



wwPDB EM Validation Summary Report ⓘ

Nov 6, 2023 – 12:48 PM JST

PDB ID : 8J6Z
EMDB ID : EMD-36021
Title : Cryo-EM structure of the Arabidopsis thaliana photosystem I(PSI-LHCII-ST2)
Authors : Chen, S.J.B.; Wu, J.H.; Sui, S.F.; Zhang, L.X.
Deposited on : 2023-04-26
Resolution : 2.79 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.dev70
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) : 2.36

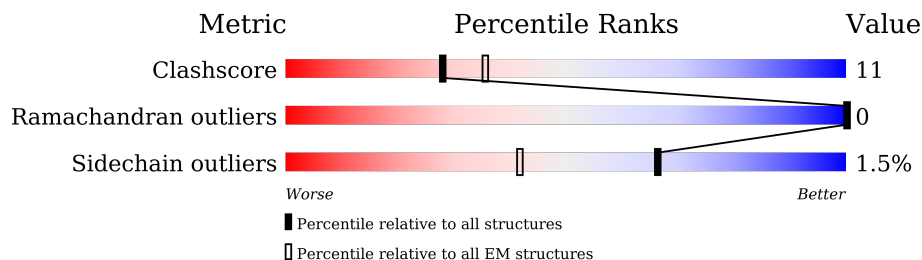
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.79 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	241	64% 15% 20%
2	2	257	65% 12% 22%
3	3	273	69% 11% 20%
4	4	251	71% 7% 22%
5	A	750	89% 9%
6	B	734	90% 10%
7	C	81	90% 7%
8	D	204	66% 30%

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Mol	Chain	Length	Quality of chain
9	E	143	
10	F	221	
11	G	160	
12	H	145	
13	I	37	
14	J	44	
15	K	130	
16	L	219	
17	O	140	
18	x	267	
18	y	267	
19	z	265	

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
20	CHL	1	601	X	-	-	-
20	CHL	1	606	X	-	-	-
20	CHL	2	601	X	-	-	-
20	CHL	2	605	X	-	-	-
20	CHL	2	606	X	-	-	-
20	CHL	2	607	X	-	-	-
20	CHL	2	615	X	-	-	-
20	CHL	3	606	X	-	-	-
20	CHL	4	605	X	-	-	-
20	CHL	4	606	X	-	-	-
20	CHL	4	607	X	-	-	-
20	CHL	4	615	X	-	-	-
20	CHL	x	601	X	-	-	-
20	CHL	x	605	X	-	-	-
20	CHL	x	606	X	-	-	-
20	CHL	x	607	X	-	-	-
20	CHL	x	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CHL	x	609	X	-	-	-
20	CHL	y	601	X	-	-	-
20	CHL	y	605	X	-	-	-
20	CHL	y	606	X	-	-	-
20	CHL	y	607	X	-	-	-
20	CHL	y	608	X	-	-	-
20	CHL	y	609	X	-	-	-
20	CHL	z	601	X	-	-	-
20	CHL	z	605	X	-	-	-
20	CHL	z	606	X	-	-	-
20	CHL	z	607	X	-	-	-
20	CHL	z	608	X	-	-	-
20	CHL	z	609	X	-	-	-
21	CLA	1	602	X	-	-	-
21	CLA	1	603	X	-	-	-
21	CLA	1	604	X	-	-	-
21	CLA	1	605	X	-	-	-
21	CLA	1	607	X	-	-	-
21	CLA	1	608	X	-	-	-
21	CLA	1	609	X	-	-	-
21	CLA	1	610	X	-	-	-
21	CLA	1	611	X	-	-	-
21	CLA	1	612	X	-	-	-
21	CLA	1	613	X	-	-	-
21	CLA	2	602	X	-	-	-
21	CLA	2	603	X	-	-	-
21	CLA	2	604	X	-	-	-
21	CLA	2	608	X	-	-	-
21	CLA	2	609	X	-	-	-
21	CLA	2	610	X	-	-	-
21	CLA	2	611	X	-	-	-
21	CLA	2	612	X	-	-	-
21	CLA	2	613	X	-	-	-
21	CLA	3	601	X	-	-	-
21	CLA	3	602	X	-	-	-
21	CLA	3	603	X	-	-	-
21	CLA	3	604	X	-	-	-
21	CLA	3	605	X	-	-	-
21	CLA	3	607	X	-	-	-
21	CLA	3	608	X	-	-	-
21	CLA	3	609	X	-	-	-
21	CLA	3	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	3	611	X	-	-	-
21	CLA	3	612	X	-	-	-
21	CLA	4	601	X	-	-	-
21	CLA	4	602	X	-	-	-
21	CLA	4	603	X	-	-	-
21	CLA	4	604	X	-	-	-
21	CLA	4	608	X	-	-	-
21	CLA	4	609	X	-	-	-
21	CLA	4	610	X	-	-	-
21	CLA	4	611	X	-	-	-
21	CLA	4	612	X	-	-	-
21	CLA	4	613	X	-	-	-
21	CLA	4	614	X	-	-	-
21	CLA	A	802	X	-	-	-
21	CLA	A	803	X	-	-	-
21	CLA	A	804	X	-	-	-
21	CLA	A	805	X	-	-	-
21	CLA	A	806	X	-	-	-
21	CLA	A	807	X	-	-	-
21	CLA	A	808	X	-	-	-
21	CLA	A	809	X	-	-	-
21	CLA	A	810	X	-	-	-
21	CLA	A	811	X	-	-	-
21	CLA	A	812	X	-	-	-
21	CLA	A	813	X	-	-	-
21	CLA	A	814	X	-	-	-
21	CLA	A	815	X	-	-	-
21	CLA	A	816	X	-	-	-
21	CLA	A	817	X	-	-	-
21	CLA	A	818	X	-	-	-
21	CLA	A	819	X	-	-	-
21	CLA	A	820	X	-	-	-
21	CLA	A	821	X	-	-	-
21	CLA	A	822	X	-	-	-
21	CLA	A	823	X	-	-	-
21	CLA	A	824	X	-	-	-
21	CLA	A	825	X	-	-	-
21	CLA	A	826	X	-	-	-
21	CLA	A	827	X	-	-	-
21	CLA	A	828	X	-	-	-
21	CLA	A	829	X	-	-	-
21	CLA	A	830	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	A	831	X	-	-	-
21	CLA	A	832	X	-	-	-
21	CLA	A	833	X	-	-	-
21	CLA	A	834	X	-	-	-
21	CLA	A	835	X	-	-	-
21	CLA	A	836	X	-	-	-
21	CLA	A	837	X	-	-	-
21	CLA	A	838	X	-	-	-
21	CLA	A	839	X	-	-	-
21	CLA	A	840	X	-	-	-
21	CLA	A	841	X	-	-	-
21	CLA	A	842	X	-	-	-
21	CLA	A	843	X	-	-	-
21	CLA	A	844	X	-	-	-
21	CLA	A	845	X	-	-	-
21	CLA	B	802	X	-	-	-
21	CLA	B	803	X	-	-	-
21	CLA	B	804	X	-	-	-
21	CLA	B	805	X	-	-	-
21	CLA	B	806	X	-	-	-
21	CLA	B	807	X	-	-	-
21	CLA	B	808	X	-	-	-
21	CLA	B	809	X	-	-	-
21	CLA	B	810	X	-	-	-
21	CLA	B	811	X	-	-	-
21	CLA	B	812	X	-	-	-
21	CLA	B	813	X	-	-	-
21	CLA	B	814	X	-	-	-
21	CLA	B	815	X	-	-	-
21	CLA	B	816	X	-	-	-
21	CLA	B	817	X	-	-	-
21	CLA	B	818	X	-	-	-
21	CLA	B	819	X	-	-	-
21	CLA	B	820	X	-	-	-
21	CLA	B	821	X	-	-	-
21	CLA	B	822	X	-	-	-
21	CLA	B	823	X	-	-	-
21	CLA	B	824	X	-	-	-
21	CLA	B	825	X	-	-	-
21	CLA	B	826	X	-	-	-
21	CLA	B	827	X	-	-	-
21	CLA	B	828	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	B	829	X	-	-	-
21	CLA	B	830	X	-	-	-
21	CLA	B	831	X	-	-	-
21	CLA	B	832	X	-	-	-
21	CLA	B	833	X	-	-	-
21	CLA	B	834	X	-	-	-
21	CLA	B	835	X	-	-	-
21	CLA	B	836	X	-	-	-
21	CLA	B	837	X	-	-	-
21	CLA	B	838	X	-	-	-
21	CLA	B	839	X	-	-	-
21	CLA	B	840	X	-	-	-
21	CLA	B	841	X	-	-	-
21	CLA	F	301	X	-	-	-
21	CLA	F	302	X	-	-	-
21	CLA	F	303	X	-	-	-
21	CLA	G	201	X	-	-	-
21	CLA	G	202	X	-	-	-
21	CLA	G	203	X	-	-	-
21	CLA	H	201	X	-	-	-
21	CLA	J	101	X	-	-	-
21	CLA	K	201	X	-	-	-
21	CLA	K	203	X	-	-	-
21	CLA	K	204	X	-	-	-
21	CLA	K	206	X	-	-	-
21	CLA	L	302	X	-	-	-
21	CLA	L	303	X	-	-	-
21	CLA	L	304	X	-	-	-
21	CLA	O	201	X	-	-	-
21	CLA	O	202	X	-	-	-
21	CLA	O	203	X	-	-	-
21	CLA	x	602	X	-	-	-
21	CLA	x	603	X	-	-	-
21	CLA	x	604	X	-	-	-
21	CLA	x	610	X	-	-	-
21	CLA	x	611	X	-	-	-
21	CLA	x	612	X	-	-	-
21	CLA	x	613	X	-	-	-
21	CLA	x	614	X	-	-	-
21	CLA	y	602	X	-	-	-
21	CLA	y	603	X	-	-	-
21	CLA	y	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	y	610	X	-	-	-
21	CLA	y	611	X	-	-	-
21	CLA	y	612	X	-	-	-
21	CLA	y	613	X	-	-	-
21	CLA	y	614	X	-	-	-
21	CLA	z	602	X	-	-	-
21	CLA	z	603	X	-	-	-
21	CLA	z	604	X	-	-	-
21	CLA	z	610	X	-	-	-
21	CLA	z	611	X	-	-	-
21	CLA	z	612	X	-	-	-
21	CLA	z	613	X	-	-	-
21	CLA	z	614	X	-	-	-
27	CL0	A	801	X	-	-	-
28	SF4	A	854	-	-	X	-
28	SF4	C	101	-	-	X	-
28	SF4	C	102	-	-	X	-

2 Entry composition [i](#)

There are 31 unique types of molecules in this entry. The entry contains 43924 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 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	193	1496	975	248	268	5	0	0

- Molecule 2 is a protein called Photosystem I chlorophyll a/b-binding protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	201	1566	1024	256	282	4	0	0

- Molecule 3 is a protein called Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	218	1666	1088	270	303	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	196	1551	1013	253	282	3	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	737	5807	3807	986	996	18	0	0

- 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	732	5854	3842	997	1001	14	0	0

- Molecule 7 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	C	80	616	381	107	117	11	0	0

- Molecule 8 is a protein called Photosystem I reaction center subunit II-2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	D	143	1128	723	195	206	4	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	E	64	517	331	92	94	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	F	152	1208	789	207	209	3	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	G	91	708	458	118	132	0	0

- Molecule 12 is a protein called Photosystem I reaction center subunit VI-2, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	H	90	693	451	112	130	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	I	31	239	162	39	37	1	0	0

- 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
			327	221	50	55	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	84	Total	C	N	O	S	0	0
			593	373	104	113	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	160	Total	C	N	O	S	0	0
			1207	799	191	215	2		

- Molecule 17 is a protein called Photosystem I subunit O.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	86	Total	C	N	O	S	0	0
			686	456	114	115	1		

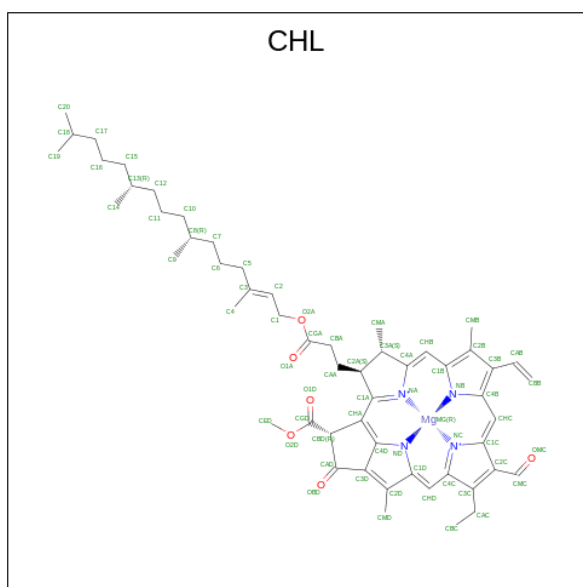
- Molecule 18 is a protein called Chlorophyll a-b binding protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	x	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
18	y	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		

- Molecule 19 is a protein called Chlorophyll a-b binding protein 2.1, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	z	227	Total	C	N	O	P	S	0	0
			1759	1140	286	327	1	5		

- Molecule 20 is CHLOROPHYLL B (three-letter code: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



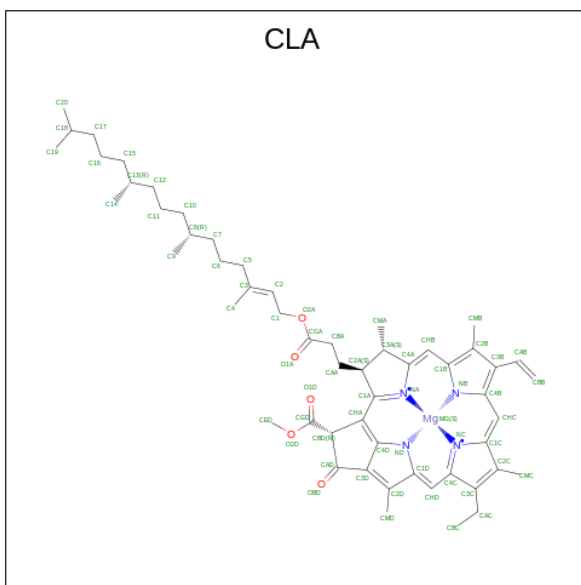
Mol	Chain	Residues	Atoms				AltConf	
20	1	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
20	1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
20	2	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
20	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
20	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
20	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
20	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
20	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
20	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
20	4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
20	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	x	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
20	x	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

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Mol	Chain	Residues	Atoms				AltConf	
20	x	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
20	x	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	x	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
20	x	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
20	y	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
20	y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	y	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
20	y	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
20	y	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
20	y	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
20	z	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	z	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
20	z	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
20	z	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
20	z	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
20	z	1	Total	C	Mg	N	O	0
			52	41	1	4	6	

- Molecule 21 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf	
21	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
21	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
21	1	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
21	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
21	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	2	1	38	30	1	4	3	0
21	2	1	65	55	1	4	5	0
21	2	1	44	34	1	4	5	0
21	2	1	45	35	1	4	5	0
21	2	1	47	37	1	4	5	0
21	2	1	43	35	1	4	3	0
21	3	1	60	50	1	4	5	0
21	3	1	36	30	1	4	1	0
21	3	1	41	33	1	4	3	0
21	3	1	45	35	1	4	5	0
21	3	1	40	32	1	4	3	0
21	3	1	45	35	1	4	5	0
21	3	1	41	33	1	4	3	0
21	3	1	40	32	1	4	3	0
21	3	1	55	45	1	4	5	0
21	3	1	54	44	1	4	5	0
21	3	1	41	33	1	4	3	0
21	4	1	45	35	1	4	5	0
21	4	1	54	44	1	4	5	0
21	4	1	45	35	1	4	5	0
21	4	1	44	34	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	4	1	41	33	1	4	3	0
21	4	1	57	47	1	4	5	0
21	4	1	46	36	1	4	5	0
21	4	1	60	50	1	4	5	0
21	4	1	42	34	1	4	3	0
21	4	1	50	40	1	4	5	0
21	4	1	43	33	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	50	40	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	54	44	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	60	50	1	4	5	0
21	A	1	50	40	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	A	1	65	55	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	42	34	1	4	3	0
21	A	1	41	33	1	4	3	0
21	A	1	59	49	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	55	45	1	4	5	0
21	A	1	52	42	1	4	5	0
21	A	1	45	35	1	4	5	0
21	A	1	42	34	1	4	3	0
21	A	1	65	55	1	4	5	0
21	A	1	59	49	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	45	35	1	4	5	0
21	A	1	45	35	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	50	40	1	4	5	0
21	A	1	51	41	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	56	46	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	A	1	65	55	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	45	35	1	4	5	0
21	A	1	50	40	1	4	5	0
21	A	1	45	35	1	4	5	0
21	A	1	52	42	1	4	5	0
21	A	1	65	55	1	4	5	0
21	A	1	55	45	1	4	5	0
21	B	1	55	45	1	4	5	0
21	B	1	65	55	1	4	5	0
21	B	1	50	40	1	4	5	0
21	B	1	41	33	1	4	3	0
21	B	1	65	55	1	4	5	0
21	B	1	65	55	1	4	5	0
21	B	1	59	49	1	4	5	0
21	B	1	65	55	1	4	5	0
21	B	1	56	46	1	4	5	0
21	B	1	43	35	1	4	3	0
21	B	1	65	55	1	4	5	0
21	B	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	B	1	43	35	1	4	3	0
21	B	1	54	44	1	4	5	0
21	B	1	45	35	1	4	5	0
21	B	1	62	52	1	4	5	0
21	B	1	50	40	1	4	5	0
21	B	1	47	37	1	4	5	0
21	B	1	65	55	1	4	5	0
21	B	1	52	42	1	4	5	0
21	B	1	65	55	1	4	5	0
21	B	1	42	34	1	4	3	0
21	B	1	47	37	1	4	5	0
21	B	1	62	52	1	4	5	0
21	B	1	65	55	1	4	5	0
21	B	1	65	55	1	4	5	0
21	B	1	45	35	1	4	5	0
21	B	1	65	55	1	4	5	0
21	B	1	55	45	1	4	5	0
21	B	1	60	50	1	4	5	0
21	B	1	65	55	1	4	5	0
21	B	1	65	55	1	4	5	0
21	B	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	B	1	65	55	1	4	5	0
21	B	1	43	35	1	4	3	0
21	B	1	65	55	1	4	5	0
21	B	1	65	55	1	4	5	0
21	B	1	60	50	1	4	5	0
21	B	1	43	35	1	4	3	0
21	B	1	65	55	1	4	5	0
21	F	1	51	41	1	4	5	0
21	F	1	41	33	1	4	3	0
21	F	1	57	47	1	4	5	0
21	G	1	45	35	1	4	5	0
21	G	1	42	34	1	4	3	0
21	G	1	45	35	1	4	5	0
21	H	1	60	50	1	4	5	0
21	J	1	51	41	1	4	5	0
21	K	1	37	31	1	4	1	0
21	K	1	46	36	1	4	5	0
21	K	1	39	31	1	4	3	0
21	K	1	45	35	1	4	5	0
21	L	1	45	35	1	4	5	0
21	L	1	65	55	1	4	5	0

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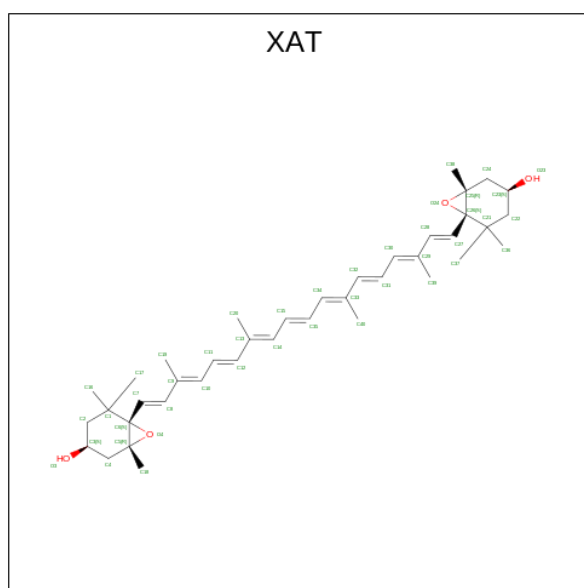
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	L	1	45	35	1	4	5	0
21	O	1	38	30	1	4	3	0
21	O	1	38	30	1	4	3	0
21	O	1	65	55	1	4	5	0
21	x	1	65	55	1	4	5	0
21	x	1	52	42	1	4	5	0
21	x	1	45	35	1	4	5	0
21	x	1	65	55	1	4	5	0
21	x	1	45	35	1	4	5	0
21	x	1	59	49	1	4	5	0
21	x	1	45	35	1	4	5	0
21	x	1	60	50	1	4	5	0
21	y	1	53	43	1	4	5	0
21	y	1	58	48	1	4	5	0
21	y	1	45	35	1	4	5	0
21	y	1	45	35	1	4	5	0
21	y	1	65	55	1	4	5	0
21	y	1	51	41	1	4	5	0
21	y	1	65	55	1	4	5	0
21	y	1	45	35	1	4	5	0
21	z	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	z	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
21	z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	z	1	Total	C	Mg	N	O	0
			57	47	1	4	5	

- Molecule 22 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).



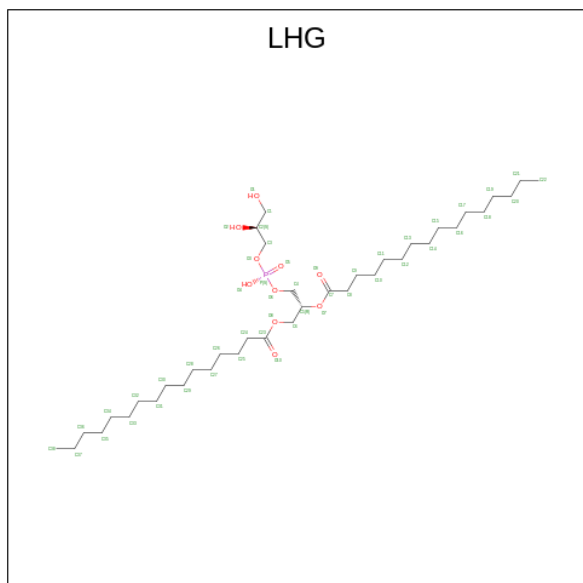
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
22	1	1	Total	C	O	0
			44	40	4	
22	2	1	Total	C	O	0
			44	40	4	
22	4	1	Total	C	O	0
			44	40	4	
22	x	1	Total	C	O	0
			44	40	4	

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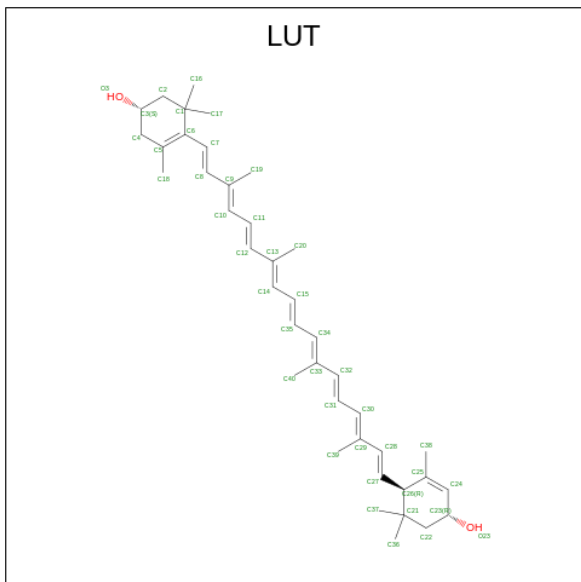
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
22	y	1	44	40	4	0
22	z	1	44	40	4	0

- Molecule 23 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



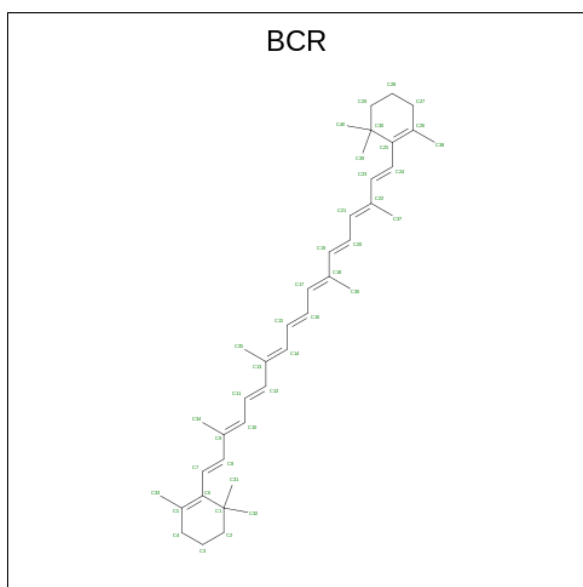
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
23	1	1	49	38	10	1	0
23	2	1	37	26	10	1	0
23	A	1	30	19	10	1	0
23	A	1	49	38	10	1	0
23	B	1	38	27	10	1	0
23	B	1	49	38	10	1	0
23	x	1	49	38	10	1	0
23	y	1	49	38	10	1	0
23	z	1	49	38	10	1	0

- Molecule 24 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
24	1	1	Total	C	O	0
			42	40	2	
24	2	1	Total	C	O	0
			42	40	2	
24	2	1	Total	C	O	0
			42	40	2	
24	3	1	Total	C	O	0
			42	40	2	
24	4	1	Total	C	O	0
			42	40	2	
24	x	1	Total	C	O	0
			42	40	2	
24	x	1	Total	C	O	0
			42	40	2	
24	y	1	Total	C	O	0
			42	40	2	
24	y	1	Total	C	O	0
			42	40	2	
24	z	1	Total	C	O	0
			42	40	2	
24	z	1	Total	C	O	0
			42	40	2	

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



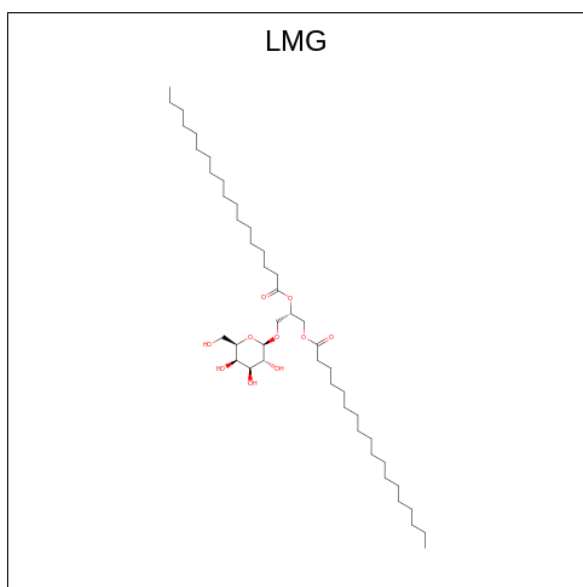
Mol	Chain	Residues	Atoms	AltConf
25	3	1	Total C 40 40	0
25	4	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C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

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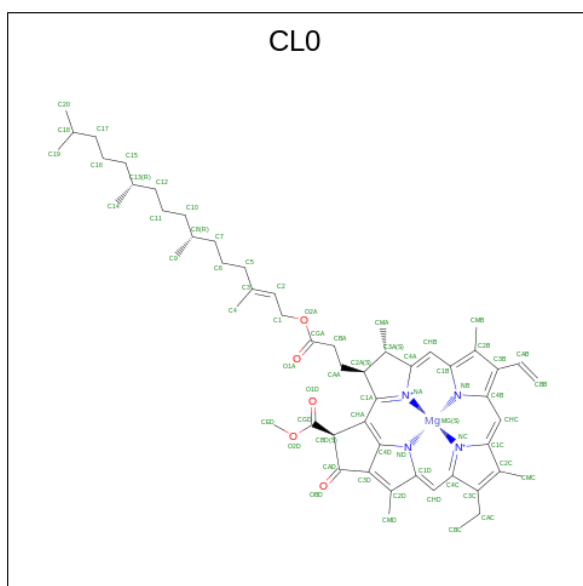
Mol	Chain	Residues	Atoms	AltConf
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	F	1	Total C 40 40	0
25	G	1	Total C 40 40	0
25	I	1	Total C 40 40	0
25	J	1	Total C 40 40	0
25	K	1	Total C 40 40	0
25	K	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	O	1	Total C 40 40	0
25	O	1	Total C 40 40	0

- Molecule 26 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



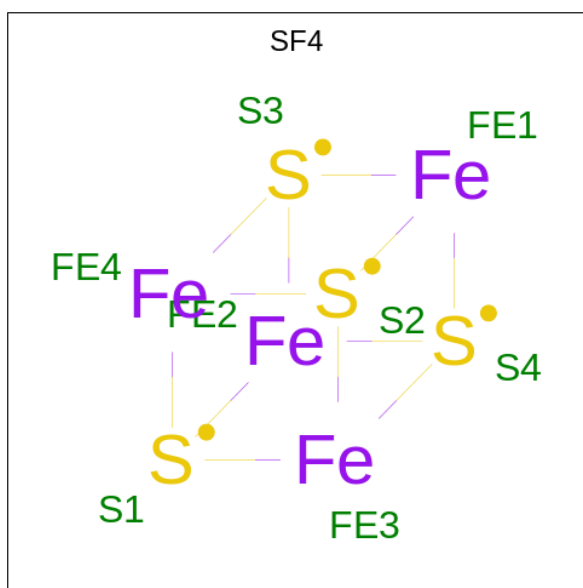
Mol	Chain	Residues	Atoms			AltConf
26	4	1	Total	C	O	0
			39	29	10	
26	4	1	Total	C	O	0
			33	23	10	

- Molecule 27 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



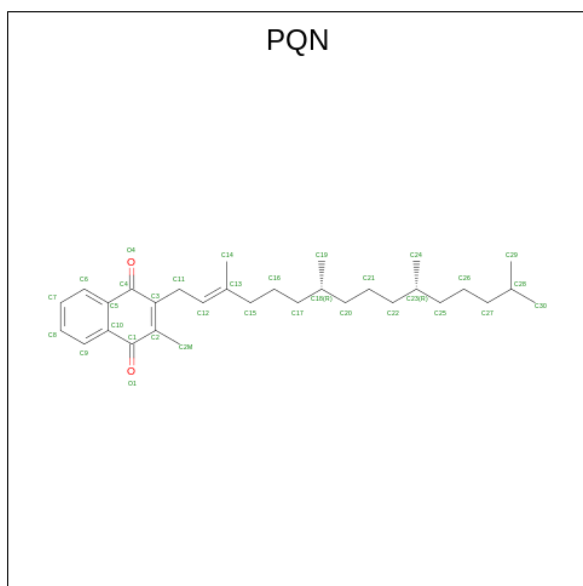
Mol	Chain	Residues	Atoms				AltConf	
27	A	1	Total	C	Mg	N	O	0
			61	53	1	4	3	

- Molecule 28 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



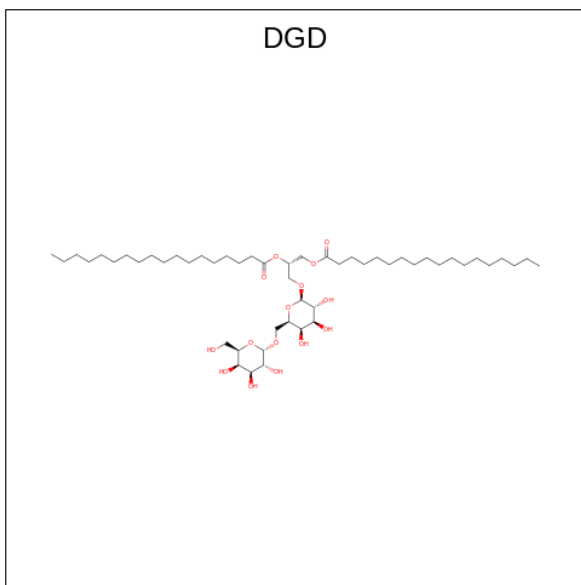
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	Fe	S	0
			8	4	4	
28	C	1	Total	Fe	S	0
			8	4	4	
28	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 29 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



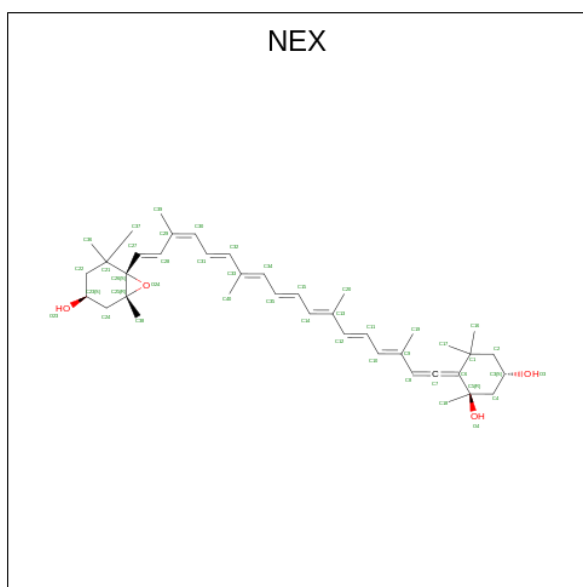
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			33	31	2	
29	B	1	Total	C	O	0
			33	31	2	

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

- Molecule 31 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-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: $C_{40}H_{56}O_4$).

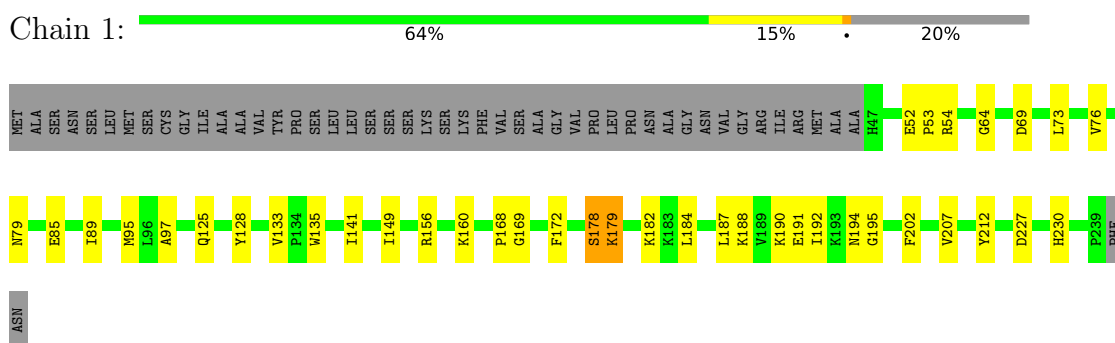


Mol	Chain	Residues	Atoms			AltConf
31	x	1	Total	C	O	0
			44	40	4	
31	y	1	Total	C	O	0
			44	40	4	
31	z	1	Total	C	O	0
			44	40	4	

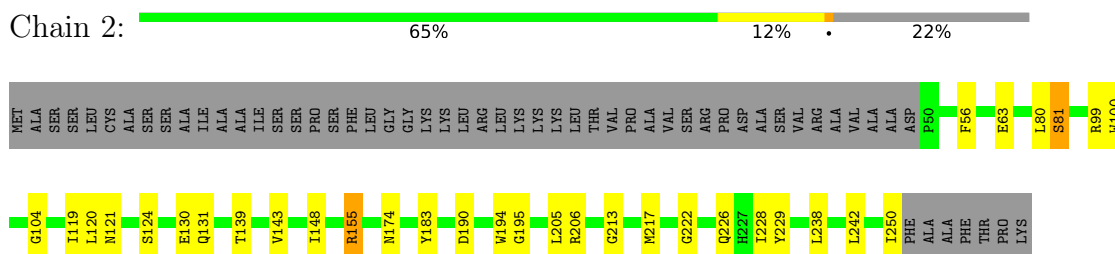
3 Residue-property plots [i](#)

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.

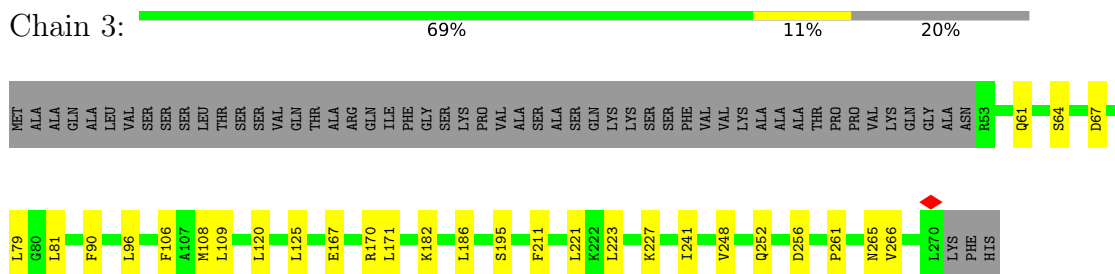
- Molecule 1: Chlorophyll a-b binding protein 6, chloroplastic



- Molecule 2: Photosystem I chlorophyll a/b-binding protein 2, chloroplastic

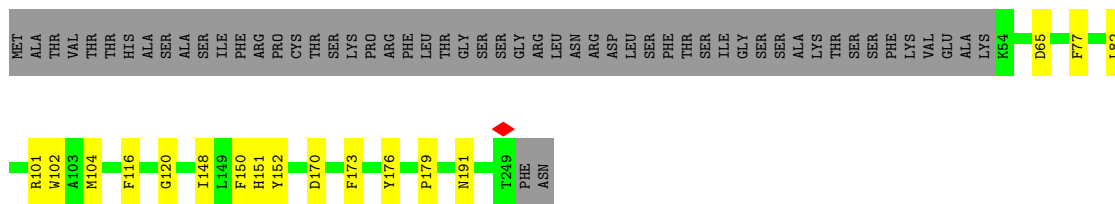


- Molecule 3: Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic

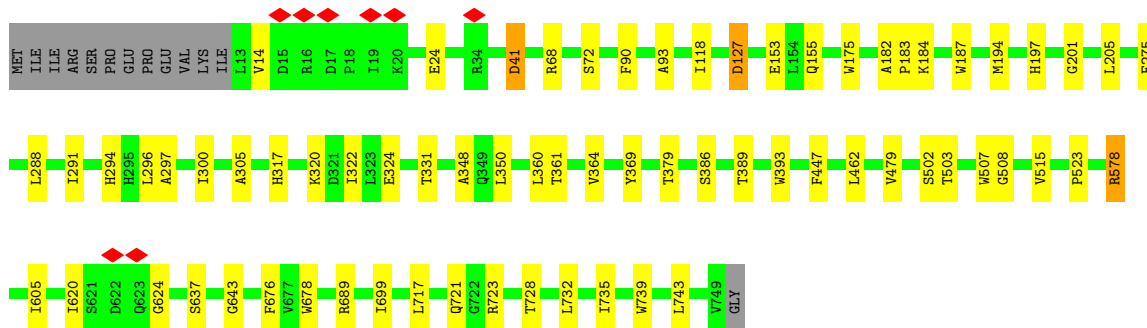
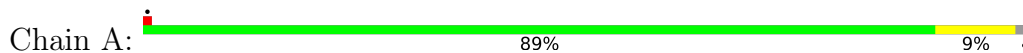


- Molecule 4: Chlorophyll a-b binding protein 4, chloroplastic

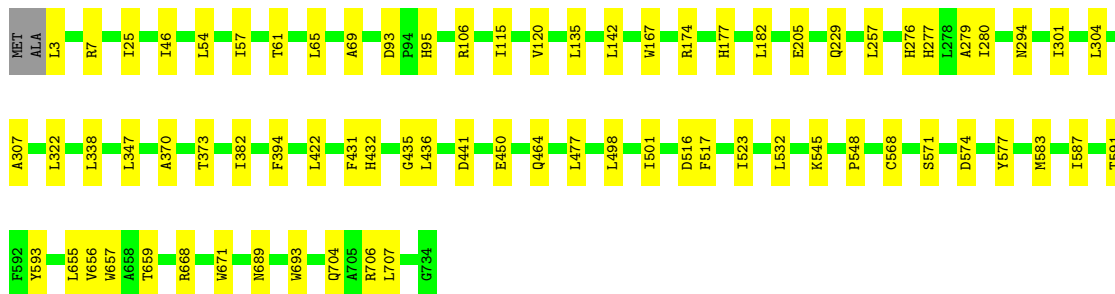
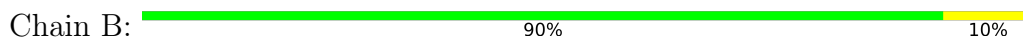




• Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1



• Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2



• Molecule 7: Photosystem I iron-sulfur center

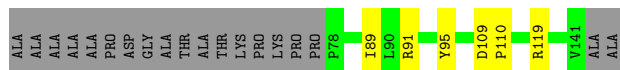


• Molecule 8: Photosystem I reaction center subunit II-2, chloroplastic





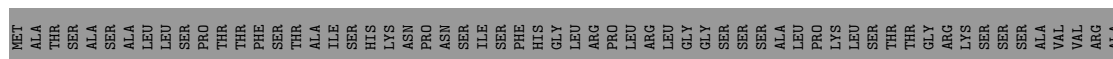
- Molecule 9: Photosystem I reaction center subunit IV A, chloroplastic



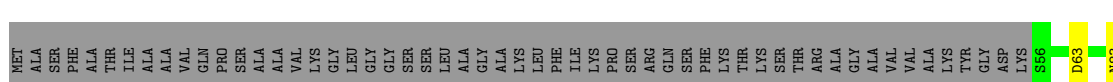
- Molecule 10: Photosystem I reaction center subunit III, chloroplastic



- Molecule 11: Photosystem I reaction center subunit V, chloroplastic



- Molecule 12: Photosystem I reaction center subunit VI-2, chloroplastic



- Molecule 13: Photosystem I reaction center subunit VIII



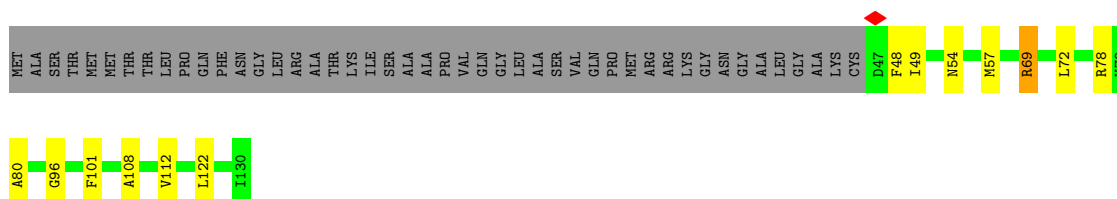
- Molecule 14: Photosystem I reaction center subunit IX

Chain J:  68% 25% 7%



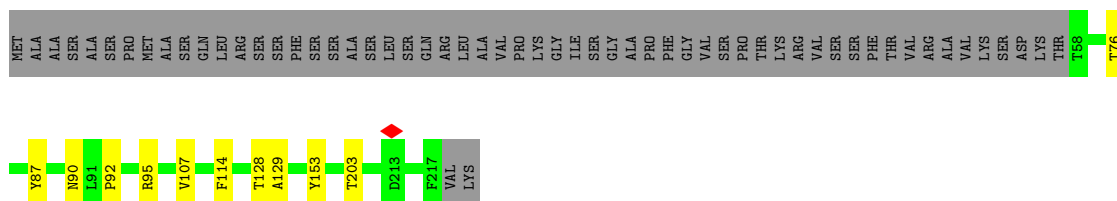
- Molecule 15: Photosystem I reaction center subunit psaK, chloroplastic

Chain K:  55% 9% 35%



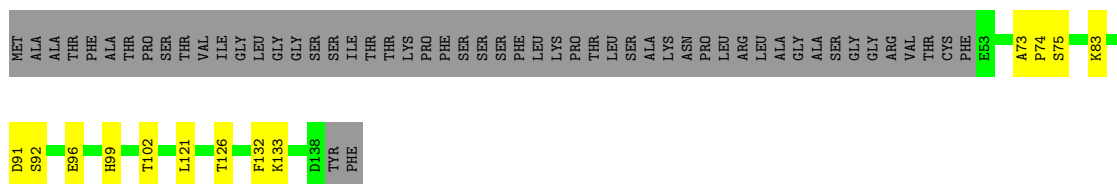
- Molecule 16: Photosystem I reaction center subunit XI, chloroplastic

Chain L:  68% 5% 27%




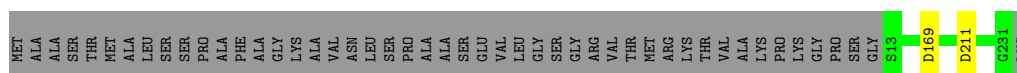
- Molecule 17: Photosystem I subunit O

Chain O:  52% 9% 39%




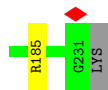
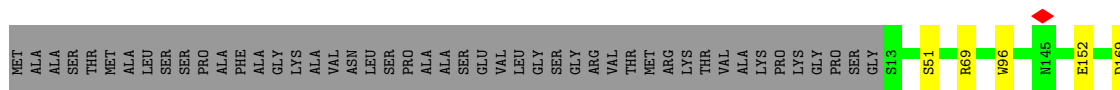
- Molecule 18: Chlorophyll a-b binding protein 2, chloroplastic

Chain x:  81% 18%



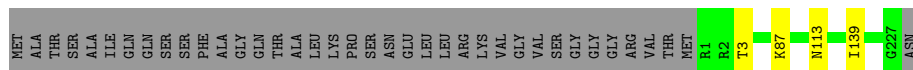
- Molecule 18: Chlorophyll a-b binding protein 2, chloroplastic

Chain y:  80% 18%



- Molecule 19: Chlorophyll a-b binding protein 2.1, chloroplastic

Chain z: 84% 14%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	188490	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 ($e^-/\text{\AA}^2$)	50.5	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	38.962	Depositor
Minimum map value	-20.964	Depositor
Average map value	0.022	Depositor
Map value standard deviation	1.157	Depositor
Recommended contour level	3.59	Depositor
Map size (Å)	365.232, 365.232, 365.232	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	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: XAT, SF4, LUT, CL0, LMG, DGD, PQN, BCR, TPO, CHL, NEX, CLA, LHG

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	0.29	0/1546	0.44	0/2110
2	2	0.43	0/1622	0.66	3/2219 (0.1%)
3	3	0.31	0/1717	0.49	0/2336
4	4	0.28	0/1599	0.42	0/2178
5	A	0.32	0/6005	0.52	5/8194 (0.1%)
6	B	0.32	0/6065	0.53	2/8279 (0.0%)
7	C	0.47	0/629	1.04	5/852 (0.6%)
8	D	0.49	0/1157	0.77	3/1563 (0.2%)
9	E	0.30	0/528	0.50	0/715
10	F	0.27	0/1238	0.47	0/1670
11	G	0.29	0/724	0.45	0/981
12	H	0.42	0/713	0.56	0/968
13	I	0.27	0/245	0.43	0/333
14	J	0.25	0/336	0.46	0/458
15	K	0.48	0/599	0.82	2/809 (0.2%)
16	L	0.31	0/1244	0.48	0/1700
17	O	0.29	0/710	0.49	0/969
18	x	0.37	0/1716	0.59	1/2336 (0.0%)
18	y	0.47	0/1716	0.73	2/2336 (0.1%)
19	z	0.34	0/1802	0.52	0/2450
All	All	0.35	0/31911	0.56	23/43456 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	A	0	1
7	C	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	44	ARG	NE-CZ-NH2	10.05	125.33	120.30
7	C	81	TYR	CB-CG-CD2	-9.85	115.09	121.00
15	K	78	ARG	NE-CZ-NH2	8.36	124.48	120.30
5	A	127	ASP	CB-CG-OD1	8.14	125.63	118.30
8	D	150	ARG	NE-CZ-NH2	8.04	124.32	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	A	578	ARG	Sidechain
7	C	44	ARG	Sidechain

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	1496	0	1471	38	0
2	2	1566	0	1519	32	0
3	3	1666	0	1627	29	0
4	4	1551	0	1508	18	0
5	A	5807	0	5657	54	0
6	B	5854	0	5645	68	0
7	C	616	0	595	7	0
8	D	1128	0	1134	2	0
9	E	517	0	526	3	0
10	F	1208	0	1243	12	0
11	G	708	0	700	2	0
12	H	693	0	690	4	0
13	I	239	0	258	4	0
14	J	327	0	342	11	0
15	K	593	0	614	19	0
16	L	1207	0	1209	9	0
17	O	686	0	677	6	0
18	x	1666	0	1593	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	y	1666	0	1593	0	0
19	z	1759	0	1693	0	0
20	1	93	0	62	7	0
20	2	226	0	150	12	0
20	3	45	0	30	2	0
20	4	169	0	100	5	0
20	x	293	0	212	0	0
20	y	296	0	215	0	0
20	z	295	0	213	0	0
21	1	496	0	354	31	0
21	2	434	0	352	43	0
21	3	498	0	377	35	0
21	4	527	0	412	21	0
21	A	2533	0	2495	134	0
21	B	2284	0	2242	123	0
21	F	149	0	123	9	0
21	G	132	0	97	3	0
21	H	60	0	59	4	0
21	J	51	0	41	1	0
21	K	167	0	116	16	0
21	L	155	0	138	7	0
21	O	141	0	110	3	0
21	x	436	0	403	0	0
21	y	427	0	384	0	0
21	z	438	0	409	0	0
22	1	44	0	56	13	0
22	2	44	0	56	5	0
22	4	44	0	54	6	0
22	x	44	0	56	0	0
22	y	44	0	56	0	0
22	z	44	0	56	0	0
23	1	49	0	74	12	0
23	2	37	0	44	2	0
23	A	79	0	104	8	0
23	B	87	0	120	6	0
23	x	49	0	74	0	0
23	y	49	0	74	0	0
23	z	49	0	74	0	0
24	1	42	0	56	3	0
24	2	84	0	112	11	0
24	3	42	0	56	8	0
24	4	42	0	56	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	x	84	0	112	0	0
24	y	84	0	112	0	0
24	z	84	0	112	0	0
25	3	40	0	56	6	0
25	4	40	0	56	6	0
25	A	240	0	336	27	0
25	B	320	0	448	46	0
25	F	40	0	56	2	0
25	G	40	0	56	4	0
25	I	40	0	56	2	0
25	J	40	0	56	5	0
25	K	80	0	112	10	0
25	L	120	0	168	14	0
25	O	80	0	112	3	0
26	4	72	0	84	0	0
27	A	61	0	68	15	0
28	A	8	0	0	2	0
28	C	16	0	0	5	0
29	A	33	0	46	3	0
29	B	33	0	46	3	0
30	B	66	0	96	5	0
31	x	44	0	56	0	0
31	y	44	0	56	0	0
31	z	44	0	56	0	0
All	All	43924	0	42922	712	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 11.

The worst 5 of 712 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)
4:4:77:PHE:HE2	22:4:617:XAT:H383	1.22	1.05
4:4:77:PHE:CE2	22:4:617:XAT:H383	1.91	1.05
21:A:803:CLA:HBA2	6:B:655:LEU:HB2	1.52	0.90
21:B:814:CLA:H3A	25:B:845:BCR:H393	1.53	0.90
2:2:143:VAL:HG22	21:4:613:CLA:HBA2	1.58	0.85

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	191/241 (79%)	190 (100%)	1 (0%)	0	100	100
2	2	199/257 (77%)	196 (98%)	3 (2%)	0	100	100
3	3	216/273 (79%)	214 (99%)	2 (1%)	0	100	100
4	4	194/251 (77%)	190 (98%)	4 (2%)	0	100	100
5	A	735/750 (98%)	723 (98%)	12 (2%)	0	100	100
6	B	730/734 (100%)	718 (98%)	12 (2%)	0	100	100
7	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
8	D	141/204 (69%)	137 (97%)	4 (3%)	0	100	100
9	E	62/143 (43%)	61 (98%)	1 (2%)	0	100	100
10	F	150/221 (68%)	148 (99%)	2 (1%)	0	100	100
11	G	89/160 (56%)	88 (99%)	1 (1%)	0	100	100
12	H	88/145 (61%)	88 (100%)	0	0	100	100
13	I	29/37 (78%)	29 (100%)	0	0	100	100
14	J	39/44 (89%)	37 (95%)	2 (5%)	0	100	100
15	K	82/130 (63%)	81 (99%)	1 (1%)	0	100	100
16	L	158/219 (72%)	156 (99%)	2 (1%)	0	100	100
17	O	84/140 (60%)	83 (99%)	1 (1%)	0	100	100
18	x	217/267 (81%)	212 (98%)	5 (2%)	0	100	100
18	y	217/267 (81%)	209 (96%)	8 (4%)	0	100	100
19	z	224/265 (84%)	211 (94%)	13 (6%)	0	100	100
All	All	3923/4829 (81%)	3845 (98%)	78 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	153/190 (80%)	149 (97%)	4 (3%)	46	79
2	2	163/205 (80%)	159 (98%)	4 (2%)	47	80
3	3	167/211 (79%)	166 (99%)	1 (1%)	86	96
4	4	163/210 (78%)	161 (99%)	2 (1%)	71	92
5	A	598/610 (98%)	592 (99%)	6 (1%)	76	93
6	B	599/600 (100%)	594 (99%)	5 (1%)	81	94
7	C	70/71 (99%)	69 (99%)	1 (1%)	67	90
8	D	121/170 (71%)	119 (98%)	2 (2%)	60	87
9	E	57/114 (50%)	56 (98%)	1 (2%)	59	86
10	F	125/185 (68%)	121 (97%)	4 (3%)	39	73
11	G	77/133 (58%)	72 (94%)	5 (6%)	17	44
12	H	75/113 (66%)	74 (99%)	1 (1%)	69	91
13	I	27/33 (82%)	27 (100%)	0	100	100
14	J	36/39 (92%)	35 (97%)	1 (3%)	43	77
15	K	61/95 (64%)	61 (100%)	0	100	100
16	L	126/174 (72%)	125 (99%)	1 (1%)	81	94
17	O	72/114 (63%)	69 (96%)	3 (4%)	30	63
18	x	167/201 (83%)	166 (99%)	1 (1%)	86	96
18	y	167/201 (83%)	163 (98%)	4 (2%)	49	81
19	z	179/208 (86%)	176 (98%)	3 (2%)	60	87
All	All	3203/3877 (83%)	3154 (98%)	49 (2%)	66	89

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	F	194	SER
12	H	63	ASP
10	F	210	GLU

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Mol	Chain	Res	Type
11	G	121	SER
16	L	114	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	237	ASN
3	3	252	GLN
18	y	102	GLN

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	$\# Z > 2$
19	TPO	z	3	19	8,10,11	1.07	0	10,14,16	1.92	2 (20%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	TPO	z	3	19	-	2/9/11/13	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	z	3	TPO	P-OG1-CB	-5.31	107.17	123.21
19	z	3	TPO	CG2-CB-CA	-2.07	109.09	113.16

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	z	3	TPO	O-C-CA-CB
19	z	3	TPO	CB-OG1-P-O2P

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](#)

263 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
21	CLA	G	203	11	45,53,73	1.74	6 (13%)	52,89,113	1.65	7 (13%)
21	CLA	B	814	-	65,73,73	1.42	6 (9%)	76,113,113	1.48	9 (11%)
21	CLA	K	201	15	38,45,73	1.90	8 (21%)	43,78,113	1.70	6 (13%)
25	BCR	A	853	-	41,41,41	1.81	8 (19%)	56,56,56	1.78	14 (25%)
21	CLA	3	603	-	45,53,73	1.77	5 (11%)	52,89,113	1.60	7 (13%)
21	CLA	A	841	-	65,73,73	1.42	6 (9%)	76,113,113	1.45	8 (10%)
21	CLA	A	833	-	56,64,73	1.57	7 (12%)	65,102,113	1.51	7 (10%)
21	CLA	x	613	-	59,67,73	1.54	7 (11%)	68,105,113	1.47	8 (11%)
23	LHG	x	619	21	48,48,48	0.28	0	51,54,54	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	B	801	-	41,41,41	1.79	8 (19%)	56,56,56	1.82	14 (25%)
25	BCR	B	848	-	41,41,41	1.72	8 (19%)	56,56,56	1.56	11 (19%)
21	CLA	A	843	-	65,73,73	1.43	6 (9%)	76,113,113	1.43	6 (7%)
21	CLA	2	612	2	65,73,73	1.45	7 (10%)	76,113,113	1.43	7 (9%)
25	BCR	A	850	-	41,41,41	1.82	8 (19%)	56,56,56	1.93	12 (21%)
20	CHL	y	608	-	49,57,74	2.20	15 (30%)	52,93,114	2.70	17 (32%)
20	CHL	4	615	4	40,49,74	2.20	13 (32%)	45,84,114	2.92	18 (40%)
21	CLA	A	842	-	65,73,73	1.44	6 (9%)	76,113,113	1.55	9 (11%)
20	CHL	z	601	19	53,61,74	2.22	16 (30%)	57,98,114	2.69	24 (42%)
21	CLA	1	602	1	54,62,73	1.60	7 (12%)	62,99,113	1.50	8 (12%)
20	CHL	x	601	18	53,61,74	2.24	16 (30%)	57,98,114	2.64	23 (40%)
21	CLA	F	303	10	41,49,73	1.83	5 (12%)	47,84,113	1.65	7 (14%)
21	CLA	H	201	12	60,68,73	1.53	6 (10%)	70,107,113	1.38	6 (8%)
24	LUT	y	615	-	42,43,43	1.65	7 (16%)	51,60,60	2.14	13 (25%)
21	CLA	A	830	-	65,73,73	1.46	7 (10%)	76,113,113	1.58	10 (13%)
21	CLA	B	819	-	55,63,73	1.60	7 (12%)	64,101,113	1.53	9 (14%)
21	CLA	B	815	-	43,51,73	1.73	7 (16%)	49,86,113	1.69	6 (12%)
20	CHL	z	606	-	46,54,74	2.31	16 (34%)	49,90,114	2.76	16 (32%)
22	XAT	z	617	-	39,47,47	1.66	8 (20%)	54,74,74	1.76	12 (22%)
23	LHG	B	852	-	48,48,48	0.27	0	51,54,54	0.34	0
21	CLA	L	302	16	45,53,73	1.79	7 (15%)	52,89,113	1.62	8 (15%)
25	BCR	B	845	-	41,41,41	1.79	8 (19%)	56,56,56	1.89	13 (23%)
21	CLA	z	611	-	45,53,73	1.76	9 (20%)	52,89,113	1.59	6 (11%)
21	CLA	A	820	-	65,73,73	1.45	7 (10%)	76,113,113	1.51	8 (10%)
21	CLA	A	837	5	45,53,73	1.76	6 (13%)	52,89,113	1.62	7 (13%)
21	CLA	y	602	18	65,73,73	1.44	7 (10%)	76,113,113	1.41	7 (9%)
21	CLA	B	809	6	65,73,73	1.44	6 (9%)	76,113,113	1.45	7 (9%)
21	CLA	A	803	-	65,73,73	1.47	8 (12%)	76,113,113	1.36	7 (9%)
24	LUT	3	613	-	42,43,43	1.68	8 (19%)	51,60,60	2.01	14 (27%)
21	CLA	4	604	-	43,51,73	1.89	7 (16%)	54,87,113	1.63	8 (14%)
21	CLA	B	833	-	45,53,73	1.75	6 (13%)	52,89,113	1.72	11 (21%)
20	CHL	2	615	2	43,51,74	2.27	15 (34%)	45,86,114	2.89	19 (42%)
21	CLA	1	604	-	49,57,73	1.69	6 (12%)	55,93,113	1.62	8 (14%)
21	CLA	A	811	-	65,73,73	1.45	6 (9%)	76,113,113	1.41	8 (10%)
30	DGD	B	850	-	67,67,67	0.83	2 (2%)	81,81,81	0.97	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	O	204	-	41,41,41	1.73	8 (19%)	56,56,56	1.53	9 (16%)
21	CLA	3	605	-	41,49,73	1.88	7 (17%)	51,84,113	1.70	9 (17%)
21	CLA	G	202	-	42,50,73	1.81	6 (14%)	48,85,113	1.59	6 (12%)
21	CLA	A	840	-	52,60,73	1.66	7 (13%)	60,97,113	1.50	8 (13%)
21	CLA	4	614	-	50,58,73	1.67	6 (12%)	58,95,113	1.59	8 (13%)
21	CLA	B	805	-	65,73,73	1.48	8 (12%)	76,113,113	1.41	9 (11%)
21	CLA	A	813	-	54,62,73	1.63	8 (14%)	62,99,113	1.51	8 (12%)
21	CLA	2	613	-	43,51,73	1.79	6 (13%)	49,86,113	1.57	7 (14%)
21	CLA	2	610	23	38,45,73	2.90	11 (28%)	41,76,113	1.46	7 (17%)
21	CLA	A	805	21	52,60,73	1.62	6 (11%)	60,97,113	1.57	9 (15%)
21	CLA	4	603	-	44,52,73	1.83	8 (18%)	55,88,113	1.63	9 (16%)
22	XAT	y	617	-	39,47,47	1.73	8 (20%)	54,74,74	2.01	14 (25%)
21	CLA	4	601	4	46,54,73	1.74	7 (15%)	53,90,113	1.54	6 (11%)
21	CLA	3	612	-	39,48,73	1.81	7 (17%)	44,83,113	1.79	7 (15%)
21	CLA	A	810	5	50,58,73	1.68	7 (14%)	58,95,113	1.71	12 (20%)
24	LUT	4	616	-	42,43,43	1.62	8 (19%)	51,60,60	1.57	10 (19%)
21	CLA	A	806	-	65,73,73	1.46	7 (10%)	76,113,113	1.42	8 (10%)
21	CLA	3	610	-	39,48,73	1.90	6 (15%)	44,83,113	1.69	7 (15%)
21	CLA	2	604	-	43,51,73	1.78	9 (20%)	48,86,113	1.61	6 (12%)
21	CLA	B	813	-	65,73,73	1.45	7 (10%)	76,113,113	1.56	9 (11%)
21	CLA	A	844	-	65,73,73	1.50	9 (13%)	76,113,113	1.40	7 (9%)
21	CLA	G	201	-	45,53,73	1.80	5 (11%)	52,89,113	1.60	7 (13%)
25	BCR	B	844	-	41,41,41	1.75	8 (19%)	56,56,56	1.87	13 (23%)
21	CLA	x	603	-	60,68,73	1.50	7 (11%)	70,107,113	1.48	8 (11%)
22	XAT	4	617	-	39,47,47	5.32	25 (64%)	54,74,74	5.60	38 (70%)
21	CLA	2	611	-	44,52,73	1.80	7 (15%)	51,88,113	1.64	8 (15%)
21	CLA	A	839	-	55,63,73	1.56	6 (10%)	64,101,113	1.54	7 (10%)
21	CLA	B	834	-	60,68,73	1.55	6 (10%)	70,107,113	1.43	8 (11%)
20	CHL	2	606	-	43,51,74	2.24	15 (34%)	45,86,114	2.91	18 (40%)
31	NEX	x	618	-	38,46,46	1.60	7 (18%)	50,70,70	1.86	13 (26%)
21	CLA	y	611	-	45,53,73	1.75	6 (13%)	52,89,113	1.61	6 (11%)
21	CLA	B	818	-	60,68,73	1.48	7 (11%)	70,107,113	1.51	9 (12%)
24	LUT	z	615	-	42,43,43	1.69	8 (19%)	51,60,60	1.76	10 (19%)
21	CLA	A	812	21	65,73,73	1.49	6 (9%)	76,113,113	1.36	7 (9%)
21	CLA	B	839	-	65,73,73	1.46	6 (9%)	76,113,113	1.37	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	3	614	-	41,41,41	1.73	8 (19%)	56,56,56	1.58	12 (21%)
21	CLA	A	831	-	65,73,73	1.45	6 (9%)	76,113,113	1.44	6 (7%)
20	CHL	4	606	-	41,49,74	2.21	13 (31%)	51,84,114	2.83	18 (35%)
21	CLA	A	832	-	50,58,73	1.66	6 (12%)	58,95,113	1.59	9 (15%)
21	CLA	z	602	-	65,73,73	1.43	8 (12%)	76,113,113	1.48	9 (11%)
20	CHL	x	605	-	53,61,74	2.05	14 (26%)	57,98,114	2.76	22 (38%)
25	BCR	J	102	-	41,41,41	1.75	8 (19%)	56,56,56	1.76	13 (23%)
21	CLA	z	614	-	65,73,73	1.47	8 (12%)	76,113,113	1.42	7 (9%)
25	BCR	K	205	-	41,41,41	1.73	8 (19%)	56,56,56	2.02	16 (28%)
21	CLA	K	204	-	46,54,73	1.77	7 (15%)	53,90,113	1.58	7 (13%)
21	CLA	1	607	-	43,52,73	1.80	6 (13%)	49,88,113	1.63	6 (12%)
28	SF4	C	102	7	0,12,12	-	-	-	-	-
23	LHG	1	615	21	48,48,48	0.93	2 (4%)	51,54,54	1.04	3 (5%)
20	CHL	2	601	2	47,55,74	2.15	14 (29%)	50,91,114	2.98	22 (44%)
25	BCR	G	204	-	41,41,41	1.72	8 (19%)	56,56,56	1.68	10 (17%)
21	CLA	1	610	23	37,46,73	1.99	8 (21%)	46,81,113	1.71	9 (19%)
23	LHG	z	619	-	48,48,48	0.29	0	51,54,54	0.38	0
25	BCR	O	205	-	41,41,41	1.70	8 (19%)	56,56,56	1.49	9 (16%)
21	CLA	1	608	1	40,48,73	1.87	7 (17%)	50,83,113	1.71	10 (20%)
21	CLA	A	804	-	65,73,73	1.45	7 (10%)	76,113,113	1.52	10 (13%)
22	XAT	x	617	-	39,47,47	1.74	8 (20%)	54,74,74	2.05	14 (25%)
20	CHL	4	607	-	46,54,74	2.24	15 (32%)	49,90,114	2.87	19 (38%)
21	CLA	3	604	-	40,49,73	1.85	7 (17%)	45,84,113	1.61	6 (13%)
21	CLA	A	807	-	65,73,73	1.48	8 (12%)	76,113,113	1.33	8 (10%)
21	CLA	B	840	-	65,73,73	1.47	7 (10%)	76,113,113	1.37	7 (9%)
21	CLA	B	831	-	43,51,73	1.74	5 (11%)	49,86,113	1.69	7 (14%)
21	CLA	A	816	-	42,50,73	1.77	6 (14%)	48,85,113	1.66	6 (12%)
20	CHL	3	606	-	45,53,74	2.24	15 (33%)	52,89,114	2.64	21 (40%)
21	CLA	J	101	-	51,59,73	1.69	5 (9%)	59,96,113	1.50	7 (11%)
21	CLA	A	826	-	65,73,73	1.46	6 (9%)	76,113,113	1.40	6 (7%)
21	CLA	A	827	-	59,67,73	1.53	6 (10%)	68,105,113	1.48	8 (11%)
21	CLA	y	603	-	53,61,73	1.62	8 (15%)	61,98,113	1.51	8 (13%)
21	CLA	B	802	-	65,73,73	1.48	7 (10%)	76,113,113	1.39	9 (11%)
21	CLA	x	612	-	45,53,73	1.74	6 (13%)	52,89,113	1.58	7 (13%)
24	LUT	1	616	-	42,43,43	1.69	7 (16%)	51,60,60	2.07	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	A	818	-	60,68,73	1.51	7 (11%)	70,107,113	5.15	10 (14%)
21	CLA	B	821	-	47,55,73	1.70	6 (12%)	54,91,113	1.70	10 (18%)
20	CHL	z	609	-	53,61,74	2.31	16 (30%)	57,98,114	2.70	21 (36%)
24	LUT	x	616	-	42,43,43	1.65	8 (19%)	51,60,60	1.84	11 (21%)
29	PQN	A	855	-	34,34,34	0.40	0	42,45,45	0.42	0
25	BCR	4	618	-	41,41,41	1.72	8 (19%)	56,56,56	1.69	11 (19%)
21	CLA	1	611	-	45,53,73	1.79	6 (13%)	52,89,113	1.53	6 (11%)
21	CLA	B	838	-	47,55,73	1.75	7 (14%)	54,91,113	1.58	8 (14%)
21	CLA	A	828	-	65,73,73	1.45	6 (9%)	76,113,113	1.43	8 (10%)
21	CLA	1	609	-	42,50,73	1.74	9 (21%)	48,85,113	1.98	9 (18%)
21	CLA	B	803	-	65,73,73	1.46	8 (12%)	76,113,113	1.44	8 (10%)
23	LHG	2	618	21	36,36,48	0.32	0	39,42,54	0.50	0
21	CLA	L	304	-	45,53,73	1.79	6 (13%)	52,89,113	1.55	7 (13%)
21	CLA	A	836	-	45,53,73	1.77	6 (13%)	52,89,113	1.62	7 (13%)
21	CLA	B	837	-	65,73,73	1.45	5 (7%)	76,113,113	1.47	9 (11%)
21	CLA	B	841	23	65,73,73	1.46	6 (9%)	76,113,113	1.40	8 (10%)
21	CLA	B	826	-	62,70,73	1.49	7 (11%)	72,109,113	1.45	7 (9%)
21	CLA	B	810	-	65,73,73	1.46	6 (9%)	76,113,113	1.40	10 (13%)
25	BCR	B	846	-	41,41,41	1.76	8 (19%)	56,56,56	1.73	11 (19%)
21	CLA	3	601	-	60,68,73	1.49	7 (11%)	70,107,113	1.48	7 (10%)
21	CLA	B	811	-	54,62,73	1.64	7 (12%)	67,100,113	1.58	8 (11%)
21	CLA	A	823	-	42,50,73	1.77	5 (11%)	48,85,113	1.67	7 (14%)
21	CLA	y	612	-	45,53,73	1.76	7 (15%)	52,89,113	1.57	6 (11%)
20	CHL	2	607	-	51,59,74	2.10	14 (27%)	55,96,114	2.77	22 (40%)
23	LHG	A	847	21	29,29,48	0.35	0	32,35,54	0.49	0
28	SF4	C	101	7	0,12,12	-	-	-	-	-
25	BCR	L	306	-	41,41,41	1.77	8 (19%)	56,56,56	2.04	16 (28%)
21	CLA	z	610	-	45,53,73	1.74	7 (15%)	52,89,113	1.63	8 (15%)
31	NEX	z	618	-	38,46,46	1.63	7 (18%)	50,70,70	1.60	9 (18%)
21	CLA	A	802	-	65,73,73	1.44	8 (12%)	76,113,113	1.52	9 (11%)
21	CLA	3	611	-	37,44,73	1.95	7 (18%)	42,77,113	1.65	8 (19%)
21	CLA	3	602	-	55,63,73	1.61	6 (10%)	64,101,113	1.44	7 (10%)
21	CLA	B	823	-	45,53,73	1.78	7 (15%)	52,89,113	1.53	7 (13%)
24	LUT	2	616	-	42,43,43	1.65	8 (19%)	51,60,60	2.13	13 (25%)
20	CHL	z	605	-	42,50,74	2.38	15 (35%)	44,85,114	2.98	21 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	F	302	-	51,59,73	1.67	7 (13%)	59,96,113	1.60	8 (13%)
24	LUT	y	616	-	42,43,43	1.66	8 (19%)	51,60,60	1.72	11 (21%)
25	BCR	I	101	-	41,41,41	1.72	8 (19%)	56,56,56	1.52	9 (16%)
21	CLA	B	830	-	43,51,73	1.77	6 (13%)	49,86,113	1.62	7 (14%)
20	CHL	y	601	18	53,61,74	2.24	16 (30%)	57,98,114	2.69	23 (40%)
21	CLA	B	804	-	41,49,73	1.79	6 (14%)	47,84,113	1.76	9 (19%)
20	CHL	x	609	18	46,54,74	2.25	16 (34%)	49,90,114	2.84	20 (40%)
20	CHL	z	608	-	49,57,74	2.14	15 (30%)	52,93,114	2.82	21 (40%)
21	CLA	A	822	-	65,73,73	1.46	6 (9%)	76,113,113	1.41	7 (9%)
28	SF4	A	854	6,5	0,12,12	-	-	-	-	-
25	BCR	B	847	-	41,41,41	1.73	8 (19%)	56,56,56	1.55	10 (17%)
20	CHL	x	608	18	42,50,74	2.34	15 (35%)	44,85,114	3.00	21 (47%)
20	CHL	y	605	18	42,50,74	2.39	15 (35%)	44,85,114	2.94	20 (45%)
21	CLA	2	608	-	45,53,73	1.74	7 (15%)	52,89,113	1.59	7 (13%)
22	XAT	2	617	-	39,47,47	1.79	8 (20%)	54,74,74	2.18	16 (29%)
20	CHL	y	606	-	46,54,74	2.28	14 (30%)	49,90,114	2.90	20 (40%)
21	CLA	B	808	-	65,73,73	1.44	9 (13%)	76,113,113	1.46	9 (11%)
26	LMG	4	619	-	39,39,55	0.23	0	47,47,63	0.24	0
21	CLA	B	835	-	42,50,73	1.83	6 (14%)	48,85,113	1.59	7 (14%)
21	CLA	3	607	-	45,53,73	1.80	7 (15%)	52,89,113	1.60	7 (13%)
21	CLA	1	603	-	54,62,73	1.59	7 (12%)	62,99,113	1.49	7 (11%)
21	CLA	A	825	-	55,63,73	1.59	6 (10%)	64,101,113	1.45	9 (14%)
21	CLA	B	829	-	56,64,73	1.57	7 (12%)	65,102,113	1.54	8 (12%)
21	CLA	z	603	-	57,65,73	1.54	7 (12%)	66,103,113	1.51	7 (10%)
21	CLA	B	836	-	50,58,73	1.68	7 (14%)	58,95,113	3.66	12 (20%)
21	CLA	A	819	-	59,67,73	1.56	7 (11%)	68,105,113	1.43	8 (11%)
20	CHL	4	605	-	40,49,74	2.31	13 (32%)	42,84,114	2.87	18 (42%)
21	CLA	A	809	5	65,73,73	1.41	6 (9%)	76,113,113	1.48	8 (10%)
23	LHG	A	846	-	48,48,48	0.28	0	51,54,54	0.35	0
24	LUT	z	616	-	42,43,43	1.66	8 (19%)	51,60,60	1.80	11 (21%)
21	CLA	x	604	-	52,60,73	1.64	6 (11%)	60,97,113	1.59	8 (13%)
25	BCR	A	848	-	41,41,41	1.75	8 (19%)	56,56,56	1.69	12 (21%)
29	PQN	B	842	-	34,34,34	0.42	0	42,45,45	0.42	0
21	CLA	x	614	-	45,53,73	1.76	6 (13%)	52,89,113	1.62	7 (13%)
25	BCR	B	843	-	41,41,41	1.74	8 (19%)	56,56,56	2.05	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CHL	1	606	-	40,49,74	2.49	16 (40%)	41,84,114	2.86	19 (46%)
21	CLA	3	608	-	41,49,73	1.78	7 (17%)	47,84,113	1.88	10 (21%)
21	CLA	O	202	-	36,46,73	1.91	7 (19%)	41,80,113	1.72	8 (19%)
21	CLA	4	611	-	40,49,73	1.85	7 (17%)	45,84,113	1.62	6 (13%)
25	BCR	B	849	-	41,41,41	1.76	8 (19%)	56,56,56	1.92	13 (23%)
20	CHL	y	609	18	53,61,74	2.31	16 (30%)	57,98,114	2.72	23 (40%)
21	CLA	4	609	4	54,62,73	1.60	9 (16%)	62,99,113	1.47	10 (16%)
21	CLA	L	303	-	65,73,73	1.45	6 (9%)	76,113,113	1.47	9 (11%)
21	CLA	1	612	-	46,54,73	1.76	7 (15%)	53,90,113	1.70	8 (15%)
25	BCR	A	851	-	41,41,41	1.85	9 (21%)	56,56,56	2.71	20 (35%)
21	CLA	z	612	-	45,53,73	1.77	8 (17%)	52,89,113	1.55	7 (13%)
21	CLA	B	820	-	50,58,73	1.65	7 (14%)	58,95,113	1.61	10 (17%)
21	CLA	B	816	-	55,63,73	1.58	6 (10%)	64,101,113	1.56	9 (14%)
21	CLA	B	825	-	62,70,73	1.48	6 (9%)	72,109,113	1.52	9 (12%)
21	CLA	B	827	-	65,73,73	1.46	7 (10%)	76,113,113	1.40	8 (10%)
21	CLA	K	203	-	45,53,73	1.74	6 (13%)	52,89,113	1.75	10 (19%)
21	CLA	A	835	-	65,73,73	1.46	8 (12%)	76,113,113	1.48	9 (11%)
25	BCR	L	301	-	41,41,41	1.77	8 (19%)	56,56,56	2.30	12 (21%)
21	CLA	4	602	4	60,68,73	1.49	7 (11%)	70,107,113	1.47	8 (11%)
21	CLA	x	610	-	65,73,73	1.43	7 (10%)	76,113,113	1.37	6 (7%)
21	CLA	z	613	19	65,73,73	1.43	7 (10%)	76,113,113	1.46	7 (9%)
27	CL0	A	801	-	62,69,73	1.88	14 (22%)	72,107,113	4.08	30 (41%)
21	CLA	B	828	-	65,73,73	1.46	6 (9%)	76,113,113	1.36	7 (9%)
21	CLA	2	602	2	65,73,73	1.46	7 (10%)	76,113,113	1.40	7 (9%)
25	BCR	L	305	-	41,41,41	1.77	8 (19%)	56,56,56	1.79	15 (26%)
21	CLA	z	604	-	51,59,73	1.64	6 (11%)	59,96,113	1.60	7 (11%)
20	CHL	1	601	1	51,60,74	2.17	16 (31%)	54,97,114	2.66	22 (40%)
21	CLA	A	845	23	50,58,73	1.69	7 (14%)	58,95,113	1.61	9 (15%)
23	LHG	y	619	-	48,48,48	0.29	0	51,54,54	0.35	0
21	CLA	4	608	4	45,53,73	1.77	6 (13%)	52,89,113	1.59	6 (11%)
22	XAT	1	614	-	39,47,47	0.82	1 (2%)	54,74,74	3.18	19 (35%)
21	CLA	A	815	-	45,53,73	1.73	6 (13%)	52,89,113	1.69	8 (15%)
21	CLA	2	609	-	47,55,73	1.68	7 (14%)	54,91,113	1.61	7 (12%)
21	CLA	B	807	-	52,60,73	1.62	6 (11%)	60,97,113	1.57	8 (13%)
21	CLA	A	817	-	45,53,73	1.80	6 (13%)	52,89,113	1.57	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	A	824	-	41,49,73	1.82	7 (17%)	47,84,113	1.69	10 (21%)
21	CLA	y	614	-	65,73,73	1.49	7 (10%)	76,113,113	1.45	7 (9%)
21	CLA	F	301	-	57,65,73	1.60	6 (10%)	66,103,113	1.41	8 (12%)
21	CLA	B	822	-	65,73,73	1.51	7 (10%)	76,113,113	1.53	9 (11%)
21	CLA	A	814	-	65,73,73	1.49	8 (12%)	76,113,113	1.35	7 (9%)
21	CLA	x	611	23	45,53,73	1.74	6 (13%)	52,89,113	1.60	8 (15%)
20	CHL	y	607	-	53,61,74	2.10	14 (26%)	57,98,114	2.71	23 (40%)
21	CLA	A	834	-	65,73,73	1.47	6 (9%)	76,113,113	1.38	8 (10%)
21	CLA	2	603	-	43,52,73	1.81	10 (23%)	49,88,113	1.59	7 (14%)
21	CLA	B	812	-	43,51,73	1.80	7 (16%)	49,86,113	1.59	6 (12%)
21	CLA	4	613	-	45,53,73	1.76	8 (17%)	52,89,113	1.82	8 (15%)
21	CLA	A	829	-	65,73,73	1.47	6 (9%)	76,113,113	1.36	7 (9%)
21	CLA	B	817	-	59,67,73	1.53	6 (10%)	68,105,113	1.46	7 (10%)
21	CLA	B	824	-	65,73,73	1.46	5 (7%)	76,113,113	1.46	7 (9%)
21	CLA	B	832	-	65,73,73	1.48	8 (12%)	76,113,113	1.34	6 (7%)
21	CLA	A	808	-	50,58,73	1.67	6 (12%)	58,95,113	1.53	9 (15%)
21	CLA	1	613	-	37,46,73	1.98	7 (18%)	46,81,113	1.76	10 (21%)
26	LMG	4	620	-	33,33,55	0.26	0	41,41,63	0.59	1 (2%)
21	CLA	1	605	-	46,54,73	1.75	7 (15%)	53,90,113	1.58	6 (11%)
20	CHL	2	605	-	42,50,74	2.24	13 (30%)	45,85,114	2.92	19 (42%)
20	CHL	x	606	-	46,54,74	2.20	14 (30%)	49,90,114	2.87	17 (34%)
23	LHG	B	851	21	37,37,48	0.31	0	40,43,54	0.51	0
24	LUT	x	615	-	42,43,43	1.64	8 (19%)	51,60,60	1.58	11 (21%)
21	CLA	O	201	-	65,73,73	1.49	6 (9%)	76,113,113	1.34	7 (9%)
21	CLA	O	203	-	37,46,73	1.96	7 (18%)	46,81,113	1.75	10 (21%)
25	BCR	A	849	-	41,41,41	1.76	8 (19%)	56,56,56	2.00	13 (23%)
31	NEX	y	618	-	38,46,46	1.60	7 (18%)	50,70,70	1.64	9 (18%)
25	BCR	K	202	-	41,41,41	1.74	8 (19%)	56,56,56	2.07	15 (26%)
21	CLA	x	602	-	65,73,73	1.43	7 (10%)	76,113,113	1.47	8 (10%)
21	CLA	y	610	18	58,66,73	1.55	6 (10%)	67,104,113	1.48	7 (10%)
21	CLA	y	613	-	45,53,73	1.76	6 (13%)	52,89,113	1.63	7 (13%)
20	CHL	z	607	-	52,60,74	2.10	14 (26%)	56,97,114	2.85	22 (39%)
20	CHL	x	607	-	53,61,74	2.19	15 (28%)	57,98,114	2.68	23 (40%)
25	BCR	A	852	-	41,41,41	1.75	9 (21%)	56,56,56	1.94	14 (25%)
25	BCR	F	304	-	41,41,41	1.87	8 (19%)	56,56,56	2.16	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	y	604	-	51,59,73	1.61	6 (11%)	59,96,113	1.62	9 (15%)
21	CLA	4	612	-	57,65,73	1.55	7 (12%)	66,103,113	1.54	8 (12%)
21	CLA	A	821	-	45,53,73	1.79	6 (13%)	52,89,113	1.59	6 (11%)
21	CLA	K	206	15	37,47,73	1.92	6 (16%)	42,81,113	1.68	8 (19%)
21	CLA	4	610	-	42,50,73	1.80	7 (16%)	48,85,113	1.56	6 (12%)
24	LUT	2	619	-	42,43,43	1.67	8 (19%)	51,60,60	1.93	12 (23%)
21	CLA	3	609	-	53,62,73	1.63	7 (13%)	61,100,113	1.47	8 (13%)
21	CLA	A	838	-	51,59,73	1.65	7 (13%)	59,96,113	1.50	7 (11%)
21	CLA	B	806	6	65,73,73	1.43	6 (9%)	76,113,113	1.39	10 (13%)

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
21	CLA	G	203	11	1/1/11/20	3/13/91/115	-
21	CLA	B	814	-	1/1/15/20	17/37/115/115	-
21	CLA	K	201	15	1/1/8/20	0/2/76/115	-
25	BCR	A	853	-	-	5/29/63/63	0/2/2/2
21	CLA	3	603	-	1/1/11/20	7/13/91/115	-
21	CLA	A	841	-	1/1/15/20	17/37/115/115	-
21	CLA	A	833	-	1/1/13/20	5/27/105/115	-
21	CLA	x	613	-	1/1/13/20	13/30/108/115	-
23	LHG	x	619	21	-	7/53/53/53	-
25	BCR	B	801	-	-	6/29/63/63	0/2/2/2
25	BCR	B	848	-	-	2/29/63/63	0/2/2/2
21	CLA	A	843	-	1/1/15/20	13/37/115/115	-
21	CLA	2	612	2	1/1/15/20	21/37/115/115	-
25	BCR	A	850	-	-	4/29/63/63	0/2/2/2
20	CHL	y	608	-	3/3/16/26	8/19/117/137	-
20	CHL	4	615	4	3/3/15/26	1/10/106/137	-
21	CLA	A	842	-	1/1/15/20	12/37/115/115	-
20	CHL	z	601	19	3/3/17/26	8/24/122/137	-
21	CLA	1	602	1	1/1/12/20	7/24/102/115	-
20	CHL	x	601	18	3/3/17/26	11/24/122/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	F	303	10	1/1/10/20	2/8/86/115	-
21	CLA	H	201	12	1/1/14/20	14/31/109/115	-
24	LUT	y	615	-	-	5/29/67/67	0/2/2/2
21	CLA	A	830	-	1/1/15/20	14/37/115/115	-
21	CLA	B	819	-	1/1/13/20	5/25/103/115	-
21	CLA	B	815	-	1/1/10/20	2/11/89/115	-
20	CHL	z	606	-	3/3/16/26	4/15/113/137	-
22	XAT	z	617	-	-	0/31/93/93	0/4/4/4
23	LHG	B	852	-	-	17/53/53/53	-
21	CLA	L	302	16	1/1/11/20	1/13/91/115	-
25	BCR	B	845	-	-	9/29/63/63	0/2/2/2
21	CLA	z	611	-	1/1/11/20	0/13/91/115	-
21	CLA	A	820	-	1/1/15/20	16/37/115/115	-
21	CLA	A	837	5	1/1/11/20	2/13/91/115	-
21	CLA	y	602	18	1/1/15/20	21/37/115/115	-
21	CLA	B	809	6	1/1/15/20	15/37/115/115	-
21	CLA	A	803	-	1/1/15/20	18/37/115/115	-
24	LUT	3	613	-	-	7/29/67/67	0/2/2/2
21	CLA	4	604	-	1/1/11/20	6/11/87/115	-
21	CLA	B	833	-	1/1/11/20	4/13/91/115	-
20	CHL	2	615	2	3/3/15/26	2/12/110/137	-
21	CLA	1	604	-	1/1/11/20	8/18/96/115	-
21	CLA	A	811	-	1/1/15/20	13/37/115/115	-
30	DGD	B	850	-	-	14/55/95/95	0/2/2/2
25	BCR	O	204	-	-	2/29/63/63	0/2/2/2
21	CLA	3	605	-	1/1/10/20	6/10/86/115	-
21	CLA	G	202	-	1/1/10/20	2/10/88/115	-
21	CLA	A	840	-	1/1/12/20	5/22/100/115	-
21	CLA	4	614	-	1/1/12/20	7/19/97/115	-
21	CLA	B	805	-	1/1/15/20	13/37/115/115	-
21	CLA	A	813	-	1/1/12/20	9/24/102/115	-
21	CLA	2	613	-	1/1/10/20	4/11/89/115	-
21	CLA	2	610	23	1/1/7/20	2/10/70/115	-
21	CLA	A	805	21	1/1/12/20	7/22/100/115	-
21	CLA	4	603	-	1/1/11/20	4/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	XAT	y	617	-	-	4/31/93/93	0/4/4/4
21	CLA	4	601	4	1/1/11/20	5/15/93/115	-
21	CLA	3	612	-	1/1/10/20	1/6/84/115	-
21	CLA	A	810	5	1/1/12/20	4/19/97/115	-
24	LUT	4	616	-	-	2/29/67/67	0/2/2/2
21	CLA	A	806	-	1/1/15/20	14/37/115/115	-
21	CLA	3	610	-	1/1/10/20	0/6/84/115	-
21	CLA	2	604	-	1/1/10/20	6/9/88/115	-
21	CLA	B	813	-	1/1/15/20	12/37/115/115	-
21	CLA	A	844	-	1/1/15/20	9/37/115/115	-
21	CLA	G	201	-	1/1/11/20	7/13/91/115	-
25	BCR	B	844	-	-	12/29/63/63	0/2/2/2
21	CLA	x	603	-	1/1/14/20	10/31/109/115	-
22	XAT	4	617	-	-	1/31/93/93	0/4/4/4
21	CLA	2	611	-	1/1/11/20	6/11/89/115	-
21	CLA	A	839	-	1/1/13/20	7/25/103/115	-
21	CLA	B	834	-	1/1/14/20	7/31/109/115	-
20	CHL	2	606	-	3/3/15/26	2/12/110/137	-
31	NEX	x	618	-	-	8/27/83/83	0/3/3/3
21	CLA	y	611	-	1/1/11/20	7/13/91/115	-
21	CLA	B	818	-	1/1/14/20	11/31/109/115	-
24	LUT	z	615	-	-	4/29/67/67	0/2/2/2
21	CLA	A	812	21	1/1/15/20	20/37/115/115	-
21	CLA	B	839	-	1/1/15/20	8/37/115/115	-
25	BCR	3	614	-	-	5/29/63/63	0/2/2/2
21	CLA	A	831	-	1/1/15/20	8/37/115/115	-
20	CHL	4	606	-	3/3/15/26	2/10/106/137	-
21	CLA	A	832	-	1/1/12/20	4/19/97/115	-
21	CLA	z	602	-	1/1/15/20	13/37/115/115	-
20	CHL	x	605	-	3/3/17/26	13/24/122/137	-
25	BCR	J	102	-	-	2/29/63/63	0/2/2/2
21	CLA	z	614	-	1/1/15/20	11/37/115/115	-
25	BCR	K	205	-	-	8/29/63/63	0/2/2/2
21	CLA	K	204	-	1/1/11/20	8/15/93/115	-
21	CLA	1	607	-	1/1/11/20	7/11/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	SF4	C	102	7	-	-	0/6/5/5
23	LHG	1	615	21	-	30/53/53/53	-
20	CHL	2	601	2	3/3/16/26	6/17/115/137	-
25	BCR	G	204	-	-	4/29/63/63	0/2/2/2
21	CLA	1	610	23	1/1/10/20	0/4/80/115	-
23	LHG	z	619	-	-	10/53/53/53	-
25	BCR	O	205	-	-	0/29/63/63	0/2/2/2
21	CLA	1	608	1	1/1/10/20	3/8/84/115	-
21	CLA	A	804	-	1/1/15/20	18/37/115/115	-
22	XAT	x	617	-	-	8/31/93/93	0/4/4/4
20	CHL	4	607	-	3/3/16/26	5/15/113/137	-
21	CLA	3	604	-	1/1/10/20	0/8/86/115	-
21	CLA	A	807	-	1/1/15/20	13/37/115/115	-
21	CLA	B	840	-	1/1/15/20	13/37/115/115	-
21	CLA	B	831	-	1/1/10/20	2/11/89/115	-
21	CLA	A	816	-	1/1/10/20	2/10/88/115	-
20	CHL	3	606	-	3/3/16/26	5/13/111/137	-
21	CLA	J	101	-	1/1/12/20	6/21/99/115	-
21	CLA	A	826	-	1/1/15/20	10/37/115/115	-
21	CLA	A	827	-	1/1/13/20	5/30/108/115	-
21	CLA	y	603	-	1/1/12/20	5/23/101/115	-
21	CLA	B	802	-	1/1/15/20	16/37/115/115	-
21	CLA	x	612	-	1/1/11/20	6/13/91/115	-
24	LUT	1	616	-	-	2/29/67/67	0/2/2/2
21	CLA	A	818	-	1/1/14/20	14/31/109/115	-
21	CLA	B	821	-	1/1/11/20	3/16/94/115	-
20	CHL	z	609	-	3/3/17/26	13/24/122/137	-
24	LUT	x	616	-	-	2/29/67/67	0/2/2/2
29	PQN	A	855	-	-	1/23/43/43	0/2/2/2
25	BCR	4	618	-	-	8/29/63/63	0/2/2/2
21	CLA	1	611	-	1/1/11/20	4/13/91/115	-
21	CLA	B	838	-	1/1/11/20	1/16/94/115	-
21	CLA	A	828	-	1/1/15/20	12/37/115/115	-
21	CLA	1	609	-	1/1/10/20	5/9/87/115	-
21	CLA	B	803	-	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LHG	2	618	21	-	10/41/41/53	-
21	CLA	L	304	-	1/1/11/20	1/13/91/115	-
21	CLA	A	836	-	1/1/11/20	4/13/91/115	-
21	CLA	B	837	-	1/1/15/20	9/37/115/115	-
21	CLA	B	841	23	1/1/15/20	23/37/115/115	-
21	CLA	B	826	-	1/1/14/20	7/34/112/115	-
21	CLA	B	810	-	1/1/15/20	14/37/115/115	-
25	BCR	B	846	-	-	8/29/63/63	0/2/2/2
21	CLA	3	601	-	1/1/14/20	17/31/109/115	-
21	CLA	B	811	-	1/1/13/20	10/25/101/115	-
21	CLA	A	823	-	1/1/10/20	5/10/88/115	-
21	CLA	y	612	-	1/1/11/20	6/13/91/115	-
20	CHL	2	607	-	3/3/17/26	7/21/119/137	-
23	LHG	A	847	21	-	3/34/34/53	-
28	SF4	C	101	7	-	-	0/6/5/5
25	BCR	L	306	-	-	5/29/63/63	0/2/2/2
21	CLA	z	610	-	1/1/11/20	5/13/91/115	-
31	NEX	z	618	-	-	2/27/83/83	0/3/3/3
21	CLA	A	802	-	1/1/15/20	19/37/115/115	-
21	CLA	3	611	-	1/1/8/20	0/0/74/115	-
21	CLA	3	602	-	1/1/13/20	11/25/103/115	-
21	CLA	B	823	-	1/1/11/20	5/13/91/115	-
24	LUT	2	616	-	-	7/29/67/67	0/2/2/2
20	CHL	z	605	-	3/3/15/26	4/10/108/137	-
21	CLA	F	302	-	1/1/12/20	6/21/99/115	-
24	LUT	y	616	-	-	6/29/67/67	0/2/2/2
25	BCR	I	101	-	-	0/29/63/63	0/2/2/2
21	CLA	B	830	-	1/1/10/20	2/11/89/115	-
20	CHL	y	601	18	3/3/17/26	10/24/122/137	-
21	CLA	B	804	-	1/1/10/20	2/8/86/115	-
20	CHL	x	609	18	3/3/16/26	5/15/113/137	-
20	CHL	z	608	-	3/3/16/26	4/19/117/137	-
21	CLA	A	822	-	1/1/15/20	11/37/115/115	-
28	SF4	A	854	6,5	-	-	0/6/5/5
25	BCR	B	847	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CHL	x	608	18	3/3/15/26	3/10/108/137	-
20	CHL	y	605	18	3/3/15/26	2/10/108/137	-
21	CLA	2	608	-	1/1/11/20	7/13/91/115	-
22	XAT	2	617	-	-	15/31/93/93	0/4/4/4
20	CHL	y	606	-	3/3/16/26	2/15/113/137	-
21	CLA	B	808	-	1/1/15/20	15/37/115/115	-
26	LMG	4	619	-	-	6/34/54/70	0/1/1/1
21	CLA	B	835	-	1/1/10/20	4/10/88/115	-
21	CLA	3	607	-	1/1/11/20	4/13/91/115	-
21	CLA	1	603	-	1/1/12/20	8/24/102/115	-
21	CLA	A	825	-	1/1/13/20	12/25/103/115	-
21	CLA	B	829	-	1/1/13/20	7/27/105/115	-
21	CLA	z	603	-	1/1/13/20	8/28/106/115	-
21	CLA	B	836	-	1/1/12/20	5/19/97/115	-
21	CLA	A	819	-	1/1/13/20	15/30/108/115	-
20	CHL	4	605	-	3/3/15/26	2/8/106/137	-
21	CLA	A	809	5	1/1/15/20	9/37/115/115	-
23	LHG	A	846	-	-	4/53/53/53	-
24	LUT	z	616	-	-	3/29/67/67	0/2/2/2
21	CLA	x	604	-	1/1/12/20	8/22/100/115	-
25	BCR	A	848	-	-	2/29/63/63	0/2/2/2
29	PQN	B	842	-	-	6/23/43/43	0/2/2/2
21	CLA	x	614	-	1/1/11/20	7/13/91/115	-
25	BCR	B	843	-	-	1/29/63/63	0/2/2/2
20	CHL	1	606	-	3/3/15/26	0/8/106/137	-
21	CLA	3	608	-	1/1/10/20	3/8/86/115	-
21	CLA	O	202	-	1/1/9/20	0/4/78/115	-
21	CLA	4	611	-	1/1/10/20	2/8/86/115	-
25	BCR	B	849	-	-	7/29/63/63	0/2/2/2
20	CHL	y	609	18	3/3/17/26	16/24/122/137	-
21	CLA	4	609	4	1/1/12/20	4/24/102/115	-
21	CLA	L	303	-	1/1/15/20	10/37/115/115	-
21	CLA	1	612	-	1/1/11/20	5/15/93/115	-
25	BCR	A	851	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	z	612	-	1/1/11/20	2/13/91/115	-
21	CLA	B	820	-	1/1/12/20	7/19/97/115	-
21	CLA	B	816	-	1/1/13/20	6/25/103/115	-
21	CLA	B	825	-	1/1/14/20	13/34/112/115	-
21	CLA	B	827	-	1/1/15/20	16/37/115/115	-
21	CLA	K	203	-	1/1/11/20	7/13/91/115	-
21	CLA	A	835	-	1/1/15/20	20/37/115/115	-
25	BCR	L	301	-	-	3/29/63/63	0/2/2/2
21	CLA	4	602	4	1/1/14/20	6/31/109/115	-
21	CLA	x	610	-	1/1/15/20	17/37/115/115	-
21	CLA	z	613	19	1/1/15/20	15/37/115/115	-
27	CL0	A	801	-	2/2/18/25	14/31/125/135	-
21	CLA	B	828	-	1/1/15/20	15/37/115/115	-
21	CLA	2	602	2	1/1/15/20	16/37/115/115	-
25	BCR	L	305	-	-	2/29/63/63	0/2/2/2
21	CLA	z	604	-	1/1/12/20	11/21/99/115	-
20	CHL	1	601	1	3/3/17/26	7/22/120/137	-
21	CLA	A	845	23	1/1/12/20	8/19/97/115	-
23	LHG	y	619	-	-	11/53/53/53	-
21	CLA	4	608	4	1/1/11/20	4/13/91/115	-
22	XAT	1	614	-	-	9/31/93/93	0/4/4/4
21	CLA	A	815	-	1/1/11/20	8/13/91/115	-
21	CLA	2	609	-	1/1/11/20	9/16/94/115	-
21	CLA	B	807	-	1/1/12/20	4/22/100/115	-
21	CLA	A	817	-	1/1/11/20	2/13/91/115	-
21	CLA	A	824	-	1/1/10/20	2/8/86/115	-
21	CLA	y	614	-	1/1/15/20	18/37/115/115	-
21	CLA	F	301	-	1/1/13/20	13/28/106/115	-
21	CLA	B	822	-	1/1/15/20	23/37/115/115	-
21	CLA	A	814	-	1/1/15/20	14/37/115/115	-
21	CLA	x	611	23	1/1/11/20	2/13/91/115	-
20	CHL	y	607	-	3/3/17/26	12/24/122/137	-
21	CLA	A	834	-	1/1/15/20	7/37/115/115	-
21	CLA	2	603	-	1/1/11/20	3/11/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	812	-	1/1/10/20	0/11/89/115	-
21	CLA	4	613	-	1/1/11/20	5/13/91/115	-
21	CLA	A	829	-	1/1/15/20	15/37/115/115	-
21	CLA	B	817	-	1/1/13/20	11/30/108/115	-
21	CLA	B	824	-	1/1/15/20	12/37/115/115	-
21	CLA	B	832	-	1/1/15/20	16/37/115/115	-
21	CLA	A	808	-	1/1/12/20	1/19/97/115	-
21	CLA	1	613	-	1/1/10/20	0/4/80/115	-
26	LMG	4	620	-	-	8/28/48/70	0/1/1/1
21	CLA	1	605	-	1/1/11/20	8/15/93/115	-
20	CHL	2	605	-	3/3/15/26	2/10/108/137	-
20	CHL	x	606	-	3/3/16/26	6/15/113/137	-
23	LHG	B	851	21	-	5/42/42/53	-
24	LUT	x	615	-	-	0/29/67/67	0/2/2/2
21	CLA	O	201	-	1/1/15/20	15/37/115/115	-
21	CLA	O	203	-	1/1/10/20	0/4/80/115	-
25	BCR	A	849	-	-	6/29/63/63	0/2/2/2
31	NEX	y	618	-	-	2/27/83/83	0/3/3/3
25	BCR	K	202	-	-	2/29/63/63	0/2/2/2
21	CLA	x	602	-	1/1/15/20	13/37/115/115	-
21	CLA	y	610	18	1/1/13/20	13/29/107/115	-
21	CLA	y	613	-	1/1/11/20	5/13/91/115	-
20	CHL	z	607	-	3/3/17/26	7/23/121/137	-
20	CHL	x	607	-	3/3/17/26	11/24/122/137	-
25	BCR	A	852	-	-	13/29/63/63	0/2/2/2
25	BCR	F	304	-	-	13/29/63/63	0/2/2/2
21	CLA	y	604	-	1/1/12/20	9/21/99/115	-
21	CLA	4	612	-	1/1/13/20	12/28/106/115	-
21	CLA	A	821	-	1/1/11/20	4/13/91/115	-
21	CLA	K	206	15	1/1/9/20	0/6/80/115	-
21	CLA	4	610	-	1/1/10/20	4/10/88/115	-
24	LUT	2	619	-	-	4/29/67/67	0/2/2/2
21	CLA	3	609	-	1/1/13/20	5/23/101/115	-
21	CLA	A	838	-	1/1/12/20	8/21/99/115	-
21	CLA	B	806	6	1/1/15/20	15/37/115/115	-

The worst 5 of 1974 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	617	XAT	O4-C5	-12.41	1.28	1.46
21	2	610	CLA	C1A-NA	12.18	1.40	1.29
22	4	617	XAT	O24-C25	-10.96	1.30	1.46
22	4	617	XAT	C4-C3	-9.80	1.38	1.52
22	4	617	XAT	C2-C3	-8.85	1.39	1.52

The worst 5 of 2575 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	818	CLA	O2D-CGD-CBD	25.89	157.28	111.27
21	A	818	CLA	O2D-CGD-O1D	-25.26	74.45	123.84
22	4	617	XAT	O24-C25-C24	23.78	131.25	113.38
21	A	818	CLA	O1D-CGD-CBD	-20.36	82.83	124.48
27	A	801	CL0	C1D-ND-C4D	-17.19	94.13	106.33

5 of 260 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	1	601	CHL	ND
20	1	601	CHL	NA
20	1	601	CHL	NC
20	1	606	CHL	ND
20	1	606	CHL	NA

5 of 1936 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	2	605	CHL	C3C-C2C-CMC-OMC
20	2	607	CHL	C1A-C2A-CAA-CBA
20	2	607	CHL	CBD-CGD-O2D-CED
20	3	606	CHL	C2A-CAA-CBA-CGA
20	3	606	CHL	CHA-CBD-CGD-O1D

There are no ring outliers.

