



wwPDB EM Validation Summary Report ⓘ

Oct 12, 2024 – 09:47 pm BST

PDB ID : 6ZZX
EMDB ID : EMD-11588
Title : Structure of low-light grown *Chlorella ohadii* Photosystem I
Authors : Caspy, I.; Nelson, N.; Nechushtai, R.; Neumann, E.; Shkolnisky, Y.
Deposited on : 2020-08-05
Resolution : 2.70 Å (reported)
Based on initial model : 6IJO

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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

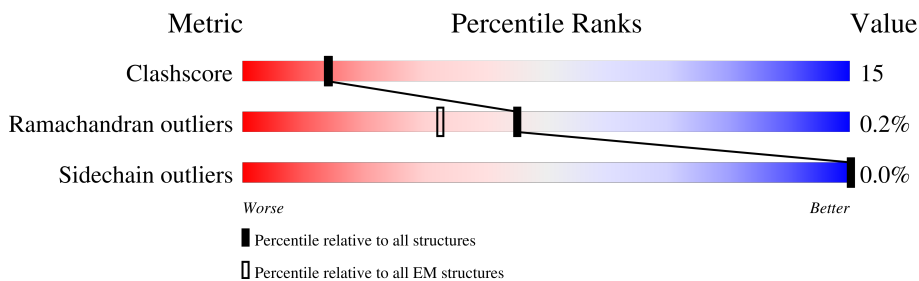
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	741	
2	B	731	
3	C	80	
4	D	143	
5	E	64	
6	F	165	
7	G	99	
8	H	94	

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Mol	Chain	Length	Quality of chain
9	J	41	
10	K	86	
11	L	157	
12	M	31	
13	I	35	
14	O	87	
15	1	192	
15	a	192	
16	3	241	
17	4	207	
18	5	229	
19	6	231	
20	7	221	
21	8	219	
22	2	215	
23	9	183	

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
24	CL0	A	1011	X	-	-	-
25	CLA	1	601	X	-	-	-
25	CLA	1	602	X	-	-	-
25	CLA	1	603	X	-	-	-
25	CLA	1	605	X	-	-	-
25	CLA	1	606	X	-	-	-
25	CLA	1	607	X	-	-	-
25	CLA	1	608	X	-	-	-
25	CLA	1	612	X	-	-	-
25	CLA	1	615	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	2	601	X	-	-	-
25	CLA	2	602	X	-	-	-
25	CLA	2	603	X	-	-	-
25	CLA	2	604	X	-	-	-
25	CLA	2	605	X	-	-	-
25	CLA	2	606	X	-	-	-
25	CLA	2	607	X	-	-	-
25	CLA	2	608	X	-	-	-
25	CLA	2	612	X	-	-	-
25	CLA	2	615	X	-	-	-
25	CLA	2	621	X	-	-	-
25	CLA	3	601	X	-	-	-
25	CLA	3	602	X	-	-	-
25	CLA	3	605	X	-	-	-
25	CLA	3	606	X	-	-	-
25	CLA	3	607	X	-	-	-
25	CLA	3	610	X	-	-	-
25	CLA	3	612	X	-	-	-
25	CLA	3	613	X	-	-	-
25	CLA	3	616	X	-	-	-
25	CLA	3	618	X	-	-	-
25	CLA	4	601	X	-	-	-
25	CLA	4	602	X	-	-	-
25	CLA	4	603	X	-	-	-
25	CLA	4	604	X	-	-	-
25	CLA	4	605	X	-	-	-
25	CLA	4	606	X	-	-	-
25	CLA	4	607	X	-	-	-
25	CLA	4	608	X	-	-	-
25	CLA	4	610	X	-	-	-
25	CLA	4	611	X	-	-	-
25	CLA	4	612	X	-	-	-
25	CLA	4	615	X	-	-	-
25	CLA	4	616	X	-	-	-
25	CLA	4	617	X	-	-	-
25	CLA	5	601	X	-	-	-
25	CLA	5	602	X	-	-	-
25	CLA	5	603	X	-	-	-
25	CLA	5	604	X	-	-	-
25	CLA	5	605	X	-	-	-
25	CLA	5	606	X	-	-	-
25	CLA	5	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	5	608	X	-	-	-
25	CLA	5	609	X	-	-	-
25	CLA	5	612	X	-	-	-
25	CLA	5	614	X	-	-	-
25	CLA	5	615	X	-	-	-
25	CLA	6	601	X	-	-	-
25	CLA	6	602	X	-	-	-
25	CLA	6	603	X	-	-	-
25	CLA	6	604	X	-	-	-
25	CLA	6	605	X	-	-	-
25	CLA	6	606	X	-	-	-
25	CLA	6	607	X	-	-	-
25	CLA	6	608	X	-	-	-
25	CLA	6	612	X	-	-	-
25	CLA	6	615	X	-	-	-
25	CLA	6	618	X	-	-	-
25	CLA	7	601	X	-	-	-
25	CLA	7	602	X	-	-	-
25	CLA	7	603	X	-	-	-
25	CLA	7	604	X	-	-	-
25	CLA	7	605	X	-	-	-
25	CLA	7	606	X	-	-	-
25	CLA	7	607	X	-	-	-
25	CLA	7	608	X	-	-	-
25	CLA	7	610	X	-	-	-
25	CLA	7	612	X	-	-	-
25	CLA	8	602	X	-	-	-
25	CLA	8	605	X	-	-	-
25	CLA	8	606	X	-	-	-
25	CLA	8	607	X	-	-	-
25	CLA	8	608	X	-	-	-
25	CLA	8	609	X	-	-	-
25	CLA	8	611	X	-	-	-
25	CLA	8	612	X	-	-	-
25	CLA	8	615	X	-	-	-
25	CLA	8	618	X	-	-	-
25	CLA	8	620	X	-	-	-
25	CLA	9	602	X	-	-	-
25	CLA	9	604	X	-	-	-
25	CLA	9	605	X	-	-	-
25	CLA	9	606	X	-	-	-
25	CLA	9	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	9	609	X	-	-	-
25	CLA	9	612	X	-	-	-
25	CLA	A	1012	X	-	-	-
25	CLA	A	1013	X	-	-	-
25	CLA	A	1101	X	-	-	-
25	CLA	A	1102	X	-	-	-
25	CLA	A	1103	X	-	-	-
25	CLA	A	1104	X	-	-	-
25	CLA	A	1105	X	-	-	-
25	CLA	A	1106	X	-	-	-
25	CLA	A	1107	X	-	-	-
25	CLA	A	1108	X	-	-	-
25	CLA	A	1109	X	-	-	-
25	CLA	A	1110	X	-	-	-
25	CLA	A	1111	X	-	-	-
25	CLA	A	1112	X	-	-	-
25	CLA	A	1113	X	-	-	-
25	CLA	A	1115	X	-	-	-
25	CLA	A	1116	X	-	-	-
25	CLA	A	1117	X	-	-	-
25	CLA	A	1118	X	-	-	-
25	CLA	A	1119	X	-	-	-
25	CLA	A	1120	X	-	-	-
25	CLA	A	1121	X	-	-	-
25	CLA	A	1122	X	-	-	-
25	CLA	A	1123	X	-	-	-
25	CLA	A	1124	X	-	-	-
25	CLA	A	1125	X	-	-	-
25	CLA	A	1126	X	-	-	-
25	CLA	A	1127	X	-	-	-
25	CLA	A	1128	X	-	-	-
25	CLA	A	1129	X	-	-	-
25	CLA	A	1130	X	-	-	-
25	CLA	A	1131	X	-	-	-
25	CLA	A	1132	X	-	-	-
25	CLA	A	1133	X	-	-	-
25	CLA	A	1134	X	-	-	-
25	CLA	A	1135	X	-	-	-
25	CLA	A	1136	X	-	-	-
25	CLA	A	1137	X	-	-	-
25	CLA	A	1138	X	-	-	-
25	CLA	A	1139	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	A	1140	X	-	-	-
25	CLA	A	1141	X	-	-	-
25	CLA	B	1021	X	-	-	-
25	CLA	B	1022	X	-	-	-
25	CLA	B	1023	X	-	-	-
25	CLA	B	1201	X	-	-	-
25	CLA	B	1202	X	-	-	-
25	CLA	B	1203	X	-	-	-
25	CLA	B	1204	X	-	-	-
25	CLA	B	1205	X	-	-	-
25	CLA	B	1206	X	-	-	-
25	CLA	B	1207	X	-	-	-
25	CLA	B	1208	X	-	-	-
25	CLA	B	1209	X	-	-	-
25	CLA	B	1210	X	-	-	-
25	CLA	B	1211	X	-	-	-
25	CLA	B	1212	X	-	-	-
25	CLA	B	1213	X	-	-	-
25	CLA	B	1214	X	-	-	-
25	CLA	B	1215	X	-	-	-
25	CLA	B	1216	X	-	-	-
25	CLA	B	1217	X	-	-	-
25	CLA	B	1218	X	-	-	-
25	CLA	B	1219	X	-	-	-
25	CLA	B	1220	X	-	-	-
25	CLA	B	1221	X	-	-	-
25	CLA	B	1222	X	-	-	-
25	CLA	B	1223	X	-	-	-
25	CLA	B	1224	X	-	-	-
25	CLA	B	1225	X	-	-	-
25	CLA	B	1226	X	-	-	-
25	CLA	B	1227	X	-	-	-
25	CLA	B	1228	X	-	-	-
25	CLA	B	1229	X	-	-	-
25	CLA	B	1230	X	-	-	-
25	CLA	B	1231	X	-	-	-
25	CLA	B	1232	X	-	-	-
25	CLA	B	1235	X	-	-	-
25	CLA	B	1236	X	-	-	-
25	CLA	B	1237	X	-	-	-
25	CLA	B	1238	X	-	-	-
25	CLA	B	1239	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	1240	X	-	-	-
25	CLA	F	1301	X	-	-	-
25	CLA	F	1302	X	-	-	-
25	CLA	G	1601	X	-	-	-
25	CLA	G	1602	X	-	-	-
25	CLA	G	1603	X	-	-	-
25	CLA	H	1701	X	-	-	-
25	CLA	H	1702	X	-	-	-
25	CLA	H	1703	X	-	-	-
25	CLA	J	1901	X	-	-	-
25	CLA	K	1401	X	-	-	-
25	CLA	K	1402	X	-	-	-
25	CLA	K	1403	X	-	-	-
25	CLA	K	1404	X	-	-	-
25	CLA	L	1501	X	-	-	-
25	CLA	L	1502	X	-	-	-
25	CLA	L	1503	X	-	-	-
25	CLA	L	1504	X	-	-	-
25	CLA	O	1801	X	-	-	-
25	CLA	O	1802	X	-	-	-
25	CLA	O	1803	X	-	-	-
25	CLA	a	601	X	-	-	-
25	CLA	a	602	X	-	-	-
25	CLA	a	603	X	-	-	-
25	CLA	a	605	X	-	-	-
25	CLA	a	607	X	-	-	-
25	CLA	a	608	X	-	-	-
25	CLA	a	611	X	-	-	-
25	CLA	a	612	X	-	-	-
25	CLA	a	615	X	-	-	-
26	CHL	1	604	X	-	-	-
26	CHL	1	609	X	-	-	-
26	CHL	1	610	X	-	-	-
26	CHL	1	611	X	-	-	-
26	CHL	1	613	X	-	-	-
26	CHL	2	609	X	-	-	-
26	CHL	2	610	X	-	-	-
26	CHL	2	613	X	-	-	-
26	CHL	3	603	X	-	-	-
26	CHL	3	604	X	-	-	-
26	CHL	3	608	X	-	-	-
26	CHL	3	611	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CHL	4	609	X	-	-	-
26	CHL	4	613	X	-	-	-
26	CHL	4	618	X	-	-	-
26	CHL	5	610	X	-	-	-
26	CHL	5	611	X	-	-	-
26	CHL	5	613	X	-	-	-
26	CHL	5	617	X	-	-	-
26	CHL	5	618	X	-	-	-
26	CHL	6	609	X	-	-	-
26	CHL	6	610	X	-	-	-
26	CHL	6	611	X	-	-	-
26	CHL	6	613	X	-	-	-
26	CHL	6	617	X	-	-	-
26	CHL	6	619	X	-	-	-
26	CHL	7	609	X	-	-	-
26	CHL	7	611	X	-	-	-
26	CHL	7	613	X	-	-	-
26	CHL	7	615	X	-	-	-
26	CHL	7	617	X	-	-	-
26	CHL	8	601	X	-	-	-
26	CHL	8	603	X	-	-	-
26	CHL	8	604	X	-	-	-
26	CHL	8	610	X	-	-	-
26	CHL	8	613	X	-	-	-
26	CHL	9	601	X	-	-	-
26	CHL	9	603	X	-	-	-
26	CHL	9	608	X	-	-	-
26	CHL	9	610	X	-	-	-
26	CHL	9	613	X	-	-	-
26	CHL	A	1114	X	-	-	-
26	CHL	a	604	X	-	-	-
26	CHL	a	606	X	-	-	-
26	CHL	a	609	X	-	-	-
26	CHL	a	610	X	-	-	-
26	CHL	a	613	X	-	-	-
39	NEX	F	4001	X	-	-	-
40	RRX	3	506	X	-	-	-
40	RRX	J	4002	X	-	-	-
43	LUT	2	507	X	-	-	-
43	LUT	4	501	X	-	-	-
43	LUT	7	501	X	-	-	-
46	QTB	a	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
50	XAT	2	501	X	-	-	-
50	XAT	7	502	X	-	-	-
50	XAT	9	504	X	-	-	-
50	XAT	9	507	X	-	-	-

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 56369 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	741	5824	3815	988	1001	20	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	368	ALA	SER	conflict	UNP W8SY74
A	437	ILE	MET	conflict	UNP W8SY74

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	731	5796	3807	980	994	15	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	THR	deletion	UNP W8SUA3
B	5	LEU	-	insertion	UNP W8SUA3
B	241	ALA	VAL	conflict	UNP W8SUA3
B	402	ALA	GLU	conflict	UNP W8SUA3
B	403	GLN	ALA	conflict	UNP W8SUA3

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	80	601	367	104	119	11	0	0

- Molecule 4 is a protein called Photosystem I reaction center subunit chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	143	1124	716	196	208	4	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	188	ALA	VAL	conflict	UNP A0A2P6TKF8
D	320	ILE	VAL	conflict	UNP A0A2P6TKF8

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	64	509	323	91	95	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	44	GLN	THR	conflict	UNP A0A2P6U4S6
E	48	LEU	MET	conflict	UNP A0A2P6U4S6
E	96	VAL	GLU	conflict	UNP A0A2P6U4S6
E	97	ALA	GLU	conflict	UNP A0A2P6U4S6
E	98	ALA	VAL	conflict	UNP A0A2P6U4S6

- Molecule 6 is a protein called PSI-F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	165	1277	830	216	228	3	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	346	LEU	MET	conflict	UNP A0A2P6TPV8
F	348	ASN	LYS	conflict	UNP A0A2P6TPV8
F	351	ALA	GLU	conflict	UNP A0A2P6TPV8
F	352	ASP	GLY	conflict	UNP A0A2P6TPV8
F	360	LYS	GLN	conflict	UNP A0A2P6TPV8
F	364	ALA	ASP	conflict	UNP A0A2P6TPV8
F	367	GLU	ASN	conflict	UNP A0A2P6TPV8
F	430	ALA	SER	conflict	UNP A0A2P6TPV8
F	431	ALA	SER	conflict	UNP A0A2P6TPV8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	432	THR	MET	conflict	UNP A0A2P6TPV8
F	433	ALA	THR	conflict	UNP A0A2P6TPV8

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	99	Total	C	N	O	S	0	0
			727	466	127	130	4		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	1229	ALA	SER	conflict	UNP A0A2P6TZI8
G	1272	LEU	MET	conflict	UNP A0A2P6TZI8
G	1285	ILE	VAL	conflict	UNP A0A2P6TZI8
G	1313	ILE	LEU	conflict	UNP A0A2P6TZI8
G	1317	SER	HIS	conflict	UNP A0A2P6TZI8
G	1320	GLY	GLN	conflict	UNP A0A2P6TZI8
G	1321	LEU	VAL	conflict	UNP A0A2P6TZI8
G	1324	ASN	VAL	conflict	UNP A0A2P6TZI8

- Molecule 8 is a protein called Photosystem I reaction center subunit VI-chloroplastic-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	94	Total	C	N	O	S	0	0
			729	457	132	139	1		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	92	ILE	VAL	conflict	UNP A0A2P6TPU7
H	102	GLY	LEU	conflict	UNP A0A2P6TPU7
H	105	ALA	SER	conflict	UNP A0A2P6TPU7
H	106	ALA	SER	conflict	UNP A0A2P6TPU7
H	109	ARG	SER	conflict	UNP A0A2P6TPU7
H	?	-	ILE	deletion	UNP A0A2P6TPU7
H	113	VAL	LYS	conflict	UNP A0A2P6TPU7

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	41	Total	C	N	O	S	0	0
			316	212	46	57	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	86	Total	C	N	O	S	0	0
			613	390	106	115	2		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	74	ALA	GLU	conflict	UNP A0A2P6U0J1
K	103	LEU	ILE	conflict	UNP A0A2P6U0J1
K	105	CYS	VAL	conflict	UNP A0A2P6U0J1
K	107	ILE	VAL	conflict	UNP A0A2P6U0J1
K	108	VAL	ILE	conflict	UNP A0A2P6U0J1
K	112	LYS	ARG	conflict	UNP A0A2P6U0J1
K	113	SER	GLY	conflict	UNP A0A2P6U0J1

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	157	Total	C	N	O	S	0	0
			1165	758	192	211	4		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	350	TYR	PHE	conflict	UNP A0A2P6TC44
L	364	ASP	ASN	conflict	UNP A0A2P6TC44
L	?	-	ALA	deletion	UNP A0A2P6TC44
L	421	ASP	GLU	conflict	UNP A0A2P6TC44
L	443	LEU	ILE	conflict	UNP A0A2P6TC44

- Molecule 12 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	31	Total	C	N	O	S	0	0
			239	163	36	39	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	35	Total	C	N	O	S	0	0
			270	183	37	47	3		

- Molecule 14 is a protein called Photosystem I subunit O.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	87	Total	C	N	O	S	0	0
			679	453	109	115	2		

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1	192	Total	C	N	O	S	0	0
			1405	900	237	261	7		
15	a	192	Total	C	N	O	S	0	0
			1405	900	237	261	7		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	166	SER	LEU	conflict	UNP A0A2P6TT36
1	167	LYS	GLU	conflict	UNP A0A2P6TT36
1	171	THR	VAL	conflict	UNP A0A2P6TT36
1	194	THR	ASN	conflict	UNP A0A2P6TT36
1	196	ALA	GLN	conflict	UNP A0A2P6TT36
1	204	SER	ALA	conflict	UNP A0A2P6TT36
1	210	MET	LEU	conflict	UNP A0A2P6TT36
a	166	SER	LEU	conflict	UNP A0A2P6TT36
a	167	LYS	GLU	conflict	UNP A0A2P6TT36
a	171	THR	VAL	conflict	UNP A0A2P6TT36
a	194	THR	ASN	conflict	UNP A0A2P6TT36
a	196	ALA	GLN	conflict	UNP A0A2P6TT36
a	204	SER	ALA	conflict	UNP A0A2P6TT36
a	210	MET	LEU	conflict	UNP A0A2P6TT36

- Molecule 16 is a protein called Glutathione reductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	3	241	Total	C	N	O	S	0	0
			1844	1194	302	337	11		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	314	CYS	GLY	conflict	UNP A0A2P6TMT4
3	329	ILE	VAL	conflict	UNP A0A2P6TMT4
3	339	THR	SER	conflict	UNP A0A2P6TMT4
3	359	LYS	ASN	conflict	UNP A0A2P6TMT4
3	405	GLY	ALA	conflict	UNP A0A2P6TMT4
3	429	GLU	ALA	conflict	UNP A0A2P6TMT4
3	484	THR	ARG	conflict	UNP A0A2P6TMT4
3	485	ILE	ARG	conflict	UNP A0A2P6TMT4
3	486	LEU	ARG	conflict	UNP A0A2P6TMT4
3	487	LYS	ALA	conflict	UNP A0A2P6TMT4

- Molecule 17 is a protein called Lhca4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	4	207	1631	1056	277	294	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	5	229	1786	1146	310	317	13	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	32	LYS	ASP	conflict	UNP A0A2P6U4K1
5	38	VAL	ALA	conflict	UNP A0A2P6U4K1
5	40	ALA	SER	conflict	UNP A0A2P6U4K1
5	42	GLY	ALA	conflict	UNP A0A2P6U4K1
5	113	SER	GLY	conflict	UNP A0A2P6U4K1
5	127	ILE	LEU	conflict	UNP A0A2P6U4K1
5	195	VAL	ILE	conflict	UNP A0A2P6U4K1

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	6	231	1787	1168	295	314	10	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	83	CYS	ALA	conflict	UNP A0A2P6TPR7
6	94	LEU	MET	conflict	UNP A0A2P6TPR7
6	196	ILE	VAL	conflict	UNP A0A2P6TPR7
6	201	ALA	GLY	conflict	UNP A0A2P6TPR7
6	250	GLN	ASN	conflict	UNP A0A2P6TPR7

- Molecule 20 is a protein called Lhca7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	7	221	1698	1090	294	308	6	0	0

- Molecule 21 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	8	219	1669	1073	285	305	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
8	103	GLU	ASP	conflict	UNP A0A2P6TZ50

- Molecule 22 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	2	215	1666	1074	277	309	6	0	0

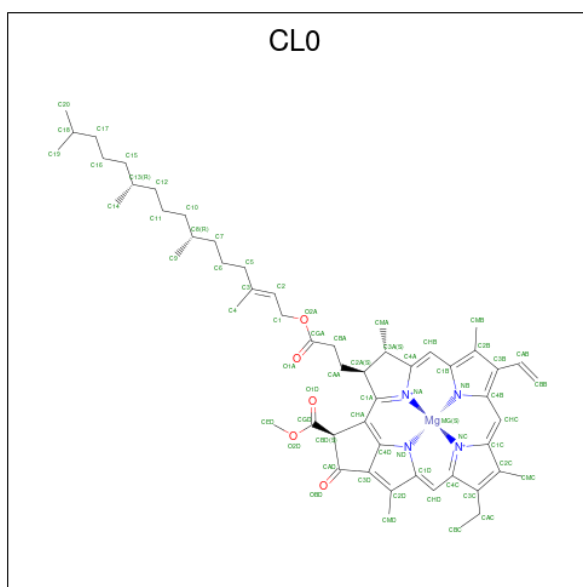
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	64	ASP	GLU	conflict	UNP A0A2P6TMX4
2	97	PRO	ASN	conflict	UNP A0A2P6TMX4

- Molecule 23 is a protein called Chlorophyll a-b binding protein, chloroplastic.

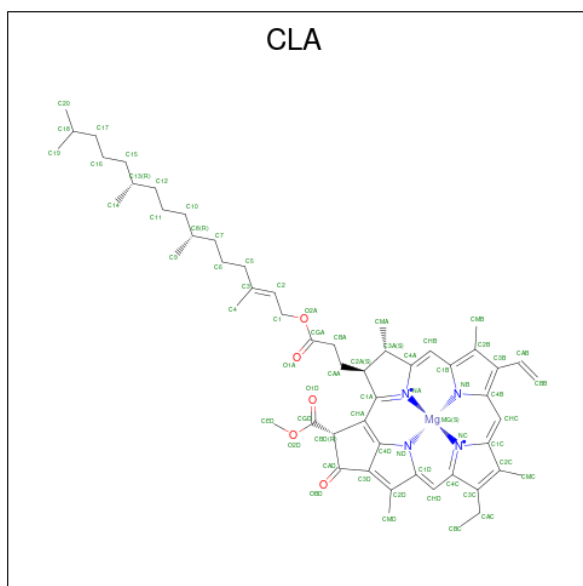
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	9	183	1406	909	237	254	6	0	0

- Molecule 24 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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

- Molecule 25 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	A	1	65	55	1	4	5	0
25	A	1	65	55	1	4	5	0
25	A	1	57	47	1	4	5	0
25	A	1	65	55	1	4	5	0
25	A	1	55	45	1	4	5	0
25	A	1	65	55	1	4	5	0
25	A	1	65	55	1	4	5	0
25	A	1	54	44	1	4	5	0
25	A	1	65	55	1	4	5	0
25	A	1	55	45	1	4	5	0
25	A	1	60	50	1	4	5	0
25	A	1	60	50	1	4	5	0
25	A	1	60	50	1	4	5	0
25	A	1	65	55	1	4	5	0
25	A	1	55	45	1	4	5	0
25	A	1	65	55	1	4	5	0
25	A	1	49	39	1	4	5	0
25	A	1	60	50	1	4	5	0
25	A	1	60	50	1	4	5	0
25	A	1	65	55	1	4	5	0
25	A	1	55	45	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	A	1	65	55	1	4	5	0
25	A	1	65	55	1	4	5	0
25	A	1	65	55	1	4	5	0
25	A	1	65	55	1	4	5	0
25	A	1	50	40	1	4	5	0
25	A	1	56	46	1	4	5	0
25	A	1	65	55	1	4	5	0
25	A	1	65	55	1	4	5	0
25	A	1	65	55	1	4	5	0
25	A	1	60	50	1	4	5	0
25	A	1	51	41	1	4	5	0
25	A	1	65	55	1	4	5	0
25	A	1	60	50	1	4	5	0
25	A	1	65	55	1	4	5	0
25	A	1	55	45	1	4	5	0
25	A	1	55	45	1	4	5	0
25	A	1	65	55	1	4	5	0
25	A	1	45	35	1	4	5	0
25	B	1	65	55	1	4	5	0
25	B	1	65	55	1	4	5	0
25	B	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	B	1	Total 57	C 47	Mg 1	N 4	O 5	0
25	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	B	1	Total	C	N	O		0
			64	55	4	5		
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	F	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	F	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	G	1	60	50	1	4	5	0
25	G	1	45	35	1	4	5	0
25	H	1	55	45	1	4	5	0
25	H	1	46	36	1	4	5	0
25	H	1	55	45	1	4	5	0
25	J	1	42	34	1	4	3	0
25	K	1	46	36	1	4	5	0
25	K	1	60	50	1	4	5	0
25	K	1	49	39	1	4	5	0
25	K	1	45	35	1	4	5	0
25	L	1	50	40	1	4	5	0
25	L	1	60	50	1	4	5	0
25	L	1	45	35	1	4	5	0
25	L	1	50	40	1	4	5	0
25	O	1	38	30	1	4	3	0
25	O	1	55	45	1	4	5	0
25	O	1	41	33	1	4	3	0
25	1	1	60	50	1	4	5	0
25	1	1	45	35	1	4	5	0
25	1	1	65	55	1	4	5	0
25	1	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	1	1	57	47	1	4	5	0
25	1	1	65	55	1	4	5	0
25	1	1	60	50	1	4	5	0
25	1	1	65	55	1	4	5	0
25	1	1	46	36	1	4	5	0
25	a	1	60	50	1	4	5	0
25	a	1	50	40	1	4	5	0
25	a	1	65	55	1	4	5	0
25	a	1	55	45	1	4	5	0
25	a	1	58	48	1	4	5	0
25	a	1	55	45	1	4	5	0
25	a	1	50	40	1	4	5	0
25	a	1	57	47	1	4	5	0
25	a	1	46	36	1	4	5	0
25	3	1	65	55	1	4	5	0
25	3	1	46	36	1	4	5	0
25	3	1	65	55	1	4	5	0
25	3	1	65	55	1	4	5	0
25	3	1	65	55	1	4	5	0
25	3	1	57	47	1	4	5	0
25	3	1	50	40	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	3	1	61	51	1	4	5	0
25	3	1	46	36	1	4	5	0
25	3	1	56	46	1	4	5	0
25	4	1	60	50	1	4	5	0
25	4	1	52	42	1	4	5	0
25	4	1	56	46	1	4	5	0
25	4	1	60	50	1	4	5	0
25	4	1	46	36	1	4	5	0
25	4	1	50	40	1	4	5	0
25	4	1	55	45	1	4	5	0
25	4	1	51	41	1	4	5	0
25	4	1	65	55	1	4	5	0
25	4	1	56	46	1	4	5	0
25	4	1	62	52	1	4	5	0
25	4	1	60	50	1	4	5	0
25	4	1	50	40	1	4	5	0
25	4	1	45	35	1	4	5	0
25	5	1	60	50	1	4	5	0
25	5	1	52	42	1	4	5	0
25	5	1	56	46	1	4	5	0
25	5	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	5	1	46	36	1	4	5	0
25	5	1	50	40	1	4	5	0
25	5	1	60	50	1	4	5	0
25	5	1	45	35	1	4	5	0
25	5	1	51	41	1	4	5	0
25	5	1	65	55	1	4	5	0
25	5	1	46	36	1	4	5	0
25	5	1	46	36	1	4	5	0
25	6	1	55	45	1	4	5	0
25	6	1	60	50	1	4	5	0
25	6	1	52	42	1	4	5	0
25	6	1	65	55	1	4	5	0
25	6	1	65	55	1	4	5	0
25	6	1	46	36	1	4	5	0
25	6	1	65	55	1	4	5	0
25	6	1	55	45	1	4	5	0
25	6	1	50	40	1	4	5	0
25	6	1	65	55	1	4	5	0
25	6	1	46	36	1	4	5	0
25	7	1	60	50	1	4	5	0
25	7	1	44	34	1	4	5	0

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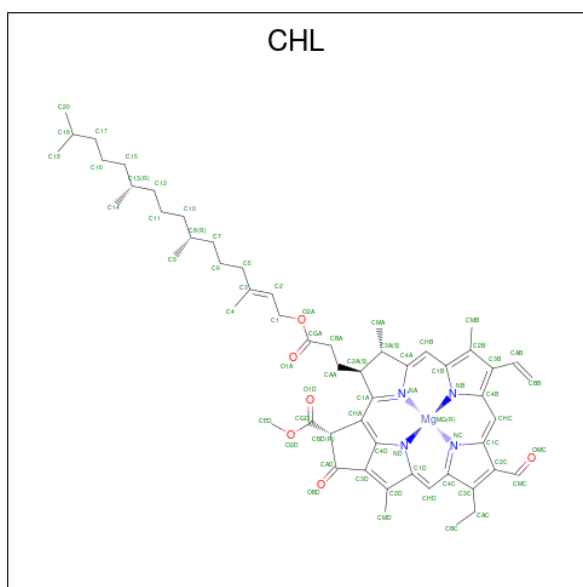
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	7	1	Total 44	C 34	Mg 1	N 4	O 5	0
25	7	1	Total 54	C 44	Mg 1	N 4	O 5	0
25	7	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	8	1	Total 52	C 42	Mg 1	N 4	O 5	0
25	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	8	1	Total 57	C 47	Mg 1	N 4	O 5	0
25	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	8	1	Total 52	C 42	Mg 1	N 4	O 5	0
25	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	2	1	Total 52	C 42	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	2	1	60	50	1	4	5	0
25	2	1	56	46	1	4	5	0
25	2	1	60	50	1	4	5	0
25	2	1	46	36	1	4	5	0
25	2	1	65	55	1	4	5	0
25	2	1	45	35	1	4	5	0
25	2	1	50	40	1	4	5	0
25	2	1	56	46	1	4	5	0
25	2	1	65	55	1	4	5	0
25	9	1	46	36	1	4	5	0
25	9	1	60	50	1	4	5	0
25	9	1	60	50	1	4	5	0
25	9	1	55	45	1	4	5	0
25	9	1	47	37	1	4	5	0
25	9	1	46	36	1	4	5	0
25	9	1	65	55	1	4	5	0

- Molecule 26 is CHLOROPHYLL B (three-letter code: CHL) (formula: C₅₅H₇₀MgN₄O₆).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Mg	N		O
26	A	1	66	55	1	4	6	0
26	1	1	66	55	1	4	6	0
26	1	1	48	37	1	4	6	0
26	1	1	56	45	1	4	6	0
26	1	1	48	37	1	4	6	0
26	1	1	66	55	1	4	6	0
26	a	1	61	50	1	4	6	0
26	a	1	56	45	1	4	6	0
26	a	1	53	42	1	4	6	0
26	a	1	48	37	1	4	6	0
26	a	1	46	35	1	4	6	0
26	3	1	66	55	1	4	6	0
26	3	1	66	55	1	4	6	0
26	3	1	43	34	1	4	4	0

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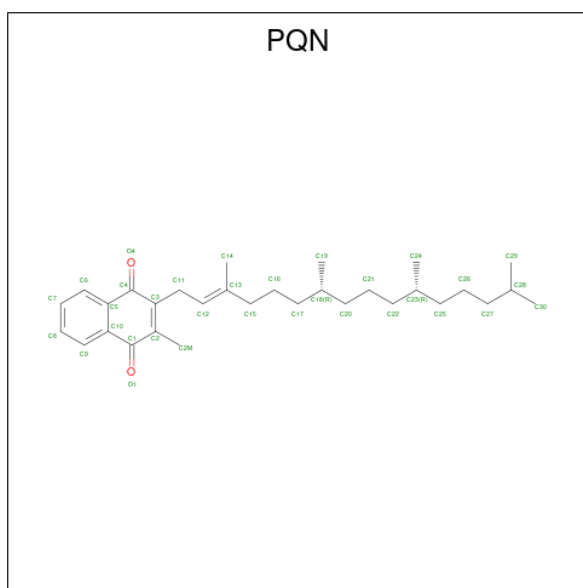
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	3	1	61	50	1	4	6	0
26	4	1	52	41	1	4	6	0
26	4	1	56	45	1	4	6	0
26	4	1	66	55	1	4	6	0
26	5	1	66	55	1	4	6	0
26	5	1	51	40	1	4	6	0
26	5	1	56	45	1	4	6	0
26	5	1	47	36	1	4	6	0
26	5	1	51	40	1	4	6	0
26	6	1	66	55	1	4	6	0
26	6	1	56	45	1	4	6	0
26	6	1	51	40	1	4	6	0
26	6	1	51	40	1	4	6	0
26	6	1	43	34	1	4	4	0
26	6	1	66	55	1	4	6	0
26	7	1	62	51	1	4	6	0
26	7	1	56	45	1	4	6	0
26	7	1	61	50	1	4	6	0
26	7	1	51	40	1	4	6	0
26	7	1	66	55	1	4	6	0
26	8	1	61	50	1	4	6	0

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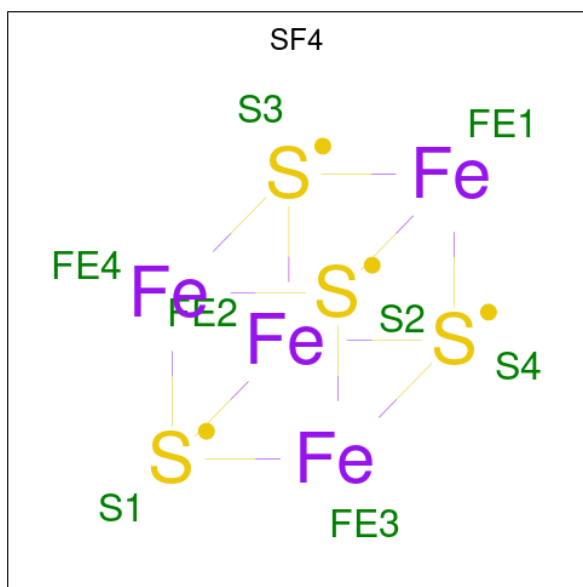
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	8	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
26	8	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
26	8	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
26	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	2	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
26	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
26	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	9	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
26	9	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
26	9	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

- Molecule 27 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



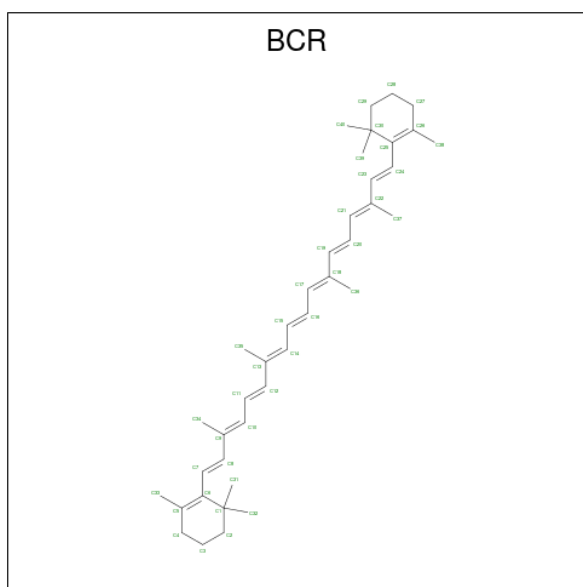
Mol	Chain	Residues	Atoms			AltConf
27	A	1	Total	C	O	0
			33	31	2	
27	B	1	Total	C	O	0
			33	31	2	

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



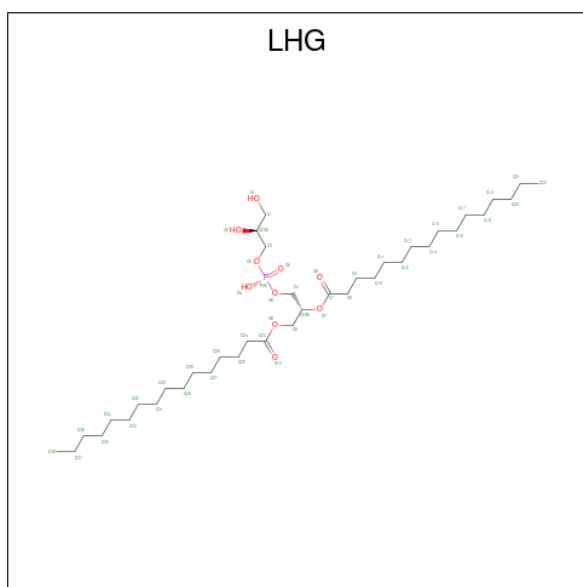
Mol	Chain	Residues	Atoms	AltConf
29	A	1	Total C 40 40	0
29	A	1	Total C 40 40	0
29	A	1	Total C 40 40	0
29	A	1	Total C 40 40	0
29	A	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	G	1	Total C 40 40	0
29	H	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
29	J	1	Total C 40 40	0
29	K	1	Total C 40 40	0
29	K	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	I	1	Total C 40 40	0
29	O	1	Total C 40 40	0
29	3	1	Total C 40 40	0
29	3	1	Total C 40 40	0
29	3	1	Total C 40 40	0
29	4	1	Total C 40 40	0
29	5	1	Total C 40 40	0
29	5	1	Total C 40 40	0
29	6	1	Total C 40 40	0
29	6	1	Total C 40 40	0
29	7	1	Total C 40 40	0
29	8	1	Total C 40 40	0

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



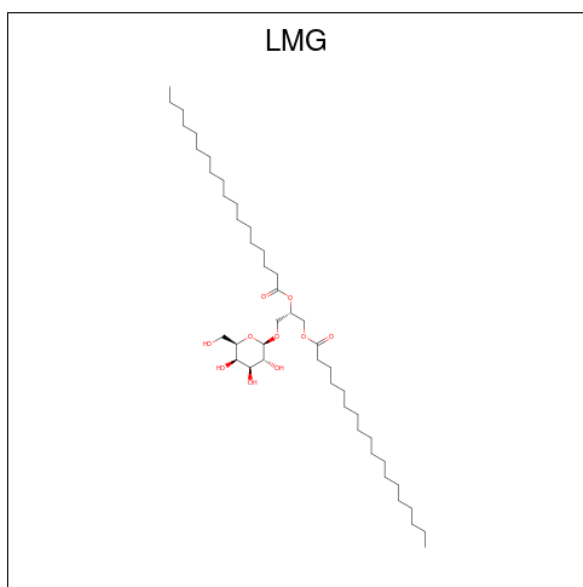
Mol	Chain	Residues	Atoms			AltConf	
			Total	C	O		P
30	A	1	49	38	10	1	0
30	A	1	49	38	10	1	0
30	A	1	46	35	10	1	0
30	B	1	49	38	10	1	0
30	B	1	49	38	10	1	0
30	F	1	36	25	10	1	0
30	F	1	43	32	10	1	0
30	1	1	35	24	10	1	0
30	1	1	49	38	10	1	0
30	a	1	35	24	10	1	0
30	3	1	49	38	10	1	0
30	4	1	32	21	10	1	0
30	4	1	49	38	10	1	0
30	5	1	49	38	10	1	0

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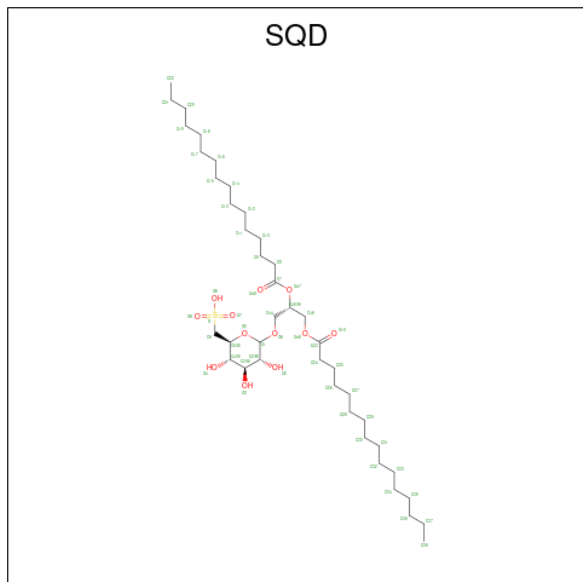
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
30	6	1	Total 37	C 26	O 10	P 1	0
30	6	1	Total 49	C 38	O 10	P 1	0
30	7	1	Total 37	C 26	O 10	P 1	0
30	7	1	Total 36	C 25	O 10	P 1	0
30	7	1	Total 35	C 24	O 10	P 1	0
30	8	1	Total 37	C 26	O 10	P 1	0
30	2	1	Total 49	C 38	O 10	P 1	0
30	2	1	Total 49	C 38	O 10	P 1	0
30	9	1	Total 49	C 38	O 10	P 1	0
30	9	1	Total 33	C 22	O 10	P 1	0

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



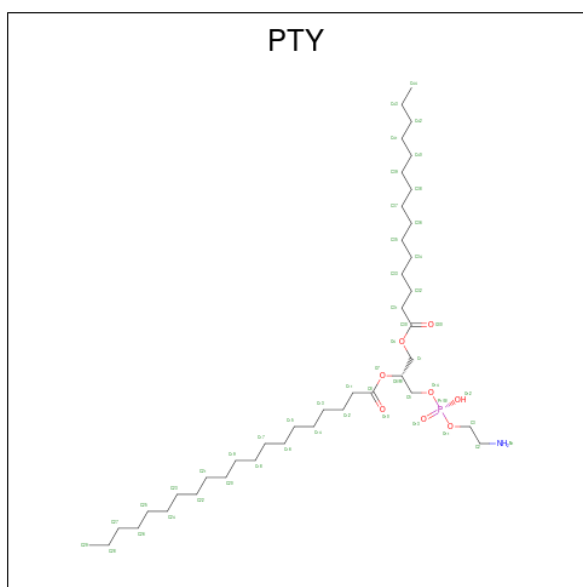
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
31	A	1	Total 42	C 32	O 10	0

- Molecule 32 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



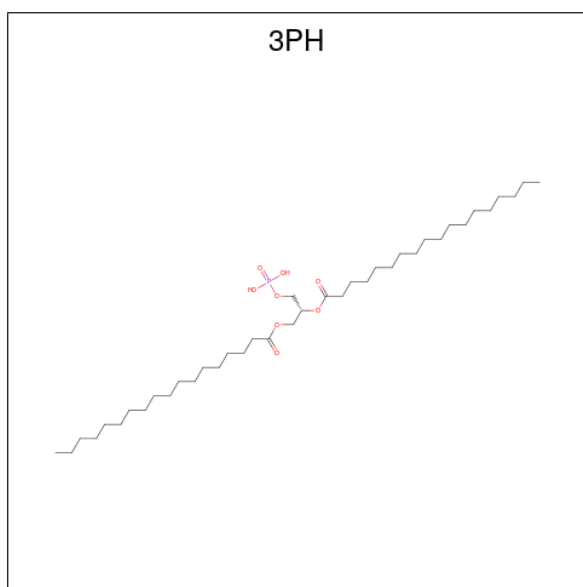
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
32	A	1	54	41	12	1	0
32	G	1	46	33	12	1	0
32	H	1	45	32	12	1	0
32	I	1	54	41	12	1	0
32	7	1	39	26	12	1	0

- Molecule 33 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



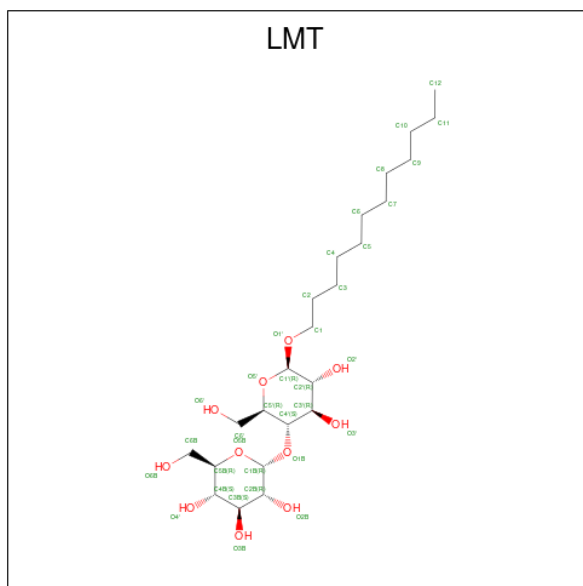
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
33	A	1	Total 34	C 24	N 1	O 8	P 1	0
33	B	1	Total 42	C 32	N 1	O 8	P 1	0
33	G	1	Total 28	C 18	N 1	O 8	P 1	0
33	G	1	Total 28	C 18	N 1	O 8	P 1	0
33	J	1	Total 28	C 18	N 1	O 8	P 1	0
33	a	1	Total 38	C 28	N 1	O 8	P 1	0
33	a	1	Total 38	C 28	N 1	O 8	P 1	0
33	3	1	Total 38	C 28	N 1	O 8	P 1	0
33	5	1	Total 38	C 28	N 1	O 8	P 1	0
33	7	1	Total 33	C 23	N 1	O 8	P 1	0
33	9	1	Total 48	C 38	N 1	O 8	P 1	0

- Molecule 34 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: C₃₉H₇₇O₈P).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
34	A	1	33	24	8	1	0

- Molecule 35 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



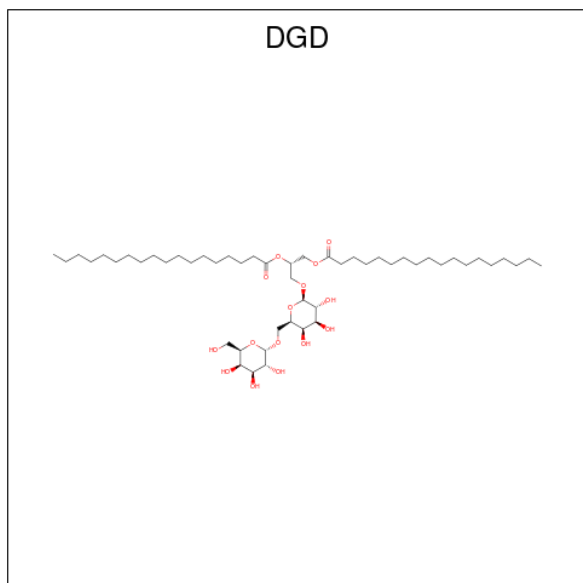
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	A	1	35	24	11	0
35	B	1	35	24	11	0

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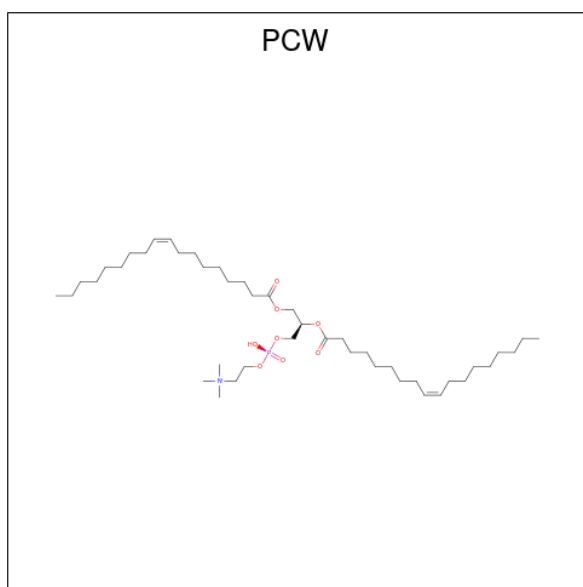
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	1	1	35	24	11	0
35	2	1	35	24	11	0

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



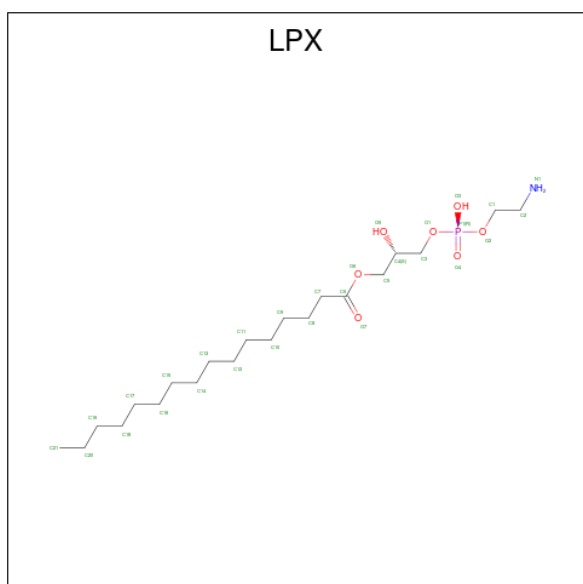
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
36	B	1	66	51	15	0
36	7	1	50	35	15	0
36	8	1	59	44	15	0
36	8	1	46	31	15	0

- Molecule 37 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).



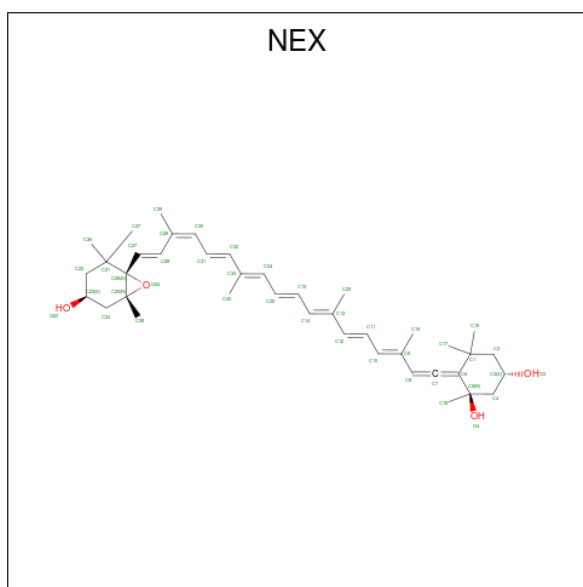
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
37	B	1	39	29	1	8	1	0
37	K	1	36	26	1	8	1	0
37	K	1	41	31	1	8	1	0
37	6	1	36	26	1	8	1	0

- Molecule 38 is (2S)-3-[[[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy]-2-hydroxypropyl hexadecanoate (three-letter code: LPX) (formula: C₂₁H₄₄NO₇P).



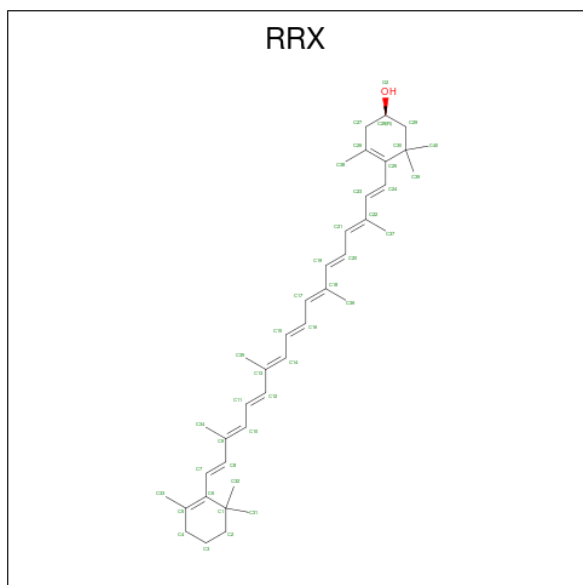
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
38	F	1	30	21	1	7	1	0

- Molecule 39 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: C₄₀H₅₆O₄).



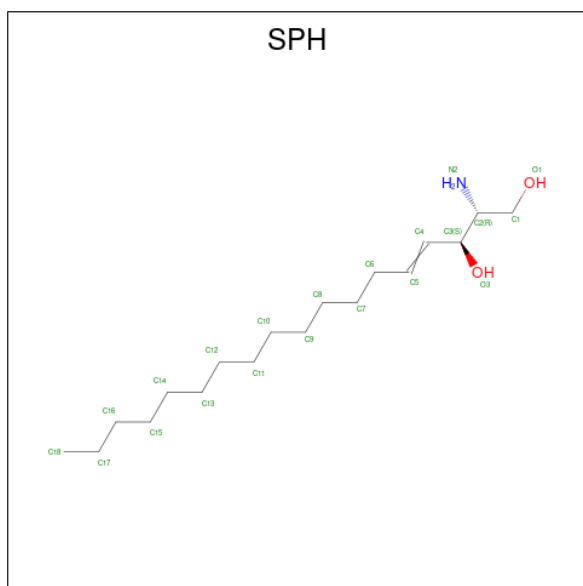
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
39	F	1	44	40	4	0

- Molecule 40 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: C₄₀H₅₆O).



Mol	Chain	Residues	Atoms			AltConf
40	J	1	Total	C	O	0
			41	40	1	
40	3	1	Total	C	O	0
			41	40	1	

- Molecule 41 is SPHINGOSINE (three-letter code: SPH) (formula: $C_{18}H_{37}NO_2$).



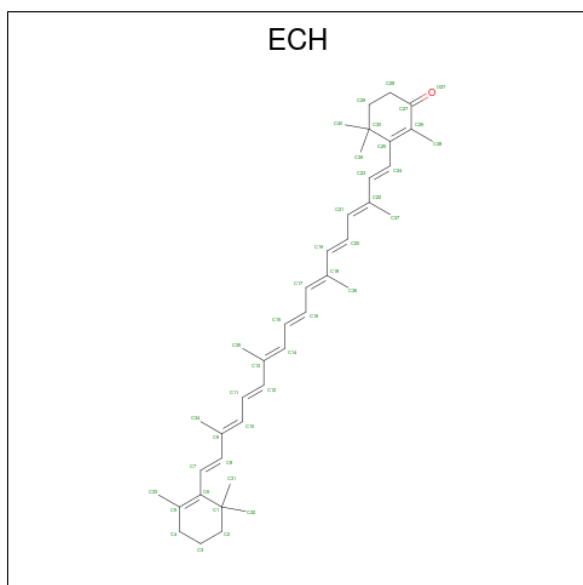
Mol	Chain	Residues	Atoms				AltConf
41	J	1	Total	C	N	O	0
			21	18	1	2	
41	4	1	Total	C	N	O	0
			21	18	1	2	

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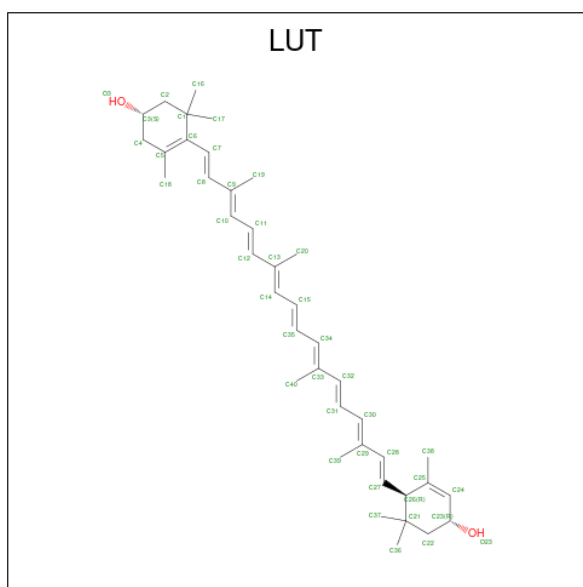
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
41	6	1	21	18	1	2	0
41	9	1	21	18	1	2	0

- Molecule 42 is beta,beta-caroten-4-one (three-letter code: ECH) (formula: C₄₀H₅₄O).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
42	M	1	41	40	1	0

- Molecule 43 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



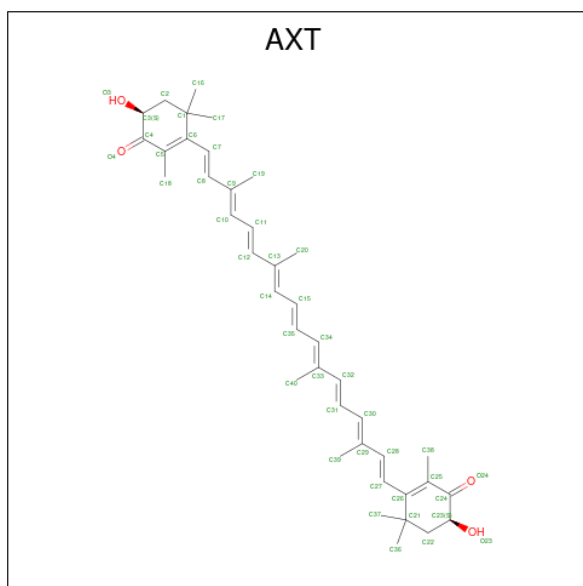
Mol	Chain	Residues	Atoms			AltConf
43	1	1	Total	C	O	0
			42	40	2	
43	1	1	Total	C	O	0
			42	40	2	
43	a	1	Total	C	O	0
			42	40	2	
43	a	1	Total	C	O	0
			42	40	2	
43	a	1	Total	C	O	0
			42	40	2	
43	3	1	Total	C	O	0
			42	40	2	
43	3	1	Total	C	O	0
			42	40	2	
43	4	1	Total	C	O	0
			42	40	2	
43	4	1	Total	C	O	0
			42	40	2	
43	5	1	Total	C	O	0
			42	40	2	
43	5	1	Total	C	O	0
			42	40	2	
43	5	1	Total	C	O	0
			42	40	2	
43	6	1	Total	C	O	0
			42	40	2	
43	6	1	Total	C	O	0
			42	40	2	

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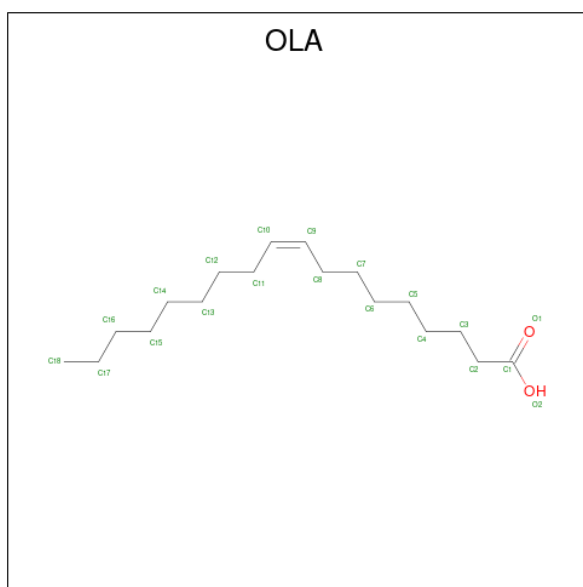
Mol	Chain	Residues	Atoms			AltConf
43	7	1	Total	C	O	0
			42	40	2	
43	8	1	Total	C	O	0
			42	40	2	
43	8	1	Total	C	O	0
			42	40	2	
43	2	1	Total	C	O	0
			42	40	2	
43	2	1	Total	C	O	0
			42	40	2	
43	9	1	Total	C	O	0
			42	40	2	
43	9	1	Total	C	O	0
			42	40	2	

- Molecule 44 is ASTAXANTHIN (three-letter code: AXT) (formula: $C_{40}H_{52}O_4$).



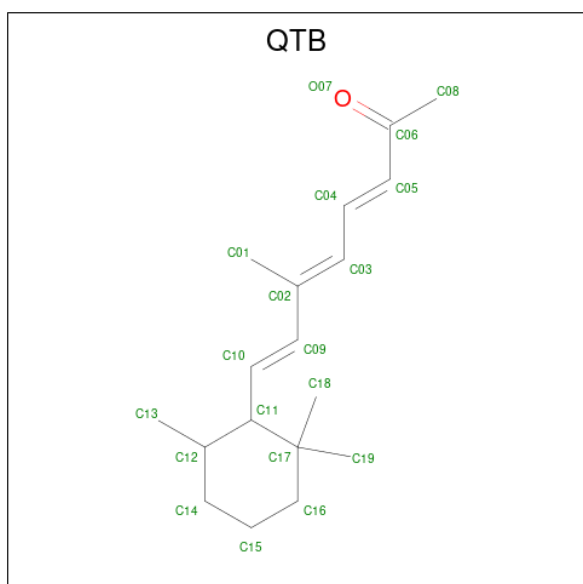
Mol	Chain	Residues	Atoms			AltConf
44	1	1	Total	C	O	0
			43	40	3	
44	7	1	Total	C	O	0
			43	40	3	

- Molecule 45 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



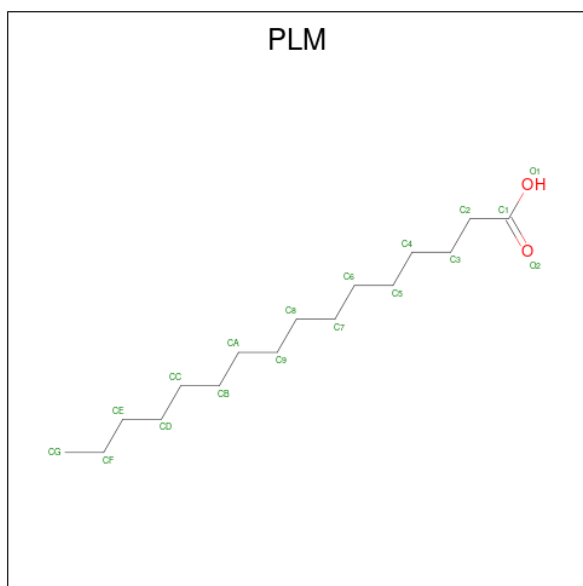
Mol	Chain	Residues	Atoms		AltConf
45	1	1	Total	C O	0
			20	18 2	
45	a	1	Total	C O	0
			20	18 2	
45	8	1	Total	C O	0
			20	18 2	
45	8	1	Total	C O	0
			20	18 2	

- Molecule 46 is (3 {E},5 {E},7 {E})-6-methyl-8-[(6 {R})-2,2,6-trimethylcyclohexyl]octa-3,5,7-trien-2-one (three-letter code: QTB) (formula: C₁₈H₂₈O).



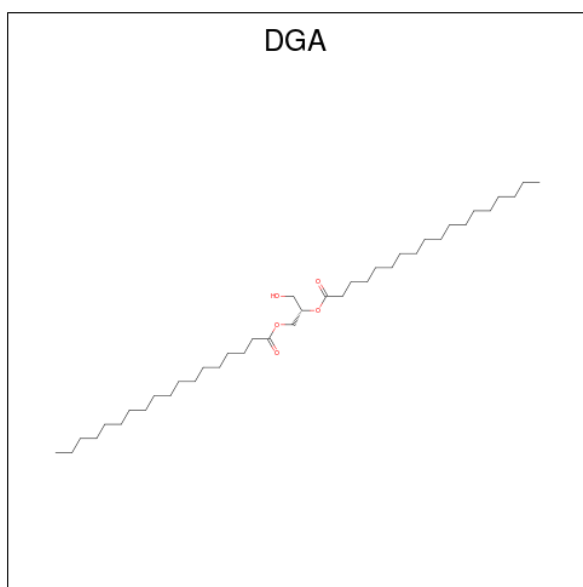
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
46	a	1	19	18	1	0

- Molecule 47 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



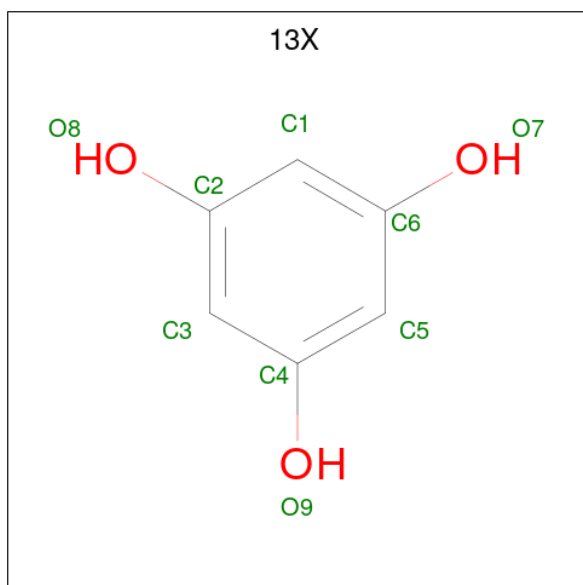
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
47	a	1	17	16	1	0
47	4	1	18	16	2	0
47	4	1	17	16	1	0
47	5	1	18	16	2	0
47	6	1	18	16	2	0
47	8	1	17	16	1	0
47	8	1	18	16	2	0

- Molecule 48 is DIACYL GLYCEROL (three-letter code: DGA) (formula: $C_{39}H_{76}O_5$).



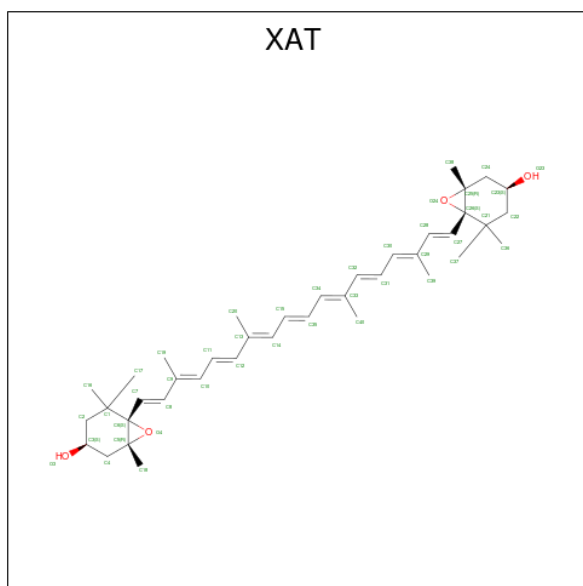
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
48	3	1	24	19	5	0
48	5	1	23	18	5	0
48	8	1	40	35	5	0
48	2	1	37	32	5	0

- Molecule 49 is benzene-1,3,5-triol (three-letter code: 13X) (formula: C₆H₆O₃).



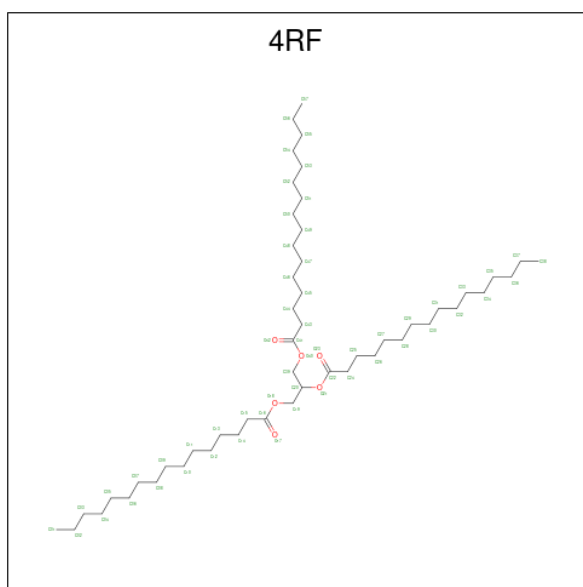
Mol	Chain	Residues	Atoms			AltConf
49	6	1	Total	C	O	0
			9	6	3	

- Molecule 50 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).



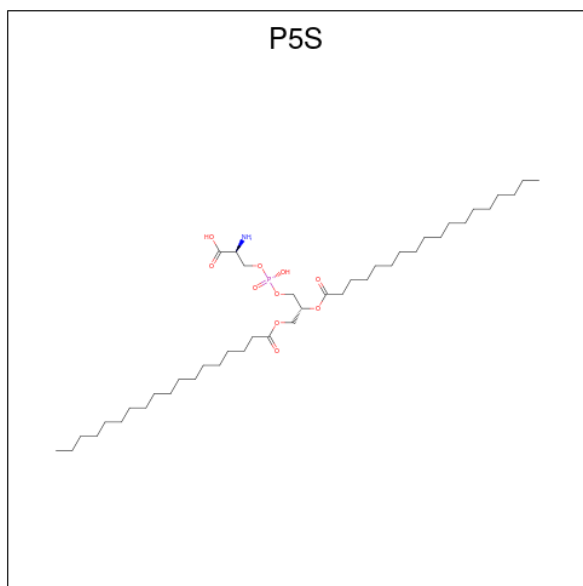
Mol	Chain	Residues	Atoms			AltConf
50	7	1	Total	C	O	0
			44	40	4	
50	2	1	Total	C	O	0
			44	40	4	
50	9	1	Total	C	O	0
			44	40	4	
50	9	1	Total	C	O	0
			44	40	4	

- Molecule 51 is Tripalmitoylglycerol (three-letter code: 4RF) (formula: C₅₁H₉₈O₆).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
51	7	1	37	31	6	0

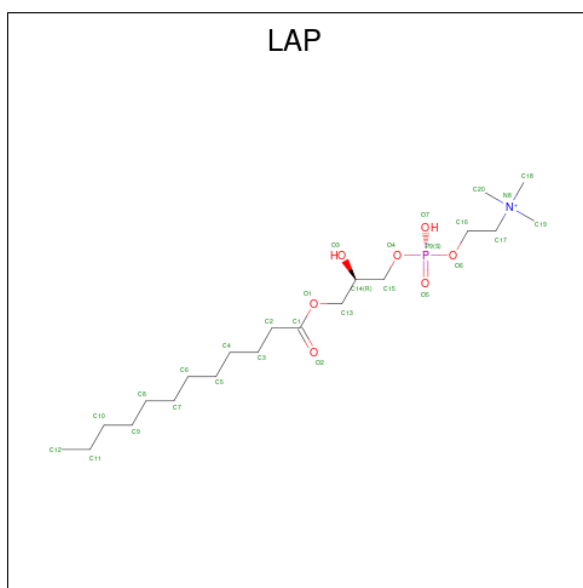
- Molecule 52 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (three-letter code: P5S) (formula: $C_{42}H_{82}NO_{10}P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
52	8	1	37	25	1	10	1	0

- Molecule 53 is [2-((1-OXODODECANOXY-(2-HYDROXY-3-PROPANYL))-PHOSPHONATE-OXY)-ETHYL]-TRIMETHYLAMMONIUM (three-letter code: LAP) (formula:

C₂₀H₄₃NO₇P).



Mol	Chain	Residues	Atoms				AltConf	
53	8	1	Total	C	N	O	P	0
			29	20	1	7	1	

- Molecule 54 is water.

Mol	Chain	Residues	Atoms		AltConf
54	A	20	Total	O	0
			20	20	
54	A	1	Total	O	0
			1	1	
54	B	2	Total	O	0
			2	2	
54	B	2	Total	O	0
			2	2	
54	B	5	Total	O	0
			5	5	
54	B	6	Total	O	0
			6	6	
54	B	4	Total	O	0
			4	4	
54	B	3	Total	O	0
			3	3	
54	B	1	Total	O	0
			1	1	
54	B	1	Total	O	0
			1	1	

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Mol	Chain	Residues	Atoms	AltConf
54	C	1	Total O 1 1	0
54	C	1	Total O 1 1	0
54	D	1	Total O 1 1	0
54	D	1	Total O 1 1	0
54	E	1	Total O 1 1	0
54	F	1	Total O 1 1	0
54	F	1	Total O 1 1	0
54	F	1	Total O 1 1	0
54	G	1	Total O 1 1	0
54	G	2	Total O 2 2	0
54	H	1	Total O 1 1	0
54	J	1	Total O 1 1	0
54	K	3	Total O 3 3	0
54	L	1	Total O 1 1	0
54	L	1	Total O 1 1	0
54	M	1	Total O 1 1	0
54	1	5	Total O 5 5	0
54	a	1	Total O 1 1	0
54	3	4	Total O 4 4	0
54	3	1	Total O 1 1	0
54	4	3	Total O 3 3	0

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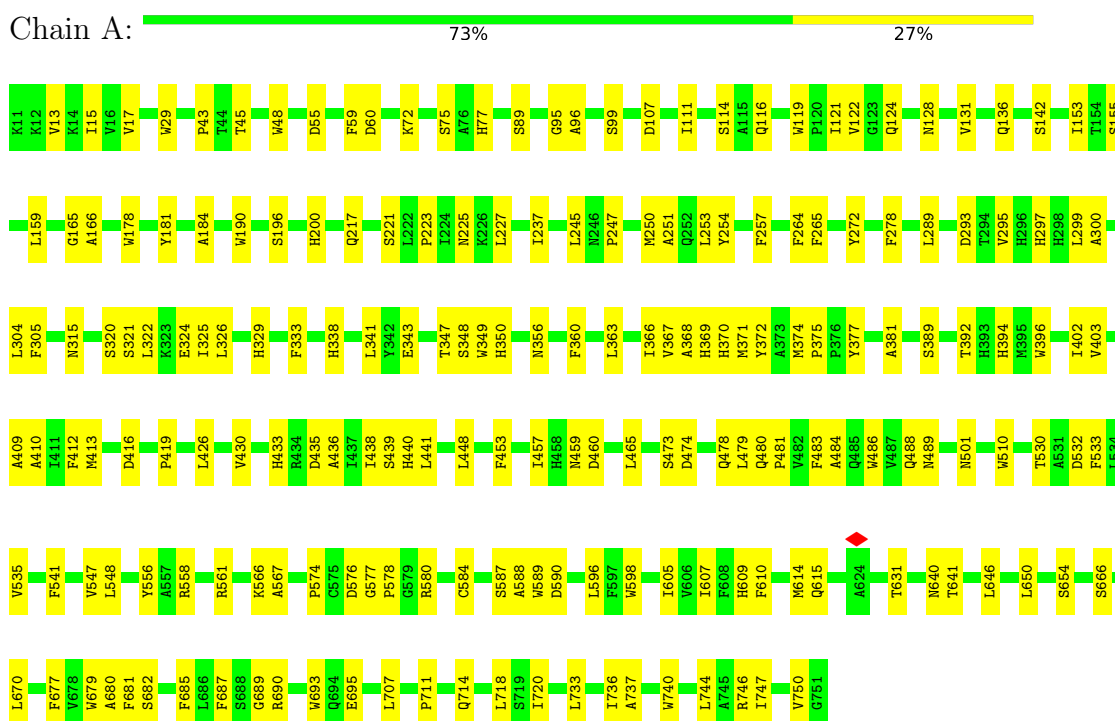
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Mol	Chain	Residues	Atoms		AltConf
54	4	1	Total 1	O 1	0
54	5	3	Total 3	O 3	0
54	6	7	Total 7	O 7	0
54	7	2	Total 2	O 2	0
54	8	1	Total 1	O 1	0
54	8	1	Total 1	O 1	0
54	2	4	Total 4	O 4	0
54	9	1	Total 1	O 1	0
54	9	1	Total 1	O 1	0

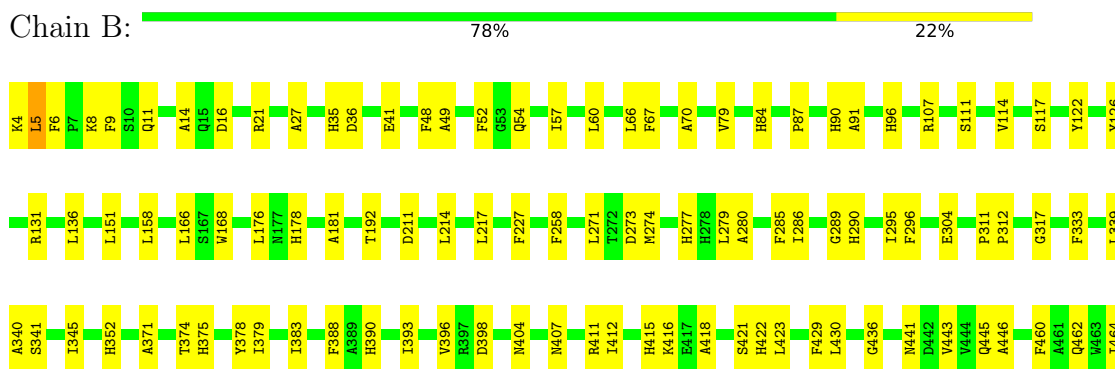
3 Residue-property plots [i](#)

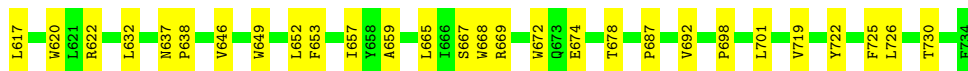
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

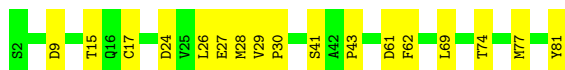
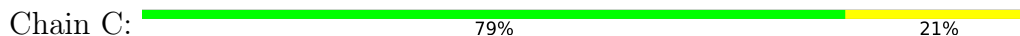


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

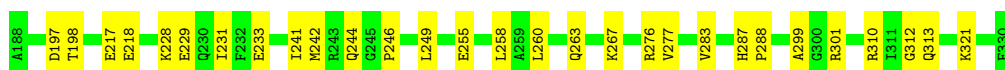
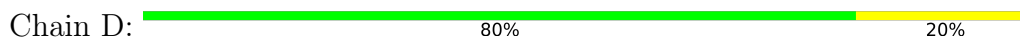




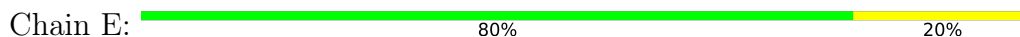
- Molecule 3: Photosystem I iron-sulfur center



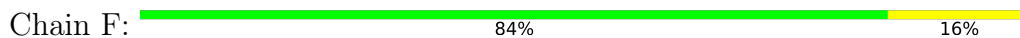
- Molecule 4: Photosystem I reaction center subunit chloroplastic



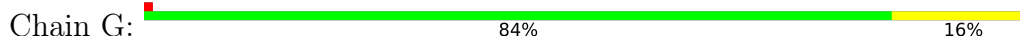
- Molecule 5: Photosystem I reaction center subunit IV



- Molecule 6: PSI-F



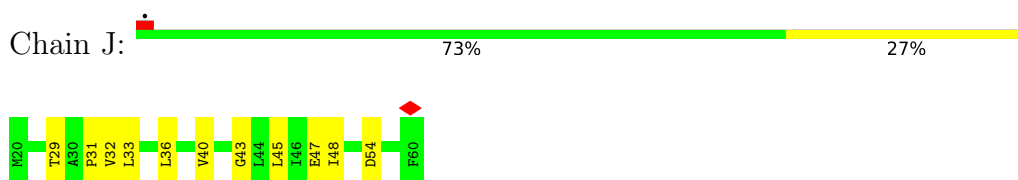
- Molecule 7: Photosystem I reaction center subunit chloroplastic



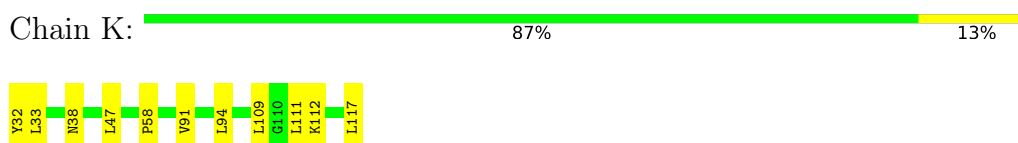
- Molecule 8: Photosystem I reaction center subunit VI-chloroplastic-like



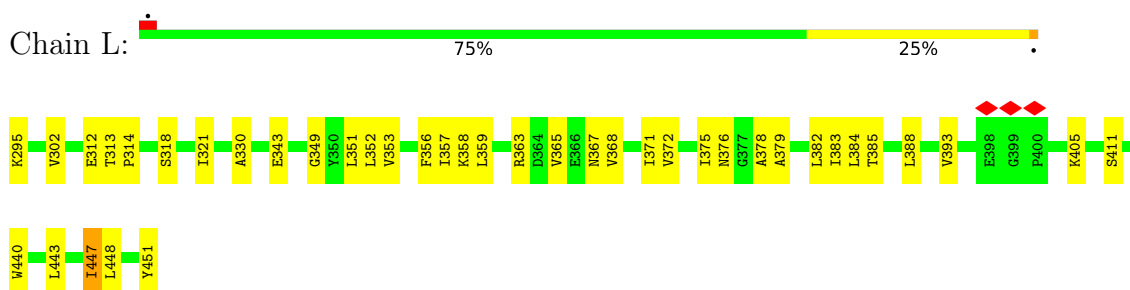
- Molecule 9: Photosystem I reaction center subunit IX



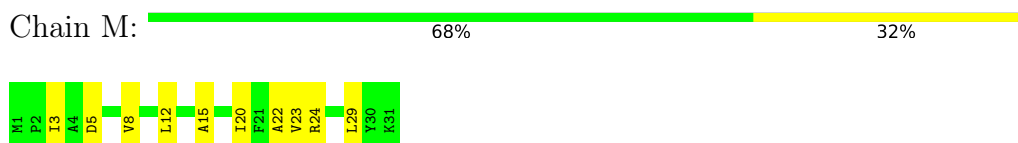
- Molecule 10: Photosystem I reaction center subunit chloroplastic



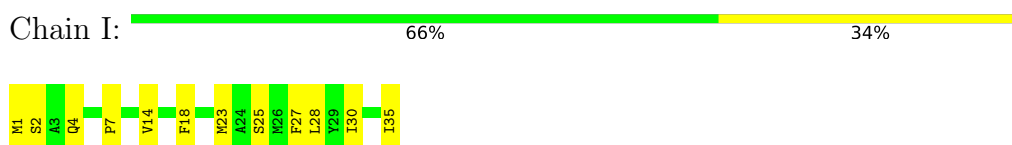
- Molecule 11: Photosystem I reaction center subunit XI



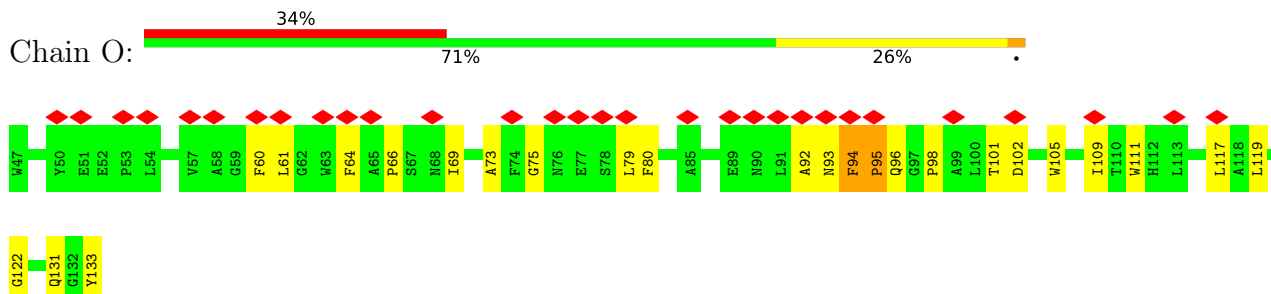
- Molecule 12: Photosystem I reaction center subunit XII



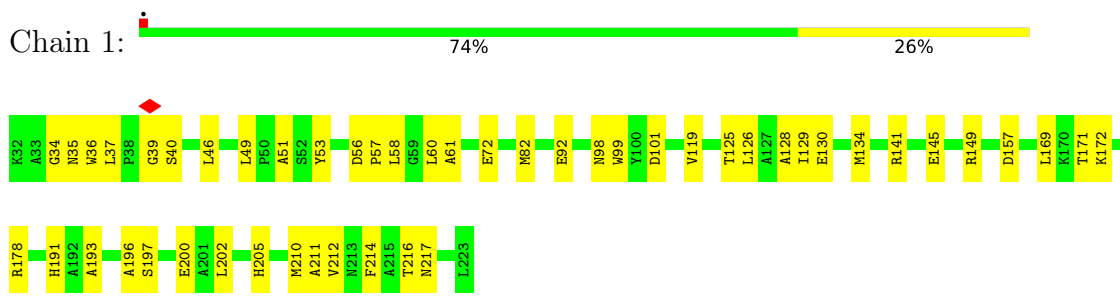
- Molecule 13: Photosystem I reaction center subunit VIII



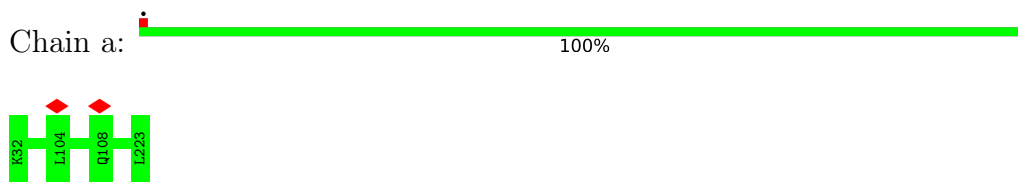
- Molecule 14: Photosystem I subunit O



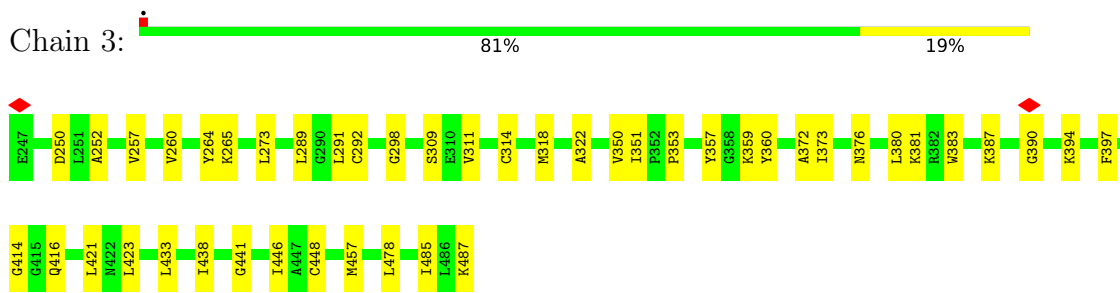
• Molecule 15: Chlorophyll a-b binding protein, chloroplastic



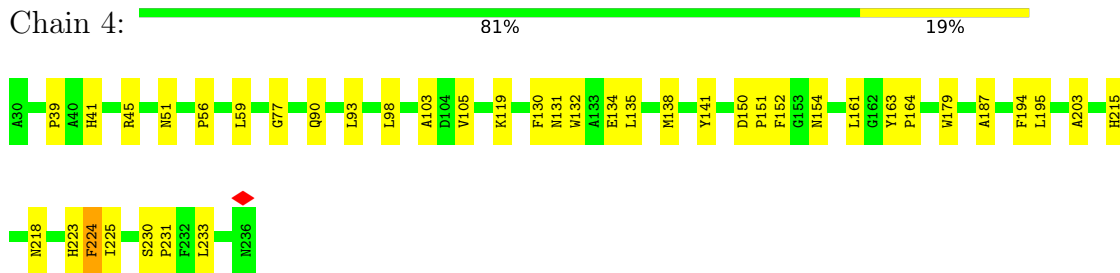
• Molecule 15: Chlorophyll a-b binding protein, chloroplastic



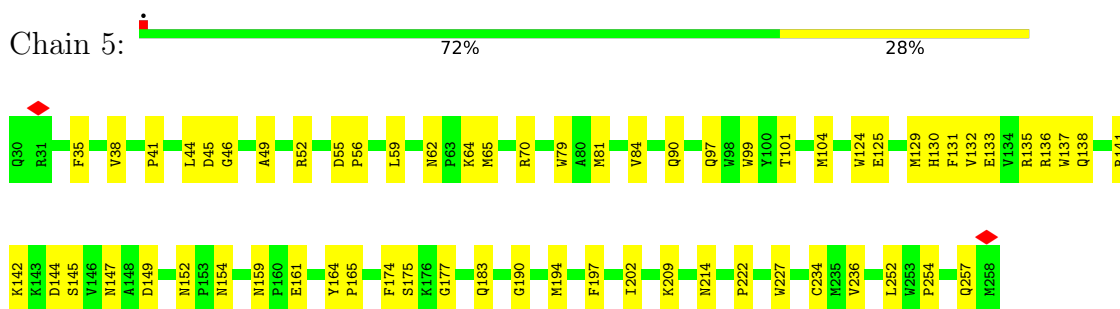
• Molecule 16: Glutathione reductase



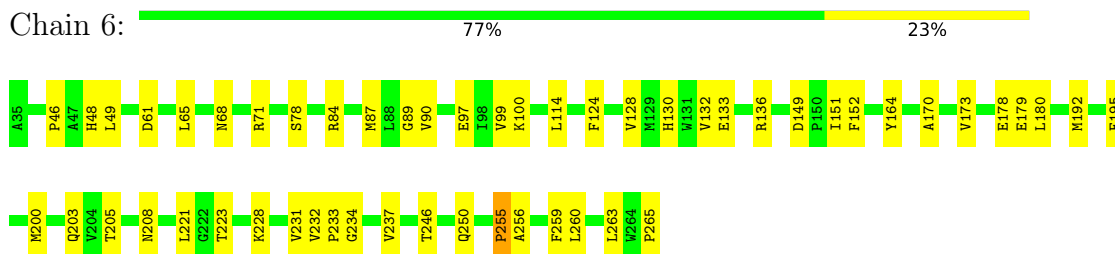
• Molecule 17: Lhca4



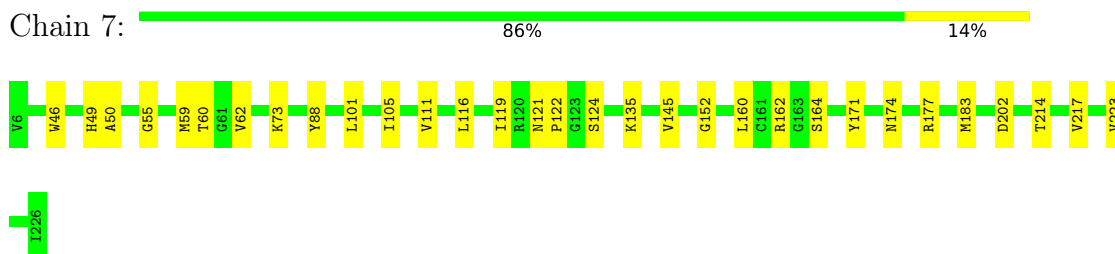
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic



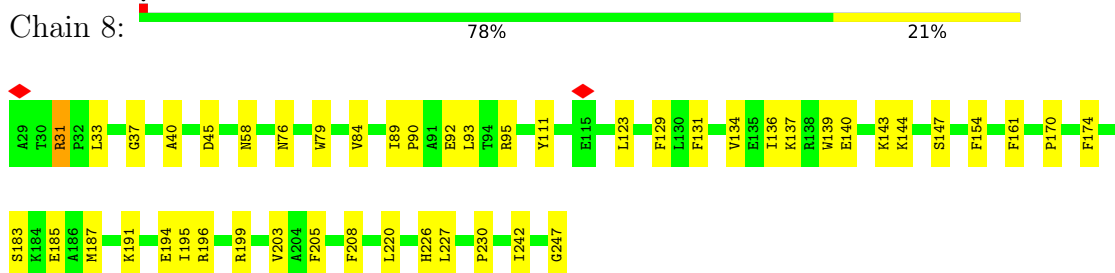
- Molecule 19: Chlorophyll a-b binding protein, chloroplastic



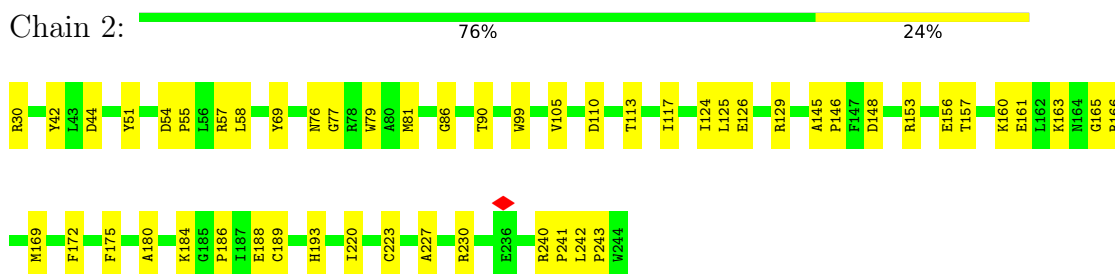
- Molecule 20: Lhca7



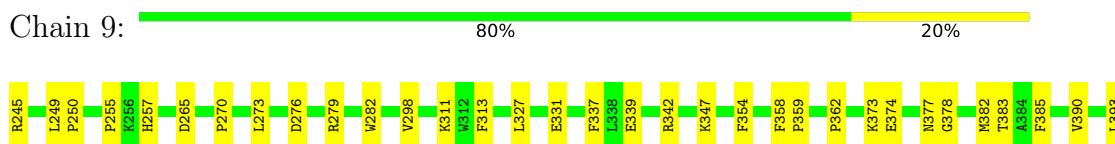
- Molecule 21: Chlorophyll a-b binding protein, chloroplastic



- Molecule 22: Chlorophyll a-b binding protein, chloroplastic



- Molecule 23: Chlorophyll a-b binding protein, chloroplastic





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	185138	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.05	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.091	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0112	Depositor
Map size (\AA)	394.56, 394.56, 394.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.82199997, 0.82199997, 0.82199997	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: PQN, PTY, DGD, SF4, CLA, SPH, PCW, LMT, XAT, OLA, LMG, CHL, PLM, LHG, 3PH, CLO, NEX, LAP, DGA, P5S, SQD, BCR, 4RF, ECH, AXT, 13X, QTB, LPX, LUT, RRX

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.27	0/6022	0.47	0/8215
2	B	0.27	0/6006	0.48	1/8205 (0.0%)
3	C	0.26	0/611	0.53	0/828
4	D	0.27	0/1150	0.52	0/1551
5	E	0.28	0/520	0.55	0/705
6	F	0.26	0/1309	0.47	0/1771
7	G	0.25	0/743	0.46	0/1007
8	H	0.27	0/744	0.54	0/1000
9	J	0.27	0/322	0.51	0/439
10	K	0.26	0/622	0.46	0/844
11	L	0.28	0/1195	0.51	0/1635
12	M	0.28	0/244	0.41	0/330
13	I	0.27	0/276	0.48	0/373
14	O	0.27	0/703	0.52	0/956
15	1	0.27	0/1443	0.48	0/1960
15	a	0.27	0/1443	0.47	0/1960
16	3	0.27	0/1896	0.46	0/2573
17	4	0.26	0/1681	0.44	0/2285
18	5	0.26	0/1842	0.45	0/2505
19	6	0.27	0/1845	0.48	0/2515
20	7	0.28	0/1748	0.49	0/2372
21	8	0.28	0/1717	0.48	0/2330
22	2	0.26	0/1708	0.47	0/2318
23	9	0.26	0/1444	0.45	0/1957
All	All	0.27	0/37234	0.48	1/50634 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5	LEU	CA-CB-CG	5.50	127.94	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5824	0	5675	174	0
2	B	5796	0	5576	146	0
3	C	601	0	576	13	0
4	D	1124	0	1129	20	0
5	E	509	0	507	8	0
6	F	1277	0	1296	19	0
7	G	727	0	724	15	0
8	H	729	0	705	26	0
9	J	316	0	332	9	0
10	K	613	0	639	11	0
11	L	1165	0	1181	39	0
12	M	239	0	255	11	0
13	I	270	0	287	12	0
14	O	679	0	661	24	0
15	1	1405	0	1370	46	0
15	a	1405	0	1370	0	0
16	3	1844	0	1805	39	0
17	4	1631	0	1575	34	0
18	5	1786	0	1736	53	0
19	6	1787	0	1760	45	0
20	7	1698	0	1640	30	0
21	8	1669	0	1619	53	0
22	2	1666	0	1657	50	0
23	9	1406	0	1385	35	0
24	A	65	0	72	6	0
25	1	528	0	523	52	0
25	2	615	0	568	44	0
25	3	576	0	555	37	0
25	4	768	0	685	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	5	642	0	564	38	0
25	6	624	0	591	34	0
25	7	566	0	525	39	0
25	8	573	0	480	42	0
25	9	379	0	338	29	0
25	A	2532	0	2566	221	0
25	B	2583	0	2685	203	0
25	F	105	0	88	8	0
25	G	155	0	130	9	0
25	H	156	0	130	8	0
25	J	42	0	30	1	0
25	K	200	0	161	12	0
25	L	205	0	168	16	0
25	O	134	0	95	5	0
25	a	496	0	443	0	0
26	1	284	0	248	31	0
26	2	165	0	137	7	0
26	3	236	0	223	21	0
26	4	174	0	154	15	0
26	5	271	0	217	18	0
26	6	333	0	284	25	0
26	7	296	0	267	24	0
26	8	296	0	265	19	0
26	9	273	0	233	26	0
26	A	66	0	69	9	0
26	a	264	0	205	0	0
27	A	33	0	46	7	0
27	B	33	0	46	5	0
28	A	8	0	0	0	0
28	C	16	0	0	1	0
29	3	120	0	158	12	0
29	4	40	0	53	8	0
29	5	80	0	103	10	0
29	6	80	0	106	8	0
29	7	40	0	52	9	0
29	8	40	0	53	3	0
29	A	200	0	264	24	0
29	B	280	0	371	34	0
29	G	40	0	53	5	0
29	H	40	0	53	4	0
29	I	40	0	52	2	0
29	J	40	0	53	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	K	80	0	106	8	0
29	L	120	0	159	6	0
29	O	40	0	52	1	0
30	1	84	0	114	6	0
30	2	98	0	148	11	0
30	3	49	0	74	1	0
30	4	81	0	108	4	0
30	5	49	0	74	2	0
30	6	86	0	118	6	0
30	7	108	0	126	3	0
30	8	37	0	44	1	0
30	9	82	0	110	7	0
30	A	144	0	213	11	0
30	B	98	0	148	7	0
30	F	79	0	101	4	0
30	a	35	0	40	0	0
31	A	42	0	54	0	0
32	7	39	0	41	1	0
32	A	54	0	77	8	0
32	G	46	0	55	4	0
32	H	45	0	53	3	0
32	I	54	0	77	5	0
33	3	38	0	49	3	0
33	5	38	0	49	3	0
33	7	33	0	39	0	0
33	9	48	0	72	3	0
33	A	34	0	41	4	0
33	B	42	0	60	4	0
33	G	56	0	62	2	0
33	J	28	0	29	2	0
33	a	76	0	98	0	0
34	A	33	0	39	3	0
35	1	35	0	46	5	0
35	2	35	0	45	5	0
35	A	35	0	45	1	0
35	B	35	0	45	2	0
36	7	50	0	58	3	0
36	8	105	0	126	8	0
36	B	66	0	96	4	0
37	6	36	0	44	4	0
37	B	39	0	50	1	0
37	K	77	0	99	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	F	30	0	43	2	0
39	F	44	0	54	5	0
40	3	41	0	56	1	0
40	J	41	0	56	2	0
41	4	21	0	37	0	0
41	6	21	0	37	1	0
41	9	21	0	37	2	0
41	J	21	0	37	1	0
42	M	41	0	54	5	0
43	1	84	0	110	7	0
43	2	84	0	110	11	0
43	3	84	0	110	7	0
43	4	84	0	110	10	0
43	5	126	0	165	13	0
43	6	84	0	110	10	0
43	7	42	0	55	5	0
43	8	84	0	110	11	0
43	9	84	0	110	17	0
43	a	126	0	165	0	0
44	1	43	0	52	3	0
44	7	43	0	52	10	0
45	1	20	0	33	2	0
45	8	40	0	66	1	0
45	a	20	0	33	0	0
46	a	19	0	0	0	0
47	4	35	0	62	3	0
47	5	18	0	31	3	0
47	6	18	0	31	1	0
47	8	35	0	62	6	0
47	a	17	0	31	0	0
48	2	37	0	56	6	0
48	3	24	0	30	3	0
48	5	23	0	28	3	0
48	8	40	0	65	5	0
49	6	9	0	6	0	0
50	2	44	0	56	2	0
50	7	44	0	56	3	0
50	9	88	0	112	8	0
51	7	37	0	49	6	0
52	8	37	0	40	2	0
53	8	29	0	42	5	0
54	1	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	2	4	0	0	0	0
54	3	5	0	0	0	0
54	4	4	0	0	0	0
54	5	3	0	0	0	0
54	6	7	0	0	0	0
54	7	2	0	0	0	0
54	8	2	0	0	0	0
54	9	2	0	0	0	0
54	A	21	0	0	1	0
54	B	24	0	0	0	0
54	C	2	0	0	0	0
54	D	2	0	0	0	0
54	E	1	0	0	0	0
54	F	3	0	0	0	0
54	G	3	0	0	0	0
54	H	1	0	0	0	0
54	J	1	0	0	0	0
54	K	3	0	0	0	0
54	L	2	0	0	0	0
54	M	1	0	0	0	0
54	a	1	0	0	0	0
All	All	56369	0	56465	1650	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 15.

The worst 5 of 1650 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)
11:L:295:LYS:N	14:O:133:TYR:HH	1.63	0.94
50:9:504:XAT:H32	50:9:507:XAT:H10	1.50	0.94
1:A:396:TRP:CD1	25:A:1126:CLA:HAB	2.04	0.92
18:5:161:GLU:OE2	18:5:183:GLN:NE2	2.05	0.89
11:L:356:PHE:HB2	11:L:372:VAL:HG13	1.55	0.89

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/741 (100%)	709 (96%)	30 (4%)	0	100	100
2	B	729/731 (100%)	697 (96%)	32 (4%)	0	100	100
3	C	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
4	D	141/143 (99%)	129 (92%)	12 (8%)	0	100	100
5	E	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
6	F	163/165 (99%)	154 (94%)	9 (6%)	0	100	100
7	G	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
8	H	92/94 (98%)	80 (87%)	11 (12%)	1 (1%)	12	30
9	J	39/41 (95%)	39 (100%)	0	0	100	100
10	K	84/86 (98%)	79 (94%)	5 (6%)	0	100	100
11	L	155/157 (99%)	144 (93%)	10 (6%)	1 (1%)	22	45
12	M	29/31 (94%)	29 (100%)	0	0	100	100
13	I	33/35 (94%)	29 (88%)	4 (12%)	0	100	100
14	O	85/87 (98%)	66 (78%)	16 (19%)	3 (4%)	3	7
15	1	190/192 (99%)	174 (92%)	15 (8%)	1 (0%)	25	49
15	a	190/192 (99%)	171 (90%)	19 (10%)	0	100	100
16	3	239/241 (99%)	225 (94%)	13 (5%)	1 (0%)	30	55
17	4	205/207 (99%)	184 (90%)	19 (9%)	2 (1%)	13	33
18	5	227/229 (99%)	214 (94%)	13 (6%)	0	100	100
19	6	229/231 (99%)	213 (93%)	15 (7%)	1 (0%)	30	55
20	7	219/221 (99%)	207 (94%)	11 (5%)	1 (0%)	25	49
21	8	217/219 (99%)	207 (95%)	10 (5%)	0	100	100
22	2	213/215 (99%)	197 (92%)	16 (8%)	0	100	100
23	9	181/183 (99%)	171 (94%)	10 (6%)	0	100	100
All	All	4636/4684 (99%)	4348 (94%)	277 (6%)	11 (0%)	45	68

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	118	PRO
14	O	93	ASN
14	O	95	PRO
15	1	36	TRP
17	4	224	PHE

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	A	600/600 (100%)	600 (100%)	0	100	100
2	B	588/588 (100%)	588 (100%)	0	100	100
3	C	69/69 (100%)	69 (100%)	0	100	100
4	D	121/121 (100%)	121 (100%)	0	100	100
5	E	55/55 (100%)	55 (100%)	0	100	100
6	F	126/126 (100%)	126 (100%)	0	100	100
7	G	71/71 (100%)	71 (100%)	0	100	100
8	H	71/71 (100%)	71 (100%)	0	100	100
9	J	35/35 (100%)	35 (100%)	0	100	100
10	K	66/66 (100%)	66 (100%)	0	100	100
11	L	122/122 (100%)	122 (100%)	0	100	100
12	M	23/23 (100%)	23 (100%)	0	100	100
13	I	30/30 (100%)	30 (100%)	0	100	100
14	O	66/66 (100%)	66 (100%)	0	100	100
15	1	134/134 (100%)	134 (100%)	0	100	100
15	a	134/134 (100%)	134 (100%)	0	100	100
16	3	186/186 (100%)	186 (100%)	0	100	100
17	4	165/165 (100%)	165 (100%)	0	100	100
18	5	185/185 (100%)	185 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	6	187/187 (100%)	187 (100%)	0	100	100
20	7	176/176 (100%)	176 (100%)	0	100	100
21	8	168/168 (100%)	167 (99%)	1 (1%)	84	94
22	2	173/173 (100%)	173 (100%)	0	100	100
23	9	141/141 (100%)	141 (100%)	0	100	100
All	All	3692/3692 (100%)	3691 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	8	31	ARG

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

Mol	Chain	Res	Type
14	O	131	GLN
15	a	35	ASN
17	4	131	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

403 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
25	CLA	G	1602	7	60,68,73	1.40	8 (13%)	70,107,113	2.05	18 (25%)
43	LUT	4	501	-	42,43,43	2.36	1 (2%)	51,60,60	2.01	12 (23%)
25	CLA	9	607	-	47,55,73	1.59	9 (19%)	54,91,113	2.16	15 (27%)
26	CHL	1	611	-	56,64,74	0.92	3 (5%)	61,102,114	1.33	9 (14%)
47	PLM	8	806	-	16,16,17	0.42	0	15,15,17	0.92	0
25	CLA	B	1204	-	65,73,73	1.36	9 (13%)	76,113,113	2.01	18 (23%)
25	CLA	A	1141	-	45,53,73	1.62	9 (20%)	52,89,113	2.21	12 (23%)
26	CHL	6	619	19	66,74,74	0.80	2 (3%)	73,114,114	1.35	11 (15%)
33	PTY	G	5002	-	27,27,49	1.03	2 (7%)	28,31,54	1.07	1 (3%)
25	CLA	a	601	-	60,68,73	1.40	9 (15%)	70,107,113	2.06	18 (25%)
26	CHL	a	606	-	56,64,74	0.93	3 (5%)	61,102,114	1.37	12 (19%)
26	CHL	6	613	-	51,59,74	0.91	2 (3%)	55,96,114	1.42	11 (20%)
26	CHL	8	603	21	66,74,74	0.91	4 (6%)	73,114,114	1.21	9 (12%)
41	SPH	6	806	-	19,20,20	0.64	0	18,21,21	1.07	1 (5%)
25	CLA	6	608	-	55,63,73	1.47	10 (18%)	64,101,113	2.14	16 (25%)
43	LUT	a	503	-	42,43,43	2.36	1 (2%)	51,60,60	2.28	15 (29%)
30	LHG	F	5001	-	42,42,48	0.42	0	45,48,54	1.10	2 (4%)
25	CLA	3	610	16	57,65,73	1.43	8 (14%)	66,103,113	2.10	18 (27%)
25	CLA	G	1603	-	45,53,73	1.63	8 (17%)	52,89,113	2.11	14 (26%)
29	BCR	A	4005	-	41,41,41	1.83	4 (9%)	56,56,56	4.22	13 (23%)
25	CLA	A	1102	25	55,63,73	1.45	6 (10%)	64,101,113	2.20	17 (26%)
25	CLA	O	1803	-	41,49,73	1.70	9 (21%)	47,84,113	2.24	15 (31%)
25	CLA	A	1118	-	55,63,73	1.48	9 (16%)	64,101,113	2.08	15 (23%)
25	CLA	A	1116	-	60,68,73	1.42	9 (15%)	70,107,113	2.00	15 (21%)
27	PQN	A	2001	-	34,34,34	0.37	0	42,45,45	1.14	2 (4%)
25	CLA	9	605	-	60,68,73	1.42	8 (13%)	70,107,113	2.04	18 (25%)
34	3PH	A	5007	-	32,32,47	1.02	4 (12%)	36,37,52	1.20	2 (5%)
26	CHL	9	601	-	66,74,74	0.81	2 (3%)	73,114,114	1.27	11 (15%)
26	CHL	9	613	-	42,50,74	1.16	4 (9%)	44,85,114	1.47	8 (18%)
29	BCR	B	4004	-	41,41,41	1.83	4 (9%)	56,56,56	4.26	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CHL	2	610	-	48,56,74	0.96	3 (6%)	51,92,114	1.42	10 (19%)
30	LHG	8	801	25	36,36,48	0.44	0	39,42,54	1.15	3 (7%)
25	CLA	7	602	-	44,52,73	1.63	7 (15%)	51,88,113	2.11	13 (25%)
41	SPH	9	804	-	19,20,20	0.65	0	18,21,21	1.08	0
25	CLA	A	1111	-	65,73,73	1.34	7 (10%)	76,113,113	2.02	18 (23%)
25	CLA	9	612	-	65,73,73	1.36	9 (13%)	76,113,113	1.95	16 (21%)
26	CHL	8	610	-	56,64,74	0.90	3 (5%)	61,102,114	1.40	13 (21%)
25	CLA	5	607	-	60,68,73	1.41	8 (13%)	70,107,113	2.05	17 (24%)
25	CLA	2	608	-	45,53,73	1.63	8 (17%)	52,89,113	2.10	12 (23%)
25	CLA	4	610	-	65,73,73	1.37	8 (12%)	76,113,113	2.01	16 (21%)
35	LMT	2	804	-	36,36,36	1.19	6 (16%)	47,47,47	1.06	2 (4%)
52	P5S	8	805	-	35,36,53	1.16	3 (8%)	39,43,60	1.22	2 (5%)
25	CLA	8	608	-	52,60,73	1.51	7 (13%)	60,97,113	2.18	17 (28%)
25	CLA	B	1235	-	65,73,73	1.35	8 (12%)	76,113,113	2.03	17 (22%)
47	PLM	4	803	-	16,16,17	0.42	0	15,15,17	0.93	0
26	CHL	7	611	-	56,64,74	0.91	3 (5%)	61,102,114	1.33	10 (16%)
25	CLA	A	1121	-	60,68,73	1.41	8 (13%)	70,107,113	2.10	18 (25%)
26	CHL	7	617	20	66,74,74	0.83	3 (4%)	73,114,114	1.20	9 (12%)
28	SF4	C	3002	3	0,12,12	-	-	-	-	-
26	CHL	6	610	-	56,64,74	0.93	3 (5%)	61,102,114	1.34	11 (18%)
30	LHG	3	801	25	48,48,48	0.40	0	51,54,54	1.03	3 (5%)
25	CLA	a	608	-	55,63,73	1.48	9 (16%)	64,101,113	2.08	15 (23%)
25	CLA	8	618	21	60,68,73	1.41	8 (13%)	70,107,113	2.09	16 (22%)
39	NEX	F	4001	-	38,46,46	3.37	9 (23%)	50,70,70	4.73	16 (32%)
30	LHG	9	801	-	32,32,48	0.47	0	35,38,54	1.18	3 (8%)
26	CHL	6	609	19	66,74,74	0.77	2 (3%)	73,114,114	1.25	12 (16%)
33	PTY	3	802	-	37,37,49	0.99	4 (10%)	40,42,54	1.10	2 (5%)
25	CLA	B	1240	30	65,73,73	1.36	8 (12%)	76,113,113	2.00	18 (23%)
25	CLA	B	1239	-	65,73,73	1.35	8 (12%)	76,113,113	1.95	17 (22%)
25	CLA	3	613	-	61,69,73	1.38	8 (13%)	71,108,113	2.03	17 (23%)
50	XAT	2	501	-	39,47,47	0.69	1 (2%)	54,74,74	1.98	14 (25%)
53	LAP	8	810	-	28,28,28	1.22	2 (7%)	33,35,35	0.99	1 (3%)
25	CLA	B	1225	-	65,73,73	1.36	7 (10%)	76,113,113	1.91	16 (21%)
25	CLA	6	604	19	65,73,73	1.36	8 (12%)	76,113,113	1.95	19 (25%)
25	CLA	5	614	18	46,54,73	1.61	8 (17%)	53,90,113	2.08	13 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	4	608	-	51,59,73	1.53	9 (17%)	59,96,113	2.18	16 (27%)
25	CLA	A	1112	-	55,63,73	1.46	6 (10%)	64,101,113	2.22	17 (26%)
25	CLA	K	1401	-	46,54,73	1.60	7 (15%)	53,90,113	2.06	12 (22%)
25	CLA	7	601	20	60,68,73	1.40	8 (13%)	70,107,113	2.07	17 (24%)
36	DGD	B	5003	-	67,67,67	1.18	7 (10%)	81,81,81	1.02	3 (3%)
32	SQD	H	5001	-	44,45,54	0.85	0	53,56,65	0.97	2 (3%)
25	CLA	B	1217	-	56,64,73	1.46	10 (17%)	65,102,113	2.14	17 (26%)
29	BCR	5	504	-	41,41,41	1.84	4 (9%)	56,56,56	4.54	19 (33%)
30	LHG	A	5002	-	48,48,48	0.39	0	51,54,54	1.00	3 (5%)
36	DGD	8	802	-	60,60,67	1.08	5 (8%)	74,74,81	1.09	5 (6%)
25	CLA	A	1104	1	65,73,73	1.35	8 (12%)	76,113,113	1.95	17 (22%)
25	CLA	A	1137	-	60,68,73	1.42	8 (13%)	70,107,113	2.06	20 (28%)
25	CLA	4	606	-	50,58,73	1.53	8 (16%)	58,95,113	2.25	17 (29%)
30	LHG	a	801	-	34,34,48	0.45	0	37,40,54	1.10	3 (8%)
33	PTY	9	803	-	47,47,49	0.89	4 (8%)	50,52,54	1.11	2 (4%)
27	PQN	B	2002	-	34,34,34	0.37	0	42,45,45	1.05	3 (7%)
25	CLA	2	604	-	56,64,73	1.44	7 (12%)	65,102,113	2.18	18 (27%)
32	SQD	G	5001	-	45,46,54	0.84	0	54,57,65	0.95	2 (3%)
29	BCR	B	4003	-	41,41,41	1.86	4 (9%)	56,56,56	4.33	17 (30%)
37	PCW	6	803	-	35,35,53	1.29	4 (11%)	41,43,61	1.13	2 (4%)
25	CLA	8	606	-	57,65,73	1.42	6 (10%)	66,103,113	2.09	17 (25%)
48	DGA	2	803	-	36,36,43	1.19	3 (8%)	38,38,45	1.34	3 (7%)
25	CLA	1	615	15	46,54,73	1.59	7 (15%)	53,90,113	2.17	14 (26%)
25	CLA	2	605	-	60,68,73	1.42	9 (15%)	70,107,113	2.04	19 (27%)
29	BCR	A	4003	-	41,41,41	1.85	4 (9%)	56,56,56	4.42	17 (30%)
25	CLA	2	621	22	65,73,73	1.37	9 (13%)	76,113,113	2.02	16 (21%)
26	CHL	7	615	20	51,59,74	0.96	3 (5%)	55,96,114	1.38	11 (20%)
25	CLA	4	601	-	60,68,73	1.39	7 (11%)	70,107,113	2.09	19 (27%)
44	AXT	7	504	-	44,44,45	2.41	17 (38%)	55,62,64	2.40	17 (30%)
25	CLA	8	605	-	55,63,73	1.48	9 (16%)	64,101,113	2.10	16 (25%)
25	CLA	B	1202	-	65,73,73	1.35	9 (13%)	76,113,113	1.94	16 (21%)
29	BCR	5	503	-	41,41,41	1.83	4 (9%)	56,56,56	4.34	17 (30%)
26	CHL	A	1114	-	66,74,74	0.87	3 (4%)	73,114,114	1.32	9 (12%)
45	OLA	8	809	-	19,19,19	0.57	0	19,19,19	1.00	0
26	CHL	a	610	-	48,56,74	0.97	3 (6%)	51,92,114	1.37	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	2	612	-	50,58,73	1.56	9 (18%)	58,95,113	2.14	15 (25%)
26	CHL	9	603	-	66,74,74	0.88	3 (4%)	73,114,114	1.16	8 (10%)
25	CLA	8	615	21	46,54,73	1.60	8 (17%)	53,90,113	2.19	14 (26%)
30	LHG	7	803	-	34,34,48	0.44	0	37,40,54	1.15	3 (8%)
25	CLA	B	1206	2	65,73,73	1.34	7 (10%)	76,113,113	2.03	16 (21%)
25	CLA	B	1229	-	65,73,73	1.36	8 (12%)	76,113,113	2.00	19 (25%)
25	CLA	B	1220	-	60,68,73	1.41	9 (15%)	70,107,113	2.00	15 (21%)
43	LUT	2	502	-	42,43,43	2.37	1 (2%)	51,60,60	1.93	13 (25%)
25	CLA	K	1403	10	49,57,73	1.56	8 (16%)	55,93,113	2.24	16 (29%)
25	CLA	2	601	-	60,68,73	1.40	8 (13%)	70,107,113	2.18	18 (25%)
26	CHL	1	613	-	48,56,74	0.92	2 (4%)	51,92,114	1.39	9 (17%)
51	4RF	7	807	-	36,36,56	1.07	6 (16%)	39,39,59	1.14	3 (7%)
30	LHG	B	5001	25	48,48,48	0.40	0	51,54,54	0.98	3 (5%)
25	CLA	9	609	23	46,54,73	1.58	7 (15%)	53,90,113	2.18	15 (28%)
25	CLA	4	603	17	56,64,73	1.47	9 (16%)	65,102,113	2.03	16 (24%)
30	LHG	7	801	25	36,36,48	0.44	0	39,42,54	1.11	2 (5%)
25	CLA	B	1230	-	58,66,73	1.41	6 (10%)	67,104,113	2.13	18 (26%)
25	CLA	B	1226	-	65,73,73	1.37	8 (12%)	76,113,113	1.97	17 (22%)
25	CLA	B	1213	-	55,63,73	1.45	7 (12%)	64,101,113	2.13	17 (26%)
43	LUT	9	502	-	42,43,43	2.32	1 (2%)	51,60,60	1.85	12 (23%)
33	PTY	G	5003	-	27,27,49	1.02	2 (7%)	28,31,54	1.07	1 (3%)
30	LHG	4	801	-	48,48,48	0.39	0	51,54,54	0.99	2 (3%)
25	CLA	B	1234	-	63,69,73	1.22	5 (7%)	71,99,113	2.17	17 (23%)
25	CLA	F	1302	-	55,63,73	1.46	7 (12%)	64,101,113	2.13	17 (26%)
29	BCR	I	4001	-	41,41,41	1.84	4 (9%)	56,56,56	4.29	16 (28%)
26	CHL	5	611	-	51,59,74	1.05	4 (7%)	55,96,114	1.40	9 (16%)
25	CLA	2	603	22	60,68,73	1.40	8 (13%)	70,107,113	2.17	20 (28%)
29	BCR	H	4001	-	41,41,41	1.86	4 (9%)	56,56,56	7.67	20 (35%)
25	CLA	B	1201	-	65,73,73	1.34	7 (10%)	76,113,113	4.36	21 (27%)
43	LUT	1	503	-	42,43,43	2.38	1 (2%)	51,60,60	2.22	17 (33%)
25	CLA	8	612	-	50,58,73	1.53	7 (14%)	58,95,113	2.15	14 (24%)
25	CLA	6	606	19	65,73,73	1.37	9 (13%)	76,113,113	2.00	18 (23%)
43	LUT	1	501	-	42,43,43	2.36	1 (2%)	51,60,60	1.96	15 (29%)
25	CLA	5	604	18	65,73,73	1.35	8 (12%)	76,113,113	1.98	16 (21%)
30	LHG	2	802	-	48,48,48	0.39	0	51,54,54	1.12	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	BCR	G	4001	-	41,41,41	1.87	4 (9%)	56,56,56	4.42	15 (26%)
32	SQD	A	5005	-	53,54,54	0.79	0	62,65,65	0.91	2 (3%)
30	LHG	A	5001	-	48,48,48	0.39	0	51,54,54	1.10	3 (5%)
25	CLA	4	611	-	56,64,73	1.46	7 (12%)	65,102,113	2.11	17 (26%)
36	DGD	8	803	-	47,47,67	0.81	1 (2%)	61,61,81	1.09	3 (4%)
33	PTY	B	5005	-	41,41,49	0.93	4 (9%)	44,46,54	1.13	2 (4%)
25	CLA	7	606	-	54,62,73	1.48	7 (12%)	63,100,113	2.09	15 (23%)
47	PLM	8	807	-	17,17,17	0.56	0	17,17,17	1.13	0
26	CHL	5	610	-	66,74,74	0.83	3 (4%)	73,114,114	1.24	12 (16%)
25	CLA	A	1122	-	60,68,73	1.42	9 (15%)	70,107,113	1.98	16 (22%)
29	BCR	6	503	-	41,41,41	1.85	4 (9%)	56,56,56	4.24	14 (25%)
37	PCW	K	5002	-	35,35,53	1.31	4 (11%)	41,43,61	1.07	2 (4%)
26	CHL	3	608	-	43,51,74	1.04	3 (6%)	45,86,114	1.48	9 (20%)
29	BCR	3	505	-	41,41,41	1.83	4 (9%)	56,56,56	4.28	15 (26%)
25	CLA	B	1208	-	54,62,73	1.41	7 (12%)	67,100,113	2.11	18 (26%)
25	CLA	K	1402	-	60,68,73	1.42	9 (15%)	70,107,113	2.05	17 (24%)
29	BCR	J	4001	-	41,41,41	1.83	4 (9%)	56,56,56	4.26	17 (30%)
26	CHL	8	604	21	62,70,74	0.97	4 (6%)	68,109,114	1.34	10 (14%)
43	LUT	8	501	-	42,43,43	2.35	1 (2%)	51,60,60	1.90	13 (25%)
25	CLA	1	612	15	65,73,73	1.36	8 (12%)	76,113,113	1.95	16 (21%)
26	CHL	a	609	15	53,61,74	0.87	2 (3%)	57,98,114	1.34	12 (21%)
25	CLA	A	1131	-	65,73,73	1.36	9 (13%)	76,113,113	1.97	15 (19%)
25	CLA	A	1133	-	65,73,73	1.37	9 (13%)	76,113,113	1.90	14 (18%)
25	CLA	4	617	-	45,53,73	1.62	8 (17%)	52,89,113	2.15	14 (26%)
26	CHL	5	613	-	56,64,74	0.85	2 (3%)	61,102,114	1.37	11 (18%)
25	CLA	A	1108	-	65,73,73	1.36	8 (12%)	76,113,113	1.91	16 (21%)
25	CLA	7	603	20	65,73,73	1.36	9 (13%)	76,113,113	2.00	17 (22%)
26	CHL	a	604	-	61,69,74	0.97	4 (6%)	67,108,114	1.39	9 (13%)
30	LHG	A	5003	-	45,45,48	0.40	0	48,51,54	1.04	3 (6%)
43	LUT	3	501	-	42,43,43	2.36	1 (2%)	51,60,60	1.96	14 (27%)
26	CHL	5	618	-	51,59,74	0.99	3 (5%)	55,96,114	1.44	11 (20%)
25	CLA	3	616	-	56,64,73	1.45	7 (12%)	65,102,113	2.15	17 (26%)
25	CLA	B	1216	-	65,73,73	1.34	7 (10%)	76,113,113	1.94	18 (23%)
25	CLA	1	605	-	65,73,73	1.33	9 (13%)	76,113,113	2.08	19 (25%)
25	CLA	3	601	16	65,73,73	1.35	7 (10%)	76,113,113	1.96	17 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	A	1136	-	65,73,73	1.36	8 (12%)	76,113,113	2.00	15 (19%)
25	CLA	J	1901	9	42,50,73	1.68	8 (19%)	48,85,113	2.20	13 (27%)
25	CLA	7	610	-	60,68,73	1.41	9 (15%)	70,107,113	2.04	16 (22%)
48	DGA	8	804	-	39,39,43	1.16	3 (7%)	41,41,45	1.57	3 (7%)
25	CLA	8	609	21	60,68,73	1.41	8 (13%)	70,107,113	2.08	17 (24%)
25	CLA	a	603	-	65,73,73	1.35	7 (10%)	76,113,113	2.05	17 (22%)
25	CLA	G	1601	-	50,58,73	1.55	8 (16%)	58,95,113	2.18	16 (27%)
29	BCR	A	4001	-	41,41,41	1.82	4 (9%)	56,56,56	4.26	17 (30%)
25	CLA	A	1128	-	65,73,73	1.36	8 (12%)	76,113,113	2.02	16 (21%)
25	CLA	8	611	-	50,58,73	1.52	7 (14%)	58,95,113	2.21	17 (29%)
25	CLA	B	1223	-	65,73,73	1.37	9 (13%)	76,113,113	2.00	17 (22%)
47	PLM	a	804	-	16,16,17	0.42	0	15,15,17	0.95	0
43	LUT	a	501	-	42,43,43	2.36	1 (2%)	51,60,60	2.07	12 (23%)
25	CLA	A	1107	1	55,63,73	1.47	8 (14%)	64,101,113	2.11	18 (28%)
25	CLA	L	1504	-	50,58,73	1.56	8 (16%)	58,95,113	2.19	15 (25%)
25	CLA	4	604	-	60,68,73	1.40	9 (15%)	70,107,113	2.06	17 (24%)
25	CLA	B	1215	-	60,68,73	1.40	7 (11%)	70,107,113	1.97	13 (18%)
41	SPH	J	5002	-	19,20,20	0.67	0	18,21,21	0.91	0
35	LMT	B	5006	-	36,36,36	1.17	6 (16%)	47,47,47	0.95	1 (2%)
47	PLM	6	804	-	17,17,17	0.56	0	17,17,17	1.14	1 (5%)
25	CLA	B	1232	-	45,53,73	1.62	8 (17%)	52,89,113	2.10	13 (25%)
25	CLA	5	606	-	50,58,73	1.54	9 (18%)	58,95,113	2.23	17 (29%)
25	CLA	B	1238	-	65,73,73	1.36	9 (13%)	76,113,113	1.97	16 (21%)
25	CLA	5	603	18	56,64,73	1.46	10 (17%)	65,102,113	2.11	17 (26%)
26	CHL	a	613	-	46,54,74	0.98	3 (6%)	49,90,114	1.38	10 (20%)
25	CLA	A	1119	-	65,73,73	1.35	8 (12%)	76,113,113	1.91	16 (21%)
25	CLA	3	606	-	65,73,73	1.34	7 (10%)	76,113,113	1.96	15 (19%)
38	LPX	F	5003	-	29,29,29	1.00	2 (6%)	31,33,33	0.93	1 (3%)
25	CLA	a	611	-	50,58,73	1.54	9 (18%)	58,95,113	2.19	16 (27%)
25	CLA	3	618	16	46,54,73	1.61	8 (17%)	53,90,113	2.10	13 (24%)
25	CLA	9	604	23	60,68,73	1.40	7 (11%)	70,107,113	2.06	19 (27%)
30	LHG	6	801	25	48,48,48	0.40	0	51,54,54	1.05	3 (5%)
28	SF4	A	3001	1,2	0,12,12	-	-	-	-	-
25	CLA	B	1210	-	65,73,73	1.35	8 (12%)	76,113,113	2.00	19 (25%)
33	PTY	7	804	-	32,32,49	1.05	4 (12%)	35,37,54	1.19	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	2	606	-	46,54,73	1.60	7 (15%)	53,90,113	2.14	15 (28%)
25	CLA	A	1135	-	51,59,73	1.55	9 (17%)	59,96,113	2.20	17 (28%)
25	CLA	6	603	-	65,73,73	1.35	10 (15%)	76,113,113	1.97	16 (21%)
40	RRX	3	506	-	42,42,42	4.92	24 (57%)	57,58,58	2.81	21 (36%)
26	CHL	9	608	-	48,56,74	0.98	3 (6%)	51,92,114	1.41	10 (19%)
26	CHL	4	613	-	52,60,74	0.95	3 (5%)	56,97,114	1.34	10 (17%)
25	CLA	5	608	-	45,53,73	1.63	8 (17%)	52,89,113	2.04	12 (23%)
25	CLA	A	1140	-	55,63,73	1.48	8 (14%)	64,101,113	2.11	17 (26%)
25	CLA	5	612	18	65,73,73	1.34	9 (13%)	76,113,113	1.97	17 (22%)
26	CHL	9	610	-	51,59,74	0.96	3 (5%)	55,96,114	1.42	12 (21%)
26	CHL	4	618	-	56,64,74	0.93	3 (5%)	61,102,114	1.31	11 (18%)
30	LHG	F	5002	-	35,35,48	0.43	0	38,41,54	1.19	3 (7%)
29	BCR	B	4006	-	41,41,41	1.83	4 (9%)	56,56,56	4.24	14 (25%)
26	CHL	6	611	-	51,59,74	0.97	3 (5%)	55,96,114	1.43	11 (20%)
29	BCR	B	4005	-	41,41,41	1.84	4 (9%)	56,56,56	4.28	12 (21%)
25	CLA	6	602	-	52,60,73	1.52	9 (17%)	60,97,113	2.13	17 (28%)
25	CLA	A	1109	25	65,73,73	1.35	8 (12%)	76,113,113	2.04	18 (23%)
25	CLA	B	1203	2	65,73,73	1.35	8 (12%)	76,113,113	1.91	15 (19%)
49	13X	6	805	-	9,9,9	0.88	0	12,12,12	0.38	0
25	CLA	L	1503	-	45,53,73	1.60	8 (17%)	52,89,113	2.16	15 (28%)
25	CLA	2	602	-	52,60,73	1.52	8 (15%)	60,97,113	2.14	17 (28%)
26	CHL	3	611	-	61,69,74	0.96	3 (4%)	67,108,114	1.32	10 (14%)
25	CLA	A	1127	-	65,73,73	1.36	6 (9%)	76,113,113	1.89	15 (19%)
25	CLA	4	616	-	50,58,73	1.56	8 (16%)	58,95,113	2.16	16 (27%)
25	CLA	3	602	-	46,54,73	1.58	8 (17%)	53,90,113	2.15	16 (30%)
43	LUT	2	507	-	42,43,43	2.38	1 (2%)	51,60,60	2.56	18 (35%)
25	CLA	8	602	-	52,60,73	1.51	8 (15%)	60,97,113	2.16	16 (26%)
25	CLA	A	1110	-	54,62,73	1.49	10 (18%)	62,99,113	2.13	16 (25%)
25	CLA	4	602	-	52,60,73	1.51	8 (15%)	60,97,113	2.14	17 (28%)
25	CLA	3	612	16	50,58,73	1.52	7 (14%)	58,95,113	2.20	15 (25%)
25	CLA	8	607	30	46,54,73	1.61	8 (17%)	53,90,113	2.12	11 (20%)
33	PTY	a	803	-	37,37,49	1.00	4 (10%)	40,42,54	1.08	2 (5%)
25	CLA	6	601	-	60,68,73	1.40	8 (13%)	70,107,113	2.05	19 (27%)
31	LMG	A	5004	-	42,42,55	0.78	2 (4%)	50,50,63	1.07	2 (4%)
33	PTY	A	5006	-	33,33,49	1.05	4 (12%)	36,38,54	1.10	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	K	1404	10	45,53,73	1.62	10 (22%)	52,89,113	2.14	13 (25%)
25	CLA	7	612	-	60,68,73	1.42	8 (13%)	70,107,113	2.01	16 (22%)
47	PLM	4	804	-	17,17,17	0.57	0	17,17,17	1.06	0
33	PTY	J	5001	-	27,27,49	1.15	4 (14%)	30,32,54	1.20	2 (6%)
45	OLA	1	803	-	19,19,19	0.56	0	19,19,19	1.03	0
24	CL0	A	1011	-	65,73,73	2.37	18 (27%)	76,113,113	2.50	21 (27%)
25	CLA	7	608	-	55,63,73	1.48	8 (14%)	64,101,113	2.10	16 (25%)
26	CHL	6	617	19	43,51,74	1.02	3 (6%)	45,86,114	1.44	9 (20%)
25	CLA	B	1022	54	65,73,73	1.38	9 (13%)	76,113,113	1.92	17 (22%)
29	BCR	O	4001	-	41,41,41	1.85	4 (9%)	56,56,56	4.63	14 (25%)
32	SQD	7	805	-	38,39,54	0.90	0	47,50,65	1.01	3 (6%)
40	RRX	J	4002	-	42,42,42	4.90	24 (57%)	57,58,58	2.66	21 (36%)
25	CLA	A	1103	-	65,73,73	1.33	7 (10%)	76,113,113	2.01	16 (21%)
30	LHG	4	802	-	31,31,48	0.46	0	34,37,54	1.22	3 (8%)
25	CLA	1	603	-	65,73,73	1.34	7 (10%)	76,113,113	1.98	16 (21%)
25	CLA	B	1212	-	57,65,73	1.43	7 (12%)	66,103,113	2.15	19 (28%)
25	CLA	B	1023	-	65,73,73	1.35	7 (10%)	76,113,113	1.96	16 (21%)
25	CLA	A	1012	-	65,73,73	1.37	8 (12%)	76,113,113	1.98	15 (19%)
25	CLA	A	1115	-	60,68,73	1.41	8 (13%)	70,107,113	2.01	16 (22%)
25	CLA	B	1224	-	65,73,73	1.36	8 (12%)	76,113,113	1.98	17 (22%)
25	CLA	B	1228	-	65,73,73	1.33	7 (10%)	76,113,113	2.04	19 (25%)
50	XAT	9	507	-	39,47,47	0.69	1 (2%)	54,74,74	1.98	14 (25%)
43	LUT	5	505	-	42,43,43	2.38	1 (2%)	51,60,60	2.28	14 (27%)
29	BCR	K	4001	-	41,41,41	1.83	4 (9%)	56,56,56	4.32	15 (26%)
25	CLA	1	608	-	60,68,73	1.40	9 (15%)	70,107,113	1.99	14 (20%)
25	CLA	a	615	15	46,54,73	1.61	8 (17%)	53,90,113	2.11	12 (22%)
30	LHG	2	801	25	48,48,48	0.36	0	51,54,54	1.03	2 (3%)
25	CLA	A	1139	-	55,63,73	1.49	9 (16%)	64,101,113	2.08	15 (23%)
25	CLA	B	1231	-	65,73,73	1.36	9 (13%)	76,113,113	1.92	14 (18%)
48	DGA	5	803	-	22,22,43	1.43	3 (13%)	24,24,45	1.33	2 (8%)
25	CLA	A	1134	1	60,68,73	1.42	9 (15%)	70,107,113	2.09	18 (25%)
25	CLA	5	605	-	46,54,73	1.61	9 (19%)	53,90,113	2.11	14 (26%)
37	PCW	B	5004	-	38,38,53	1.29	4 (10%)	44,46,61	1.07	2 (4%)
25	CLA	1	607	30	65,73,73	1.36	9 (13%)	76,113,113	1.92	15 (19%)
25	CLA	A	1125	-	65,73,73	1.38	10 (15%)	76,113,113	1.93	16 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	3	607	30	65,73,73	1.35	8 (12%)	76,113,113	1.92	16 (21%)
30	LHG	7	802	-	35,35,48	0.44	0	38,41,54	1.07	2 (5%)
29	BCR	B	4002	-	41,41,41	1.84	4 (9%)	56,56,56	4.34	14 (25%)
43	LUT	8	502	-	42,43,43	2.33	1 (2%)	51,60,60	1.90	12 (23%)
25	CLA	6	605	-	46,54,73	1.60	9 (19%)	53,90,113	2.15	14 (26%)
25	CLA	6	607	30	55,63,73	1.48	8 (14%)	64,101,113	2.05	16 (25%)
25	CLA	A	1113	-	60,68,73	1.40	7 (11%)	70,107,113	2.07	19 (27%)
41	SPH	4	805	-	19,20,20	0.64	0	18,21,21	1.08	1 (5%)
43	LUT	6	501	-	42,43,43	2.34	1 (2%)	51,60,60	1.88	14 (27%)
25	CLA	9	606	-	55,63,73	1.47	6 (10%)	64,101,113	2.06	16 (25%)
25	CLA	2	607	30	65,73,73	1.36	8 (12%)	76,113,113	1.99	16 (21%)
29	BCR	L	4002	-	41,41,41	1.83	4 (9%)	56,56,56	4.33	15 (26%)
48	DGA	3	803	-	23,23,43	1.41	3 (13%)	25,25,45	1.34	2 (8%)
25	CLA	3	605	-	65,73,73	1.34	7 (10%)	76,113,113	1.98	17 (22%)
25	CLA	L	1501	11	50,58,73	1.55	8 (16%)	58,95,113	2.22	16 (27%)
25	CLA	L	1502	-	60,68,73	1.39	8 (13%)	70,107,113	2.09	18 (25%)
26	CHL	1	609	15	66,74,74	0.86	3 (4%)	73,114,114	1.16	9 (12%)
25	CLA	6	615	54	65,73,73	1.36	8 (12%)	76,113,113	2.02	16 (21%)
26	CHL	3	604	16	66,74,74	0.92	4 (6%)	73,114,114	1.38	9 (12%)
25	CLA	A	1124	-	55,63,73	1.48	8 (14%)	64,101,113	2.09	16 (25%)
25	CLA	A	1101	-	65,73,73	1.35	8 (12%)	76,113,113	1.96	18 (23%)
25	CLA	5	601	18	60,68,73	1.40	8 (13%)	70,107,113	2.08	20 (28%)
25	CLA	O	1802	-	55,63,73	1.47	8 (14%)	64,101,113	2.19	20 (31%)
50	XAT	7	502	-	39,47,47	0.70	1 (2%)	54,74,74	1.93	11 (20%)
43	LUT	6	502	-	42,43,43	2.32	1 (2%)	51,60,60	1.98	14 (27%)
43	LUT	9	501	-	42,43,43	2.35	1 (2%)	51,60,60	1.92	13 (25%)
26	CHL	2	609	22	66,74,74	0.88	4 (6%)	73,114,114	1.23	10 (13%)
45	OLA	a	805	-	19,19,19	0.56	0	19,19,19	1.01	0
29	BCR	6	504	-	41,41,41	1.85	4 (9%)	56,56,56	4.42	17 (30%)
25	CLA	B	1207	-	60,68,73	1.41	7 (11%)	70,107,113	1.97	15 (21%)
25	CLA	A	1129	-	50,58,73	1.54	9 (18%)	58,95,113	2.19	17 (29%)
43	LUT	3	502	-	42,43,43	2.39	1 (2%)	51,60,60	1.96	13 (25%)
26	CHL	5	617	18	47,55,74	0.98	3 (6%)	50,91,114	1.46	11 (22%)
26	CHL	1	610	-	48,56,74	0.90	2 (4%)	51,92,114	1.46	12 (23%)
32	SQD	I	5001	-	53,54,54	0.80	0	62,65,65	0.89	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	A	1117	-	65,73,73	1.34	7 (10%)	76,113,113	2.11	17 (22%)
26	CHL	3	603	16	66,74,74	0.92	4 (6%)	73,114,114	1.16	8 (10%)
25	CLA	a	607	-	58,66,73	1.44	9 (15%)	67,104,113	2.08	16 (23%)
29	BCR	A	4002	-	41,41,41	1.80	4 (9%)	56,56,56	4.10	14 (25%)
25	CLA	B	1219	2	59,67,73	1.42	8 (13%)	68,105,113	2.07	17 (25%)
25	CLA	A	1120	-	49,57,73	1.55	8 (16%)	55,93,113	2.26	16 (29%)
35	LMT	A	5008	-	36,36,36	1.18	6 (16%)	47,47,47	1.00	2 (4%)
30	LHG	B	5002	-	48,48,48	0.39	0	51,54,54	1.07	3 (5%)
25	CLA	B	1211	-	55,63,73	1.46	8 (14%)	64,101,113	2.14	20 (31%)
25	CLA	B	1222	-	58,66,73	1.42	7 (12%)	67,104,113	2.09	17 (25%)
29	BCR	L	4001	-	41,41,41	1.83	4 (9%)	56,56,56	4.29	16 (28%)
45	OLA	8	808	-	19,19,19	0.56	0	19,19,19	1.03	0
25	CLA	a	612	15	57,65,73	1.45	9 (15%)	66,103,113	2.02	15 (22%)
25	CLA	B	1214	-	59,67,73	1.43	8 (13%)	68,105,113	2.09	16 (23%)
25	CLA	4	605	-	46,54,73	1.61	8 (17%)	53,90,113	2.11	13 (24%)
25	CLA	4	607	-	55,63,73	1.48	8 (14%)	64,101,113	2.11	17 (26%)
25	CLA	6	612	-	50,58,73	1.54	8 (16%)	58,95,113	2.19	15 (25%)
25	CLA	7	604	20	65,73,73	1.35	8 (12%)	76,113,113	2.01	17 (22%)
29	BCR	L	4003	-	41,41,41	1.85	4 (9%)	56,56,56	4.35	15 (26%)
33	PTY	5	802	-	37,37,49	0.99	4 (10%)	40,42,54	1.16	2 (5%)
44	AXT	1	502	-	44,44,45	2.95	15 (34%)	55,62,64	1.98	13 (23%)
25	CLA	B	1021	-	65,73,73	1.36	8 (12%)	76,113,113	1.95	15 (19%)
26	CHL	1	604	-	66,74,74	0.92	4 (6%)	73,114,114	1.32	9 (12%)
25	CLA	4	615	17	60,68,73	1.42	8 (13%)	70,107,113	1.96	15 (21%)
30	LHG	6	802	-	36,36,48	0.43	0	39,42,54	1.24	3 (7%)
28	SF4	C	3003	3	0,12,12	-	-	-	-	-
42	ECH	M	4001	-	42,42,42	0.87	1 (2%)	55,58,58	2.00	14 (25%)
25	CLA	A	1105	-	57,65,73	1.45	9 (15%)	66,103,113	2.07	15 (22%)
50	XAT	9	504	-	39,47,47	0.66	1 (2%)	54,74,74	6.69	16 (29%)
25	CLA	B	1205	-	65,73,73	1.35	10 (15%)	76,113,113	2.03	16 (21%)
25	CLA	O	1801	-	36,46,73	1.77	8 (22%)	41,80,113	2.17	12 (29%)
43	LUT	4	502	-	42,43,43	2.34	1 (2%)	51,60,60	1.93	13 (25%)
25	CLA	B	1237	-	65,73,73	1.36	9 (13%)	76,113,113	1.92	15 (19%)
30	LHG	9	802	-	48,48,48	0.38	0	51,54,54	1.13	3 (5%)
43	LUT	5	501	-	42,43,43	2.34	1 (2%)	51,60,60	1.92	14 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	1	602	-	45,53,73	1.63	9 (20%)	52,89,113	2.10	13 (25%)
46	QTB	a	504	-	19,19,19	2.54	5 (26%)	20,26,26	2.83	8 (40%)
25	CLA	B	1221	-	65,73,73	1.34	10 (15%)	76,113,113	2.03	18 (23%)
25	CLA	F	1301	-	50,58,73	1.55	7 (14%)	58,95,113	2.20	15 (25%)
29	BCR	3	504	-	41,41,41	1.84	4 (9%)	56,56,56	4.33	17 (30%)
25	CLA	5	615	18	46,54,73	1.61	8 (17%)	53,90,113	2.12	13 (24%)
43	LUT	a	502	-	42,43,43	2.35	1 (2%)	51,60,60	1.97	14 (27%)
25	CLA	B	1209	-	65,73,73	1.36	8 (12%)	76,113,113	1.98	16 (21%)
25	CLA	1	601	-	60,68,73	1.40	8 (13%)	70,107,113	2.03	17 (24%)
29	BCR	B	4001	-	41,41,41	1.83	4 (9%)	56,56,56	4.28	13 (23%)
25	CLA	A	1130	-	56,64,73	1.46	7 (12%)	65,102,113	2.08	15 (23%)
25	CLA	A	1013	-	65,73,73	1.33	7 (10%)	76,113,113	1.91	17 (22%)
29	BCR	7	503	-	41,41,41	1.82	4 (9%)	56,56,56	4.31	17 (30%)
25	CLA	7	605	-	43,52,73	1.65	8 (18%)	49,88,113	2.06	15 (30%)
25	CLA	7	607	30	59,67,73	1.42	8 (13%)	68,105,113	2.04	13 (19%)
25	CLA	4	612	17	62,70,73	1.37	7 (11%)	72,109,113	2.07	17 (23%)
37	PCW	K	5001	-	40,40,53	1.26	4 (10%)	46,48,61	1.08	2 (4%)
25	CLA	A	1106	1	65,73,73	1.35	8 (12%)	76,113,113	2.02	17 (22%)
25	CLA	A	1123	-	65,73,73	1.36	10 (15%)	76,113,113	2.02	16 (21%)
29	BCR	B	4007	-	41,41,41	1.83	4 (9%)	56,56,56	4.34	15 (26%)
47	PLM	5	804	-	17,17,17	0.57	0	17,17,17	1.13	0
26	CHL	2	613	-	51,59,74	0.96	3 (5%)	55,96,114	1.38	9 (16%)
25	CLA	a	605	-	55,63,73	1.46	8 (14%)	64,101,113	2.14	18 (28%)
25	CLA	5	609	18	51,59,73	1.53	7 (13%)	59,96,113	2.15	17 (28%)
26	CHL	7	609	20	62,70,74	0.89	3 (4%)	68,109,114	1.26	10 (14%)
25	CLA	H	1701	-	55,63,73	1.47	7 (12%)	64,101,113	2.12	15 (23%)
25	CLA	A	1126	-	65,73,73	1.37	9 (13%)	76,113,113	1.98	17 (22%)
25	CLA	B	1218	-	55,63,73	1.46	7 (12%)	64,101,113	2.23	18 (28%)
25	CLA	H	1703	-	55,63,73	1.47	8 (14%)	64,101,113	2.09	15 (23%)
35	LMT	1	804	-	36,36,36	1.16	6 (16%)	47,47,47	1.02	3 (6%)
43	LUT	7	501	-	42,43,43	2.38	1 (2%)	51,60,60	2.06	11 (21%)
29	BCR	3	503	-	41,41,41	1.83	4 (9%)	56,56,56	4.31	15 (26%)
33	PTY	a	802	-	37,37,49	1.00	4 (10%)	40,42,54	1.10	2 (5%)
29	BCR	4	503	-	41,41,41	1.85	4 (9%)	56,56,56	4.37	12 (21%)
43	LUT	5	502	-	42,43,43	2.33	1 (2%)	51,60,60	1.90	11 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	A	1138	-	65,73,73	1.35	9 (13%)	76,113,113	1.89	16 (21%)
25	CLA	8	620	-	45,53,73	1.62	10 (22%)	52,89,113	2.16	15 (28%)
26	CHL	7	613	-	61,69,74	0.92	4 (6%)	67,108,114	1.23	11 (16%)
25	CLA	1	606	-	57,65,73	1.42	8 (14%)	66,103,113	2.19	17 (25%)
29	BCR	8	503	-	41,41,41	1.85	4 (9%)	56,56,56	4.24	12 (21%)
25	CLA	H	1702	8	46,54,73	1.60	9 (19%)	53,90,113	2.20	13 (24%)
25	CLA	B	1236	-	53,61,73	1.50	9 (16%)	61,98,113	2.11	17 (27%)
29	BCR	K	4002	-	41,41,41	1.84	4 (9%)	56,56,56	4.29	16 (28%)
25	CLA	5	602	-	52,60,73	1.51	8 (15%)	60,97,113	2.12	16 (26%)
25	CLA	a	602	-	50,58,73	1.55	8 (16%)	58,95,113	2.17	17 (29%)
29	BCR	A	4004	-	41,41,41	1.83	4 (9%)	56,56,56	4.31	18 (32%)
36	DGD	7	806	-	51,51,67	0.92	3 (5%)	65,65,81	1.03	3 (4%)
26	CHL	4	609	17	66,74,74	0.84	3 (4%)	73,114,114	1.25	10 (13%)
25	CLA	B	1227	-	50,58,73	1.55	9 (18%)	58,95,113	2.24	18 (31%)
25	CLA	6	618	-	46,54,73	1.61	8 (17%)	53,90,113	2.08	13 (24%)
25	CLA	2	615	-	56,64,73	1.46	8 (14%)	65,102,113	2.12	16 (24%)
30	LHG	1	802	-	48,48,48	0.40	0	51,54,54	1.00	3 (5%)
30	LHG	1	801	25	34,34,48	0.44	0	37,40,54	1.15	3 (8%)
30	LHG	5	801	-	48,48,48	0.38	0	51,54,54	1.08	3 (5%)
25	CLA	A	1132	-	65,73,73	1.34	8 (12%)	76,113,113	2.00	17 (22%)
26	CHL	8	601	21	61,69,74	0.99	4 (6%)	67,108,114	1.41	9 (13%)
26	CHL	8	613	-	51,59,74	0.97	3 (5%)	55,96,114	1.39	9 (16%)
25	CLA	9	602	-	46,54,73	1.58	7 (15%)	53,90,113	2.13	16 (30%)

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
25	CLA	G	1602	7	1/1/14/20	12/31/109/115	-
43	LUT	4	501	-	1/1/12/27	6/29/67/67	0/2/2/2
25	CLA	9	607	-	1/1/11/20	8/16/94/115	-
26	CHL	1	611	-	4/4/18/26	4/27/125/137	-
47	PLM	8	806	-	-	6/13/14/15	-
25	CLA	B	1204	-	1/1/15/20	19/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	A	1141	-	1/1/11/20	7/13/91/115	-
26	CHL	6	619	19	5/5/20/26	10/39/137/137	-
33	PTY	G	5002	-	-	10/30/30/53	-
25	CLA	a	601	-	1/1/14/20	9/31/109/115	-
26	CHL	a	606	-	4/4/18/26	6/27/125/137	-
26	CHL	6	613	-	3/3/17/26	1/21/119/137	-
26	CHL	8	603	21	4/4/20/26	8/39/137/137	-
41	SPH	6	806	-	-	9/21/21/21	-
25	CLA	6	608	-	1/1/13/20	7/25/103/115	-
43	LUT	a	503	-	-	6/29/67/67	0/2/2/2
30	LHG	F	5001	-	-	28/47/47/53	-
25	CLA	3	610	16	1/1/13/20	13/28/106/115	-
25	CLA	G	1603	-	1/1/11/20	5/13/91/115	-
29	BCR	A	4005	-	-	16/29/63/63	0/2/2/2
25	CLA	A	1102	25	1/1/13/20	10/25/103/115	-
25	CLA	O	1803	-	1/1/10/20	5/8/86/115	-
25	CLA	A	1118	-	1/1/13/20	13/25/103/115	-
25	CLA	A	1116	-	1/1/14/20	13/31/109/115	-
27	PQN	A	2001	-	-	7/23/43/43	0/2/2/2
25	CLA	9	605	-	1/1/14/20	12/31/109/115	-
34	3PH	A	5007	-	-	17/34/34/49	-
26	CHL	9	601	-	4/4/20/26	8/39/137/137	-
26	CHL	9	613	-	3/3/15/26	0/10/108/137	-
29	BCR	B	4004	-	-	9/29/63/63	0/2/2/2
26	CHL	2	610	-	4/4/16/26	0/18/116/137	-
30	LHG	8	801	25	-	28/41/41/53	-
25	CLA	7	602	-	1/1/11/20	4/11/89/115	-
41	SPH	9	804	-	-	13/21/21/21	-
25	CLA	A	1111	-	1/1/15/20	21/37/115/115	-
25	CLA	9	612	-	1/1/15/20	13/37/115/115	-
26	CHL	8	610	-	5/5/18/26	4/27/125/137	-
25	CLA	5	607	-	1/1/14/20	15/31/109/115	-
25	CLA	2	608	-	1/1/11/20	7/13/91/115	-
25	CLA	4	610	-	1/1/15/20	20/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LMT	2	804	-	-	6/21/61/61	0/2/2/2
52	P5S	8	805	-	-	23/42/42/59	-
25	CLA	8	608	-	1/1/12/20	8/22/100/115	-
25	CLA	B	1235	-	1/1/15/20	21/37/115/115	-
47	PLM	4	803	-	-	5/13/14/15	-
26	CHL	7	611	-	4/4/18/26	7/27/125/137	-
25	CLA	A	1121	-	1/1/14/20	19/31/109/115	-
26	CHL	7	617	20	4/4/20/26	13/39/137/137	-
28	SF4	C	3002	3	-	-	0/6/5/5
26	CHL	6	610	-	4/4/18/26	6/27/125/137	-
30	LHG	3	801	25	-	33/53/53/53	-
25	CLA	a	608	-	1/1/13/20	10/25/103/115	-
25	CLA	8	618	21	1/1/14/20	17/31/109/115	-
39	NEX	F	4001	-	1/1/12/25	14/27/83/83	0/3/3/3
30	LHG	9	801	-	-	18/37/37/53	-
26	CHL	6	609	19	4/4/20/26	10/39/137/137	-
33	PTY	3	802	-	-	17/41/41/53	-
25	CLA	B	1240	30	1/1/15/20	12/37/115/115	-
25	CLA	B	1239	-	1/1/15/20	18/37/115/115	-
25	CLA	3	613	-	1/1/14/20	12/33/111/115	-
50	XAT	2	501	-	2/2/12/26	0/31/93/93	0/4/4/4
53	LAP	8	810	-	-	15/30/30/30	-
25	CLA	B	1225	-	1/1/15/20	6/37/115/115	-
25	CLA	6	604	19	1/1/15/20	16/37/115/115	-
25	CLA	5	614	18	1/1/11/20	6/15/93/115	-
25	CLA	4	608	-	1/1/12/20	6/21/99/115	-
25	CLA	A	1112	-	1/1/13/20	16/25/103/115	-
25	CLA	K	1401	-	1/1/11/20	6/15/93/115	-
25	CLA	7	601	20	1/1/14/20	16/31/109/115	-
36	DGD	B	5003	-	-	22/55/95/95	0/2/2/2
32	SQD	H	5001	-	-	8/40/60/69	0/1/1/1
25	CLA	B	1217	-	1/1/13/20	12/27/105/115	-
29	BCR	5	504	-	-	12/29/63/63	0/2/2/2
30	LHG	A	5002	-	-	37/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	DGD	8	802	-	-	18/48/88/95	0/2/2/2
25	CLA	A	1104	1	1/1/15/20	17/37/115/115	-
25	CLA	A	1137	-	1/1/14/20	14/31/109/115	-
25	CLA	4	606	-	1/1/12/20	8/19/97/115	-
30	LHG	a	801	-	-	24/39/39/53	-
33	PTY	9	803	-	-	26/51/51/53	-
27	PQN	B	2002	-	-	8/23/43/43	0/2/2/2
25	CLA	2	604	-	1/1/13/20	13/27/105/115	-
32	SQD	G	5001	-	-	20/41/61/69	0/1/1/1
29	BCR	B	4003	-	-	7/29/63/63	0/2/2/2
37	PCW	6	803	-	-	22/39/39/57	-
25	CLA	8	606	-	1/1/13/20	15/28/106/115	-
48	DGA	2	803	-	-	28/38/38/45	-
25	CLA	1	615	15	1/1/11/20	12/15/93/115	-
25	CLA	2	605	-	1/1/14/20	18/31/109/115	-
29	BCR	A	4003	-	-	12/29/63/63	0/2/2/2
25	CLA	2	621	22	1/1/15/20	16/37/115/115	-
26	CHL	7	615	20	3/3/17/26	5/21/119/137	-
25	CLA	4	601	-	1/1/14/20	10/31/109/115	-
44	AXT	7	504	-	-	14/29/71/75	0/2/2/2
25	CLA	8	605	-	1/1/13/20	13/25/103/115	-
25	CLA	B	1202	-	1/1/15/20	17/37/115/115	-
29	BCR	5	503	-	-	13/29/63/63	0/2/2/2
26	CHL	A	1114	-	4/4/20/26	9/39/137/137	-
45	OLA	8	809	-	-	11/17/17/17	-
26	CHL	a	610	-	3/3/16/26	0/18/116/137	-
25	CLA	2	612	-	1/1/12/20	10/19/97/115	-
26	CHL	9	603	-	4/4/20/26	8/39/137/137	-
25	CLA	8	615	21	1/1/11/20	9/15/93/115	-
30	LHG	7	803	-	-	22/39/39/53	-
25	CLA	B	1206	2	1/1/15/20	23/37/115/115	-
25	CLA	B	1229	-	1/1/15/20	12/37/115/115	-
25	CLA	B	1220	-	1/1/14/20	15/31/109/115	-
43	LUT	2	502	-	-	2/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	K	1403	10	1/1/11/20	11/18/96/115	-
25	CLA	2	601	-	1/1/14/20	11/31/109/115	-
26	CHL	1	613	-	3/3/16/26	2/18/116/137	-
51	4RF	7	807	-	-	19/39/39/59	-
30	LHG	B	5001	25	-	34/53/53/53	-
25	CLA	9	609	23	1/1/11/20	6/15/93/115	-
25	CLA	4	603	17	1/1/13/20	9/27/105/115	-
30	LHG	7	801	25	-	26/41/41/53	-
25	CLA	B	1230	-	1/1/13/20	11/29/107/115	-
25	CLA	B	1226	-	1/1/15/20	11/37/115/115	-
25	CLA	B	1213	-	1/1/13/20	14/25/103/115	-
43	LUT	9	502	-	-	3/29/67/67	0/2/2/2
33	PTY	G	5003	-	-	13/30/30/53	-
30	LHG	4	801	-	-	30/53/53/53	-
25	CLA	B	1234	-	-	21/48/87/115	0/5/5/9
25	CLA	F	1302	-	1/1/13/20	10/25/103/115	-
29	BCR	I	4001	-	-	15/29/63/63	0/2/2/2
26	CHL	5	611	-	3/3/17/26	1/21/119/137	-
25	CLA	2	603	22	1/1/14/20	12/31/109/115	-
29	BCR	H	4001	-	-	12/29/63/63	0/2/2/2
25	CLA	B	1201	-	1/1/15/20	21/37/115/115	-
43	LUT	1	503	-	-	8/29/67/67	0/2/2/2
25	CLA	8	612	-	1/1/12/20	8/19/97/115	-
25	CLA	6	606	19	1/1/15/20	14/37/115/115	-
43	LUT	1	501	-	-	3/29/67/67	0/2/2/2
25	CLA	5	604	18	1/1/15/20	13/37/115/115	-
30	LHG	2	802	-	-	39/53/53/53	-
29	BCR	G	4001	-	-	12/29/63/63	0/2/2/2
32	SQD	A	5005	-	-	20/49/69/69	0/1/1/1
30	LHG	A	5001	-	-	32/53/53/53	-
25	CLA	4	611	-	1/1/13/20	9/27/105/115	-
36	DGD	8	803	-	-	18/35/75/95	0/2/2/2
33	PTY	B	5005	-	-	20/45/45/53	-
25	CLA	7	606	-	1/1/13/20	12/23/101/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	PLM	8	807	-	-	5/15/15/15	-
26	CHL	5	610	-	4/4/20/26	10/39/137/137	-
25	CLA	A	1122	-	1/1/14/20	19/31/109/115	-
29	BCR	6	503	-	-	16/29/63/63	0/2/2/2
37	PCW	K	5002	-	-	17/39/39/57	-
26	CHL	3	608	-	3/3/15/26	1/12/110/137	-
29	BCR	3	505	-	-	11/29/63/63	0/2/2/2
25	CLA	B	1208	-	1/1/13/20	11/25/101/115	-
25	CLA	K	1402	-	1/1/14/20	10/31/109/115	-
29	BCR	J	4001	-	-	11/29/63/63	0/2/2/2
26	CHL	8	604	21	4/4/19/26	13/35/133/137	-
43	LUT	8	501	-	-	3/29/67/67	0/2/2/2
25	CLA	1	612	15	1/1/15/20	21/37/115/115	-
26	CHL	a	609	15	3/3/17/26	4/24/122/137	-
25	CLA	A	1131	-	1/1/15/20	12/37/115/115	-
25	CLA	A	1133	-	1/1/15/20	20/37/115/115	-
25	CLA	4	617	-	1/1/11/20	6/13/91/115	-
26	CHL	5	613	-	4/4/18/26	3/27/125/137	-
25	CLA	A	1108	-	1/1/15/20	16/37/115/115	-
25	CLA	7	603	20	1/1/15/20	24/37/115/115	-
26	CHL	a	604	-	4/4/19/26	7/33/131/137	-
30	LHG	A	5003	-	-	26/50/50/53	-
43	LUT	3	501	-	-	3/29/67/67	0/2/2/2
26	CHL	5	618	-	3/3/17/26	2/21/119/137	-
25	CLA	3	616	-	1/1/13/20	13/27/105/115	-
25	CLA	B	1216	-	1/1/15/20	20/37/115/115	-
25	CLA	1	605	-	1/1/15/20	20/37/115/115	-
25	CLA	3	601	16	1/1/15/20	14/37/115/115	-
25	CLA	A	1136	-	1/1/15/20	15/37/115/115	-
25	CLA	J	1901	9	1/1/10/20	6/10/88/115	-
25	CLA	7	610	-	1/1/14/20	17/31/109/115	-
48	DGA	8	804	-	-	23/41/41/45	-
25	CLA	8	609	21	1/1/14/20	15/31/109/115	-
25	CLA	a	603	-	1/1/15/20	18/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	G	1601	-	1/1/12/20	11/19/97/115	-
29	BCR	A	4001	-	-	13/29/63/63	0/2/2/2
25	CLA	A	1128	-	1/1/15/20	20/37/115/115	-
25	CLA	8	611	-	1/1/12/20	6/19/97/115	-
25	CLA	B	1223	-	1/1/15/20	13/37/115/115	-
47	PLM	a	804	-	-	4/13/14/15	-
43	LUT	a	501	-	-	5/29/67/67	0/2/2/2
25	CLA	A	1107	1	1/1/13/20	9/25/103/115	-
25	CLA	L	1504	-	1/1/12/20	9/19/97/115	-
25	CLA	4	604	-	1/1/14/20	11/31/109/115	-
25	CLA	B	1215	-	1/1/14/20	16/31/109/115	-
41	SPH	J	5002	-	-	12/21/21/21	-
35	LMT	B	5006	-	-	9/21/61/61	0/2/2/2
47	PLM	6	804	-	-	8/15/15/15	-
25	CLA	B	1232	-	1/1/11/20	7/13/91/115	-
25	CLA	5	606	-	1/1/12/20	10/19/97/115	-
25	CLA	B	1238	-	1/1/15/20	9/37/115/115	-
25	CLA	5	603	18	1/1/13/20	16/27/105/115	-
26	CHL	a	613	-	3/3/16/26	6/15/113/137	-
25	CLA	A	1119	-	1/1/15/20	20/37/115/115	-
25	CLA	3	606	-	1/1/15/20	16/37/115/115	-
38	LPX	F	5003	-	-	12/31/31/31	-
25	CLA	a	611	-	1/1/12/20	8/19/97/115	-
25	CLA	3	618	16	1/1/11/20	4/15/93/115	-
25	CLA	9	604	23	1/1/14/20	7/31/109/115	-
30	LHG	6	801	25	-	34/53/53/53	-
28	SF4	A	3001	1,2	-	-	0/6/5/5
25	CLA	B	1210	-	1/1/15/20	21/37/115/115	-
33	PTY	7	804	-	-	16/36/36/53	-
25	CLA	2	606	-	1/1/11/20	4/15/93/115	-
25	CLA	A	1135	-	1/1/12/20	7/21/99/115	-
25	CLA	6	603	-	1/1/15/20	15/37/115/115	-
40	RRX	3	506	-	1/1/11/25	11/29/65/65	0/2/2/2
26	CHL	9	608	-	3/3/16/26	5/18/116/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CHL	4	613	-	3/3/17/26	4/23/121/137	-
25	CLA	5	608	-	1/1/11/20	6/13/91/115	-
25	CLA	A	1140	-	1/1/13/20	11/25/103/115	-
25	CLA	5	612	18	1/1/15/20	24/37/115/115	-
26	CHL	9	610	-	3/3/17/26	2/21/119/137	-
26	CHL	4	618	-	4/4/18/26	4/27/125/137	-
30	LHG	F	5002	-	-	19/40/40/53	-
29	BCR	B	4006	-	-	15/29/63/63	0/2/2/2
26	CHL	6	611	-	3/3/17/26	5/21/119/137	-
29	BCR	B	4005	-	-	15/29/63/63	0/2/2/2
25	CLA	6	602	-	1/1/12/20	8/22/100/115	-
25	CLA	A	1109	25	1/1/15/20	19/37/115/115	-
25	CLA	B	1203	2	1/1/15/20	13/37/115/115	-
49	13X	6	805	-	-	-	0/1/1/1
25	CLA	L	1503	-	1/1/11/20	7/13/91/115	-
25	CLA	2	602	-	1/1/12/20	11/22/100/115	-
26	CHL	3	611	-	4/4/19/26	9/33/131/137	-
25	CLA	A	1127	-	1/1/15/20	17/37/115/115	-
25	CLA	4	616	-	1/1/12/20	6/19/97/115	-
25	CLA	3	602	-	1/1/11/20	5/15/93/115	-
43	LUT	2	507	-	1/1/12/27	19/29/67/67	0/2/2/2
25	CLA	8	602	-	1/1/12/20	4/22/100/115	-
25	CLA	A	1110	-	1/1/12/20	9/24/102/115	-
25	CLA	4	602	-	1/1/12/20	7/22/100/115	-
25	CLA	3	612	16	1/1/12/20	6/19/97/115	-
25	CLA	8	607	30	1/1/11/20	6/15/93/115	-
33	PTY	a	803	-	-	24/41/41/53	-
25	CLA	6	601	-	1/1/14/20	13/31/109/115	-
31	LMG	A	5004	-	-	4/37/57/70	0/1/1/1
33	PTY	A	5006	-	-	14/37/37/53	-
25	CLA	K	1404	10	1/1/11/20	5/13/91/115	-
25	CLA	7	612	-	1/1/14/20	15/31/109/115	-
47	PLM	4	804	-	-	9/15/15/15	-
33	PTY	J	5001	-	-	21/31/31/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	OLA	1	803	-	-	6/17/17/17	-
24	CL0	A	1011	-	3/3/20/25	10/37/135/135	-
25	CLA	7	608	-	1/1/13/20	10/25/103/115	-
26	CHL	6	617	19	3/3/15/26	1/12/110/137	-
25	CLA	B	1022	54	1/1/15/20	13/37/115/115	-
29	BCR	O	4001	-	-	13/29/63/63	0/2/2/2
32	SQD	7	805	-	-	10/34/54/69	0/1/1/1
40	RRX	J	4002	-	1/1/11/25	13/29/65/65	0/2/2/2
25	CLA	A	1103	-	1/1/15/20	19/37/115/115	-
30	LHG	4	802	-	-	23/36/36/53	-
25	CLA	1	603	-	1/1/15/20	15/37/115/115	-
25	CLA	B	1212	-	1/1/13/20	12/28/106/115	-
25	CLA	B	1023	-	1/1/15/20	17/37/115/115	-
25	CLA	A	1012	-	1/1/15/20	13/37/115/115	-
25	CLA	A	1115	-	1/1/14/20	15/31/109/115	-
25	CLA	B	1224	-	1/1/15/20	21/37/115/115	-
25	CLA	B	1228	-	1/1/15/20	18/37/115/115	-
50	XAT	9	507	-	1/1/12/26	8/31/93/93	0/4/4/4
43	LUT	5	505	-	-	10/29/67/67	0/2/2/2
29	BCR	K	4001	-	-	10/29/63/63	0/2/2/2
25	CLA	1	608	-	1/1/14/20	15/31/109/115	-
25	CLA	a	615	15	1/1/11/20	4/15/93/115	-
30	LHG	2	801	25	-	31/53/53/53	-
25	CLA	A	1139	-	1/1/13/20	11/25/103/115	-
25	CLA	B	1231	-	1/1/15/20	17/37/115/115	-
48	DGA	5	803	-	-	14/24/24/45	-
25	CLA	A	1134	1	1/1/14/20	14/31/109/115	-
25	CLA	5	605	-	1/1/11/20	3/15/93/115	-
37	PCW	B	5004	-	-	24/42/42/57	-
25	CLA	1	607	30	1/1/15/20	18/37/115/115	-
25	CLA	A	1125	-	1/1/15/20	25/37/115/115	-
25	CLA	3	607	30	1/1/15/20	18/37/115/115	-
30	LHG	7	802	-	-	20/40/40/53	-
29	BCR	B	4002	-	-	16/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	LUT	8	502	-	-	5/29/67/67	0/2/2/2
25	CLA	6	605	-	1/1/11/20	6/15/93/115	-
25	CLA	6	607	30	1/1/13/20	10/25/103/115	-
25	CLA	A	1113	-	1/1/14/20	14/31/109/115	-
41	SPH	4	805	-	-	9/21/21/21	-
43	LUT	6	501	-	-	3/29/67/67	0/2/2/2
25	CLA	9	606	-	1/1/13/20	7/25/103/115	-
25	CLA	2	607	30	1/1/15/20	15/37/115/115	-
29	BCR	L	4002	-	-	11/29/63/63	0/2/2/2
48	DGA	3	803	-	-	14/25/25/45	-
25	CLA	3	605	-	1/1/15/20	16/37/115/115	-
25	CLA	L	1501	11	1/1/12/20	10/19/97/115	-
25	CLA	L	1502	-	1/1/14/20	14/31/109/115	-
26	CHL	1	609	15	4/4/20/26	12/39/137/137	-
25	CLA	6	615	54	1/1/15/20	15/37/115/115	-
26	CHL	3	604	16	4/4/20/26	8/39/137/137	-
25	CLA	A	1124	-	1/1/13/20	7/25/103/115	-
25	CLA	A	1101	-	1/1/15/20	24/37/115/115	-
25	CLA	5	601	18	1/1/14/20	12/31/109/115	-
25	CLA	O	1802	-	1/1/13/20	13/25/103/115	-
50	XAT	7	502	-	2/2/12/26	0/31/93/93	0/4/4/4
43	LUT	6	502	-	-	3/29/67/67	0/2/2/2
43	LUT	9	501	-	-	3/29/67/67	0/2/2/2
26	CHL	2	609	22	4/4/20/26	11/39/137/137	-
45	OLA	a	805	-	-	7/17/17/17	-
29	BCR	6	504	-	-	13/29/63/63	0/2/2/2
25	CLA	B	1207	-	1/1/14/20	18/31/109/115	-
25	CLA	A	1129	-	1/1/12/20	9/19/97/115	-
43	LUT	3	502	-	-	2/29/67/67	0/2/2/2
26	CHL	5	617	18	3/3/16/26	1/17/115/137	-
26	CHL	1	610	-	3/3/16/26	2/18/116/137	-
32	SQD	I	5001	-	-	23/49/69/69	0/1/1/1
25	CLA	A	1117	-	1/1/15/20	18/37/115/115	-
26	CHL	3	603	16	4/4/20/26	8/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	a	607	-	1/1/13/20	14/29/107/115	-
29	BCR	A	4002	-	-	9/29/63/63	0/2/2/2
25	CLA	B	1219	2	1/1/13/20	14/30/108/115	-
25	CLA	A	1120	-	1/1/11/20	7/18/96/115	-
35	LMT	A	5008	-	-	10/21/61/61	0/2/2/2
30	LHG	B	5002	-	-	29/53/53/53	-
25	CLA	B	1211	-	1/1/13/20	11/25/103/115	-
25	CLA	B	1222	-	1/1/13/20	8/29/107/115	-
29	BCR	L	4001	-	-	12/29/63/63	0/2/2/2
45	OLA	8	808	-	-	5/17/17/17	-
25	CLA	a	612	15	1/1/13/20	10/28/106/115	-
25	CLA	B	1214	-	1/1/13/20	17/30/108/115	-
25	CLA	4	605	-	1/1/11/20	5/15/93/115	-
25	CLA	4	607	-	1/1/13/20	9/25/103/115	-
25	CLA	6	612	-	1/1/12/20	11/19/97/115	-
25	CLA	7	604	20	1/1/15/20	16/37/115/115	-
29	BCR	L	4003	-	-	10/29/63/63	0/2/2/2
33	PTY	5	802	-	-	23/41/41/53	-
44	AXT	1	502	-	-	10/29/71/75	0/2/2/2
25	CLA	B	1021	-	1/1/15/20	18/37/115/115	-
26	CHL	1	604	-	4/4/20/26	10/39/137/137	-
25	CLA	4	615	17	1/1/14/20	13/31/109/115	-
30	LHG	6	802	-	-	25/41/41/53	-
28	SF4	C	3003	3	-	-	0/6/5/5
42	ECH	M	4001	-	-	5/29/66/66	0/2/2/2
25	CLA	A	1105	-	1/1/13/20	4/28/106/115	-
50	XAT	9	504	-	1/1/12/26	13/31/93/93	0/4/4/4
25	CLA	B	1205	-	1/1/15/20	12/37/115/115	-
25	CLA	O	1801	-	1/1/9/20	0/4/78/115	-
43	LUT	4	502	-	-	4/29/67/67	0/2/2/2
25	CLA	B	1237	-	1/1/15/20	20/37/115/115	-
30	LHG	9	802	-	-	27/53/53/53	-
43	LUT	5	501	-	-	2/29/67/67	0/2/2/2
25	CLA	1	602	-	1/1/11/20	6/13/91/115	-
46	QTB	a	504	-	1/1/5/10	1/11/28/28	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	1221	-	1/1/15/20	9/37/115/115	-
25	CLA	F	1301	-	1/1/12/20	11/19/97/115	-
29	BCR	3	504	-	-	11/29/63/63	0/2/2/2
25	CLA	5	615	18	1/1/11/20	8/15/93/115	-
43	LUT	a	502	-	-	1/29/67/67	0/2/2/2
25	CLA	B	1209	-	1/1/15/20	16/37/115/115	-
25	CLA	1	601	-	1/1/14/20	14/31/109/115	-
29	BCR	B	4001	-	-	11/29/63/63	0/2/2/2
25	CLA	A	1130	-	1/1/13/20	11/27/105/115	-
25	CLA	A	1013	-	1/1/15/20	18/37/115/115	-
29	BCR	7	503	-	-	11/29/63/63	0/2/2/2
25	CLA	7	605	-	1/1/11/20	4/11/89/115	-
25	CLA	7	607	30	1/1/13/20	11/29/107/115	-
25	CLA	4	612	17	1/1/14/20	17/34/112/115	-
37	PCW	K	5001	-	-	22/44/44/57	-
25	CLA	A	1106	1	1/1/15/20	19/37/115/115	-
25	CLA	A	1123	-	1/1/15/20	11/37/115/115	-
29	BCR	B	4007	-	-	7/29/63/63	0/2/2/2
47	PLM	5	804	-	-	3/15/15/15	-
26	CHL	2	613	-	3/3/17/26	1/21/119/137	-
25	CLA	a	605	-	1/1/13/20	10/25/103/115	-
25	CLA	5	609	18	1/1/12/20	12/21/99/115	-
26	CHL	7	609	20	4/4/19/26	10/35/133/137	-
25	CLA	H	1701	-	1/1/13/20	10/25/103/115	-
25	CLA	A	1126	-	1/1/15/20	22/37/115/115	-
25	CLA	B	1218	-	1/1/13/20	7/25/103/115	-
25	CLA	H	1703	-	1/1/13/20	9/25/103/115	-
35	LMT	1	804	-	-	12/21/61/61	0/2/2/2
43	LUT	7	501	-	1/1/12/27	6/29/67/67	0/2/2/2
29	BCR	3	503	-	-	12/29/63/63	0/2/2/2
33	PTY	a	802	-	-	22/41/41/53	-
29	BCR	4	503	-	-	15/29/63/63	0/2/2/2
43	LUT	5	502	-	-	3/29/67/67	0/2/2/2
25	CLA	A	1138	-	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	8	620	-	1/1/11/20	8/13/91/115	-
26	CHL	7	613	-	4/4/19/26	4/33/131/137	-
25	CLA	1	606	-	1/1/13/20	12/28/106/115	-
29	BCR	8	503	-	-	16/29/63/63	0/2/2/2
25	CLA	H	1702	8	1/1/11/20	8/15/93/115	-
25	CLA	B	1236	-	1/1/12/20	9/23/101/115	-
29	BCR	K	4002	-	-	11/29/63/63	0/2/2/2
25	CLA	5	602	-	1/1/12/20	10/22/100/115	-
25	CLA	a	602	-	1/1/12/20	8/19/97/115	-
29	BCR	A	4004	-	-	12/29/63/63	0/2/2/2
36	DGD	7	806	-	-	13/39/79/95	0/2/2/2
26	CHL	4	609	17	4/4/20/26	12/39/137/137	-
25	CLA	B	1227	-	1/1/12/20	13/19/97/115	-
25	CLA	6	618	-	1/1/11/20	8/15/93/115	-
25	CLA	2	615	-	1/1/13/20	6/27/105/115	-
30	LHG	1	802	-	-	34/53/53/53	-
30	LHG	1	801	25	-	25/39/39/53	-
30	LHG	5	801	-	-	35/53/53/53	-
25	CLA	A	1132	-	1/1/15/20	15/37/115/115	-
26	CHL	8	601	21	4/4/19/26	4/33/131/137	-
26	CHL	8	613	-	3/3/17/26	2/21/119/137	-
25	CLA	9	602	-	1/1/11/20	4/15/93/115	-

