



wwPDB EM Validation Summary Report ⓘ

Nov 8, 2022 – 10:27 AM JST

PDB ID : 5ZJI
EMDB ID : EMD-6932
Title : Structure of photosystem I supercomplex with light-harvesting complexes I and II
Authors : Pan, X.W.; Ma, J.; Su, X.D.; Cao, P.; Liu, Z.F.; Zhang, X.Z.; Li, M.
Deposited on : 2018-03-20
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

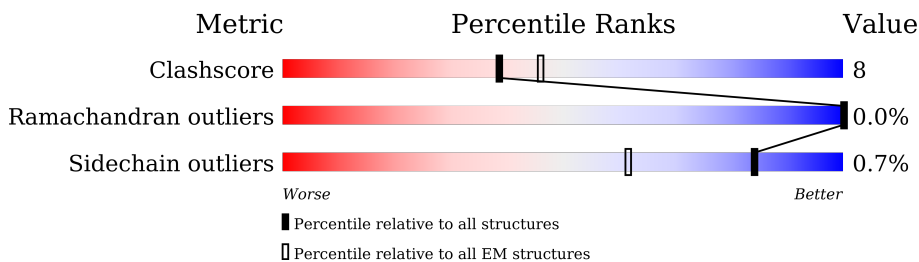
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	245	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">22%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 22%, orange 22%, yellow 22%, green 22%, grey 22%);"></div> <div style="text-align: center;">68%</div> <div style="text-align: center;">12%</div> <div style="text-align: center;">20%</div> </div>
2	2	270	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">11%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 11%, orange 11%, yellow 11%, green 11%, grey 11%);"></div> <div style="text-align: center;">66%</div> <div style="text-align: center;">10%</div> <div style="text-align: center;">23%</div> </div>
3	3	267	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">20%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 20%, orange 20%, yellow 20%, green 20%, grey 20%);"></div> <div style="text-align: center;">73%</div> <div style="text-align: center;">9%</div> <div style="text-align: center;">17%</div> </div>
4	4	252	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">13%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 13%, orange 13%, yellow 13%, green 13%, grey 13%);"></div> <div style="text-align: center;">69%</div> <div style="text-align: center;">10%</div> <div style="text-align: center;">21%</div> </div>
5	A	750	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">7%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 7%, orange 7%, yellow 7%, green 7%, grey 7%);"></div> <div style="text-align: center;">83%</div> <div style="text-align: center;">16%</div> <div style="text-align: center;">•</div> </div>
6	B	734	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">•</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 0%, orange 0%, yellow 0%, green 0%, grey 0%);"></div> <div style="text-align: center;">86%</div> <div style="text-align: center;">14%</div> <div style="text-align: center;">•</div> </div>
7	C	81	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">6%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 6%, orange 6%, yellow 6%, green 6%, grey 6%);"></div> <div style="text-align: center;">83%</div> <div style="text-align: center;">16%</div> <div style="text-align: center;">•</div> </div>
8	D	199	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">7%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 7%, orange 7%, yellow 7%, green 7%, grey 7%);"></div> <div style="text-align: center;">64%</div> <div style="text-align: center;">7%</div> <div style="text-align: center;">29%</div> <div style="text-align: center;">•</div> </div>

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Mol	Chain	Length	Quality of chain
9	E	136	
10	F	225	
11	G	145	
12	H	142	
13	I	36	
14	J	42	
15	K	134	
16	L	211	
17	O	127	
18	N	145	
19	X	232	
19	Z	232	
20	Y	228	

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
21	CHL	1	601	X	-	-	-
21	CHL	1	607	X	-	-	-
21	CHL	2	601	X	-	-	-
21	CHL	2	606	X	-	-	-
21	CHL	2	607	X	-	-	-
21	CHL	2	608	X	-	-	-
21	CHL	2	618	X	-	-	-
21	CHL	3	608	X	-	-	-
21	CHL	4	606	X	-	-	-
21	CHL	4	607	X	-	-	-
21	CHL	4	608	X	-	-	-
21	CHL	4	618	X	-	-	-
21	CHL	X	601	X	-	-	-
21	CHL	X	605	X	-	-	-
21	CHL	X	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CHL	X	607	X	-	-	-
21	CHL	X	608	X	-	-	-
21	CHL	X	609	X	-	-	-
21	CHL	Y	601	X	-	-	-
21	CHL	Y	605	X	-	-	-
21	CHL	Y	606	X	-	-	-
21	CHL	Y	607	X	-	-	-
21	CHL	Y	608	X	-	-	-
21	CHL	Y	609	X	-	-	-
21	CHL	Z	601	X	-	-	-
21	CHL	Z	605	X	-	-	-
21	CHL	Z	606	X	-	-	-
21	CHL	Z	607	X	-	-	-
21	CHL	Z	608	X	-	-	-
21	CHL	Z	609	X	-	-	-
22	CLA	1	602	X	-	-	-
22	CLA	1	603	X	-	-	-
22	CLA	1	604	X	-	-	-
22	CLA	1	606	X	-	-	-
22	CLA	1	608	X	-	-	-
22	CLA	1	609	X	-	-	-
22	CLA	1	610	X	-	-	-
22	CLA	1	611	X	-	-	-
22	CLA	1	612	X	-	-	-
22	CLA	1	613	X	-	-	-
22	CLA	1	614	X	-	-	-
22	CLA	2	602	X	-	-	-
22	CLA	2	603	X	-	-	-
22	CLA	2	604	X	-	-	-
22	CLA	2	609	X	-	-	-
22	CLA	2	610	X	-	-	-
22	CLA	2	611	X	-	-	-
22	CLA	2	612	X	-	-	-
22	CLA	2	613	X	-	-	-
22	CLA	2	614	X	-	-	-
22	CLA	3	602	X	-	-	-
22	CLA	3	603	X	-	-	-
22	CLA	3	604	X	-	-	-
22	CLA	3	606	X	-	-	-
22	CLA	3	607	X	-	-	-
22	CLA	3	609	X	-	-	-
22	CLA	3	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	3	613	X	-	-	-
22	CLA	3	614	X	-	-	-
22	CLA	3	615	X	-	-	-
22	CLA	3	617	X	-	-	-
22	CLA	4	601	X	-	-	-
22	CLA	4	602	X	-	-	-
22	CLA	4	603	X	-	-	-
22	CLA	4	604	X	-	-	-
22	CLA	4	609	X	-	-	-
22	CLA	4	610	X	-	-	-
22	CLA	4	611	X	-	-	-
22	CLA	4	612	X	-	-	-
22	CLA	4	613	X	-	-	-
22	CLA	4	614	X	-	-	-
22	CLA	4	617	X	-	-	-
22	CLA	A	802	X	-	-	-
22	CLA	A	803	X	-	-	-
22	CLA	A	804	X	-	-	-
22	CLA	A	805	X	-	-	-
22	CLA	A	806	X	-	-	-
22	CLA	A	807	X	-	-	-
22	CLA	A	808	X	-	-	-
22	CLA	A	809	X	-	-	-
22	CLA	A	810	X	-	-	-
22	CLA	A	811	X	-	-	-
22	CLA	A	812	X	-	-	-
22	CLA	A	813	X	-	-	-
22	CLA	A	814	X	-	-	-
22	CLA	A	815	X	-	-	-
22	CLA	A	816	X	-	-	-
22	CLA	A	817	X	-	-	-
22	CLA	A	818	X	-	-	-
22	CLA	A	819	X	-	-	-
22	CLA	A	820	X	-	-	-
22	CLA	A	821	X	-	-	-
22	CLA	A	822	X	-	-	-
22	CLA	A	823	X	-	-	-
22	CLA	A	824	X	-	-	-
22	CLA	A	825	X	-	-	-
22	CLA	A	826	X	-	-	-
22	CLA	A	827	X	-	-	-
22	CLA	A	828	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	829	X	-	-	-
22	CLA	A	830	X	-	-	-
22	CLA	A	831	X	-	-	-
22	CLA	A	832	X	-	-	-
22	CLA	A	833	X	-	-	-
22	CLA	A	834	X	-	-	-
22	CLA	A	835	X	-	-	-
22	CLA	A	836	X	-	-	-
22	CLA	A	837	X	-	-	-
22	CLA	A	838	X	-	-	-
22	CLA	A	839	X	-	-	-
22	CLA	A	840	X	-	-	-
22	CLA	A	841	X	-	-	-
22	CLA	A	842	X	-	-	-
22	CLA	A	843	X	-	-	-
22	CLA	A	845	X	-	-	-
22	CLA	A	854	X	-	-	-
22	CLA	B	802	X	-	-	-
22	CLA	B	803	X	-	-	-
22	CLA	B	804	X	-	-	-
22	CLA	B	805	X	-	-	-
22	CLA	B	806	X	-	-	-
22	CLA	B	808	X	-	-	-
22	CLA	B	809	X	-	-	-
22	CLA	B	810	X	-	-	-
22	CLA	B	811	X	-	-	-
22	CLA	B	812	X	-	-	-
22	CLA	B	813	X	-	-	-
22	CLA	B	814	X	-	-	-
22	CLA	B	815	X	-	-	-
22	CLA	B	816	X	-	-	-
22	CLA	B	817	X	-	-	-
22	CLA	B	818	X	-	-	-
22	CLA	B	819	X	-	-	-
22	CLA	B	820	X	-	-	-
22	CLA	B	821	X	-	-	-
22	CLA	B	822	X	-	-	-
22	CLA	B	823	X	-	-	-
22	CLA	B	824	X	-	-	-
22	CLA	B	825	X	-	-	-
22	CLA	B	826	X	-	-	-
22	CLA	B	827	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	828	X	-	-	-
22	CLA	B	829	X	-	-	-
22	CLA	B	830	X	-	-	-
22	CLA	B	831	X	-	-	-
22	CLA	B	832	X	-	-	-
22	CLA	B	833	X	-	-	-
22	CLA	B	834	X	-	-	-
22	CLA	B	835	X	-	-	-
22	CLA	B	836	X	-	-	-
22	CLA	B	837	X	-	-	-
22	CLA	B	838	X	-	-	-
22	CLA	B	839	X	-	-	-
22	CLA	B	840	X	-	-	-
22	CLA	B	841	X	-	-	-
22	CLA	F	301	X	-	-	-
22	CLA	F	303	X	-	-	-
22	CLA	F	304	X	-	-	-
22	CLA	G	201	X	-	-	-
22	CLA	G	203	X	-	-	-
22	CLA	G	204	X	-	-	-
22	CLA	H	201	X	-	-	-
22	CLA	J	101	X	-	-	-
22	CLA	K	201	X	-	-	-
22	CLA	K	203	X	-	-	-
22	CLA	K	204	X	-	-	-
22	CLA	K	206	X	-	-	-
22	CLA	L	302	X	-	-	-
22	CLA	L	303	X	-	-	-
22	CLA	L	304	X	-	-	-
22	CLA	N	1002	X	-	-	-
22	CLA	O	2001	X	-	-	-
22	CLA	O	2002	X	-	-	-
22	CLA	X	602	X	-	-	-
22	CLA	X	603	X	-	-	-
22	CLA	X	604	X	-	-	-
22	CLA	X	610	X	-	-	-
22	CLA	X	611	X	-	-	-
22	CLA	X	612	X	-	-	-
22	CLA	X	613	X	-	-	-
22	CLA	X	614	X	-	-	-
22	CLA	Y	602	X	-	-	-
22	CLA	Y	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	Y	604	X	-	-	-
22	CLA	Y	610	X	-	-	-
22	CLA	Y	611	X	-	-	-
22	CLA	Y	612	X	-	-	-
22	CLA	Y	613	X	-	-	-
22	CLA	Y	614	X	-	-	-
22	CLA	Z	602	X	-	-	-
22	CLA	Z	603	X	-	-	-
22	CLA	Z	604	X	-	-	-
22	CLA	Z	610	X	-	-	-
22	CLA	Z	611	X	-	-	-
22	CLA	Z	612	X	-	-	-
22	CLA	Z	613	X	-	-	-
22	CLA	Z	614	X	-	-	-
28	CL0	A	801	X	-	X	-

2 Entry composition [i](#)

There are 33 unique types of molecules in this entry. The entry contains 44708 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	196	1522	991	253	272	6	0	0

- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	207	1624	1064	263	293	4	0	0

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	221	1720	1130	276	307	7	0	0

- Molecule 4 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	199	1566	1020	257	285	4	0	0

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	A	742	5836	3824	992	1002	18	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASN	deletion	UNP P04966

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	B	733	5866	3849	997	1007	13	0	0

- Molecule 7 is a protein called photosystem I subunit VII.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	C	81	612	377	105	118	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	D	142	1115	717	193	202	3	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	E	68	540	344	97	99	0	0

- Molecule 10 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	F	158	1238	805	212	218	3	0	0

- Molecule 11 is a protein called Photosystem I reaction center subunit V.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	G	97	752	489	125	138	0	0

- Molecule 12 is a protein called Photosystem I reaction center subunit VI, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	H	95	729	477	116	136	0	0

- Molecule 13 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	33	Total	C	N	O	S	0	0
			260	178	38	43	1		

- Molecule 14 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	41	Total	C	N	O	S	0	0
			325	220	50	54	1		

- Molecule 15 is a protein called Photosystem I reaction center subunit psaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	84	Total	C	N	O	S	0	0
			589	372	102	112	3		

- Molecule 16 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	166	Total	C	N	O	S	0	0
			1246	820	198	226	2		

- Molecule 17 is a protein called 16kDa membrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	76	Total	C	N	O	S	0	0
			621	418	101	101	1		

- Molecule 18 is a protein called Photosystem I reaction center subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	84	Total	C	N	O	S	0	0
			685	439	112	129	5		

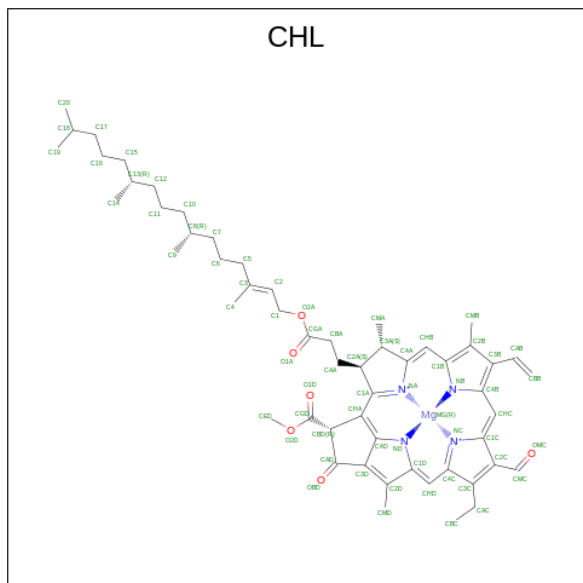
- Molecule 19 is a protein called Chlorophyll a-b binding protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	218	Total	C	N	O	S	0	0
			1661	1080	269	306	6		
19	Z	218	Total	C	N	O	S	0	0
			1661	1080	269	306	6		

- Molecule 20 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	P			S
20	Y	228	1751	1132	290	322	1	6	0	0

- Molecule 21 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	1	1	Total	C	Mg	N	O	0
			96	76	2	8	10	
21	1	1	Total	C	Mg	N	O	0
			96	76	2	8	10	
21	2	1	Total	C	Mg	N	O	0
			240	191	5	20	24	
21	2	1	Total	C	Mg	N	O	0
			240	191	5	20	24	
21	2	1	Total	C	Mg	N	O	0
			240	191	5	20	24	
21	2	1	Total	C	Mg	N	O	0
			240	191	5	20	24	
21	2	1	Total	C	Mg	N	O	0
			240	191	5	20	24	
21	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			169	132	4	16	17	
21	4	1	Total	C	Mg	N	O	0
			169	132	4	16	17	
21	4	1	Total	C	Mg	N	O	0
			169	132	4	16	17	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	4	1	Total 169	C 132	Mg 4	N 16	O 17	0
21	X	1	Total 235	C 189	Mg 6	N 24	O 16	0
21	X	1	Total 235	C 189	Mg 6	N 24	O 16	0
21	X	1	Total 235	C 189	Mg 6	N 24	O 16	0
21	X	1	Total 235	C 189	Mg 6	N 24	O 16	0
21	X	1	Total 235	C 189	Mg 6	N 24	O 16	0
21	X	1	Total 235	C 189	Mg 6	N 24	O 16	0
21	Y	1	Total 259	C 208	Mg 6	N 24	O 21	0
21	Y	1	Total 259	C 208	Mg 6	N 24	O 21	0
21	Y	1	Total 259	C 208	Mg 6	N 24	O 21	0
21	Y	1	Total 259	C 208	Mg 6	N 24	O 21	0
21	Y	1	Total 259	C 208	Mg 6	N 24	O 21	0
21	Y	1	Total 259	C 208	Mg 6	N 24	O 21	0
21	Y	1	Total 259	C 208	Mg 6	N 24	O 21	0
21	Z	1	Total 250	C 195	Mg 6	N 24	O 25	0
21	Z	1	Total 250	C 195	Mg 6	N 24	O 25	0
21	Z	1	Total 250	C 195	Mg 6	N 24	O 25	0
21	Z	1	Total 250	C 195	Mg 6	N 24	O 25	0
21	Z	1	Total 250	C 195	Mg 6	N 24	O 25	0
21	Z	1	Total 250	C 195	Mg 6	N 24	O 25	0

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	1	1	Total	C	Mg	N	O	0
			577	465	12	48	52	
22	1	1	Total	C	Mg	N	O	0
			577	465	12	48	52	
22	1	1	Total	C	Mg	N	O	0
			577	465	12	48	52	
22	1	1	Total	C	Mg	N	O	0
			577	465	12	48	52	
22	1	1	Total	C	Mg	N	O	0
			577	465	12	48	52	
22	1	1	Total	C	Mg	N	O	0
			577	465	12	48	52	
22	1	1	Total	C	Mg	N	O	0
			577	465	12	48	52	
22	1	1	Total	C	Mg	N	O	0
			577	465	12	48	52	
22	1	1	Total	C	Mg	N	O	0
			577	465	12	48	52	
22	1	1	Total	C	Mg	N	O	0
			577	465	12	48	52	
22	2	1	Total	C	Mg	N	O	0
			442	357	9	36	40	
22	2	1	Total	C	Mg	N	O	0
			442	357	9	36	40	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	2	1	442	357	9	36	40	0
22	2	1	442	357	9	36	40	0
22	2	1	442	357	9	36	40	0
22	2	1	442	357	9	36	40	0
22	2	1	442	357	9	36	40	0
22	2	1	442	357	9	36	40	0
22	2	1	442	357	9	36	40	0
22	2	1	442	357	9	36	40	0
22	3	1	538	434	12	48	44	0
22	3	1	538	434	12	48	44	0
22	3	1	538	434	12	48	44	0
22	3	1	538	434	12	48	44	0
22	3	1	538	434	12	48	44	0
22	3	1	538	434	12	48	44	0
22	3	1	538	434	12	48	44	0
22	3	1	538	434	12	48	44	0
22	3	1	538	434	12	48	44	0
22	3	1	538	434	12	48	44	0
22	3	1	538	434	12	48	44	0
22	3	1	538	434	12	48	44	0
22	3	1	538	434	12	48	44	0
22	4	1	527	421	11	44	51	0
22	4	1	527	421	11	44	51	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	4	1	527	421	11	44	51	0
22	4	1	527	421	11	44	51	0
22	4	1	527	421	11	44	51	0
22	4	1	527	421	11	44	51	0
22	4	1	527	421	11	44	51	0
22	4	1	527	421	11	44	51	0
22	4	1	527	421	11	44	51	0
22	4	1	527	421	11	44	51	0
22	4	1	527	421	11	44	51	0
22	A	1	2533	2099	44	176	214	0
22	A	1	2533	2099	44	176	214	0
22	A	1	2533	2099	44	176	214	0
22	A	1	2533	2099	44	176	214	0
22	A	1	2533	2099	44	176	214	0
22	A	1	2533	2099	44	176	214	0
22	A	1	2533	2099	44	176	214	0
22	A	1	2533	2099	44	176	214	0
22	A	1	2533	2099	44	176	214	0
22	A	1	2533	2099	44	176	214	0
22	A	1	2533	2099	44	176	214	0
22	A	1	2533	2099	44	176	214	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0
22	A	1	Total 2533	C 2099	Mg 44	N 176	O 214	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	A	1	2533	2099	44	176	214	0
22	A	1	2533	2099	44	176	214	0
22	A	1	2533	2099	44	176	214	0
22	A	1	2533	2099	44	176	214	0
22	A	1	2533	2099	44	176	214	0
22	A	1	2533	2099	44	176	214	0
22	A	1	2533	2099	44	176	214	0
22	A	1	2533	2099	44	176	214	0
22	A	1	2533	2099	44	176	214	0
22	A	1	2533	2099	44	176	214	0
22	A	1	2533	2099	44	176	214	0
22	A	1	2533	2099	44	176	214	0
22	B	1	2261	1875	40	160	186	0
22	B	1	2261	1875	40	160	186	0
22	B	1	2261	1875	40	160	186	0
22	B	1	2261	1875	40	160	186	0
22	B	1	2261	1875	40	160	186	0
22	B	1	2261	1875	40	160	186	0
22	B	1	2261	1875	40	160	186	0
22	B	1	2261	1875	40	160	186	0
22	B	1	2261	1875	40	160	186	0
22	B	1	2261	1875	40	160	186	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	B	1	Total 2261	C 1875	Mg 40	N 160	O 186	0
22	F	1	Total 140	C 114	Mg 3	N 12	O 11	0
22	F	1	Total 140	C 114	Mg 3	N 12	O 11	0
22	F	1	Total 140	C 114	Mg 3	N 12	O 11	0
22	G	1	Total 132	C 104	Mg 3	N 12	O 13	0
22	G	1	Total 132	C 104	Mg 3	N 12	O 13	0
22	G	1	Total 132	C 104	Mg 3	N 12	O 13	0
22	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	K	1	Total 167	C 133	Mg 4	N 16	O 14	0
22	K	1	Total 167	C 133	Mg 4	N 16	O 14	0
22	K	1	Total 167	C 133	Mg 4	N 16	O 14	0
22	K	1	Total 167	C 133	Mg 4	N 16	O 14	0

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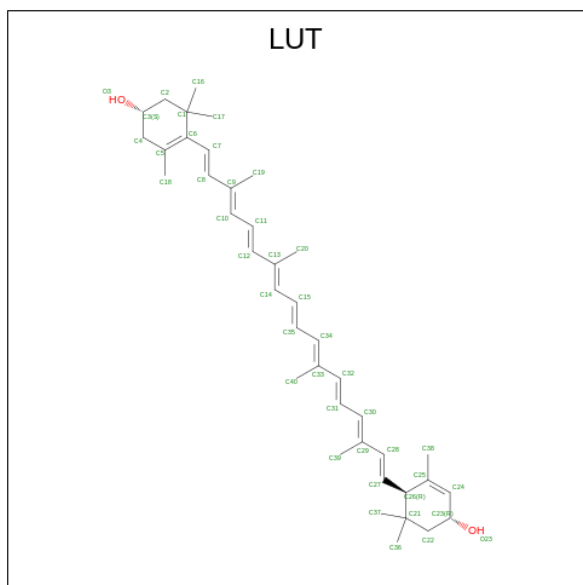
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	L	1	150	120	3	12	15	0
22	L	1	150	120	3	12	15	0
22	L	1	150	120	3	12	15	0
22	O	1	76	60	2	8	6	0
22	O	1	76	60	2	8	6	0
22	N	1	95	75	2	8	10	0
22	N	1	95	75	2	8	10	0
22	X	1	305	248	8	32	17	0
22	X	1	305	248	8	32	17	0
22	X	1	305	248	8	32	17	0
22	X	1	305	248	8	32	17	0
22	X	1	305	248	8	32	17	0
22	X	1	305	248	8	32	17	0
22	X	1	305	248	8	32	17	0
22	X	1	305	248	8	32	17	0
22	X	1	305	248	8	32	17	0
22	Y	1	325	257	8	32	28	0
22	Y	1	325	257	8	32	28	0
22	Y	1	325	257	8	32	28	0
22	Y	1	325	257	8	32	28	0
22	Y	1	325	257	8	32	28	0
22	Y	1	325	257	8	32	28	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	Y	1	Total 325	C 257	Mg 8	N 32	O 28	0
22	Y	1	Total 325	C 257	Mg 8	N 32	O 28	0
22	Z	1	Total 339	C 274	Mg 8	N 32	O 25	0
22	Z	1	Total 339	C 274	Mg 8	N 32	O 25	0
22	Z	1	Total 339	C 274	Mg 8	N 32	O 25	0
22	Z	1	Total 339	C 274	Mg 8	N 32	O 25	0
22	Z	1	Total 339	C 274	Mg 8	N 32	O 25	0
22	Z	1	Total 339	C 274	Mg 8	N 32	O 25	0
22	Z	1	Total 339	C 274	Mg 8	N 32	O 25	0
22	Z	1	Total 339	C 274	Mg 8	N 32	O 25	0
22	Z	1	Total 339	C 274	Mg 8	N 32	O 25	0

- Molecule 23 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



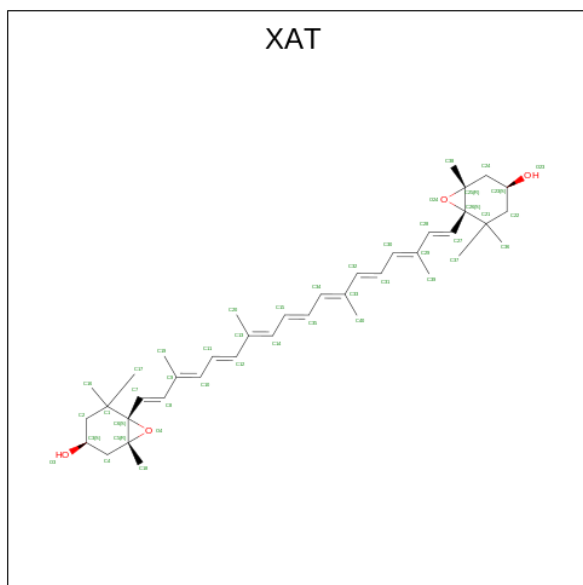
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
23	1	1	Total 84	C 80	O 4	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
23	1	1	84	80	4	0
23	2	1	42	40	2	0
23	3	1	42	40	2	0
23	4	1	42	40	2	0
23	X	1	84	80	4	0
23	X	1	84	80	4	0
23	Y	1	84	80	4	0
23	Y	1	84	80	4	0
23	Z	1	84	80	4	0
23	Z	1	84	80	4	0

- Molecule 24 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 (three-letter code: XAT) (formula: C₄₀H₅₆O₄).



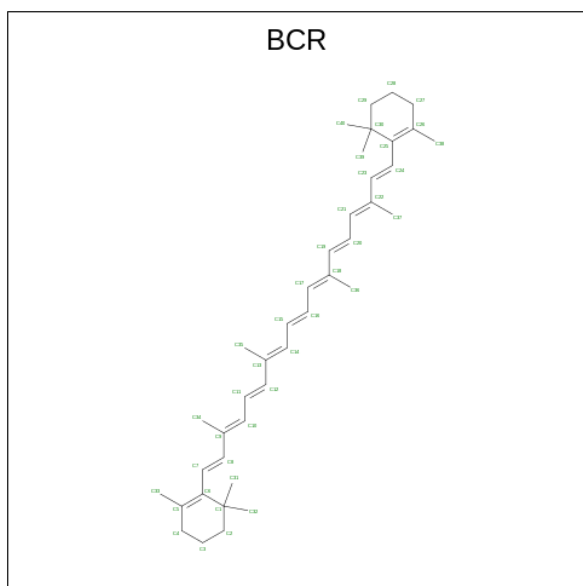
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
24	1	1	44	40	4	0

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Mol	Chain	Residues	Atoms			AltConf
24	2	1	Total	C	O	0
			44	40	4	
24	3	1	Total	C	O	0
			44	40	4	
24	4	1	Total	C	O	0
			44	40	4	
24	X	1	Total	C	O	0
			44	40	4	
24	Y	1	Total	C	O	0
			44	40	4	
24	Z	1	Total	C	O	0
			44	40	4	

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



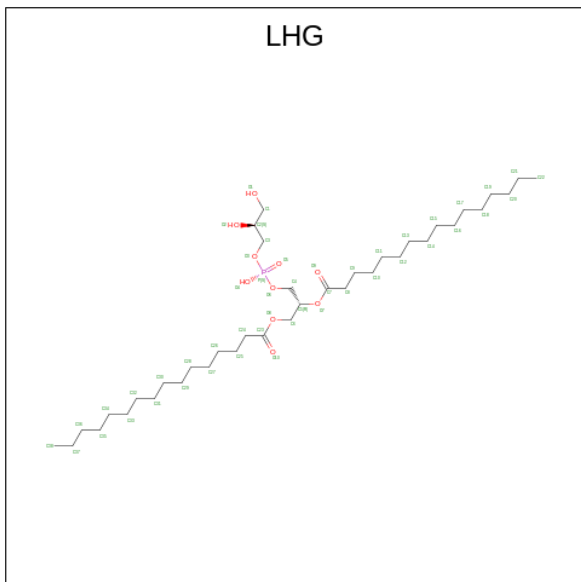
Mol	Chain	Residues	Atoms		AltConf
25	1	1	Total	C	0
			40	40	
25	2	1	Total	C	0
			40	40	
25	3	1	Total	C	0
			40	40	
25	4	1	Total	C	0
			40	40	
25	A	1	Total	C	0
			240	240	

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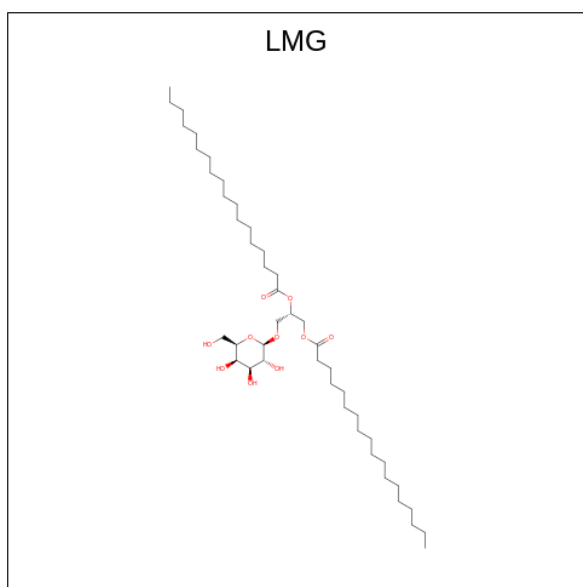
Mol	Chain	Residues	Atoms		AltConf
25	A	1	Total 240	C 240	0
25	A	1	Total 240	C 240	0
25	A	1	Total 240	C 240	0
25	A	1	Total 240	C 240	0
25	A	1	Total 240	C 240	0
25	B	1	Total 280	C 280	0
25	B	1	Total 280	C 280	0
25	B	1	Total 280	C 280	0
25	B	1	Total 280	C 280	0
25	B	1	Total 280	C 280	0
25	B	1	Total 280	C 280	0
25	B	1	Total 280	C 280	0
25	B	1	Total 280	C 280	0
25	F	1	Total 40	C 40	0
25	G	1	Total 40	C 40	0
25	I	1	Total 40	C 40	0
25	J	1	Total 40	C 40	0
25	K	1	Total 80	C 80	0
25	K	1	Total 80	C 80	0
25	L	1	Total 120	C 120	0
25	L	1	Total 120	C 120	0
25	L	1	Total 120	C 120	0

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



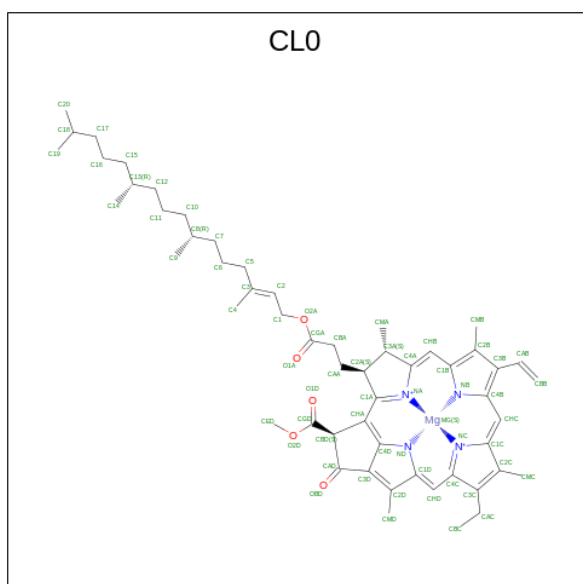
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
26	1	1	49	38	10	1	0
26	2	1	37	26	10	1	0
26	A	1	79	57	20	2	0
26	A	1	79	57	20	2	0
26	B	1	38	27	10	1	0
26	X	1	22	11	10	1	0
26	Y	1	45	34	10	1	0
26	Z	1	23	12	10	1	0

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



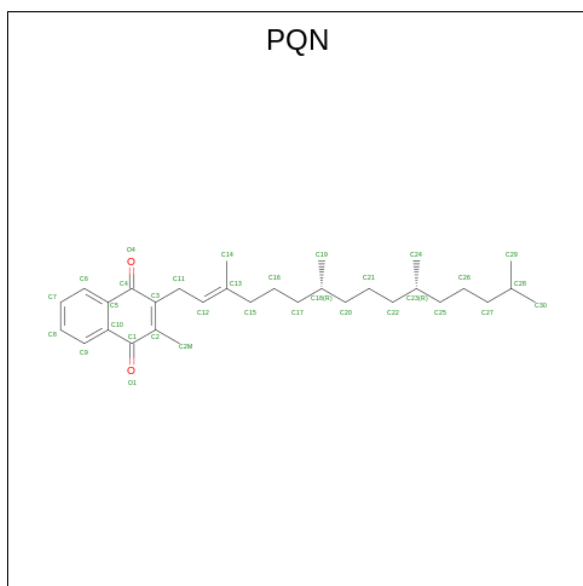
Mol	Chain	Residues	Atoms			AltConf
27	1	1	Total	C	O	0
			53	43	10	
27	2	1	Total	C	O	0
			36	26	10	
27	4	1	Total	C	O	0
			72	52	20	
27	4	1	Total	C	O	0
			72	52	20	
27	G	1	Total	C	O	0
			38	28	10	

- Molecule 28 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



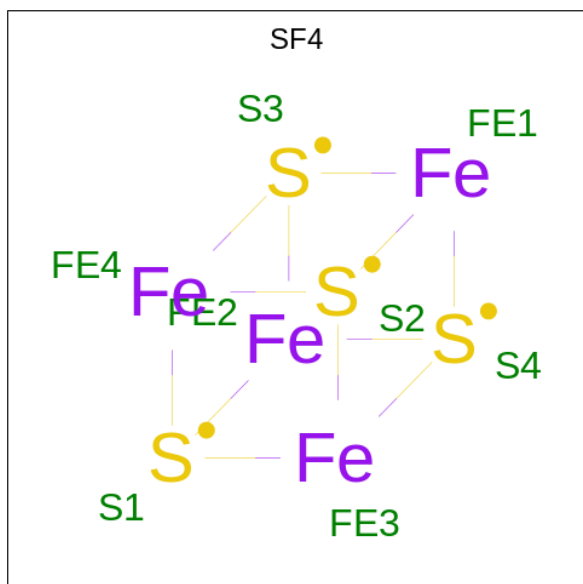
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Mg	N		O
28	A	1	65	55	1	4	5	0

- Molecule 29 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



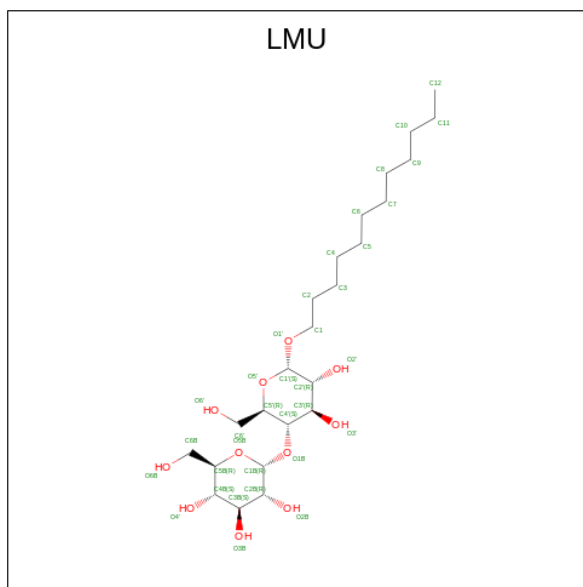
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
29	A	1	33	31	2	0
29	B	1	33	31	2	0

- Molecule 30 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



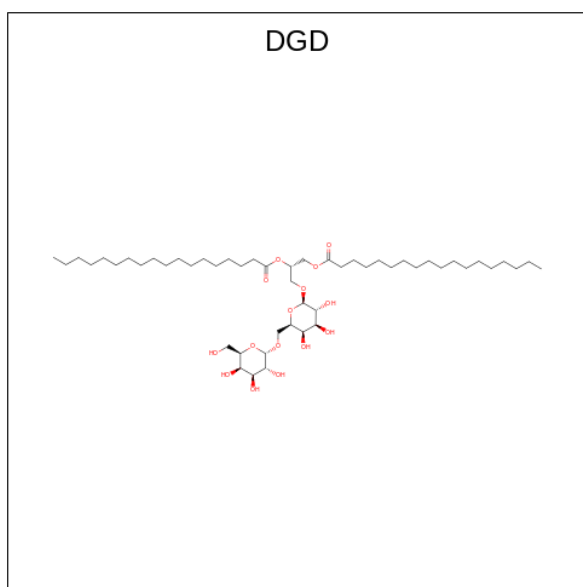
Mol	Chain	Residues	Atoms			AltConf
30	A	1	Total	Fe	S	0
			8	4	4	
30	C	1	Total	Fe	S	0
			16	8	8	
30	C	1	Total	Fe	S	0
			16	8	8	

- Molecule 31 is DODECYL-ALPHA-D-MALTOSE (three-letter code: LMU) (formula: $C_{24}H_{46}O_{11}$).



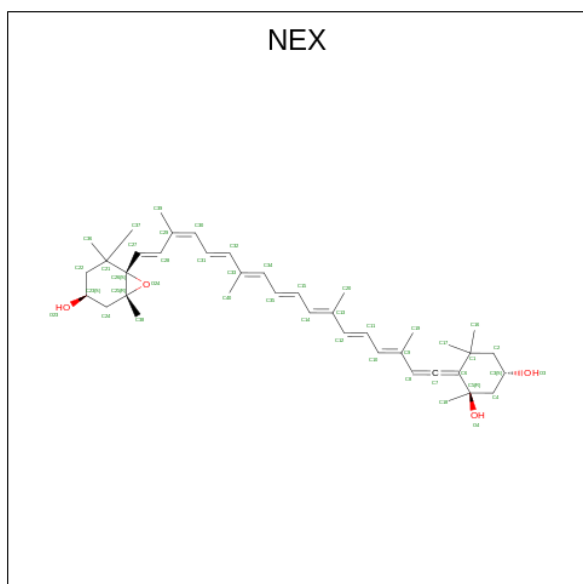
Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			30	19	11	
31	B	1	Total	C	O	0
			35	24	11	

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
32	B	1	Total	C	O	0
			66	51	15	
32	J	1	Total	C	O	0
			66	51	15	

- Molecule 33 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADEC-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C₄₀H₅₆O₄).

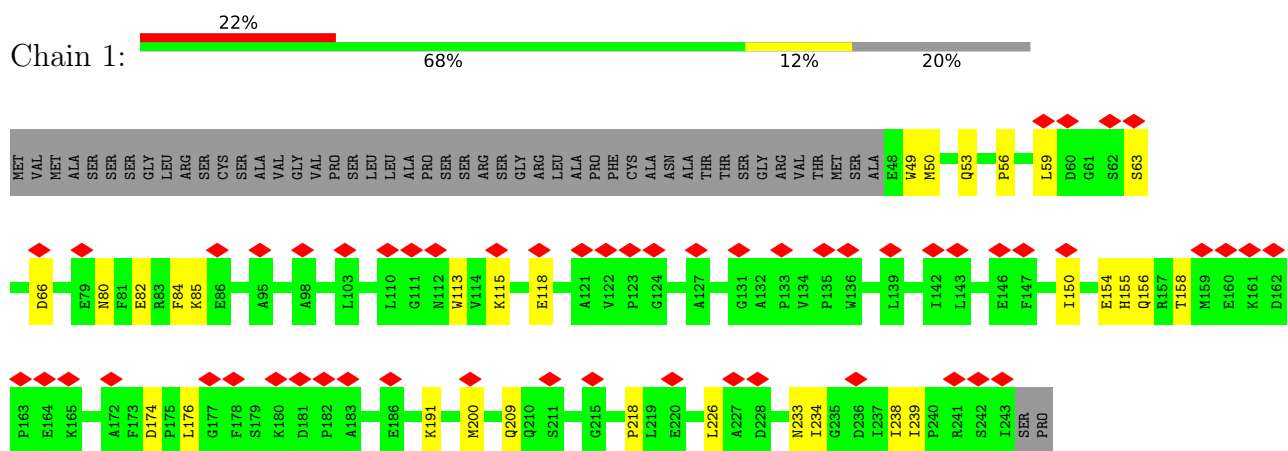


Mol	Chain	Residues	Atoms			AltConf
33	X	1	Total 44	C 40	O 4	0
33	Y	1	Total 44	C 40	O 4	0
33	Z	1	Total 44	C 40	O 4	0

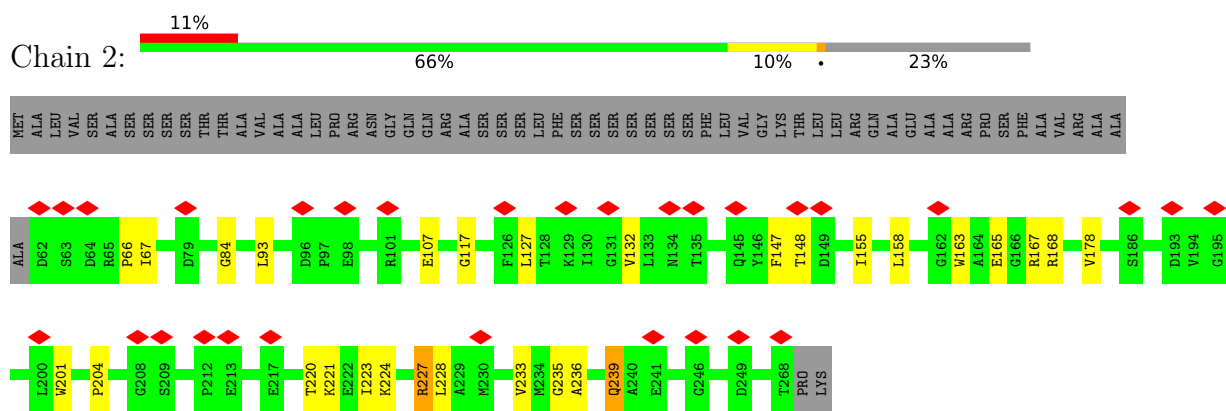
3 Residue-property plots (i)

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.

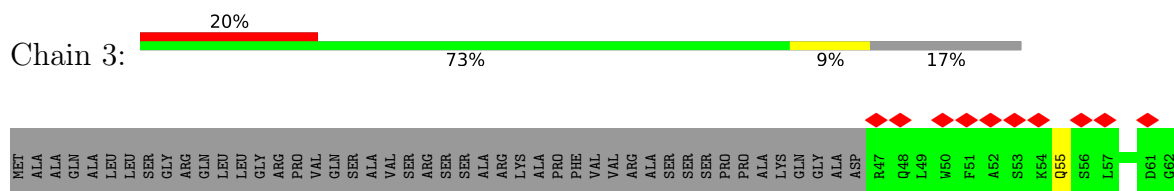
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

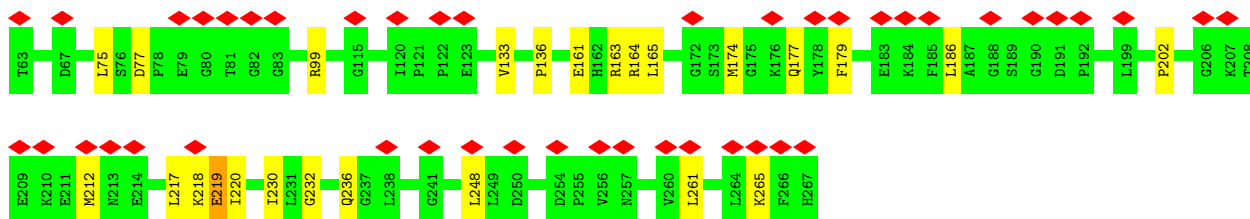


- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

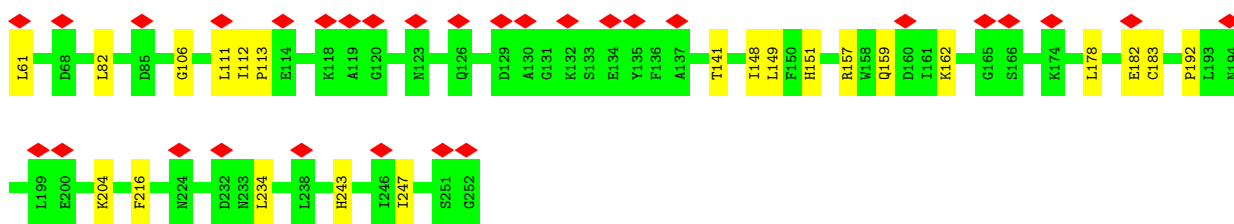
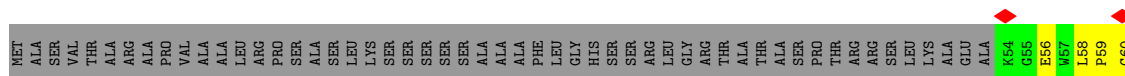


- Molecule 3: Chlorophyll a-b binding protein, chloroplastic

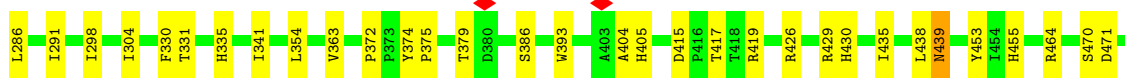
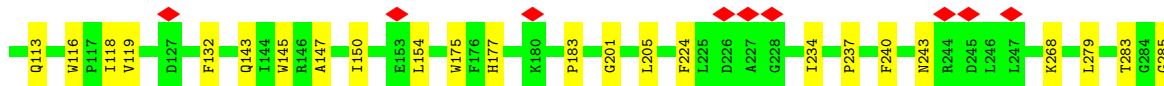
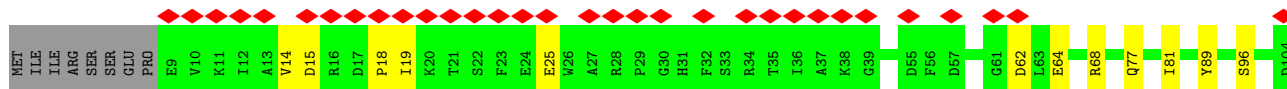
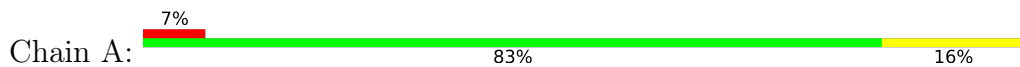




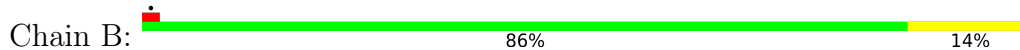
• Molecule 4: Chlorophyll a-b binding protein, chloroplastic

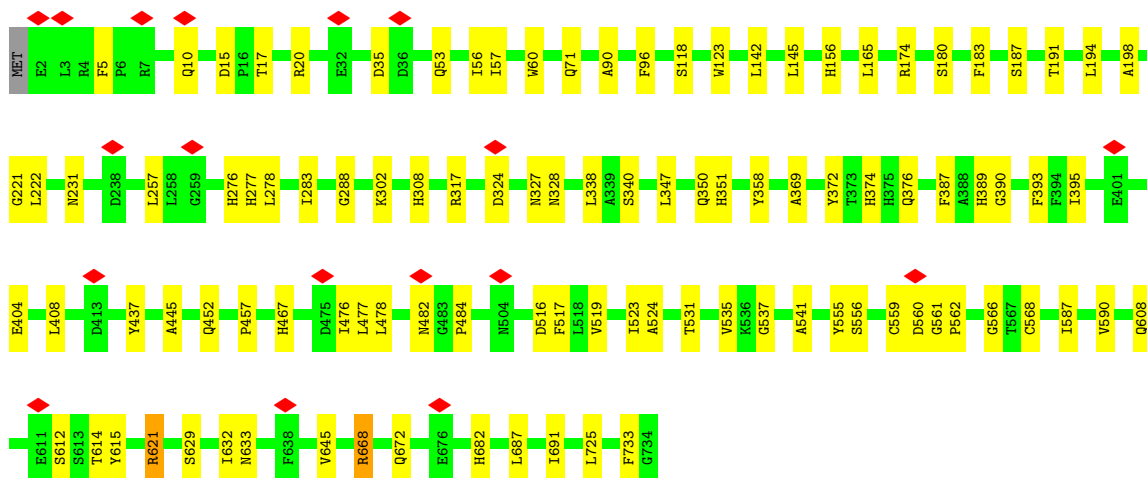


• Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1

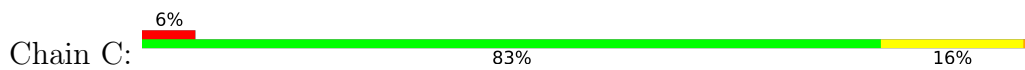


• Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2

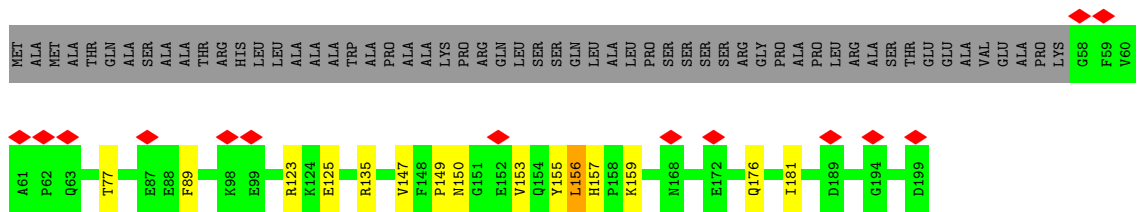




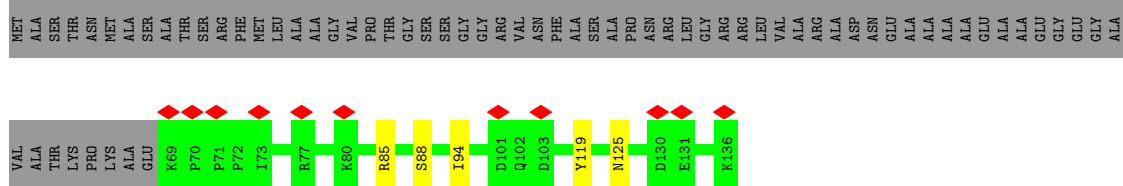
• Molecule 7: photosystem I subunit VII



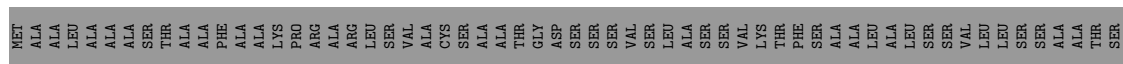
• Molecule 8: Photosystem I reaction center subunit II

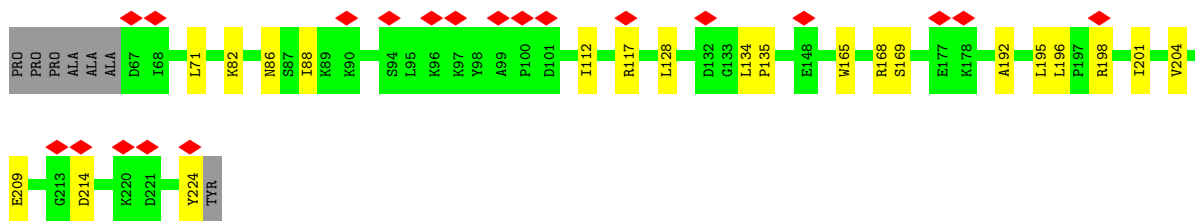


• Molecule 9: Photosystem I reaction center subunit IV A

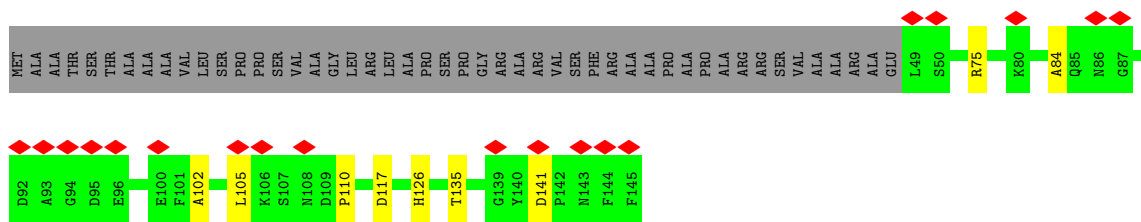


• Molecule 10: Photosystem I reaction center subunit III

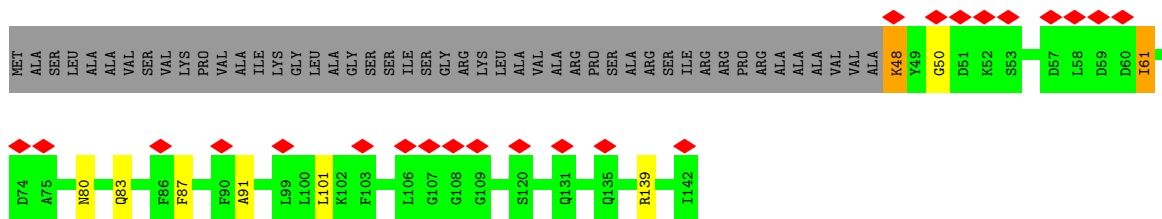




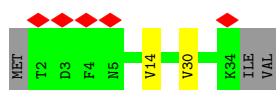
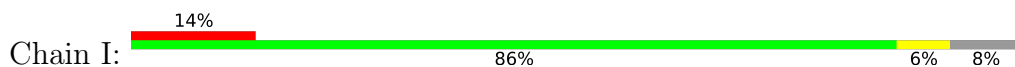
- Molecule 11: Photosystem I reaction center subunit V



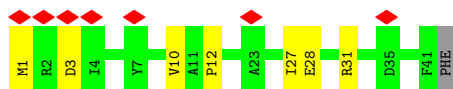
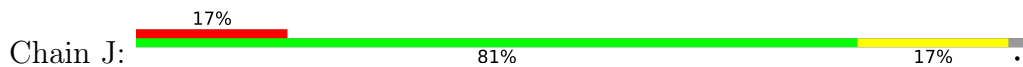
- Molecule 12: Photosystem I reaction center subunit VI, chloroplastic



- Molecule 13: Photosystem I reaction center subunit VIII

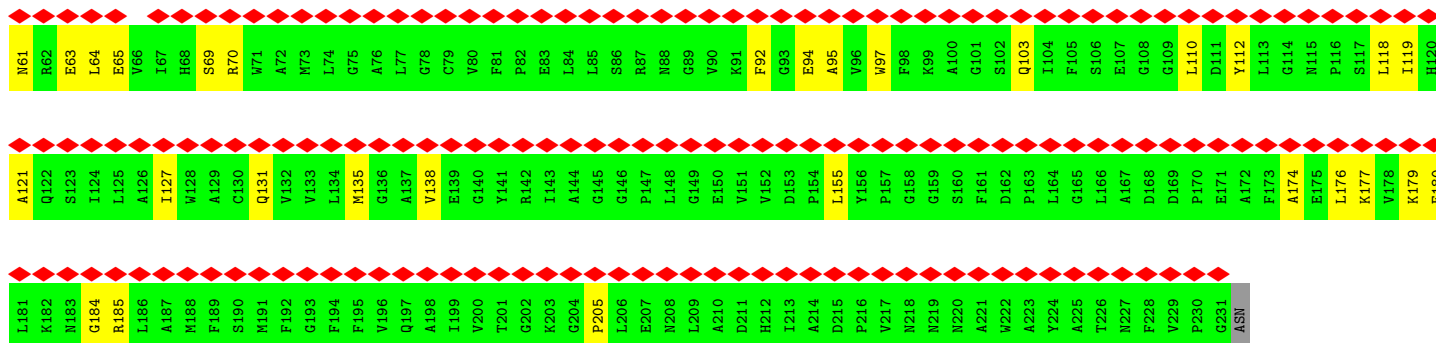


- Molecule 14: Photosystem I reaction center subunit IX

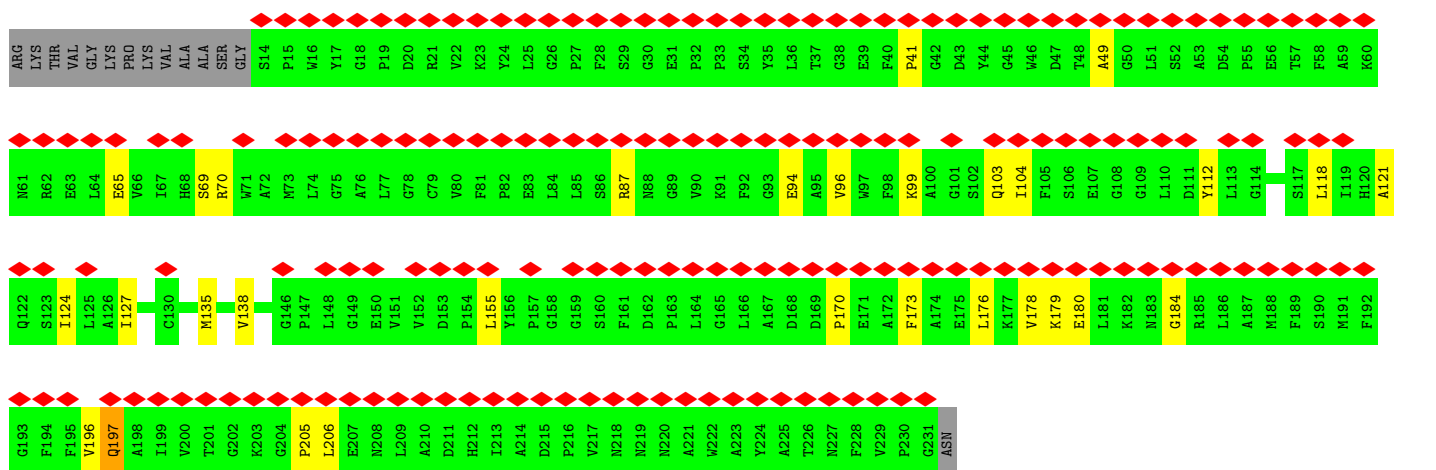
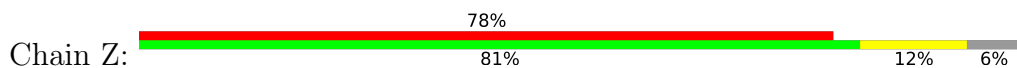


- Molecule 15: Photosystem I reaction center subunit psaK

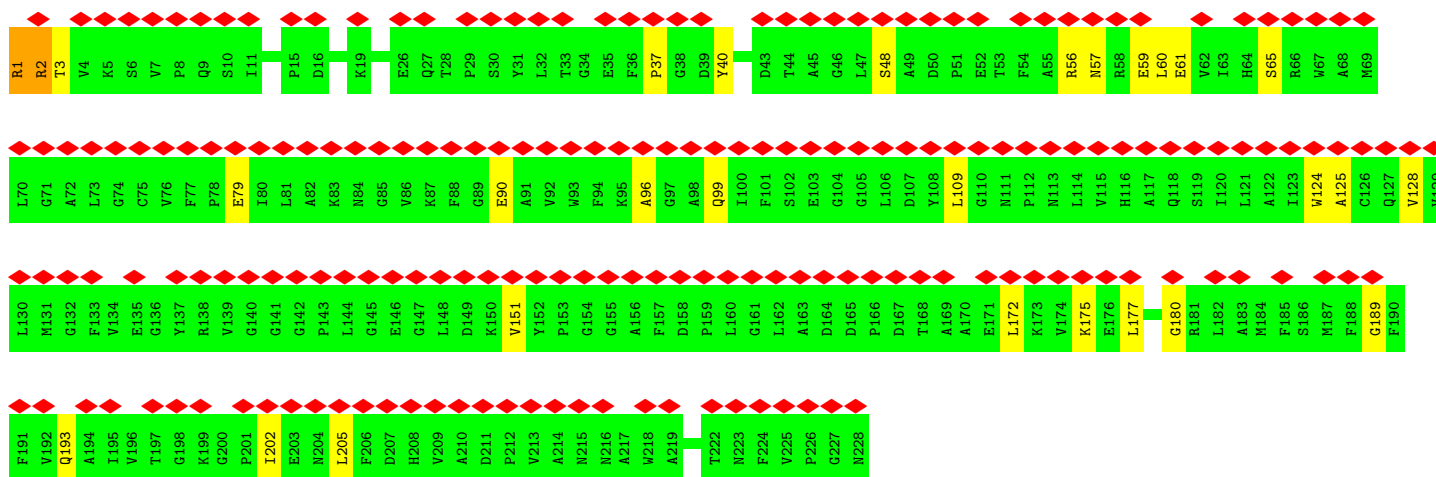
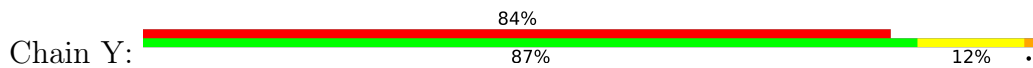




• Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic



• Molecule 20: Chlorophyll a-b binding protein, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	635845	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.292	Depositor
Minimum map value	-0.111	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	296.8, 296.8, 296.8	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CL0, PQN, CHL, LMU, LMG, DGD, XAT, SF4, LHG, NEX, LUT, TPO, BCR, CLA

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	0.37	0/1574	0.57	0/2146
2	2	0.38	0/1684	0.59	1/2305 (0.0%)
3	3	0.41	0/1775	0.65	2/2410 (0.1%)
4	4	0.36	0/1617	0.61	1/2208 (0.0%)
5	A	0.45	0/6034	0.61	0/8229
6	B	0.44	0/6077	0.62	1/8300 (0.0%)
7	C	0.50	1/623 (0.2%)	0.70	1/844 (0.1%)
8	D	0.41	0/1144	0.71	1/1547 (0.1%)
9	E	0.41	0/553	0.56	0/754
10	F	0.36	0/1267	0.60	0/1713
11	G	0.34	0/771	0.53	0/1046
12	H	0.34	0/752	0.58	0/1022
13	I	0.43	0/267	0.82	0/364
14	J	0.37	0/334	0.58	0/455
15	K	0.33	0/595	0.72	1/806 (0.1%)
16	L	0.40	0/1284	0.67	0/1758
17	O	0.36	0/646	0.75	1/882 (0.1%)
18	N	0.34	0/701	0.63	1/938 (0.1%)
19	X	0.32	0/1714	0.51	0/2336
19	Z	0.33	0/1714	0.53	0/2336
20	Y	0.35	0/1792	0.54	0/2437
All	All	0.40	1/32918 (0.0%)	0.61	10/44836 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	58	CYS	C-N	5.41	1.44	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	K	123	LEU	CA-CB-CG	7.30	132.08	115.30
8	D	156	LEU	N-CA-C	6.90	129.63	111.00
3	3	219	GLU	CA-CB-CG	6.44	127.56	113.40
4	4	111	LEU	CA-CB-CG	5.96	129.00	115.30
7	C	63	LEU	CA-CB-CG	5.94	128.97	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1522	0	1484	24	0
2	2	1624	0	1555	35	0
3	3	1720	0	1686	20	0
4	4	1566	0	1520	27	0
5	A	5836	0	5689	105	0
6	B	5866	0	5644	81	0
7	C	612	0	607	16	0
8	D	1115	0	1118	18	0
9	E	540	0	539	6	0
10	F	1238	0	1272	12	0
11	G	752	0	731	7	0
12	H	729	0	724	9	0
13	I	260	0	274	2	0
14	J	325	0	340	6	0
15	K	589	0	612	8	0
16	L	1246	0	1242	15	0
17	O	621	0	606	11	0
18	N	685	0	658	16	0
19	X	1661	0	1593	26	0
19	Z	1661	0	1593	23	0
20	Y	1751	0	1688	27	0
21	1	96	0	68	4	0
21	2	240	0	176	8	0
21	3	45	0	30	1	0
21	4	169	0	100	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	X	235	0	128	4	0
21	Y	259	0	156	2	0
21	Z	250	0	144	0	0
22	1	577	0	453	18	0
22	2	442	0	366	7	0
22	3	538	0	399	10	0
22	4	527	0	412	15	0
22	A	2533	0	2495	96	0
22	B	2261	0	2201	78	0
22	F	140	0	113	4	0
22	G	132	0	97	4	0
22	H	60	0	59	5	0
22	J	42	0	31	0	0
22	K	167	0	116	4	0
22	L	150	0	125	7	0
22	N	95	0	69	3	0
22	O	76	0	38	1	0
22	X	305	0	181	7	0
22	Y	325	0	194	6	0
22	Z	339	0	228	8	0
23	1	84	0	112	7	0
23	2	42	0	56	9	0
23	3	42	0	56	3	0
23	4	42	0	56	4	0
23	X	84	0	112	5	0
23	Y	84	0	112	5	0
23	Z	84	0	112	6	0
24	1	44	0	56	0	0
24	2	44	0	56	4	0
24	3	44	0	56	4	0
24	4	44	0	56	5	0
24	X	44	0	56	3	0
24	Y	44	0	56	2	0
24	Z	44	0	56	1	0
25	1	40	0	56	0	0
25	2	40	0	56	4	0
25	3	40	0	56	3	0
25	4	40	0	56	1	0
25	A	240	0	336	26	0
25	B	280	0	392	22	0
25	F	40	0	56	2	0
25	G	40	0	56	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	I	40	0	56	3	0
25	J	40	0	56	1	0
25	K	80	0	112	7	0
25	L	120	0	168	8	0
26	1	49	0	74	6	0
26	2	37	0	44	3	0
26	A	79	0	104	5	0
26	B	38	0	46	1	0
26	X	22	0	16	1	0
26	Y	45	0	60	3	0
26	Z	23	0	16	1	0
27	1	53	0	79	2	0
27	2	36	0	42	1	0
27	4	72	0	84	3	0
27	G	38	0	46	1	0
28	A	65	0	72	25	0
29	A	33	0	46	6	0
29	B	33	0	46	7	0
30	A	8	0	0	0	0
30	C	16	0	0	1	0
31	A	30	0	33	4	0
31	B	35	0	46	5	0
32	B	66	0	96	8	0
32	J	66	0	96	2	0
33	X	44	0	56	3	0
33	Y	44	0	56	2	0
33	Z	44	0	56	2	0
All	All	44708	0	43232	693	0

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

The worst 5 of 693 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)
2:2:239:GLN:NE2	23:2:619:LUT:H42	1.53	1.21
2:2:235:GLY:O	2:2:239:GLN:HG2	1.62	0.97
2:2:236:ALA:HA	2:2:239:GLN:HG3	1.50	0.90
2:2:239:GLN:HE22	23:2:619:LUT:H42	1.38	0.89
5:A:678:TRP:CE3	28:A:801:CLO:H4	2.10	0.87

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	194/245 (79%)	177 (91%)	17 (9%)	0	100	100
2	2	205/270 (76%)	199 (97%)	6 (3%)	0	100	100
3	3	219/267 (82%)	205 (94%)	14 (6%)	0	100	100
4	4	197/252 (78%)	182 (92%)	15 (8%)	0	100	100
5	A	740/750 (99%)	705 (95%)	35 (5%)	0	100	100
6	B	731/734 (100%)	699 (96%)	32 (4%)	0	100	100
7	C	79/81 (98%)	72 (91%)	7 (9%)	0	100	100
8	D	140/199 (70%)	126 (90%)	14 (10%)	0	100	100
9	E	66/136 (48%)	61 (92%)	5 (8%)	0	100	100
10	F	156/225 (69%)	148 (95%)	8 (5%)	0	100	100
11	G	95/145 (66%)	91 (96%)	4 (4%)	0	100	100
12	H	93/142 (66%)	84 (90%)	9 (10%)	0	100	100
13	I	31/36 (86%)	26 (84%)	5 (16%)	0	100	100
14	J	39/42 (93%)	38 (97%)	1 (3%)	0	100	100
15	K	82/134 (61%)	75 (92%)	7 (8%)	0	100	100
16	L	164/211 (78%)	155 (94%)	9 (6%)	0	100	100
17	O	72/127 (57%)	60 (83%)	12 (17%)	0	100	100
18	N	82/145 (57%)	69 (84%)	13 (16%)	0	100	100
19	X	216/232 (93%)	202 (94%)	14 (6%)	0	100	100
19	Z	216/232 (93%)	205 (95%)	11 (5%)	0	100	100
20	Y	225/228 (99%)	202 (90%)	22 (10%)	1 (0%)	34	66
All	All	4042/4833 (84%)	3781 (94%)	260 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	Y	2	ARG

5.3.2 Protein sidechains [i](#)

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	156/194 (80%)	156 (100%)	0	100	100
2	2	167/215 (78%)	165 (99%)	2 (1%)	71	83
3	3	176/210 (84%)	176 (100%)	0	100	100
4	4	166/204 (81%)	165 (99%)	1 (1%)	86	91
5	A	599/607 (99%)	596 (100%)	3 (0%)	88	93
6	B	599/600 (100%)	594 (99%)	5 (1%)	81	89
7	C	71/71 (100%)	70 (99%)	1 (1%)	67	82
8	D	119/159 (75%)	118 (99%)	1 (1%)	81	89
9	E	59/103 (57%)	59 (100%)	0	100	100
10	F	127/171 (74%)	125 (98%)	2 (2%)	62	79
11	G	79/110 (72%)	79 (100%)	0	100	100
12	H	78/110 (71%)	76 (97%)	2 (3%)	46	71
13	I	30/33 (91%)	30 (100%)	0	100	100
14	J	35/36 (97%)	35 (100%)	0	100	100
15	K	59/96 (62%)	57 (97%)	2 (3%)	37	65
16	L	130/164 (79%)	129 (99%)	1 (1%)	81	89
17	O	66/110 (60%)	65 (98%)	1 (2%)	65	81
18	N	73/111 (66%)	72 (99%)	1 (1%)	67	82
19	X	168/178 (94%)	168 (100%)	0	100	100
19	Z	168/178 (94%)	167 (99%)	1 (1%)	86	91
20	Y	175/175 (100%)	174 (99%)	1 (1%)	86	91
All	All	3300/3835 (86%)	3276 (99%)	24 (1%)	84	90

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	F	168	ARG
15	K	53	ASN
12	H	61	ILE
15	K	77	ARG
6	B	96	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
6	B	327	ASN
20	Y	57	ASN
6	B	452	GLN
19	Z	61	ASN
18	N	140	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	TPO	Y	3	20	8,10,11	1.06	0	10,14,16	1.63	1 (10%)

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	TPO	Y	3	20	-	0/9/11/13	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Y	3	TPO	P-OG1-CB	-4.53	109.54	123.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

271 ligands 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
22	CLA	A	806	-	65,73,73	1.42	9 (13%)	76,113,113	1.66	9 (11%)
22	CLA	B	810	-	65,73,73	1.45	8 (12%)	76,113,113	1.51	11 (14%)
28	CL0	A	801	-	65,73,73	2.06	16 (24%)	76,113,113	2.71	31 (40%)
22	CLA	3	614	-	39,48,73	1.85	7 (17%)	44,83,113	1.78	7 (15%)
26	LHG	X	2630	22	21,21,48	0.85	1 (4%)	22,26,54	1.12	1 (4%)
22	CLA	A	814	-	65,73,73	1.41	8 (12%)	76,113,113	1.44	9 (11%)
21	CHL	Y	609	20	39,48,74	2.28	14 (35%)	42,82,114	2.95	17 (40%)
24	XAT	X	7622	-	39,47,47	0.93	0	54,74,74	2.95	19 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	A	827	-	59,67,73	1.51	9 (15%)	68,105,113	1.43	9 (13%)
22	CLA	A	821	-	45,53,73	1.76	9 (20%)	52,89,113	1.71	7 (13%)
21	CHL	Z	605	19	37,46,74	2.37	14 (37%)	46,81,114	3.02	19 (41%)
22	CLA	K	203	-	45,53,73	1.74	9 (20%)	52,89,113	1.64	10 (19%)
22	CLA	B	821	-	47,55,73	1.64	9 (19%)	54,91,113	1.77	9 (16%)
25	BCR	B	846	-	41,41,41	0.83	0	56,56,56	2.02	22 (39%)
22	CLA	B	816	-	55,63,73	1.54	7 (12%)	64,101,113	1.73	6 (9%)
22	CLA	A	830	-	65,73,73	1.45	10 (15%)	76,113,113	1.49	10 (13%)
22	CLA	B	820	-	50,58,73	1.66	8 (16%)	58,95,113	1.65	6 (10%)
22	CLA	3	609	3	45,53,73	1.81	11 (24%)	52,89,113	1.83	11 (21%)
27	LMG	G	202	-	38,38,55	1.00	1 (2%)	46,46,63	1.22	6 (13%)
22	CLA	X	604	-	36,43,73	2.01	8 (22%)	45,76,113	1.78	9 (20%)
22	CLA	A	839	-	55,63,73	1.61	9 (16%)	64,101,113	1.50	8 (12%)
22	CLA	Y	611	26	39,48,73	1.94	7 (17%)	48,83,113	1.74	9 (18%)
22	CLA	2	614	-	43,51,73	1.73	7 (16%)	49,86,113	1.93	11 (22%)
22	CLA	A	836	-	45,53,73	1.74	10 (22%)	52,89,113	1.70	6 (11%)
22	CLA	A	815	-	45,53,73	1.70	9 (20%)	52,89,113	1.83	10 (19%)
22	CLA	A	833	-	56,64,73	1.52	8 (14%)	65,102,113	1.69	7 (10%)
23	LUT	X	2620	-	42,43,43	0.70	0	51,60,60	1.65	9 (17%)
21	CHL	Z	607	-	43,52,74	5.32	15 (34%)	49,88,114	3.07	19 (38%)
22	CLA	3	607	3	41,49,73	1.87	7 (17%)	51,84,113	1.76	10 (19%)
22	CLA	B	836	-	50,58,73	1.61	8 (16%)	58,95,113	1.82	11 (18%)
22	CLA	H	201	-	60,68,73	1.51	8 (13%)	70,107,113	1.48	8 (11%)
22	CLA	G	201	-	45,53,73	1.76	9 (20%)	52,89,113	1.70	8 (15%)
22	CLA	Z	603	-	41,49,73	1.87	8 (19%)	51,84,113	1.82	11 (21%)
22	CLA	A	811	-	65,73,73	1.45	10 (15%)	76,113,113	1.43	7 (9%)
22	CLA	A	834	-	65,73,73	1.46	8 (12%)	76,113,113	1.50	10 (13%)
22	CLA	B	818	-	60,68,73	1.47	10 (16%)	70,107,113	1.59	9 (12%)
22	CLA	A	804	-	65,73,73	1.42	8 (12%)	76,113,113	1.62	9 (11%)
22	CLA	2	604	-	43,51,73	1.79	7 (16%)	48,86,113	1.70	6 (12%)
22	CLA	A	842	-	65,73,73	1.45	8 (12%)	76,113,113	1.54	9 (11%)
22	CLA	B	838	-	47,55,73	1.71	8 (17%)	54,91,113	1.69	8 (14%)
22	CLA	B	826	-	62,70,73	1.50	9 (14%)	72,109,113	1.54	10 (13%)
23	LUT	3	618	-	42,43,43	0.74	0	51,60,60	1.58	10 (19%)
25	BCR	B	844	-	41,41,41	0.74	0	56,56,56	1.97	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LMG	1	622	-	53,53,55	0.84	2 (3%)	61,61,63	1.28	5 (8%)
22	CLA	A	807	5	65,73,73	1.47	10 (15%)	76,113,113	1.41	7 (9%)
22	CLA	A	845	26	50,58,73	1.66	8 (16%)	58,95,113	1.63	10 (17%)
22	CLA	A	838	-	51,59,73	1.55	7 (13%)	59,96,113	1.91	14 (23%)
22	CLA	K	204	-	46,54,73	1.70	8 (17%)	53,90,113	1.63	7 (13%)
22	CLA	2	609	2	45,53,73	1.71	7 (15%)	52,89,113	1.80	10 (19%)
22	CLA	4	609	4	45,53,73	1.78	10 (22%)	52,89,113	1.84	9 (17%)
25	BCR	A	848	-	41,41,41	0.81	0	56,56,56	1.84	13 (23%)
21	CHL	2	601	2	61,69,74	1.88	14 (22%)	67,108,114	2.67	23 (34%)
21	CHL	2	607	-	43,51,74	2.14	12 (27%)	45,86,114	3.00	17 (37%)
22	CLA	A	808	-	50,58,73	1.61	8 (16%)	58,95,113	1.68	8 (13%)
22	CLA	1	616	1	43,51,73	1.86	8 (18%)	54,87,113	1.70	10 (18%)
27	LMG	2	623	-	36,36,55	1.01	2 (5%)	44,44,63	1.15	3 (6%)
22	CLA	Z	611	26	39,47,73	1.95	7 (17%)	49,82,113	1.81	11 (22%)
25	BCR	A	852	-	41,41,41	0.74	0	56,56,56	1.98	11 (19%)
22	CLA	B	803	-	65,73,73	1.44	8 (12%)	76,113,113	1.91	12 (15%)
21	CHL	Y	608	-	39,48,74	2.24	15 (38%)	45,83,114	3.02	16 (35%)
22	CLA	X	610	19	39,47,73	1.86	6 (15%)	42,81,113	1.87	7 (16%)
22	CLA	B	822	-	42,50,73	1.79	8 (19%)	48,85,113	1.71	9 (18%)
22	CLA	4	611	-	42,50,73	1.78	7 (16%)	48,85,113	1.71	9 (18%)
32	DGD	J	103	-	67,67,67	0.95	4 (5%)	81,81,81	1.45	8 (9%)
25	BCR	G	205	-	41,41,41	0.75	0	56,56,56	1.90	16 (28%)
22	CLA	1	603	-	55,63,73	1.65	8 (14%)	64,101,113	1.54	9 (14%)
22	CLA	4	602	4	60,68,73	1.49	7 (11%)	70,107,113	1.60	10 (14%)
22	CLA	4	610	4	54,62,73	1.60	10 (18%)	62,99,113	1.62	6 (9%)
22	CLA	3	612	3	43,51,73	1.82	6 (13%)	49,86,113	1.80	9 (18%)
22	CLA	J	101	14	42,50,73	1.80	6 (14%)	48,85,113	1.73	8 (16%)
25	BCR	K	205	-	41,41,41	0.72	0	56,56,56	1.95	14 (25%)
33	NEX	Y	4623	-	38,46,46	0.89	1 (2%)	50,70,70	2.37	19 (38%)
22	CLA	2	603	-	43,52,73	1.78	10 (23%)	49,88,113	1.74	9 (18%)
22	CLA	X	602	19	40,49,73	1.91	8 (20%)	45,84,113	1.62	6 (13%)
21	CHL	X	601	19	37,46,74	2.29	13 (35%)	44,80,114	3.06	20 (45%)
22	CLA	Y	604	-	42,50,73	1.80	7 (16%)	48,85,113	1.90	8 (16%)
25	BCR	B	843	-	41,41,41	0.84	1 (2%)	56,56,56	2.01	16 (28%)
22	CLA	B	808	-	65,73,73	1.46	11 (16%)	76,113,113	1.75	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	Z	602	19	52,60,73	1.72	8 (15%)	64,97,113	1.59	8 (12%)
26	LHG	A	847	22	29,29,48	0.87	1 (3%)	32,35,54	1.26	3 (9%)
22	CLA	Y	603	-	38,47,73	1.91	7 (18%)	43,82,113	1.74	7 (16%)
22	CLA	3	610	3	41,49,73	1.79	8 (19%)	47,84,113	1.80	8 (17%)
25	BCR	B	847	-	41,41,41	1.03	3 (7%)	56,56,56	2.52	25 (44%)
22	CLA	A	824	-	41,49,73	1.84	9 (21%)	47,84,113	1.79	11 (23%)
22	CLA	G	204	11	45,53,73	1.78	9 (20%)	52,89,113	1.64	7 (13%)
22	CLA	F	303	-	42,50,73	1.81	7 (16%)	48,85,113	1.71	8 (16%)
22	CLA	X	611	26	38,47,73	1.94	6 (15%)	44,81,113	1.64	7 (15%)
25	BCR	A	850	-	41,41,41	0.89	2 (4%)	56,56,56	2.25	19 (33%)
22	CLA	2	612	2	44,52,73	1.79	8 (18%)	51,88,113	1.69	7 (13%)
27	LMG	4	622	-	39,39,55	0.90	1 (2%)	47,47,63	1.24	4 (8%)
22	CLA	A	813	-	54,62,73	1.59	8 (14%)	62,99,113	1.66	6 (9%)
22	CLA	A	840	-	52,60,73	1.63	8 (15%)	60,97,113	1.73	8 (13%)
22	CLA	2	611	26	38,45,73	2.94	10 (26%)	41,76,113	1.52	9 (21%)
22	CLA	L	302	16	45,53,73	1.76	9 (20%)	52,89,113	1.76	9 (17%)
22	CLA	A	803	-	65,73,73	1.47	10 (15%)	76,113,113	1.47	7 (9%)
22	CLA	B	840	-	65,73,73	1.50	10 (15%)	76,113,113	1.52	6 (7%)
25	BCR	A	851	-	41,41,41	0.78	0	56,56,56	1.97	12 (21%)
21	CHL	4	608	-	46,54,74	2.16	15 (32%)	49,90,114	2.83	18 (36%)
22	CLA	B	813	-	65,73,73	1.42	11 (16%)	76,113,113	1.54	13 (17%)
23	LUT	X	2621	-	42,43,43	0.76	0	51,60,60	1.57	8 (15%)
25	BCR	L	306	-	41,41,41	0.76	0	56,56,56	1.84	13 (23%)
33	NEX	X	2623	-	38,46,46	0.86	1 (2%)	50,70,70	2.27	15 (30%)
24	XAT	1	618	-	39,47,47	0.99	2 (5%)	54,74,74	2.58	18 (33%)
25	BCR	I	101	-	41,41,41	0.83	0	56,56,56	2.14	18 (32%)
22	CLA	A	835	-	65,73,73	1.43	11 (16%)	76,113,113	1.67	13 (17%)
25	BCR	F	305	-	41,41,41	0.78	0	56,56,56	1.84	13 (23%)
25	BCR	L	305	-	41,41,41	0.74	0	56,56,56	1.92	12 (21%)
26	LHG	Y	4630	22	44,44,48	0.60	0	47,50,54	1.23	4 (8%)
22	CLA	O	2002	-	37,46,73	1.96	7 (18%)	46,81,113	2.02	11 (23%)
22	CLA	Y	610	20	39,47,73	1.93	7 (17%)	49,82,113	1.89	11 (22%)
21	CHL	3	608	-	45,53,74	2.13	14 (31%)	52,89,114	2.78	21 (40%)
30	SF4	A	853	-	0,12,12	-	-	-	-	-
22	CLA	O	2001	-	36,46,73	1.93	6 (16%)	41,80,113	1.67	7 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	2	613	2	65,73,73	1.48	9 (13%)	76,113,113	1.52	7 (9%)
21	CHL	1	601	1	54,63,74	2.09	16 (29%)	58,101,114	2.43	19 (32%)
22	CLA	A	825	-	55,63,73	1.59	10 (18%)	64,101,113	1.65	11 (17%)
21	CHL	X	607	-	41,49,74	2.39	15 (36%)	48,84,114	2.91	20 (41%)
22	CLA	A	837	5	45,53,73	1.78	7 (15%)	52,89,113	1.69	7 (13%)
22	CLA	1	610	1	59,67,73	1.50	7 (11%)	69,106,113	1.55	7 (10%)
22	CLA	G	203	-	42,50,73	1.77	7 (16%)	48,85,113	1.68	9 (18%)
22	CLA	Z	612	19	37,46,73	1.98	8 (21%)	48,80,113	1.78	12 (25%)
22	CLA	Z	613	19	43,51,73	1.78	6 (13%)	49,86,113	1.77	8 (16%)
22	CLA	A	831	-	65,73,73	1.55	11 (16%)	76,113,113	1.65	8 (10%)
27	LMG	4	623	-	33,33,55	1.15	3 (9%)	41,41,63	1.20	6 (14%)
26	LHG	B	851	22	37,37,48	0.67	1 (2%)	40,43,54	1.23	4 (10%)
30	SF4	C	102	-	0,12,12	-	-	-	-	-
25	BCR	B	845	-	41,41,41	0.74	0	56,56,56	1.96	13 (23%)
22	CLA	A	819	-	59,67,73	1.63	10 (16%)	68,105,113	1.42	8 (11%)
32	DGD	B	850	-	67,67,67	1.07	5 (7%)	81,81,81	1.44	13 (16%)
23	LUT	2	619	-	42,43,43	0.78	0	51,60,60	1.60	10 (19%)
22	CLA	B	812	-	43,51,73	1.69	7 (16%)	49,86,113	1.95	7 (14%)
21	CHL	Y	607	-	40,48,74	2.28	12 (30%)	47,83,114	3.09	21 (44%)
25	BCR	1	619	-	41,41,41	0.67	0	56,56,56	1.80	13 (23%)
24	XAT	4	620	-	39,47,47	0.95	2 (5%)	54,74,74	2.59	19 (35%)
22	CLA	4	617	-	50,58,73	1.67	10 (20%)	58,95,113	1.50	9 (15%)
22	CLA	B	830	-	43,51,73	1.77	10 (23%)	49,86,113	1.66	7 (14%)
21	CHL	Y	601	20	62,71,74	1.85	13 (20%)	76,111,114	2.32	21 (27%)
23	LUT	Z	7620	-	42,43,43	0.75	0	51,60,60	1.56	12 (23%)
22	CLA	4	601	4	46,54,73	1.74	10 (21%)	53,90,113	1.61	9 (16%)
22	CLA	A	826	-	65,73,73	1.43	8 (12%)	76,113,113	1.54	9 (11%)
22	CLA	Z	604	-	46,54,73	1.78	8 (17%)	57,90,113	1.68	9 (15%)
22	CLA	F	304	-	41,49,73	1.79	9 (21%)	47,84,113	1.76	7 (14%)
22	CLA	3	617	-	39,48,73	1.84	8 (20%)	44,83,113	1.76	8 (18%)
21	CHL	Y	605	20	37,46,74	2.46	14 (37%)	46,81,114	2.92	20 (43%)
21	CHL	X	606	-	38,47,74	2.31	14 (36%)	45,81,114	3.14	23 (51%)
22	CLA	B	815	-	43,51,73	1.69	9 (20%)	49,86,113	1.86	7 (14%)
22	CLA	K	206	15	37,47,73	1.92	6 (16%)	42,81,113	1.81	10 (23%)
24	XAT	Y	2622	-	39,47,47	0.84	0	54,74,74	2.61	18 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	A	817	-	45,53,73	1.75	9 (20%)	52,89,113	1.75	9 (17%)
22	CLA	X	603	-	39,48,73	1.89	6 (15%)	44,83,113	1.83	9 (20%)
22	CLA	A	828	-	65,73,73	1.44	9 (13%)	76,113,113	1.42	6 (7%)
21	CHL	4	606	-	40,49,74	2.22	13 (32%)	42,84,114	2.89	18 (42%)
22	CLA	B	811	-	54,62,73	1.63	9 (16%)	67,100,113	1.57	9 (13%)
22	CLA	B	817	-	59,67,73	1.52	10 (16%)	68,105,113	1.50	7 (10%)
22	CLA	X	613	19	37,44,73	1.94	6 (16%)	42,77,113	1.91	8 (19%)
22	CLA	1	609	1	40,48,73	1.90	8 (20%)	50,83,113	1.86	10 (20%)
26	LHG	Z	7630	22	22,22,48	0.90	1 (4%)	25,28,54	1.18	1 (4%)
22	CLA	A	832	-	50,58,73	1.65	9 (18%)	58,95,113	1.76	11 (18%)
22	CLA	A	854	-	65,73,73	1.46	8 (12%)	76,113,113	1.47	8 (10%)
22	CLA	X	614	-	38,47,73	1.98	7 (18%)	48,81,113	1.70	10 (20%)
25	BCR	4	621	-	41,41,41	0.73	0	56,56,56	2.02	18 (32%)
31	LMU	B	849	-	36,36,36	1.19	2 (5%)	47,47,47	0.93	1 (2%)
22	CLA	B	832	-	65,73,73	1.40	7 (10%)	76,113,113	1.55	9 (11%)
22	CLA	A	816	-	42,50,73	1.74	7 (16%)	48,85,113	1.84	8 (16%)
21	CHL	Z	606	-	38,47,74	2.30	14 (36%)	41,81,114	2.97	20 (48%)
26	LHG	A	846	-	48,48,48	0.75	1 (2%)	51,54,54	1.31	5 (9%)
22	CLA	Y	613	20	42,51,73	1.92	7 (16%)	52,87,113	1.77	8 (15%)
29	PQN	A	844	-	34,34,34	2.88	11 (32%)	42,45,45	2.13	6 (14%)
24	XAT	Z	4622	-	39,47,47	0.98	0	54,74,74	2.88	18 (33%)
22	CLA	A	809	5	65,73,73	1.44	10 (15%)	76,113,113	1.44	9 (11%)
22	CLA	K	201	15	38,45,73	1.92	10 (26%)	43,78,113	1.86	9 (20%)
23	LUT	Y	4620	-	42,43,43	0.75	0	51,60,60	1.63	13 (25%)
22	CLA	B	824	-	65,73,73	1.46	10 (15%)	76,113,113	1.51	7 (9%)
22	CLA	1	604	-	49,57,73	1.69	8 (16%)	55,93,113	1.66	7 (12%)
21	CHL	1	607	1	40,49,74	2.42	16 (40%)	41,84,114	2.85	20 (48%)
22	CLA	Y	614	-	38,47,73	1.93	7 (18%)	47,82,113	1.84	10 (21%)
22	CLA	3	606	3	40,49,73	1.82	10 (25%)	45,84,113	1.78	11 (24%)
22	CLA	B	833	-	45,53,73	1.76	10 (22%)	52,89,113	1.67	11 (21%)
24	XAT	3	619	-	39,47,47	0.92	2 (5%)	54,74,74	2.51	19 (35%)
22	CLA	A	841	-	65,73,73	1.42	9 (13%)	76,113,113	1.52	9 (11%)
22	CLA	B	828	-	65,73,73	1.44	11 (16%)	76,113,113	1.55	13 (17%)
21	CHL	X	605	19	41,50,74	2.25	13 (31%)	49,85,114	2.68	16 (32%)
25	BCR	J	102	-	41,41,41	0.81	0	56,56,56	2.02	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	L	301	-	41,41,41	0.80	0	56,56,56	1.88	18 (32%)
22	CLA	B	841	26	65,73,73	1.43	9 (13%)	76,113,113	1.46	8 (10%)
25	BCR	A	856	-	41,41,41	0.73	0	56,56,56	1.88	14 (25%)
22	CLA	A	818	-	60,68,73	1.44	7 (11%)	70,107,113	1.83	12 (17%)
22	CLA	1	606	-	39,48,73	1.82	7 (17%)	45,82,113	1.77	9 (20%)
21	CHL	4	607	-	41,49,74	2.23	14 (34%)	51,84,114	2.82	18 (35%)
21	CHL	2	618	2	43,51,74	2.22	15 (34%)	45,86,114	3.04	20 (44%)
22	CLA	L	303	-	60,68,73	1.51	9 (15%)	70,107,113	1.50	10 (14%)
25	BCR	B	848	-	41,41,41	0.79	0	56,56,56	2.01	16 (28%)
29	PQN	B	842	-	34,34,34	2.89	11 (32%)	42,45,45	2.08	5 (11%)
21	CHL	2	606	-	42,50,74	2.21	13 (30%)	45,85,114	2.94	19 (42%)
24	XAT	2	620	-	39,47,47	0.98	1 (2%)	54,74,74	2.75	23 (42%)
22	CLA	A	812	-	65,73,73	1.46	7 (10%)	76,113,113	1.50	7 (9%)
22	CLA	B	835	-	42,50,73	1.86	9 (21%)	48,85,113	1.64	7 (14%)
22	CLA	1	613	-	65,73,73	1.45	10 (15%)	76,113,113	1.46	7 (9%)
26	LHG	1	620	22	48,48,48	0.64	1 (2%)	51,54,54	1.20	5 (9%)
21	CHL	Y	606	-	37,46,74	2.42	13 (35%)	46,81,114	3.02	18 (39%)
21	CHL	2	608	-	51,59,74	2.03	14 (27%)	55,96,114	2.80	20 (36%)
22	CLA	X	612	19	37,44,73	1.98	7 (18%)	46,77,113	1.84	10 (21%)
26	LHG	2	622	22	36,36,48	0.74	1 (2%)	39,42,54	1.29	5 (12%)
22	CLA	A	802	-	65,73,73	1.47	10 (15%)	76,113,113	1.76	15 (19%)
22	CLA	Y	612	20	37,46,73	2.03	8 (21%)	46,81,113	1.93	12 (26%)
31	LMU	A	857	-	31,31,36	1.37	3 (9%)	42,42,47	1.55	8 (19%)
22	CLA	3	602	3	60,68,73	1.57	8 (13%)	70,107,113	1.47	8 (11%)
23	LUT	1	617	-	42,43,43	0.79	0	51,60,60	1.71	15 (29%)
30	SF4	C	101	-	0,12,12	-	-	-	-	-
22	CLA	B	802	-	65,73,73	1.49	10 (15%)	76,113,113	1.33	5 (6%)
22	CLA	A	805	-	52,60,73	1.64	8 (15%)	60,97,113	1.68	8 (13%)
22	CLA	B	804	-	41,49,73	1.76	7 (17%)	47,84,113	1.96	8 (17%)
22	CLA	B	814	-	65,73,73	1.45	9 (13%)	76,113,113	1.58	8 (10%)
22	CLA	N	1001	18	44,53,73	1.77	8 (18%)	50,89,113	1.65	7 (14%)
22	CLA	L	304	-	45,53,73	1.70	8 (17%)	52,89,113	1.88	9 (17%)
23	LUT	Y	4621	-	42,43,43	0.75	0	51,60,60	1.51	10 (19%)
22	CLA	2	610	2	55,63,73	1.54	10 (18%)	64,101,113	1.54	8 (12%)
22	CLA	N	1002	-	50,58,73	1.66	7 (14%)	58,95,113	1.71	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	1	611	26	37,46,73	1.94	9 (24%)	46,81,113	1.80	9 (19%)
22	CLA	F	301	-	57,65,73	1.60	9 (15%)	66,103,113	1.53	8 (12%)
22	CLA	A	810	5	50,58,73	1.68	10 (20%)	58,95,113	1.52	9 (15%)
22	CLA	B	823	-	45,53,73	1.74	9 (20%)	52,89,113	1.73	7 (13%)
22	CLA	B	829	-	56,64,73	1.76	10 (17%)	65,102,113	1.89	10 (15%)
21	CHL	X	608	-	38,47,74	2.40	15 (39%)	41,81,114	2.97	19 (46%)
21	CHL	X	609	19	37,44,74	2.23	13 (35%)	46,77,114	2.91	24 (52%)
22	CLA	3	603	3	55,63,73	1.61	10 (18%)	64,101,113	1.63	13 (20%)
22	CLA	B	807	6	52,60,73	1.61	9 (17%)	60,97,113	1.63	8 (13%)
22	CLA	1	612	1	45,53,73	1.79	7 (15%)	52,89,113	1.69	8 (15%)
22	CLA	B	827	-	65,73,73	1.39	8 (12%)	76,113,113	1.55	8 (10%)
33	NEX	Z	7623	-	38,46,46	0.90	1 (2%)	50,70,70	2.34	17 (34%)
22	CLA	1	614	-	37,46,73	1.99	8 (21%)	46,81,113	1.81	10 (21%)
22	CLA	1	602	1	61,69,73	1.51	6 (9%)	71,108,113	1.46	9 (12%)
23	LUT	1	621	-	42,43,43	0.74	0	51,60,60	1.57	10 (19%)
22	CLA	A	829	-	65,73,73	1.42	7 (10%)	76,113,113	1.67	10 (13%)
22	CLA	B	837	-	65,73,73	1.43	7 (10%)	76,113,113	1.64	11 (14%)
22	CLA	B	839	-	65,73,73	1.44	8 (12%)	76,113,113	1.49	8 (10%)
23	LUT	4	619	-	42,43,43	0.82	0	51,60,60	1.70	12 (23%)
21	CHL	Z	608	-	44,53,74	2.20	13 (29%)	46,89,114	2.93	17 (36%)
22	CLA	2	602	2	65,73,73	1.49	10 (15%)	76,113,113	1.36	7 (9%)
22	CLA	A	822	-	65,73,73	1.49	10 (15%)	76,113,113	1.45	6 (7%)
25	BCR	B	801	-	41,41,41	0.78	0	56,56,56	2.09	12 (21%)
22	CLA	B	819	-	55,63,73	1.63	11 (20%)	64,101,113	1.60	7 (10%)
23	LUT	Z	7621	-	42,43,43	0.80	1 (2%)	51,60,60	1.59	11 (21%)
22	CLA	4	613	-	57,65,73	1.55	7 (12%)	66,103,113	1.58	9 (13%)
25	BCR	A	849	-	41,41,41	0.89	2 (4%)	56,56,56	2.04	19 (33%)
22	CLA	B	831	-	43,51,73	1.78	7 (16%)	49,86,113	1.77	7 (14%)
22	CLA	Z	610	19	37,44,73	2.02	8 (21%)	41,77,113	1.85	8 (19%)
22	CLA	A	823	-	42,50,73	1.75	7 (16%)	48,85,113	1.82	7 (14%)
22	CLA	Y	602	20	45,53,73	1.81	9 (20%)	52,89,113	1.57	8 (15%)
22	CLA	3	615	-	37,44,73	1.89	7 (18%)	42,77,113	1.83	7 (16%)
22	CLA	B	834	-	60,68,73	1.50	8 (13%)	70,107,113	1.56	9 (12%)
22	CLA	B	825	-	62,70,73	1.45	8 (12%)	72,109,113	1.46	11 (15%)
22	CLA	4	604	-	43,51,73	1.82	8 (18%)	54,87,113	1.69	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	806	6	65,73,73	1.45	8 (12%)	76,113,113	1.46	6 (7%)
22	CLA	4	614	-	45,53,73	1.79	7 (15%)	52,89,113	1.65	10 (19%)
22	CLA	4	603	4	44,52,73	1.87	9 (20%)	55,88,113	1.65	11 (20%)
21	CHL	Z	601	19	41,50,74	2.38	16 (39%)	42,85,114	2.84	18 (42%)
21	CHL	Z	609	19	41,50,74	2.27	12 (29%)	42,85,114	3.00	17 (40%)
22	CLA	1	608	-	43,52,73	1.80	6 (13%)	49,88,113	1.54	7 (14%)
21	CHL	4	618	4	40,49,74	2.16	12 (30%)	45,84,114	3.04	20 (44%)
22	CLA	A	843	-	65,73,73	1.49	10 (15%)	76,113,113	1.44	7 (9%)
22	CLA	B	809	6	65,73,73	1.49	10 (15%)	76,113,113	1.41	7 (9%)
22	CLA	A	820	-	65,73,73	1.50	10 (15%)	76,113,113	1.64	8 (10%)
22	CLA	3	613	3	53,62,73	1.61	8 (15%)	61,100,113	1.53	6 (9%)
22	CLA	Z	614	-	44,52,73	1.81	6 (13%)	51,88,113	1.60	6 (11%)
25	BCR	K	202	-	41,41,41	0.78	0	56,56,56	2.25	14 (25%)
22	CLA	4	612	4	40,49,73	1.83	7 (17%)	45,84,113	1.72	8 (17%)
25	BCR	2	621	-	41,41,41	0.71	0	56,56,56	1.87	11 (19%)
25	BCR	3	620	-	41,41,41	0.74	0	56,56,56	1.99	16 (28%)
22	CLA	B	805	-	65,73,73	1.37	7 (10%)	76,113,113	1.69	11 (14%)
22	CLA	3	604	-	41,50,73	1.89	8 (19%)	51,86,113	1.73	8 (15%)

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
22	CLA	A	806	-	1/1/15/20	20/37/115/115	-
22	CLA	B	810	-	1/1/15/20	13/37/115/115	-
28	CL0	A	801	-	3/3/20/25	7/37/135/135	-
22	CLA	3	614	-	1/1/10/20	1/6/84/115	-
26	LHG	X	2630	22	-	8/25/25/53	-
22	CLA	A	814	-	1/1/15/20	18/37/115/115	-
21	CHL	Y	609	20	3/3/14/26	0/6/104/137	-
24	XAT	X	7622	-	-	1/31/93/93	0/4/4/4
22	CLA	A	827	-	1/1/13/20	11/30/108/115	-
22	CLA	A	821	-	1/1/11/20	0/13/91/115	-
21	CHL	Z	605	19	3/3/15/26	1/4/100/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	K	203	-	1/1/11/20	4/13/91/115	-
22	CLA	B	821	-	1/1/11/20	6/16/94/115	-
25	BCR	B	846	-	-	1/29/63/63	0/2/2/2
22	CLA	B	816	-	1/1/13/20	6/25/103/115	-
22	CLA	A	830	-	1/1/15/20	14/37/115/115	-
22	CLA	B	820	-	1/1/12/20	6/19/97/115	-
22	CLA	3	609	3	1/1/11/20	5/13/91/115	-
27	LMG	G	202	-	-	20/33/53/70	0/1/1/1
22	CLA	X	604	-	1/1/8/20	-	-
22	CLA	A	839	-	1/1/13/20	7/25/103/115	-
22	CLA	Y	611	26	1/1/10/20	1/8/84/115	-
22	CLA	2	614	-	1/1/10/20	3/11/89/115	-
22	CLA	A	836	-	1/1/11/20	1/13/91/115	-
22	CLA	A	815	-	1/1/11/20	6/13/91/115	-
22	CLA	A	833	-	1/1/13/20	8/27/105/115	-
23	LUT	X	2620	-	-	4/29/67/67	0/2/2/2
21	CHL	Z	607	-	3/3/16/26	5/13/109/137	-
22	CLA	3	607	3	1/1/10/20	2/10/86/115	-
22	CLA	B	836	-	1/1/12/20	3/19/97/115	-
22	CLA	H	201	-	1/1/14/20	14/31/109/115	-
22	CLA	G	201	-	1/1/11/20	4/13/91/115	-
22	CLA	Z	603	-	1/1/10/20	4/10/86/115	-
22	CLA	A	811	-	1/1/15/20	16/37/115/115	-
22	CLA	A	834	-	1/1/15/20	15/37/115/115	-
22	CLA	B	818	-	1/1/14/20	18/31/109/115	-
22	CLA	A	804	-	1/1/15/20	12/37/115/115	-
22	CLA	2	604	-	1/1/10/20	5/9/88/115	-
22	CLA	A	842	-	1/1/15/20	9/37/115/115	-
22	CLA	B	838	-	1/1/11/20	7/16/94/115	-
22	CLA	B	826	-	1/1/14/20	14/34/112/115	-
23	LUT	3	618	-	-	4/29/67/67	0/2/2/2
25	BCR	B	844	-	-	8/29/63/63	0/2/2/2
27	LMG	1	622	-	-	26/48/68/70	0/1/1/1
22	CLA	A	807	5	1/1/15/20	19/37/115/115	-
22	CLA	A	845	26	1/1/12/20	8/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	838	-	1/1/12/20	7/21/99/115	-
22	CLA	K	204	-	1/1/11/20	11/15/93/115	-
22	CLA	2	609	2	1/1/11/20	6/13/91/115	-
22	CLA	4	609	4	1/1/11/20	6/13/91/115	-
25	BCR	A	848	-	-	4/29/63/63	0/2/2/2
21	CHL	2	601	2	4/4/19/26	16/33/131/137	-
21	CHL	2	607	-	3/3/15/26	4/12/110/137	-
22	CLA	A	808	-	1/1/12/20	2/19/97/115	-
22	CLA	1	616	1	-	6/11/87/115	-
27	LMG	2	623	-	-	16/31/51/70	0/1/1/1
22	CLA	Z	611	26	1/1/10/20	2/6/82/115	-
25	BCR	A	852	-	-	8/29/63/63	0/2/2/2
22	CLA	B	803	-	1/1/15/20	15/37/115/115	-
21	CHL	Y	608	-	3/3/15/26	2/8/104/137	-
22	CLA	X	610	19	1/1/9/20	0/2/82/115	-
22	CLA	B	822	-	1/1/10/20	4/10/88/115	-
22	CLA	4	611	-	1/1/10/20	6/10/88/115	-
32	DGD	J	103	-	-	29/55/95/95	0/2/2/2
25	BCR	G	205	-	-	0/29/63/63	0/2/2/2
22	CLA	1	603	-	1/1/13/20	11/25/103/115	-
22	CLA	4	602	4	1/1/14/20	12/31/109/115	-
22	CLA	4	610	4	1/1/12/20	6/24/102/115	-
22	CLA	3	612	3	-	4/11/89/115	-
22	CLA	J	101	14	1/1/10/20	5/10/88/115	-
25	BCR	K	205	-	-	8/29/63/63	0/2/2/2
33	NEX	Y	4623	-	-	5/27/83/83	0/3/3/3
22	CLA	2	603	-	1/1/11/20	2/11/89/115	-
22	CLA	X	602	19	1/1/10/20	3/8/86/115	-
21	CHL	X	601	19	3/3/14/26	2/4/100/137	-
22	CLA	Y	604	-	1/1/10/20	7/10/88/115	-
25	BCR	B	843	-	-	5/29/63/63	0/2/2/2
22	CLA	B	808	-	1/1/15/20	16/37/115/115	-
22	CLA	Z	602	19	1/1/12/20	7/22/98/115	-
26	LHG	A	847	22	-	14/34/34/53	-
22	CLA	Y	603	-	1/1/10/20	1/4/82/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	3	610	3	1/1/10/20	3/8/86/115	-
25	BCR	B	847	-	-	2/29/63/63	0/2/2/2
22	CLA	A	824	-	1/1/10/20	2/8/86/115	-
22	CLA	G	204	11	1/1/11/20	8/13/91/115	-
22	CLA	F	303	-	1/1/10/20	4/10/88/115	-
22	CLA	X	611	26	1/1/9/20	1/6/80/115	-
25	BCR	A	850	-	-	3/29/63/63	0/2/2/2
22	CLA	2	612	2	1/1/11/20	7/11/89/115	-
27	LMG	4	622	-	-	12/34/54/70	0/1/1/1
22	CLA	A	813	-	1/1/12/20	3/24/102/115	-
22	CLA	A	840	-	1/1/12/20	3/22/100/115	-
22	CLA	2	611	26	1/1/7/20	3/10/70/115	-
22	CLA	L	302	16	1/1/11/20	5/13/91/115	-
22	CLA	A	803	-	1/1/15/20	5/37/115/115	-
22	CLA	B	840	-	1/1/15/20	13/37/115/115	-
25	BCR	A	851	-	-	6/29/63/63	0/2/2/2
21	CHL	4	608	-	3/3/16/26	5/15/113/137	-
22	CLA	B	813	-	1/1/15/20	18/37/115/115	-
23	LUT	X	2621	-	-	5/29/67/67	0/2/2/2
25	BCR	L	306	-	-	6/29/63/63	0/2/2/2
33	NEX	X	2623	-	-	5/27/83/83	0/3/3/3
24	XAT	1	618	-	-	3/31/93/93	0/4/4/4
25	BCR	I	101	-	-	3/29/63/63	0/2/2/2
22	CLA	A	835	-	1/1/15/20	19/37/115/115	-
25	BCR	F	305	-	-	2/29/63/63	0/2/2/2
25	BCR	L	305	-	-	10/29/63/63	0/2/2/2
26	LHG	Y	4630	22	-	13/49/49/53	-
22	CLA	O	2002	-	1/1/10/20	0/4/80/115	-
22	CLA	Y	610	20	1/1/10/20	3/6/82/115	-
21	CHL	3	608	-	3/3/16/26	7/13/111/137	-
30	SF4	A	853	-	-	-	0/6/5/5
22	CLA	O	2001	-	1/1/9/20	2/4/78/115	-
22	CLA	2	613	2	1/1/15/20	10/37/115/115	-
21	CHL	1	601	1	4/4/18/26	14/25/123/137	-
22	CLA	A	825	-	1/1/13/20	16/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CHL	X	607	-	3/3/15/26	4/10/106/137	-
22	CLA	A	837	5	1/1/11/20	7/13/91/115	-
22	CLA	1	610	1	1/1/14/20	2/29/107/115	-
22	CLA	G	203	-	1/1/10/20	3/10/88/115	-
22	CLA	Z	612	19	1/1/9/20	2/4/80/115	-
22	CLA	Z	613	19	1/1/10/20	1/11/89/115	-
22	CLA	A	831	-	1/1/15/20	12/37/115/115	-
27	LMG	4	623	-	-	11/28/48/70	0/1/1/1
26	LHG	B	851	22	-	19/42/42/53	-
32	DGD	B	850	-	-	22/55/95/95	0/2/2/2
25	BCR	B	845	-	-	6/29/63/63	0/2/2/2
22	CLA	A	819	-	1/1/13/20	9/30/108/115	-
23	LUT	2	619	-	-	2/29/67/67	0/2/2/2
22	CLA	B	812	-	1/1/10/20	4/11/89/115	-
21	CHL	Y	607	-	3/3/15/26	4/8/104/137	-
25	BCR	1	619	-	-	6/29/63/63	0/2/2/2
24	XAT	4	620	-	-	2/31/93/93	0/4/4/4
22	CLA	4	617	-	1/1/12/20	8/19/97/115	-
22	CLA	B	830	-	1/1/10/20	3/11/89/115	-
21	CHL	Y	601	20	4/4/20/26	18/35/131/137	-
23	LUT	Z	7620	-	-	2/29/67/67	0/2/2/2
22	CLA	4	601	4	1/1/11/20	7/15/93/115	-
22	CLA	A	826	-	1/1/15/20	17/37/115/115	-
22	CLA	Z	604	-	1/1/11/20	3/16/92/115	-
22	CLA	F	304	-	1/1/10/20	2/8/86/115	-
22	CLA	3	617	-	1/1/10/20	0/6/84/115	-
21	CHL	Y	605	20	3/3/15/26	2/4/100/137	-
21	CHL	X	606	-	3/3/14/26	0/8/100/137	-
22	CLA	B	815	-	1/1/10/20	1/11/89/115	-
22	CLA	K	206	15	1/1/9/20	0/6/80/115	-
24	XAT	Y	2622	-	-	4/31/93/93	0/4/4/4
22	CLA	A	817	-	1/1/11/20	6/13/91/115	-
22	CLA	X	603	-	1/1/10/20	2/6/84/115	-
22	CLA	A	828	-	1/1/15/20	14/37/115/115	-
21	CHL	4	606	-	3/3/15/26	4/8/106/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	811	-	1/1/13/20	10/25/101/115	-
22	CLA	B	817	-	1/1/13/20	10/30/108/115	-
22	CLA	X	613	19	1/1/8/20	0/0/74/115	-
22	CLA	1	609	1	1/1/10/20	2/8/84/115	-
26	LHG	Z	7630	22	-	13/26/26/53	-
22	CLA	A	832	-	1/1/12/20	8/19/97/115	-
22	CLA	A	854	-	1/1/15/20	16/37/115/115	-
22	CLA	X	614	-	1/1/9/20	5/8/80/115	-
25	BCR	4	621	-	-	10/29/63/63	0/2/2/2
31	LMU	B	849	-	-	11/21/61/61	0/2/2/2
22	CLA	B	832	-	1/1/15/20	9/37/115/115	-
22	CLA	A	816	-	1/1/10/20	3/10/88/115	-
21	CHL	Z	606	-	3/3/14/26	2/4/102/137	-
26	LHG	A	846	-	-	29/53/53/53	-
22	CLA	Y	613	20	1/1/11/20	4/11/87/115	-
29	PQN	A	844	-	-	11/23/43/43	0/2/2/2
24	XAT	Z	4622	-	-	3/31/93/93	0/4/4/4
22	CLA	A	809	5	1/1/15/20	12/37/115/115	-
22	CLA	K	201	15	1/1/8/20	0/2/76/115	-
23	LUT	Y	4620	-	-	7/29/67/67	0/2/2/2
22	CLA	B	824	-	1/1/15/20	12/37/115/115	-
22	CLA	1	604	-	1/1/11/20	10/18/96/115	-
21	CHL	1	607	1	3/3/15/26	2/8/106/137	-
22	CLA	Y	614	-	1/1/10/20	4/6/82/115	-
22	CLA	3	606	3	1/1/10/20	5/8/86/115	-
22	CLA	B	833	-	1/1/11/20	6/13/91/115	-
24	XAT	3	619	-	-	2/31/93/93	0/4/4/4
22	CLA	A	841	-	1/1/15/20	13/37/115/115	-
22	CLA	B	828	-	1/1/15/20	16/37/115/115	-
21	CHL	X	605	19	3/3/15/26	5/7/105/137	-
25	BCR	J	102	-	-	7/29/63/63	0/2/2/2
25	BCR	L	301	-	-	4/29/63/63	0/2/2/2
22	CLA	B	841	26	1/1/15/20	14/37/115/115	-
25	BCR	A	856	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	818	-	1/1/14/20	12/31/109/115	-
22	CLA	1	606	-	1/1/9/20	4/8/82/115	-
21	CHL	4	607	-	3/3/15/26	0/10/106/137	-
21	CHL	2	618	2	3/3/15/26	4/12/110/137	-
22	CLA	L	303	-	1/1/14/20	16/31/109/115	-
25	BCR	B	848	-	-	3/29/63/63	0/2/2/2
29	PQN	B	842	-	-	9/23/43/43	0/2/2/2
21	CHL	2	606	-	3/3/15/26	0/10/108/137	-
24	XAT	2	620	-	-	3/31/93/93	0/4/4/4
22	CLA	A	812	-	1/1/15/20	14/37/115/115	-
22	CLA	B	835	-	1/1/10/20	4/10/88/115	-
22	CLA	1	613	-	1/1/15/20	12/37/115/115	-
26	LHG	1	620	22	-	23/53/53/53	-
21	CHL	Y	606	-	3/3/15/26	1/4/100/137	-
21	CHL	2	608	-	3/3/17/26	7/21/119/137	-
22	CLA	X	612	19	1/1/8/20	2/2/74/115	-
26	LHG	2	622	22	-	21/41/41/53	-
22	CLA	A	802	-	1/1/15/20	13/37/115/115	-
22	CLA	Y	612	20	1/1/10/20	0/4/80/115	-
31	LMU	A	857	-	-	8/16/56/61	0/2/2/2
22	CLA	3	602	3	1/1/14/20	10/31/109/115	-
23	LUT	1	617	-	-	4/29/67/67	0/2/2/2
30	SF4	C	101	-	-	-	0/6/5/5
22	CLA	B	802	-	1/1/15/20	18/37/115/115	-
22	CLA	A	805	-	1/1/12/20	7/22/100/115	-
22	CLA	B	804	-	1/1/10/20	2/8/86/115	-
22	CLA	B	814	-	1/1/15/20	7/37/115/115	-
22	CLA	N	1001	18	-	5/13/91/115	-
22	CLA	L	304	-	1/1/11/20	3/13/91/115	-
23	LUT	Y	4621	-	-	3/29/67/67	0/2/2/2
22	CLA	2	610	2	1/1/13/20	8/25/103/115	-
22	CLA	N	1002	-	1/1/12/20	9/19/97/115	-
22	CLA	1	611	26	1/1/10/20	1/4/80/115	-
22	CLA	F	301	-	1/1/13/20	11/28/106/115	-
22	CLA	A	810	5	1/1/12/20	8/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	823	-	1/1/11/20	4/13/91/115	-
22	CLA	B	829	-	1/1/13/20	10/27/105/115	-
21	CHL	X	608	-	3/3/14/26	1/4/102/137	-
21	CHL	X	609	19	3/3/13/26	0/2/94/137	-
22	CLA	3	603	3	1/1/13/20	8/25/103/115	-
22	CLA	B	807	6	-	4/22/100/115	-
22	CLA	1	612	1	1/1/11/20	3/13/91/115	-
22	CLA	B	827	-	1/1/15/20	20/37/115/115	-
33	NEX	Z	7623	-	-	2/27/83/83	0/3/3/3
22	CLA	1	614	-	1/1/10/20	0/4/80/115	-
22	CLA	1	602	1	1/1/14/20	5/33/111/115	-
23	LUT	1	621	-	-	2/29/67/67	0/2/2/2
30	SF4	C	102	-	-	-	0/6/5/5
22	CLA	A	829	-	1/1/15/20	13/37/115/115	-
22	CLA	B	837	-	1/1/15/20	8/37/115/115	-
22	CLA	B	839	-	1/1/15/20	13/37/115/115	-
23	LUT	4	619	-	-	2/29/67/67	0/2/2/2
21	CHL	Z	608	-	3/3/16/26	7/13/111/137	-
22	CLA	2	602	2	1/1/15/20	13/37/115/115	-
22	CLA	A	822	-	1/1/15/20	13/37/115/115	-
25	BCR	B	801	-	-	6/29/63/63	0/2/2/2
22	CLA	B	819	-	1/1/13/20	8/25/103/115	-
23	LUT	Z	7621	-	-	3/29/67/67	0/2/2/2
22	CLA	4	613	-	1/1/13/20	9/28/106/115	-
25	BCR	A	849	-	-	3/29/63/63	0/2/2/2
22	CLA	B	831	-	1/1/10/20	3/11/89/115	-
22	CLA	Z	610	19	1/1/8/20	0/0/74/115	-
22	CLA	A	823	-	1/1/10/20	6/10/88/115	-
22	CLA	Y	602	20	1/1/11/20	7/13/91/115	-
22	CLA	3	615	-	1/1/8/20	0/0/74/115	-
22	CLA	B	834	-	1/1/14/20	8/31/109/115	-
22	CLA	B	825	-	1/1/14/20	9/34/112/115	-
22	CLA	4	604	-	1/1/11/20	5/11/87/115	-
22	CLA	B	806	6	1/1/15/20	12/37/115/115	-
22	CLA	4	614	-	1/1/11/20	3/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	4	603	4	1/1/11/20	2/13/89/115	-
21	CHL	Z	601	19	3/3/15/26	4/10/108/137	-
21	CHL	Z	609	19	3/3/15/26	5/10/108/137	-
22	CLA	1	608	-	1/1/11/20	4/11/89/115	-
21	CHL	4	618	4	3/3/15/26	2/10/106/137	-
22	CLA	A	843	-	1/1/15/20	16/37/115/115	-
22	CLA	B	809	6	1/1/15/20	16/37/115/115	-
22	CLA	A	820	-	1/1/15/20	12/37/115/115	-
22	CLA	3	613	3	1/1/13/20	8/23/101/115	-
22	CLA	Z	614	-	1/1/11/20	5/11/89/115	-
25	BCR	K	202	-	-	6/29/63/63	0/2/2/2
22	CLA	4	612	4	1/1/10/20	2/8/86/115	-
25	BCR	2	621	-	-	4/29/63/63	0/2/2/2
25	BCR	3	620	-	-	5/29/63/63	0/2/2/2
22	CLA	B	805	-	1/1/15/20	15/37/115/115	-
22	CLA	3	604	-	1/1/11/20	0/9/85/115	-

The worst 5 of 1925 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Z	607	CHL	C4B-NB	29.20	1.61	1.35
22	2	611	CLA	C1A-NA	12.62	1.40	1.29
21	Z	607	CHL	C1B-NB	12.55	1.46	1.35
29	A	844	PQN	C12-C13	8.56	1.53	1.33
29	B	842	PQN	C12-C13	8.52	1.53	1.33

The worst 5 of 2886 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	X	7622	XAT	O24-C25-C24	10.93	121.59	113.38
22	B	808	CLA	C4A-NA-C1A	9.49	110.97	106.71
24	Z	4622	XAT	O24-C25-C24	9.46	120.49	113.38
33	Y	4623	NEX	O24-C25-C24	9.16	120.26	113.38
21	X	601	CHL	CMD-C2D-C1D	9.10	140.76	124.71

5 of 263 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	1	601	CHL	C8
21	1	601	CHL	NA
21	1	601	CHL	ND
21	1	601	CHL	NC
21	1	607	CHL	NA

5 of 1886 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	1	601	CHL	C1A-C2A-CAA-CBA
21	1	601	CHL	C3A-C2A-CAA-CBA
21	2	601	CHL	C1A-C2A-CAA-CBA
21	2	601	CHL	C1C-C2C-CMC-OMC
21	2	601	CHL	C3C-C2C-CMC-OMC

There are no ring outliers.

