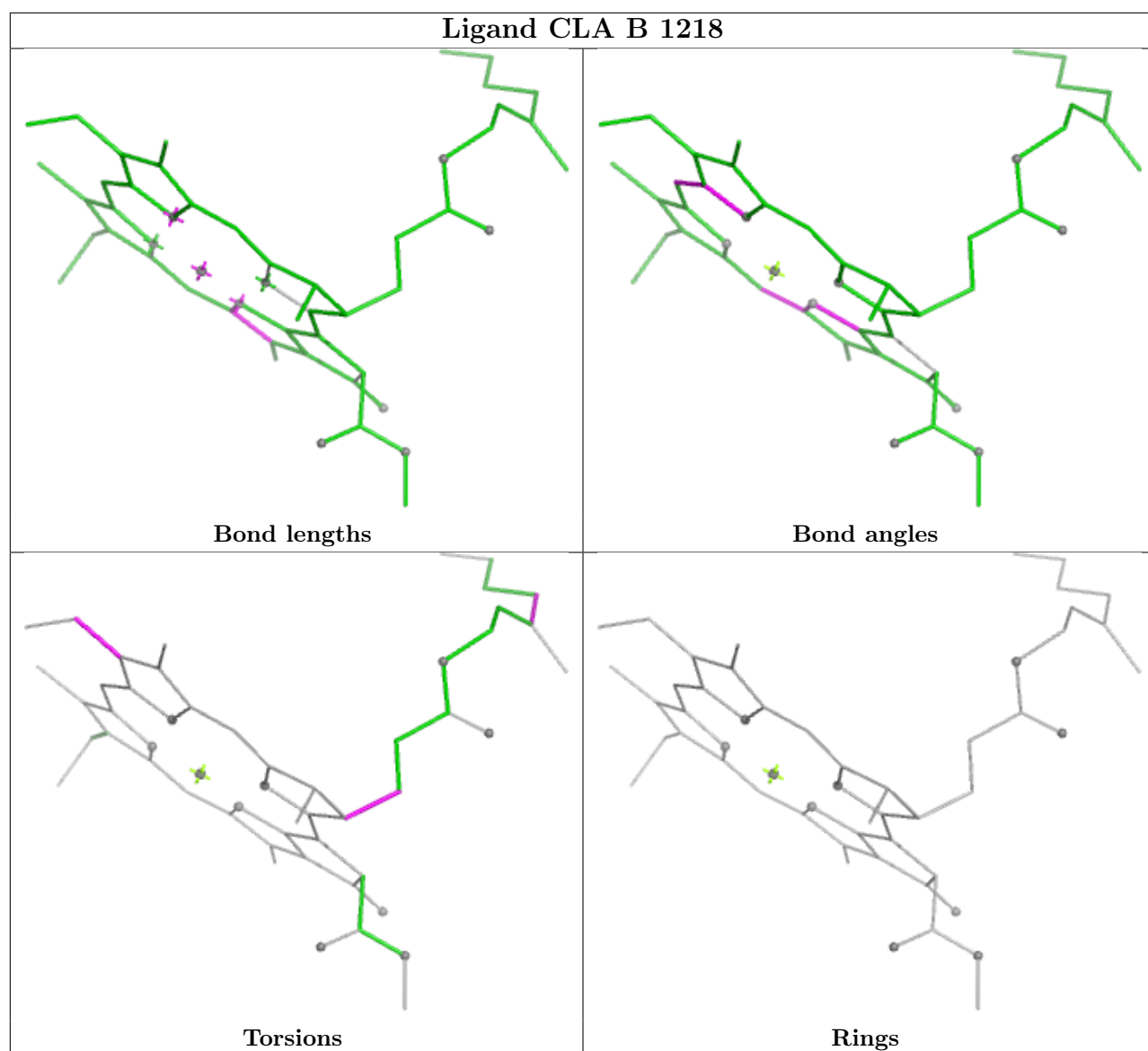


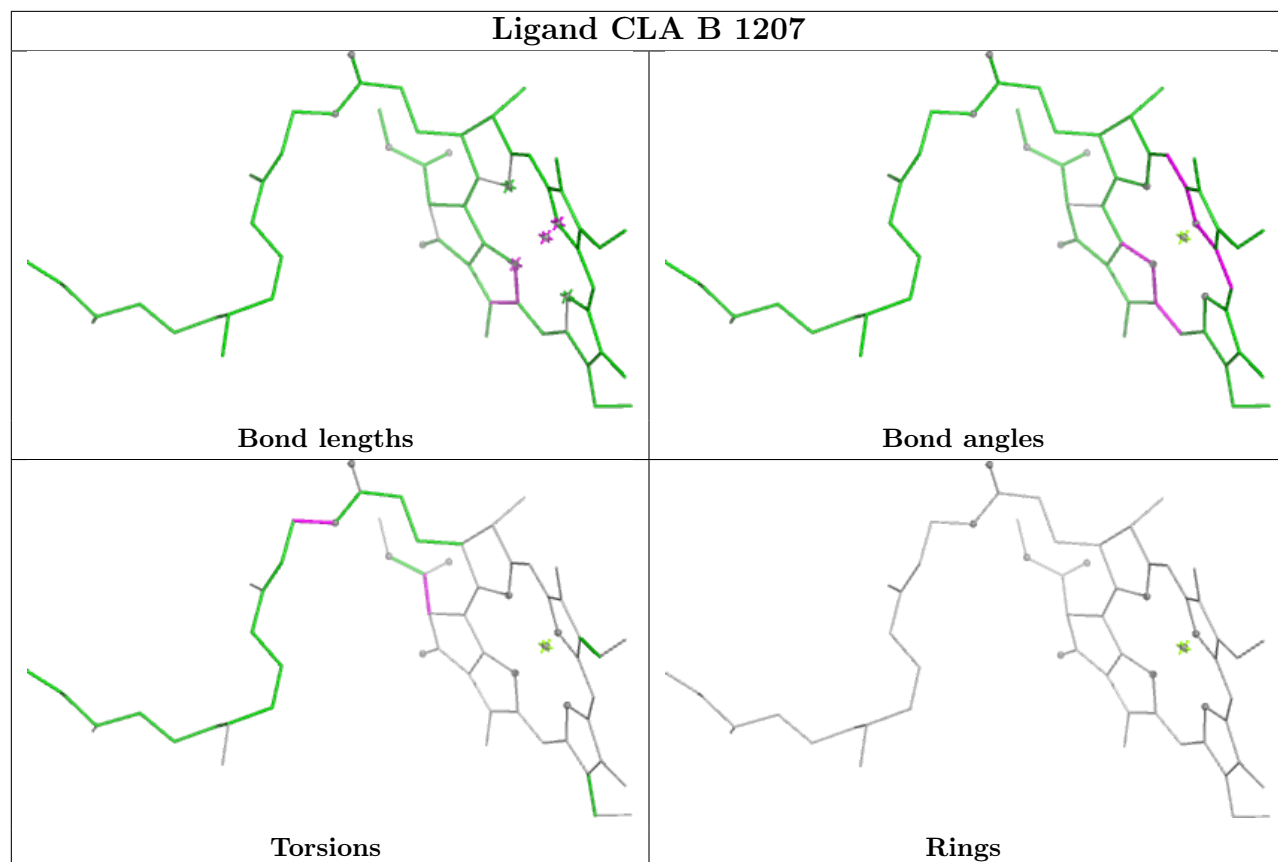


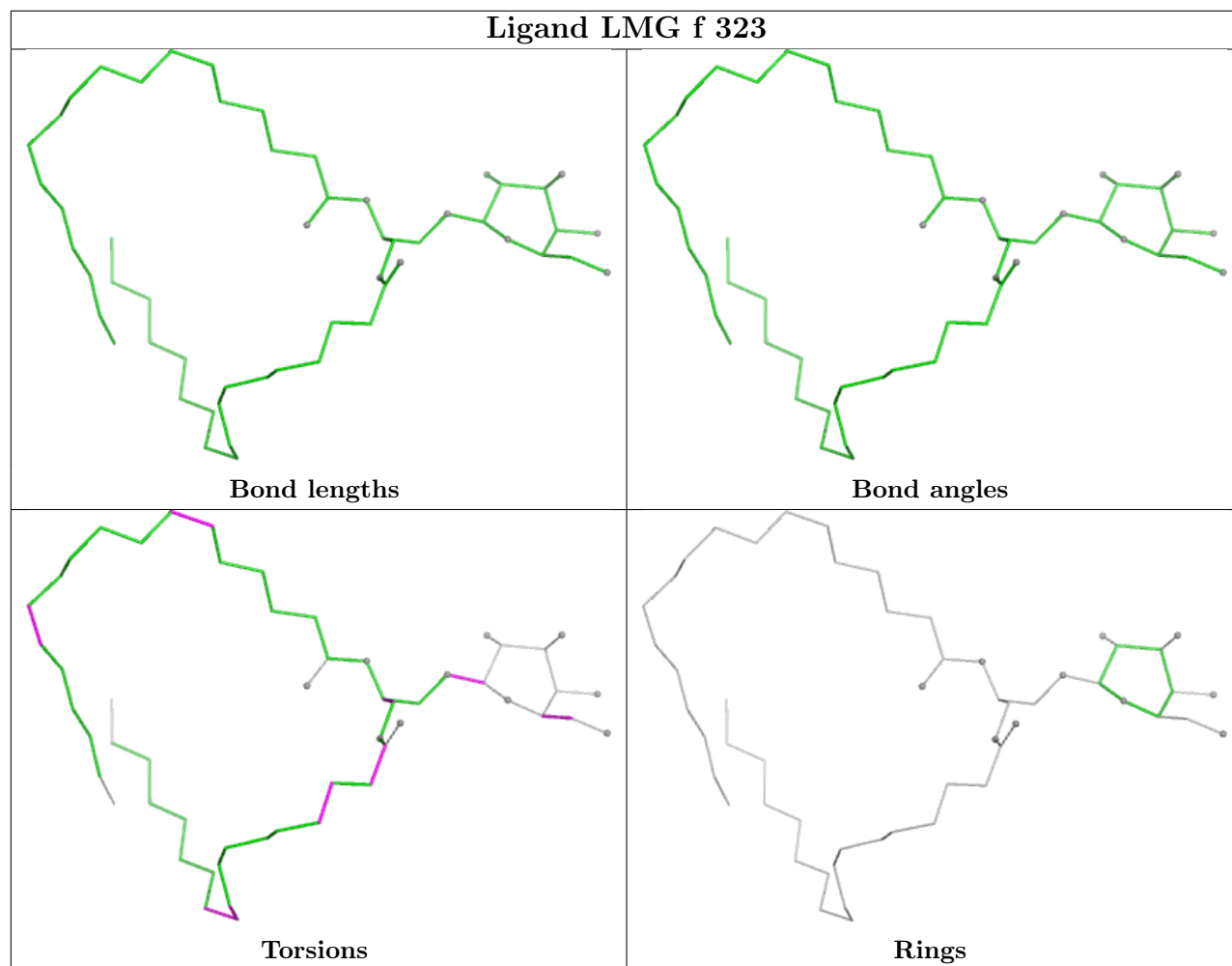
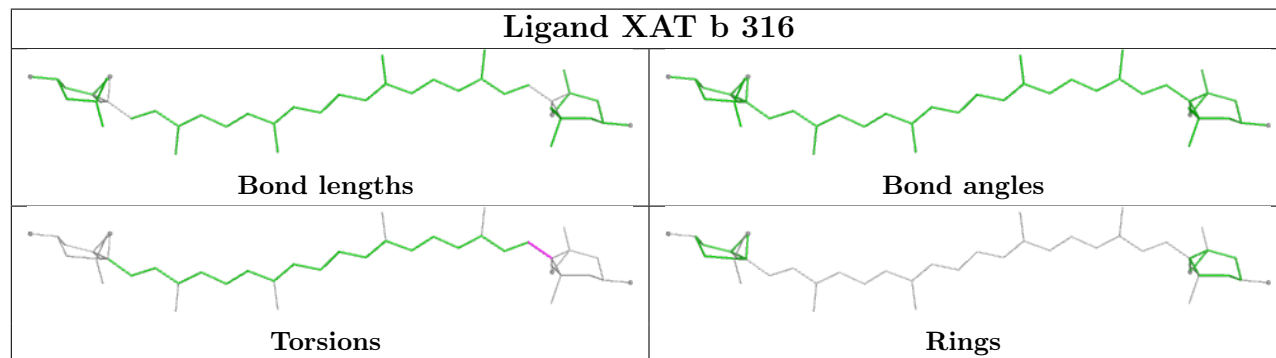




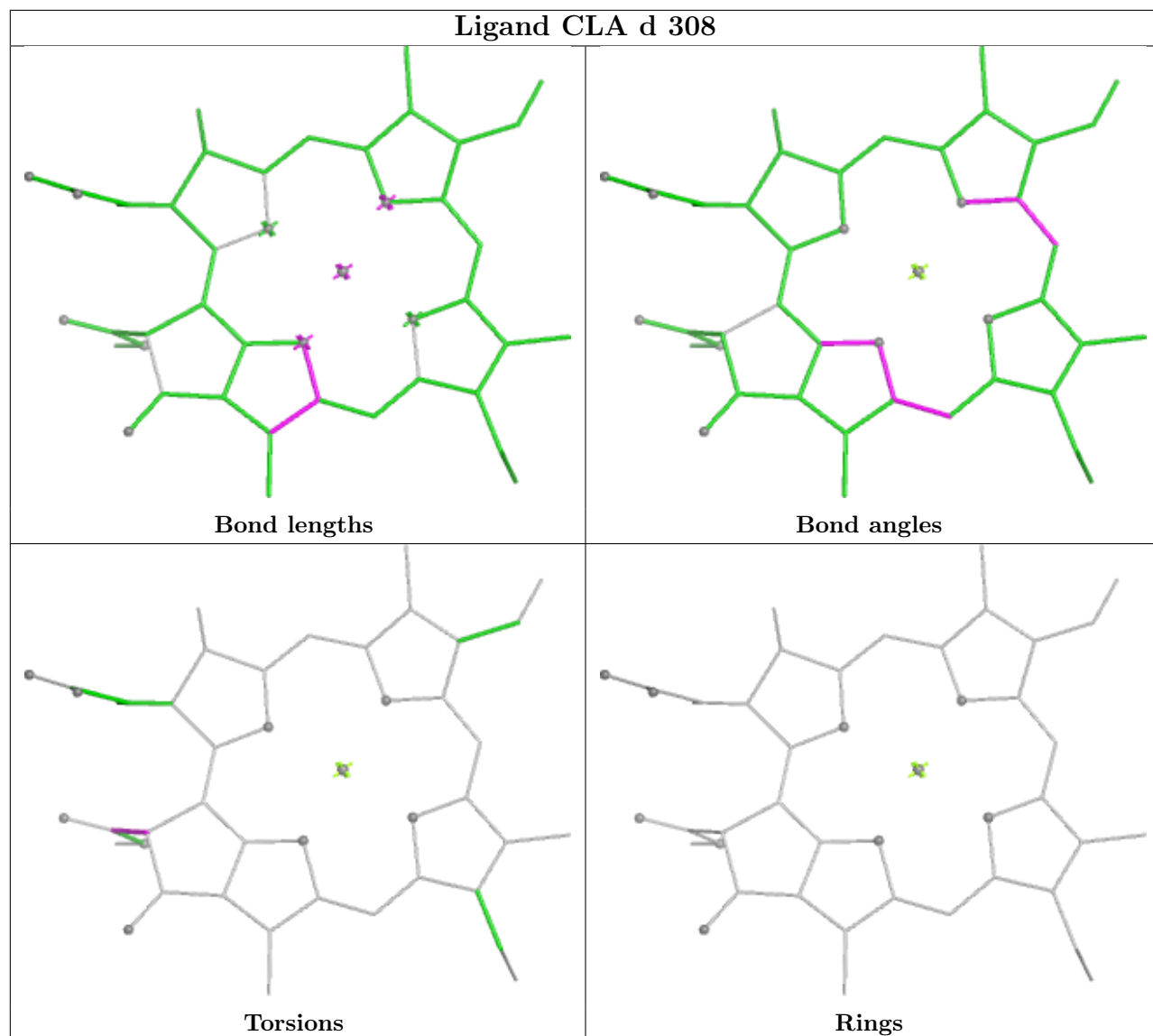


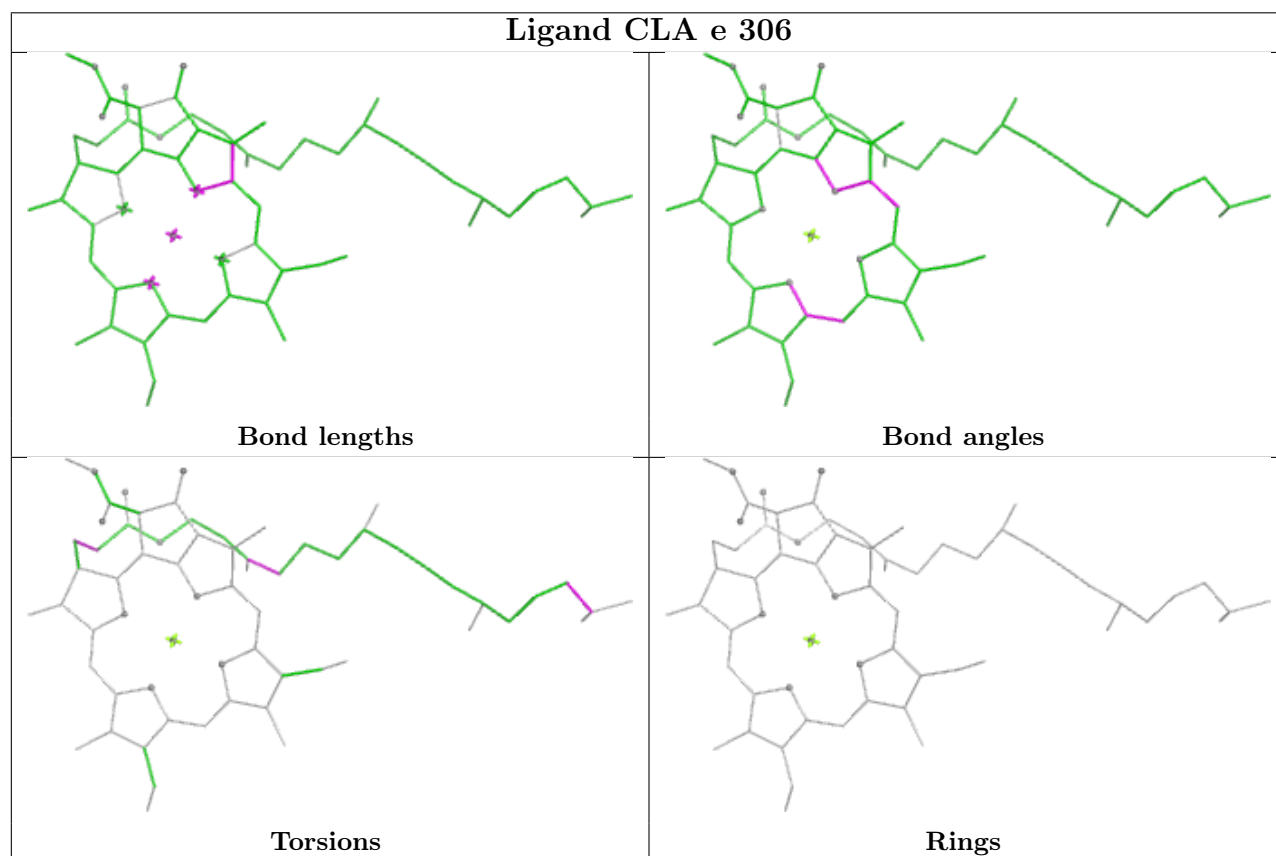
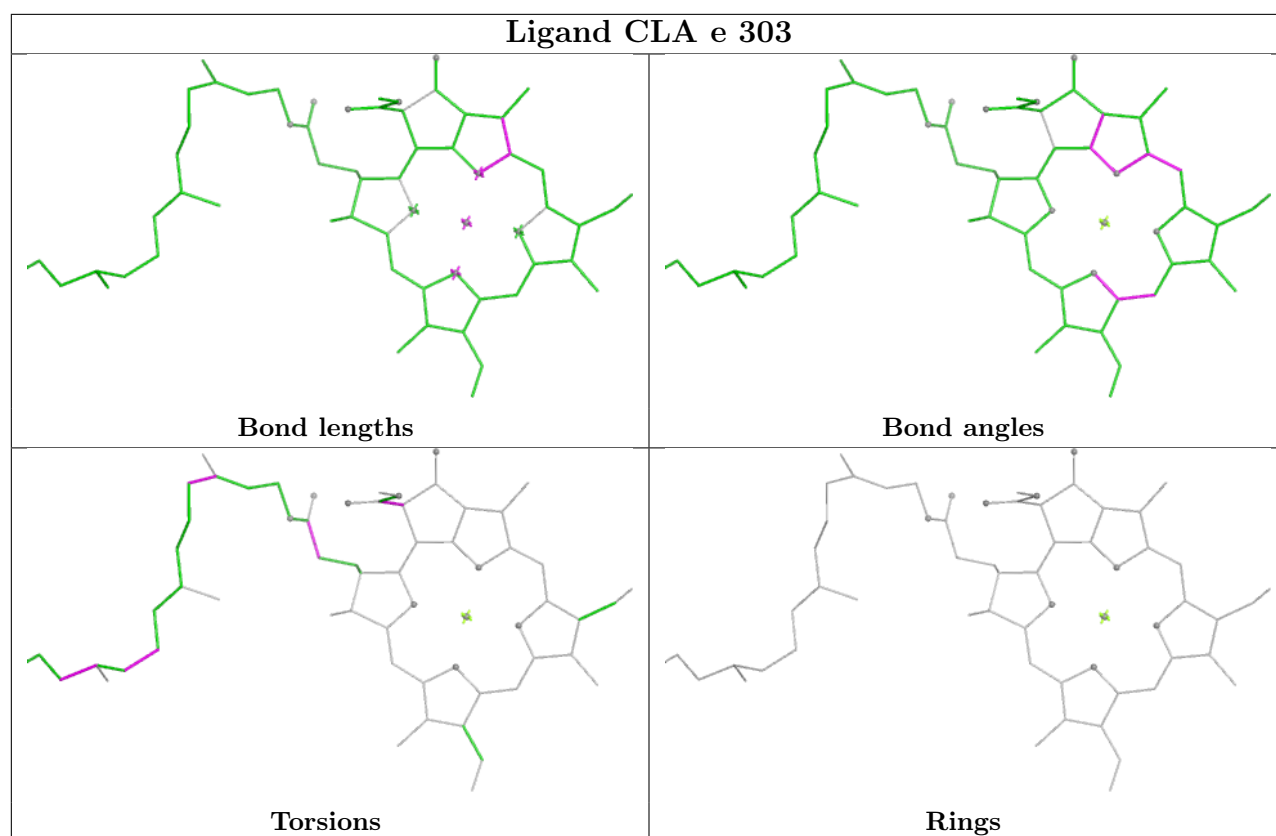




