



wwPDB EM Validation Summary Report ⓘ

Sep 10, 2026 – 11:36 pm BST

PDB ID : 6ZZY / pdb_00006zzy
EMDB ID : EMD-11589
Title : Structure of high-light grown Chlorella ohadii photosystem I
Authors : Caspy, I.; Nelson, N.; Nechushtai, R.; Shkolnisky, Y.; Neumann, E.
Deposited on : 2020-08-05
Resolution : 3.16 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.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

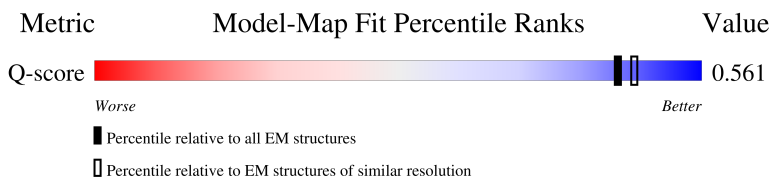
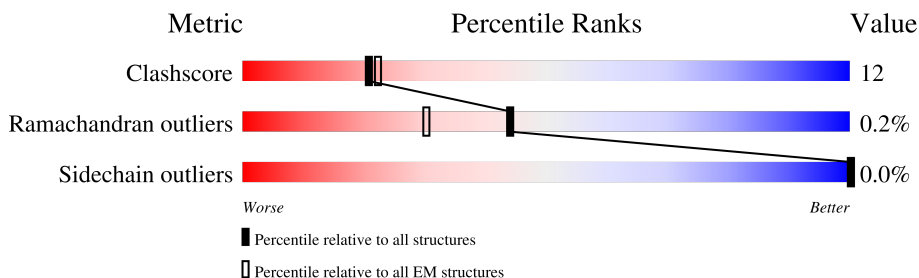
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.16 Å.

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



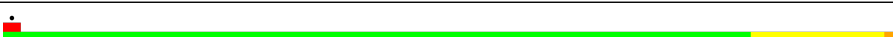
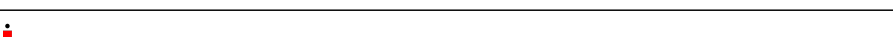
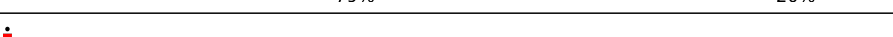
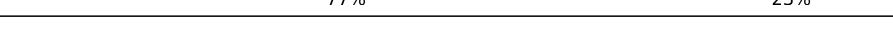
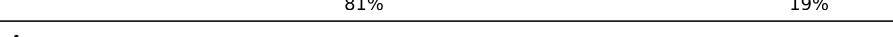
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14474 (2.66 - 3.66)

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	78% 22%
2	B	731	77% 23%
3	C	80	81% 19%
4	D	143	73% 27%

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Mol	Chain	Length	Quality of chain
5	E	64	 83%17%
6	F	165	 87%13%
7	G	99	 79%21%
8	J	41	 80%20%
9	K	86	 85%15%
10	M	31	 65%35%
11	I	35	 66%34%
12	H	94	 18%70%30%
13	L	157	 18%73%27%
14	1	192	 81%19%
14	a	192	 18%84%15%
15	3	241	 83%17%
16	4	207	 18%79%21%
17	5	227	 18%79%20%
18	6	231	 18%77%23%
19	7	221	 86%14%
20	8	219	 81%19%
21	2	215	 18%81%19%
22	9	182	 18%84%16%

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
36	ERG	G	5002	X	-	-	-
37	RRX	J	4002	X	-	-	-
40	LUT	1	503	X	-	-	-
40	LUT	6	501	X	-	-	-
40	LUT	6	502	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
40	LUT	7	501	X	-	-	-
40	LUT	9	502	X	-	-	-
41	CHL	1	609	X	-	-	-
41	CHL	4	609	X	-	-	-
41	CHL	4	618	X	-	-	-
41	CHL	5	610	X	-	-	-
41	CHL	5	613	X	-	-	-
41	CHL	6	610	X	-	-	-
41	CHL	6	619	X	-	-	-
41	CHL	7	613	X	-	-	-
41	CHL	8	601	X	-	-	-
41	CHL	8	604	X	-	-	-
41	CHL	a	606	X	-	-	-
41	CHL	a	610	X	-	-	-
41	CHL	a	613	X	-	-	-
43	QTB	3	506	X	-	-	-
43	QTB	a	504	X	-	-	-
48	XAT	7	502	X	-	-	-
49	C7Z	7	504	X	-	-	-

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 54609 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
1	A	741	Total	C	N	O	S	0	0
			5824	3815	988	1001	20		

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
3	C	80	Total	C	N	O	S	0	0
			601	367	104	119	11		

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 5 discrepancies between the modelled and reference sequences:

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

- Molecule 6 is a protein called PSI-F.

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

There are 11 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
F	432	THR	MET	variant	UNP A0A2P6TPV8
F	433	ALA	THR	variant	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	variant	UNP A0A2P6TZI8
G	1272	LEU	MET	variant	UNP A0A2P6TZI8
G	1285	ILE	VAL	variant	UNP A0A2P6TZI8
G	1313	ILE	LEU	variant	UNP A0A2P6TZI8
G	1317	SER	HIS	variant	UNP A0A2P6TZI8
G	1320	GLY	GLN	variant	UNP A0A2P6TZI8
G	1321	LEU	VAL	variant	UNP A0A2P6TZI8
G	1324	ASN	VAL	variant	UNP A0A2P6TZI8

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

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

- Molecule 9 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	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	variant	UNP A0A2P6U0J1
K	103	LEU	ILE	variant	UNP A0A2P6U0J1
K	105	CYS	VAL	variant	UNP A0A2P6U0J1
K	107	ILE	VAL	variant	UNP A0A2P6U0J1
K	108	VAL	ILE	variant	UNP A0A2P6U0J1

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Chain	Residue	Modelled	Actual	Comment	Reference
K	112	LYS	ARG	variant	UNP A0A2P6U0J1
K	113	SER	GLY	variant	UNP A0A2P6U0J1

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	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 13 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	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 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	1	192	Total	C	N	O	S	0	0
			1405	900	237	261	7		
14	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 15 is a protein called Glutathione reductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 16 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	4	207	Total	C	N	O	S	0	0
			1631	1056	277	294	4		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	37	GLU	ASP	conflict	UNP A0A2P6TQ14
4	109	ASP	ASN	conflict	UNP A0A2P6TQ14
4	112	ASN	ASP	conflict	UNP A0A2P6TQ14
4	213	GLY	SER	conflict	UNP A0A2P6TQ14
4	218	ASN	ASP	conflict	UNP A0A2P6TQ14
4	?	-	LEU	deletion	UNP A0A2P6TQ14
4	236	ASN	ARG	variant	UNP A0A2P6TQ14

- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	5	227	Total	C	N	O	S	0	0
			1769	1136	307	314	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	6	231	Total	C	N	O	S	0	0
			1787	1168	295	314	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	7	221	Total	C	N	O	S	0	0
			1698	1090	294	308	6		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7	6	VAL	ASP	conflict	UNP A0A2P6TS63
7	8	GLU	PRO	conflict	UNP A0A2P6TS63
7	17	VAL	ALA	conflict	UNP A0A2P6TS63
7	82	PHE	TYR	conflict	UNP A0A2P6TS63
7	96	ASP	SER	conflict	UNP A0A2P6TS63
7	107	MET	LEU	conflict	UNP A0A2P6TS63
7	154	TYR	PHE	conflict	UNP A0A2P6TS63
7	205	VAL	ILE	conflict	UNP A0A2P6TS63
7	209	ALA	SER	conflict	UNP A0A2P6TS63
7	218	HIS	TYR	conflict	UNP A0A2P6TS63

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	8	219	Total	C	N	O	S	0	0
			1669	1073	285	305	6		

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	2	215	Total	C	N	O	S	0	0
			1666	1074	277	309	6		

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

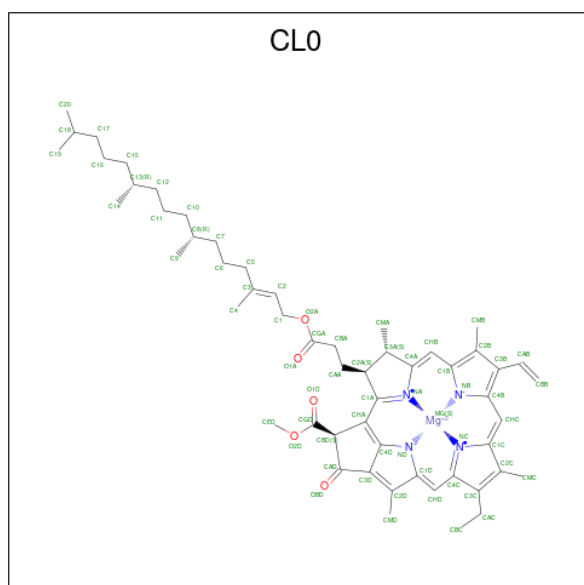
- Molecule 22 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	9	182	Total	C	N	O	S	0	0
			1397	906	231	254	6		

There is a discrepancy between the modelled and reference sequences:

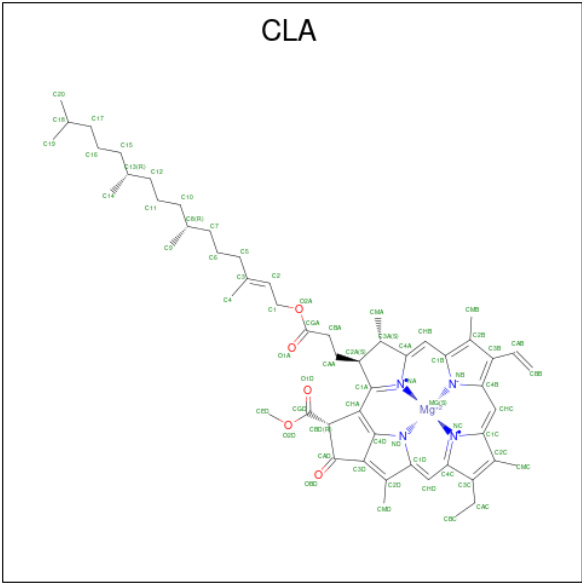
Chain	Residue	Modelled	Actual	Comment	Reference
9	257	TYR	HIS	conflict	UNP A0A2P6TMI2

- Molecule 23 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
24	A	1	Total 57	C 47	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	A	1	Total 56	C 46	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	B	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	B	1	Total 62	C 52	Mg 1	N 4	O 5	0
24	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	B	1	Total 61	C 51	Mg 1	N 4	O 5	0
24	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
24	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
24	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 53	C 43	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	F	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	F	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
24	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	K	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	K	1	Total 52	C 42	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	H	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	H	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	H	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	1	1	Total 57	C 47	Mg 1	N 4	O 5	0
24	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	a	1	Total 58	C 48	Mg 1	N 4	O 5	0
24	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	a	1	Total 57	C 47	Mg 1	N 4	O 5	0
24	a	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	3	1	Total 61	C 51	Mg 1	N 4	O 5	0
24	3	1	Total 56	C 46	Mg 1	N 4	O 5	0
24	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	4	1	Total 52	C 42	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	4	1	Total 56	C 46	Mg 1	N 4	O 5	0
24	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	4	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	4	1	Total 56	C 46	Mg 1	N 4	O 5	0
24	4	1	Total 62	C 52	Mg 1	N 4	O 5	0
24	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	5	1	Total 52	C 42	Mg 1	N 4	O 5	0
24	5	1	Total 56	C 46	Mg 1	N 4	O 5	0
24	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	5	1	Total 51	C 41	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	5	1	Total 52	C 42	Mg 1	N 4	O 5	0
24	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	6	1	Total 52	C 42	Mg 1	N 4	O 5	0
24	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	6	1	Total 52	C 42	Mg 1	N 4	O 5	0
24	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	7	1	Total 44	C 35	Mg 1	N 4	O 4	0
24	7	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	7	1	Total 44	C 34	Mg 1	N 4	O 5	0
24	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	7	1	Total 59	C 49	Mg 1	N 4	O 5	0
24	7	1	Total 42	C 34	Mg 1	N 4	O 3	0
24	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	7	1	Total 54	C 44	Mg 1	N 4	O 5	0
24	8	1	Total 52	C 42	Mg 1	N 4	O 5	0
24	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	8	1	Total 57	C 47	Mg 1	N 4	O 5	0
24	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	8	1	Total 52	C 42	Mg 1	N 4	O 5	0
24	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	8	1	Total 46	C 36	Mg 1	N 4	O 5	0

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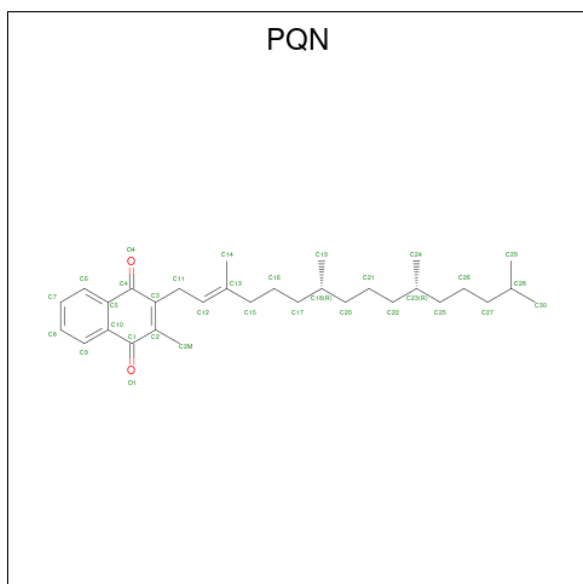
Mol	Chain	Residues	Atoms					AltConf
24	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	2	1	Total 52	C 42	Mg 1	N 4	O 5	0
24	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	2	1	Total 56	C 46	Mg 1	N 4	O 5	0
24	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
24	2	1	Total 57	C 47	Mg 1	N 4	O 5	0
24	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	9	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	9	1	Total 60	C 50	Mg 1	N 4	O 5	0

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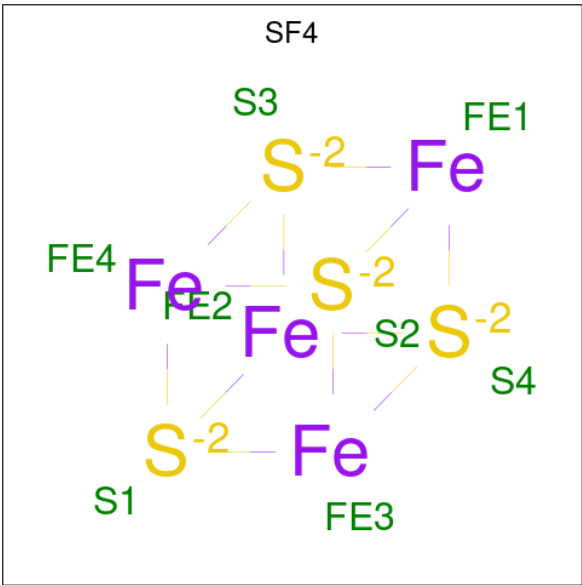
Mol	Chain	Residues	Atoms					AltConf
24	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	9	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
24	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 25 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



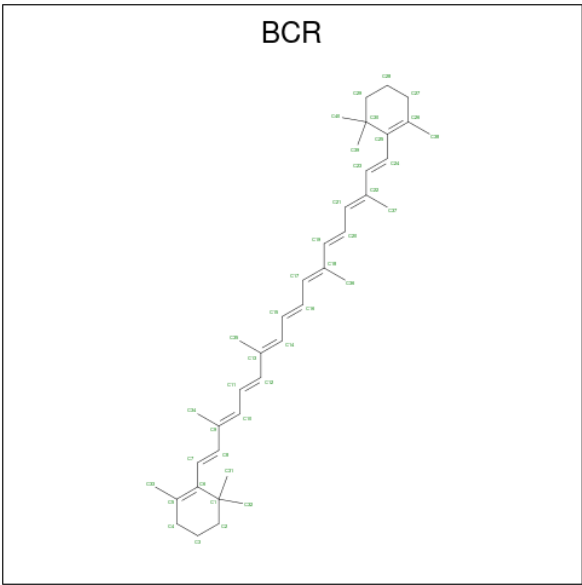
Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	C	O	0
			33	31	2	
25	B	1	Total	C	O	0
			33	31	2	

- Molecule 26 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 27 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		AltConf
27	A	1	Total	C	0
			40	40	

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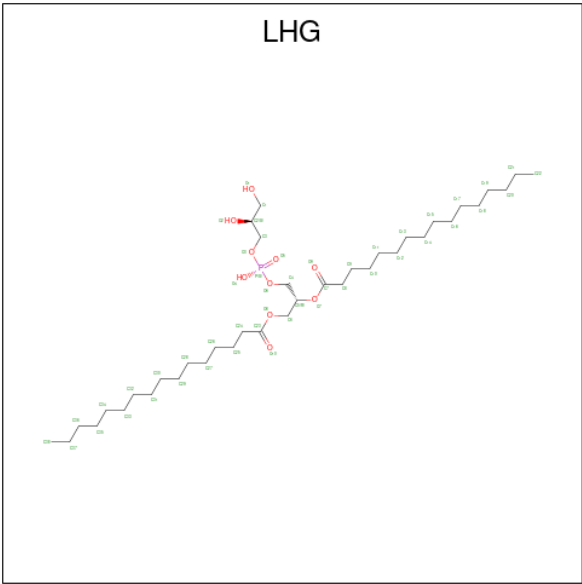
Mol	Chain	Residues	Atoms	AltConf
27	A	1	Total C 40 40	0
27	A	1	Total C 40 40	0
27	A	1	Total C 40 40	0
27	A	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	F	1	Total C 40 40	0
27	G	1	Total C 40 40	0
27	J	1	Total C 40 40	0
27	K	1	Total C 40 40	0
27	K	1	Total C 40 40	0
27	I	1	Total C 40 40	0
27	H	1	Total C 40 40	0
27	L	1	Total C 40 40	0
27	L	1	Total C 40 40	0
27	L	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms		AltConf
27	3	1	Total	C	0
			40	40	
27	3	1	Total	C	0
			40	40	
27	3	1	Total	C	0
			40	40	
27	4	1	Total	C	0
			40	40	
27	5	1	Total	C	0
			40	40	
27	5	1	Total	C	0
			40	40	
27	6	1	Total	C	0
			40	40	
27	6	1	Total	C	0
			40	40	
27	7	1	Total	C	0
			40	40	
27	8	1	Total	C	0
			40	40	

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	O	P	0
			29	18	10	1	

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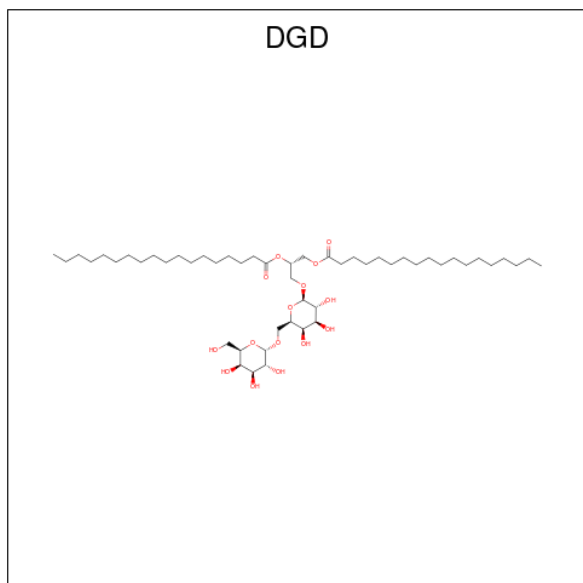
Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total 49	C 38	O 10	P 1	0
28	A	1	Total 42	C 31	O 10	P 1	0
28	B	1	Total 46	C 35	O 10	P 1	0
28	B	1	Total 49	C 38	O 10	P 1	0
28	F	1	Total 43	C 32	O 10	P 1	0
28	F	1	Total 36	C 25	O 10	P 1	0
28	1	1	Total 35	C 24	O 10	P 1	0
28	1	1	Total 42	C 31	O 10	P 1	0
28	a	1	Total 35	C 24	O 10	P 1	0
28	3	1	Total 49	C 38	O 10	P 1	0
28	4	1	Total 49	C 38	O 10	P 1	0
28	4	1	Total 32	C 21	O 10	P 1	0
28	5	1	Total 49	C 38	O 10	P 1	0
28	6	1	Total 49	C 38	O 10	P 1	0
28	6	1	Total 37	C 26	O 10	P 1	0
28	7	1	Total 49	C 38	O 10	P 1	0
28	7	1	Total 36	C 25	O 10	P 1	0
28	7	1	Total 43	C 32	O 10	P 1	0
28	8	1	Total 37	C 26	O 10	P 1	0
28	2	1	Total 49	C 38	O 10	P 1	0
28	2	1	Total 49	C 38	O 10	P 1	0

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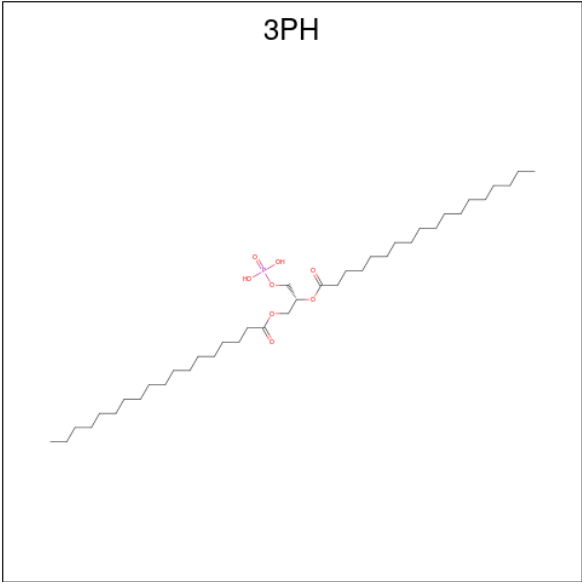
Mol	Chain	Residues	Atoms				AltConf
28	9	1	Total	C	O	P	0
			33	22	10	1	
28	9	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



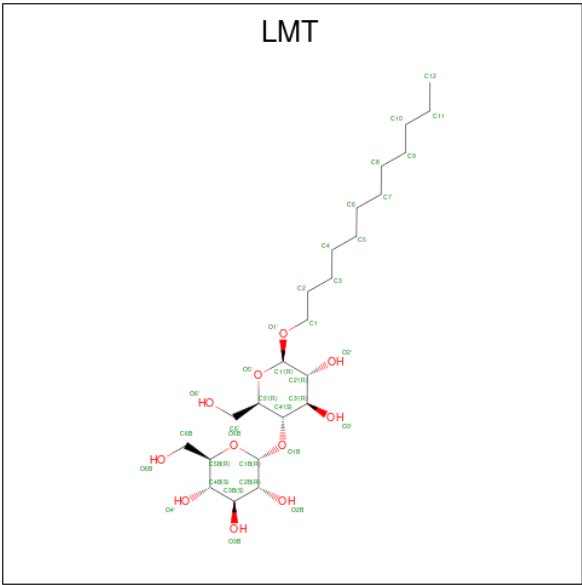
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			51	36	15	
29	B	1	Total	C	O	0
			66	51	15	
29	8	1	Total	C	O	0
			66	51	15	

- Molecule 30 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).



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

- Molecule 31 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



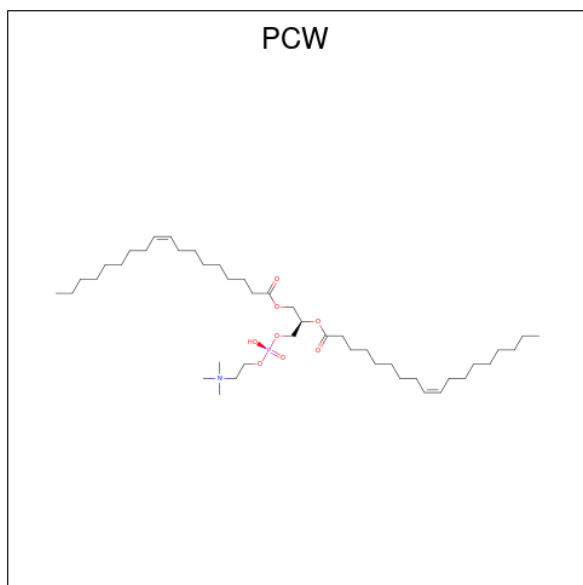
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
31	A	1	35	24	11	0
31	B	1	35	24	11	0
31	1	1	35	24	11	0

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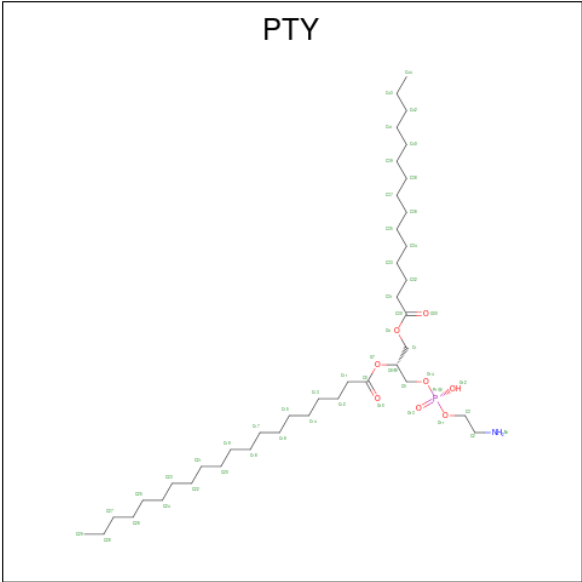
Mol	Chain	Residues	Atoms			AltConf
31	2	1	Total	C	O	0
			35	24	11	

- Molecule 32 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: $C_{44}H_{85}NO_8P$).



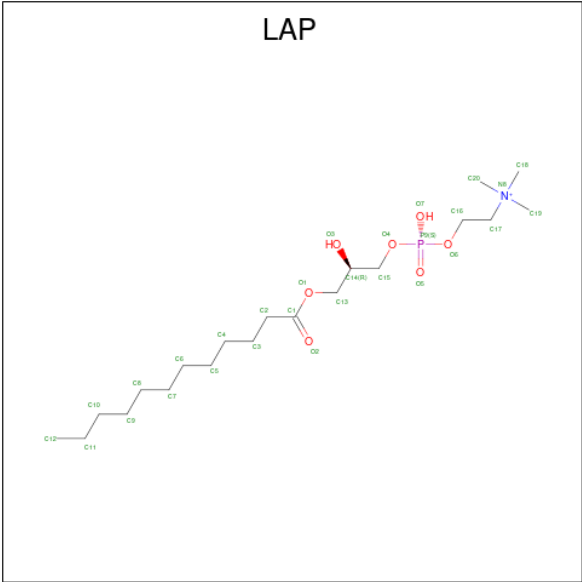
Mol	Chain	Residues	Atoms					AltConf
32	B	1	Total	C	N	O	P	0
			30	20	1	8	1	
32	6	1	Total	C	N	O	P	0
			36	26	1	8	1	

- Molecule 33 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$).



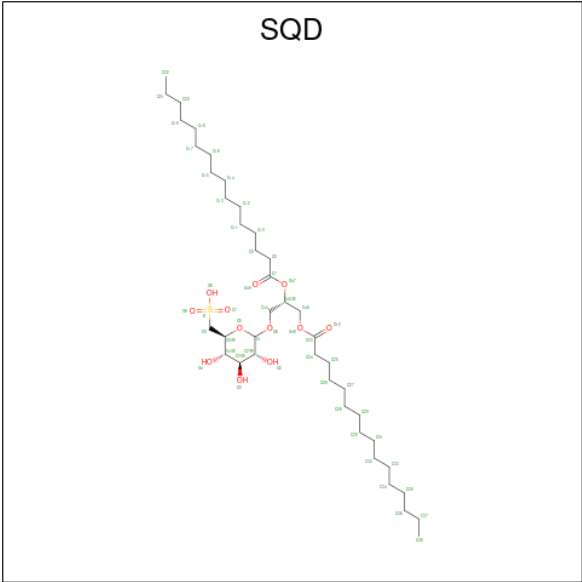
Mol	Chain	Residues	Atoms					AltConf
33	B	1	Total	C	N	O	P	0
			41	31	1	8	1	
33	3	1	Total	C	N	O	P	0
			38	28	1	8	1	
33	5	1	Total	C	N	O	P	0
			38	28	1	8	1	
33	7	1	Total	C	N	O	P	0
			33	23	1	8	1	
33	8	1	Total	C	N	O	P	0
			35	25	1	8	1	
33	9	1	Total	C	N	O	P	0
			48	38	1	8	1	

- Molecule 34 is [2-(((1-oxododecanoxy)-(2-hydroxy-3-propanyl))-phosphonate-oxy)-ethyl]-trimethylammonium (CCD ID: LAP) (formula: C₂₀H₄₃NO₇P).



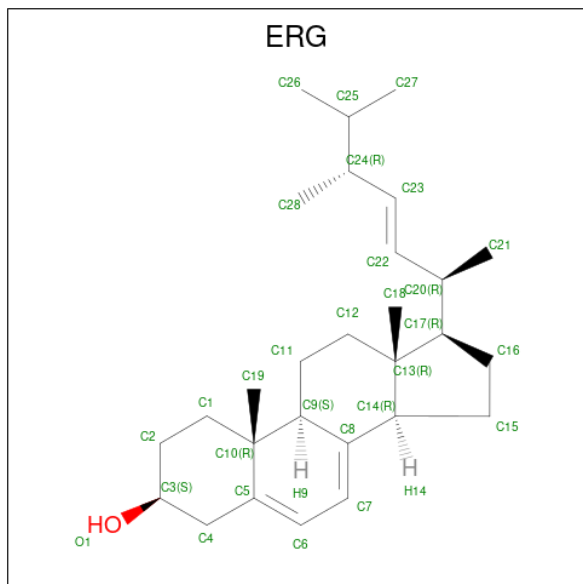
Mol	Chain	Residues	Atoms					AltConf
34	B	1	Total	C	N	O	P	0
			29	20	1	7	1	
34	F	1	Total	C	N	O	P	0
			29	20	1	7	1	
34	K	1	Total	C	N	O	P	0
			29	20	1	7	1	

- Molecule 35 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



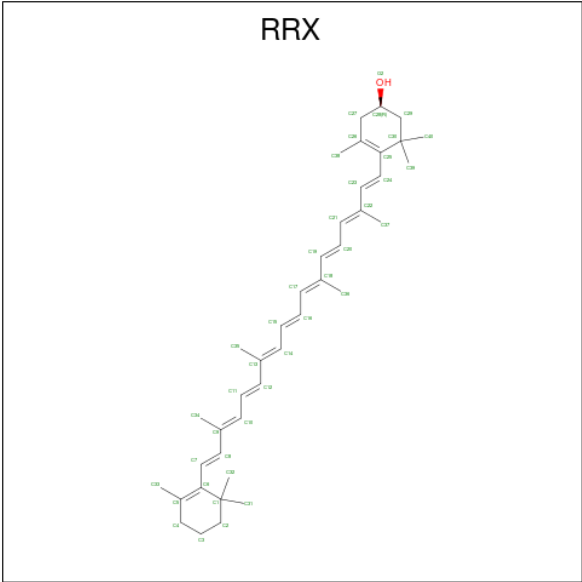
Mol	Chain	Residues	Atoms				AltConf
35	G	1	Total	C	O	S	0
			46	33	12	1	
35	H	1	Total	C	O	S	0
			45	32	12	1	
35	7	1	Total	C	O	S	0
			39	26	12	1	

- Molecule 36 is ERGOSTEROL (CCD ID: ERG) (formula: $C_{28}H_{44}O$).



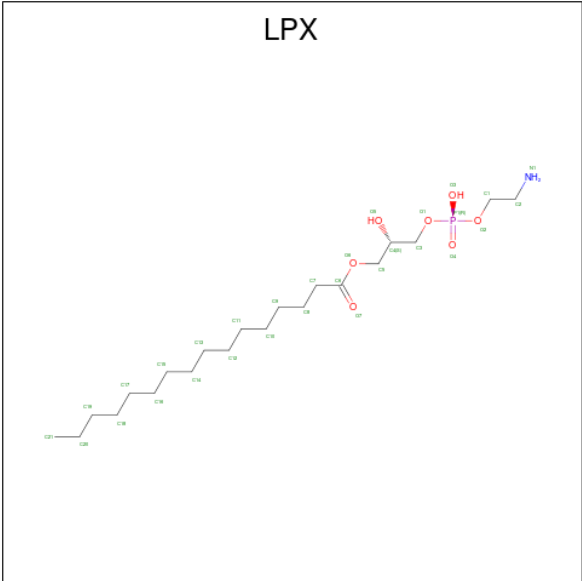
Mol	Chain	Residues	Atoms			AltConf
36	G	1	Total	C	O	0
			29	28	1	

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



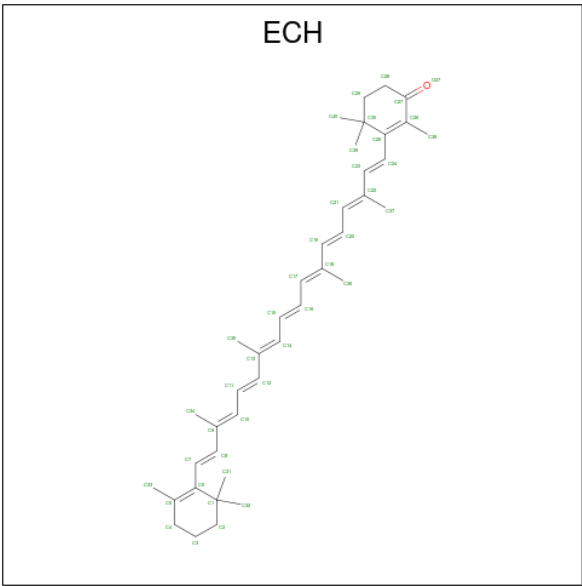
Mol	Chain	Residues	Atoms			AltConf
37	J	1	Total	C	O	0
			41	40	1	

- Molecule 38 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (CCD ID: LPX) (formula: C₂₁H₄₄NO₇P).



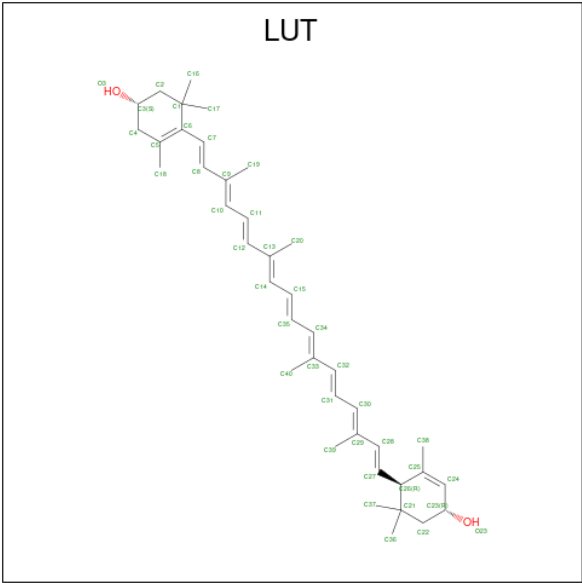
Mol	Chain	Residues	Atoms					AltConf
38	J	1	Total	C	N	O	P	0
			17	8	1	7	1	
38	a	1	Total	C	N	O	P	0
			30	21	1	7	1	

- Molecule 39 is beta,beta-caroten-4-one (CCD ID: ECH) (formula: C₄₀H₅₄O).



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

- Molecule 40 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



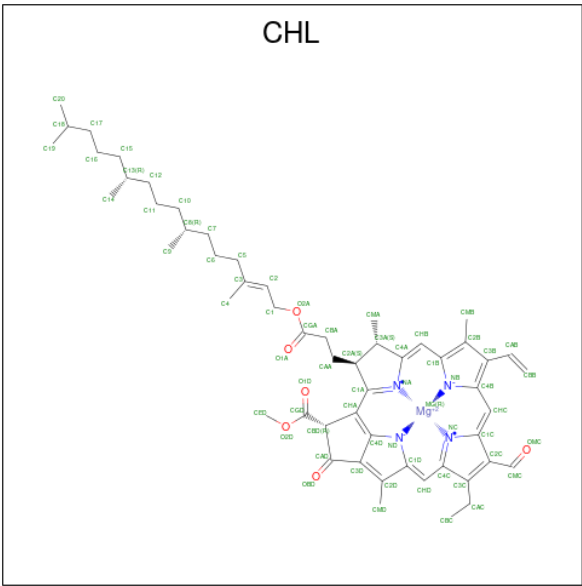
Mol	Chain	Residues	Atoms			AltConf
40	1	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
40	1	1	Total	C	O	0
			42	40	2	
40	1	1	Total	C	O	0
			42	40	2	
40	a	1	Total	C	O	0
			42	40	2	
40	a	1	Total	C	O	0
			42	40	2	
40	a	1	Total	C	O	0
			42	40	2	
40	3	1	Total	C	O	0
			42	40	2	
40	3	1	Total	C	O	0
			42	40	2	
40	4	1	Total	C	O	0
			42	40	2	
40	4	1	Total	C	O	0
			42	40	2	
40	5	1	Total	C	O	0
			42	40	2	
40	5	1	Total	C	O	0
			42	40	2	
40	5	1	Total	C	O	0
			42	40	2	
40	6	1	Total	C	O	0
			42	40	2	
40	6	1	Total	C	O	0
			42	40	2	
40	7	1	Total	C	O	0
			42	40	2	
40	8	1	Total	C	O	0
			42	40	2	
40	8	1	Total	C	O	0
			42	40	2	
40	2	1	Total	C	O	0
			42	40	2	
40	2	1	Total	C	O	0
			42	40	2	
40	9	1	Total	C	O	0
			42	40	2	
40	9	1	Total	C	O	0
			42	40	2	

- Molecule 41 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆).



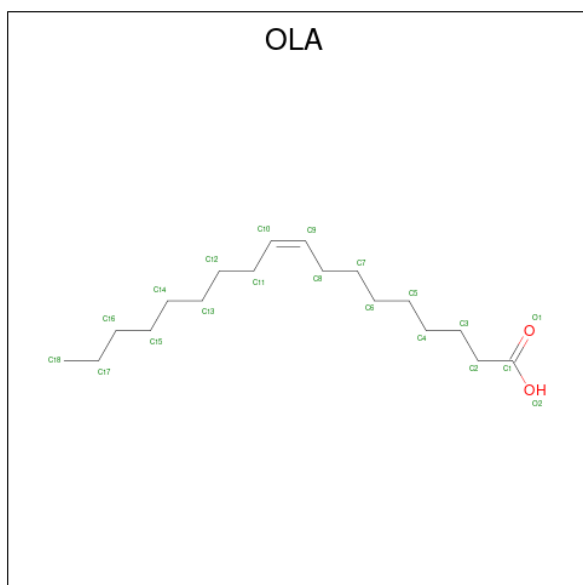
Mol	Chain	Residues	Atoms					AltConf
41	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
41	1	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
41	a	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
41	a	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
41	a	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
41	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
41	3	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
41	3	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
41	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
41	4	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
41	4	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
41	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
41	5	1	Total	C	Mg	N	O	0
			51	40	1	4	6	

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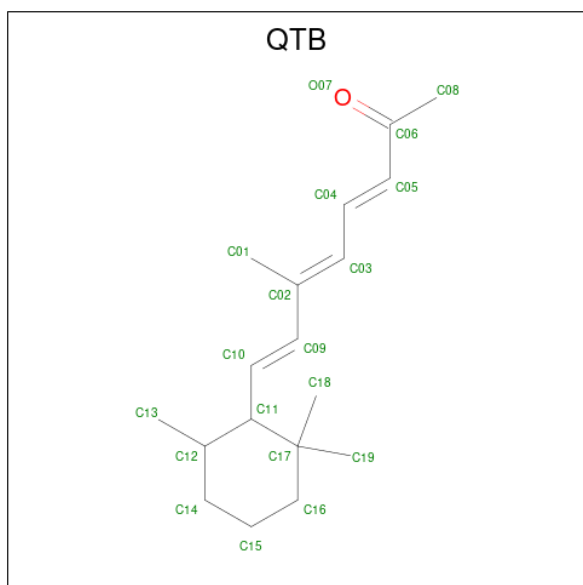
Mol	Chain	Residues	Atoms					AltConf
41	5	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
41	6	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
41	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
41	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
41	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
41	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
41	8	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
41	8	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
41	8	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
41	9	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
41	9	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

- Molecule 42 is OLEIC ACID (CCD ID: OLA) (formula: C₁₈H₃₄O₂).



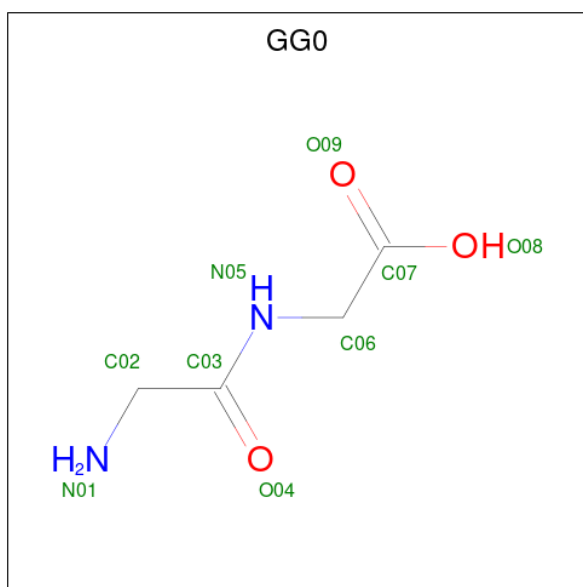
Mol	Chain	Residues	Atoms			AltConf
42	1	1	Total	C	O	0
			20	18	2	
42	8	1	Total	C	O	0
			20	18	2	

- Molecule 43 is (3 {E},5 {E},7 {E})-6-methyl-8-[(6 {R})-2,2,6-trimethylcyclohexyl]octa-3,5,7-trien-2-one (CCD ID: QTB) (formula: C₁₈H₂₈O).



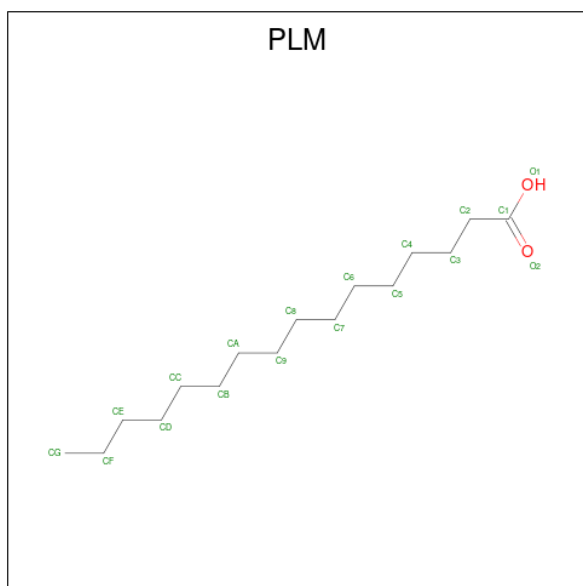
Mol	Chain	Residues	Atoms			AltConf
43	a	1	Total	C	O	0
			19	18	1	
43	3	1	Total	C	O	0
			19	18	1	

- Molecule 44 is 2-(2-azanylethanoylamino)ethanoic acid (CCD ID: GG0) (formula: C₄H₈N₂O₃).



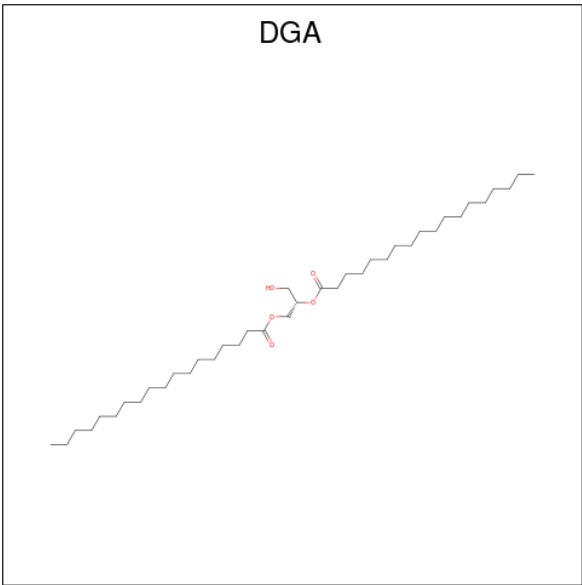
Mol	Chain	Residues	Atoms				AltConf
44	a	1	Total	C	N	O	0
			9	4	2	3	

- Molecule 45 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



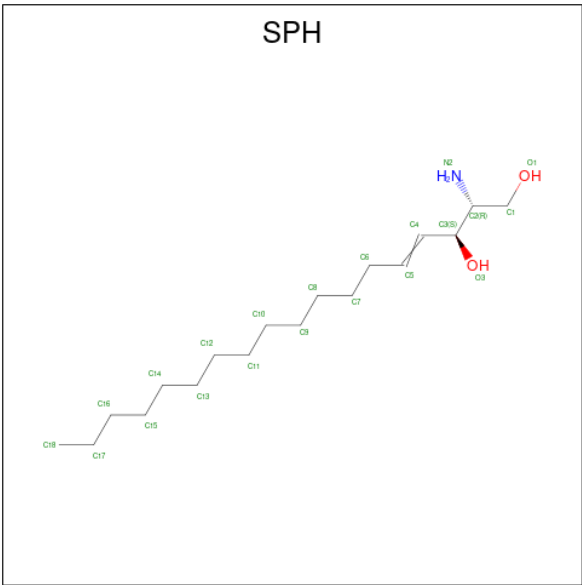
Mol	Chain	Residues	Atoms			AltConf
45	4	1	Total	C	O	0
			17	16	1	
45	6	1	Total	C	O	0
			18	16	2	

- Molecule 46 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$).



Mol	Chain	Residues	Atoms			AltConf
46	5	1	Total	C	O	0
			23	18	5	
46	8	1	Total	C	O	0
			30	25	5	

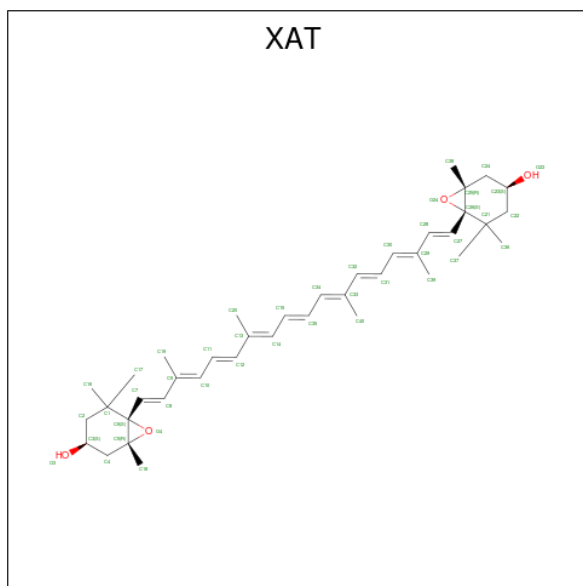
- Molecule 47 is SPHINGOSINE (CCD ID: SPH) (formula: C₁₈H₃₇NO₂).



Mol	Chain	Residues	Atoms				AltConf
47	6	1	Total	C	N	O	0
			21	18	1	2	

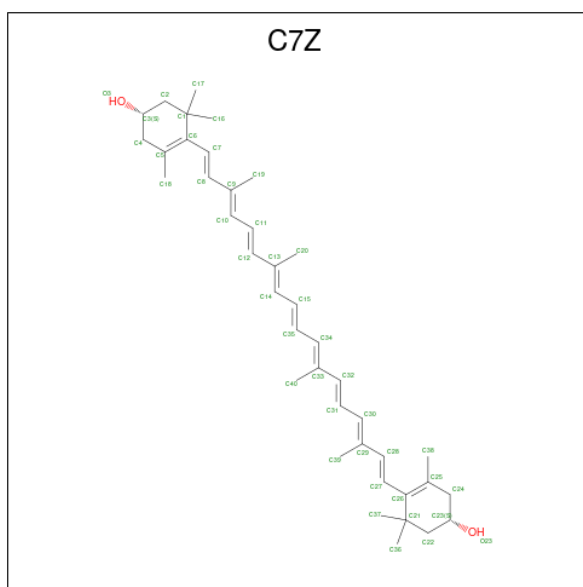
- Molecule 48 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA

,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$).