184 monomers are involved in 611 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	G	203	CLA	1	0
21	B	814	CLA	6	0
21	K	201	CLA	7	0
25	A	853	BCR	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	3	603	CLA	2	0
21	A	841	CLA	5	0
21	A	833	CLA	2	0
25	B	801	BCR	9	0
25	B	848	BCR	1	0
21	A	843	CLA	1	0
21	2	612	CLA	4	0
25	A	850	BCR	5	0
20	4	615	CHL	2	0
21	A	842	CLA	7	0
21	1	602	CLA	5	0
21	H	201	CLA	4	0
21	A	830	CLA	7	0
21	B	819	CLA	4	0
23	B	852	LHG	3	0
21	L	302	CLA	4	0
25	B	845	BCR	9	0
21	A	820	CLA	7	0
21	B	809	CLA	6	0
21	A	803	CLA	9	0
24	3	613	LUT	8	0
21	B	833	CLA	1	0
20	2	615	CHL	3	0
21	1	604	CLA	4	0
21	A	811	CLA	6	0
30	B	850	DGD	5	0
25	O	204	BCR	3	0
21	3	605	CLA	1	0
21	A	840	CLA	1	0
21	4	614	CLA	1	0
21	B	805	CLA	7	0
21	A	813	CLA	2	0
21	2	613	CLA	4	0
21	A	805	CLA	2	0
21	4	603	CLA	2	0
21	4	601	CLA	2	0
21	3	612	CLA	3	0
21	A	810	CLA	2	0
24	4	616	LUT	2	0
21	A	806	CLA	5	0
21	3	610	CLA	2	0
21	2	604	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	813	CLA	7	0
21	A	844	CLA	3	0
21	G	201	CLA	2	0
25	B	844	BCR	6	0
22	4	617	XAT	6	0
21	2	611	CLA	2	0
21	A	839	CLA	1	0
21	B	834	CLA	3	0
20	2	606	CHL	1	0
21	B	818	CLA	5	0
21	A	812	CLA	9	0
21	B	839	CLA	2	0
25	3	614	BCR	6	0
21	A	831	CLA	4	0
21	A	832	CLA	1	0
25	J	102	BCR	5	0
25	K	205	BCR	5	0
21	K	204	CLA	4	0
21	1	607	CLA	2	0
28	C	102	SF4	3	0
23	1	615	LHG	12	0
20	2	601	CHL	2	0
25	G	204	BCR	4	0
21	1	608	CLA	3	0
21	A	804	CLA	8	0
20	4	607	CHL	1	0
21	3	604	CLA	1	0
21	A	807	CLA	2	0
21	B	840	CLA	5	0
20	3	606	CHL	2	0
21	J	101	CLA	1	0
21	A	826	CLA	4	0
21	A	827	CLA	1	0
21	B	802	CLA	12	0
24	1	616	LUT	3	0
21	A	818	CLA	7	0
21	B	821	CLA	2	0
29	A	855	PQN	3	0
25	4	618	BCR	6	0
21	1	611	CLA	1	0
21	B	838	CLA	1	0
21	A	828	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	1	609	CLA	12	0
21	B	803	CLA	5	0
23	2	618	LHG	2	0
21	L	304	CLA	1	0
21	B	837	CLA	2	0
21	B	841	CLA	2	0
21	B	826	CLA	3	0
21	B	810	CLA	1	0
25	B	846	BCR	5	0
21	3	601	CLA	5	0
21	B	811	CLA	3	0
21	A	823	CLA	3	0
20	2	607	CHL	1	0
23	A	847	LHG	1	0
28	C	101	SF4	2	0
25	L	306	BCR	4	0
21	A	802	CLA	7	0
21	3	602	CLA	3	0
21	B	823	CLA	2	0
24	2	616	LUT	5	0
21	F	302	CLA	7	0
25	I	101	BCR	2	0
21	B	830	CLA	2	0
21	B	804	CLA	1	0
21	A	822	CLA	3	0
28	A	854	SF4	2	0
25	B	847	BCR	3	0
21	2	608	CLA	5	0
22	2	617	XAT	5	0
21	B	808	CLA	4	0
21	B	835	CLA	1	0
21	3	607	CLA	8	0
21	1	603	CLA	1	0
21	A	825	CLA	2	0
21	B	829	CLA	1	0
21	B	836	CLA	2	0
21	A	819	CLA	3	0
20	4	605	CHL	2	0
21	A	809	CLA	7	0
23	A	846	LHG	7	0
25	A	848	BCR	3	0
29	B	842	PQN	3	0

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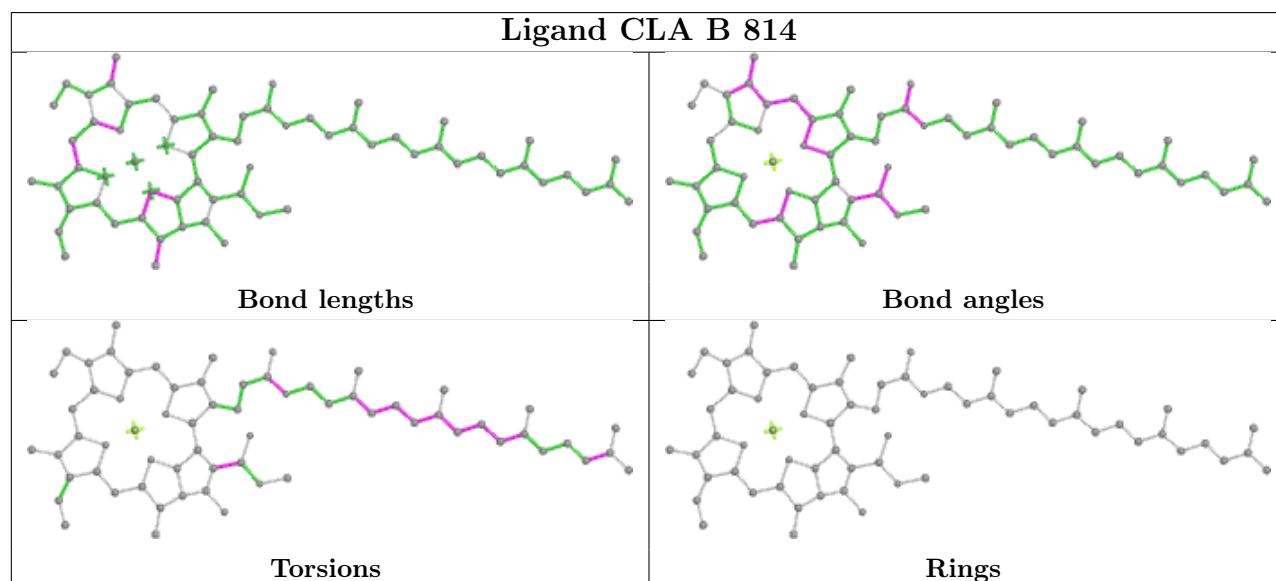
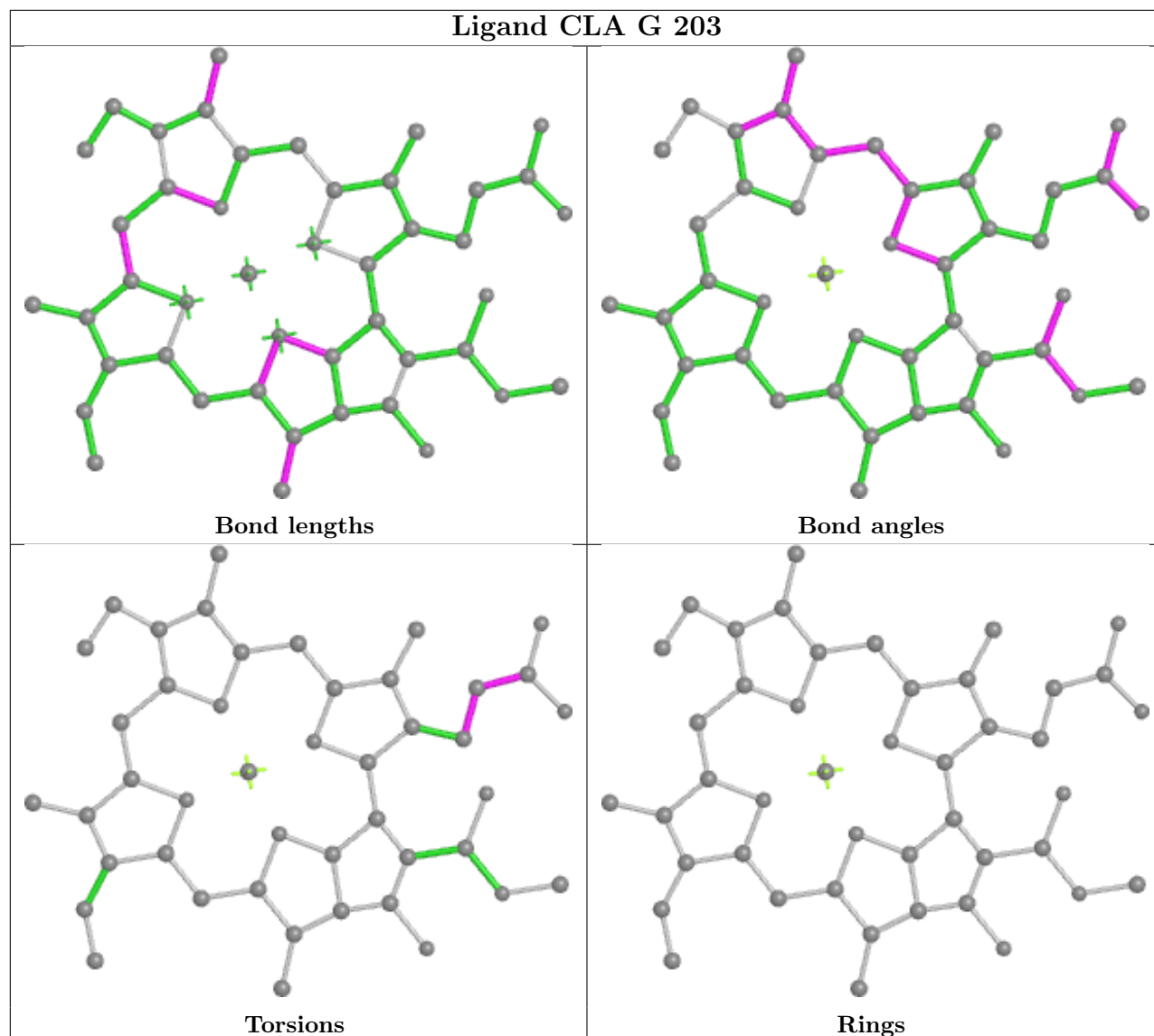
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	843	BCR	6	0
21	3	608	CLA	6	0
21	4	611	CLA	1	0
25	B	849	BCR	7	0
21	4	609	CLA	5	0
21	L	303	CLA	2	0
21	1	612	CLA	2	0
25	A	851	BCR	6	0
21	B	820	CLA	1	0
21	B	816	CLA	2	0
21	B	825	CLA	3	0
21	B	827	CLA	3	0
21	A	835	CLA	4	0
25	L	301	BCR	3	0
21	4	602	CLA	3	0
27	A	801	CL0	15	0
21	B	828	CLA	9	0
21	2	602	CLA	9	0
25	L	305	BCR	7	0
20	1	601	CHL	7	0
21	A	845	CLA	3	0
21	4	608	CLA	3	0
22	1	614	XAT	13	0
21	A	815	CLA	1	0
21	2	609	CLA	11	0
21	A	824	CLA	2	0
21	F	301	CLA	2	0
21	B	822	CLA	8	0
21	A	814	CLA	2	0
21	A	834	CLA	2	0
21	2	603	CLA	3	0
21	4	613	CLA	2	0
21	A	829	CLA	9	0
21	B	817	CLA	3	0
21	B	824	CLA	11	0
21	B	832	CLA	5	0
21	A	808	CLA	1	0
21	1	605	CLA	3	0
20	2	605	CHL	5	0
23	B	851	LHG	3	0
21	O	201	CLA	2	0
21	O	203	CLA	1	0

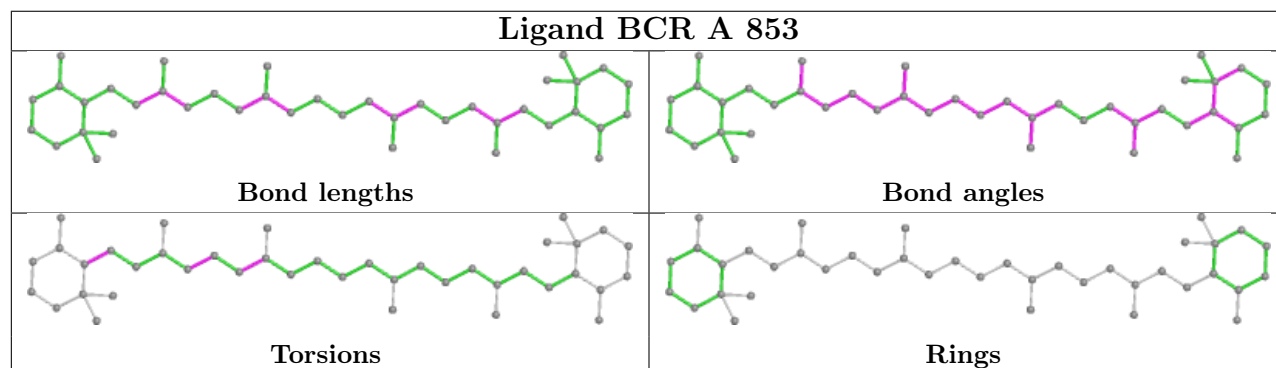
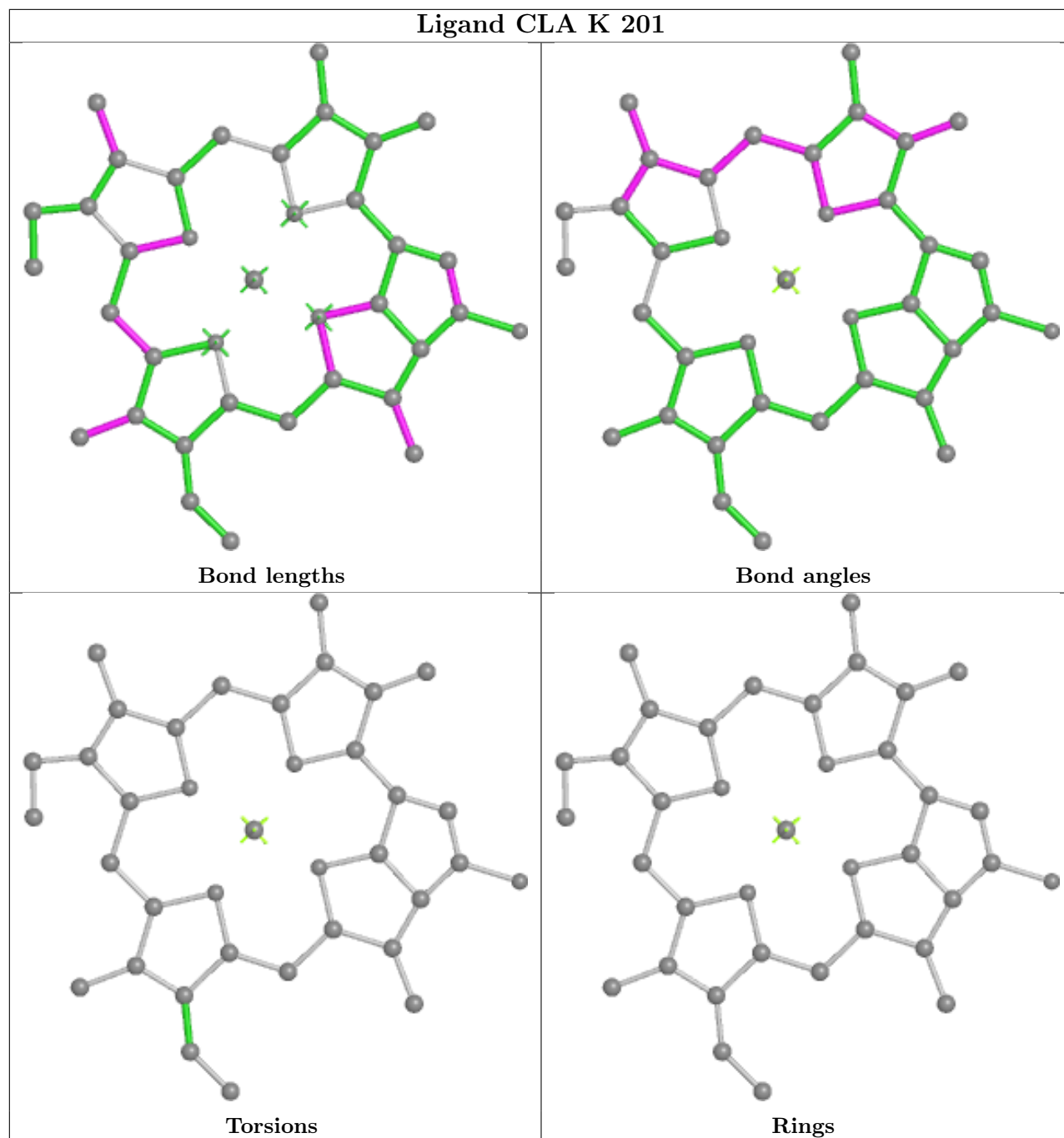
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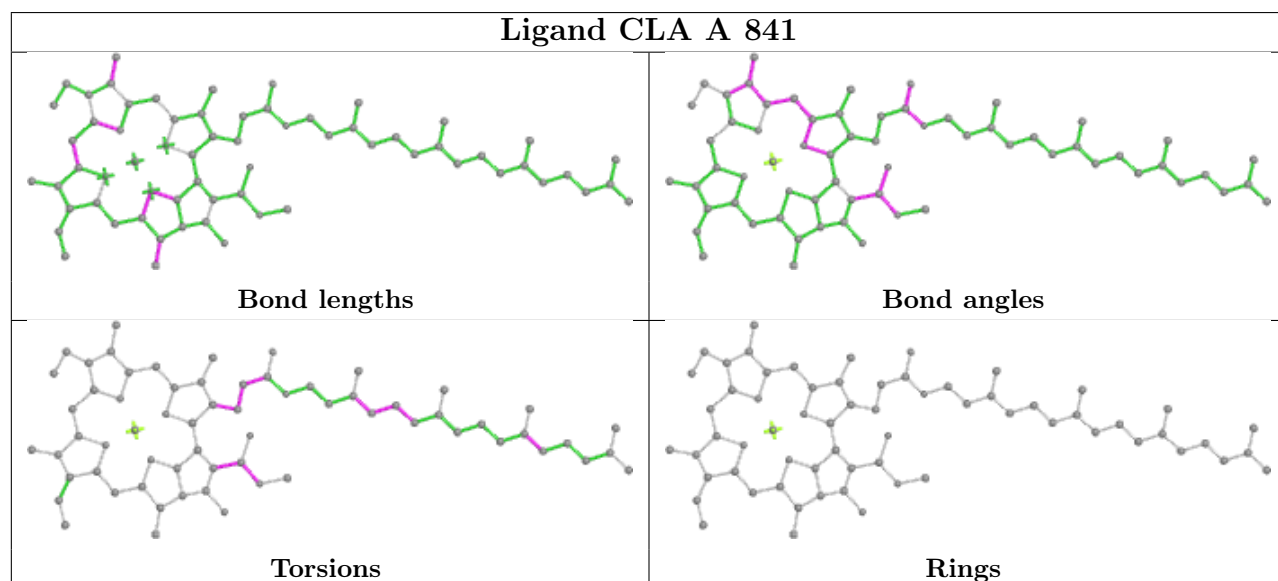
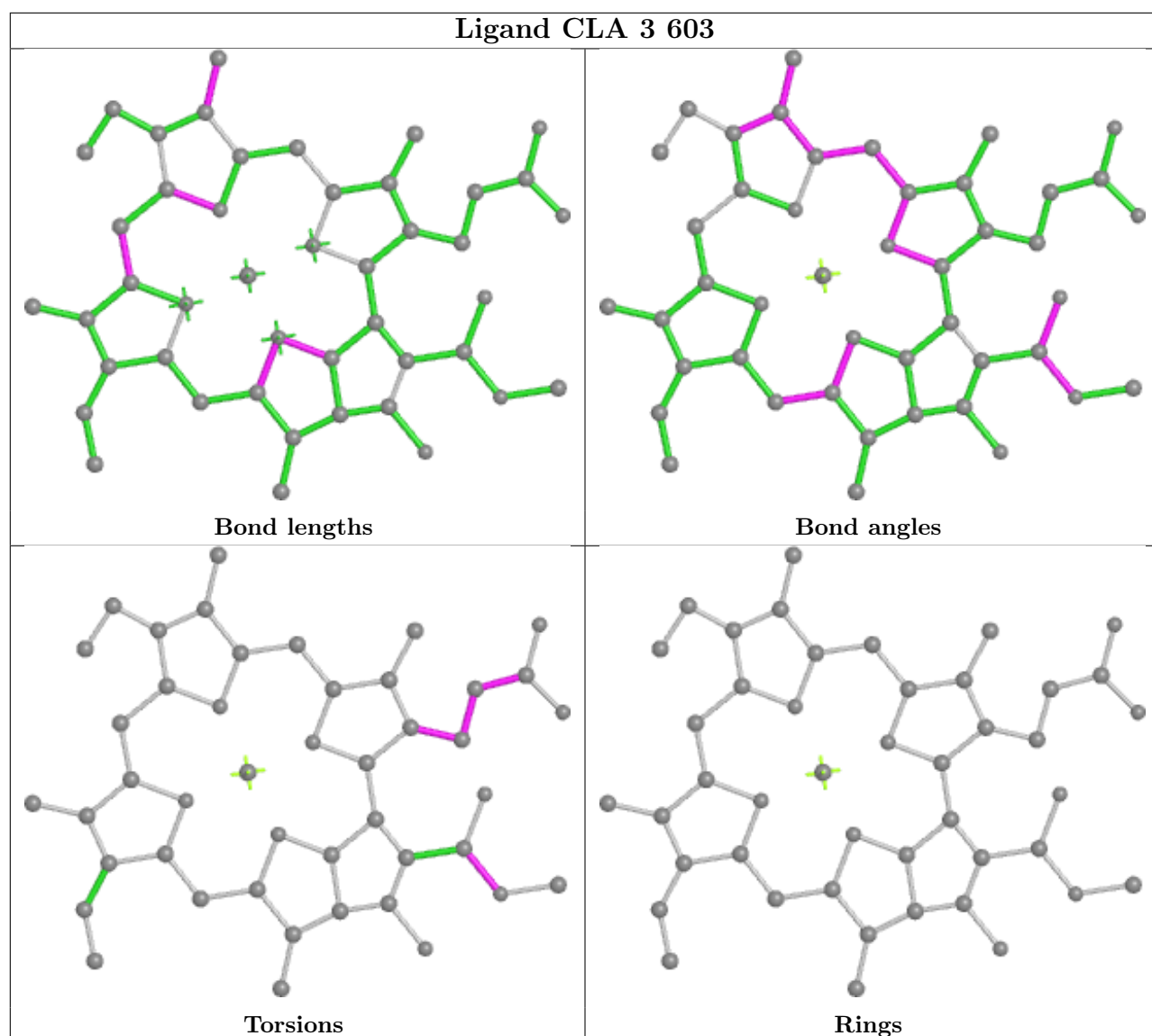
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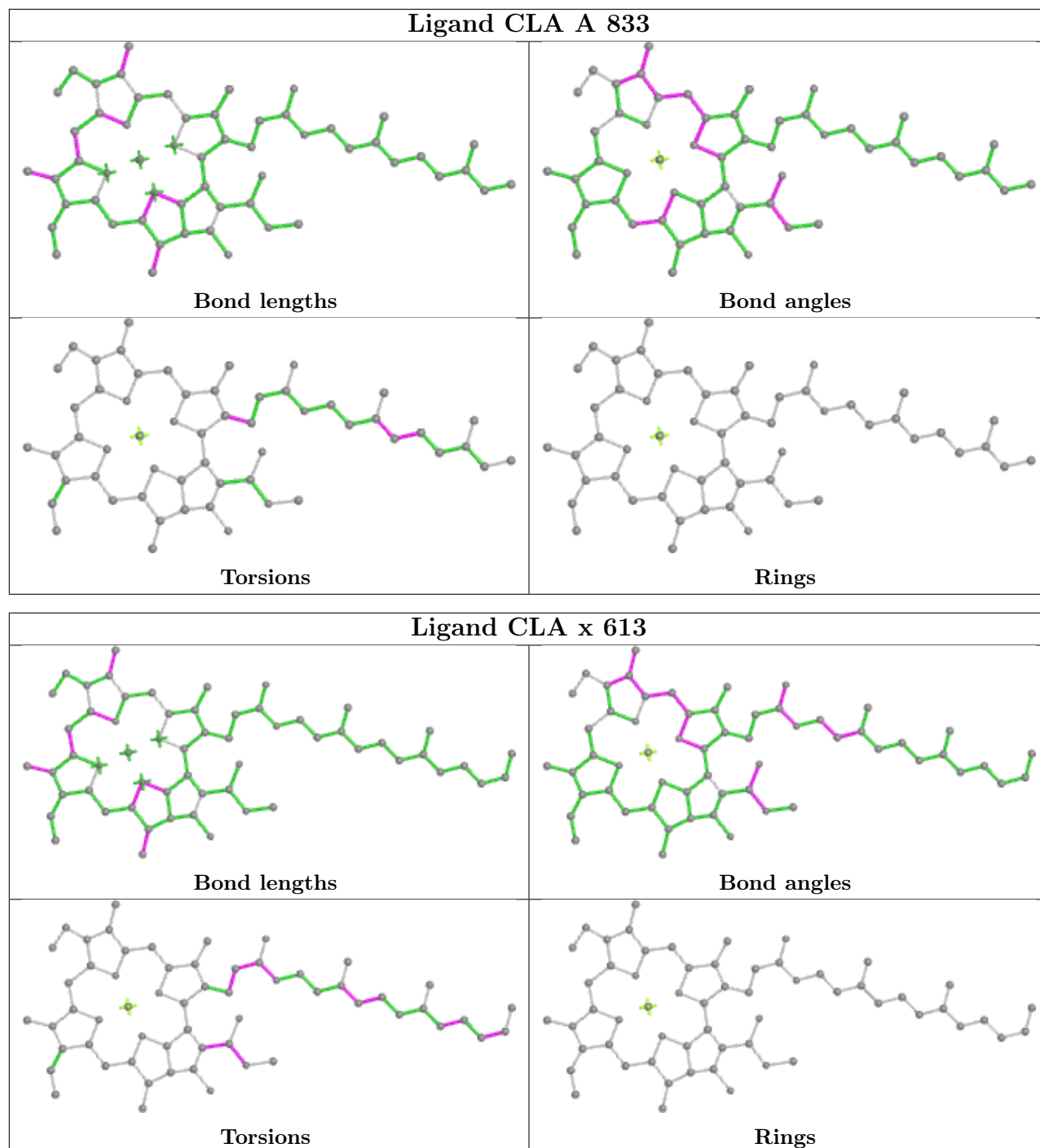
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	849	BCR	2	0
25	K	202	BCR	5	0
25	A	852	BCR	2	0
25	F	304	BCR	2	0
21	4	612	CLA	2	0
21	A	821	CLA	1	0
21	K	206	CLA	5	0
21	4	610	CLA	2	0
24	2	619	LUT	6	0
21	3	609	CLA	7	0
21	A	838	CLA	1	0
21	B	806	CLA	4	0

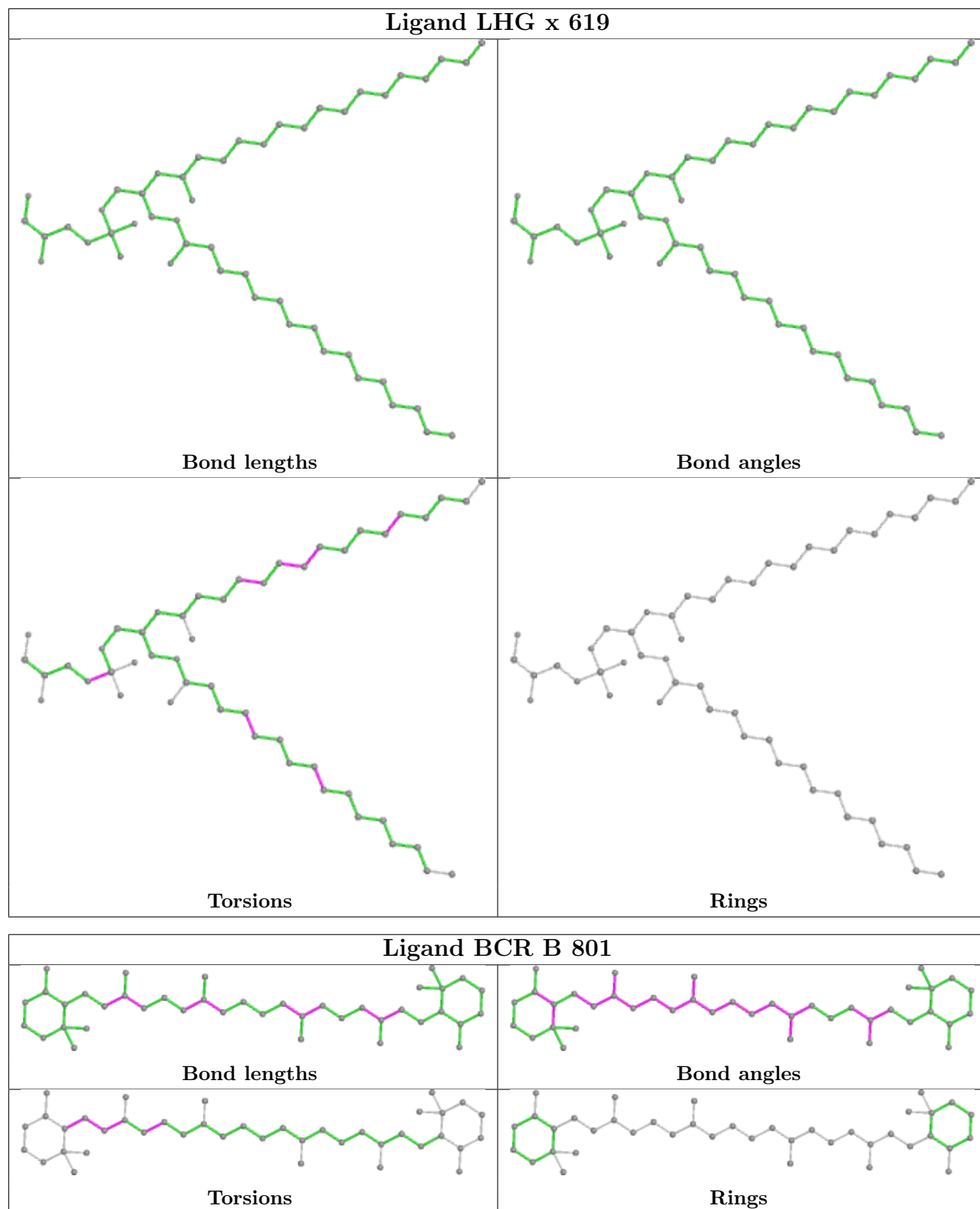
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

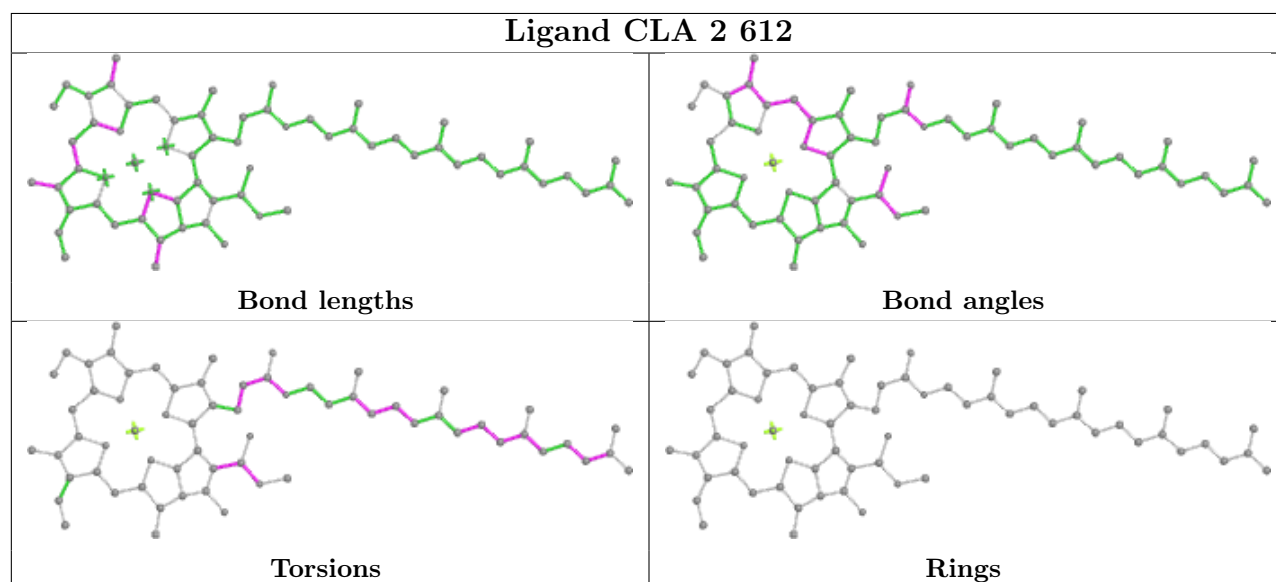
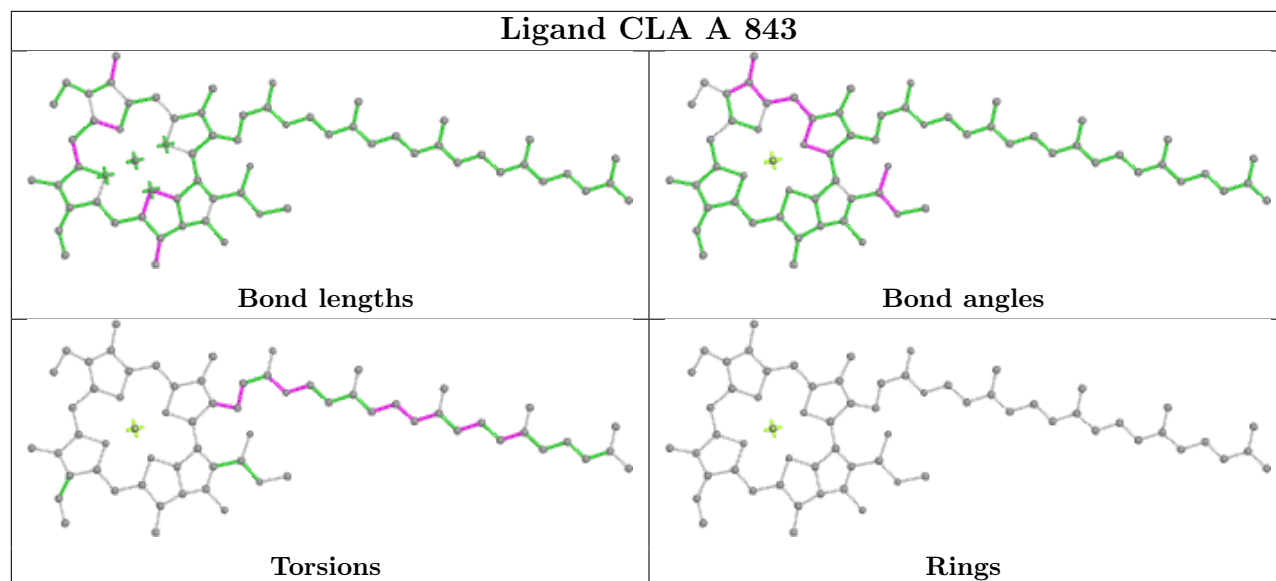
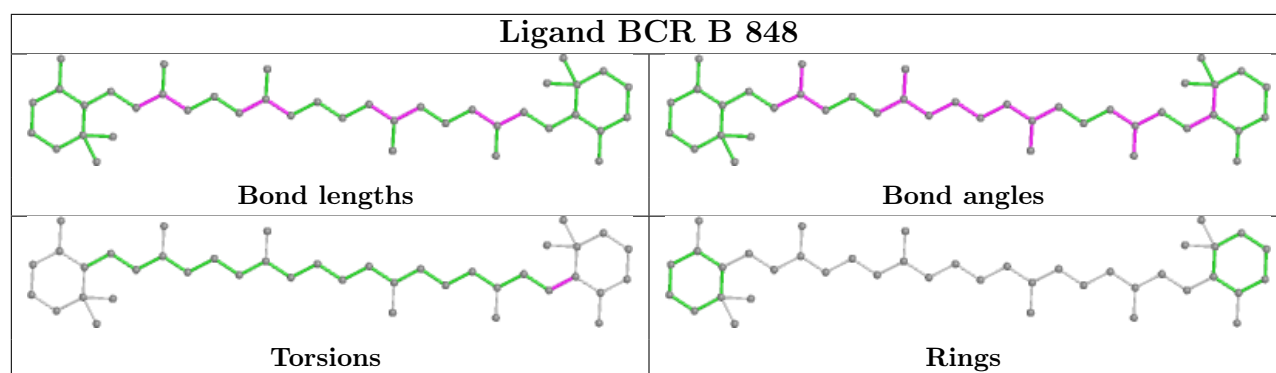


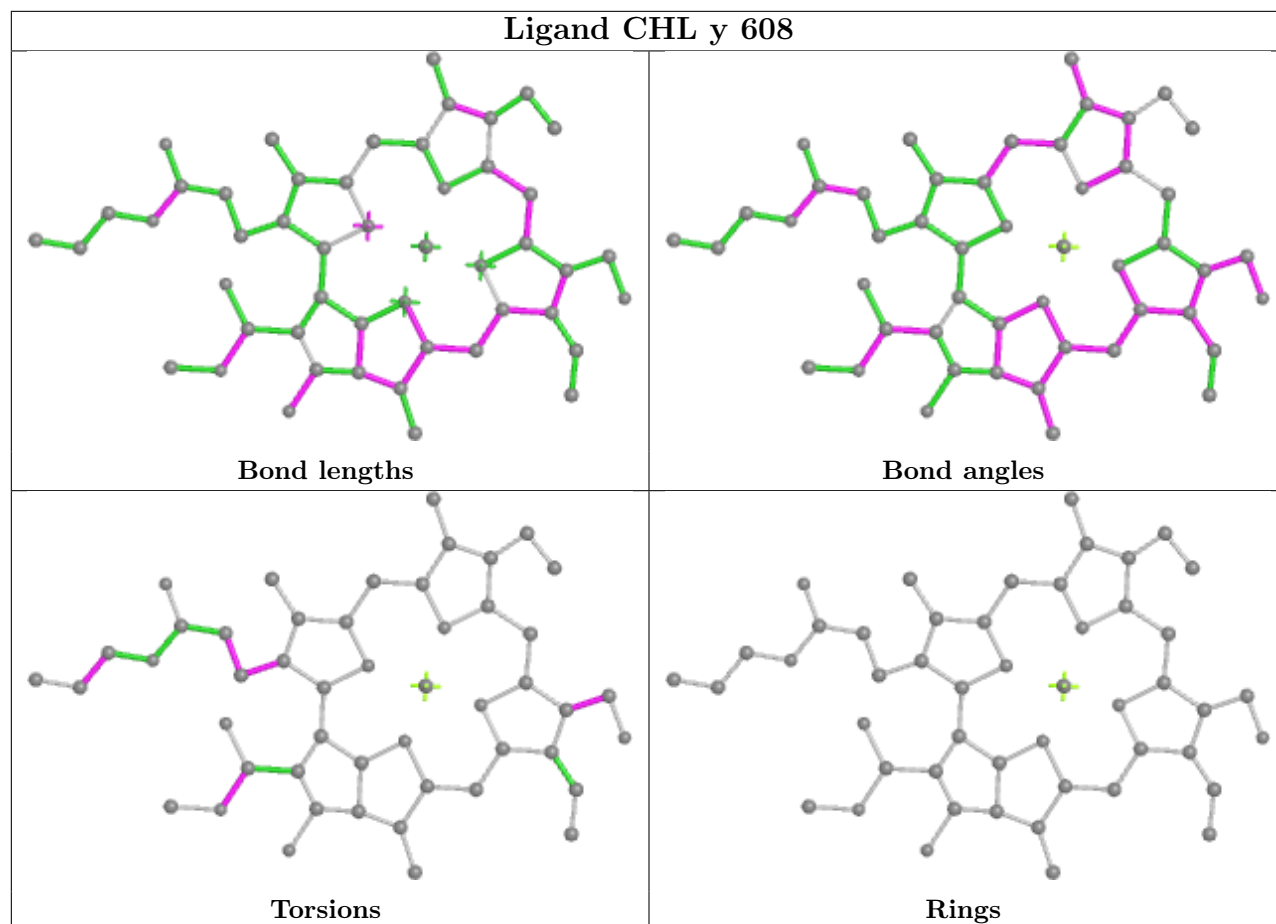
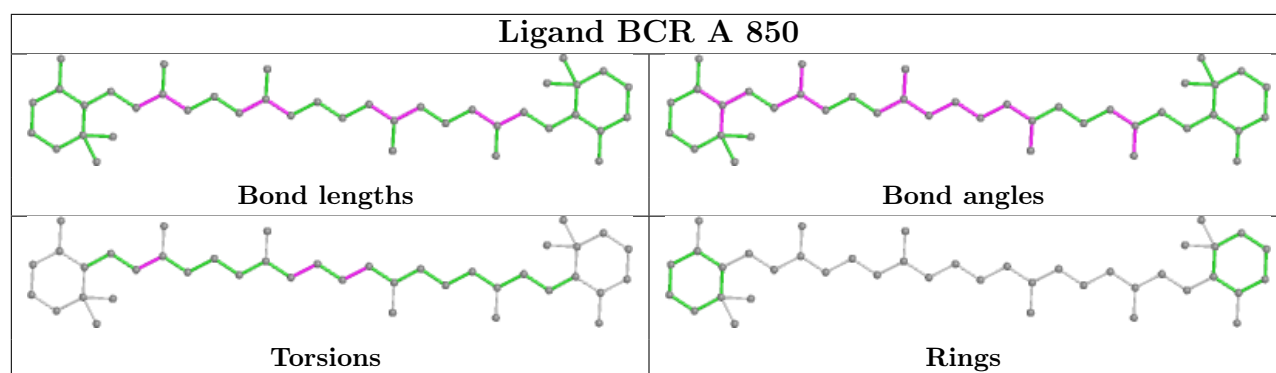


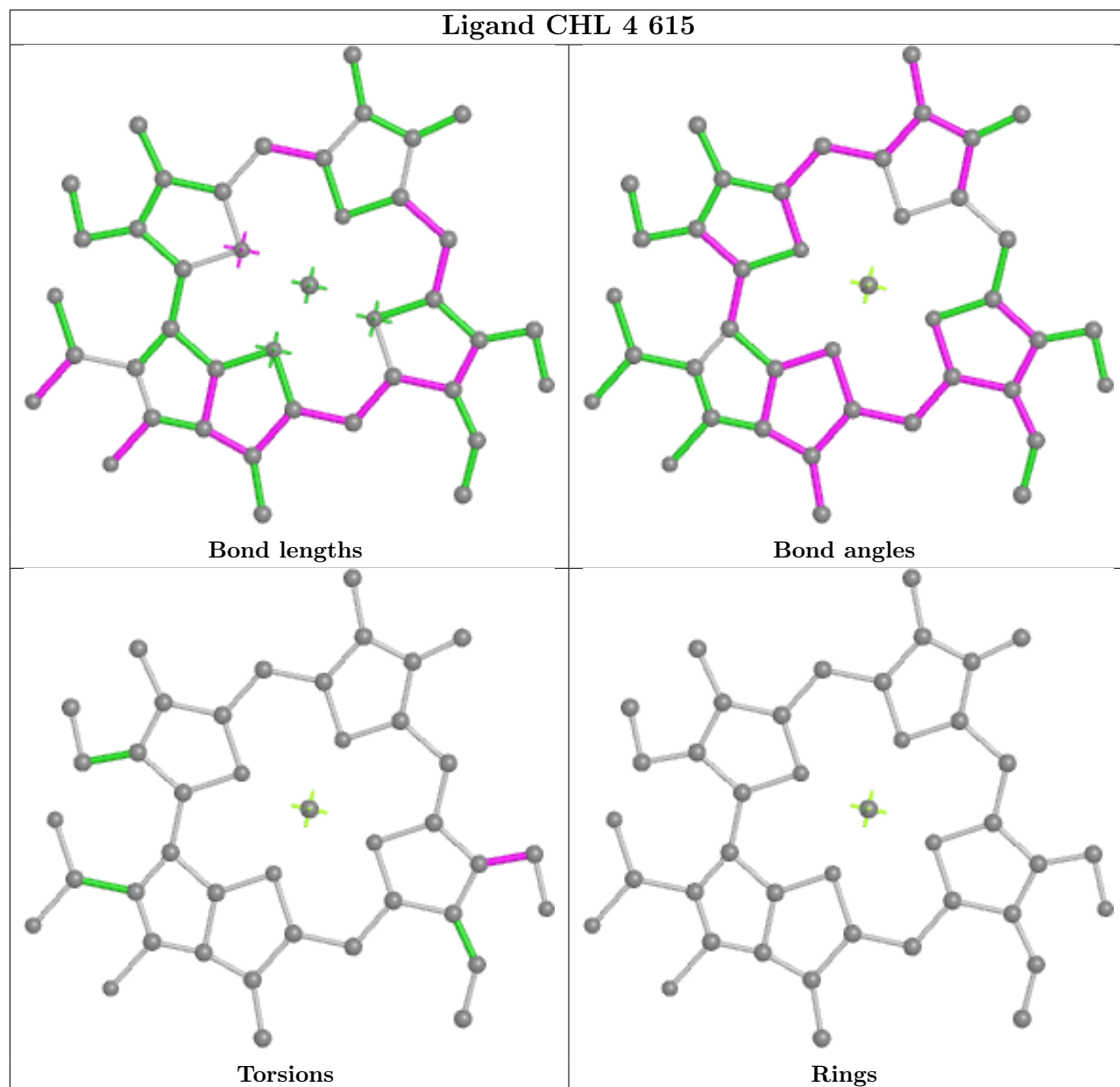


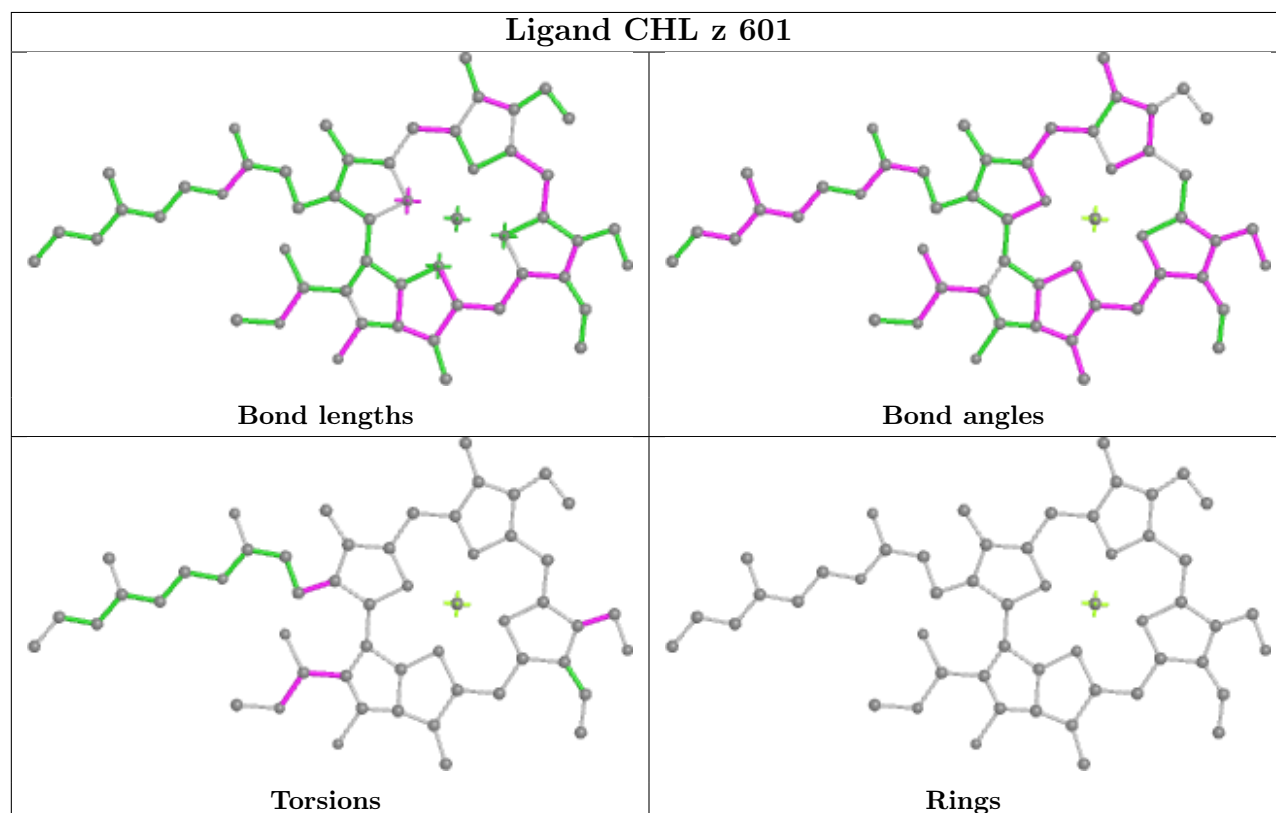
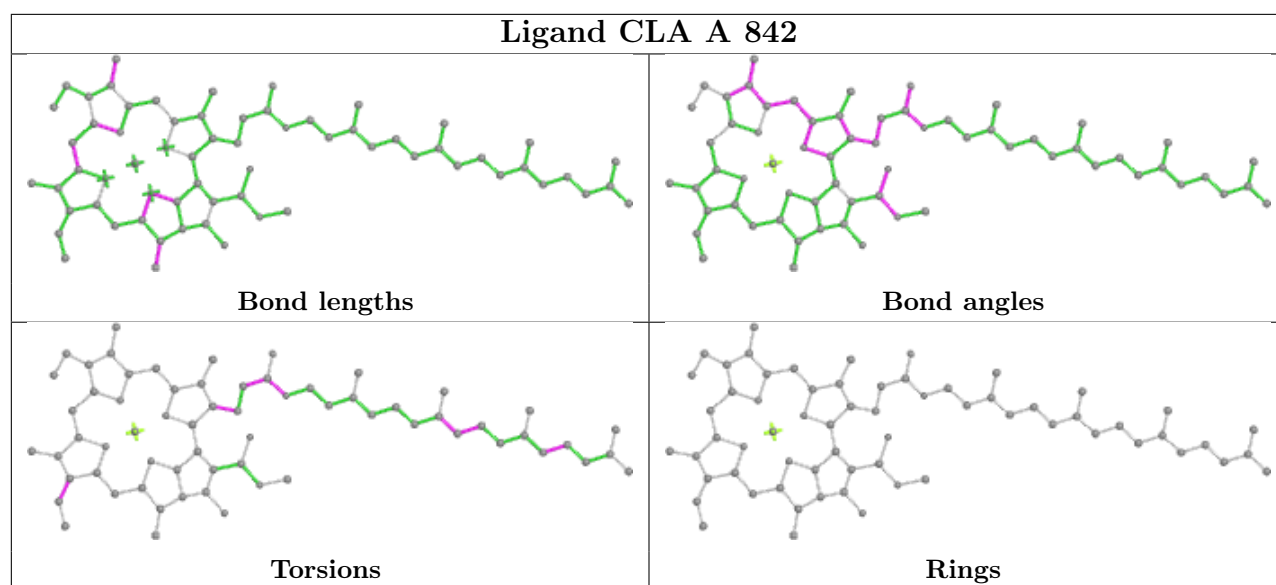


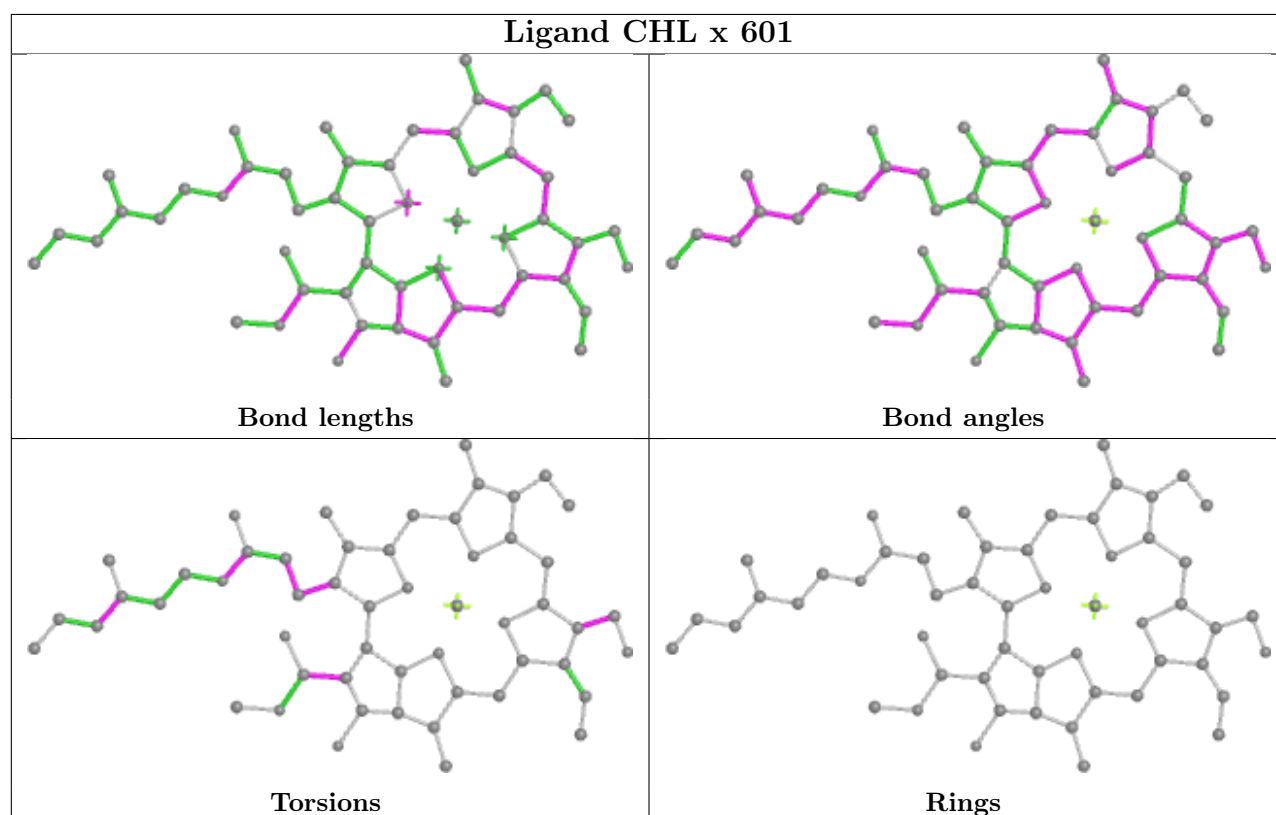
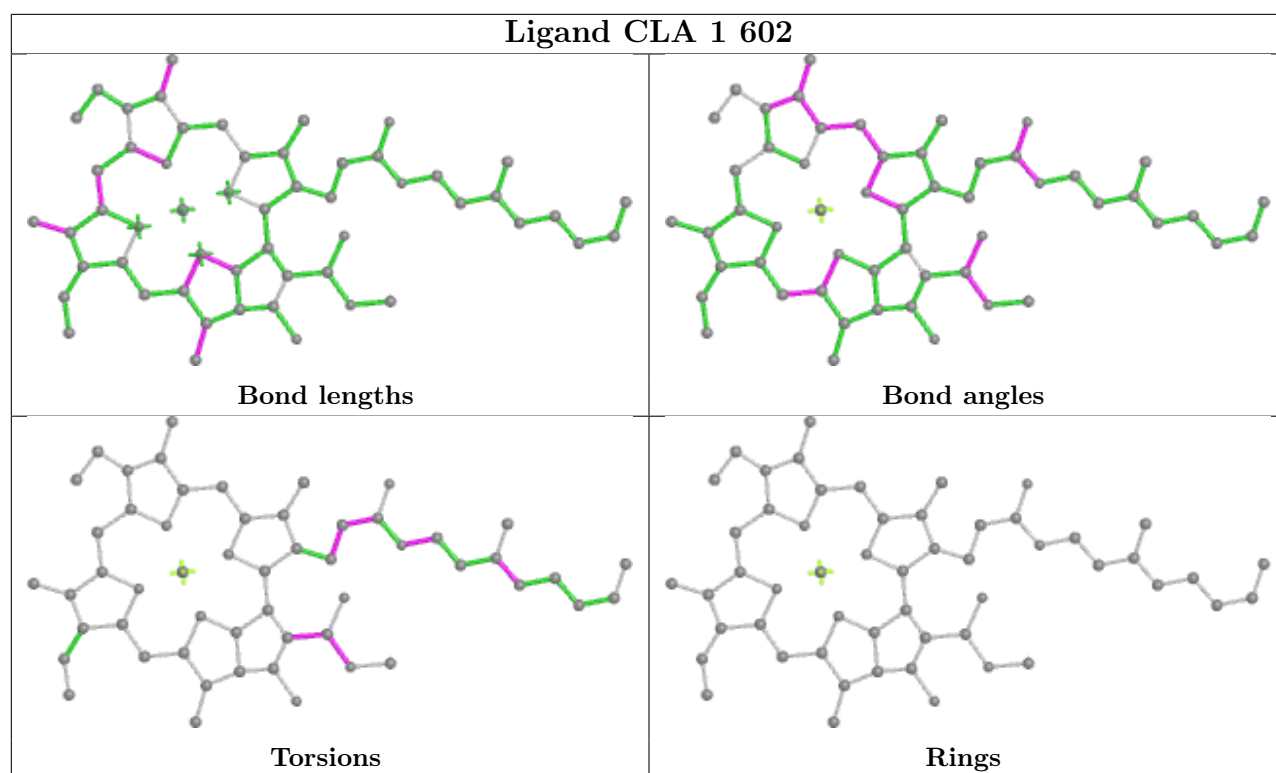


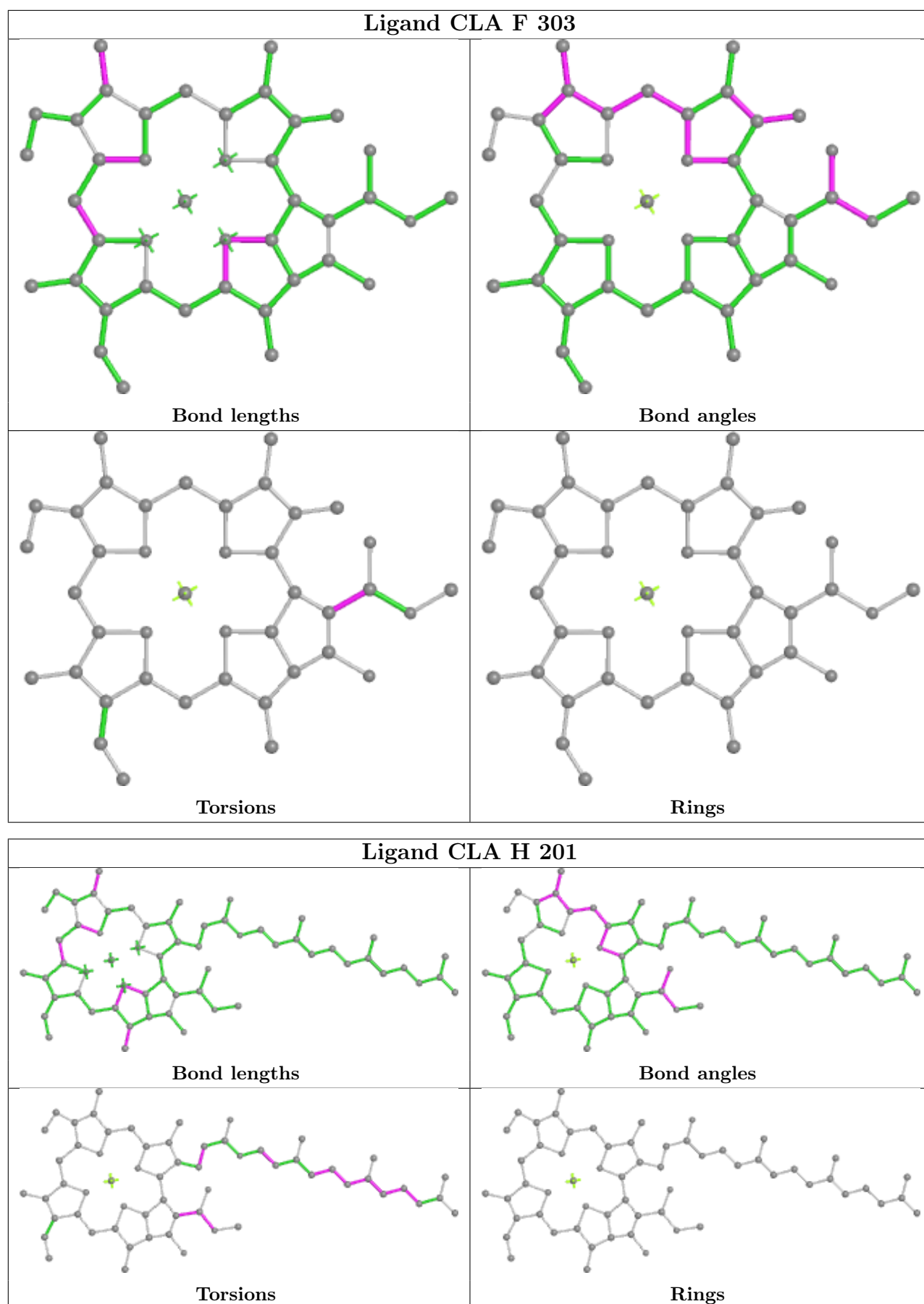


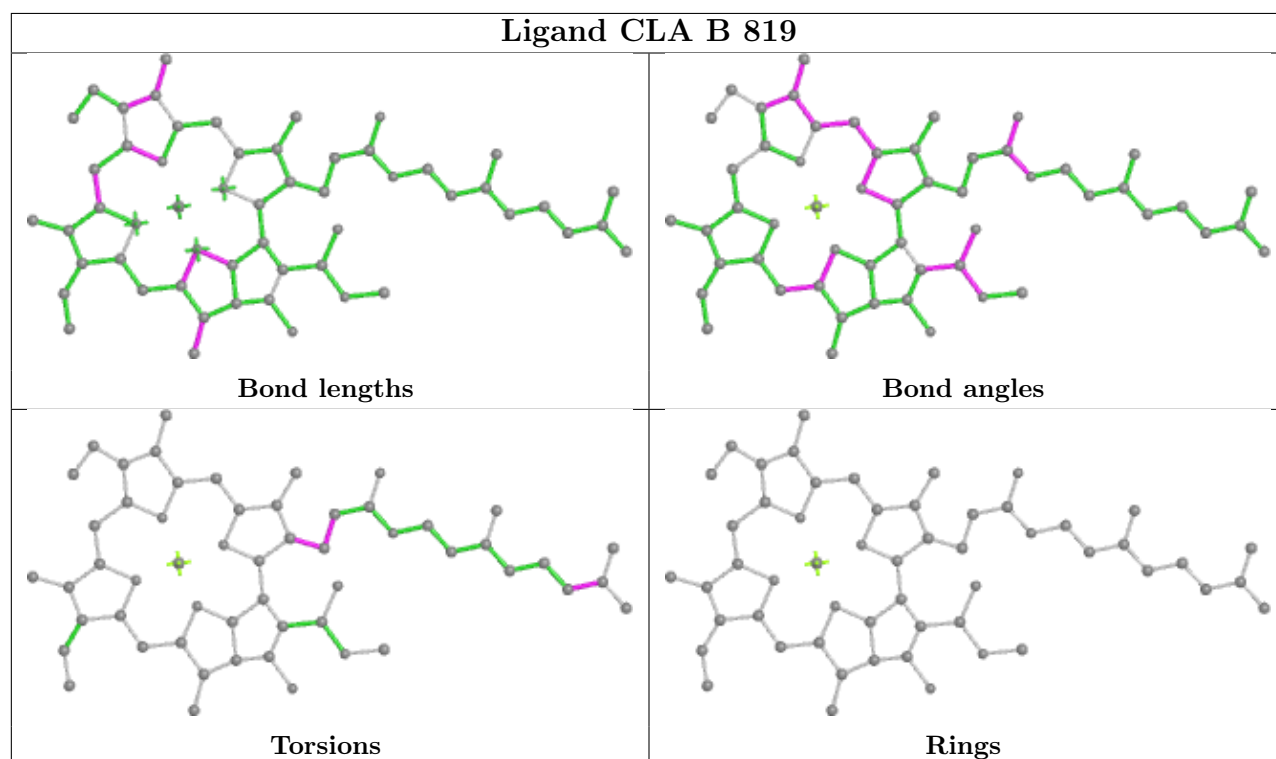
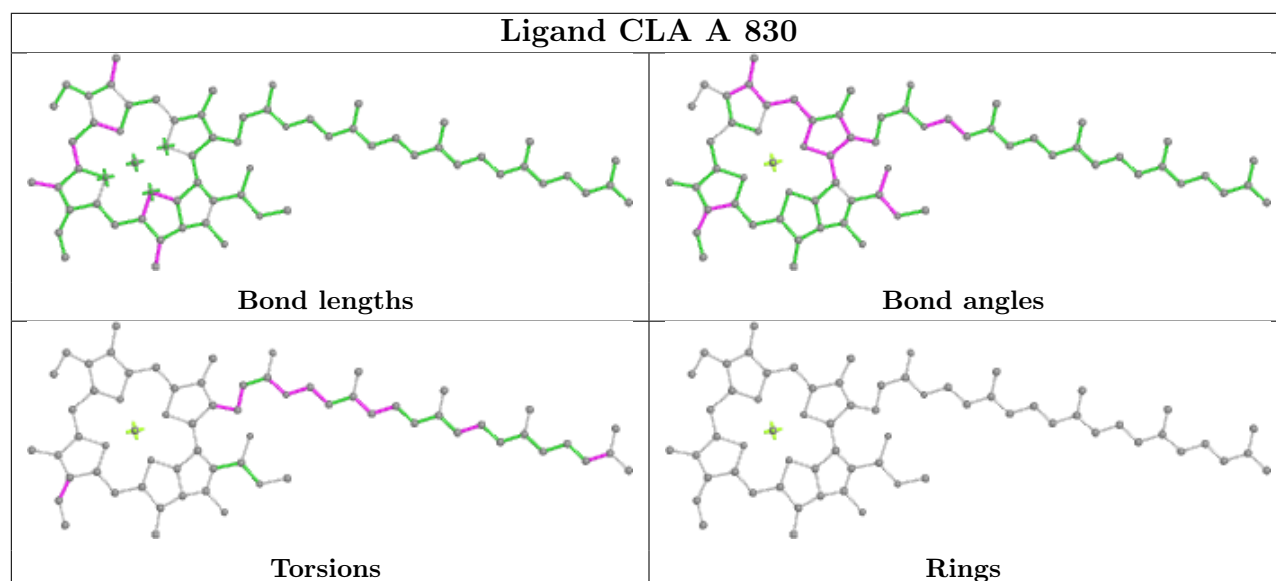
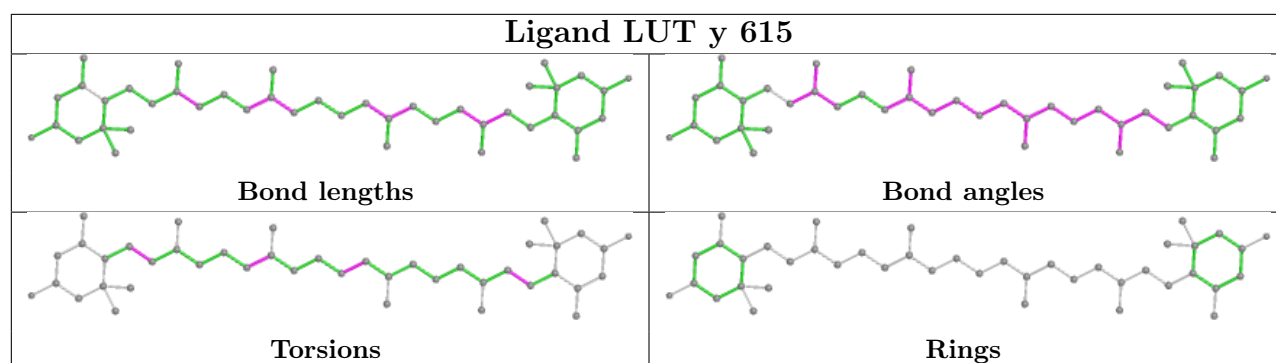