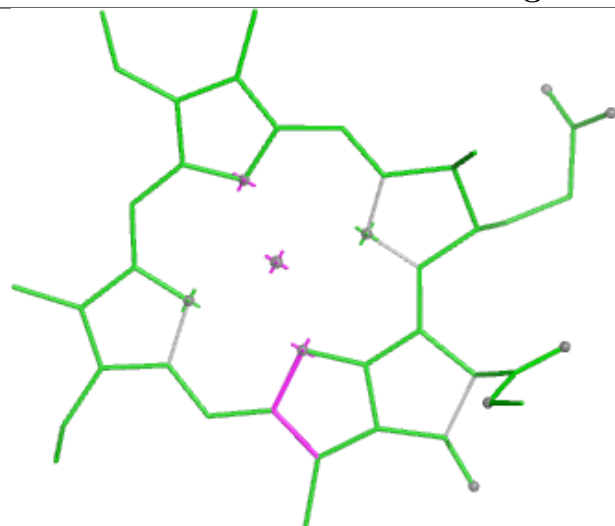
Ligand LMG f 323**Ligand XAT b 316**

Ligand CLA d 308

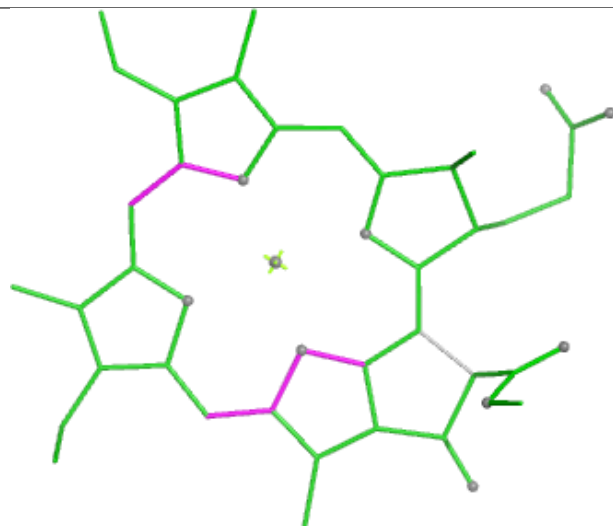




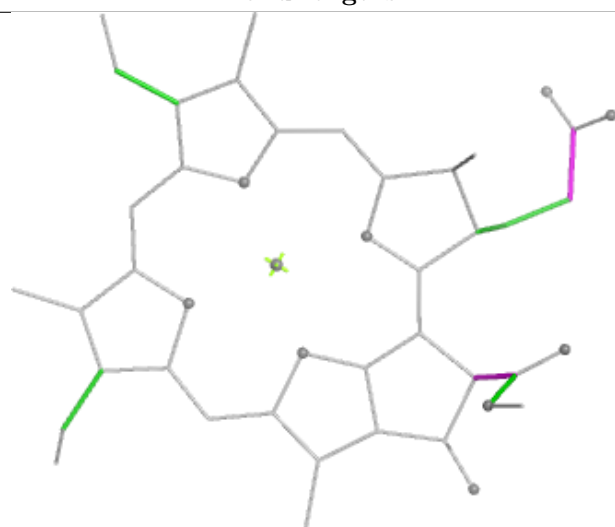
Ligand CLA f 314



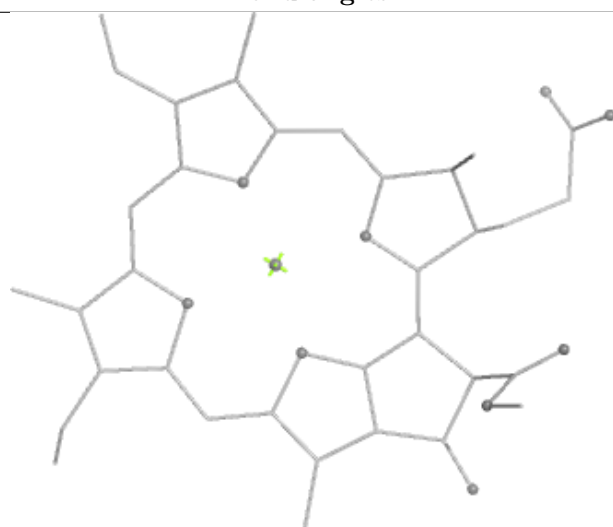
Bond lengths



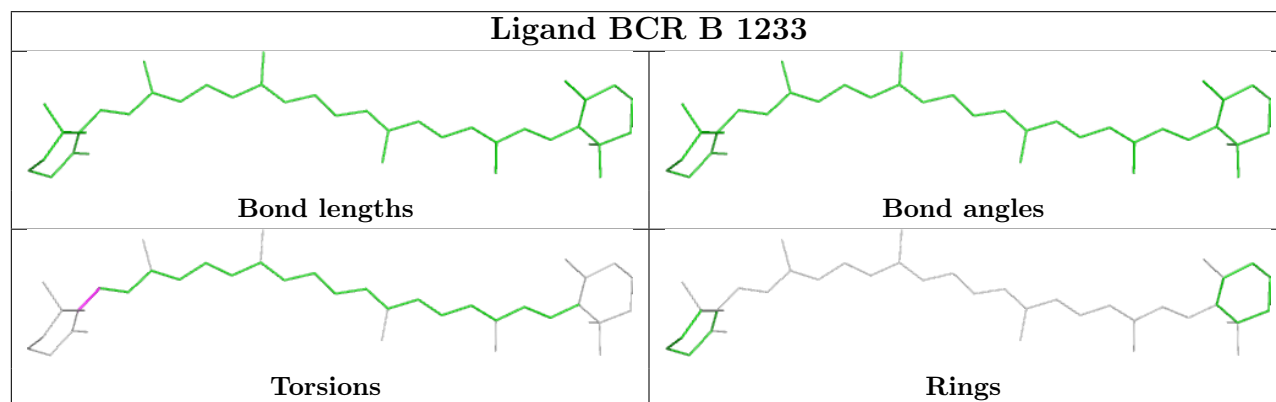
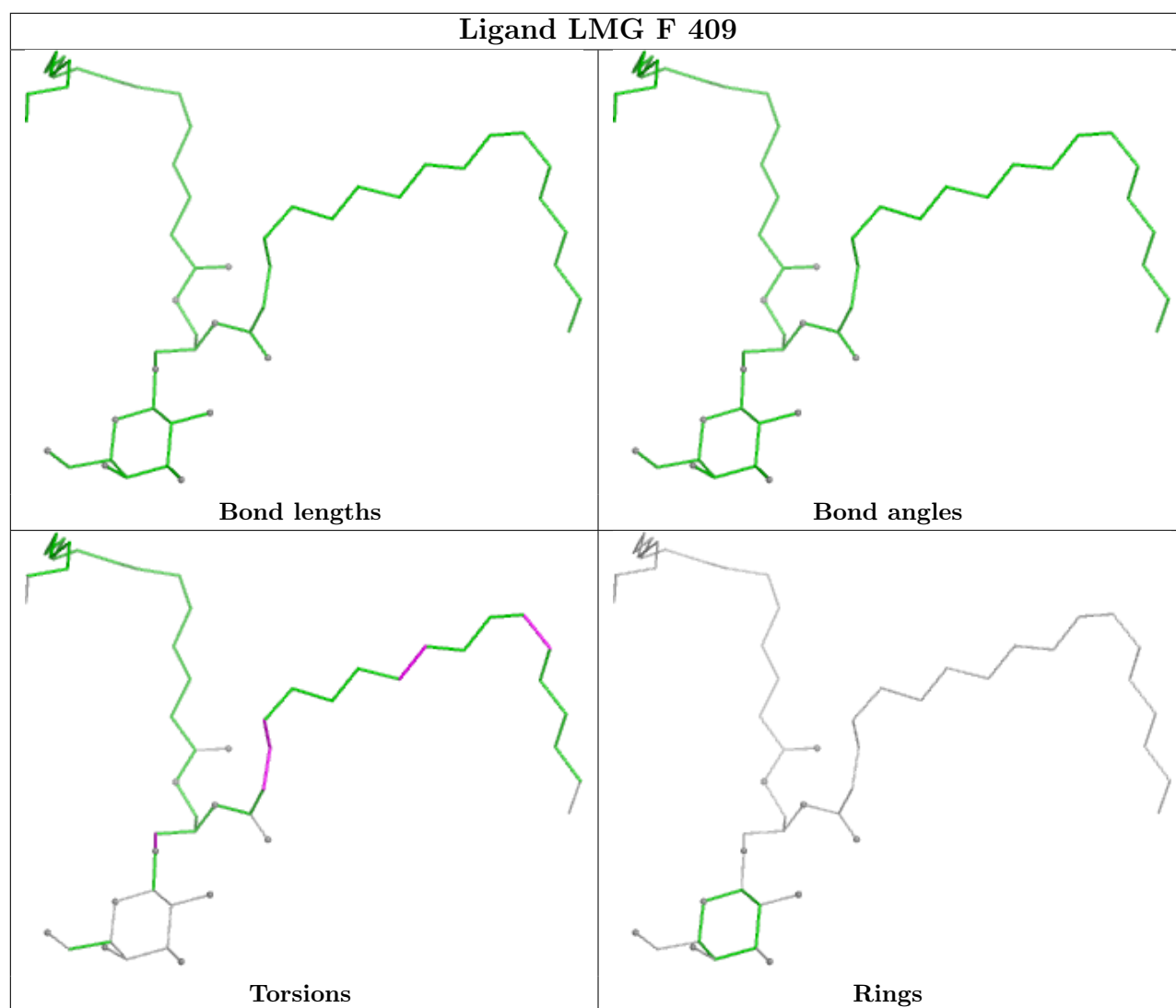
Bond angles



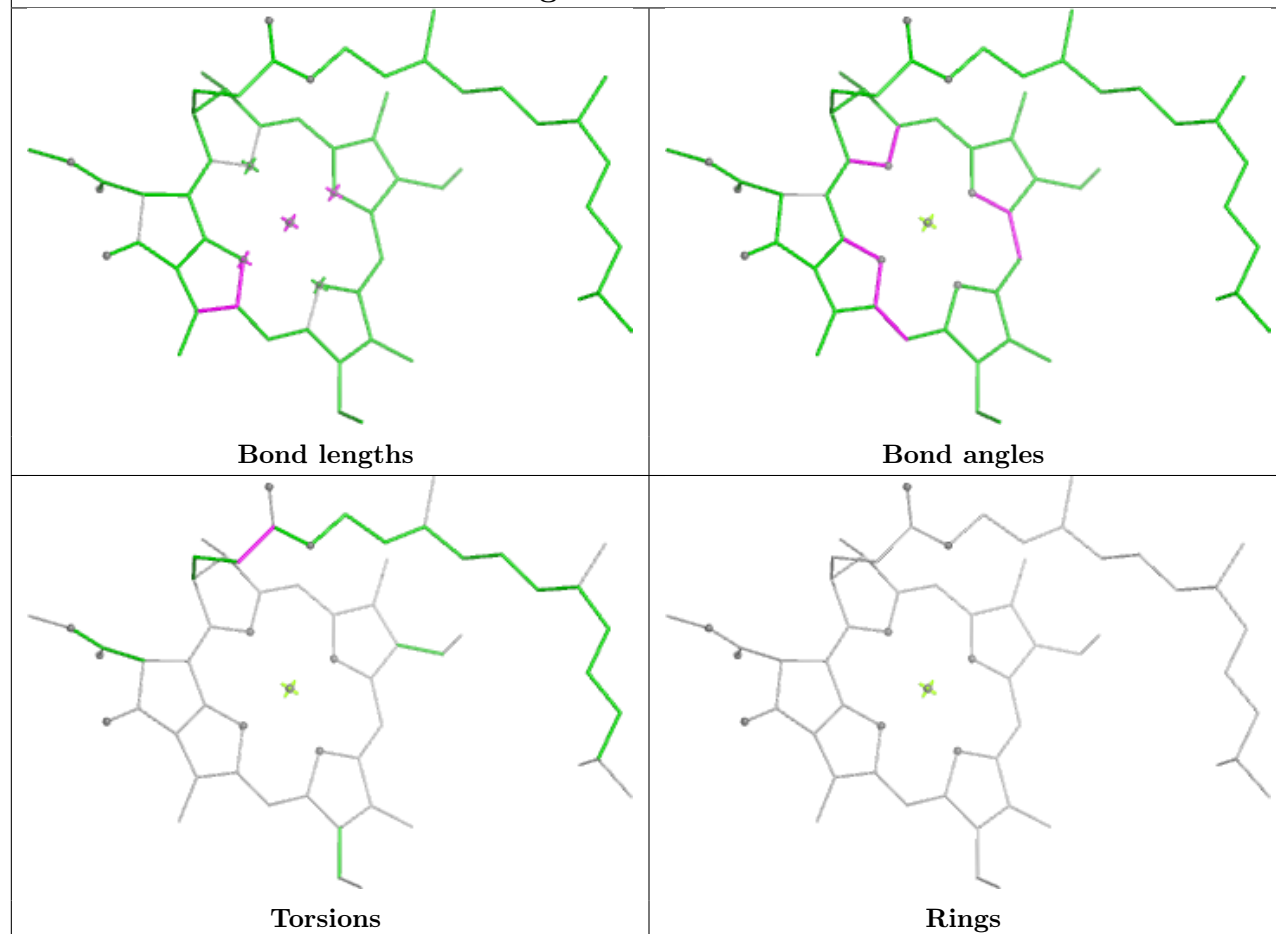
Torsions



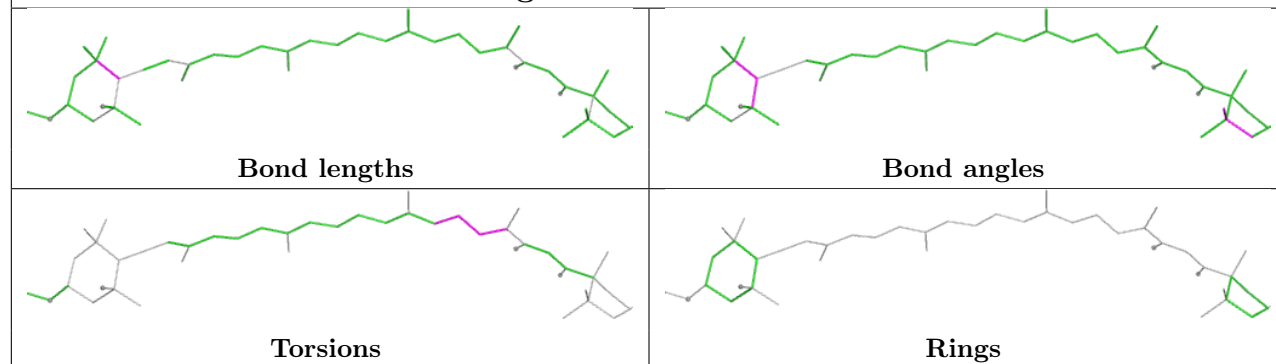
Rings



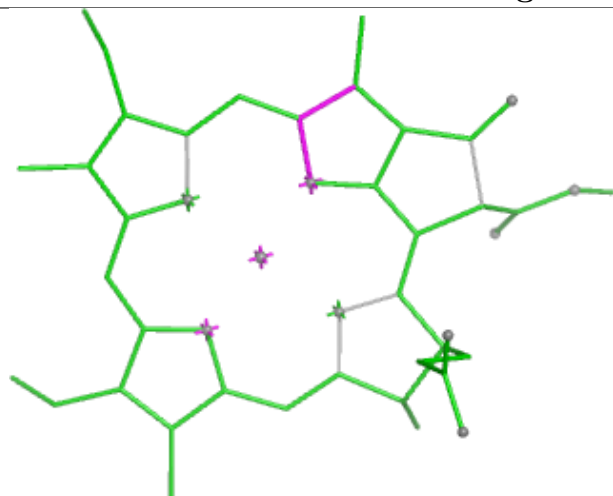
Ligand CLA f 306



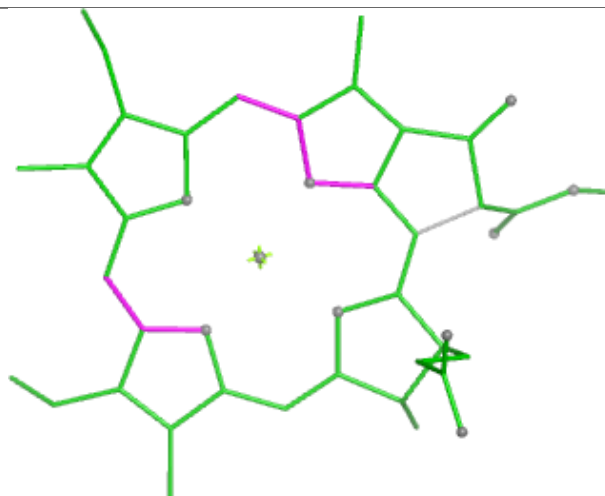
Ligand A1L6D d 314



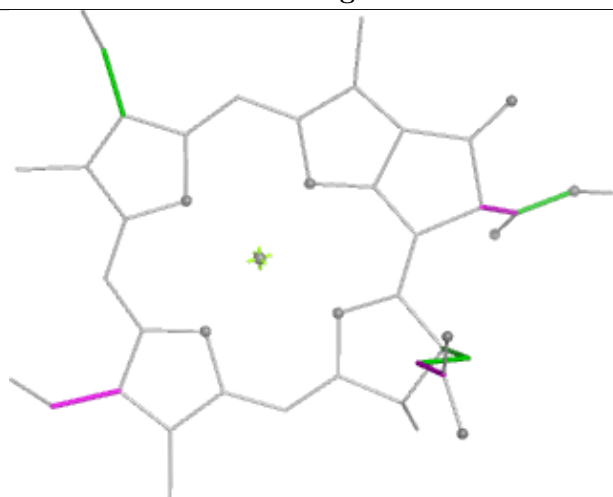
Ligand CLA L 313



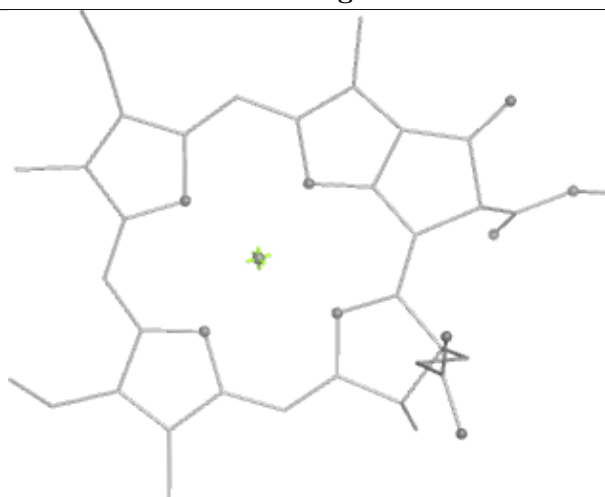
Bond lengths



Bond angles



Torsions



Rings

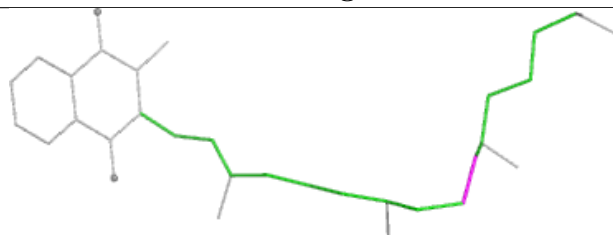
Ligand PQN A 416



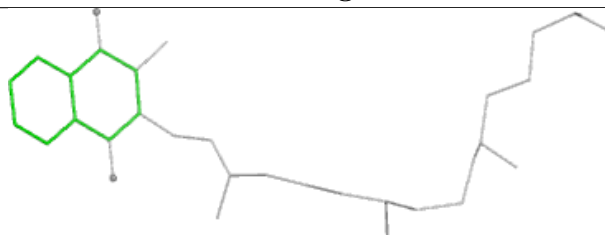
Bond lengths



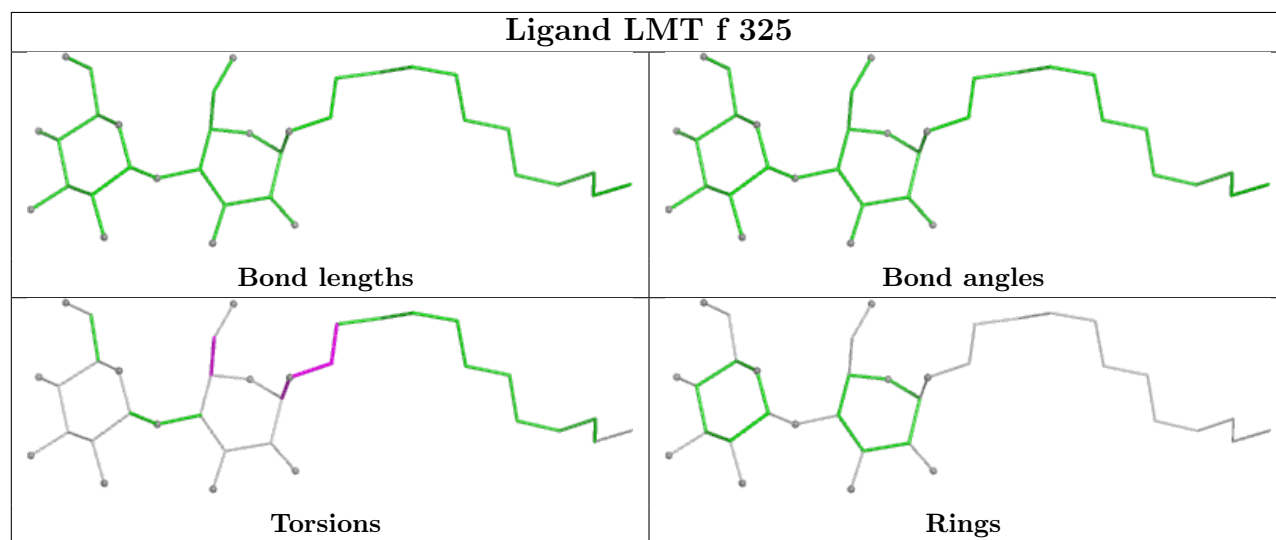
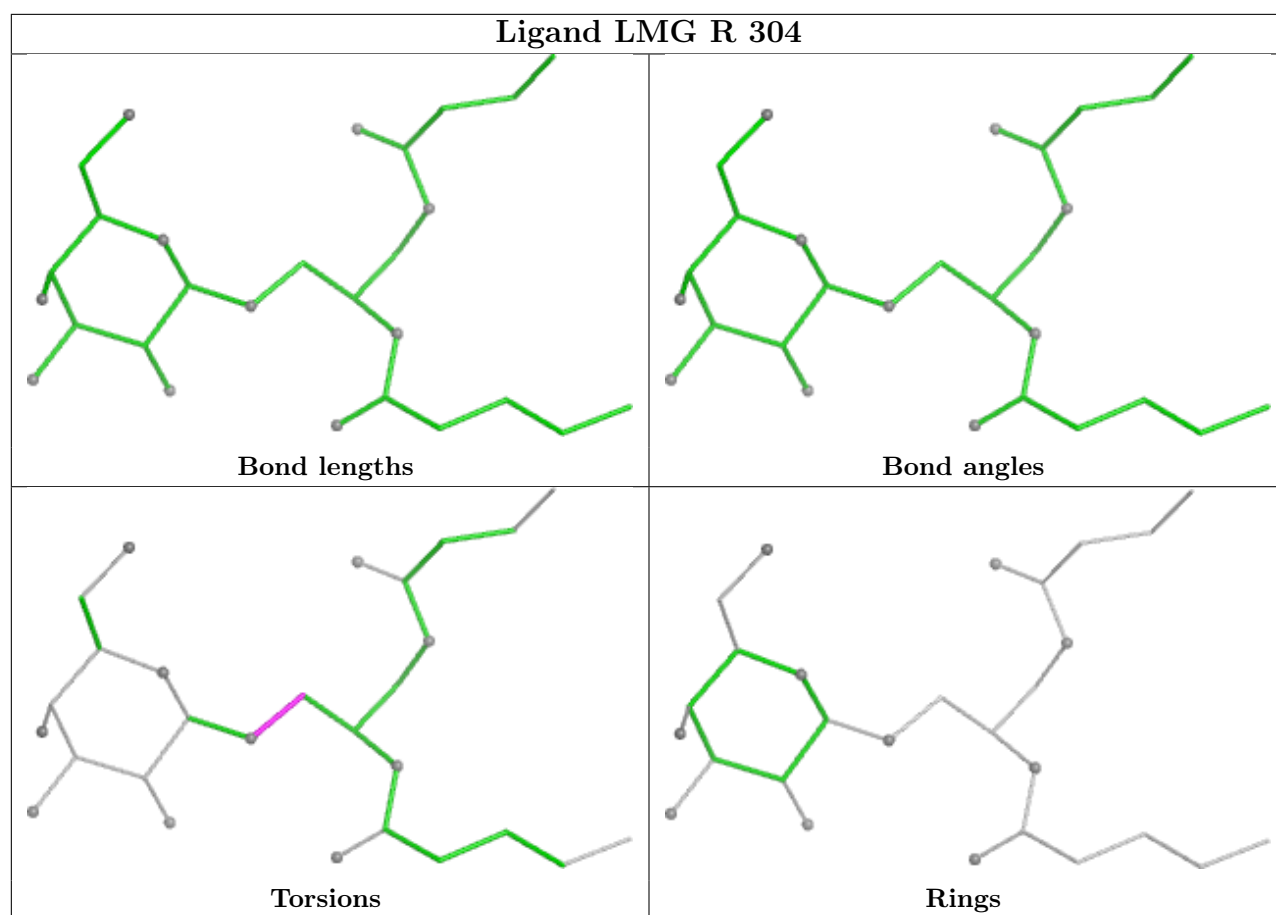
Bond angles