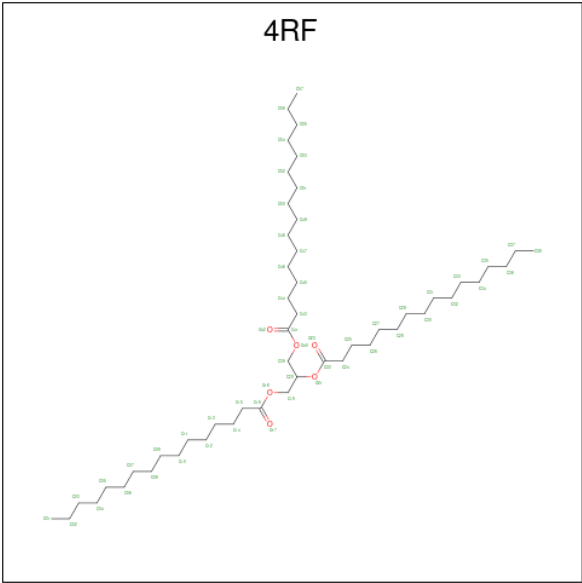
Mol	Chain	Residues	Atoms		AltConf
48	7	1	Total	C	O
			44	40	4
					0

- Molecule 49 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (CCD ID: C7Z) (formula: $C_{40}H_{56}O_2$).



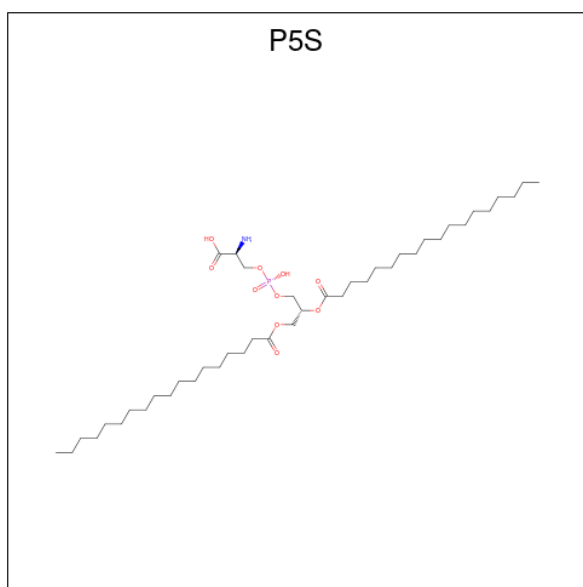
Mol	Chain	Residues	Atoms			AltConf
49	7	1	Total	C	O	0
			42	40	2	

- Molecule 50 is Tripalmitoylglycerol (CCD ID: 4RF) (formula: C₅₁H₉₈O₆).



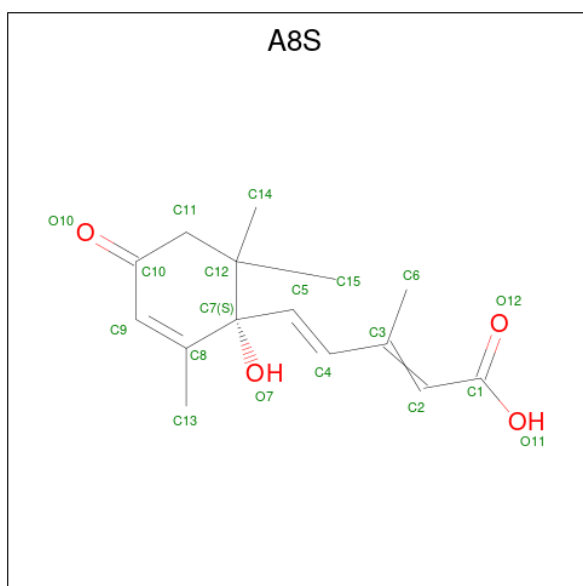
Mol	Chain	Residues	Atoms			AltConf
50	7	1	Total	C	O	0
			32	26	6	
50	8	1	Total	C	O	0
			42	36	6	
50	8	1	Total	C	O	0
			54	48	6	

- Molecule 51 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (CCD ID: P5S) (formula: C₄₂H₈₂NO₁₀P).



Mol	Chain	Residues	Atoms					AltConf
51	8	1	Total	C	N	O	P	0
			37	25	1	10	1	

- Molecule 52 is (2Z,4E)-5-[(1S)-1-hydroxy-2,6,6-trimethyl-4-oxocyclohex-2-en-1-yl]-3-methyl penta-2,4-dienoic acid (CCD ID: A8S) (formula: $C_{15}H_{20}O_4$).

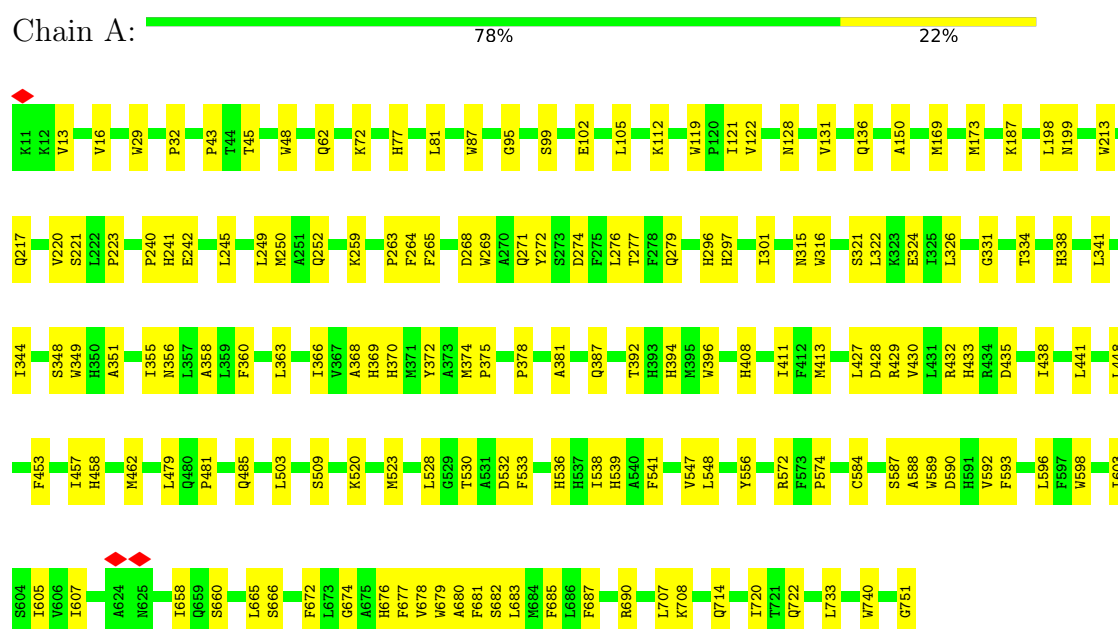


Mol	Chain	Residues	Atoms			AltConf
52	9	1	Total	C	O	0
			19	15	4	

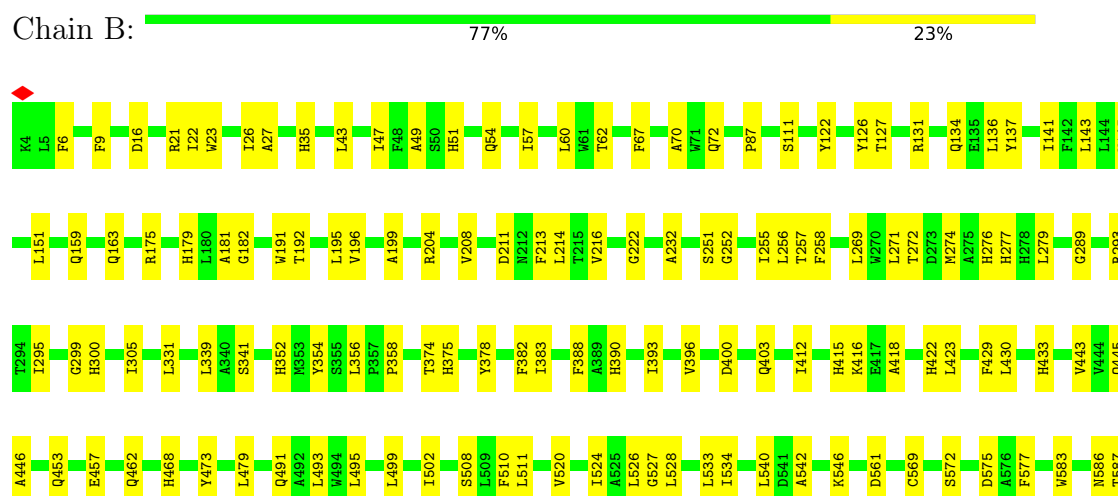
3 Residue-property plots

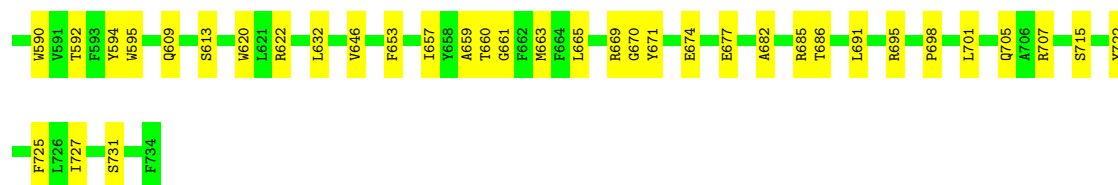
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2





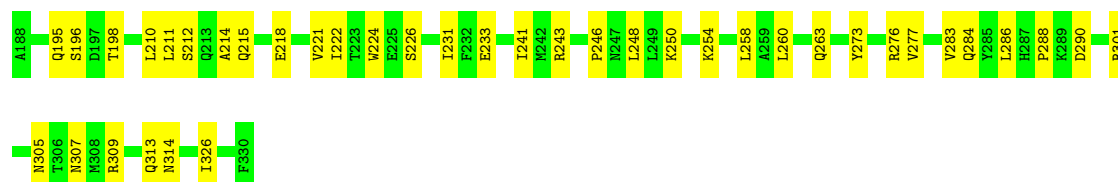
• Molecule 3: Photosystem I iron-sulfur center

Chain C: 81% 19%



• Molecule 4: Photosystem I reaction center subunit chloroplastic

Chain D: 73% 27%



• Molecule 5: Photosystem I reaction center subunit IV

Chain E: 83% 17%



• Molecule 6: PSI-F

Chain F: 87% 13%



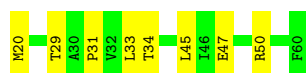
• Molecule 7: Photosystem I reaction center subunit chloroplastic

Chain G: 79% 21%



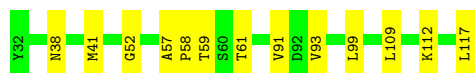
• Molecule 8: Photosystem I reaction center subunit IX

Chain J: 80% 20%



- Molecule 9: PSI-K

Chain K: 85% 15%



- Molecule 10: Photosystem I reaction center subunit XII

Chain M: 65% 35%



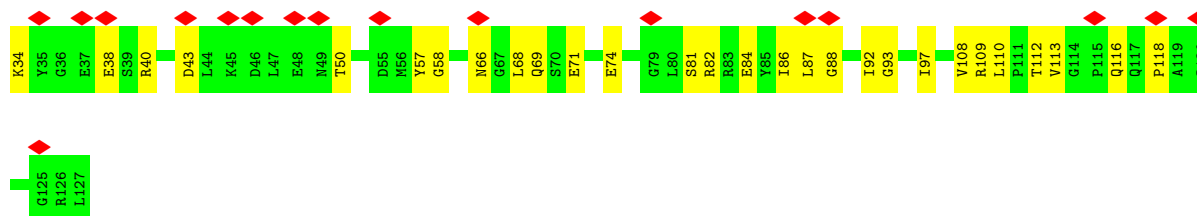
- Molecule 11: Photosystem I reaction center subunit VIII

Chain I: 66% 34%



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

Chain H: 18% 70% 30%



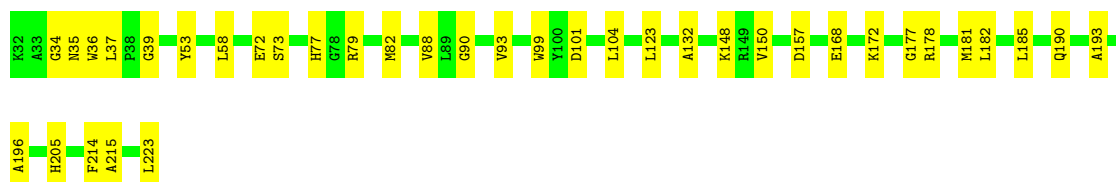
- Molecule 13: PSI subunit V

Chain L: 73% 27%



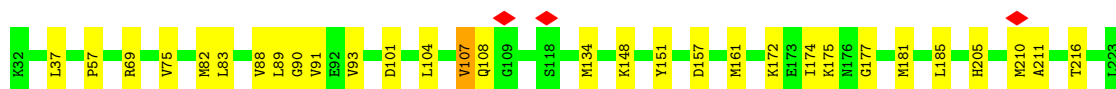
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain 1: 81% 19%



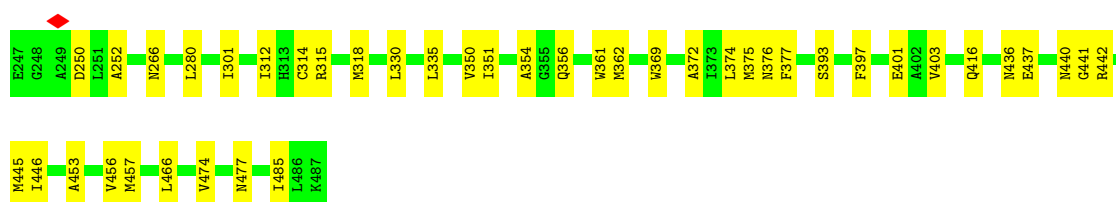
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain a: 84% 15%



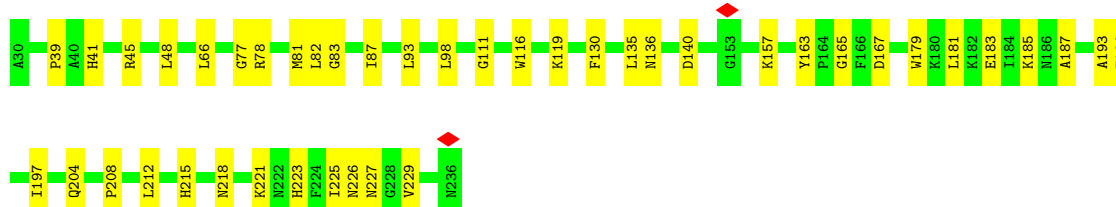
- Molecule 15: Glutathione reductase

Chain 3: 83% 17%



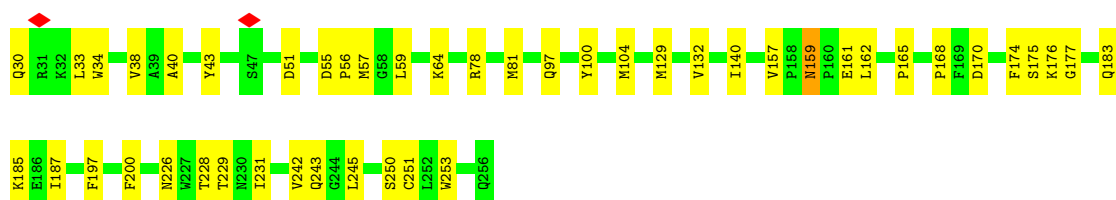
- Molecule 16: Chlorophyll a-b binding protein, chloroplastic

Chain 4: 79% 21%



- Molecule 17: Chlorophyll a-b binding protein, chloroplastic

Chain 5: 79% 20%



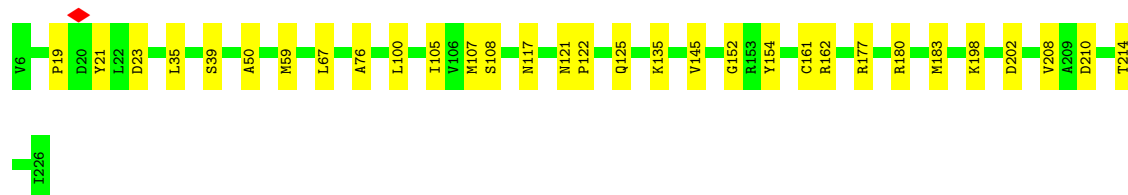
- Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 6: 77% 23%



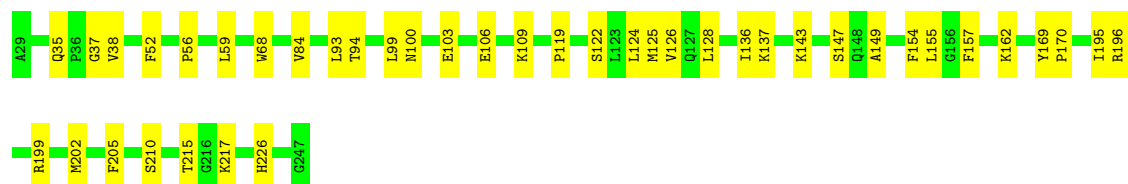
- Molecule 19: Chlorophyll a-b binding protein, chloroplastic

Chain 7: 86% 14%



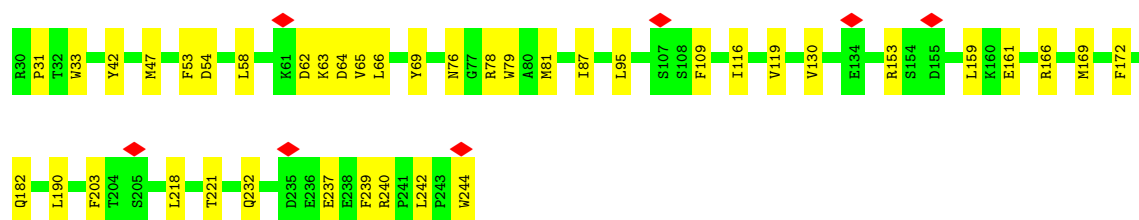
- Molecule 20: Chlorophyll a-b binding protein, chloroplastic

Chain 8: 81% 19%



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

Chain 2: 81% 19%



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

Chain 9: 84% 16%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	75049	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 ($e^-/\text{\AA}^2$)	46.04	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.082	Depositor
Minimum map value	-0.041	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.007	Depositor
Map size ($\text{\AA}$)	414.72, 414.72, 414.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.81, 0.81, 0.81	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCR, LHG, 4RF, ERG, LPX, DGD, LUT, CHL, XAT, PTY, GG0, OLA, LMT, P5S, SQD, PQN, PLM, RRX, CL0, SF4, SPH, QTB, PCW, DGA, A8S, CLA, LAP, 3PH, C7Z, ECH

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	0.15	0/6022	0.35	0/8215
2	B	0.17	0/6006	0.35	0/8205
3	C	0.11	0/611	0.34	0/828
4	D	0.14	0/1150	0.36	0/1551
5	E	0.12	0/520	0.34	0/705
6	F	0.15	0/1309	0.33	0/1771
7	G	0.16	0/743	0.42	0/1007
8	J	0.15	0/322	0.39	0/439
9	K	0.14	0/622	0.35	0/844
10	M	0.16	0/244	0.32	0/330
11	I	0.19	0/276	0.41	0/373
12	H	0.16	0/744	0.43	0/1000
13	L	0.16	0/1195	0.41	0/1635
14	1	0.18	0/1443	0.41	0/1960
14	a	0.19	0/1443	0.49	0/1960
15	3	0.17	0/1896	0.40	0/2573
16	4	0.16	0/1681	0.43	2/2285 (0.1%)
17	5	0.16	0/1825	0.38	0/2483
18	6	0.17	0/1845	0.37	0/2515
19	7	0.14	0/1748	0.34	0/2372
20	8	0.15	0/1717	0.33	0/2330
21	2	0.18	0/1708	0.44	0/2318
22	9	0.19	0/1435	0.46	1/1946 (0.1%)
All	All	0.16	0/36505	0.38	3/49645 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	9	355	LEU	CB-CA-C	-5.41	110.32	116.54
16	4	218	ASN	CA-C-N	5.21	139.49	127.00
16	4	218	ASN	C-N-CA	5.21	139.49	127.00

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	125	0
2	B	5796	0	5576	148	0
3	C	601	0	576	16	0
4	D	1124	0	1129	27	0
5	E	509	0	507	8	0
6	F	1277	0	1296	20	0
7	G	727	0	724	20	0
8	J	316	0	332	8	0
9	K	613	0	639	11	0
10	M	239	0	255	14	0
11	I	270	0	287	14	0
12	H	729	0	705	26	0
13	L	1165	0	1181	37	0
14	1	1405	0	1370	29	0
14	a	1405	0	1370	27	0
15	3	1844	0	1805	33	0
16	4	1631	0	1575	40	0
17	5	1769	0	1719	39	0
18	6	1787	0	1762	42	0
19	7	1698	0	1640	28	0
20	8	1669	0	1619	40	0
21	2	1666	0	1657	34	0
22	9	1397	0	1374	26	0
23	A	65	0	72	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	1	693	0	673	39	0
24	2	724	0	608	38	0
24	3	719	0	724	32	0
24	4	768	0	683	32	0
24	5	739	0	635	23	0
24	6	711	0	648	32	0
24	7	778	0	716	35	0
24	8	699	0	619	25	0
24	9	549	0	499	25	0
24	A	2621	0	2693	157	0
24	B	2583	0	2673	153	0
24	F	105	0	87	6	0
24	G	141	0	104	3	0
24	H	156	0	129	8	0
24	J	42	0	30	1	0
24	K	204	0	165	7	0
24	L	155	0	130	5	0
24	a	571	0	538	25	0
25	A	33	0	46	5	0
25	B	33	0	46	7	0
26	A	8	0	0	0	0
26	C	16	0	0	1	0
27	3	120	0	159	10	0
27	4	40	0	51	1	0
27	5	80	0	106	6	0
27	6	80	0	105	4	0
27	7	40	0	52	2	0
27	8	40	0	53	1	0
27	A	200	0	264	26	0
27	B	280	0	369	29	0
27	F	40	0	53	7	0
27	G	40	0	53	3	0
27	H	40	0	52	2	0
27	I	40	0	53	6	0
27	J	40	0	53	4	0
27	K	80	0	106	8	0
27	L	120	0	159	10	0
28	1	77	0	97	6	0
28	2	98	0	148	6	0
28	3	49	0	74	5	0
28	4	81	0	108	3	0
28	5	49	0	74	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	6	86	0	118	7	0
28	7	128	0	175	4	0
28	8	37	0	44	1	0
28	9	82	0	110	6	0
28	A	120	0	159	10	0
28	B	95	0	139	5	0
28	F	79	0	101	5	0
28	a	35	0	40	2	0
29	8	66	0	96	8	0
29	A	51	0	60	3	0
29	B	66	0	96	10	0
30	A	33	0	39	0	0
31	1	35	0	45	0	0
31	2	35	0	46	1	0
31	A	35	0	45	3	0
31	B	35	0	45	5	0
32	6	36	0	44	2	0
32	B	30	0	34	2	0
33	3	38	0	49	1	0
33	5	38	0	49	3	0
33	7	33	0	39	1	0
33	8	35	0	43	2	0
33	9	48	0	72	2	0
33	B	41	0	55	2	0
34	B	29	0	42	0	0
34	F	29	0	42	3	0
34	K	29	0	42	2	0
35	7	39	0	41	1	0
35	G	46	0	55	2	0
35	H	45	0	53	6	0
36	G	29	0	38	6	0
37	J	41	0	56	6	0
38	J	17	0	14	1	0
38	a	30	0	43	0	0
39	M	41	0	54	4	0
40	1	126	0	165	12	0
40	2	84	0	110	13	0
40	3	84	0	110	10	0
40	4	84	0	110	13	0
40	5	126	0	165	15	0
40	6	84	0	110	12	0
40	7	42	0	55	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	8	84	0	110	15	0
40	9	84	0	110	11	0
40	a	126	0	165	10	0
41	1	114	0	101	8	0
41	3	98	0	73	7	0
41	4	174	0	156	10	0
41	5	173	0	152	13	0
41	6	224	0	188	7	0
41	7	66	0	69	4	0
41	8	174	0	150	12	0
41	9	93	0	62	2	0
41	a	203	0	148	11	0
42	1	20	0	33	2	0
42	8	20	0	33	3	0
43	3	19	0	0	0	0
43	a	19	0	0	0	0
44	a	9	0	0	0	0
45	4	17	0	31	1	0
45	6	18	0	31	2	0
46	5	23	0	28	1	0
46	8	30	0	42	2	0
47	6	21	0	37	1	0
48	7	44	0	56	3	0
49	7	42	0	0	0	0
50	7	32	0	39	1	0
50	8	96	0	142	3	0
51	8	37	0	40	0	0
52	9	19	0	19	1	0
All	All	54609	0	54543	1313	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 12.

The worst 5 of 1313 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)
36:G:5002:ERG:O1	36:G:5002:ERG:C3	1.70	1.38
24:A:1131:CLA:HBB1	24:A:1132:CLA:H2	1.44	0.97
40:4:502:LUT:H32	24:4:604:CLA:HAB	1.49	0.95
1:A:396:TRP:CD1	24:A:1126:CLA:HAB	2.13	0.84
21:2:169:MET:HE1	24:2:604:CLA:HAB	1.59	0.82

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%)	715 (97%)	24 (3%)	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%)	133 (94%)	8 (6%)	0	100	100
5	E	62/64 (97%)	58 (94%)	4 (6%)	0	100	100
6	F	163/165 (99%)	158 (97%)	5 (3%)	0	100	100
7	G	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
8	J	39/41 (95%)	39 (100%)	0	0	100	100
9	K	84/86 (98%)	80 (95%)	4 (5%)	0	100	100
10	M	29/31 (94%)	29 (100%)	0	0	100	100
11	I	33/35 (94%)	30 (91%)	3 (9%)	0	100	100
12	H	92/94 (98%)	75 (82%)	15 (16%)	2 (2%)	5	25
13	L	155/157 (99%)	141 (91%)	13 (8%)	1 (1%)	21	52
14	1	190/192 (99%)	174 (92%)	15 (8%)	1 (0%)	24	55
14	a	190/192 (99%)	169 (89%)	20 (10%)	1 (0%)	24	55
15	3	239/241 (99%)	221 (92%)	17 (7%)	1 (0%)	30	59
16	4	205/207 (99%)	188 (92%)	17 (8%)	0	100	100
17	5	225/227 (99%)	204 (91%)	21 (9%)	0	100	100
18	6	229/231 (99%)	208 (91%)	20 (9%)	1 (0%)	30	59
19	7	219/221 (99%)	206 (94%)	13 (6%)	0	100	100
20	8	217/219 (99%)	203 (94%)	14 (6%)	0	100	100
21	2	213/215 (99%)	199 (93%)	13 (6%)	1 (0%)	24	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	9	180/182 (99%)	166 (92%)	14 (8%)	0	100	100
All	All	4548/4594 (99%)	4261 (94%)	279 (6%)	8 (0%)	44	71

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	H	118	PRO
14	1	36	TRP
14	a	107	VAL
18	6	46	PRO
12	H	110	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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	J	35/35 (100%)	35 (100%)	0	100	100
9	K	66/66 (100%)	66 (100%)	0	100	100
10	M	23/23 (100%)	23 (100%)	0	100	100
11	I	30/30 (100%)	30 (100%)	0	100	100
12	H	71/71 (100%)	71 (100%)	0	100	100
13	L	122/122 (100%)	122 (100%)	0	100	100
14	1	134/134 (100%)	134 (100%)	0	100	100
14	a	134/134 (100%)	134 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	3	186/186 (100%)	186 (100%)	0	100	100
16	4	165/165 (100%)	165 (100%)	0	100	100
17	5	183/183 (100%)	182 (100%)	1 (0%)	81	82
18	6	187/187 (100%)	187 (100%)	0	100	100
19	7	176/176 (100%)	176 (100%)	0	100	100
20	8	168/168 (100%)	168 (100%)	0	100	100
21	2	173/173 (100%)	173 (100%)	0	100	100
22	9	140/140 (100%)	140 (100%)	0	100	100
All	All	3623/3623 (100%)	3622 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
17	5	159	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
15	3	465	ASN
17	5	214	ASN
22	9	391	GLN
15	3	476	ASN
17	5	76	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