206 monomers are involved in 430 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	806	CLA	3	0
22	B	810	CLA	2	0
28	A	801	CL0	25	0
22	3	614	CLA	1	0
26	X	2630	LHG	1	0
22	A	814	CLA	3	0
21	Y	609	CHL	1	0
24	X	7622	XAT	3	0
22	A	827	CLA	1	0
22	B	821	CLA	1	0
25	B	846	BCR	2	0
22	B	816	CLA	2	0
22	A	830	CLA	4	0
22	3	609	CLA	4	0
27	G	202	LMG	1	0
22	A	839	CLA	4	0
22	A	815	CLA	1	0
22	A	833	CLA	1	0
23	X	2620	LUT	2	0
22	H	201	CLA	5	0
22	G	201	CLA	1	0
22	A	811	CLA	3	0
22	A	834	CLA	1	0
22	B	818	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	842	CLA	6	0
22	B	838	CLA	1	0
22	B	826	CLA	4	0
23	3	618	LUT	3	0
25	B	844	BCR	1	0
27	1	622	LMG	2	0
22	A	807	CLA	1	0
22	A	838	CLA	1	0
22	K	204	CLA	2	0
22	2	609	CLA	1	0
22	4	609	CLA	3	0
25	A	848	BCR	6	0
21	2	601	CHL	3	0
22	A	808	CLA	1	0
27	2	623	LMG	1	0
22	Z	611	CLA	1	0
25	A	852	BCR	5	0
22	B	803	CLA	2	0
22	X	610	CLA	2	0
22	4	611	CLA	2	0
32	J	103	DGD	2	0
25	G	205	BCR	2	0
22	1	603	CLA	3	0
22	4	602	CLA	4	0
22	4	610	CLA	2	0
22	3	612	CLA	1	0
25	K	205	BCR	2	0
33	Y	4623	NEX	2	0
22	X	602	CLA	4	0
21	X	601	CHL	2	0
22	Y	604	CLA	2	0
25	B	843	BCR	2	0
22	Z	602	CLA	2	0
26	A	847	LHG	2	0
22	3	610	CLA	2	0
25	B	847	BCR	6	0
22	A	824	CLA	1	0
22	G	204	CLA	1	0
22	F	303	CLA	1	0
25	A	850	BCR	2	0
22	2	612	CLA	1	0
27	4	622	LMG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	840	CLA	3	0
22	2	611	CLA	2	0
22	L	302	CLA	3	0
22	A	803	CLA	6	0
22	B	840	CLA	3	0
25	A	851	BCR	2	0
22	B	813	CLA	3	0
23	X	2621	LUT	3	0
25	L	306	BCR	2	0
33	X	2623	NEX	3	0
25	I	101	BCR	3	0
22	A	835	CLA	2	0
25	F	305	BCR	2	0
25	L	305	BCR	6	0
26	Y	4630	LHG	3	0
21	3	608	CHL	1	0
22	O	2001	CLA	1	0
21	1	601	CHL	4	0
22	A	825	CLA	3	0
22	A	837	CLA	1	0
22	1	610	CLA	2	0
22	G	203	CLA	2	0
22	Z	612	CLA	1	0
22	Z	613	CLA	1	0
22	A	831	CLA	6	0
27	4	623	LMG	1	0
26	B	851	LHG	1	0
30	C	102	SF4	1	0
25	B	845	BCR	5	0
22	A	819	CLA	1	0
32	B	850	DGD	8	0
23	2	619	LUT	9	0
24	4	620	XAT	5	0
22	4	617	CLA	3	0
22	B	830	CLA	2	0
21	Y	601	CHL	1	0
23	Z	7620	LUT	4	0
22	4	601	CLA	1	0
22	A	826	CLA	2	0
22	F	304	CLA	1	0
21	X	606	CHL	1	0
22	B	815	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	K	206	CLA	1	0
24	Y	2622	XAT	2	0
22	A	817	CLA	1	0
22	X	603	CLA	1	0
22	A	828	CLA	4	0
22	B	811	CLA	2	0
22	B	817	CLA	3	0
22	1	609	CLA	2	0
26	Z	7630	LHG	1	0
22	A	832	CLA	1	0
22	A	854	CLA	8	0
25	4	621	BCR	1	0
31	B	849	LMU	5	0
22	B	832	CLA	6	0
26	A	846	LHG	3	0
22	Y	613	CLA	1	0
29	A	844	PQN	6	0
24	Z	4622	XAT	1	0
22	A	809	CLA	4	0
22	K	201	CLA	1	0
23	Y	4620	LUT	3	0
22	B	824	CLA	2	0
22	3	606	CLA	1	0
22	B	833	CLA	1	0
24	3	619	XAT	4	0
22	A	841	CLA	5	0
22	B	828	CLA	4	0
21	X	605	CHL	1	0
25	J	102	BCR	1	0
22	B	841	CLA	4	0
25	A	856	BCR	5	0
22	A	818	CLA	1	0
21	2	618	CHL	1	0
22	L	303	CLA	1	0
25	B	848	BCR	3	0
29	B	842	PQN	7	0
21	2	606	CHL	2	0
24	2	620	XAT	4	0
22	A	812	CLA	4	0
22	B	835	CLA	3	0
22	1	613	CLA	2	0
26	1	620	LHG	6	0

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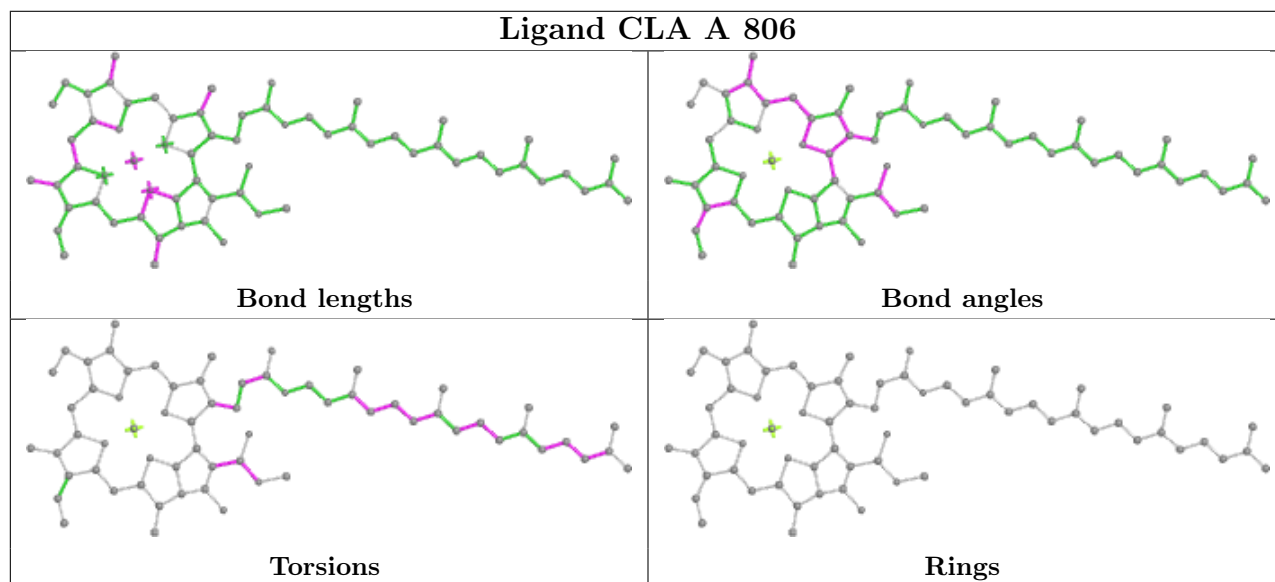
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	Y	606	CHL	1	0
21	2	608	CHL	2	0
22	X	612	CLA	1	0
26	2	622	LHG	3	0
22	A	802	CLA	3	0
22	Y	612	CLA	1	0
31	A	857	LMU	4	0
22	3	602	CLA	2	0
23	1	617	LUT	6	0
22	B	802	CLA	4	0
22	B	814	CLA	1	0
22	N	1001	CLA	1	0
22	L	304	CLA	3	0
23	Y	4621	LUT	2	0
22	2	610	CLA	3	0
22	N	1002	CLA	2	0
22	F	301	CLA	2	0
22	A	810	CLA	2	0
22	B	823	CLA	2	0
22	B	829	CLA	3	0
21	X	609	CHL	1	0
22	B	807	CLA	1	0
22	1	612	CLA	1	0
22	B	827	CLA	5	0
33	Z	7623	NEX	2	0
22	1	614	CLA	1	0
22	1	602	CLA	6	0
23	1	621	LUT	1	0
22	A	829	CLA	7	0
22	B	837	CLA	4	0
22	B	839	CLA	2	0
23	4	619	LUT	4	0
22	A	822	CLA	5	0
25	B	801	BCR	3	0
22	B	819	CLA	1	0
23	Z	7621	LUT	2	0
25	A	849	BCR	7	0
22	B	831	CLA	1	0
22	Z	610	CLA	2	0
22	A	823	CLA	1	0
22	Y	602	CLA	2	0
22	B	834	CLA	1	0

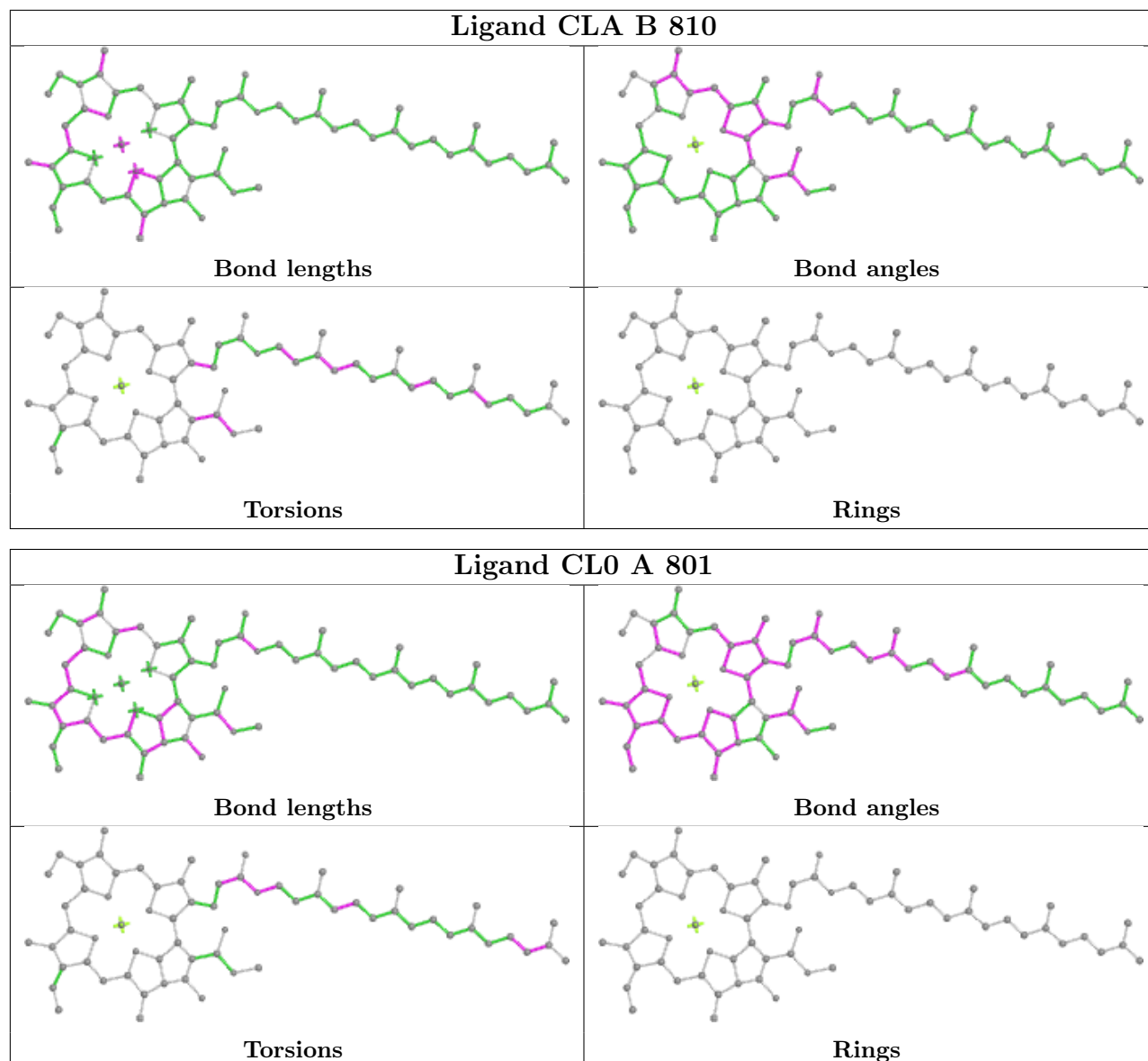
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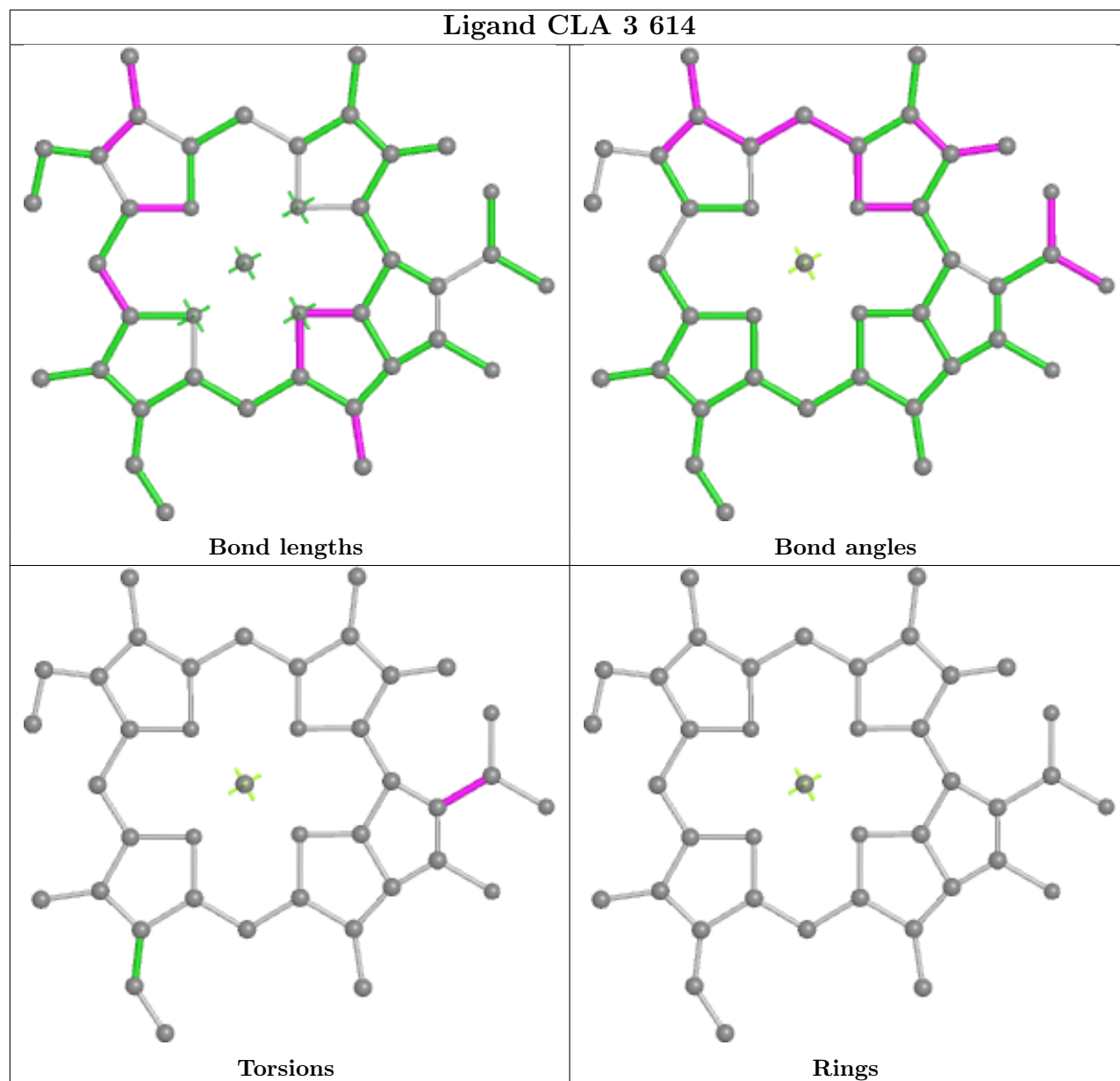
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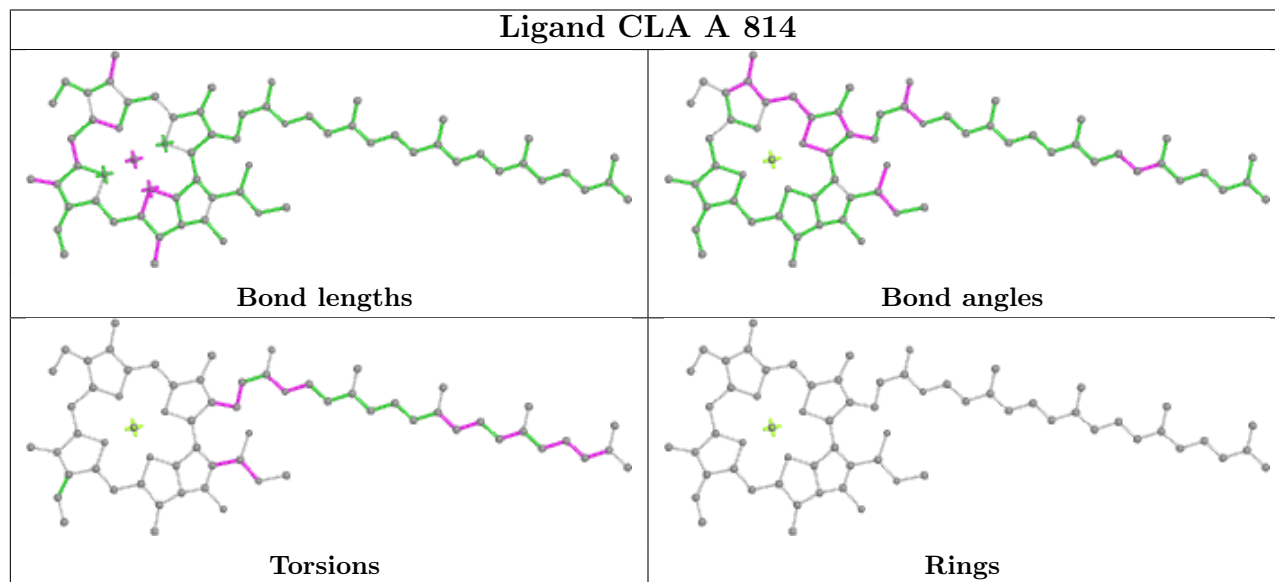
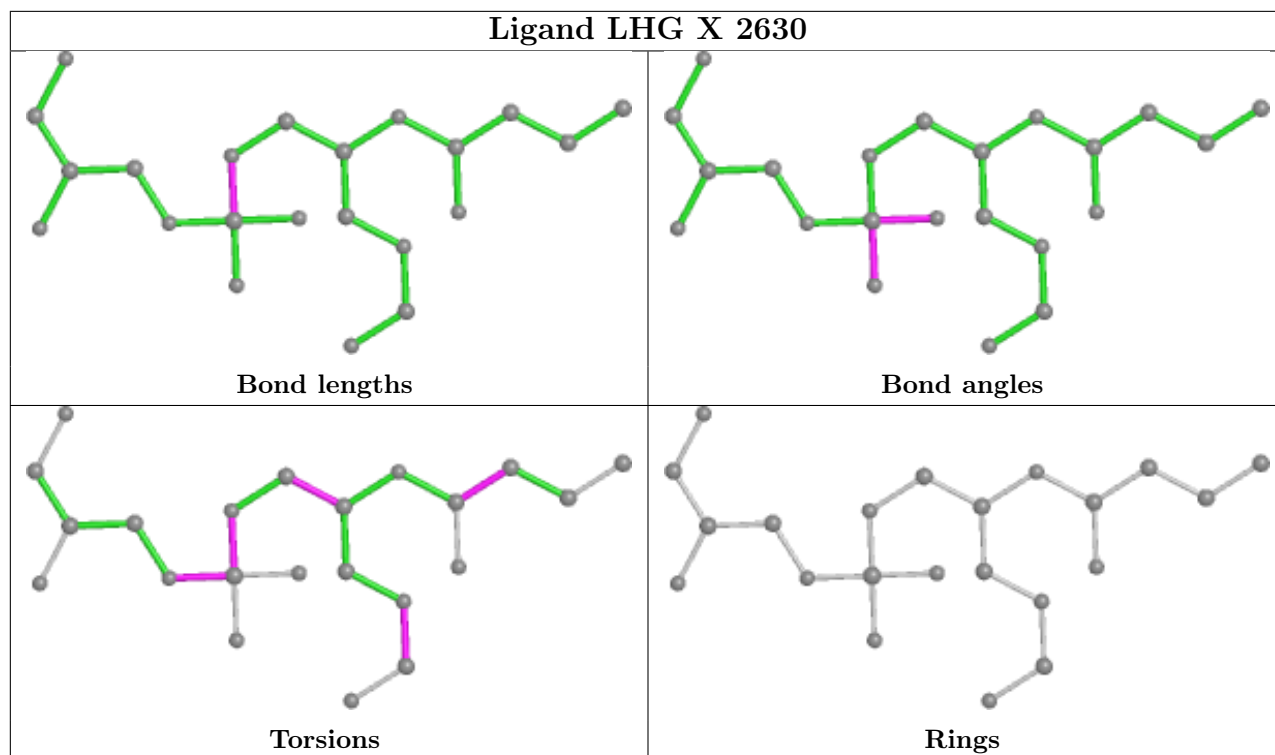
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	825	CLA	3	0
22	B	806	CLA	1	0
22	1	608	CLA	1	0
21	4	618	CHL	1	0
22	A	843	CLA	2	0
22	B	809	CLA	4	0
22	A	820	CLA	5	0
22	3	613	CLA	1	0
22	Z	614	CLA	1	0
25	K	202	BCR	5	0
22	4	612	CLA	2	0
25	2	621	BCR	4	0
25	3	620	BCR	3	0
22	B	805	CLA	2	0

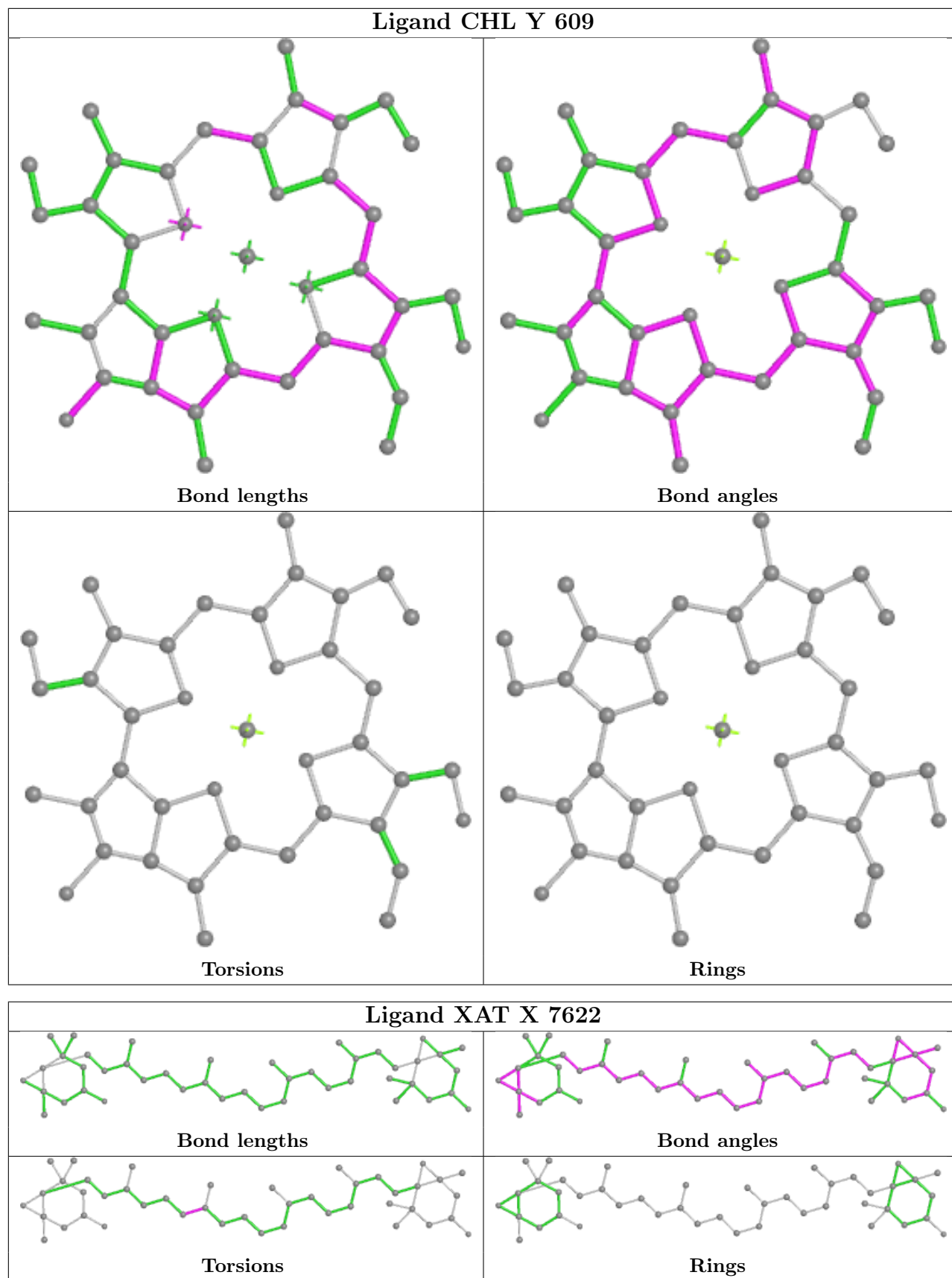
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

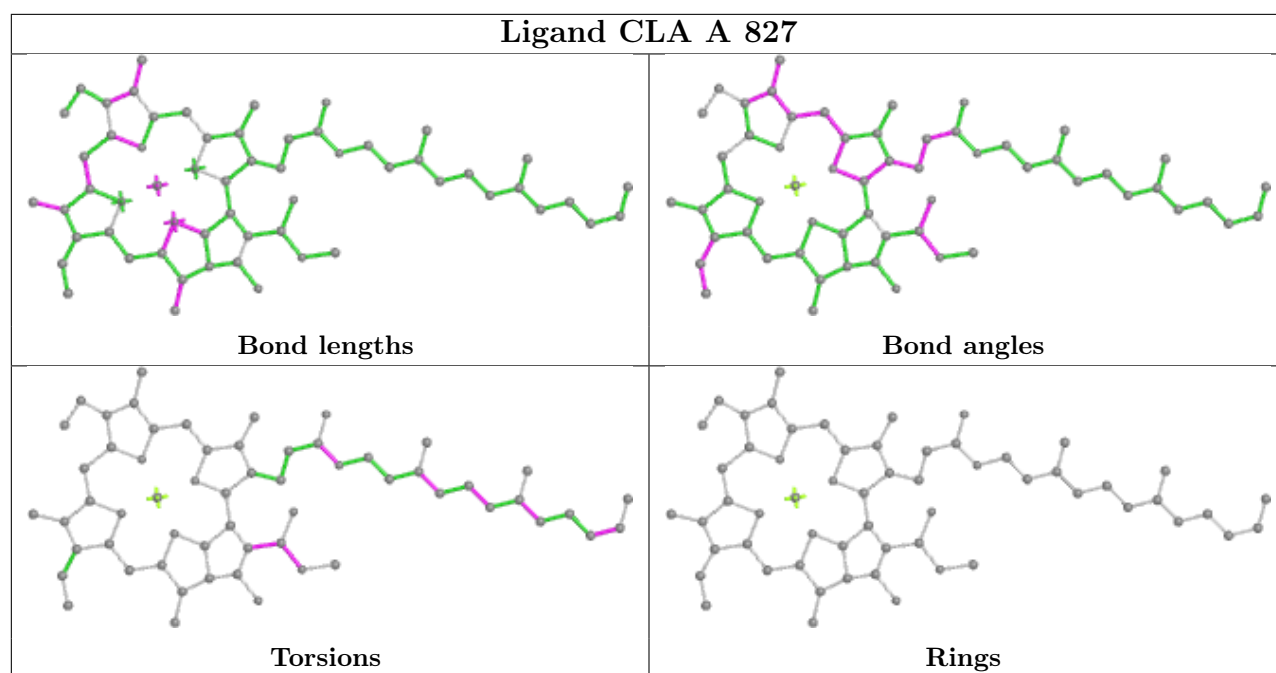


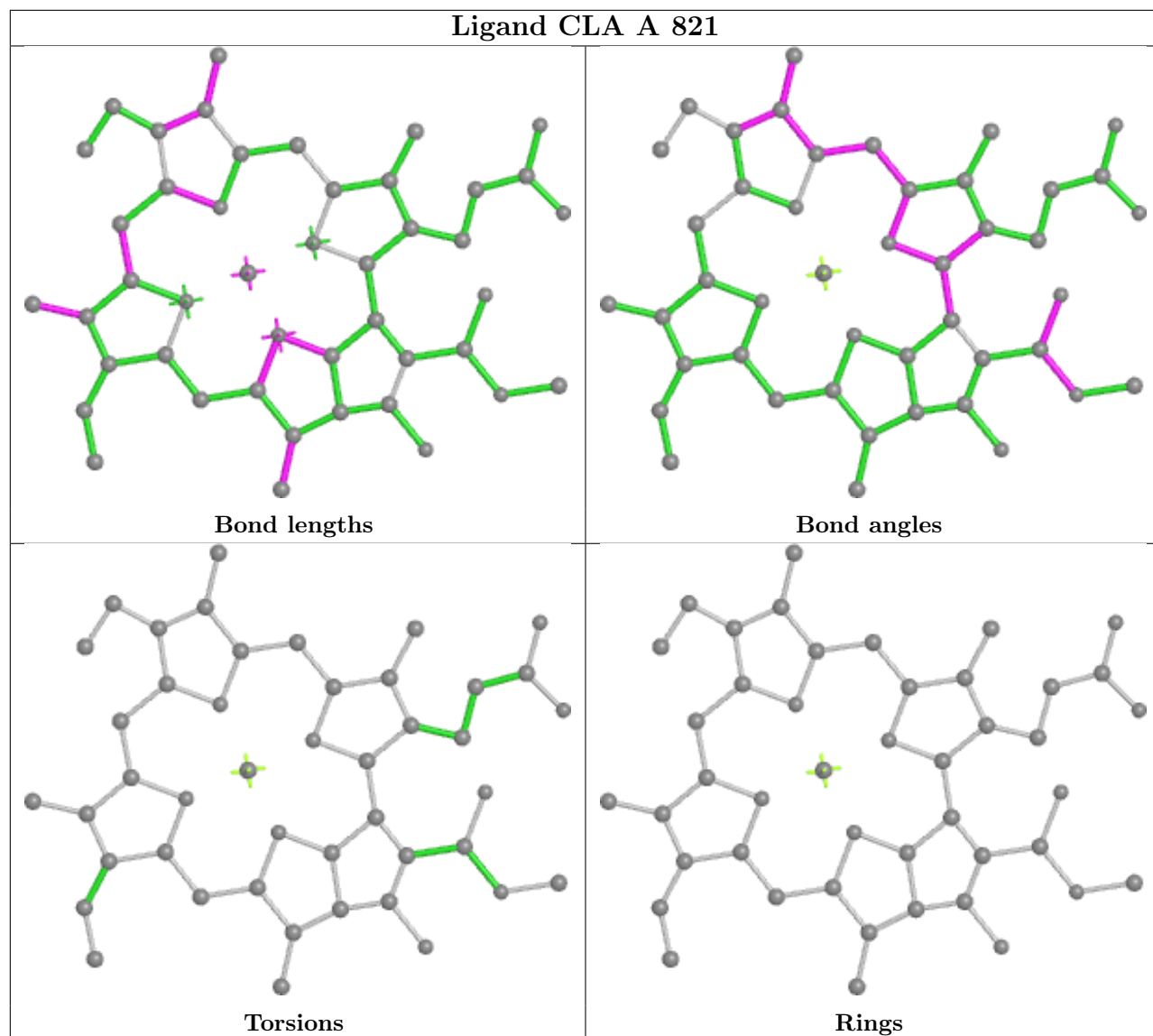


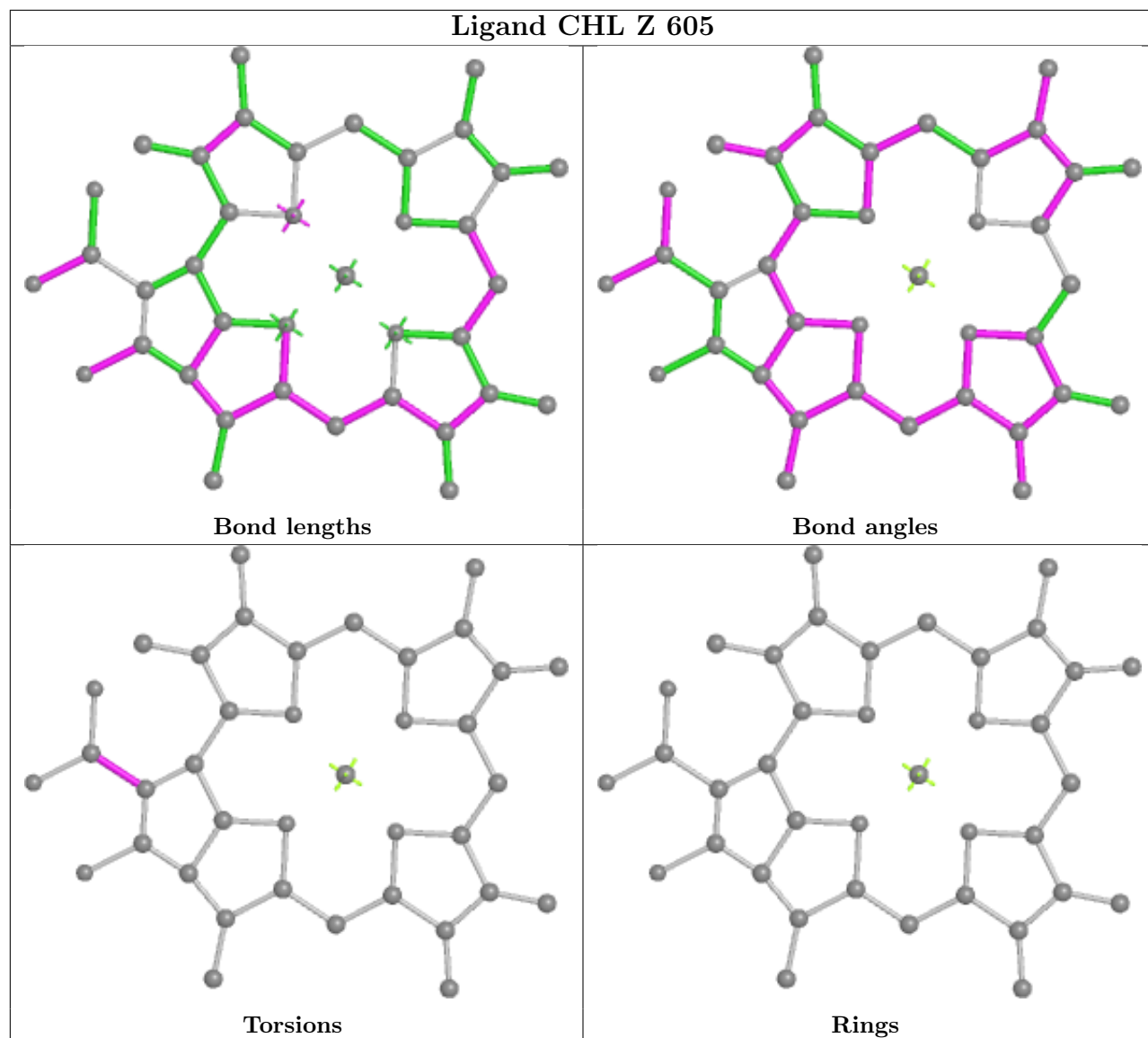


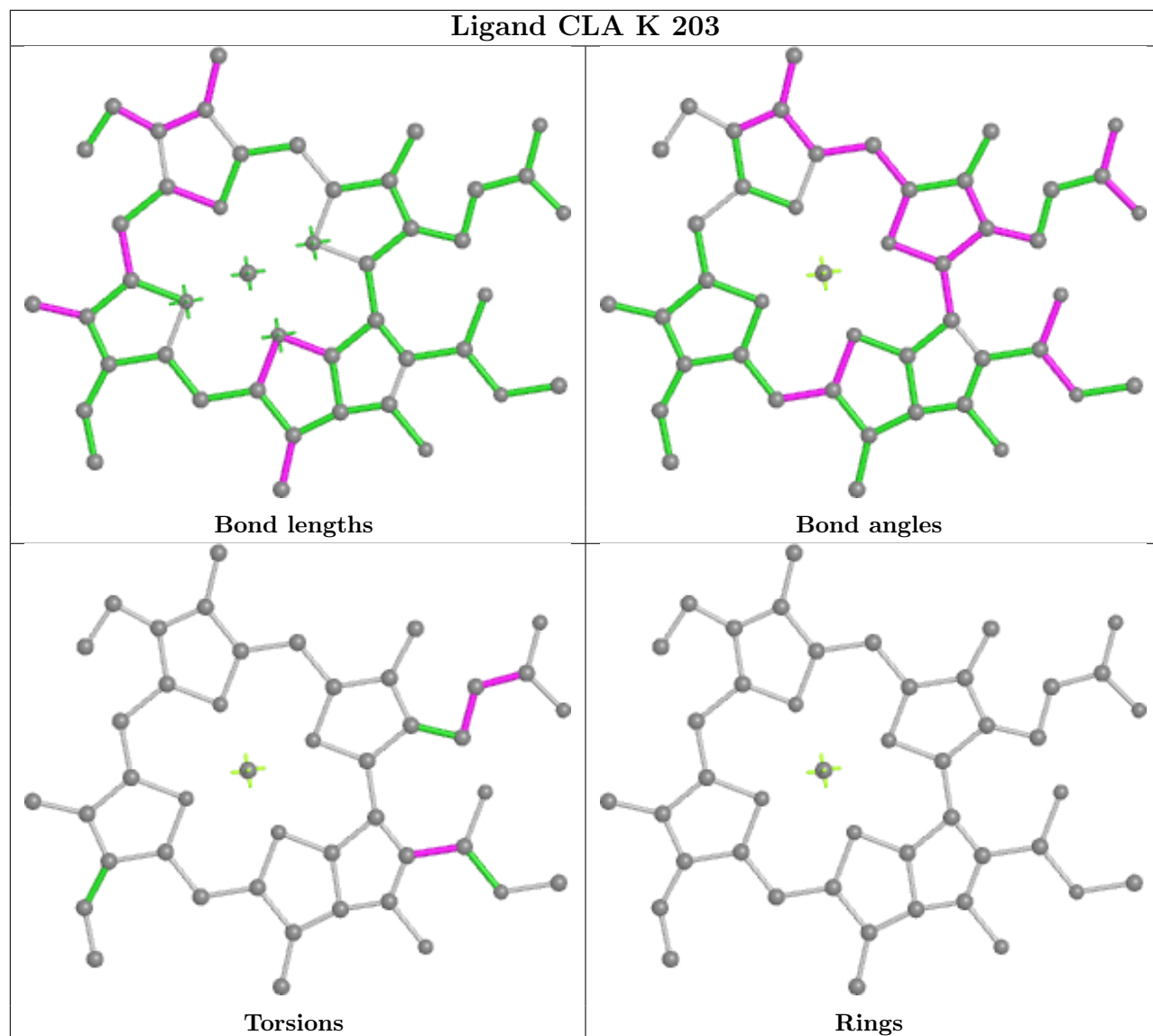


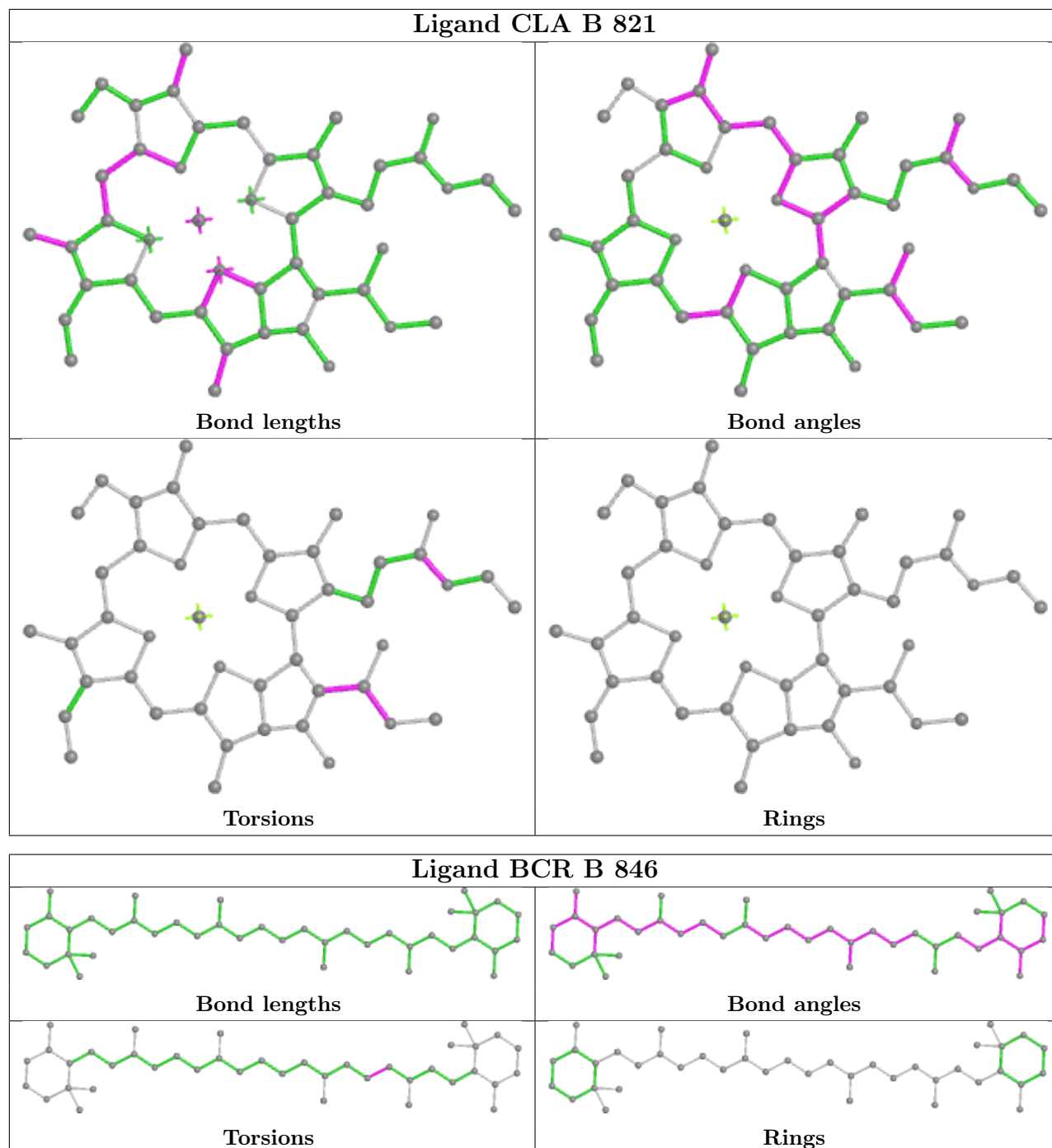


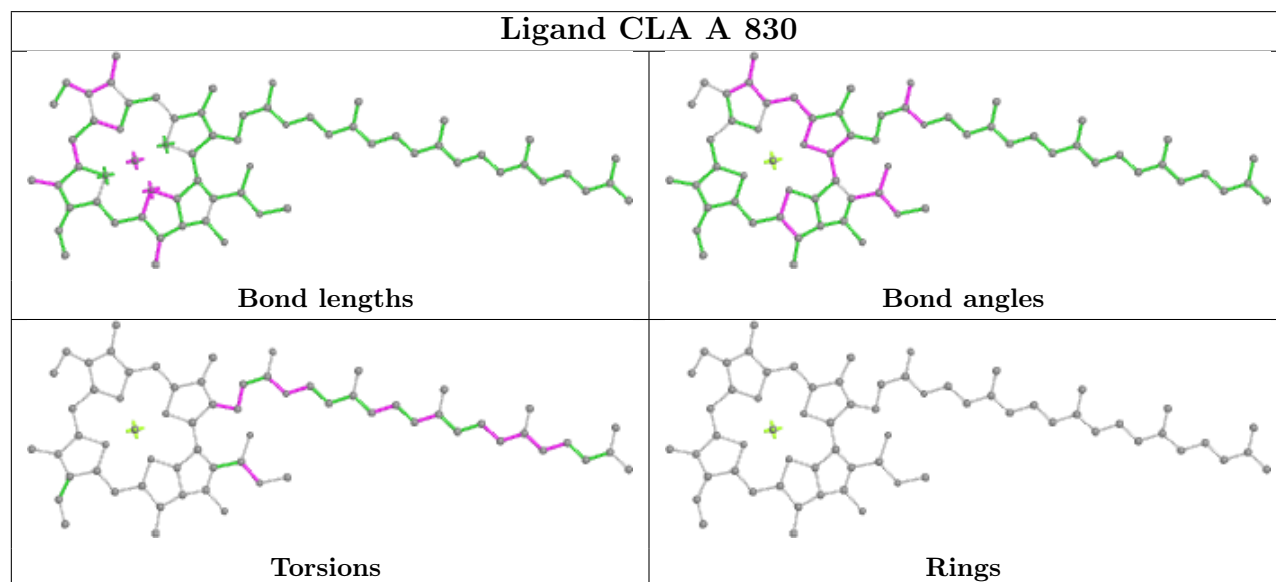
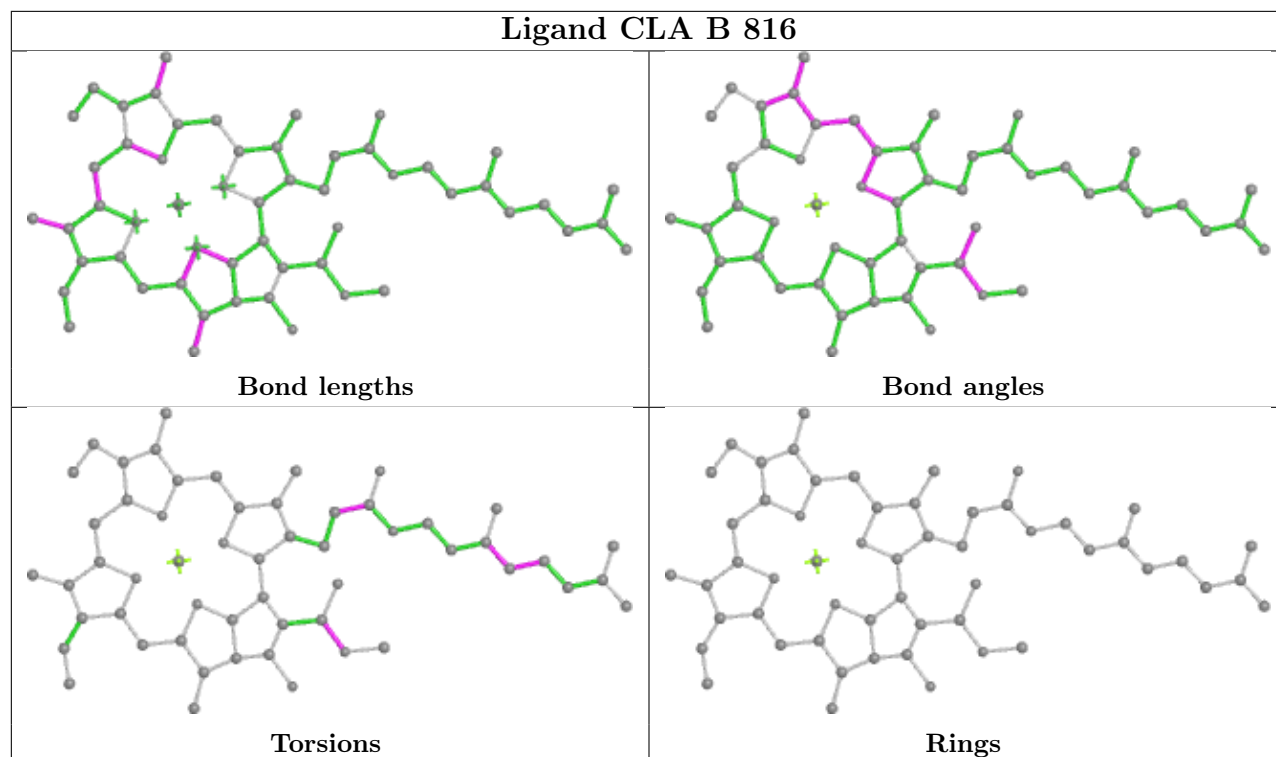


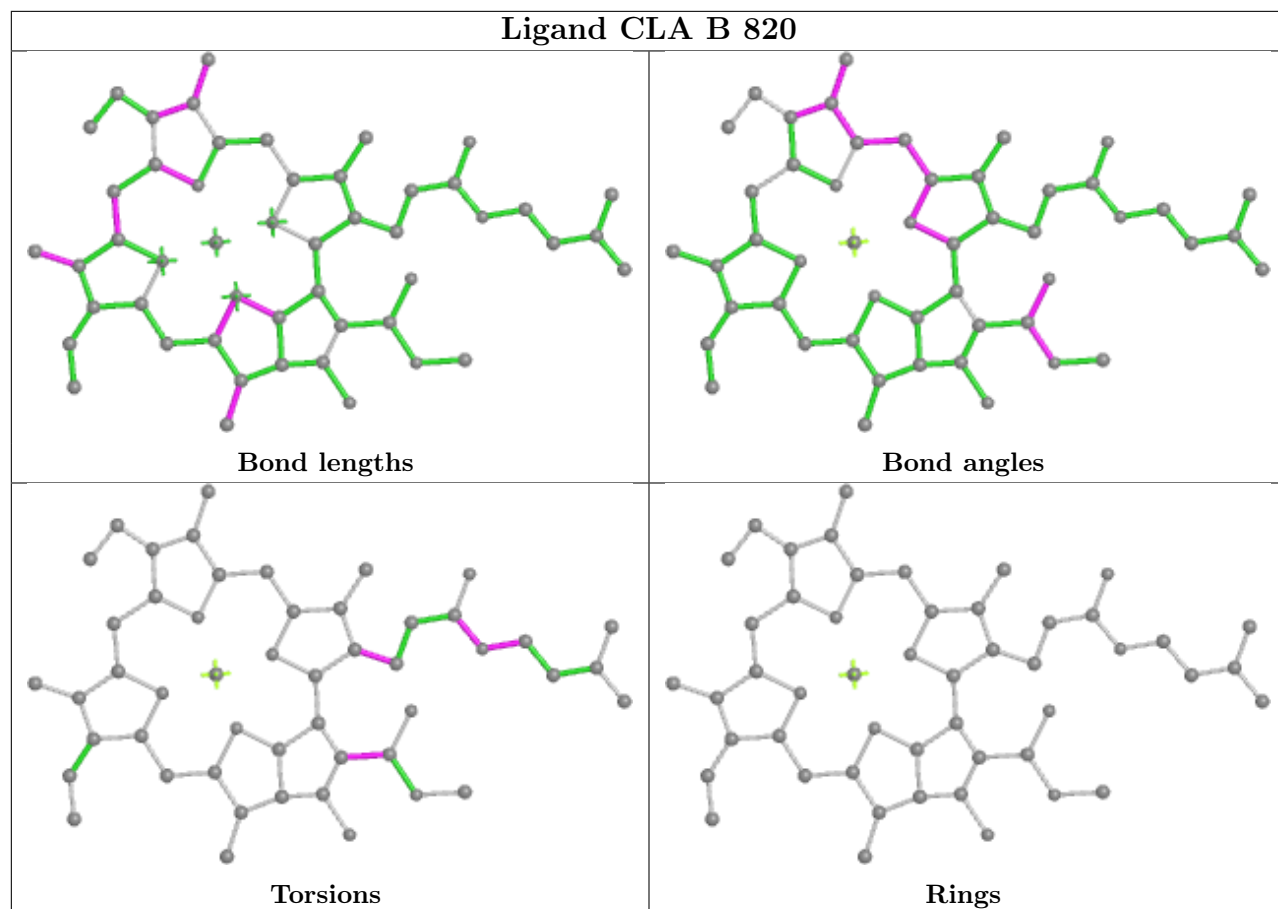


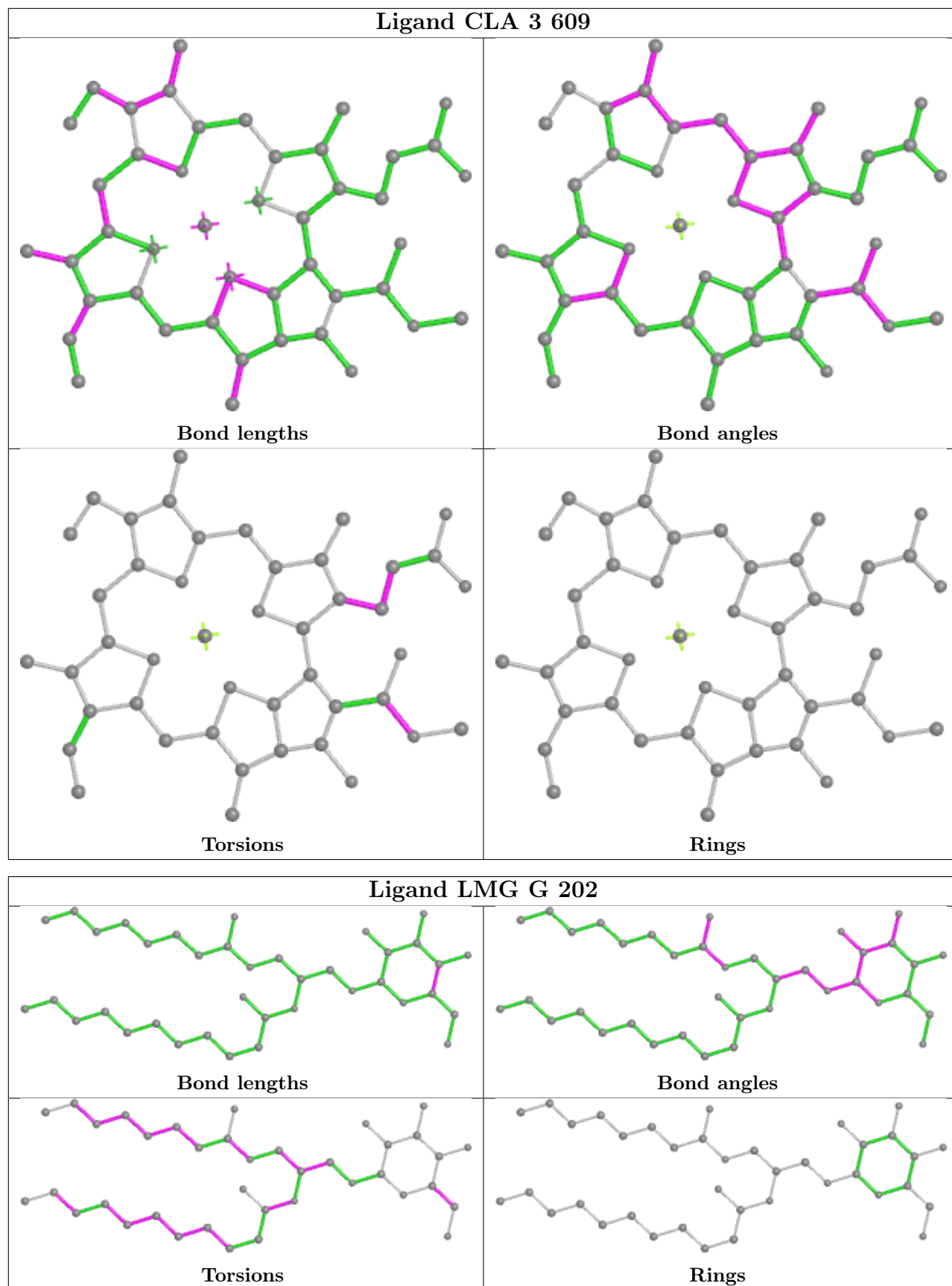


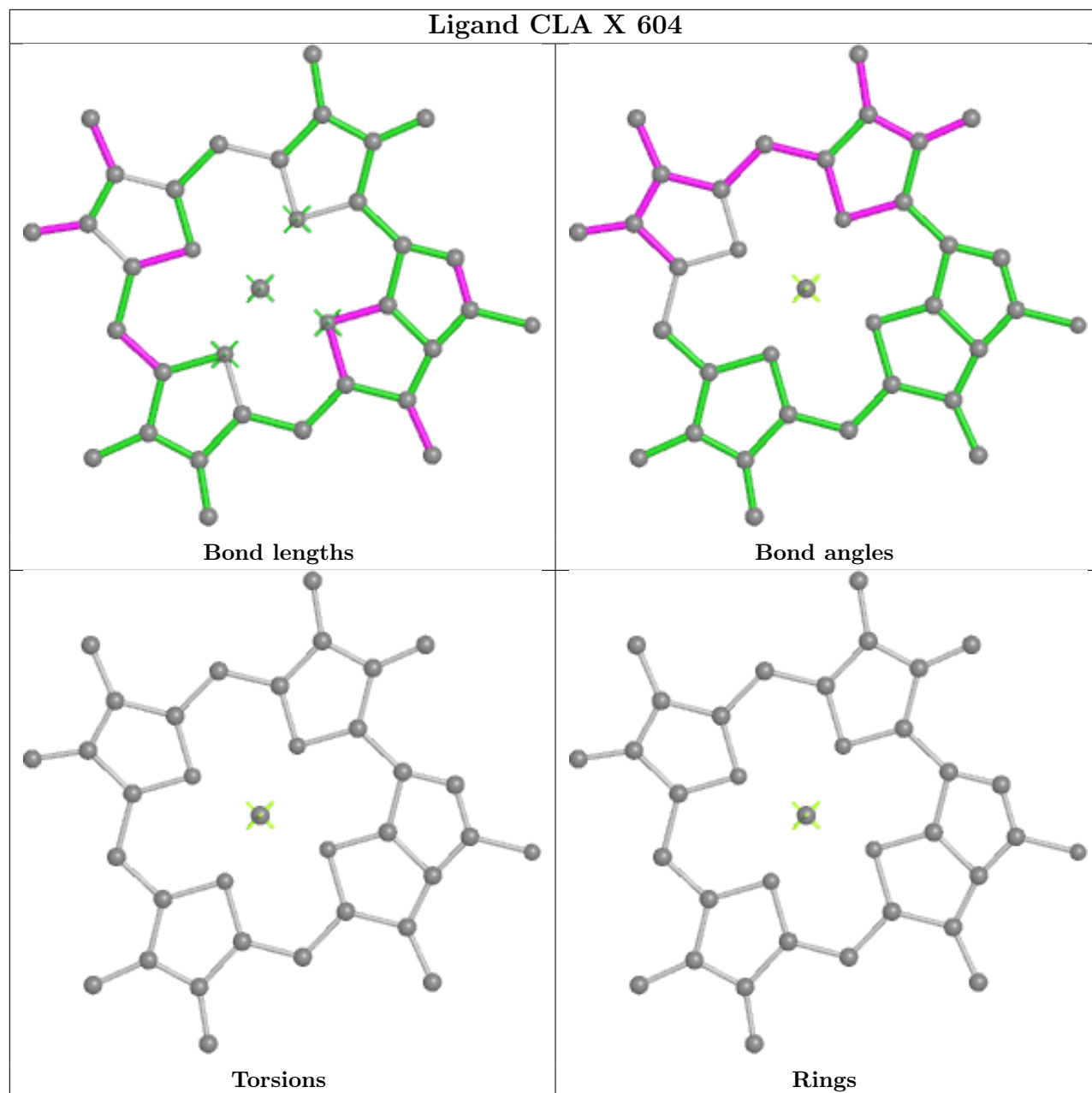


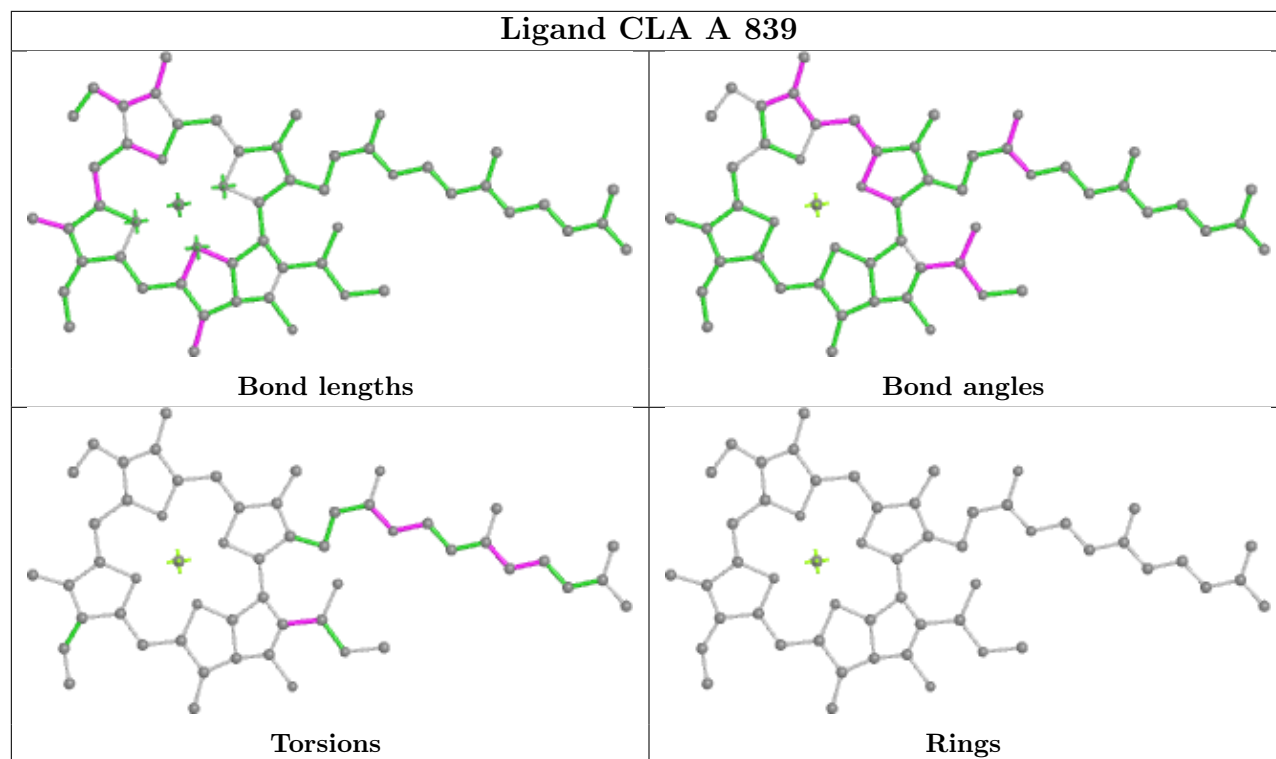


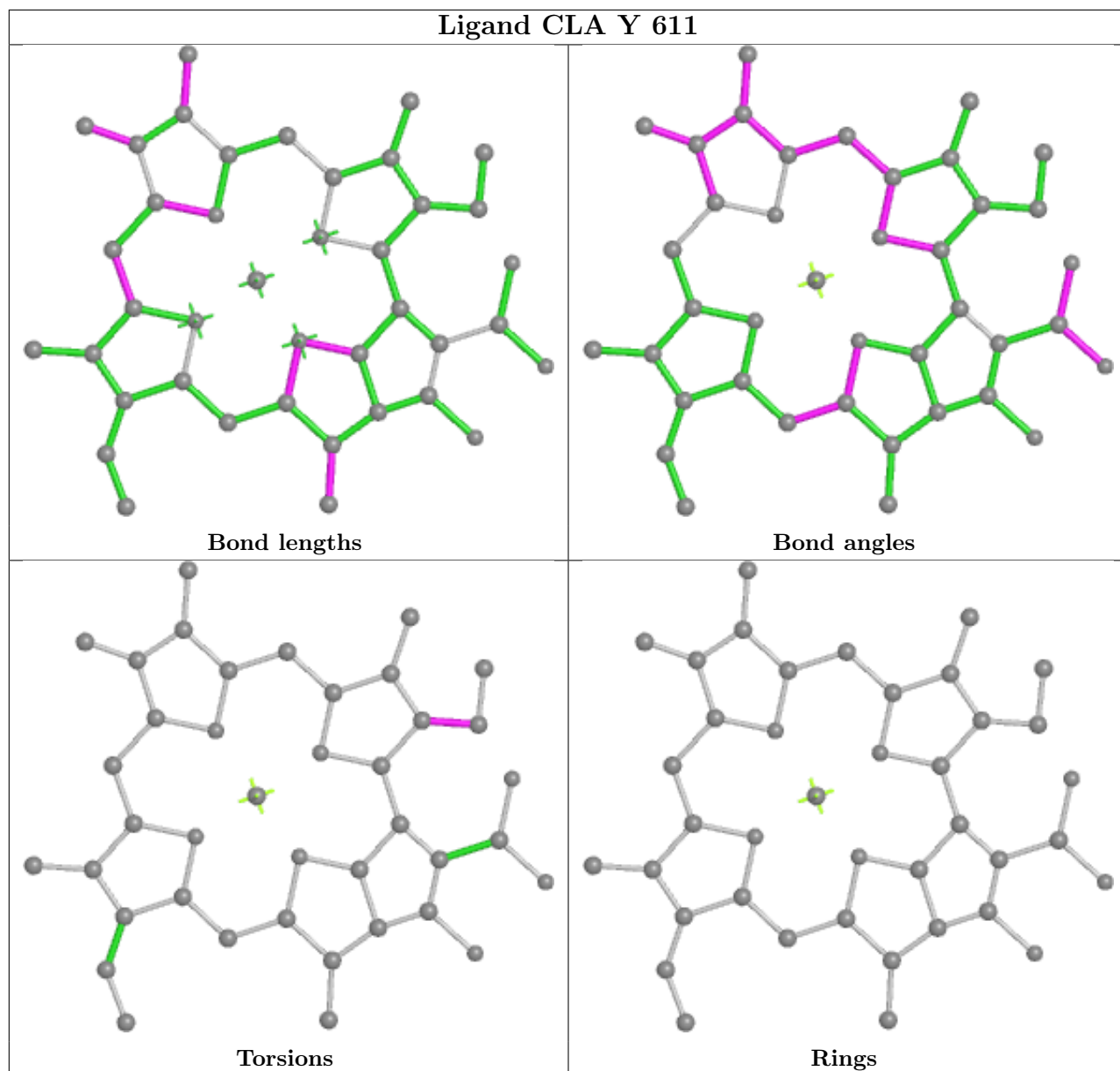


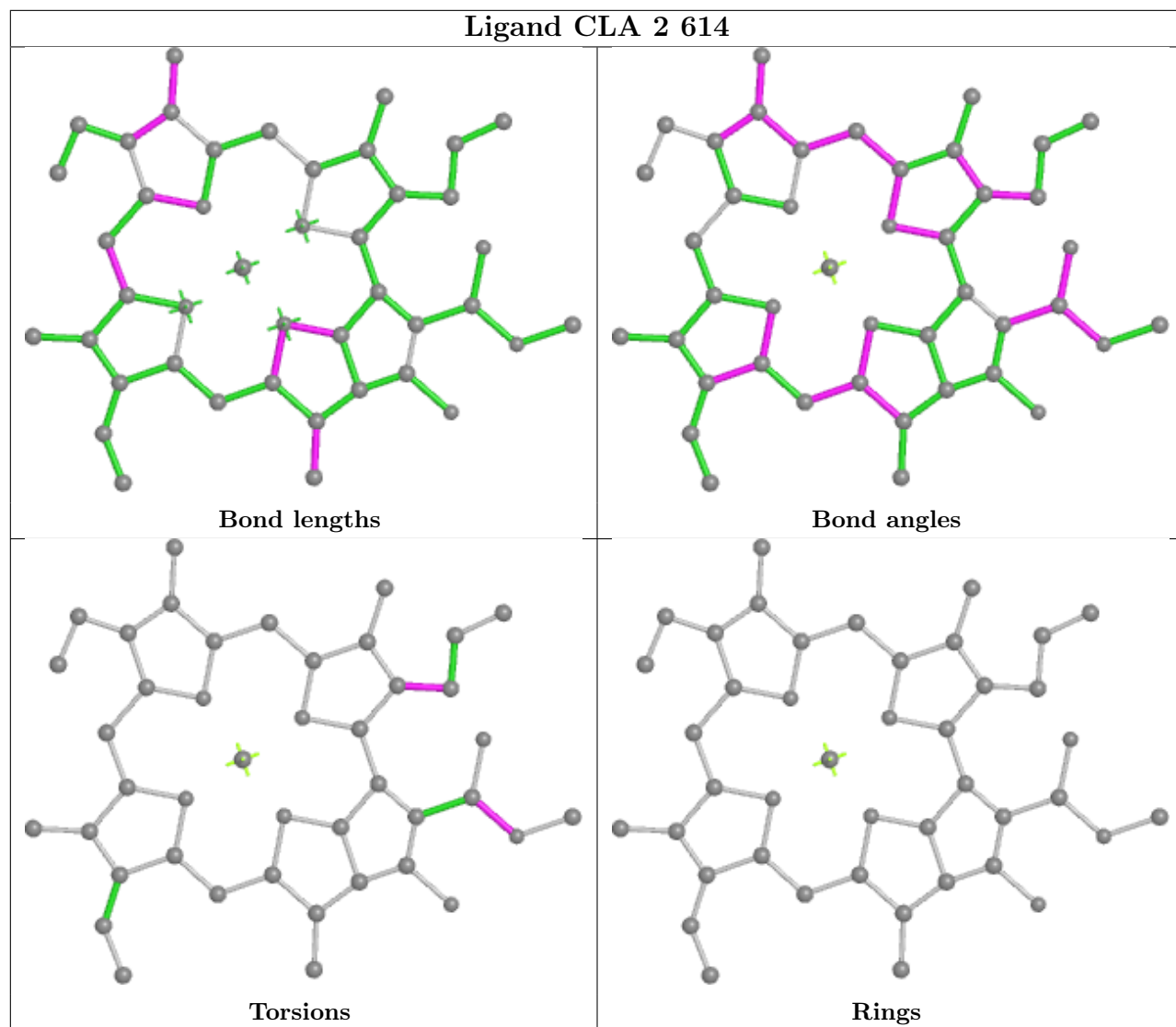


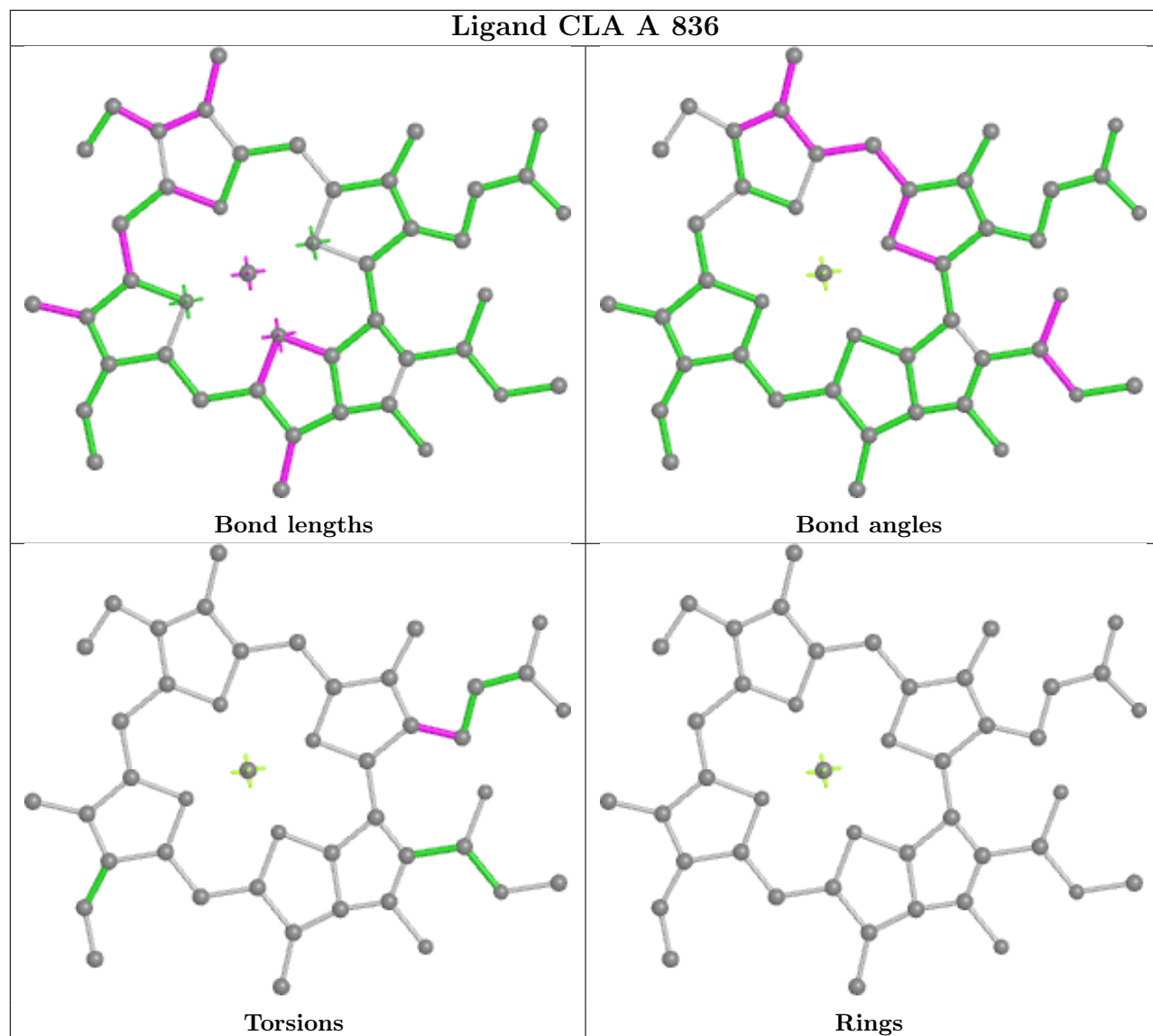


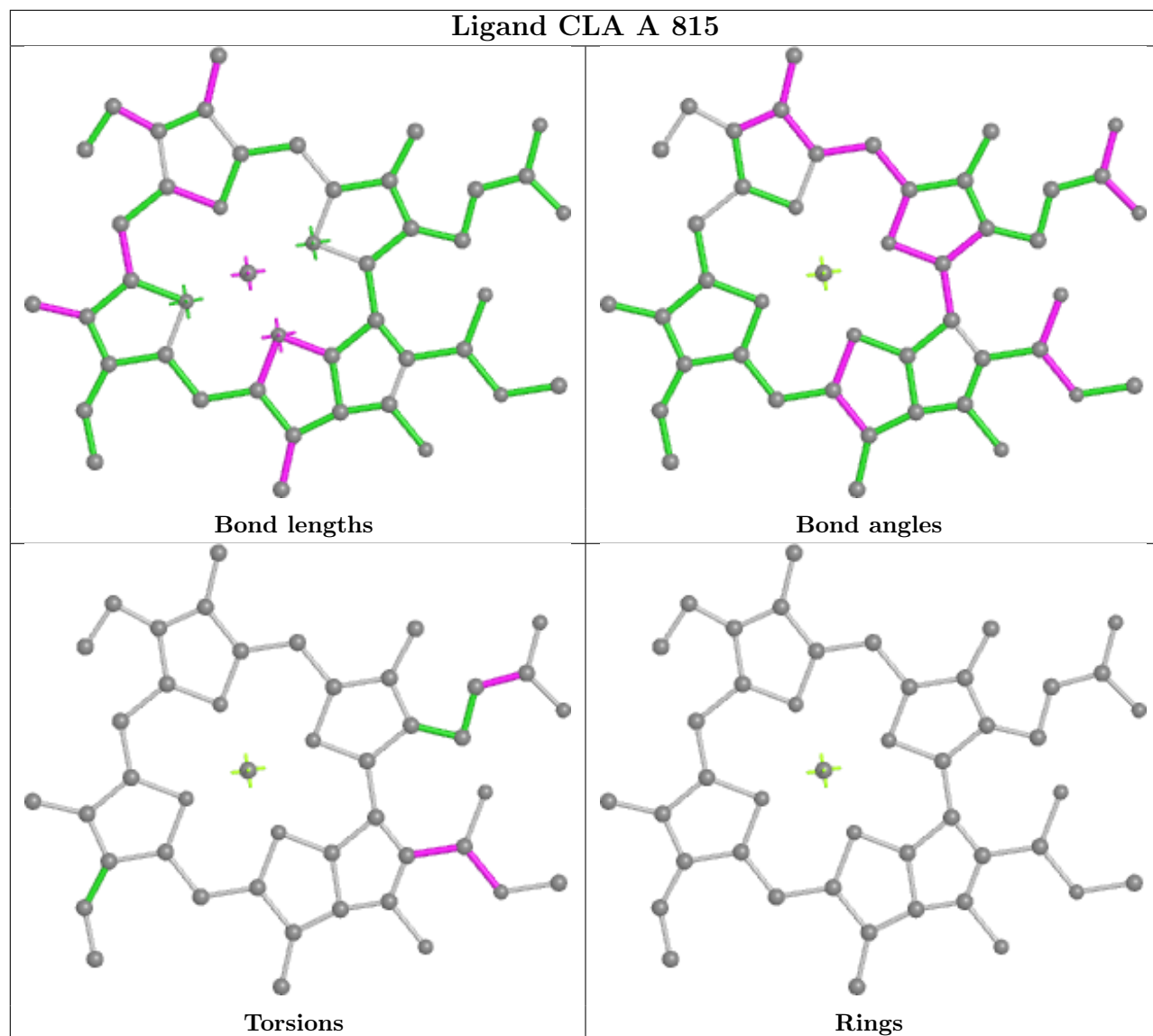


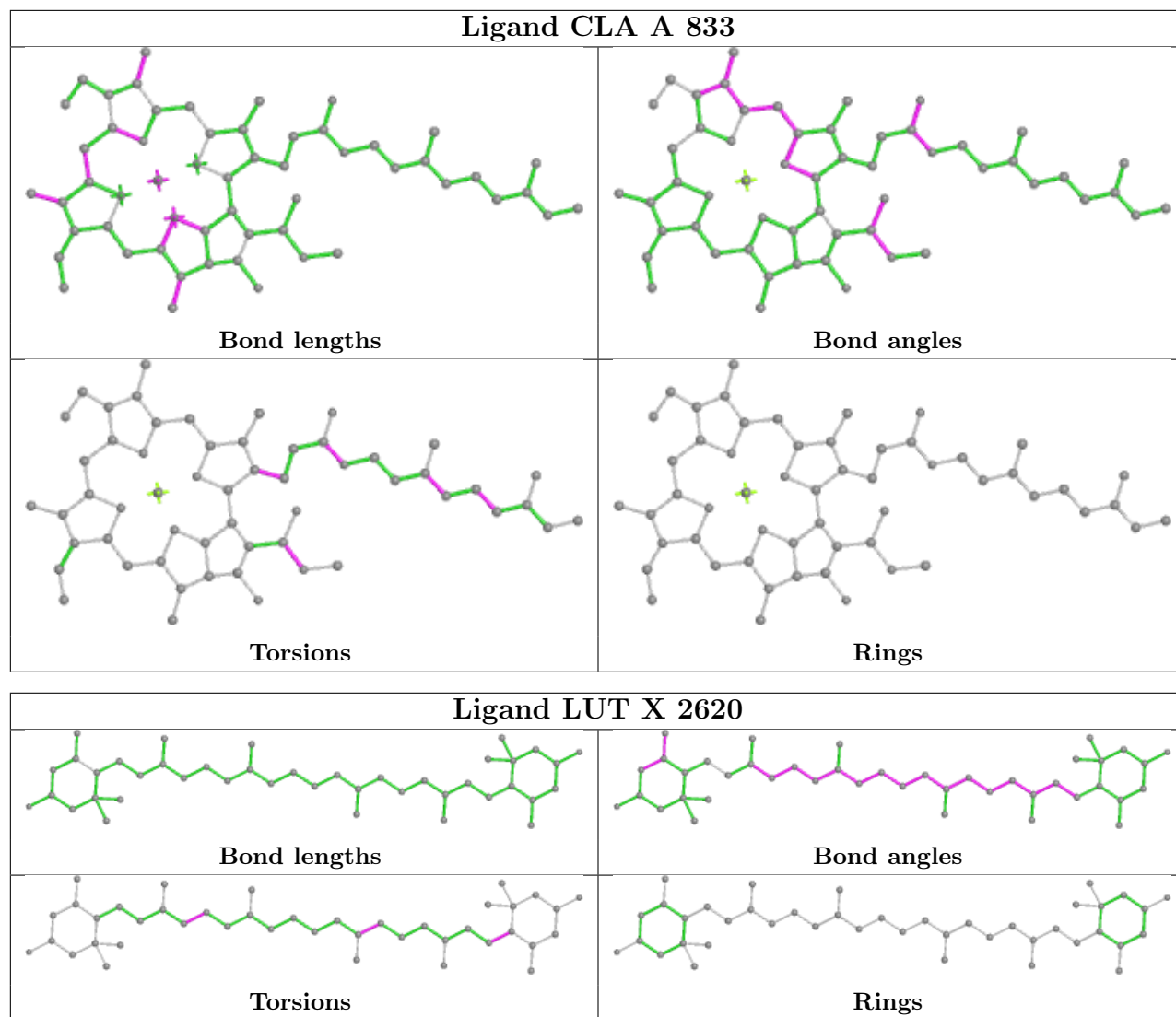


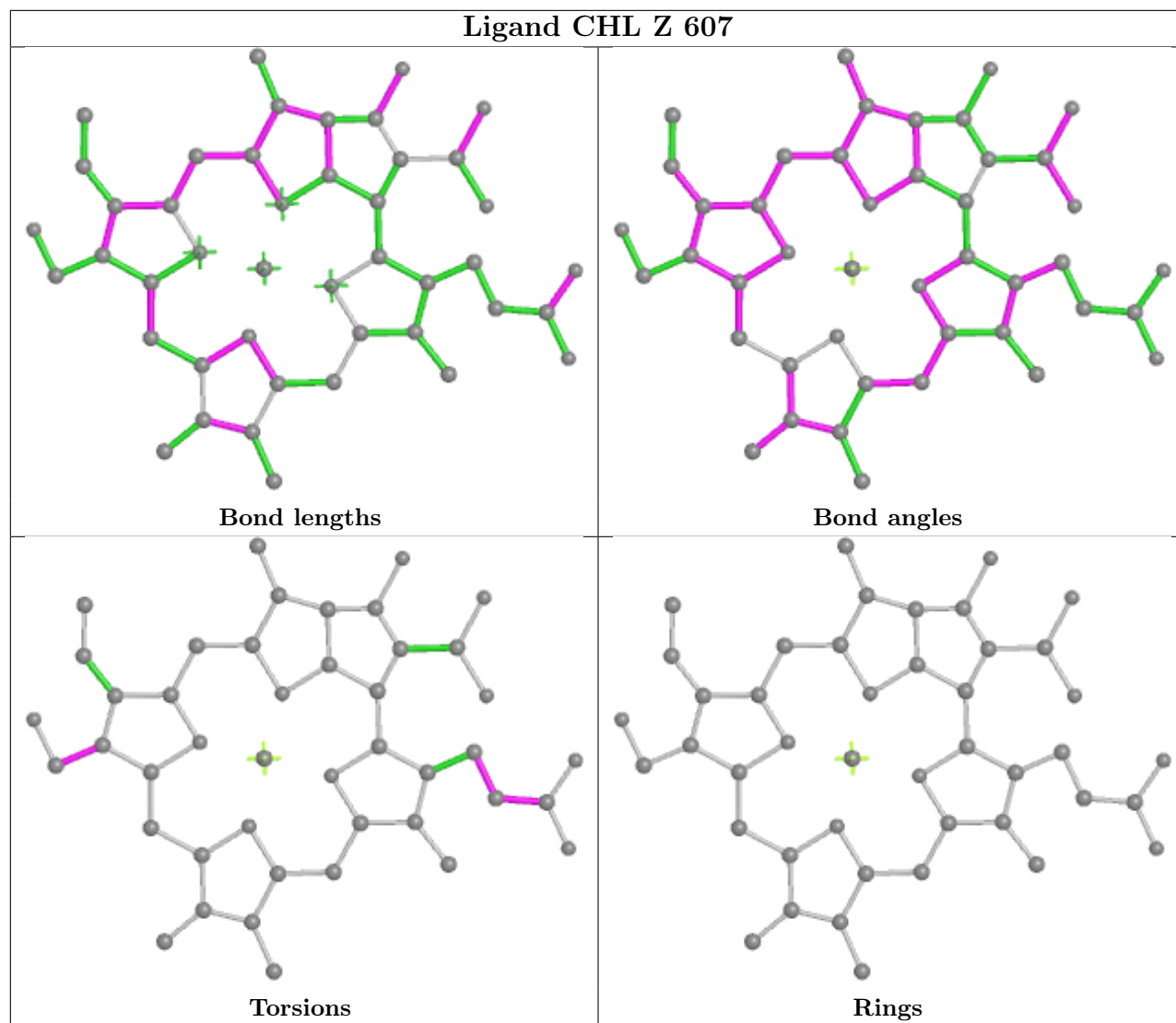


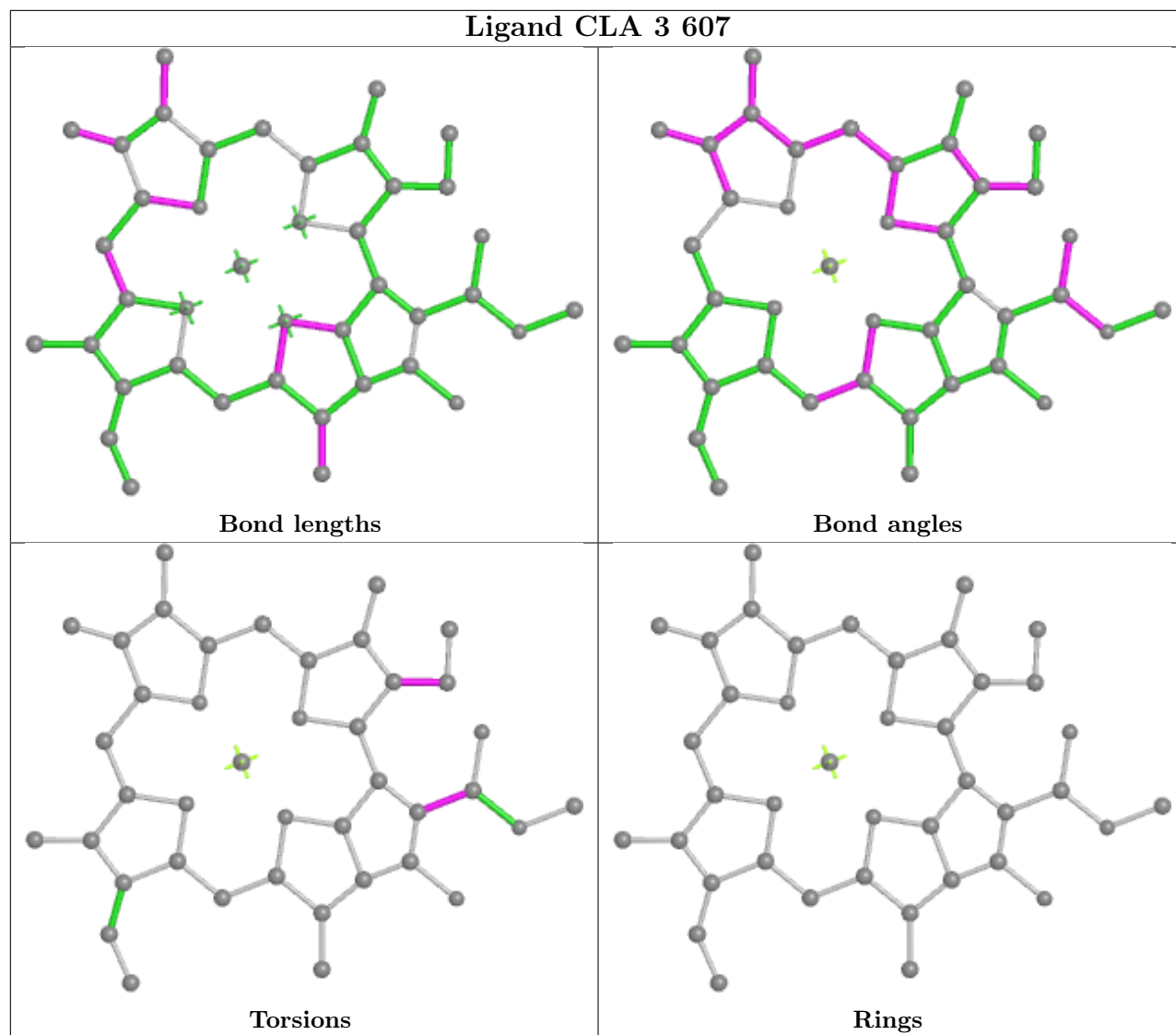


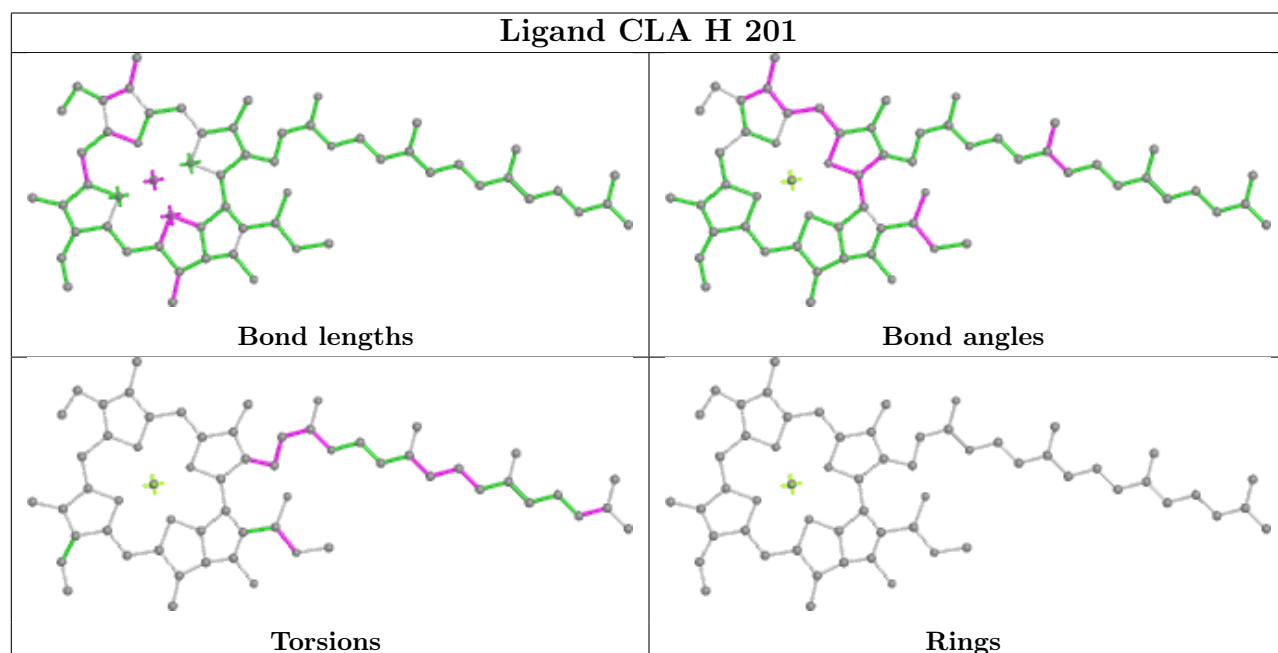
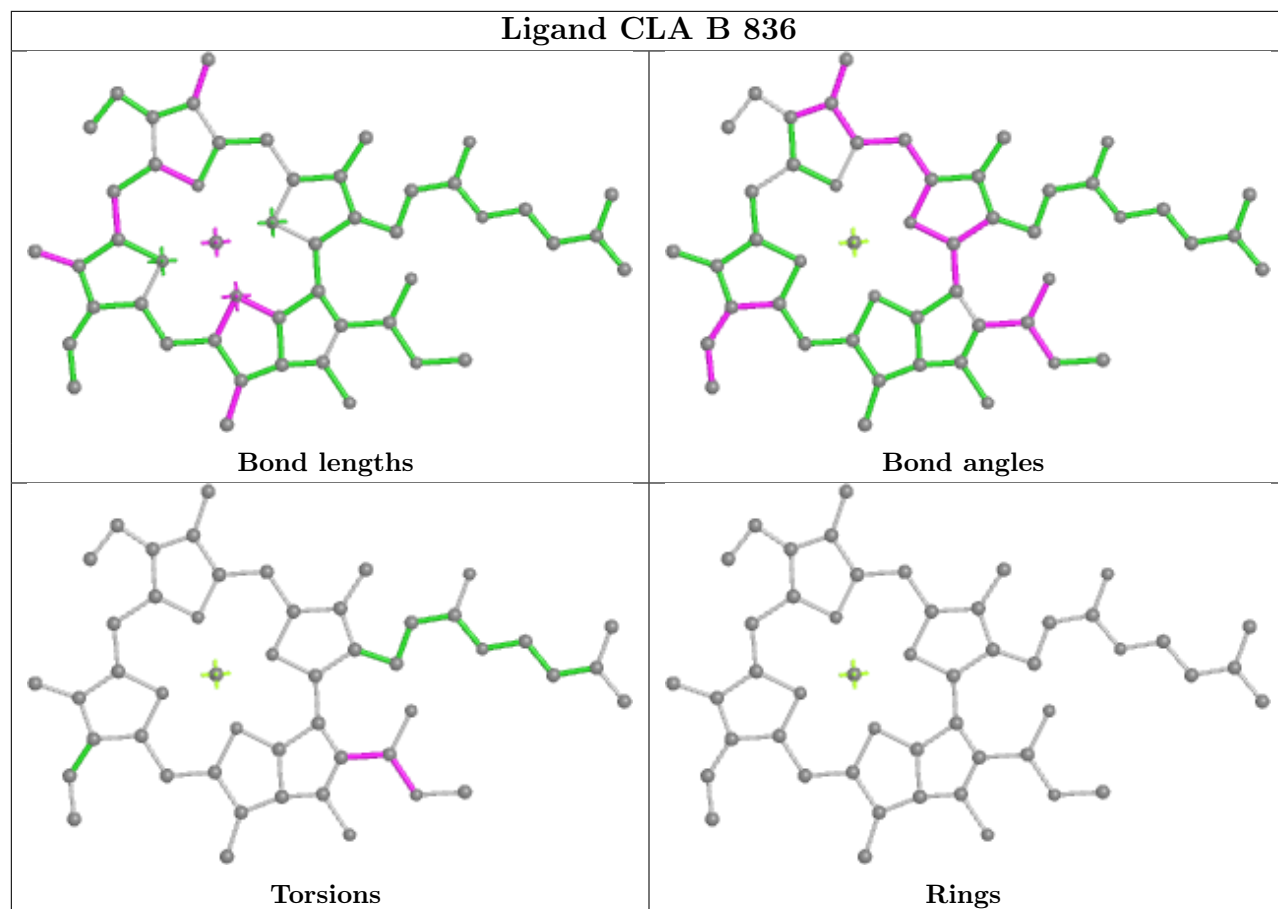