The worst 5 of 2215 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	3	506	RRX	C26-C25	15.50	1.61	1.34
40	J	4002	RRX	C26-C25	15.46	1.61	1.34
40	3	506	RRX	C5-C6	14.91	1.60	1.34
40	J	4002	RRX	C5-C6	14.73	1.59	1.34
43	3	502	LUT	C24-C25	14.67	1.51	1.33

The worst 5 of 4958 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	9	504	XAT	C20-C13-C14	-30.45	80.27	122.92
29	H	4001	BCR	C37-C22-C21	-30.28	80.51	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	H	4001	BCR	C23-C22-C21	27.27	160.78	118.94
50	9	504	XAT	C12-C13-C14	26.86	160.15	118.94
39	F	4001	NEX	C17-C1-C6	-26.13	87.08	110.47

5 of 394 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	1011	CL0	ND
24	A	1011	CL0	NC
24	A	1011	CL0	NA
25	A	1012	CLA	ND
25	A	1013	CLA	ND

5 of 4852 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	1102	CLA	C1A-C2A-CAA-CBA
25	A	1102	CLA	C3A-C2A-CAA-CBA
25	A	1103	CLA	C3A-C2A-CAA-CBA
25	A	1103	CLA	CHA-CBD-CGD-O1D
25	A	1103	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

362 monomers are involved in 1239 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	G	1602	CLA	3	0
43	4	501	LUT	4	0
25	9	607	CLA	2	0
26	1	611	CHL	6	0
47	8	806	PLM	1	0
25	B	1204	CLA	6	0
26	6	619	CHL	7	0
33	G	5002	PTY	1	0
26	6	613	CHL	5	0
26	8	603	CHL	5	0
41	6	806	SPH	1	0
25	6	608	CLA	4	0
30	F	5001	LHG	2	0
25	3	610	CLA	3	0
25	G	1603	CLA	4	0
29	A	4005	BCR	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	1102	CLA	4	0
25	O	1803	CLA	1	0
25	A	1118	CLA	3	0
25	A	1116	CLA	8	0
27	A	2001	PQN	7	0
25	9	605	CLA	6	0
34	A	5007	3PH	3	0
26	9	601	CHL	9	0
26	9	613	CHL	4	0
29	B	4004	BCR	8	0
26	2	610	CHL	2	0
30	8	801	LHG	1	0
25	7	602	CLA	2	0
41	9	804	SPH	2	0
25	A	1111	CLA	8	0
25	9	612	CLA	8	0
26	8	610	CHL	2	0
25	5	607	CLA	3	0
25	2	608	CLA	1	0
25	4	610	CLA	4	0
35	2	804	LMT	5	0
52	8	805	P5S	2	0
25	8	608	CLA	2	0
25	B	1235	CLA	6	0
26	7	611	CHL	3	0
25	A	1121	CLA	1	0
26	7	617	CHL	5	0
26	6	610	CHL	2	0
30	3	801	LHG	1	0
25	8	618	CLA	6	0
39	F	4001	NEX	5	0
30	9	801	LHG	3	0
26	6	609	CHL	7	0
33	3	802	PTY	3	0
25	B	1240	CLA	6	0
25	B	1239	CLA	4	0
25	3	613	CLA	5	0
50	2	501	XAT	2	0
53	8	810	LAP	5	0
25	B	1225	CLA	4	0
25	6	604	CLA	5	0
25	5	614	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	4	608	CLA	4	0
25	A	1112	CLA	5	0
25	K	1401	CLA	5	0
25	7	601	CLA	6	0
36	B	5003	DGD	4	0
32	H	5001	SQD	3	0
25	B	1217	CLA	4	0
29	5	504	BCR	4	0
30	A	5002	LHG	5	0
36	8	802	DGD	3	0
25	A	1104	CLA	3	0
25	A	1137	CLA	6	0
25	4	606	CLA	3	0
33	9	803	PTY	3	0
27	B	2002	PQN	5	0
25	2	604	CLA	14	0
32	G	5001	SQD	4	0
29	B	4003	BCR	1	0
37	6	803	PCW	4	0
25	8	606	CLA	5	0
48	2	803	DGA	6	0
25	1	615	CLA	2	0
25	2	605	CLA	4	0
29	A	4003	BCR	4	0
25	2	621	CLA	3	0
26	7	615	CHL	1	0
25	4	601	CLA	6	0
44	7	504	AXT	10	0
25	8	605	CLA	3	0
25	B	1202	CLA	5	0
29	5	503	BCR	6	0
26	A	1114	CHL	9	0
45	8	809	OLA	1	0
25	2	612	CLA	4	0
26	9	603	CHL	7	0
25	8	615	CLA	2	0
30	7	803	LHG	3	0
25	B	1206	CLA	7	0
25	B	1229	CLA	7	0
25	B	1220	CLA	10	0
43	2	502	LUT	4	0
25	K	1403	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	2	601	CLA	7	0
26	1	613	CHL	6	0
51	7	807	4RF	6	0
30	B	5001	LHG	6	0
25	9	609	CLA	3	0
25	4	603	CLA	3	0
25	B	1230	CLA	10	0
25	B	1226	CLA	6	0
25	B	1213	CLA	3	0
43	9	502	LUT	8	0
33	G	5003	PTY	1	0
30	4	801	LHG	4	0
25	B	1234	CLA	9	0
25	F	1302	CLA	5	0
29	I	4001	BCR	2	0
26	5	611	CHL	3	0
25	2	603	CLA	5	0
29	H	4001	BCR	4	0
25	B	1201	CLA	8	0
43	1	503	LUT	3	0
25	8	612	CLA	6	0
25	6	606	CLA	2	0
43	1	501	LUT	4	0
25	5	604	CLA	5	0
30	2	802	LHG	6	0
29	G	4001	BCR	5	0
32	A	5005	SQD	8	0
30	A	5001	LHG	3	0
25	4	611	CLA	3	0
36	8	803	DGD	5	0
33	B	5005	PTY	4	0
25	7	606	CLA	2	0
47	8	807	PLM	5	0
26	5	610	CHL	5	0
25	A	1122	CLA	5	0
29	6	503	BCR	4	0
37	K	5002	PCW	1	0
26	3	608	CHL	2	0
29	3	505	BCR	4	0
25	B	1208	CLA	4	0
25	K	1402	CLA	3	0
29	J	4001	BCR	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	8	604	CHL	3	0
43	8	501	LUT	6	0
25	1	612	CLA	16	0
25	A	1131	CLA	6	0
25	A	1133	CLA	7	0
25	4	617	CLA	1	0
26	5	613	CHL	4	0
25	A	1108	CLA	9	0
25	7	603	CLA	5	0
30	A	5003	LHG	3	0
43	3	501	LUT	3	0
26	5	618	CHL	4	0
25	3	616	CLA	3	0
25	B	1216	CLA	7	0
25	1	605	CLA	9	0
25	3	601	CLA	8	0
25	A	1136	CLA	3	0
25	J	1901	CLA	1	0
25	7	610	CLA	7	0
48	8	804	DGA	5	0
25	8	609	CLA	6	0
25	G	1601	CLA	2	0
29	A	4001	BCR	4	0
25	A	1128	CLA	8	0
25	8	611	CLA	4	0
25	B	1223	CLA	2	0
25	A	1107	CLA	3	0
25	L	1504	CLA	4	0
25	4	604	CLA	7	0
25	B	1215	CLA	4	0
41	J	5002	SPH	1	0
35	B	5006	LMT	2	0
47	6	804	PLM	1	0
25	B	1232	CLA	2	0
25	5	606	CLA	3	0
25	B	1238	CLA	2	0
25	5	603	CLA	3	0
25	A	1119	CLA	11	0
25	3	606	CLA	5	0
38	F	5003	LPX	2	0
25	3	618	CLA	1	0
25	9	604	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	6	801	LHG	6	0
25	B	1210	CLA	2	0
25	A	1135	CLA	3	0
25	6	603	CLA	5	0
40	3	506	RRX	1	0
26	9	608	CHL	2	0
26	4	613	CHL	4	0
25	5	608	CLA	2	0
25	A	1140	CLA	5	0
25	5	612	CLA	11	0
26	9	610	CHL	5	0
26	4	618	CHL	5	0
30	F	5002	LHG	2	0
29	B	4006	BCR	5	0
26	6	611	CHL	3	0
29	B	4005	BCR	6	0
25	6	602	CLA	2	0
25	A	1109	CLA	8	0
25	B	1203	CLA	1	0
25	L	1503	CLA	6	0
25	2	602	CLA	2	0
26	3	611	CHL	7	0
25	A	1127	CLA	10	0
25	4	616	CLA	3	0
25	3	602	CLA	3	0
43	2	507	LUT	7	0
25	8	602	CLA	5	0
25	A	1110	CLA	4	0
25	4	602	CLA	2	0
25	3	612	CLA	5	0
25	8	607	CLA	2	0
25	6	601	CLA	7	0
33	A	5006	PTY	4	0
25	K	1404	CLA	1	0
25	7	612	CLA	9	0
47	4	804	PLM	3	0
33	J	5001	PTY	2	0
45	1	803	OLA	2	0
24	A	1011	CL0	6	0
25	7	608	CLA	2	0
26	6	617	CHL	1	0
25	B	1022	CLA	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	O	4001	BCR	1	0
32	7	805	SQD	1	0
40	J	4002	RRX	2	0
25	A	1103	CLA	9	0
25	1	603	CLA	6	0
25	B	1212	CLA	3	0
25	B	1023	CLA	7	0
25	A	1012	CLA	12	0
25	A	1115	CLA	9	0
25	B	1224	CLA	12	0
25	B	1228	CLA	5	0
50	9	507	XAT	5	0
43	5	505	LUT	4	0
29	K	4001	BCR	5	0
25	1	608	CLA	9	0
30	2	801	LHG	5	0
25	A	1139	CLA	5	0
25	B	1231	CLA	7	0
48	5	803	DGA	3	0
25	A	1134	CLA	4	0
25	5	605	CLA	4	0
37	B	5004	PCW	1	0
25	1	607	CLA	4	0
25	A	1125	CLA	8	0
25	3	607	CLA	2	0
29	B	4002	BCR	5	0
43	8	502	LUT	5	0
25	6	605	CLA	2	0
25	A	1113	CLA	7	0
43	6	501	LUT	5	0
25	9	606	CLA	5	0
25	2	607	CLA	4	0
29	L	4002	BCR	2	0
48	3	803	DGA	3	0
25	3	605	CLA	6	0
25	L	1501	CLA	1	0
25	L	1502	CLA	7	0
26	1	609	CHL	11	0
25	6	615	CLA	8	0
26	3	604	CHL	6	0
25	A	1124	CLA	4	0
25	A	1101	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	5	601	CLA	4	0
25	O	1802	CLA	4	0
50	7	502	XAT	3	0
43	6	502	LUT	5	0
43	9	501	LUT	9	0
26	2	609	CHL	4	0
29	6	504	BCR	4	0
25	B	1207	CLA	6	0
25	A	1129	CLA	5	0
43	3	502	LUT	4	0
26	5	617	CHL	2	0
26	1	610	CHL	3	0
32	I	5001	SQD	5	0
25	A	1117	CLA	7	0
26	3	603	CHL	7	0
29	A	4002	BCR	4	0
25	B	1219	CLA	7	0
25	A	1120	CLA	4	0
35	A	5008	LMT	1	0
30	B	5002	LHG	1	0
25	B	1211	CLA	1	0
25	B	1222	CLA	6	0
29	L	4001	BCR	3	0
25	B	1214	CLA	6	0
25	4	605	CLA	3	0
25	4	607	CLA	2	0
25	6	612	CLA	2	0
25	7	604	CLA	5	0
29	L	4003	BCR	1	0
33	5	802	PTY	3	0
44	1	502	AXT	3	0
25	B	1021	CLA	9	0
26	1	604	CHL	7	0
25	4	615	CLA	3	0
28	C	3003	SF4	1	0
42	M	4001	ECH	5	0
25	A	1105	CLA	6	0
50	9	504	XAT	4	0
25	B	1205	CLA	6	0
43	4	502	LUT	6	0
25	B	1237	CLA	3	0
30	9	802	LHG	4	0

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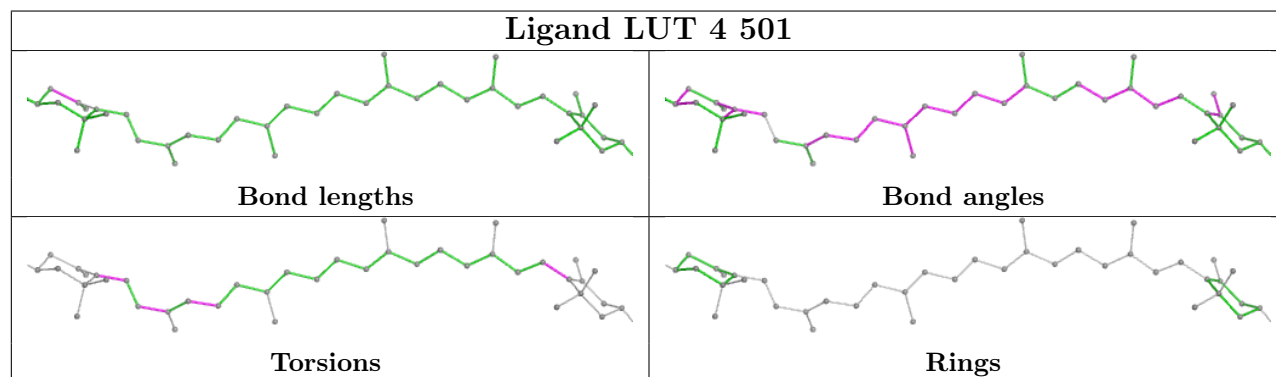
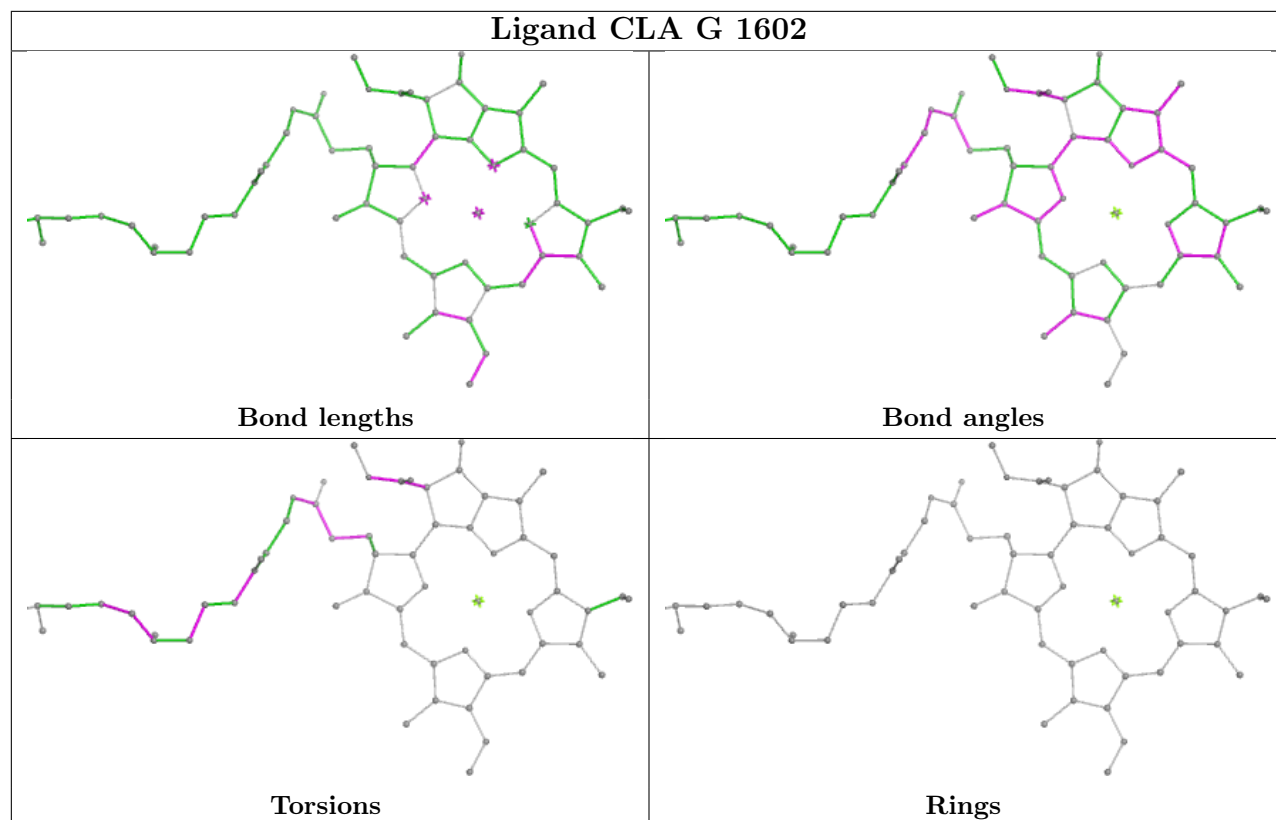
Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	5	501	LUT	5	0
25	1	602	CLA	2	0
25	B	1221	CLA	5	0
25	F	1301	CLA	3	0
29	3	504	BCR	5	0
25	5	615	CLA	1	0
25	B	1209	CLA	9	0
25	1	601	CLA	8	0
29	B	4001	BCR	5	0
25	A	1130	CLA	8	0
25	A	1013	CLA	8	0
29	7	503	BCR	9	0
25	7	605	CLA	5	0
25	7	607	CLA	3	0
25	4	612	CLA	8	0
37	K	5001	PCW	2	0
25	A	1106	CLA	7	0
25	A	1123	CLA	5	0
29	B	4007	BCR	4	0
47	5	804	PLM	3	0
26	2	613	CHL	1	0
25	5	609	CLA	2	0
26	7	609	CHL	4	0
25	H	1701	CLA	3	0
25	A	1126	CLA	13	0
25	B	1218	CLA	4	0
25	H	1703	CLA	5	0
35	1	804	LMT	5	0
43	7	501	LUT	5	0
29	3	503	BCR	3	0
29	4	503	BCR	8	0
43	5	502	LUT	4	0
25	A	1138	CLA	8	0
25	8	620	CLA	2	0
26	7	613	CHL	12	0
25	1	606	CLA	2	0
29	8	503	BCR	3	0
25	B	1236	CLA	7	0
29	K	4002	BCR	3	0
25	5	602	CLA	6	0
29	A	4004	BCR	4	0
36	7	806	DGD	3	0

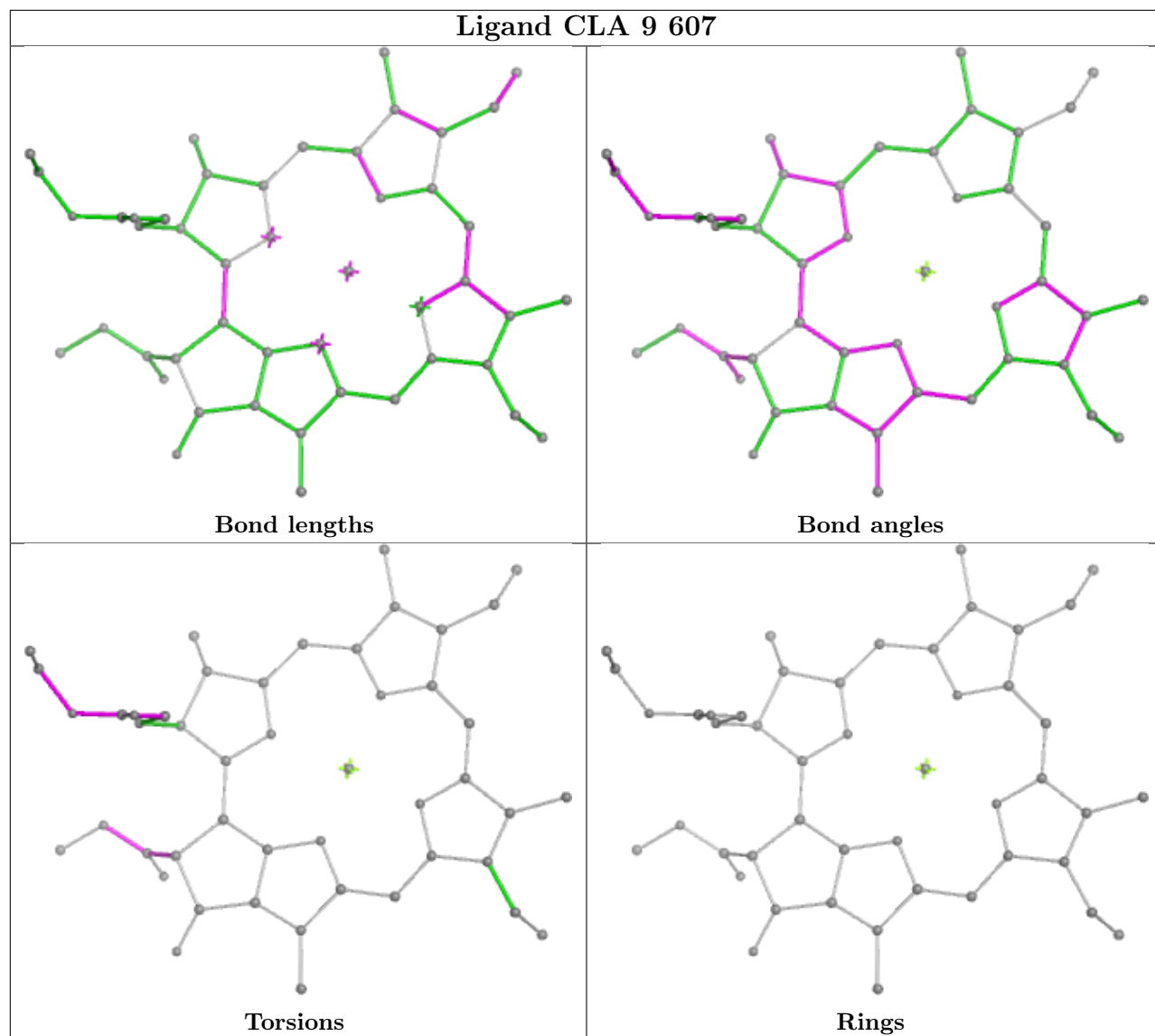
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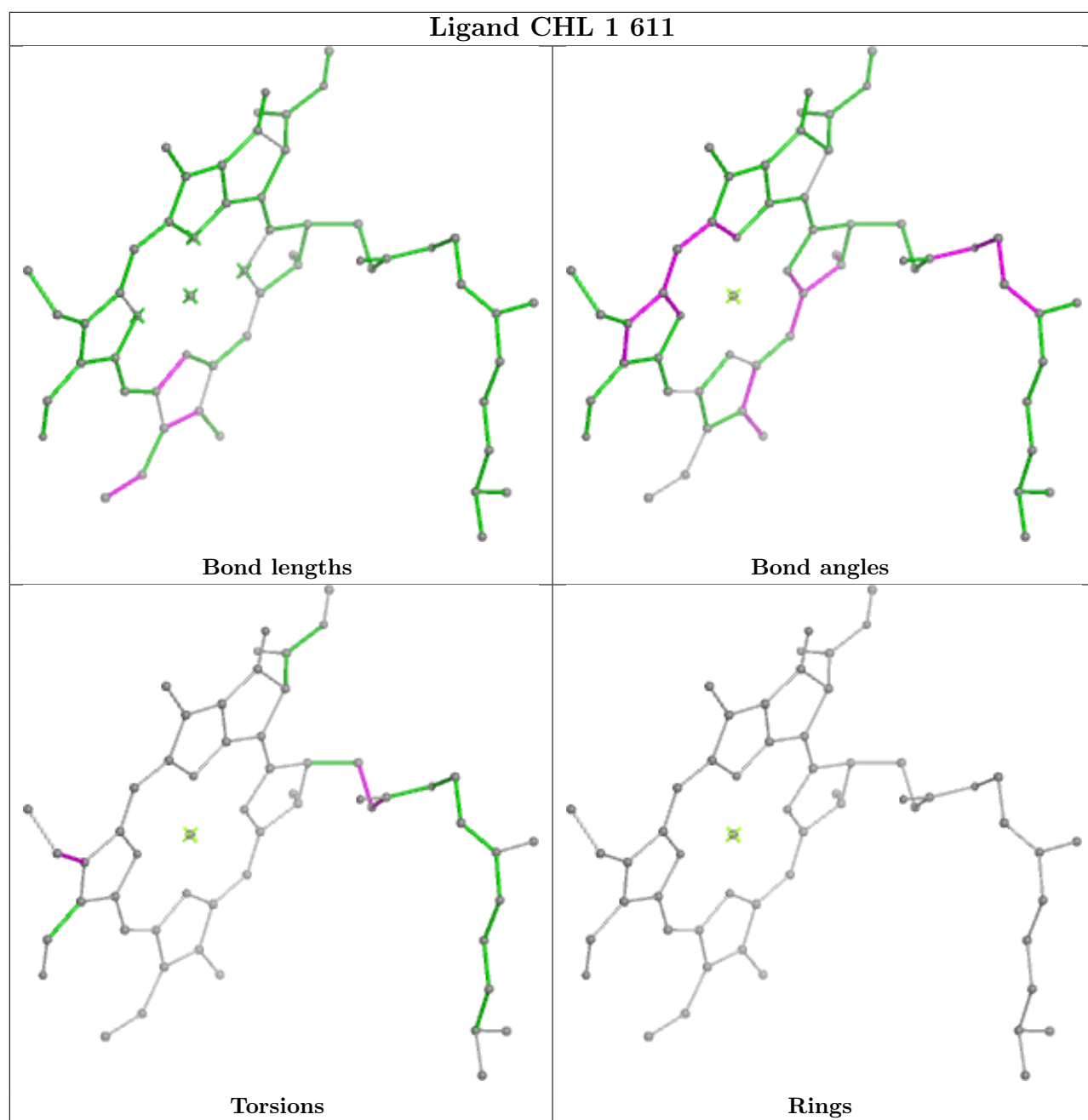
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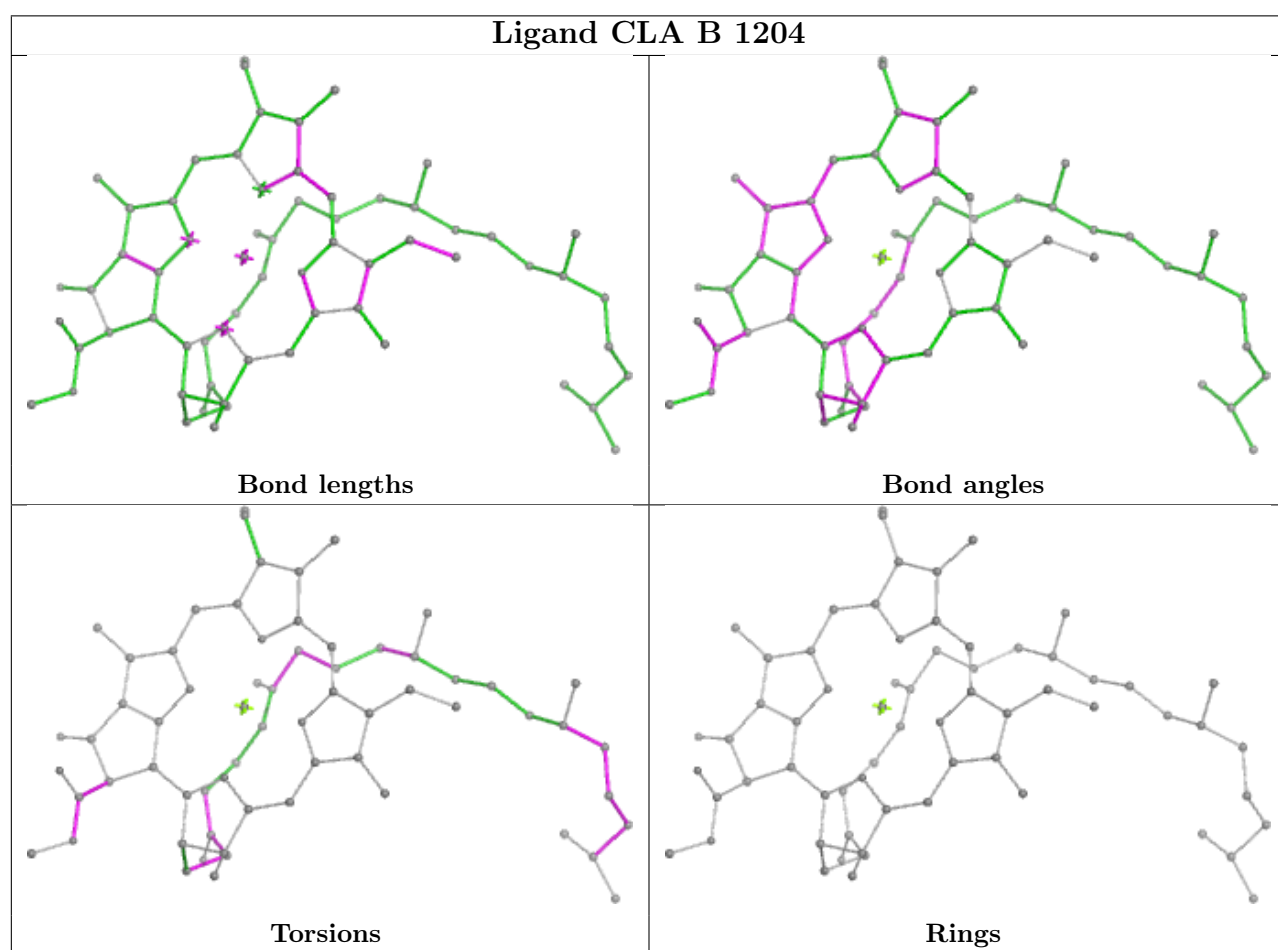
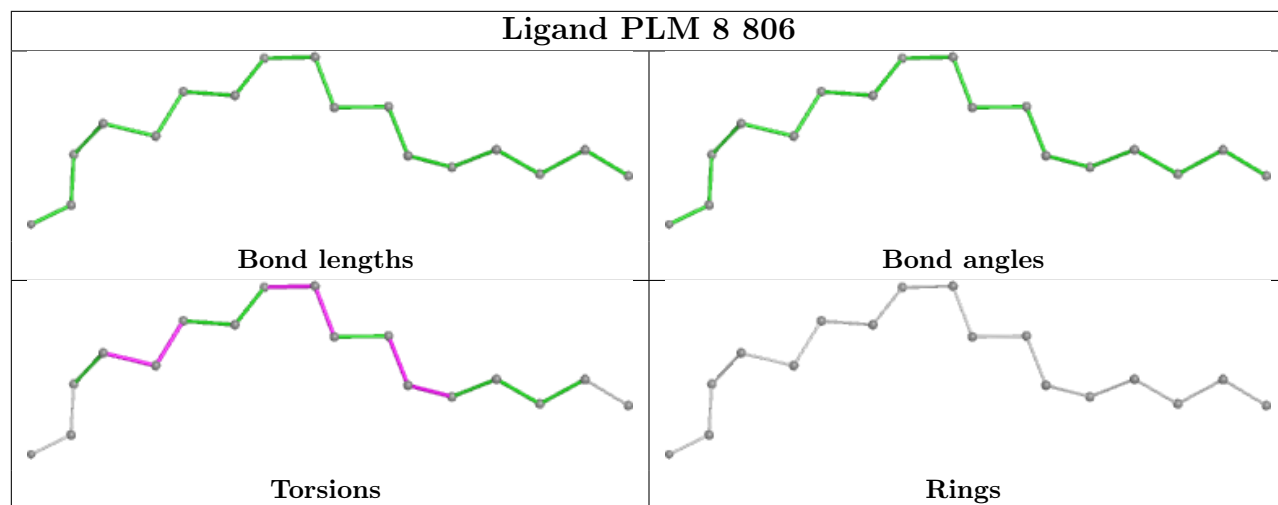
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	4	609	CHL	6	0
25	B	1227	CLA	5	0
25	2	615	CLA	3	0
30	1	802	LHG	4	0
30	1	801	LHG	2	0
30	5	801	LHG	2	0
25	A	1132	CLA	4	0
26	8	601	CHL	5	0
26	8	613	CHL	4	0
25	9	602	CLA	2	0

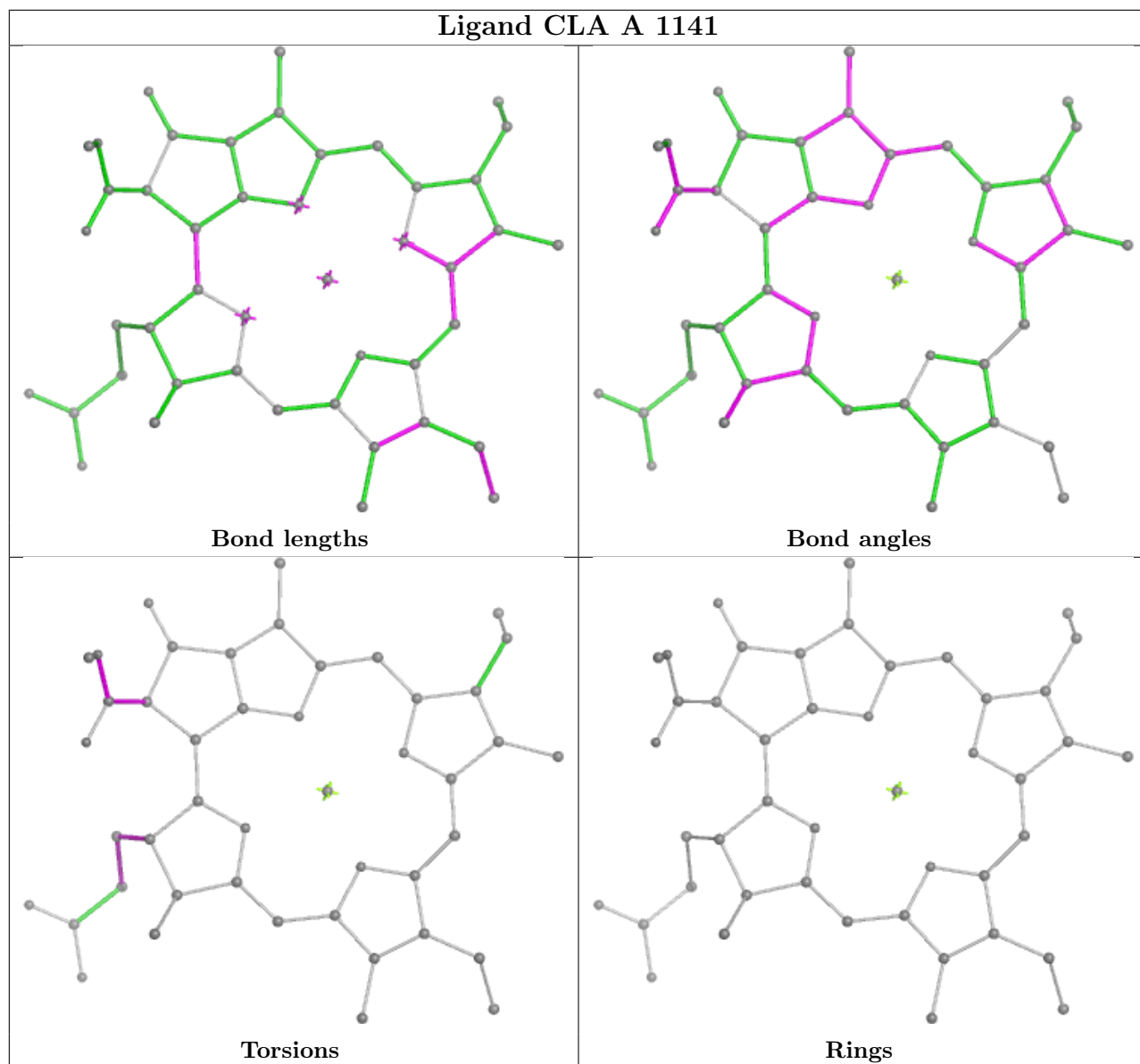
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

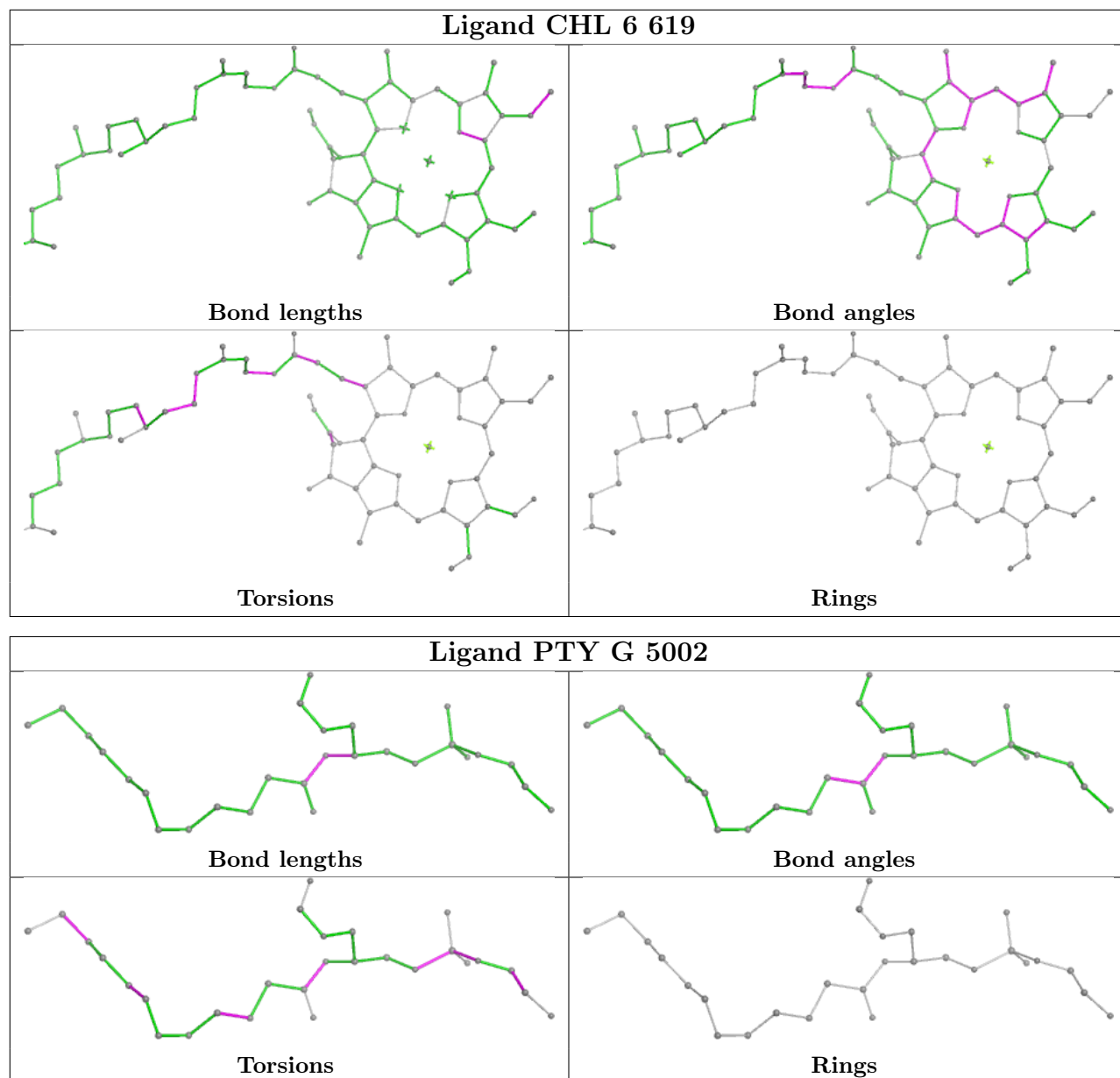


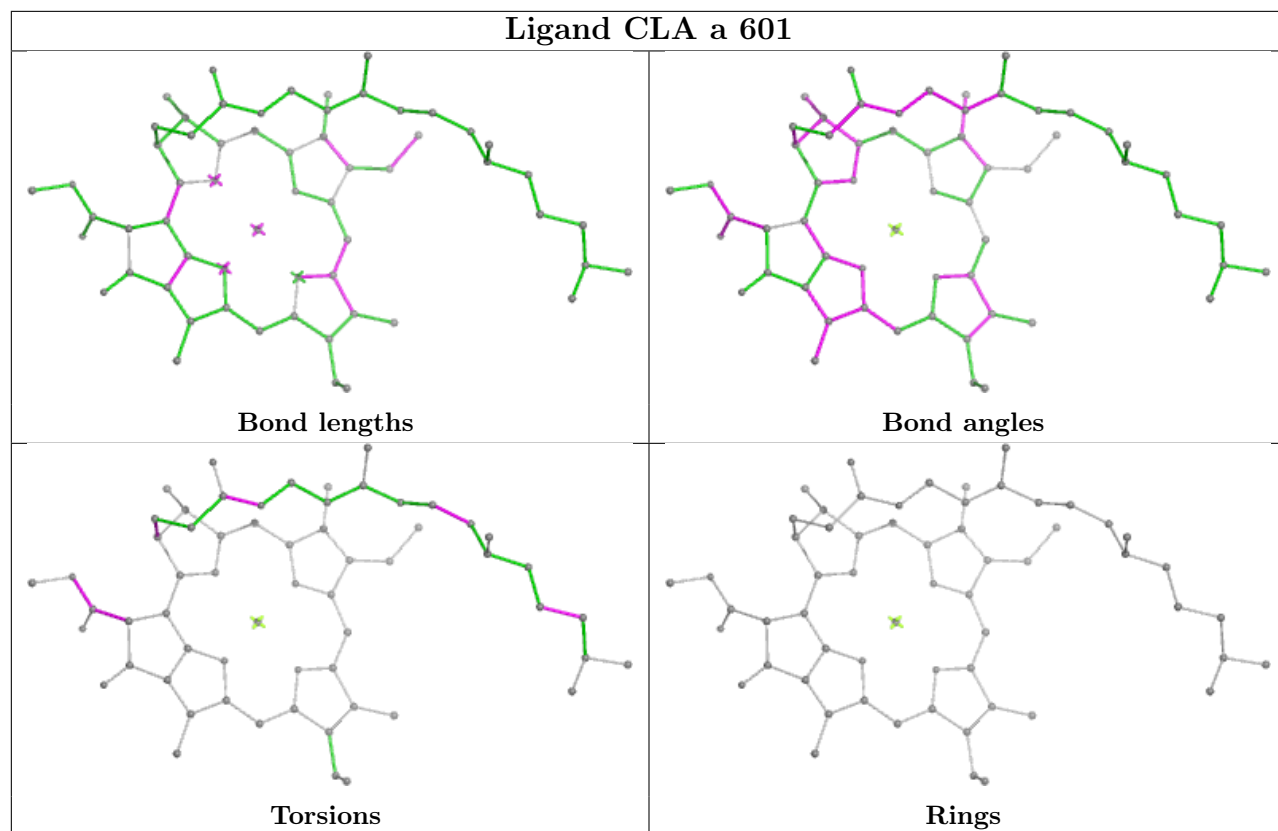


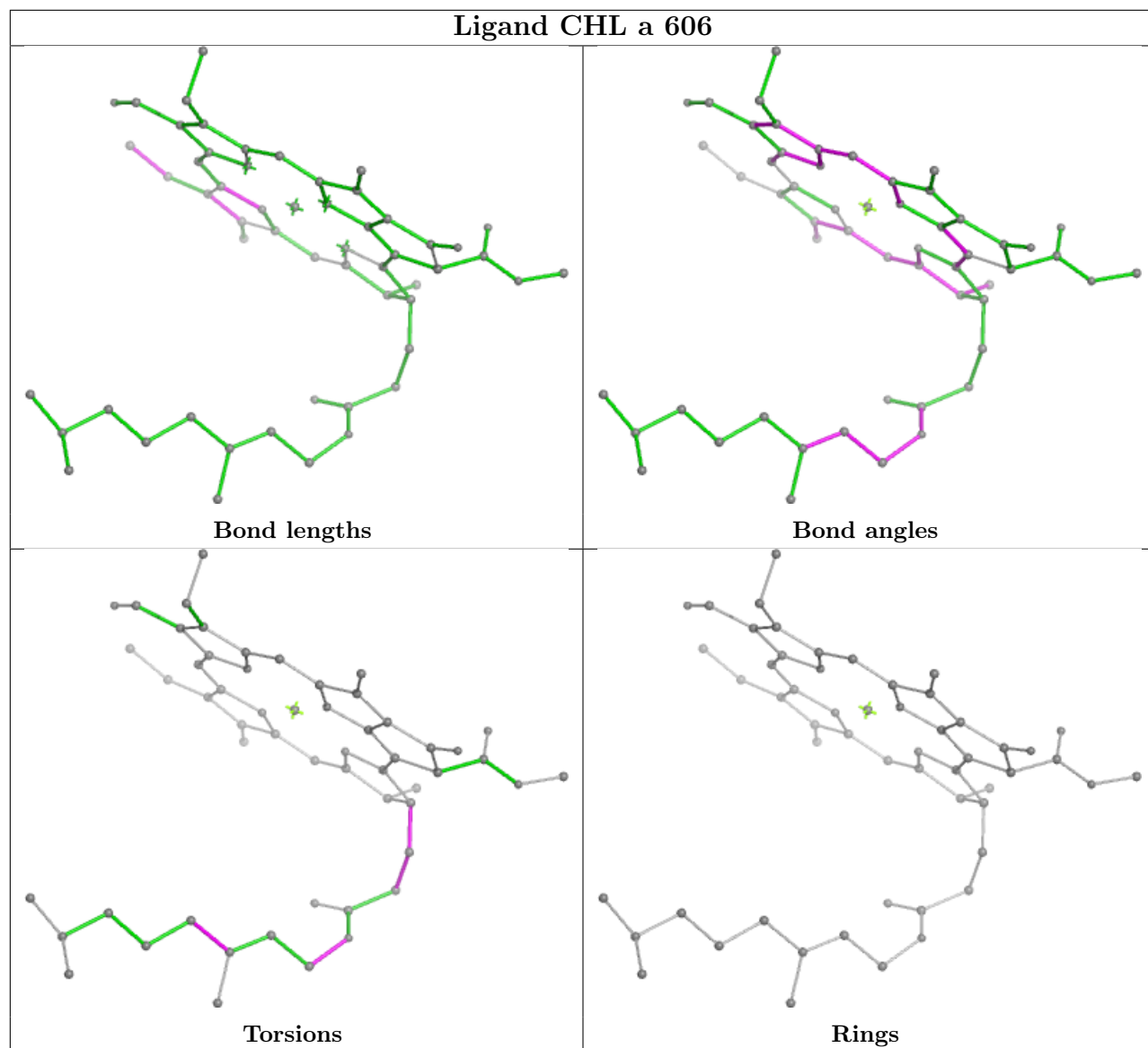


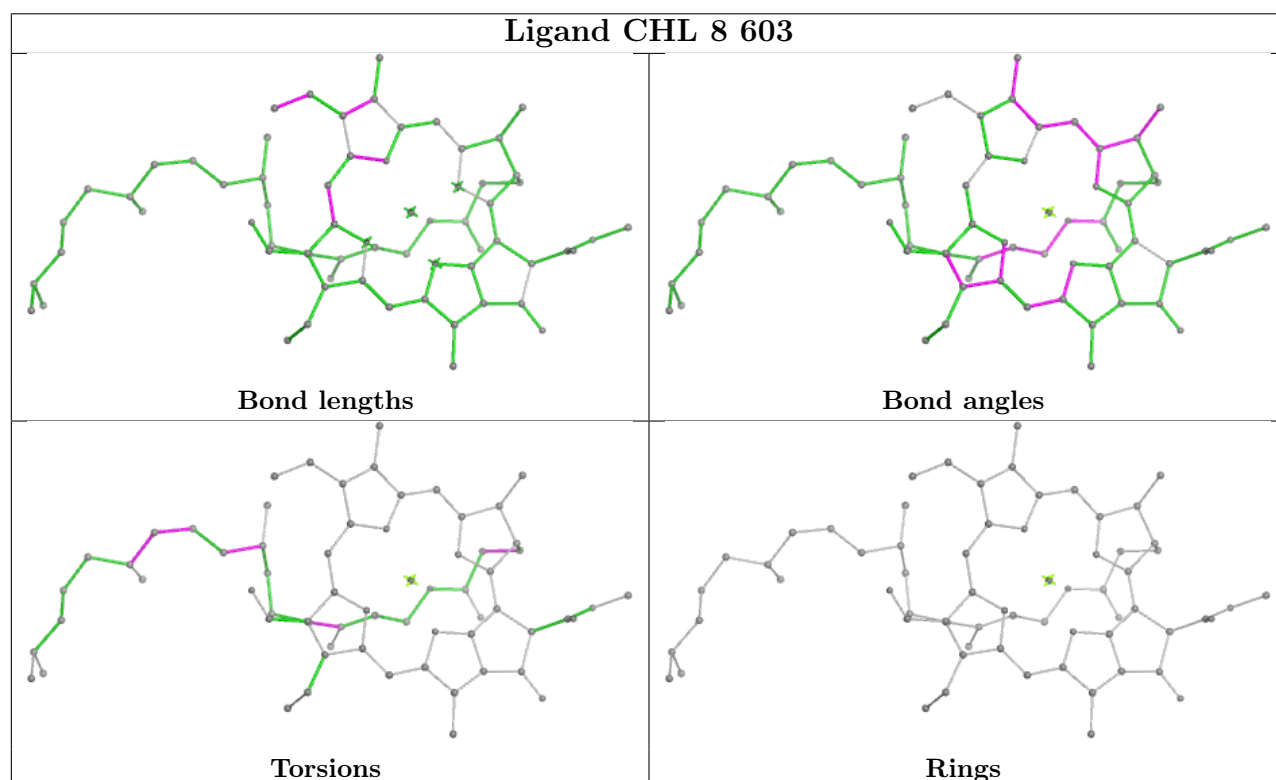
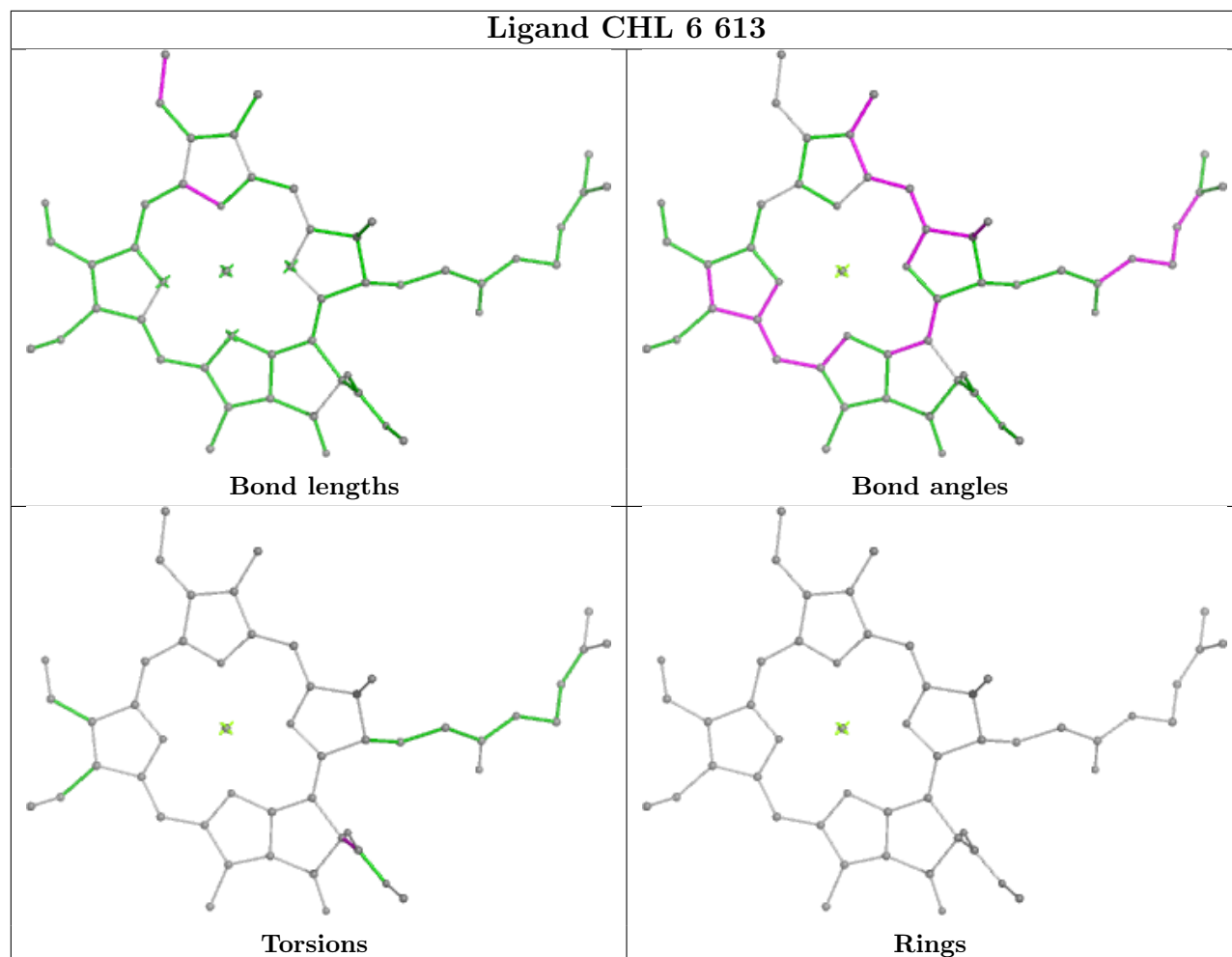


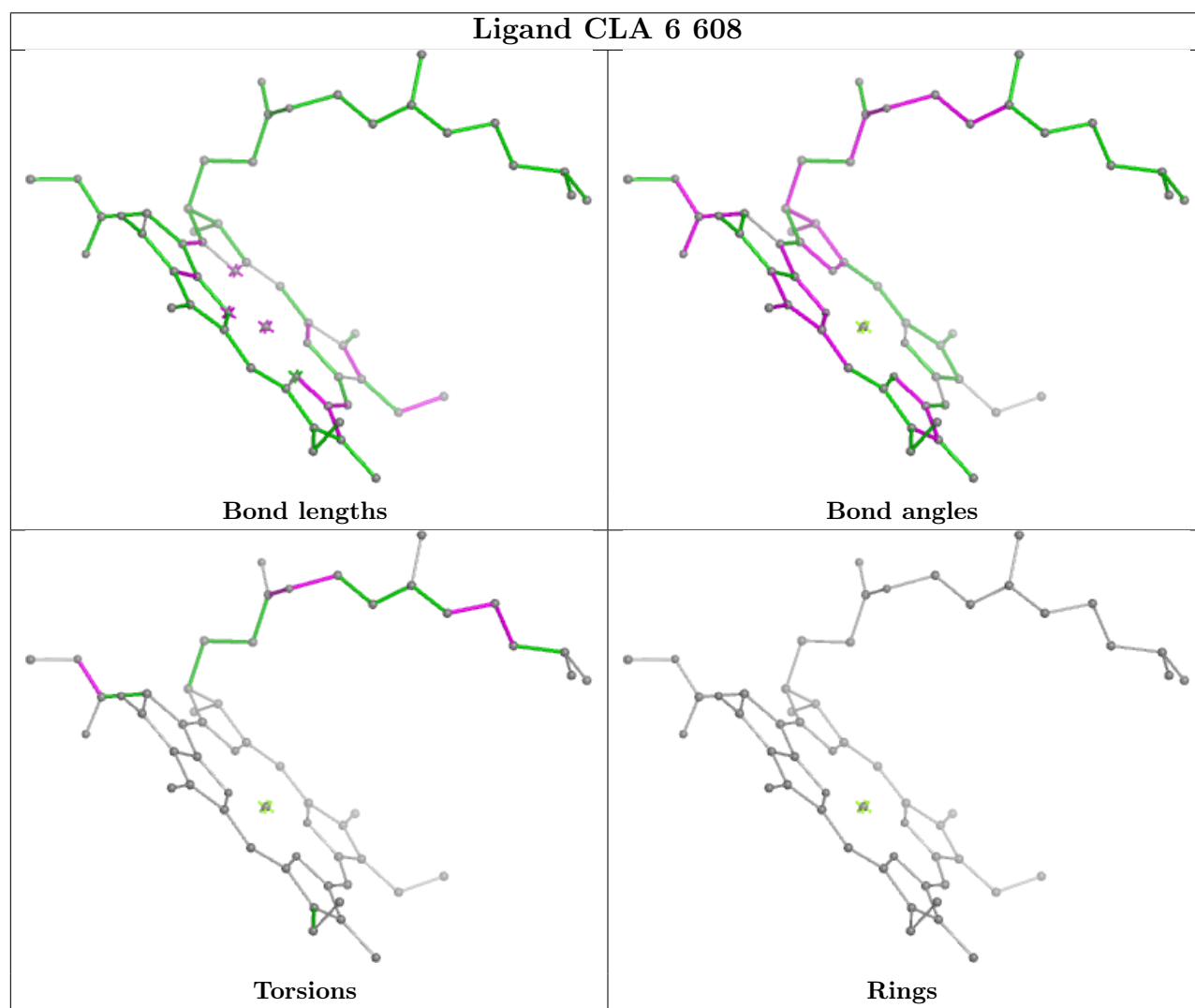
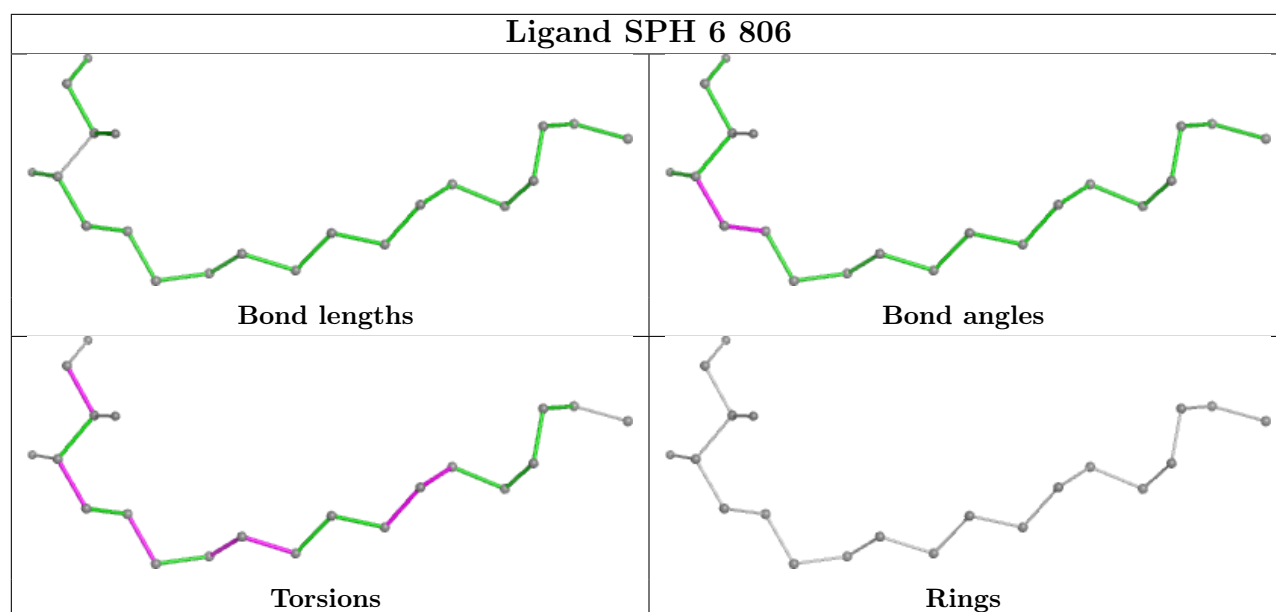


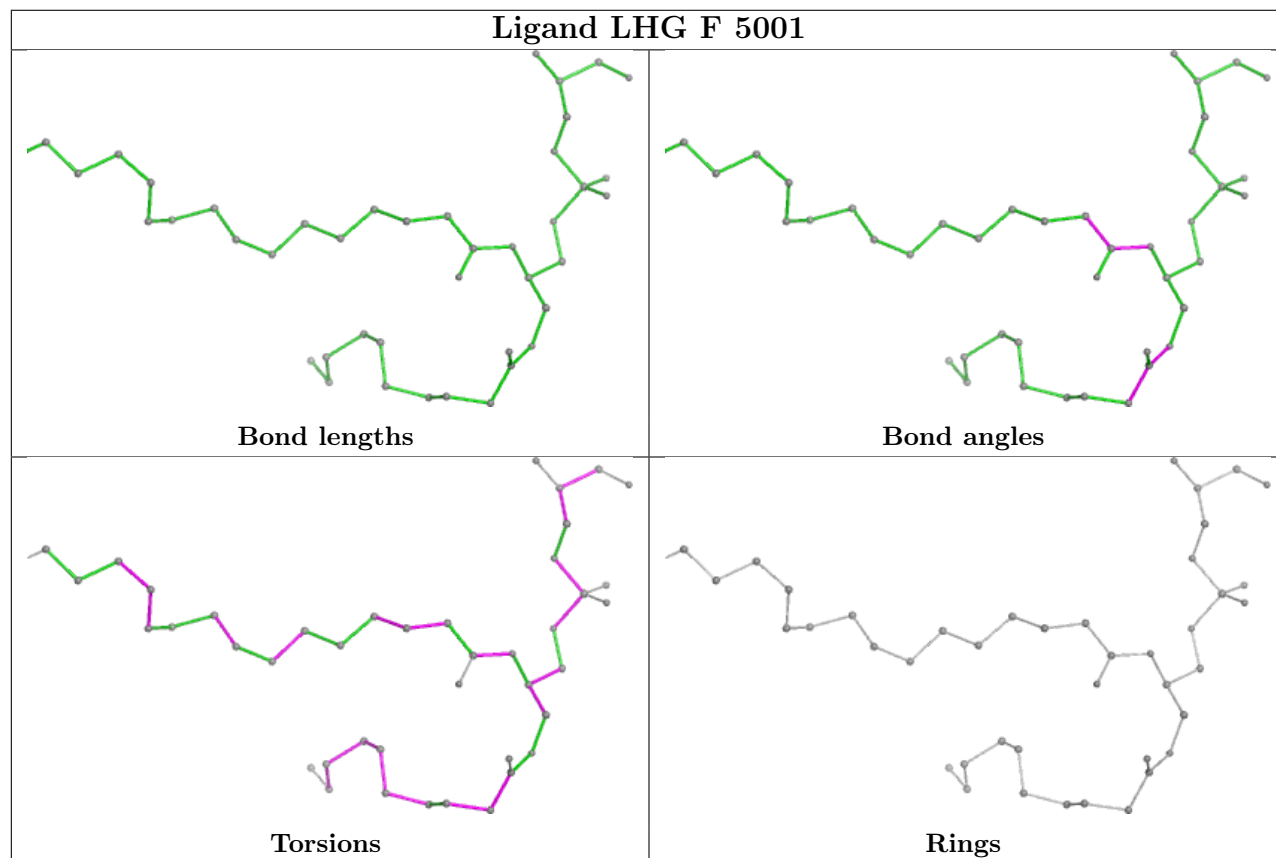
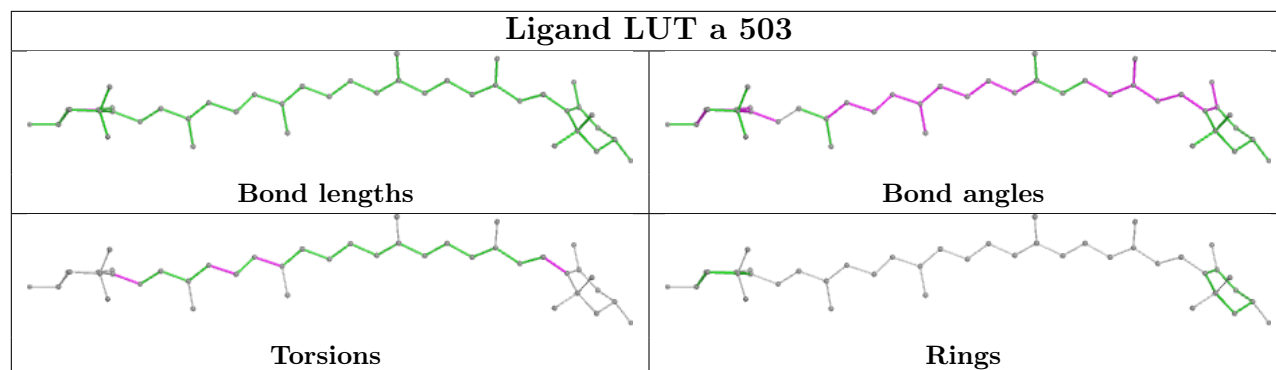


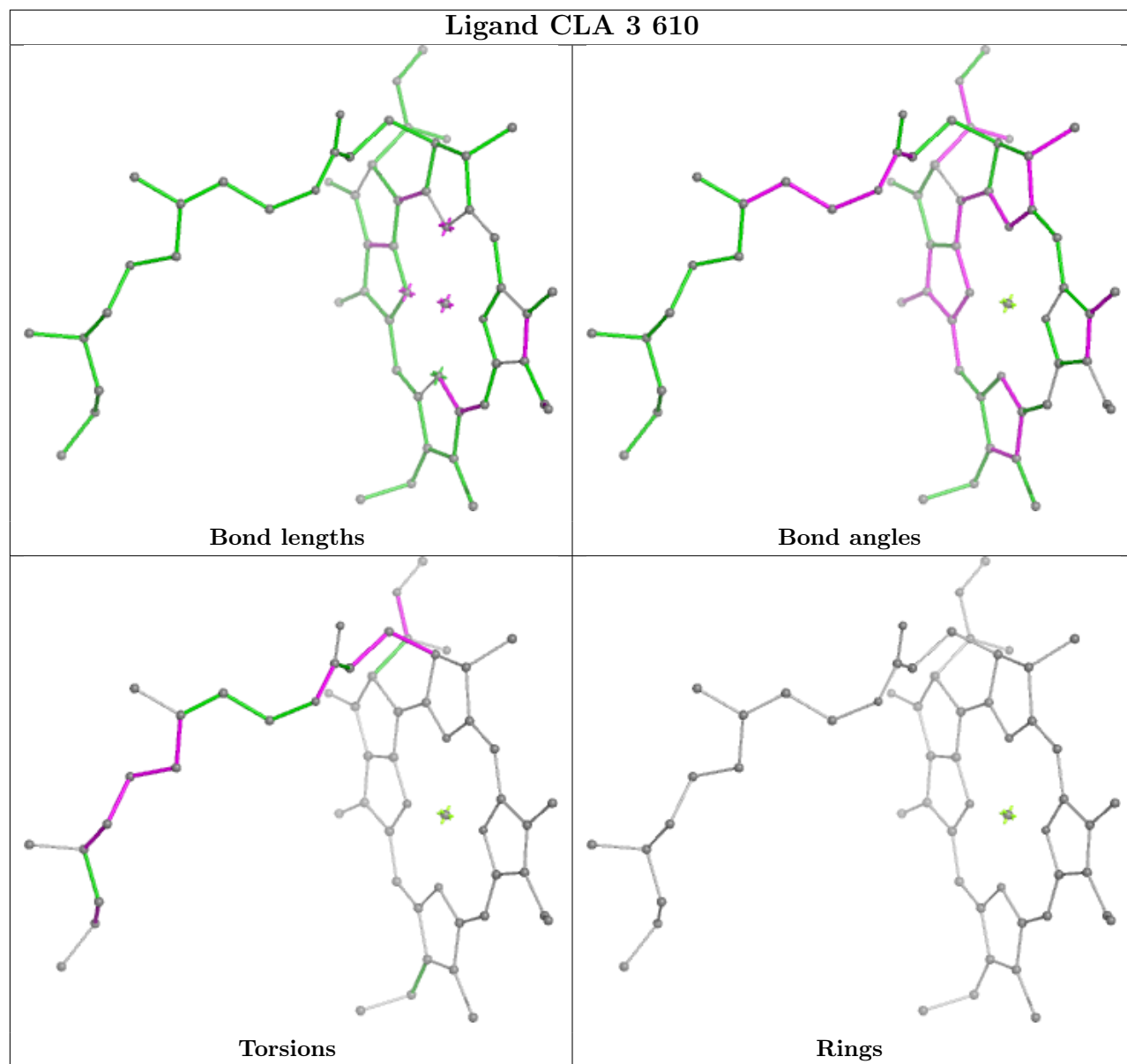


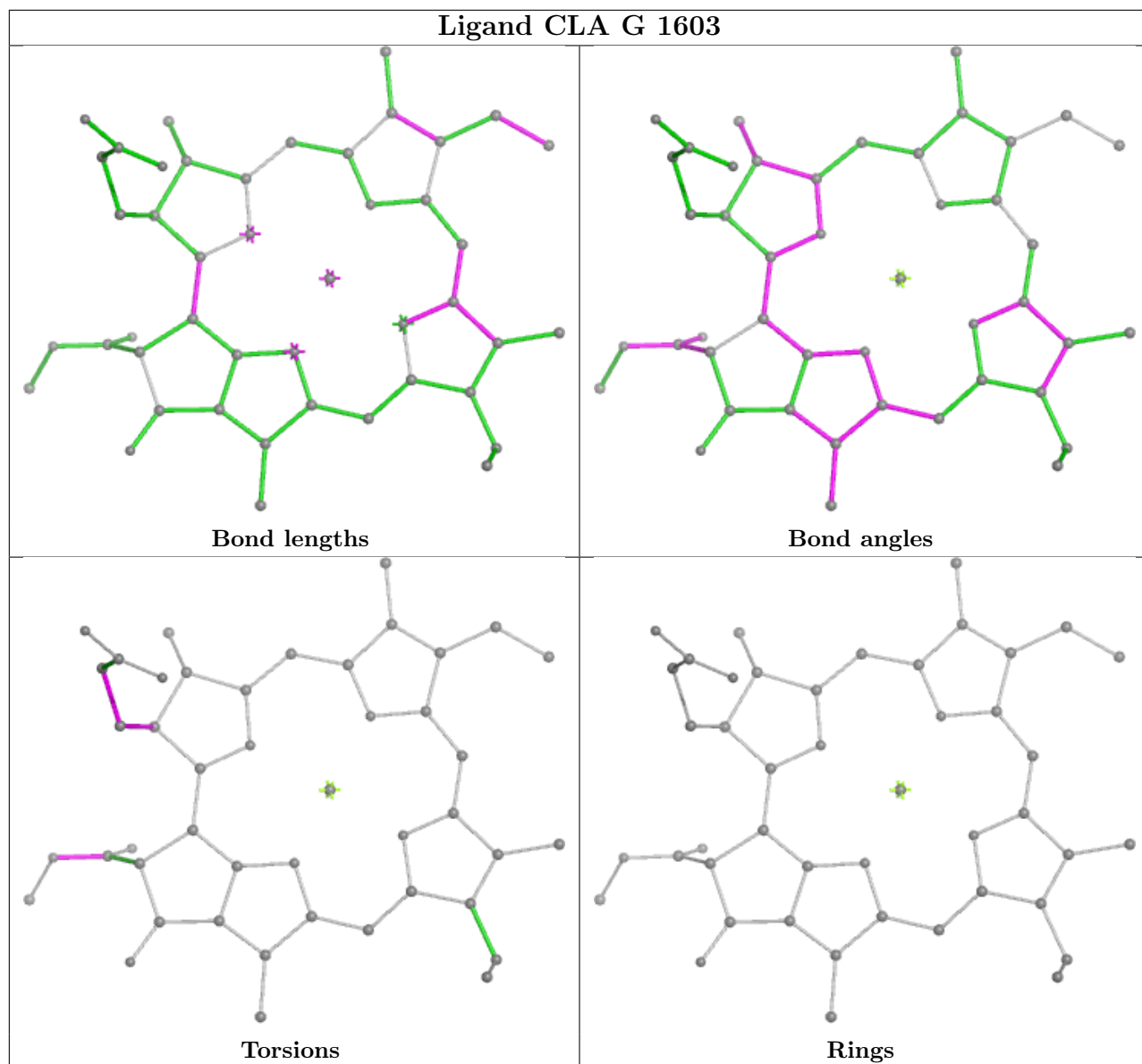


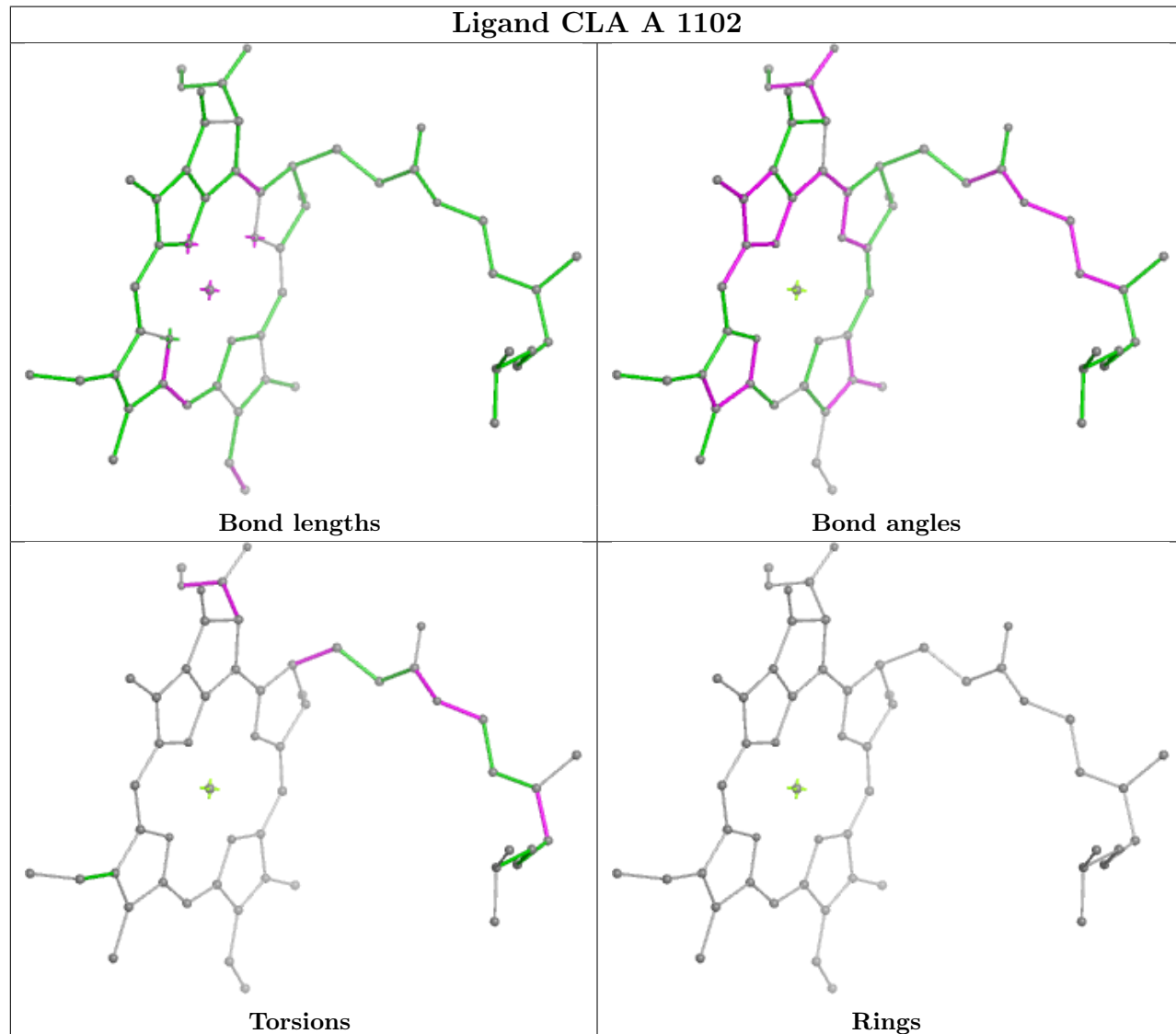
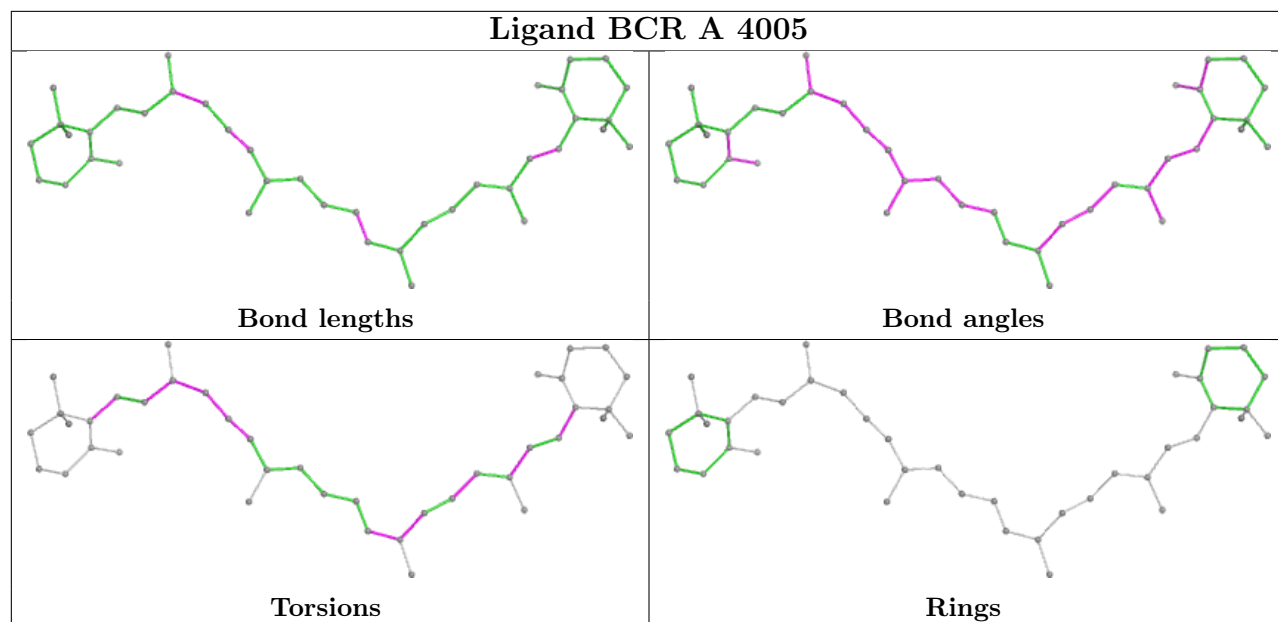


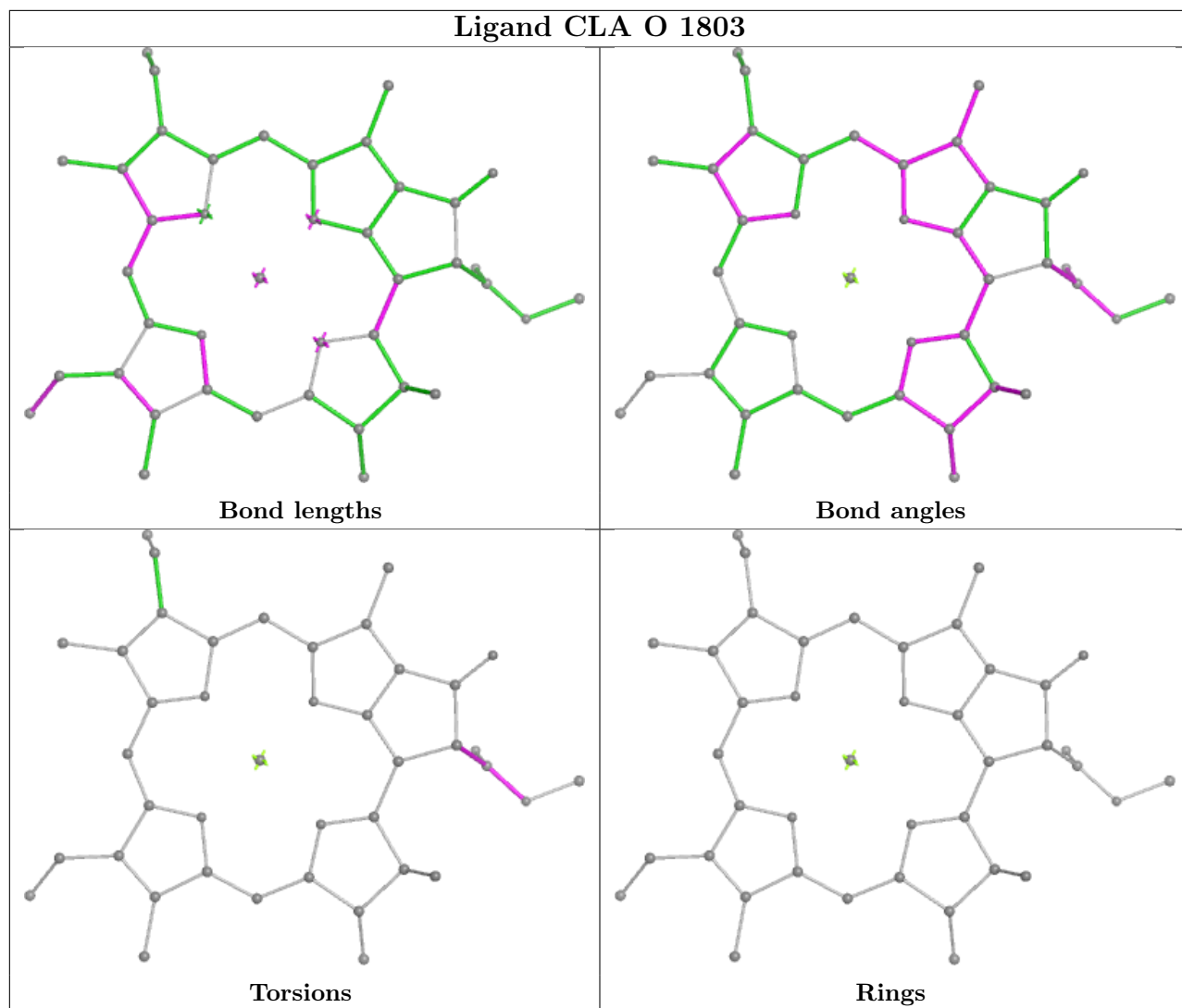


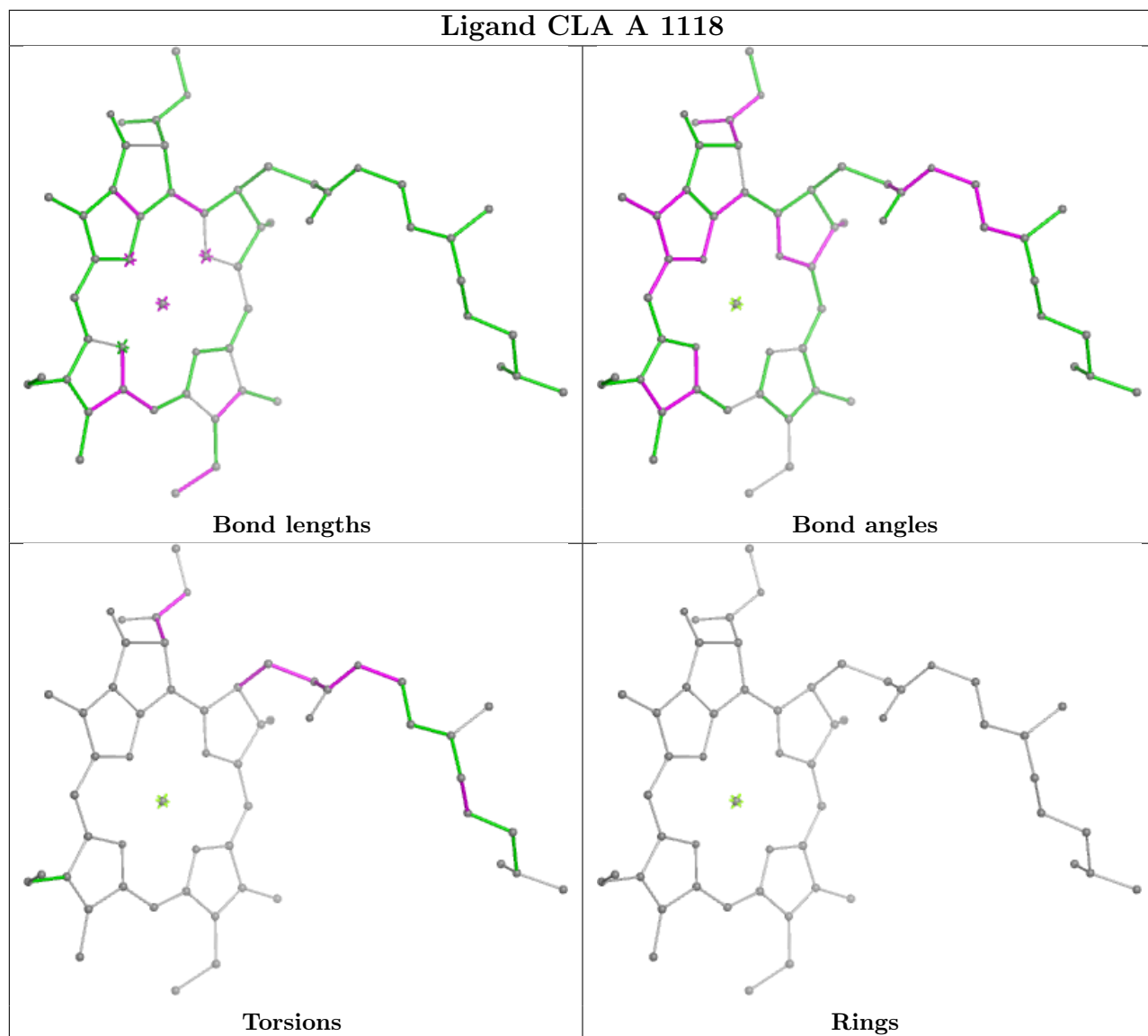


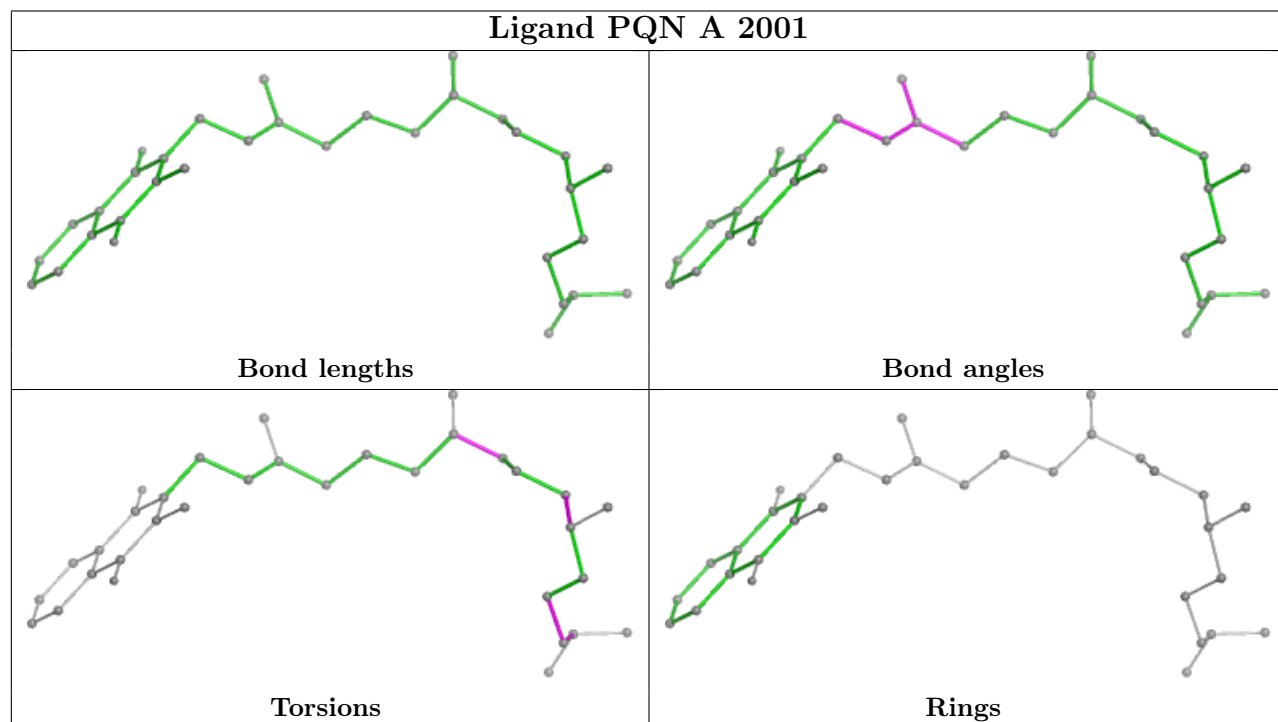
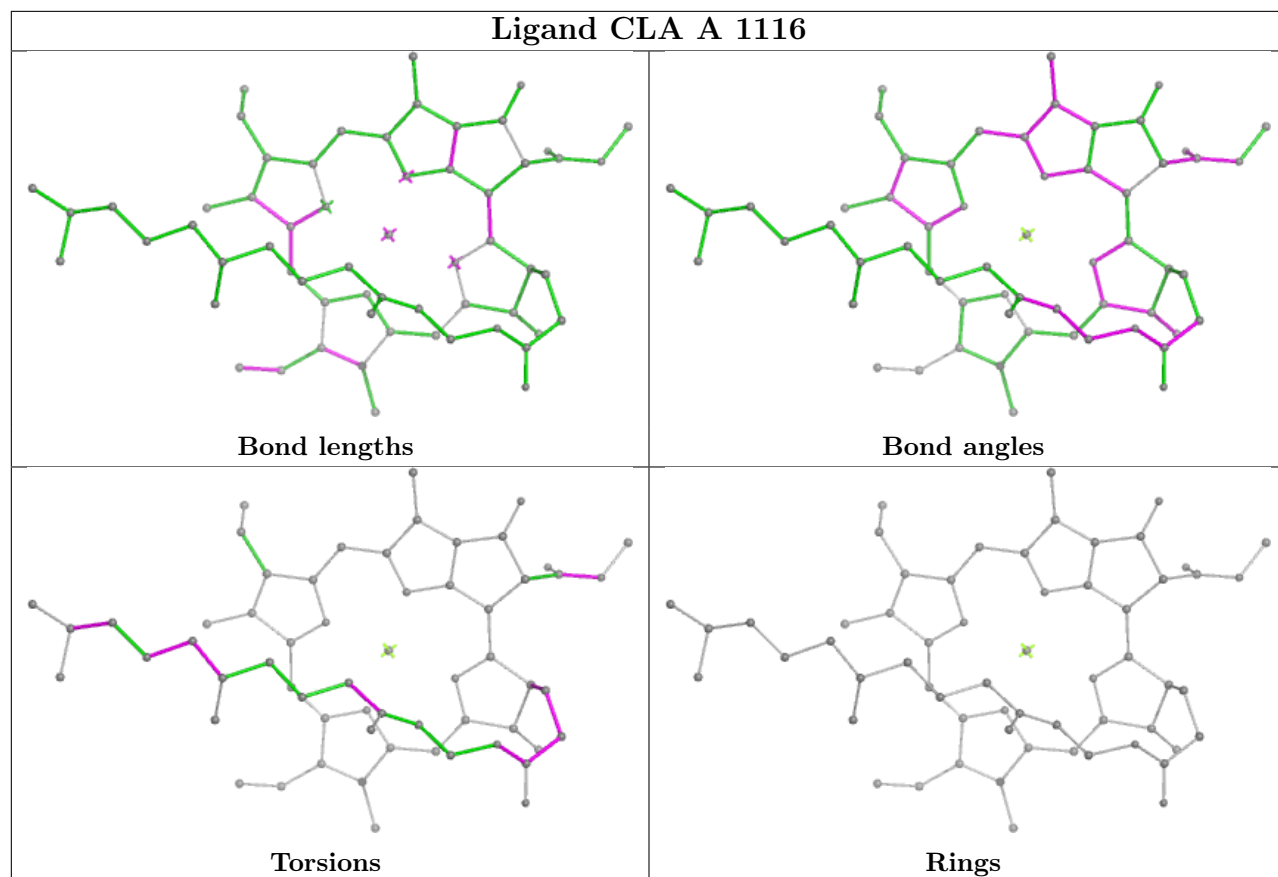


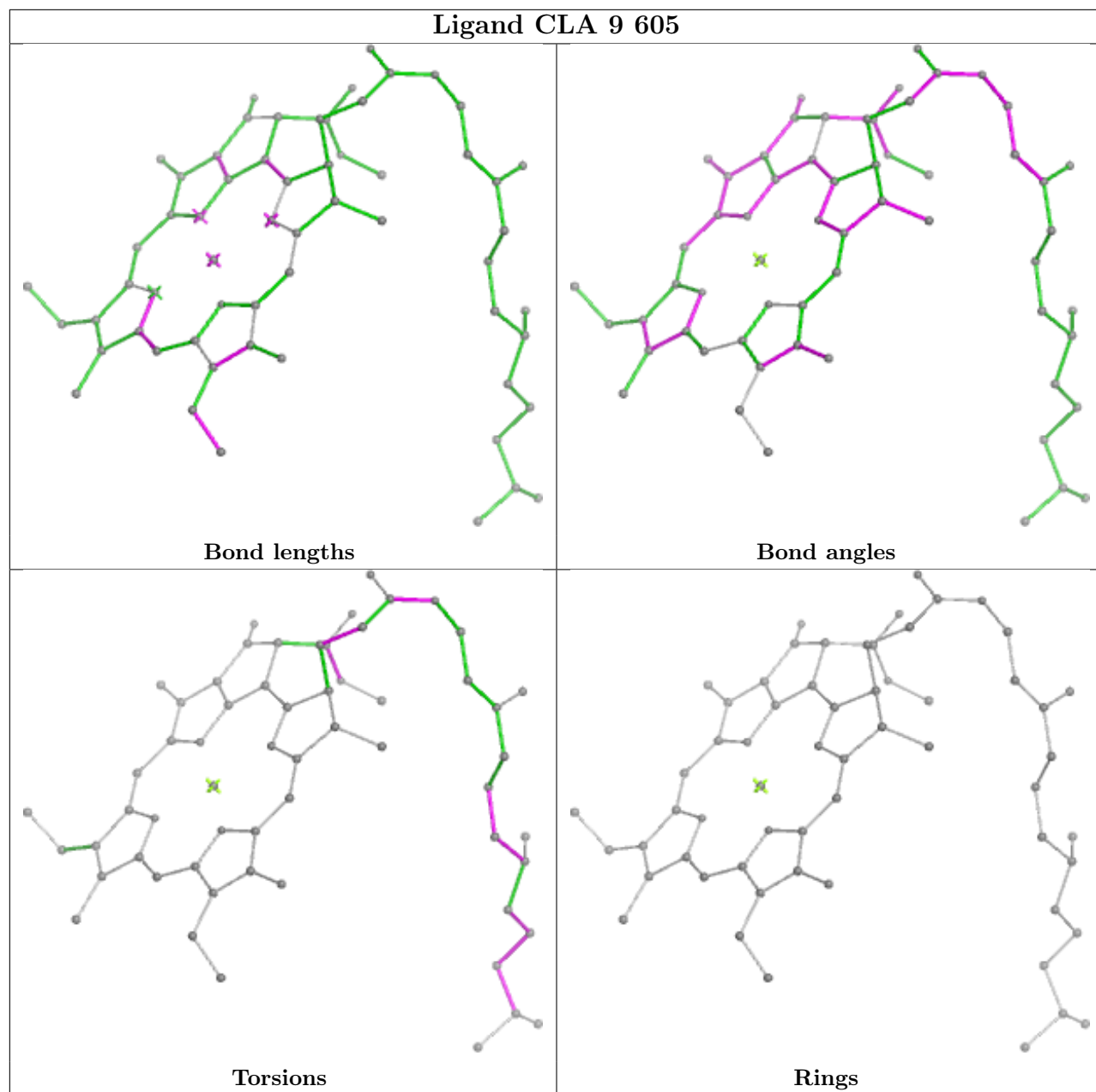


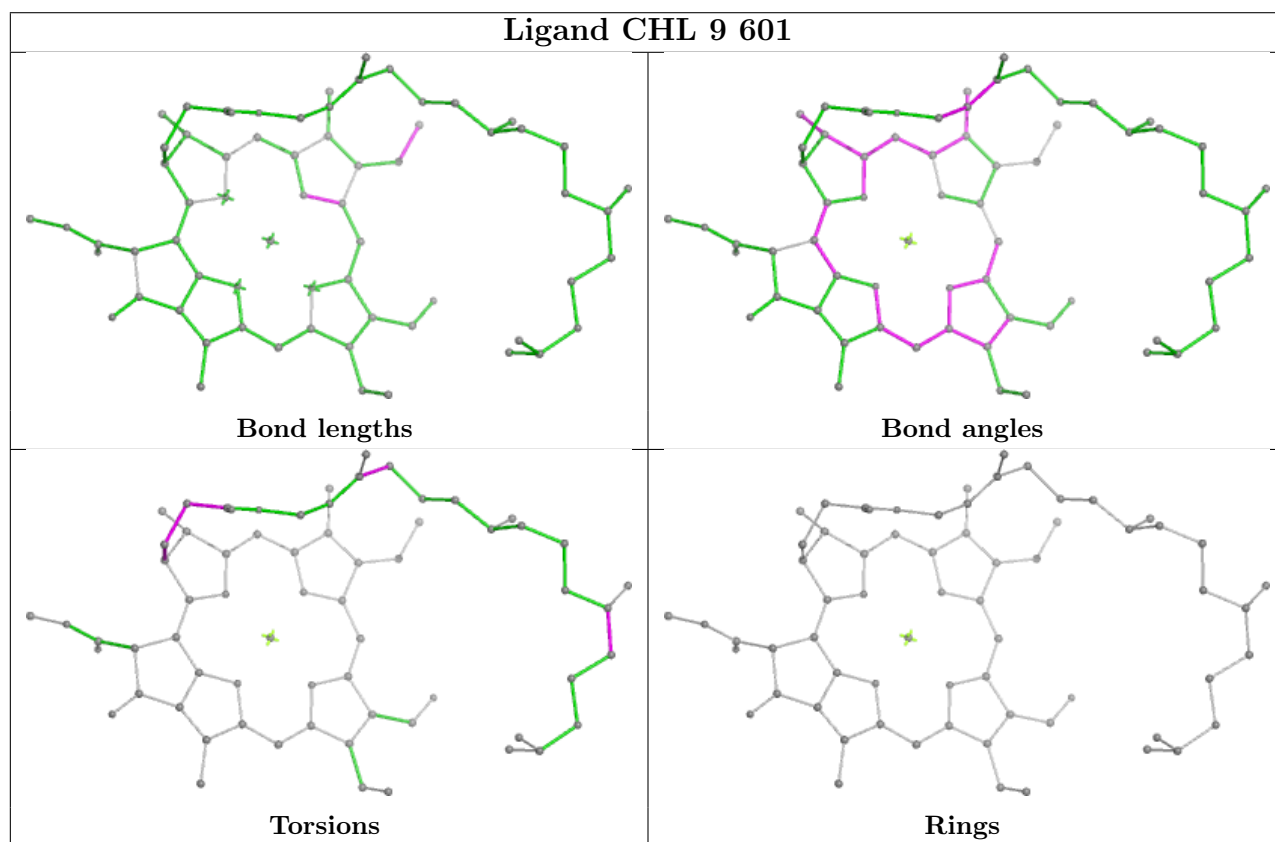
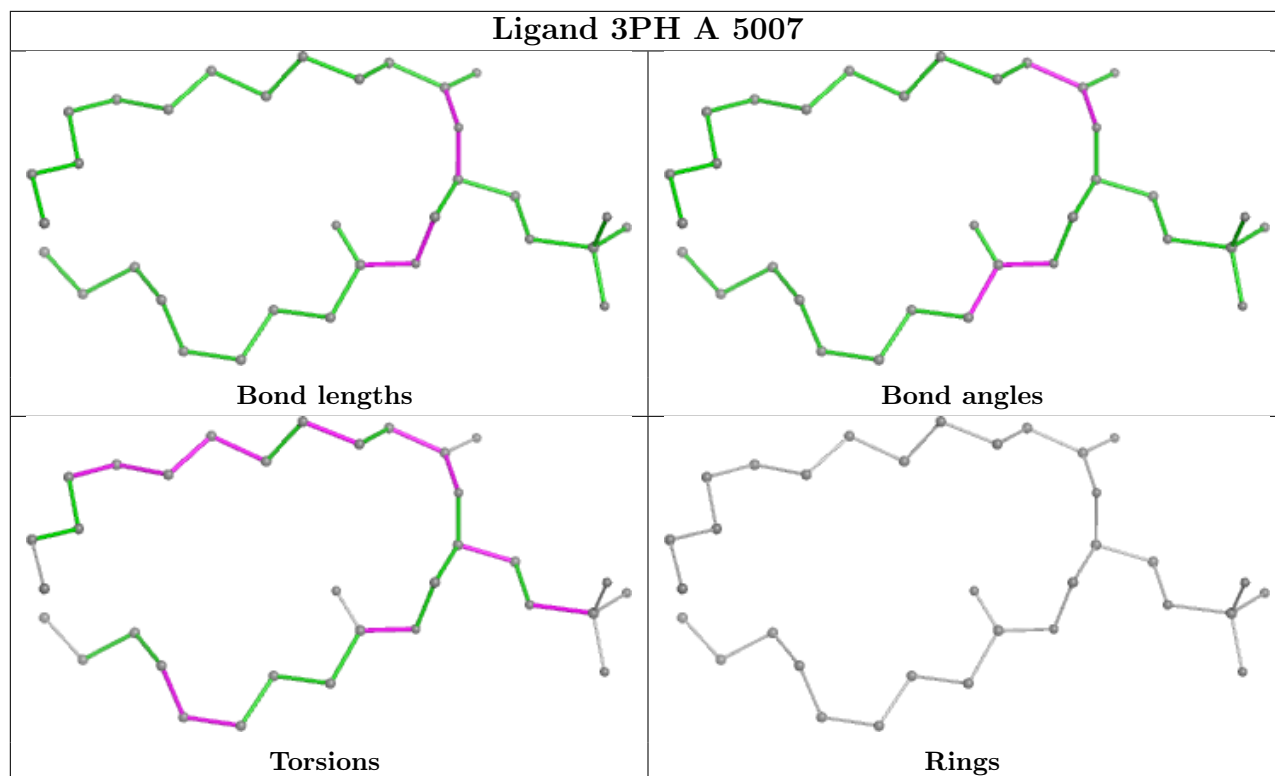


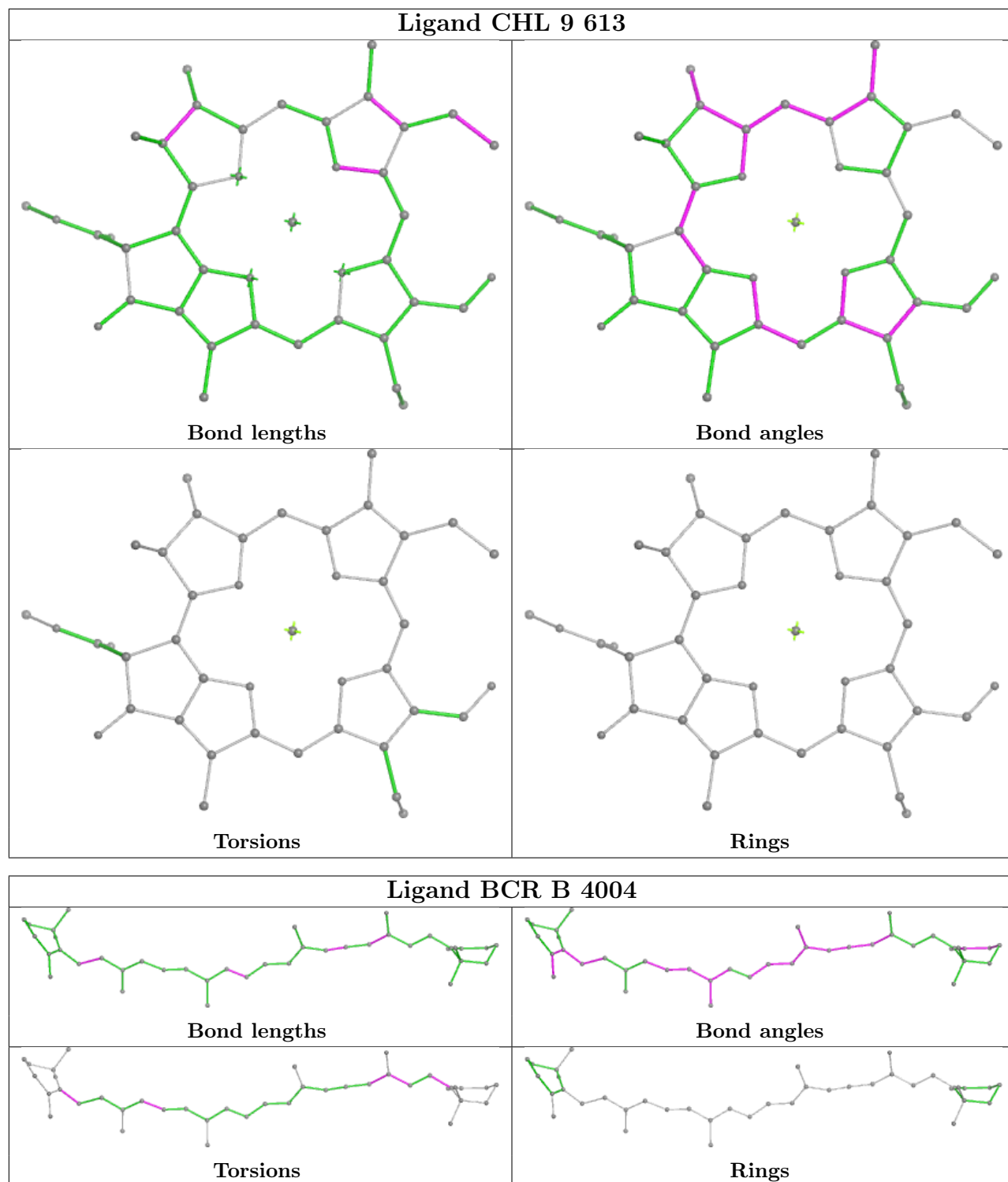


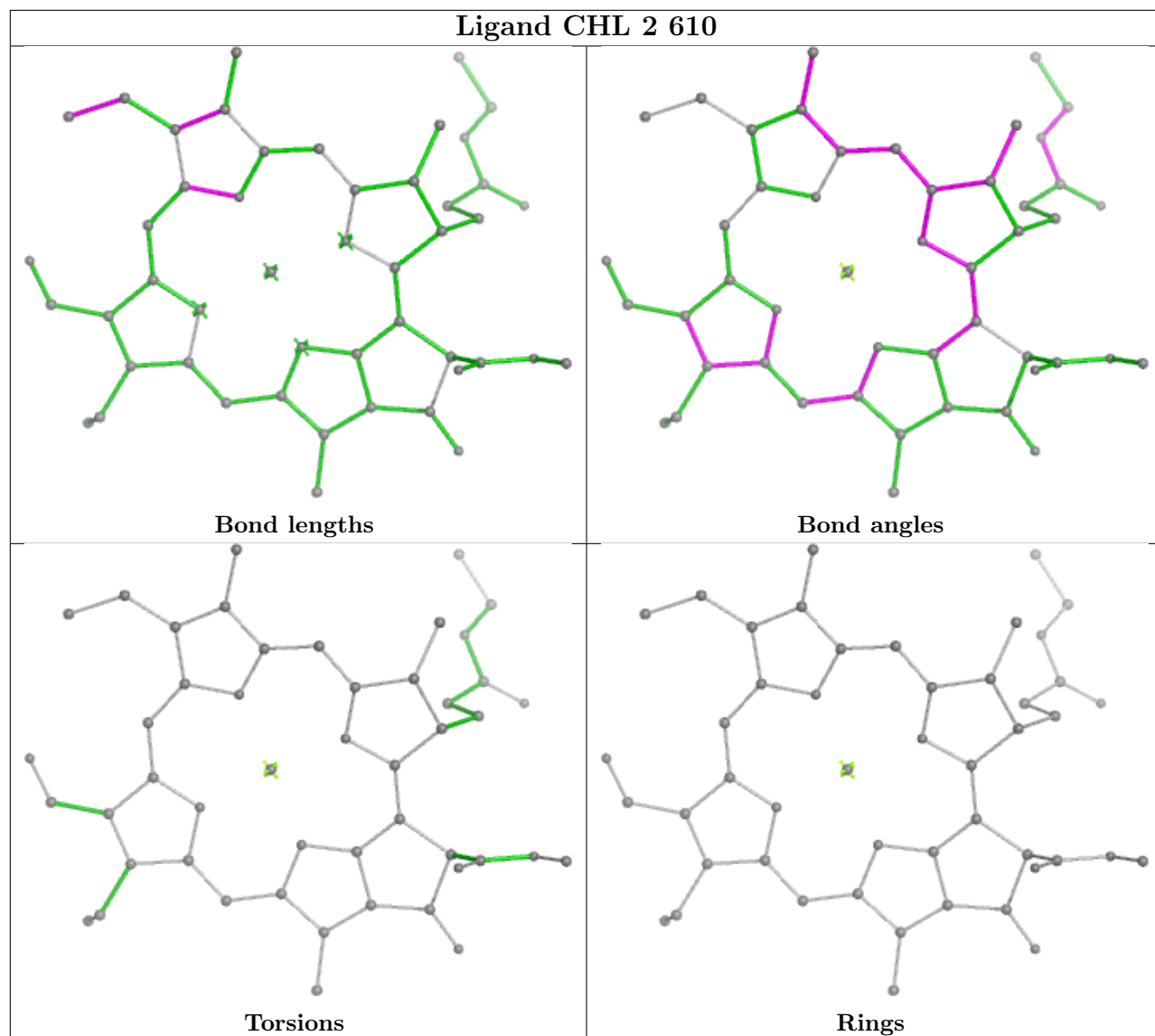


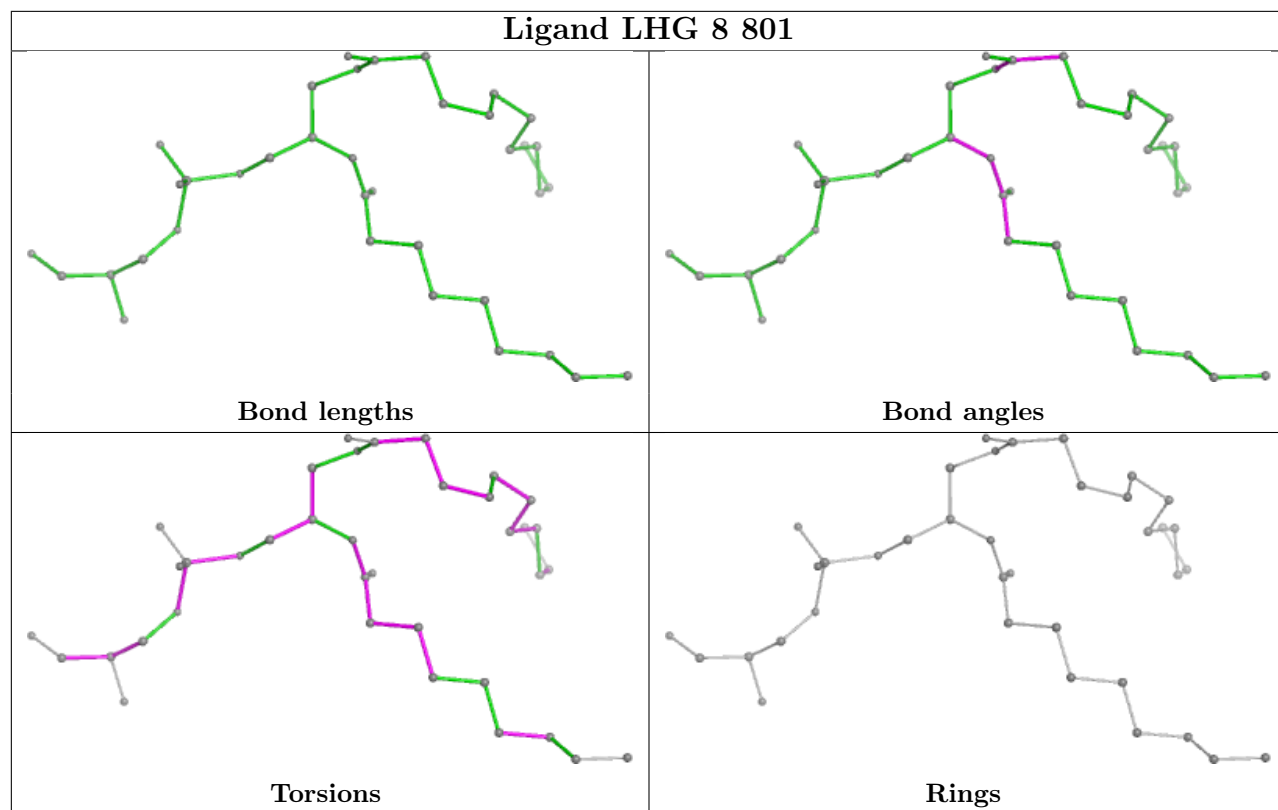


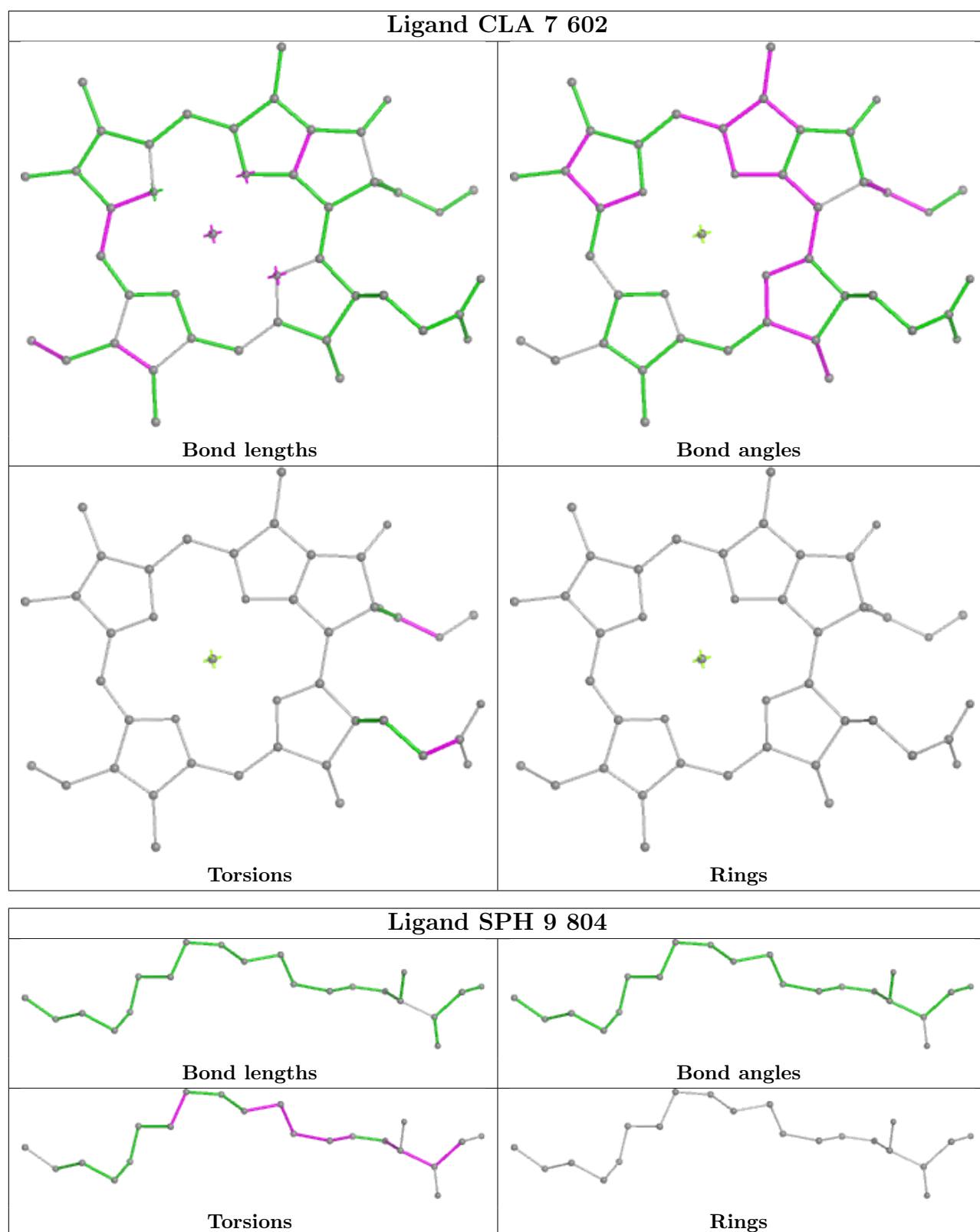


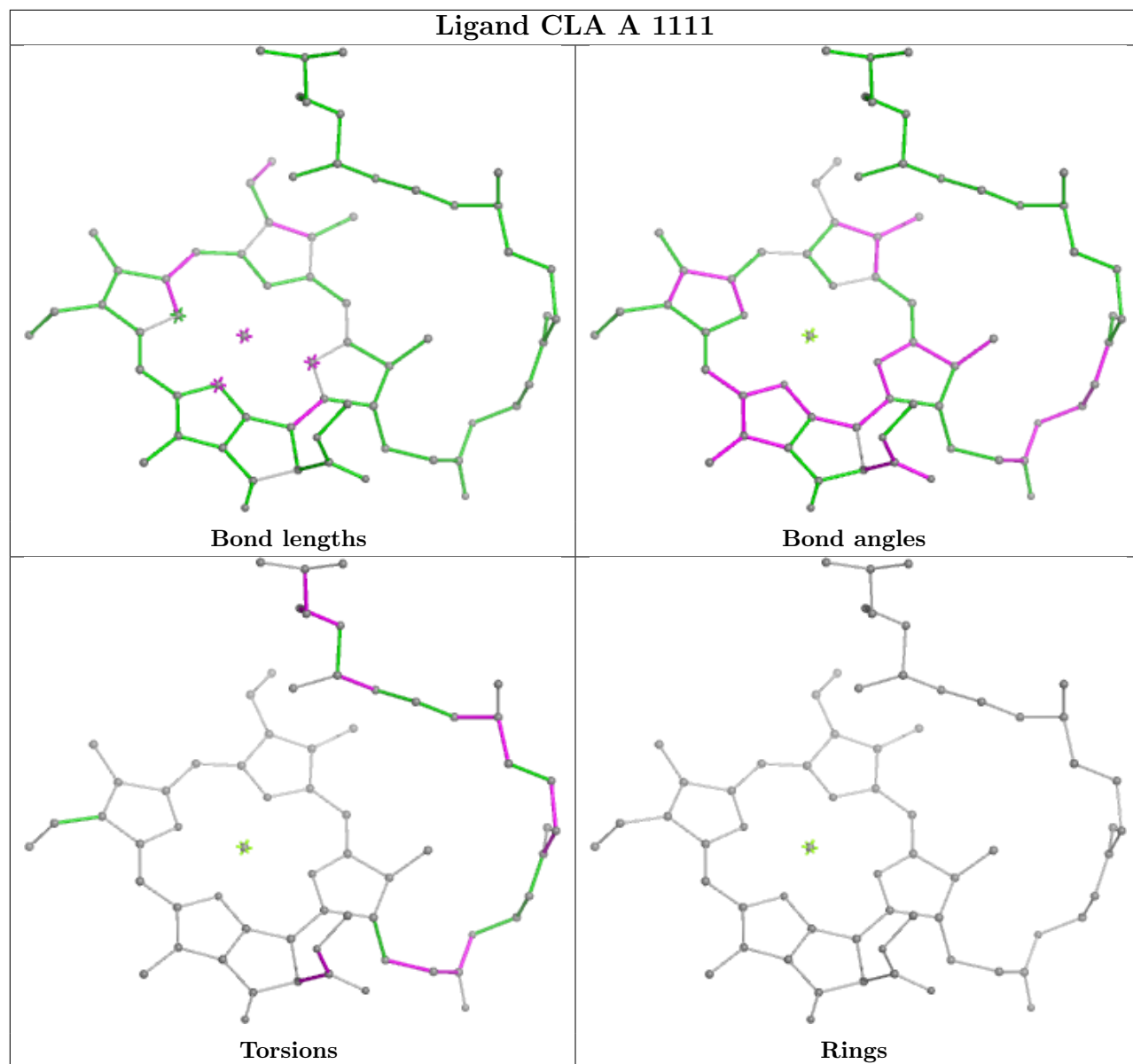


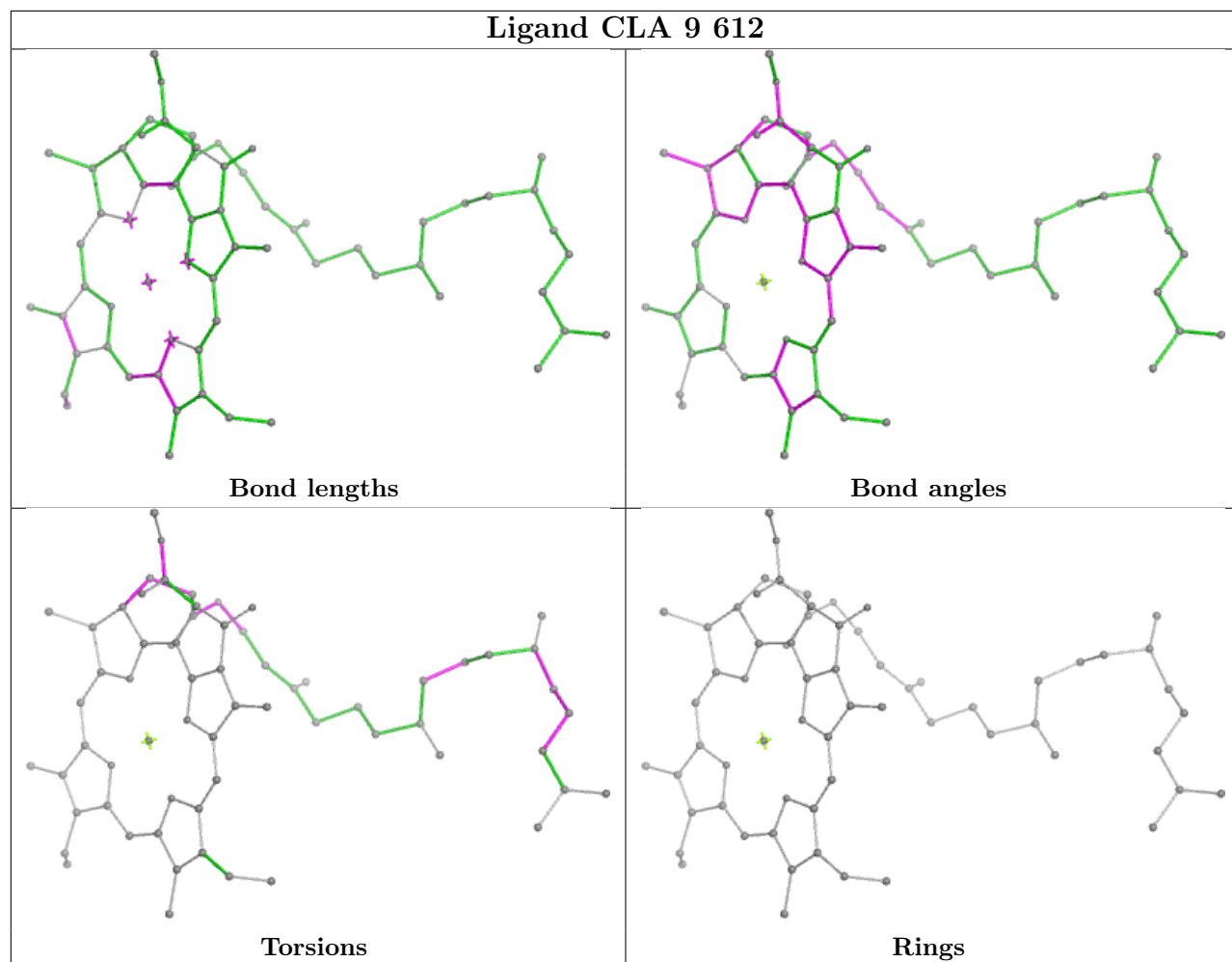


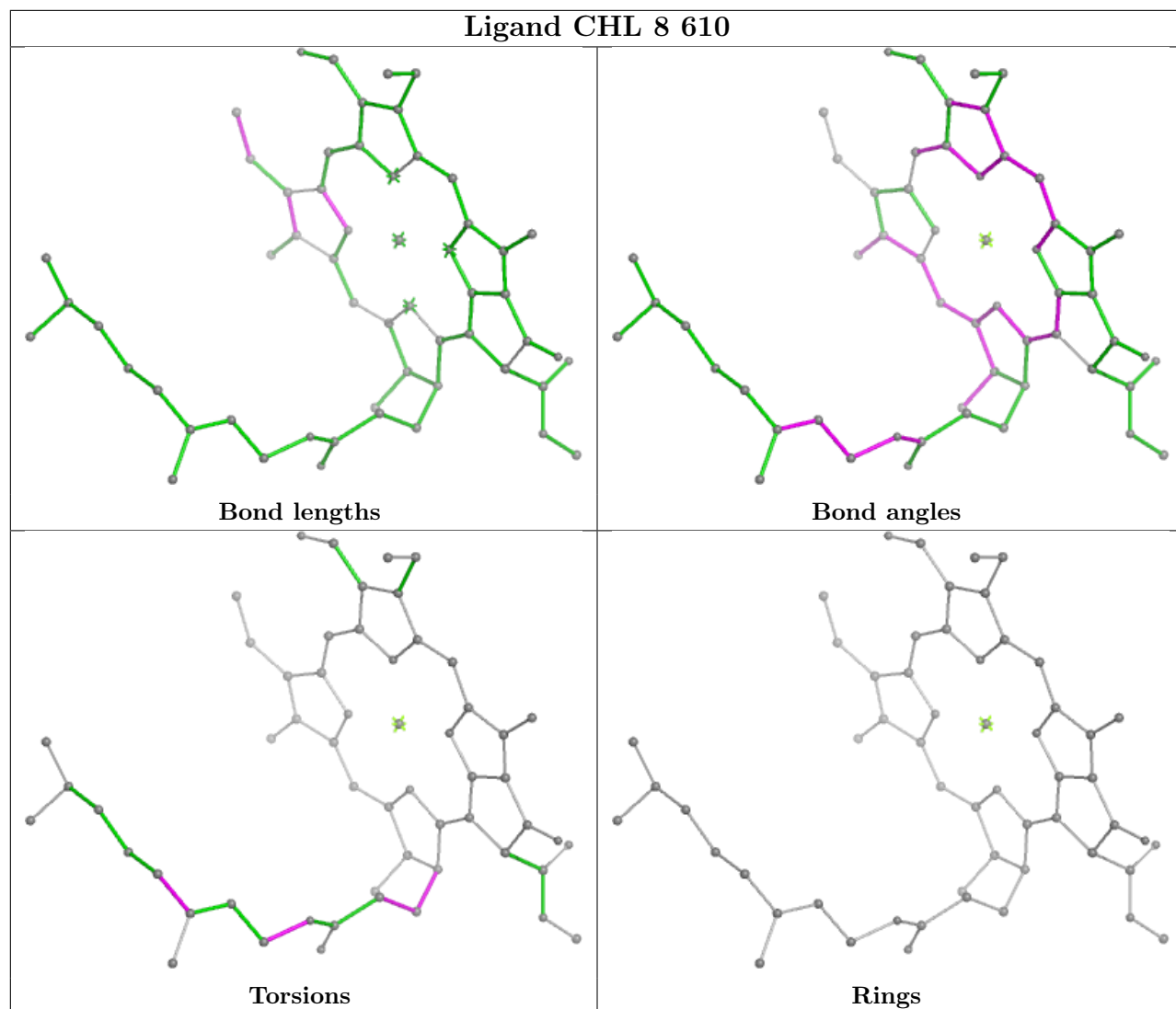


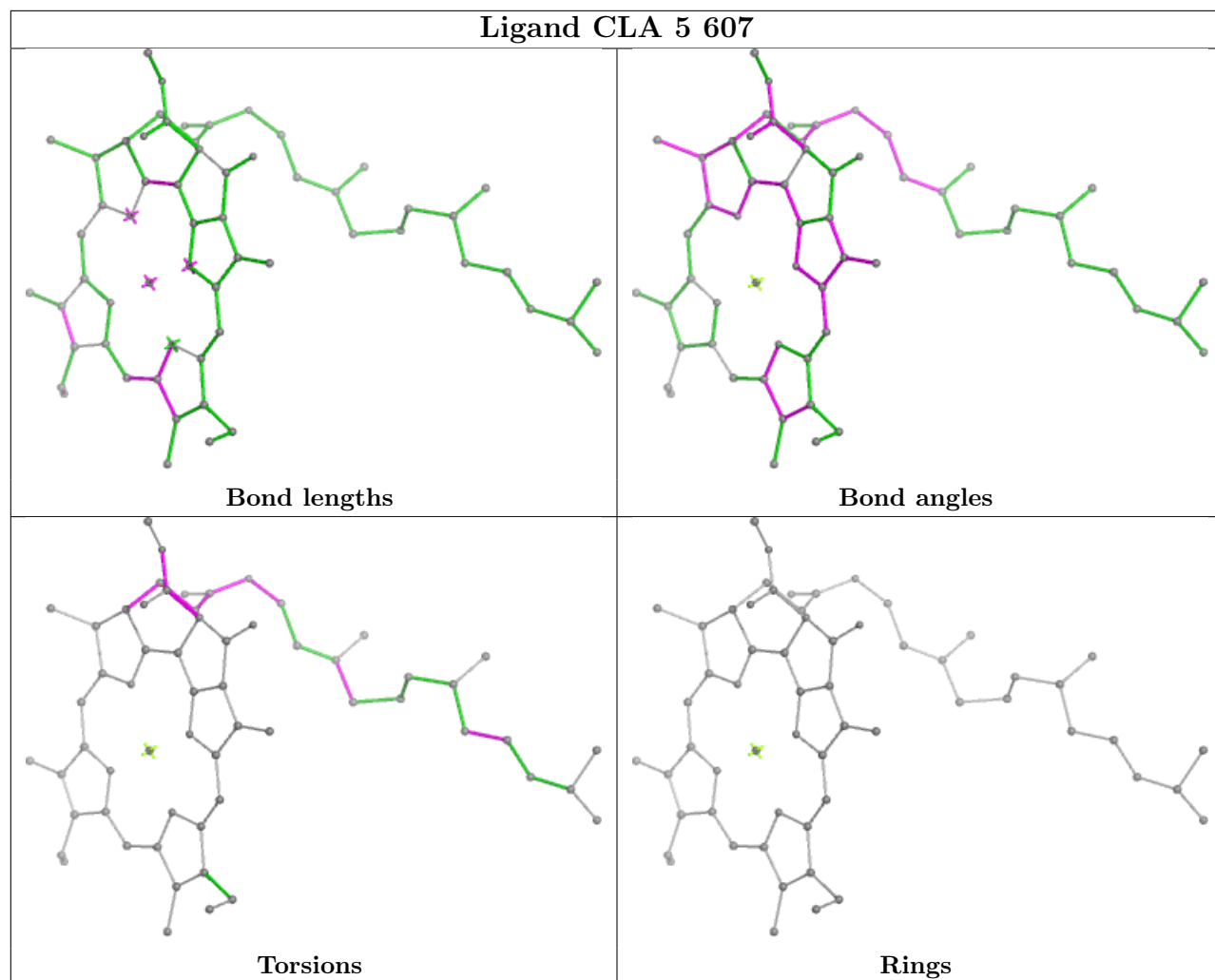


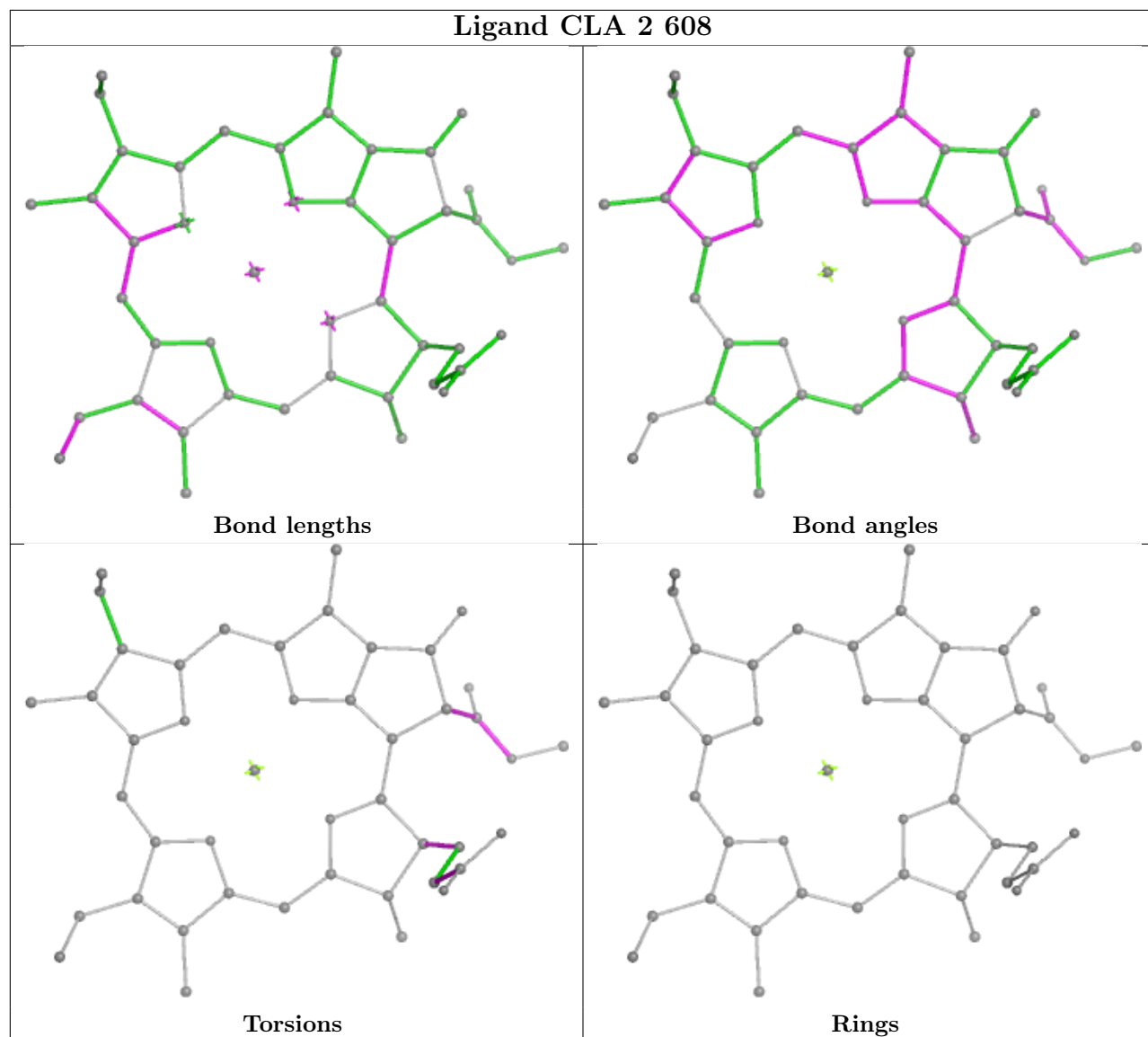


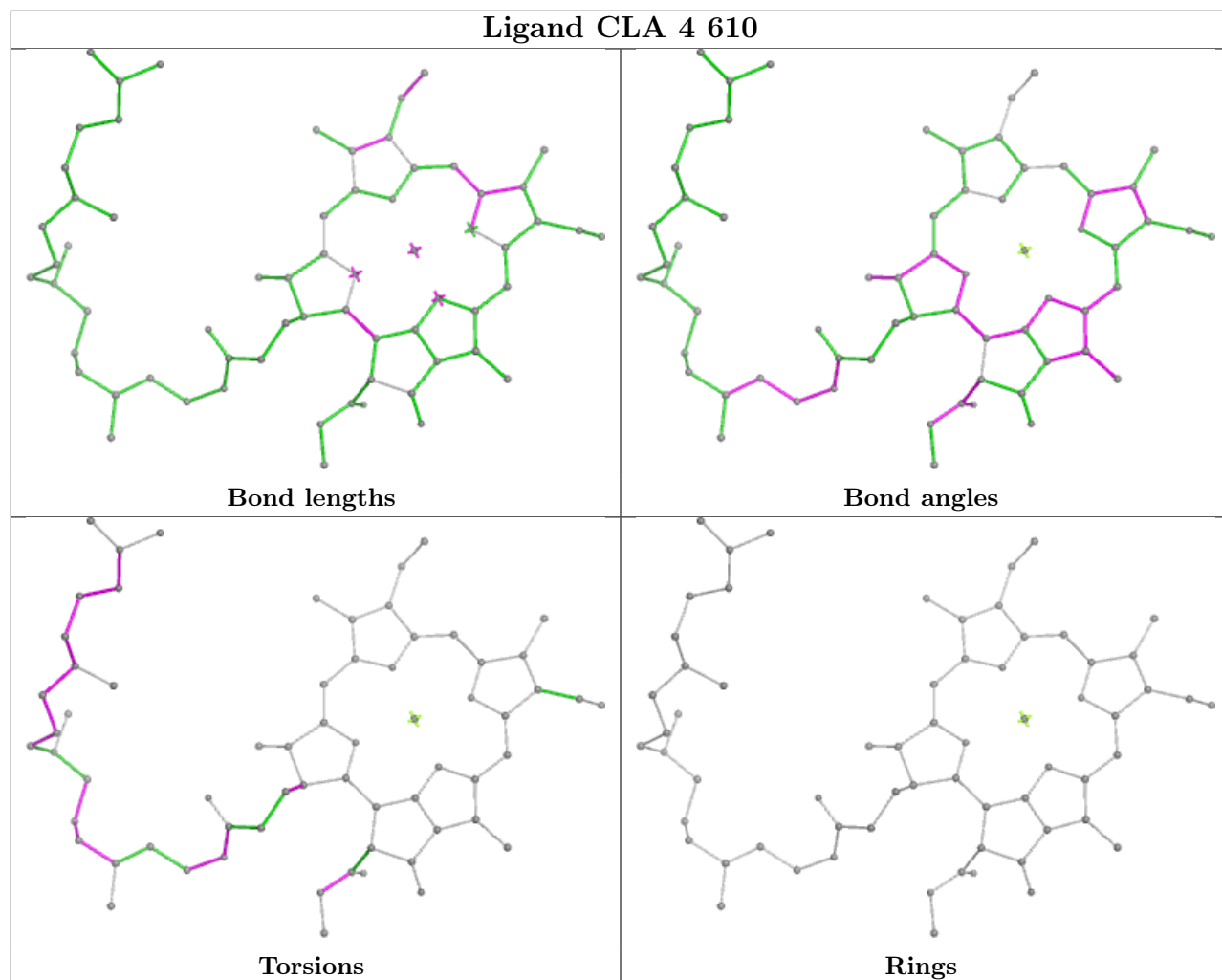


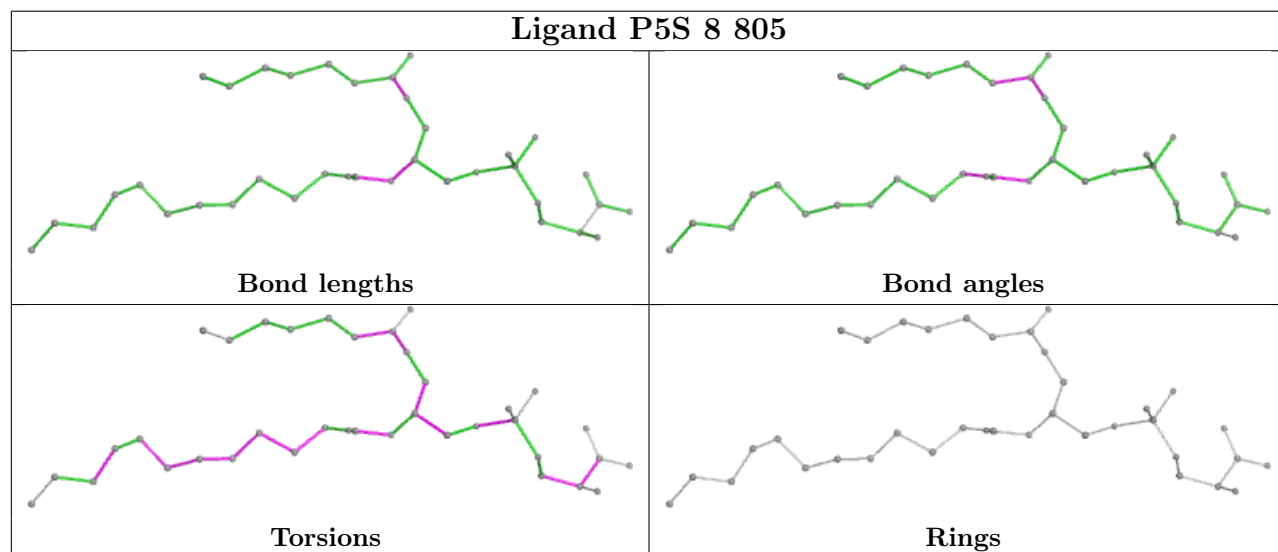
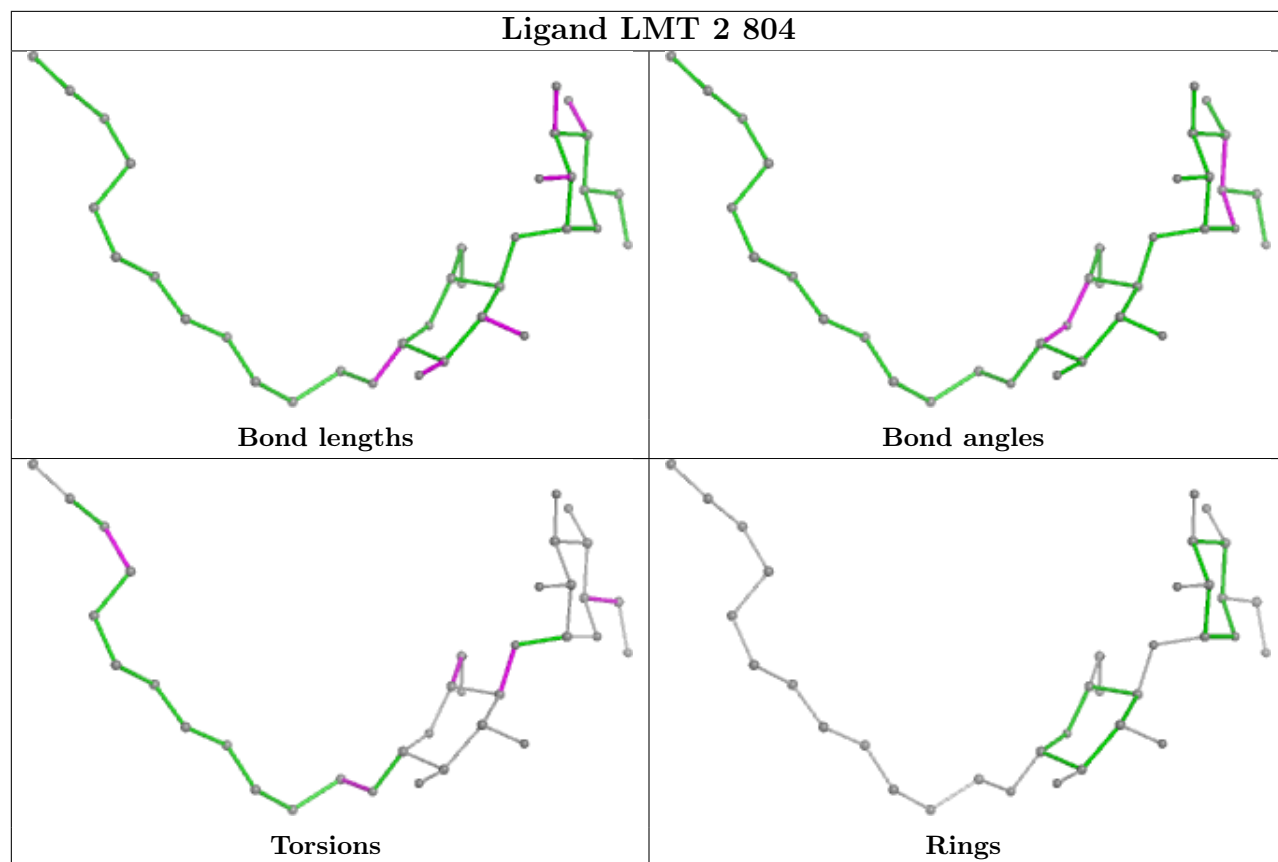


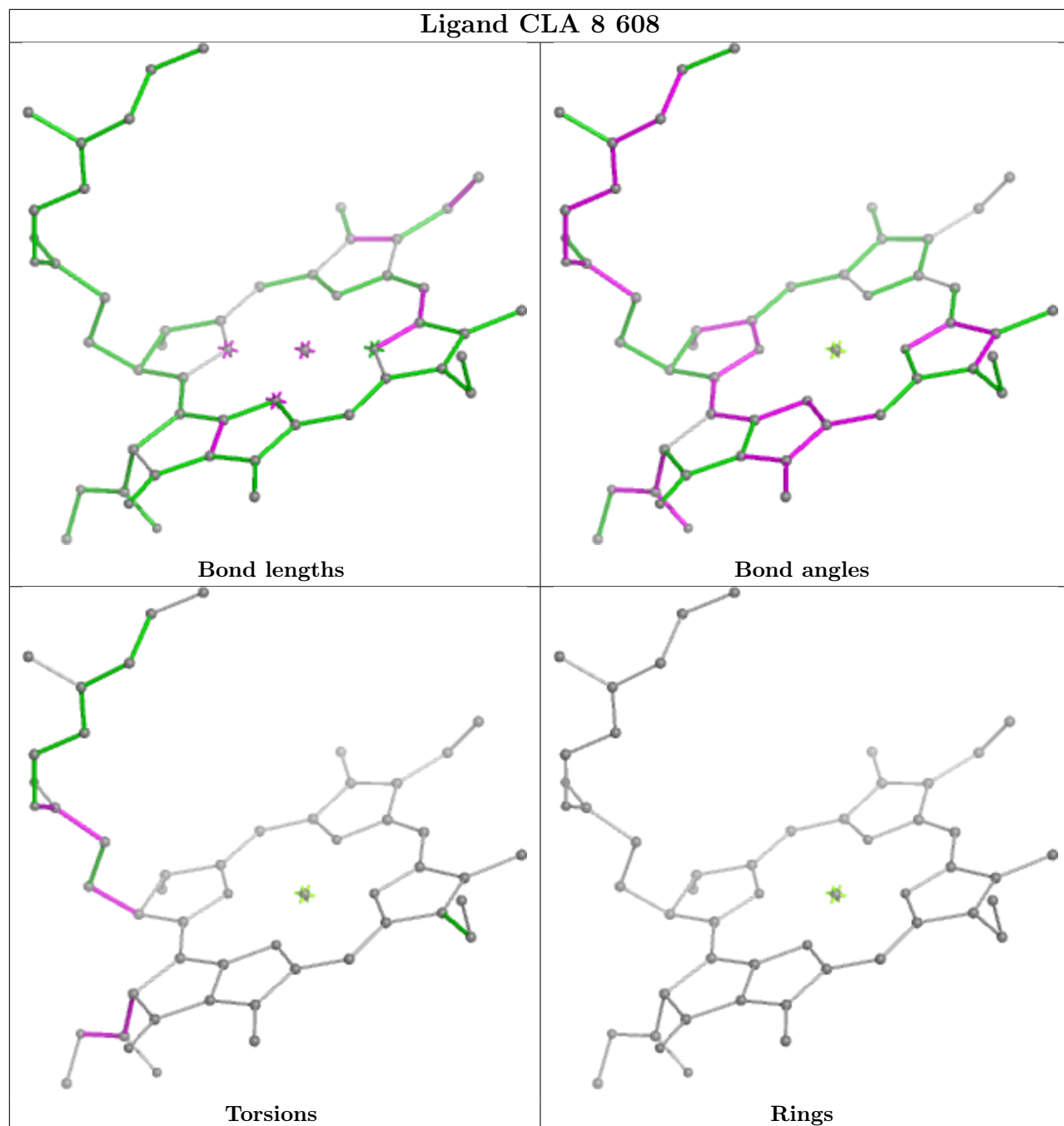


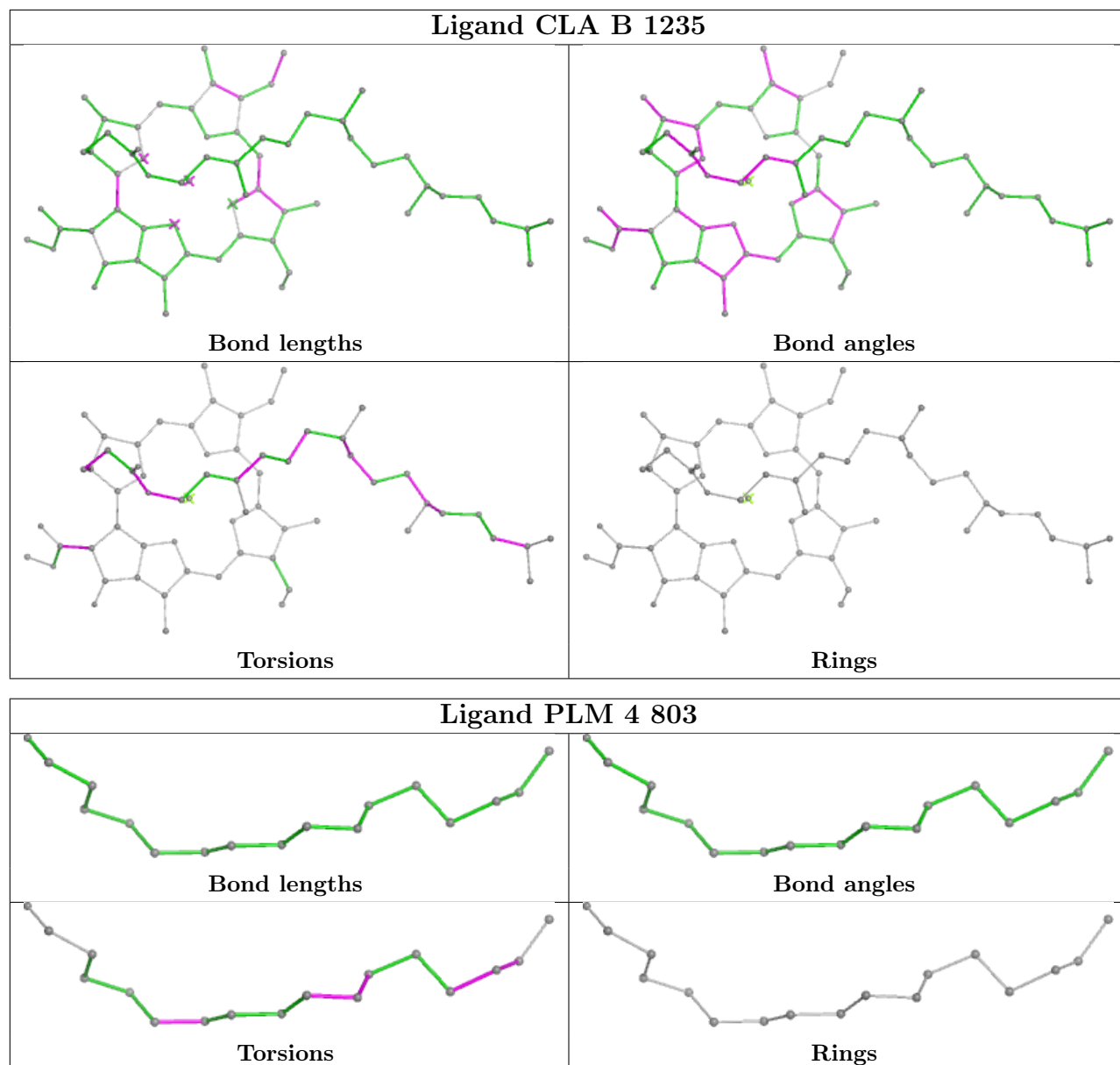


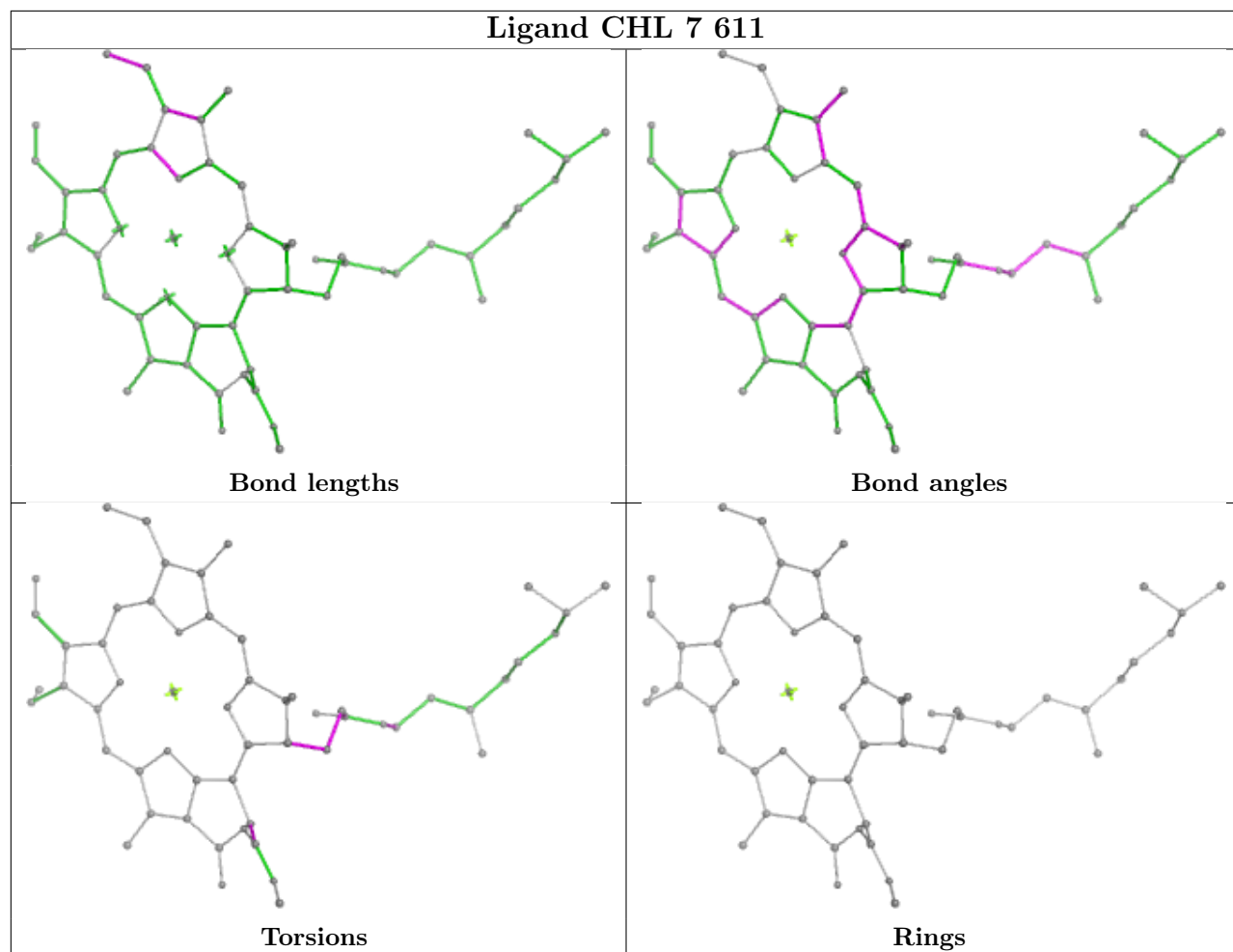


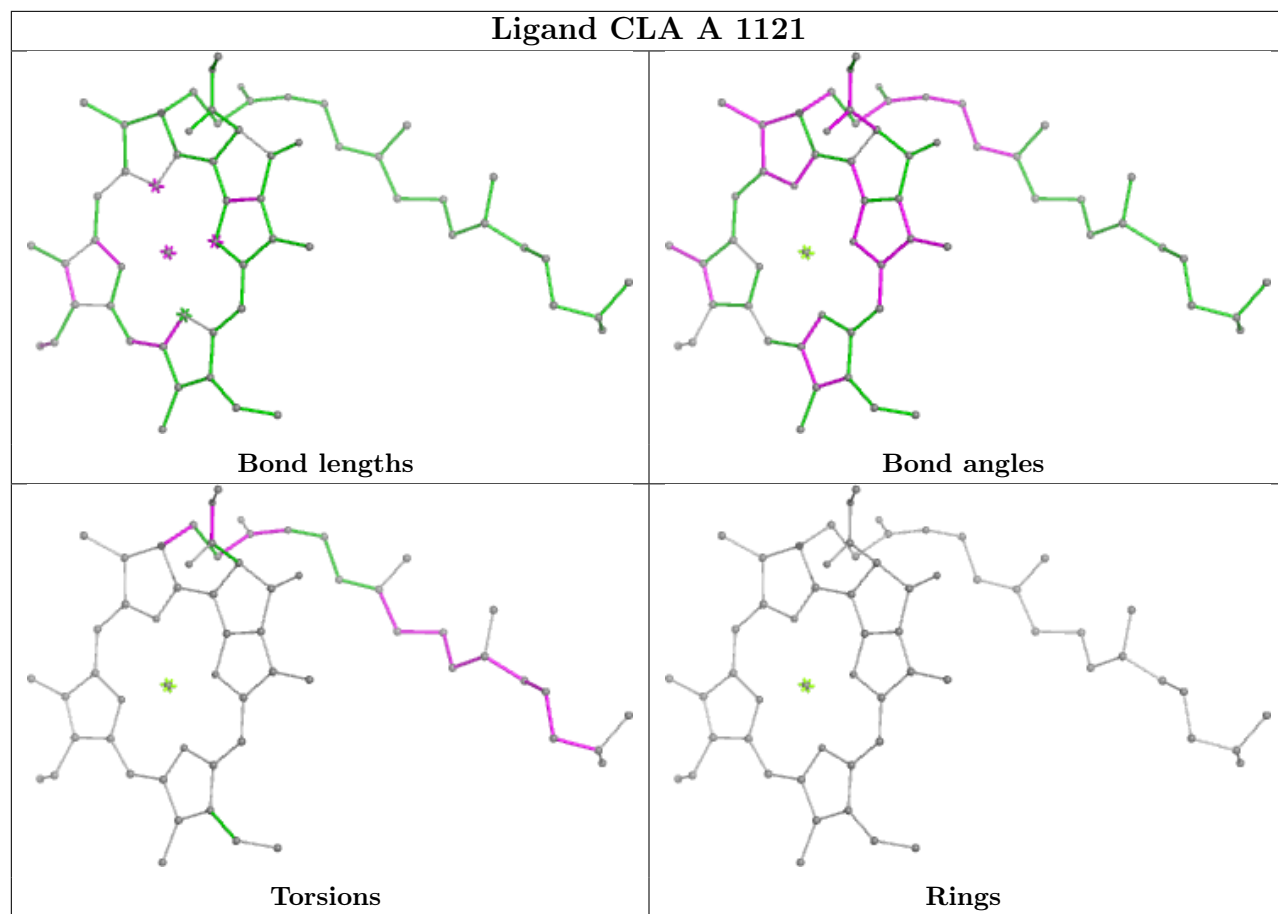


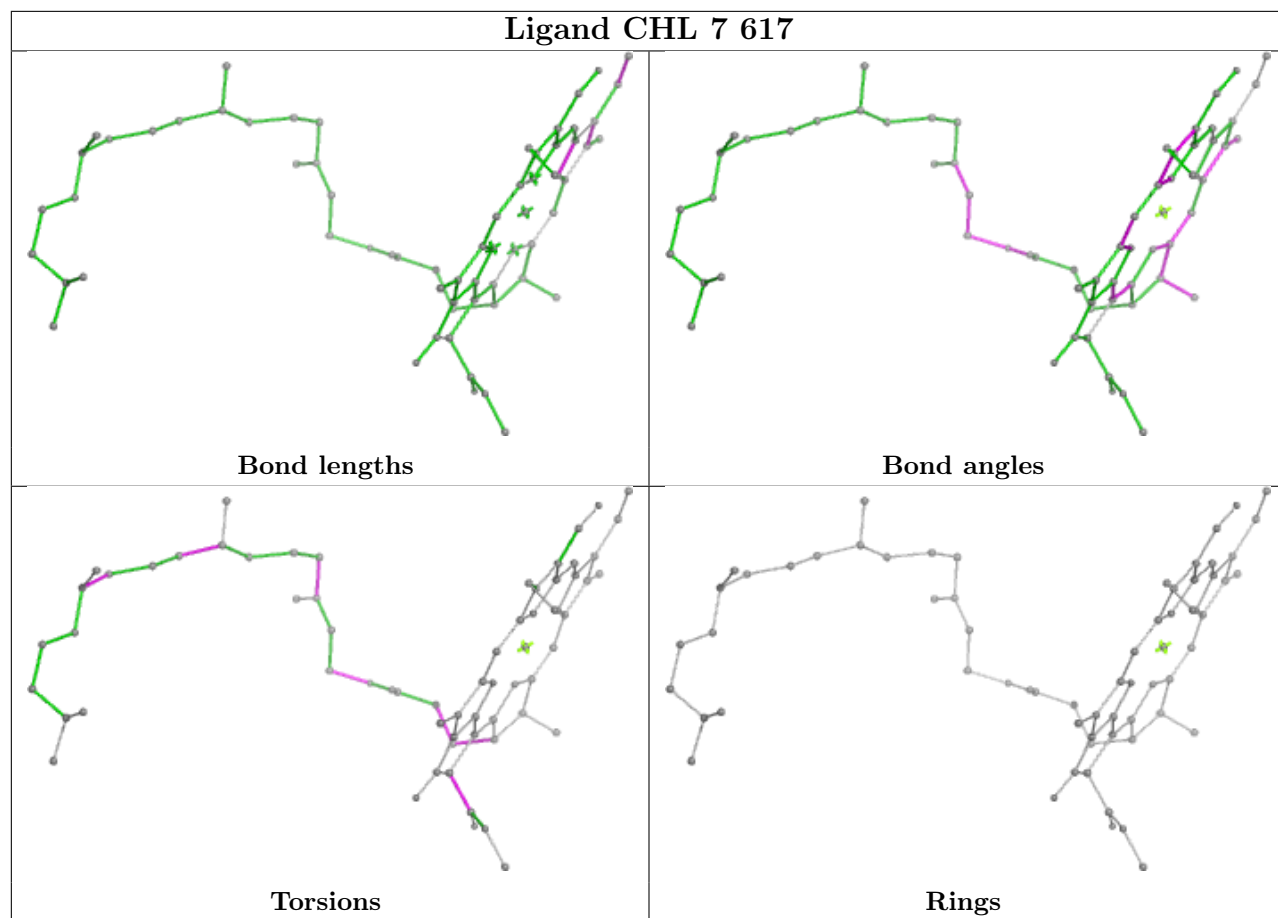


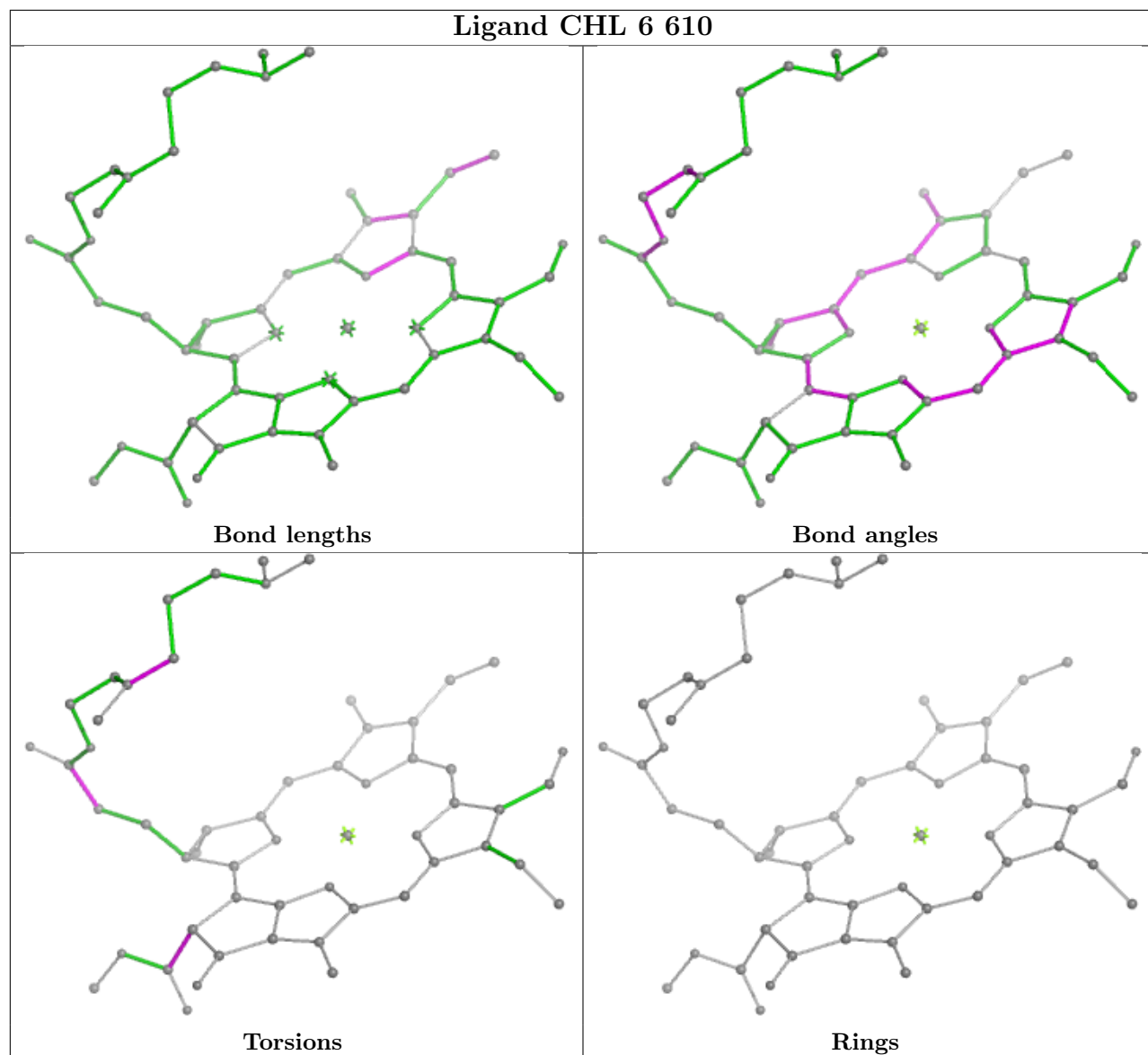


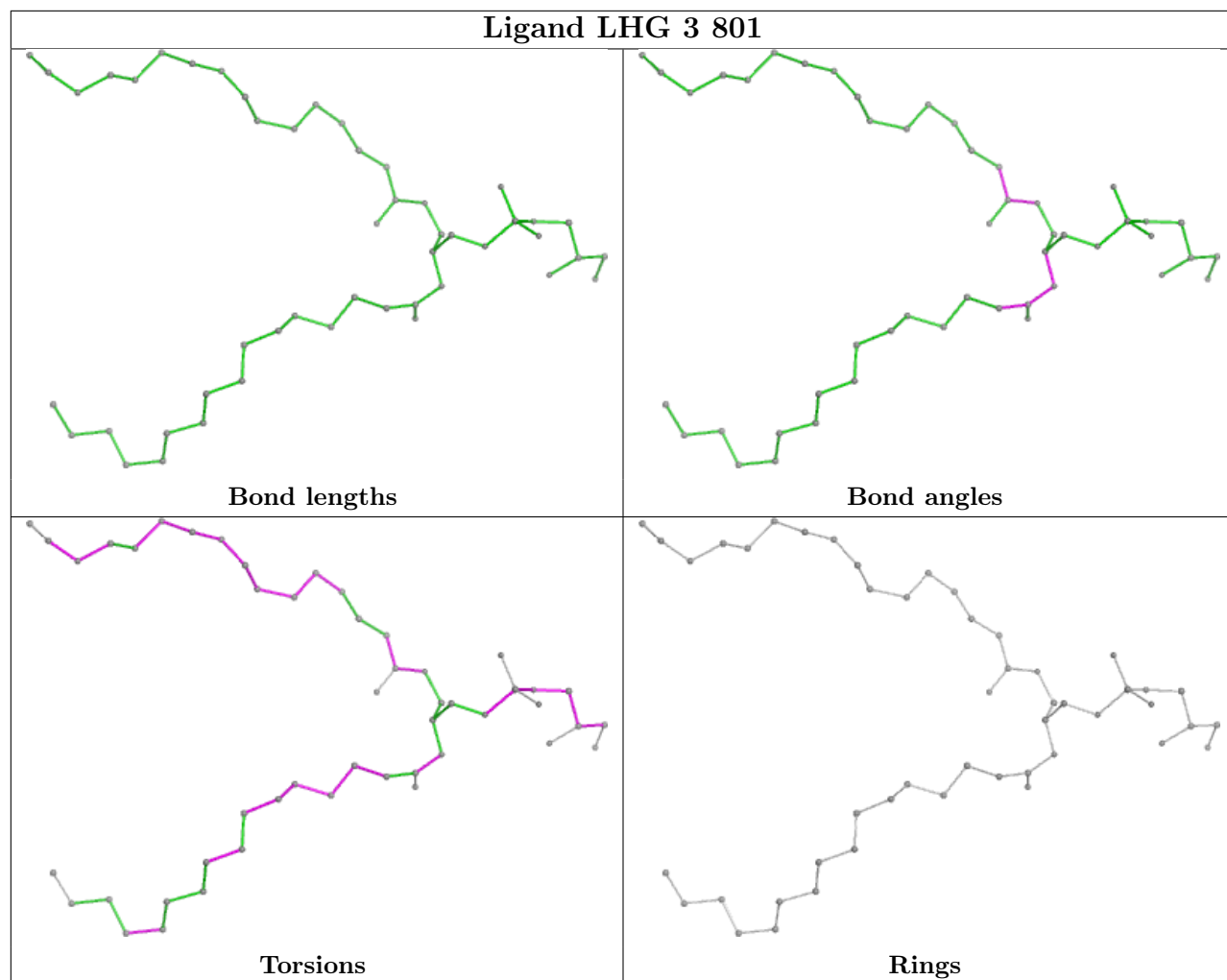


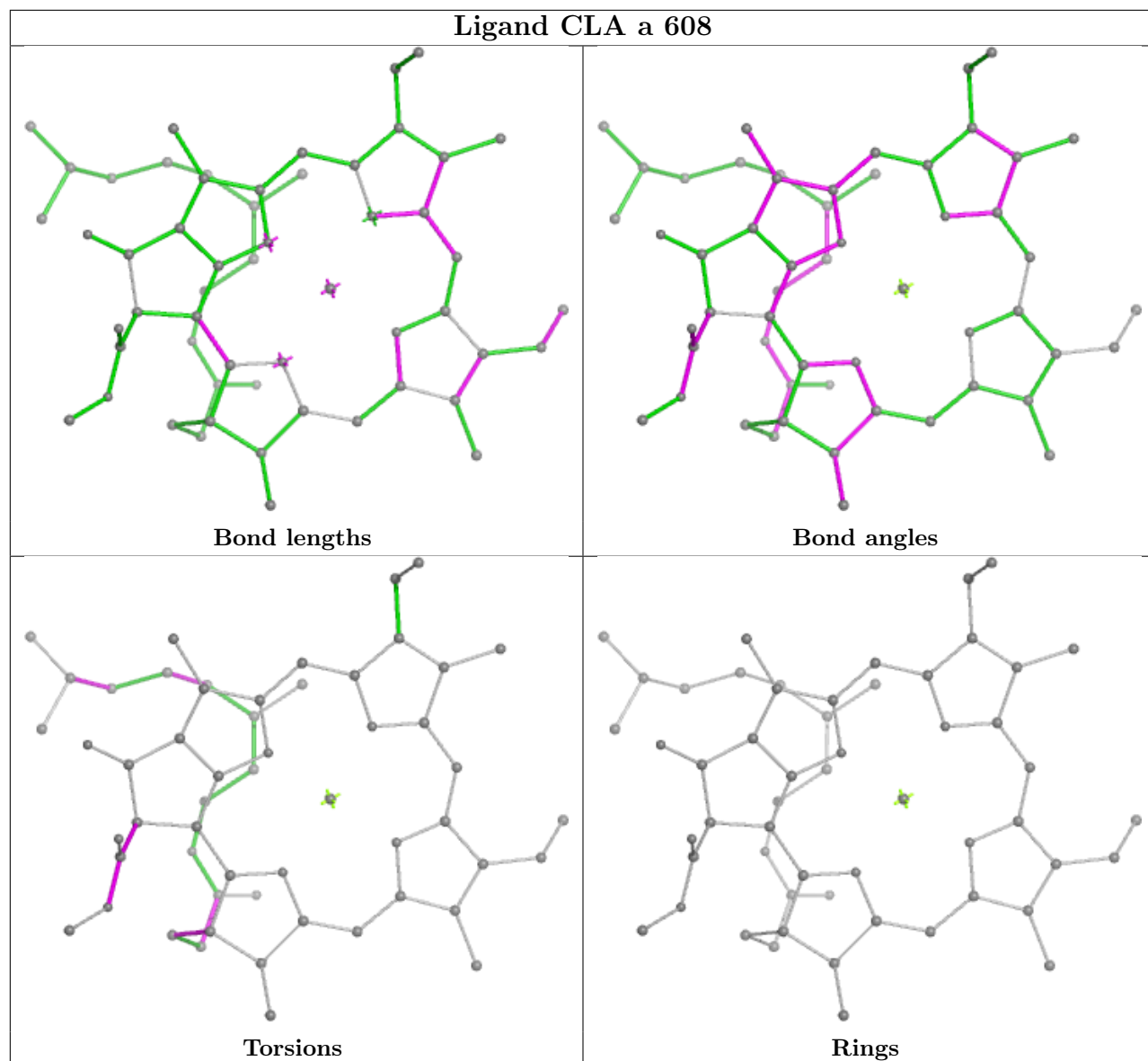


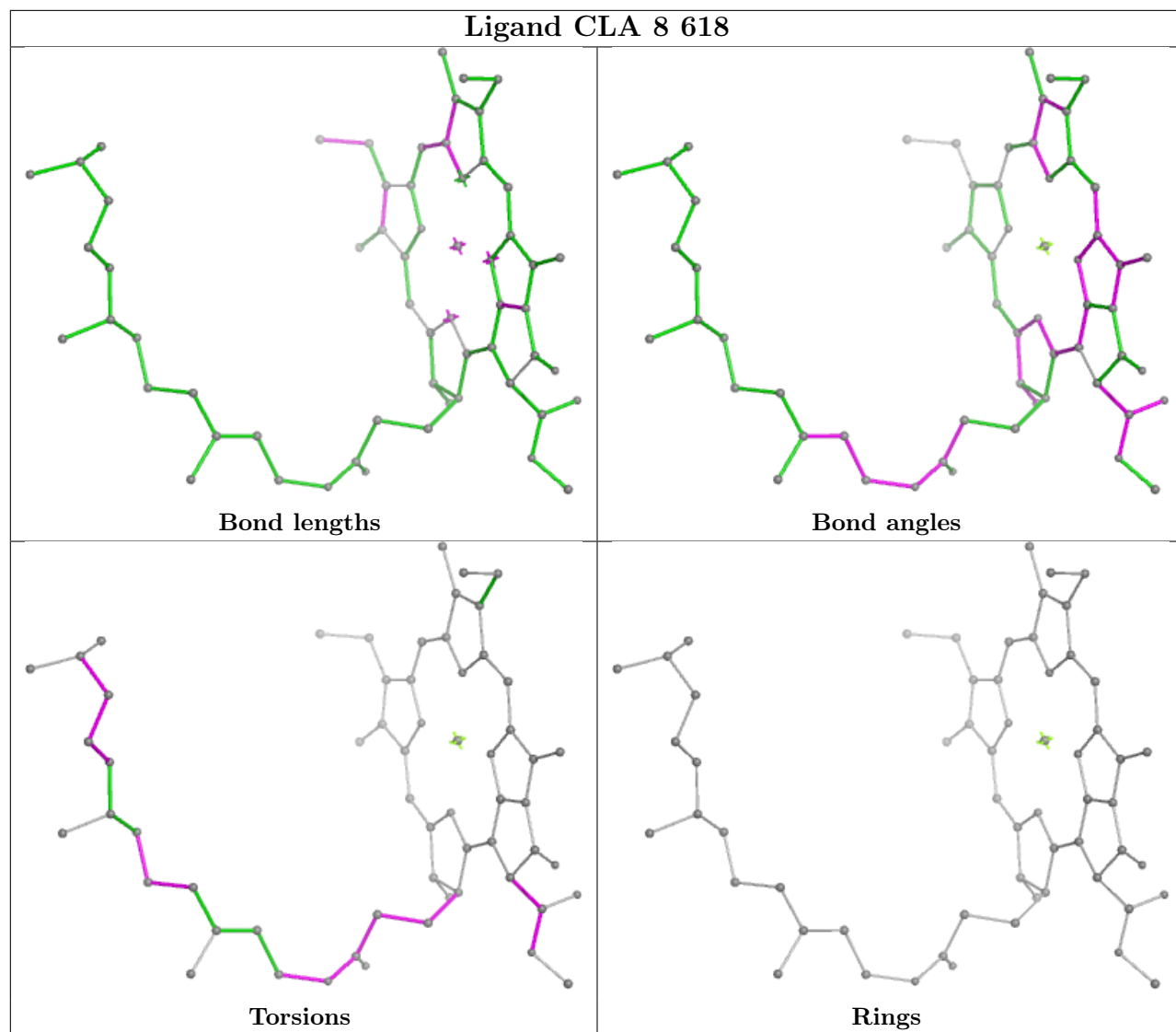


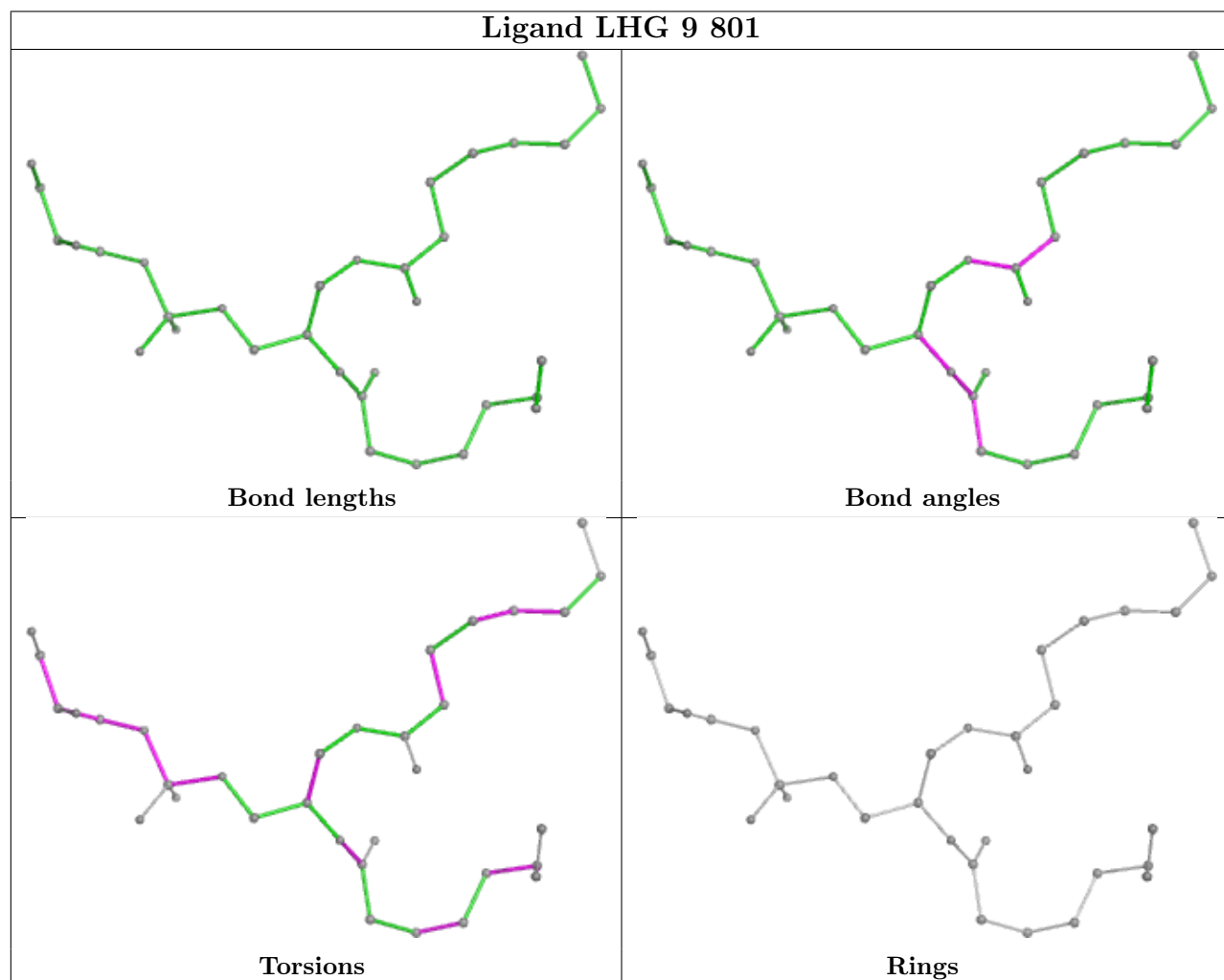
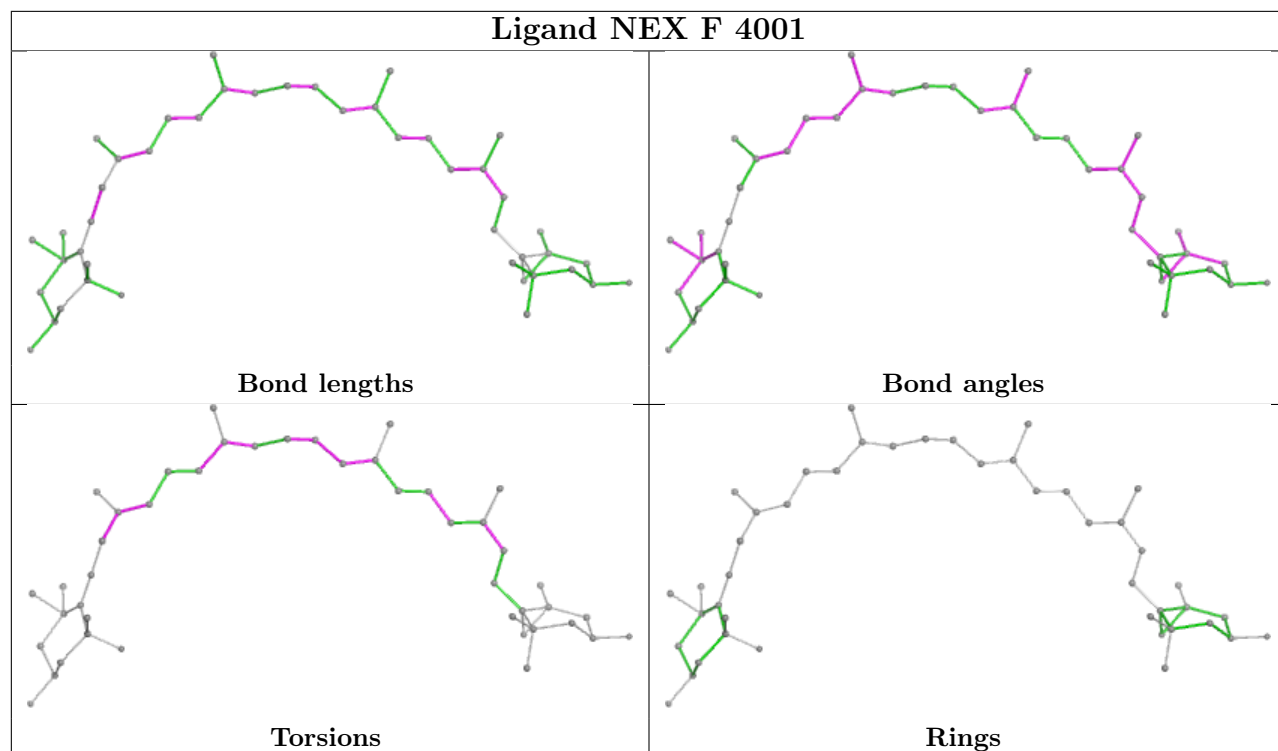