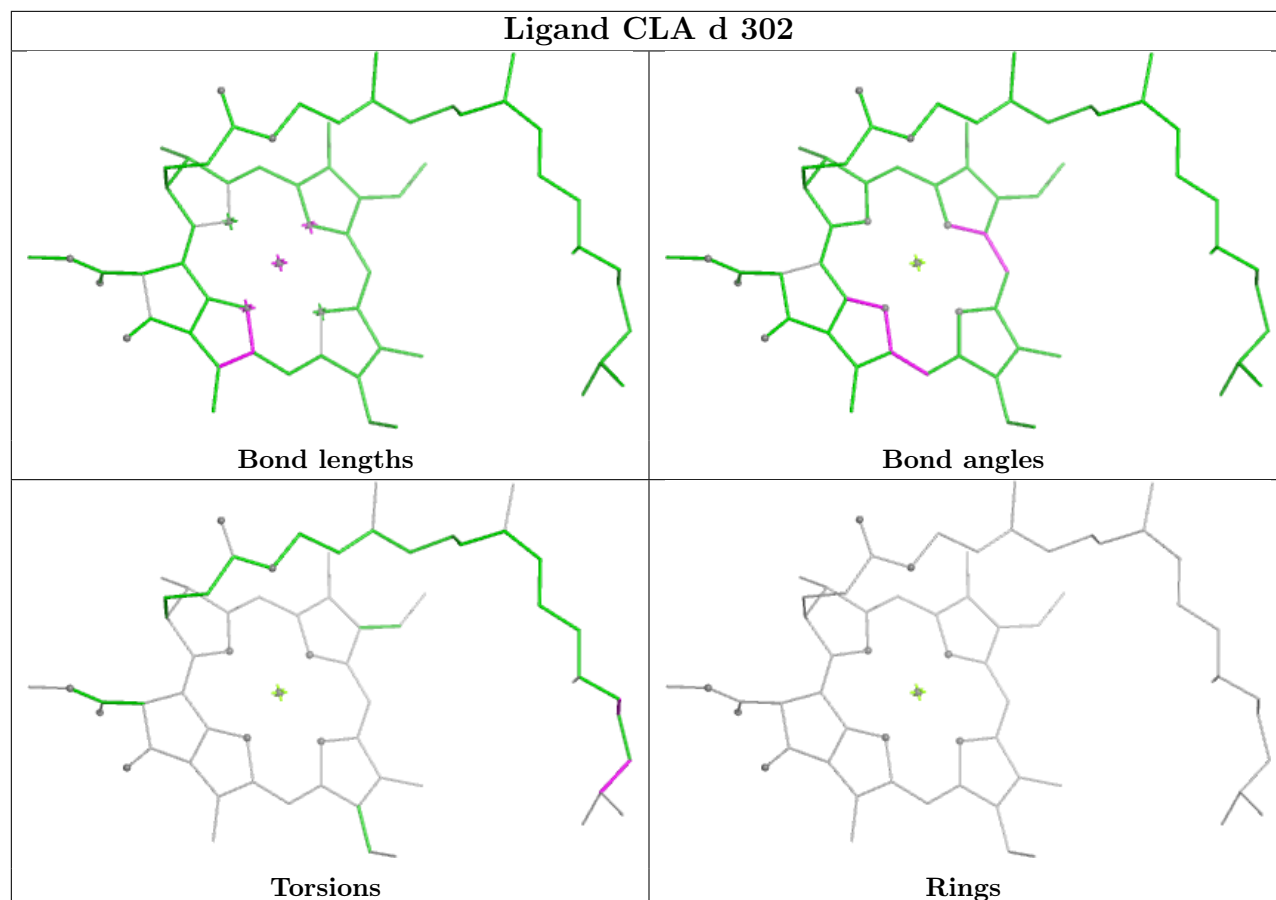
Torsions



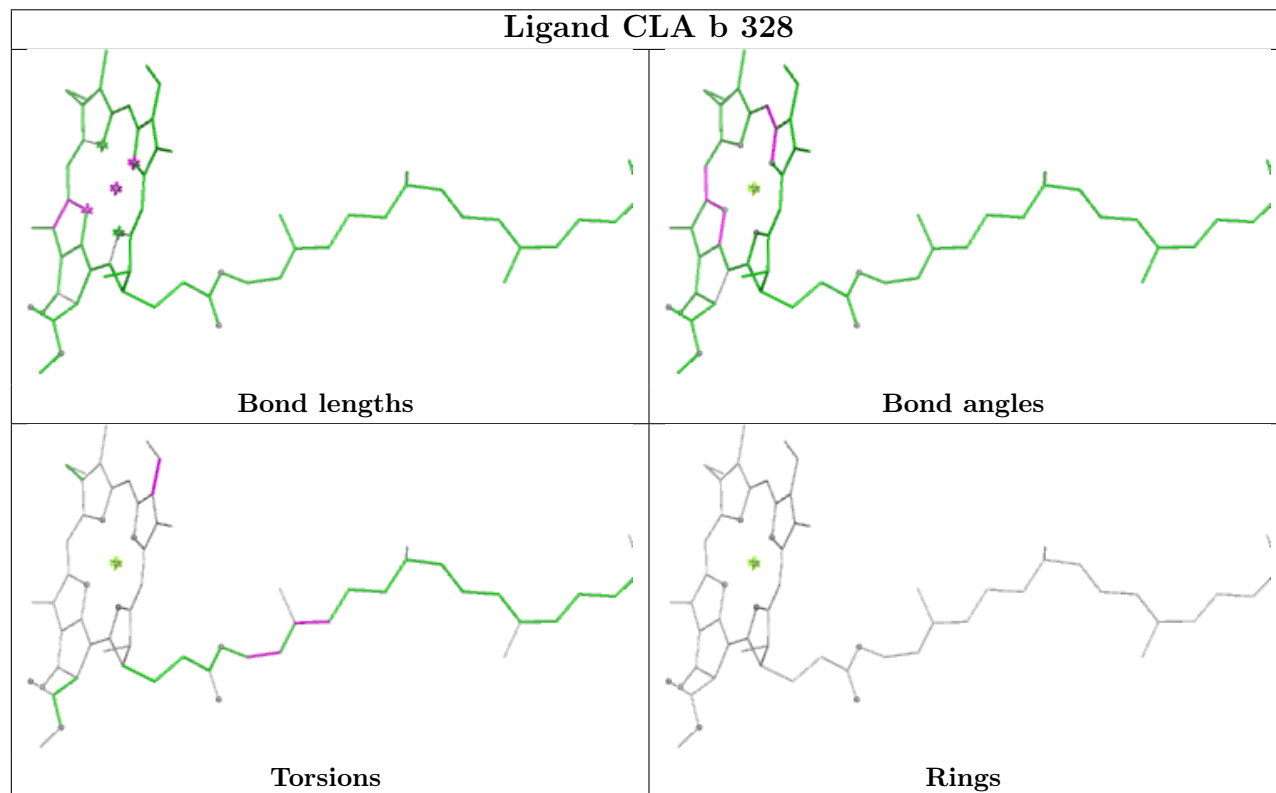
Rings

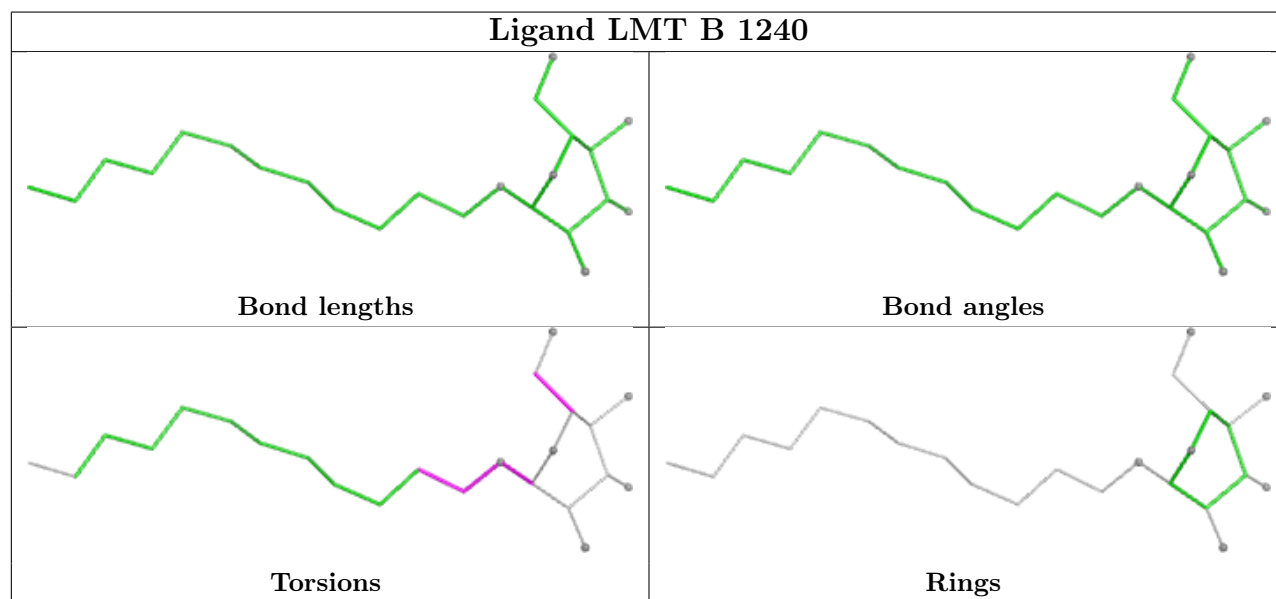
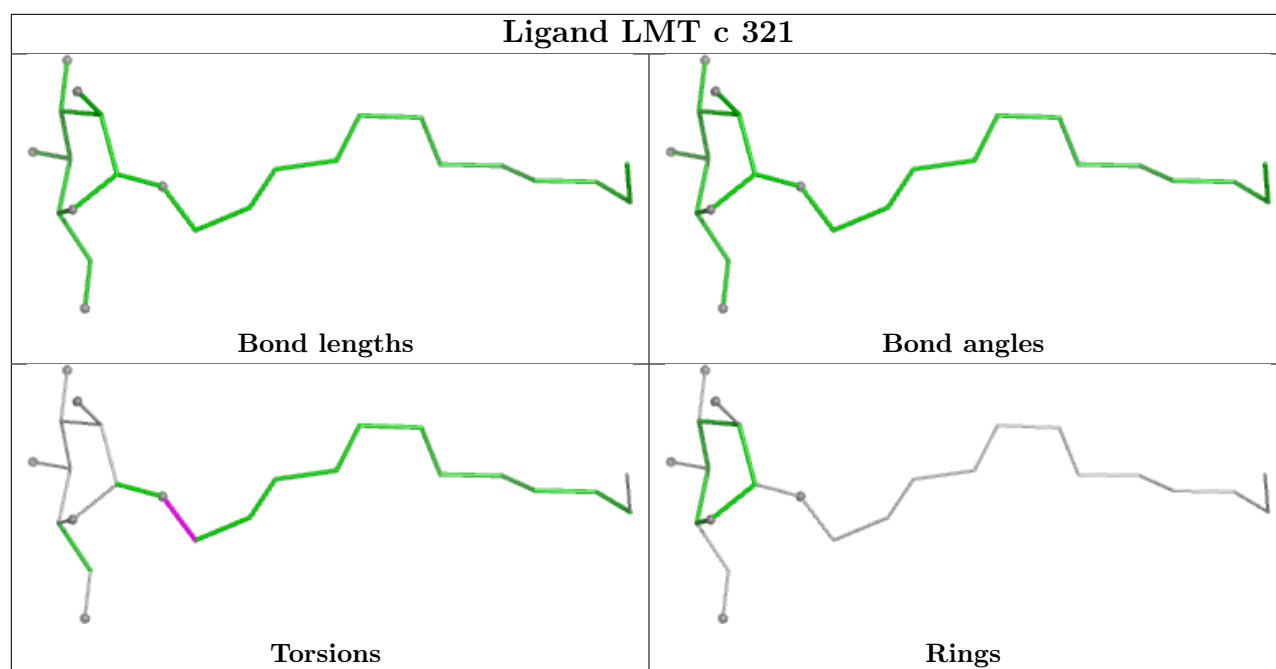


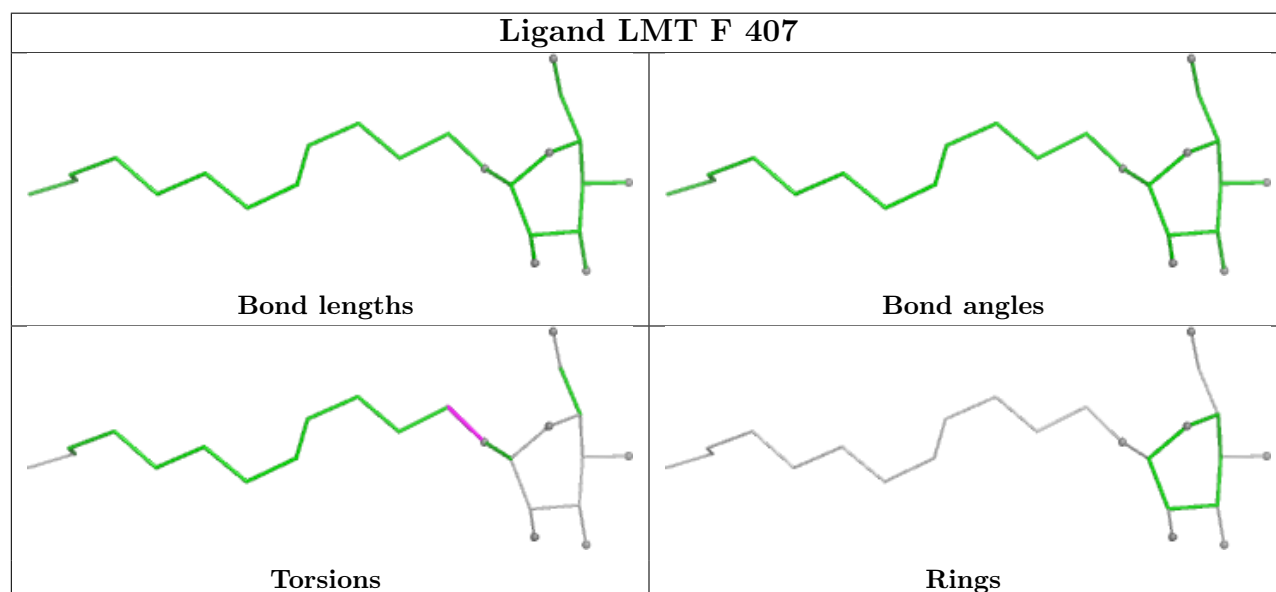
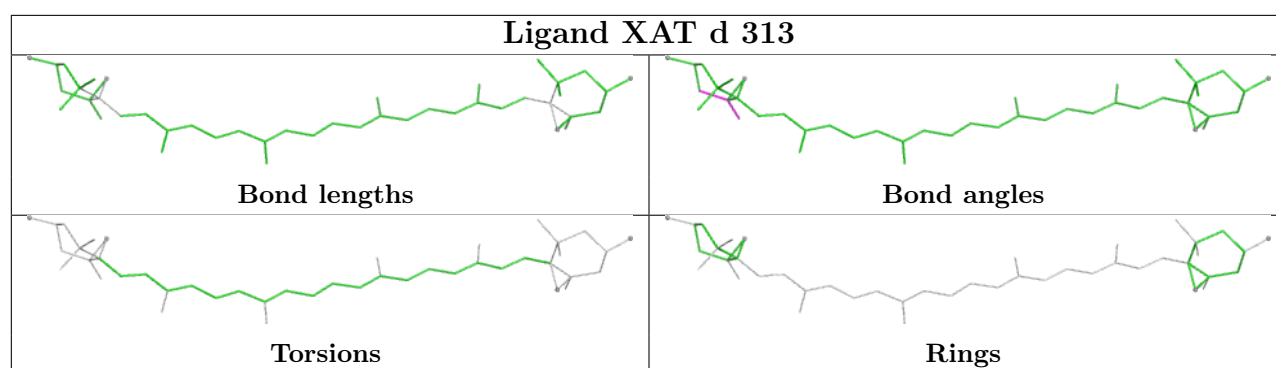
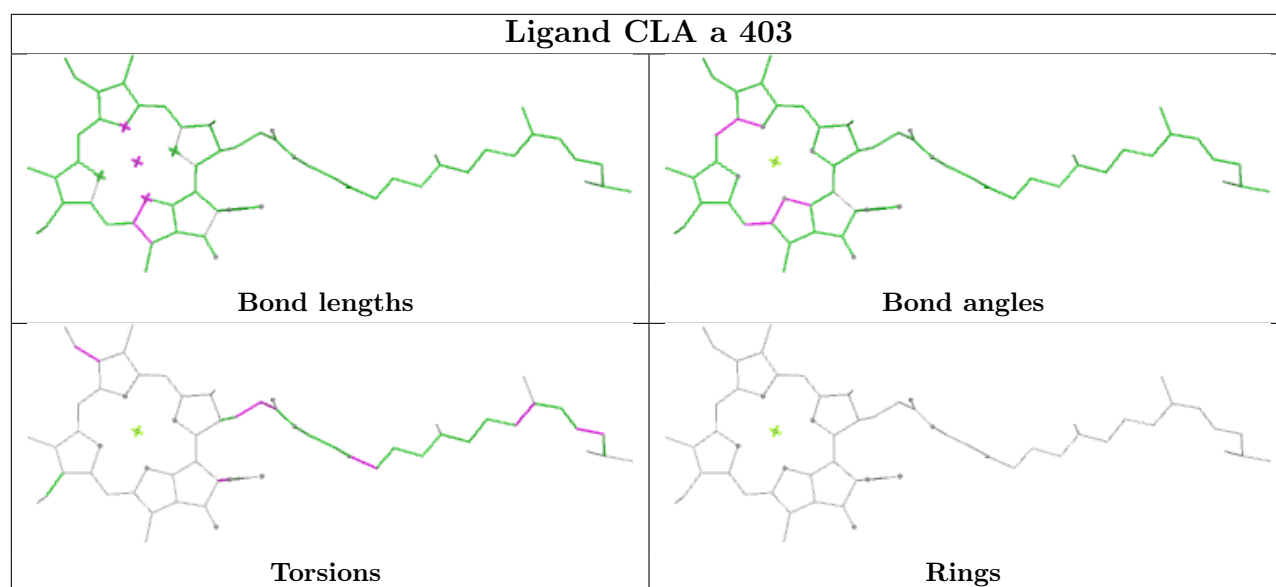
Ligand CLA d 302