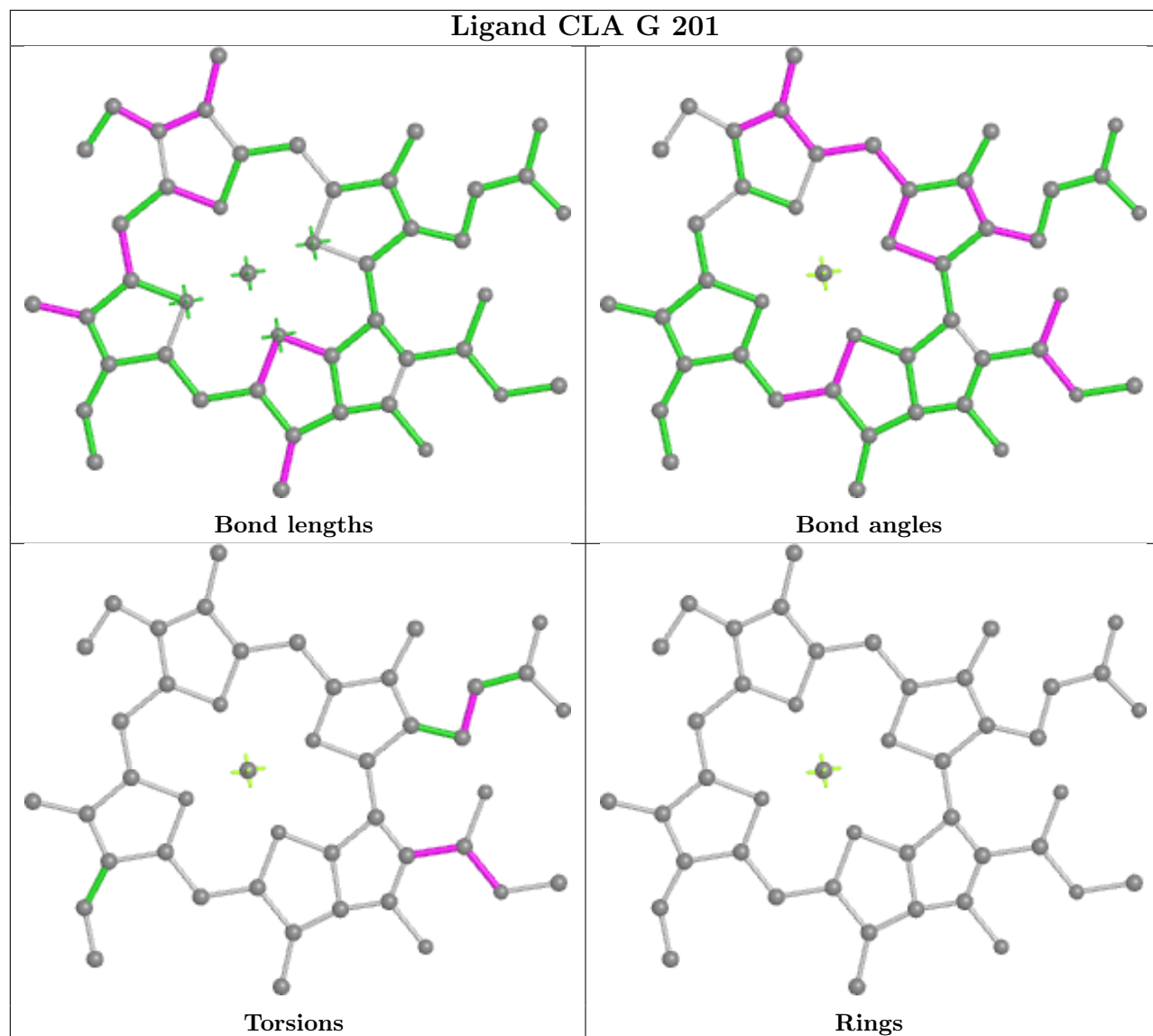


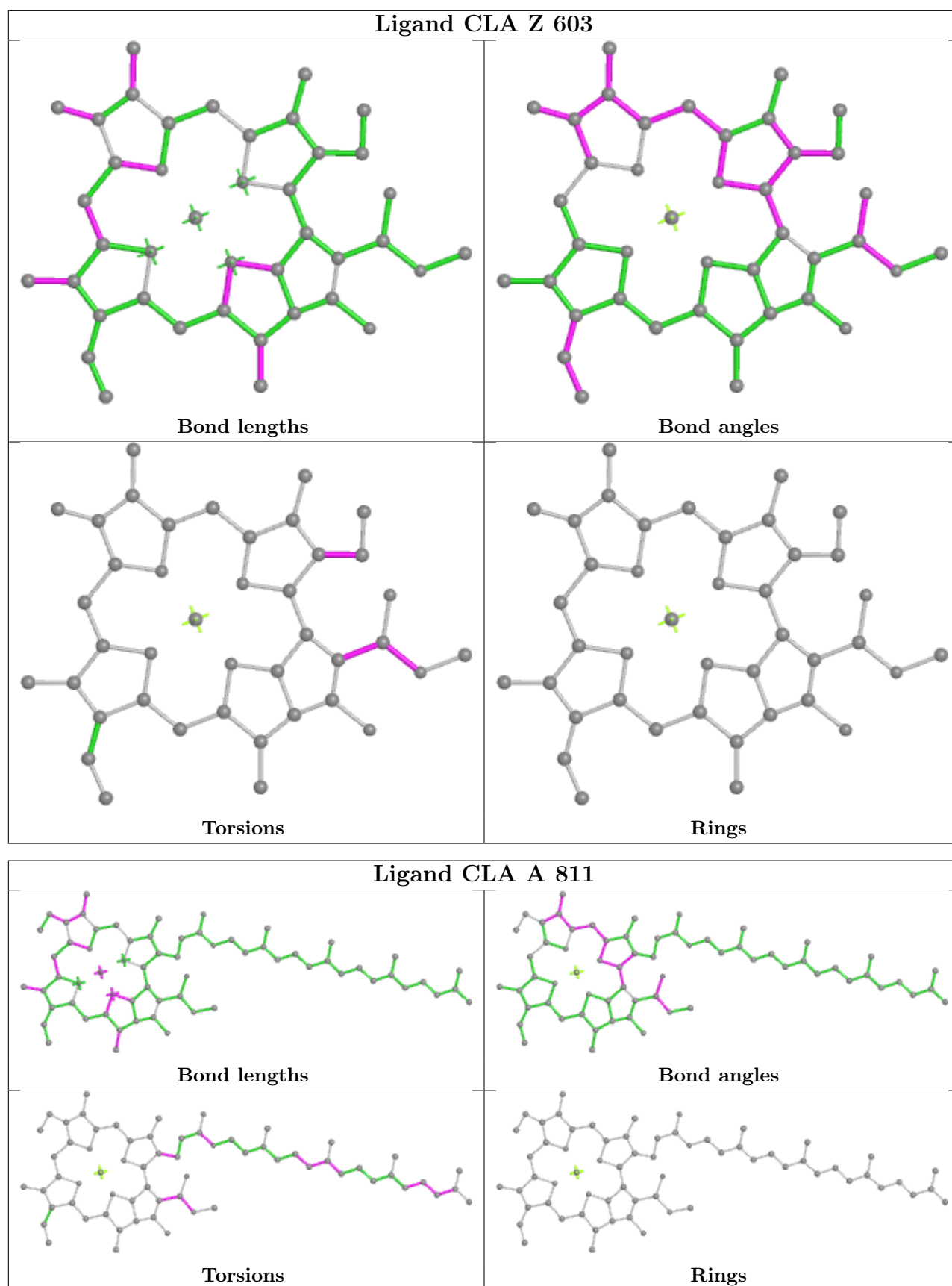


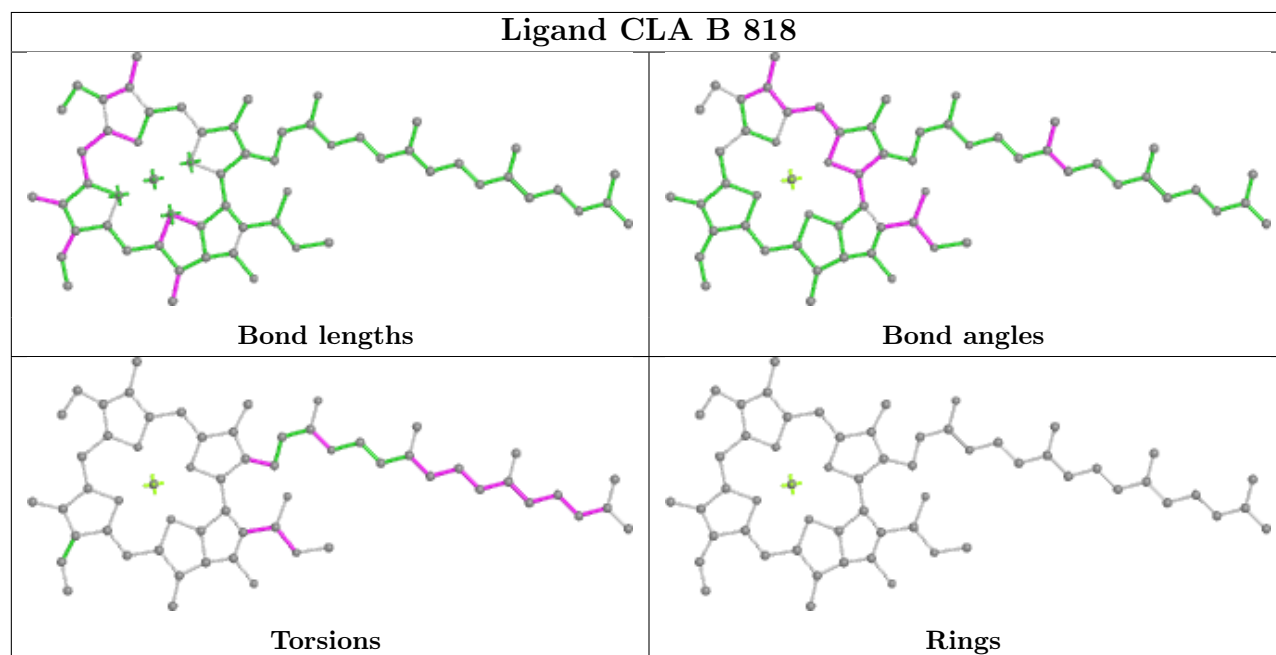
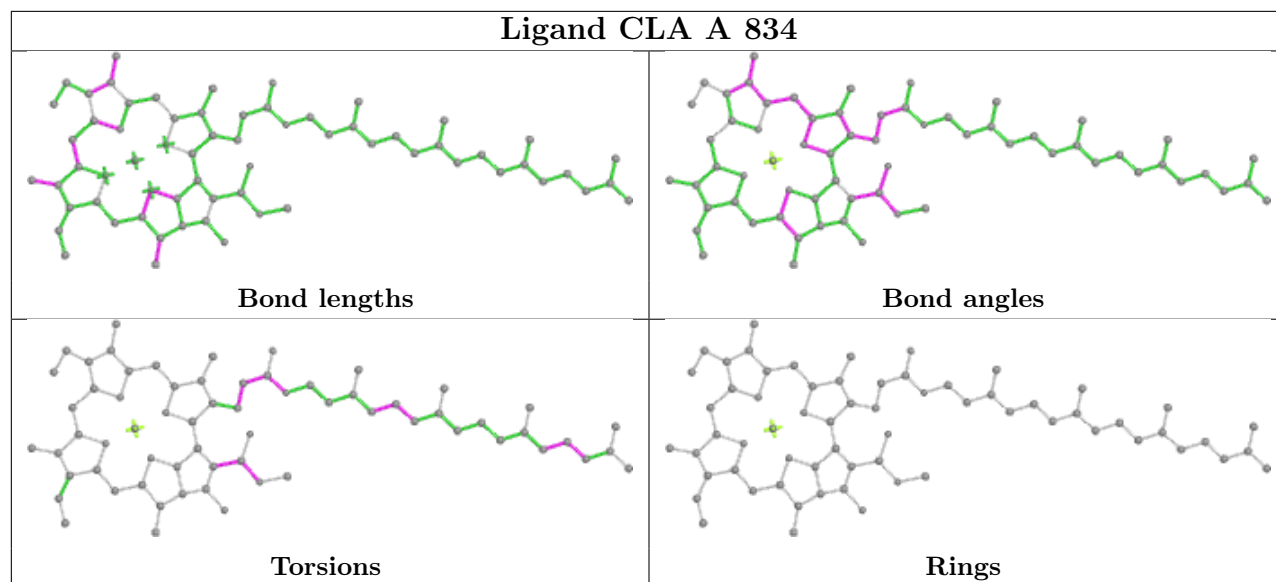


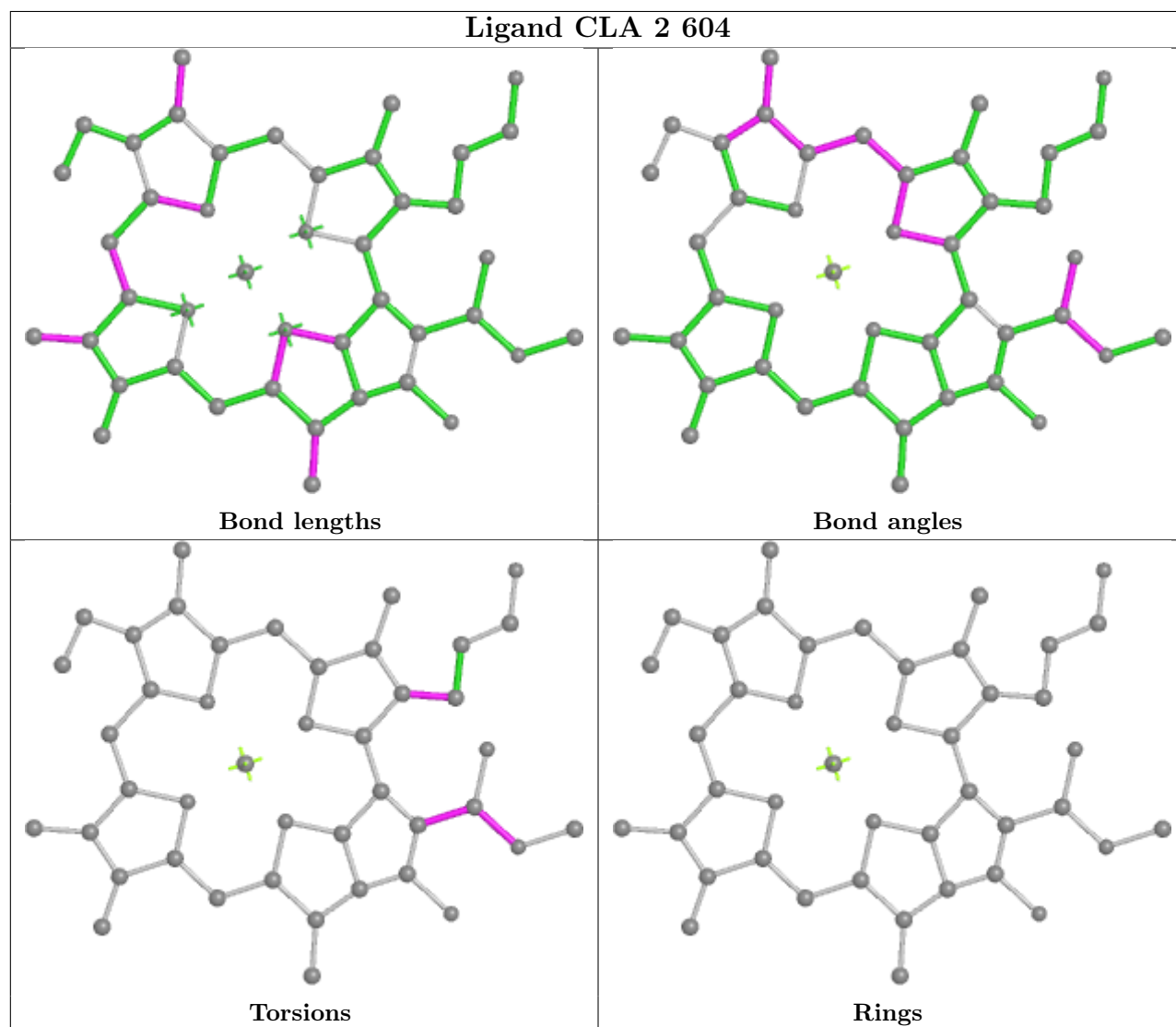
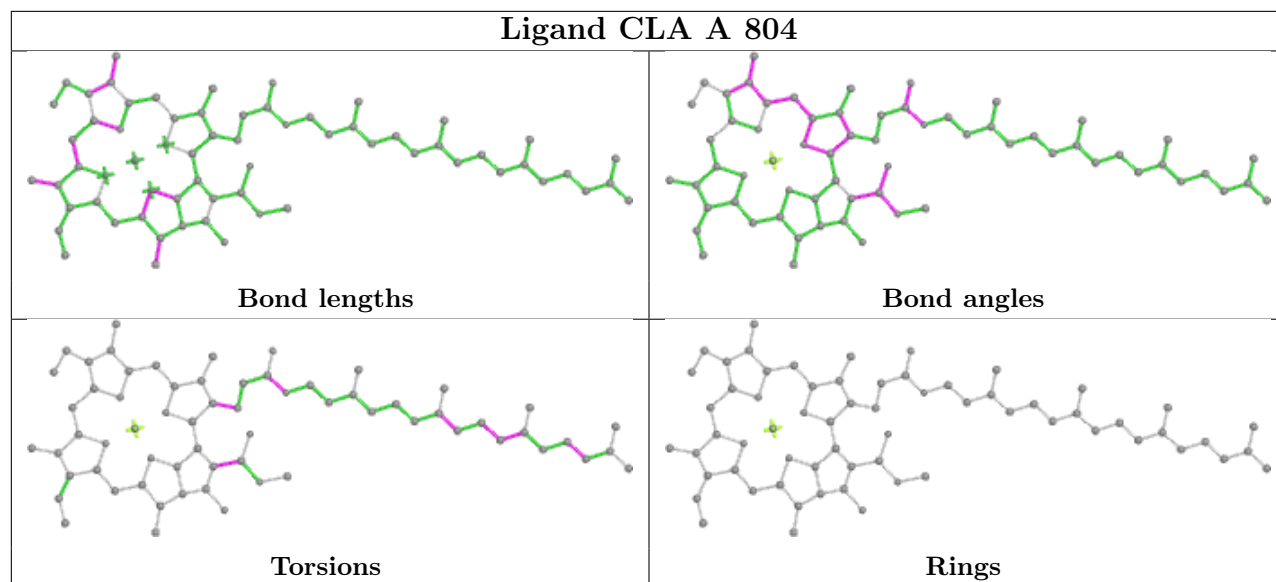


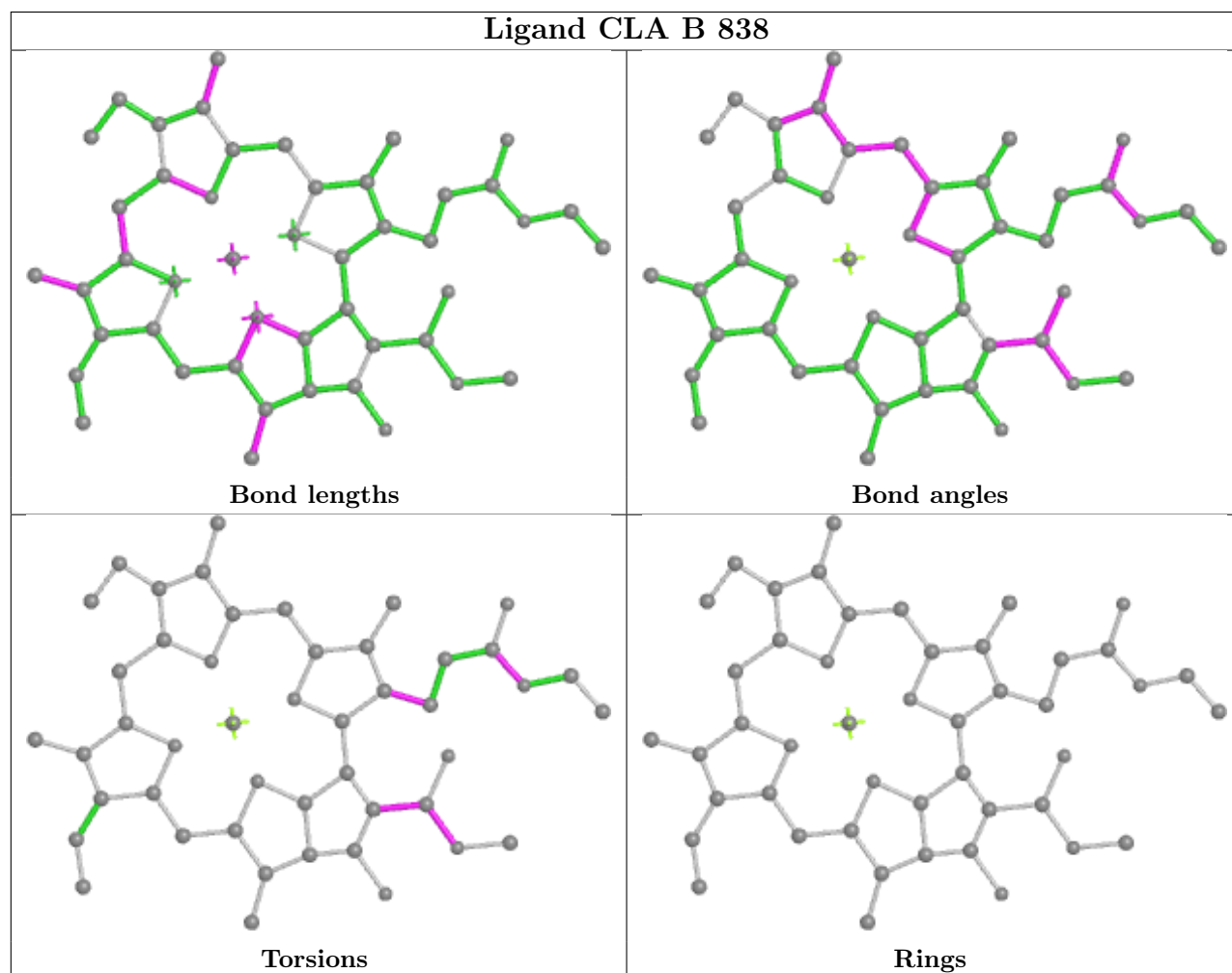
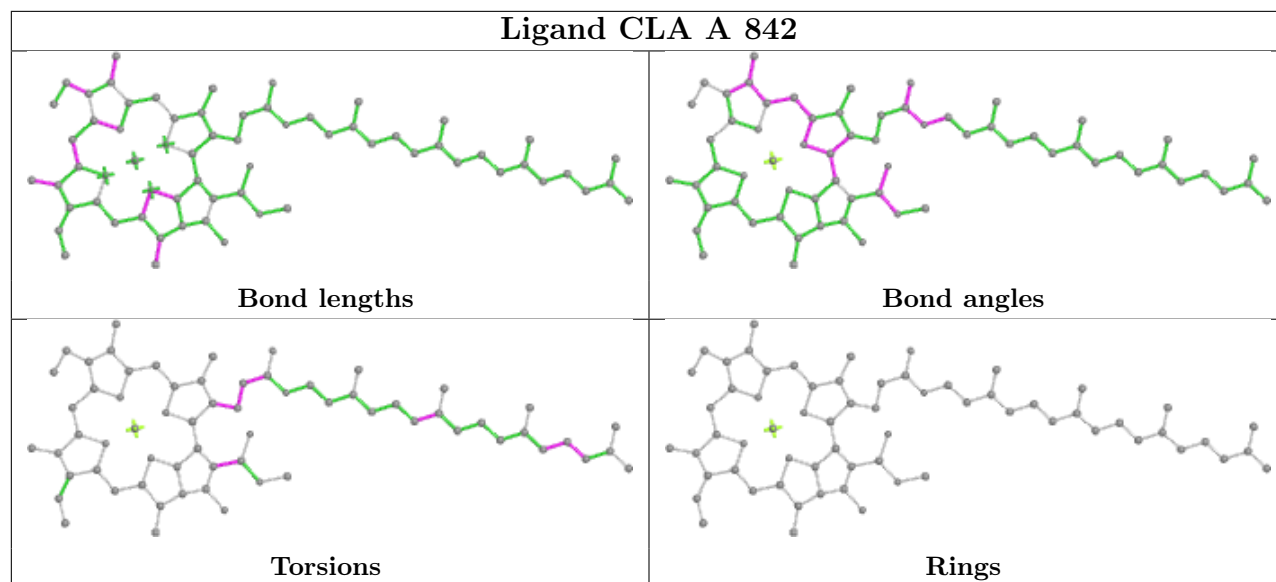


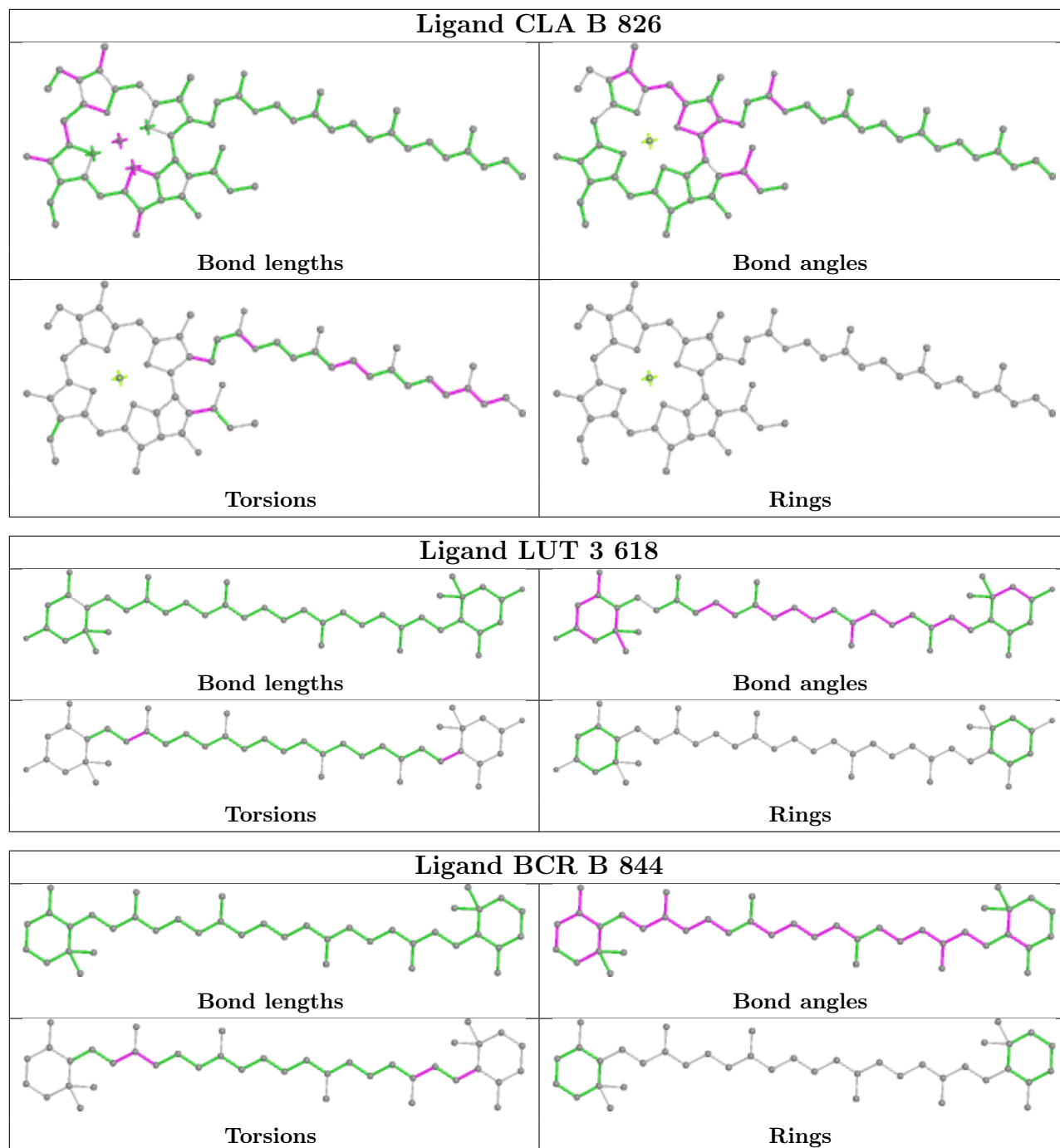


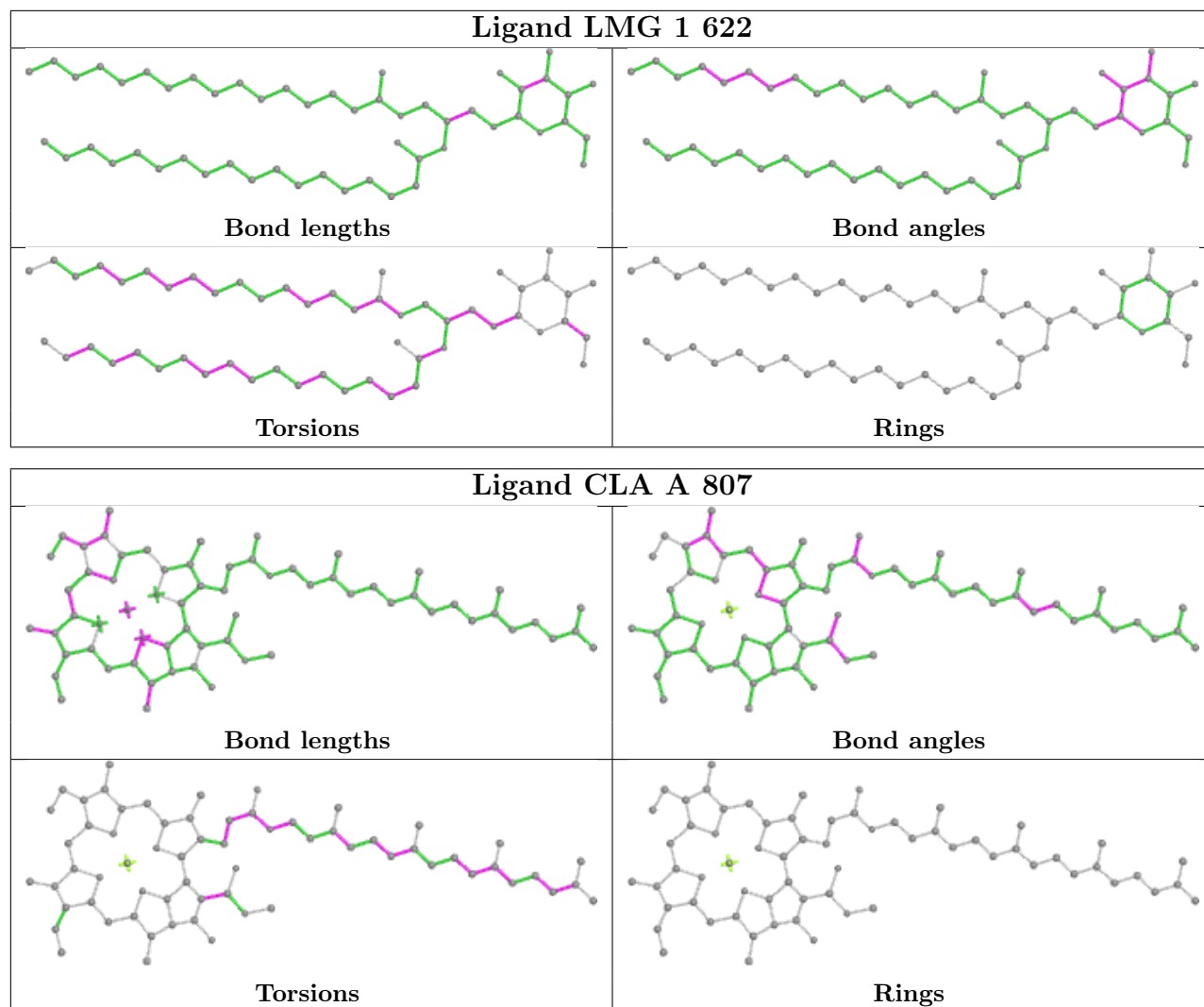


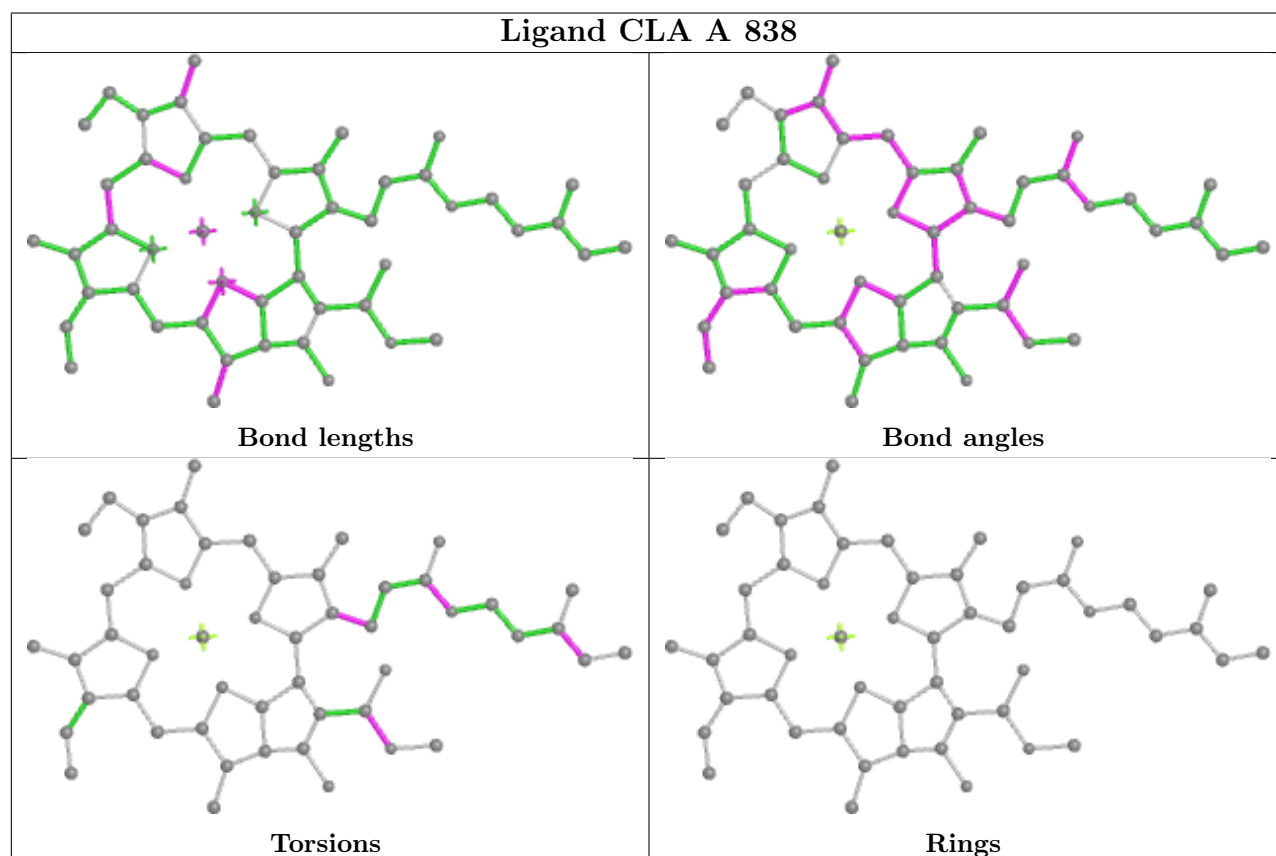
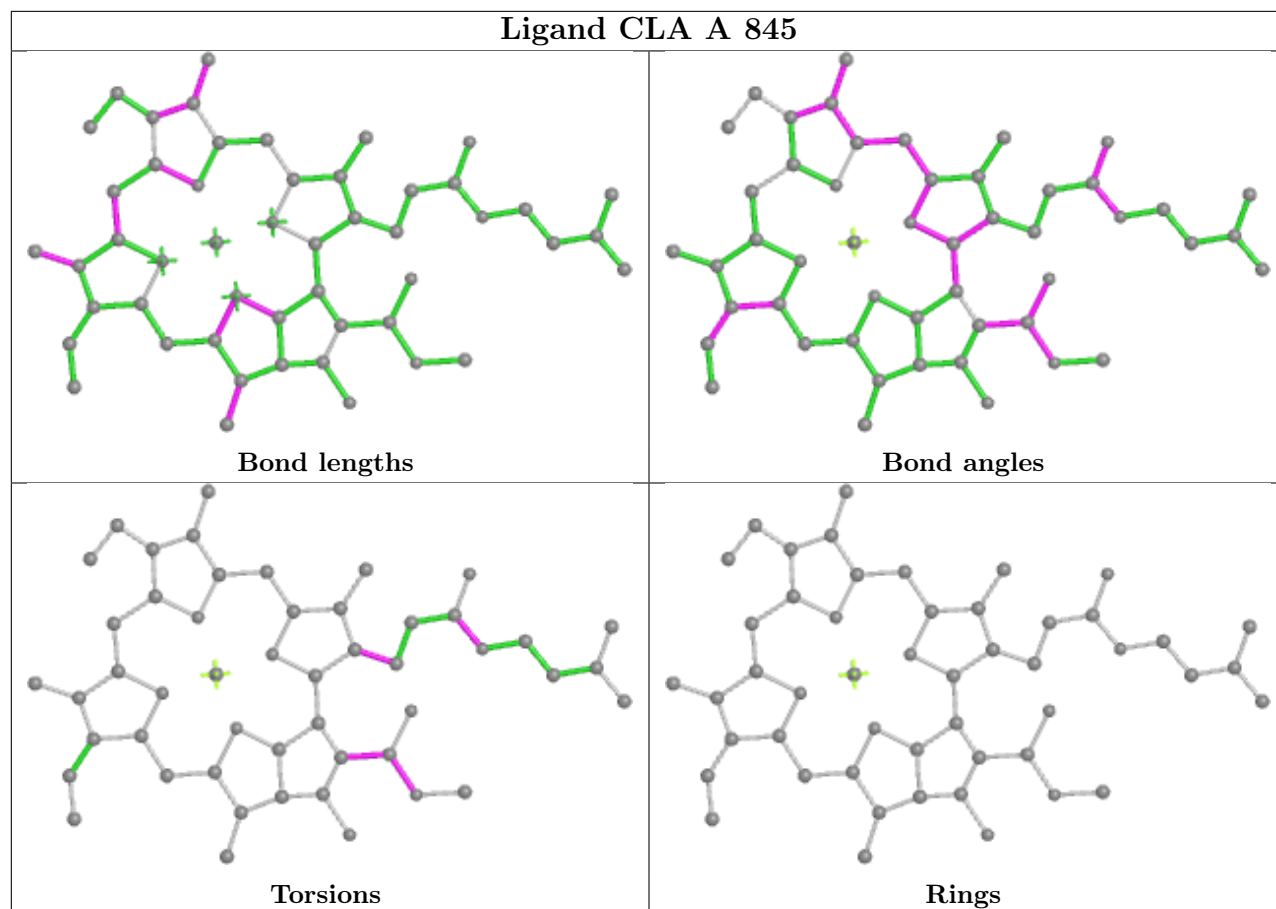


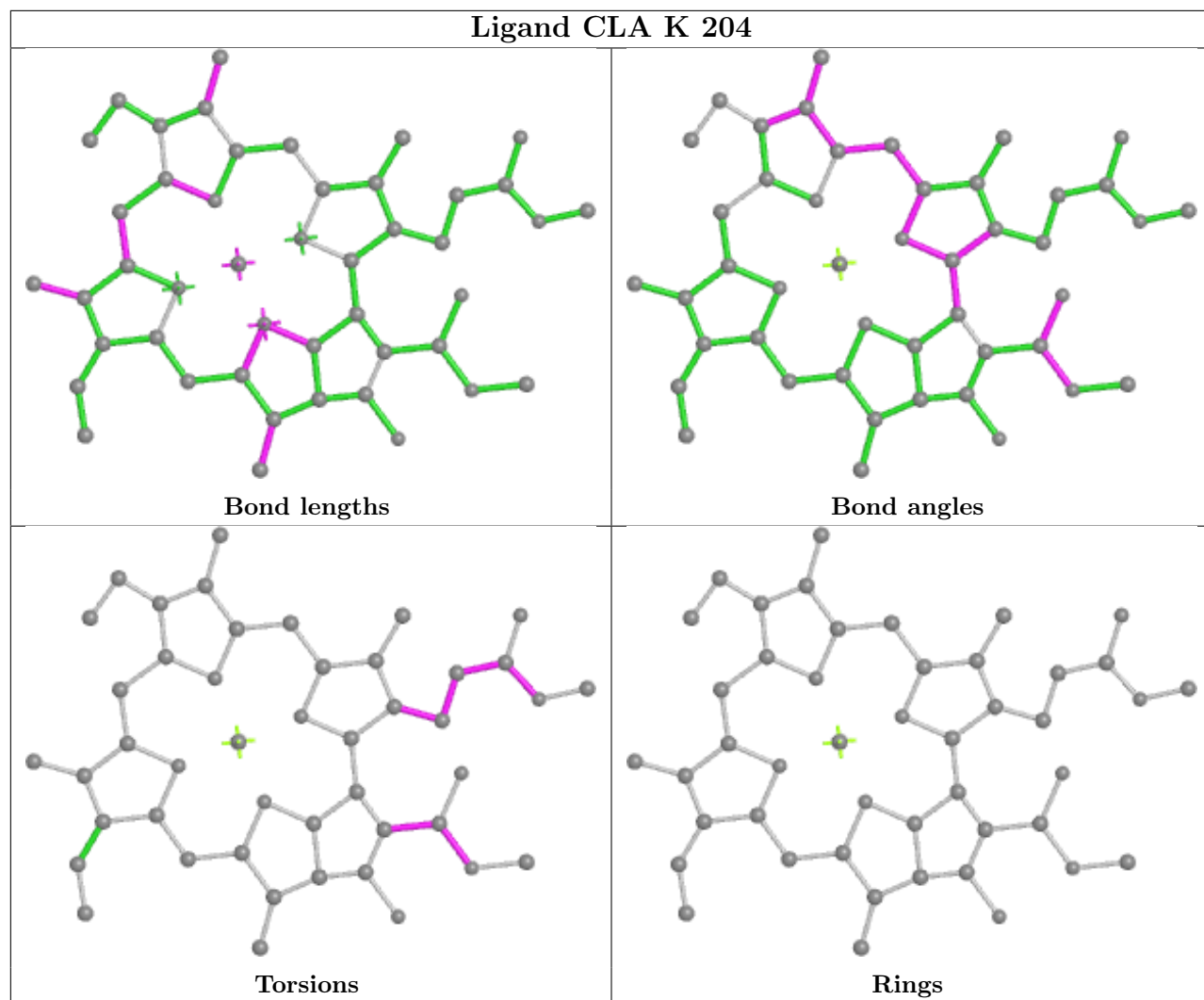


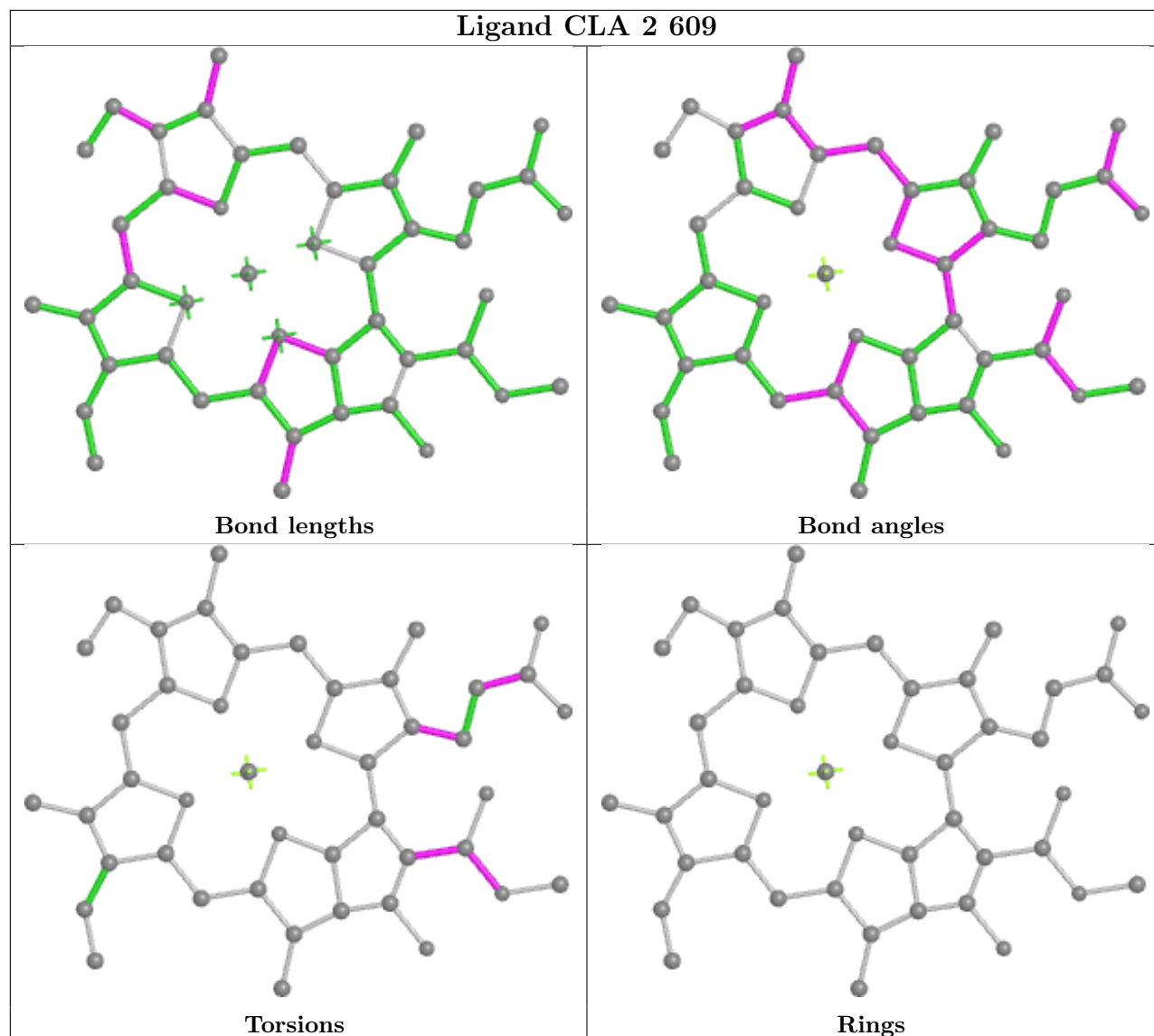


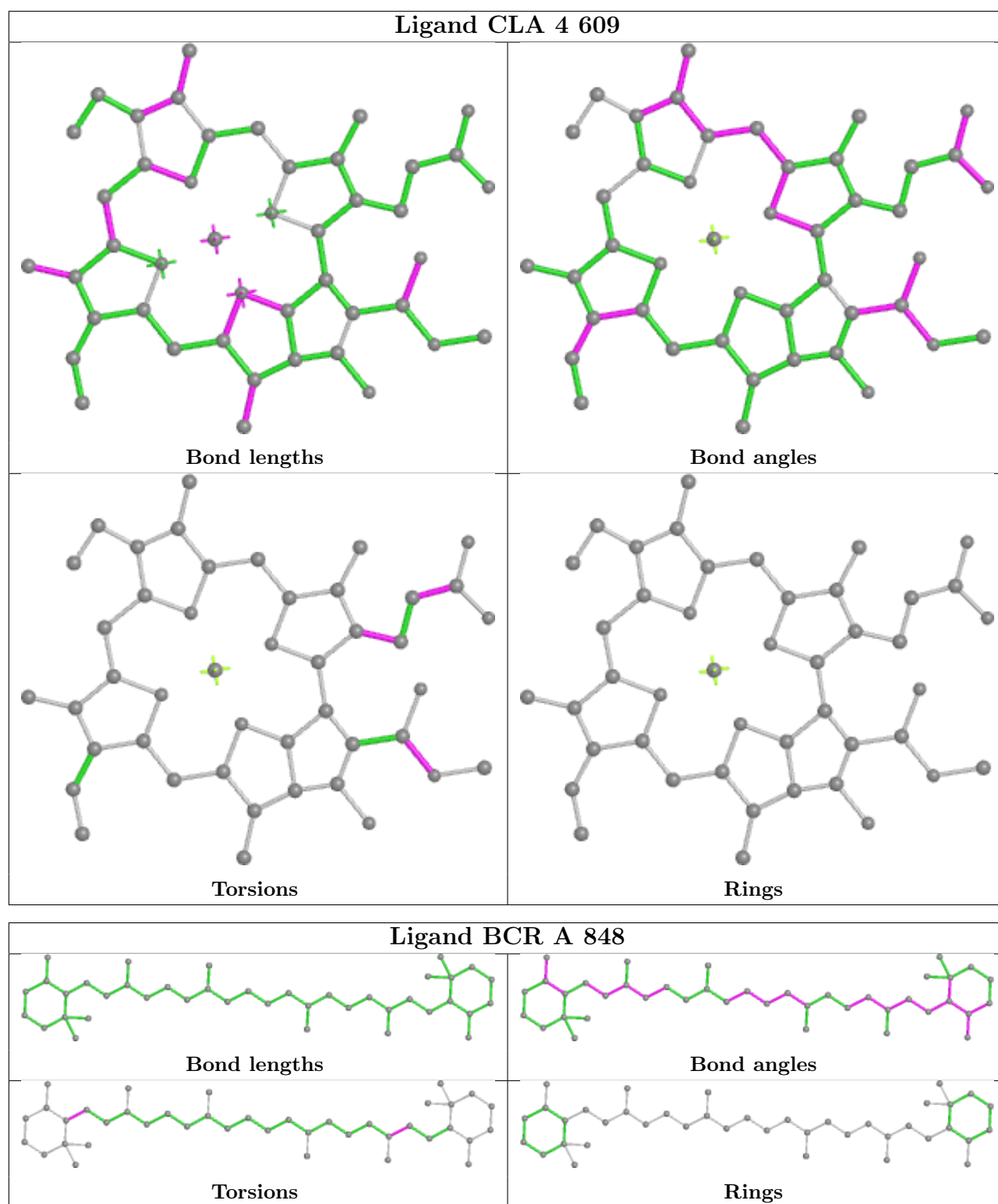


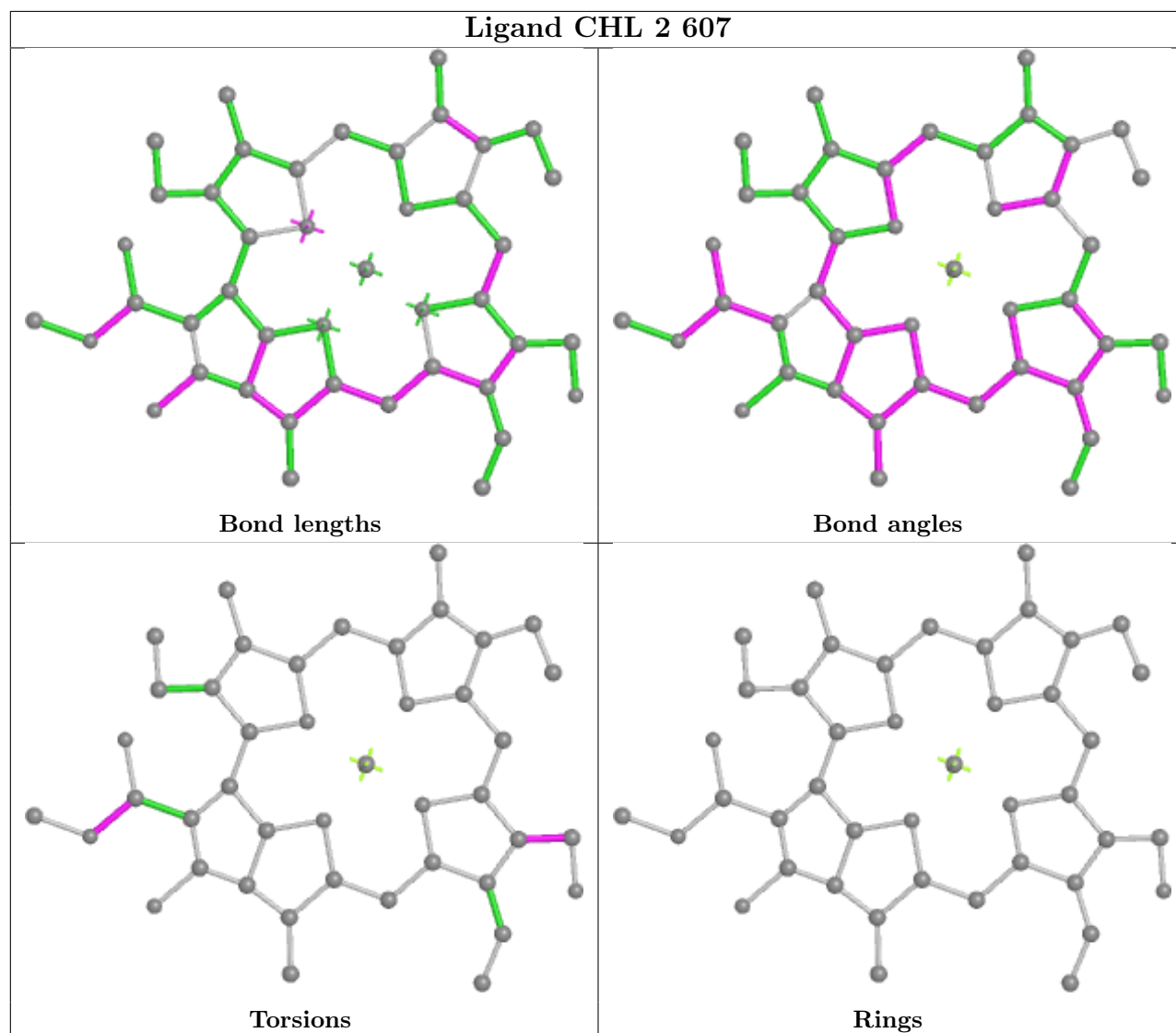
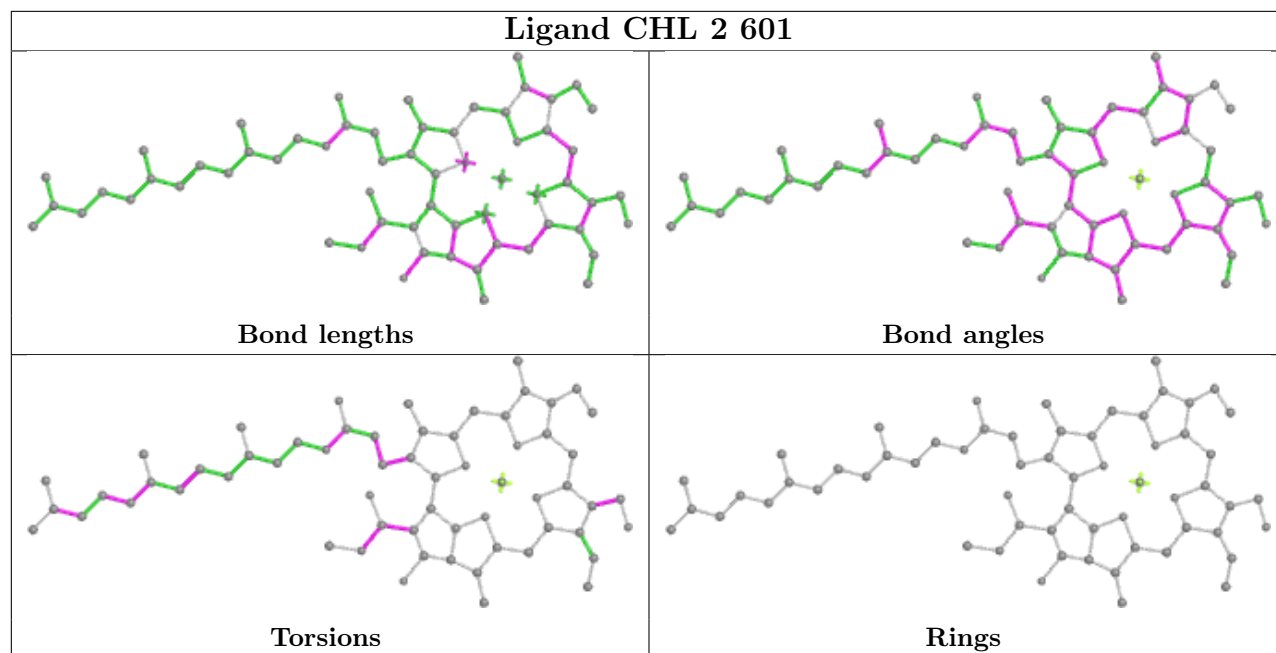


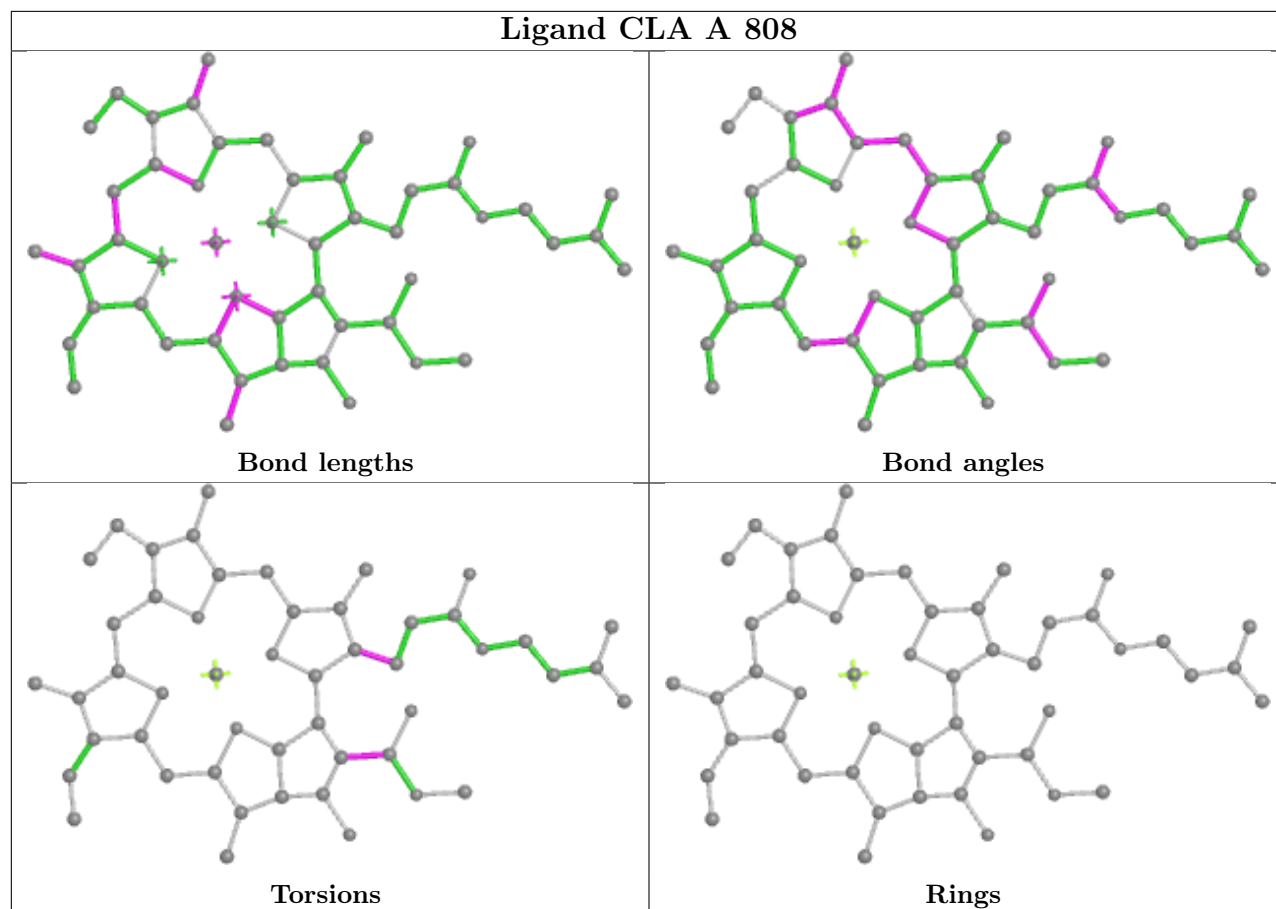


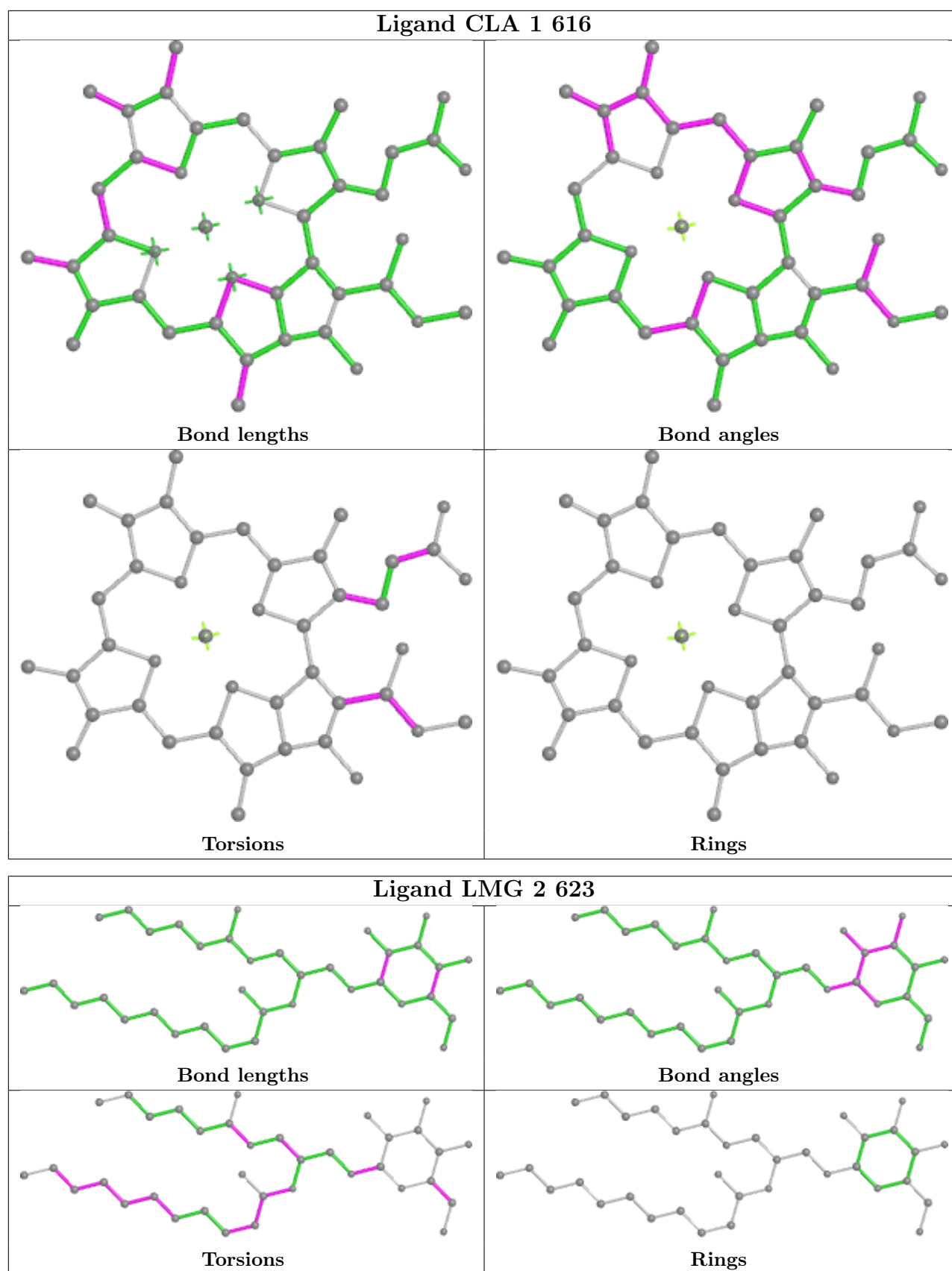


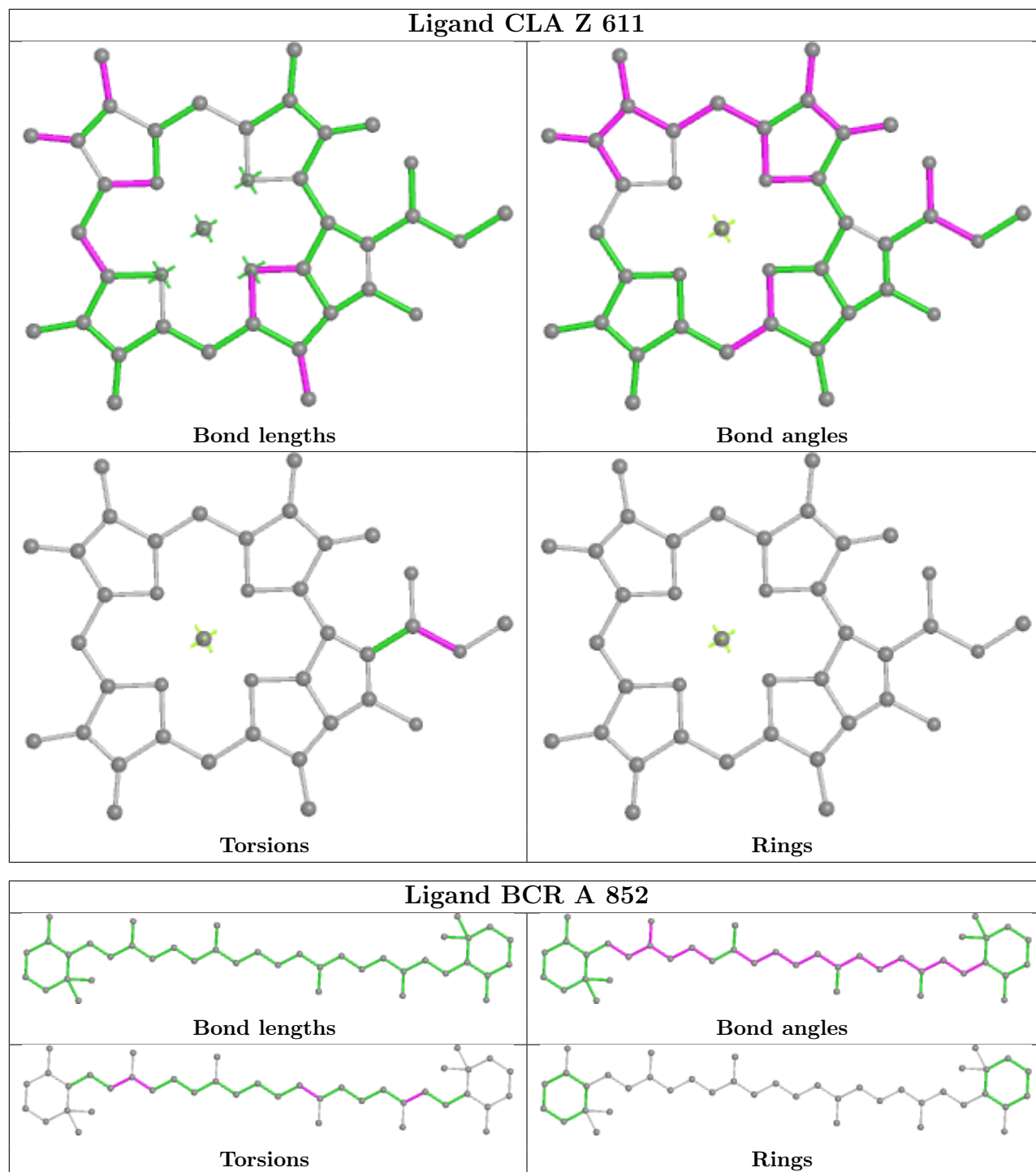


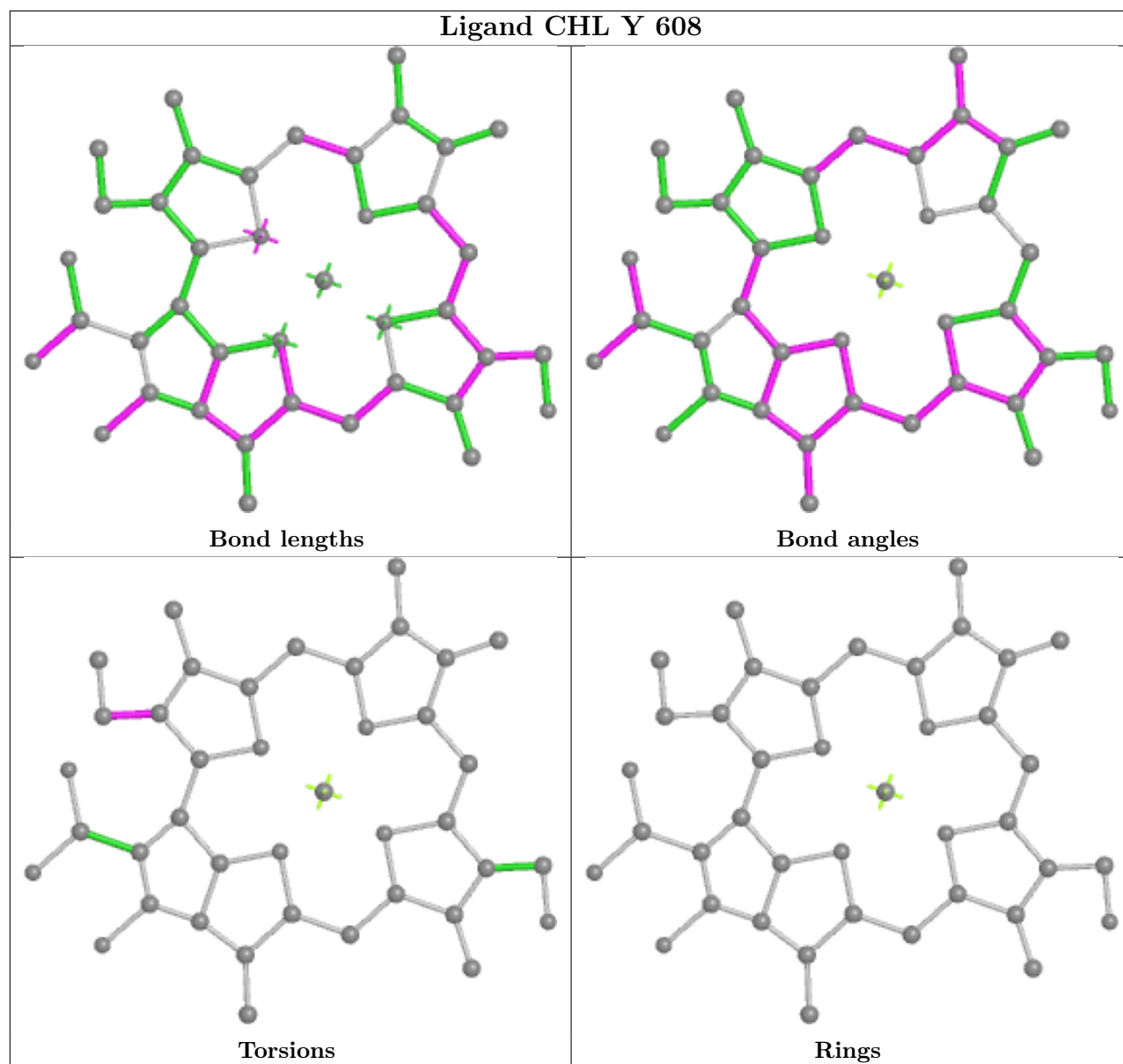
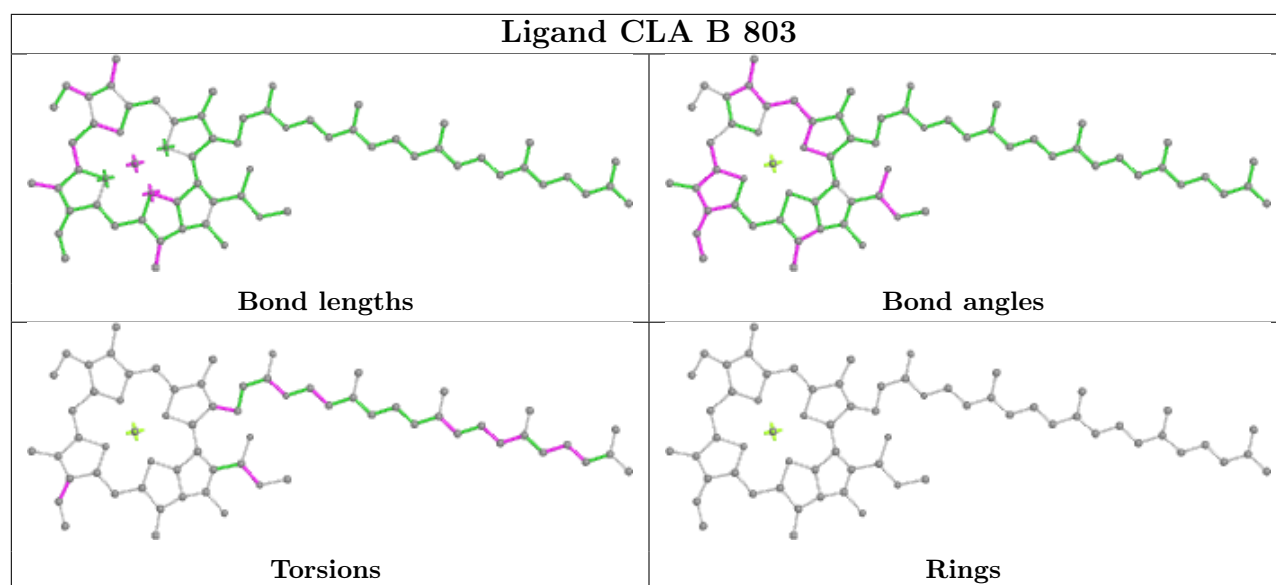


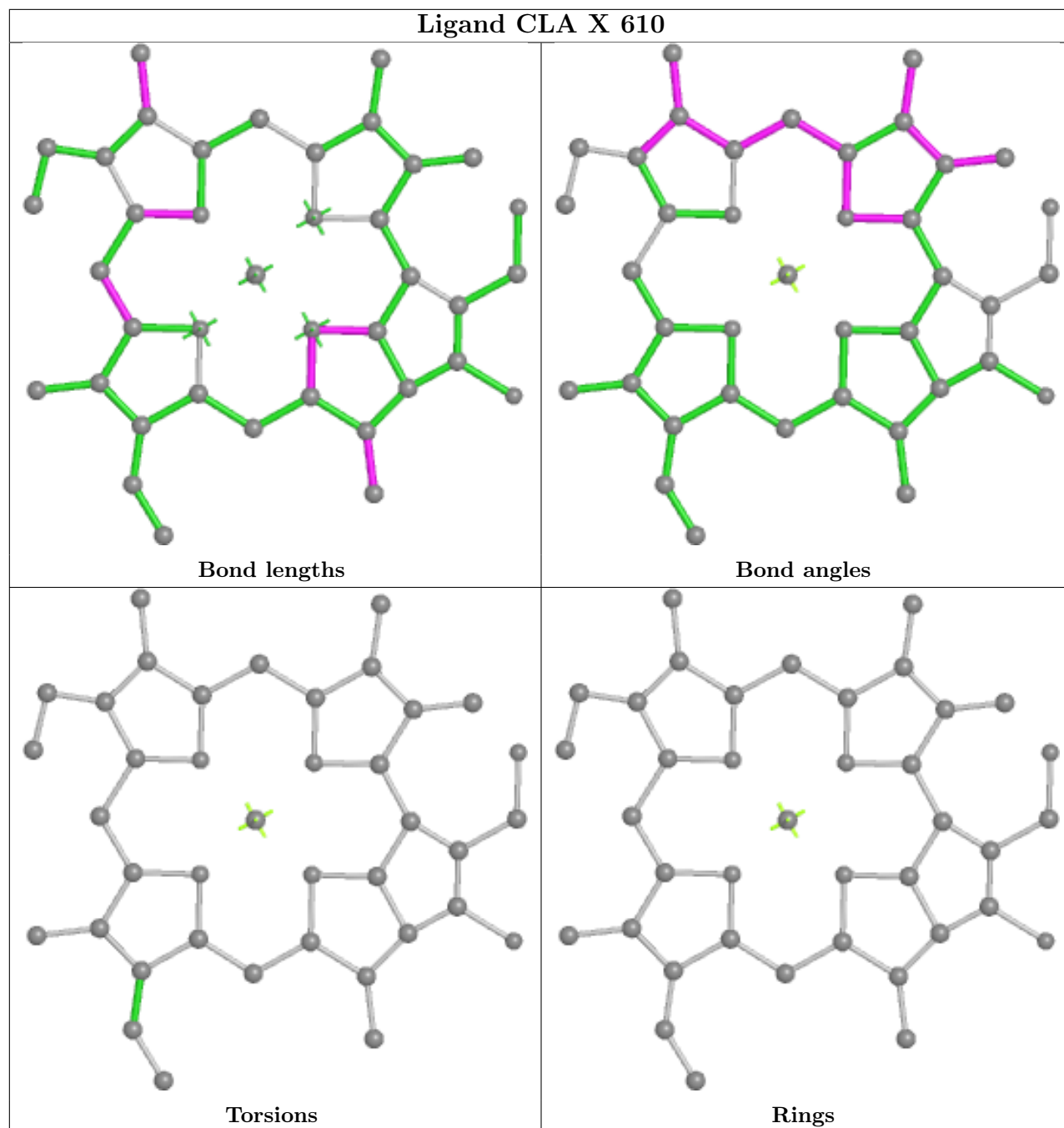


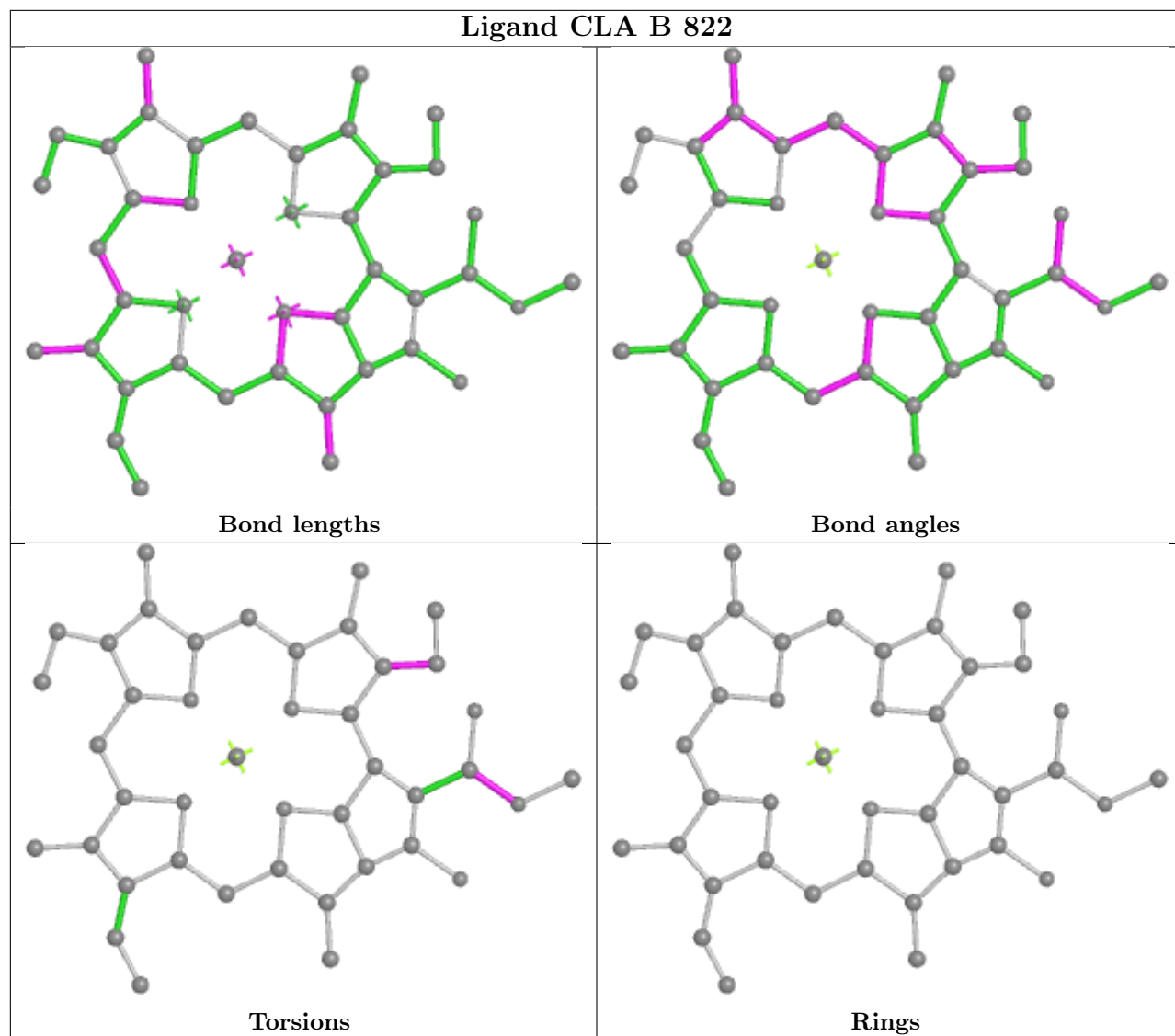


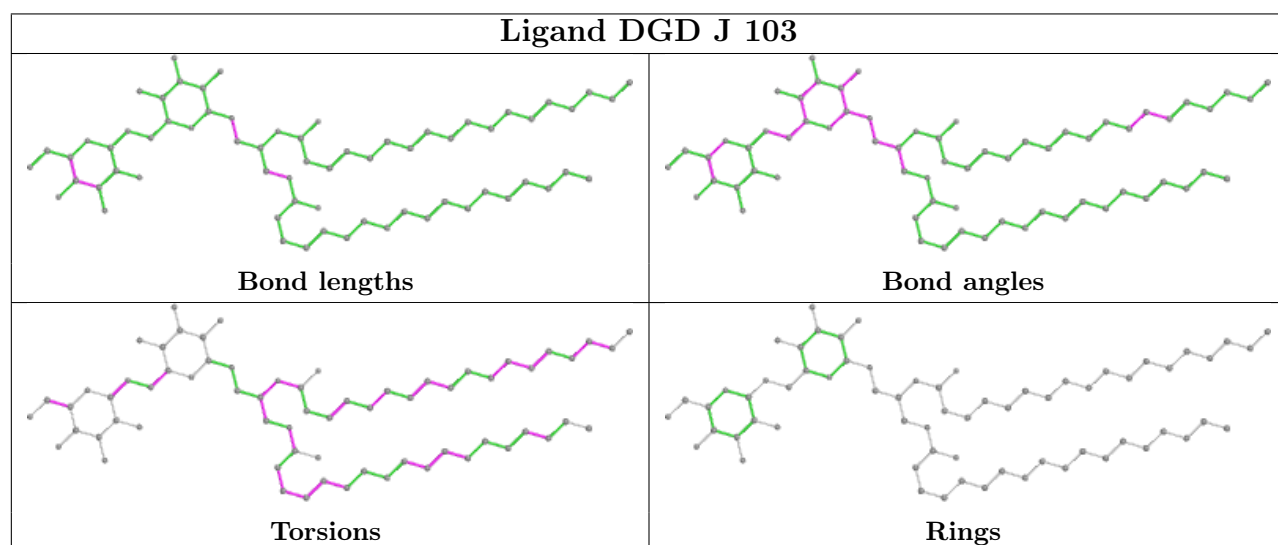
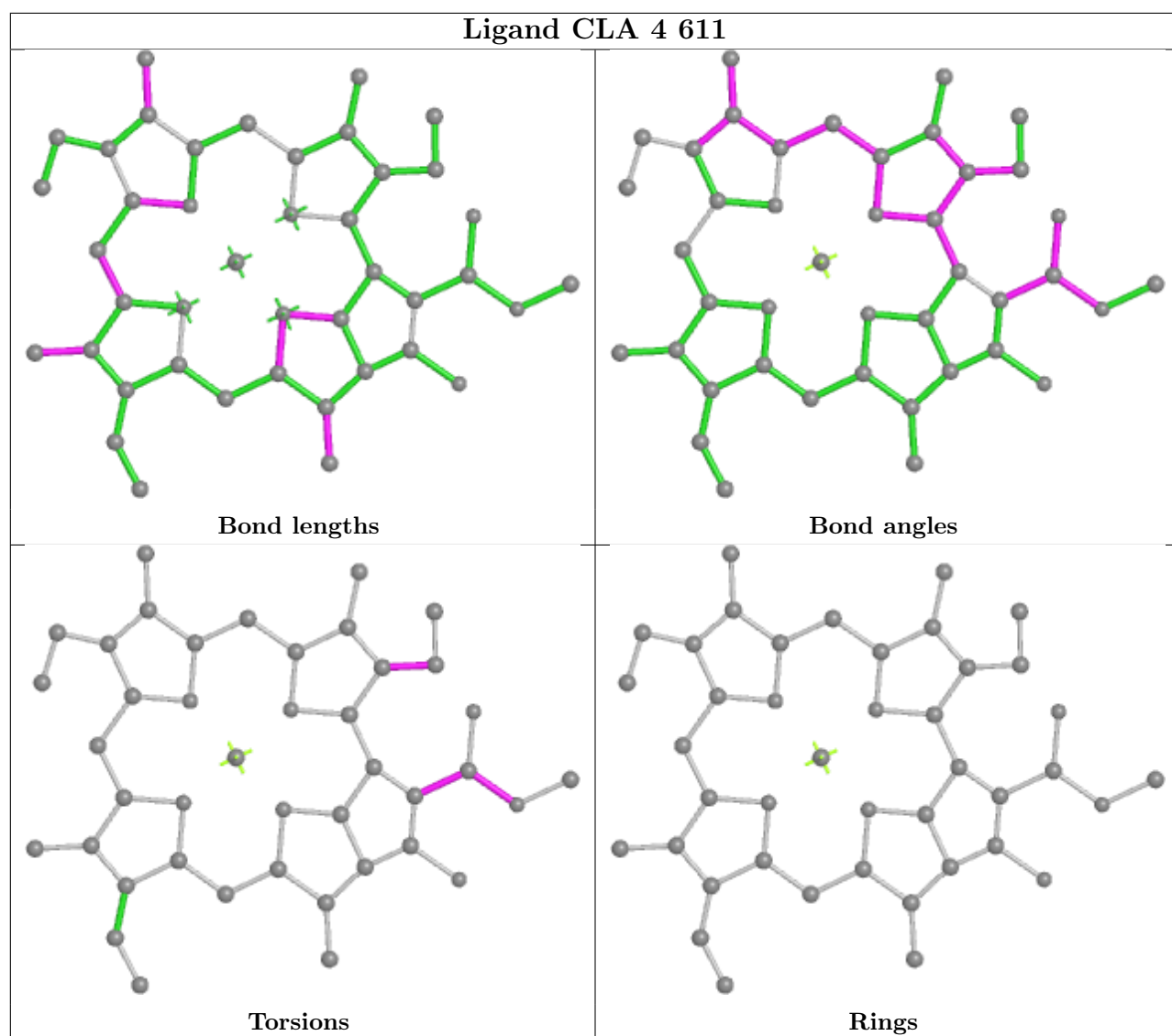


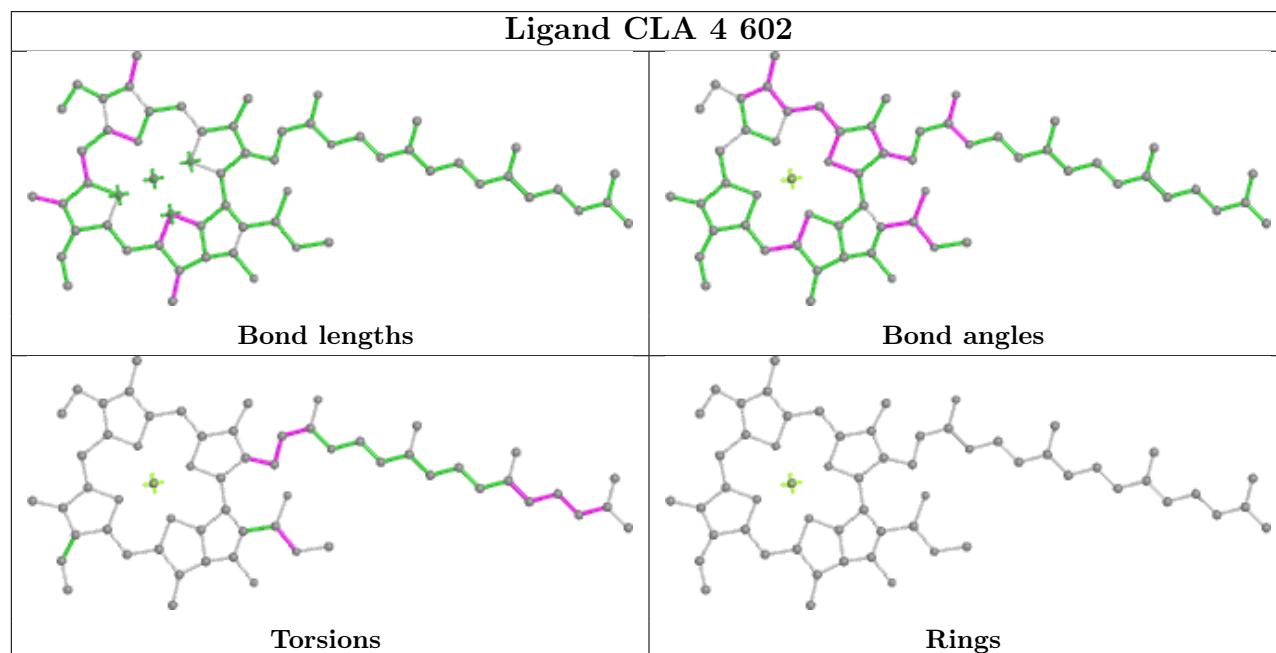
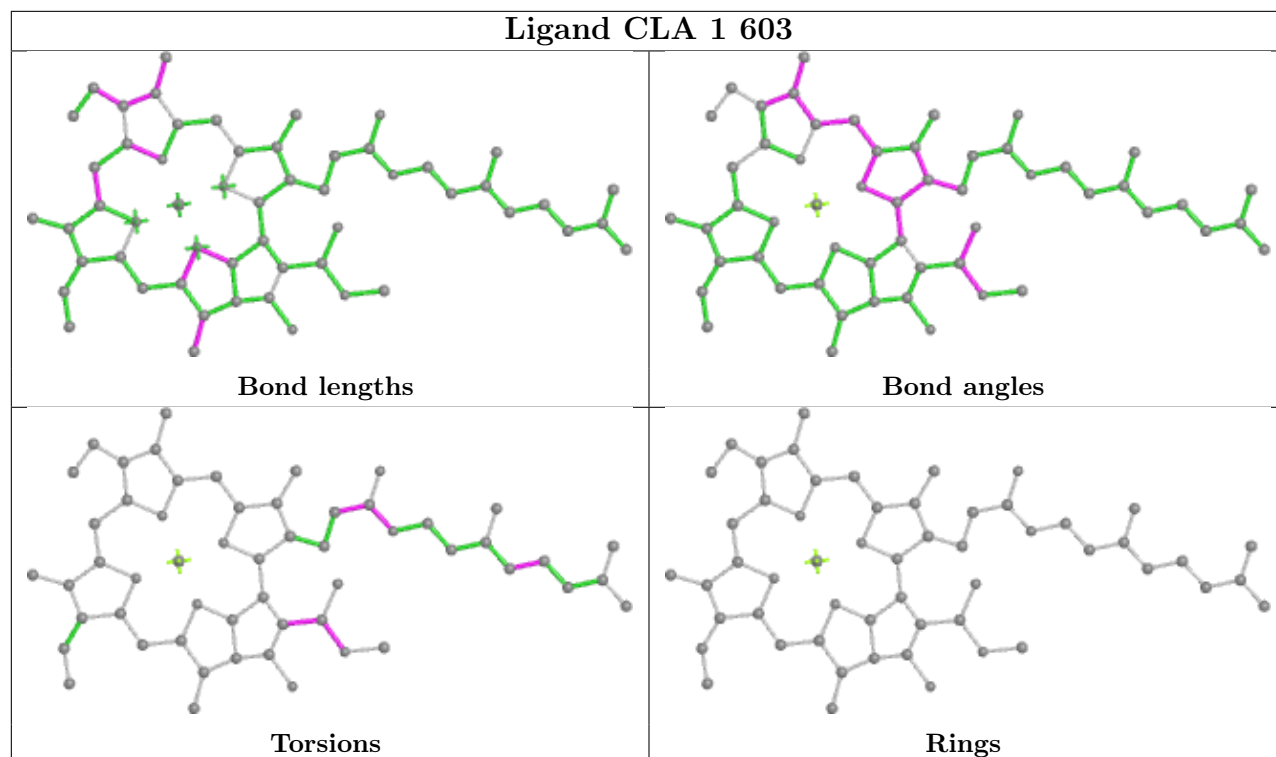
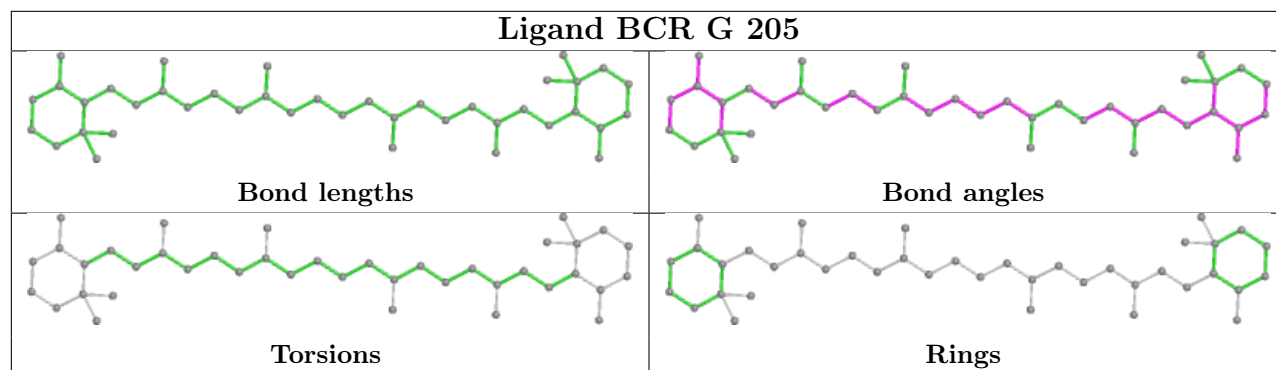


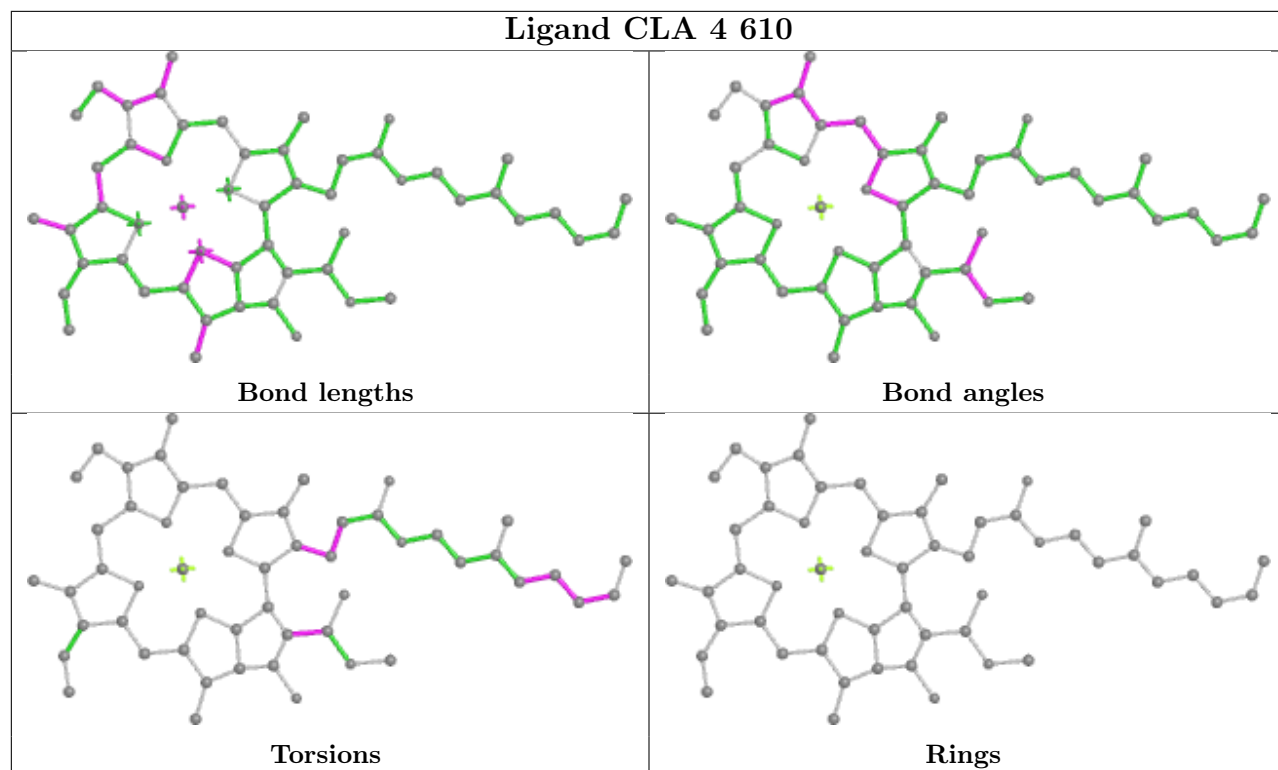


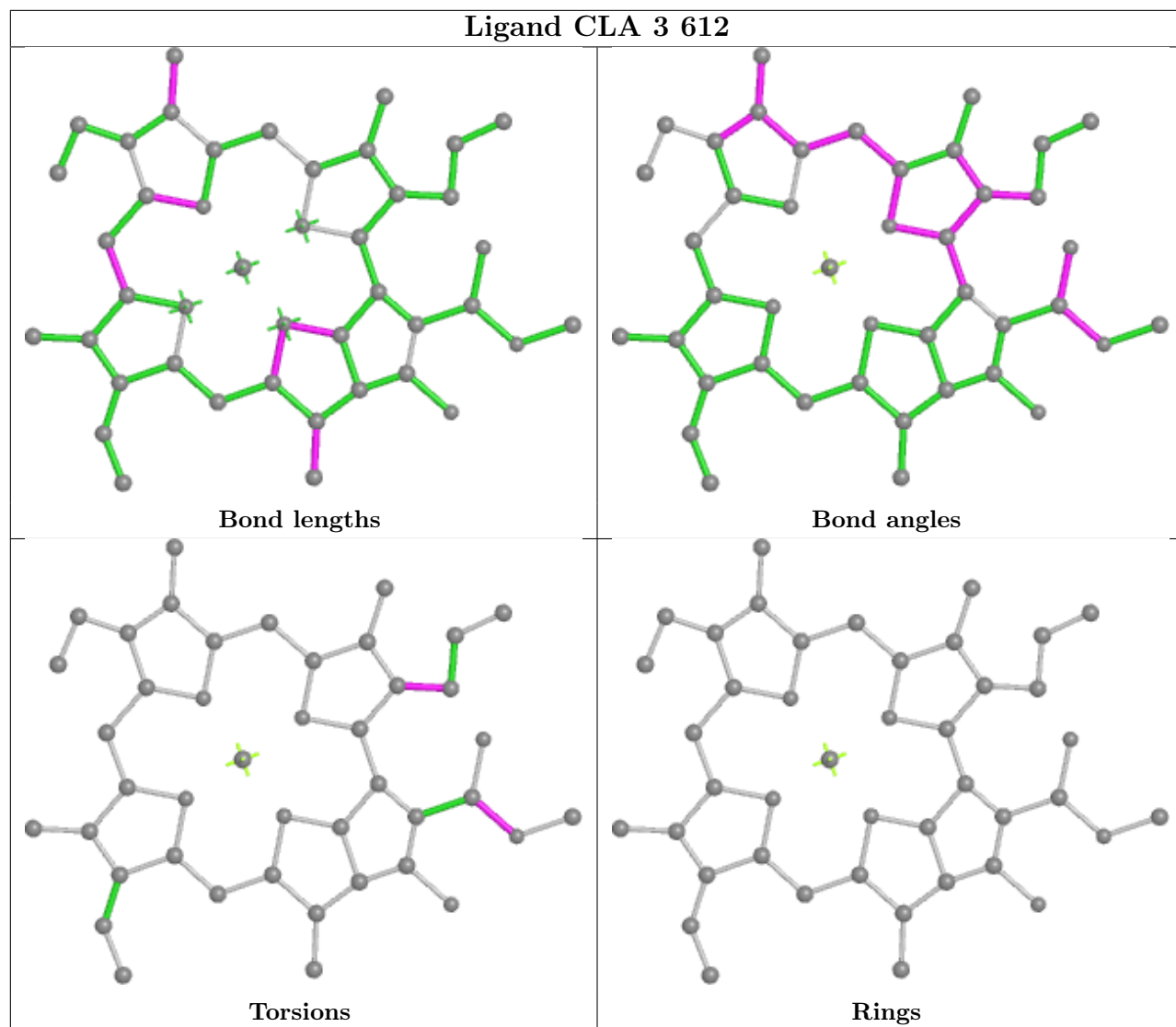


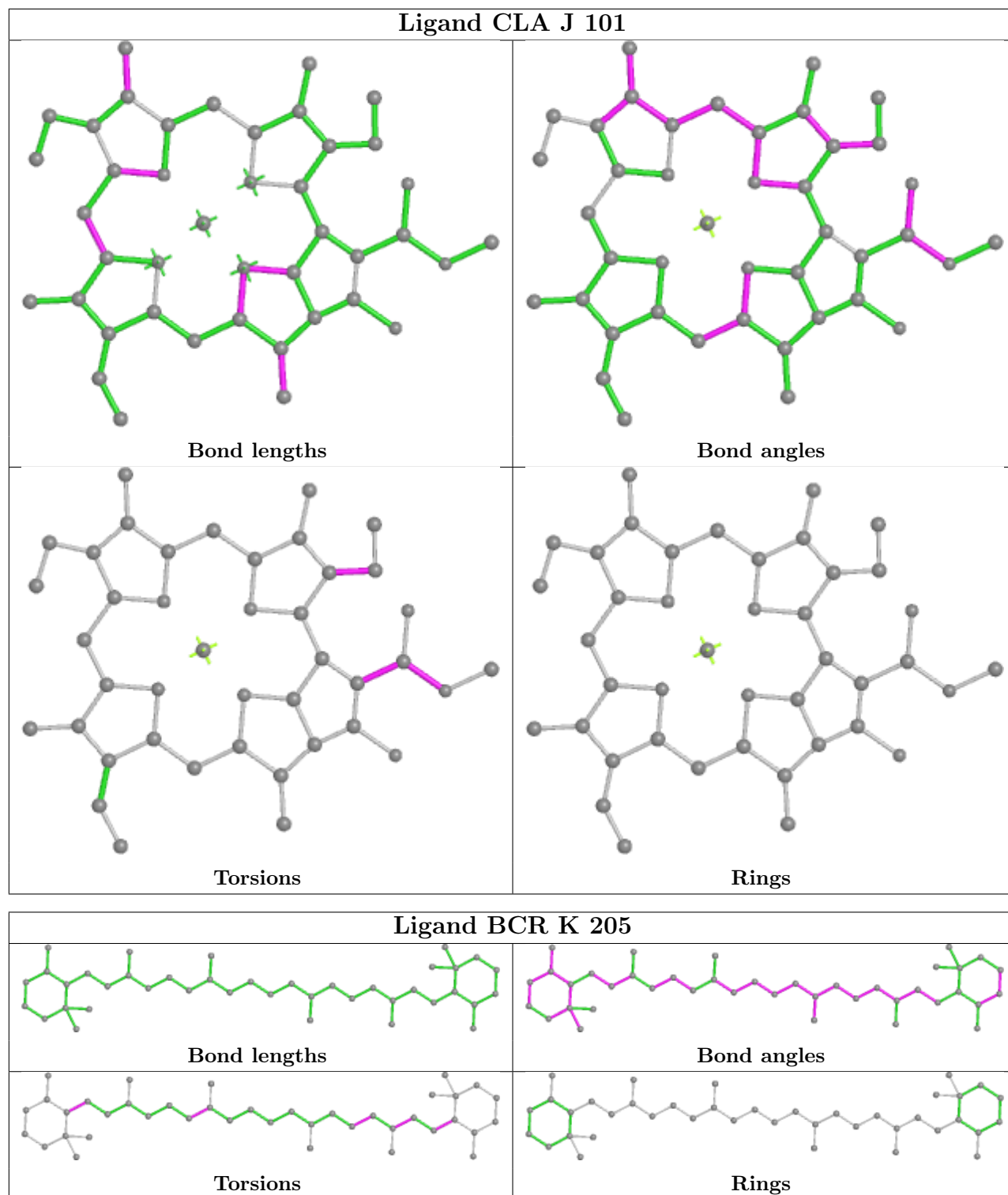


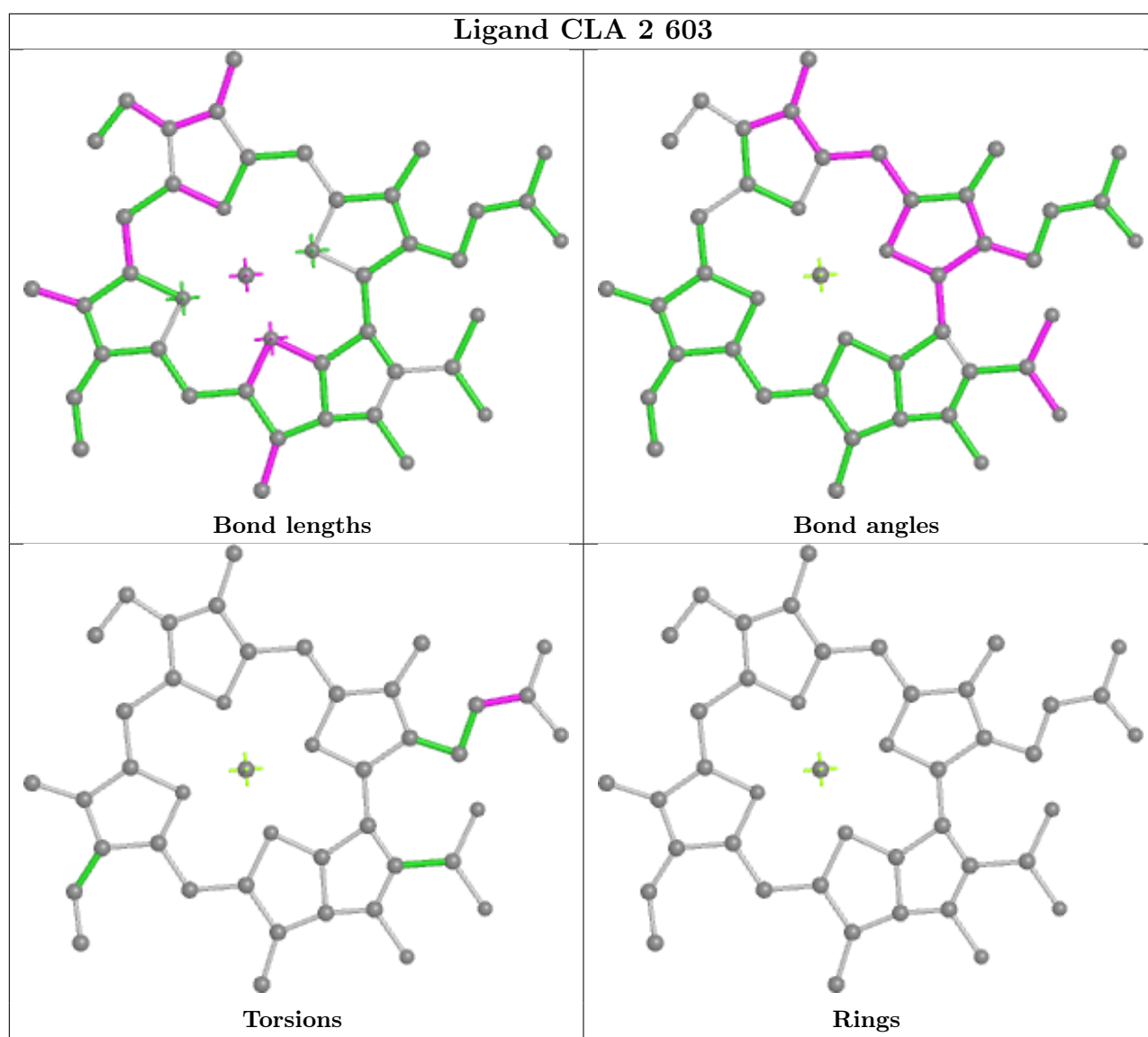
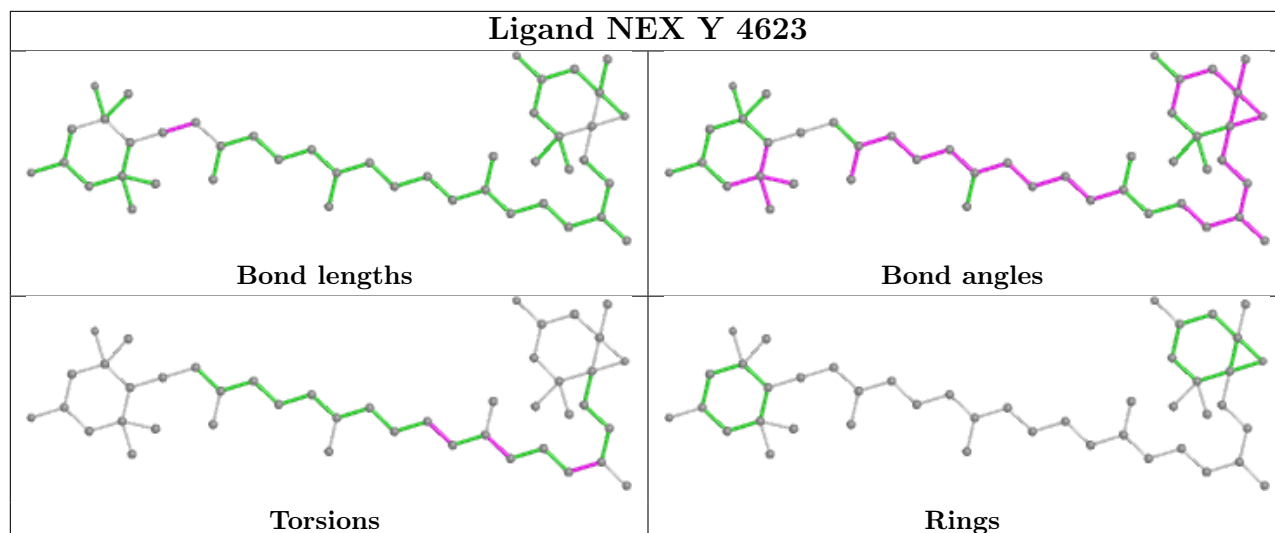