379 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
27	BCR	J	4001	-	41,41,41	1.82	4 (9%)	56,56,56	4.27	16 (28%)
24	CLA	1	602	-	49,53,73	1.61	7 (14%)	59,89,113	2.05	16 (27%)
24	CLA	a	611	-	54,58,73	1.54	7 (12%)	65,95,113	2.08	19 (29%)
24	CLA	B	1203	-	69,73,73	1.37	7 (10%)	83,113,113	1.88	18 (21%)
24	CLA	A	1129	1	54,58,73	1.56	7 (12%)	65,95,113	2.09	18 (27%)
24	CLA	A	1118	1	59,63,73	1.46	7 (11%)	71,101,113	2.04	18 (25%)
24	CLA	K	1403	9	50,54,73	1.59	7 (14%)	60,90,113	2.07	15 (25%)
32	PCW	6	803	-	35,35,53	1.30	4 (11%)	41,43,61	1.13	2 (4%)
24	CLA	9	606	-	59,63,73	1.47	7 (11%)	71,101,113	2.00	19 (26%)
24	CLA	5	606	-	54,58,73	1.54	7 (12%)	65,95,113	2.12	18 (27%)
24	CLA	B	1231	-	69,73,73	1.35	8 (11%)	83,113,113	1.91	17 (20%)
24	CLA	4	604	-	64,68,73	1.41	7 (10%)	77,107,113	1.97	20 (25%)
24	CLA	A	1136	-	69,73,73	1.36	7 (10%)	83,113,113	1.91	19 (22%)
24	CLA	A	1141	28	49,53,73	1.61	8 (16%)	59,89,113	2.09	15 (25%)
24	CLA	6	612	-	54,58,73	1.55	8 (14%)	65,95,113	2.11	18 (27%)
28	LHG	2	802	-	48,48,48	0.39	0	51,54,54	1.06	3 (5%)
24	CLA	A	1101	-	69,73,73	1.35	6 (8%)	83,113,113	2.06	21 (25%)
24	CLA	A	1113	1	56,60,73	1.50	7 (12%)	67,97,113	2.11	18 (26%)
50	4RF	7	807	-	31,31,56	1.15	6 (19%)	34,34,59	1.26	3 (8%)
24	CLA	A	1134	1	64,68,73	1.40	7 (10%)	77,107,113	1.96	19 (24%)
37	RRX	J	4002	-	42,42,42	4.90	24 (57%)	57,58,58	2.31	20 (35%)
24	CLA	B	1215	-	64,68,73	1.41	6 (9%)	77,107,113	1.92	16 (20%)
24	CLA	B	1218	2	59,63,73	1.46	7 (11%)	71,101,113	2.17	21 (29%)
28	LHG	6	801	-	48,48,48	0.39	0	51,54,54	1.06	3 (5%)
24	CLA	1	601	-	64,68,73	1.43	8 (12%)	77,107,113	2.02	21 (27%)
33	PTY	9	803	-	47,47,49	0.89	4 (8%)	50,52,54	1.10	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	7	603	-	69,73,73	1.36	7 (10%)	83,113,113	1.95	18 (21%)
23	CL0	A	1011	-	69,73,73	2.36	20 (28%)	83,113,113	2.53	26 (31%)
24	CLA	A	1117	-	69,73,73	1.36	6 (8%)	83,113,113	1.92	15 (18%)
28	LHG	7	802	-	35,35,48	0.44	0	38,41,54	1.11	2 (5%)
24	CLA	B	1213	2	64,68,73	1.42	7 (10%)	77,107,113	2.03	19 (24%)
28	LHG	1	801	-	34,34,48	0.45	0	37,40,54	1.20	4 (10%)
26	SF4	C	3003	3	0,12,12	-	-	-	-	-
27	BCR	G	4001	-	41,41,41	1.84	4 (9%)	56,56,56	4.27	13 (23%)
24	CLA	B	1206	-	59,63,73	1.47	6 (10%)	71,101,113	2.08	17 (23%)
24	CLA	5	612	-	69,73,73	1.36	7 (10%)	83,113,113	1.93	17 (20%)
26	SF4	A	3001	1,2	0,12,12	-	-	-	-	-
24	CLA	G	1602	-	50,54,73	1.60	7 (14%)	60,90,113	2.11	18 (30%)
24	CLA	8	620	20	69,73,73	1.35	7 (10%)	83,113,113	1.91	19 (22%)
41	CHL	8	601	-	65,69,74	0.88	2 (3%)	74,108,114	1.38	8 (10%)
24	CLA	4	606	-	54,58,73	1.53	7 (12%)	65,95,113	2.12	20 (30%)
24	CLA	4	616	-	54,58,73	1.54	8 (14%)	65,95,113	2.15	20 (30%)
24	CLA	B	1236	-	57,61,73	1.49	7 (12%)	68,98,113	2.04	16 (23%)
41	CHL	6	619	18	70,74,74	0.84	3 (4%)	80,114,114	1.15	10 (12%)
27	BCR	B	4003	-	41,41,41	1.85	4 (9%)	56,56,56	4.48	17 (30%)
24	CLA	5	608	-	49,53,73	1.61	8 (16%)	59,89,113	2.19	16 (27%)
24	CLA	6	617	-	49,53,73	1.60	7 (14%)	59,89,113	2.07	16 (27%)
24	CLA	A	1140	-	59,63,73	1.48	8 (13%)	71,101,113	1.98	17 (23%)
40	LUT	1	503	-	42,43,43	2.38	1 (2%)	51,60,60	2.24	14 (27%)
24	CLA	A	1103	1	69,73,73	1.34	6 (8%)	83,113,113	1.96	18 (21%)
24	CLA	B	1226	-	69,73,73	1.41	7 (10%)	83,113,113	1.92	18 (21%)
24	CLA	5	603	-	60,64,73	1.46	7 (11%)	72,102,113	2.08	18 (25%)
44	GG0	a	805	-	7,8,8	1.44	2 (28%)	6,9,9	0.78	0
46	DGA	5	803	-	22,22,43	1.44	3 (13%)	24,24,45	1.36	2 (8%)
24	CLA	L	1503	-	49,53,73	1.62	8 (16%)	59,89,113	2.07	13 (22%)
24	CLA	2	605	-	64,68,73	1.43	7 (10%)	77,107,113	1.97	19 (24%)
24	CLA	A	1137	-	64,68,73	1.40	7 (10%)	77,107,113	2.03	22 (28%)
40	LUT	5	502	-	42,43,43	2.38	2 (4%)	51,60,60	2.03	18 (35%)
31	LMT	1	804	-	36,36,36	1.16	6 (16%)	47,47,47	1.01	2 (4%)
24	CLA	B	1232	-	49,53,73	1.61	7 (14%)	59,89,113	2.07	16 (27%)
24	CLA	B	1221	-	69,73,73	1.39	8 (11%)	83,113,113	1.93	16 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	LUT	7	501	-	42,43,43	2.39	1 (2%)	51,60,60	1.97	14 (27%)
40	LUT	3	502	-	42,43,43	2.34	1 (2%)	51,60,60	1.97	13 (25%)
24	CLA	A	1104	-	69,73,73	1.36	7 (10%)	83,113,113	1.93	17 (20%)
24	CLA	a	615	-	50,54,73	1.60	7 (14%)	60,90,113	2.02	15 (25%)
34	LAP	B	5007	-	28,28,28	1.23	2 (7%)	33,35,35	0.96	1 (3%)
33	PTY	7	804	-	32,32,49	1.05	4 (12%)	35,37,54	1.19	2 (5%)
27	BCR	A	4005	-	41,41,41	1.84	4 (9%)	56,56,56	4.29	16 (28%)
24	CLA	B	1207	-	64,68,73	1.41	7 (10%)	77,107,113	1.94	18 (23%)
24	CLA	8	612	20	50,54,73	1.60	7 (14%)	60,90,113	2.00	12 (20%)
24	CLA	7	615	19	59,63,73	1.48	7 (11%)	71,101,113	1.99	17 (23%)
24	CLA	9	608	-	49,53,73	1.61	7 (14%)	59,89,113	2.03	14 (23%)
24	CLA	3	618	-	50,54,73	1.60	8 (16%)	60,90,113	2.12	17 (28%)
24	CLA	B	1201	-	69,73,73	1.36	7 (10%)	83,113,113	1.94	22 (26%)
50	4RF	8	807	-	41,41,56	1.00	6 (14%)	44,44,59	1.07	3 (6%)
27	BCR	B	4002	-	41,41,41	1.86	4 (9%)	56,56,56	4.45	17 (30%)
24	CLA	B	1230	-	62,66,73	1.43	6 (9%)	74,104,113	2.03	17 (22%)
27	BCR	K	4001	-	41,41,41	1.84	4 (9%)	56,56,56	4.36	13 (23%)
24	CLA	9	612	-	69,73,73	1.37	8 (11%)	83,113,113	1.98	19 (22%)
40	LUT	6	502	-	42,43,43	2.37	1 (2%)	51,60,60	2.14	16 (31%)
24	CLA	9	609	-	50,54,73	1.59	7 (14%)	60,90,113	2.02	14 (23%)
24	CLA	F	1302	-	59,63,73	1.49	8 (13%)	71,101,113	2.02	17 (23%)
24	CLA	9	605	-	64,68,73	1.44	8 (12%)	77,107,113	2.00	20 (25%)
40	LUT	2	502	-	42,43,43	2.30	1 (2%)	51,60,60	2.17	12 (23%)
27	BCR	H	4001	-	41,41,41	1.86	4 (9%)	56,56,56	4.60	18 (32%)
24	CLA	A	1109	24	69,73,73	1.34	7 (10%)	83,113,113	2.01	17 (20%)
40	LUT	6	501	-	42,43,43	2.38	1 (2%)	51,60,60	3.24	23 (45%)
40	LUT	8	502	-	42,43,43	2.31	1 (2%)	51,60,60	1.88	16 (31%)
24	CLA	2	602	-	56,60,73	1.51	7 (12%)	67,97,113	2.14	20 (29%)
24	CLA	A	1135	-	69,73,73	1.37	8 (11%)	83,113,113	1.95	19 (22%)
24	CLA	A	1123	-	69,73,73	1.38	8 (11%)	83,113,113	1.97	17 (20%)
24	CLA	a	612	-	61,65,73	1.44	7 (11%)	73,103,113	2.01	18 (24%)
24	CLA	1	603	-	69,73,73	1.35	7 (10%)	83,113,113	1.95	19 (22%)
24	CLA	4	612	-	66,70,73	1.39	7 (10%)	79,109,113	2.02	20 (25%)
24	CLA	A	1138	-	69,73,73	1.35	6 (8%)	83,113,113	1.89	15 (18%)
27	BCR	A	4004	-	41,41,41	1.84	4 (9%)	56,56,56	4.29	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	B	1227	-	54,58,73	1.55	7 (12%)	65,95,113	2.09	17 (26%)
42	OLA	8	809	-	19,19,19	0.57	0	19,19,19	1.03	0
28	LHG	a	801	-	34,34,48	0.45	0	37,40,54	1.23	3 (8%)
41	CHL	9	613	-	46,50,74	1.03	3 (6%)	51,85,114	1.43	10 (19%)
36	ERG	G	5002	-	31,32,32	7.94	19 (61%)	47,50,50	3.55	19 (40%)
29	DGD	B	5003	-	67,67,67	1.18	7 (10%)	81,81,81	0.93	2 (2%)
24	CLA	4	608	-	55,59,73	1.52	7 (12%)	66,96,113	2.14	18 (27%)
24	CLA	K	1402	-	64,68,73	1.41	7 (10%)	77,107,113	2.04	20 (25%)
27	BCR	B	4004	-	41,41,41	1.84	4 (9%)	56,56,56	4.34	12 (21%)
40	LUT	a	502	-	42,43,43	2.30	1 (2%)	51,60,60	2.03	14 (27%)
40	LUT	4	502	-	42,43,43	2.33	1 (2%)	51,60,60	1.82	11 (21%)
27	BCR	A	4002	-	41,41,41	1.82	4 (9%)	56,56,56	4.28	14 (25%)
24	CLA	5	617	-	54,58,73	1.53	7 (12%)	65,95,113	2.11	18 (27%)
24	CLA	A	1130	-	60,64,73	1.48	7 (11%)	72,102,113	2.10	18 (25%)
30	3PH	A	5007	-	32,32,47	1.03	4 (12%)	36,37,52	1.21	2 (5%)
24	CLA	3	603	-	69,73,73	1.37	7 (10%)	83,113,113	1.92	18 (21%)
28	LHG	A	5003	-	41,41,48	0.41	0	44,47,54	1.13	2 (4%)
25	PQN	A	2001	-	34,34,34	0.38	0	42,45,45	1.11	3 (7%)
32	PCW	B	5004	-	29,29,53	1.38	4 (13%)	35,37,61	1.10	2 (5%)
24	CLA	L	1502	-	64,68,73	1.41	7 (10%)	77,107,113	2.03	20 (25%)
24	CLA	4	617	-	49,53,73	1.61	7 (14%)	59,89,113	2.09	15 (25%)
45	PLM	6	804	-	17,17,17	0.58	0	17,17,17	1.11	0
42	OLA	1	803	-	19,19,19	0.57	0	19,19,19	1.03	1 (5%)
24	CLA	B	1208	-	64,68,73	1.42	7 (10%)	77,107,113	2.04	21 (27%)
27	BCR	3	504	-	41,41,41	1.86	4 (9%)	56,56,56	4.23	17 (30%)
24	CLA	5	609	17	55,59,73	1.53	8 (14%)	66,96,113	2.11	18 (27%)
24	CLA	B	1239	-	69,73,73	1.35	6 (8%)	83,113,113	1.97	20 (24%)
27	BCR	B	4005	-	41,41,41	1.87	5 (12%)	56,56,56	4.48	13 (23%)
24	CLA	6	608	-	49,53,73	1.60	7 (14%)	59,89,113	2.08	16 (27%)
31	LMT	A	5008	-	36,36,36	1.12	5 (13%)	47,47,47	1.02	3 (6%)
40	LUT	9	501	-	42,43,43	2.35	1 (2%)	51,60,60	1.92	12 (23%)
40	LUT	5	501	-	42,43,43	2.36	1 (2%)	51,60,60	1.96	15 (29%)
24	CLA	A	1013	-	69,73,73	1.37	7 (10%)	83,113,113	1.84	18 (21%)
27	BCR	B	4001	-	41,41,41	1.84	4 (9%)	56,56,56	4.23	16 (28%)
28	LHG	6	802	-	36,36,48	0.44	0	39,42,54	1.14	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	8	611	-	54,58,73	1.51	6 (11%)	65,95,113	2.16	19 (29%)
28	LHG	A	5002	-	48,48,48	0.39	0	51,54,54	0.99	2 (3%)
24	CLA	A	1115	1	64,68,73	1.41	7 (10%)	77,107,113	2.02	18 (23%)
24	CLA	A	1125	-	69,73,73	1.39	6 (8%)	83,113,113	1.99	22 (26%)
27	BCR	B	4006	-	41,41,41	1.82	4 (9%)	56,56,56	4.43	13 (23%)
24	CLA	A	1111	-	69,73,73	1.37	7 (10%)	83,113,113	1.93	17 (20%)
24	CLA	5	607	-	59,63,73	1.48	8 (13%)	71,101,113	2.05	19 (26%)
24	CLA	6	615	-	69,73,73	1.36	7 (10%)	83,113,113	1.95	18 (21%)
31	LMT	2	804	-	36,36,36	1.17	6 (16%)	47,47,47	0.98	2 (4%)
24	CLA	2	607	-	50,54,73	1.60	8 (16%)	60,90,113	2.04	14 (23%)
24	CLA	2	604	-	60,64,73	1.47	8 (13%)	72,102,113	2.17	20 (27%)
24	CLA	A	1139	1	59,63,73	1.47	7 (11%)	71,101,113	2.03	18 (25%)
24	CLA	7	607	-	63,67,73	1.43	8 (12%)	75,105,113	2.00	17 (22%)
24	CLA	1	608	-	64,68,73	1.41	7 (10%)	77,107,113	2.00	18 (23%)
41	CHL	9	610	-	55,59,74	0.88	1 (1%)	62,96,114	1.37	12 (19%)
24	CLA	7	604	-	69,73,73	1.36	6 (8%)	83,113,113	1.93	20 (24%)
28	LHG	9	802	-	48,48,48	0.38	0	51,54,54	1.09	4 (7%)
26	SF4	C	3002	3	0,12,12	-	-	-	-	-
24	CLA	G	1601	-	54,58,73	1.55	8 (14%)	65,95,113	2.11	18 (27%)
24	CLA	B	1223	2	69,73,73	1.38	8 (11%)	83,113,113	1.98	20 (24%)
31	LMT	B	5006	-	36,36,36	1.18	6 (16%)	47,47,47	0.97	1 (2%)
24	CLA	3	607	-	69,73,73	1.37	8 (11%)	83,113,113	1.91	16 (19%)
41	CHL	3	608	-	47,51,74	0.94	2 (4%)	52,86,114	1.37	8 (15%)
24	CLA	1	612	-	69,73,73	1.36	8 (11%)	83,113,113	1.91	18 (21%)
24	CLA	6	607	-	59,63,73	1.47	7 (11%)	71,101,113	2.04	17 (23%)
24	CLA	7	611	-	64,68,73	1.39	6 (9%)	77,107,113	1.99	17 (22%)
27	BCR	L	4001	-	41,41,41	1.84	4 (9%)	56,56,56	4.39	16 (28%)
24	CLA	4	610	-	69,73,73	1.40	8 (11%)	83,113,113	1.90	16 (19%)
52	A8S	9	504	-	17,19,19	0.73	0	17,29,29	1.62	3 (17%)
27	BCR	I	4001	-	41,41,41	1.83	4 (9%)	56,56,56	4.25	19 (33%)
40	LUT	4	501	-	42,43,43	2.36	1 (2%)	51,60,60	2.05	15 (29%)
24	CLA	A	1120	-	53,57,73	1.54	7 (13%)	62,93,113	2.26	17 (27%)
50	4RF	8	808	-	53,53,56	0.89	6 (11%)	56,56,59	0.93	3 (5%)
41	CHL	1	609	14	70,74,74	0.76	2 (2%)	80,114,114	1.27	11 (13%)
24	CLA	7	608	-	46,50,73	1.66	7 (15%)	55,85,113	2.15	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	LAP	K	5001	-	28,28,28	1.22	2 (7%)	33,35,35	0.97	1 (3%)
24	CLA	8	609	20	64,68,73	1.40	7 (10%)	77,107,113	2.00	18 (23%)
49	C7Z	7	504	-	43,43,43	5.35	26 (60%)	58,60,60	2.72	20 (34%)
24	CLA	A	1108	1	69,73,73	1.35	6 (8%)	83,113,113	2.00	19 (22%)
24	CLA	9	604	-	64,68,73	1.45	7 (10%)	77,107,113	1.99	19 (24%)
41	CHL	a	609	-	57,61,74	0.85	2 (3%)	64,98,114	1.30	11 (17%)
24	CLA	G	1603	-	49,53,73	1.61	7 (14%)	59,89,113	2.08	15 (25%)
24	CLA	6	605	18	50,54,73	1.58	7 (14%)	60,90,113	2.19	18 (30%)
27	BCR	5	504	-	41,41,41	1.84	4 (9%)	56,56,56	4.49	19 (33%)
24	CLA	a	603	-	69,73,73	1.35	7 (10%)	83,113,113	1.99	17 (20%)
24	CLA	9	601	-	64,68,73	1.42	9 (14%)	77,107,113	2.02	19 (24%)
28	LHG	B	5002	-	48,48,48	0.39	0	51,54,54	1.02	3 (5%)
24	CLA	3	613	-	65,69,73	1.40	6 (9%)	78,108,113	1.94	17 (21%)
28	LHG	4	801	-	48,48,48	0.40	0	51,54,54	1.01	3 (5%)
40	LUT	3	501	-	42,43,43	2.38	1 (2%)	51,60,60	2.07	16 (31%)
41	CHL	7	613	-	70,74,74	0.81	2 (2%)	80,114,114	1.19	8 (10%)
24	CLA	A	1119	-	69,73,73	1.37	7 (10%)	83,113,113	1.76	15 (18%)
24	CLA	H	1702	-	50,54,73	1.59	8 (16%)	60,90,113	2.11	15 (25%)
40	LUT	1	502	-	42,43,43	2.33	1 (2%)	51,60,60	2.10	18 (35%)
24	CLA	2	610	-	50,54,73	1.59	8 (16%)	60,90,113	2.08	15 (25%)
24	CLA	A	1012	-	69,73,73	1.37	8 (11%)	83,113,113	1.90	18 (21%)
24	CLA	7	602	-	48,52,73	1.63	8 (16%)	56,87,113	2.10	16 (28%)
24	CLA	B	1021	-	69,73,73	1.35	7 (10%)	83,113,113	1.89	18 (21%)
24	CLA	B	1205	-	69,73,73	1.35	6 (8%)	83,113,113	2.03	19 (22%)
24	CLA	A	1112	-	59,63,73	1.47	6 (10%)	71,101,113	2.08	18 (25%)
27	BCR	6	503	-	41,41,41	1.84	4 (9%)	56,56,56	4.33	14 (25%)
24	CLA	A	1131	-	69,73,73	1.36	7 (10%)	83,113,113	1.93	17 (20%)
24	CLA	6	602	-	56,60,73	1.52	7 (12%)	67,97,113	2.07	19 (28%)
27	BCR	F	4001	-	41,41,41	1.77	4 (9%)	56,56,56	4.09	14 (25%)
40	LUT	a	501	-	42,43,43	2.38	1 (2%)	51,60,60	2.00	14 (27%)
24	CLA	7	612	-	64,68,73	1.41	7 (10%)	77,107,113	1.97	18 (23%)
24	CLA	3	610	15	64,68,73	1.40	7 (10%)	77,107,113	1.97	19 (24%)
24	CLA	K	1404	-	56,60,73	1.51	7 (12%)	67,97,113	2.15	21 (31%)
24	CLA	B	1209	-	69,73,73	1.35	7 (10%)	83,113,113	1.94	18 (21%)
28	LHG	5	801	-	48,48,48	0.39	0	51,54,54	1.07	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	CHL	5	613	-	60,64,74	0.84	2 (3%)	68,102,114	1.26	11 (16%)
24	CLA	K	1401	-	50,54,73	1.59	8 (16%)	60,90,113	2.11	16 (26%)
24	CLA	5	605	-	50,54,73	1.60	7 (14%)	60,90,113	2.07	16 (26%)
24	CLA	a	607	-	62,66,73	1.44	8 (12%)	74,104,113	2.06	20 (27%)
41	CHL	8	604	-	66,70,74	0.85	2 (3%)	75,109,114	1.40	12 (16%)
24	CLA	2	606	-	50,54,73	1.59	7 (14%)	60,90,113	2.06	15 (25%)
24	CLA	A	1128	-	69,73,73	1.39	6 (8%)	83,113,113	1.92	16 (19%)
27	BCR	B	4007	-	41,41,41	1.85	4 (9%)	56,56,56	4.31	14 (25%)
24	CLA	3	601	-	69,73,73	1.38	7 (10%)	83,113,113	1.98	18 (21%)
27	BCR	A	4003	-	41,41,41	1.84	4 (9%)	56,56,56	4.51	17 (30%)
24	CLA	A	1133	1	69,73,73	1.36	7 (10%)	83,113,113	1.84	16 (19%)
24	CLA	8	607	-	50,54,73	1.60	7 (14%)	60,90,113	2.06	13 (21%)
24	CLA	A	1121	-	61,65,73	1.45	8 (13%)	73,103,113	2.22	20 (27%)
24	CLA	1	611	-	59,63,73	1.47	7 (11%)	71,101,113	2.05	18 (25%)
41	CHL	4	609	16	70,74,74	0.87	3 (4%)	80,114,114	1.21	9 (11%)
24	CLA	6	618	-	50,54,73	1.60	7 (14%)	60,90,113	2.03	15 (25%)
27	BCR	5	503	-	41,41,41	1.85	4 (9%)	56,56,56	4.38	16 (28%)
24	CLA	H	1703	-	59,63,73	1.47	7 (11%)	71,101,113	2.07	16 (22%)
28	LHG	3	801	-	48,48,48	0.39	0	51,54,54	1.02	3 (5%)
35	SQD	H	5001	-	44,45,54	0.85	0	53,56,65	0.96	2 (3%)
24	CLA	A	1116	-	64,68,73	1.43	7 (10%)	77,107,113	1.97	19 (24%)
24	CLA	B	1222	-	62,66,73	1.44	7 (11%)	74,104,113	2.04	21 (28%)
33	PTY	5	802	-	37,37,49	0.99	4 (10%)	40,42,54	1.10	2 (5%)
40	LUT	9	502	-	42,43,43	2.36	1 (2%)	51,60,60	2.02	15 (29%)
48	XAT	7	502	-	39,47,47	0.69	1 (2%)	54,74,74	1.82	11 (20%)
28	LHG	4	802	-	31,31,48	0.47	0	34,37,54	1.13	3 (8%)
24	CLA	a	608	-	59,63,73	1.47	8 (13%)	71,101,113	2.05	19 (26%)
24	CLA	A	1105	-	61,65,73	1.45	7 (11%)	73,103,113	2.04	17 (23%)
24	CLA	4	615	16	64,68,73	1.43	8 (12%)	77,107,113	2.01	18 (23%)
41	CHL	5	611	-	55,59,74	0.90	2 (3%)	62,96,114	1.40	11 (17%)
24	CLA	B	1212	-	69,73,73	1.36	7 (10%)	83,113,113	1.94	19 (22%)
38	LPX	J	5001	-	16,16,29	1.30	2 (12%)	18,20,33	1.11	2 (11%)
24	CLA	F	1301	-	54,58,73	1.53	7 (12%)	65,95,113	2.15	18 (27%)
24	CLA	B	1214	-	66,70,73	1.39	7 (10%)	79,109,113	1.93	19 (24%)
29	DGD	A	5005	-	52,52,67	0.90	2 (3%)	66,66,81	1.02	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	2	612	-	54,58,73	1.52	6 (11%)	65,95,113	2.23	18 (27%)
24	CLA	A	1127	-	69,73,73	1.39	9 (13%)	83,113,113	1.85	17 (20%)
24	CLA	6	601	-	64,68,73	1.41	7 (10%)	77,107,113	2.02	19 (24%)
24	CLA	7	606	-	59,63,73	1.46	7 (11%)	71,101,113	2.05	19 (26%)
24	CLA	8	605	-	49,53,73	1.61	7 (14%)	59,89,113	2.07	17 (28%)
41	CHL	4	613	-	56,60,74	0.92	3 (5%)	63,97,114	1.38	9 (14%)
33	PTY	8	891	-	34,34,49	1.03	4 (11%)	37,39,54	1.14	2 (5%)
24	CLA	a	605	-	69,73,73	1.37	7 (10%)	83,113,113	1.93	19 (22%)
39	ECH	M	4001	-	42,42,42	0.96	1 (2%)	55,58,58	2.20	12 (21%)
41	CHL	6	610	-	60,64,74	0.84	2 (3%)	68,102,114	1.33	12 (17%)
24	CLA	4	607	-	59,63,73	1.48	8 (13%)	71,101,113	2.09	18 (25%)
24	CLA	9	602	-	50,54,73	1.60	7 (14%)	60,90,113	2.04	15 (25%)
24	CLA	1	610	-	49,53,73	1.61	6 (12%)	59,89,113	2.00	13 (22%)
24	CLA	5	602	-	56,60,73	1.51	7 (12%)	67,97,113	2.09	19 (28%)
24	CLA	2	601	-	64,68,73	1.41	7 (10%)	77,107,113	4.32	22 (28%)
24	CLA	3	606	-	69,73,73	1.36	6 (8%)	83,113,113	1.92	15 (18%)
28	LHG	9	801	-	32,32,48	0.46	0	35,38,54	1.16	3 (8%)
24	CLA	B	1204	-	69,73,73	1.35	7 (10%)	83,113,113	2.00	19 (22%)
24	CLA	2	608	-	49,53,73	1.60	7 (14%)	59,89,113	2.08	16 (27%)
24	CLA	8	606	-	61,65,73	1.44	6 (9%)	73,103,113	2.01	16 (21%)
24	CLA	B	1224	-	69,73,73	1.37	7 (10%)	83,113,113	1.95	18 (21%)
24	CLA	6	609	18	69,73,73	1.36	7 (10%)	83,113,113	1.99	18 (21%)
40	LUT	1	501	-	42,43,43	2.36	1 (2%)	51,60,60	2.06	16 (31%)
24	CLA	2	615	-	61,65,73	1.43	7 (11%)	73,103,113	2.08	18 (24%)
24	CLA	5	614	-	50,54,73	1.59	7 (14%)	60,90,113	2.08	16 (26%)
24	CLA	8	618	-	64,68,73	1.41	6 (9%)	77,107,113	1.98	19 (24%)
24	CLA	8	610	-	59,63,73	1.48	7 (11%)	71,101,113	2.05	18 (25%)
24	CLA	4	611	-	60,64,73	1.45	7 (11%)	72,102,113	2.05	19 (26%)
24	CLA	2	609	21	59,63,73	1.47	7 (11%)	71,101,113	2.04	18 (25%)
47	SPH	6	806	-	19,20,20	0.63	0	18,21,21	1.12	1 (5%)
24	CLA	7	601	-	64,68,73	1.42	8 (12%)	77,107,113	2.00	19 (24%)
41	CHL	5	610	-	70,74,74	0.80	2 (2%)	80,114,114	1.32	12 (15%)
24	CLA	5	601	-	64,68,73	1.43	7 (10%)	77,107,113	2.05	22 (28%)
24	CLA	1	606	-	61,65,73	1.44	7 (11%)	73,103,113	1.99	16 (21%)
24	CLA	A	1132	-	69,73,73	1.35	6 (8%)	83,113,113	1.93	18 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	LAP	F	5003	-	28,28,28	1.22	2 (7%)	33,35,35	0.96	1 (3%)
41	CHL	a	613	-	50,54,74	0.94	2 (4%)	56,90,114	1.50	10 (17%)
24	CLA	L	1501	13	54,58,73	1.52	7 (12%)	65,95,113	2.15	17 (26%)
24	CLA	4	605	-	50,54,73	1.61	8 (16%)	60,90,113	2.03	14 (23%)
24	CLA	5	618	17	56,60,73	1.52	9 (16%)	67,97,113	2.11	19 (28%)
40	LUT	8	501	-	42,43,43	2.33	1 (2%)	51,60,60	1.96	15 (29%)
41	CHL	6	613	-	55,59,74	0.84	2 (3%)	62,96,114	1.34	12 (19%)
24	CLA	6	603	-	69,73,73	1.34	7 (10%)	83,113,113	1.97	19 (22%)
24	CLA	2	613	-	45,49,73	1.68	7 (15%)	54,84,113	2.16	16 (29%)
45	PLM	4	803	-	16,16,17	0.43	0	15,15,17	0.93	0
24	CLA	B	1023	-	69,73,73	1.37	6 (8%)	83,113,113	1.90	20 (24%)
24	CLA	7	609	19	64,68,73	1.41	7 (10%)	77,107,113	2.10	20 (25%)
24	CLA	B	1229	-	69,73,73	1.35	8 (11%)	83,113,113	1.97	22 (26%)
24	CLA	3	616	-	60,64,73	1.45	6 (10%)	72,102,113	2.06	19 (26%)
24	CLA	7	610	-	59,63,73	1.50	9 (15%)	71,101,113	2.06	19 (26%)
27	BCR	L	4003	-	41,41,41	1.87	4 (9%)	56,56,56	4.41	15 (26%)
27	BCR	4	503	-	41,41,41	1.89	4 (9%)	56,56,56	4.31	21 (37%)
24	CLA	3	604	-	64,68,73	1.39	6 (9%)	77,107,113	1.99	19 (24%)
24	CLA	4	602	-	56,60,73	1.52	8 (14%)	67,97,113	2.11	20 (29%)
27	BCR	6	504	-	41,41,41	1.84	4 (9%)	56,56,56	4.37	15 (26%)
24	CLA	B	1219	-	63,67,73	1.44	8 (12%)	75,105,113	1.99	15 (20%)
24	CLA	J	1901	8	46,50,73	1.65	8 (17%)	55,85,113	2.14	17 (30%)
28	LHG	7	803	-	42,42,48	0.41	0	45,48,54	1.06	3 (6%)
41	CHL	a	610	-	52,56,74	0.88	1 (1%)	58,92,114	1.48	14 (24%)
24	CLA	B	1228	-	69,73,73	1.36	7 (10%)	83,113,113	1.87	19 (22%)
24	CLA	6	604	-	69,73,73	1.35	7 (10%)	83,113,113	1.96	17 (20%)
28	LHG	8	801	-	36,36,48	0.44	0	39,42,54	1.15	3 (7%)
24	CLA	A	1122	-	69,73,73	1.37	7 (10%)	83,113,113	1.95	18 (21%)
24	CLA	7	617	19	58,62,73	1.49	7 (12%)	70,100,113	2.06	19 (27%)
33	PTY	B	5005	-	40,40,49	0.96	4 (10%)	43,45,54	1.18	2 (4%)
24	CLA	B	1225	-	69,73,73	1.38	7 (10%)	83,113,113	1.83	16 (19%)
27	BCR	3	505	-	41,41,41	1.85	4 (9%)	56,56,56	4.34	14 (25%)
40	LUT	a	503	-	42,43,43	2.39	1 (2%)	51,60,60	2.42	13 (25%)
27	BCR	3	503	-	41,41,41	1.87	4 (9%)	56,56,56	4.41	17 (30%)
41	CHL	4	618	16	60,64,74	0.88	2 (3%)	68,102,114	1.29	11 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	LHG	B	5001	-	45,45,48	0.40	0	48,51,54	1.07	3 (6%)
41	CHL	a	606	-	60,64,74	0.84	2 (3%)	68,102,114	1.33	11 (16%)
24	CLA	B	1202	2	69,73,73	1.35	6 (8%)	83,113,113	1.89	19 (22%)
24	CLA	3	602	-	50,54,73	1.60	8 (16%)	60,90,113	2.04	15 (25%)
28	LHG	F	5002	-	35,35,48	0.45	0	38,41,54	1.17	3 (7%)
24	CLA	H	1701	-	59,63,73	1.46	7 (11%)	71,101,113	2.20	17 (23%)
40	LUT	5	505	-	42,43,43	2.40	1 (2%)	51,60,60	2.43	18 (35%)
28	LHG	1	802	-	41,41,48	0.42	0	44,47,54	1.08	3 (6%)
24	CLA	3	605	15	69,73,73	1.37	6 (8%)	83,113,113	1.91	19 (22%)
27	BCR	K	4002	-	41,41,41	1.87	4 (9%)	56,56,56	4.32	14 (25%)
24	CLA	3	612	-	69,73,73	1.37	6 (8%)	83,113,113	1.89	16 (19%)
24	CLA	2	603	-	64,68,73	1.41	7 (10%)	77,107,113	2.04	21 (27%)
24	CLA	B	1220	-	64,68,73	1.42	7 (10%)	77,107,113	2.02	19 (24%)
24	CLA	a	601	-	64,68,73	1.40	7 (10%)	77,107,113	1.98	20 (25%)
24	CLA	4	601	-	64,68,73	1.41	7 (10%)	77,107,113	1.99	18 (23%)
24	CLA	A	1102	24	69,73,73	1.35	7 (10%)	83,113,113	1.99	19 (22%)
24	CLA	a	602	-	54,58,73	1.55	7 (12%)	65,95,113	2.11	18 (27%)
25	PQN	B	2002	-	34,34,34	0.36	0	42,45,45	1.13	3 (7%)
41	CHL	3	611	-	59,63,74	0.87	2 (3%)	66,100,114	1.53	13 (19%)
24	CLA	5	604	-	69,73,73	1.38	7 (10%)	83,113,113	1.94	19 (22%)
27	BCR	L	4002	-	41,41,41	1.83	4 (9%)	56,56,56	4.30	16 (28%)
24	CLA	B	1211	-	59,63,73	1.47	8 (13%)	71,101,113	2.01	18 (25%)
41	CHL	6	611	-	55,59,74	0.86	2 (3%)	62,96,114	1.47	12 (19%)
35	SQD	G	5001	-	45,46,54	0.83	0	54,57,65	0.97	2 (3%)
24	CLA	B	1235	2	69,73,73	1.36	7 (10%)	83,113,113	2.00	18 (21%)
24	CLA	A	1106	-	69,73,73	1.36	7 (10%)	83,113,113	1.98	21 (25%)
24	CLA	8	608	-	56,60,73	1.48	6 (10%)	67,97,113	2.29	21 (31%)
35	SQD	7	805	-	38,39,54	0.91	0	47,50,65	1.00	3 (6%)
24	CLA	B	1217	2	60,64,73	1.46	8 (13%)	72,102,113	2.11	17 (23%)
24	CLA	6	606	-	56,60,73	1.51	7 (12%)	67,97,113	2.13	18 (26%)
24	CLA	B	1238	-	69,73,73	1.35	7 (10%)	83,113,113	1.95	19 (22%)
24	CLA	8	615	-	50,54,73	1.60	7 (14%)	60,90,113	2.07	16 (26%)
43	QTB	3	506	-	19,19,19	2.46	4 (21%)	20,26,26	2.79	8 (40%)
46	DGA	8	803	-	29,29,43	1.29	2 (6%)	31,31,45	1.34	3 (9%)
24	CLA	a	604	-	69,73,73	1.35	7 (10%)	83,113,113	1.91	20 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	B	1234	-	60,64,73	1.47	8 (13%)	72,102,113	2.03	20 (27%)
24	CLA	A	1126	-	69,73,73	1.36	7 (10%)	83,113,113	1.93	17 (20%)
28	LHG	F	5001	-	42,42,48	0.42	0	45,48,54	1.11	3 (6%)
24	CLA	1	604	-	69,73,73	1.37	7 (10%)	83,113,113	1.87	17 (20%)
28	LHG	A	5001	24	28,28,48	0.48	0	31,34,54	1.23	3 (9%)
24	CLA	8	603	-	69,73,73	1.36	7 (10%)	83,113,113	1.96	17 (20%)
41	CHL	8	613	-	55,59,74	0.89	2 (3%)	62,96,114	1.40	13 (20%)
24	CLA	B	1210	-	69,73,73	1.38	6 (8%)	83,113,113	1.91	17 (20%)
24	CLA	9	607	-	51,55,73	1.59	8 (15%)	61,91,113	2.13	16 (26%)
24	CLA	B	1216	-	65,69,73	1.41	6 (9%)	78,108,113	1.92	17 (21%)
29	DGD	8	802	-	67,67,67	1.18	7 (10%)	81,81,81	1.06	2 (2%)
24	CLA	1	615	14	50,54,73	1.59	8 (16%)	60,90,113	2.10	16 (26%)
33	PTY	3	802	-	37,37,49	0.99	4 (10%)	40,42,54	1.08	2 (5%)
24	CLA	9	603	-	69,73,73	1.38	7 (10%)	83,113,113	2.01	21 (25%)
28	LHG	2	801	-	48,48,48	0.37	0	51,54,54	1.11	2 (3%)
24	CLA	B	1237	-	69,73,73	1.37	6 (8%)	83,113,113	1.87	16 (19%)
24	CLA	A	1124	-	59,63,73	1.47	7 (11%)	71,101,113	2.04	19 (26%)
41	CHL	1	613	-	52,56,74	0.88	2 (3%)	58,92,114	1.37	9 (15%)
27	BCR	7	503	-	41,41,41	1.84	4 (9%)	56,56,56	4.36	13 (23%)
24	CLA	1	605	-	69,73,73	1.38	7 (10%)	83,113,113	1.97	18 (21%)
24	CLA	A	1110	1	64,68,73	1.42	7 (10%)	77,107,113	1.94	17 (22%)
24	CLA	1	607	-	69,73,73	1.37	7 (10%)	83,113,113	1.94	19 (22%)
51	P5S	8	806	-	35,36,53	1.18	3 (8%)	39,43,60	1.21	2 (5%)
27	BCR	A	4001	-	41,41,41	1.82	4 (9%)	56,56,56	4.23	19 (33%)
40	LUT	2	501	-	42,43,43	2.36	1 (2%)	51,60,60	2.08	10 (19%)
27	BCR	8	503	-	41,41,41	1.85	4 (9%)	56,56,56	4.41	18 (32%)
24	CLA	8	602	-	56,60,73	1.52	7 (12%)	67,97,113	2.09	18 (26%)
24	CLA	2	621	-	54,58,73	1.55	8 (14%)	65,95,113	2.19	18 (27%)
28	LHG	7	801	-	48,48,48	0.39	0	51,54,54	1.09	3 (5%)
24	CLA	A	1107	1	59,63,73	1.47	6 (10%)	71,101,113	2.06	18 (25%)
38	LPX	a	804	-	29,29,29	1.02	2 (6%)	31,33,33	0.97	1 (3%)
24	CLA	7	605	-	47,52,73	1.66	8 (17%)	56,88,113	1.95	14 (25%)
24	CLA	5	616	-	50,54,73	1.61	8 (16%)	60,90,113	2.04	15 (25%)
24	CLA	B	1240	-	69,73,73	1.36	7 (10%)	83,113,113	1.97	21 (25%)
43	QTB	a	504	-	19,19,19	2.45	5 (26%)	20,26,26	2.77	8 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	4	603	-	60,64,73	1.44	7 (11%)	72,102,113	2.07	18 (25%)
24	CLA	B	1022	-	69,73,73	1.37	7 (10%)	83,113,113	1.89	21 (25%)
24	CLA	A	1114	-	69,73,73	1.36	6 (8%)	83,113,113	1.97	19 (22%)

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
27	BCR	J	4001	-	-	10/29/63/63	0/2/2/2
24	CLA	1	602	-	-	9/15/91/115	-
24	CLA	a	611	-	-	10/21/97/115	-
24	CLA	B	1203	-	-	17/39/115/115	-
24	CLA	A	1129	1	-	12/21/97/115	-
24	CLA	A	1118	1	-	16/27/103/115	-
24	CLA	K	1403	9	-	11/17/93/115	-
32	PCW	6	803	-	-	16/39/39/57	-
24	CLA	9	606	-	-	8/27/103/115	-
24	CLA	5	606	-	-	7/21/97/115	-
24	CLA	B	1231	-	-	15/39/115/115	-
24	CLA	4	604	-	-	12/33/109/115	-
24	CLA	A	1136	-	-	20/39/115/115	-
24	CLA	A	1141	28	-	12/15/91/115	-
24	CLA	6	612	-	-	12/21/97/115	-
28	LHG	2	802	-	-	35/53/53/53	-
24	CLA	A	1101	-	-	15/39/115/115	-
24	CLA	A	1113	1	-	7/24/100/115	-
50	4RF	7	807	-	-	10/34/34/59	-
24	CLA	A	1134	1	-	17/33/109/115	-
37	RRX	J	4002	-	1/1/11/25	9/29/65/65	0/2/2/2
24	CLA	B	1215	-	-	20/33/109/115	-
24	CLA	B	1218	2	-	11/27/103/115	-
28	LHG	6	801	-	-	29/53/53/53	-
24	CLA	1	601	-	-	10/33/109/115	-
33	PTY	9	803	-	-	27/51/51/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	7	603	-	-	23/39/115/115	-
23	CL0	A	1011	-	-	7/39/115/115	-
24	CLA	A	1117	-	-	23/39/115/115	-
28	LHG	7	802	-	-	20/40/40/53	-
24	CLA	B	1213	2	-	11/33/109/115	-
28	LHG	1	801	-	-	26/39/39/53	-
26	SF4	C	3003	3	-	-	0/6/5/5
27	BCR	G	4001	-	-	14/29/63/63	0/2/2/2
24	CLA	B	1206	-	-	14/27/103/115	-
24	CLA	5	612	-	-	16/39/115/115	-
26	SF4	A	3001	1,2	-	-	0/6/5/5
24	CLA	G	1602	-	-	10/17/93/115	-
24	CLA	8	620	20	-	18/39/115/115	-
41	CHL	8	601	-	1/1/14/21	6/35/111/117	-
24	CLA	4	606	-	-	6/21/97/115	-
24	CLA	4	616	-	-	8/21/97/115	-
24	CLA	B	1236	-	-	9/25/101/115	-
41	CHL	6	619	18	1/1/15/21	13/41/117/117	-
27	BCR	B	4003	-	-	12/29/63/63	0/2/2/2
24	CLA	5	608	-	-	7/15/91/115	-
24	CLA	6	617	-	-	6/15/91/115	-
40	LUT	1	503	-	1/1/12/27	4/29/67/67	0/2/2/2
24	CLA	A	1140	-	-	10/27/103/115	-
24	CLA	A	1103	1	-	24/39/115/115	-
24	CLA	B	1226	-	-	14/39/115/115	-
24	CLA	5	603	-	-	20/29/105/115	-
44	GG0	a	805	-	-	2/7/7/7	-
46	DGA	5	803	-	-	13/24/24/45	-
24	CLA	L	1503	-	-	6/15/91/115	-
24	CLA	2	605	-	-	16/33/109/115	-
24	CLA	A	1137	-	-	13/33/109/115	-
40	LUT	5	502	-	-	5/29/67/67	0/2/2/2
31	LMT	1	804	-	-	8/21/61/61	0/2/2/2
24	CLA	B	1232	-	-	9/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	1221	-	-	14/39/115/115	-
40	LUT	7	501	-	1/1/12/27	6/29/67/67	0/2/2/2
40	LUT	3	502	-	-	1/29/67/67	0/2/2/2
24	CLA	A	1104	-	-	18/39/115/115	-
24	CLA	a	615	-	-	6/17/93/115	-
34	LAP	B	5007	-	-	15/30/30/30	-
33	PTY	7	804	-	-	17/36/36/53	-
27	BCR	A	4005	-	-	15/29/63/63	0/2/2/2
24	CLA	B	1207	-	-	14/33/109/115	-
24	CLA	8	612	20	-	13/17/93/115	-
24	CLA	7	615	19	-	13/27/103/115	-
24	CLA	9	608	-	-	6/15/91/115	-
24	CLA	3	618	-	-	8/17/93/115	-
24	CLA	B	1201	-	-	14/39/115/115	-
50	4RF	8	807	-	-	25/44/44/59	-
27	BCR	B	4002	-	-	13/29/63/63	0/2/2/2
24	CLA	B	1230	-	-	15/31/107/115	-
27	BCR	K	4001	-	-	10/29/63/63	0/2/2/2
24	CLA	9	612	-	-	21/39/115/115	-
40	LUT	6	502	-	1/1/12/27	7/29/67/67	0/2/2/2
24	CLA	9	609	-	-	8/17/93/115	-
24	CLA	F	1302	-	-	11/27/103/115	-
24	CLA	9	605	-	-	15/33/109/115	-
40	LUT	2	502	-	-	3/29/67/67	0/2/2/2
27	BCR	H	4001	-	-	11/29/63/63	0/2/2/2
40	LUT	6	501	-	1/1/12/27	8/29/67/67	0/2/2/2
24	CLA	A	1109	24	-	18/39/115/115	-
40	LUT	8	502	-	-	2/29/67/67	0/2/2/2
24	CLA	2	602	-	-	9/24/100/115	-
24	CLA	A	1135	-	-	19/39/115/115	-
24	CLA	A	1123	-	-	20/39/115/115	-
24	CLA	a	612	-	-	12/30/106/115	-
24	CLA	1	603	-	-	21/39/115/115	-
24	CLA	4	612	-	-	21/36/112/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	1138	-	-	12/39/115/115	-
27	BCR	A	4004	-	-	12/29/63/63	0/2/2/2
24	CLA	B	1227	-	-	9/21/97/115	-
42	OLA	8	809	-	-	10/17/17/17	-
28	LHG	a	801	-	-	23/39/39/53	-
41	CHL	9	613	-	-	1/12/88/117	-
36	ERG	G	5002	-	4/4/11/15	7/13/71/71	0/4/4/4
29	DGD	B	5003	-	-	16/55/95/95	0/2/2/2
24	CLA	4	608	-	-	6/23/99/115	-
24	CLA	K	1402	-	-	17/33/109/115	-
27	BCR	B	4004	-	-	12/29/63/63	0/2/2/2
40	LUT	a	502	-	-	1/29/67/67	0/2/2/2
40	LUT	4	502	-	-	3/29/67/67	0/2/2/2
27	BCR	A	4002	-	-	9/29/63/63	0/2/2/2
24	CLA	5	617	-	-	11/21/97/115	-
24	CLA	A	1130	-	-	15/29/105/115	-
30	3PH	A	5007	-	-	17/34/34/49	-
24	CLA	3	603	-	-	14/39/115/115	-
28	LHG	A	5003	-	-	24/46/46/53	-
25	PQN	A	2001	-	-	8/23/43/43	0/2/2/2
32	PCW	B	5004	-	-	19/33/33/57	-
24	CLA	L	1502	-	-	17/33/109/115	-
24	CLA	4	617	-	-	9/15/91/115	-
45	PLM	6	804	-	-	4/15/15/15	-
42	OLA	1	803	-	-	5/17/17/17	-
24	CLA	B	1208	-	-	15/33/109/115	-
27	BCR	3	504	-	-	12/29/63/63	0/2/2/2
24	CLA	5	609	17	-	13/23/99/115	-
24	CLA	B	1239	-	-	15/39/115/115	-
27	BCR	B	4005	-	-	11/29/63/63	0/2/2/2
24	CLA	6	608	-	-	5/15/91/115	-
31	LMT	A	5008	-	-	8/21/61/61	0/2/2/2
40	LUT	9	501	-	-	2/29/67/67	0/2/2/2
40	LUT	5	501	-	-	3/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	1013	-	-	13/39/115/115	-
27	BCR	B	4001	-	-	10/29/63/63	0/2/2/2
28	LHG	6	802	-	-	23/41/41/53	-
24	CLA	8	611	-	-	10/21/97/115	-
28	LHG	A	5002	-	-	32/53/53/53	-
24	CLA	A	1115	1	-	18/33/109/115	-
24	CLA	A	1125	-	-	21/39/115/115	-
27	BCR	B	4006	-	-	11/29/63/63	0/2/2/2
24	CLA	A	1111	-	-	19/39/115/115	-
24	CLA	5	607	-	-	12/27/103/115	-
24	CLA	6	615	-	-	20/39/115/115	-
31	LMT	2	804	-	-	6/21/61/61	0/2/2/2
24	CLA	2	607	-	-	8/17/93/115	-
24	CLA	2	604	-	-	16/29/105/115	-
24	CLA	A	1139	1	-	14/27/103/115	-
24	CLA	7	607	-	-	18/31/107/115	-
24	CLA	1	608	-	-	17/33/109/115	-
41	CHL	9	610	-	-	4/23/99/117	-
24	CLA	7	604	-	-	13/39/115/115	-
28	LHG	9	802	-	-	31/53/53/53	-
26	SF4	C	3002	3	-	-	0/6/5/5
24	CLA	G	1601	-	-	12/21/97/115	-
24	CLA	B	1223	2	-	20/39/115/115	-
31	LMT	B	5006	-	-	15/21/61/61	0/2/2/2
24	CLA	3	607	-	-	18/39/115/115	-
41	CHL	3	608	-	-	7/14/90/117	-
24	CLA	1	612	-	-	24/39/115/115	-
24	CLA	6	607	-	-	12/27/103/115	-
24	CLA	7	611	-	-	11/33/109/115	-
27	BCR	L	4001	-	-	12/29/63/63	0/2/2/2
24	CLA	4	610	-	-	26/39/115/115	-
52	A8S	9	504	-	-	2/10/34/34	0/1/1/1
27	BCR	I	4001	-	-	12/29/63/63	0/2/2/2
40	LUT	4	501	-	-	2/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	1120	-	-	10/20/96/115	-
50	4RF	8	808	-	-	24/56/56/59	-
41	CHL	1	609	14	1/1/15/21	11/41/117/117	-
24	CLA	7	608	-	-	7/12/88/115	-
34	LAP	K	5001	-	-	12/30/30/30	-
24	CLA	8	609	20	-	21/33/109/115	-
49	C7Z	7	504	-	1/1/12/26	10/29/67/67	0/2/2/2
24	CLA	A	1108	1	-	22/39/115/115	-
24	CLA	9	604	-	-	9/33/109/115	-
41	CHL	a	609	-	-	6/26/102/117	-
24	CLA	G	1603	-	-	5/15/91/115	-
24	CLA	6	605	18	-	6/17/93/115	-
27	BCR	5	504	-	-	11/29/63/63	0/2/2/2
24	CLA	a	603	-	-	15/39/115/115	-
24	CLA	9	601	-	-	16/33/109/115	-
28	LHG	B	5002	-	-	28/53/53/53	-
24	CLA	3	613	-	-	11/35/111/115	-
28	LHG	4	801	-	-	28/53/53/53	-
40	LUT	3	501	-	-	3/29/67/67	0/2/2/2
41	CHL	7	613	-	1/1/15/21	6/41/117/117	-
24	CLA	A	1119	-	-	20/39/115/115	-
24	CLA	H	1702	-	-	9/17/93/115	-
40	LUT	1	502	-	-	1/29/67/67	0/2/2/2
24	CLA	2	610	-	-	9/17/93/115	-
24	CLA	A	1012	-	-	17/39/115/115	-
24	CLA	7	602	-	-	7/13/90/115	-
24	CLA	B	1021	-	-	19/39/115/115	-
24	CLA	B	1205	-	-	10/39/115/115	-
24	CLA	A	1112	-	-	15/27/103/115	-
27	BCR	6	503	-	-	12/29/63/63	0/2/2/2
24	CLA	A	1131	-	-	16/39/115/115	-
24	CLA	6	602	-	-	6/24/100/115	-
27	BCR	F	4001	-	-	14/29/63/63	0/2/2/2
40	LUT	a	501	-	-	8/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	7	612	-	-	13/33/109/115	-
24	CLA	3	610	15	-	13/33/109/115	-
24	CLA	K	1404	-	-	10/24/100/115	-
41	CHL	5	613	-	1/1/13/21	1/29/105/117	-
24	CLA	B	1209	-	-	16/39/115/115	-
28	LHG	5	801	-	-	26/53/53/53	-
24	CLA	K	1401	-	-	8/17/93/115	-
24	CLA	5	605	-	-	7/17/93/115	-
24	CLA	a	607	-	-	15/31/107/115	-
41	CHL	8	604	-	1/1/14/21	14/37/113/117	-
24	CLA	2	606	-	-	10/17/93/115	-
24	CLA	A	1128	-	-	15/39/115/115	-
27	BCR	B	4007	-	-	13/29/63/63	0/2/2/2
24	CLA	3	601	-	-	15/39/115/115	-
27	BCR	A	4003	-	-	11/29/63/63	0/2/2/2
24	CLA	A	1133	1	-	17/39/115/115	-
24	CLA	8	607	-	-	6/17/93/115	-
24	CLA	A	1121	-	-	16/30/106/115	-
24	CLA	1	611	-	-	10/27/103/115	-
41	CHL	4	609	16	1/1/15/21	9/41/117/117	-
24	CLA	6	618	-	-	11/17/93/115	-
27	BCR	5	503	-	-	13/29/63/63	0/2/2/2
24	CLA	H	1703	-	-	10/27/103/115	-
28	LHG	3	801	-	-	31/53/53/53	-
35	SQD	H	5001	-	-	8/40/60/69	0/1/1/1
24	CLA	A	1116	-	-	16/33/109/115	-
40	LUT	9	502	-	1/1/12/27	7/29/67/67	0/2/2/2
48	XAT	7	502	-	2/2/12/26	1/31/93/93	0/4/4/4
24	CLA	B	1222	-	-	4/31/107/115	-
33	PTY	5	802	-	-	19/41/41/53	-
28	LHG	4	802	-	-	22/36/36/53	-
24	CLA	a	608	-	-	16/27/103/115	-
24	CLA	A	1105	-	-	11/30/106/115	-
24	CLA	4	615	16	-	18/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	CHL	5	611	-	-	3/23/99/117	-
24	CLA	B	1212	-	-	22/39/115/115	-
38	LPX	J	5001	-	-	11/18/18/31	-
24	CLA	F	1301	-	-	9/21/97/115	-
24	CLA	B	1214	-	-	21/36/112/115	-
29	DGD	A	5005	-	-	12/40/80/95	0/2/2/2
24	CLA	2	612	-	-	10/21/97/115	-
24	CLA	A	1127	-	-	16/39/115/115	-
24	CLA	6	601	-	-	19/33/109/115	-
24	CLA	7	606	-	-	17/27/103/115	-
24	CLA	8	605	-	-	8/15/91/115	-
41	CHL	4	613	-	-	4/25/101/117	-
33	PTY	8	891	-	-	14/38/38/53	-
24	CLA	a	605	-	-	19/39/115/115	-
39	ECH	M	4001	-	-	5/29/66/66	0/2/2/2
41	CHL	6	610	-	1/1/13/21	6/29/105/117	-
24	CLA	4	607	-	-	15/27/103/115	-
24	CLA	9	602	-	-	6/17/93/115	-
24	CLA	1	610	-	-	9/15/91/115	-
24	CLA	5	602	-	-	9/24/100/115	-
24	CLA	2	601	-	-	15/33/109/115	-
24	CLA	3	606	-	-	21/39/115/115	-
28	LHG	9	801	-	-	22/37/37/53	-
24	CLA	B	1204	-	-	20/39/115/115	-
24	CLA	2	608	-	-	7/15/91/115	-
24	CLA	8	606	-	-	17/30/106/115	-
24	CLA	B	1224	-	-	23/39/115/115	-
24	CLA	6	609	18	-	19/39/115/115	-
40	LUT	1	501	-	-	5/29/67/67	0/2/2/2
24	CLA	2	615	-	-	15/30/106/115	-
24	CLA	5	614	-	-	6/17/93/115	-
24	CLA	8	618	-	-	17/33/109/115	-
24	CLA	8	610	-	-	18/27/103/115	-
24	CLA	4	611	-	-	11/29/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	2	609	21	-	10/27/103/115	-
47	SPH	6	806	-	-	7/21/21/21	-
24	CLA	7	601	-	-	17/33/109/115	-
41	CHL	5	610	-	1/1/15/21	7/41/117/117	-
24	CLA	5	601	-	-	13/33/109/115	-
24	CLA	1	606	-	-	16/30/106/115	-
24	CLA	A	1132	-	-	15/39/115/115	-
34	LAP	F	5003	-	-	17/30/30/30	-
41	CHL	a	613	-	1/1/11/21	5/17/93/117	-
24	CLA	L	1501	13	-	13/21/97/115	-
24	CLA	4	605	-	-	7/17/93/115	-
24	CLA	5	618	17	-	6/24/100/115	-
40	LUT	8	501	-	-	2/29/67/67	0/2/2/2
41	CHL	6	613	-	-	5/23/99/117	-
24	CLA	6	603	-	-	18/39/115/115	-
24	CLA	2	613	-	-	4/10/86/115	-
45	PLM	4	803	-	-	2/13/14/15	-
24	CLA	B	1023	-	-	13/39/115/115	-
24	CLA	7	609	19	-	17/33/109/115	-
24	CLA	B	1229	-	-	13/39/115/115	-
24	CLA	3	616	-	-	13/29/105/115	-
24	CLA	7	610	-	-	14/27/103/115	-
27	BCR	L	4003	-	-	12/29/63/63	0/2/2/2
27	BCR	4	503	-	-	13/29/63/63	0/2/2/2
24	CLA	3	604	-	-	9/33/109/115	-
24	CLA	4	602	-	-	7/24/100/115	-
27	BCR	6	504	-	-	9/29/63/63	0/2/2/2
24	CLA	B	1219	-	-	11/32/108/115	-
24	CLA	J	1901	8	-	7/12/88/115	-
28	LHG	7	803	-	-	25/47/47/53	-
41	CHL	a	610	-	1/1/11/21	1/20/96/117	-
24	CLA	B	1228	-	-	18/39/115/115	-
24	CLA	6	604	-	-	16/39/115/115	-
28	LHG	8	801	-	-	28/41/41/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	1122	-	-	17/39/115/115	-
24	CLA	7	617	19	-	15/25/101/115	-
33	PTY	B	5005	-	-	26/44/44/53	-
24	CLA	B	1225	-	-	7/39/115/115	-
27	BCR	3	505	-	-	11/29/63/63	0/2/2/2
40	LUT	a	503	-	-	5/29/67/67	0/2/2/2
27	BCR	3	503	-	-	12/29/63/63	0/2/2/2
41	CHL	4	618	16	1/1/13/21	6/29/105/117	-
28	LHG	B	5001	-	-	30/50/50/53	-
41	CHL	a	606	-	1/1/13/21	7/29/105/117	-
24	CLA	B	1202	2	-	17/39/115/115	-
24	CLA	3	602	-	-	5/17/93/115	-
28	LHG	F	5002	-	-	27/40/40/53	-
24	CLA	H	1701	-	-	12/27/103/115	-
40	LUT	5	505	-	-	7/29/67/67	0/2/2/2
28	LHG	1	802	-	-	29/46/46/53	-
24	CLA	3	605	15	-	21/39/115/115	-
27	BCR	K	4002	-	-	12/29/63/63	0/2/2/2
24	CLA	3	612	-	-	12/39/115/115	-
24	CLA	2	603	-	-	15/33/109/115	-
24	CLA	B	1220	-	-	19/33/109/115	-
24	CLA	a	601	-	-	13/33/109/115	-
24	CLA	4	601	-	-	10/33/109/115	-
24	CLA	A	1102	24	-	18/39/115/115	-
24	CLA	a	602	-	-	9/21/97/115	-
25	PQN	B	2002	-	-	5/23/43/43	0/2/2/2
41	CHL	3	611	-	-	5/28/104/117	-
24	CLA	5	604	-	-	16/39/115/115	-
27	BCR	L	4002	-	-	7/29/63/63	0/2/2/2
24	CLA	B	1211	-	-	14/27/103/115	-
41	CHL	6	611	-	-	2/23/99/117	-
35	SQD	G	5001	-	-	16/41/61/69	0/1/1/1
24	CLA	B	1235	2	-	13/39/115/115	-
24	CLA	A	1106	-	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	8	608	-	-	11/24/100/115	-
35	SQD	7	805	-	-	15/34/54/69	0/1/1/1
24	CLA	B	1217	2	-	15/29/105/115	-
24	CLA	6	606	-	-	14/24/100/115	-
24	CLA	B	1238	-	-	15/39/115/115	-
24	CLA	8	615	-	-	9/17/93/115	-
43	QTB	3	506	-	2/2/5/10	0/11/28/28	0/1/1/1
46	DGA	8	803	-	-	18/31/31/45	-
24	CLA	a	604	-	-	18/39/115/115	-
24	CLA	B	1234	-	-	11/29/105/115	-
24	CLA	A	1126	-	-	24/39/115/115	-
28	LHG	F	5001	-	-	24/47/47/53	-
24	CLA	1	604	-	-	21/39/115/115	-
28	LHG	A	5001	24	-	15/33/33/53	-
24	CLA	8	603	-	-	19/39/115/115	-
41	CHL	8	613	-	-	3/23/99/117	-
24	CLA	B	1210	-	-	20/39/115/115	-
24	CLA	9	607	-	-	13/18/94/115	-
24	CLA	B	1216	-	-	20/35/111/115	-
29	DGD	8	802	-	-	19/55/95/95	0/2/2/2
24	CLA	1	615	14	-	11/17/93/115	-
33	PTY	3	802	-	-	14/41/41/53	-
24	CLA	9	603	-	-	15/39/115/115	-
28	LHG	2	801	-	-	35/53/53/53	-
24	CLA	B	1237	-	-	21/39/115/115	-
24	CLA	A	1124	-	-	7/27/103/115	-
41	CHL	1	613	-	-	5/20/96/117	-
27	BCR	7	503	-	-	10/29/63/63	0/2/2/2
24	CLA	1	605	-	-	19/39/115/115	-
24	CLA	A	1110	1	-	15/33/109/115	-
24	CLA	1	607	-	-	8/39/115/115	-
51	P5S	8	806	-	-	16/42/42/59	-
27	BCR	A	4001	-	-	14/29/63/63	0/2/2/2
40	LUT	2	501	-	-	3/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	8	503	-	-	11/29/63/63	0/2/2/2
24	CLA	8	602	-	-	11/24/100/115	-
24	CLA	2	621	-	-	12/21/97/115	-
28	LHG	7	801	-	-	24/53/53/53	-
24	CLA	A	1107	1	-	10/27/103/115	-
38	LPX	a	804	-	-	8/31/31/31	-
24	CLA	7	605	-	-	3/13/89/115	-
24	CLA	5	616	-	-	11/17/93/115	-
24	CLA	B	1240	-	-	15/39/115/115	-
43	QTB	a	504	-	1/1/5/10	4/11/28/28	0/1/1/1
24	CLA	4	603	-	-	14/29/105/115	-
24	CLA	B	1022	-	-	14/39/115/115	-
24	CLA	A	1114	-	-	15/39/115/115	-

The worst 5 of 2027 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	G	5002	ERG	C1-C10	-23.39	1.09	1.54
36	G	5002	ERG	C10-C9	-21.00	1.27	1.55
49	7	504	C7Z	C25-C26	15.58	1.61	1.34
37	J	4002	RRX	C26-C25	15.42	1.61	1.34
49	7	504	C7Z	C5-C6	15.18	1.60	1.34

The worst 5 of 5405 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	2	601	CLA	C4-C3-C5	-22.53	77.37	115.27
24	2	601	CLA	C5-C3-C2	18.93	159.43	121.12
27	F	4001	BCR	C10-C11-C12	18.18	179.95	123.22
27	5	504	BCR	C10-C11-C12	17.97	179.29	123.22
27	H	4001	BCR	C10-C11-C12	17.82	178.83	123.22

5 of 29 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
36	G	5002	ERG	C14
36	G	5002	ERG	C24
36	G	5002	ERG	C9
36	G	5002	ERG	C20

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Mol	Chain	Res	Type	Atom
37	J	4002	RRX	C28

5 of 4852 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	1011	CL0	C2-C1-O2A-CGA
24	A	1101	CLA	C2A-CAA-CBA-CGA
24	A	1101	CLA	CBA-CGA-O2A-C1
24	A	1101	CLA	O1A-CGA-O2A-C1
24	A	1101	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