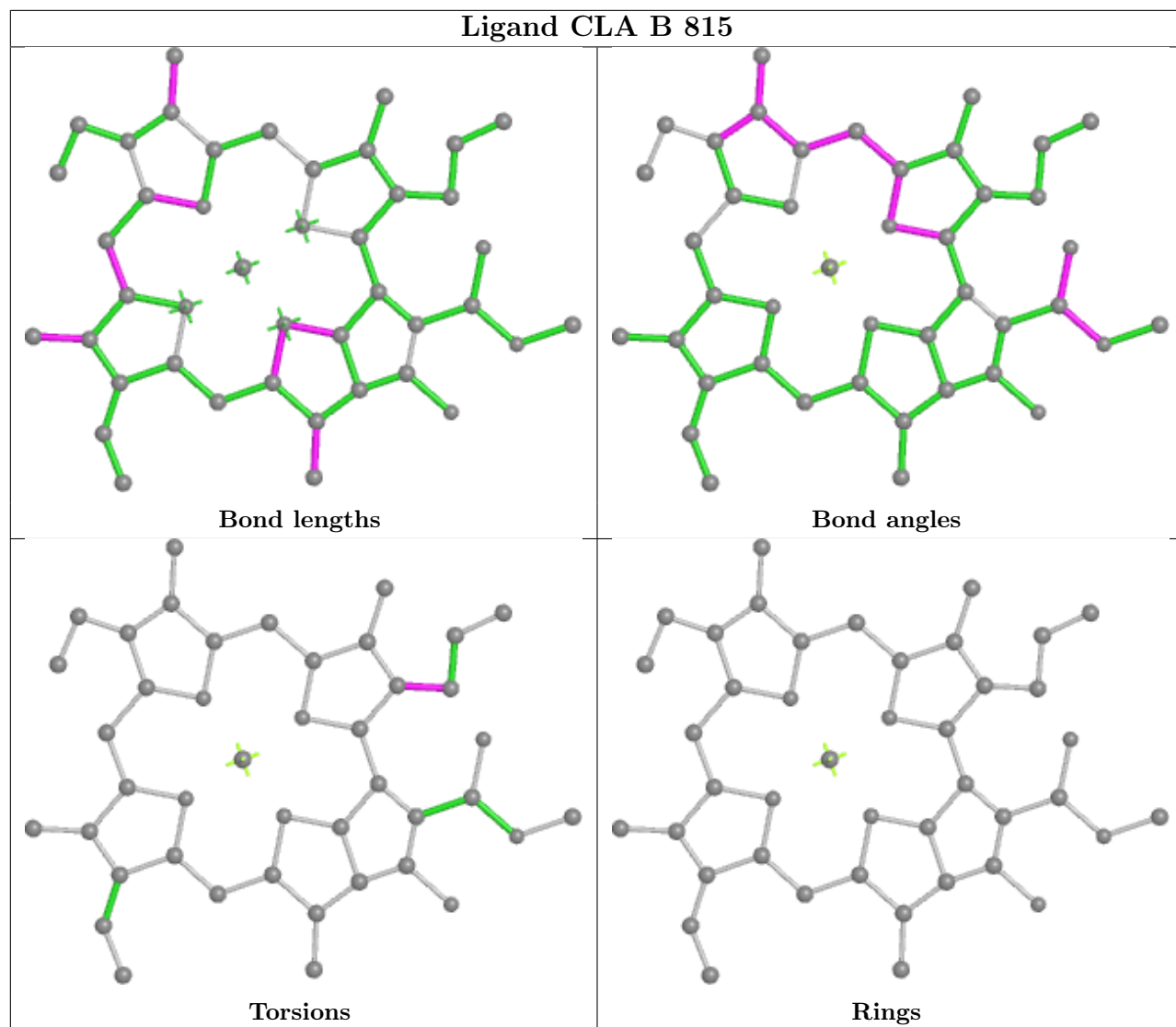


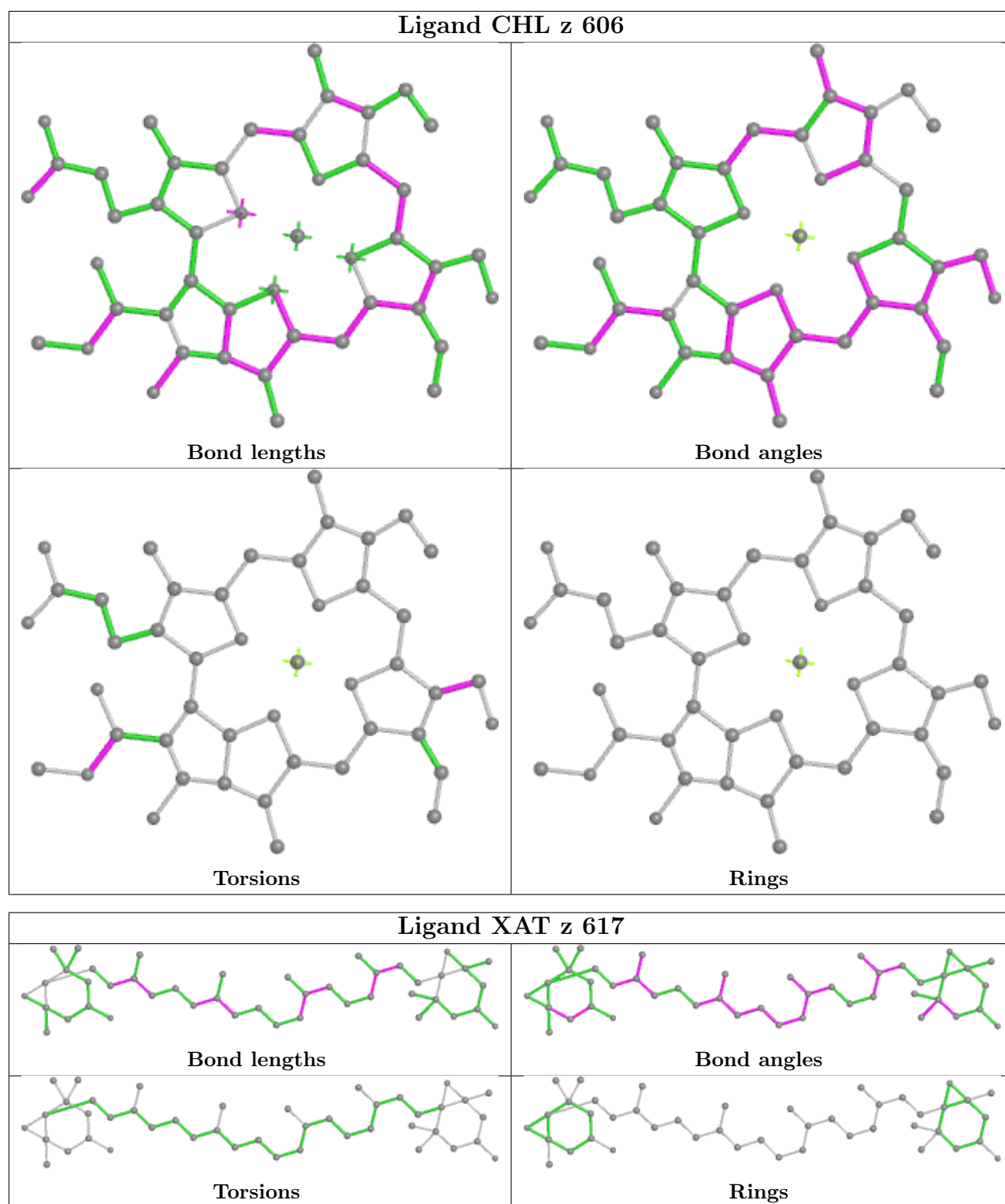


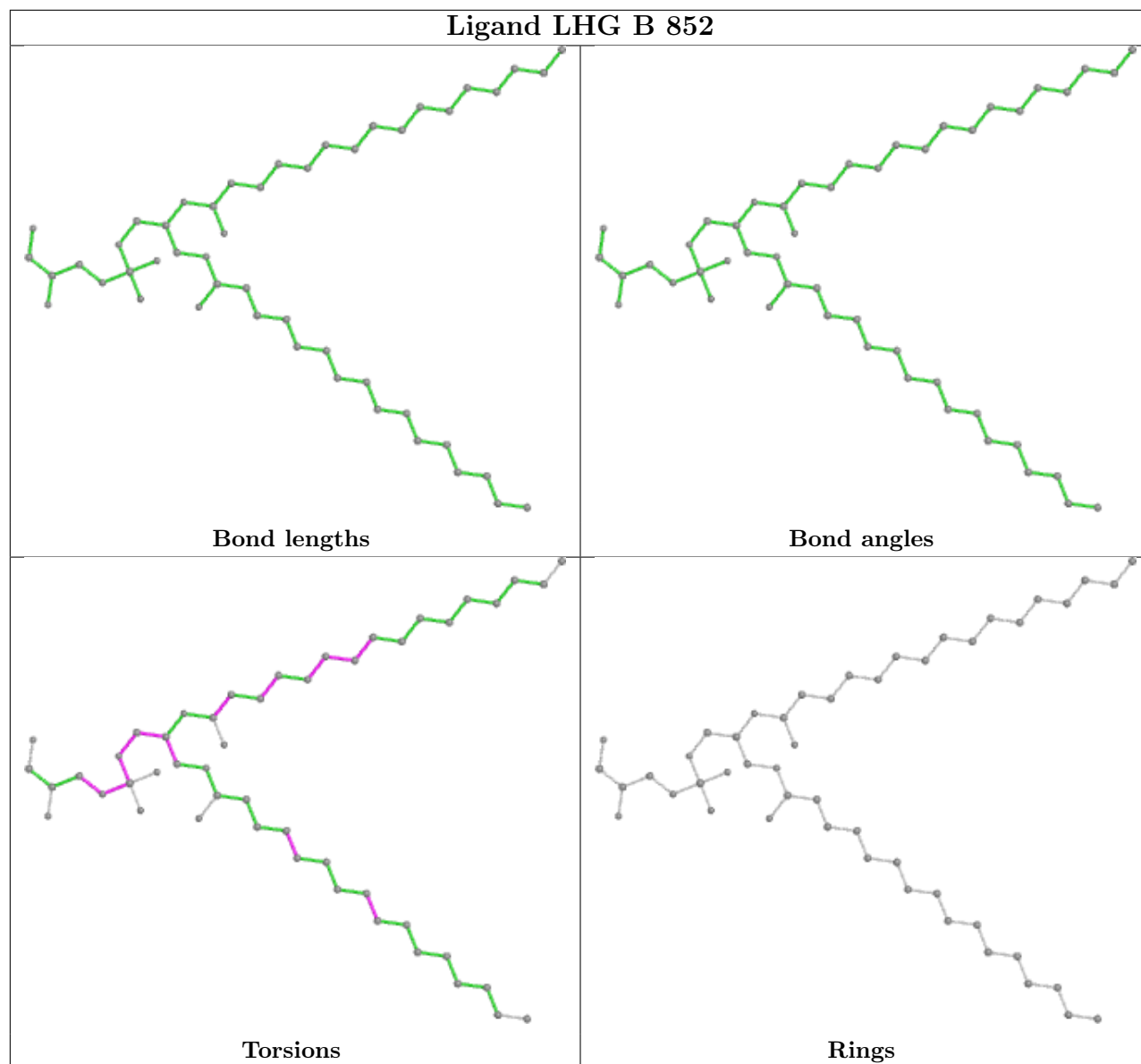


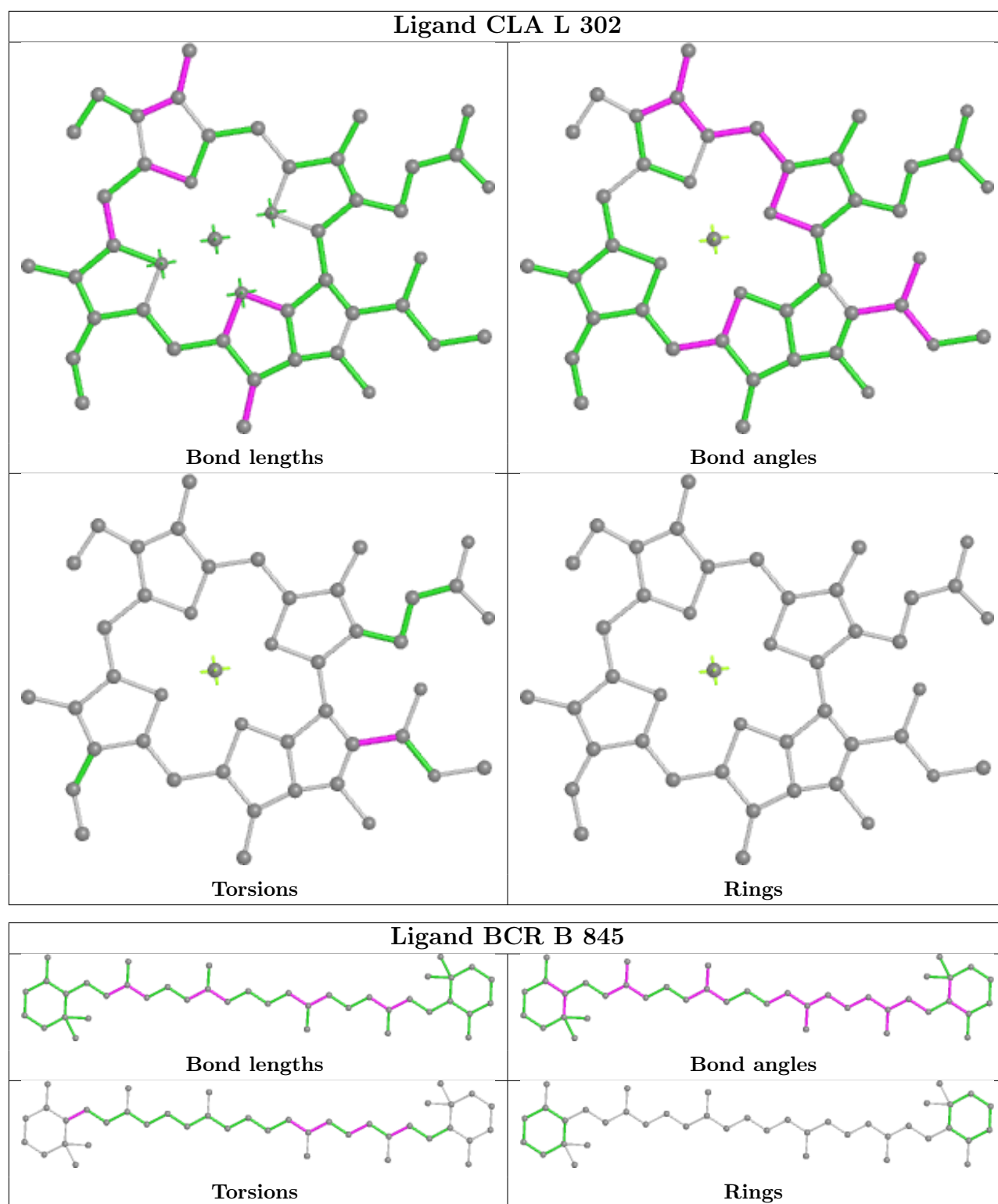


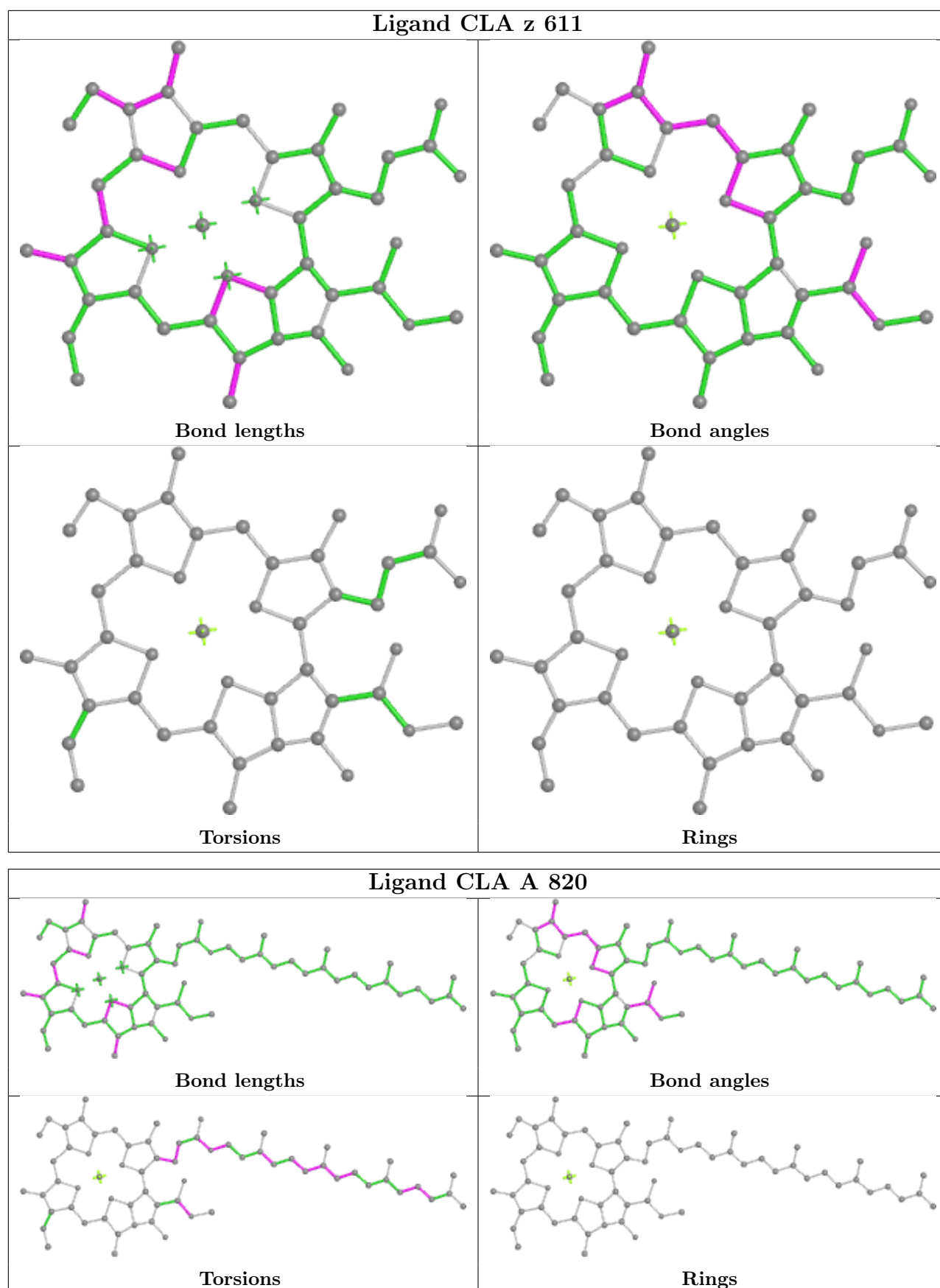


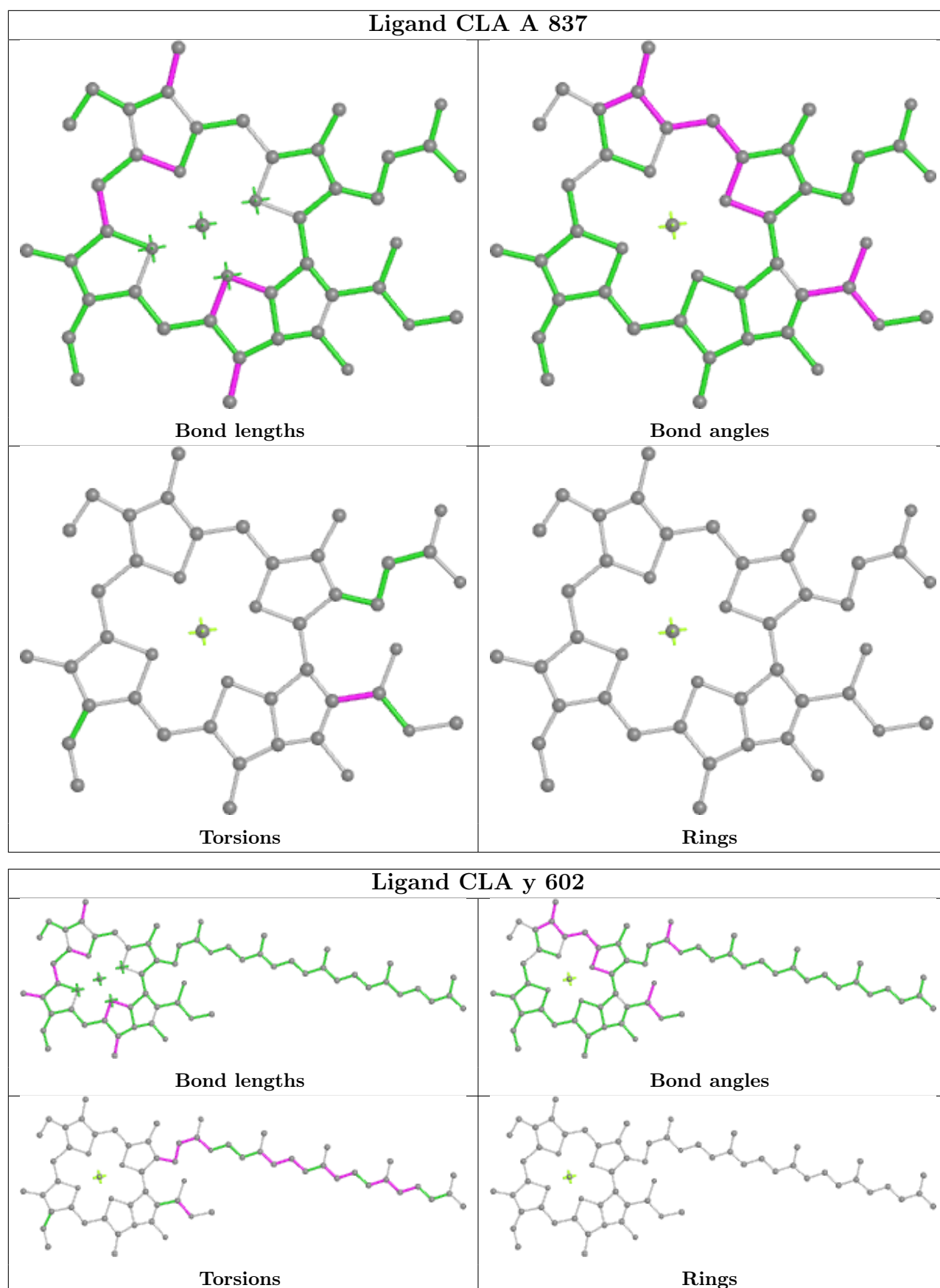


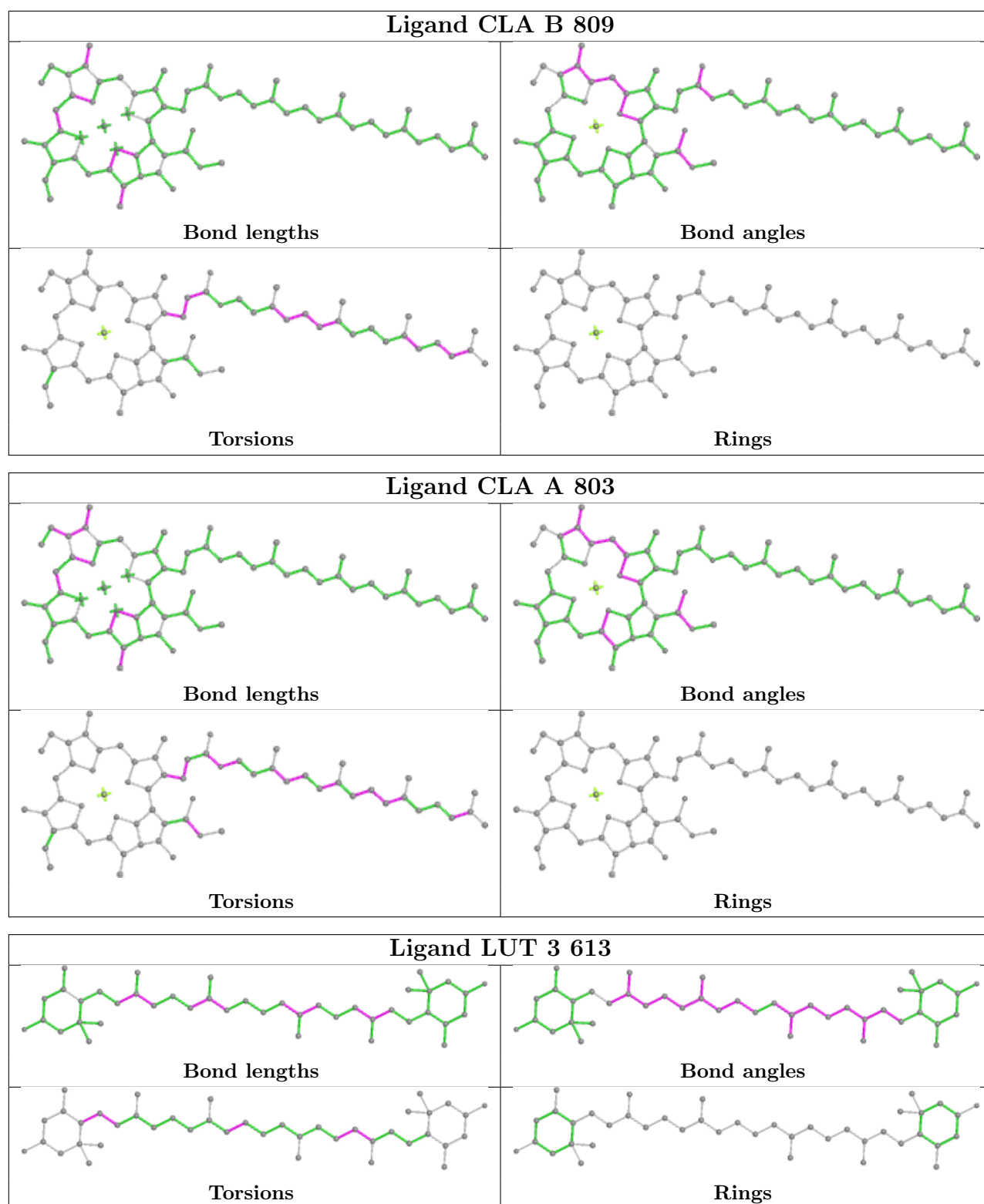


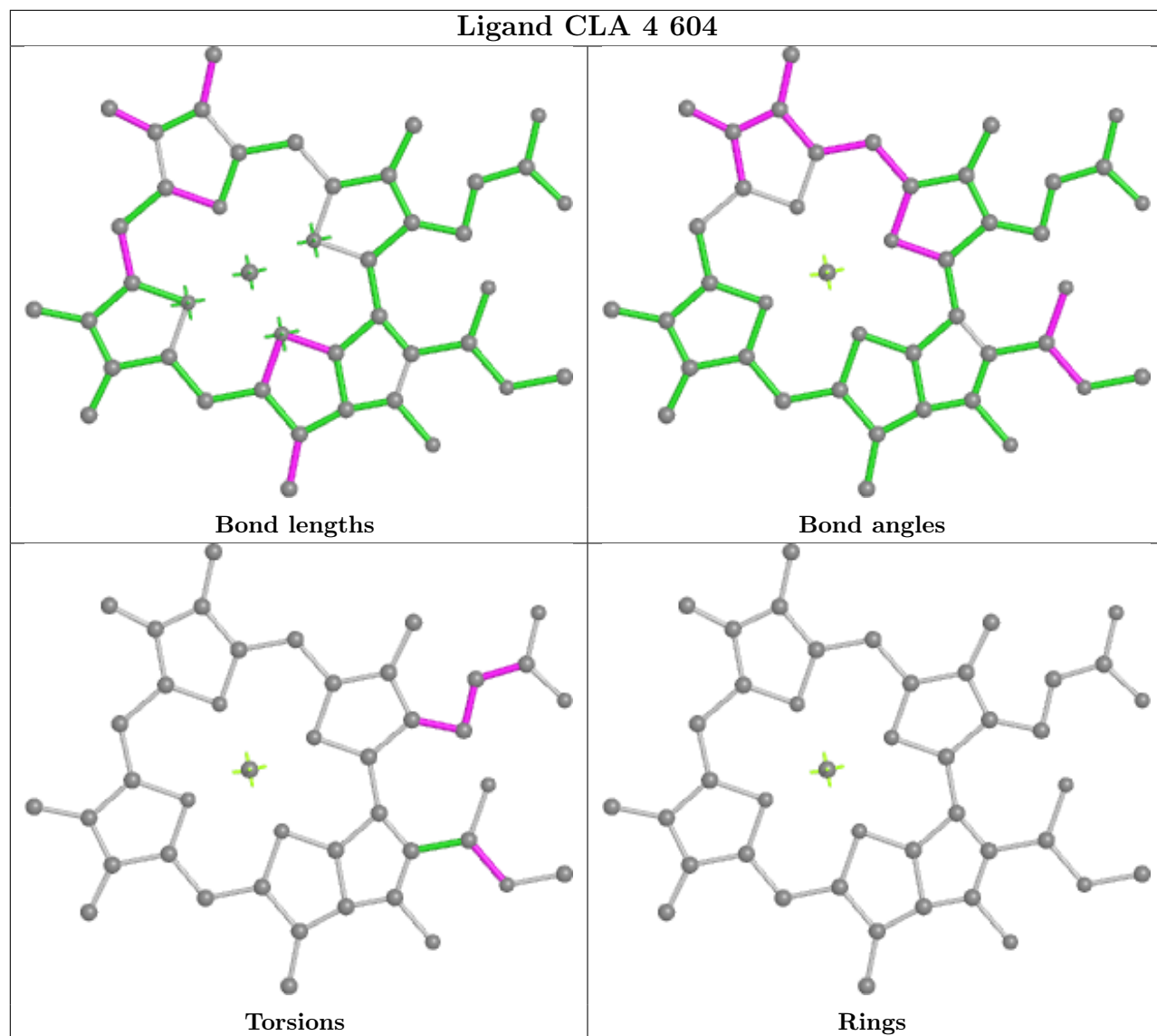


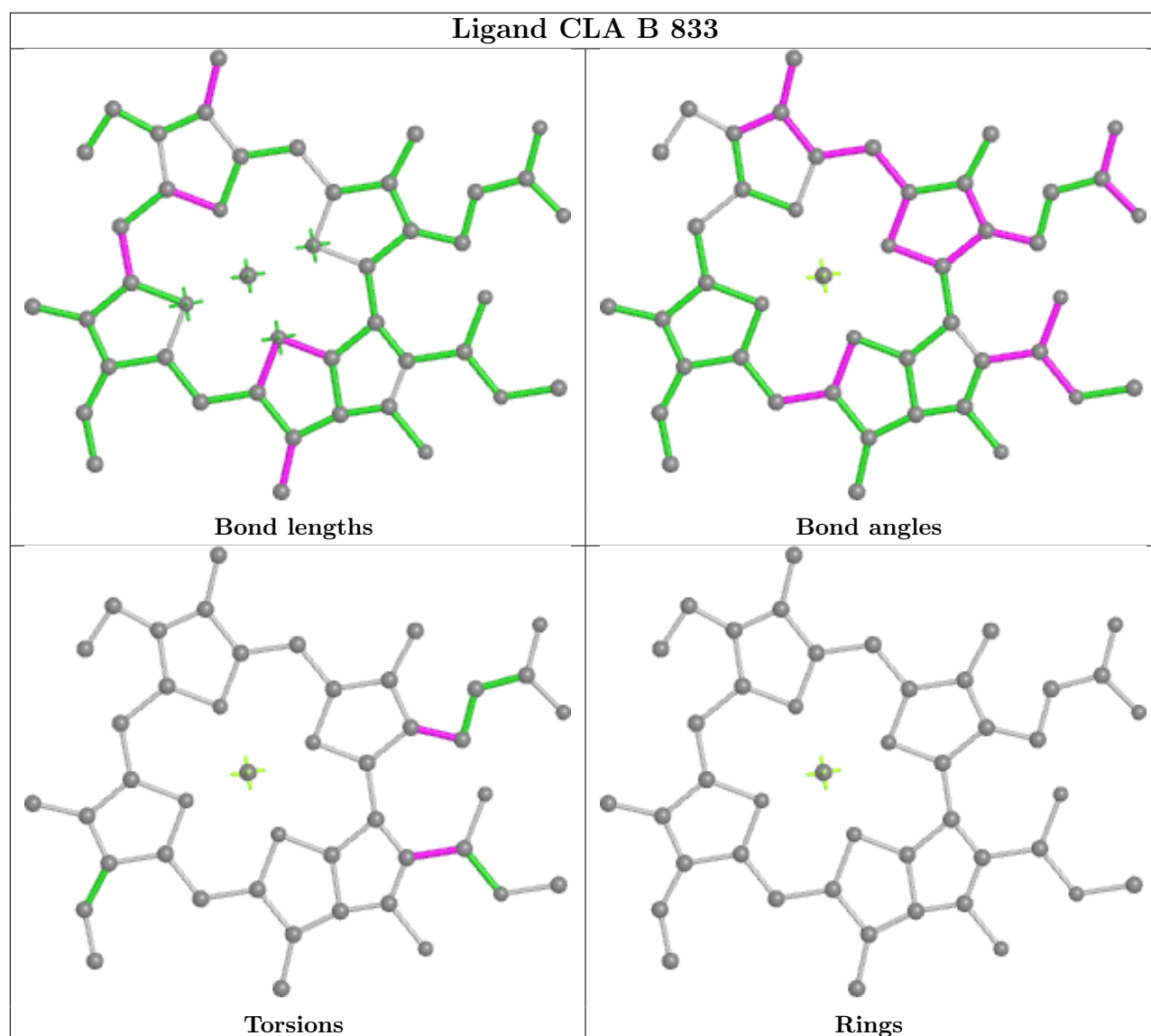


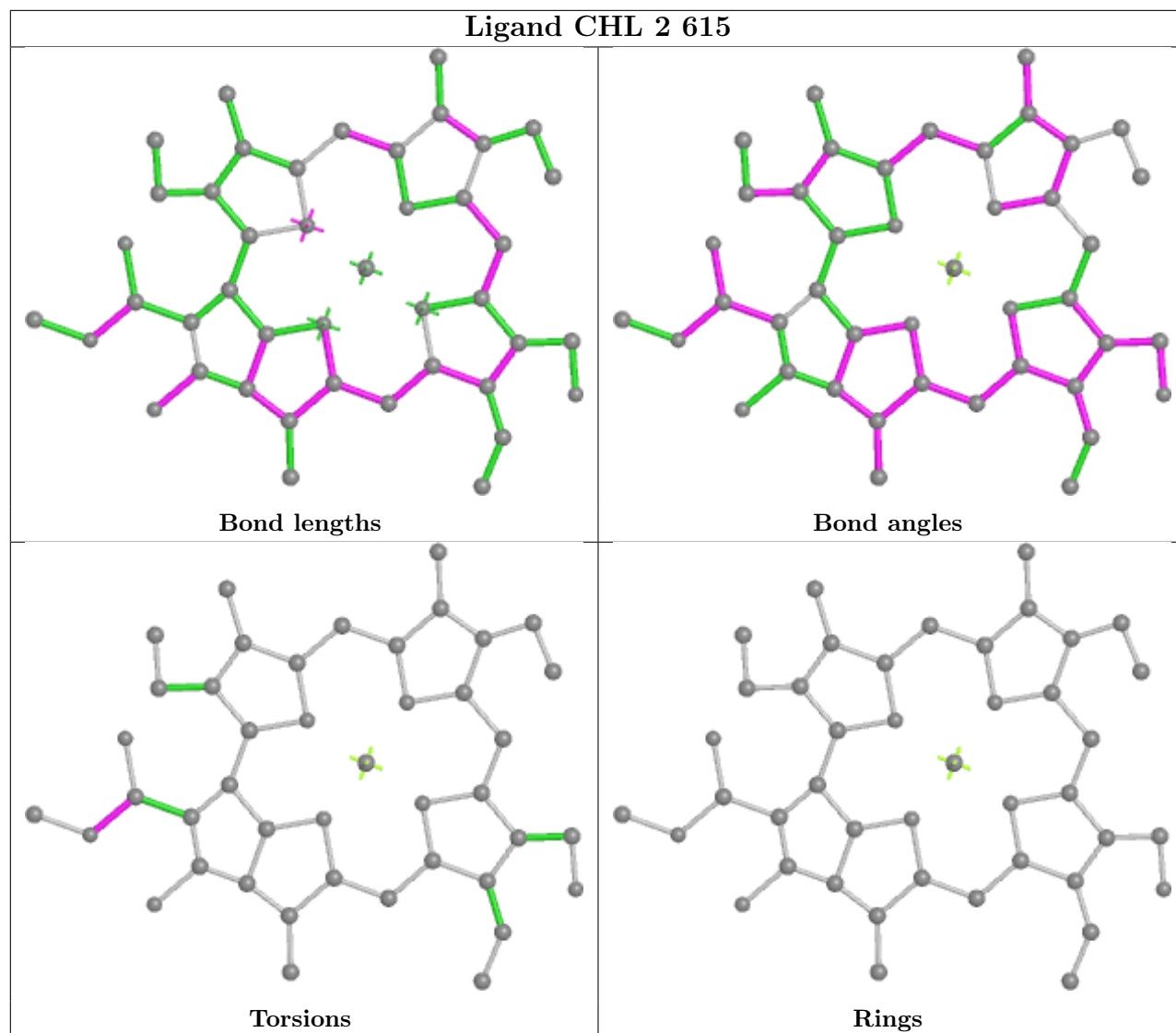


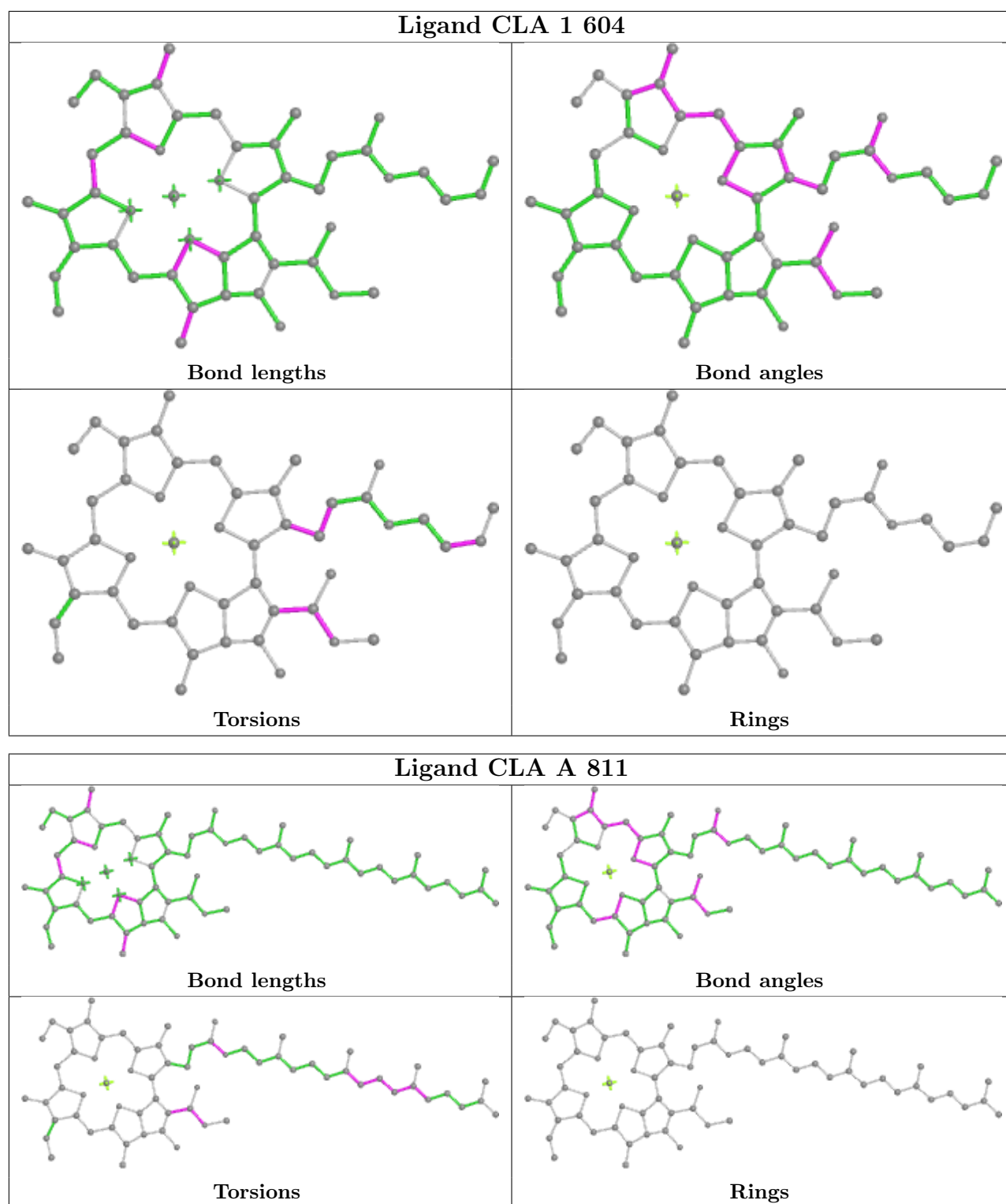


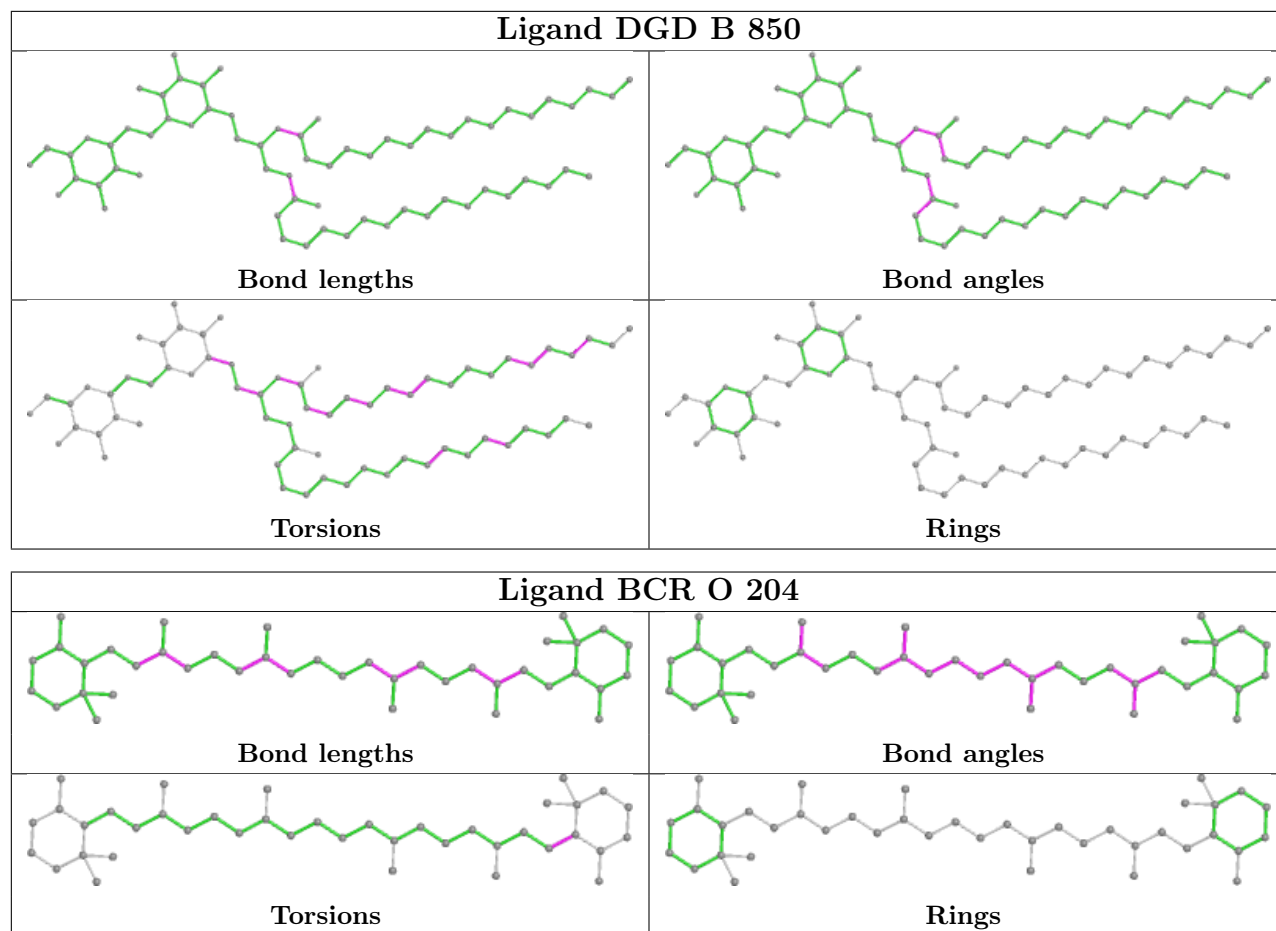


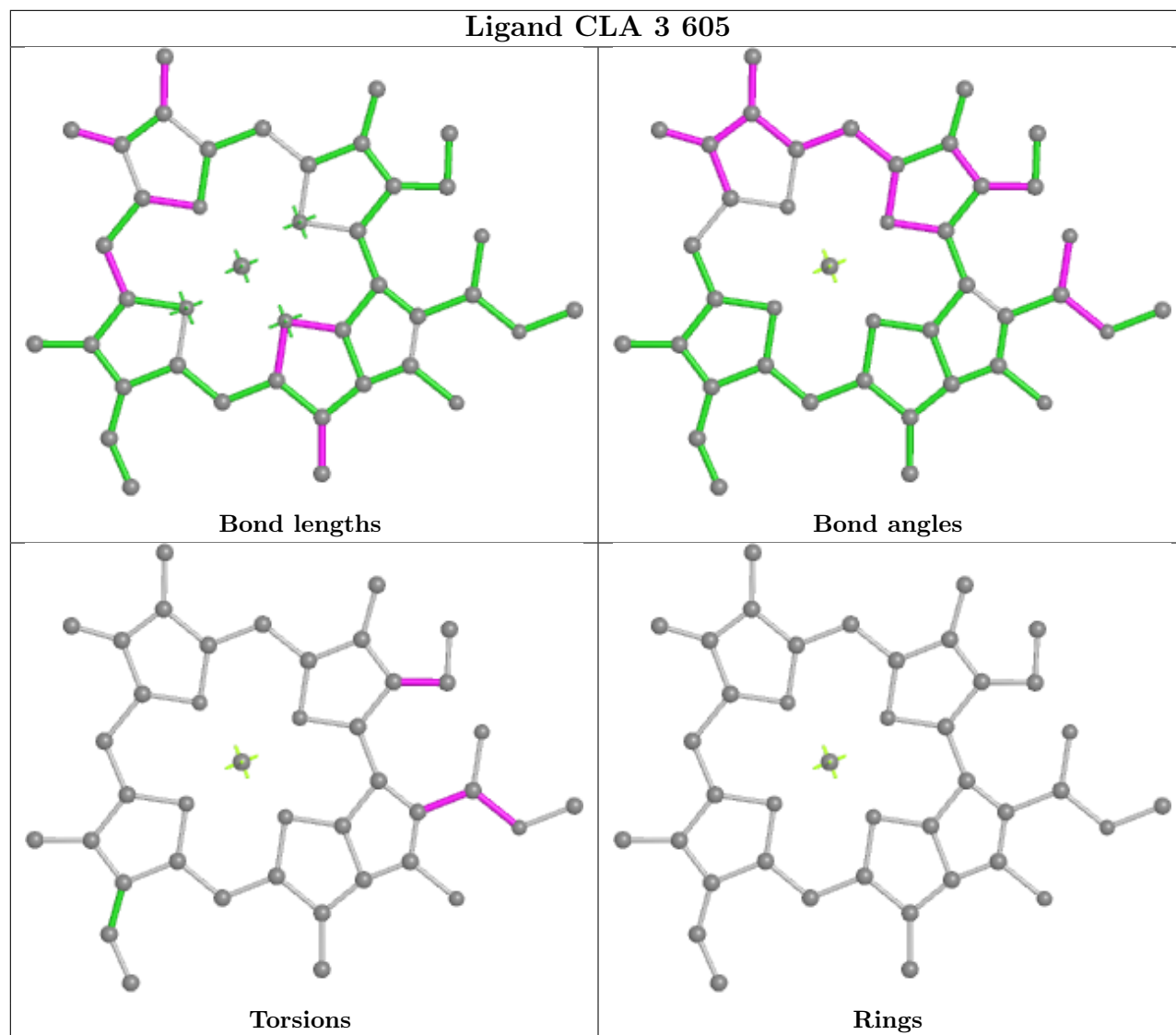


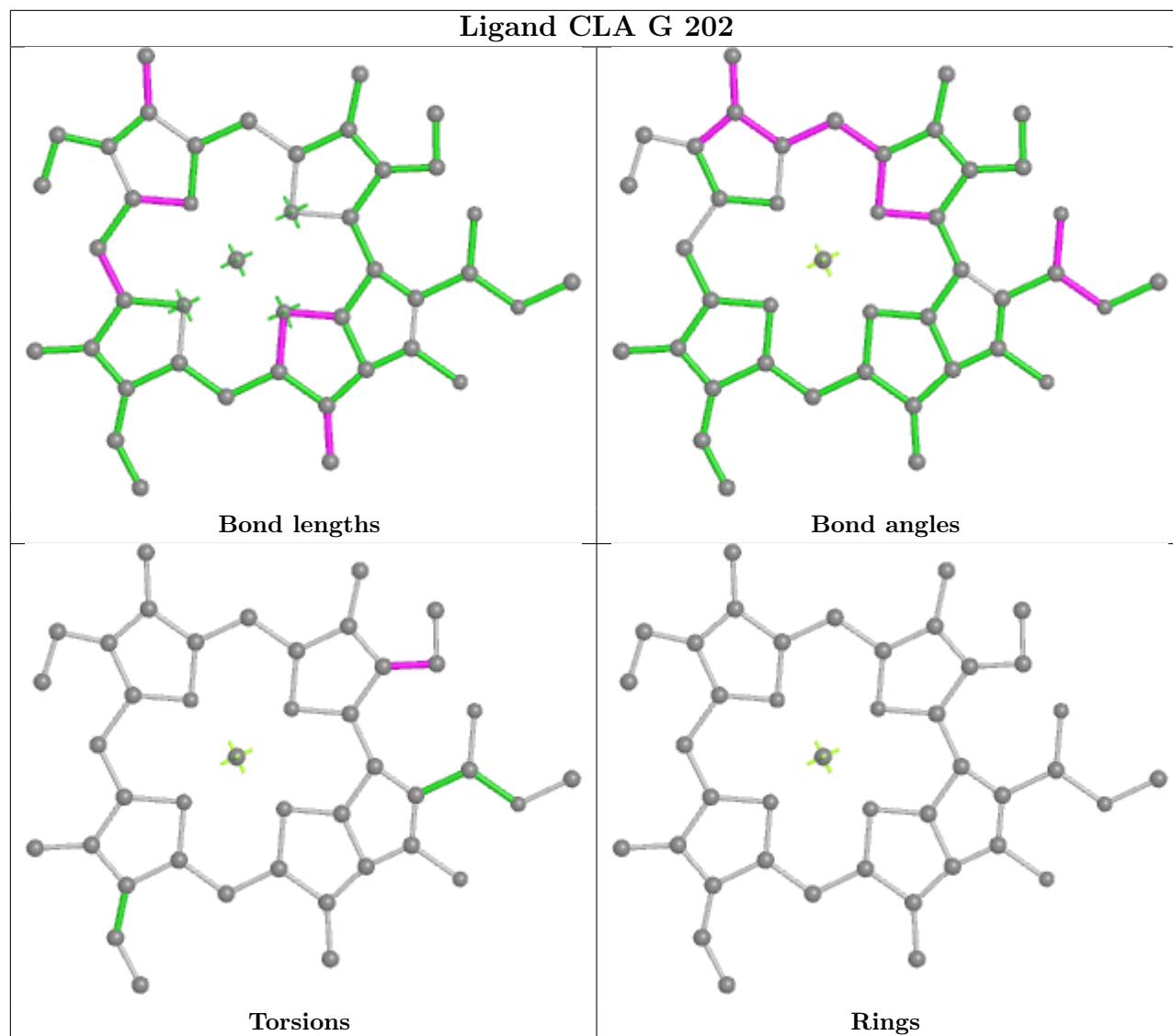


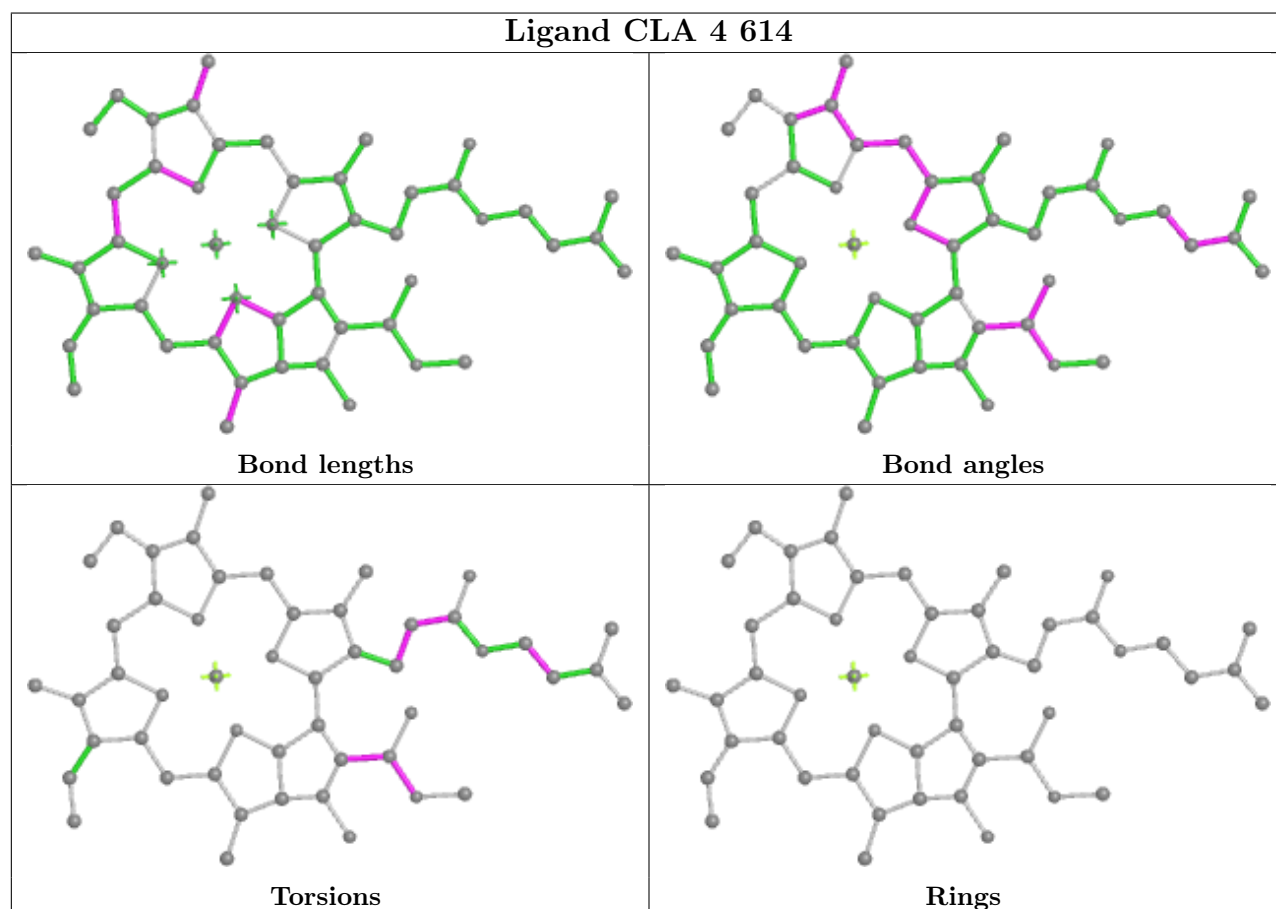
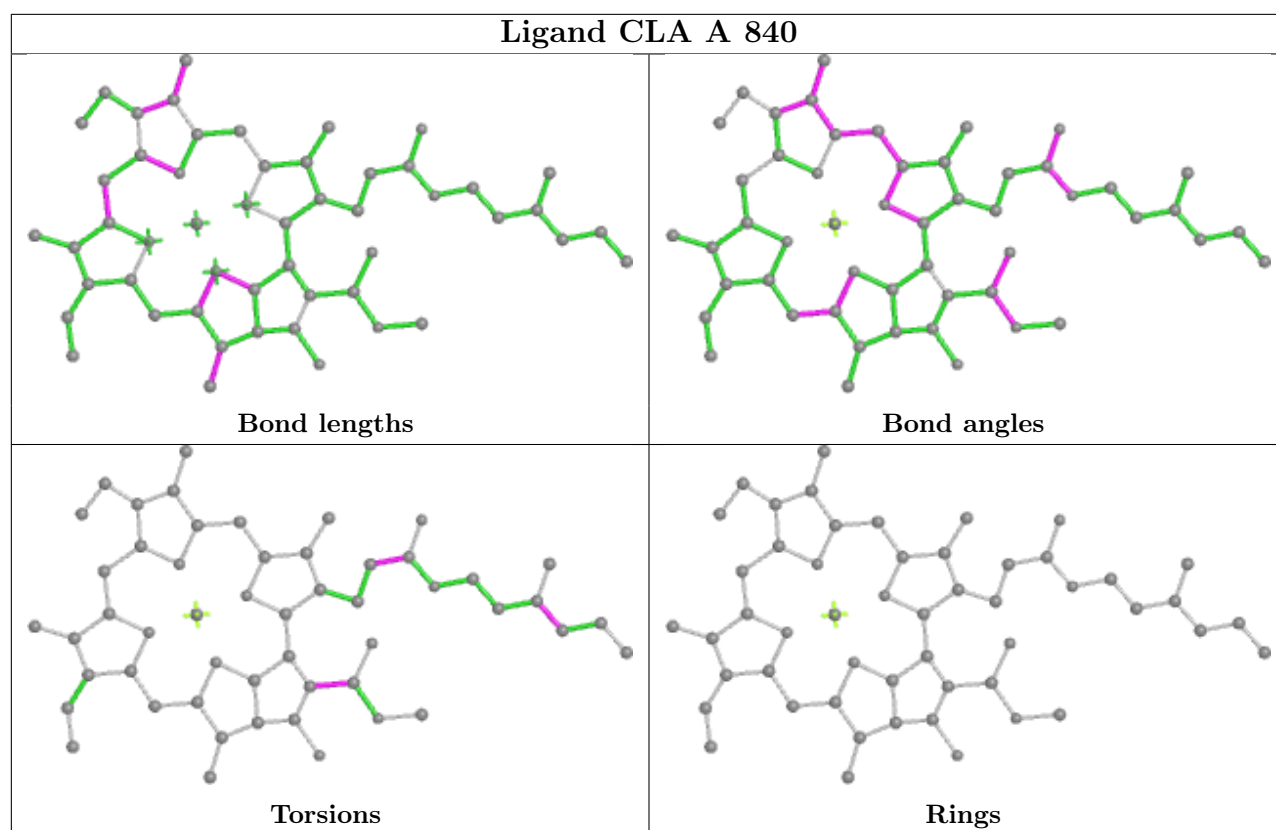


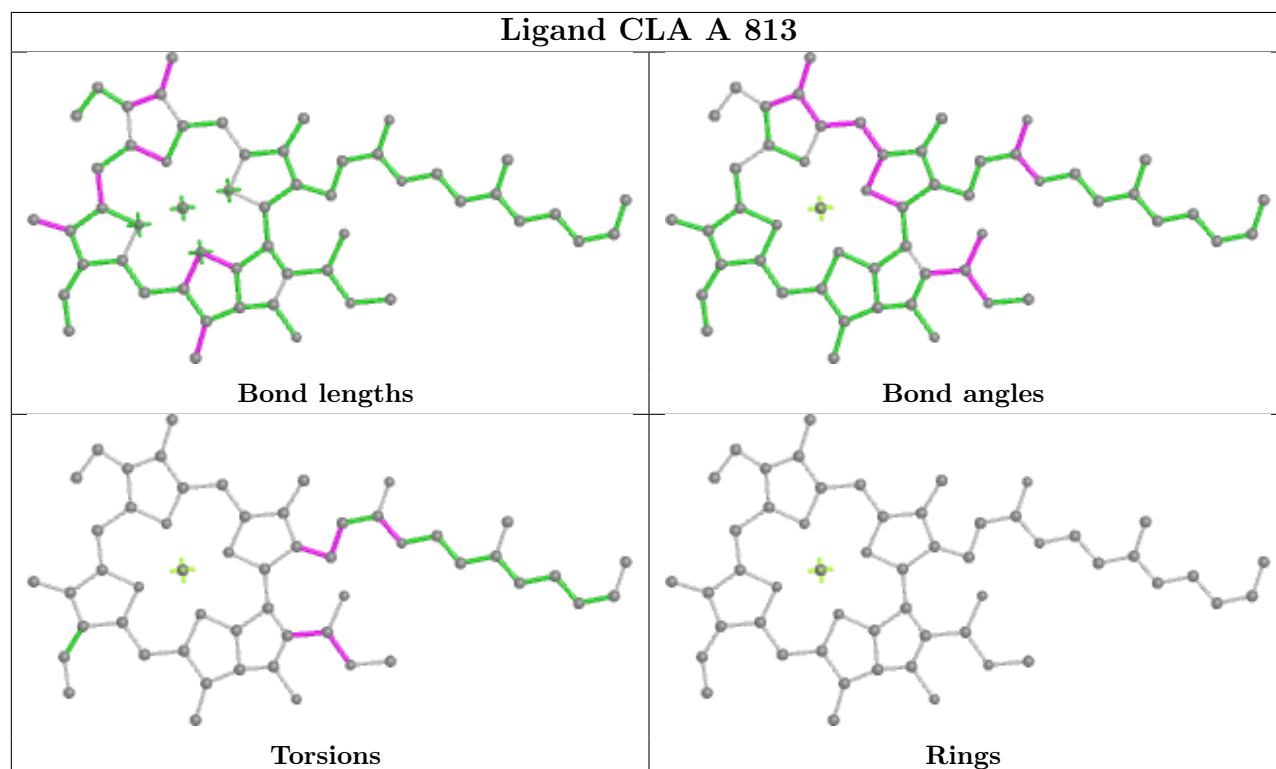
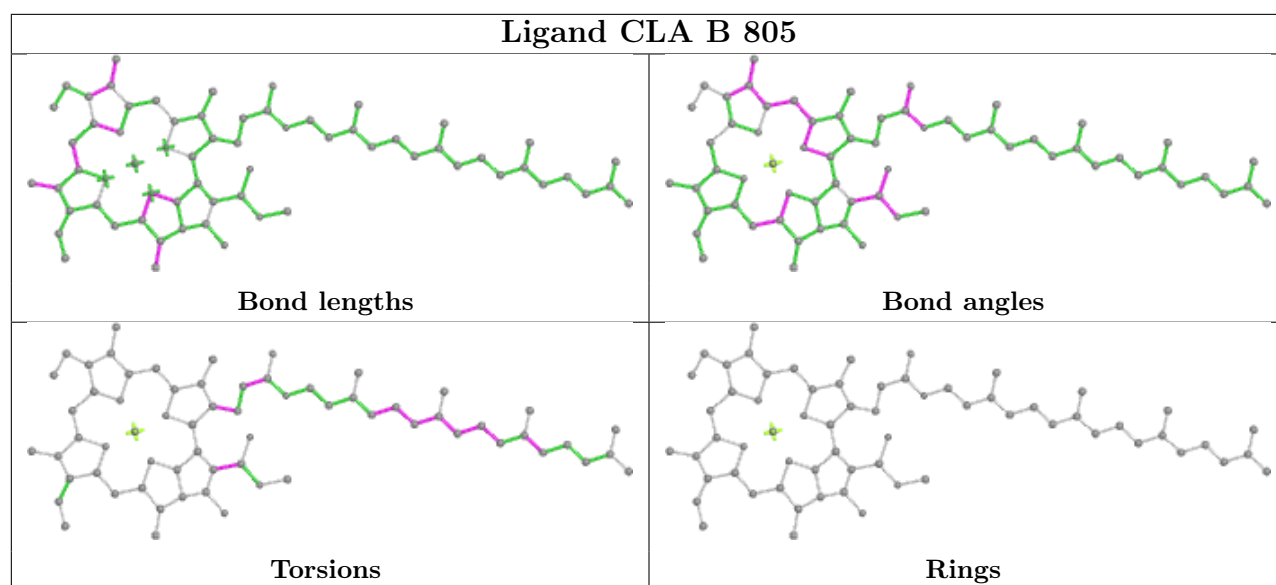


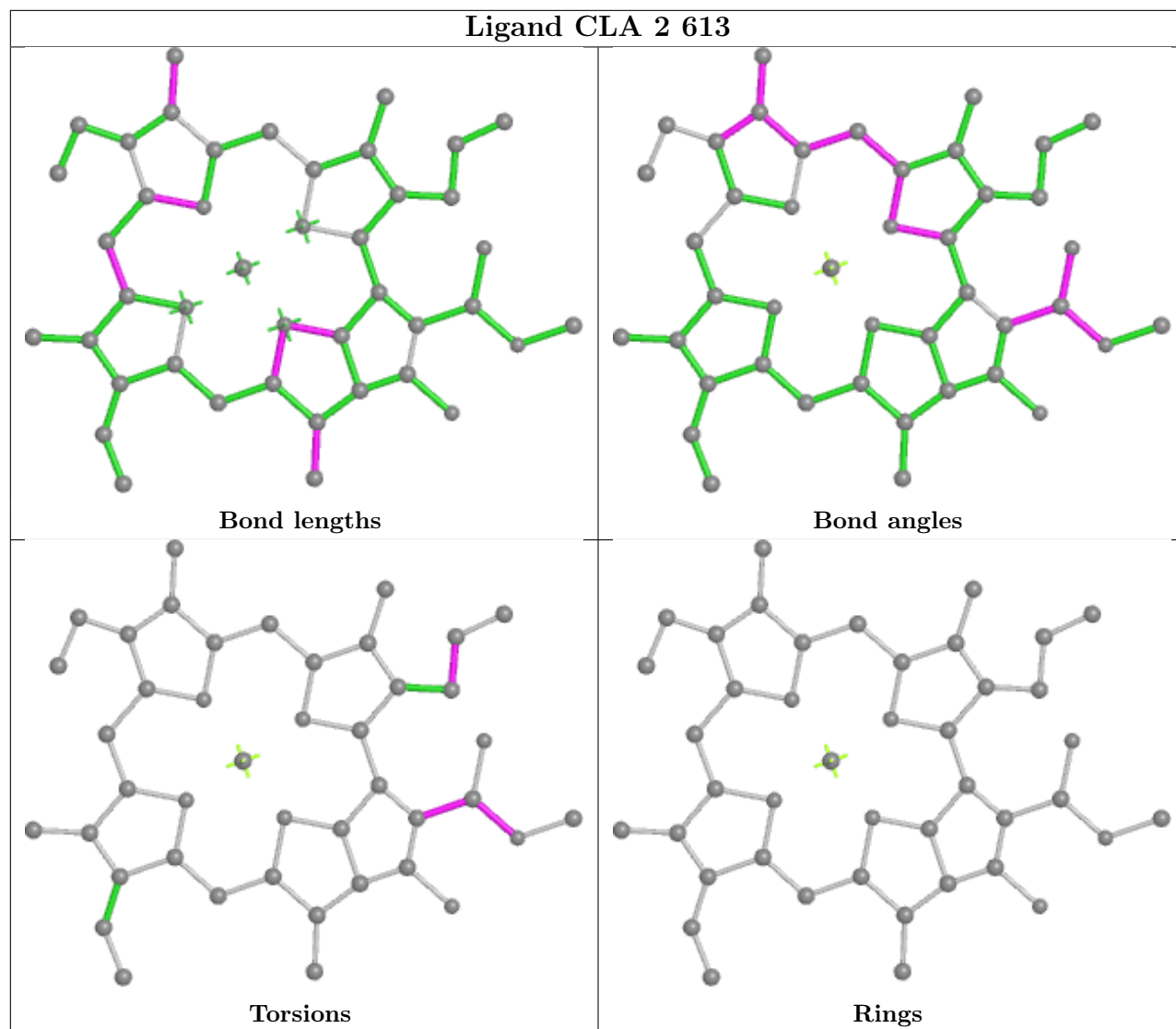


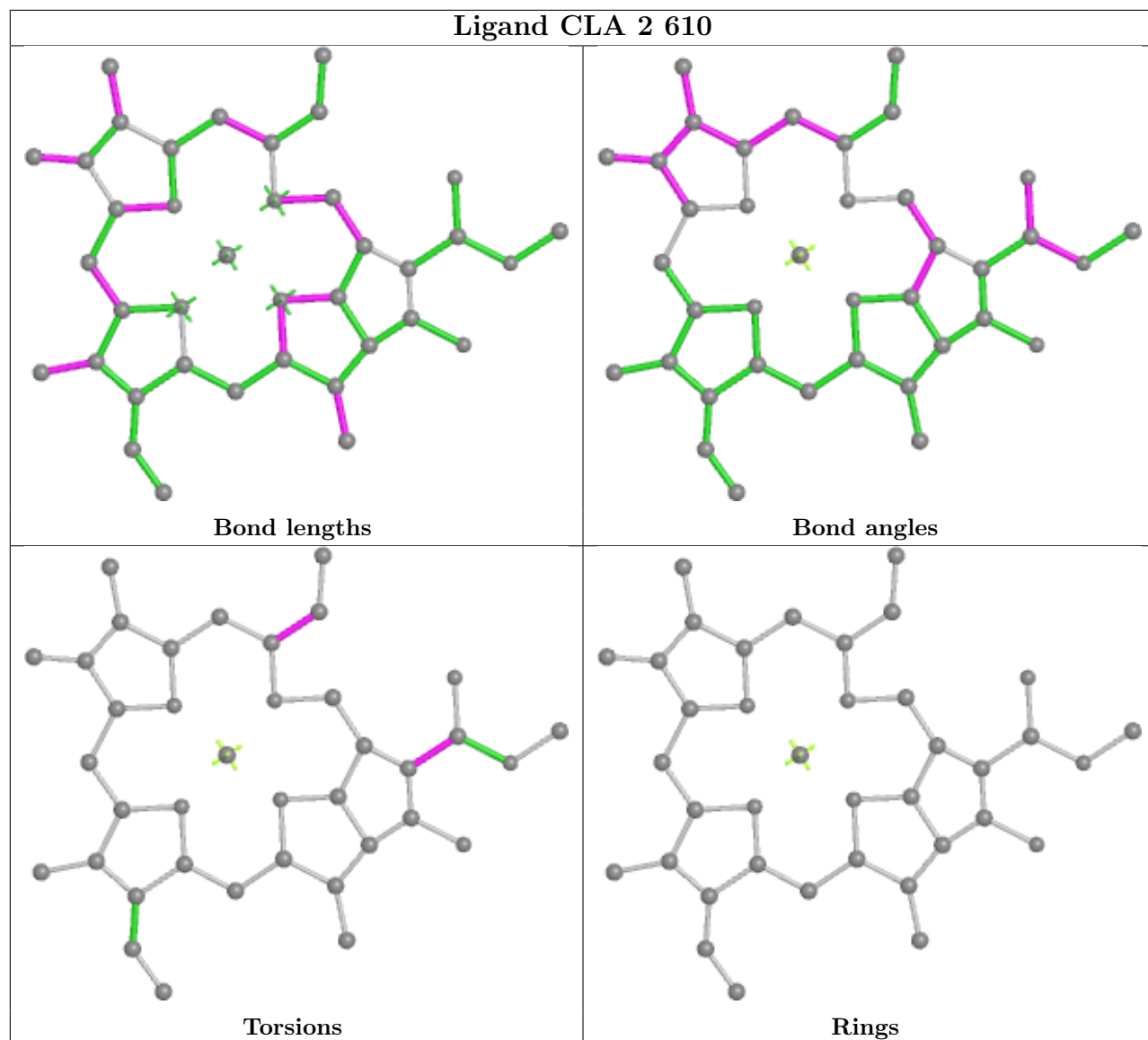


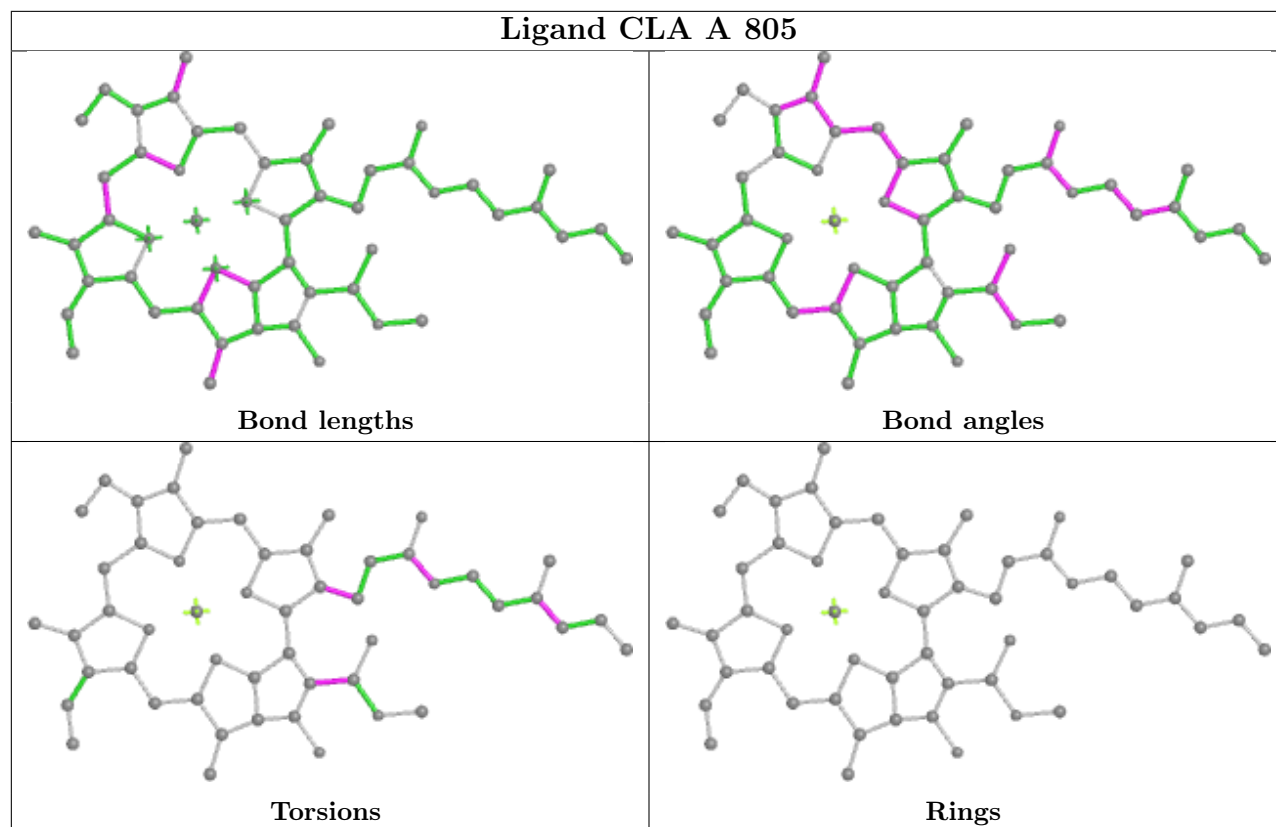


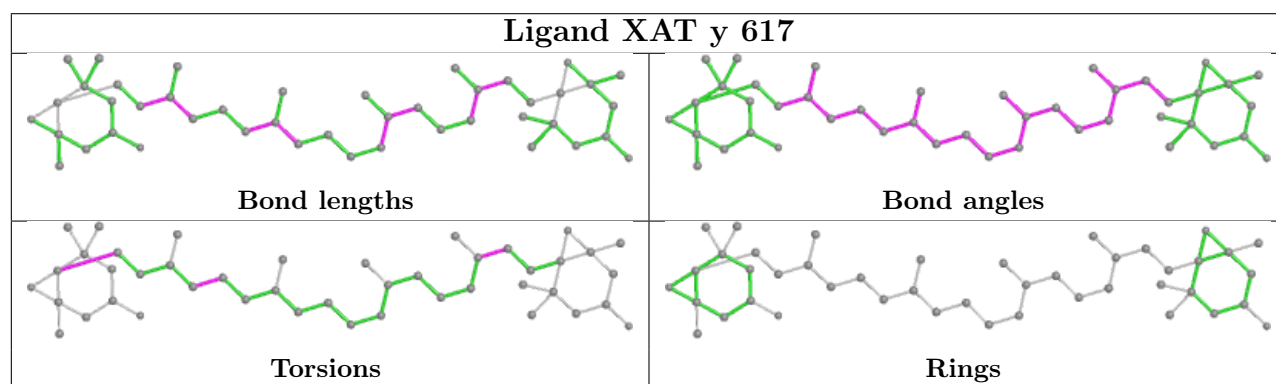
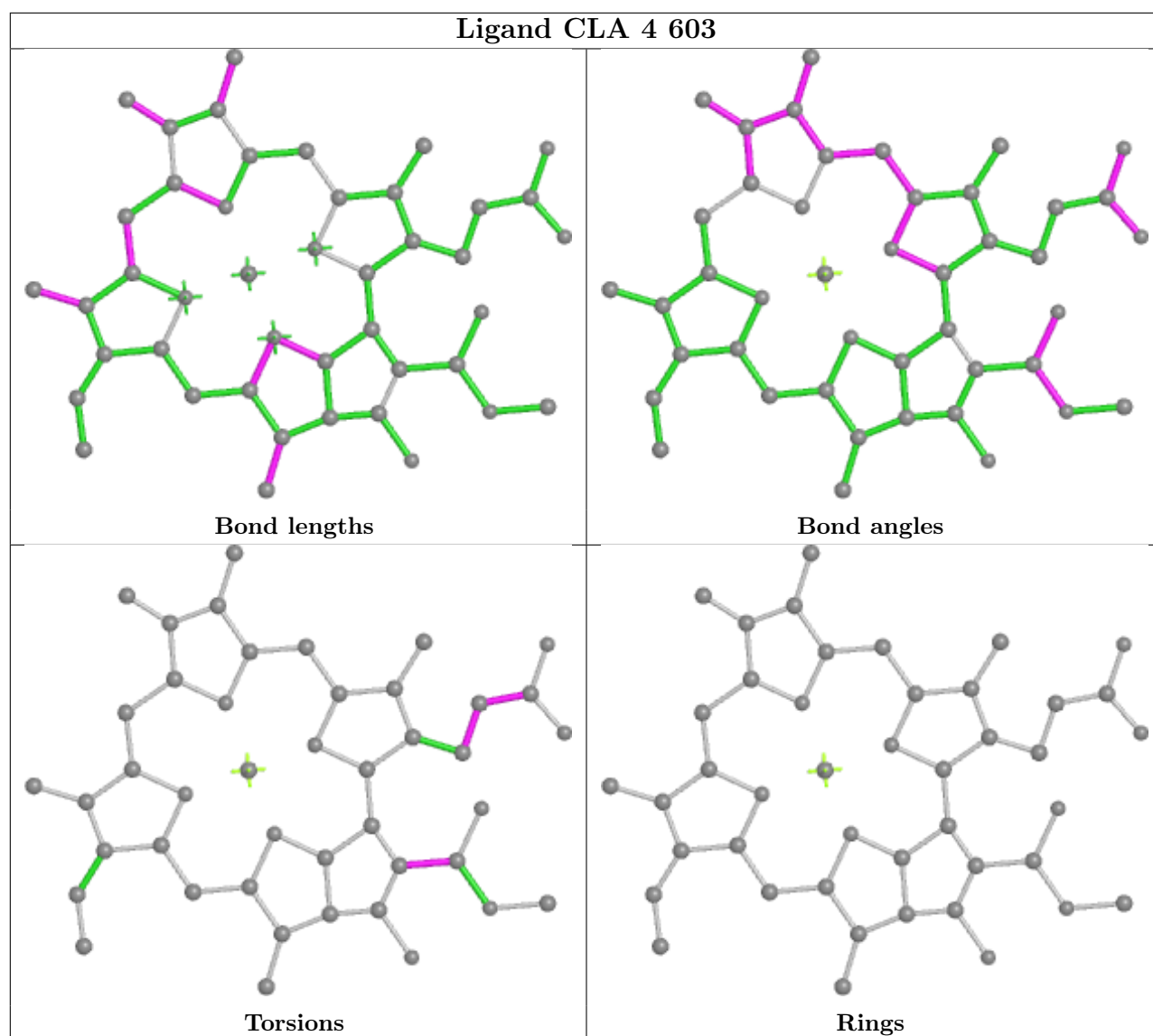


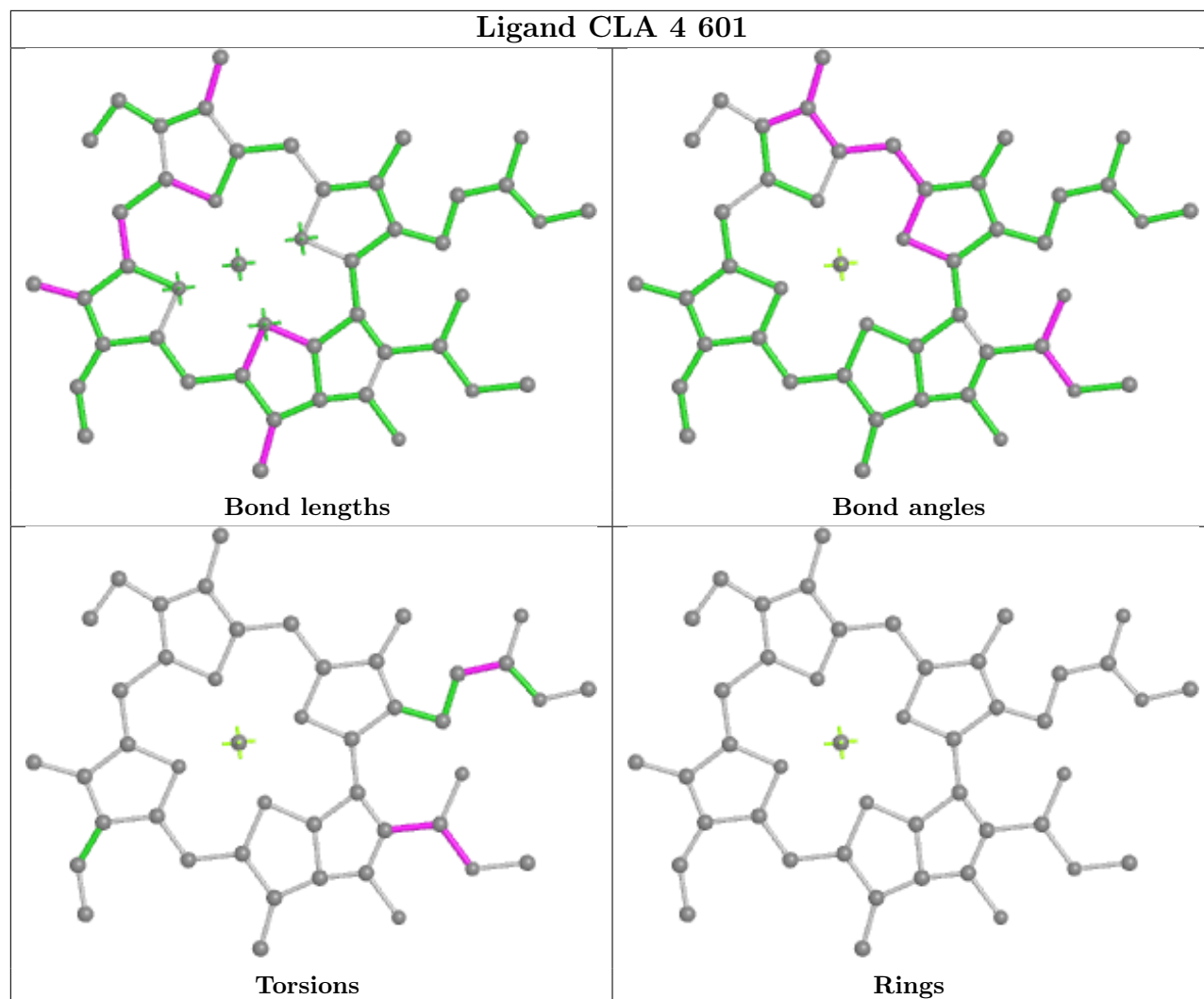


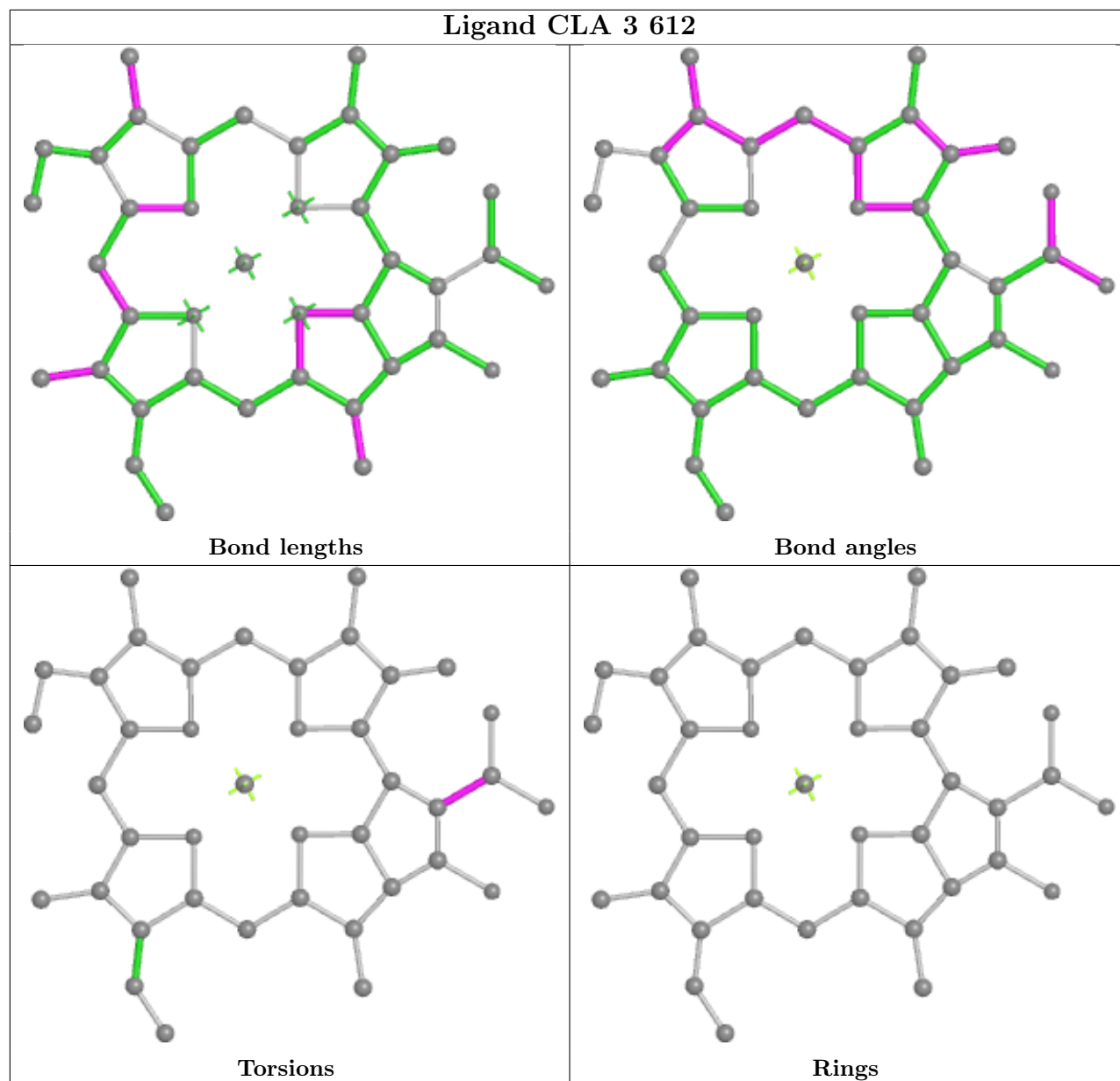


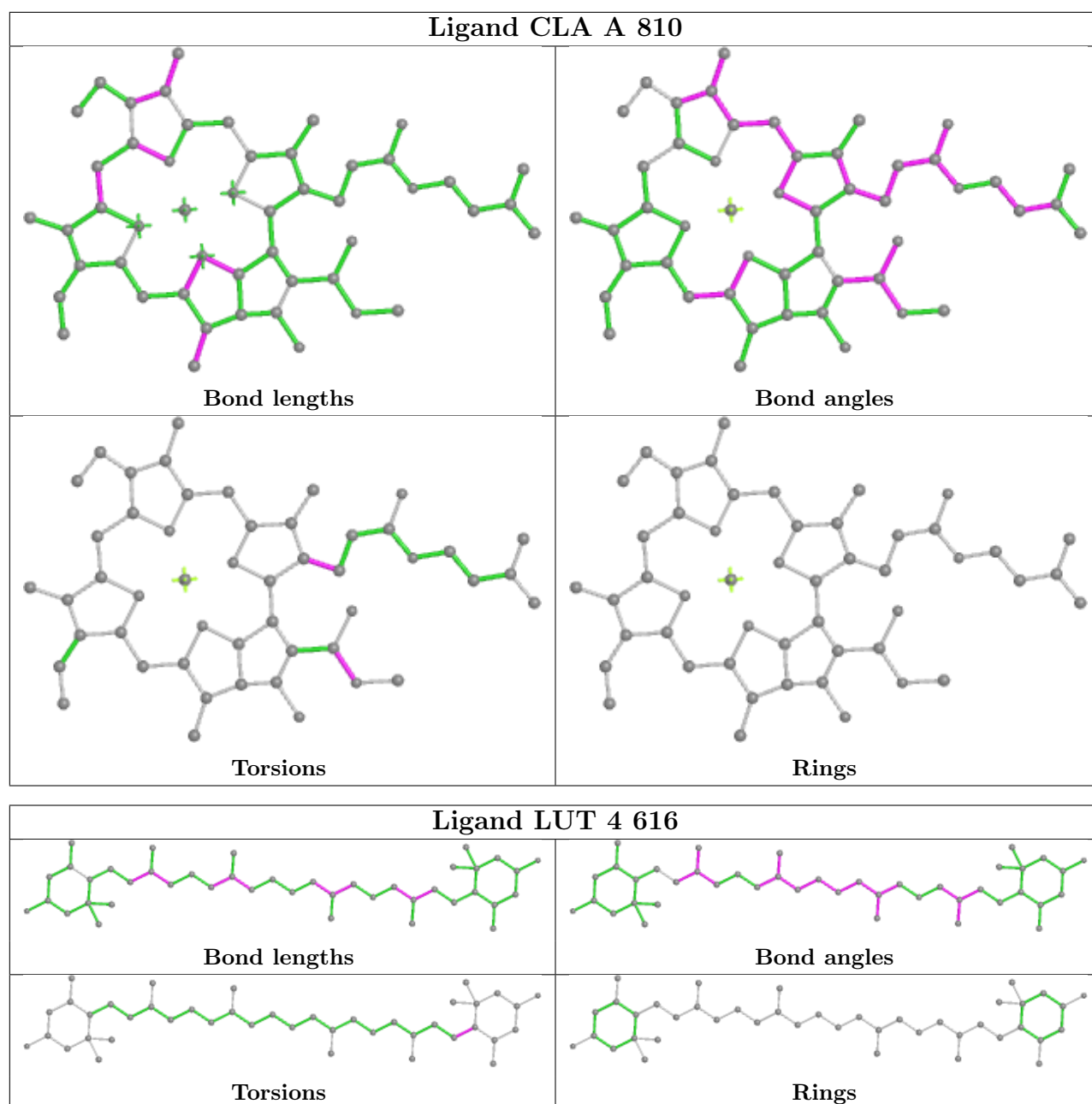


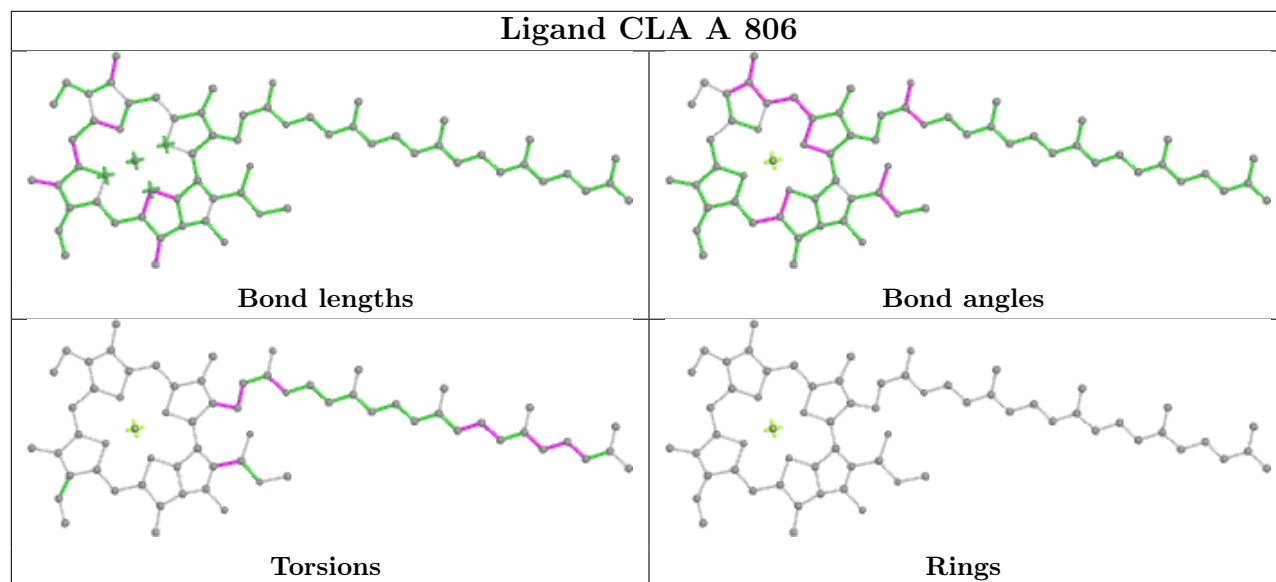


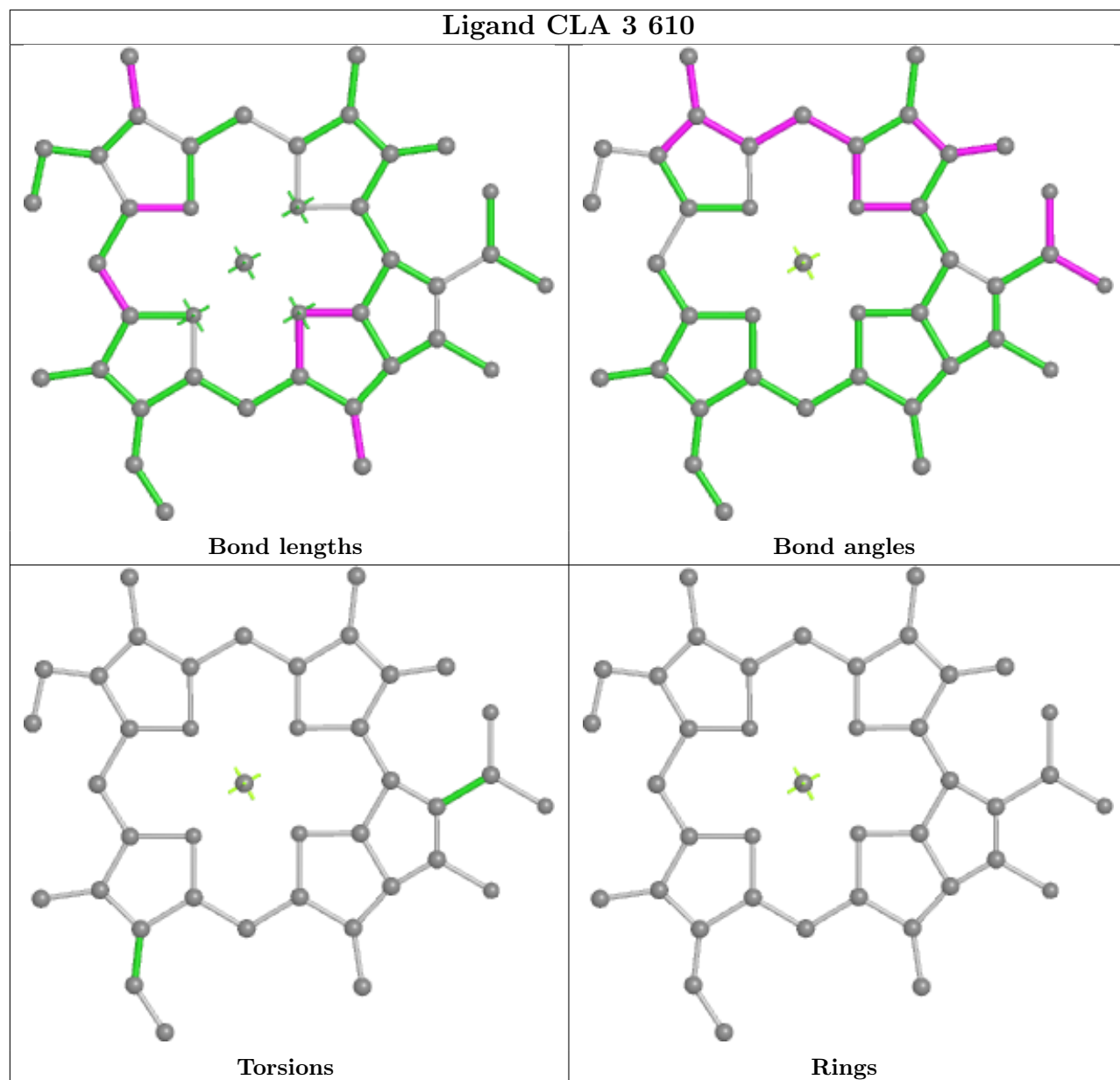


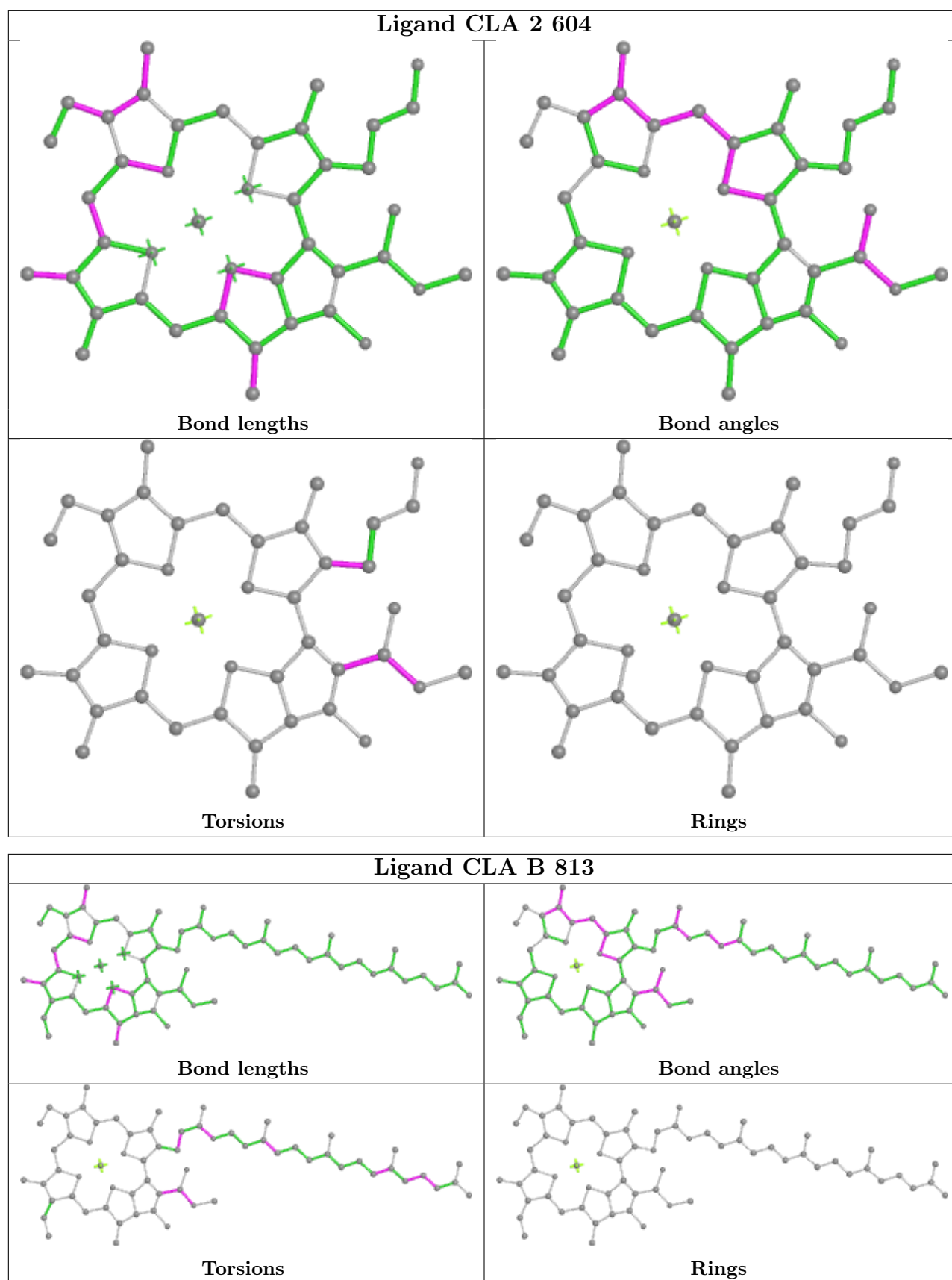


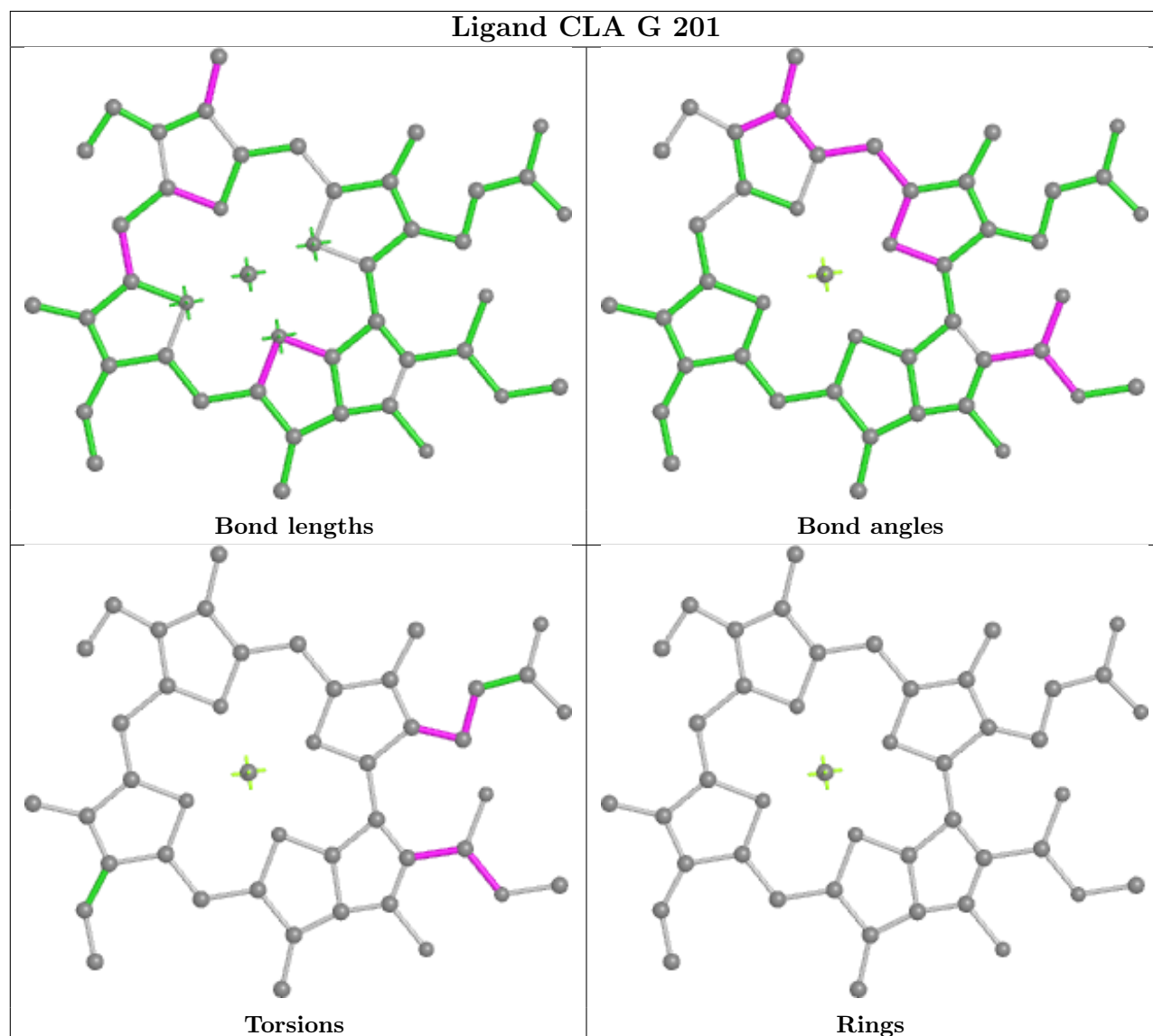
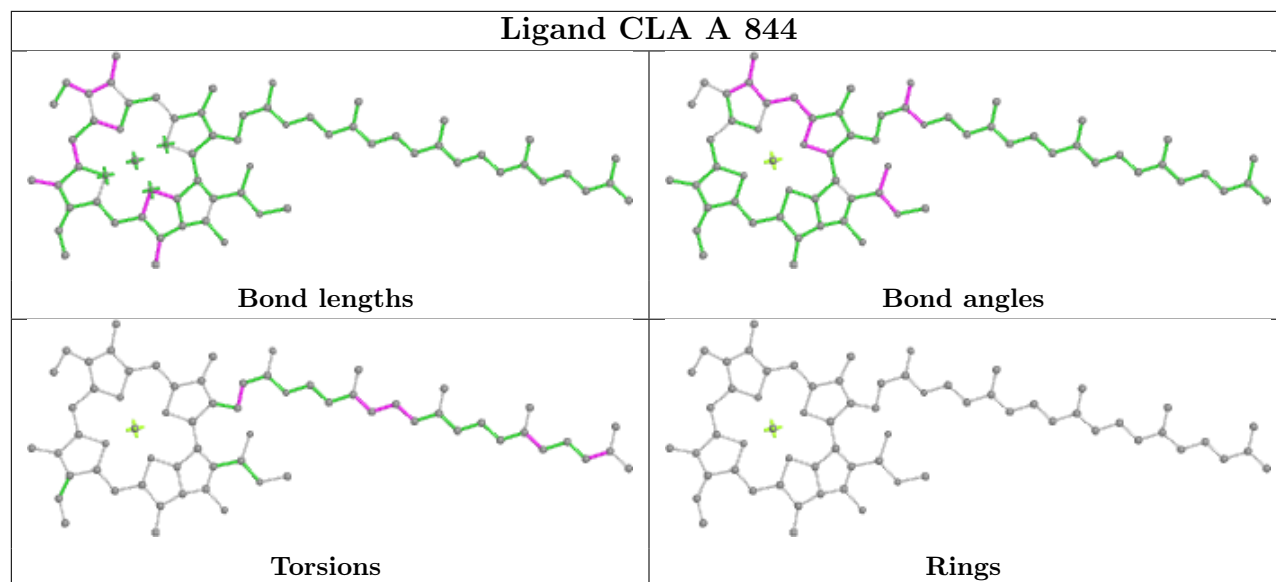


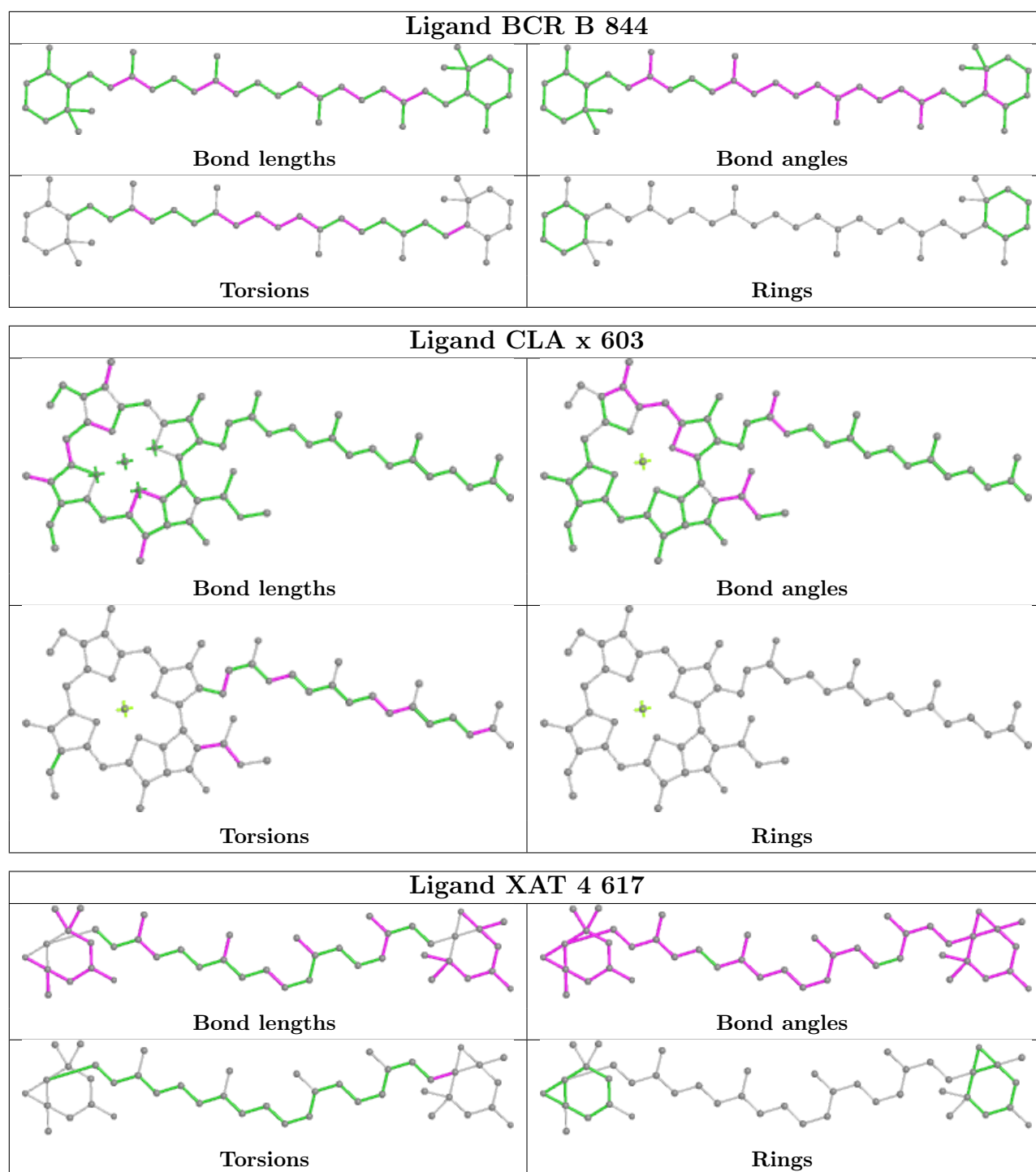


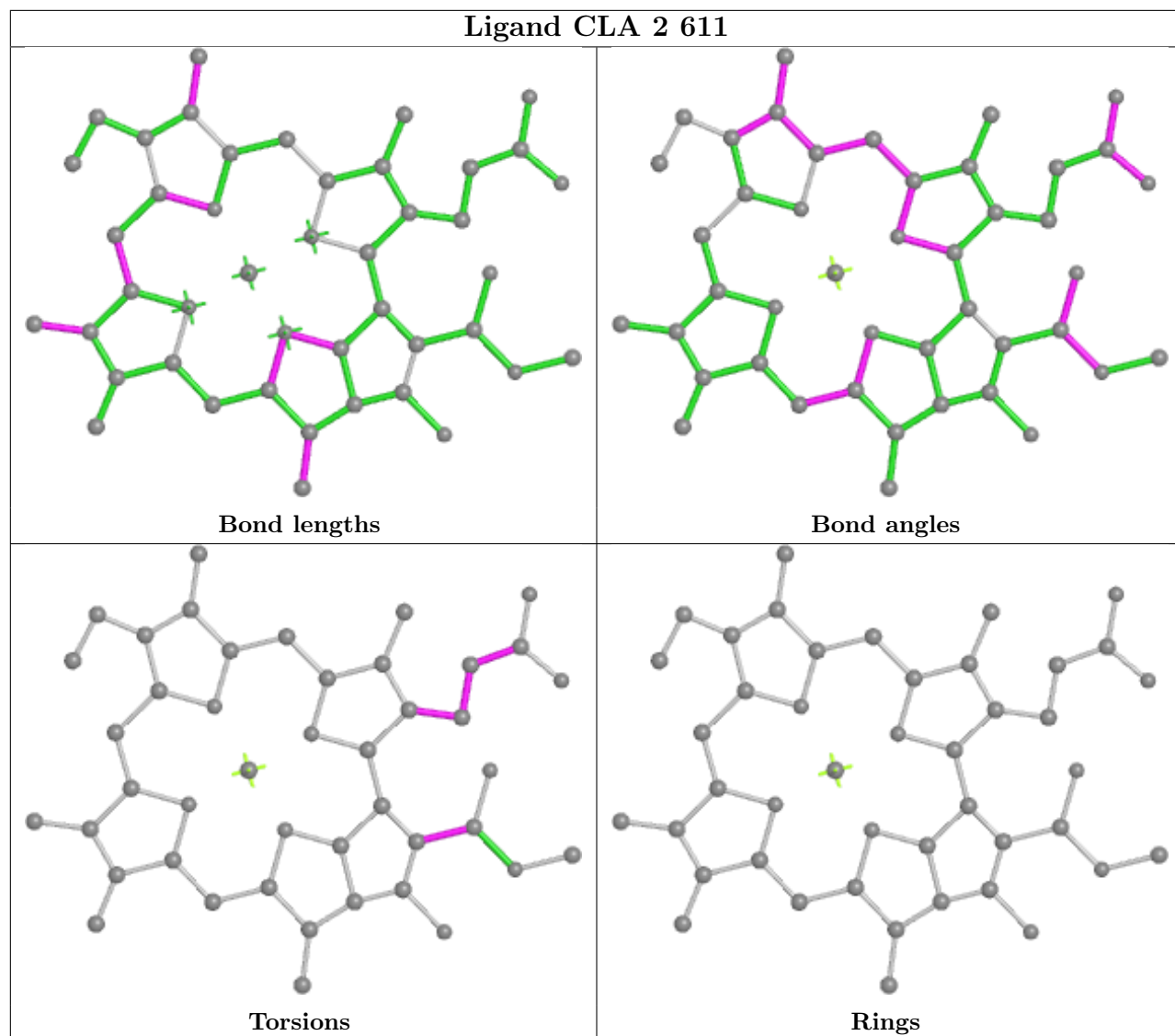


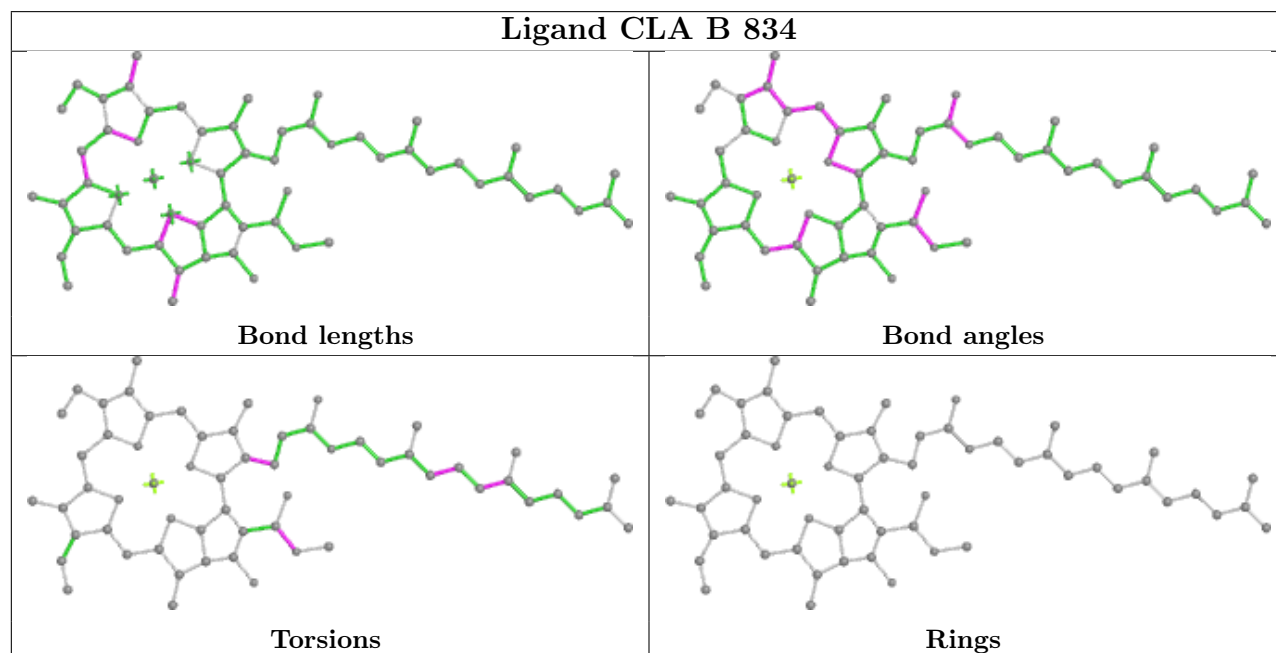
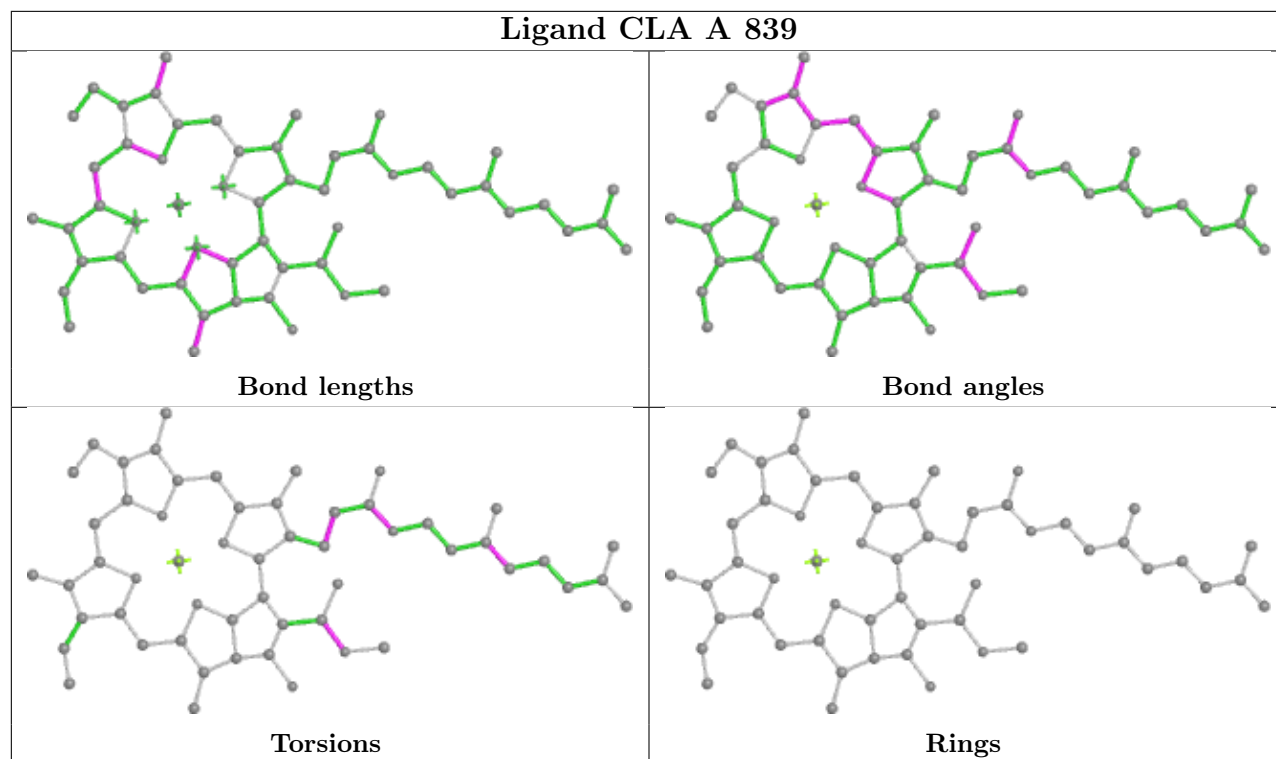