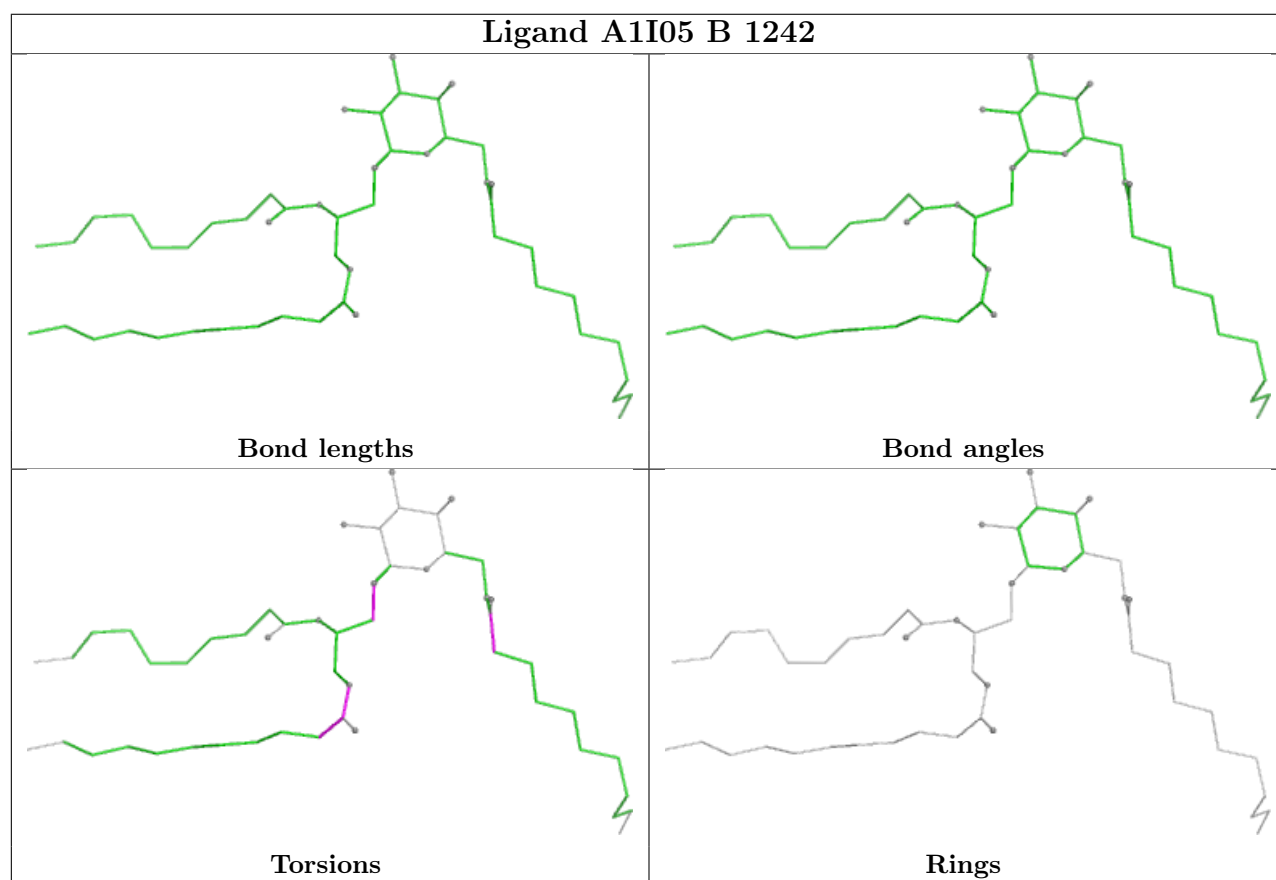
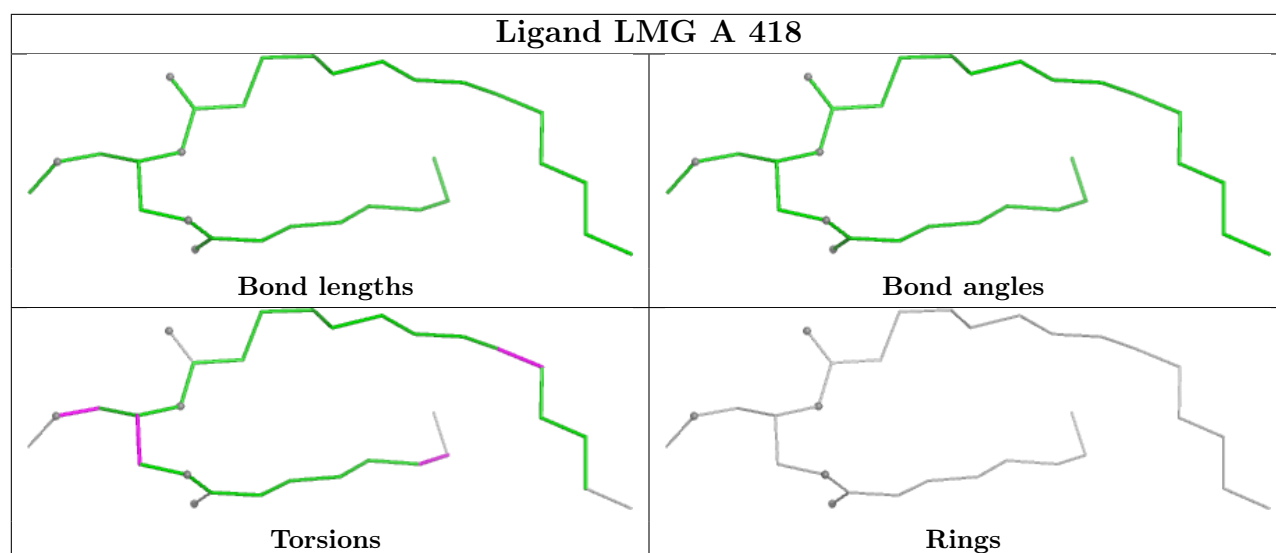


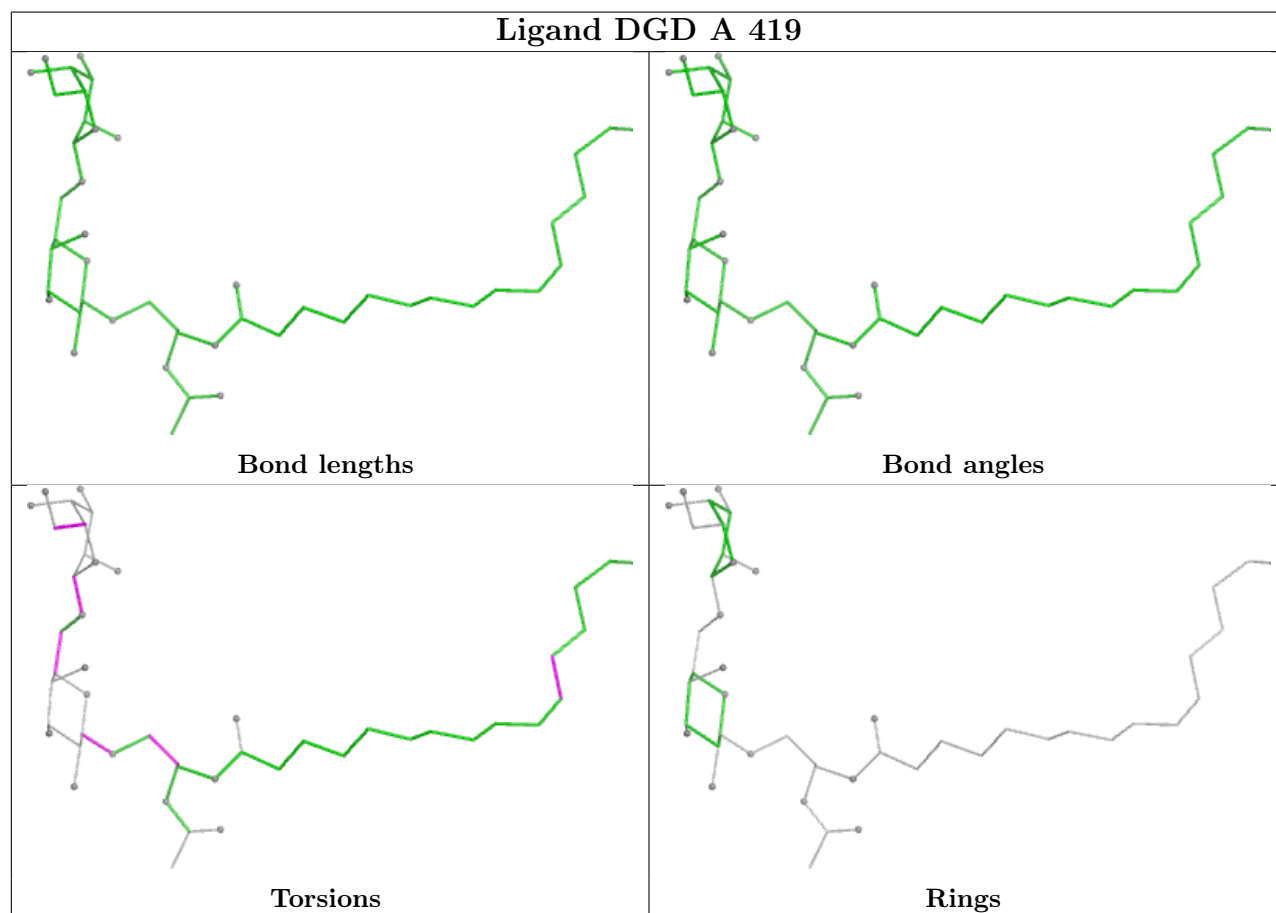
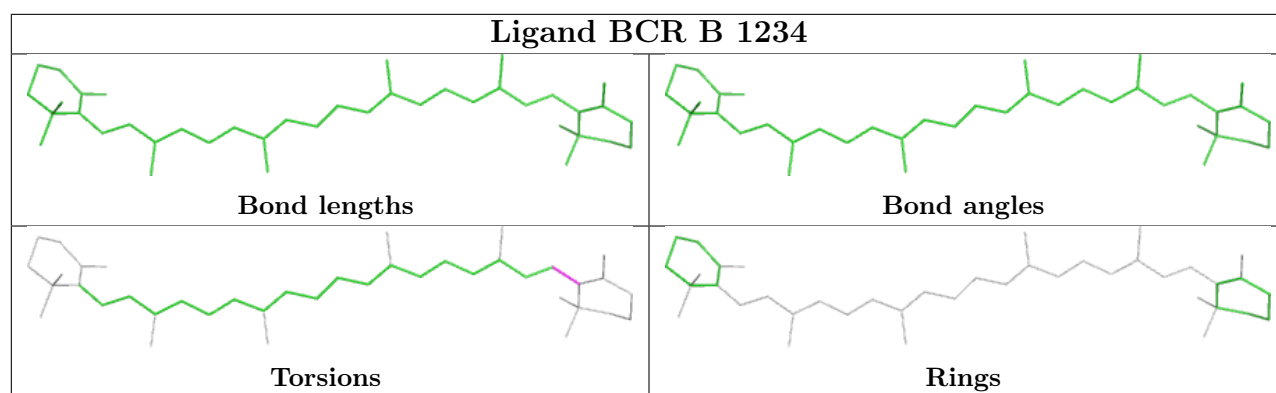
Ligand CLA b 328

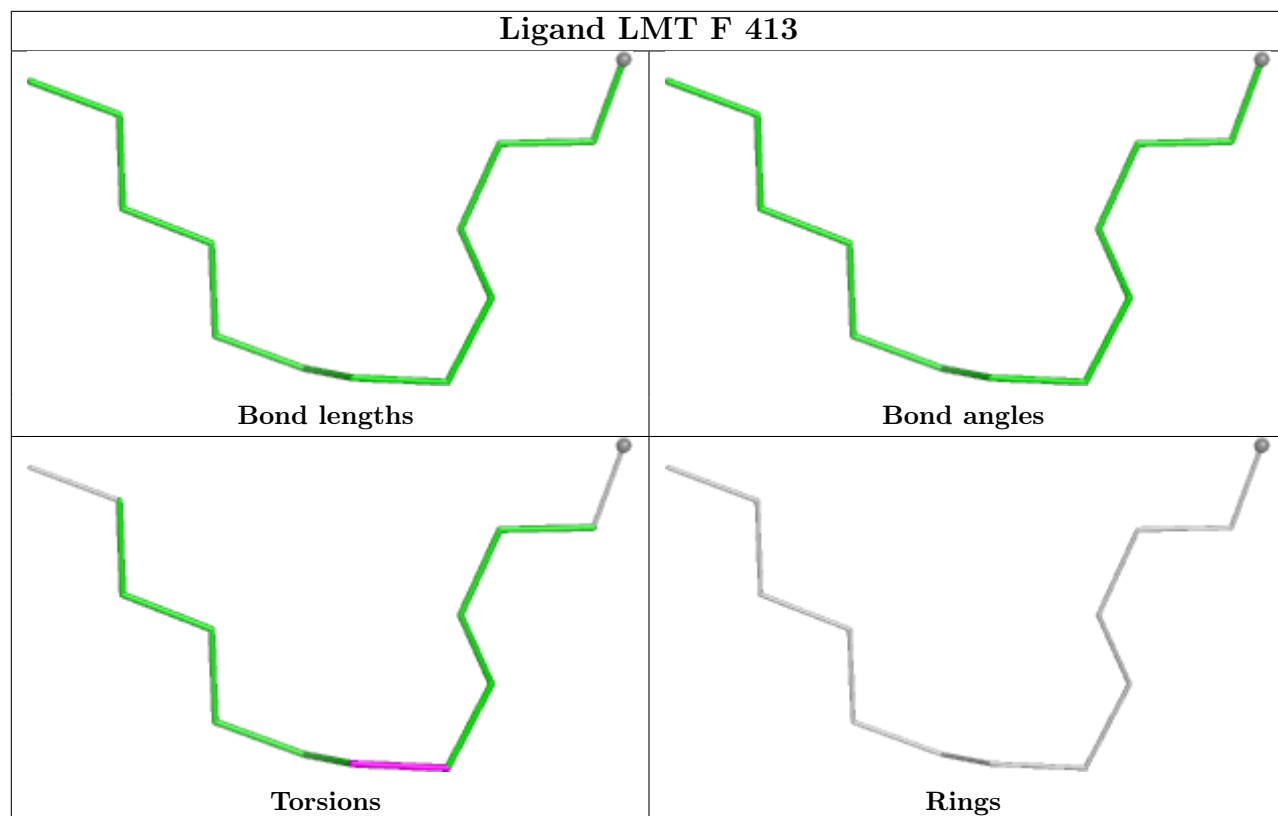




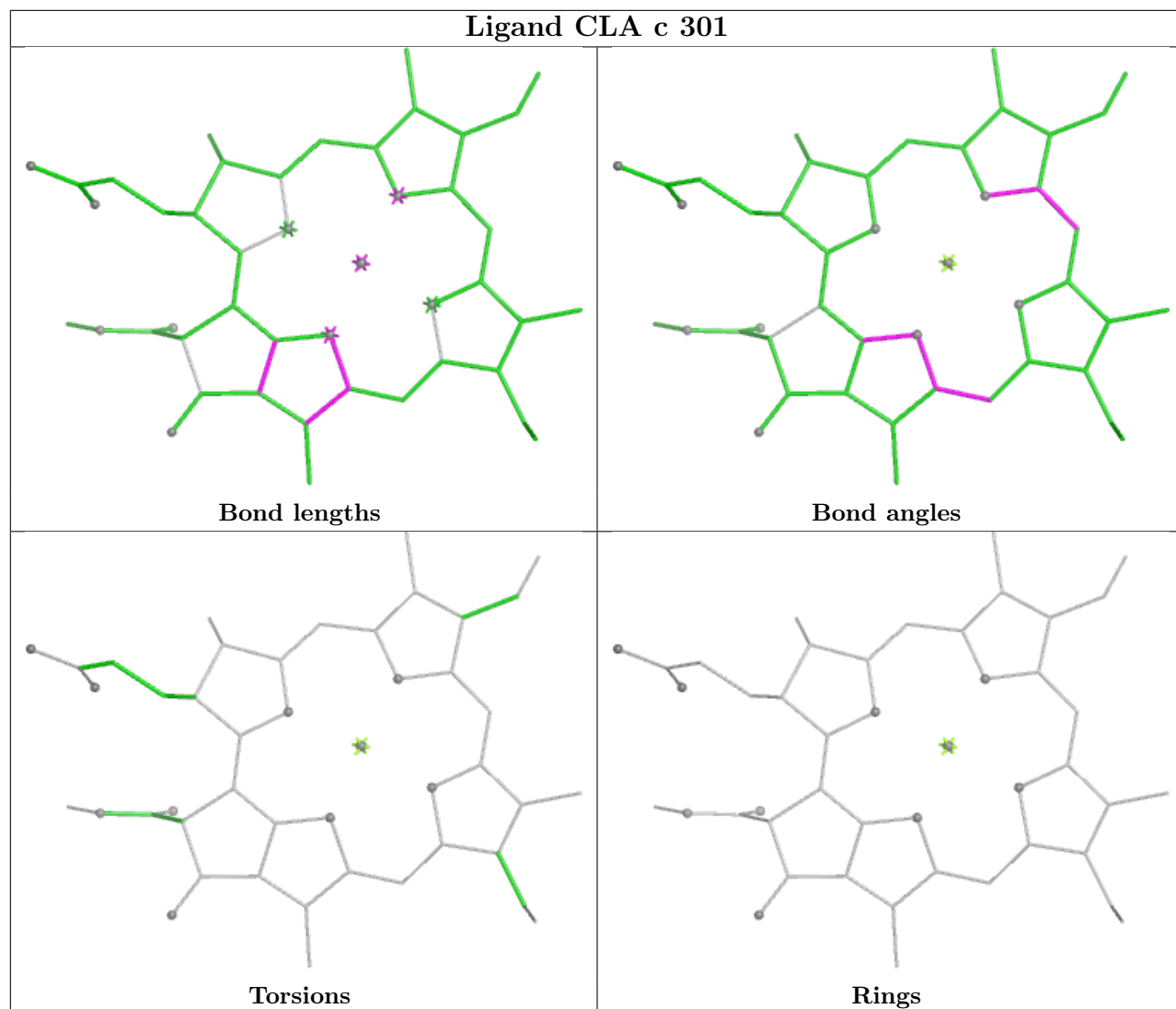


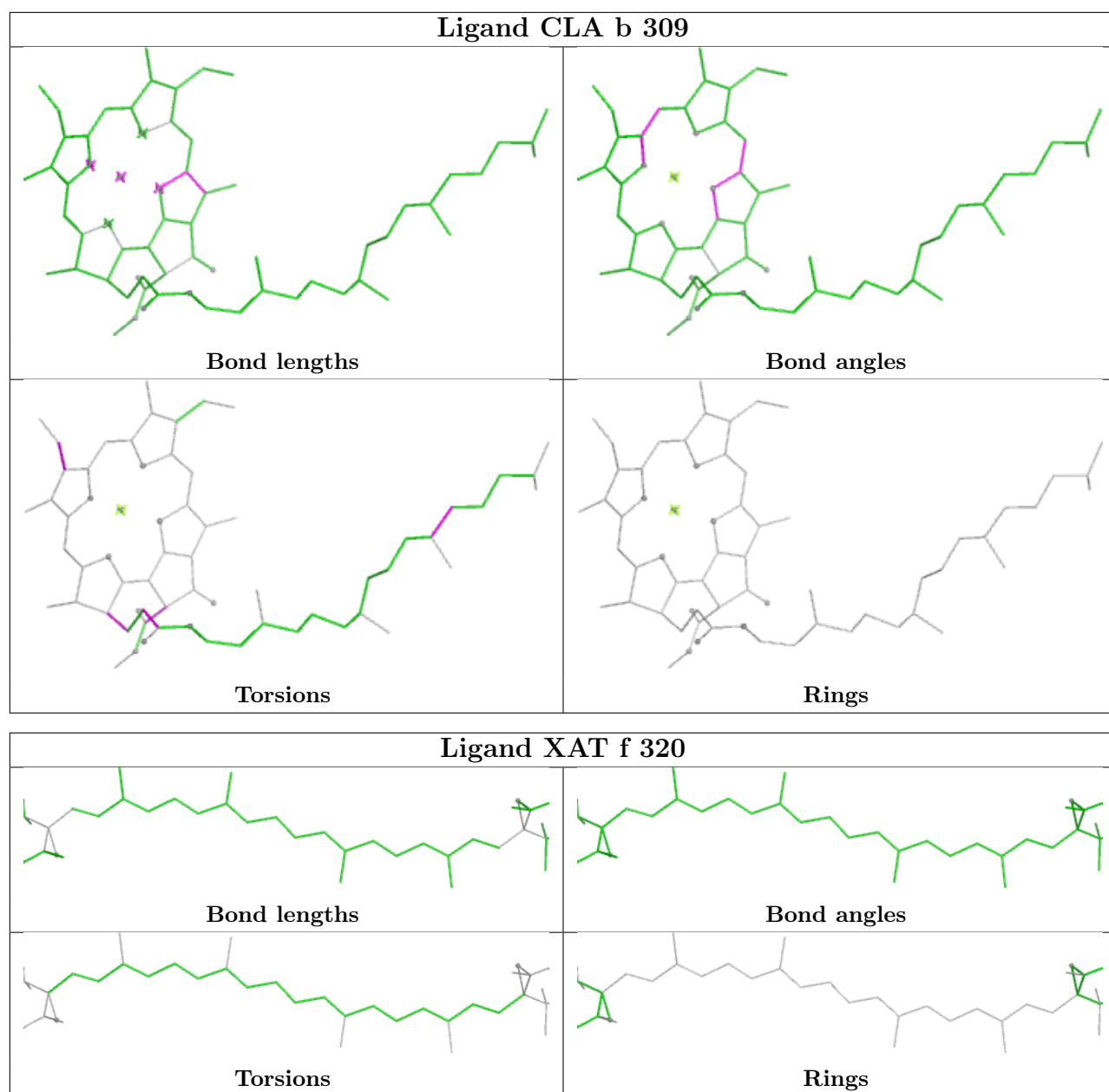


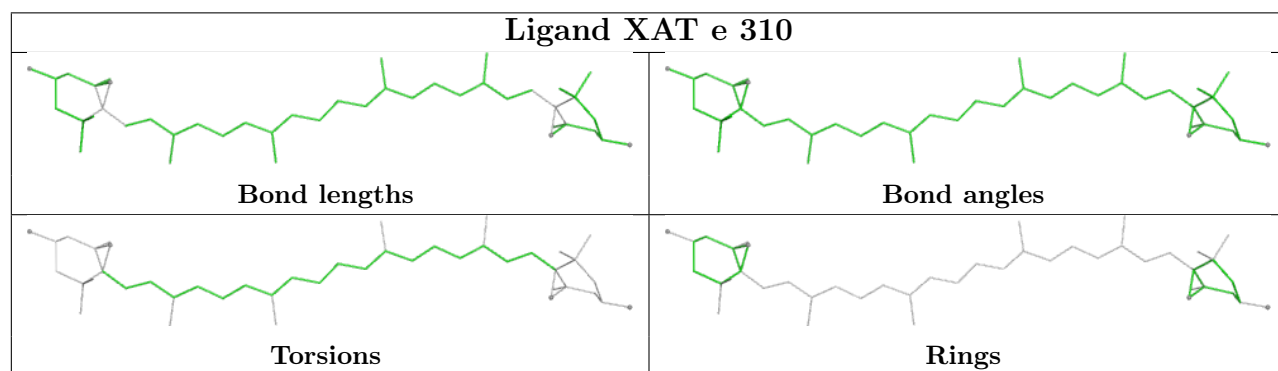
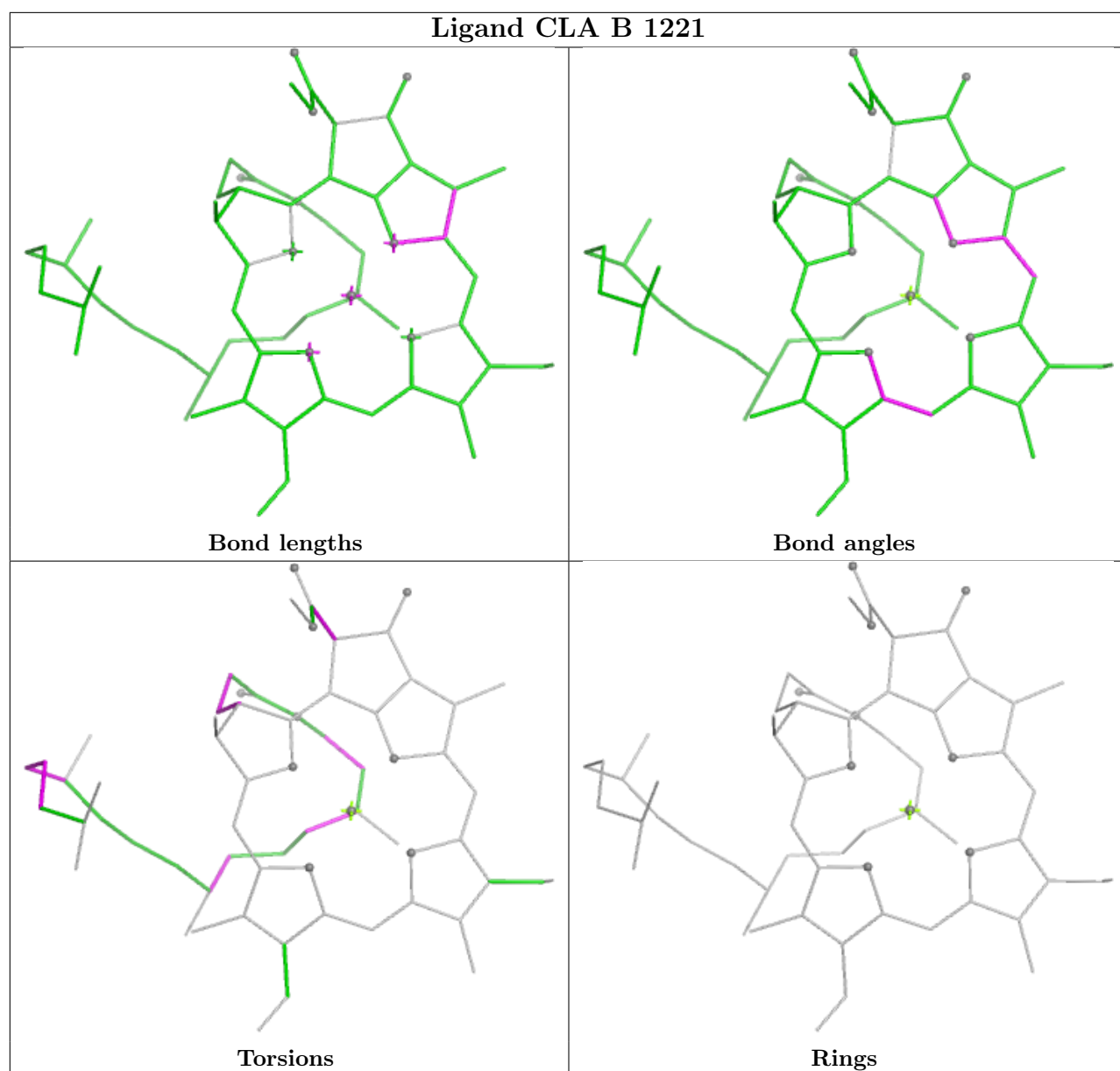