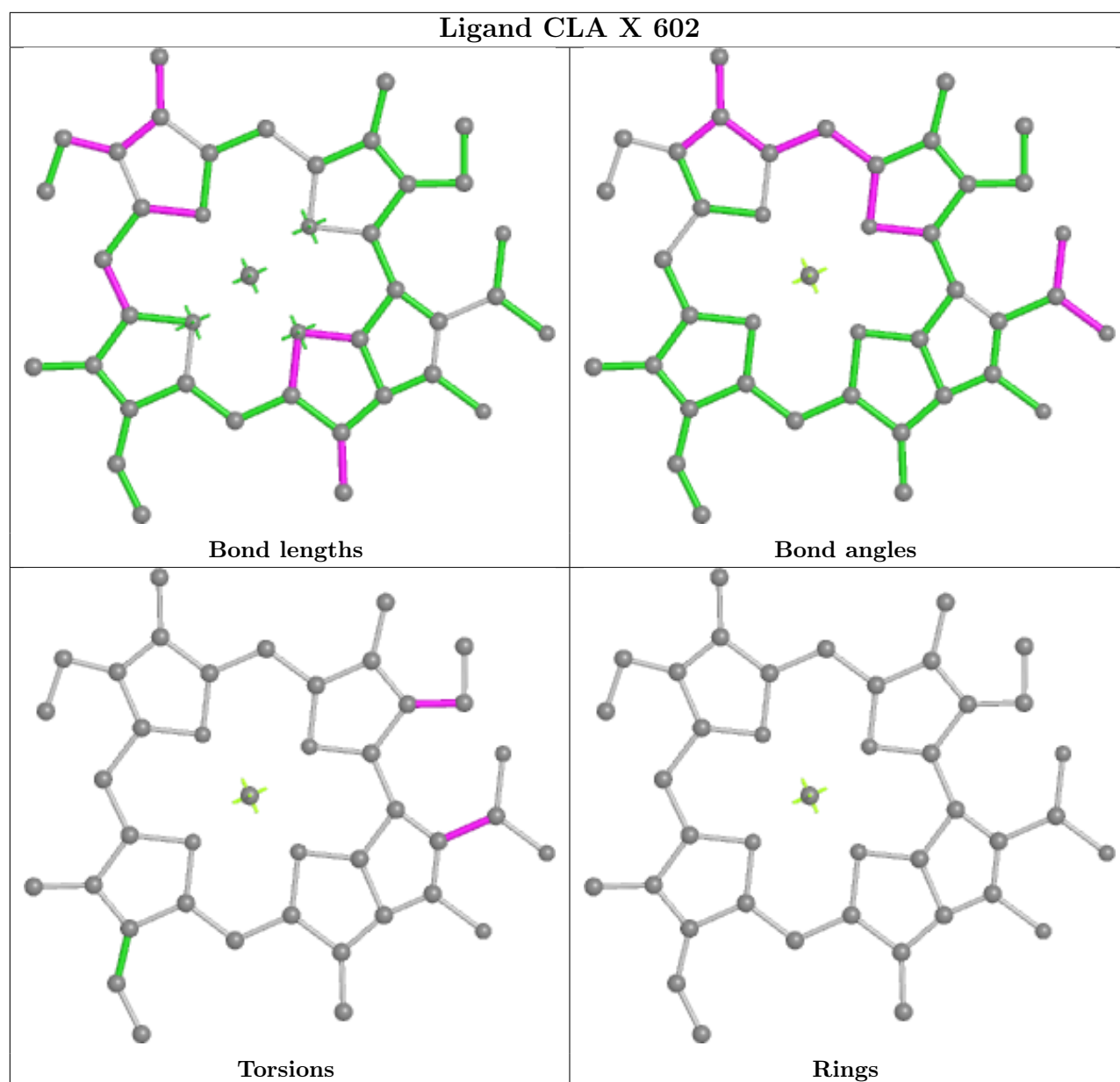


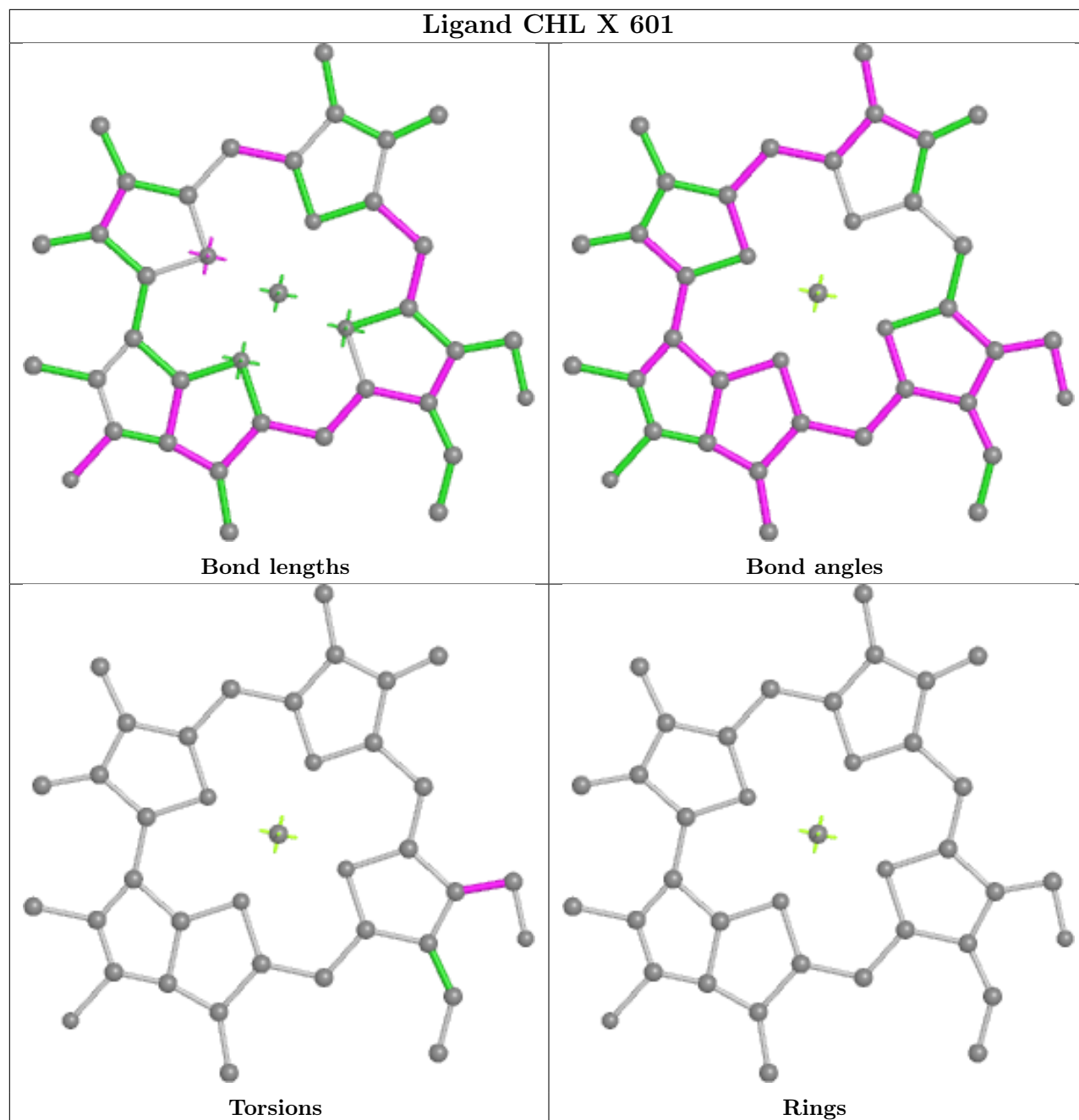


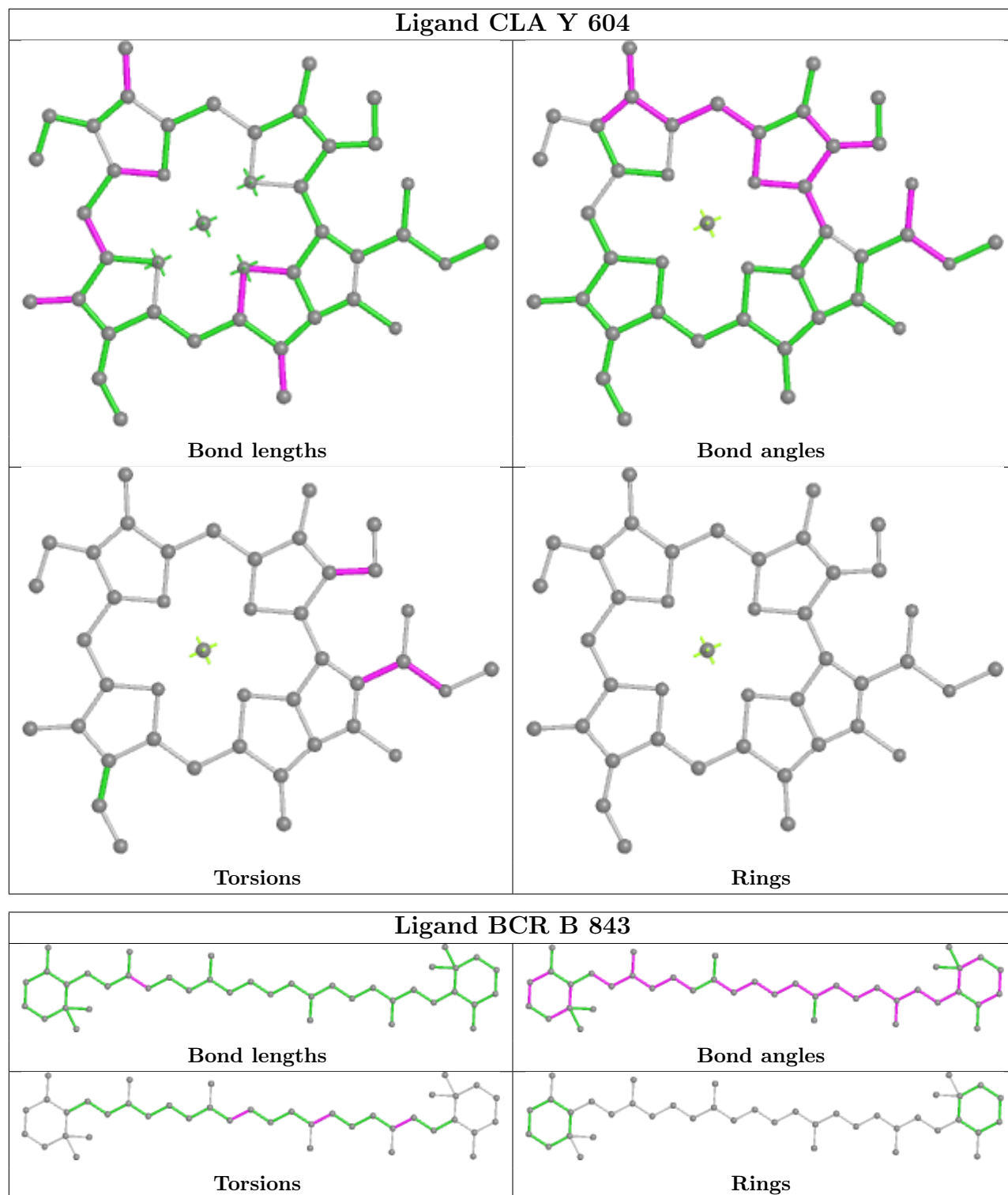


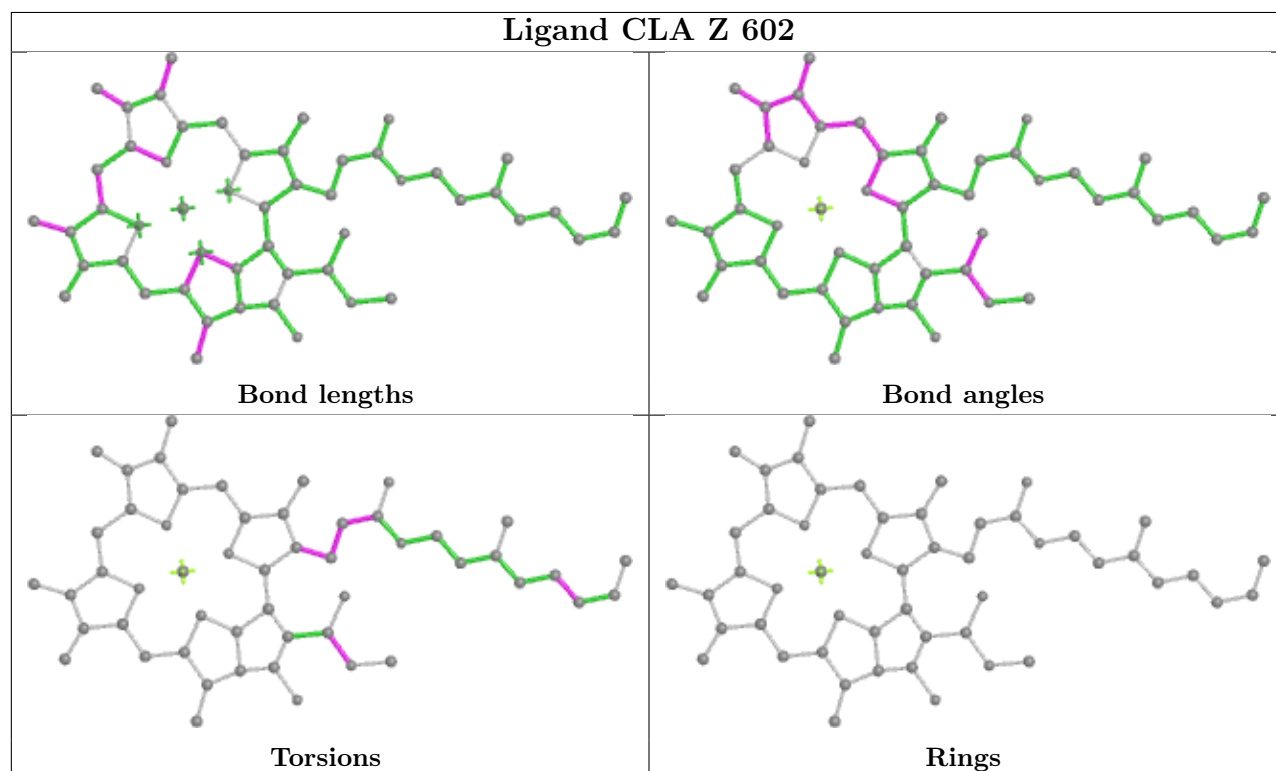
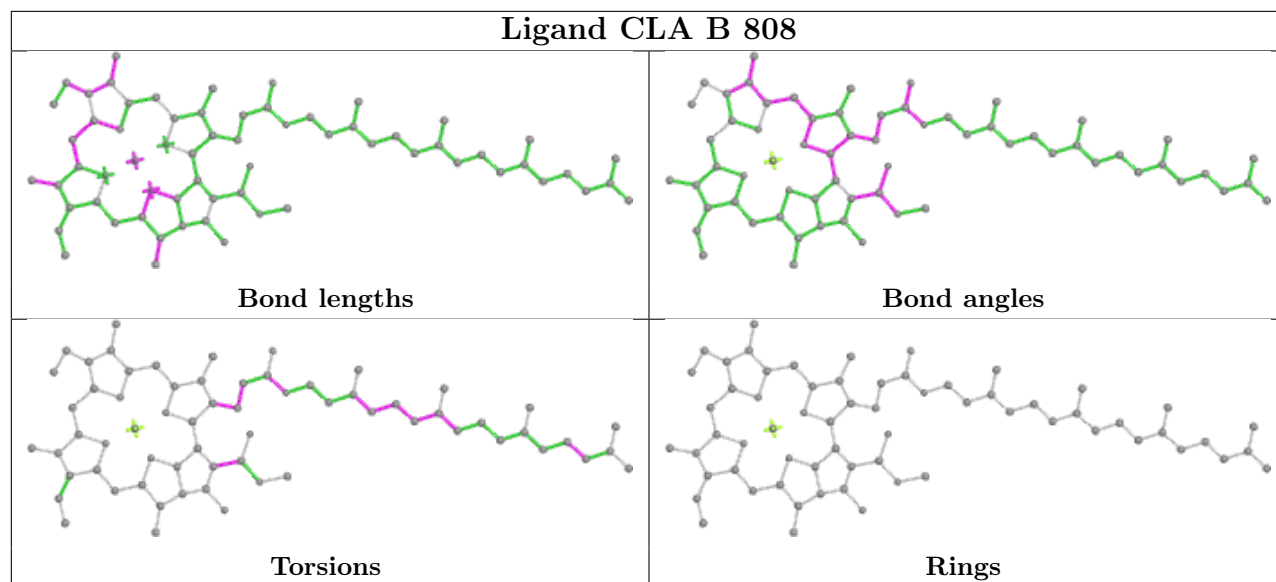


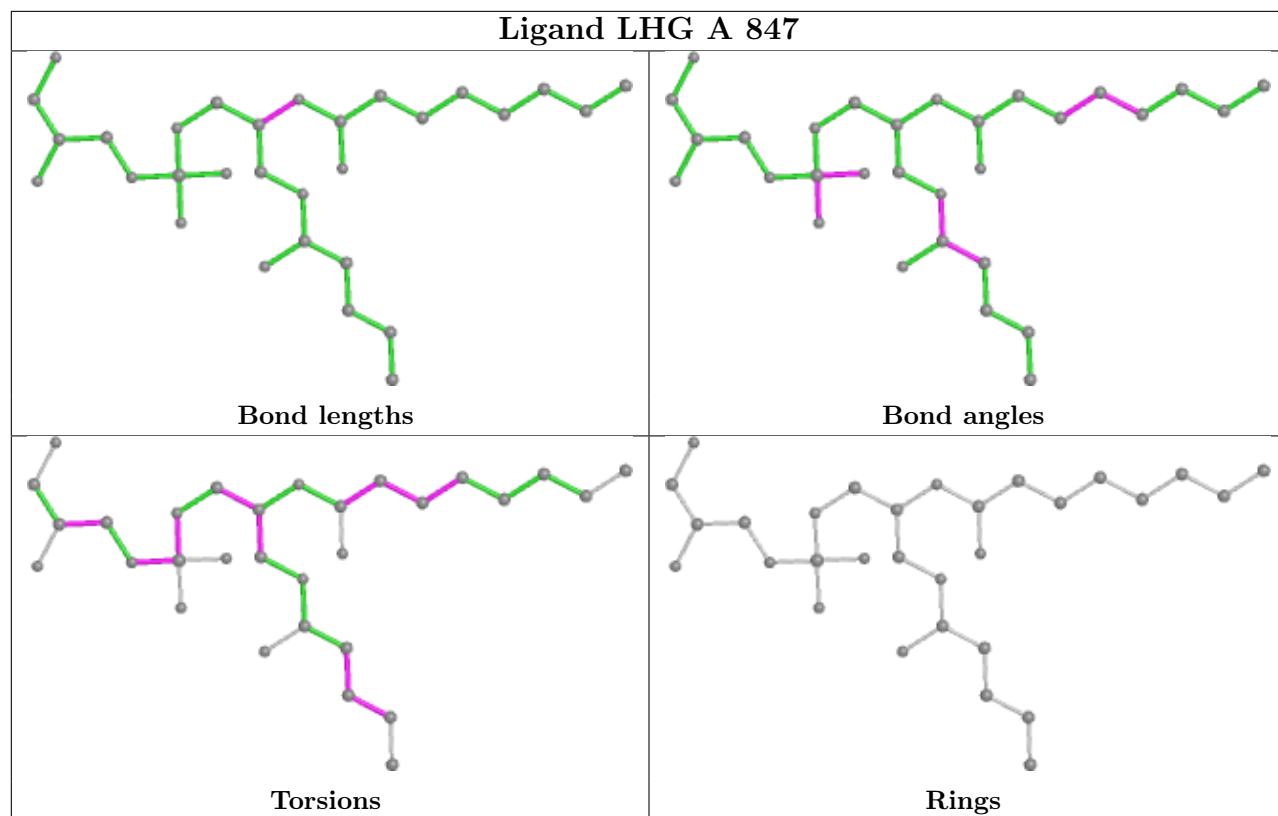


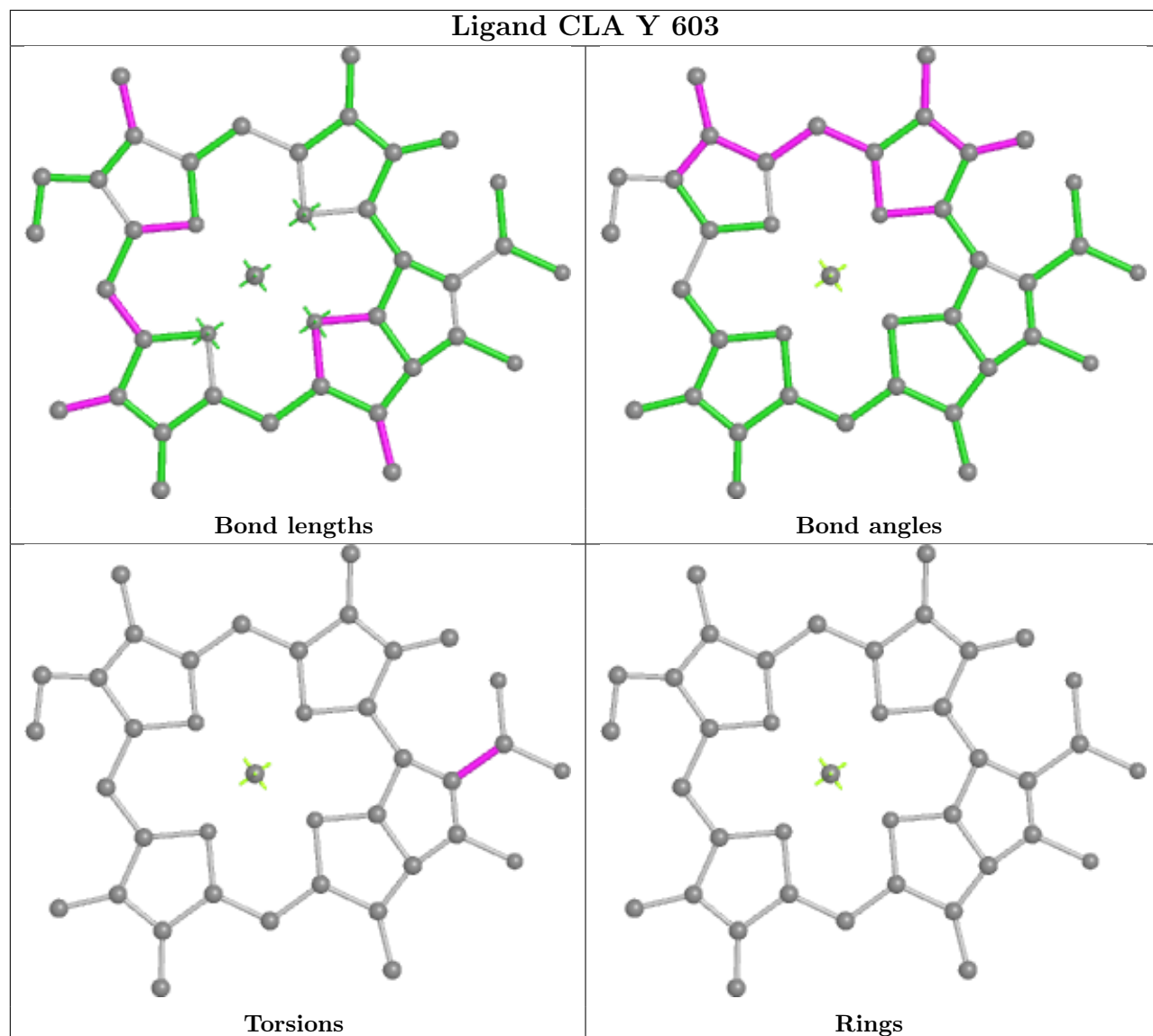


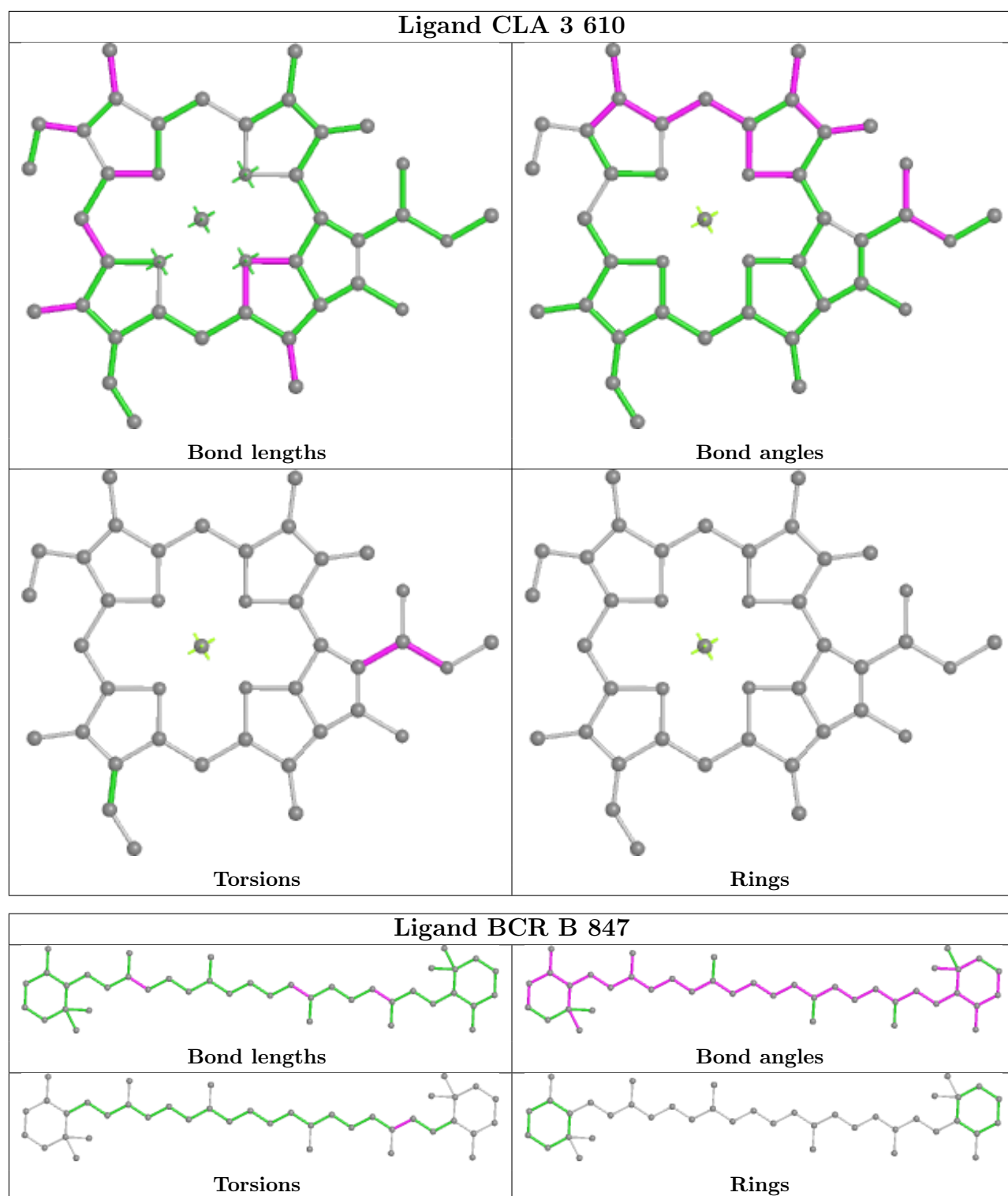


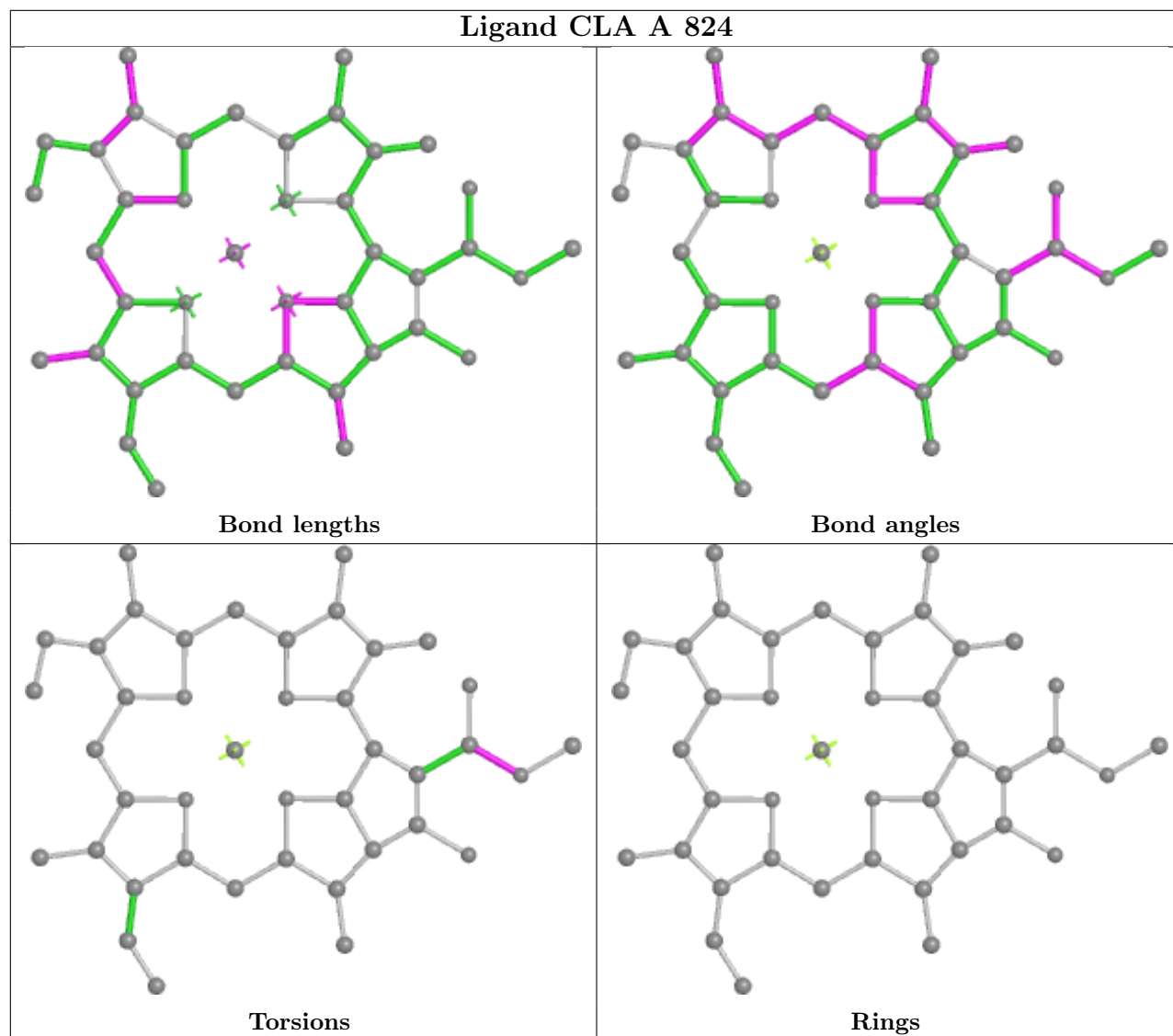


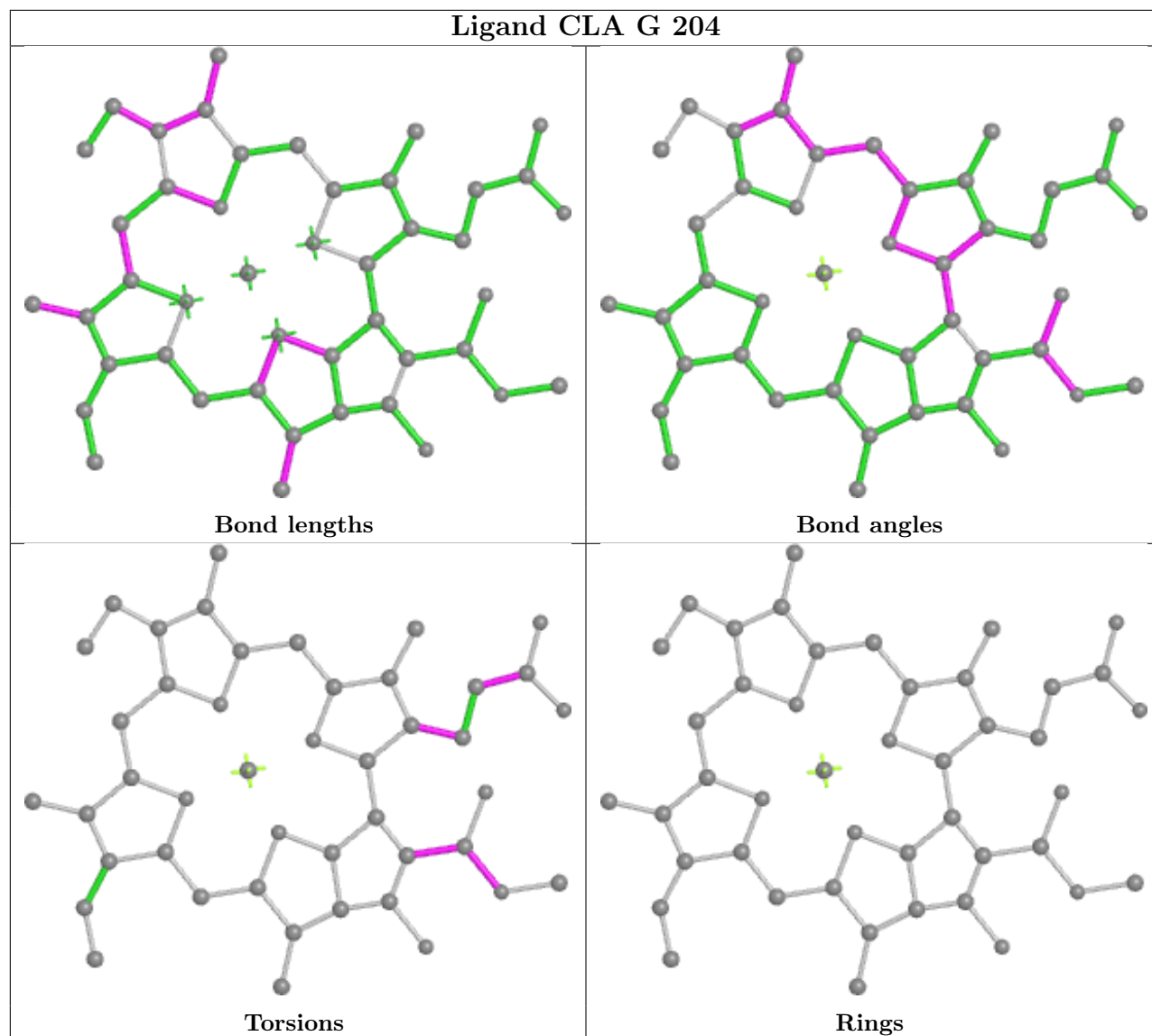


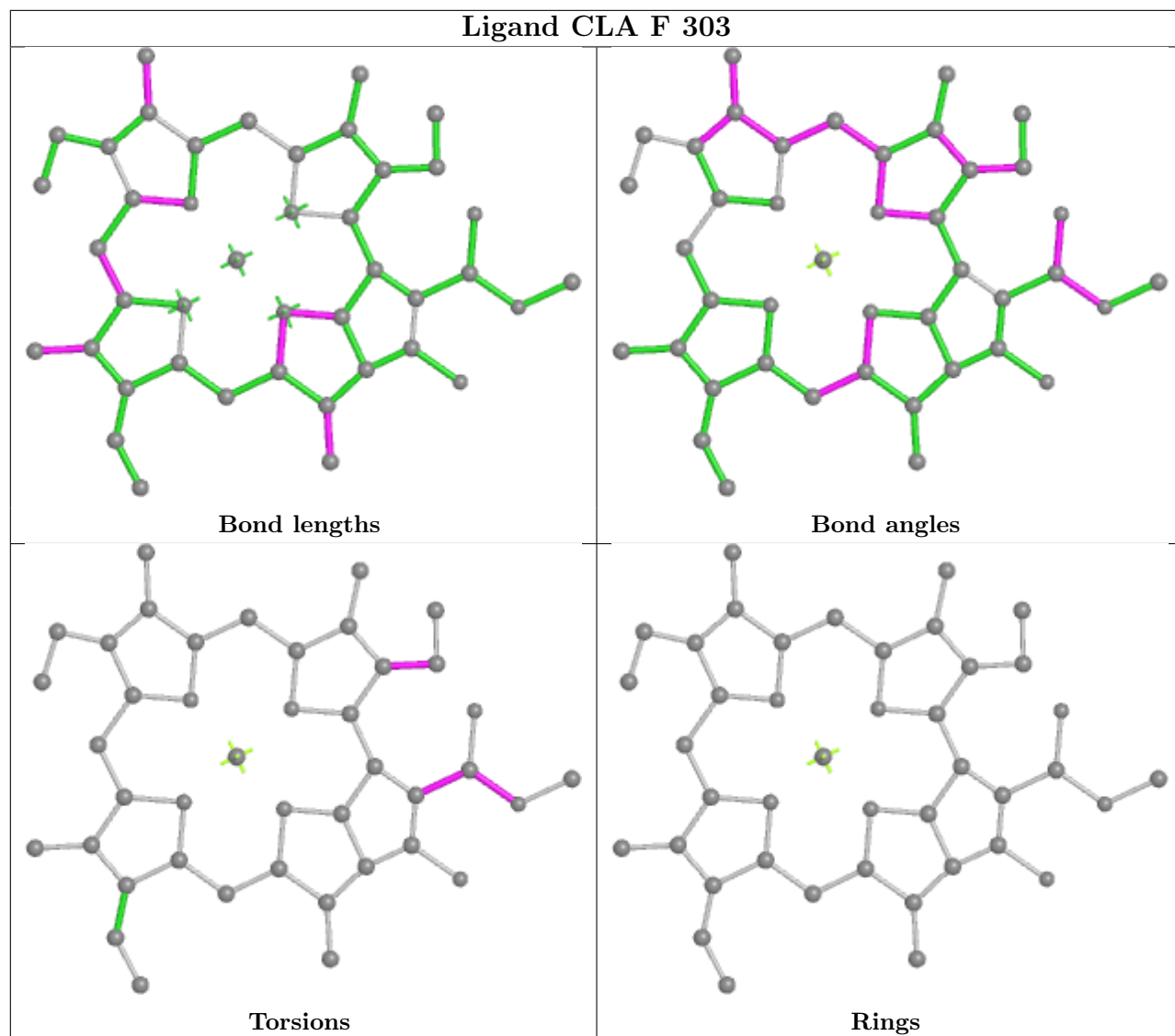


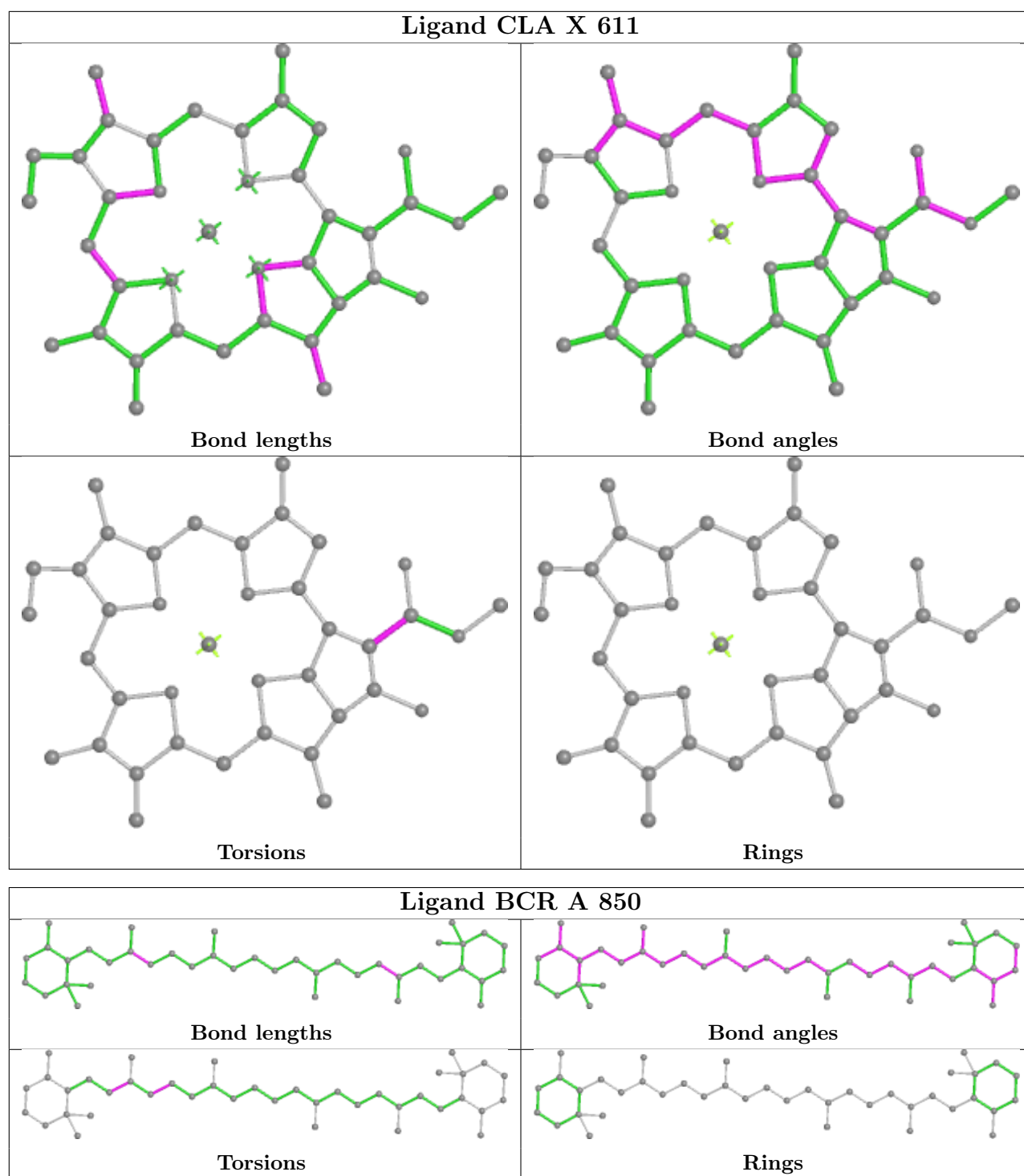


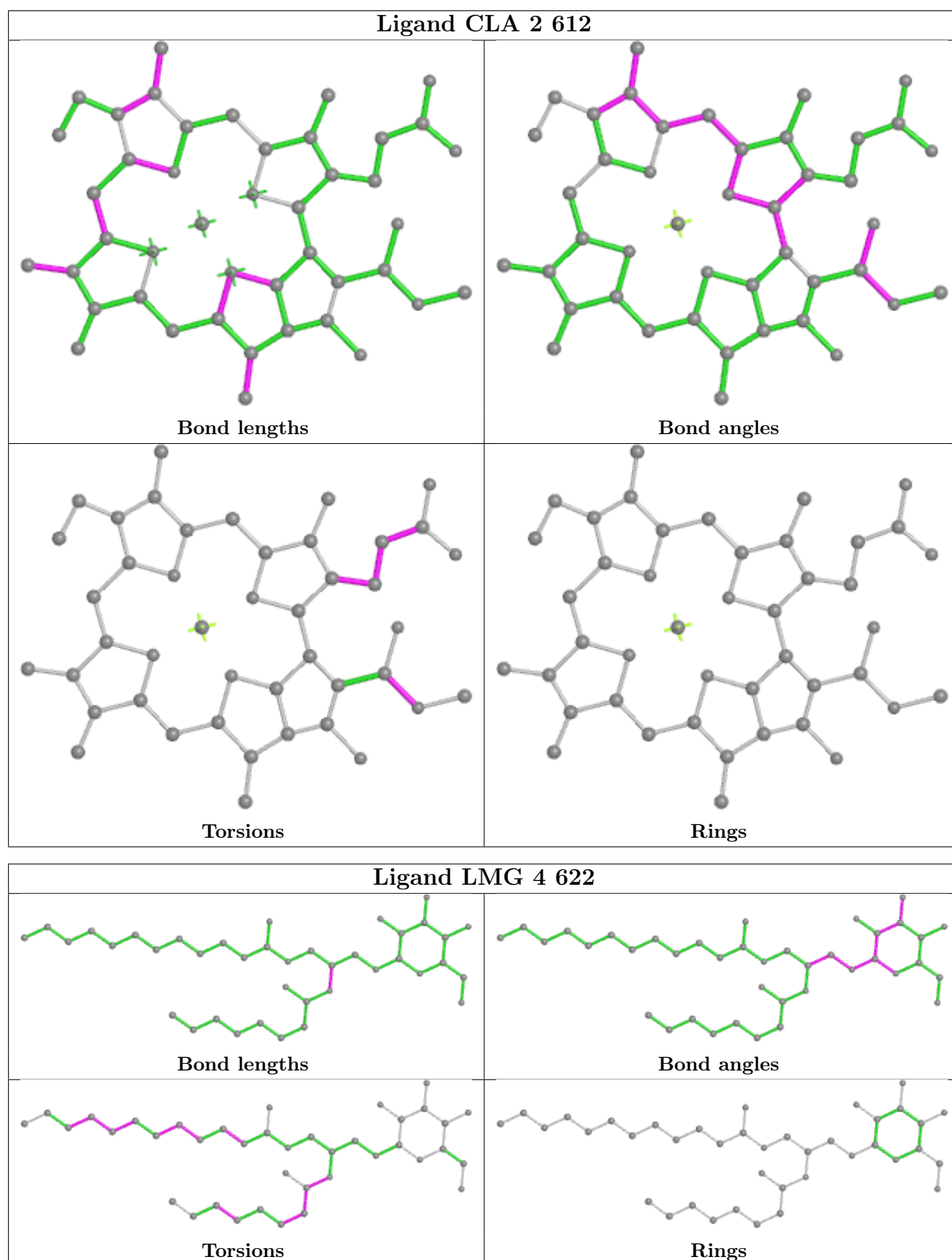


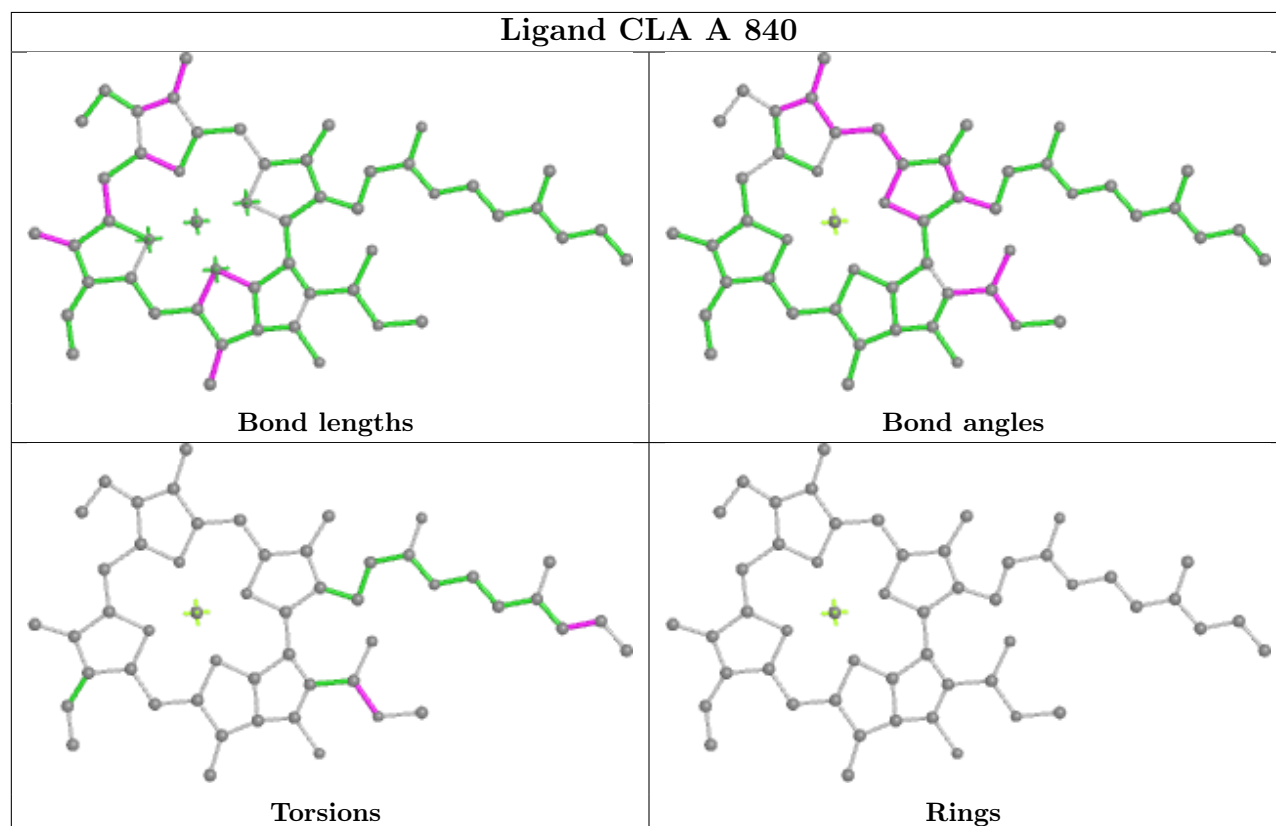
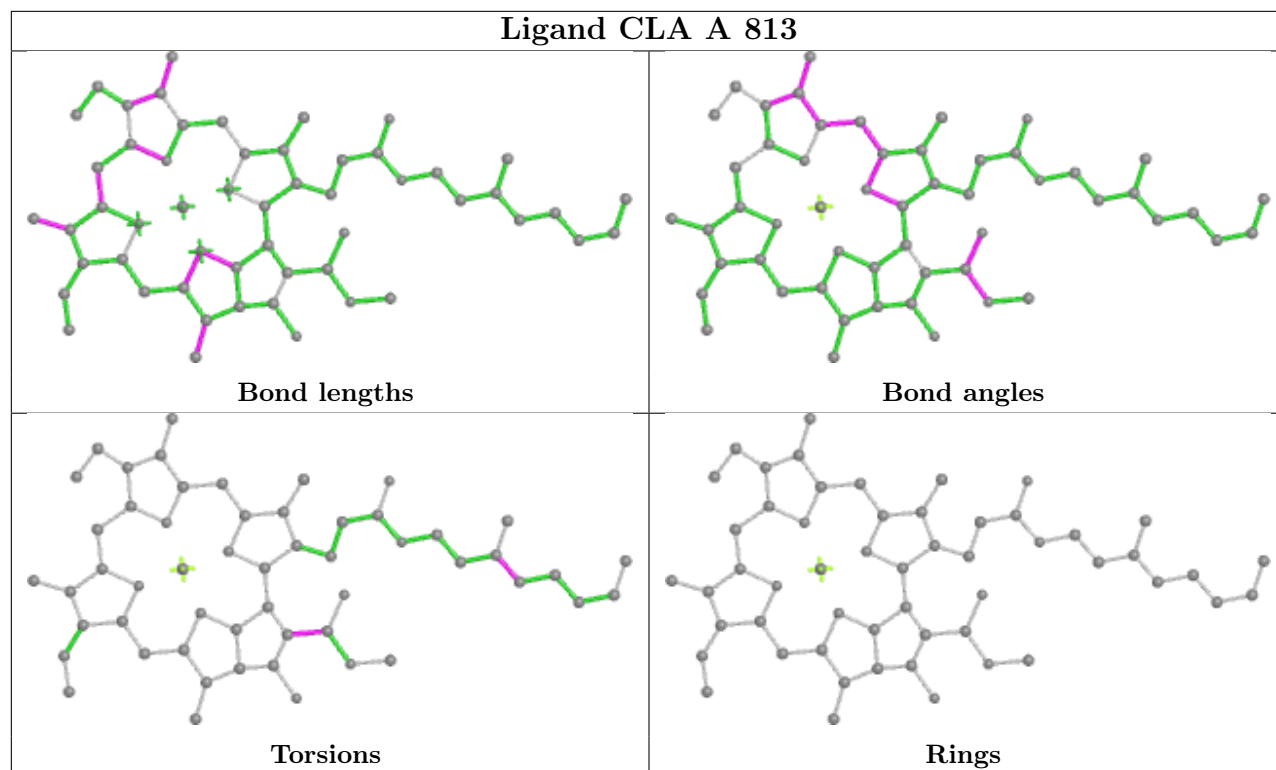


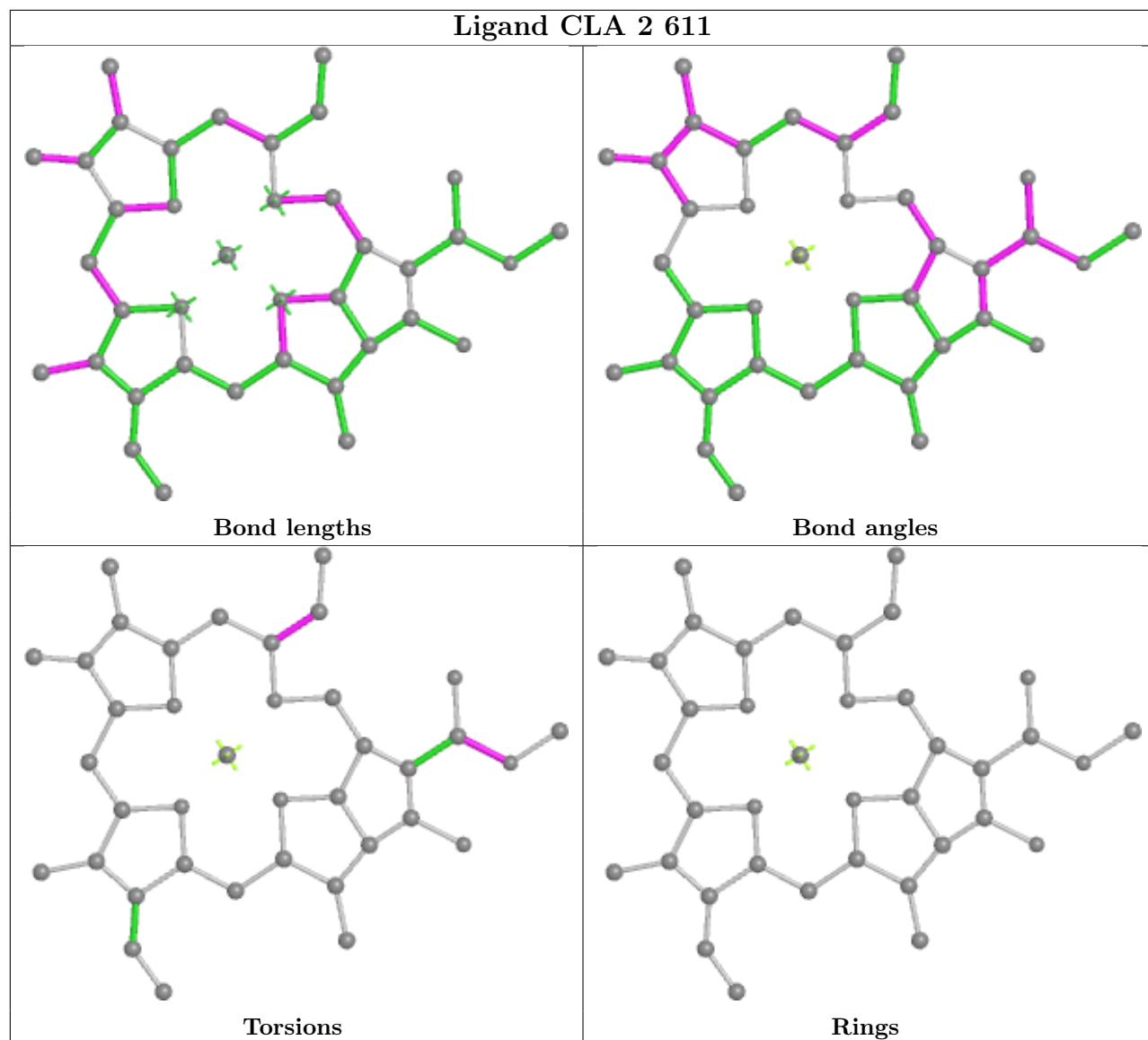


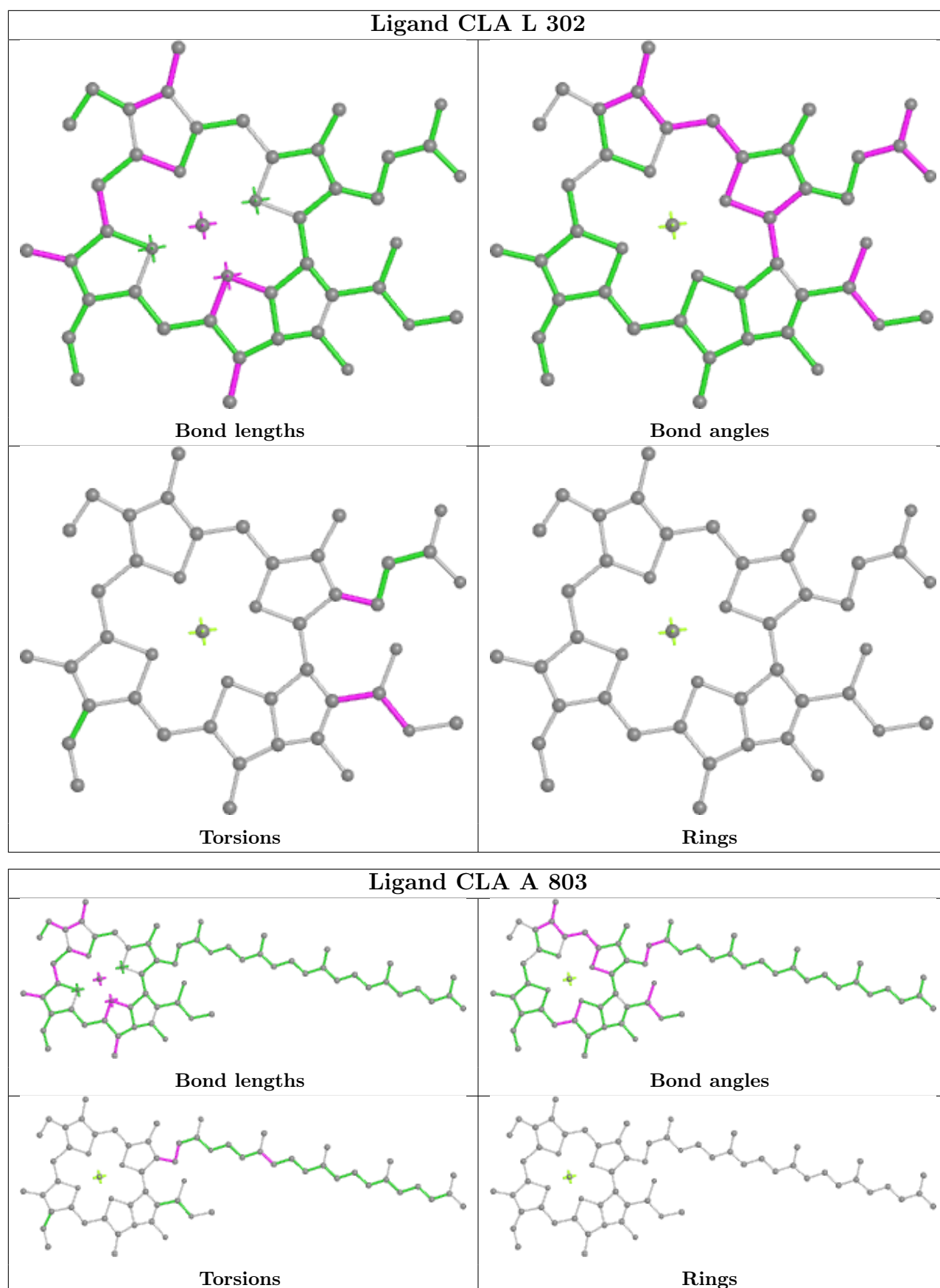


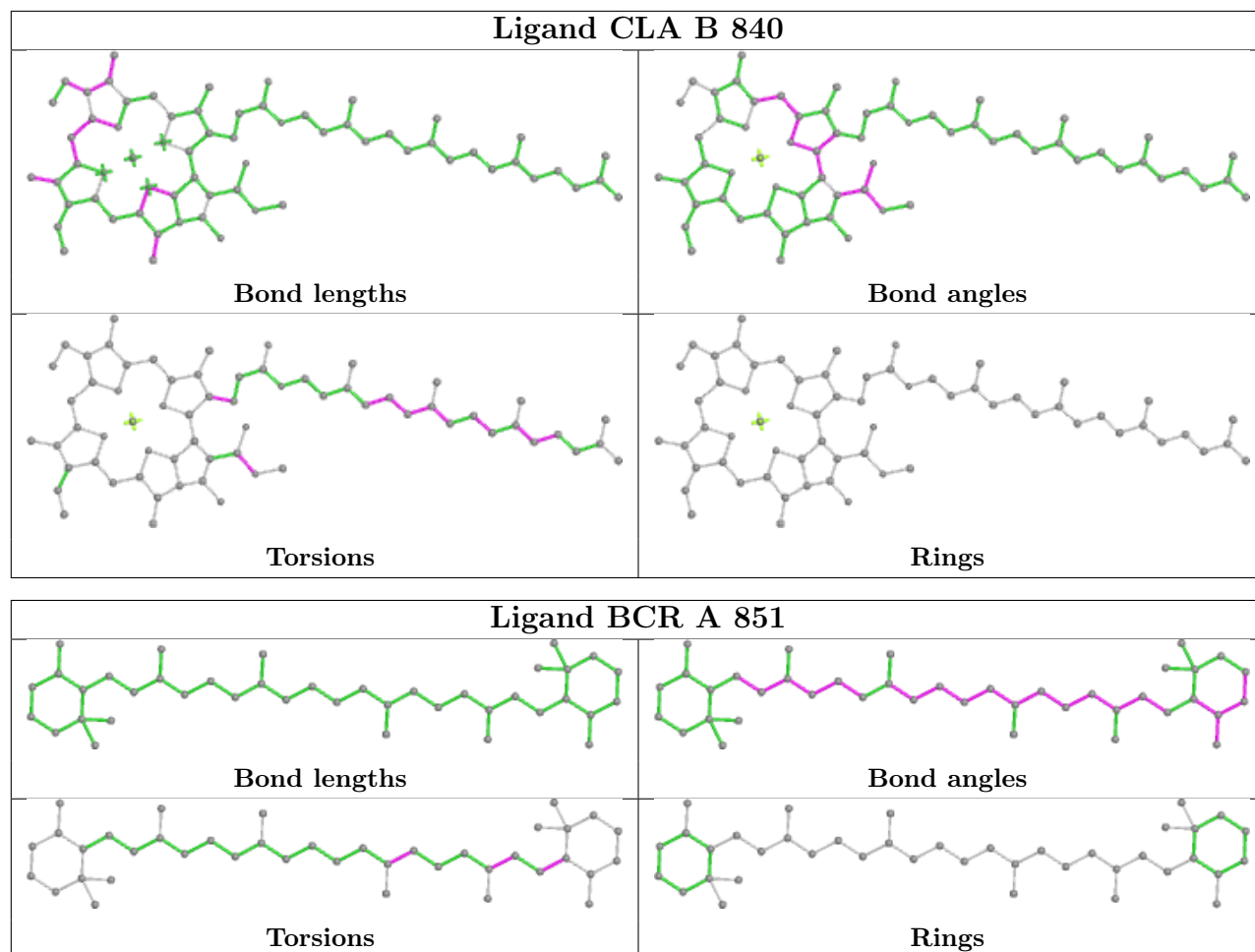


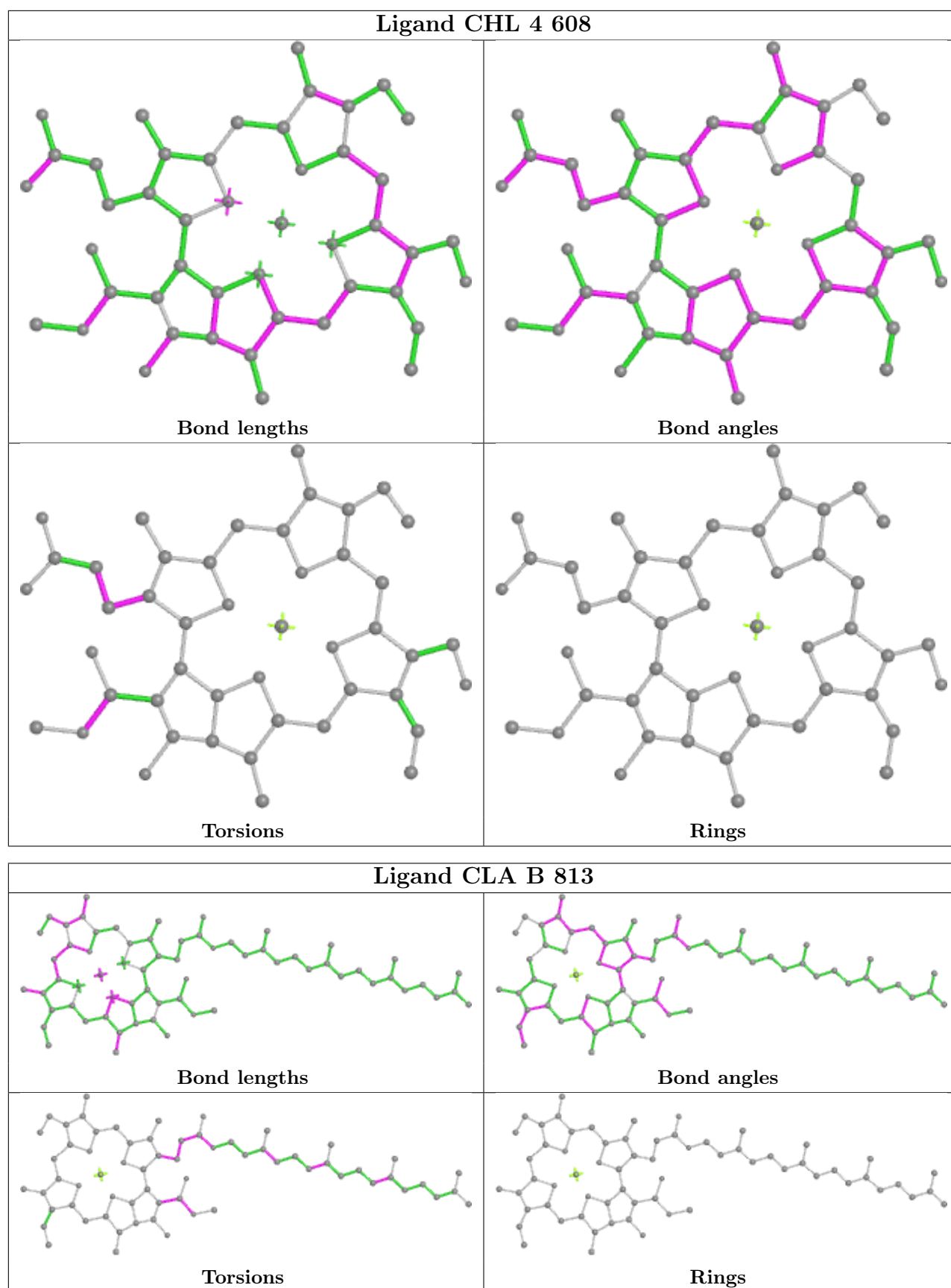


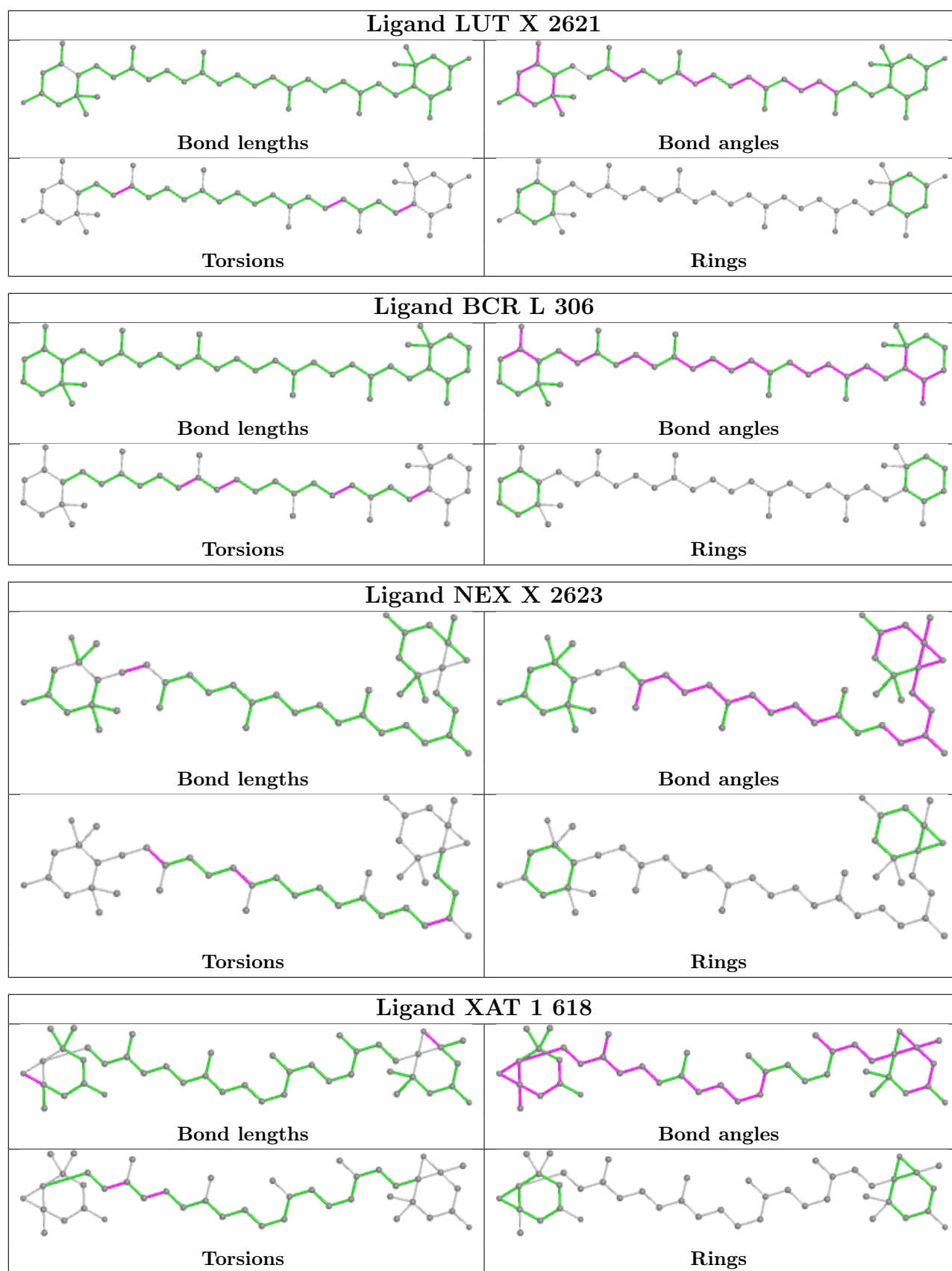


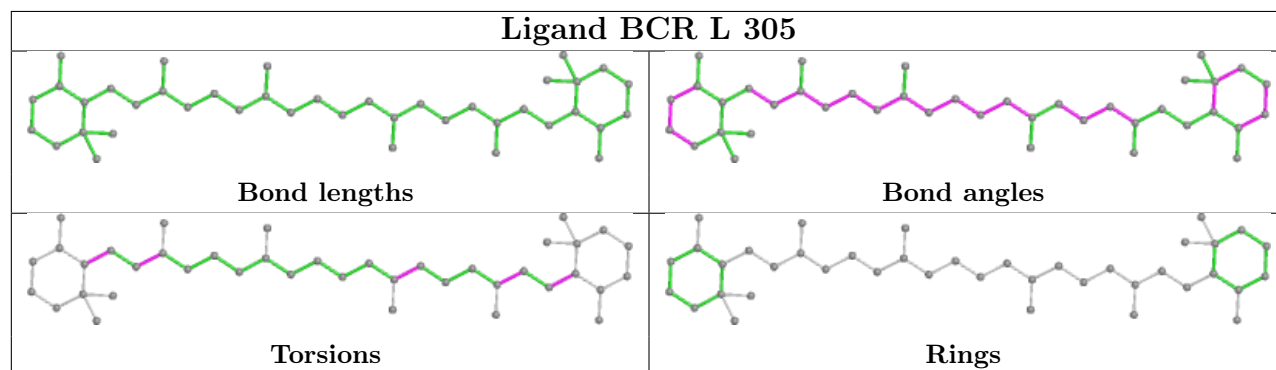
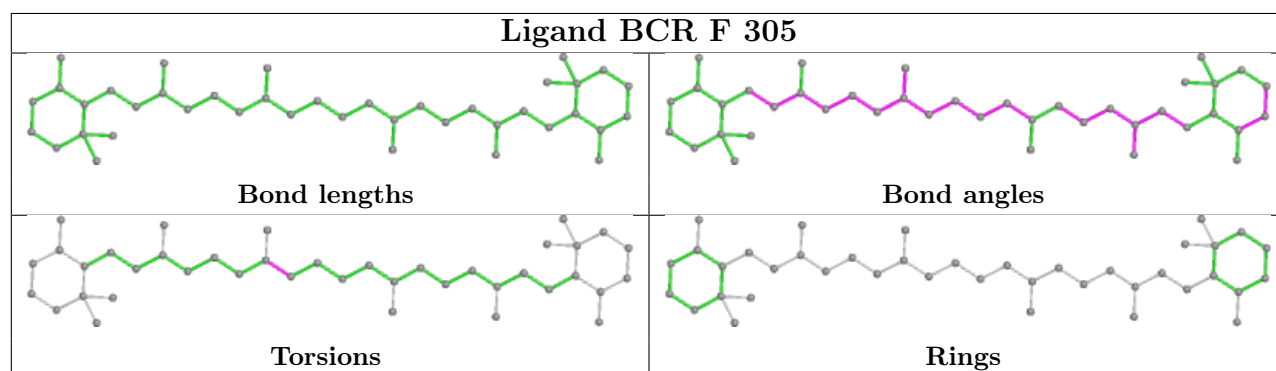
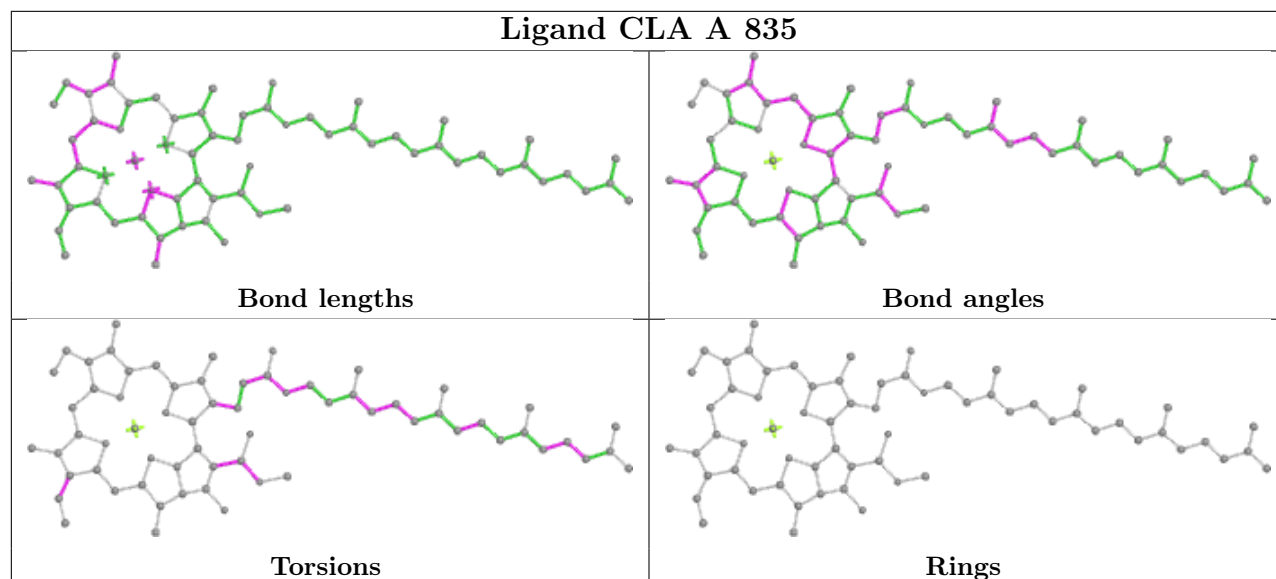
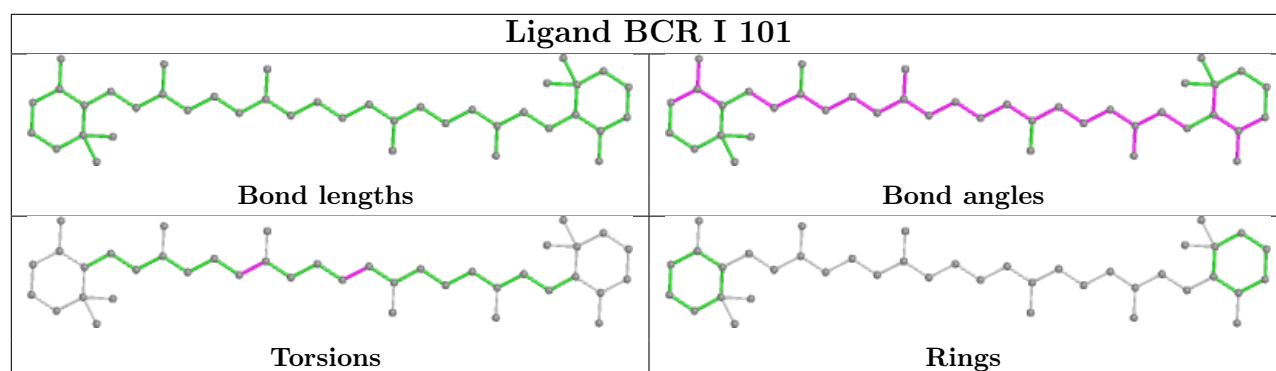


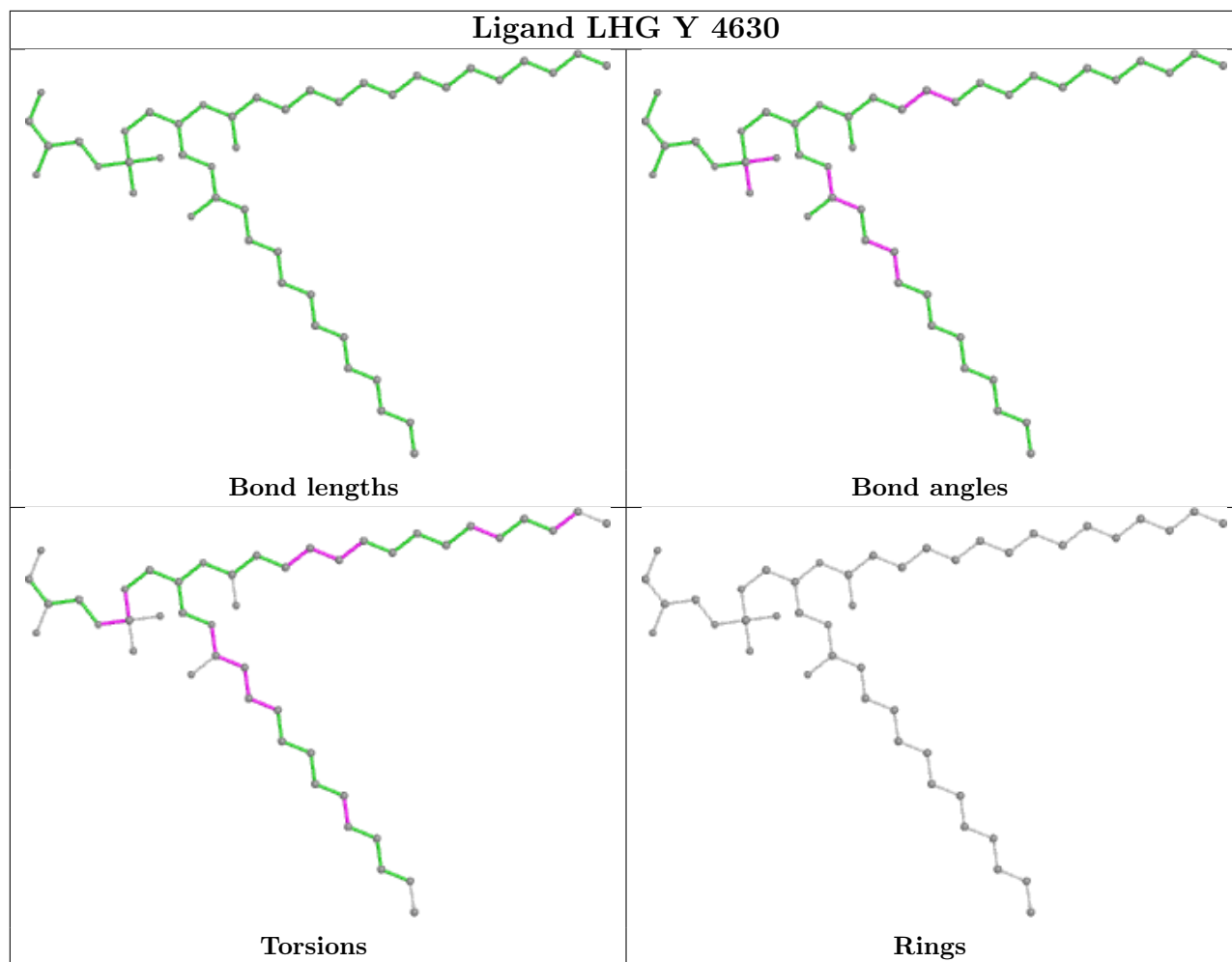


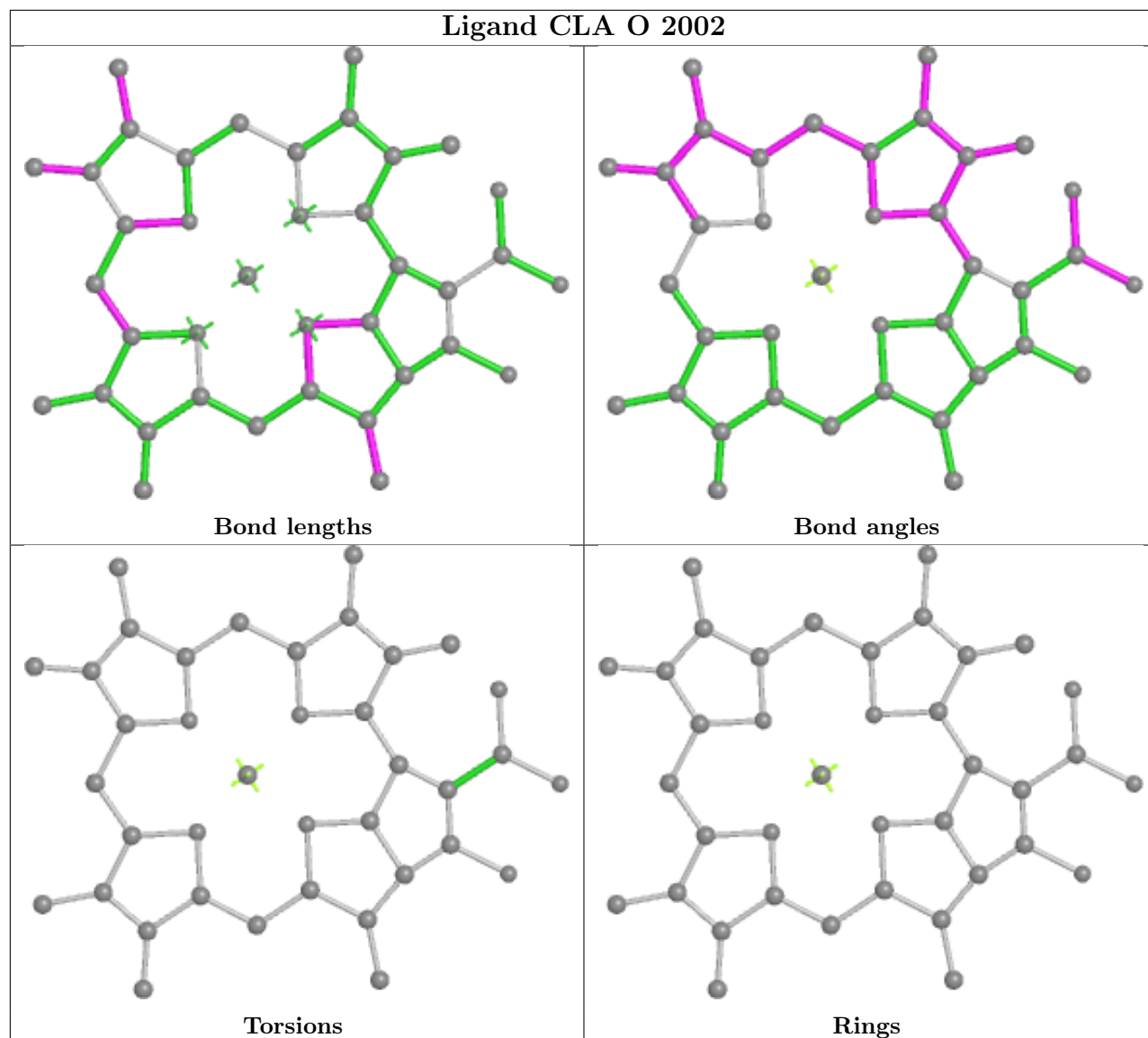


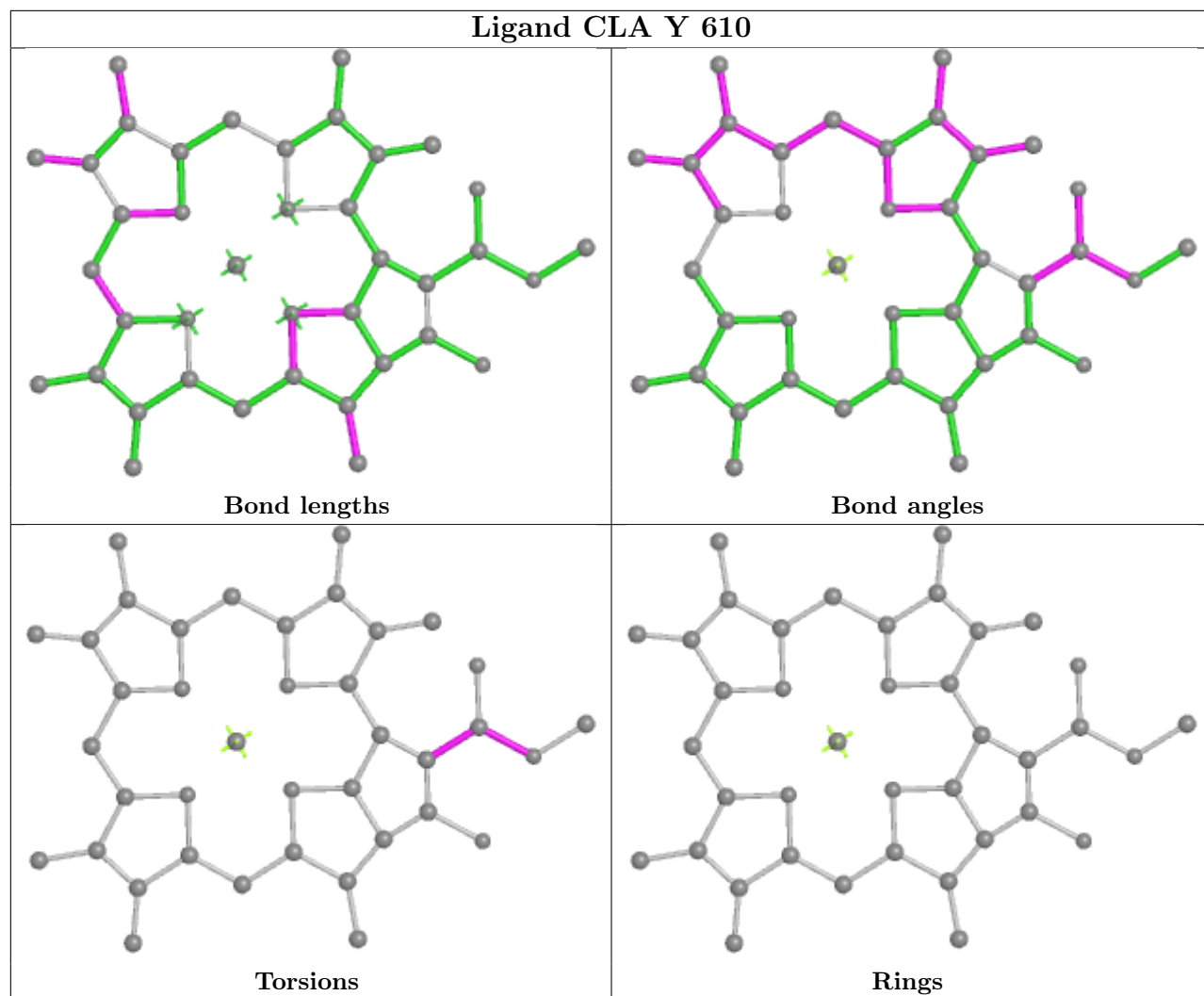


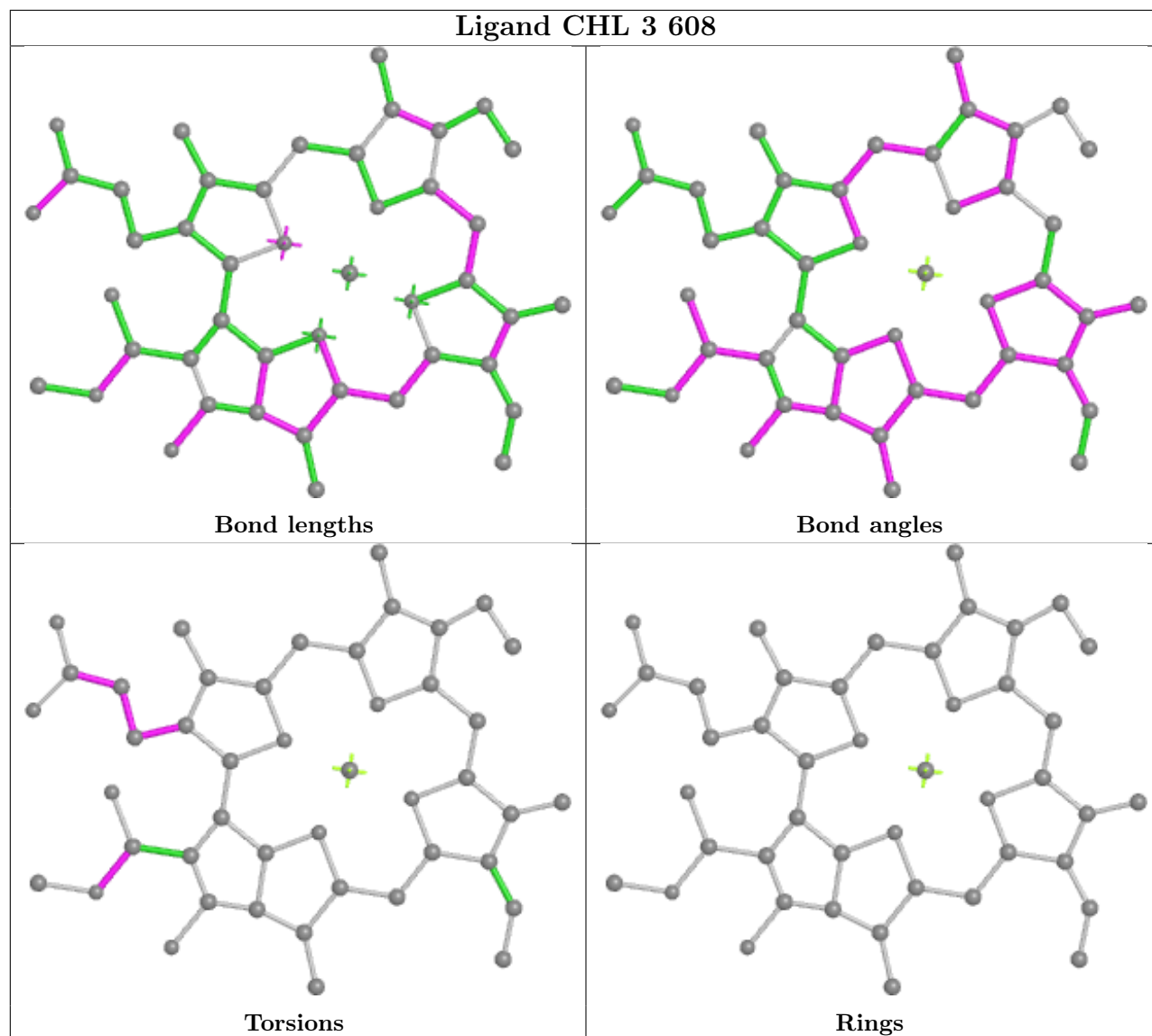


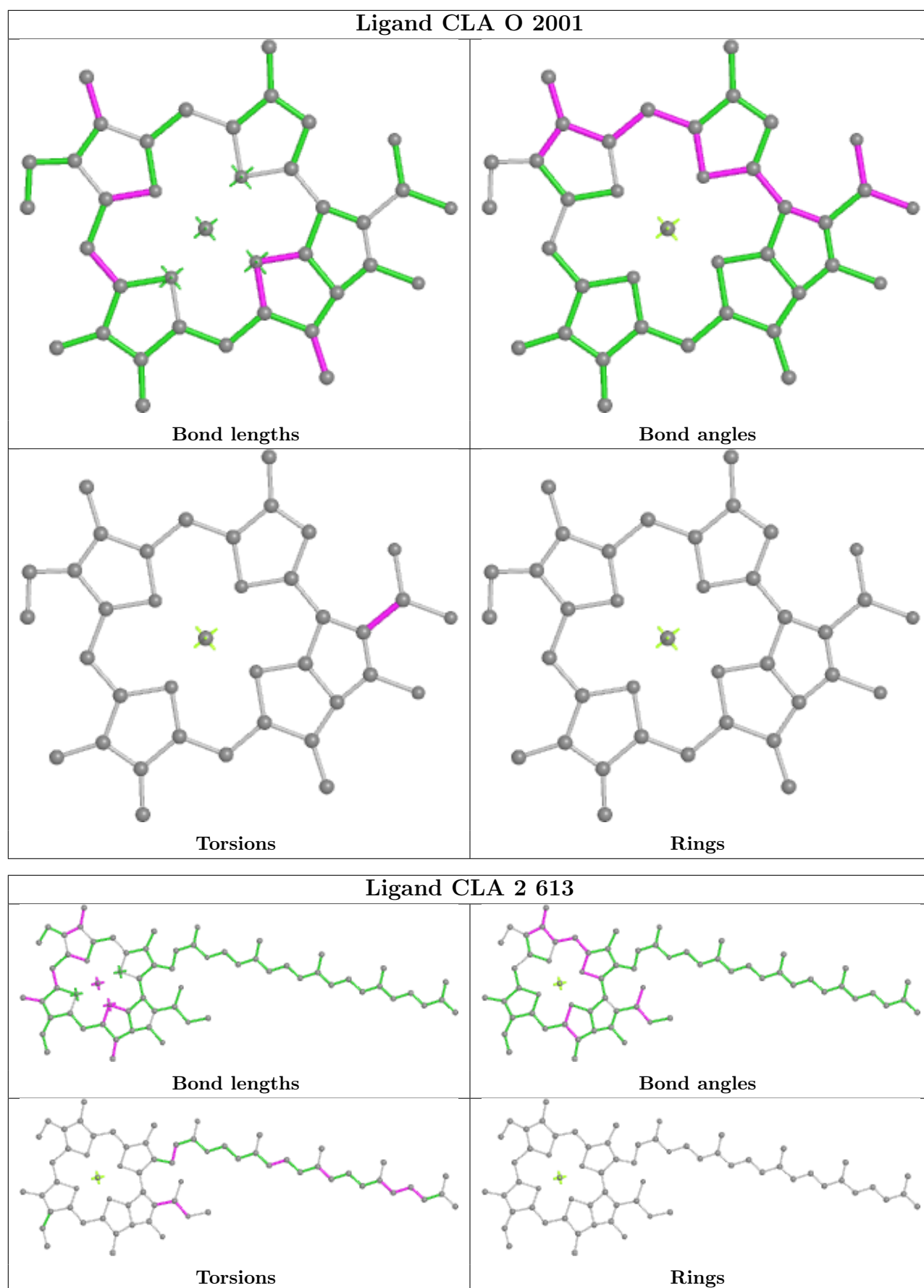


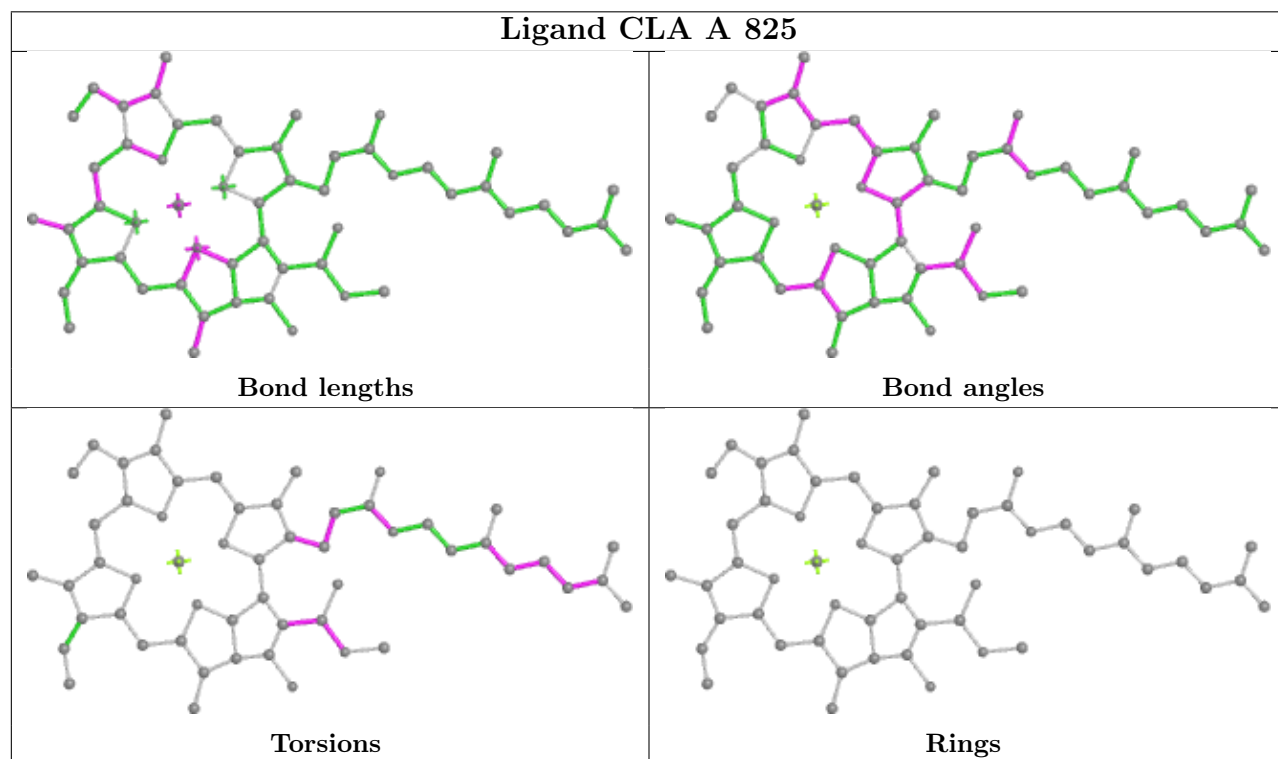
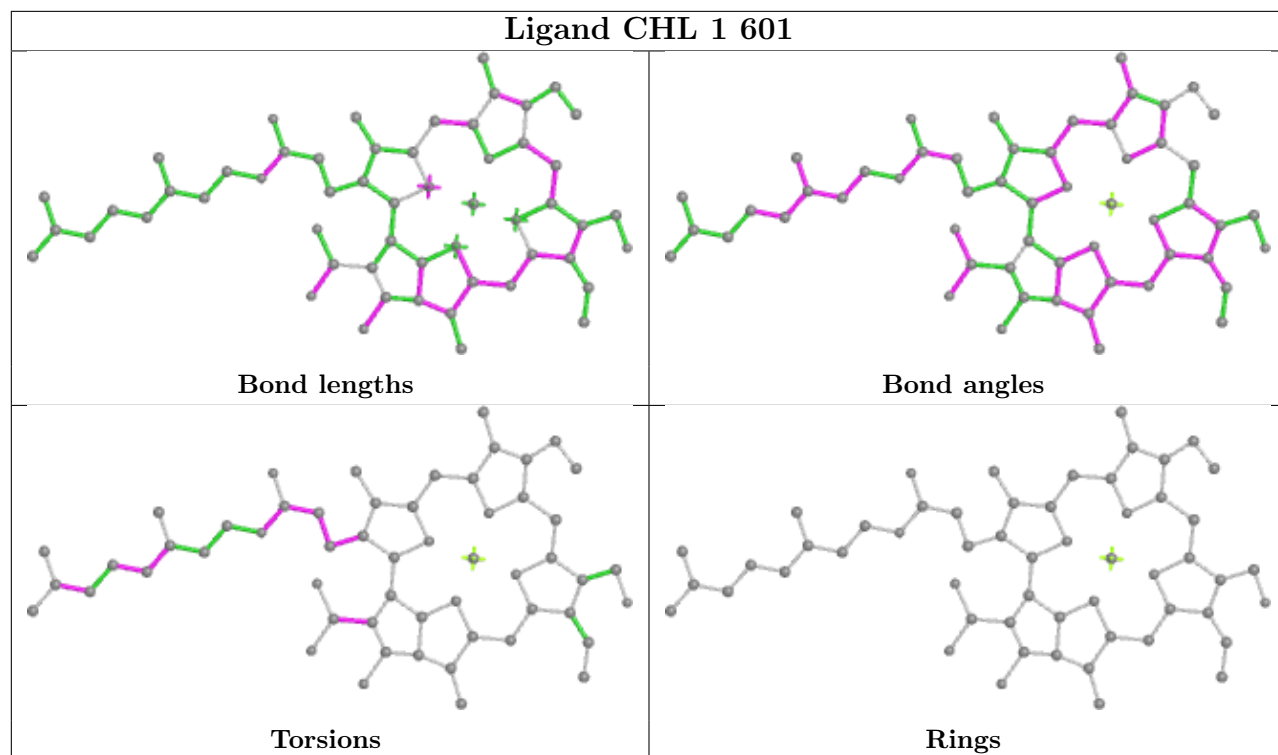