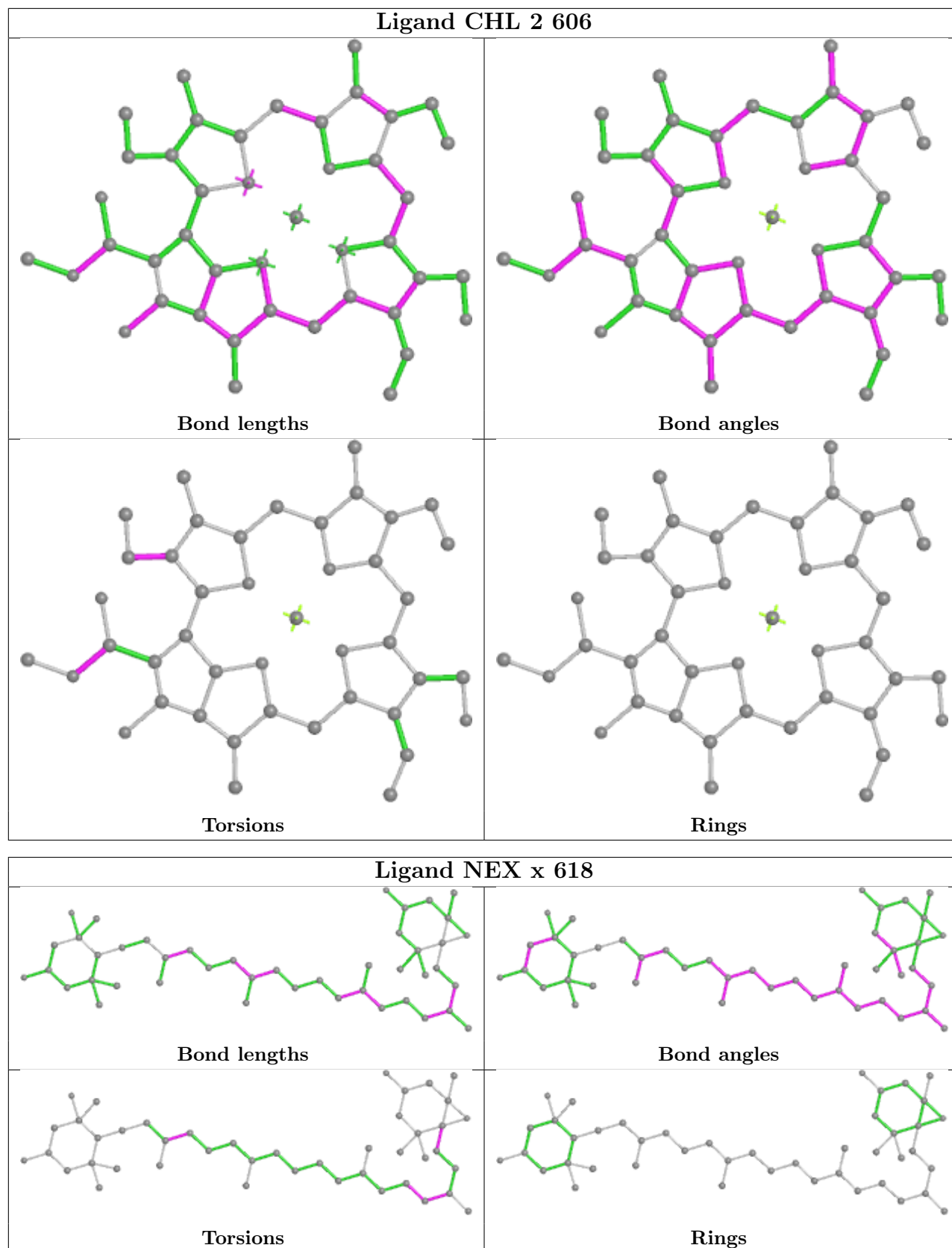


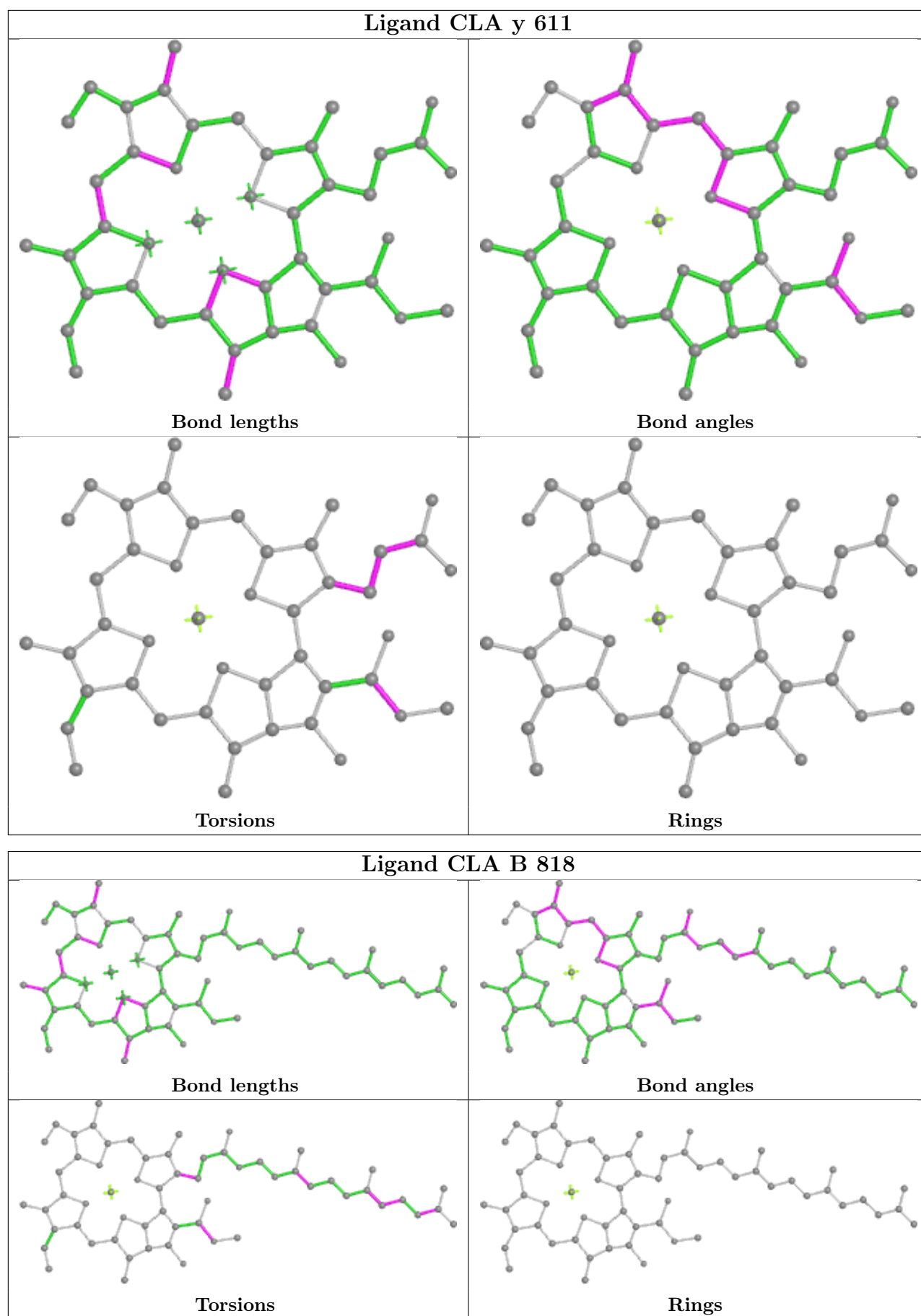


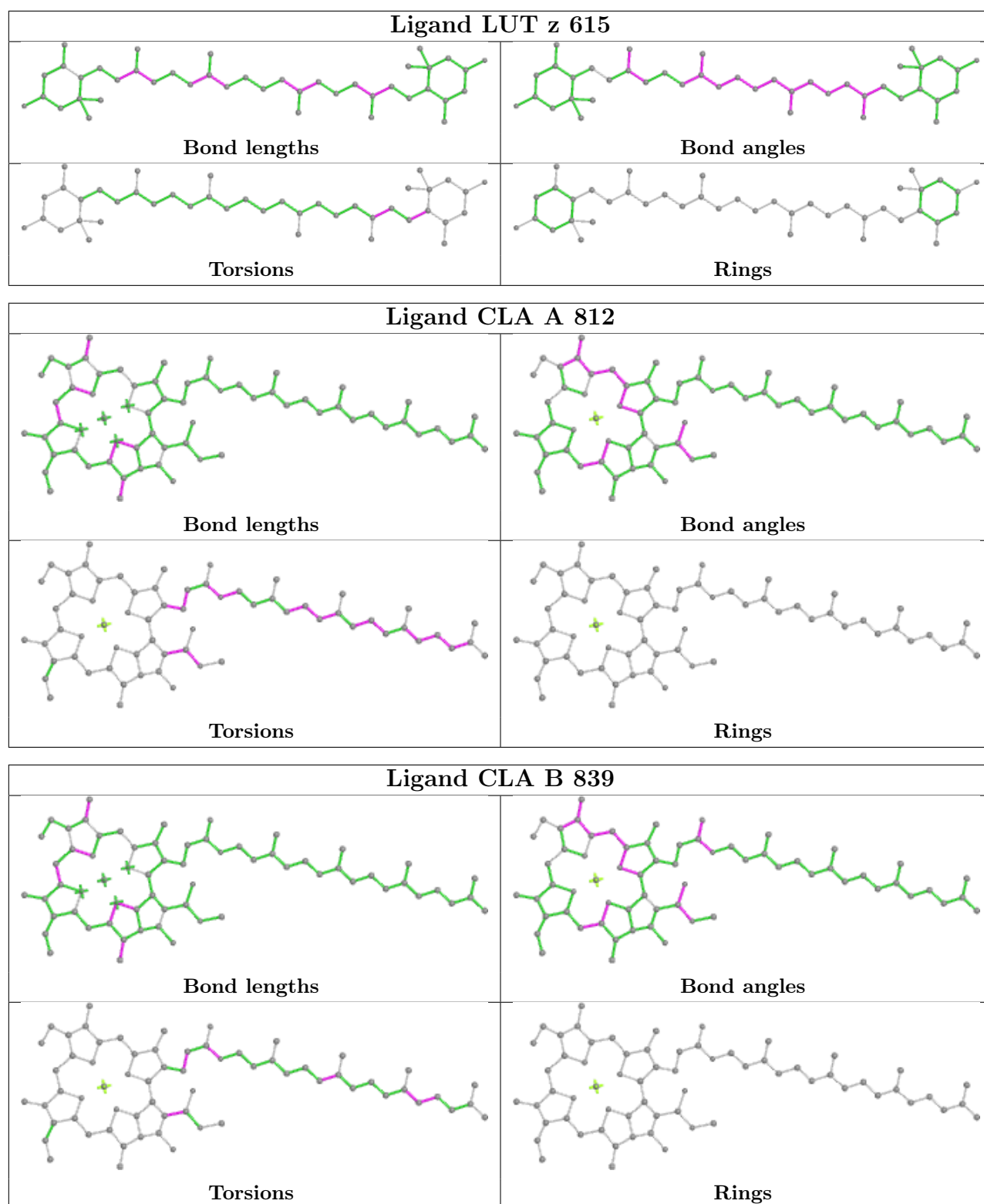


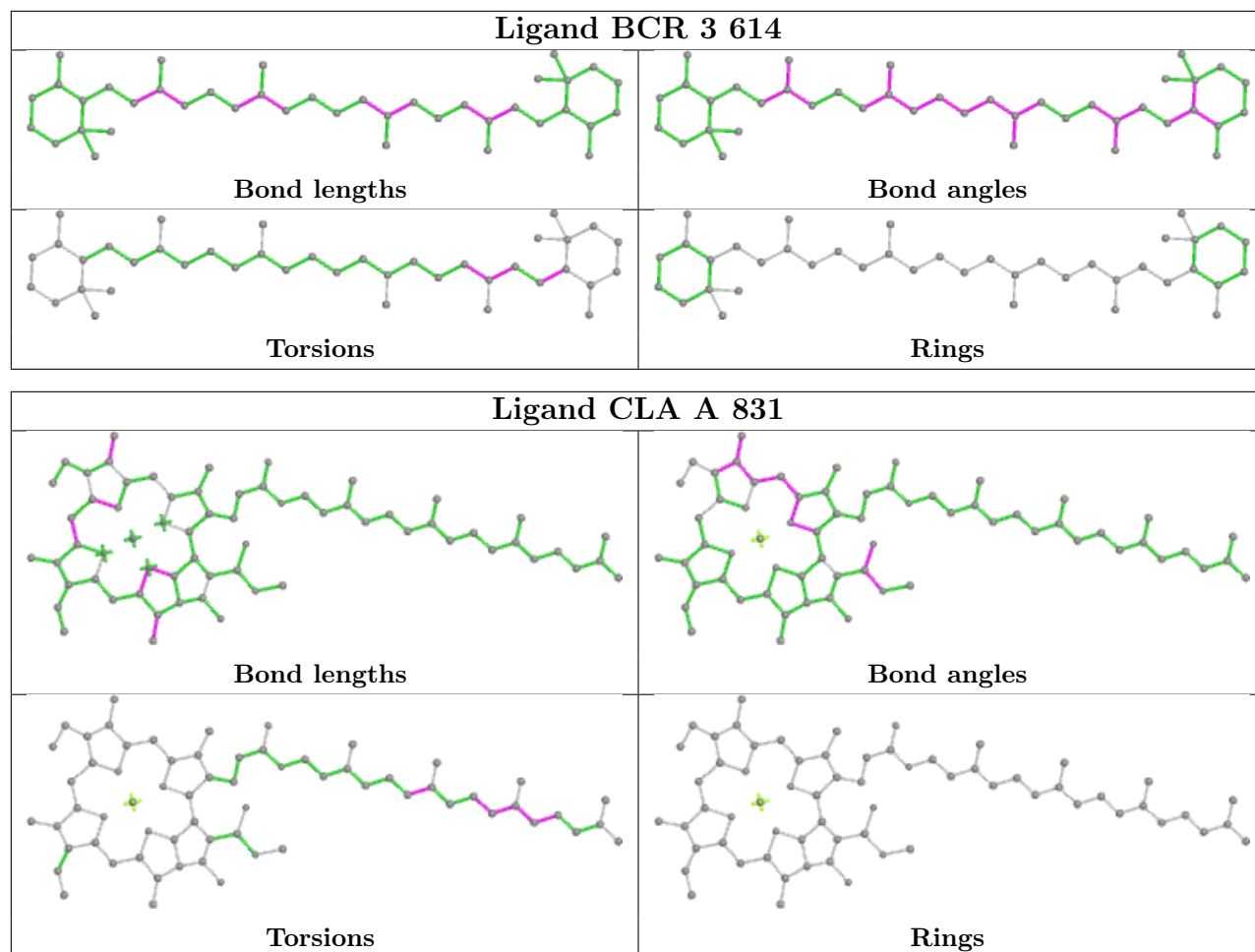


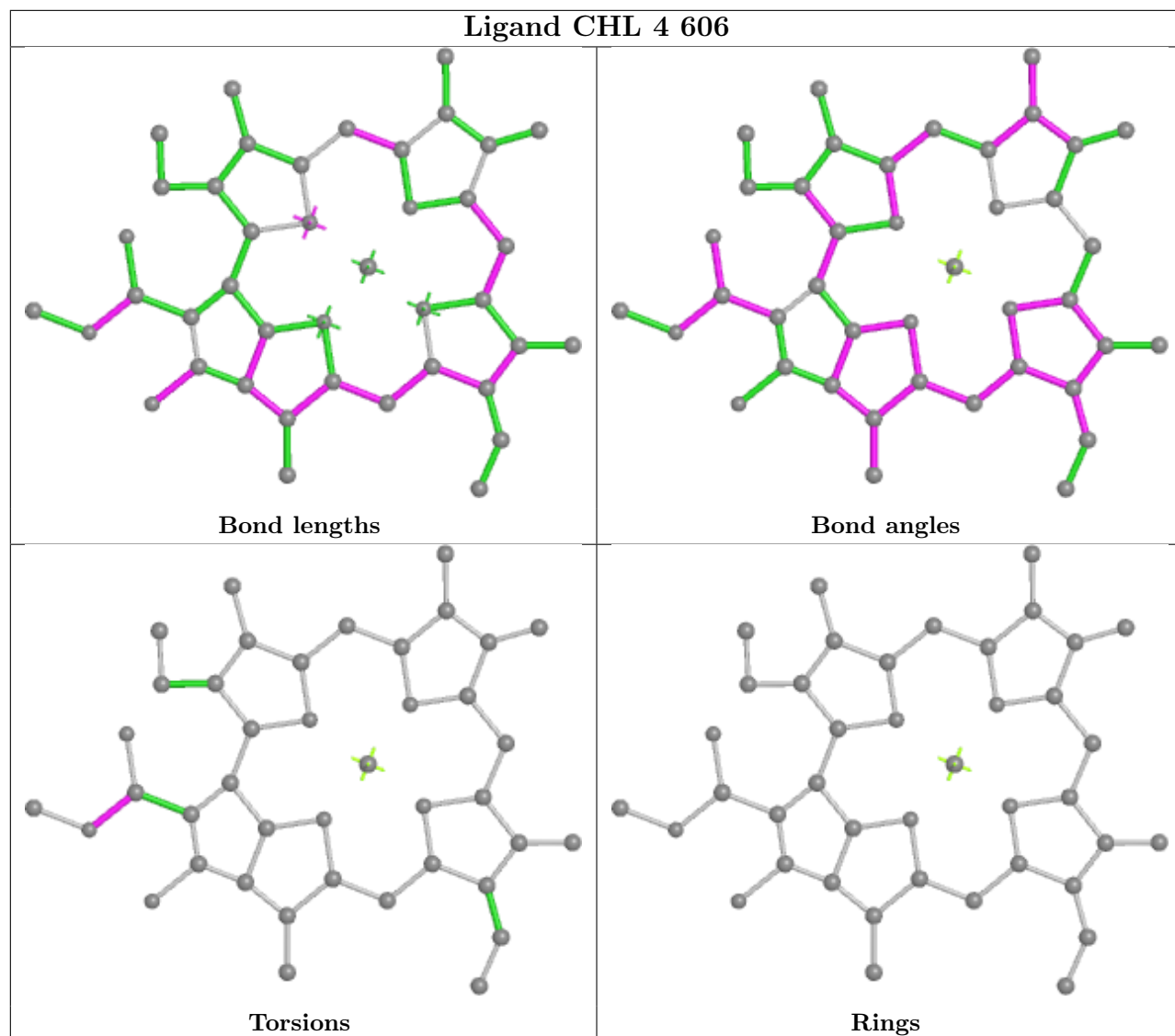


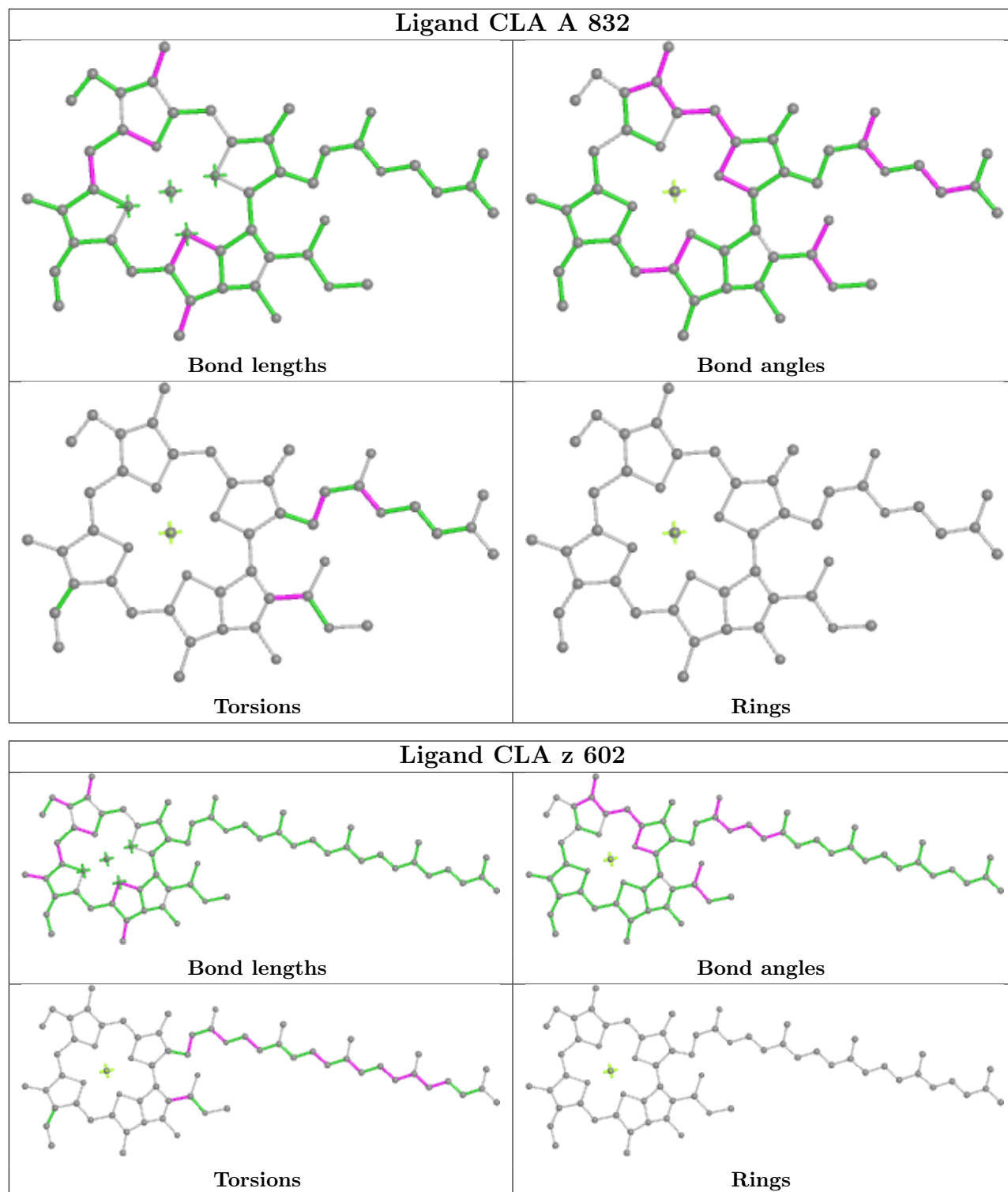


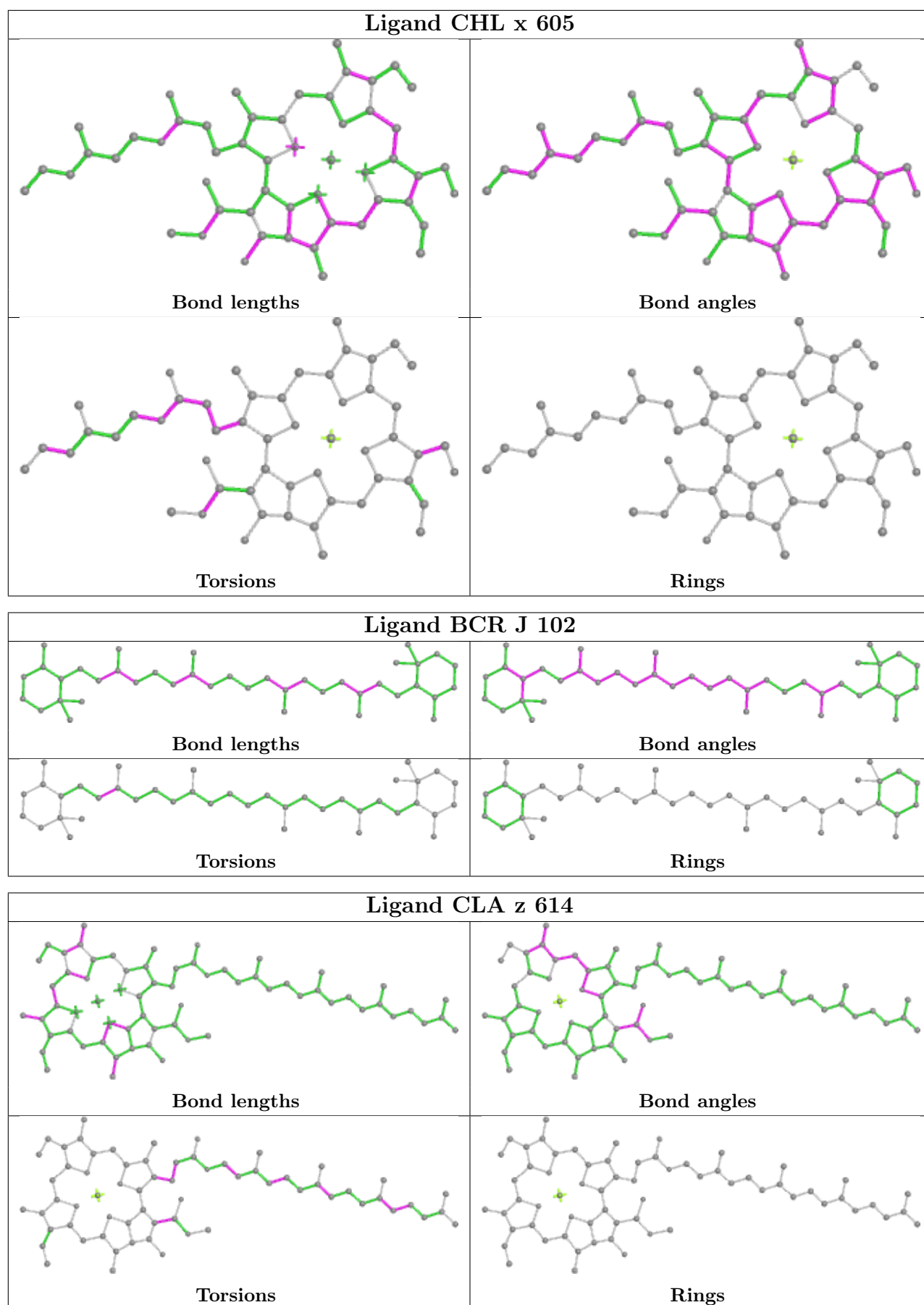


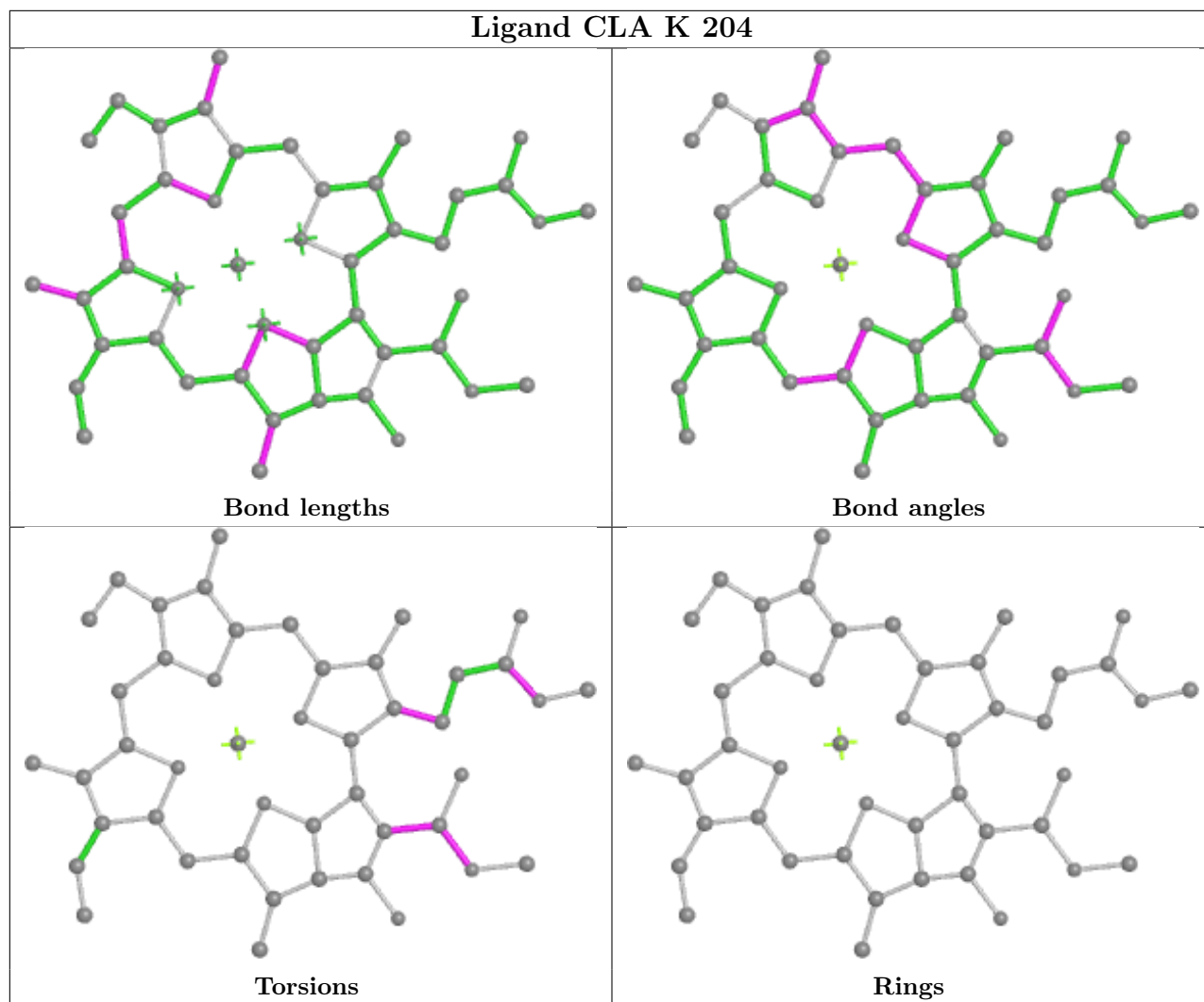
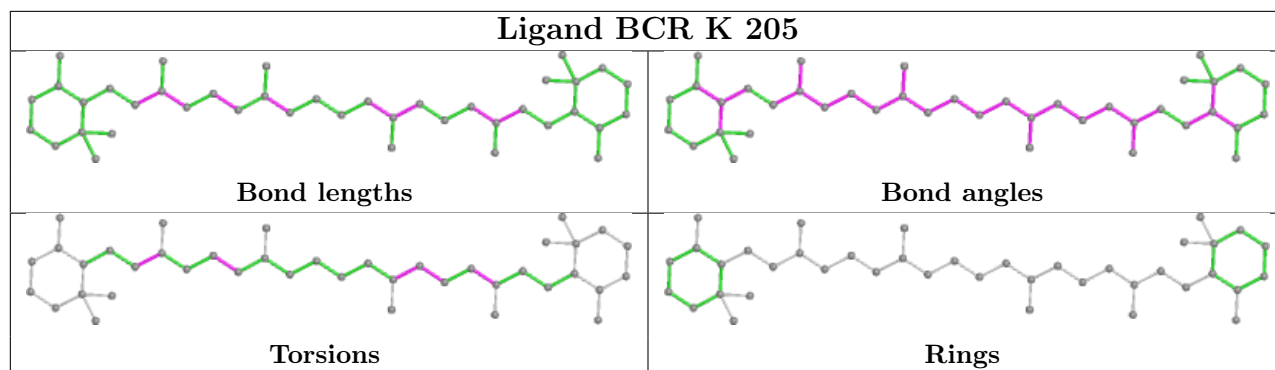


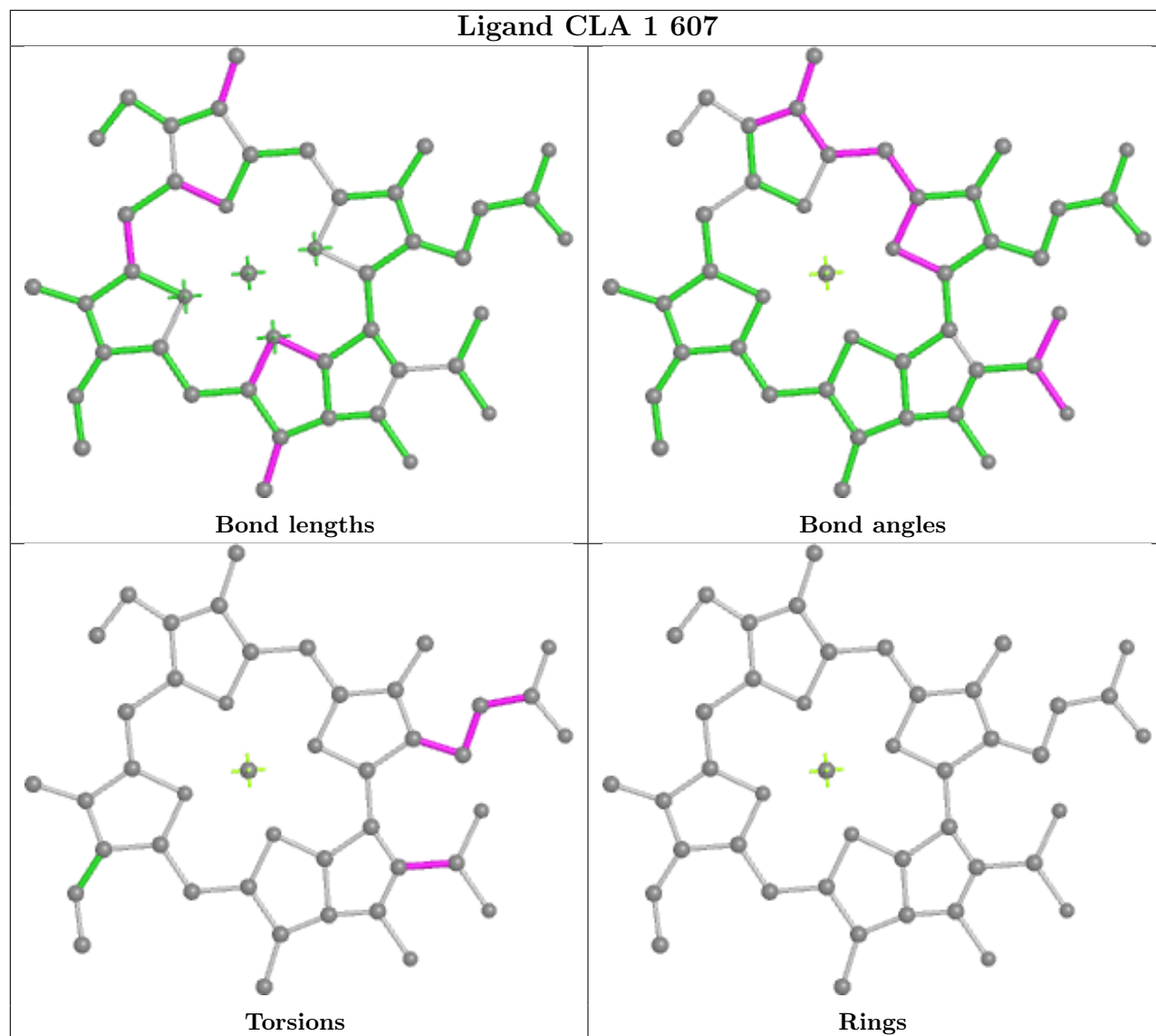


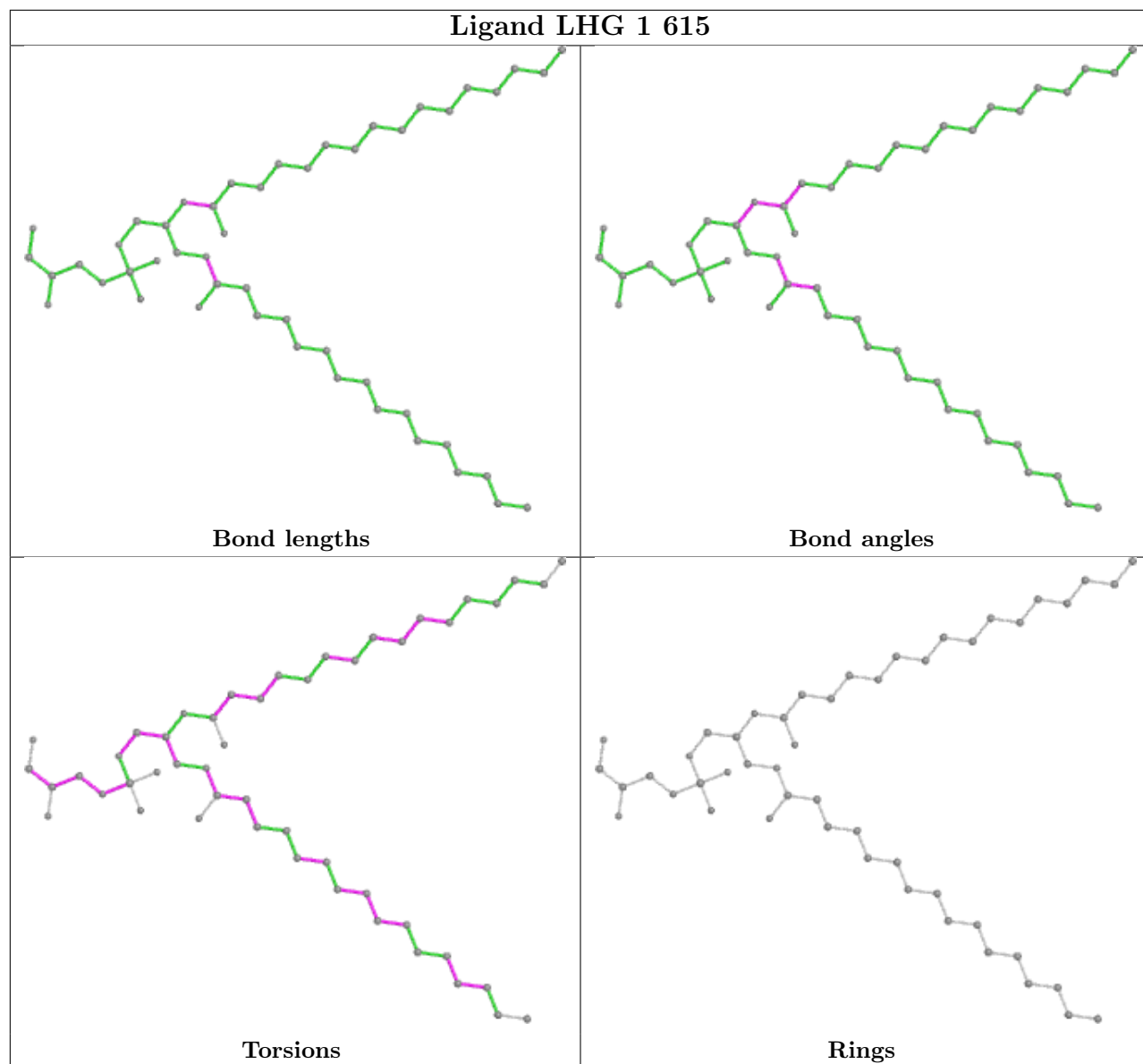


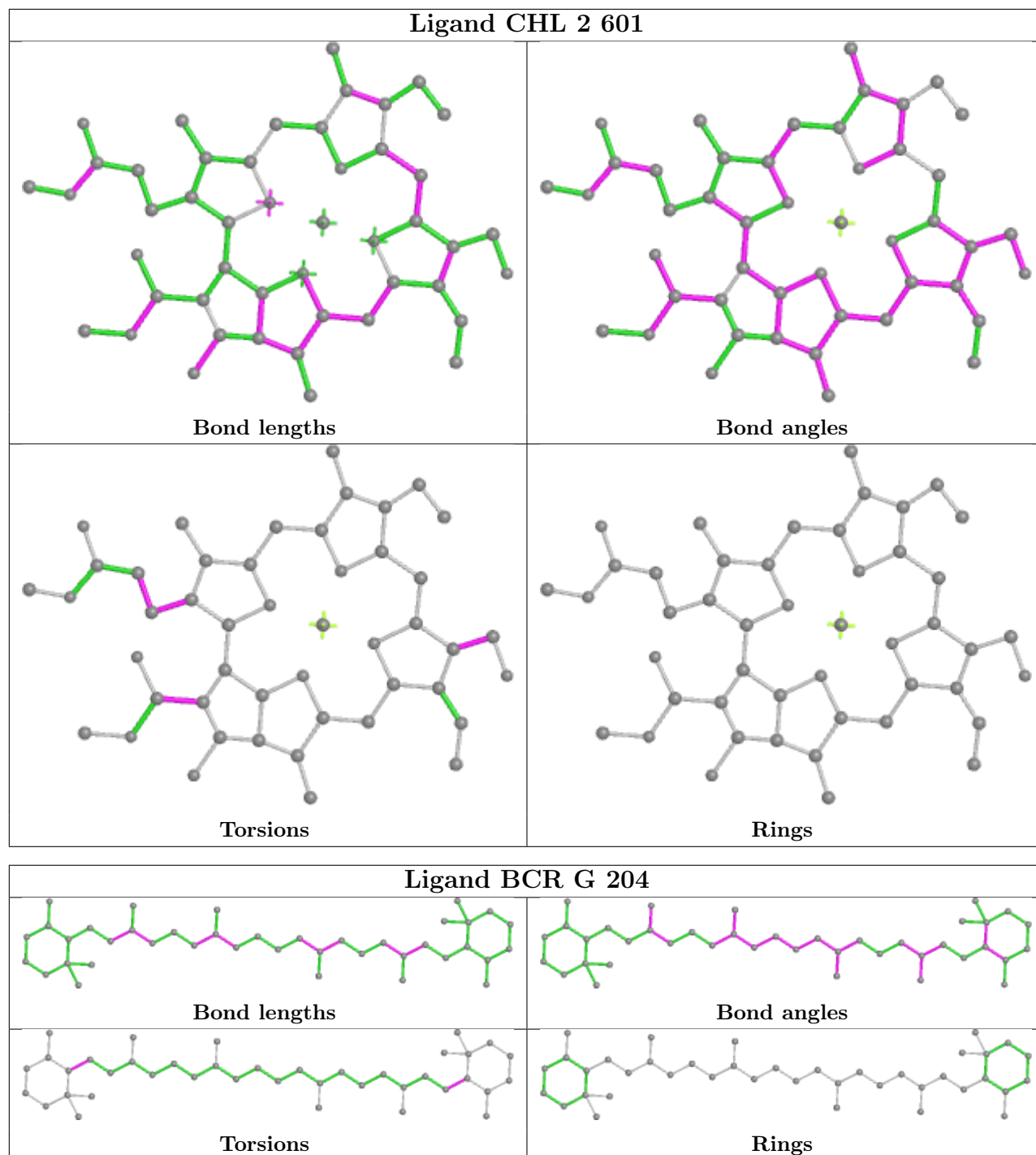


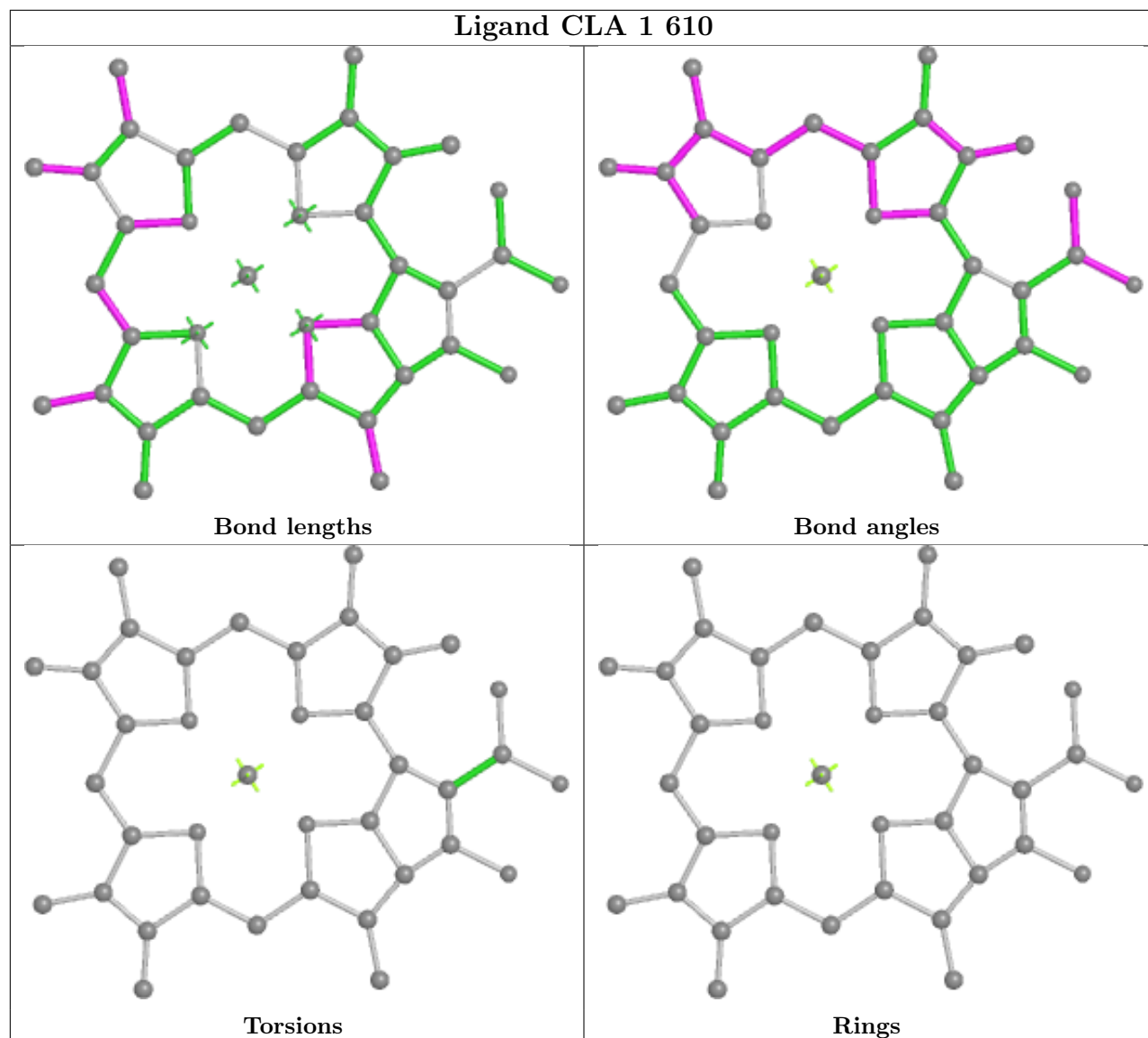


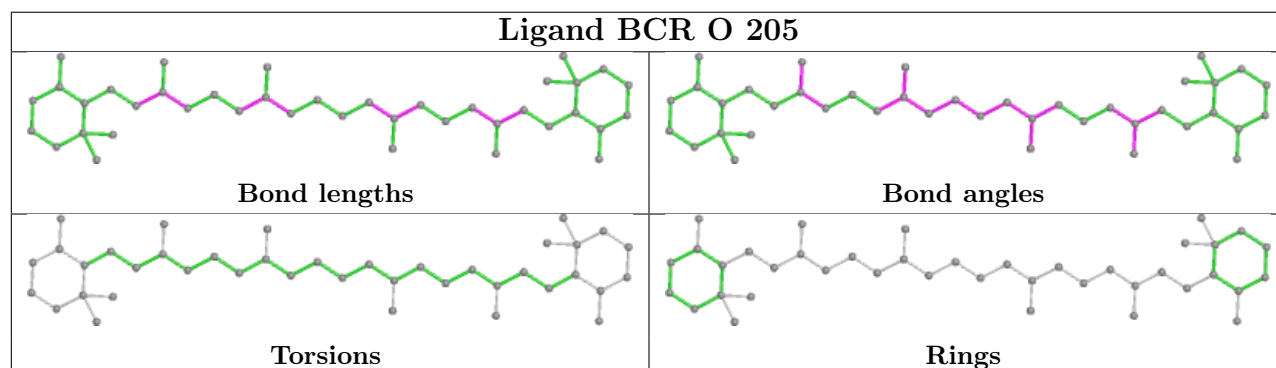
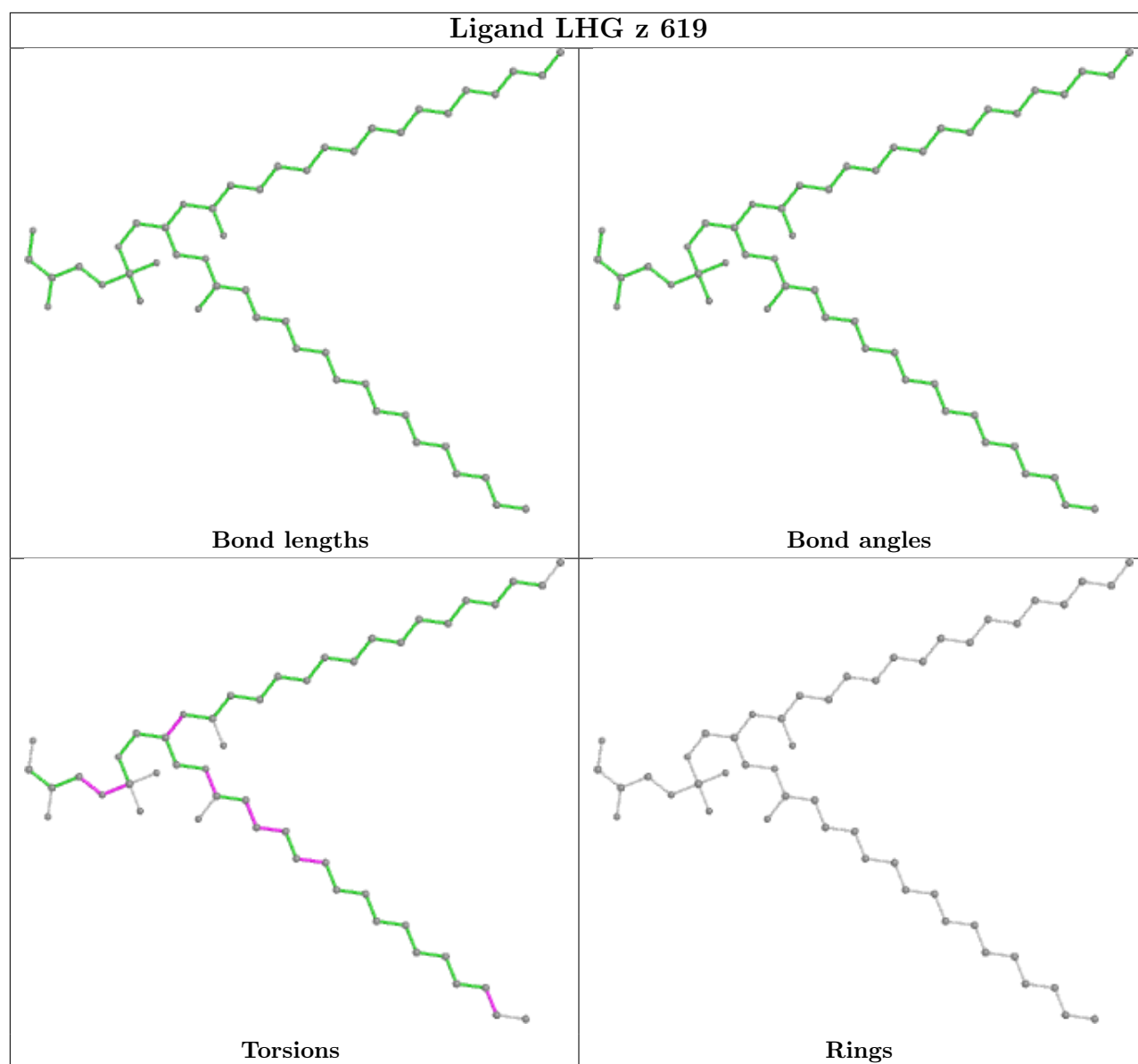


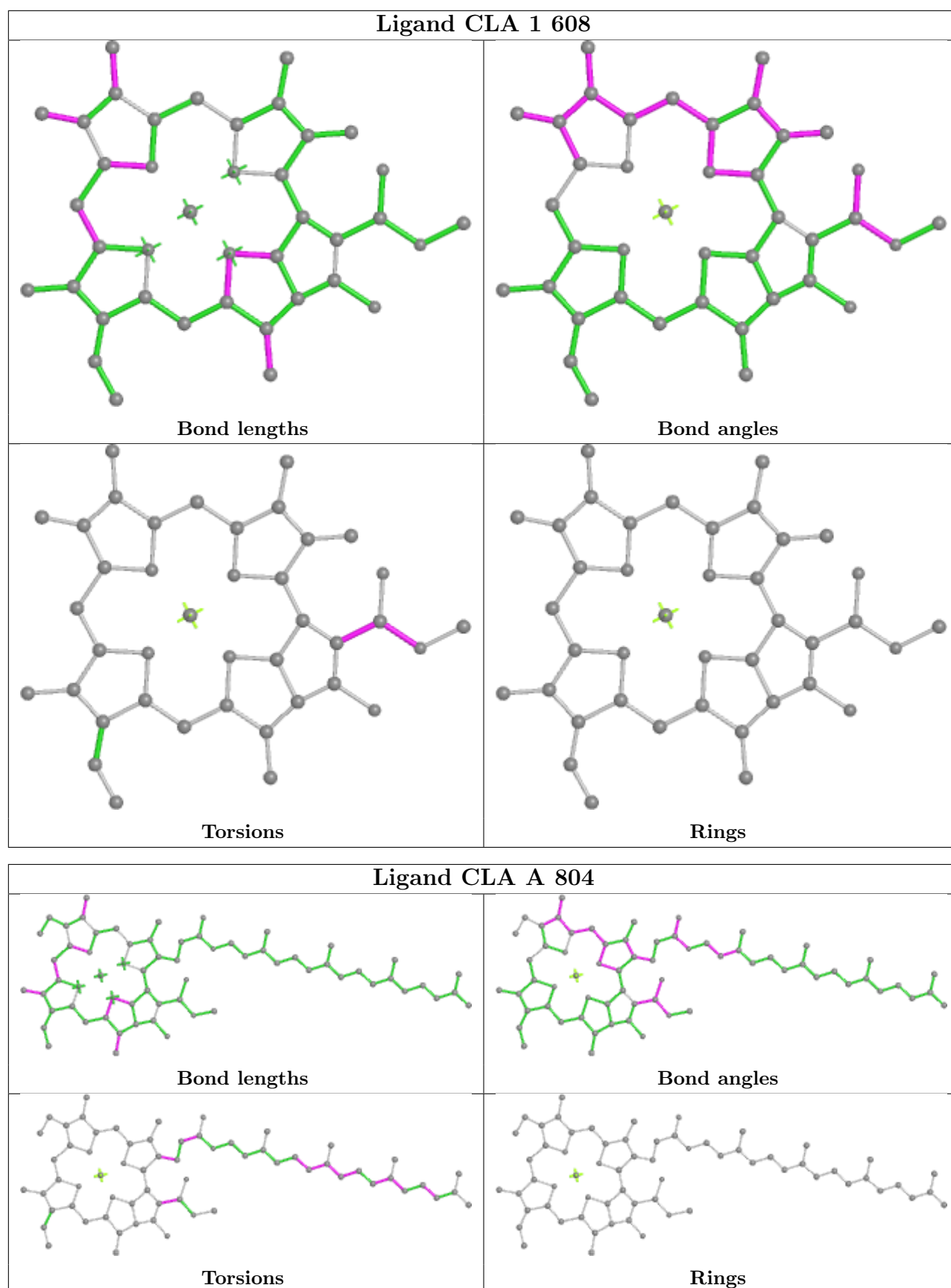


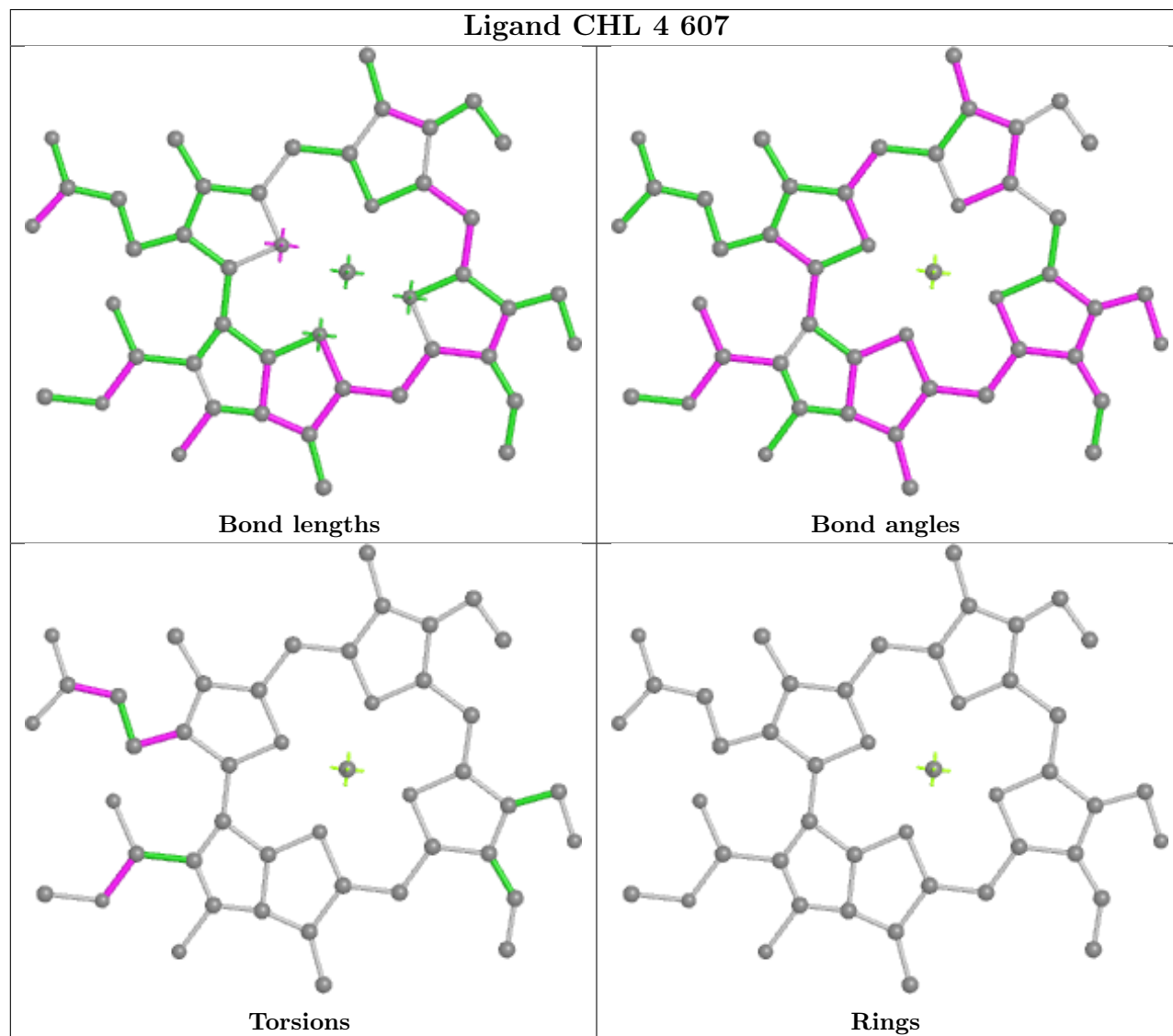
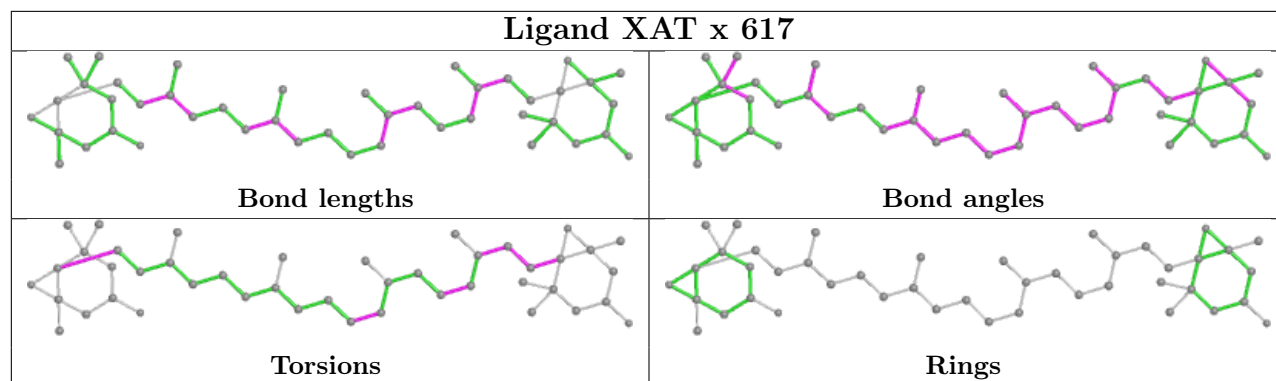


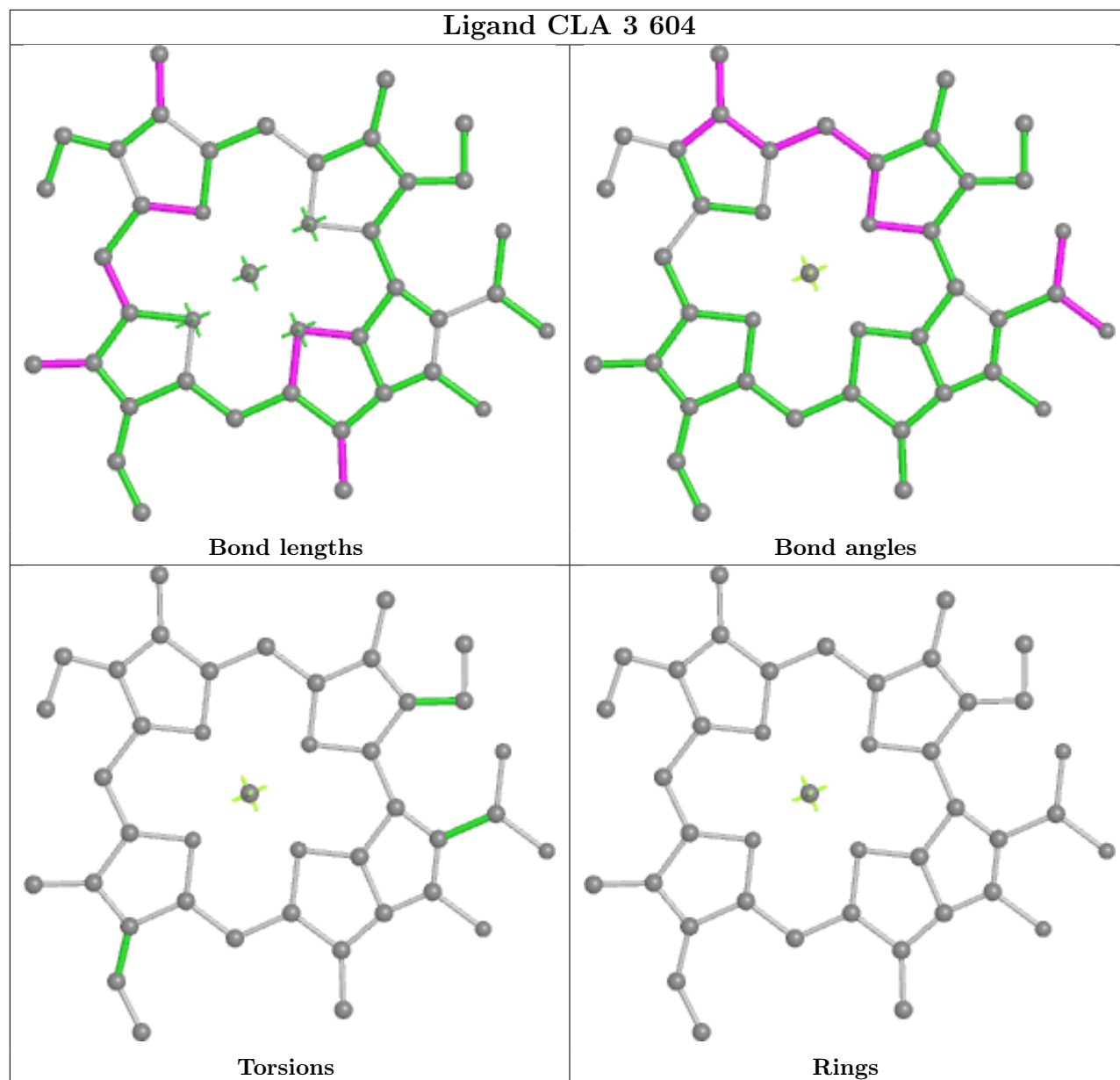


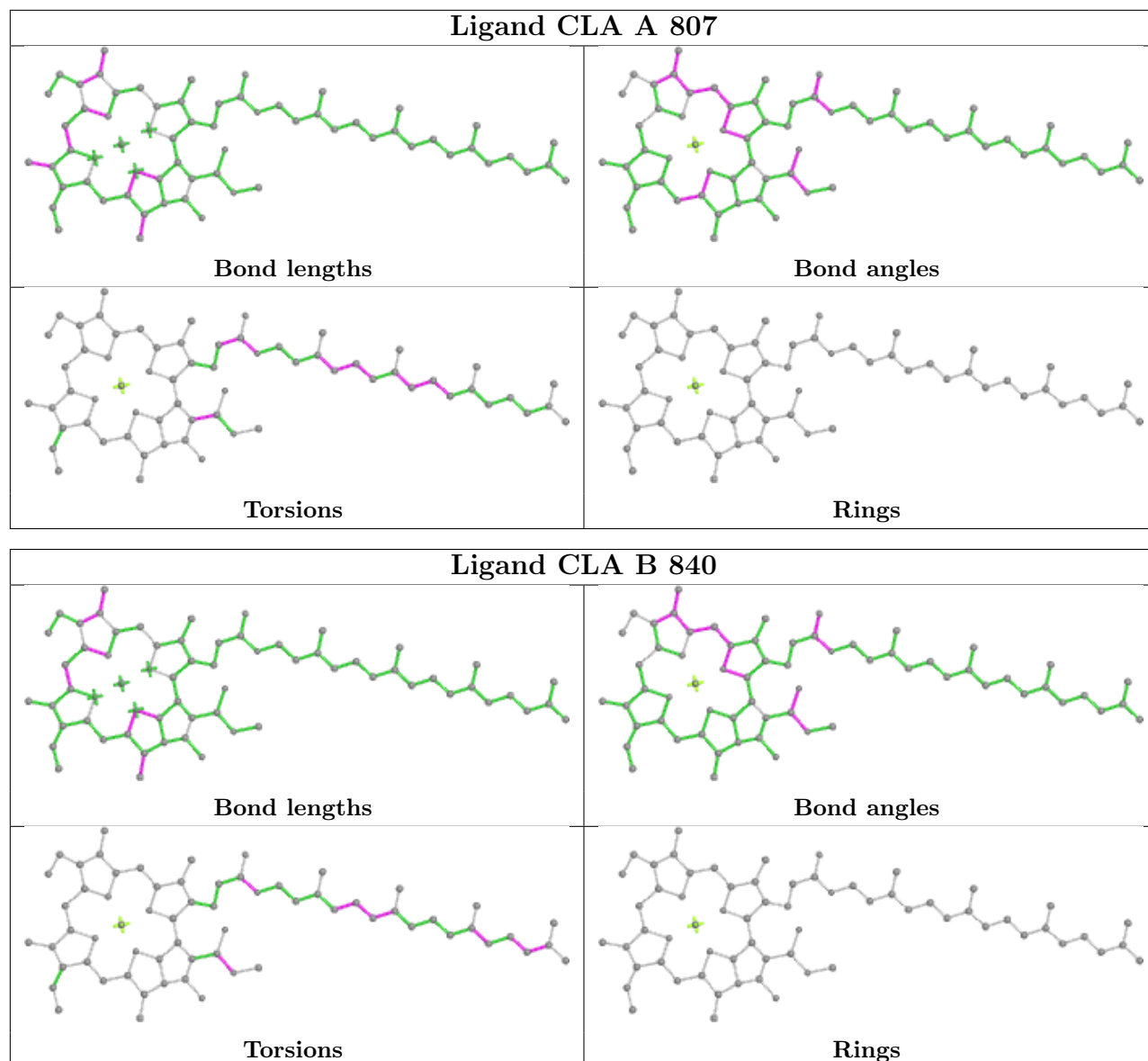


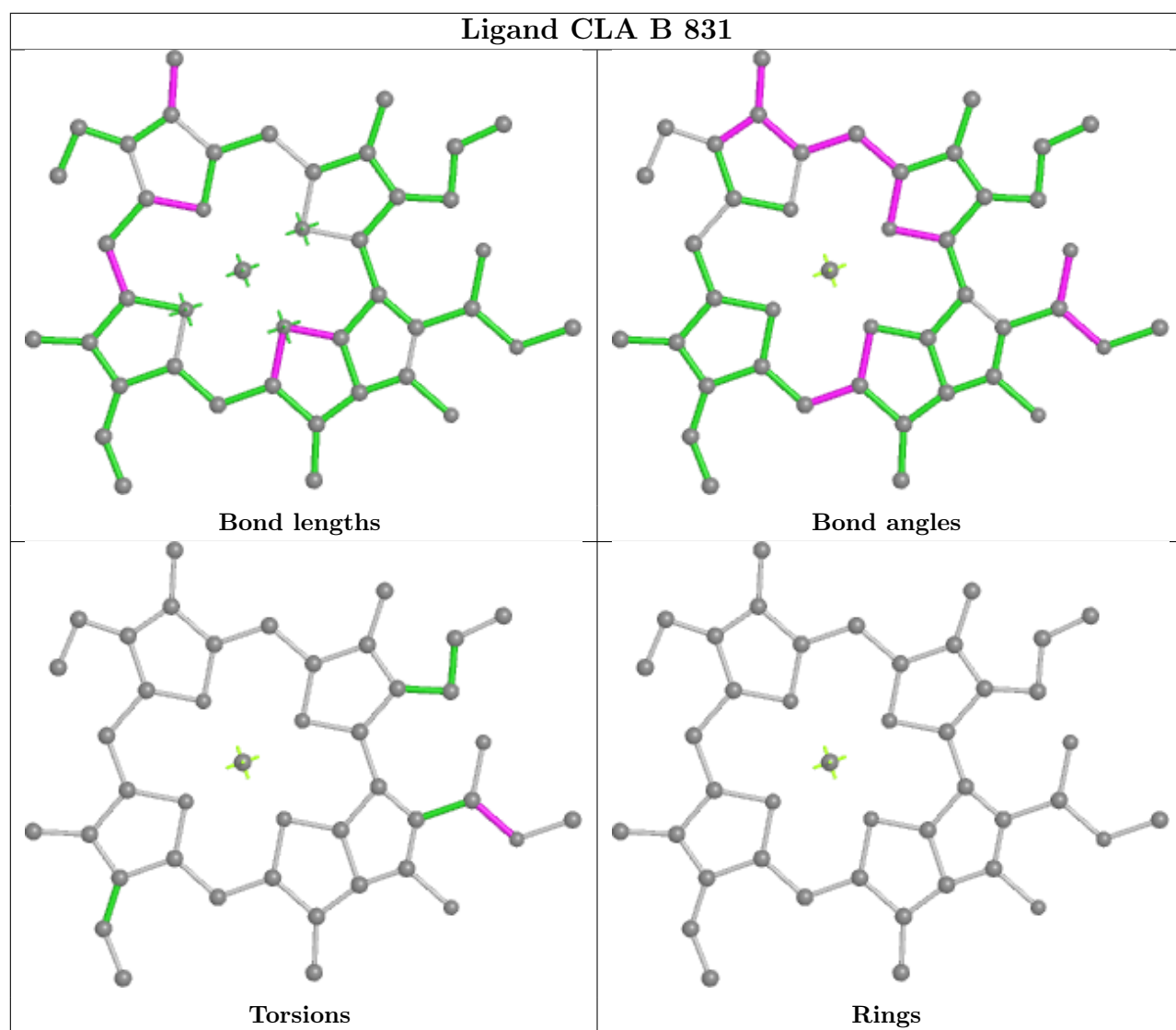


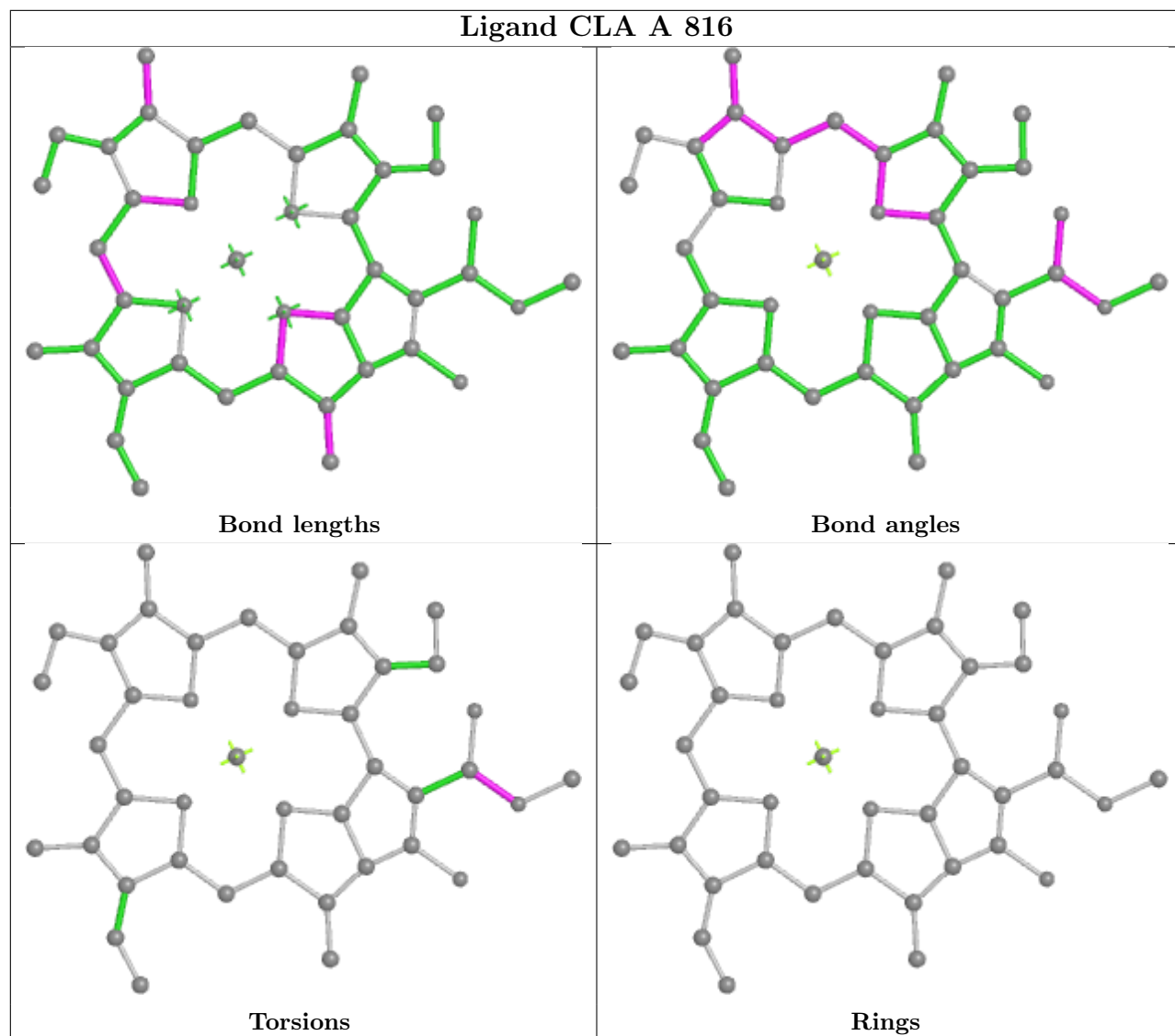


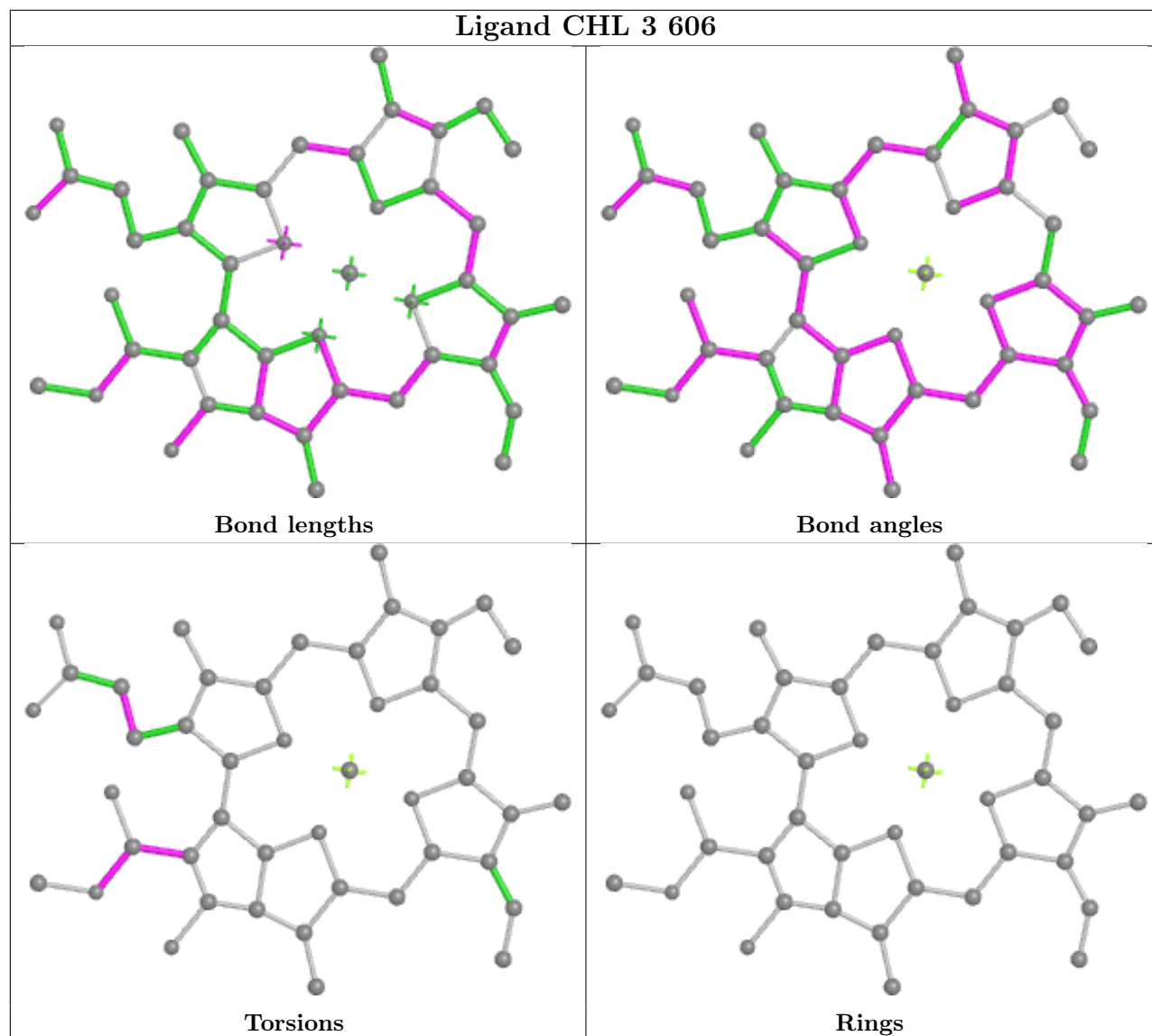


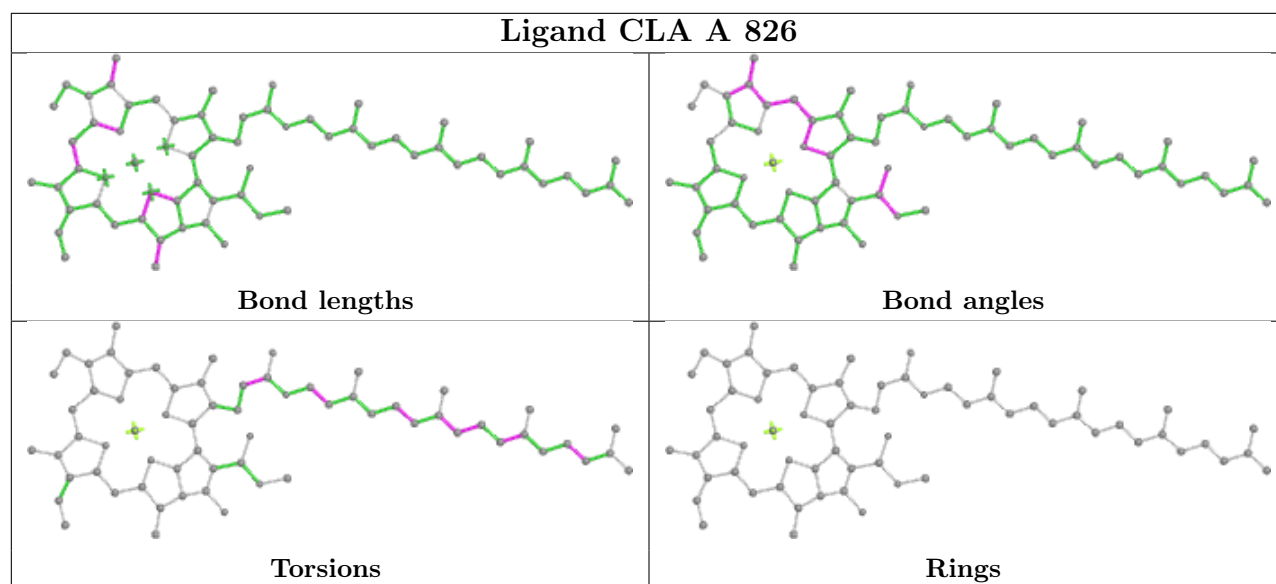
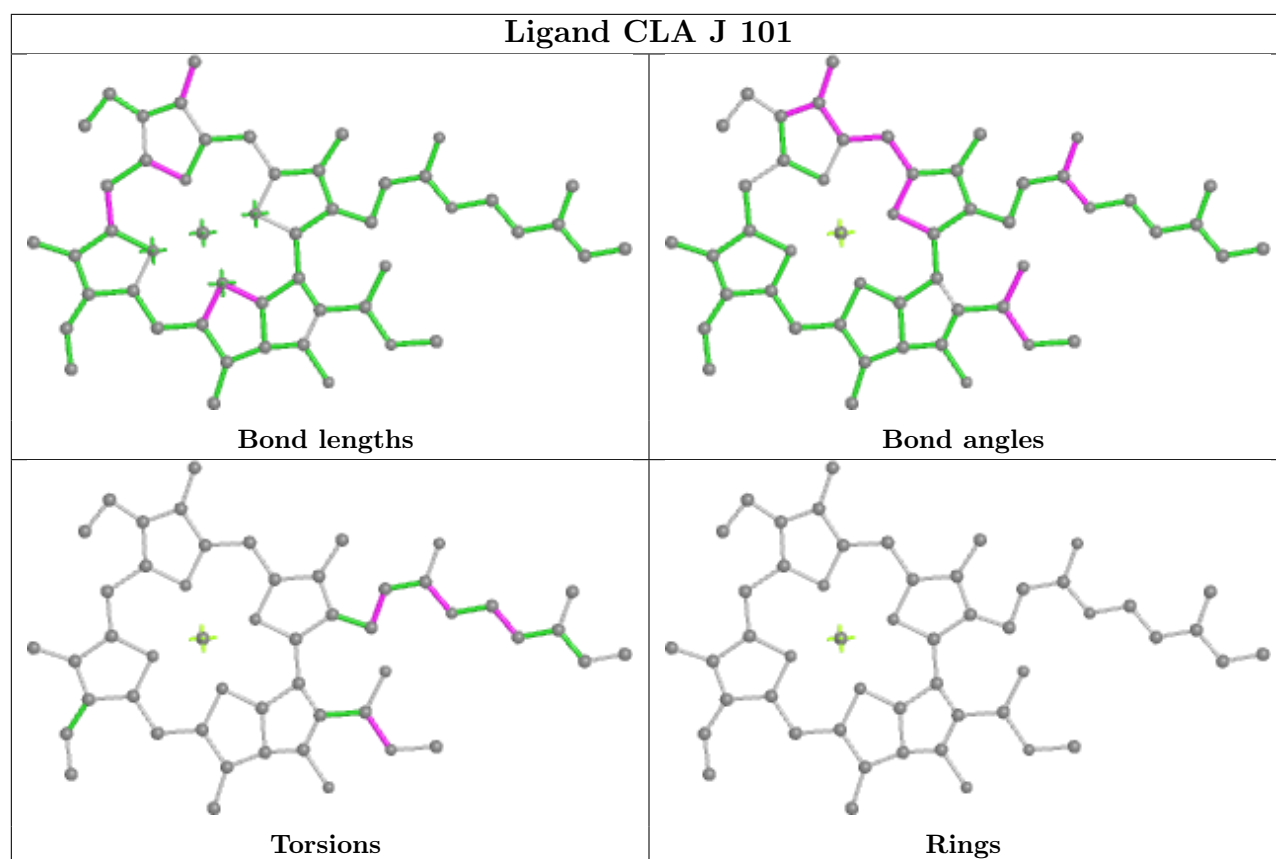


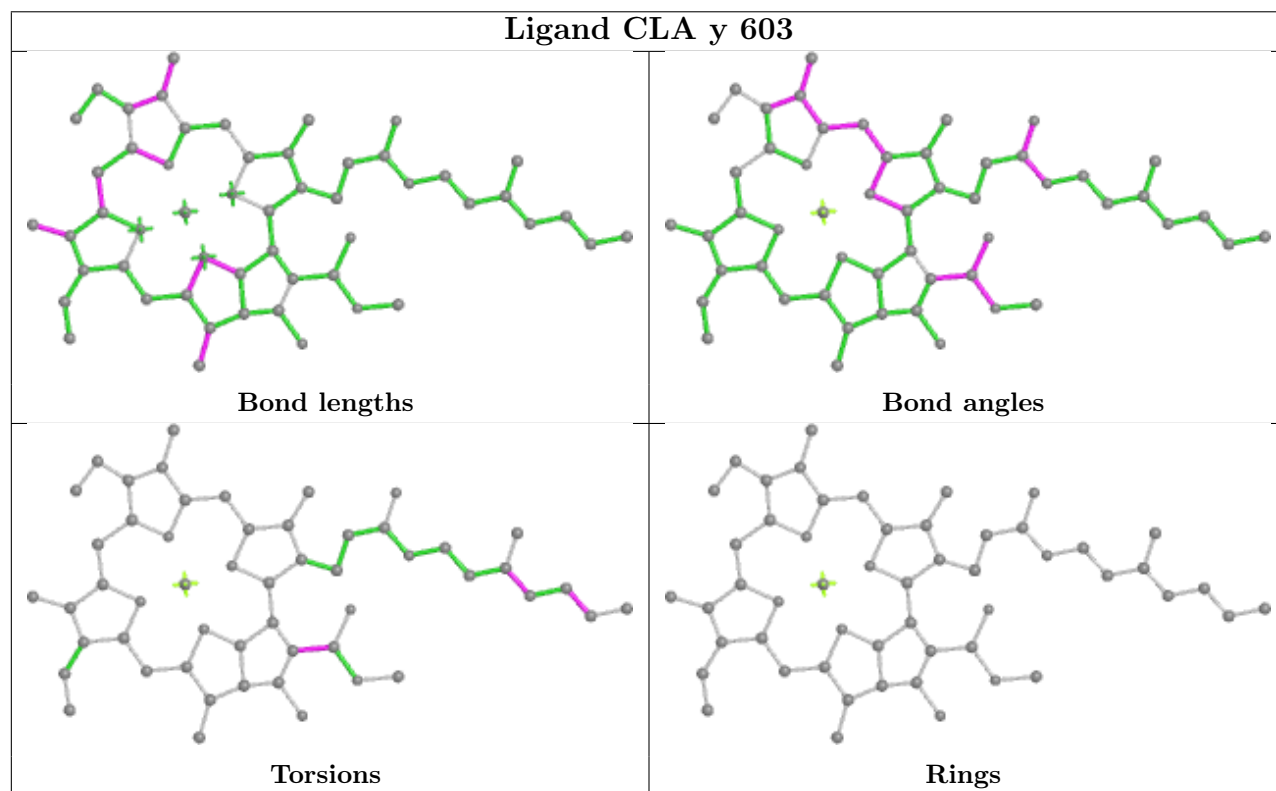
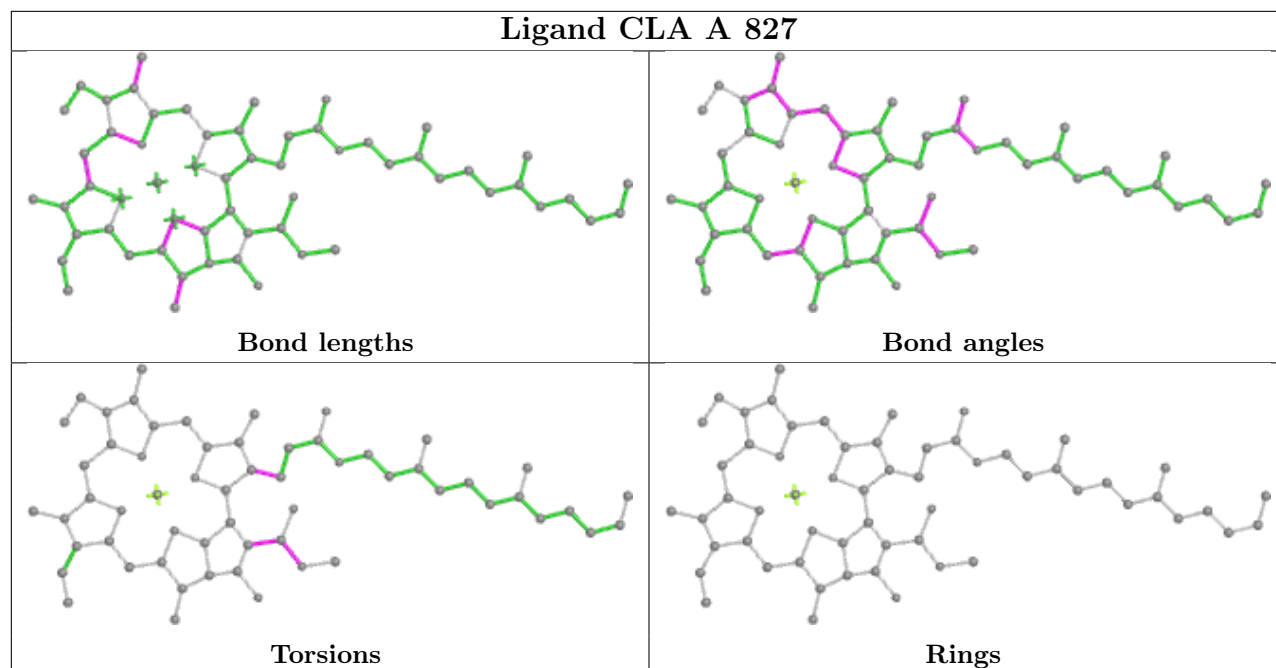


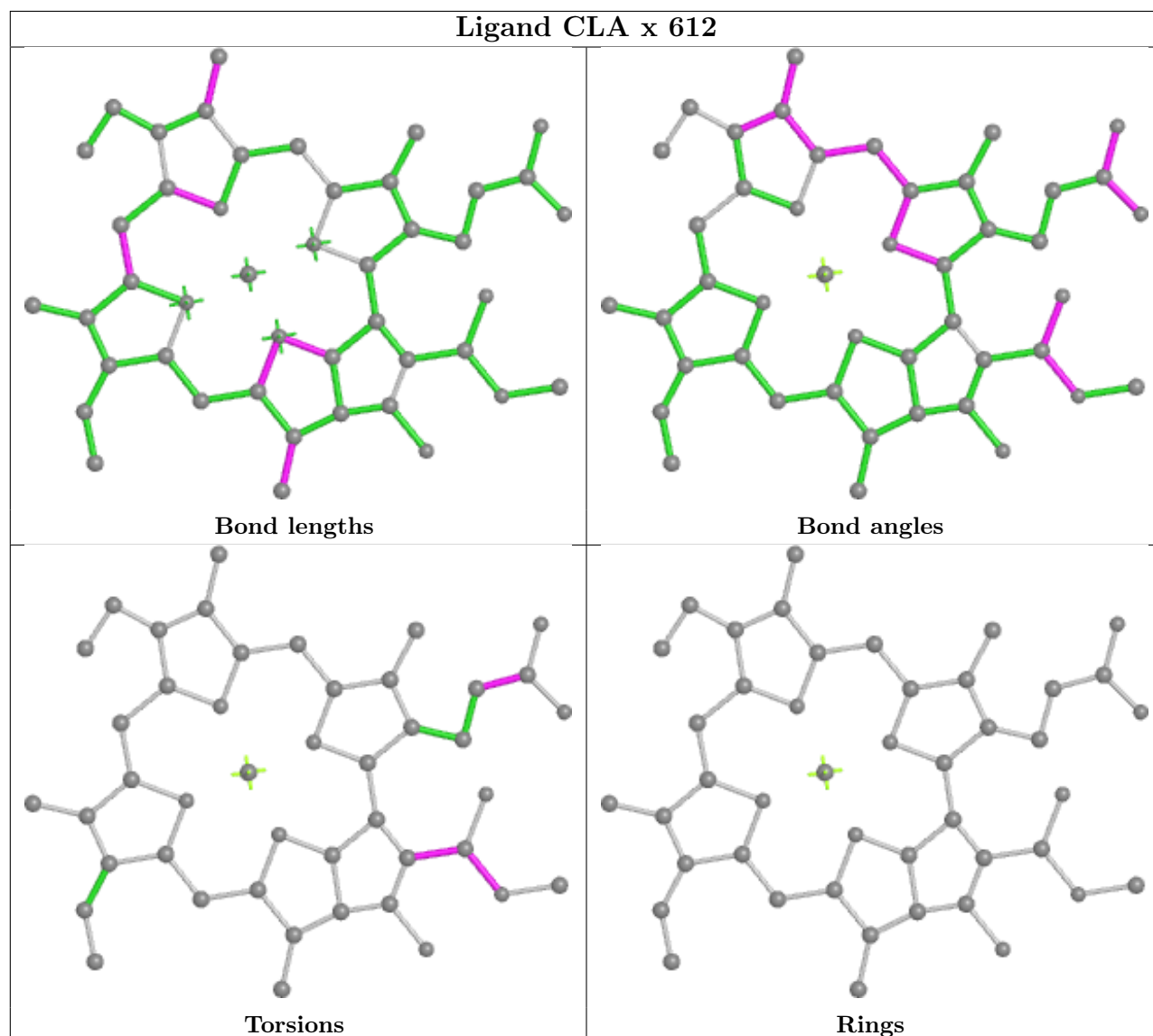
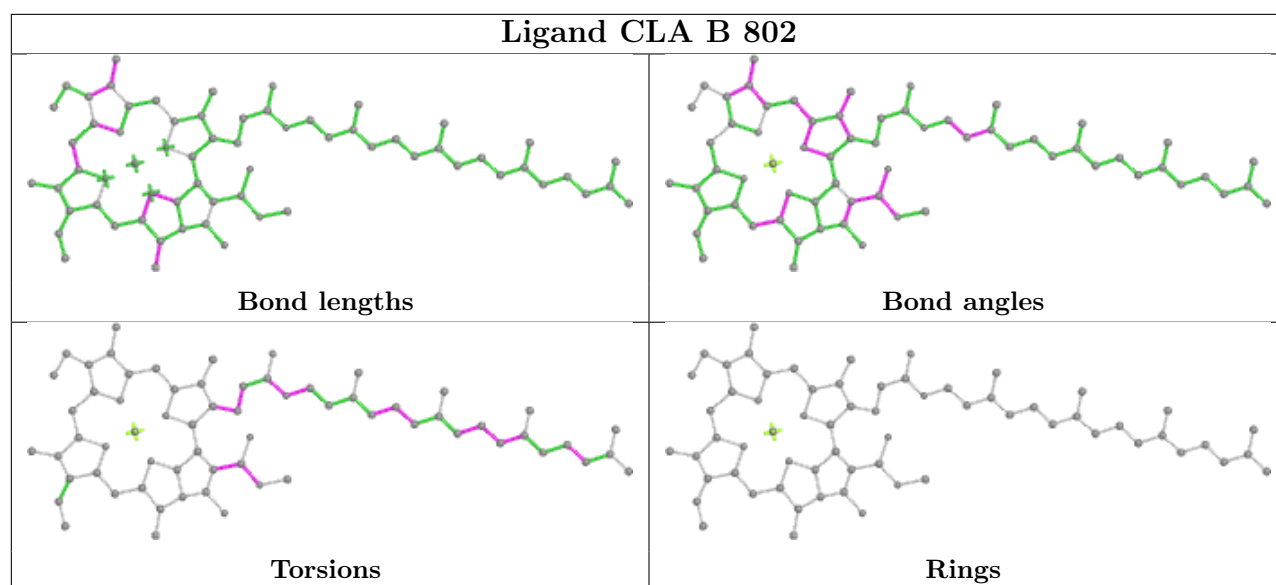