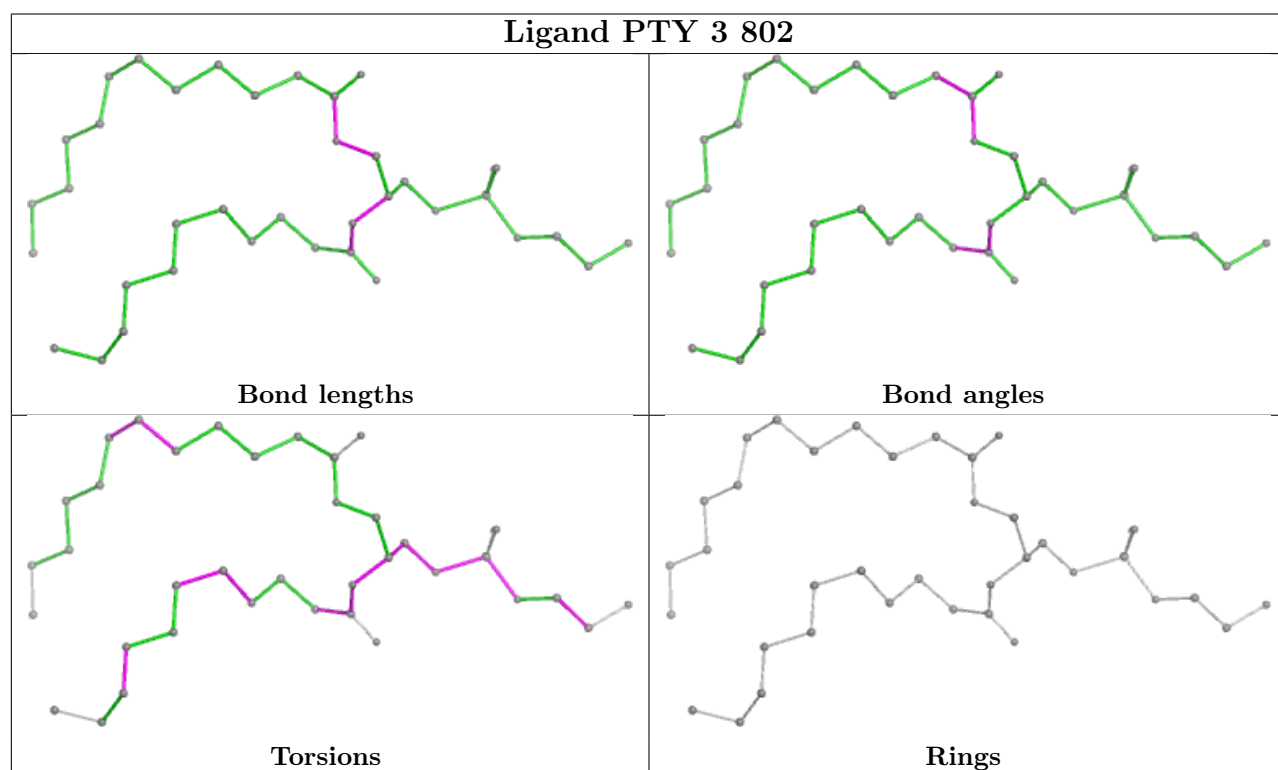
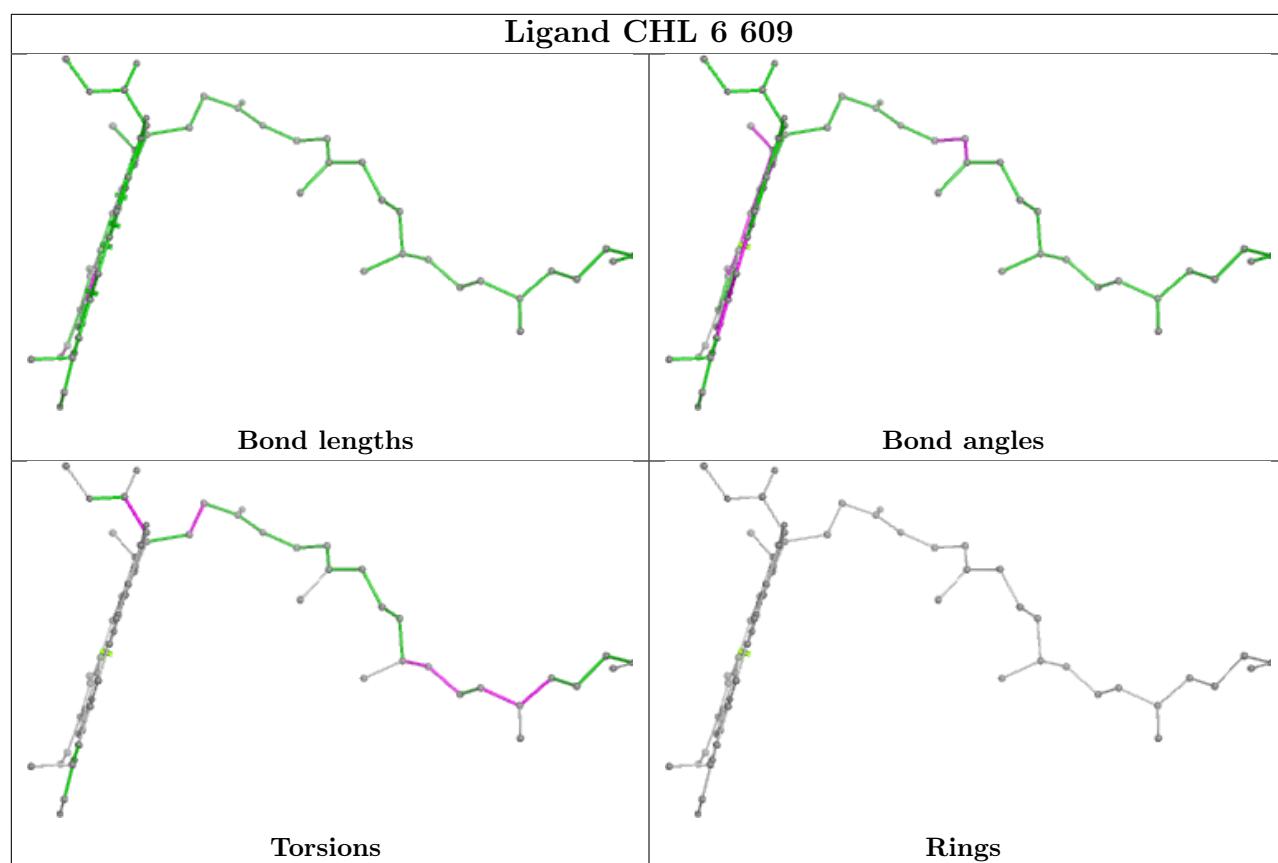


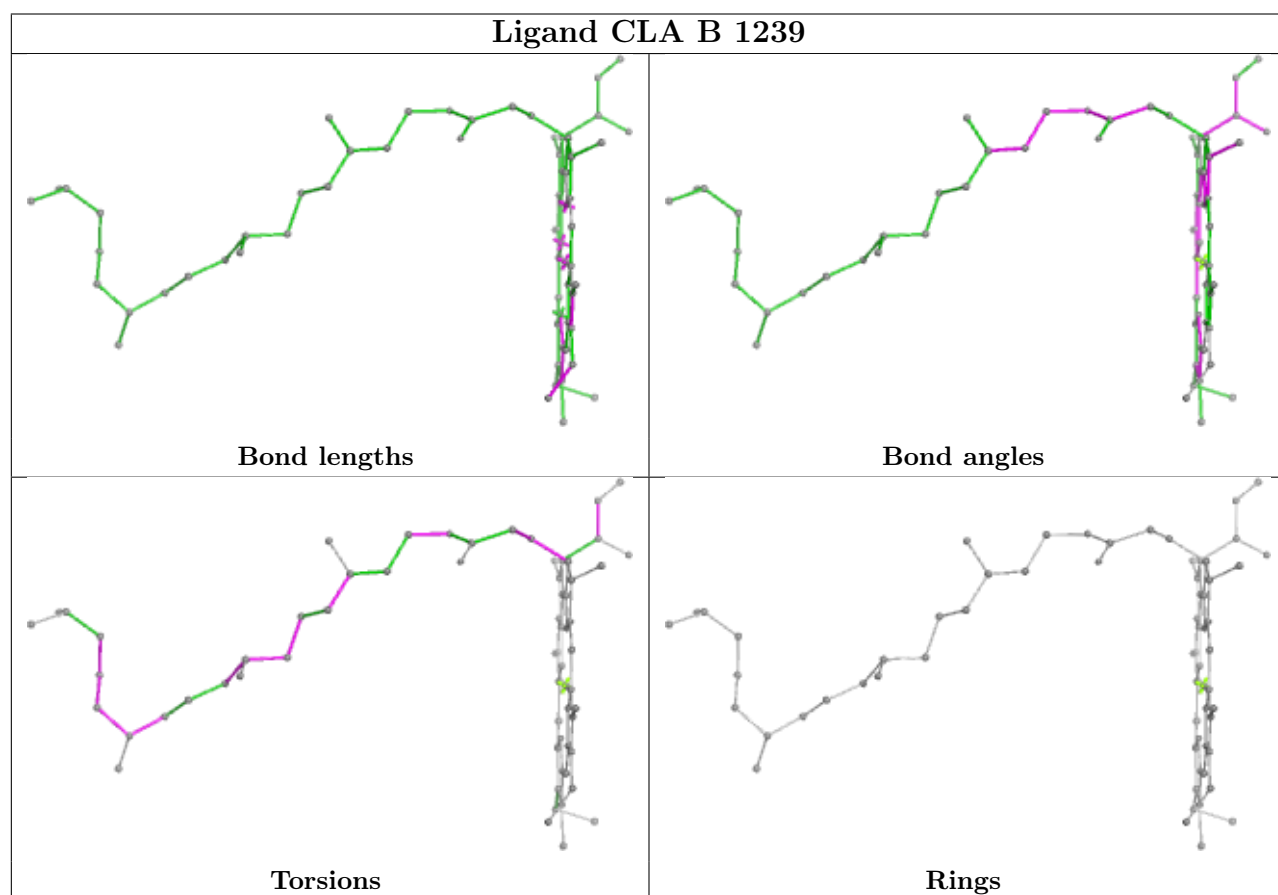
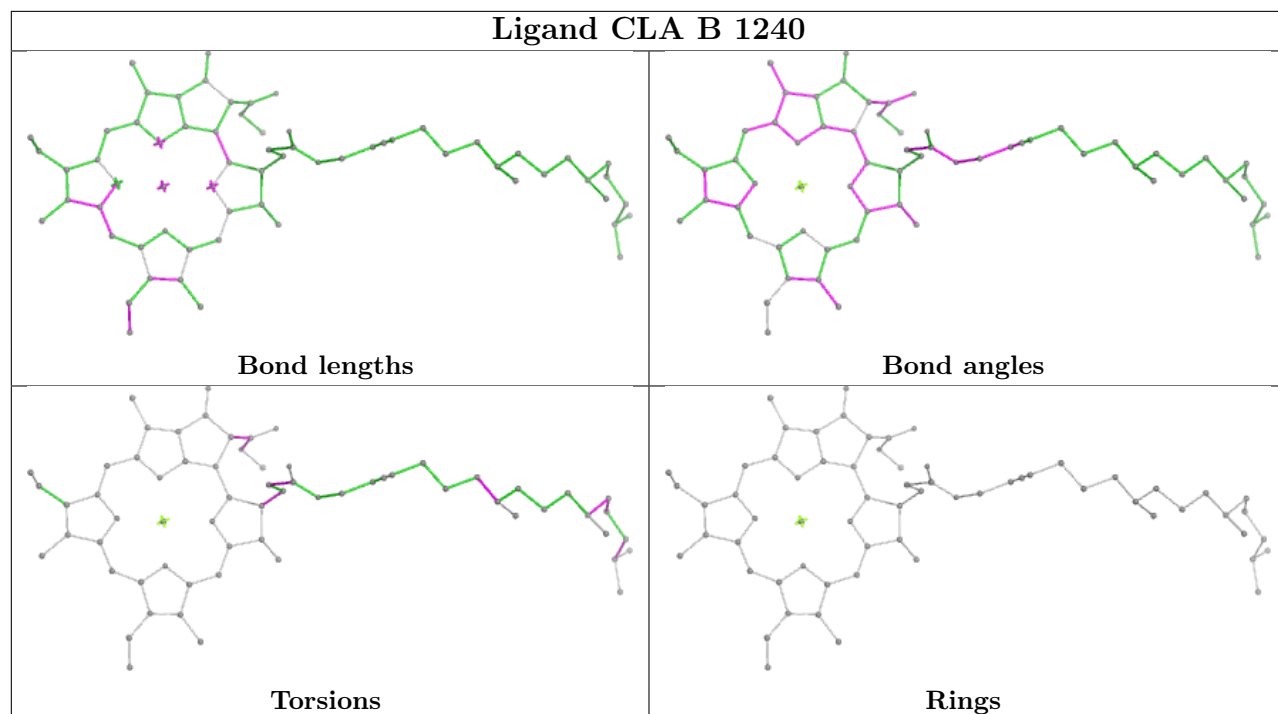


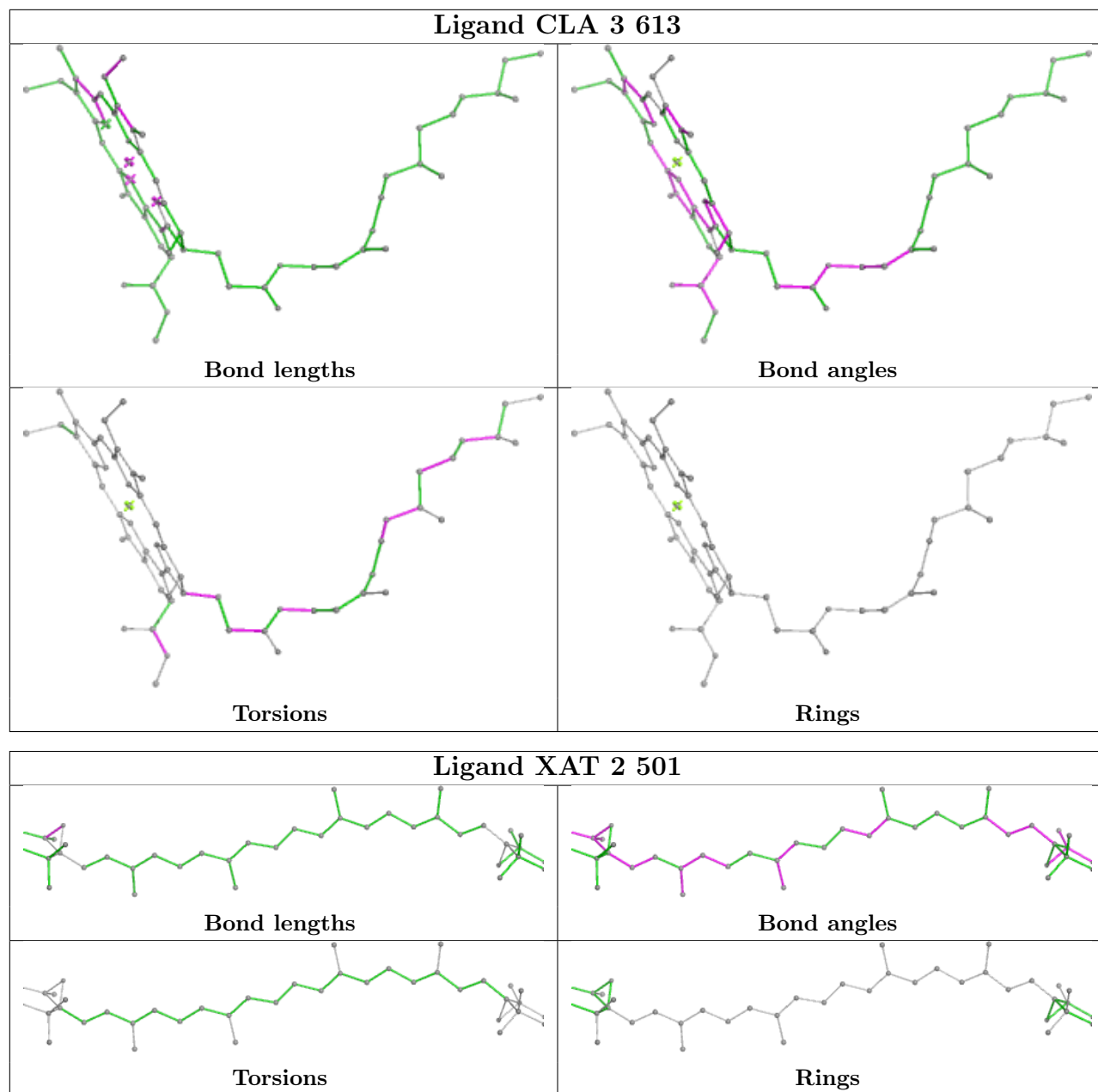


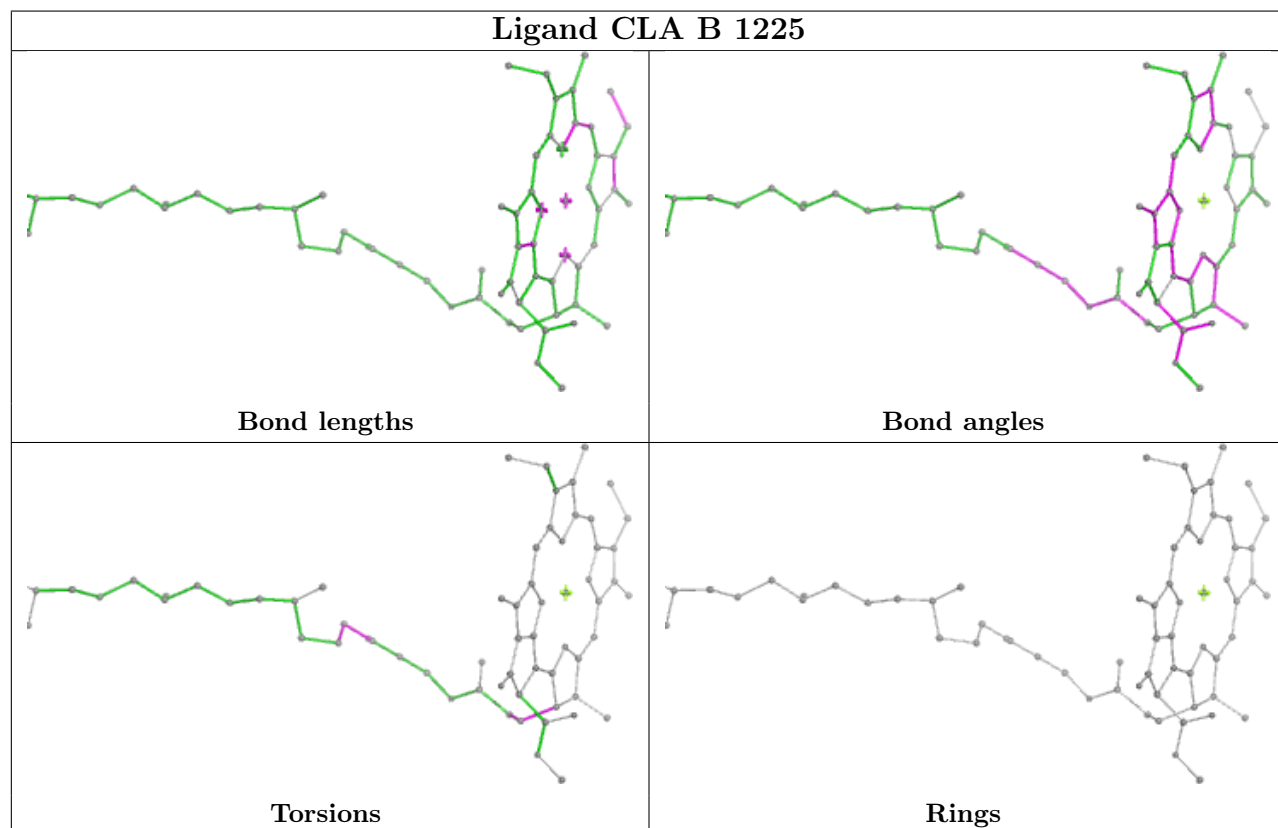
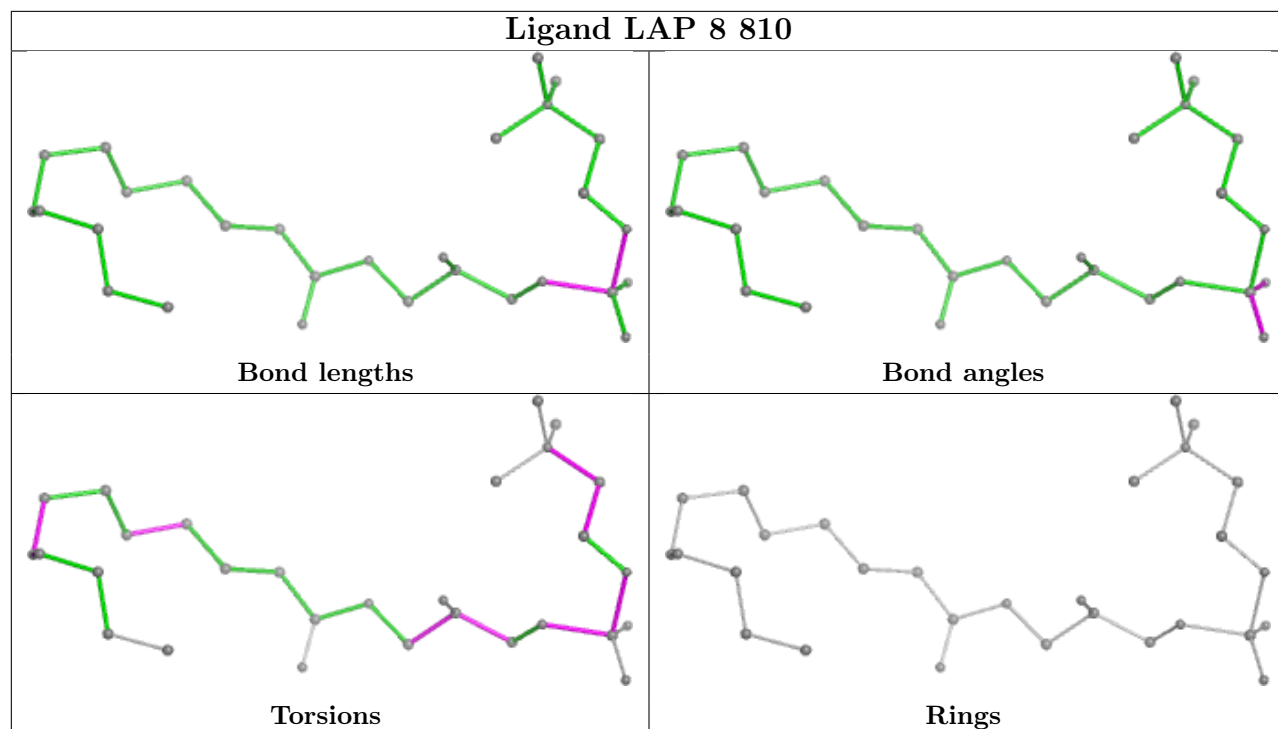


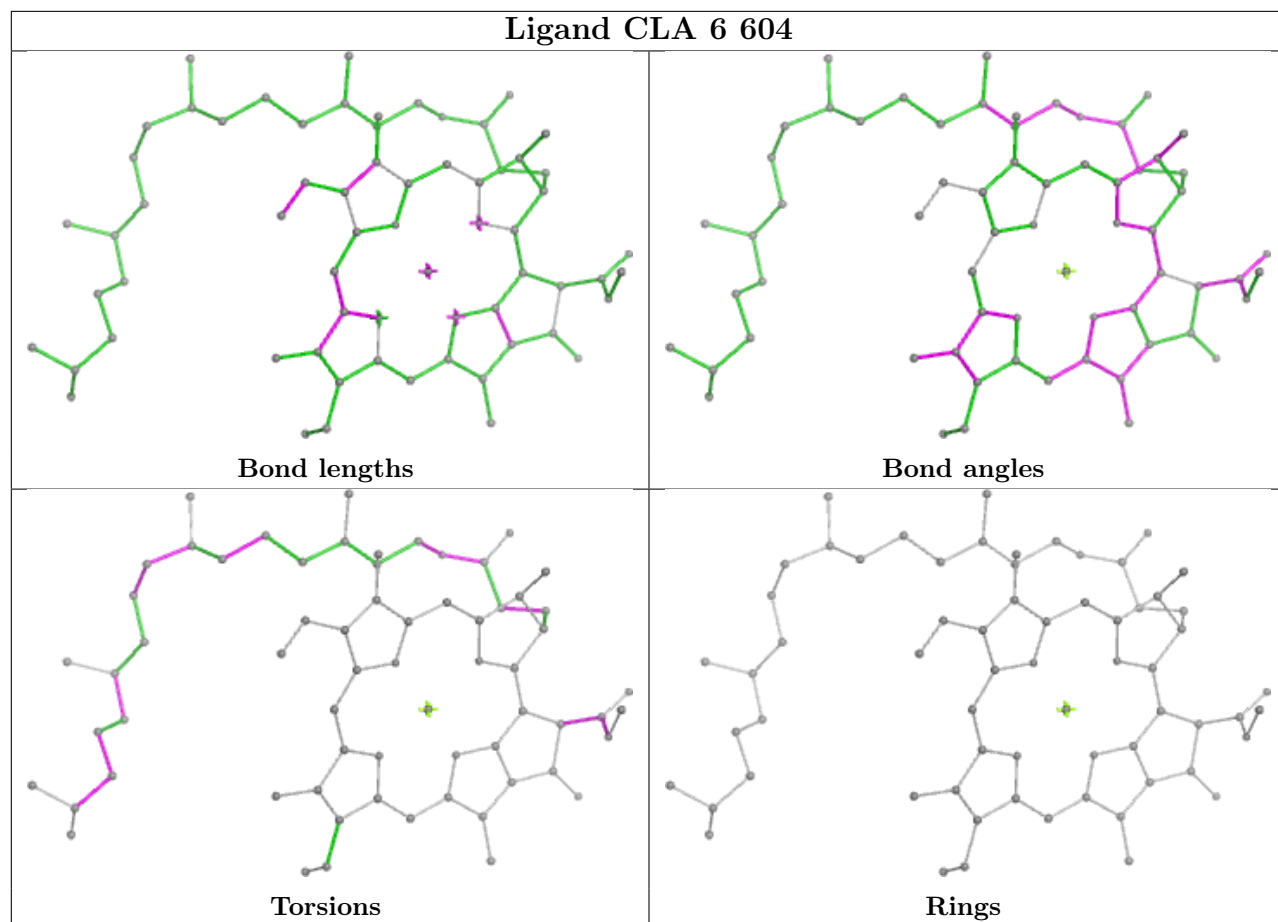


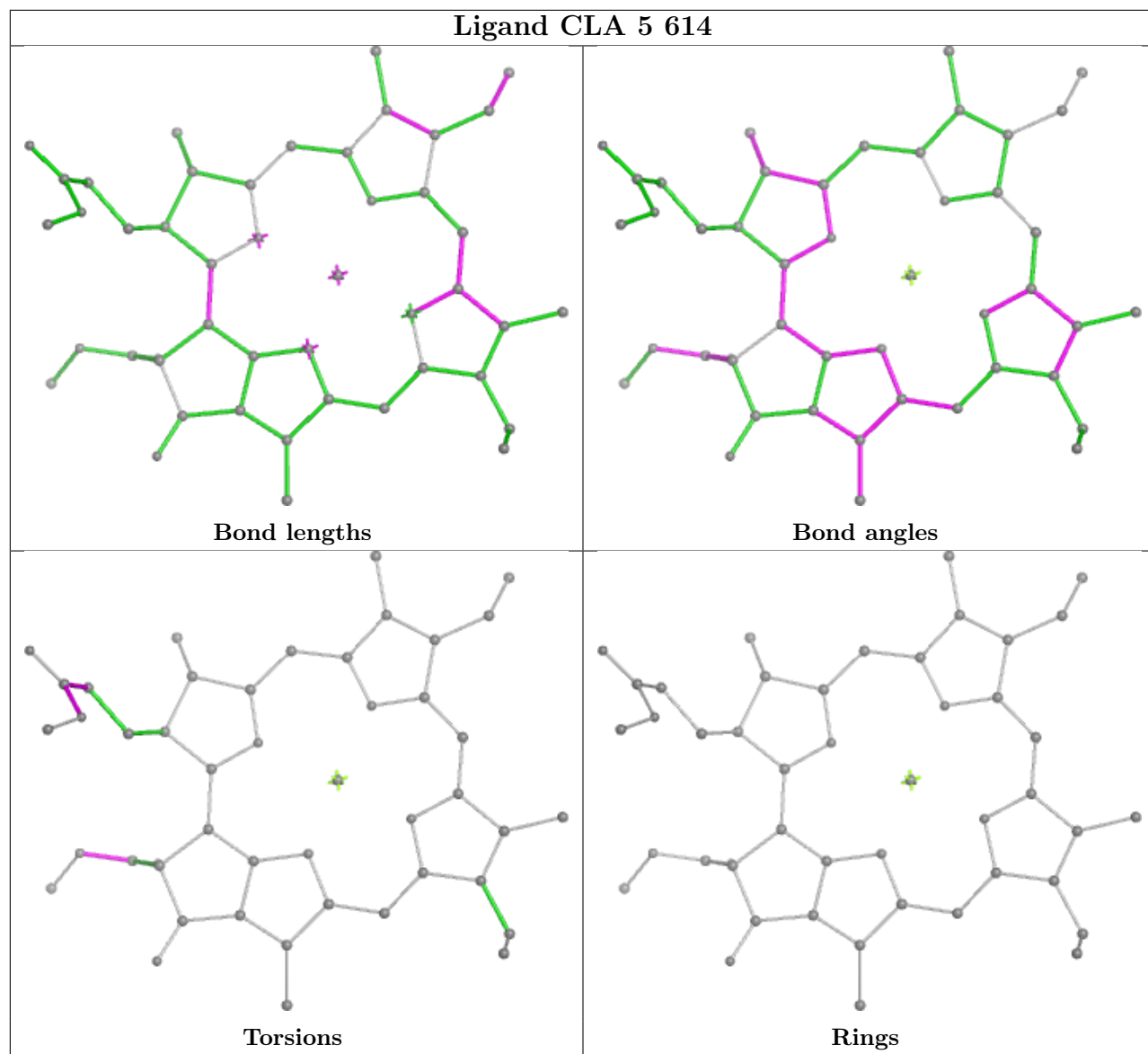


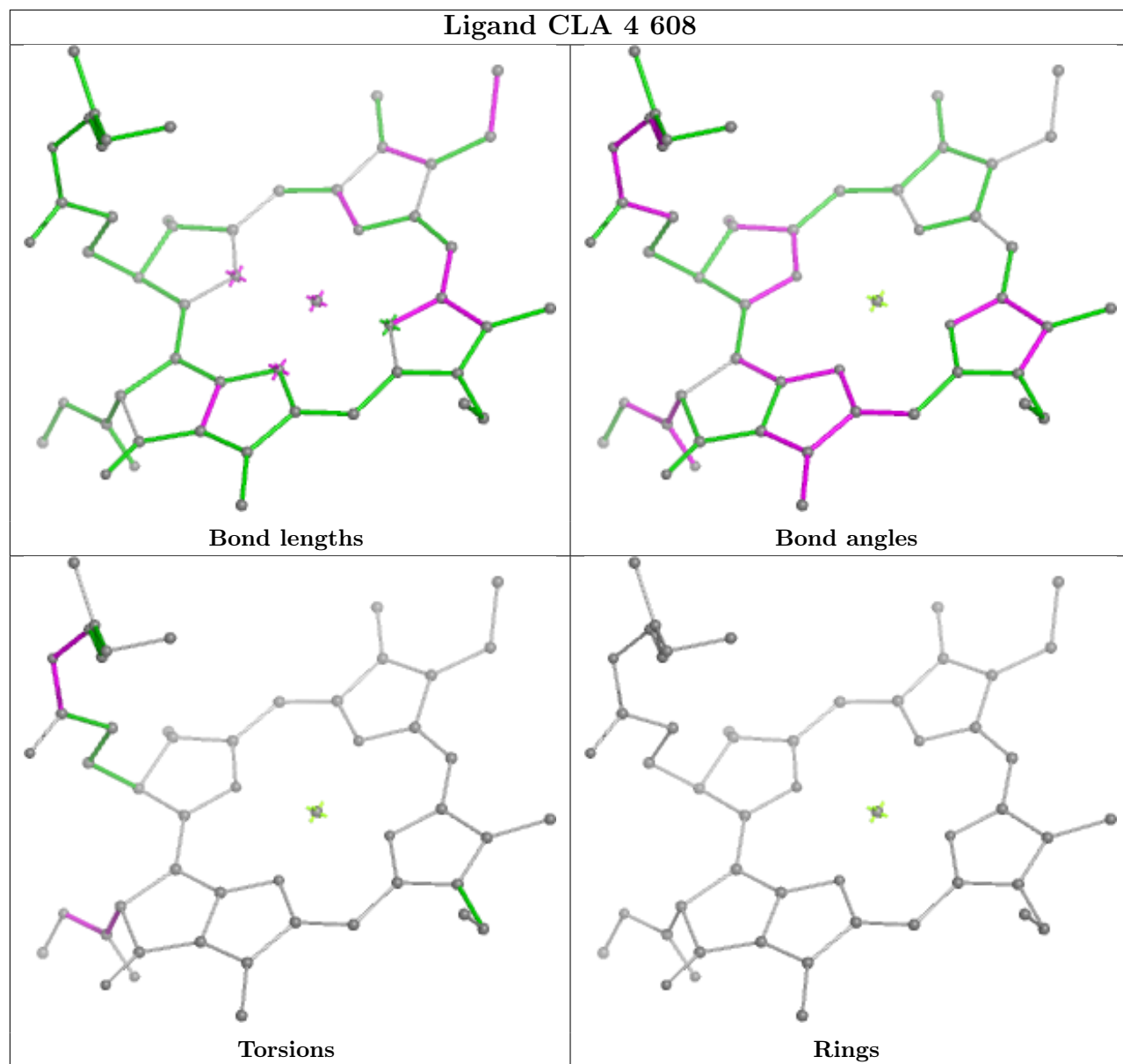


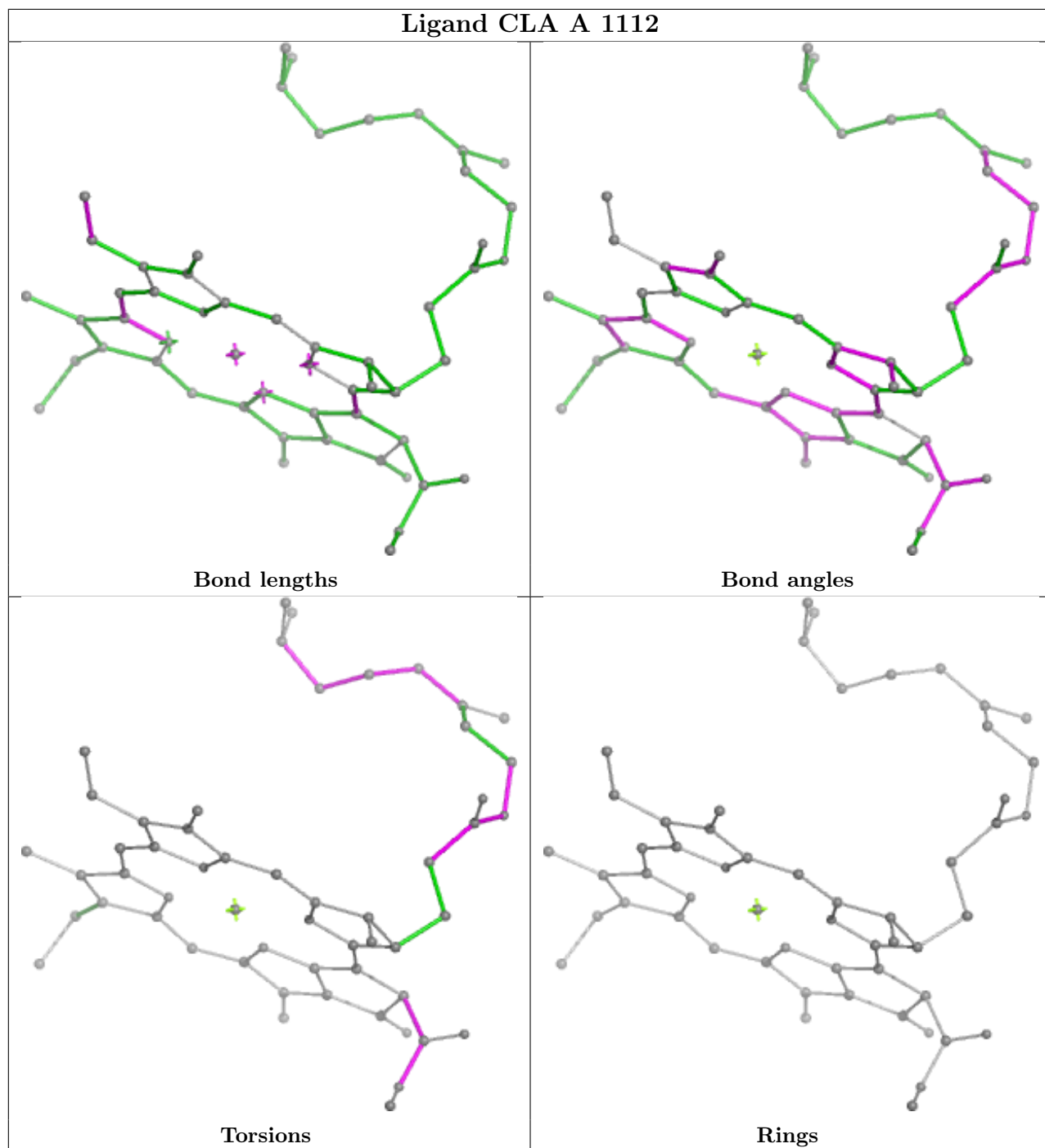


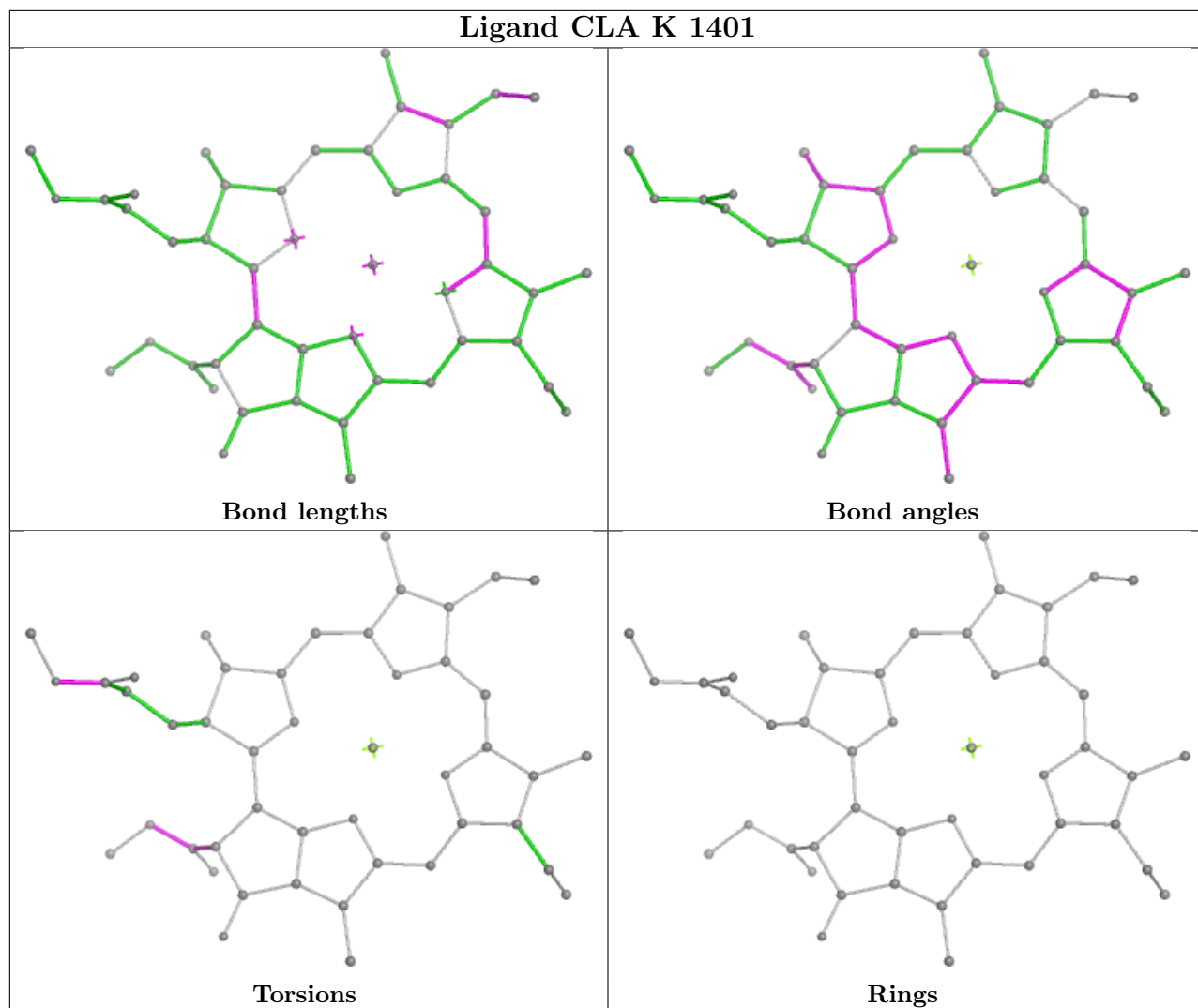


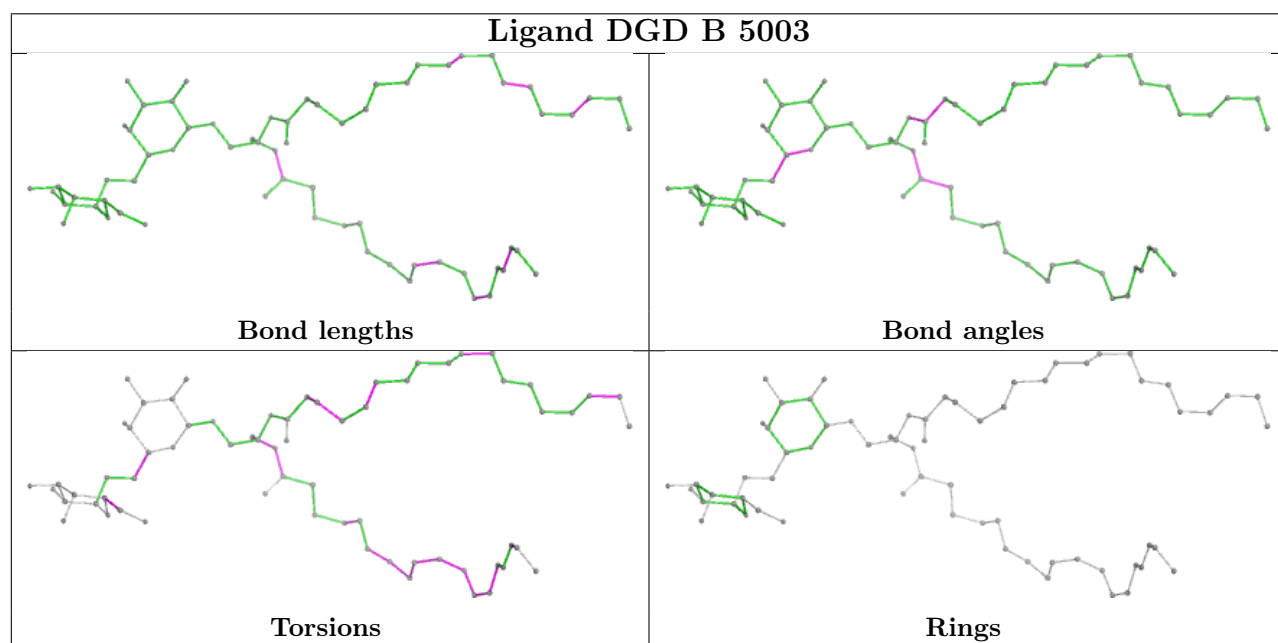
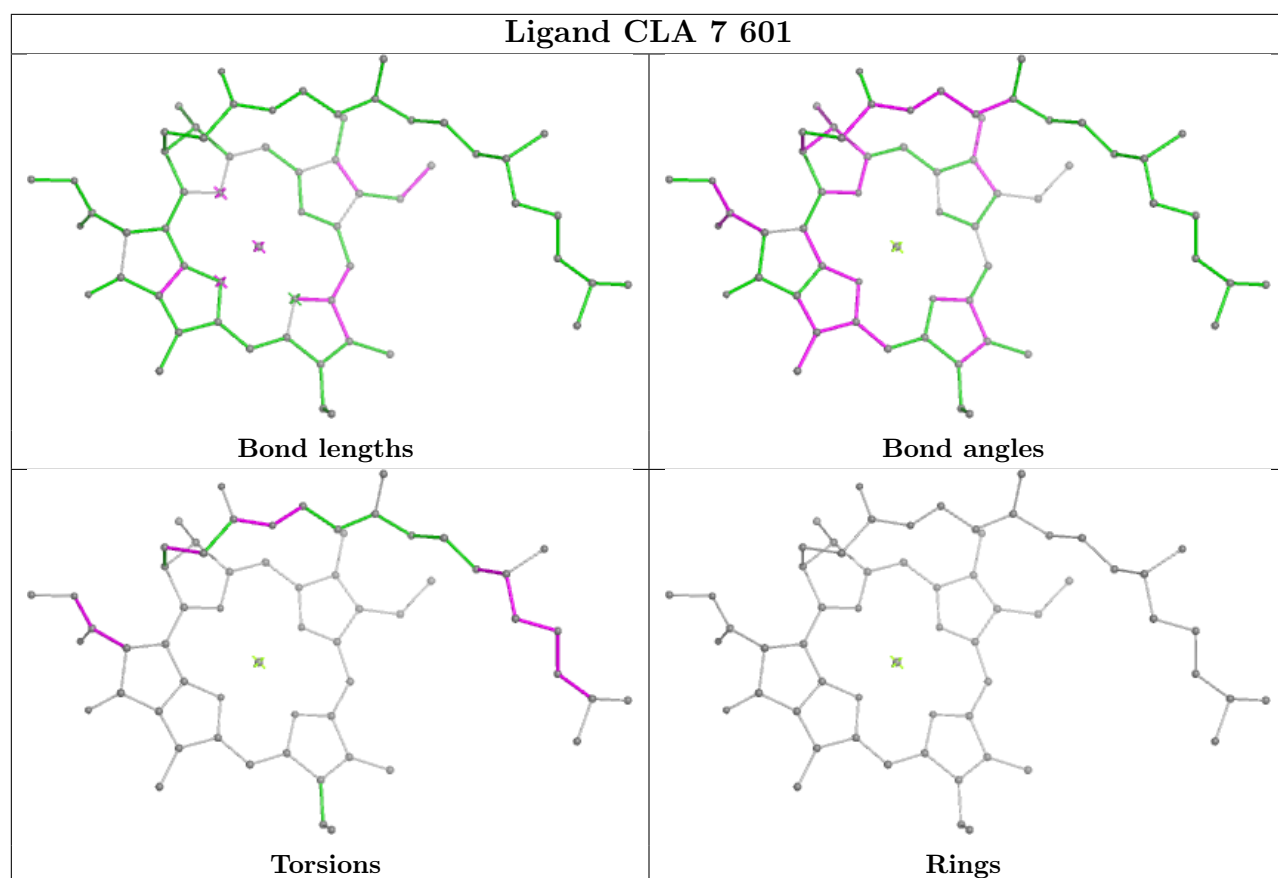


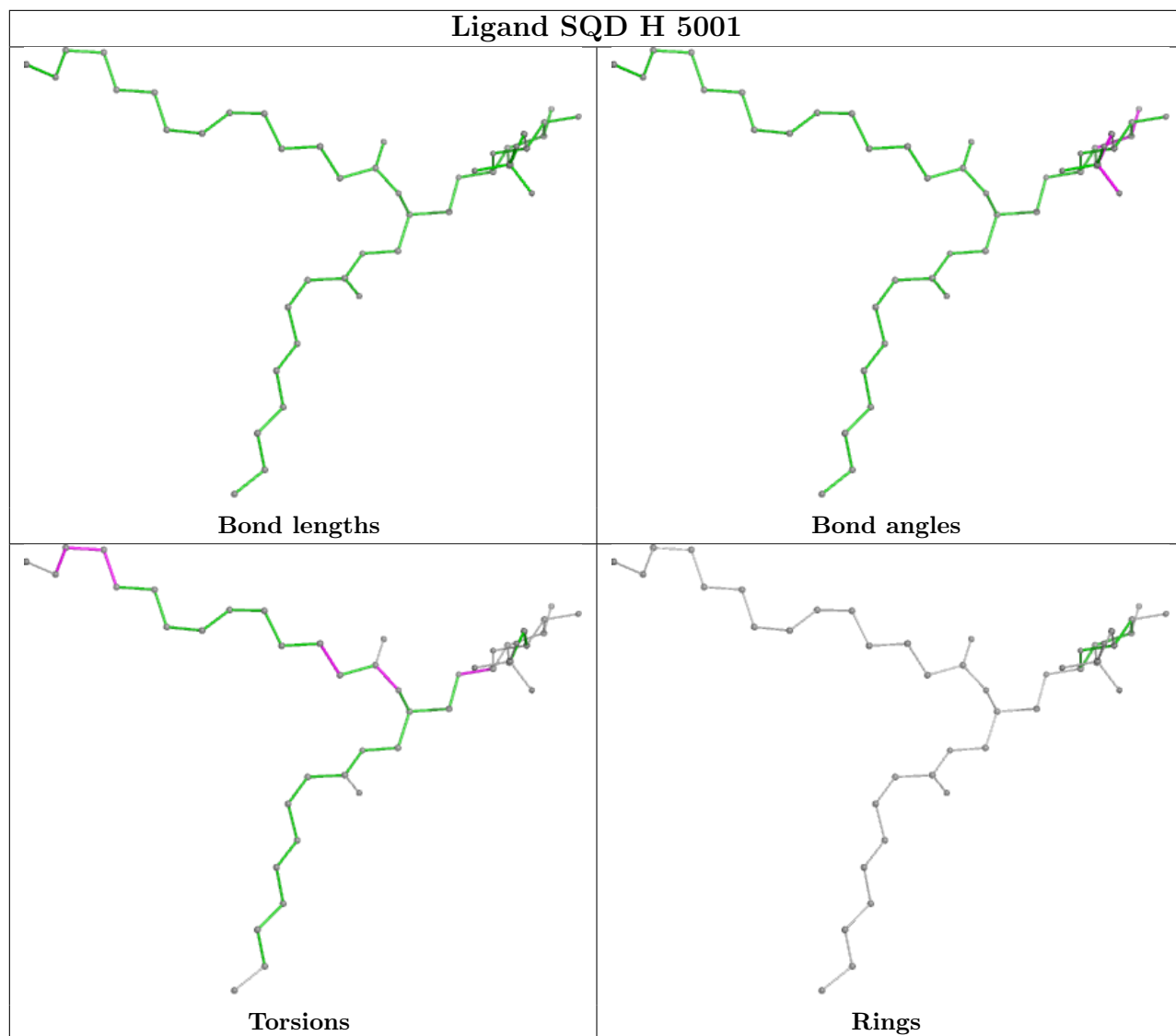


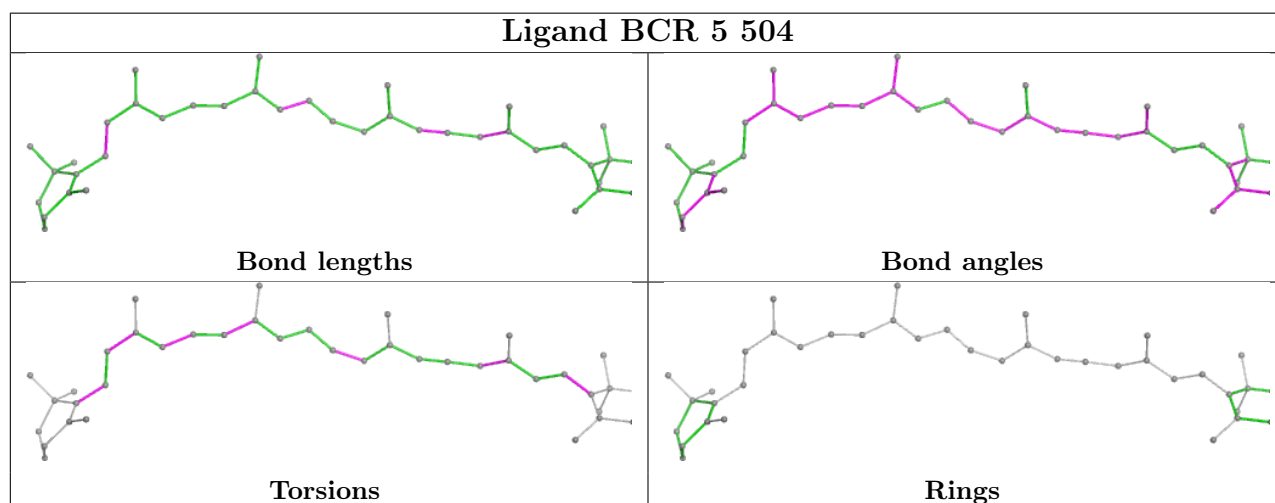
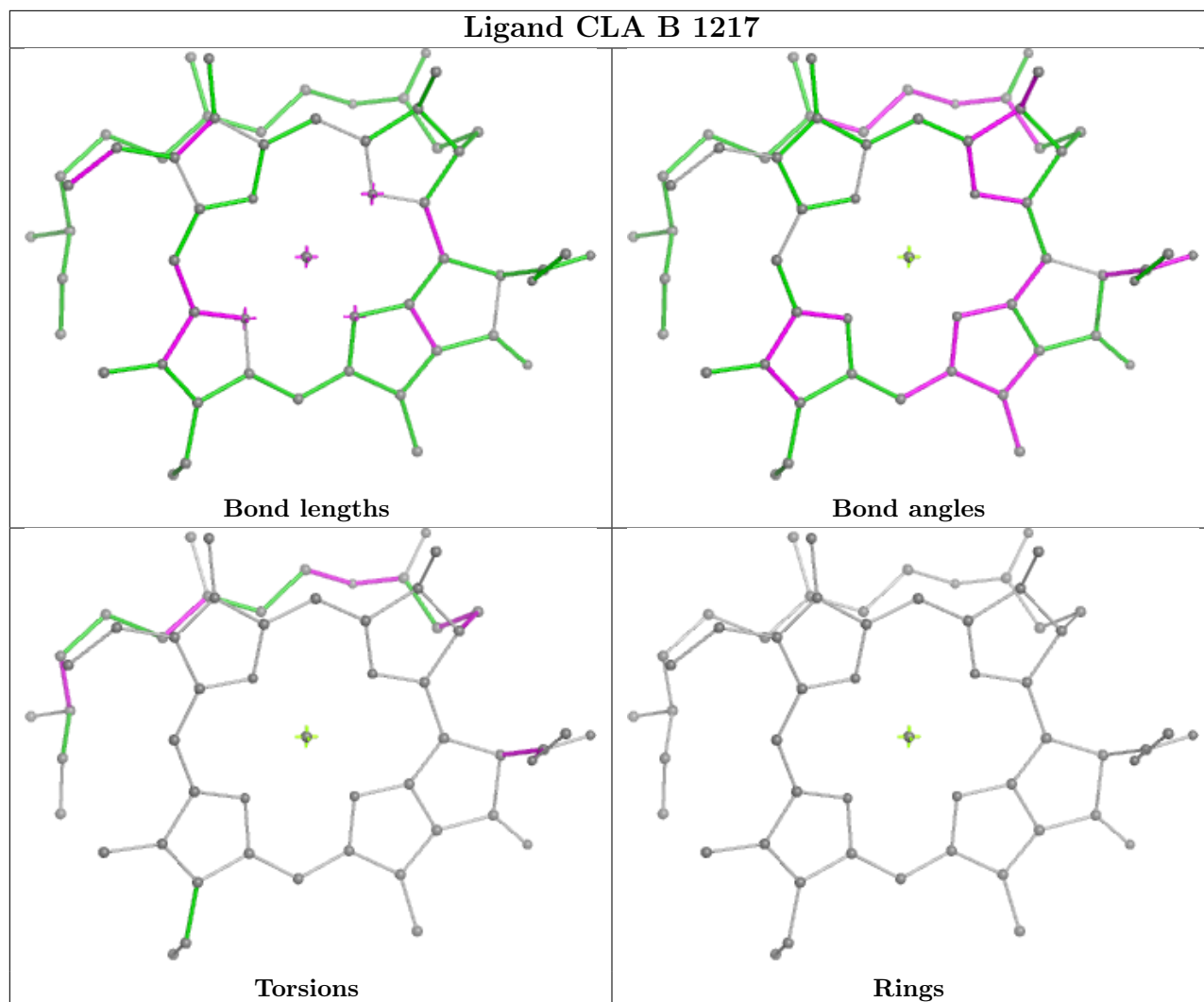


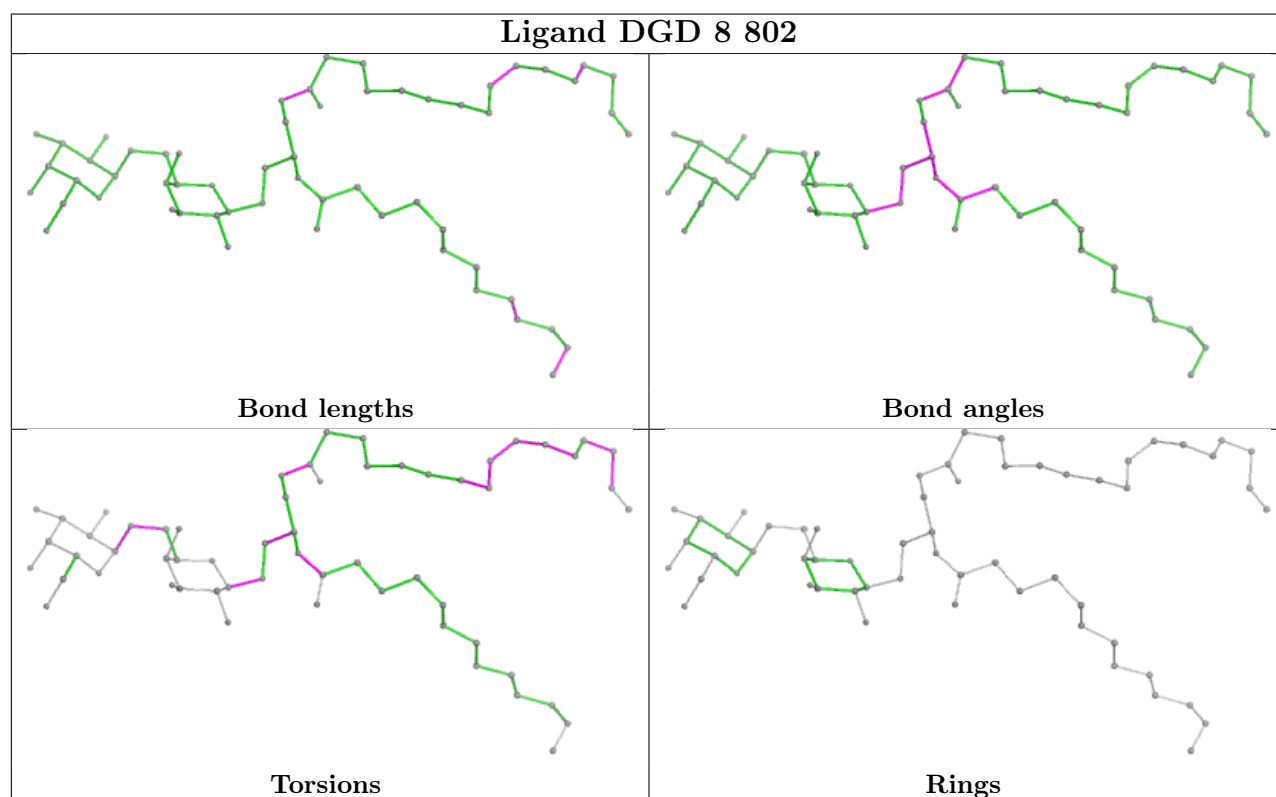
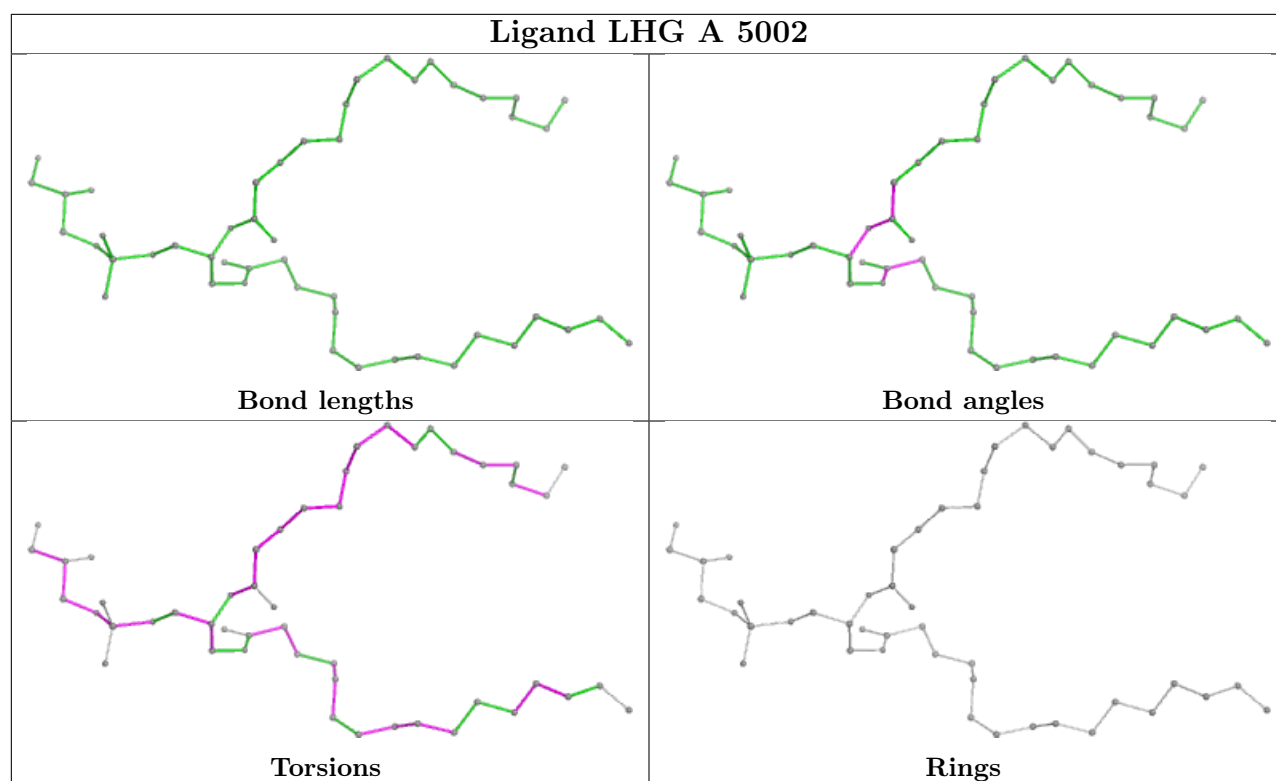


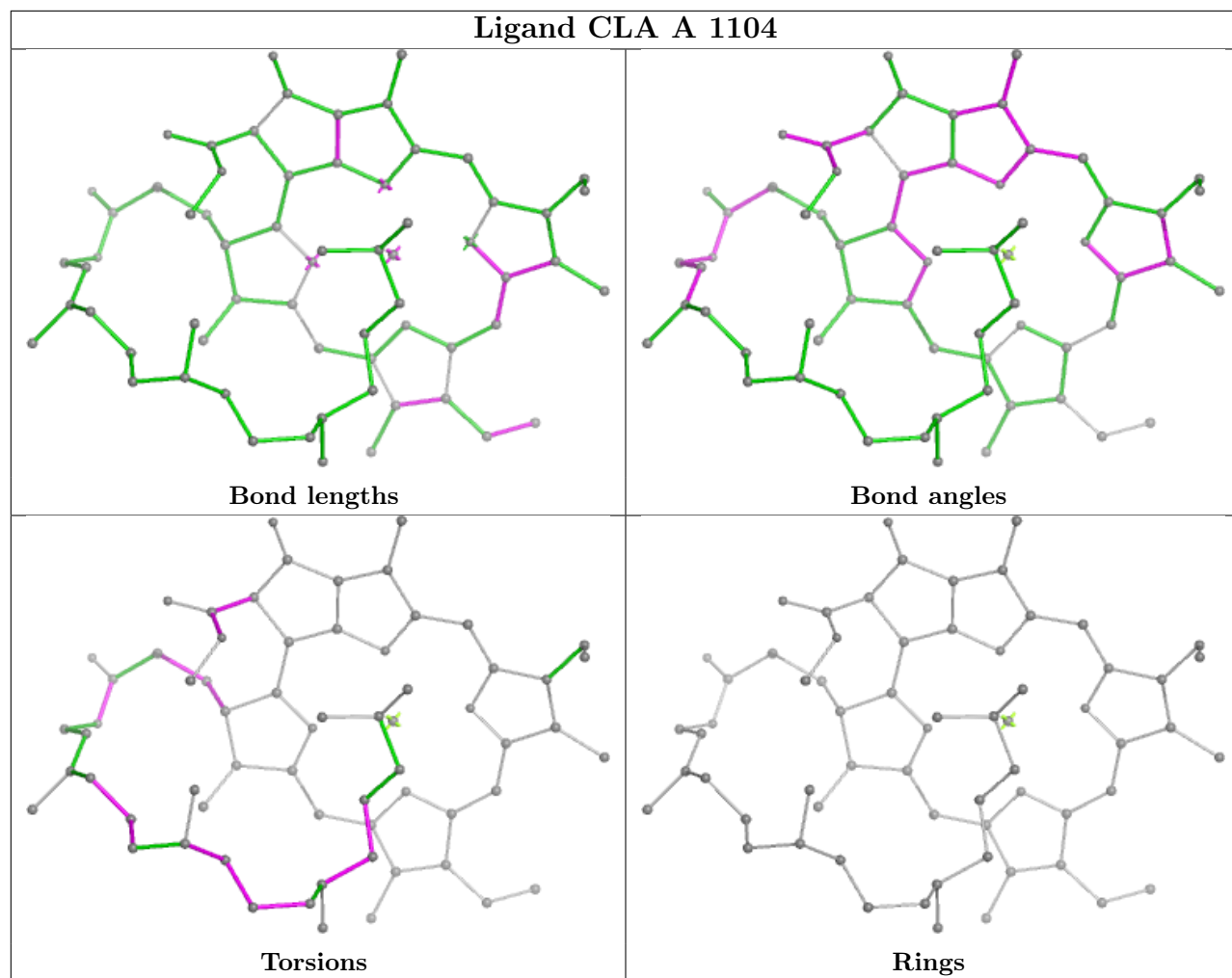


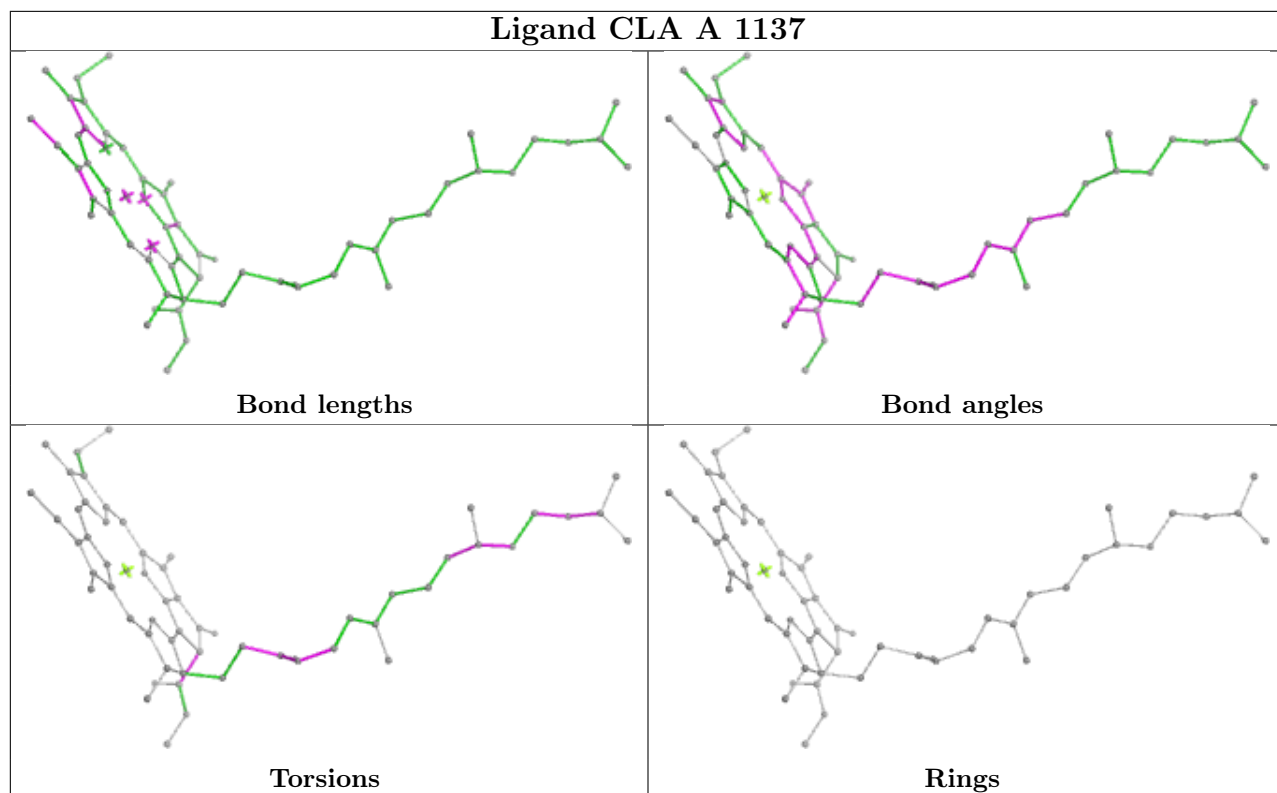


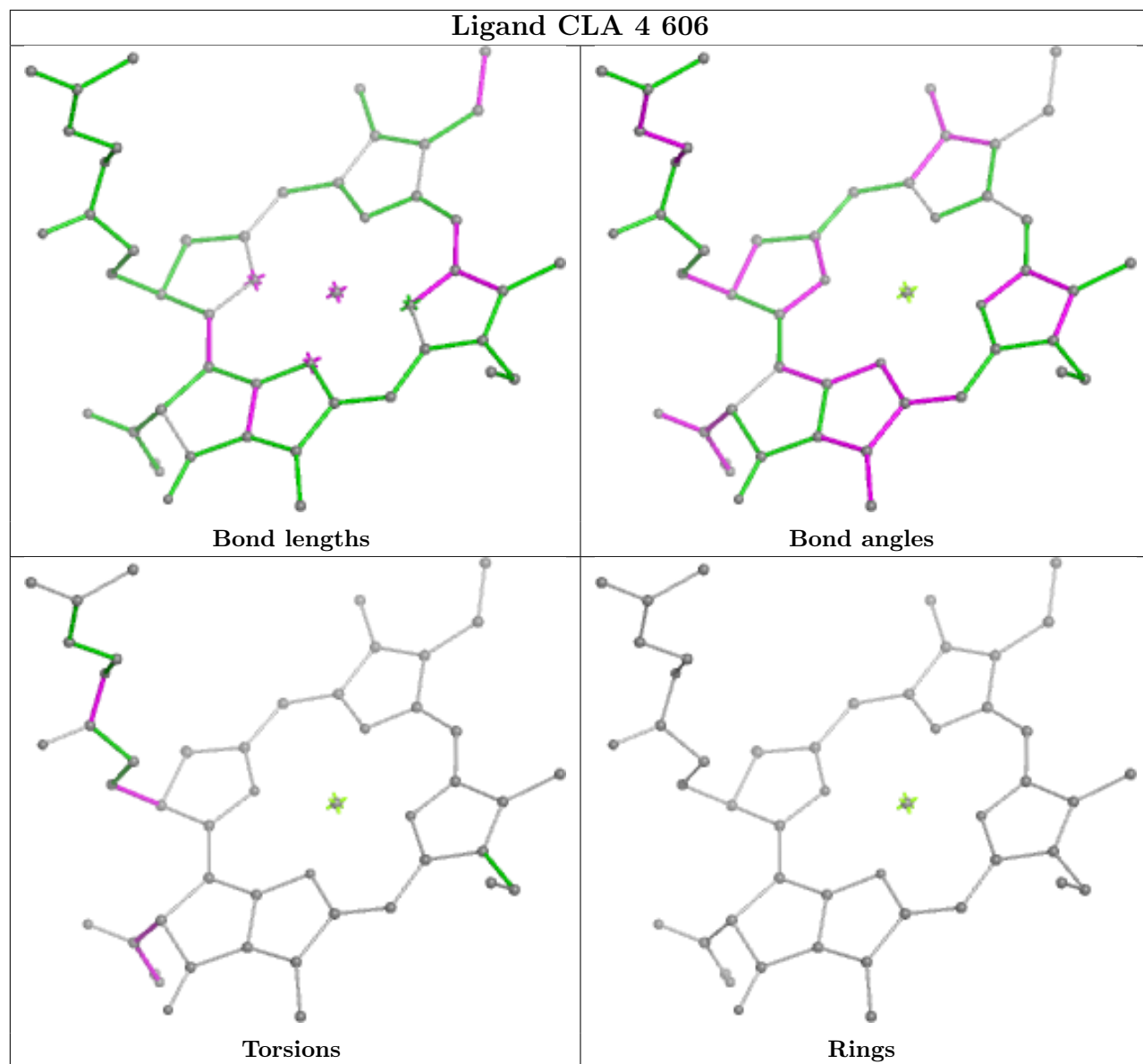


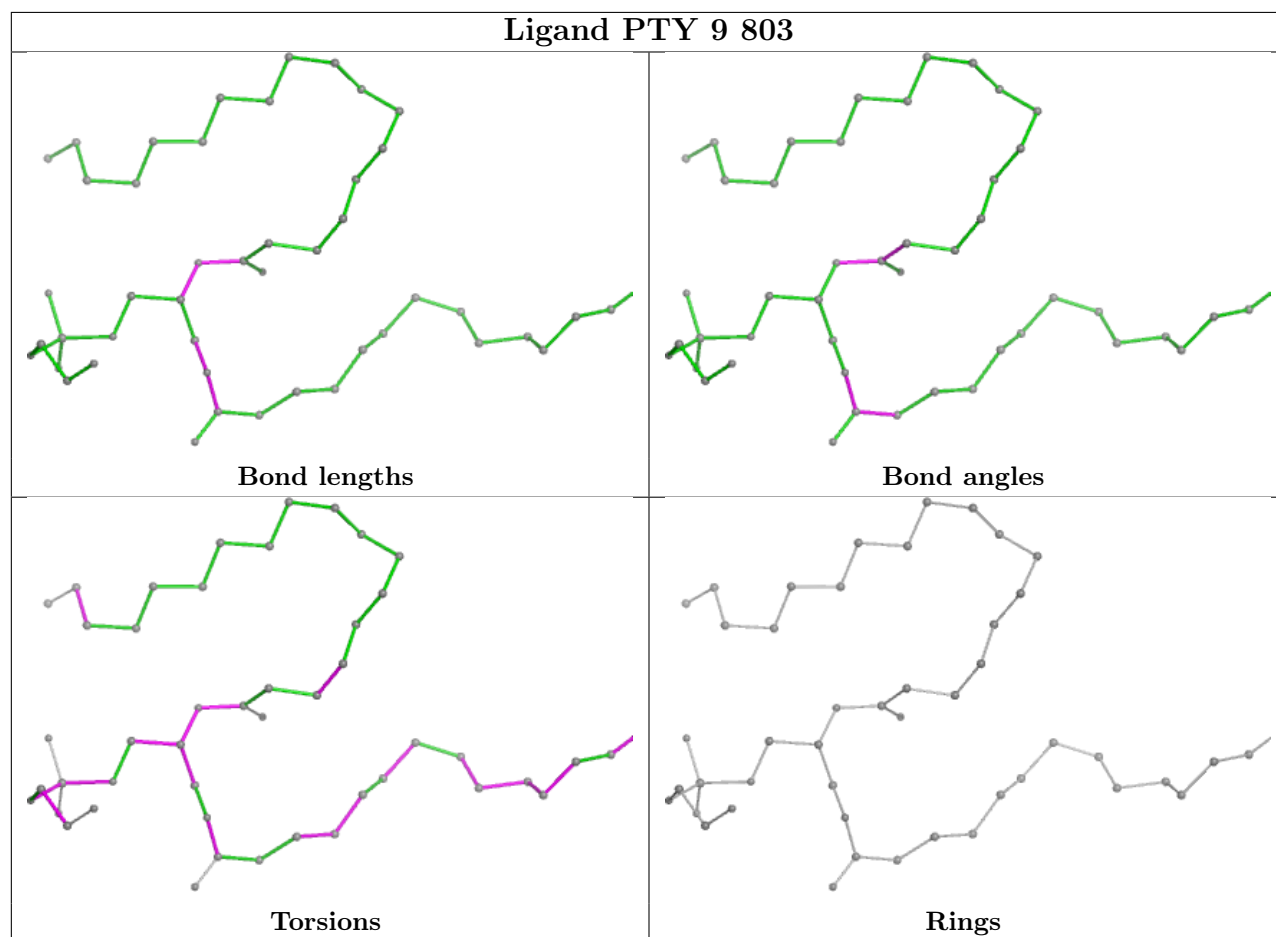
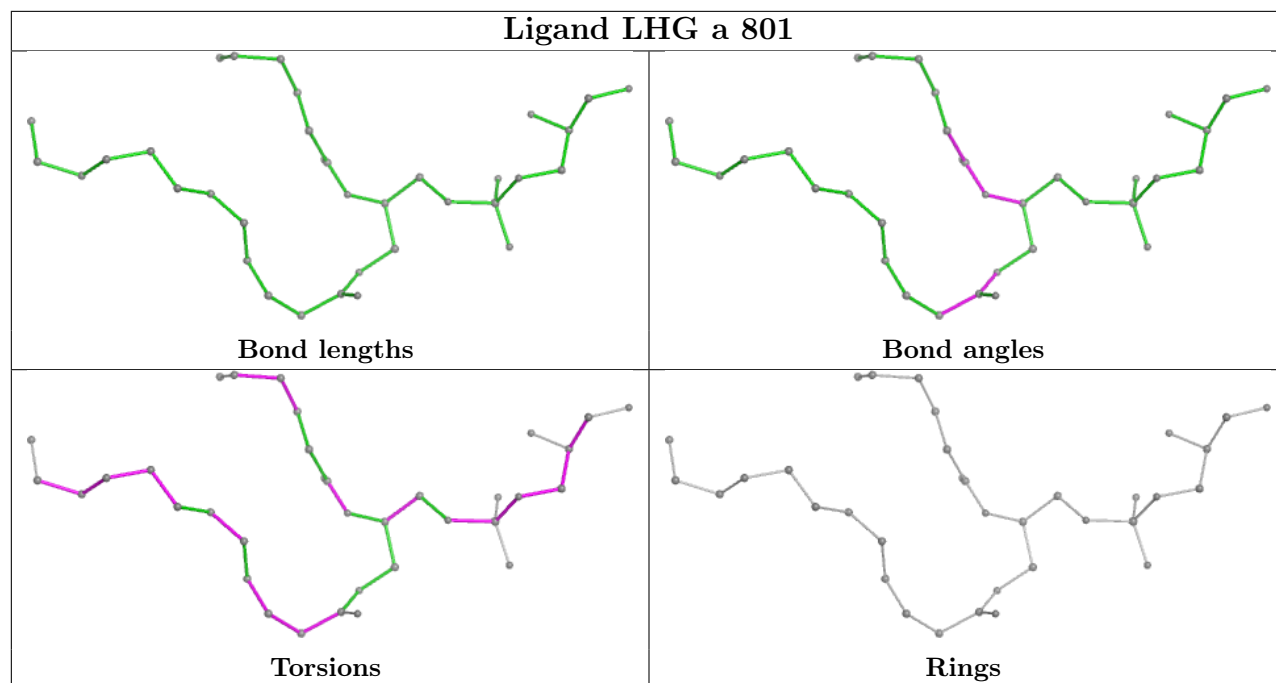


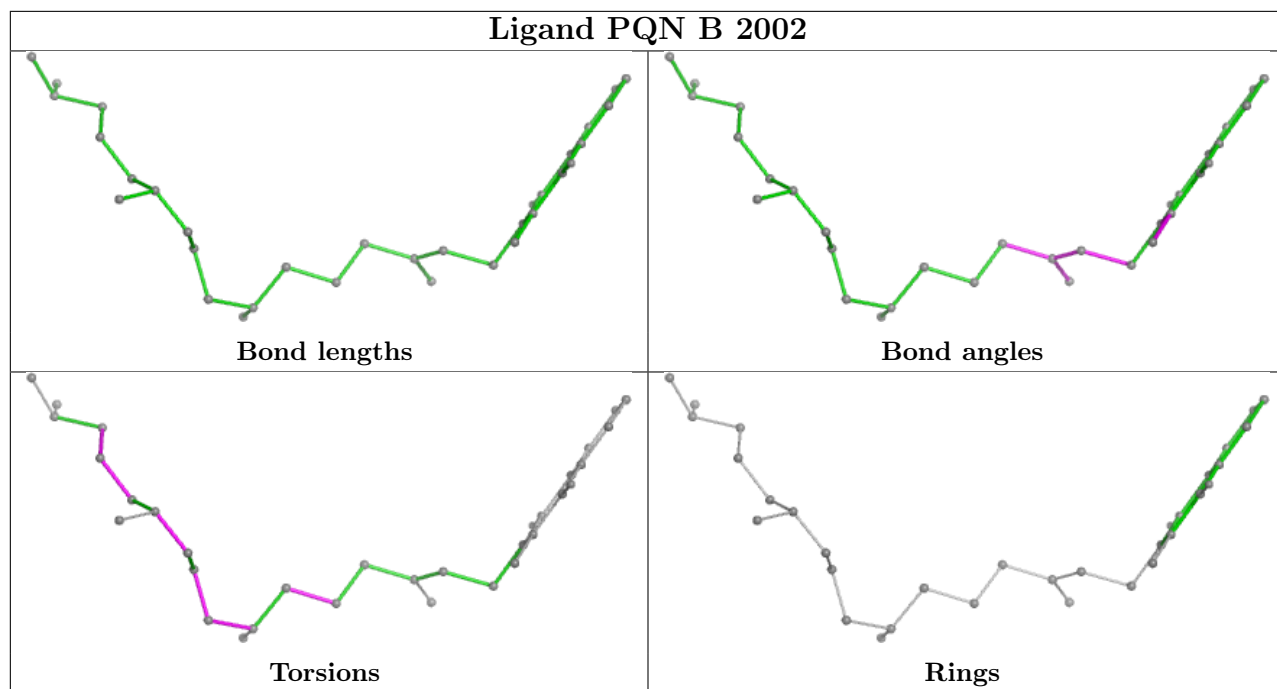


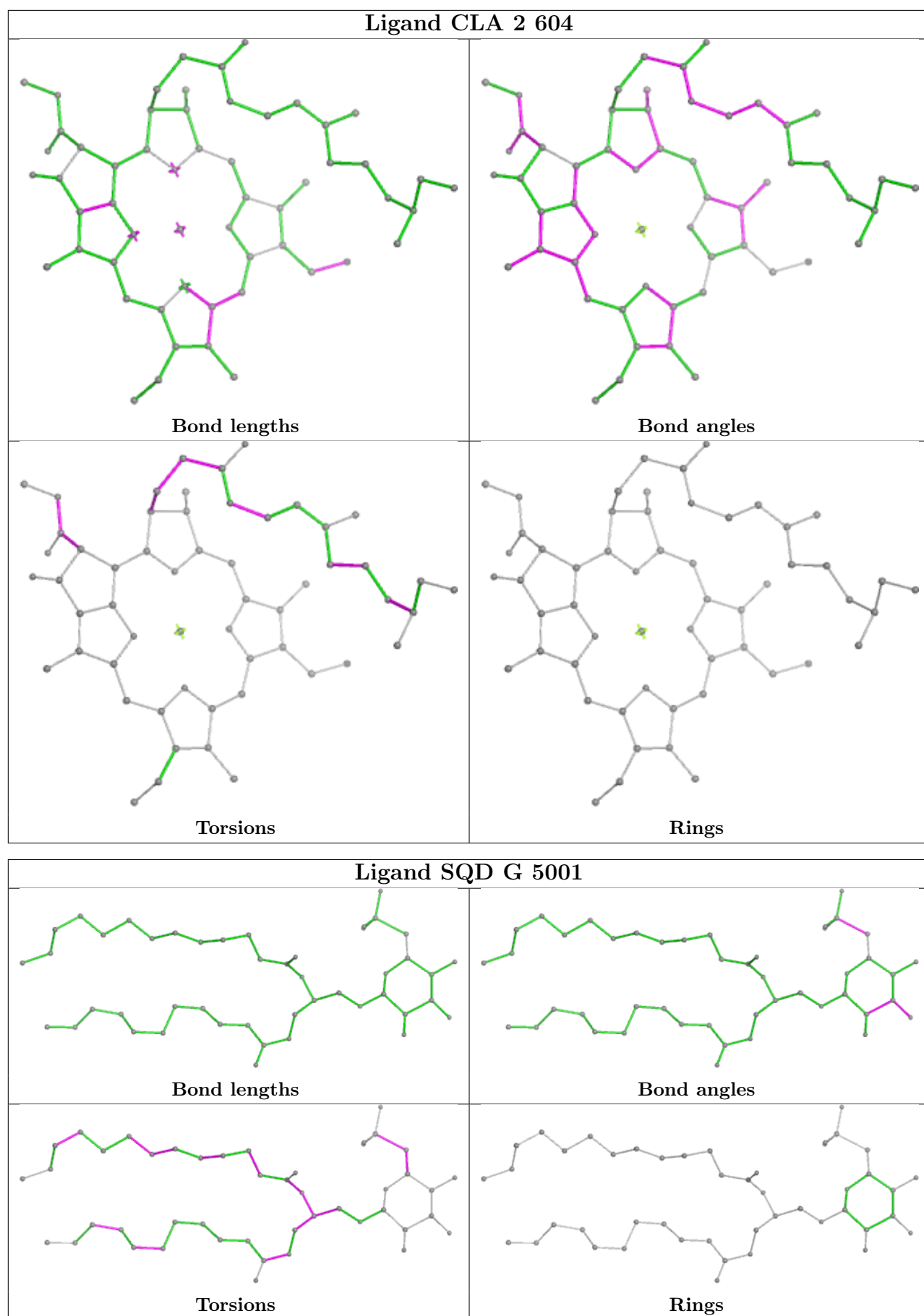


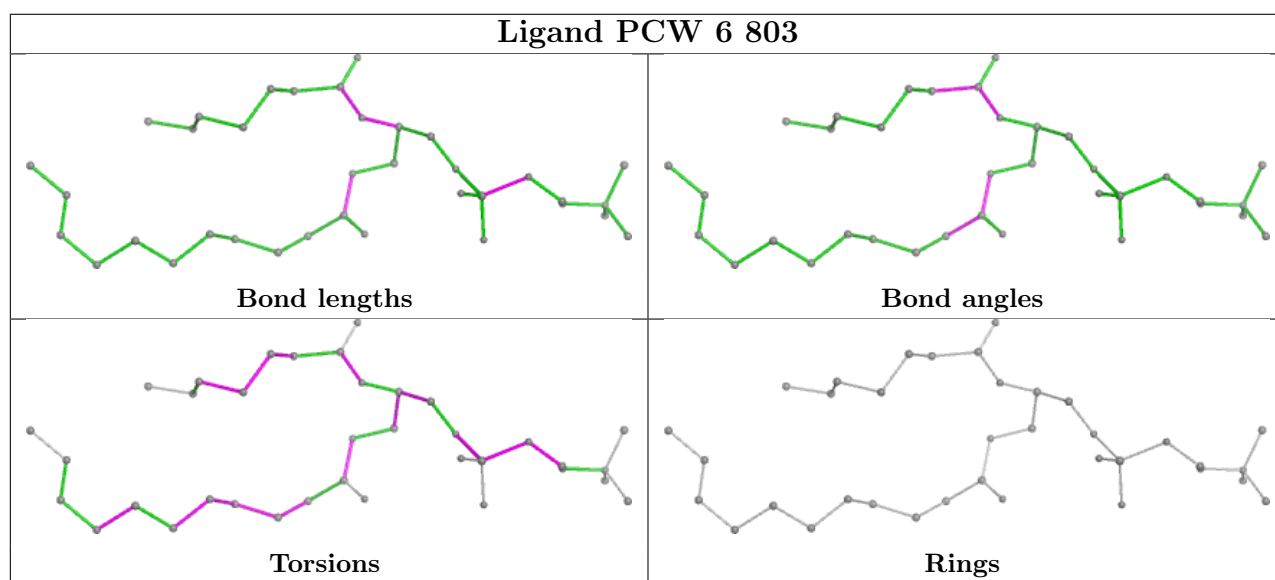
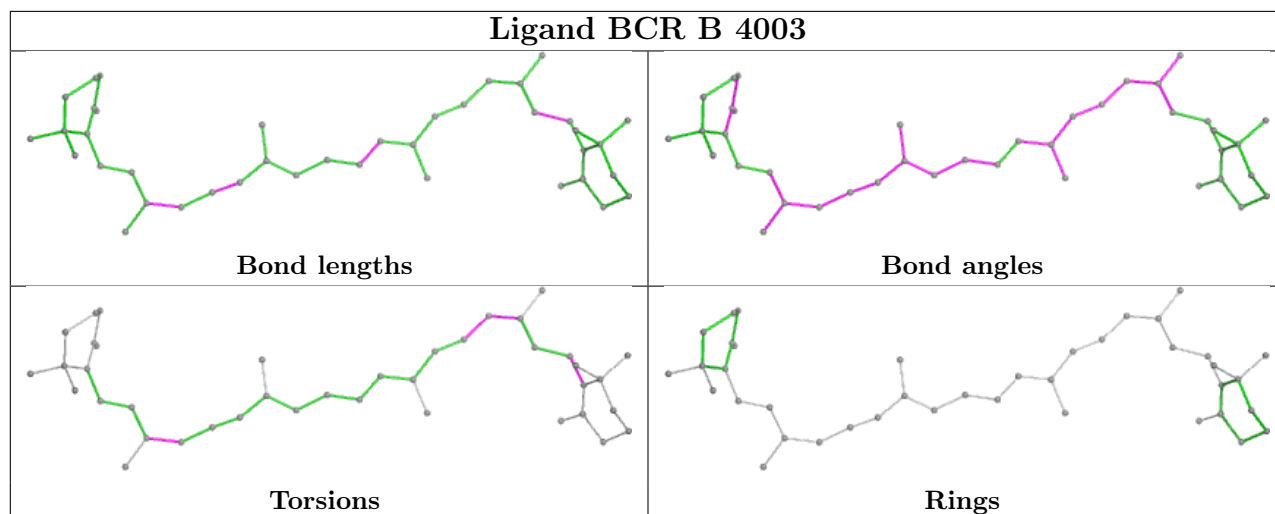


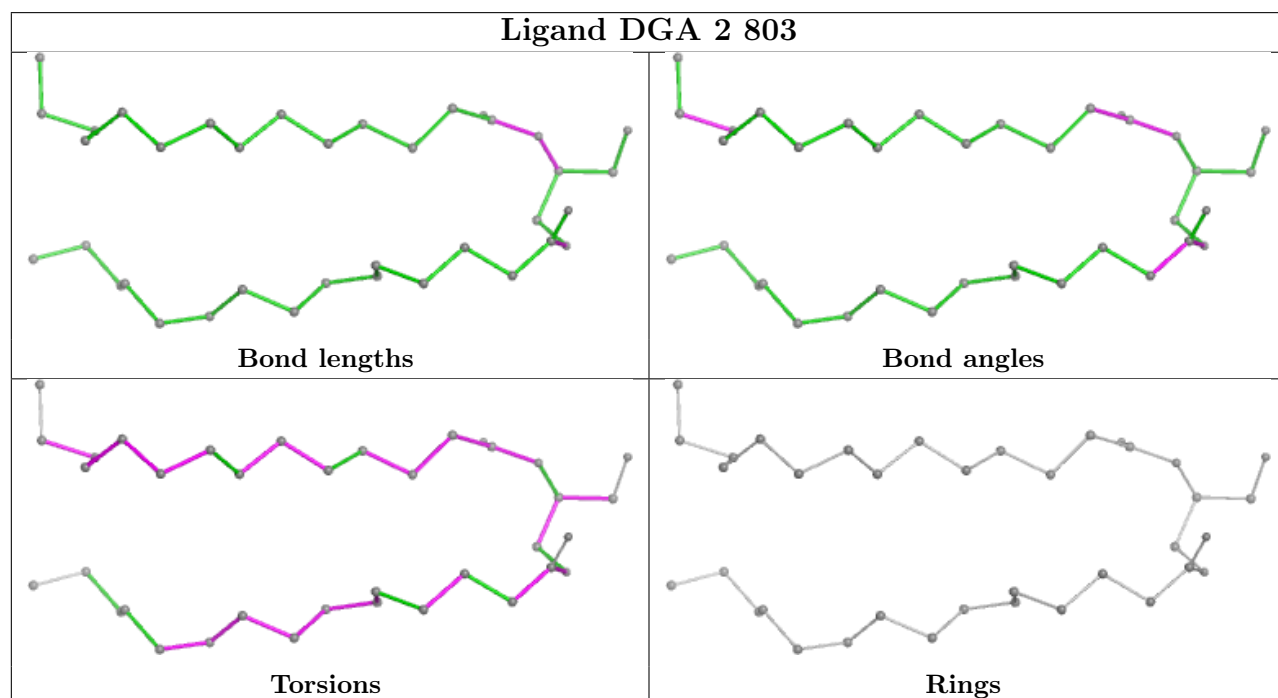
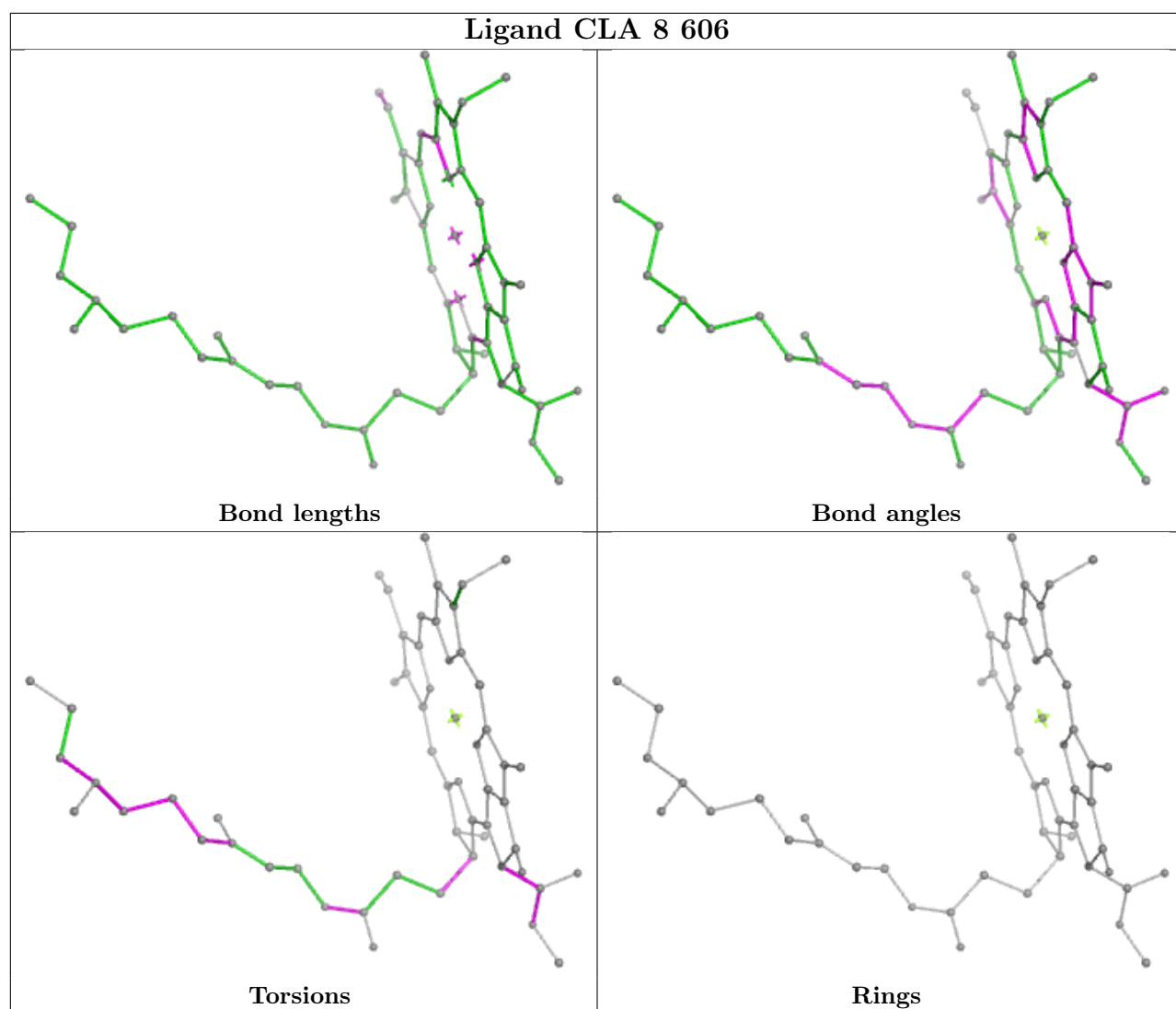


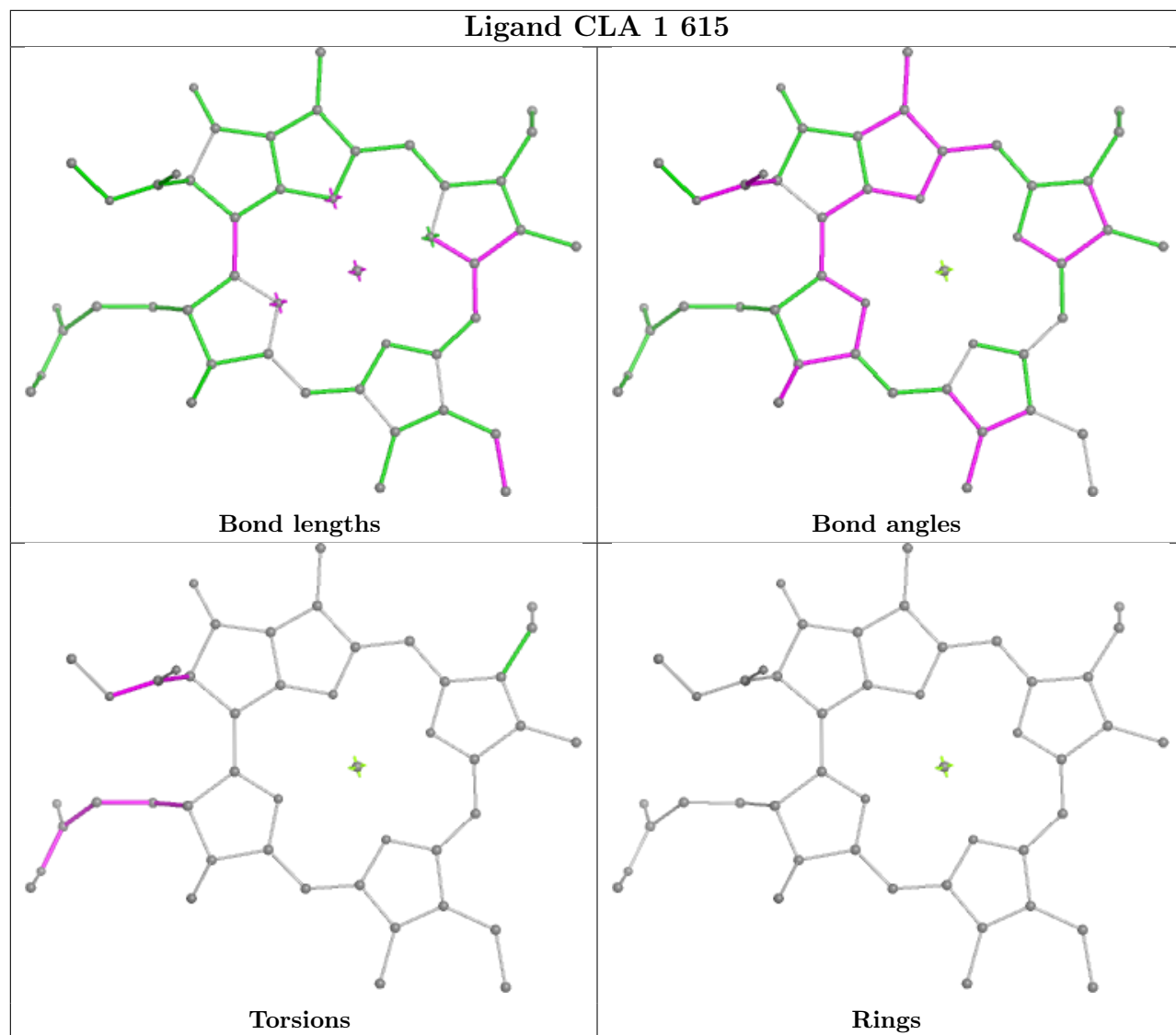


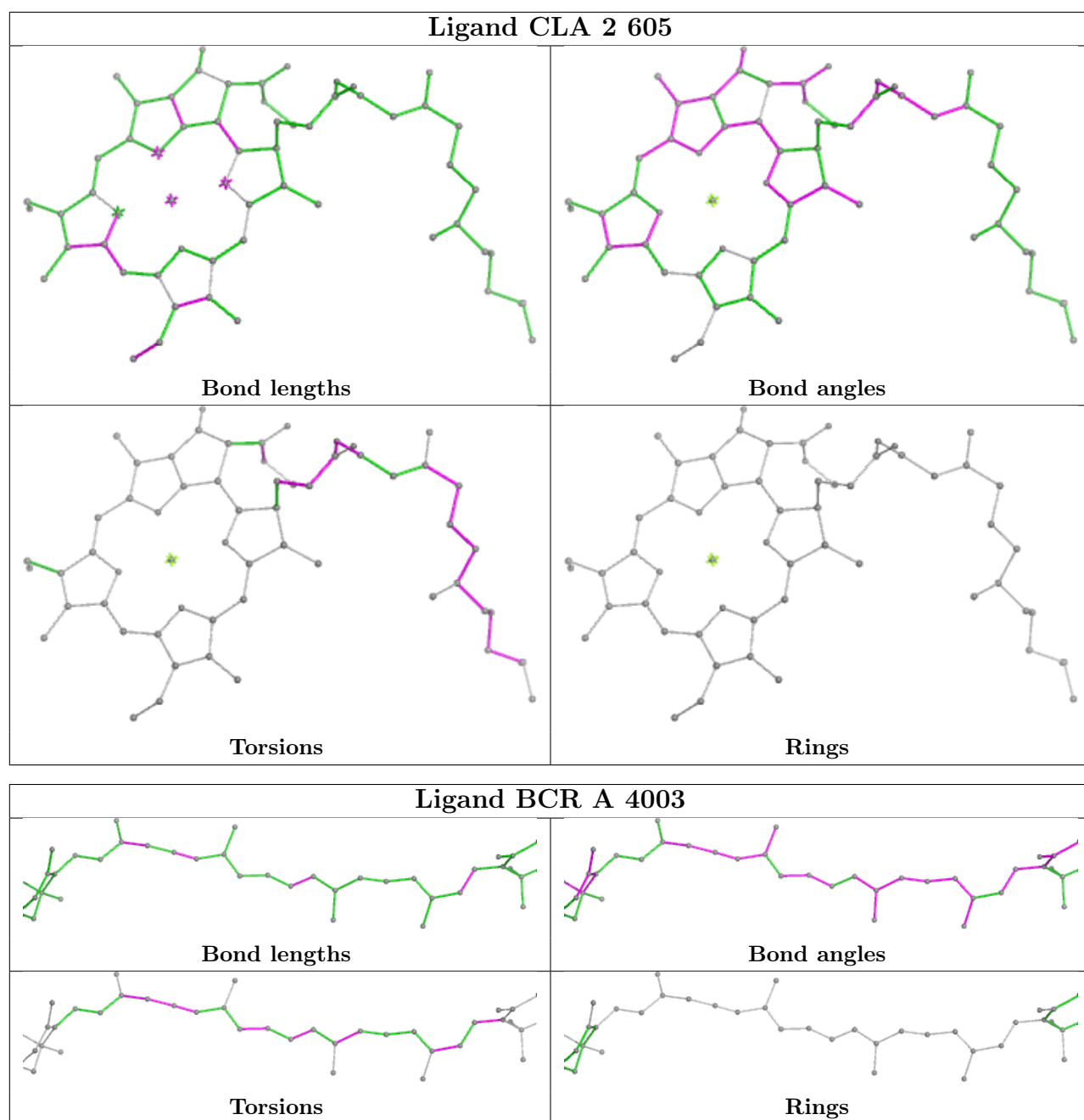


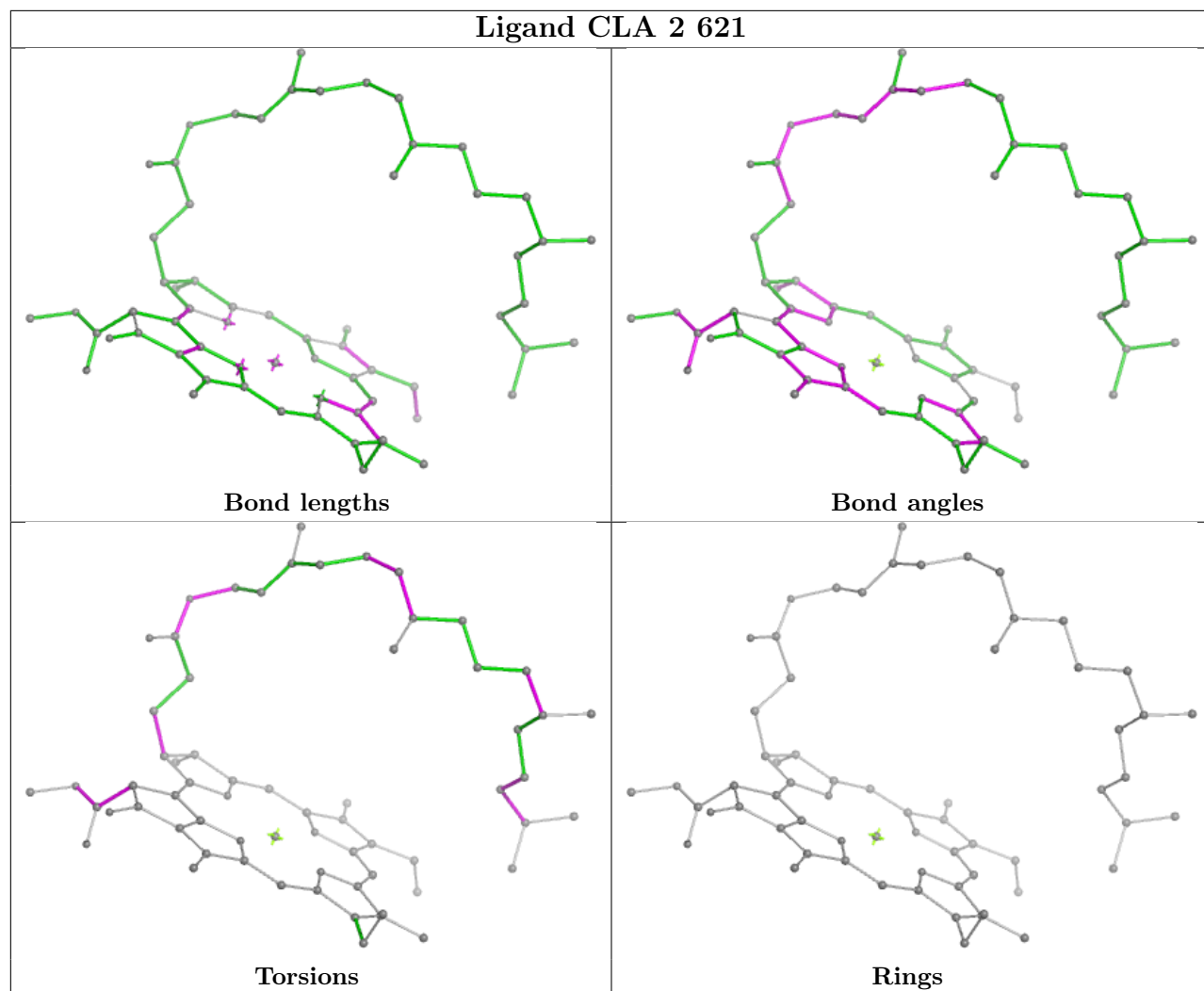


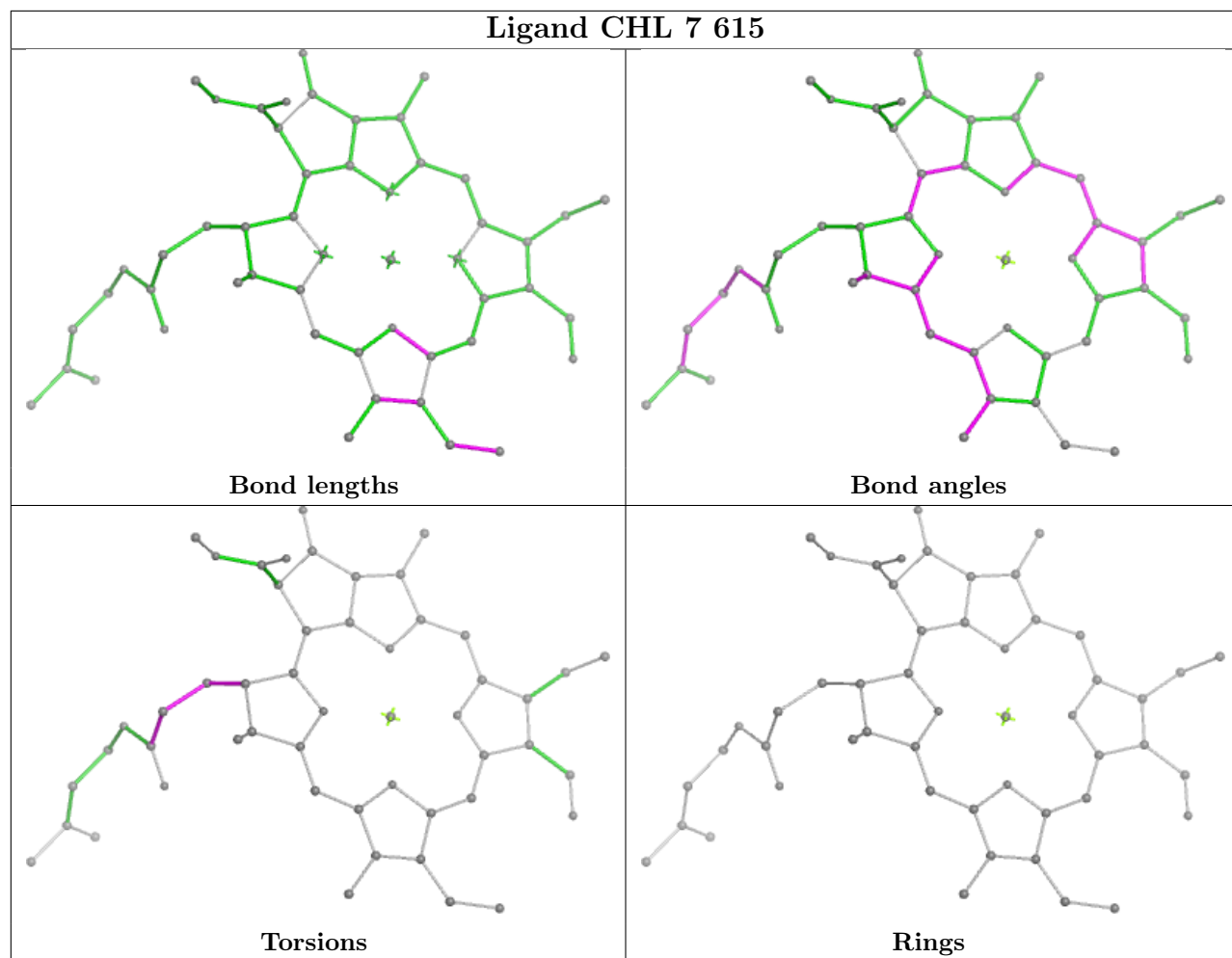


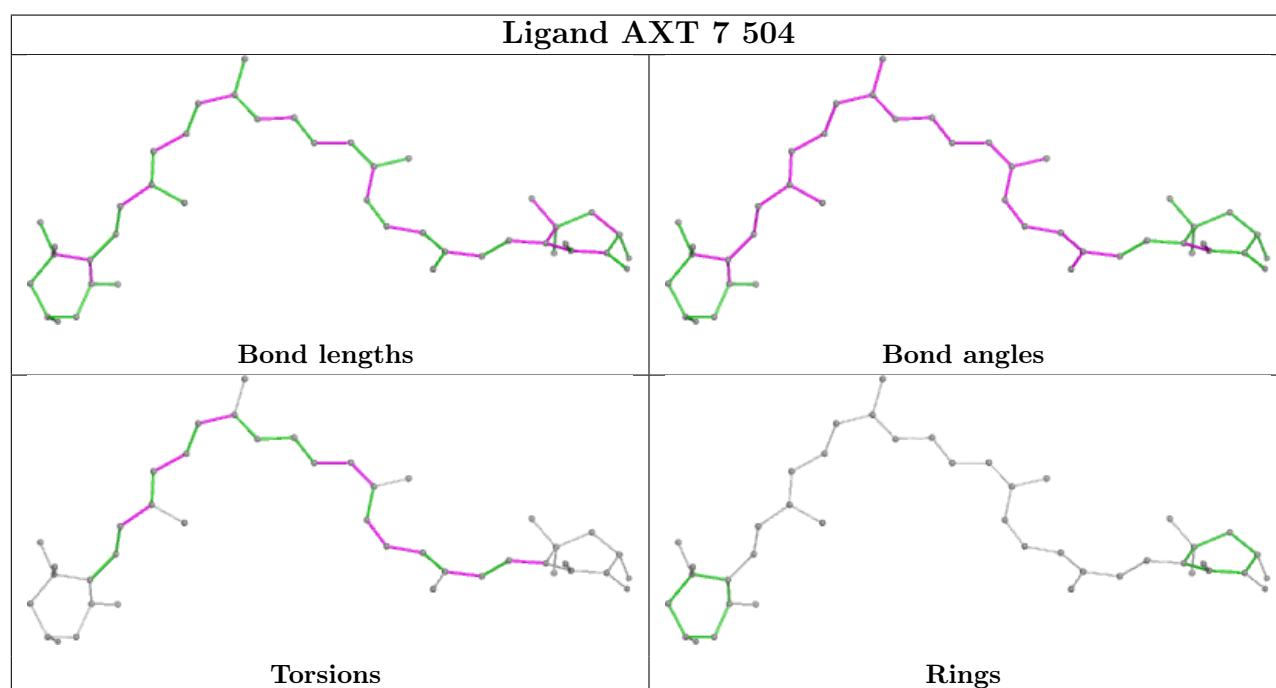
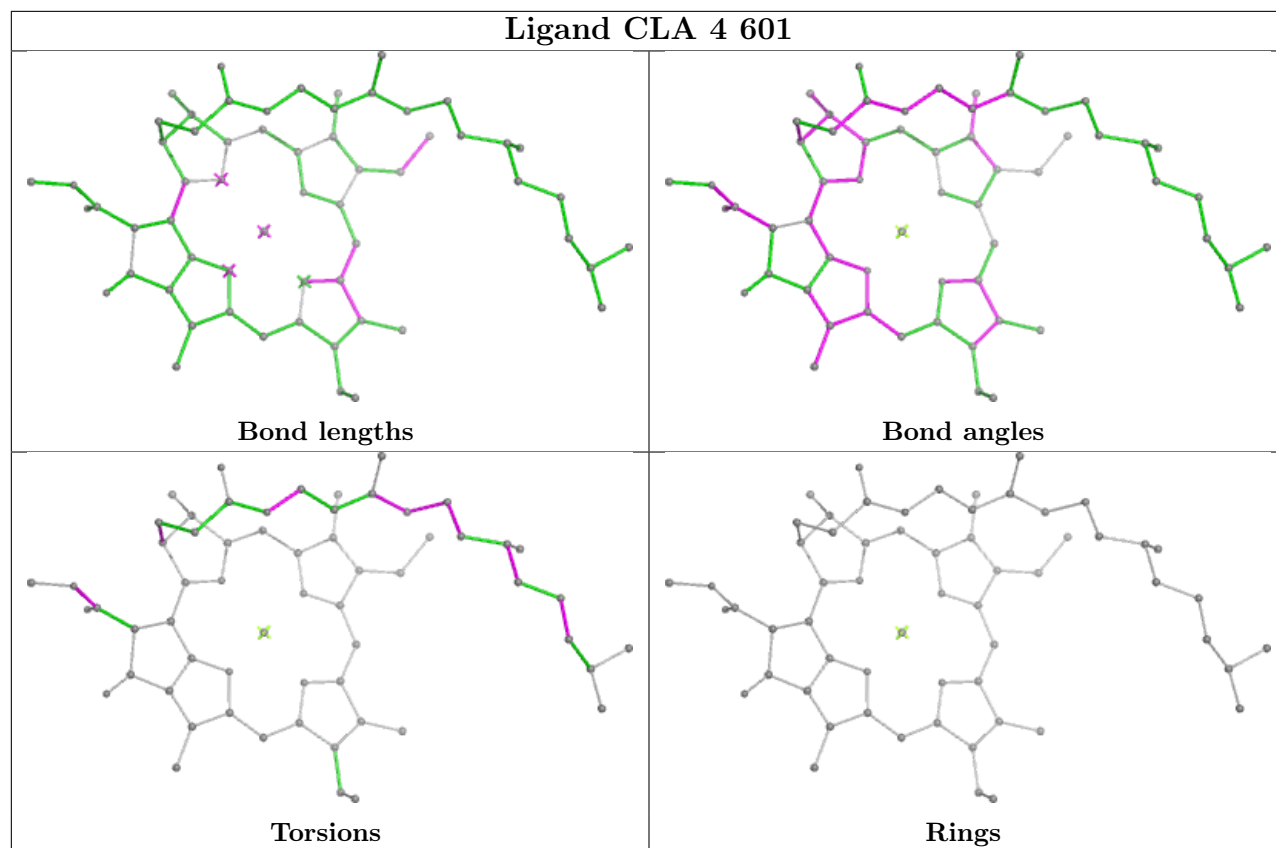


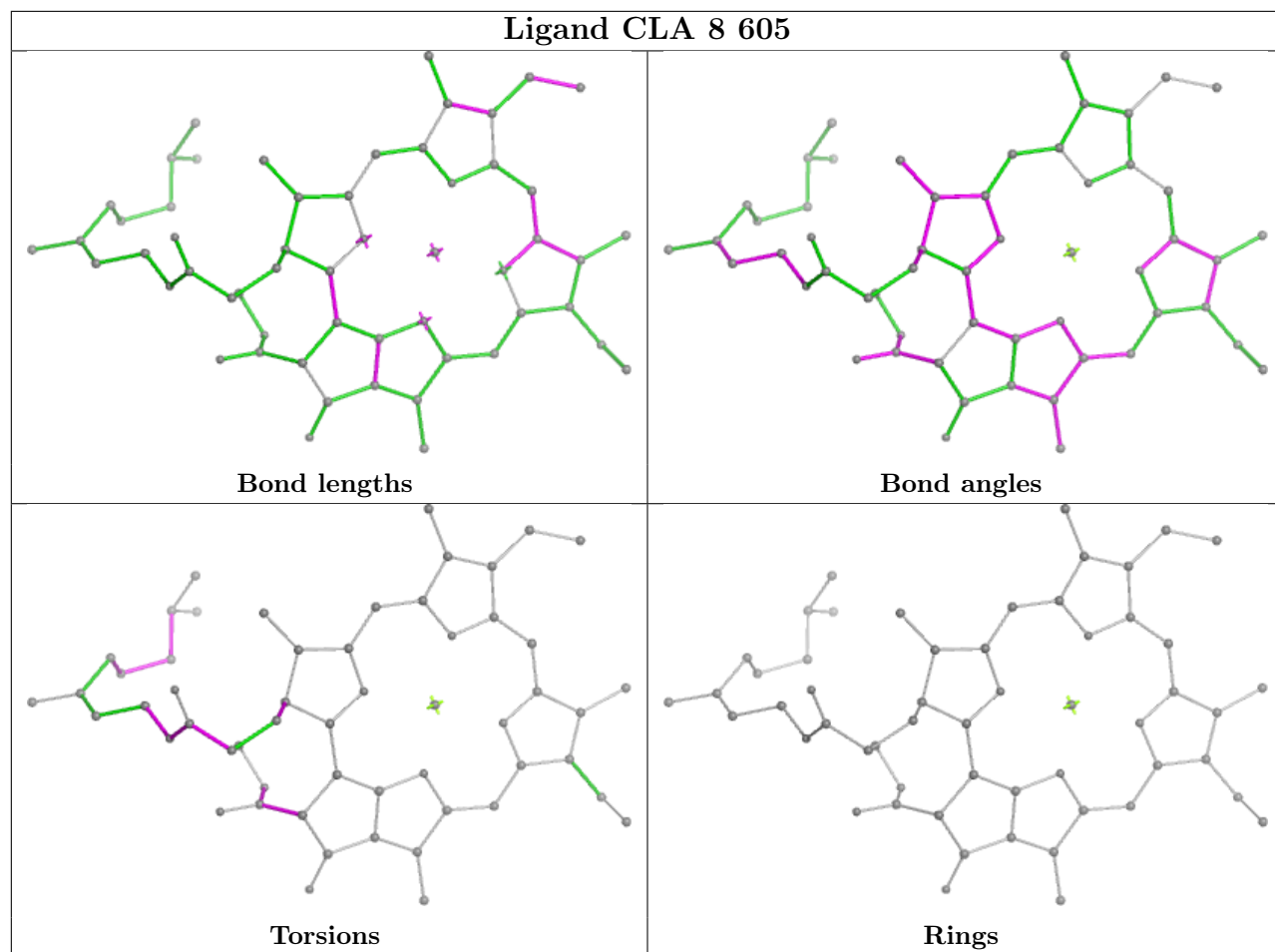


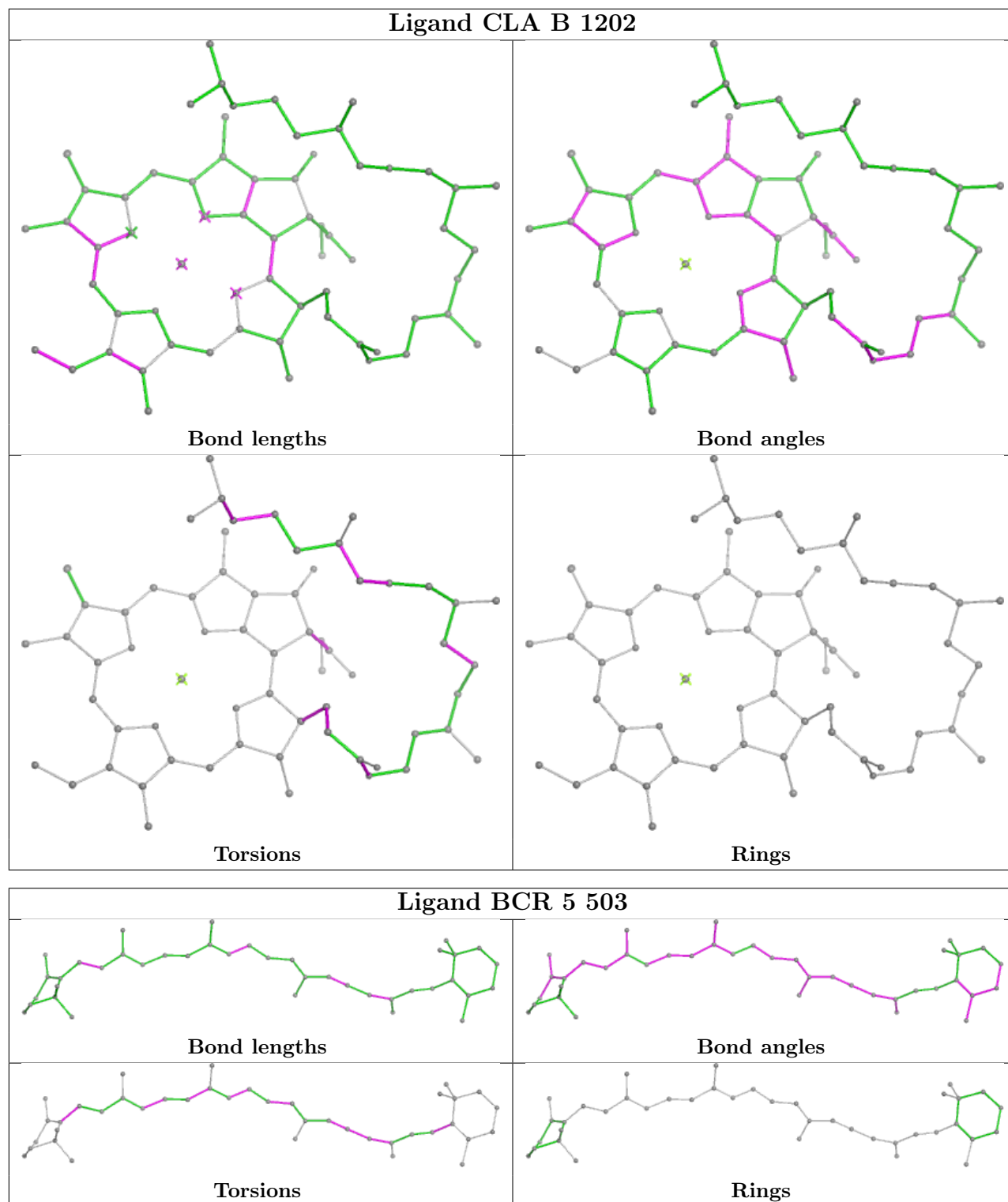


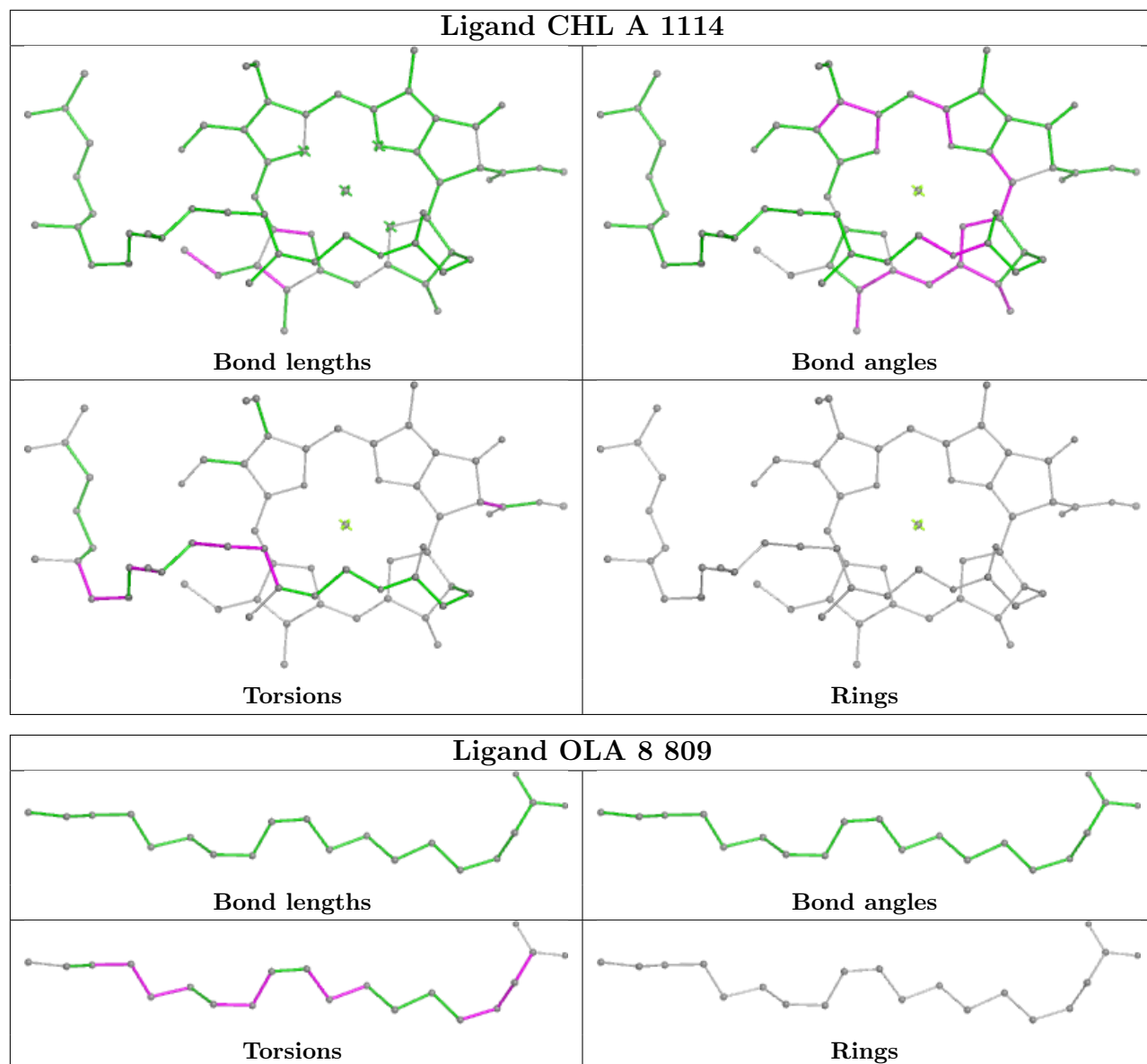


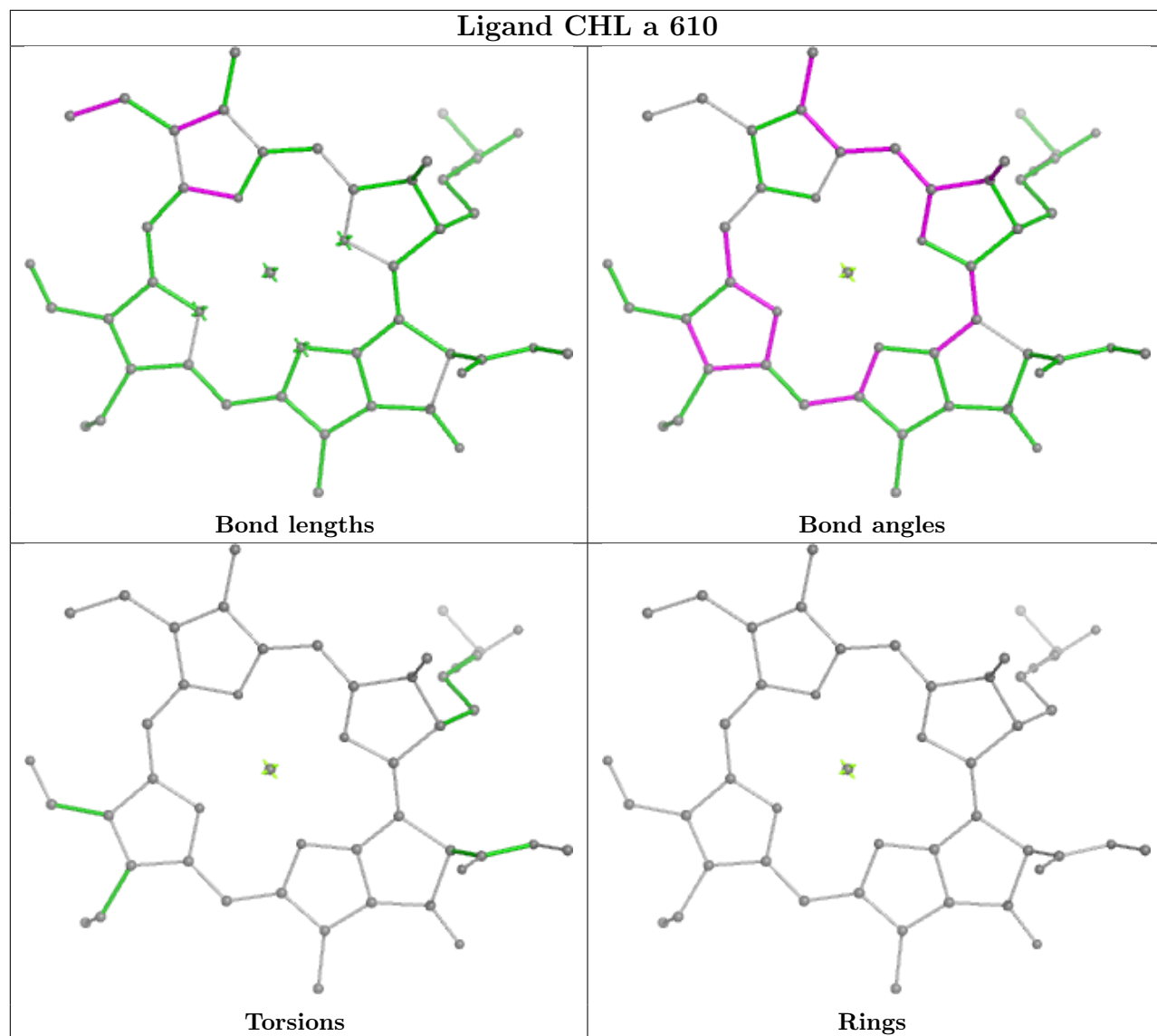


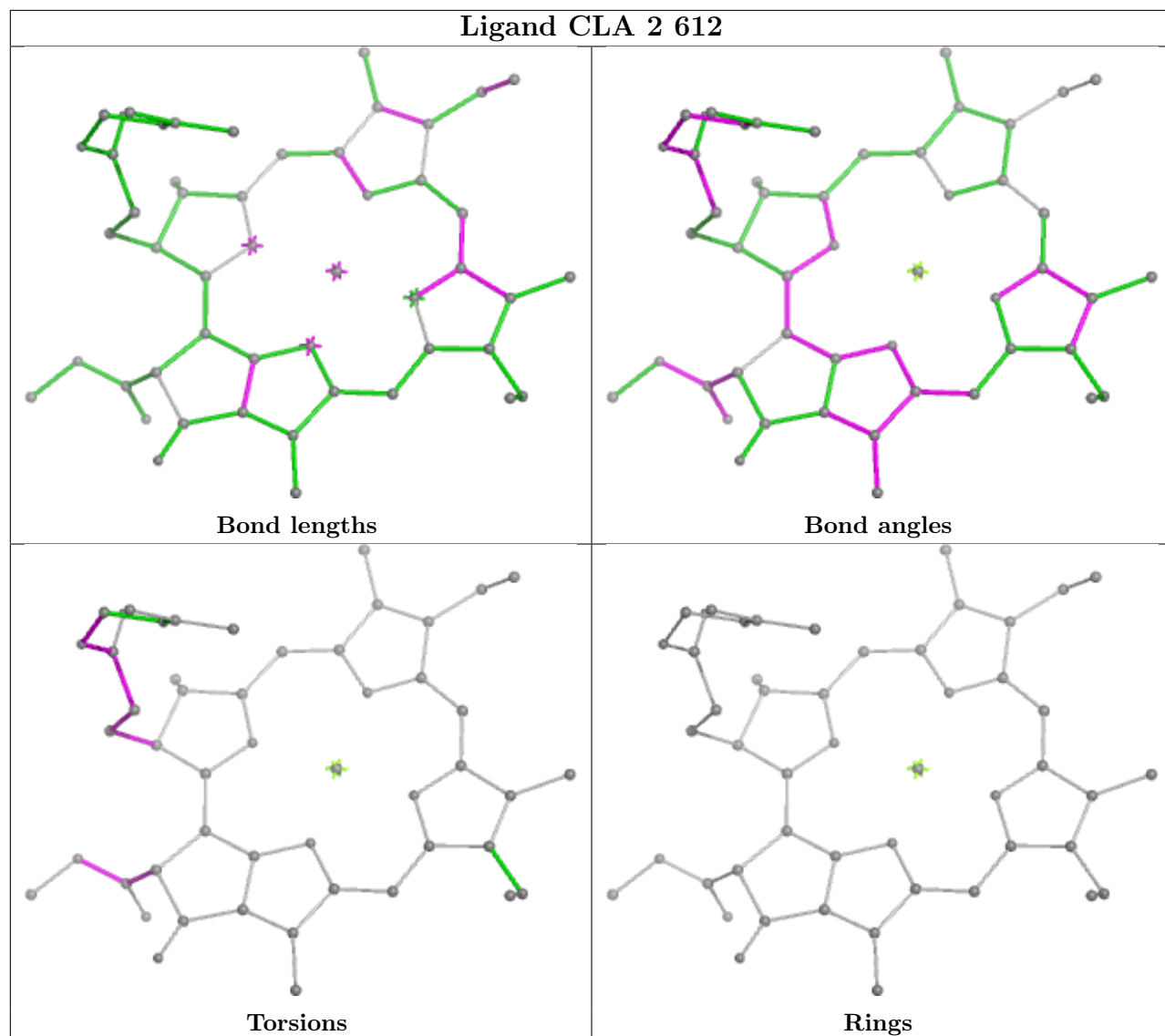


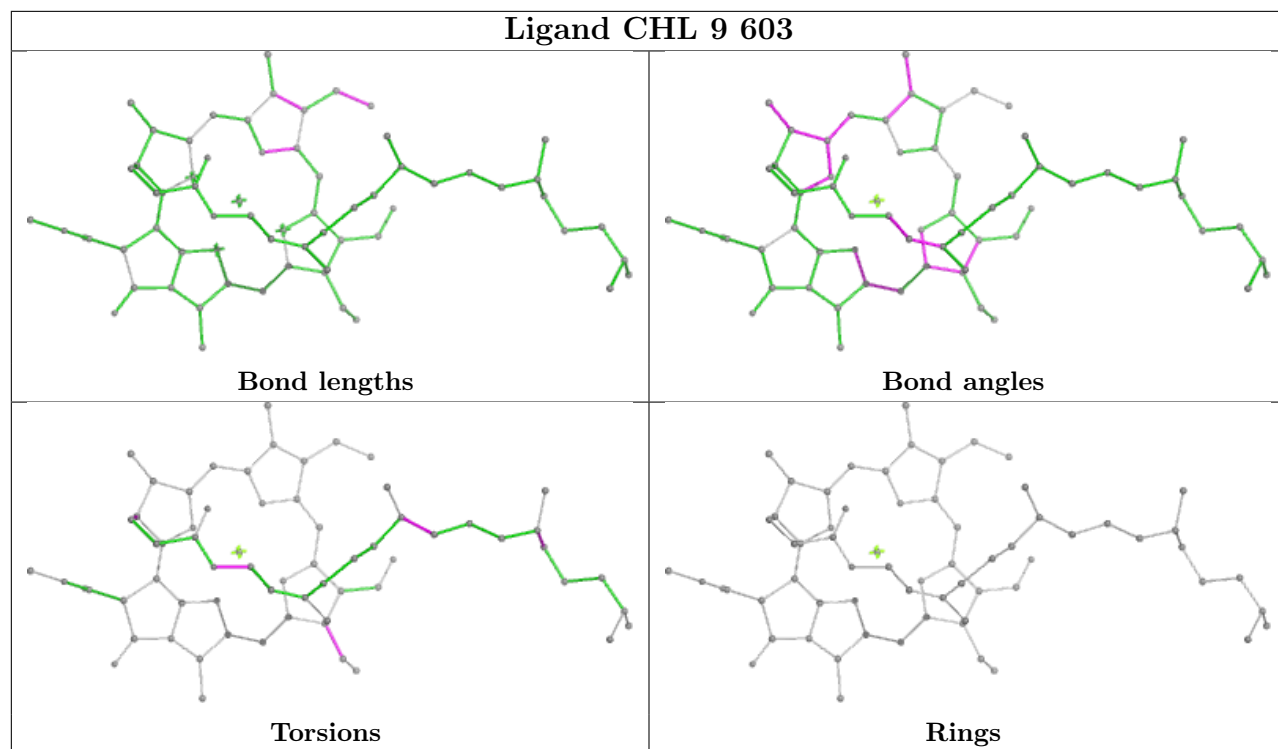


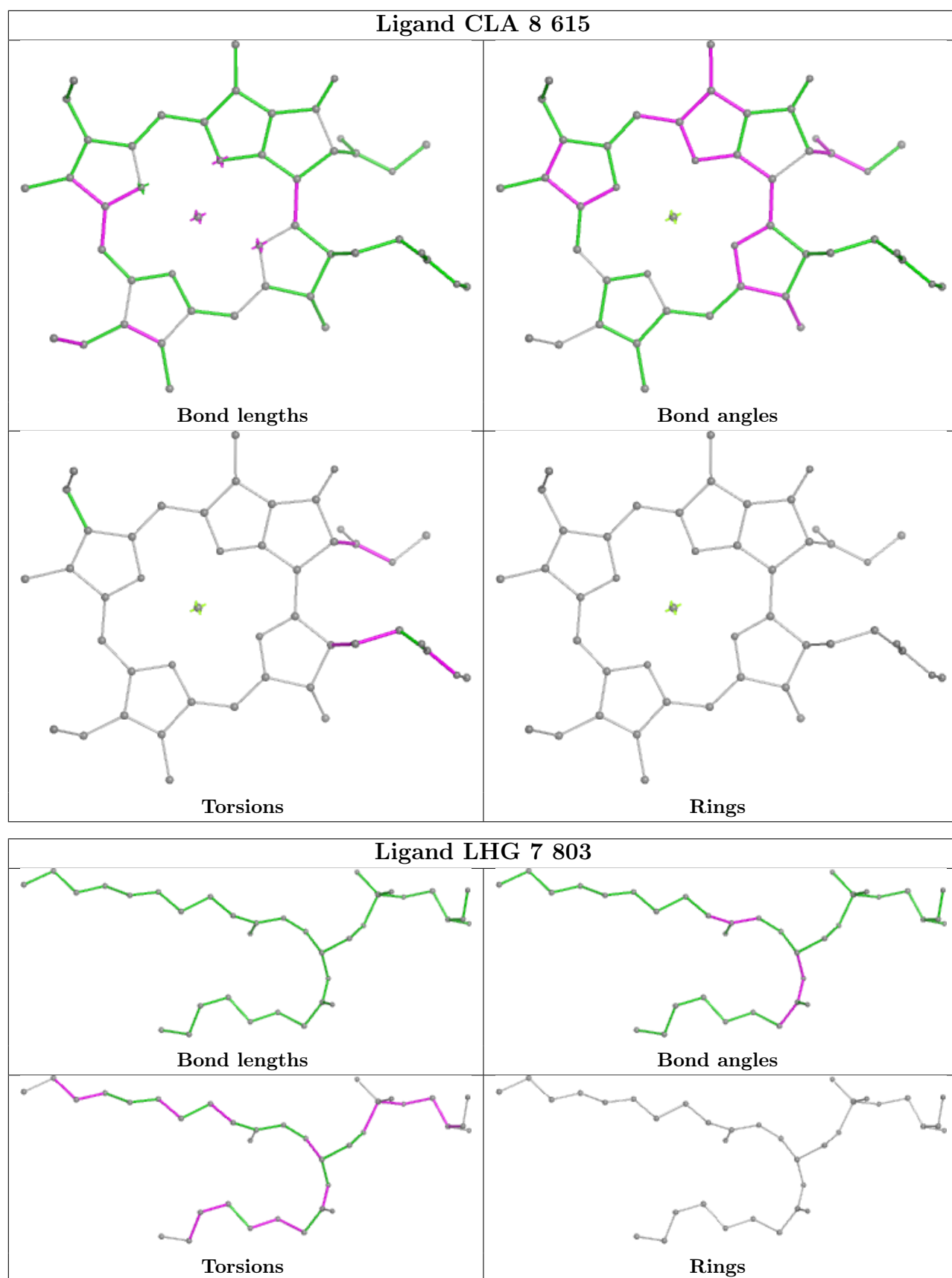


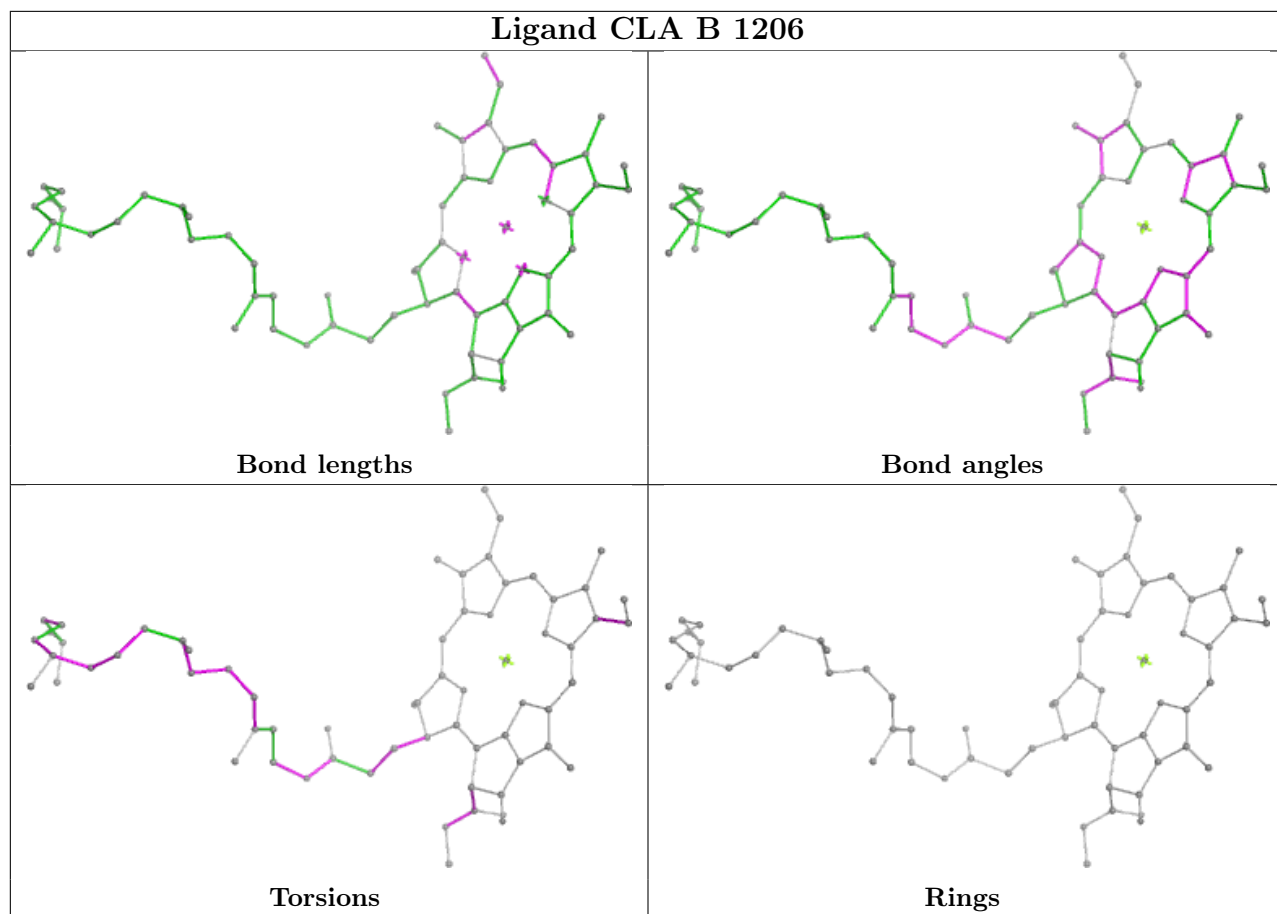


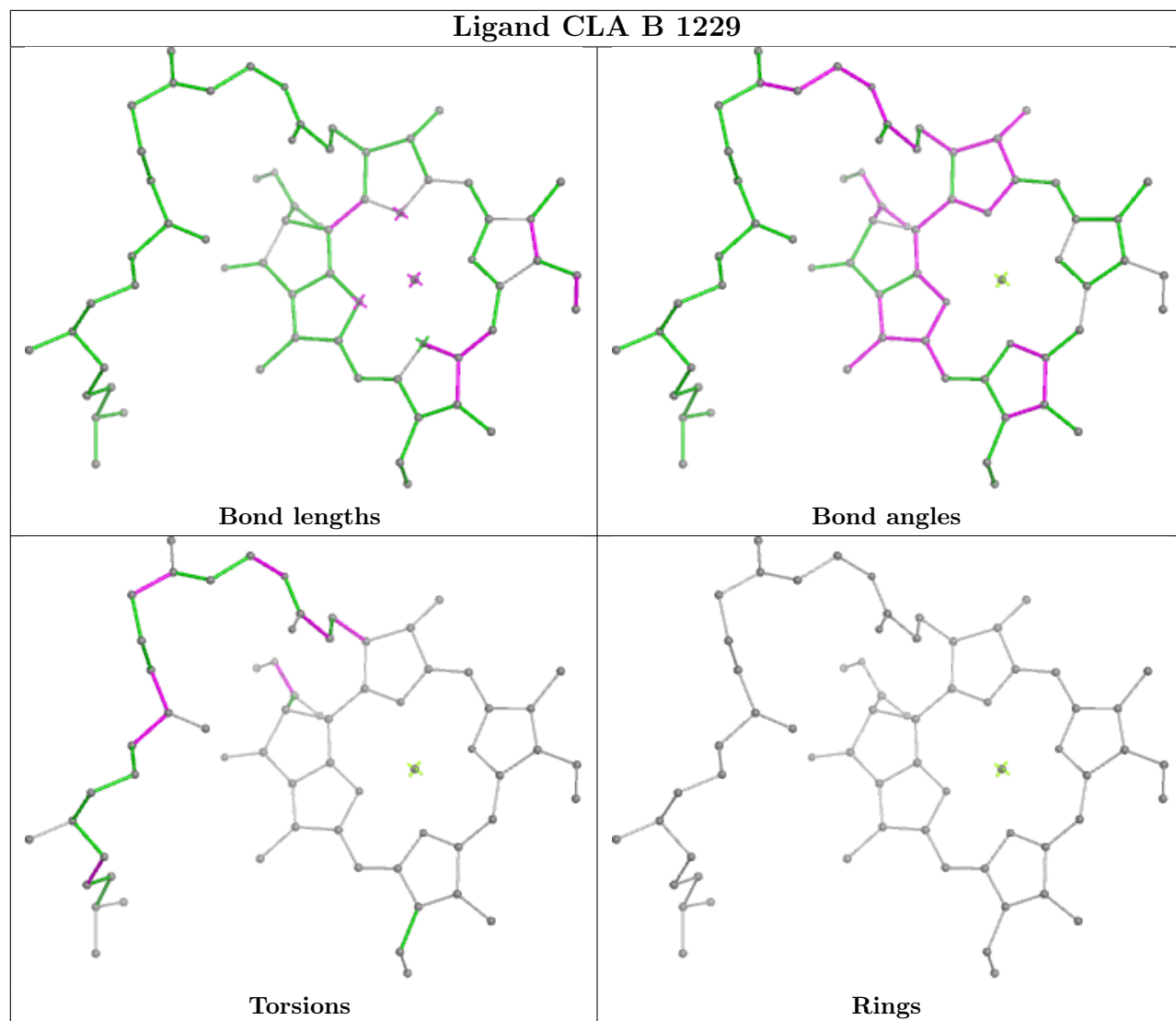


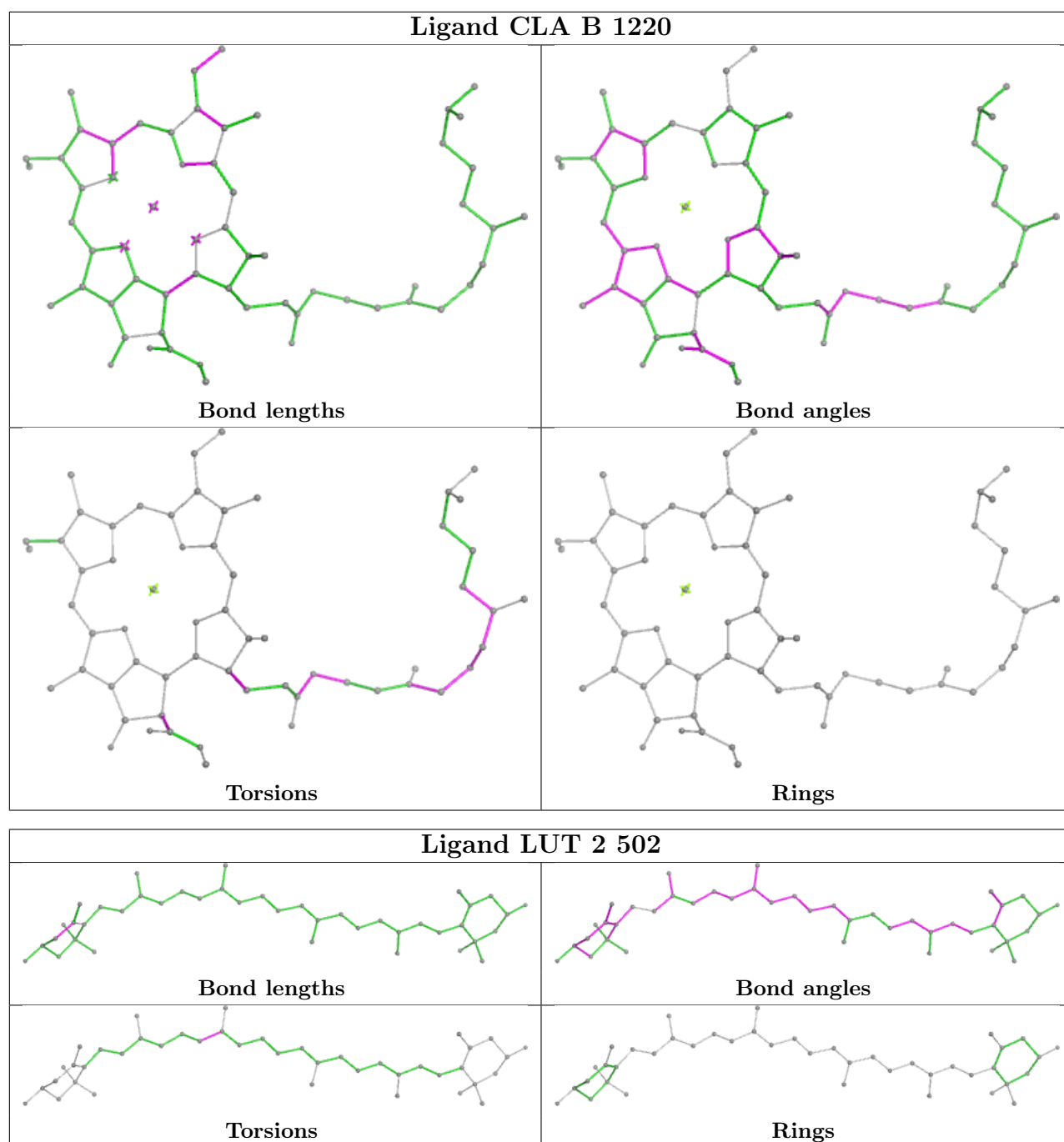


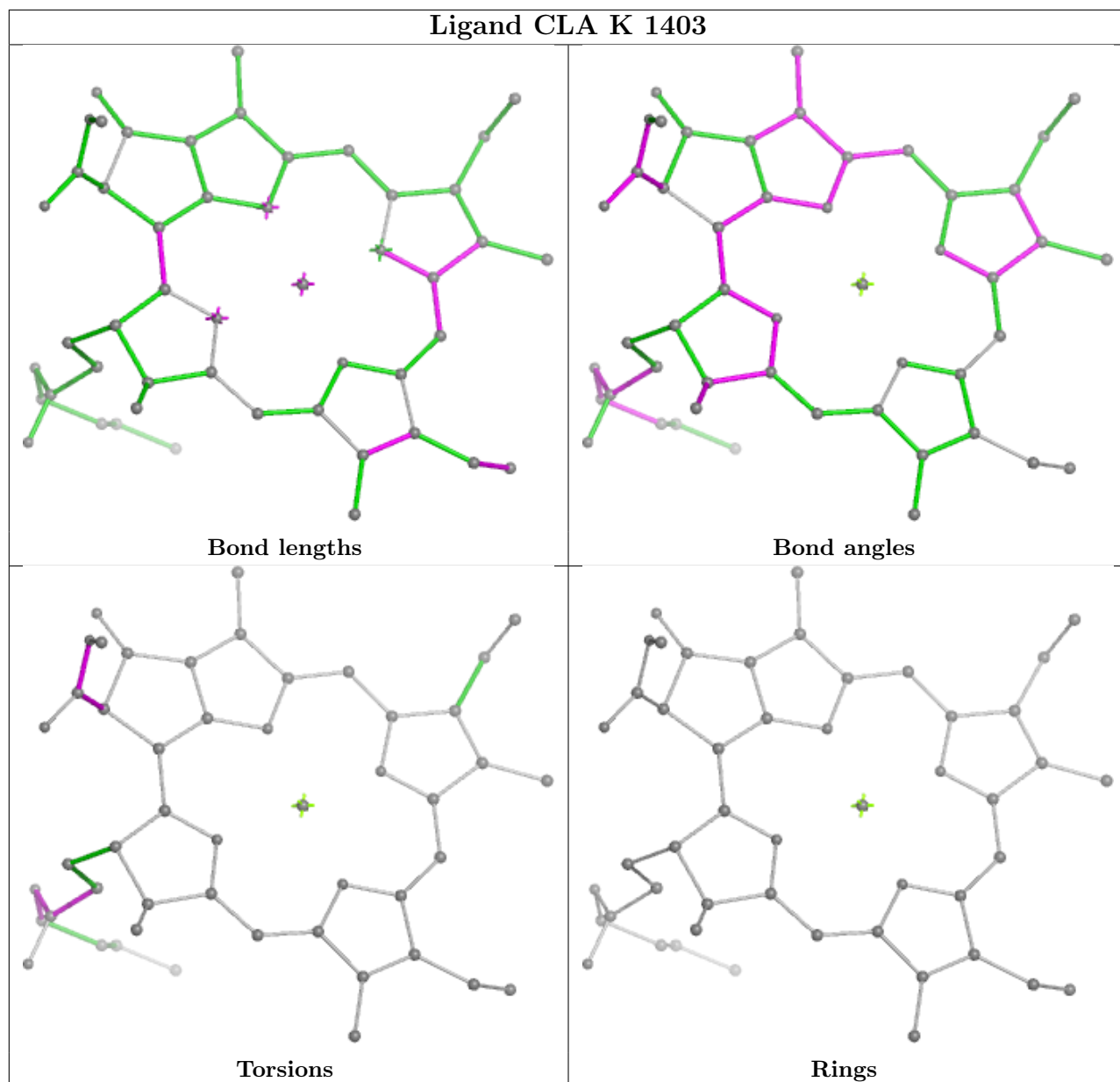


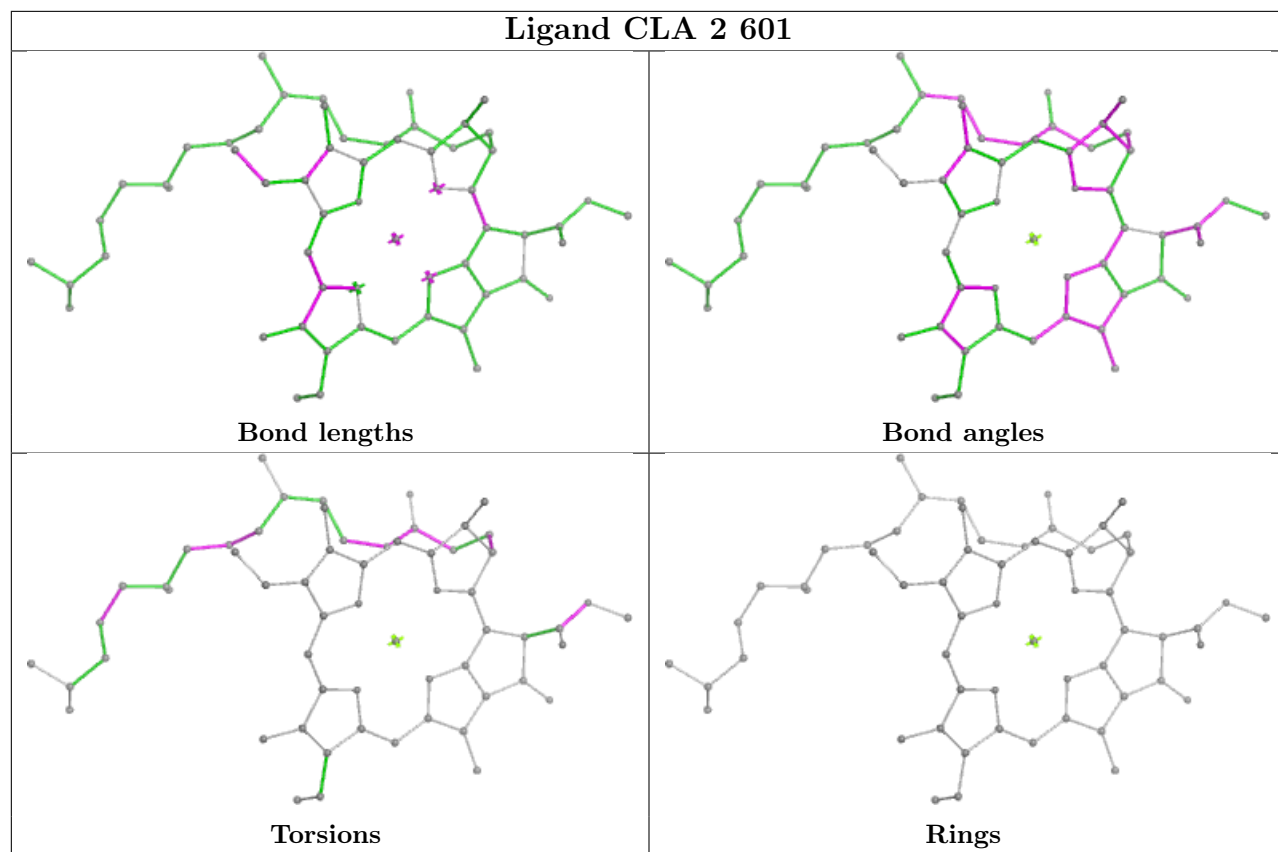


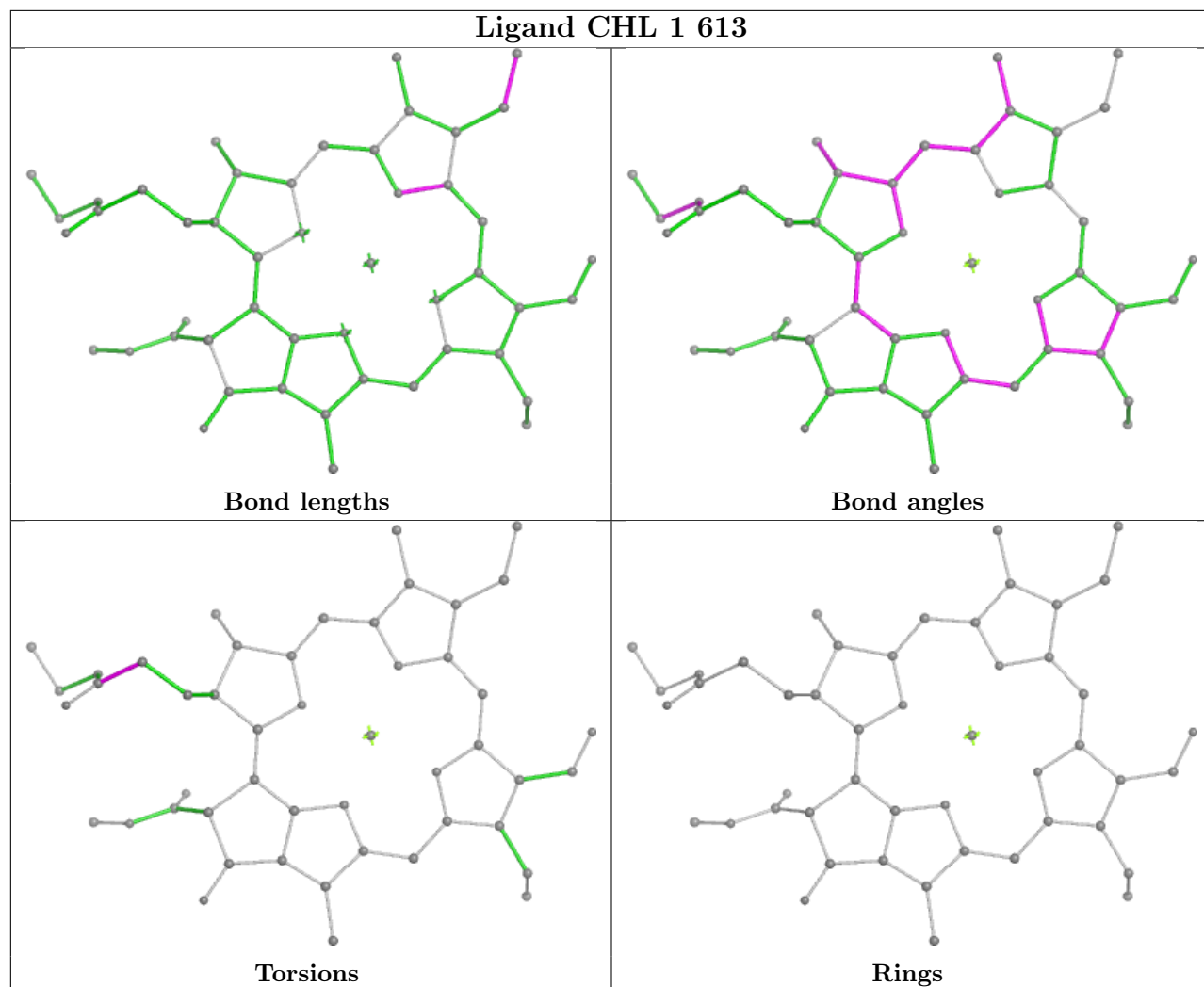


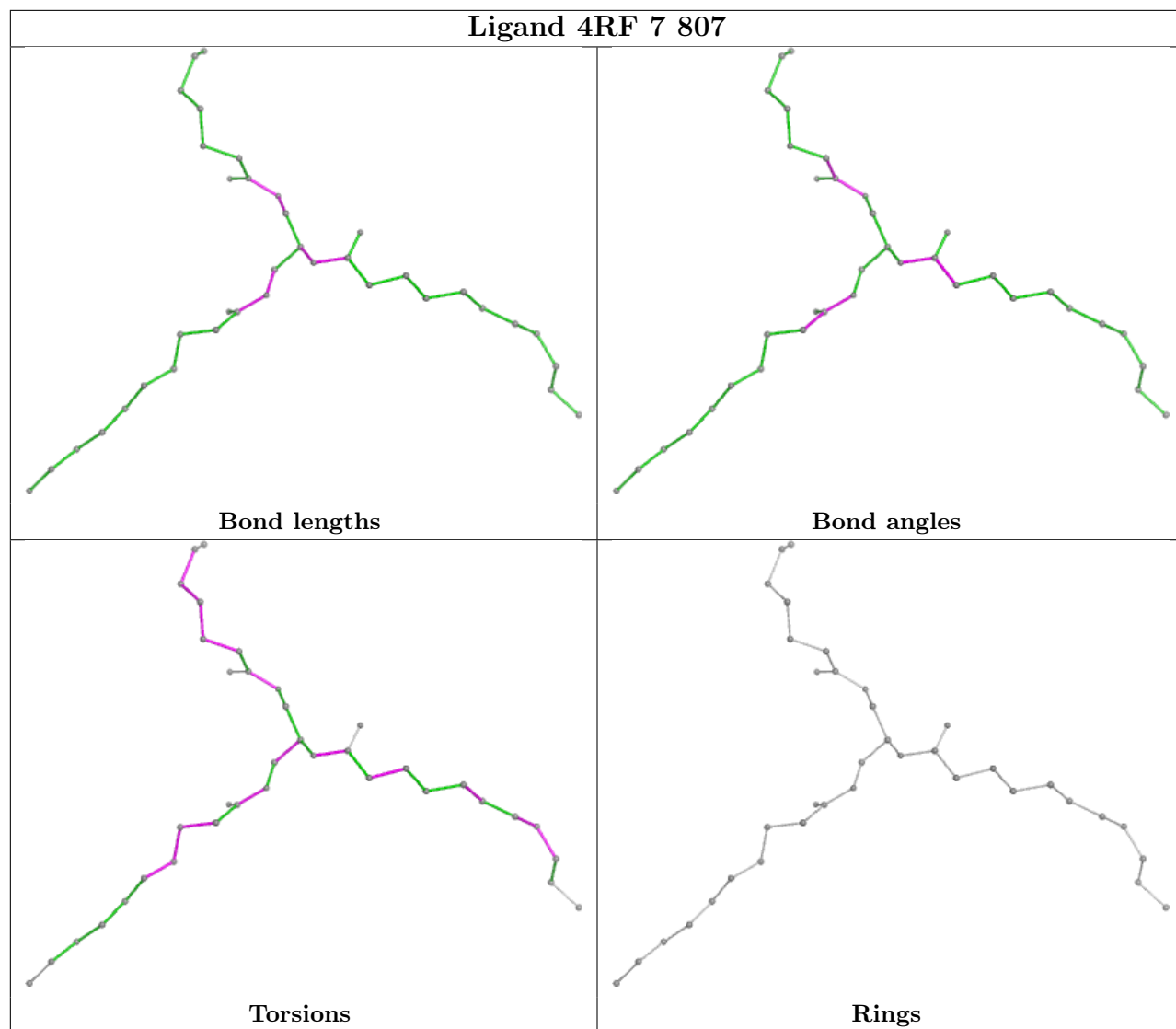


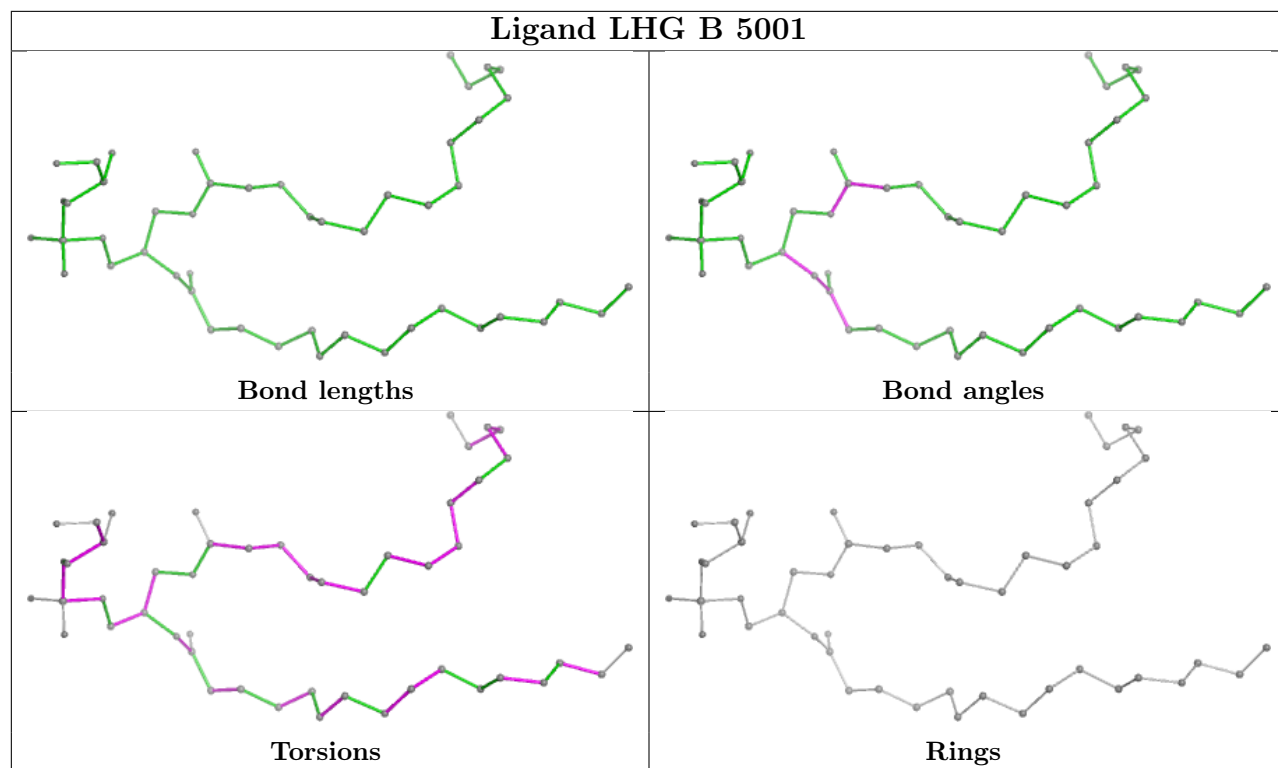


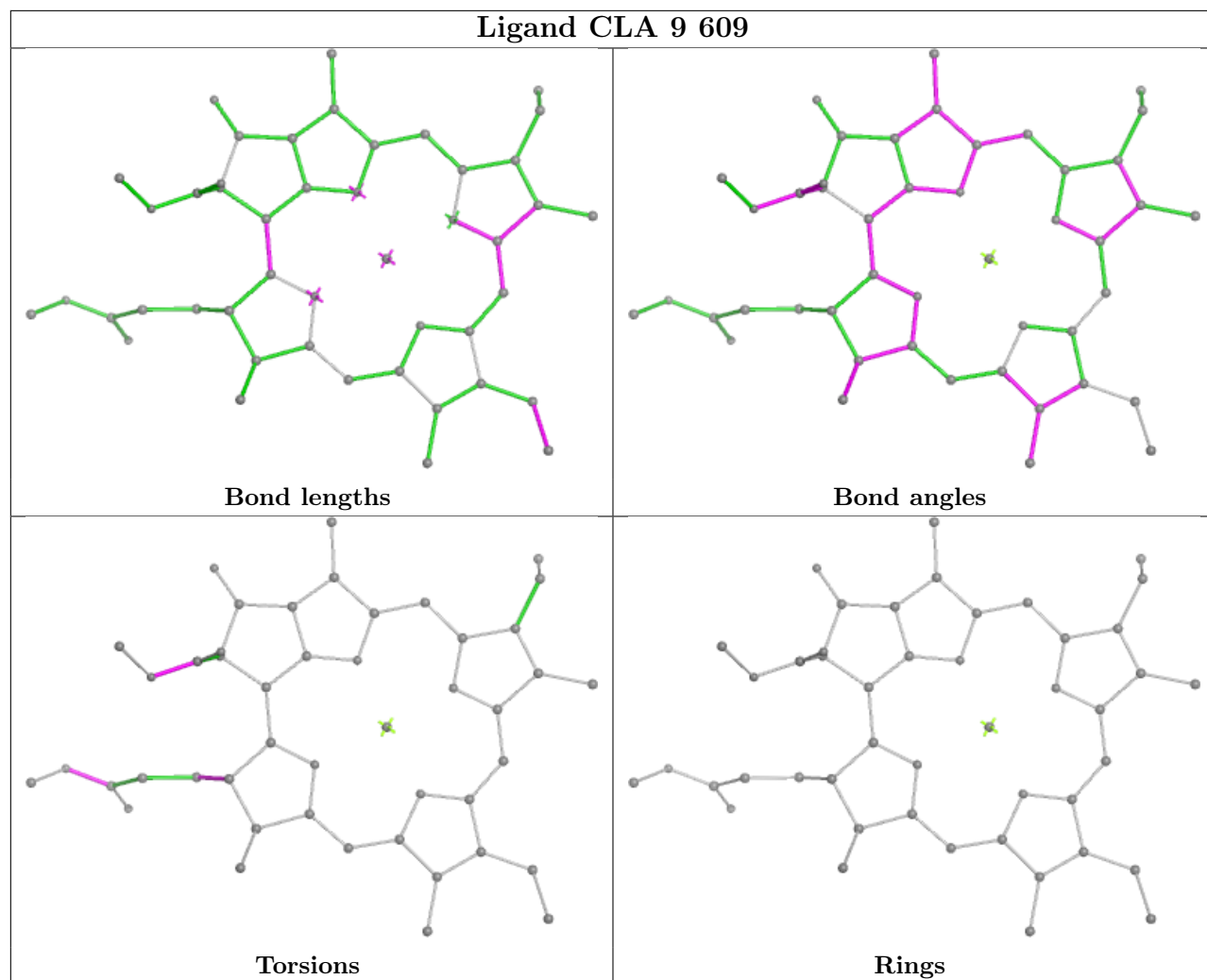


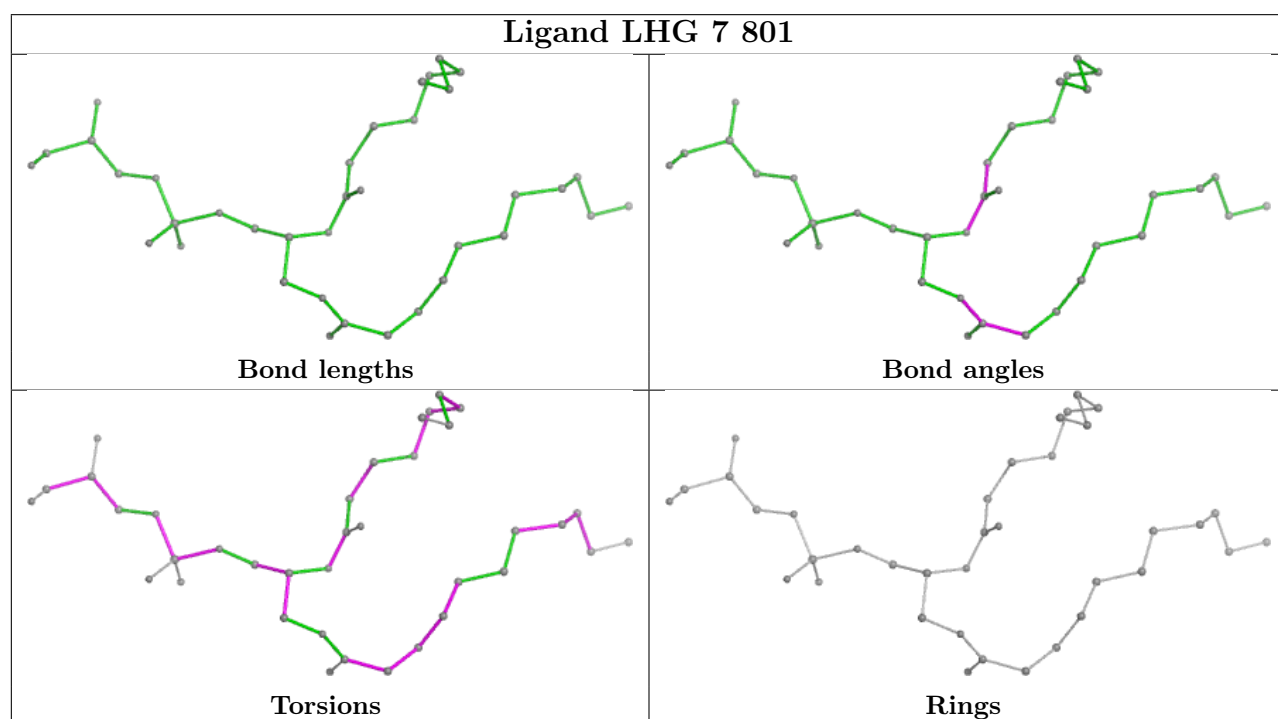
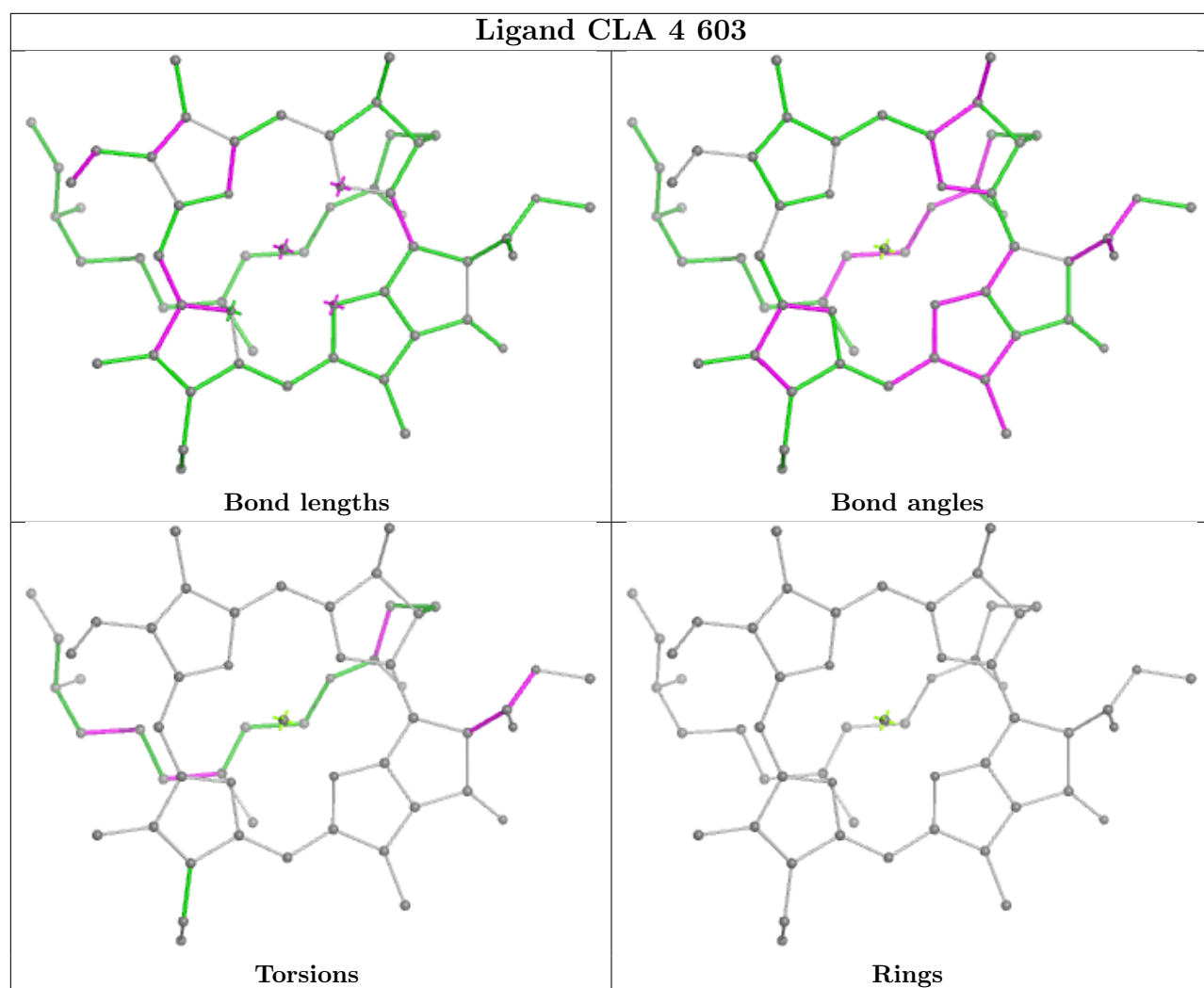