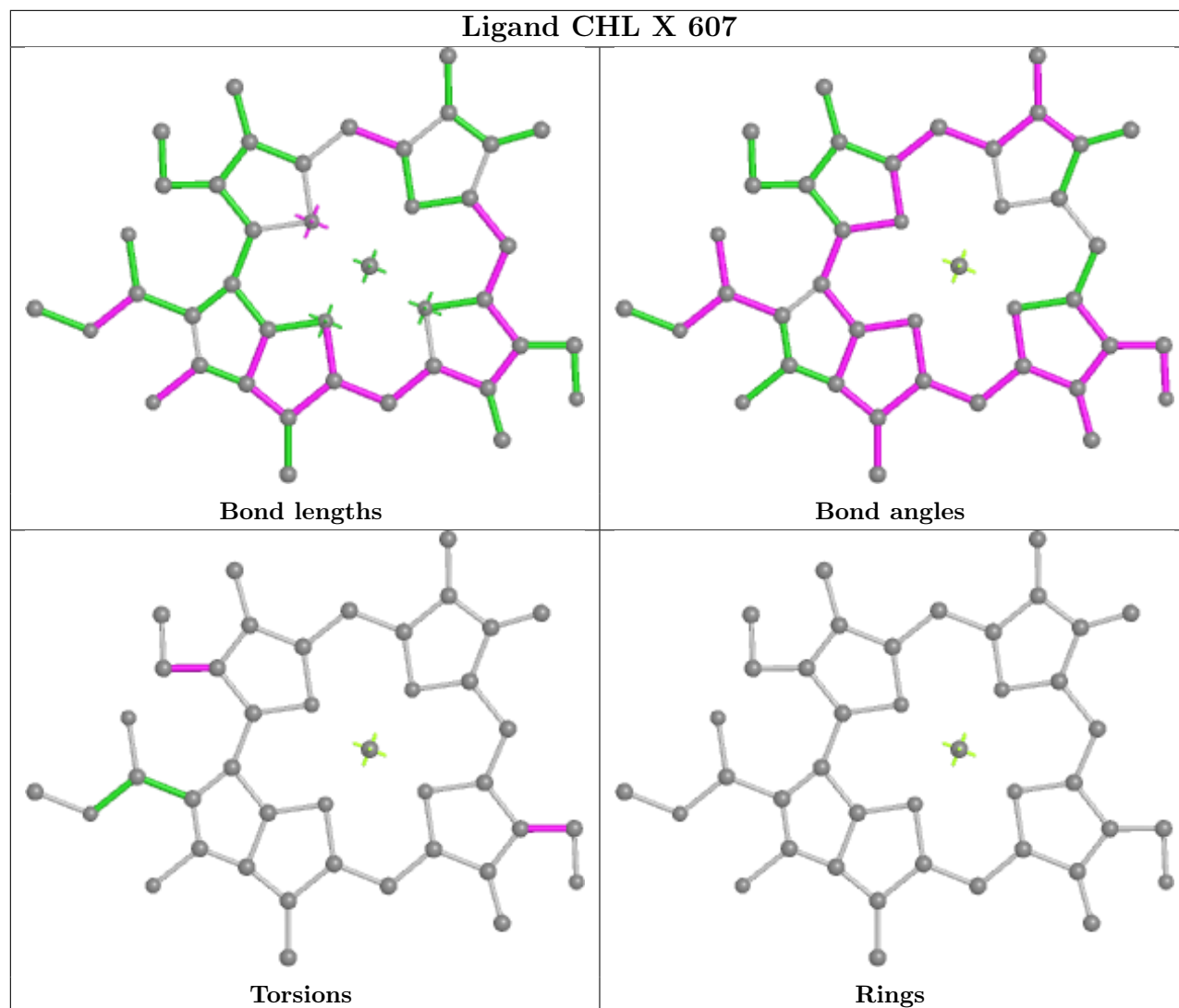


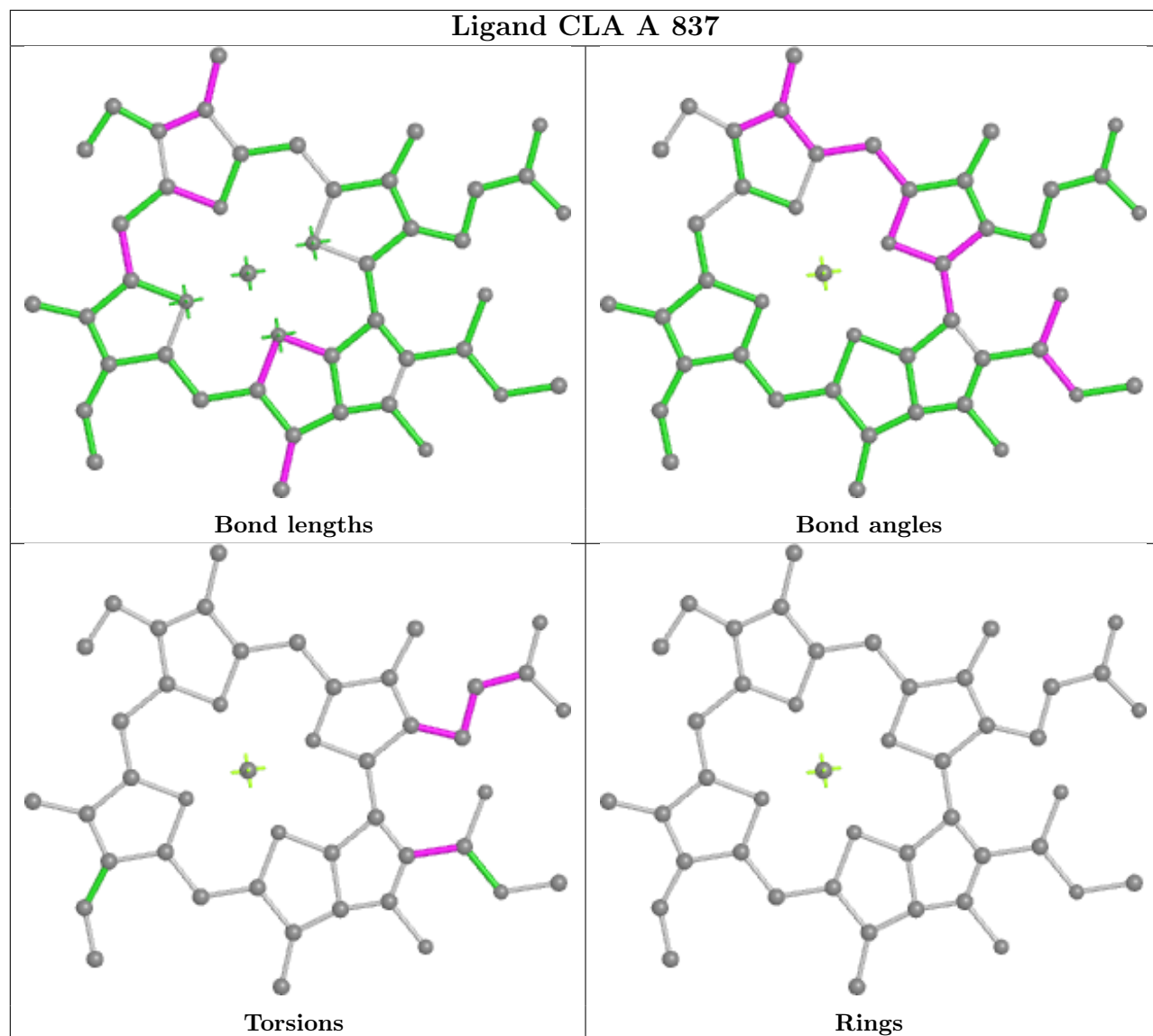


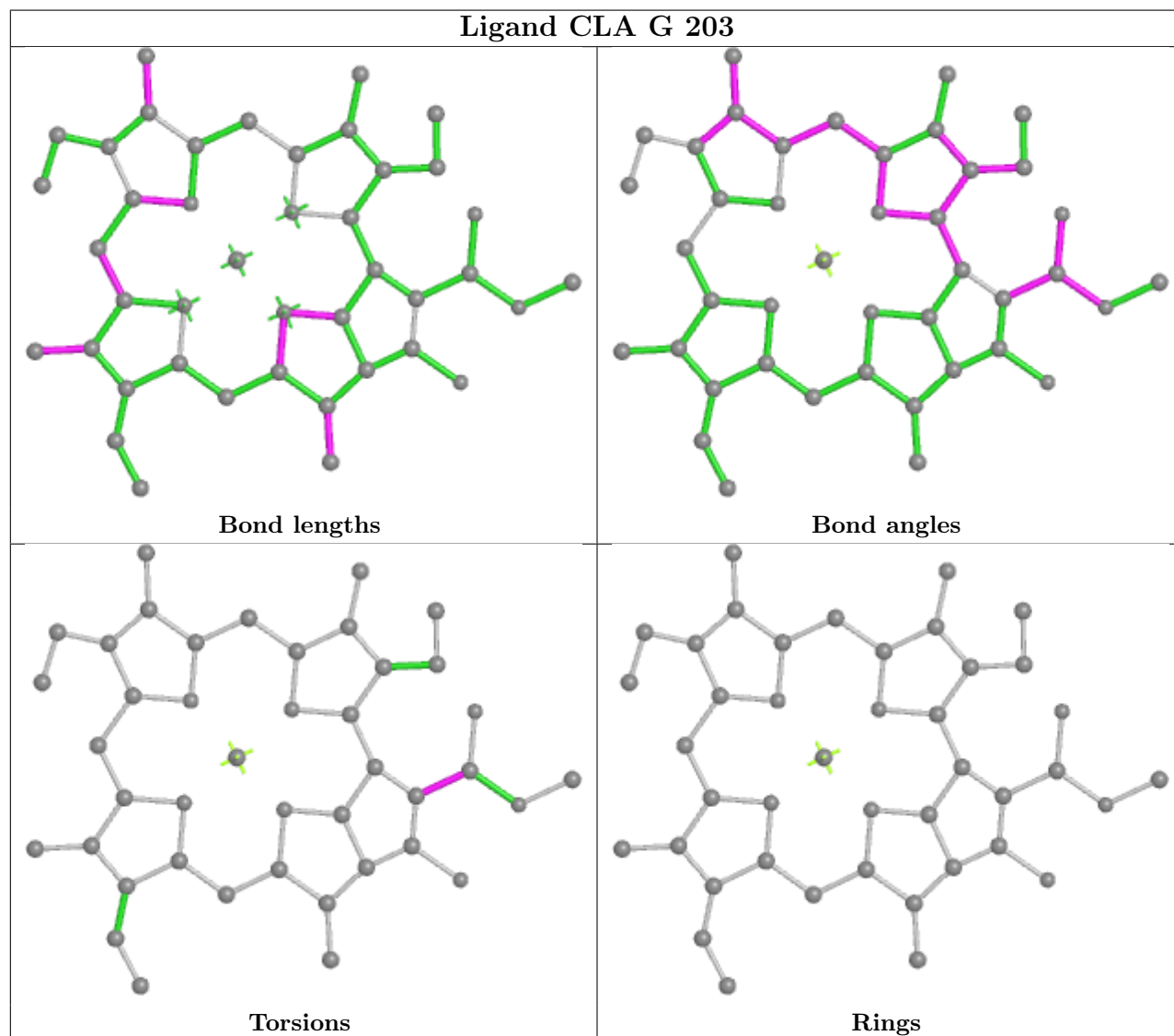
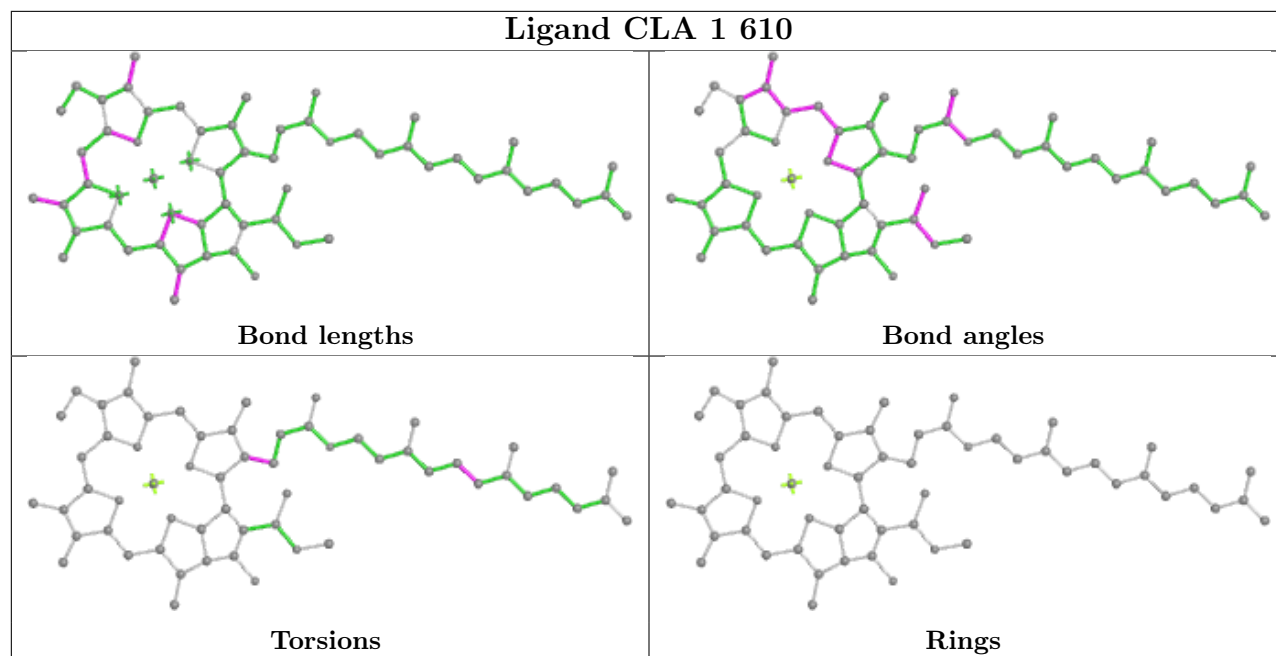


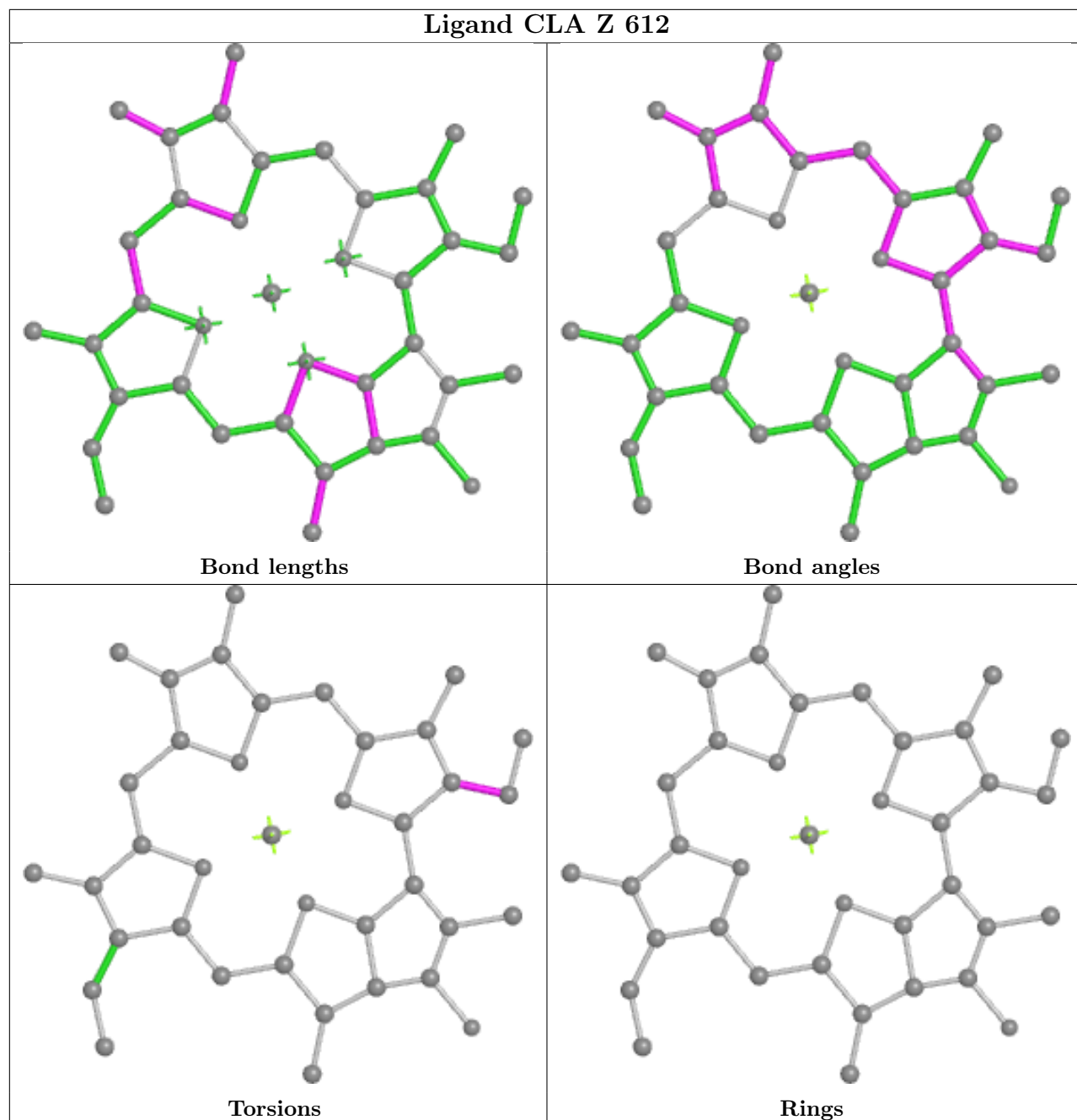


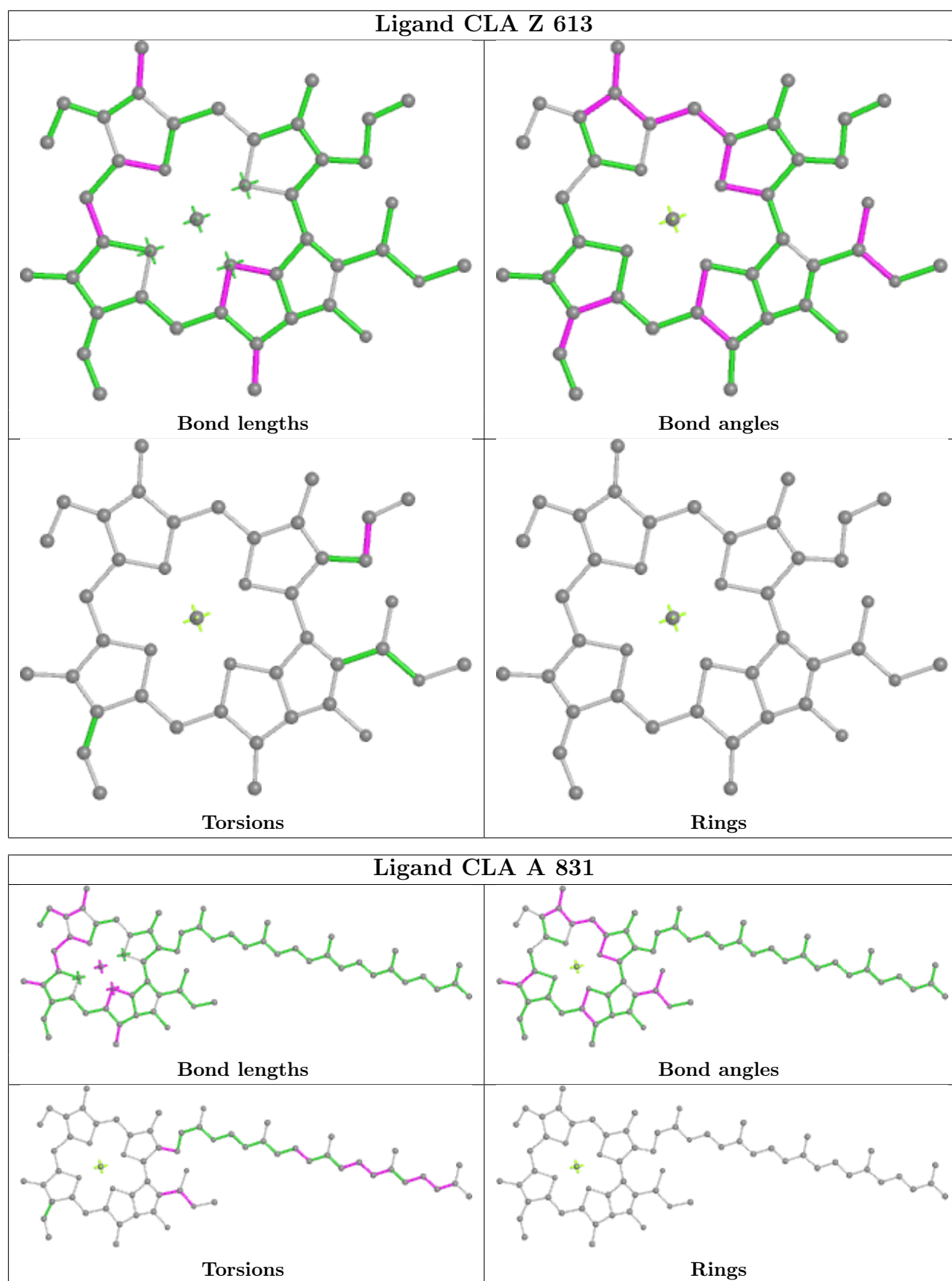


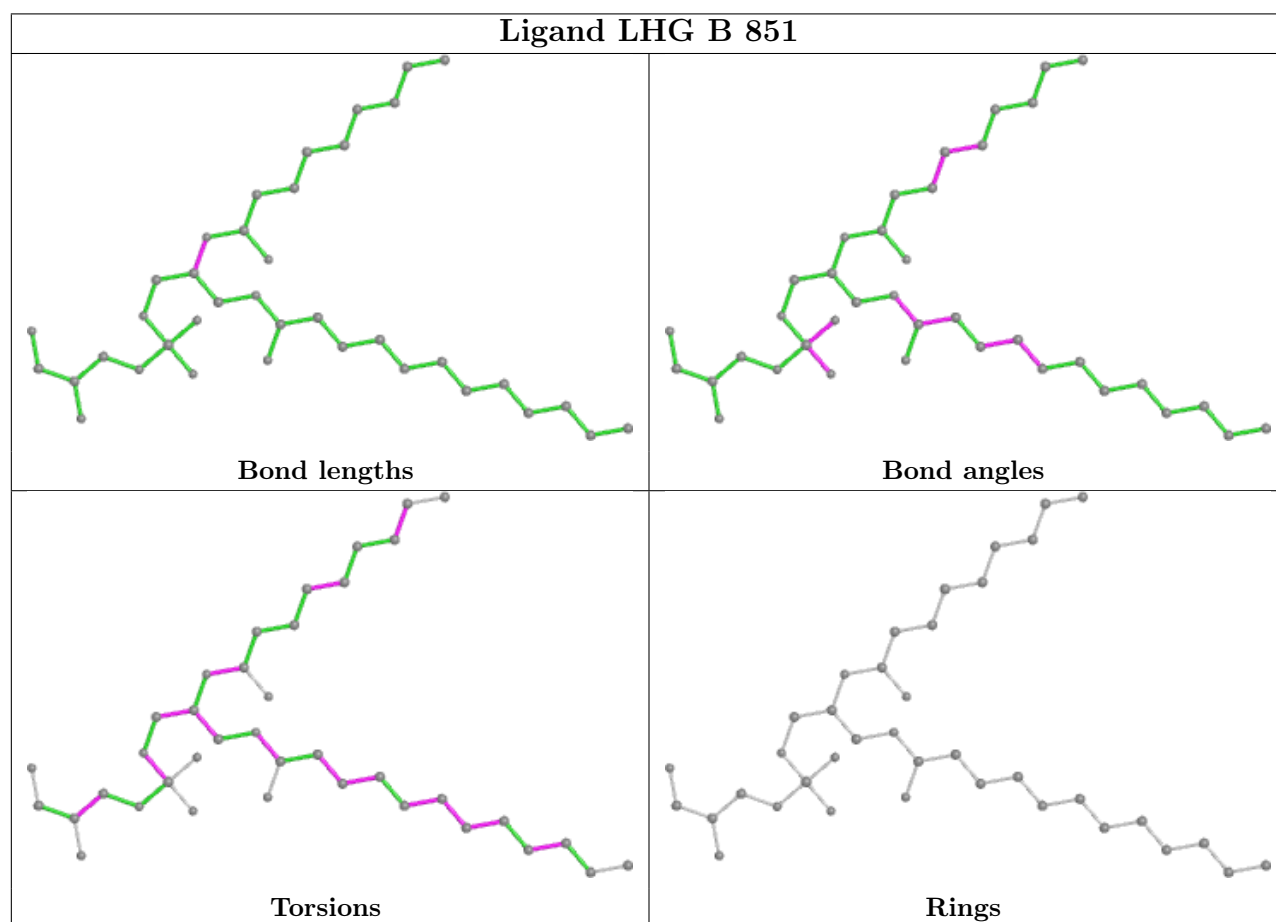
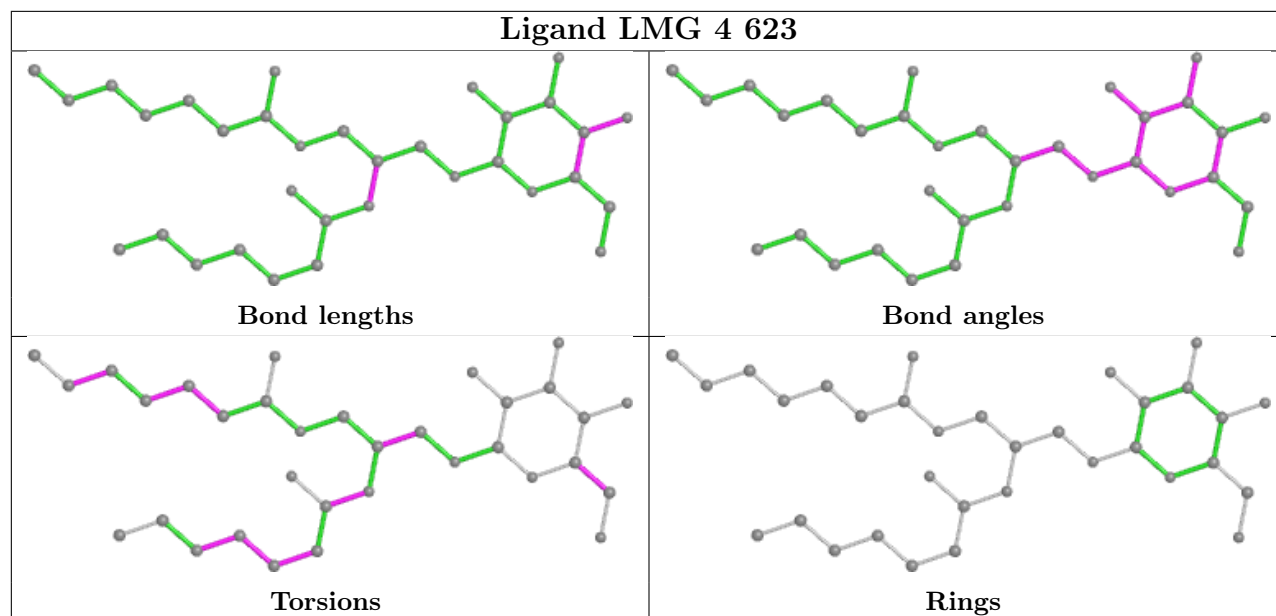


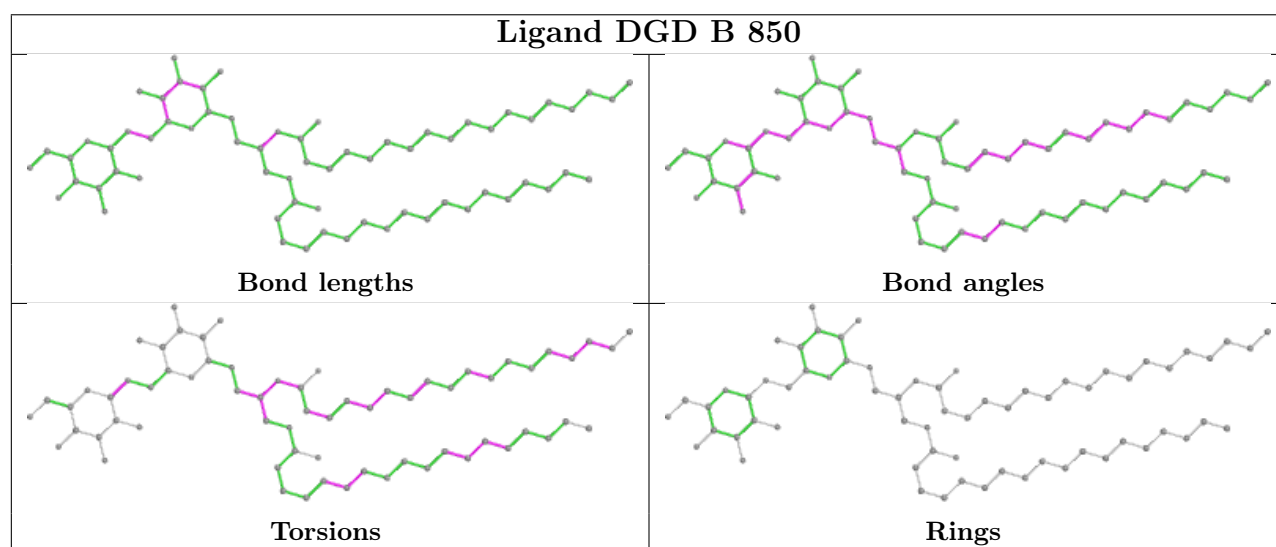
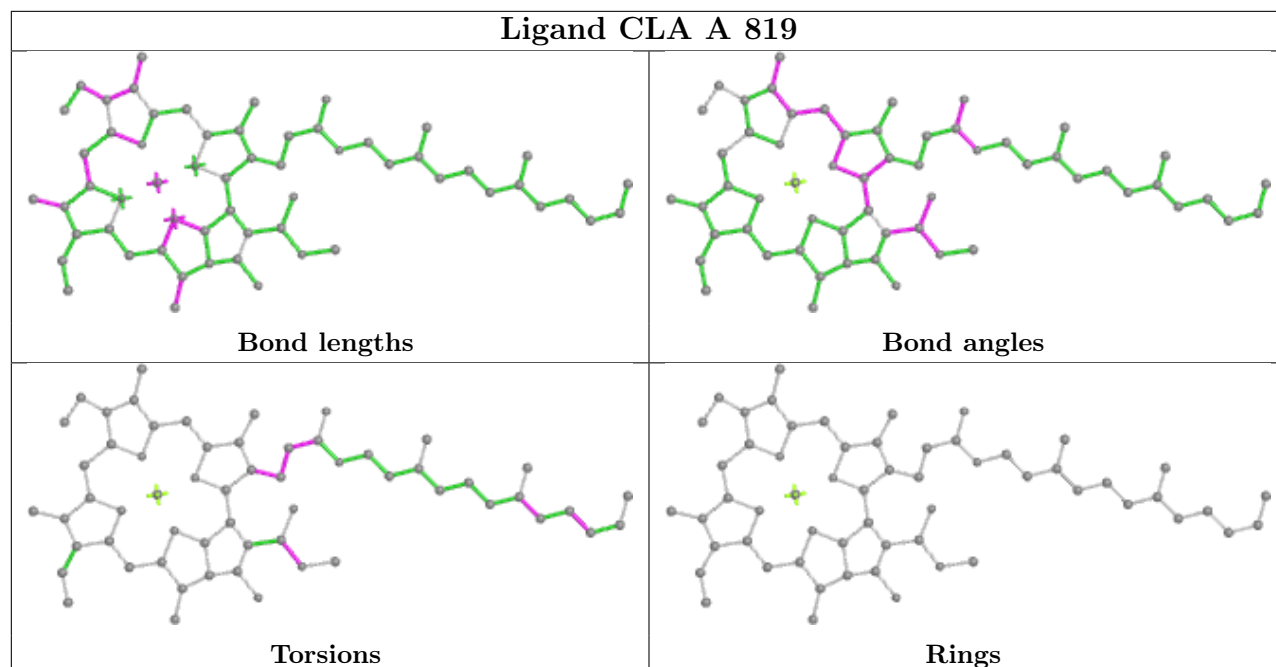
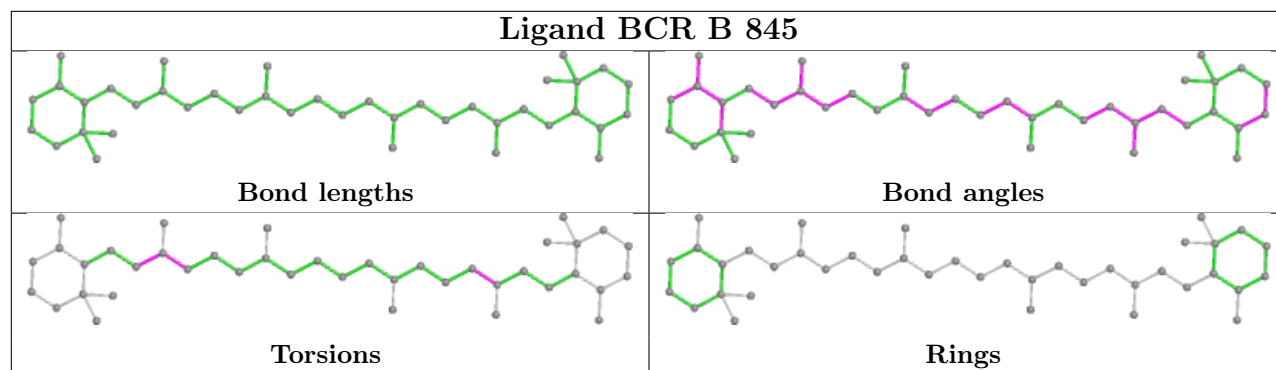


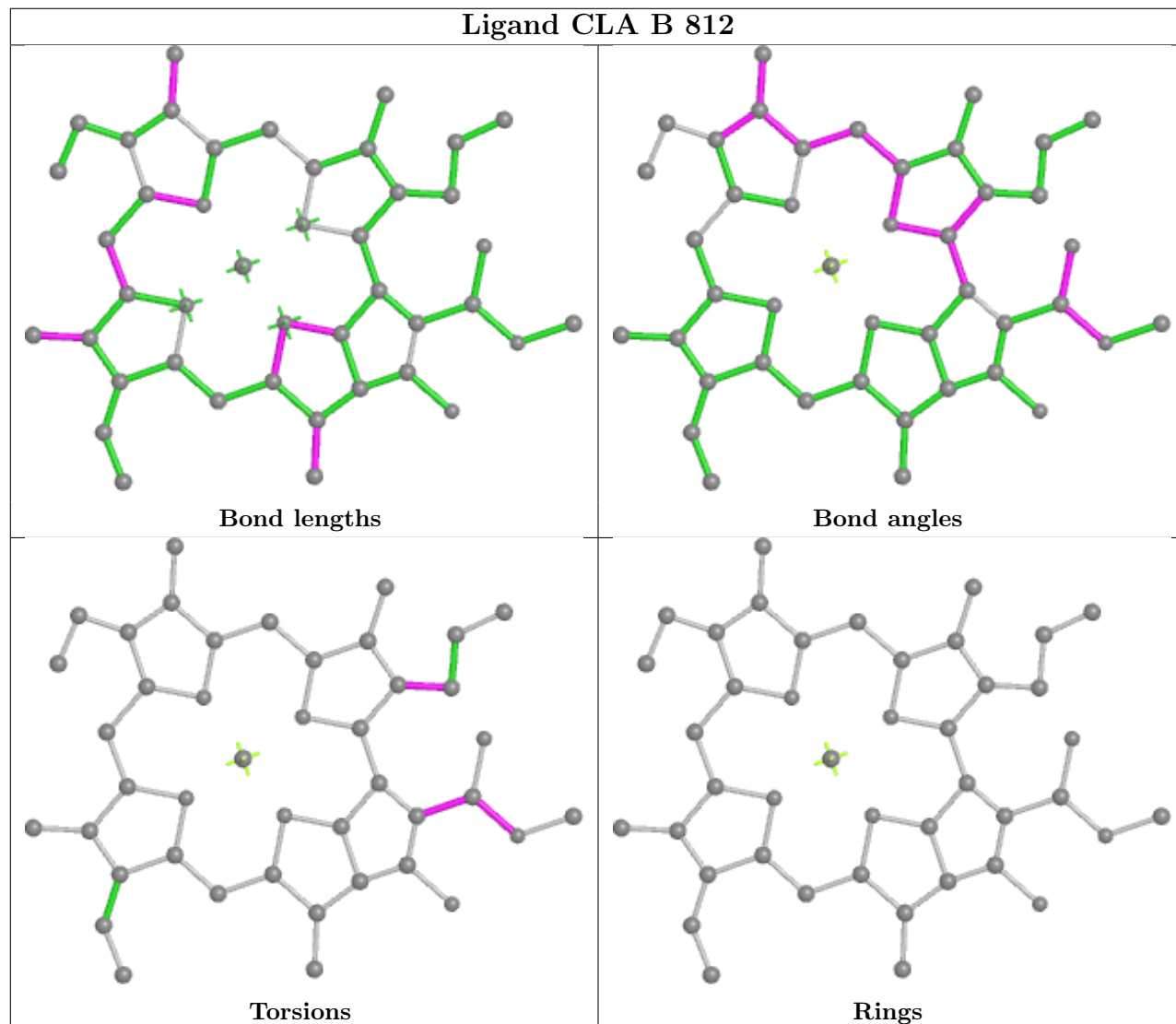
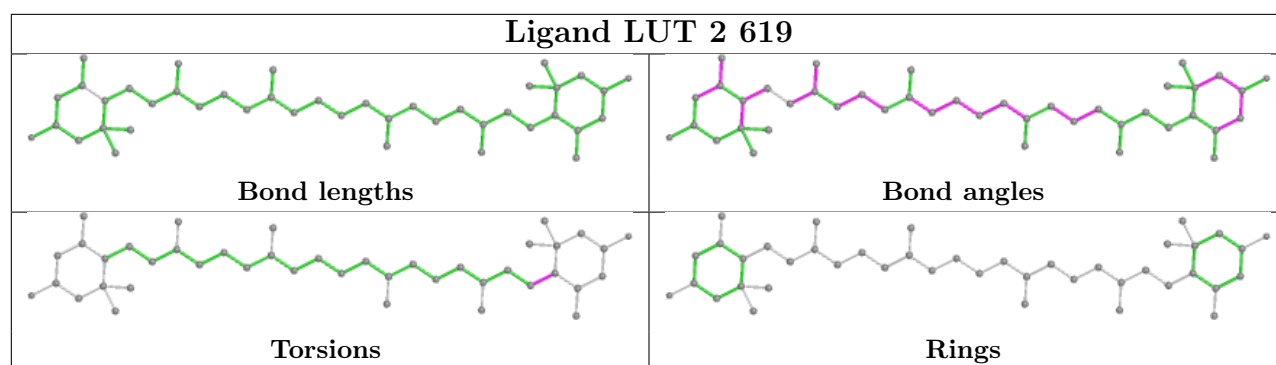


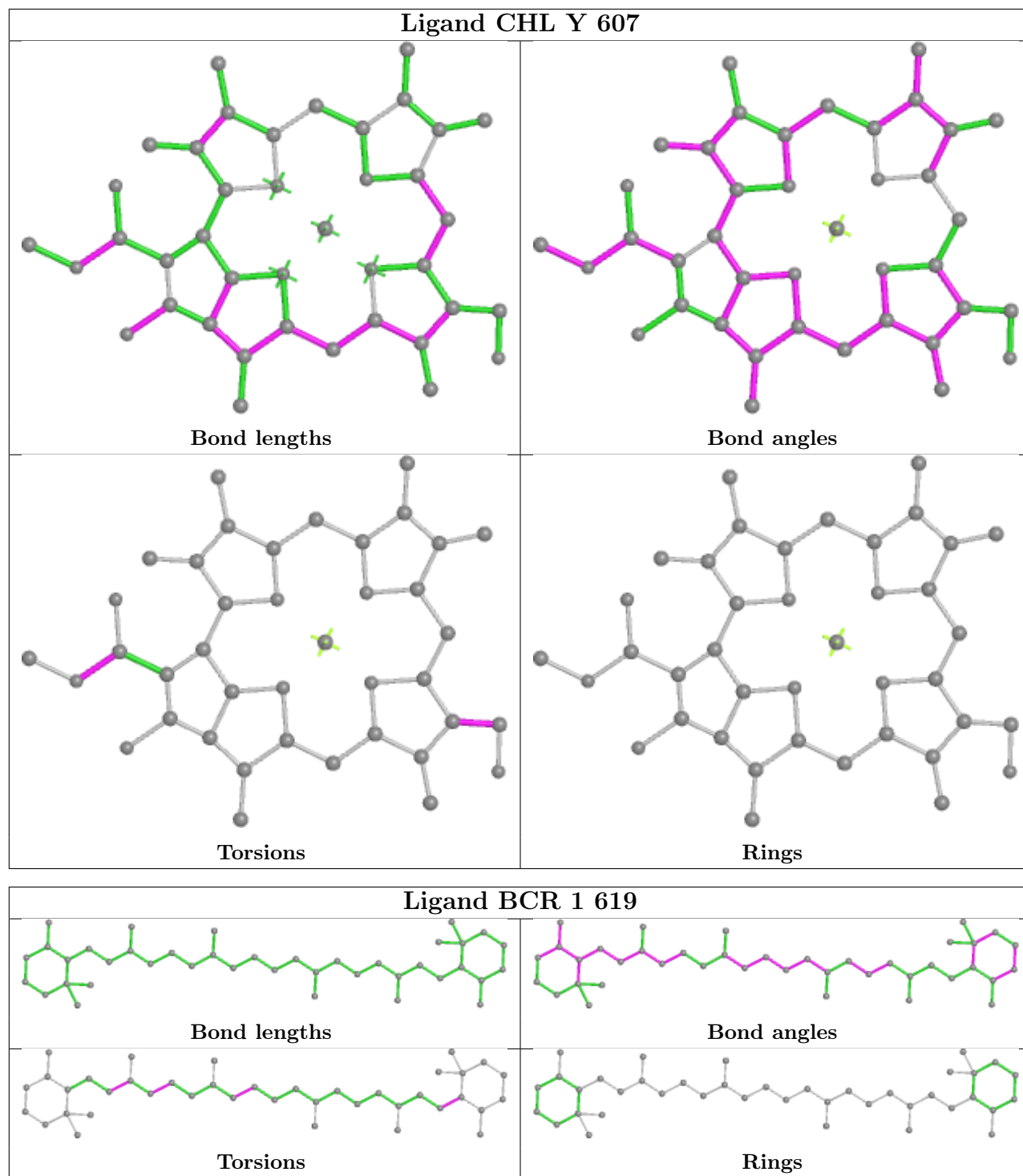


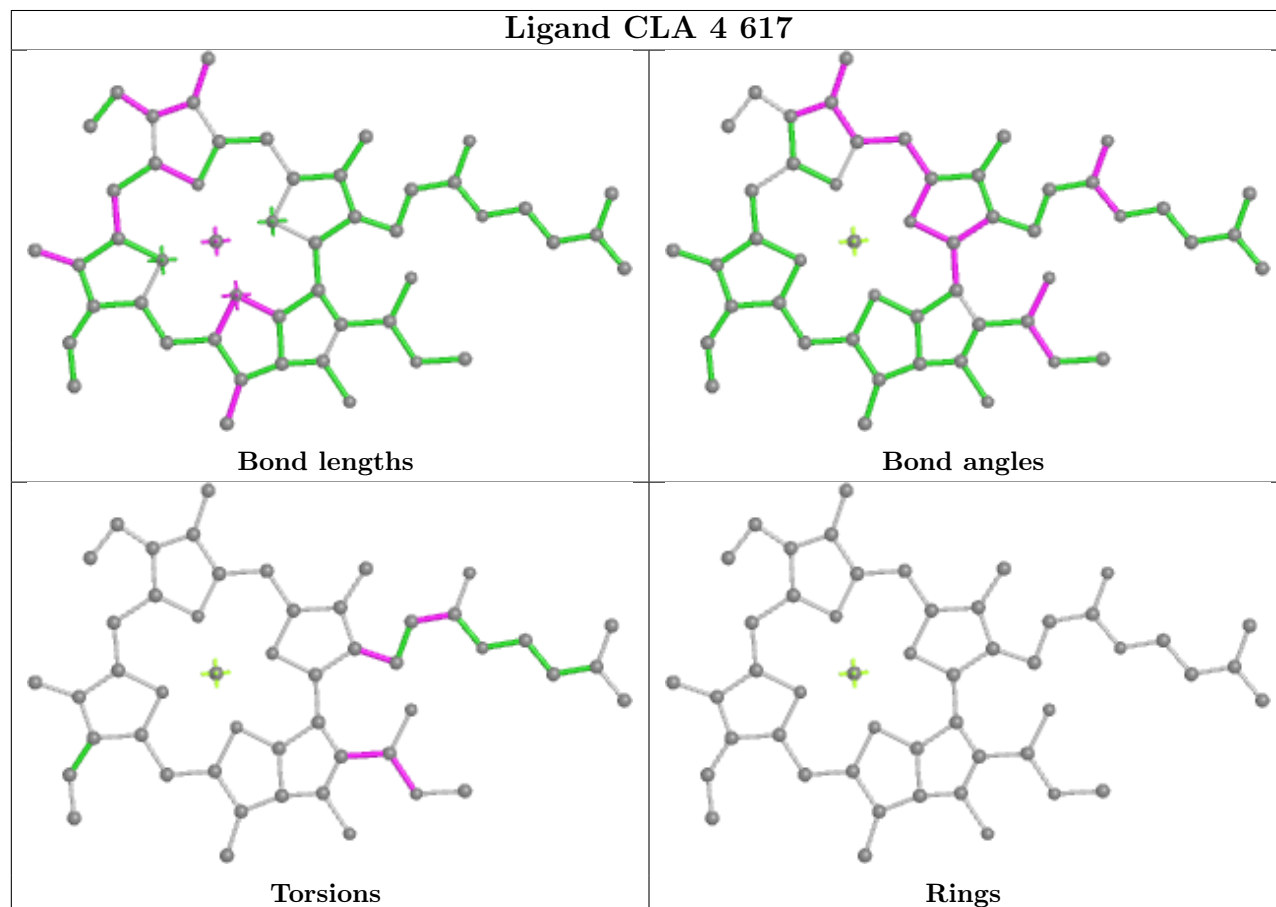
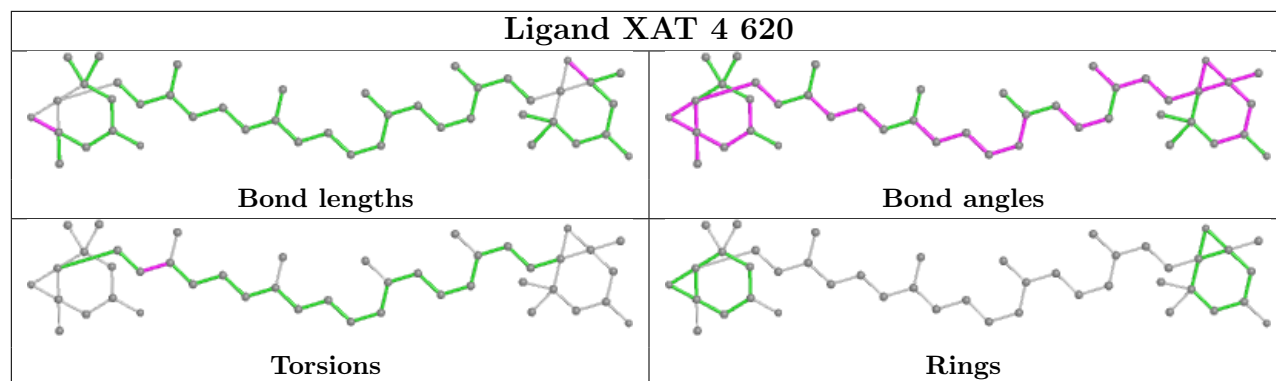


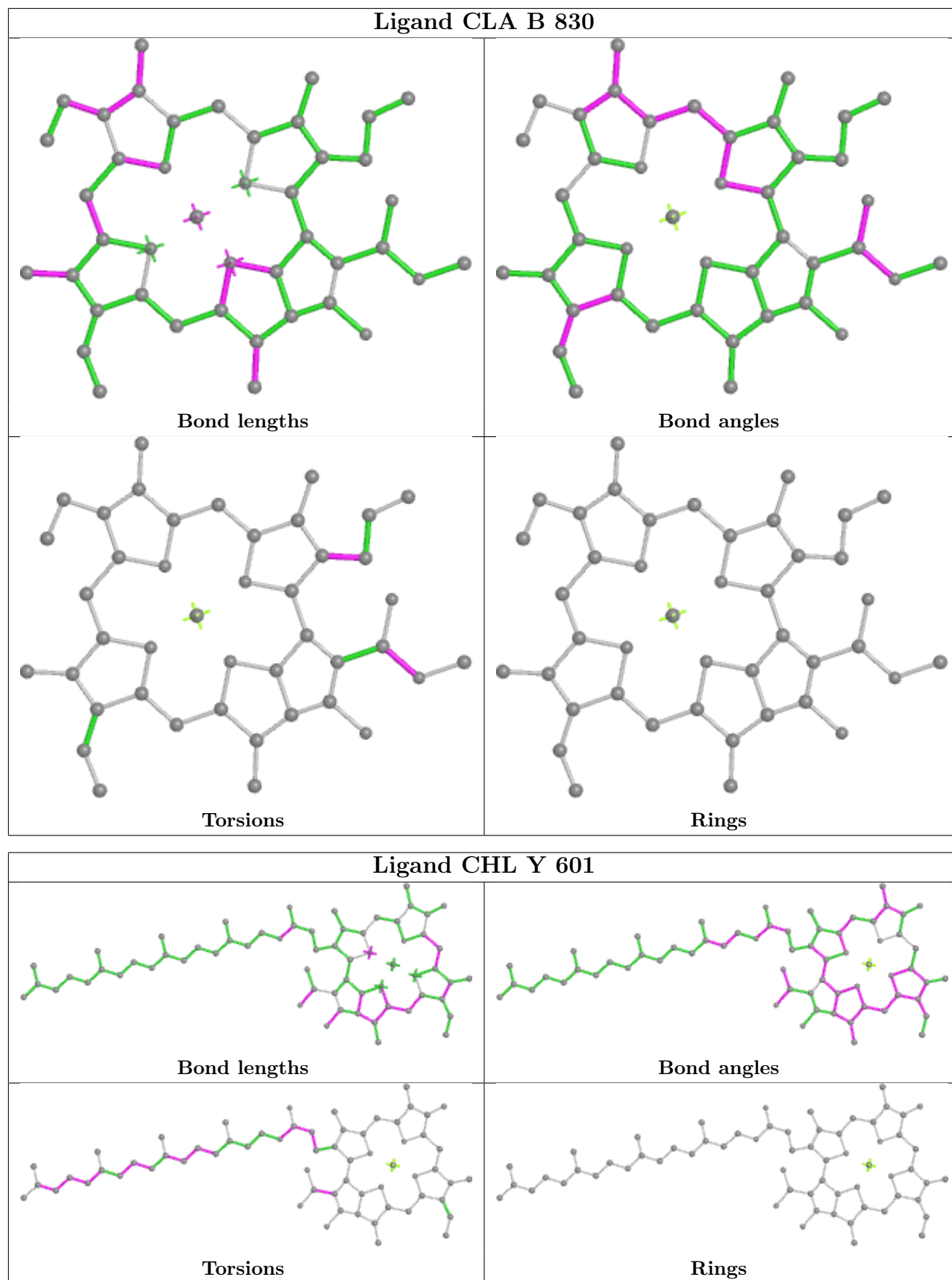


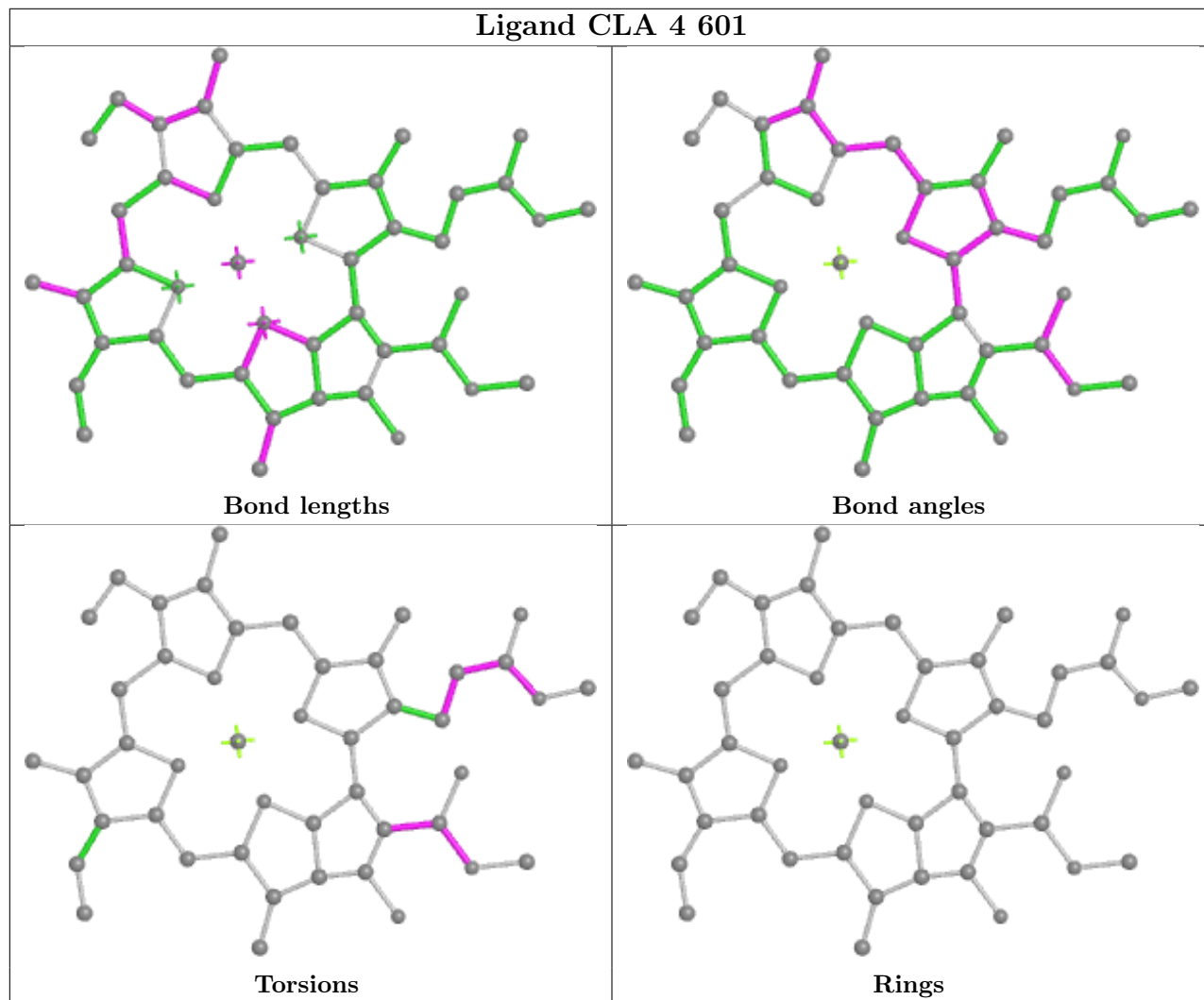
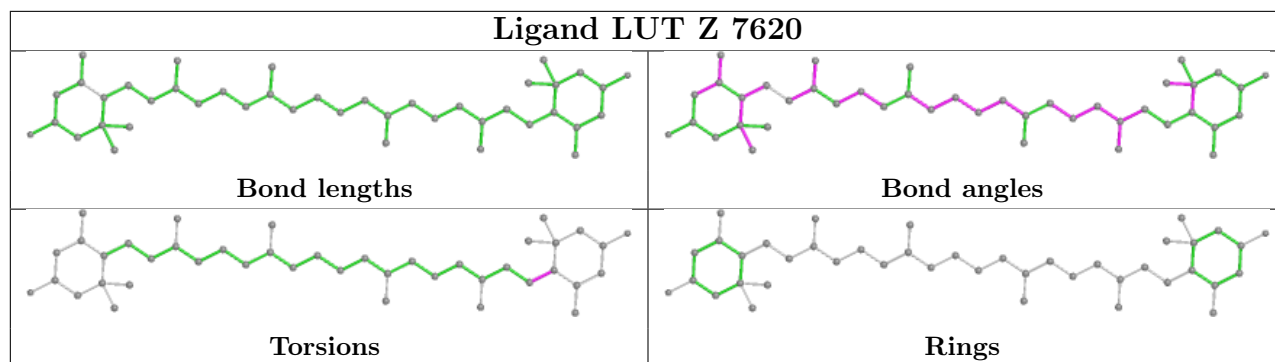


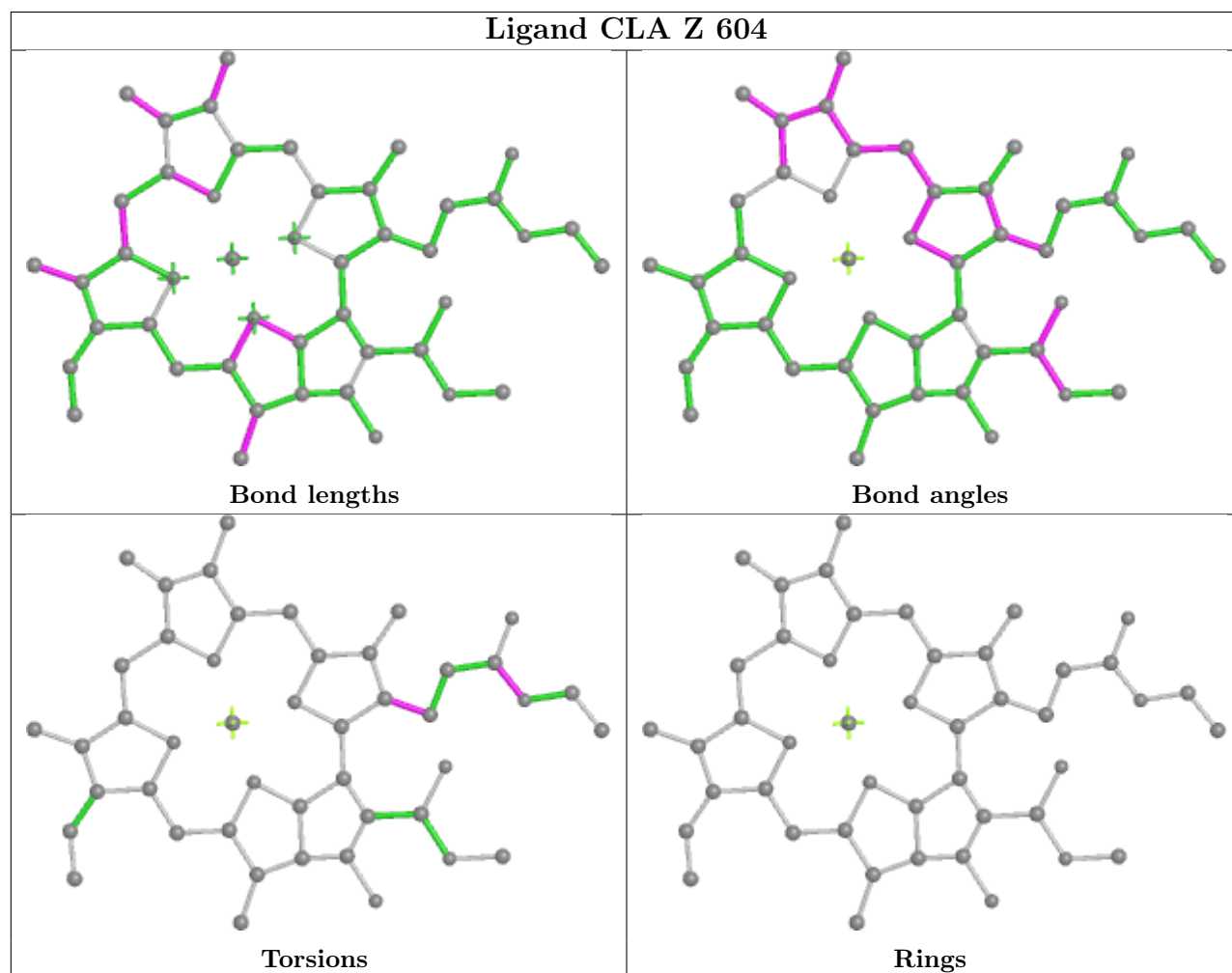
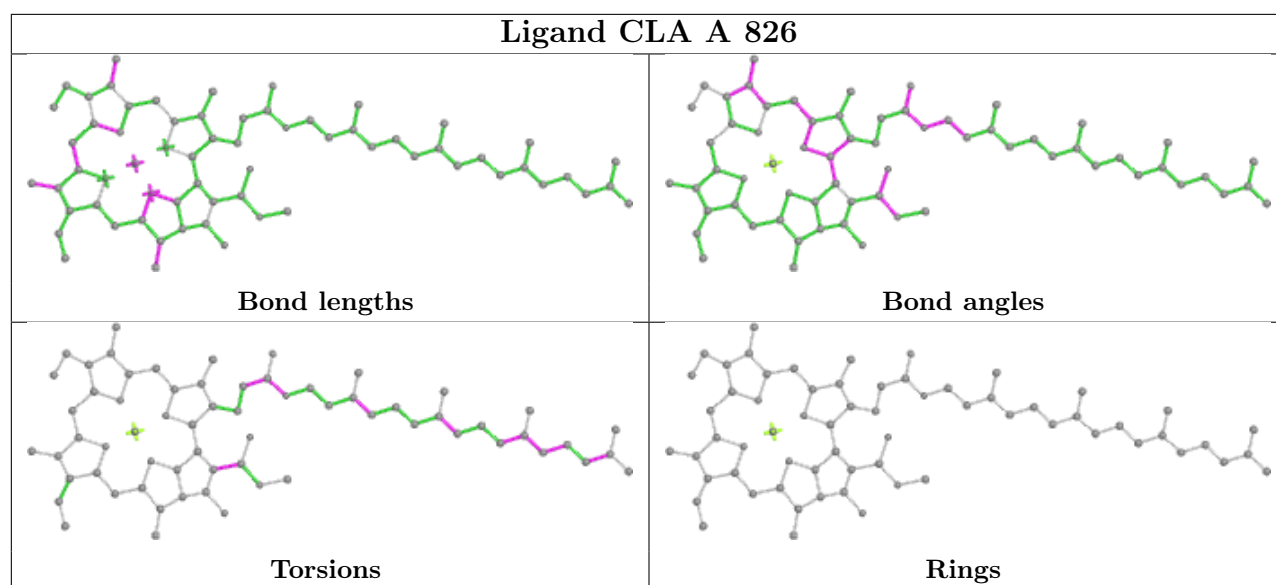


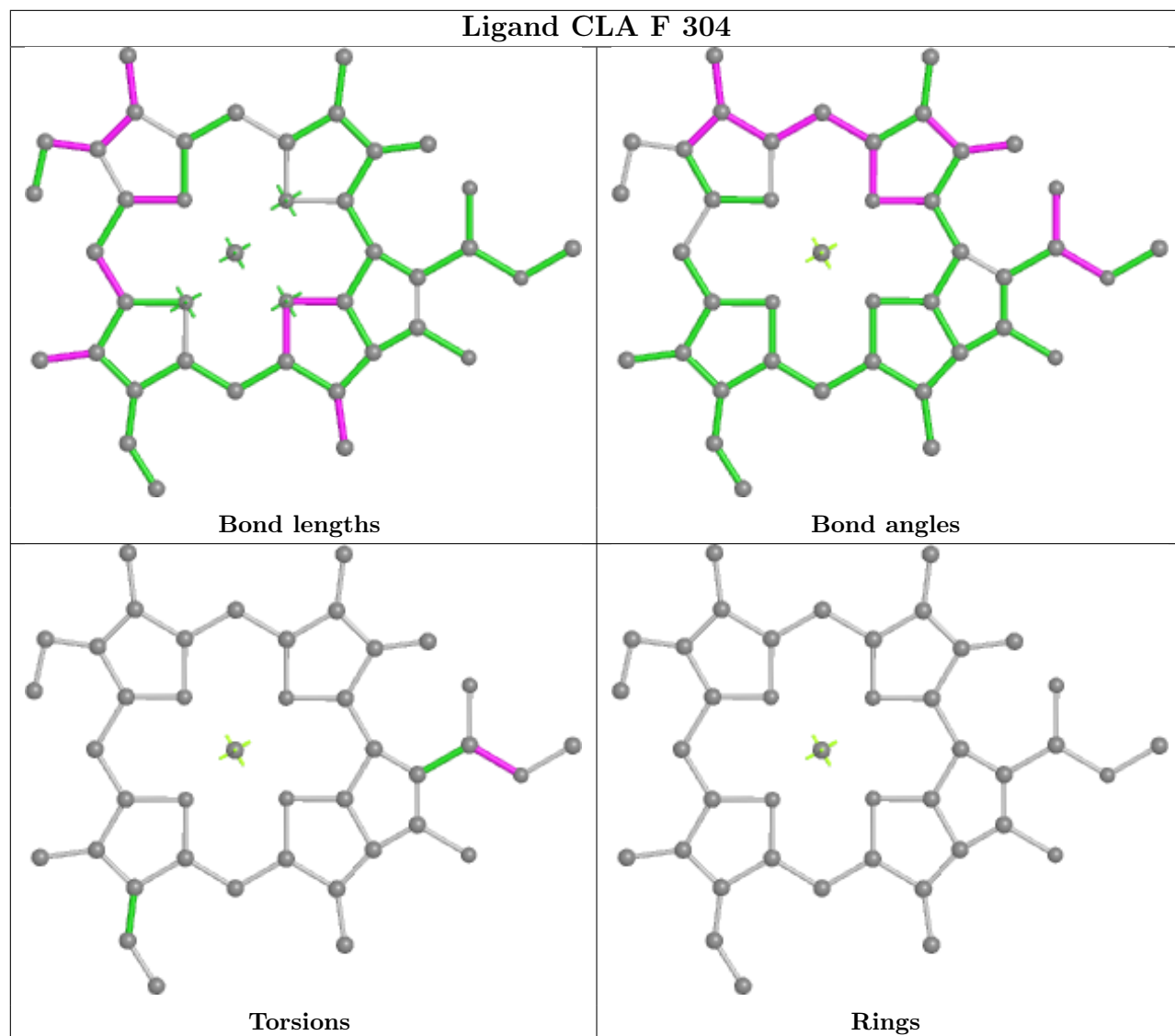


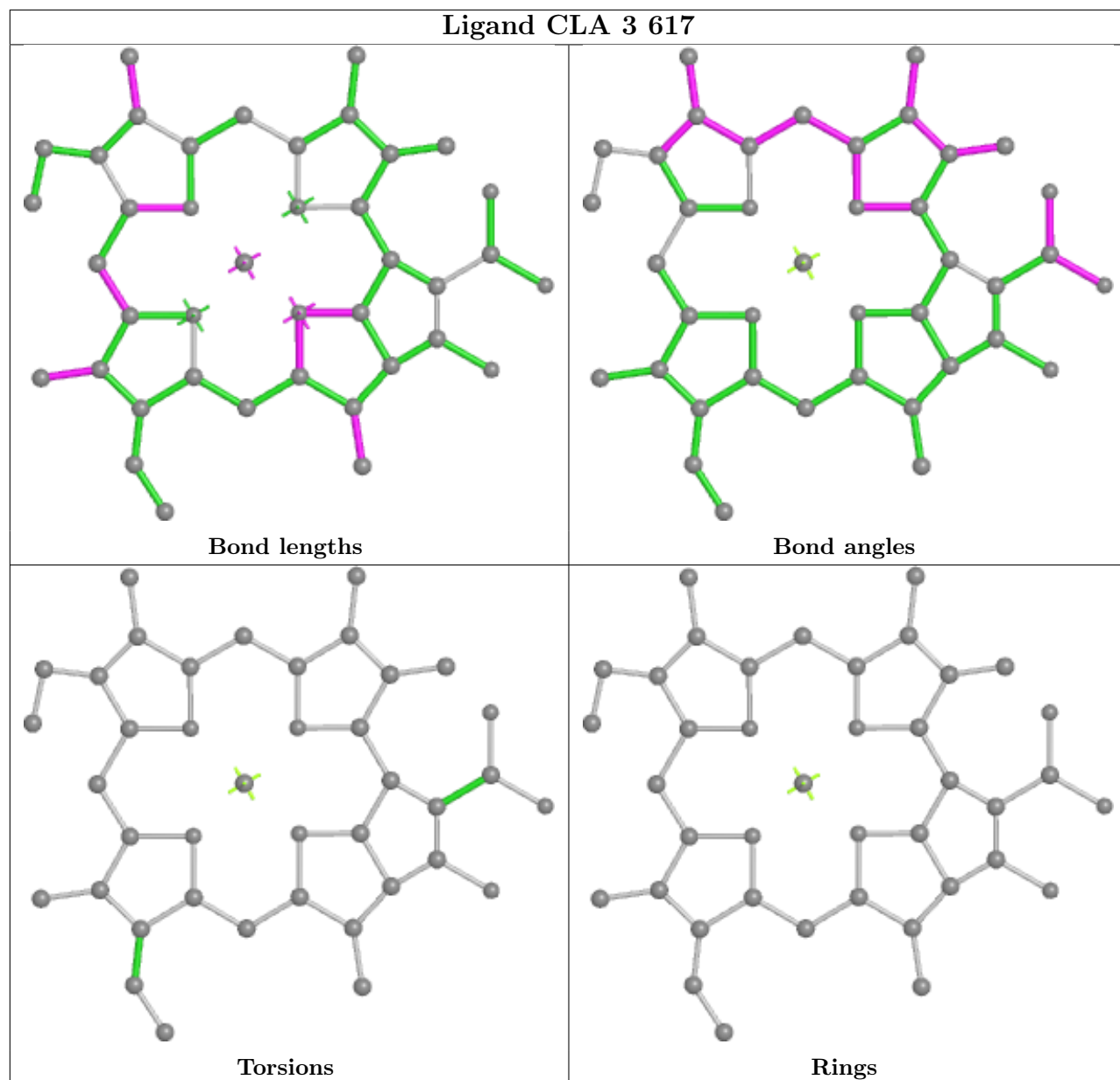


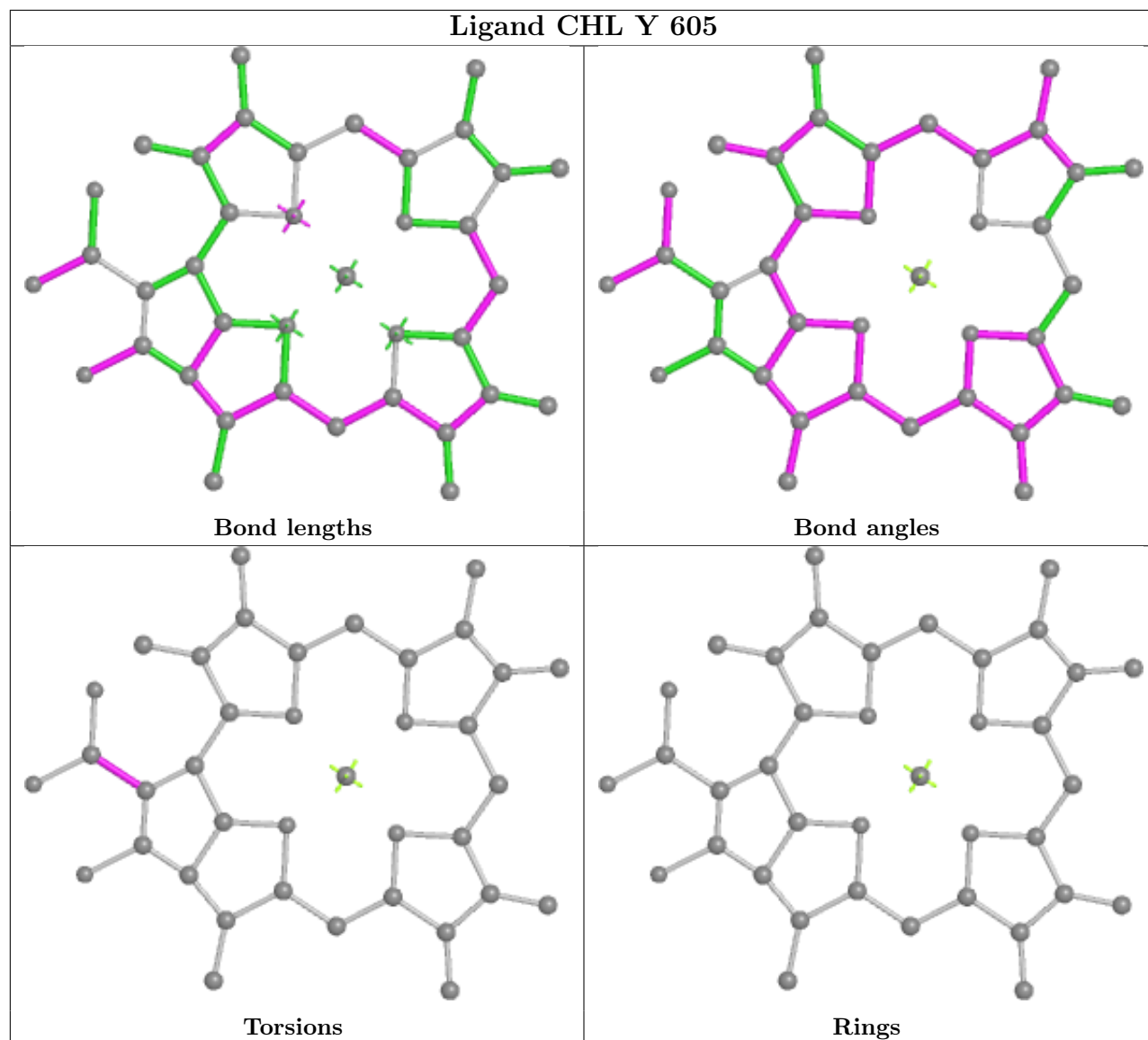


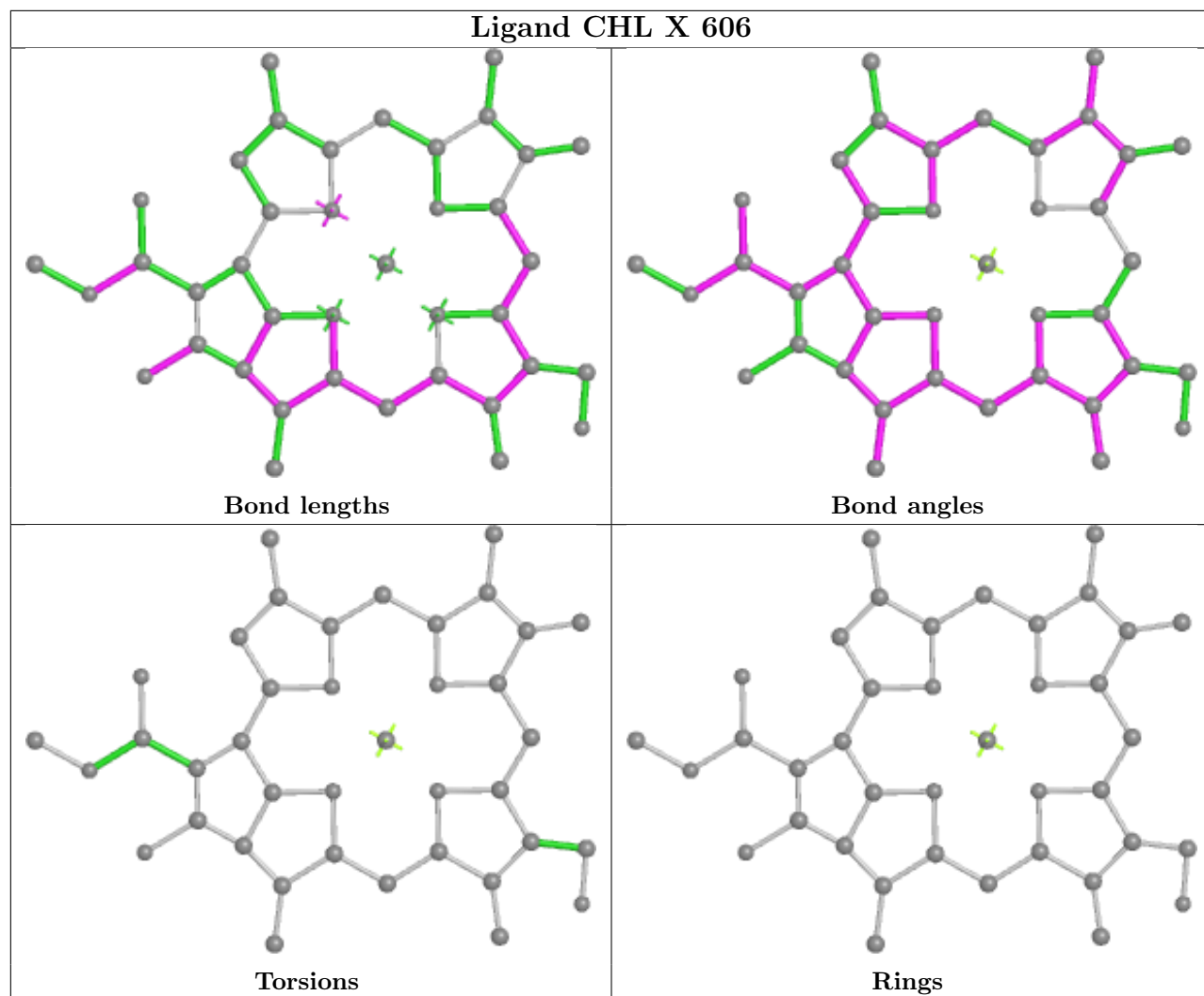


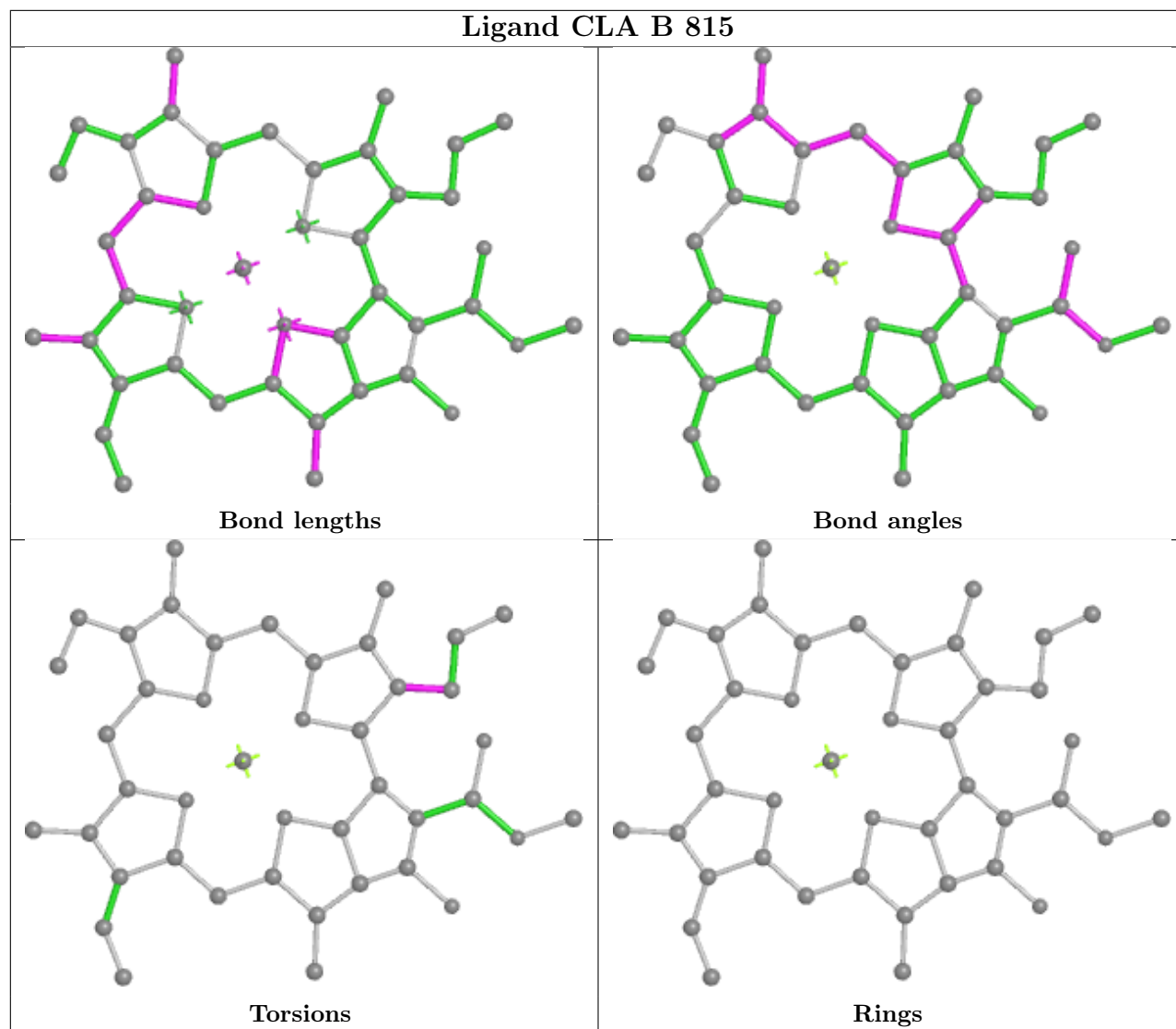


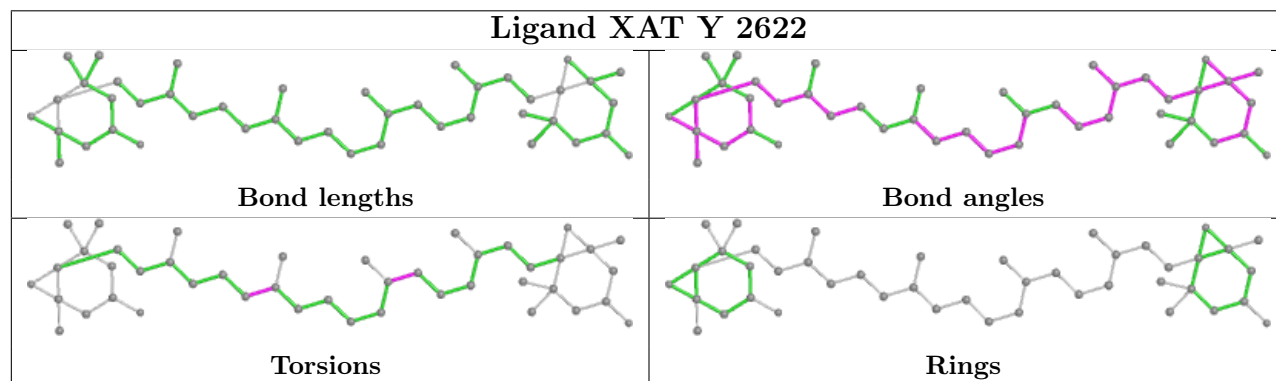
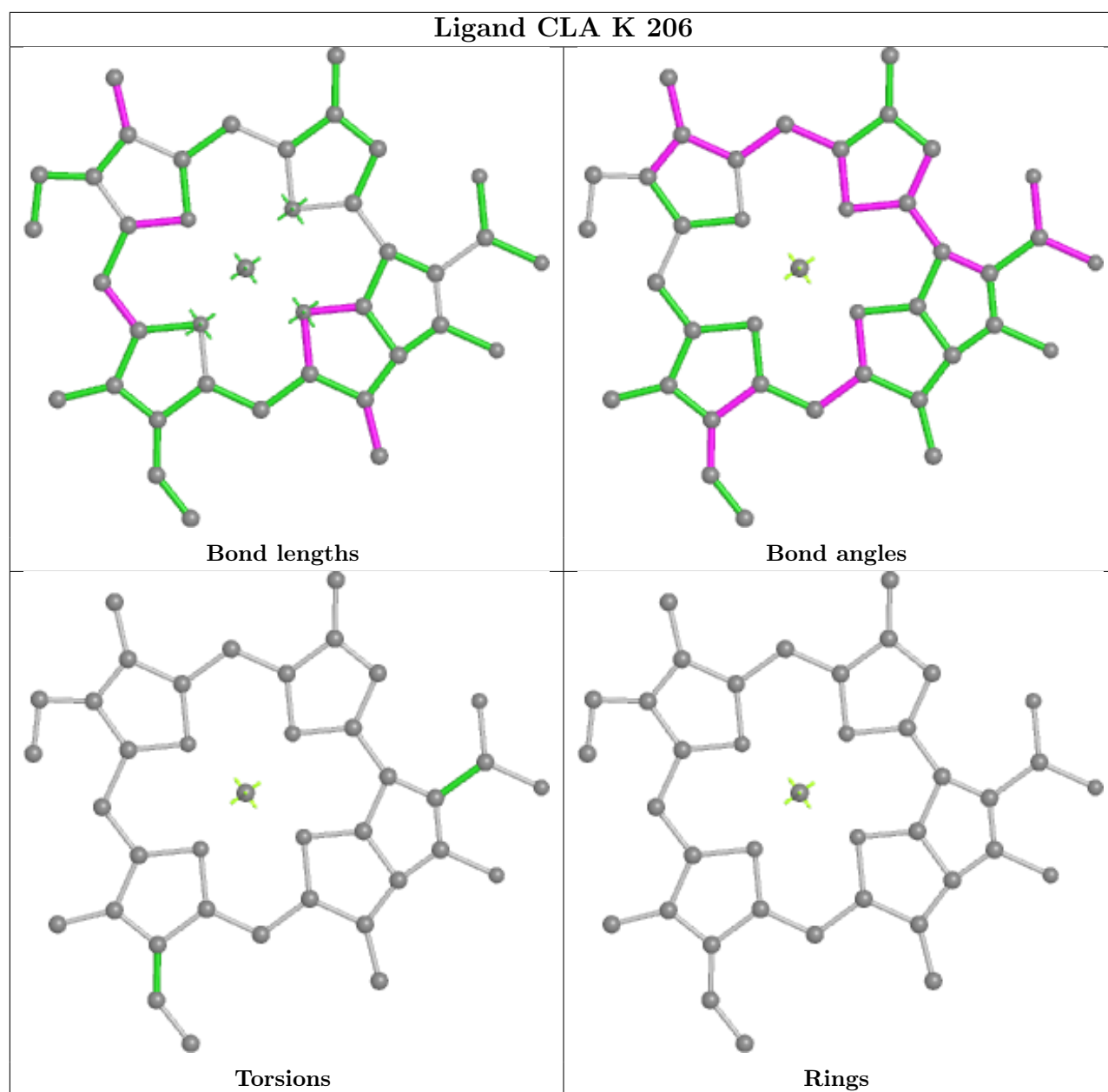


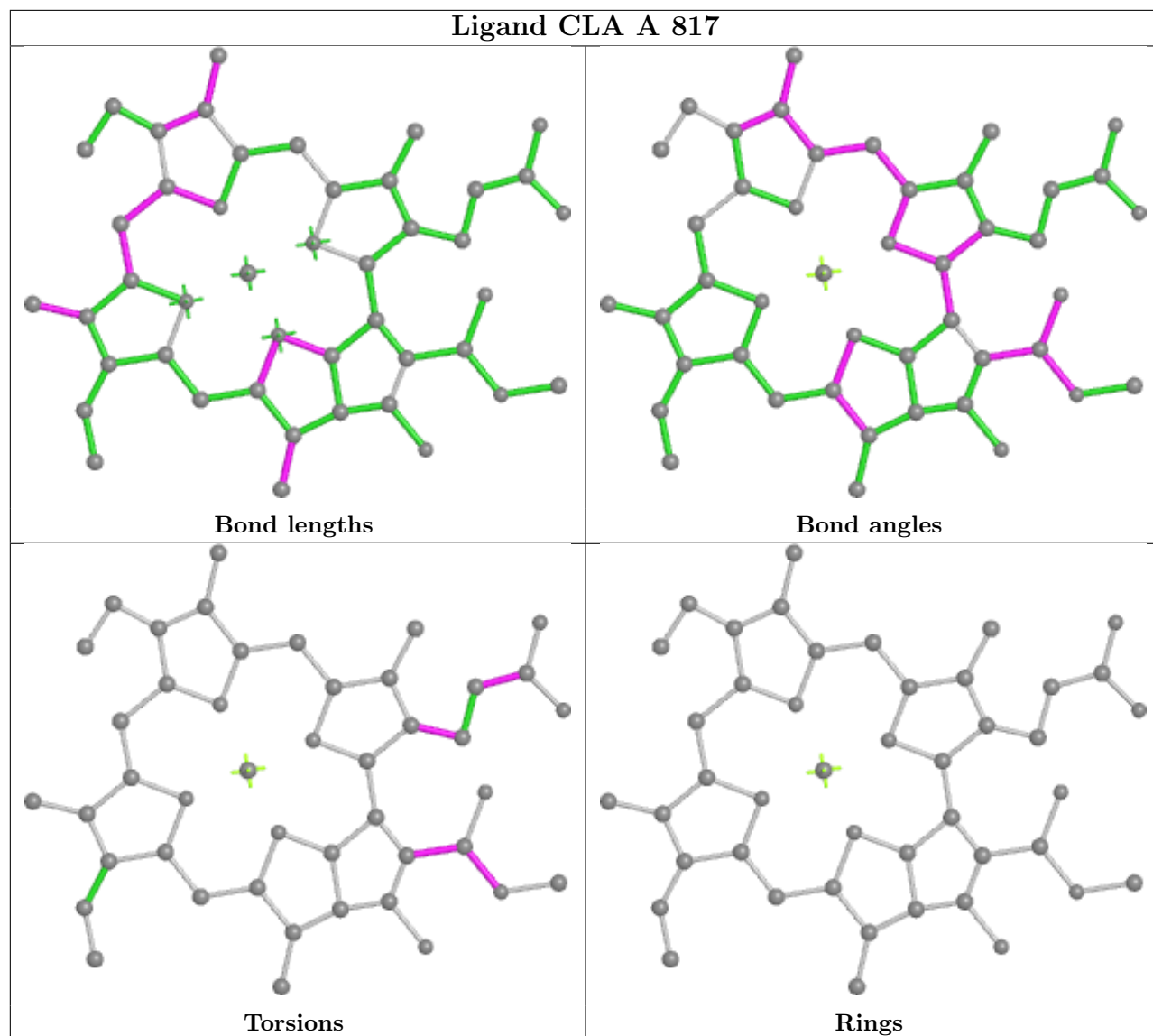


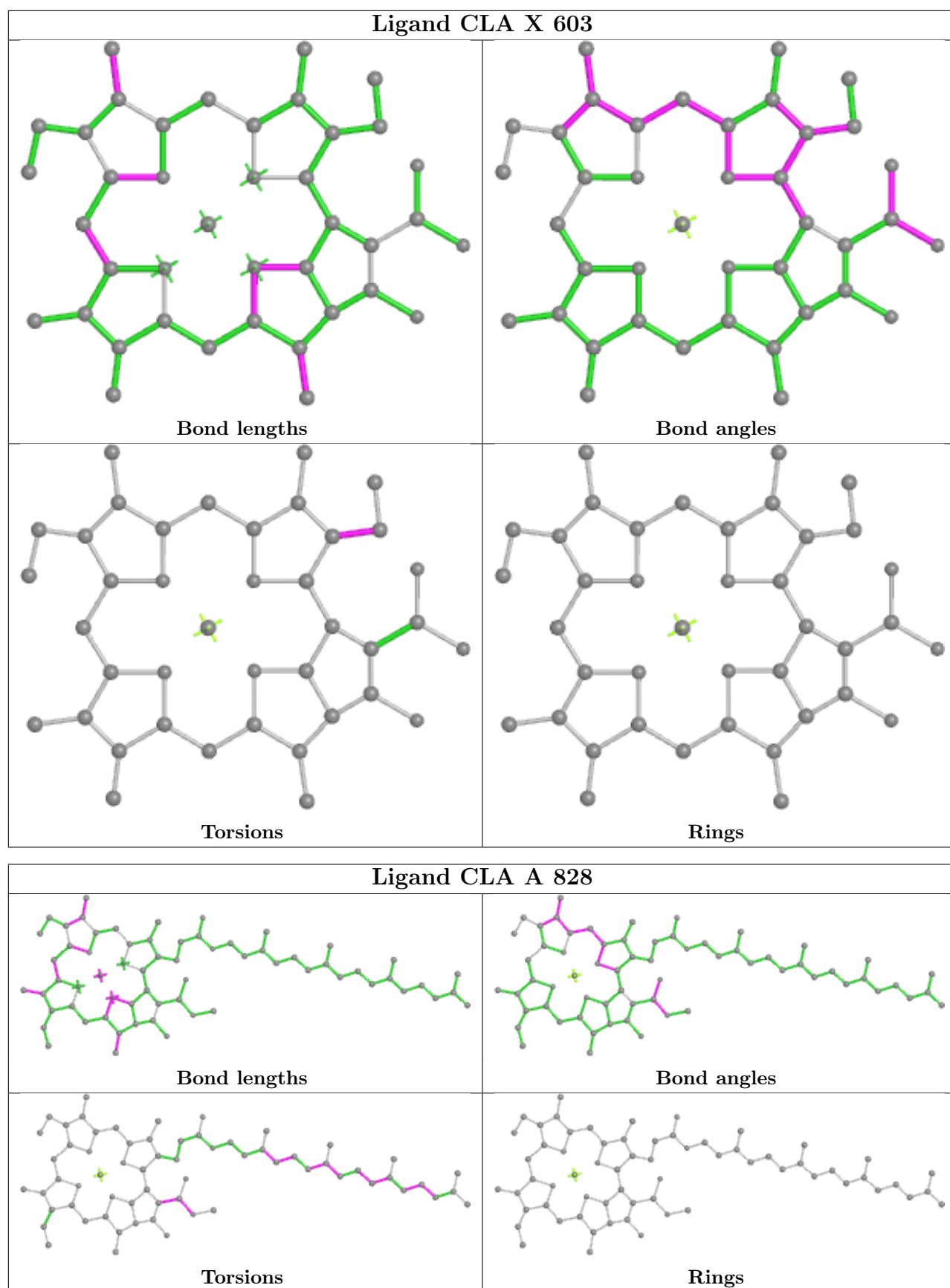


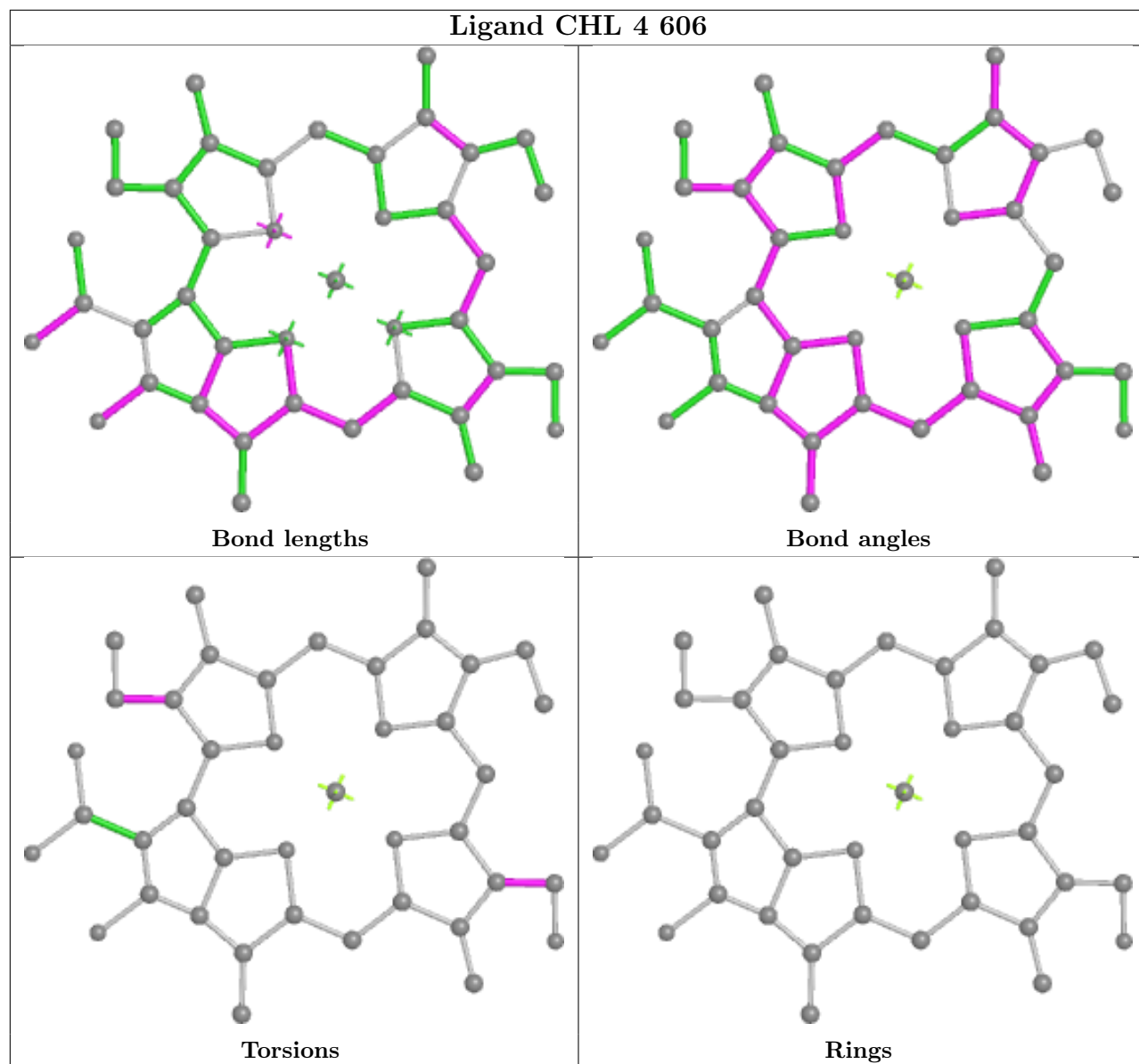


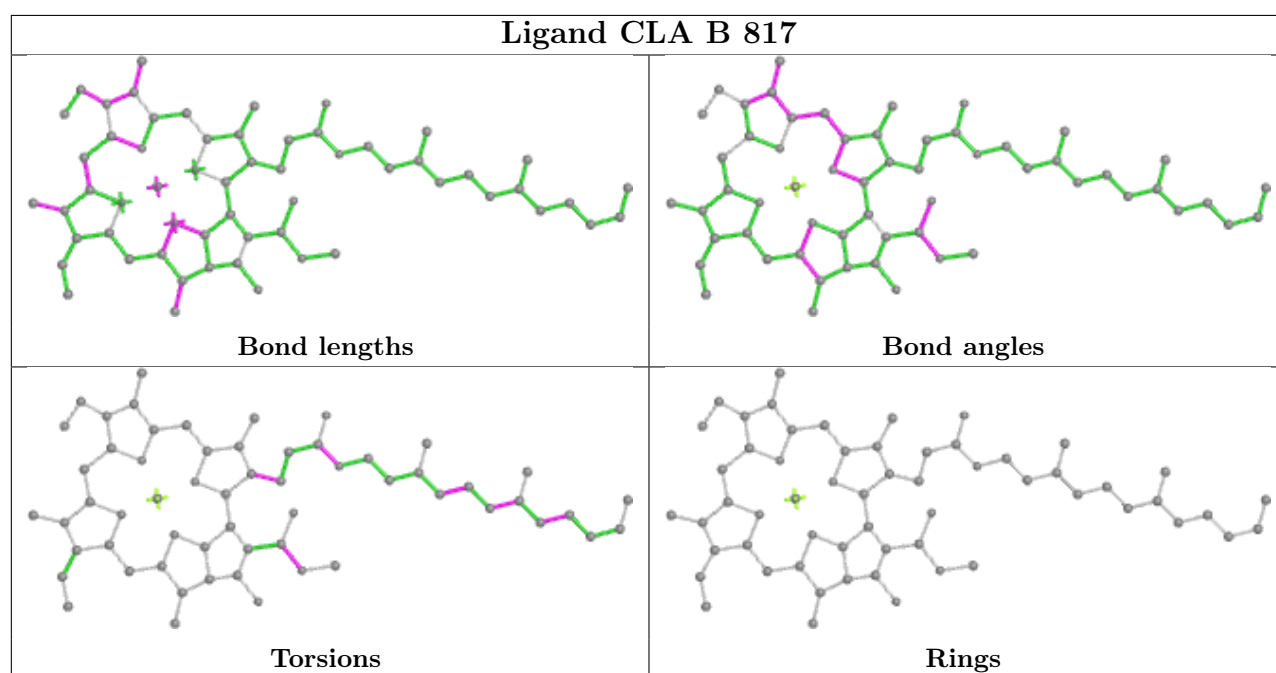
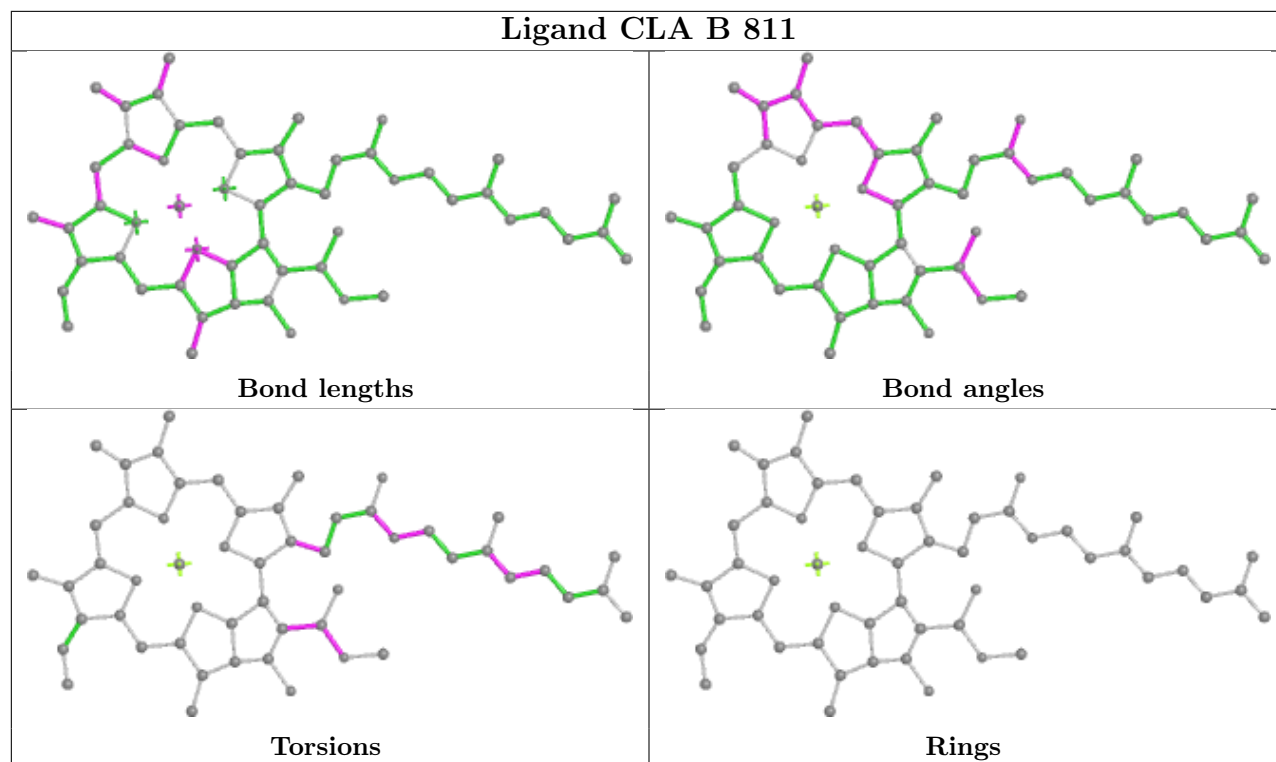