341 monomers are involved in 915 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	J	4001	BCR	4	0
24	1	602	CLA	1	0
24	a	611	CLA	1	0
24	B	1203	CLA	3	0
24	A	1129	CLA	2	0
24	A	1118	CLA	4	0
24	K	1403	CLA	1	0
32	6	803	PCW	2	0
24	9	606	CLA	2	0
24	5	606	CLA	2	0
24	B	1231	CLA	6	0
24	4	604	CLA	5	0
24	A	1136	CLA	6	0
24	A	1141	CLA	2	0
24	6	612	CLA	3	0
28	2	802	LHG	2	0
24	A	1101	CLA	5	0
24	A	1113	CLA	1	0
50	7	807	4RF	1	0
24	A	1134	CLA	3	0
37	J	4002	RRX	6	0
24	B	1215	CLA	4	0
24	B	1218	CLA	2	0
28	6	801	LHG	6	0
24	1	601	CLA	3	0
33	9	803	PTY	2	0
24	7	603	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	1011	CL0	6	0
24	A	1117	CLA	11	0
24	B	1213	CLA	1	0
28	1	801	LHG	4	0
26	C	3003	SF4	1	0
27	G	4001	BCR	3	0
24	B	1206	CLA	1	0
24	5	612	CLA	6	0
24	G	1602	CLA	1	0
24	8	620	CLA	1	0
41	8	601	CHL	5	0
24	4	606	CLA	1	0
24	B	1236	CLA	2	0
41	6	619	CHL	2	0
27	B	4003	BCR	4	0
24	5	608	CLA	1	0
24	6	617	CLA	1	0
24	A	1140	CLA	2	0
40	1	503	LUT	3	0
24	A	1103	CLA	6	0
24	B	1226	CLA	3	0
24	5	603	CLA	1	0
46	5	803	DGA	1	0
24	2	605	CLA	2	0
24	A	1137	CLA	4	0
40	5	502	LUT	4	0
24	B	1232	CLA	2	0
24	B	1221	CLA	4	0
40	7	501	LUT	3	0
40	3	502	LUT	4	0
24	A	1104	CLA	3	0
33	7	804	PTY	1	0
27	A	4005	BCR	6	0
24	B	1207	CLA	13	0
24	8	612	CLA	2	0
24	7	615	CLA	1	0
24	9	608	CLA	1	0
24	B	1201	CLA	4	0
50	8	807	4RF	1	0
27	B	4002	BCR	4	0
24	B	1230	CLA	2	0
27	K	4001	BCR	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	9	612	CLA	7	0
40	6	502	LUT	5	0
24	9	609	CLA	1	0
24	F	1302	CLA	3	0
40	2	502	LUT	9	0
27	H	4001	BCR	2	0
24	A	1109	CLA	5	0
40	6	501	LUT	7	0
40	8	502	LUT	11	0
24	A	1135	CLA	5	0
24	A	1123	CLA	6	0
24	a	612	CLA	6	0
24	1	603	CLA	7	0
24	4	612	CLA	4	0
24	A	1138	CLA	3	0
27	A	4004	BCR	6	0
24	B	1227	CLA	3	0
42	8	809	OLA	3	0
28	a	801	LHG	2	0
36	G	5002	ERG	6	0
29	B	5003	DGD	10	0
24	4	608	CLA	1	0
27	B	4004	BCR	6	0
40	a	502	LUT	5	0
40	4	502	LUT	4	0
27	A	4002	BCR	4	0
24	5	617	CLA	4	0
24	A	1130	CLA	2	0
24	3	603	CLA	6	0
28	A	5003	LHG	5	0
25	A	2001	PQN	5	0
32	B	5004	PCW	2	0
24	L	1502	CLA	2	0
45	6	804	PLM	2	0
42	1	803	OLA	2	0
24	B	1208	CLA	1	0
27	3	504	BCR	3	0
24	B	1239	CLA	4	0
27	B	4005	BCR	1	0
31	A	5008	LMT	3	0
40	9	501	LUT	4	0
40	5	501	LUT	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1013	CLA	8	0
27	B	4001	BCR	5	0
28	6	802	LHG	1	0
24	8	611	CLA	1	0
28	A	5002	LHG	2	0
24	A	1115	CLA	2	0
24	A	1125	CLA	4	0
27	B	4006	BCR	8	0
24	A	1111	CLA	5	0
24	5	607	CLA	1	0
24	6	615	CLA	5	0
31	2	804	LMT	1	0
24	2	607	CLA	1	0
24	2	604	CLA	10	0
24	A	1139	CLA	3	0
24	7	607	CLA	2	0
24	1	608	CLA	6	0
41	9	610	CHL	2	0
24	7	604	CLA	6	0
28	9	802	LHG	3	0
24	B	1223	CLA	2	0
31	B	5006	LMT	5	0
24	3	607	CLA	2	0
41	3	608	CHL	3	0
24	1	612	CLA	5	0
24	7	611	CLA	2	0
27	L	4001	BCR	5	0
24	4	610	CLA	3	0
52	9	504	A8S	1	0
27	I	4001	BCR	6	0
40	4	501	LUT	9	0
24	A	1120	CLA	4	0
50	8	808	4RF	2	0
41	1	609	CHL	6	0
24	7	608	CLA	5	0
34	K	5001	LAP	2	0
24	8	609	CLA	5	0
24	A	1108	CLA	4	0
24	9	604	CLA	4	0
41	a	609	CHL	3	0
24	G	1603	CLA	2	0
24	6	605	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	5	504	BCR	4	0
24	a	603	CLA	2	0
24	9	601	CLA	5	0
28	B	5002	LHG	2	0
24	3	613	CLA	3	0
28	4	801	LHG	3	0
40	3	501	LUT	6	0
41	7	613	CHL	4	0
24	A	1119	CLA	6	0
24	H	1702	CLA	2	0
40	1	502	LUT	4	0
24	A	1012	CLA	4	0
24	B	1021	CLA	5	0
24	B	1205	CLA	4	0
24	A	1112	CLA	2	0
27	6	503	BCR	1	0
24	A	1131	CLA	4	0
24	6	602	CLA	3	0
27	F	4001	BCR	7	0
40	a	501	LUT	2	0
24	7	612	CLA	6	0
24	3	610	CLA	2	0
24	K	1404	CLA	2	0
24	B	1209	CLA	5	0
28	5	801	LHG	1	0
41	5	613	CHL	1	0
24	K	1401	CLA	4	0
24	5	605	CLA	1	0
24	a	607	CLA	3	0
41	8	604	CHL	4	0
24	A	1128	CLA	6	0
27	B	4007	BCR	2	0
24	3	601	CLA	3	0
27	A	4003	BCR	5	0
24	A	1133	CLA	9	0
24	8	607	CLA	2	0
24	A	1121	CLA	4	0
24	1	611	CLA	2	0
41	4	609	CHL	6	0
24	6	618	CLA	2	0
27	5	503	BCR	2	0
24	H	1703	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	3	801	LHG	5	0
35	H	5001	SQD	6	0
24	A	1116	CLA	9	0
24	B	1222	CLA	5	0
33	5	802	PTY	3	0
40	9	502	LUT	7	0
48	7	502	XAT	3	0
24	A	1105	CLA	1	0
24	4	615	CLA	2	0
41	5	611	CHL	2	0
24	B	1212	CLA	4	0
38	J	5001	LPX	1	0
24	F	1301	CLA	3	0
24	B	1214	CLA	6	0
29	A	5005	DGD	3	0
24	2	612	CLA	4	0
24	A	1127	CLA	7	0
24	6	601	CLA	9	0
24	7	606	CLA	1	0
24	8	605	CLA	1	0
41	4	613	CHL	1	0
33	8	891	PTY	2	0
24	a	605	CLA	5	0
39	M	4001	ECH	4	0
41	6	610	CHL	3	0
24	4	607	CLA	1	0
24	1	610	CLA	1	0
24	5	602	CLA	1	0
24	2	601	CLA	4	0
24	3	606	CLA	4	0
28	9	801	LHG	3	0
24	B	1204	CLA	7	0
24	2	608	CLA	1	0
24	8	606	CLA	3	0
24	B	1224	CLA	7	0
24	6	609	CLA	4	0
40	1	501	LUT	5	0
24	2	615	CLA	4	0
24	8	618	CLA	2	0
24	8	610	CLA	5	0
24	4	611	CLA	5	0
24	2	609	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	6	806	SPH	1	0
24	7	601	CLA	5	0
41	5	610	CHL	10	0
24	5	601	CLA	5	0
24	1	606	CLA	2	0
24	A	1132	CLA	3	0
34	F	5003	LAP	3	0
41	a	613	CHL	2	0
24	L	1501	CLA	3	0
24	4	605	CLA	1	0
24	5	618	CLA	1	0
40	8	501	LUT	4	0
41	6	613	CHL	2	0
24	6	603	CLA	3	0
45	4	803	PLM	1	0
24	B	1023	CLA	9	0
24	7	609	CLA	3	0
24	B	1229	CLA	4	0
24	3	616	CLA	5	0
24	7	610	CLA	1	0
27	L	4003	BCR	2	0
27	4	503	BCR	1	0
24	3	604	CLA	2	0
27	6	504	BCR	3	0
24	B	1219	CLA	3	0
24	J	1901	CLA	1	0
41	a	610	CHL	1	0
24	B	1228	CLA	6	0
24	6	604	CLA	3	0
28	8	801	LHG	1	0
24	A	1122	CLA	6	0
24	7	617	CLA	4	0
33	B	5005	PTY	2	0
24	B	1225	CLA	7	0
27	3	505	BCR	3	0
40	a	503	LUT	3	0
27	3	503	BCR	4	0
41	4	618	CHL	3	0
28	B	5001	LHG	3	0
41	a	606	CHL	7	0
24	B	1202	CLA	7	0
28	F	5002	LHG	2	0

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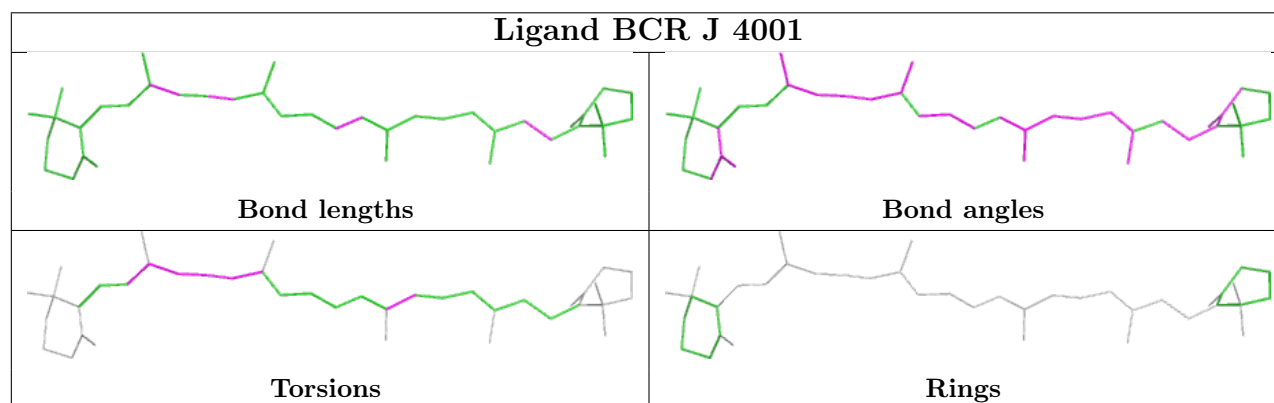
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	H	1701	CLA	3	0
40	5	505	LUT	8	0
28	1	802	LHG	2	0
24	3	605	CLA	4	0
27	K	4002	BCR	1	0
24	3	612	CLA	6	0
24	2	603	CLA	6	0
24	B	1220	CLA	8	0
24	a	601	CLA	4	0
24	4	601	CLA	7	0
24	A	1102	CLA	6	0
24	a	602	CLA	1	0
25	B	2002	PQN	7	0
41	3	611	CHL	4	0
24	5	604	CLA	1	0
27	L	4002	BCR	3	0
24	B	1211	CLA	1	0
41	6	611	CHL	2	0
35	G	5001	SQD	2	0
24	B	1235	CLA	5	0
24	A	1106	CLA	5	0
24	8	608	CLA	1	0
35	7	805	SQD	1	0
24	B	1217	CLA	3	0
24	B	1238	CLA	3	0
24	8	615	CLA	1	0
46	8	803	DGA	2	0
24	a	604	CLA	3	0
24	B	1234	CLA	4	0
24	A	1126	CLA	12	0
28	F	5001	LHG	3	0
24	1	604	CLA	7	0
28	A	5001	LHG	3	0
24	8	603	CLA	2	0
41	8	613	CHL	3	0
24	B	1210	CLA	4	0
24	B	1216	CLA	3	0
29	8	802	DGD	8	0
24	1	615	CLA	2	0
33	3	802	PTY	1	0
24	9	603	CLA	5	0
28	2	801	LHG	4	0

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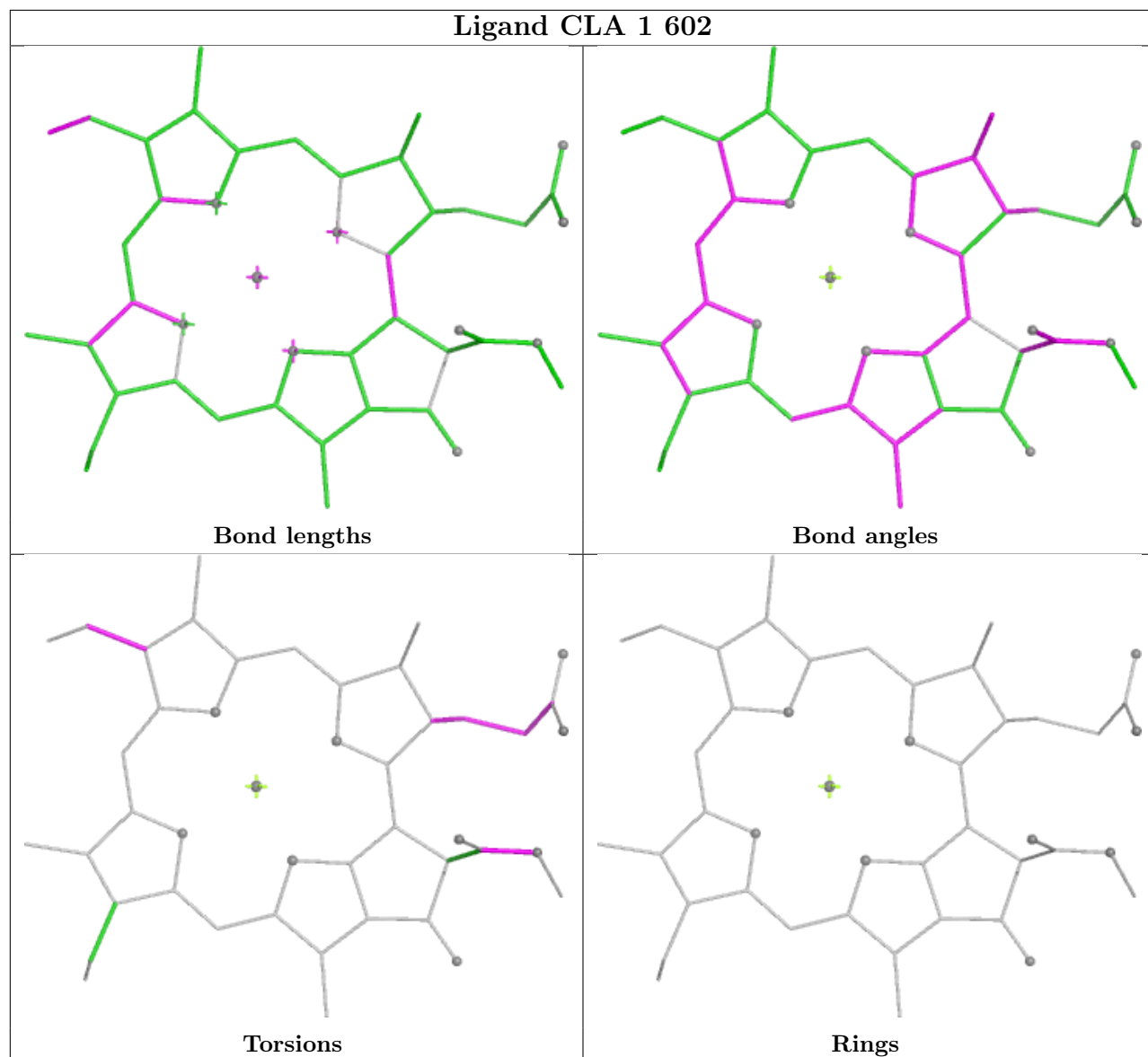
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	1237	CLA	1	0
24	A	1124	CLA	3	0
41	1	613	CHL	2	0
27	7	503	BCR	2	0
24	1	605	CLA	4	0
24	A	1110	CLA	3	0
24	1	607	CLA	2	0
27	A	4001	BCR	5	0
40	2	501	LUT	4	0
27	8	503	BCR	1	0
24	8	602	CLA	1	0
24	2	621	CLA	4	0
28	7	801	LHG	4	0
24	A	1107	CLA	3	0
24	7	605	CLA	2	0
24	5	616	CLA	1	0
24	B	1240	CLA	5	0
24	4	603	CLA	3	0
24	B	1022	CLA	4	0
24	A	1114	CLA	3	0

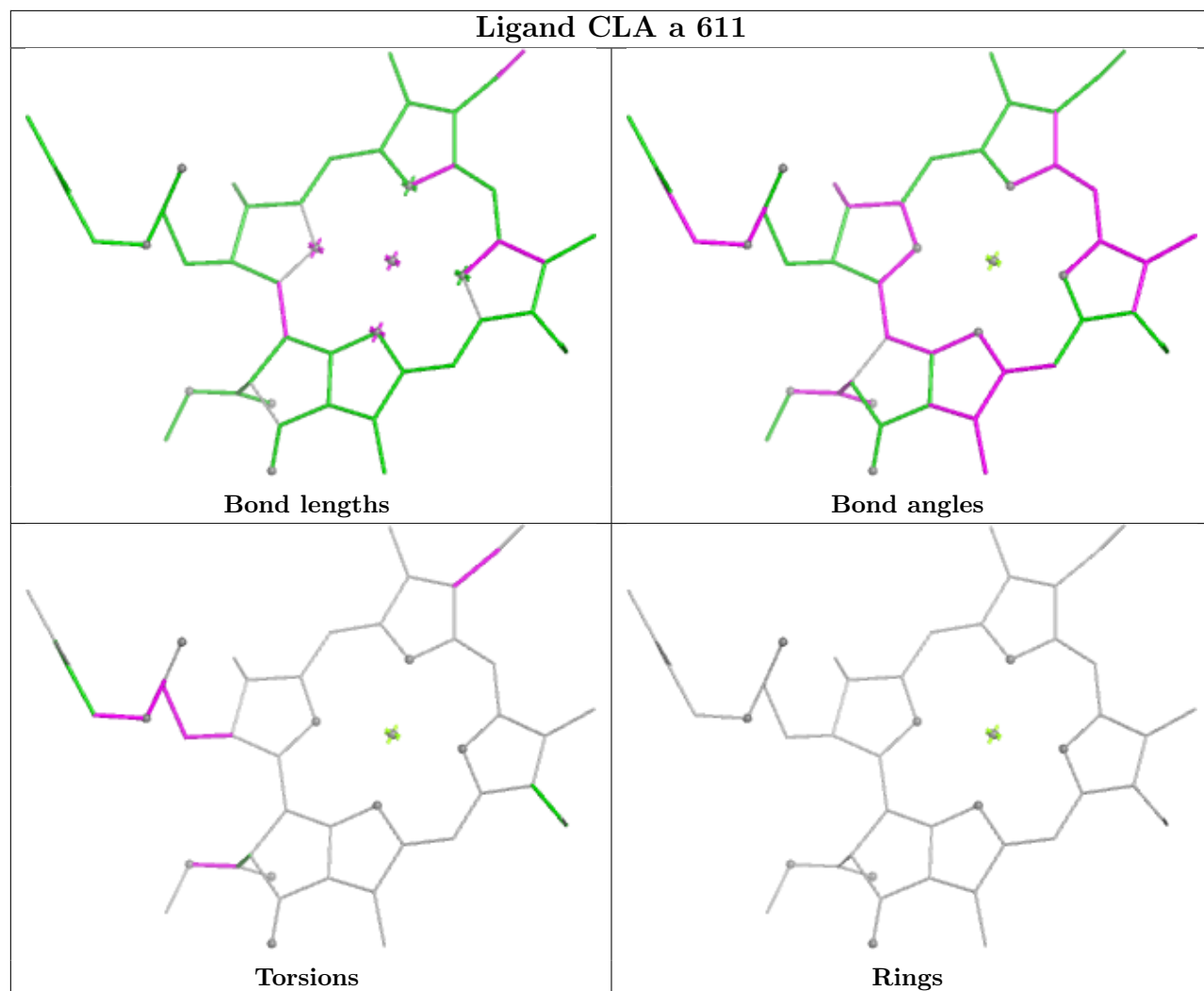
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

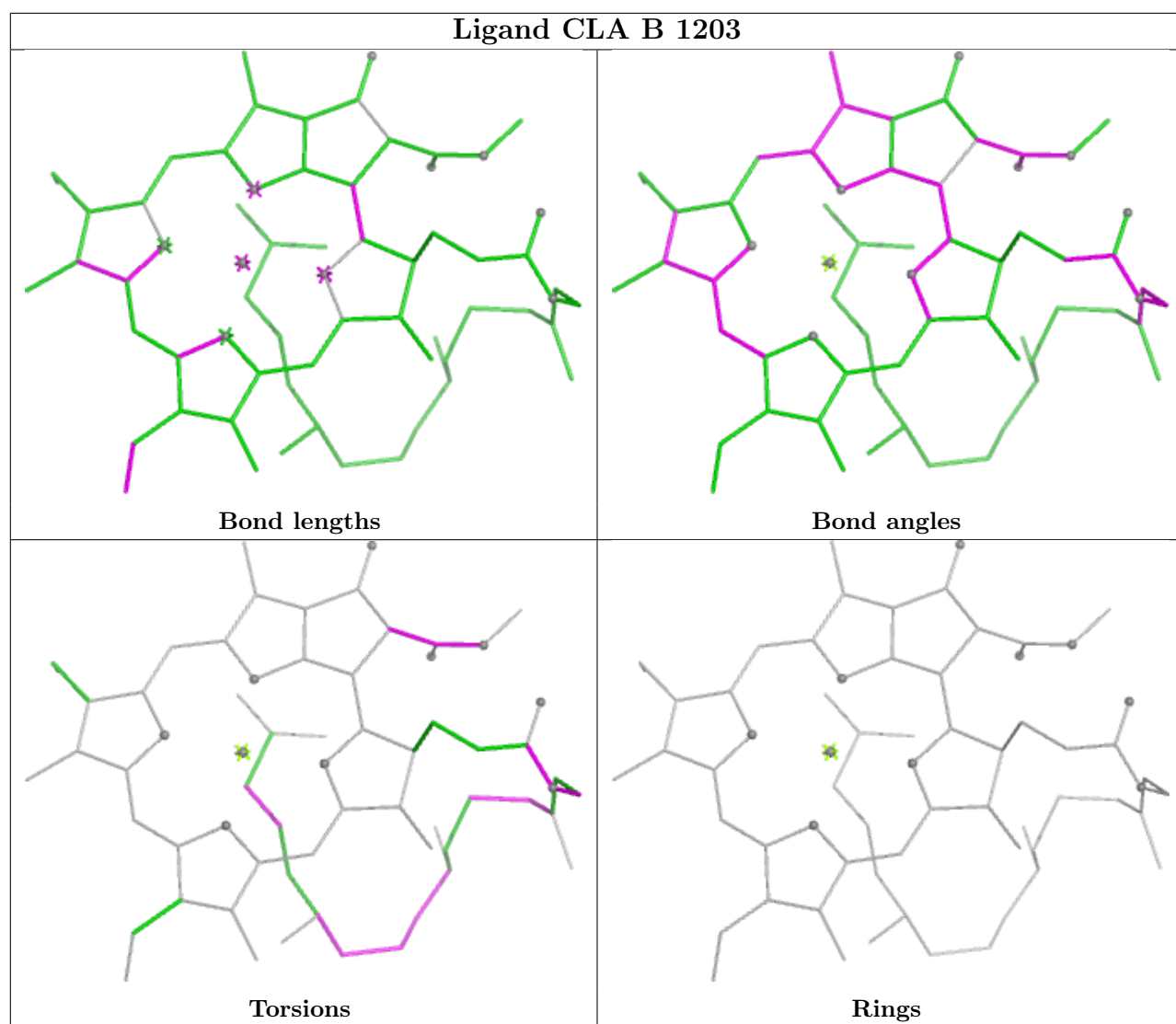


Ligand CLA 1 602

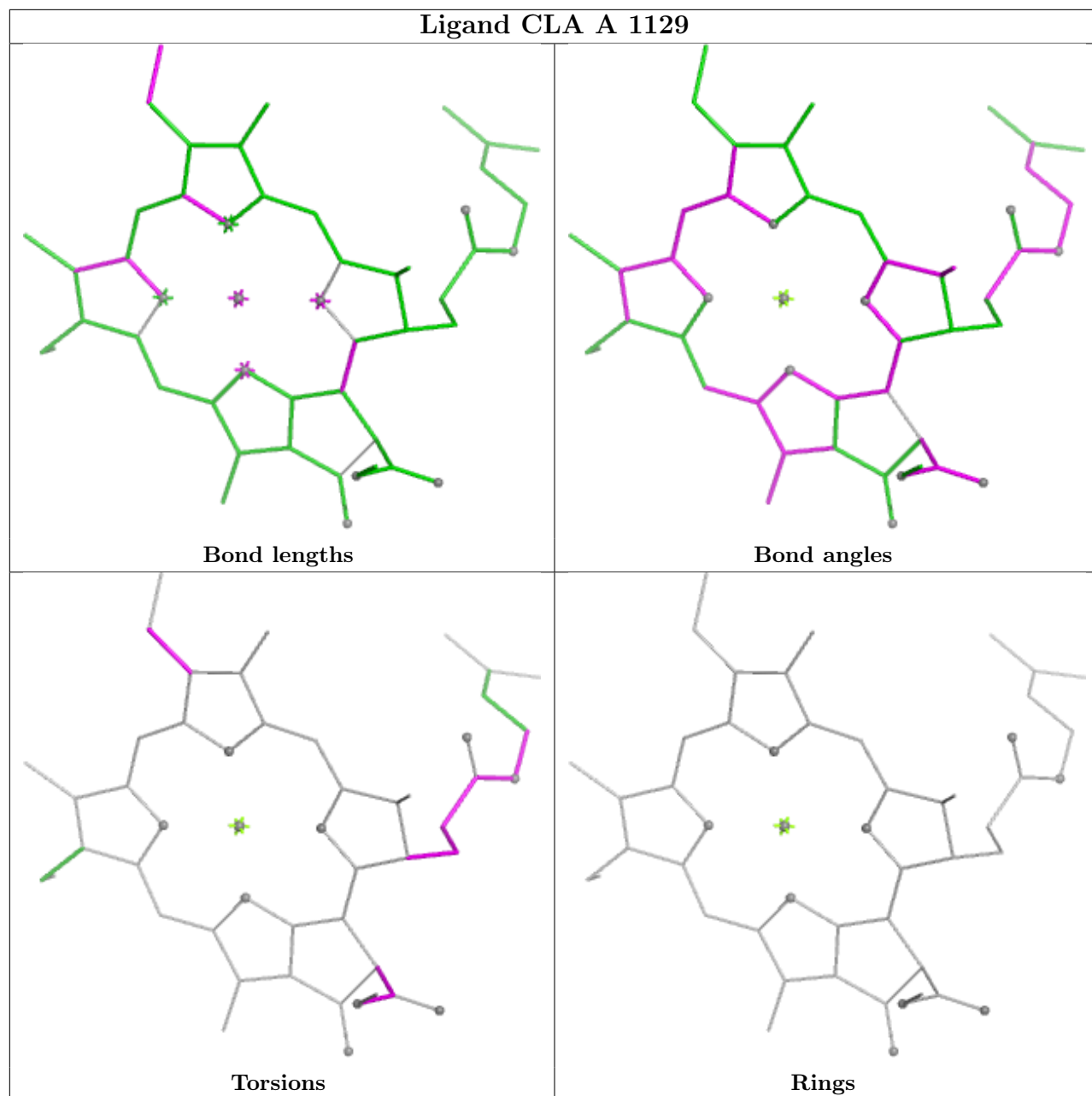


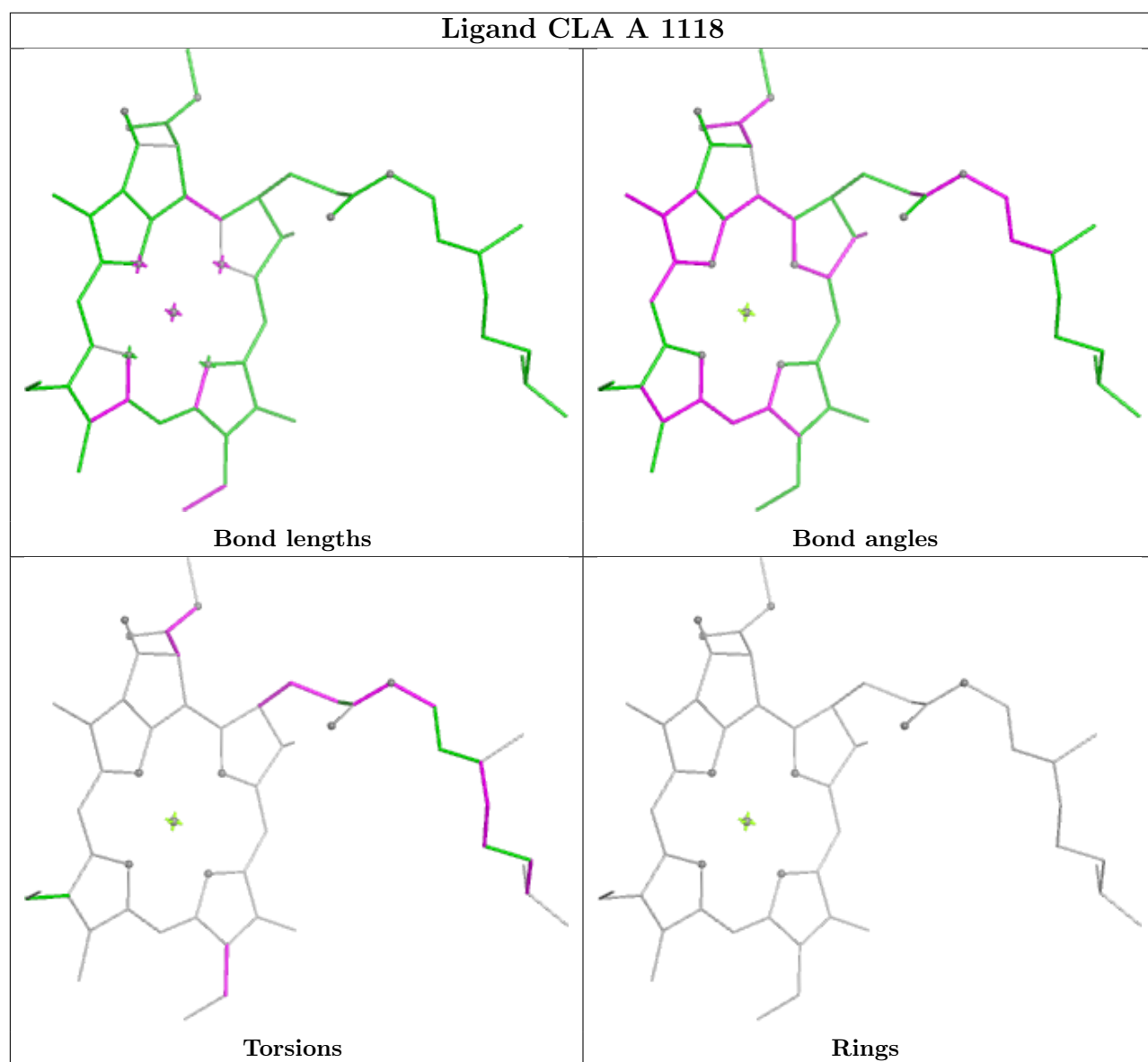
Ligand CLA a 611



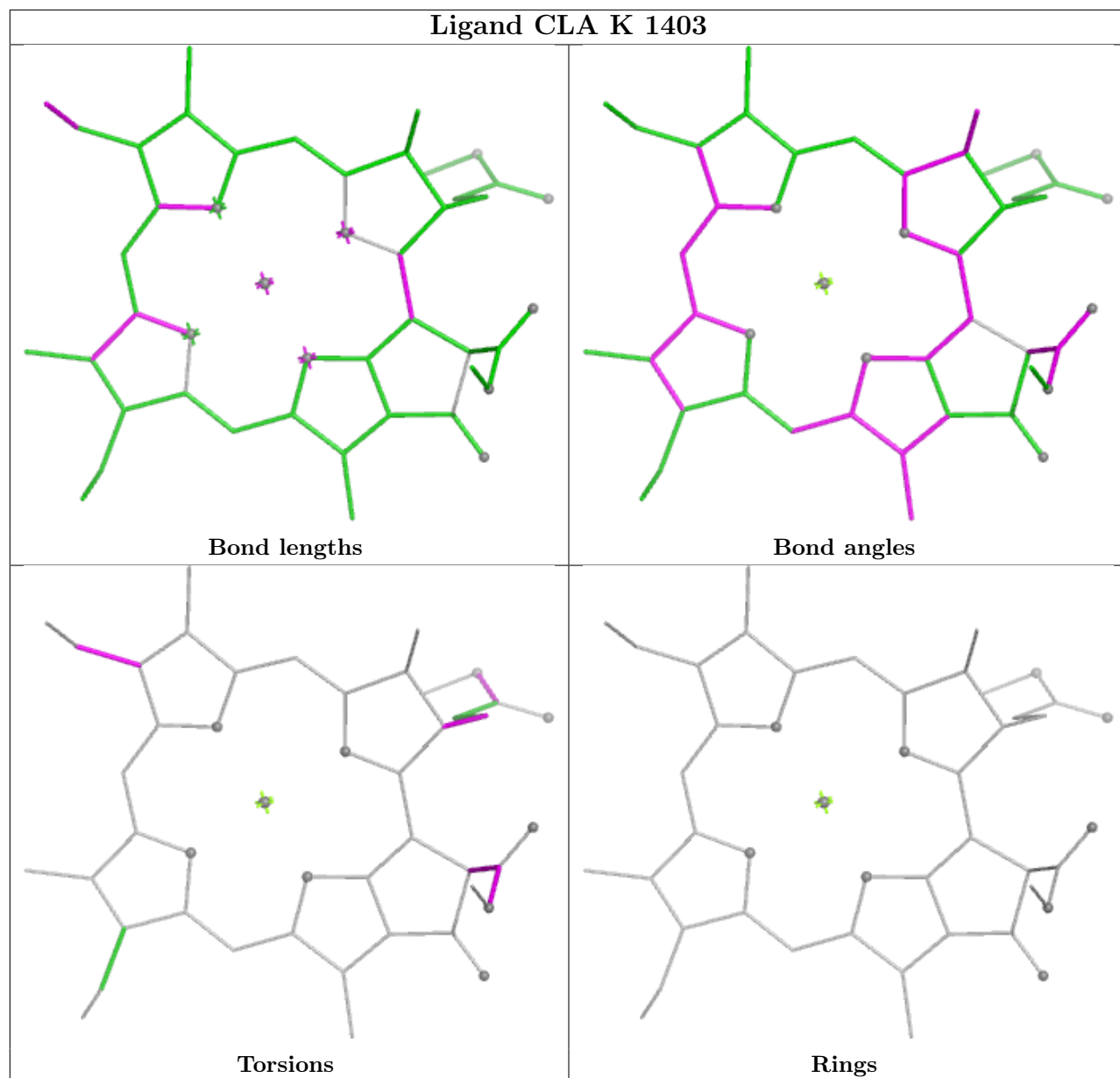


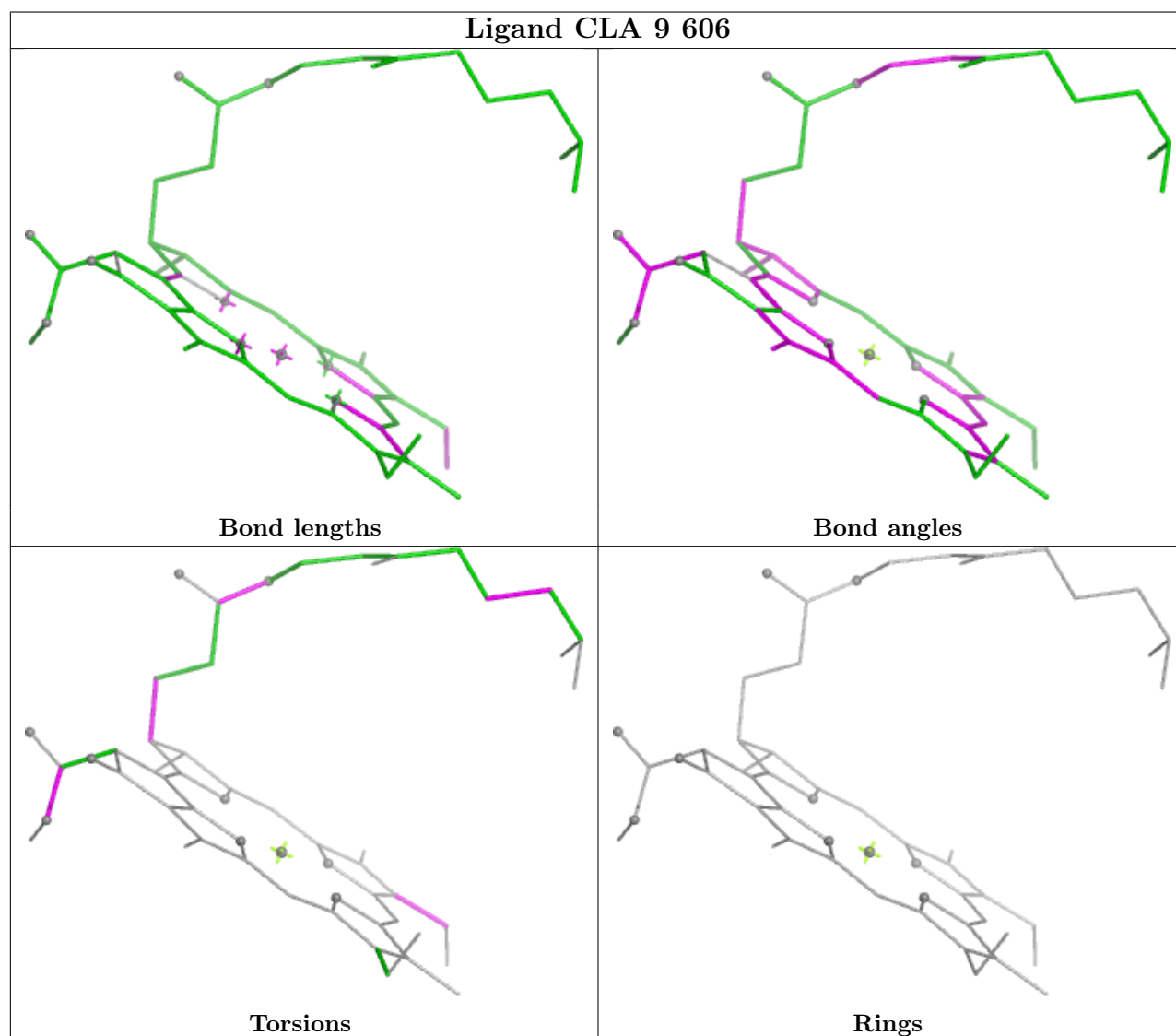
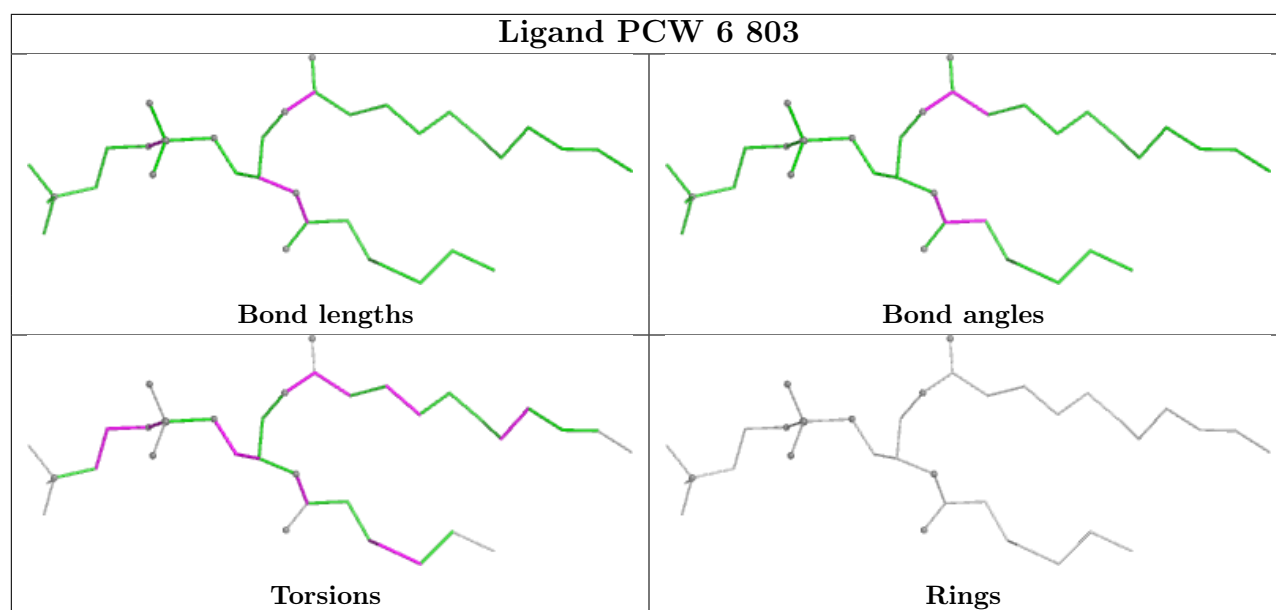
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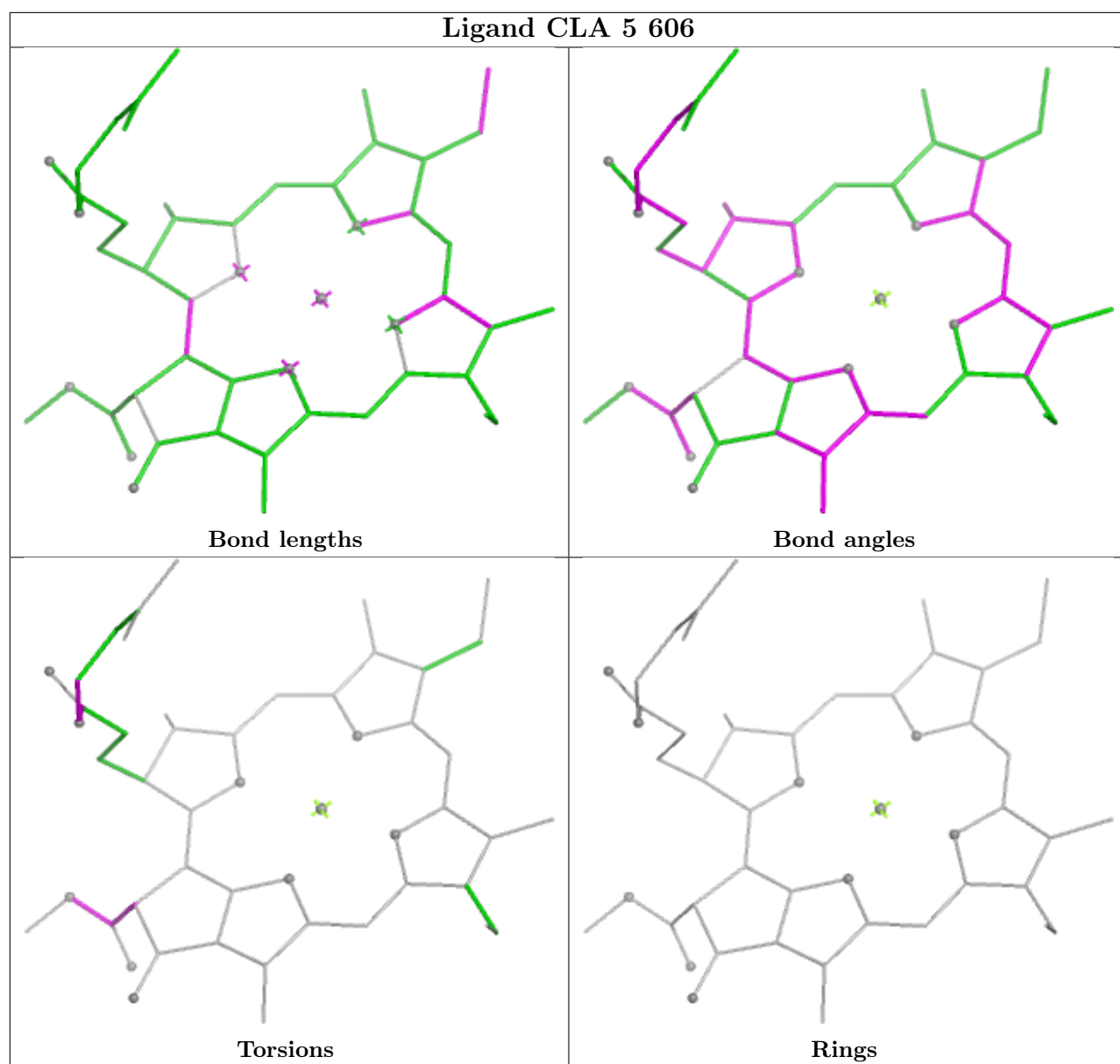