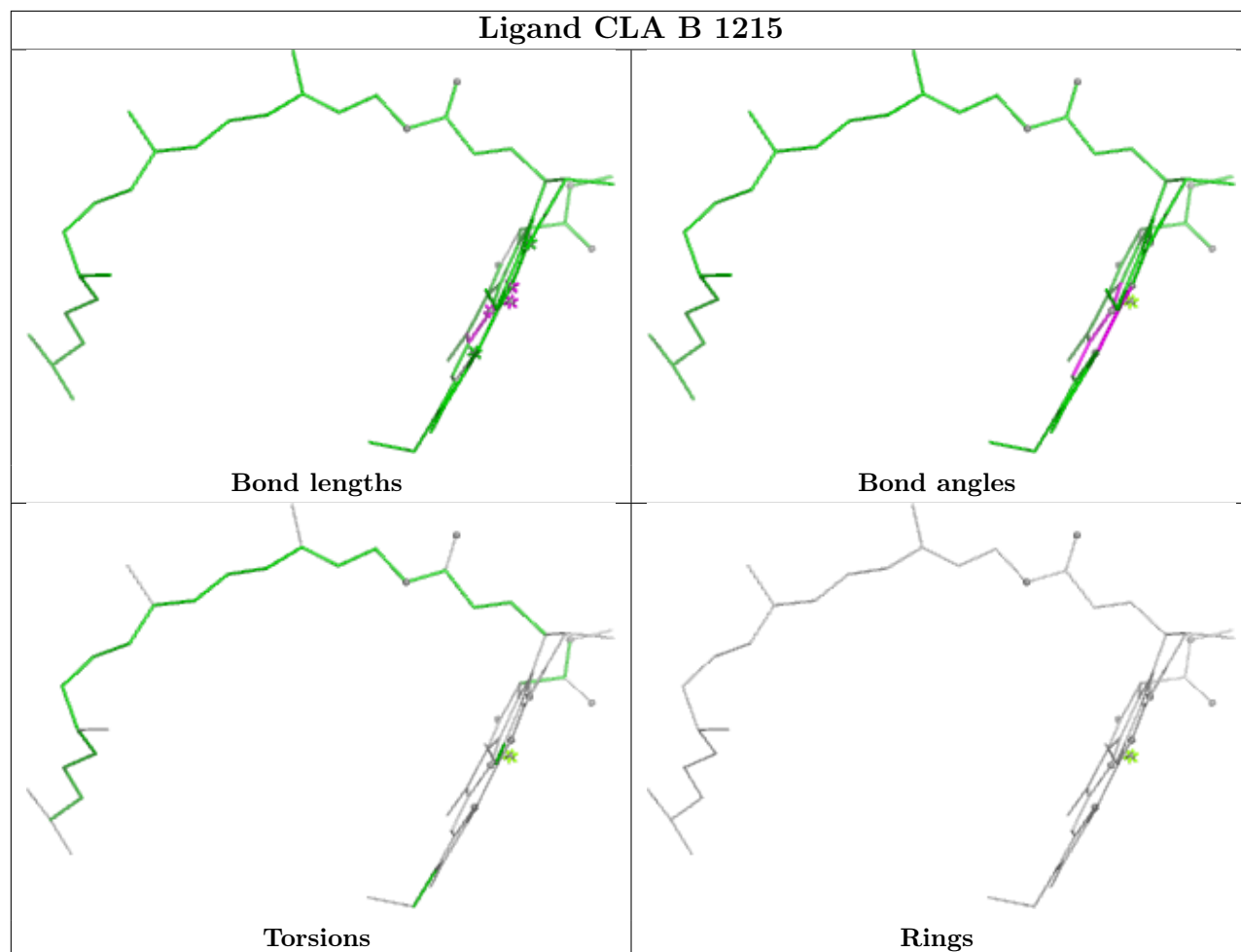
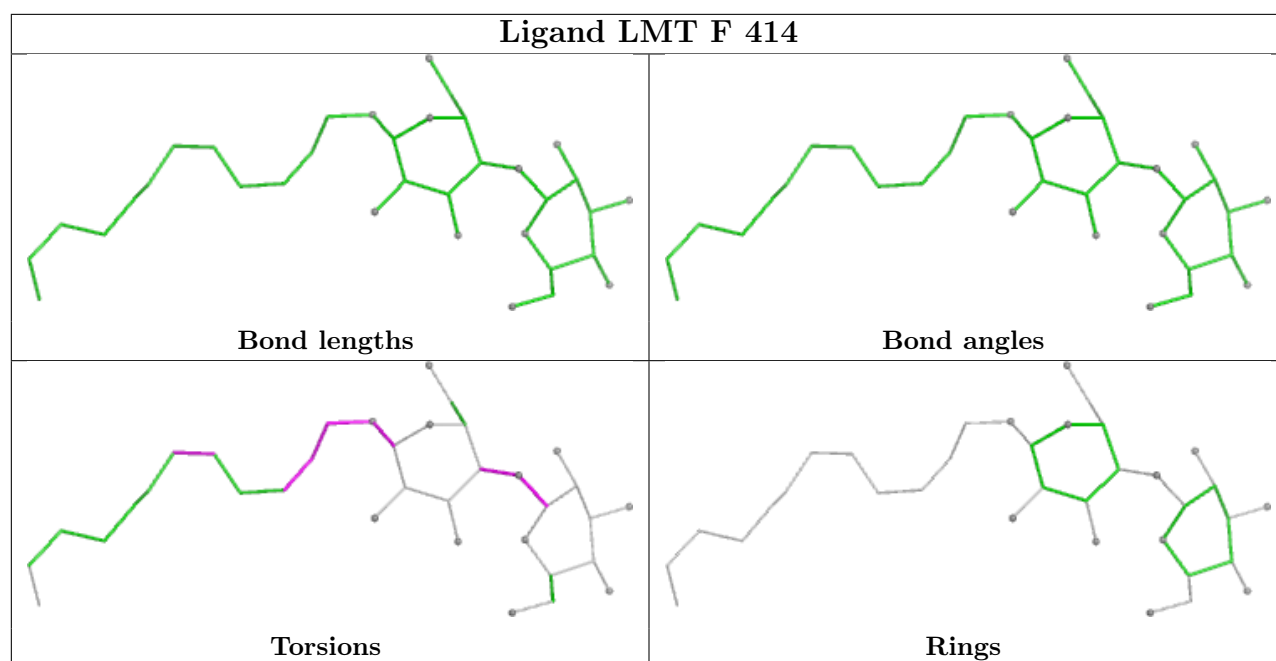


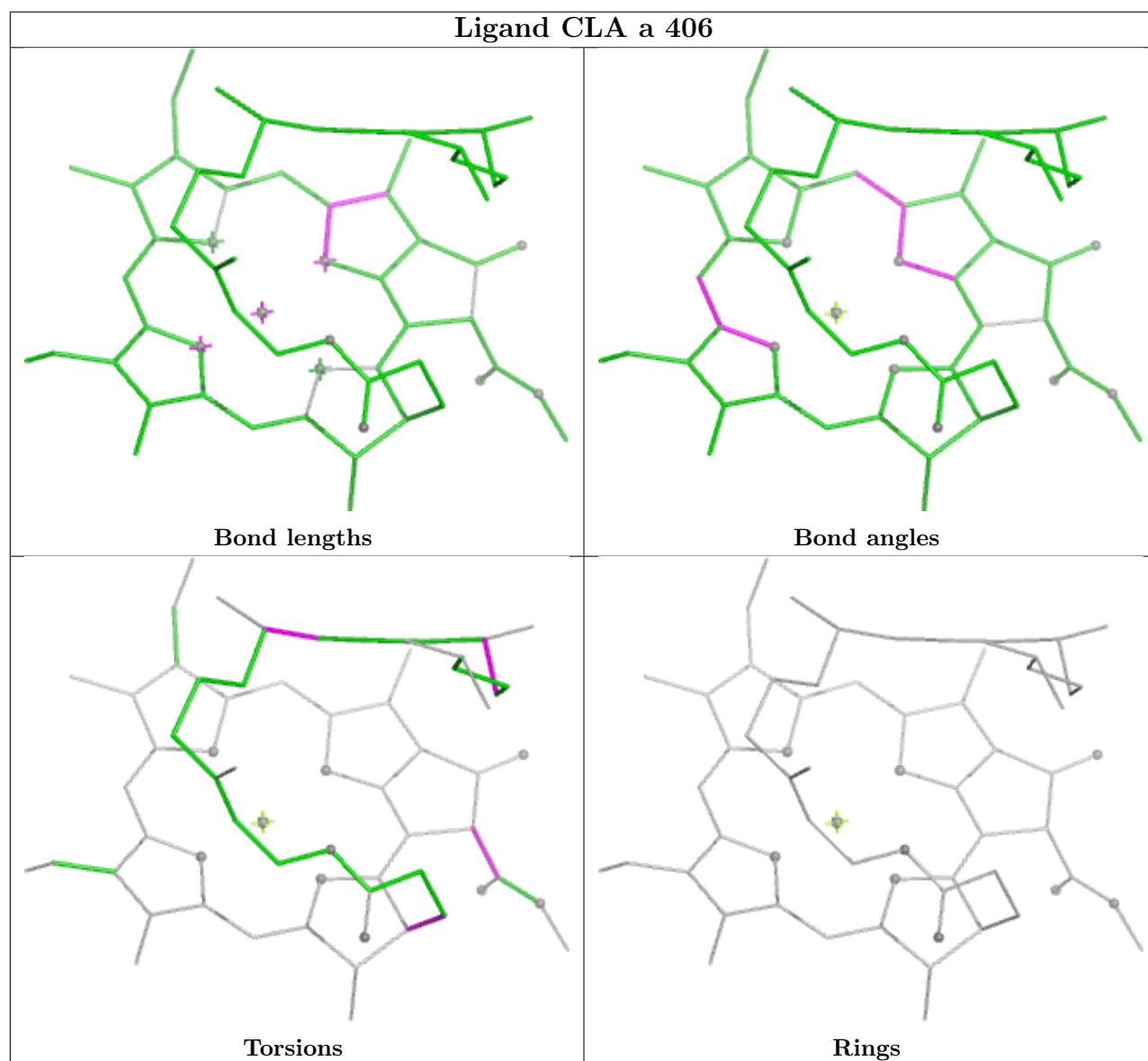
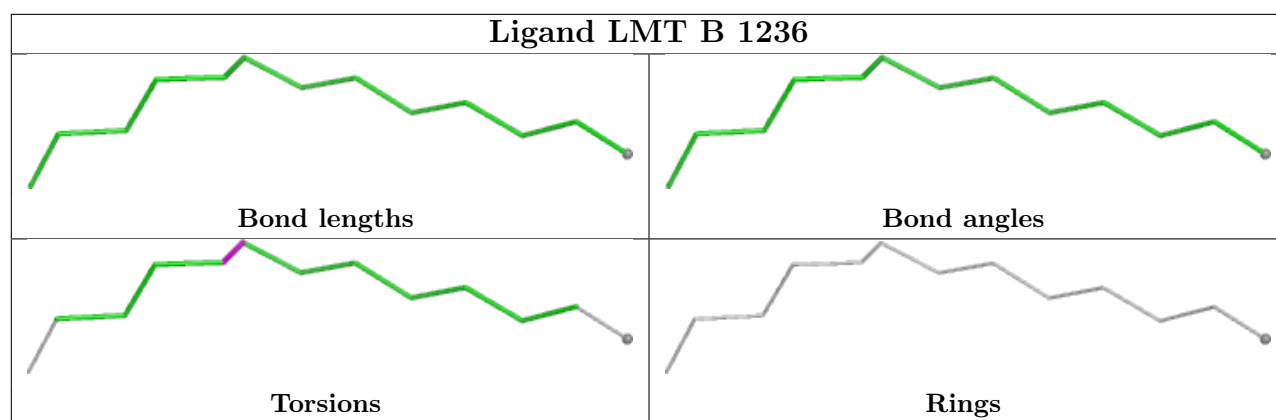
Ligand CLA c 301

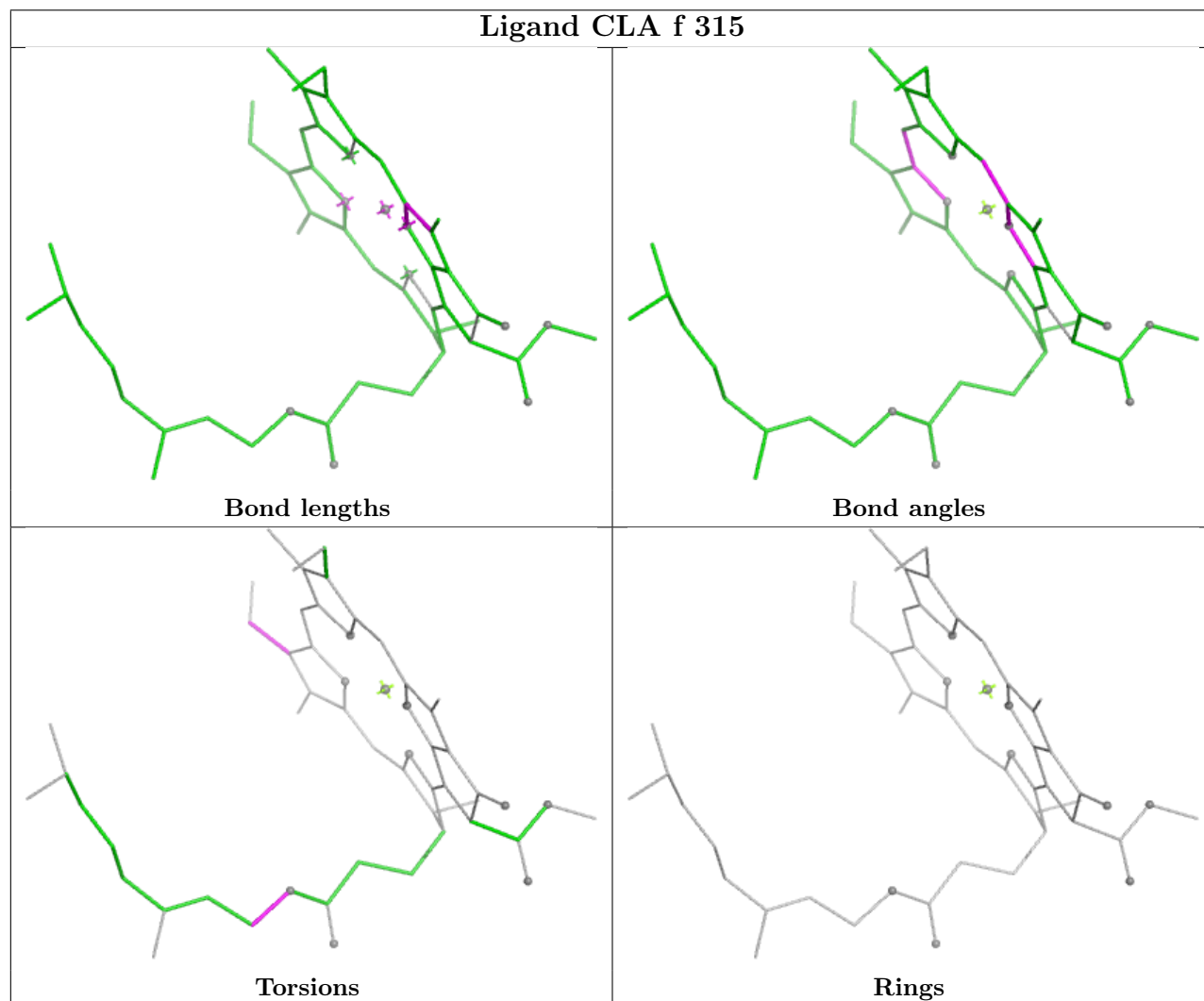
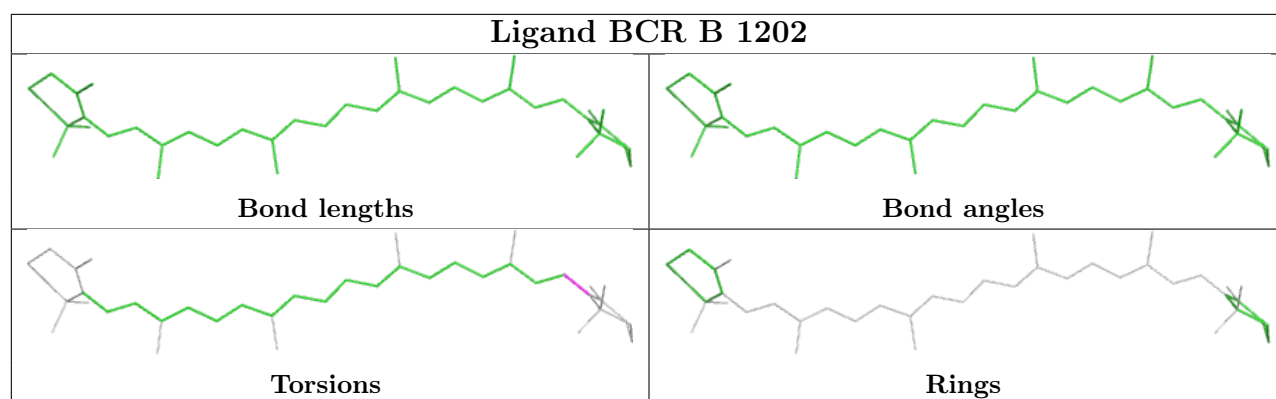