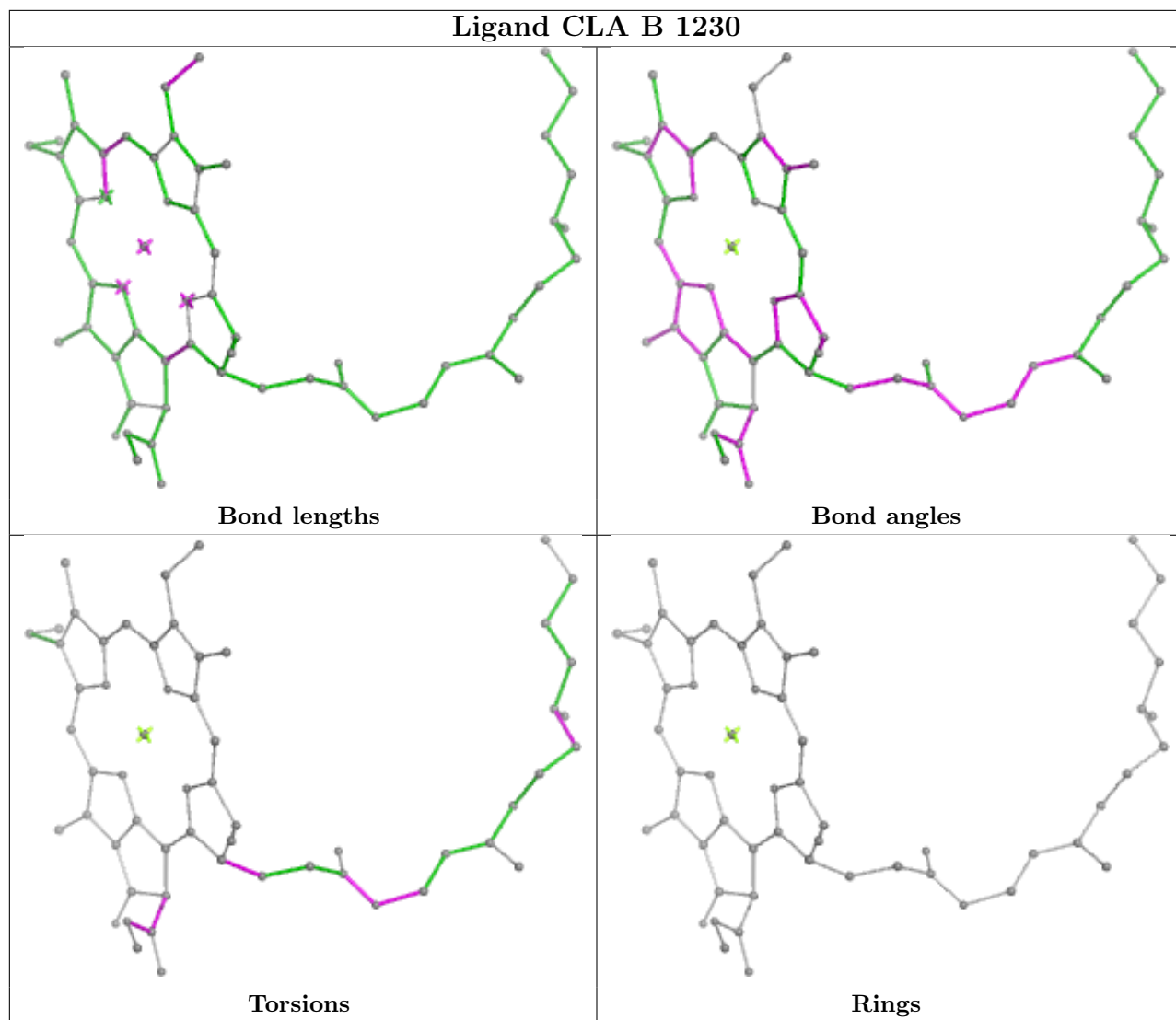


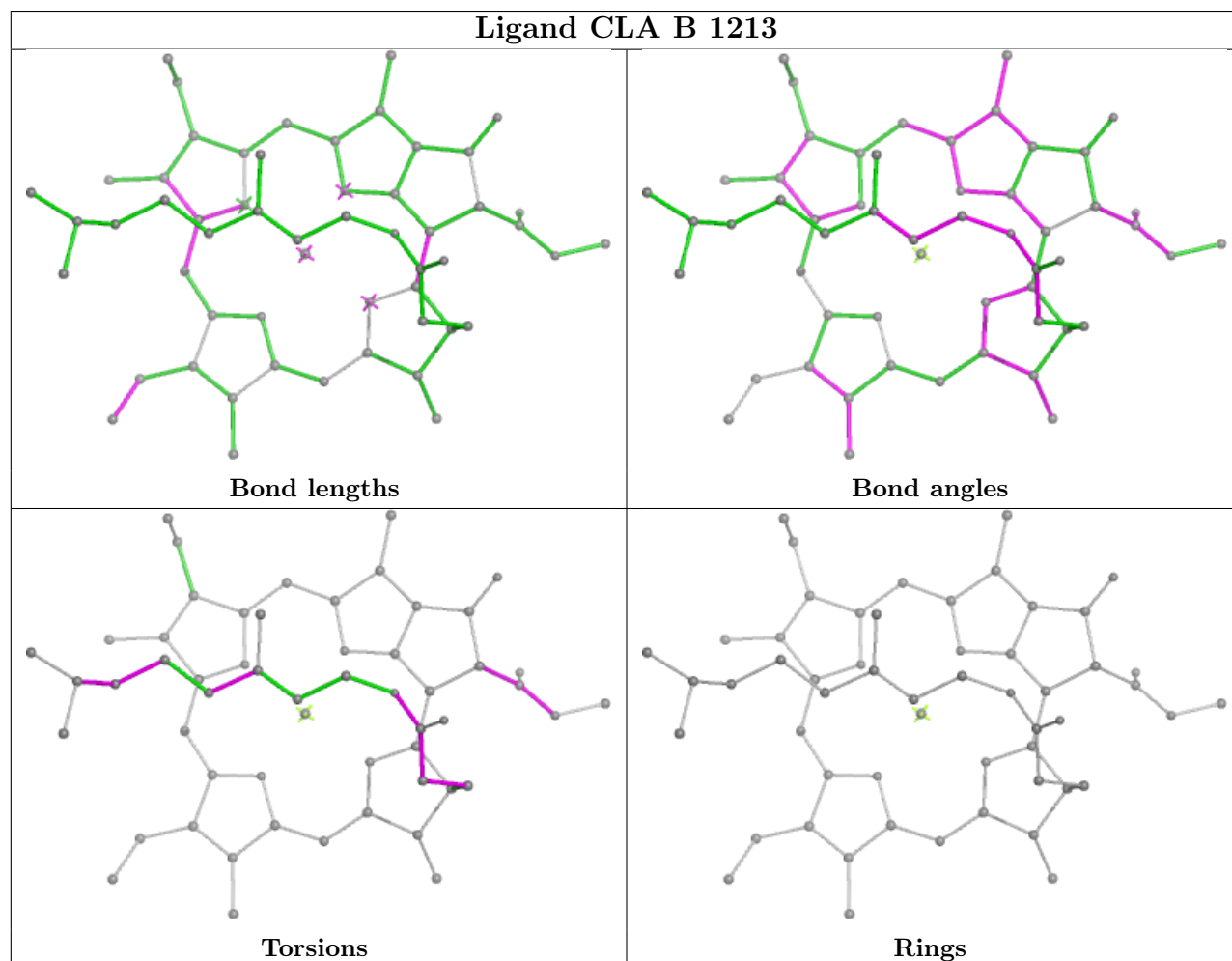
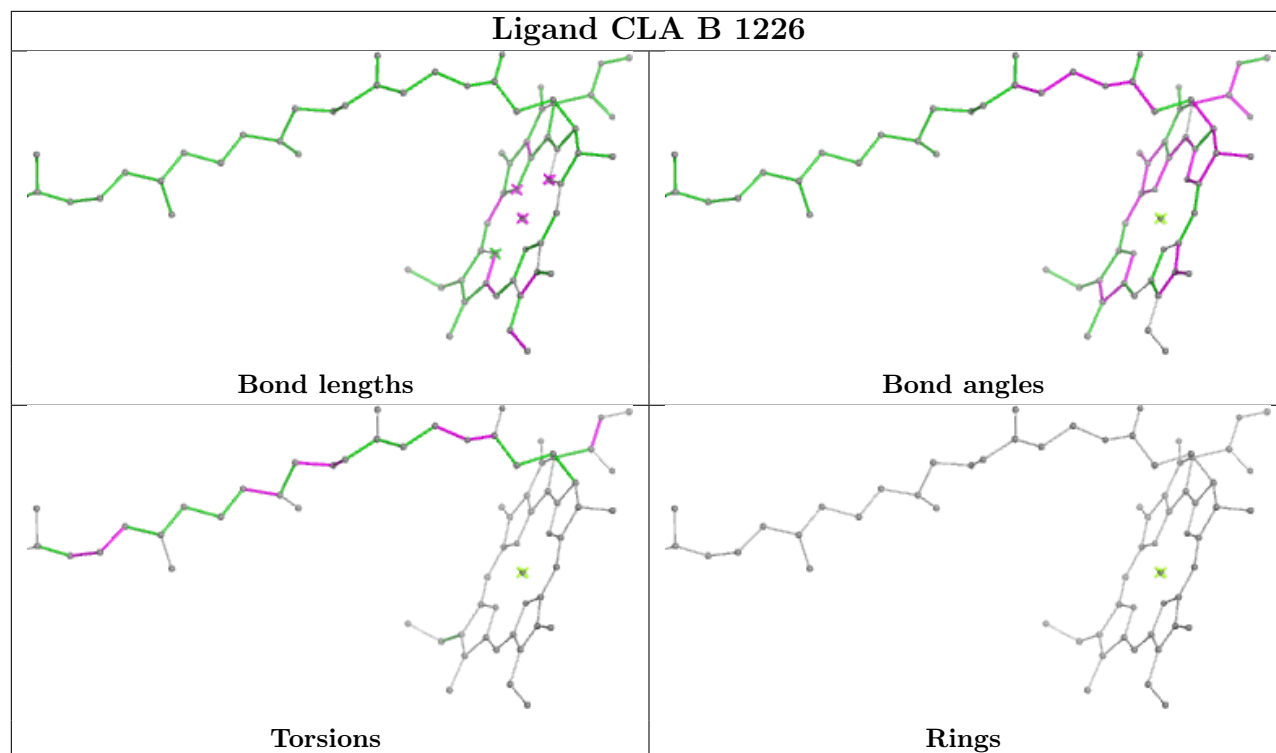


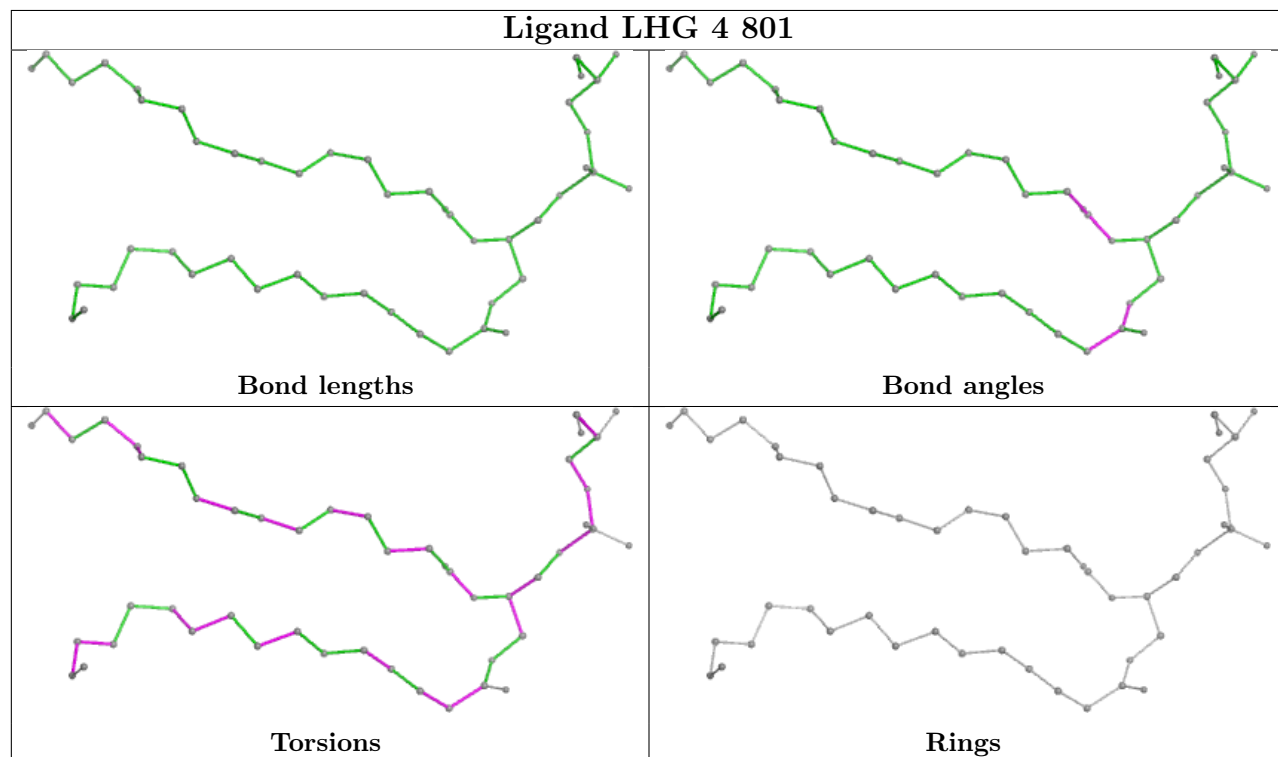
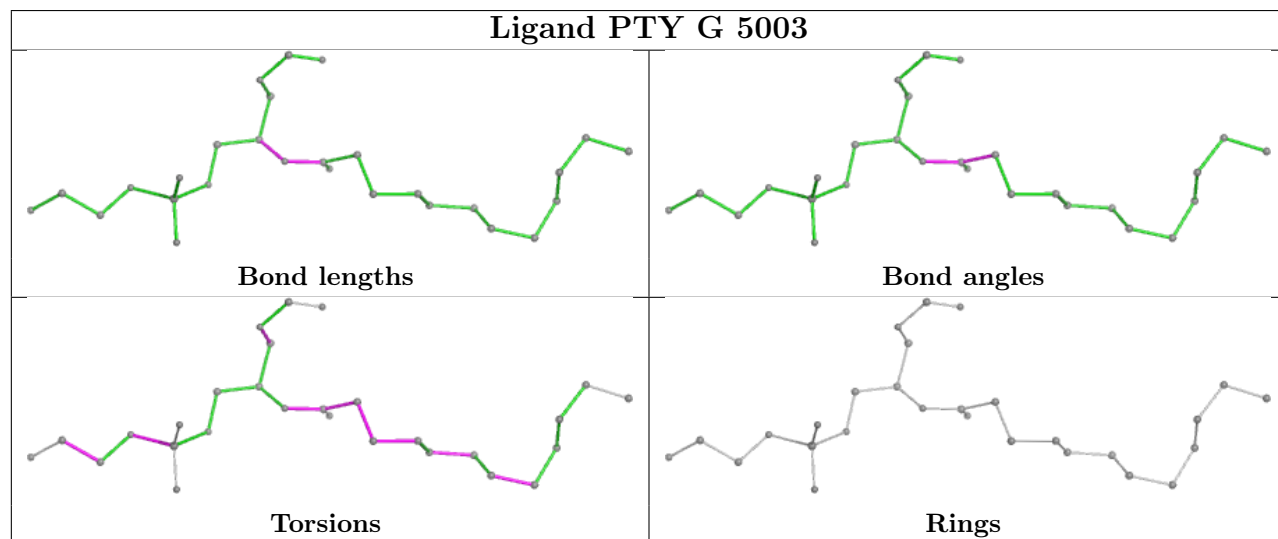
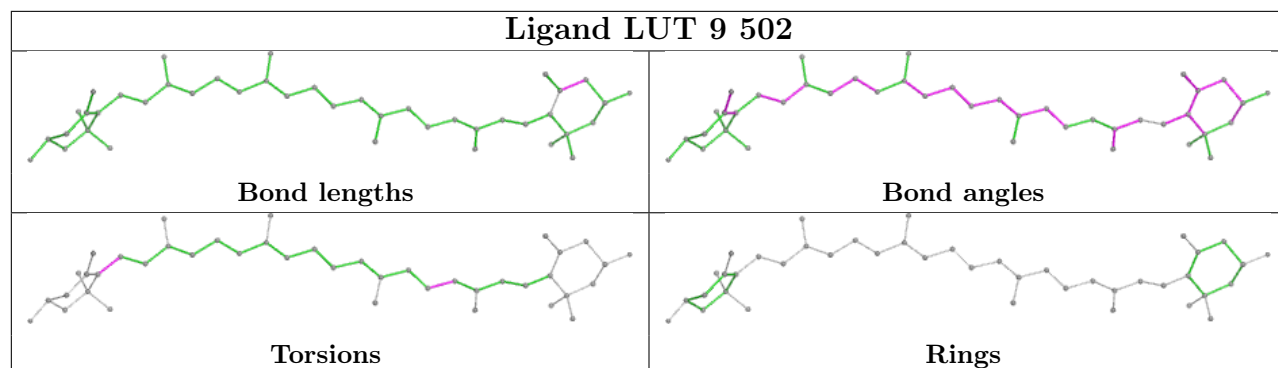


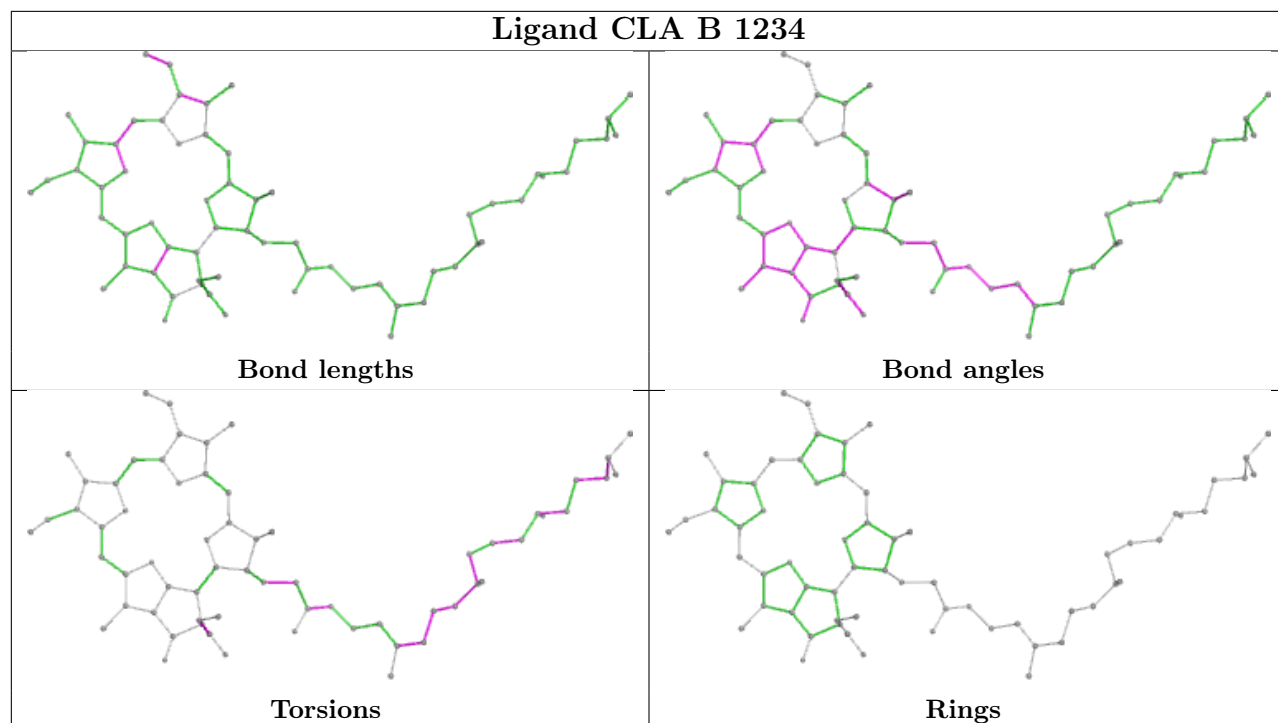


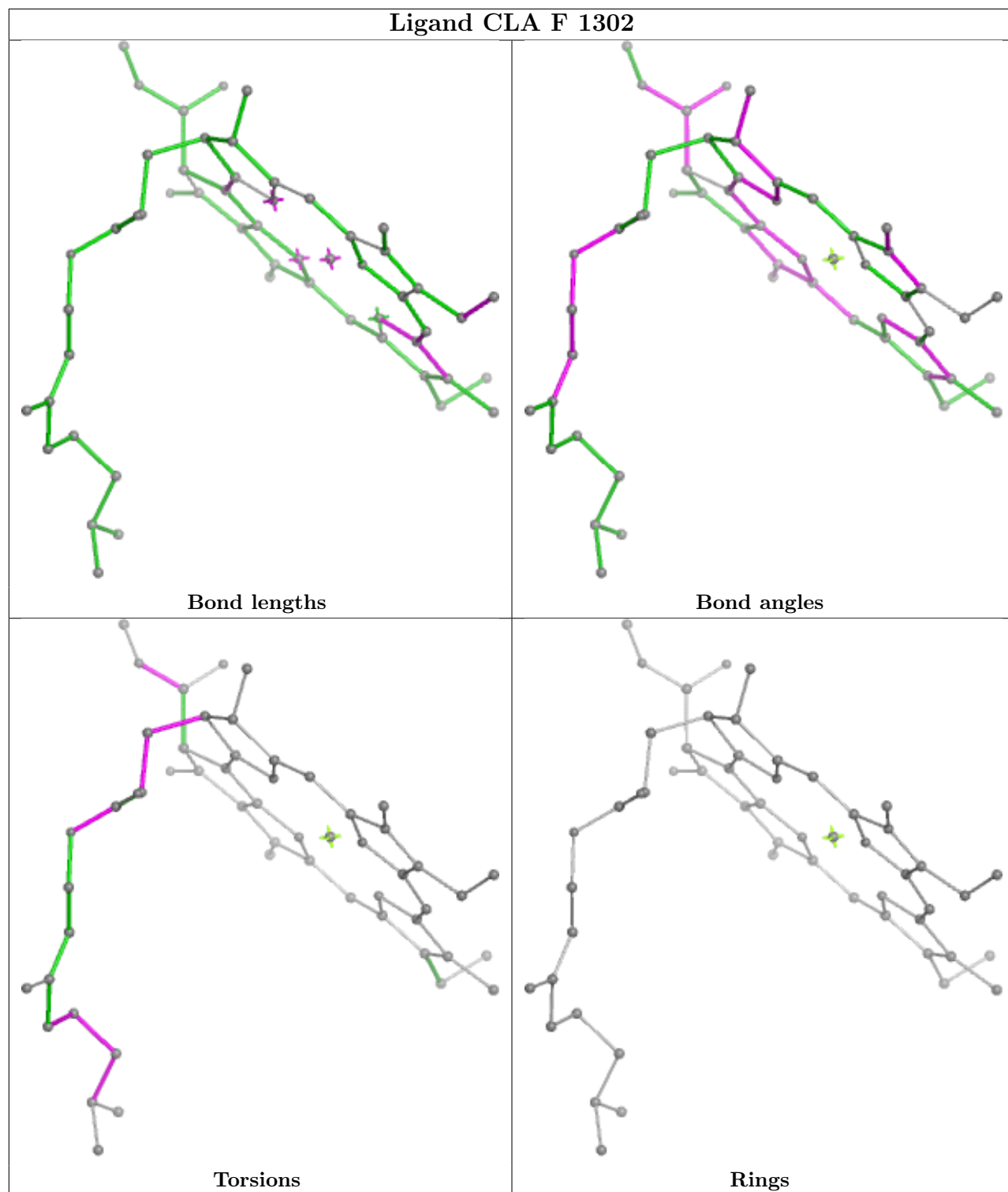


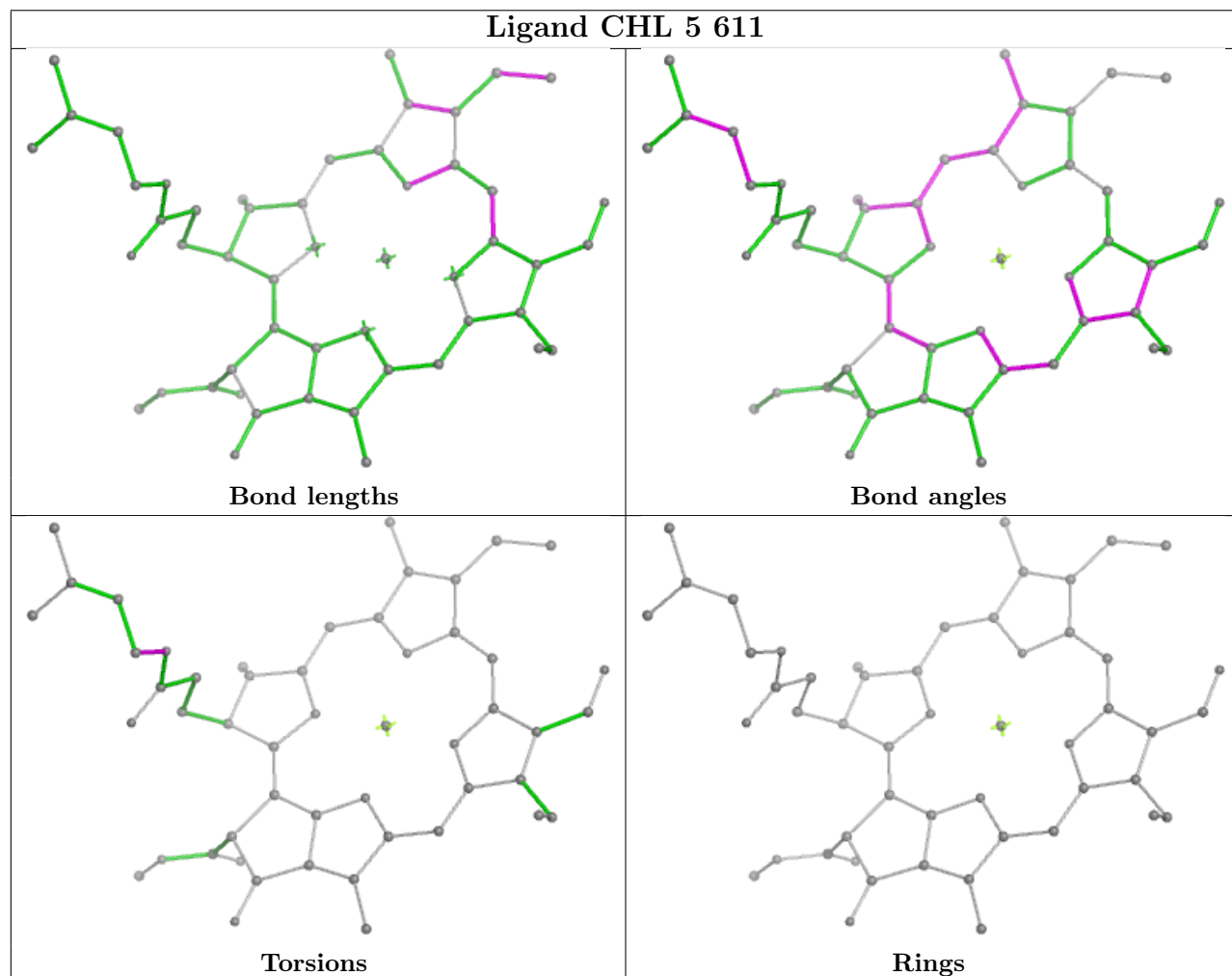
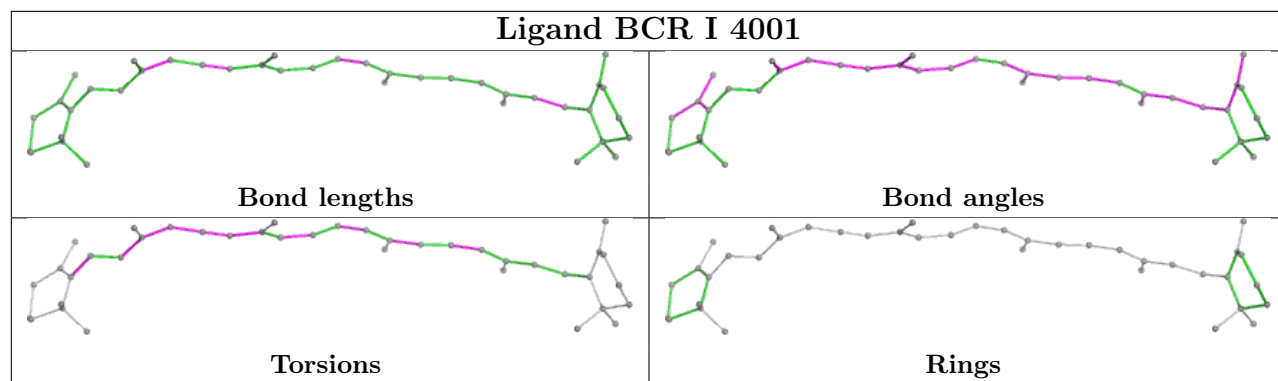


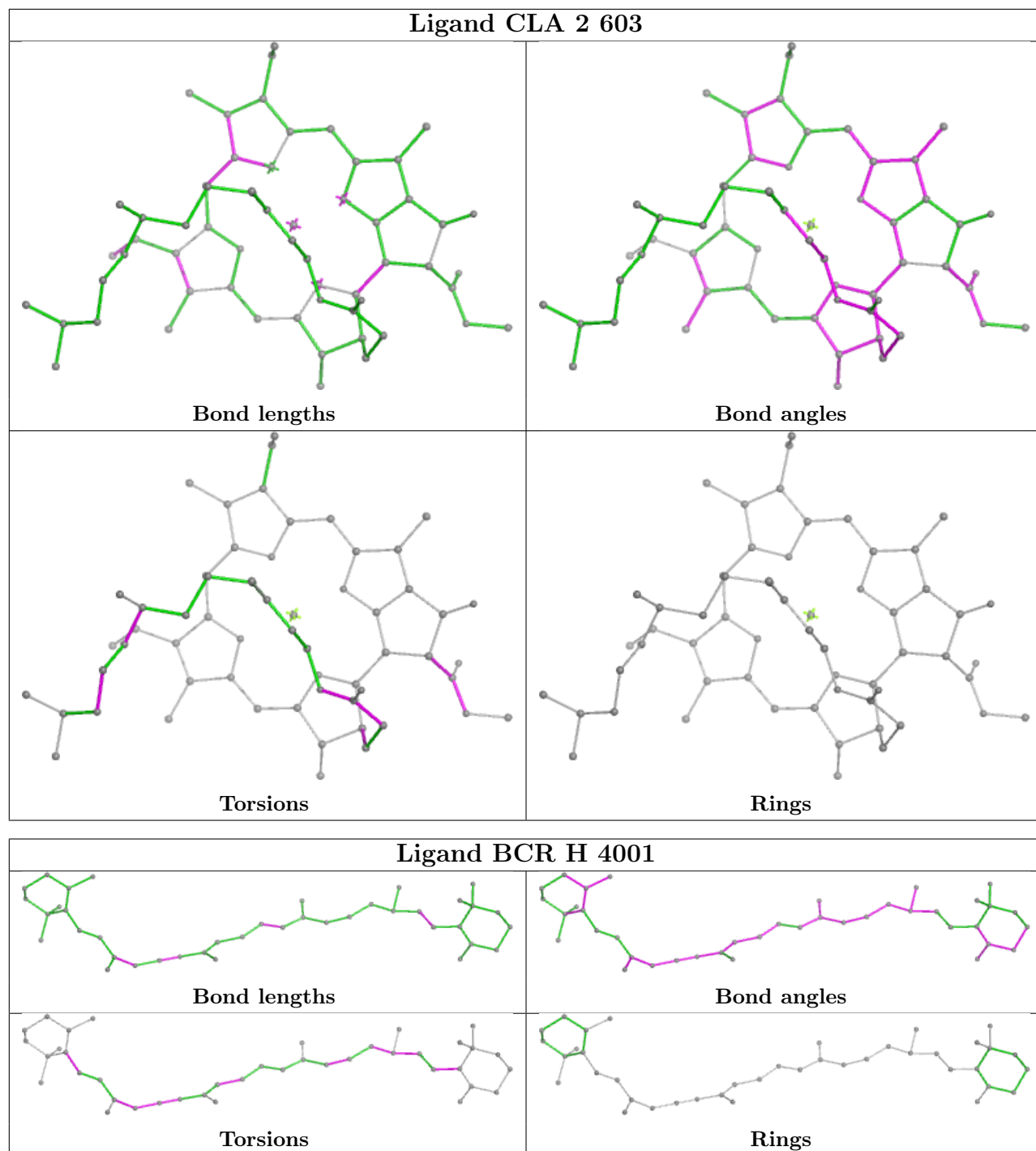


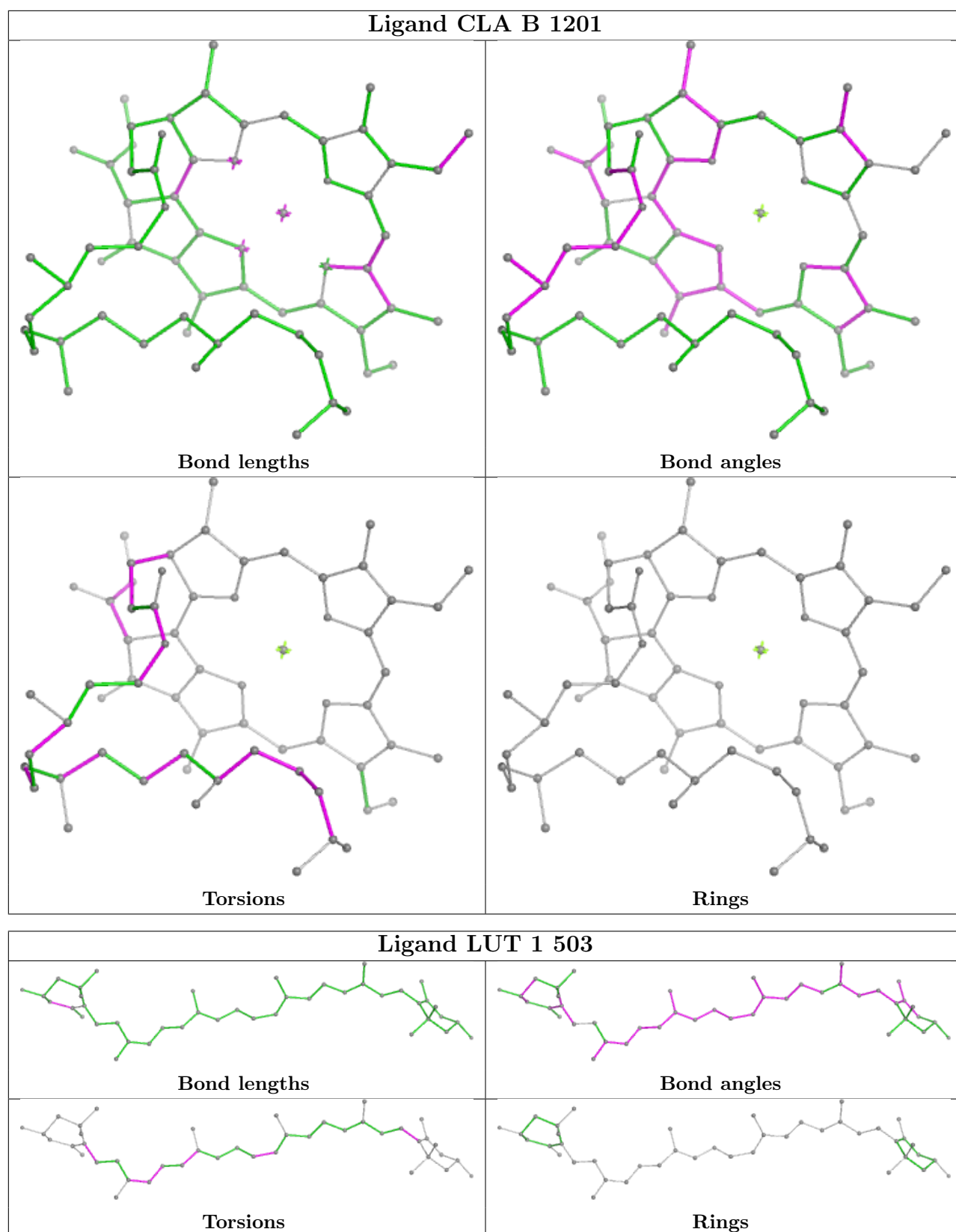


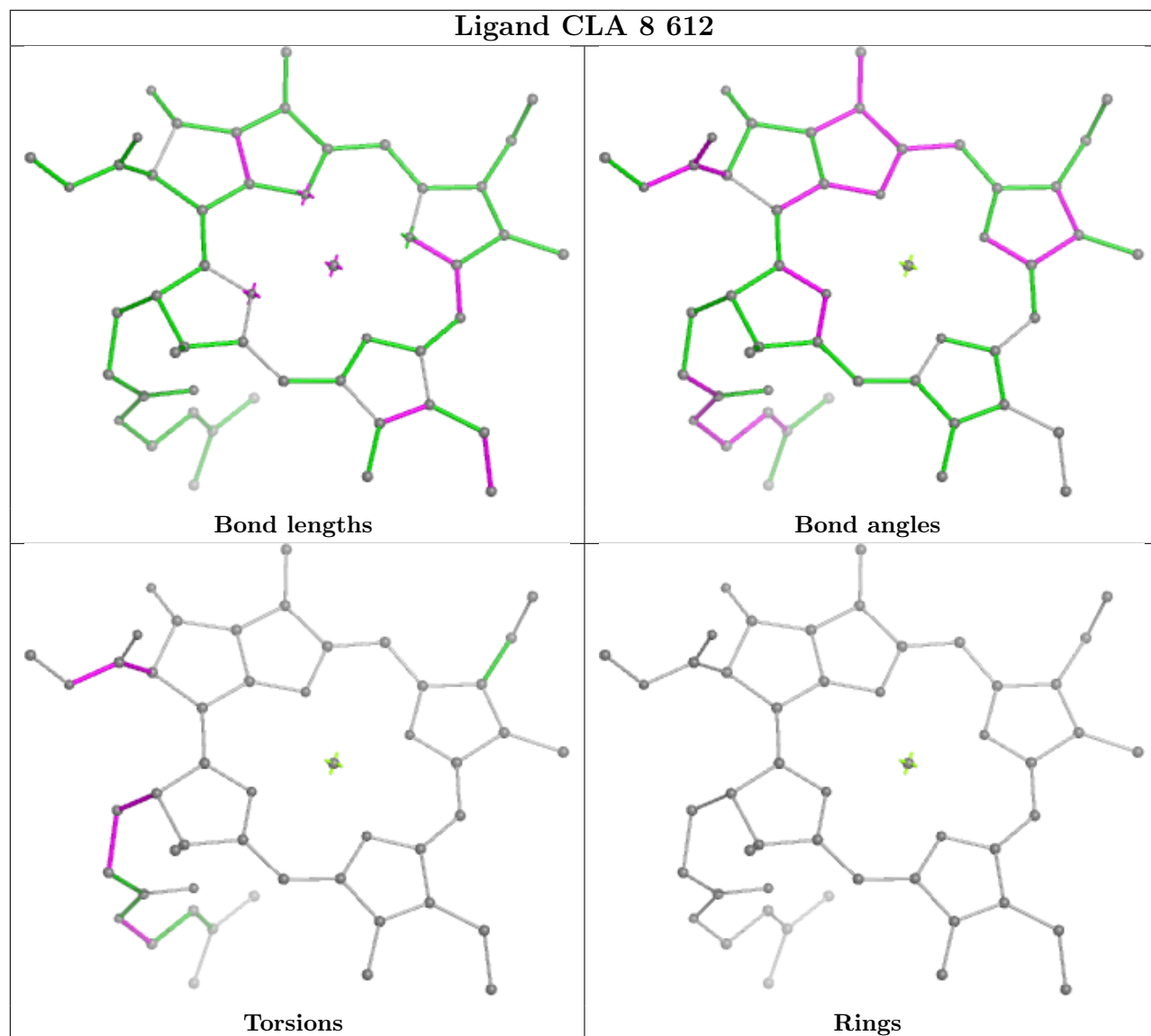


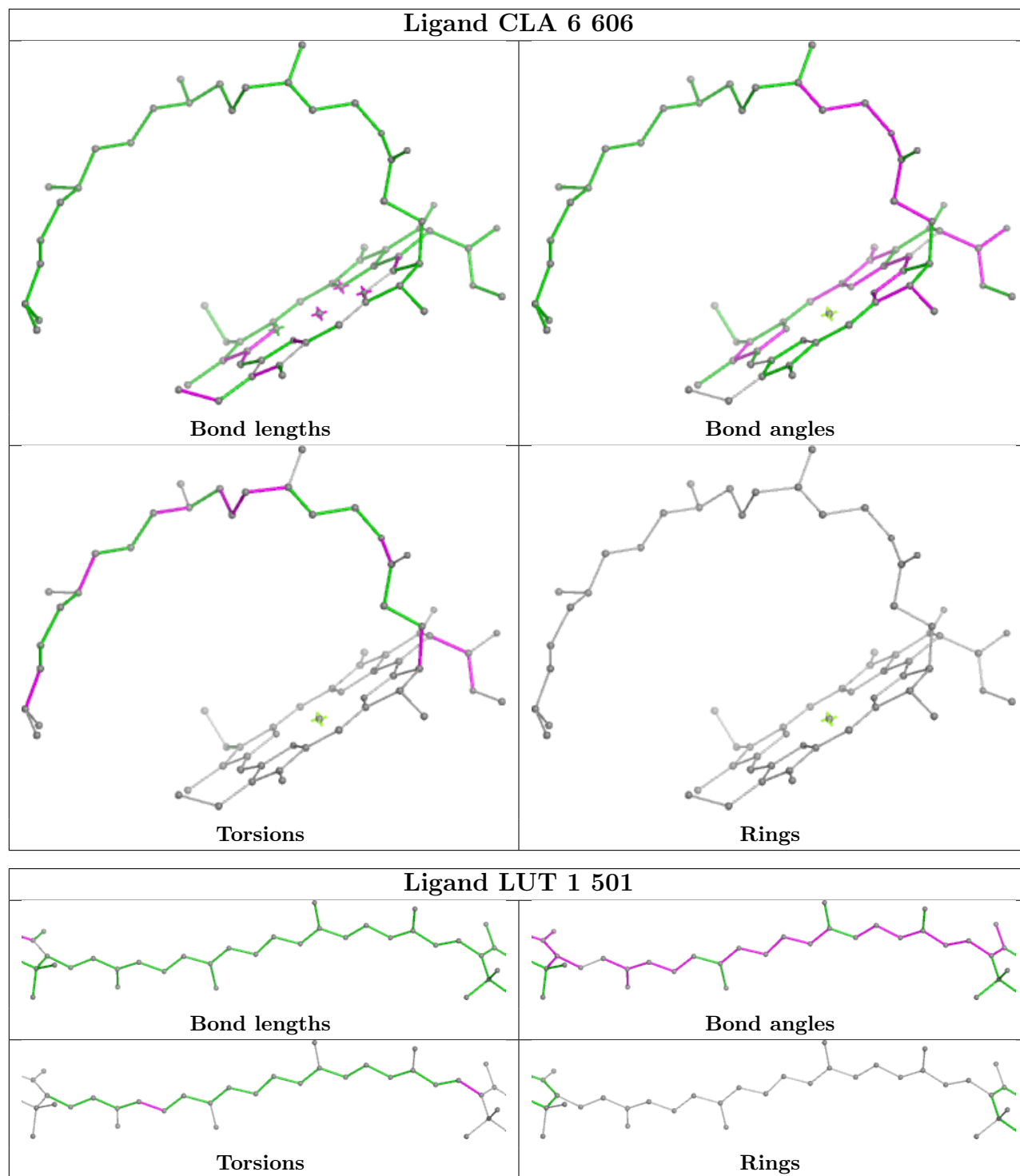


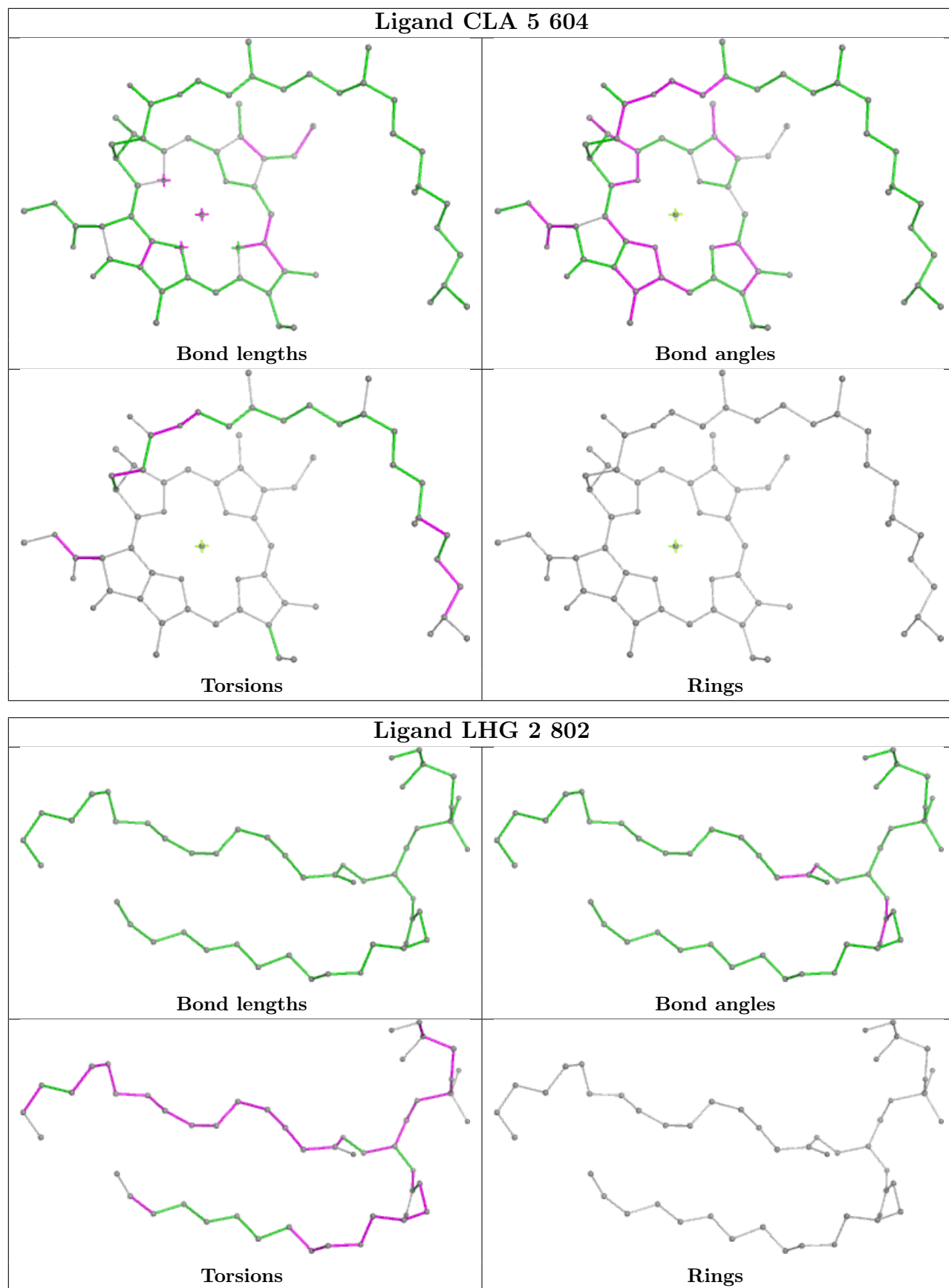


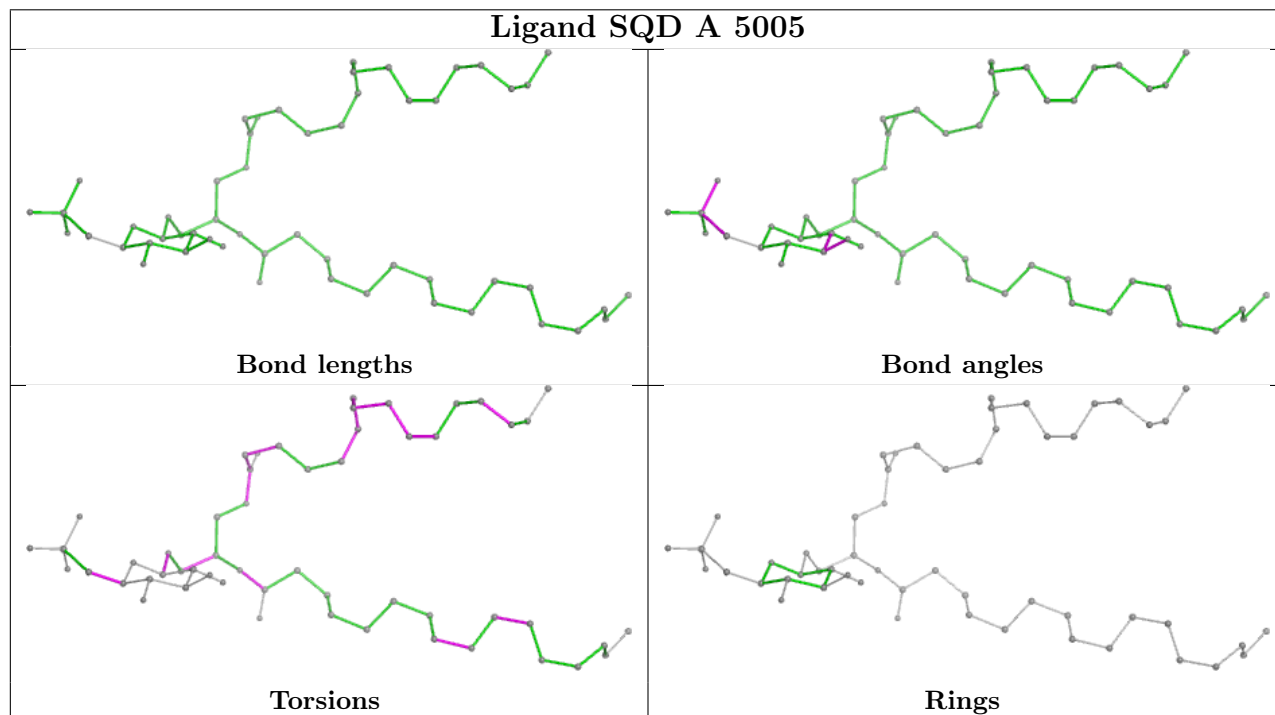
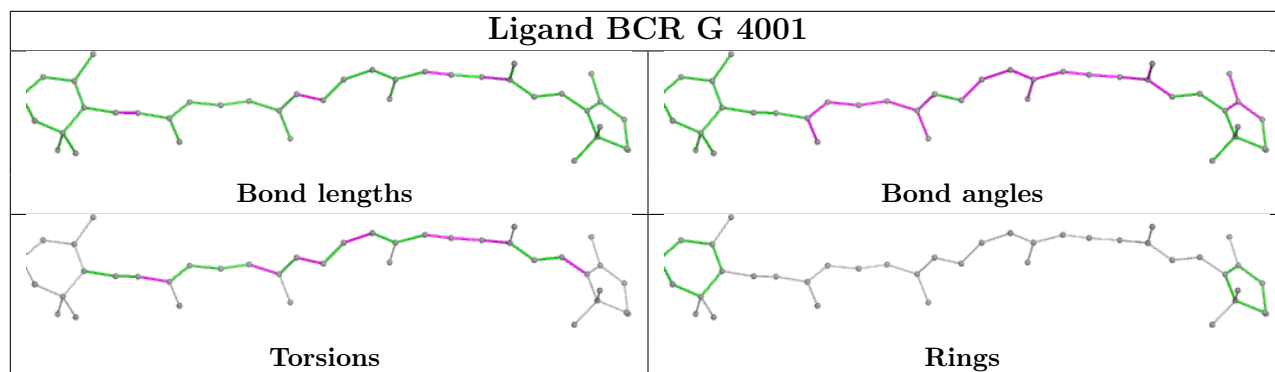


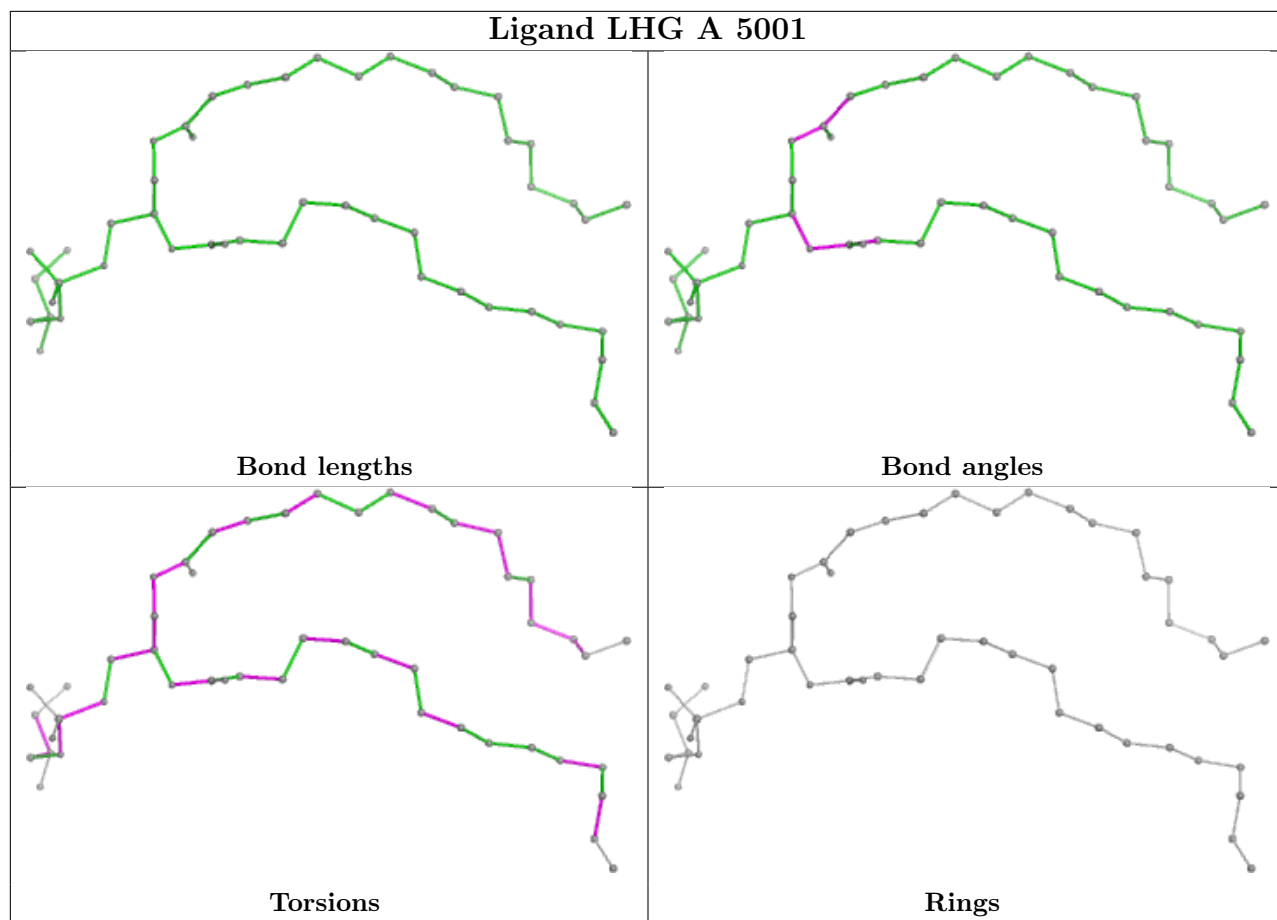


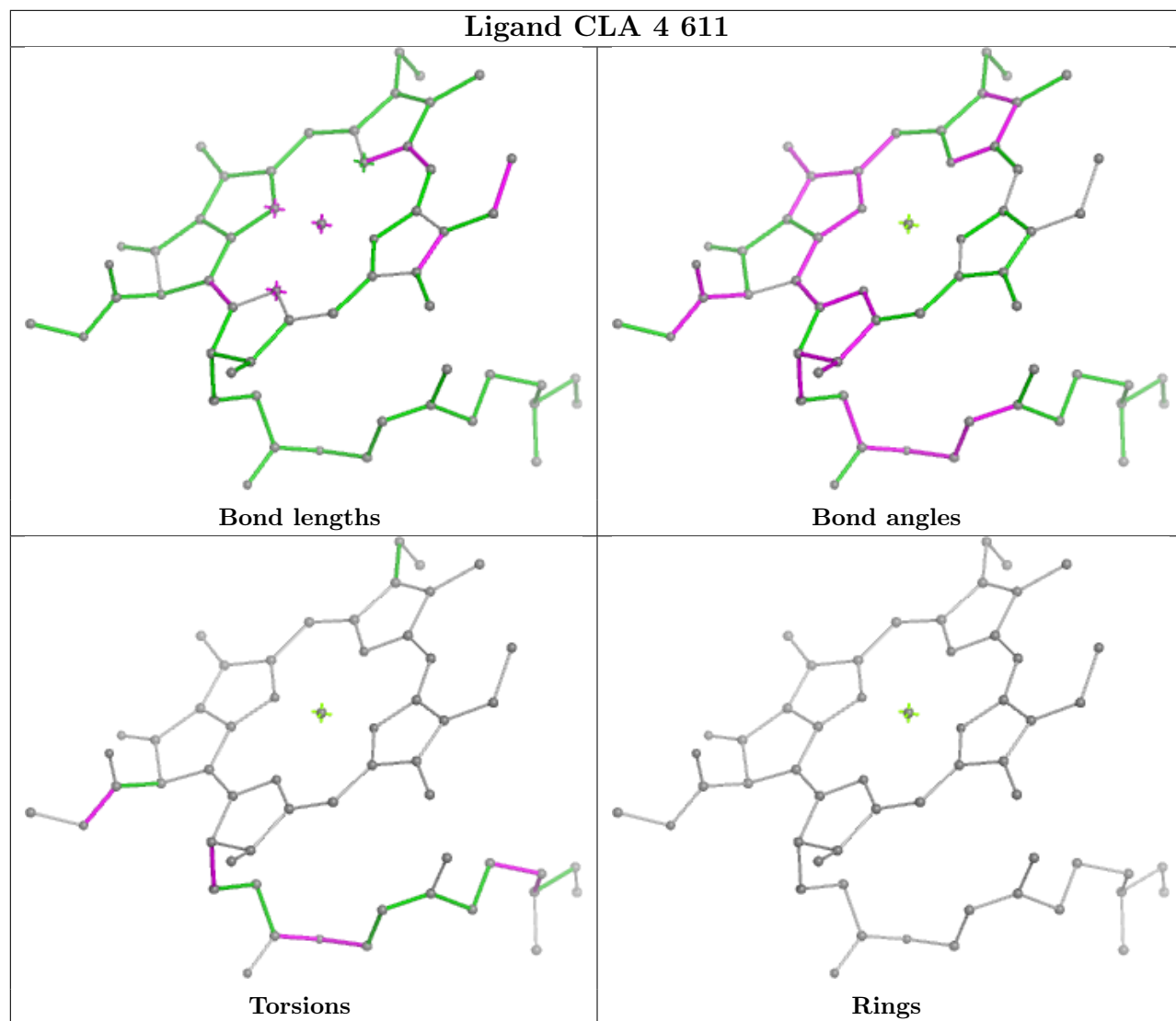


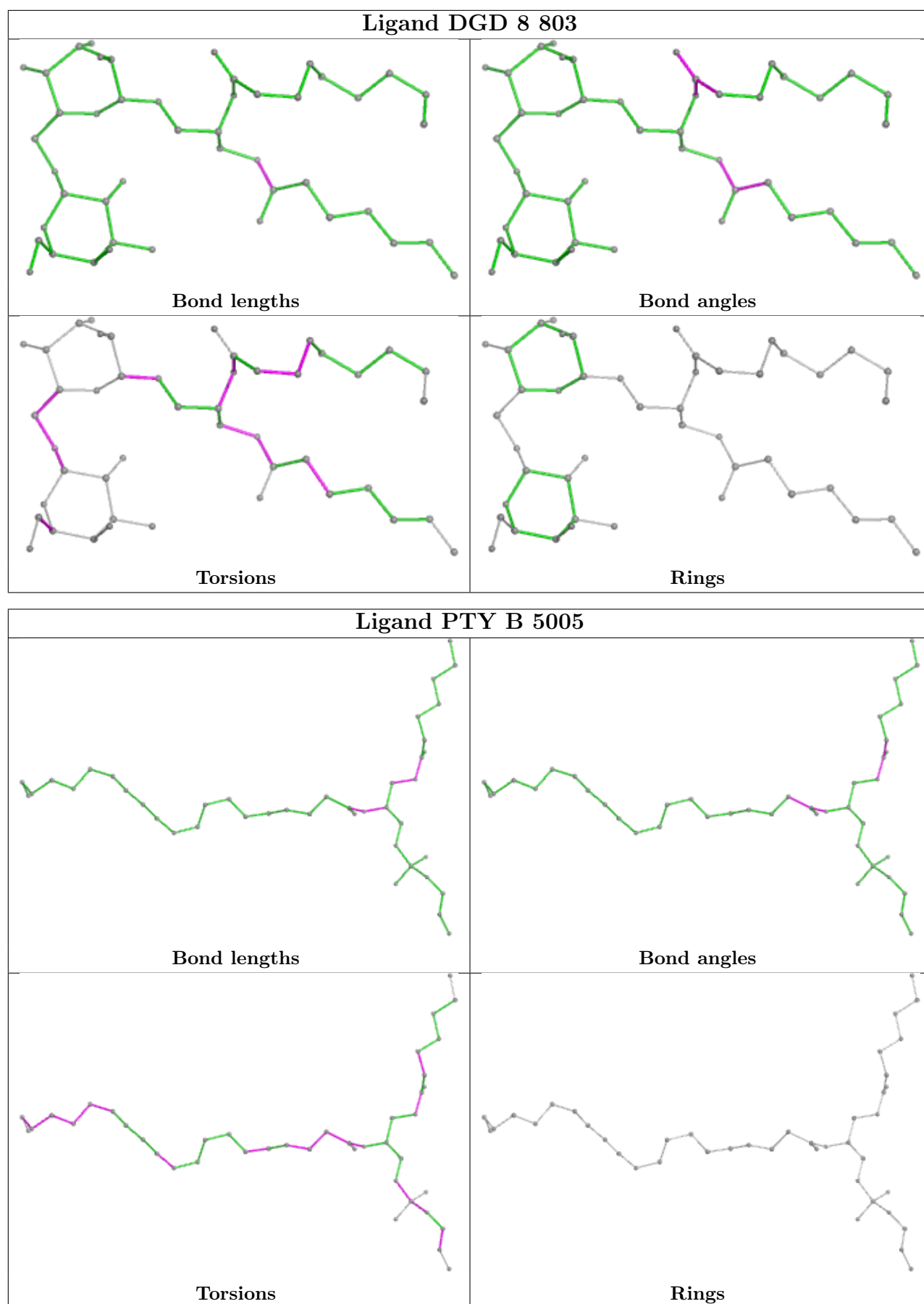


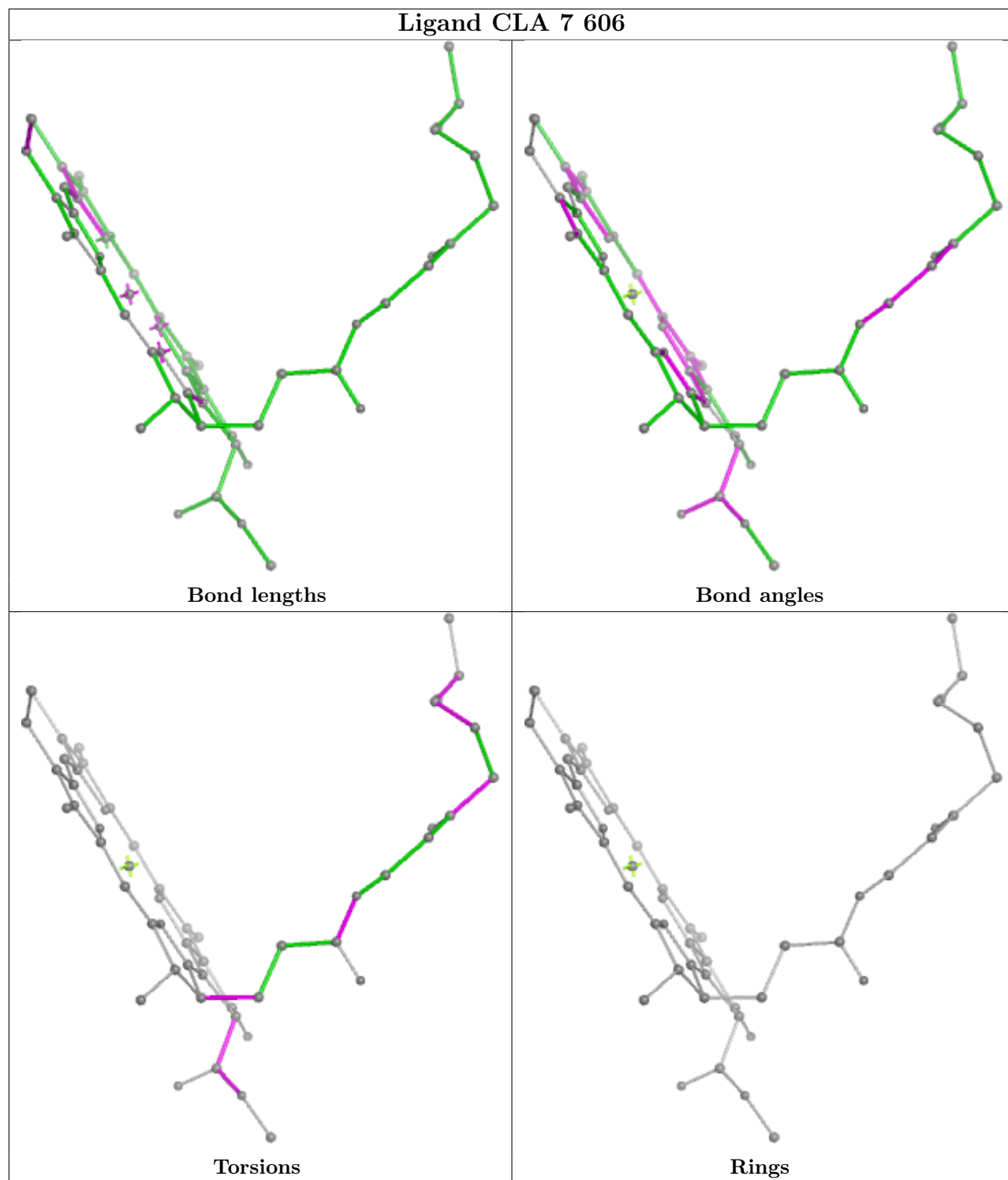


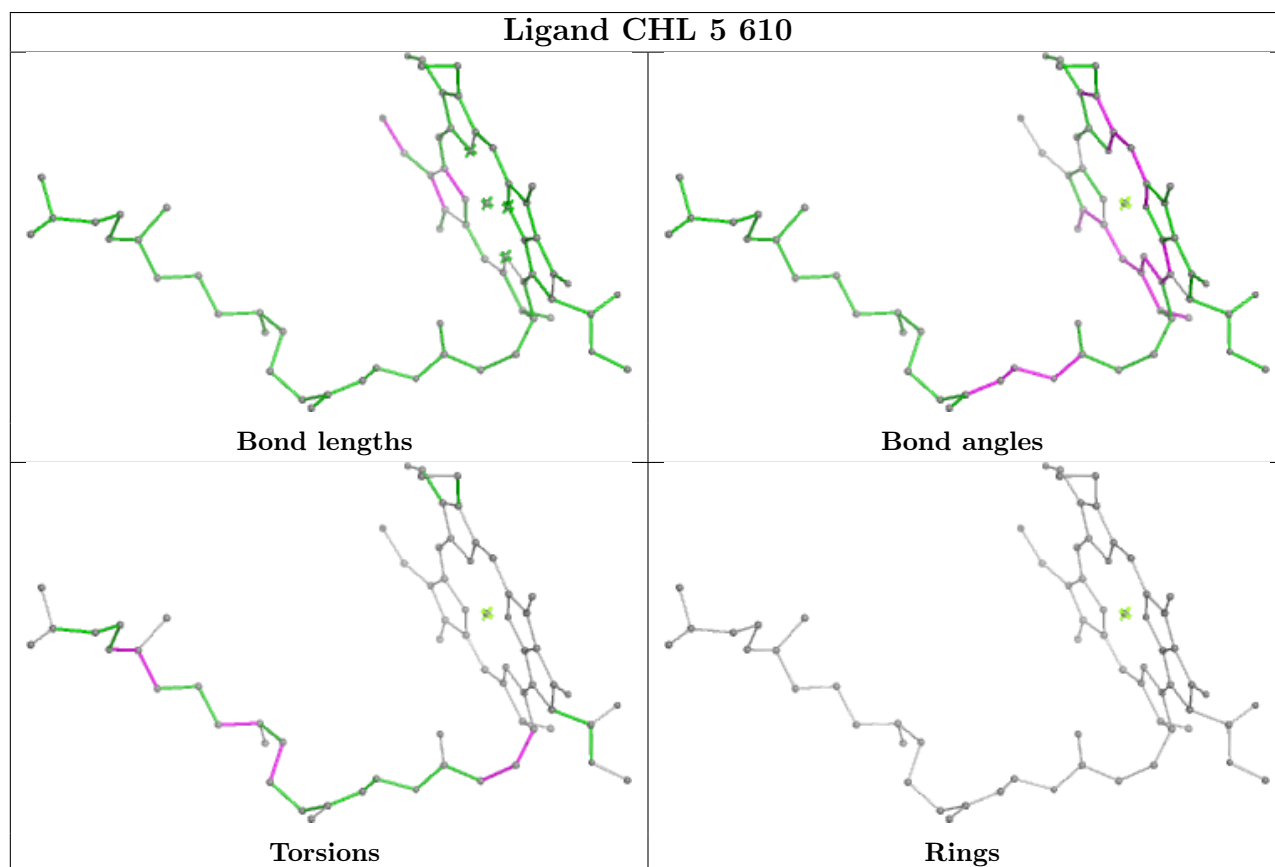
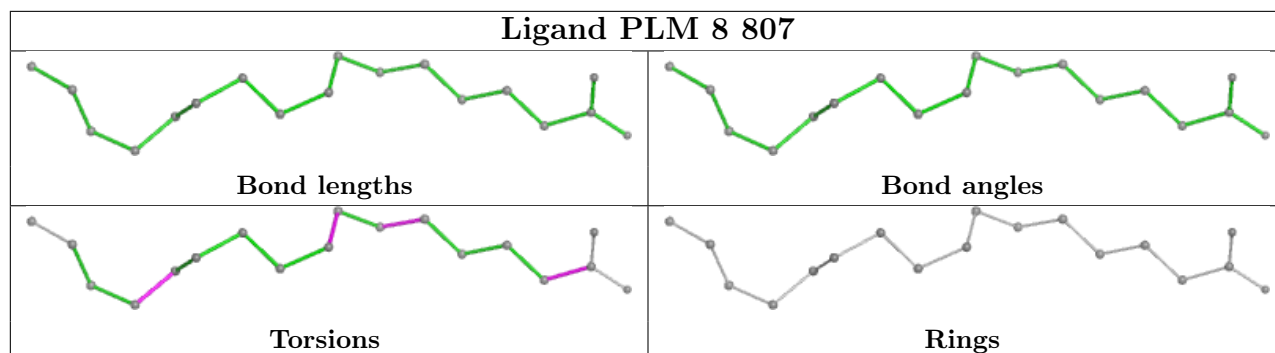


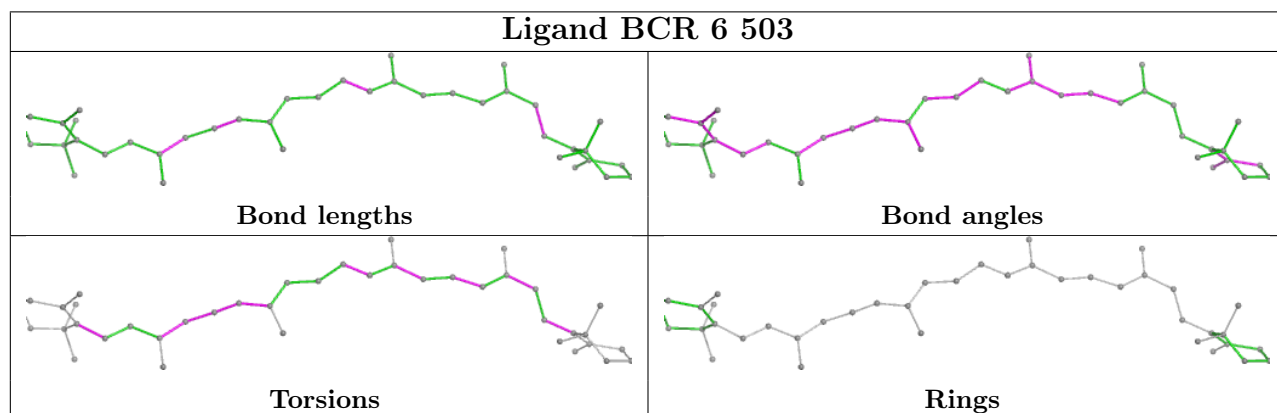
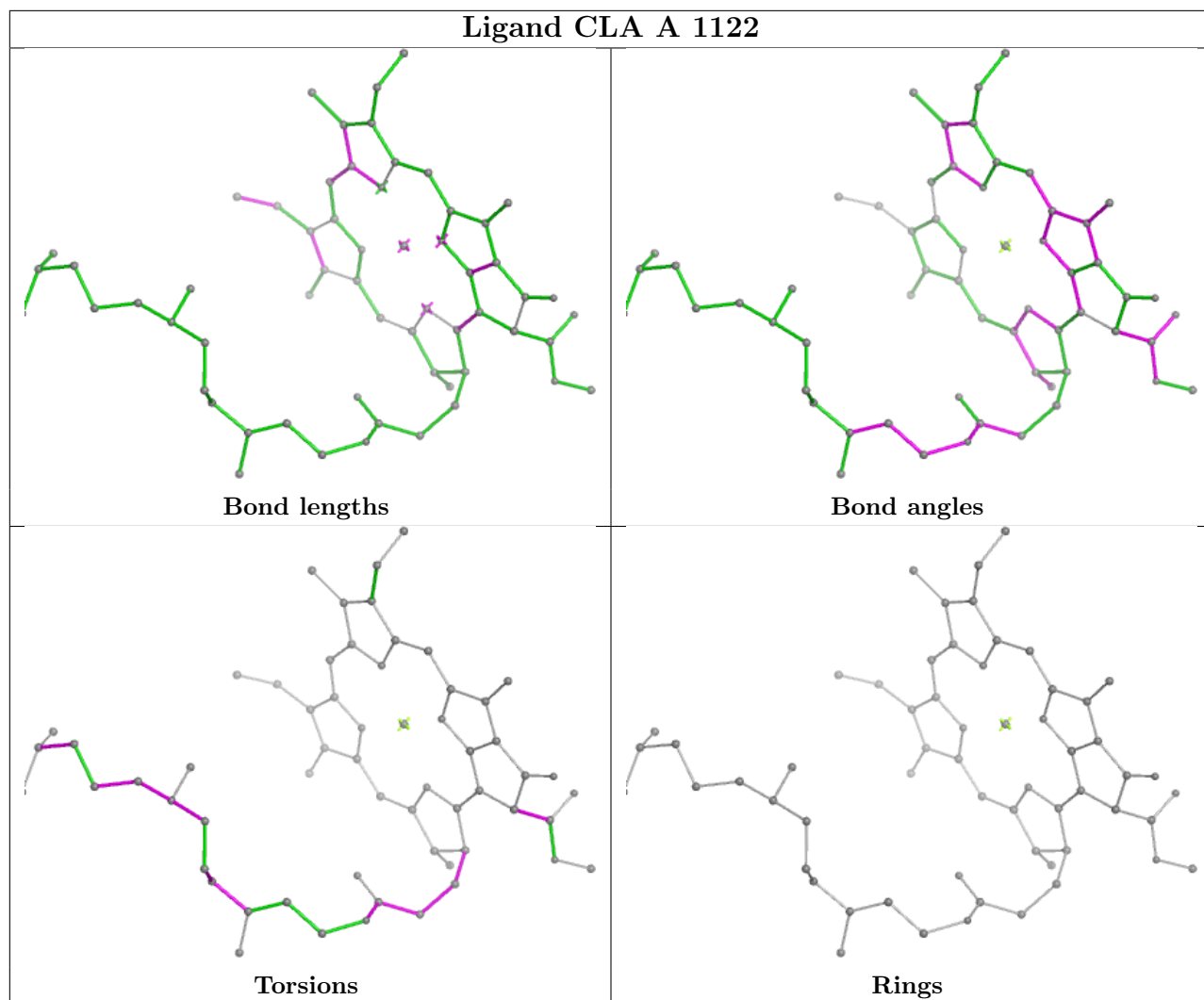


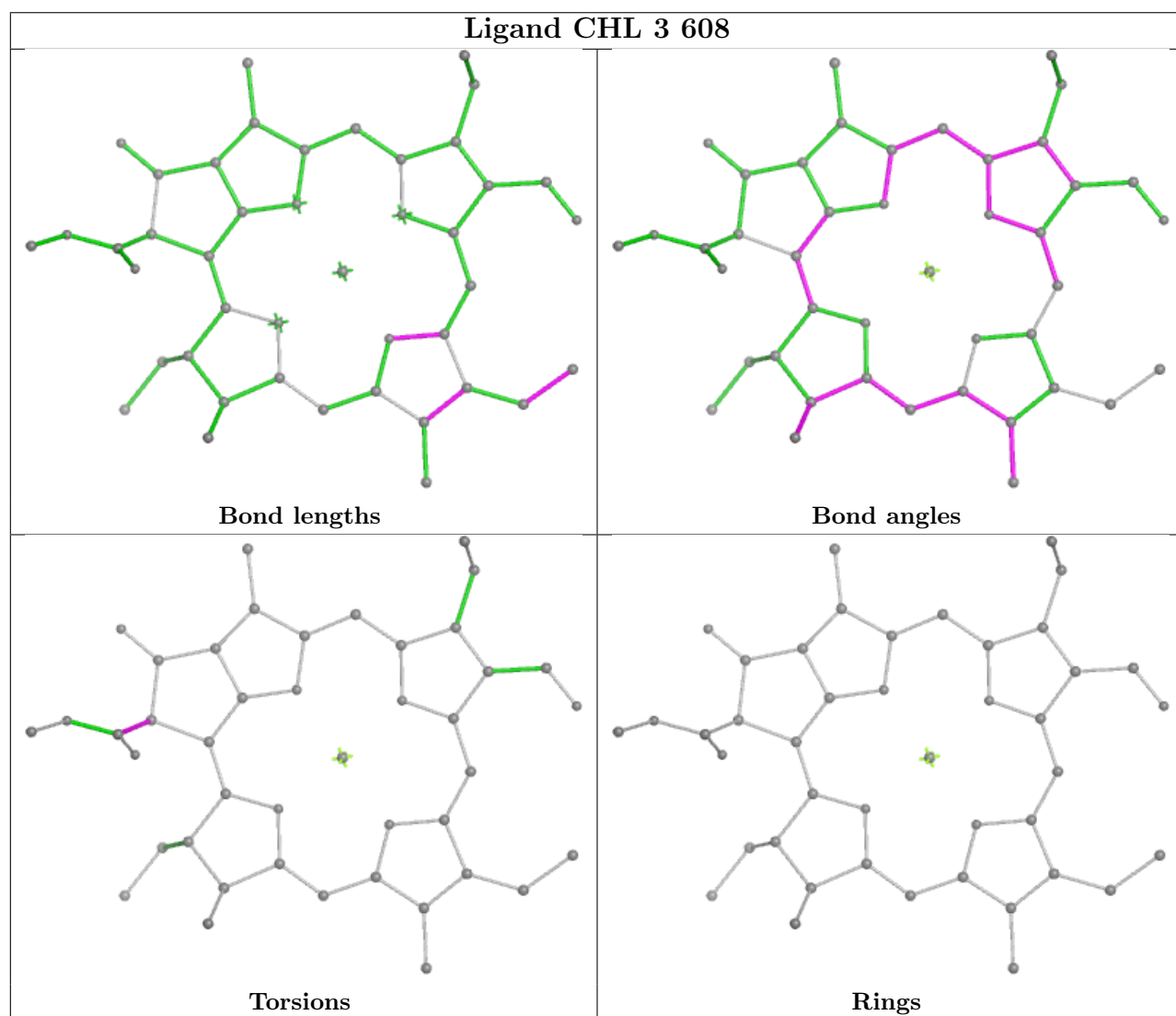
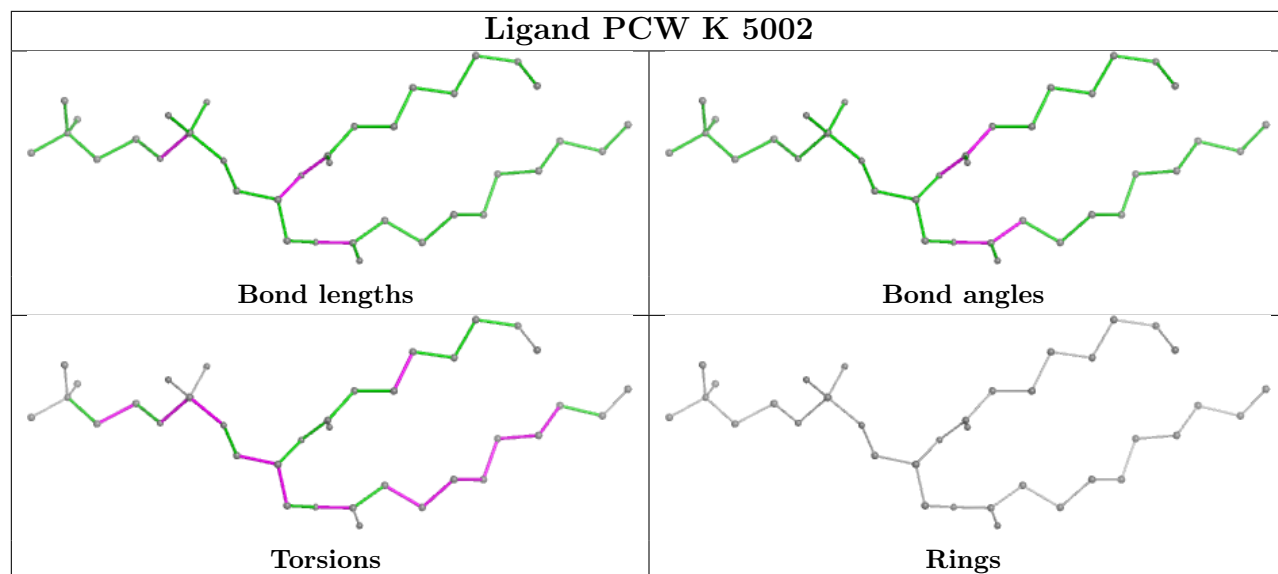


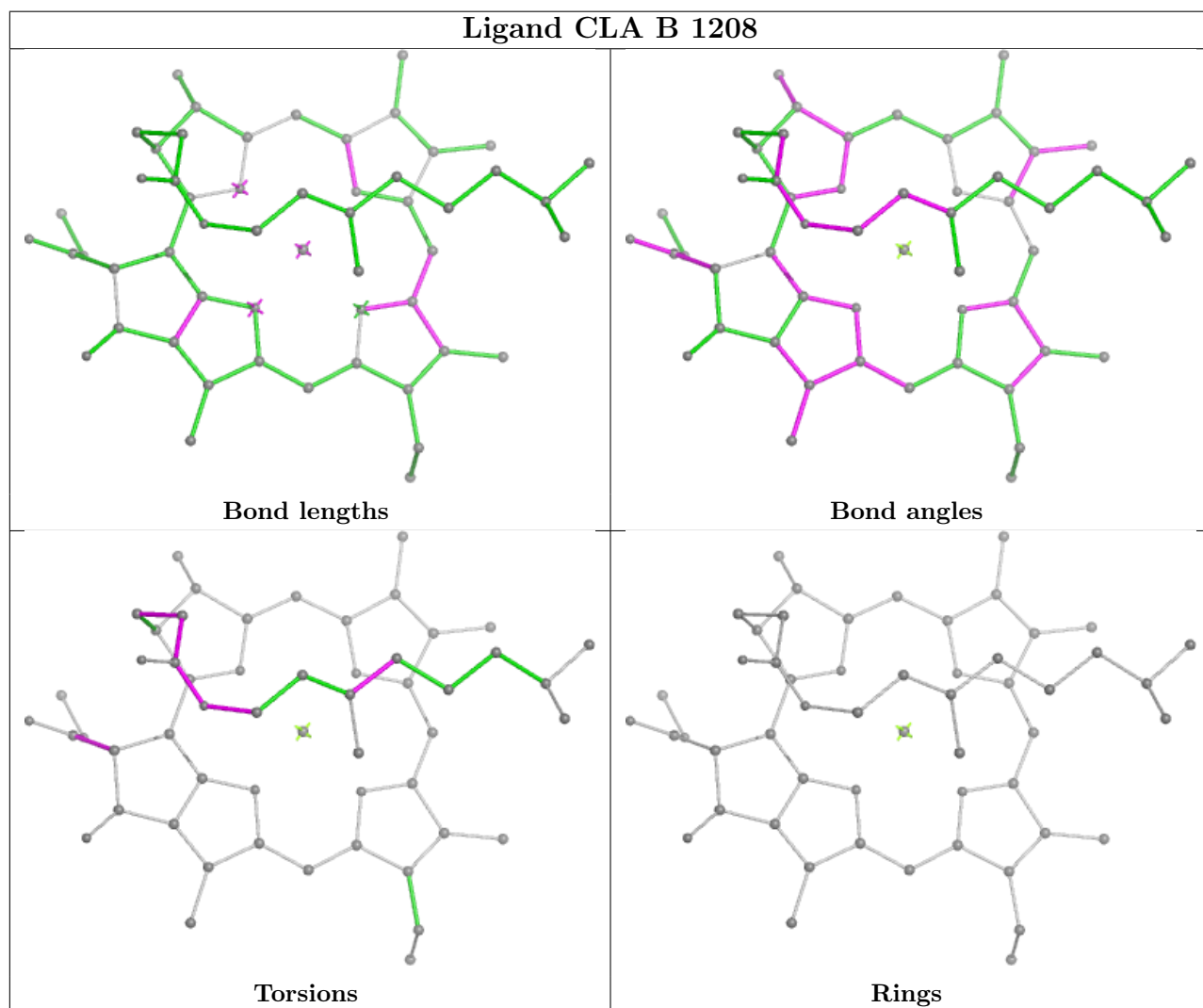
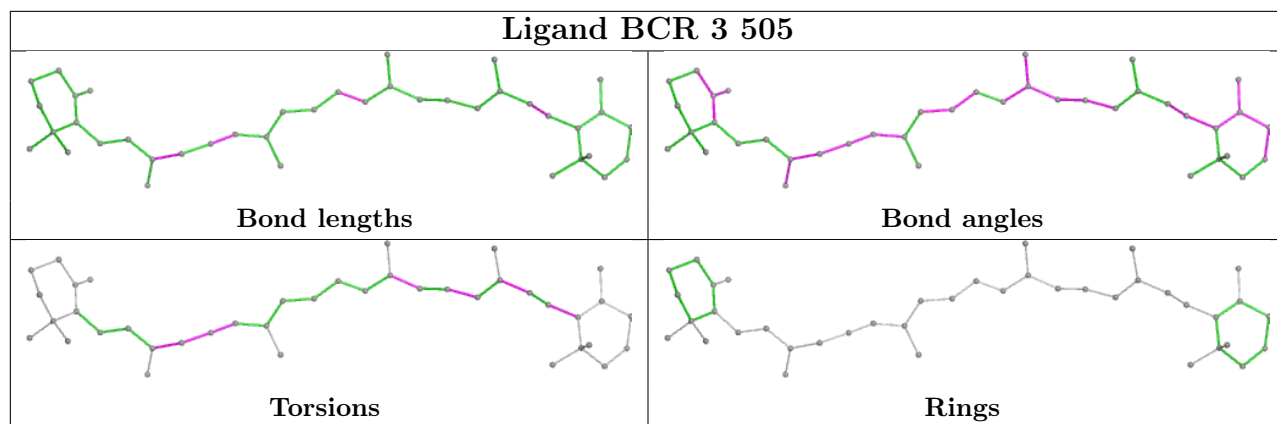


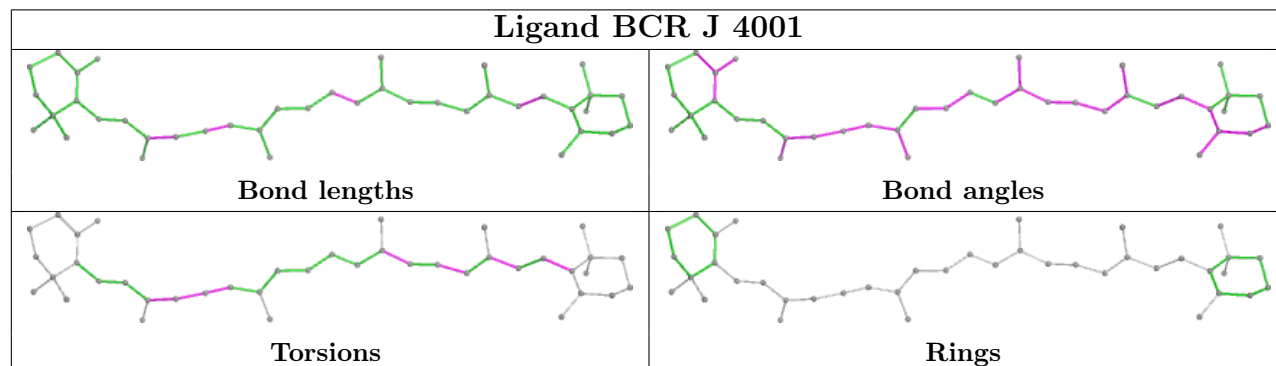
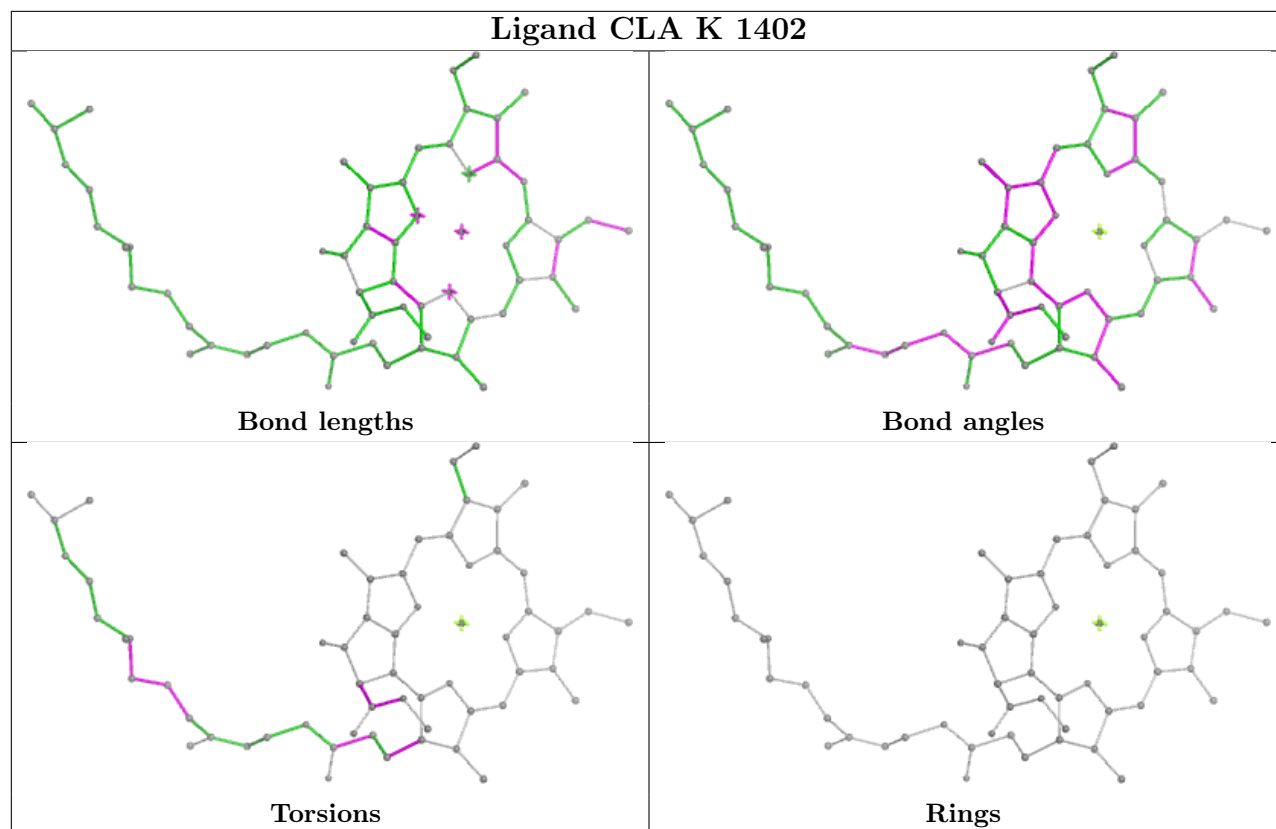


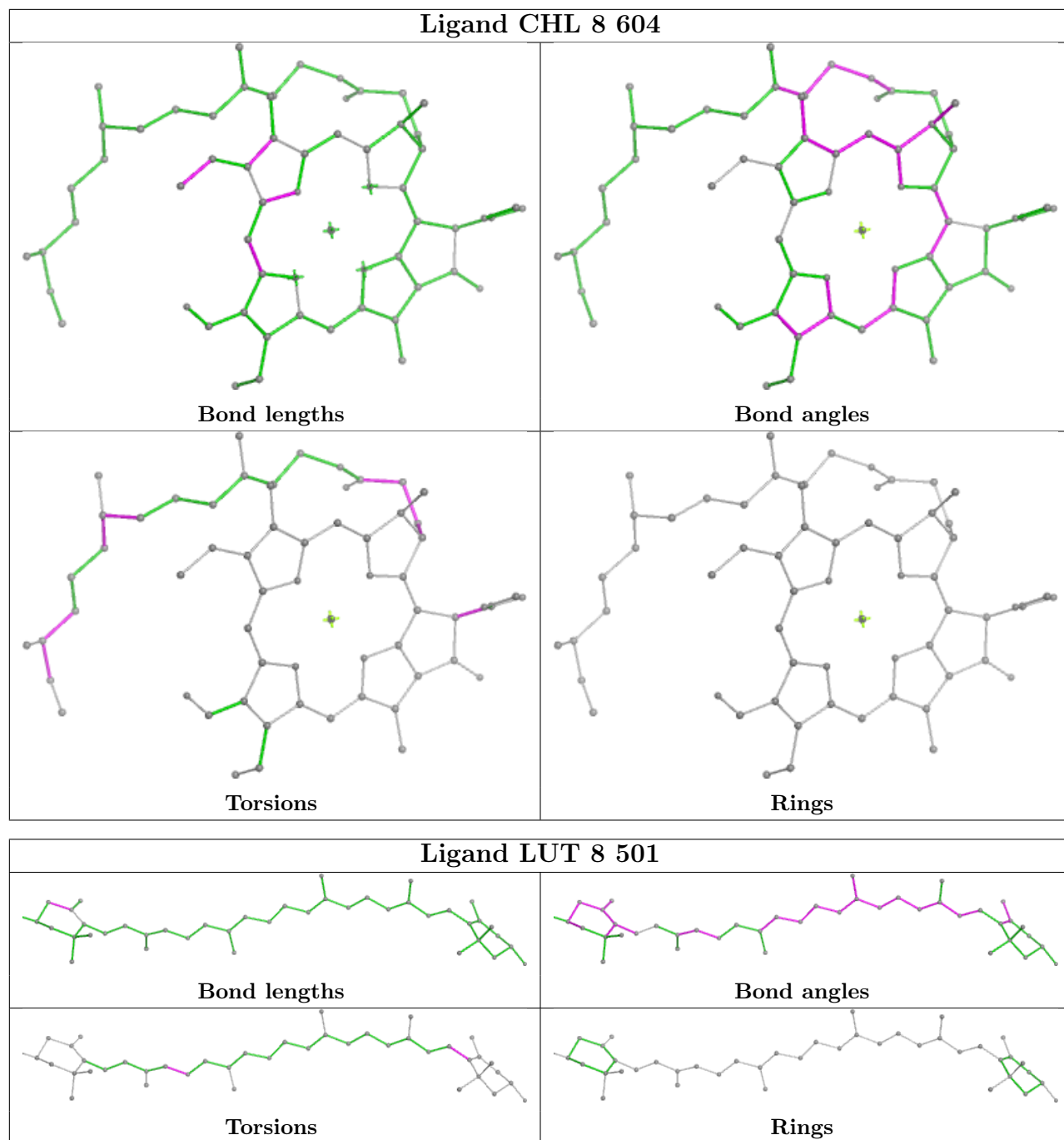


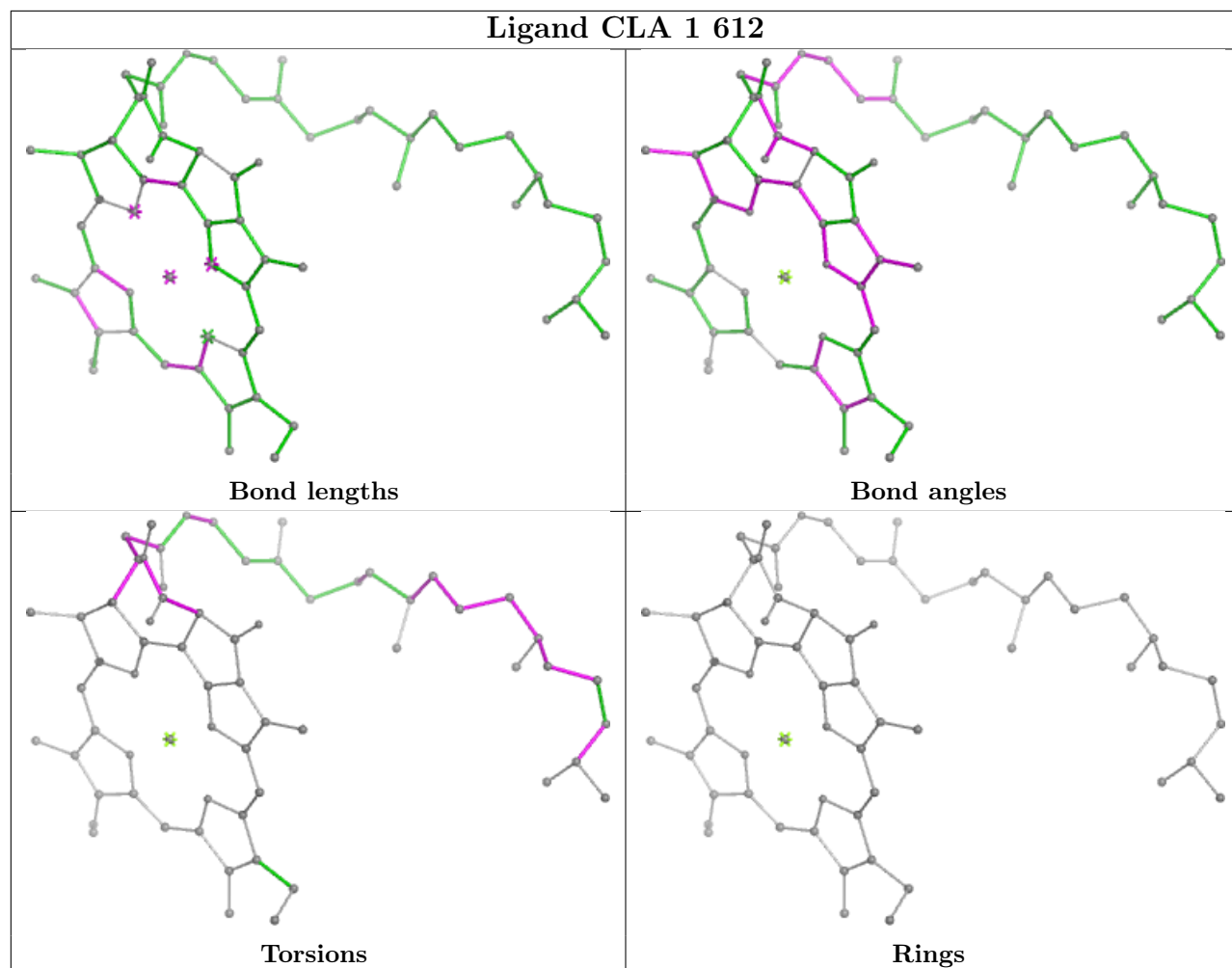


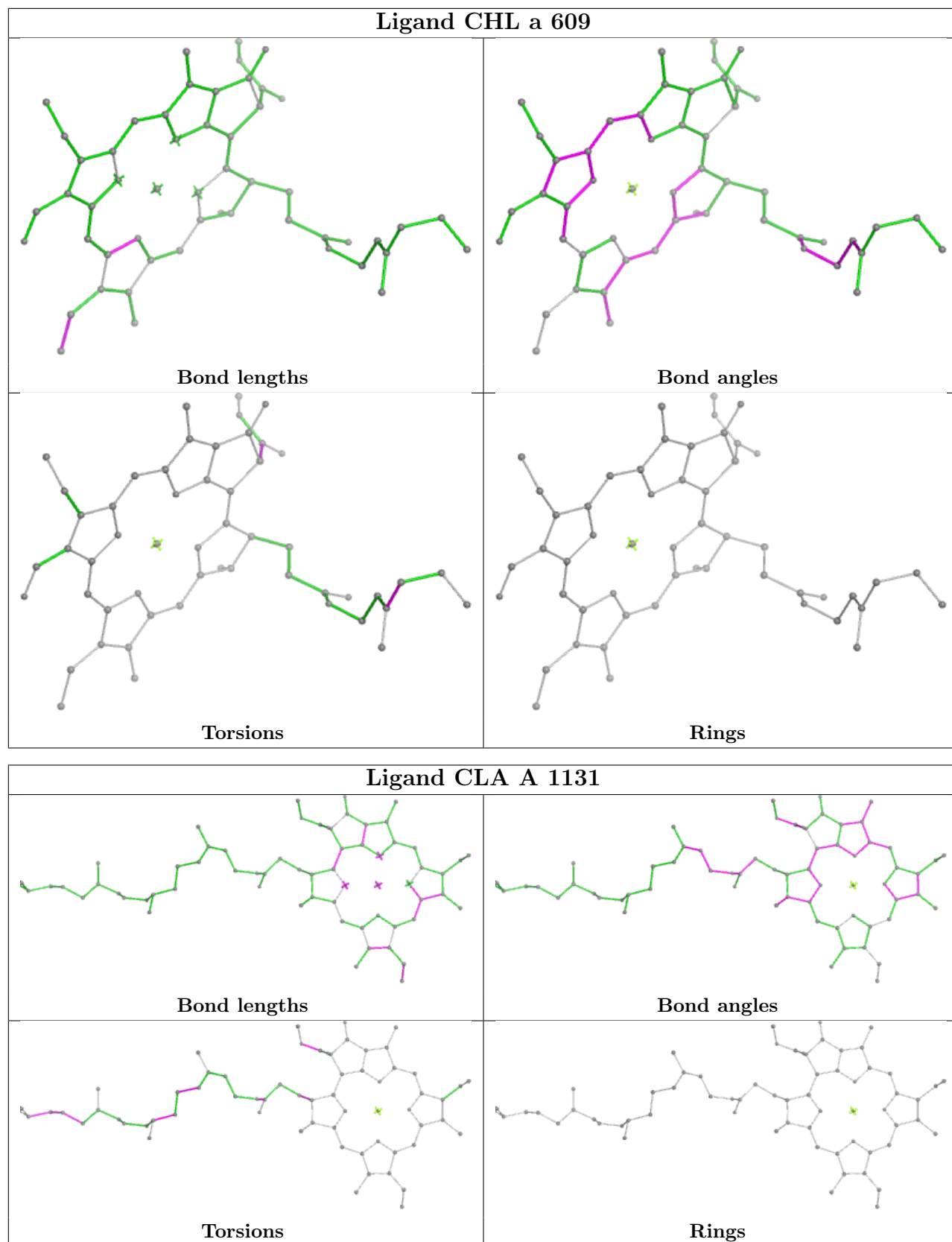


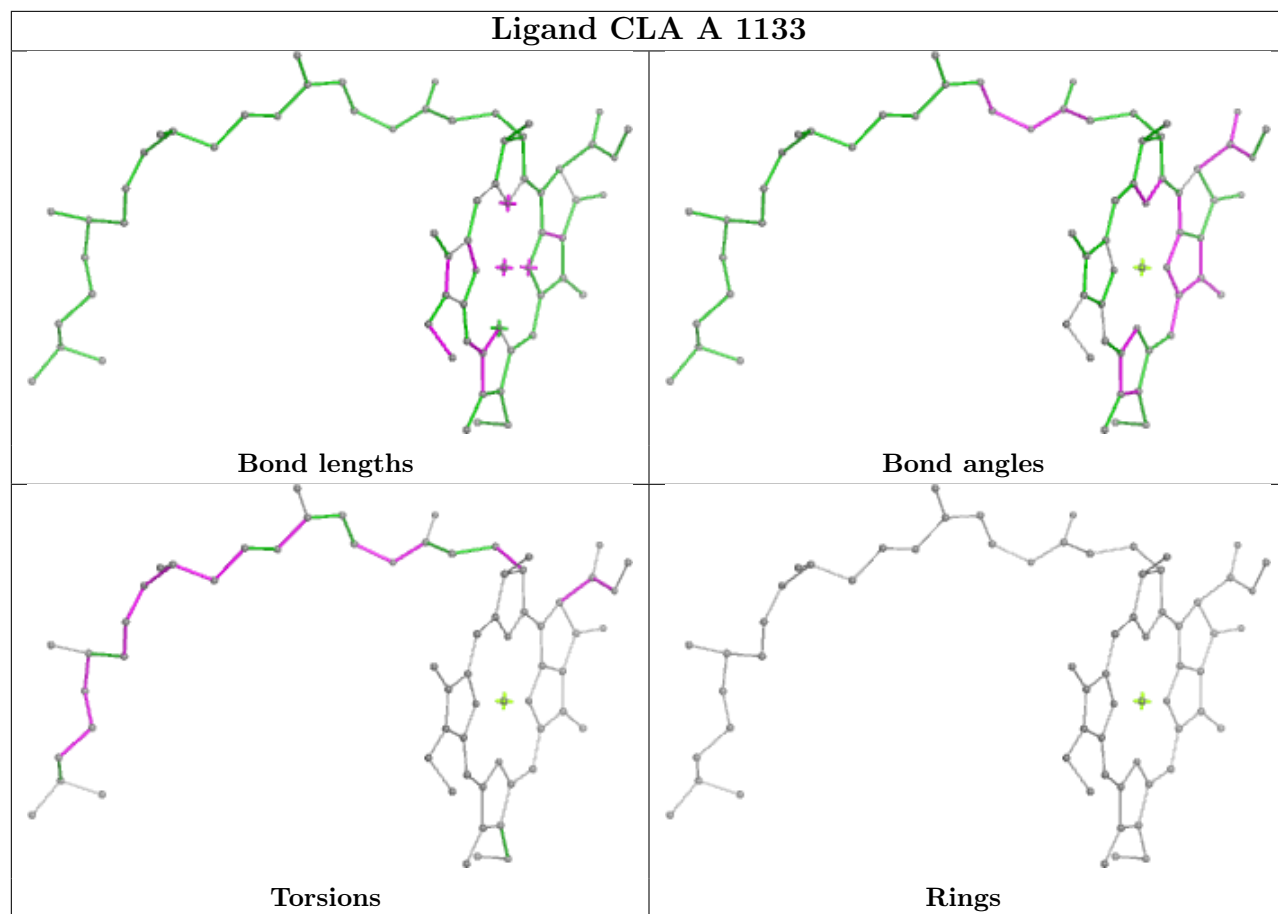


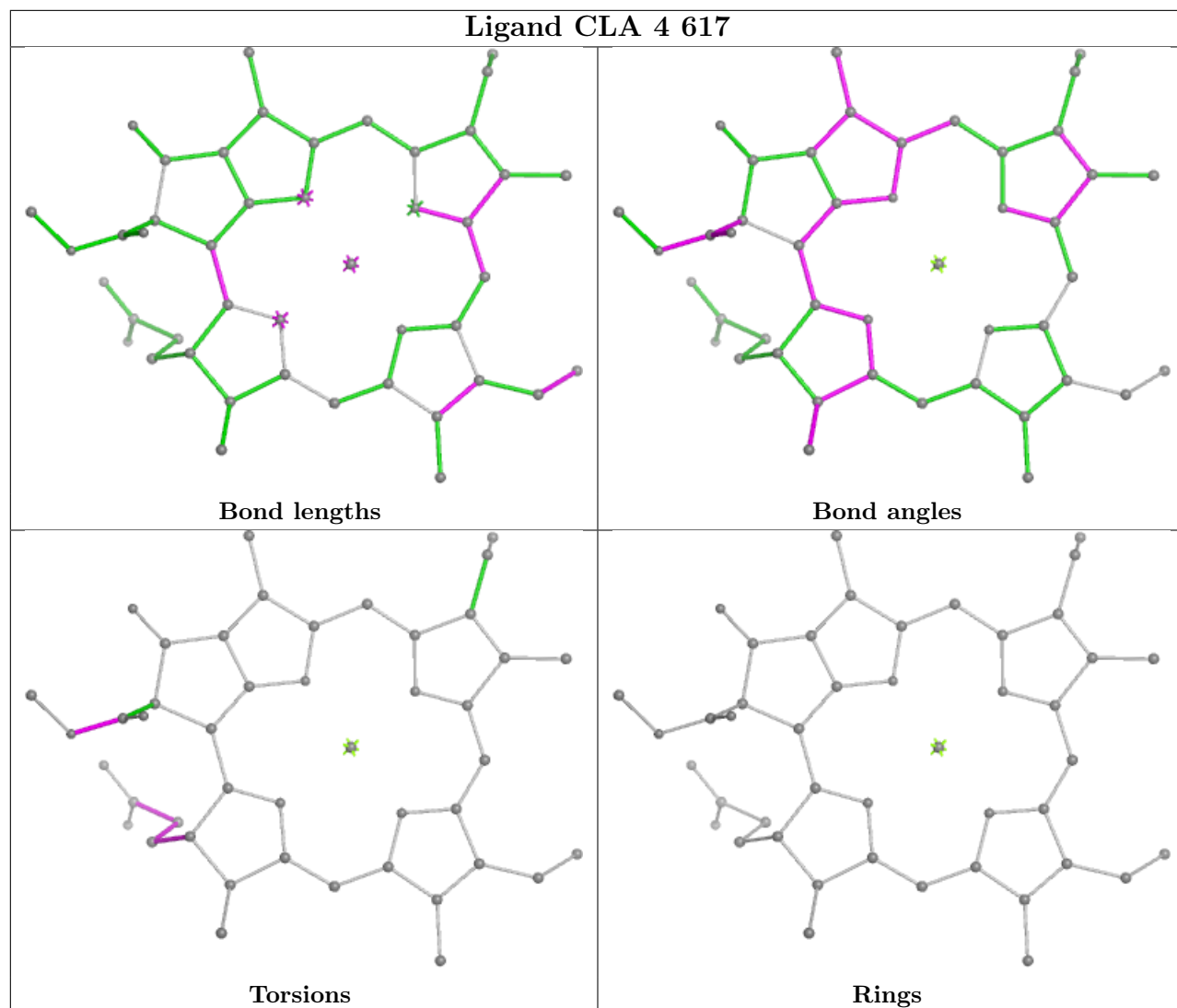


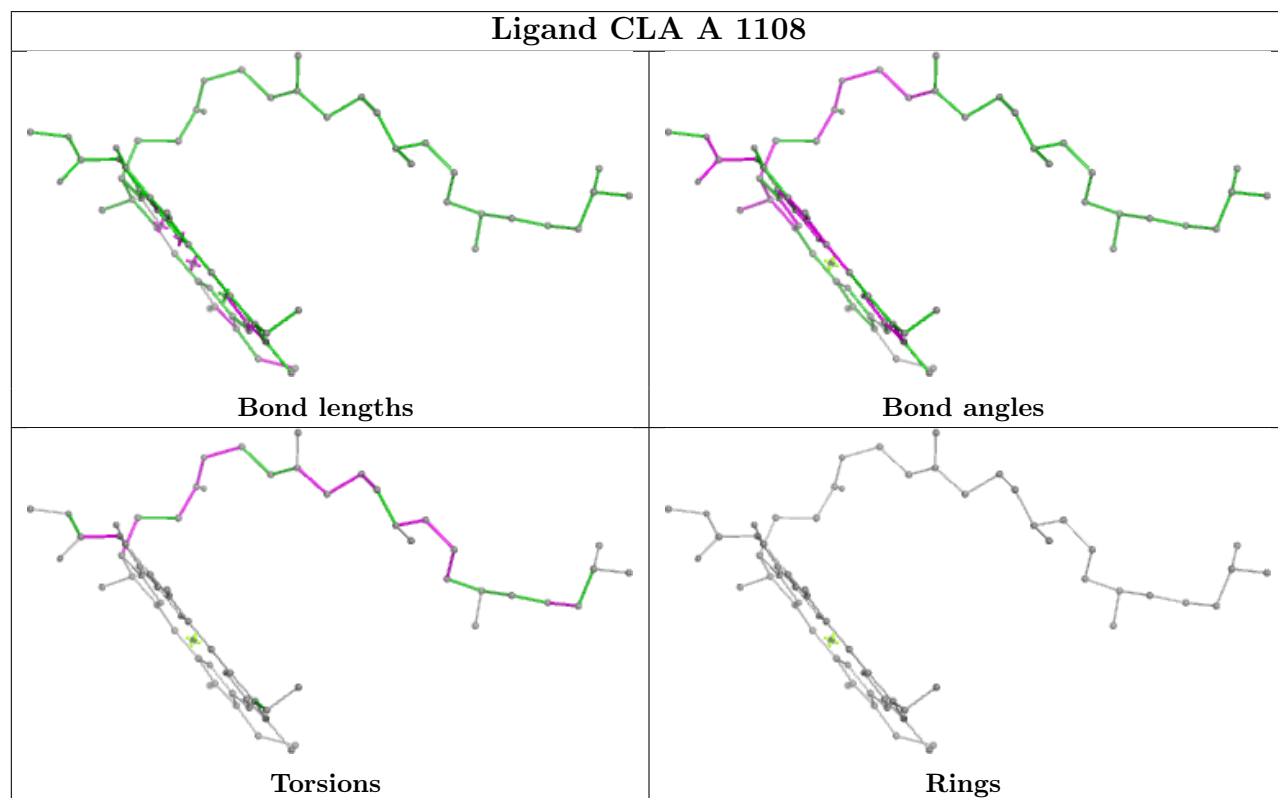
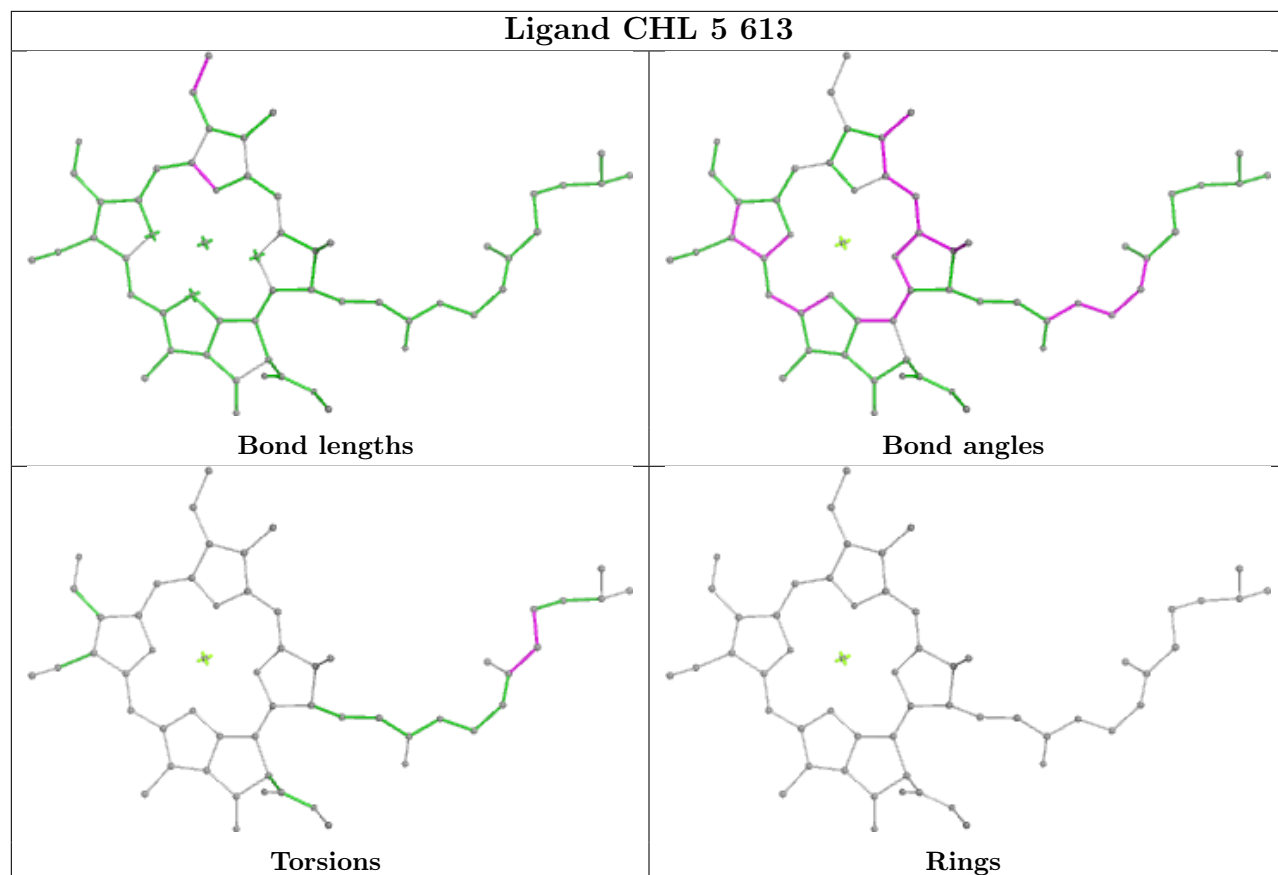


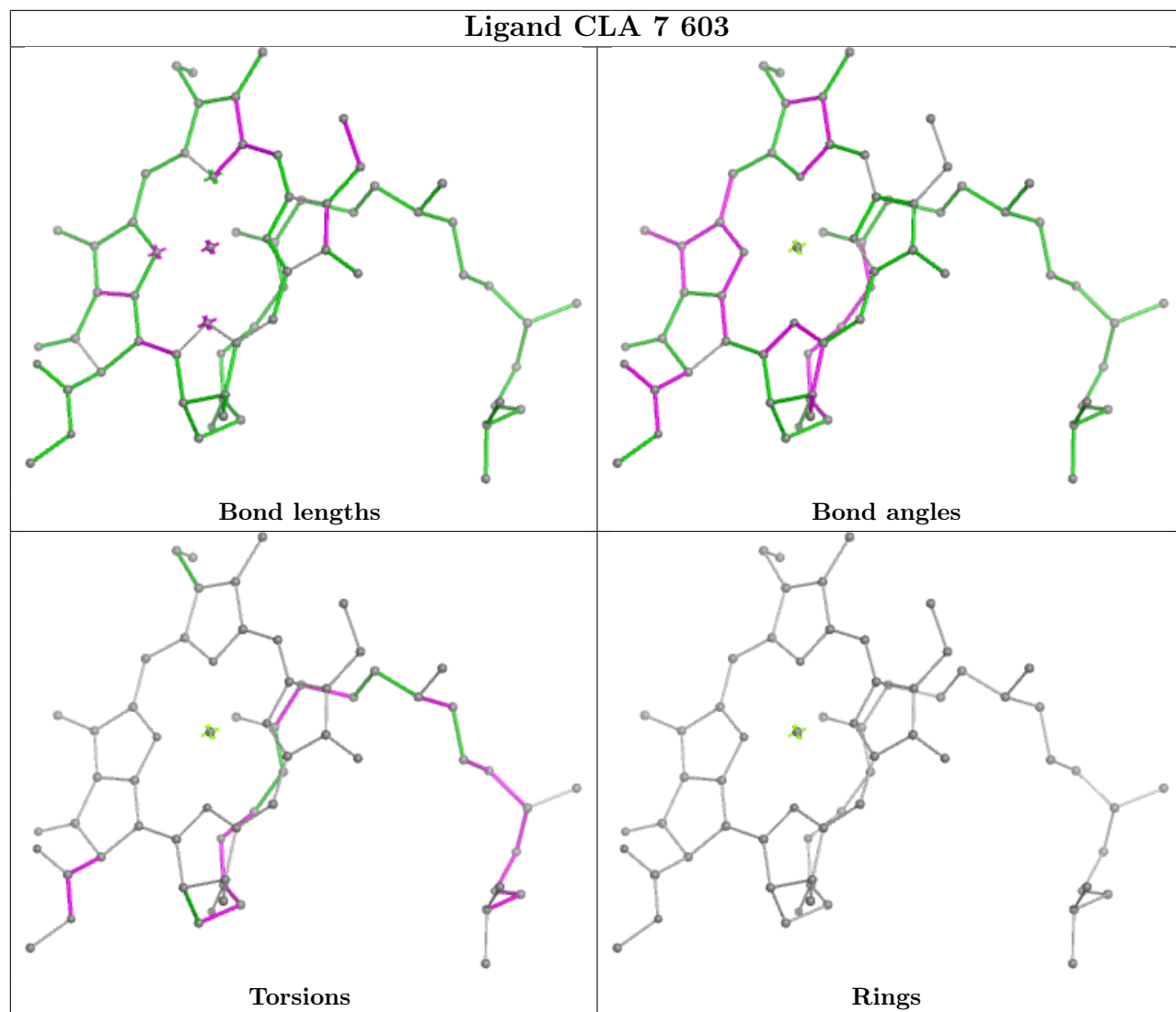


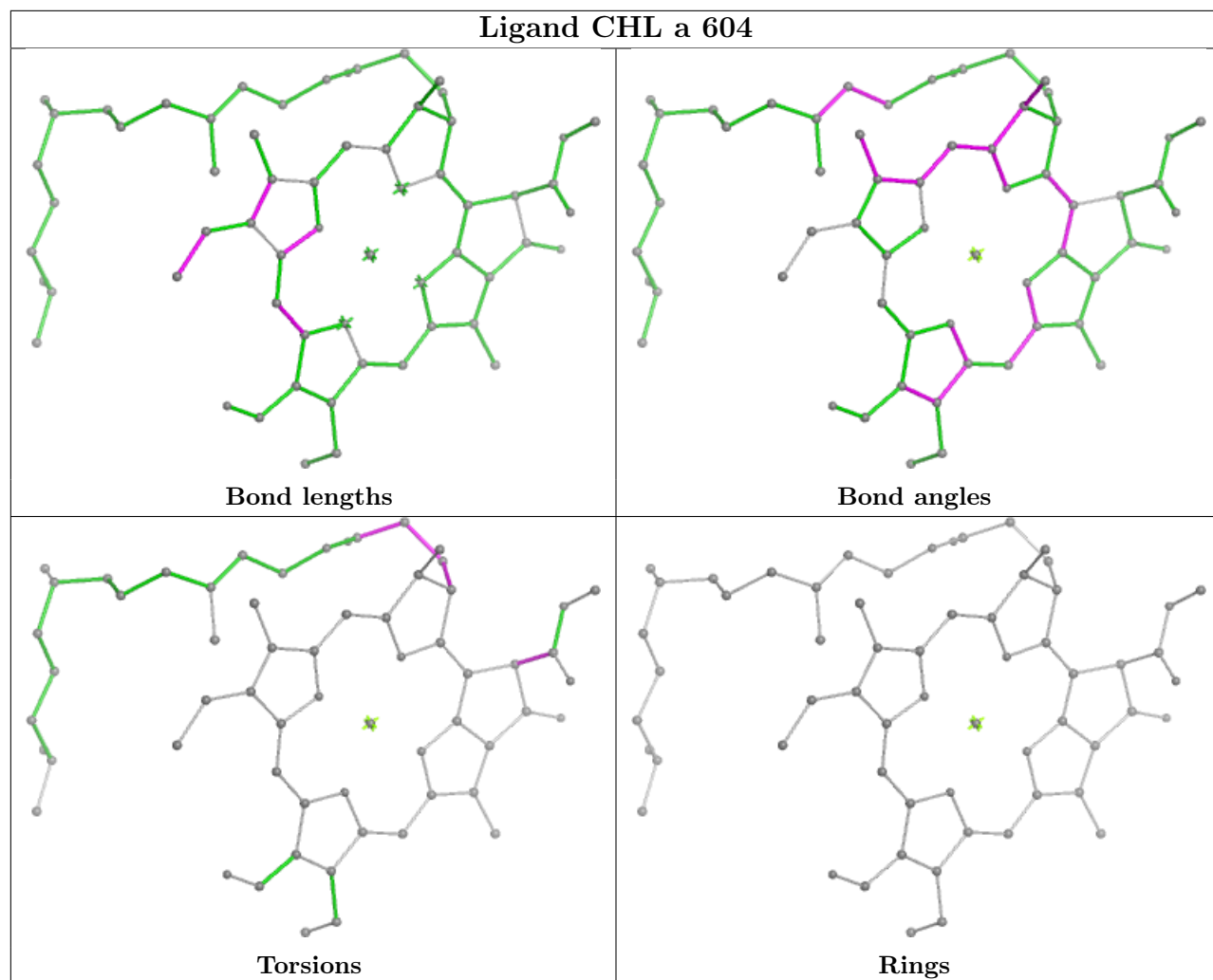


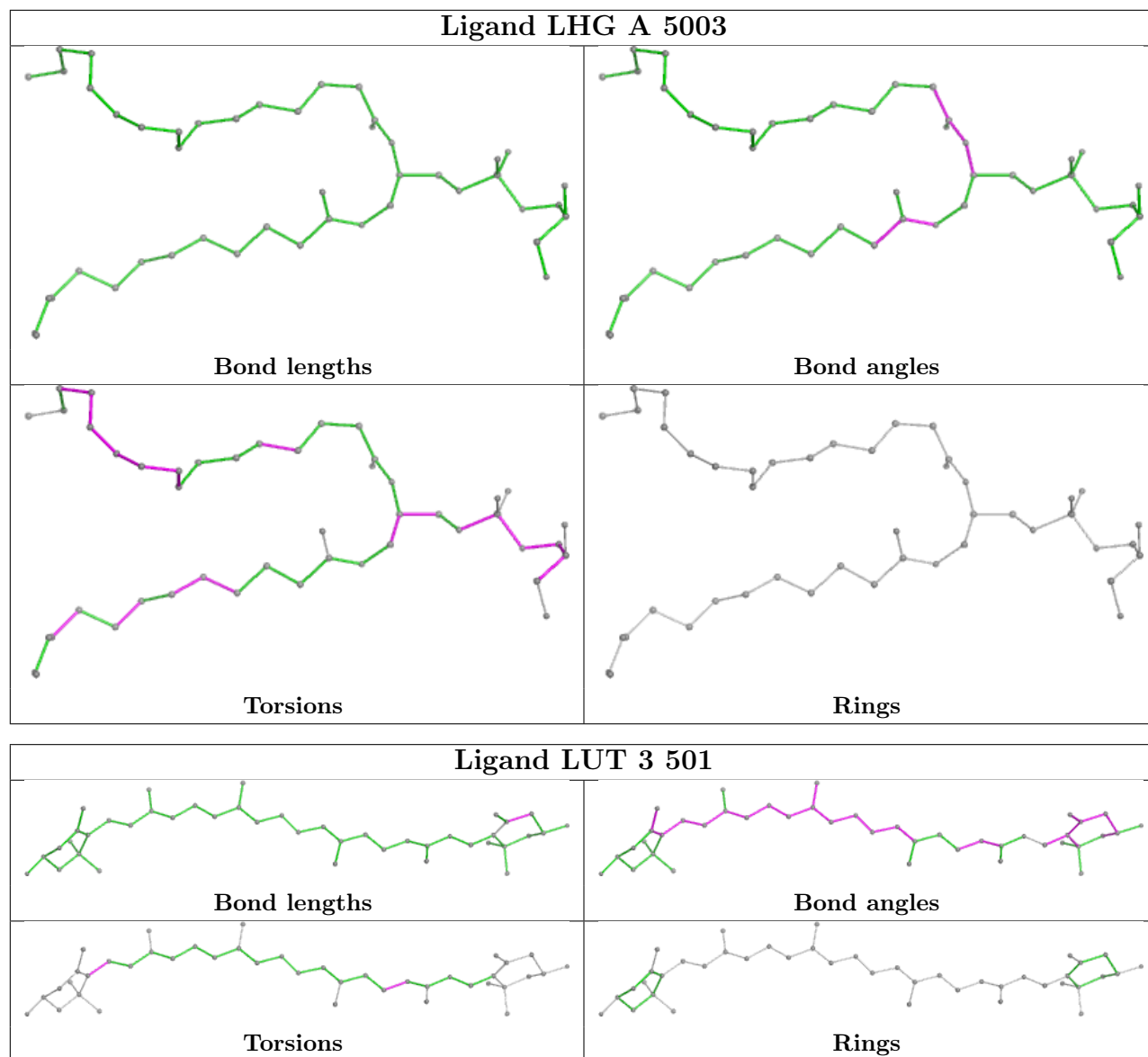


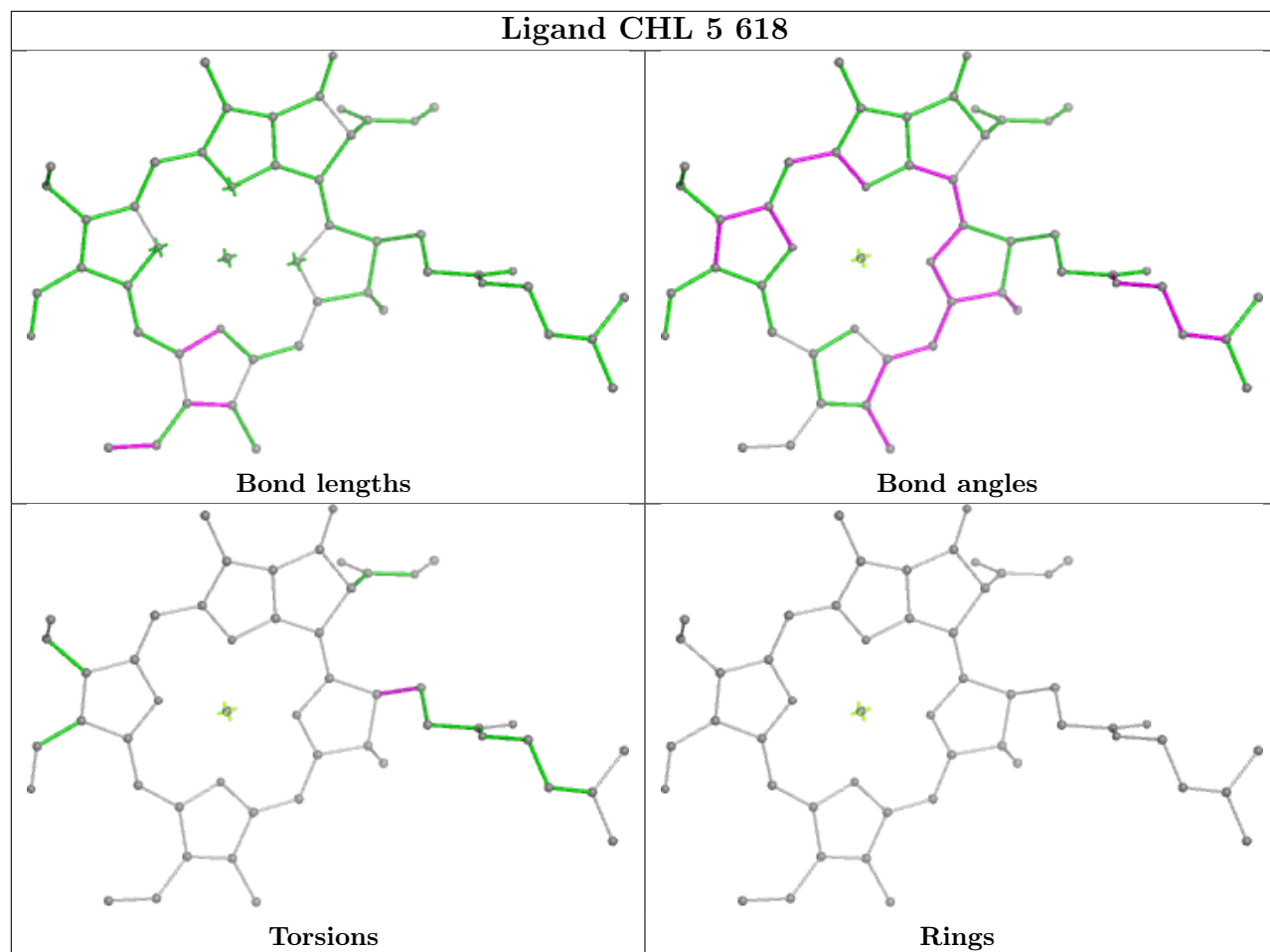


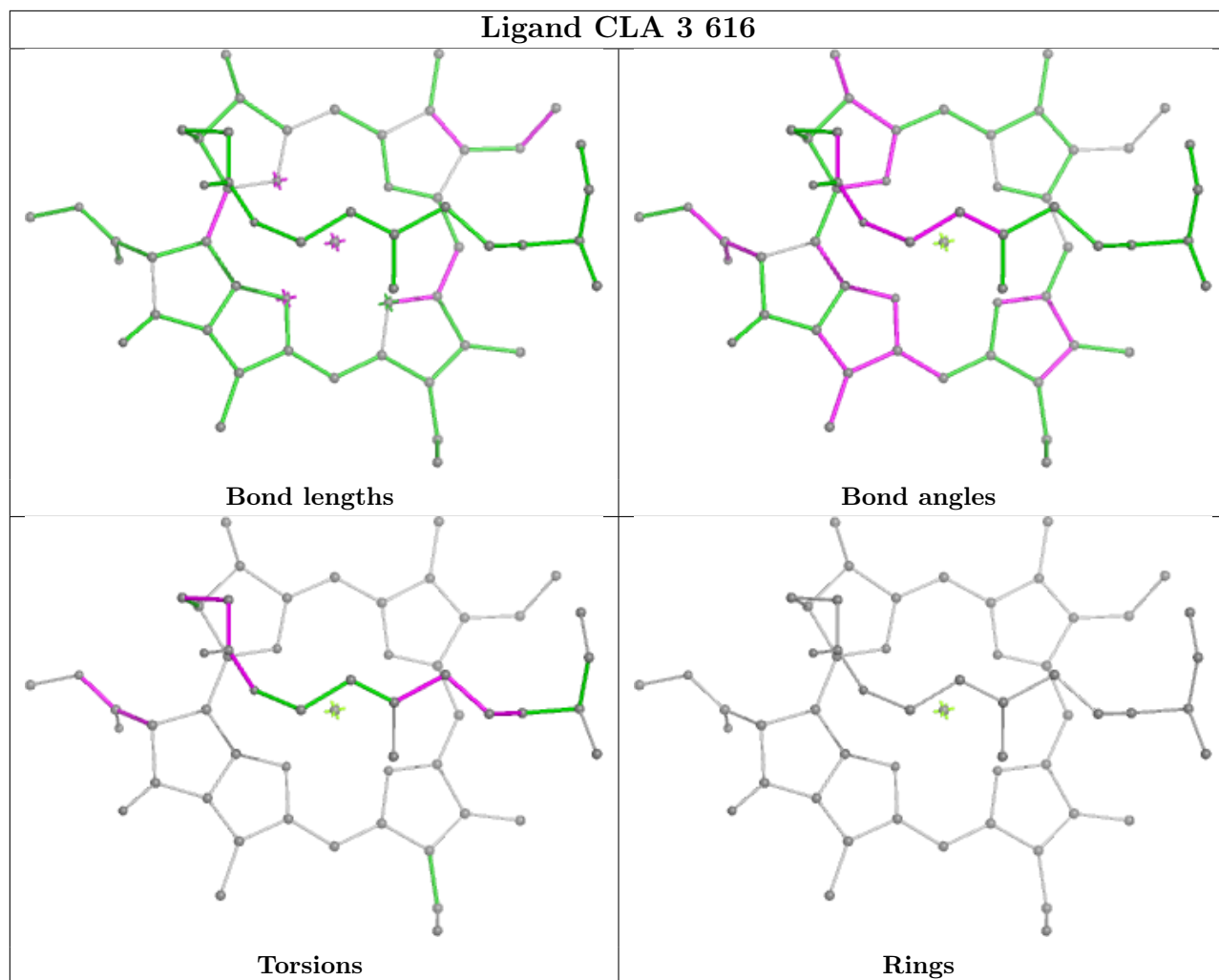


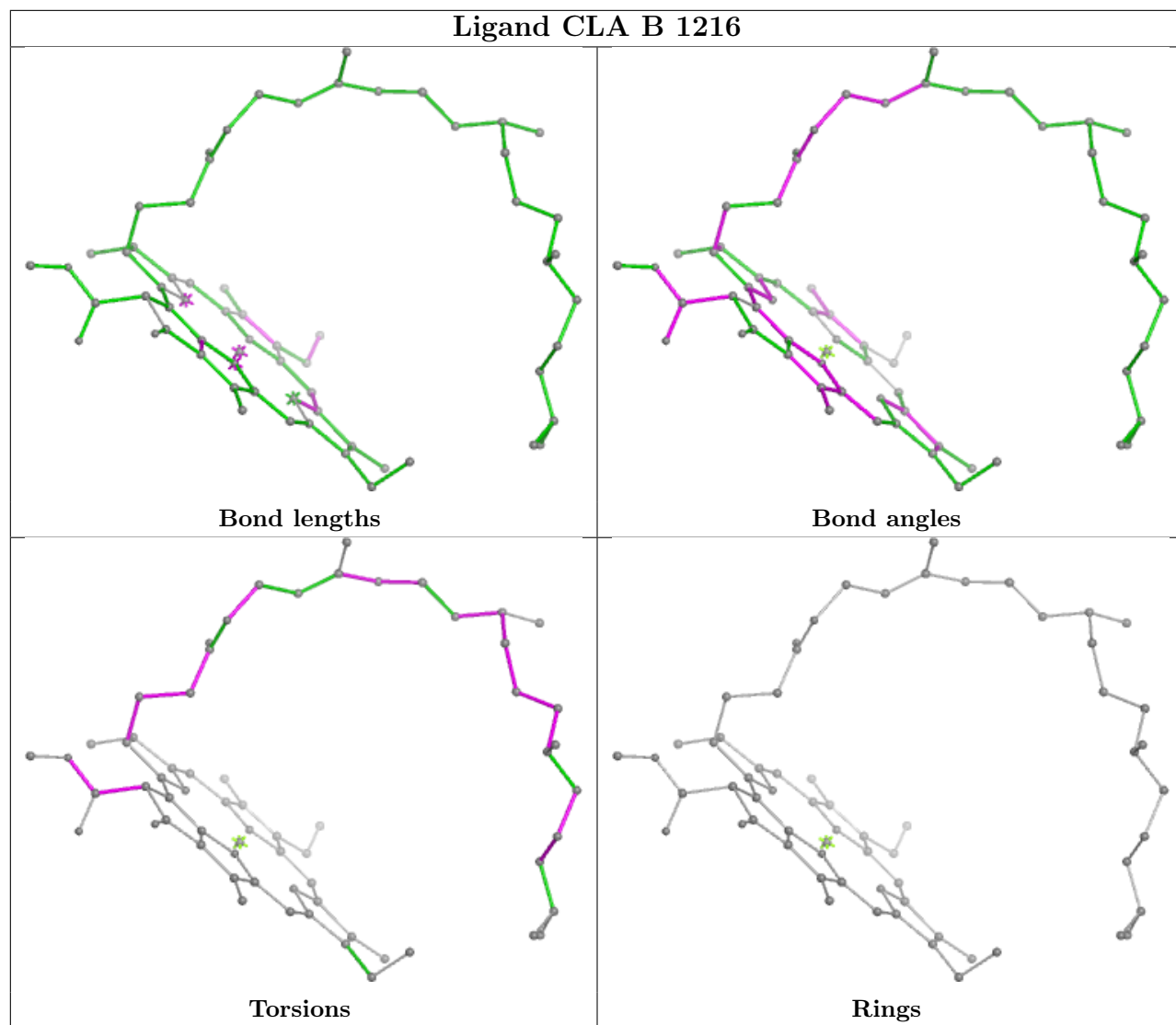


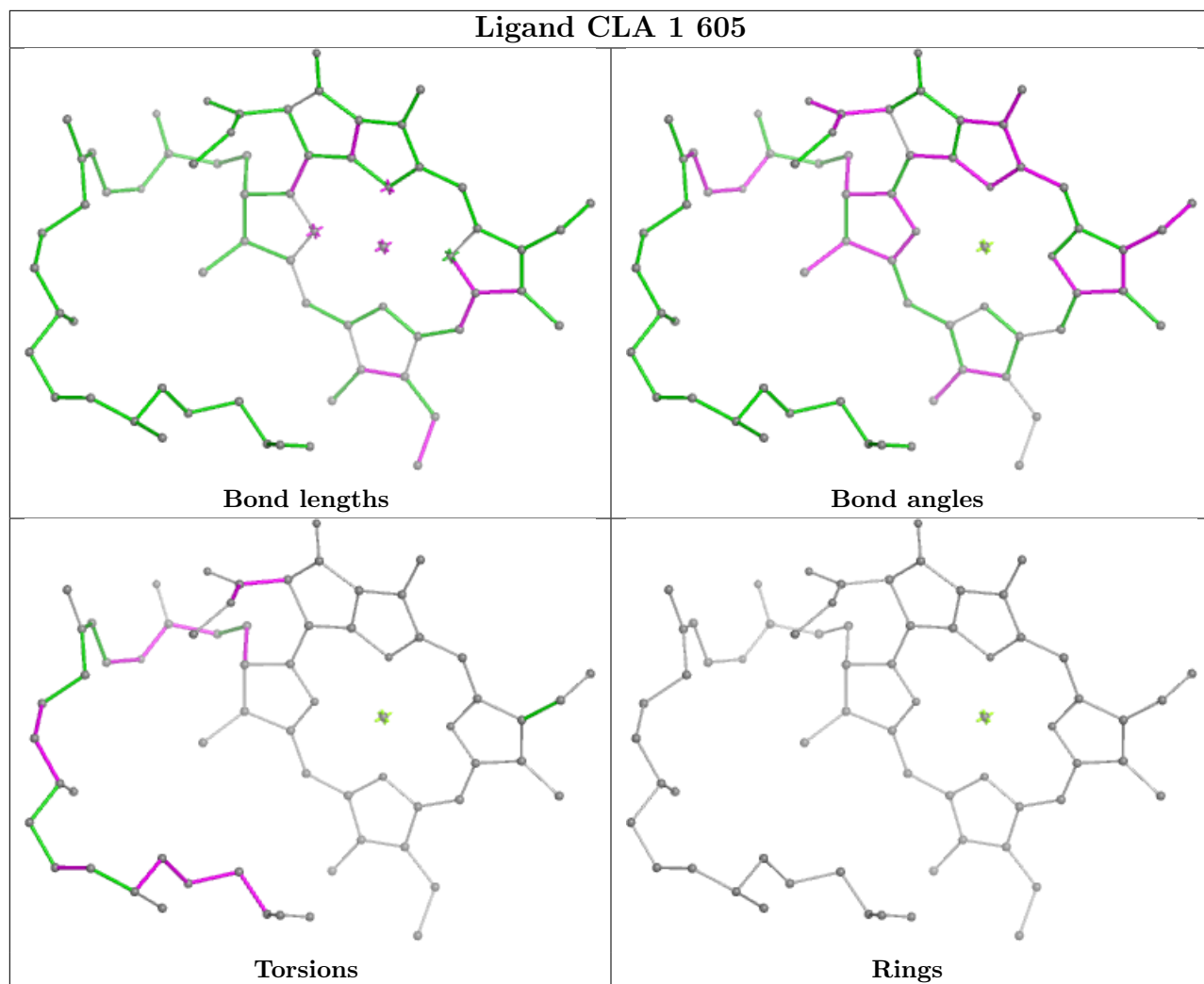


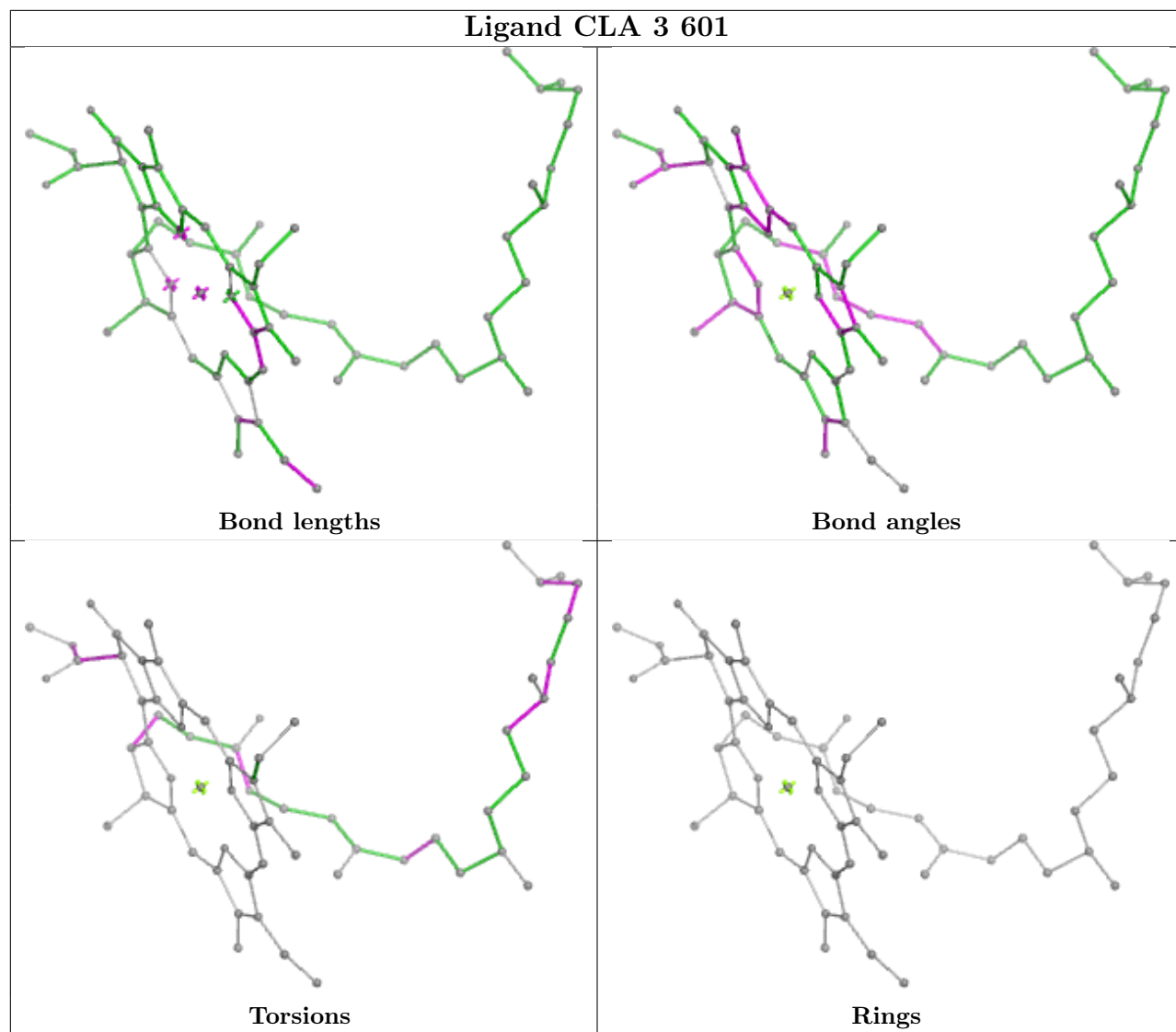


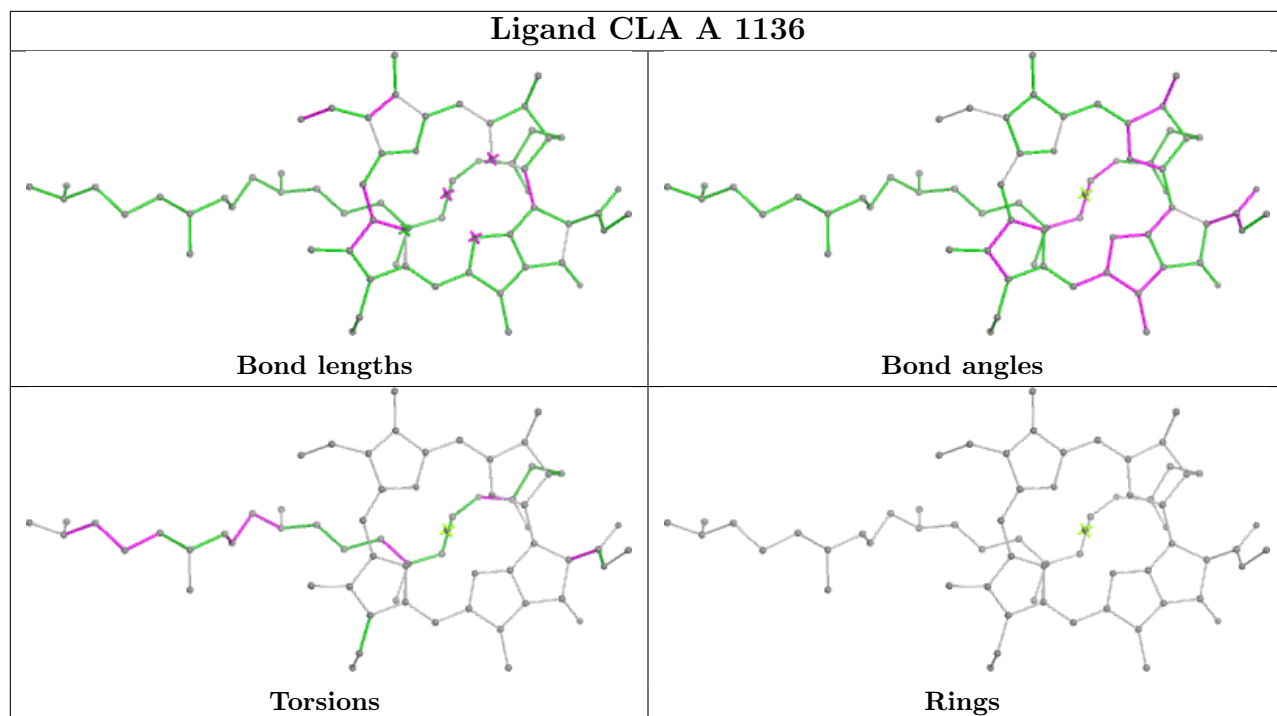


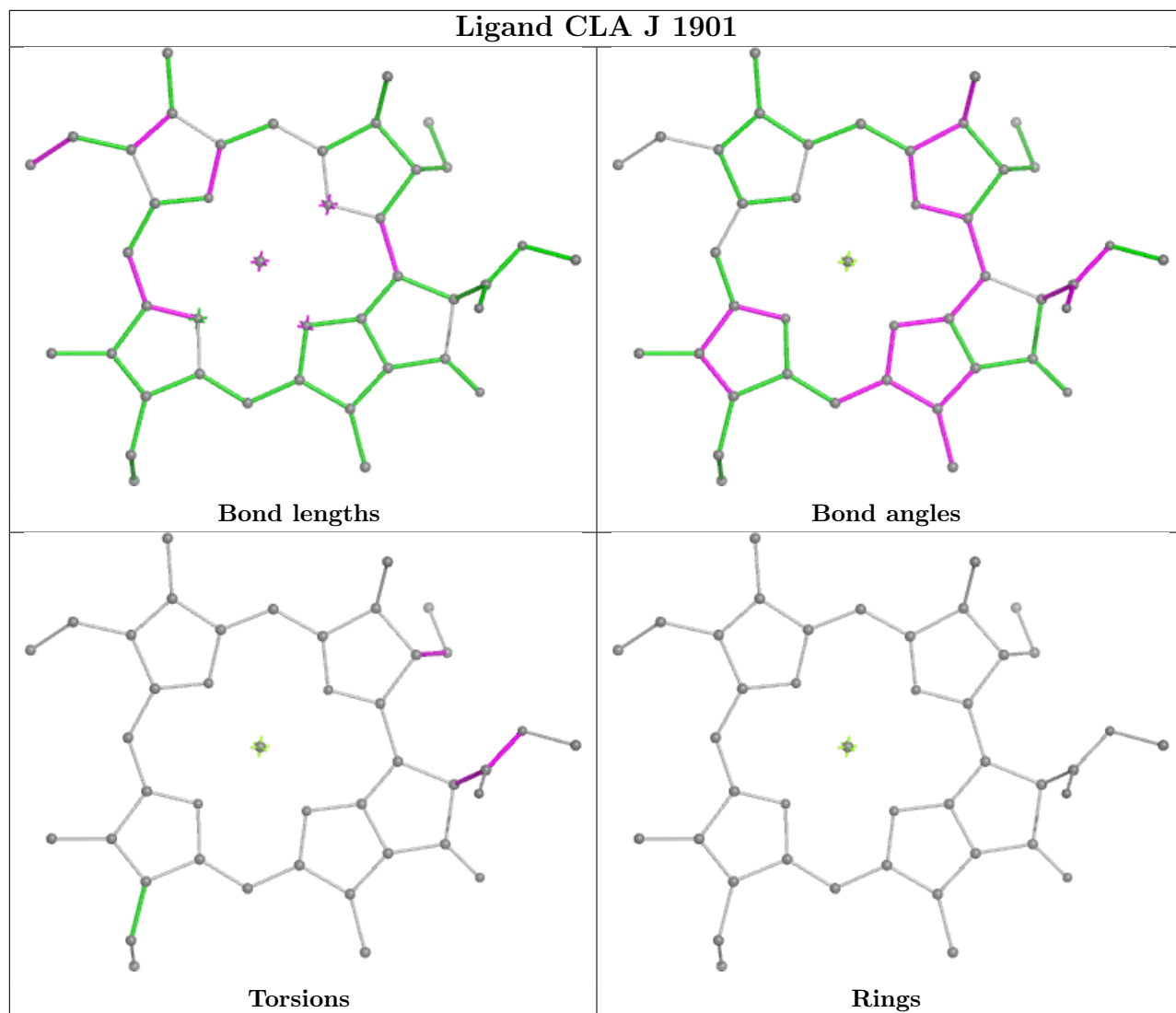


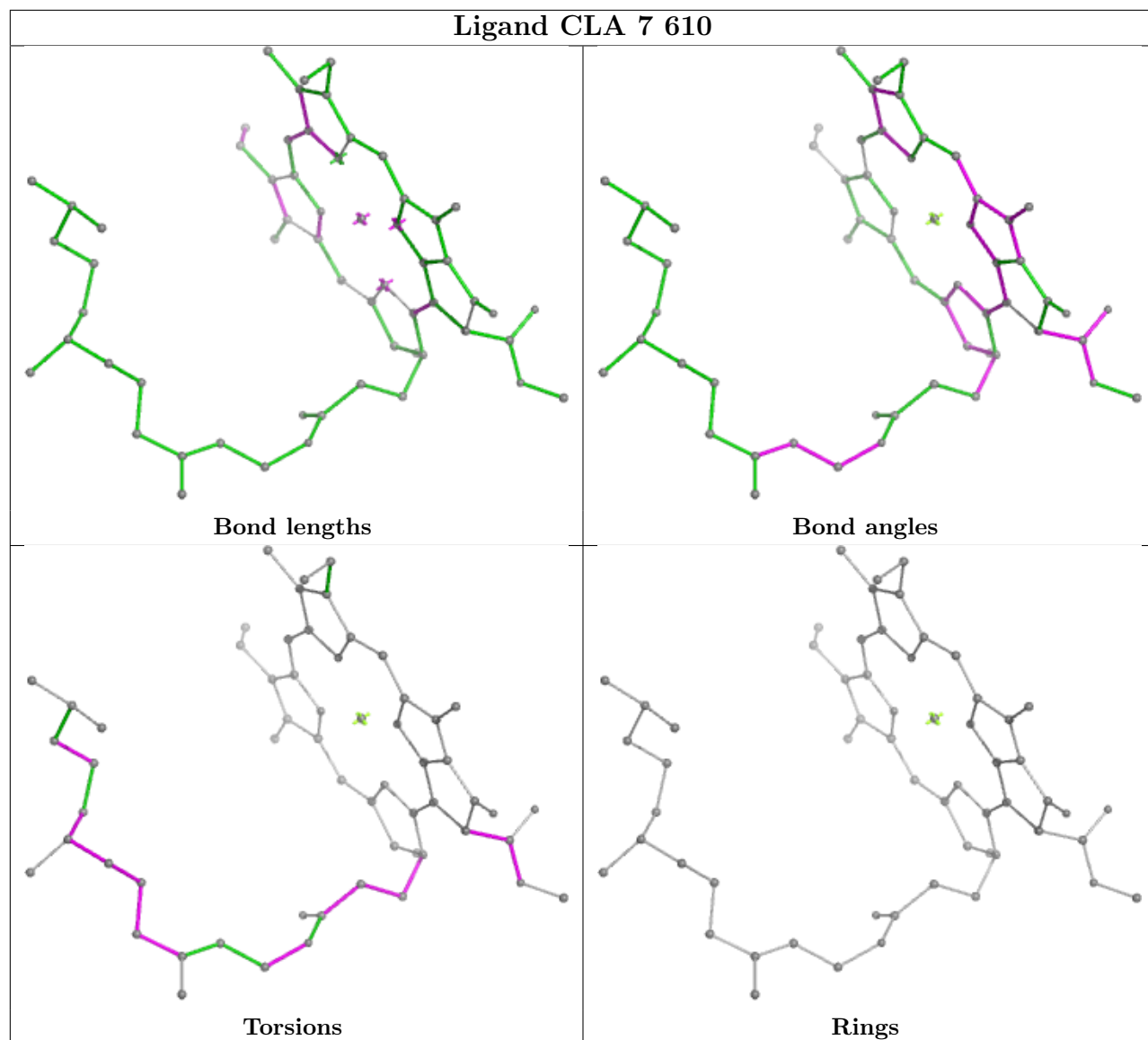


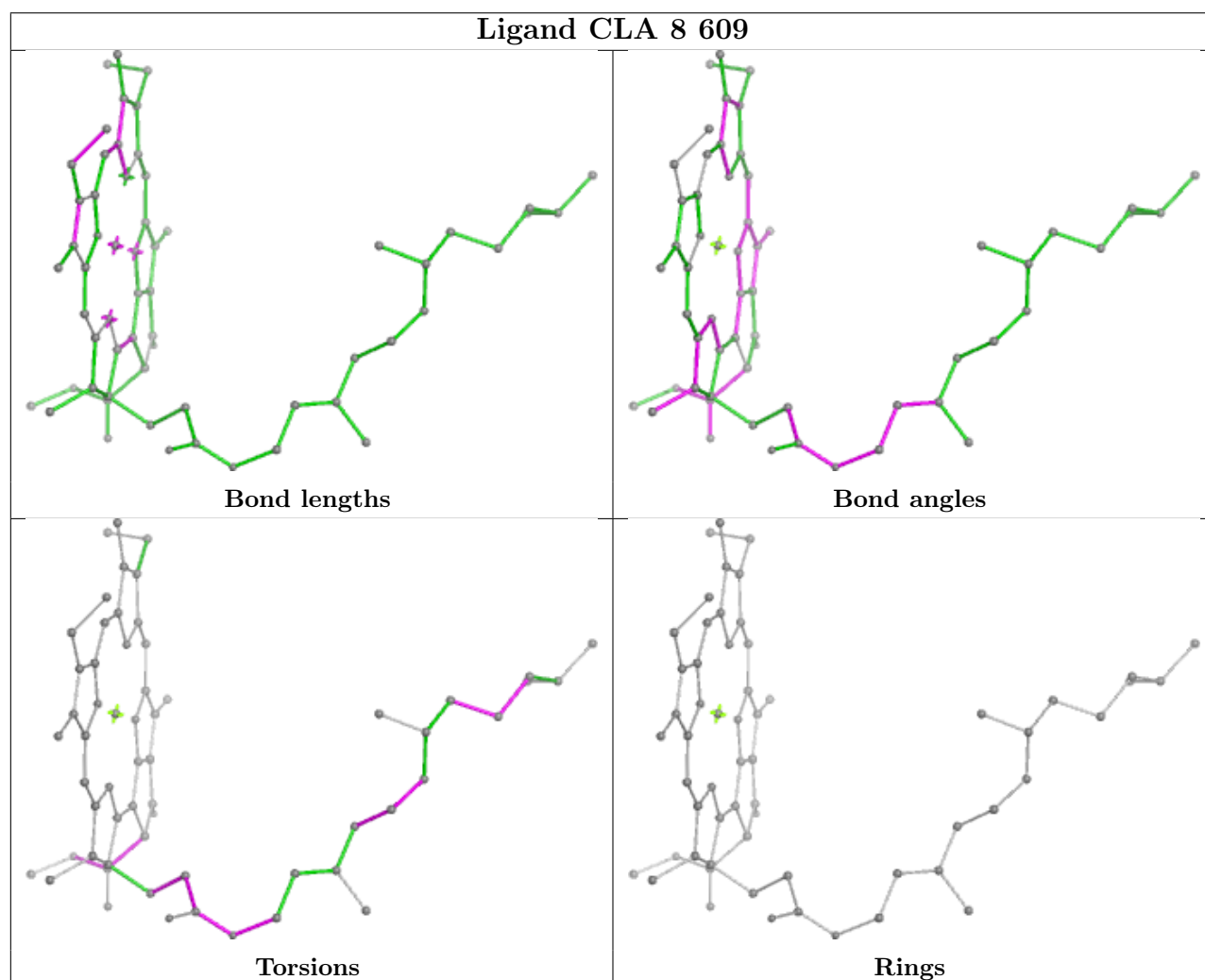
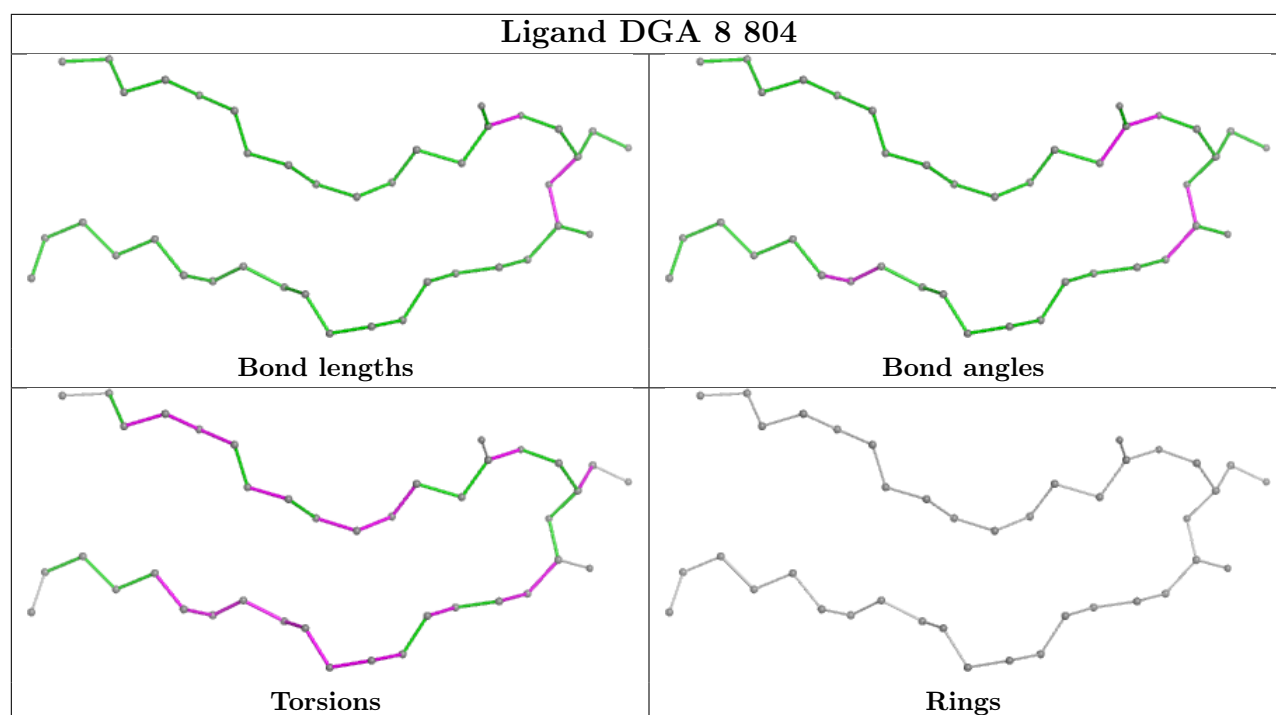