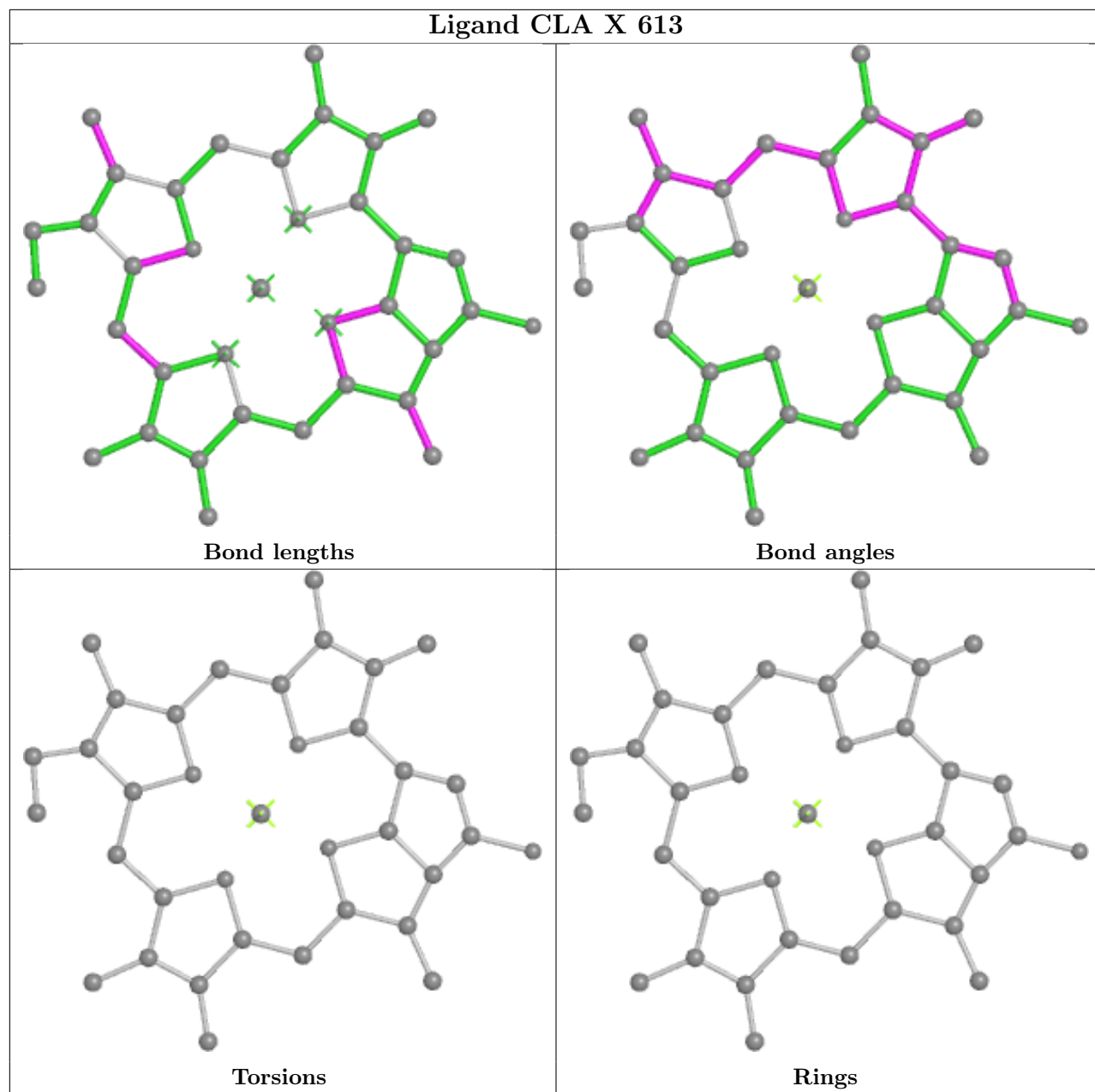


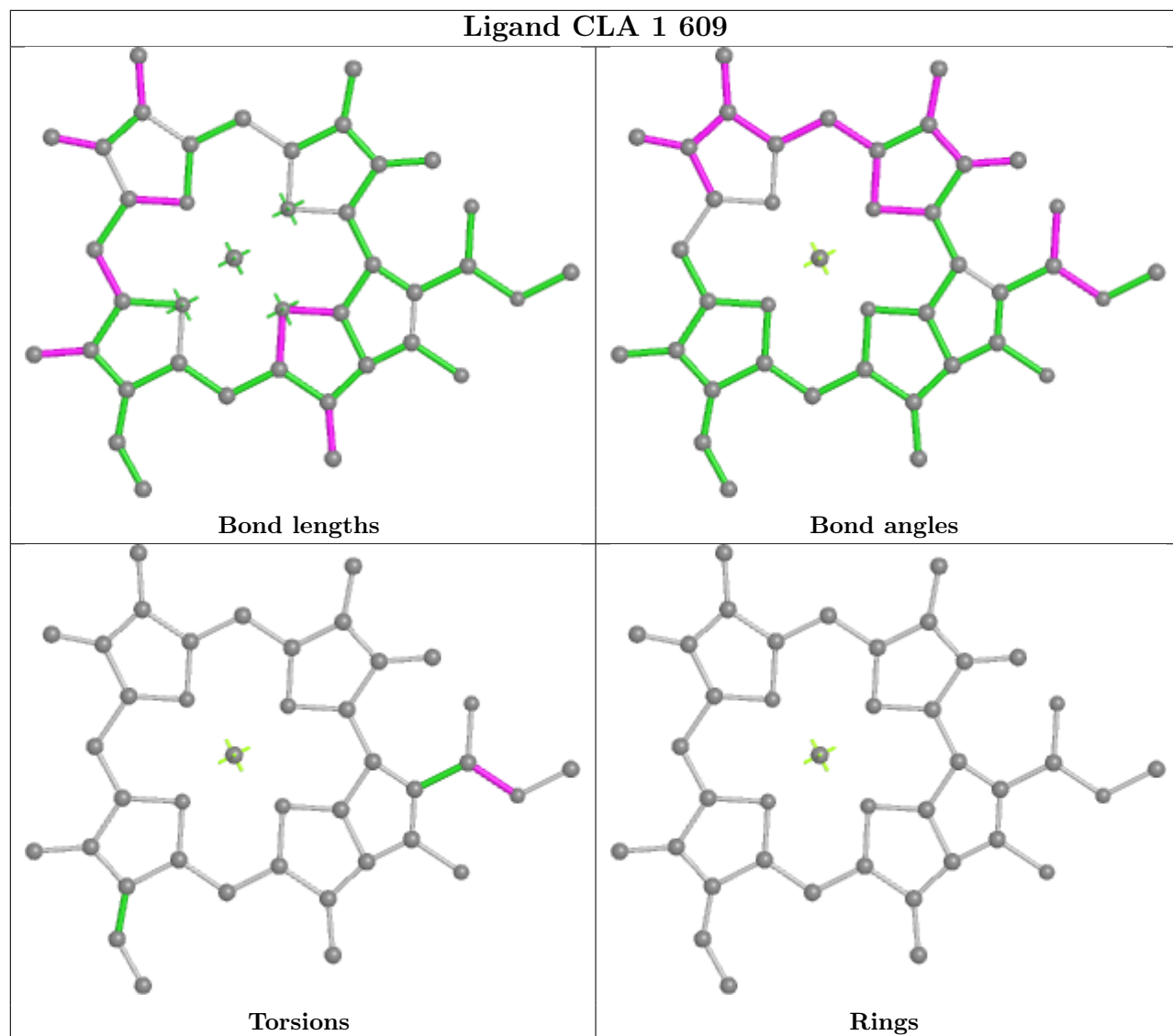


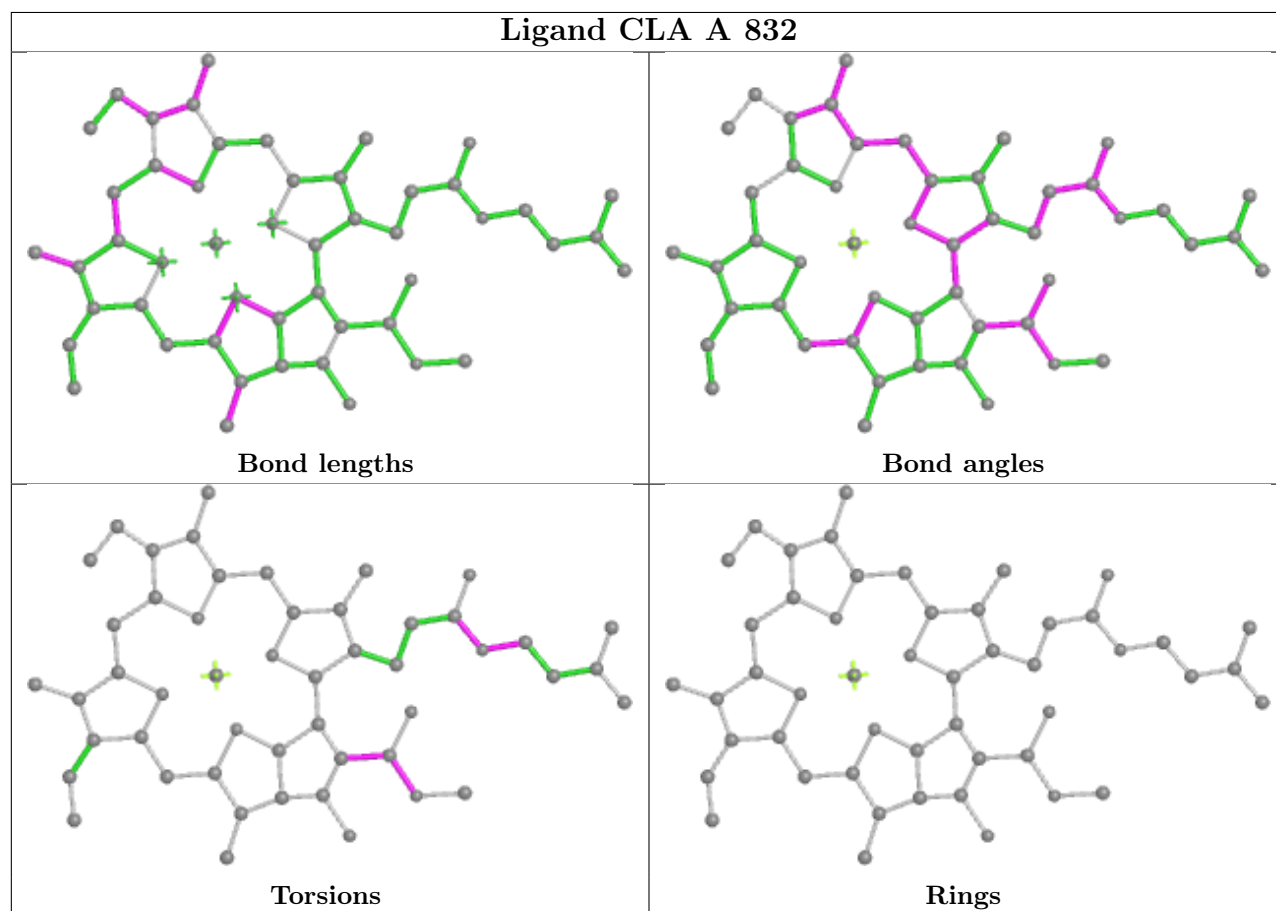
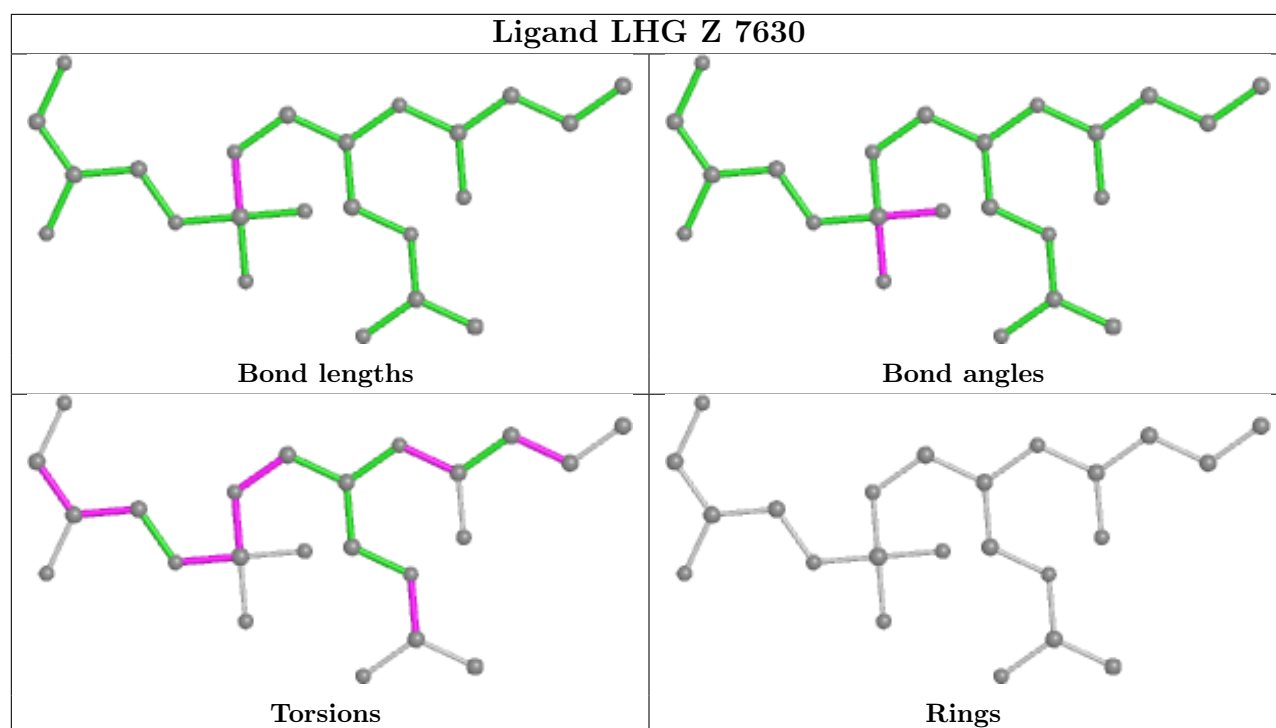


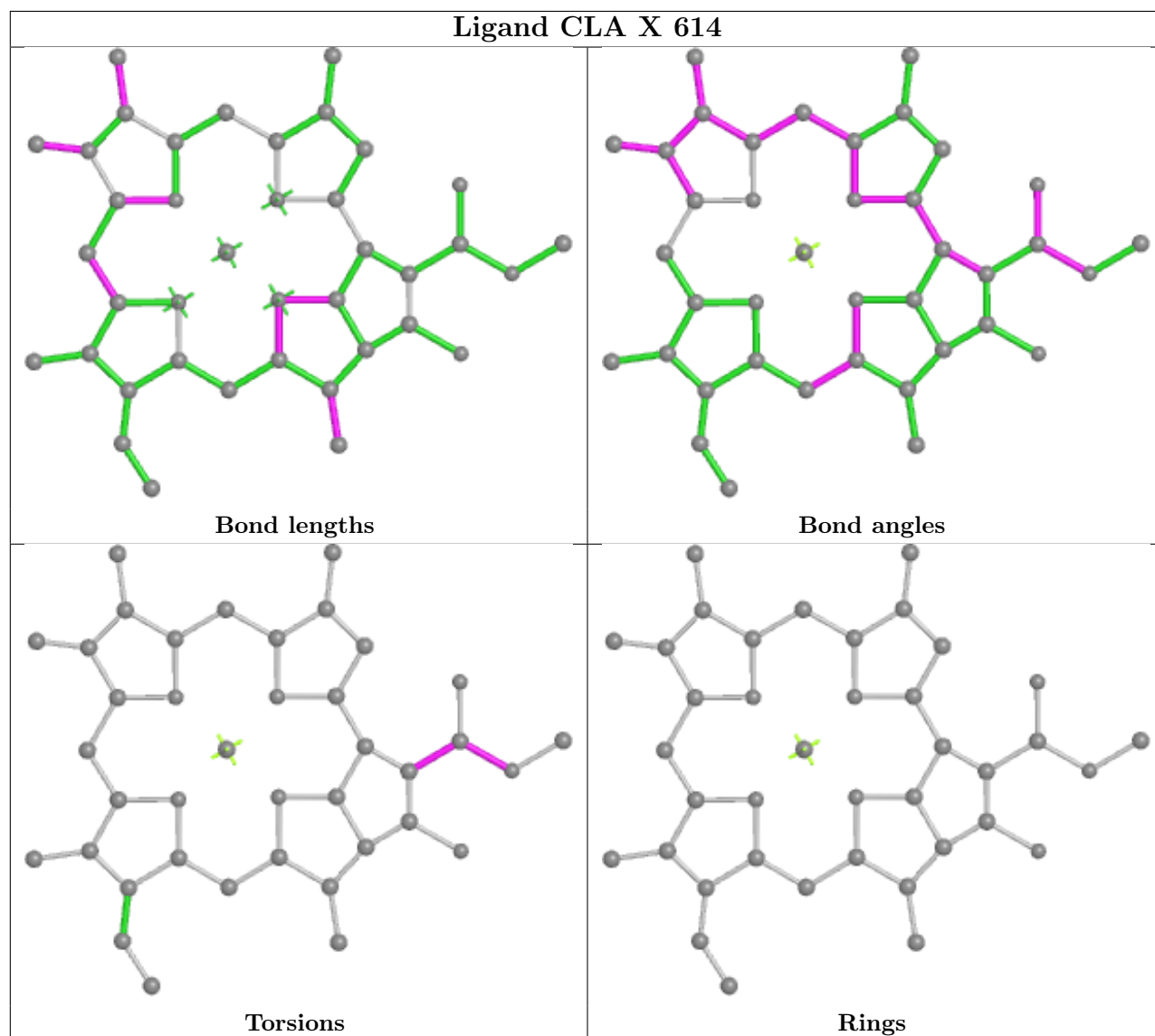
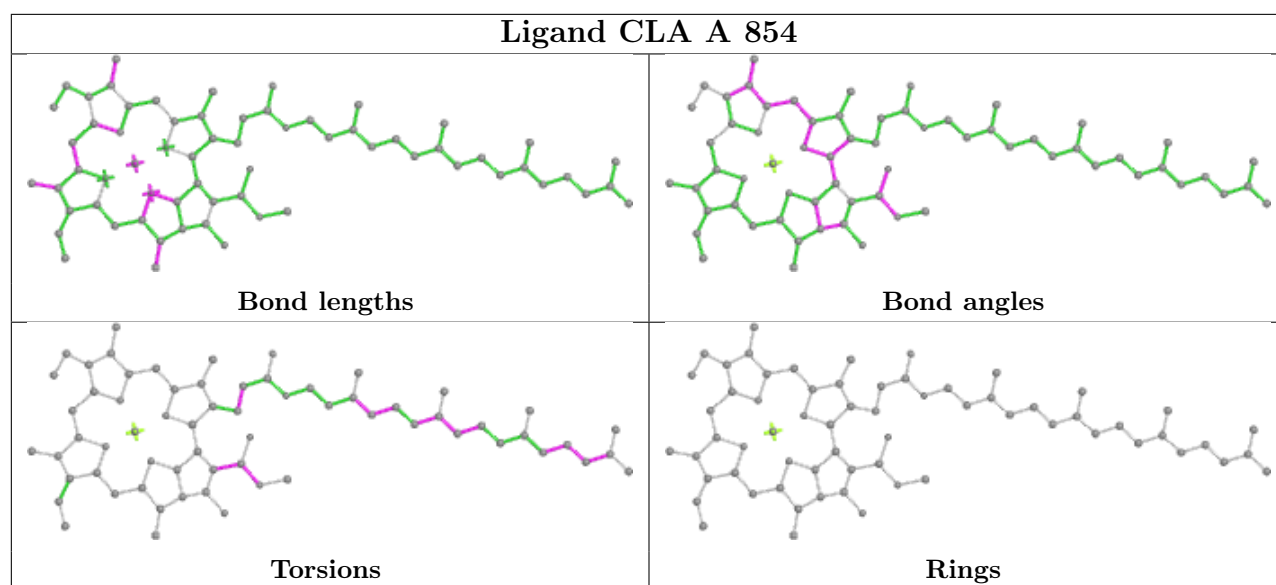


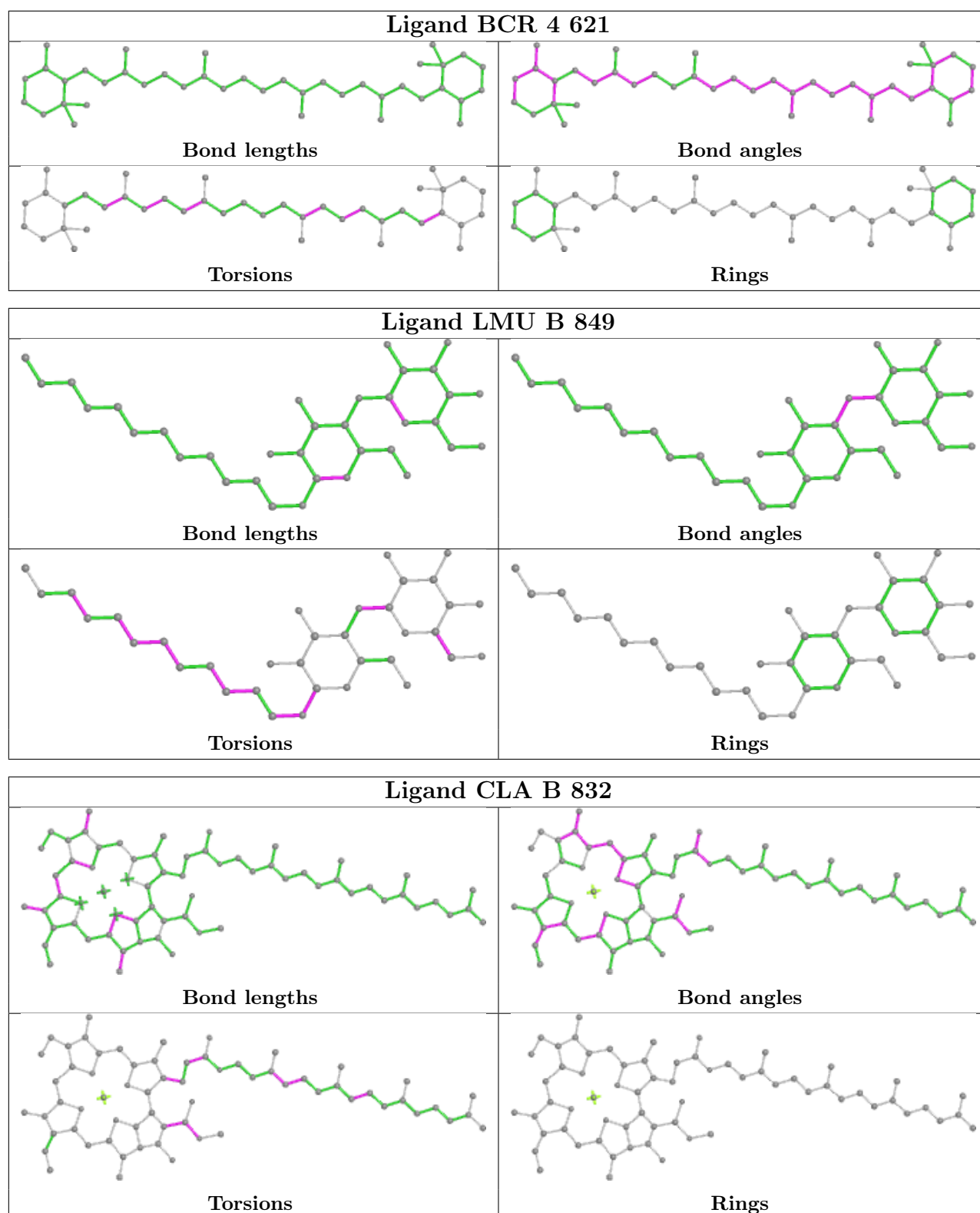


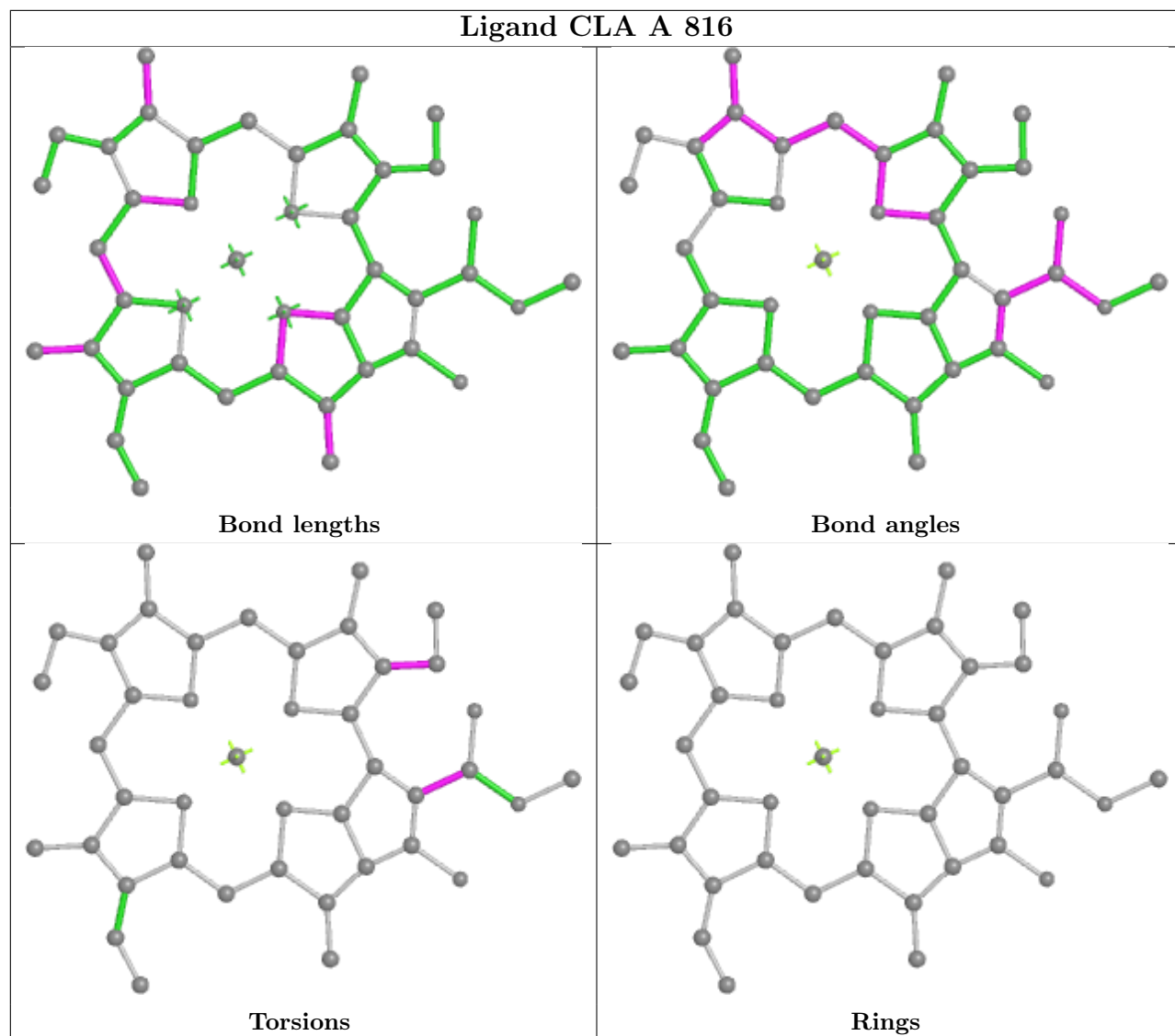


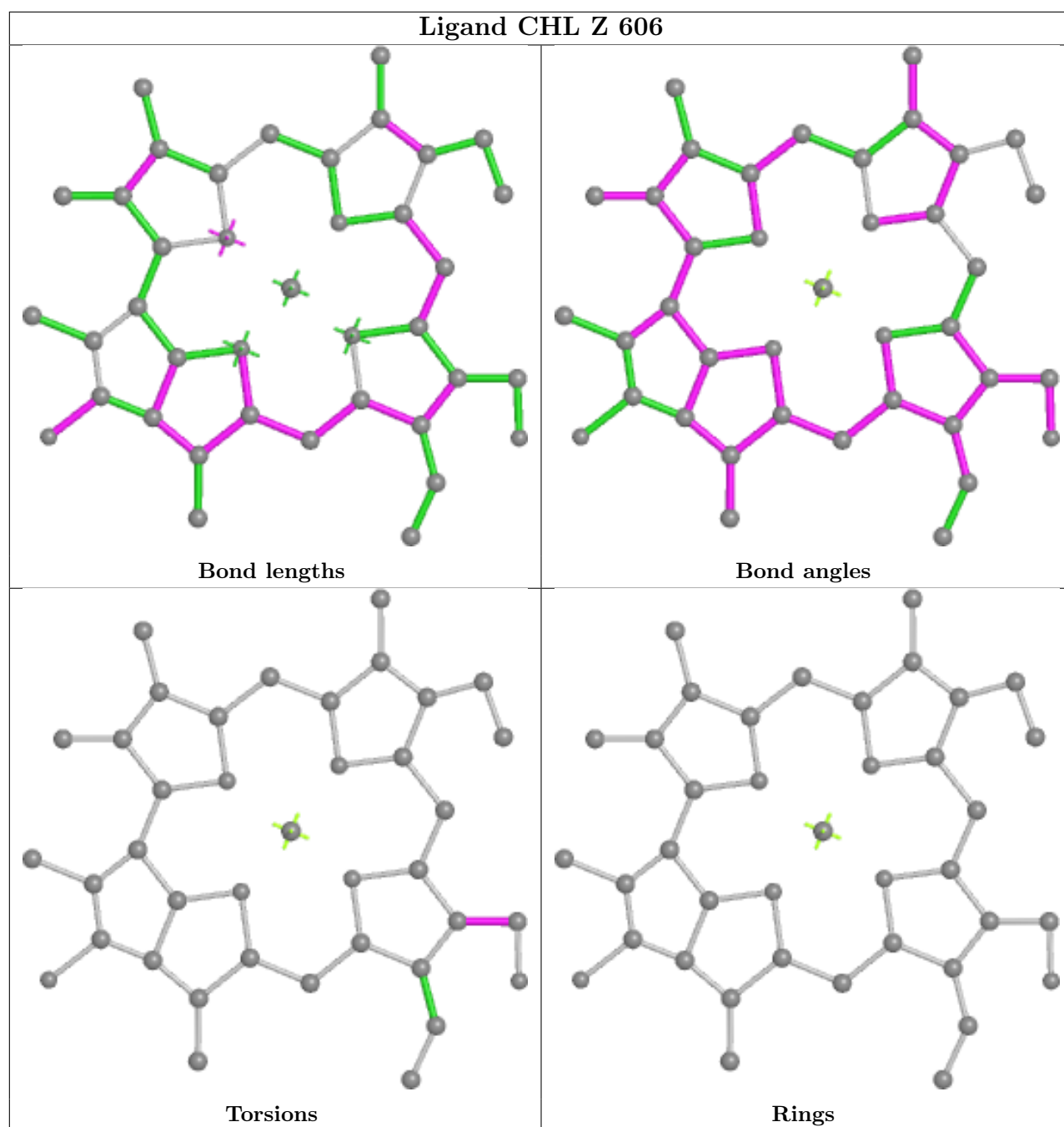


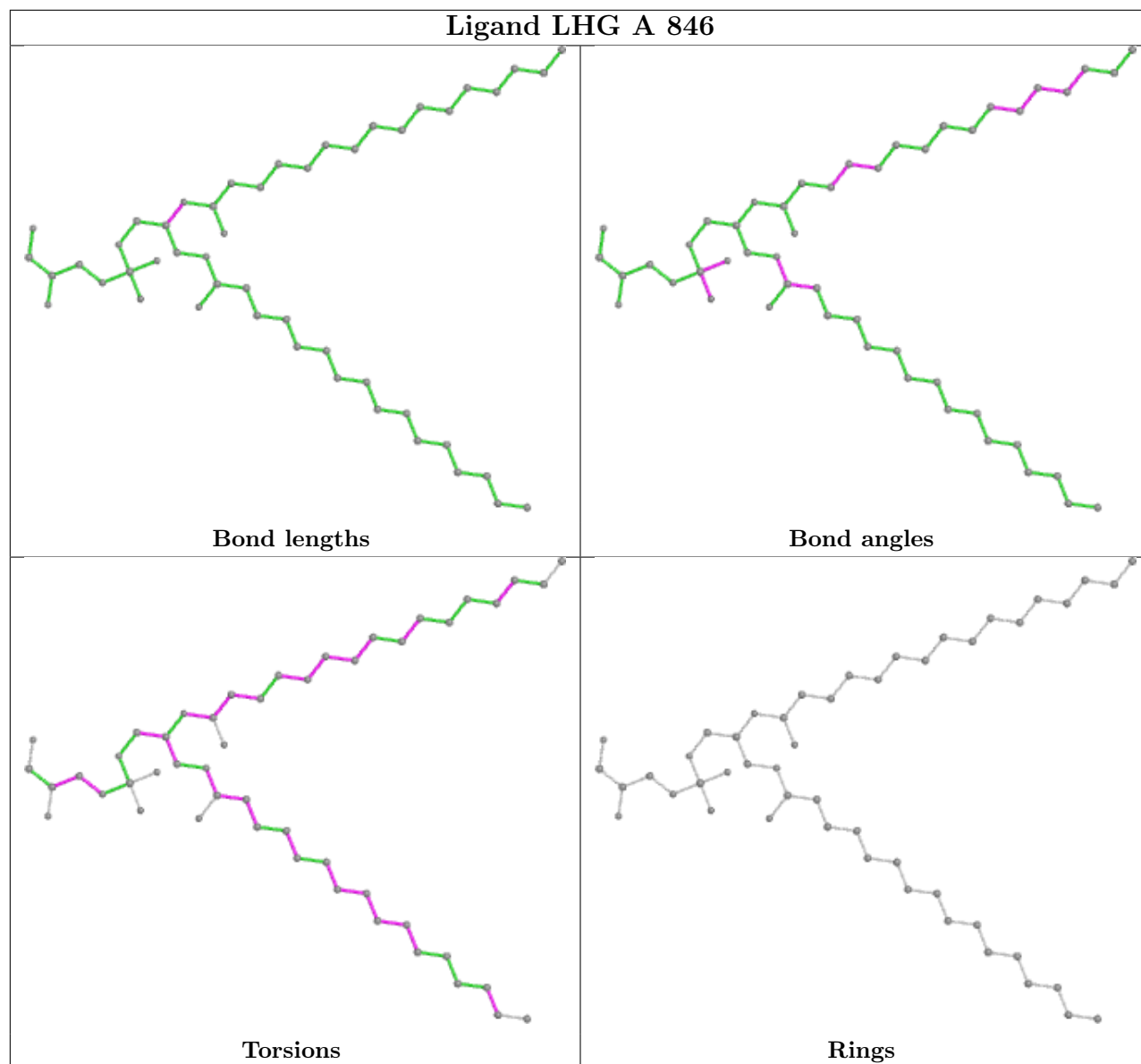


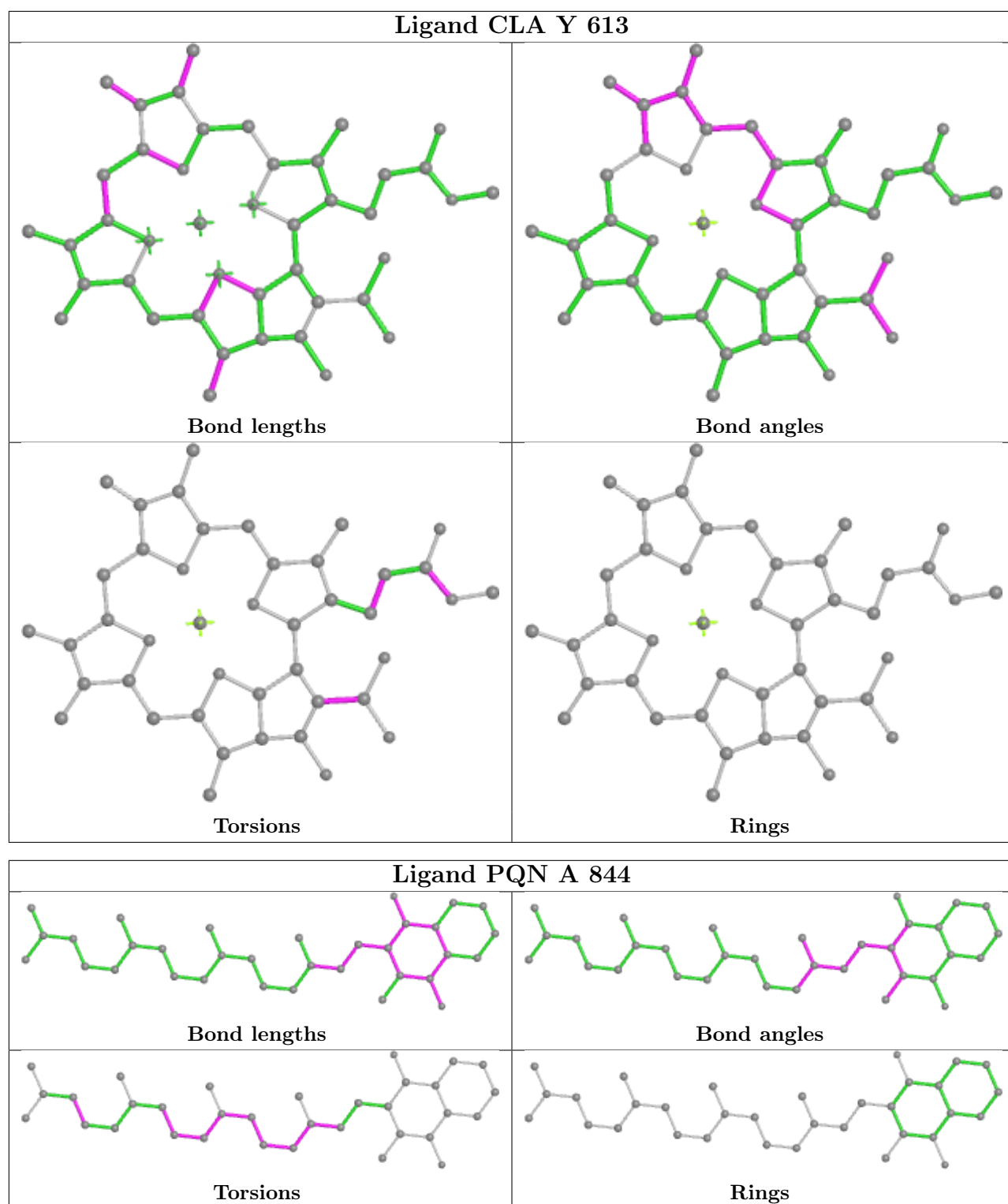


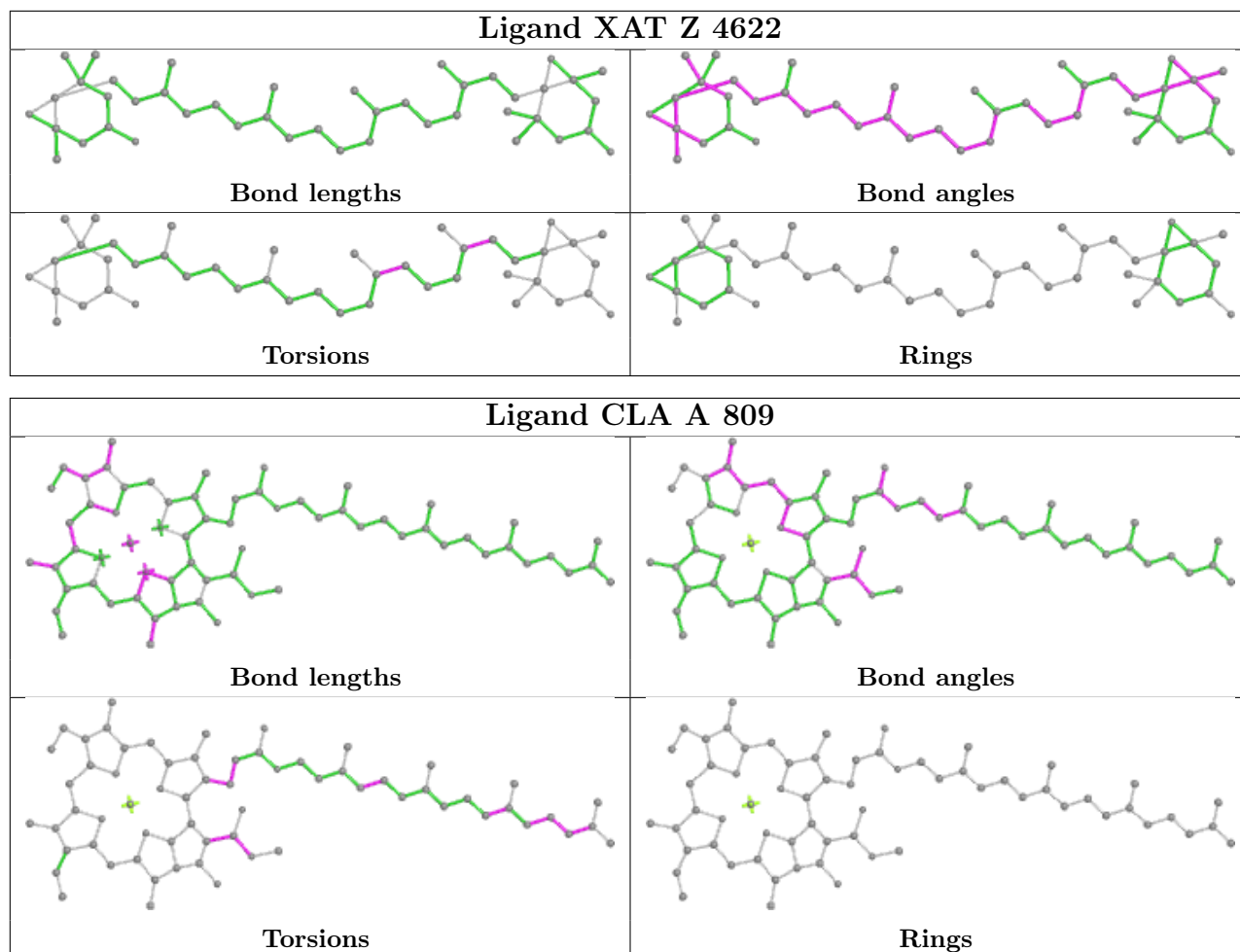


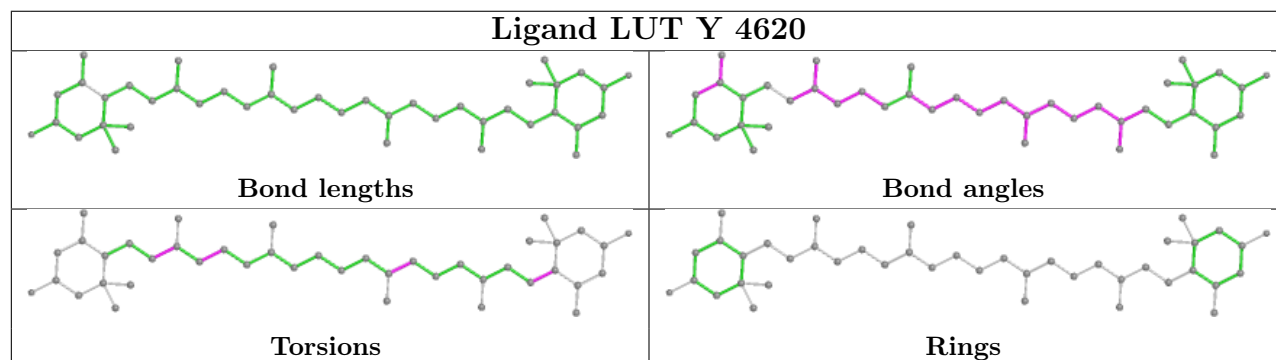
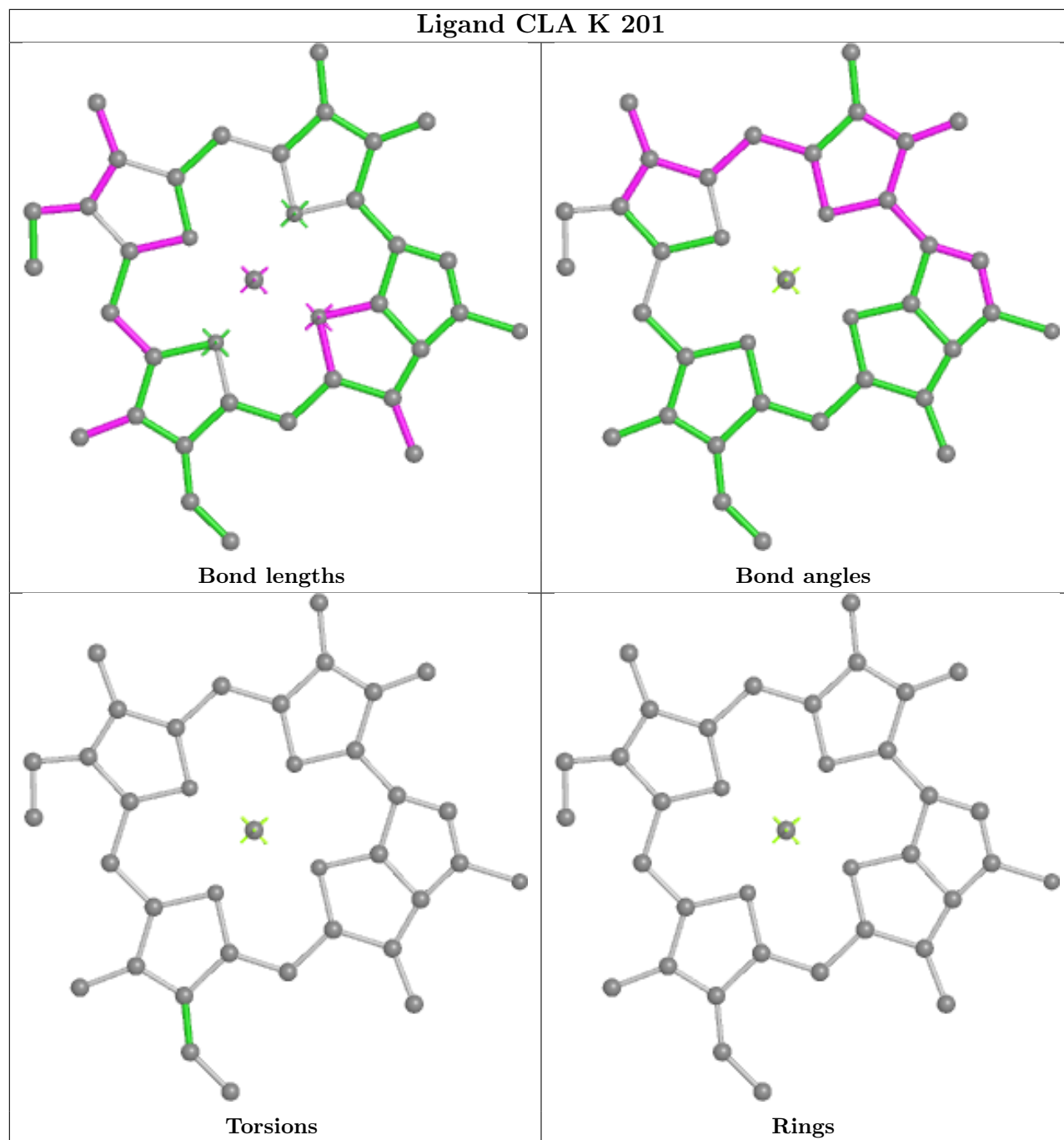


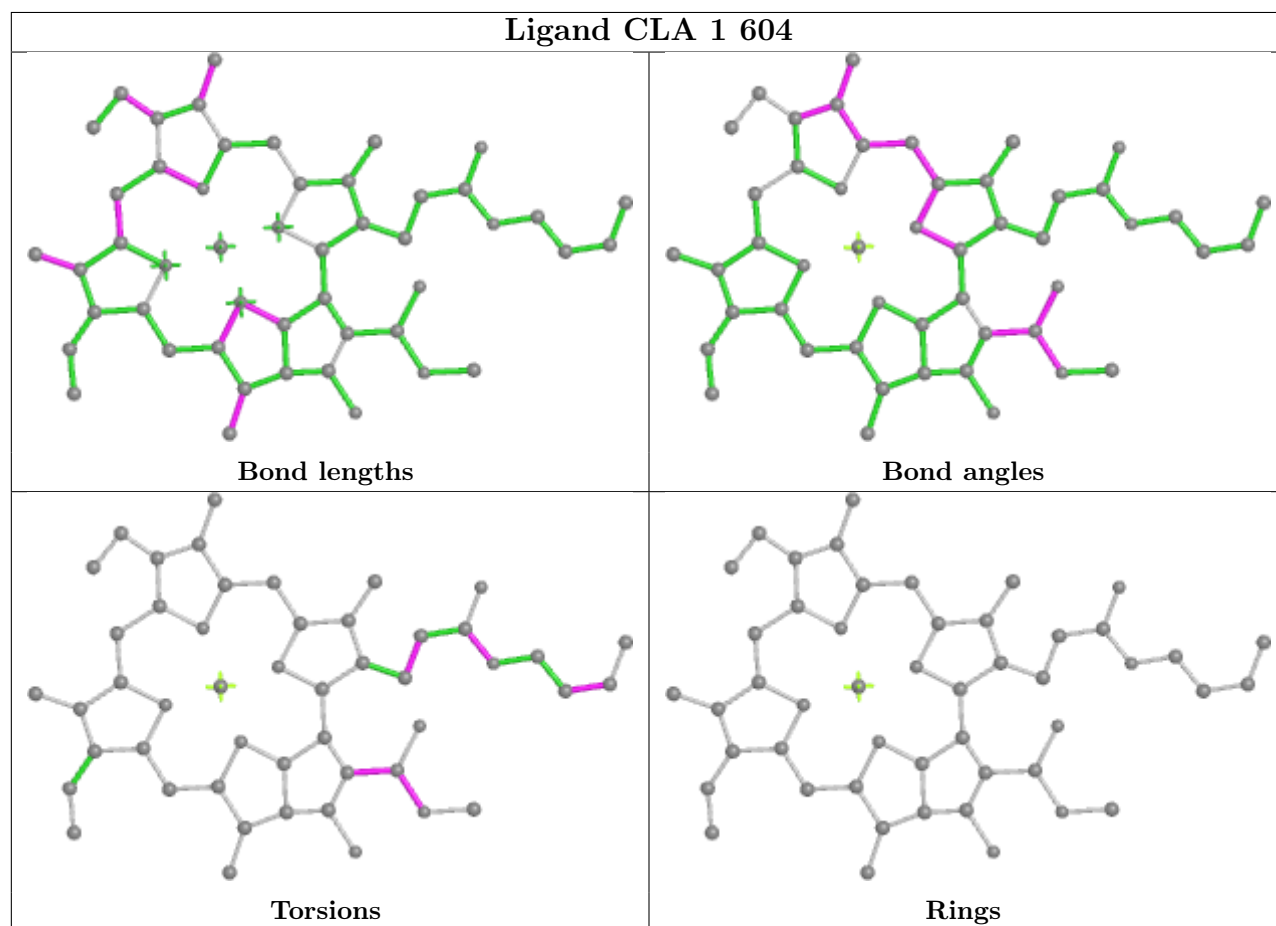
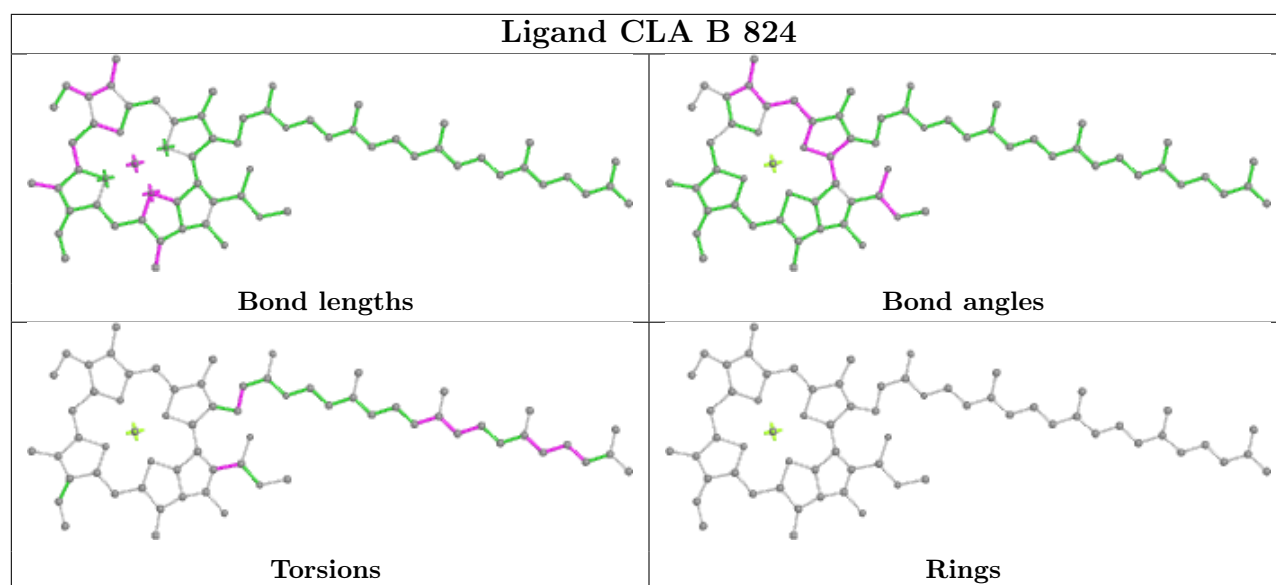


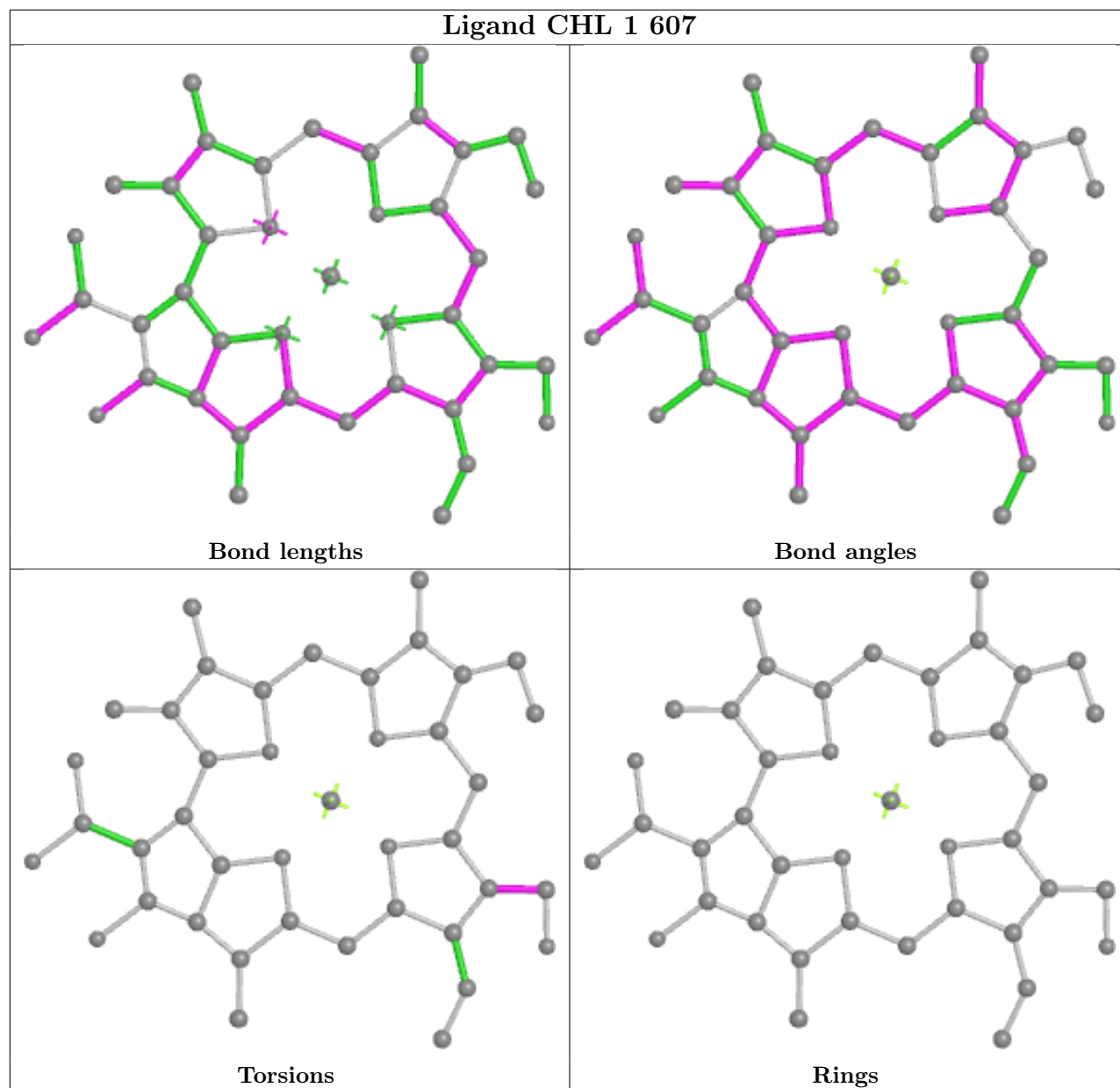


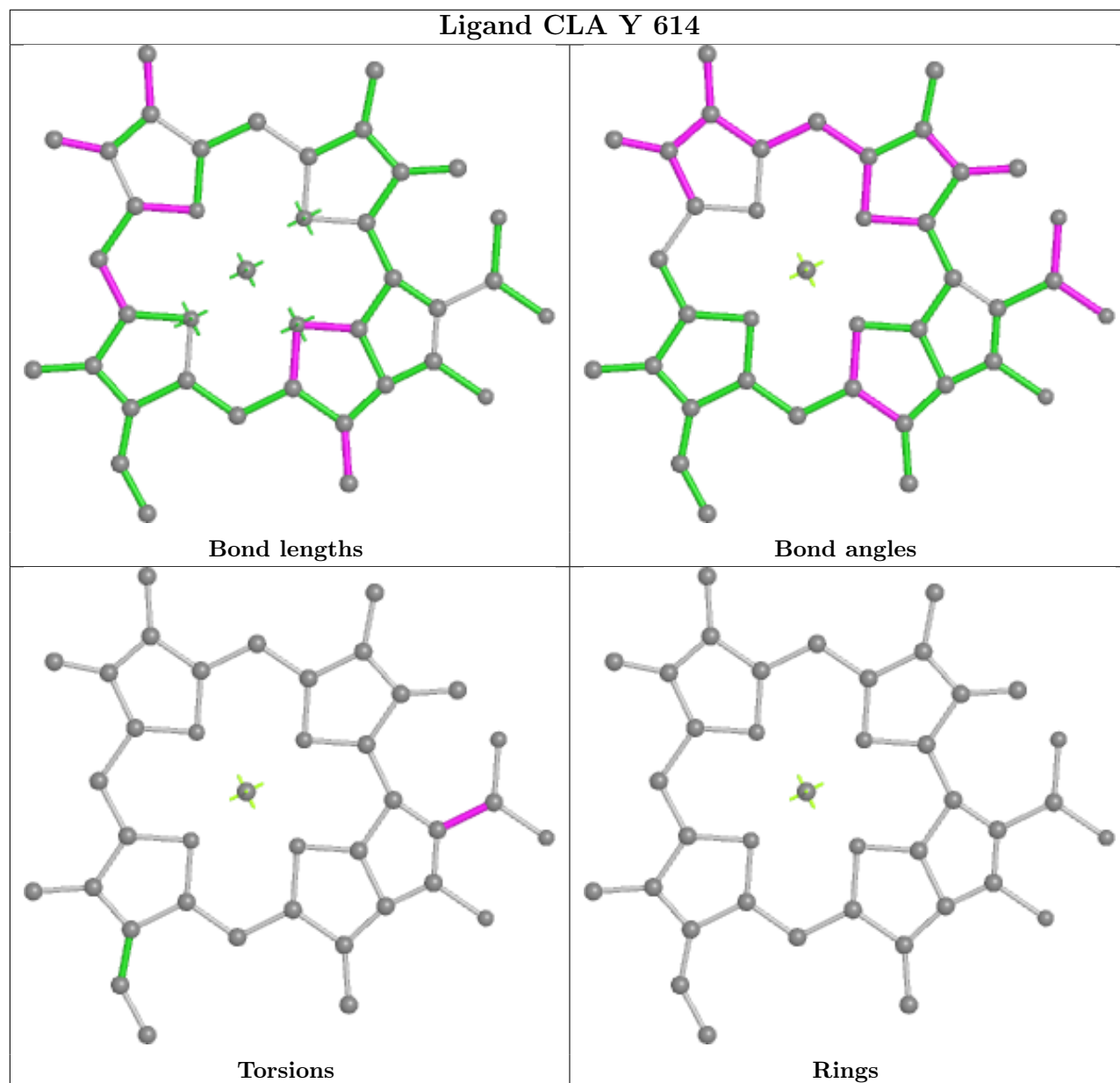


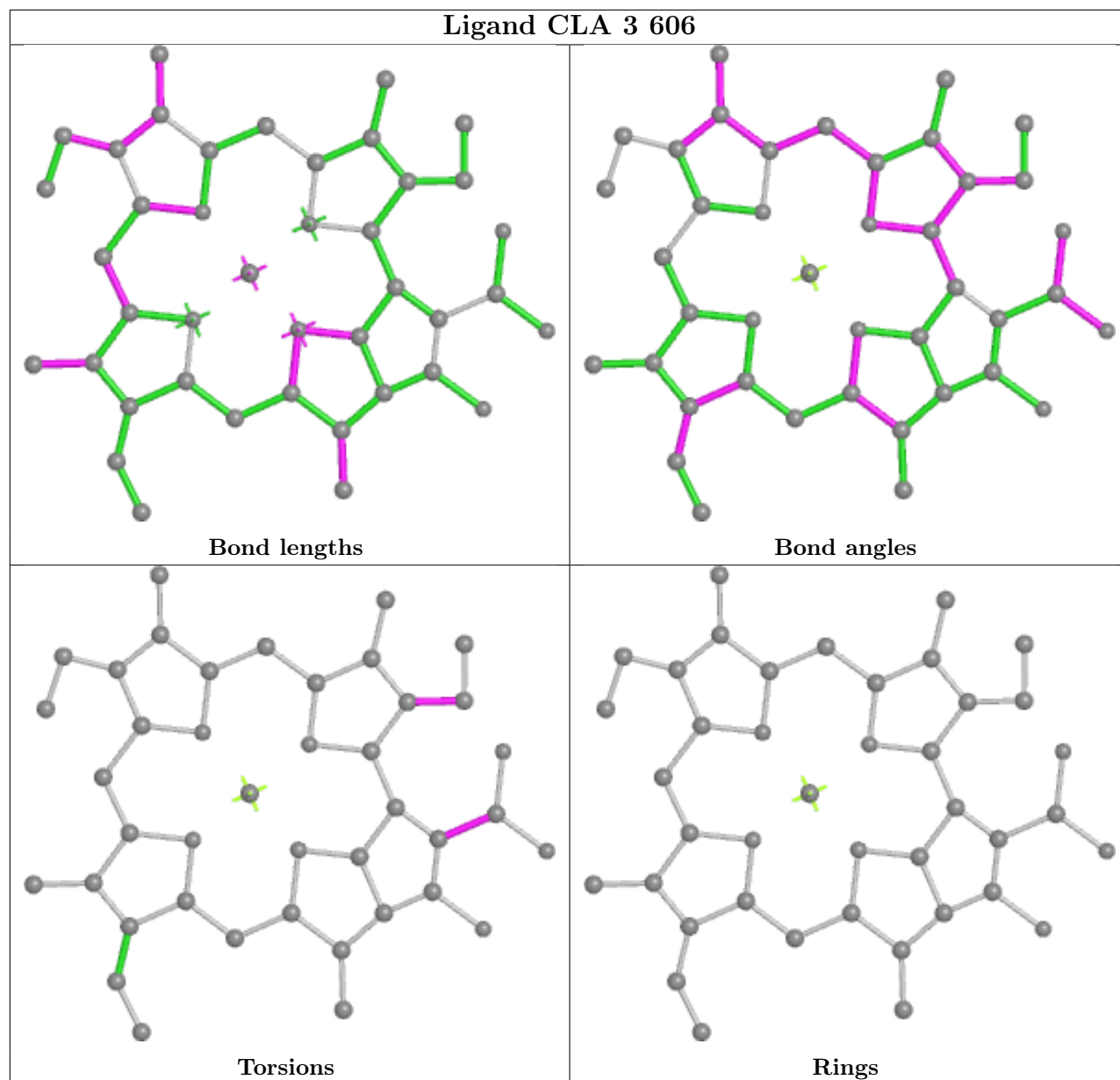


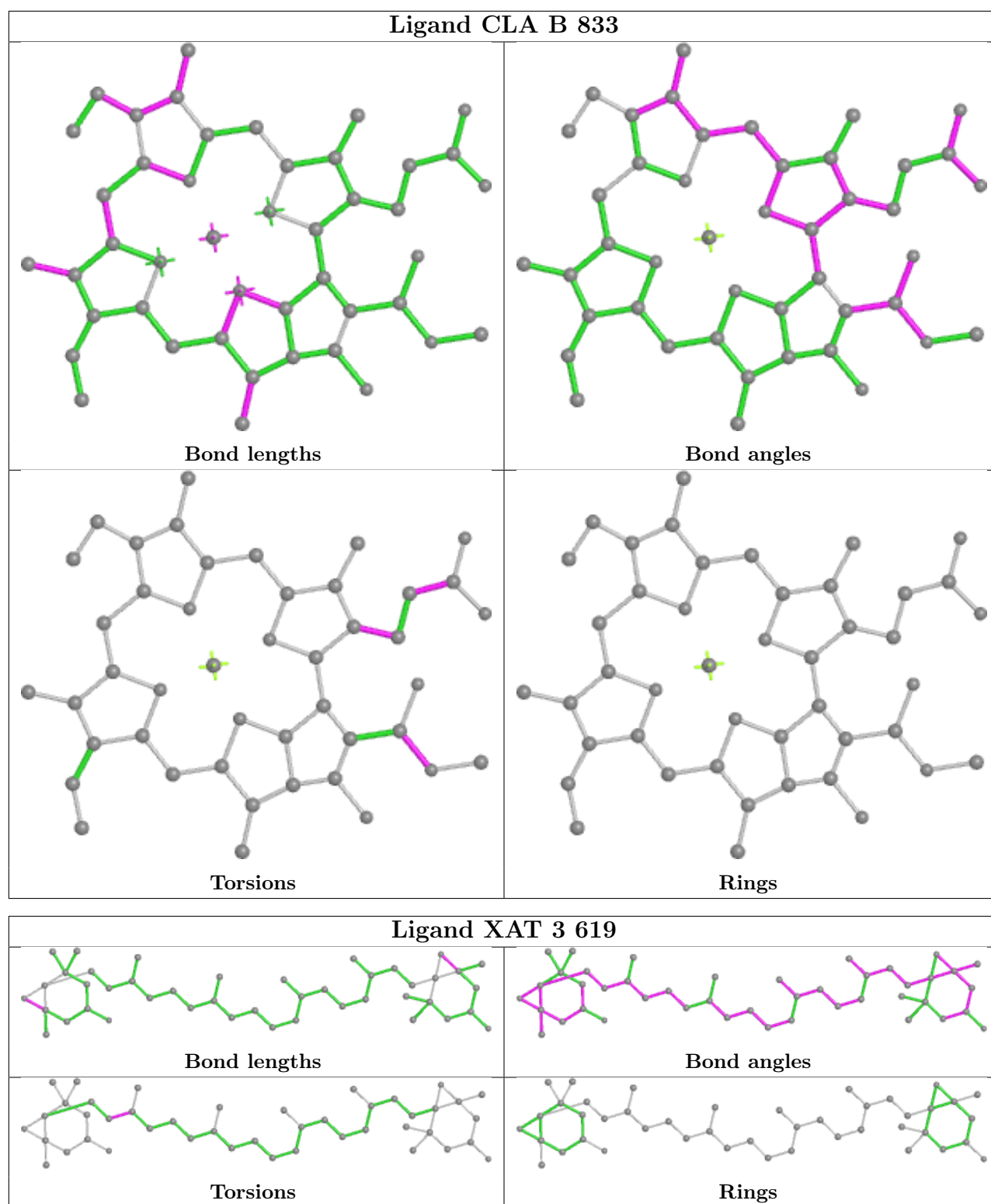


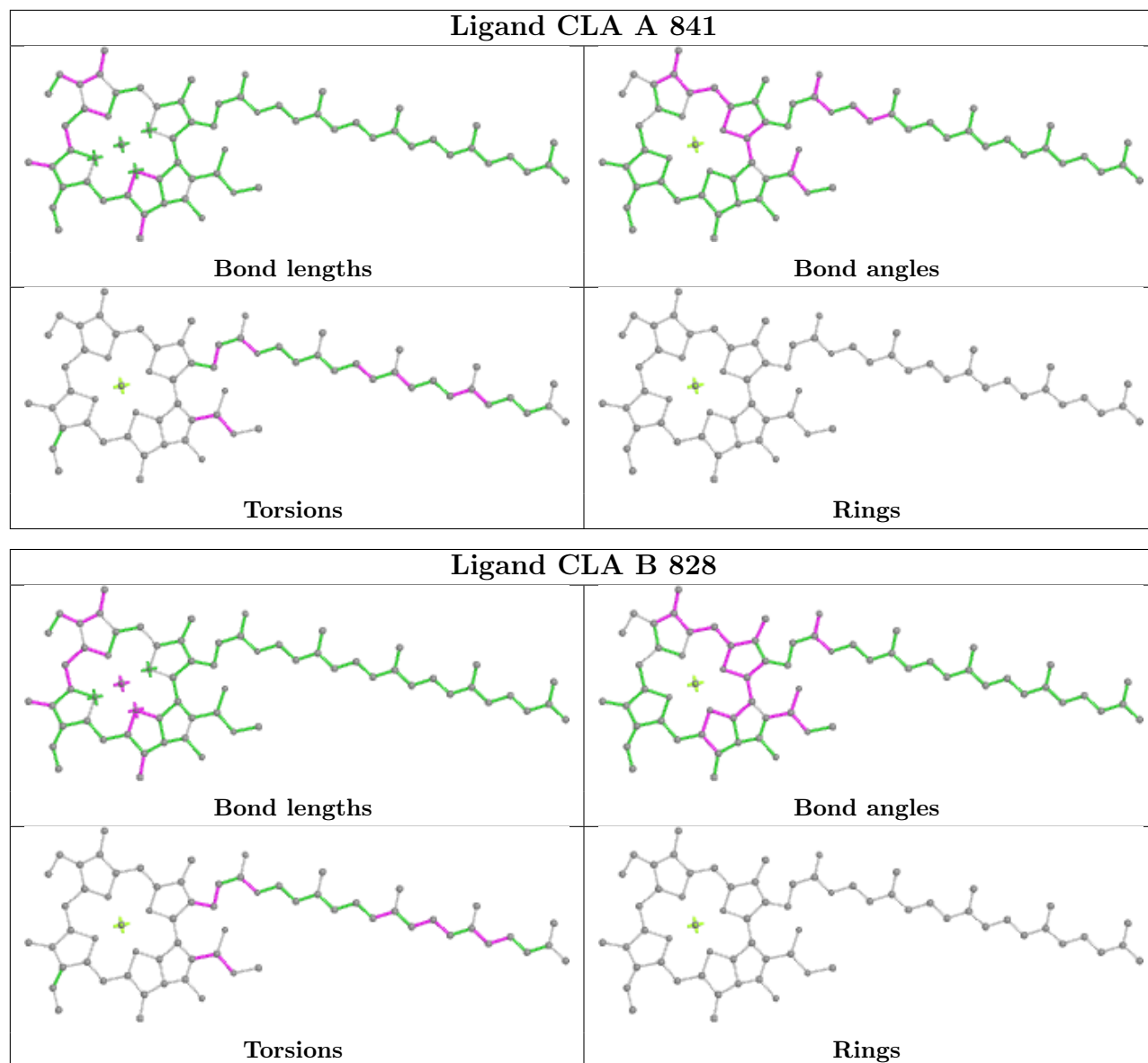


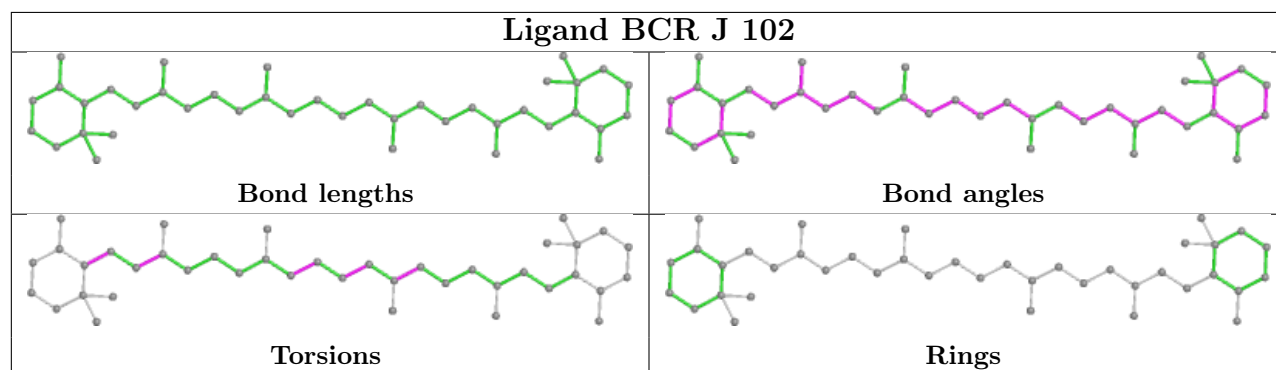
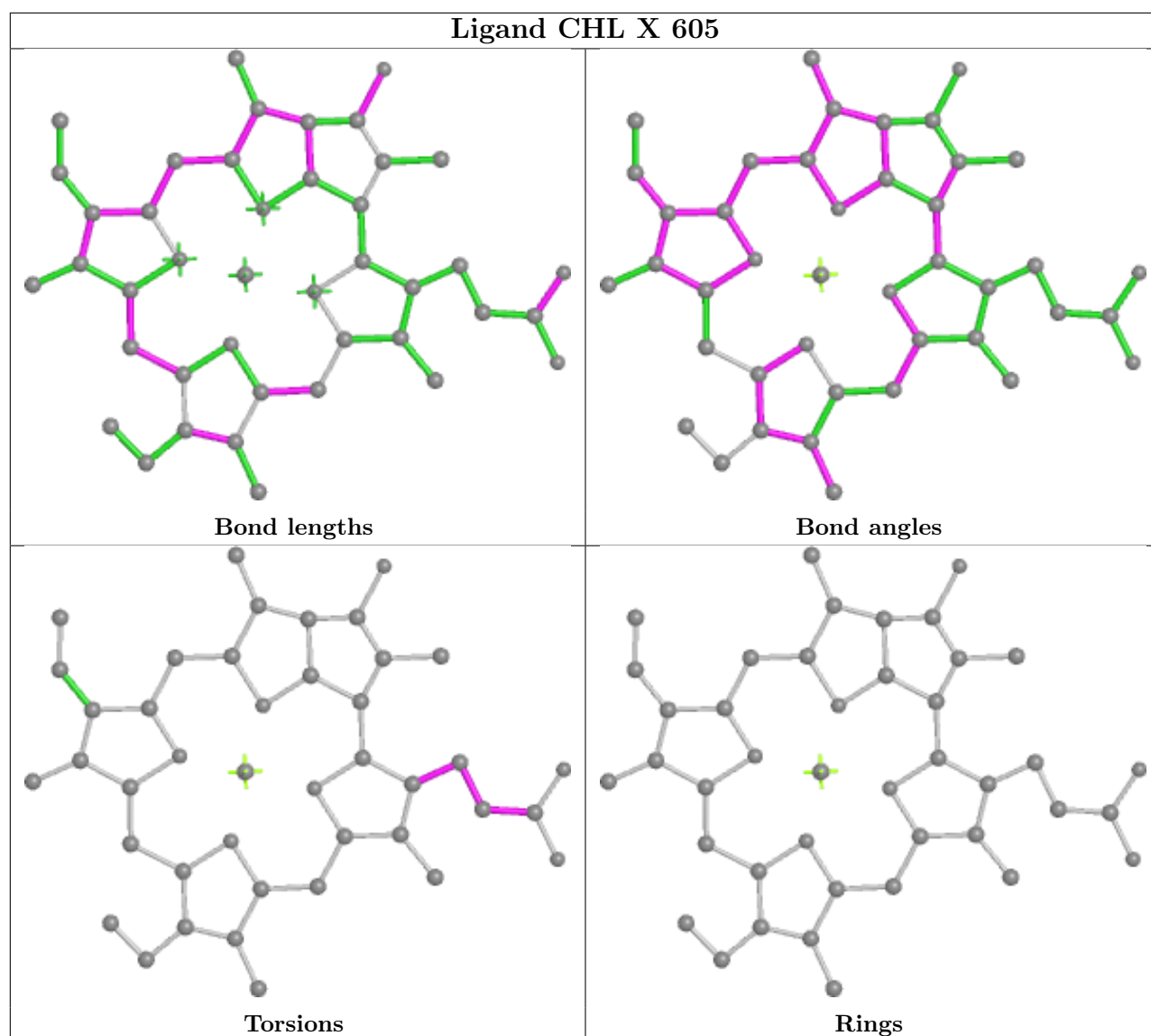


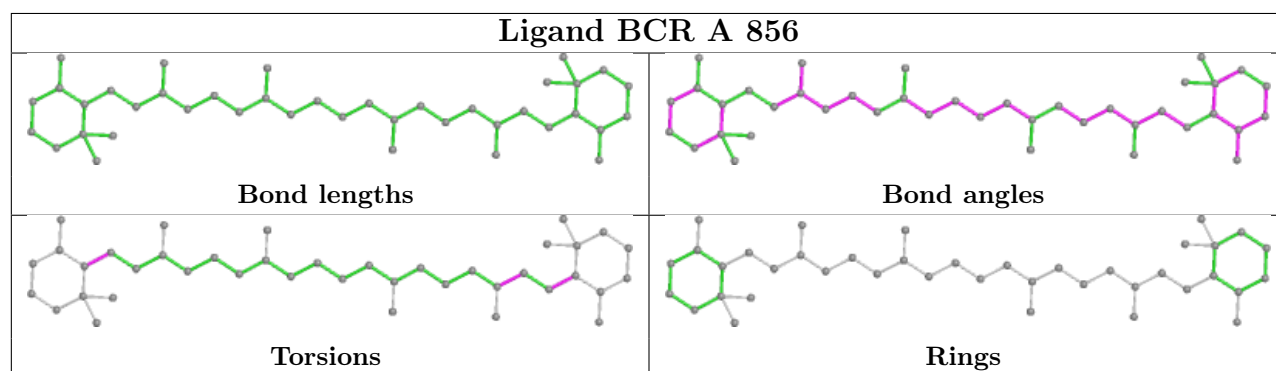
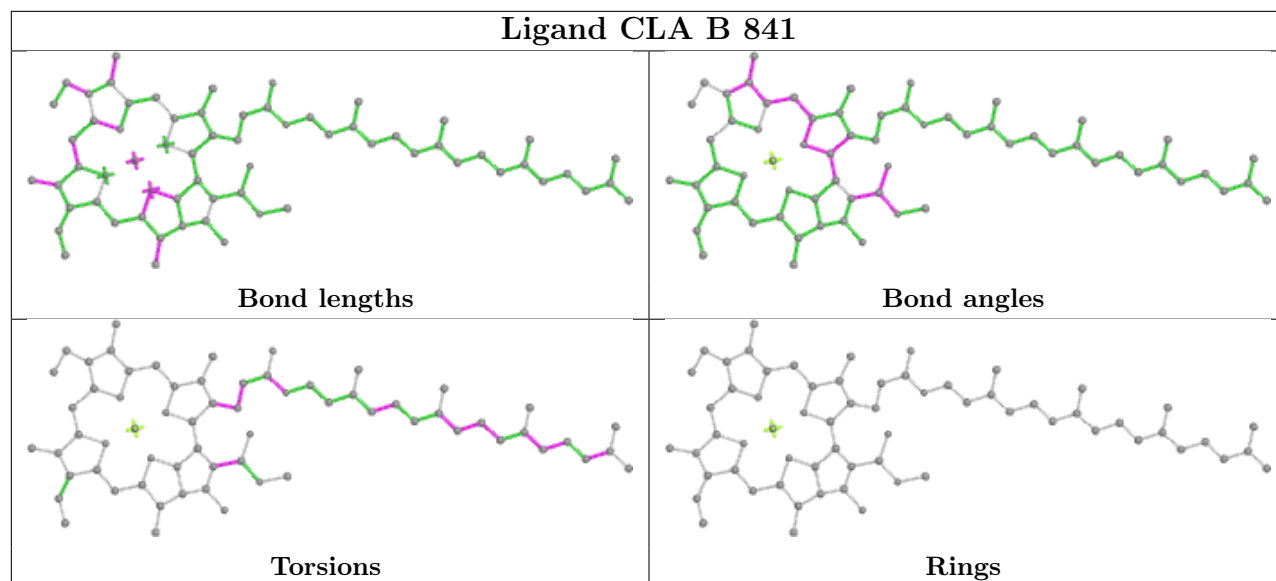
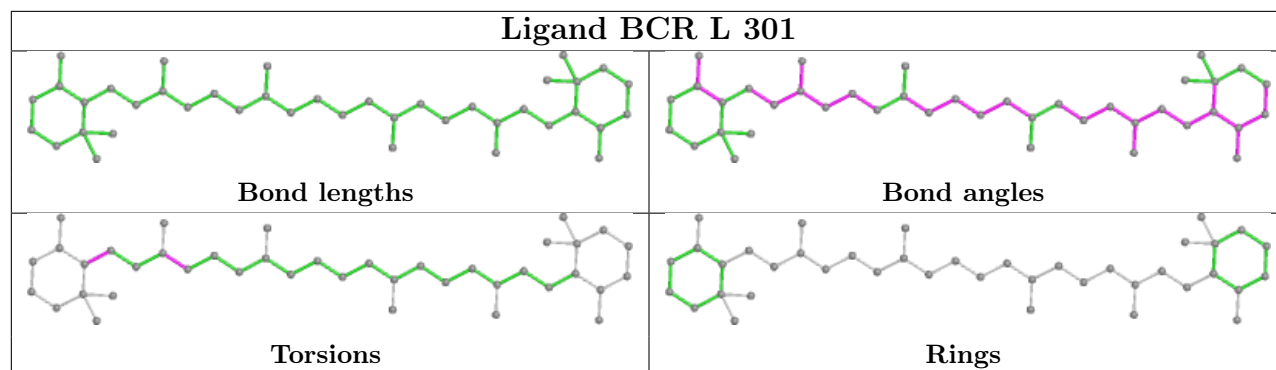


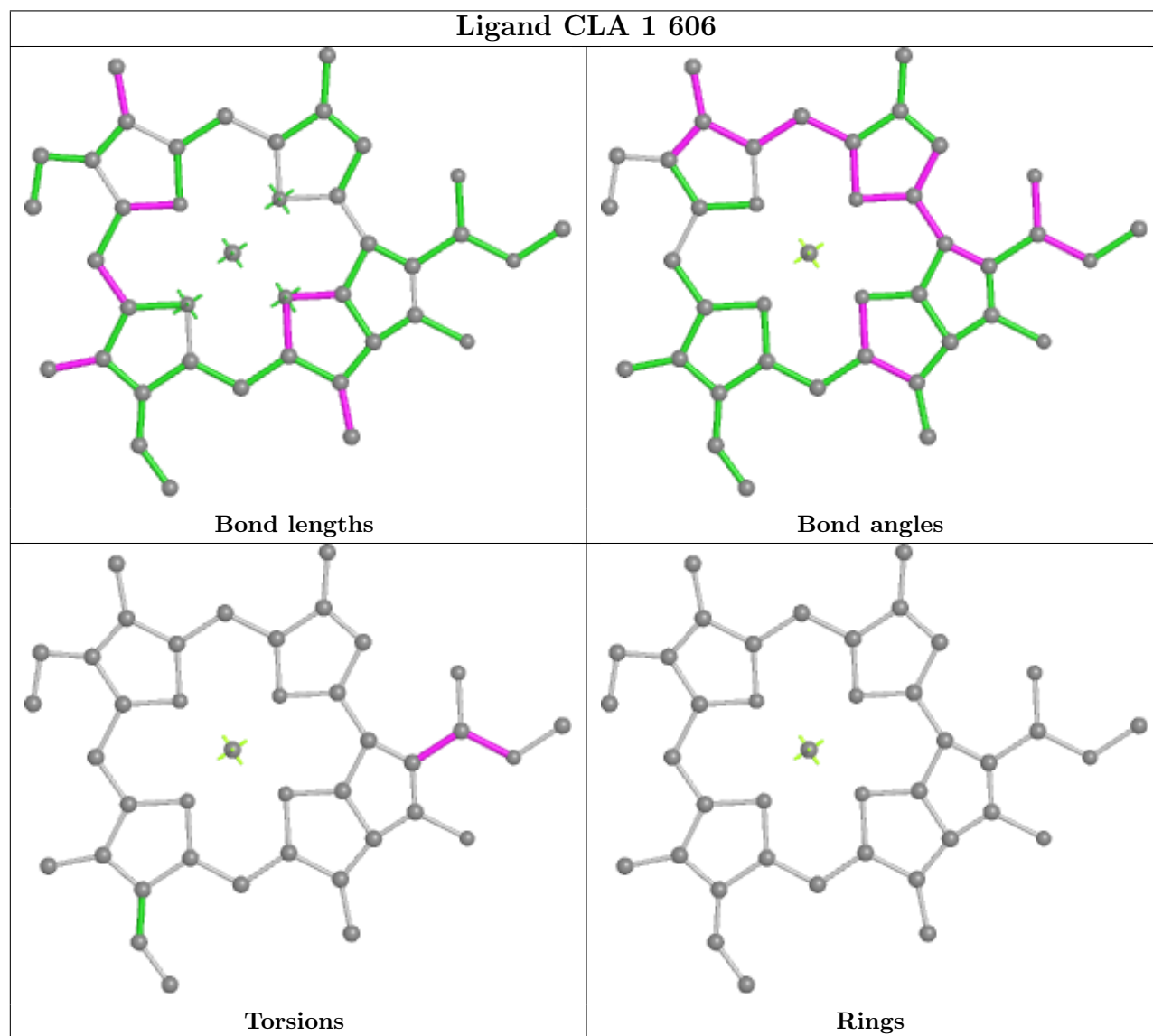
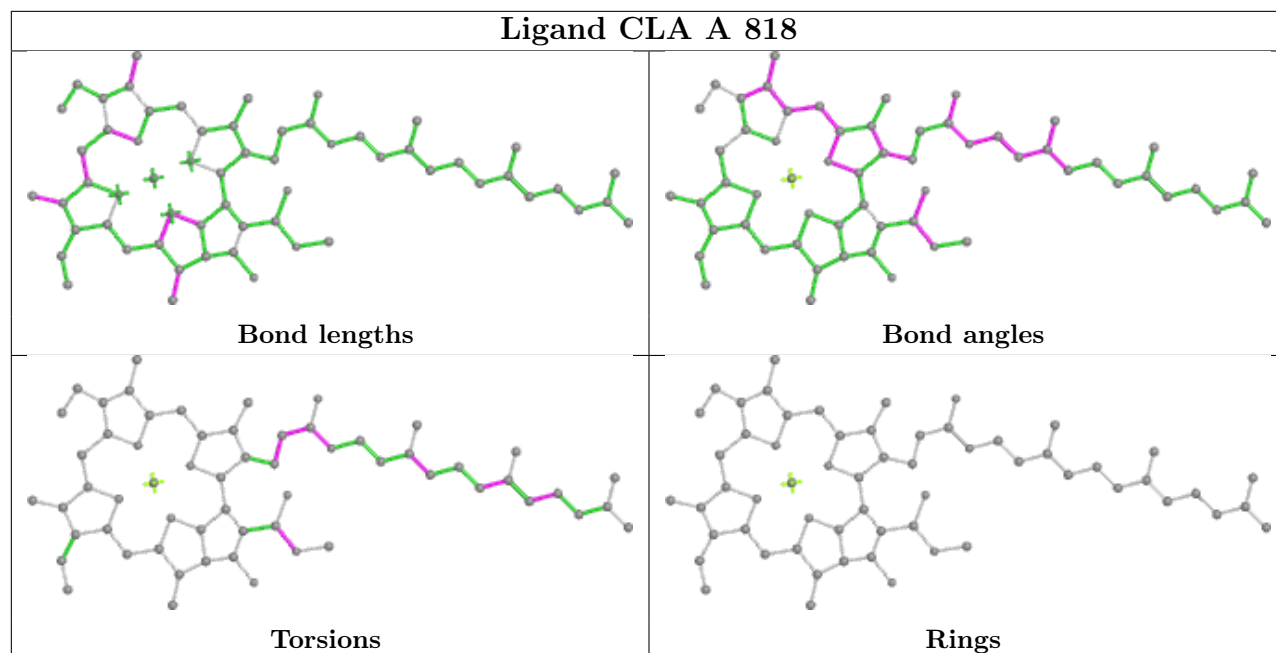


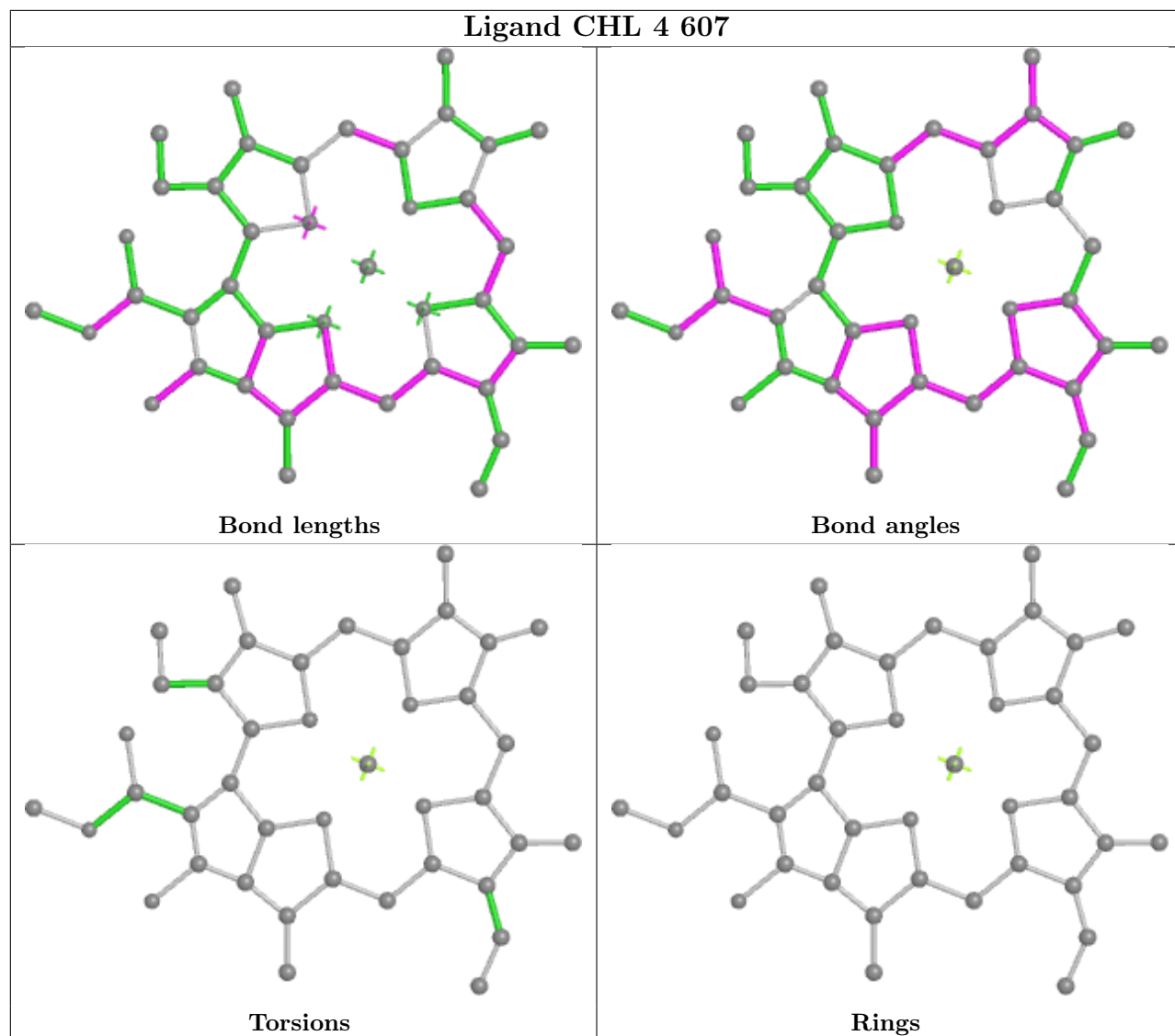


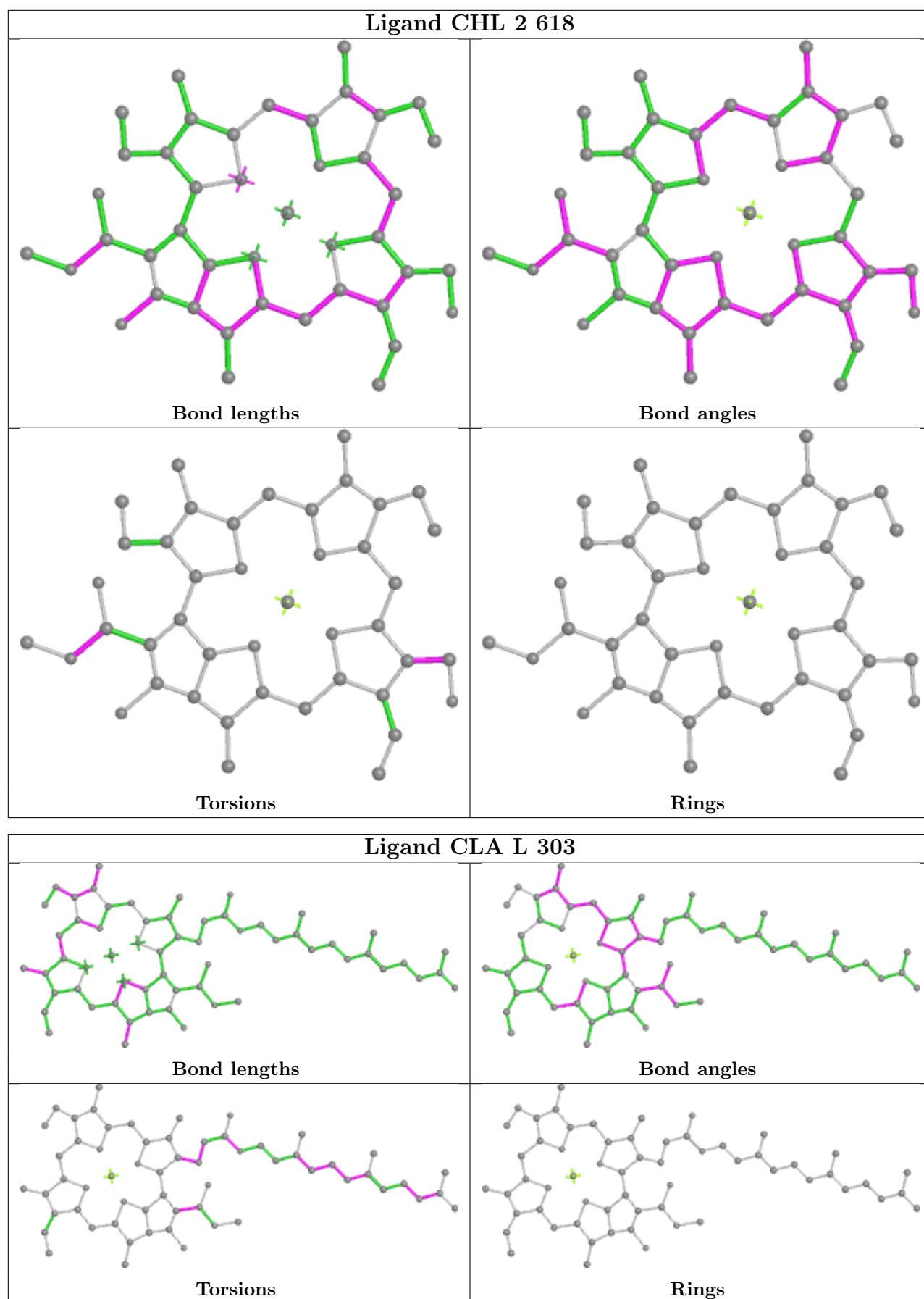


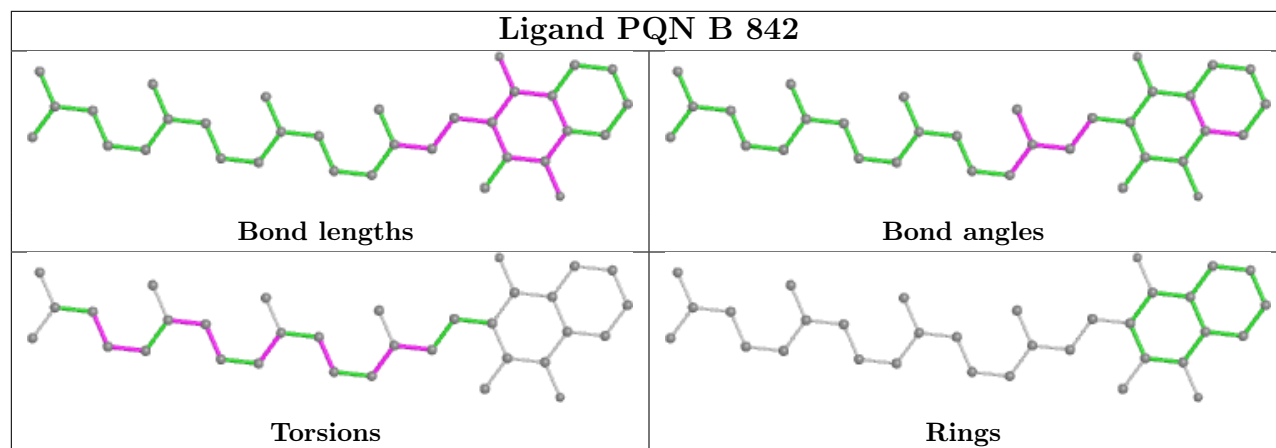
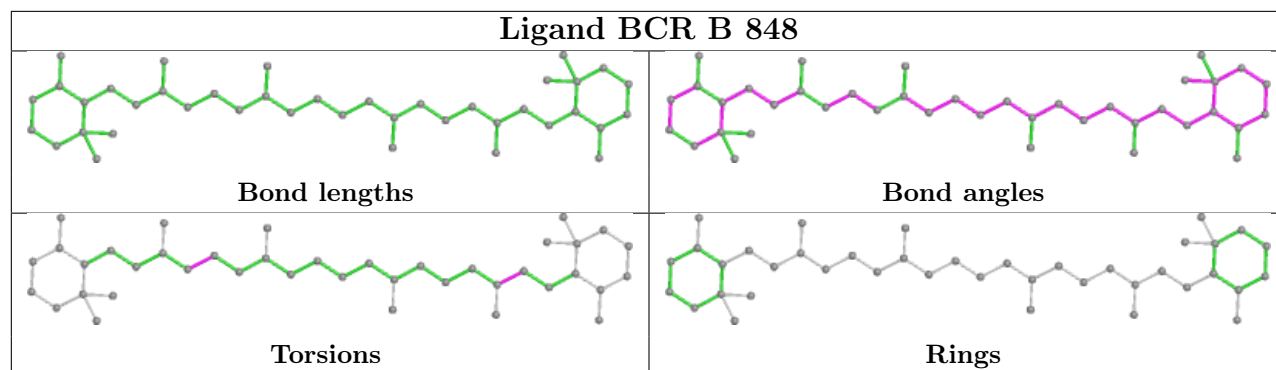


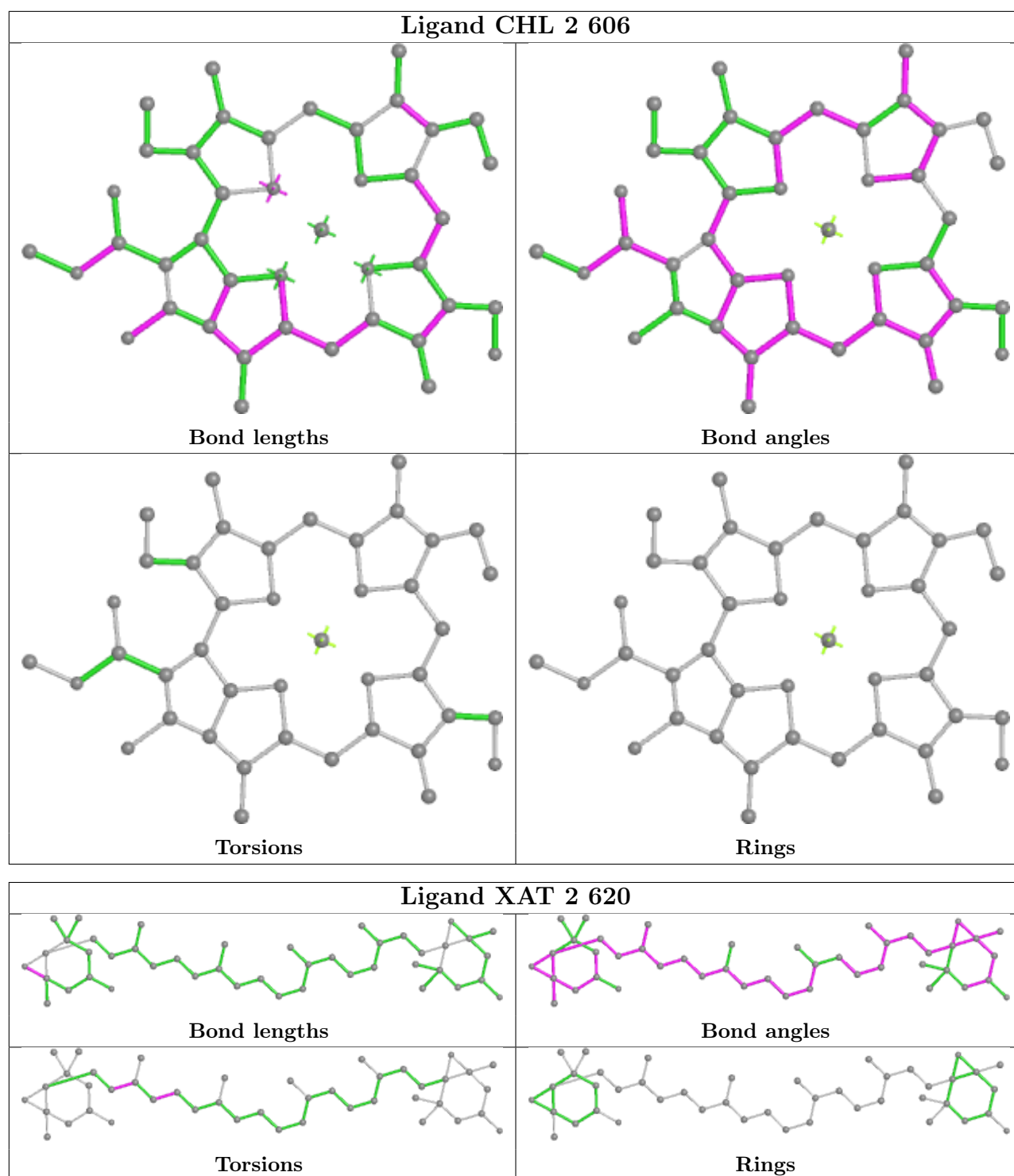


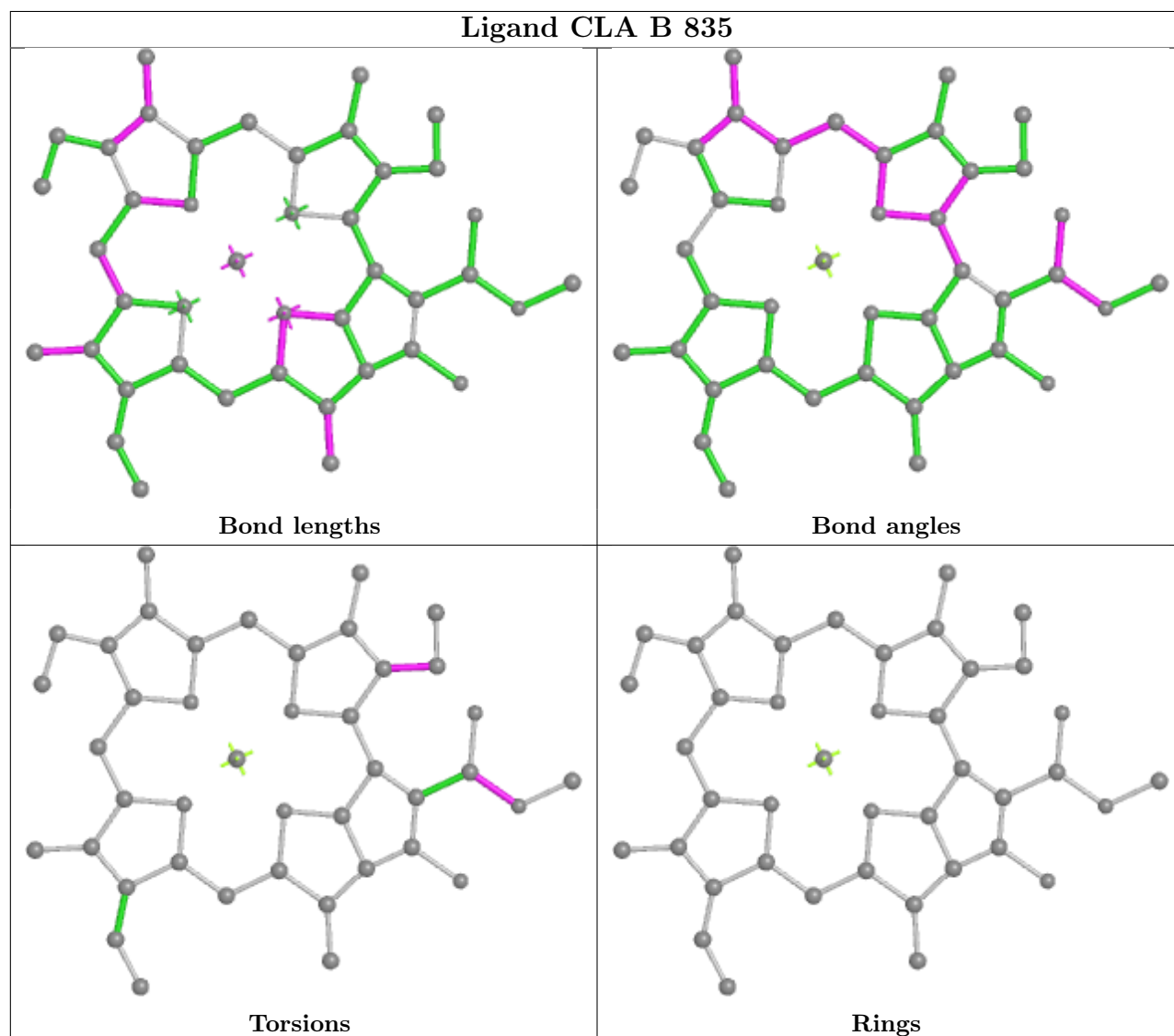
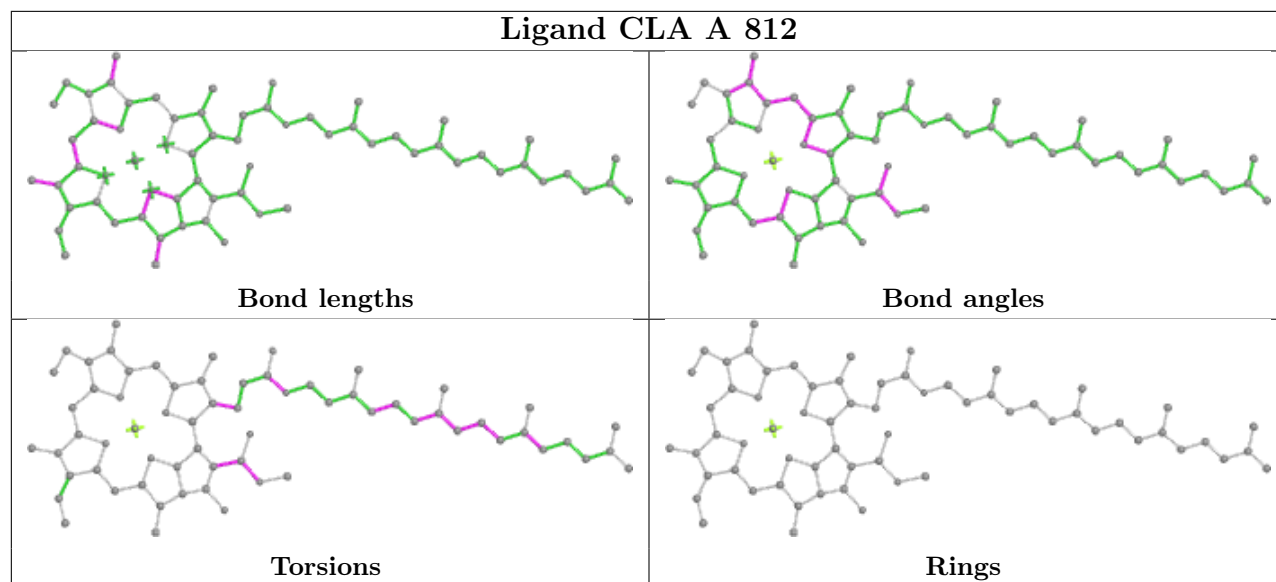