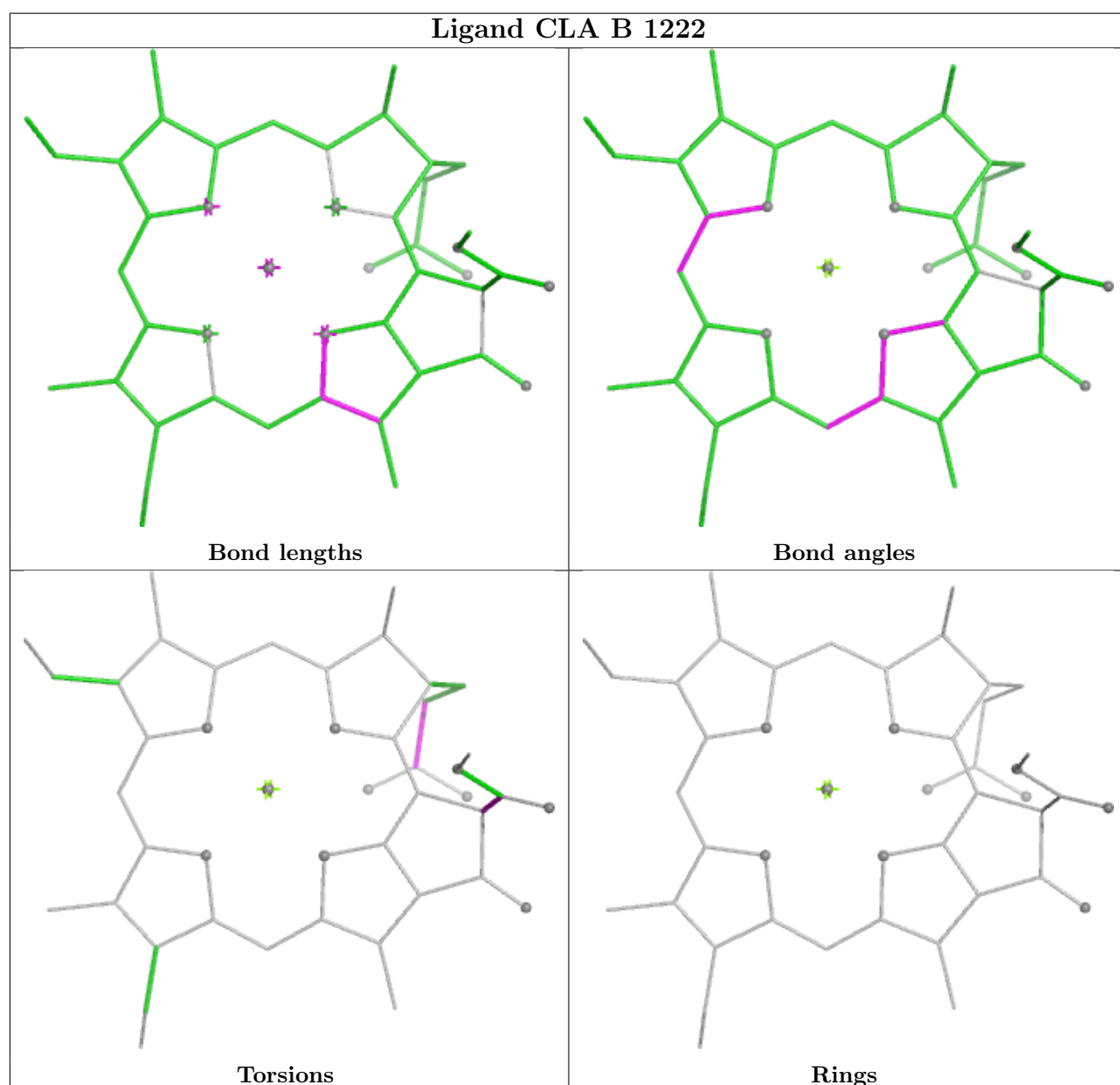
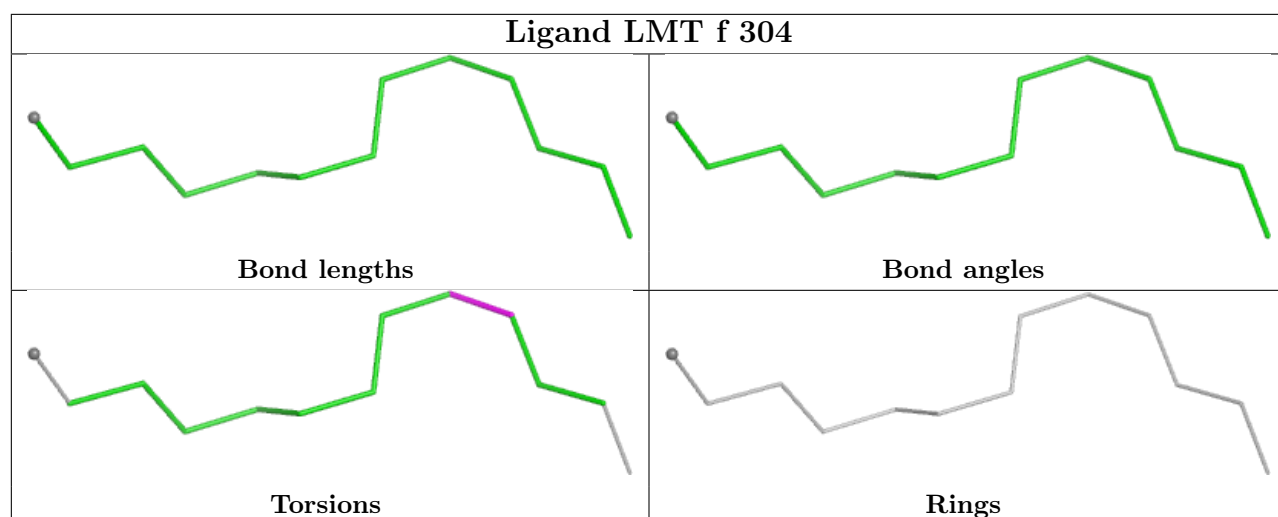


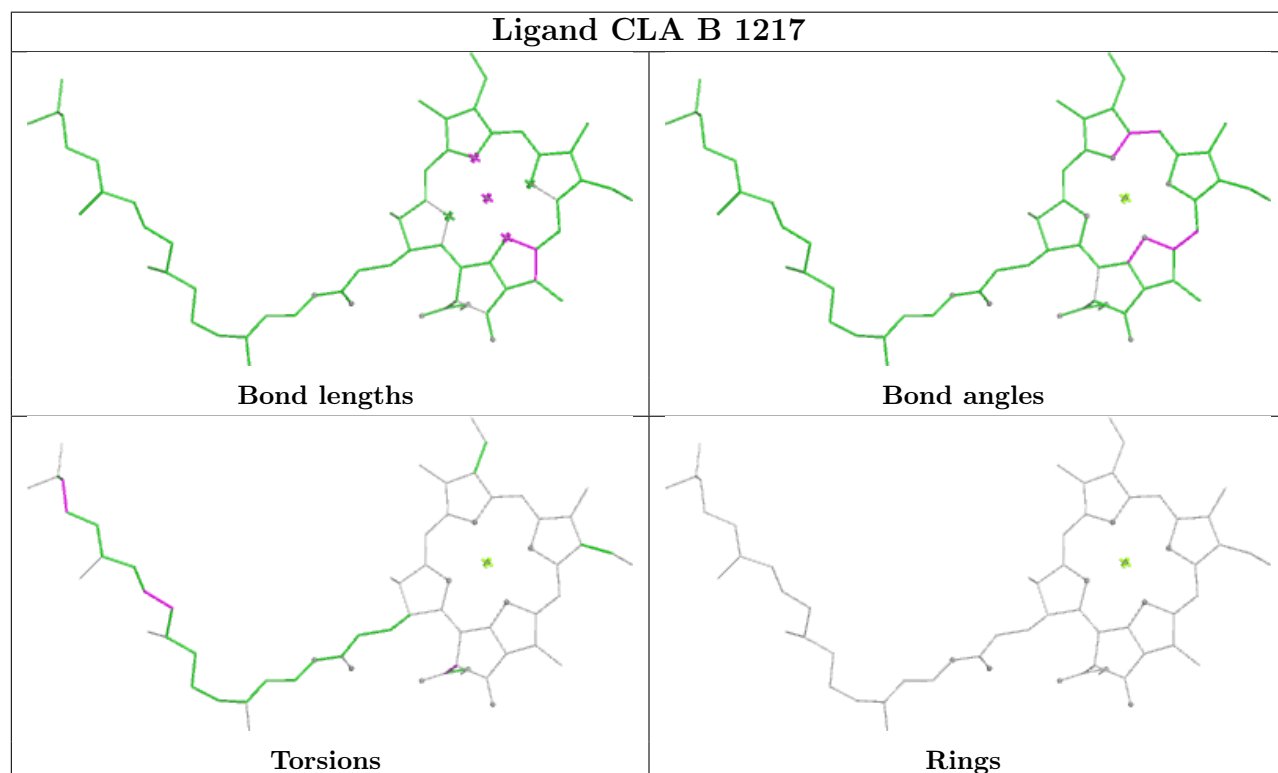
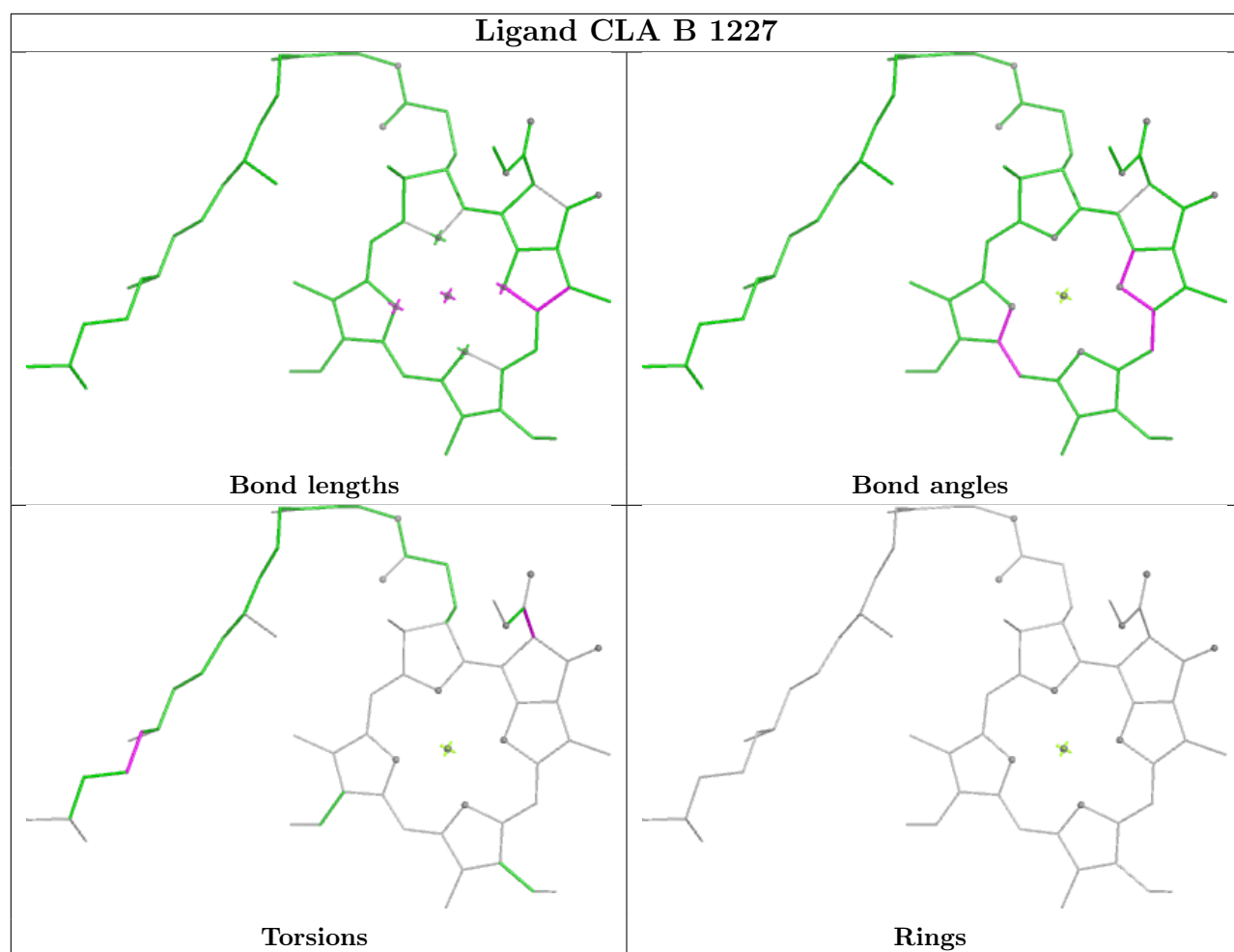


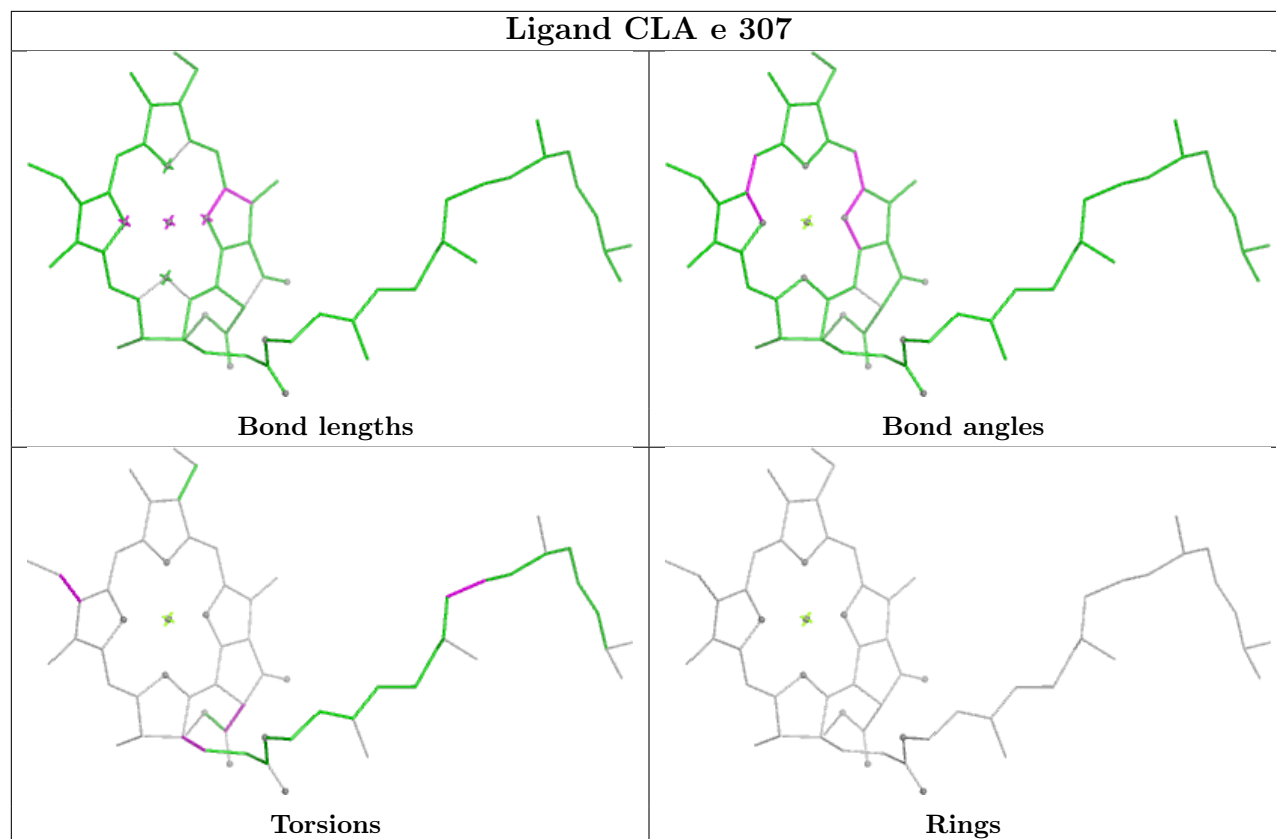
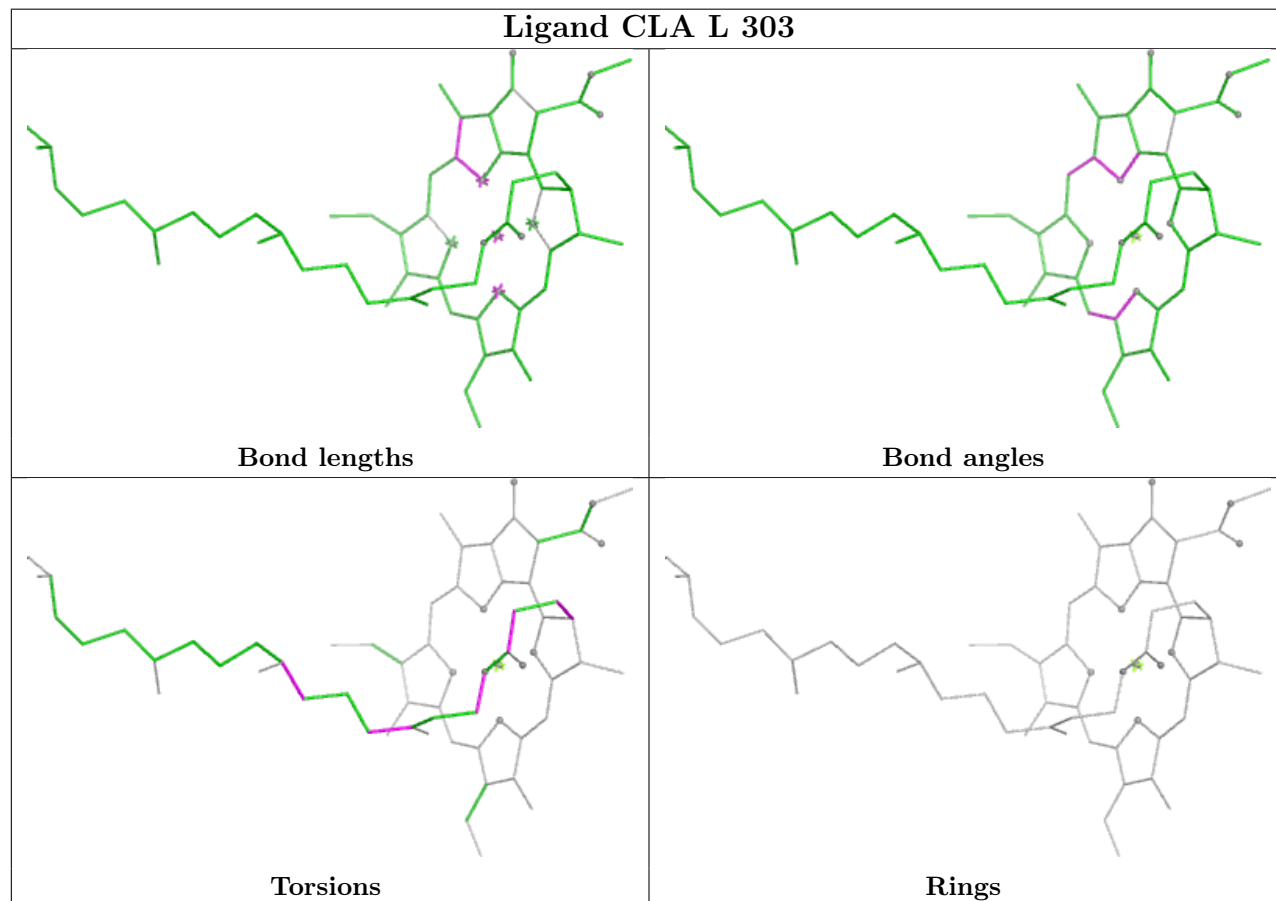


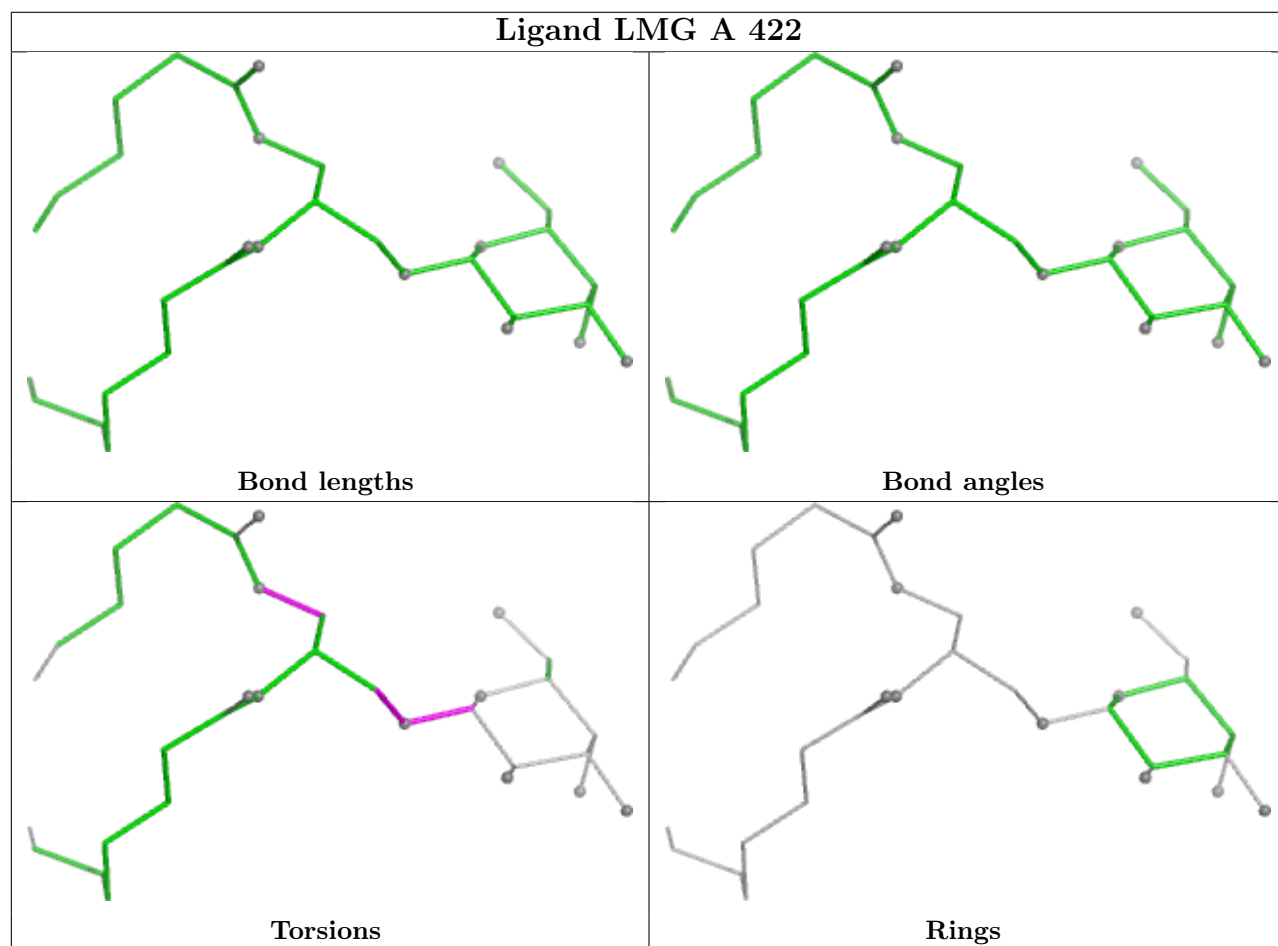
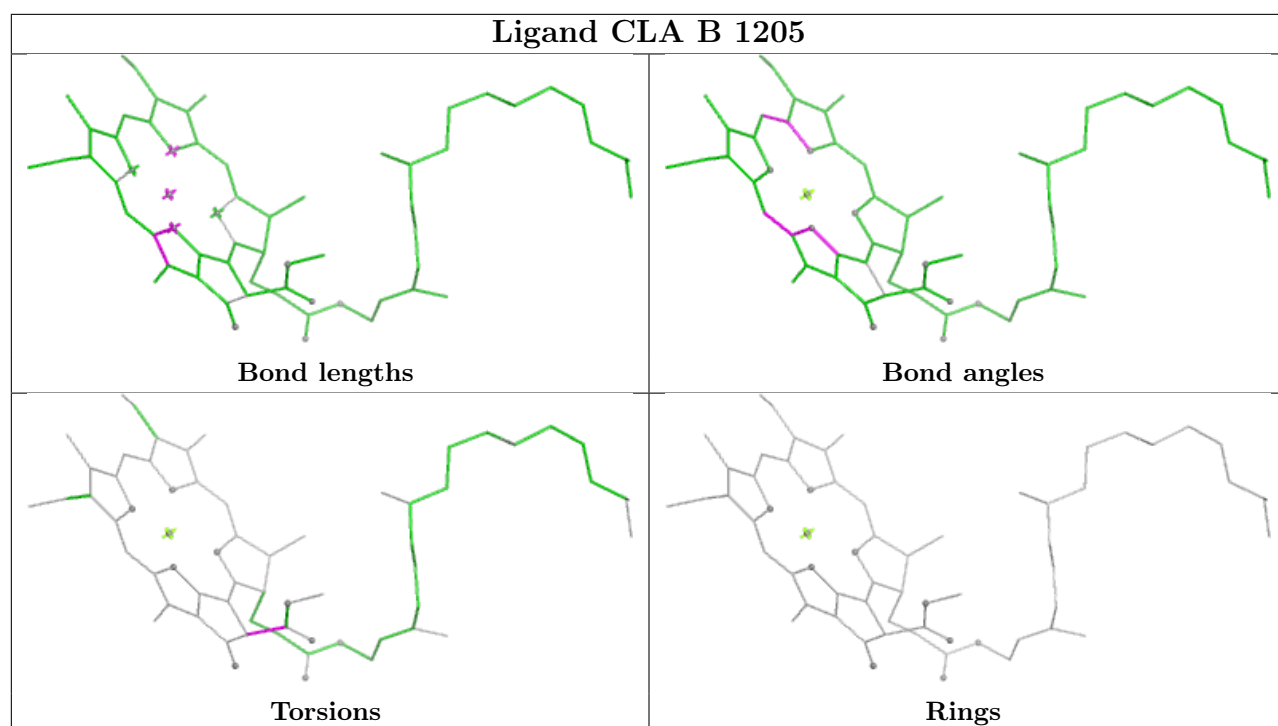