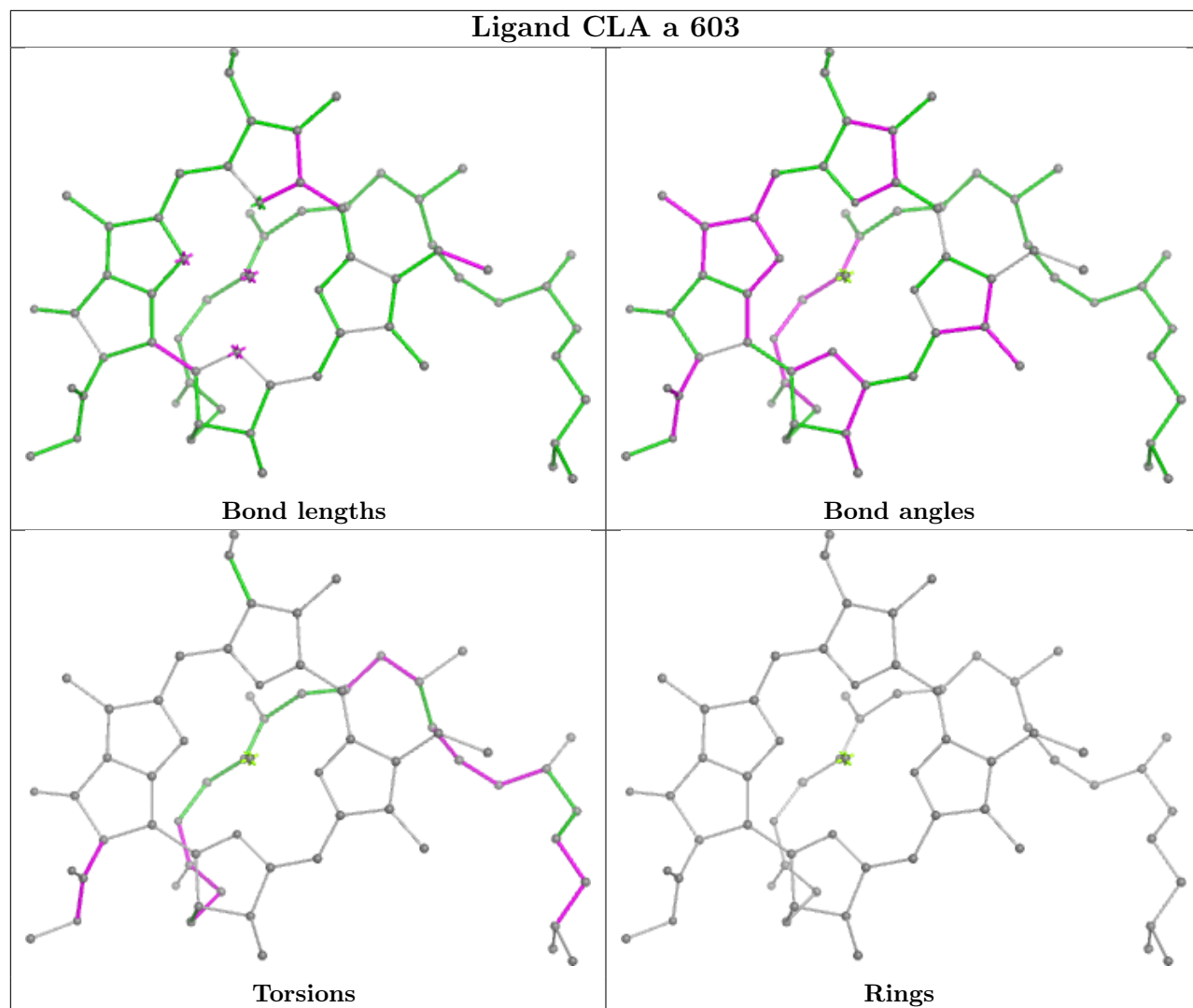


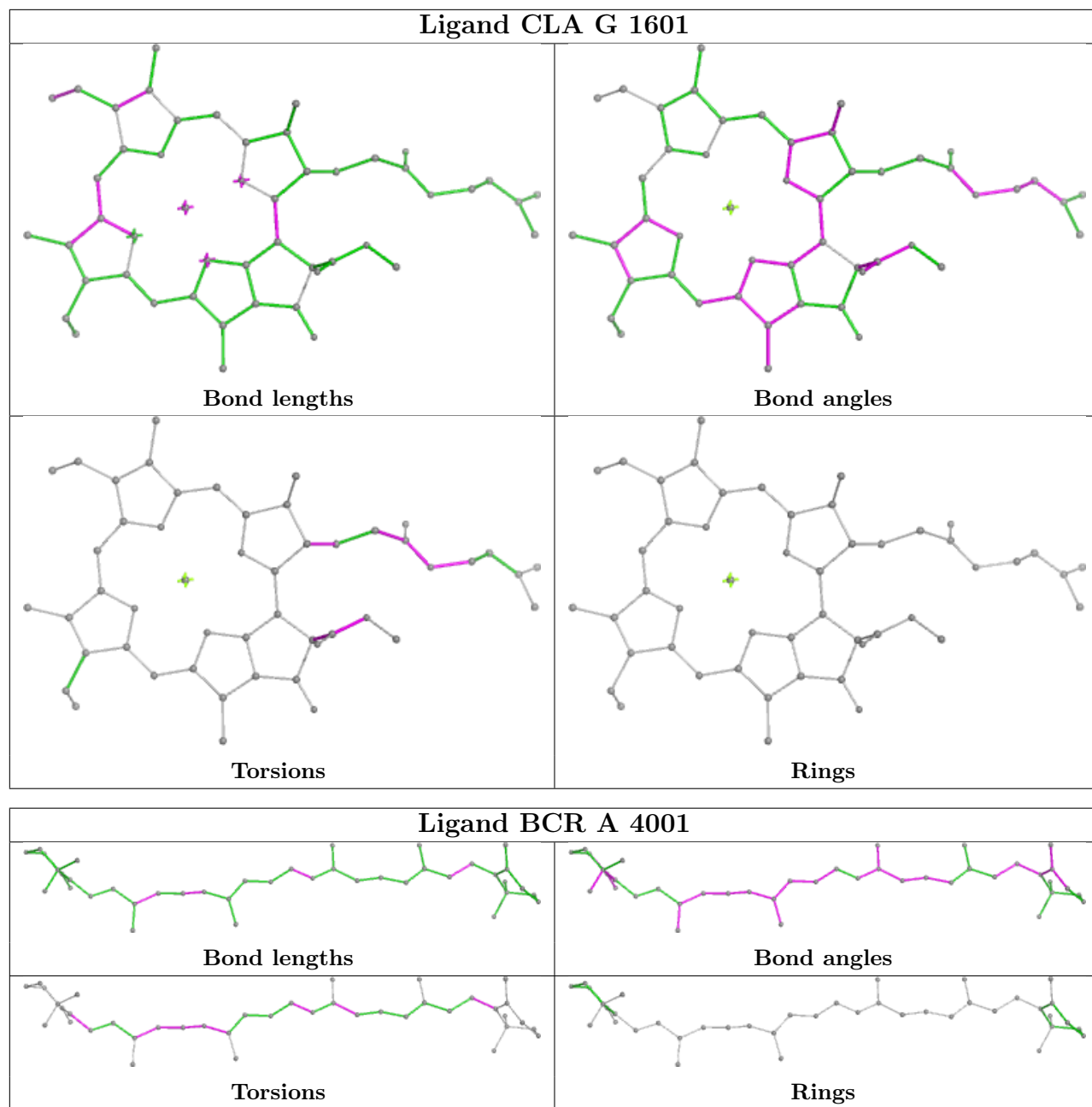


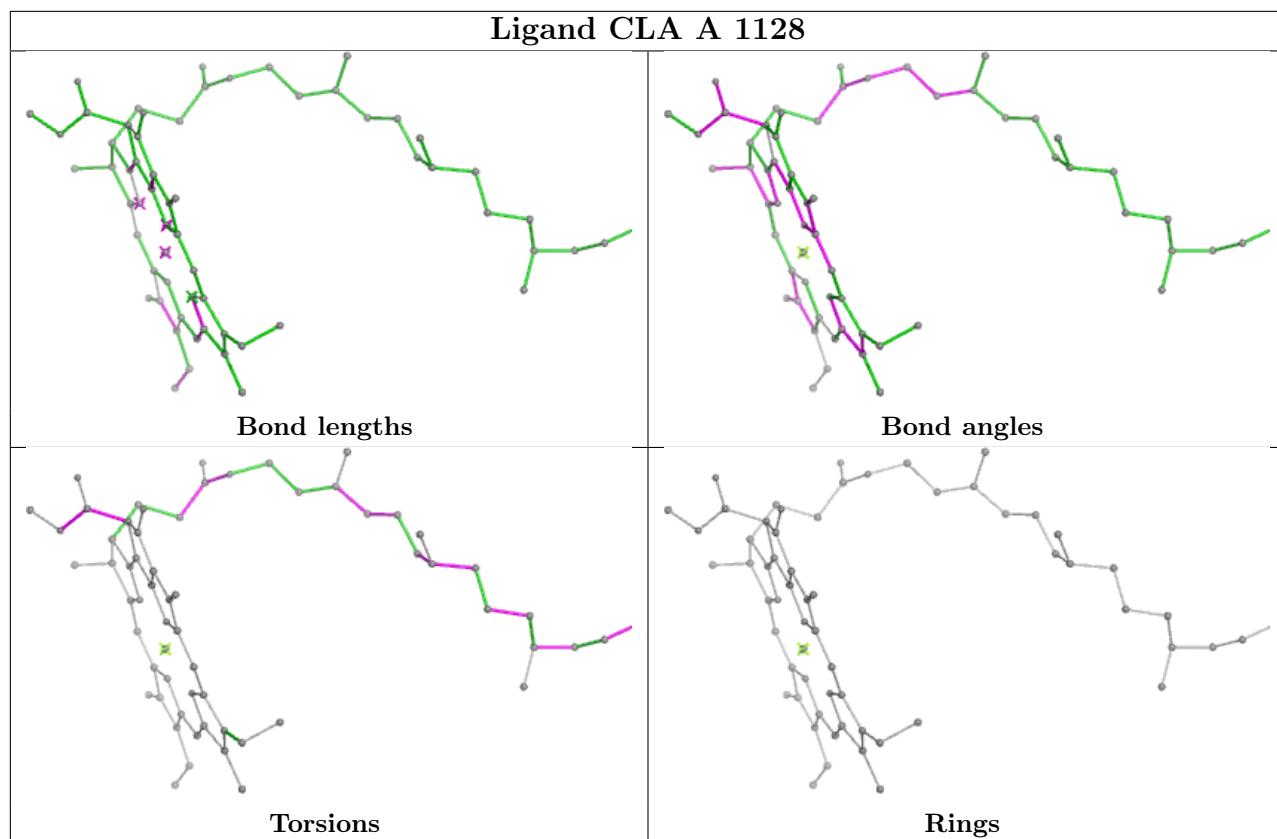


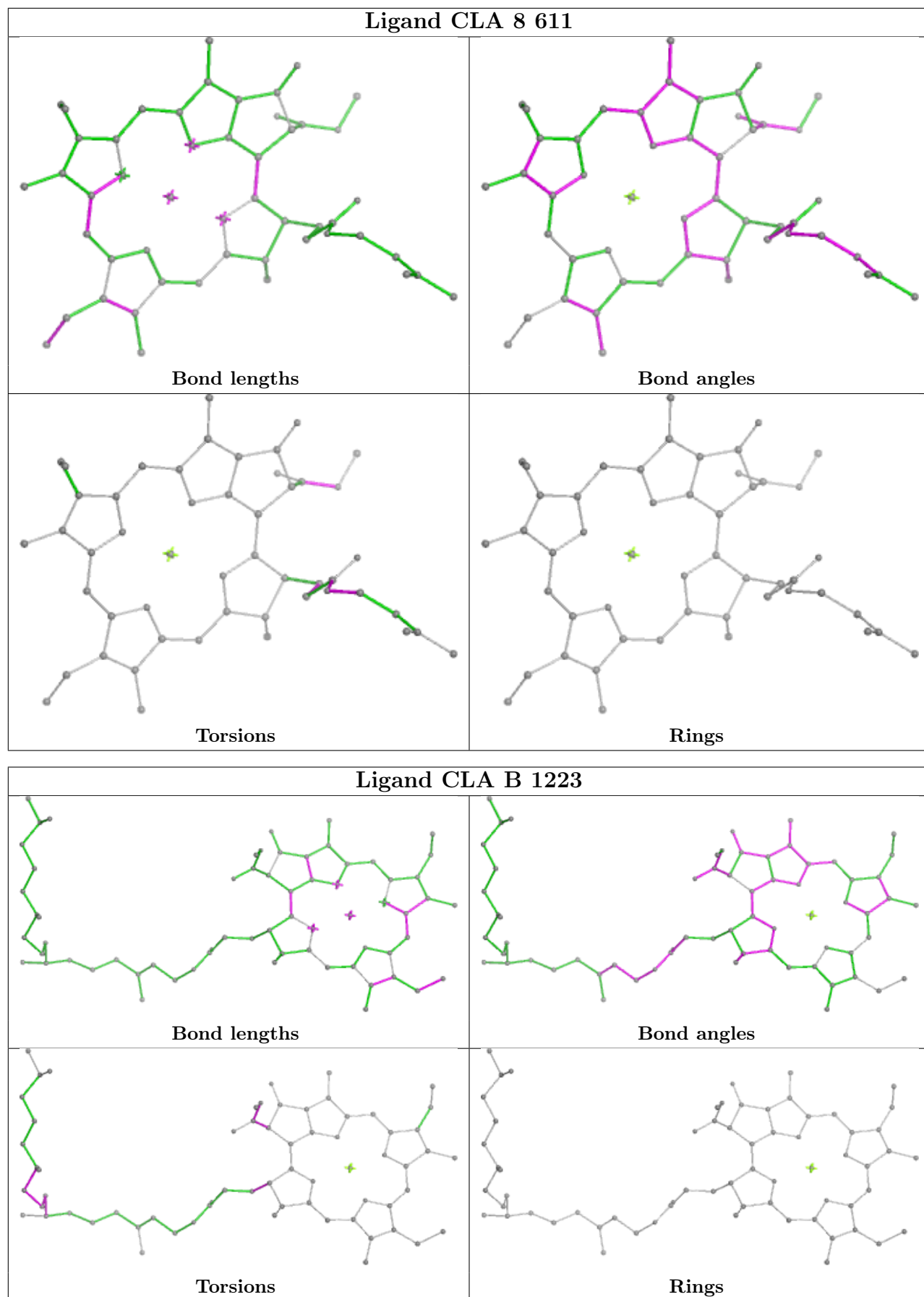


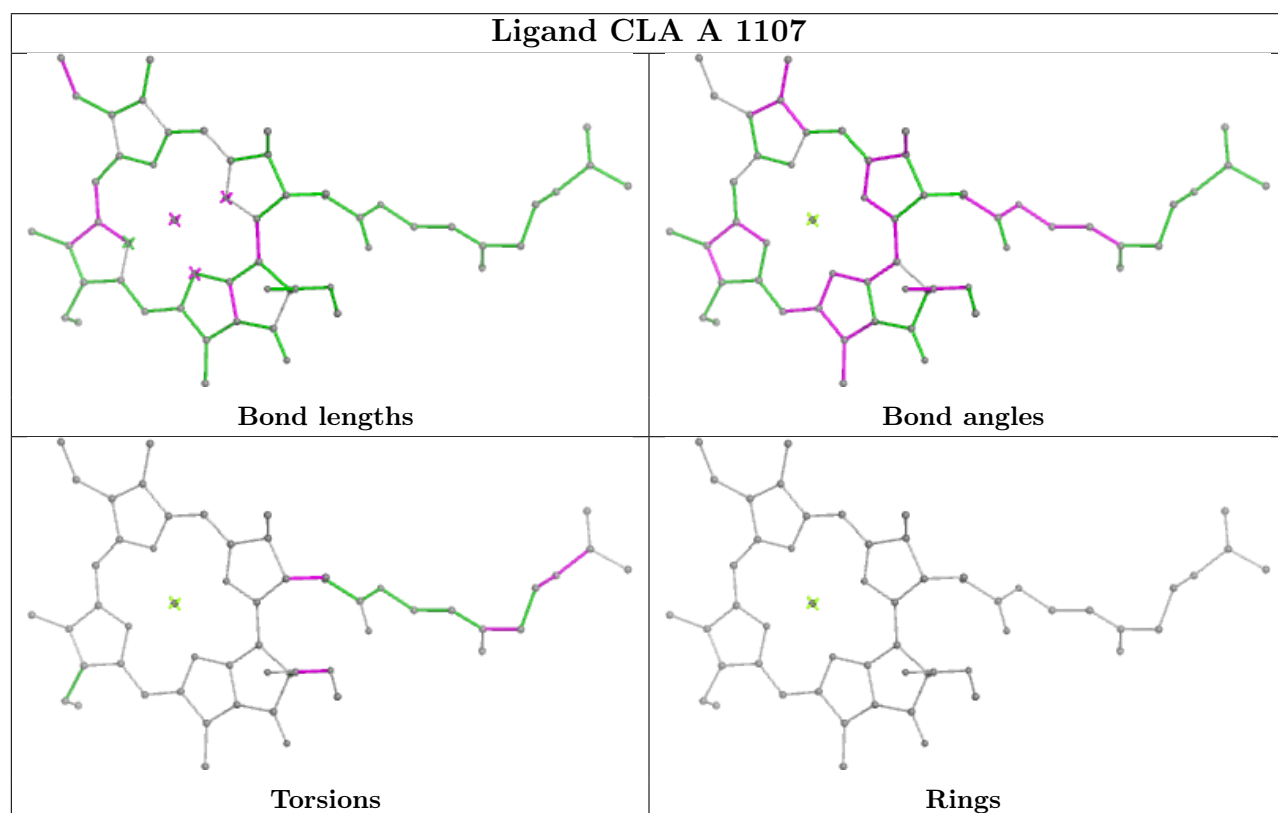
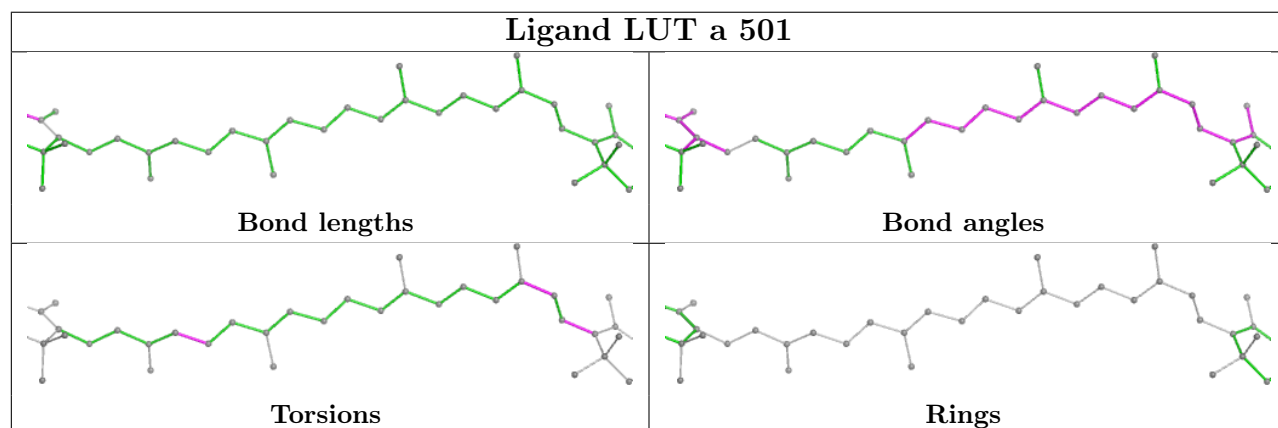
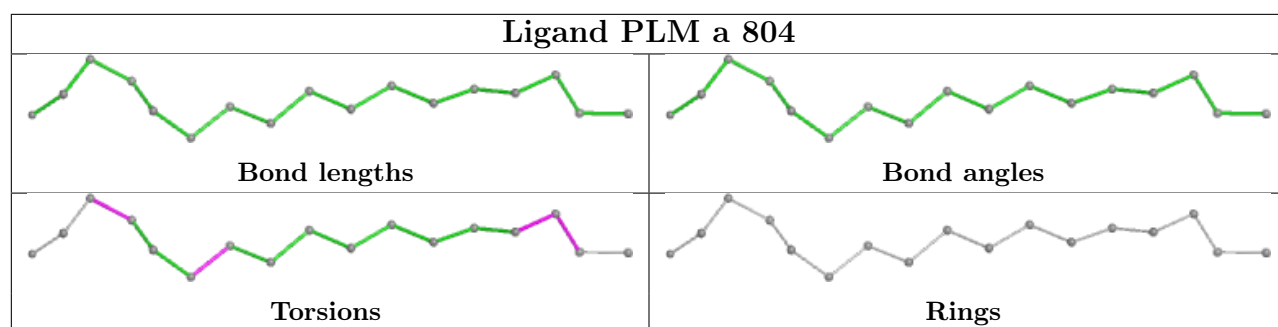


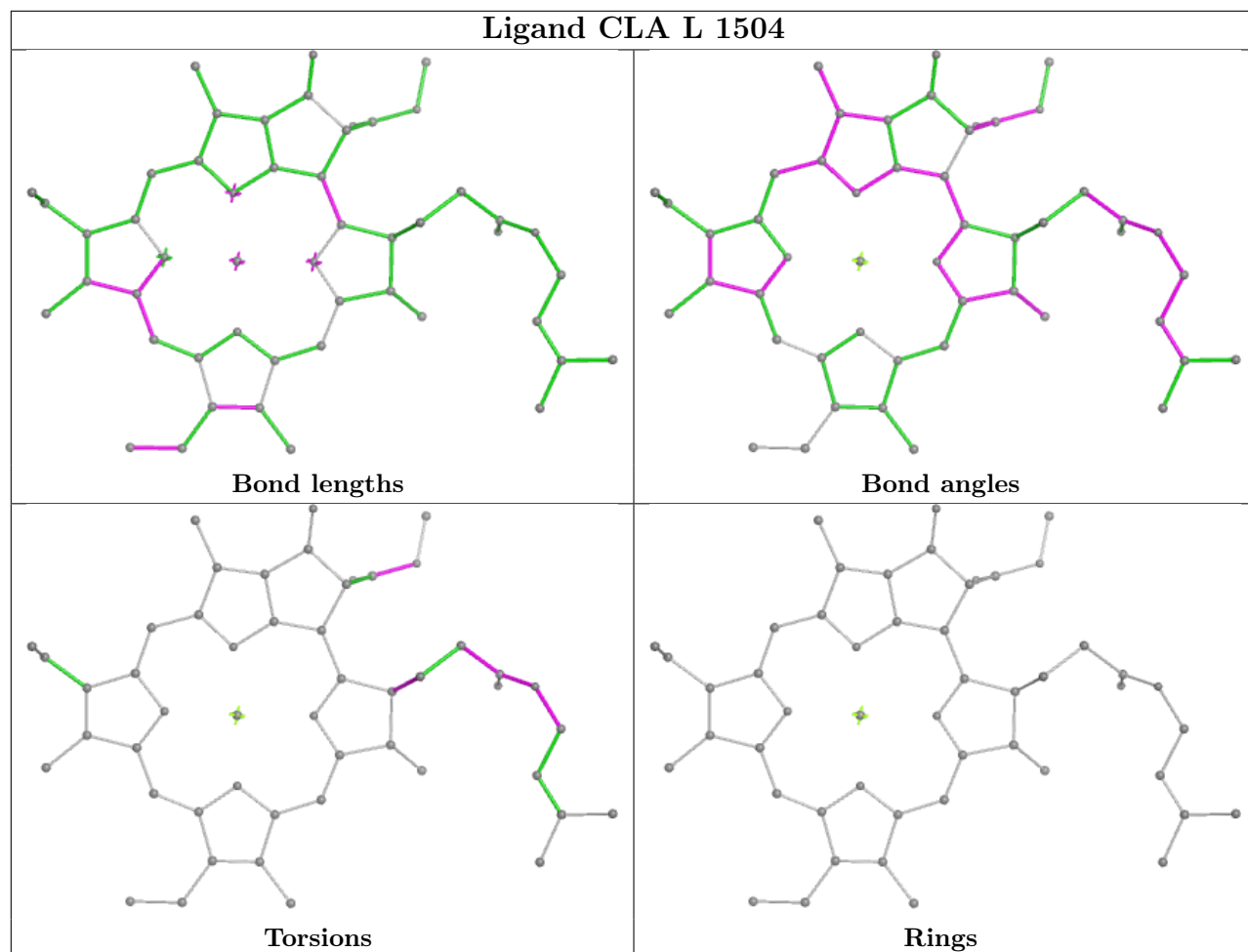


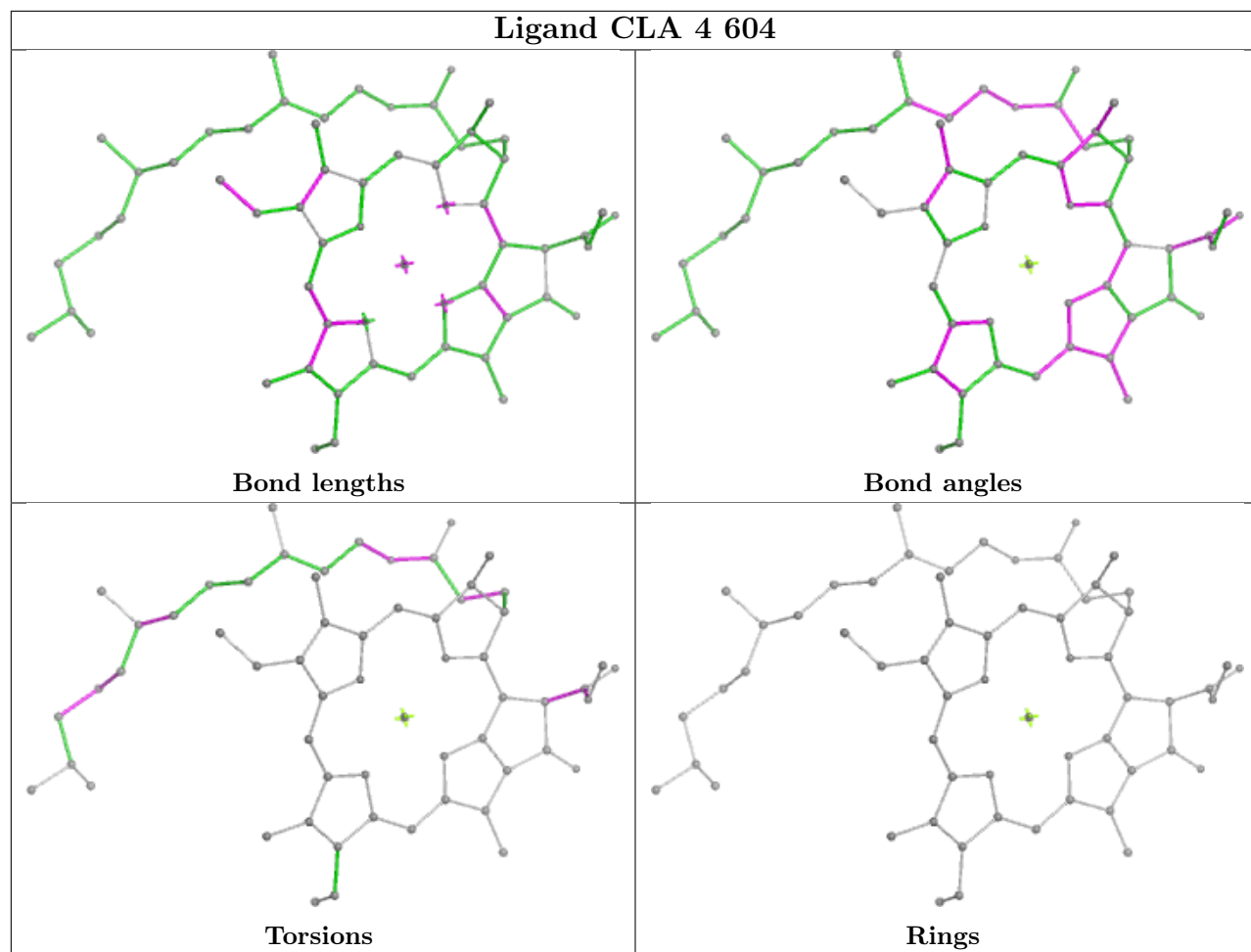


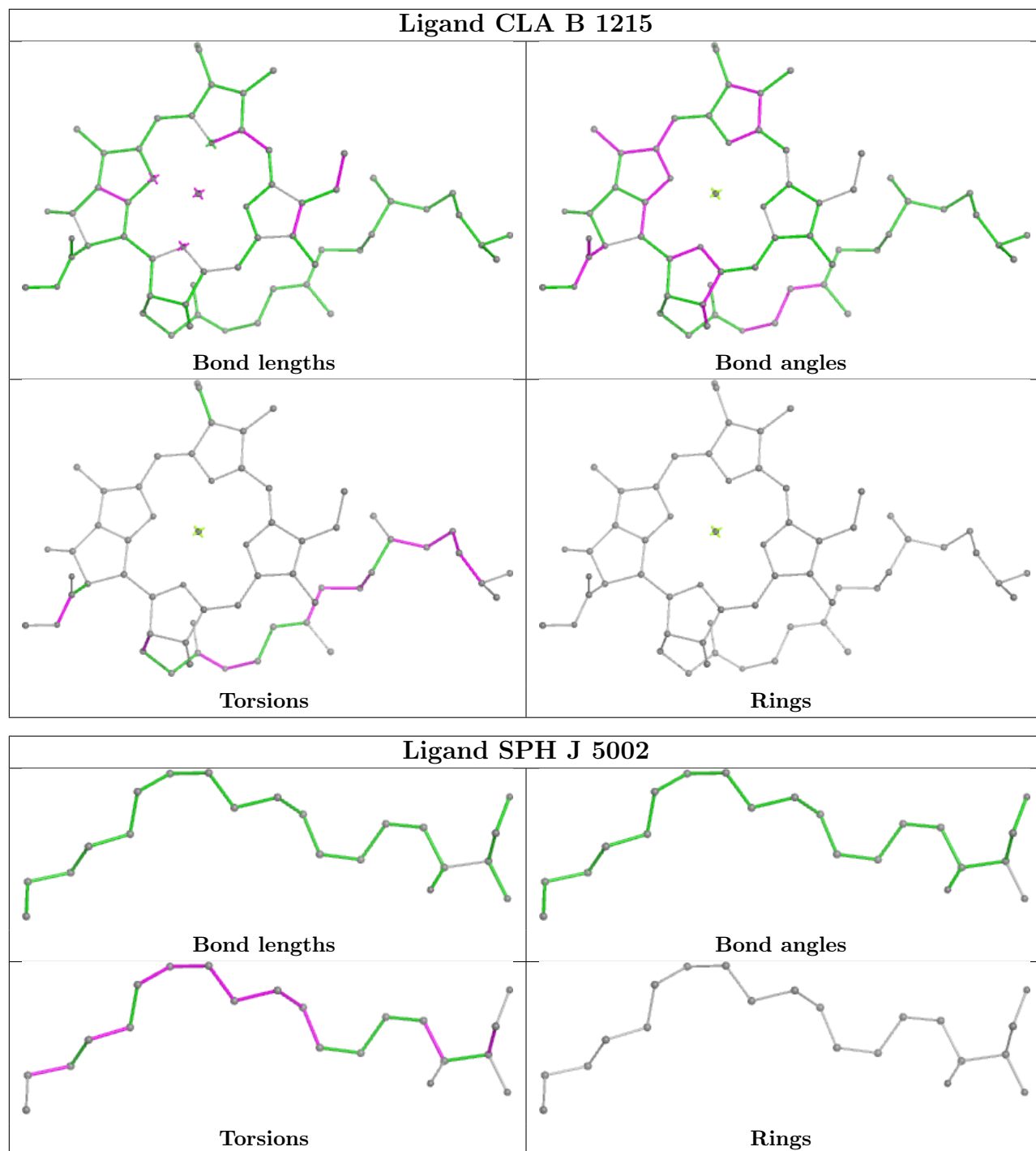


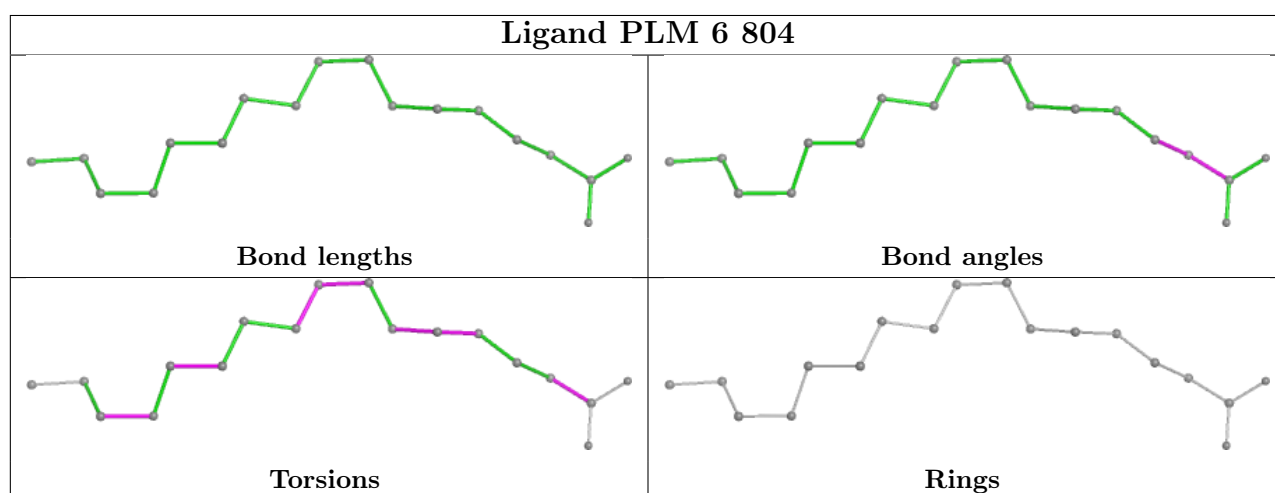
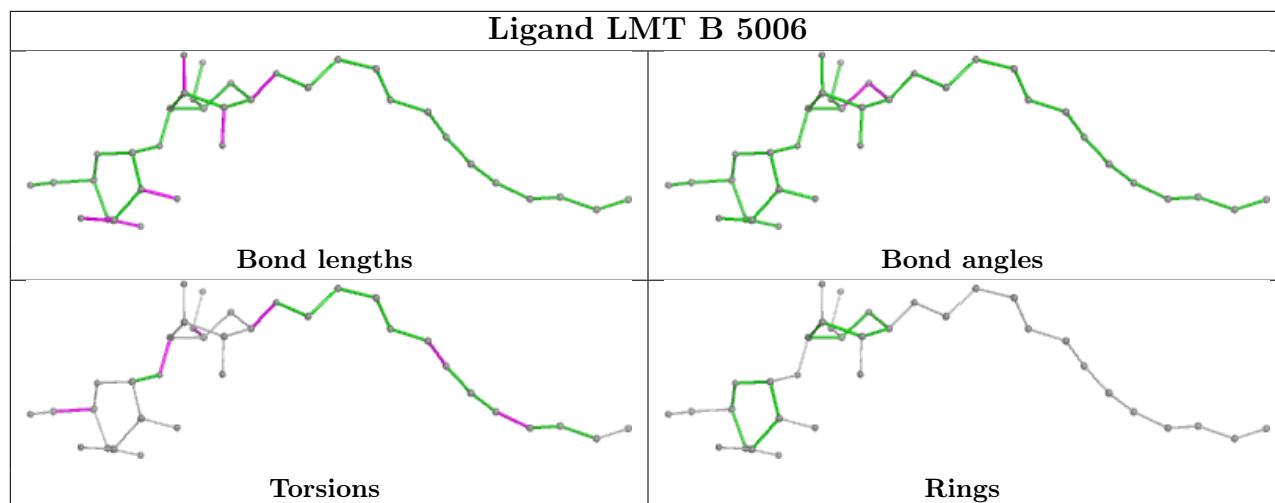


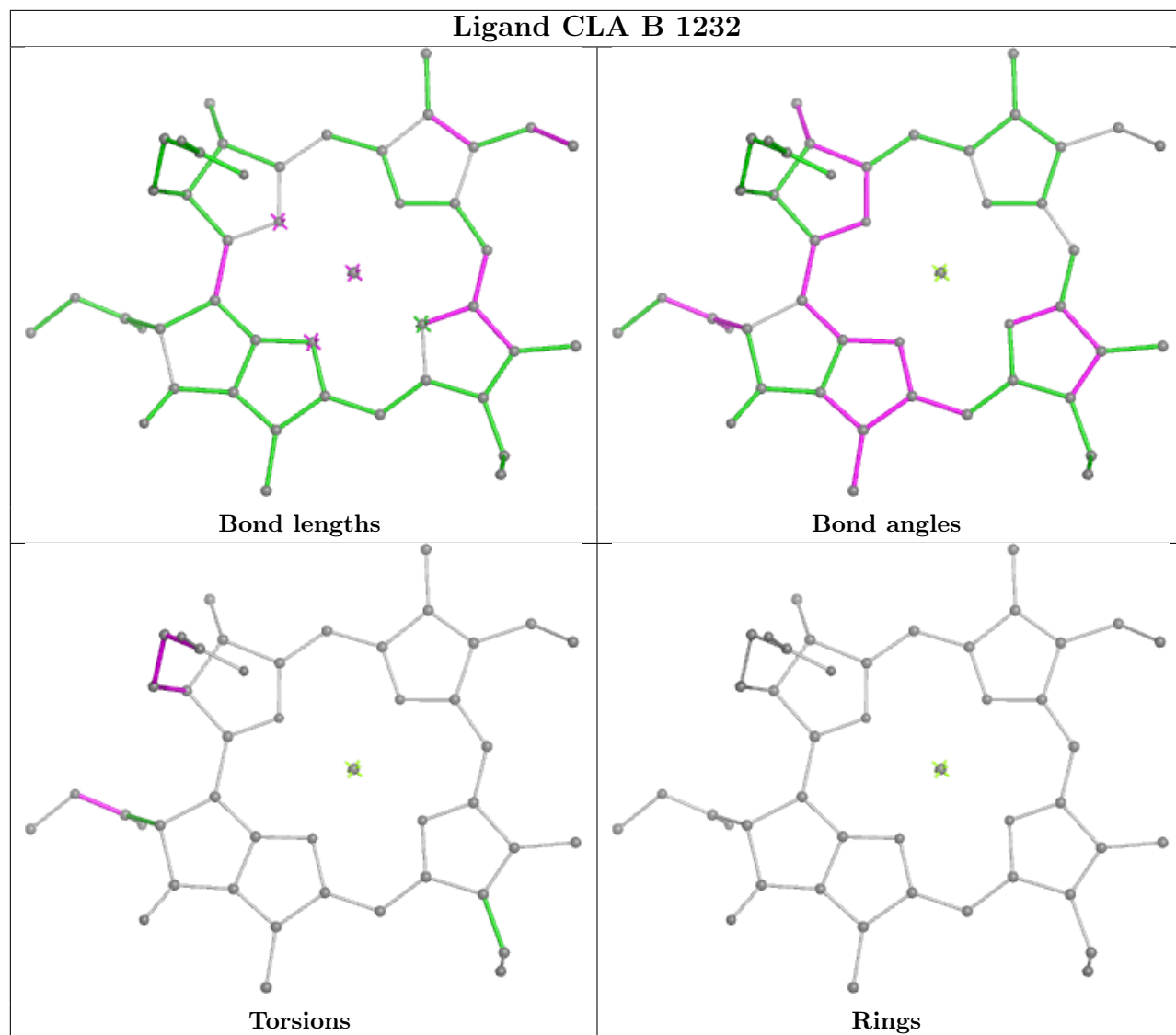


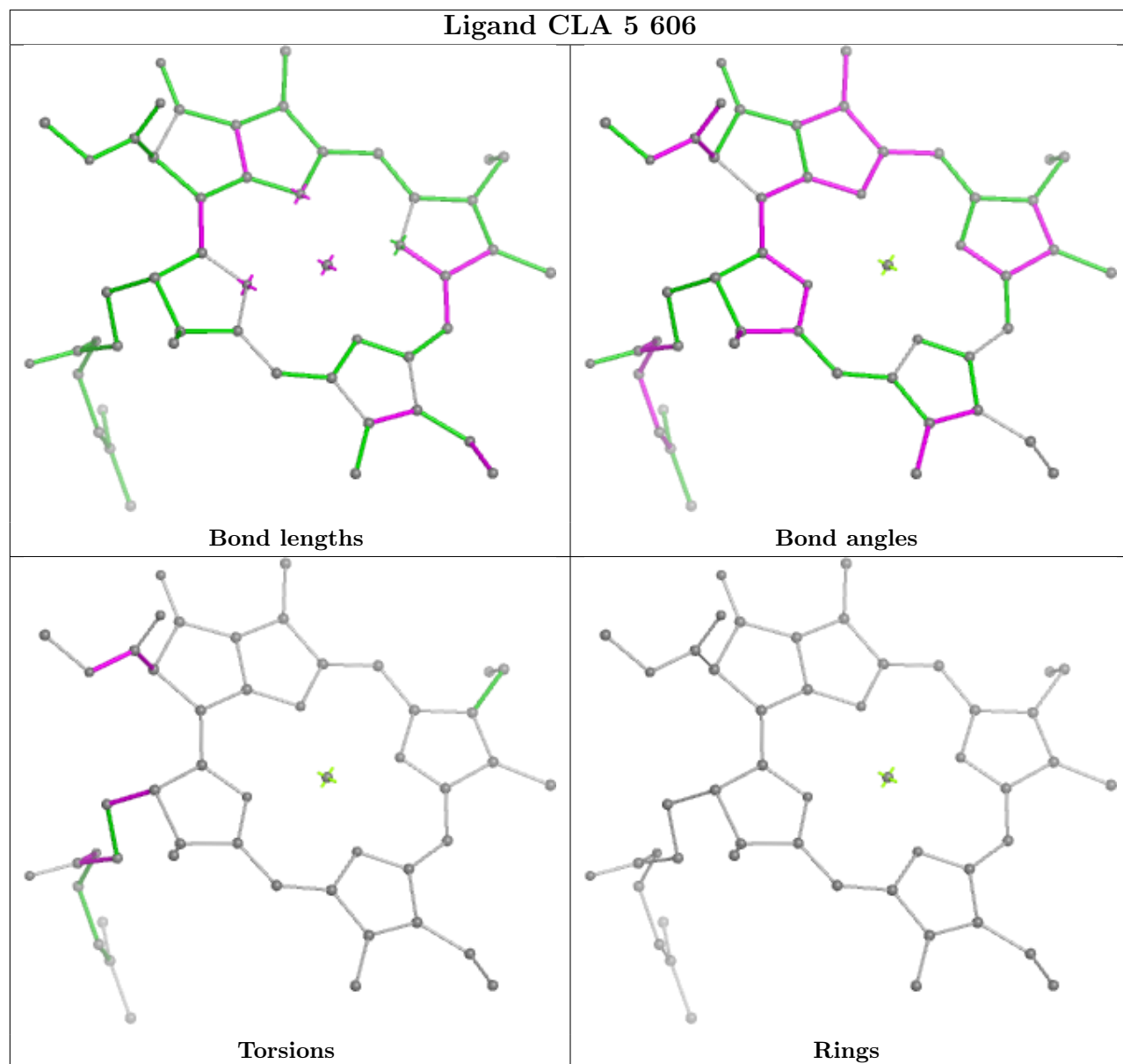


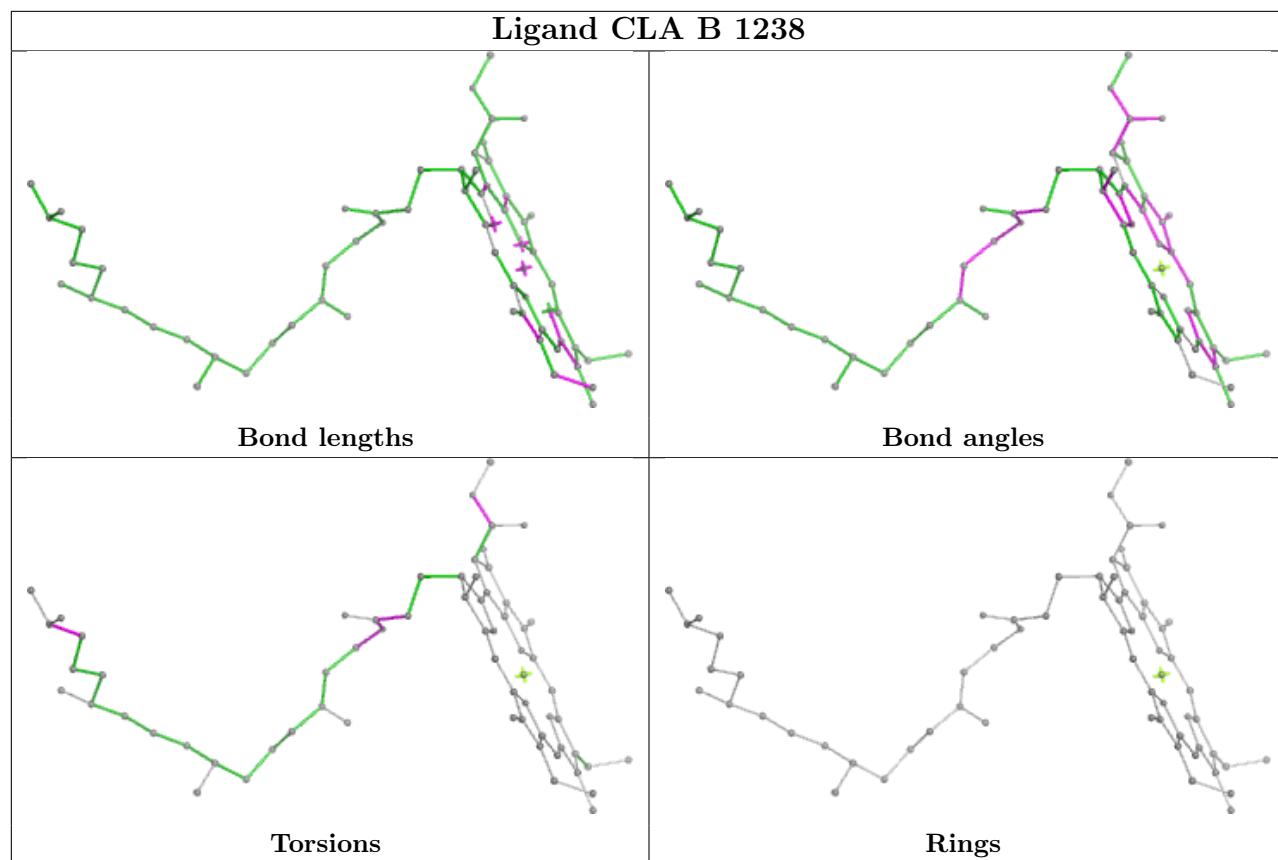


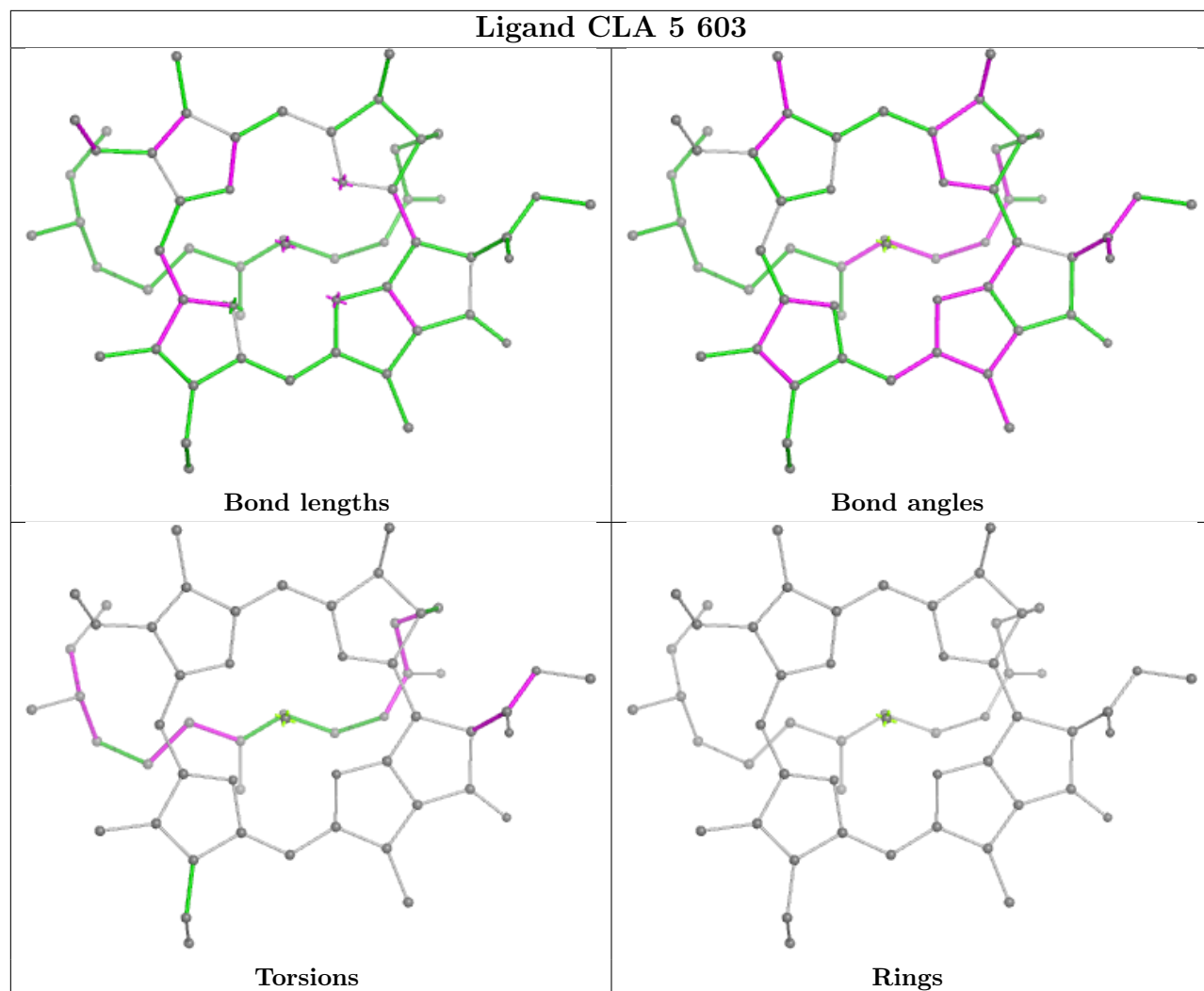


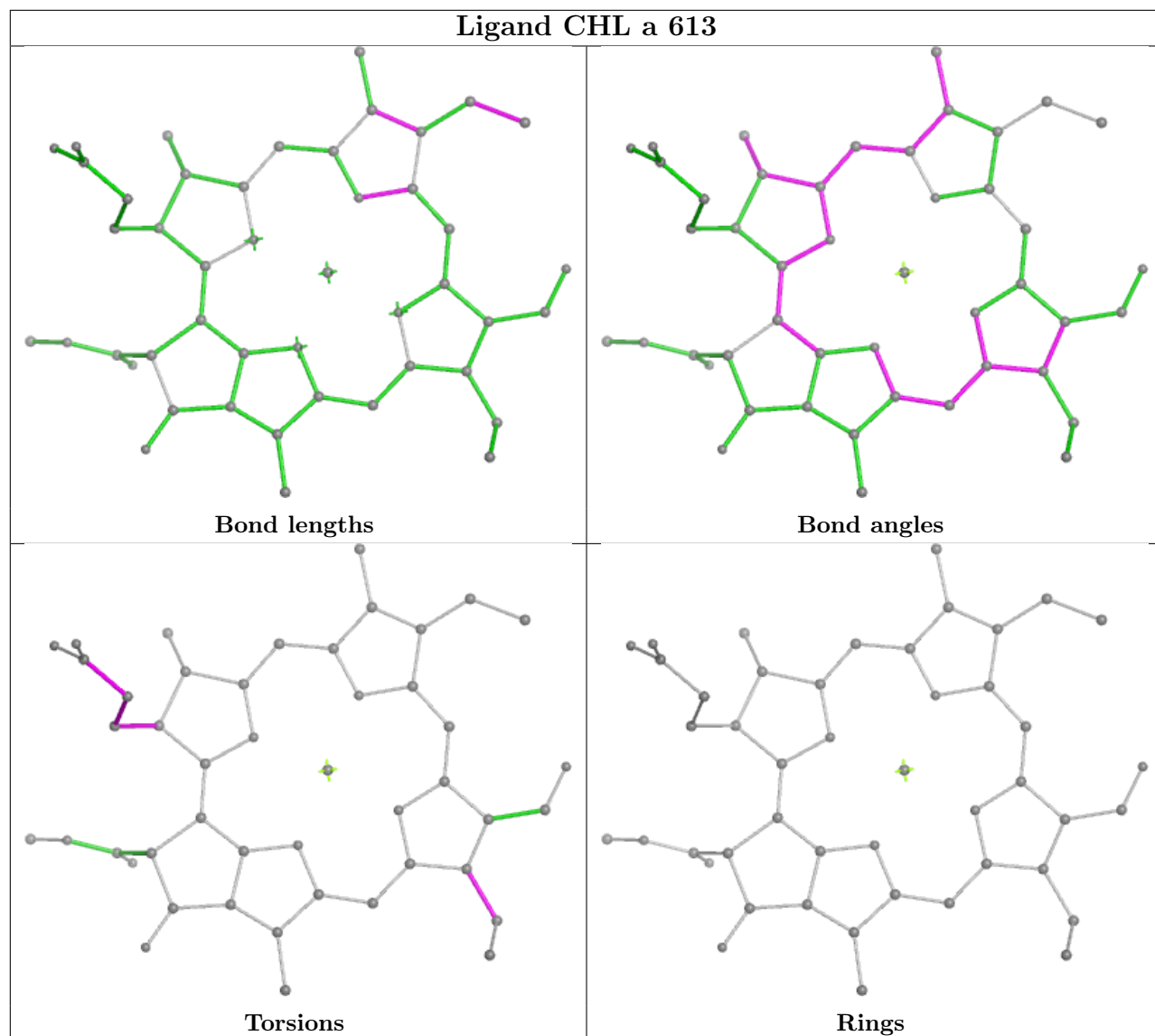


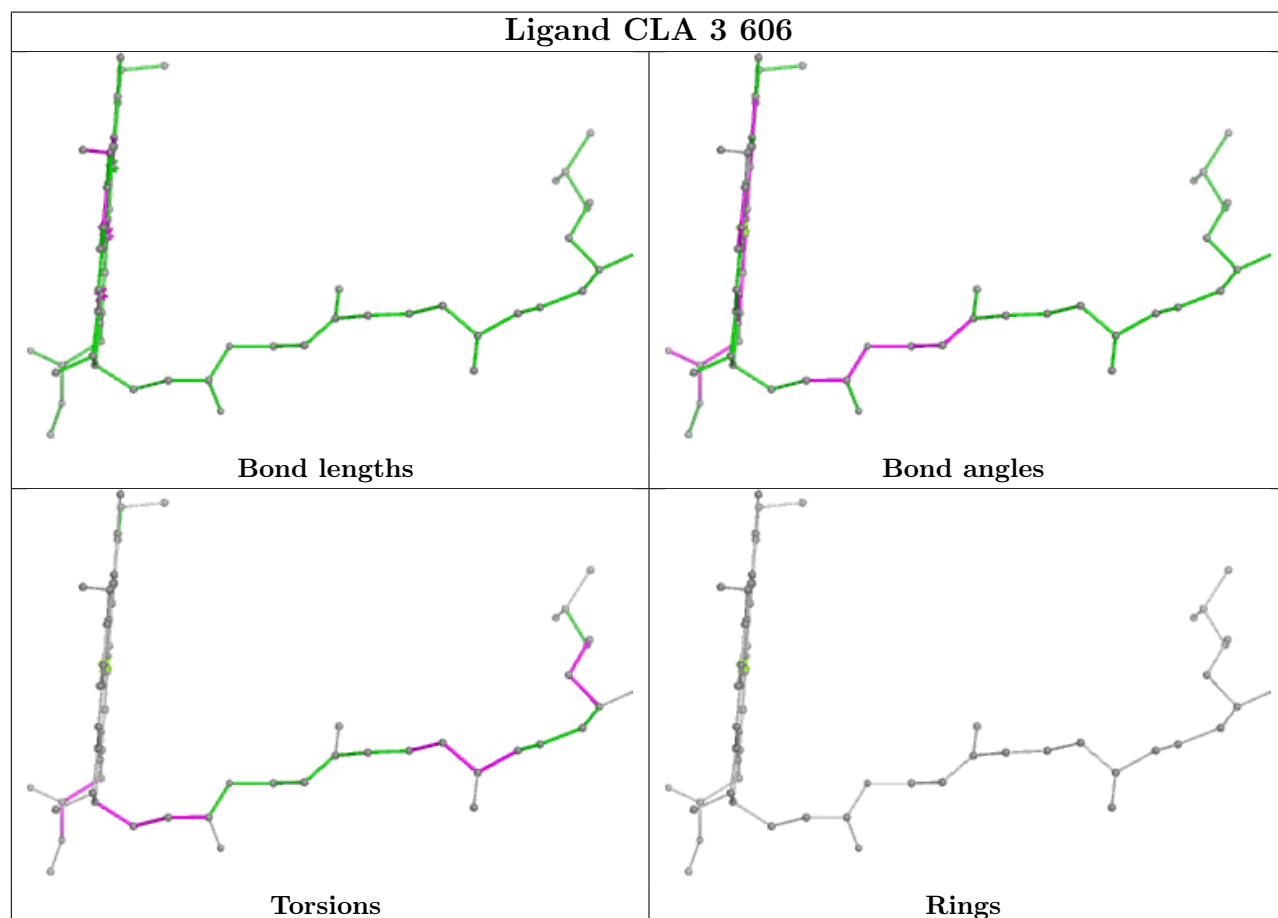
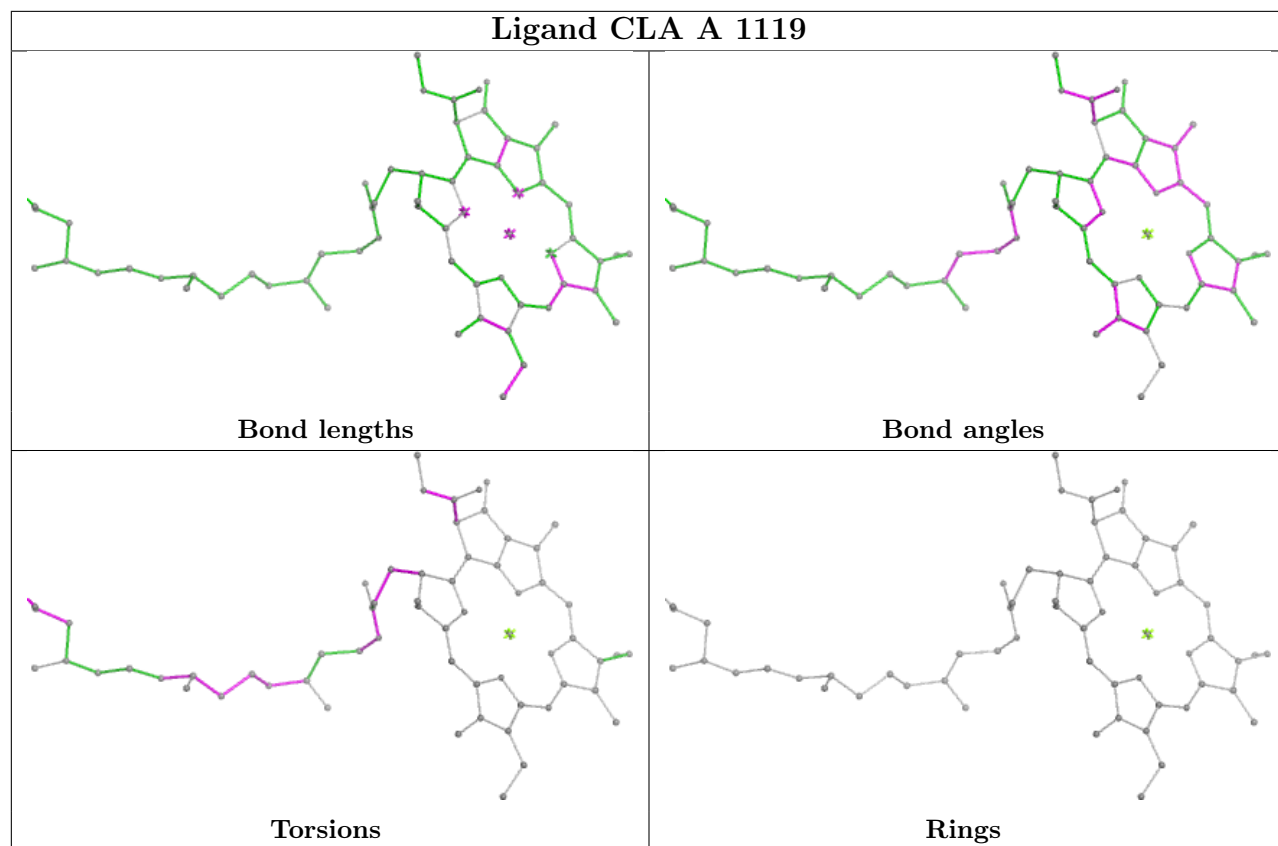


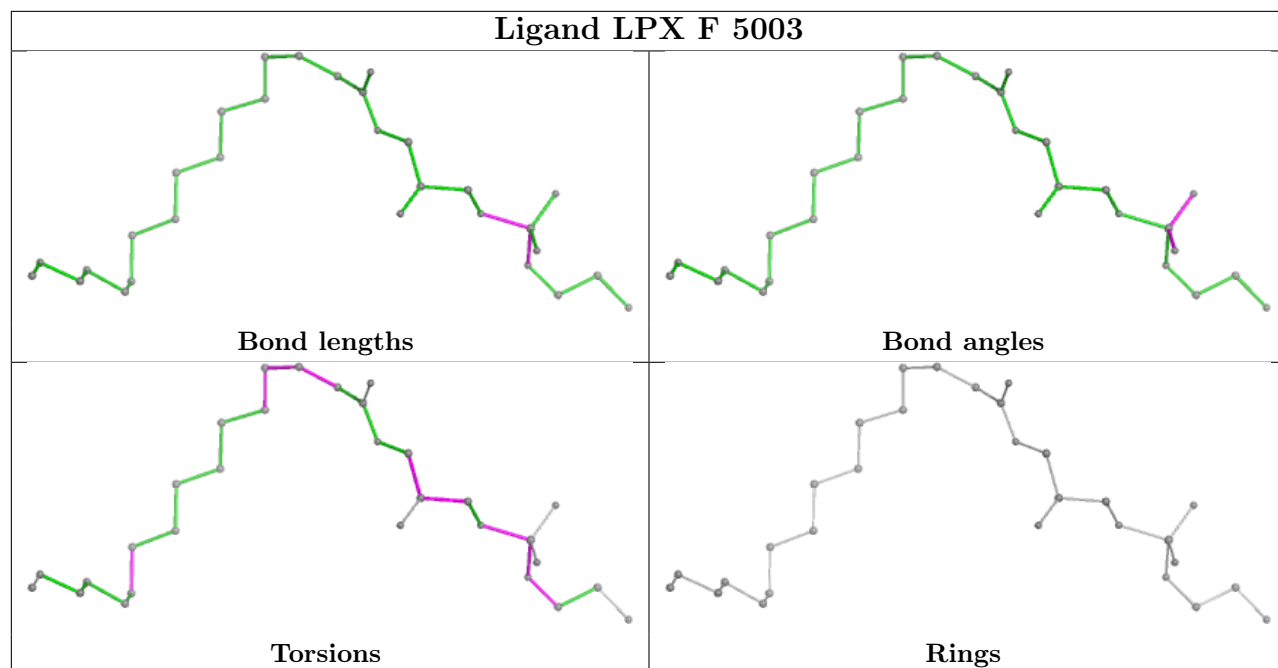


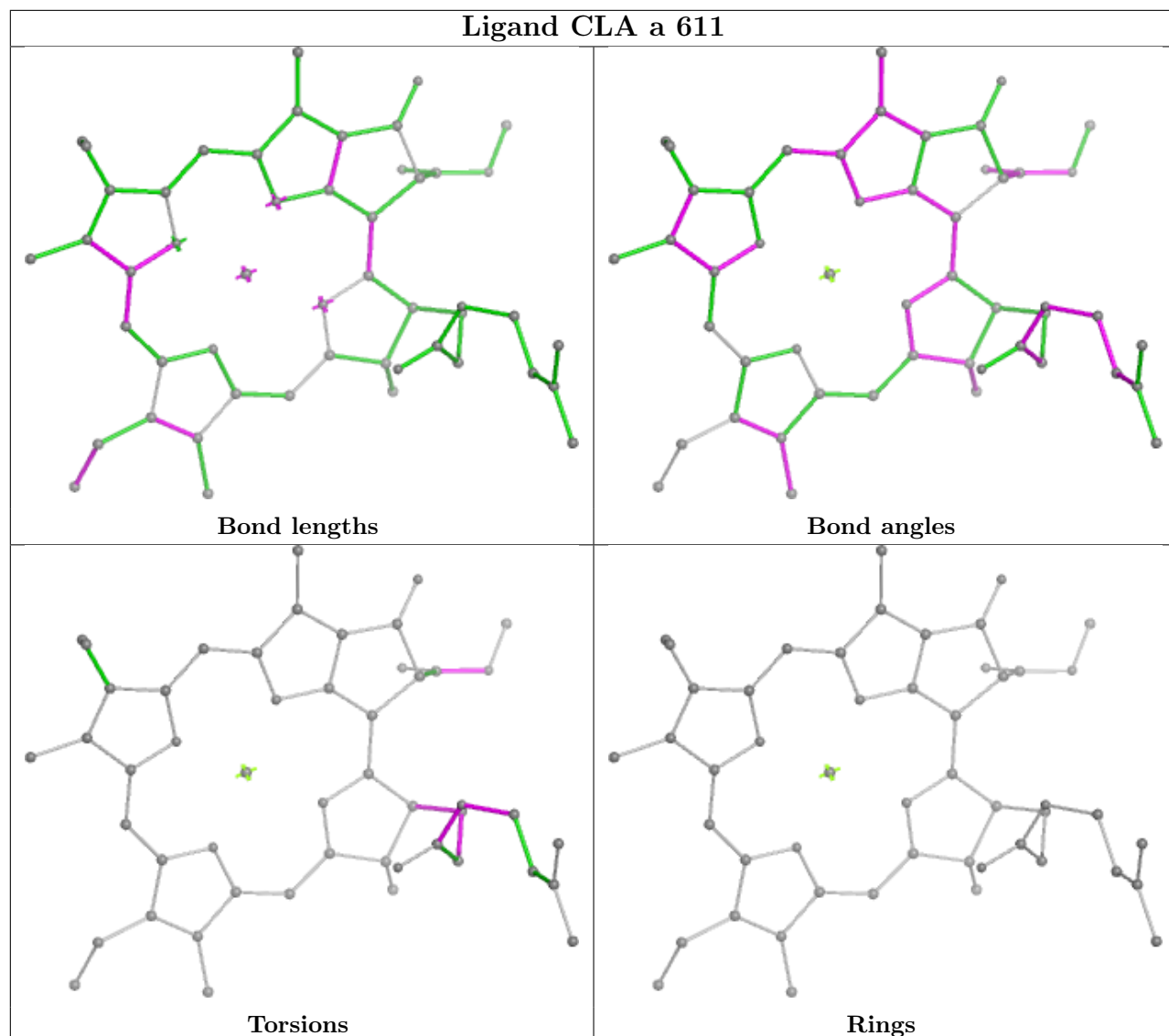


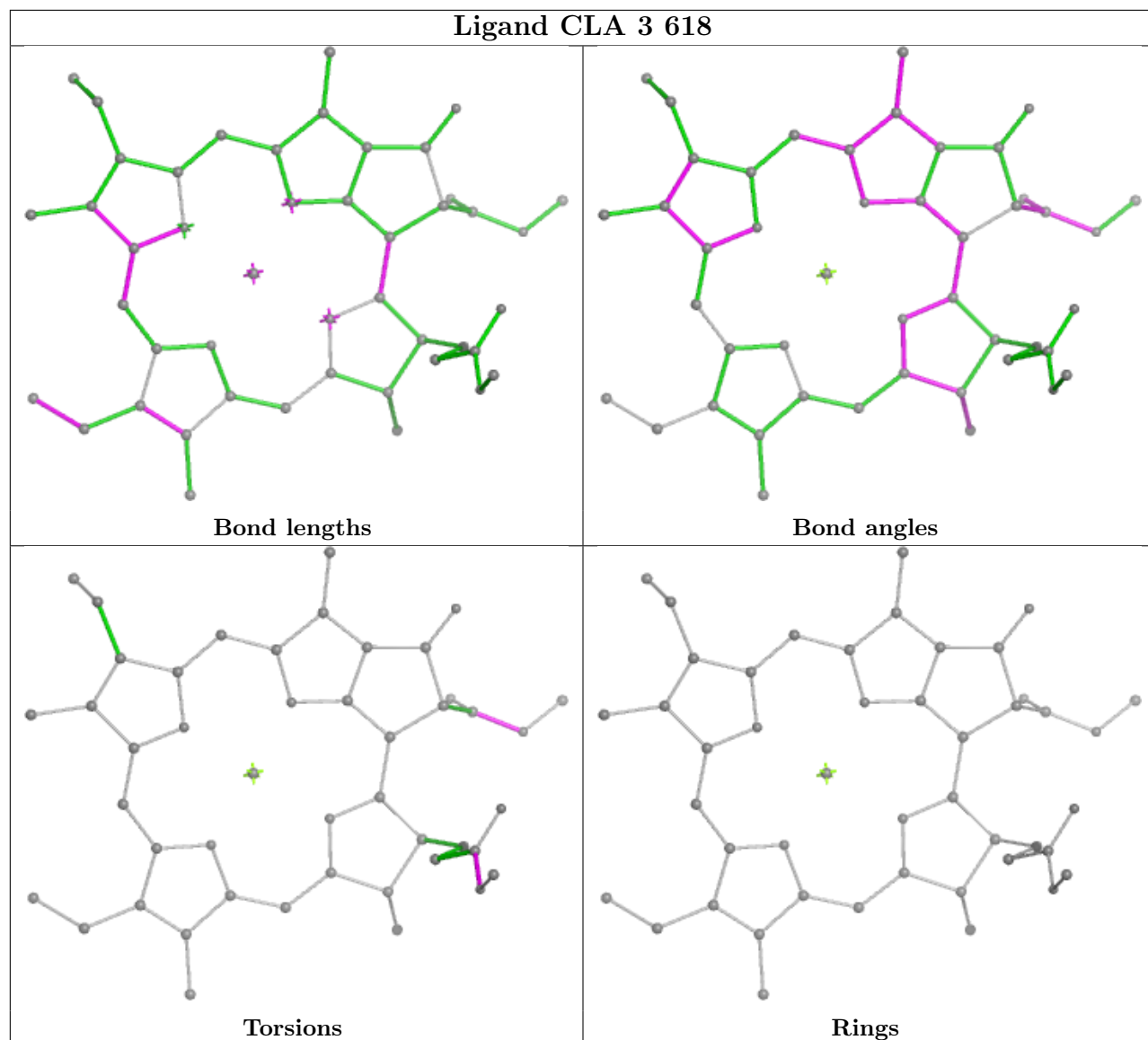


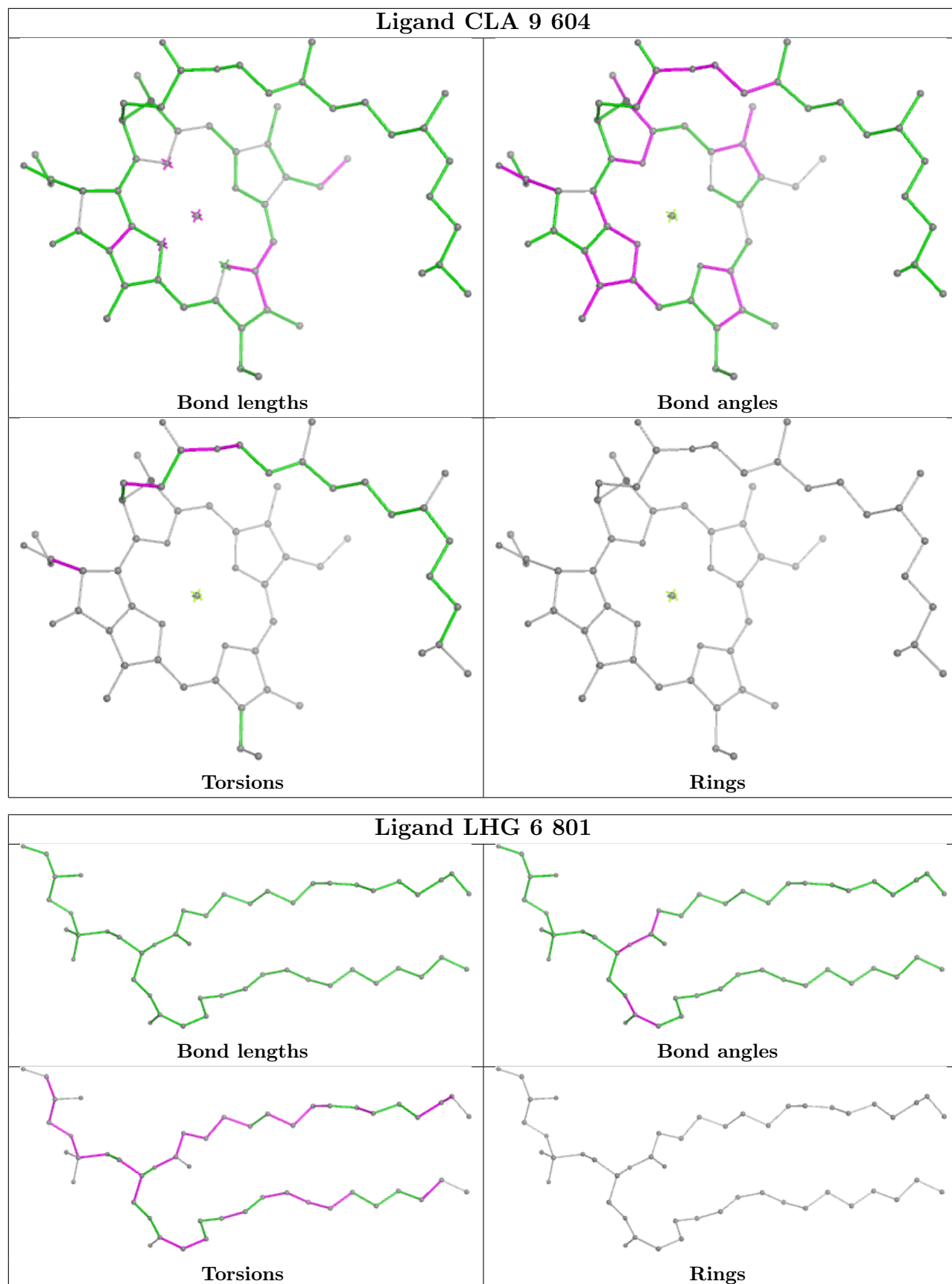


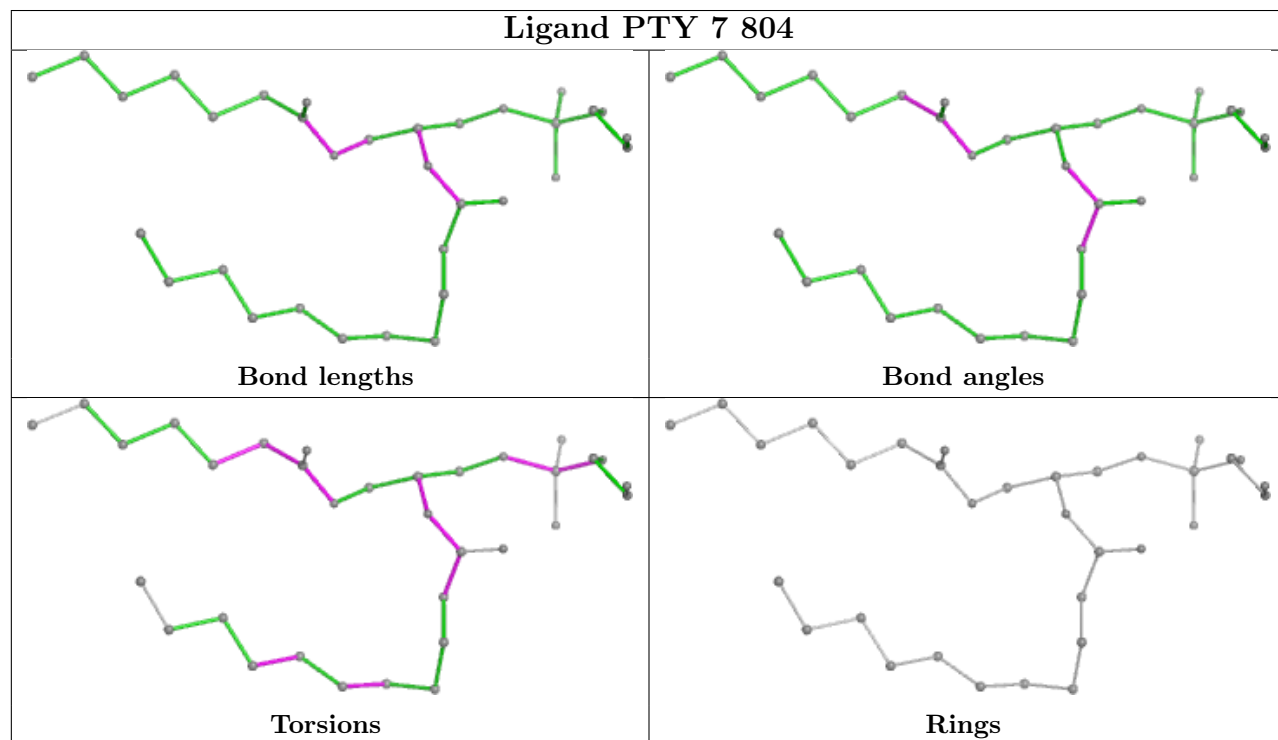
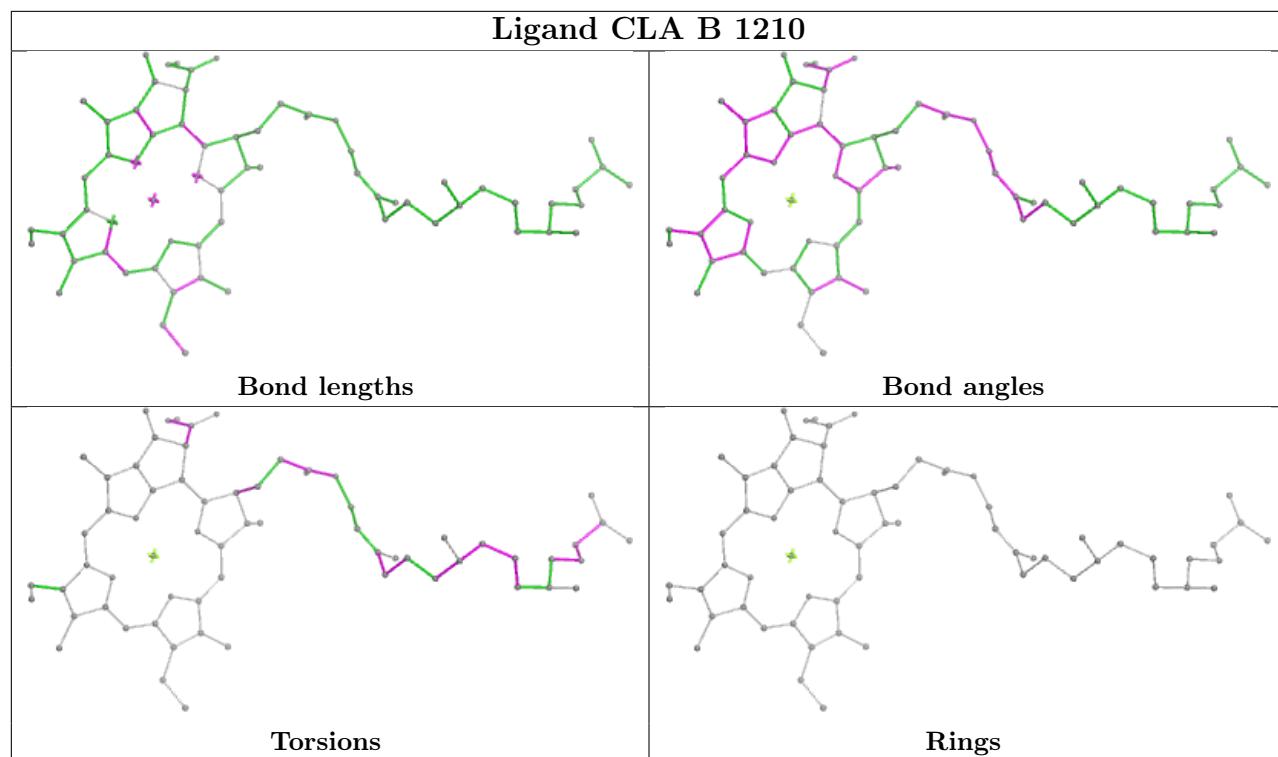


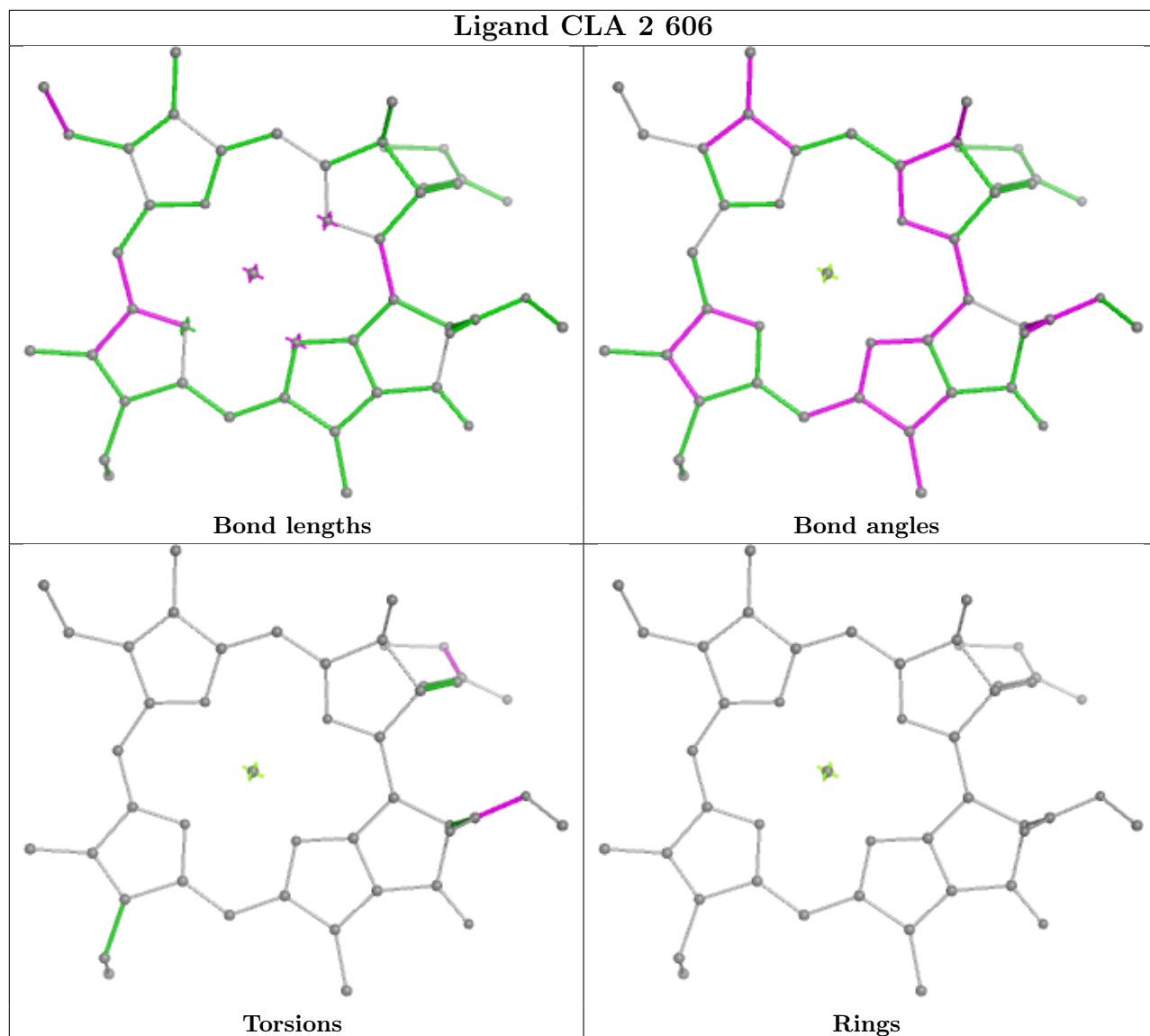


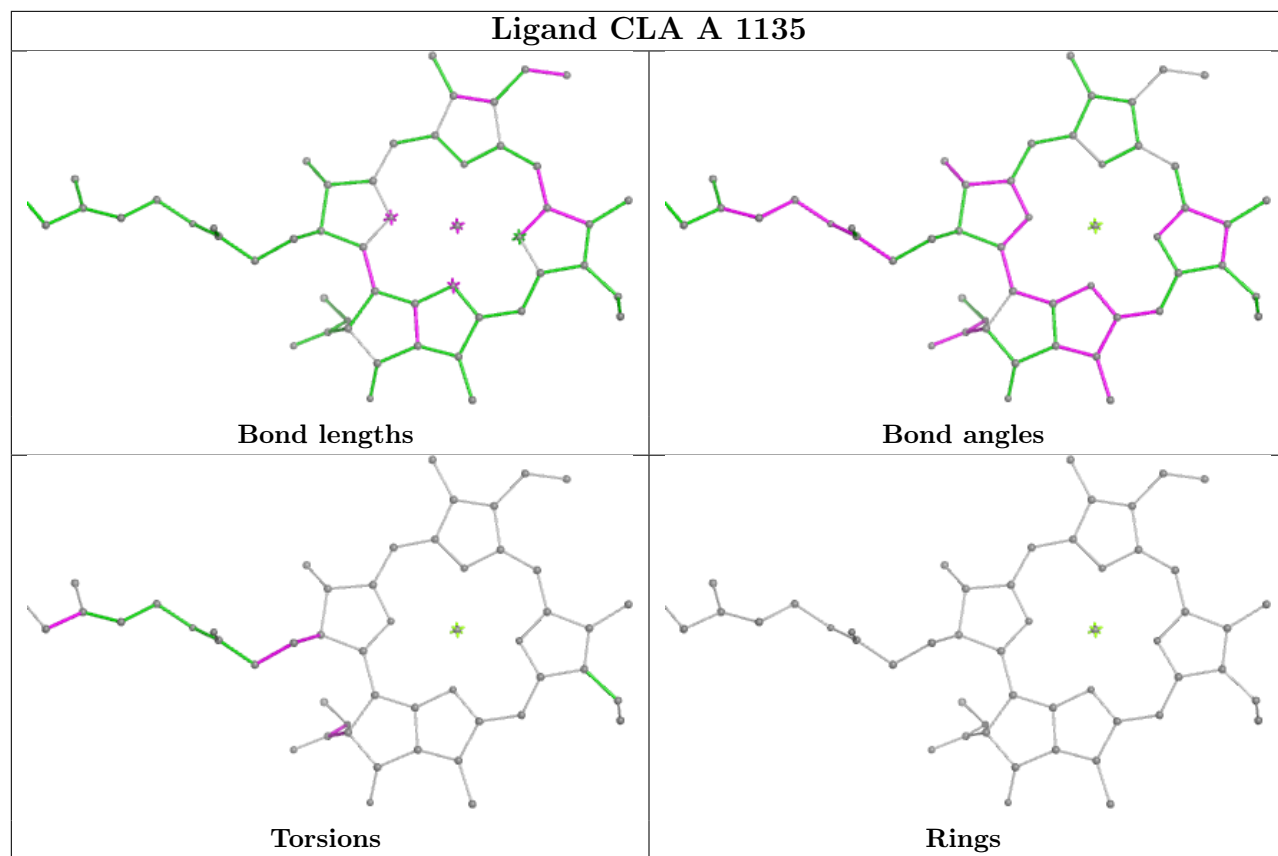


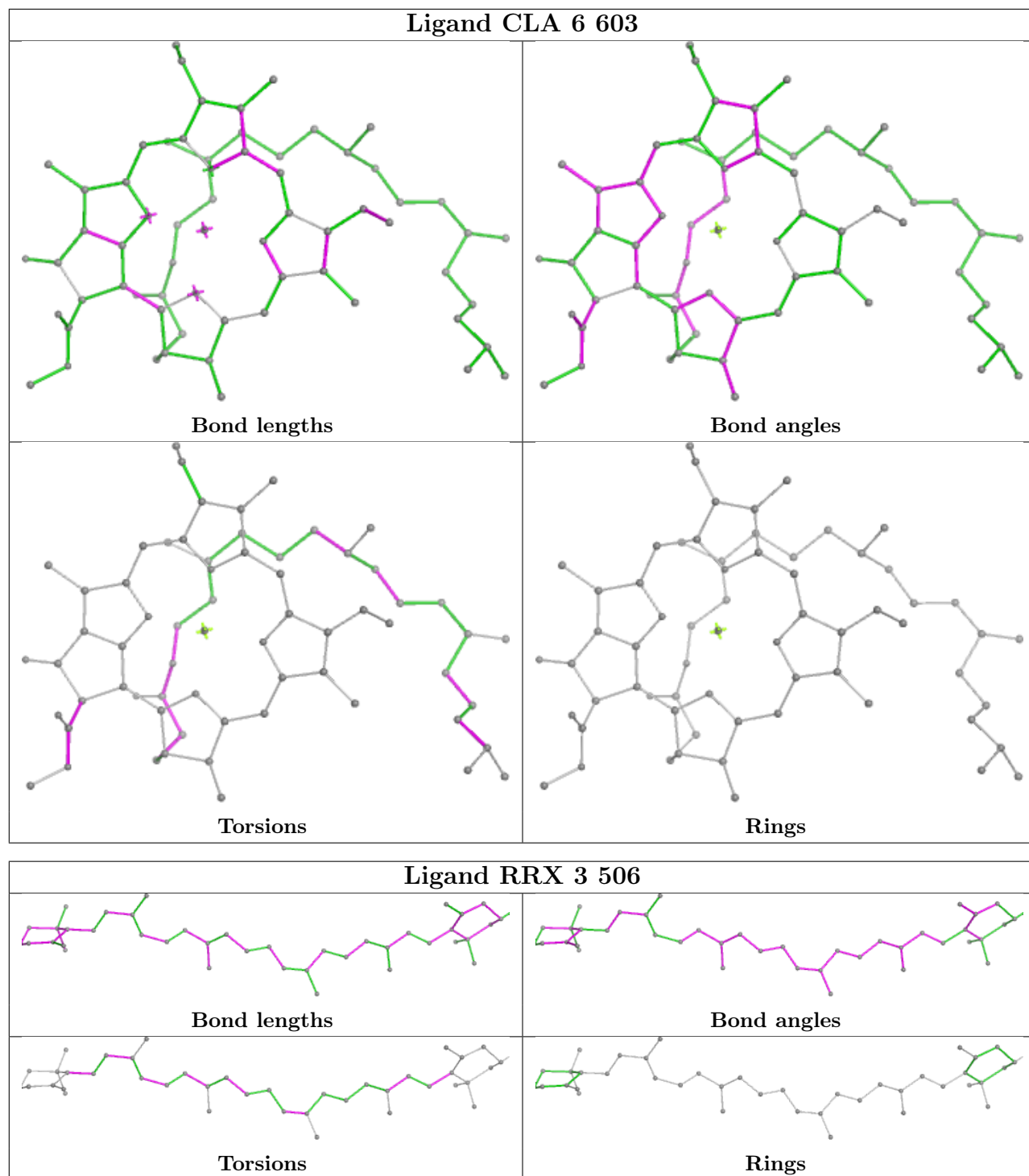


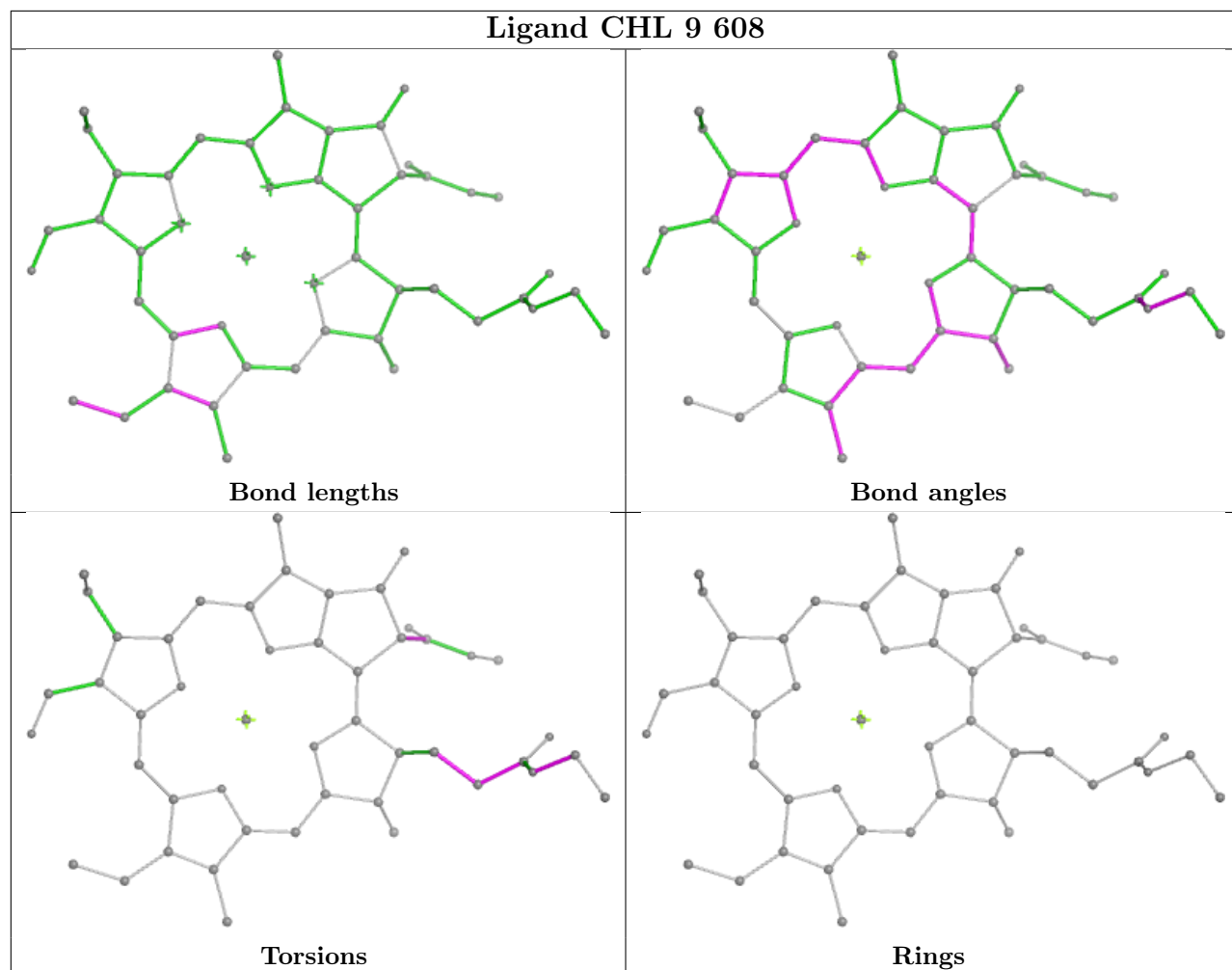


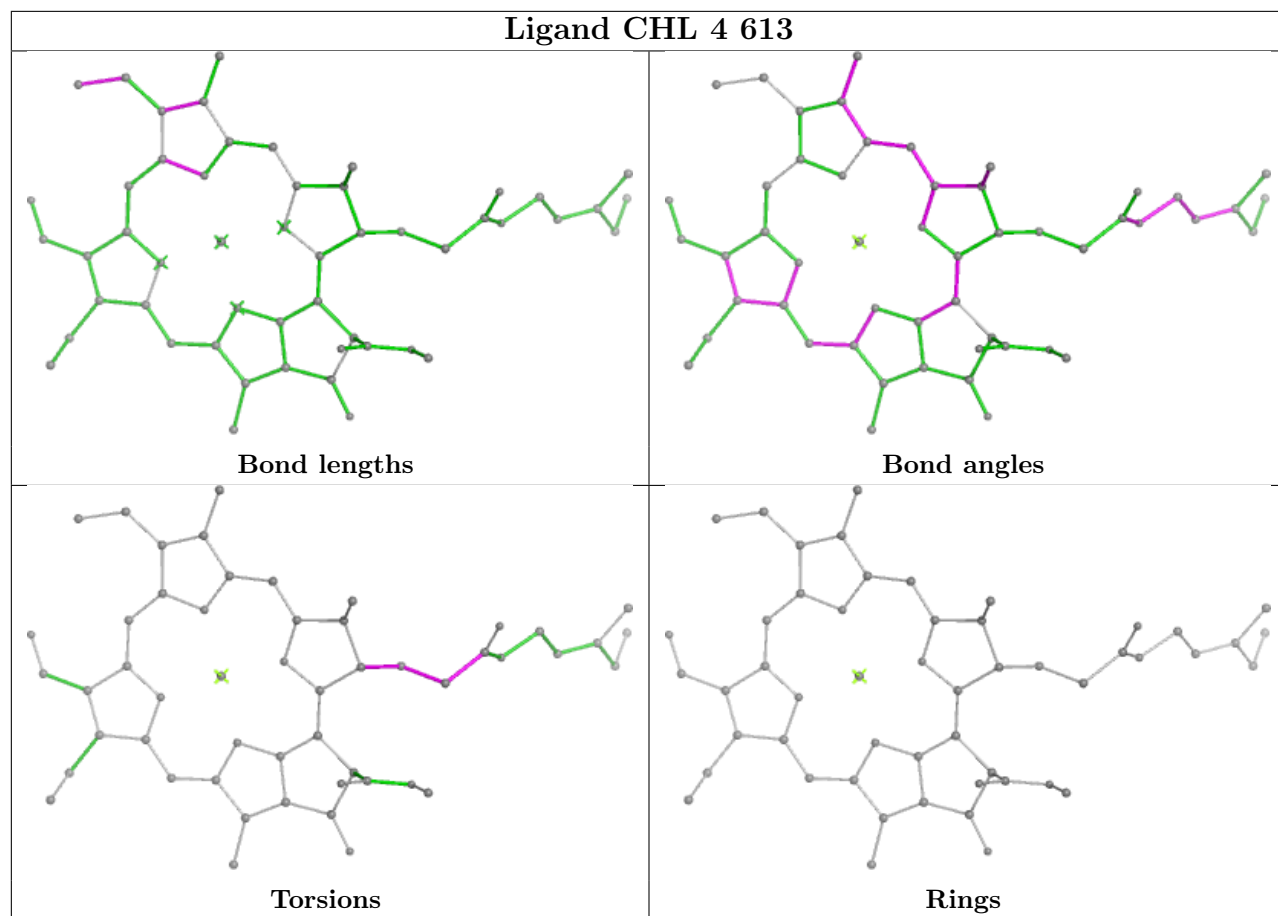


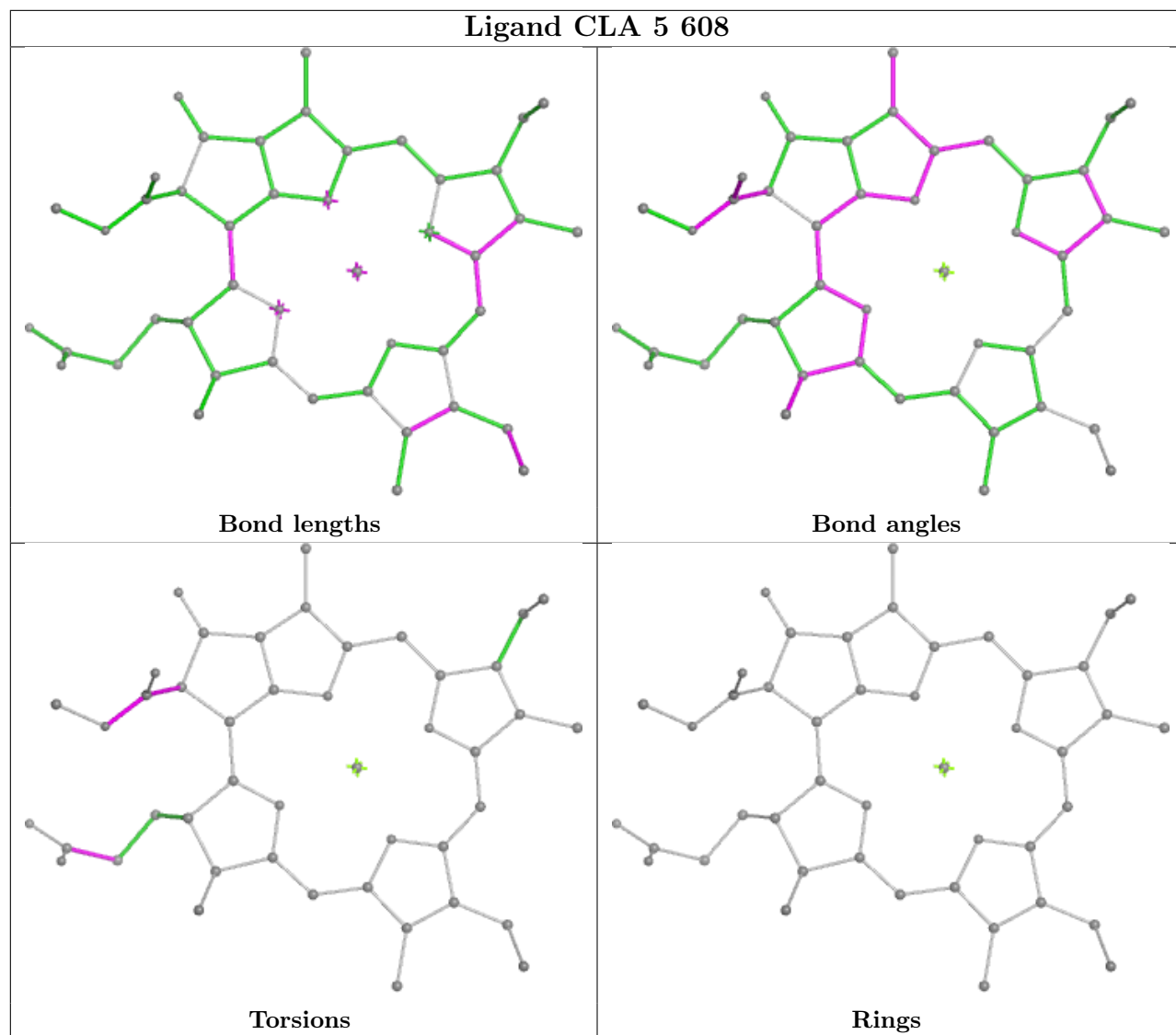


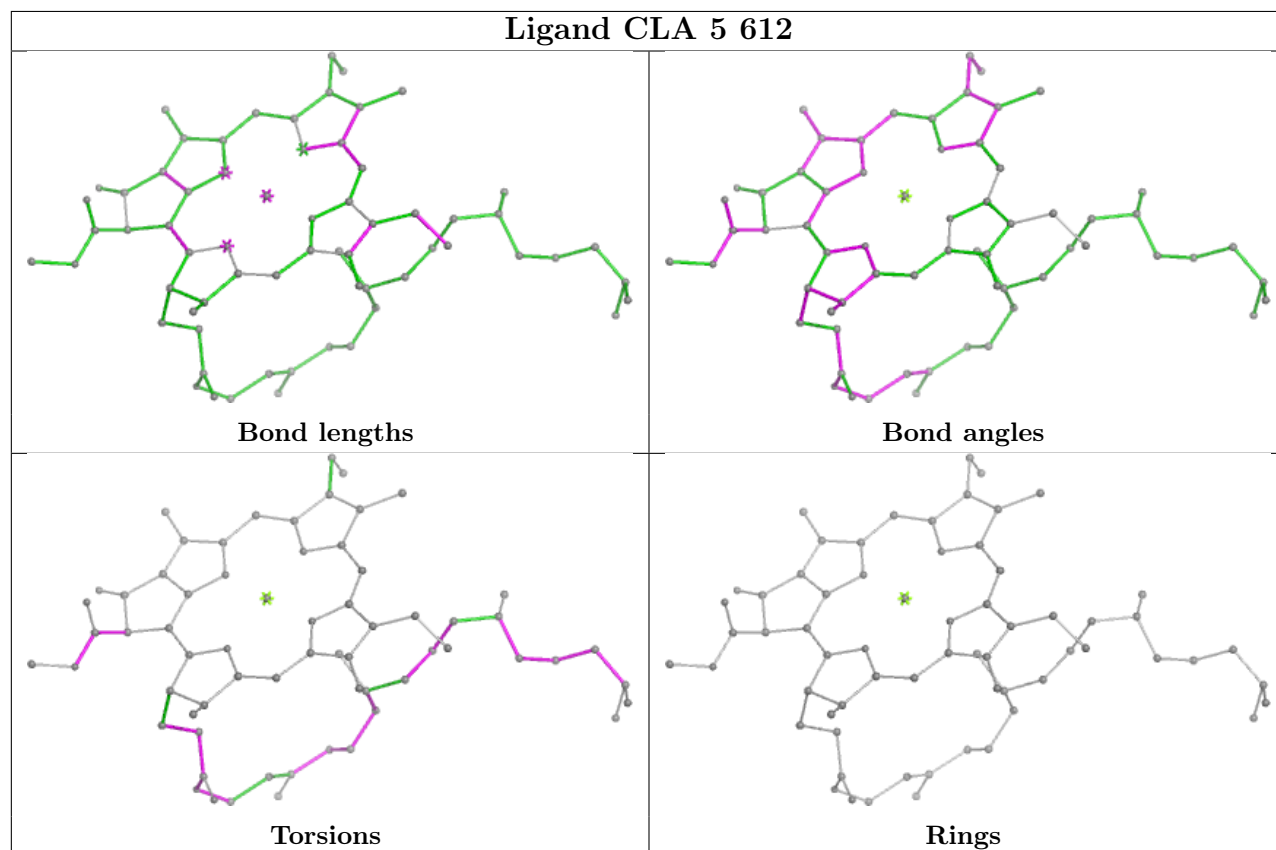
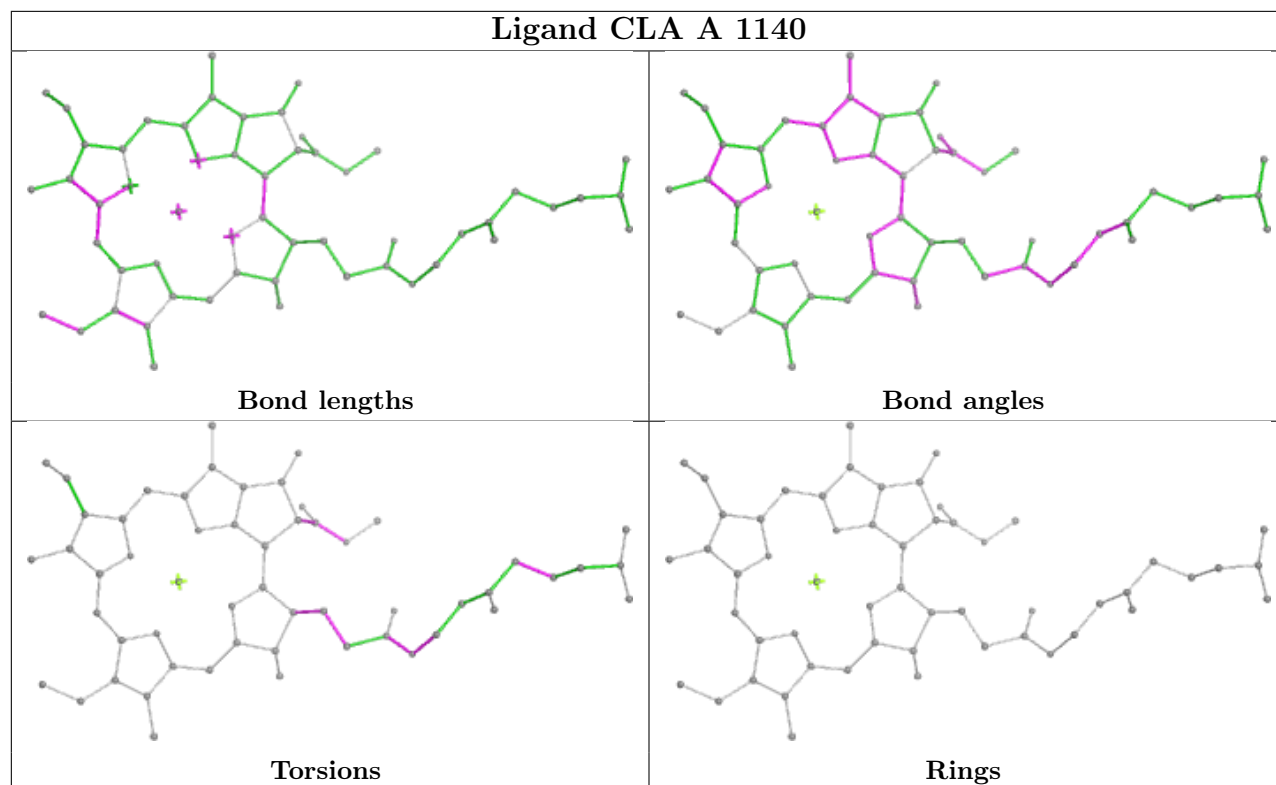


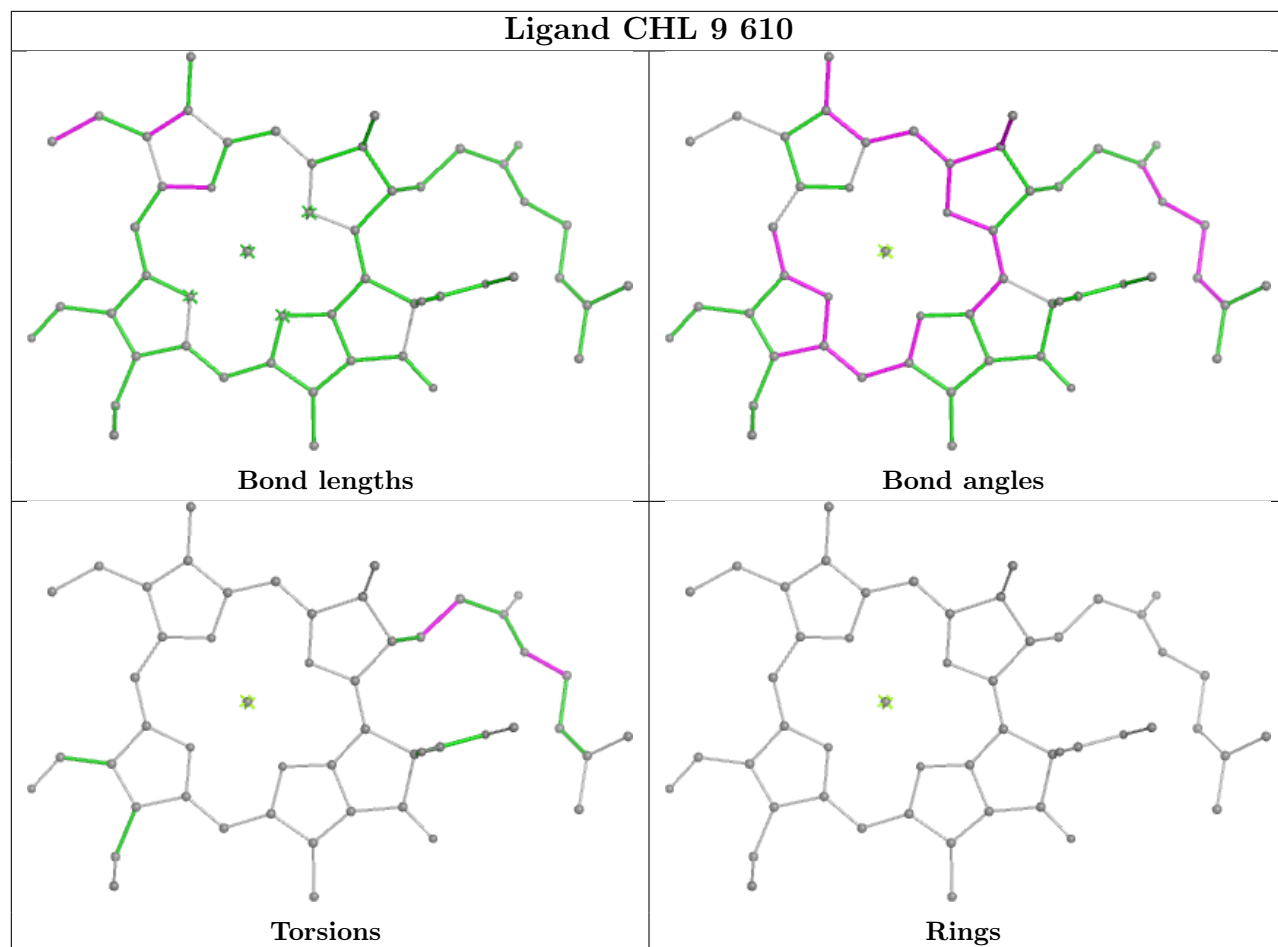


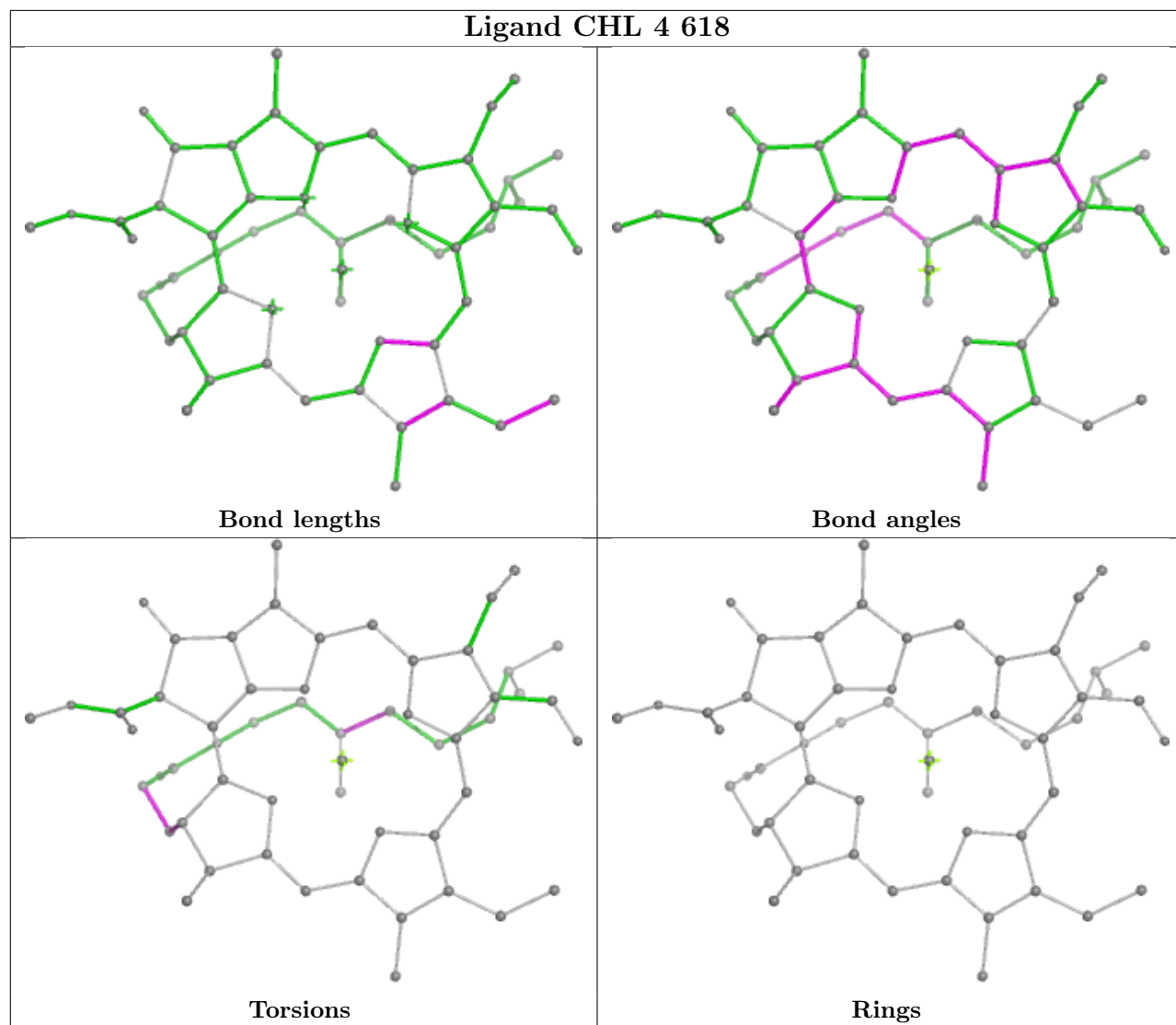


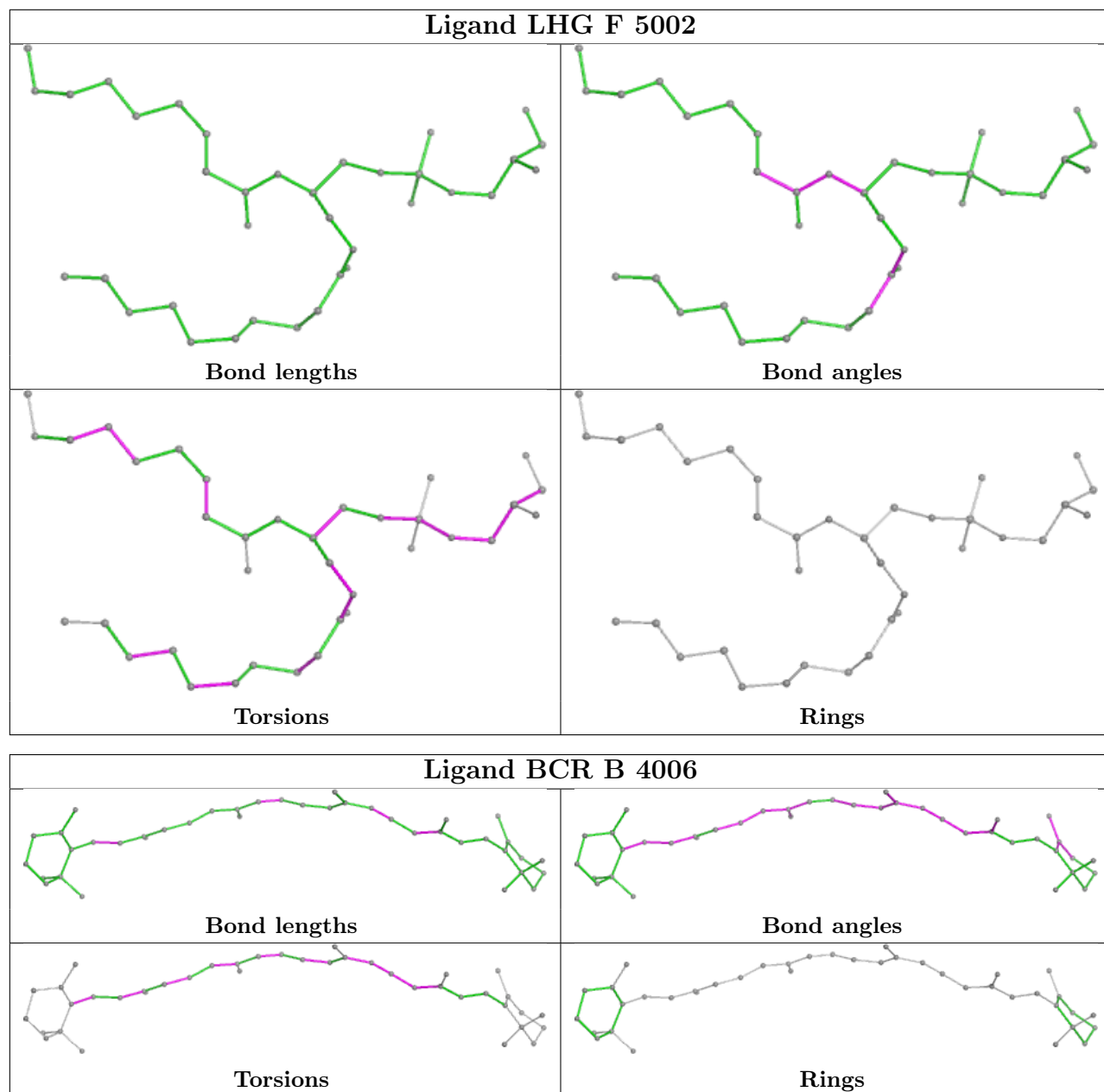


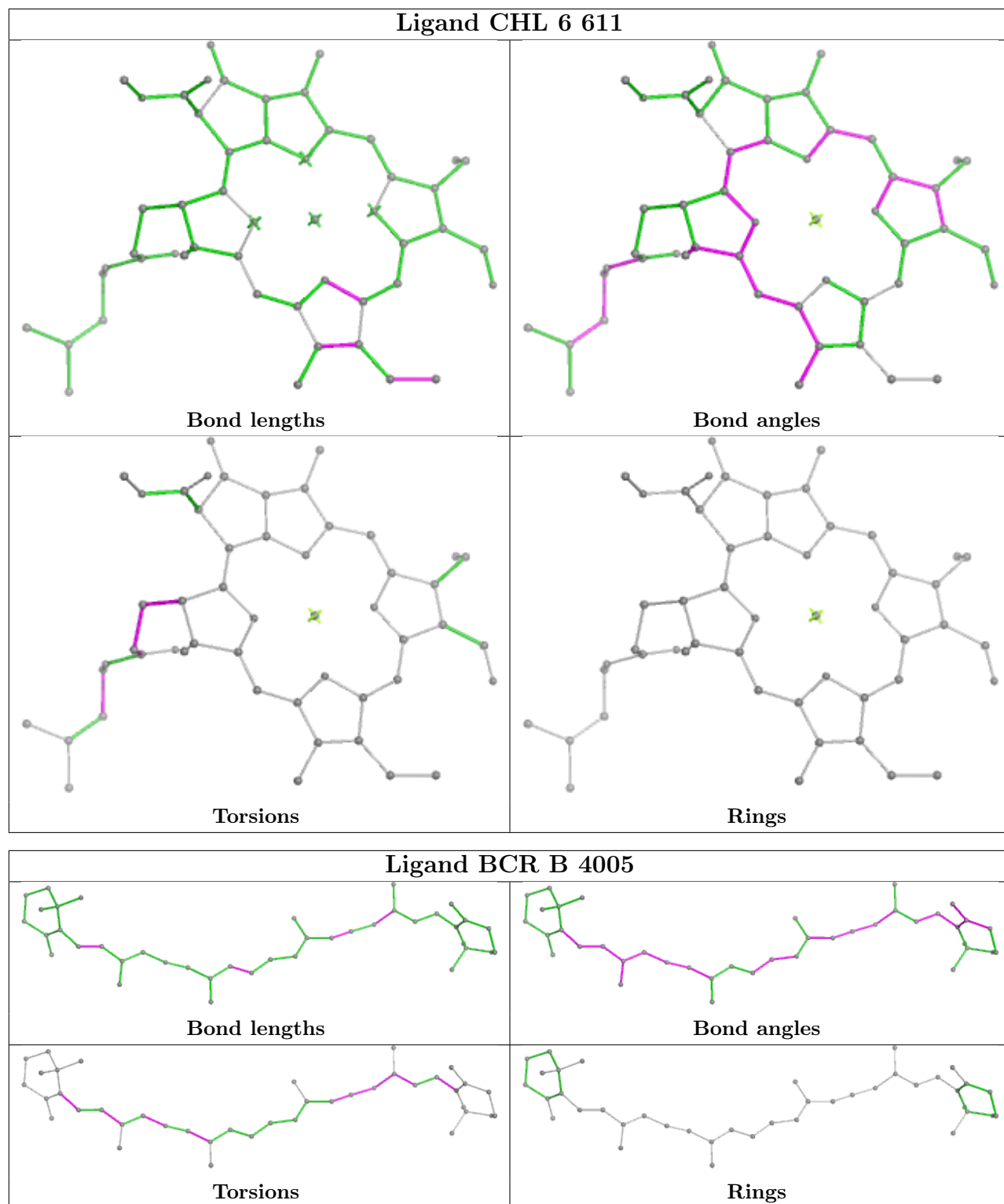


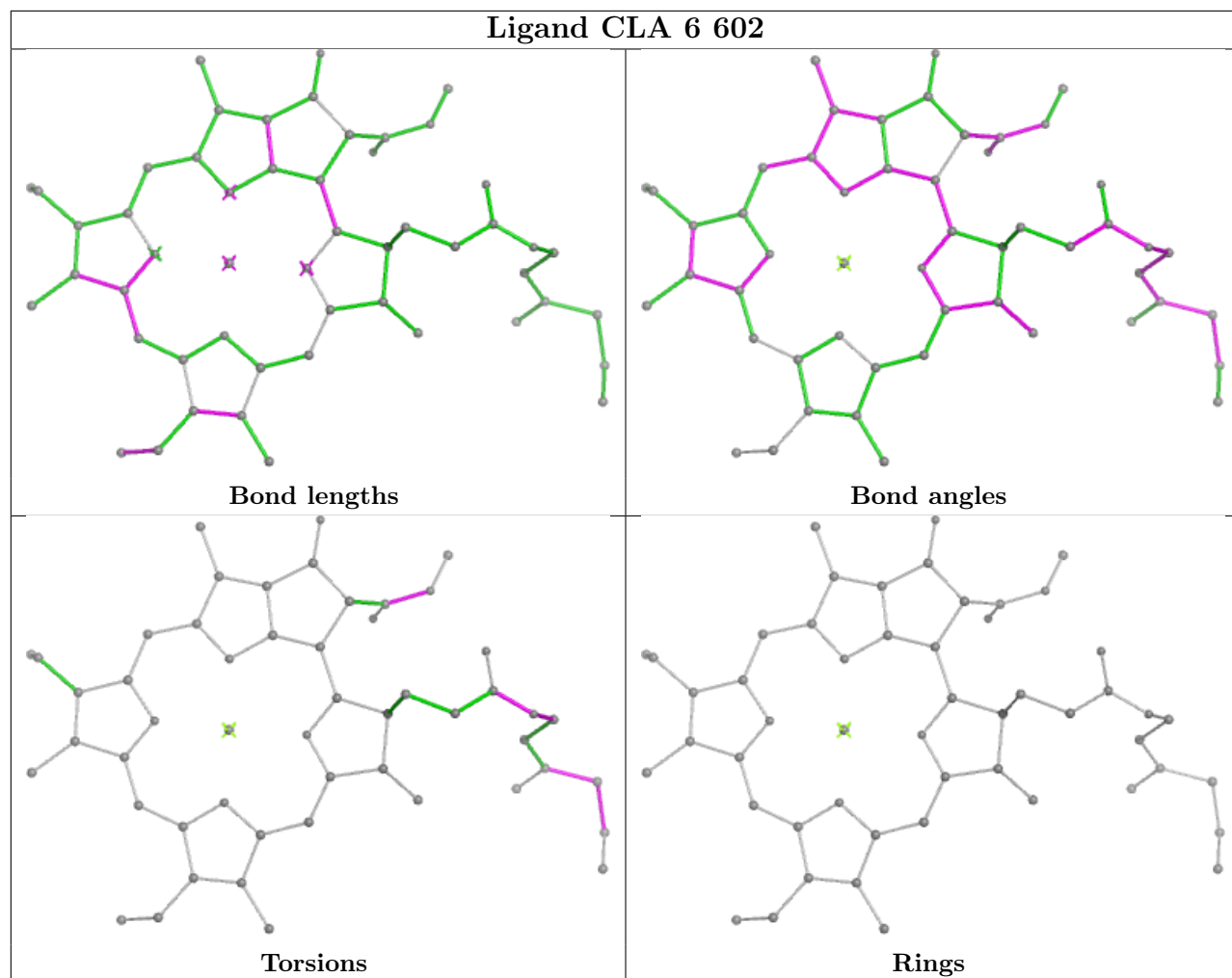


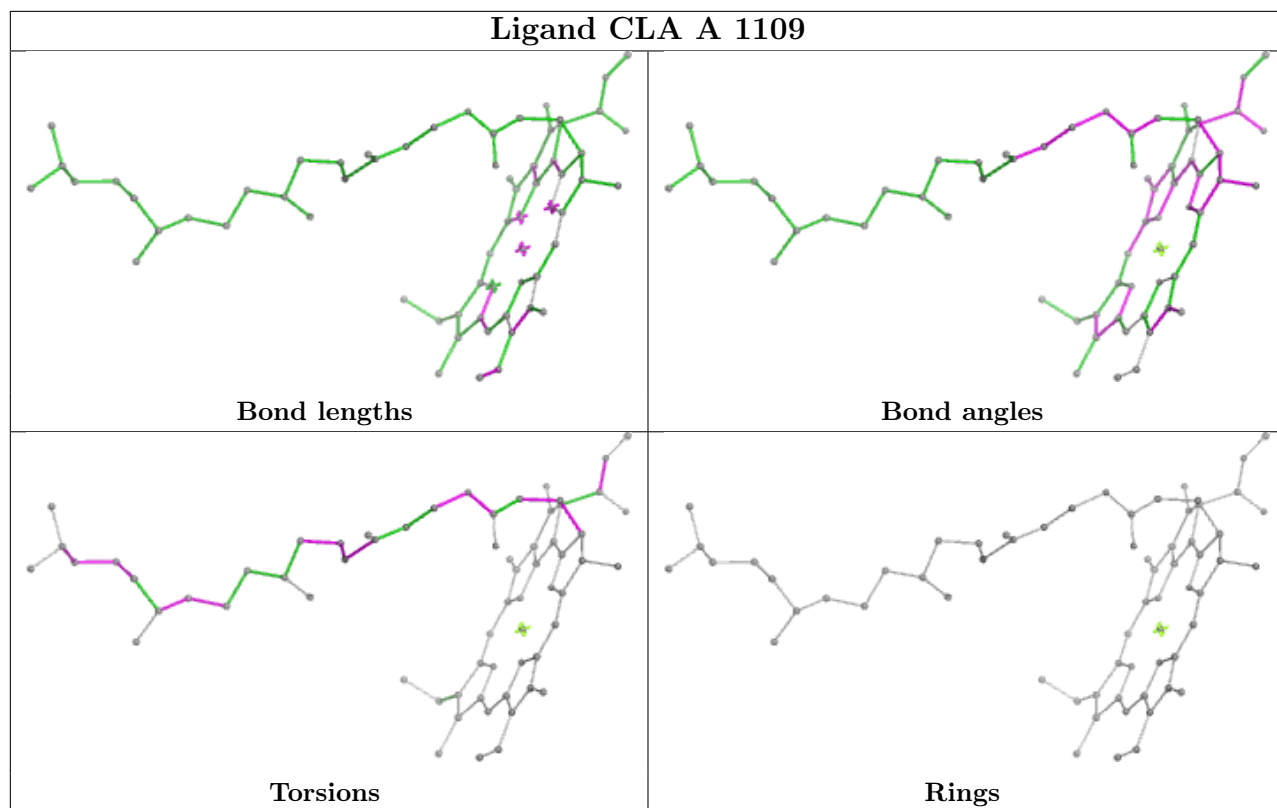


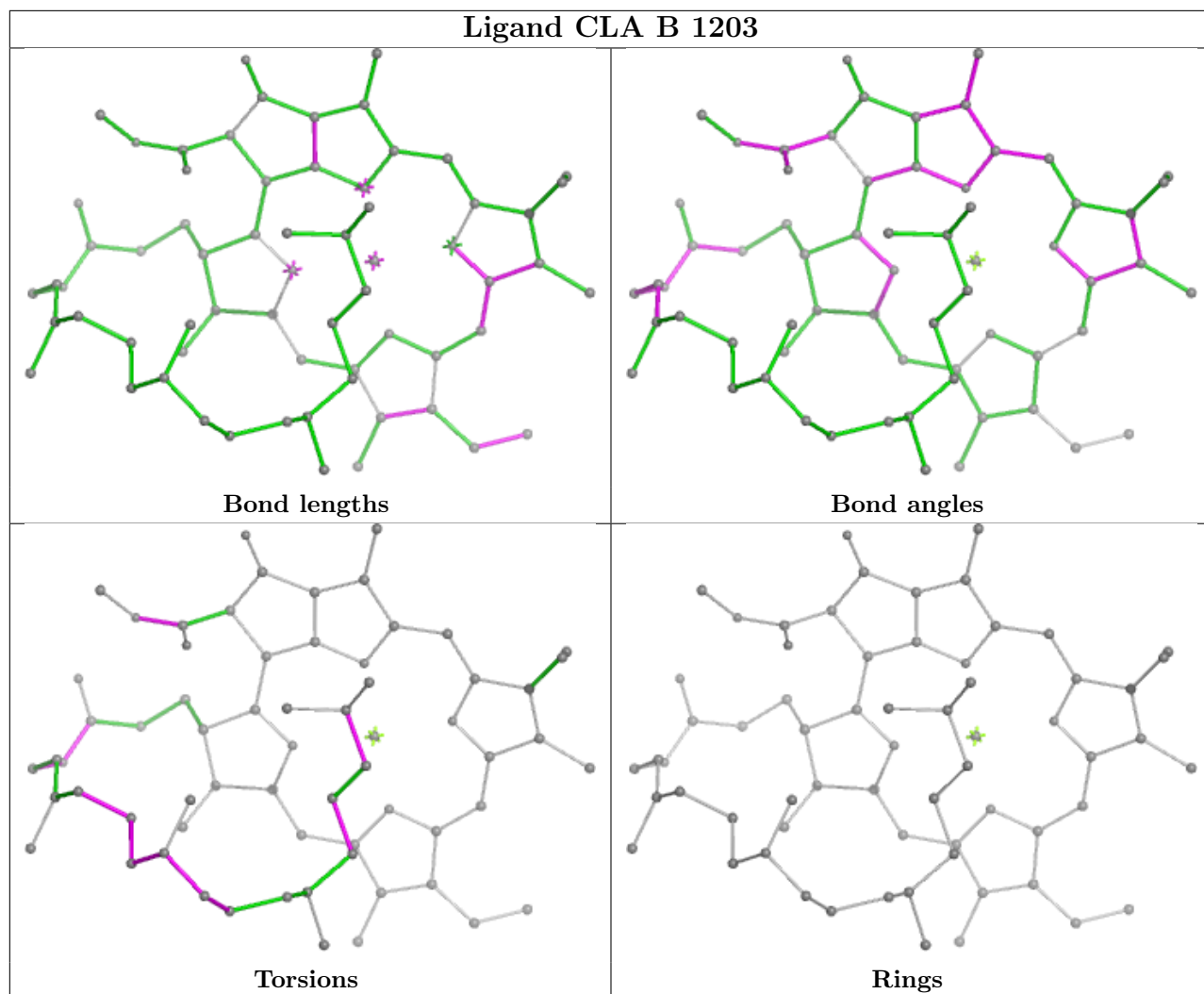


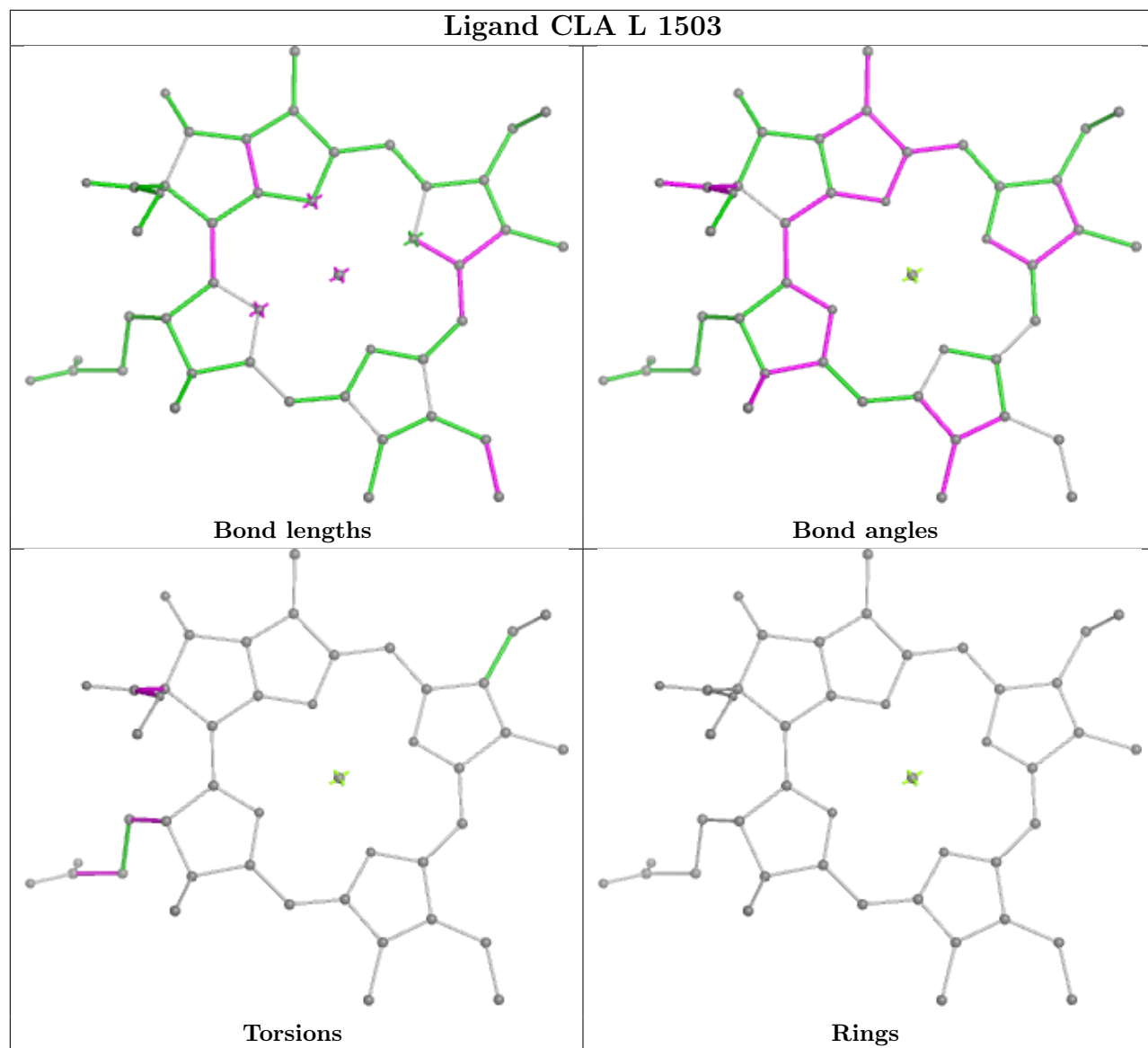


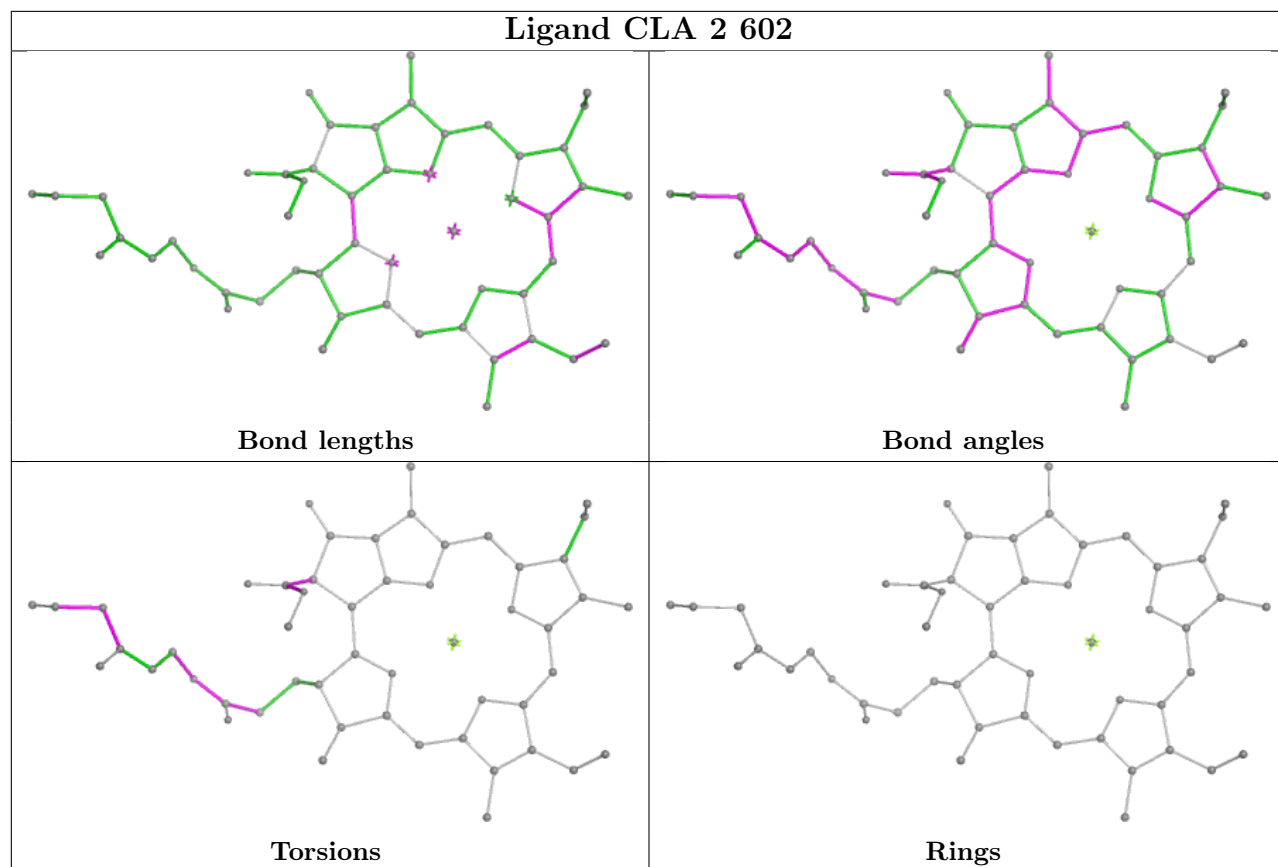


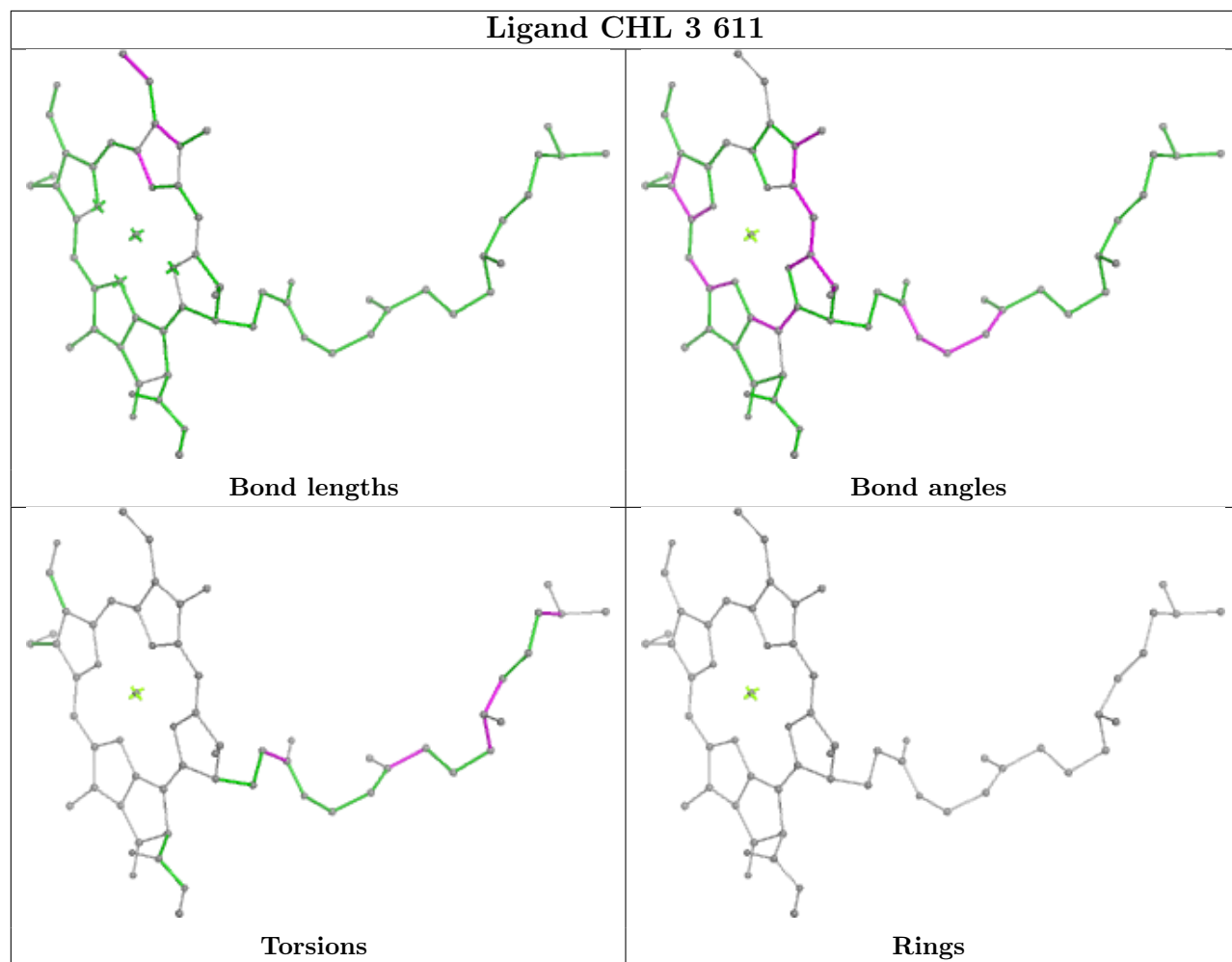


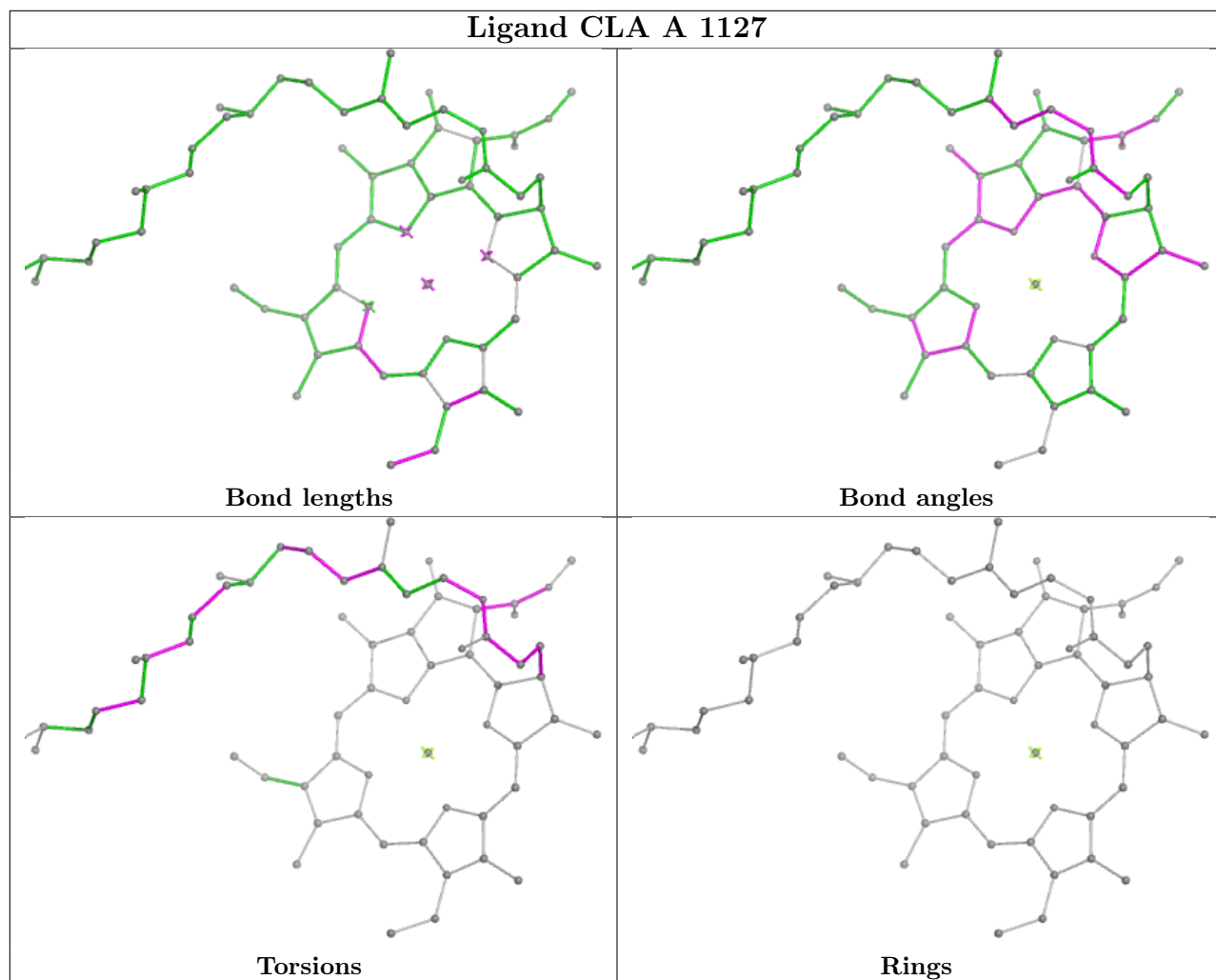


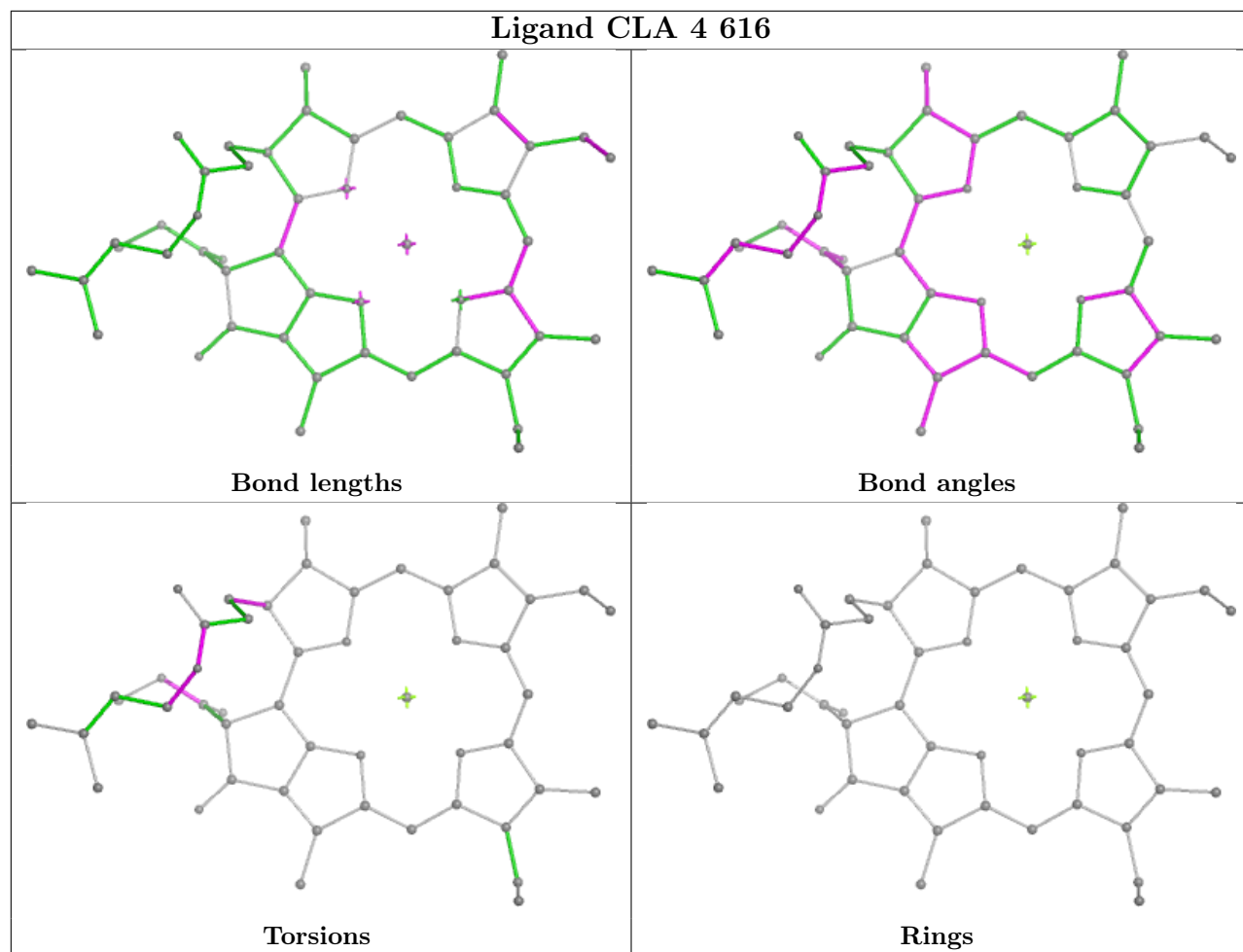


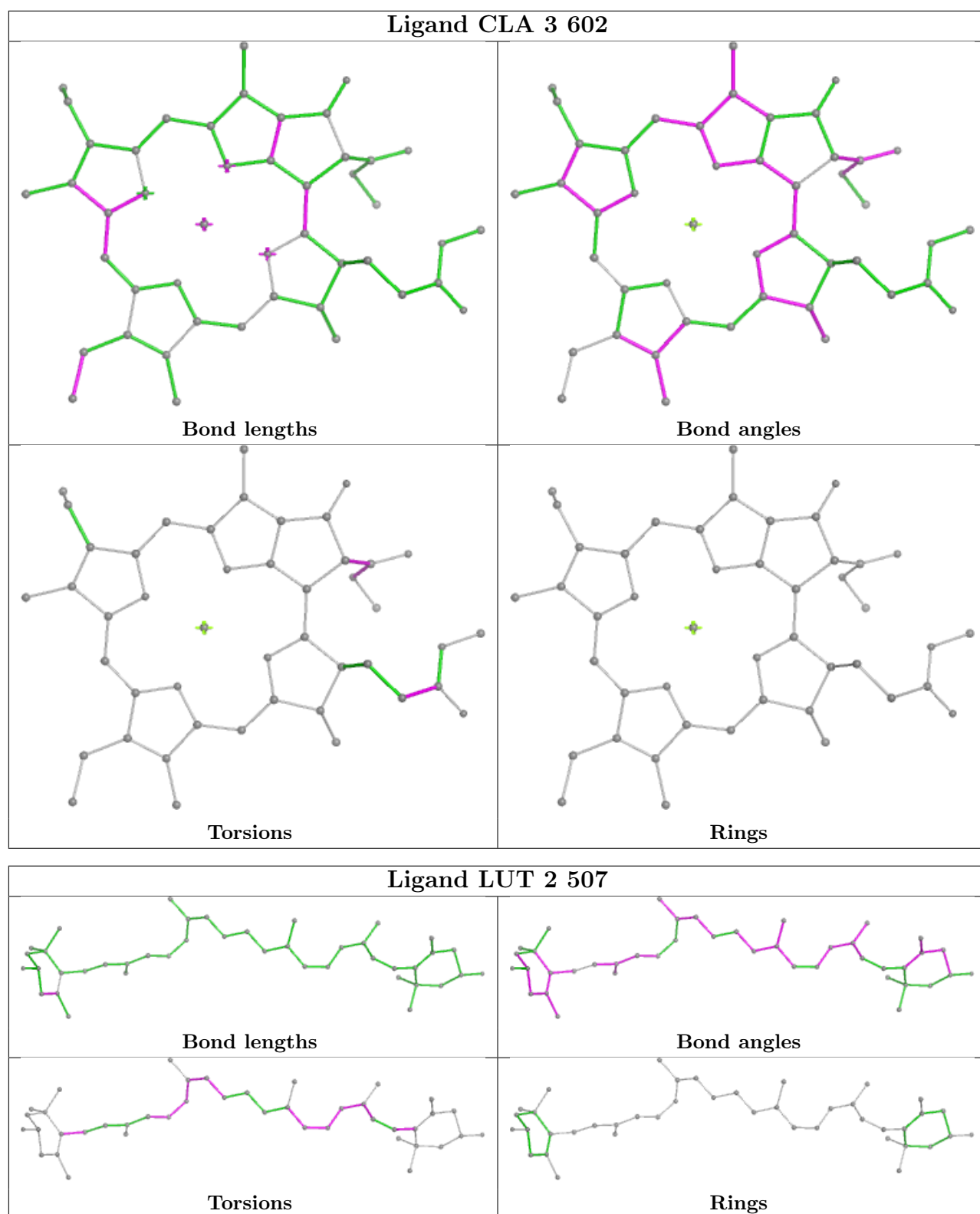


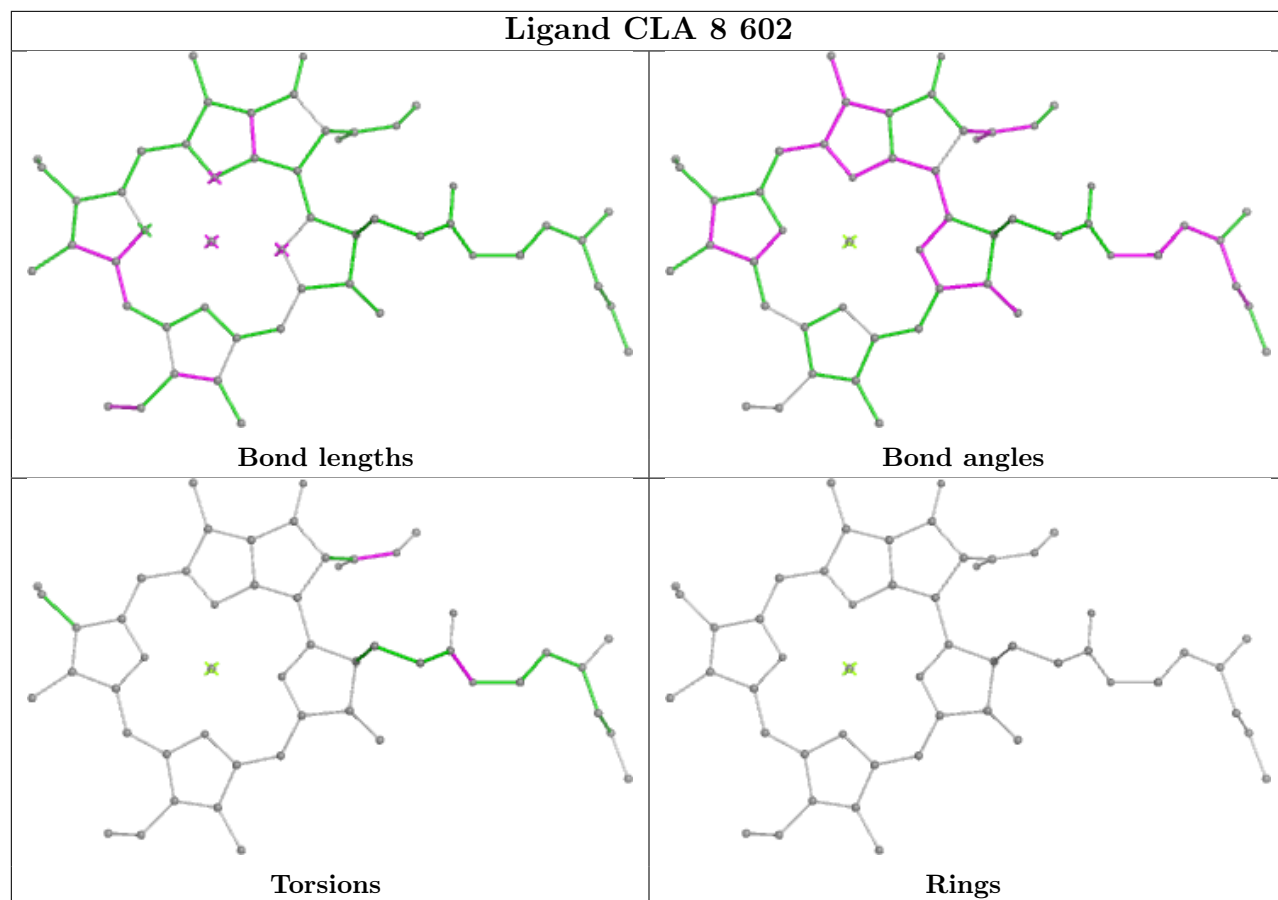


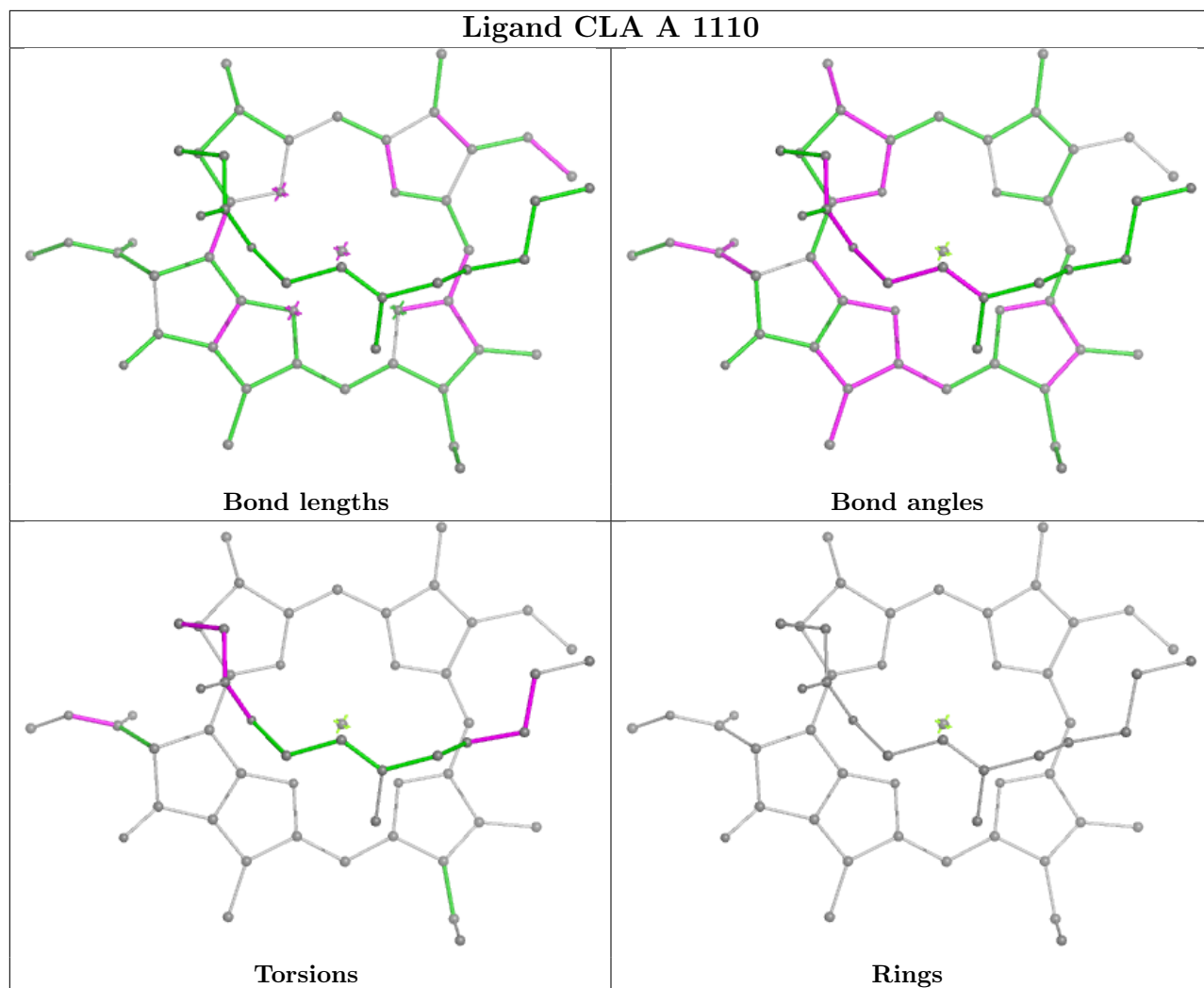


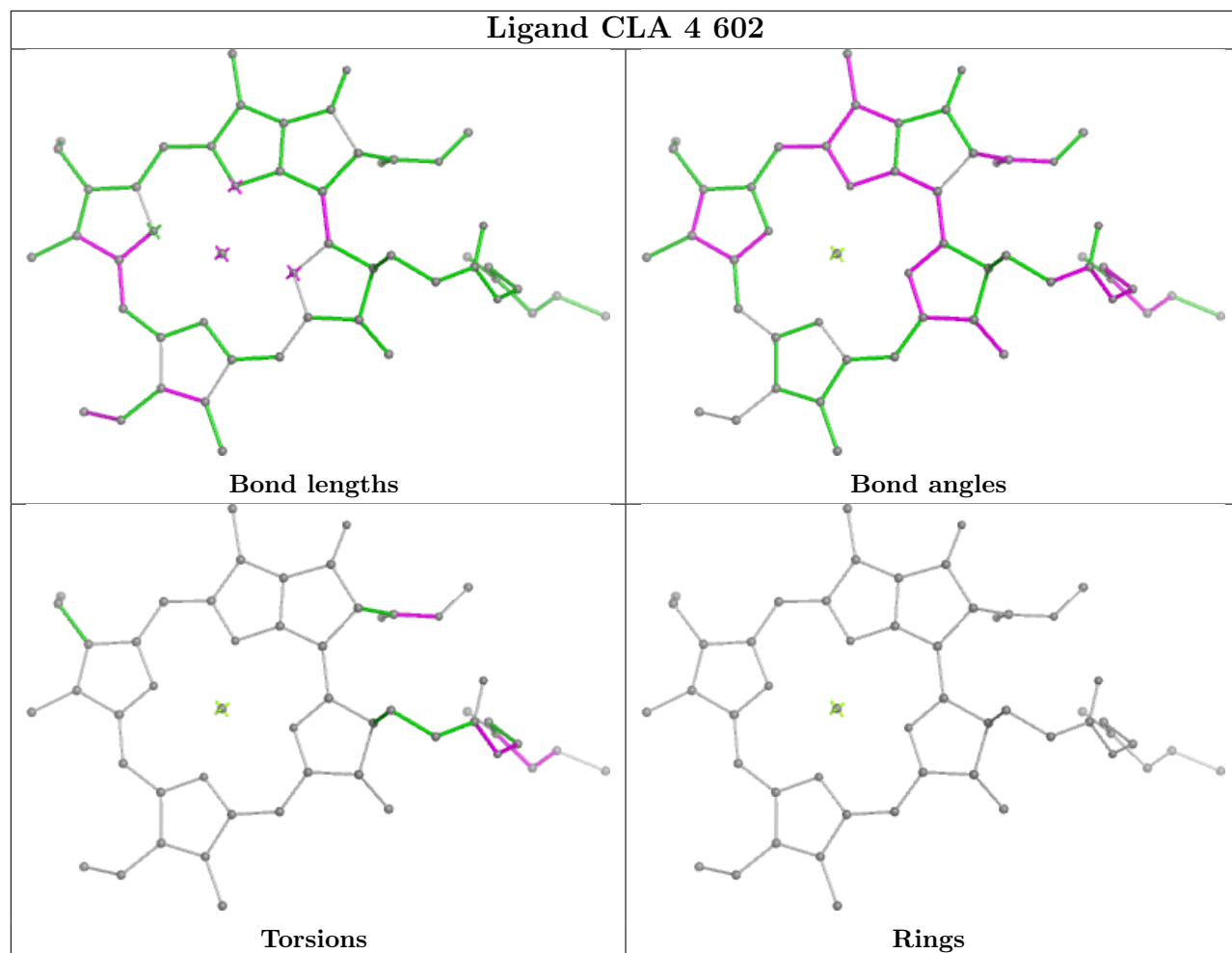


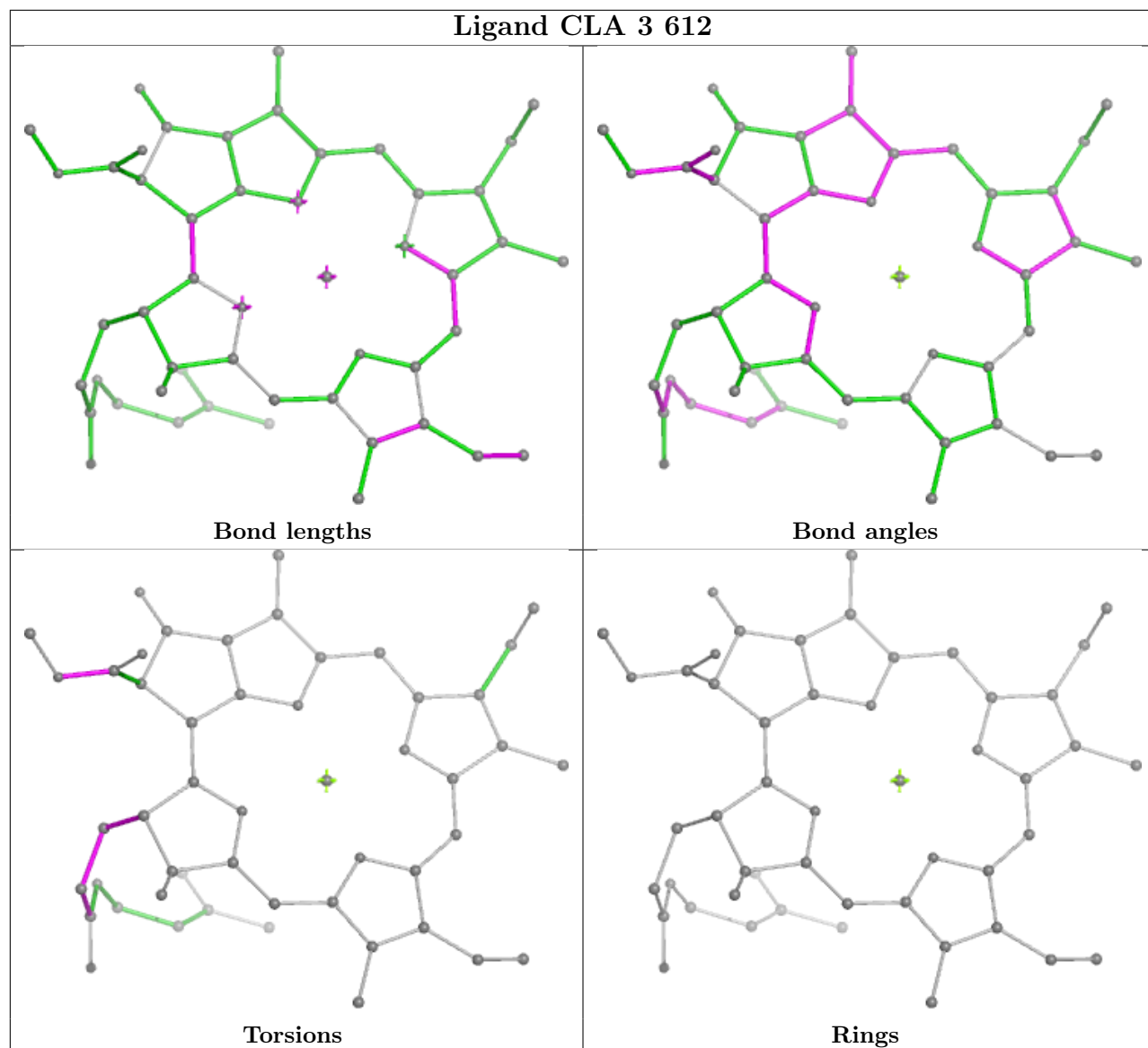


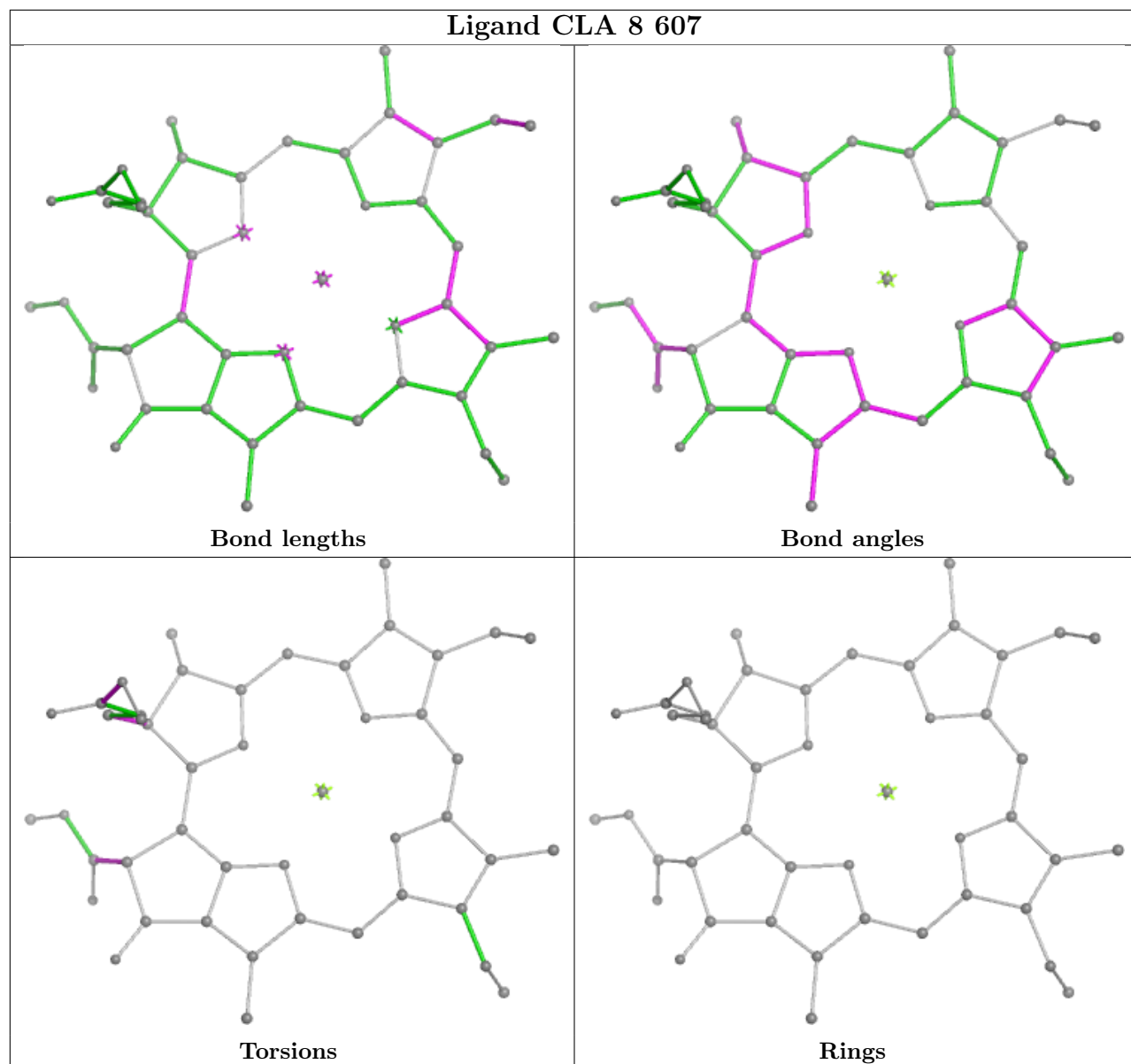


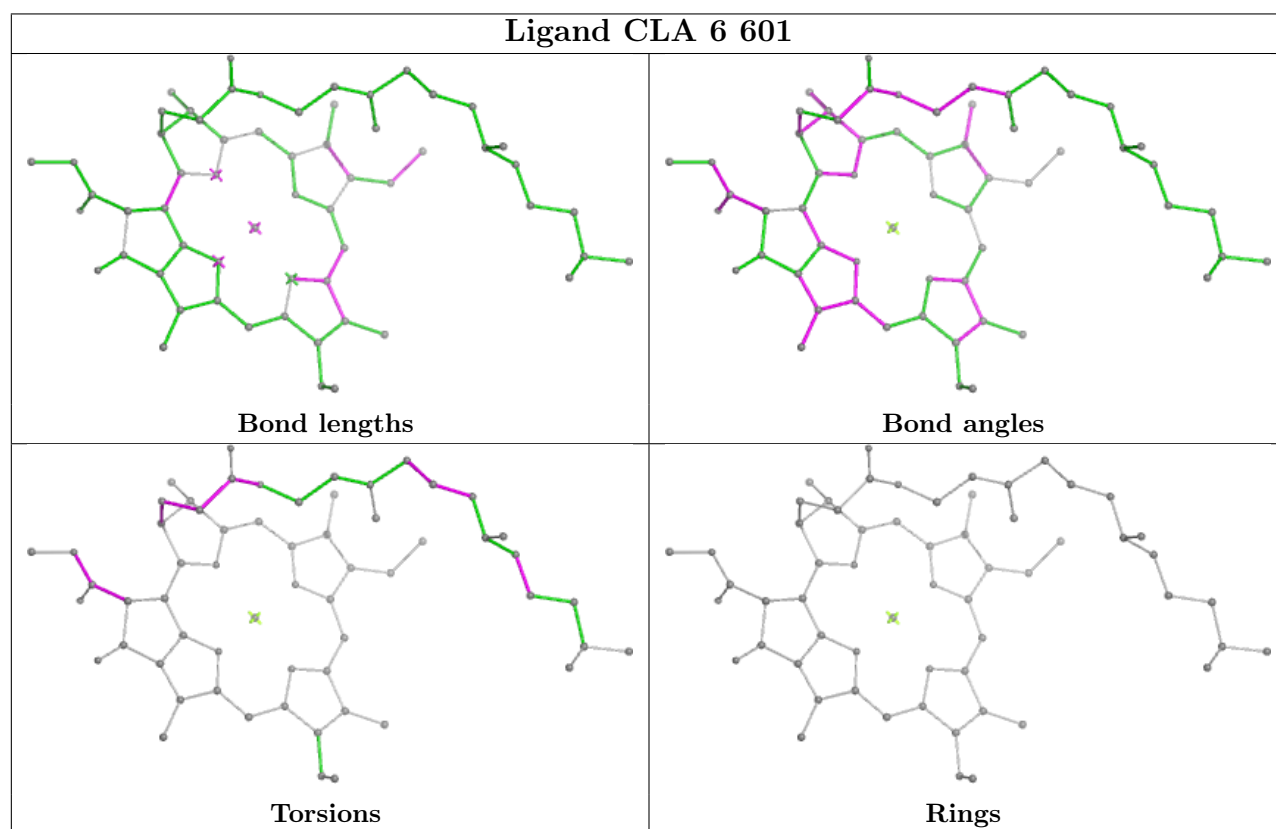
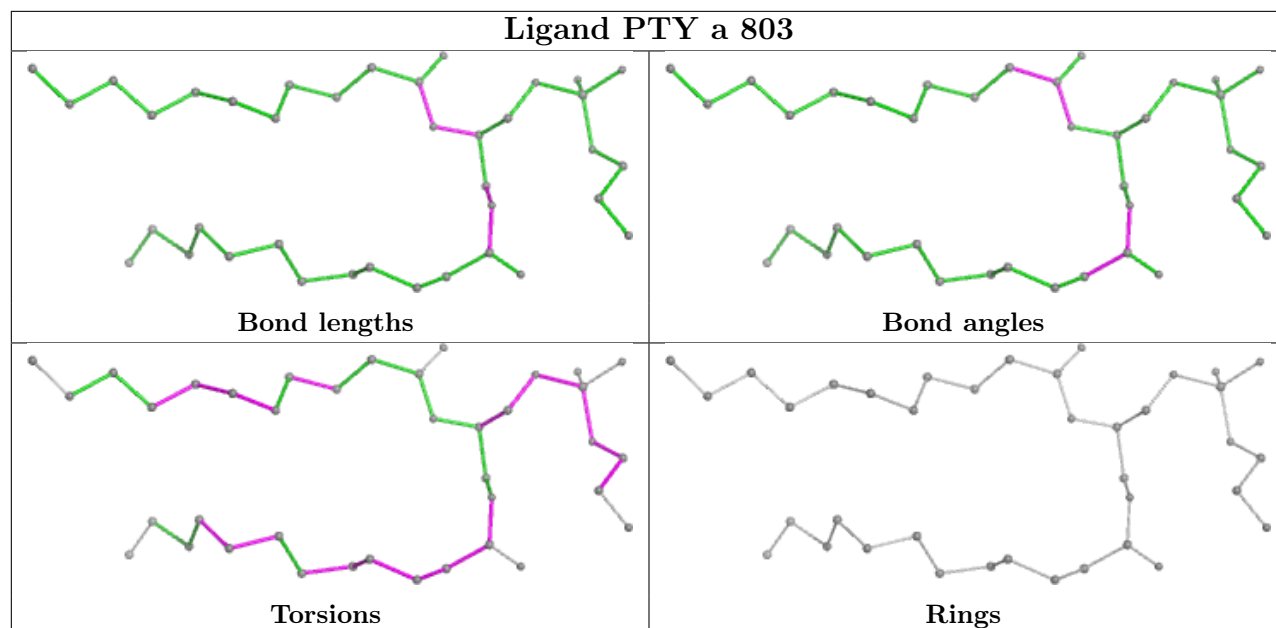