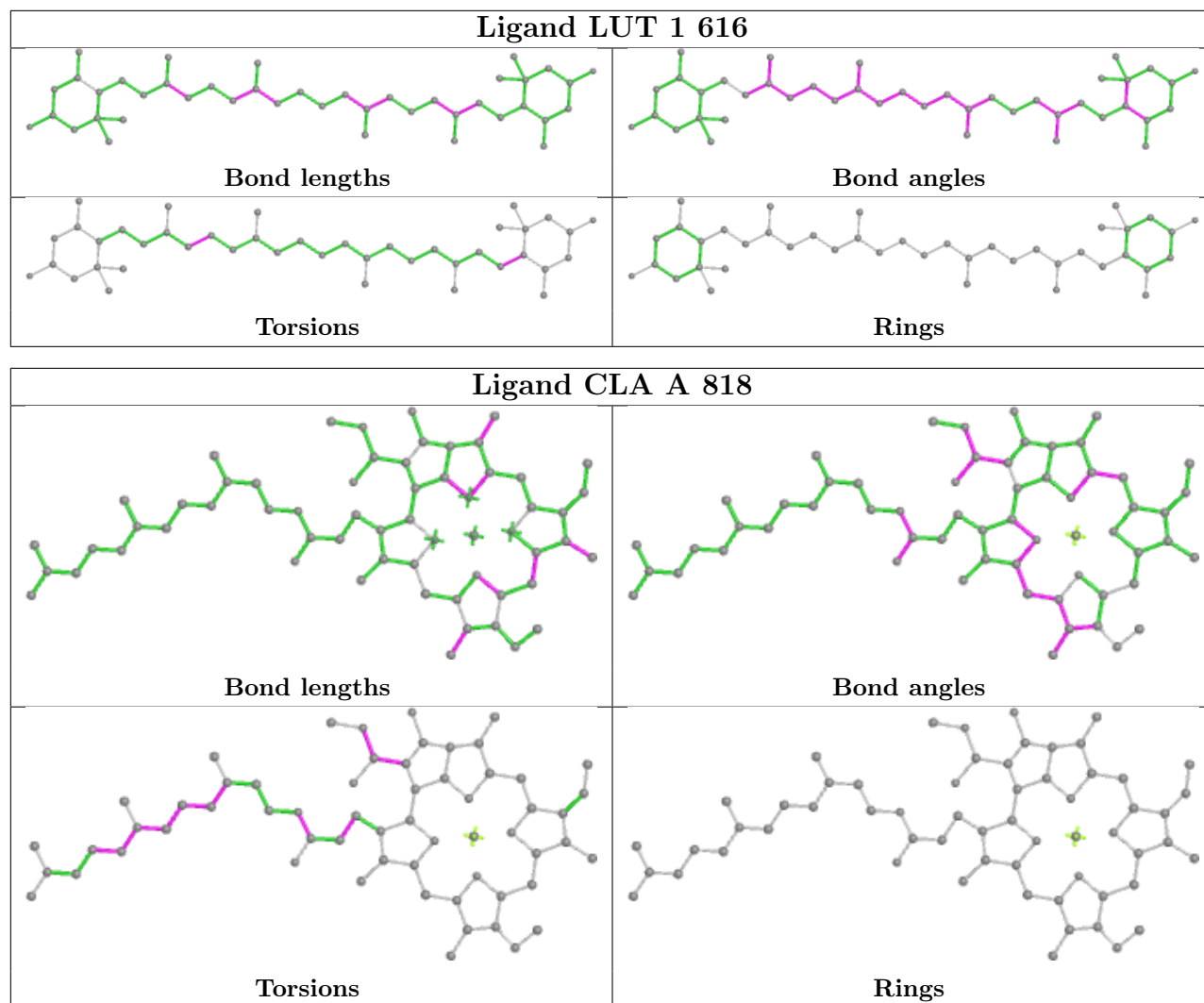


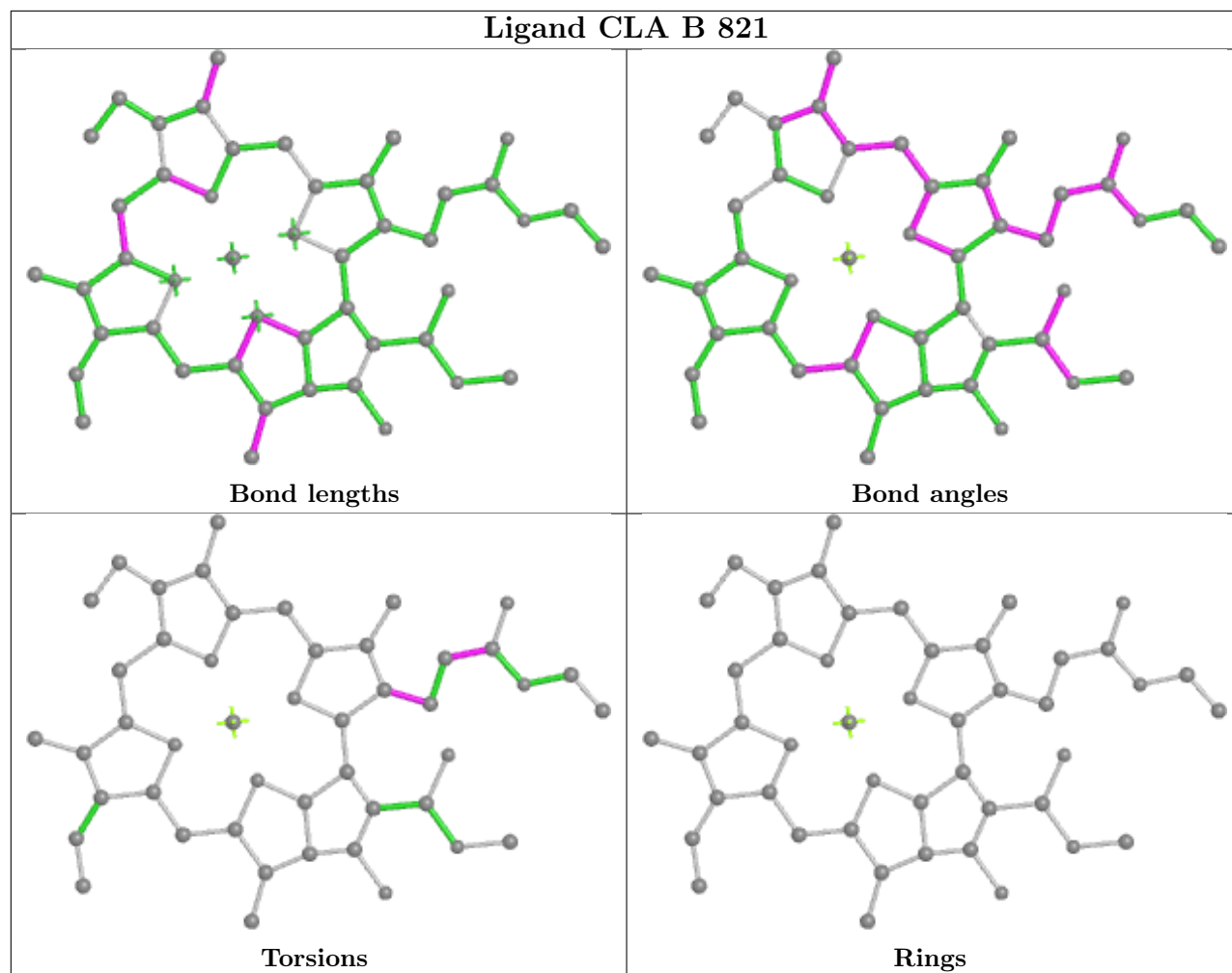


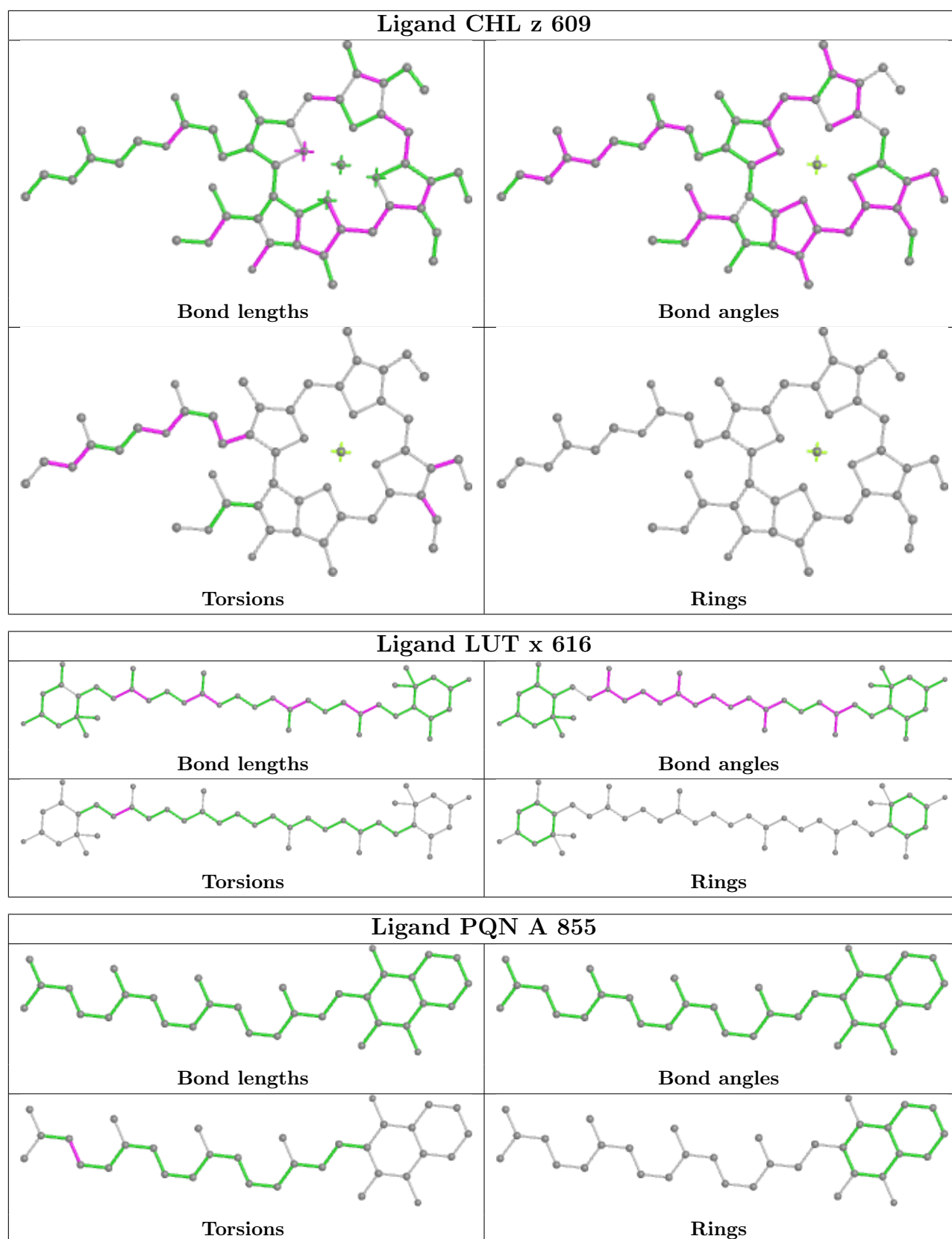


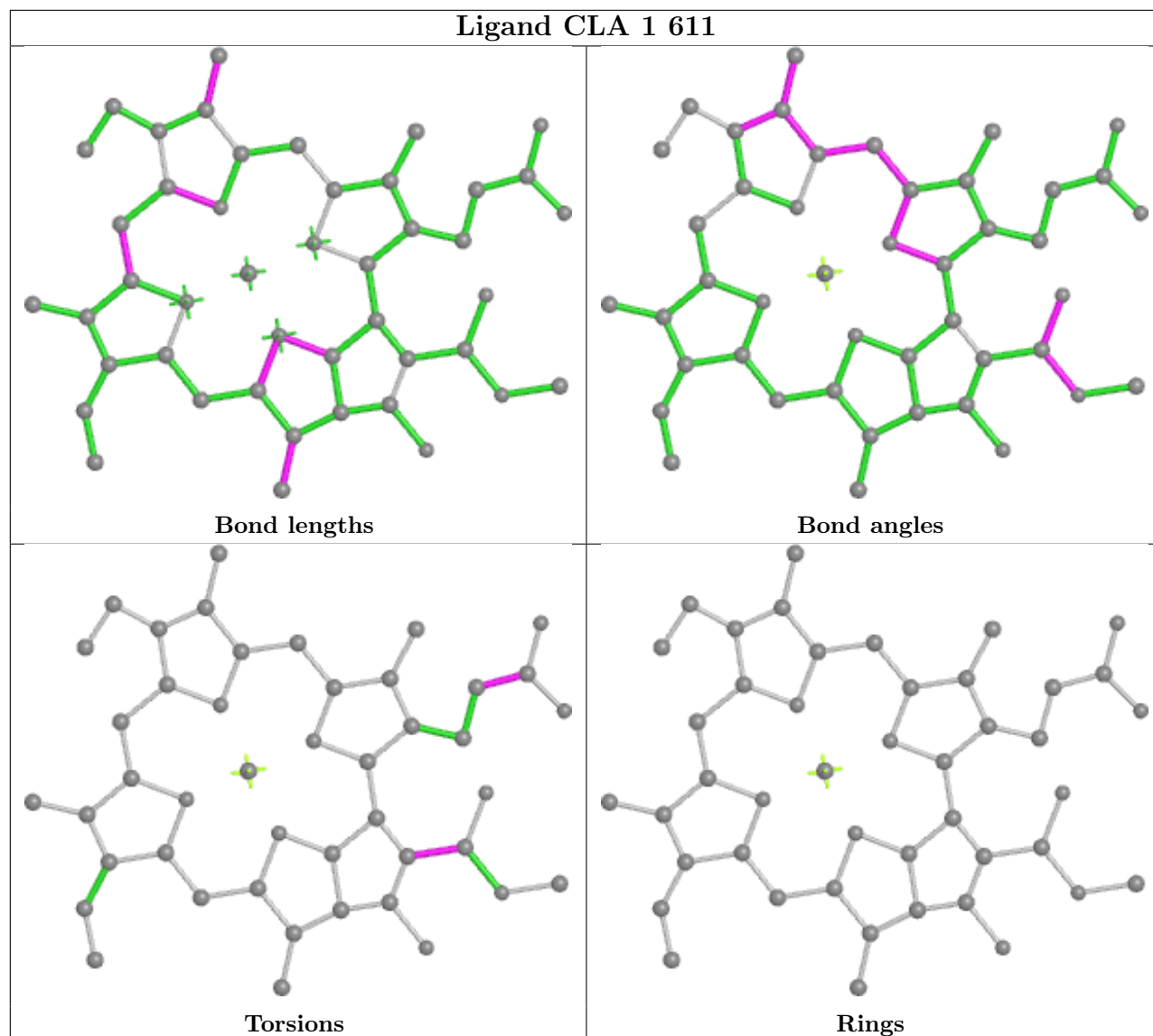
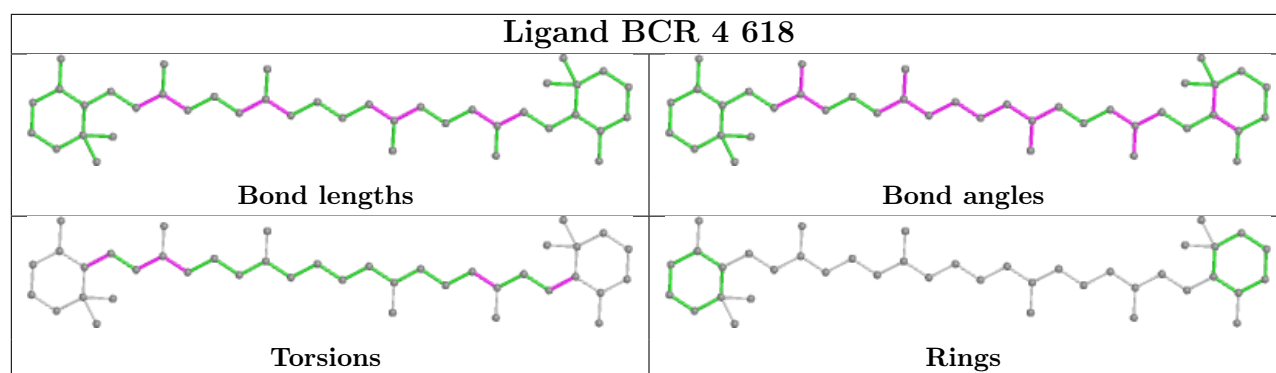


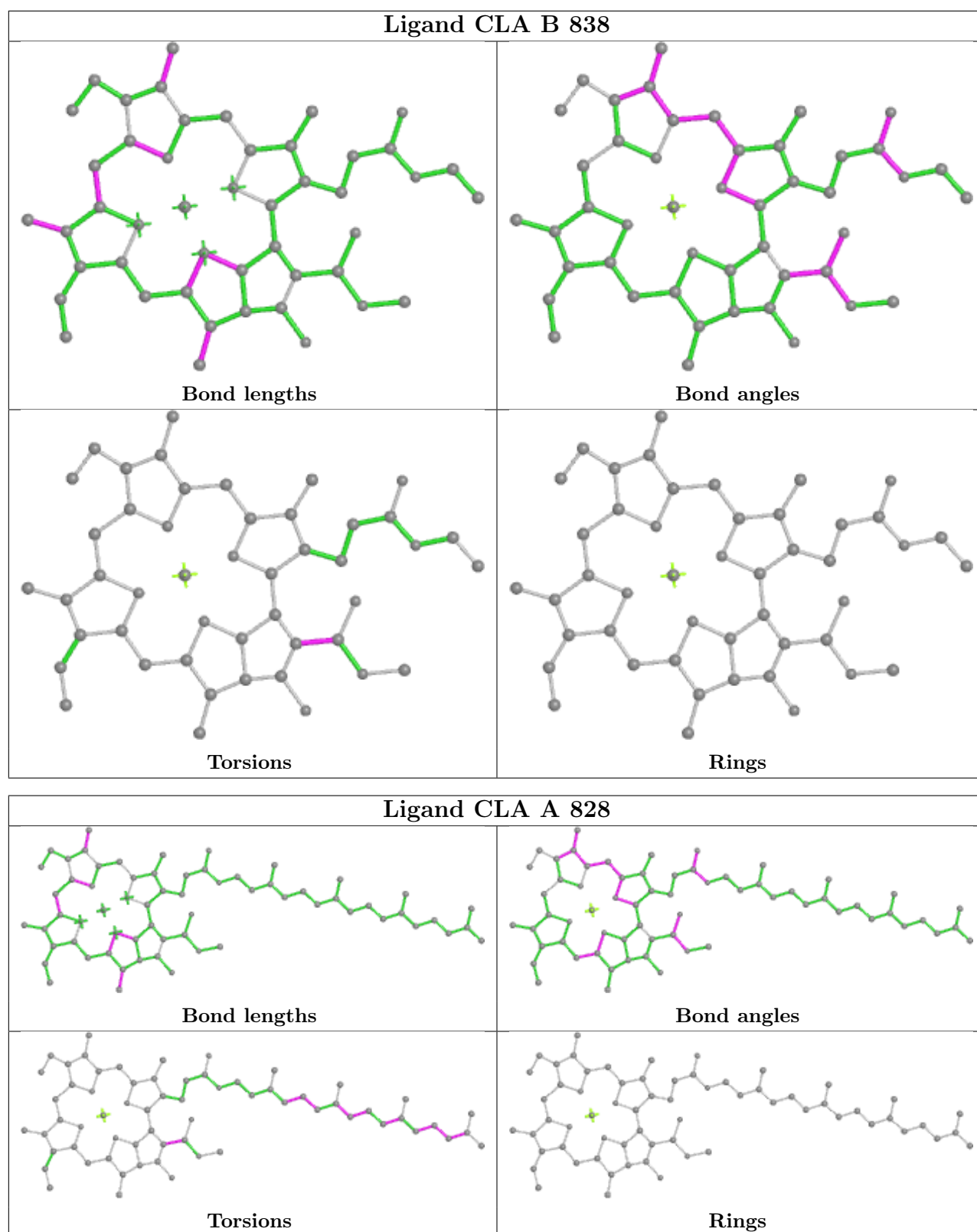


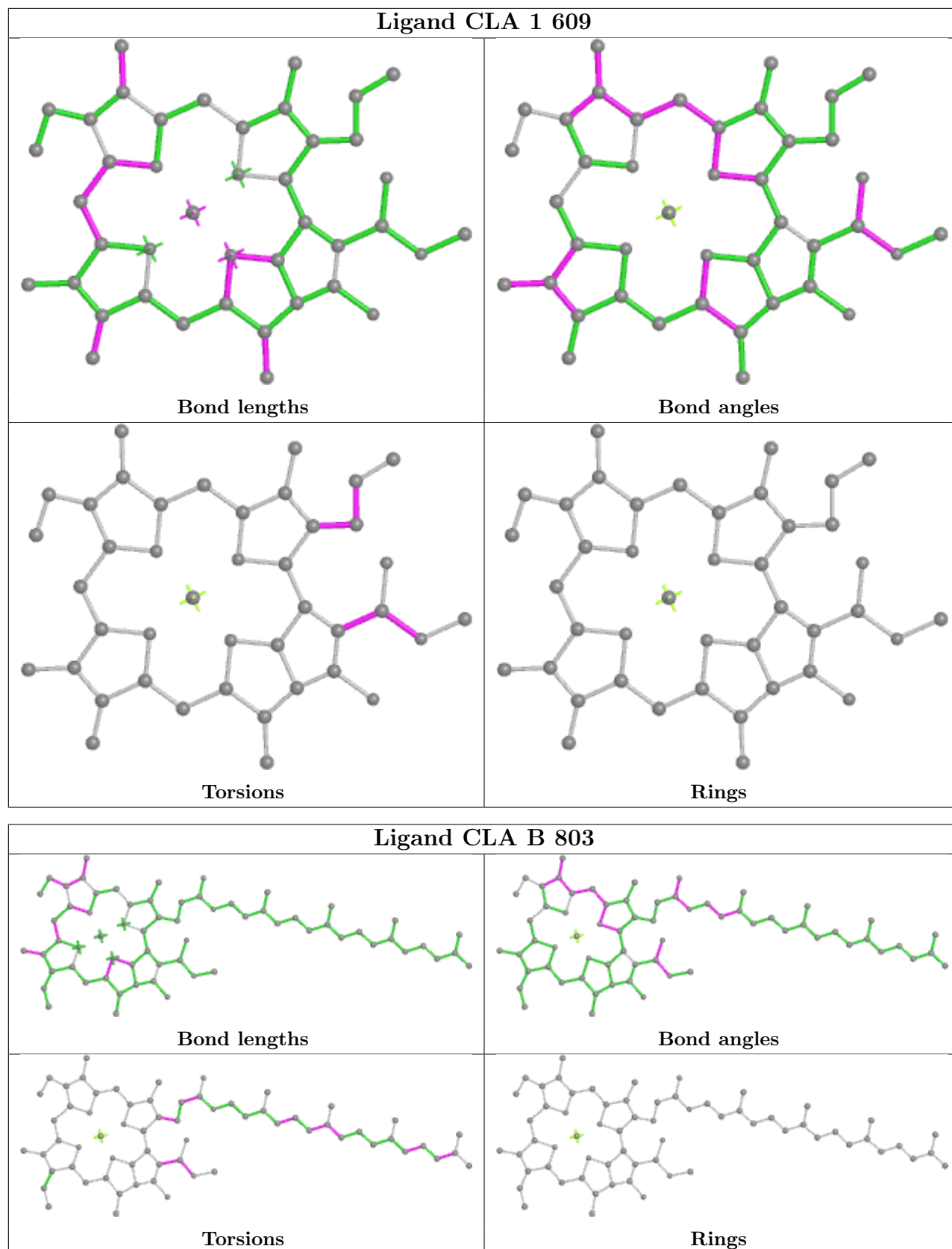


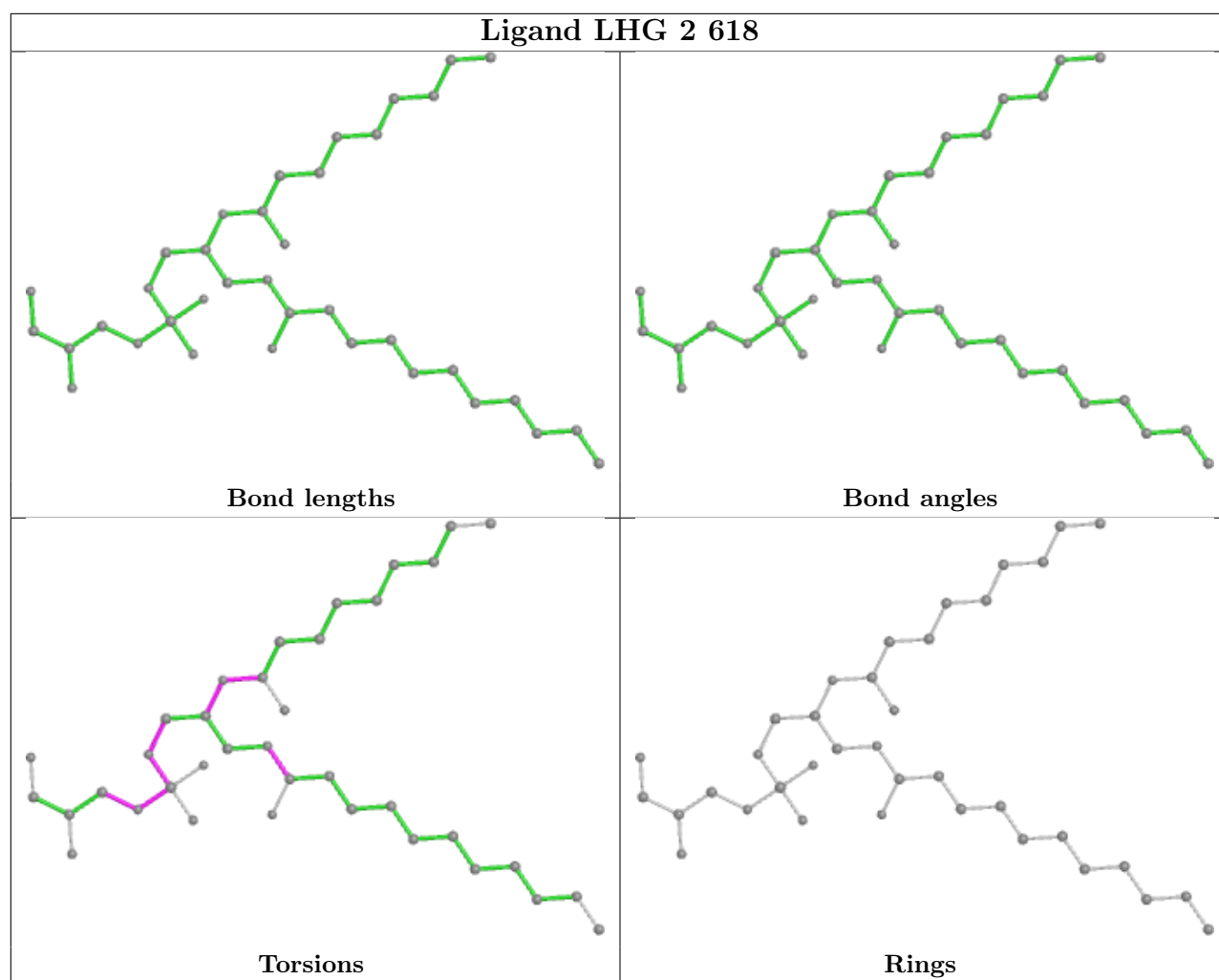


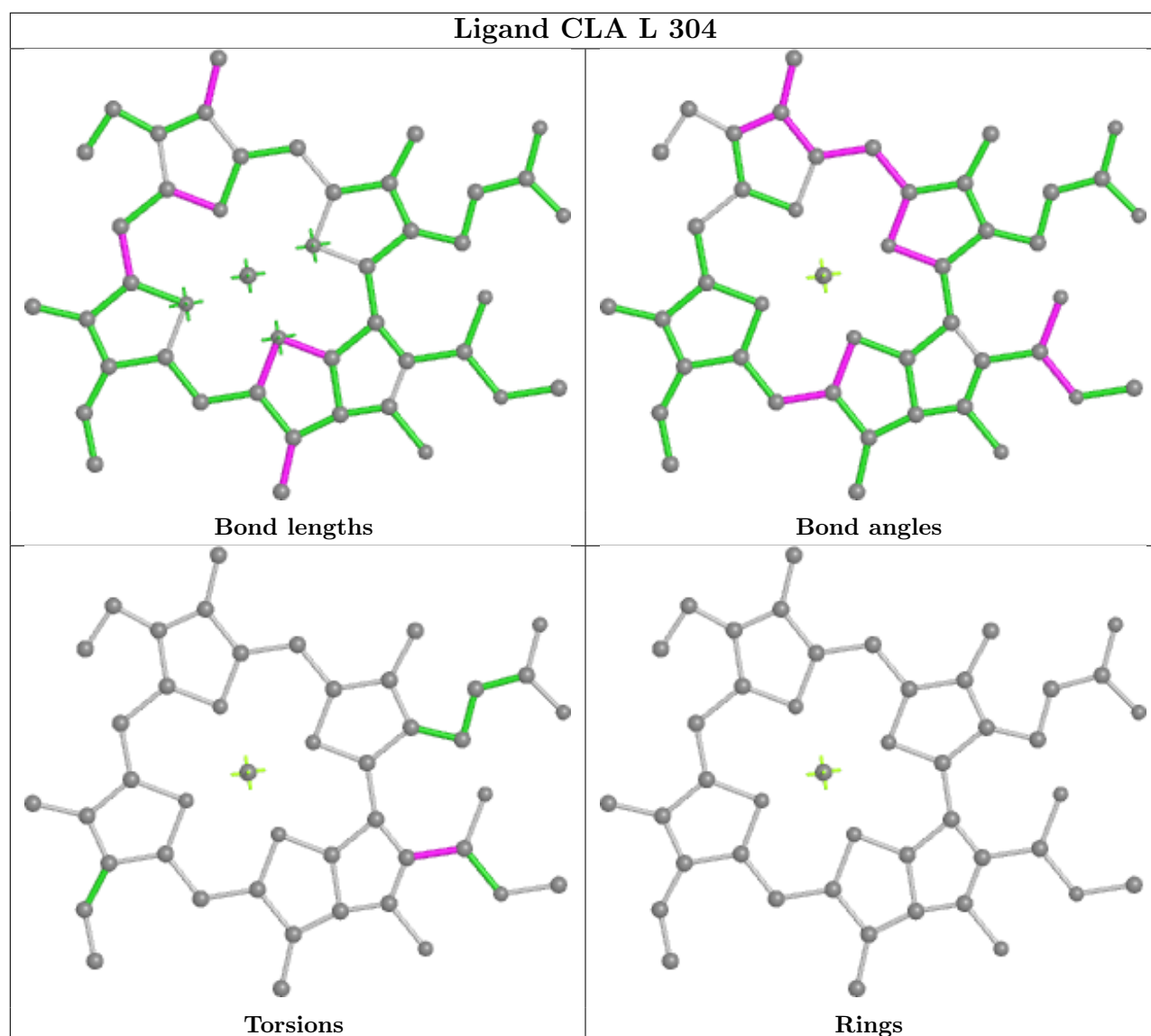


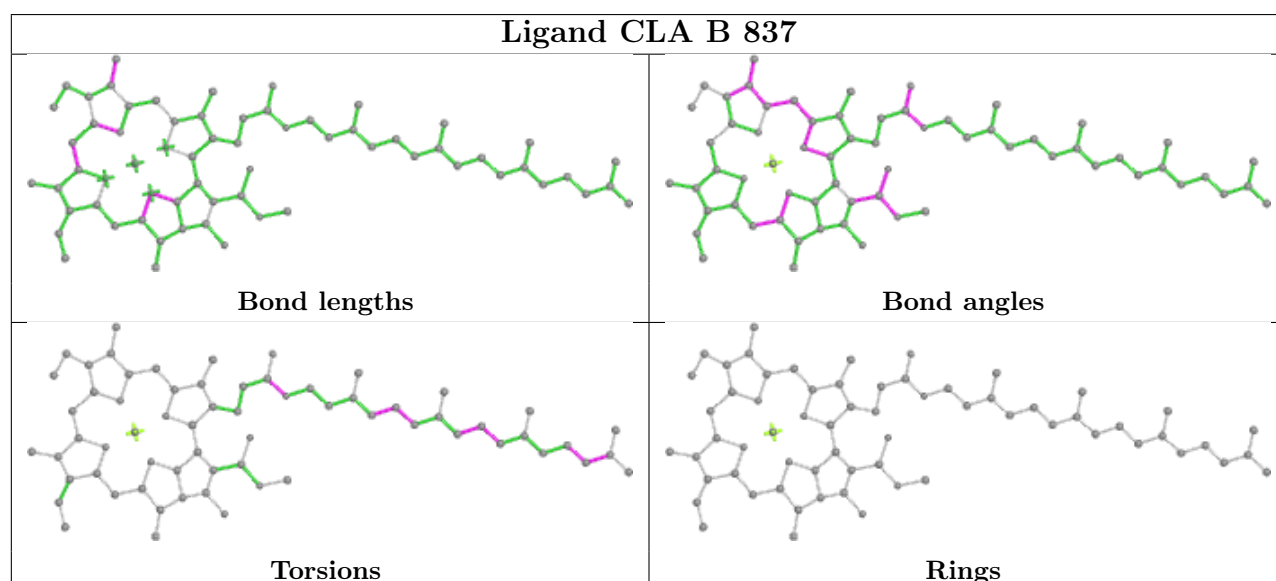
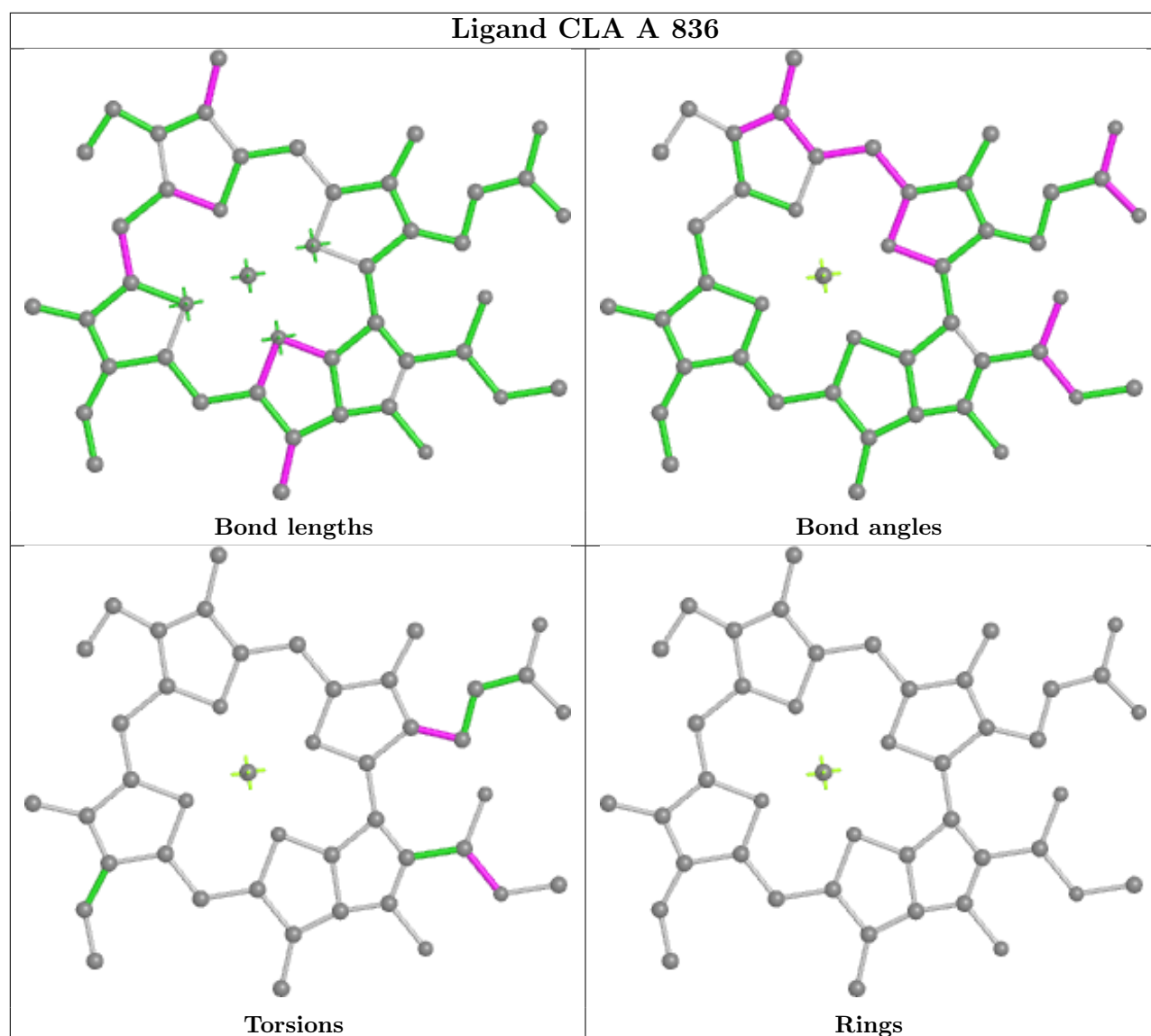


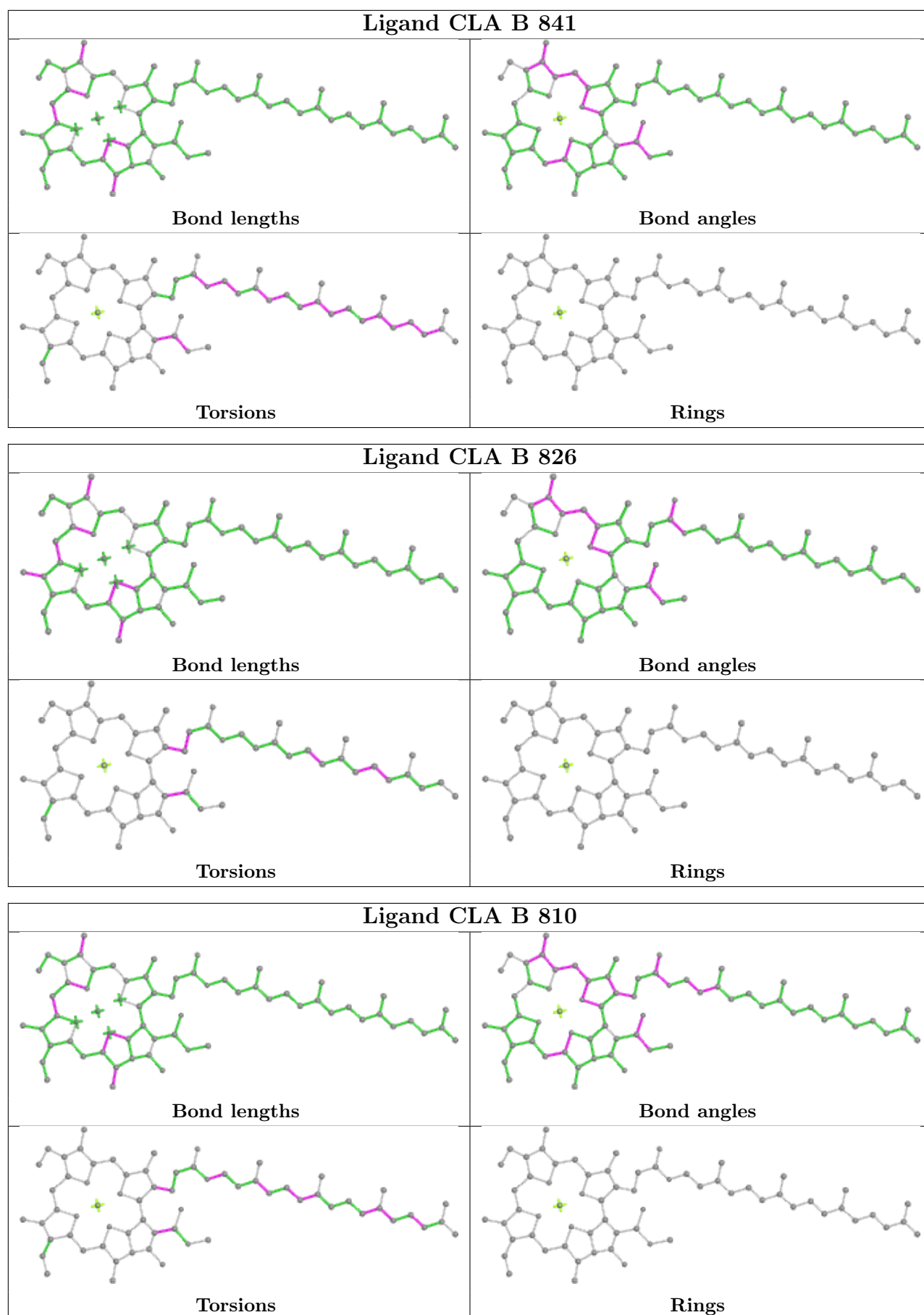


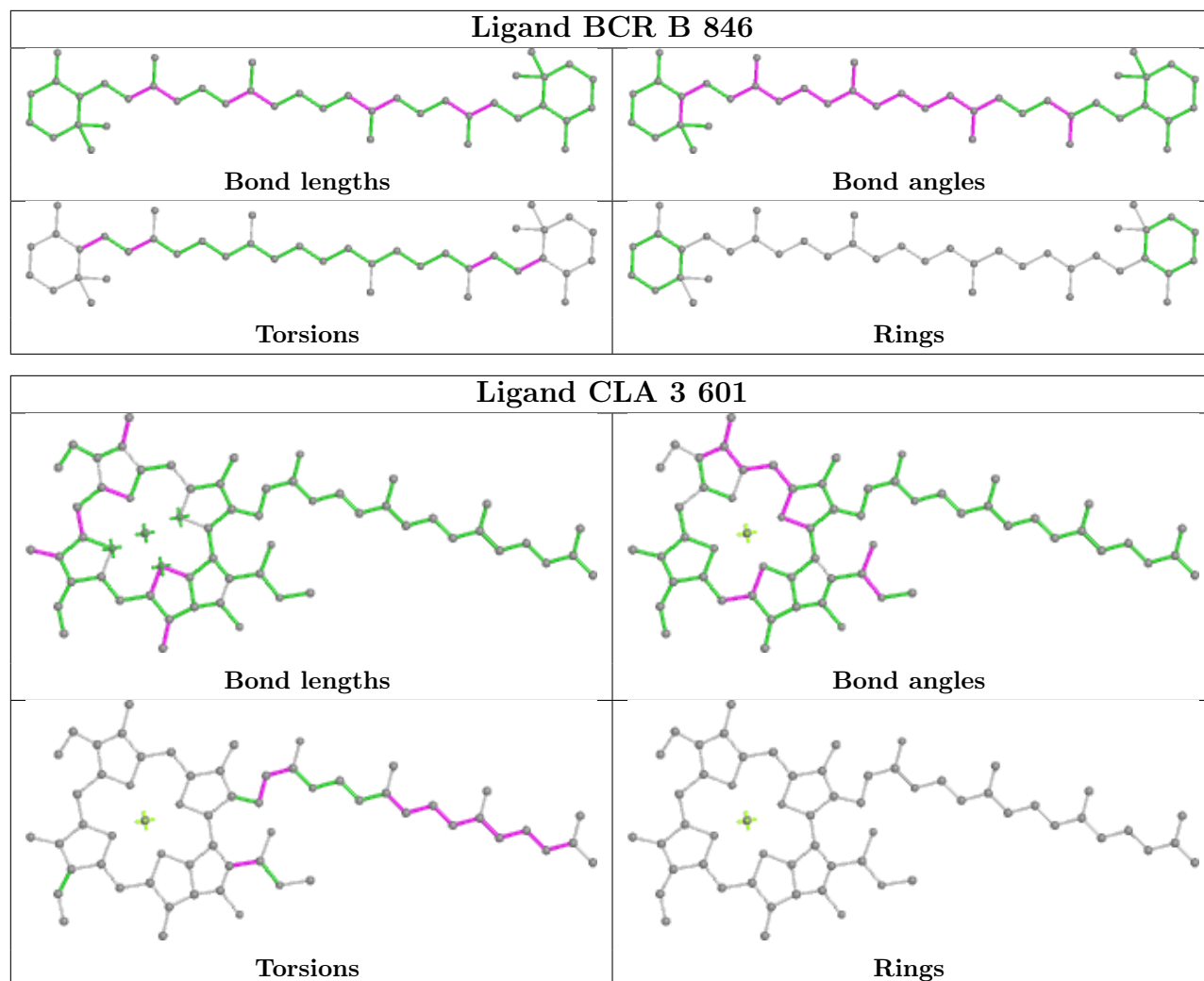


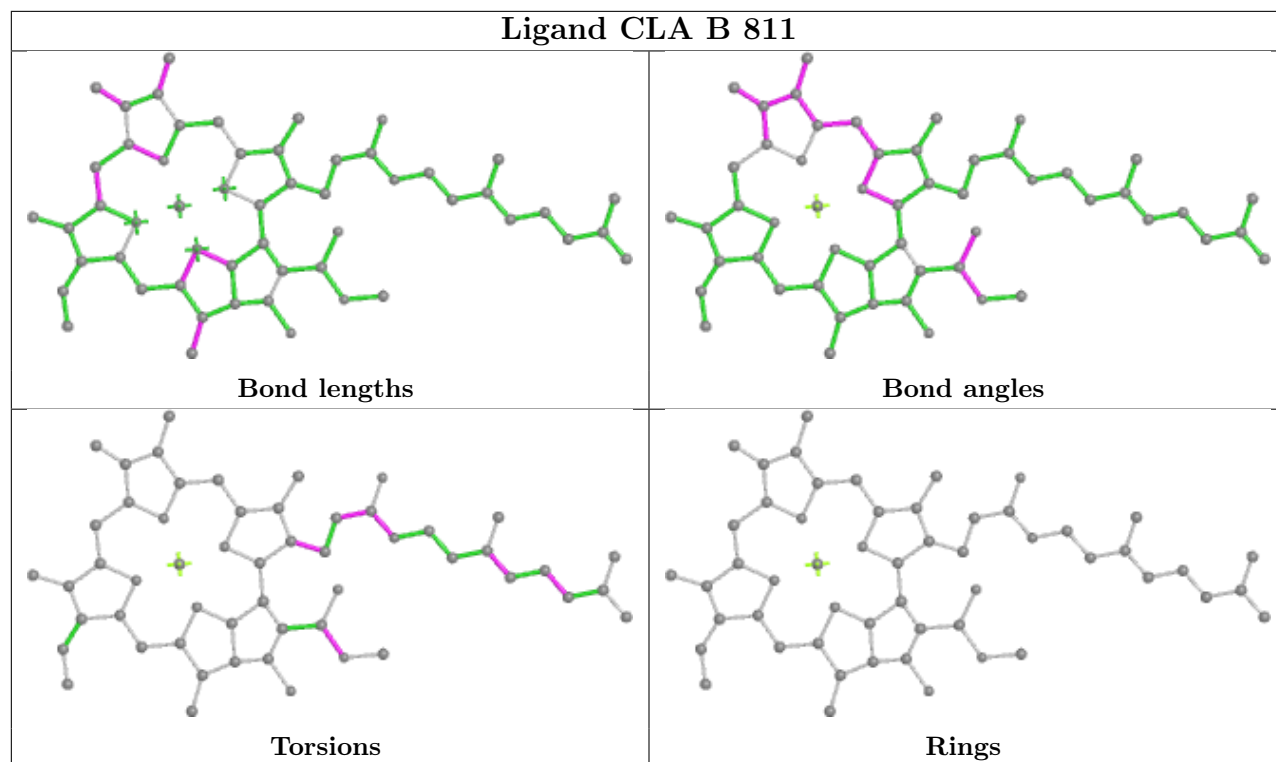


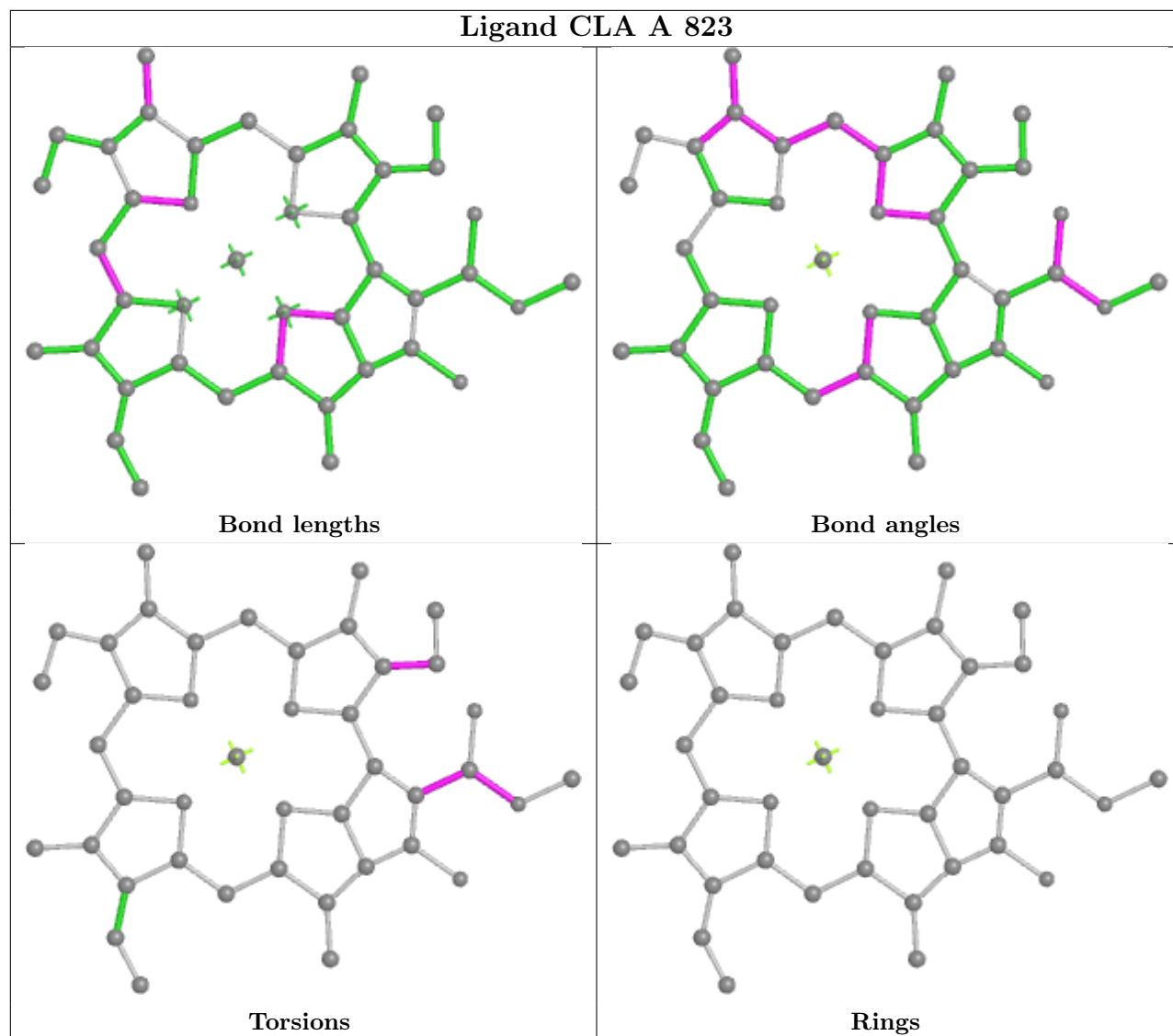


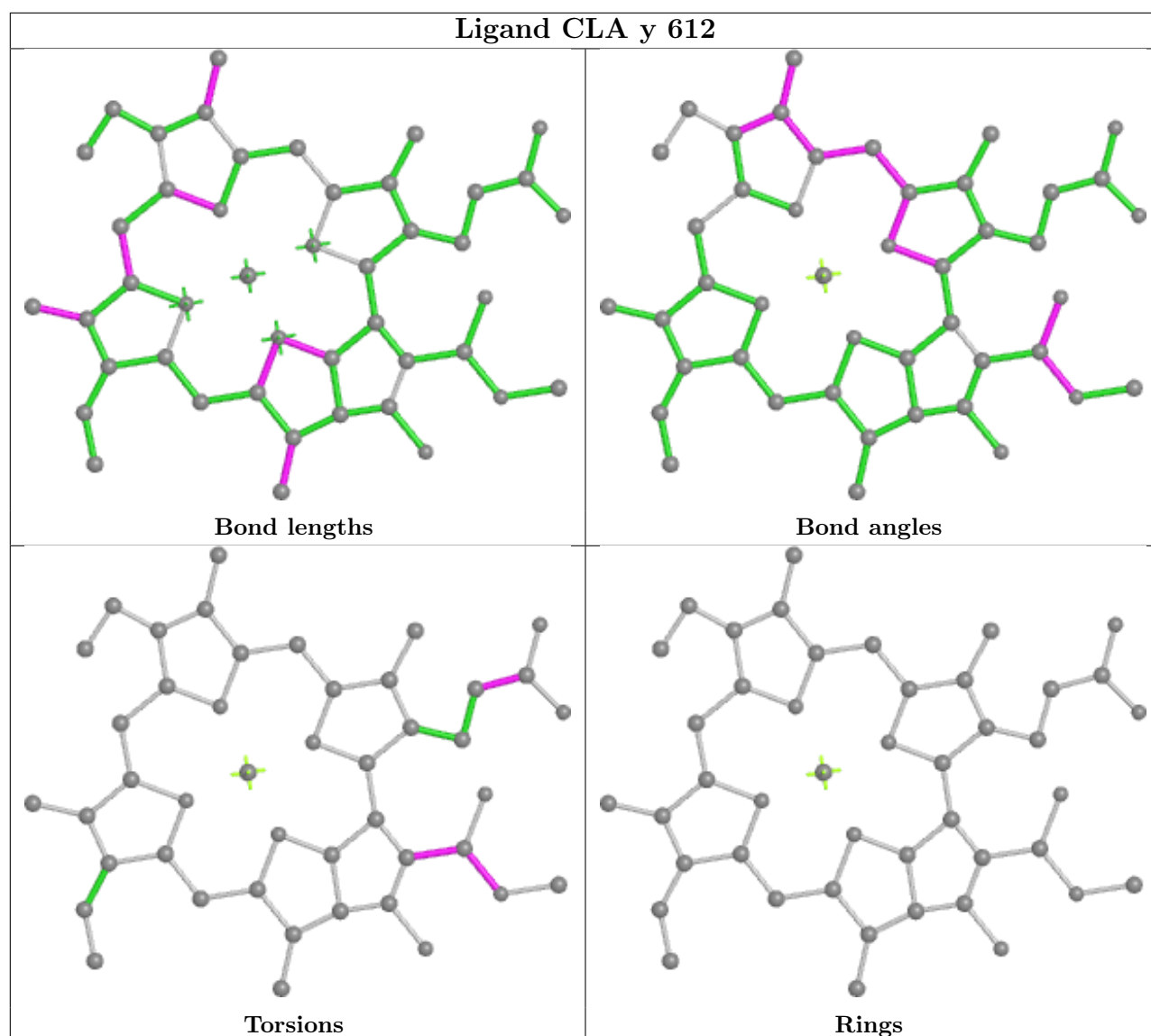


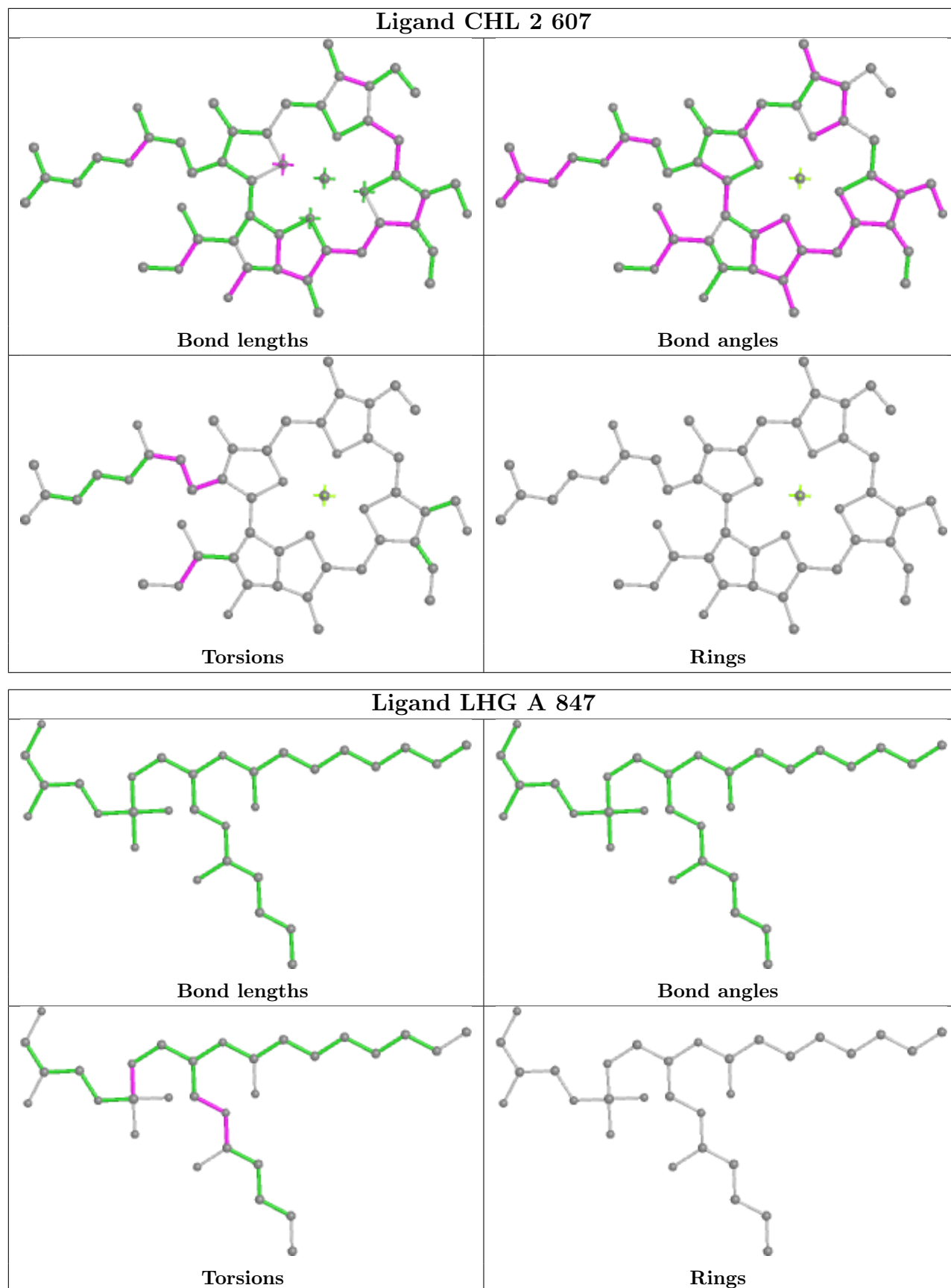


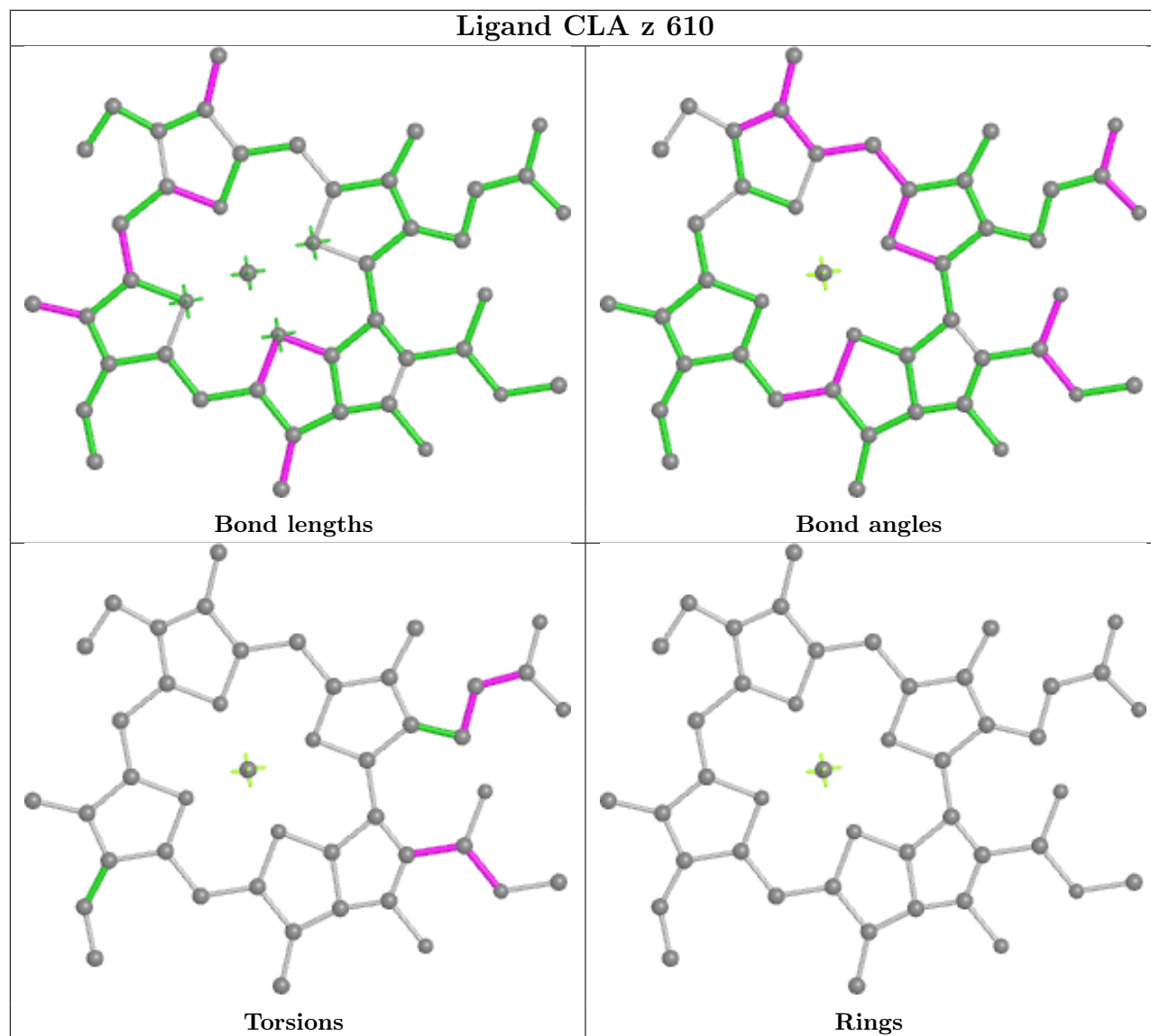
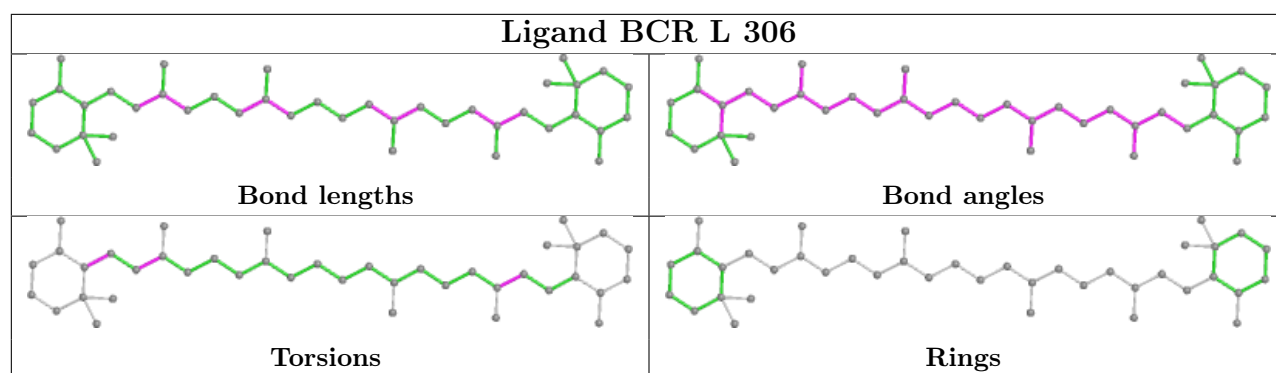


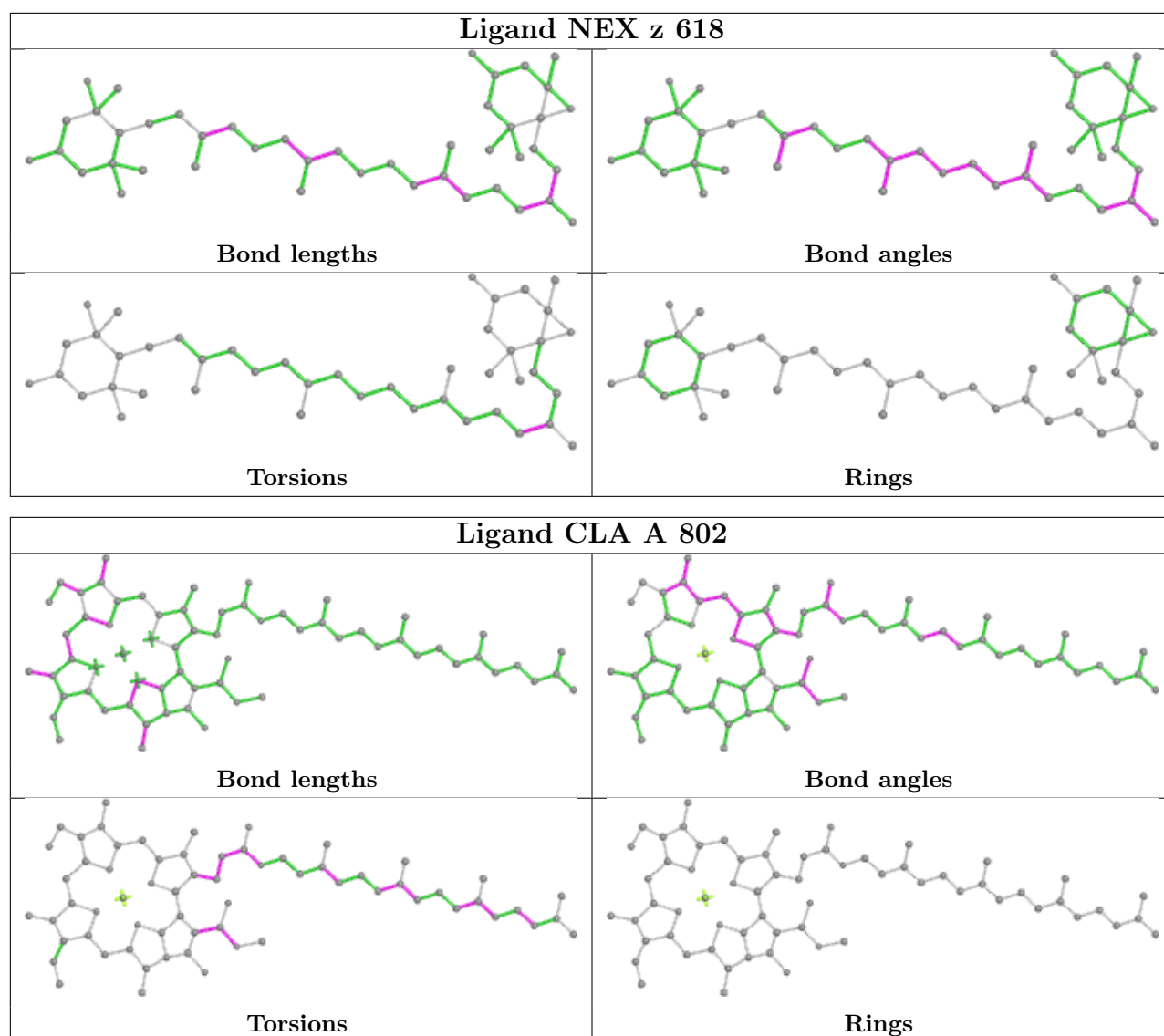


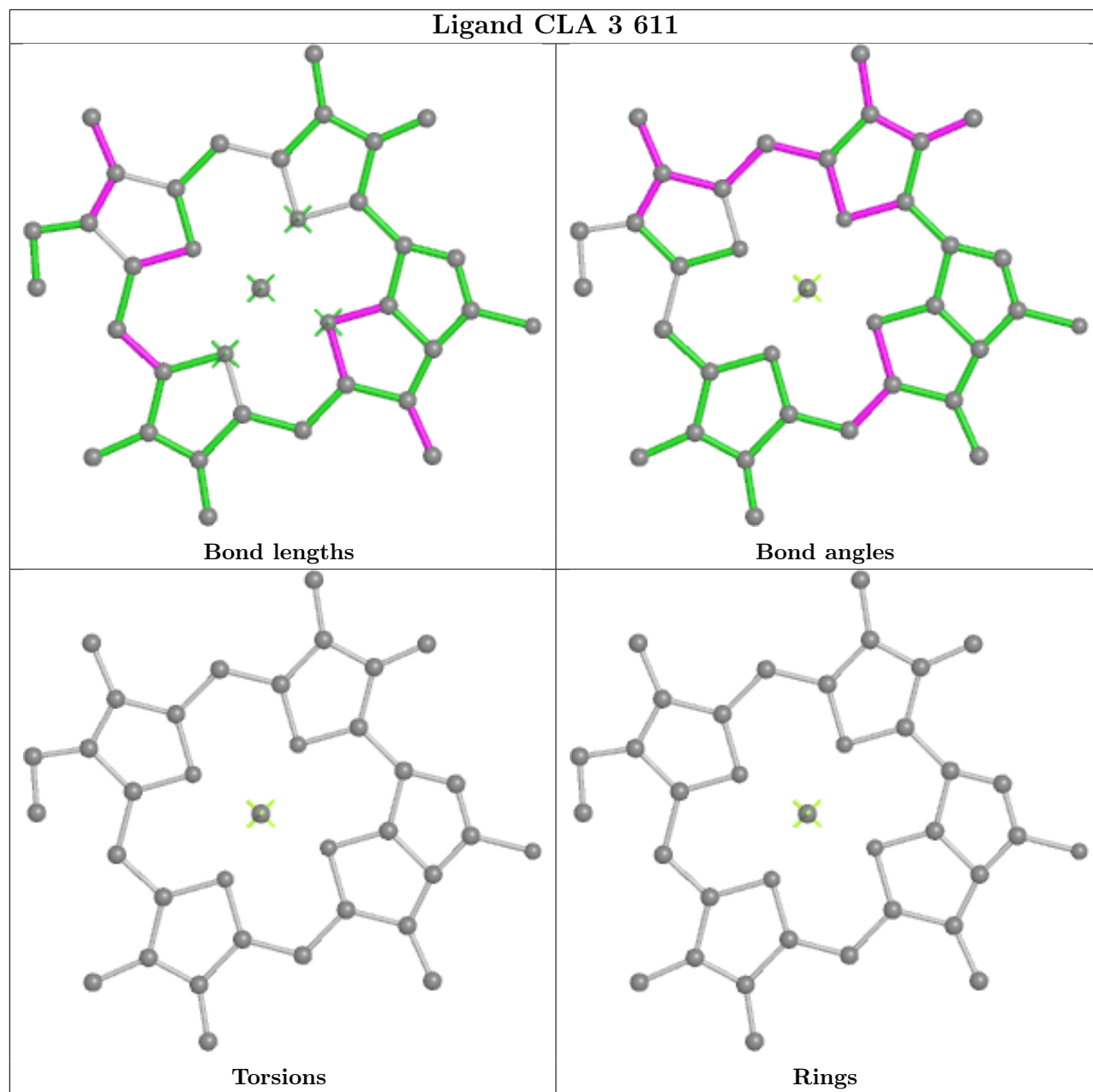


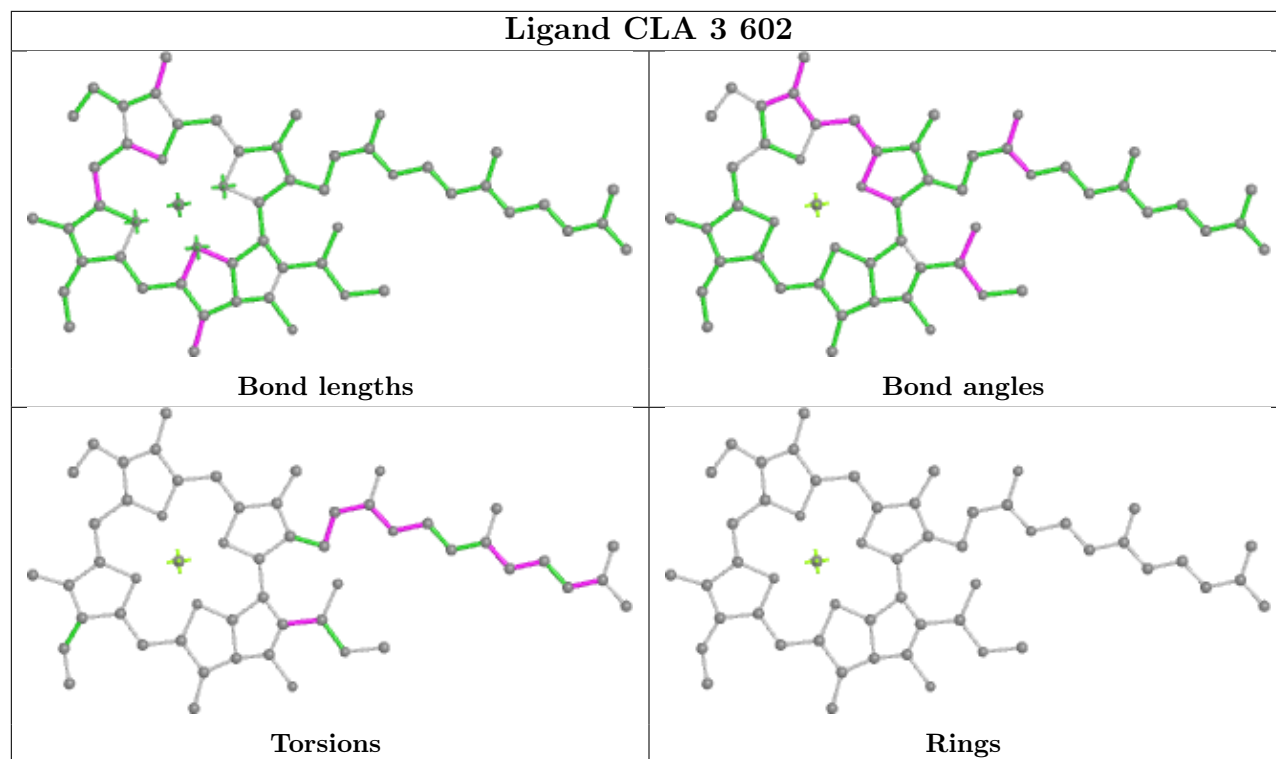


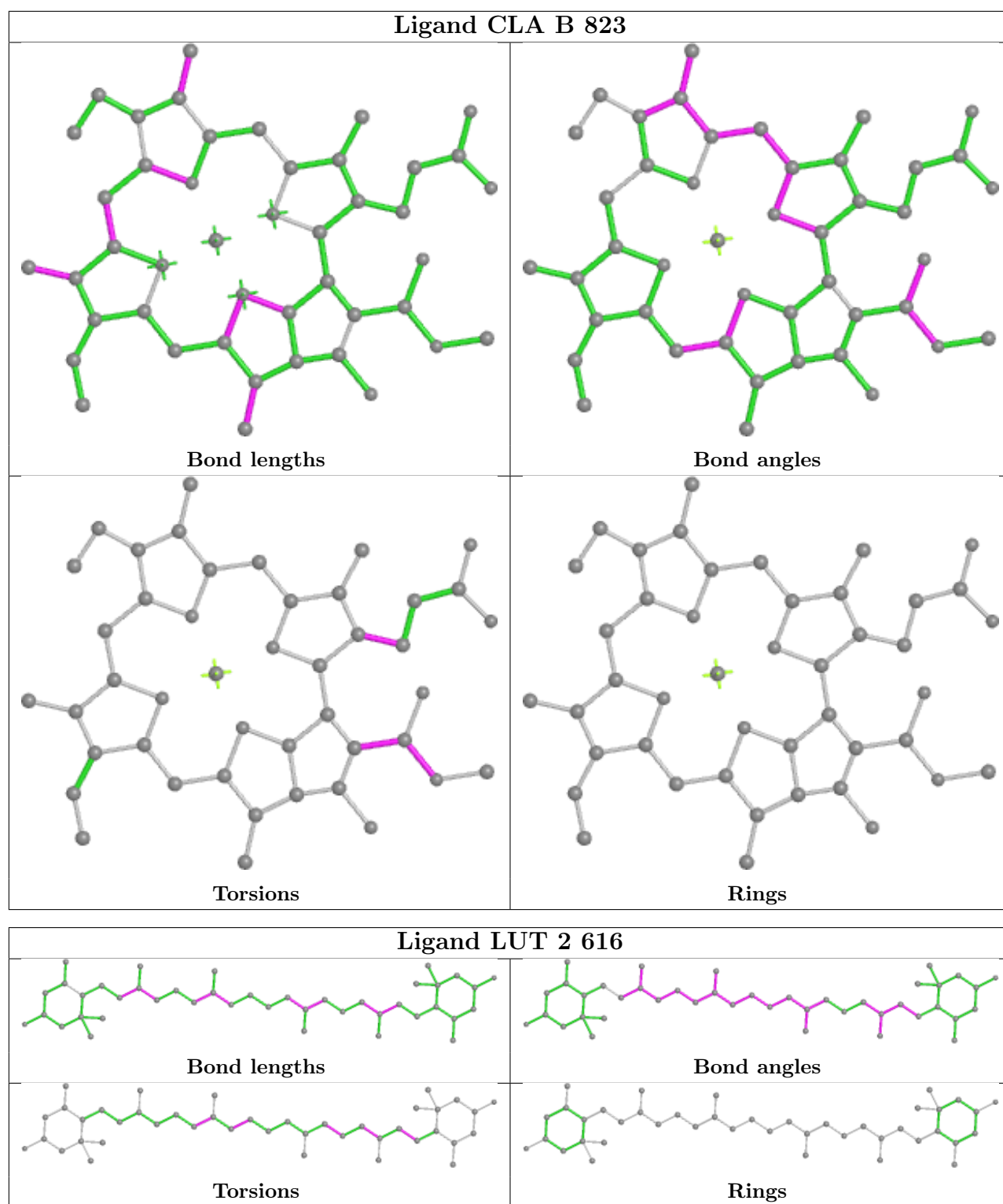


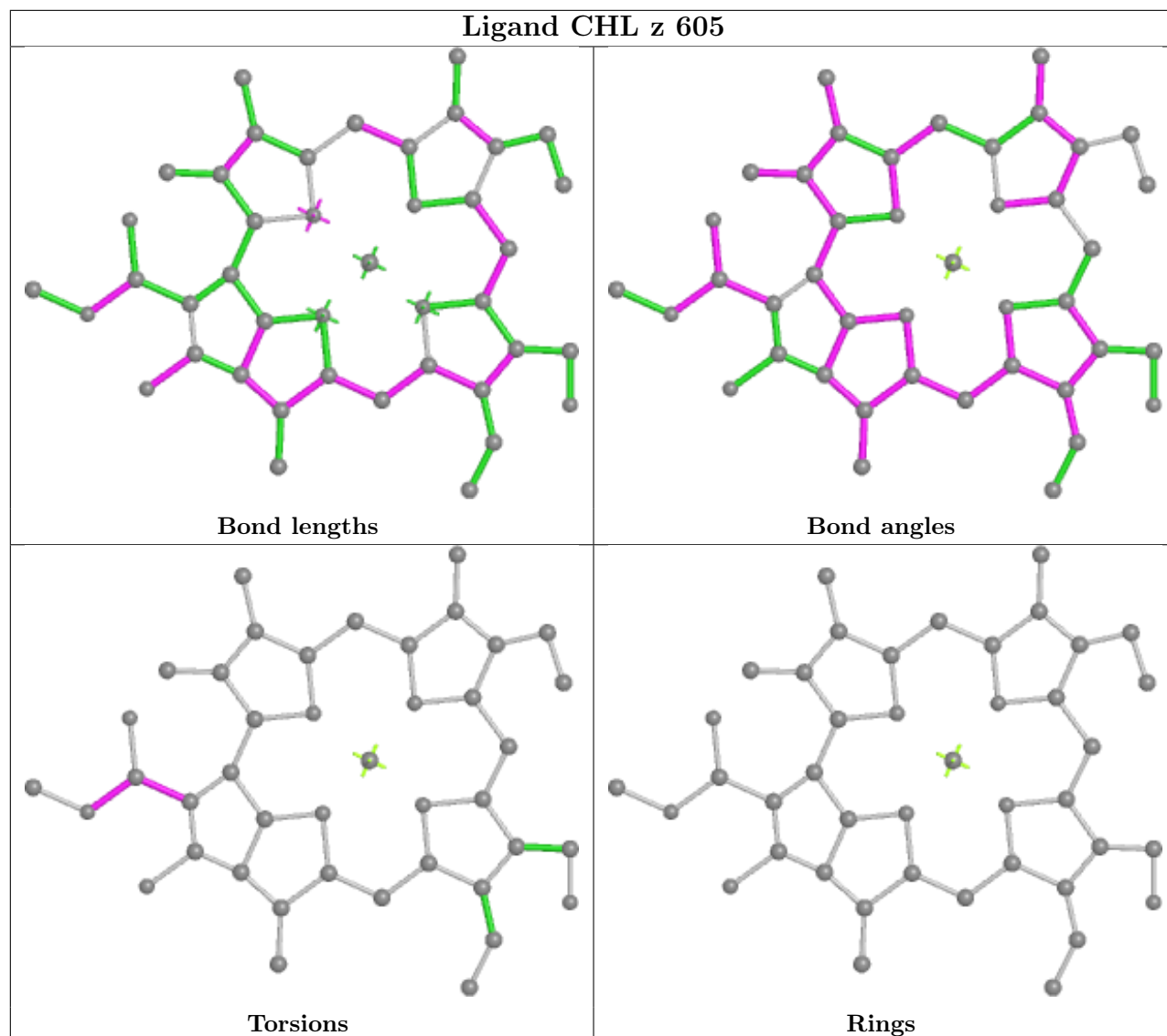


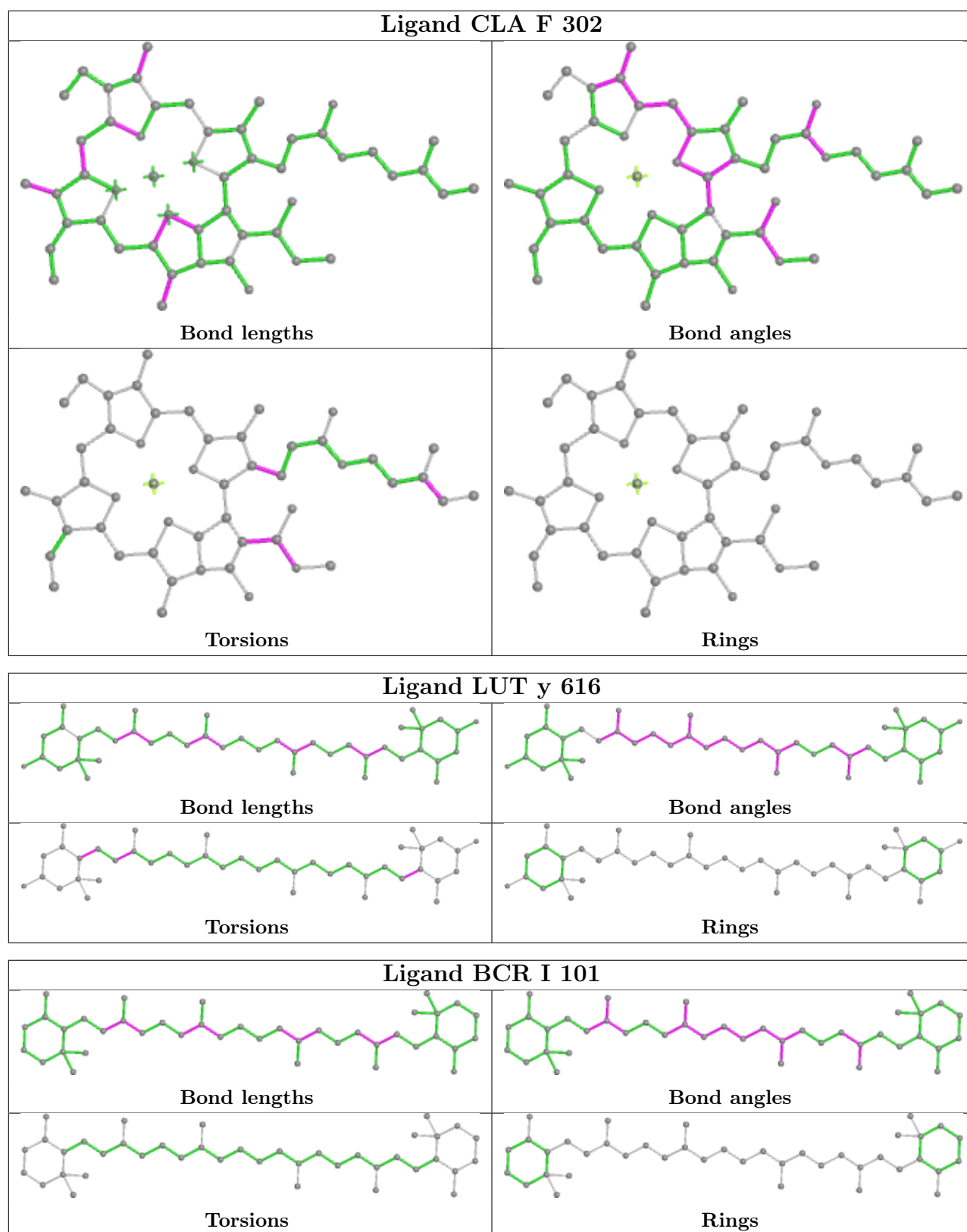


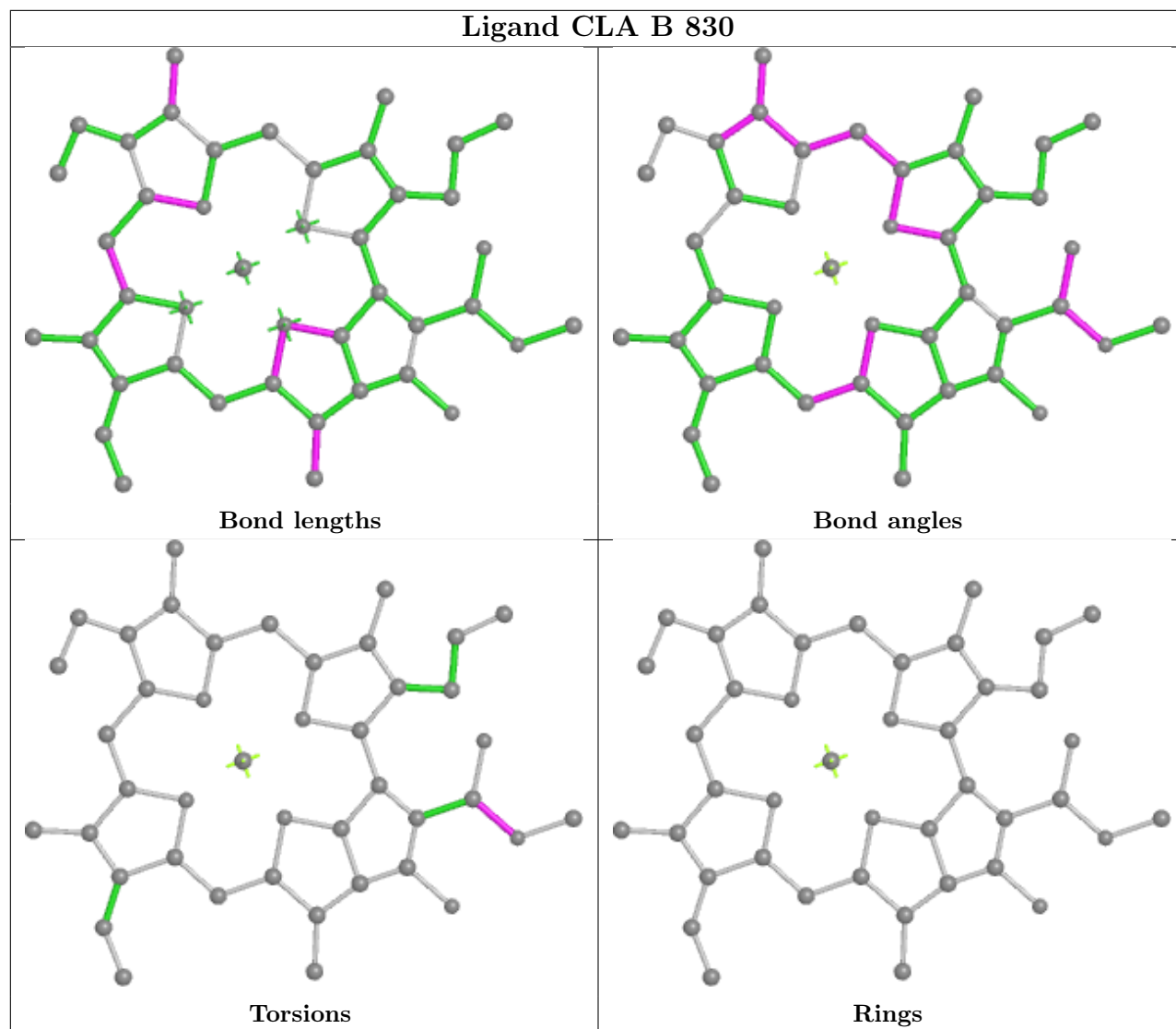


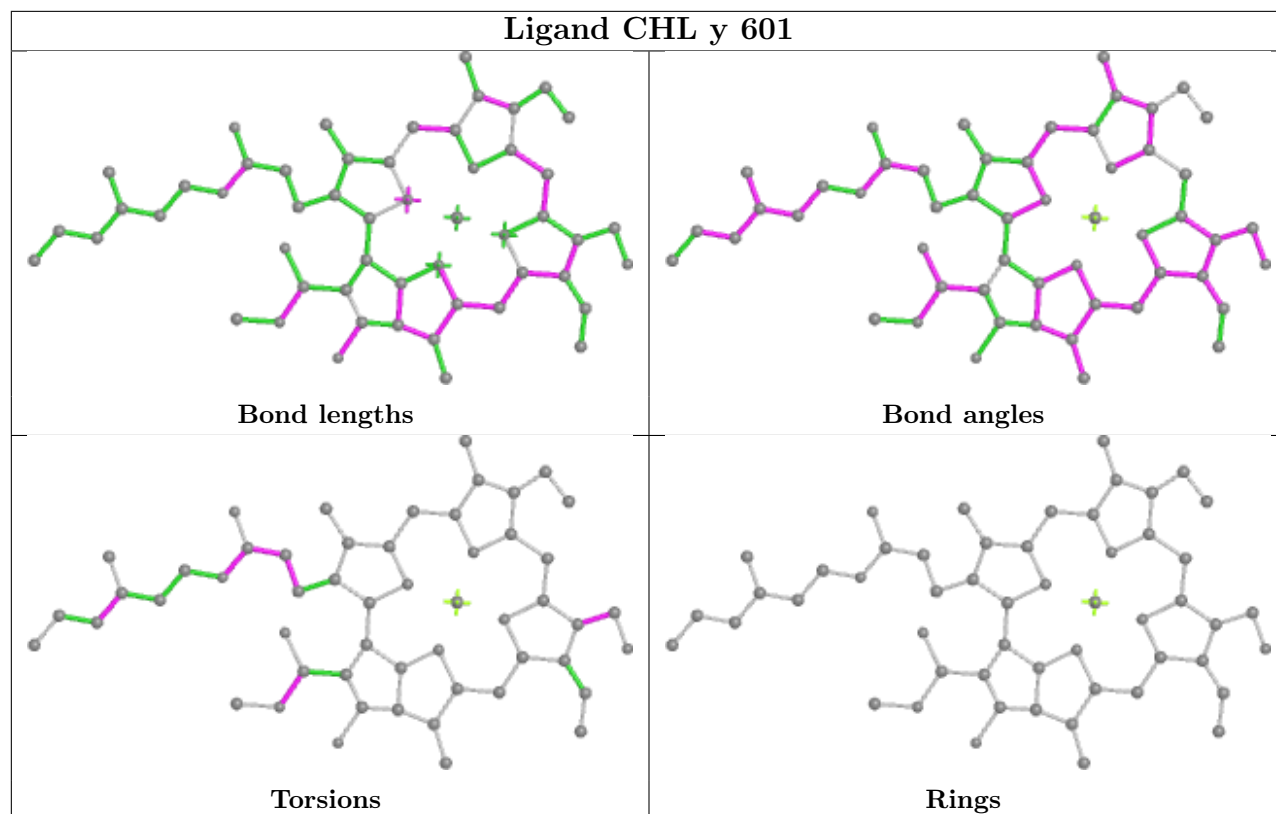


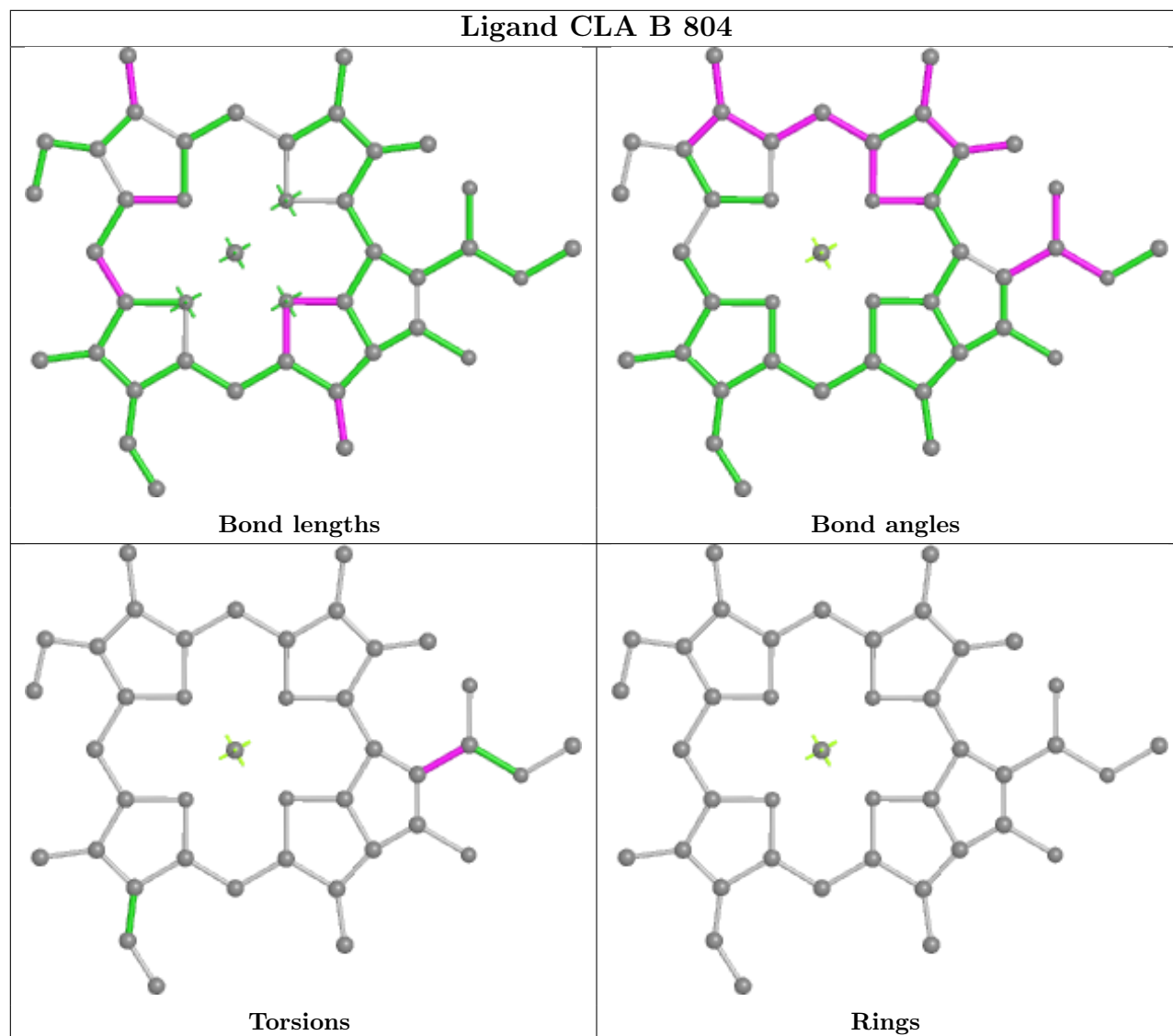


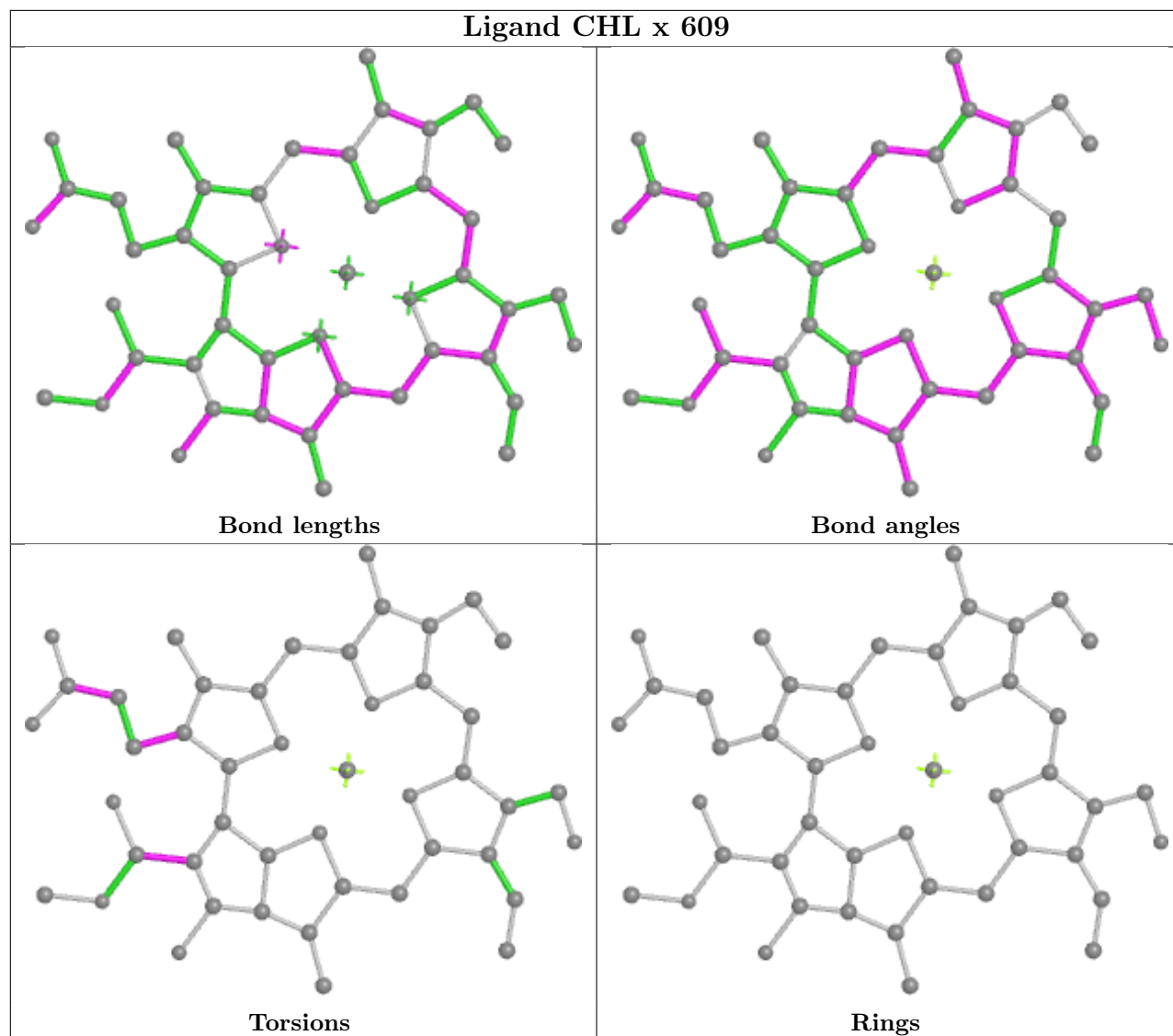


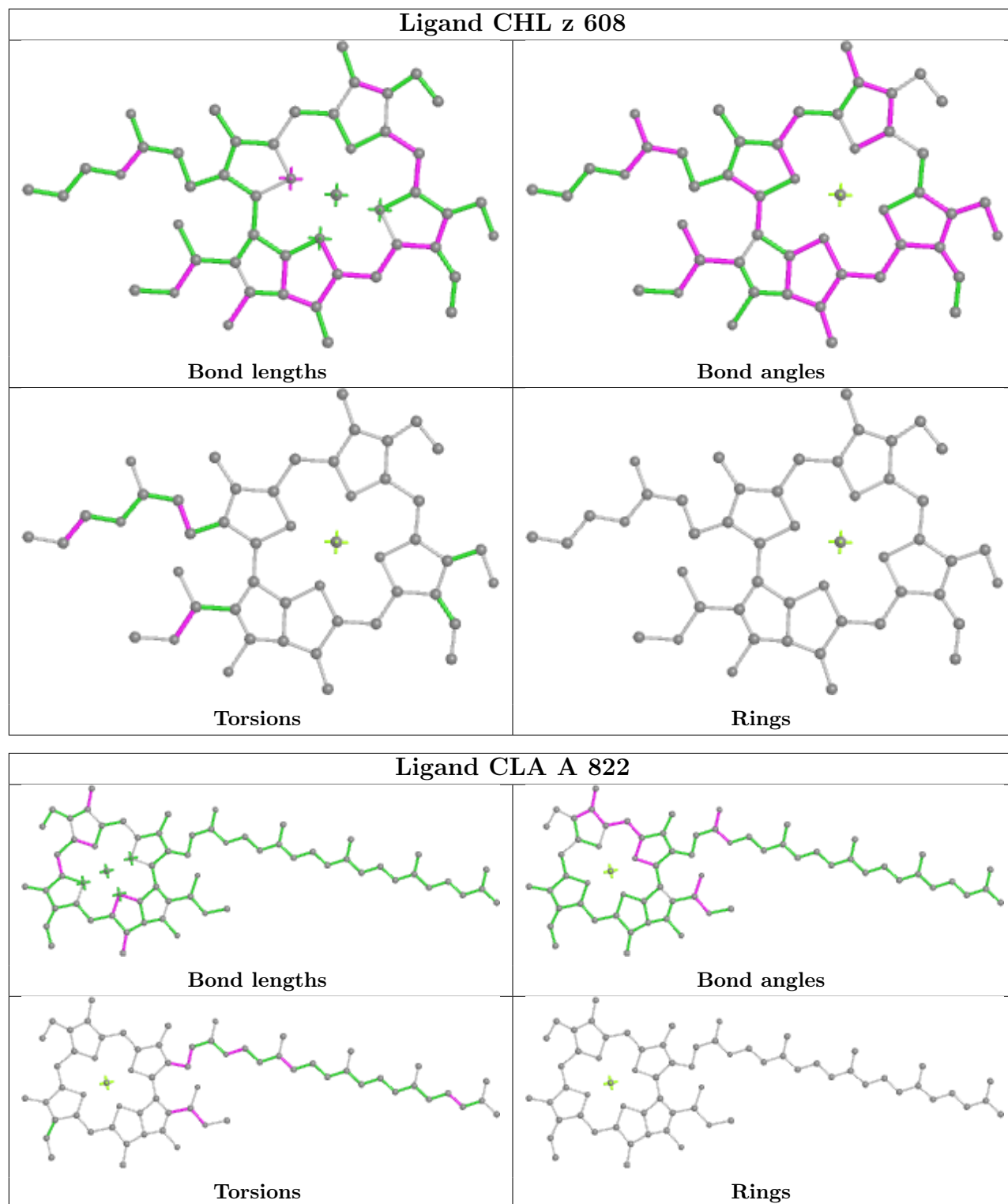


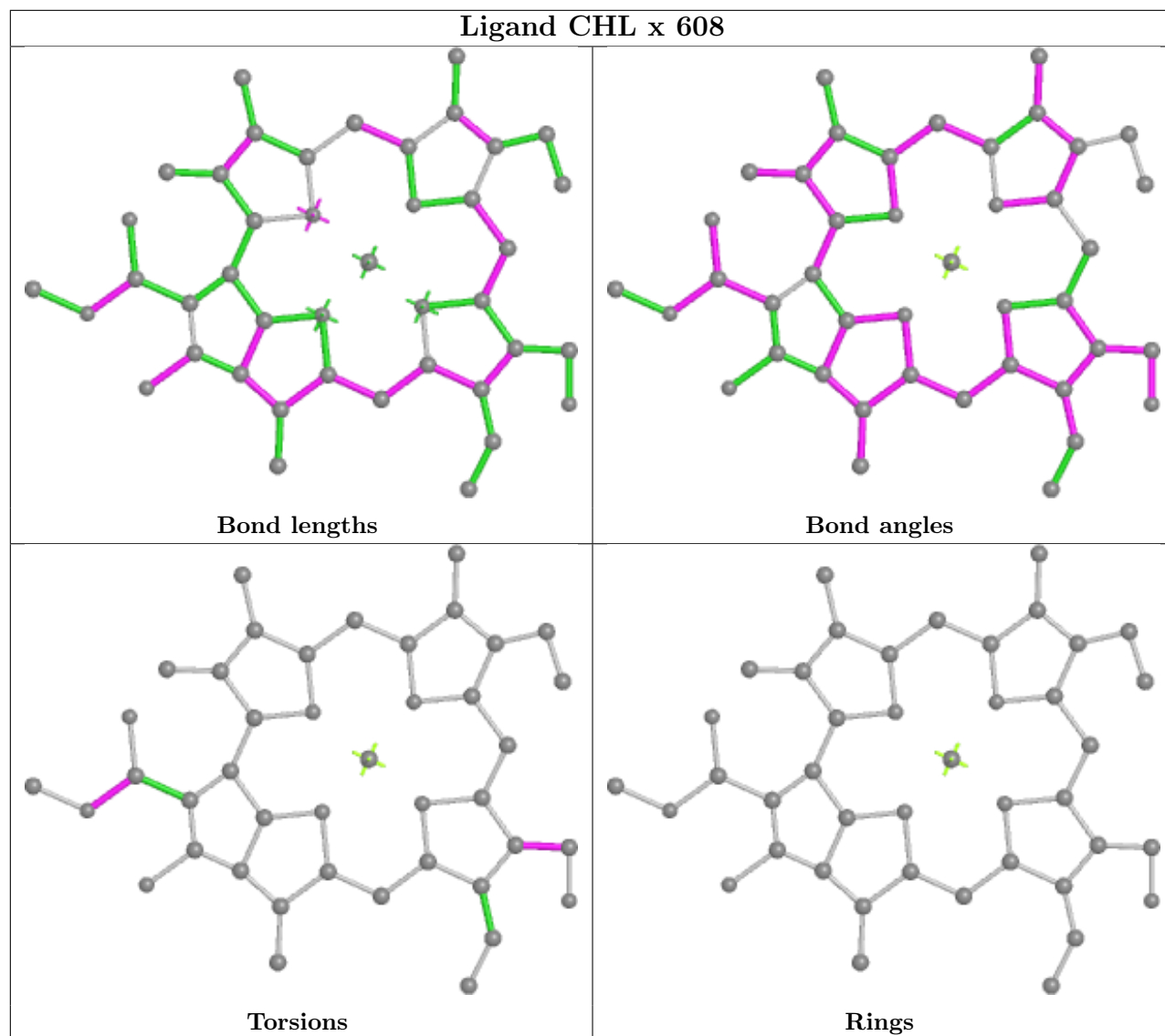
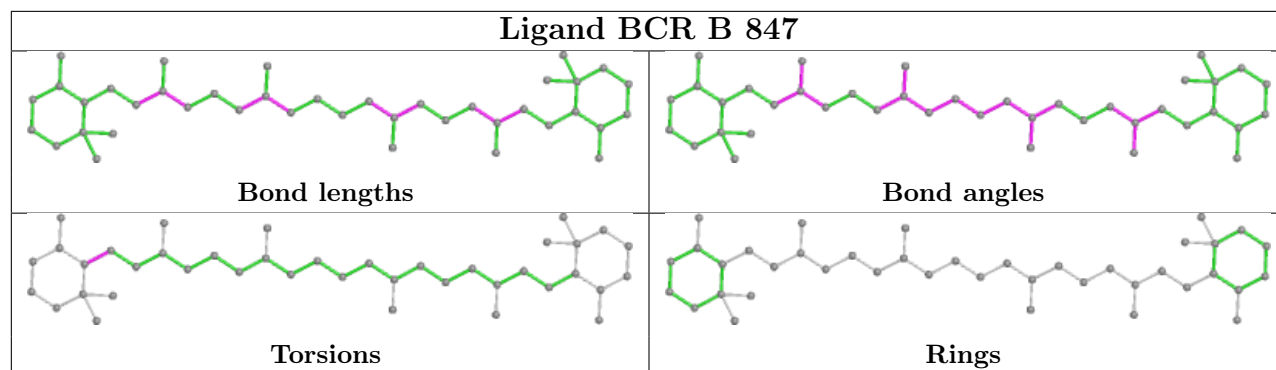