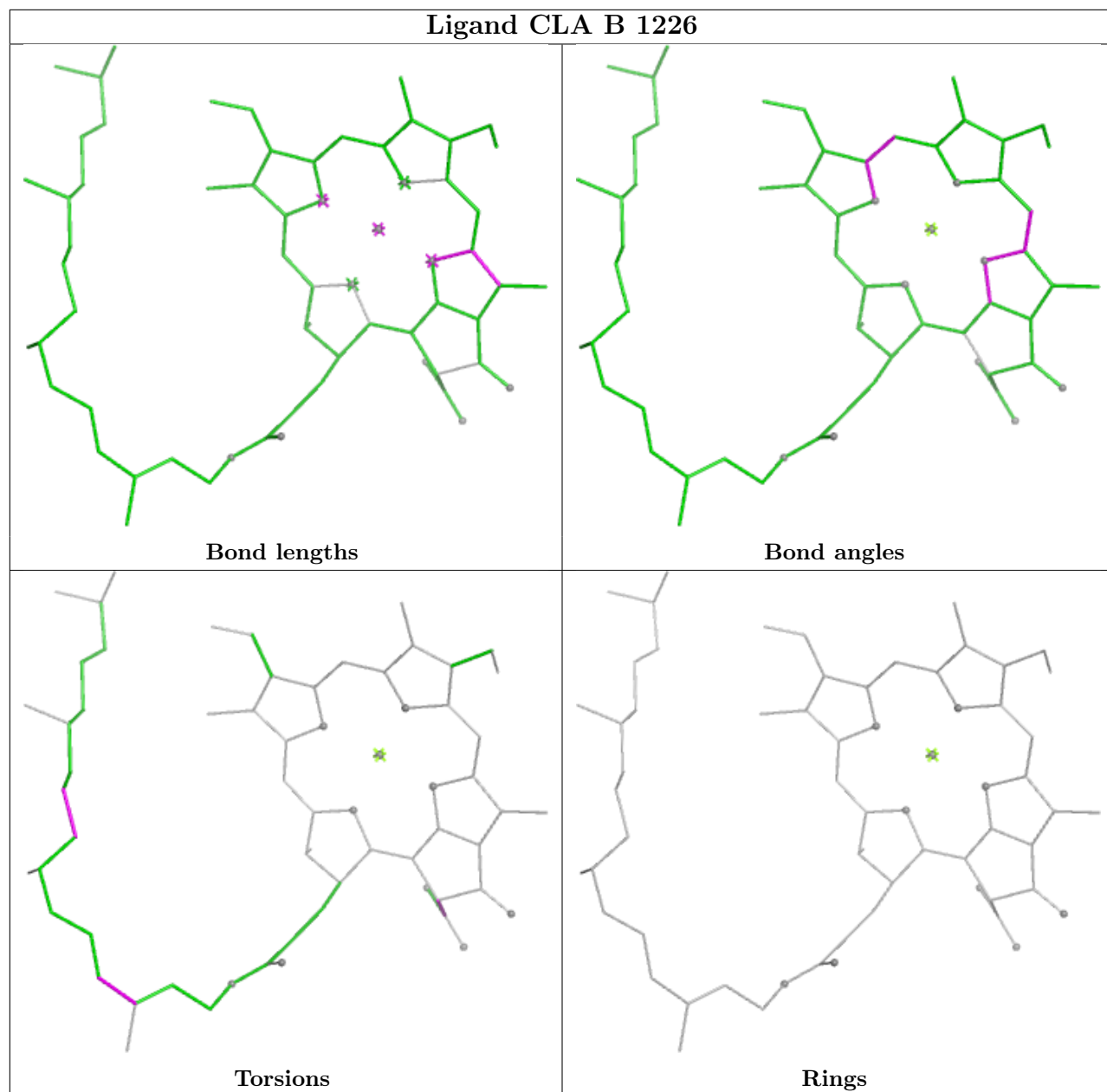




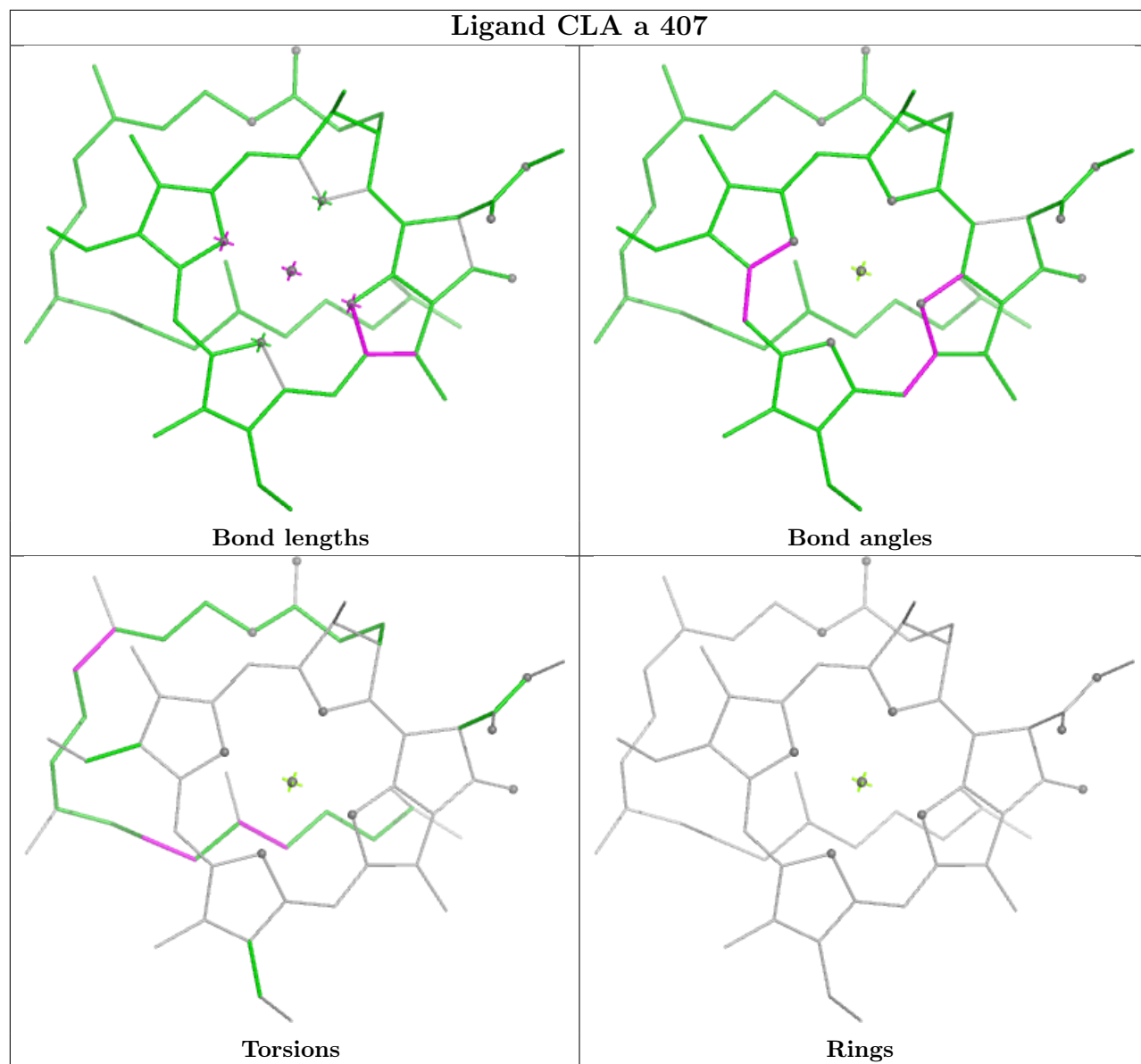


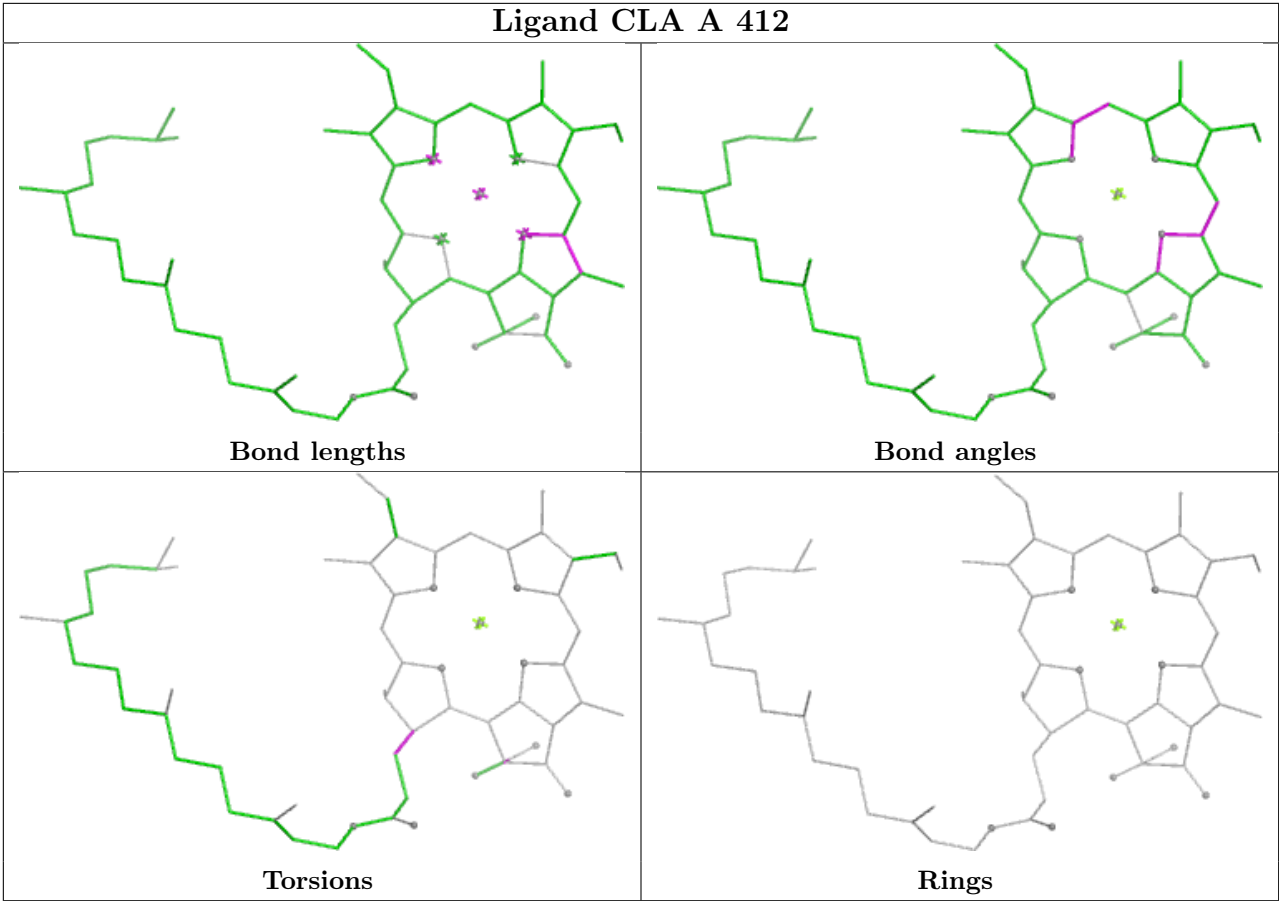
Ligand CLA e 307**Ligand CLA L 303**





Ligand CLA a 407





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
14	d	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	d	221:GLY	C	223:PHE	N	3.22

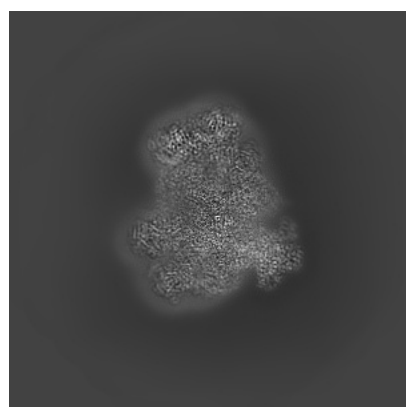
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52518. These allow visual inspection of the internal detail of the map and identification of artifacts.

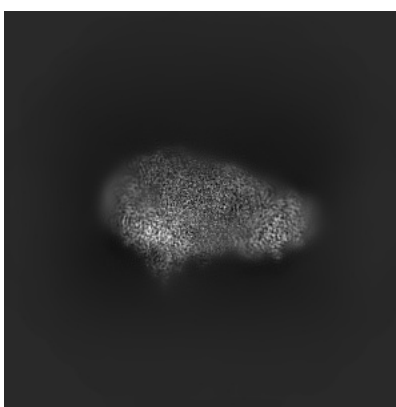
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

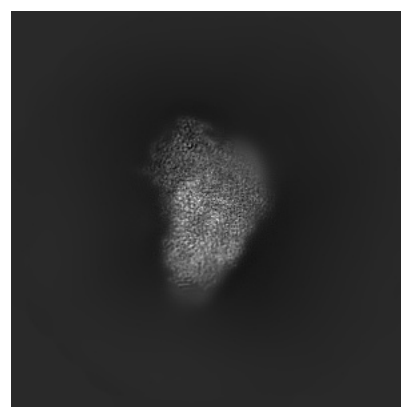
6.1.1 Primary map



X



Y

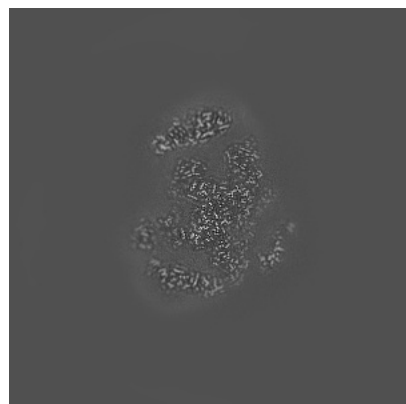


Z

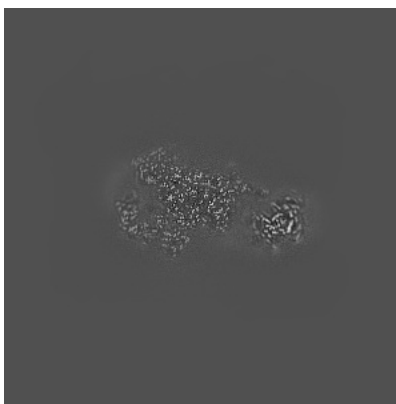
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

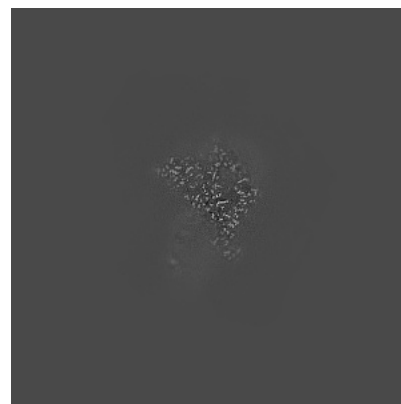
6.2.1 Primary map



X Index: 250



Y Index: 250

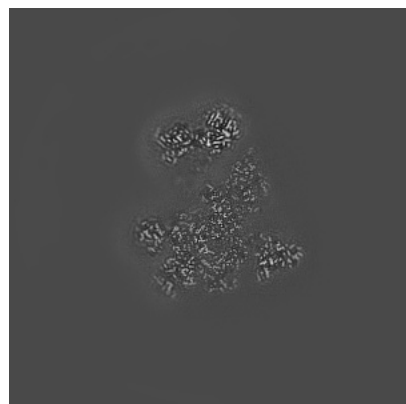


Z Index: 250

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

6.3 Largest variance slices [i](#)

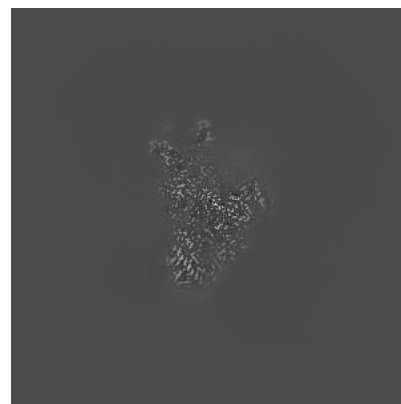
6.3.1 Primary map



X Index: 227



Y Index: 262

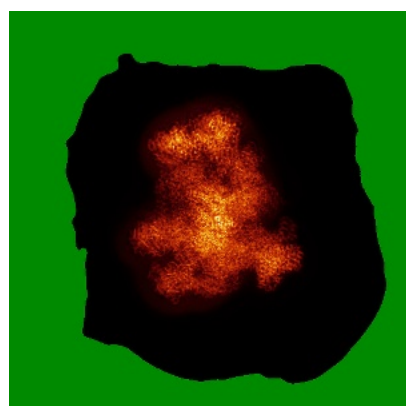


Z Index: 219

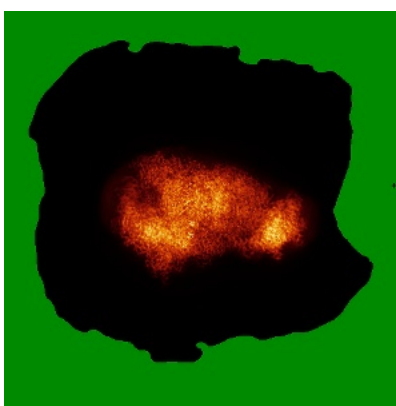
The images above show the largest variance slices of the map in three orthogonal directions.

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

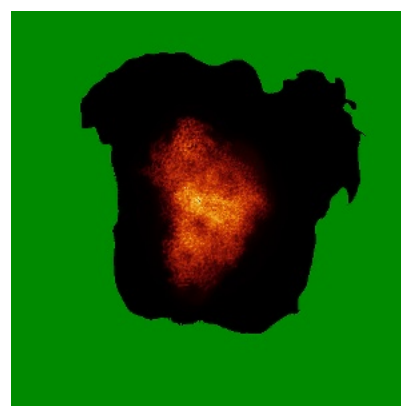
6.4.1 Primary map



X



Y

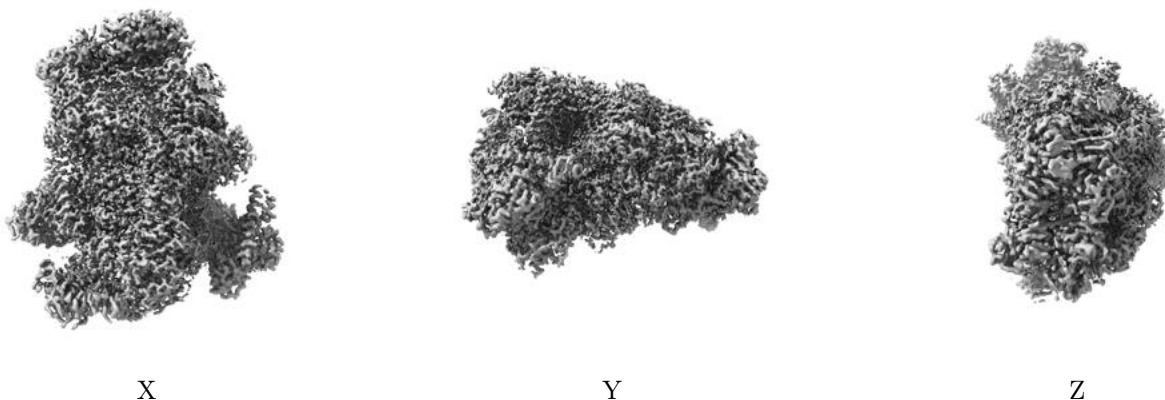


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 8.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

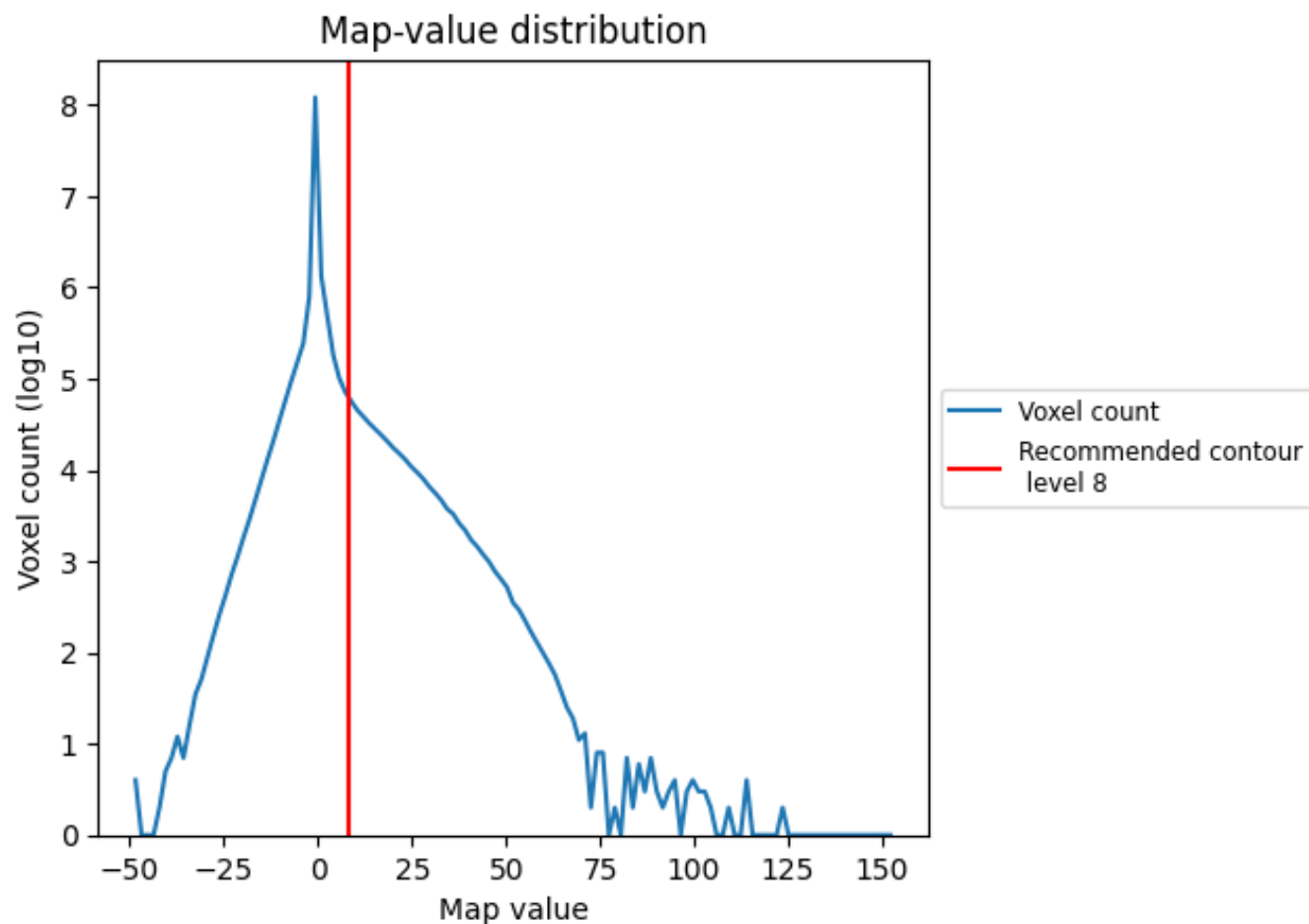
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