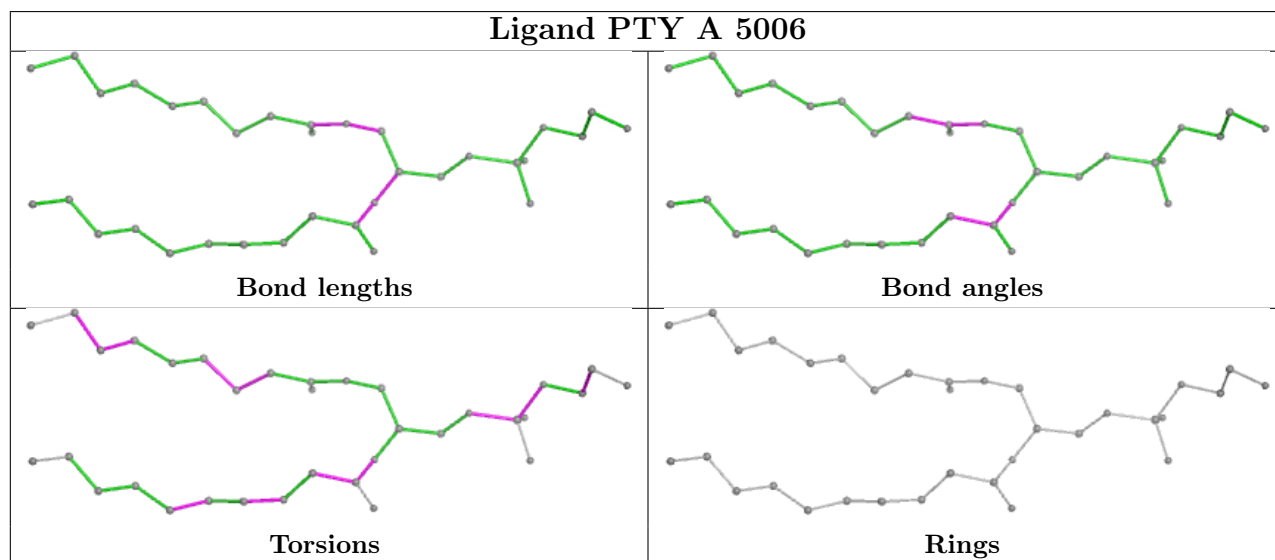
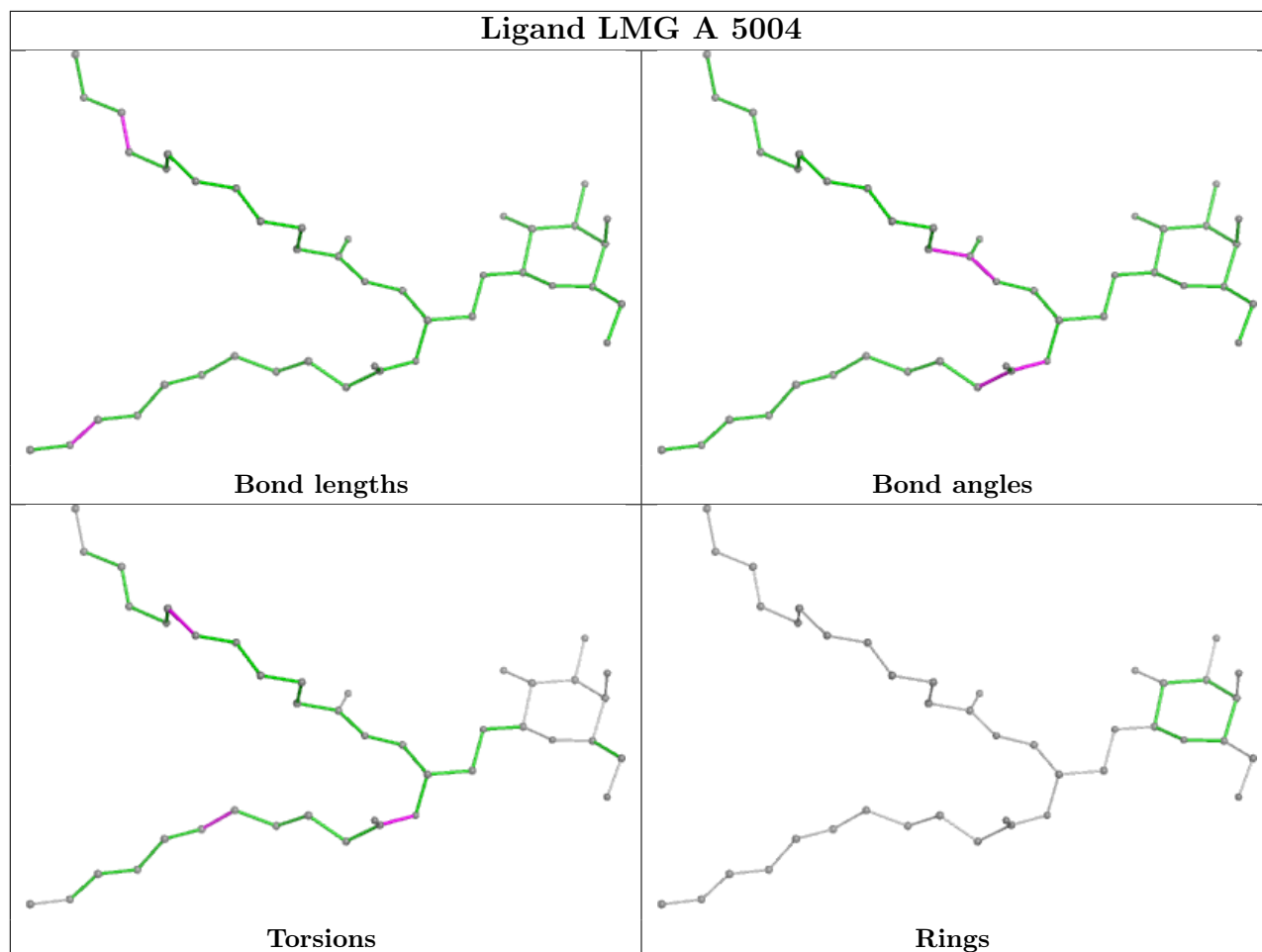


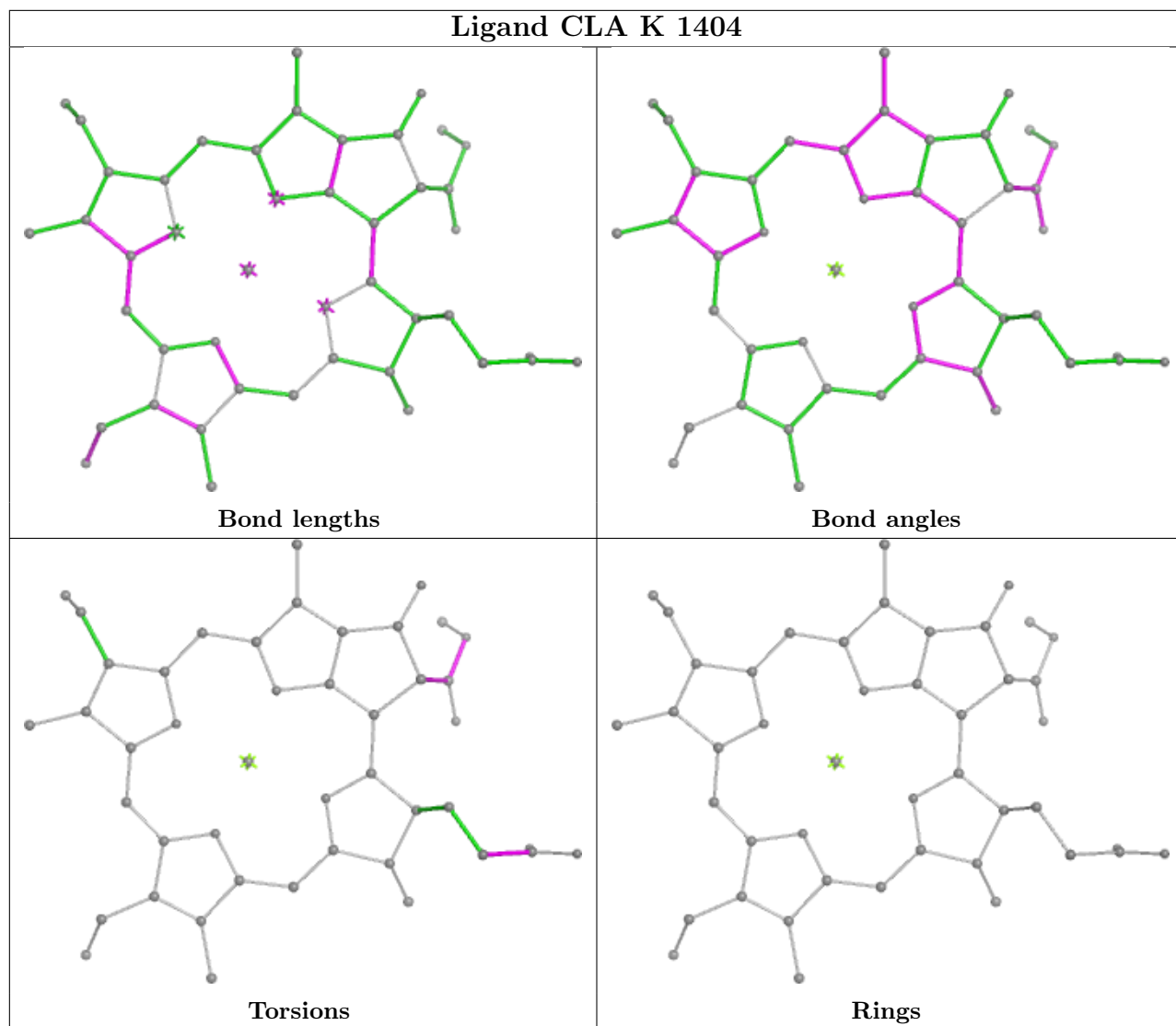




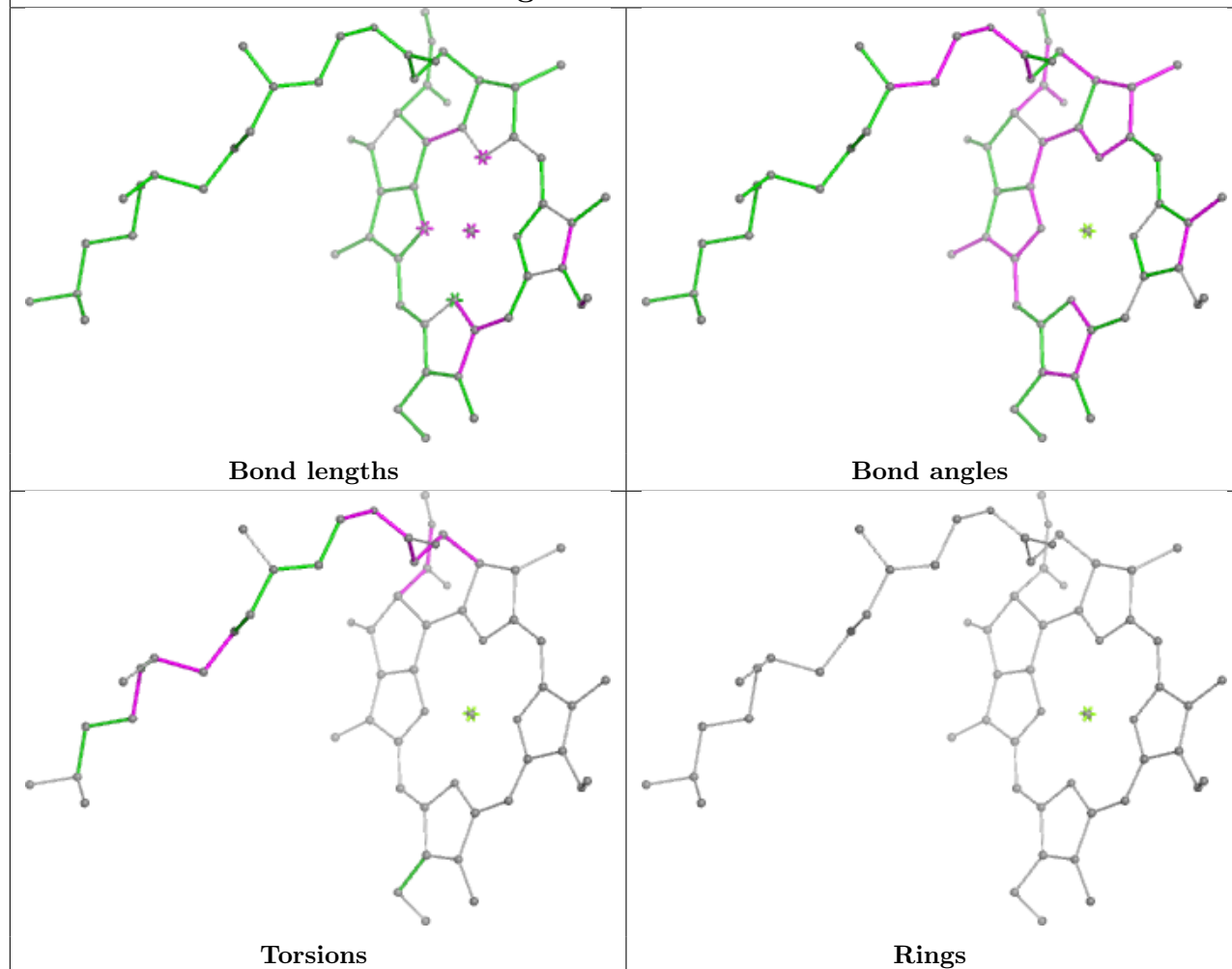




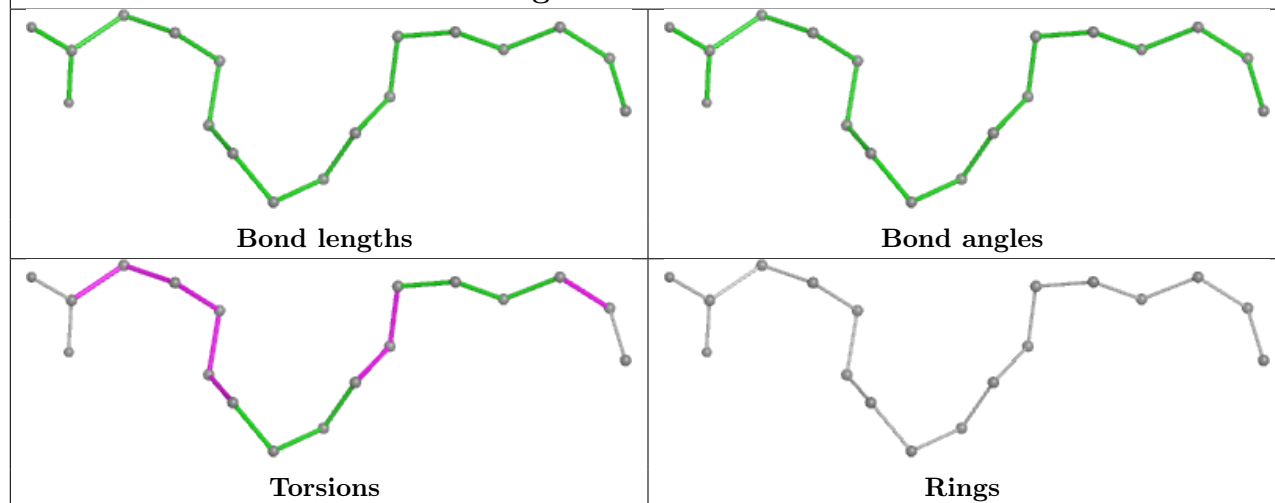


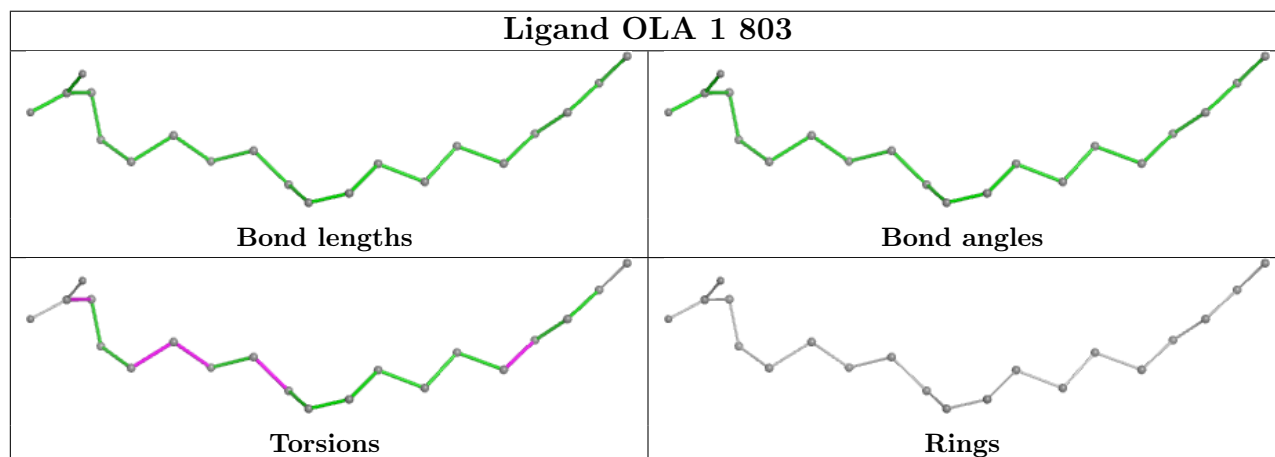
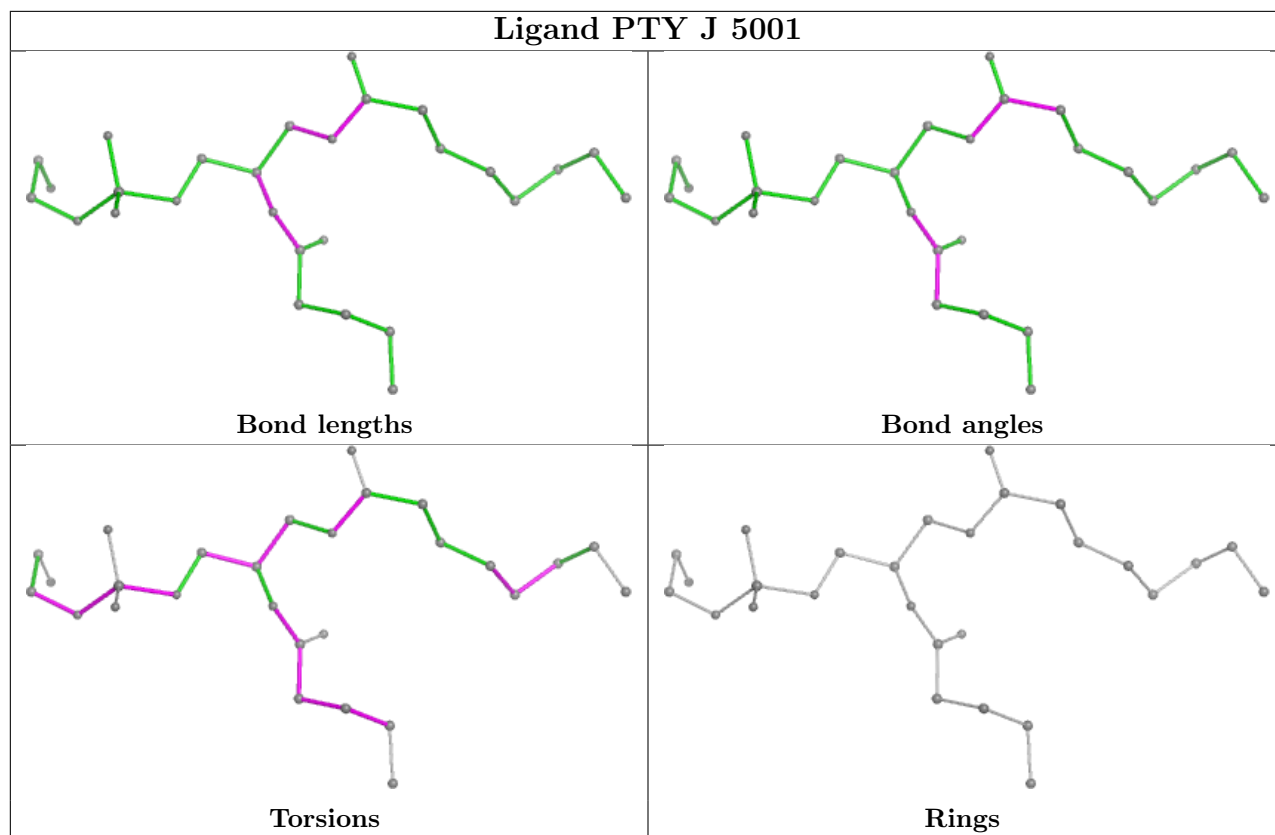


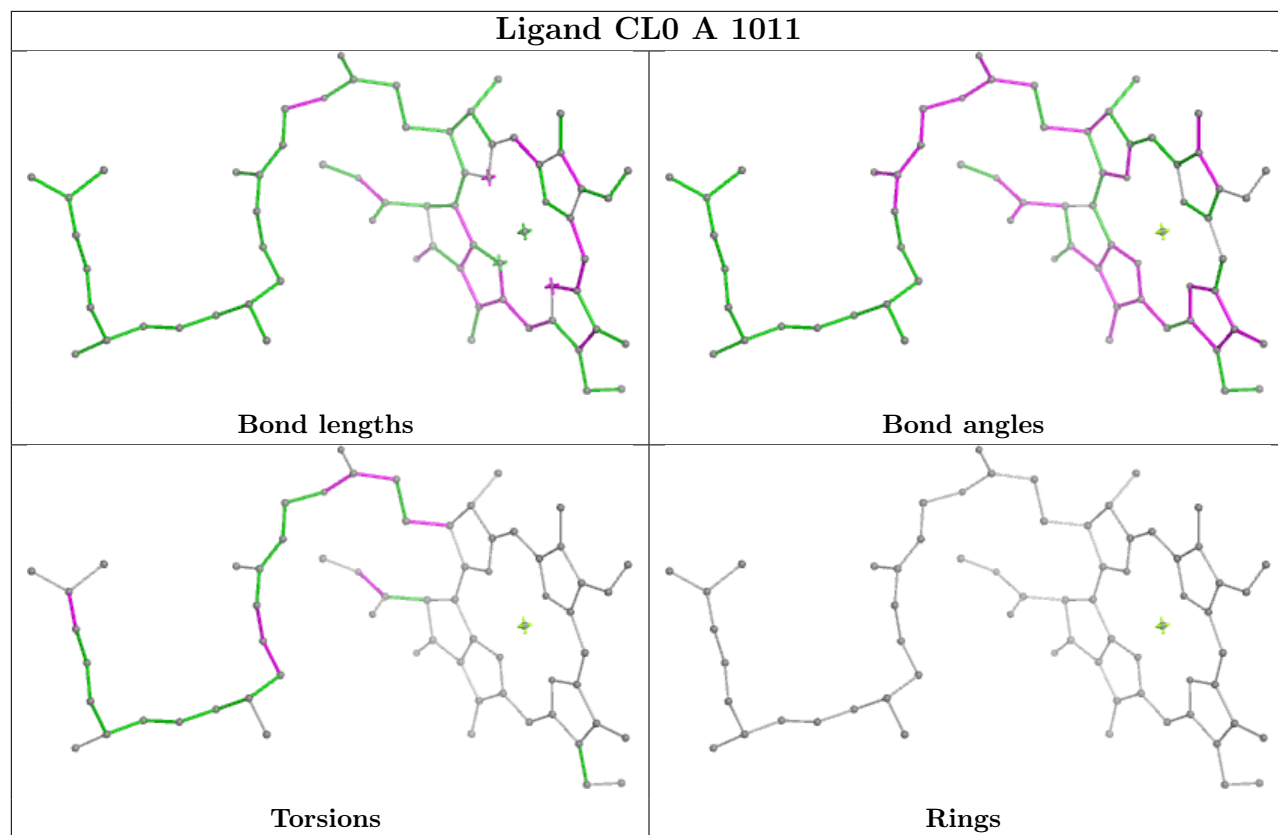
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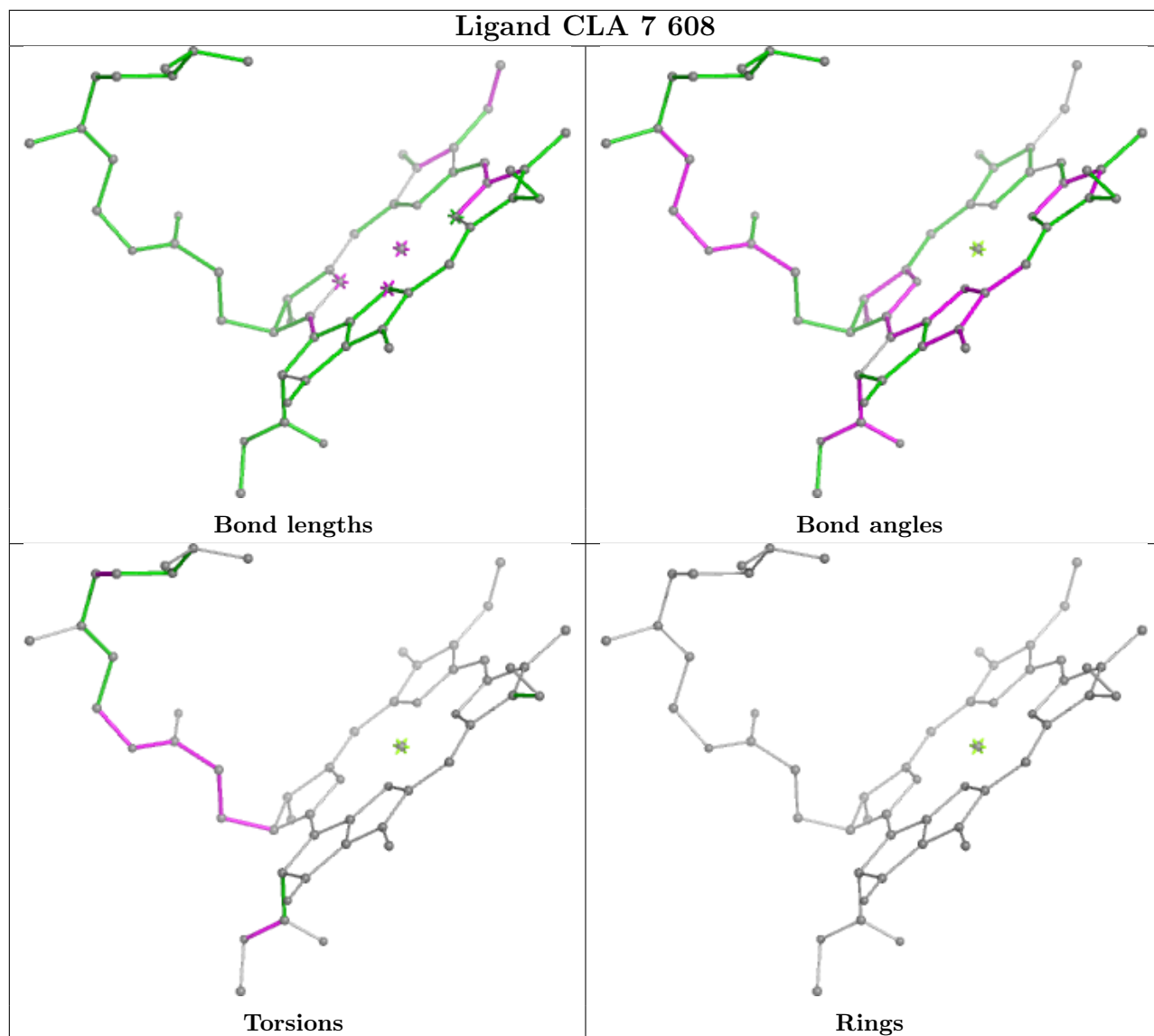


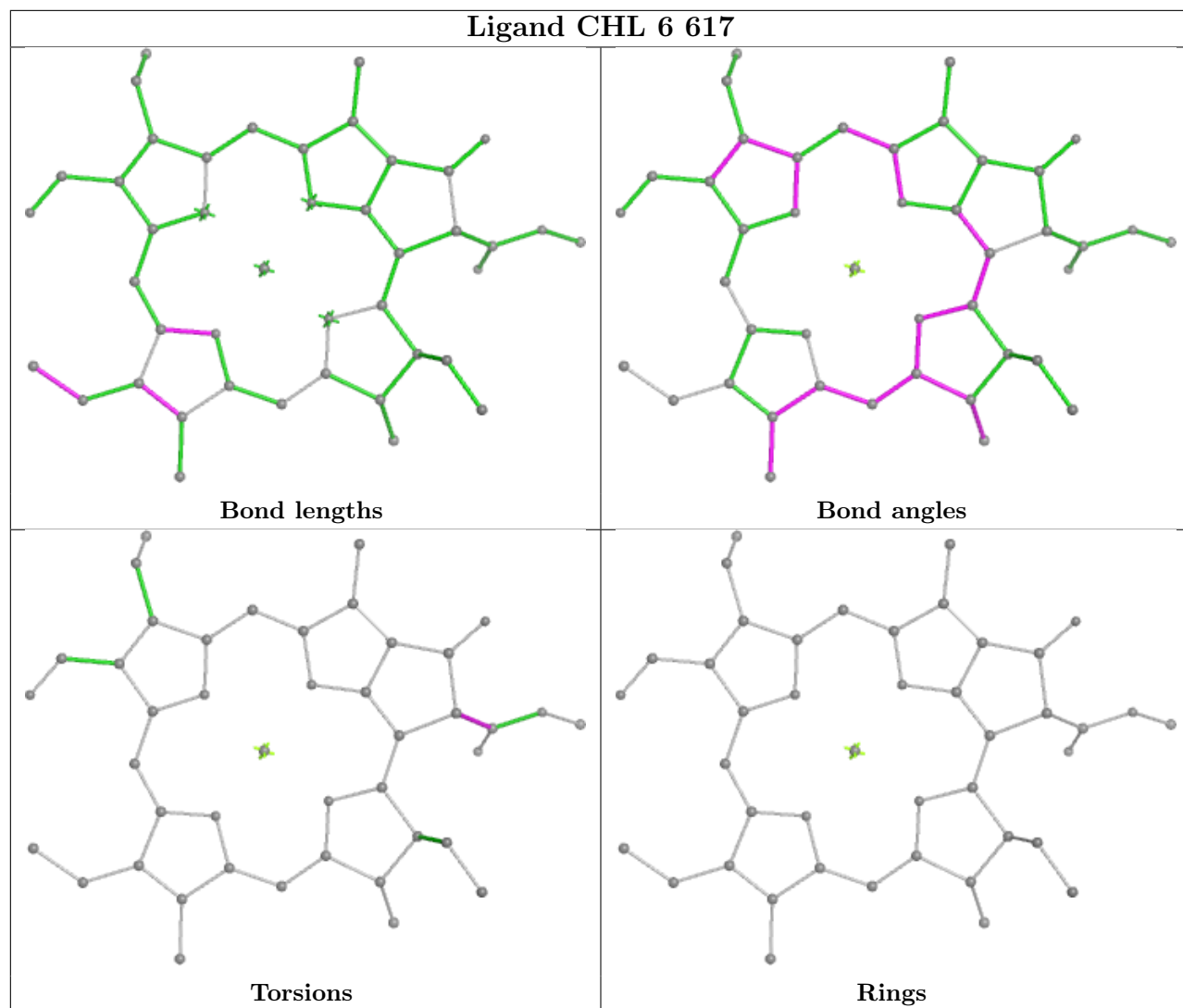
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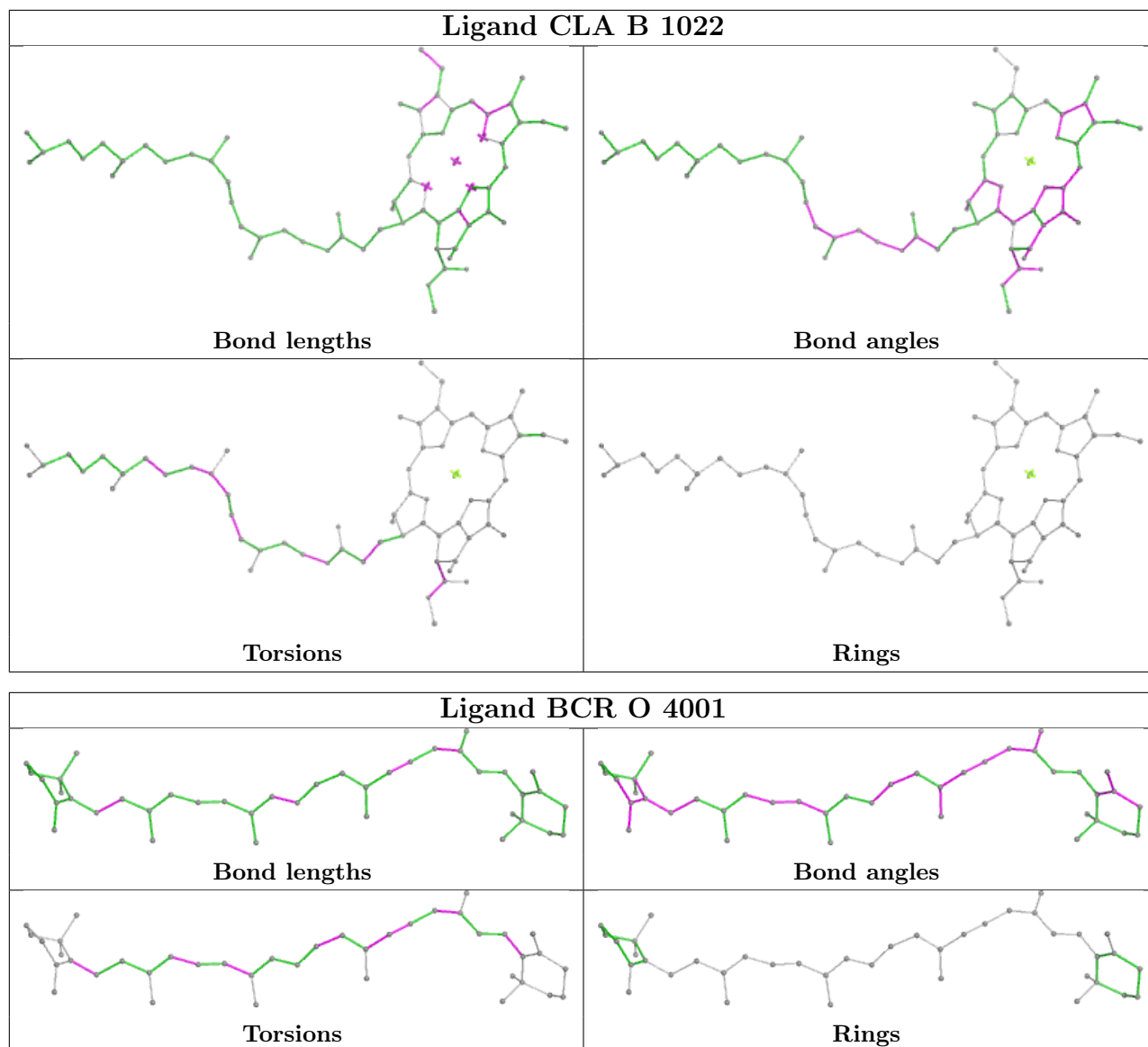


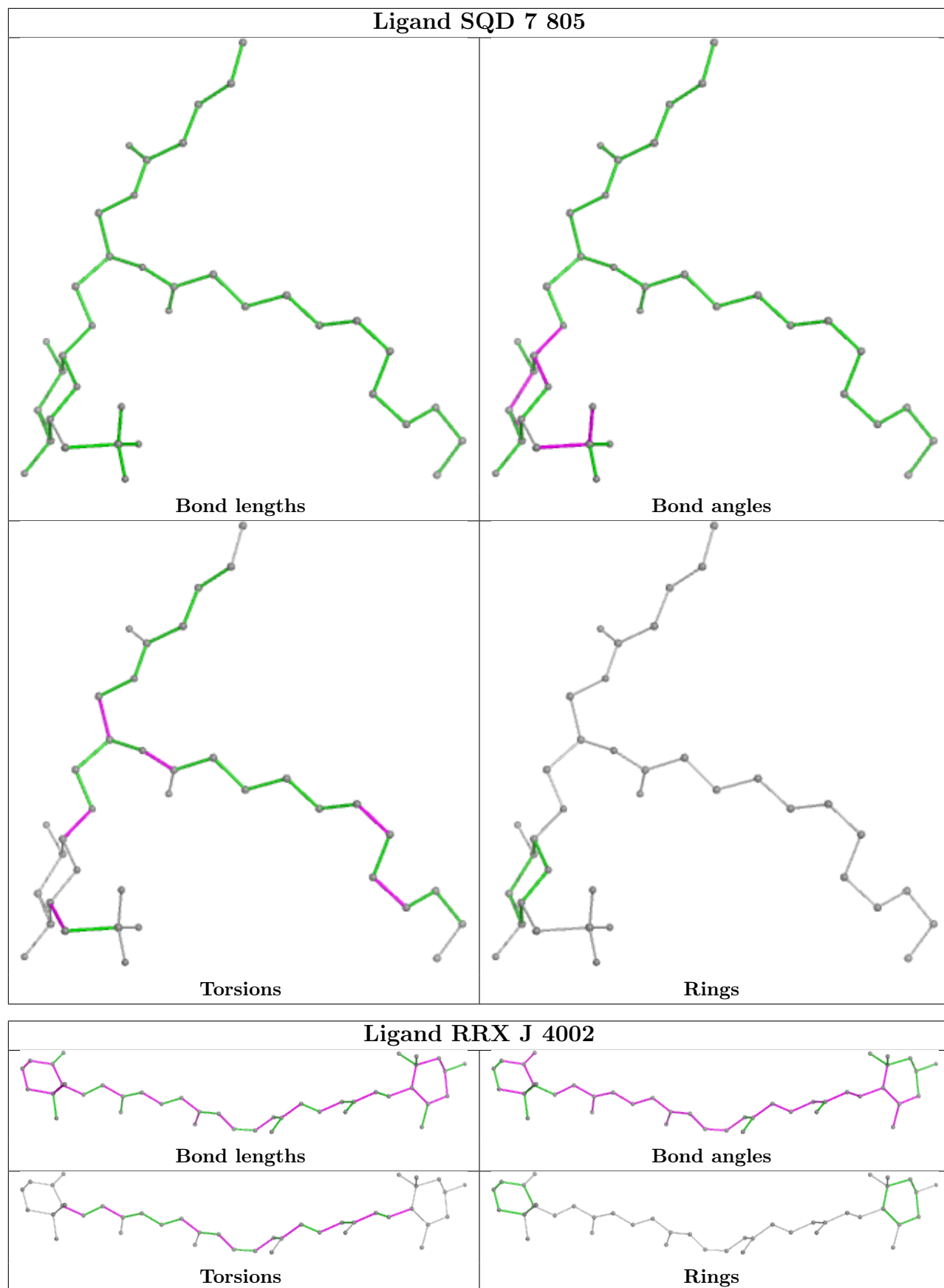


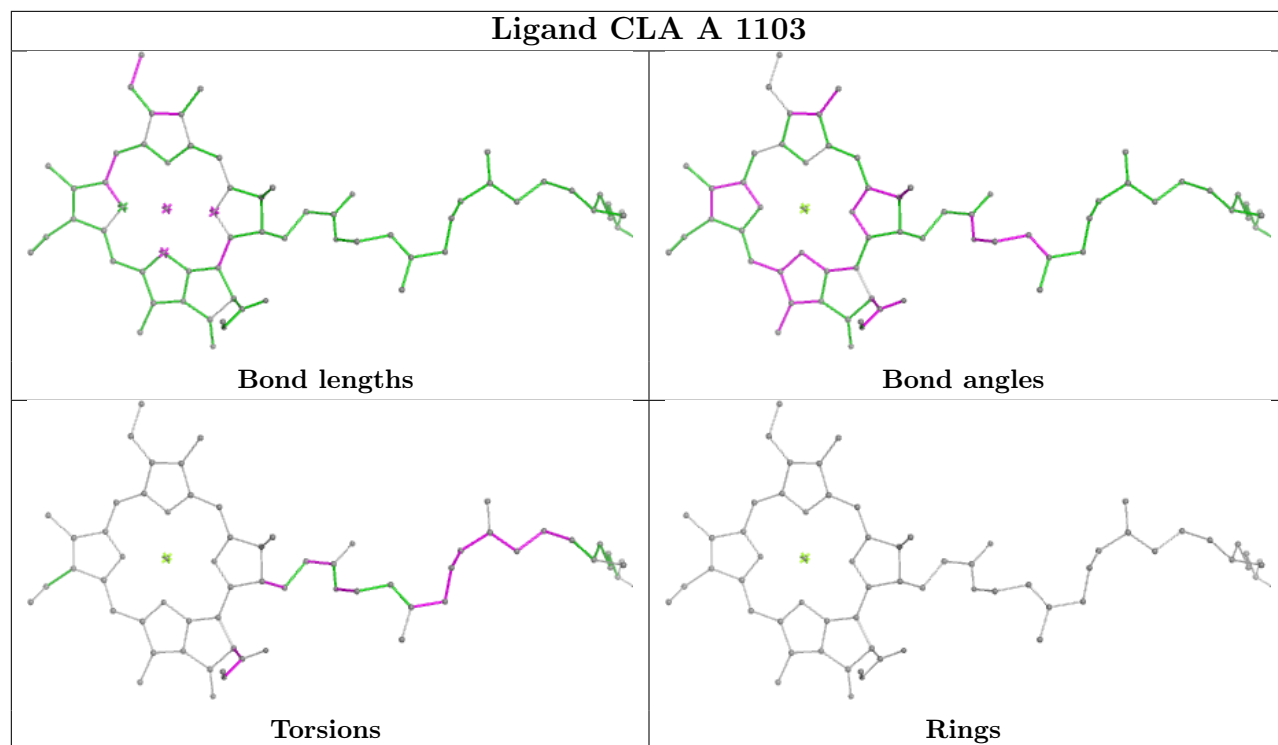


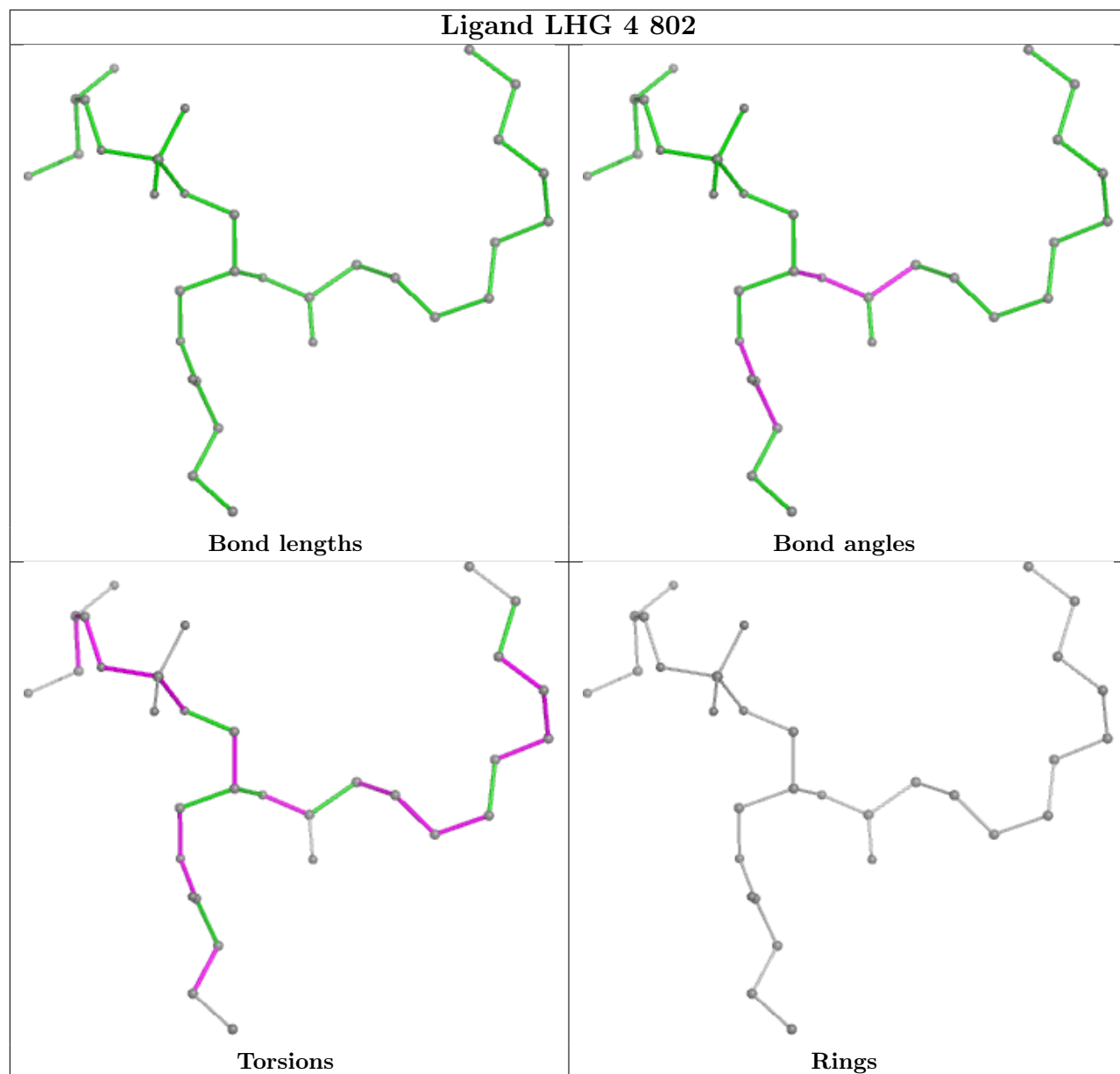


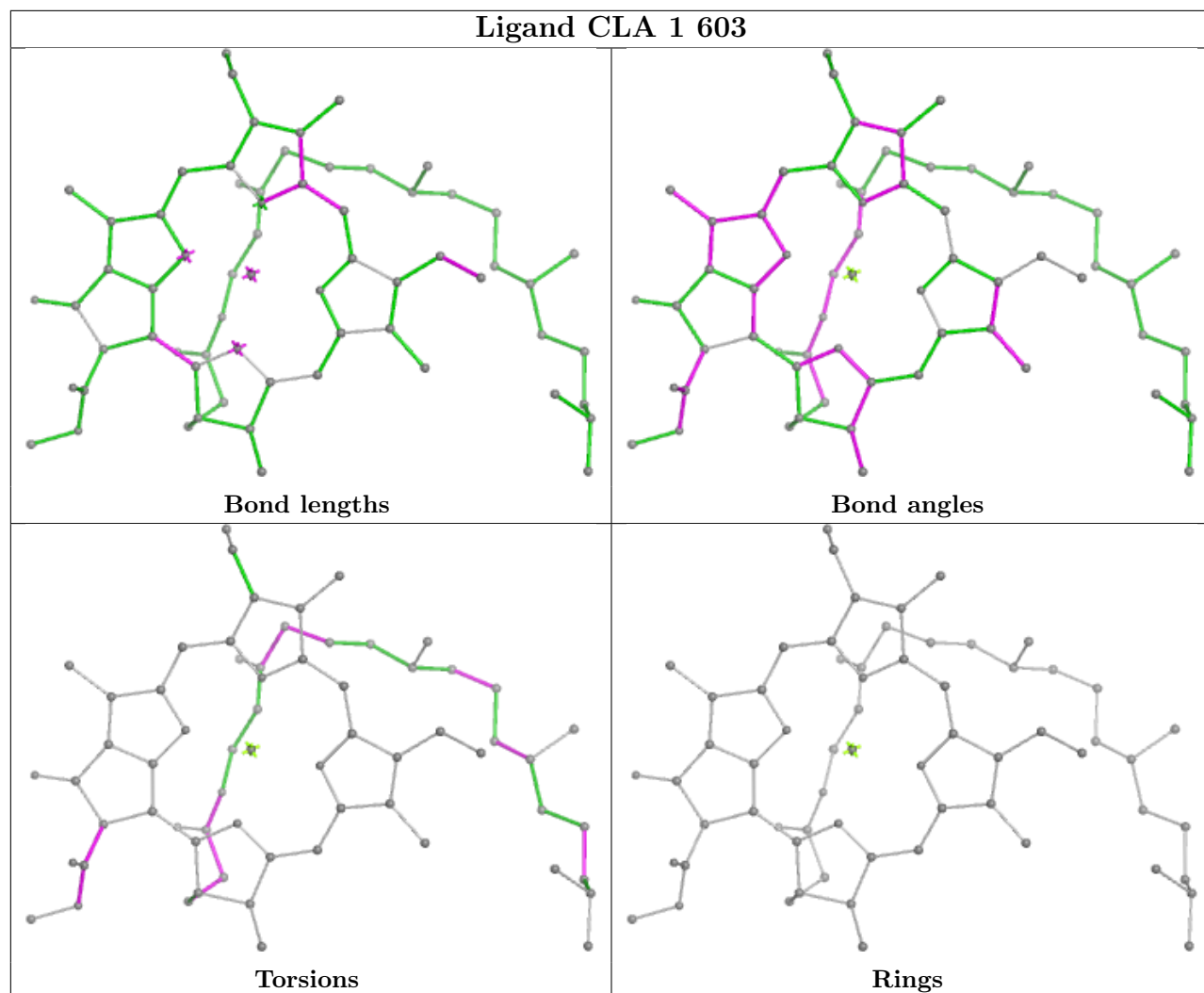


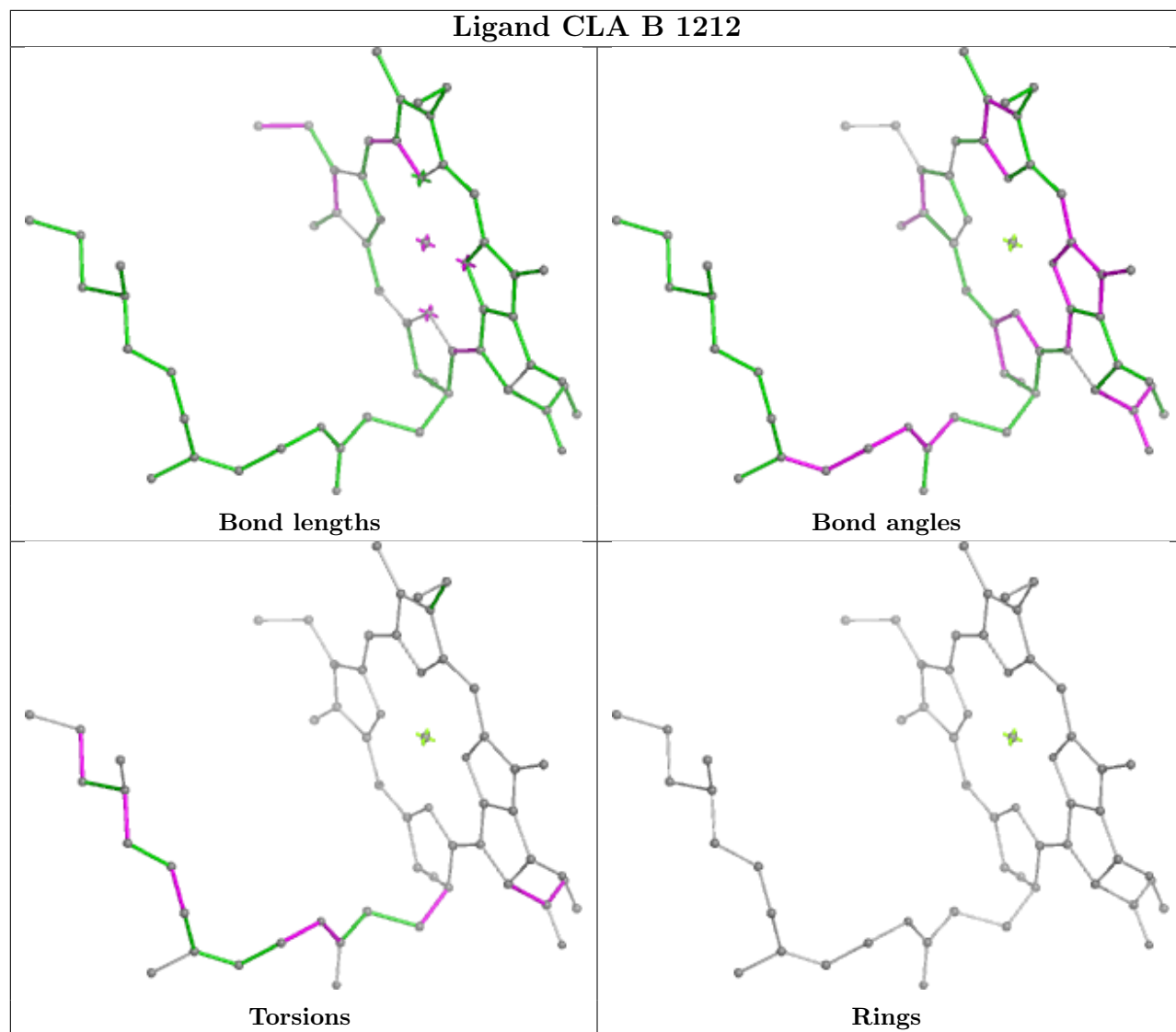


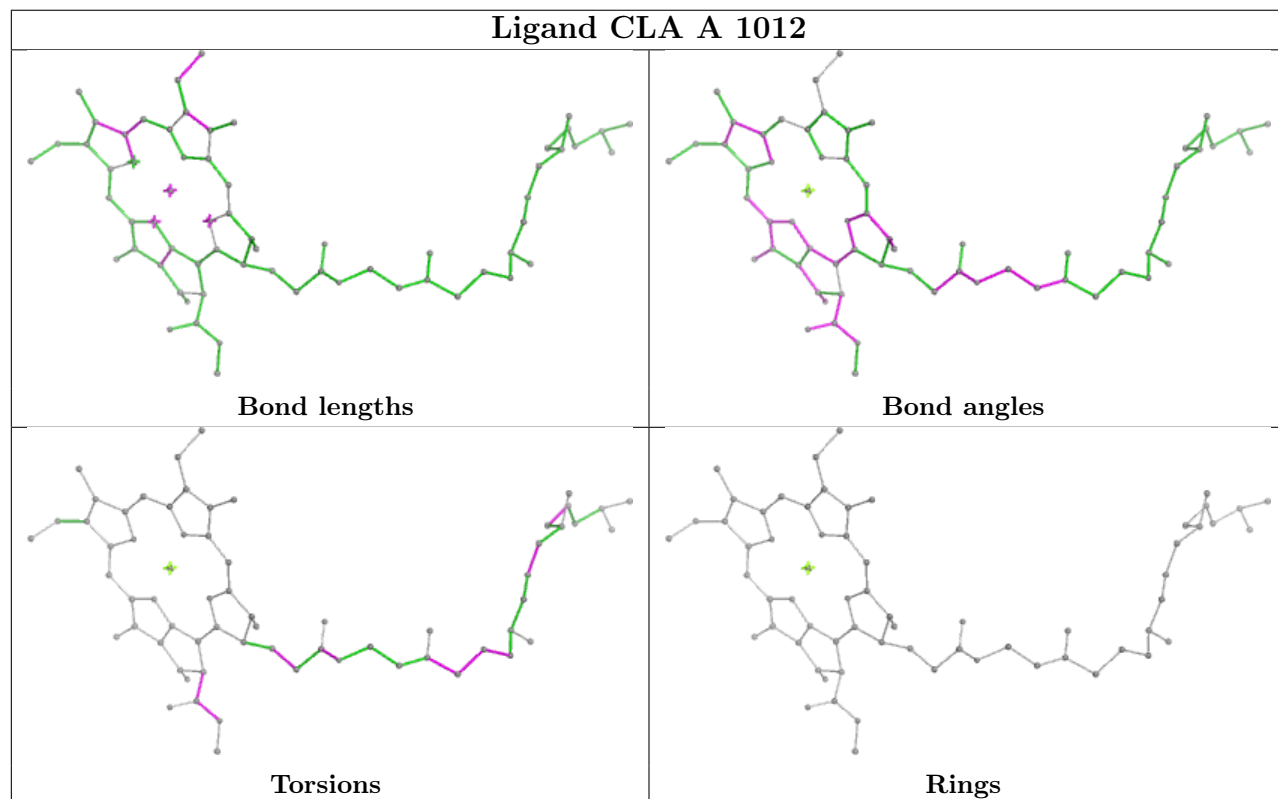
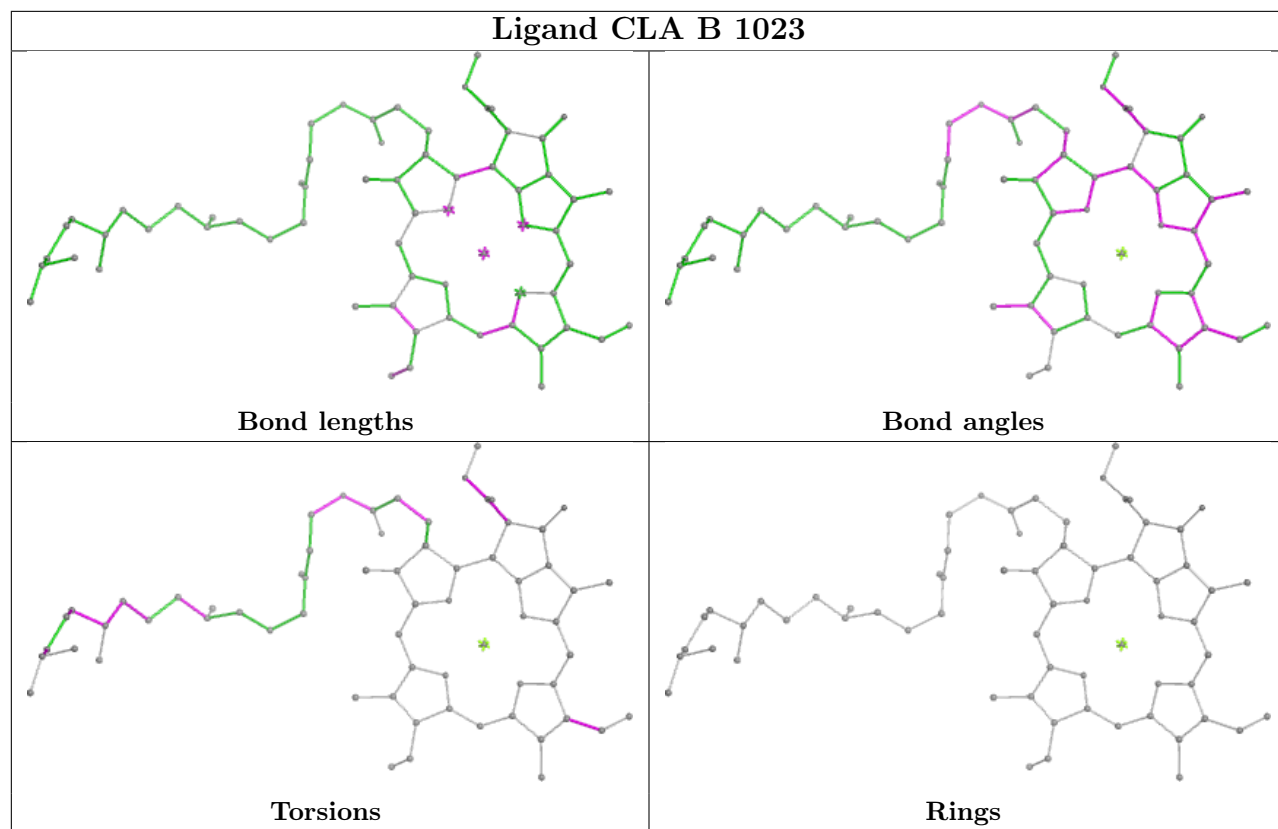


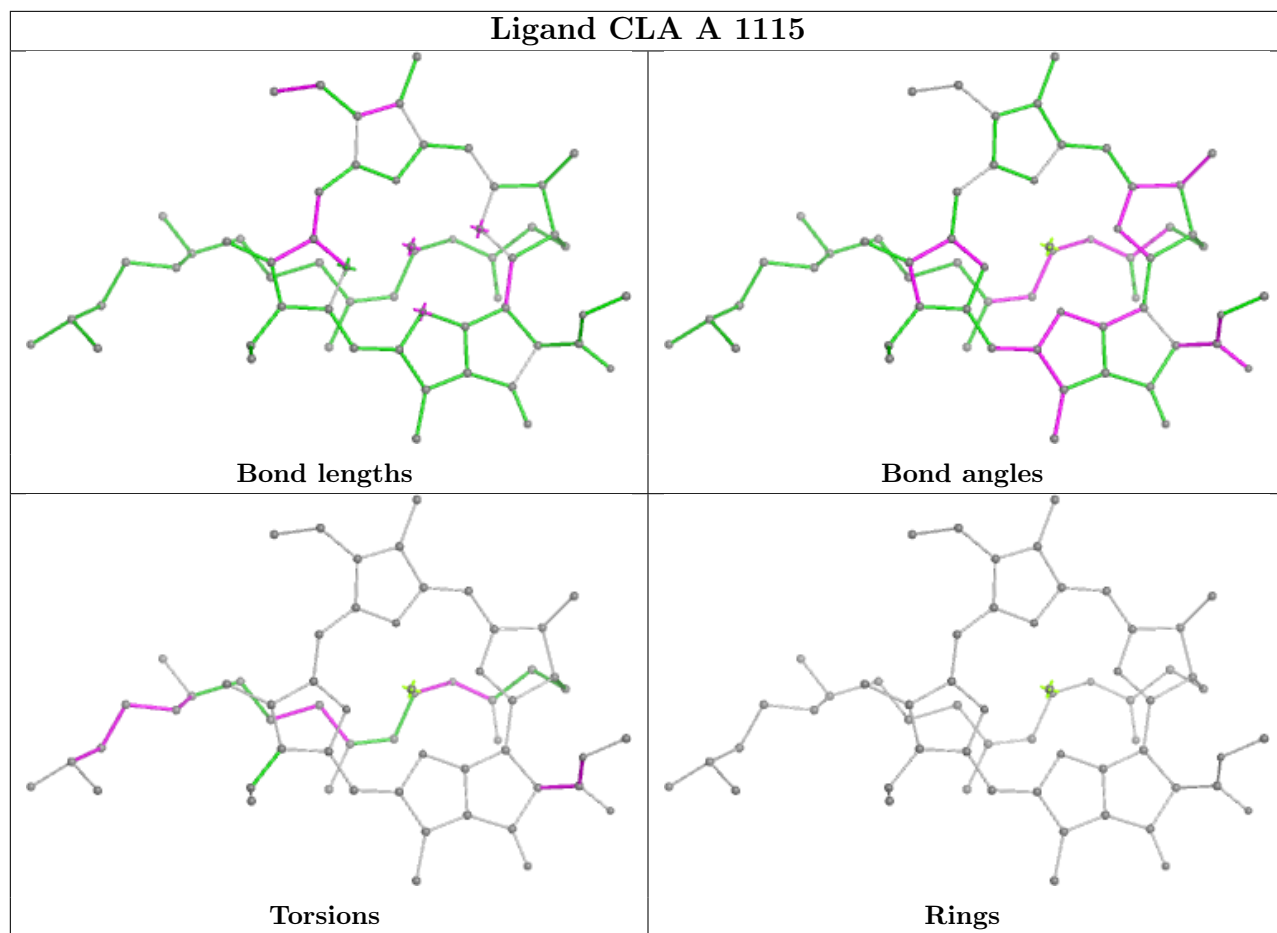


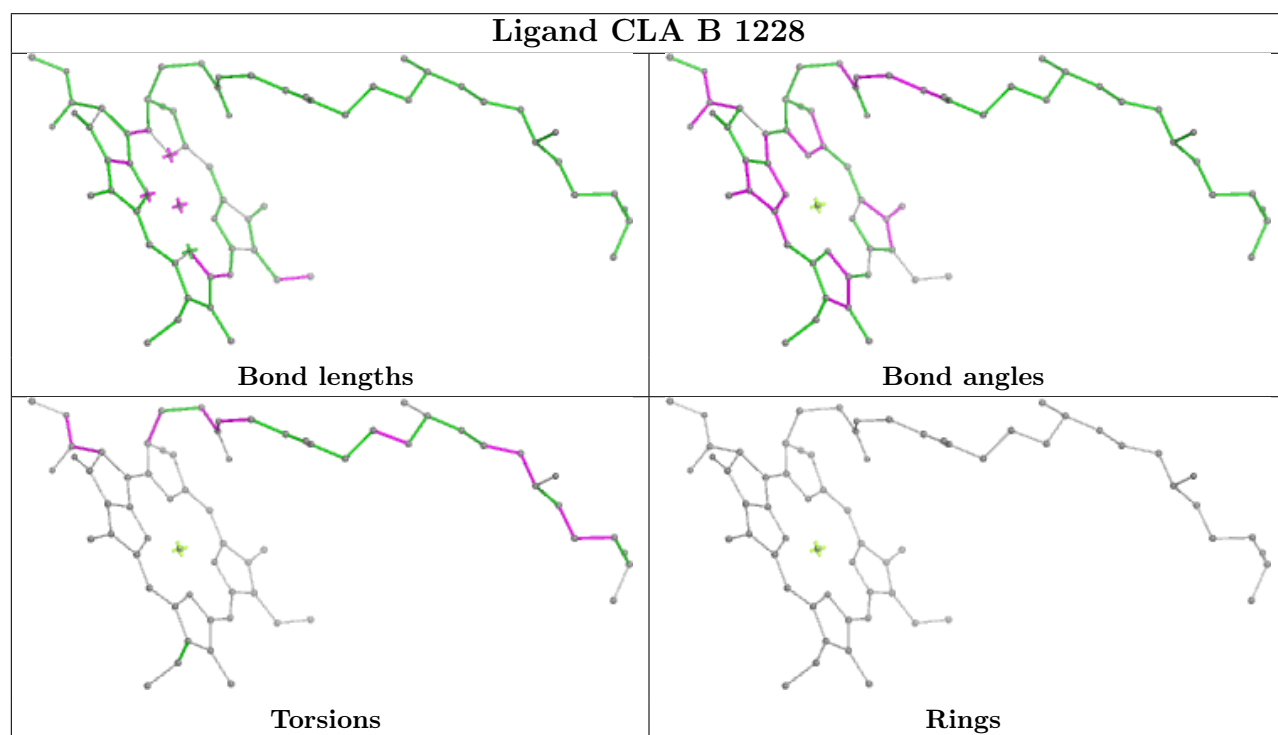
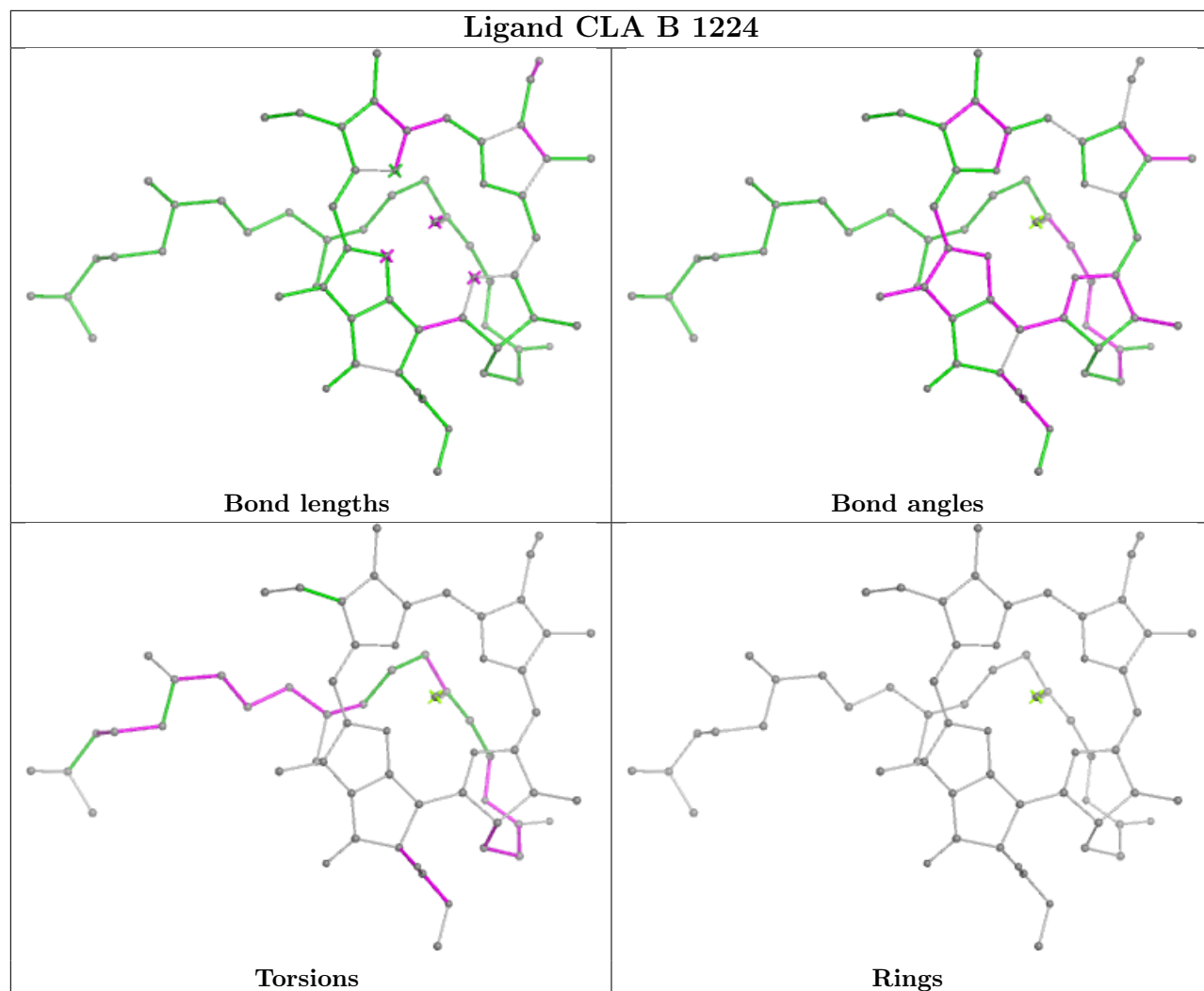


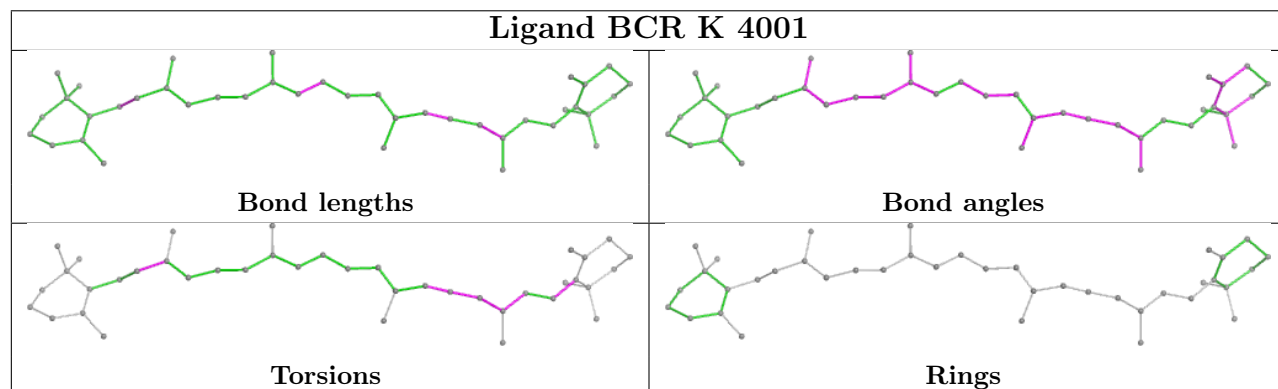
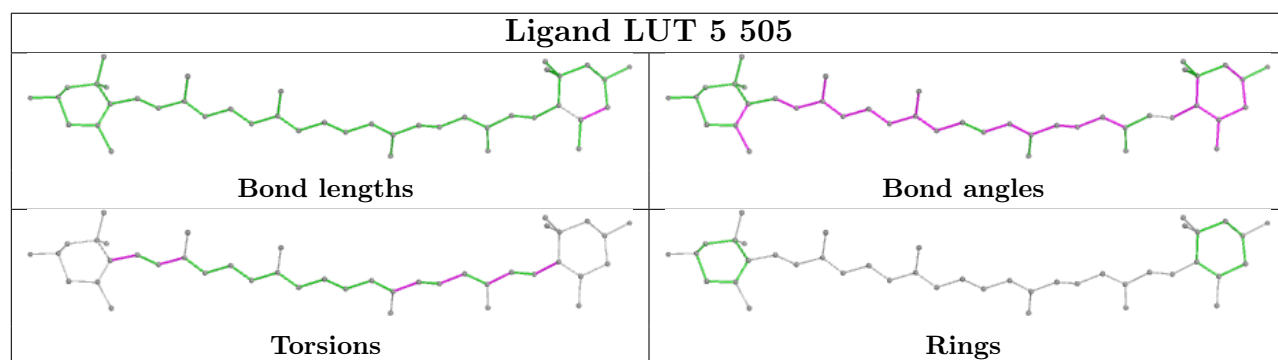
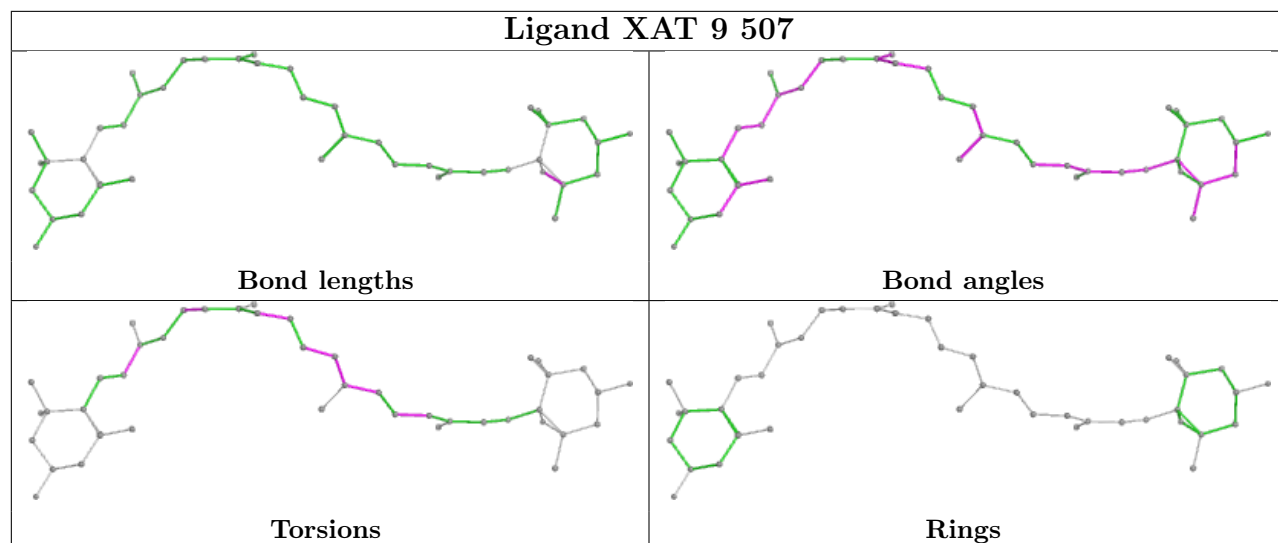


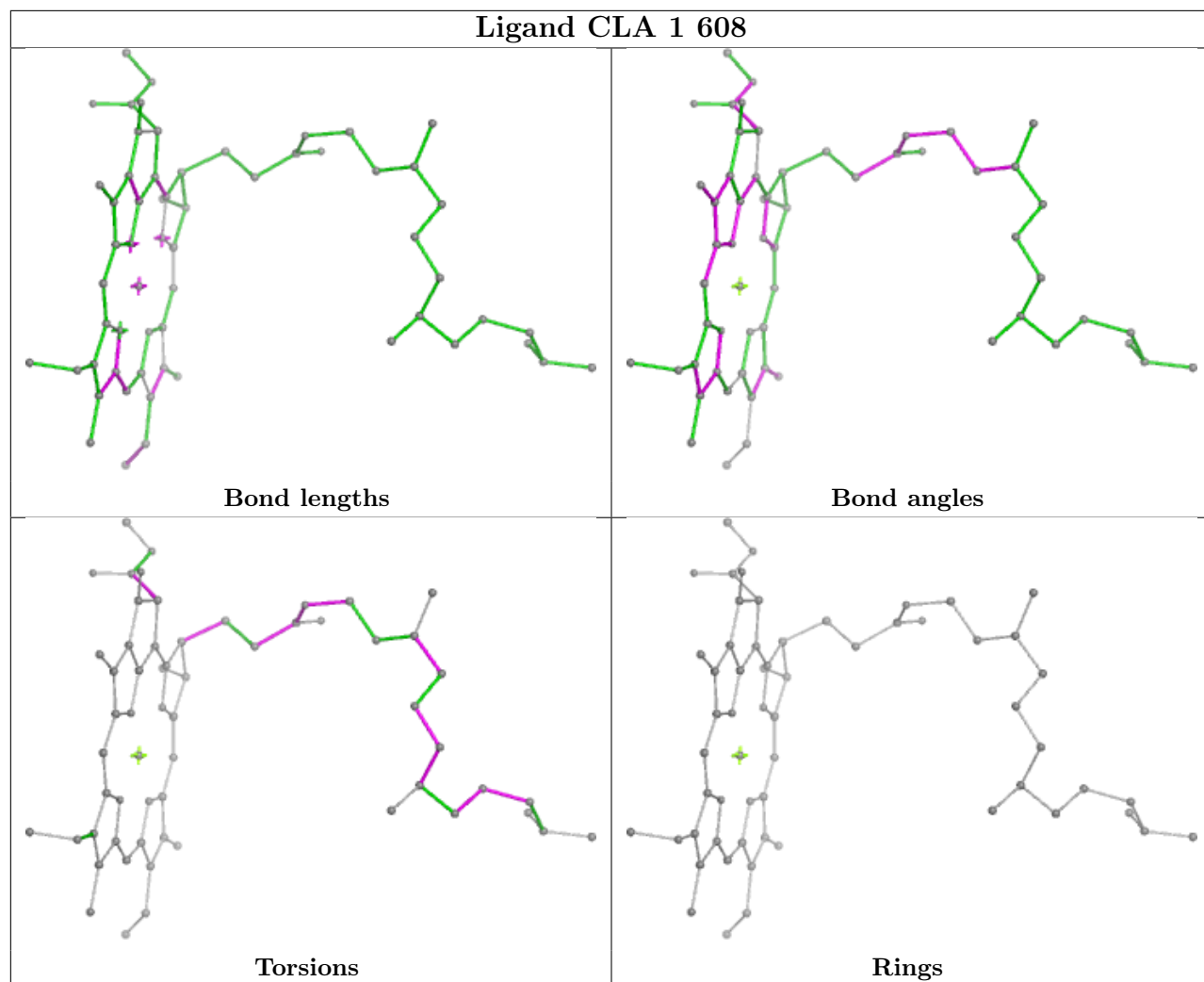


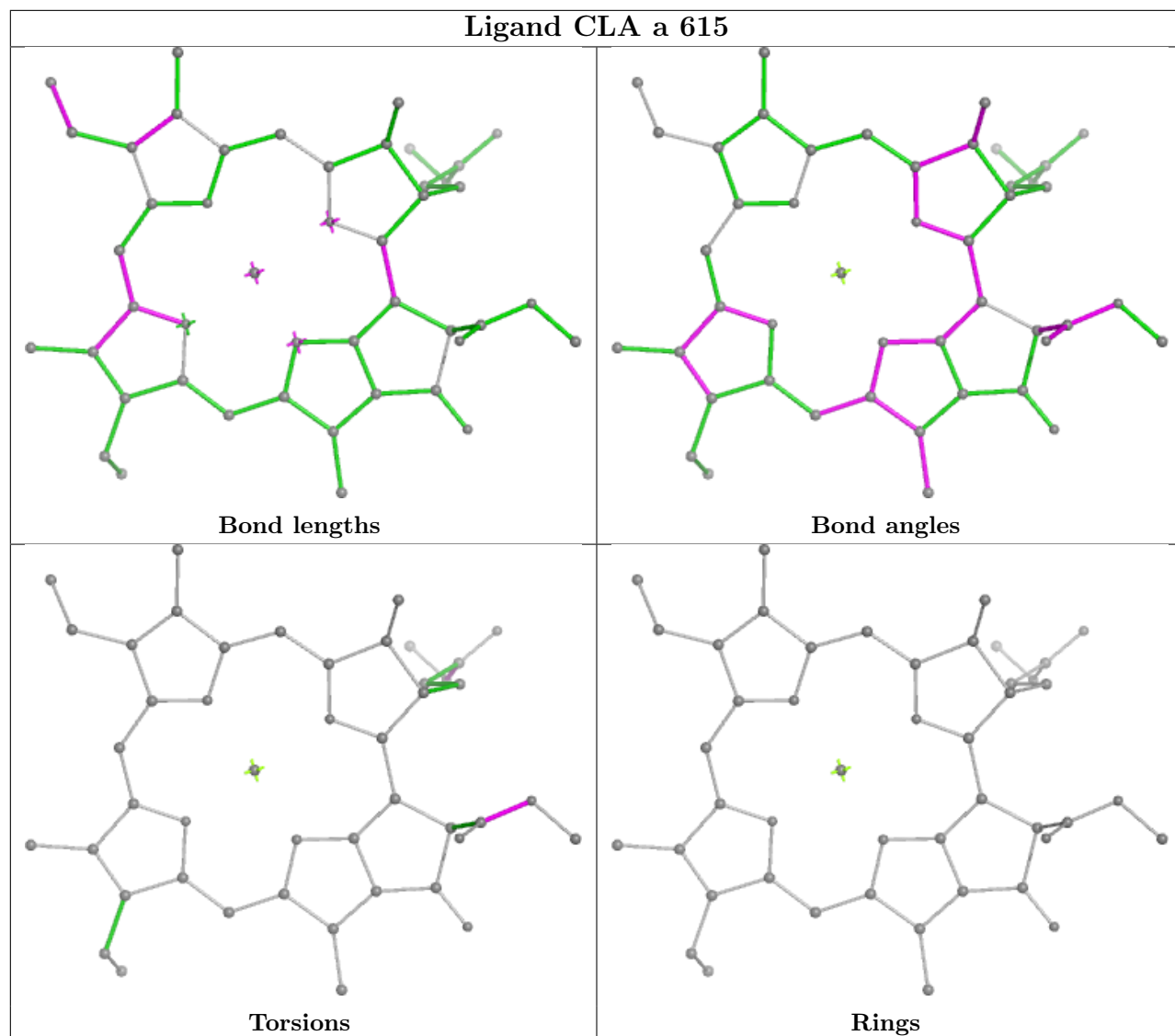


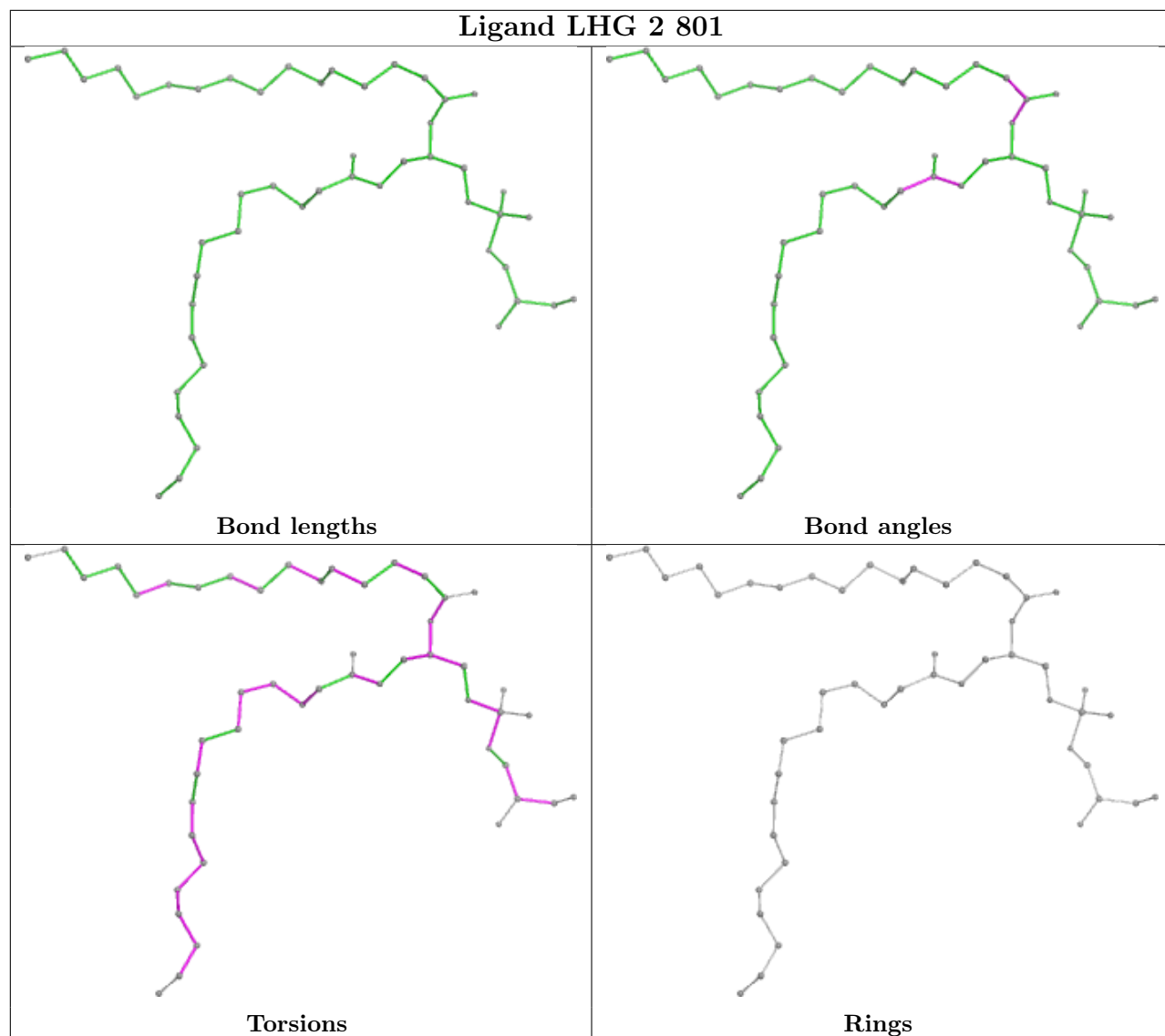


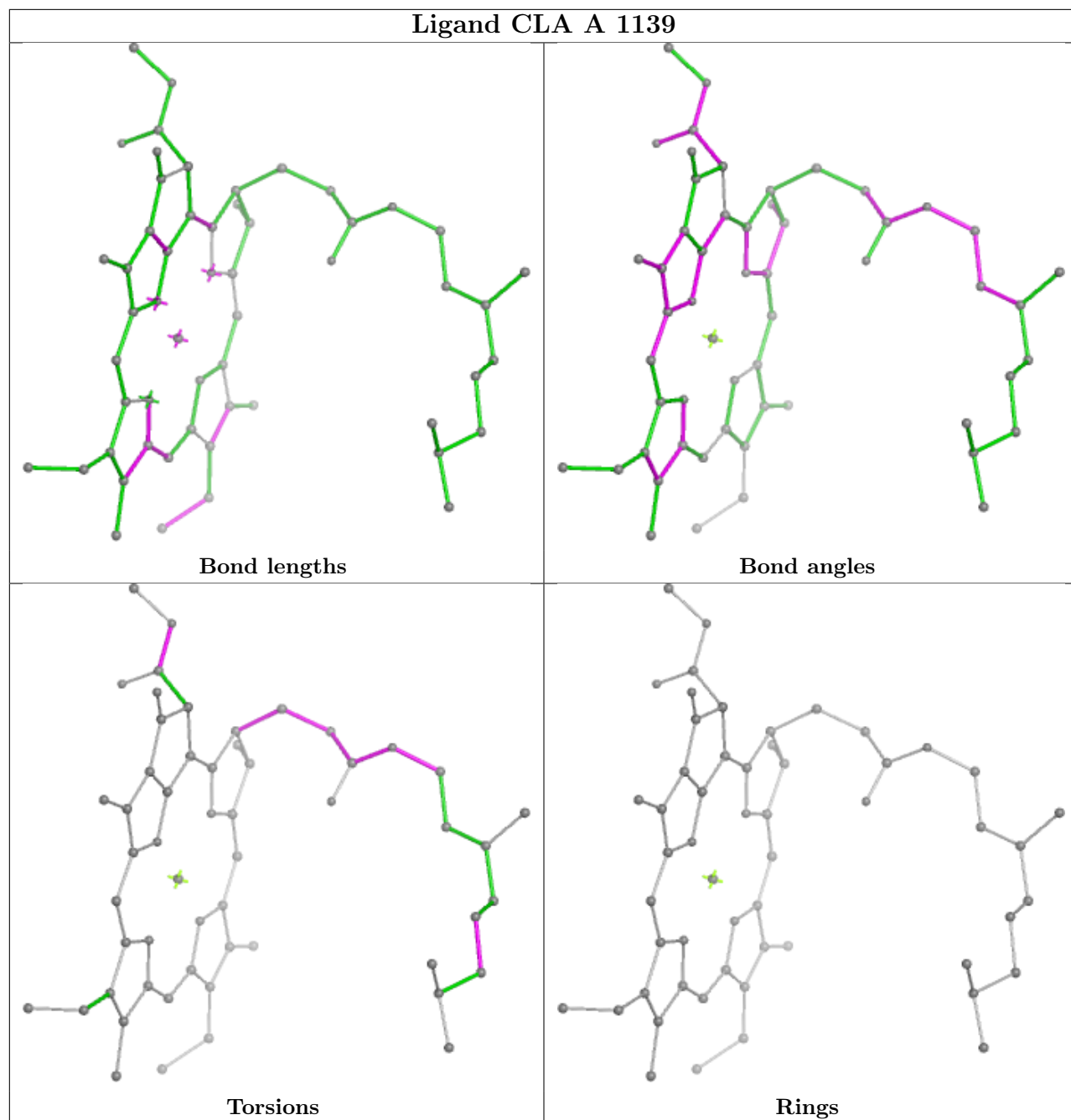


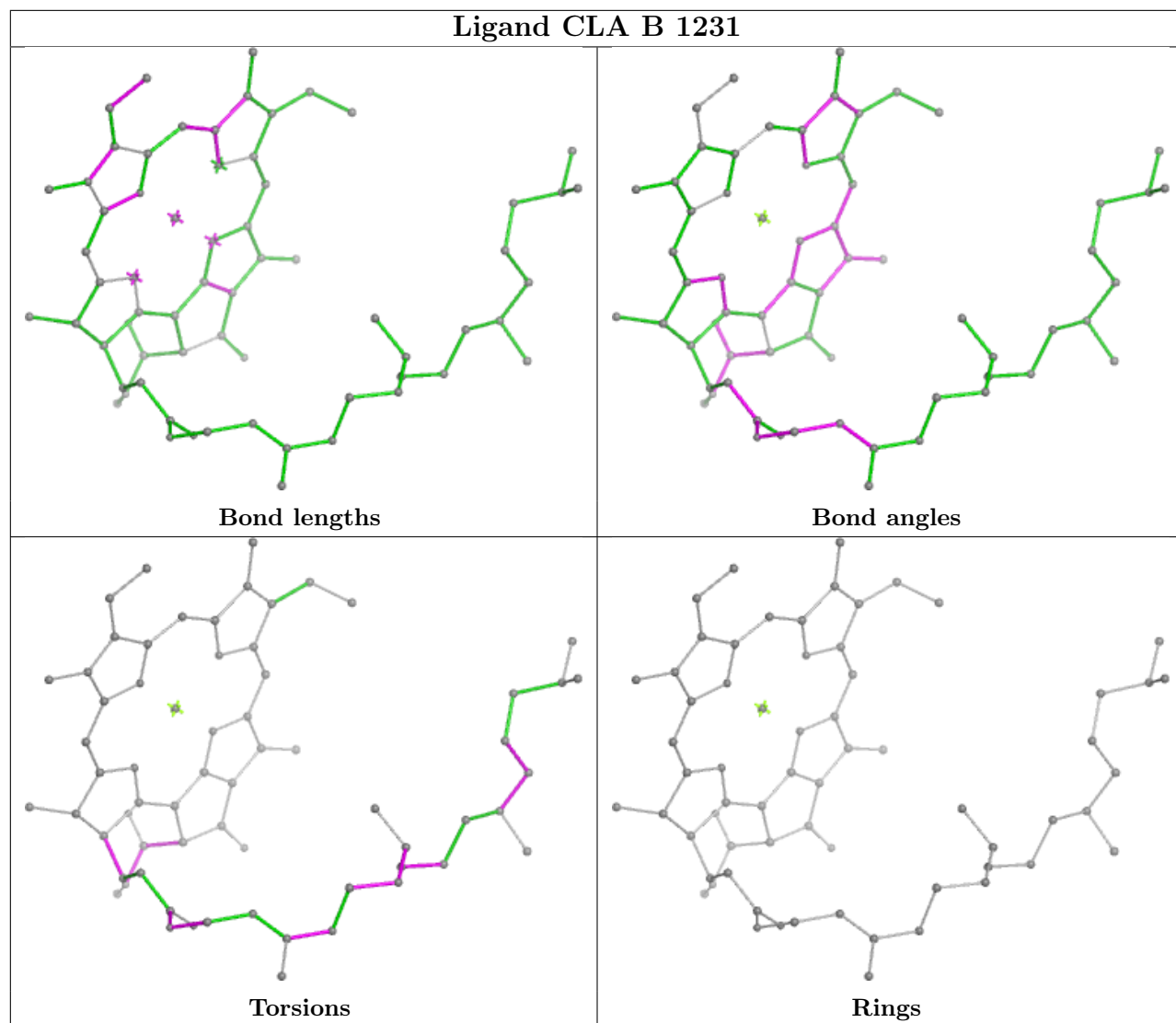


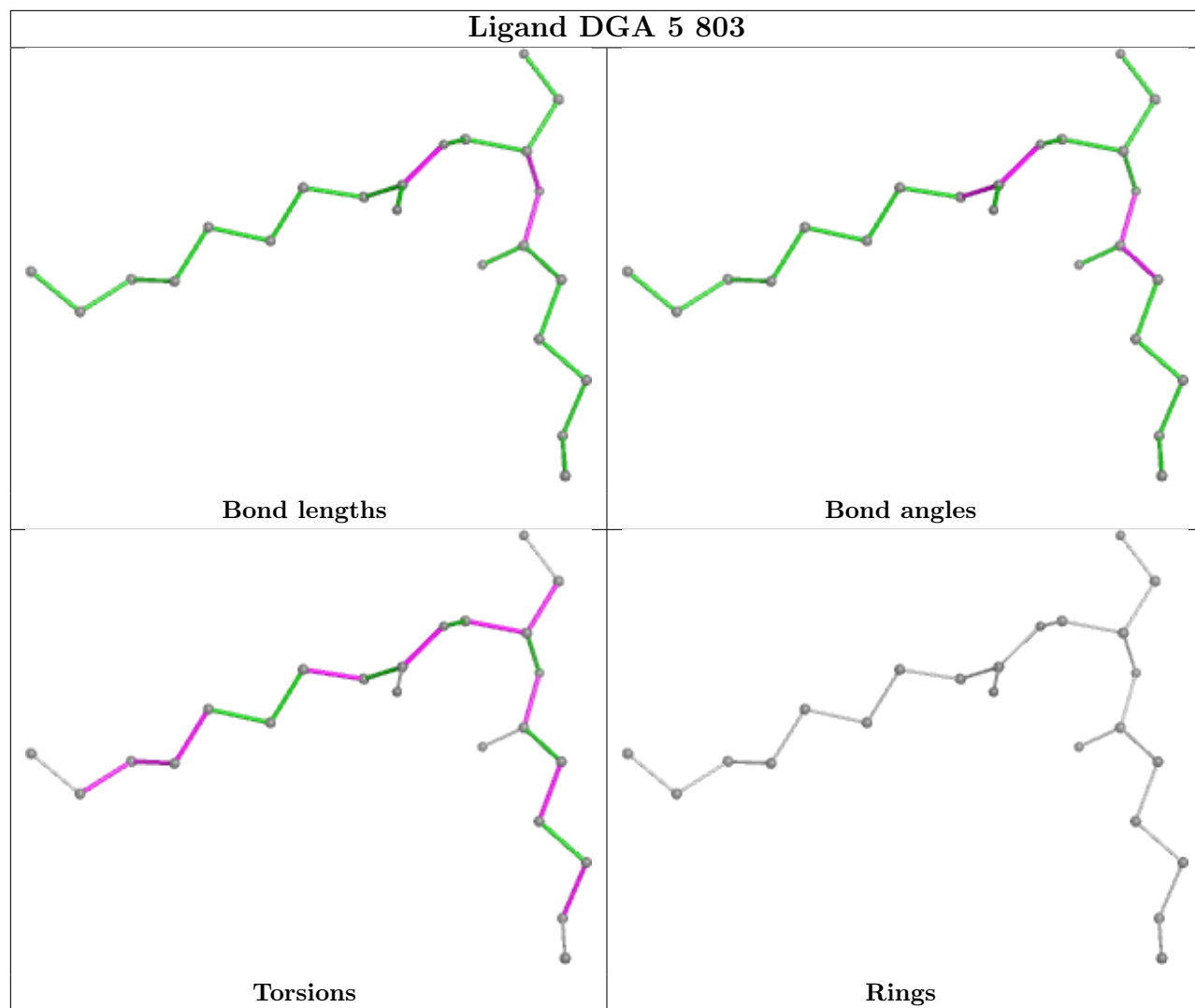


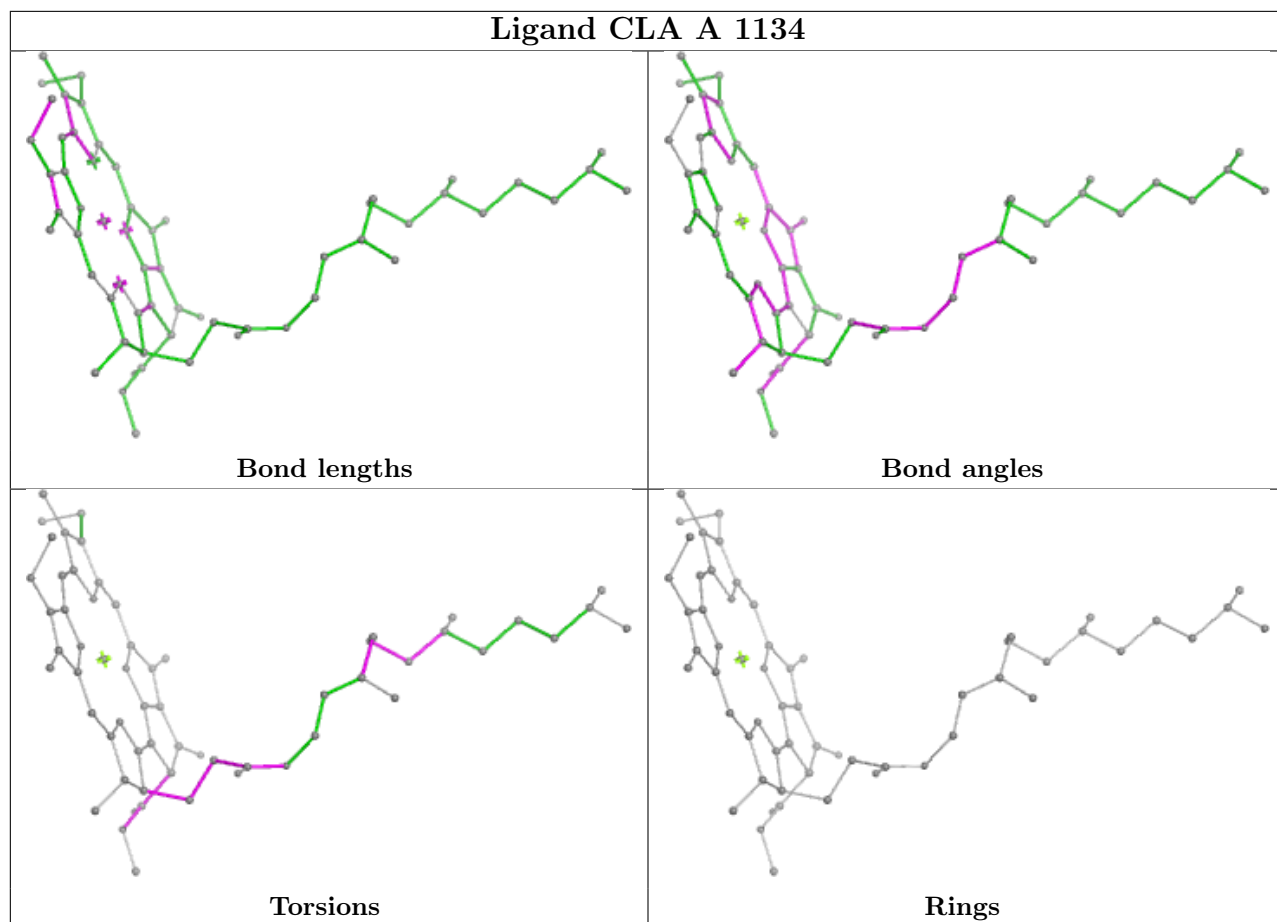


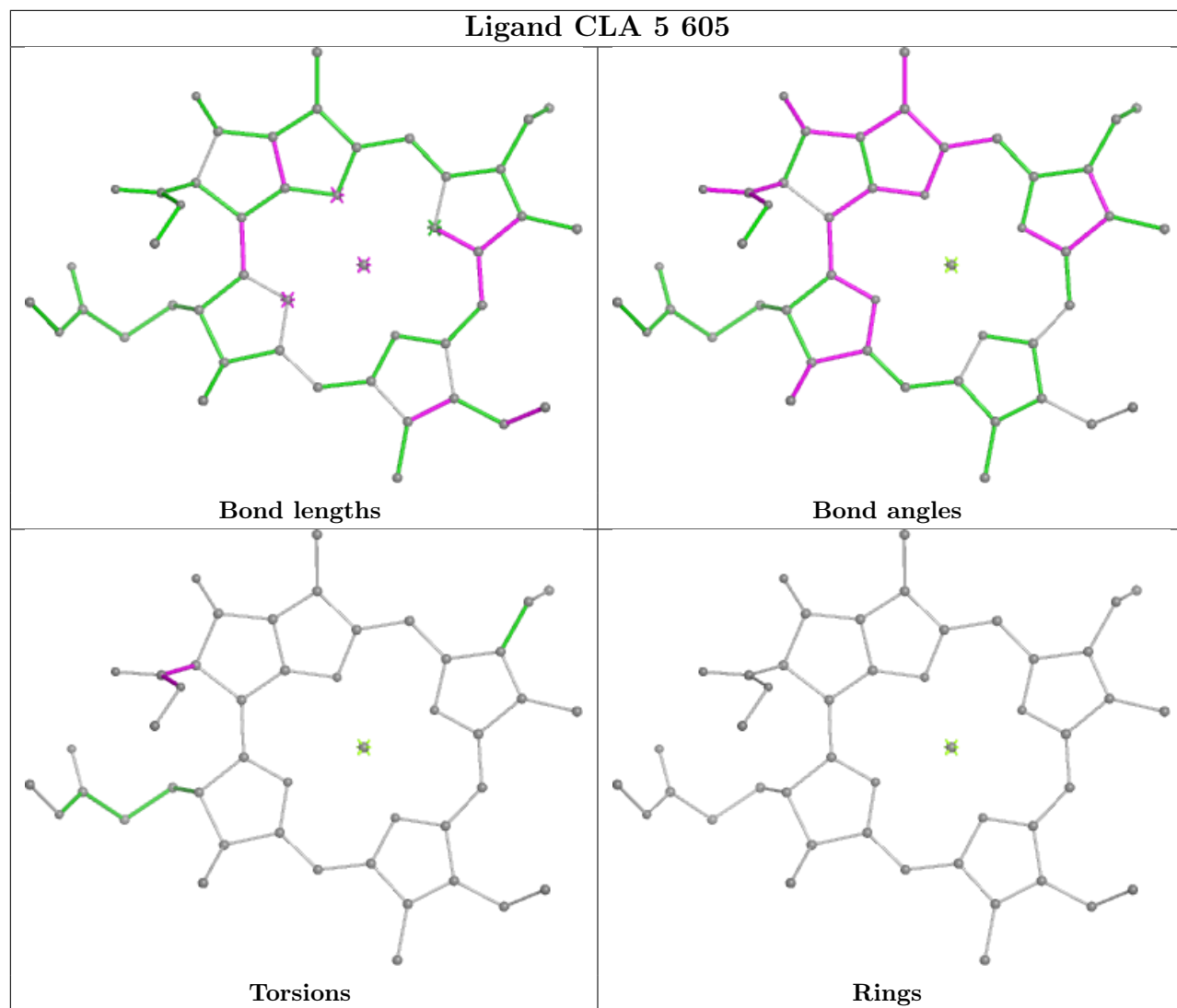


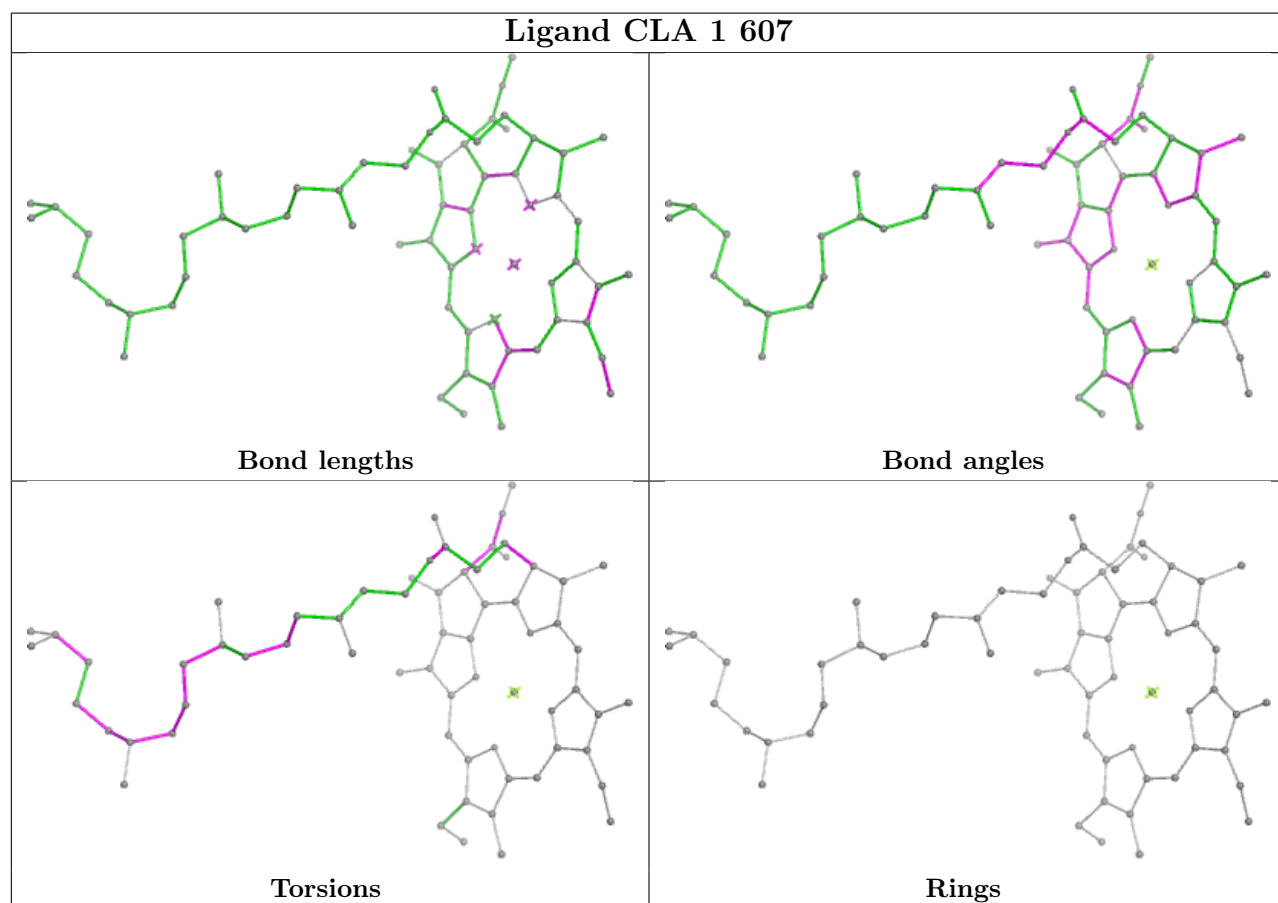
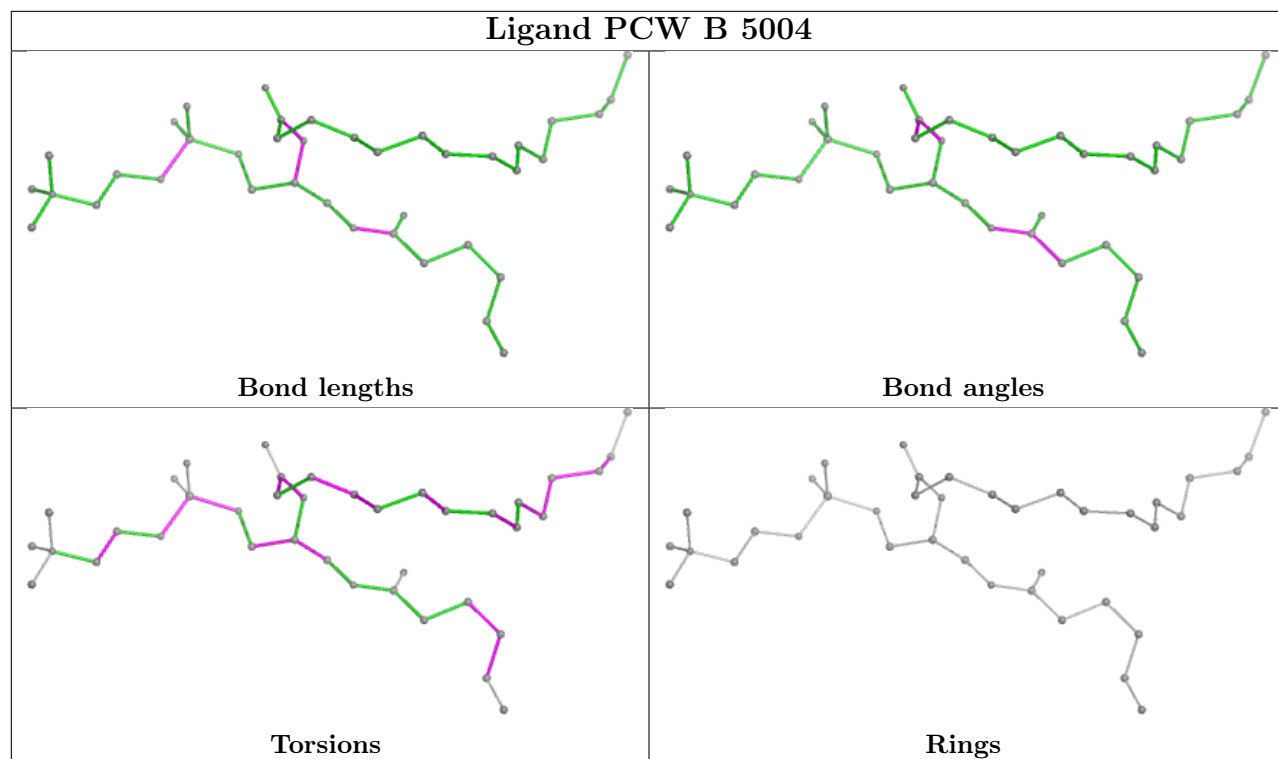


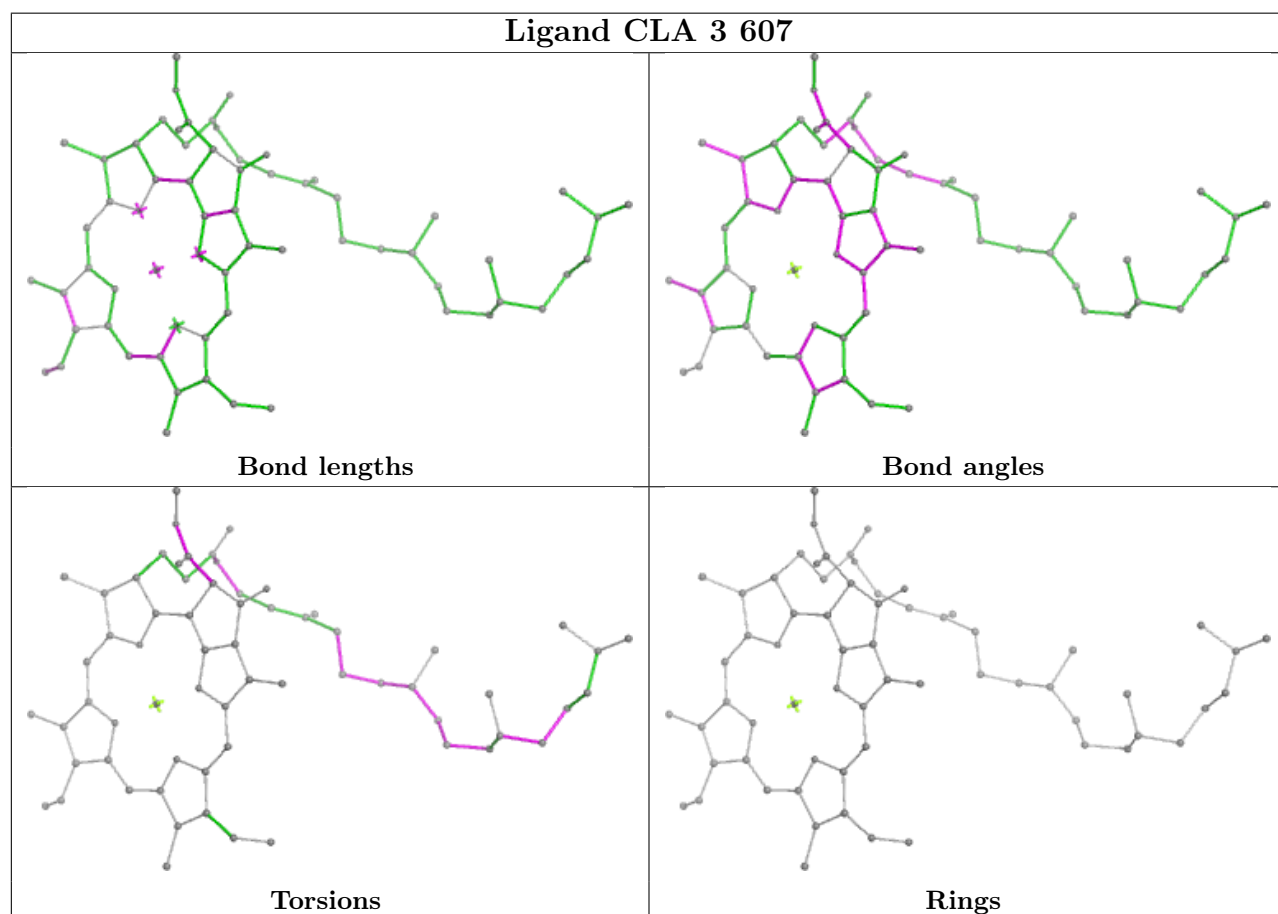
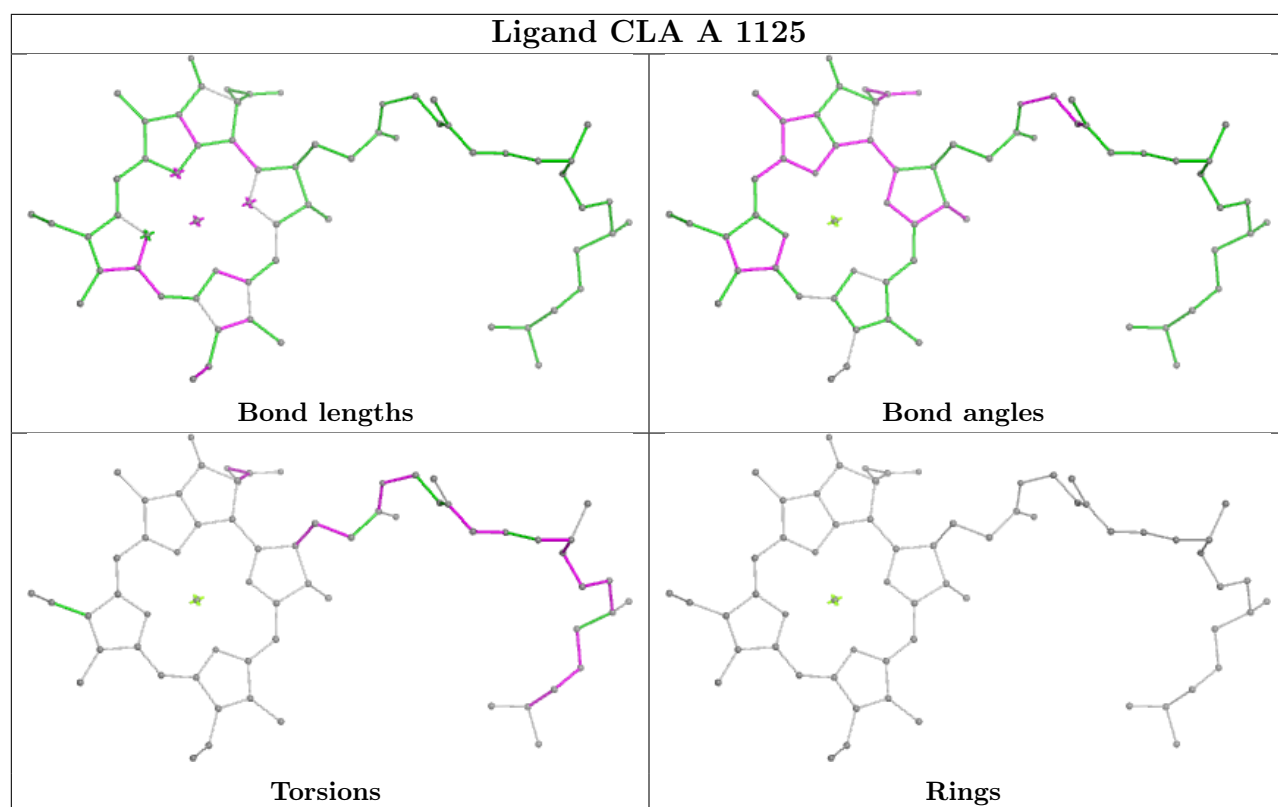


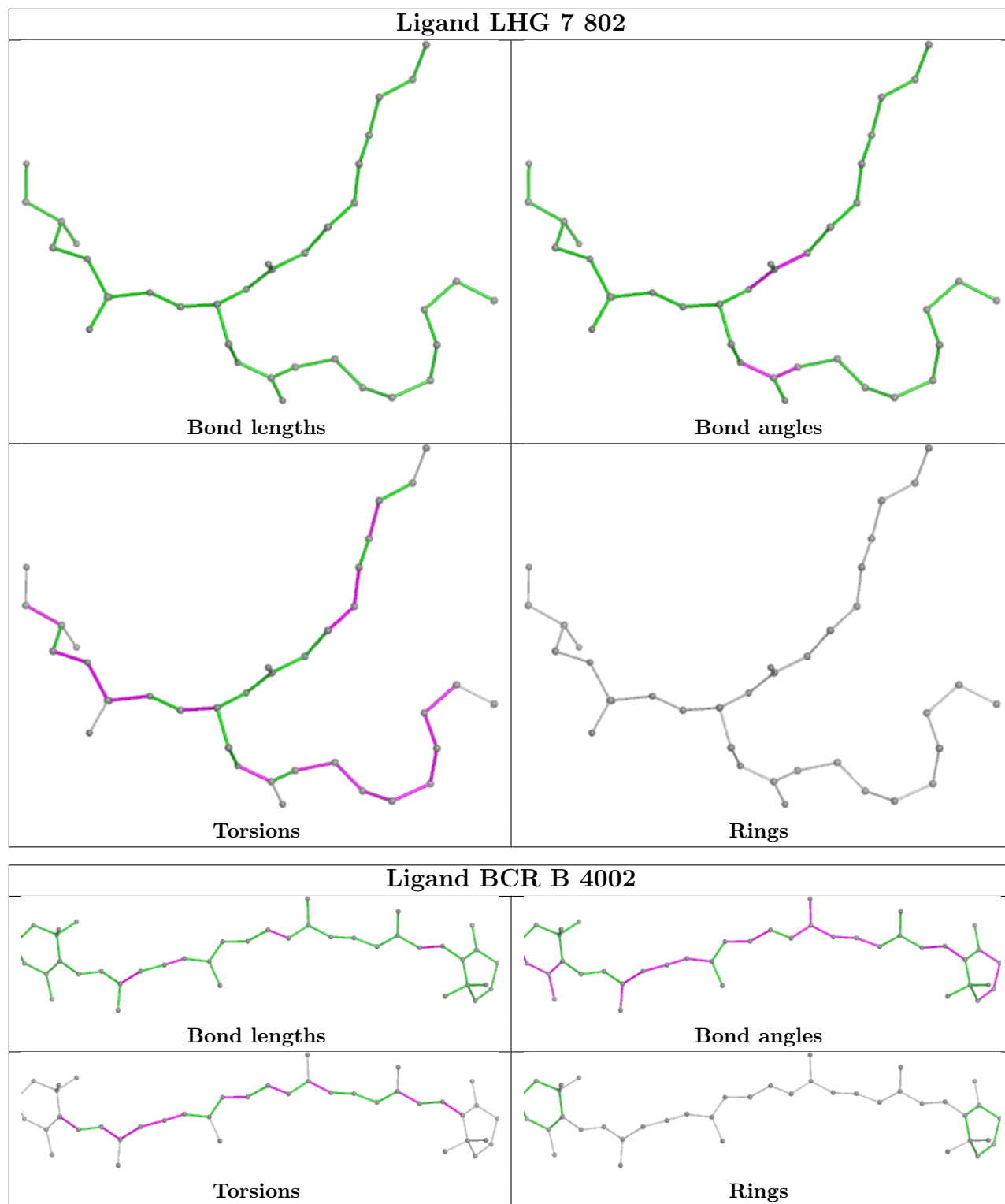


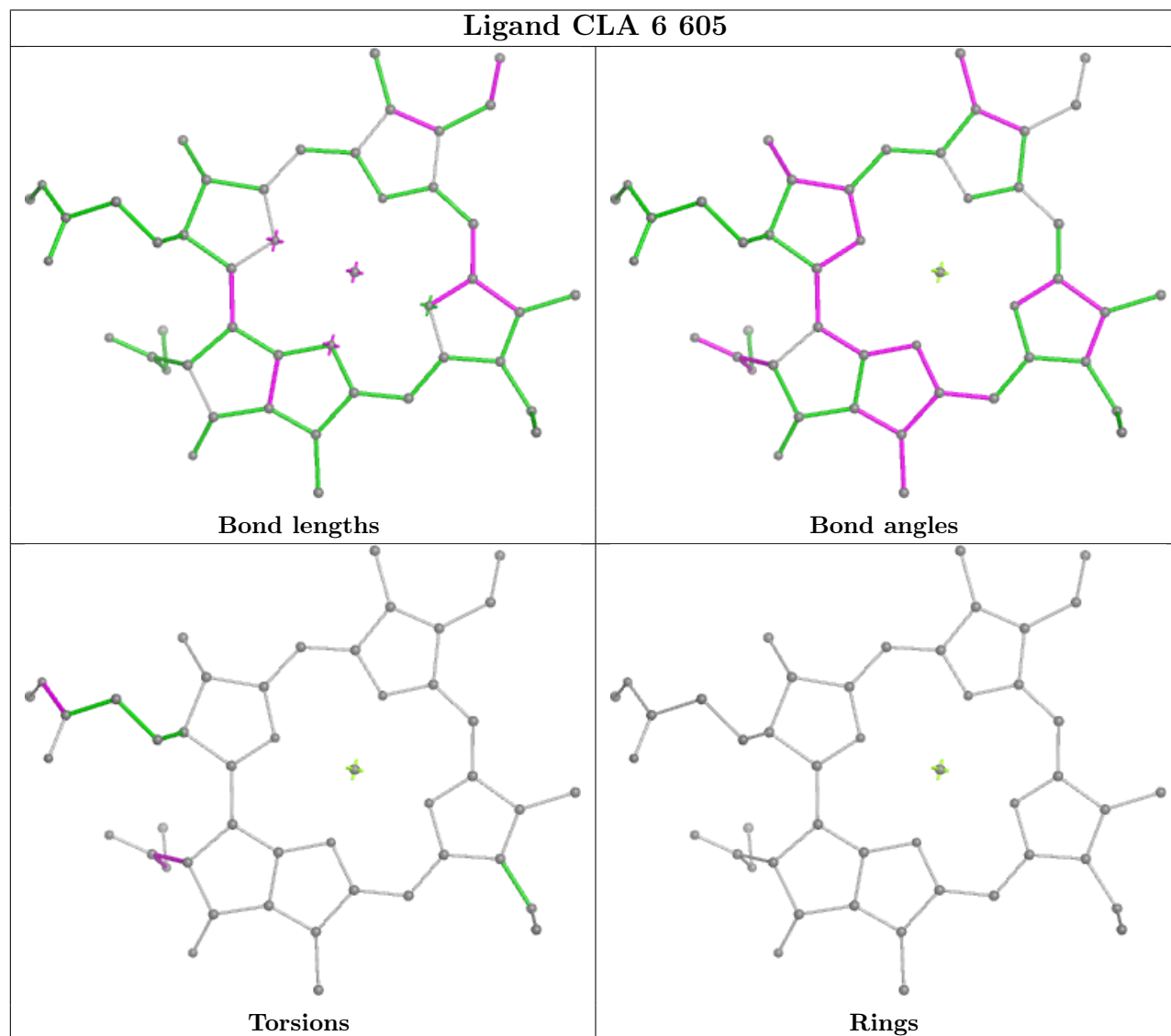
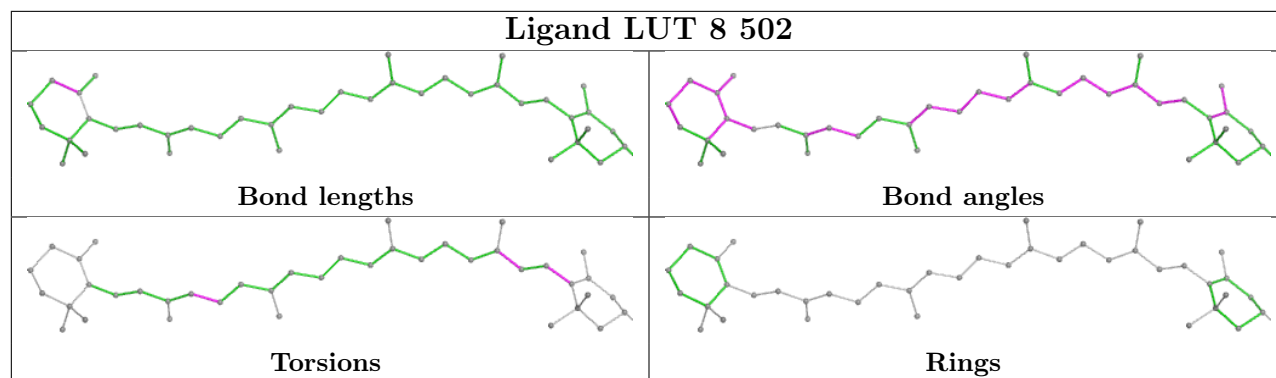


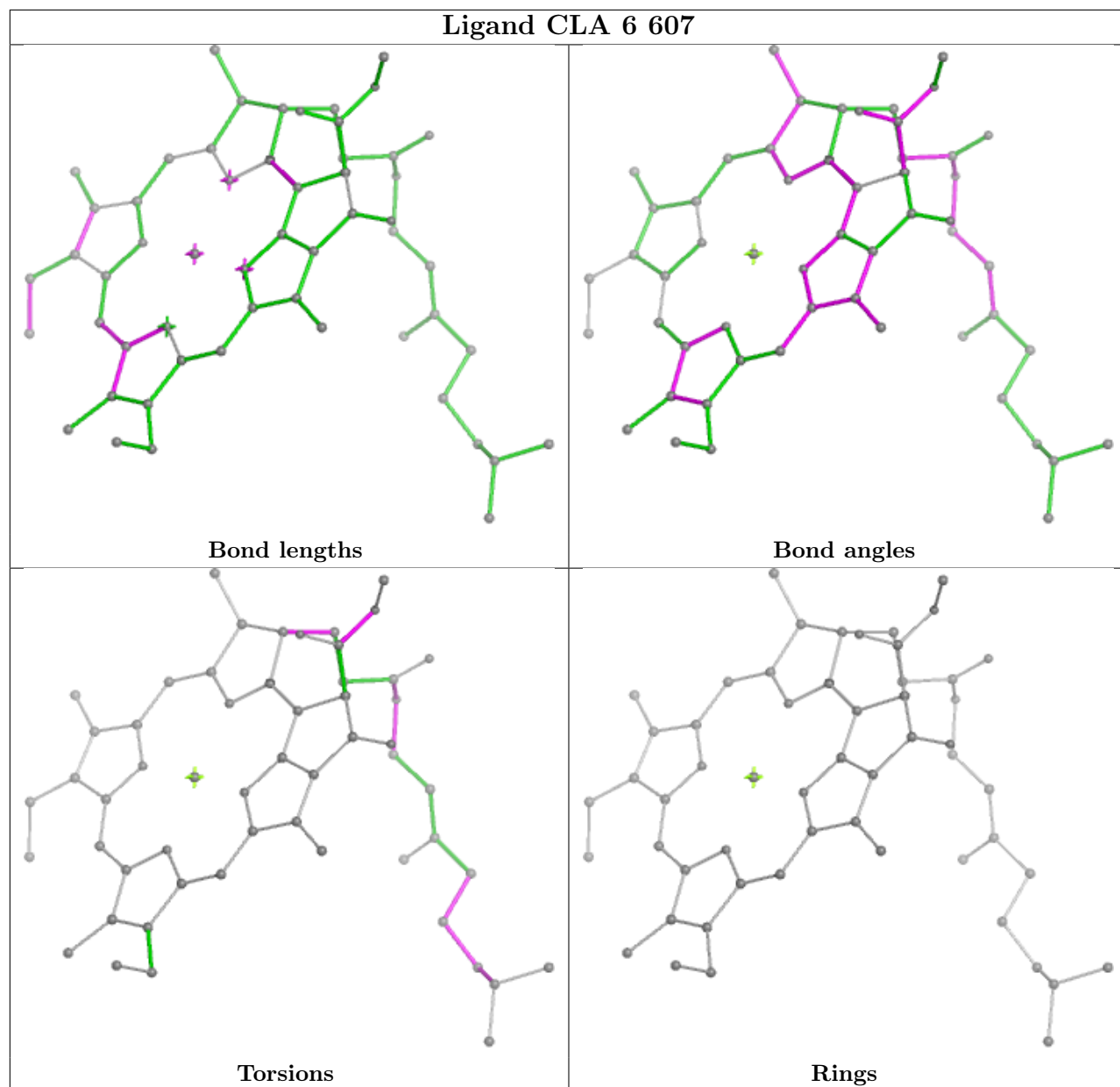


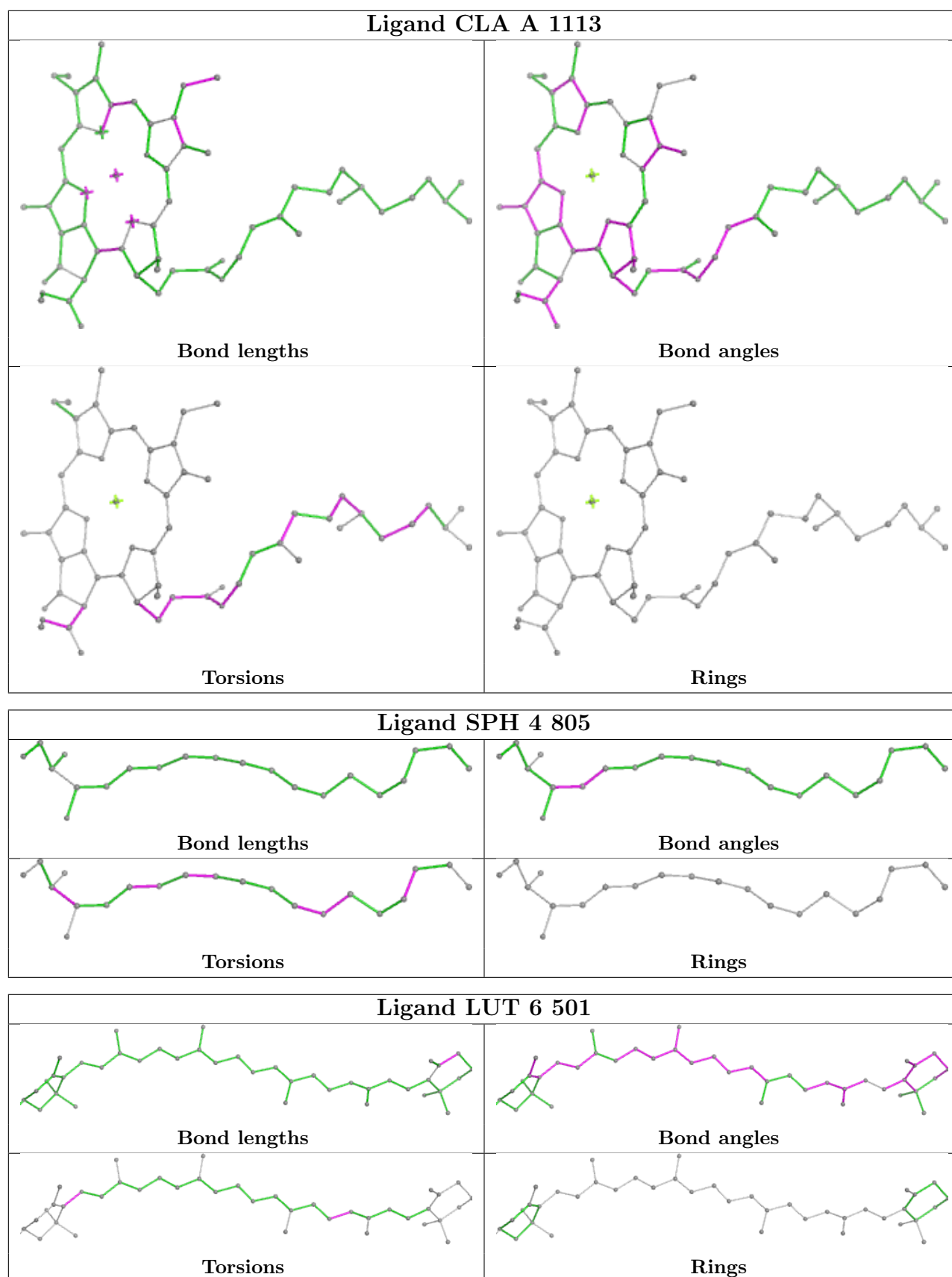


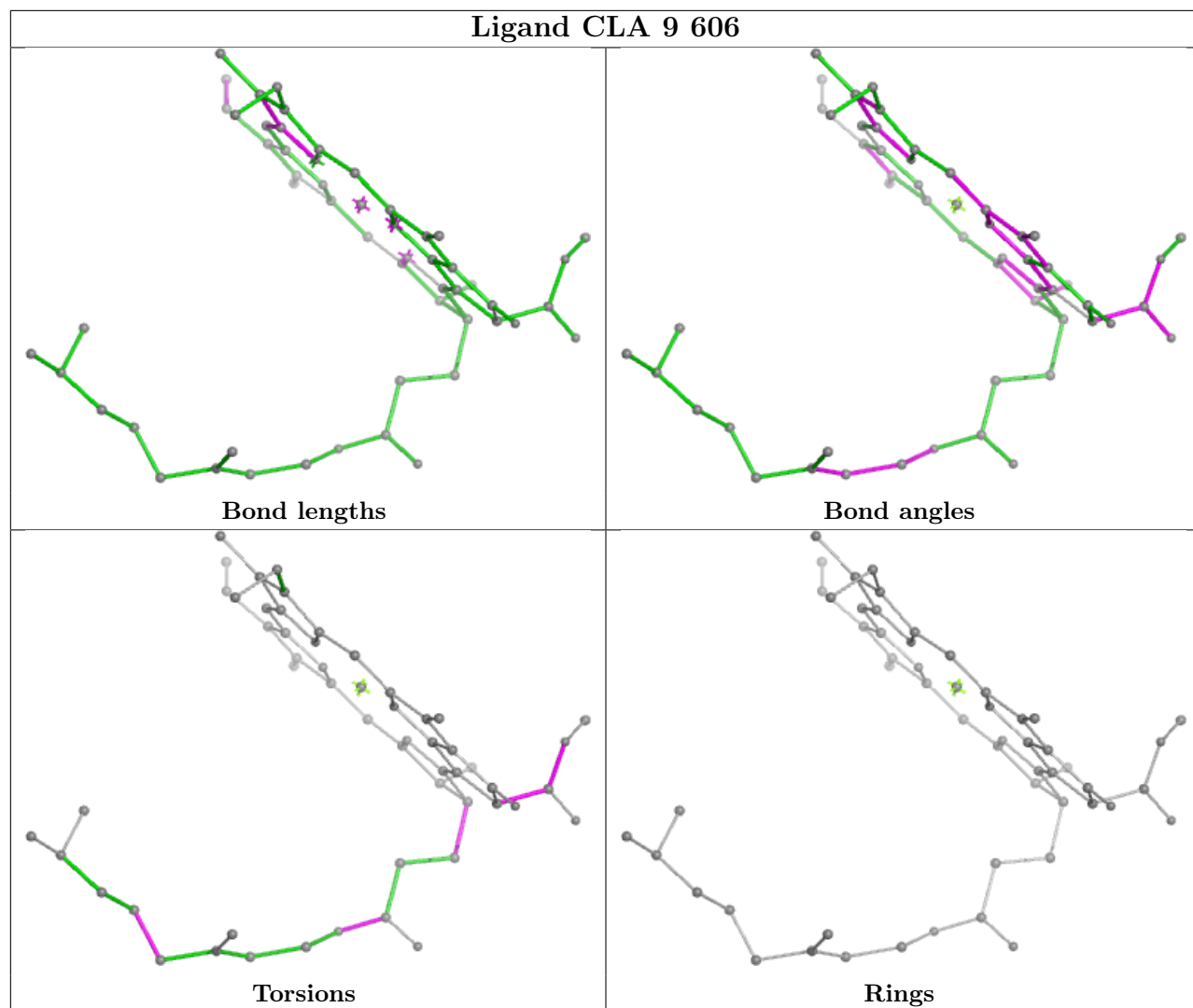


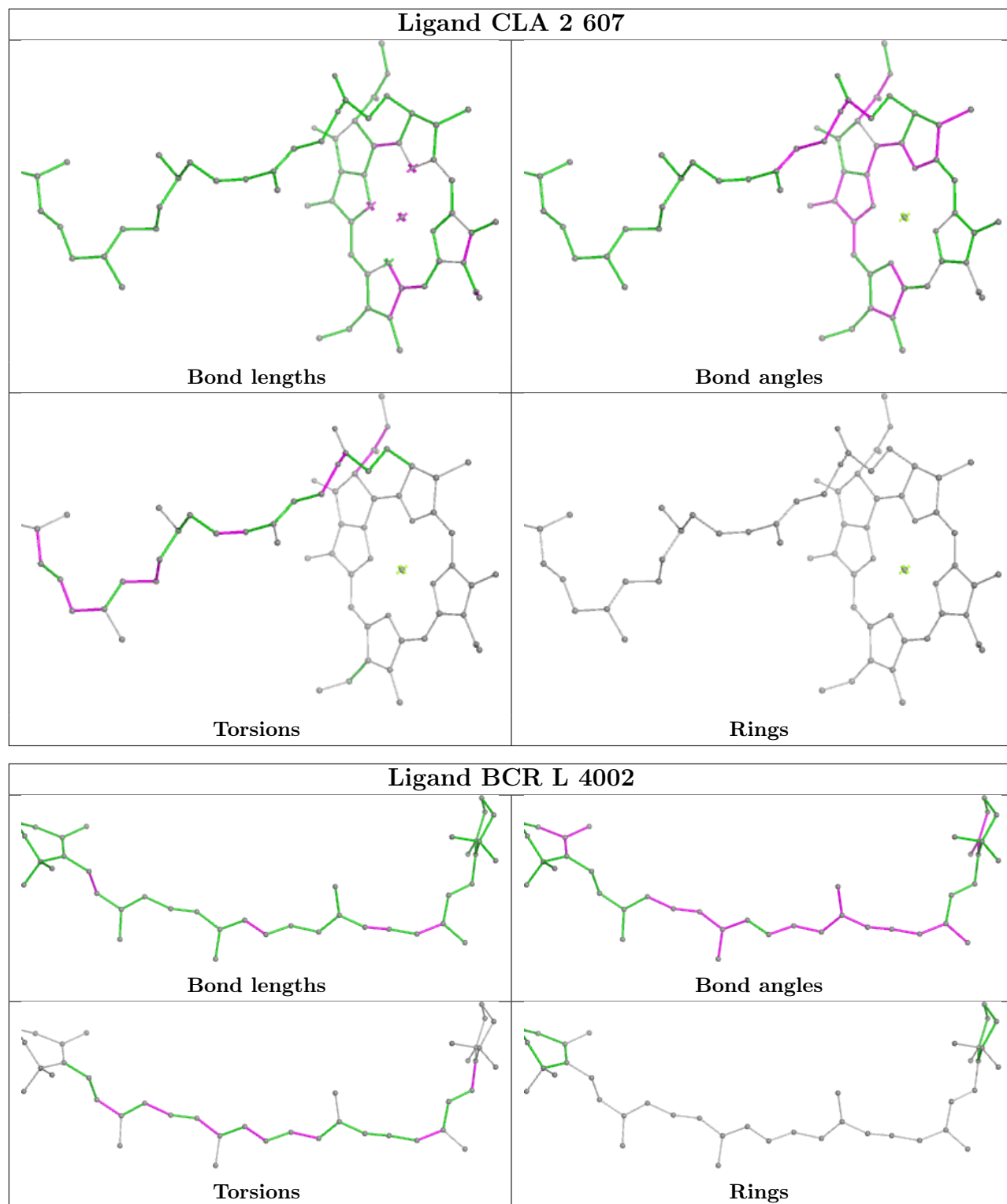


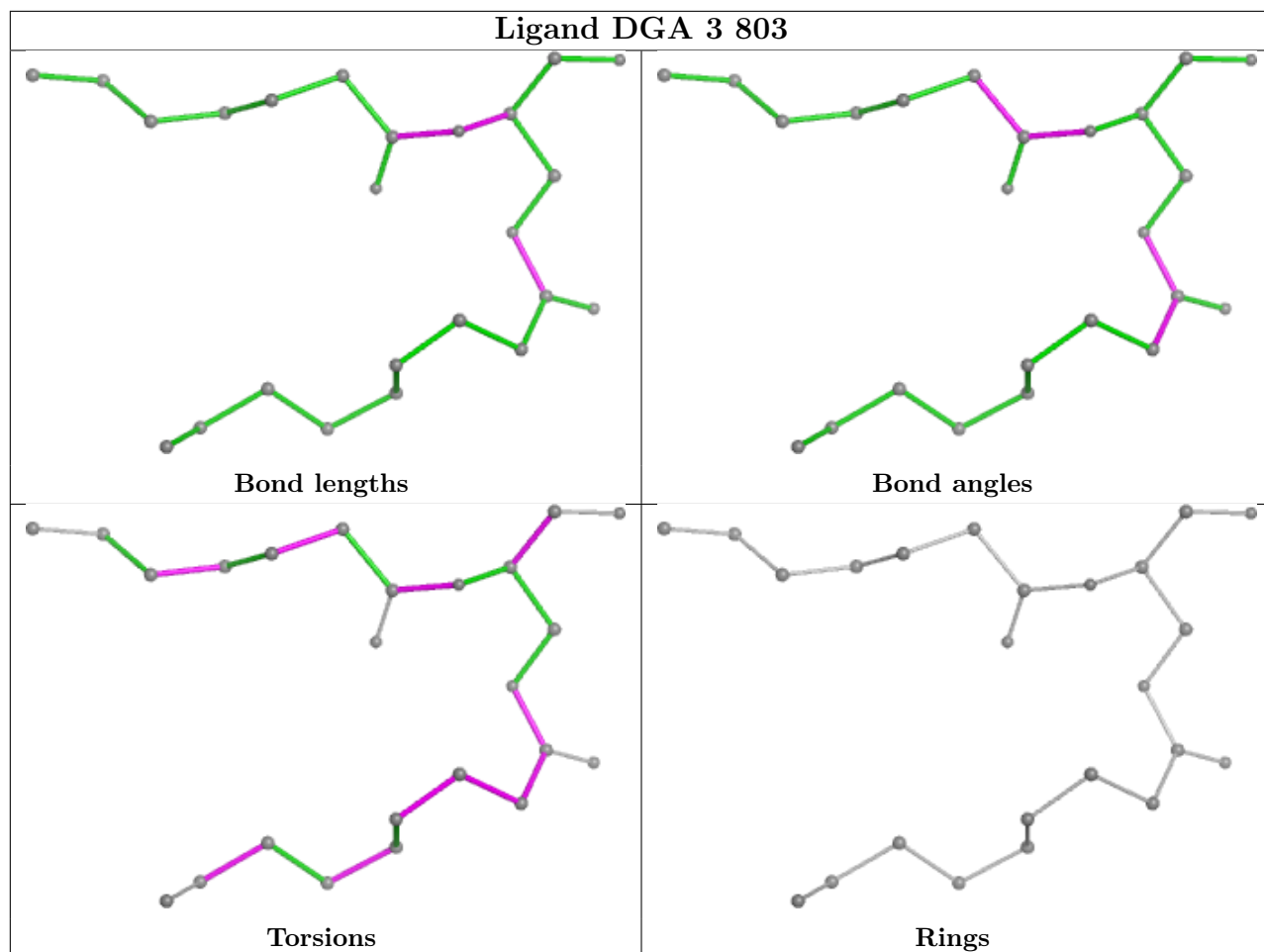


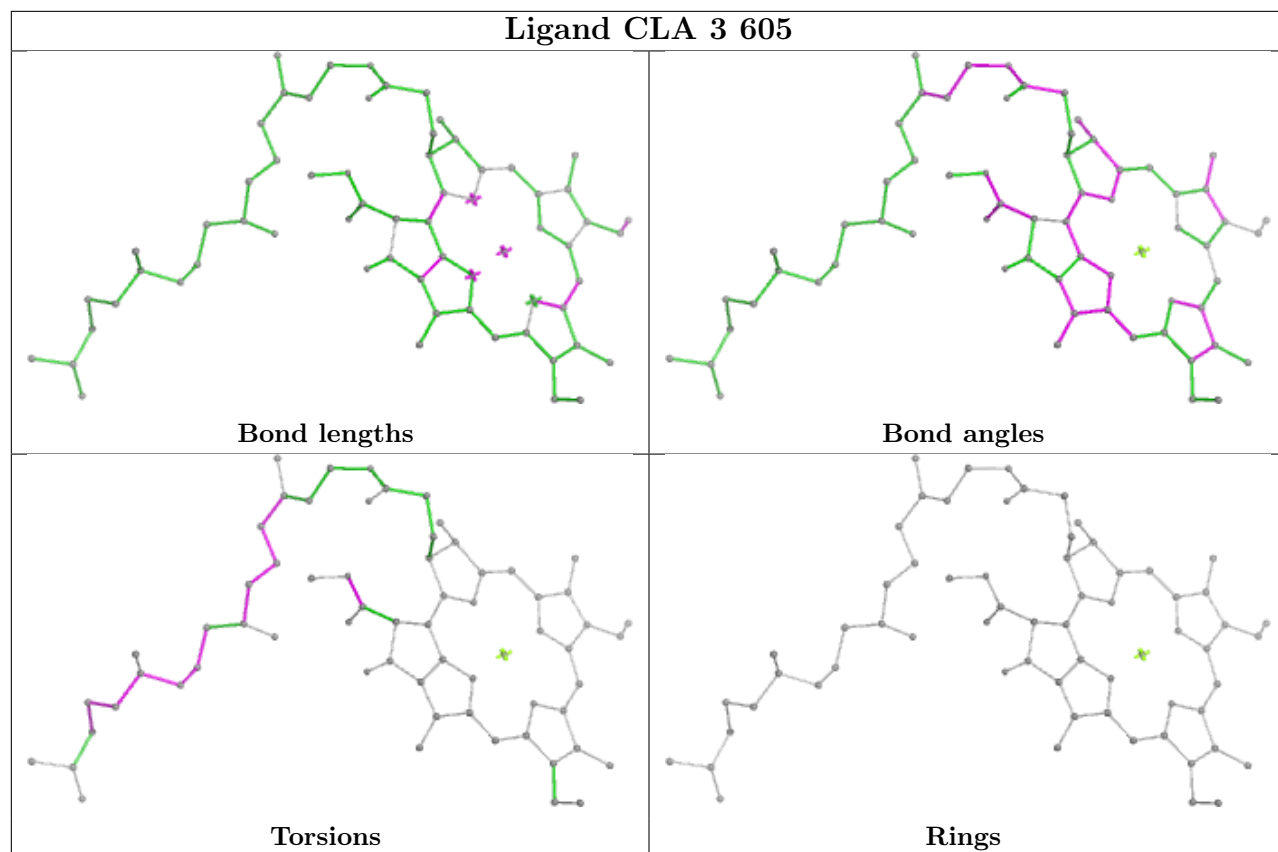


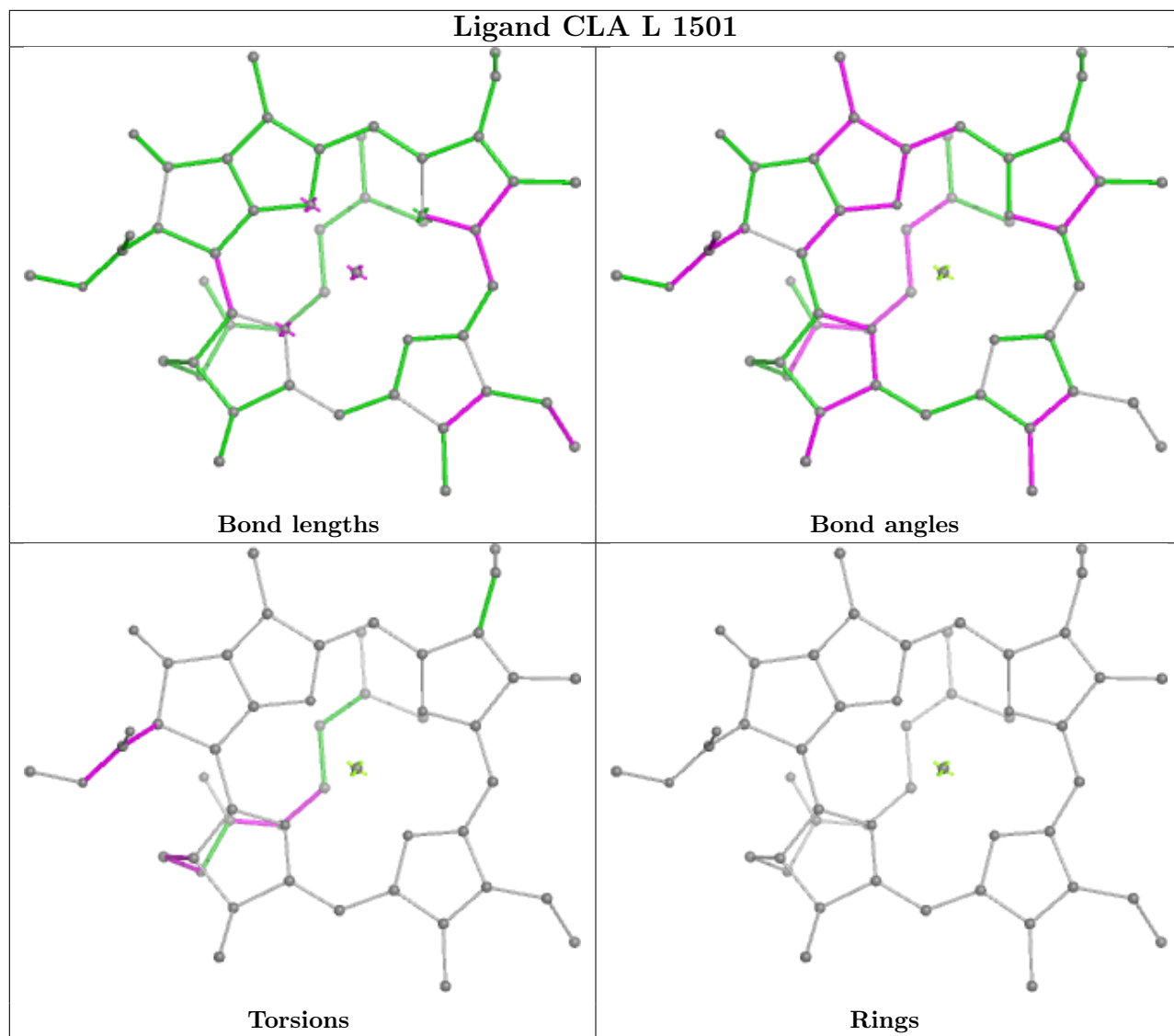


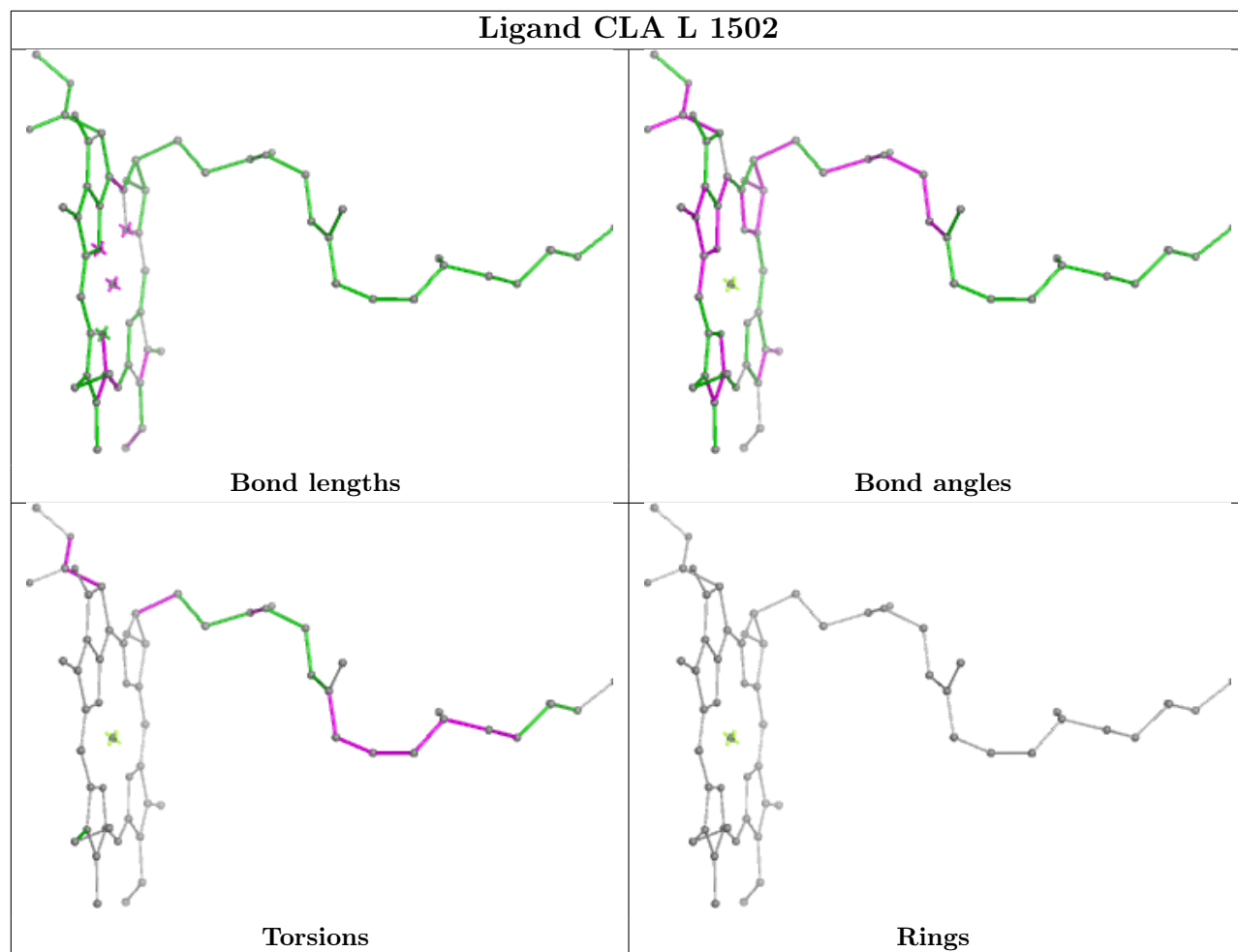


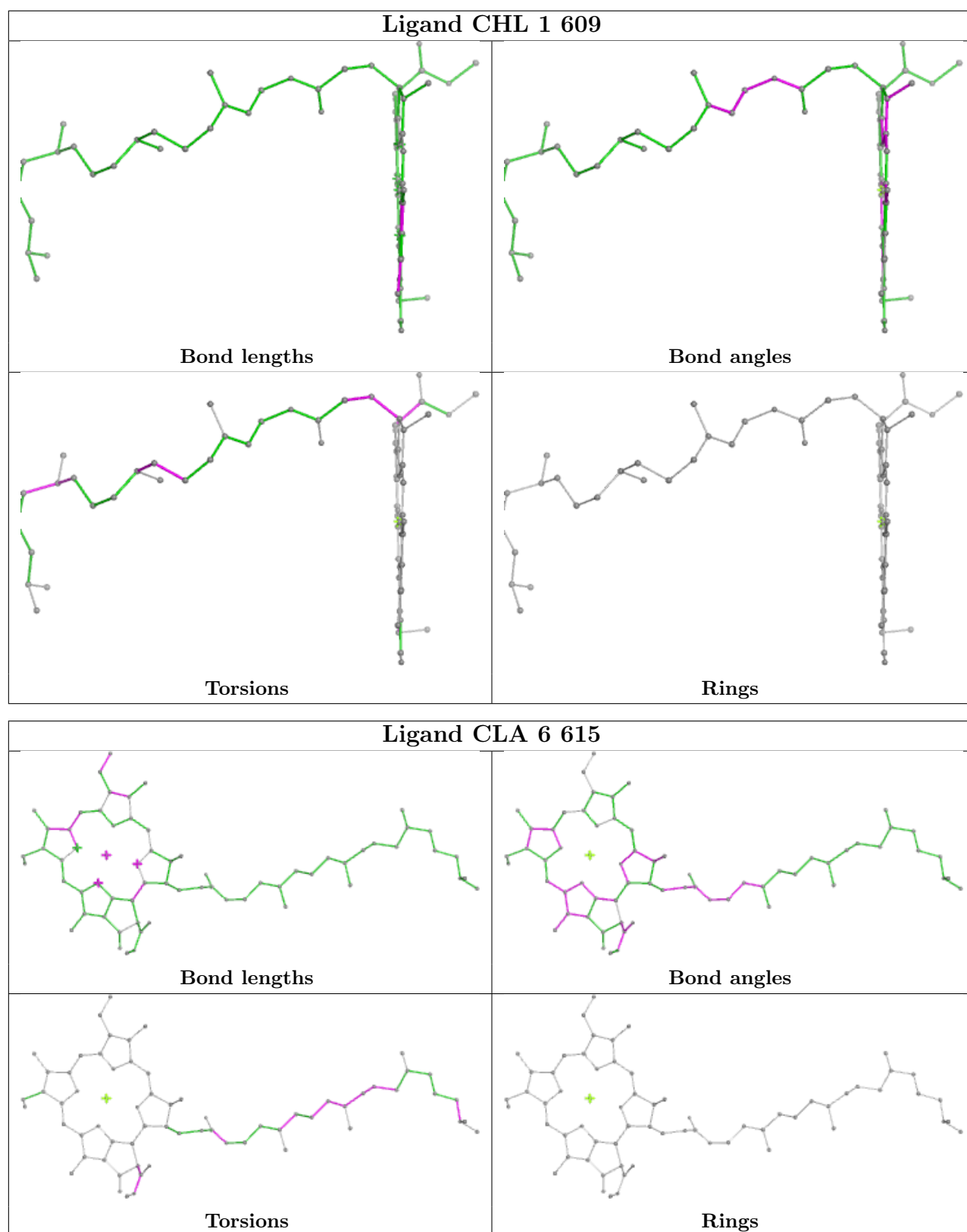


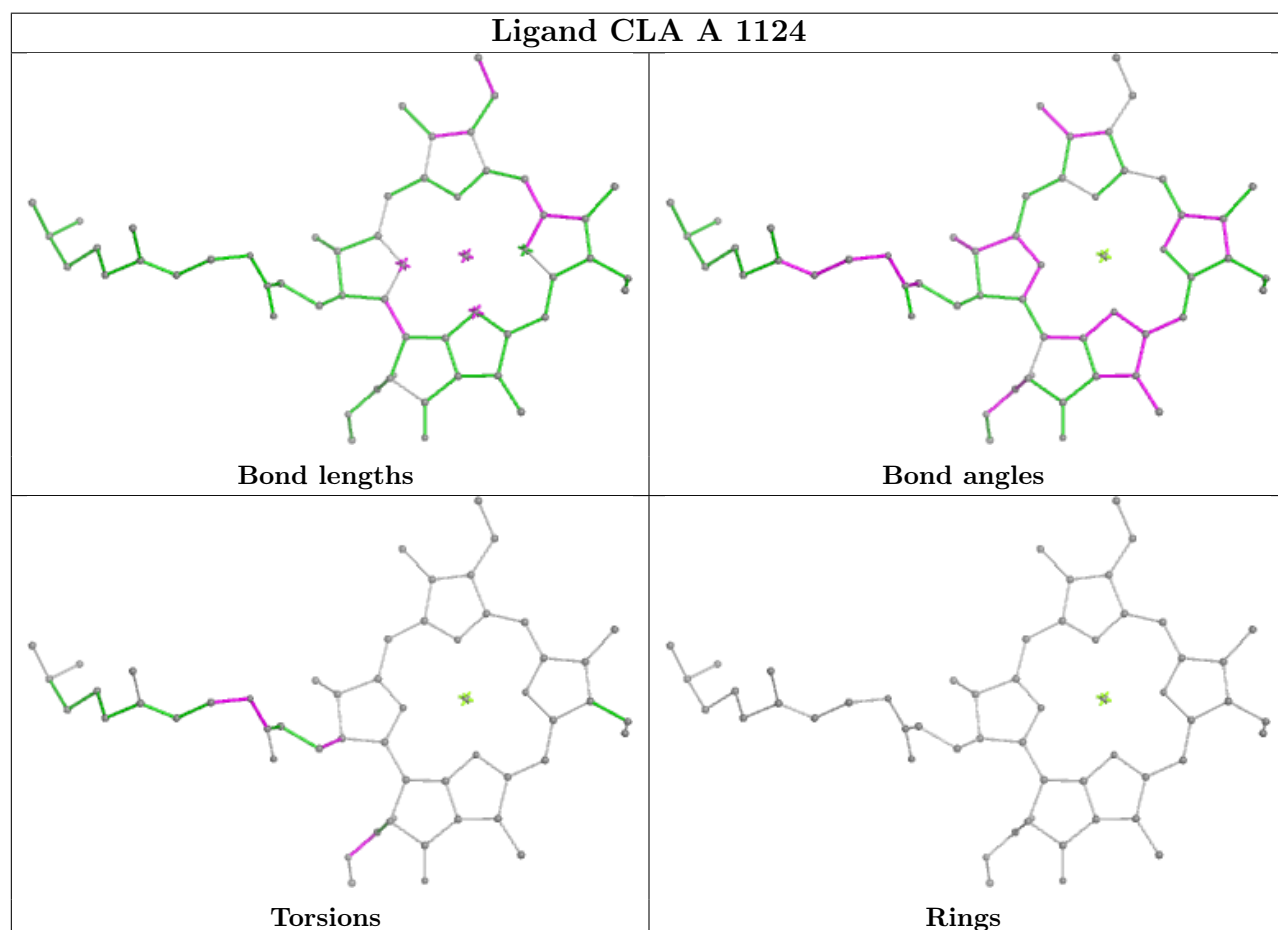
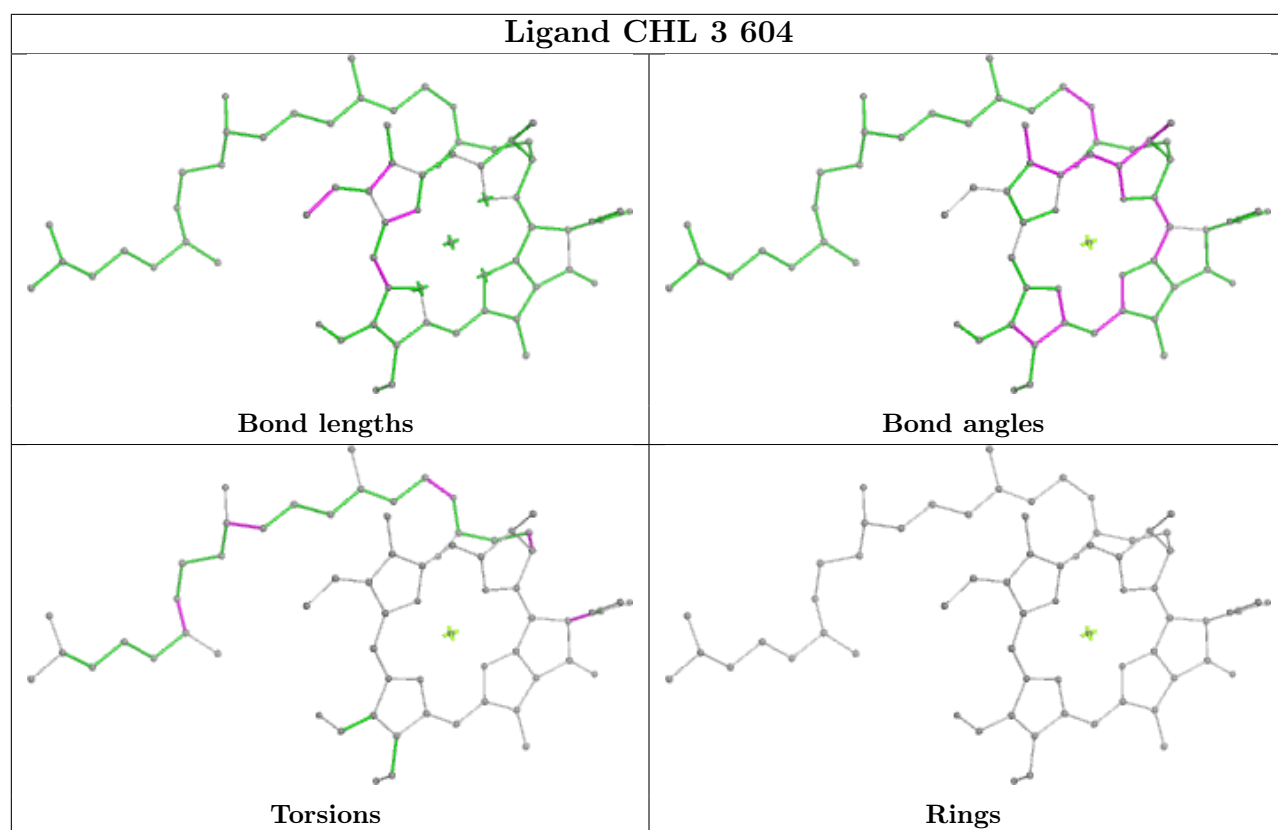