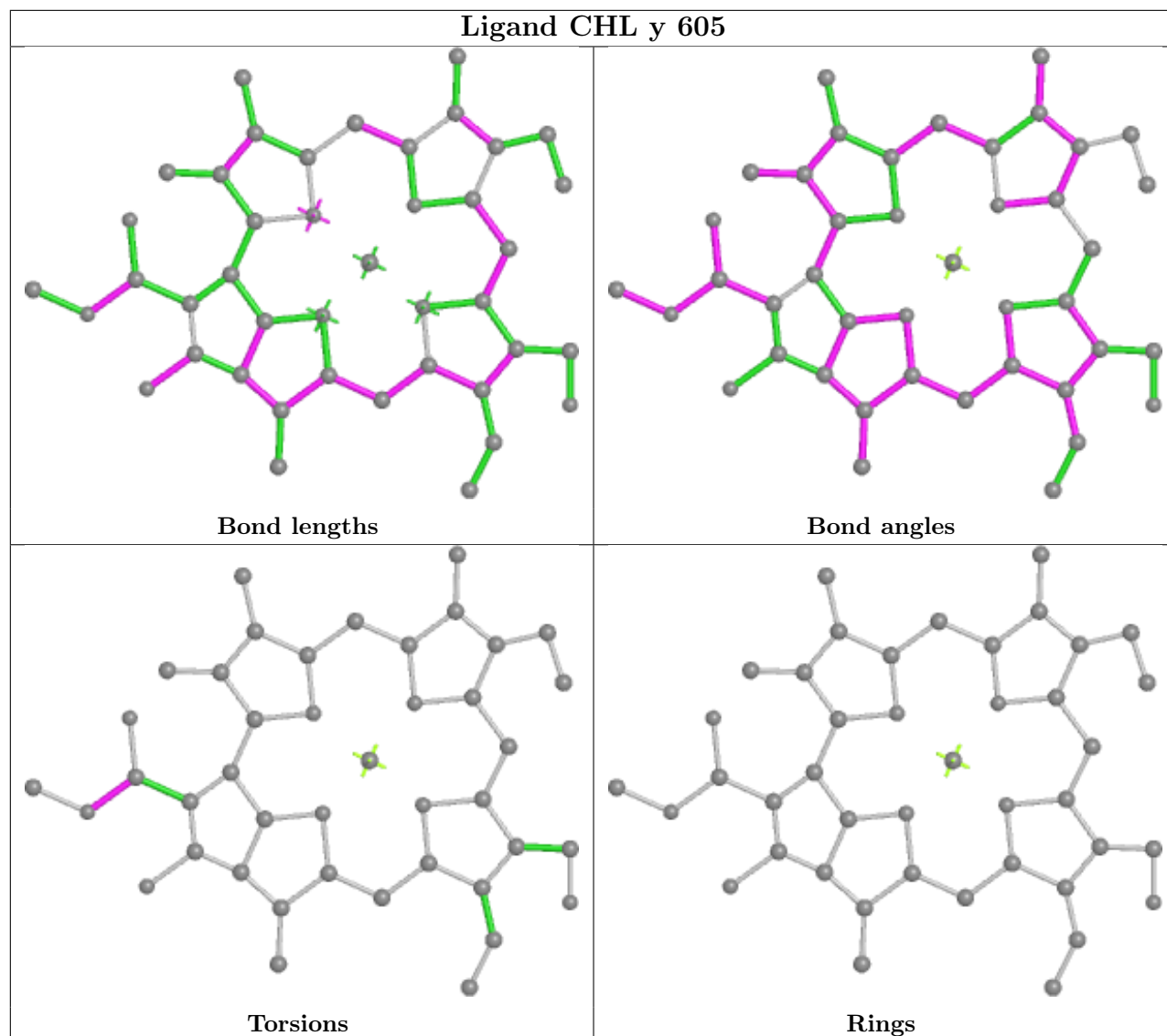


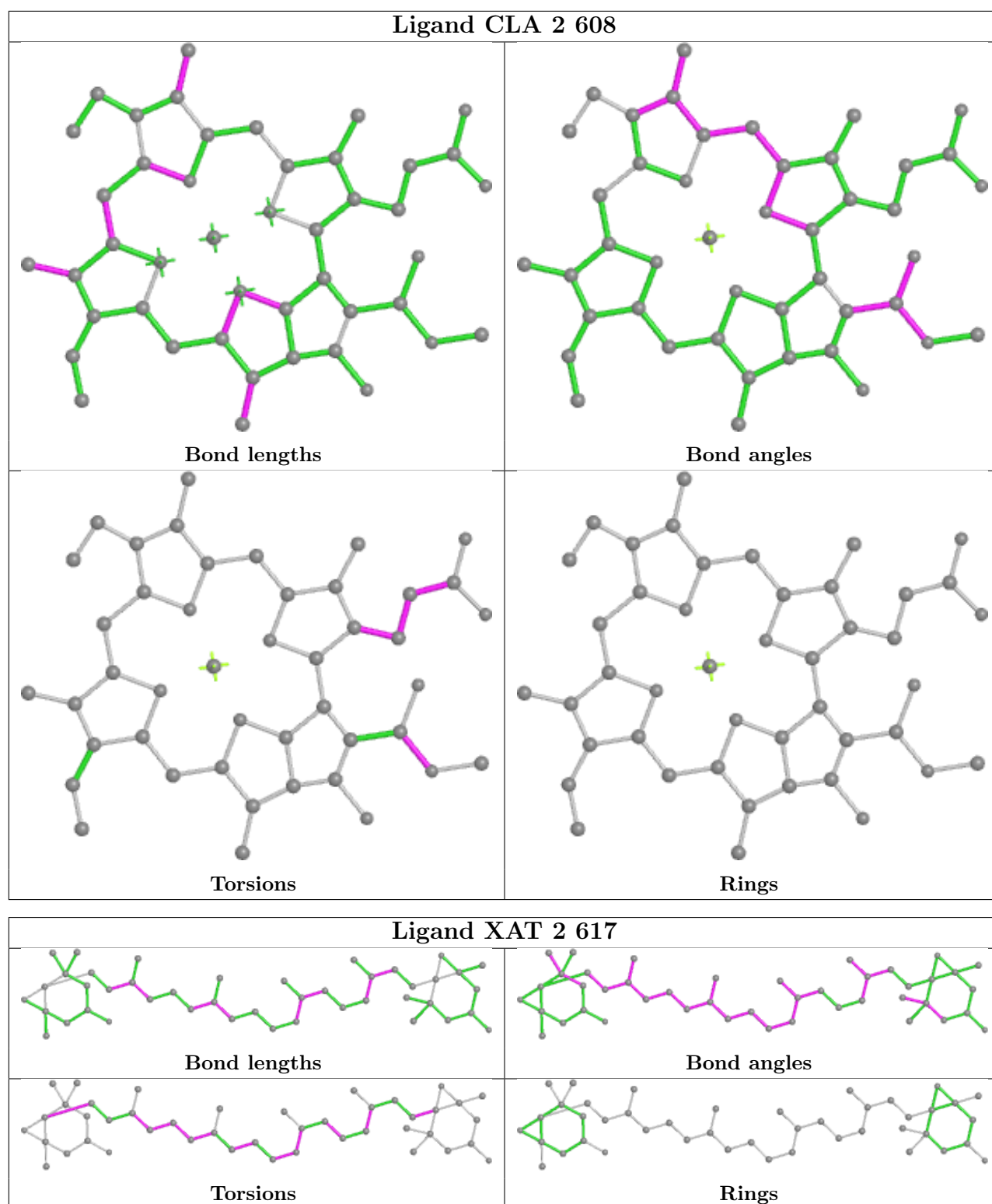


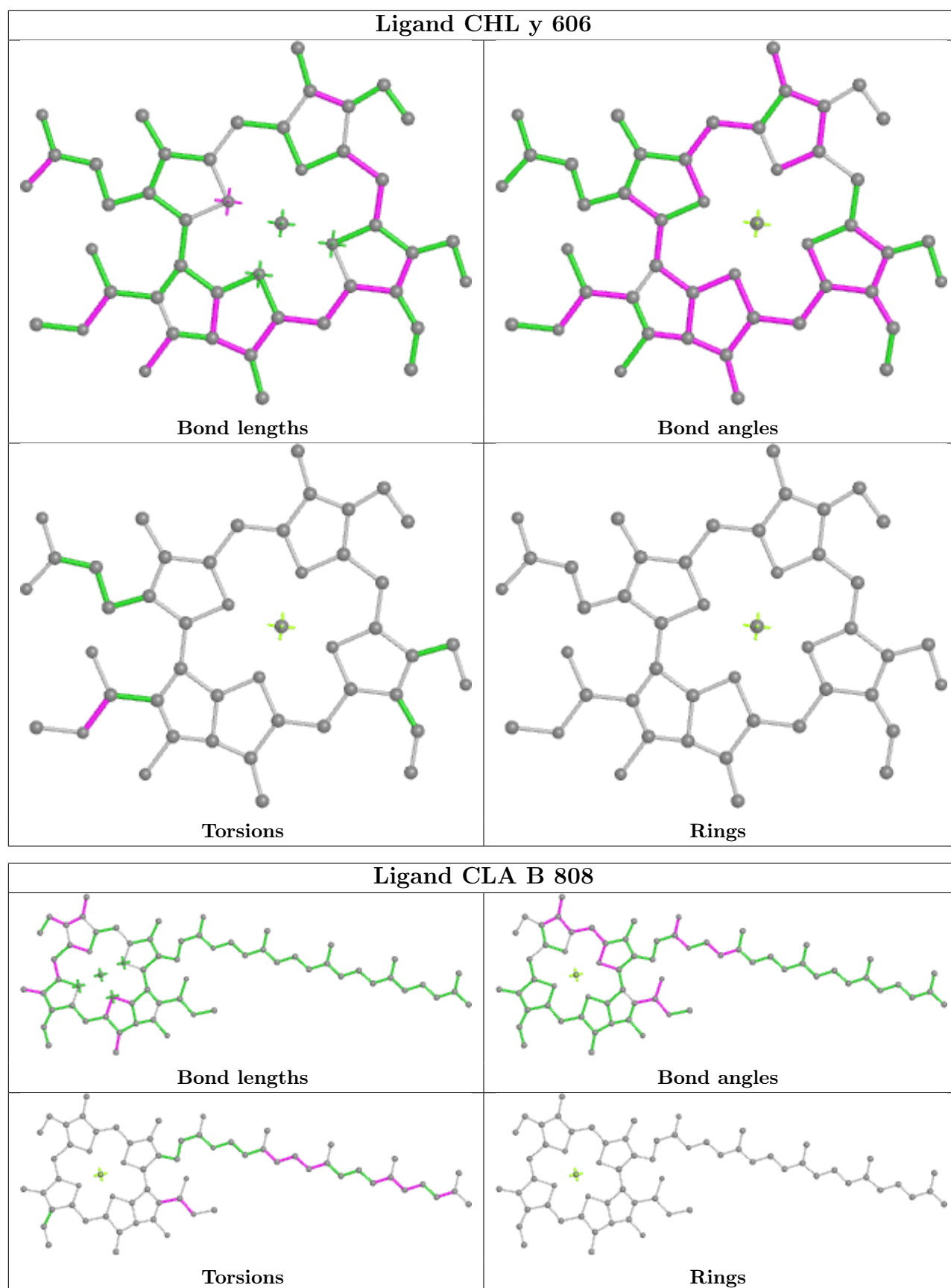


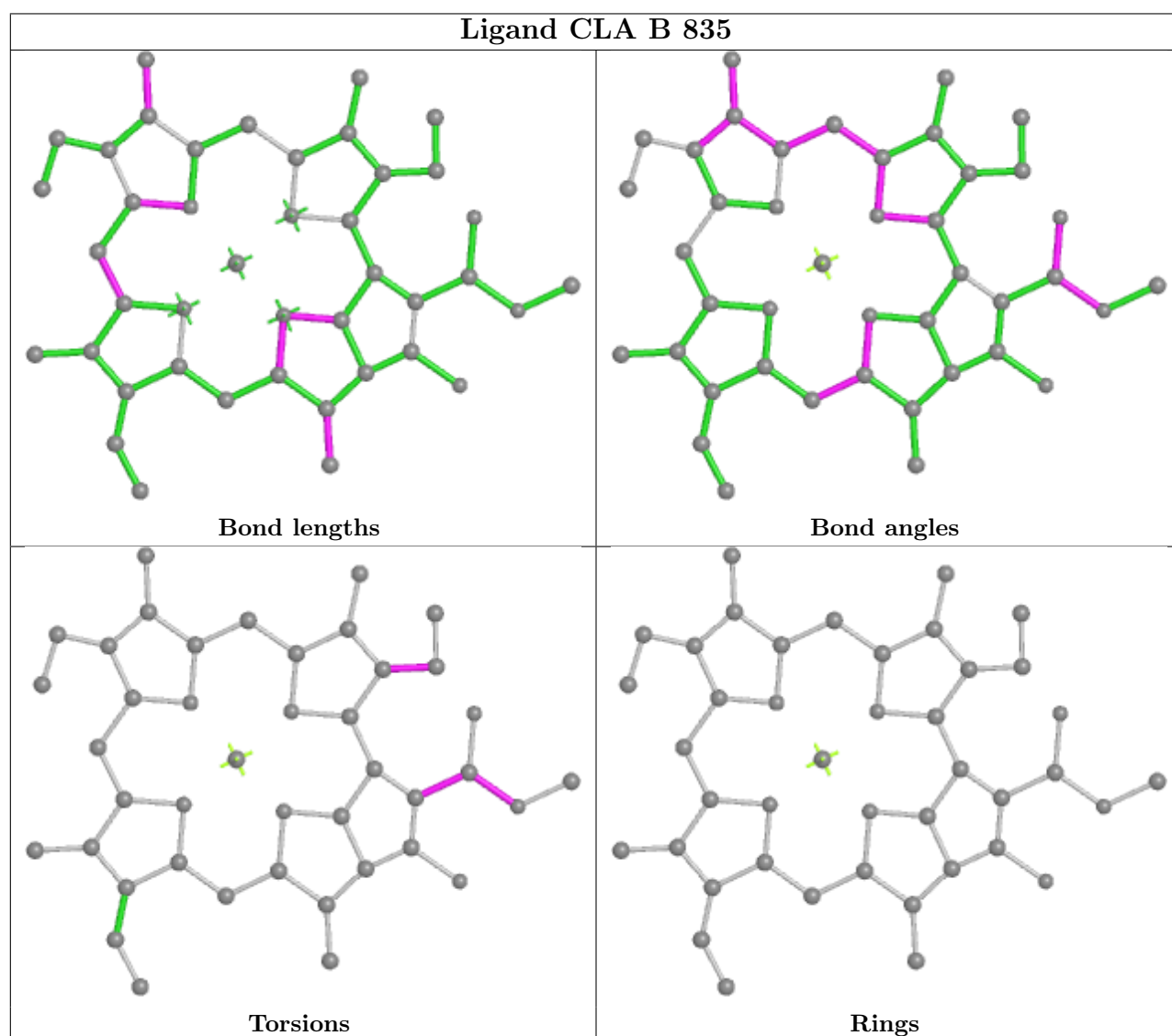
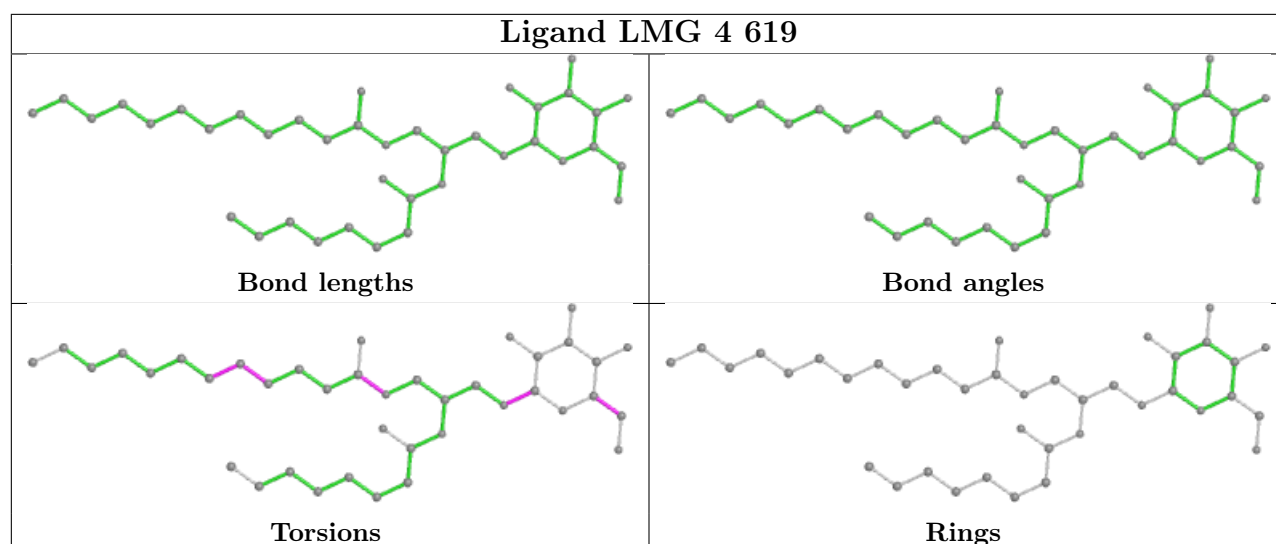


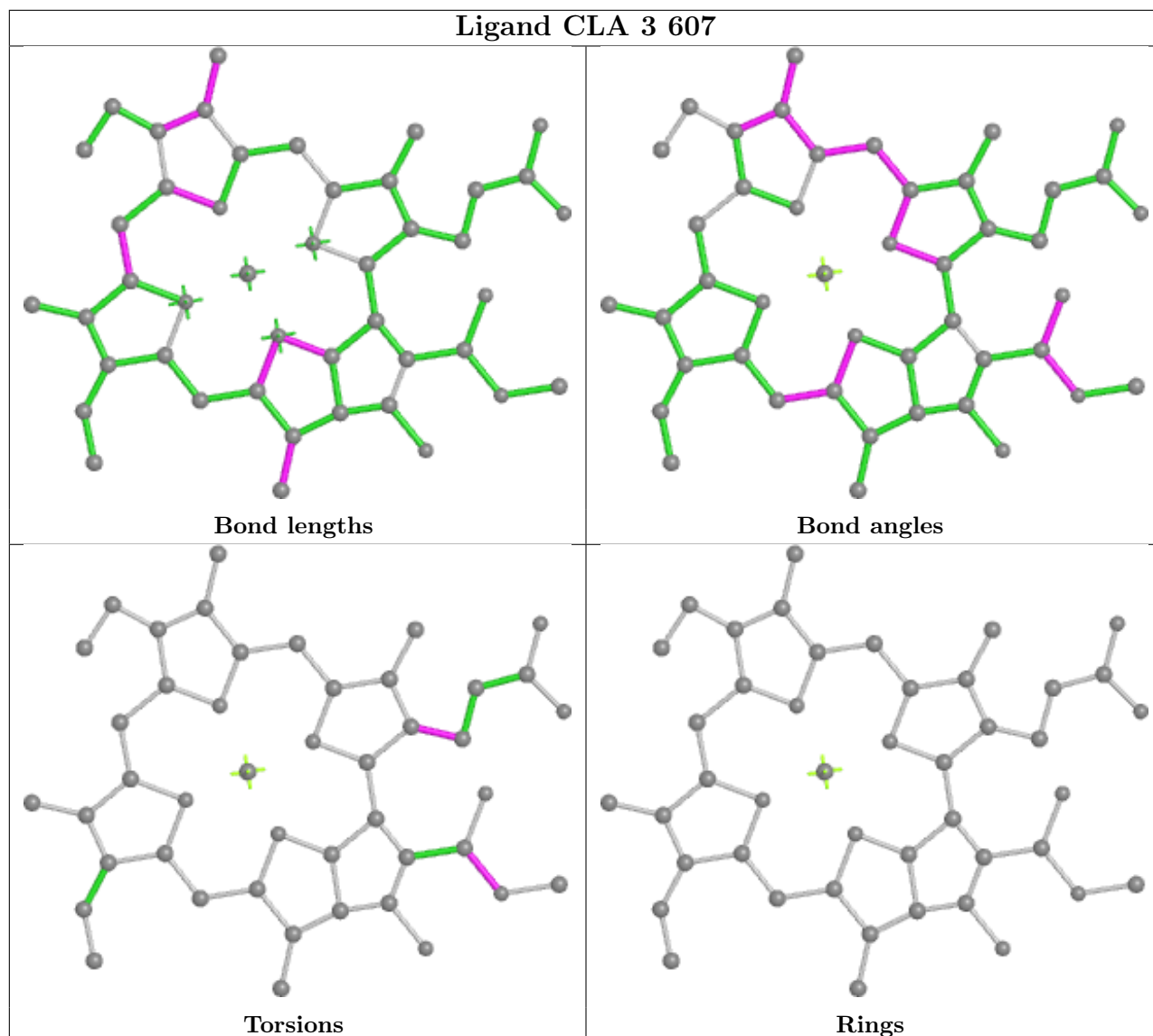


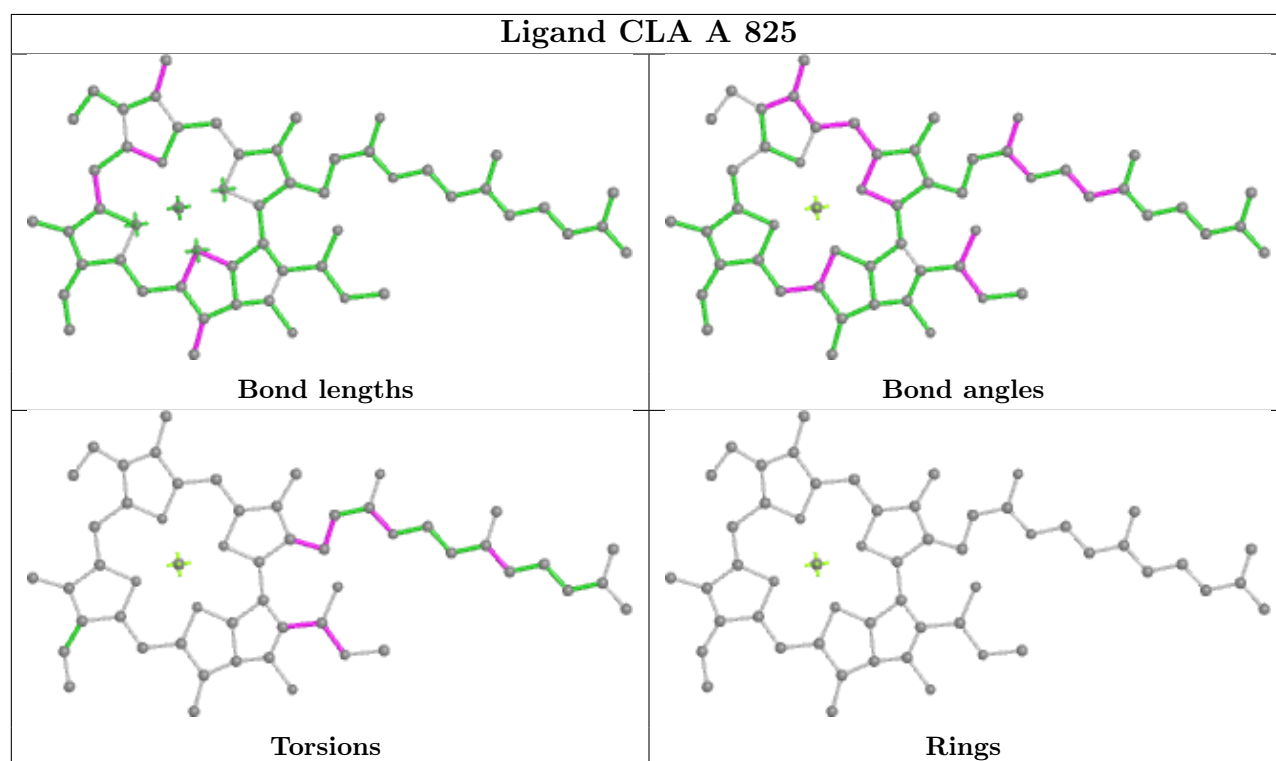
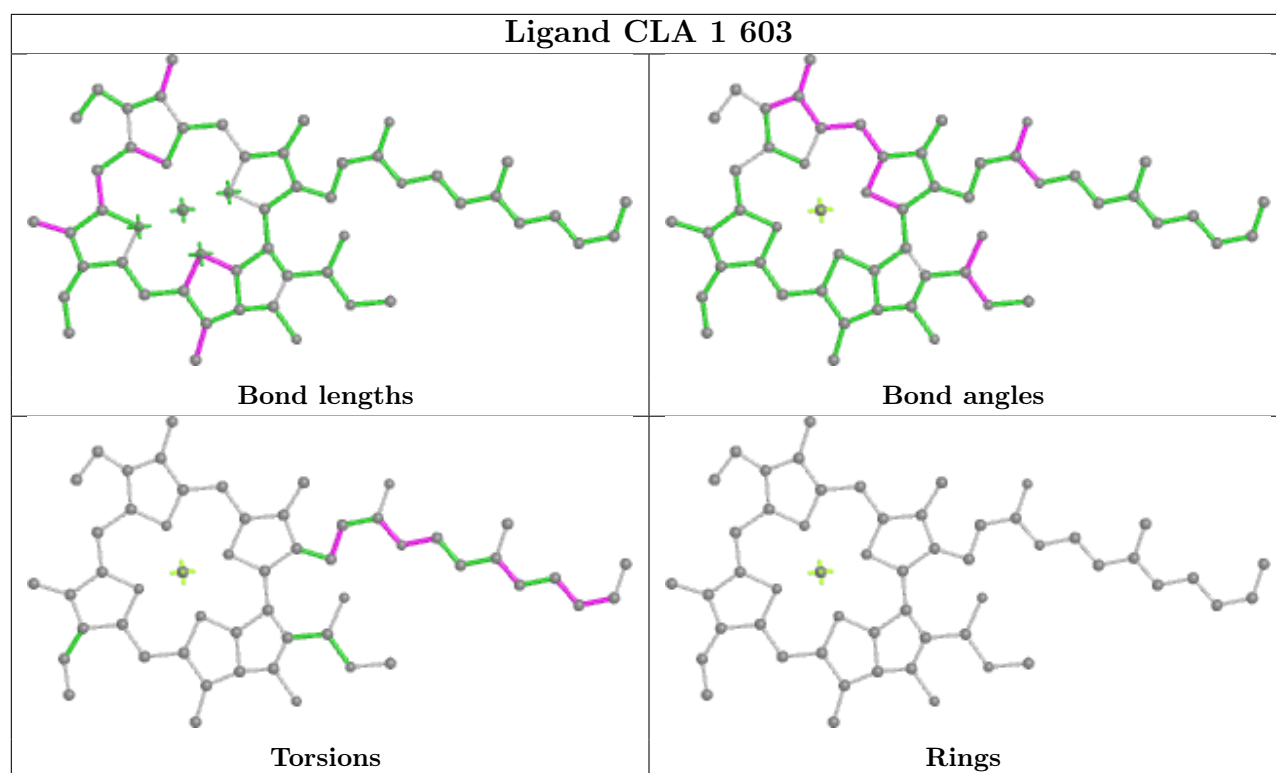


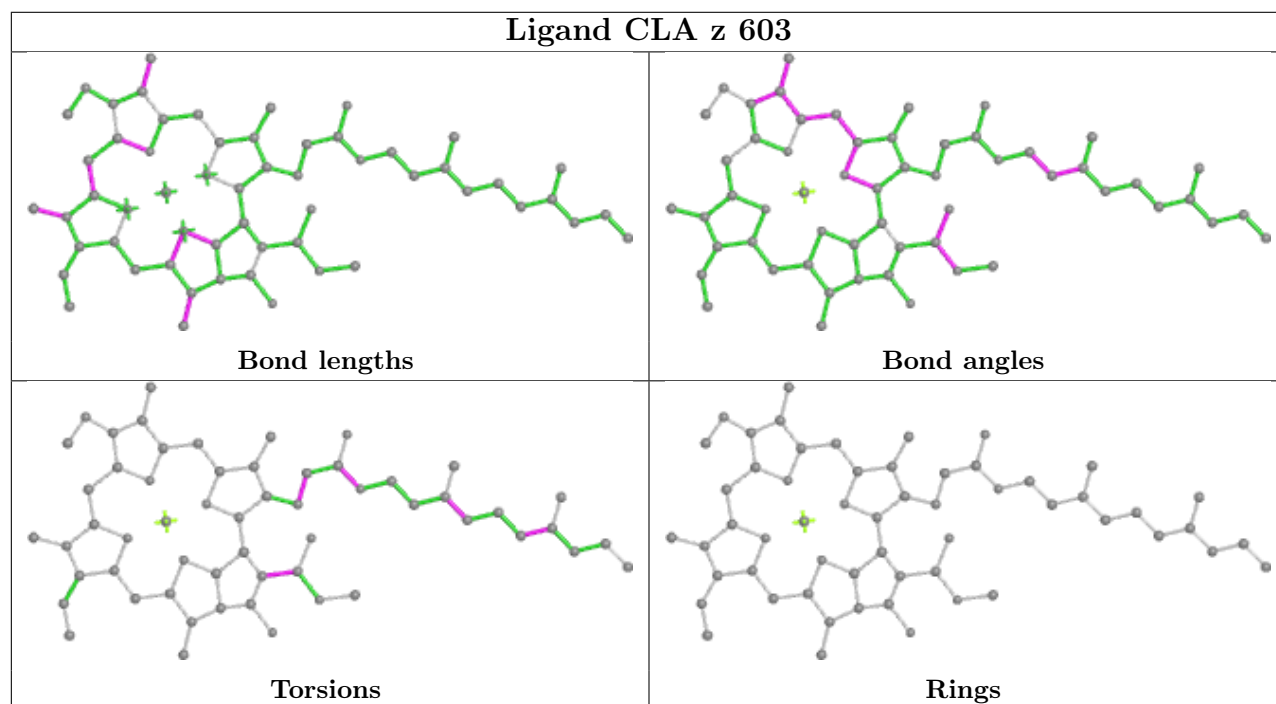
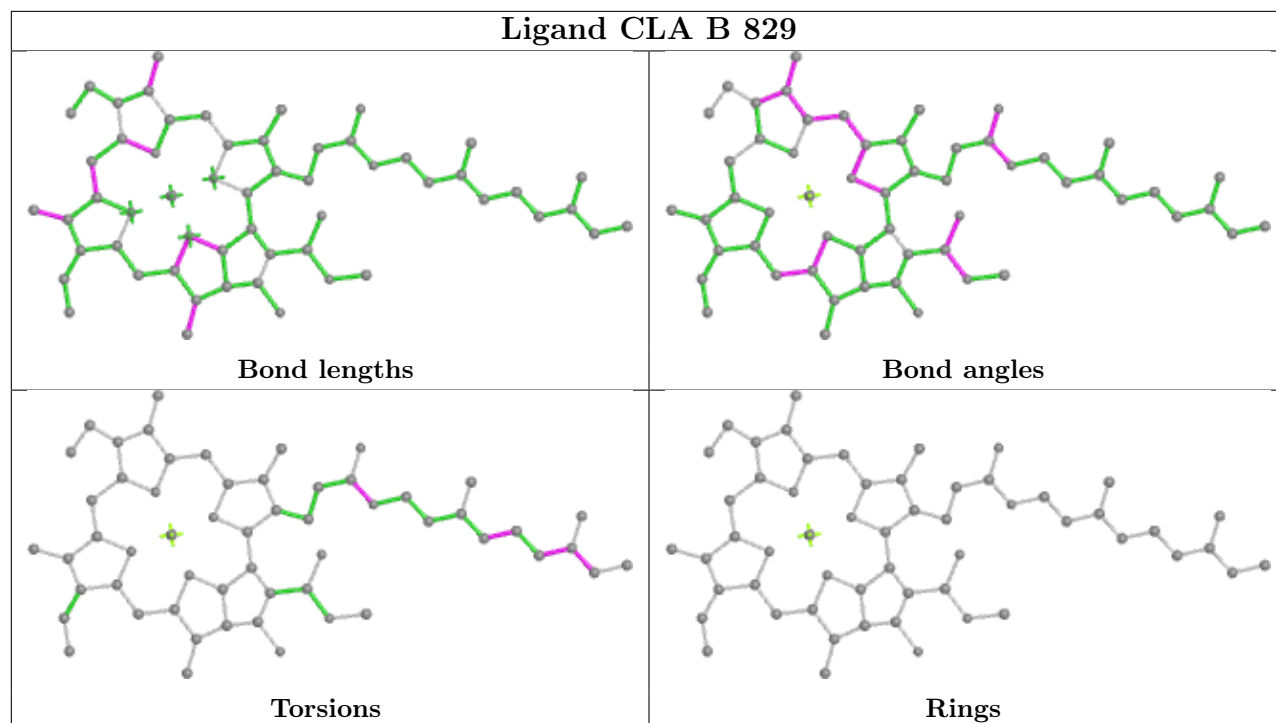


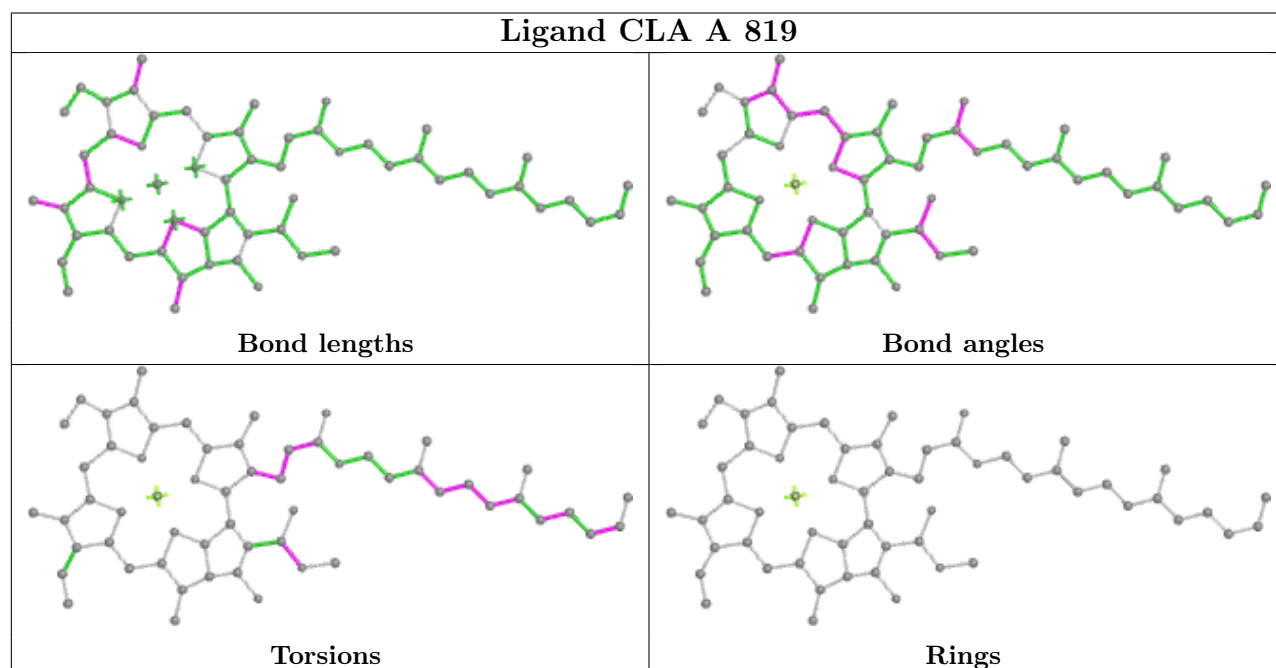
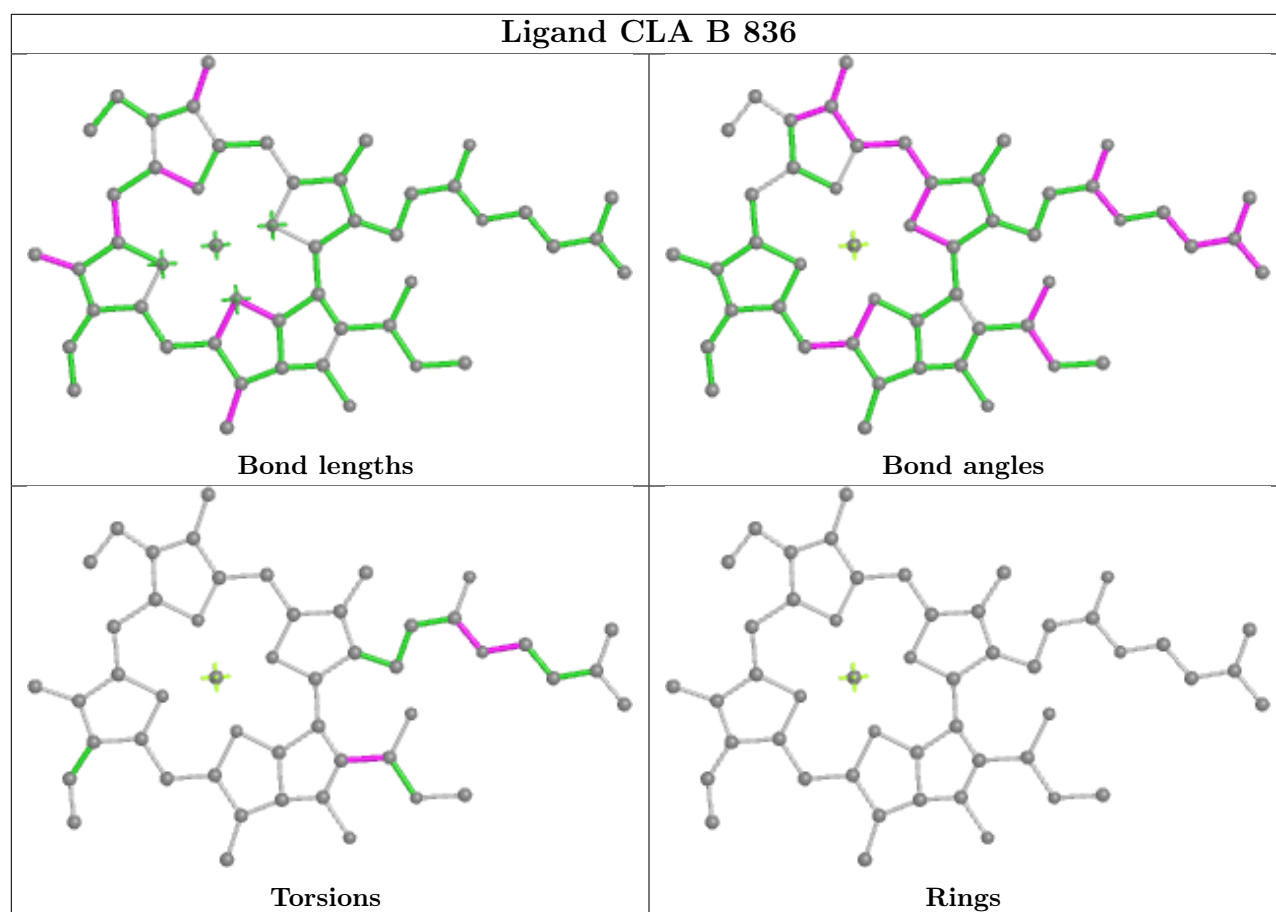


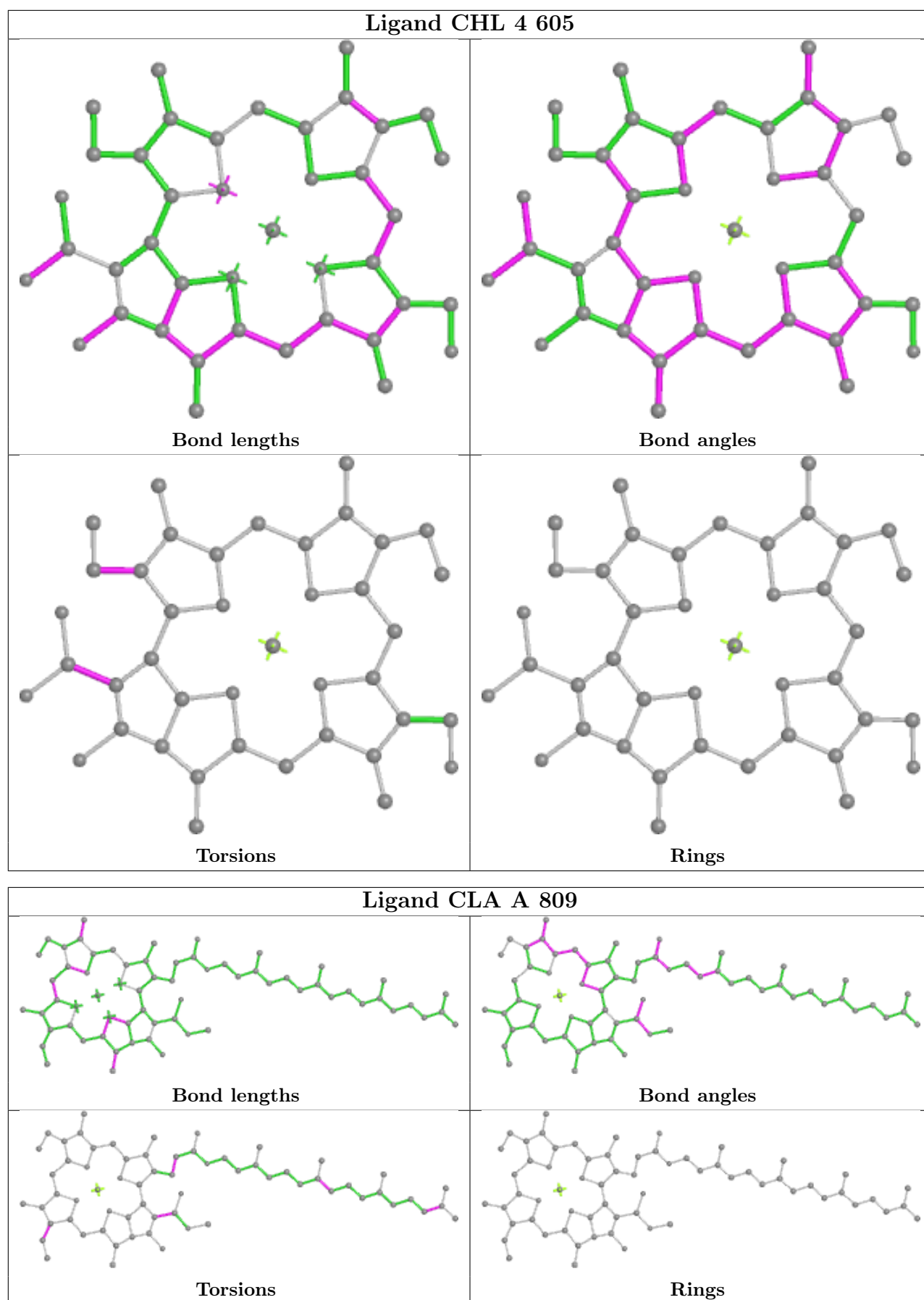


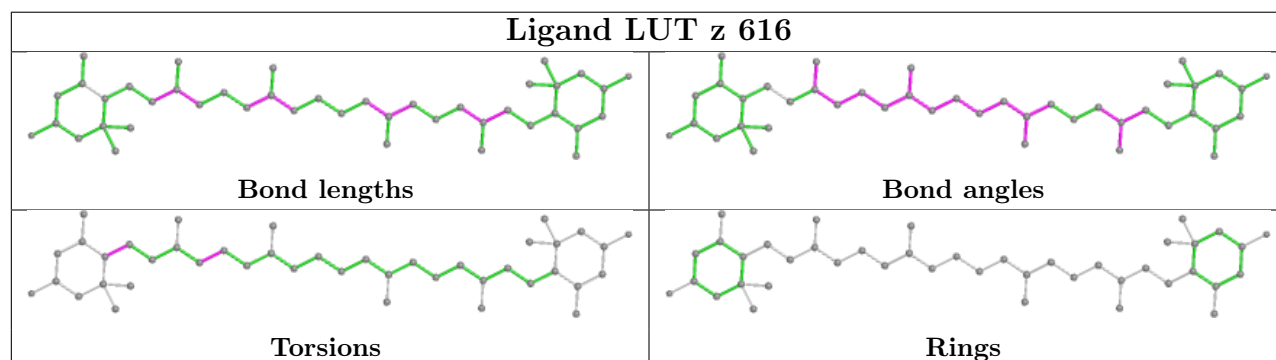
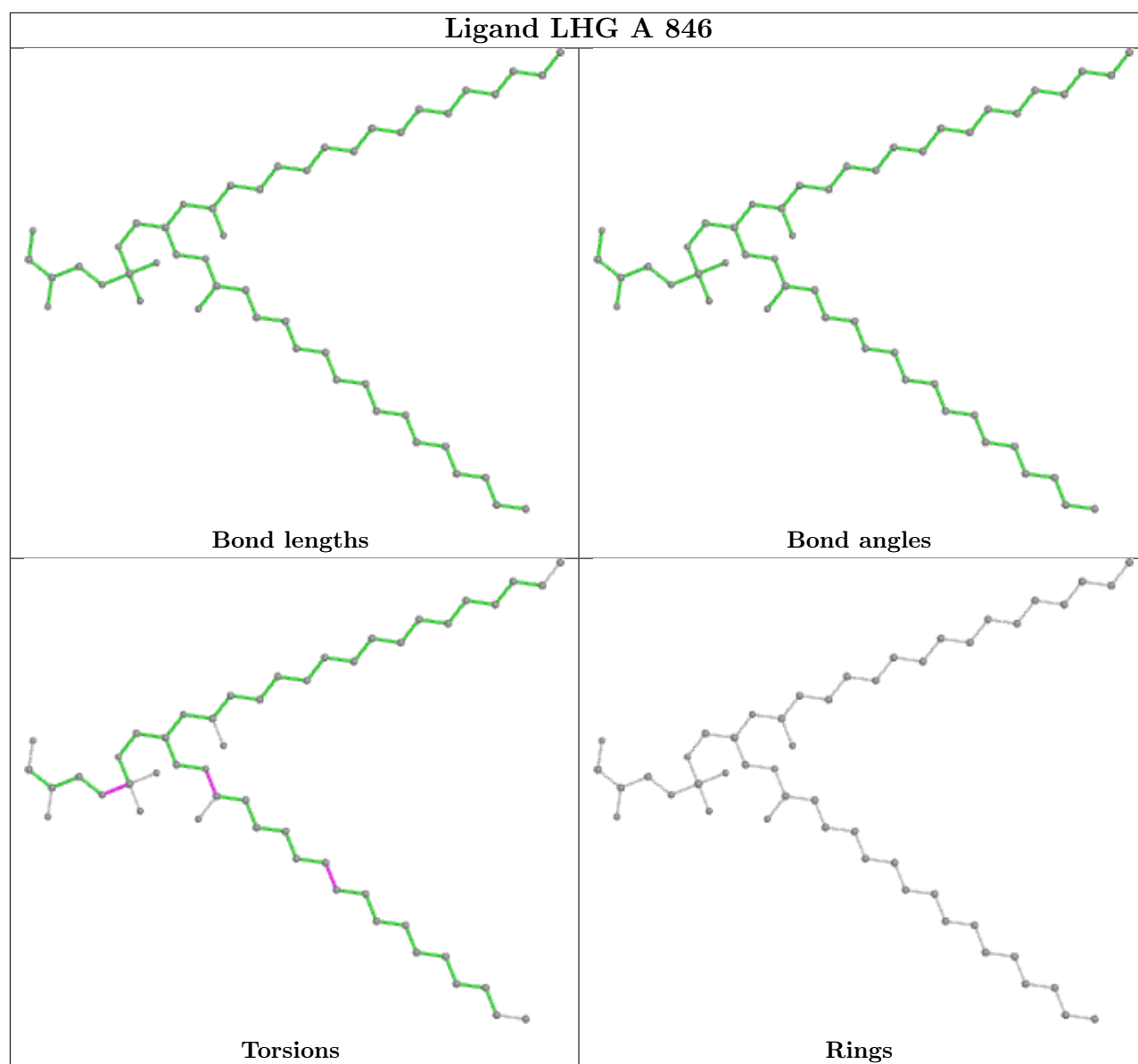


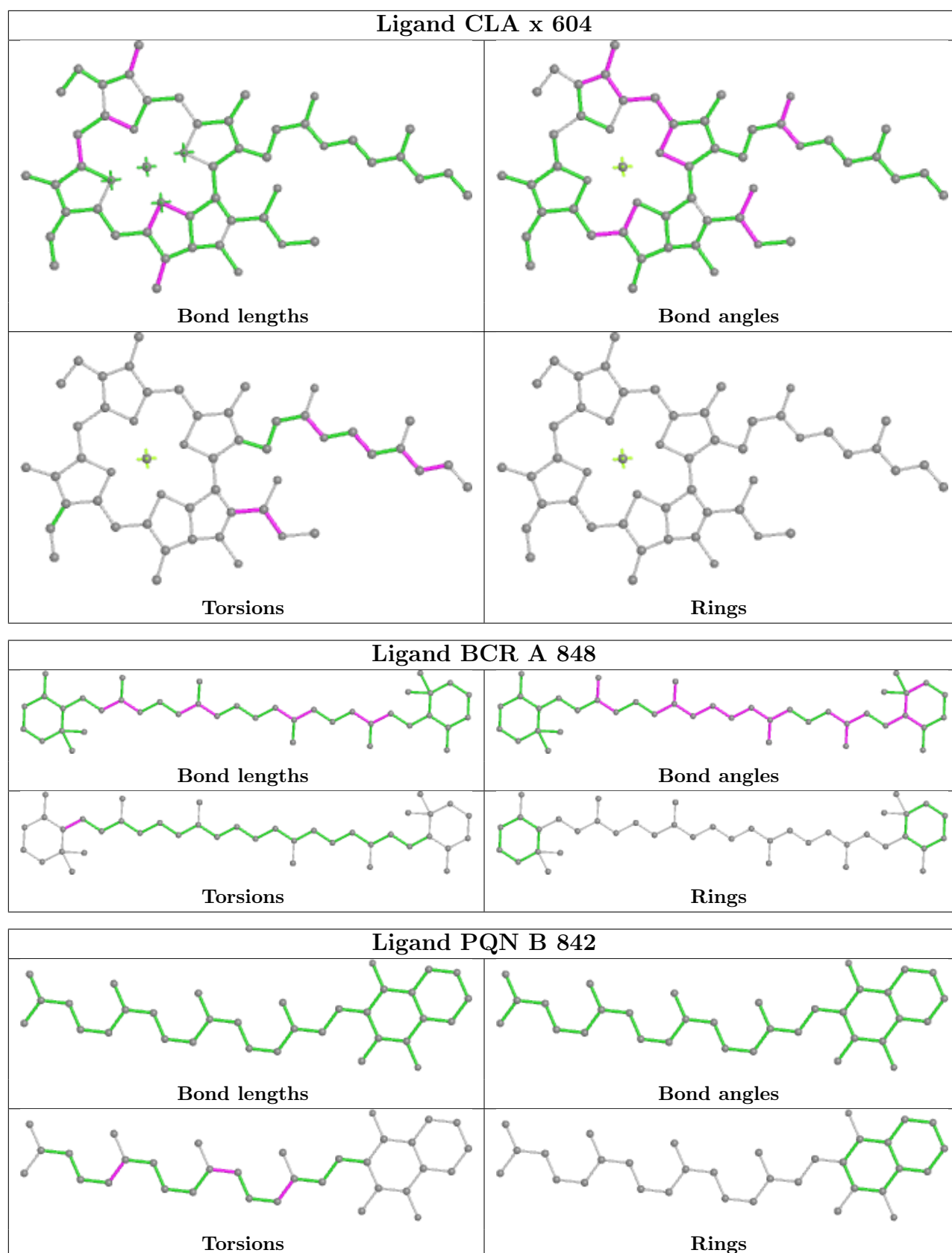


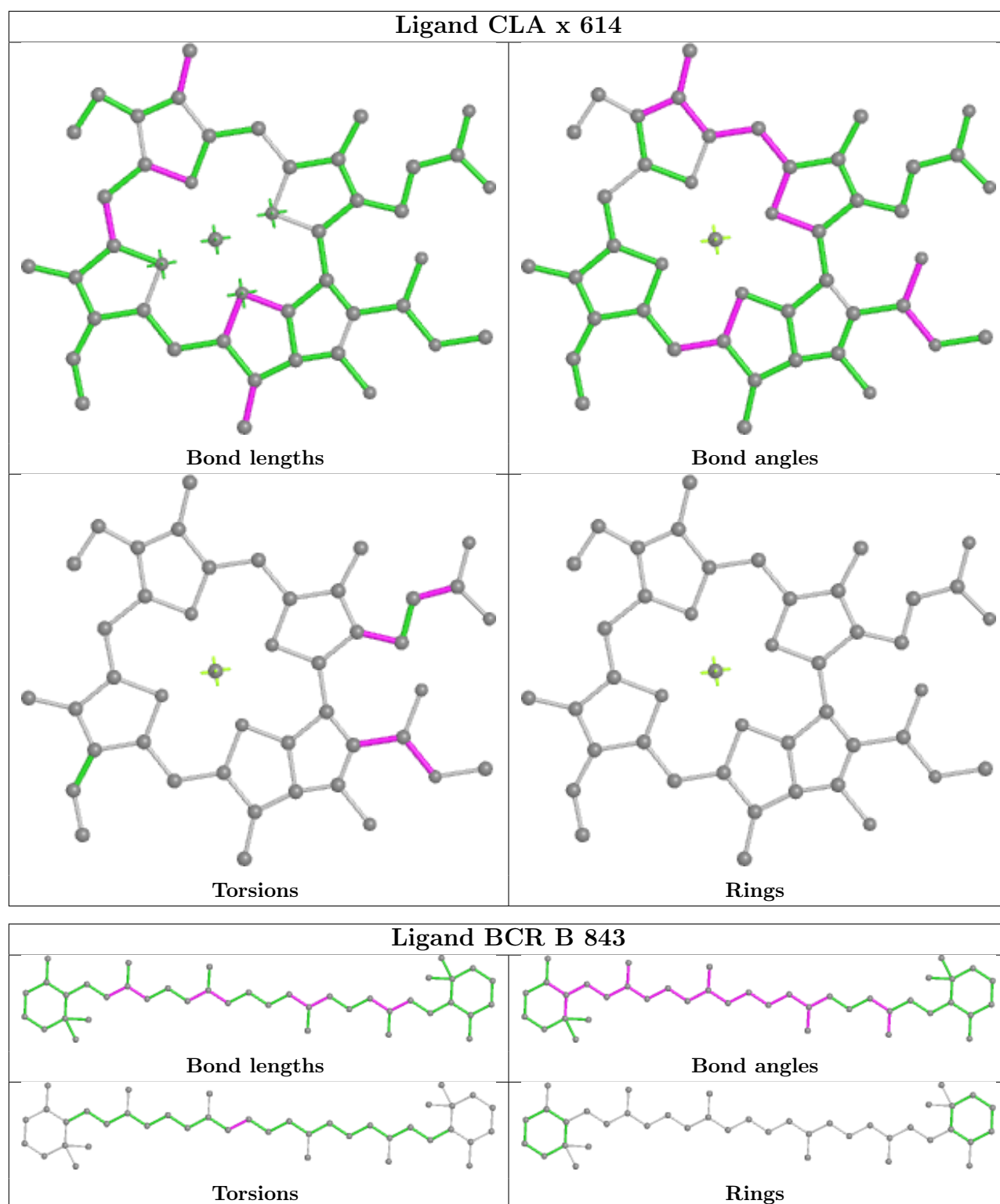


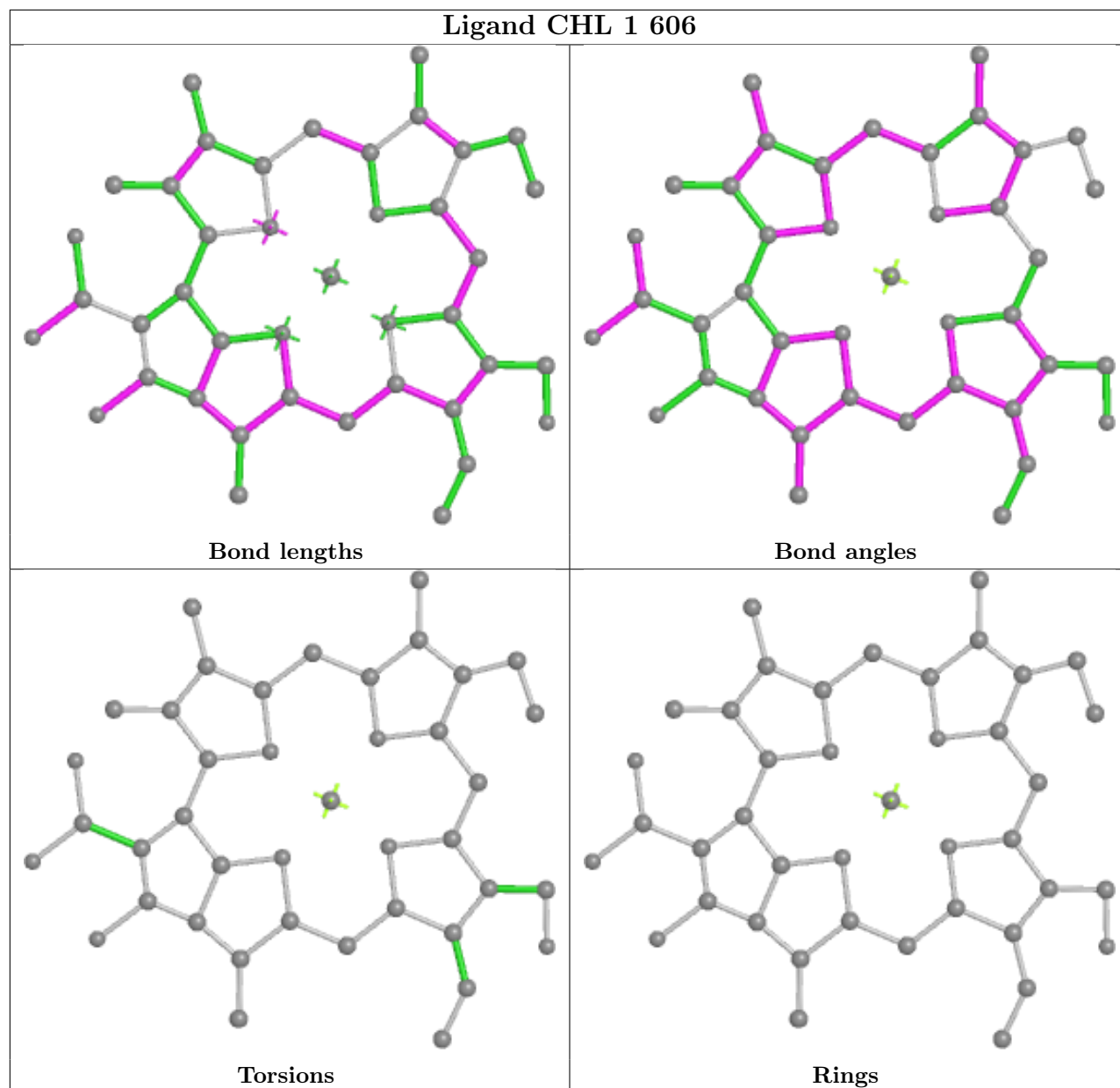


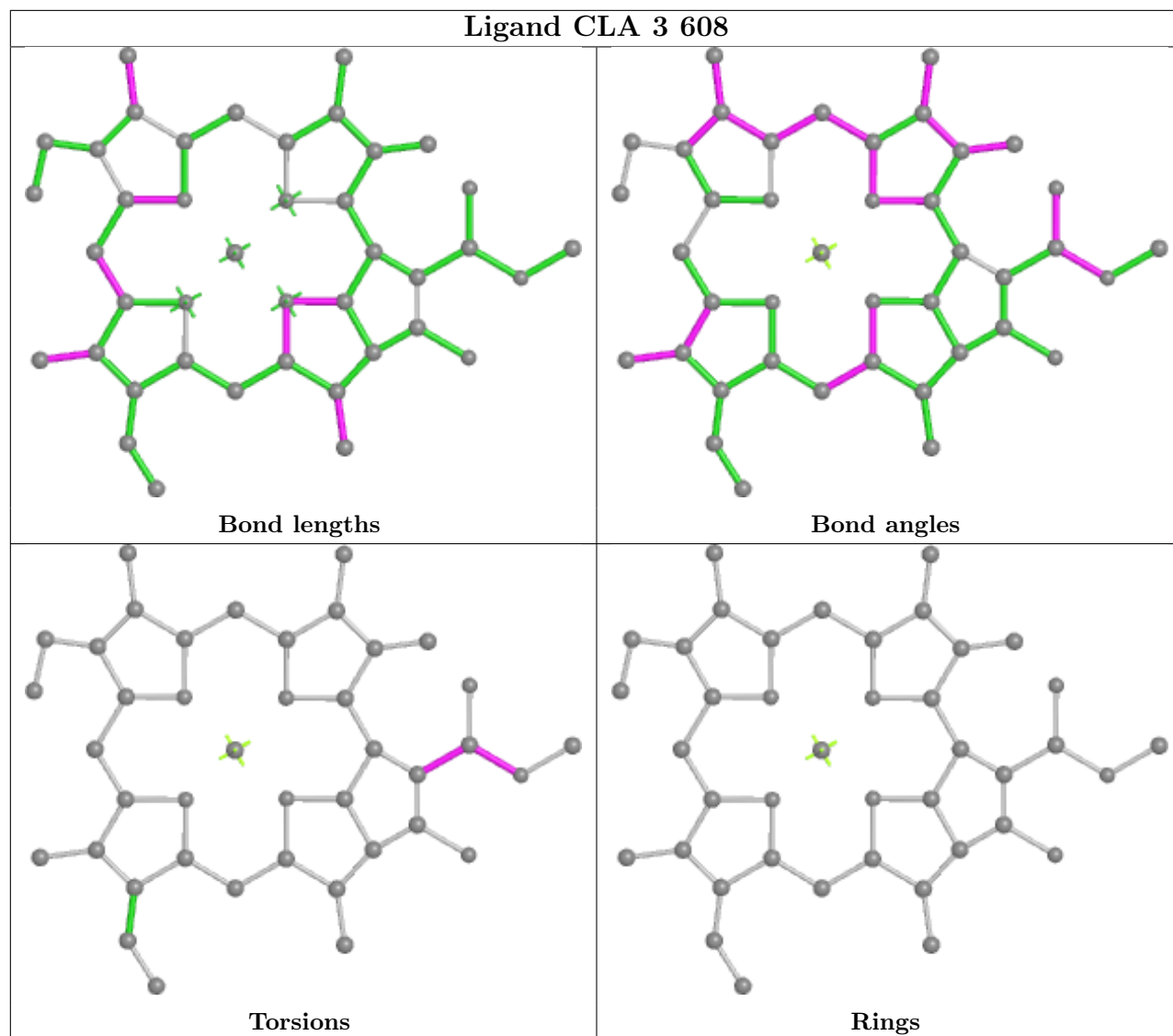


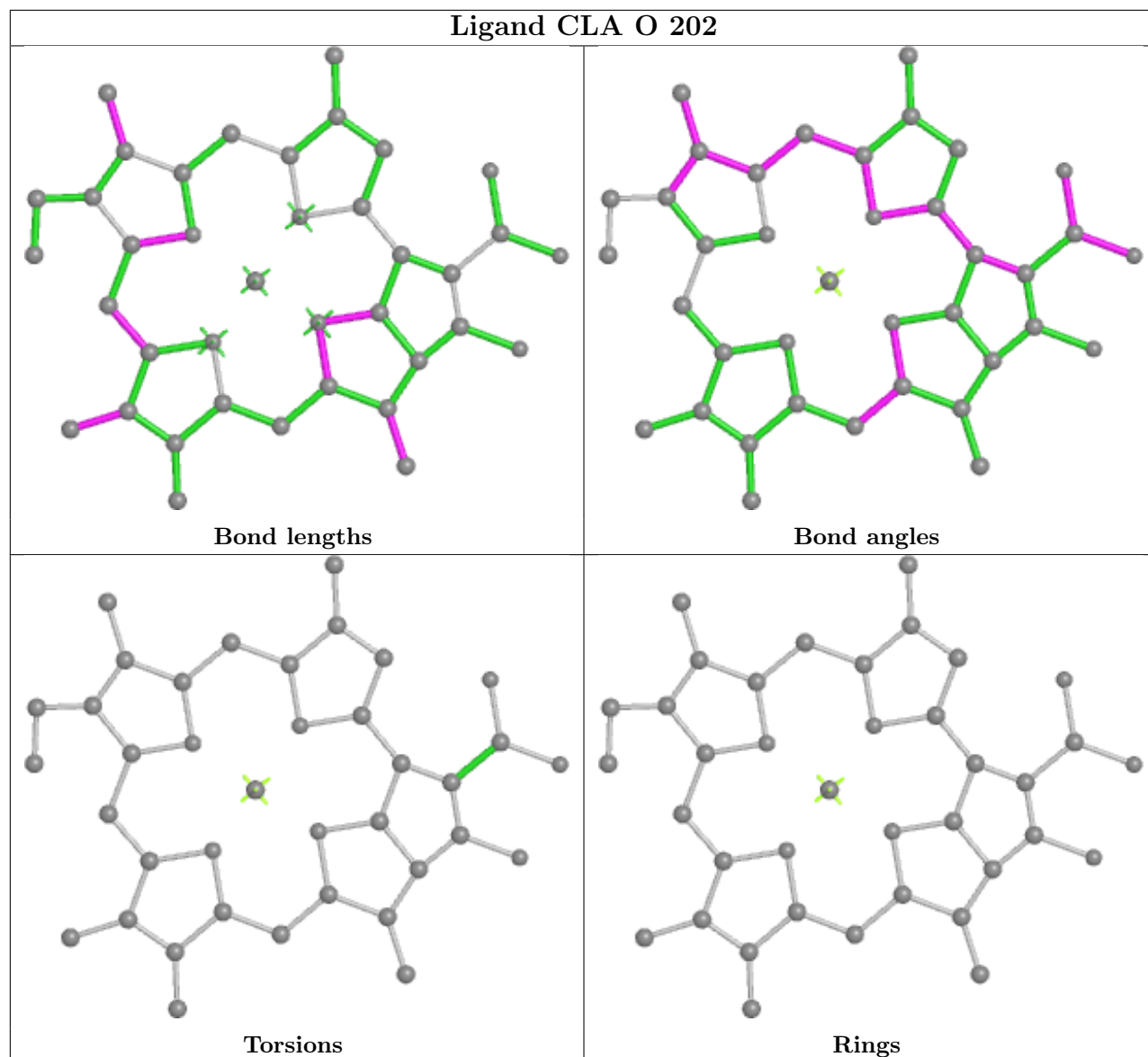


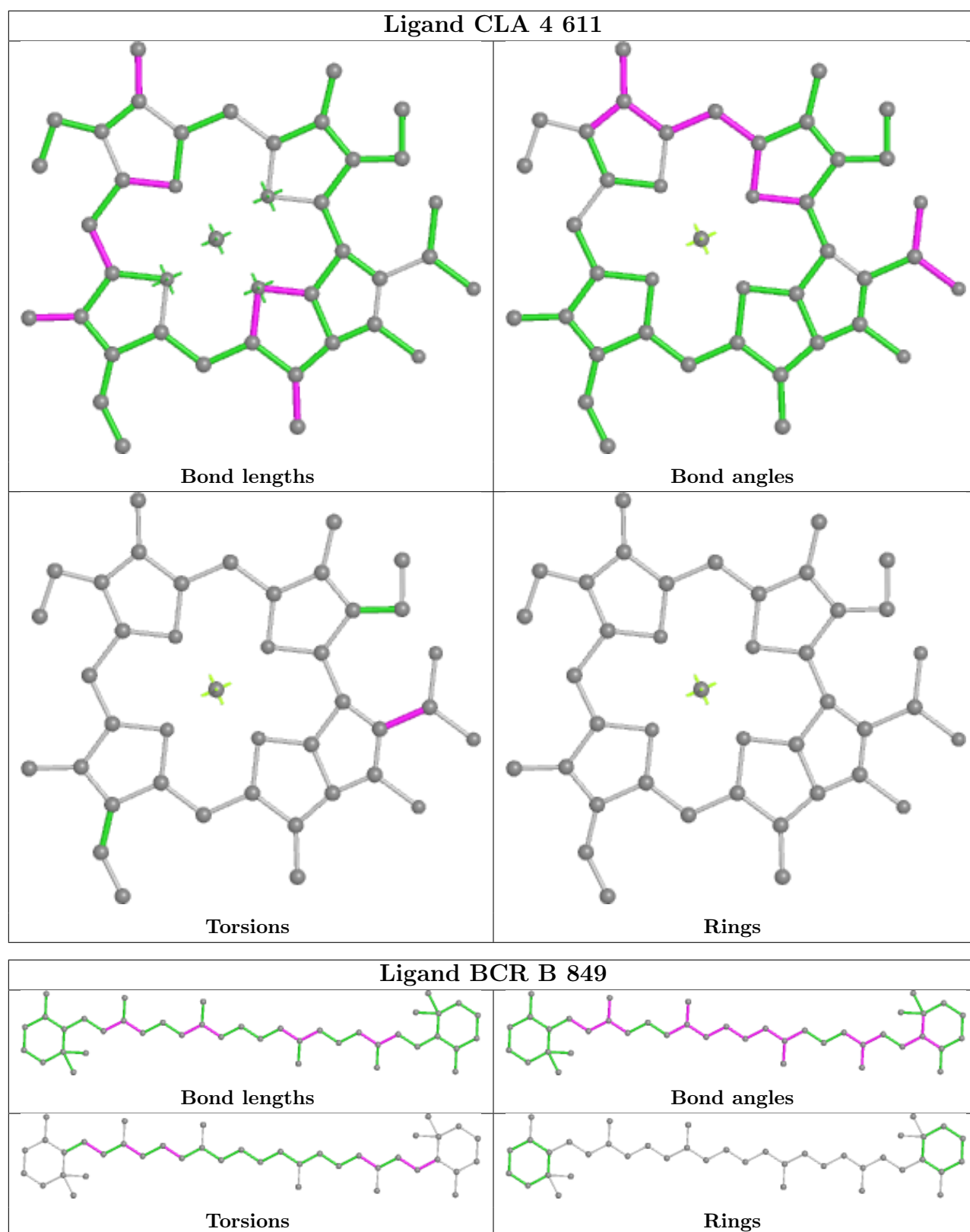


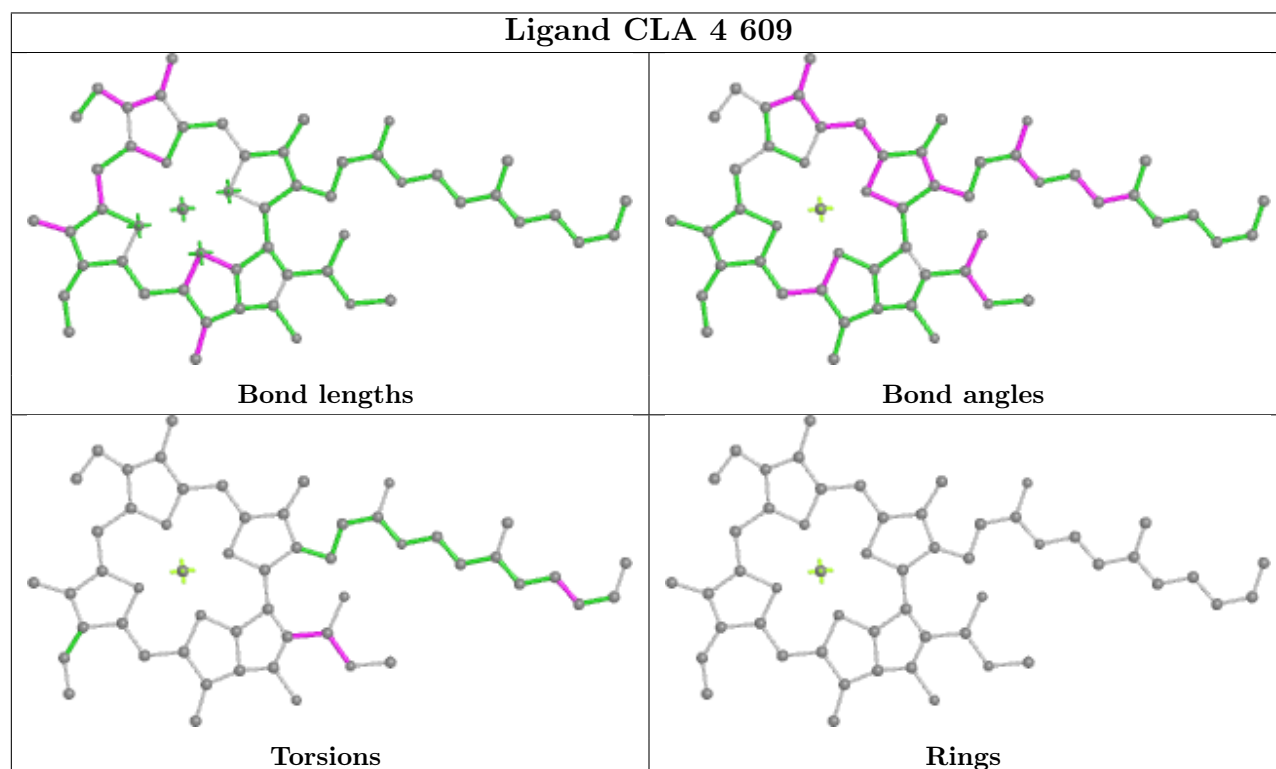
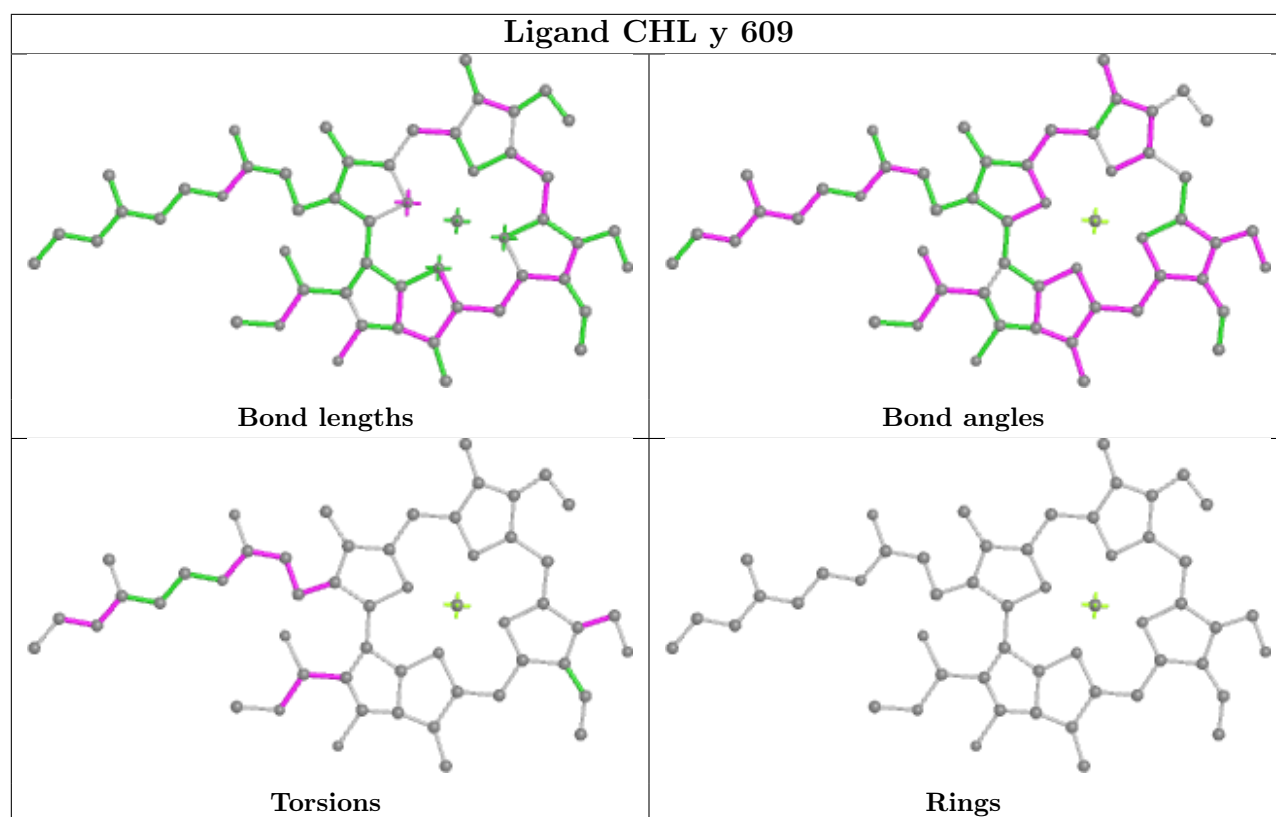


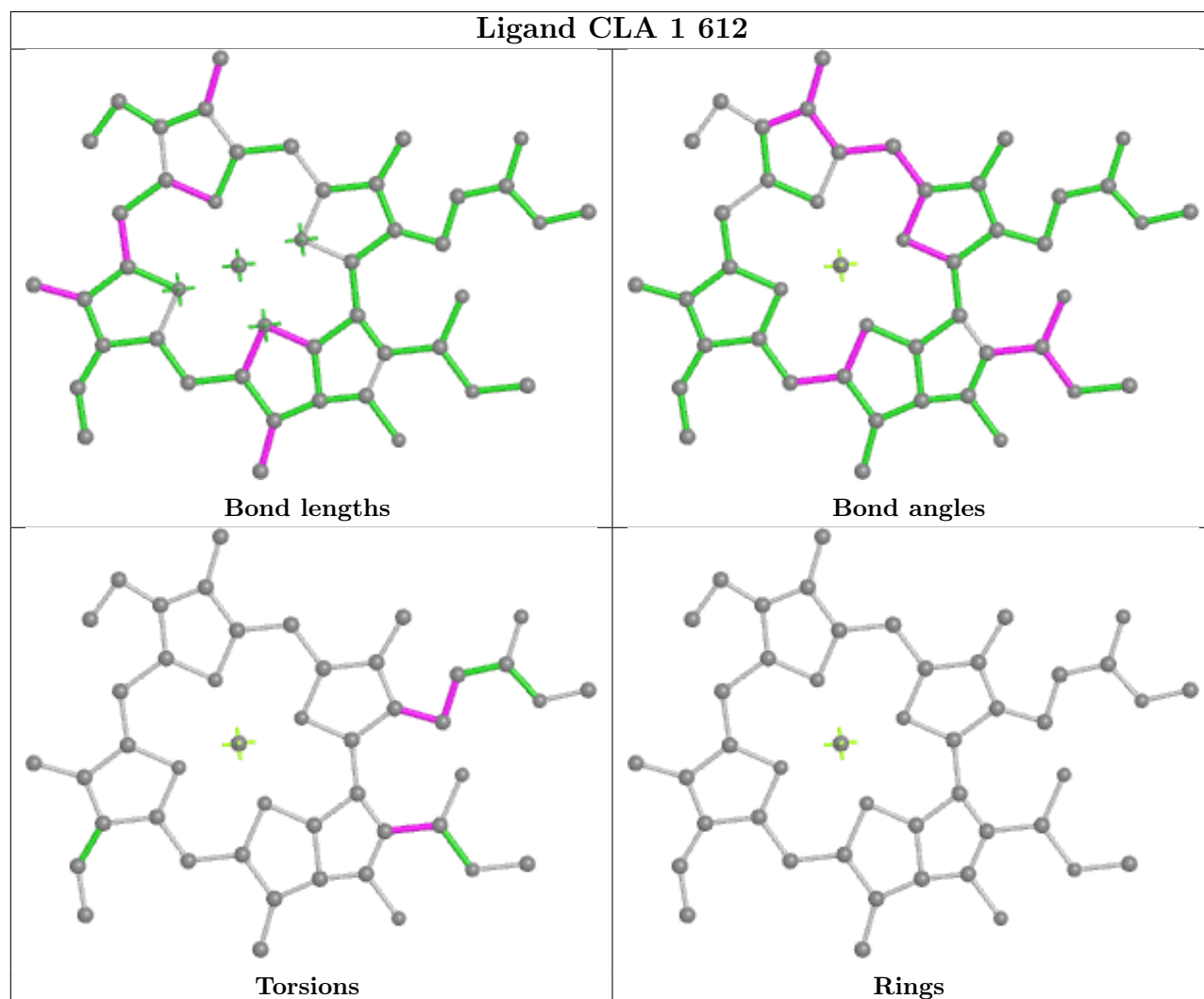
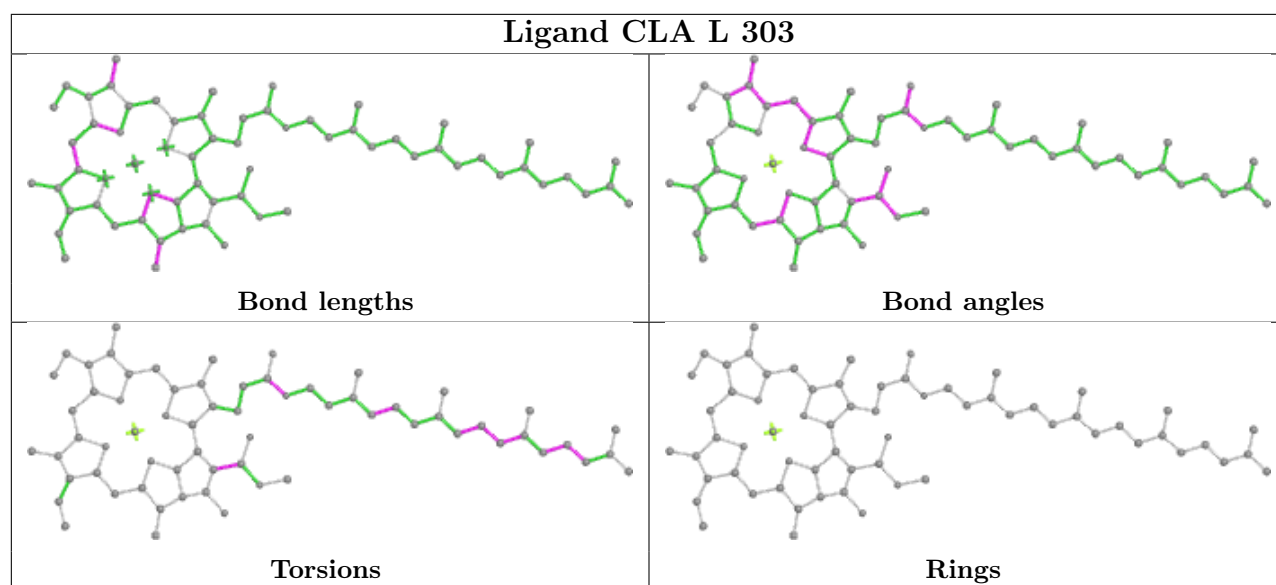


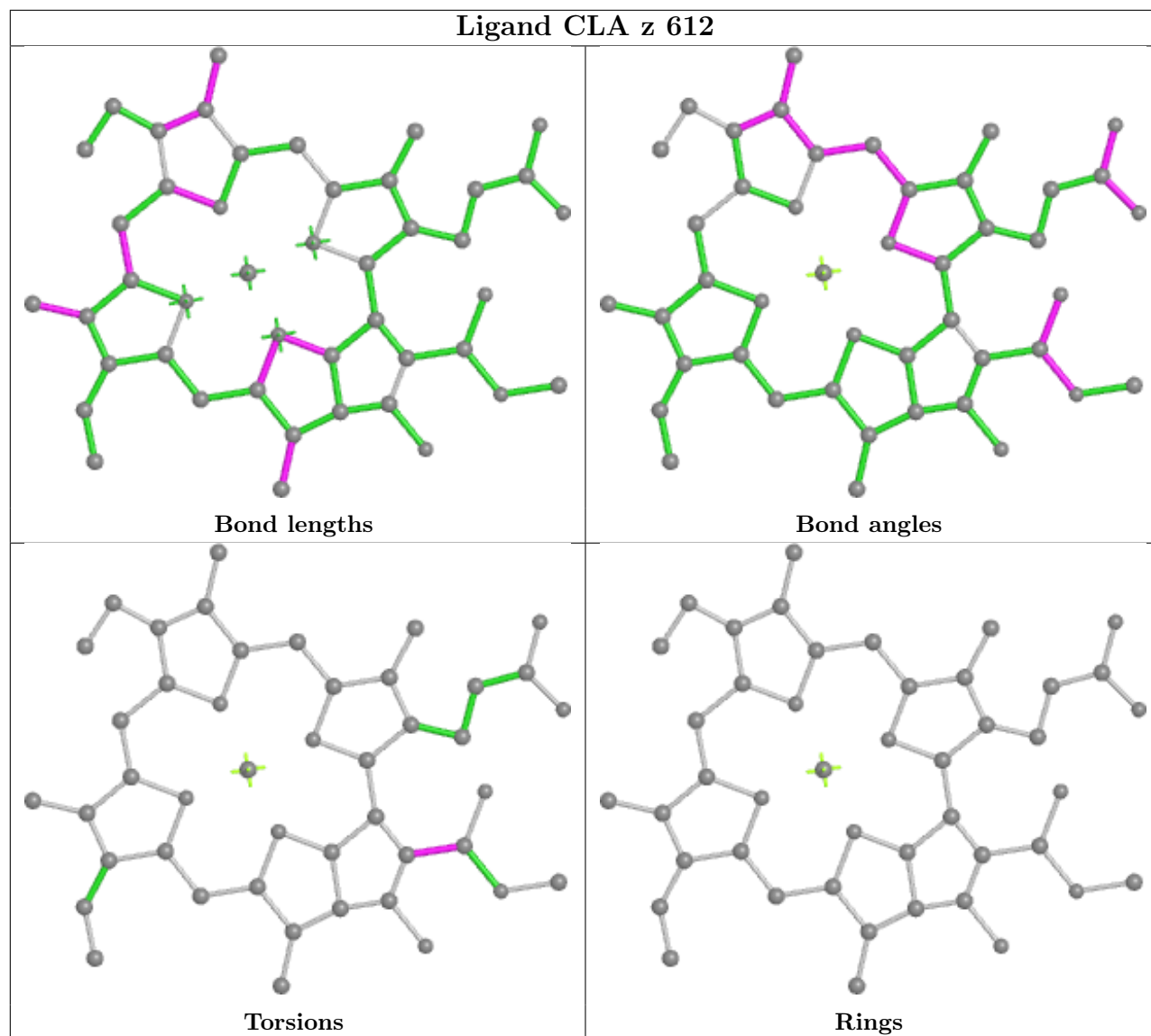
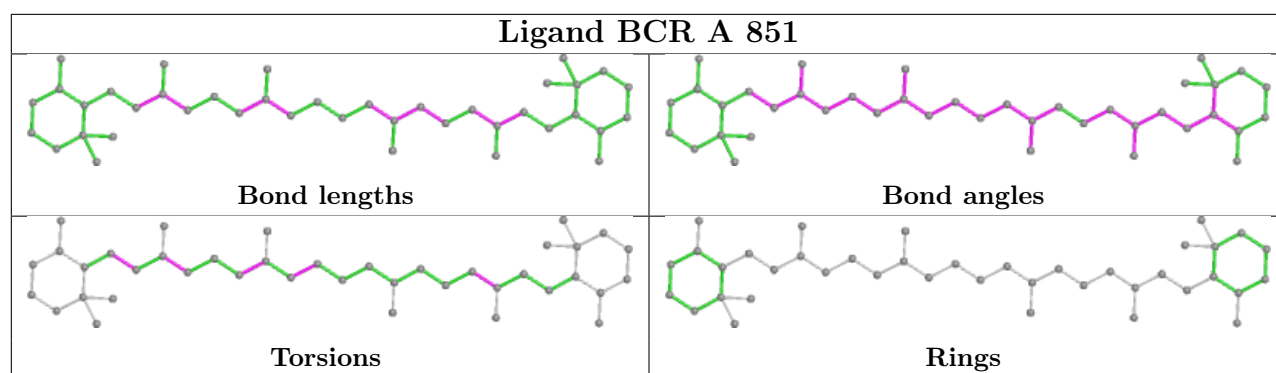