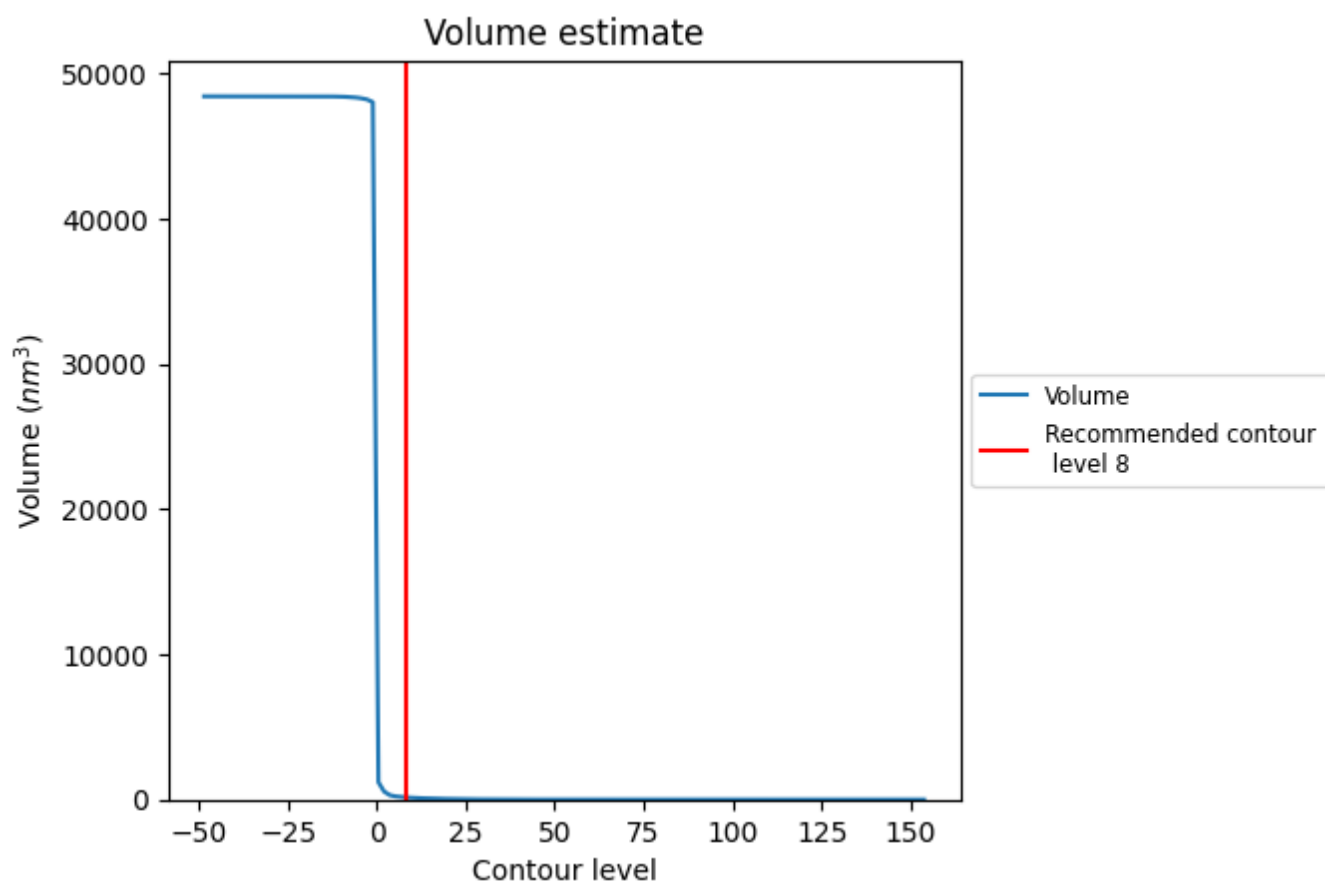
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

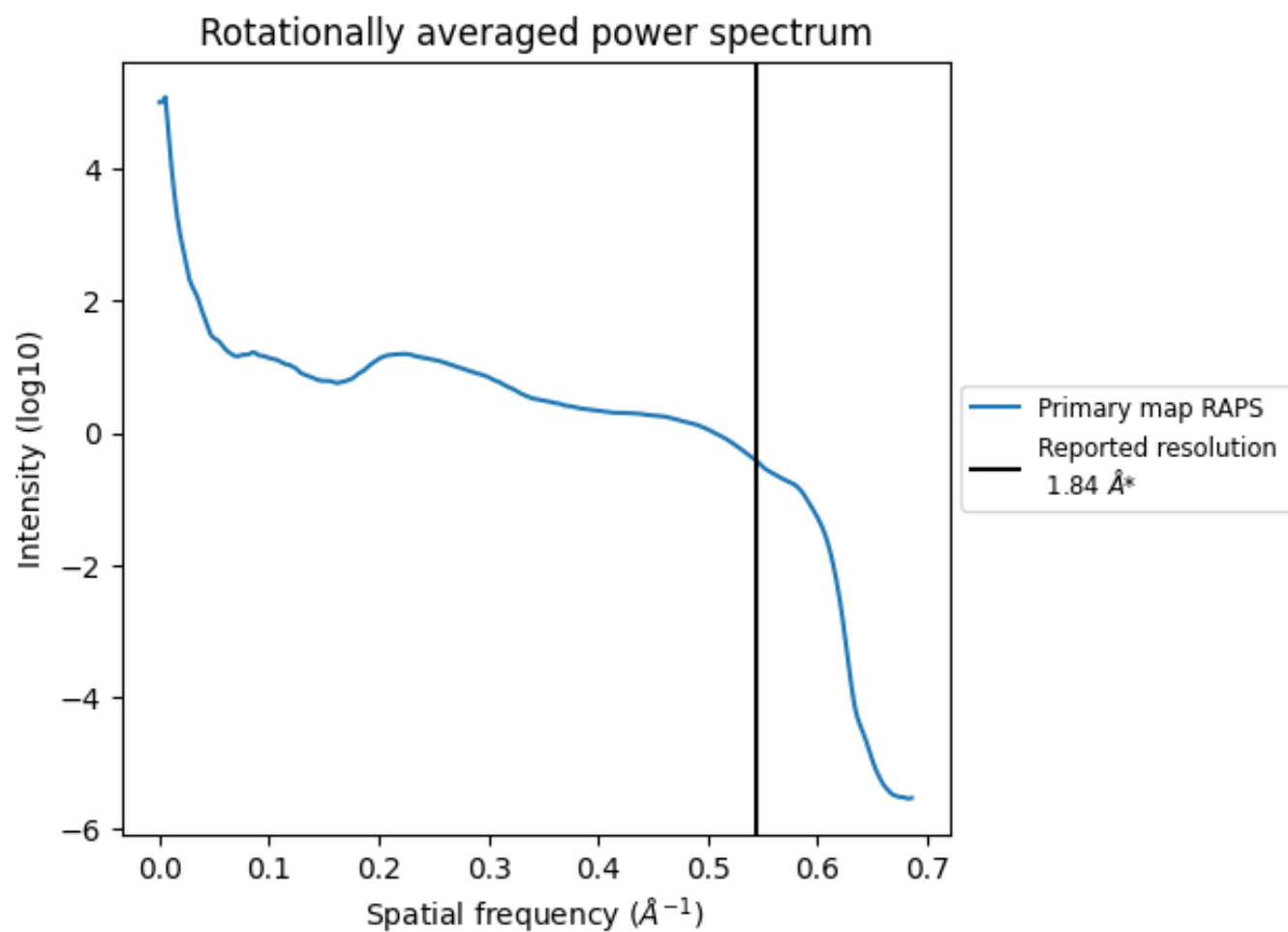
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 153 nm³; this corresponds to an approximate mass of 138 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

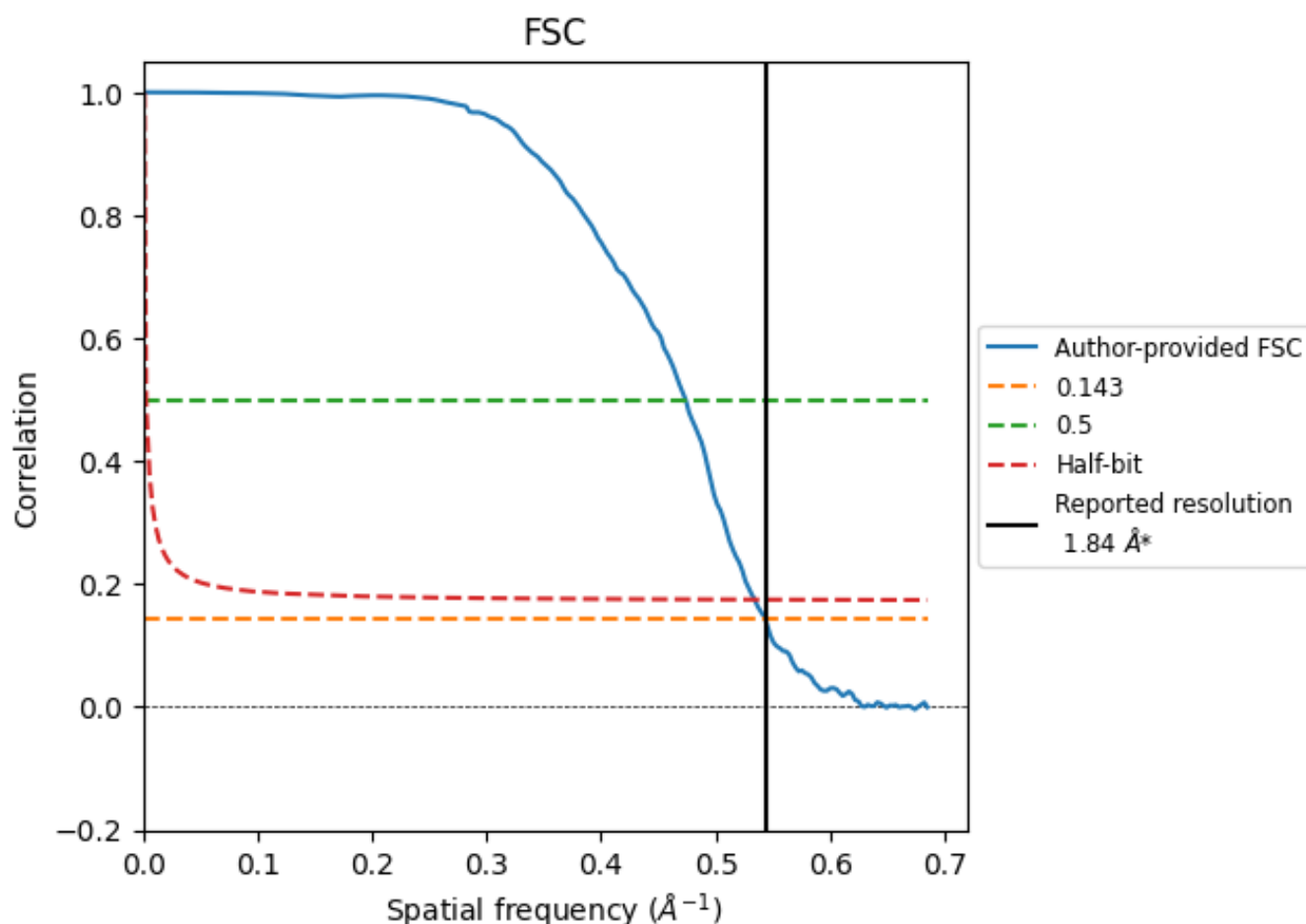


*Reported resolution corresponds to spatial frequency of 0.543 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.543 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

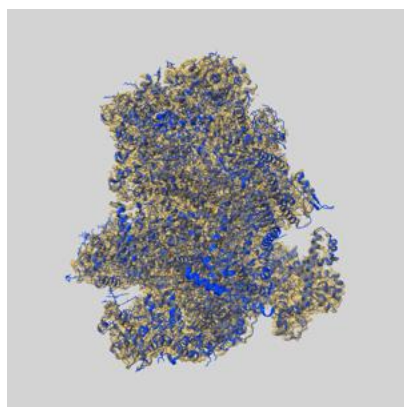
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.84	-	-
Author-provided FSC curve	1.84	2.11	1.87
Unmasked-calculated*	-	-	-

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

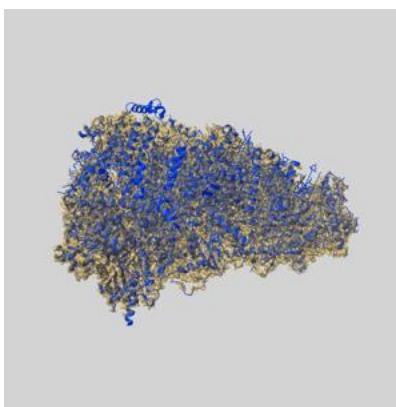
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52518 and PDB model 9HYU. Per-residue inclusion information can be found in [section 3](#) on [page 28](#).

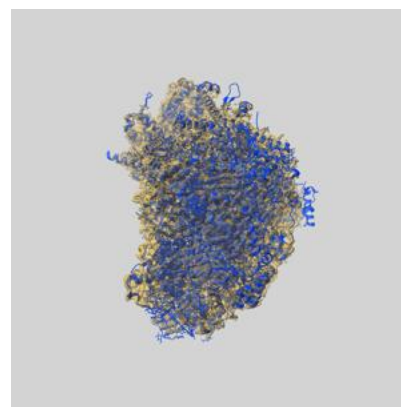
9.1 Map-model overlay [i](#)



X



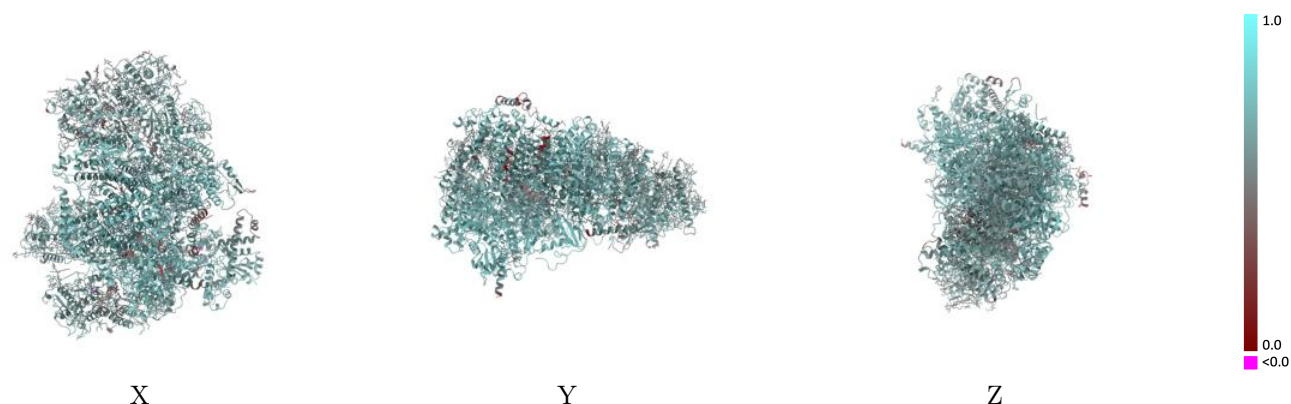
Y



Z

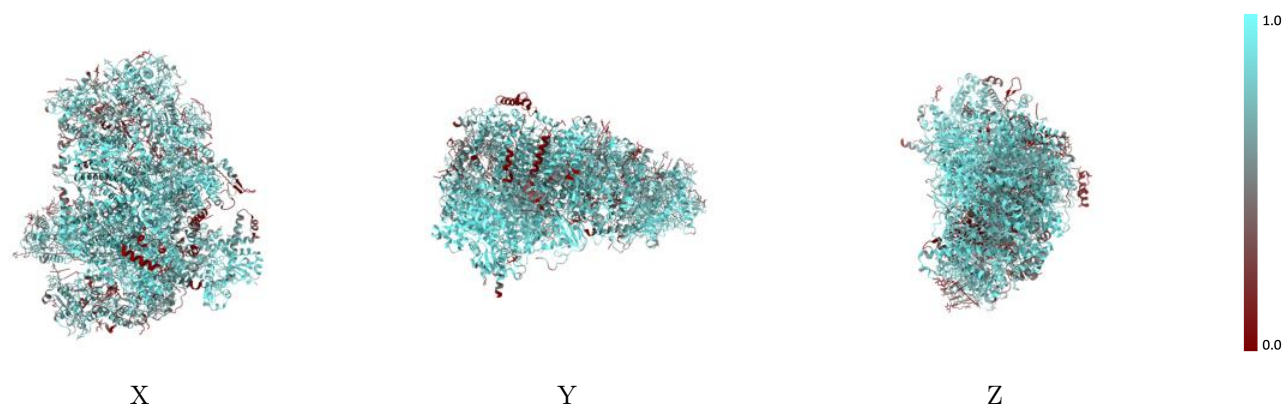
The images above show the 3D surface view of the map at the recommended contour level 8.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



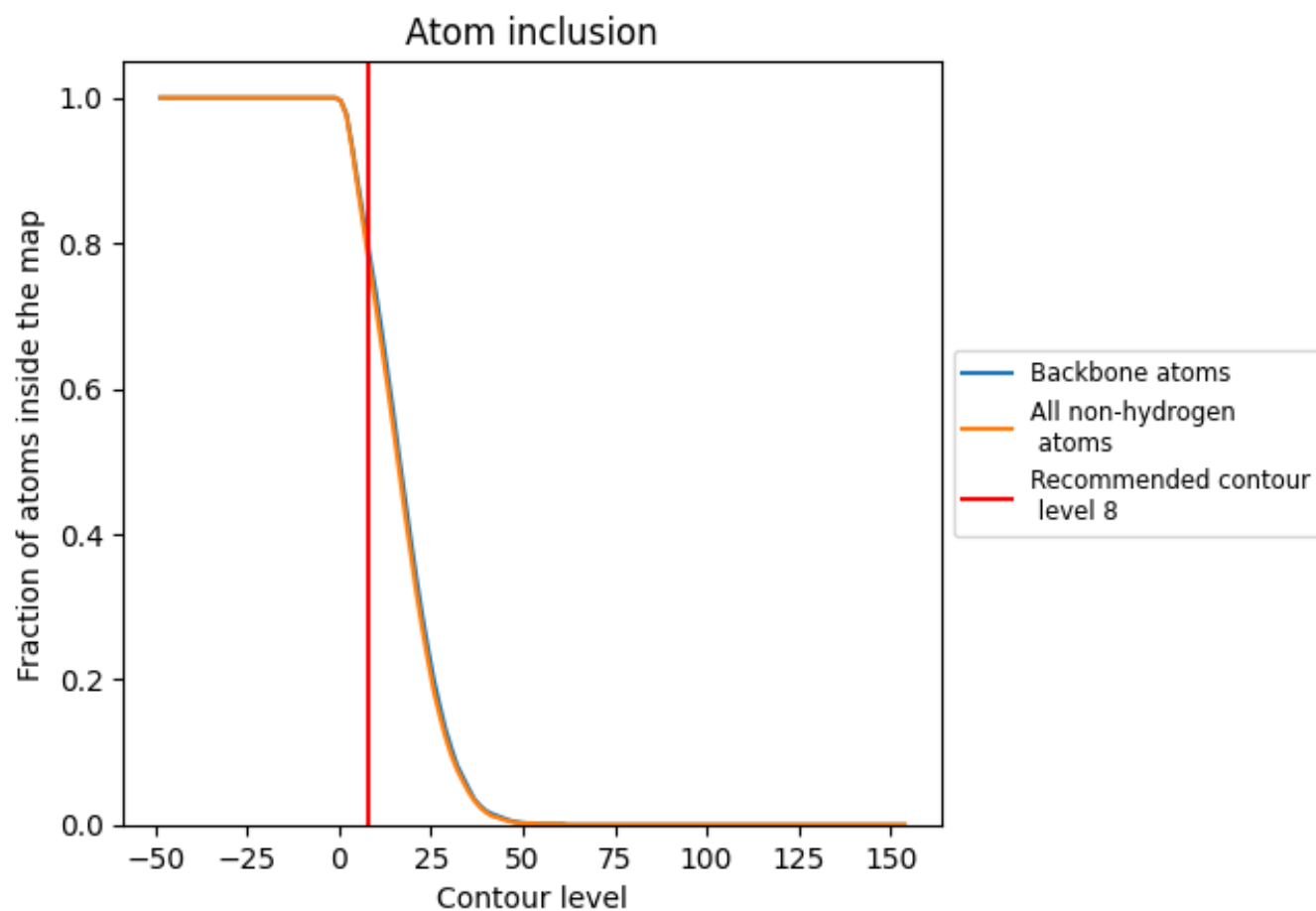
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 78% 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 (8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7790	 0.6660
1	 0.8250	 0.6980
2	 0.9220	 0.6840
A	 0.8870	 0.7260
B	 0.8250	 0.7110
C	 0.9530	 0.7620
D	 0.8920	 0.7310
E	 0.8410	 0.7250
F	 0.8070	 0.6990
G	 0.2050	 0.5160
H	 0.1070	 0.5640
I	 0.3790	 0.5480
L	 0.7430	 0.6740
M	 0.6460	 0.5660
R	 0.7390	 0.6450
a	 0.5940	 0.5960
b	 0.7250	 0.6560
c	 0.7460	 0.5820
d	 0.7380	 0.6400
e	 0.6870	 0.6180
f	 0.8030	 0.6010
u	 0.7240	 0.6410