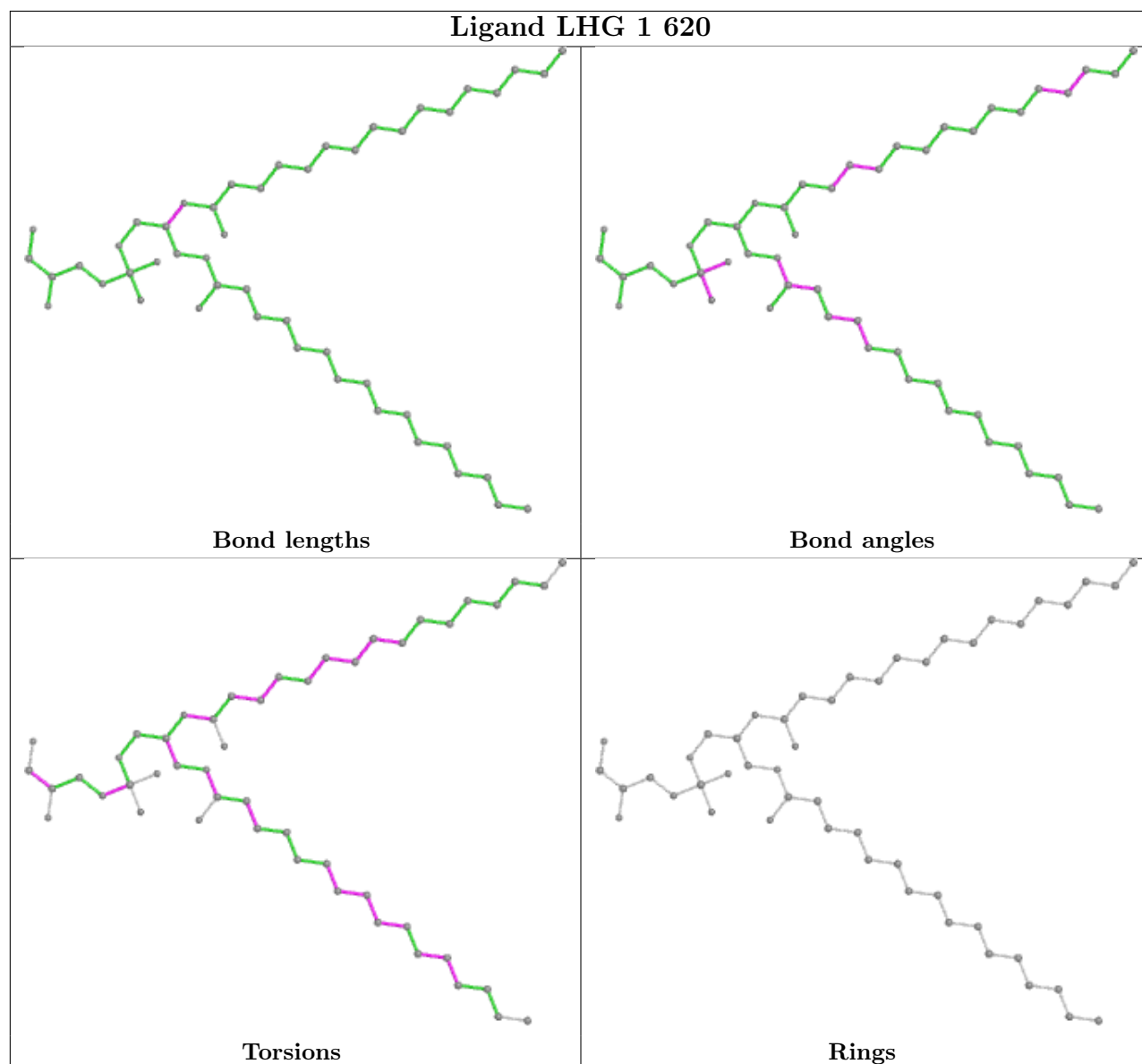
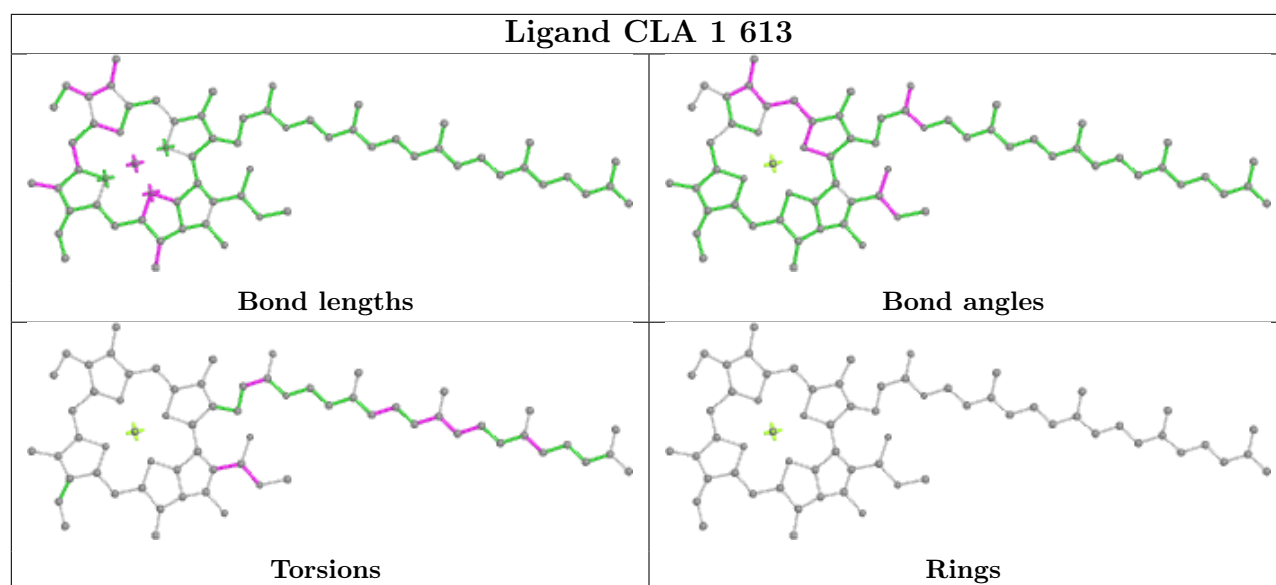


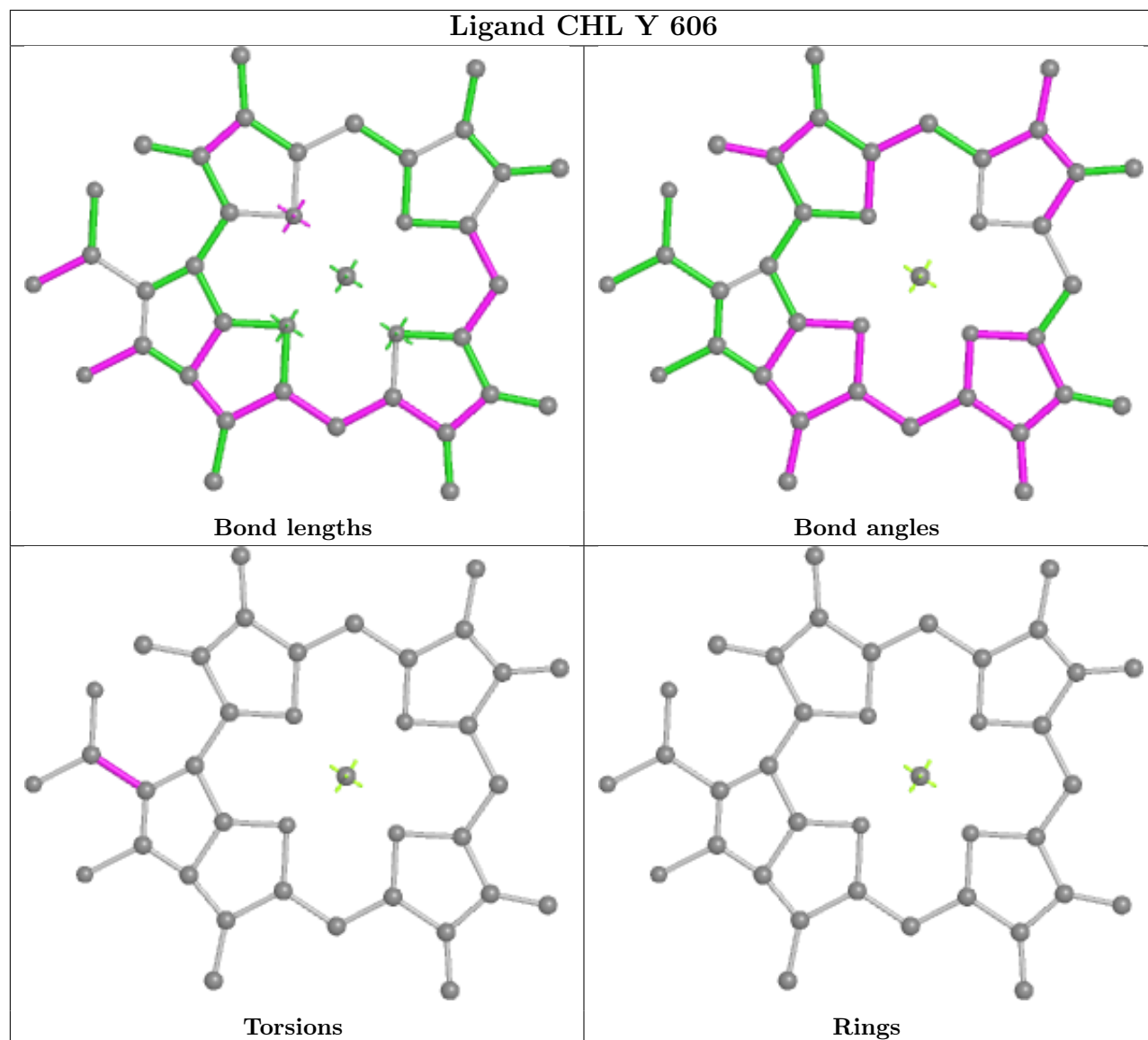


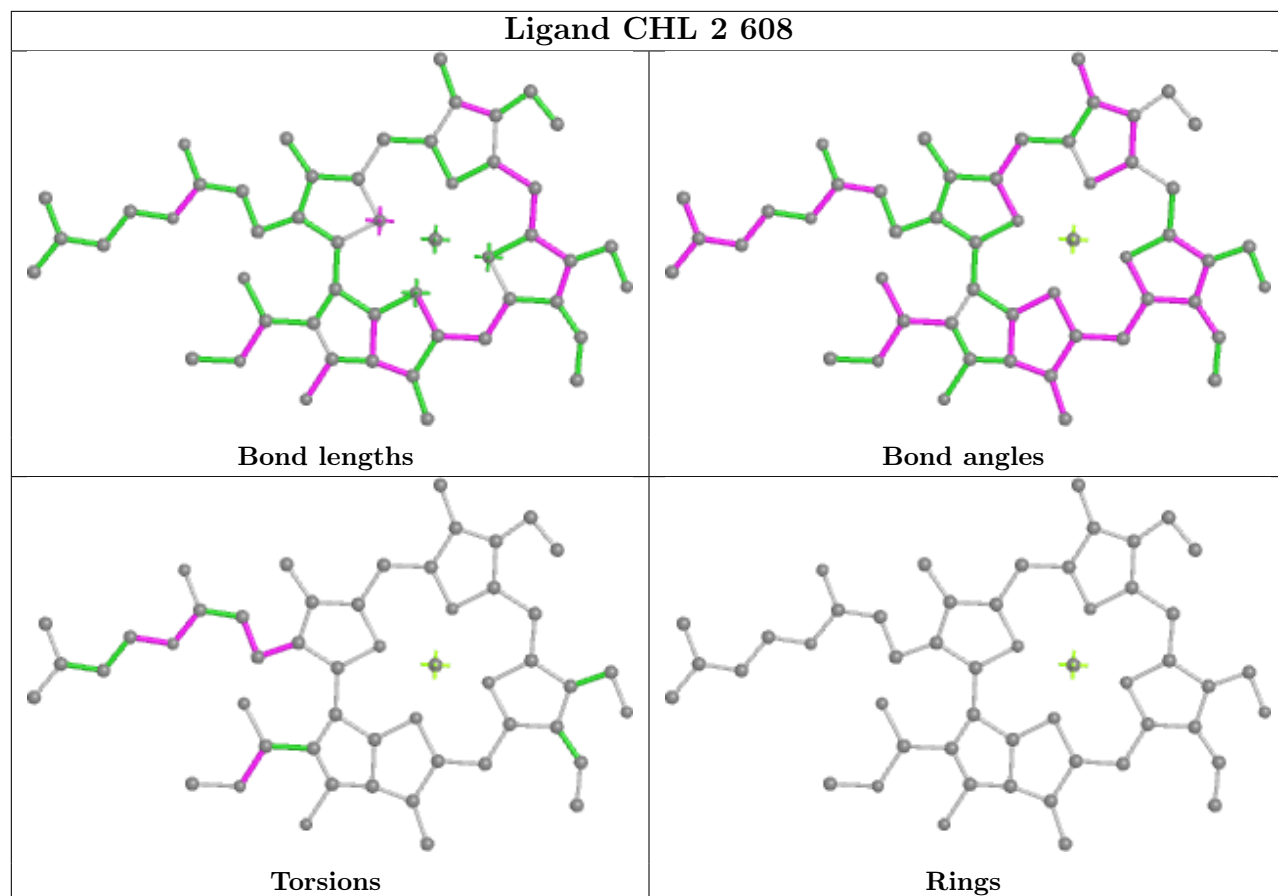


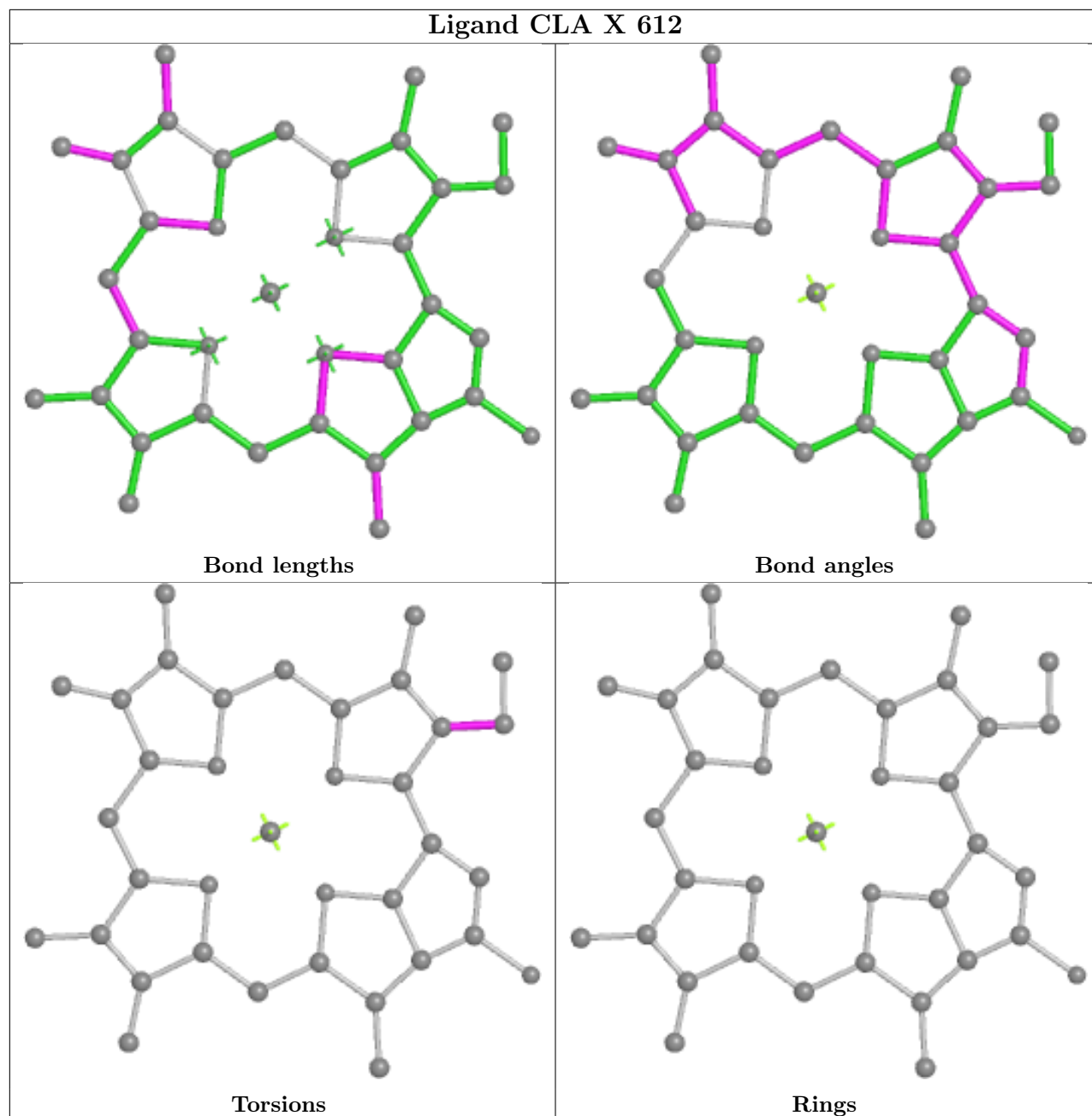


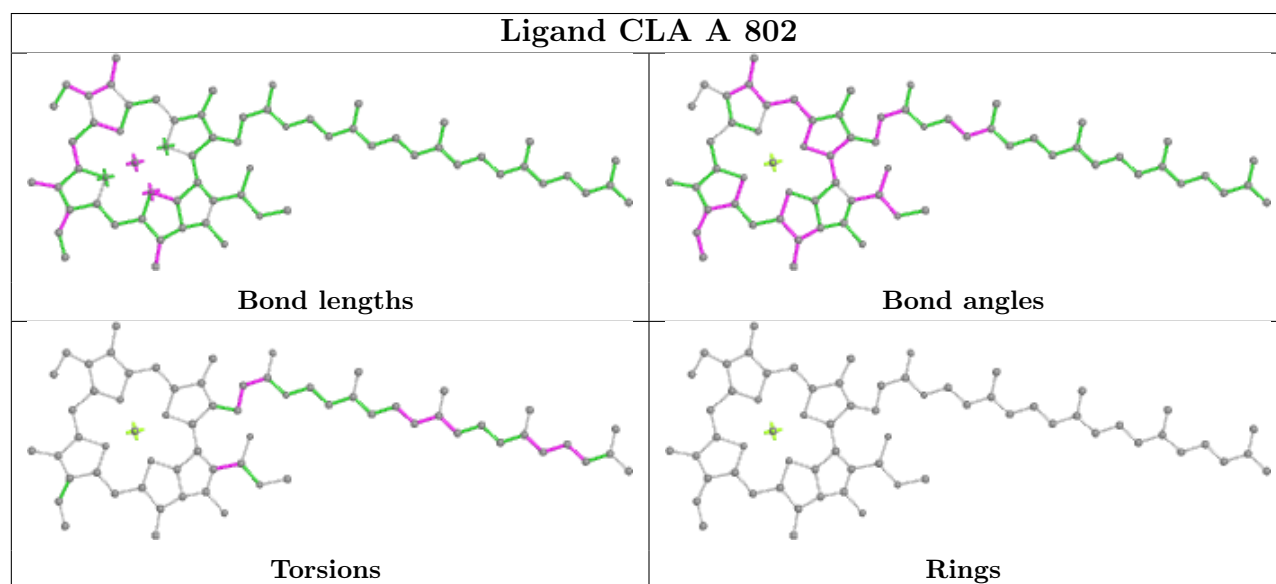
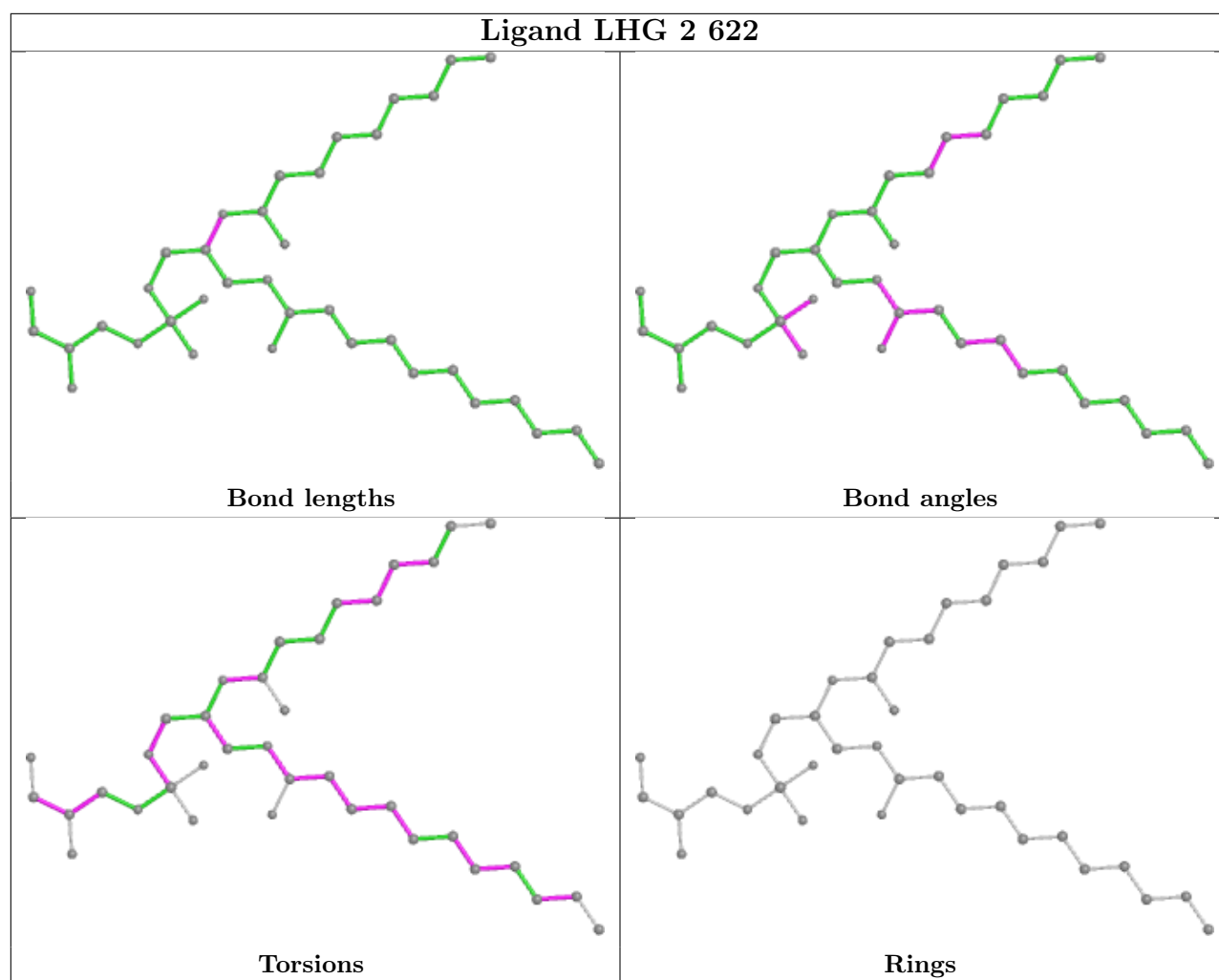


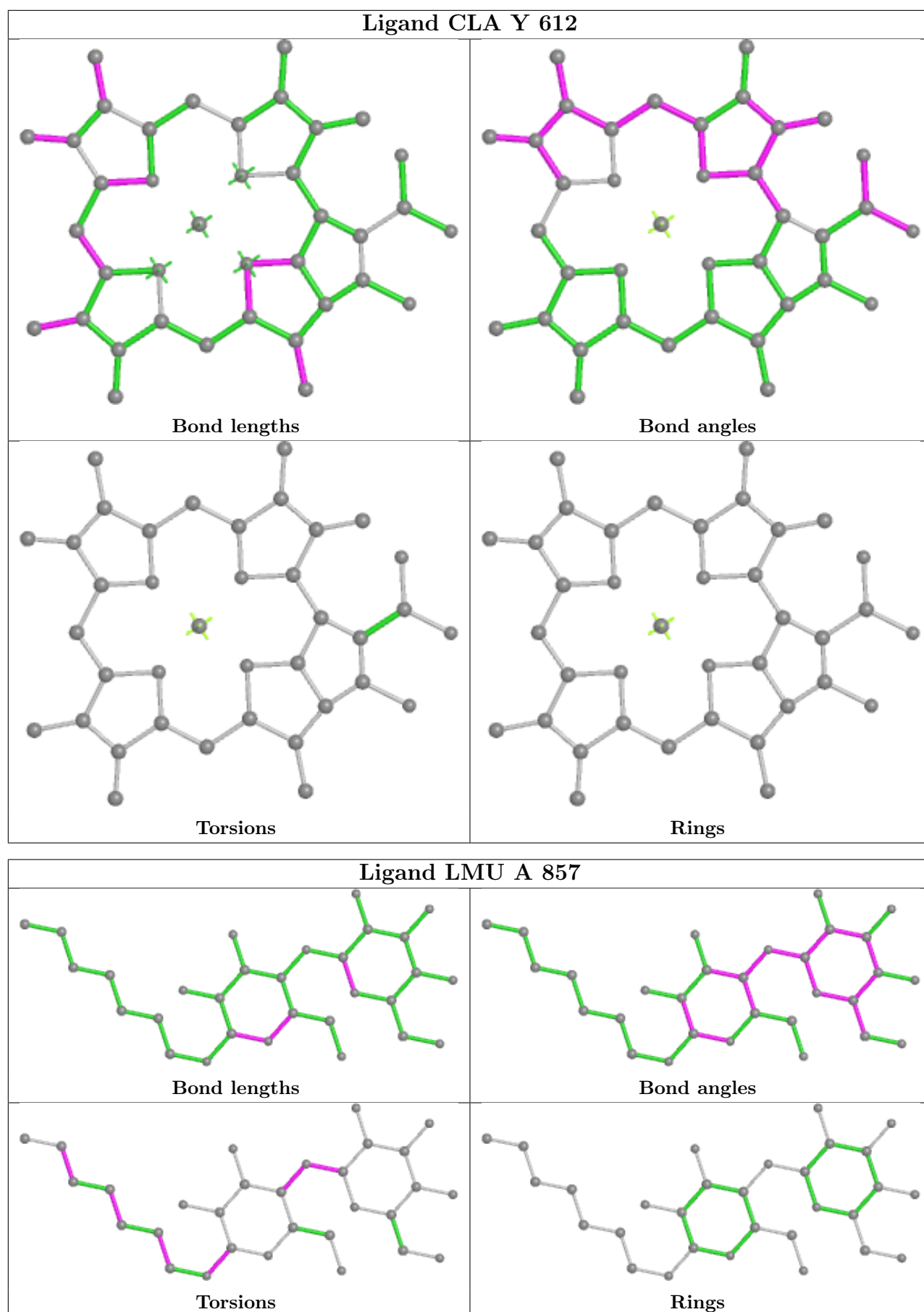


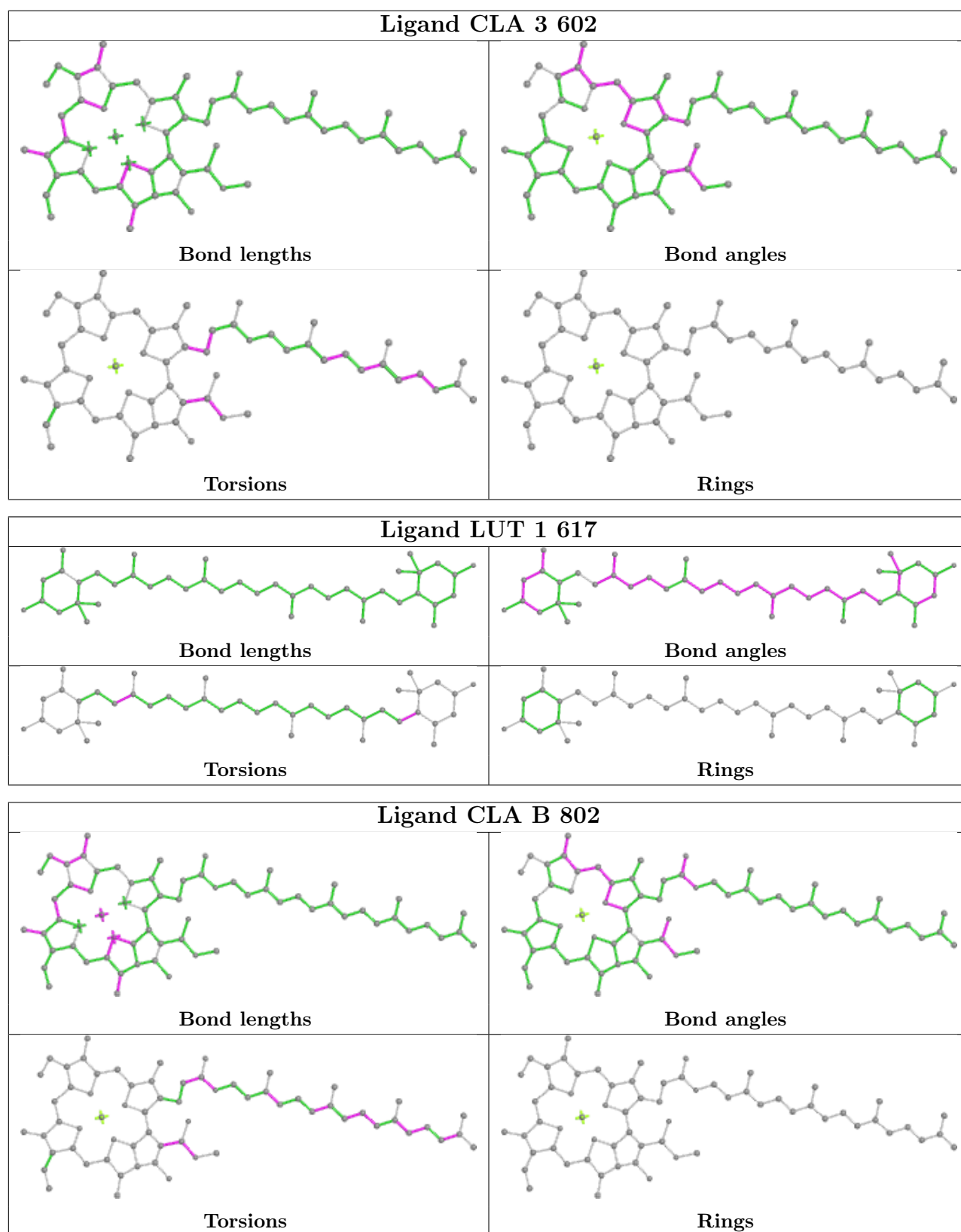


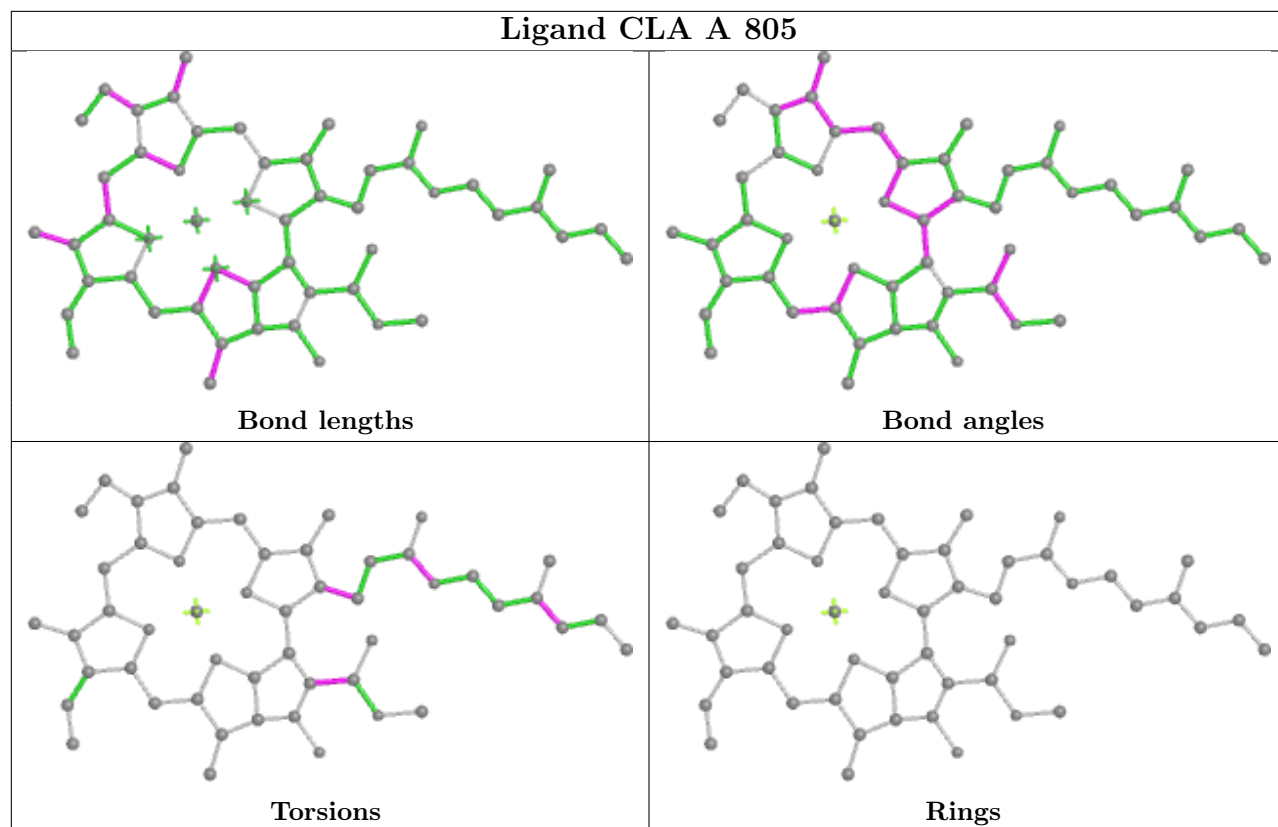


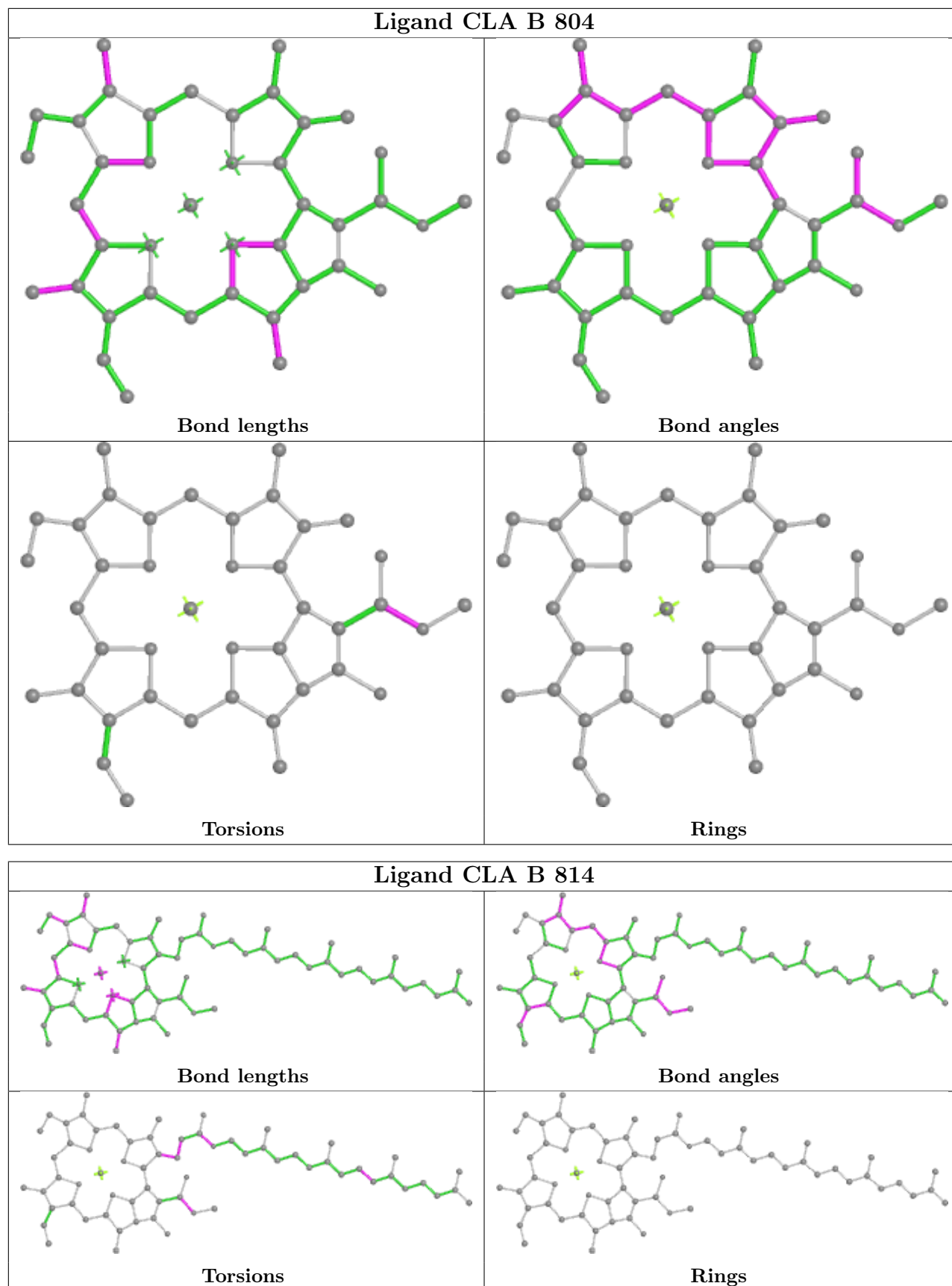


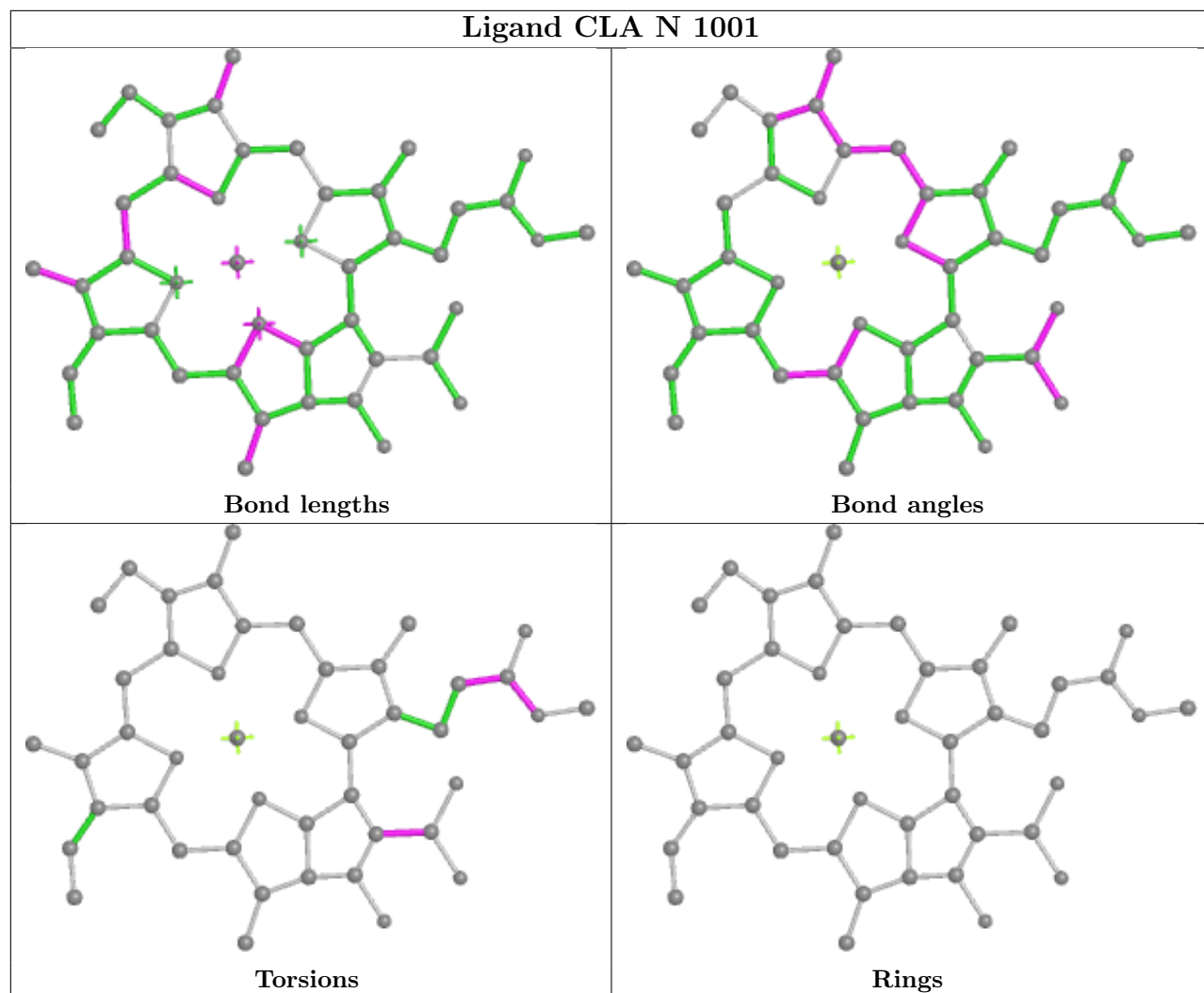


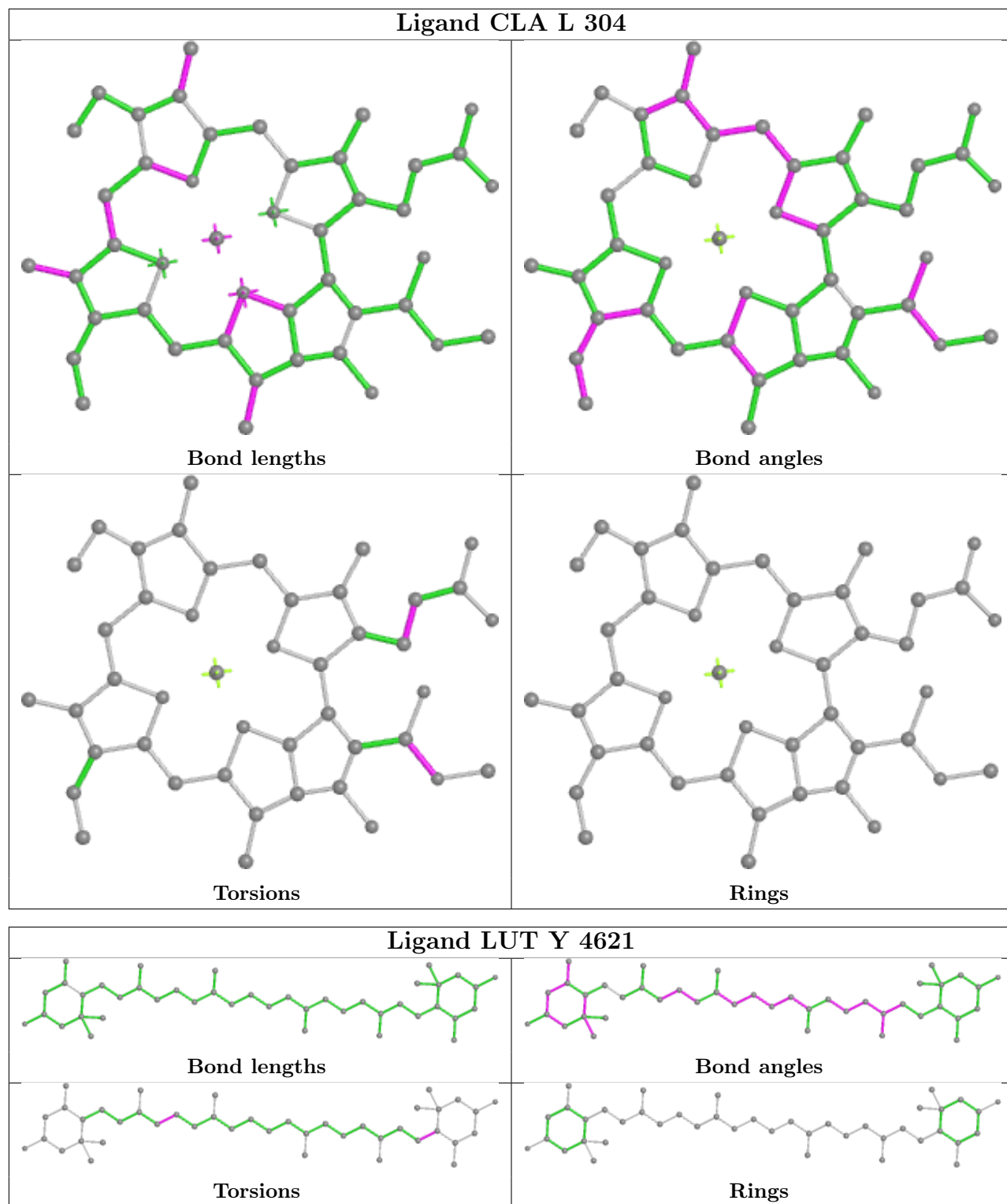


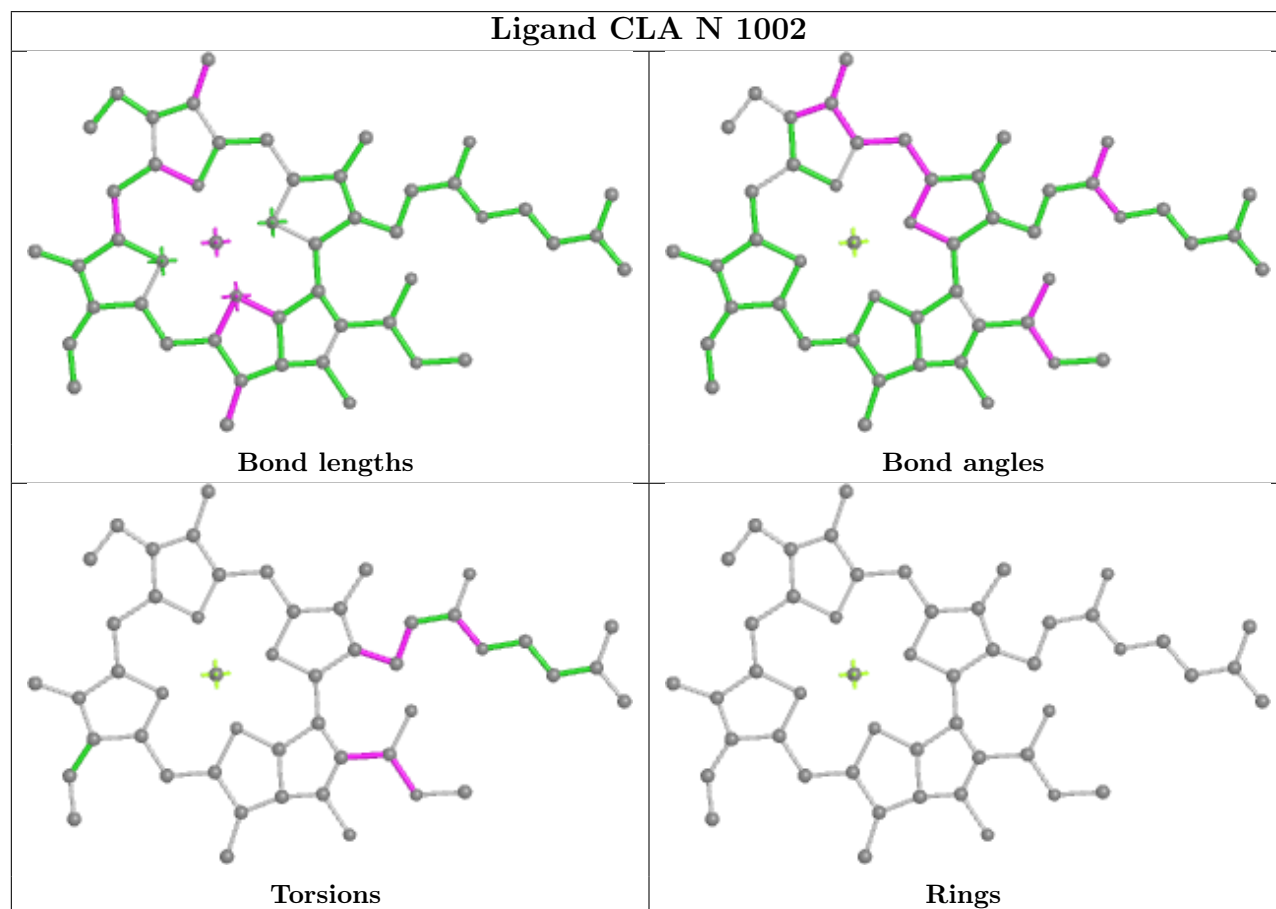
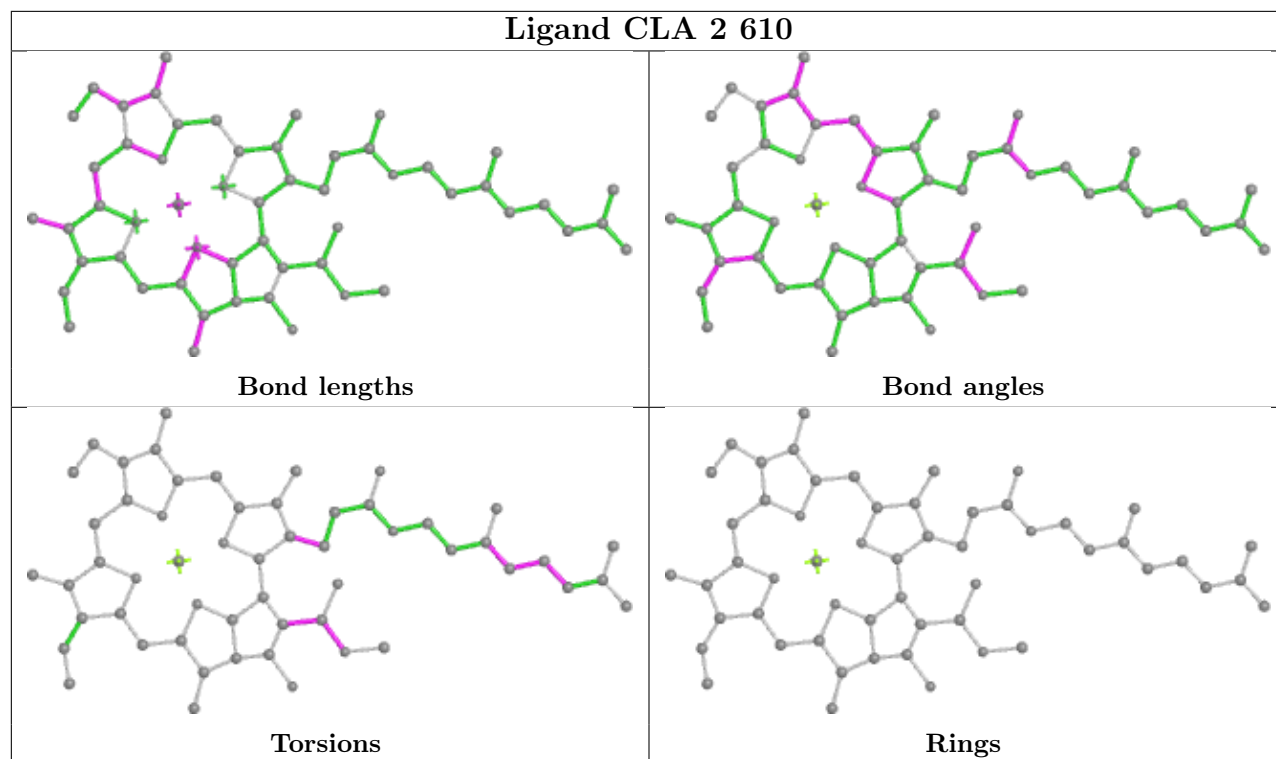


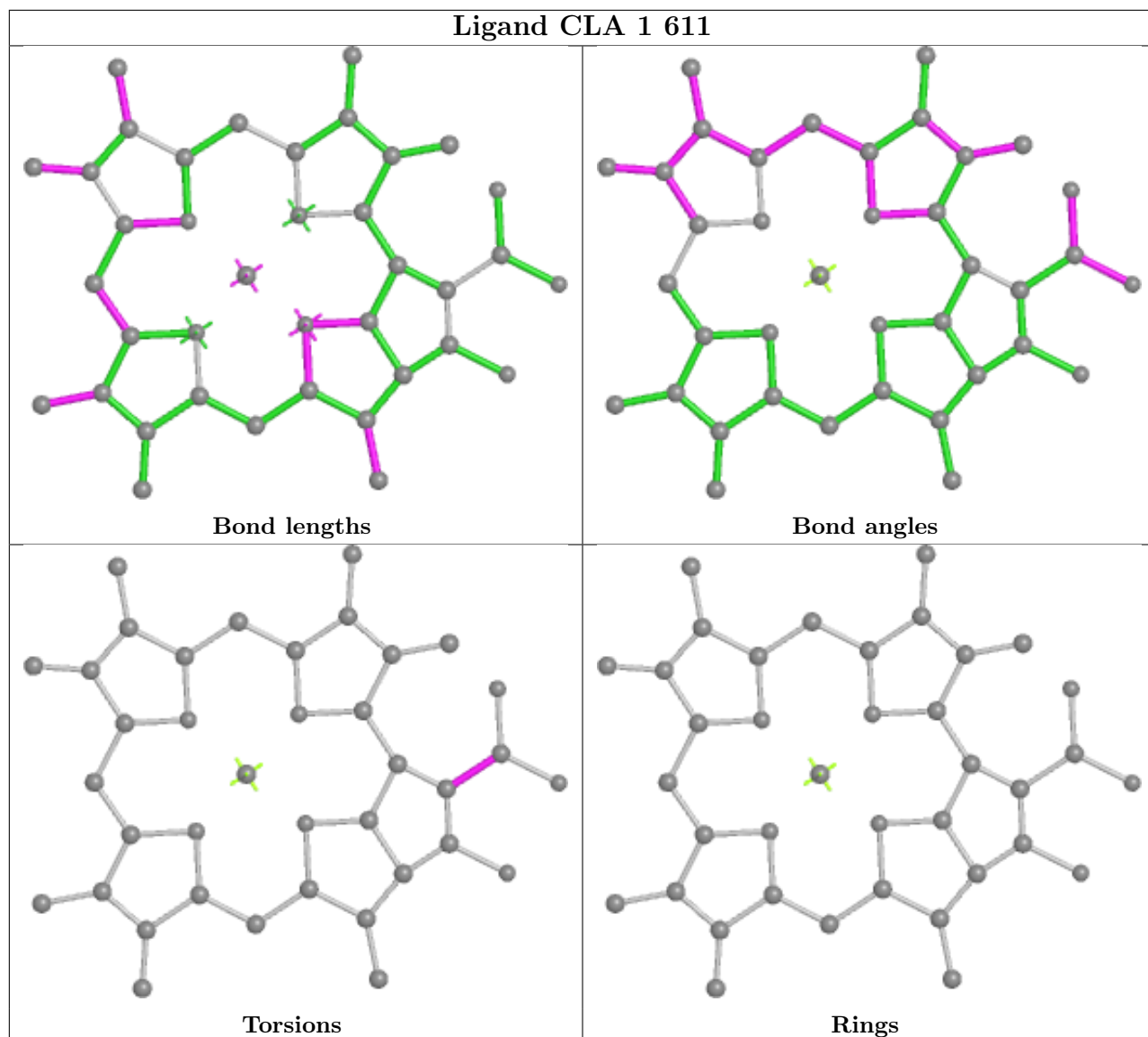


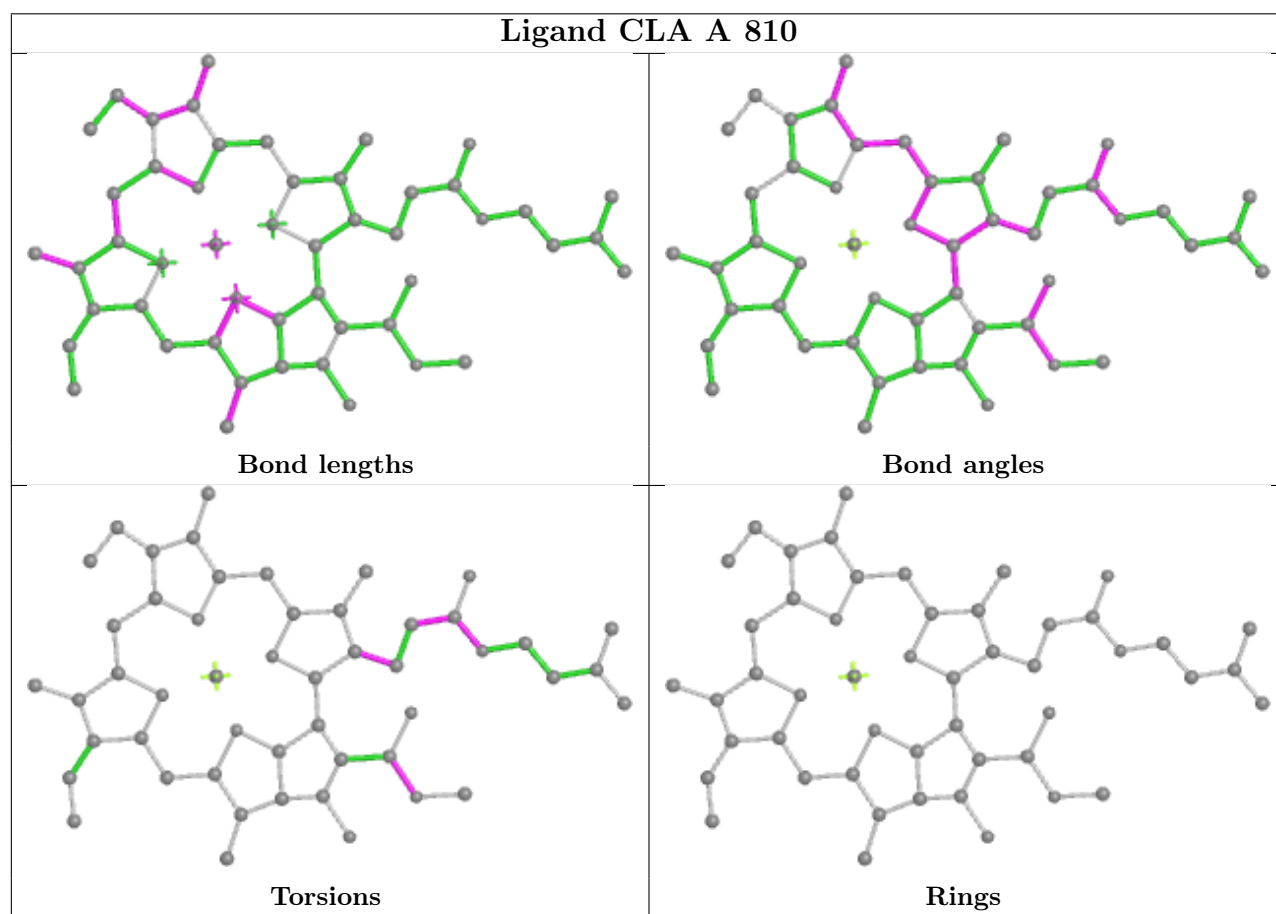
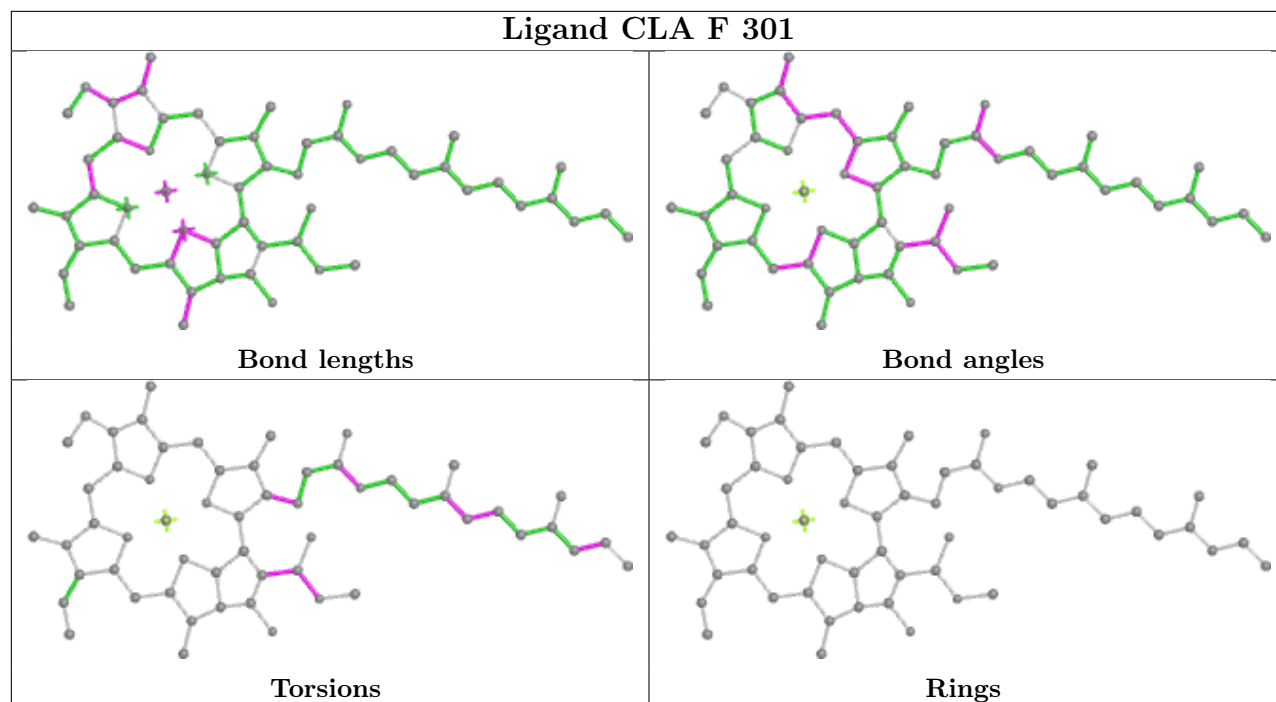


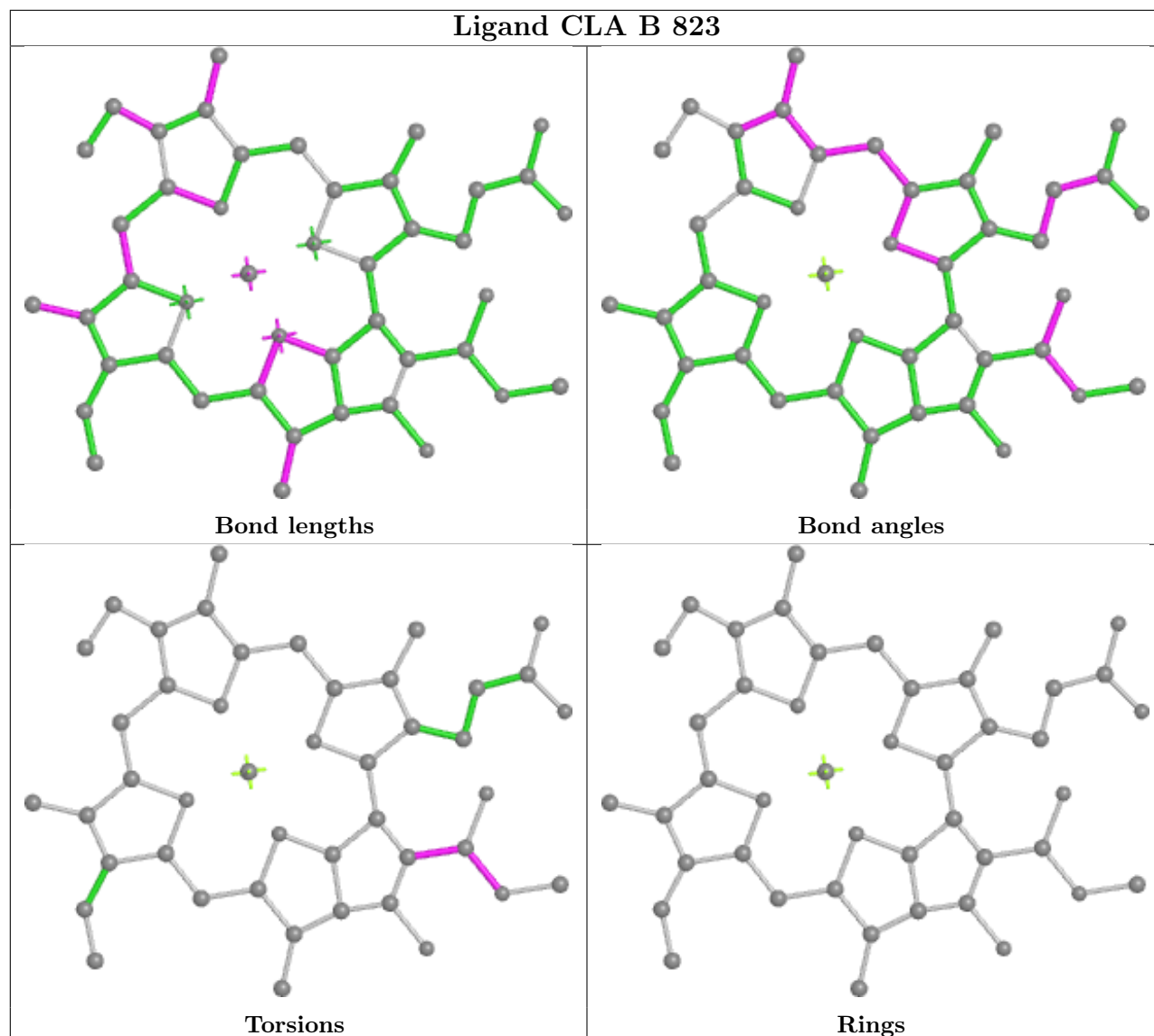


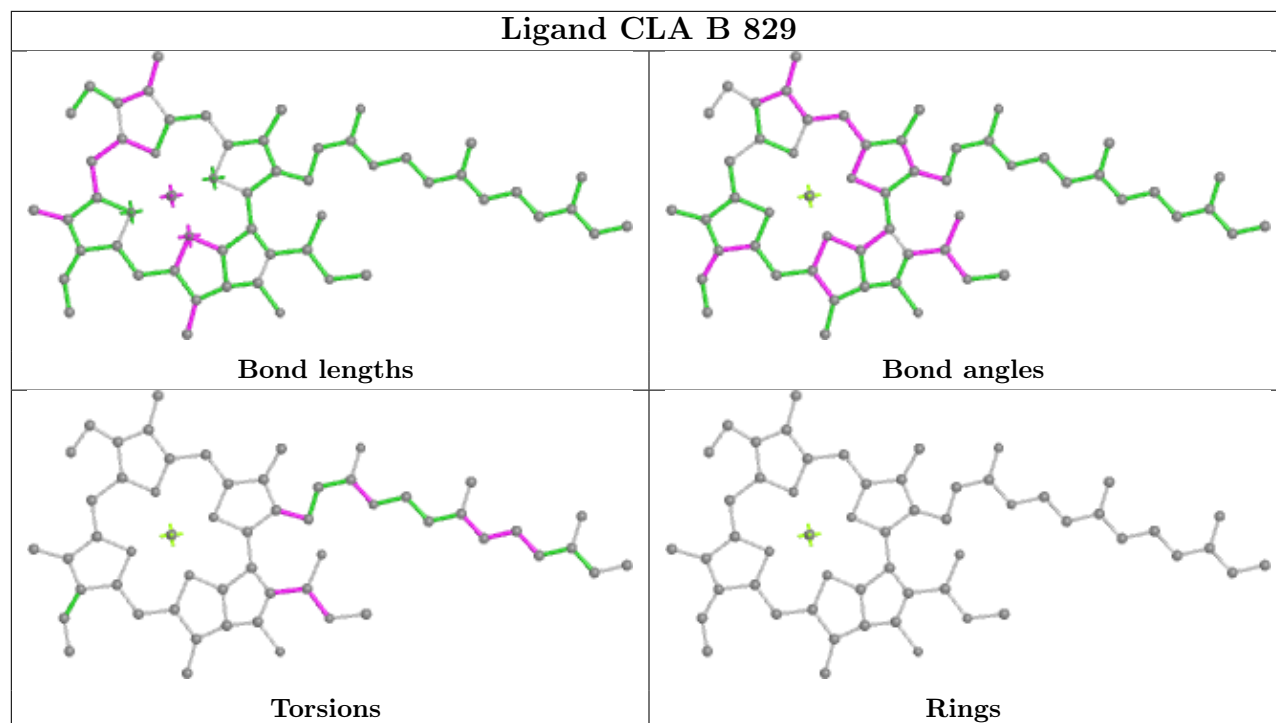


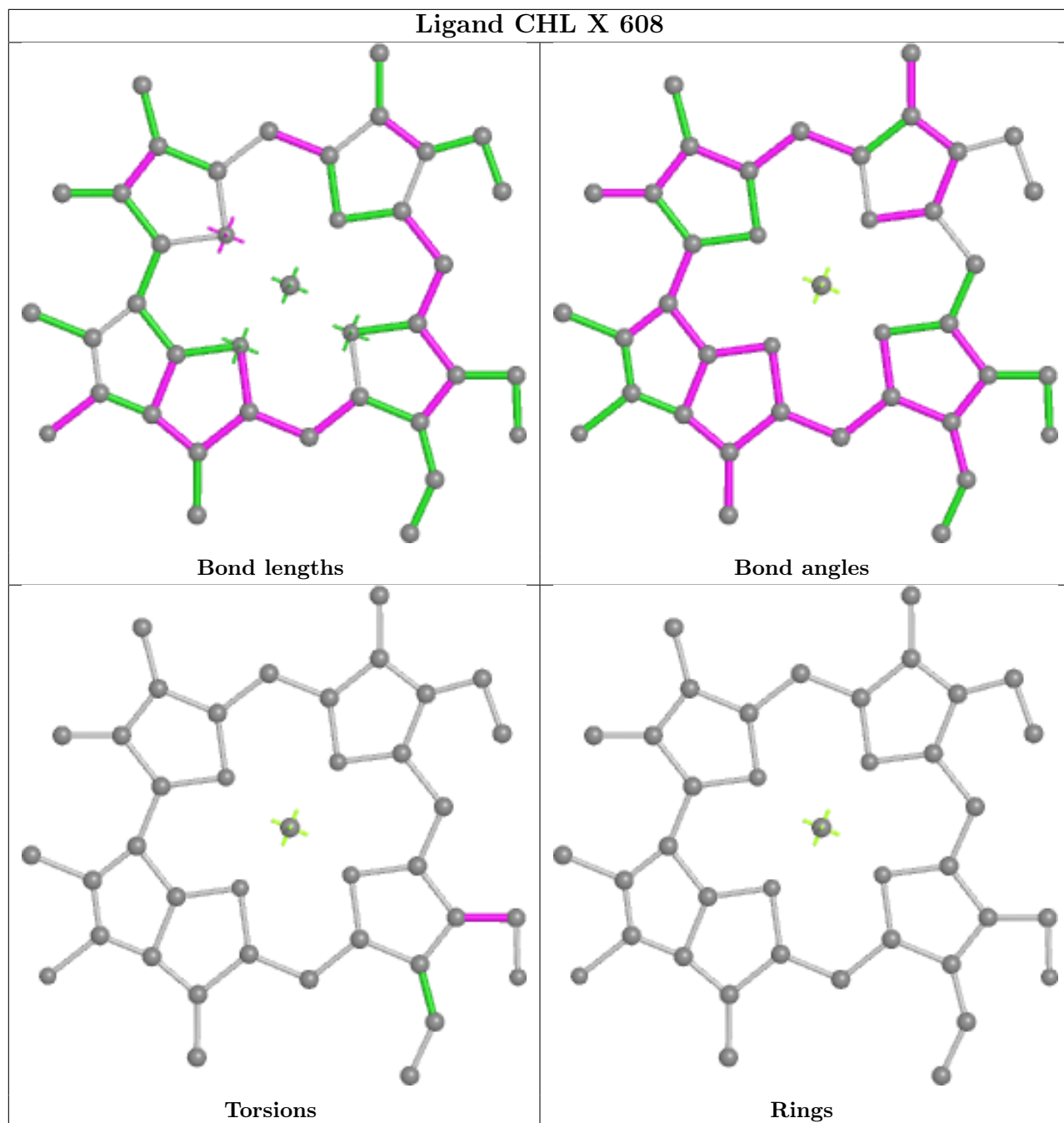


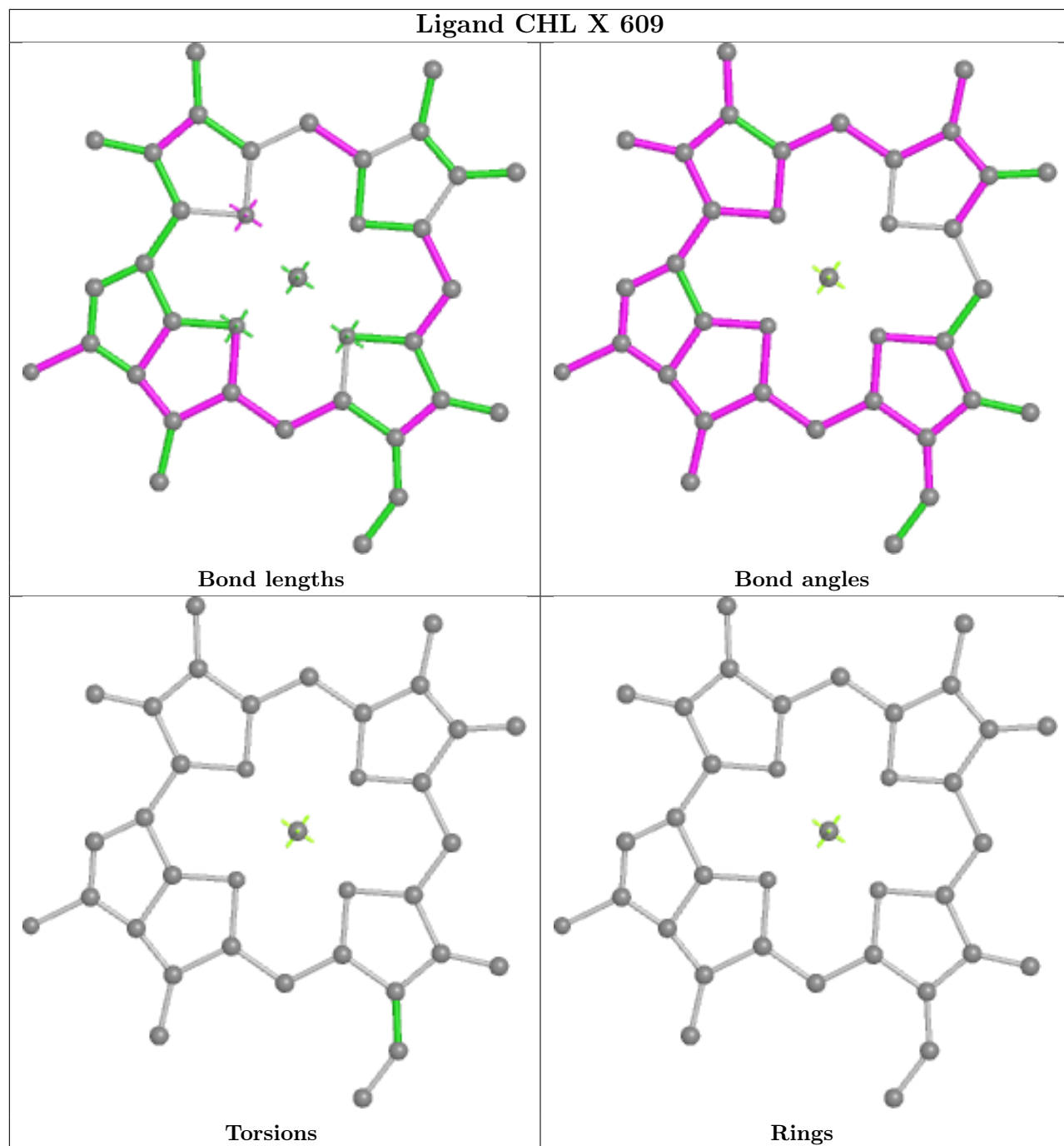


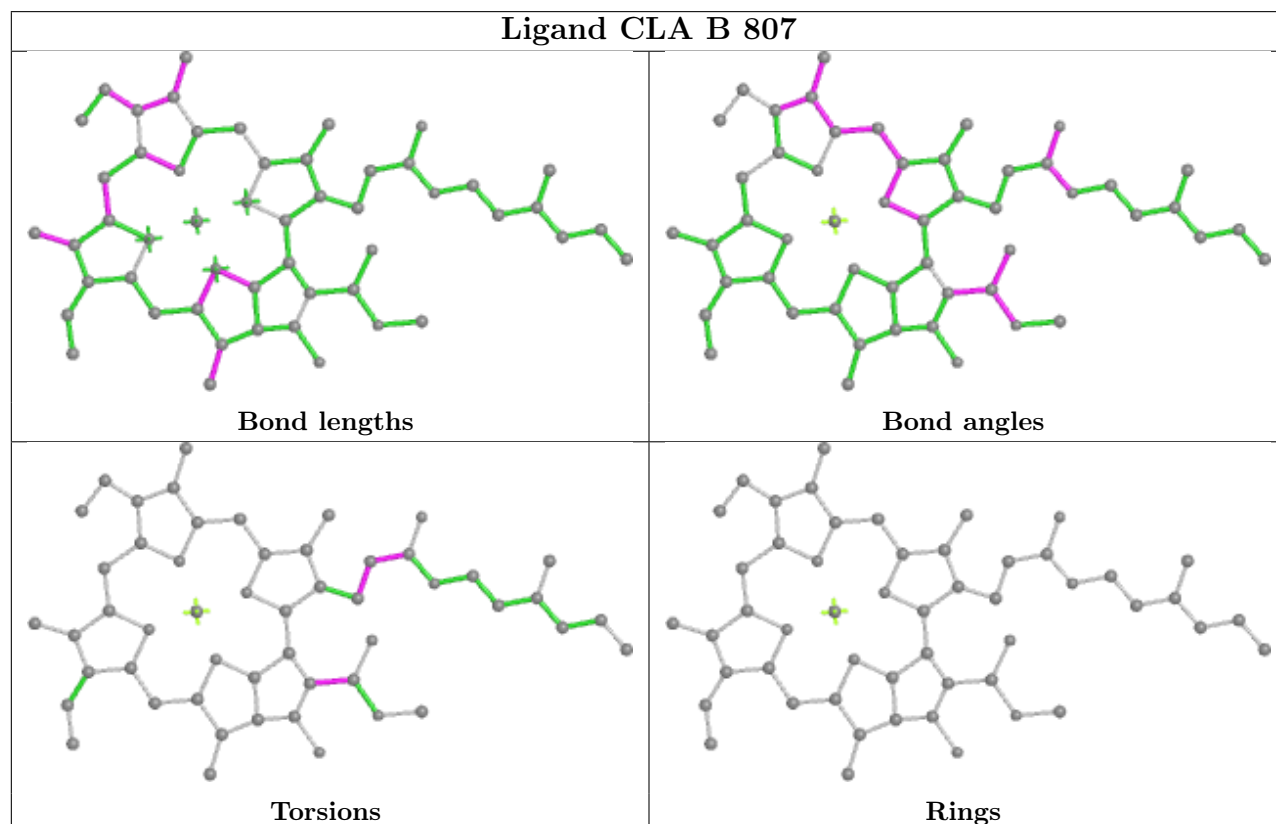
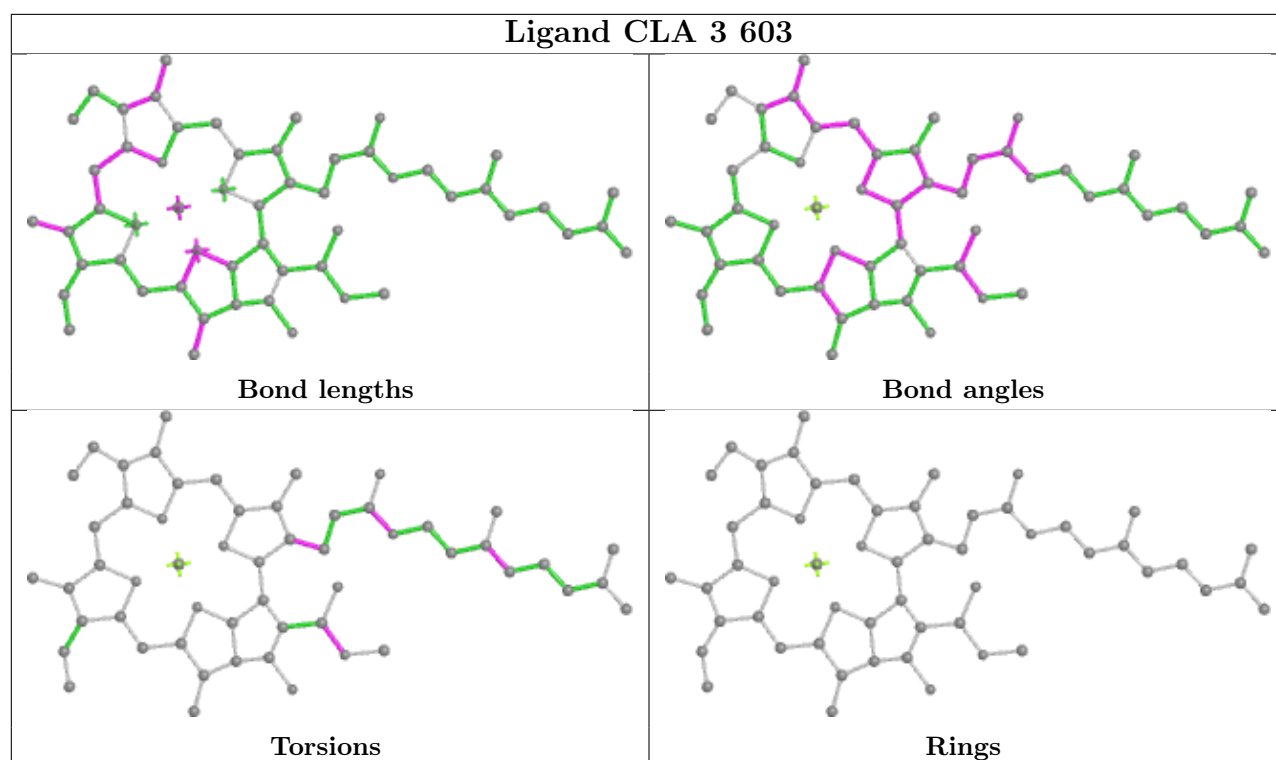


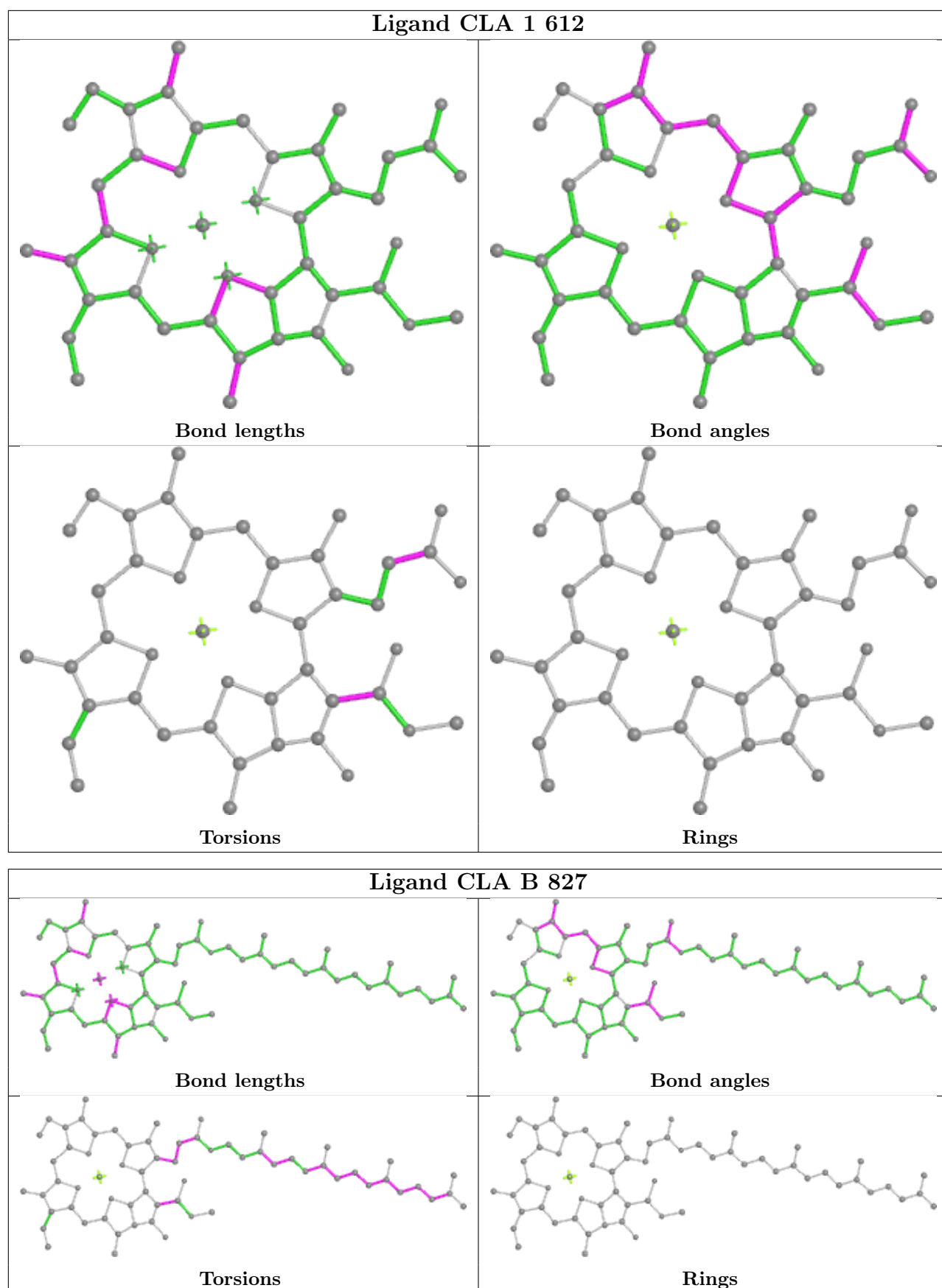


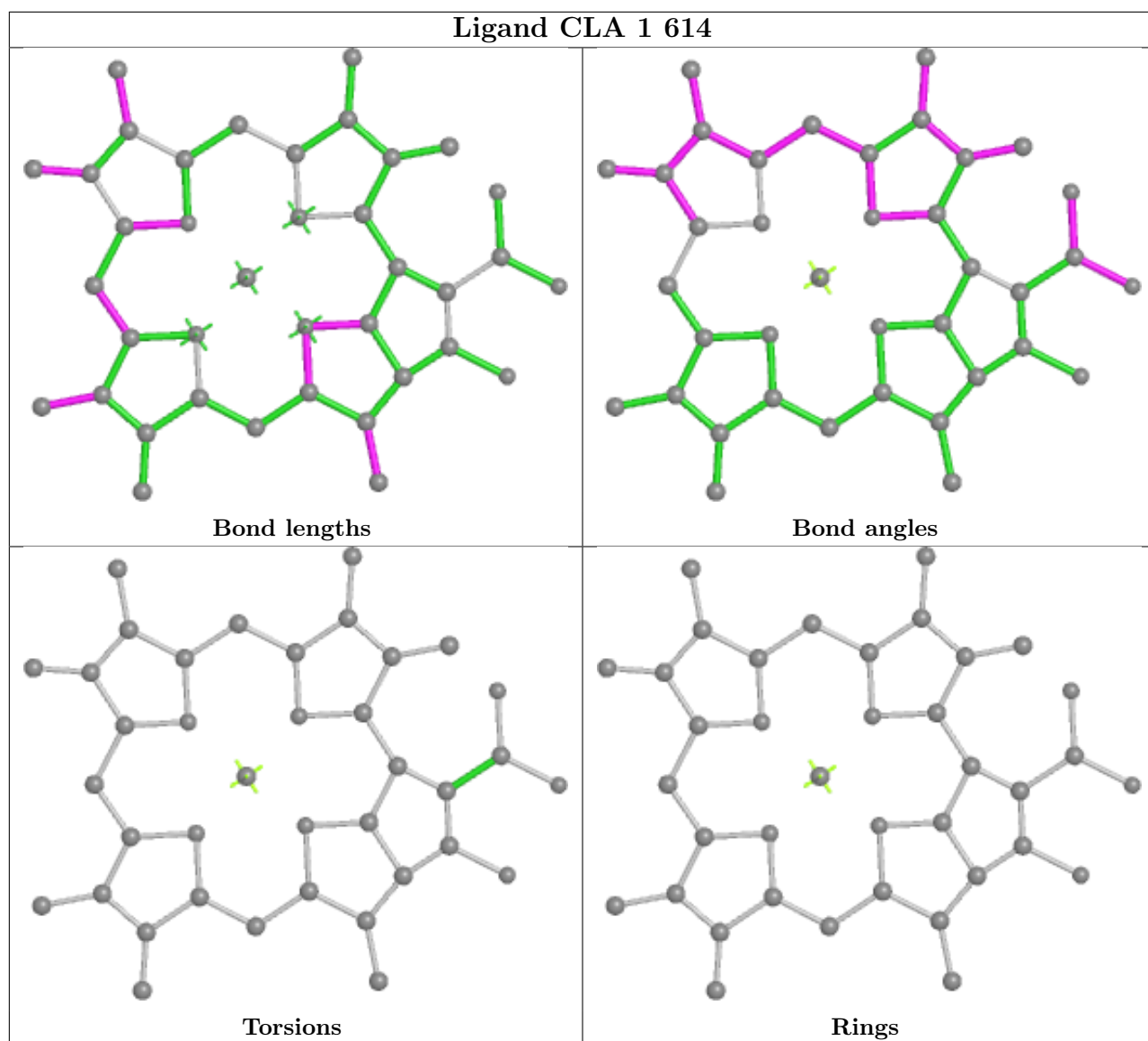
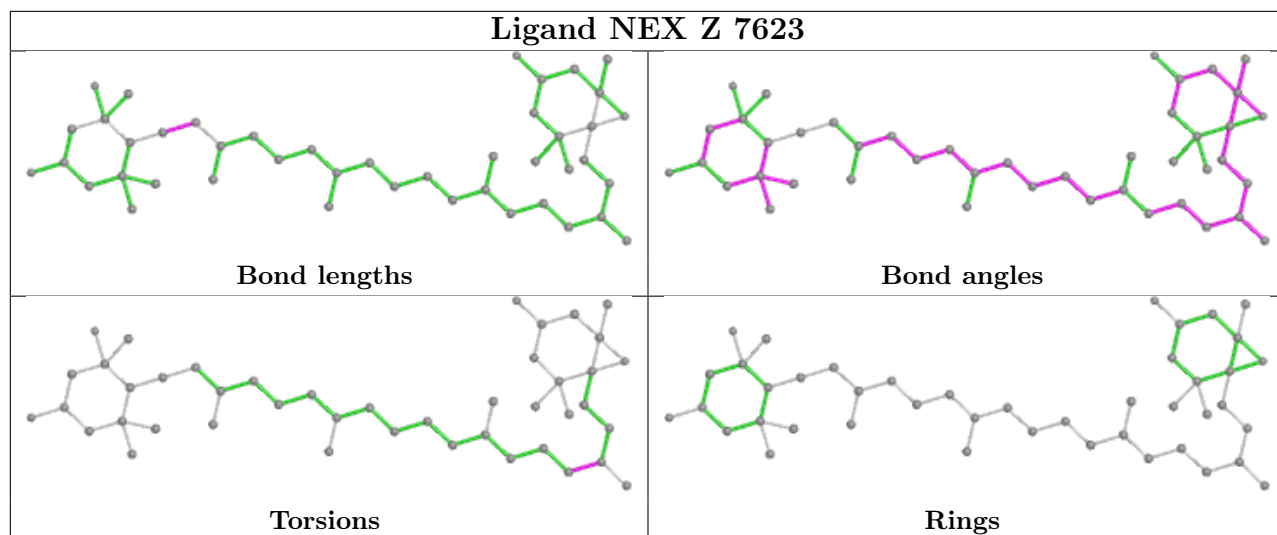


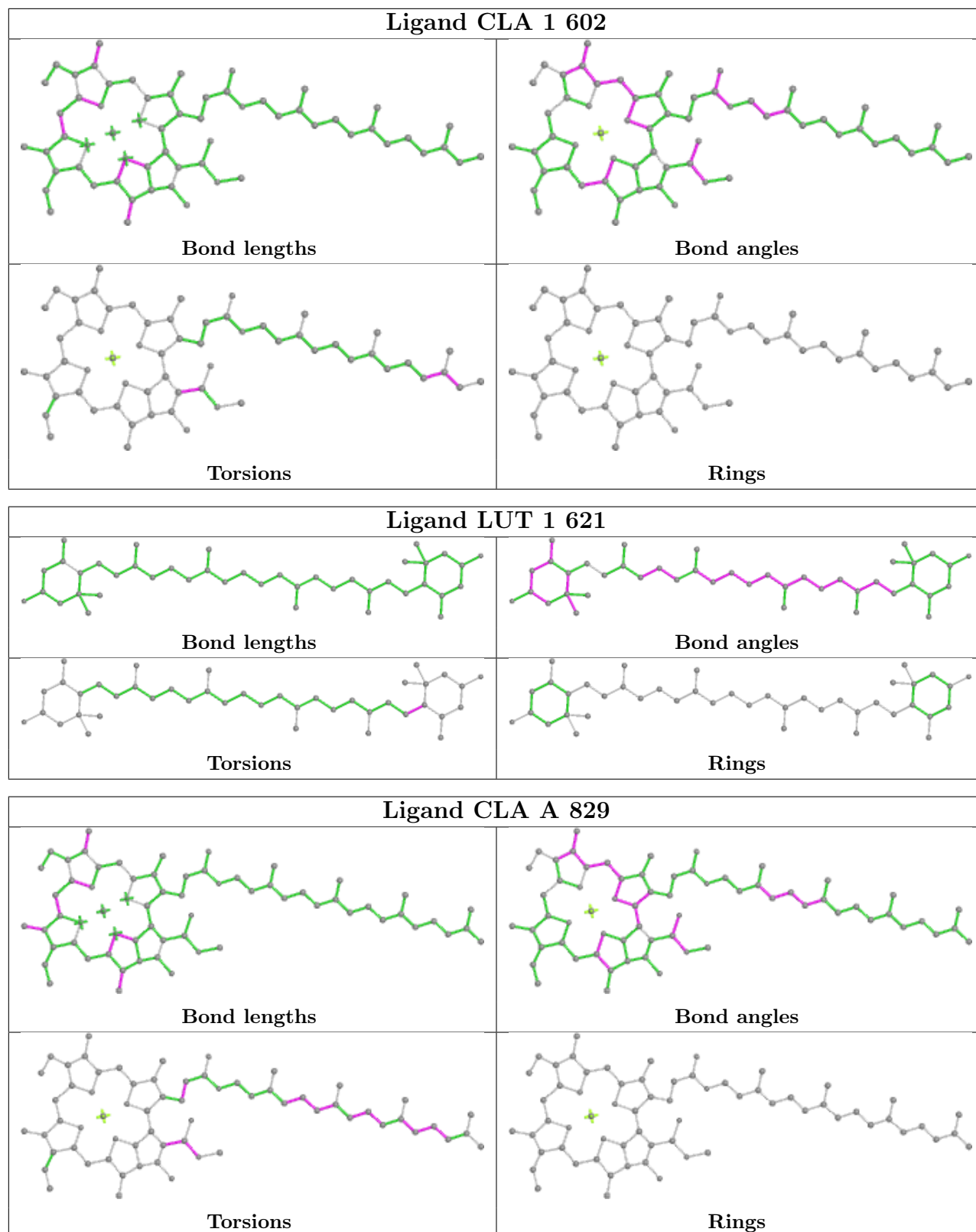


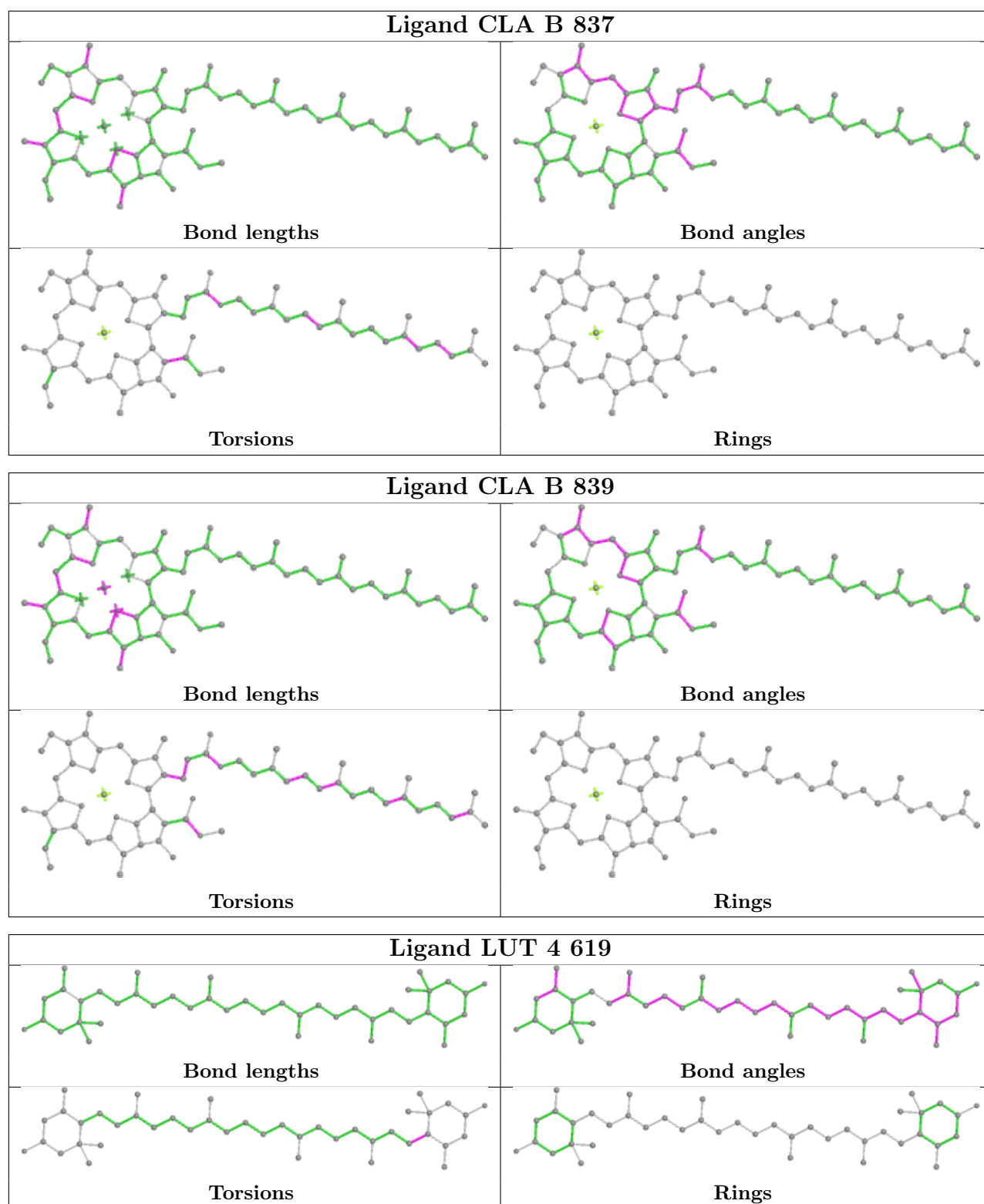


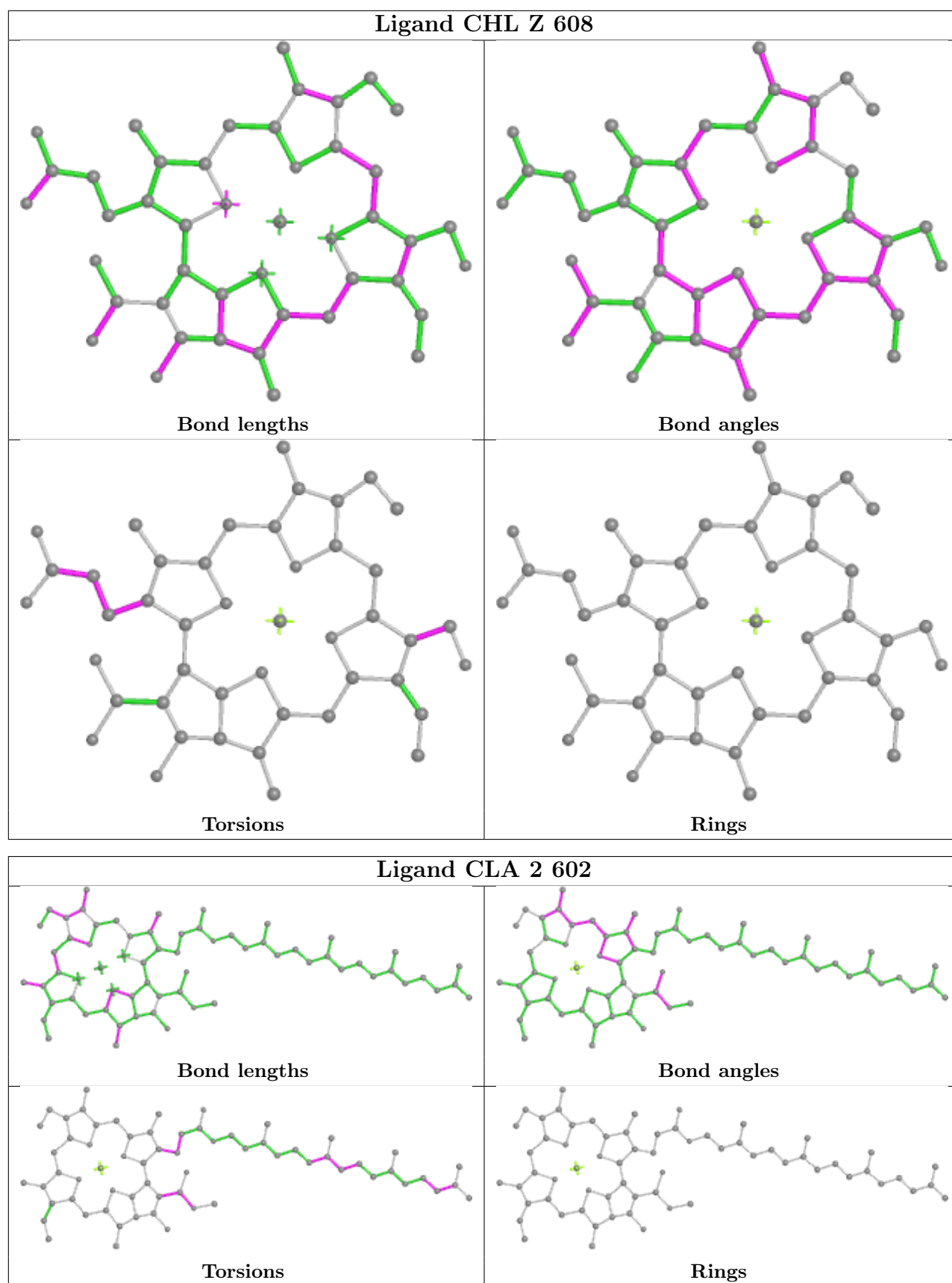


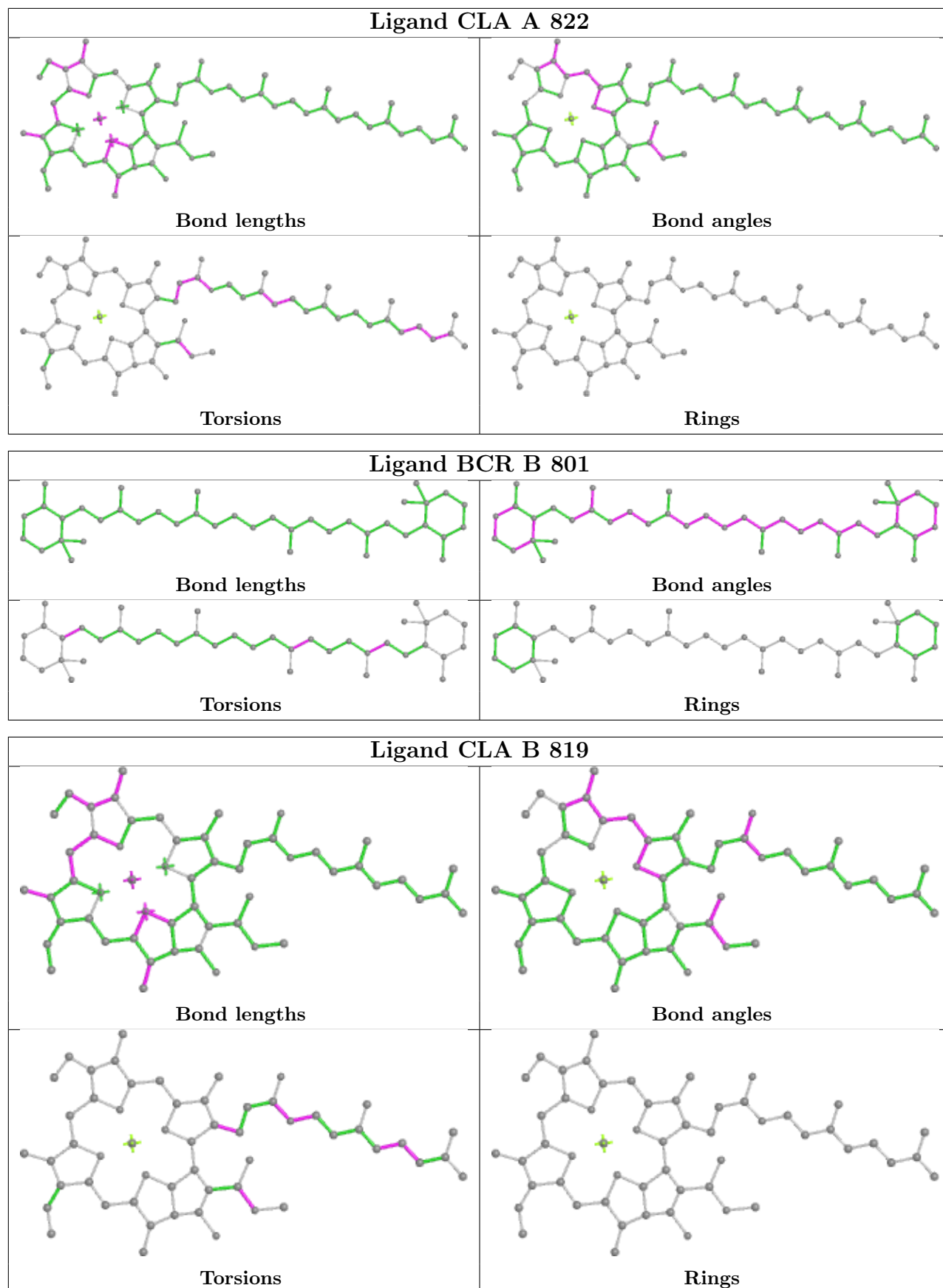


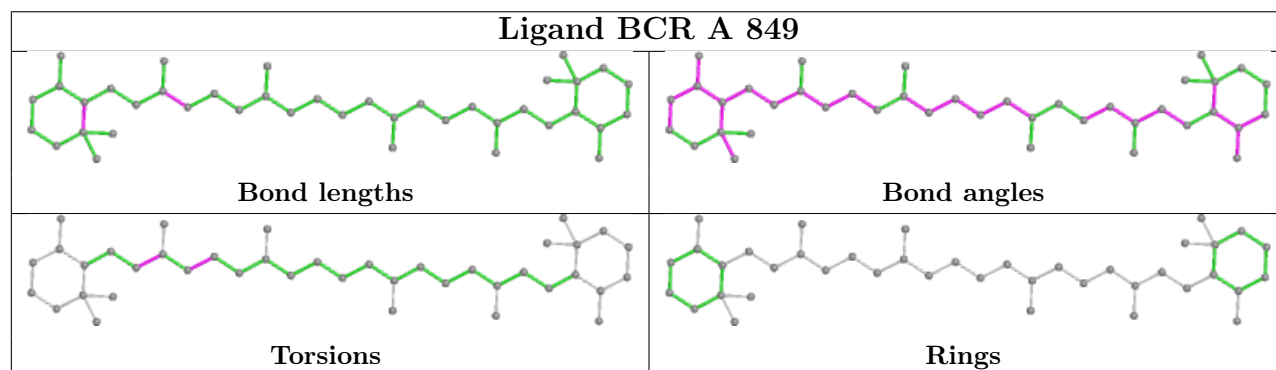
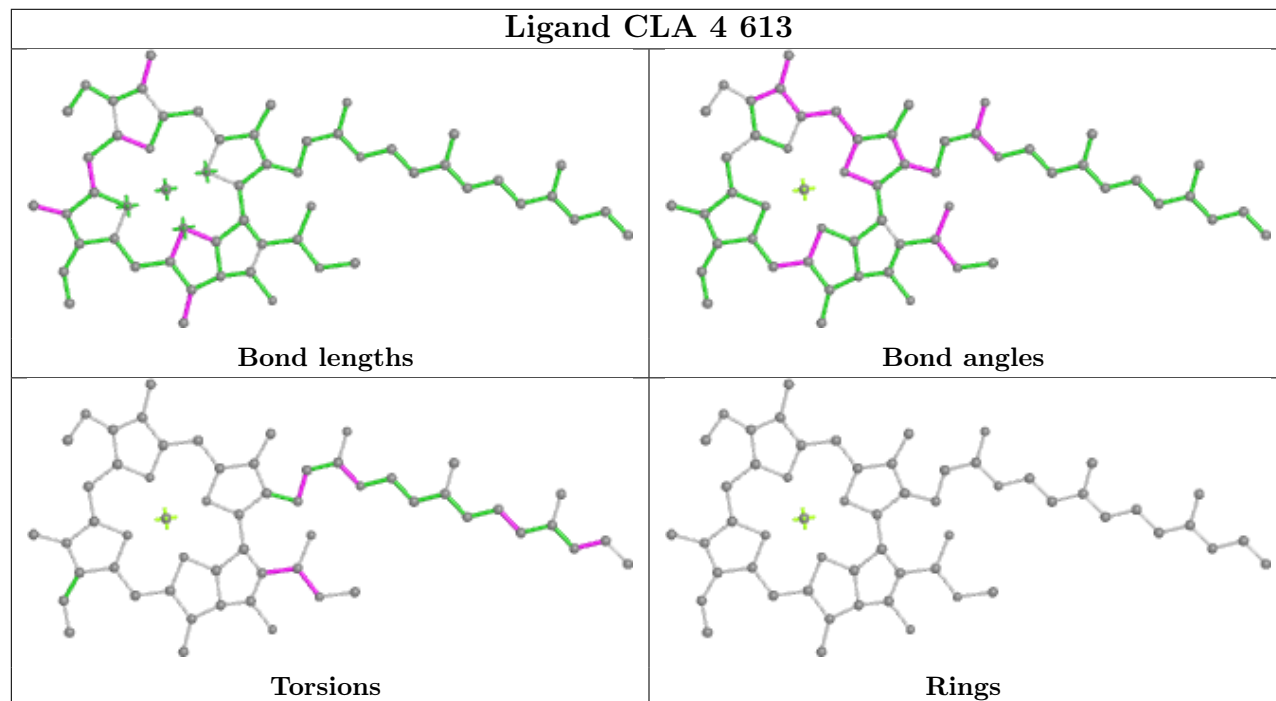
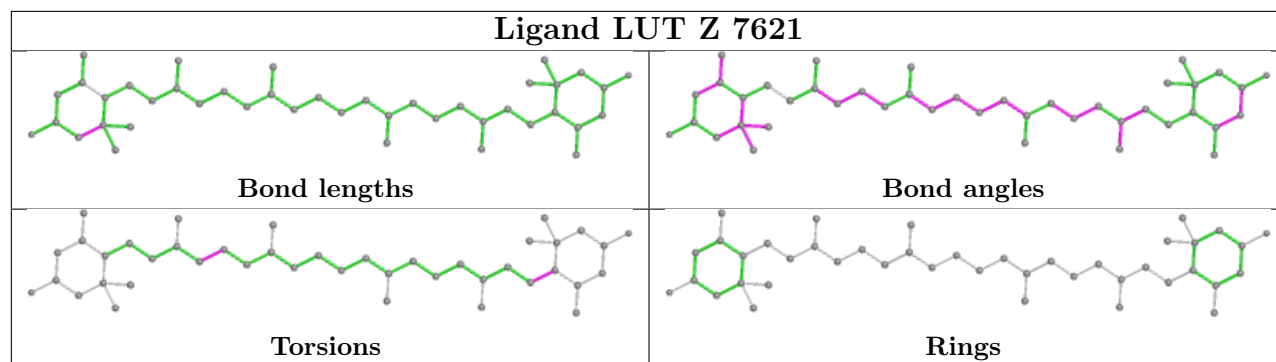