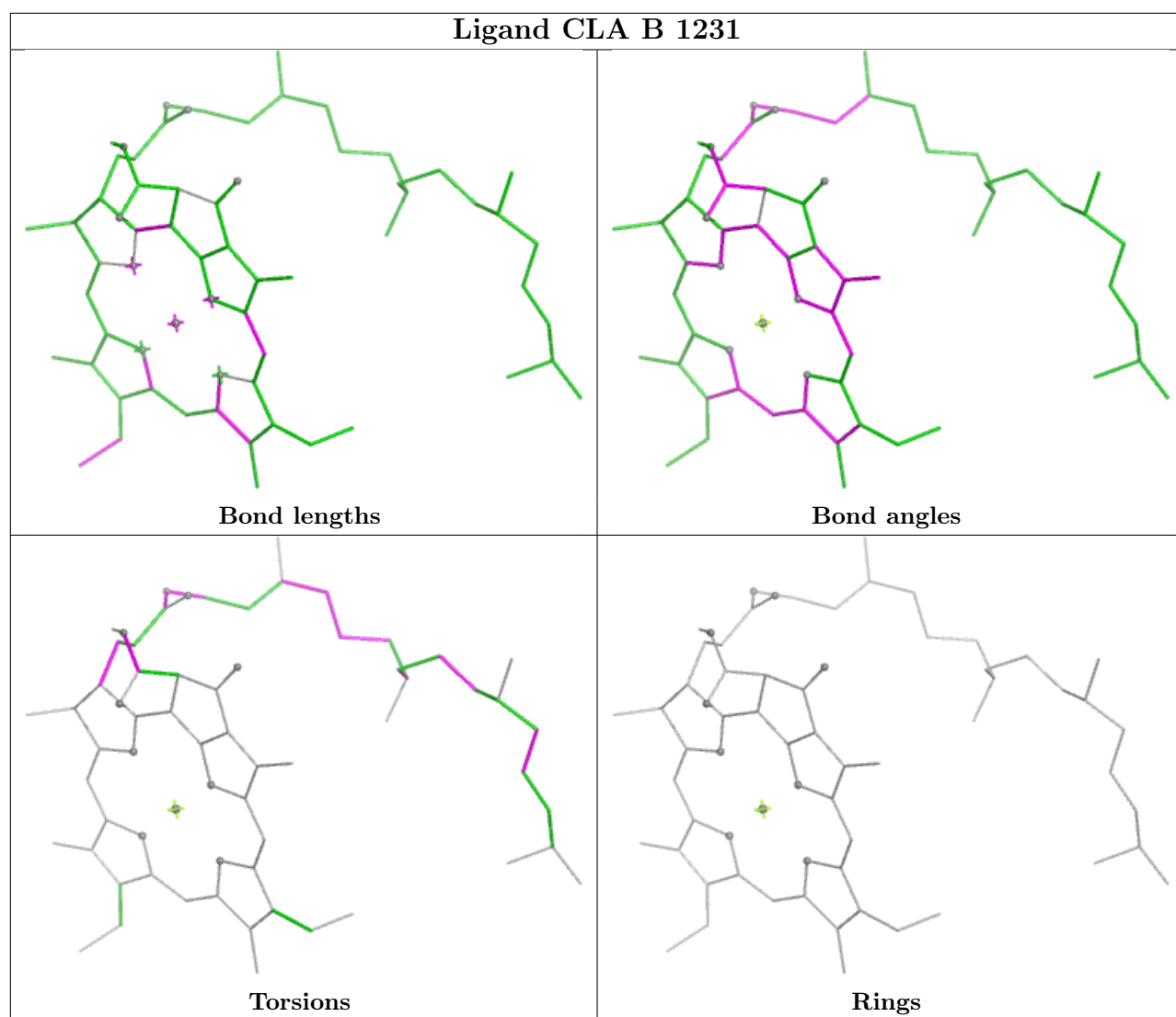


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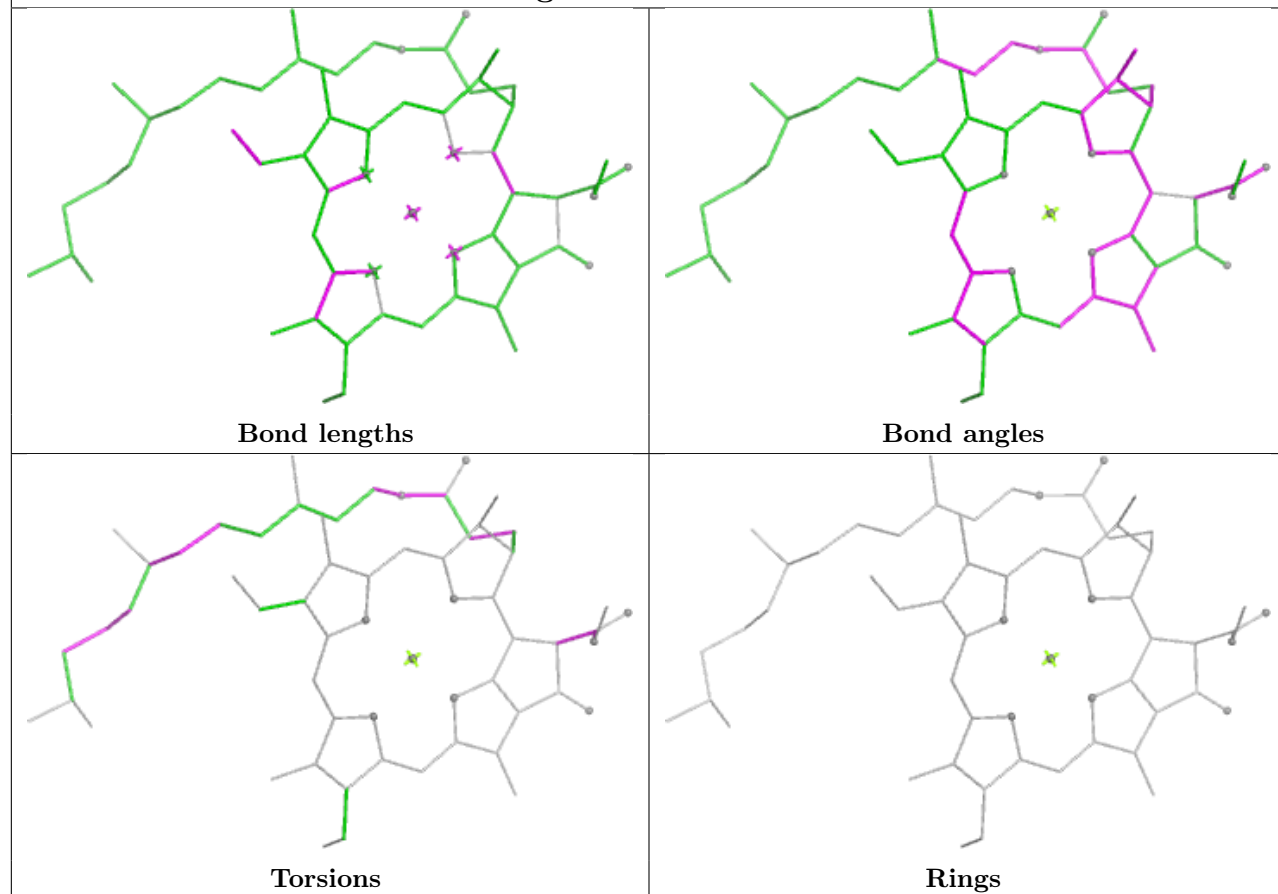




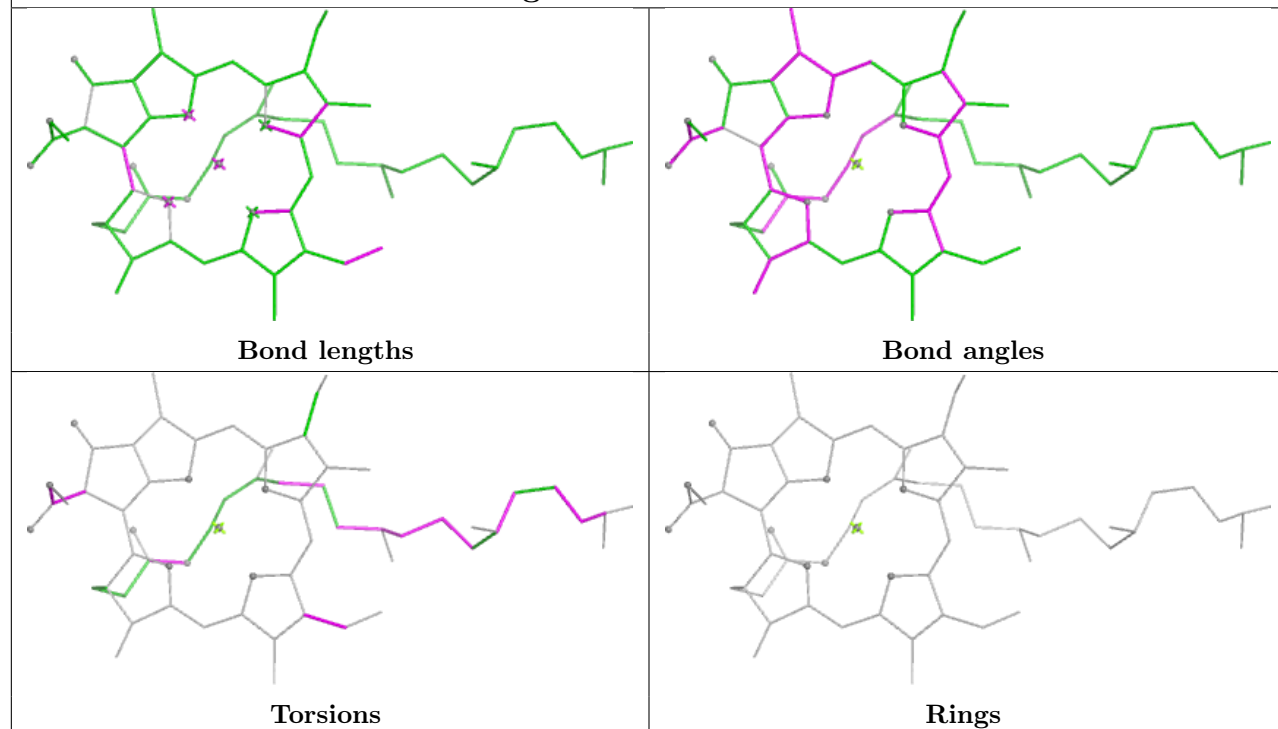


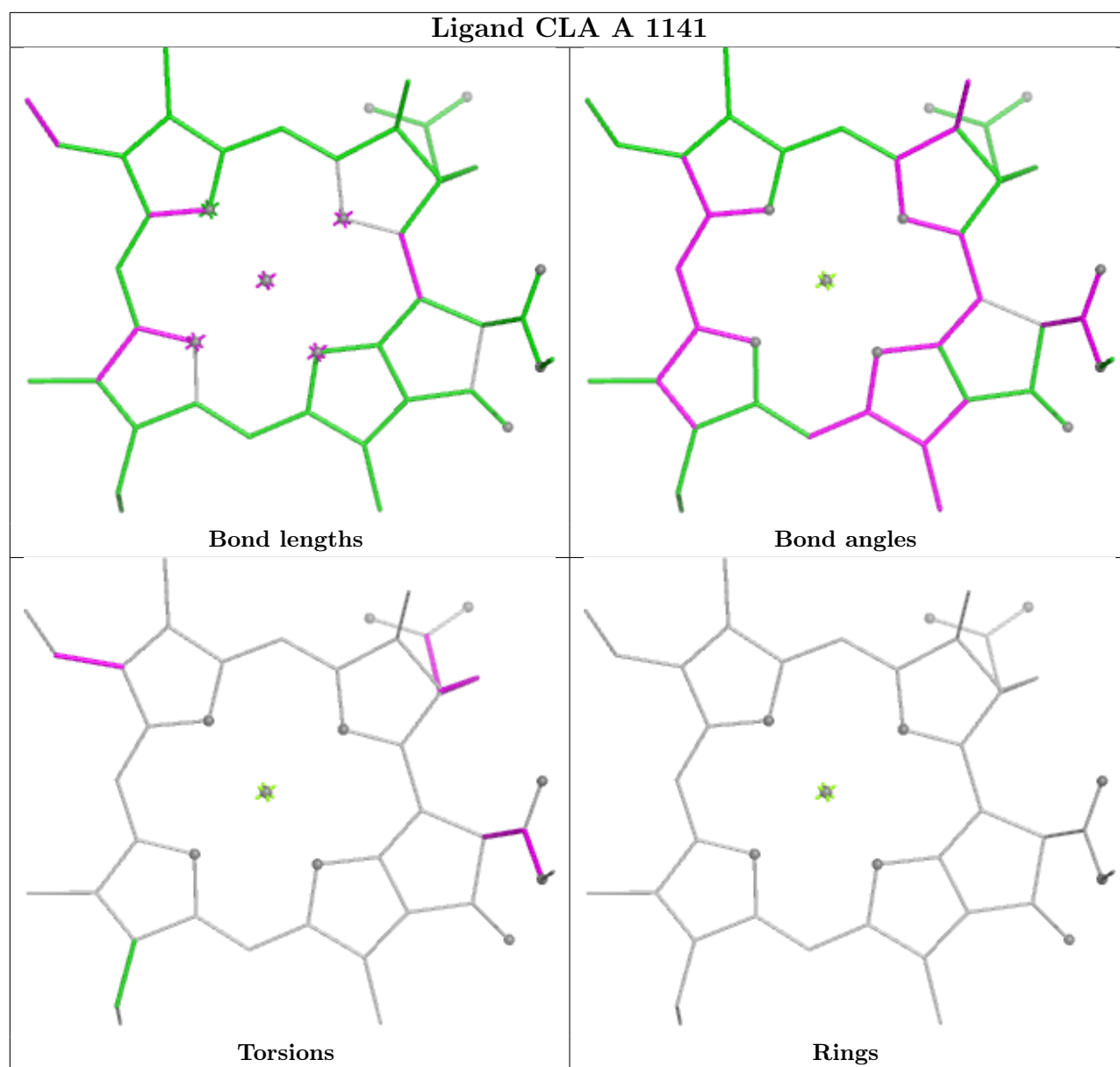


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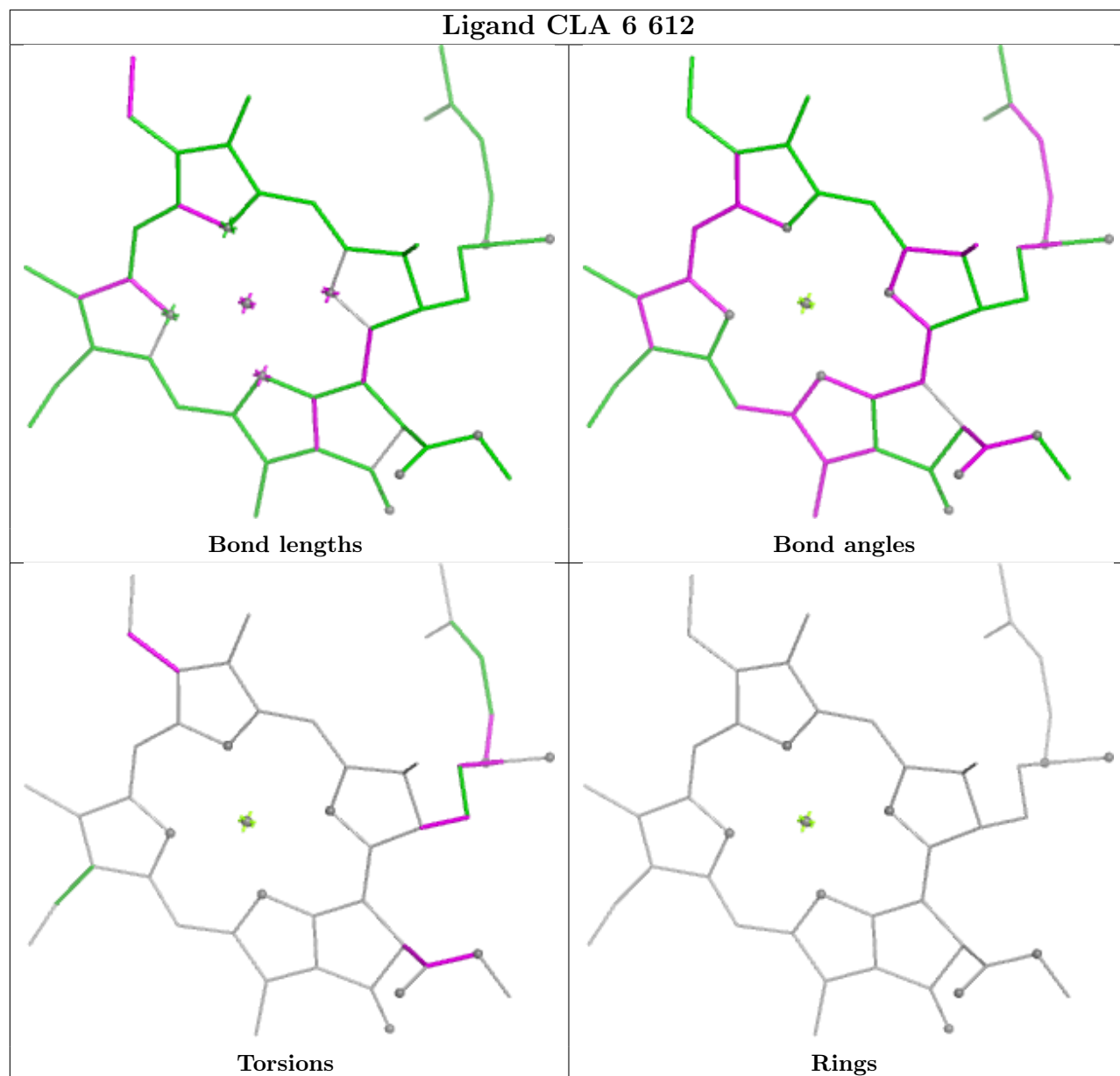


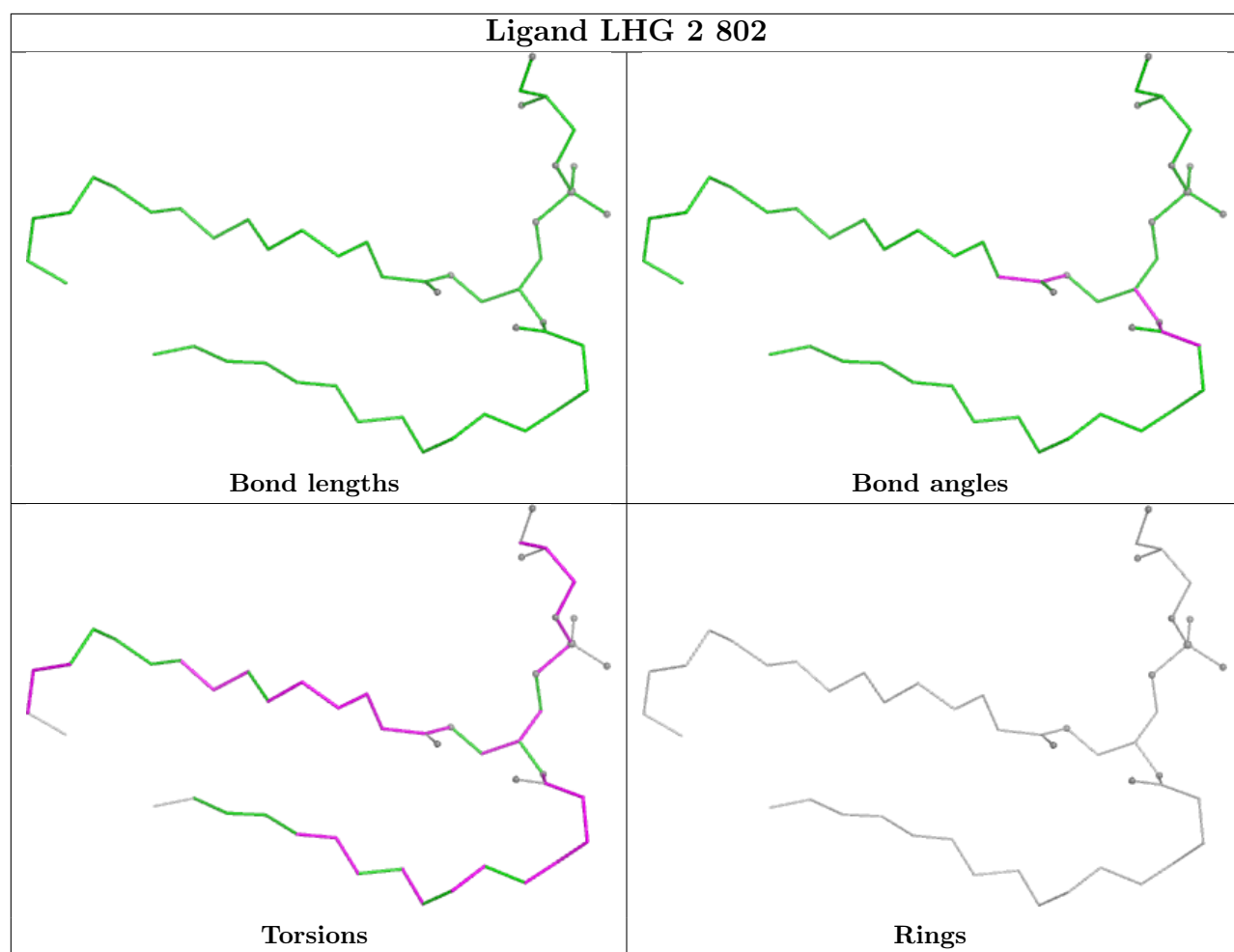
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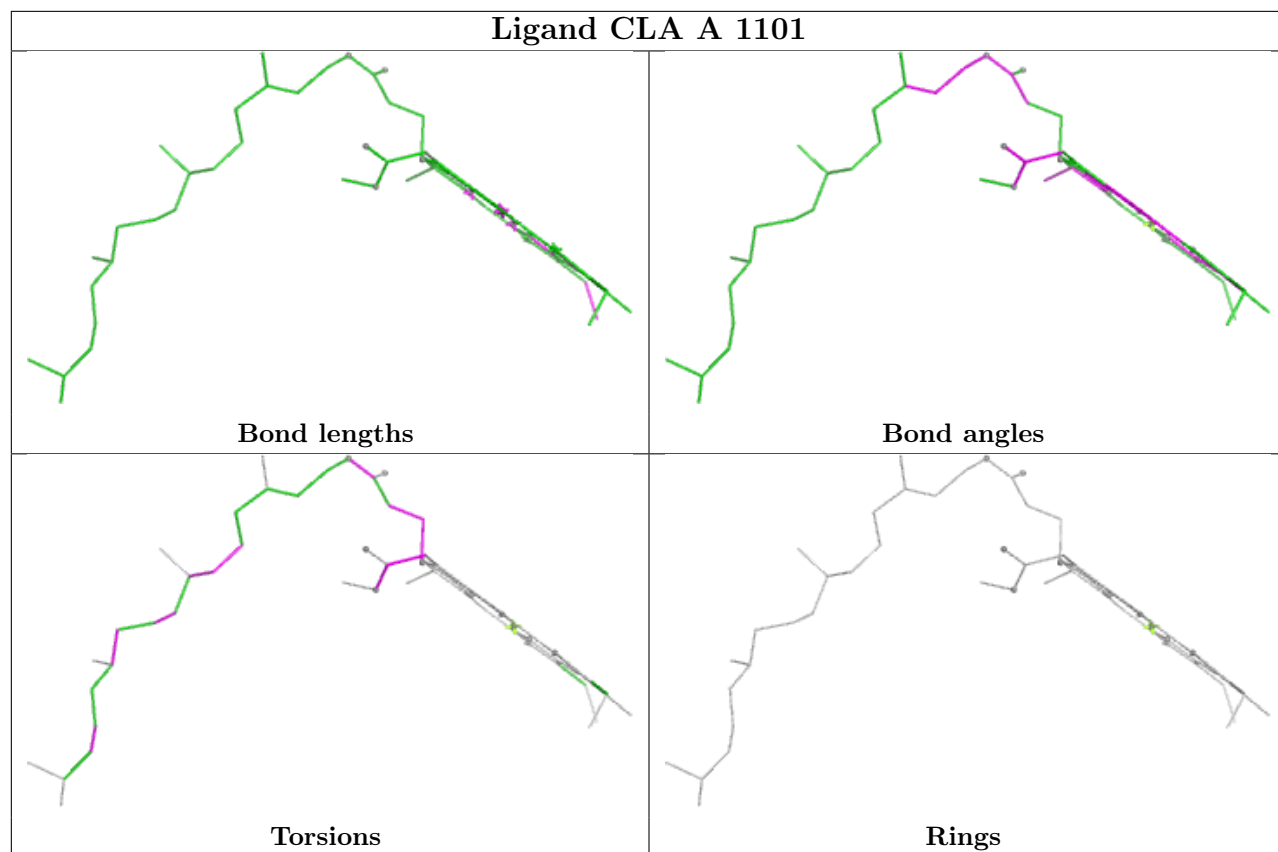


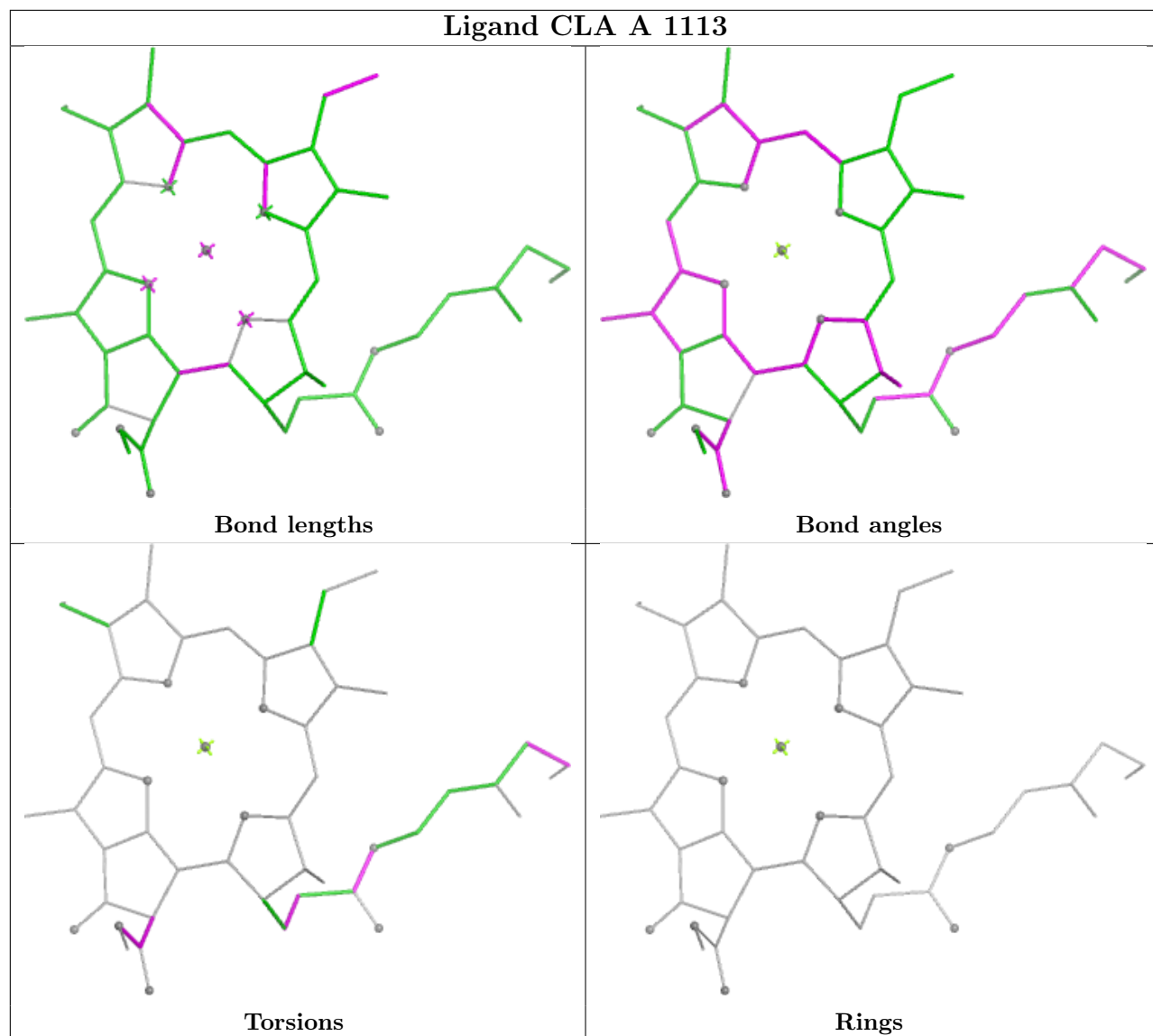


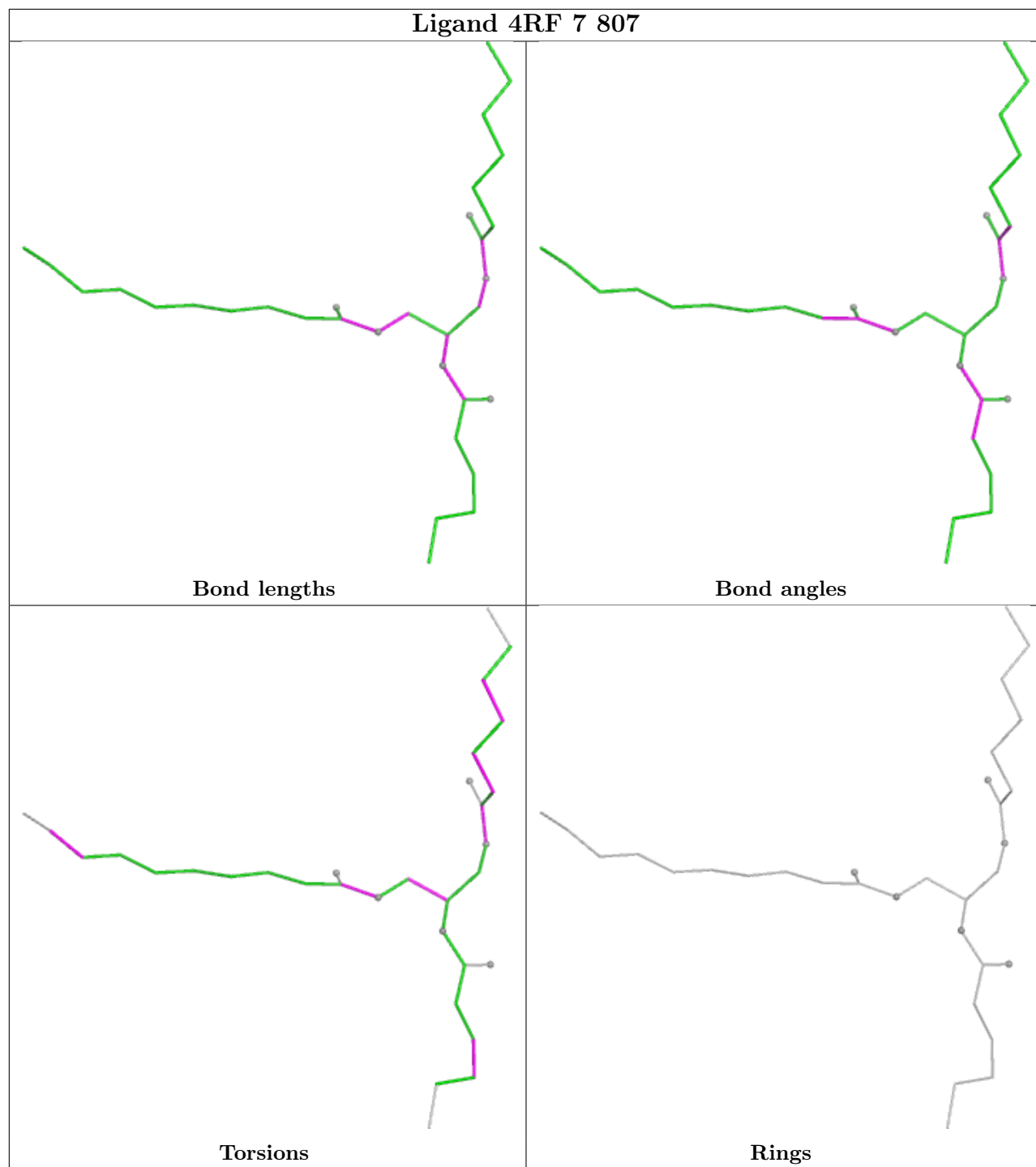
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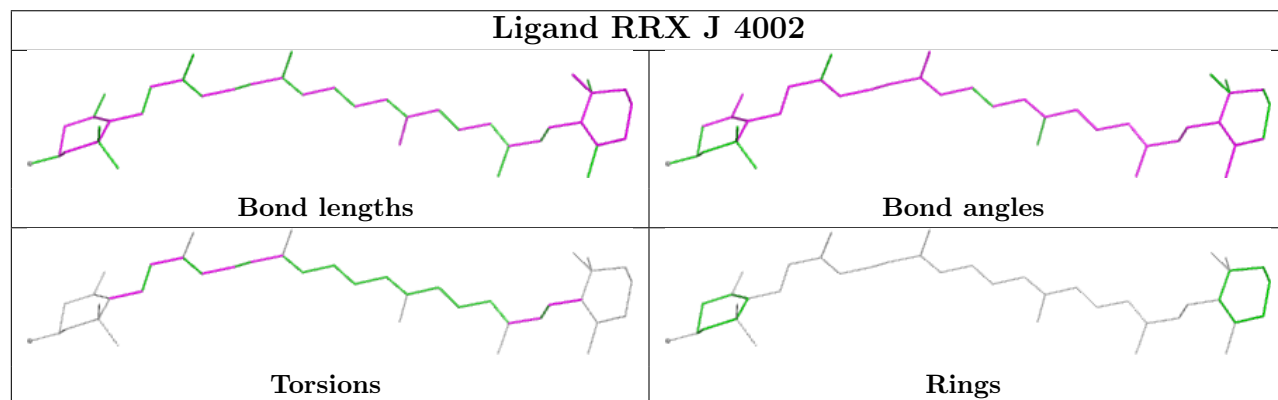
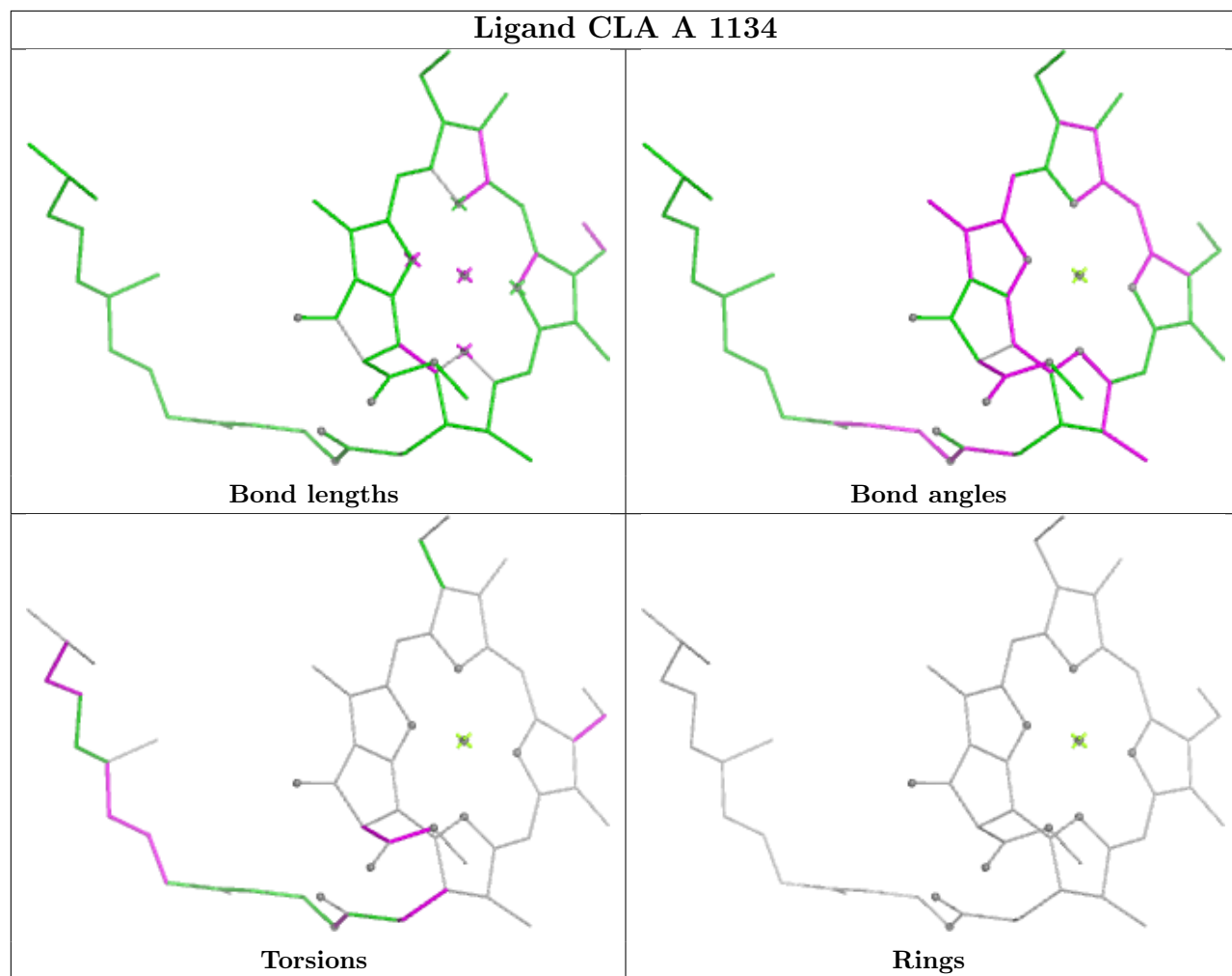


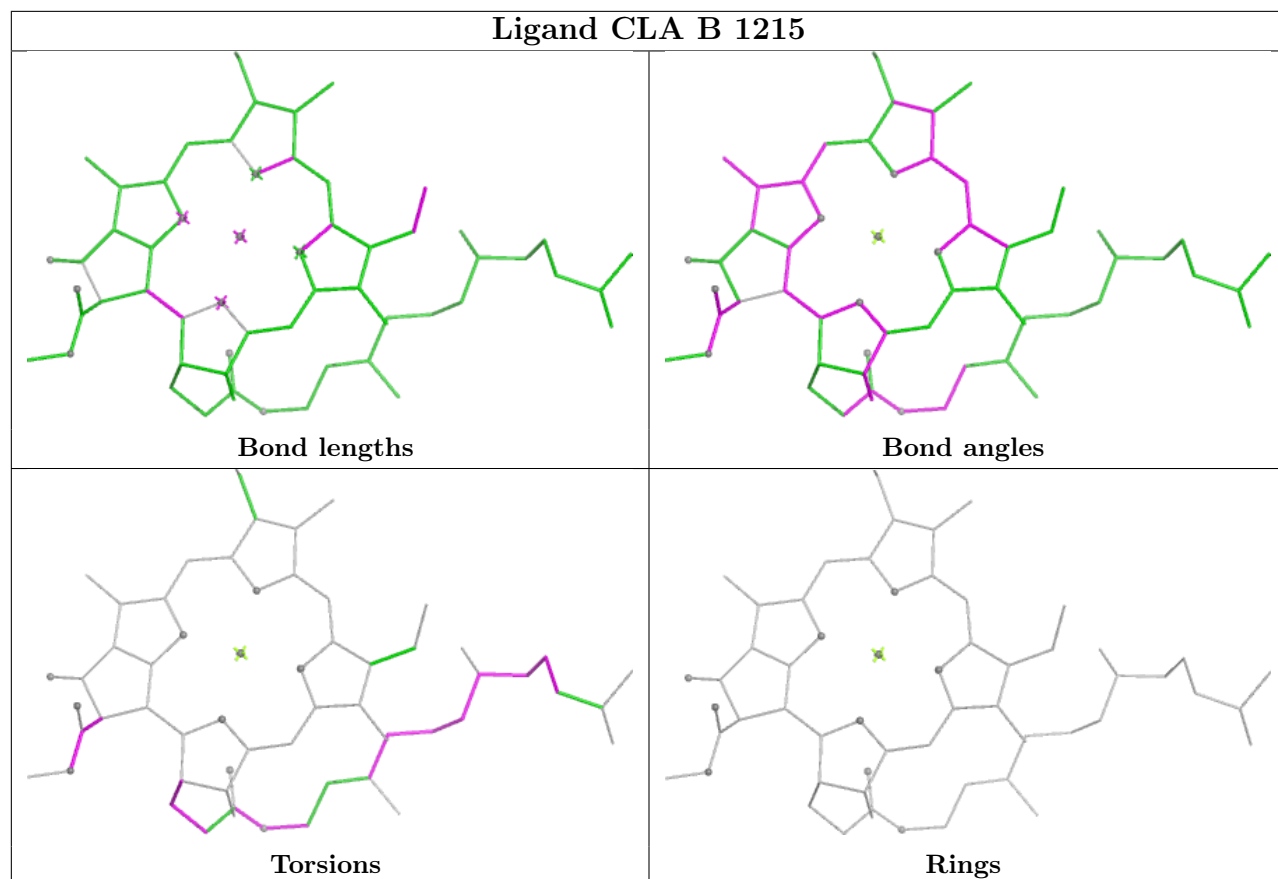


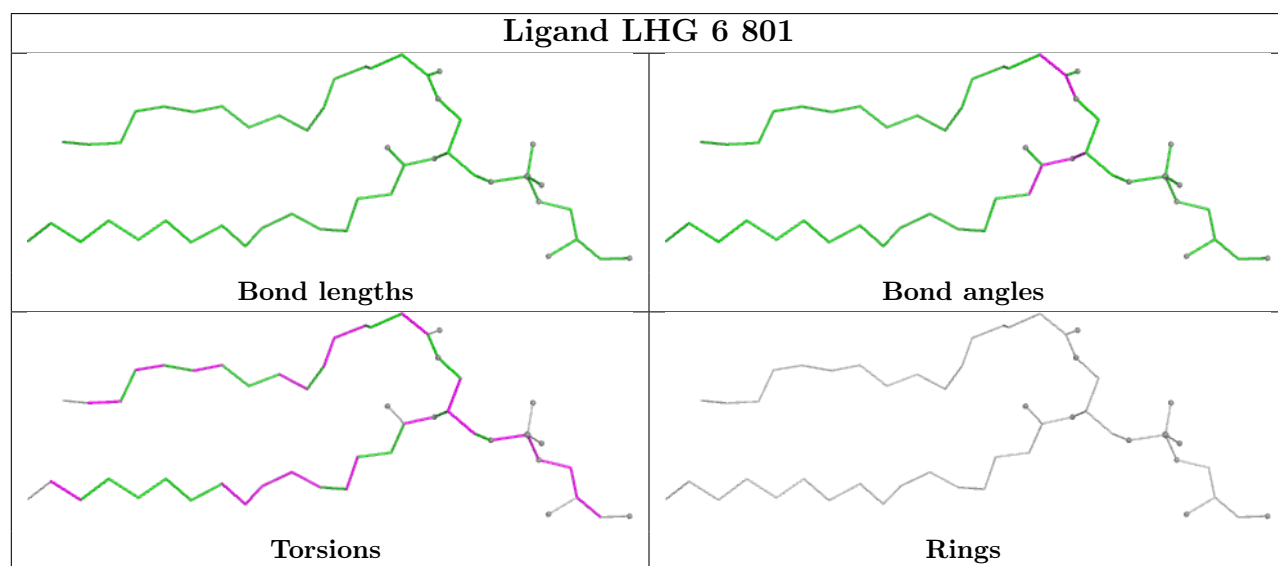
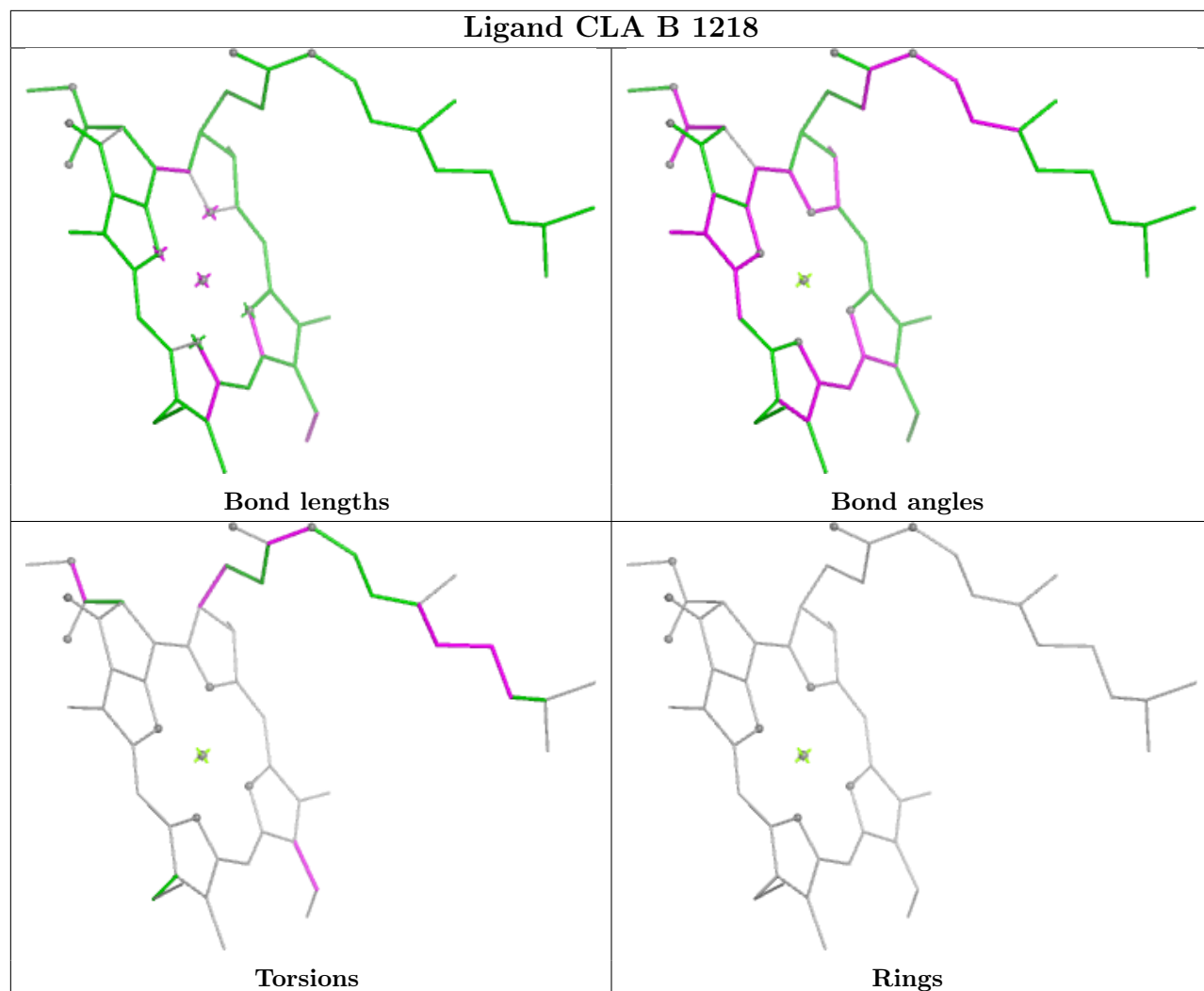


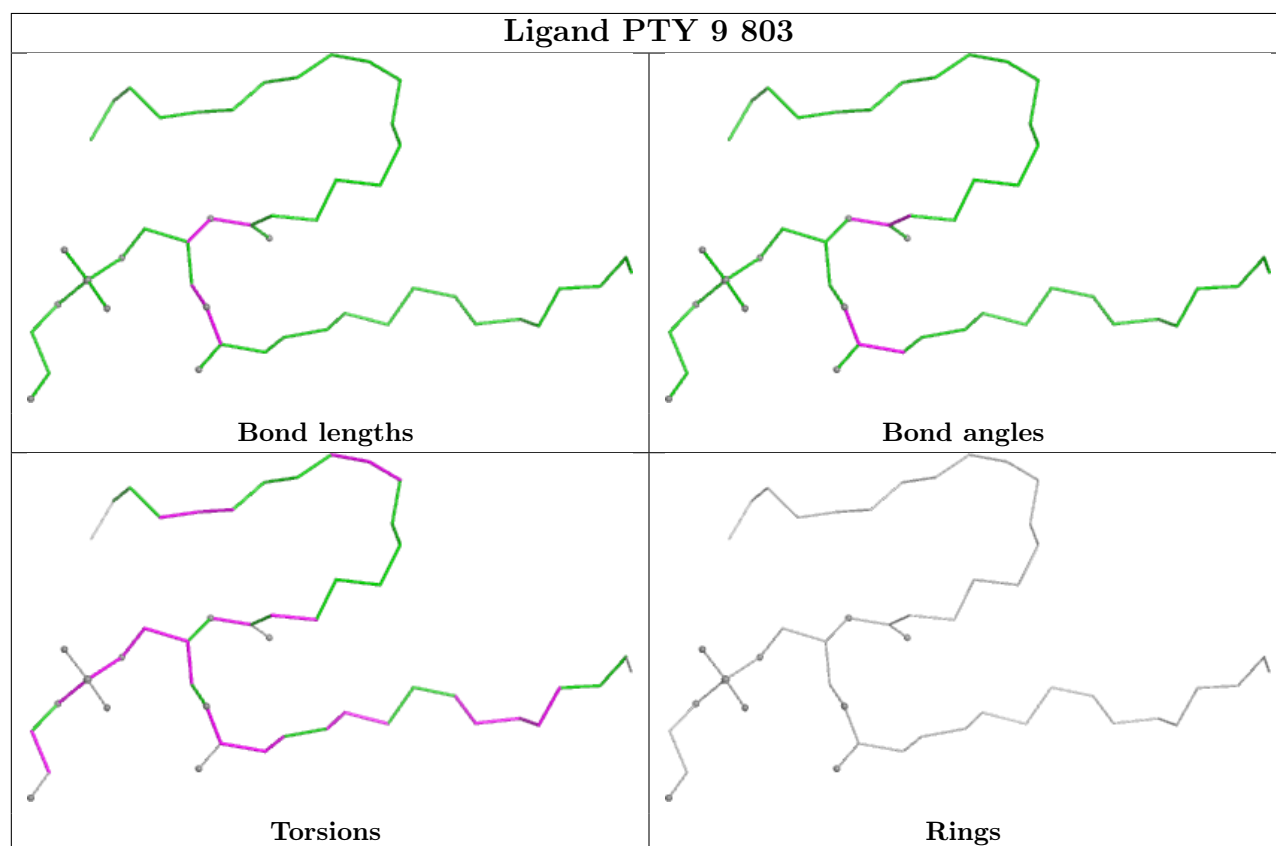
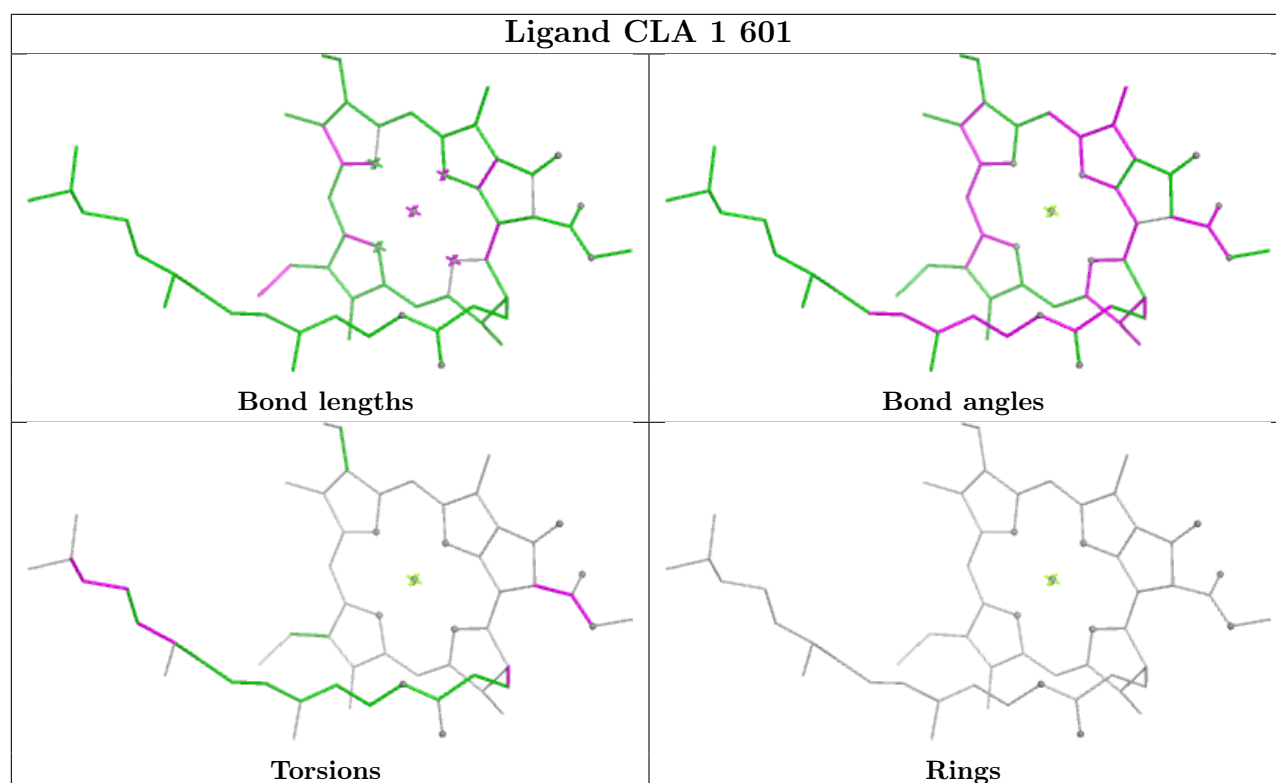