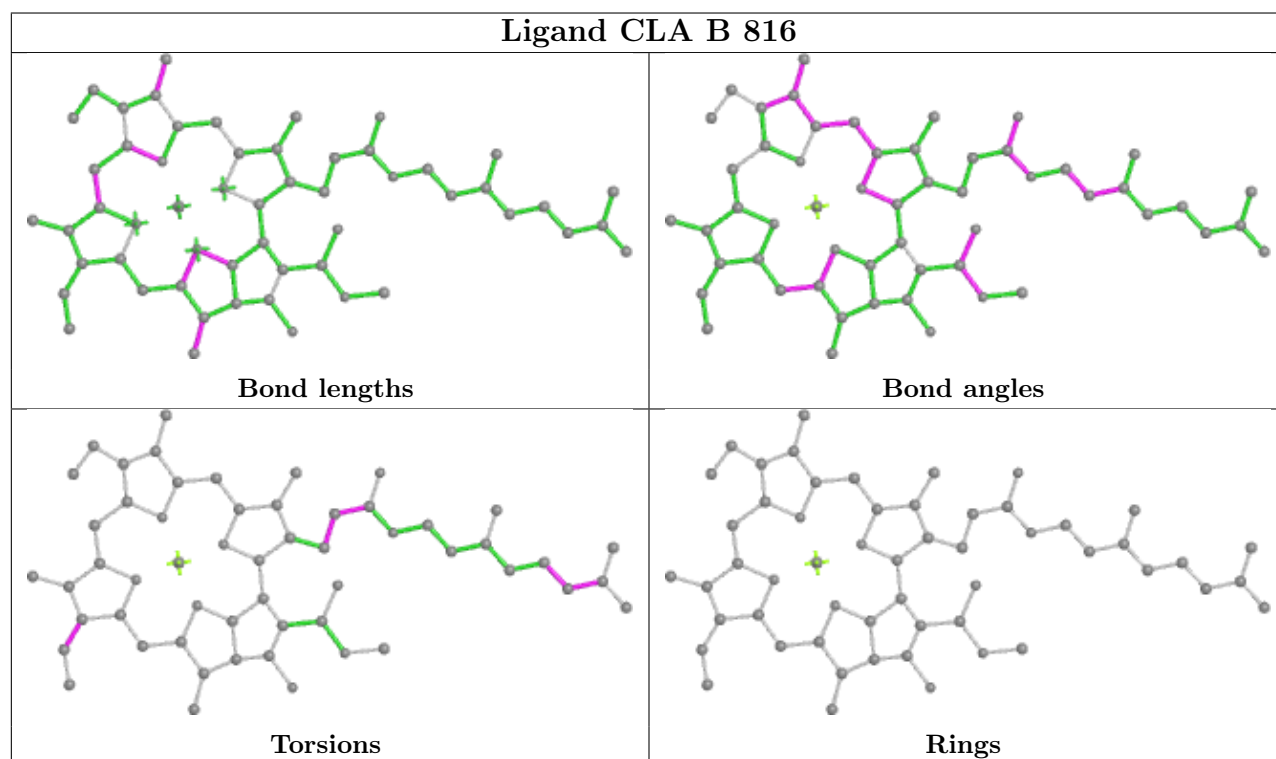
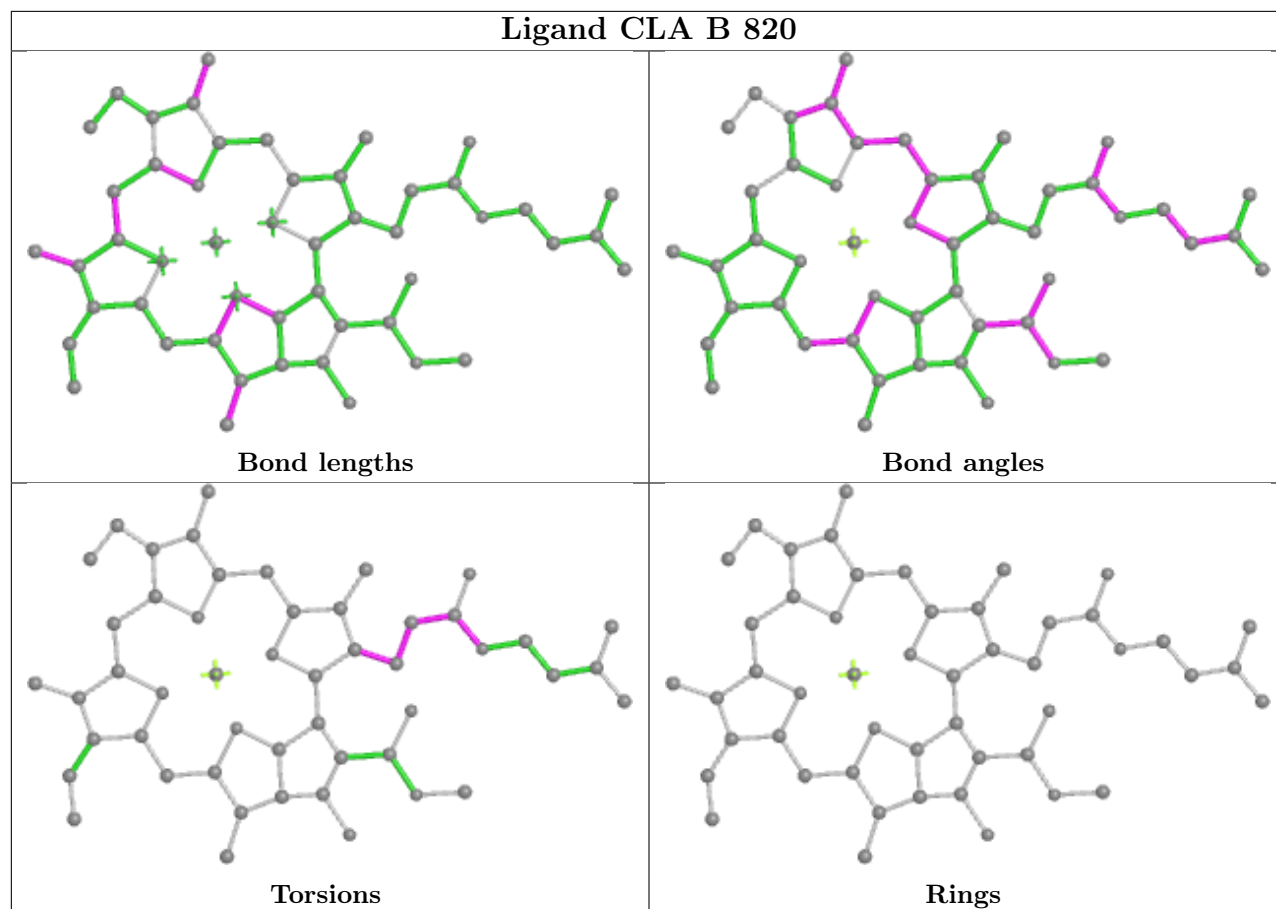


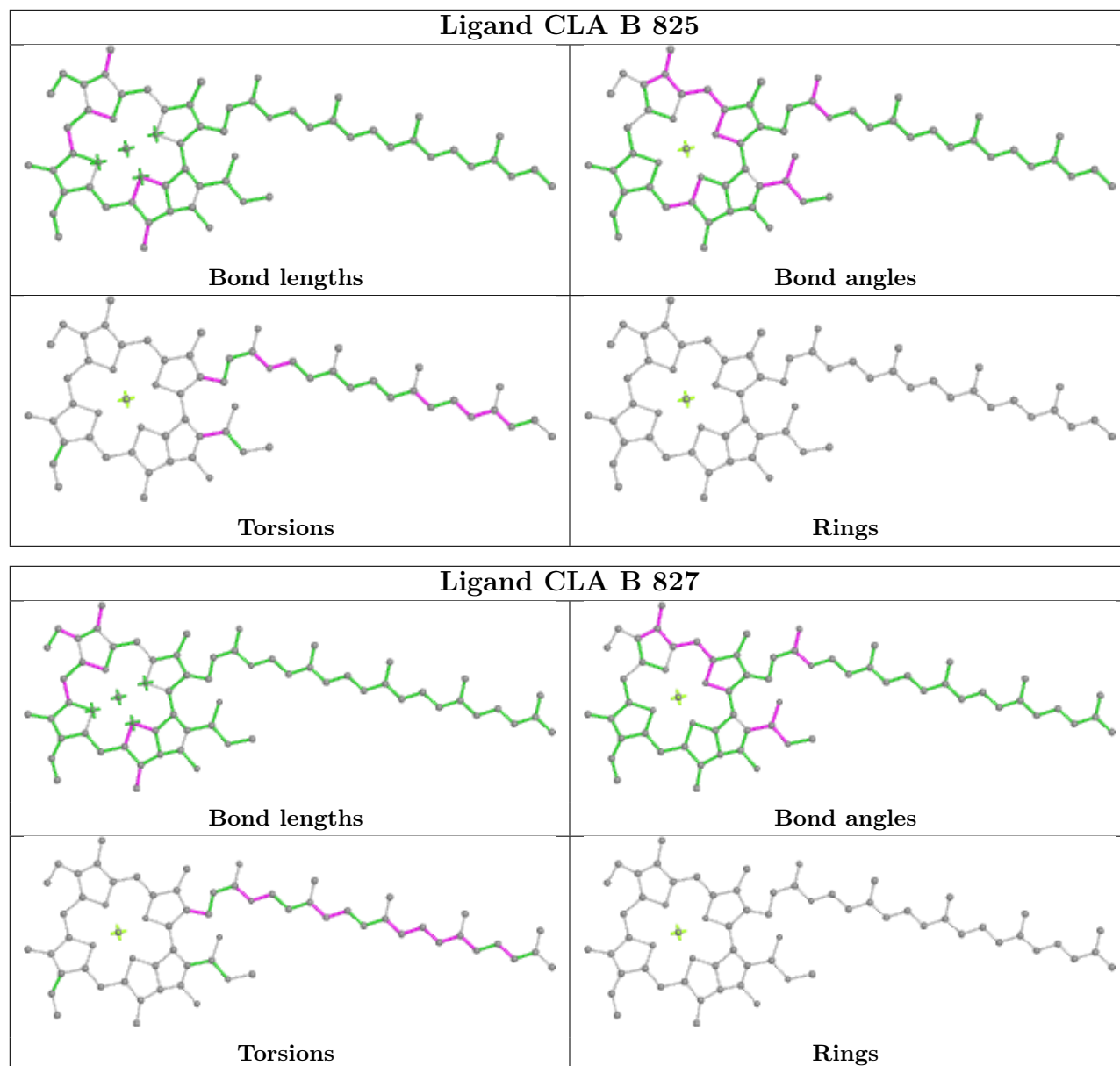


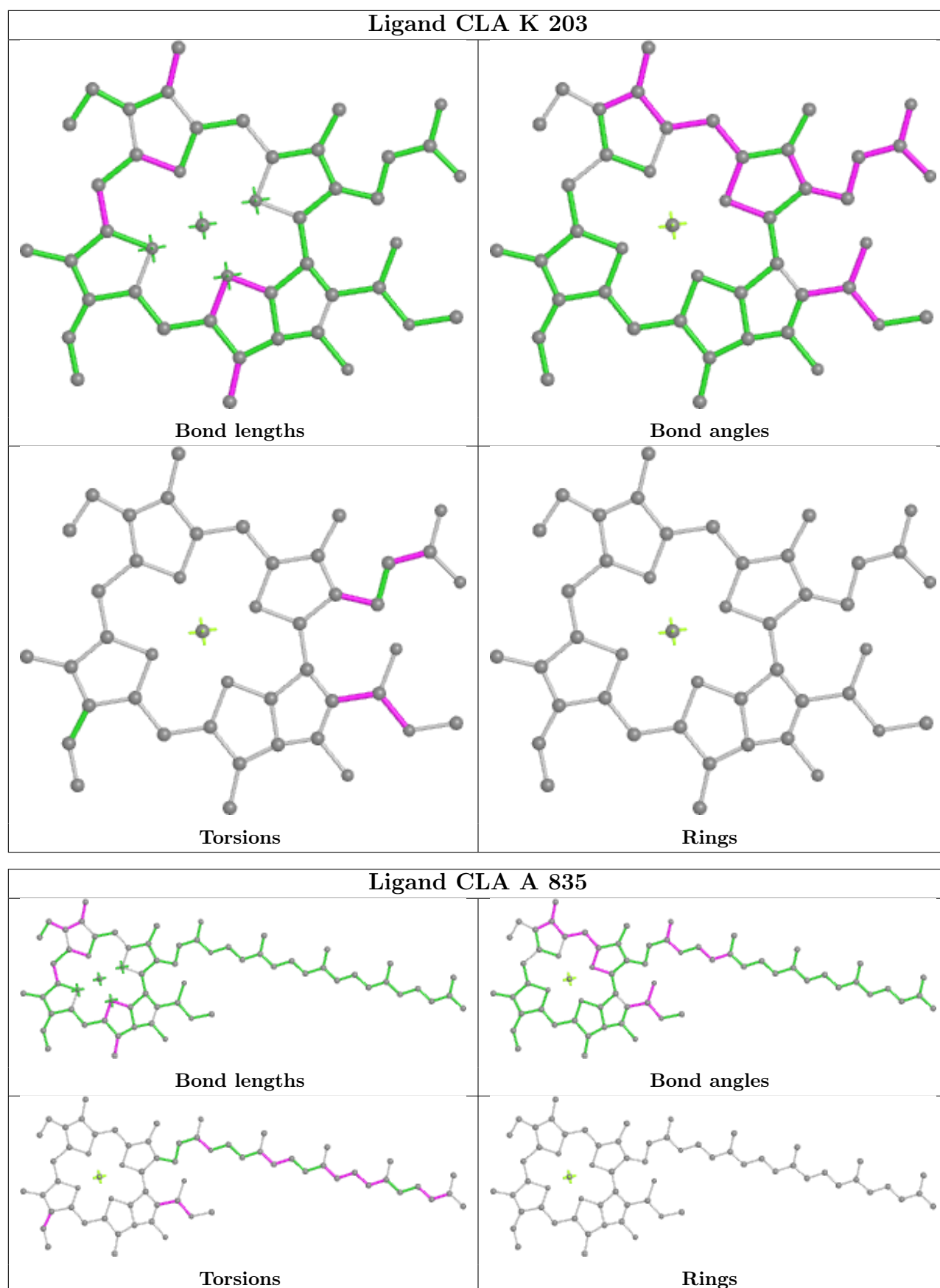


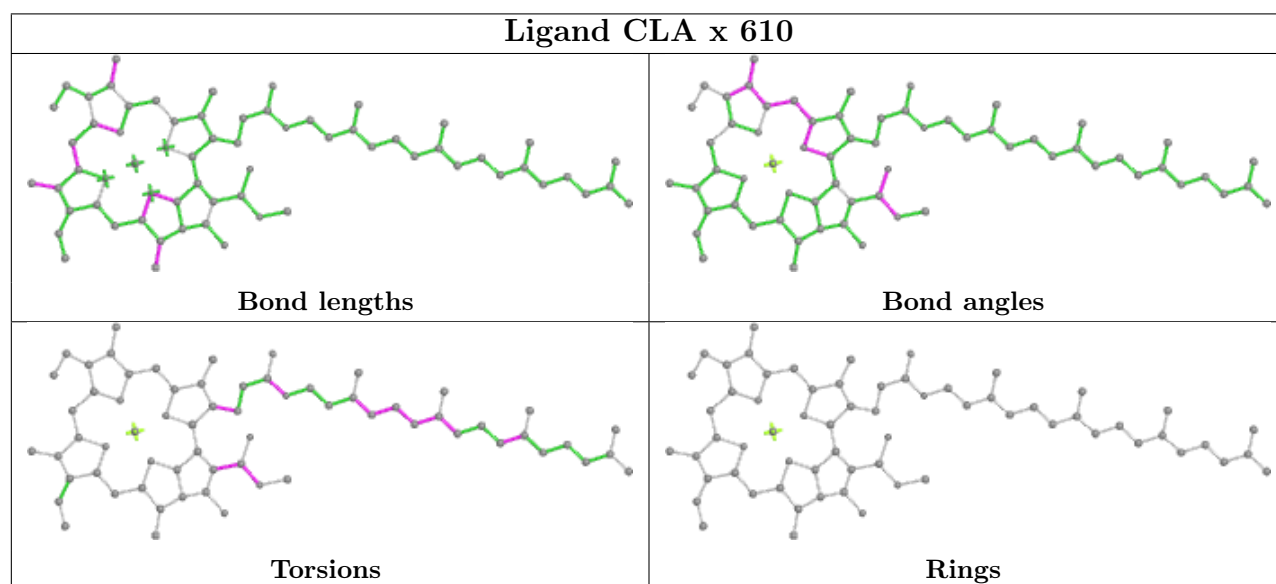
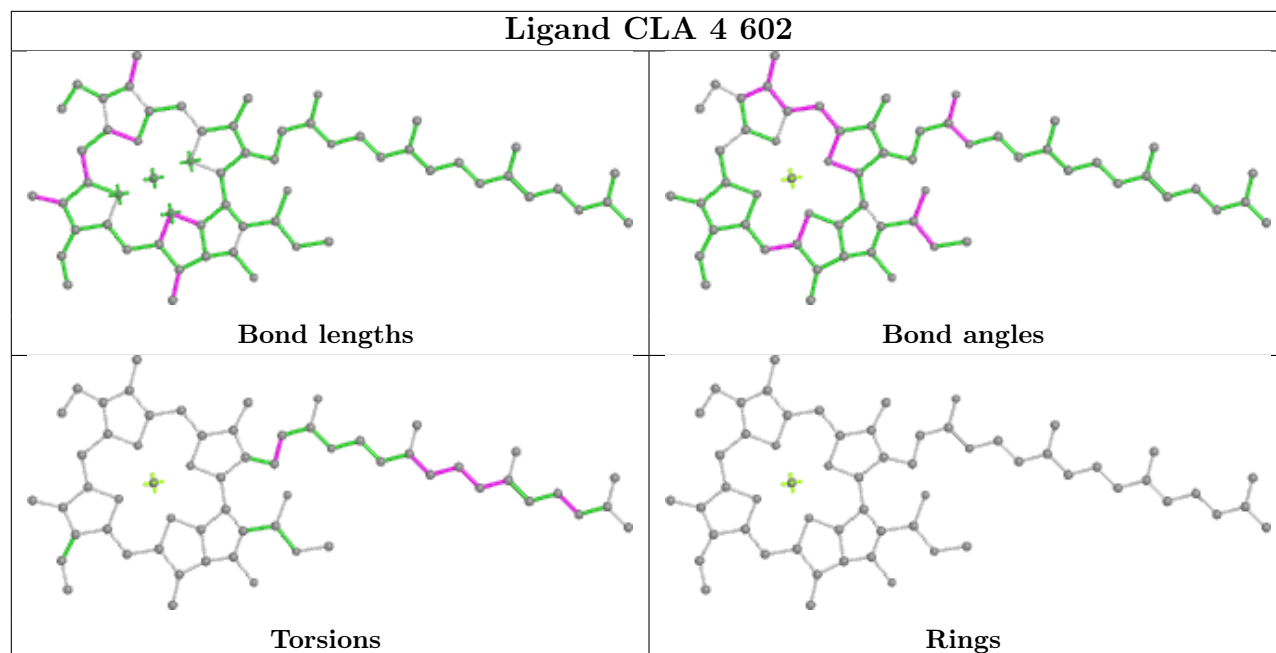
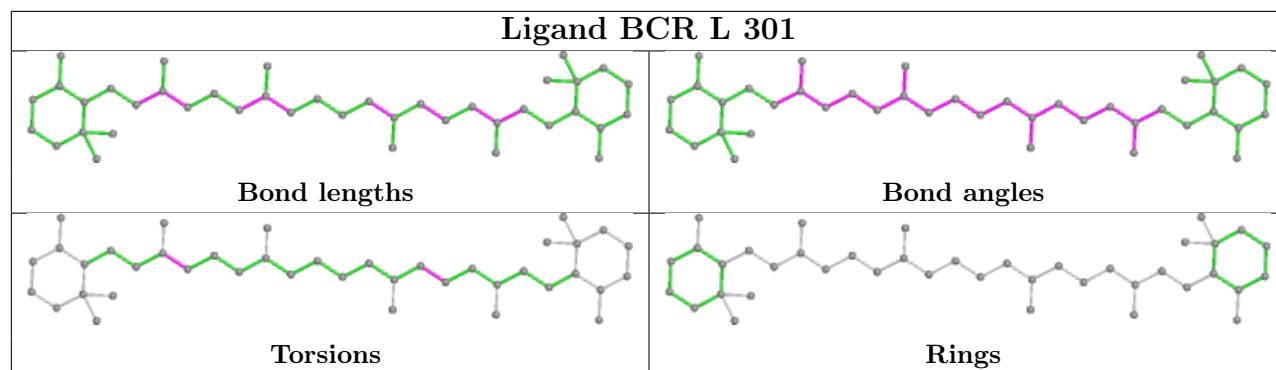


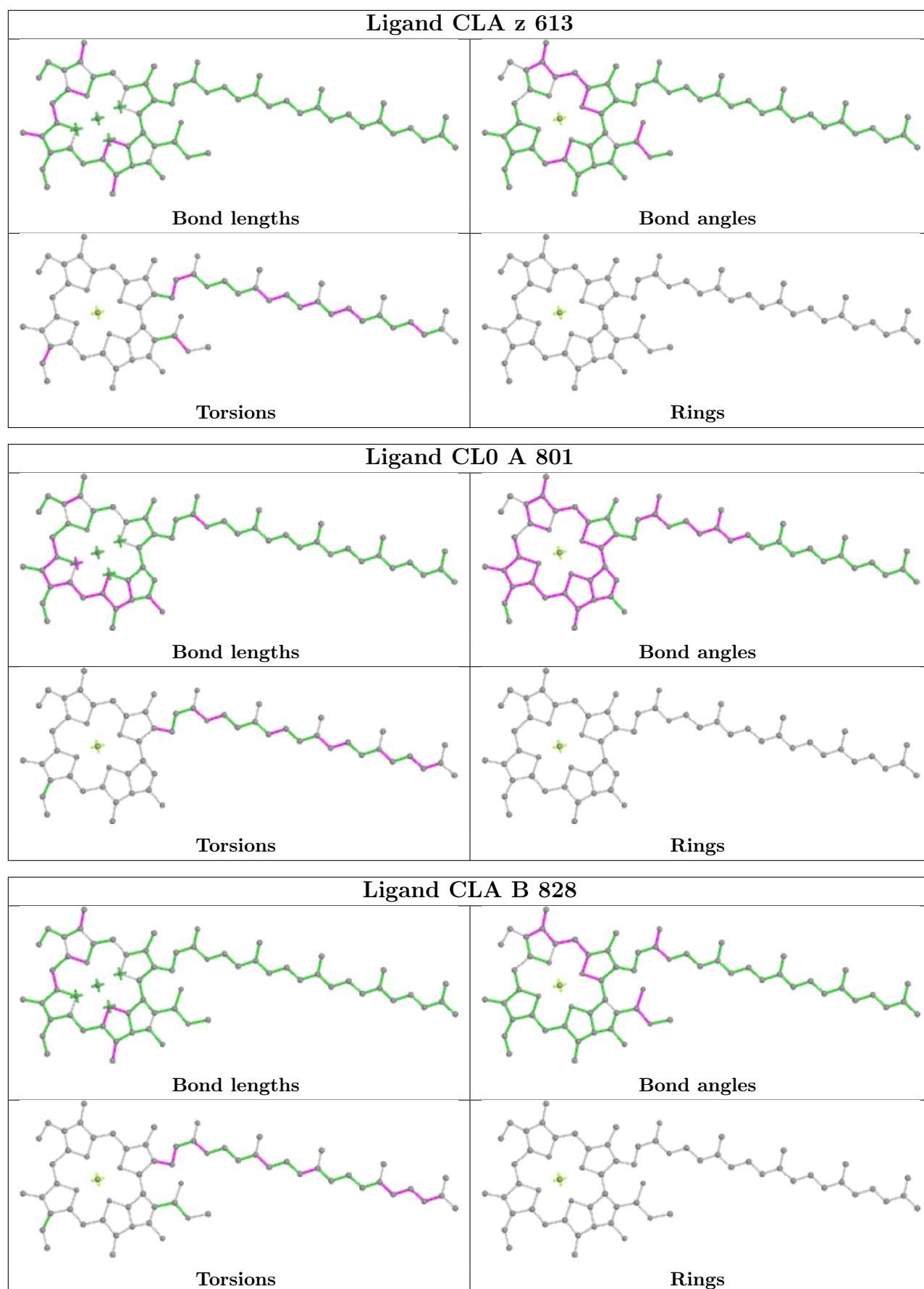


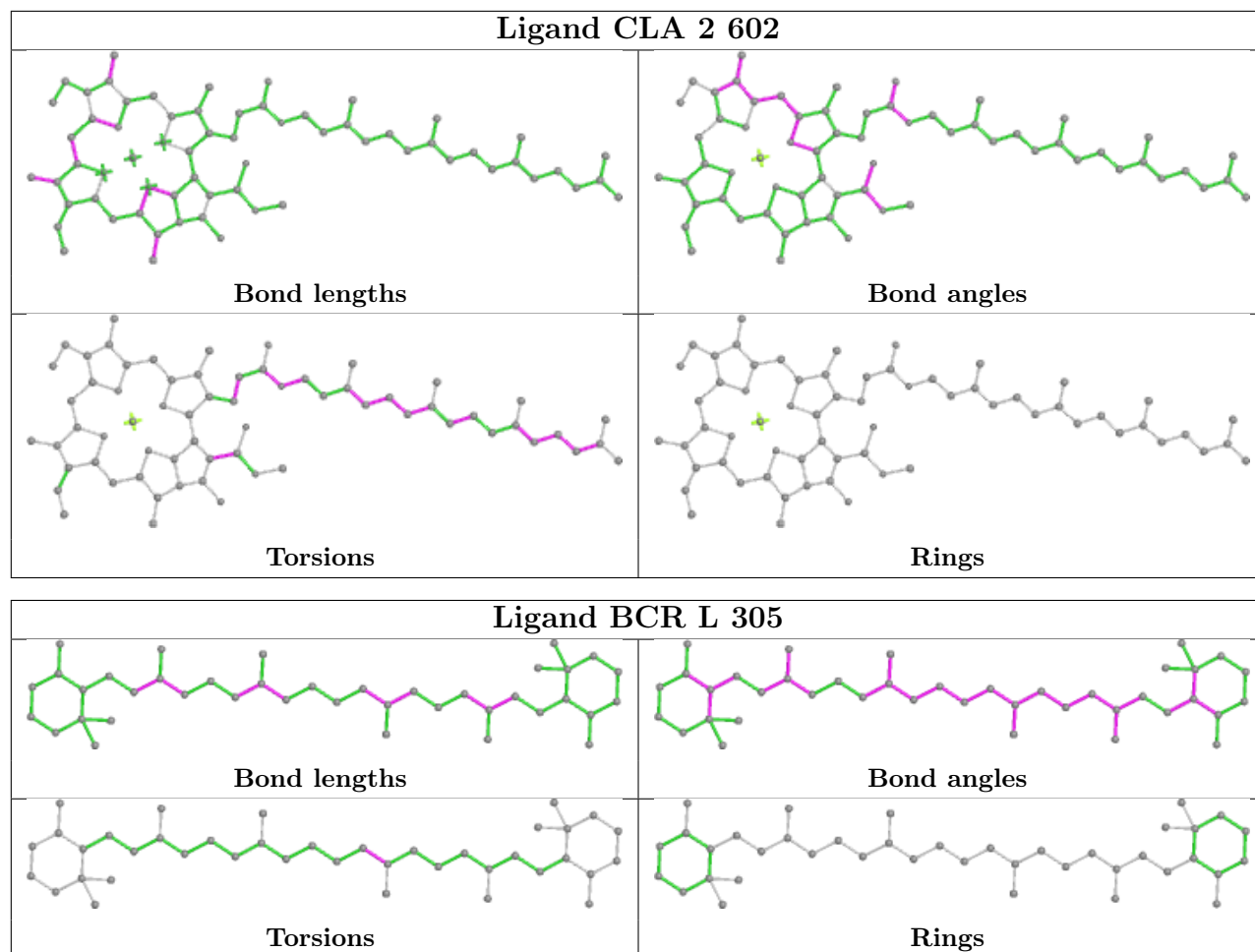


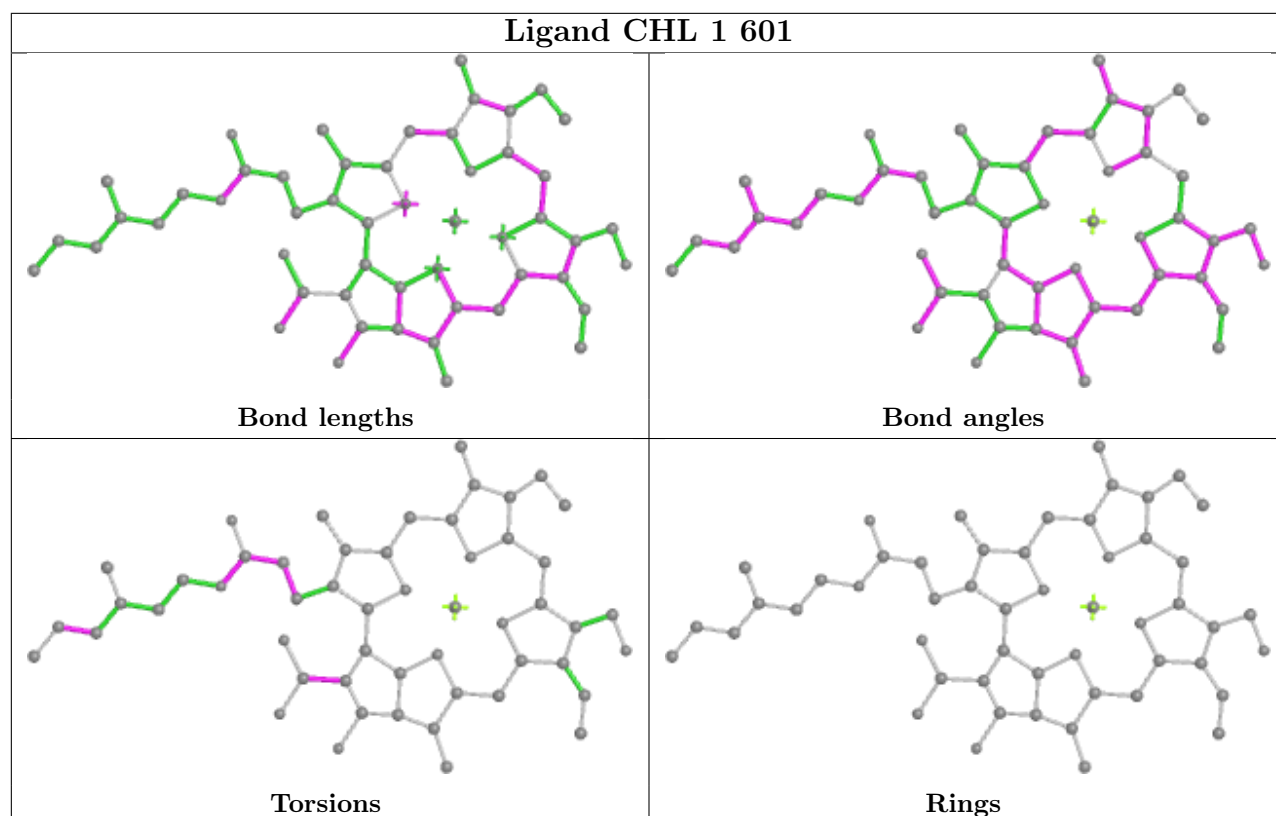
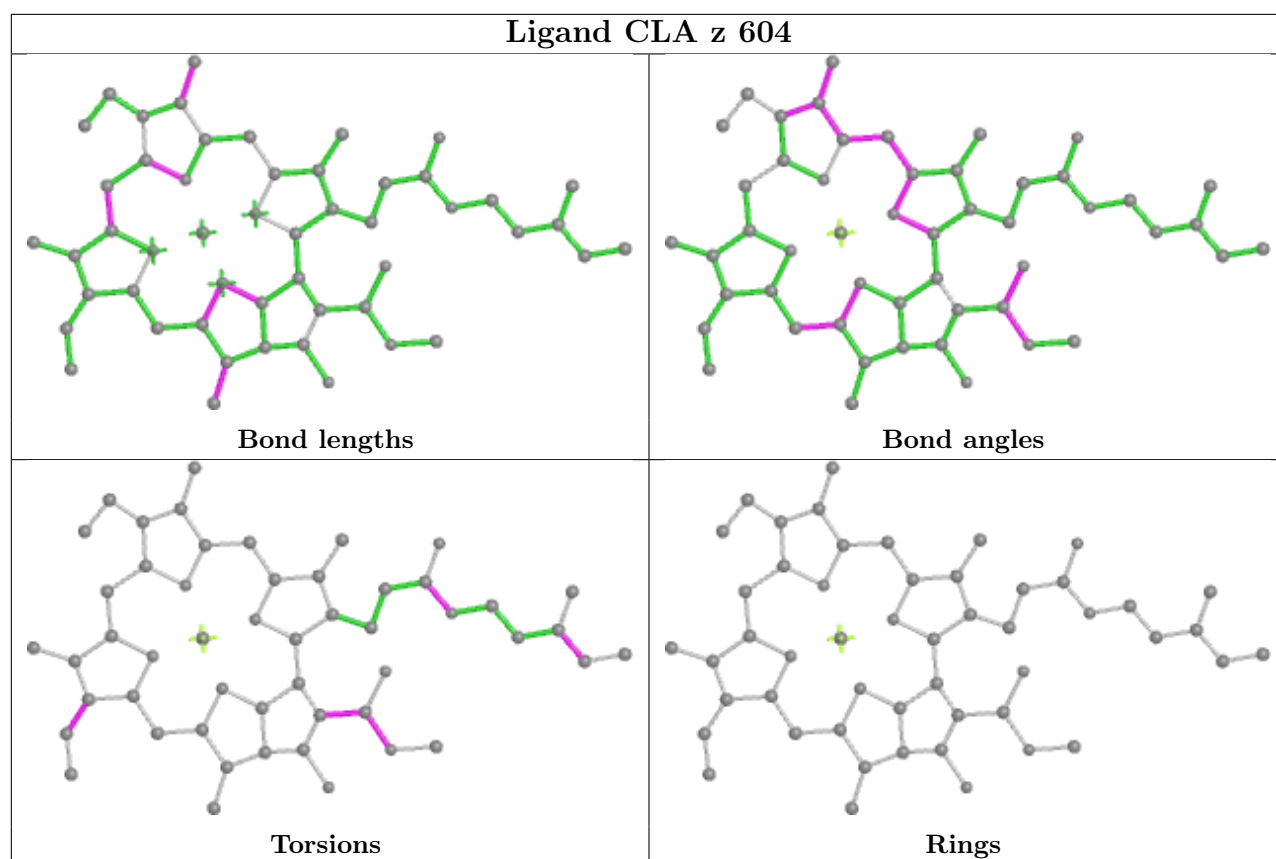


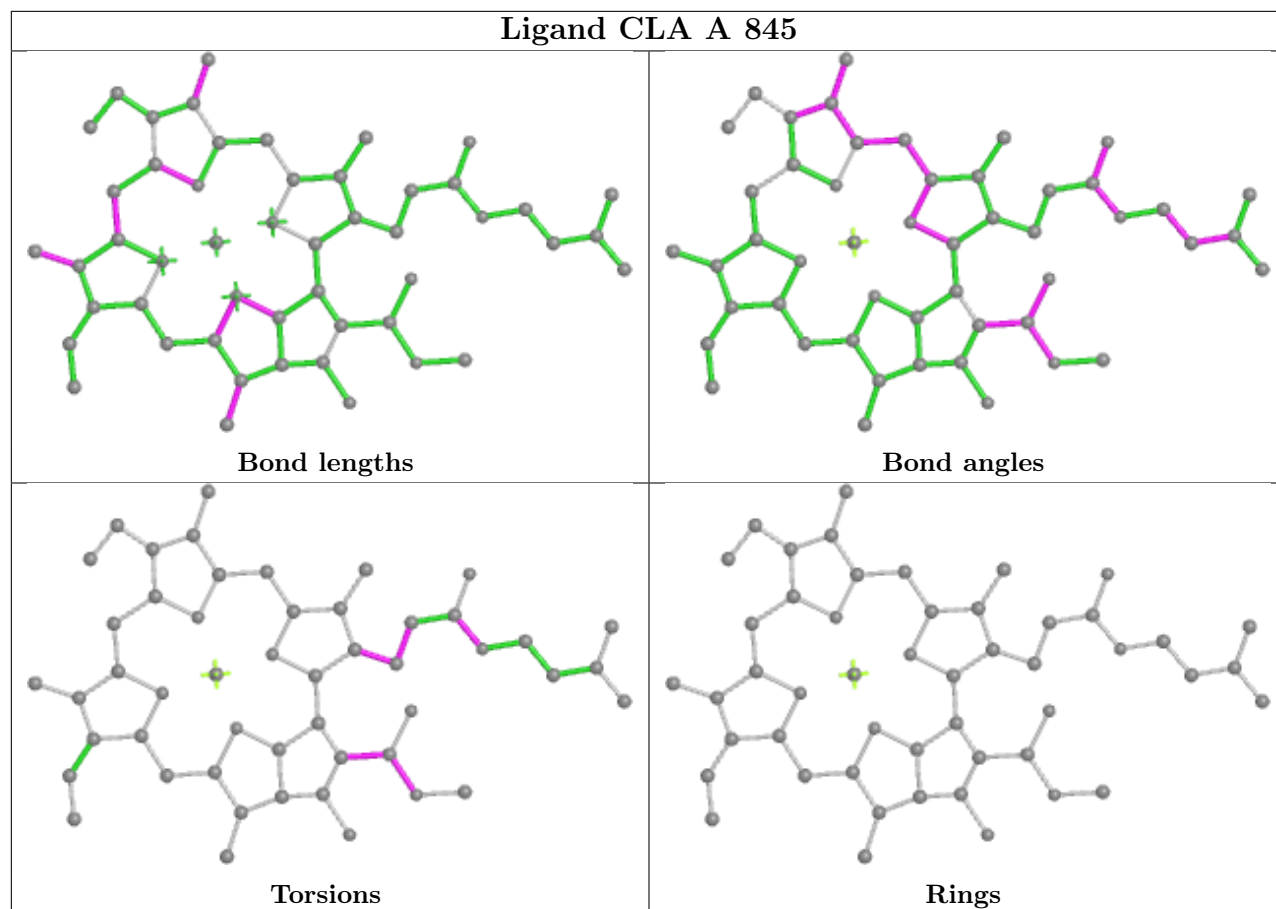


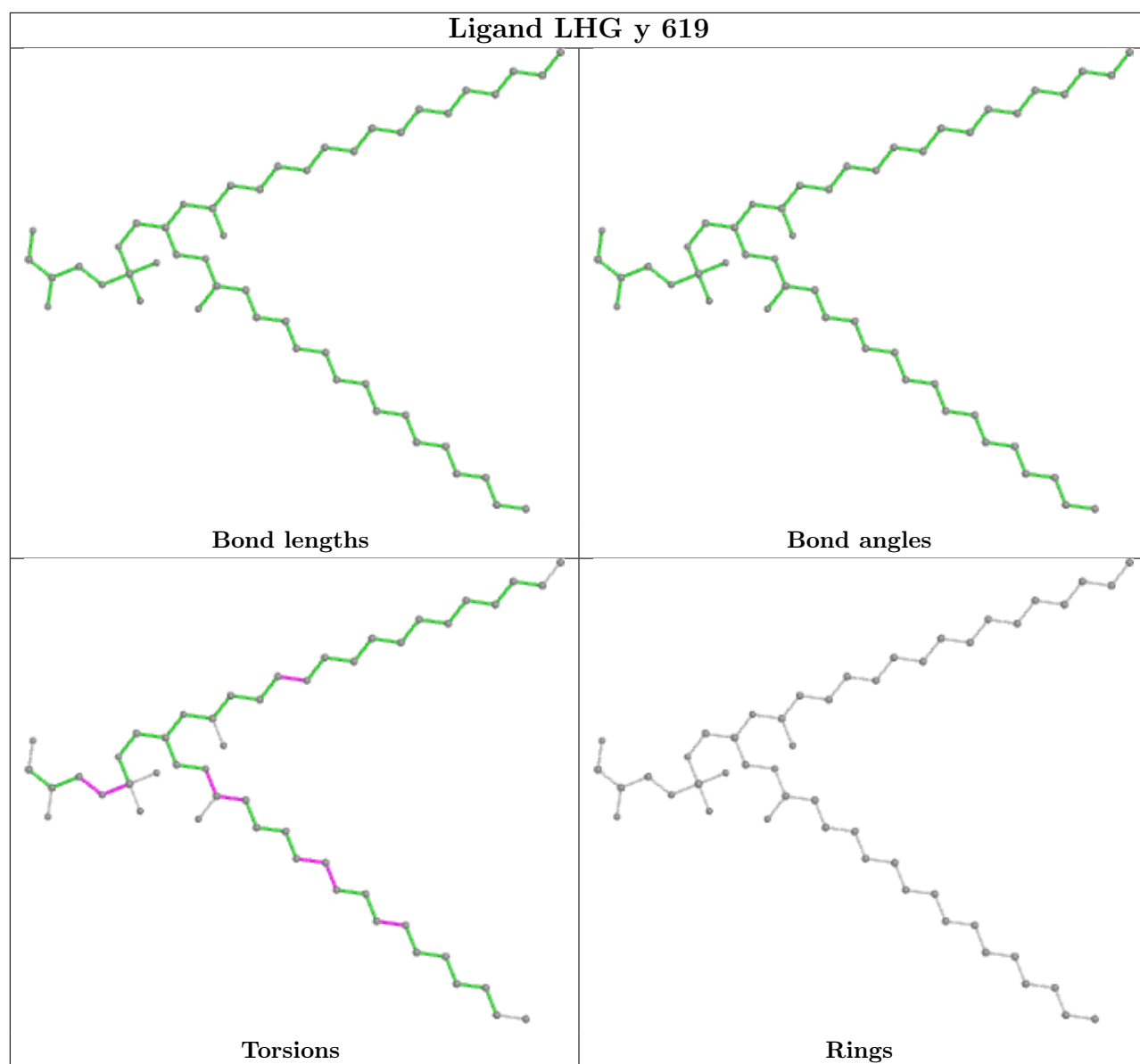


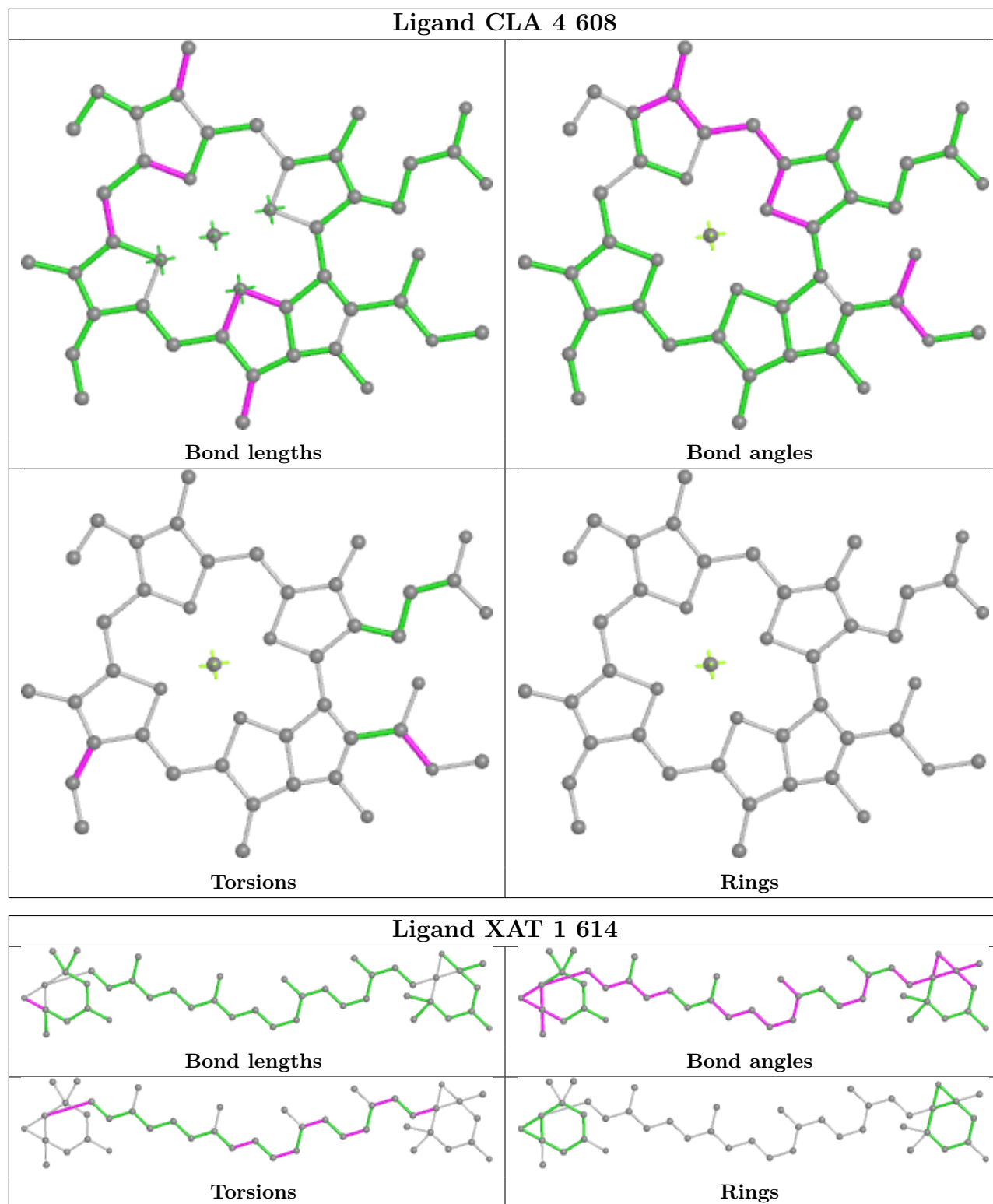


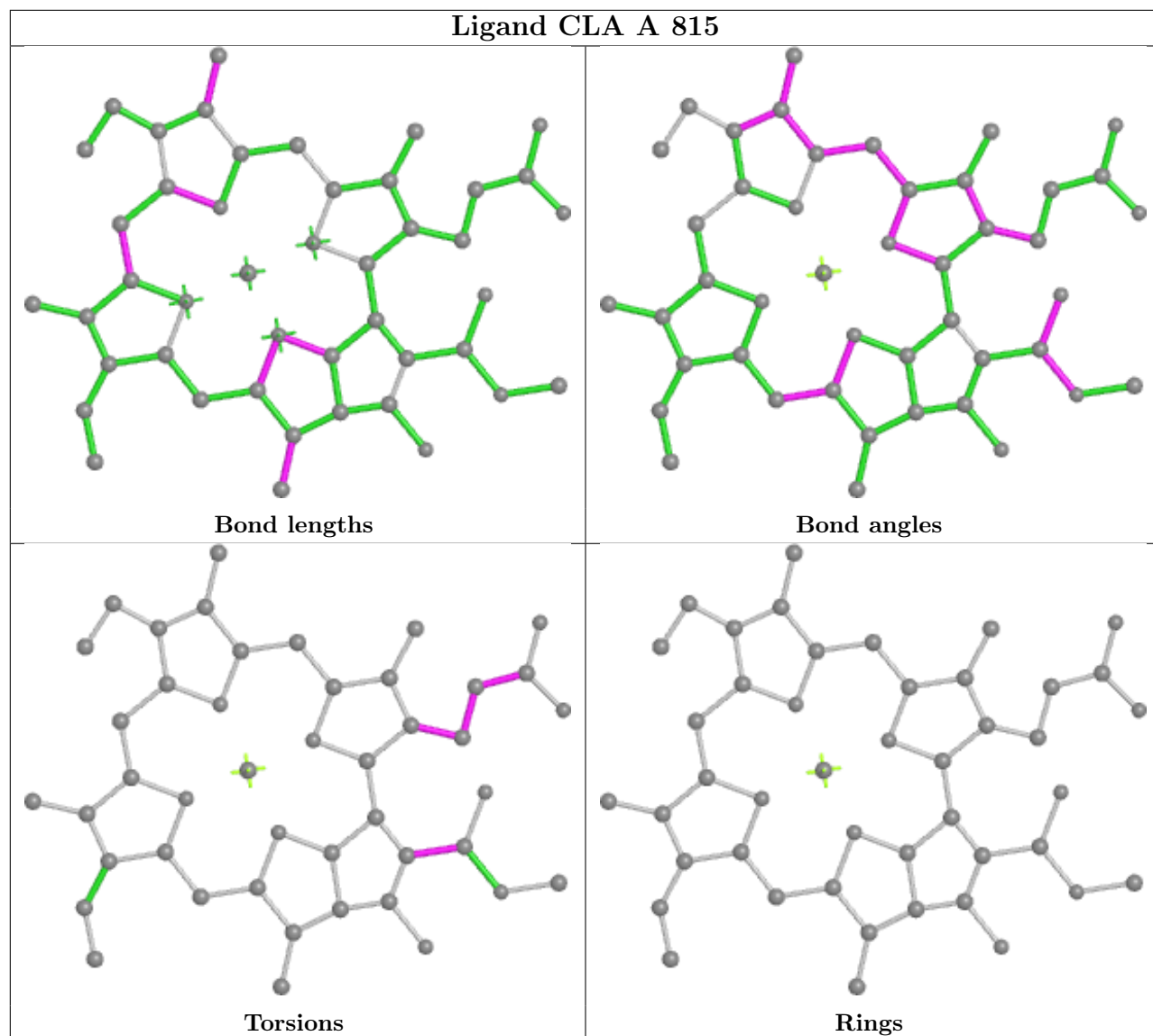


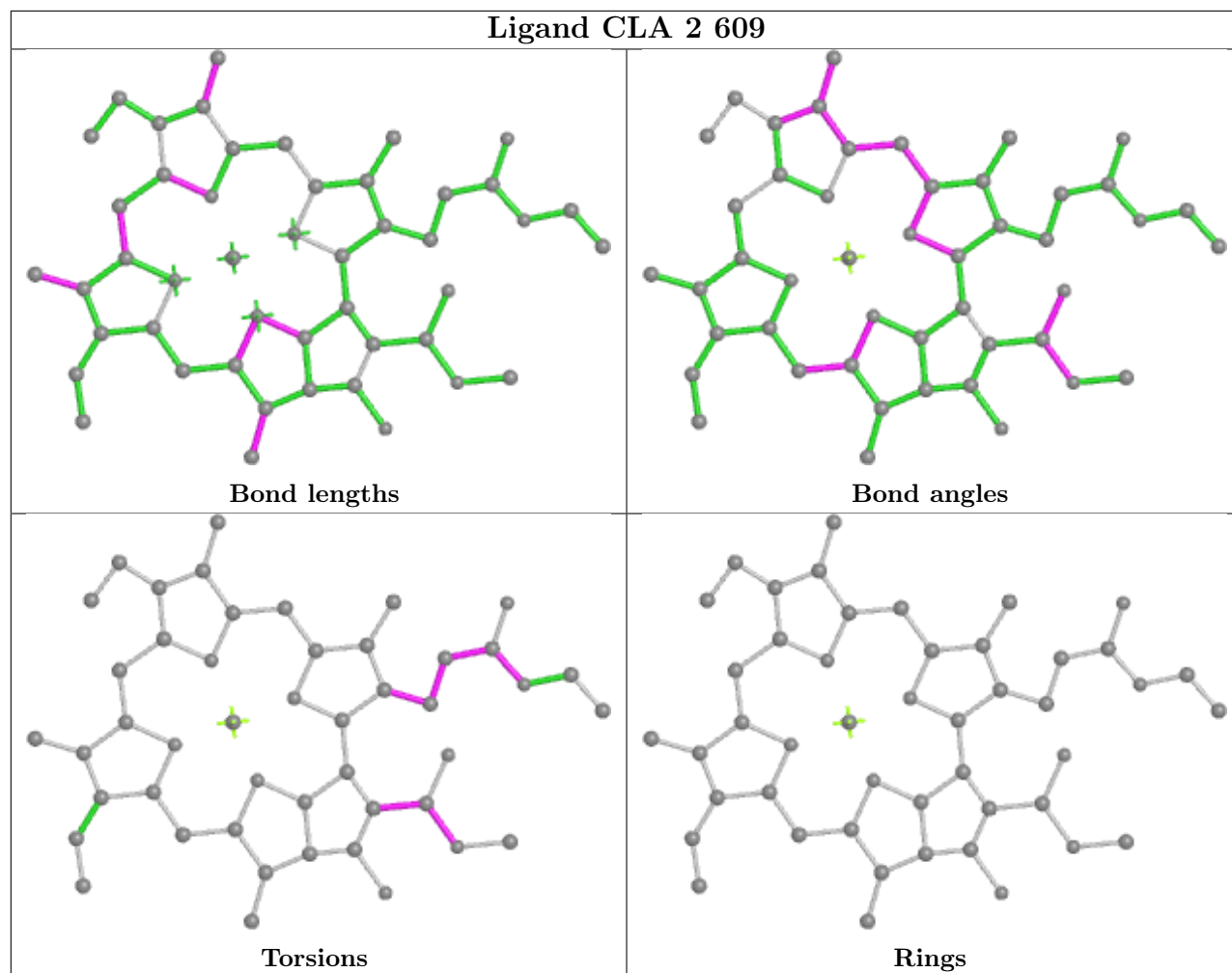


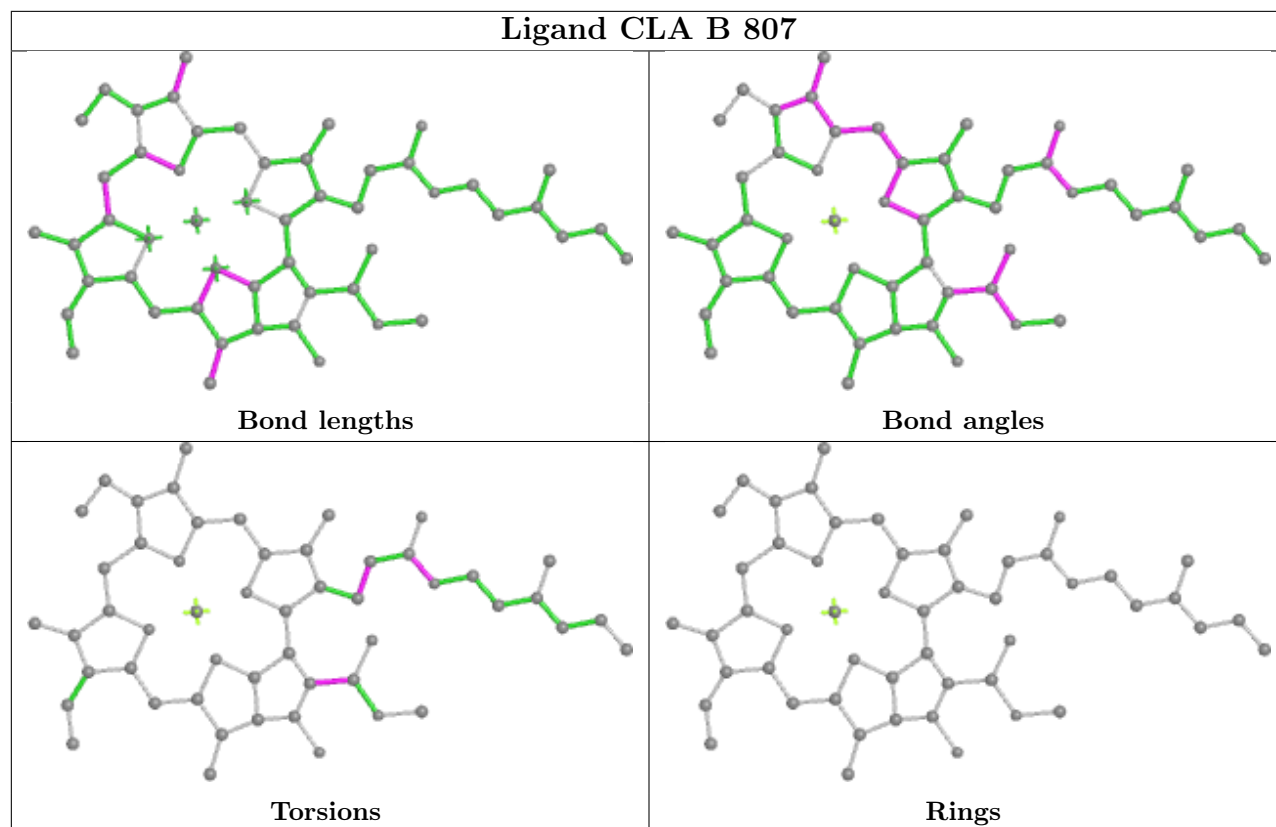


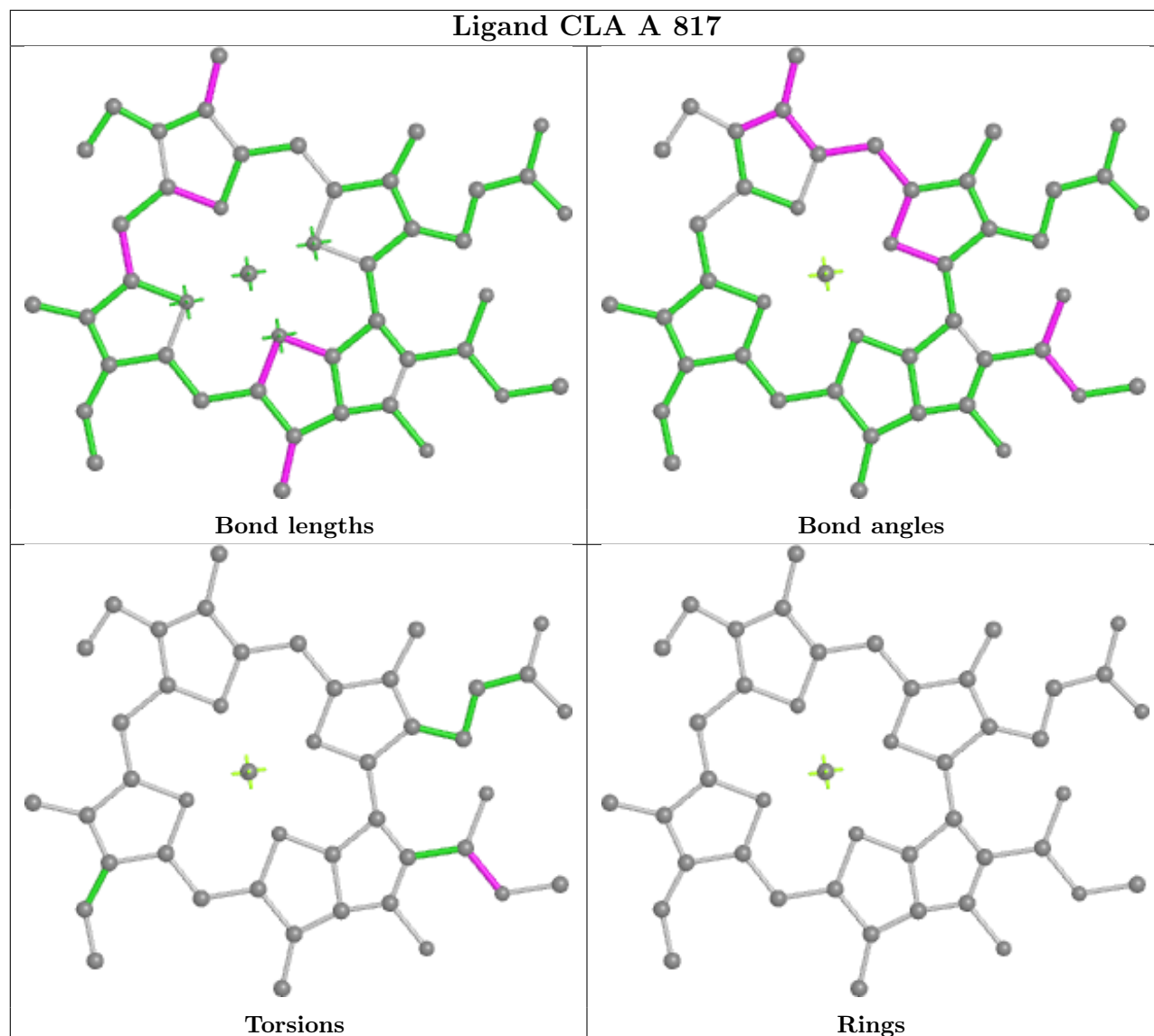


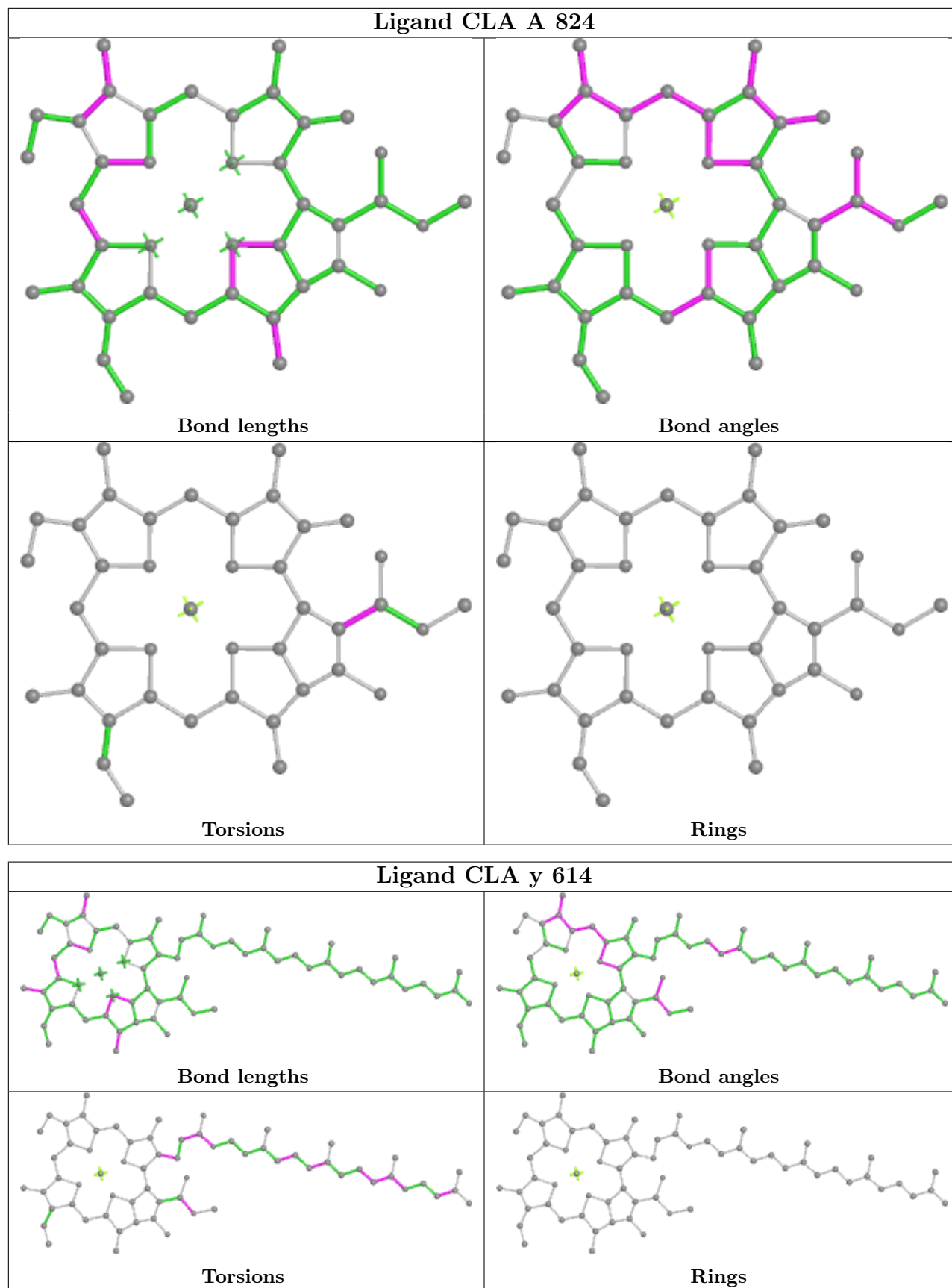


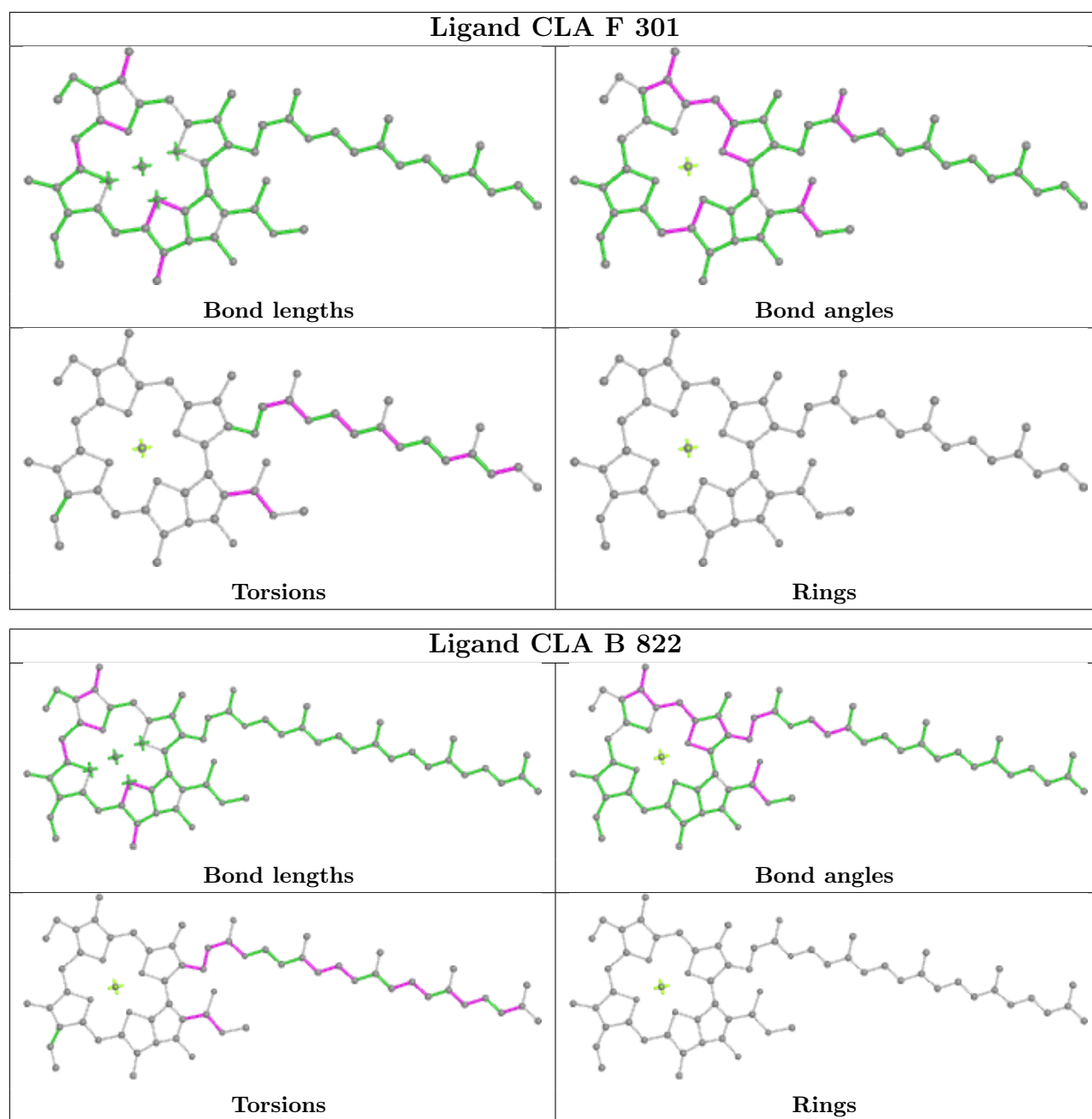


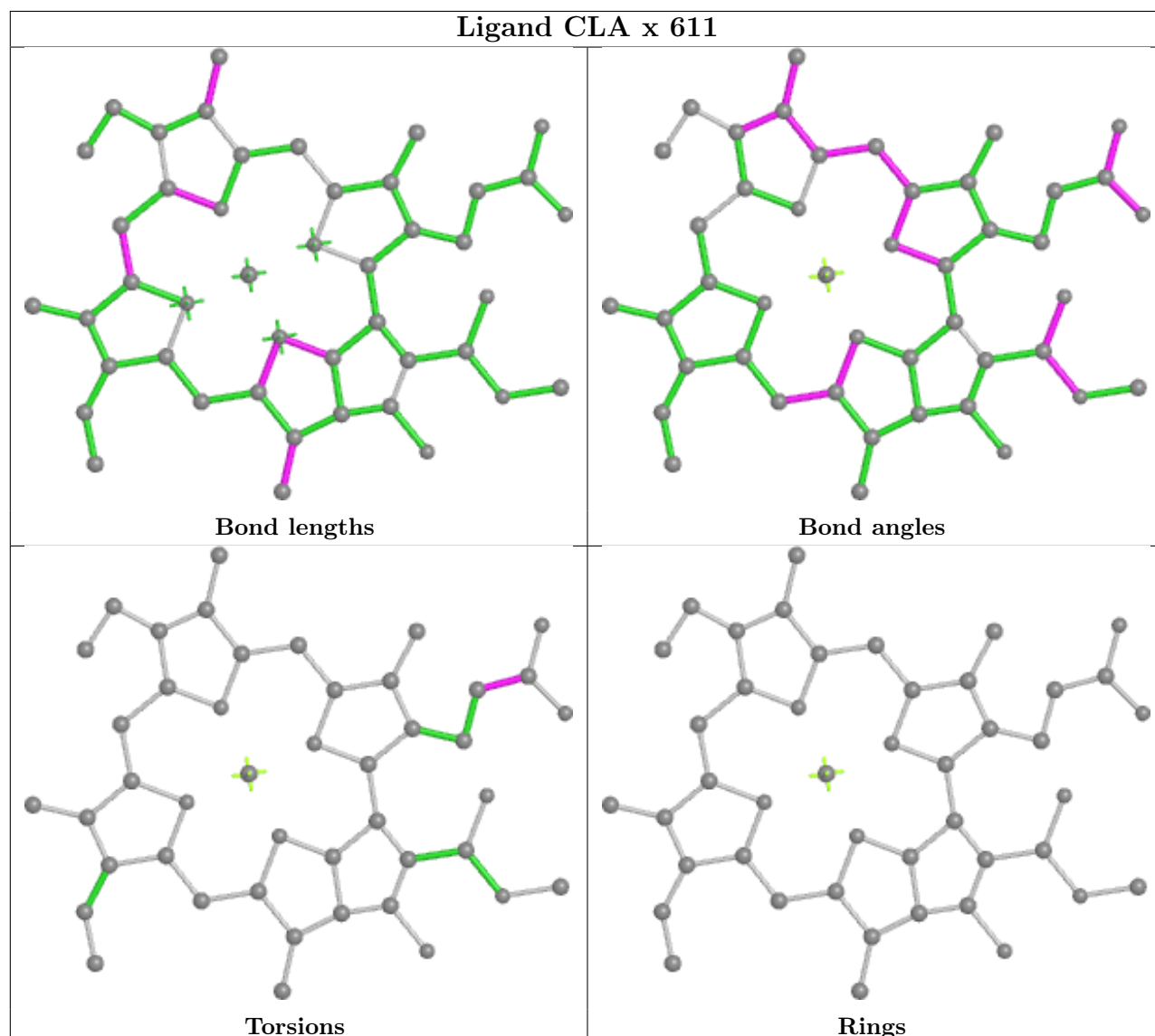
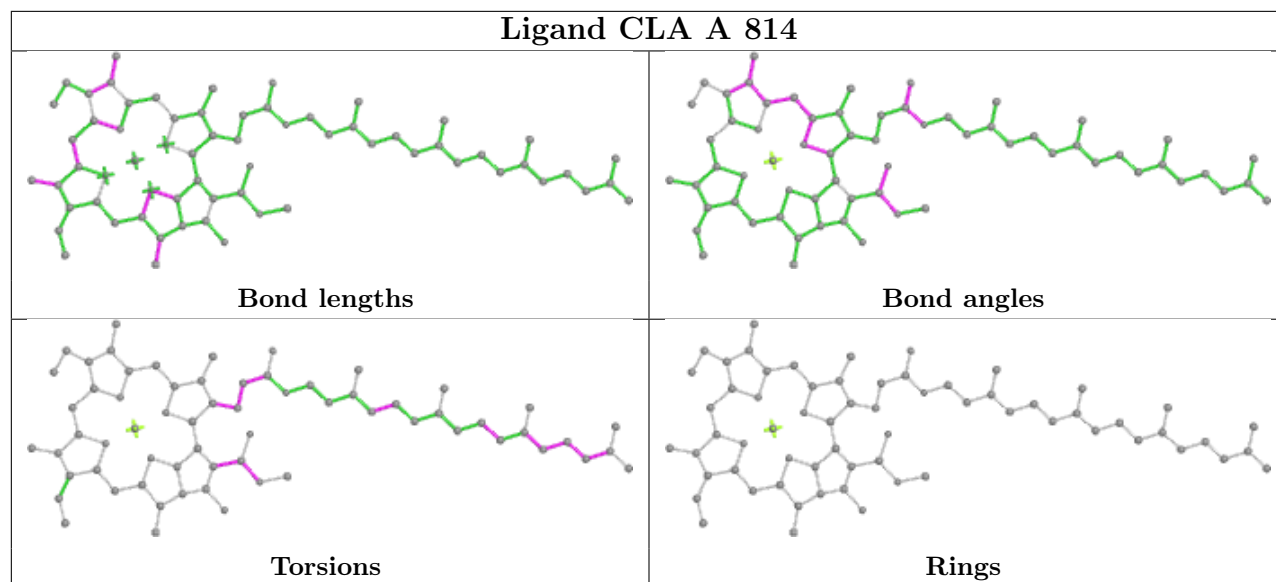


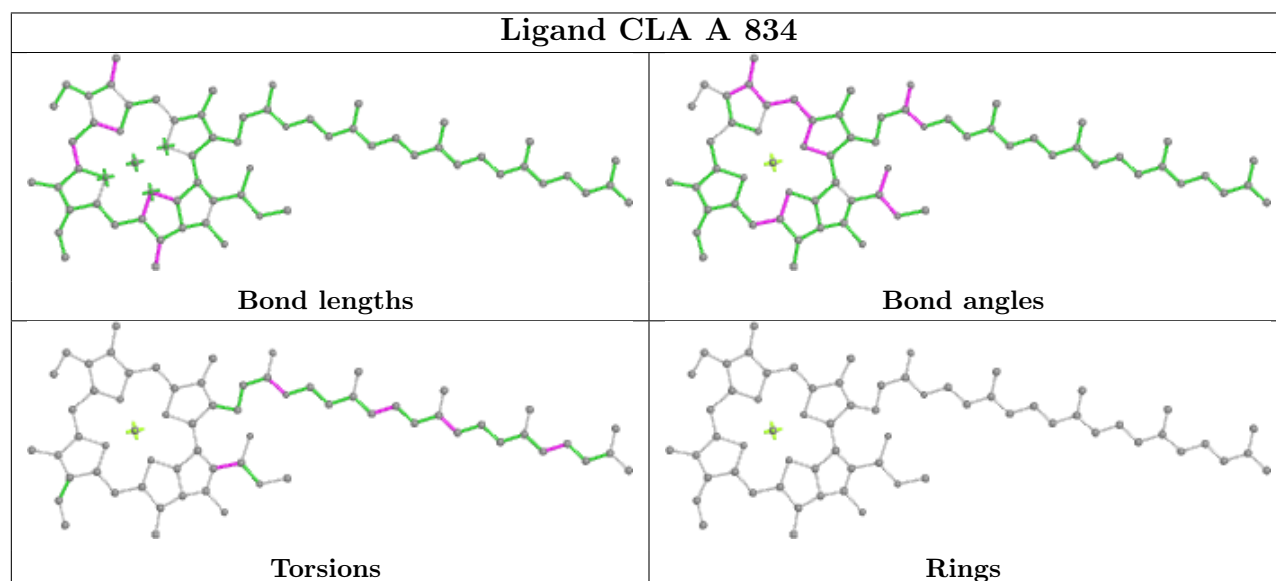
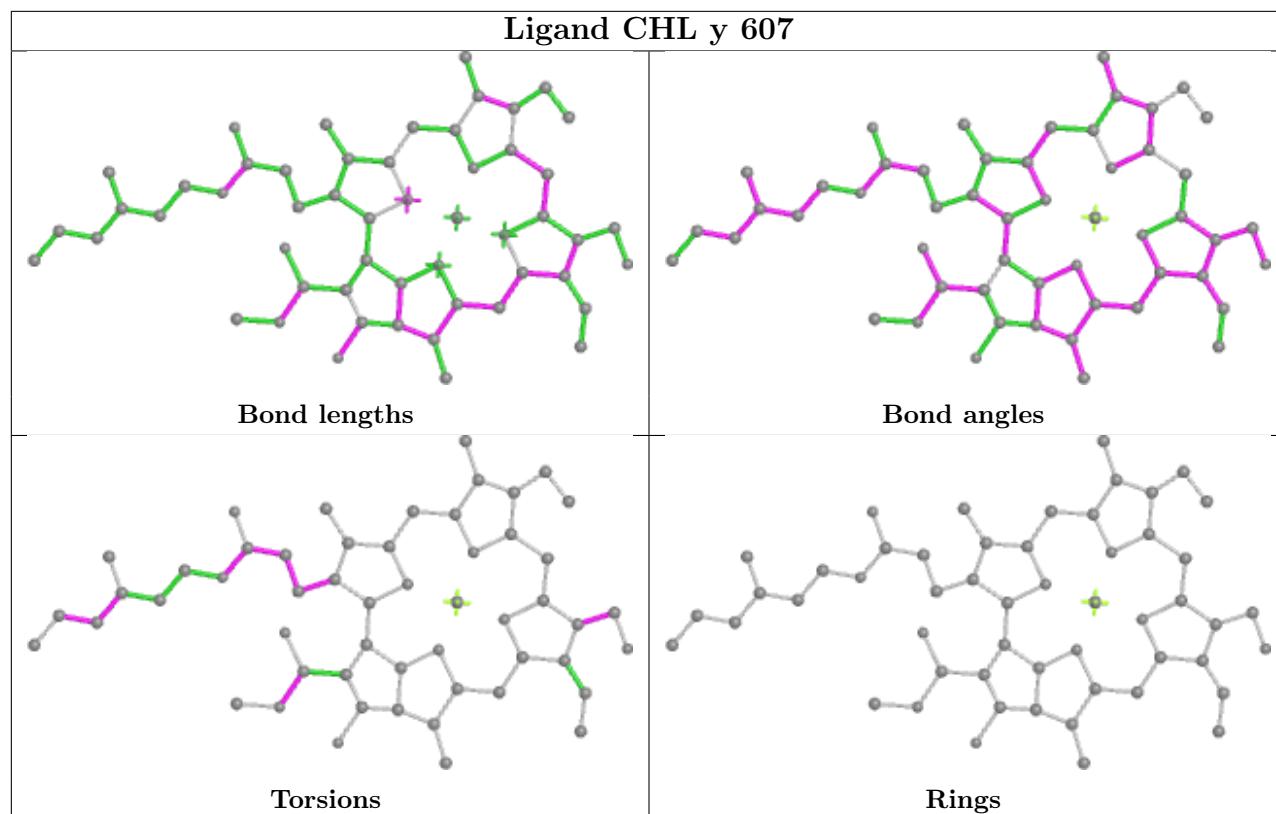


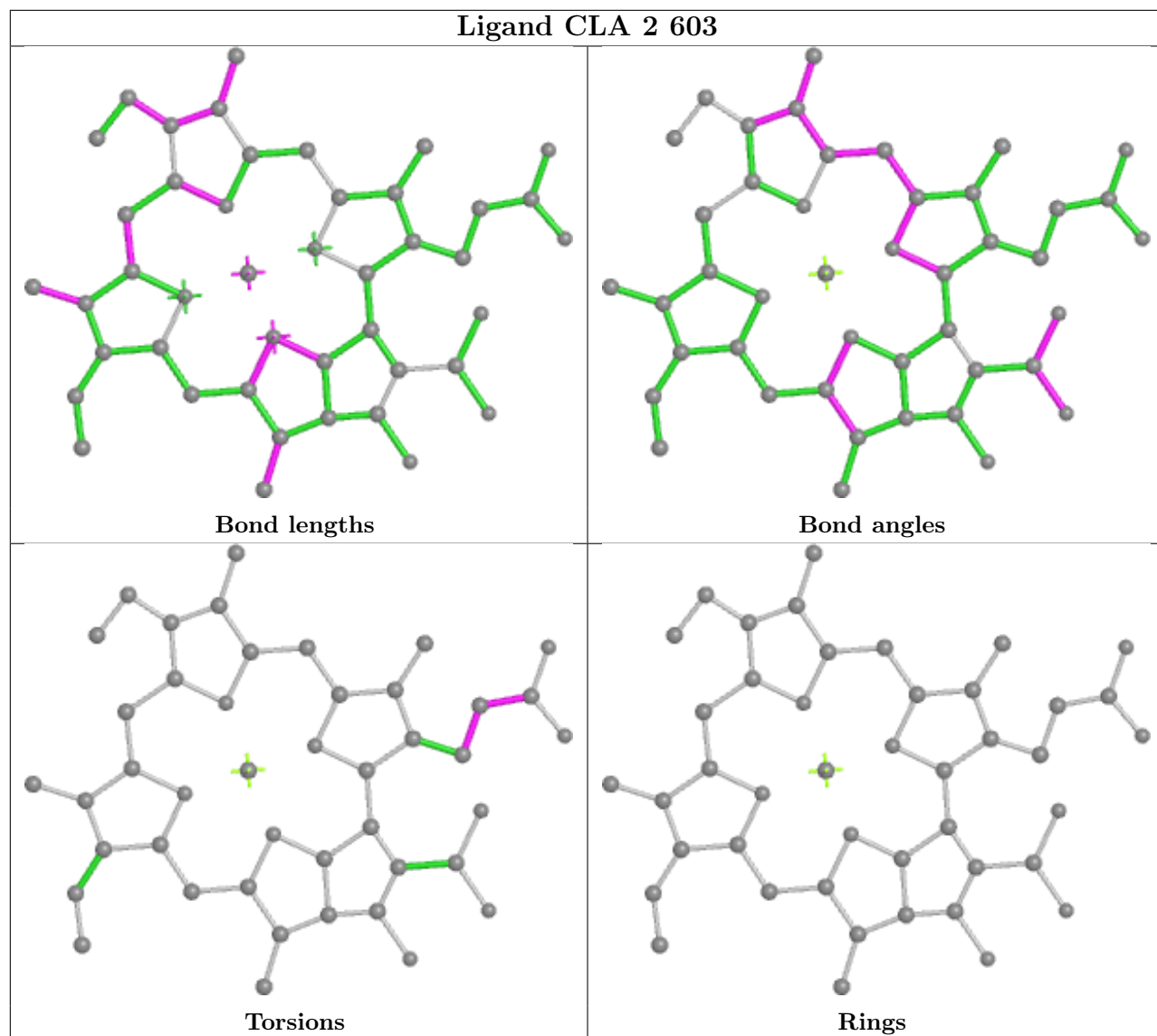


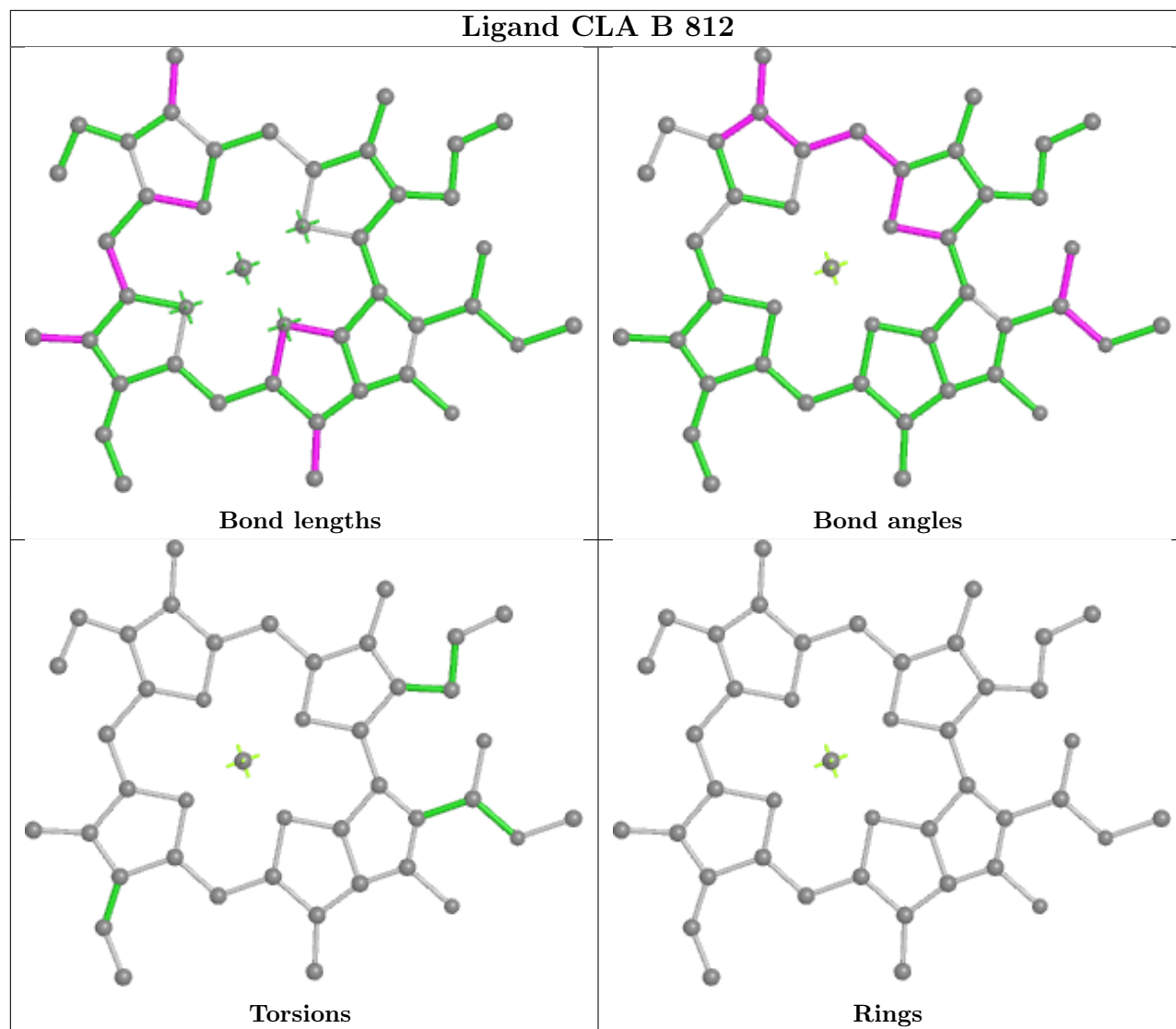


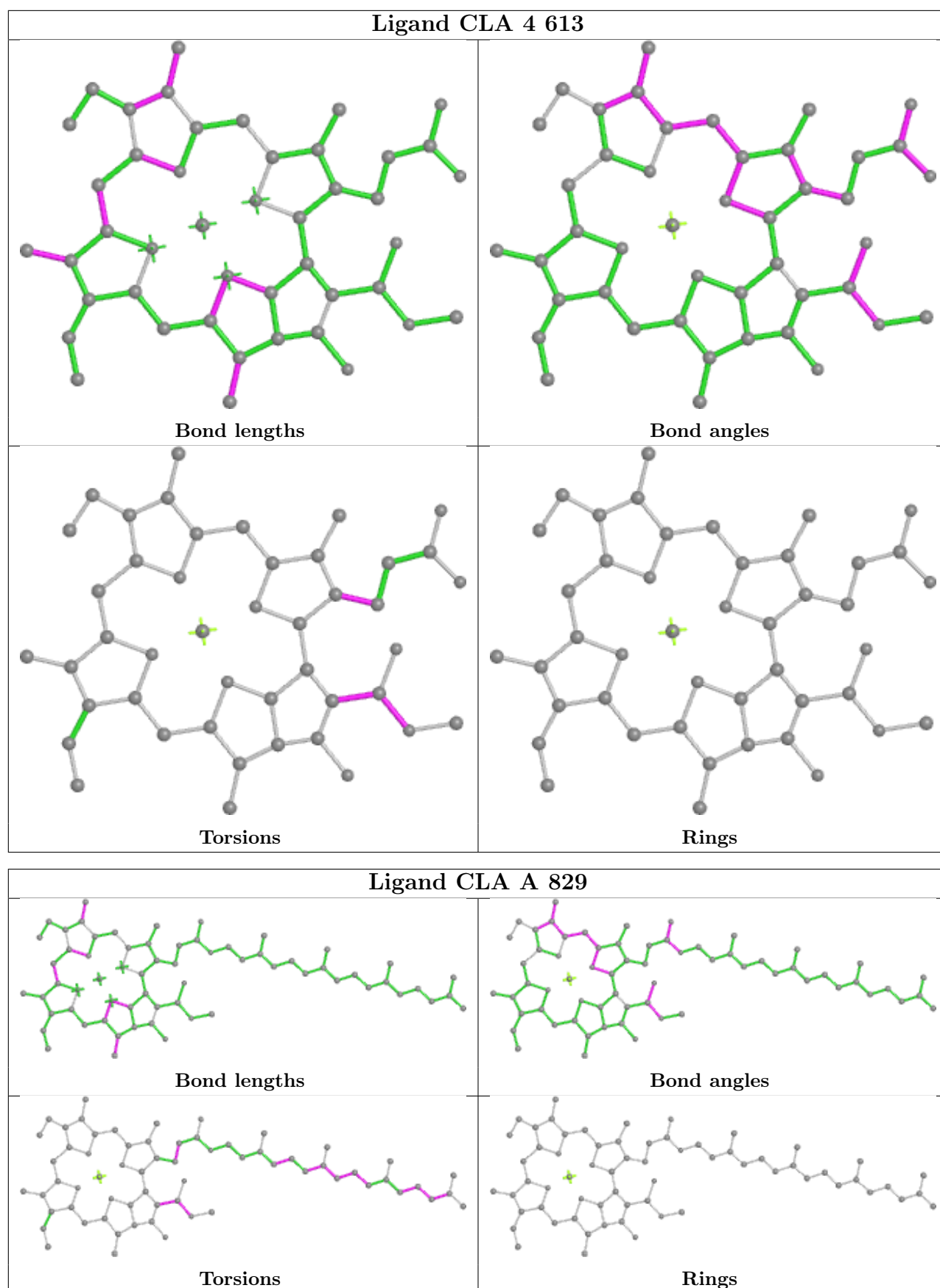


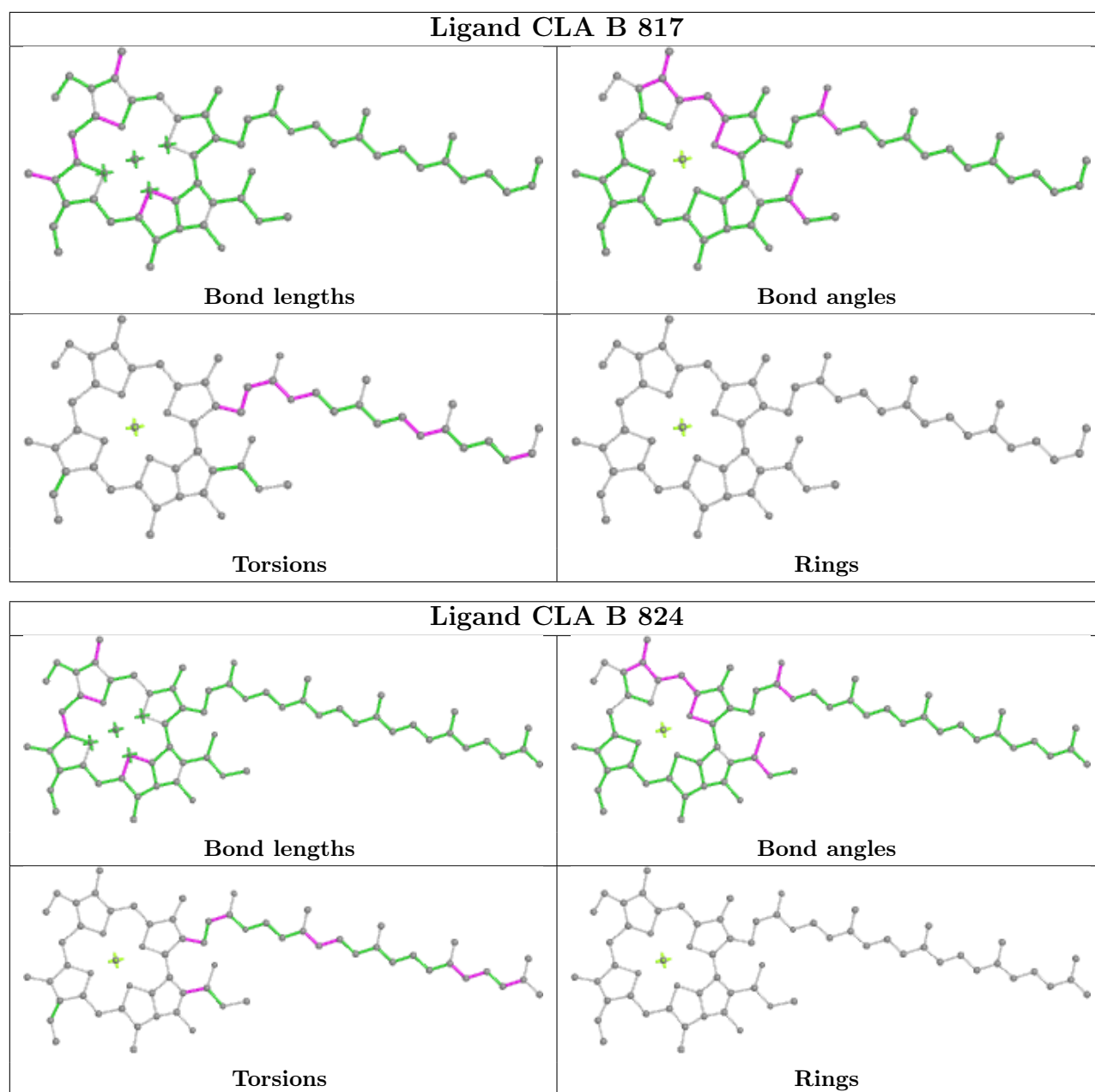


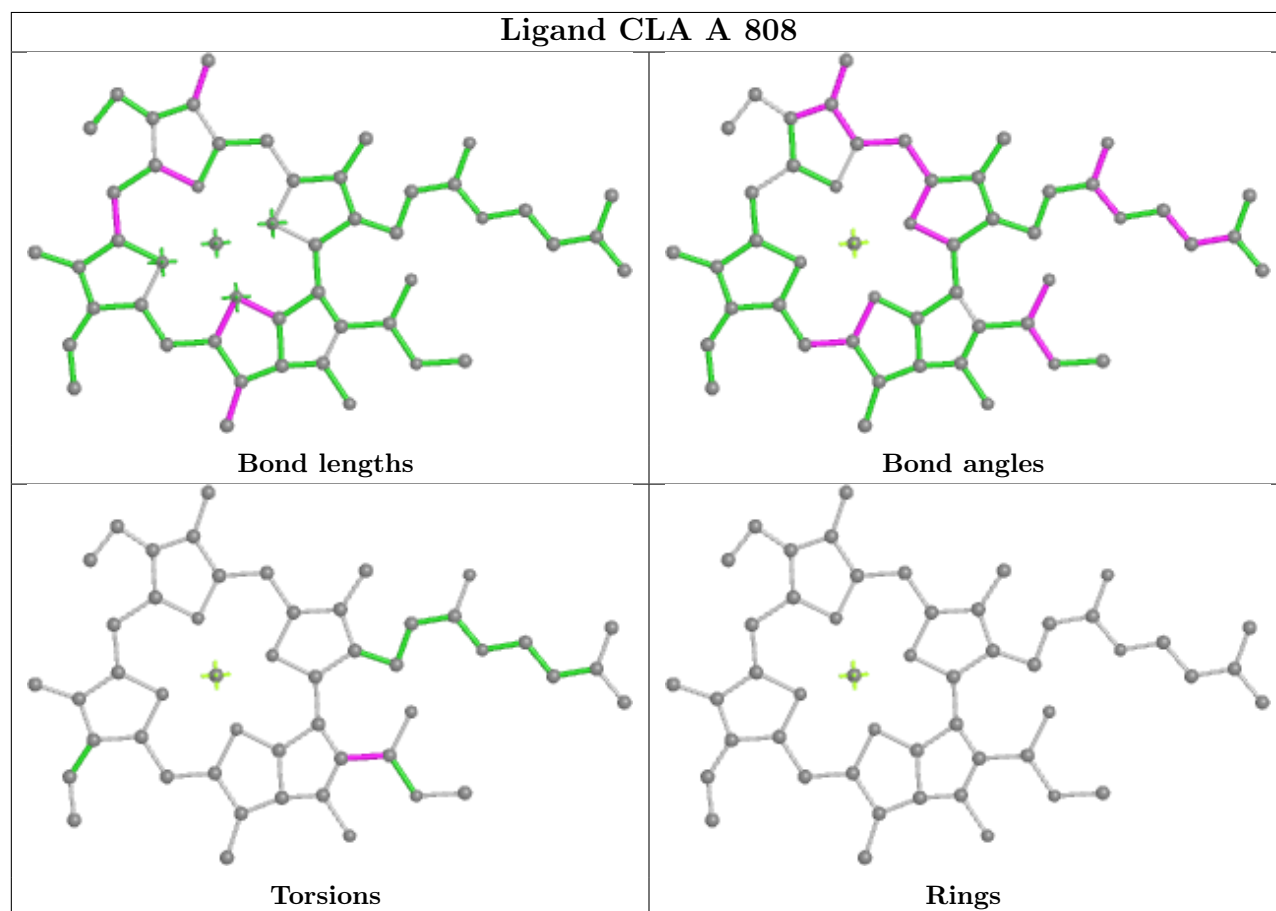
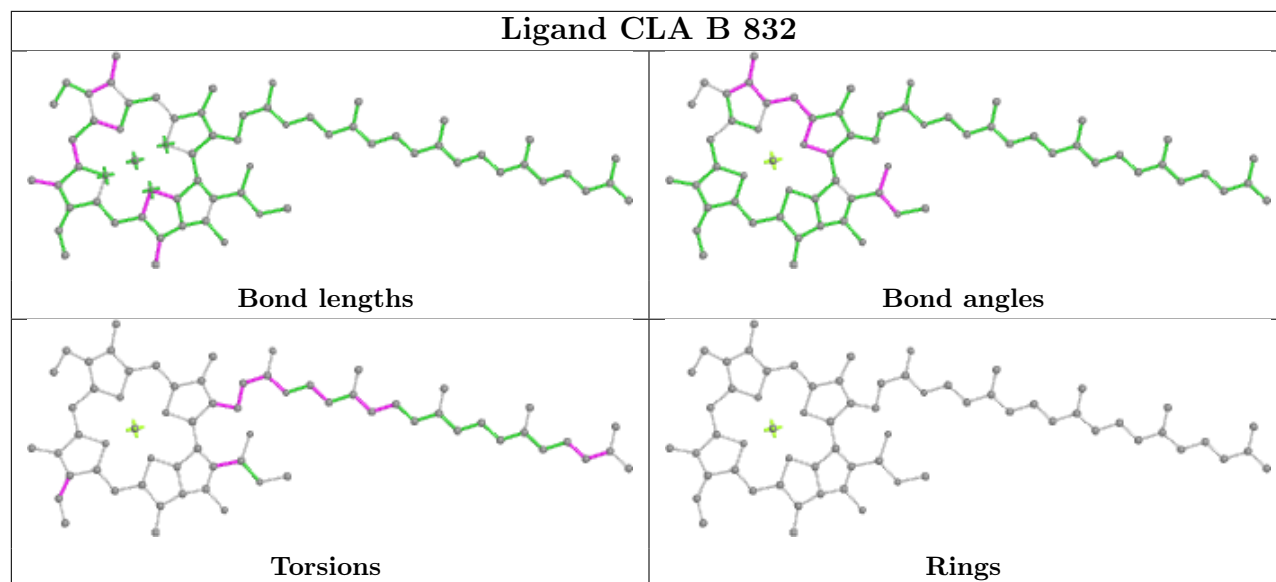