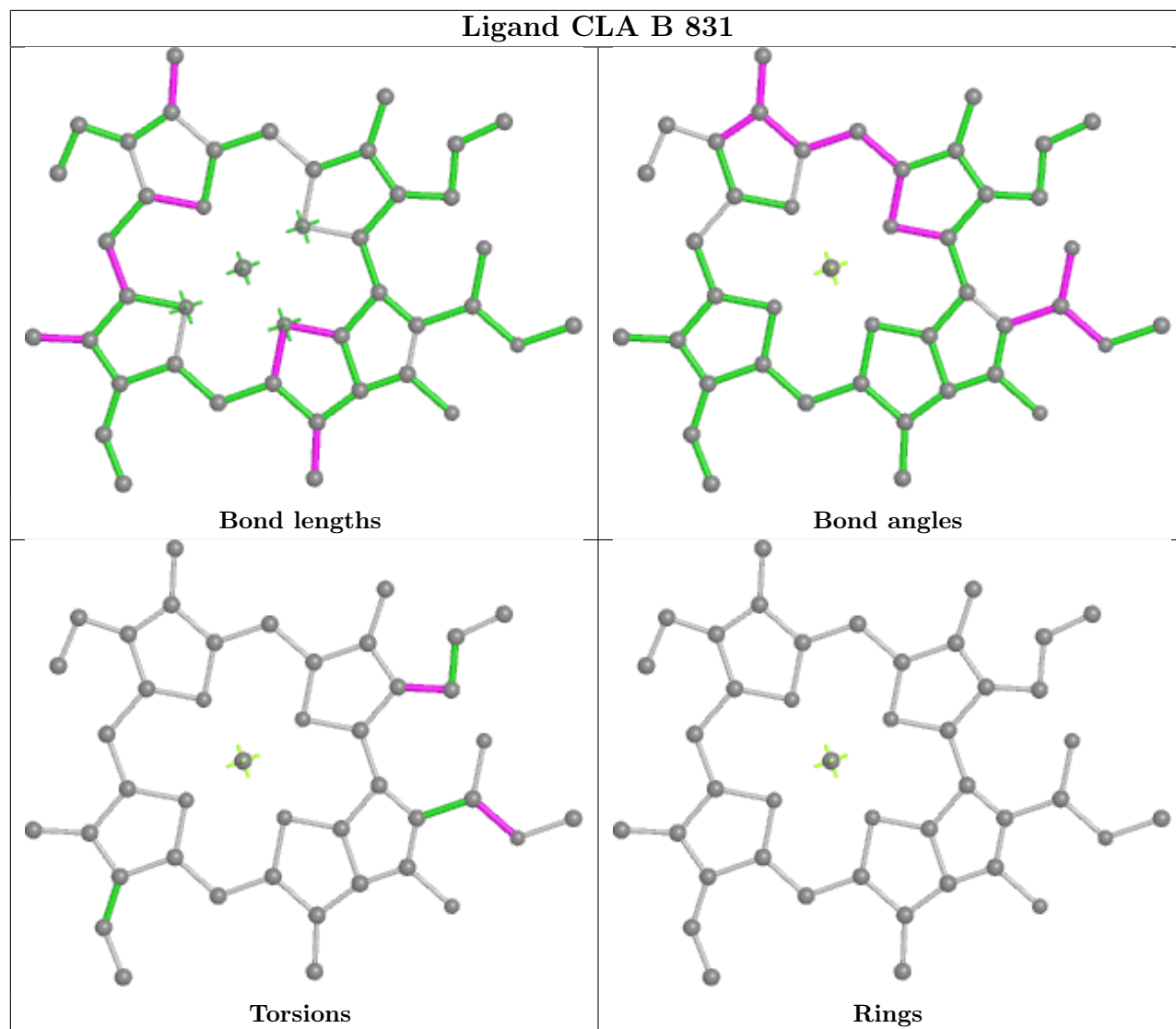




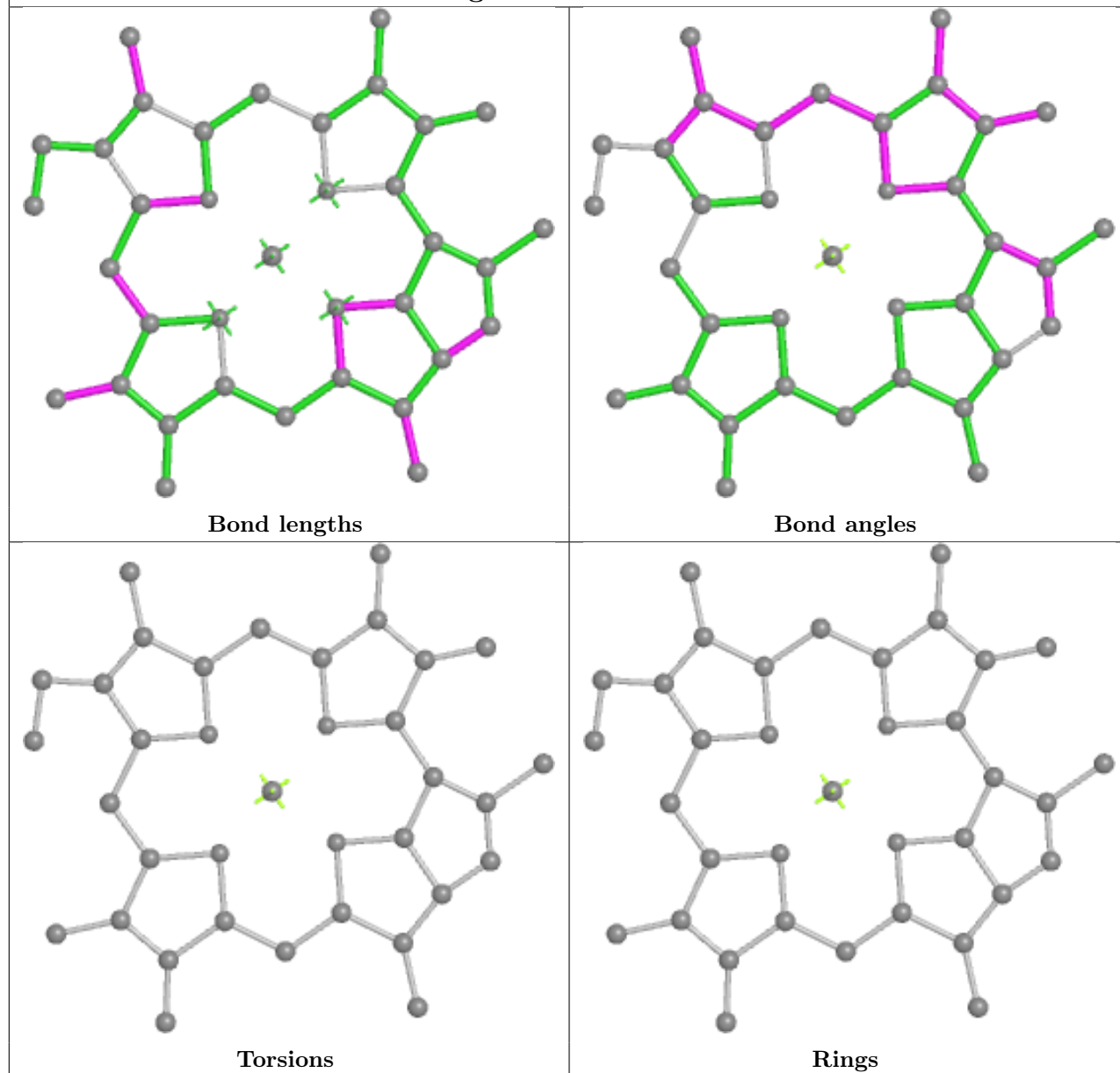


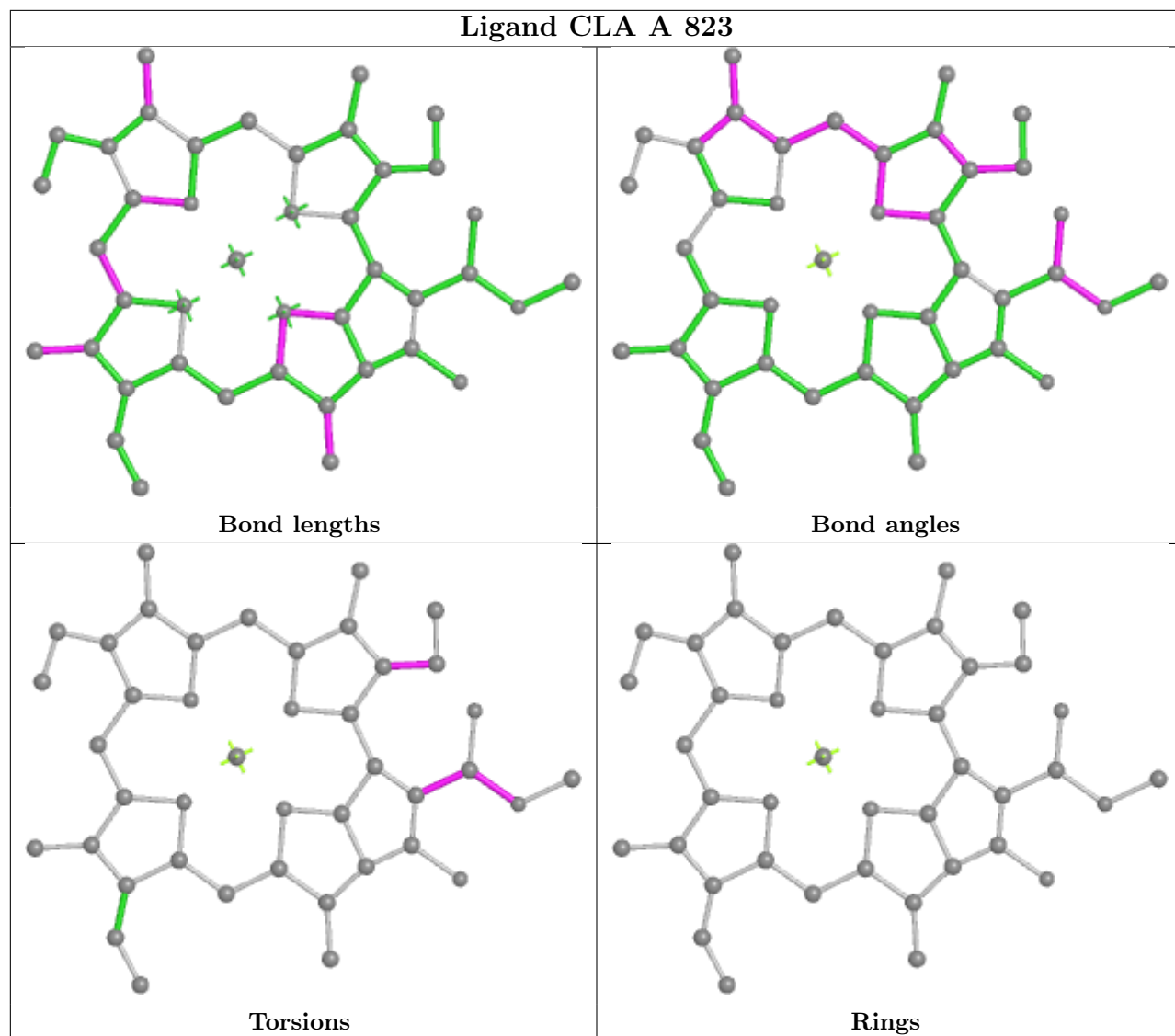


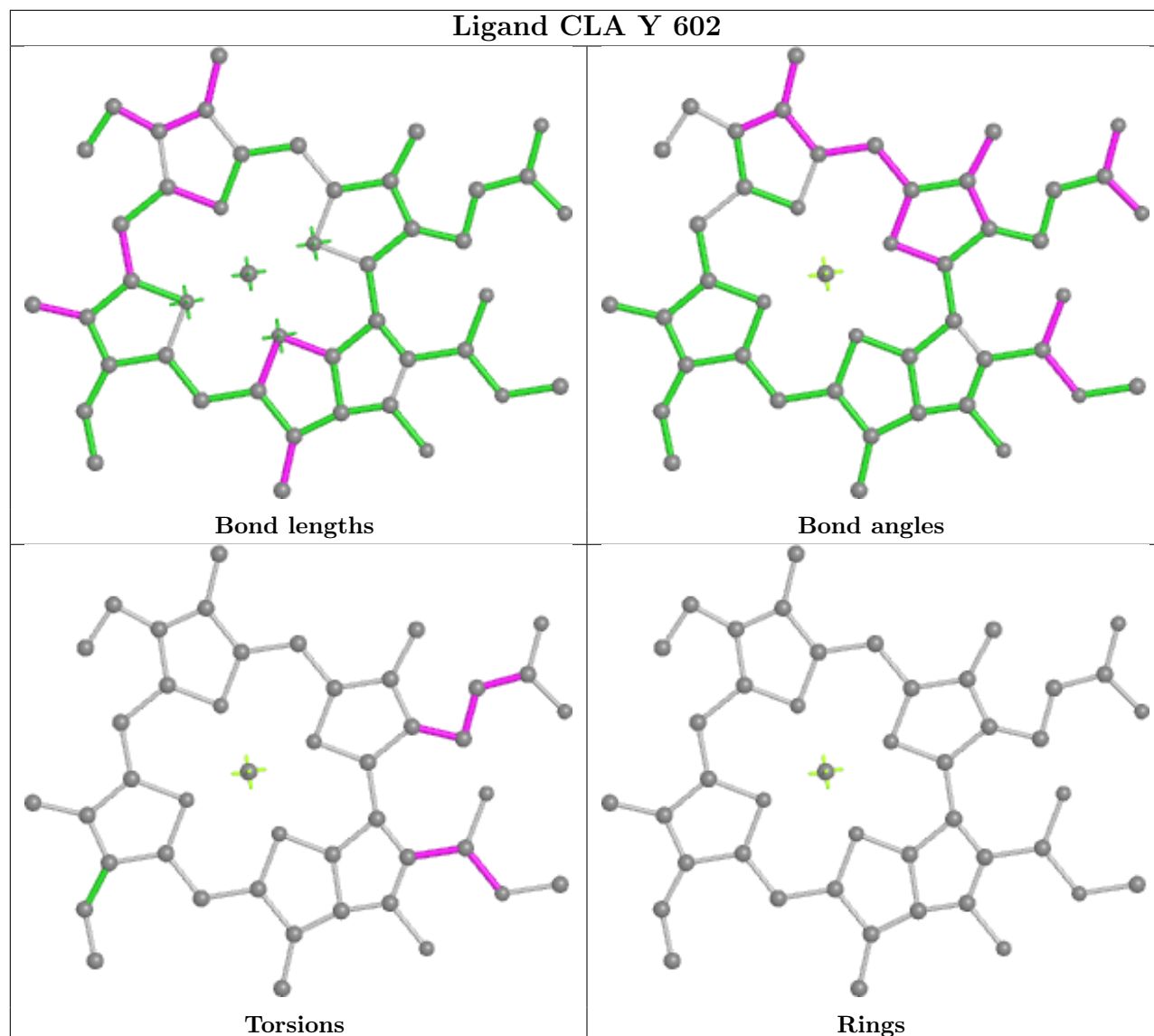


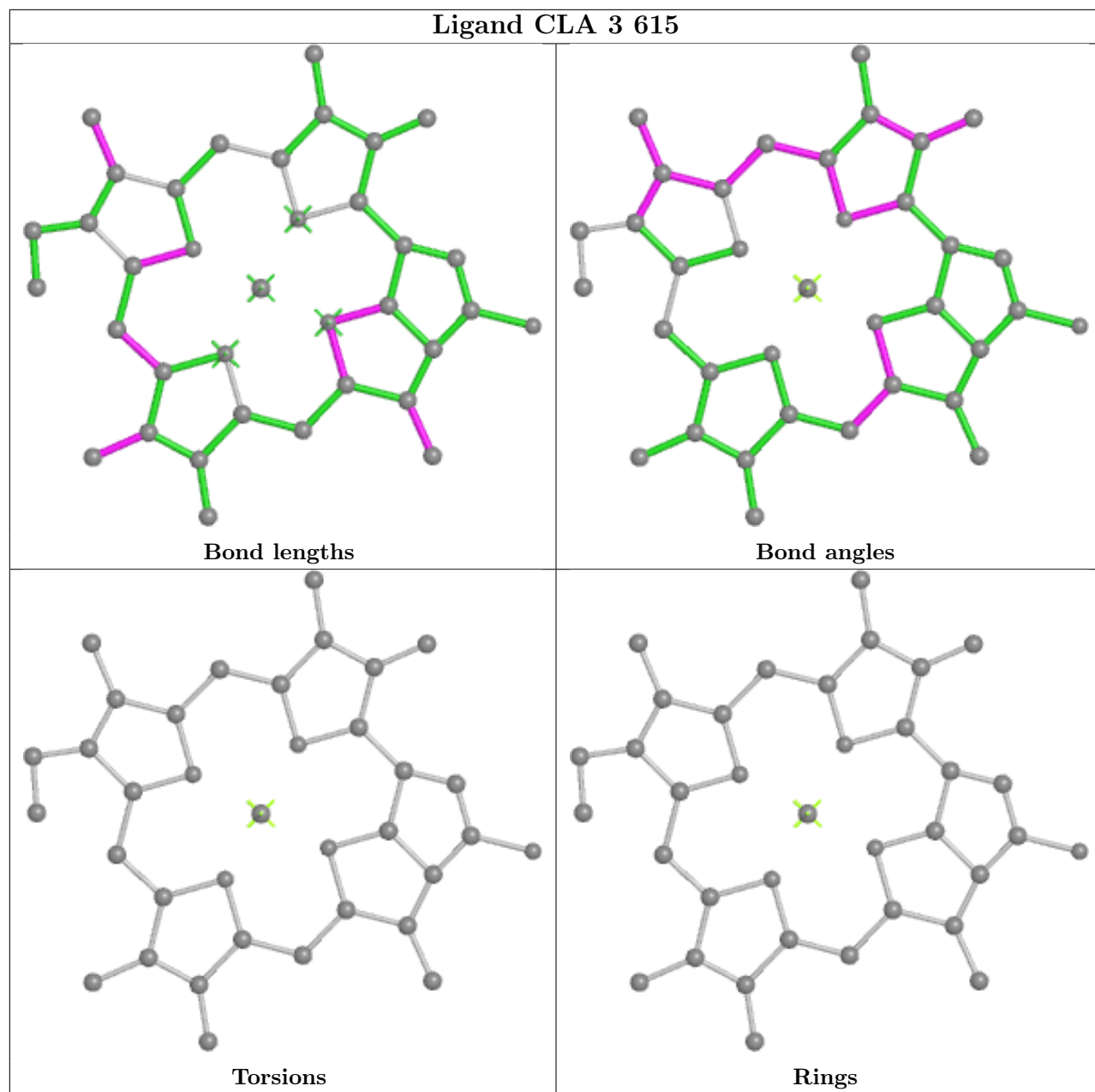


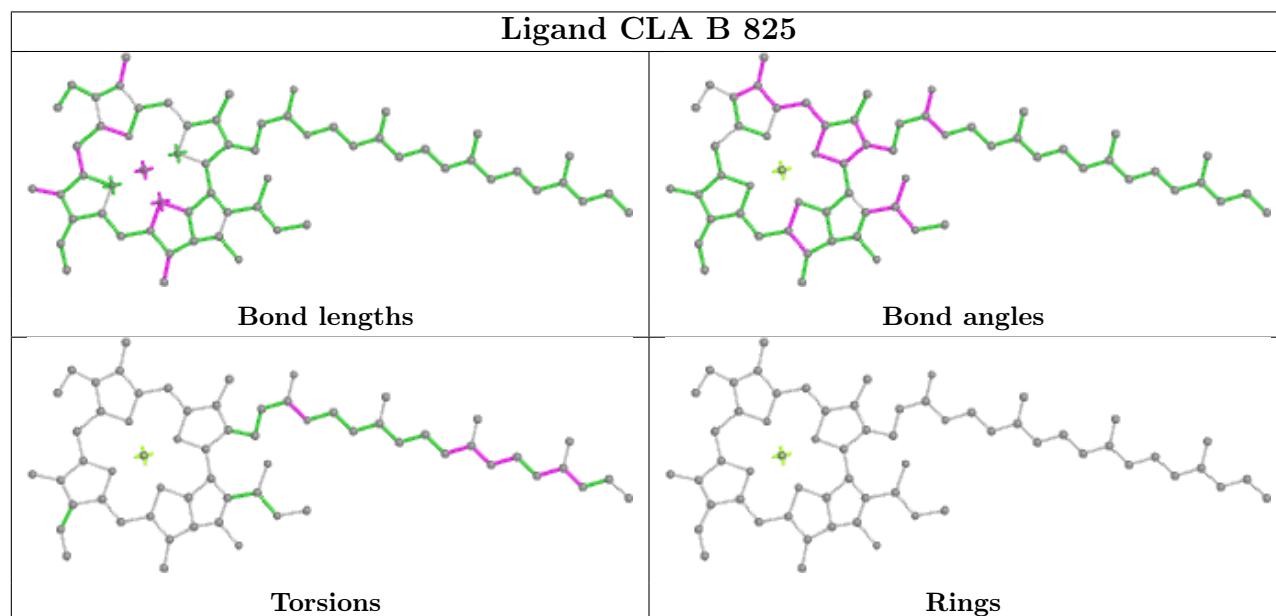
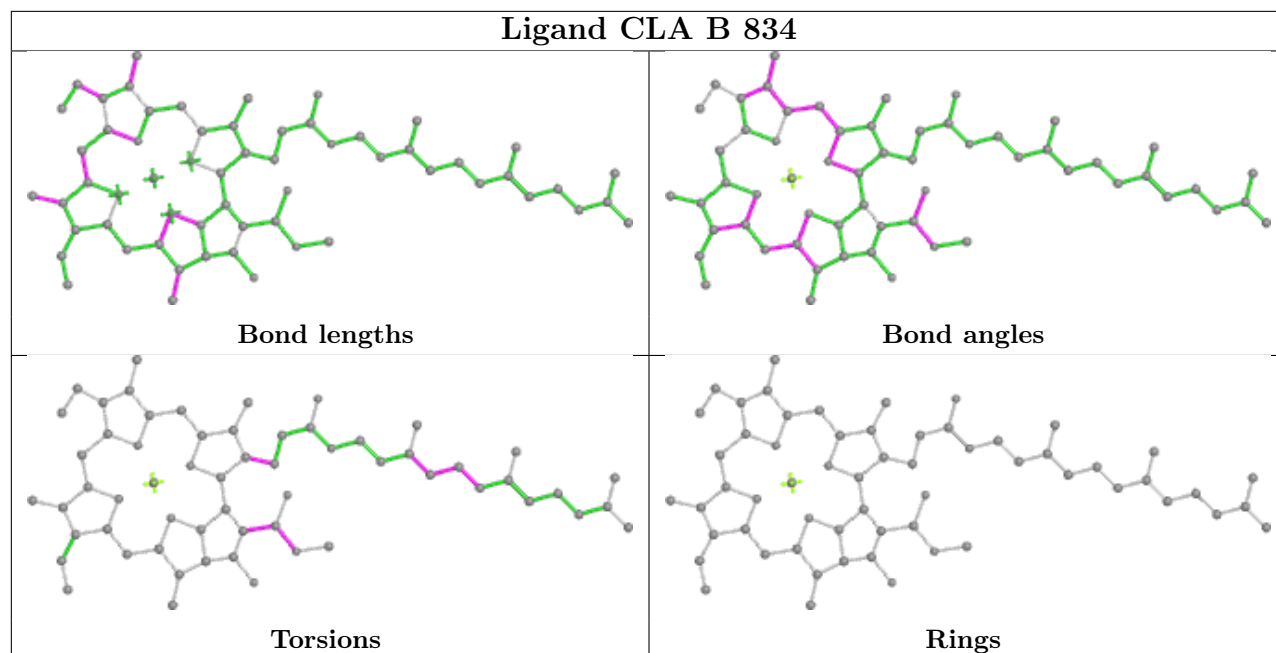
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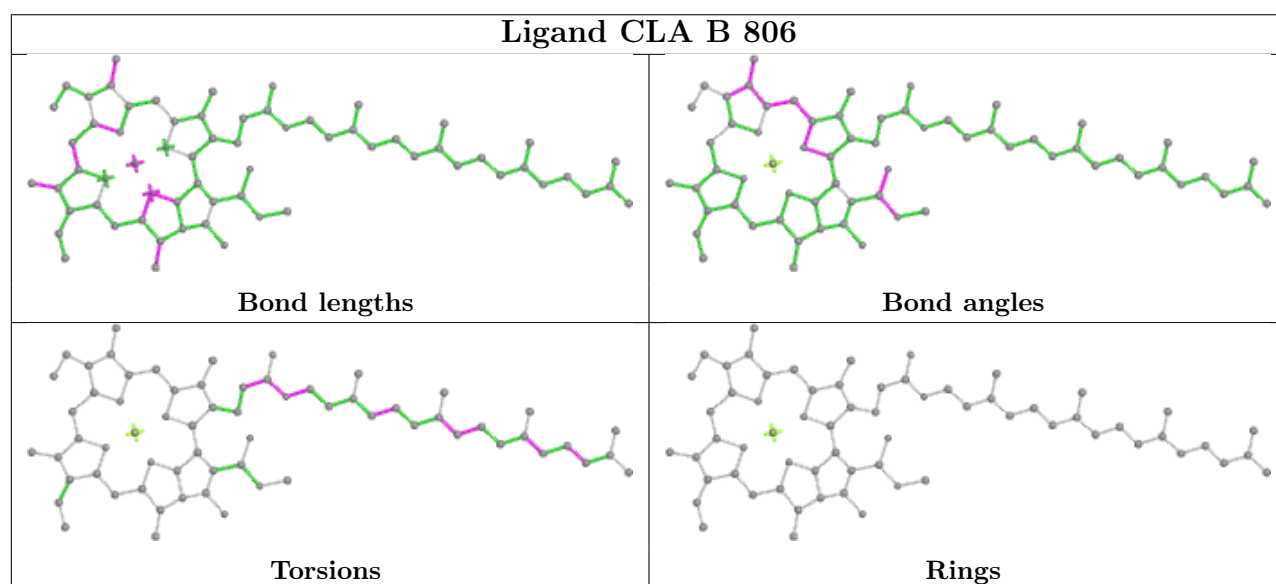
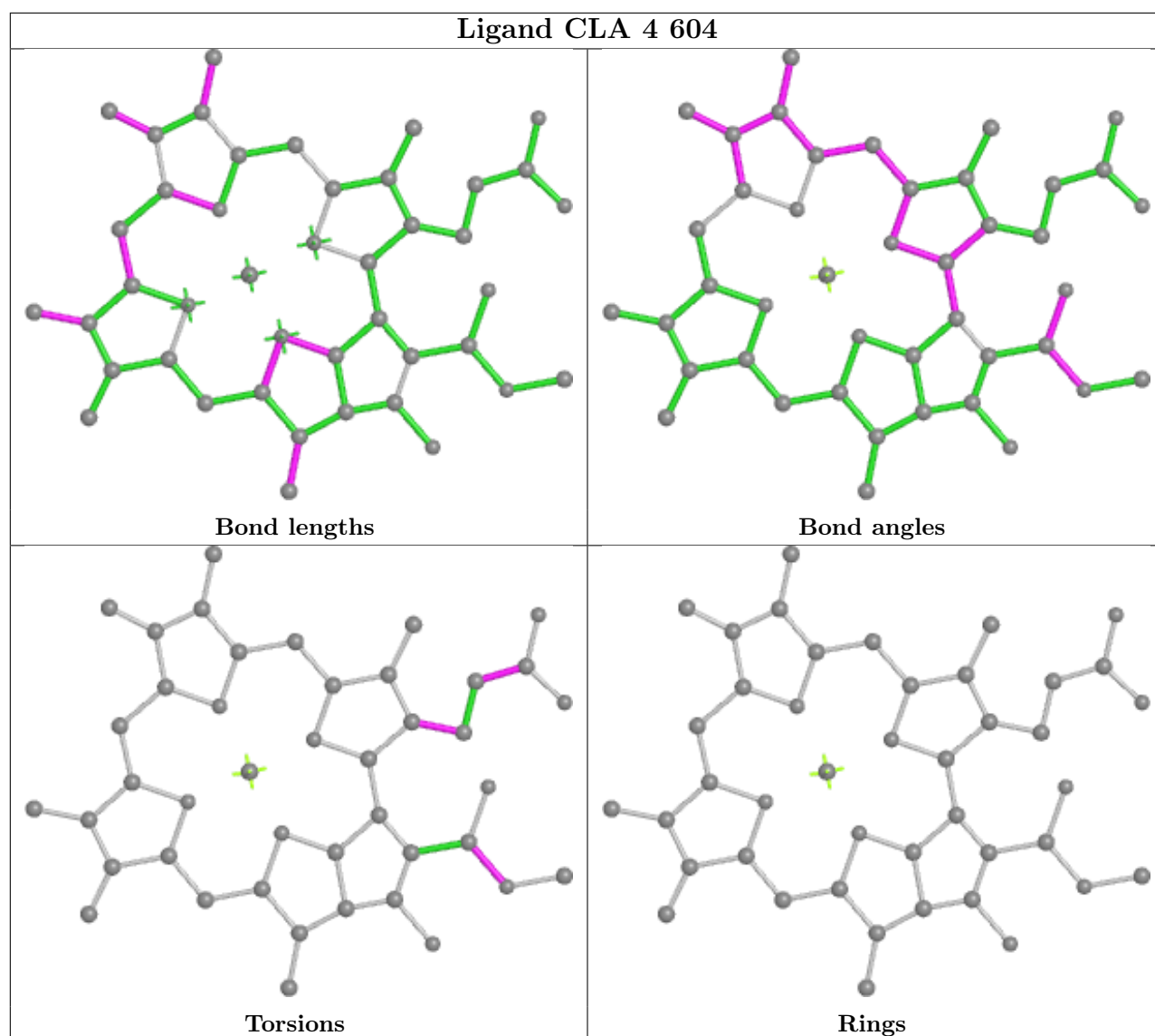


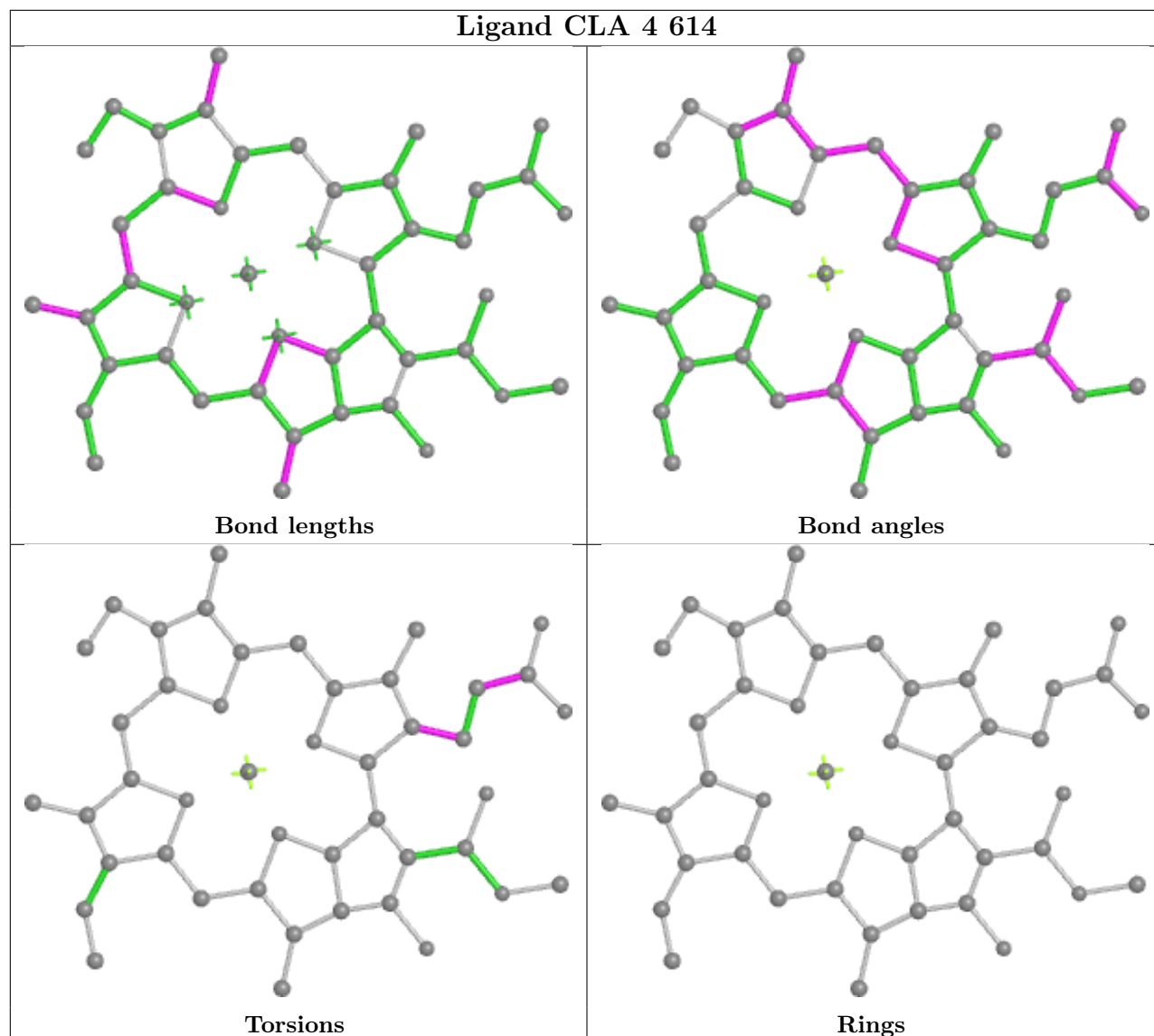


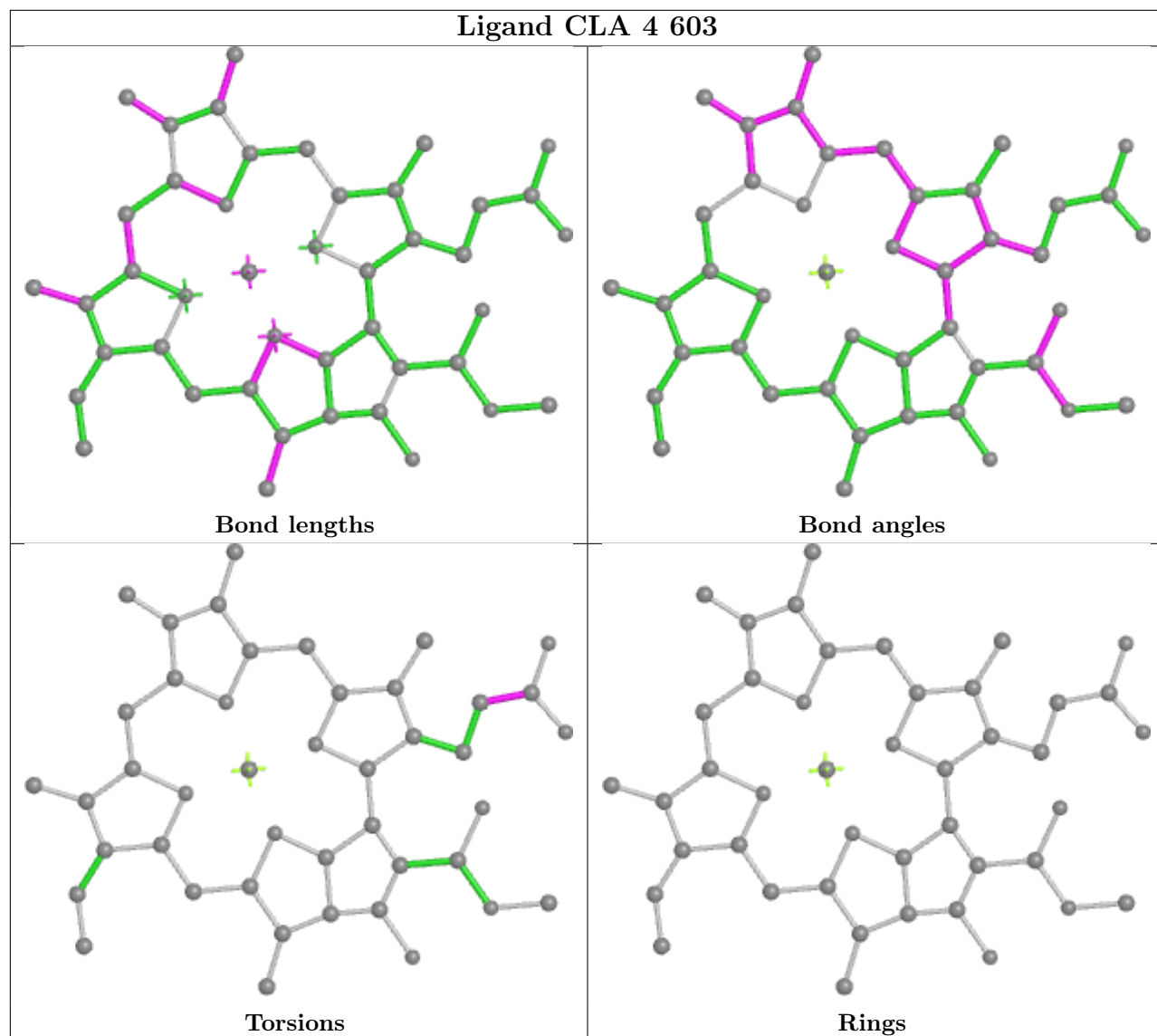


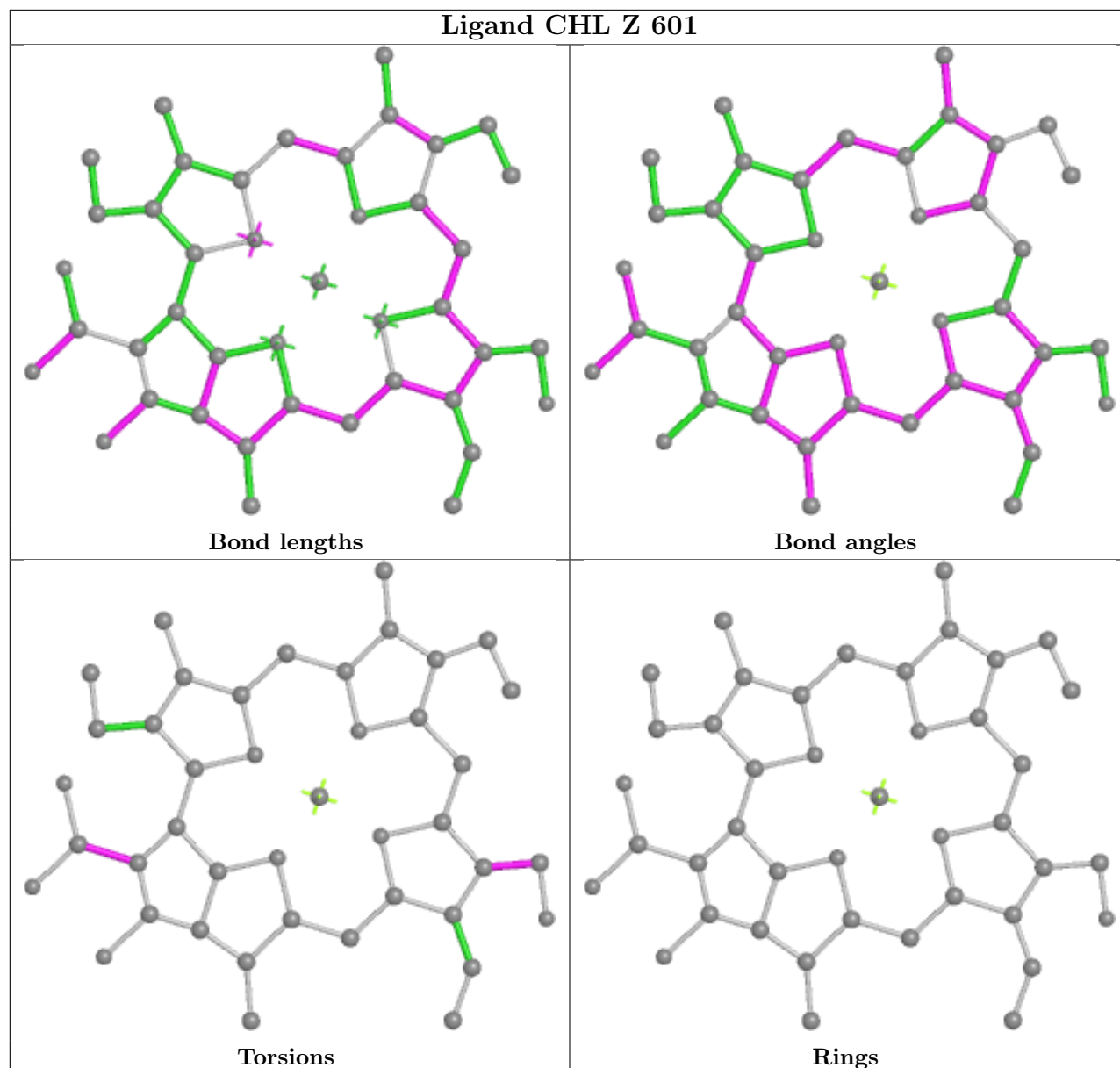


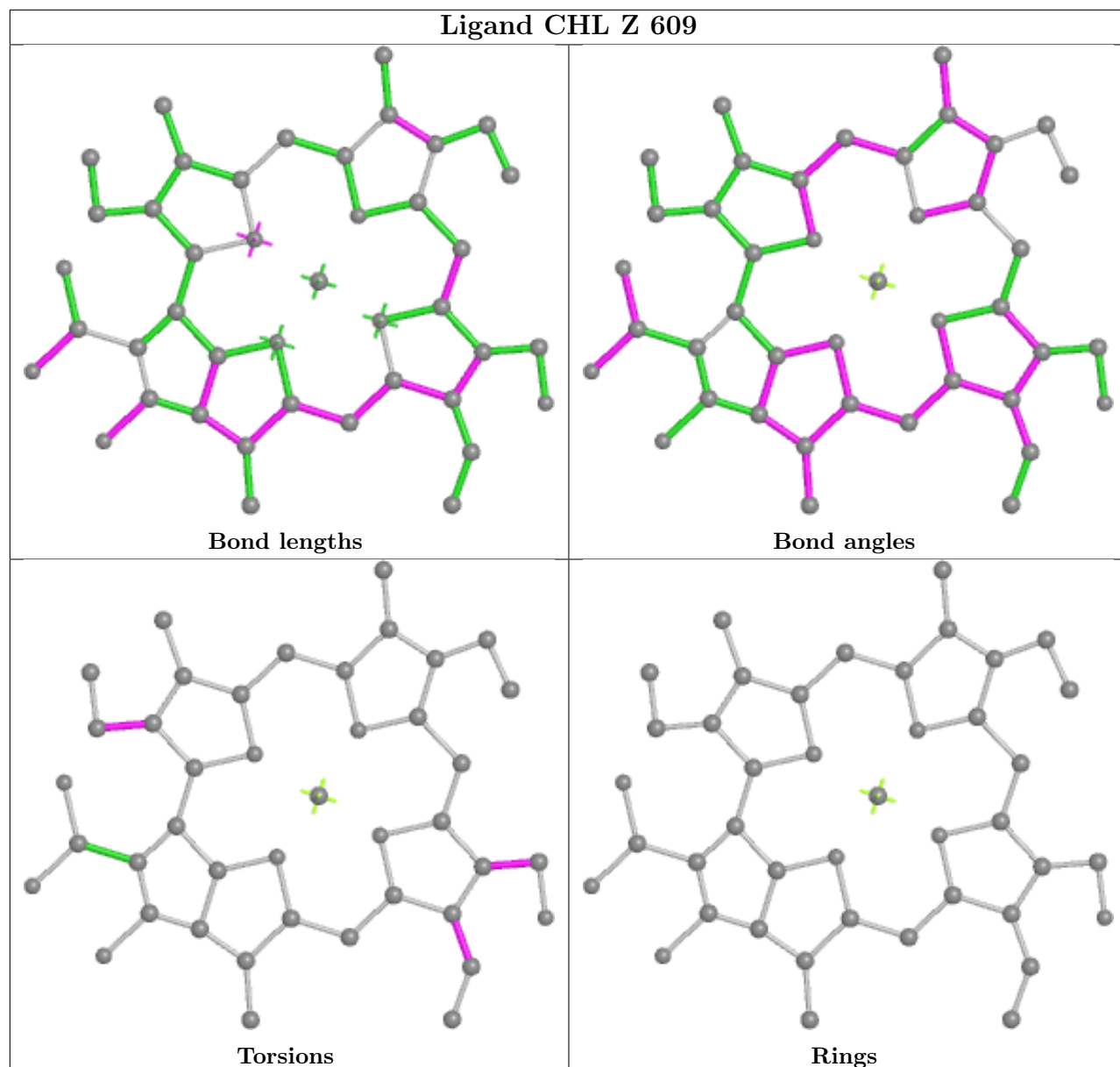


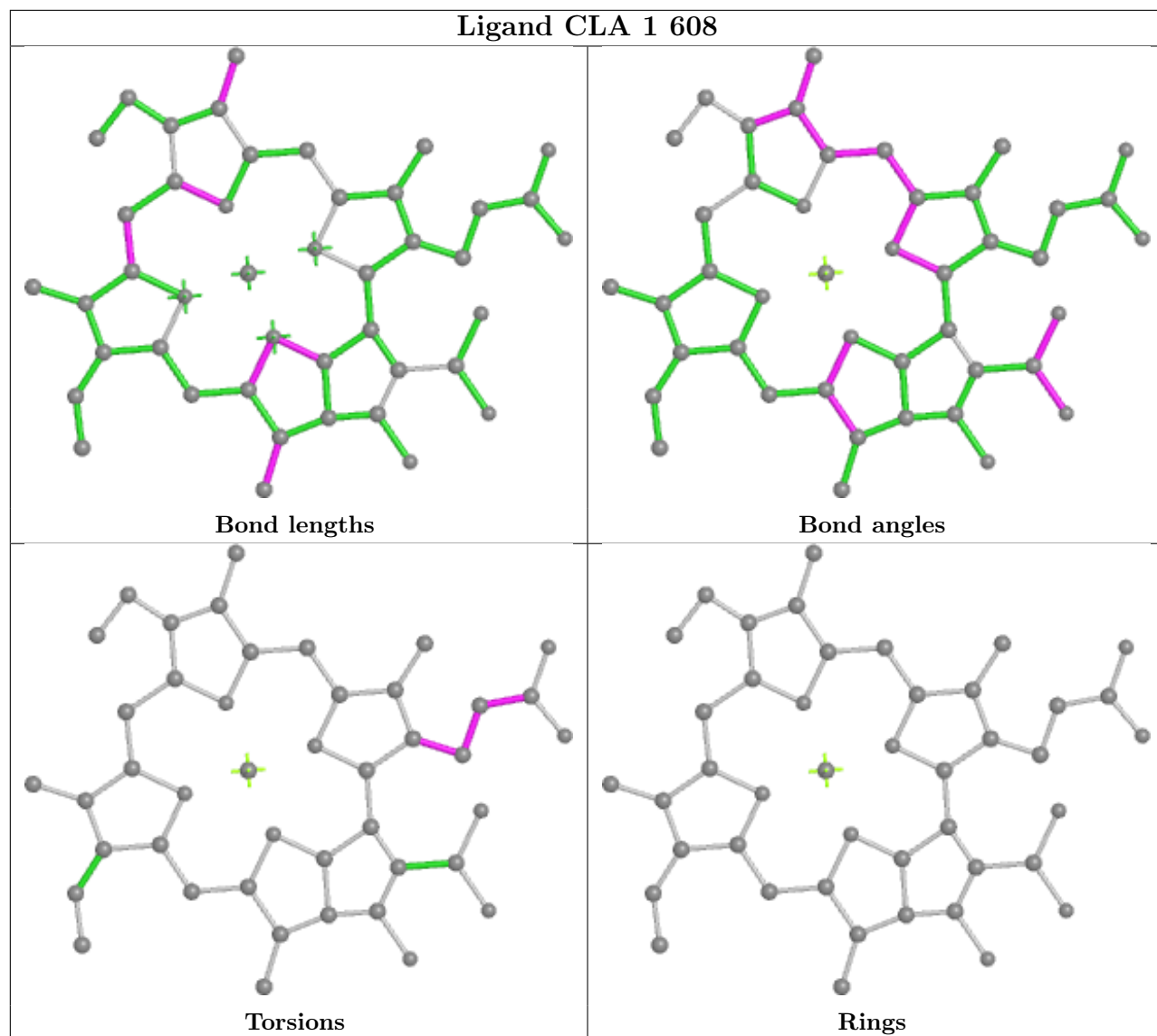


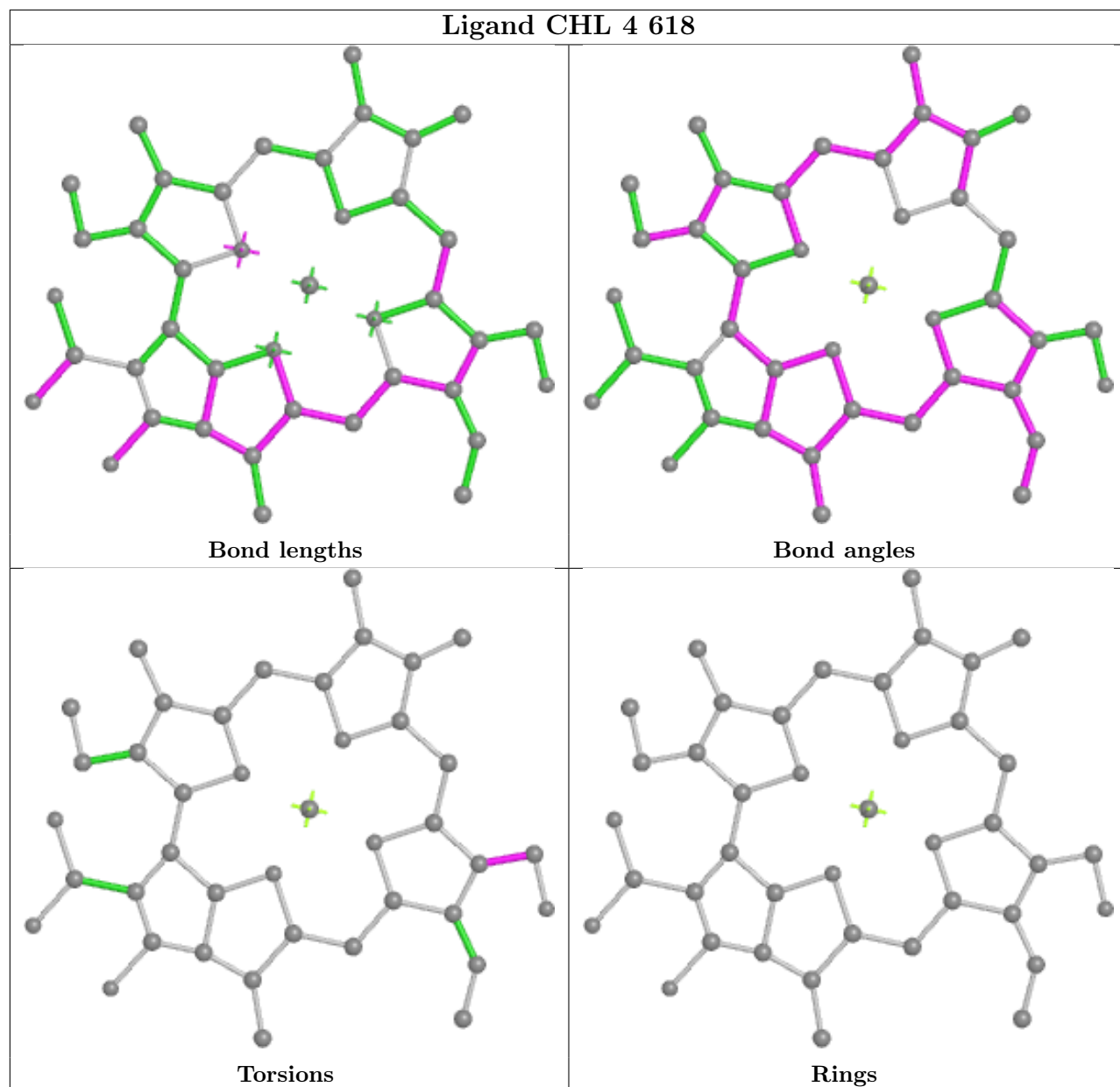


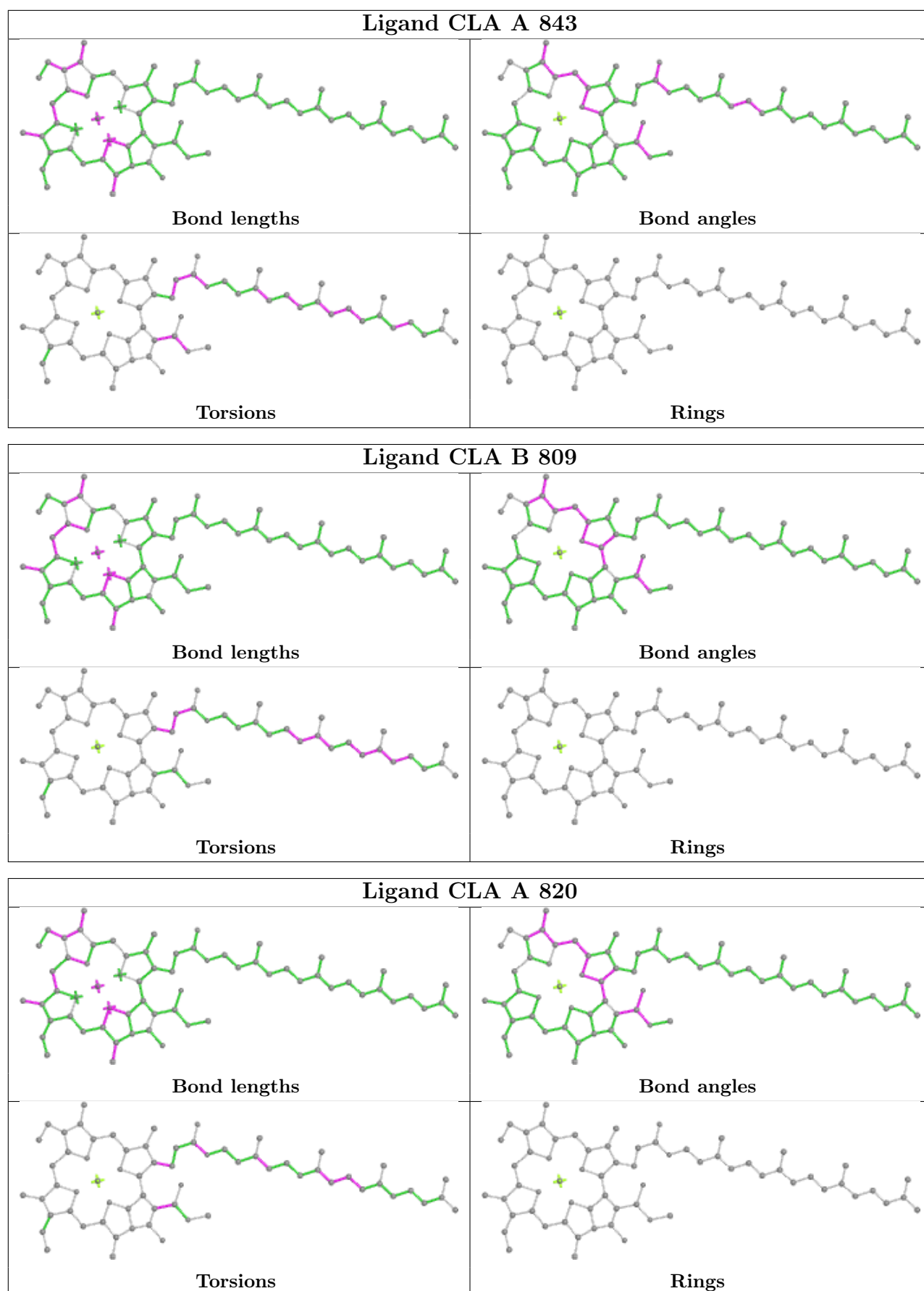


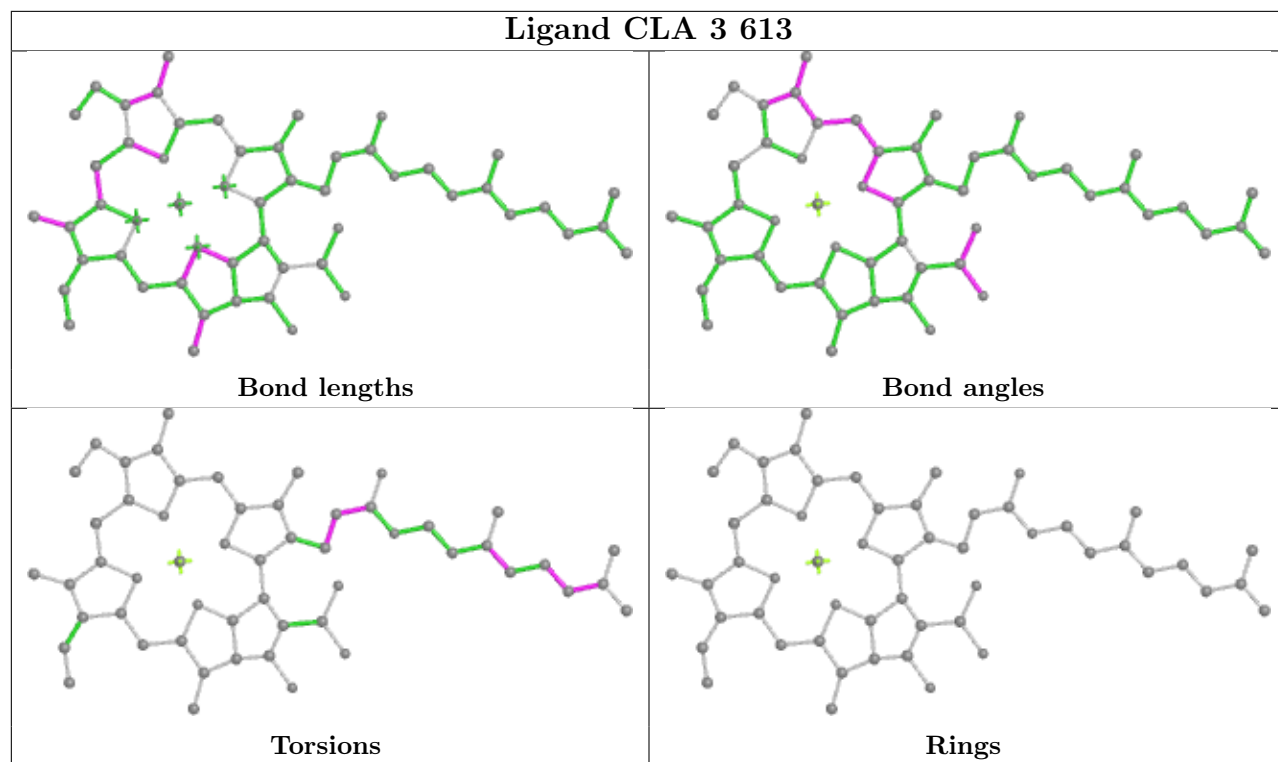


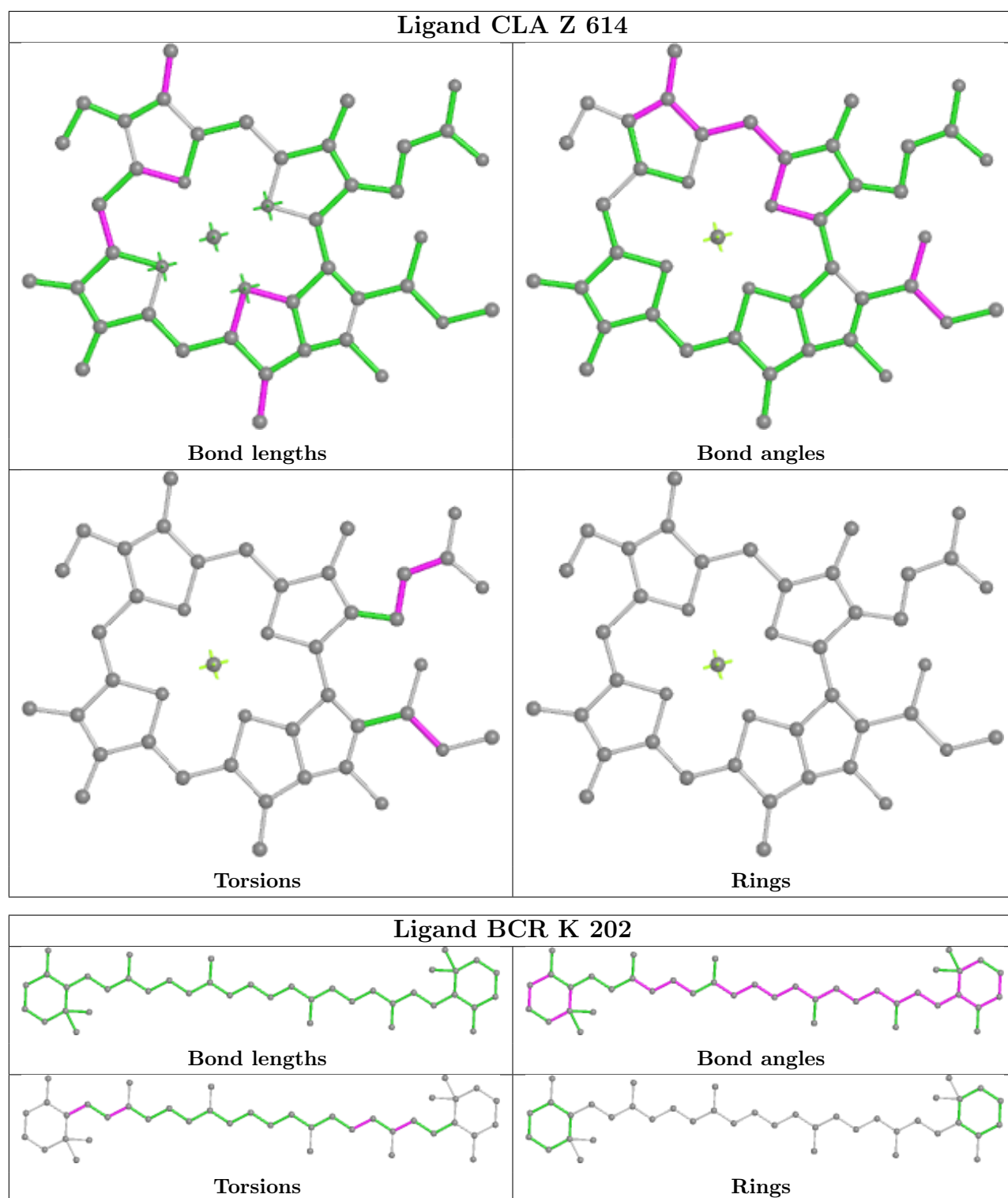


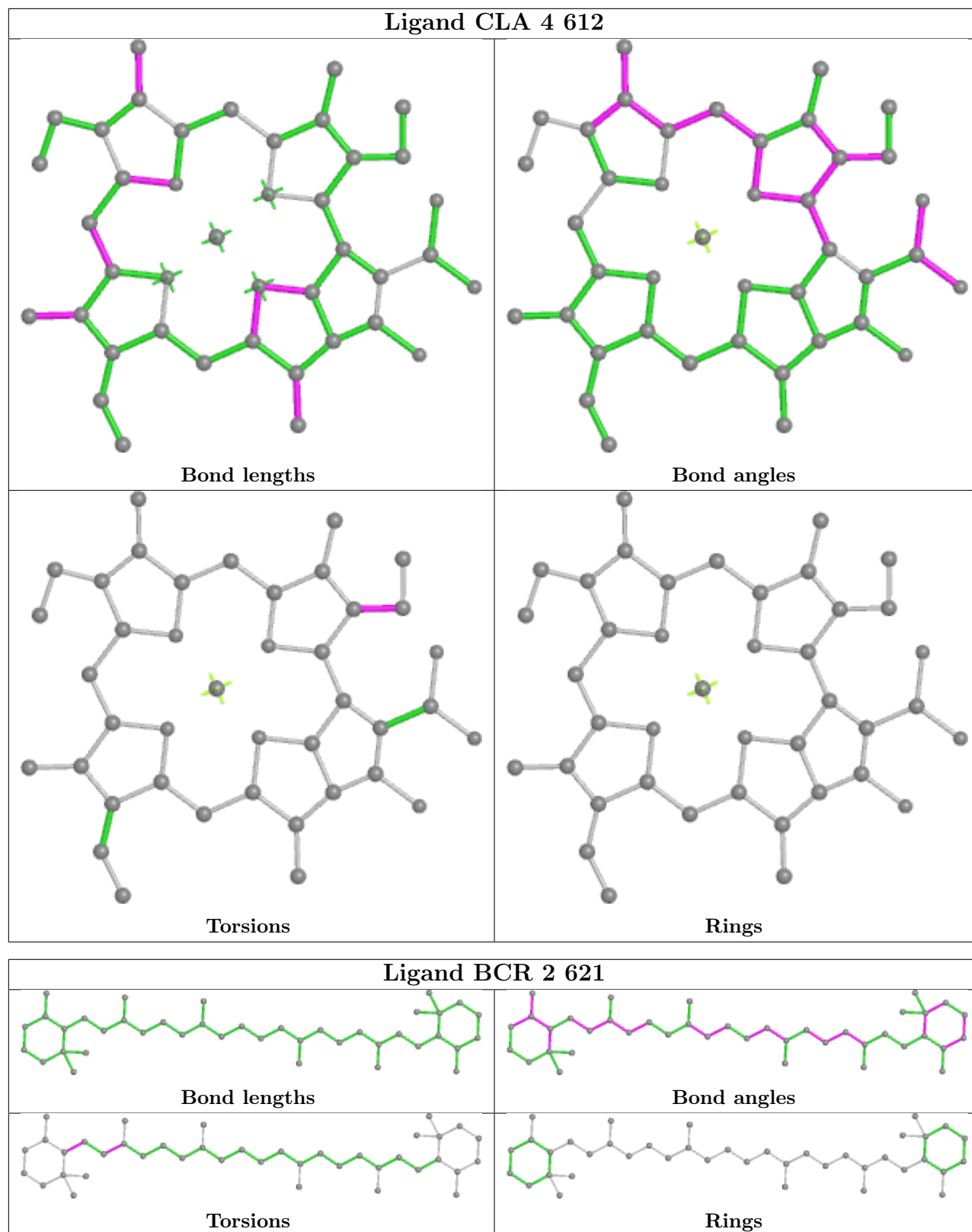


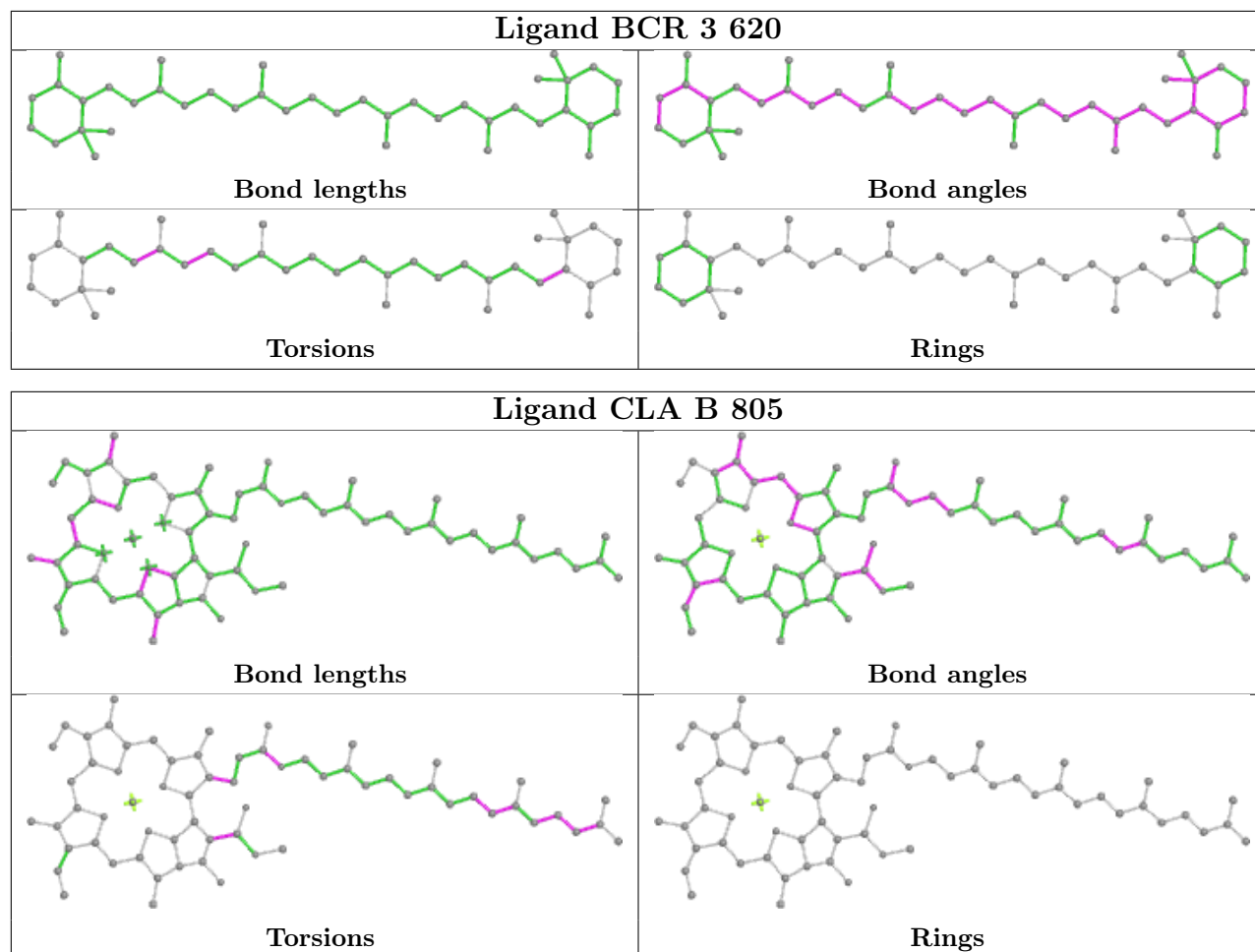


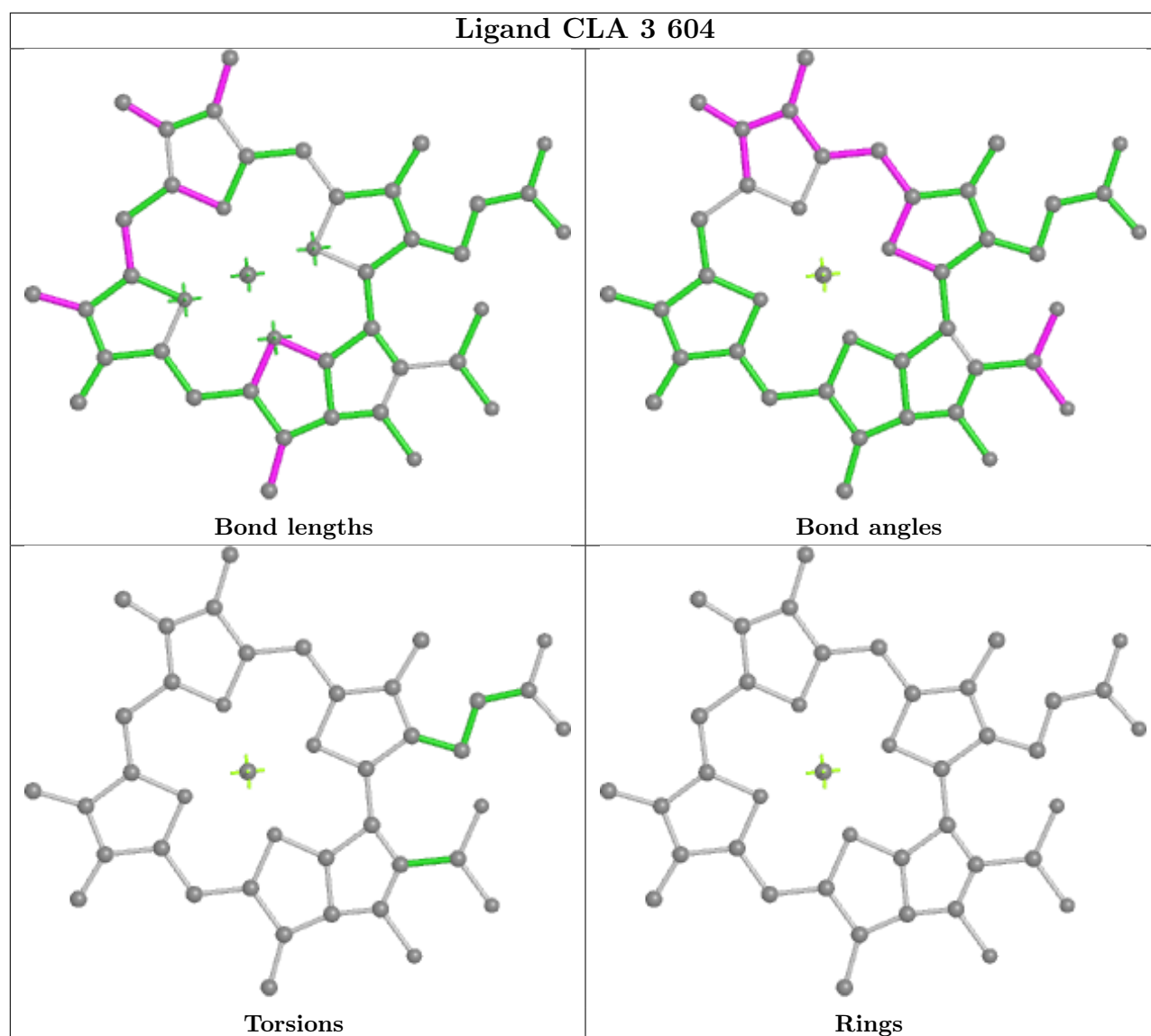












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

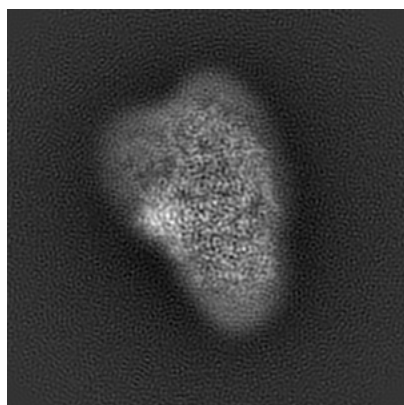
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6932. These allow visual inspection of the internal detail of the map and identification of artifacts.

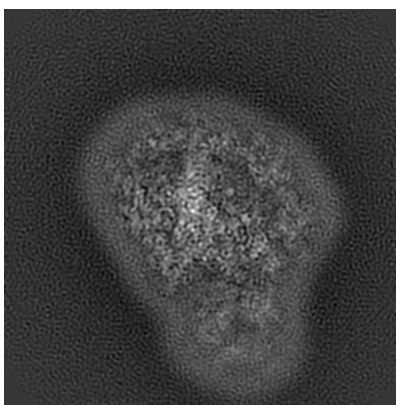
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

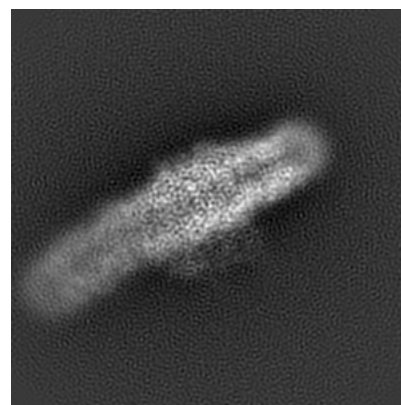
6.1.1 Primary map



X



Y

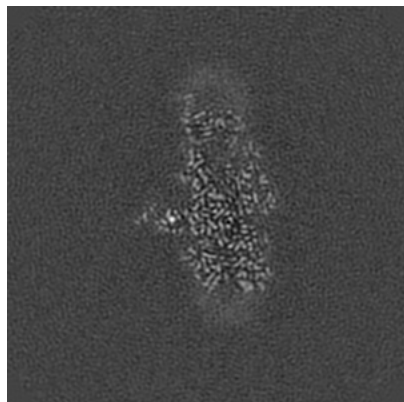


Z

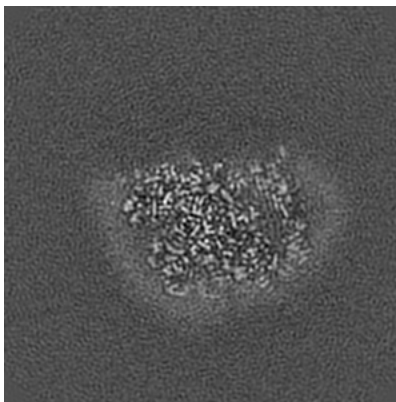
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

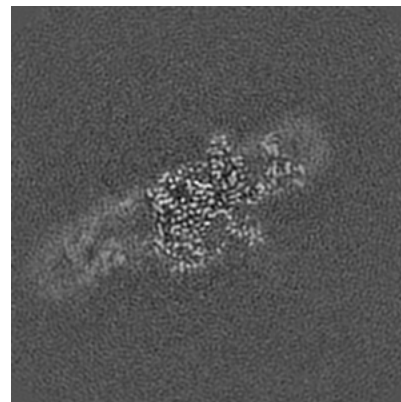
6.2.1 Primary map



X Index: 140



Y Index: 140

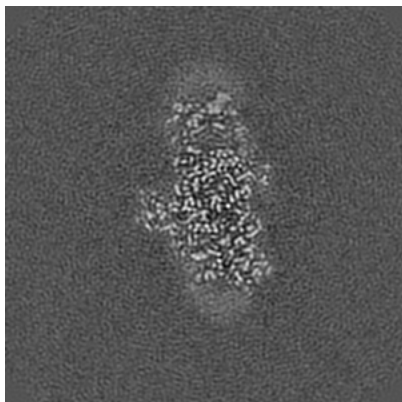


Z Index: 140

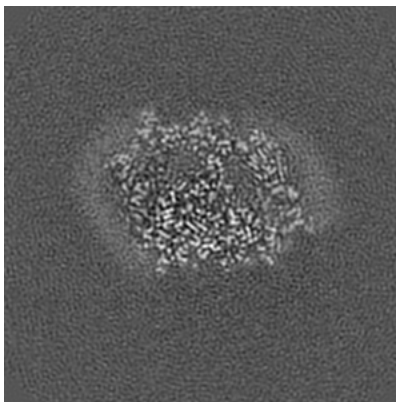
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

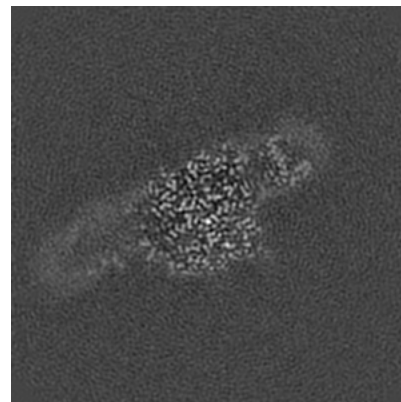
6.3.1 Primary map



X Index: 130



Y Index: 157

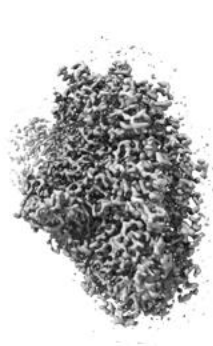


Z Index: 132

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

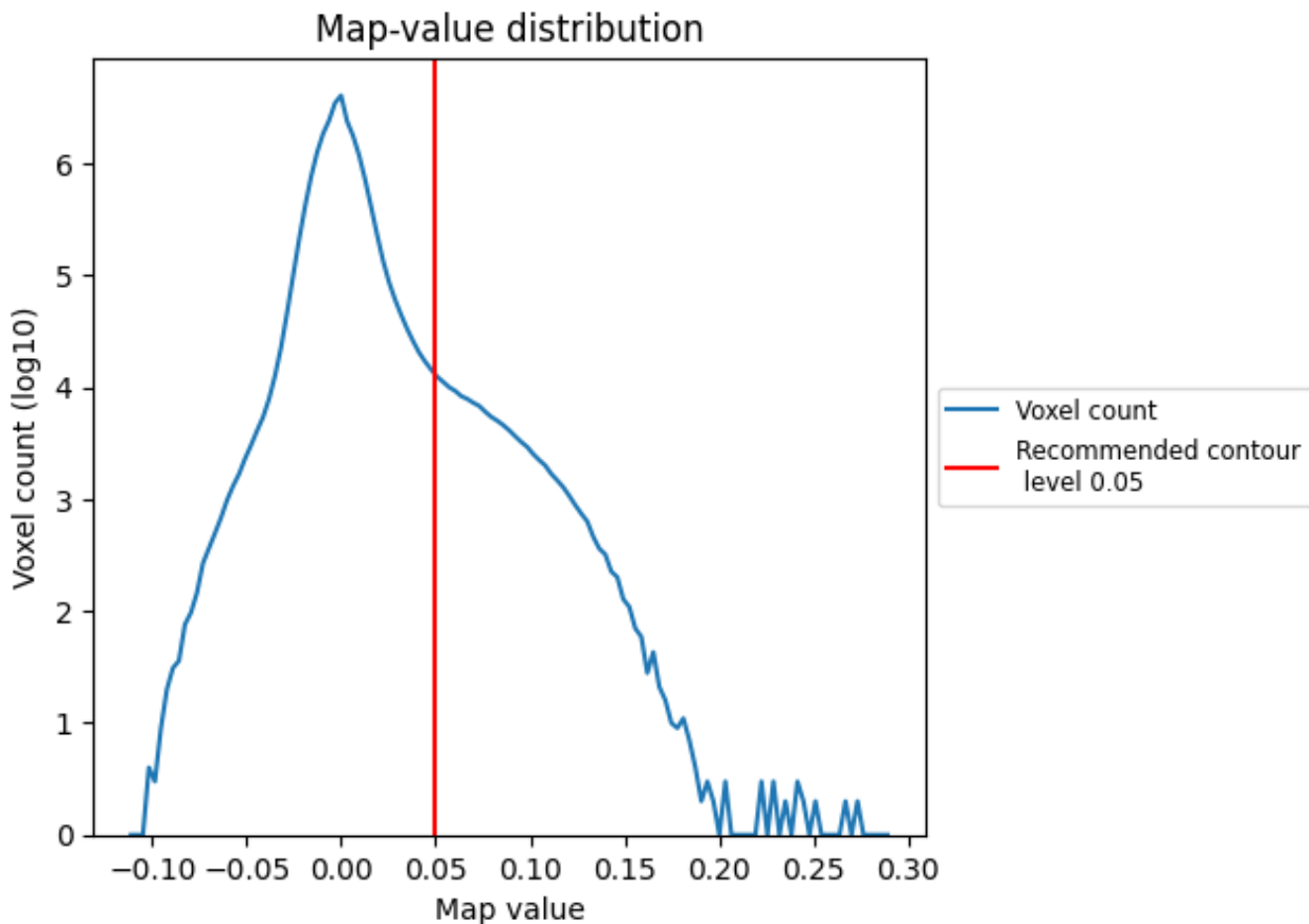
6.5 Mask visualisation

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

7 Map analysis [i](#)

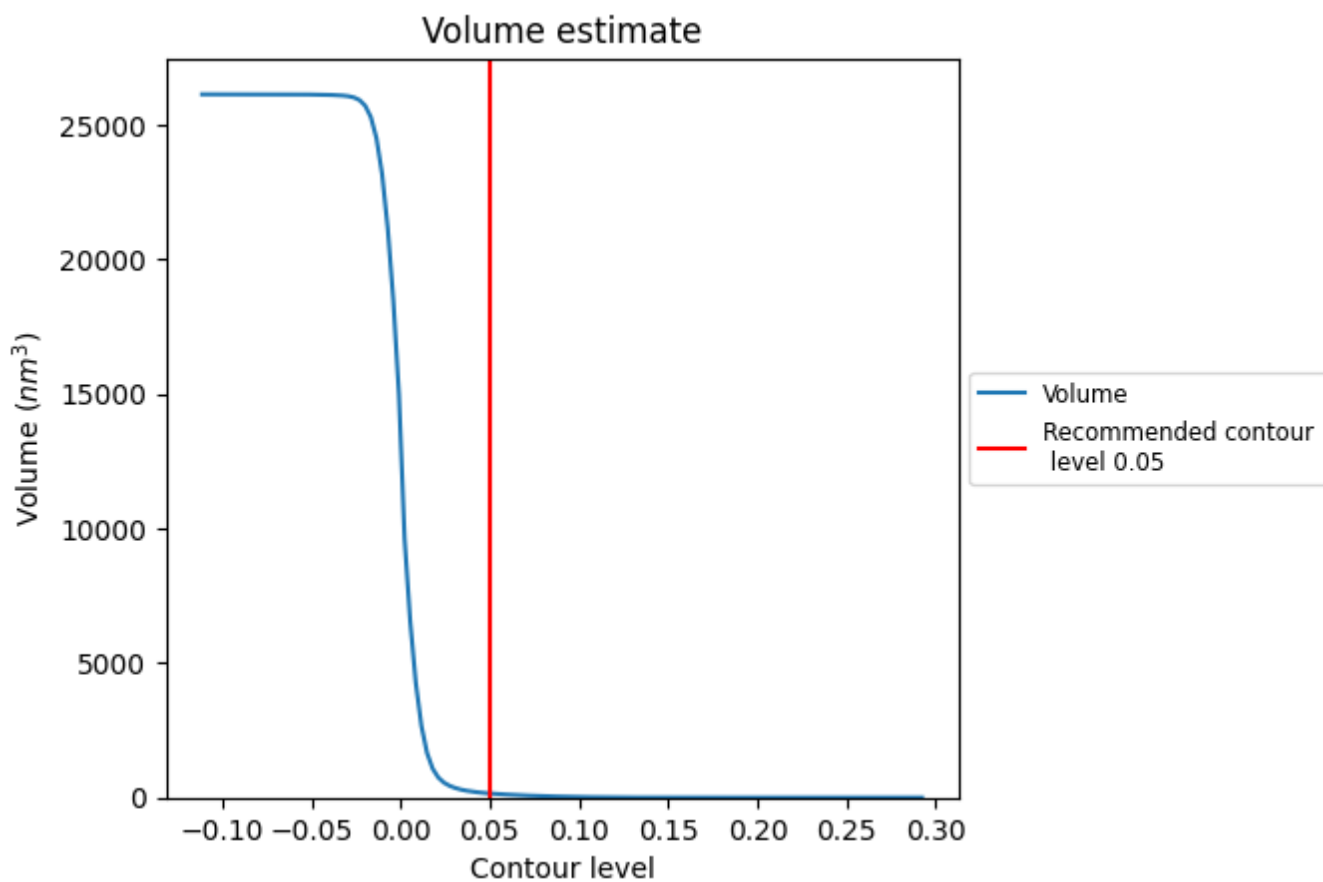
This section contains the results of statistical analysis of the map.

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.

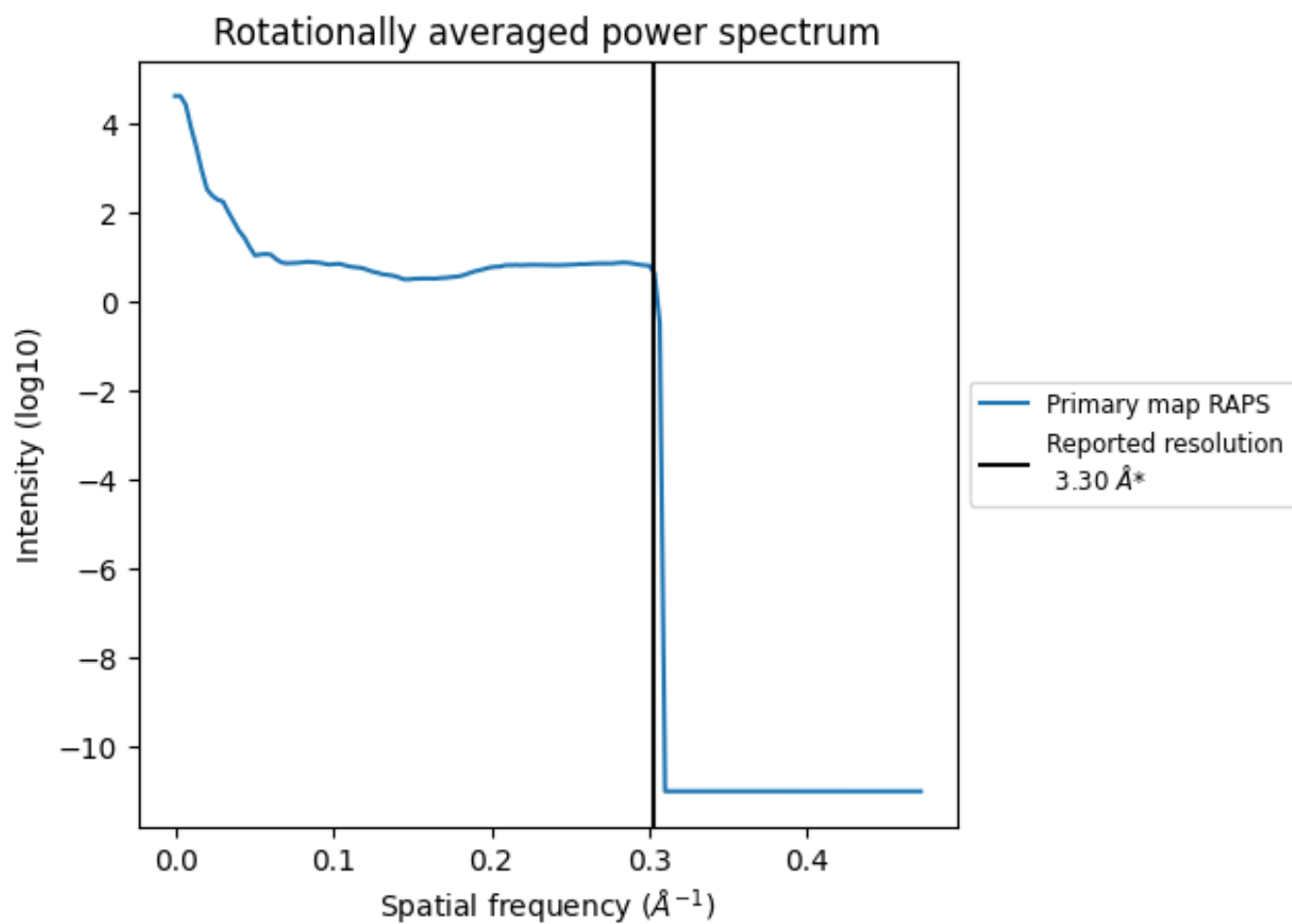
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 153 nm^3 ; 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 [\(i\)](#)



*Reported resolution corresponds to spatial frequency of 0.303\AA^{-1}

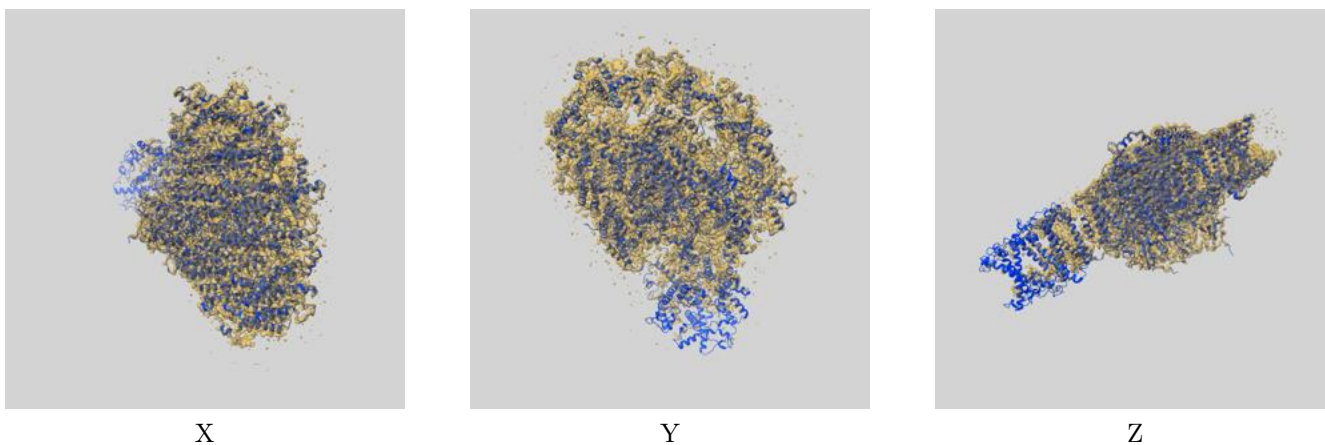
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

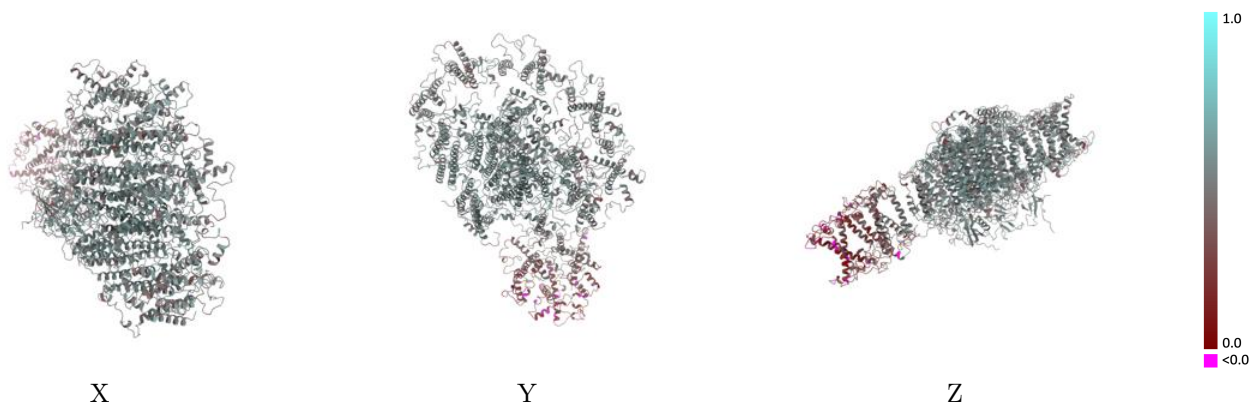
This section contains information regarding the fit between EMDB map EMD-6932 and PDB model 5ZJI. Per-residue inclusion information can be found in section 3 on page 32.

9.1 Map-model overlay [i](#)



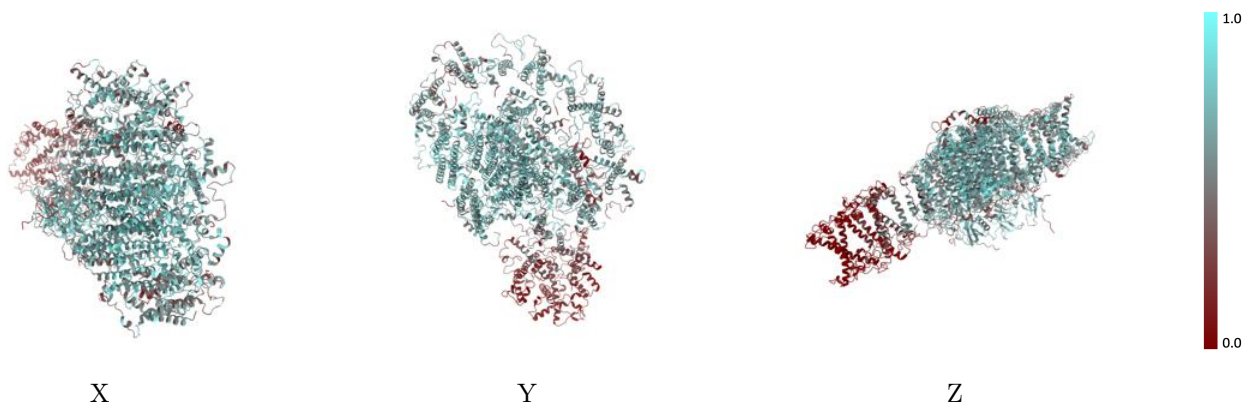
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



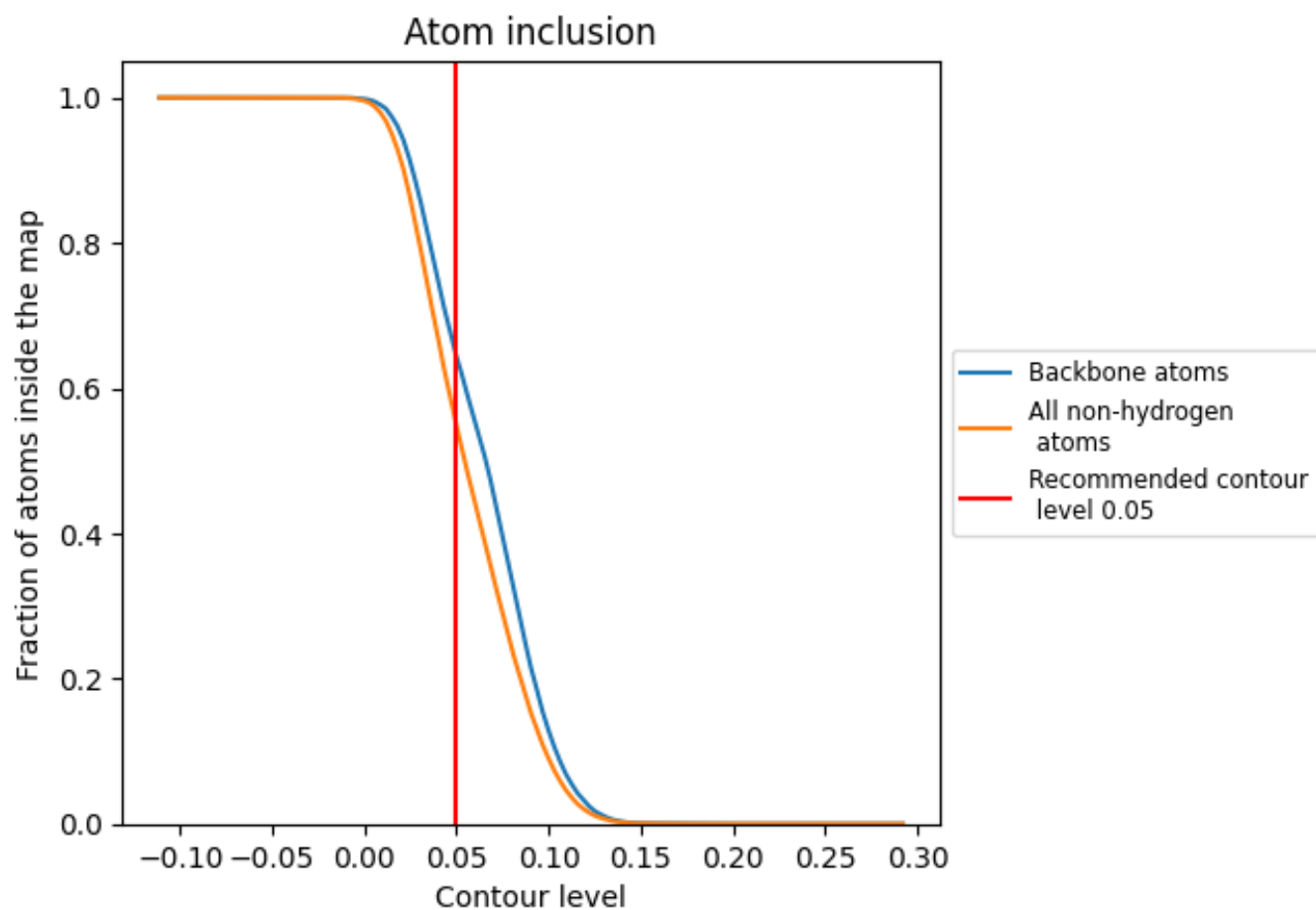
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).













































9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 55% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5481	 0.4940
1	 0.5138	 0.4870
2	 0.5880	 0.5130
3	 0.5559	 0.4990
4	 0.5961	 0.5060
A	 0.6864	 0.5560
B	 0.6974	 0.5540
C	 0.7378	 0.5320
D	 0.6538	 0.5250
E	 0.6183	 0.5170
F	 0.6226	 0.5270
G	 0.5085	 0.4990
H	 0.5290	 0.4880
I	 0.5853	 0.5160
J	 0.5640	 0.5320
K	 0.5092	 0.4850
L	 0.6202	 0.5200
N	 0.3932	 0.4840
O	 0.4859	 0.4690
X	 0.0242	 0.2260
Y	 0.2198	 0.3500
Z	 0.2095	 0.3740