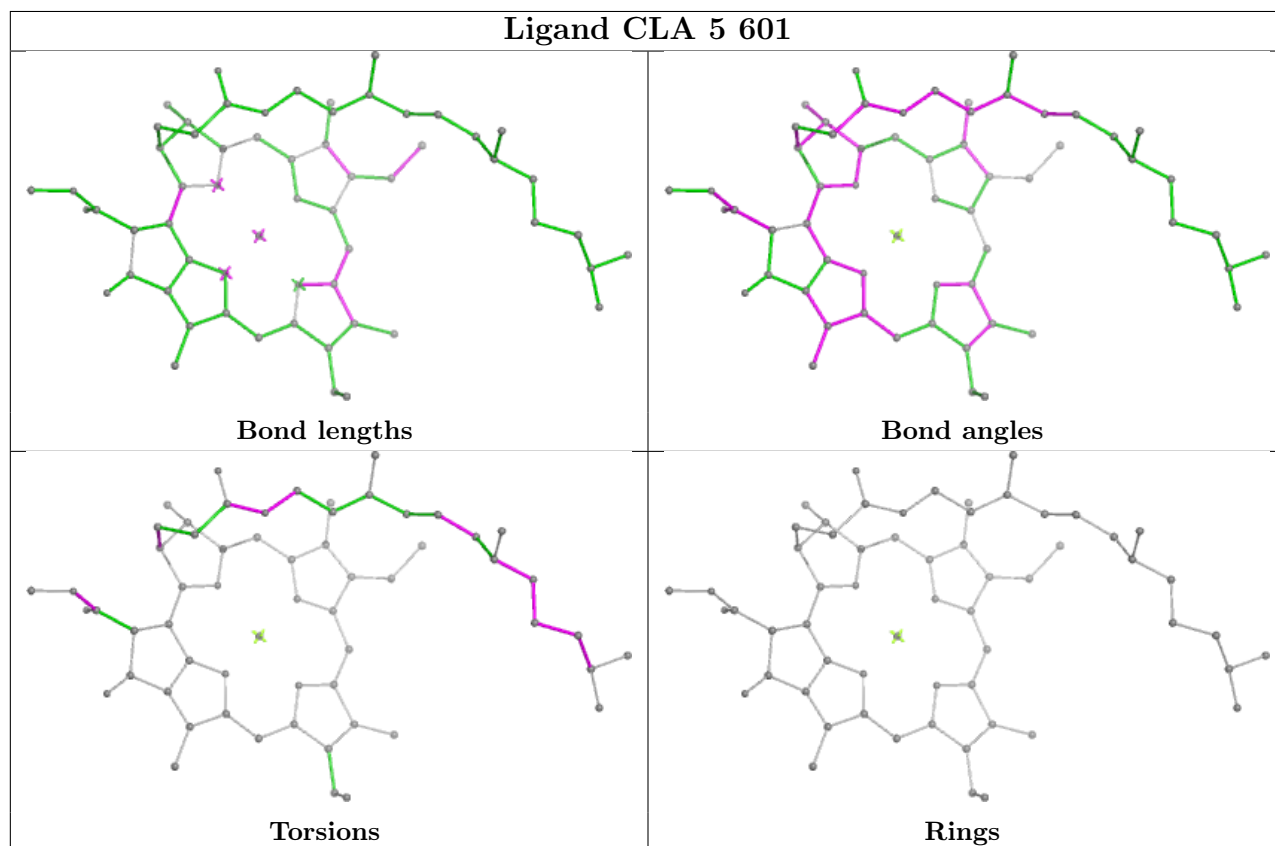
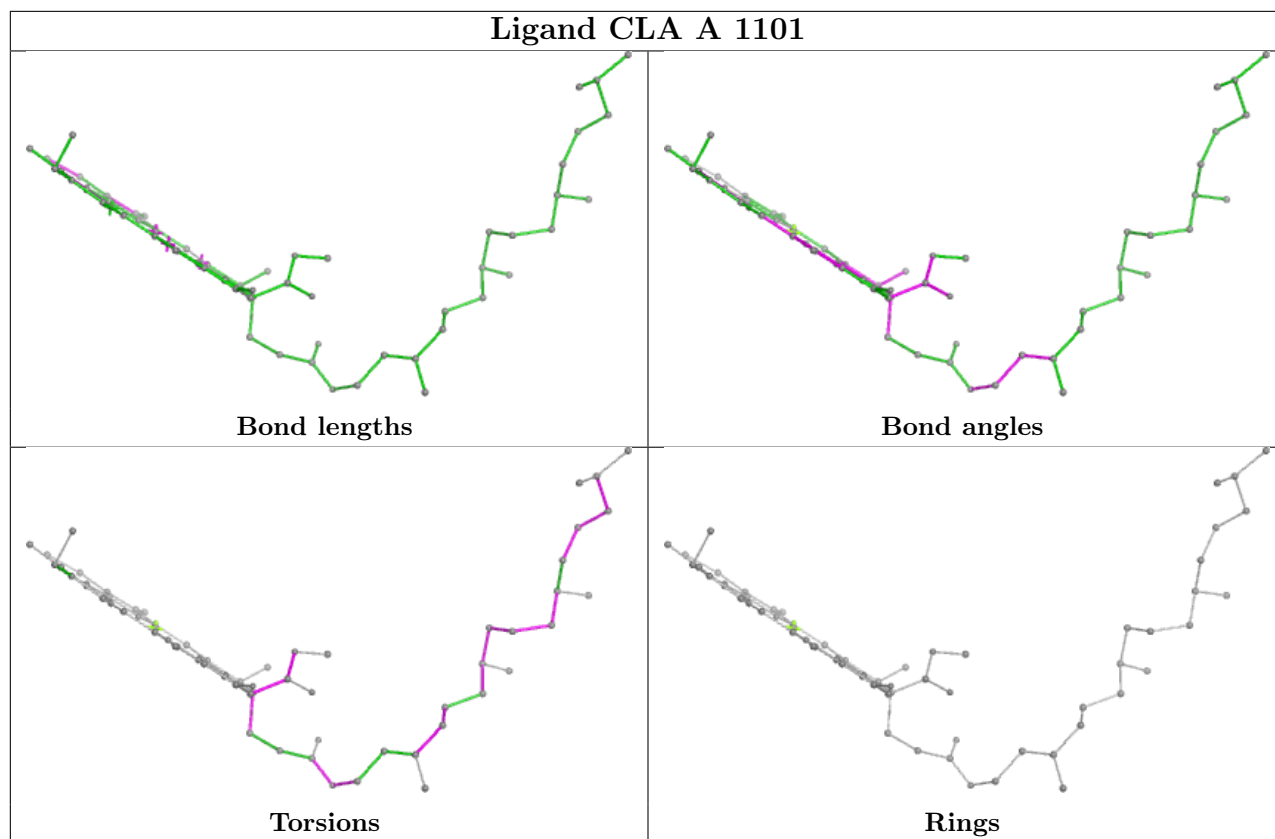


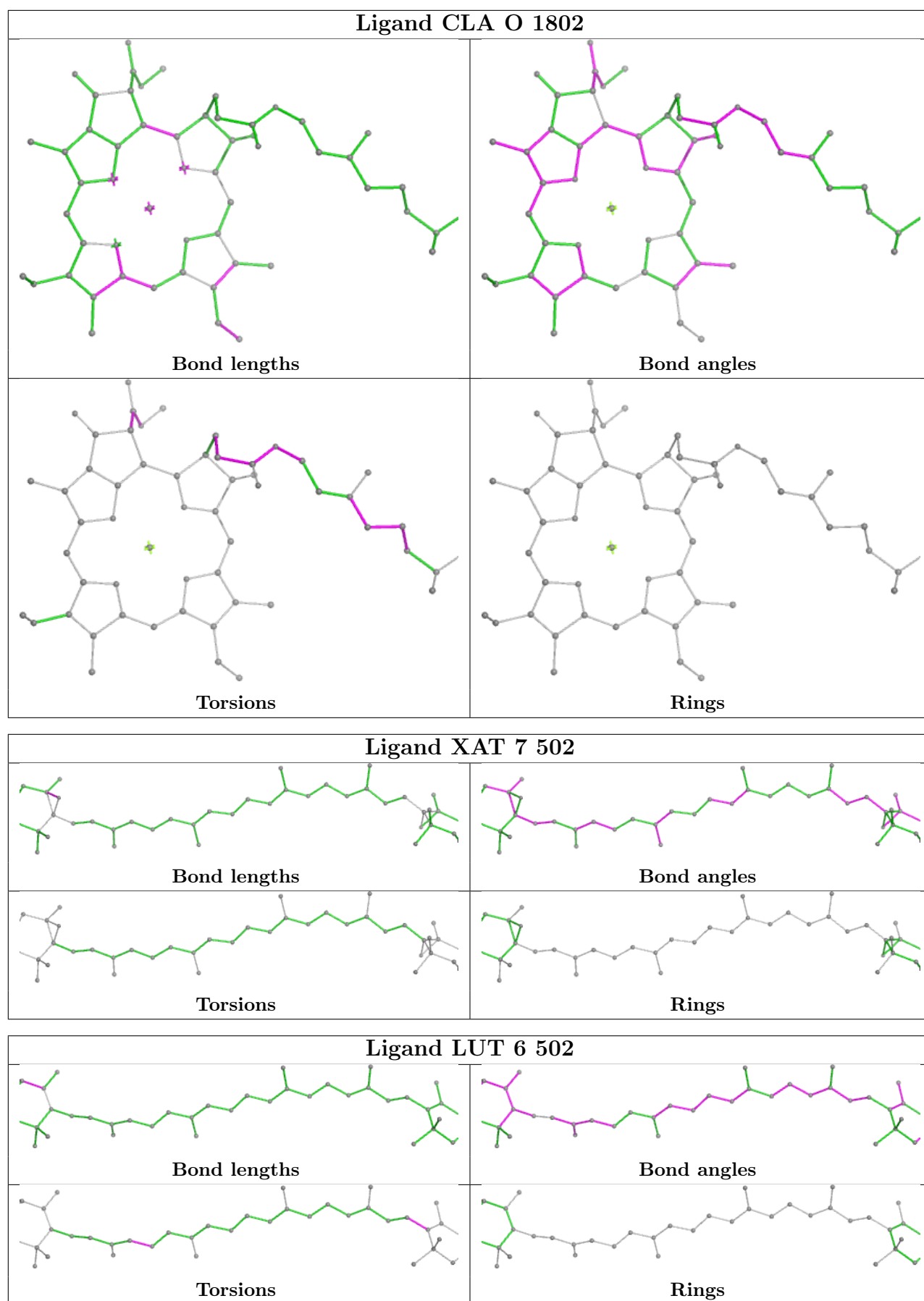


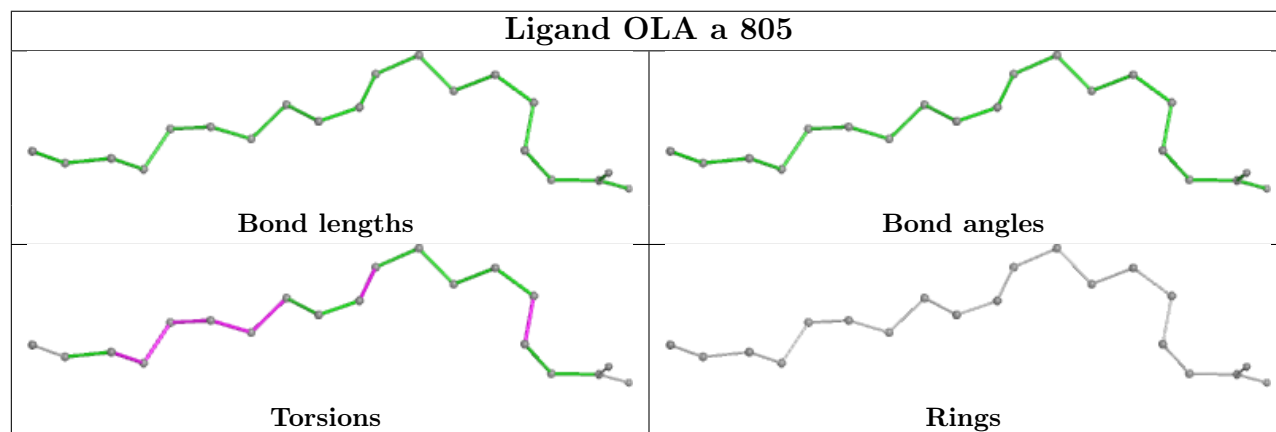
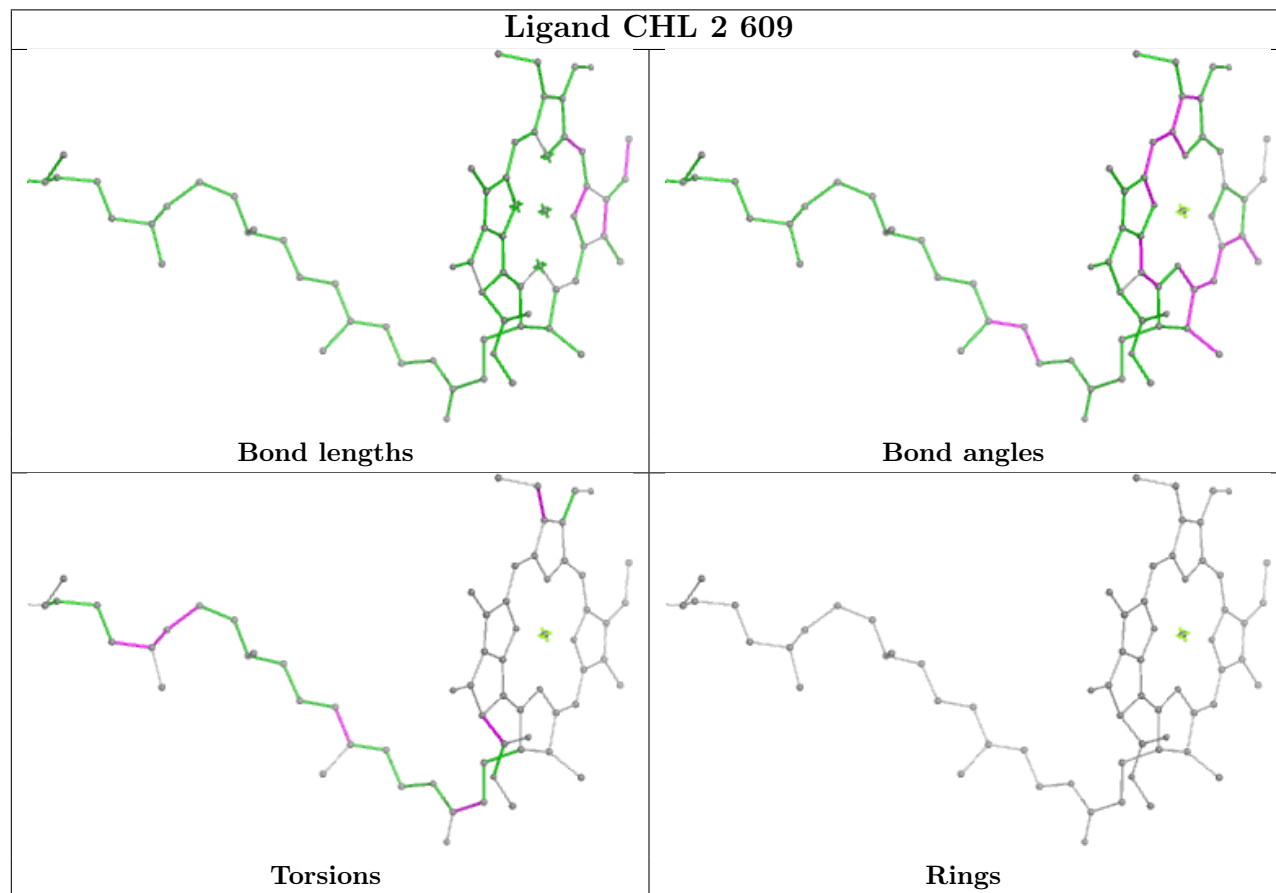
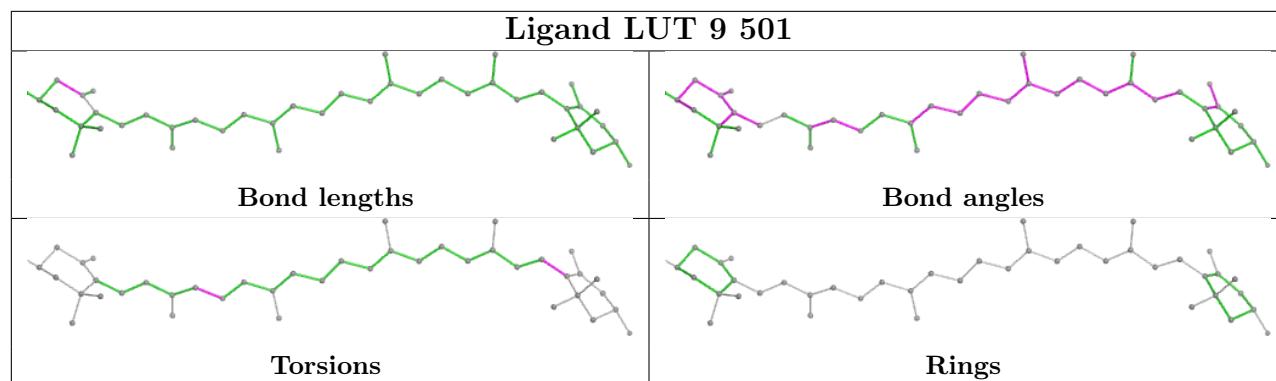


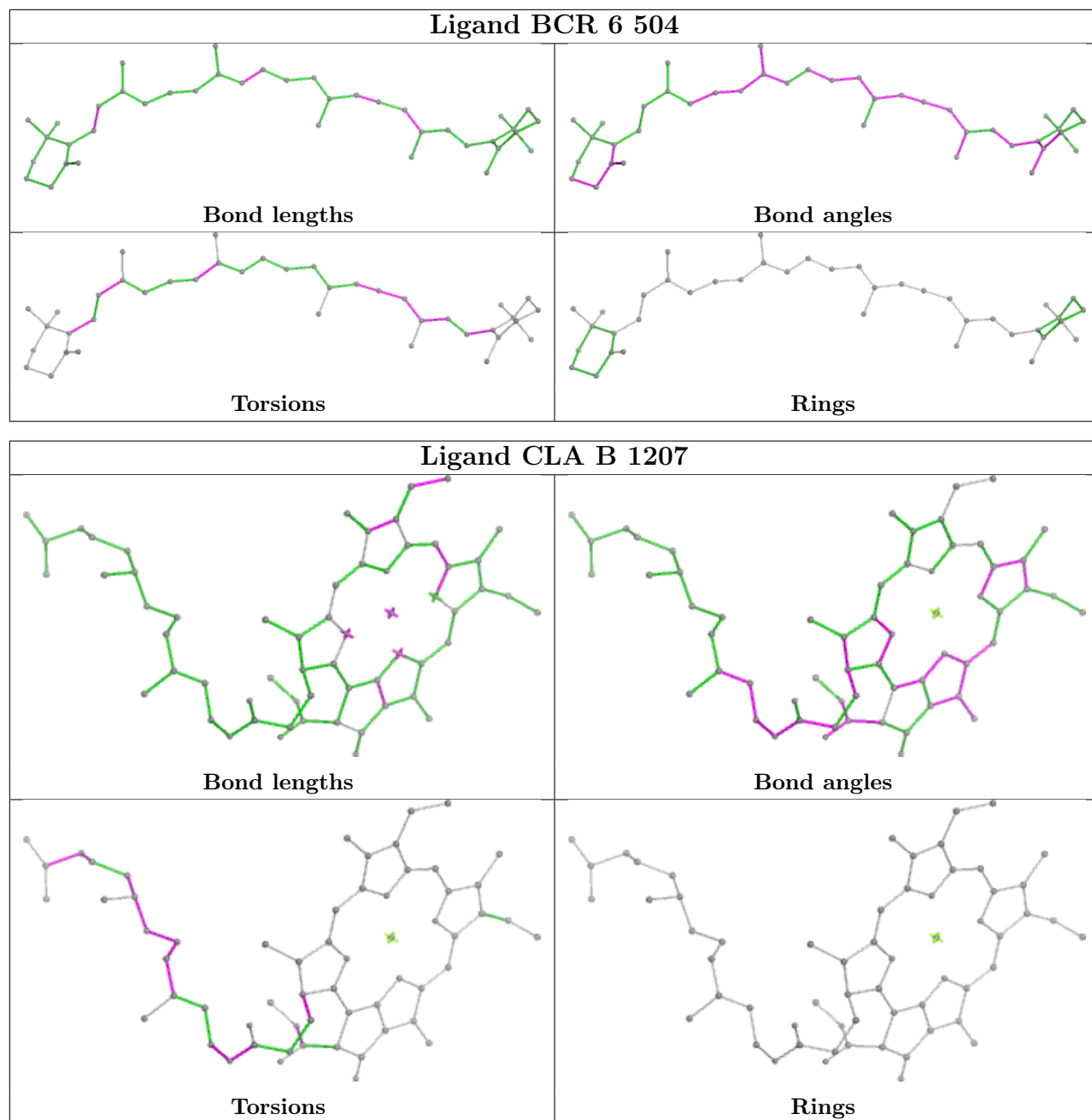


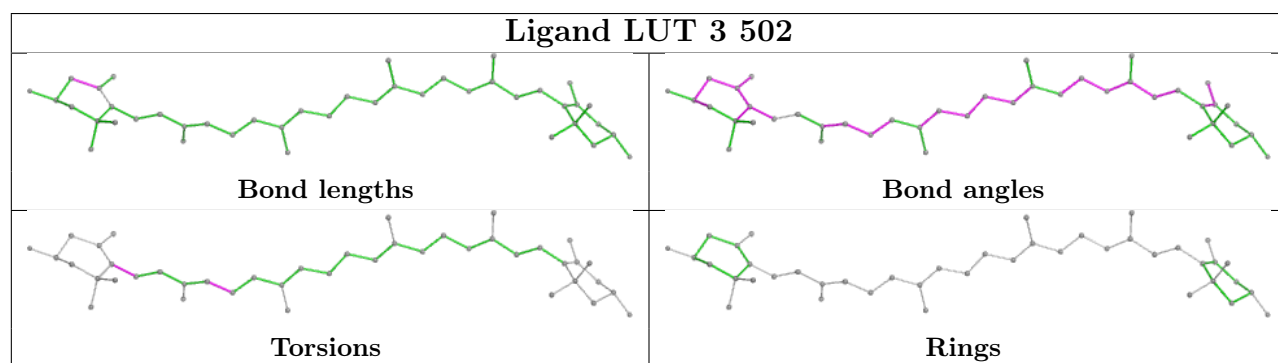
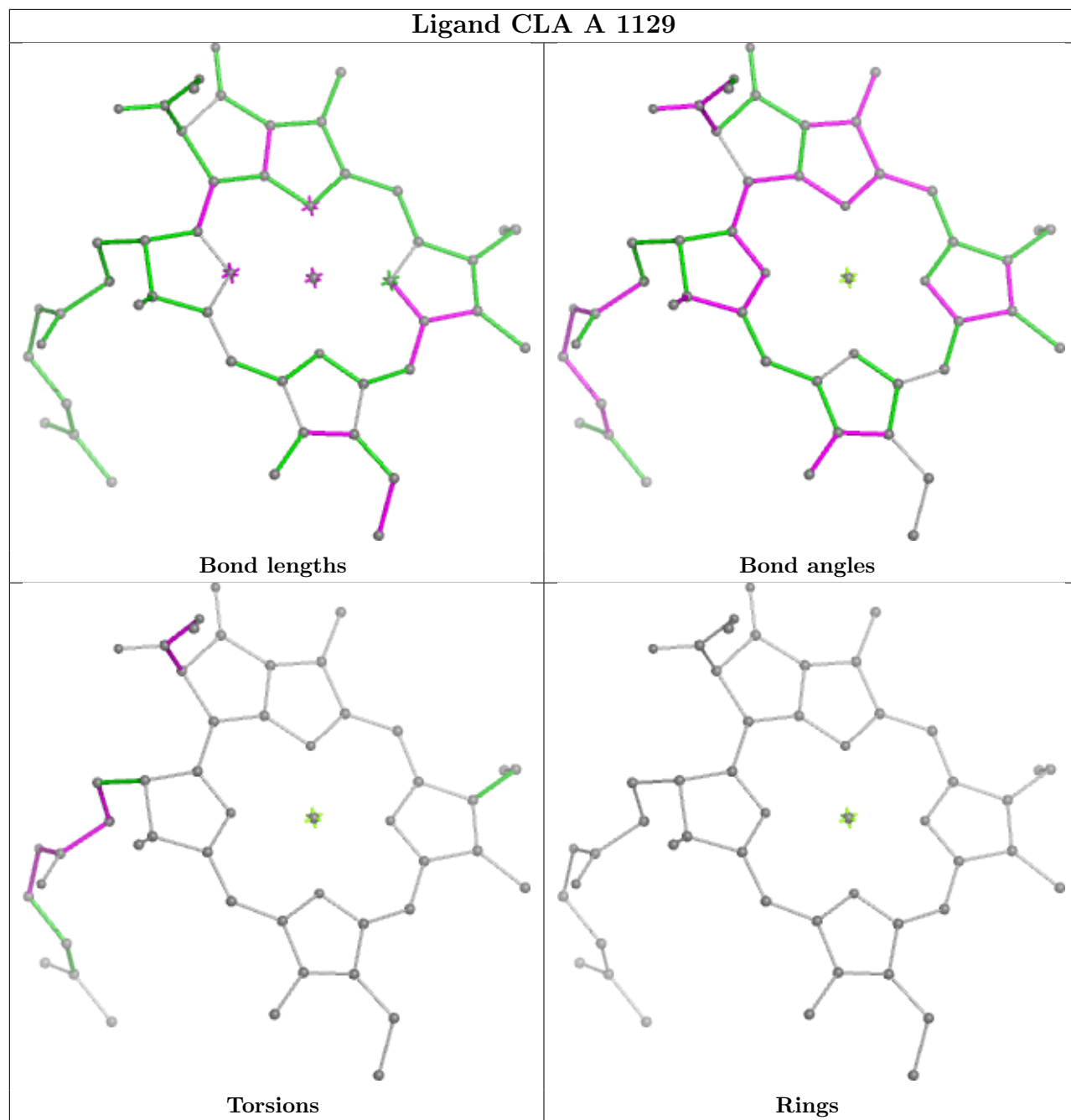




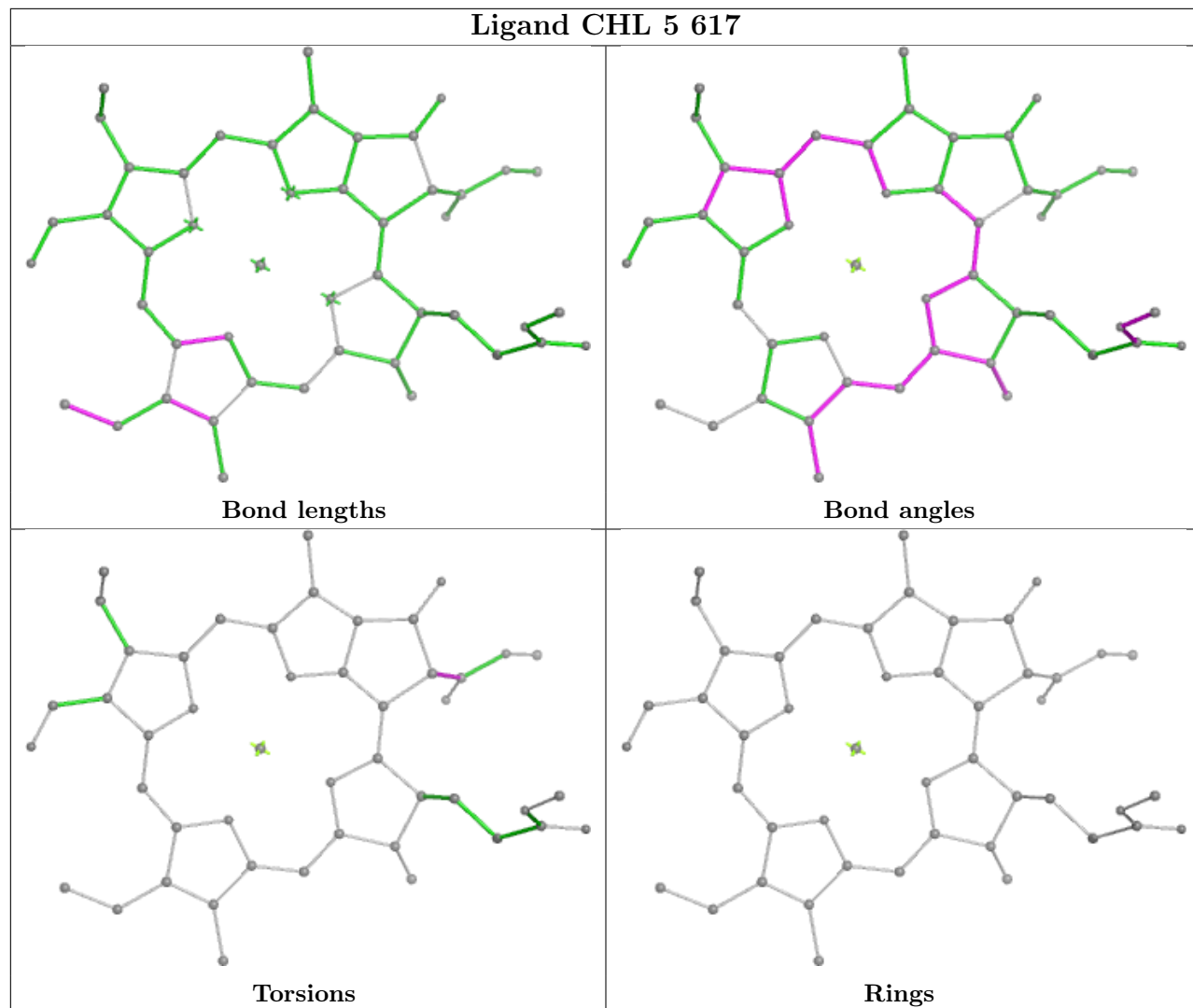


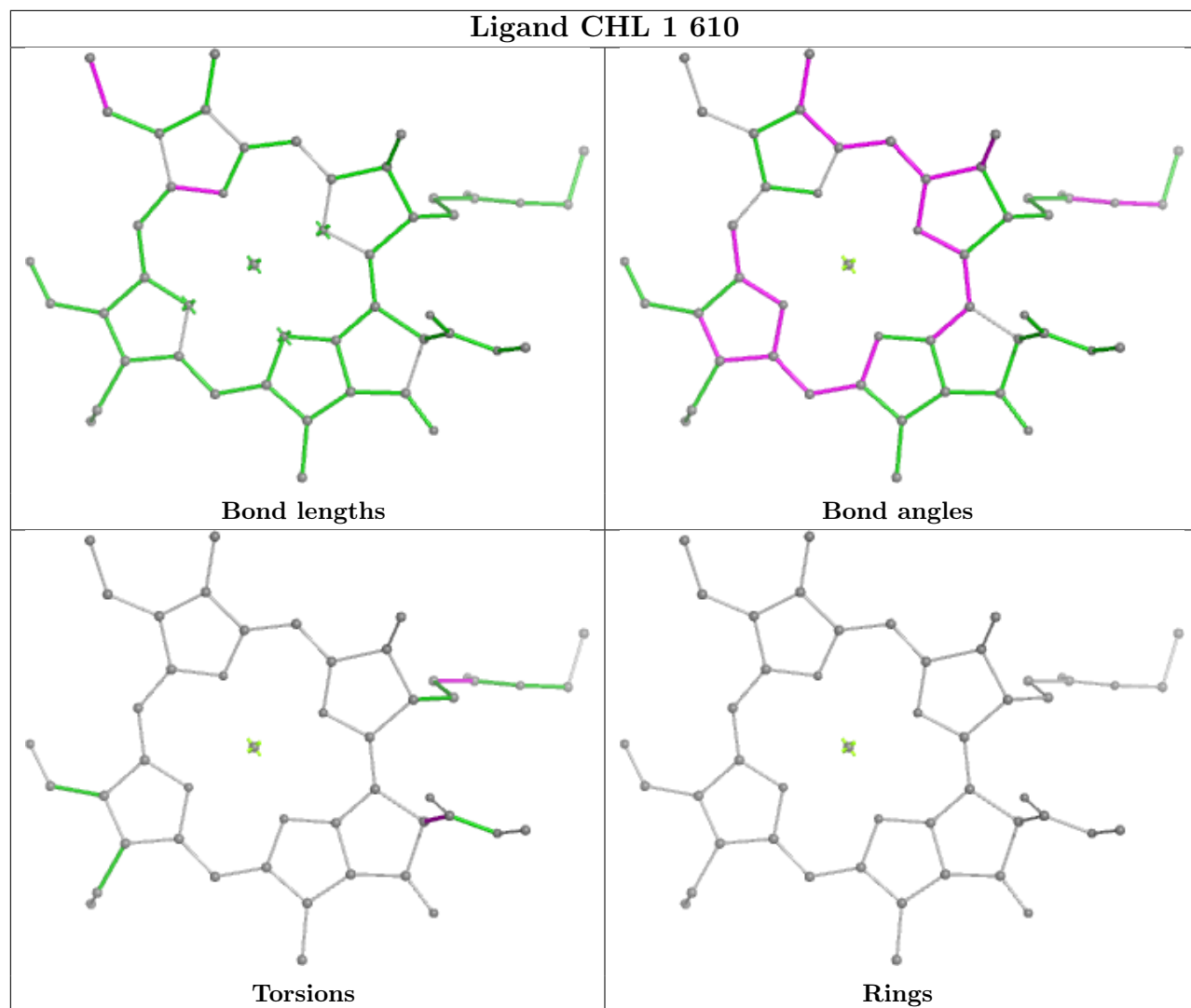


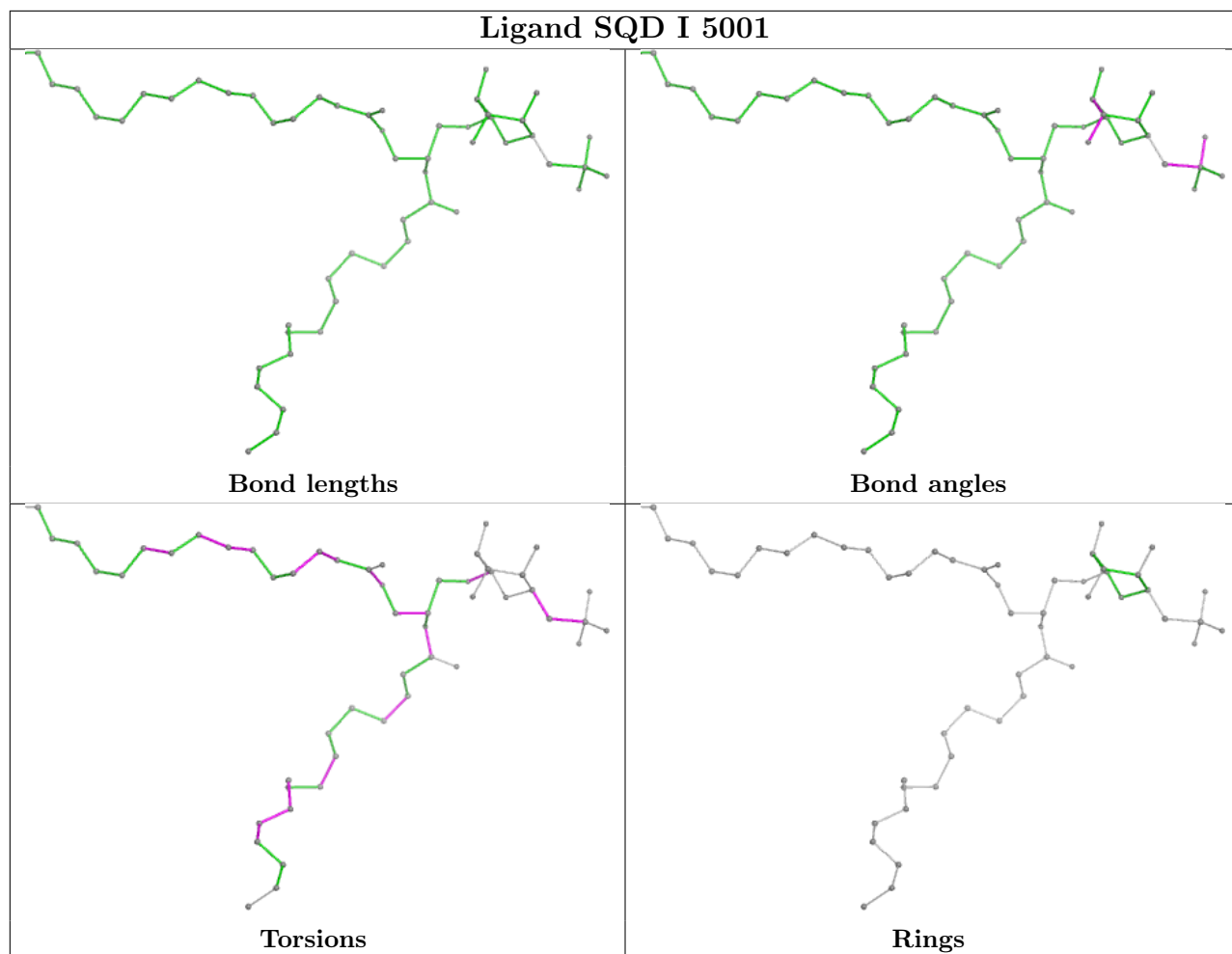


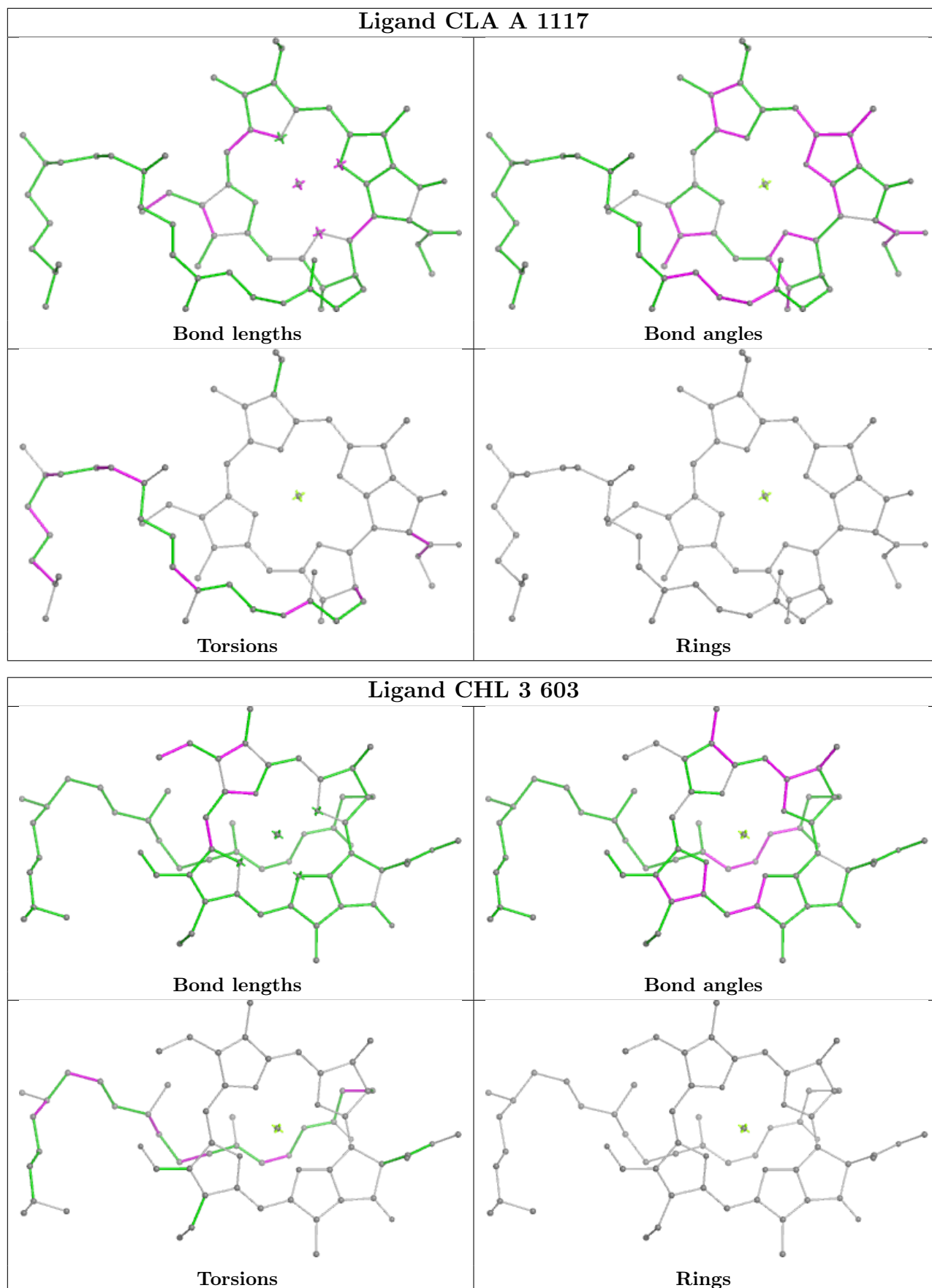


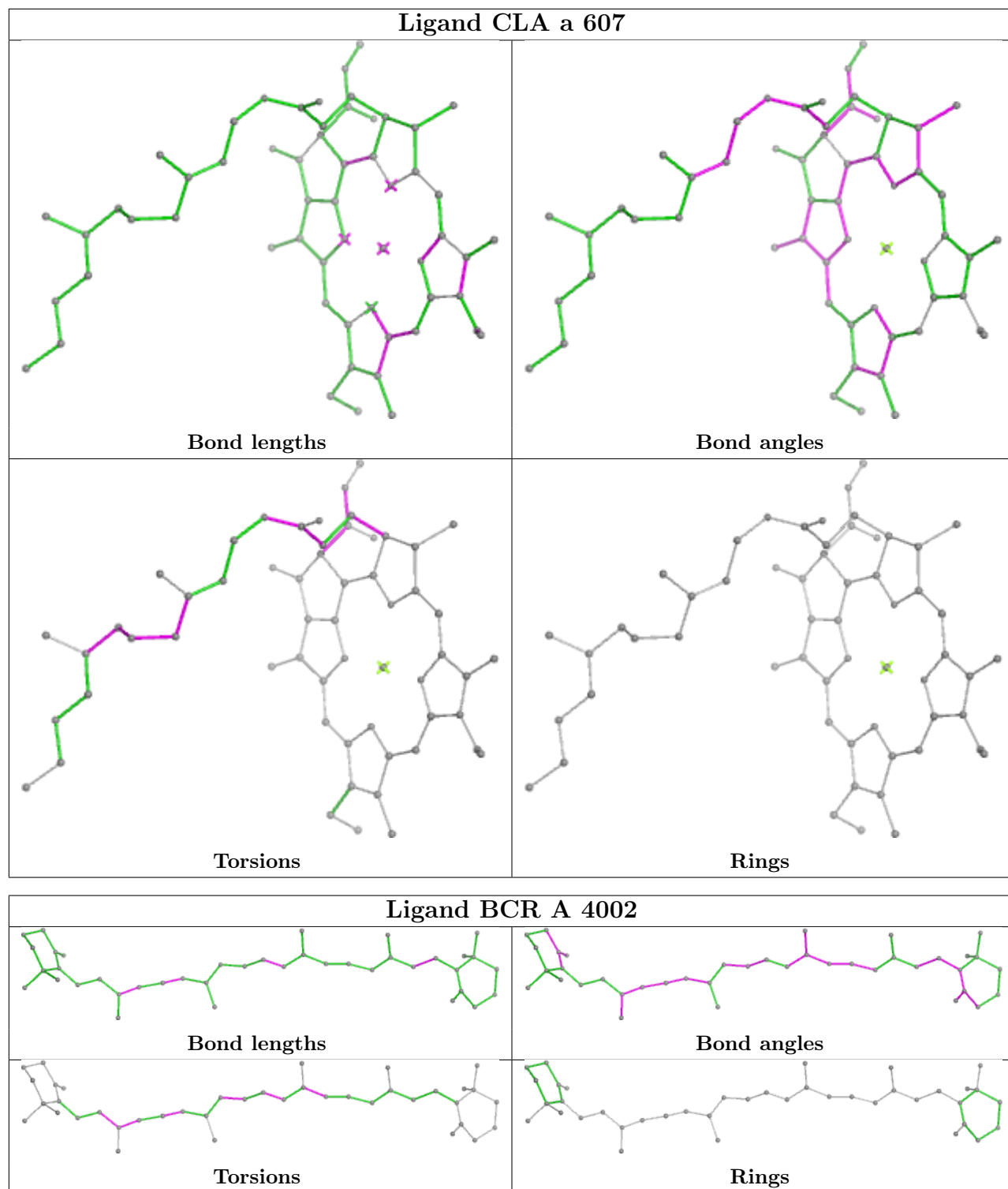
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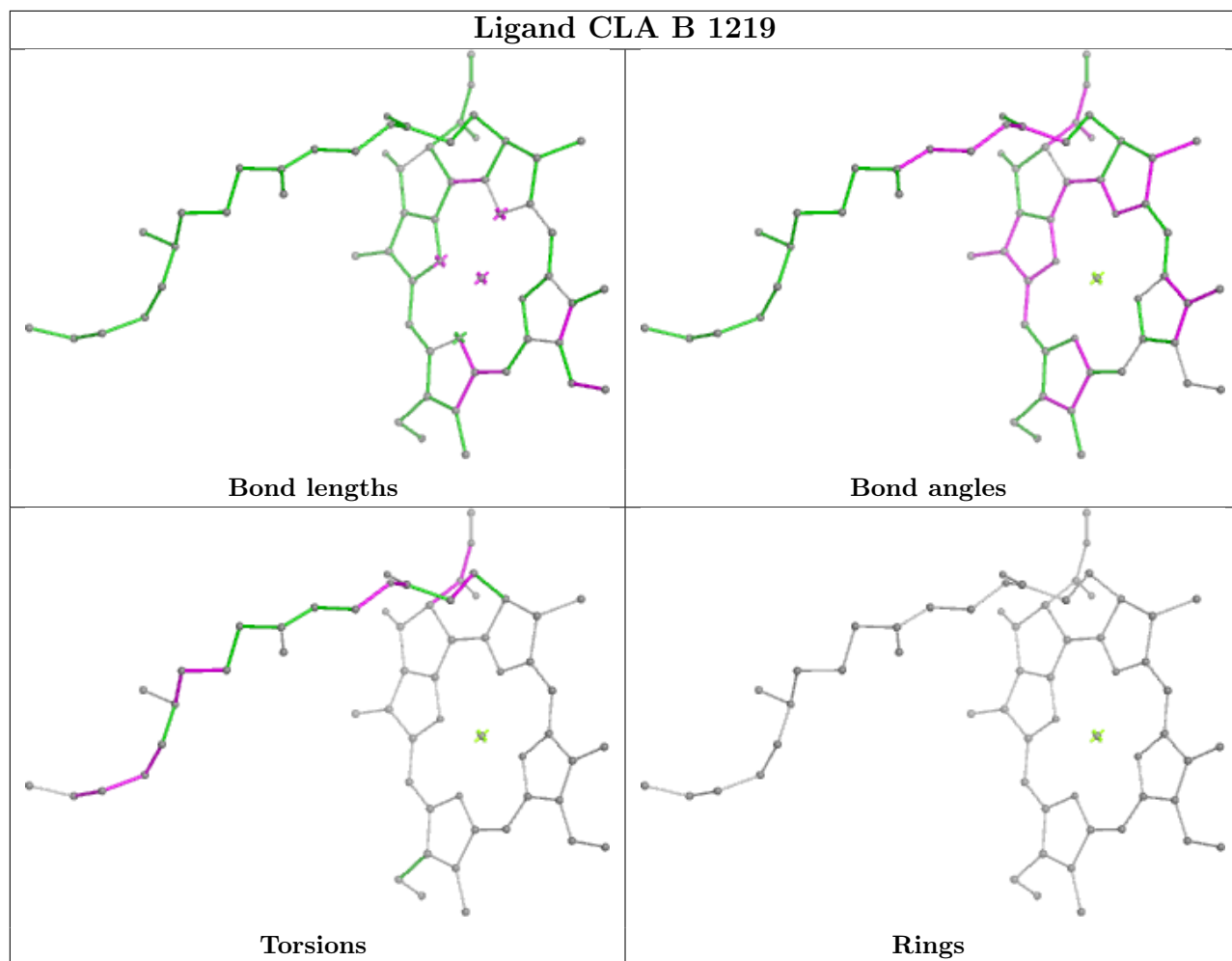


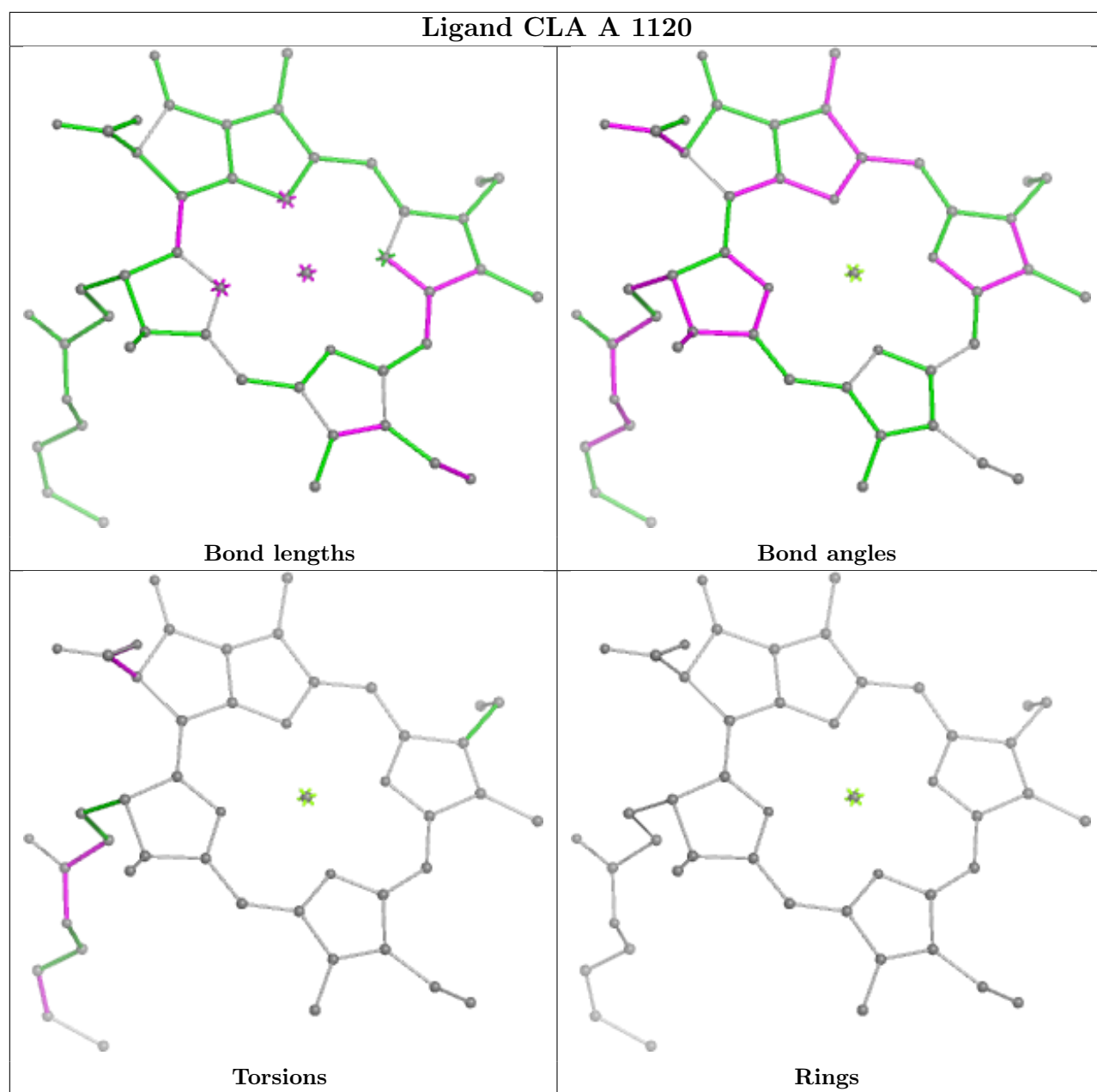


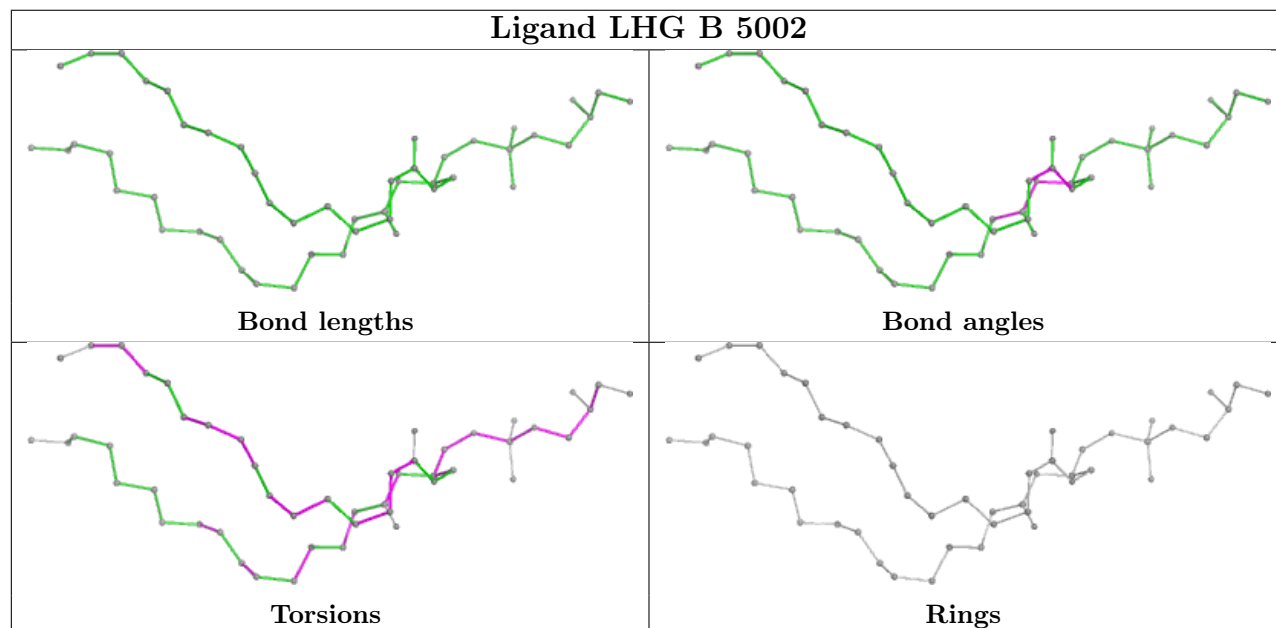
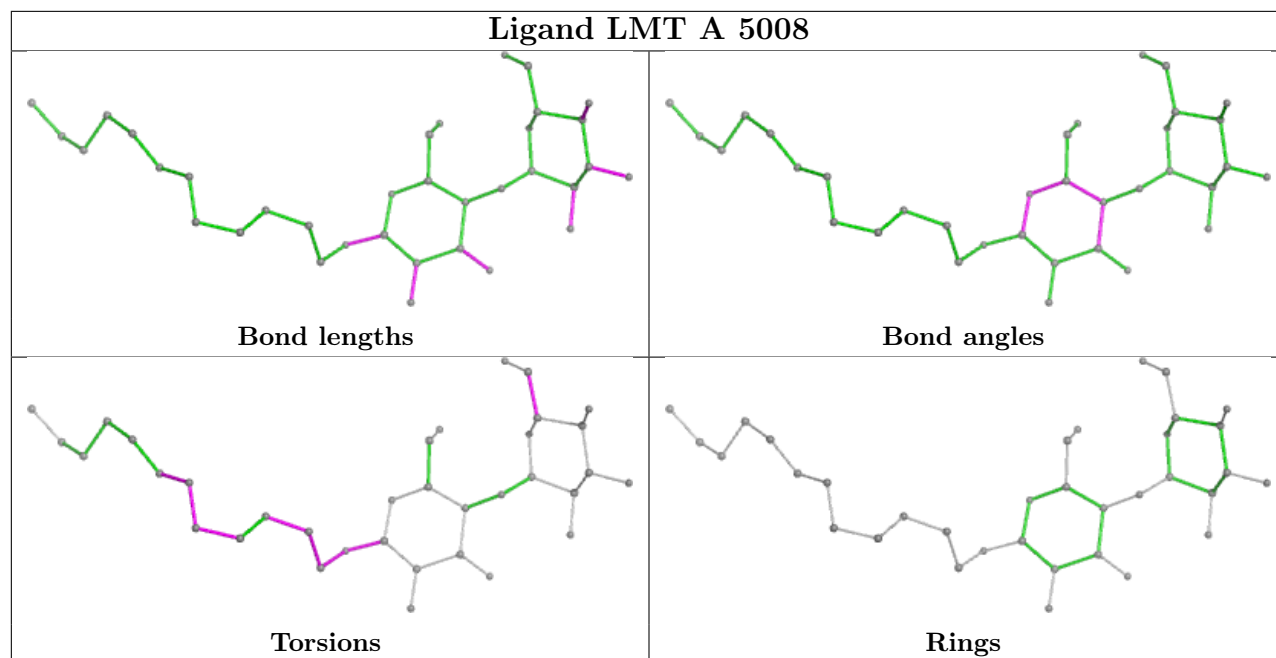


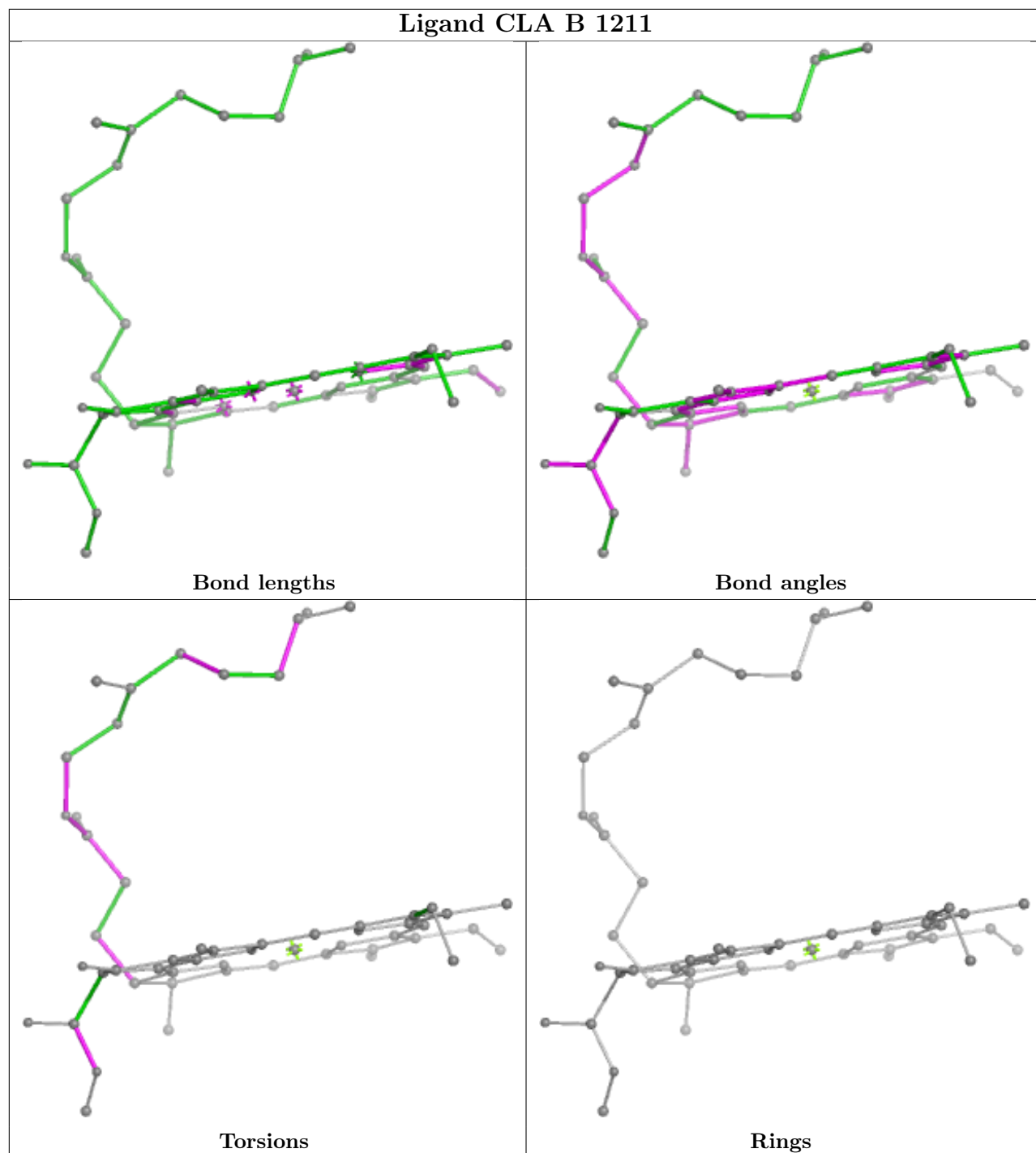


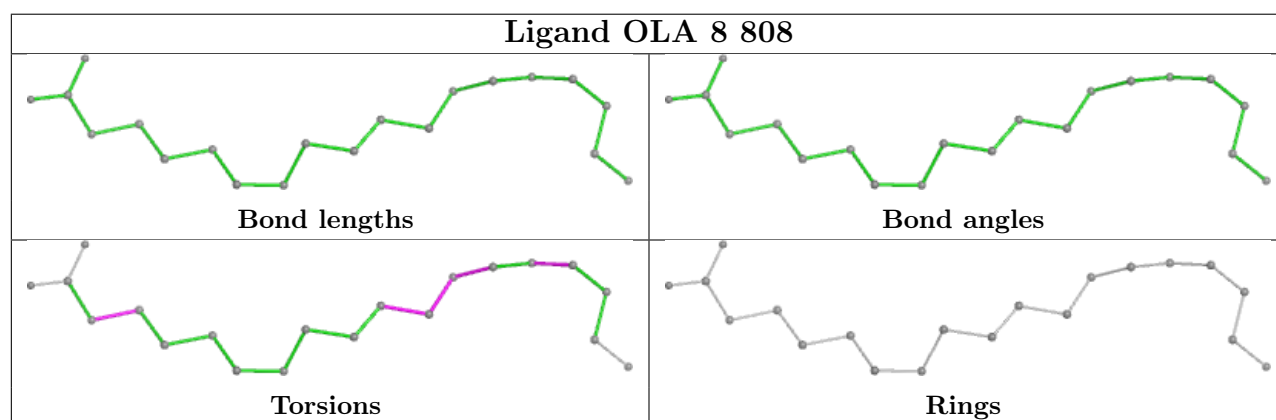
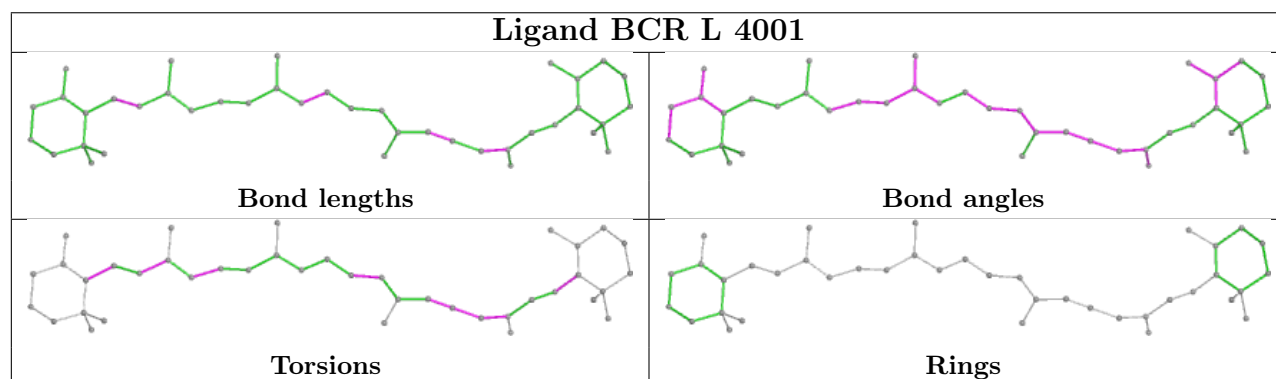
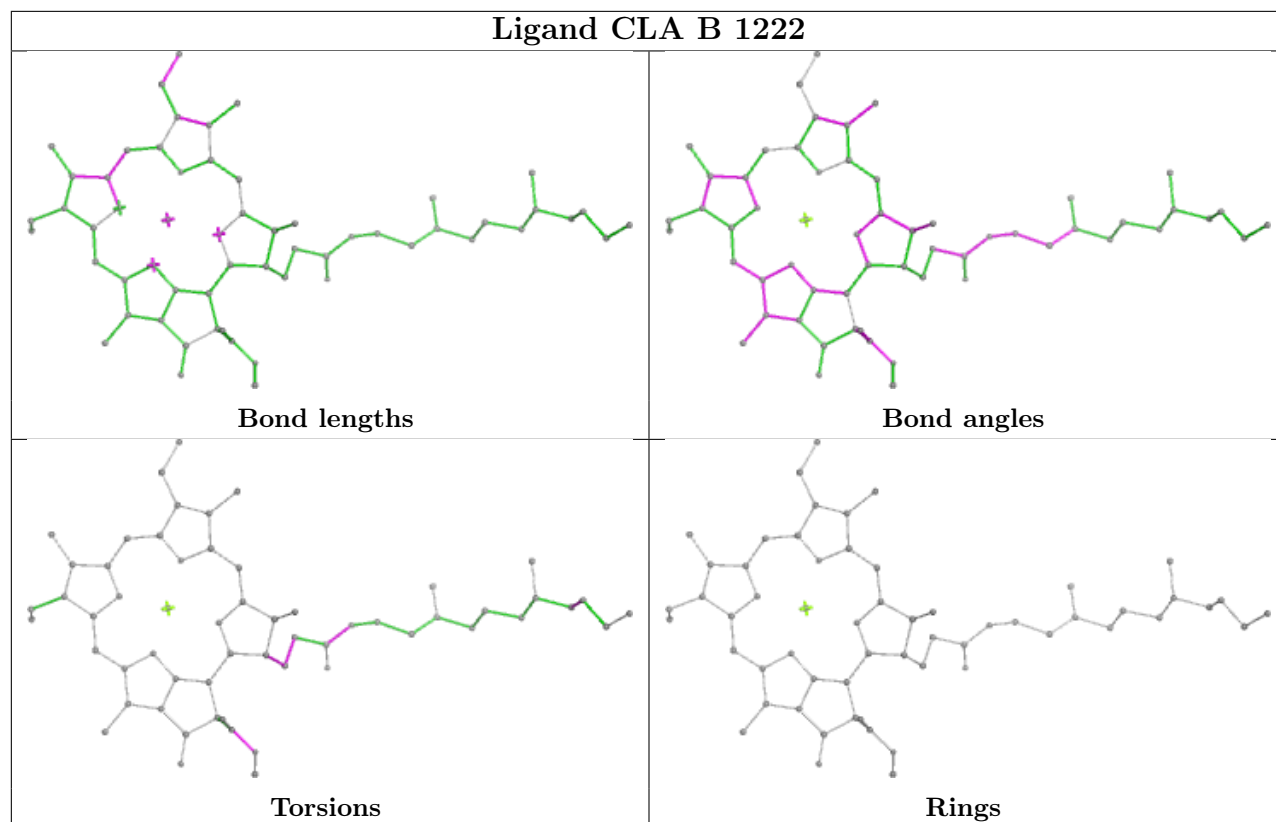


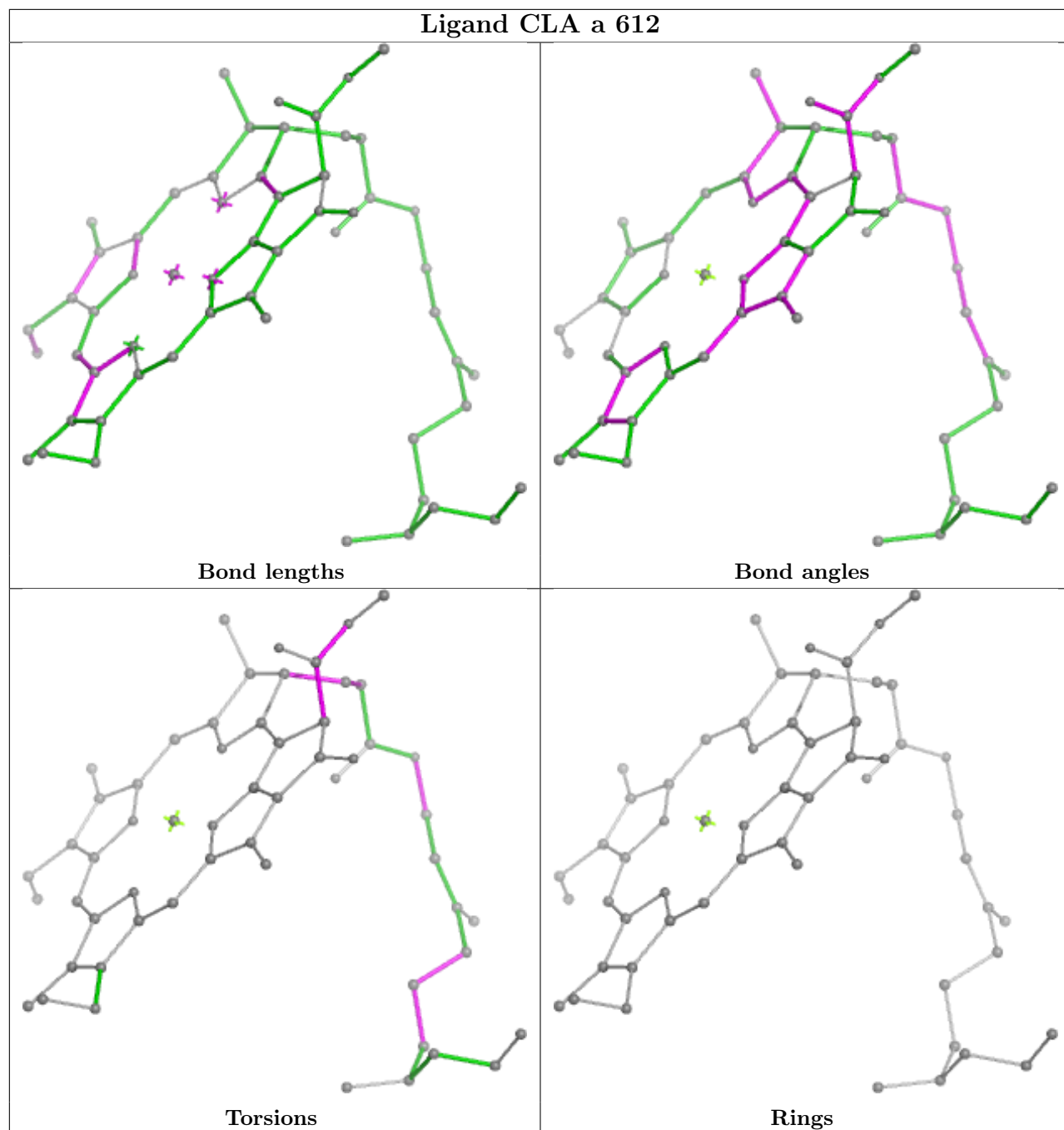


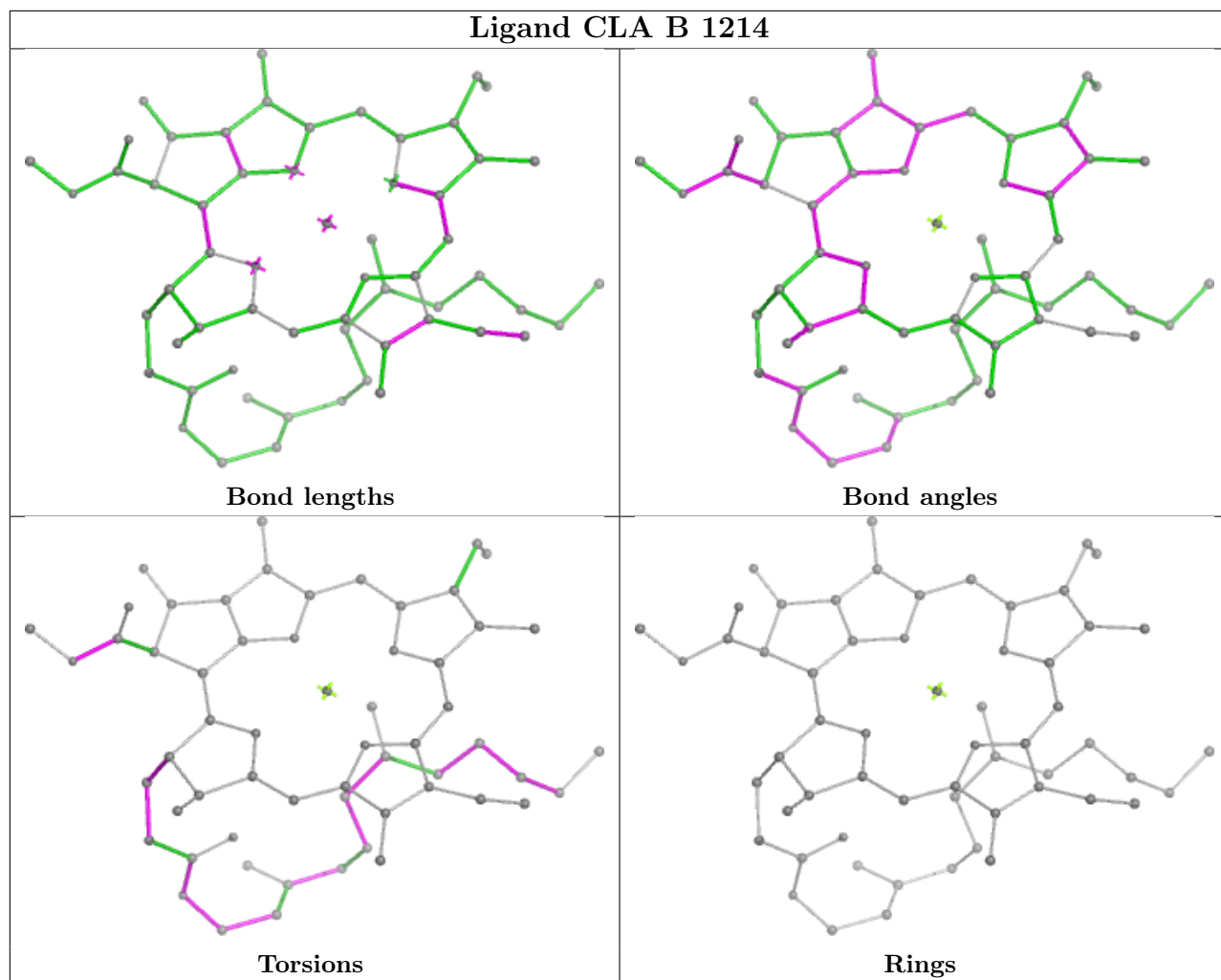


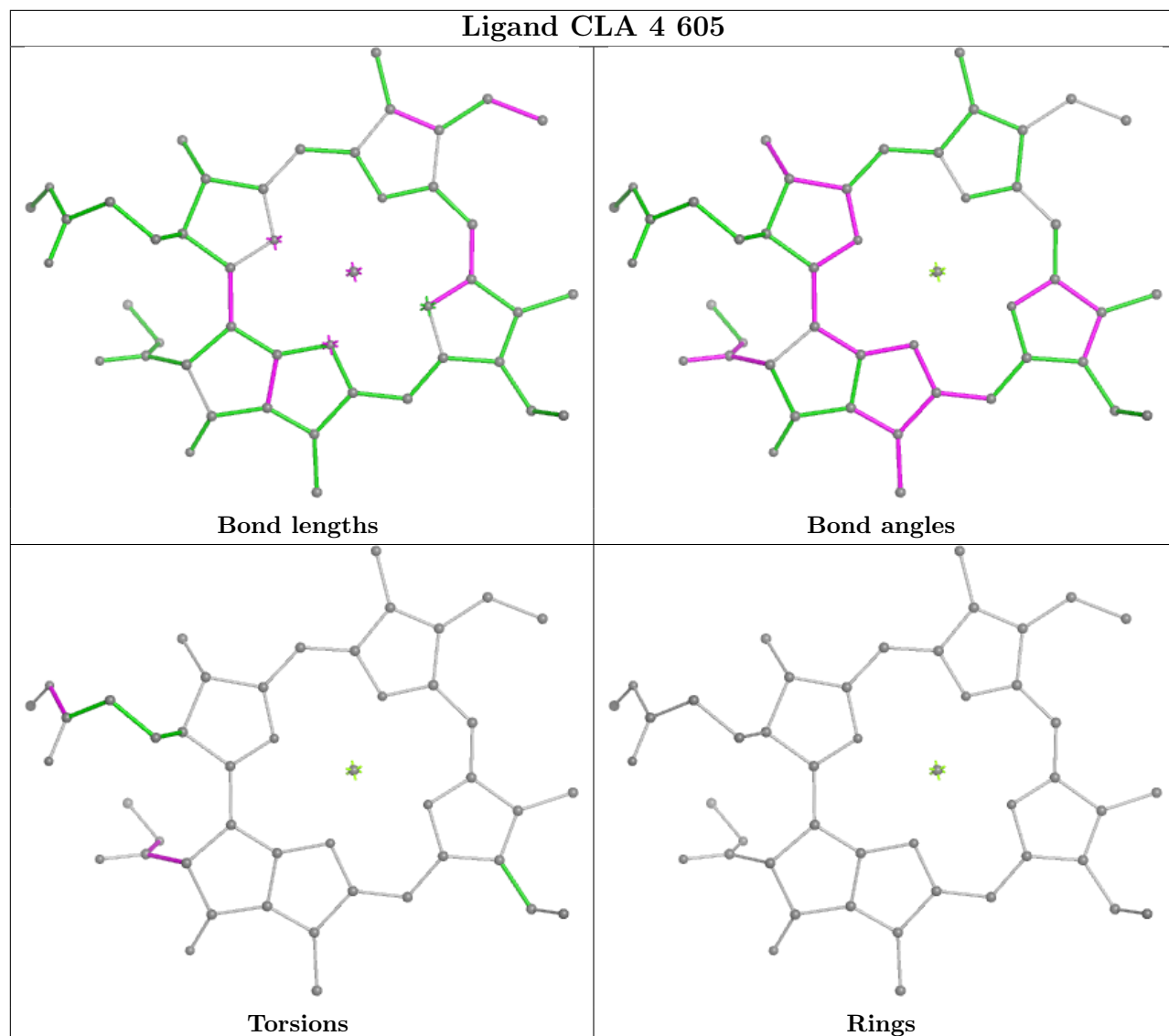


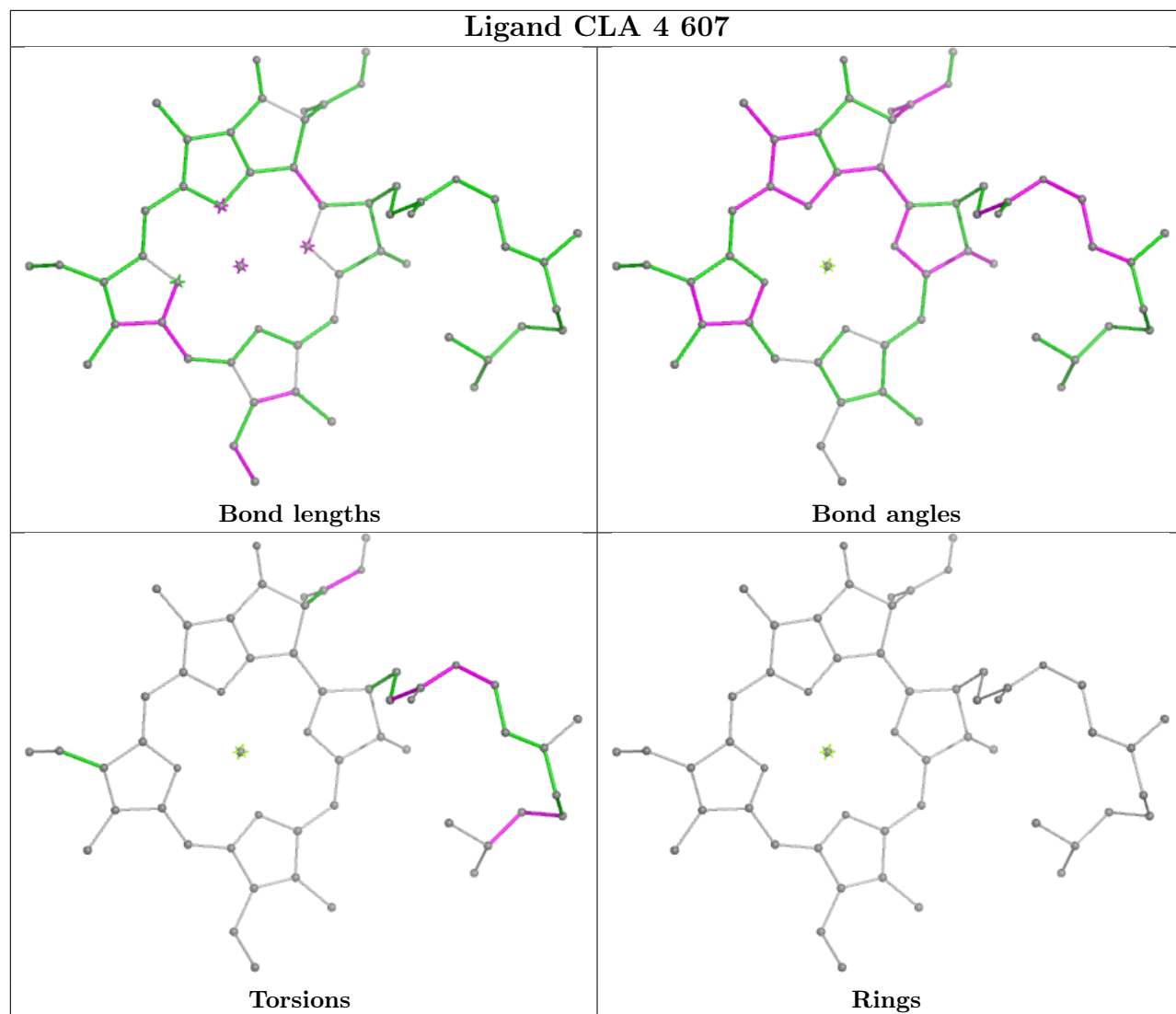


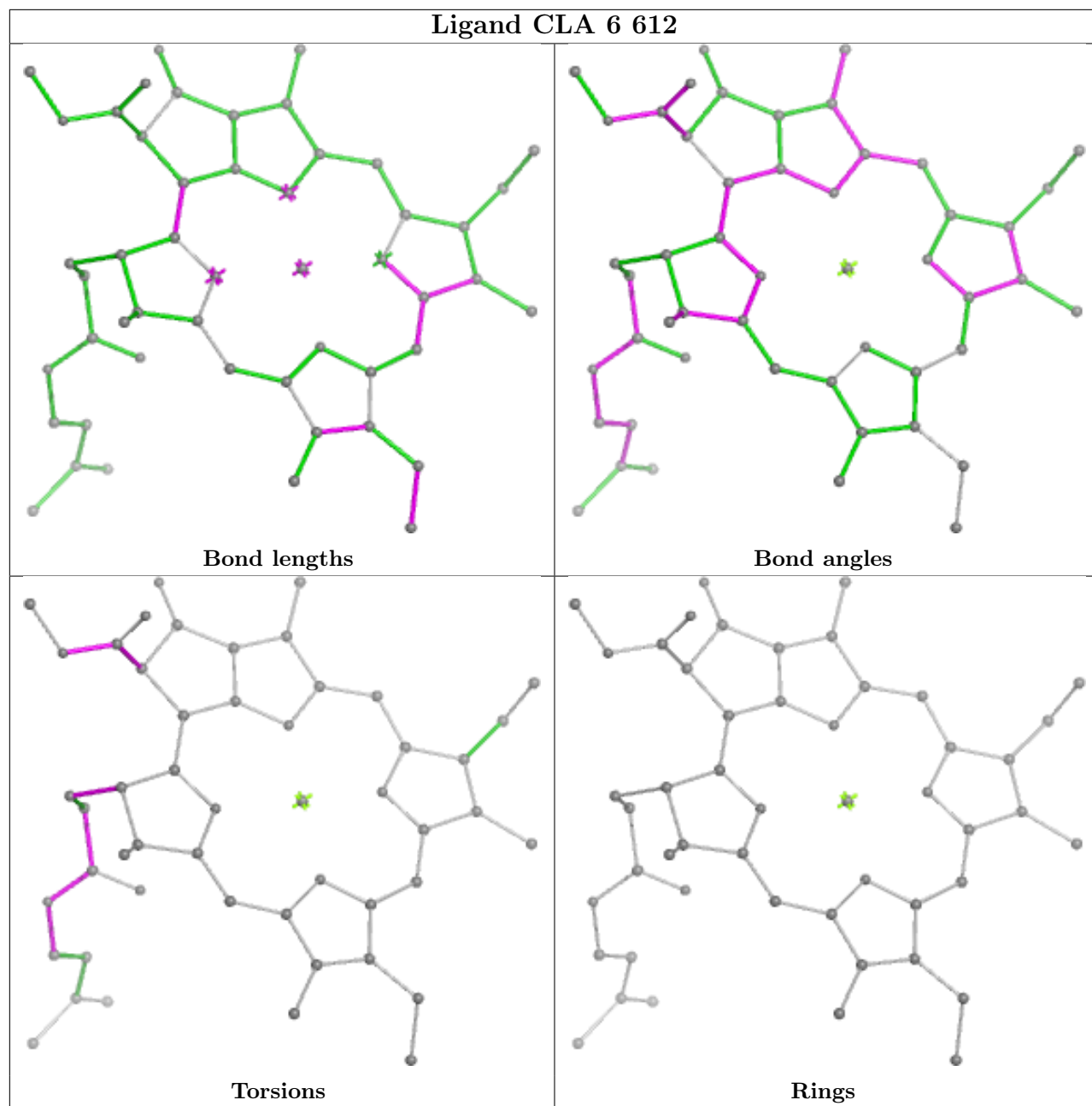


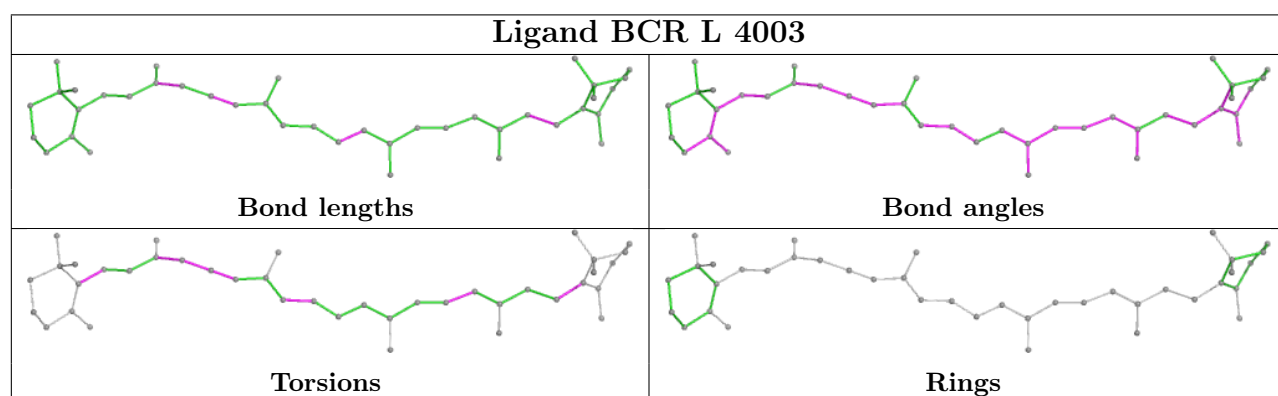
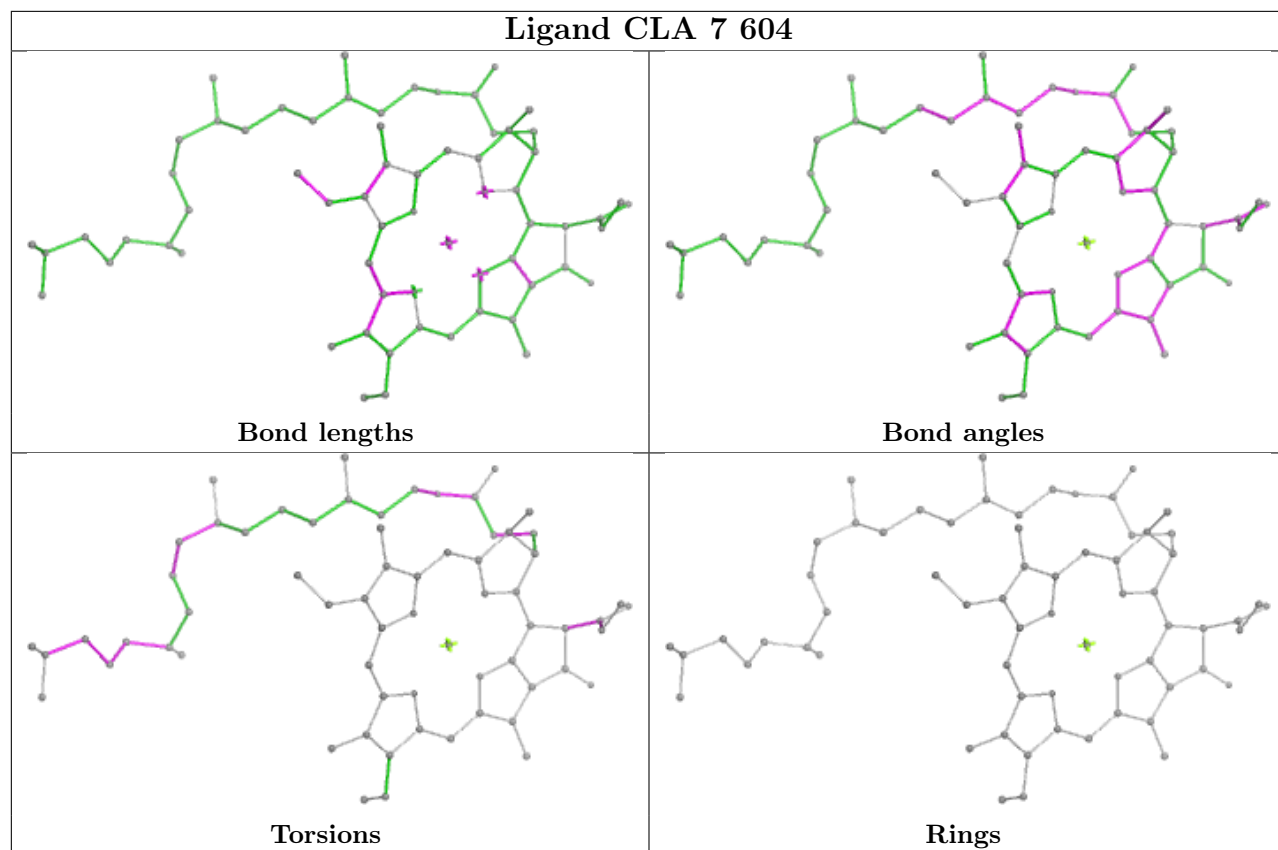


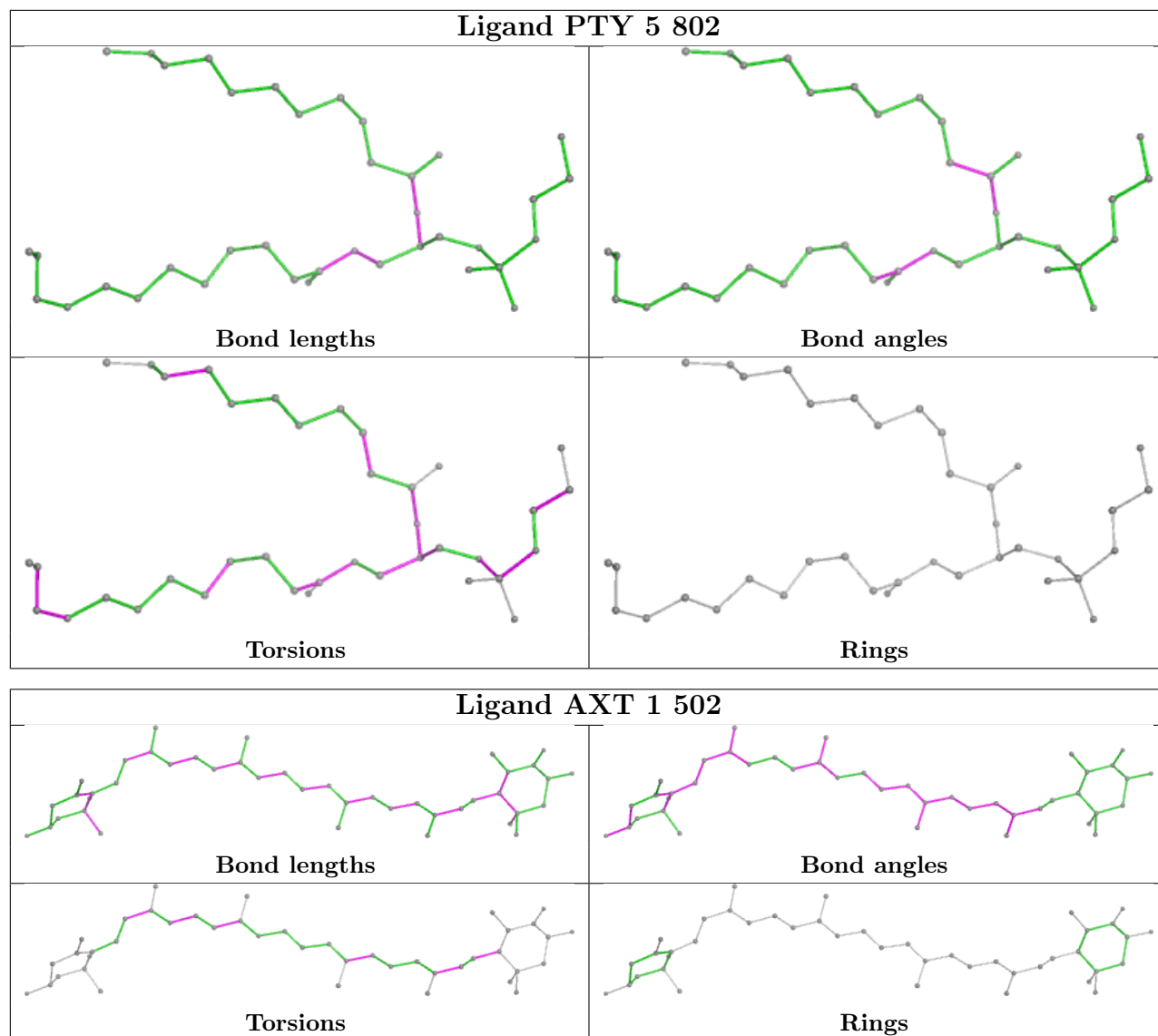


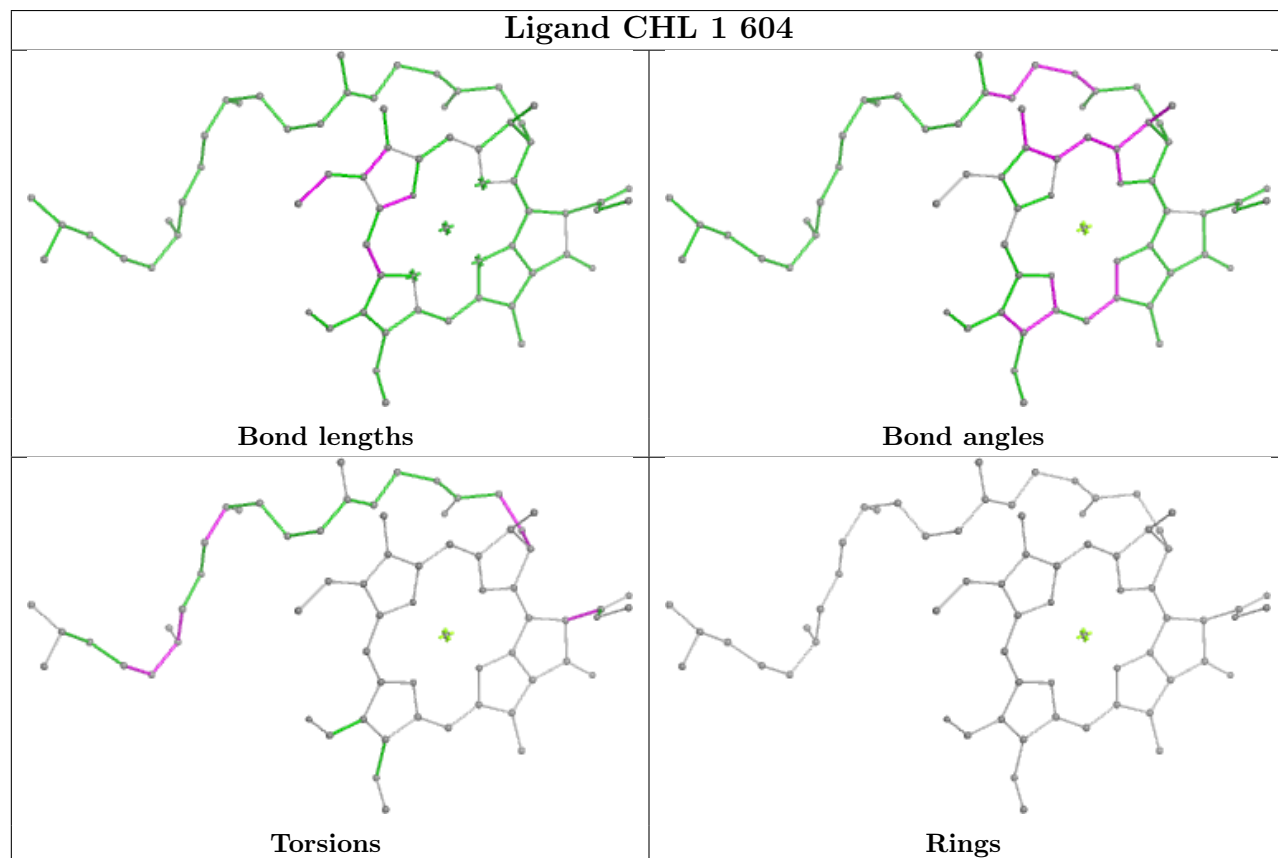
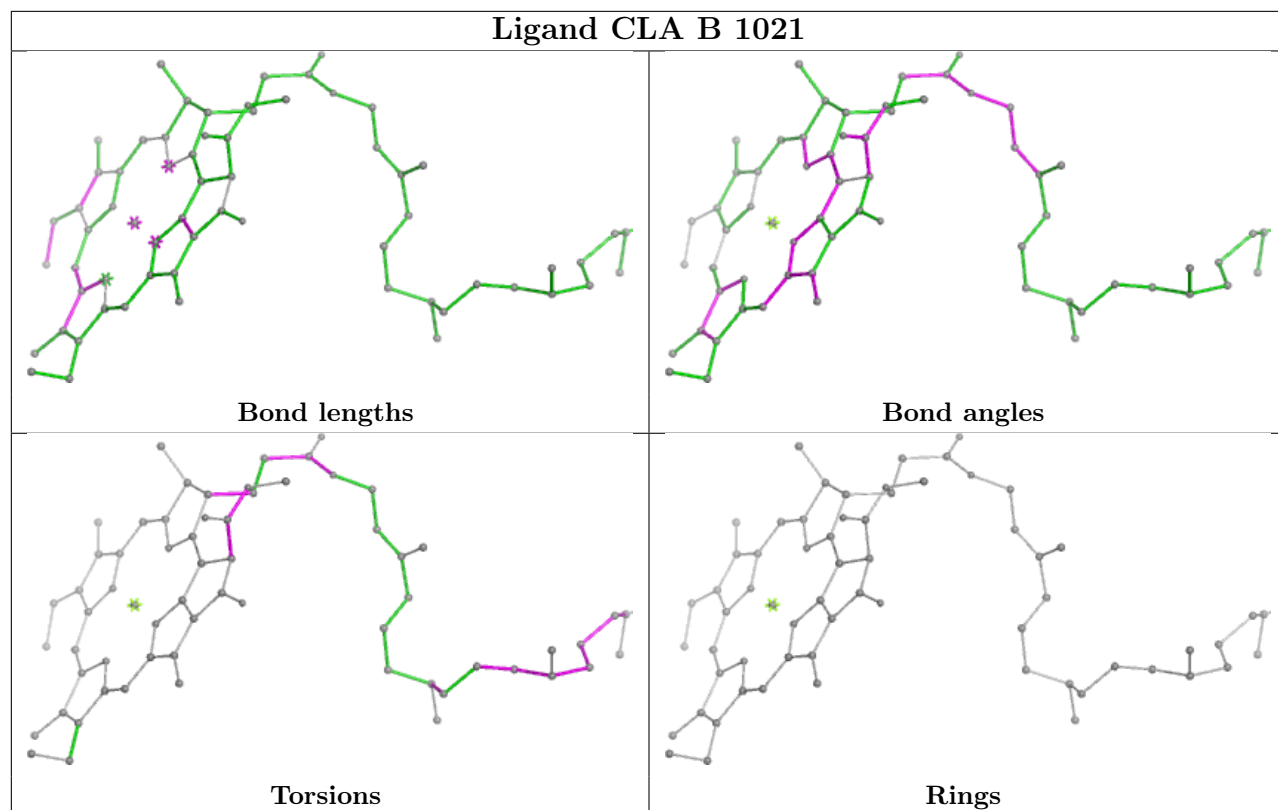


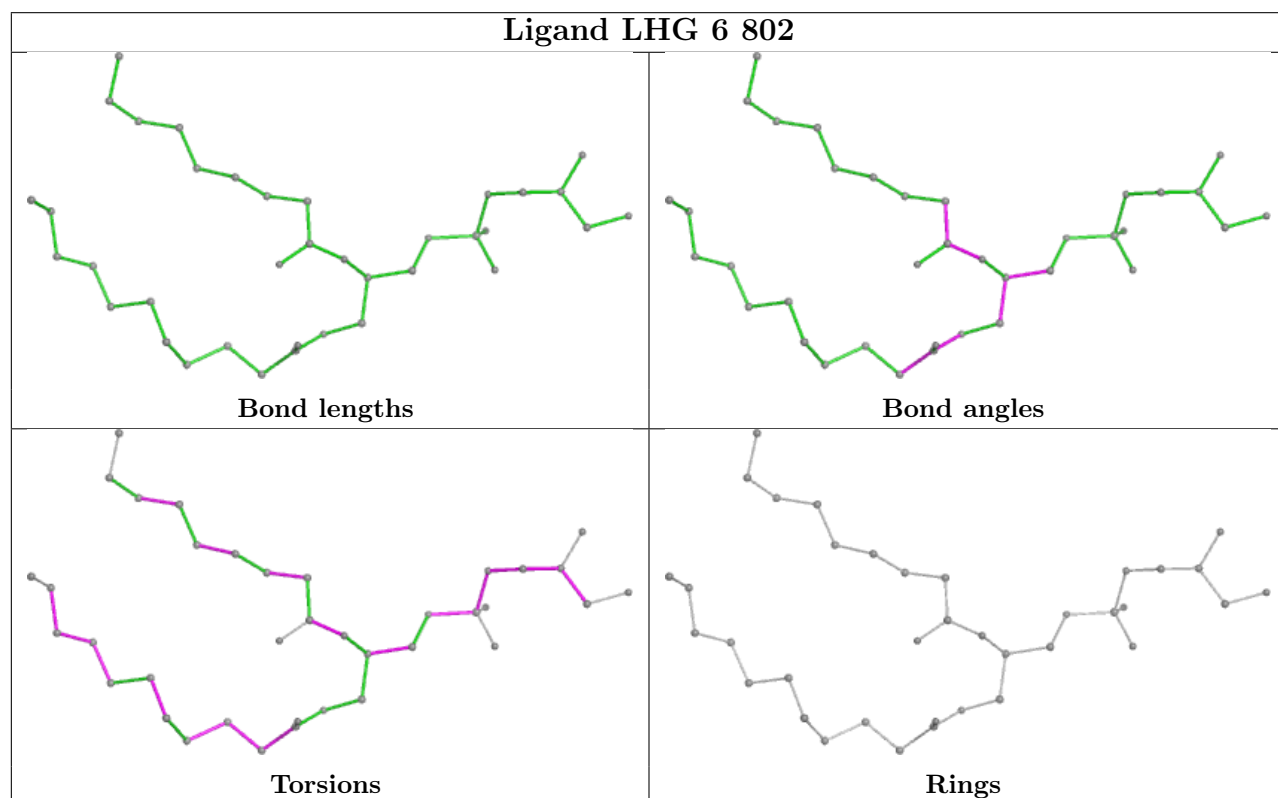
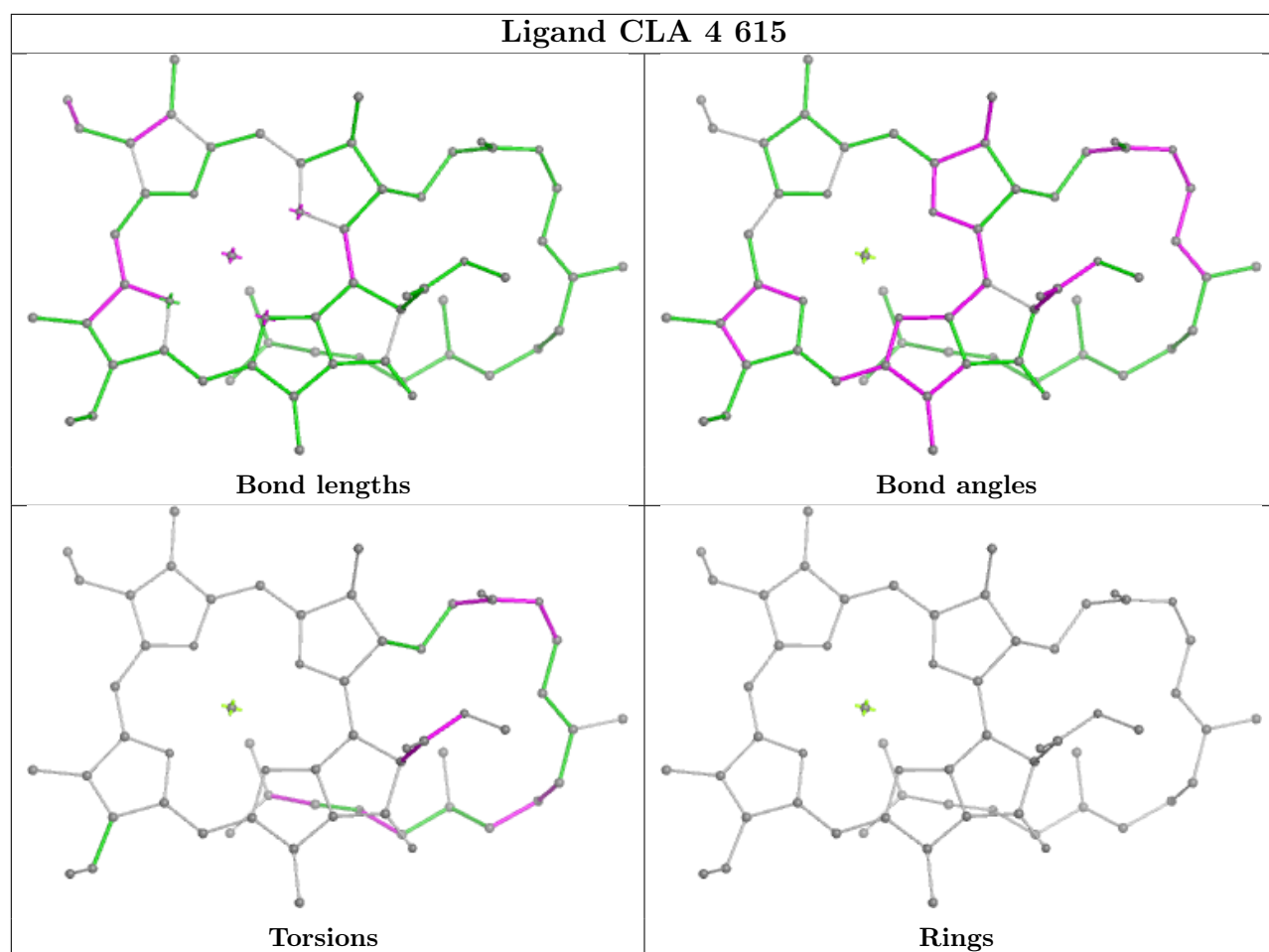


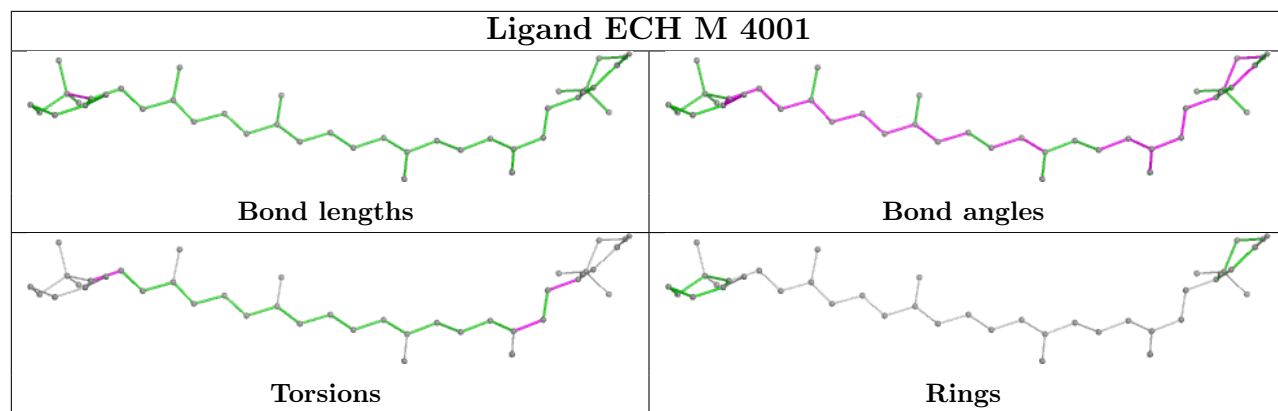


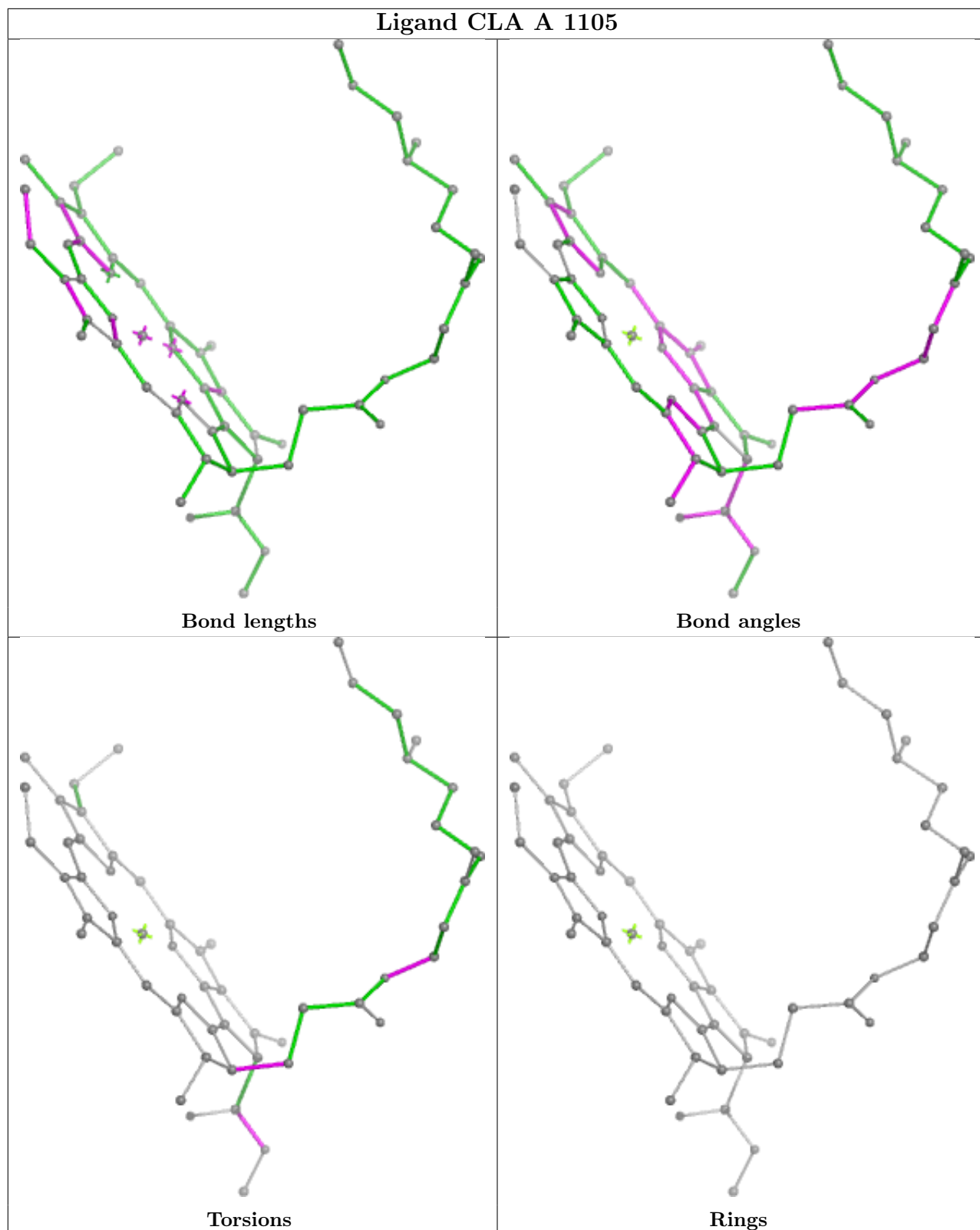


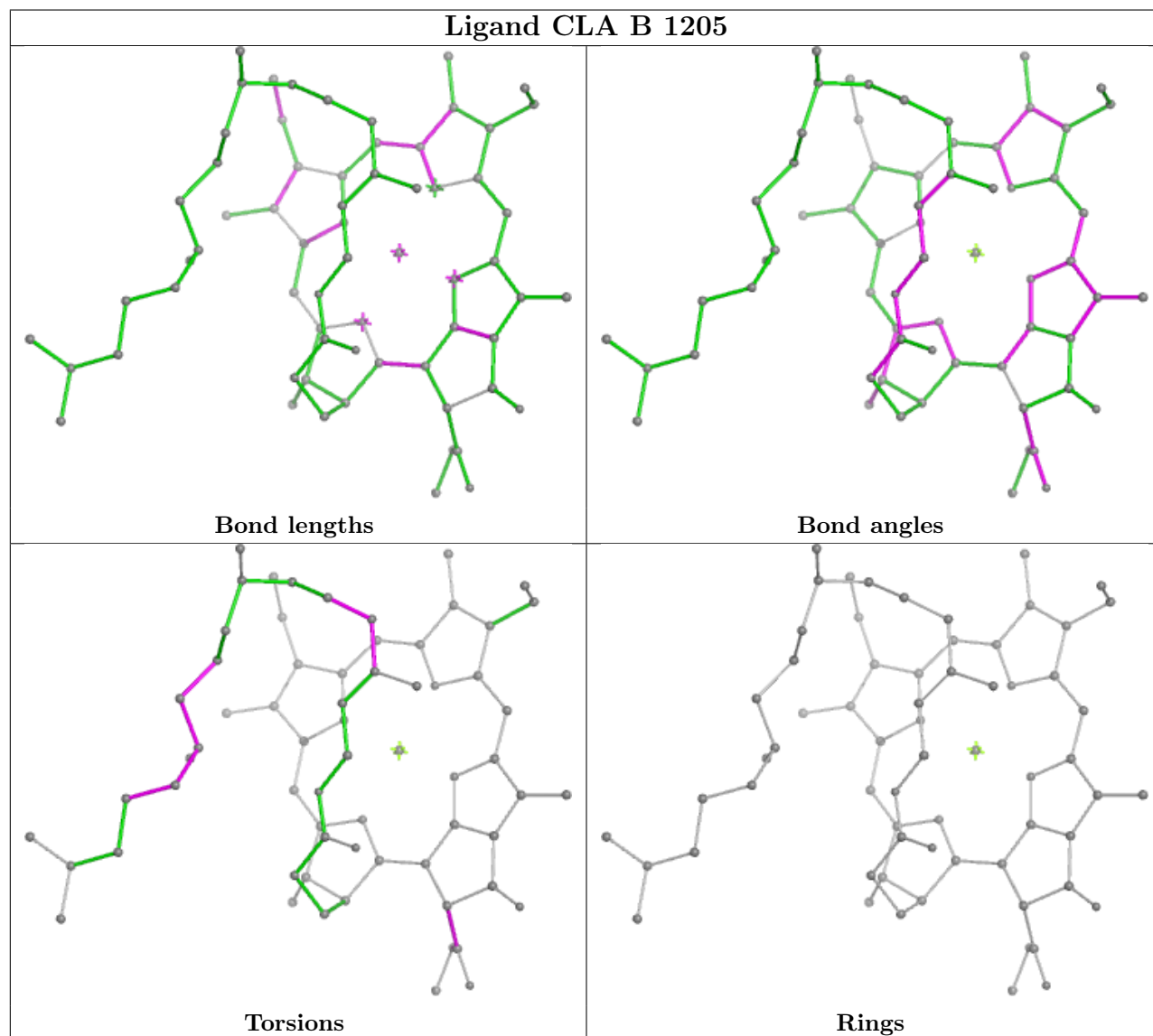
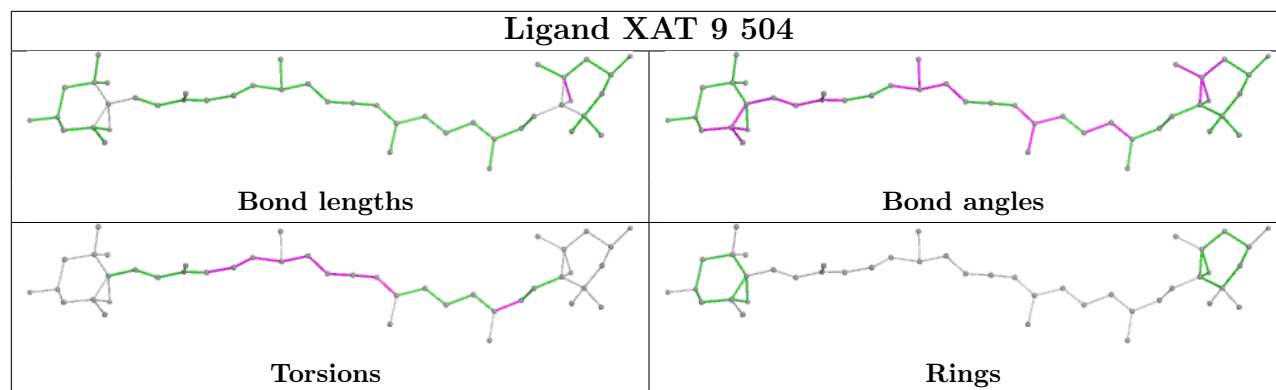


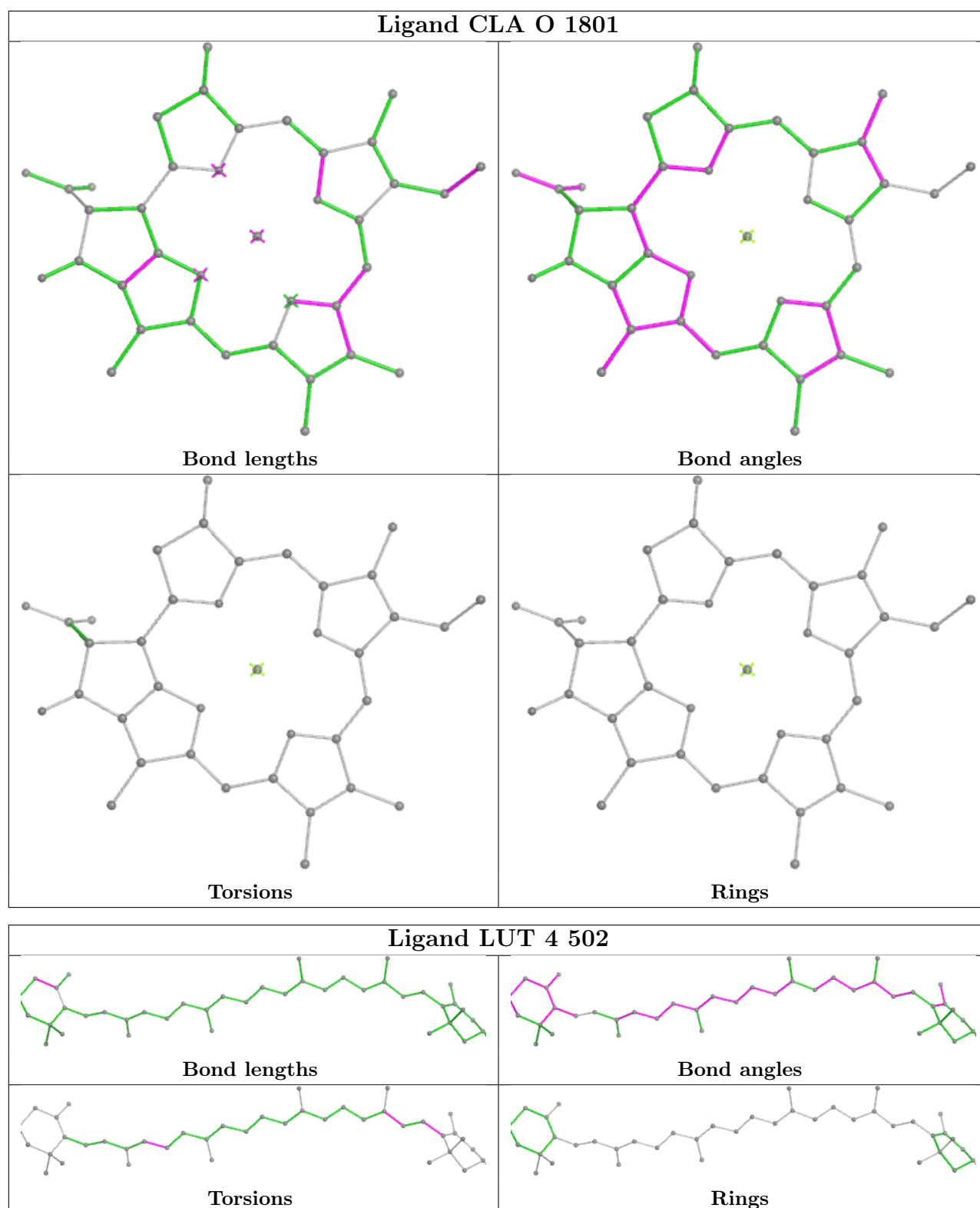


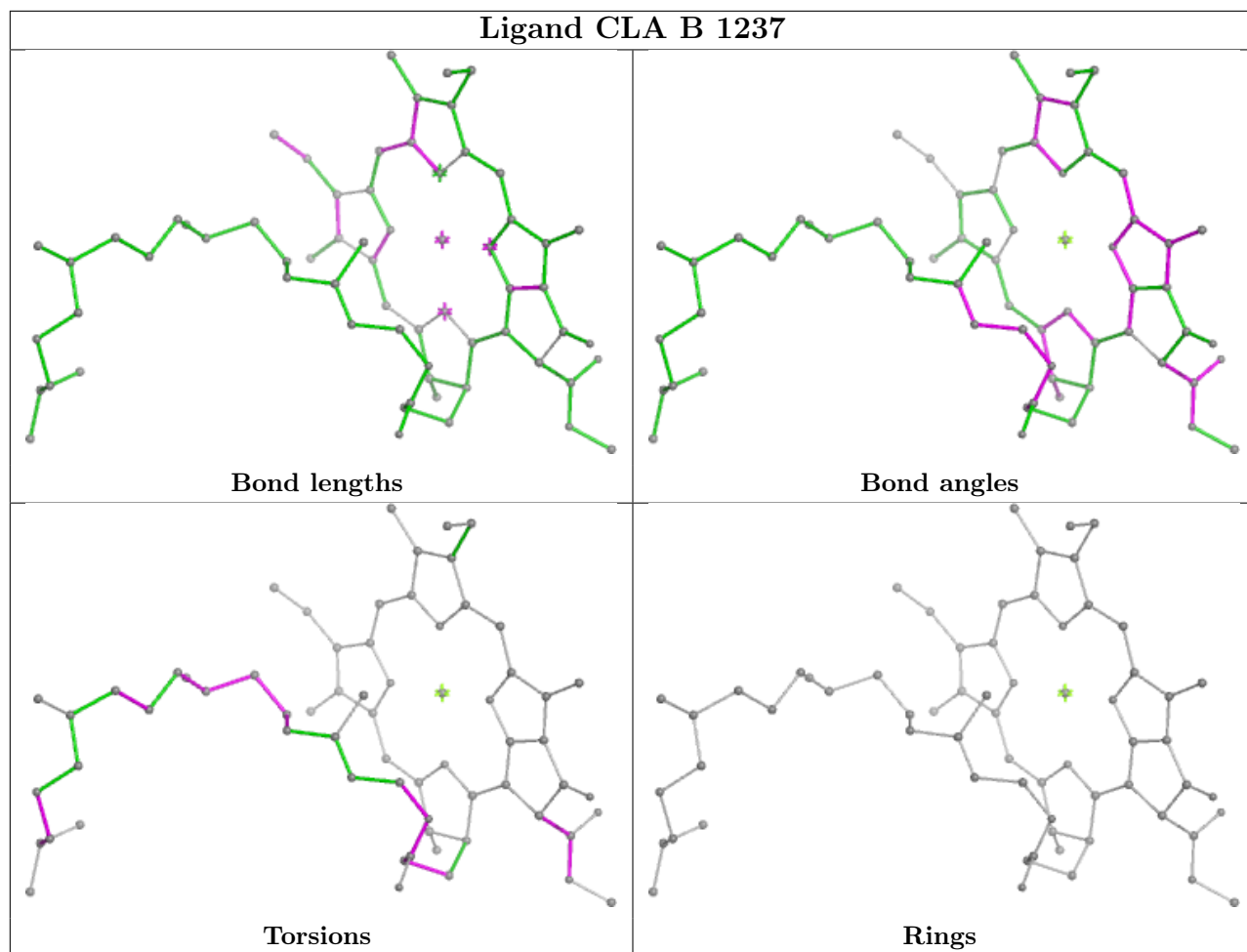


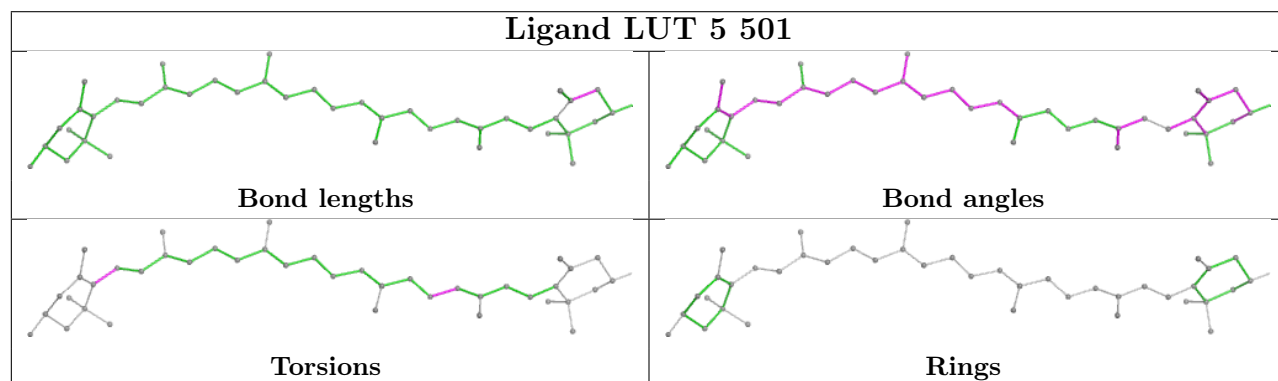
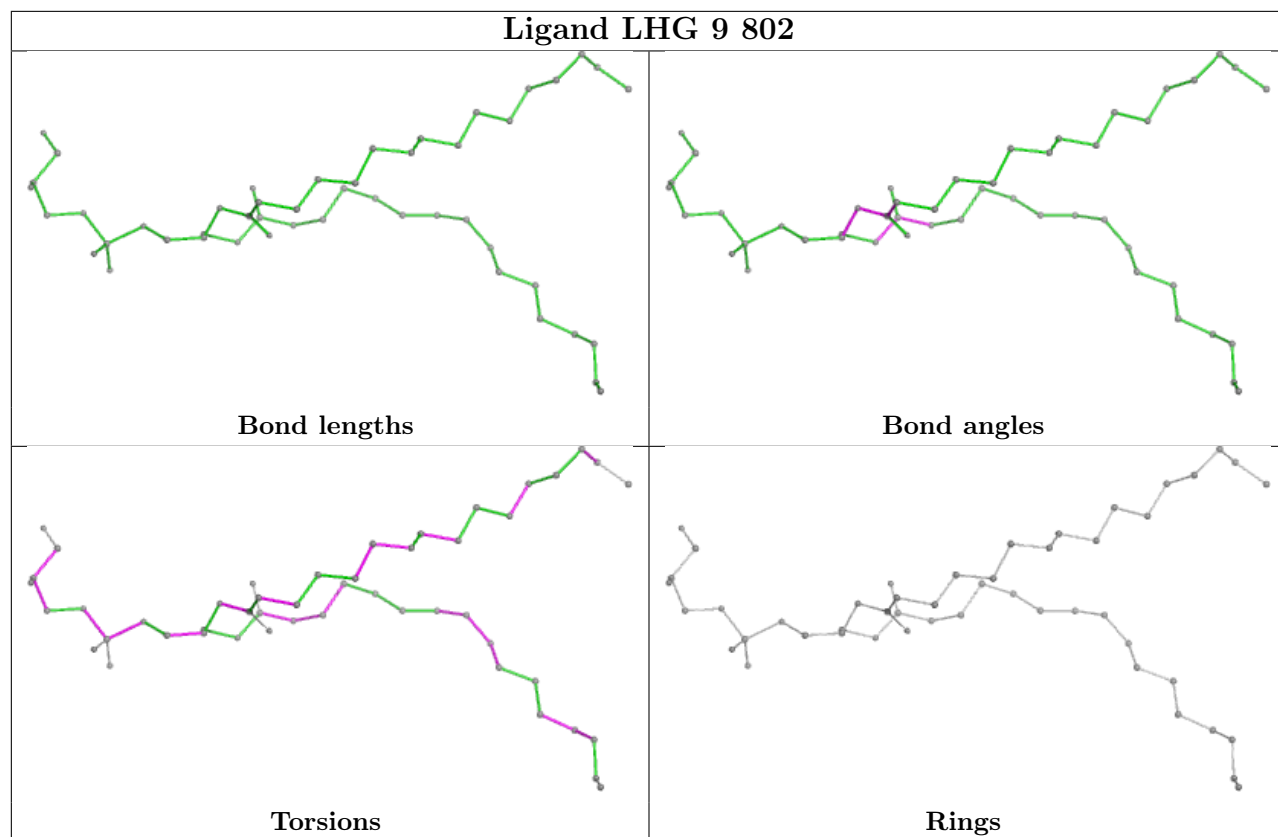


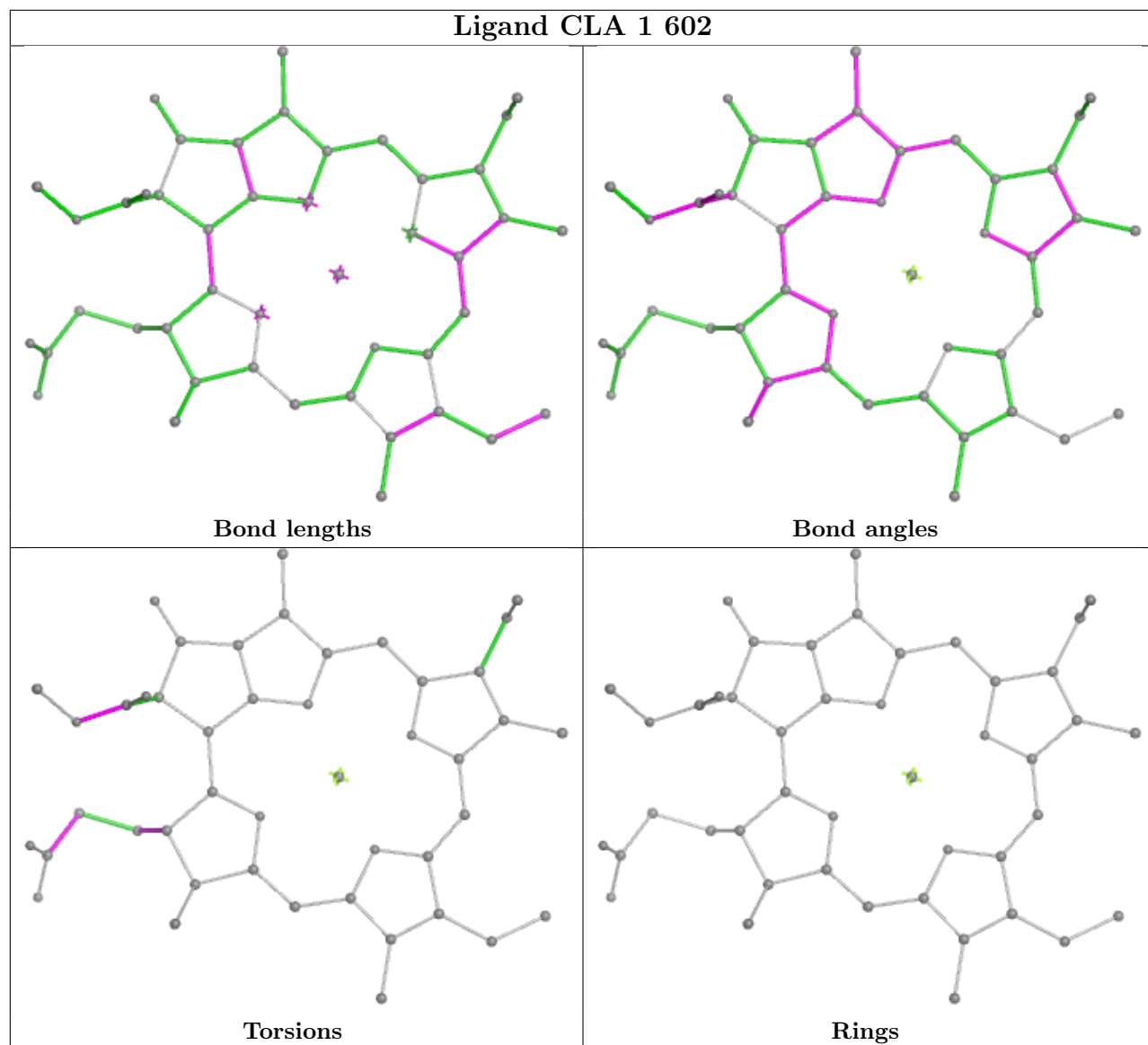


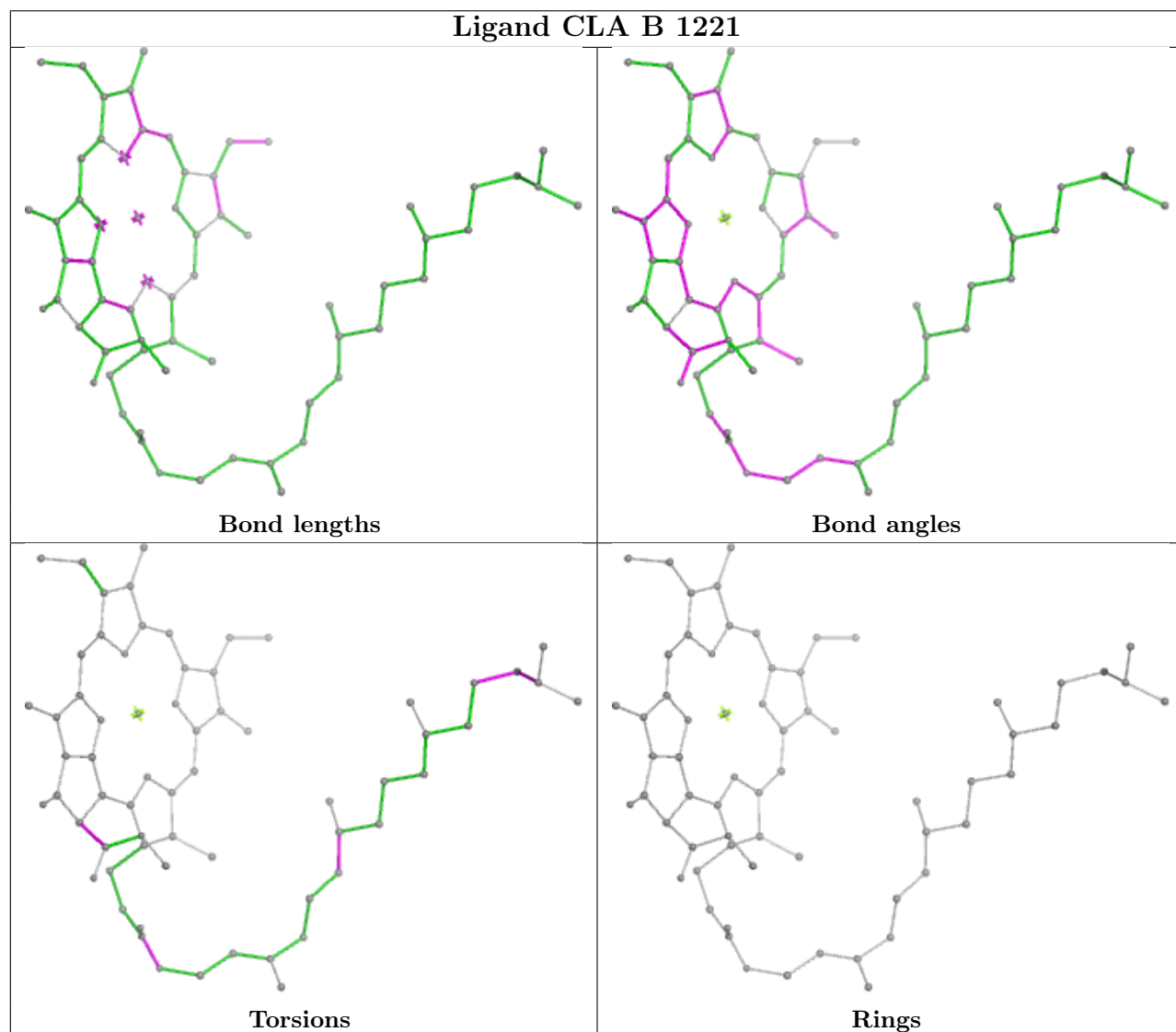
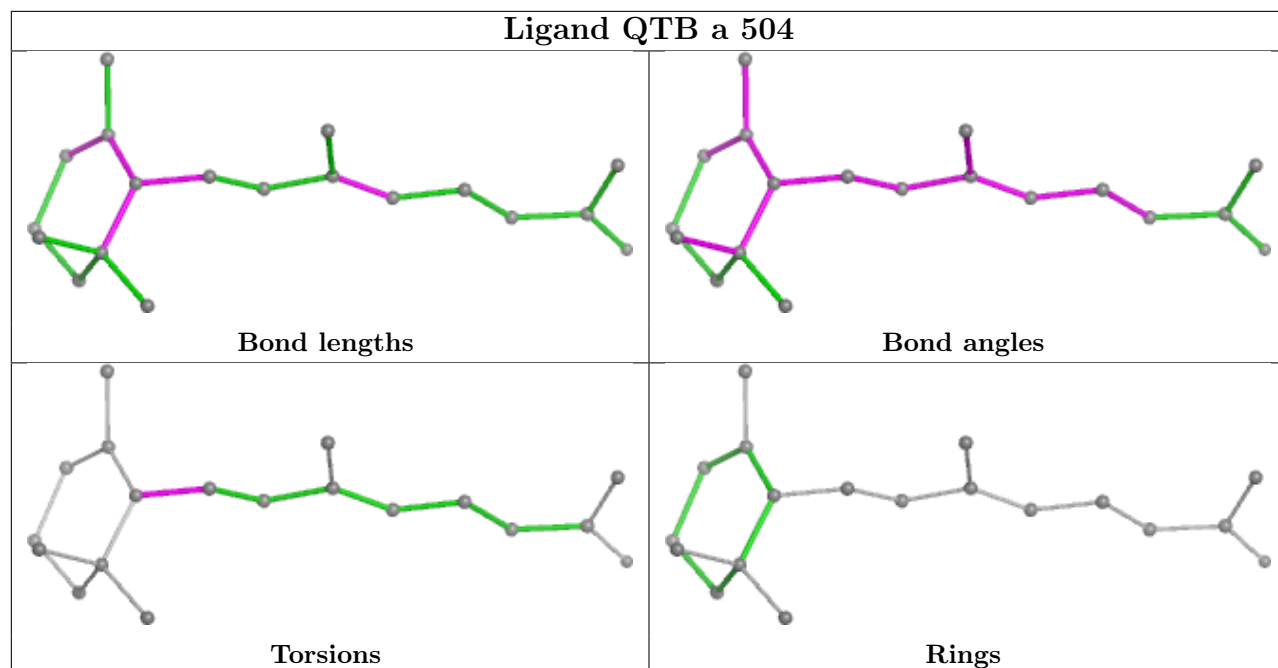


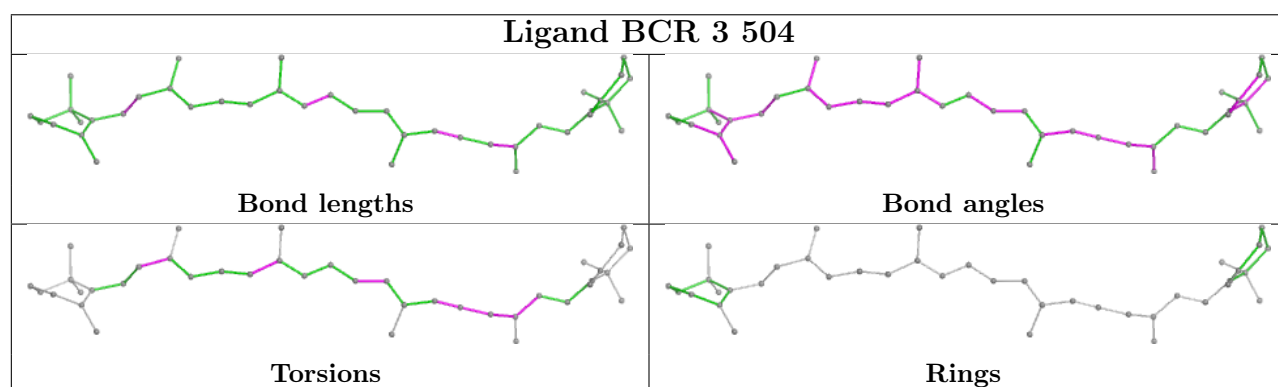
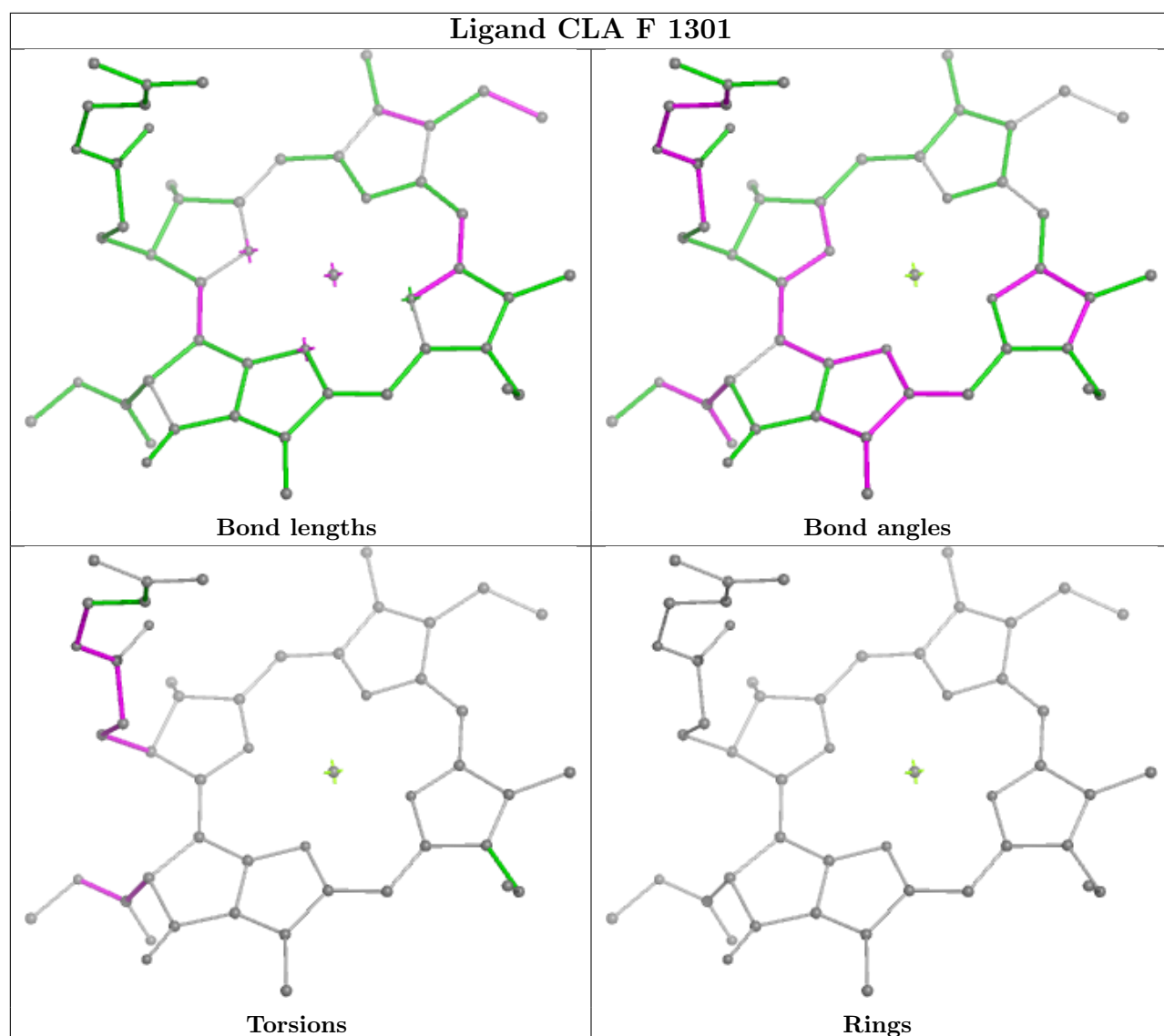


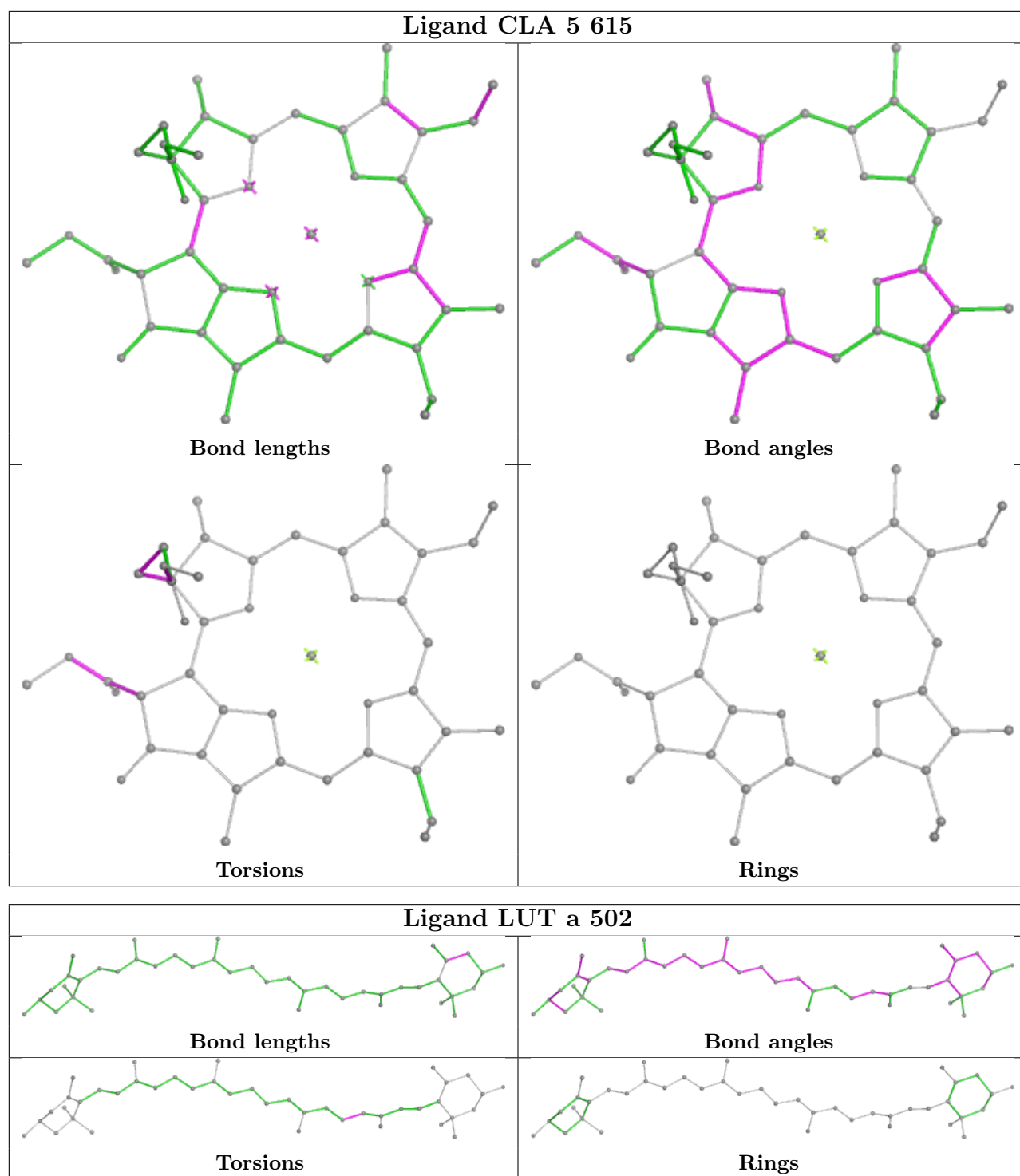


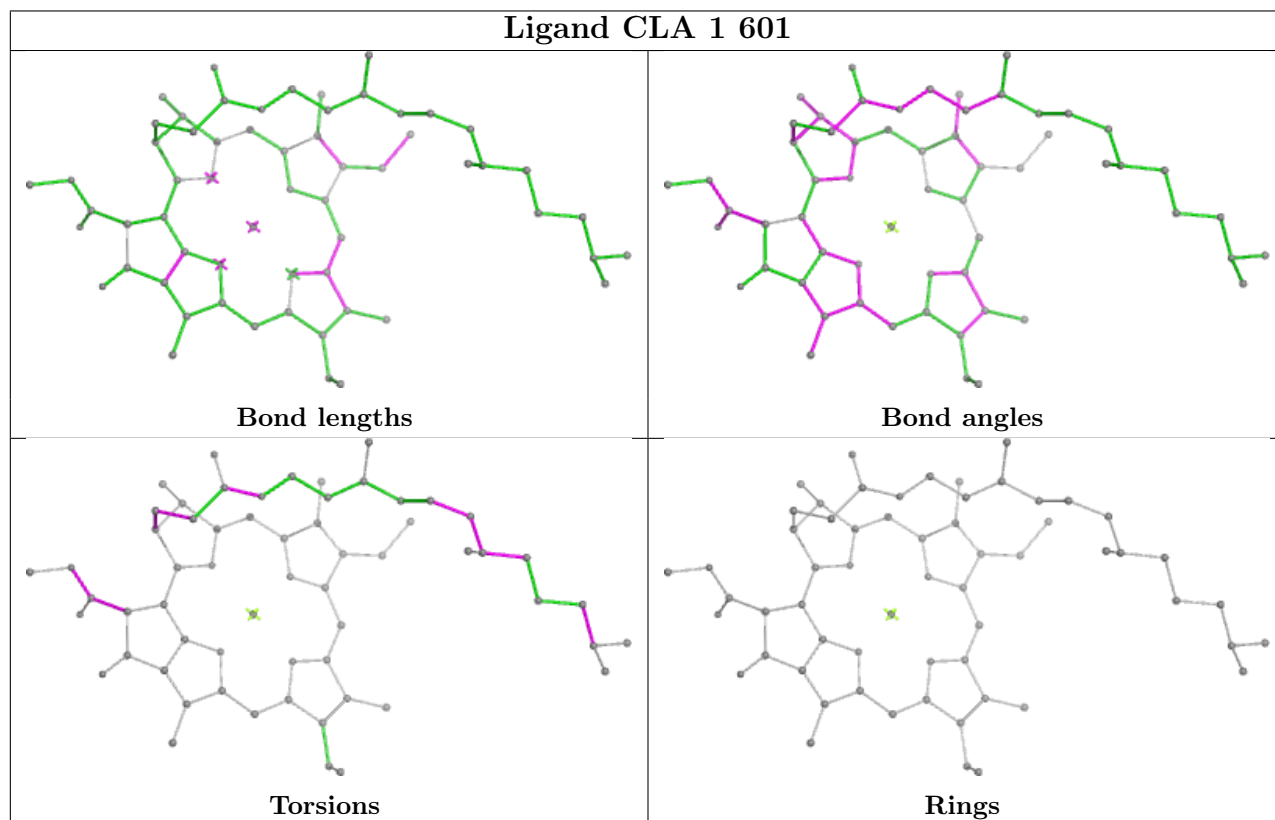
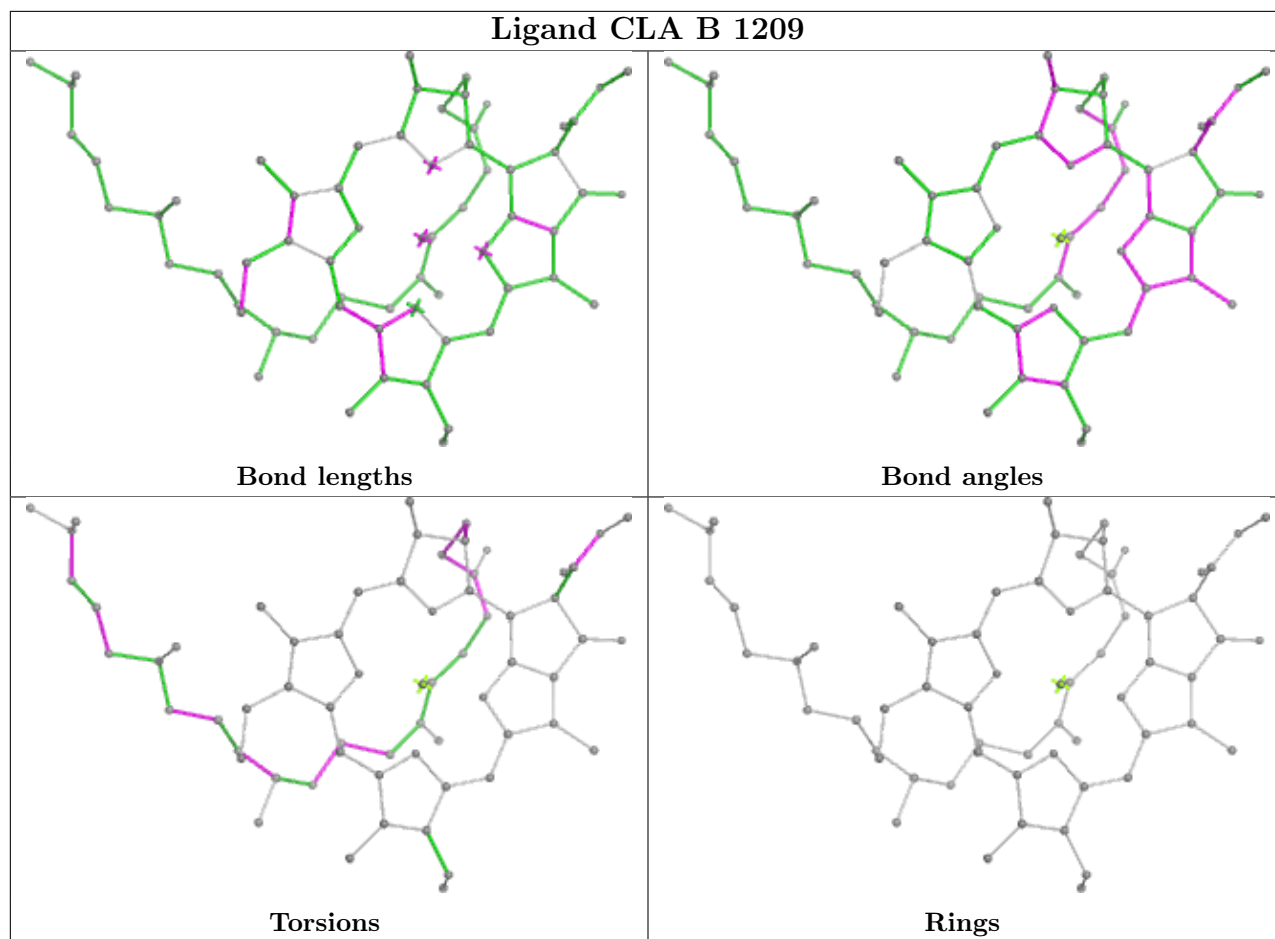


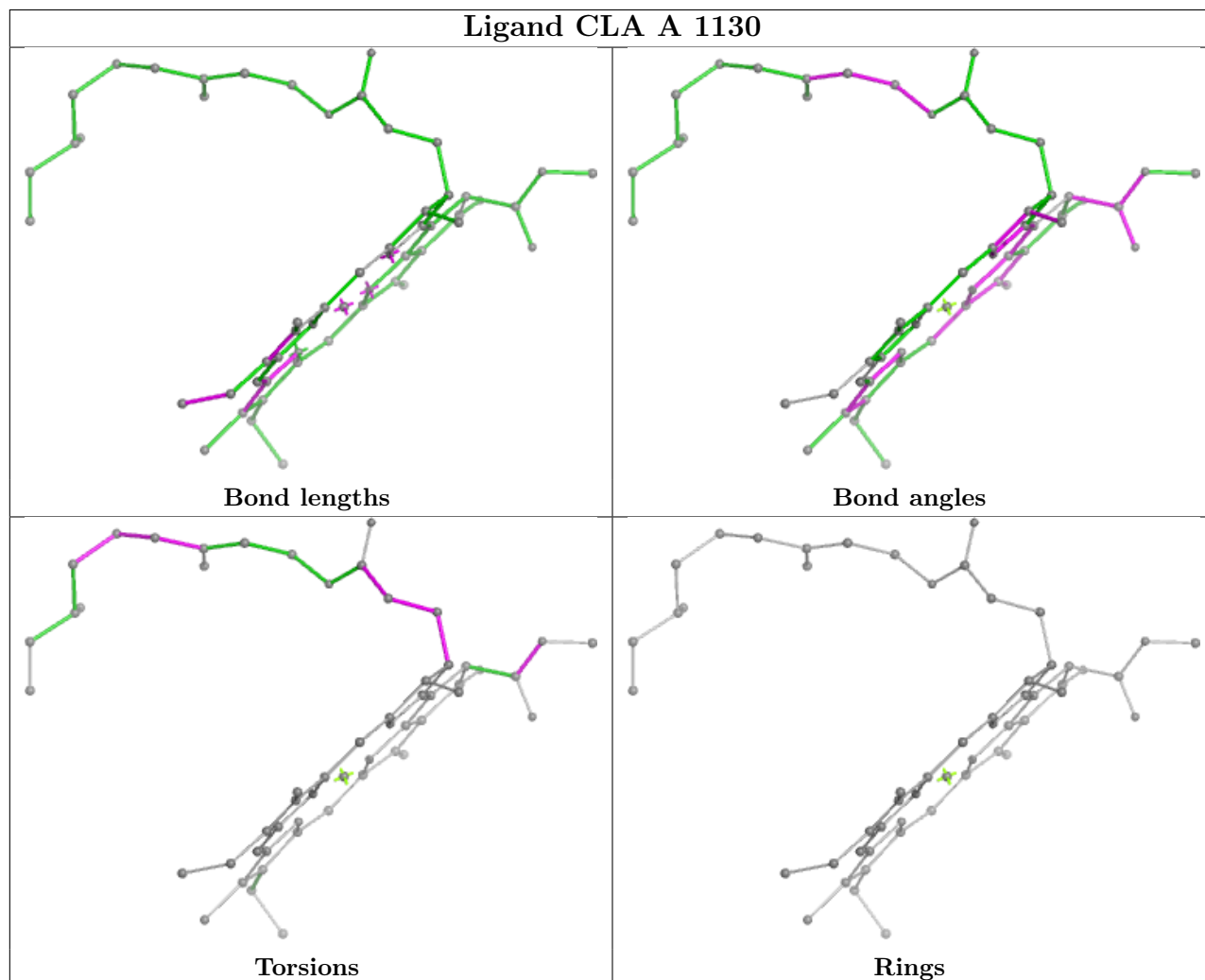
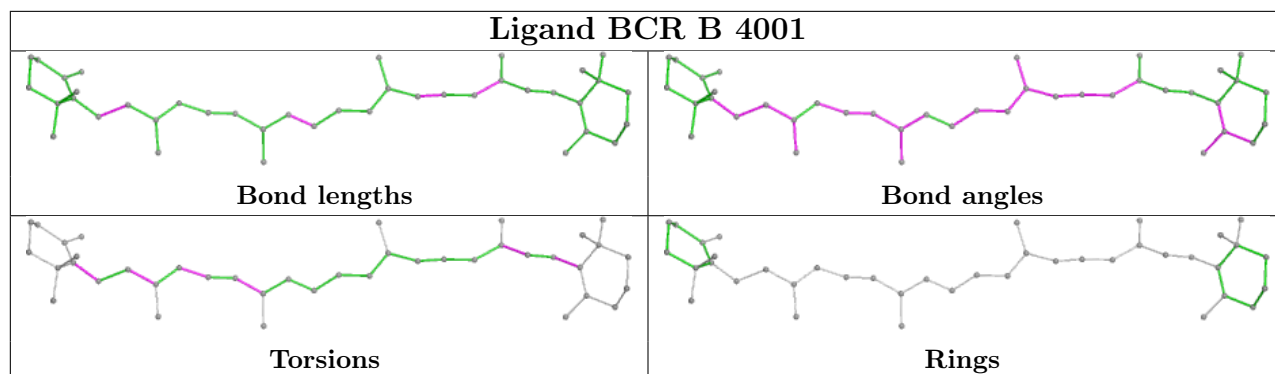


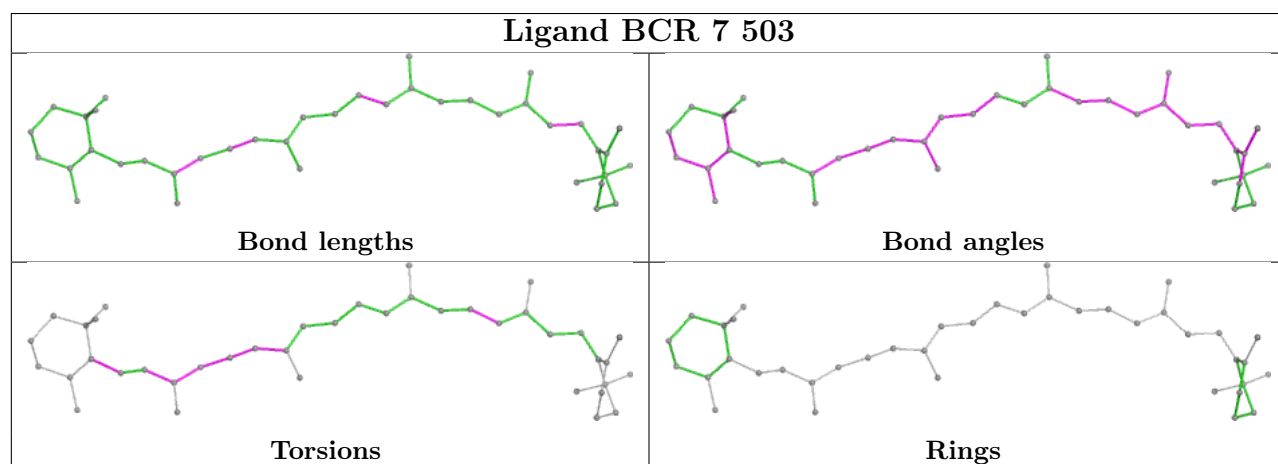
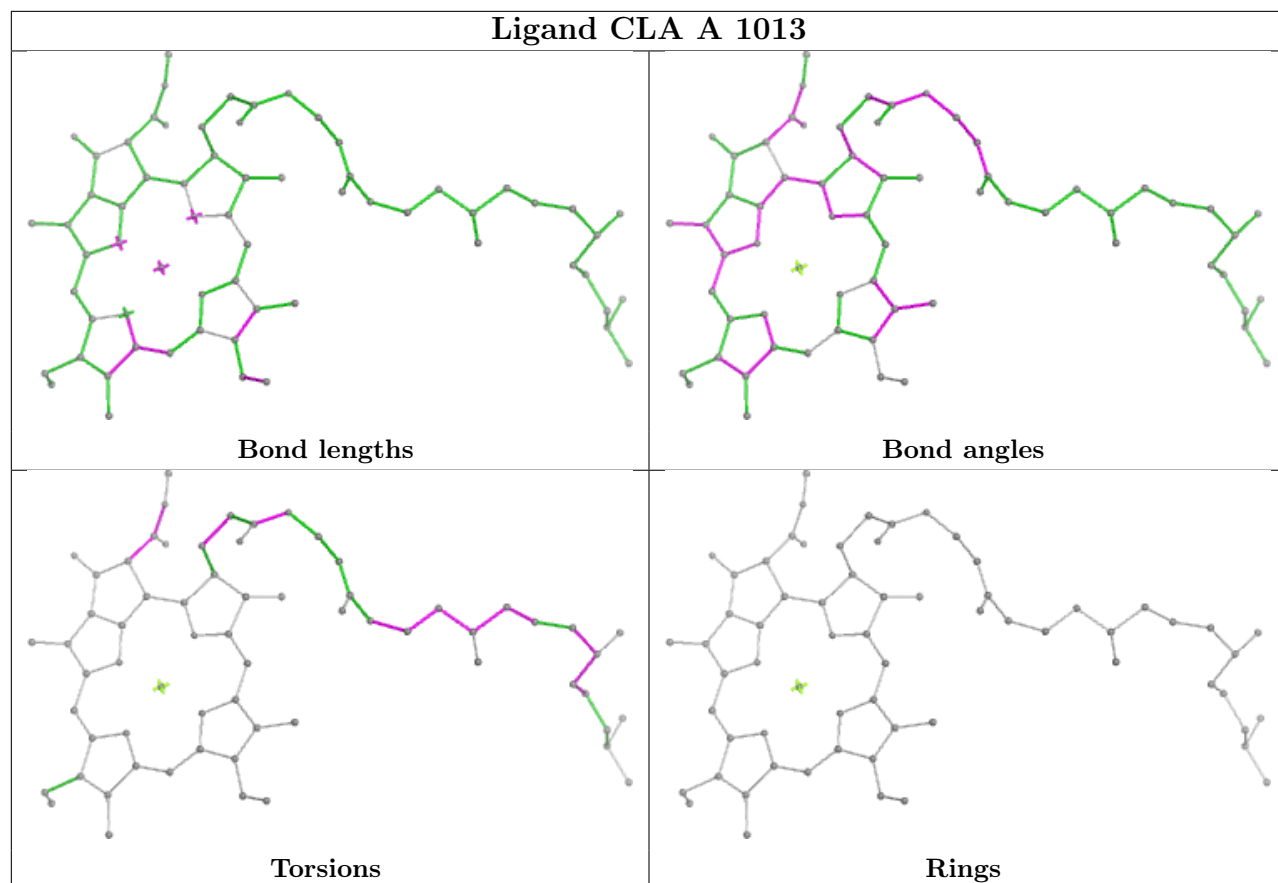