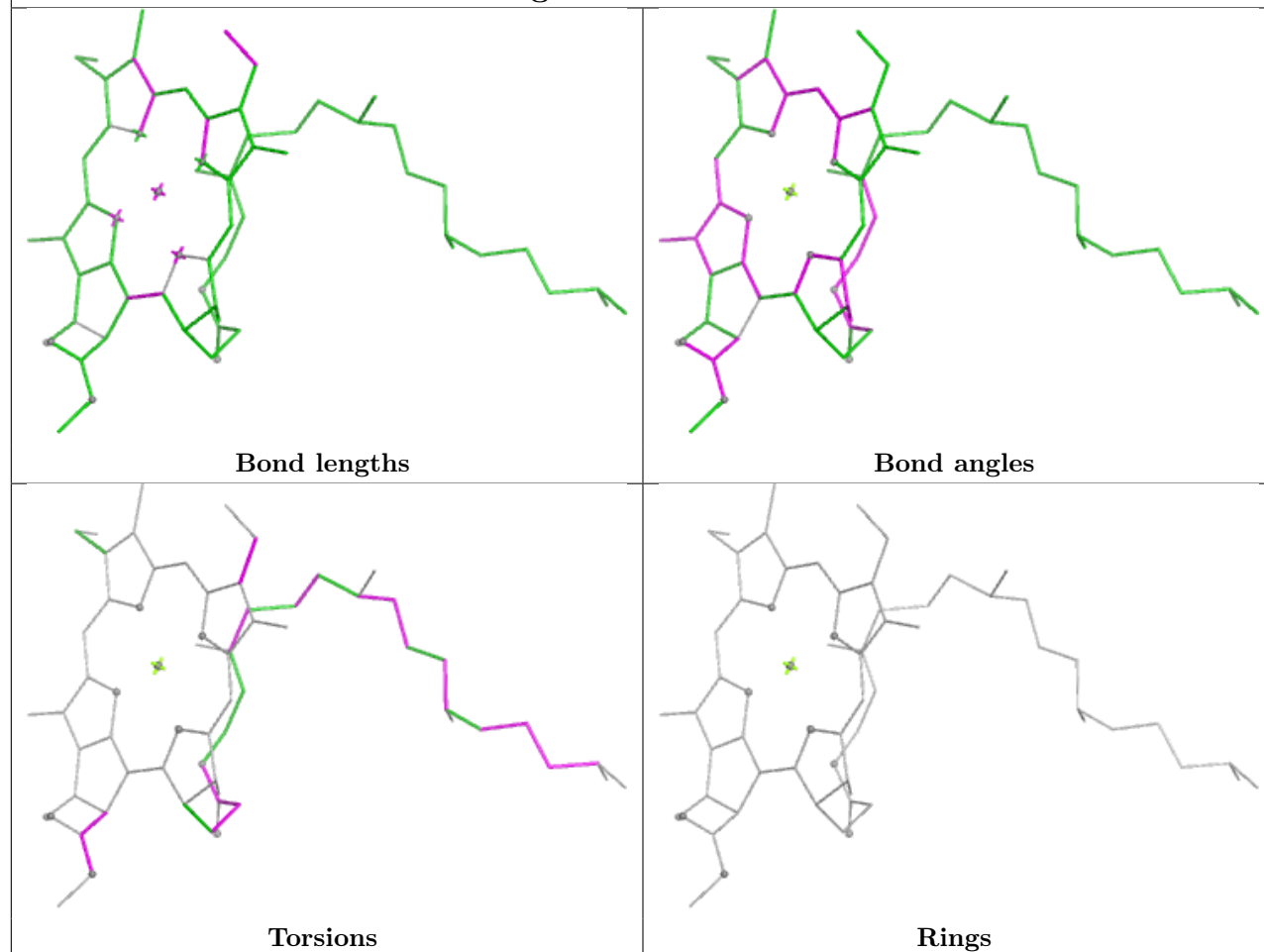




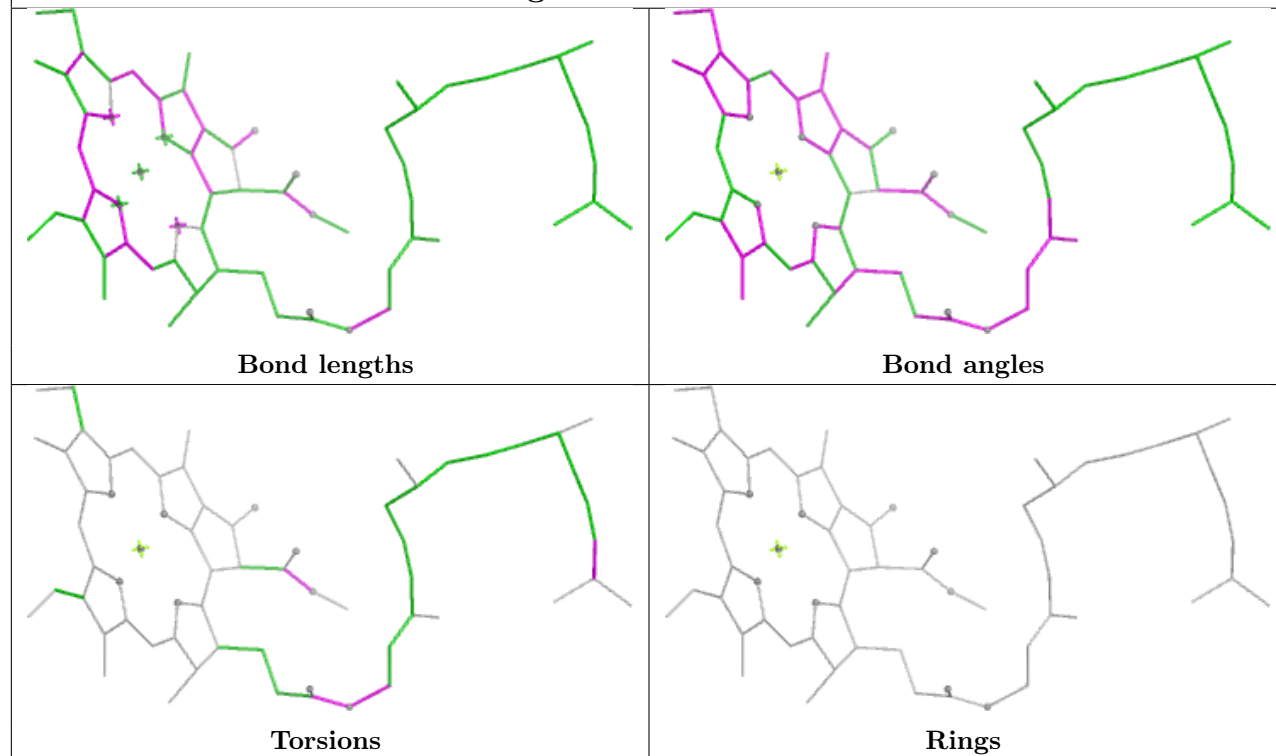


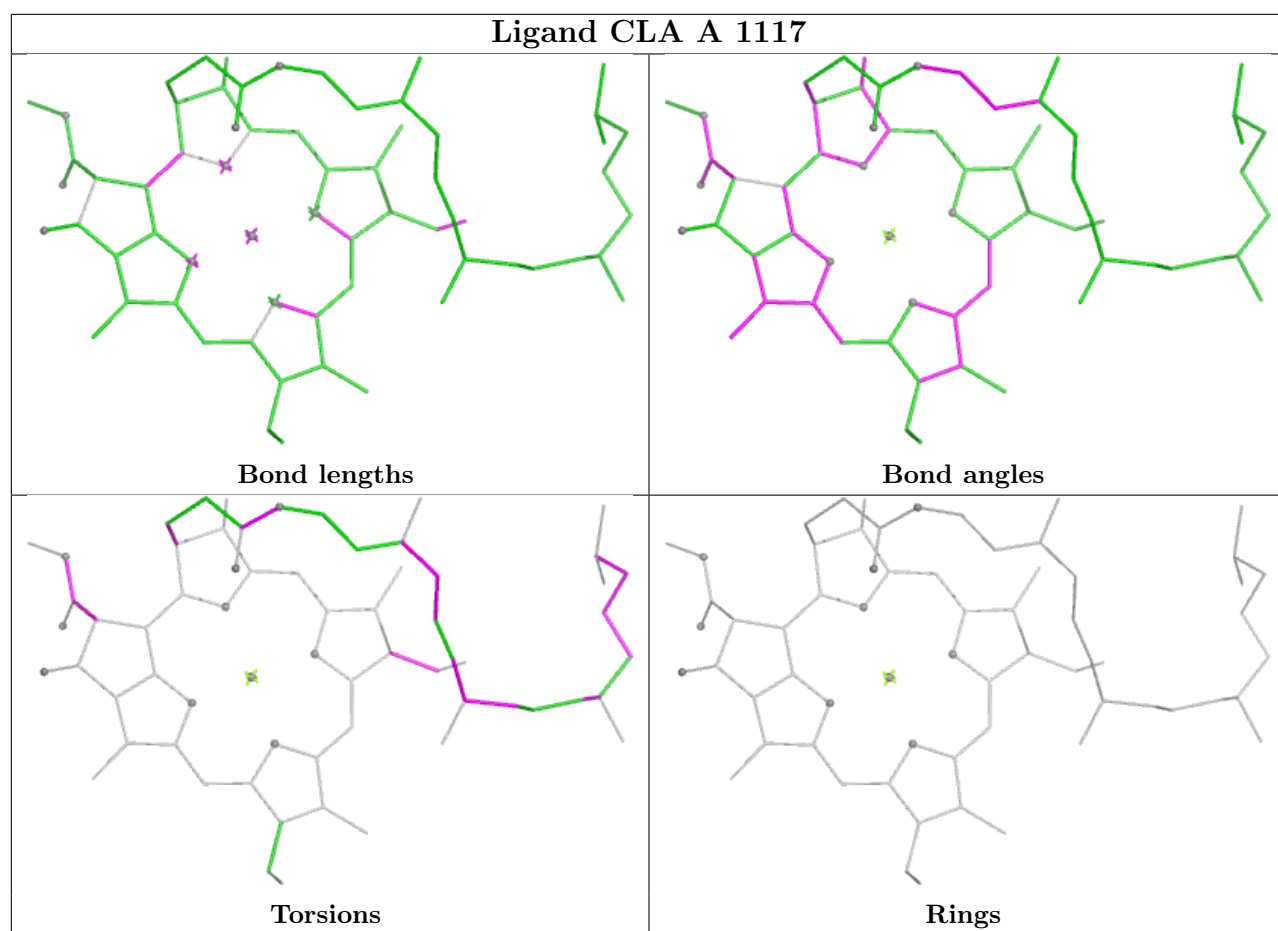


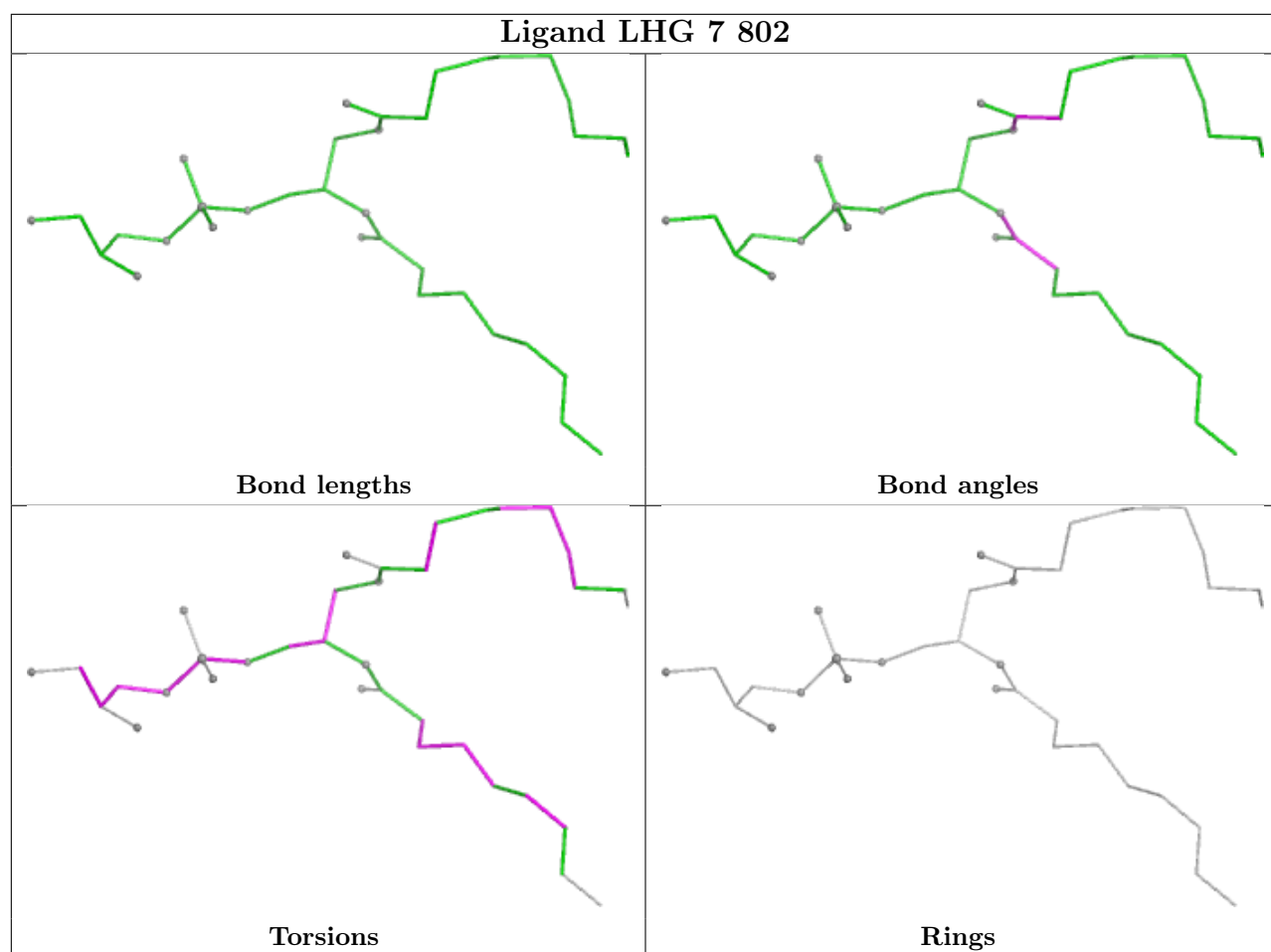
Ligand CLA 7 603

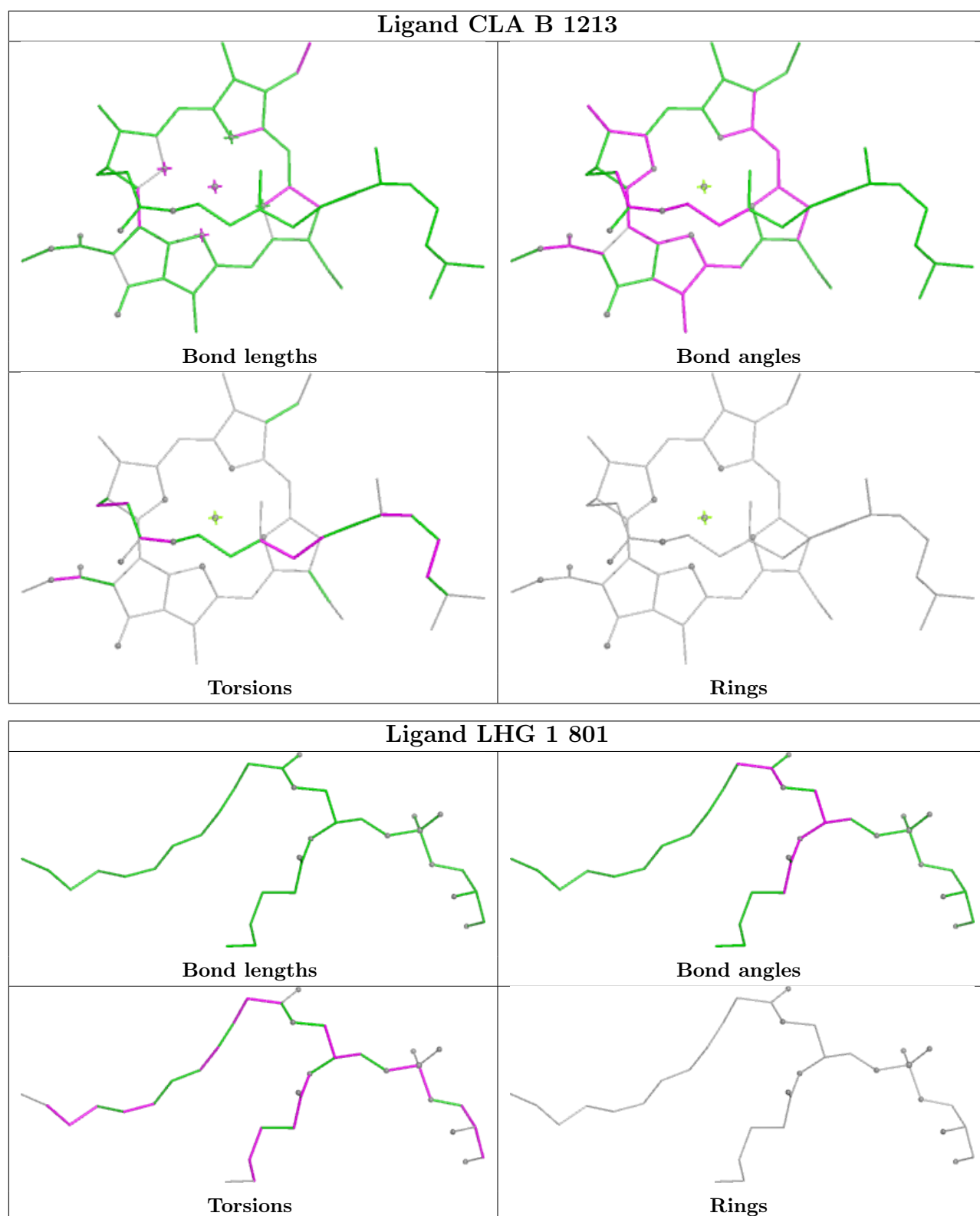


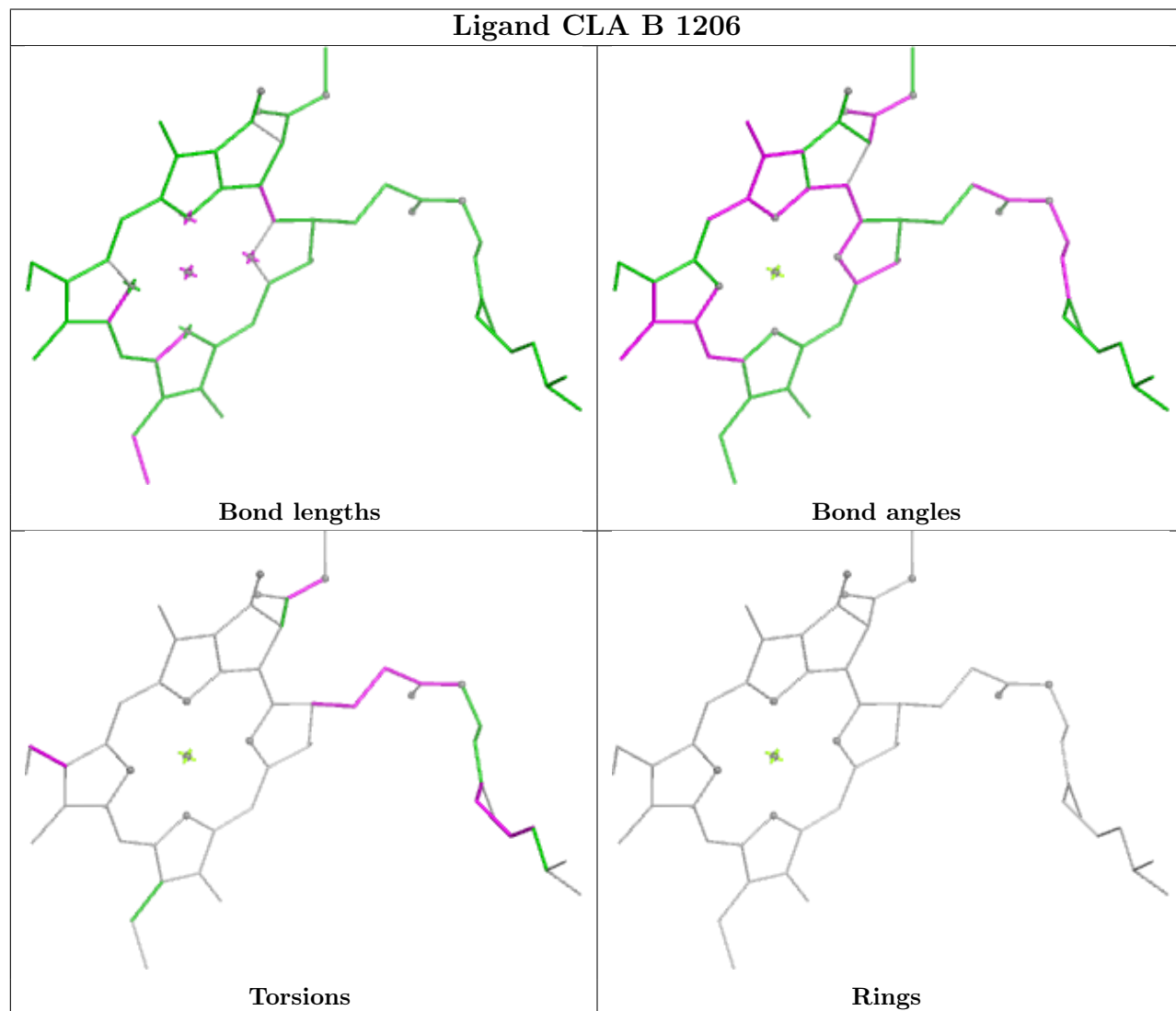
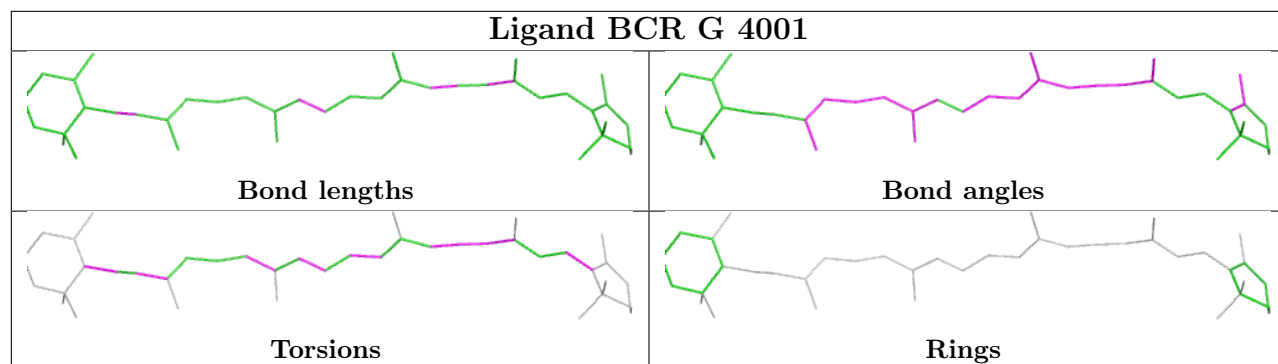
Ligand CL0 A 1011