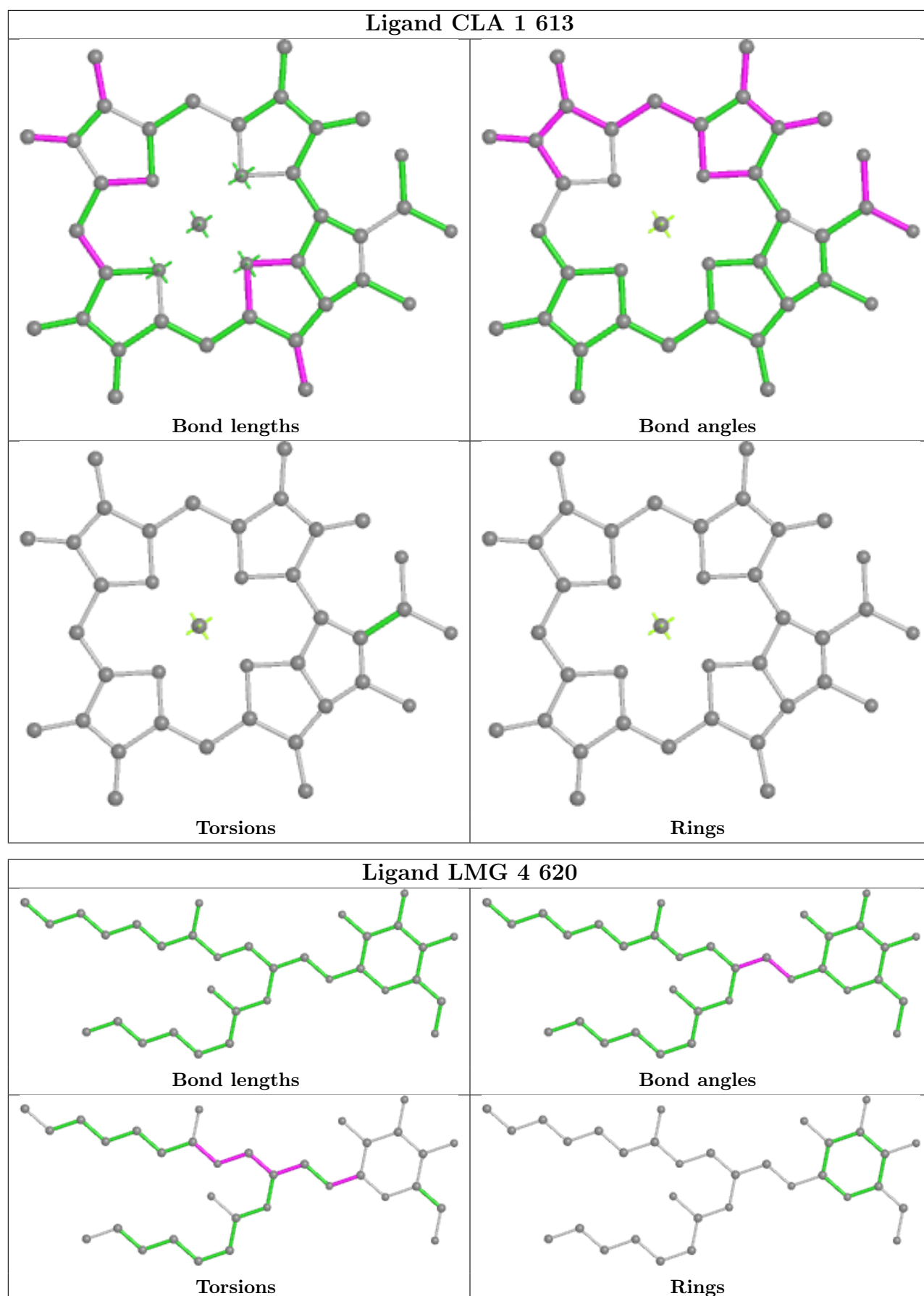


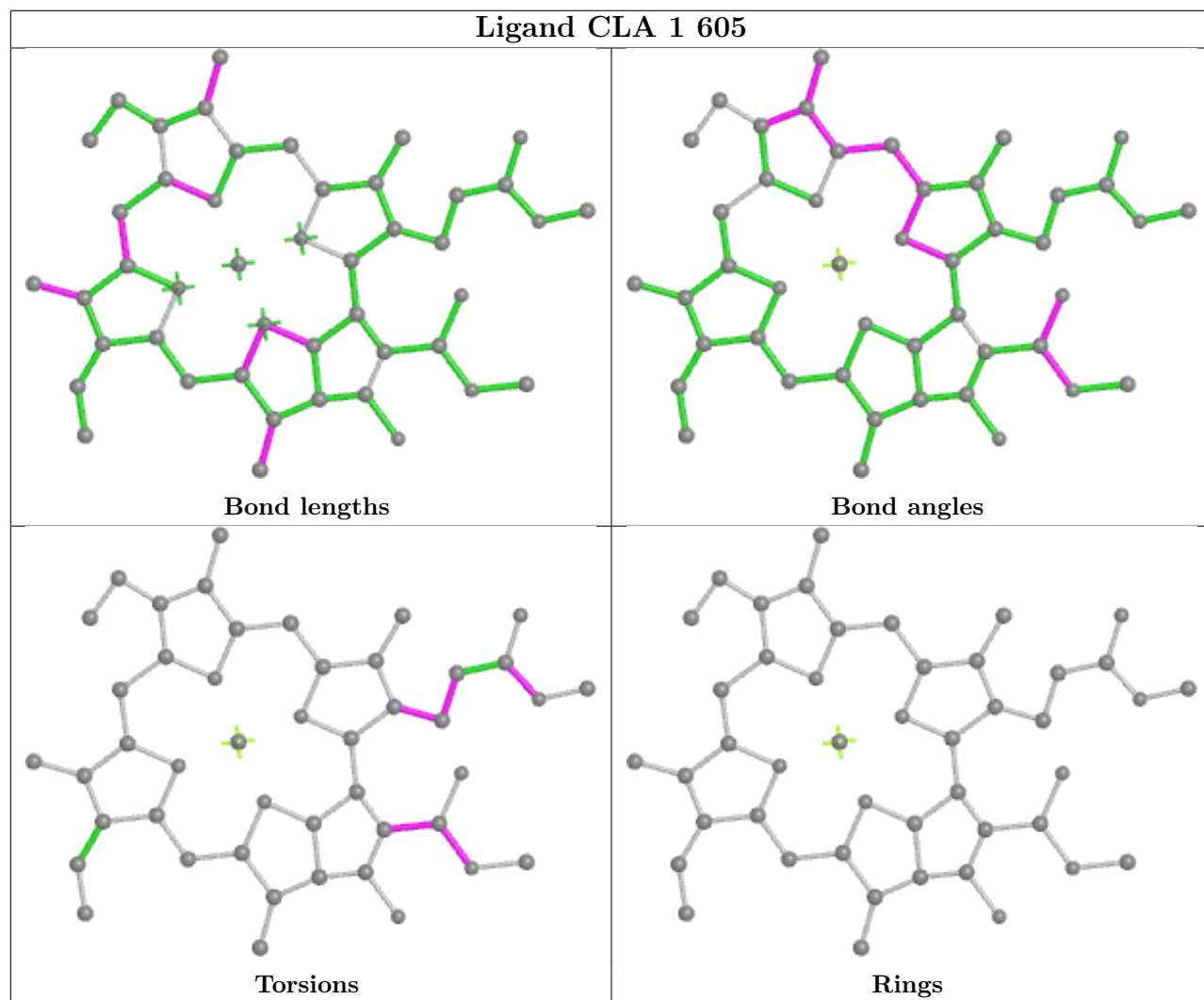


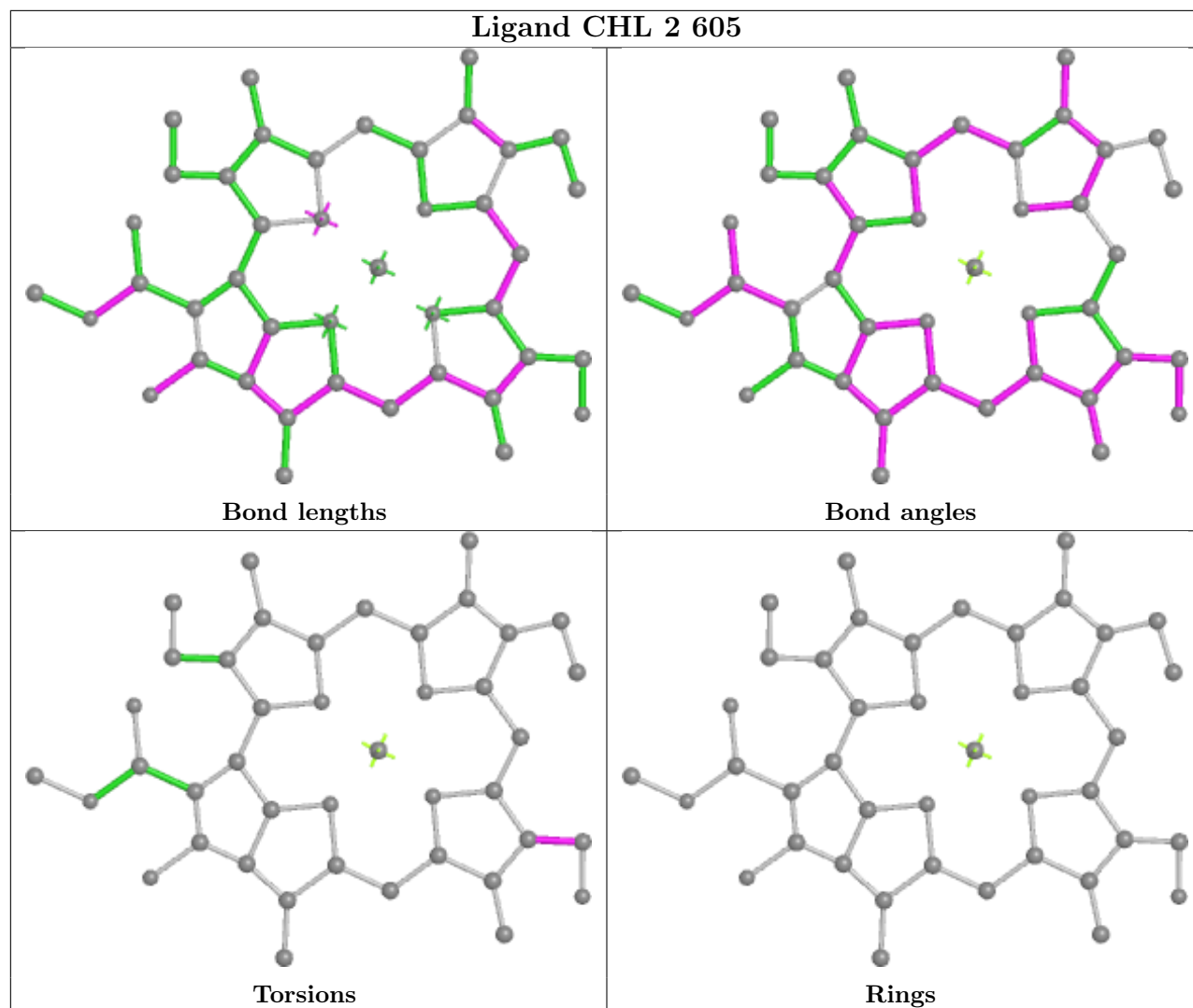


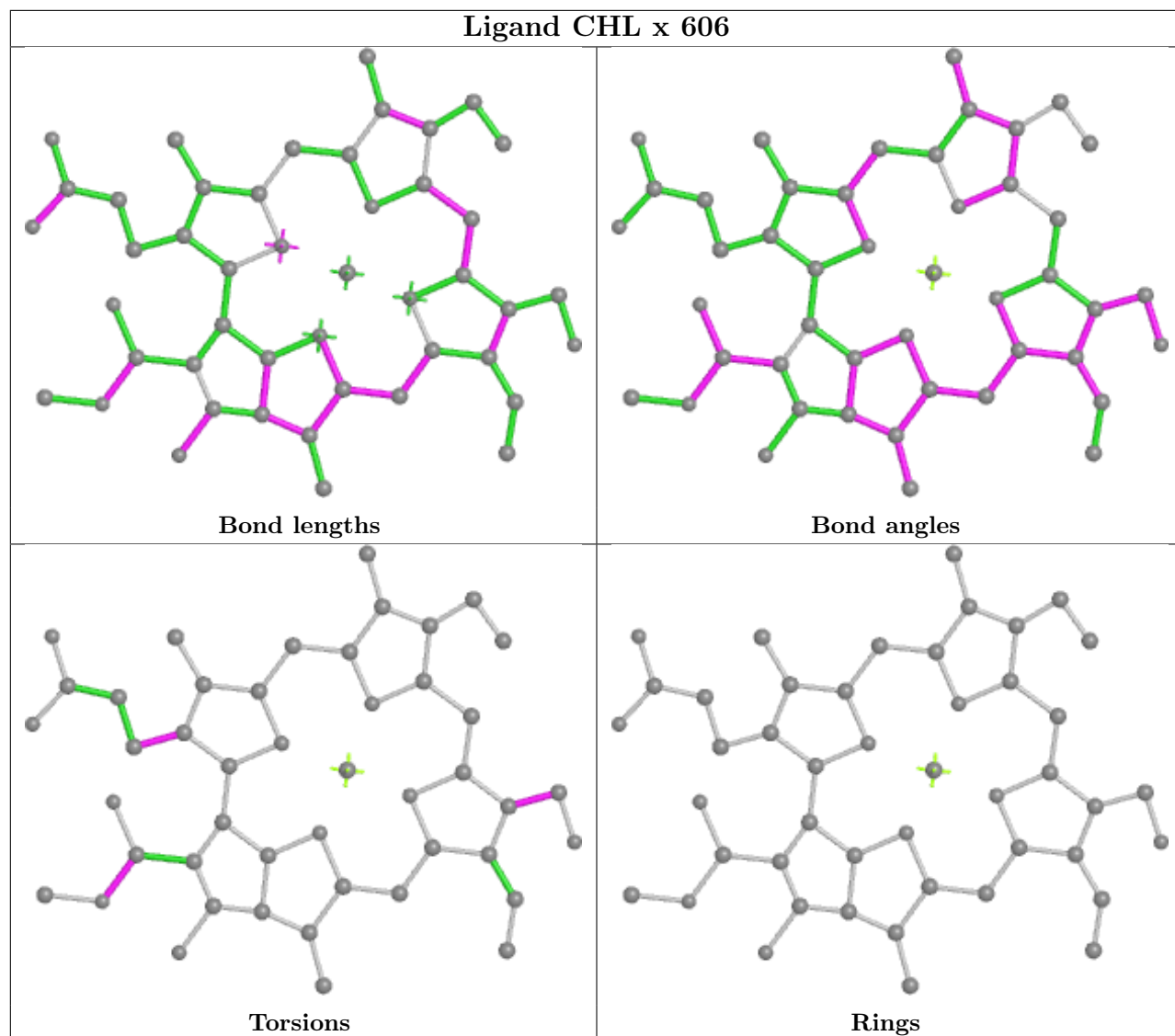


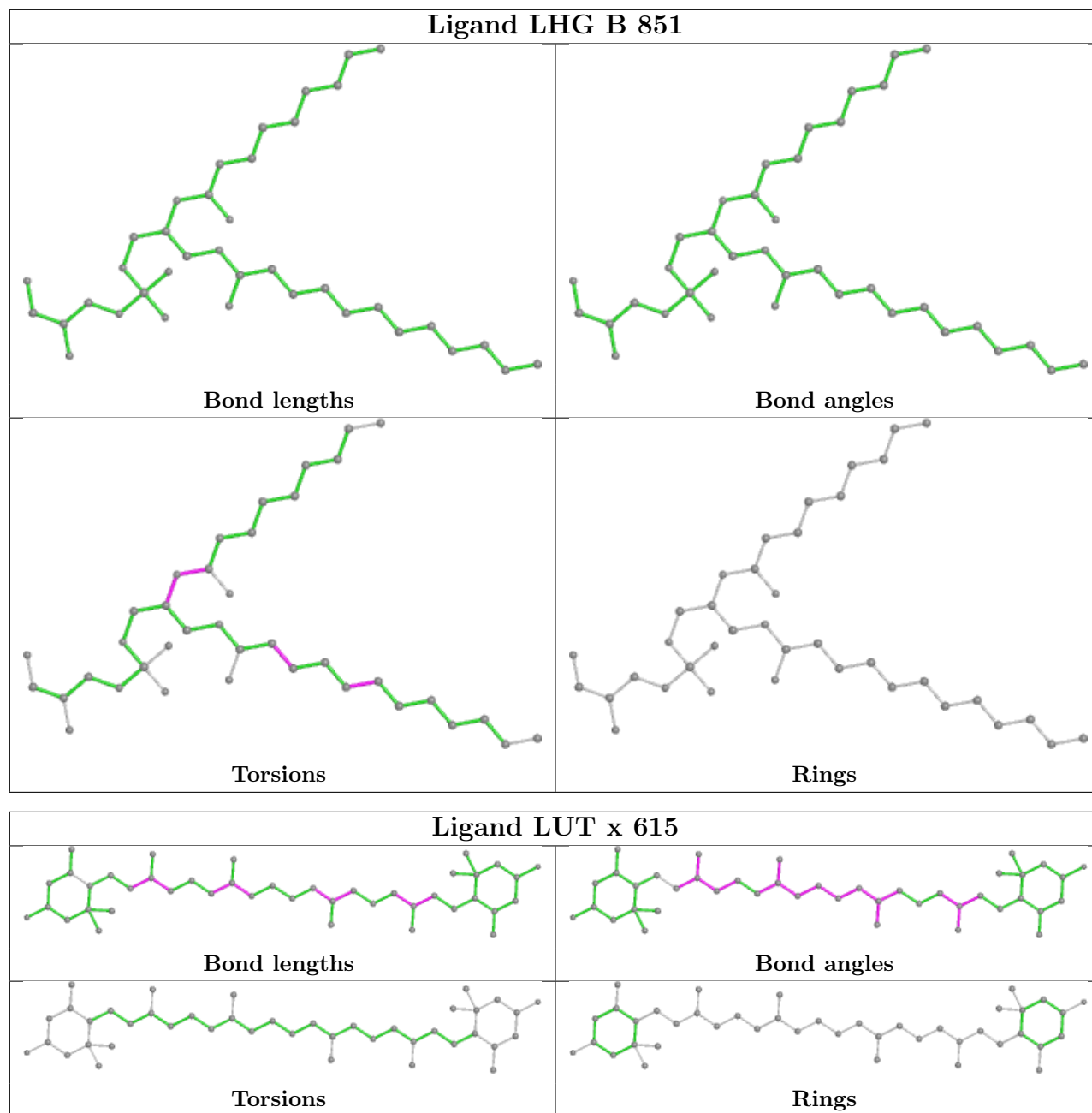


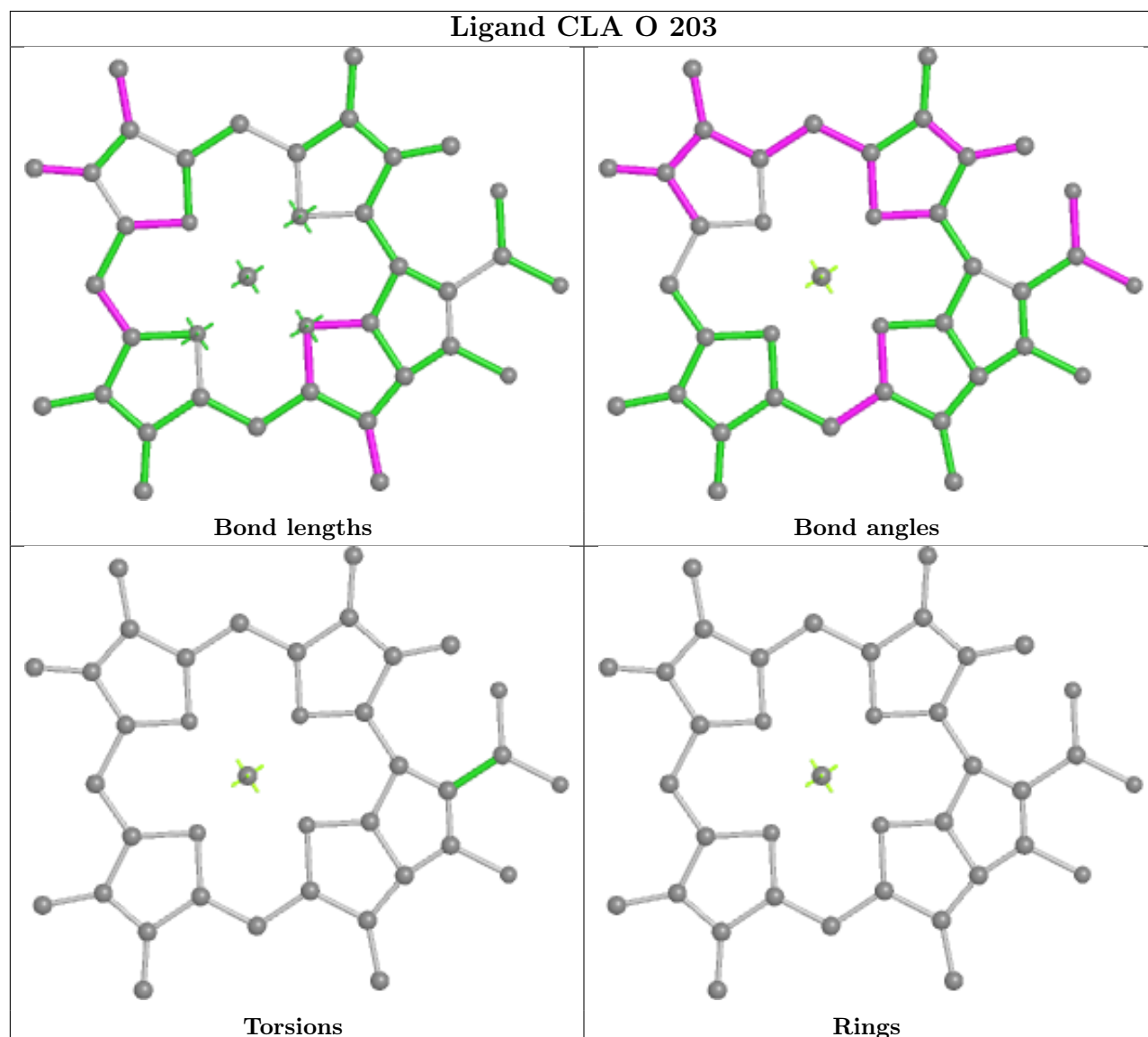
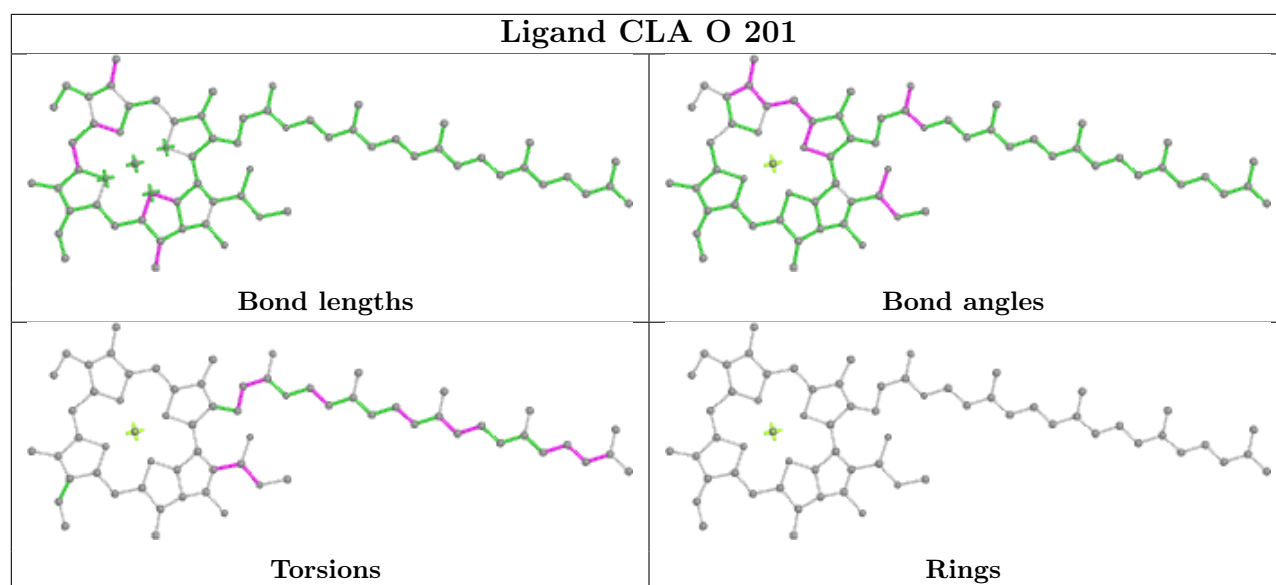


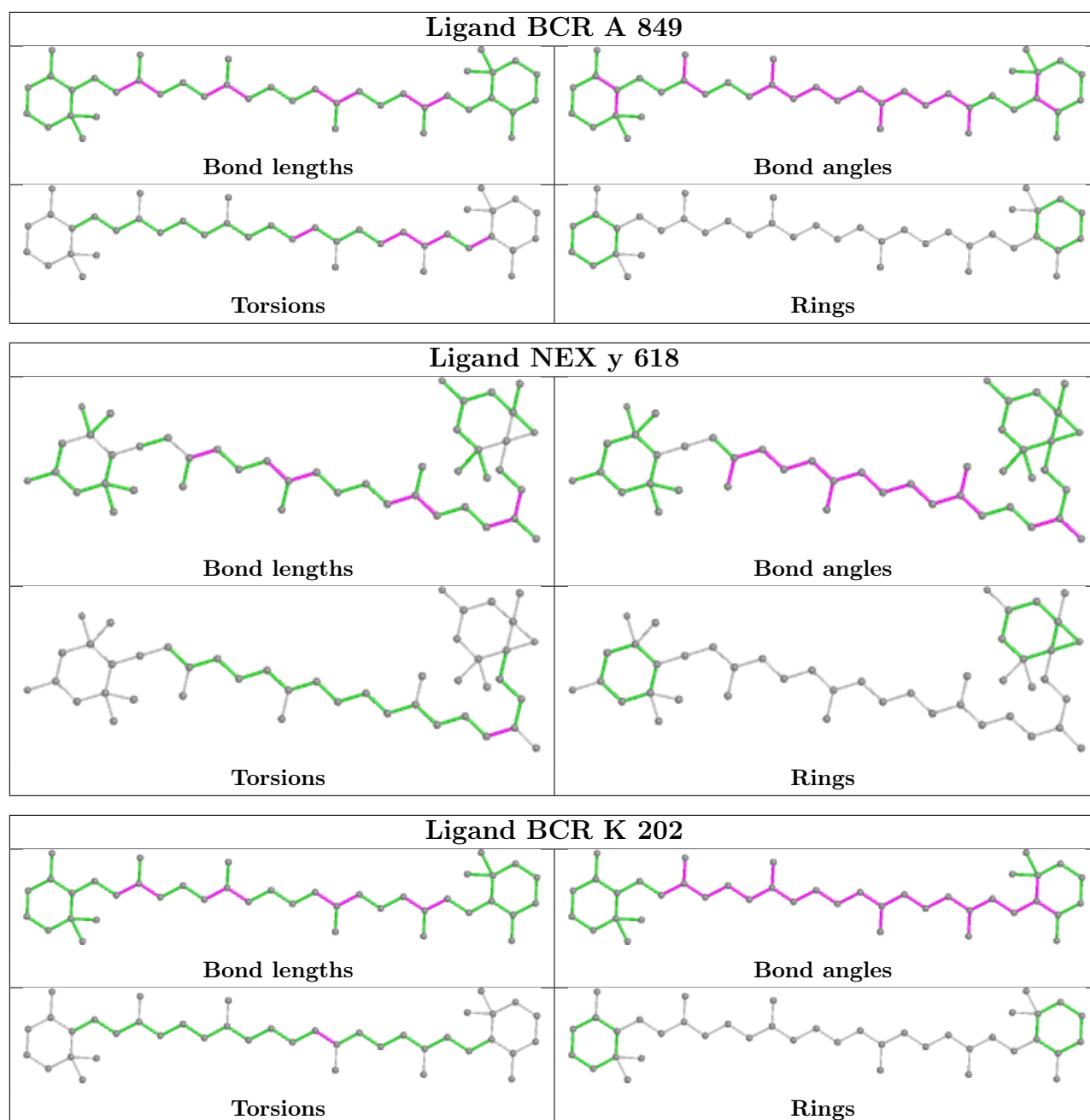


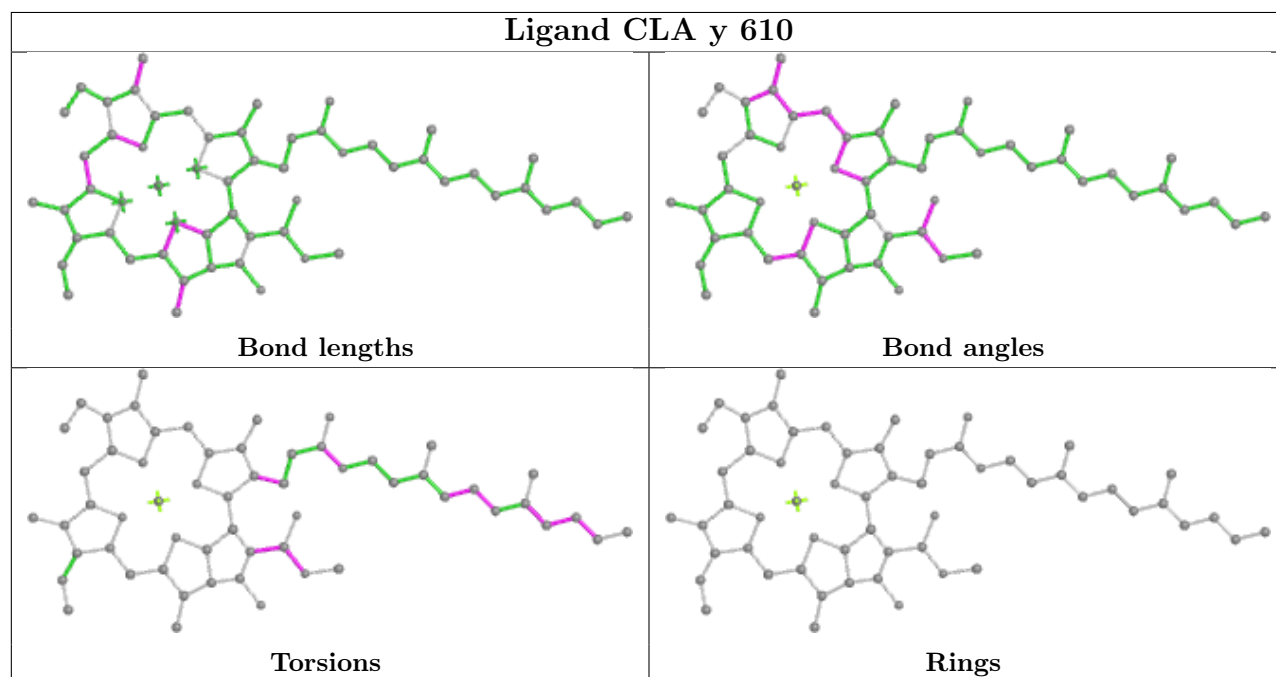
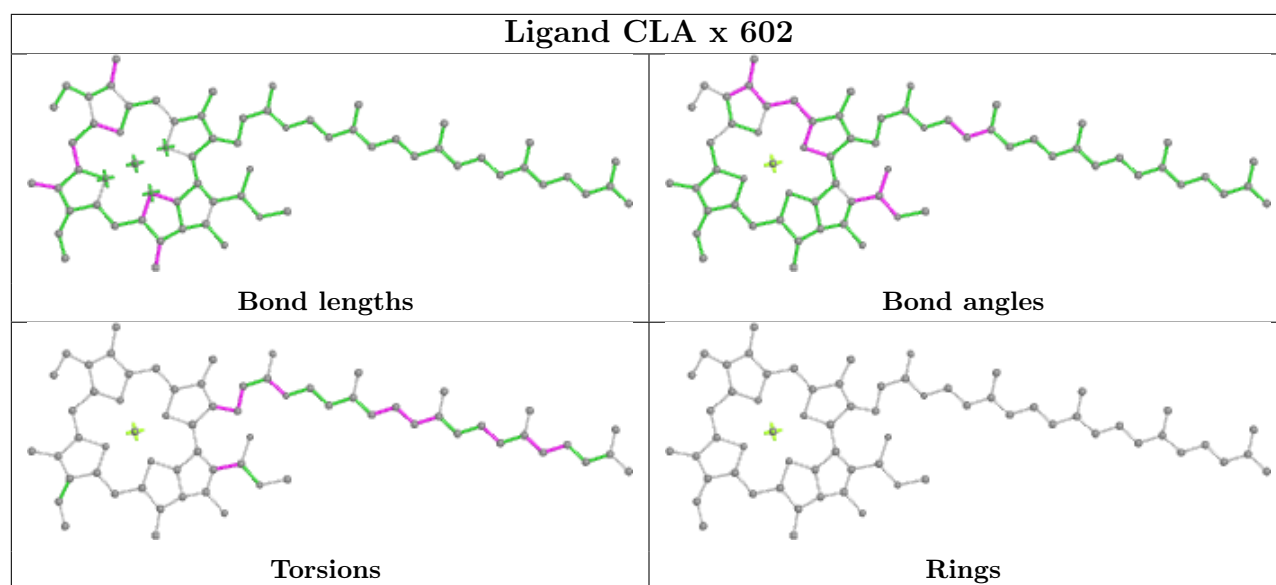


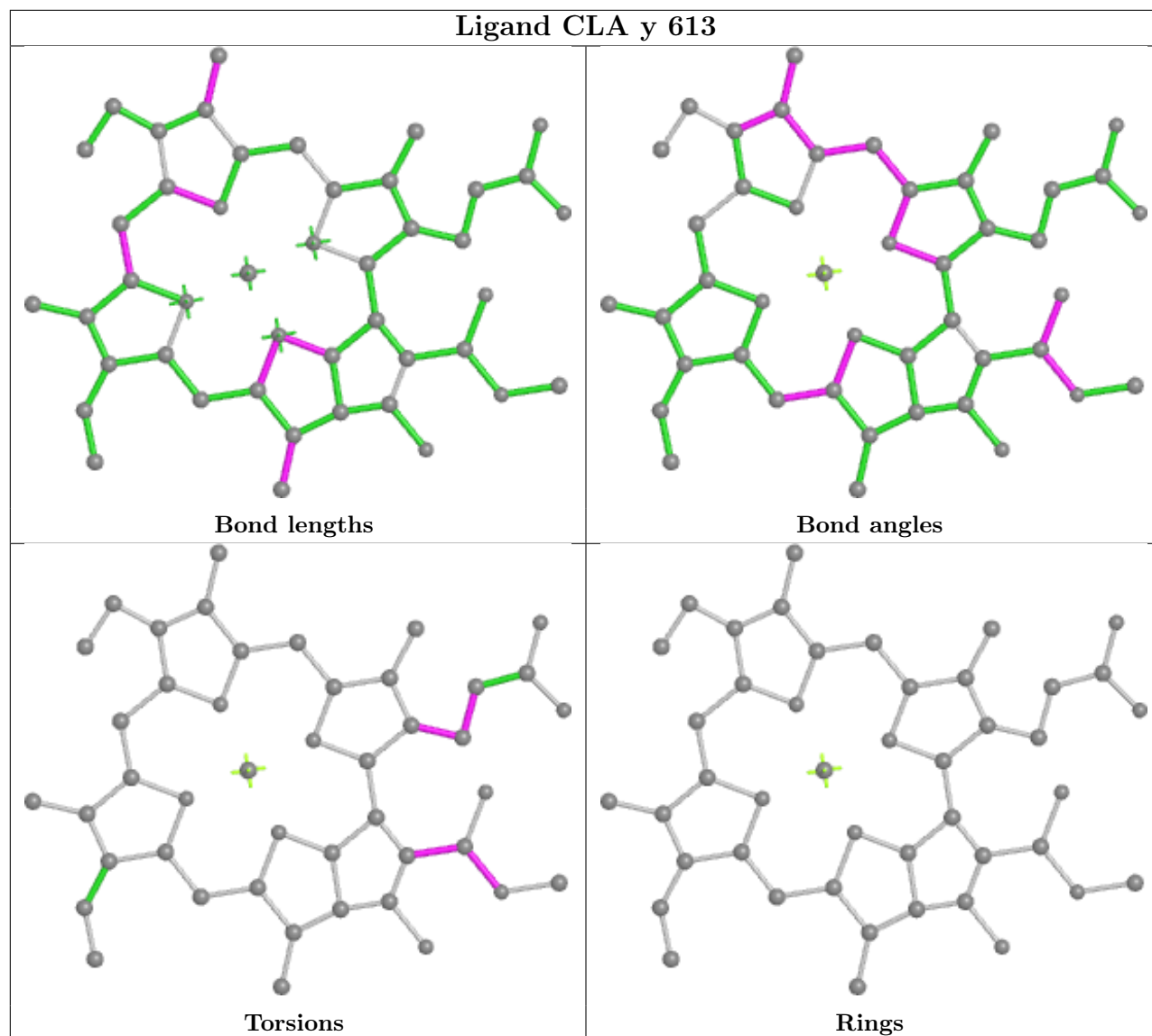


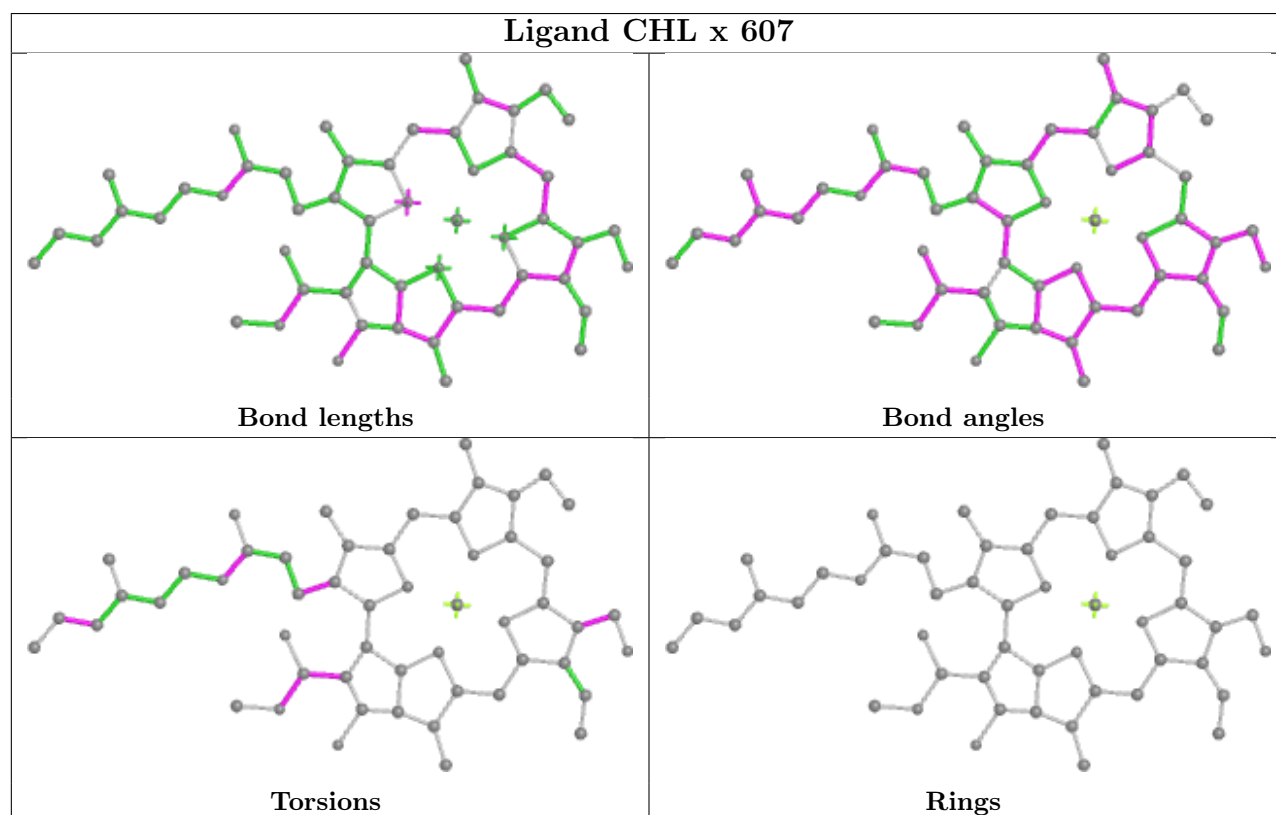
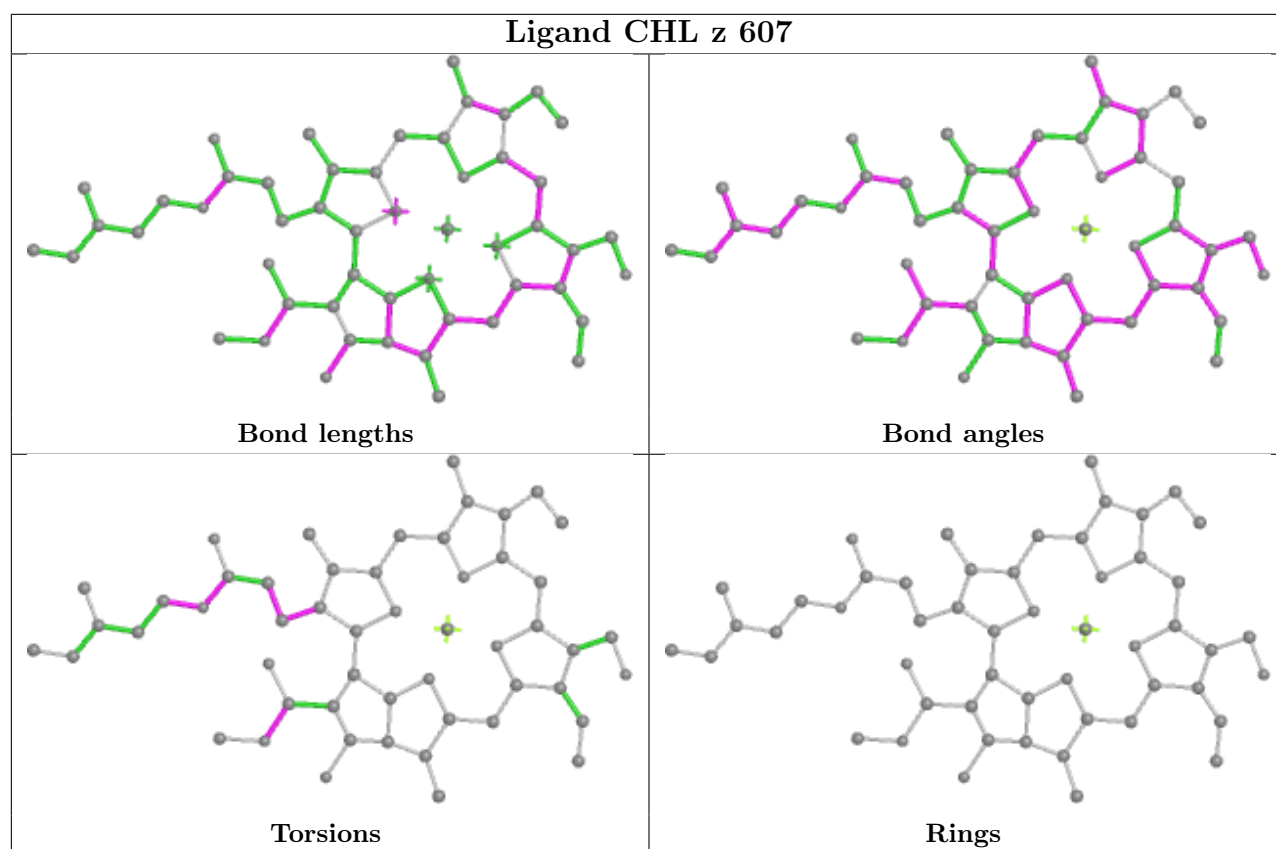


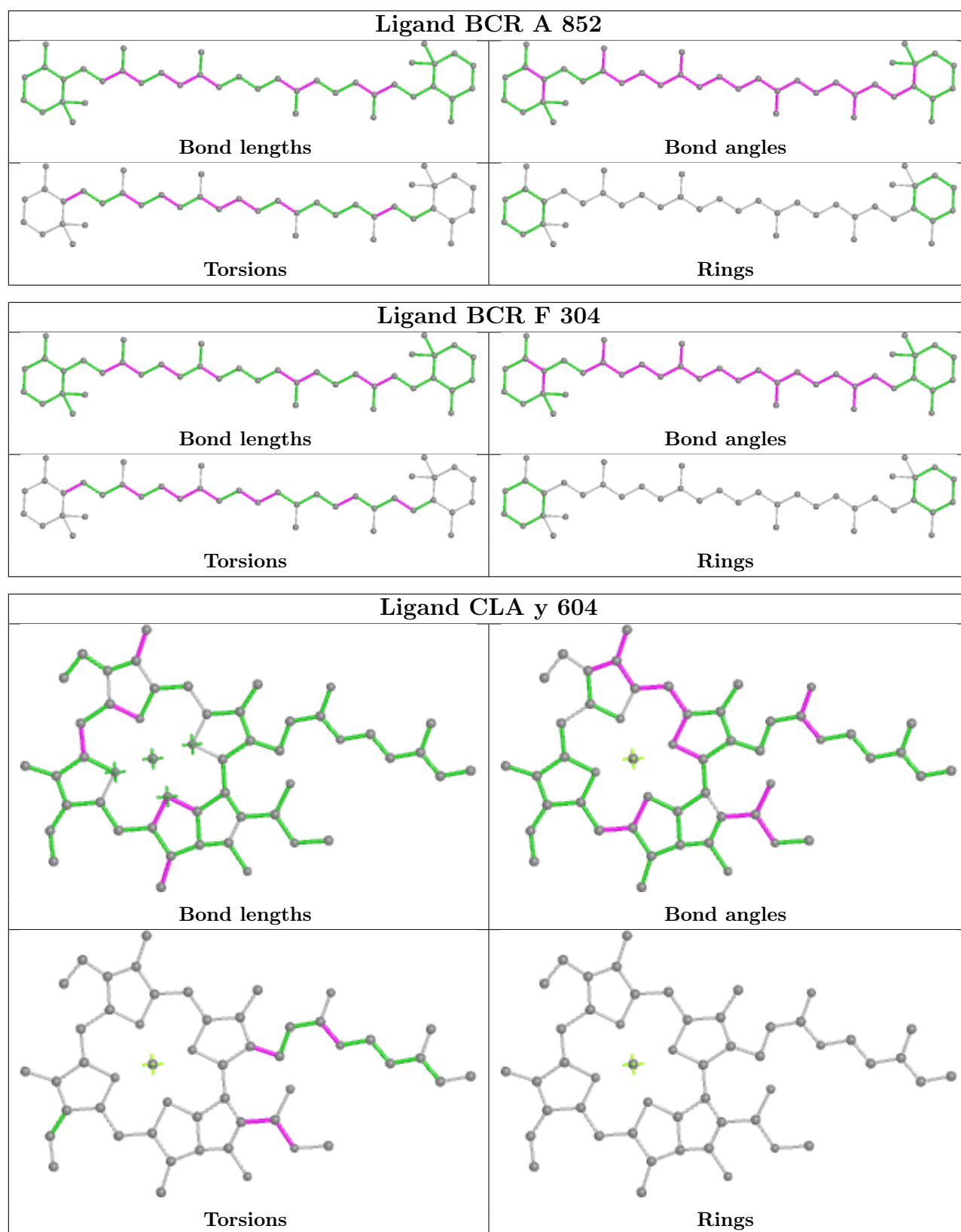


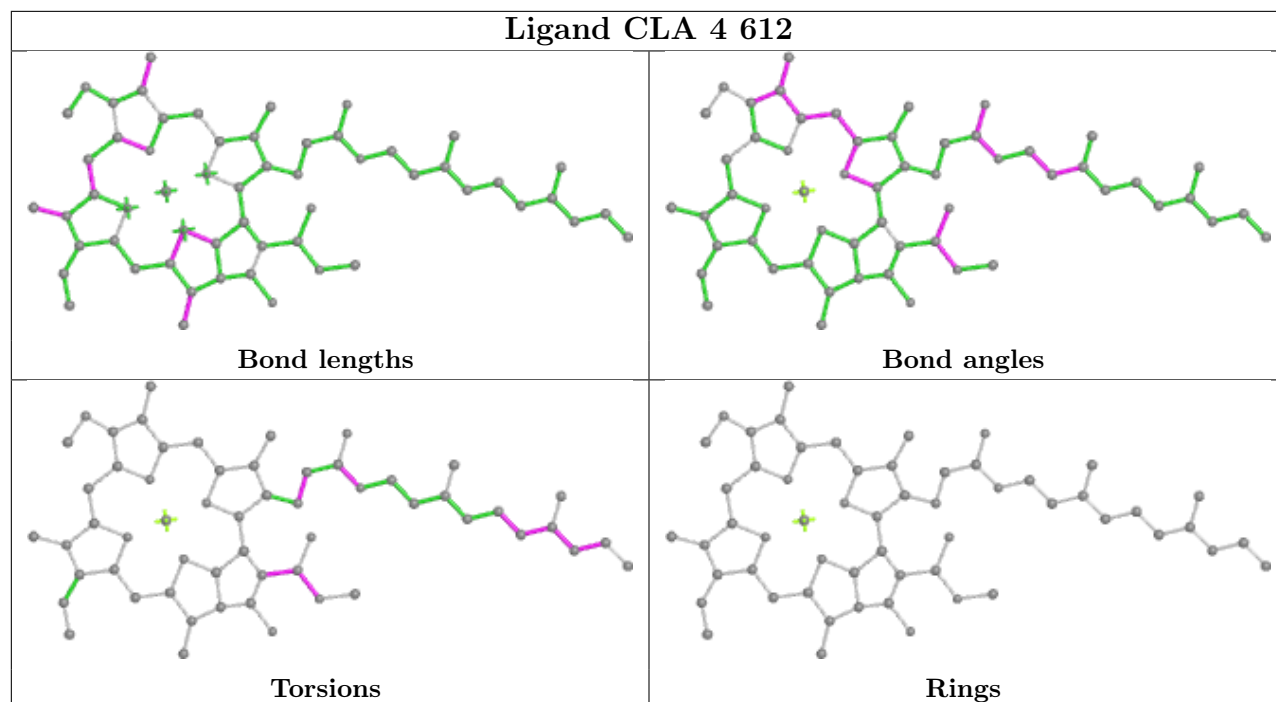


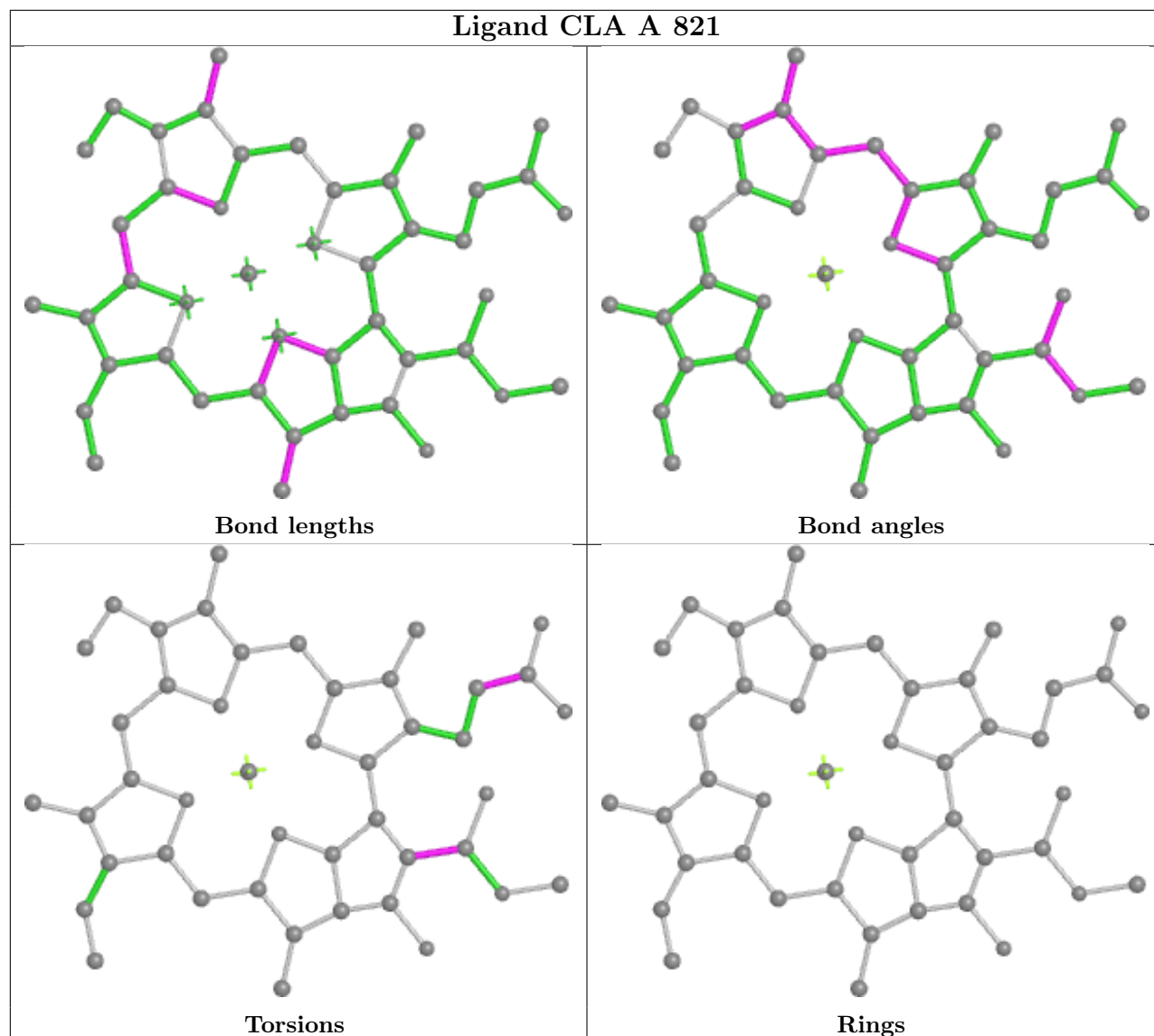


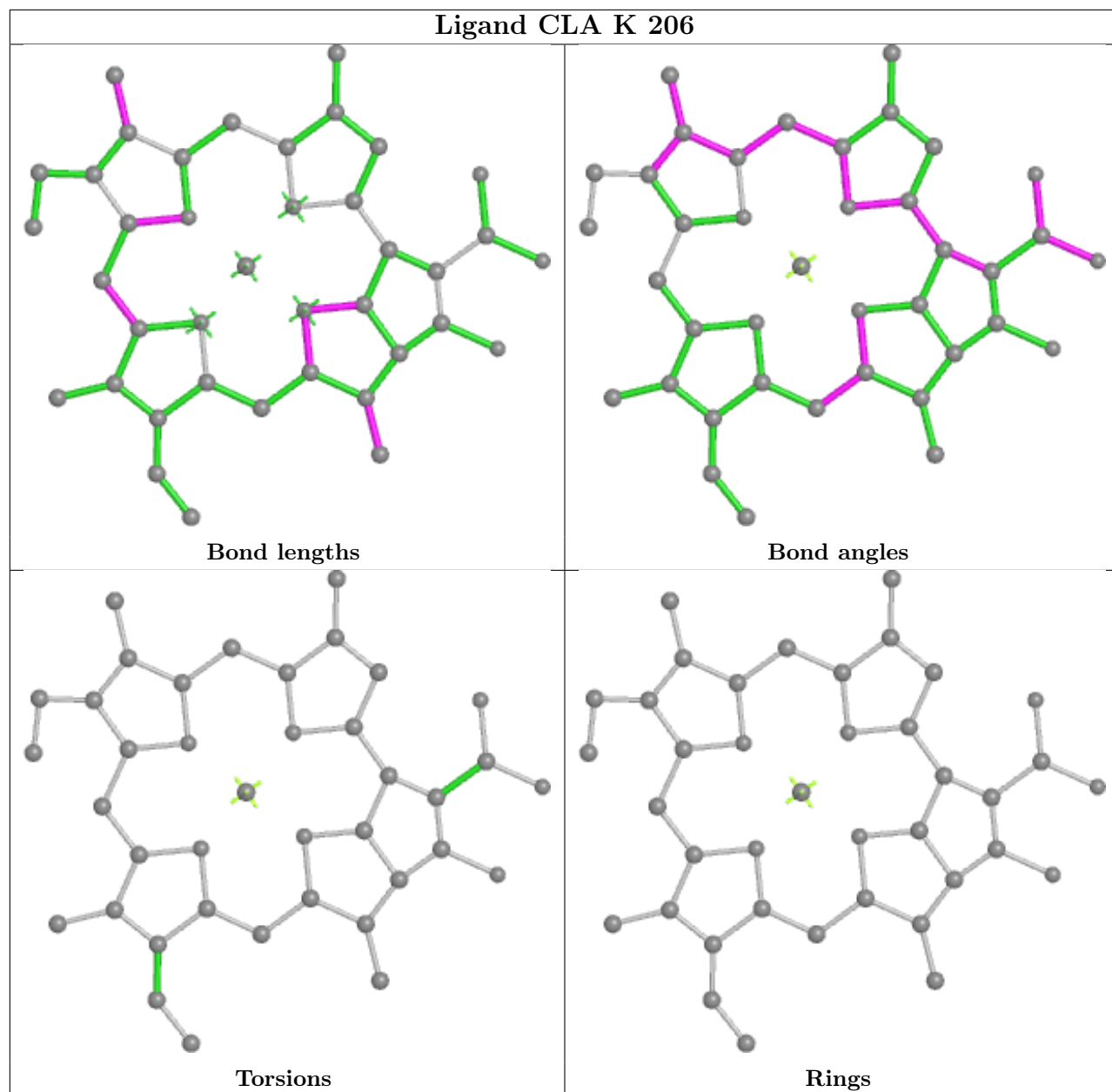


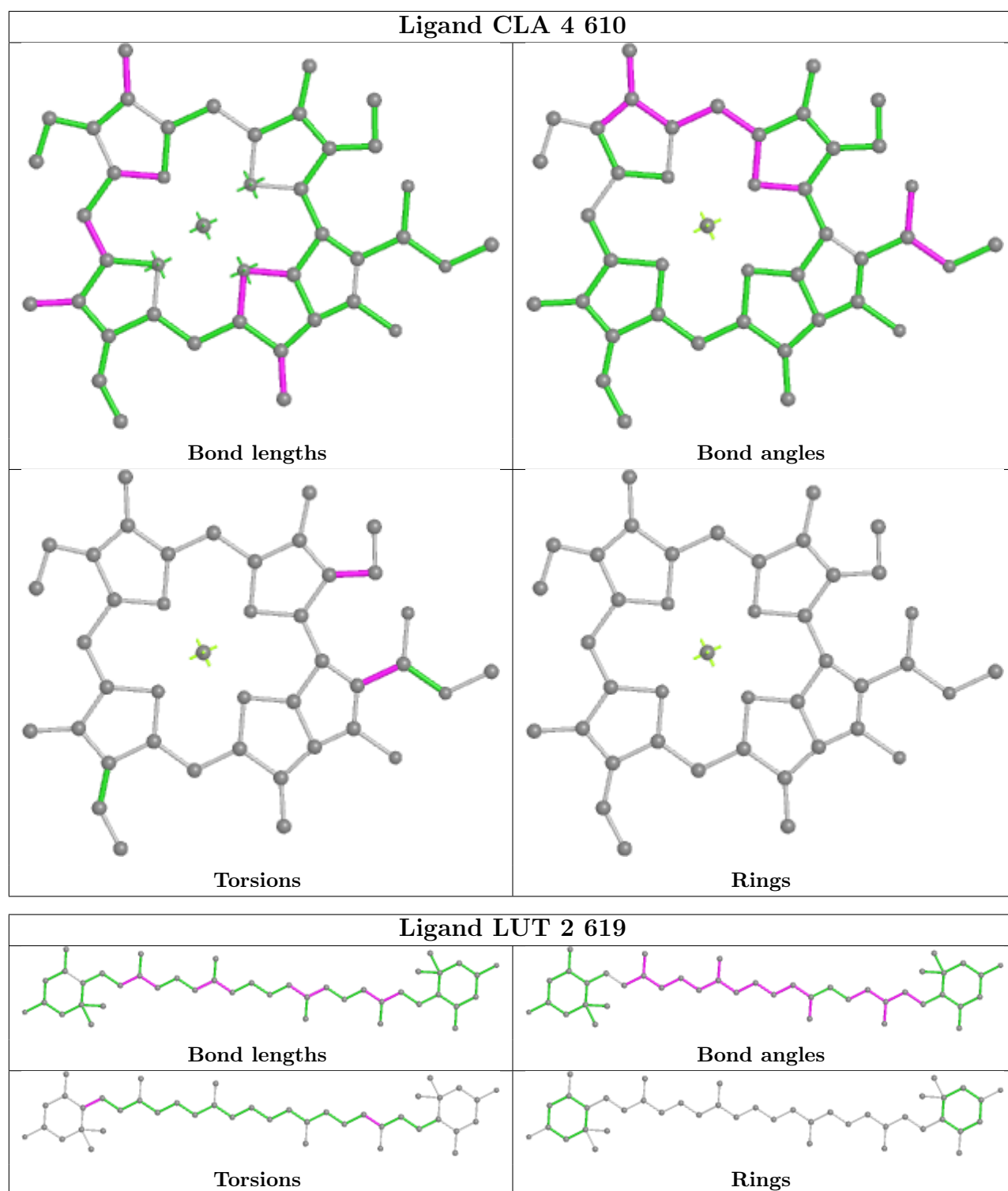


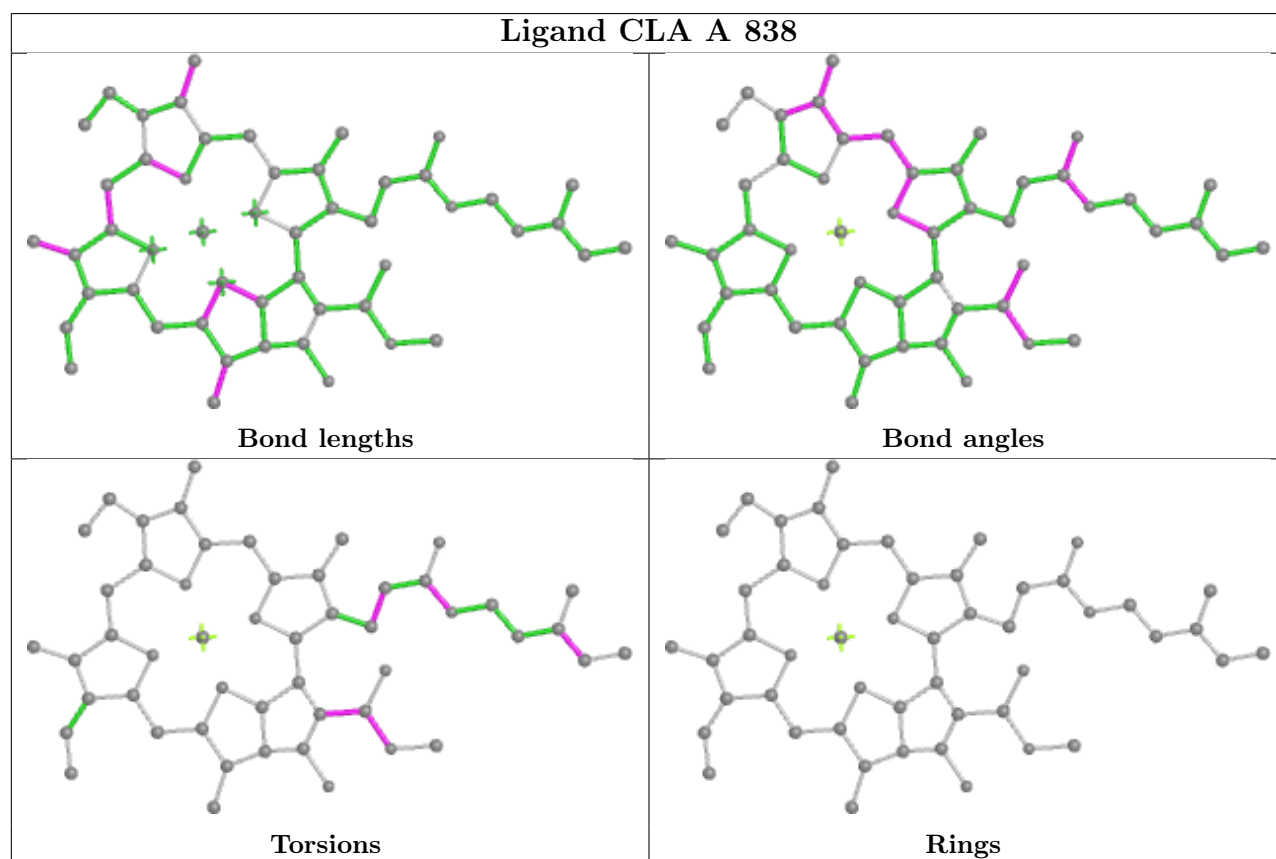
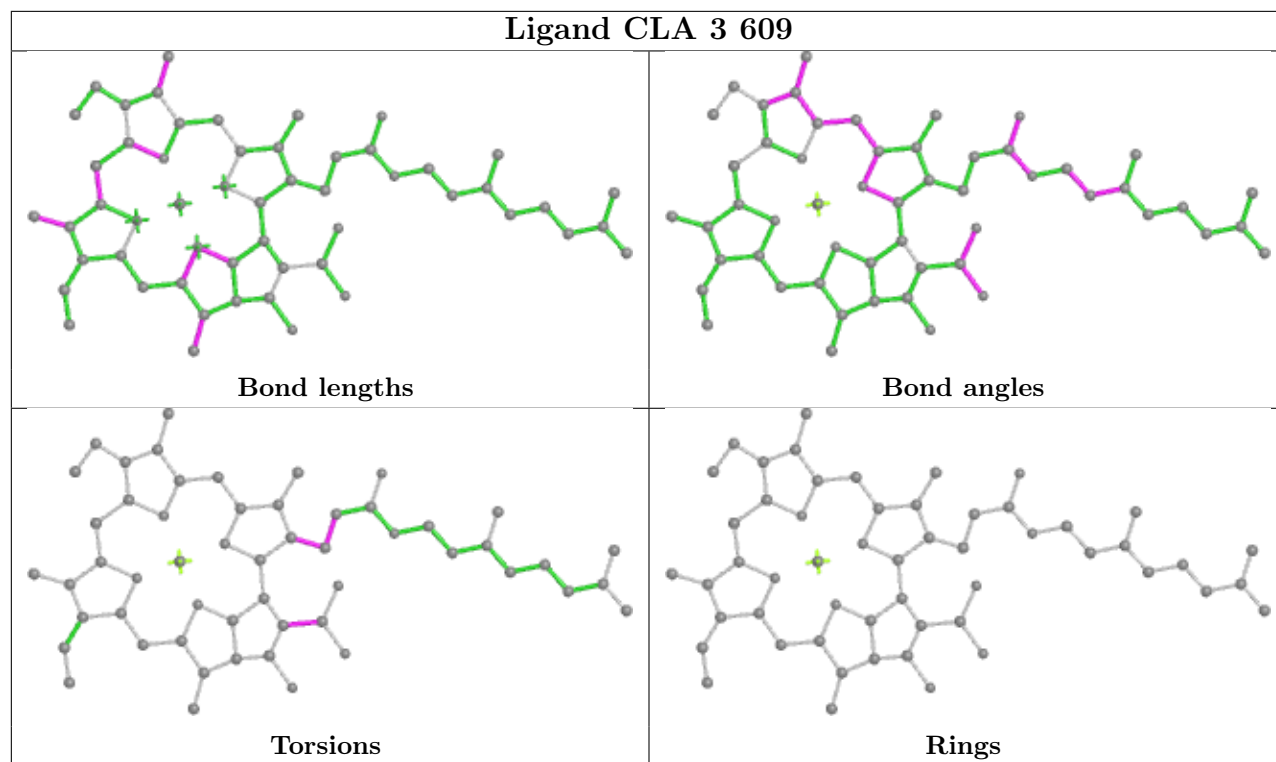


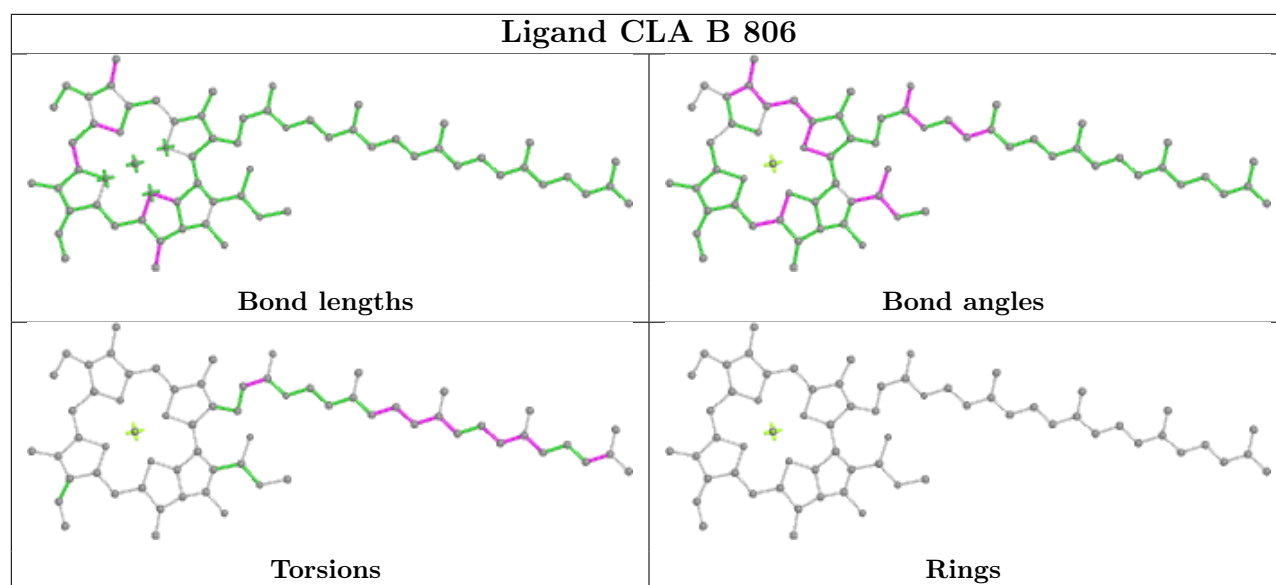












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

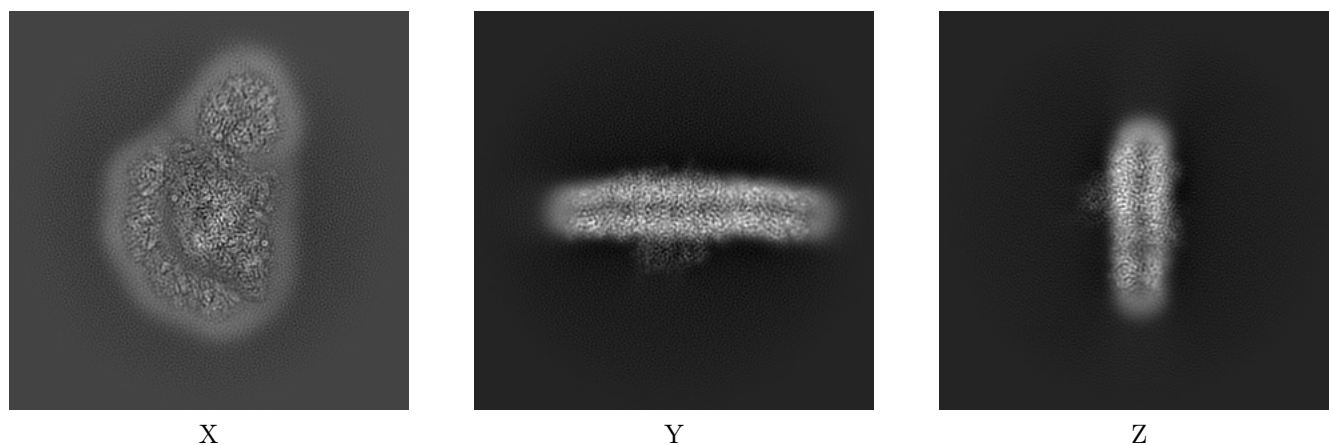
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36021. 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](#)

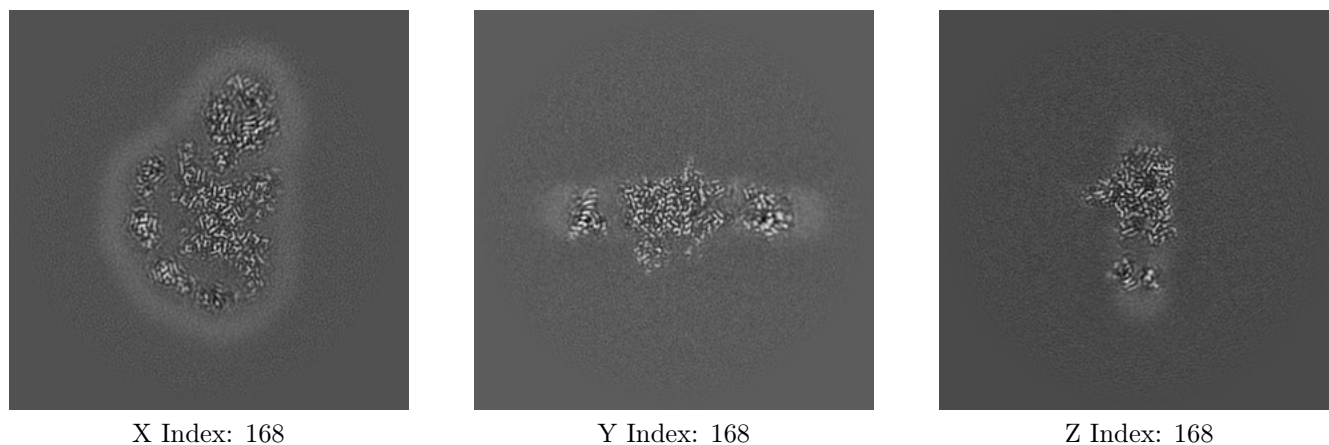
6.1.1 Primary map



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

6.2 Central slices [i](#)

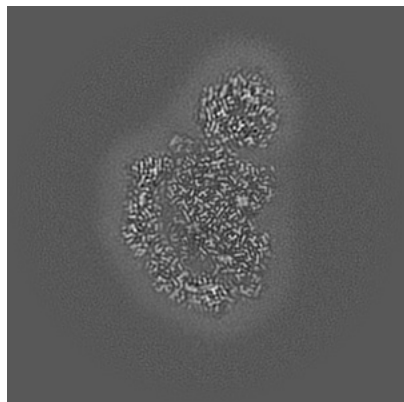
6.2.1 Primary map



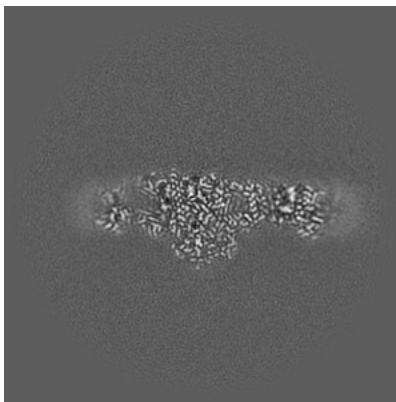
The images above show central slices of the map in three orthogonal directions.

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

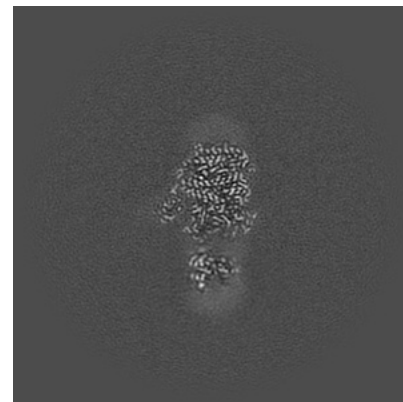
6.3.1 Primary map



X Index: 157



Y Index: 180

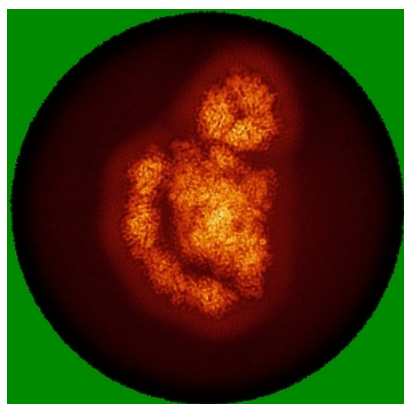


Z Index: 142

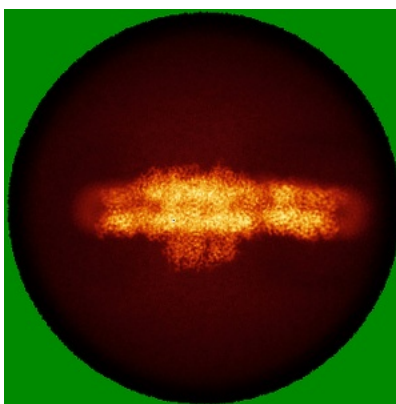
The images above show the largest variance slices of the map in three orthogonal directions.

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

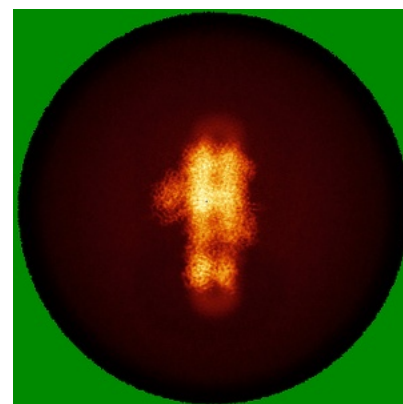
6.4.1 Primary map



X



Y

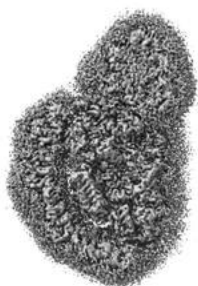


Z

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

6.5 Orthogonal surface views [i](#)

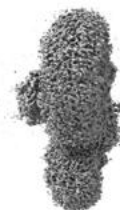
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.59. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

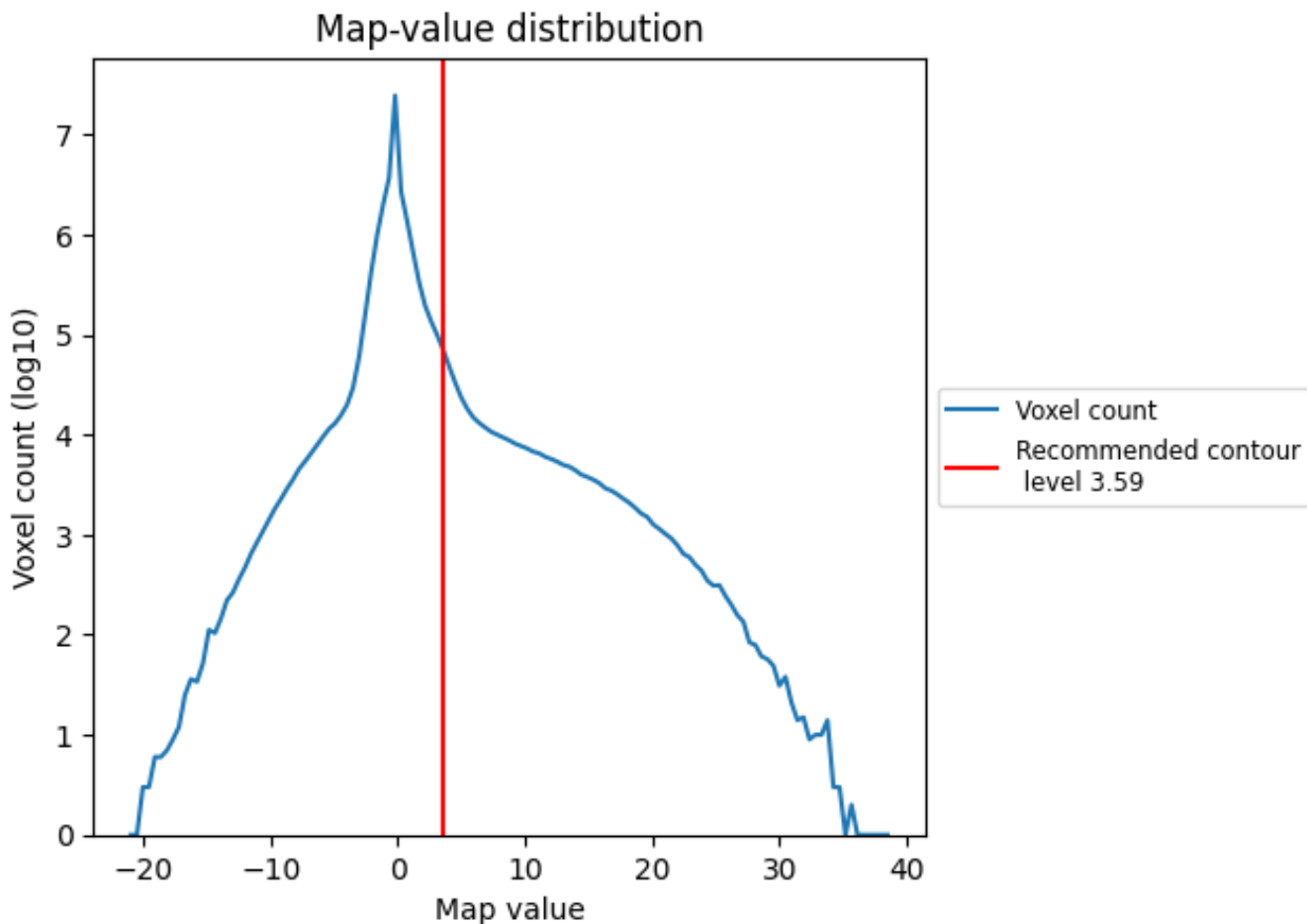
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

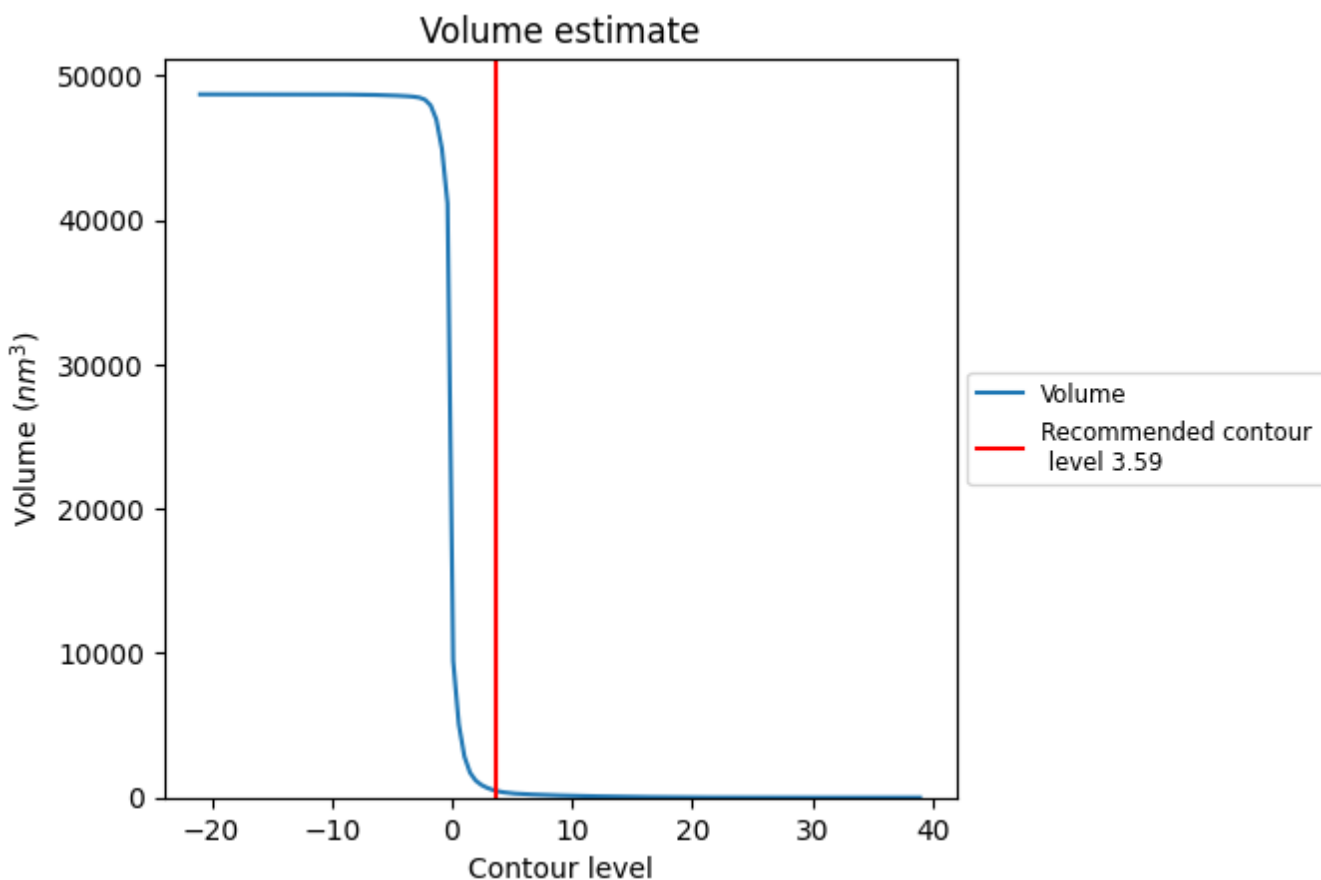
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

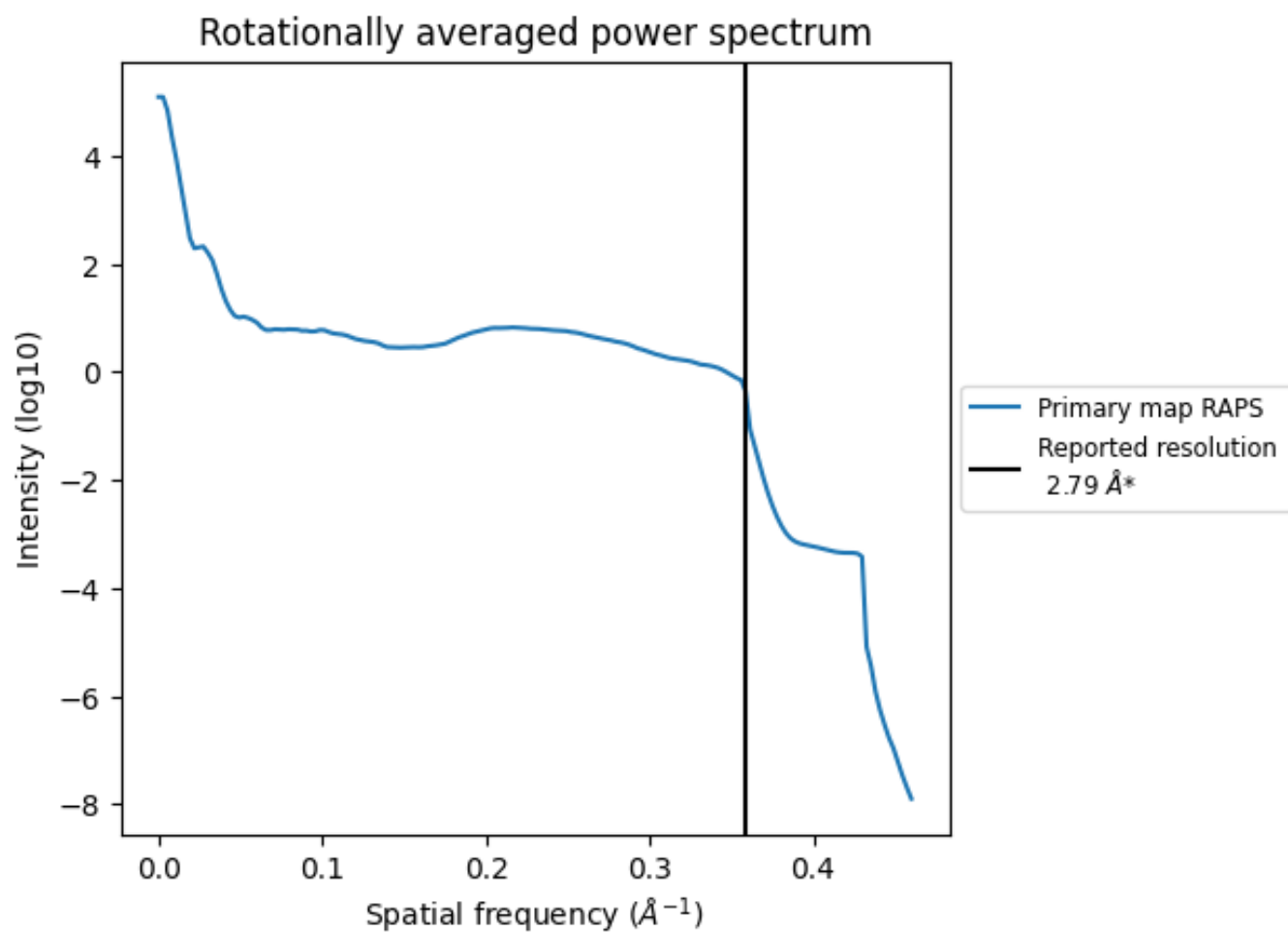
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 492 nm^3 ; this corresponds to an approximate mass of 444 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 0.358 Å⁻¹

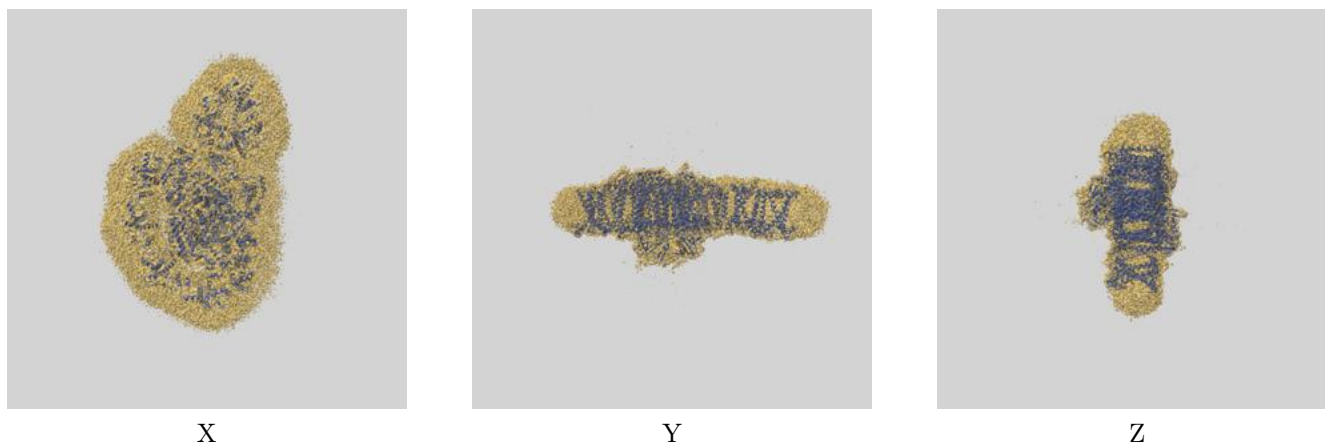
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

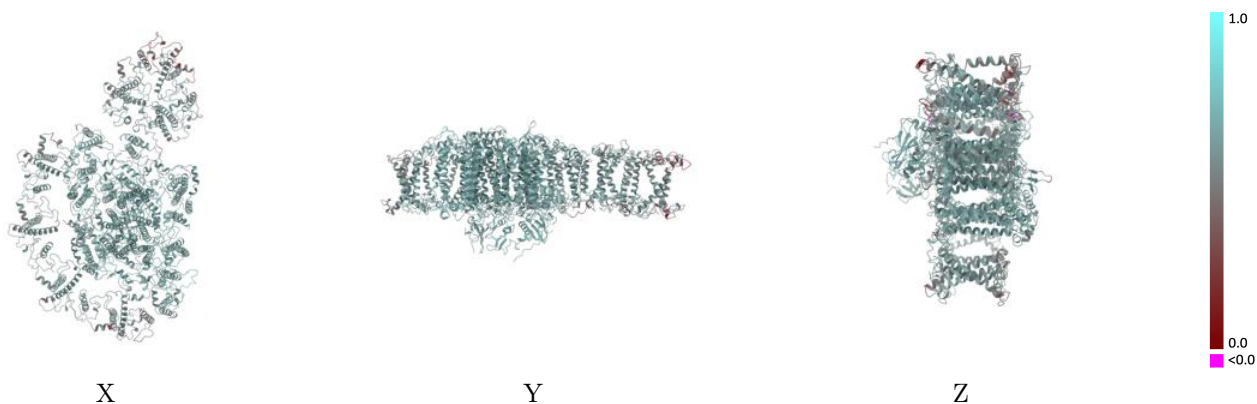
This section contains information regarding the fit between EMDB map EMD-36021 and PDB model 8J6Z. Per-residue inclusion information can be found in section 3 on page 31.

9.1 Map-model overlay [i](#)



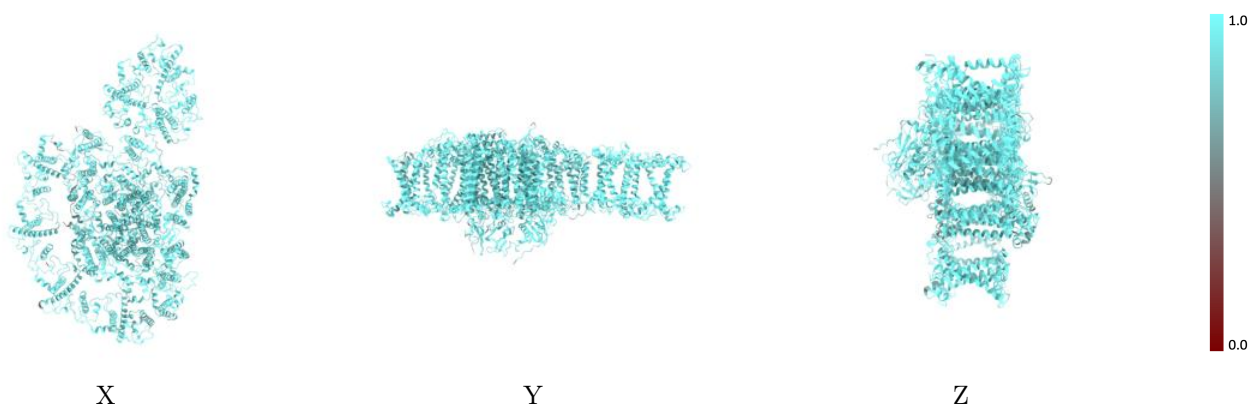
The images above show the 3D surface view of the map at the recommended contour level 3.59 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



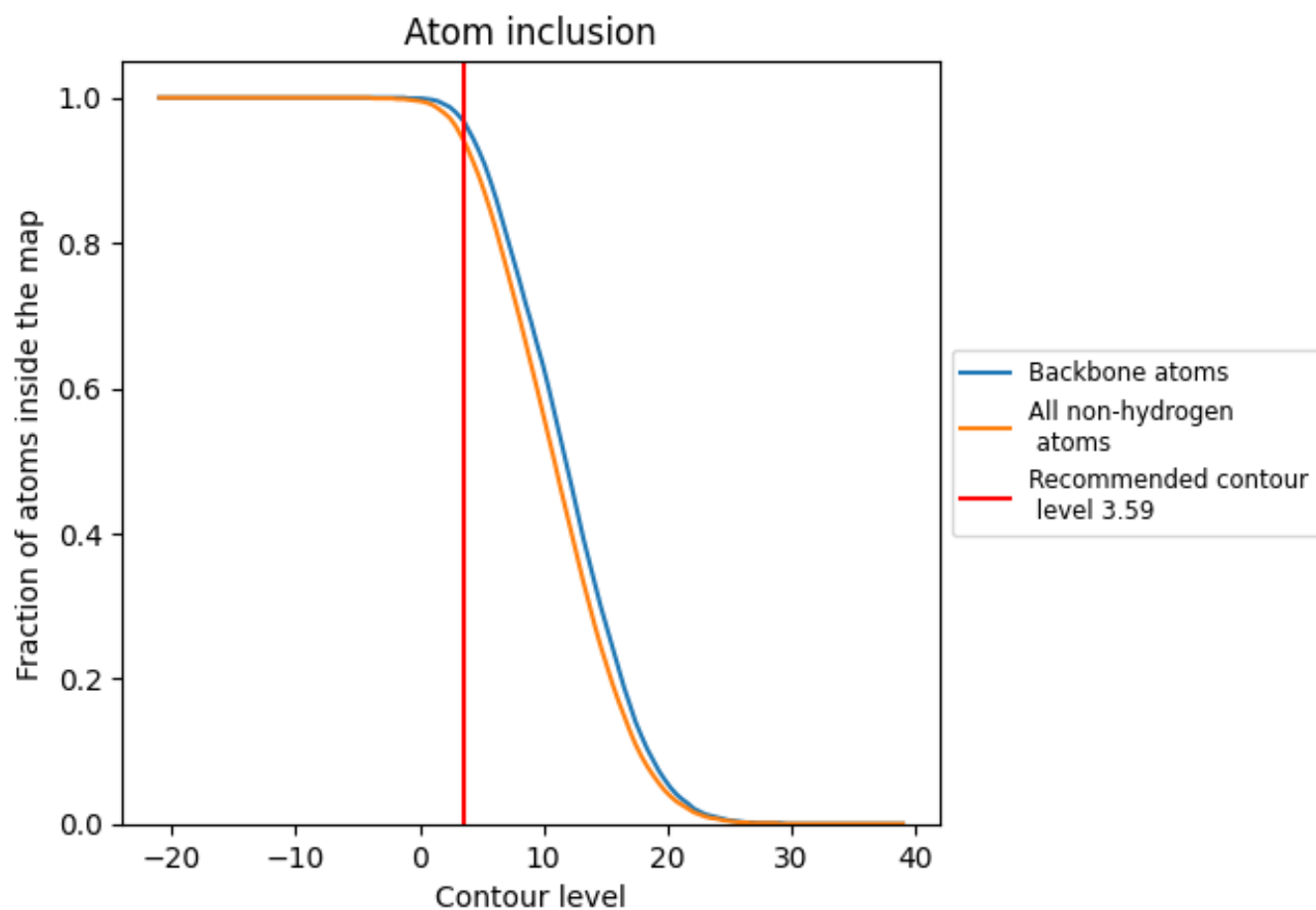
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.59).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 94% 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 (3.59) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9400	 0.5870
1	 0.9140	 0.5120
2	 0.9470	 0.5510
3	 0.9300	 0.5400
4	 0.9350	 0.5600
A	 0.9480	 0.6270
B	 0.9600	 0.6330
C	 0.9790	 0.6360
D	 0.9550	 0.6250
E	 0.9480	 0.6200
F	 0.8810	 0.5920
G	 0.9060	 0.5880
H	 0.9160	 0.5880
I	 0.9680	 0.6200
J	 0.7920	 0.5530
K	 0.8900	 0.5620
L	 0.9590	 0.6250
O	 0.9570	 0.5820
x	 0.9460	 0.5470
y	 0.9200	 0.4890
z	 0.9480	 0.5580