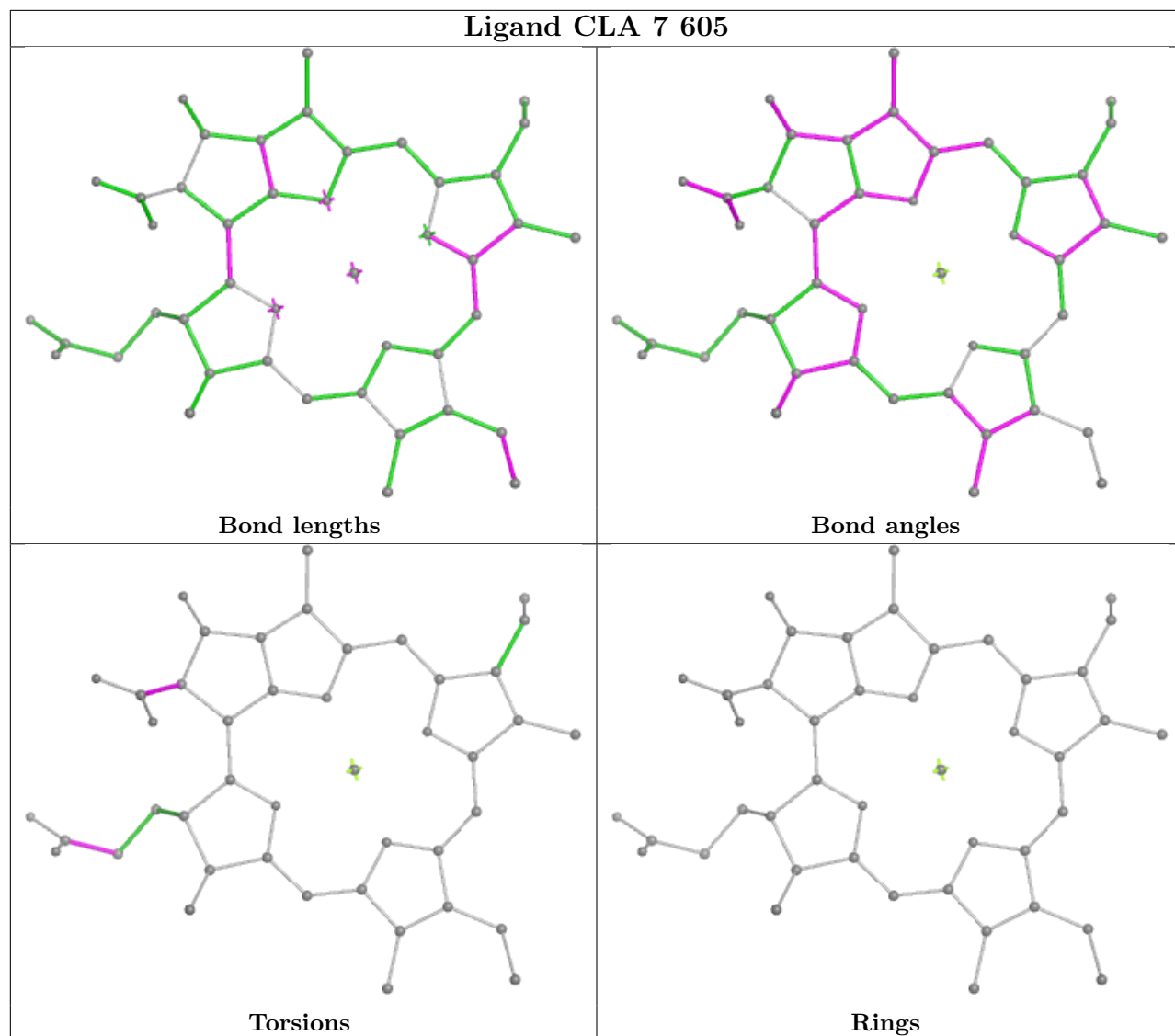


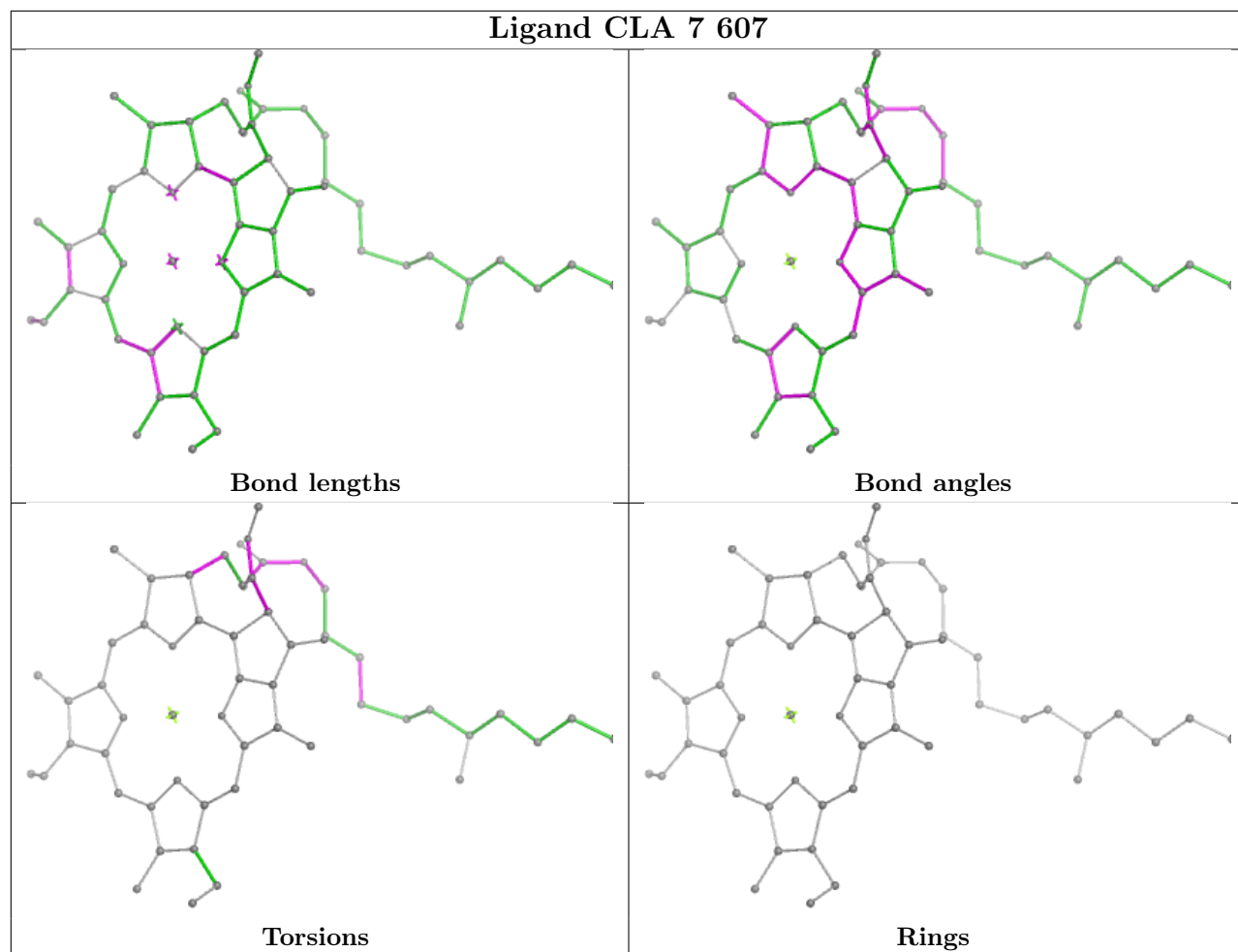


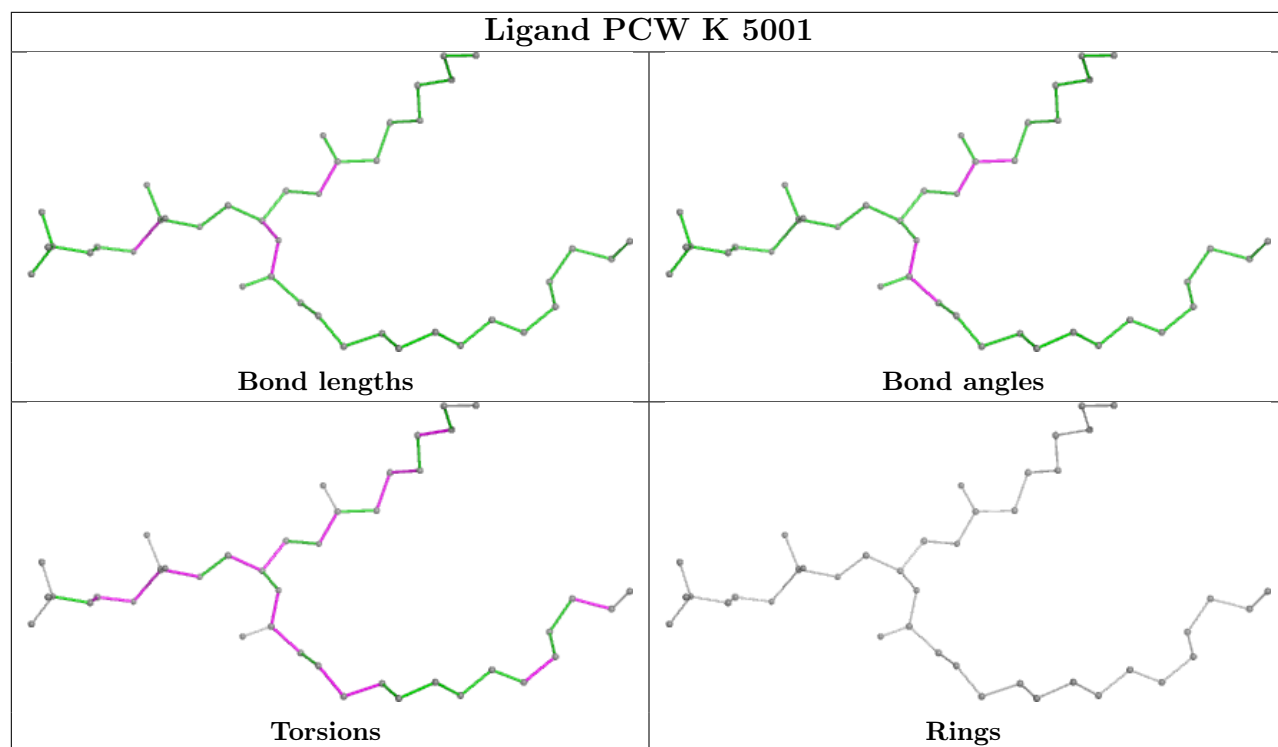
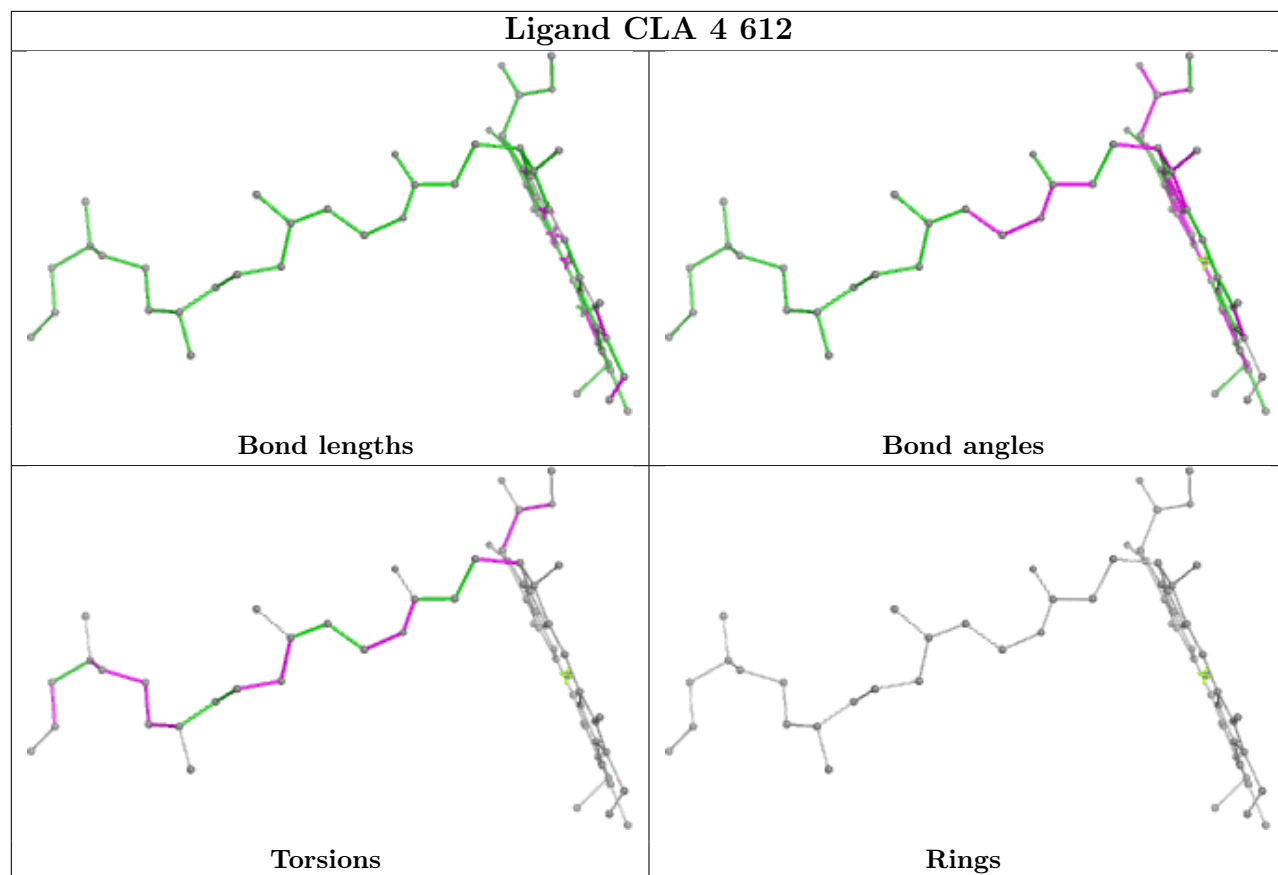


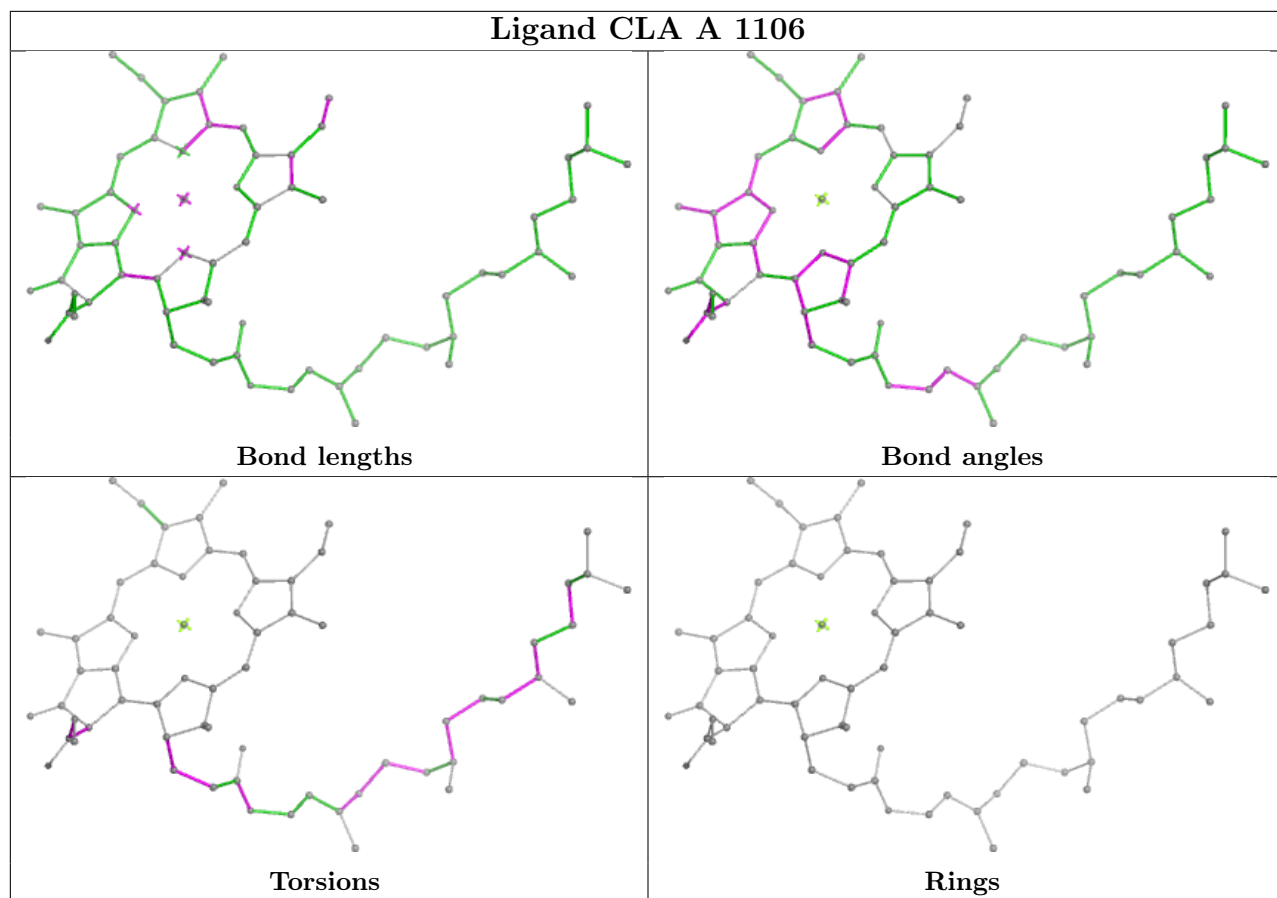


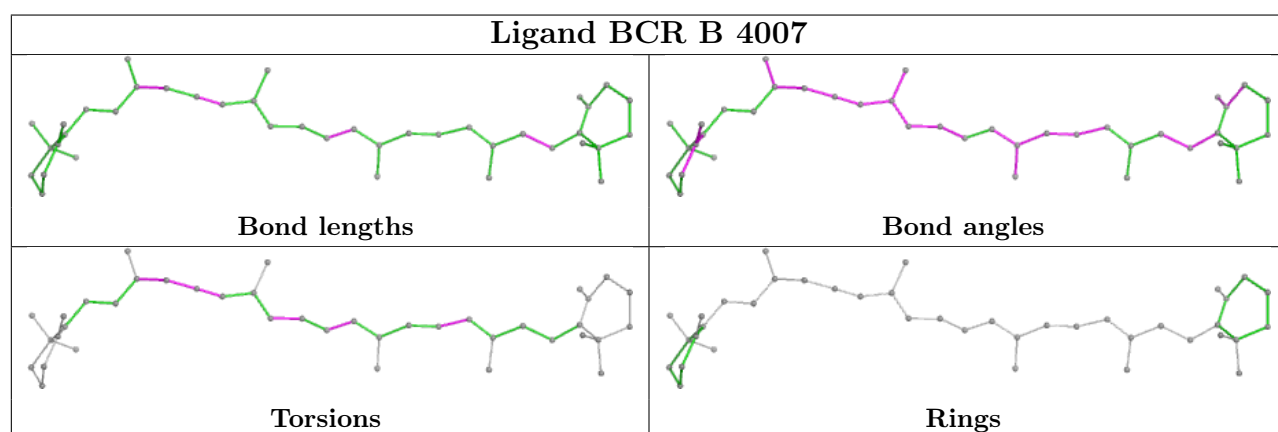
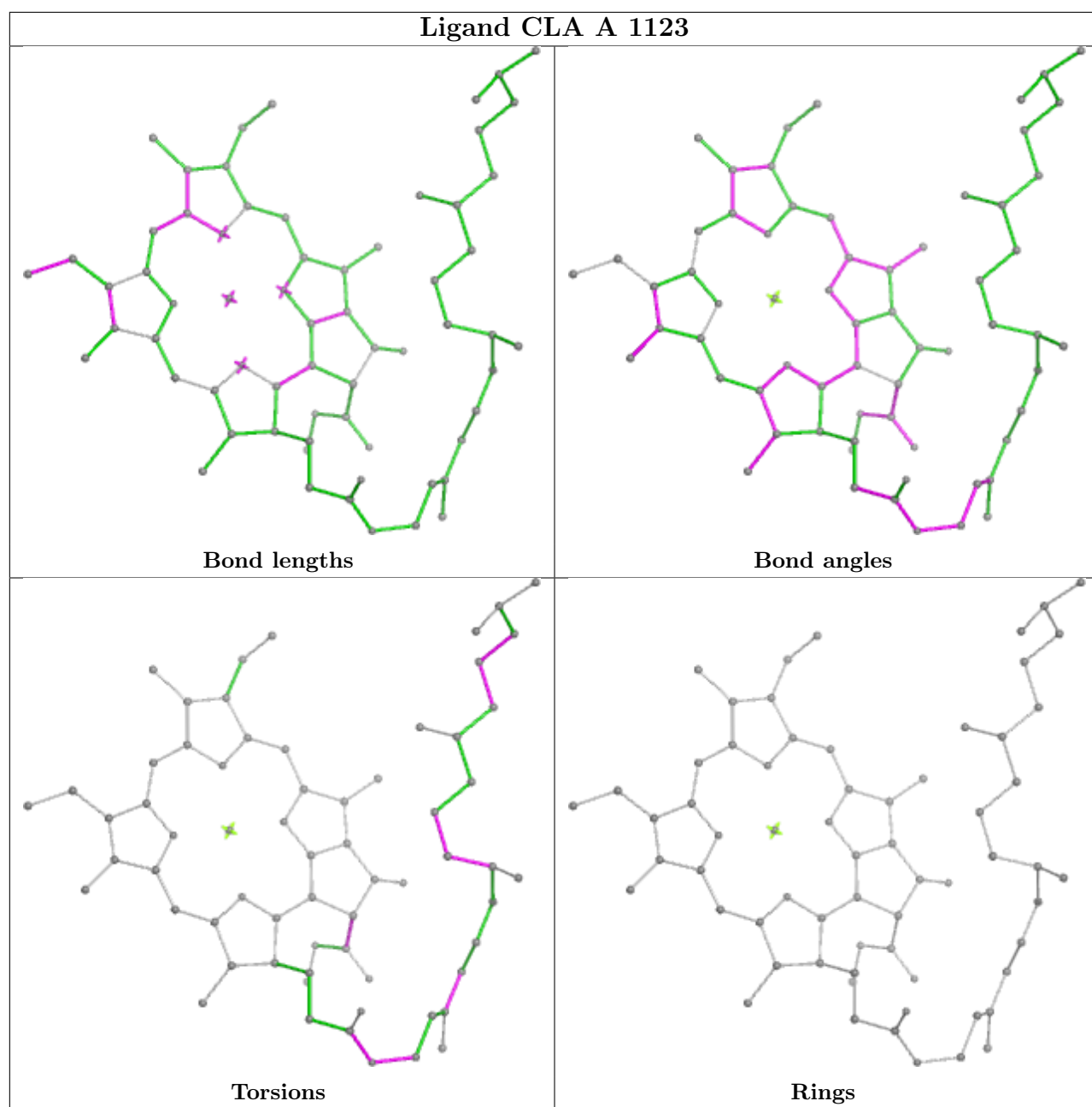


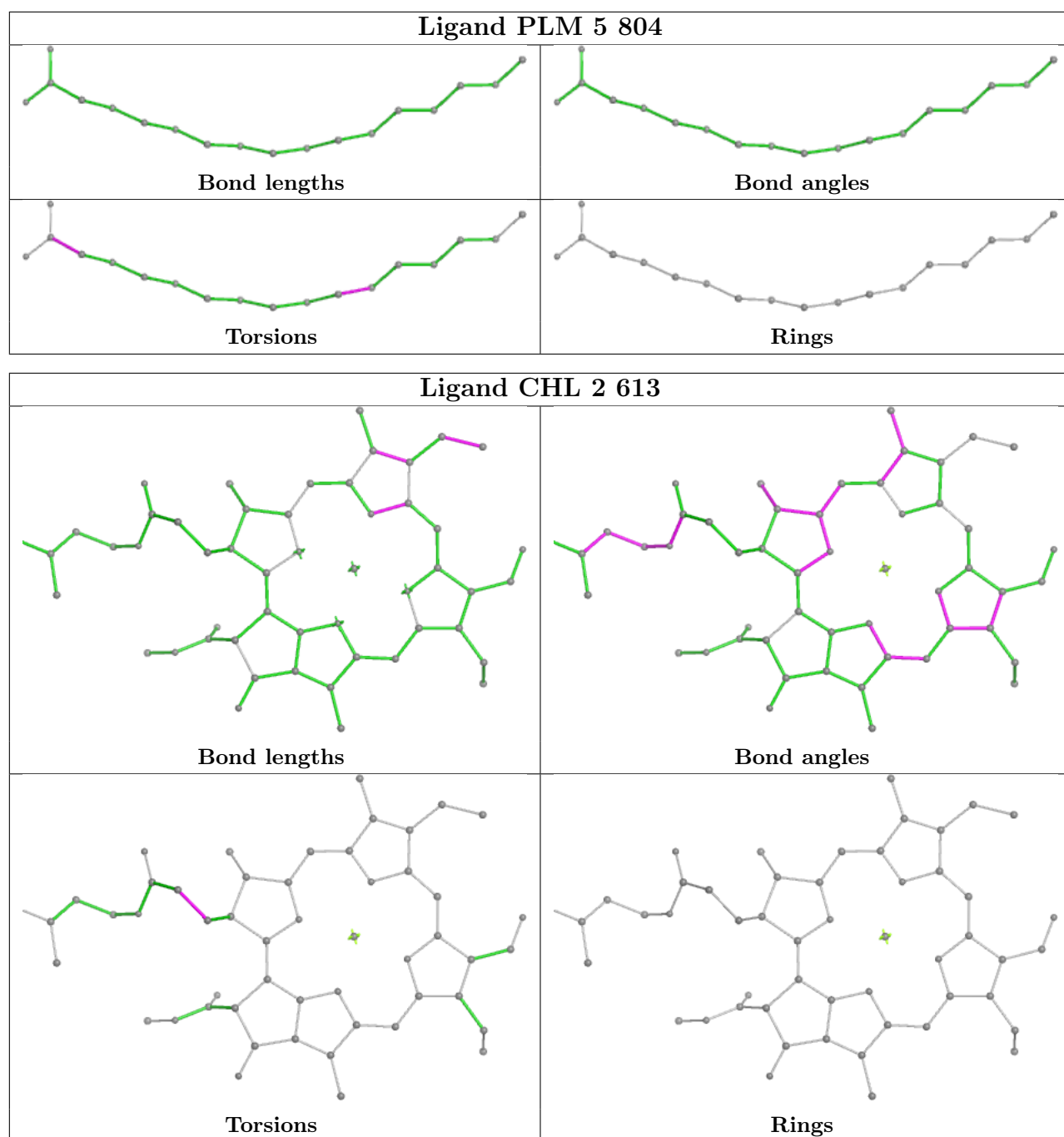


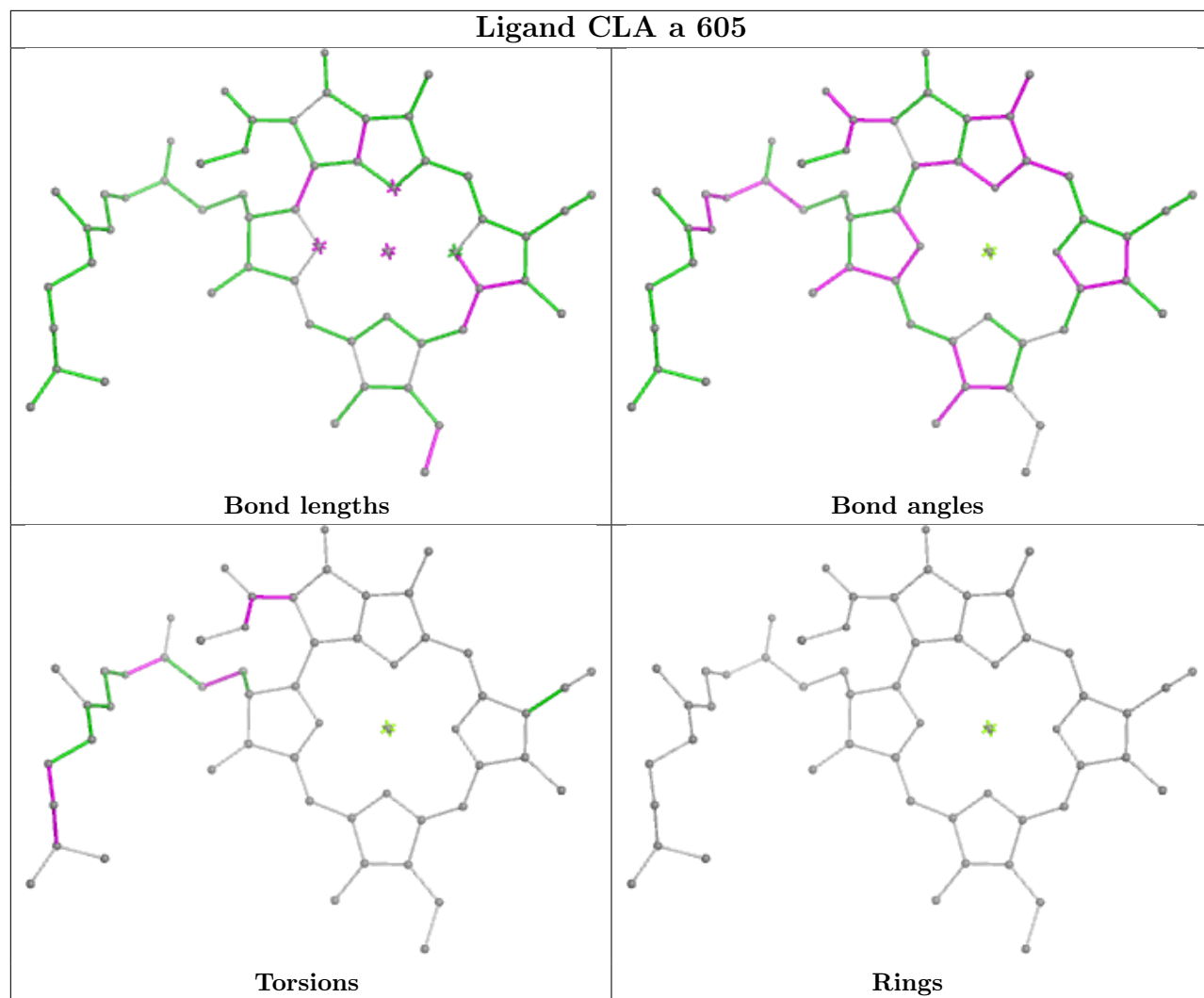


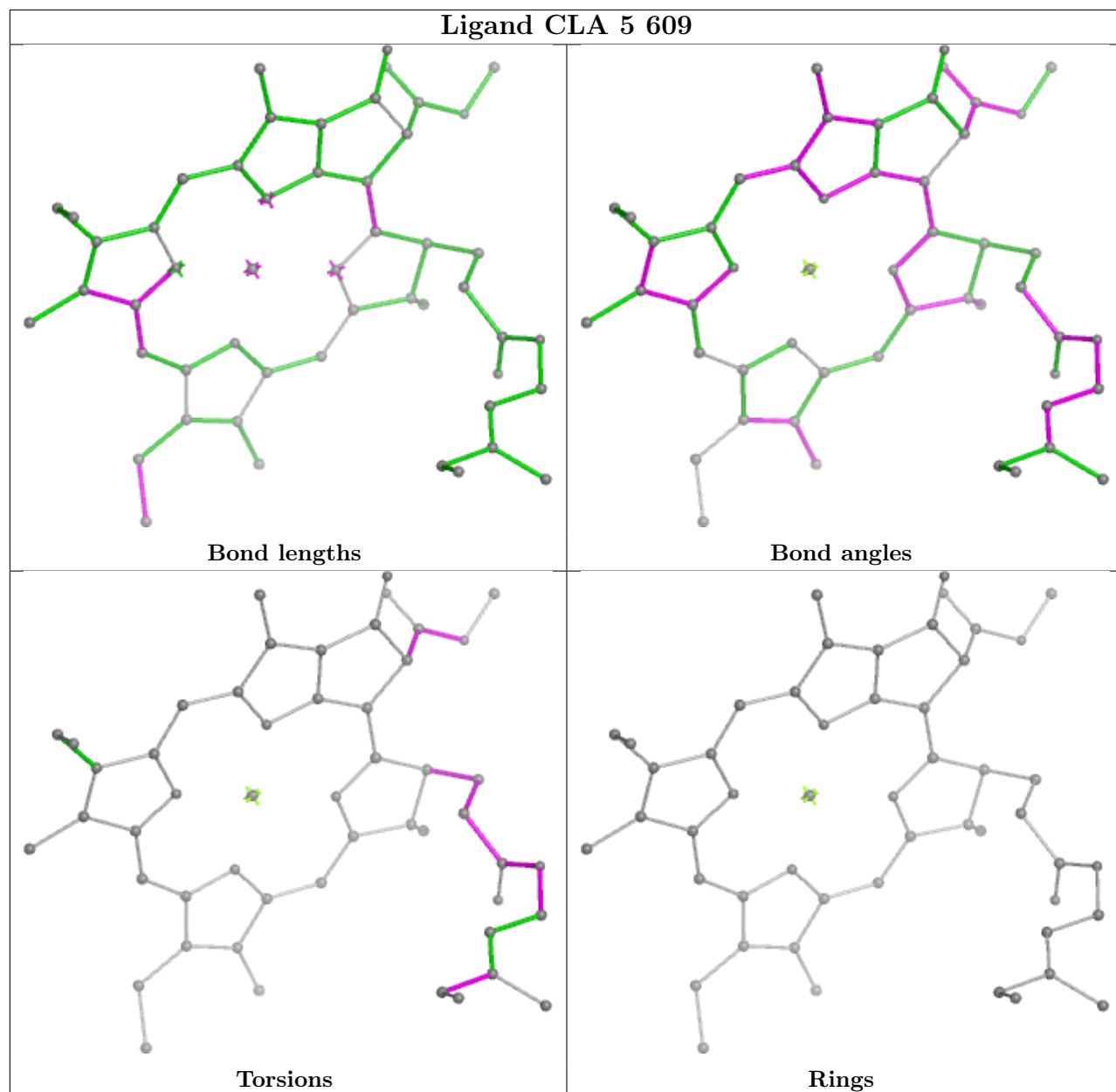


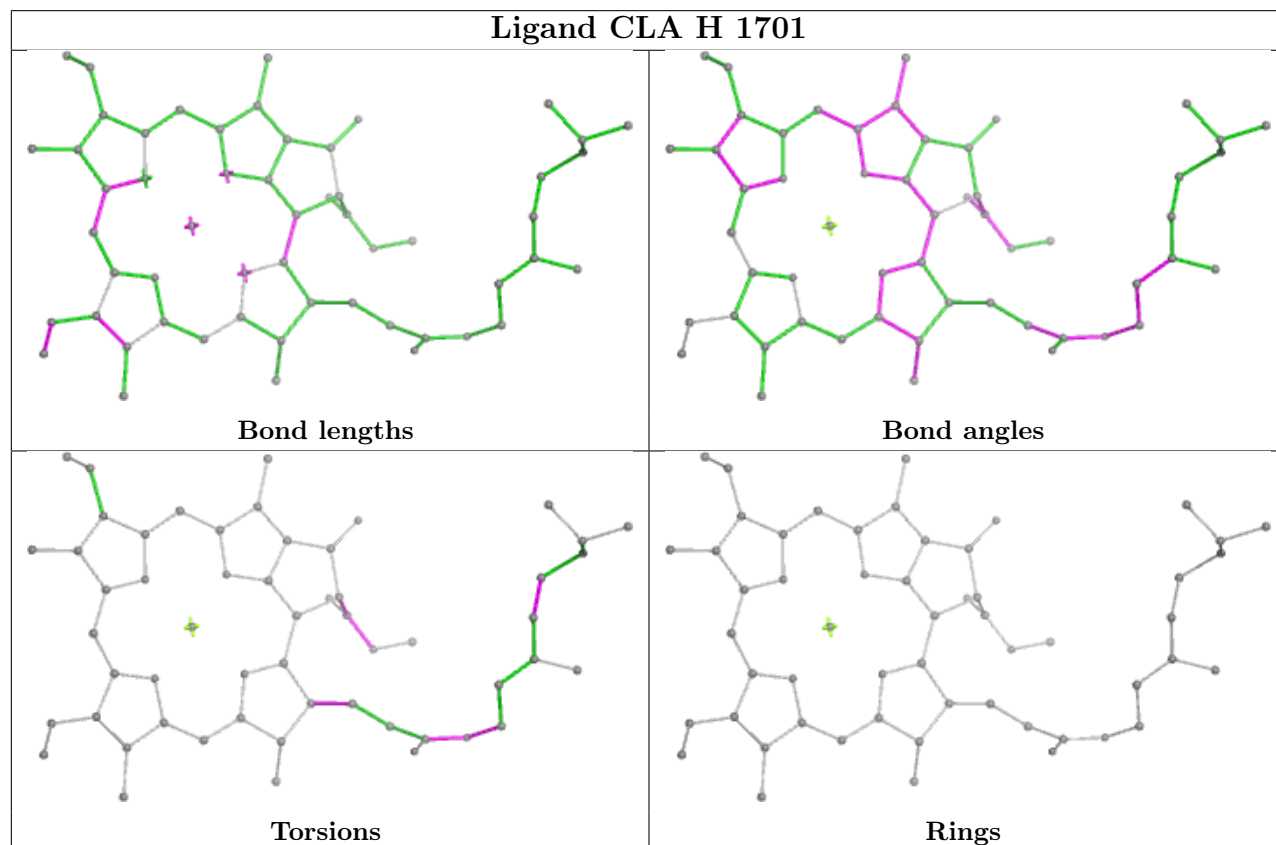
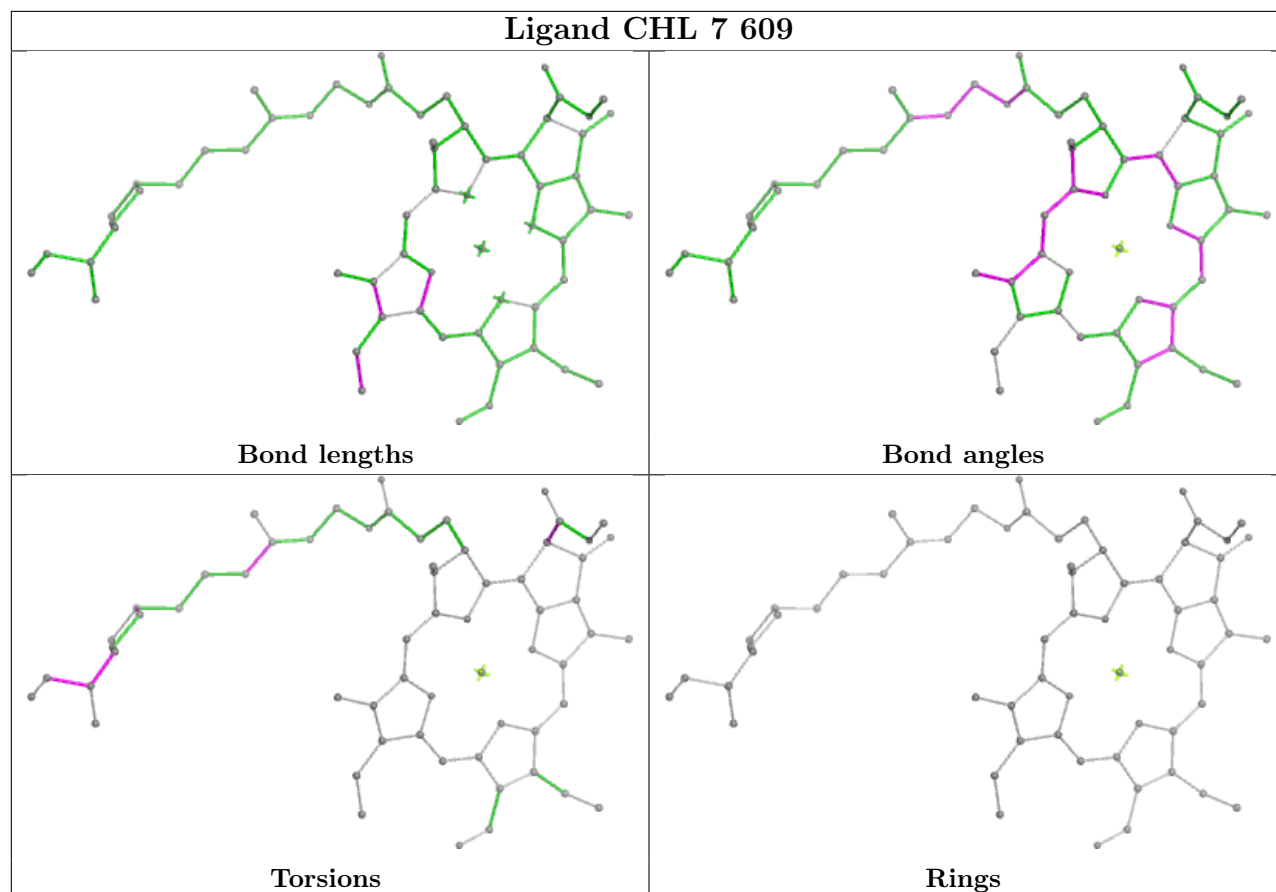


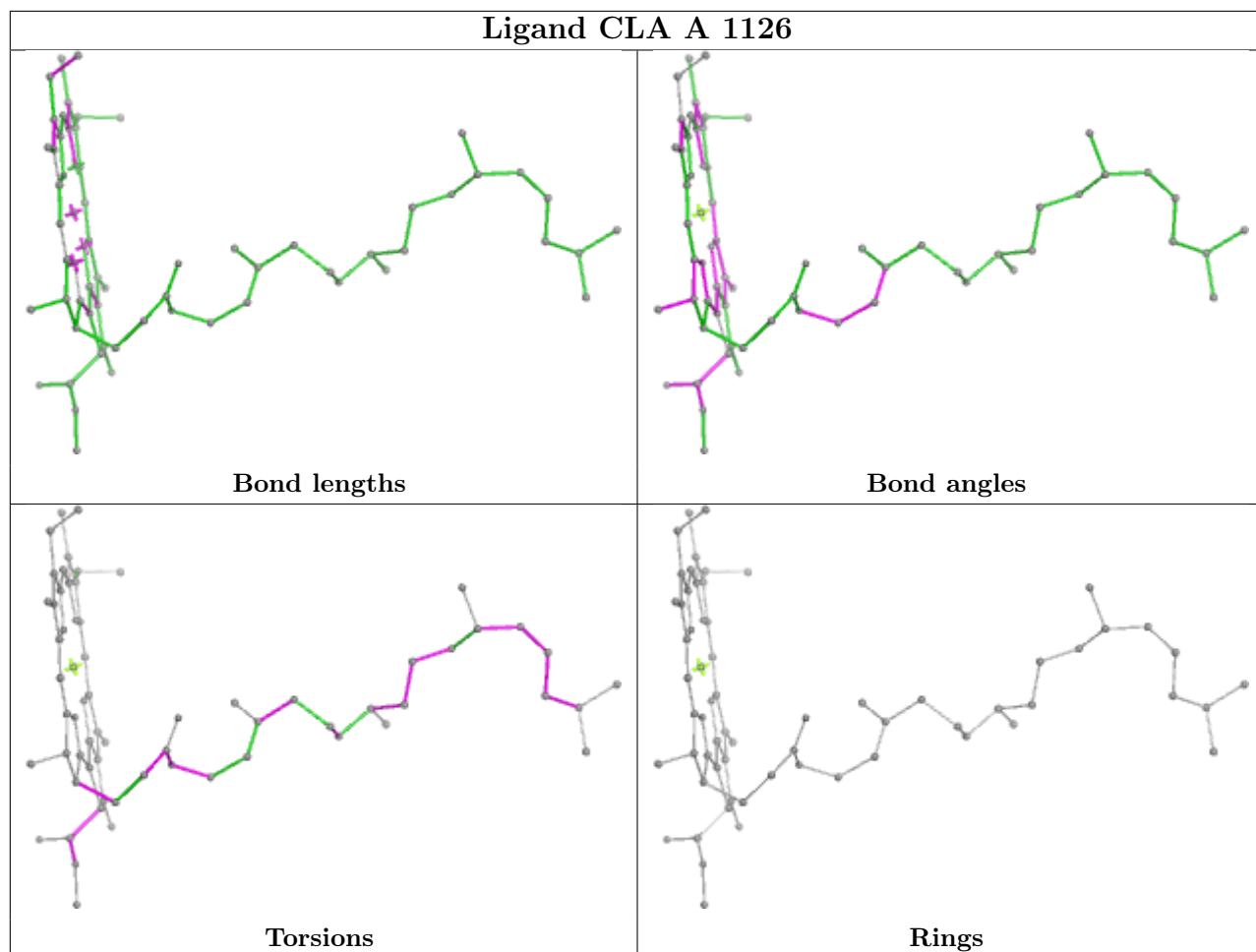


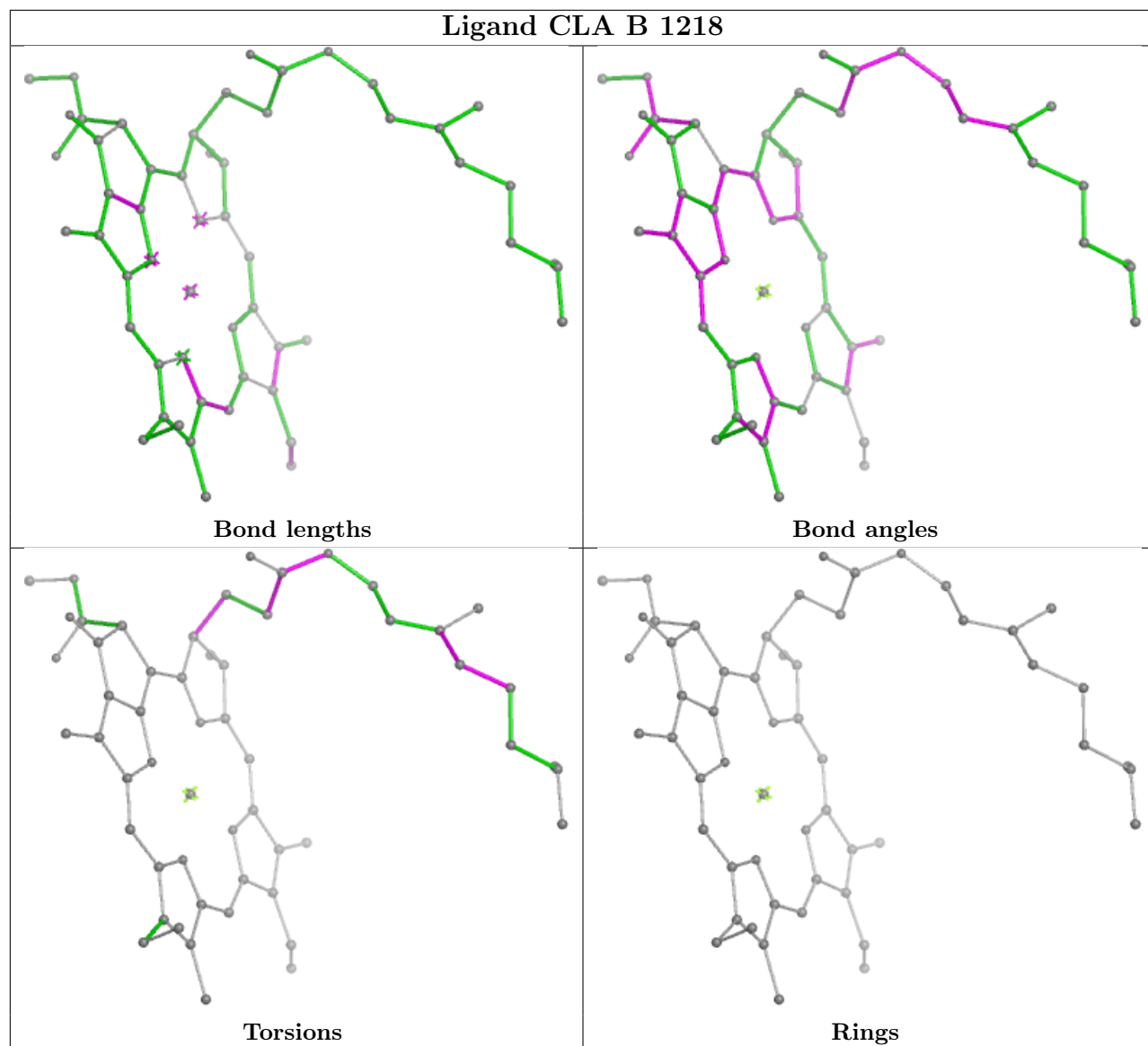


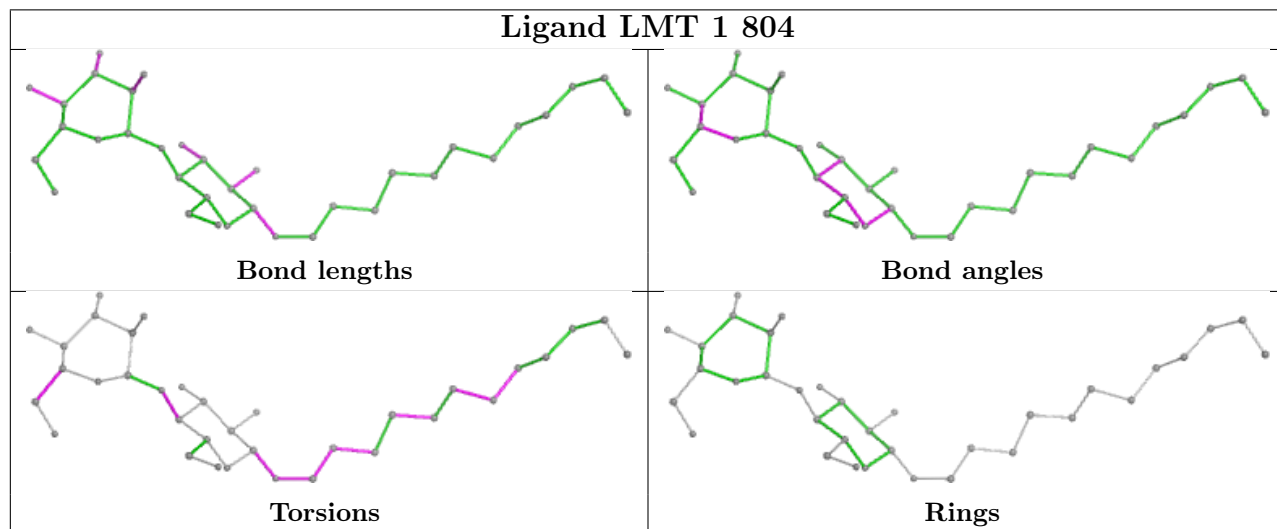
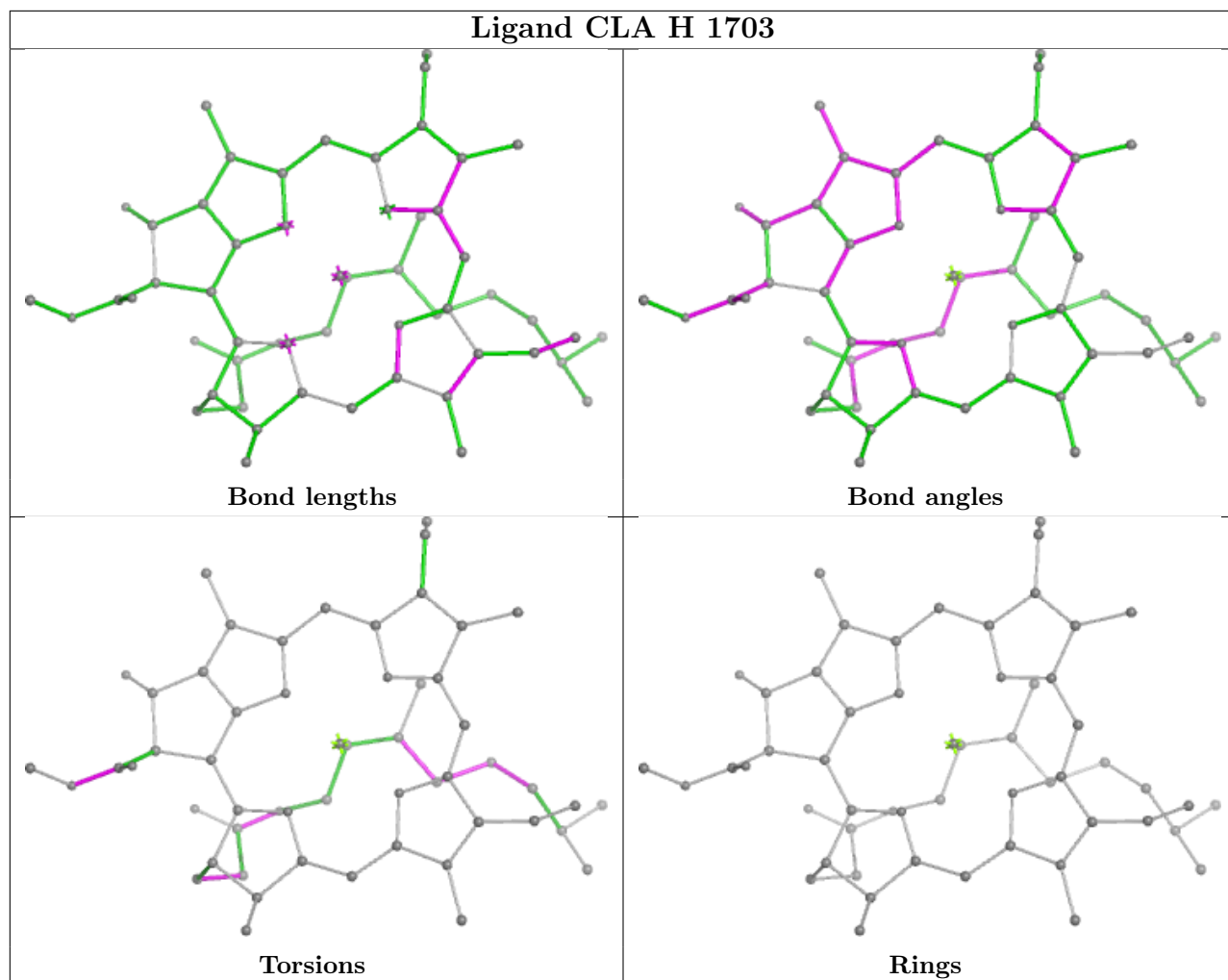


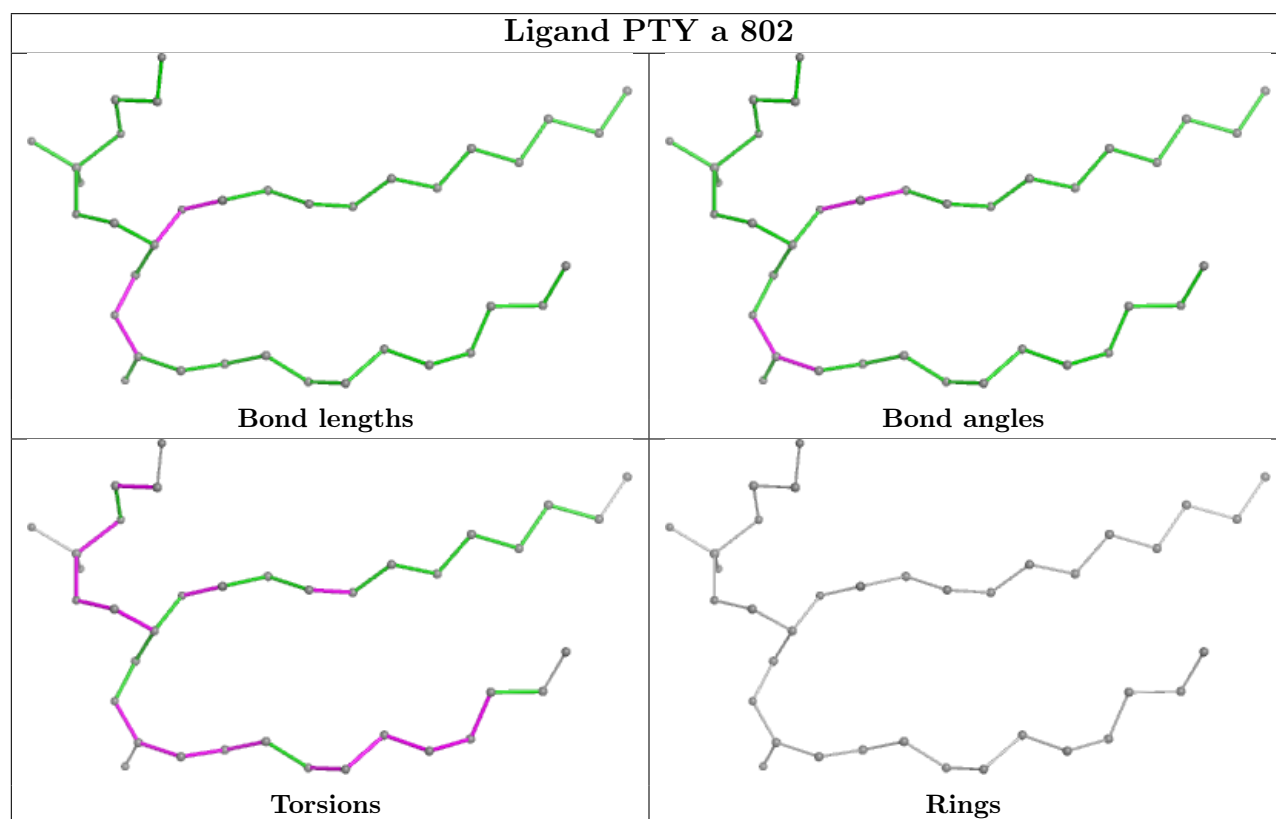
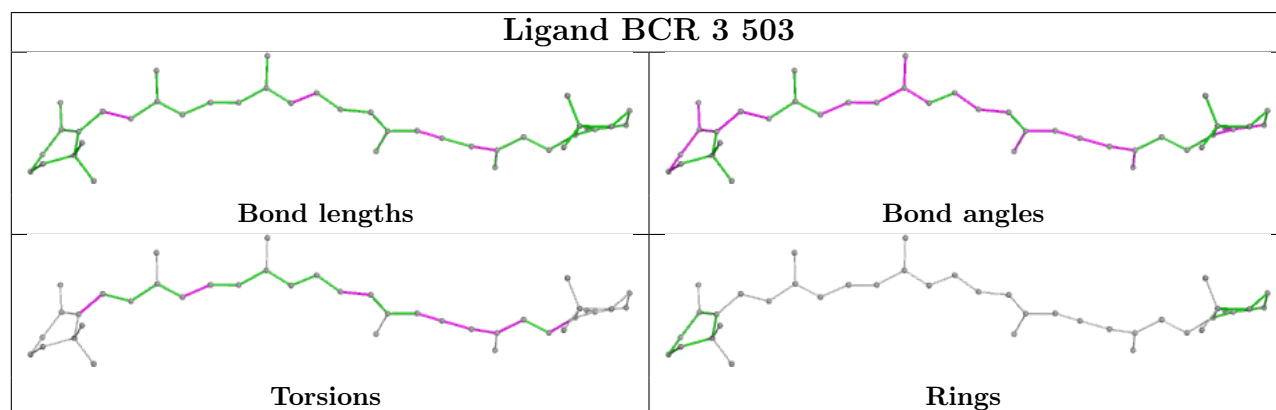
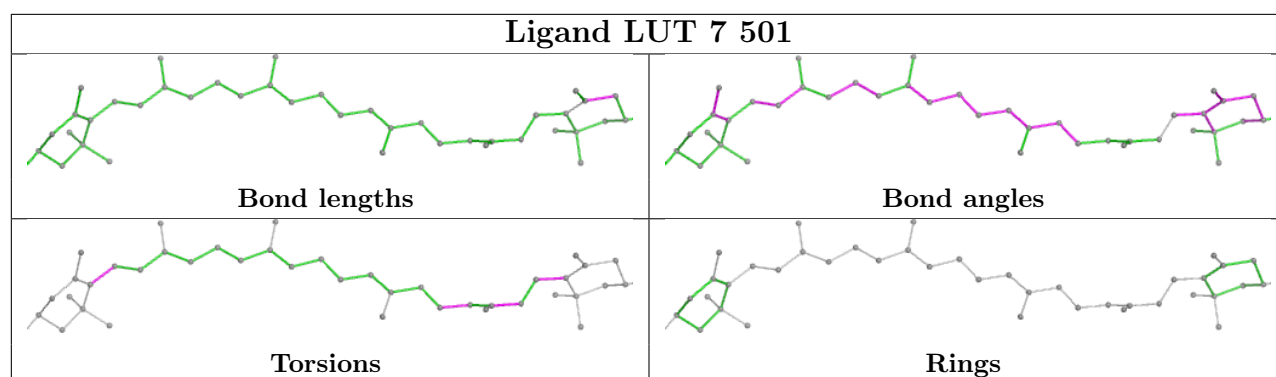


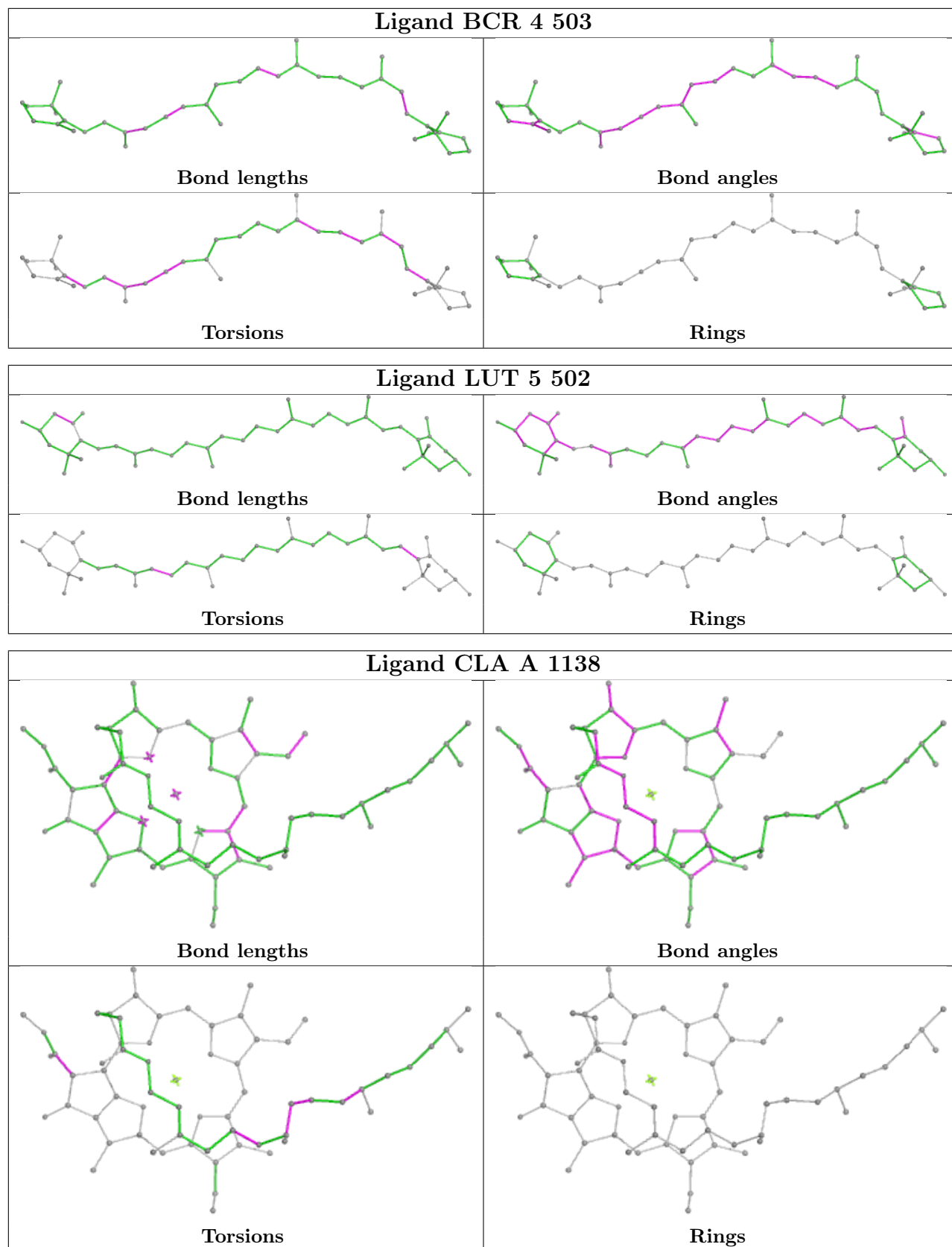




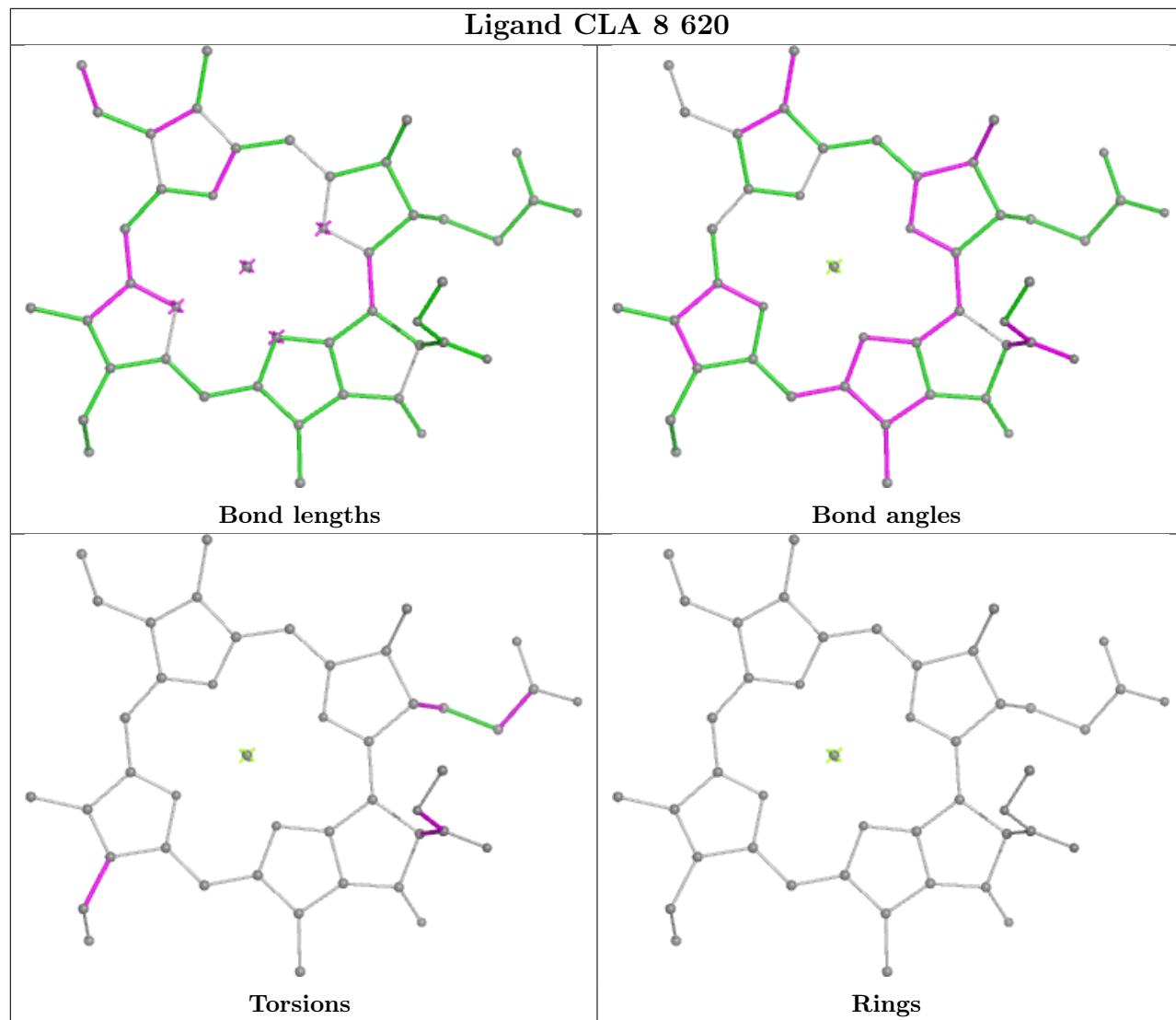


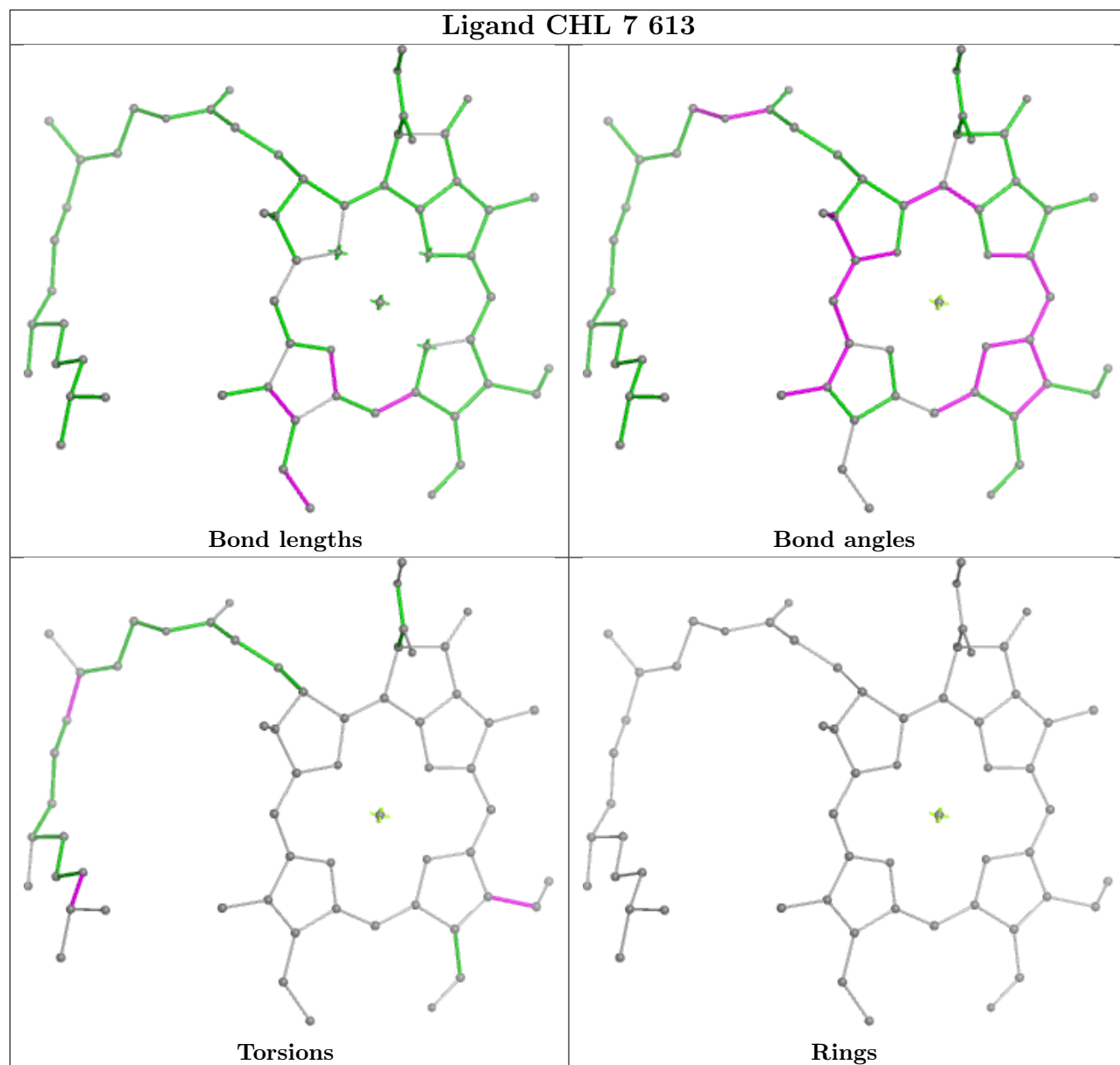


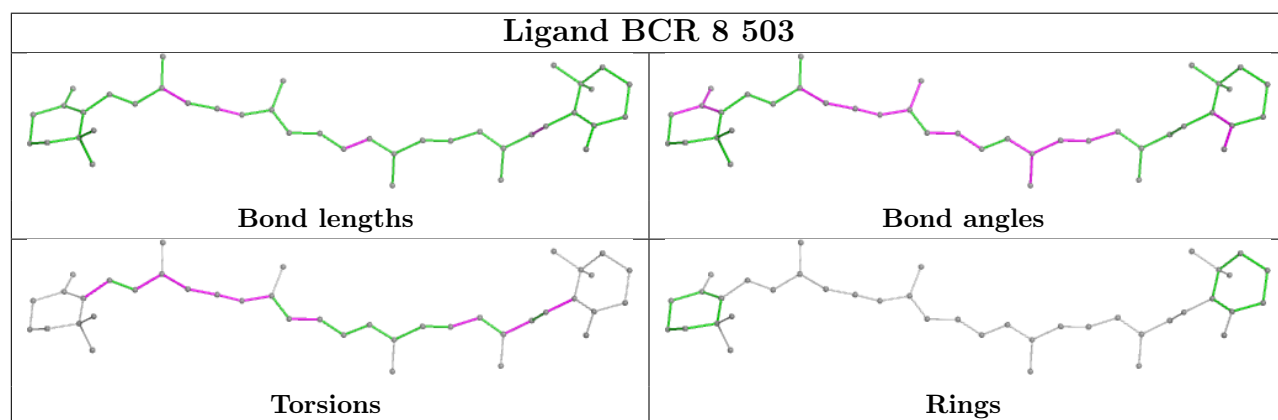
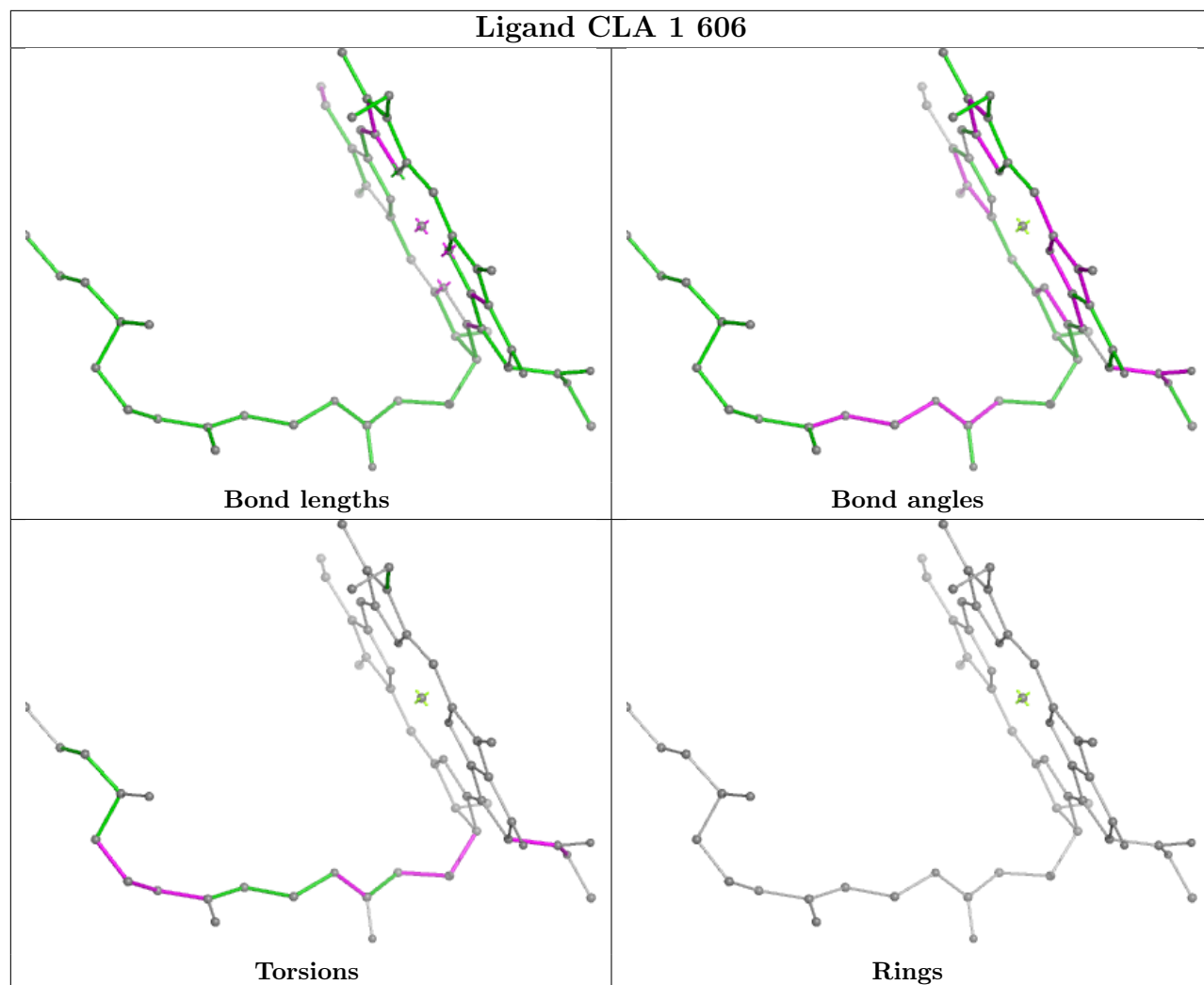


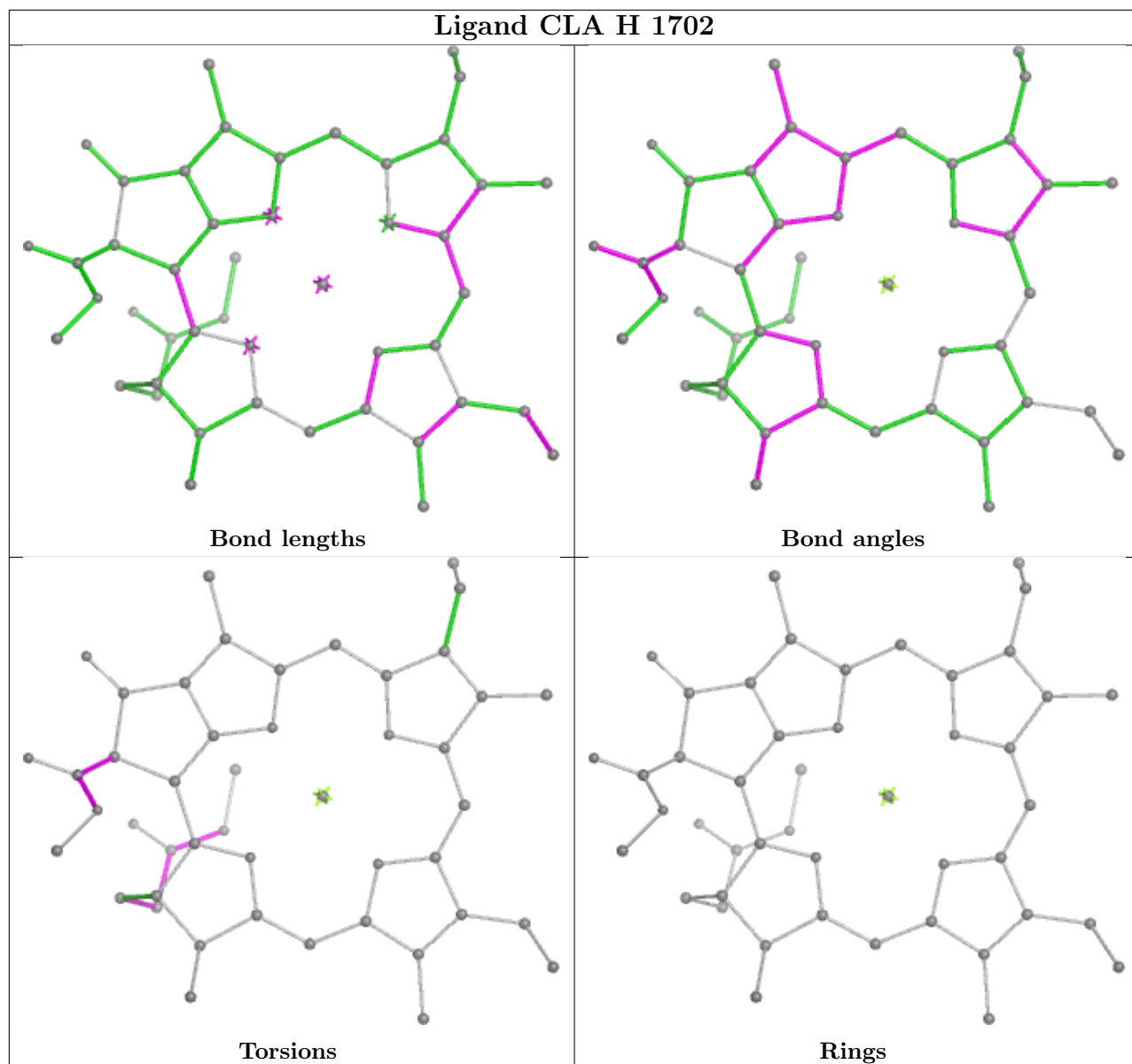


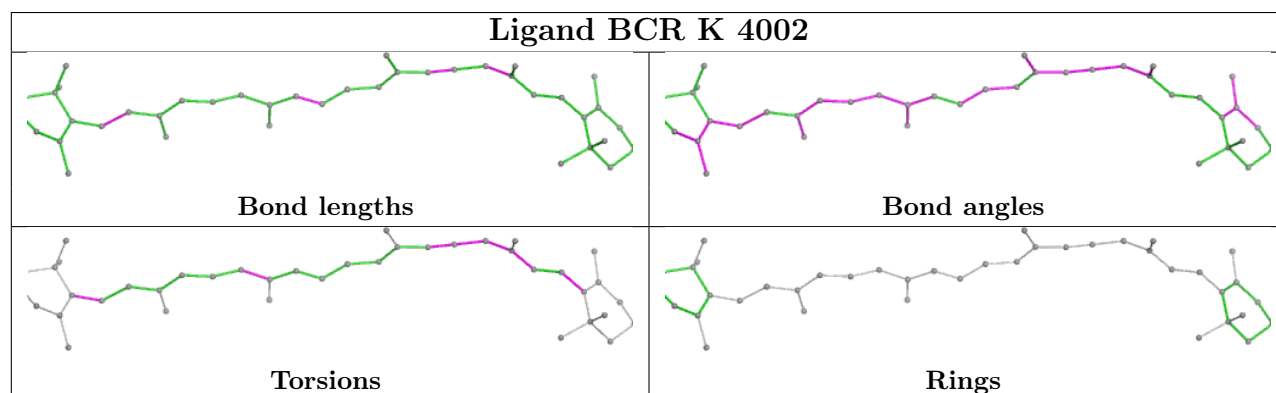
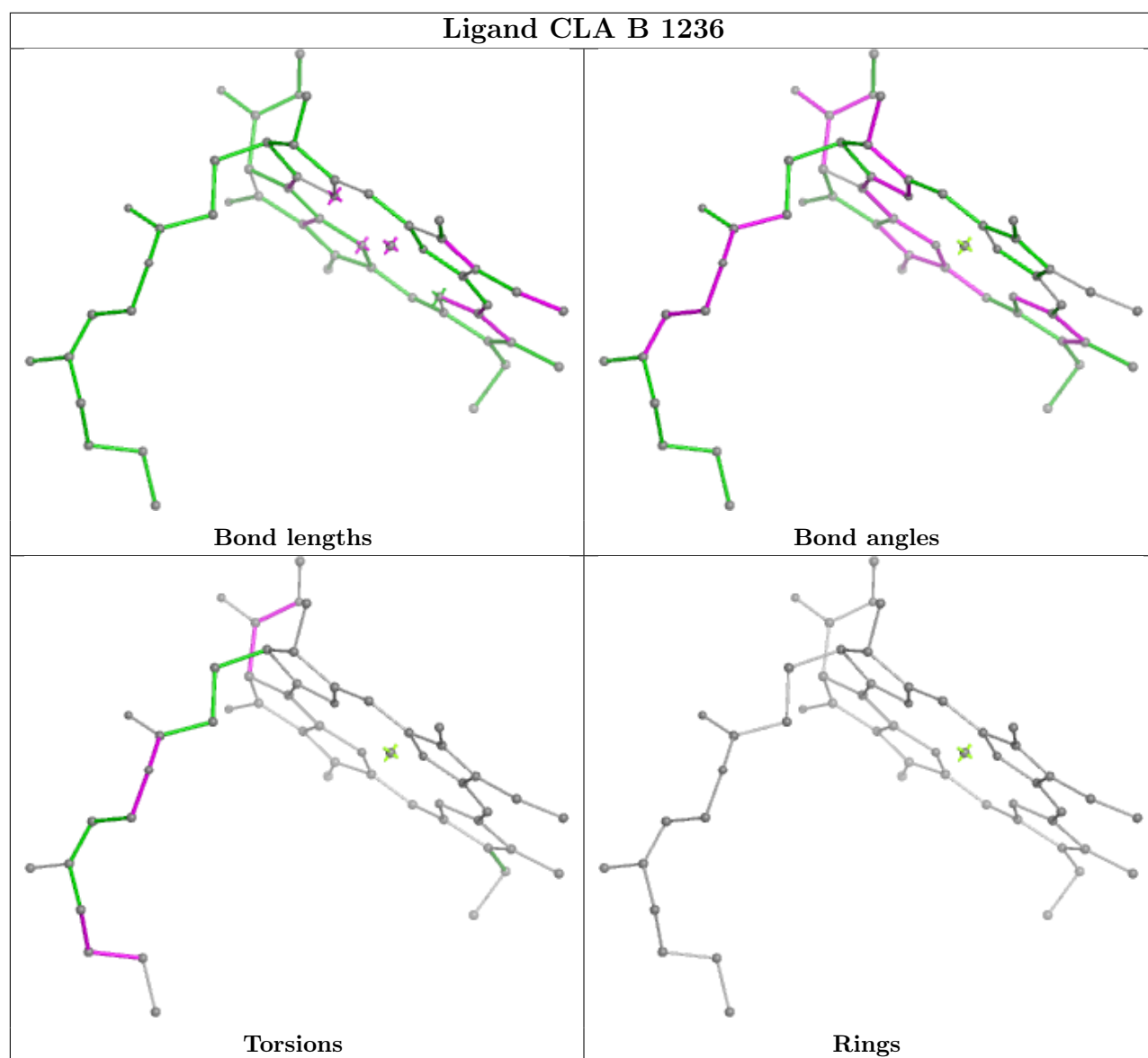
Ligand CLA 8 620

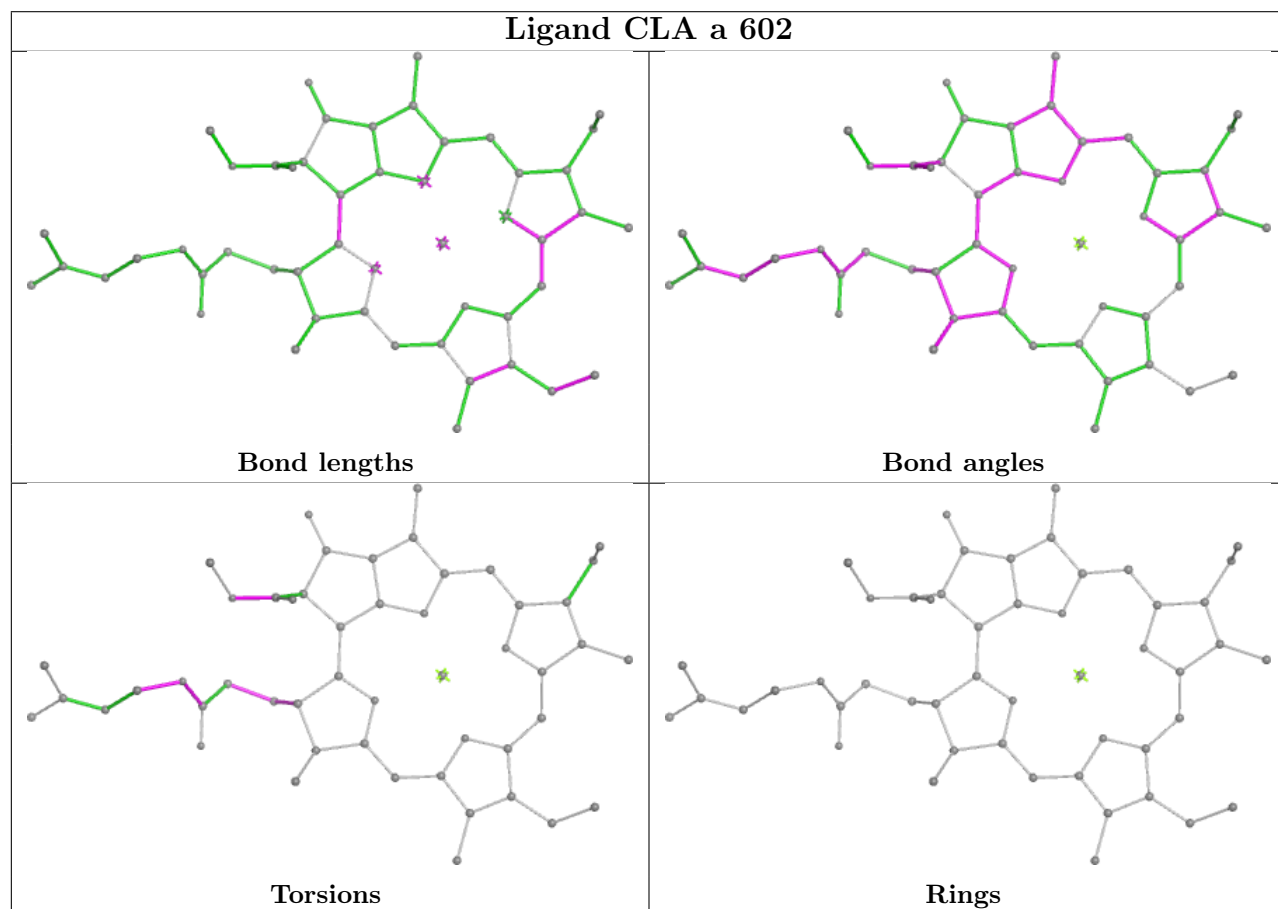
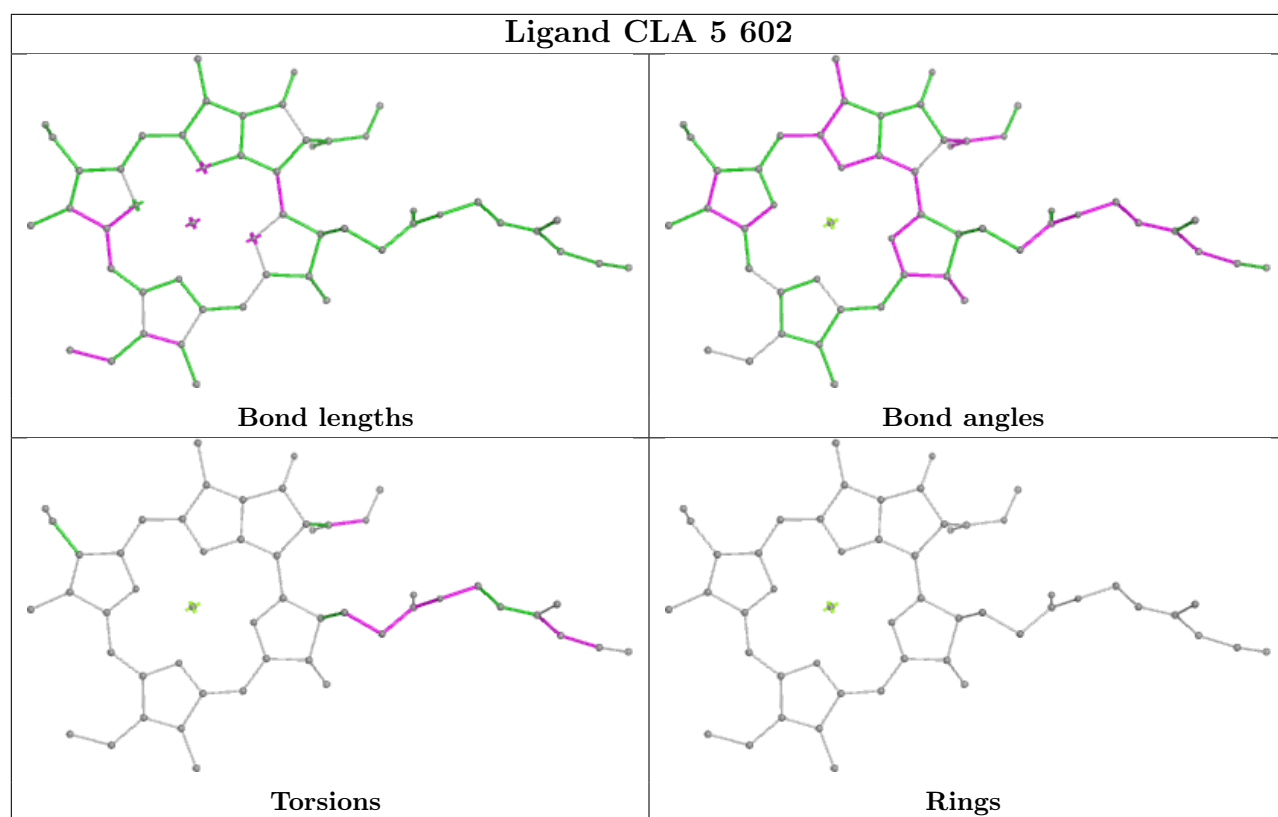


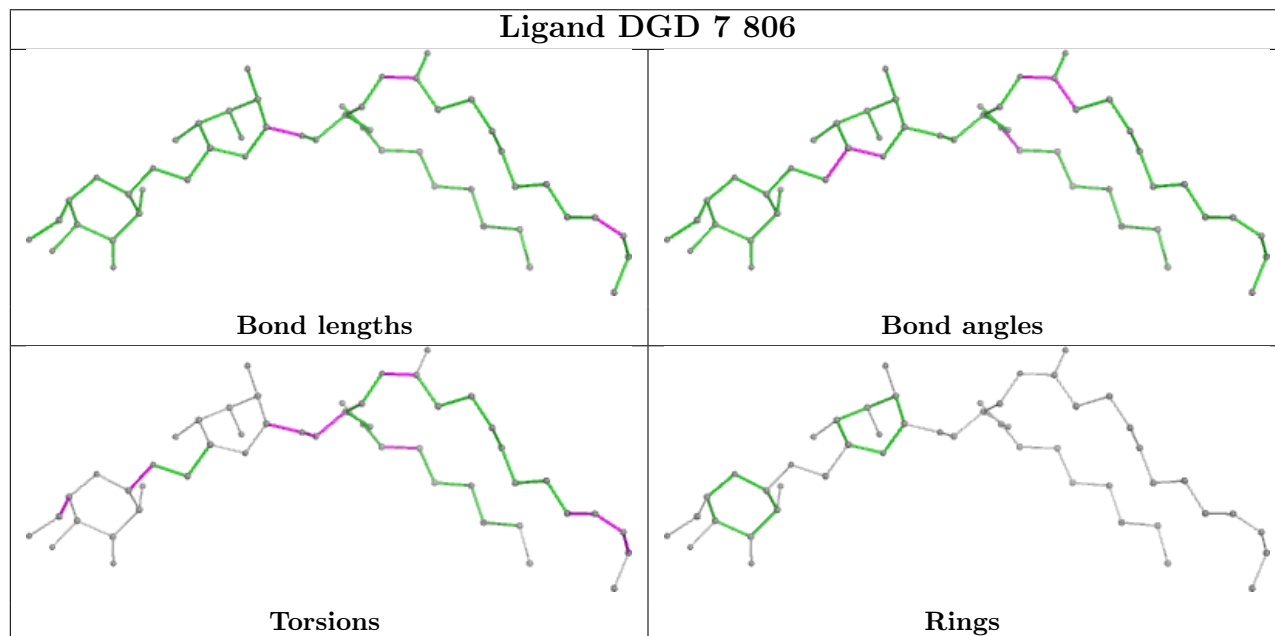
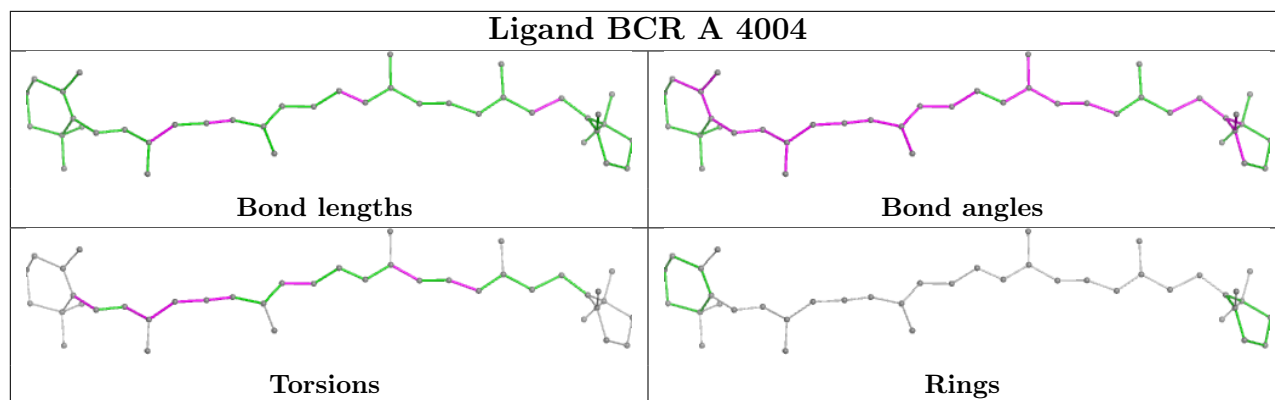


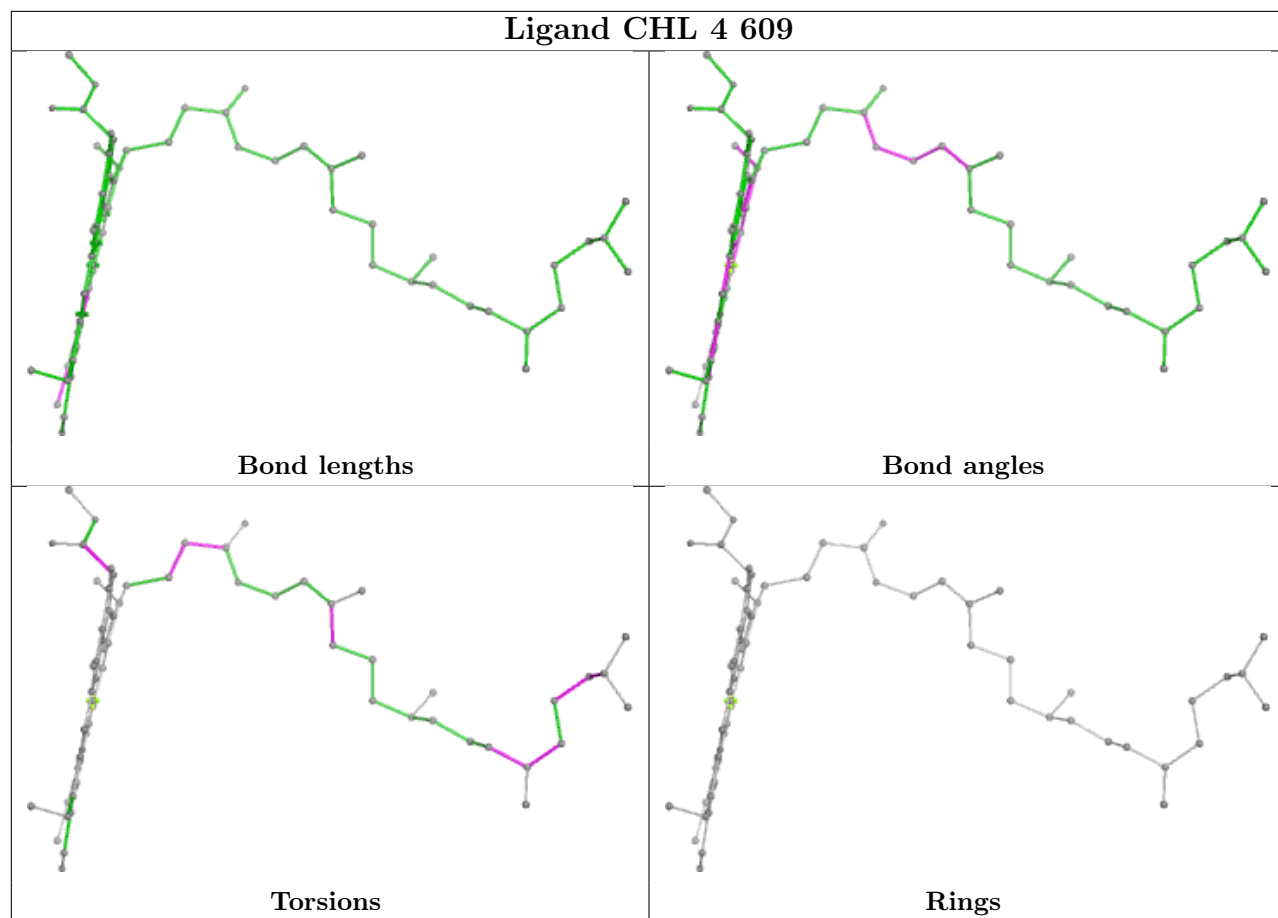


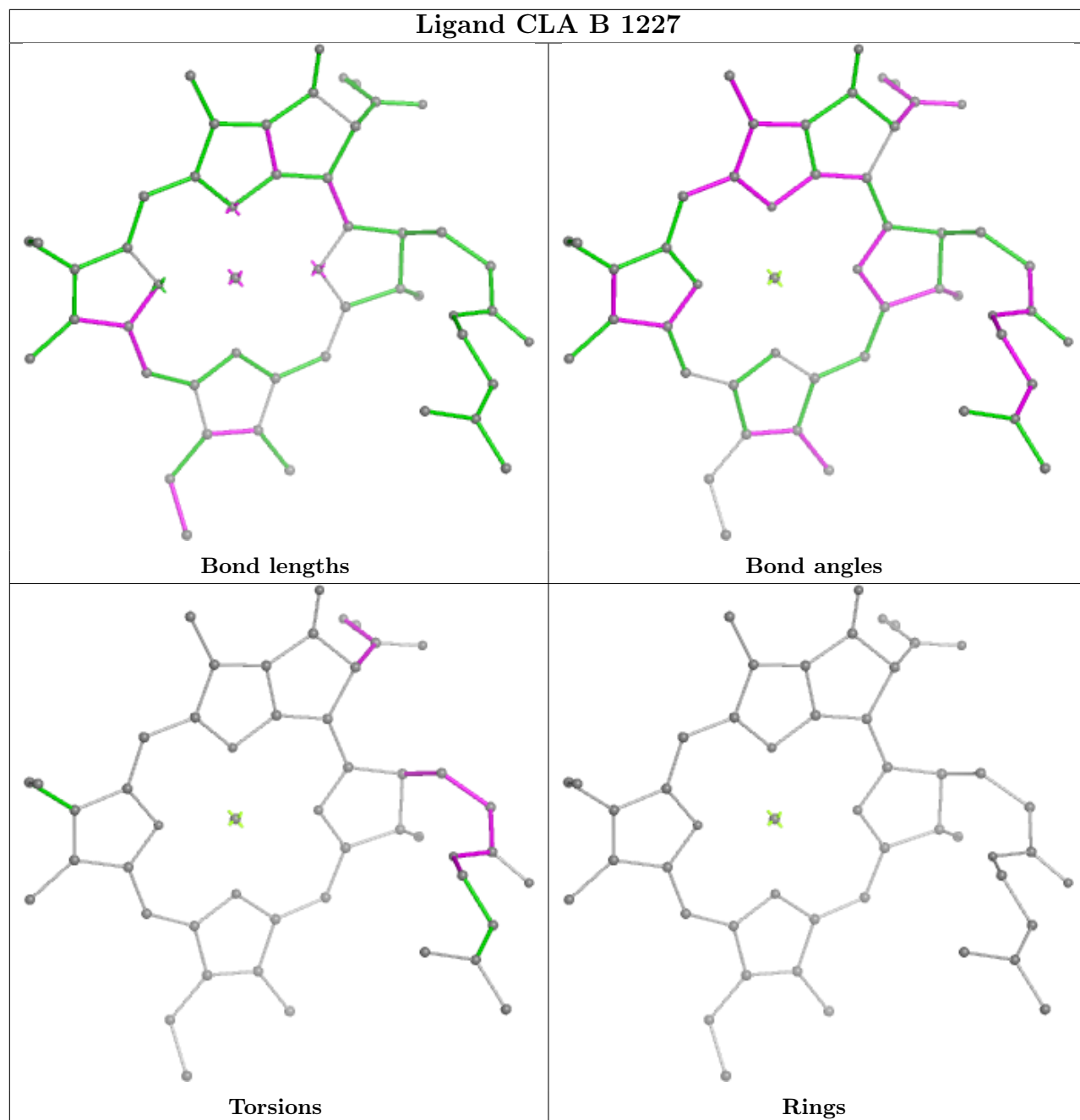


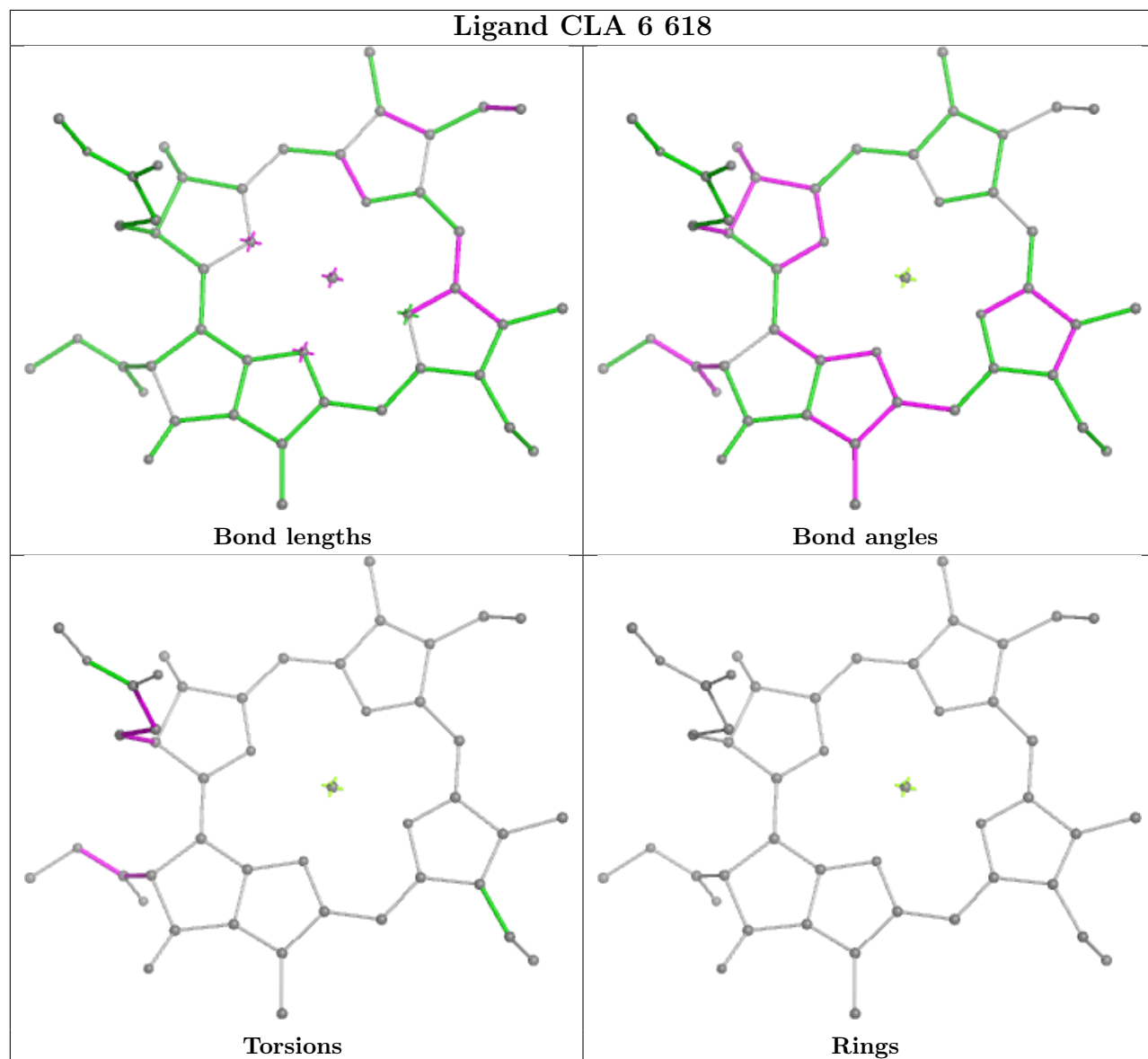


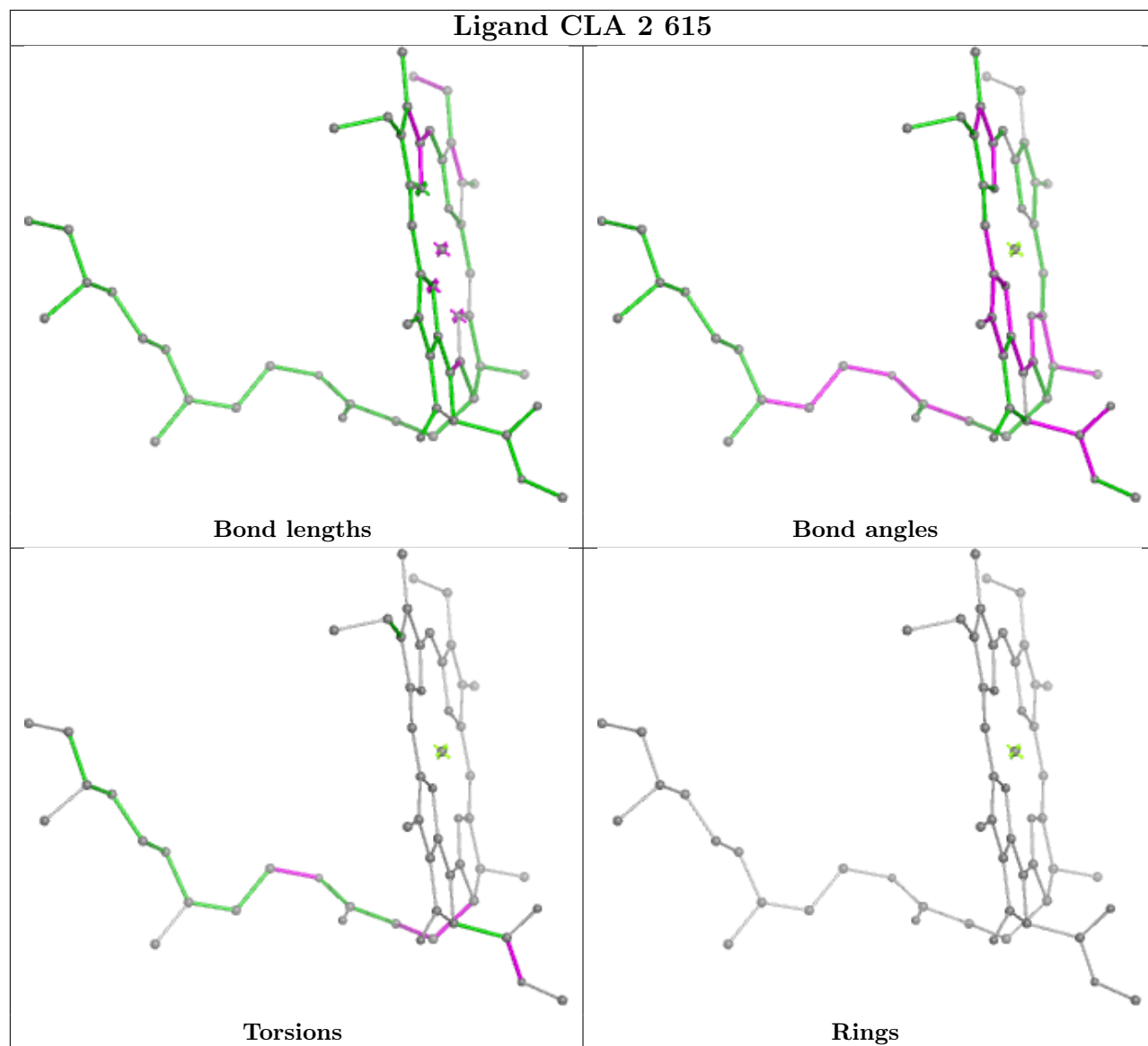


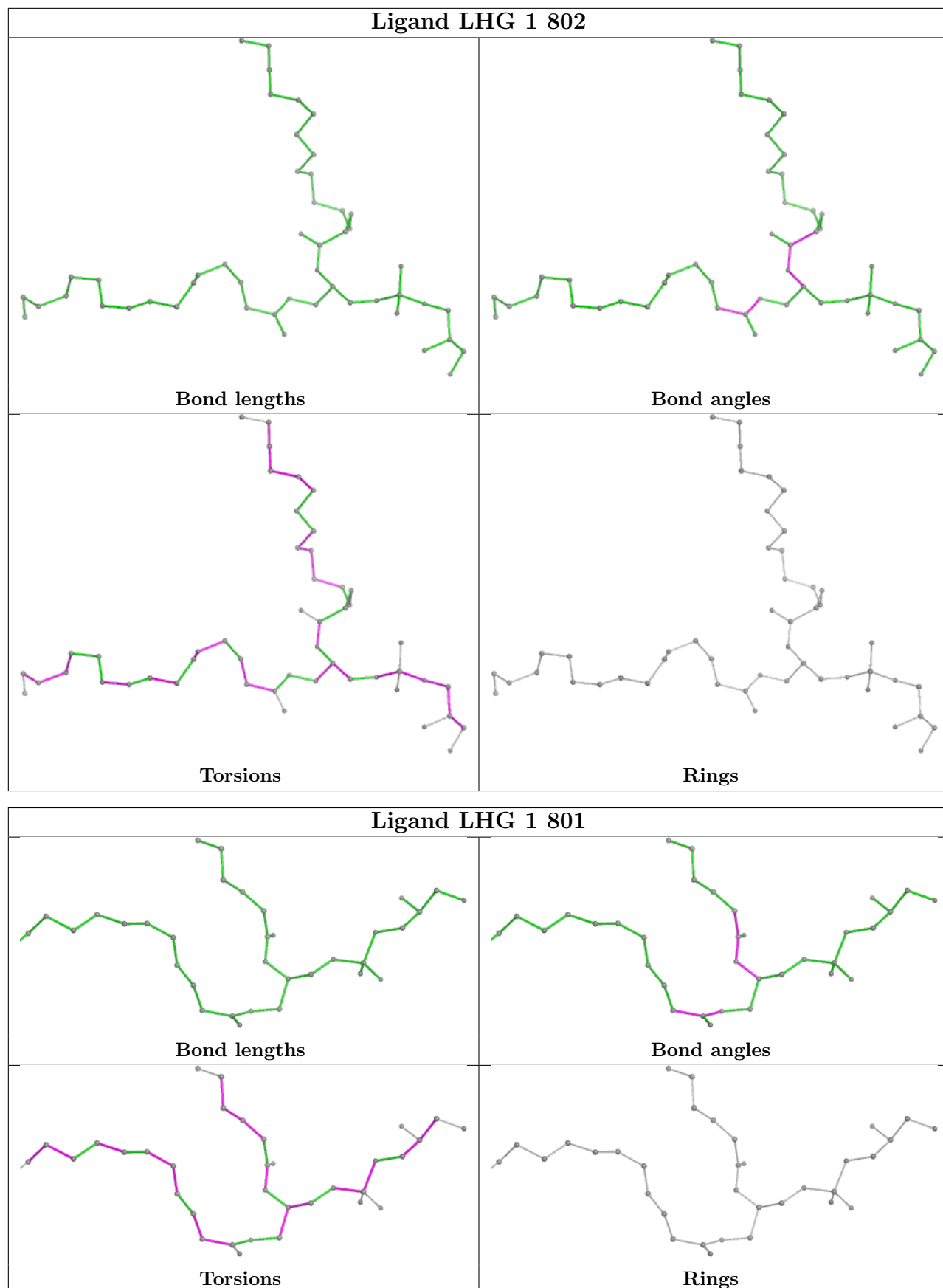


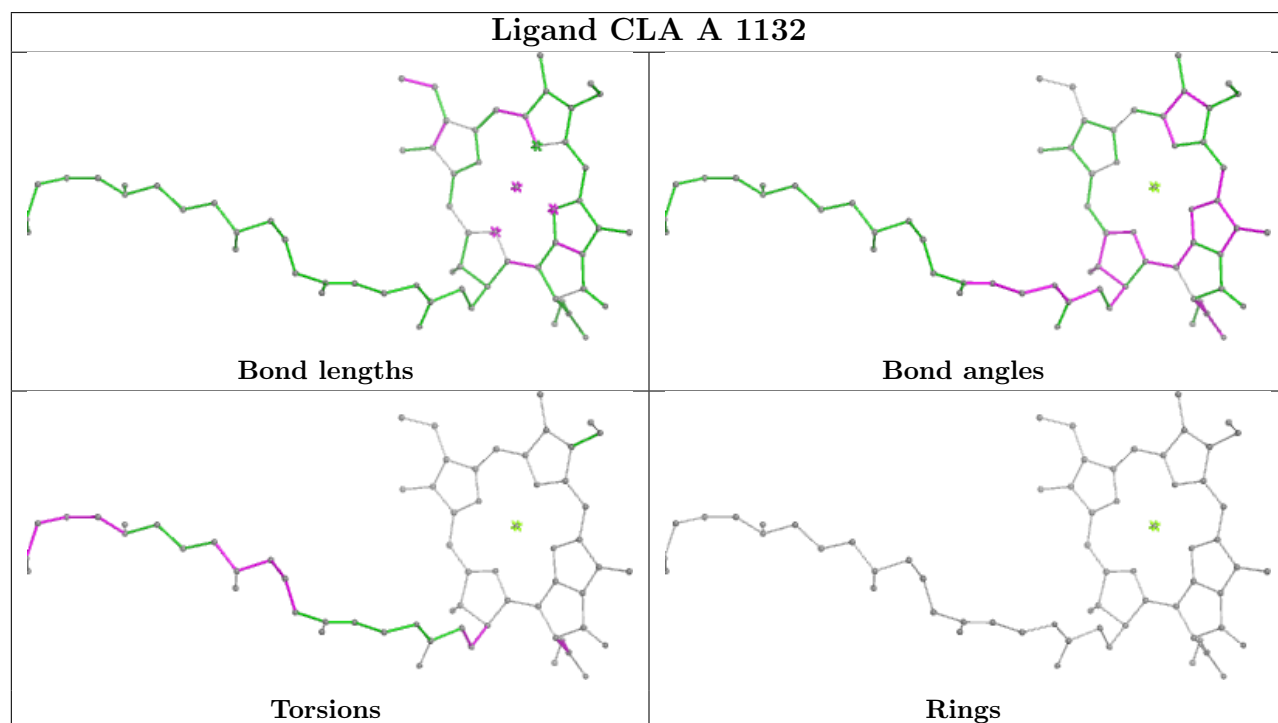
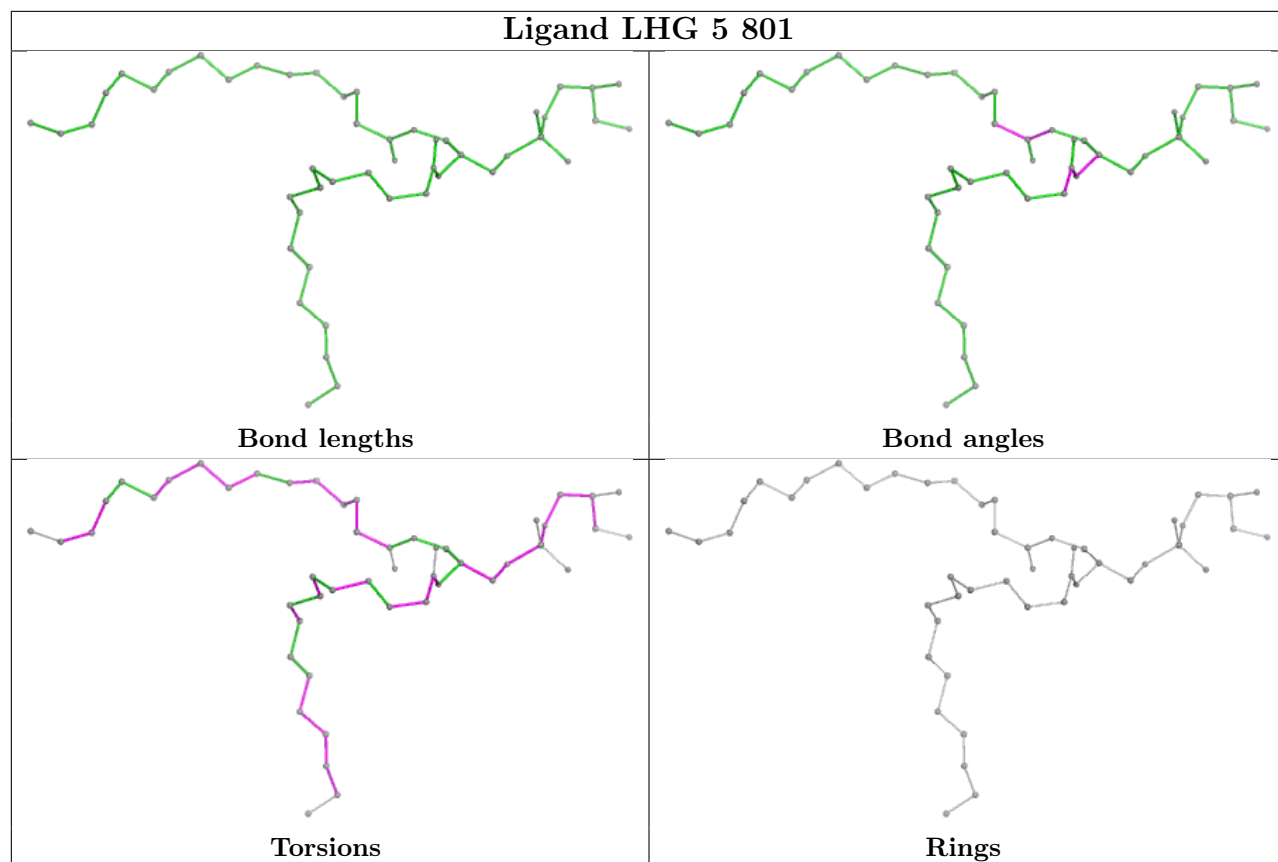


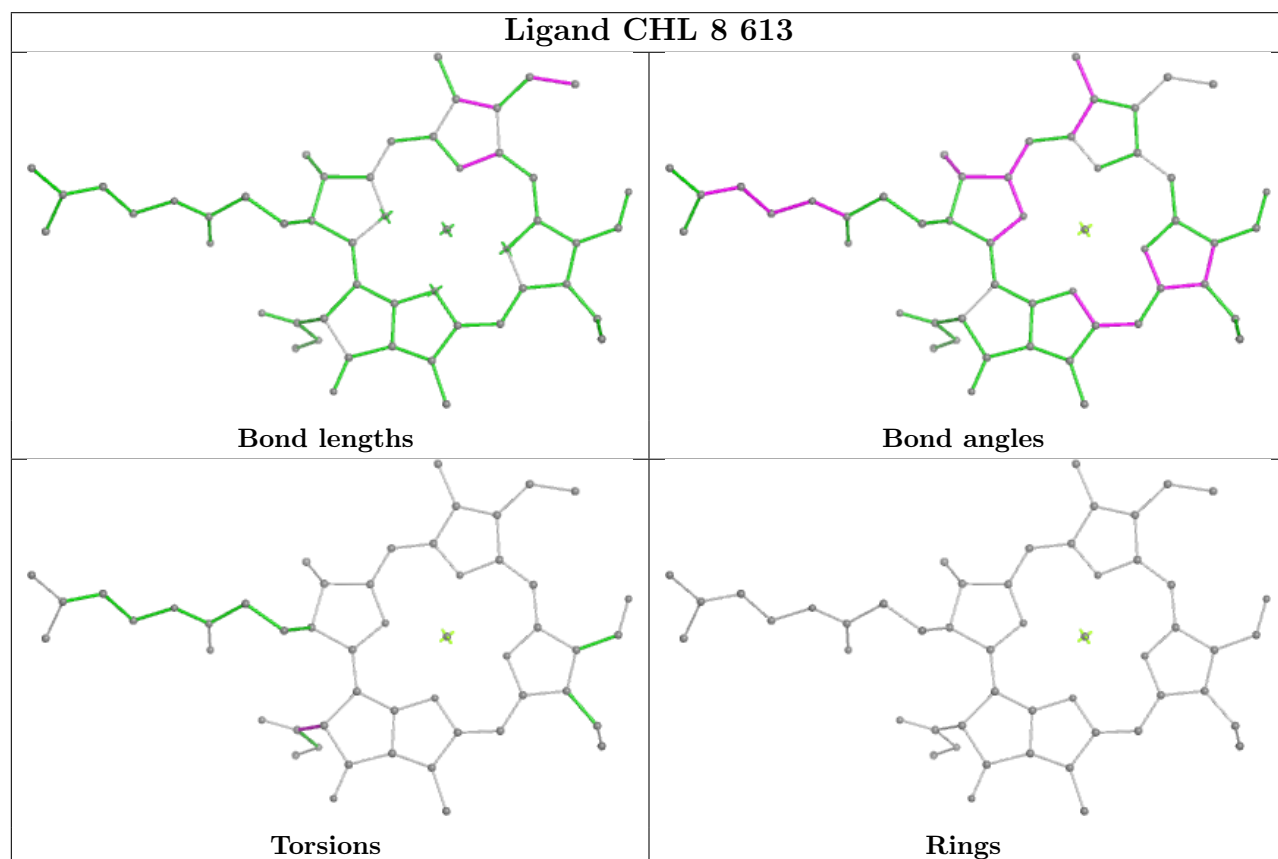
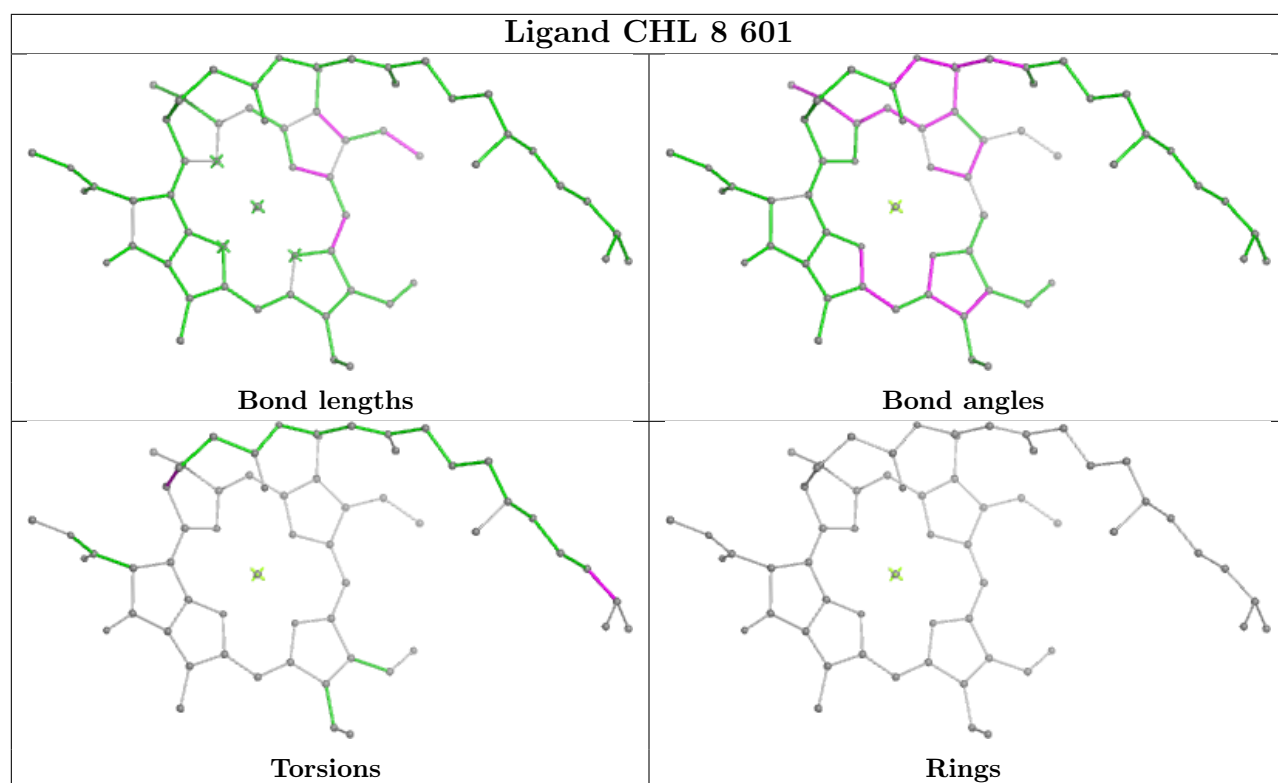


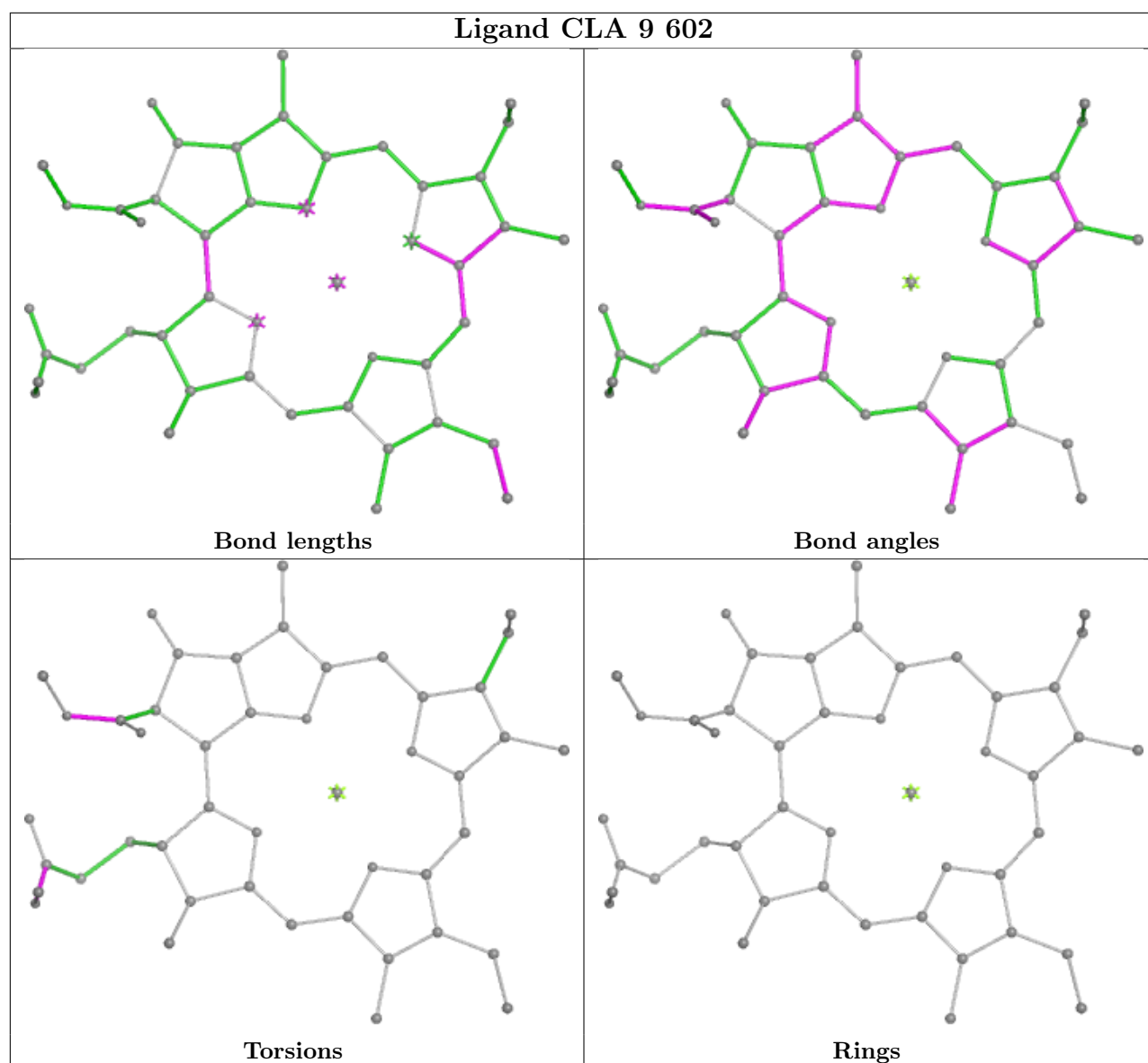












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

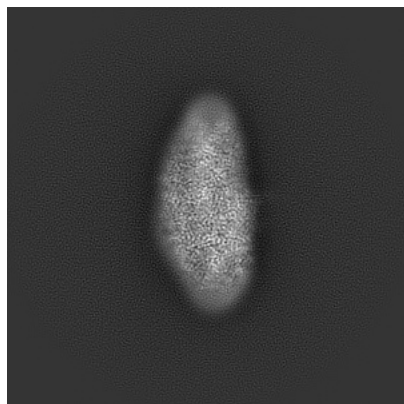
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11588. These allow visual inspection of the internal detail of the map and identification of artifacts.

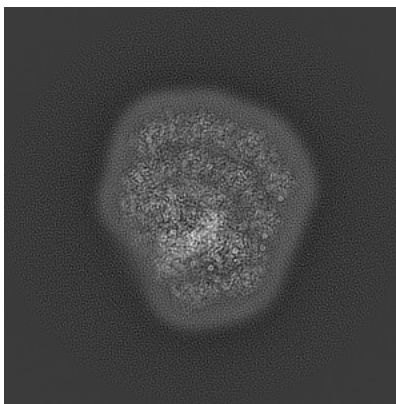
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

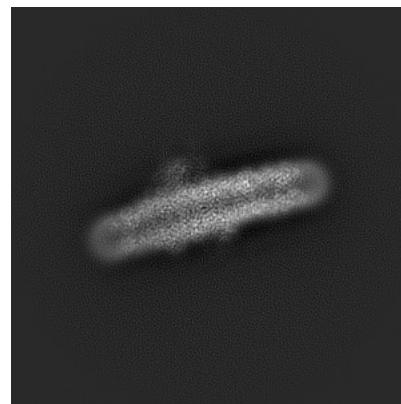
6.1.1 Primary map



X

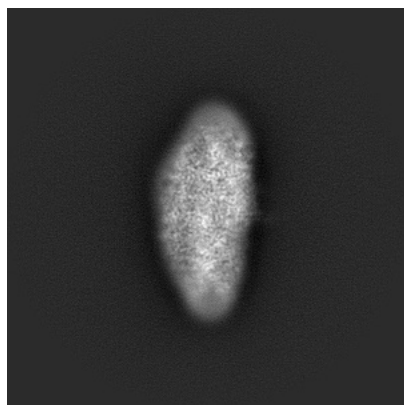


Y

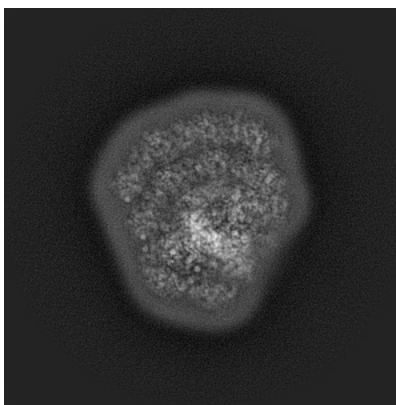


Z

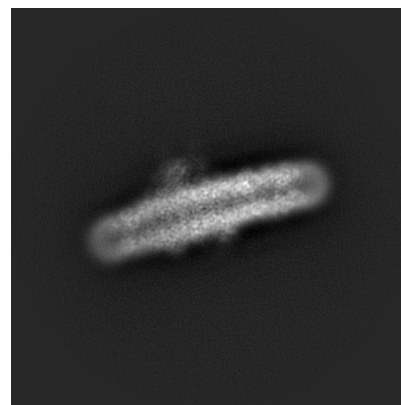
6.1.2 Raw map



X



Y

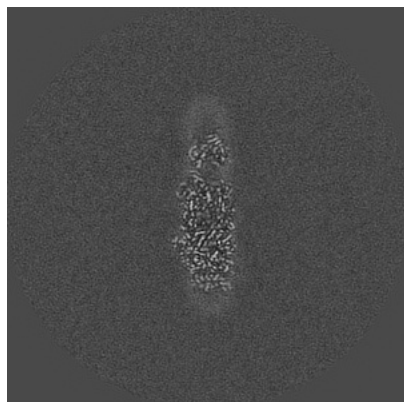


Z

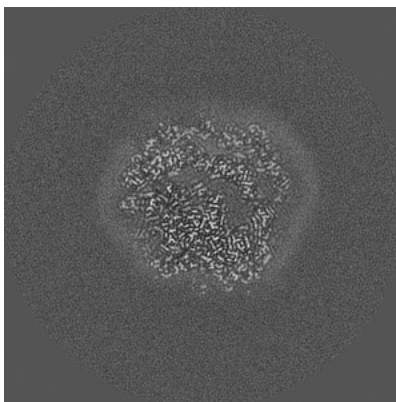
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

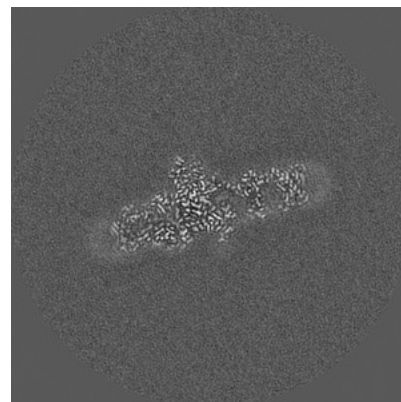
6.2.1 Primary map



X Index: 240

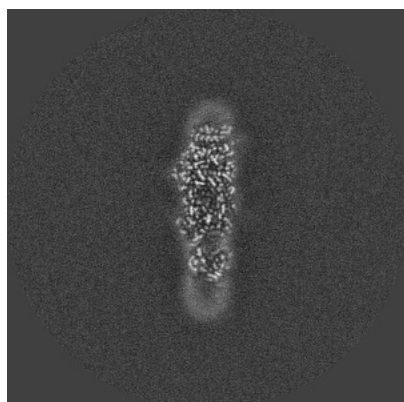


Y Index: 240

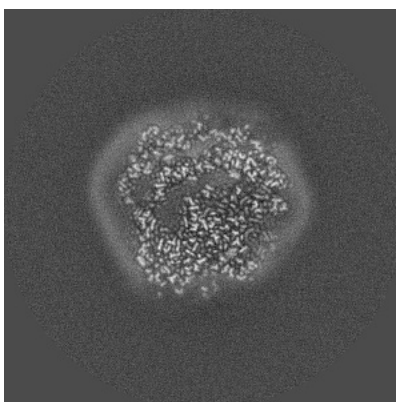


Z Index: 240

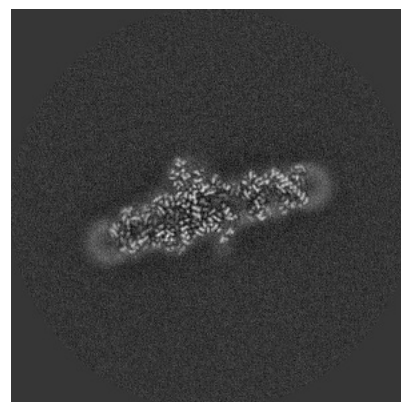
6.2.2 Raw map



X Index: 240



Y Index: 240

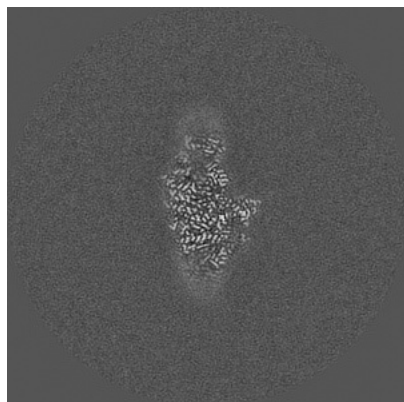


Z Index: 240

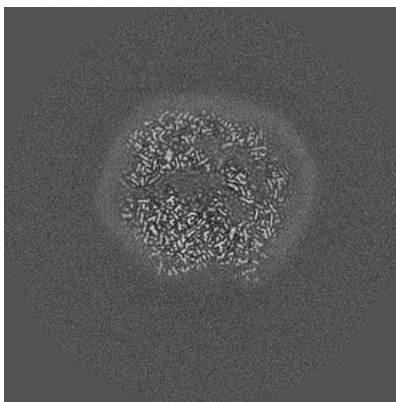
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

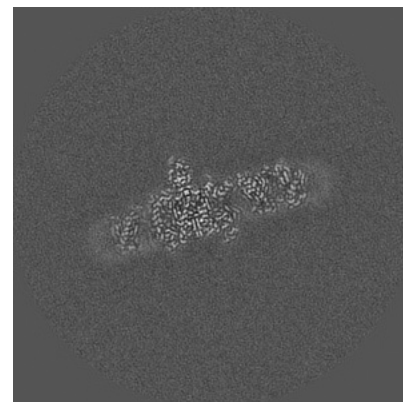
6.3.1 Primary map



X Index: 208

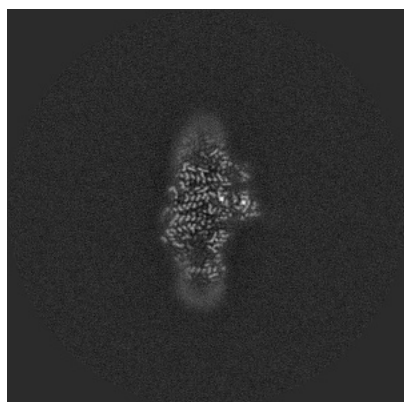


Y Index: 248

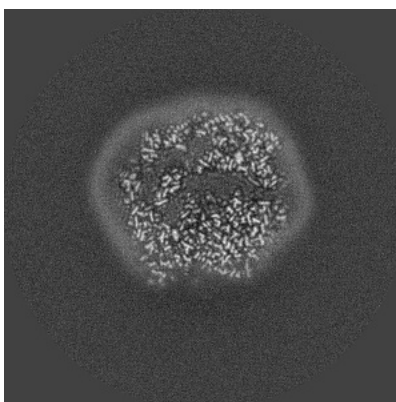


Z Index: 227

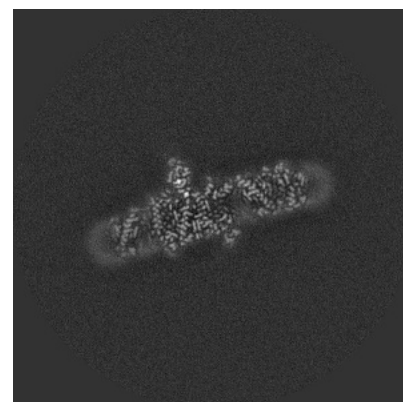
6.3.2 Raw map



X Index: 207



Y Index: 248

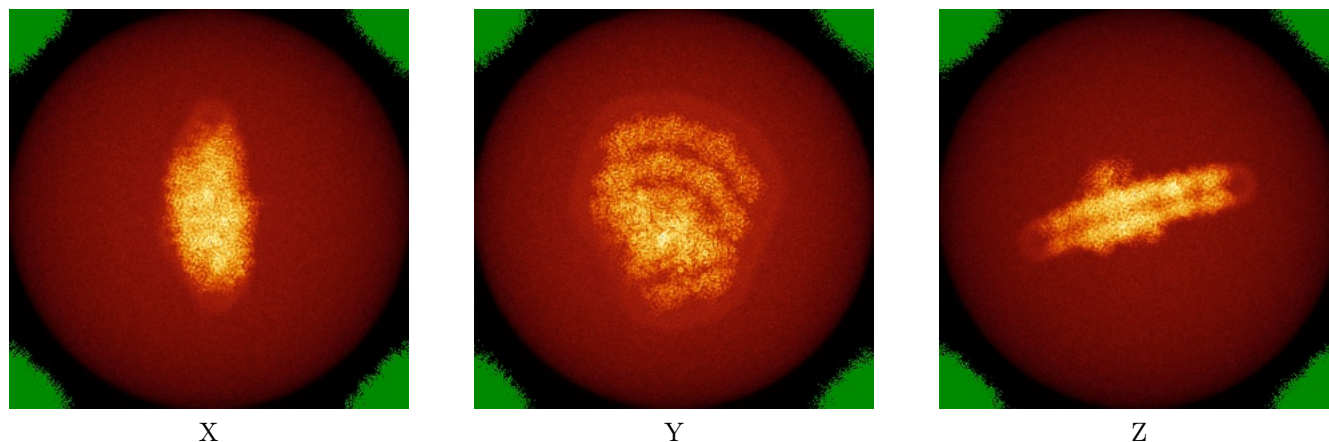


Z Index: 253

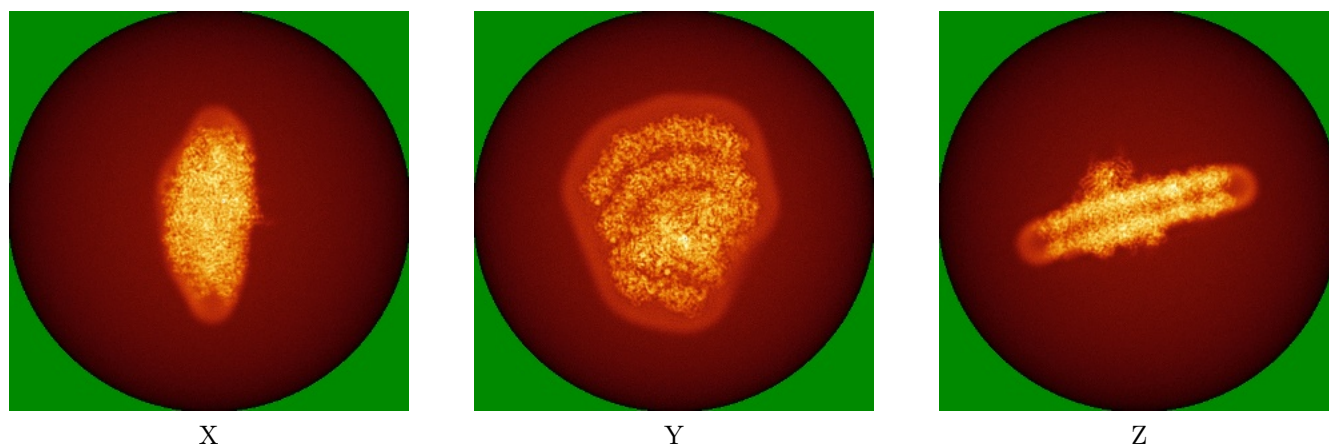
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



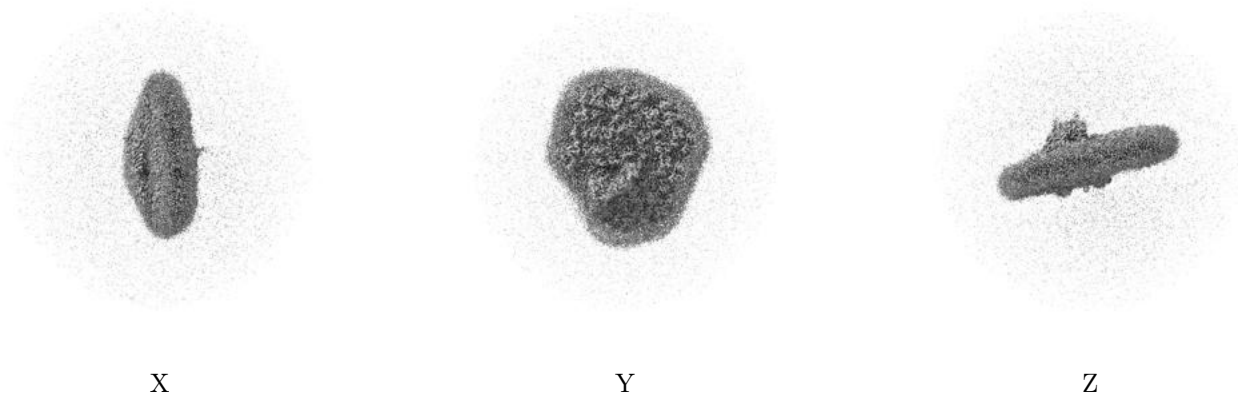
6.4.2 Raw map



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

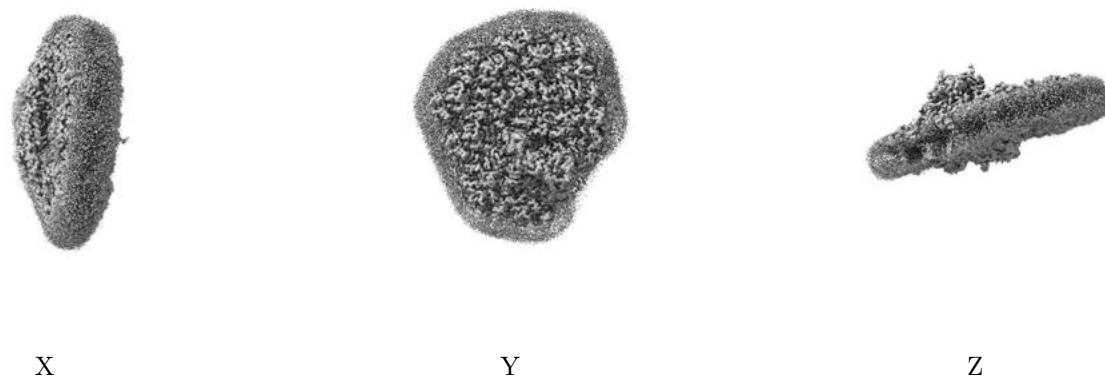
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0112. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

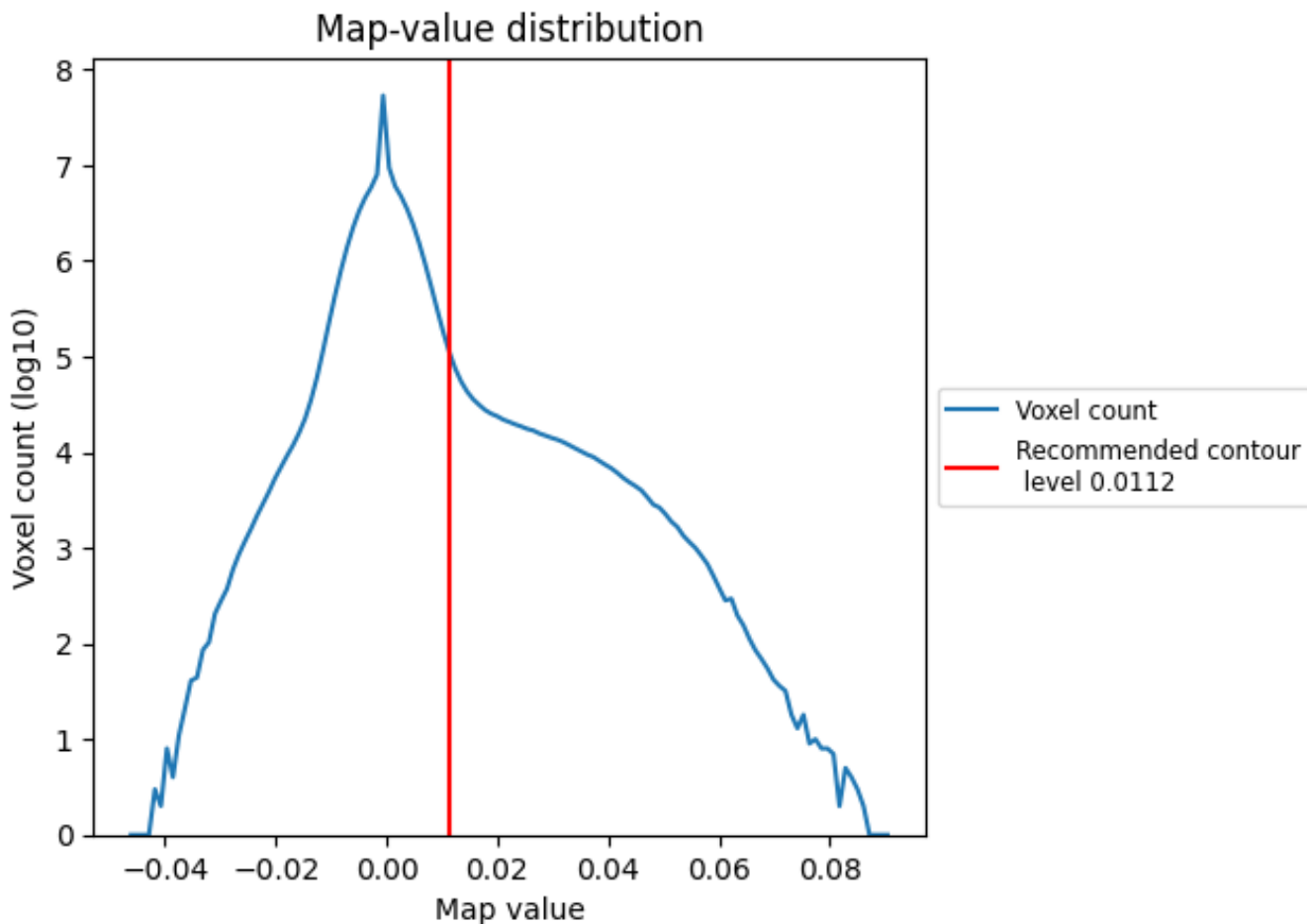
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

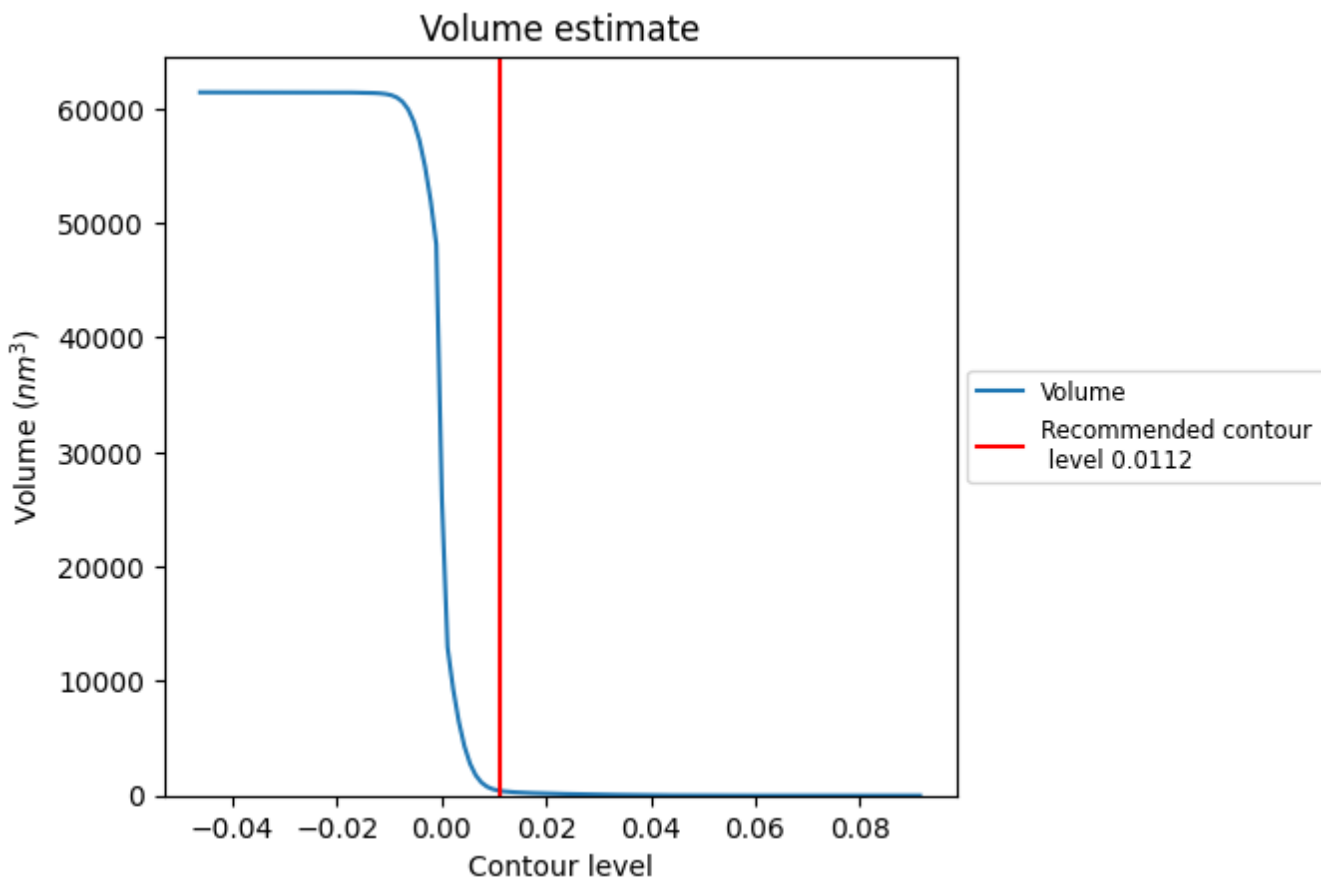
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

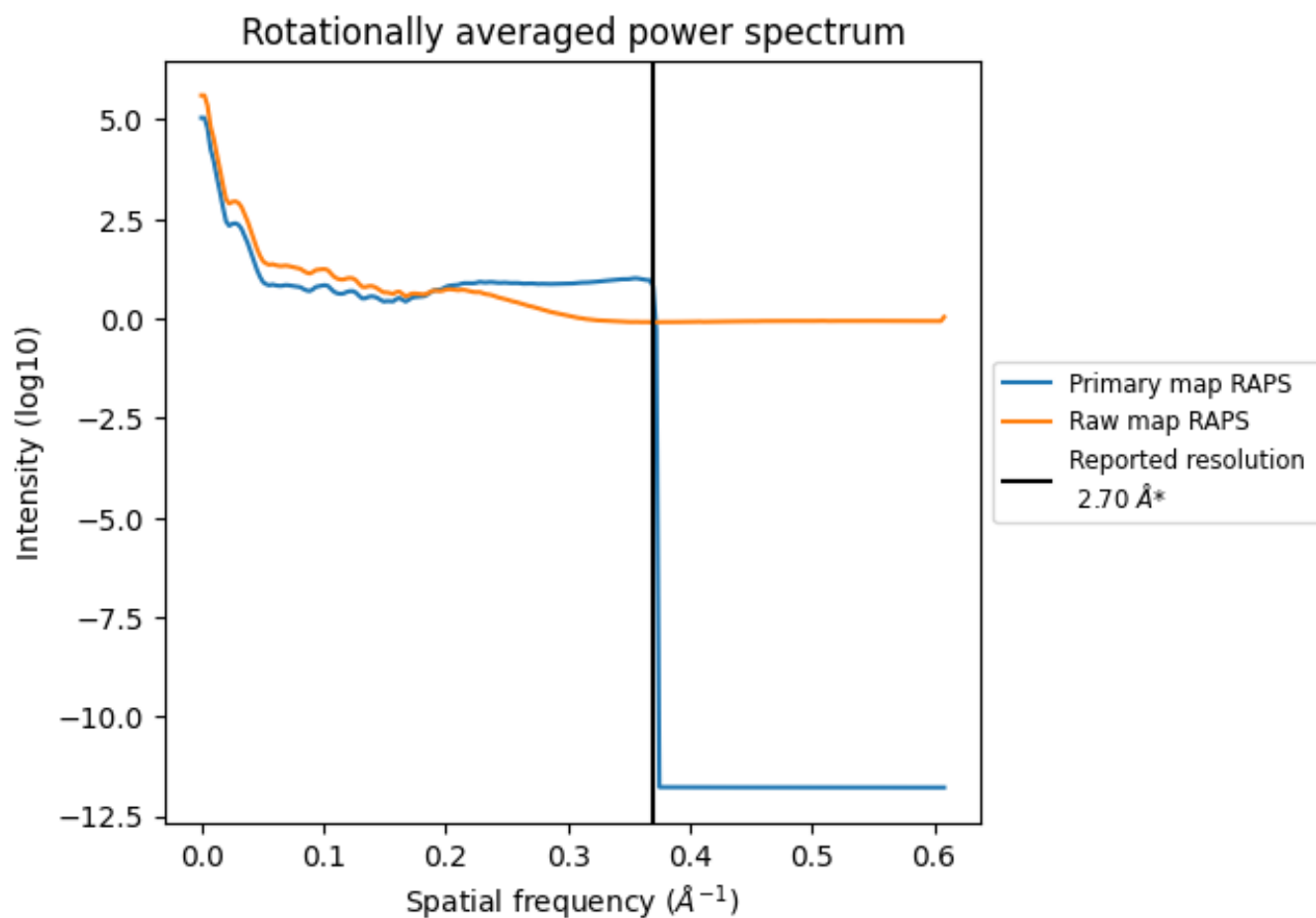
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 418 nm³; this corresponds to an approximate mass of 378 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](#)

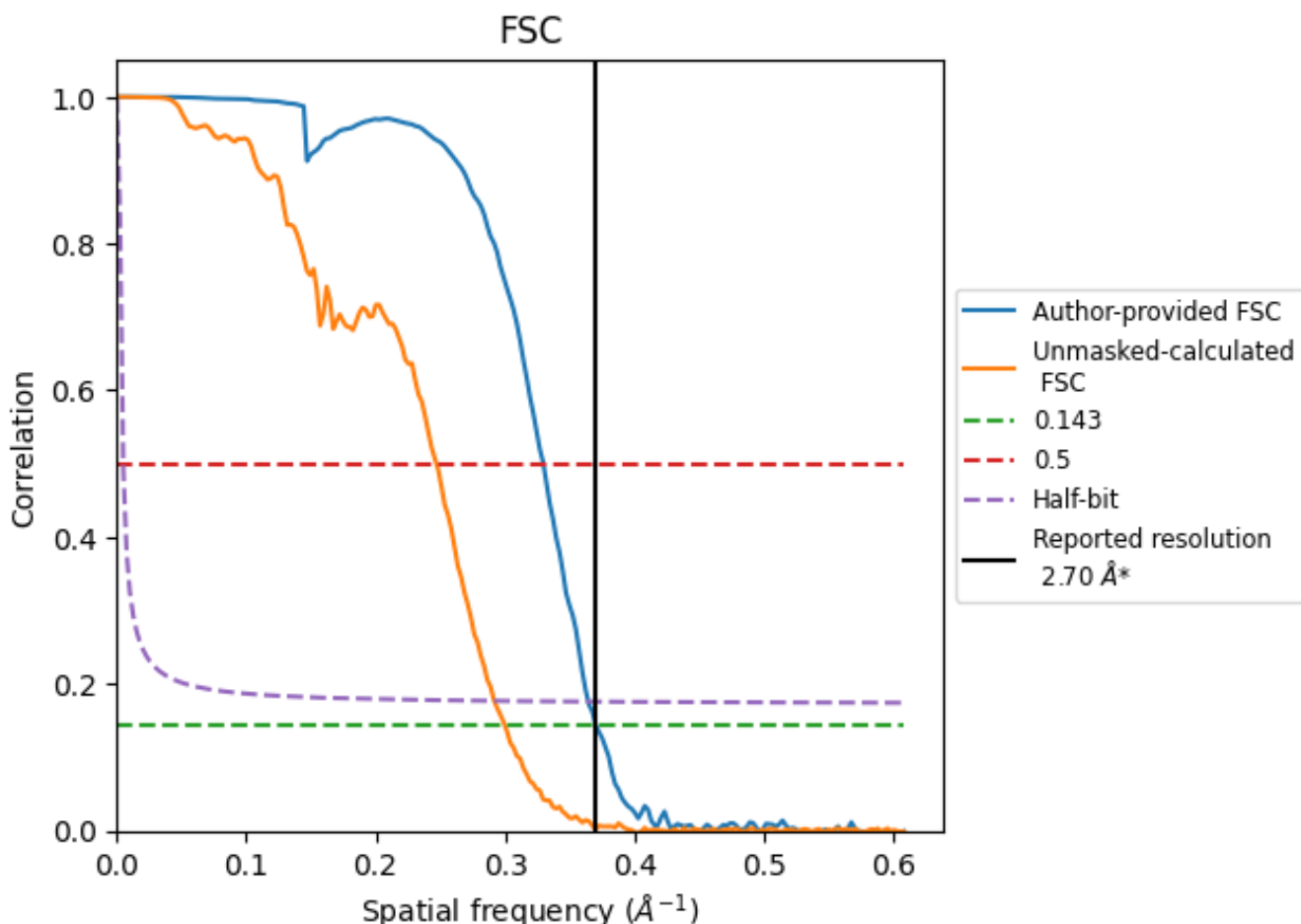


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.70	3.03	2.74
Unmasked-calculated*	3.33	4.05	3.43

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.33 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

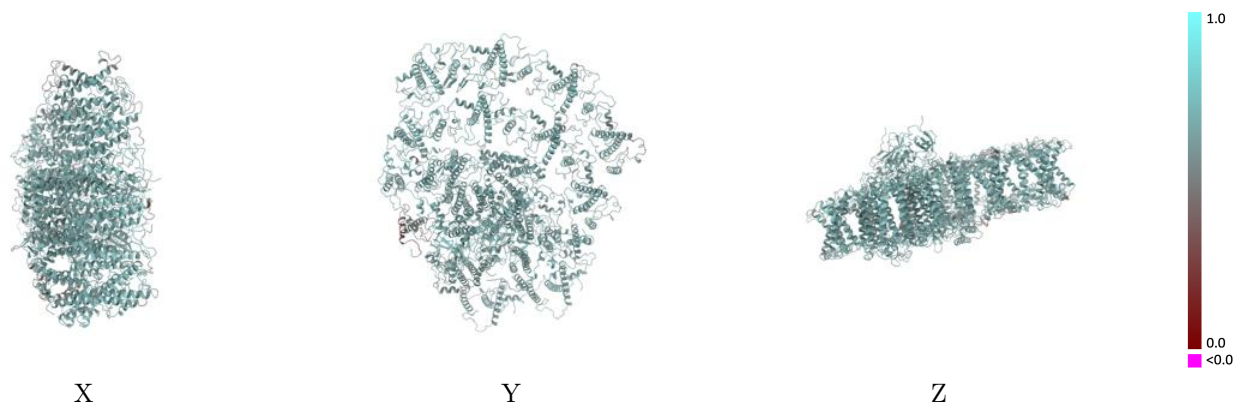
This section contains information regarding the fit between EMDB map EMD-11588 and PDB model 6ZZX. Per-residue inclusion information can be found in section 3 on page 55.

9.1 Map-model overlay [i](#)



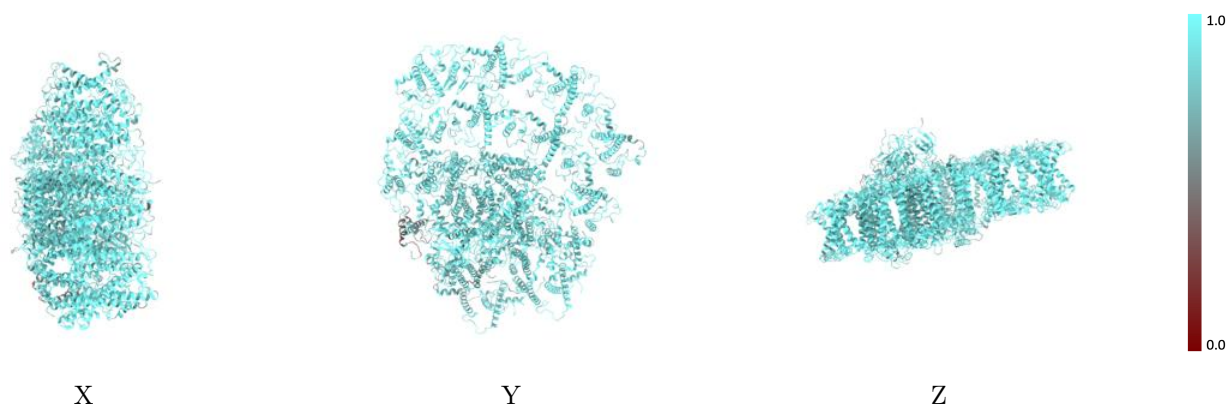
The images above show the 3D surface view of the map at the recommended contour level 0.0112 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



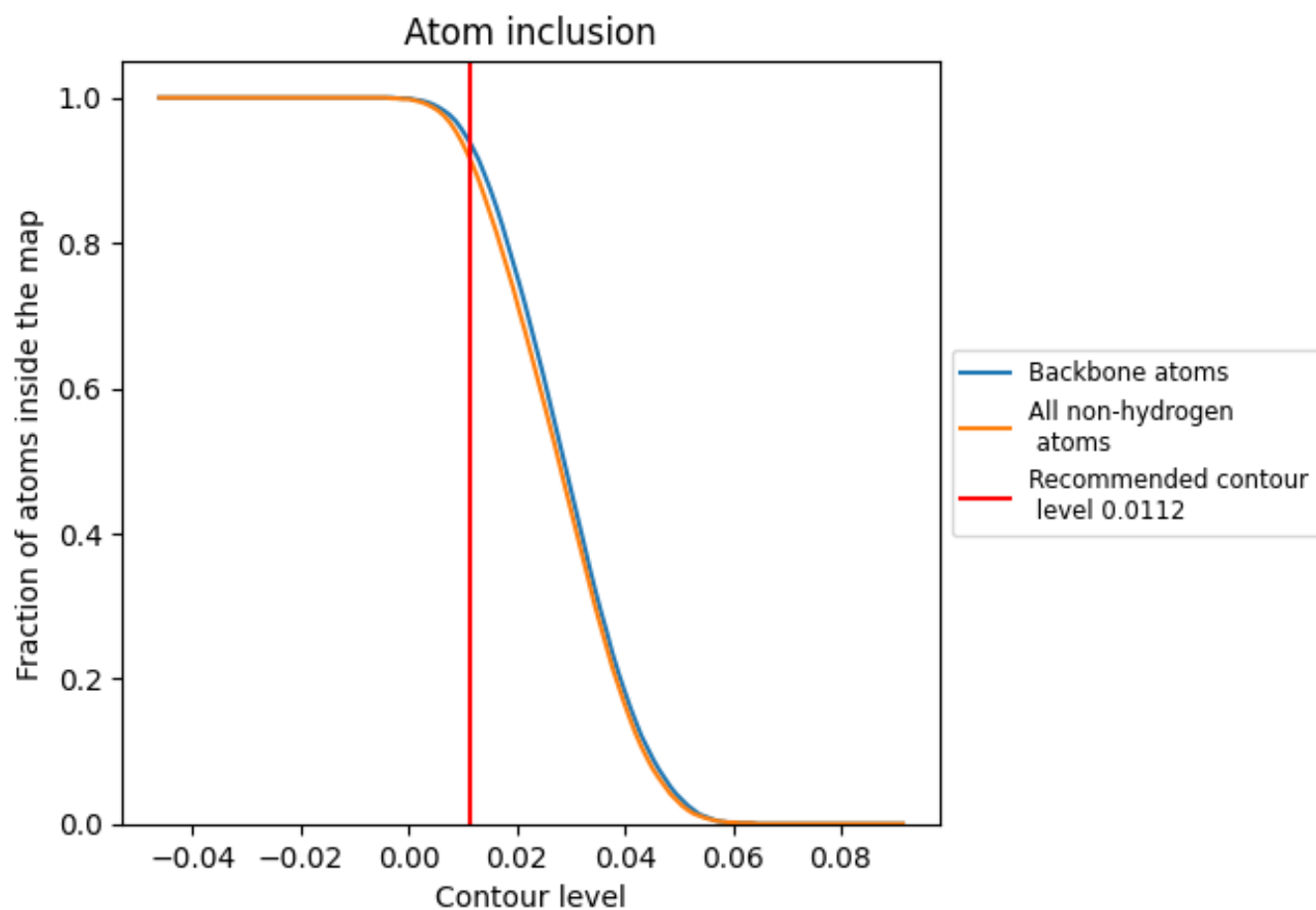
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0112).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0112) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9180	 0.6210
1	 0.9060	 0.6130
2	 0.8860	 0.6000
3	 0.9370	 0.6350
4	 0.8970	 0.5980
5	 0.9340	 0.6190
6	 0.9200	 0.6190
7	 0.9090	 0.6200
8	 0.9050	 0.6190
9	 0.9160	 0.6190
A	 0.9560	 0.6480
B	 0.9600	 0.6500
C	 0.9780	 0.6530
D	 0.9320	 0.6250
E	 0.9310	 0.6160
F	 0.9120	 0.6210
G	 0.8990	 0.6170
H	 0.7480	 0.5440
I	 0.9010	 0.6100
J	 0.9020	 0.6260
K	 0.8960	 0.6010
L	 0.8820	 0.5930
M	 0.9640	 0.6330
O	 0.5450	 0.4140
a	 0.8550	 0.5770