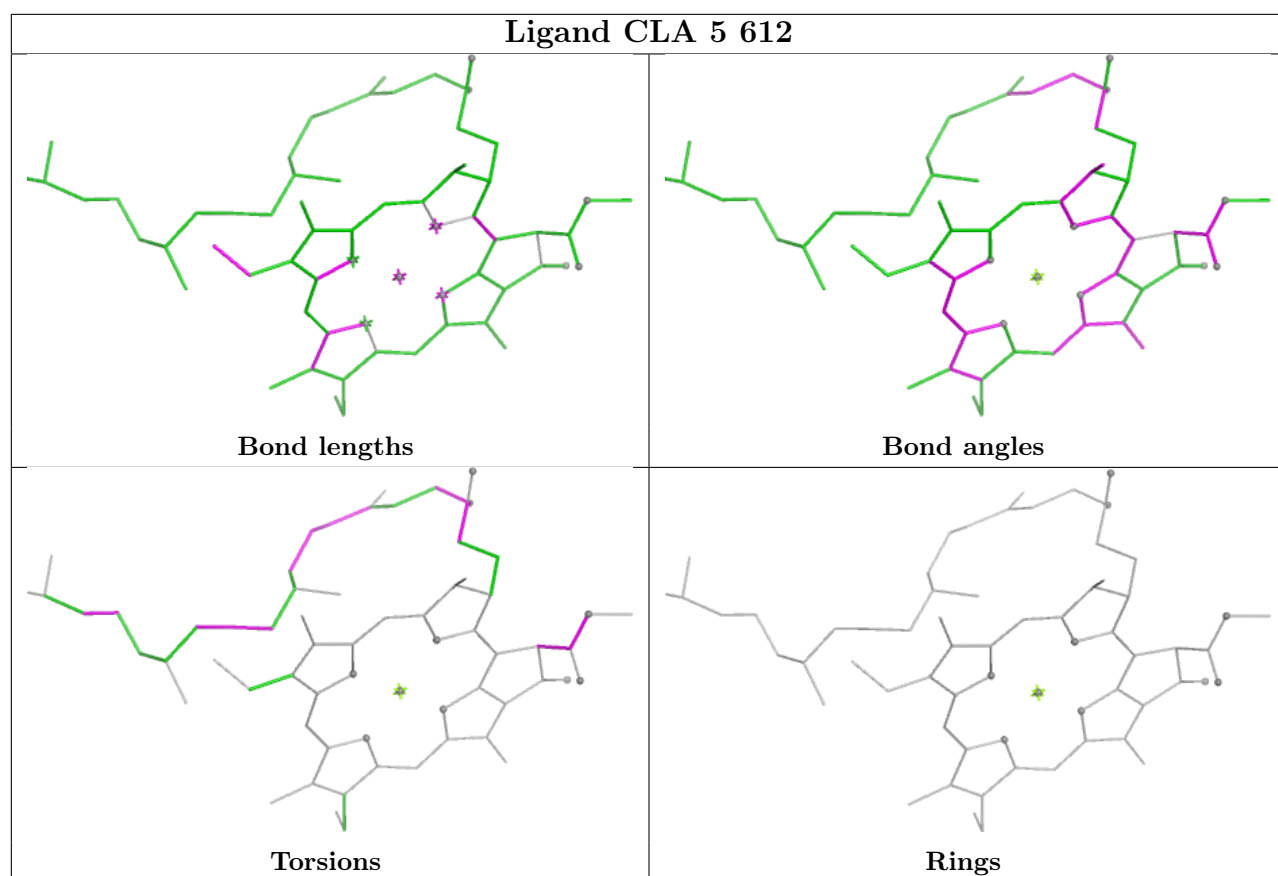


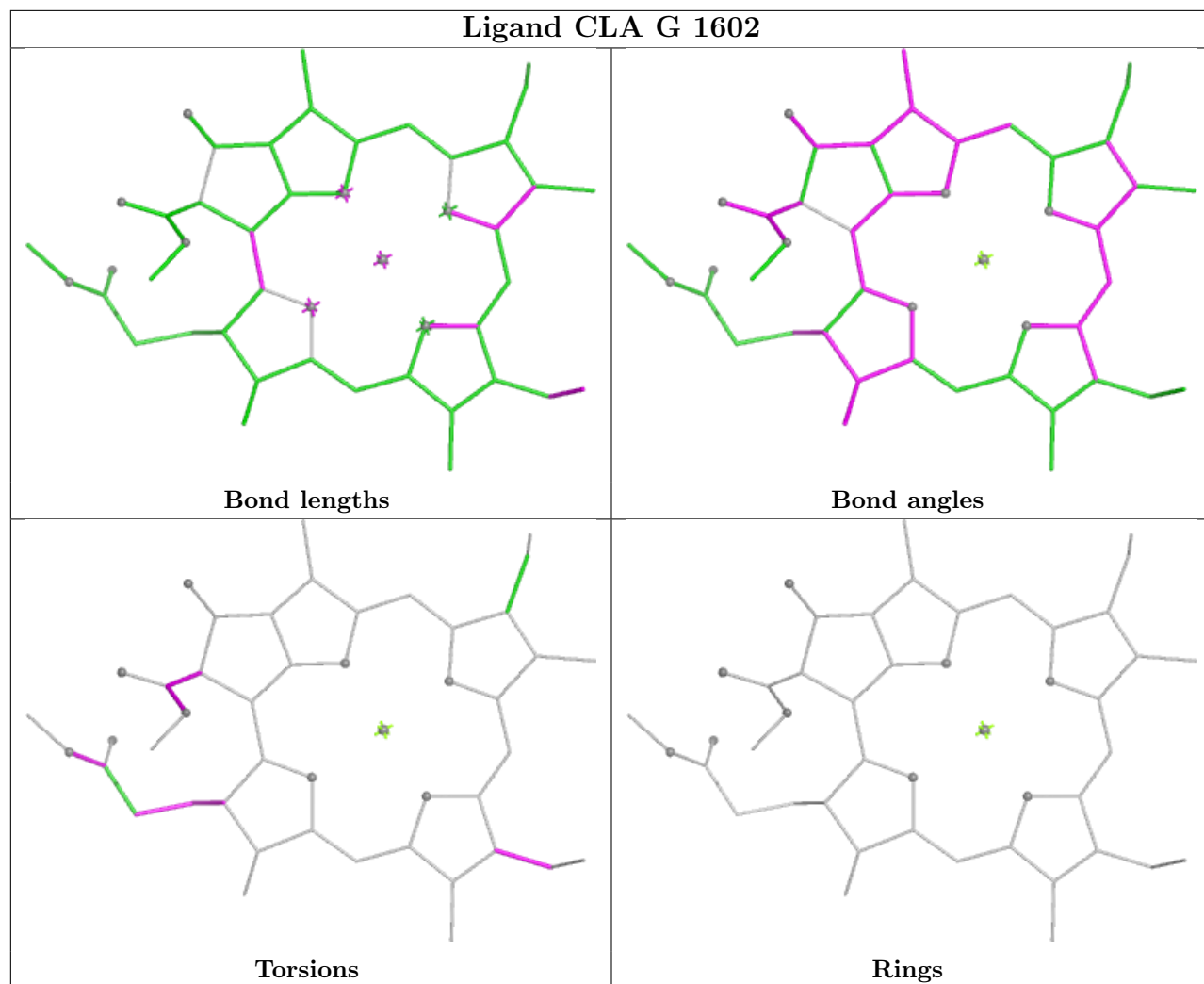




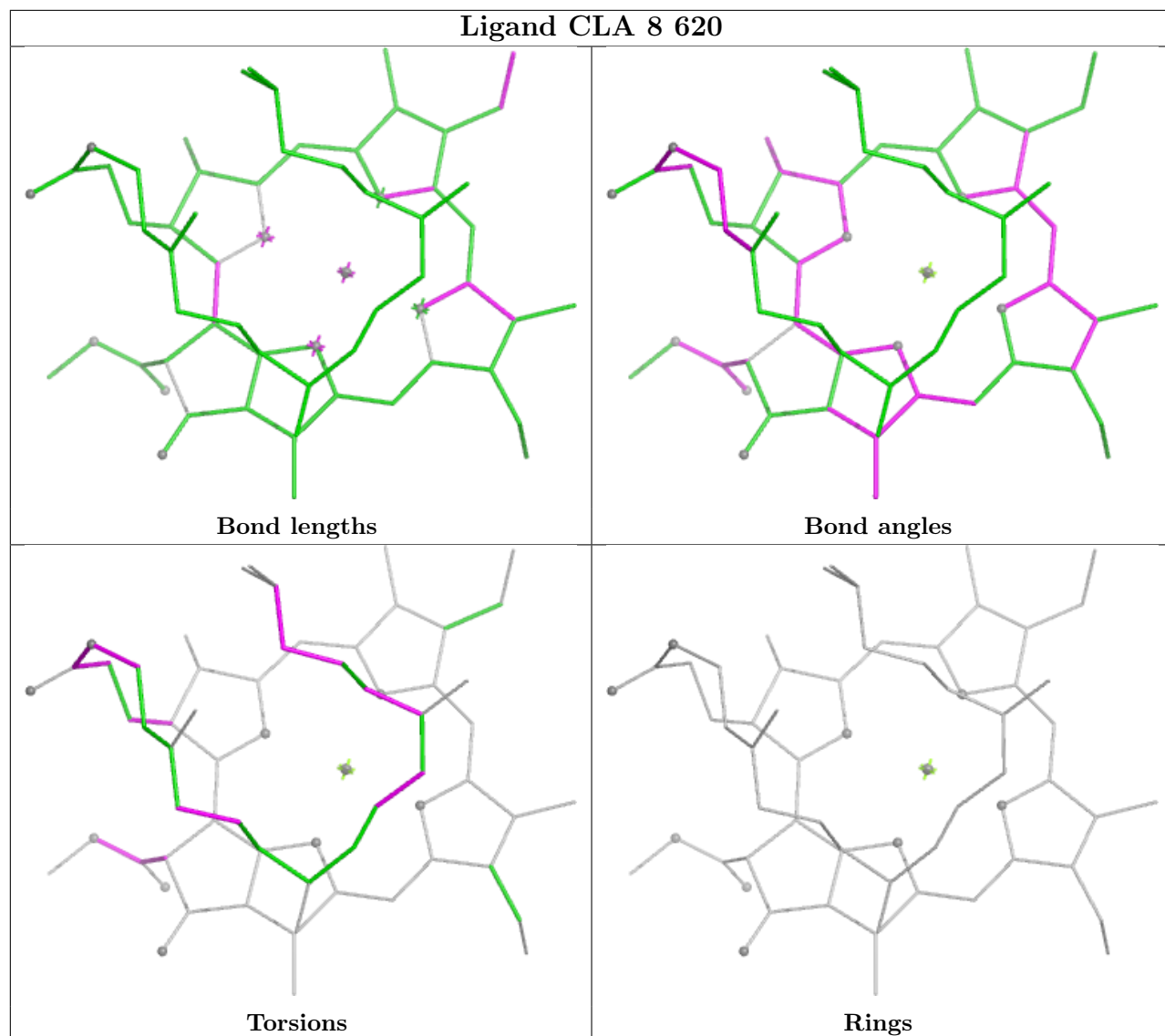


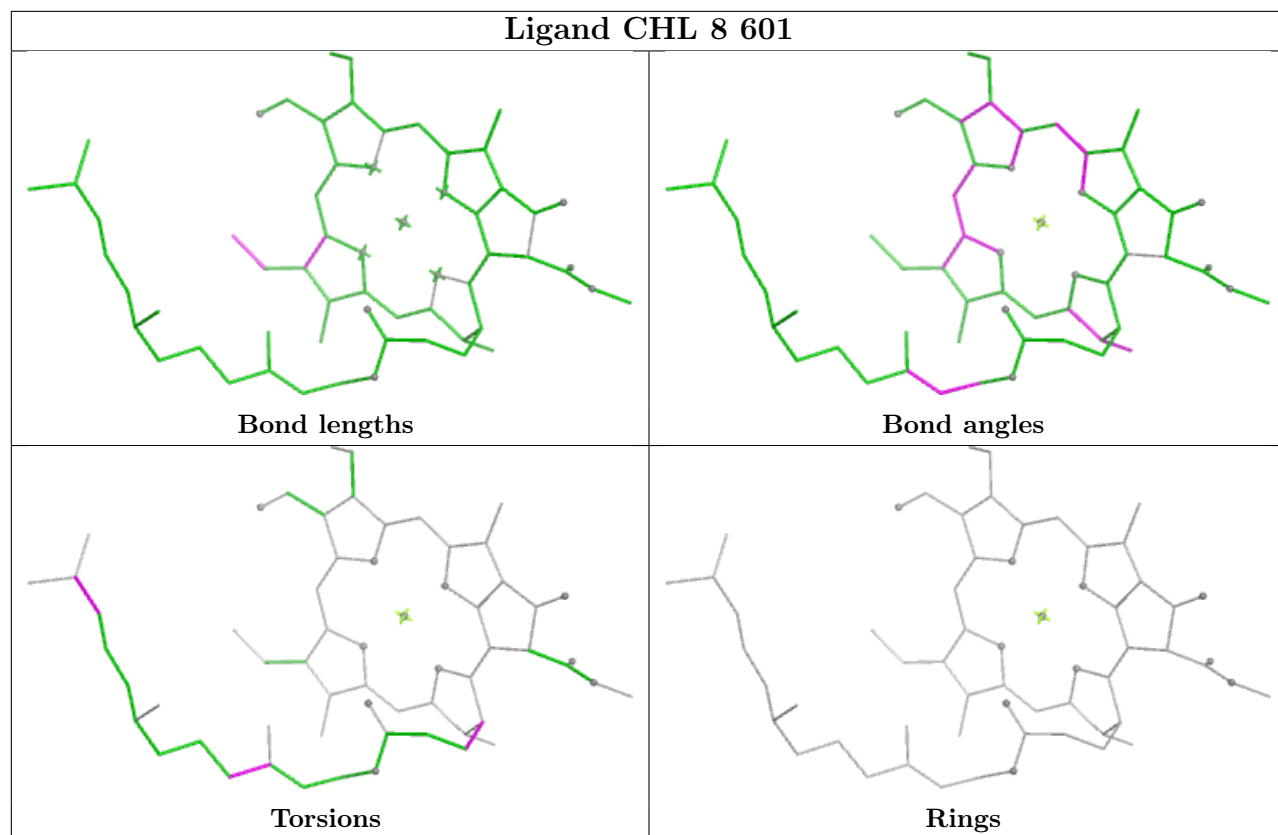




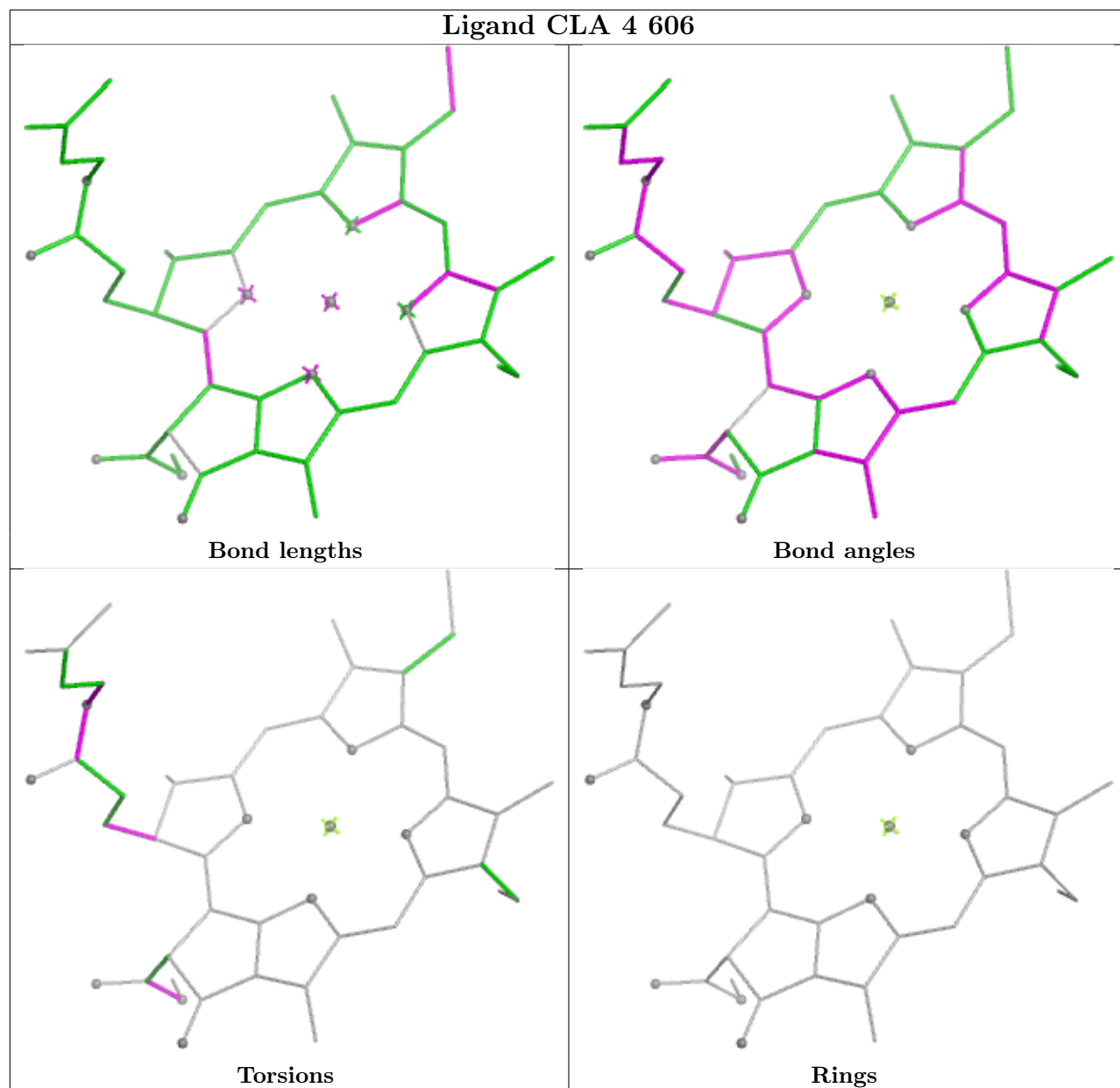


Ligand CLA 8 620

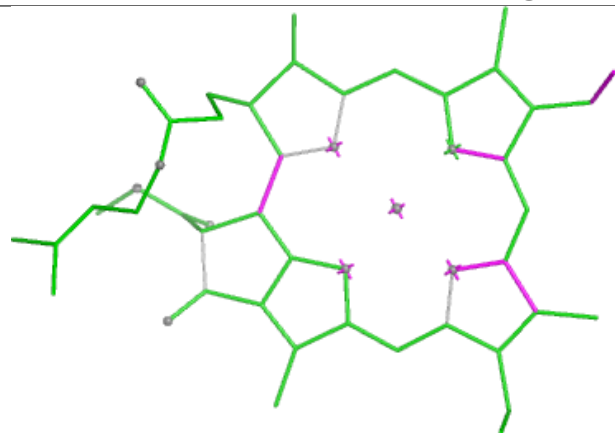




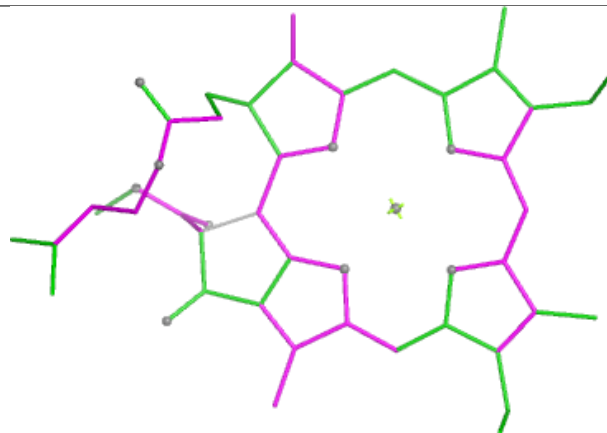
Ligand CLA 4 606



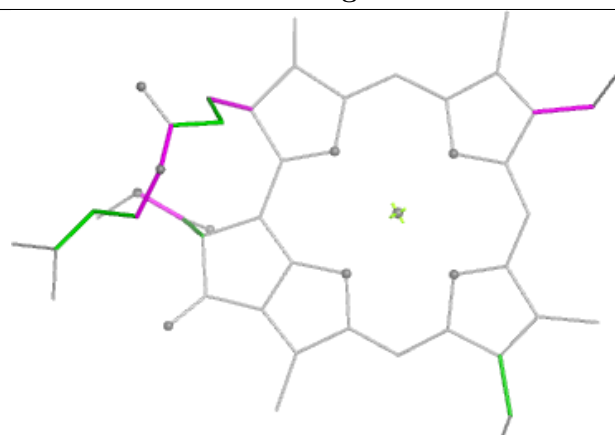
Ligand CLA 4 616



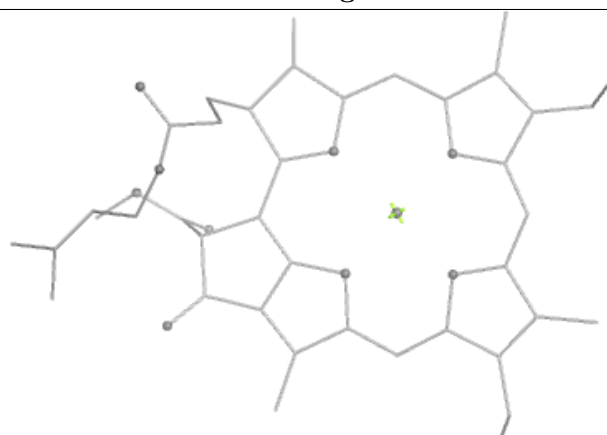
Bond lengths



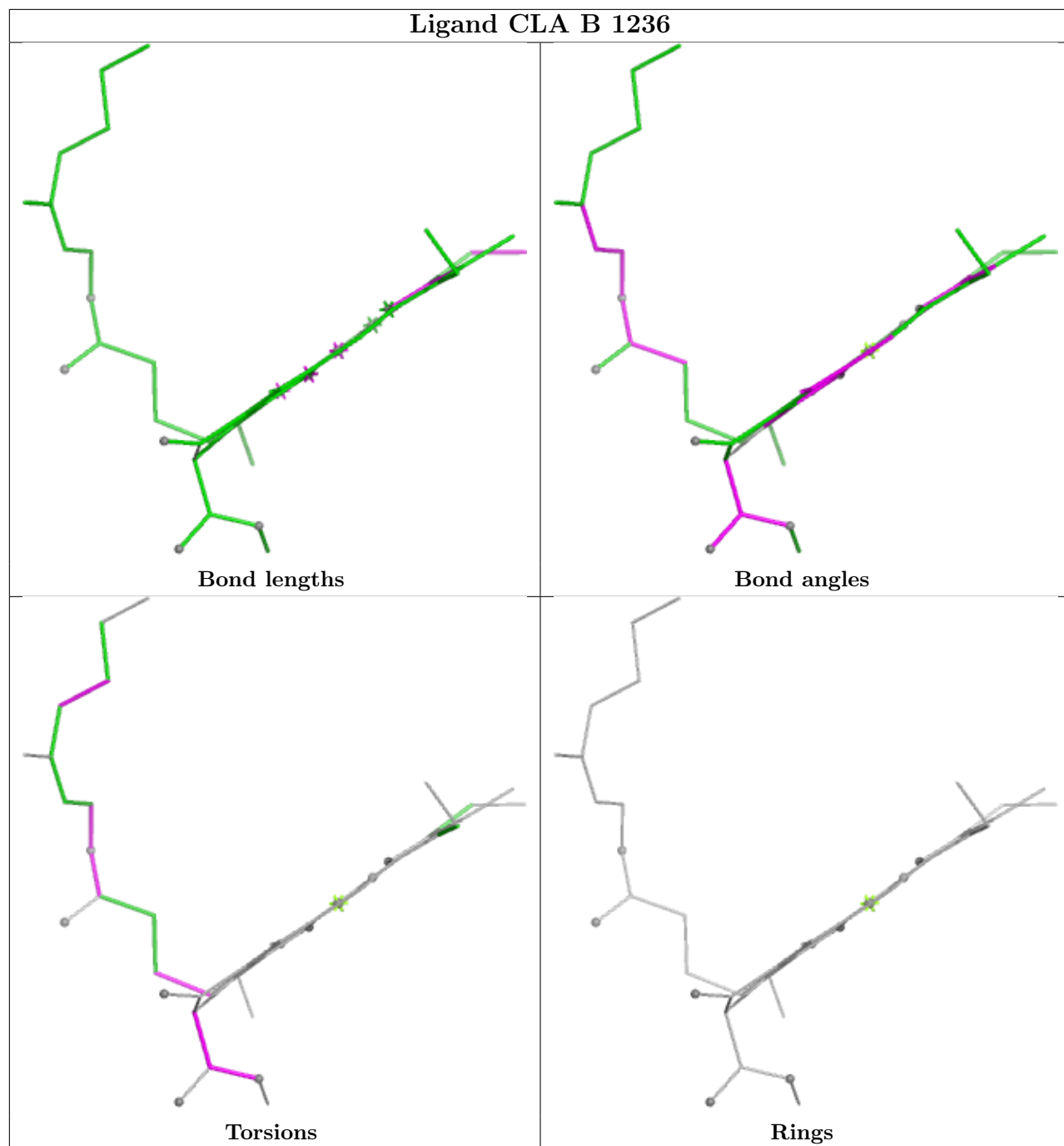
Bond angles

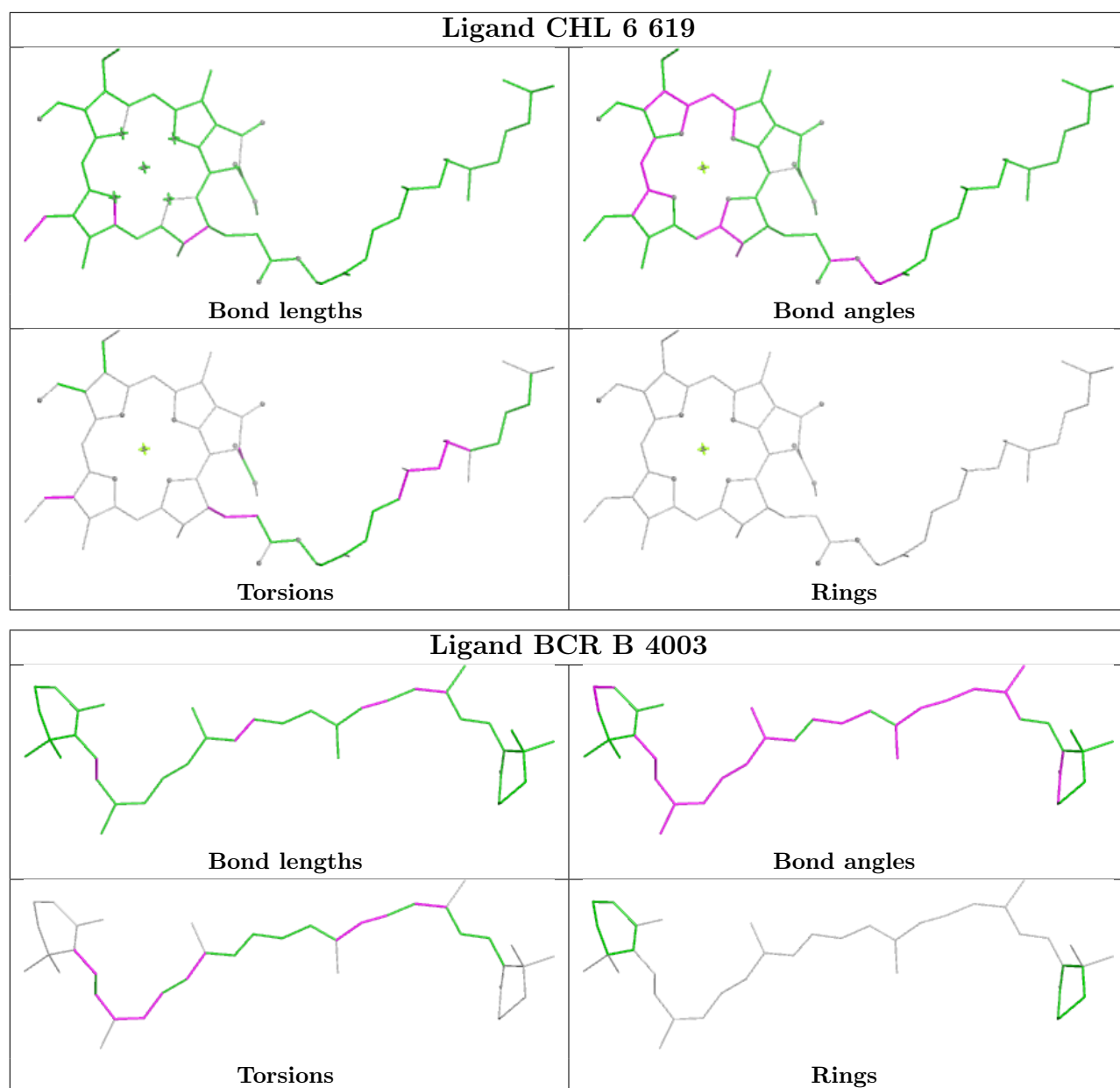


Torsions

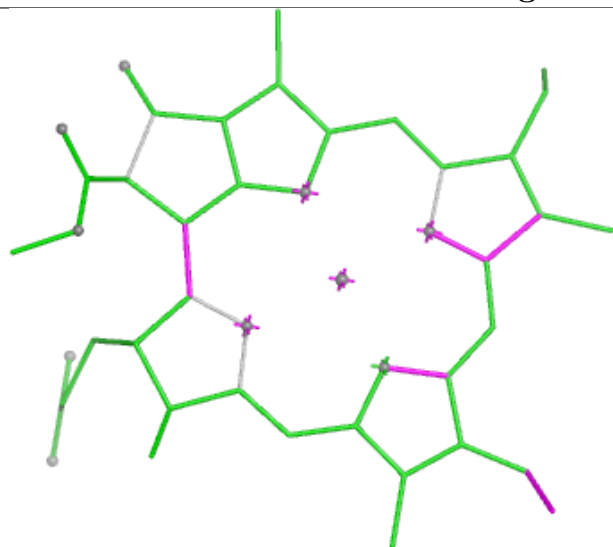


Rings

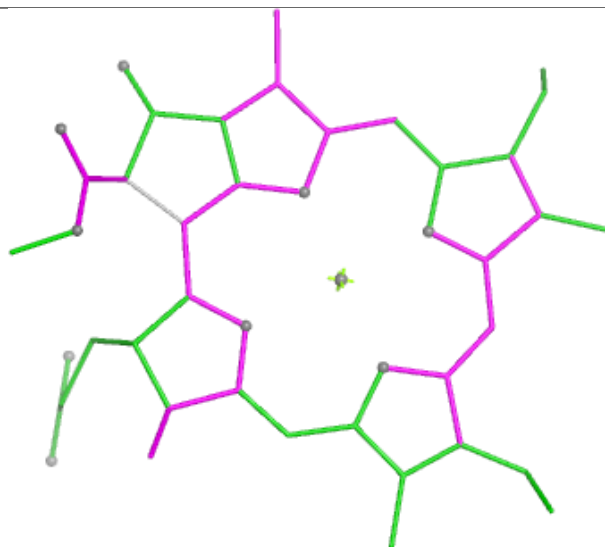




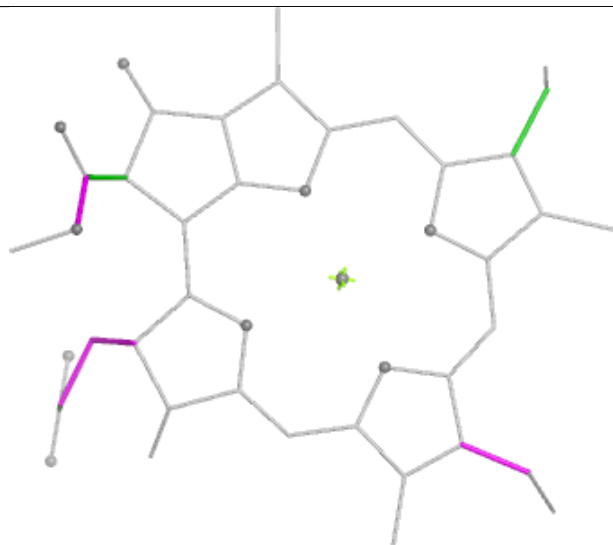
Ligand CLA 5 608



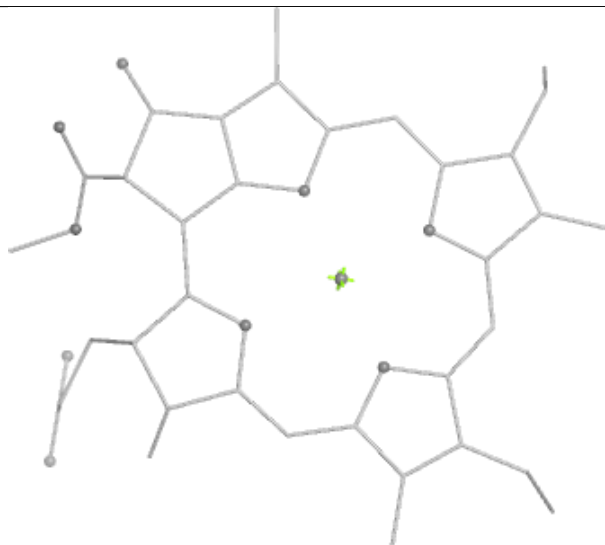
Bond lengths



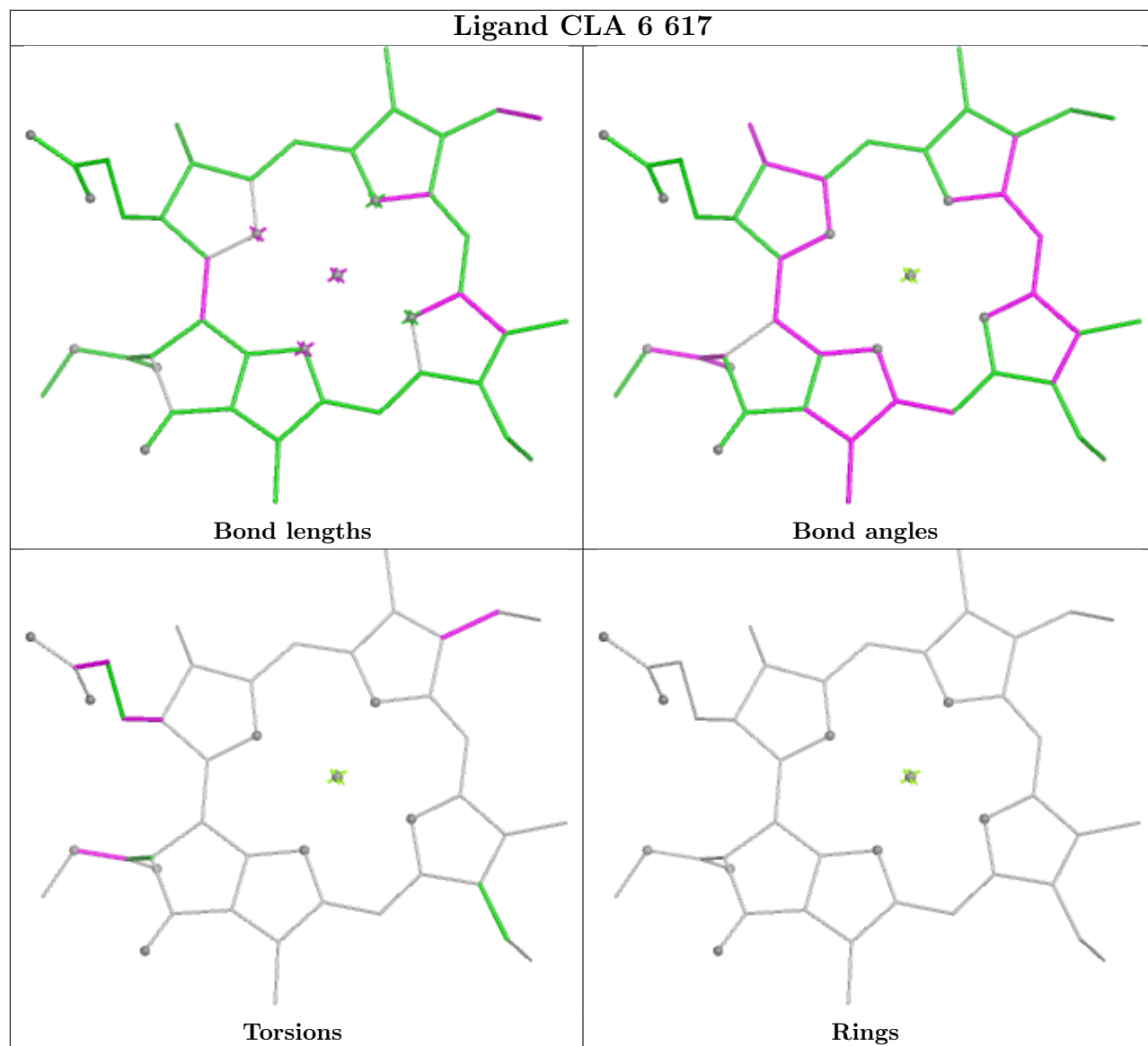
Bond angles

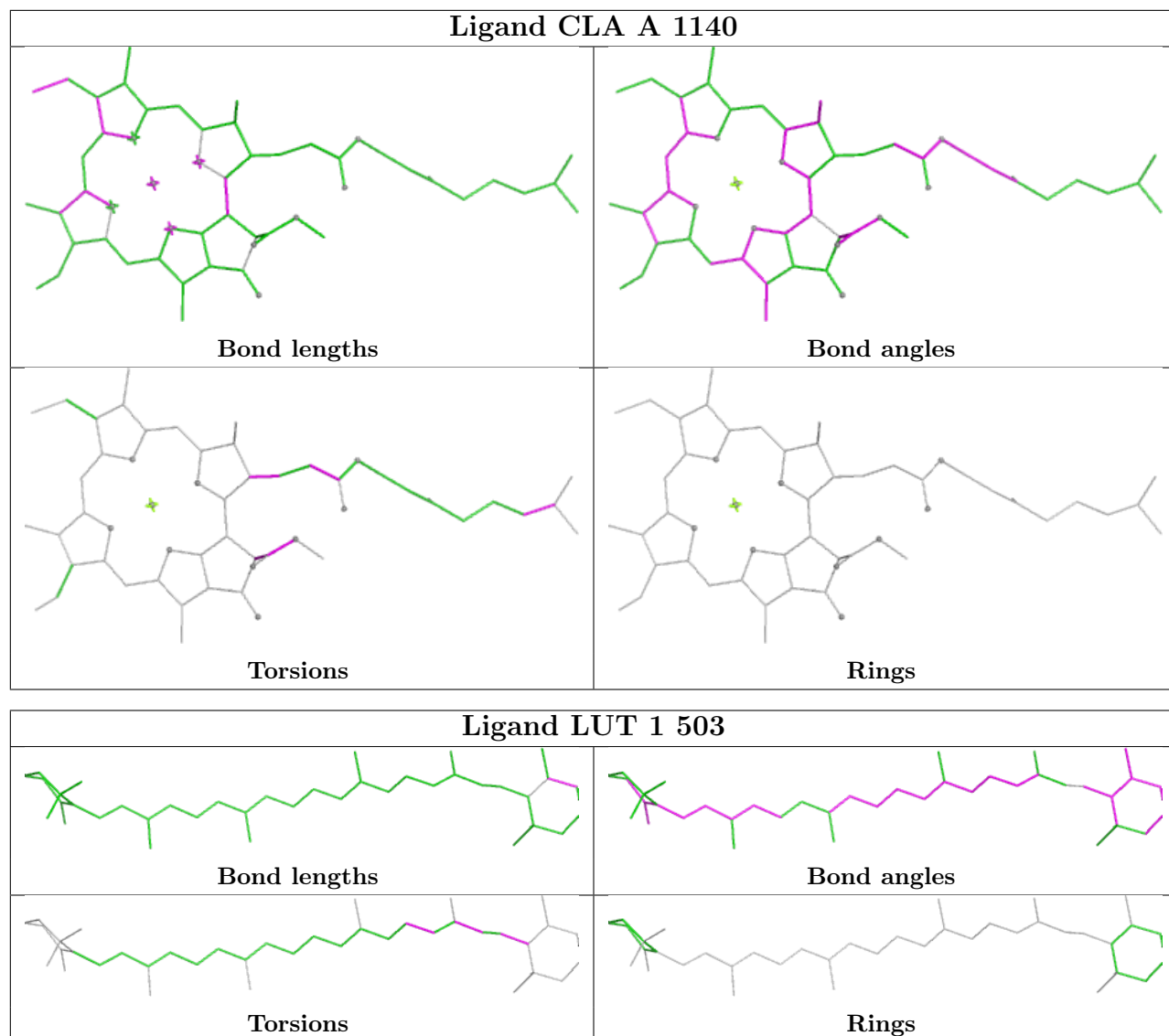


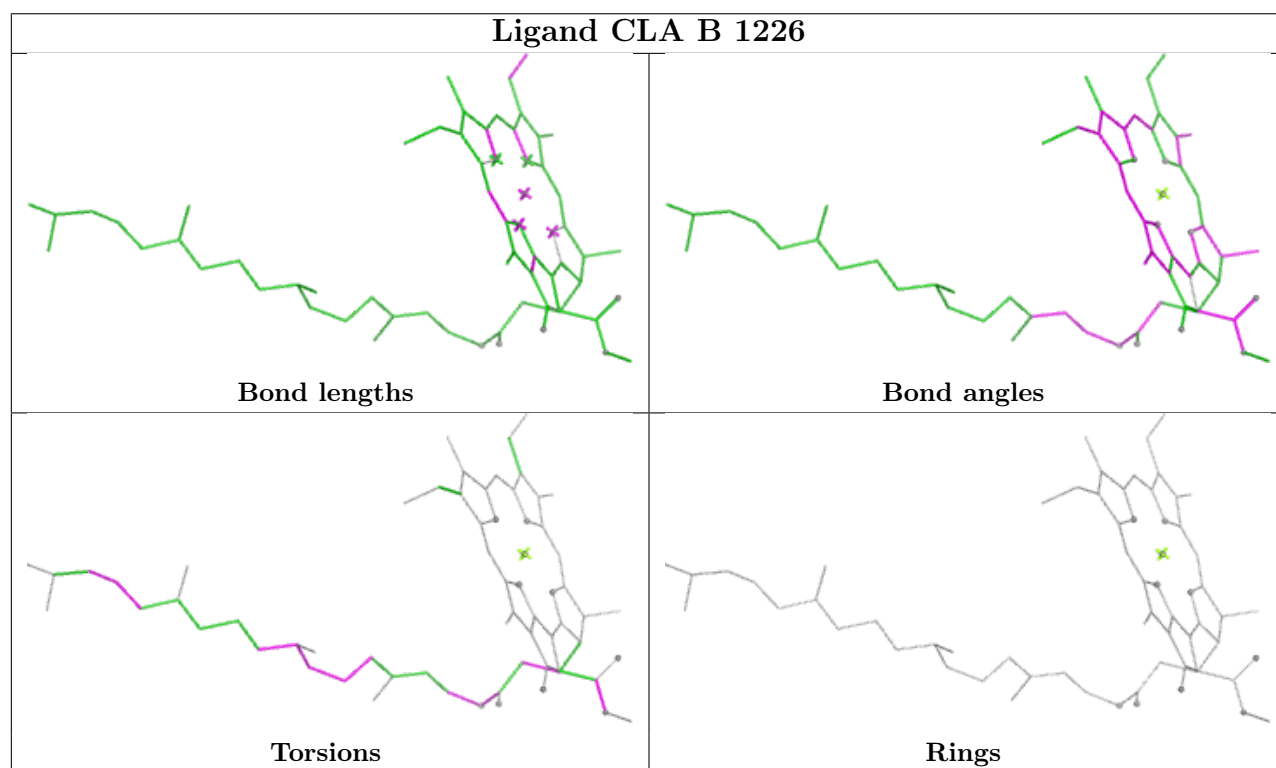
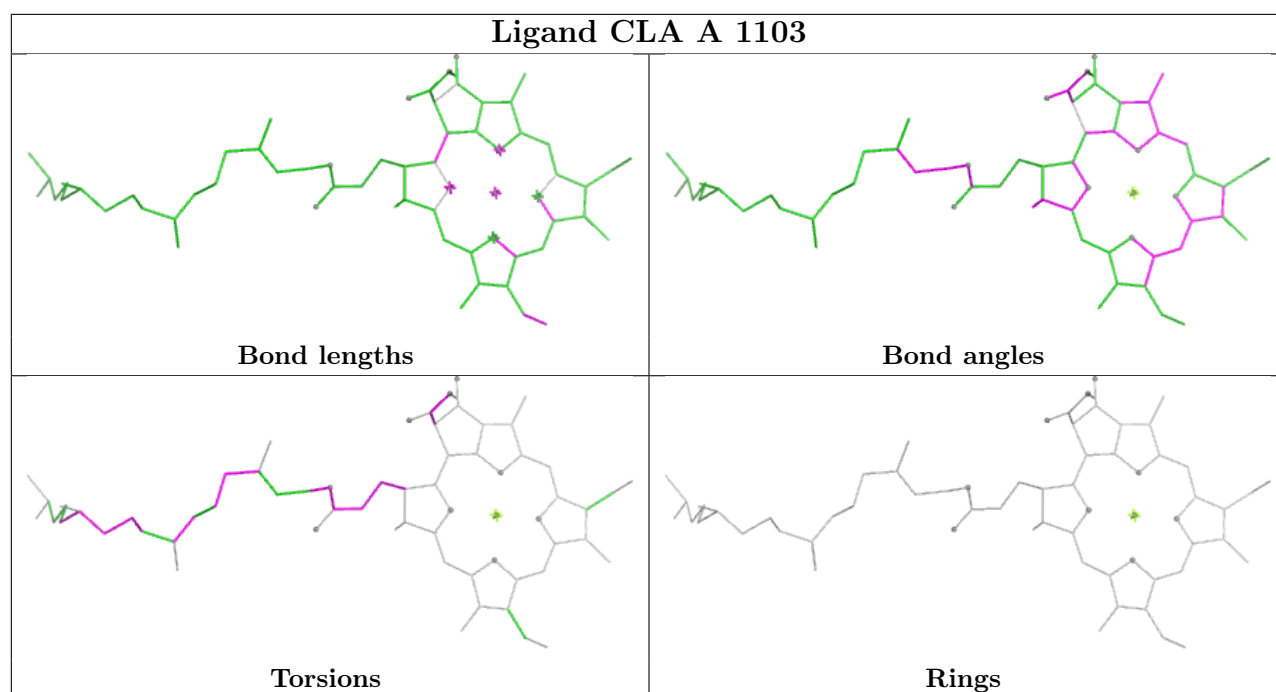
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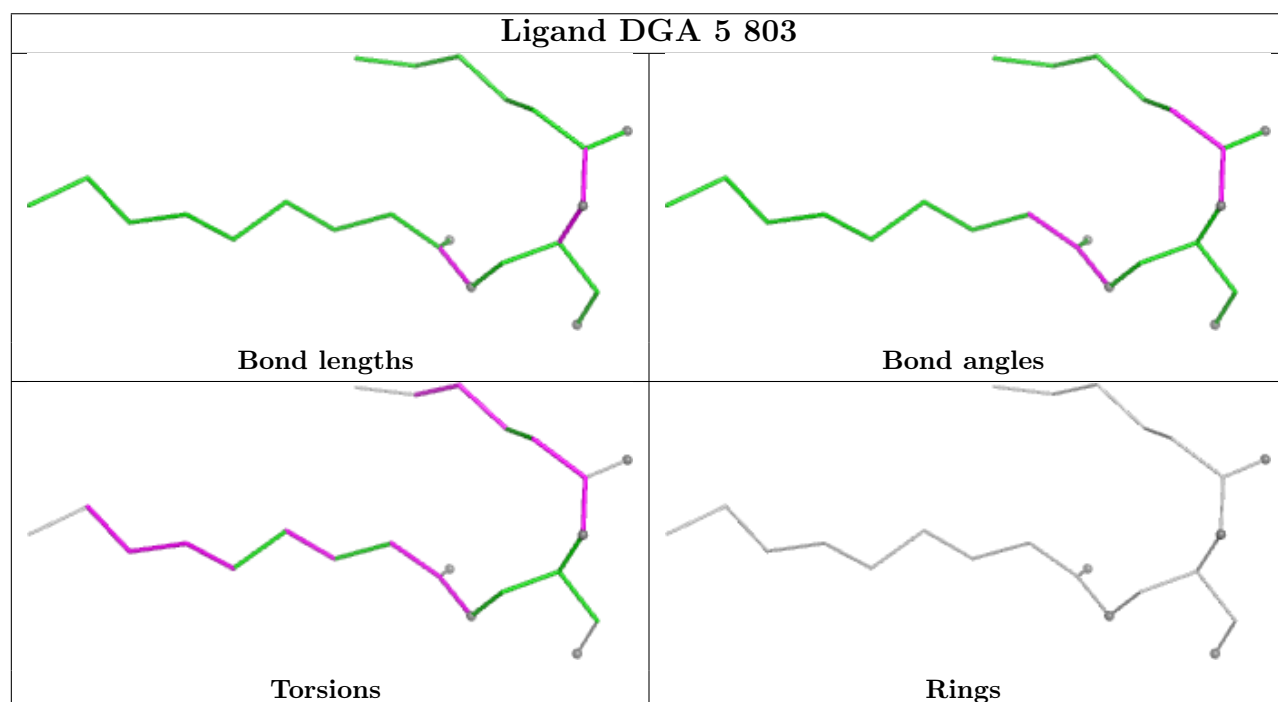
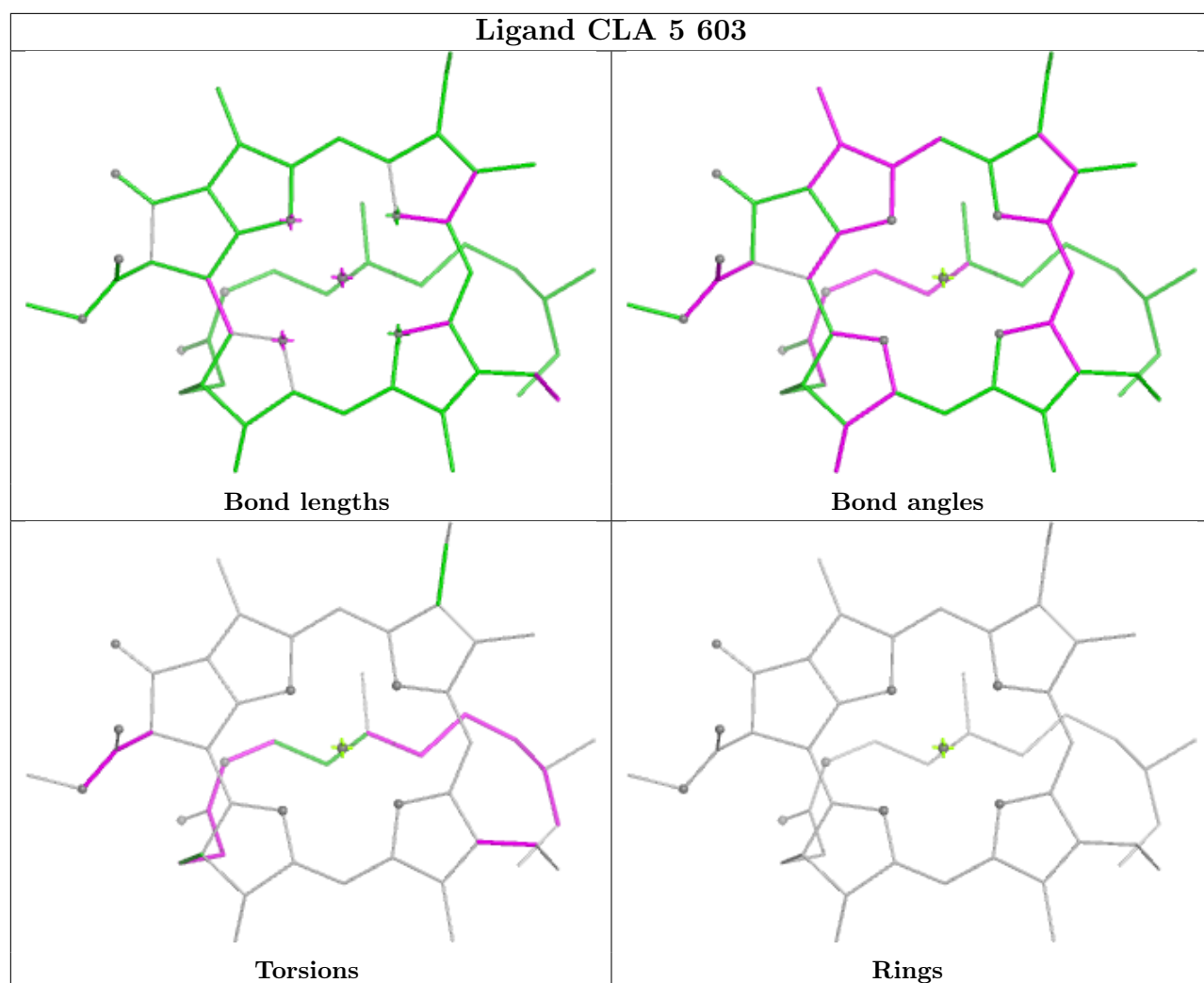


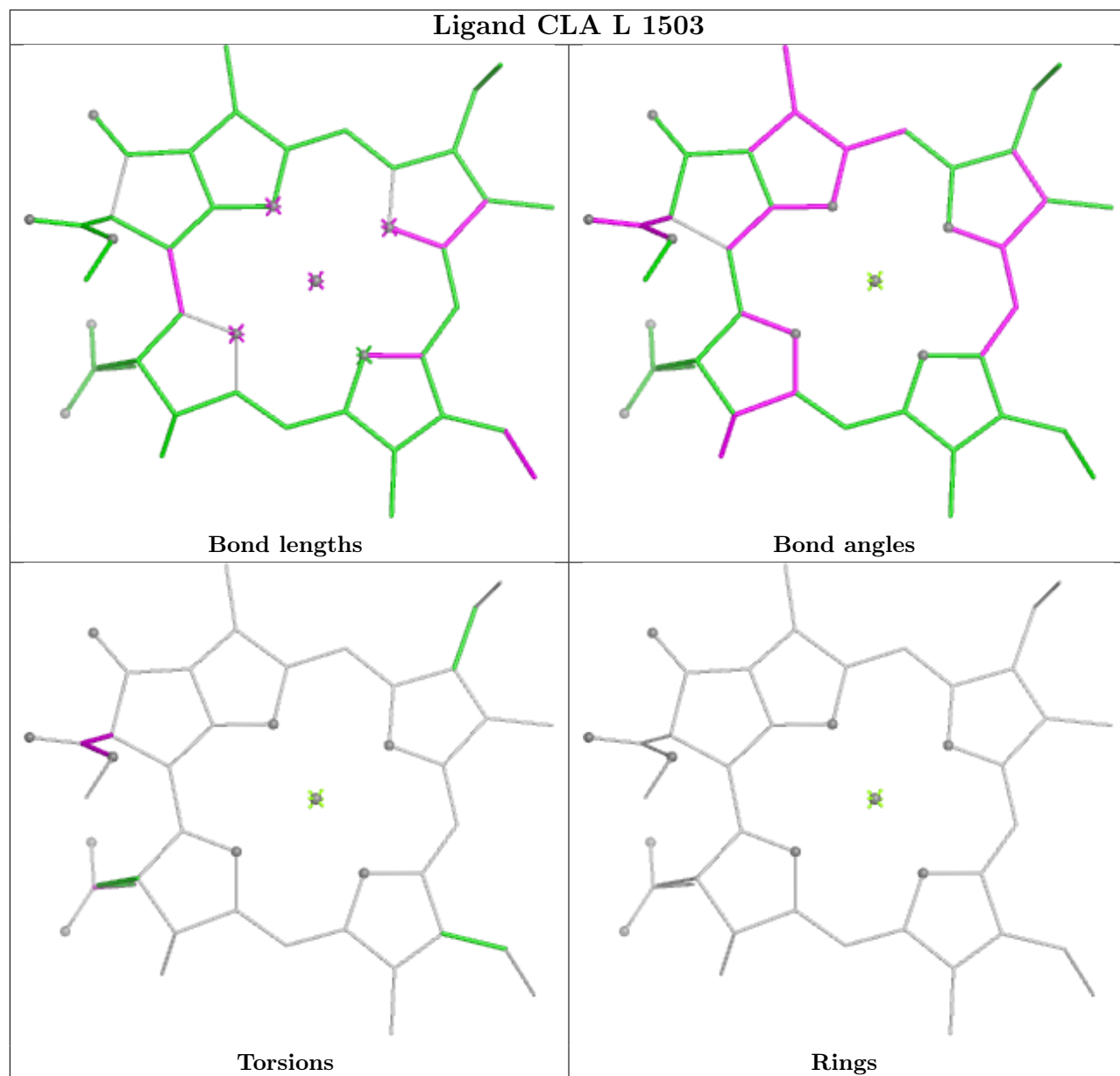
Rings

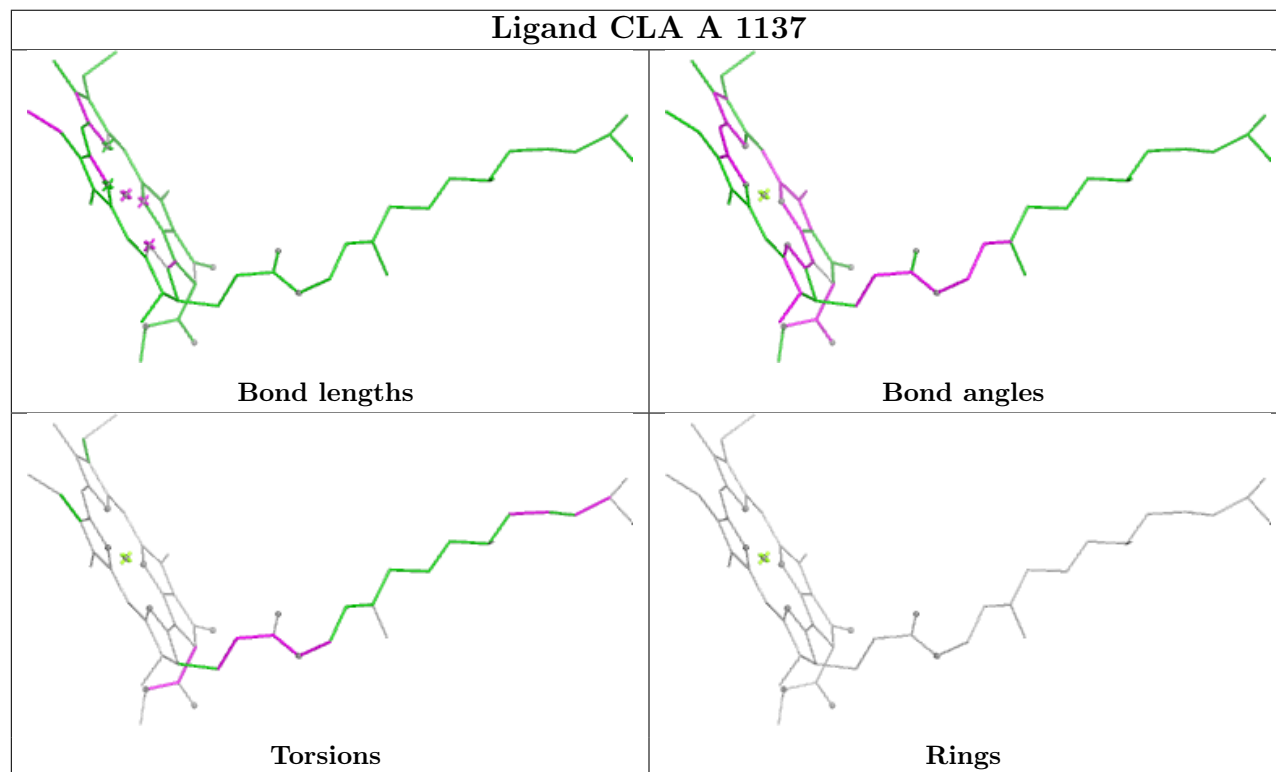
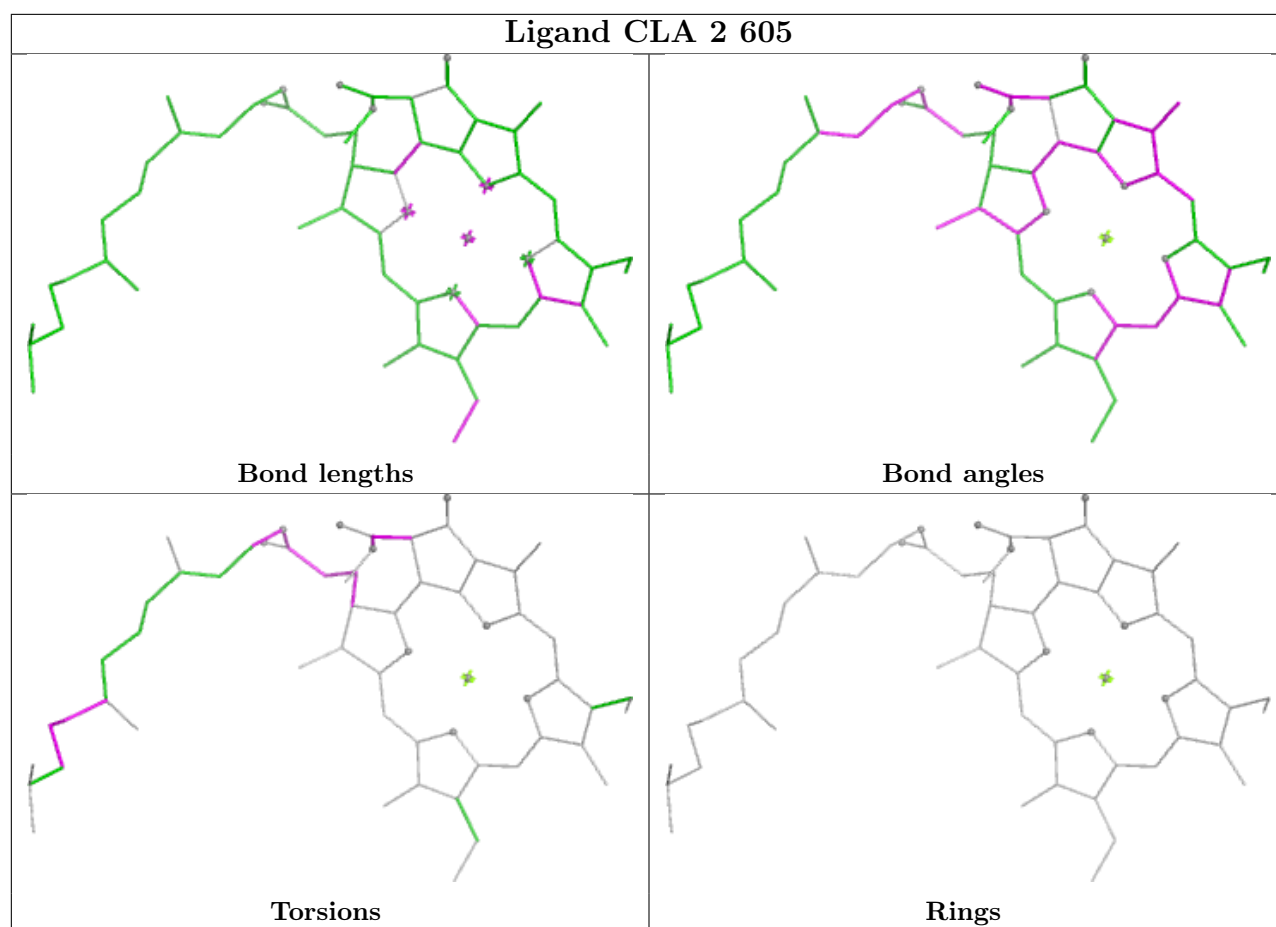


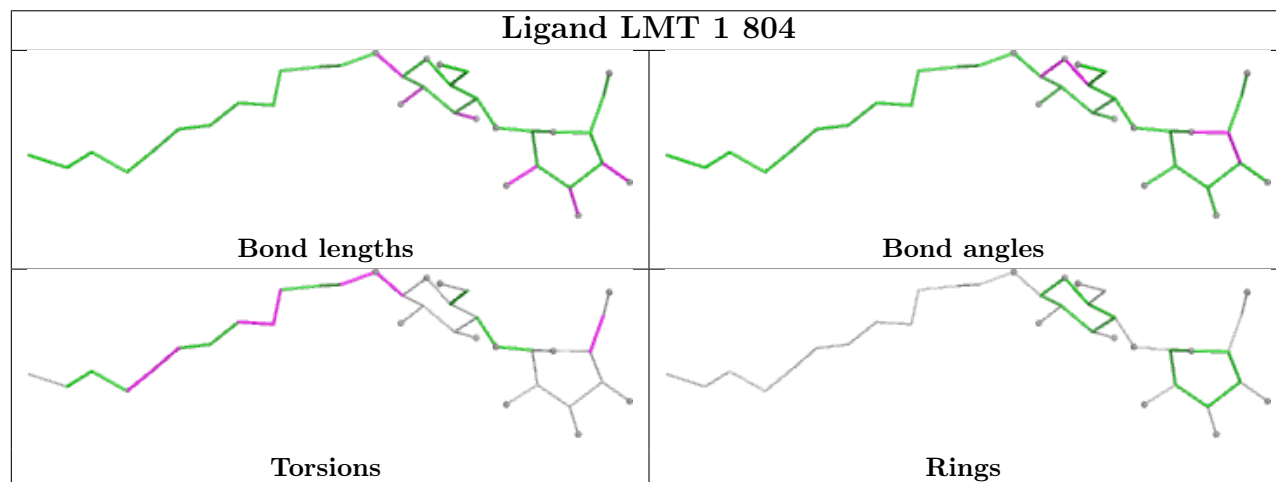
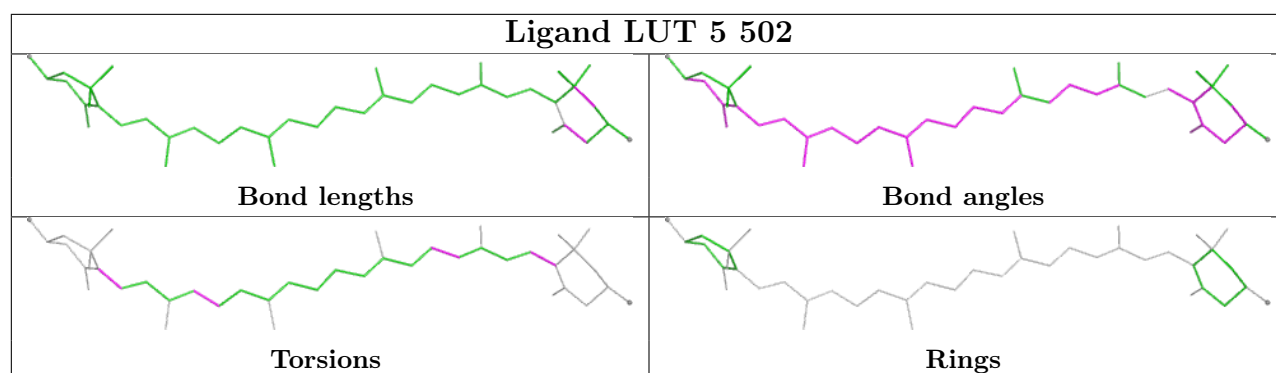


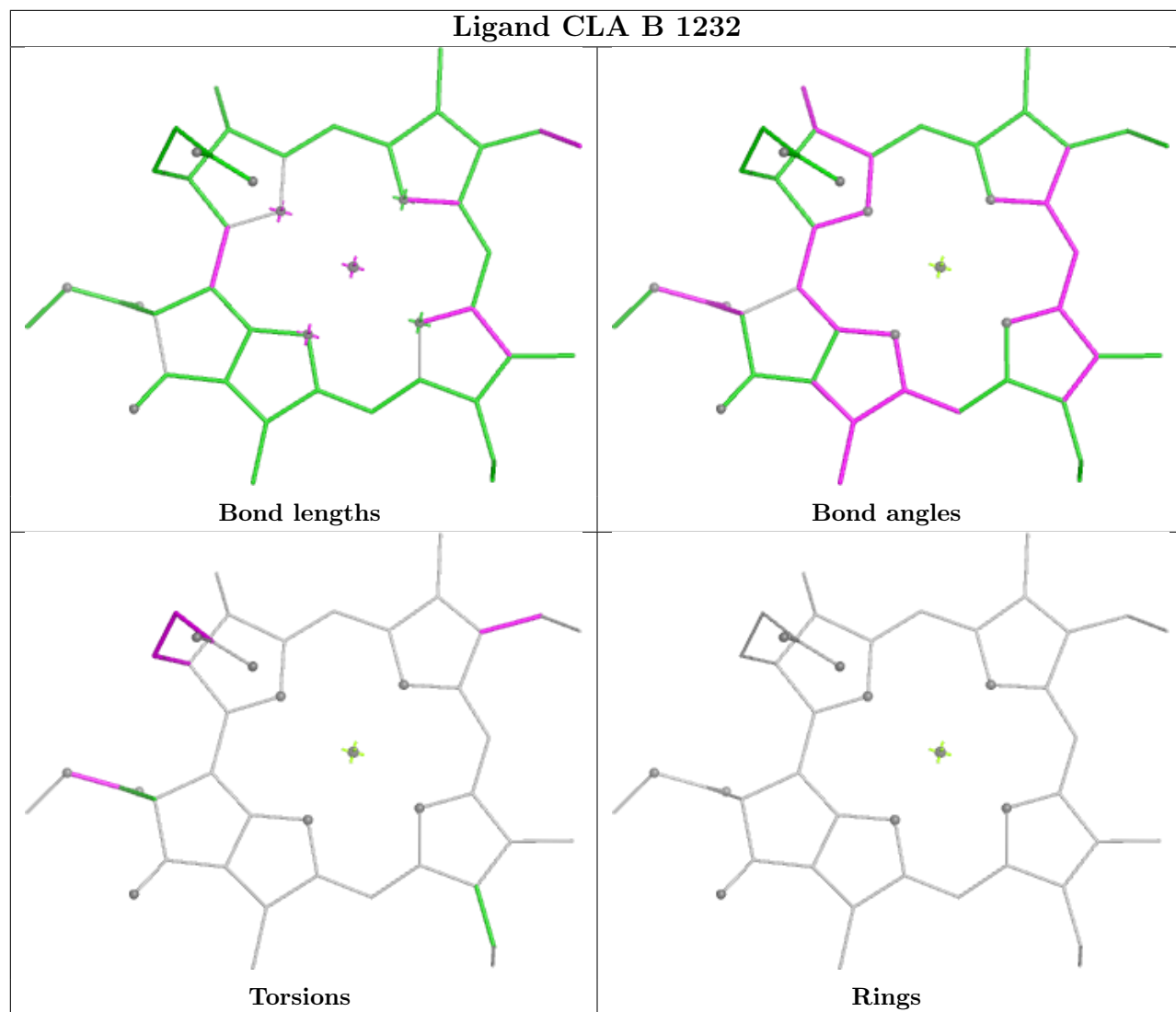


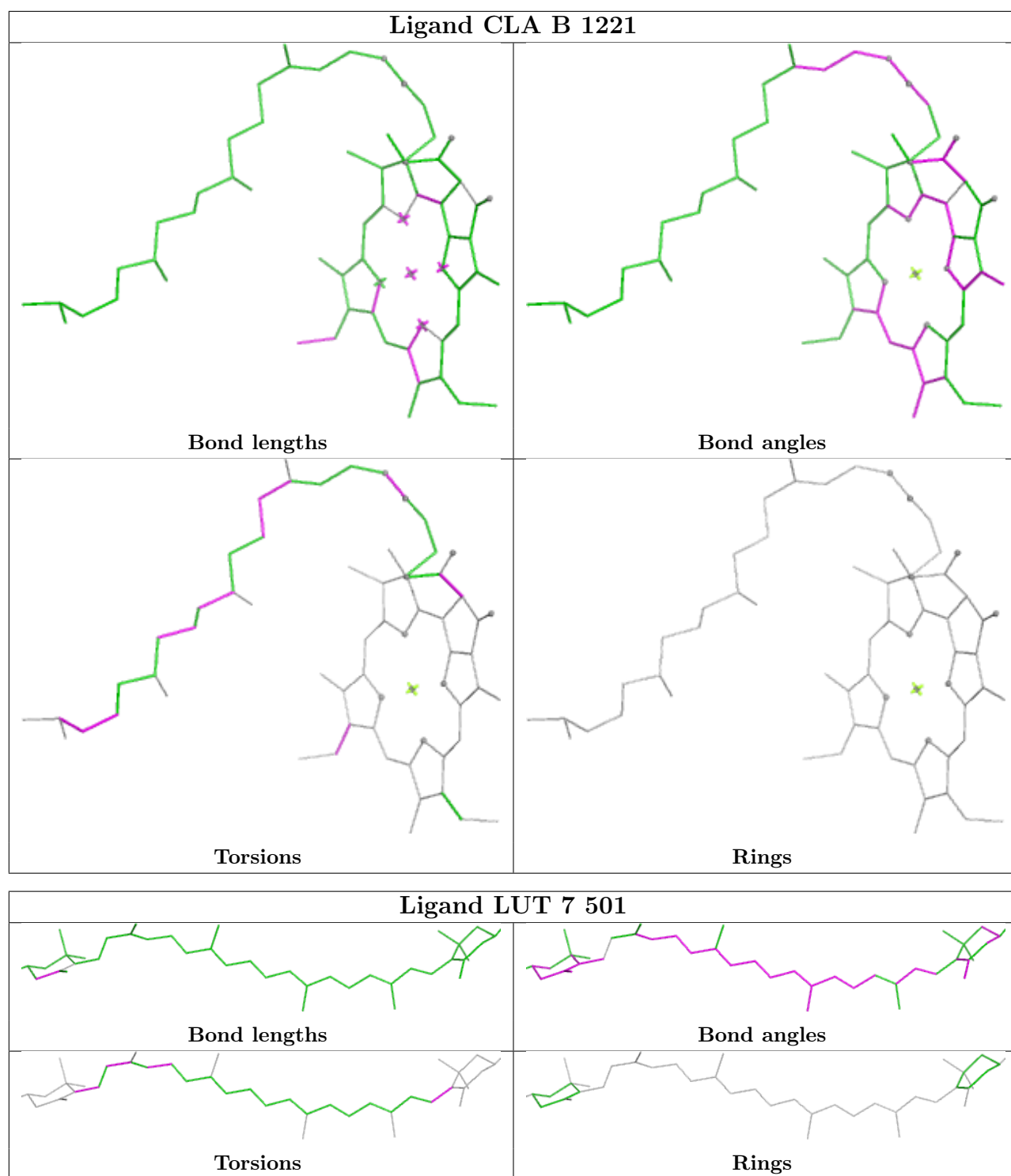


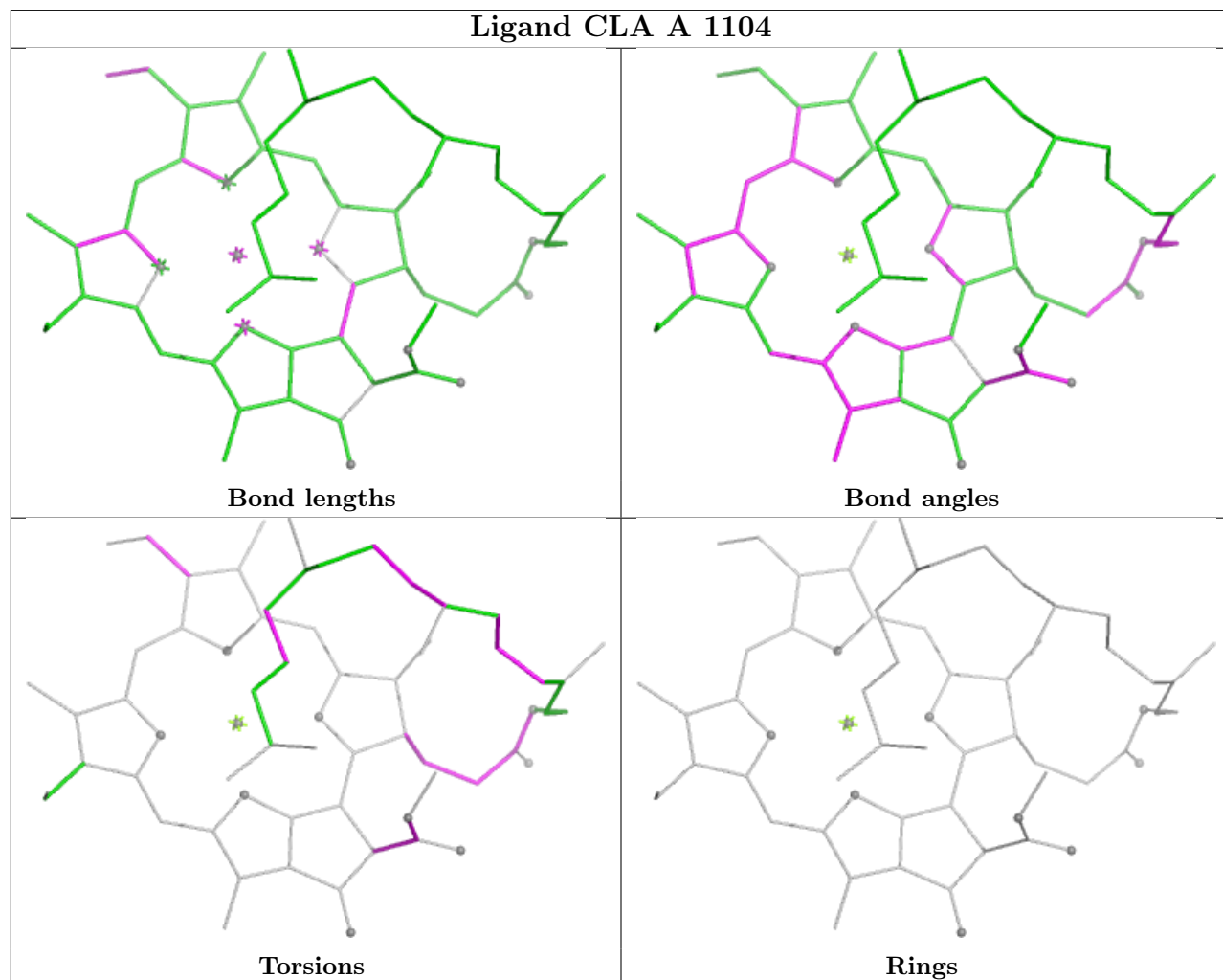
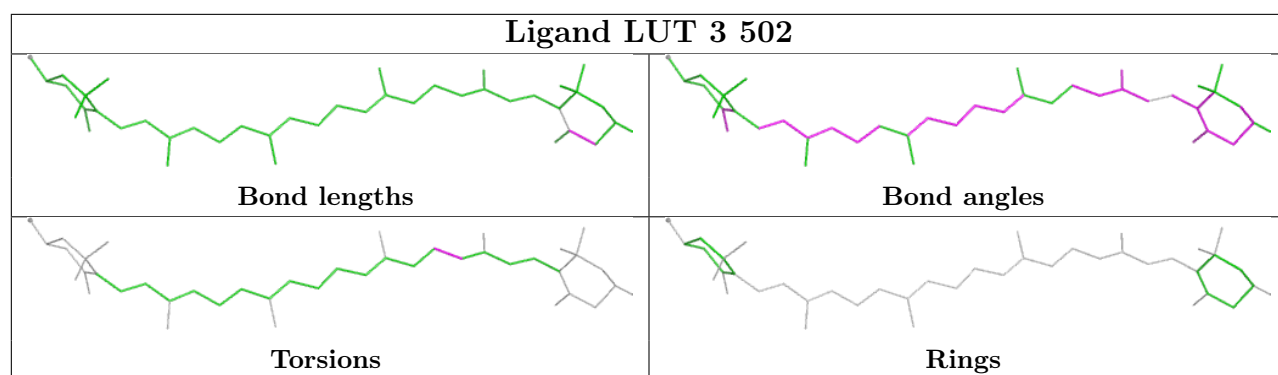


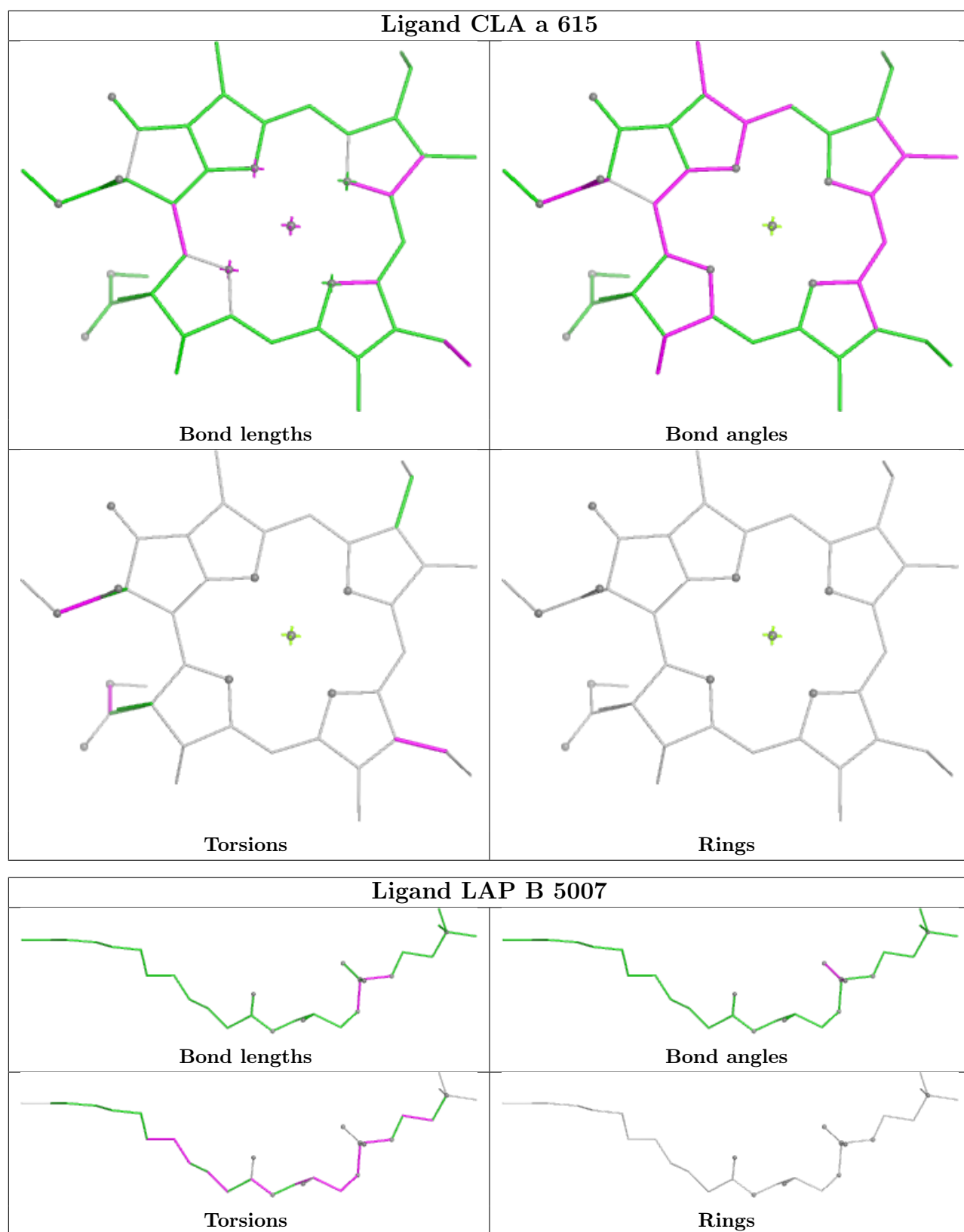


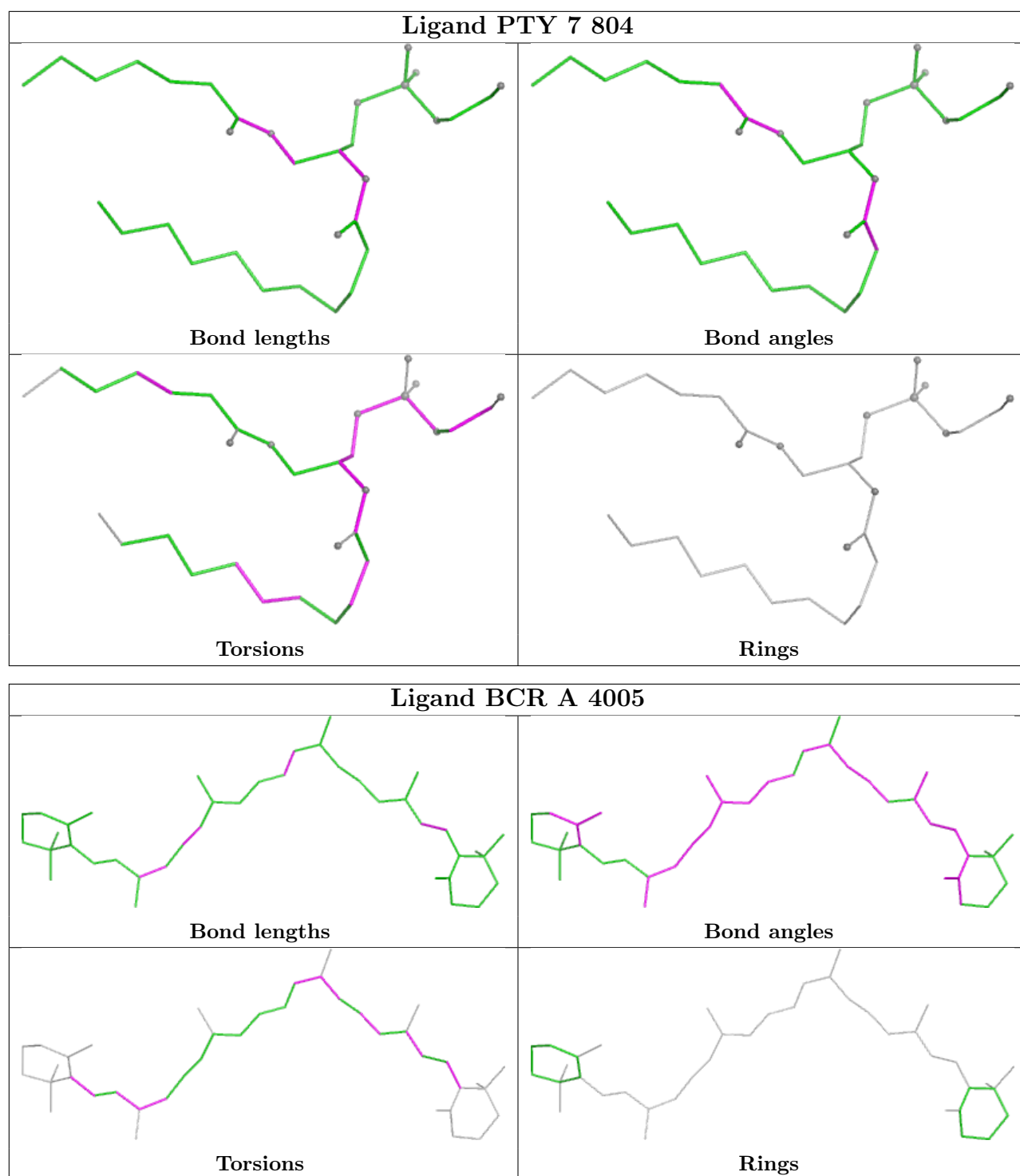


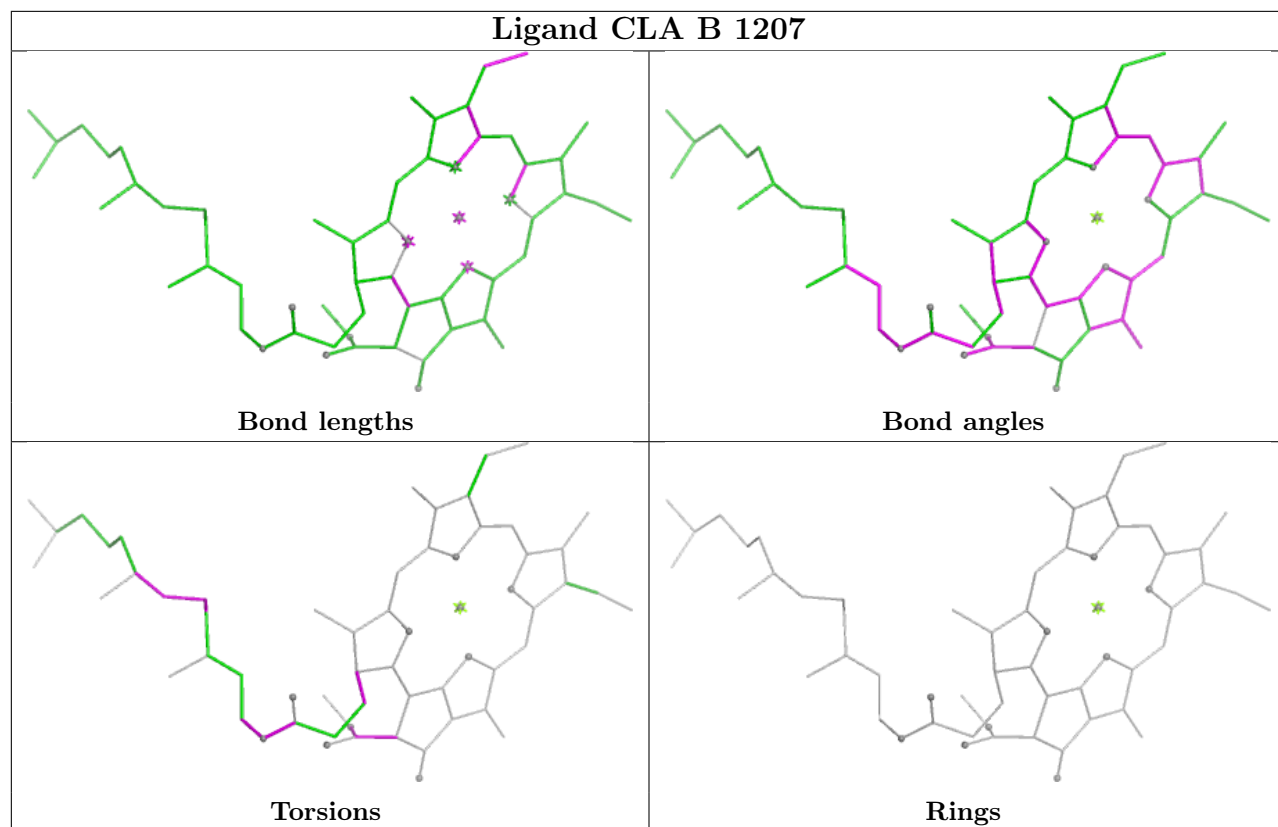




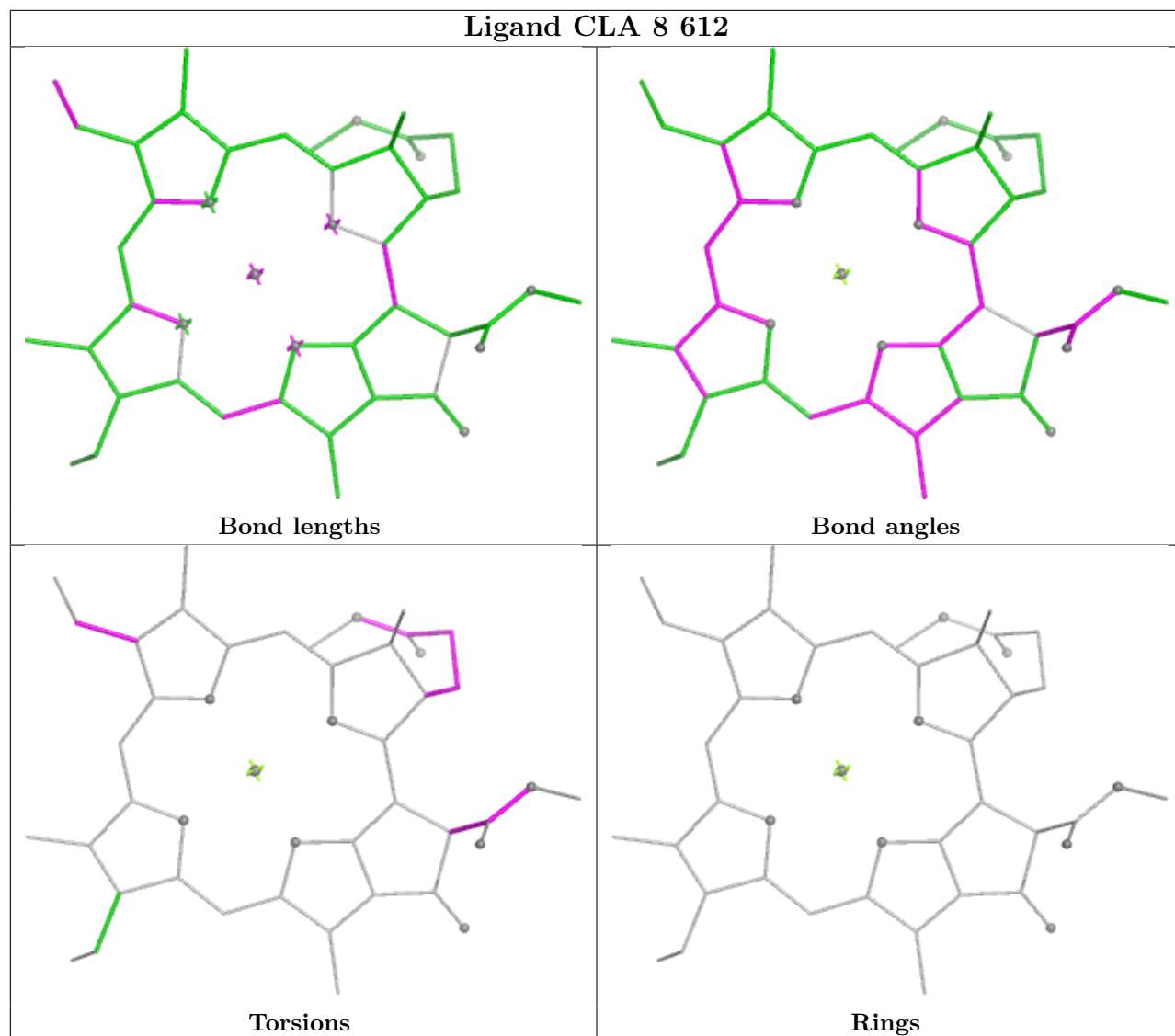




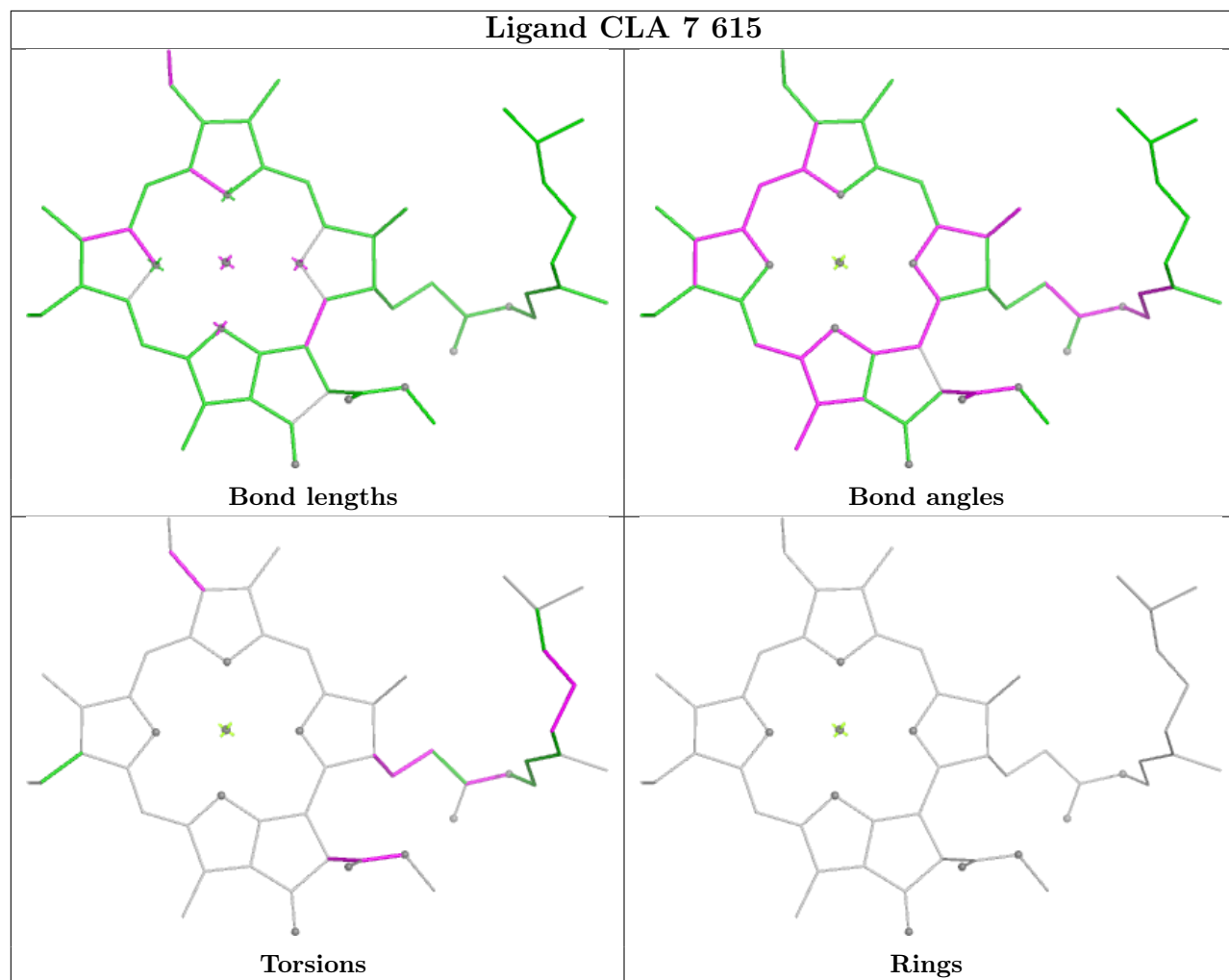




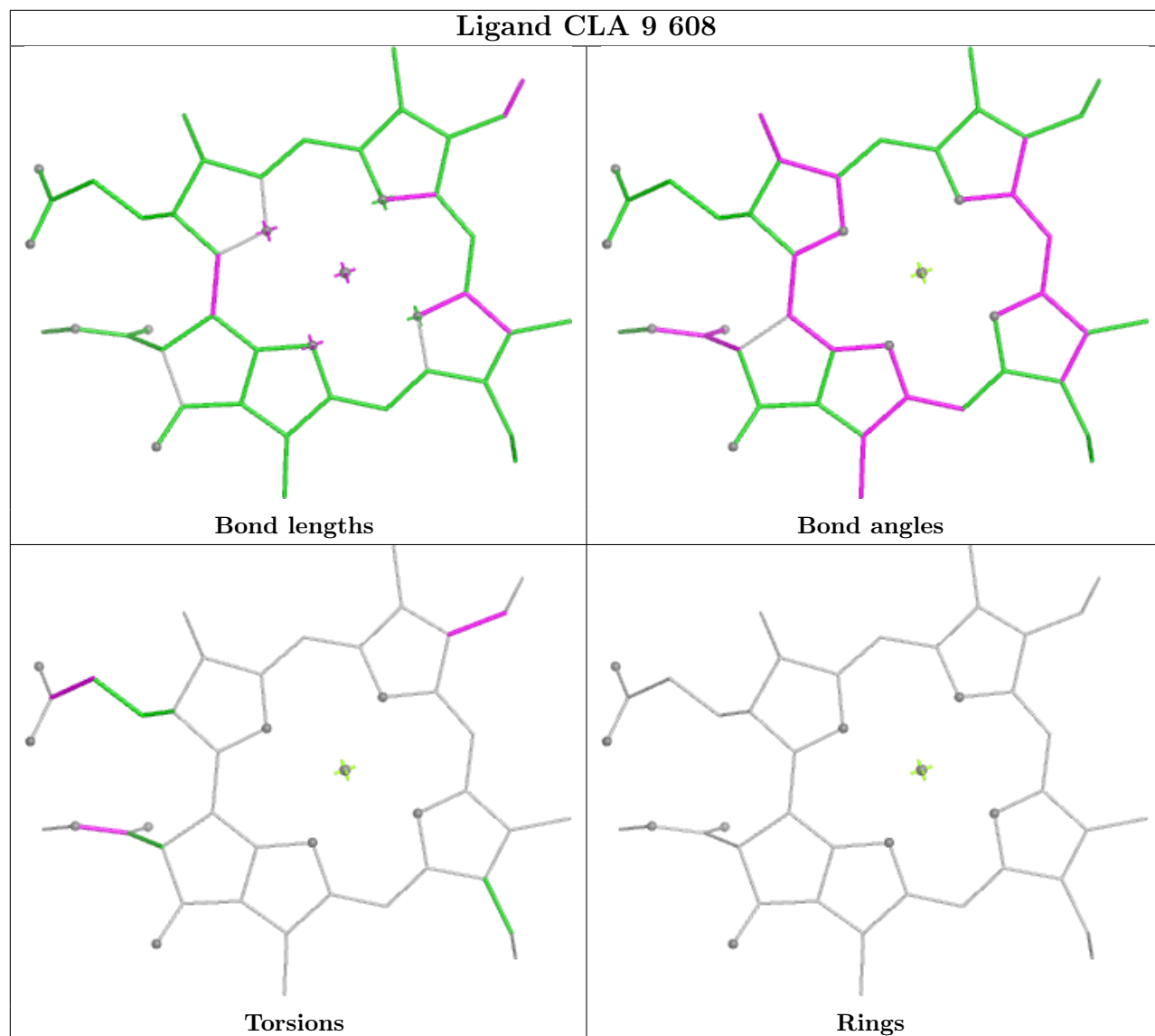
Ligand CLA 8 612



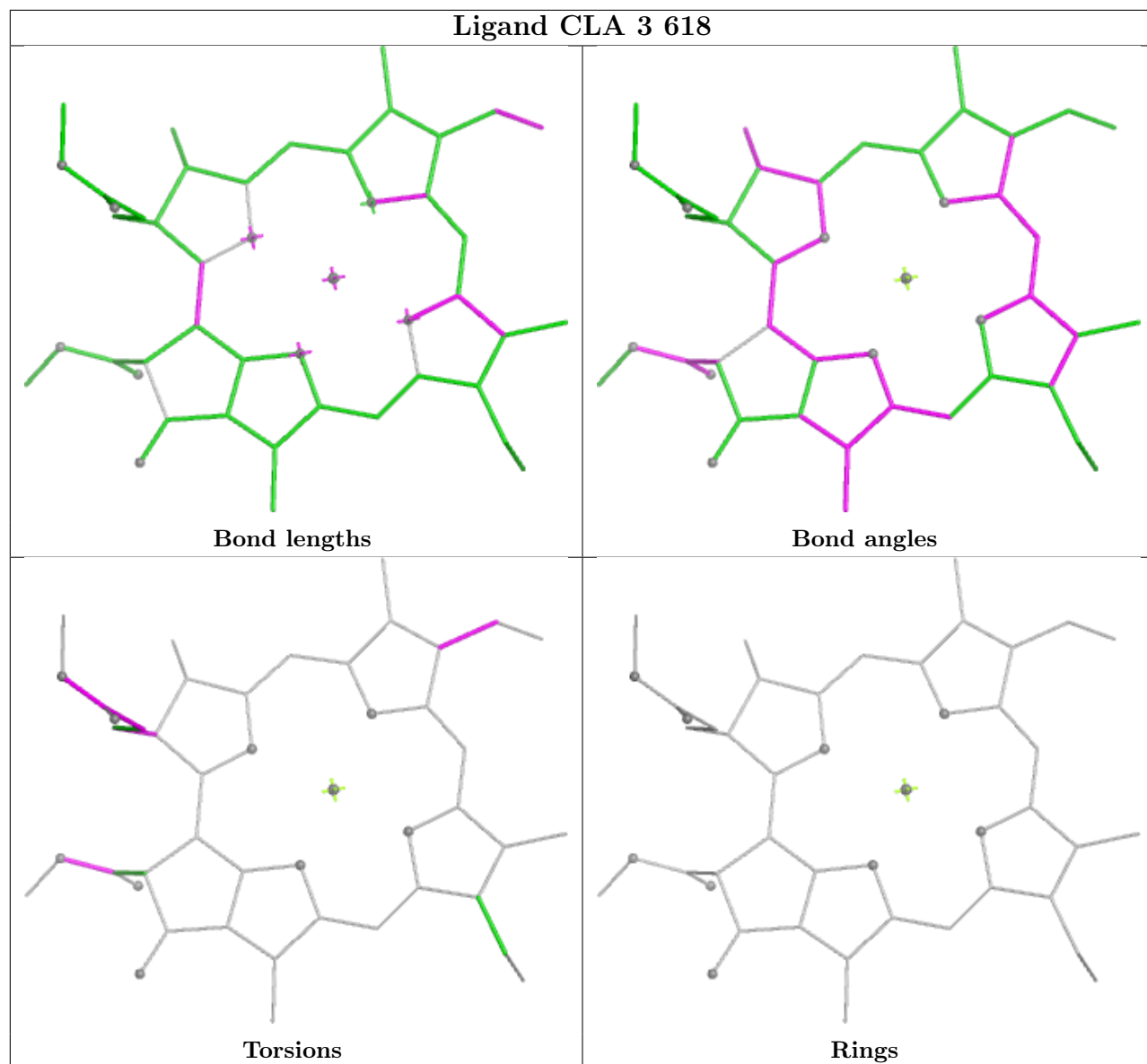
Ligand CLA 7 615

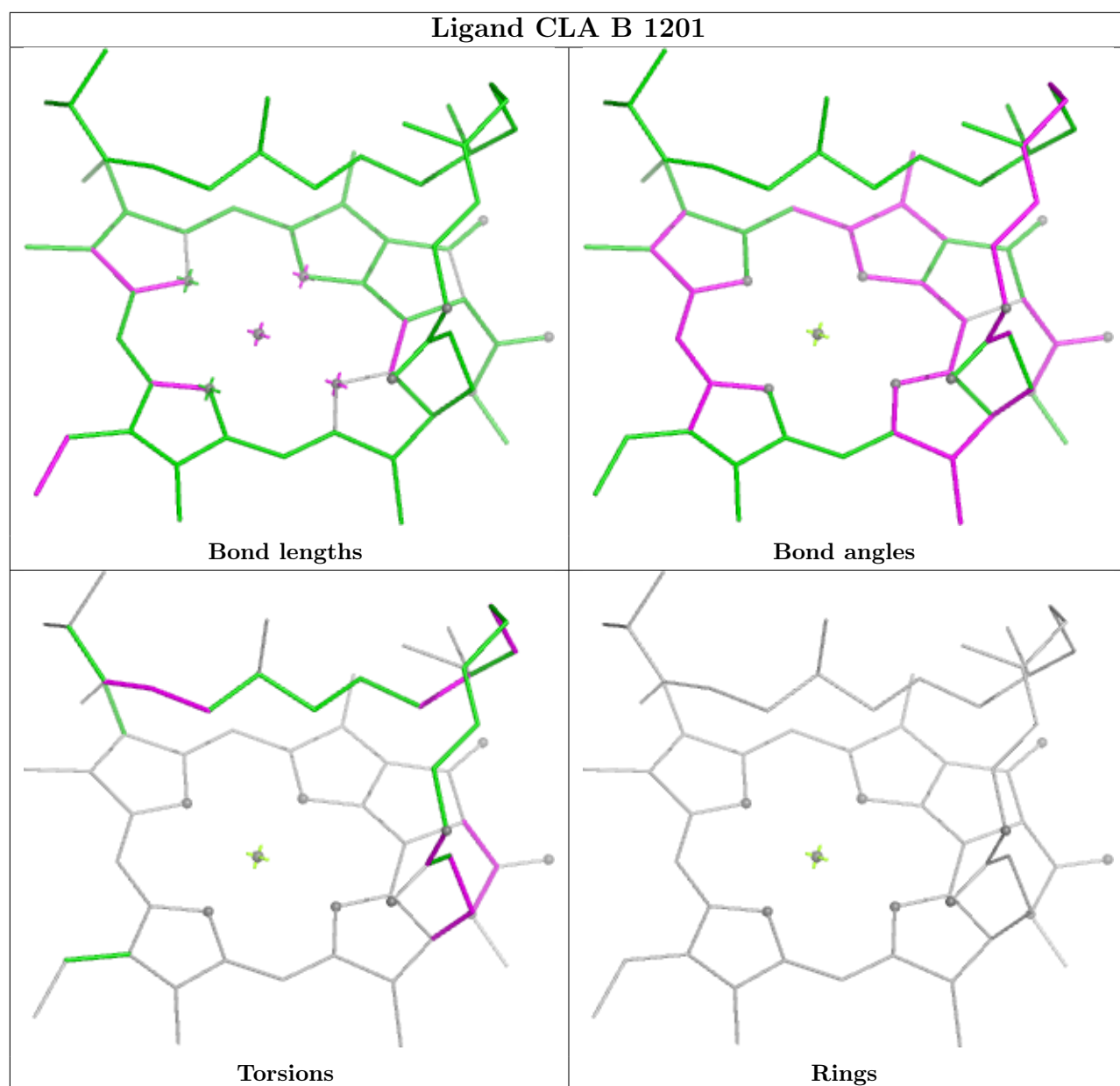


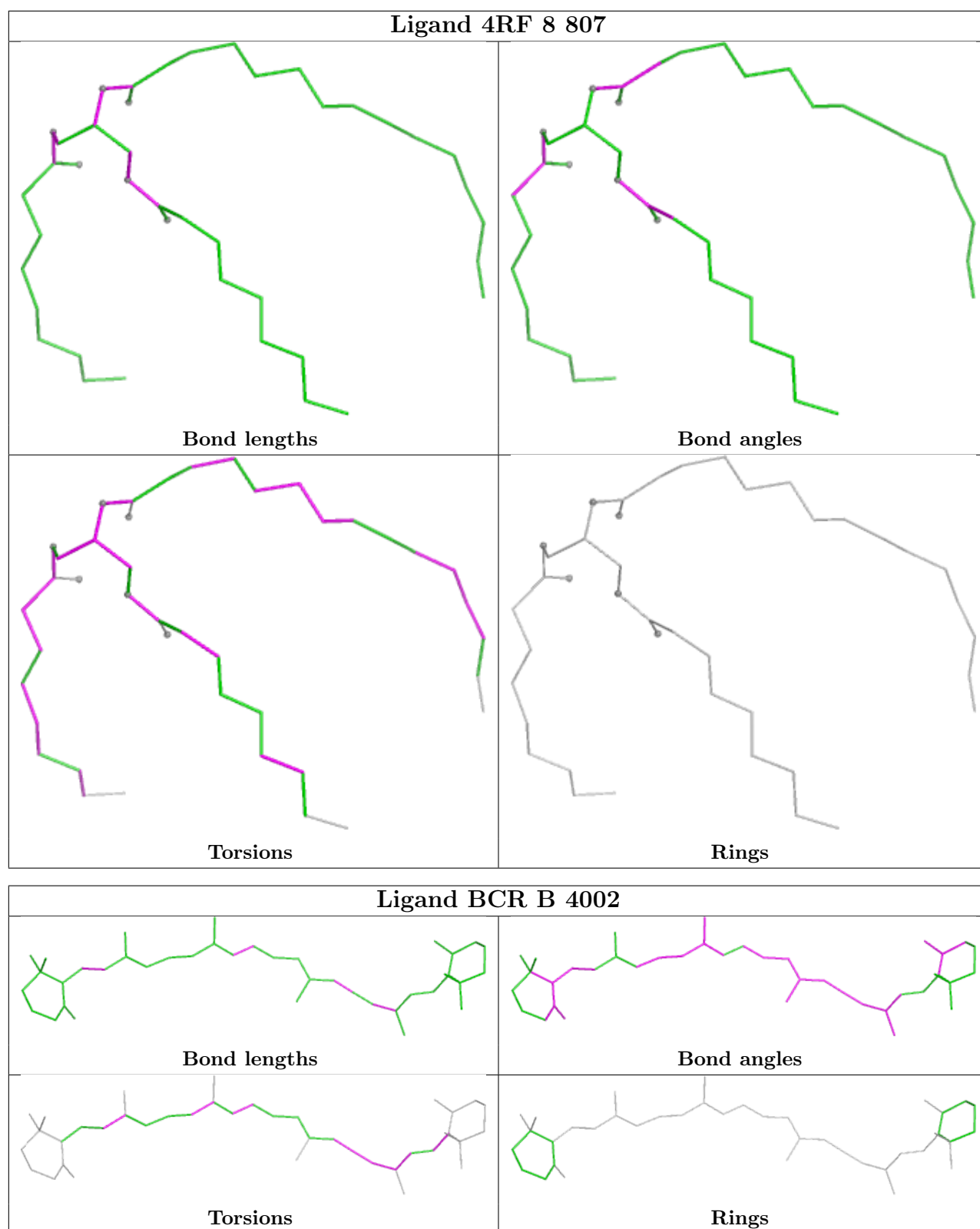
Ligand CLA 9 608

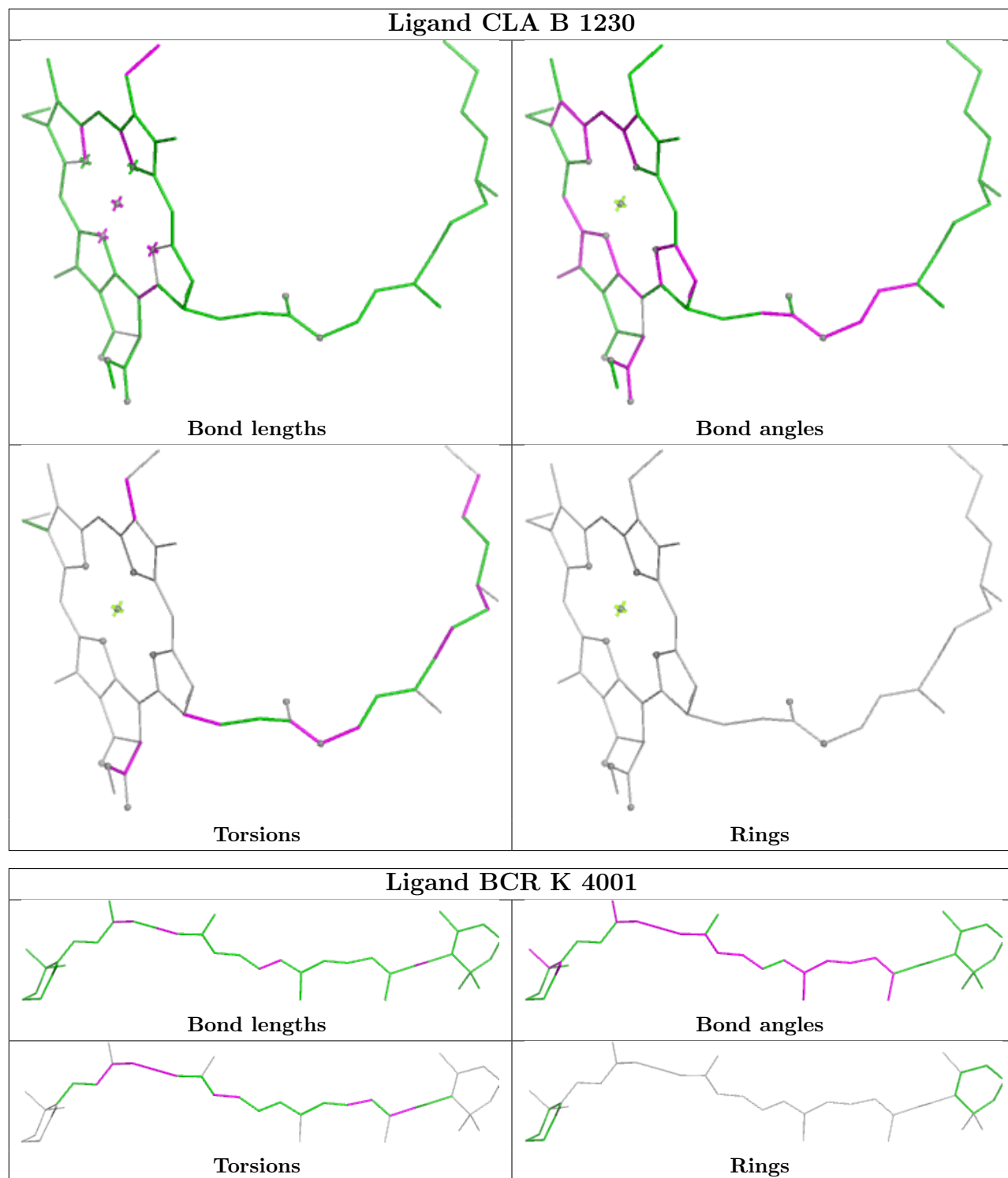


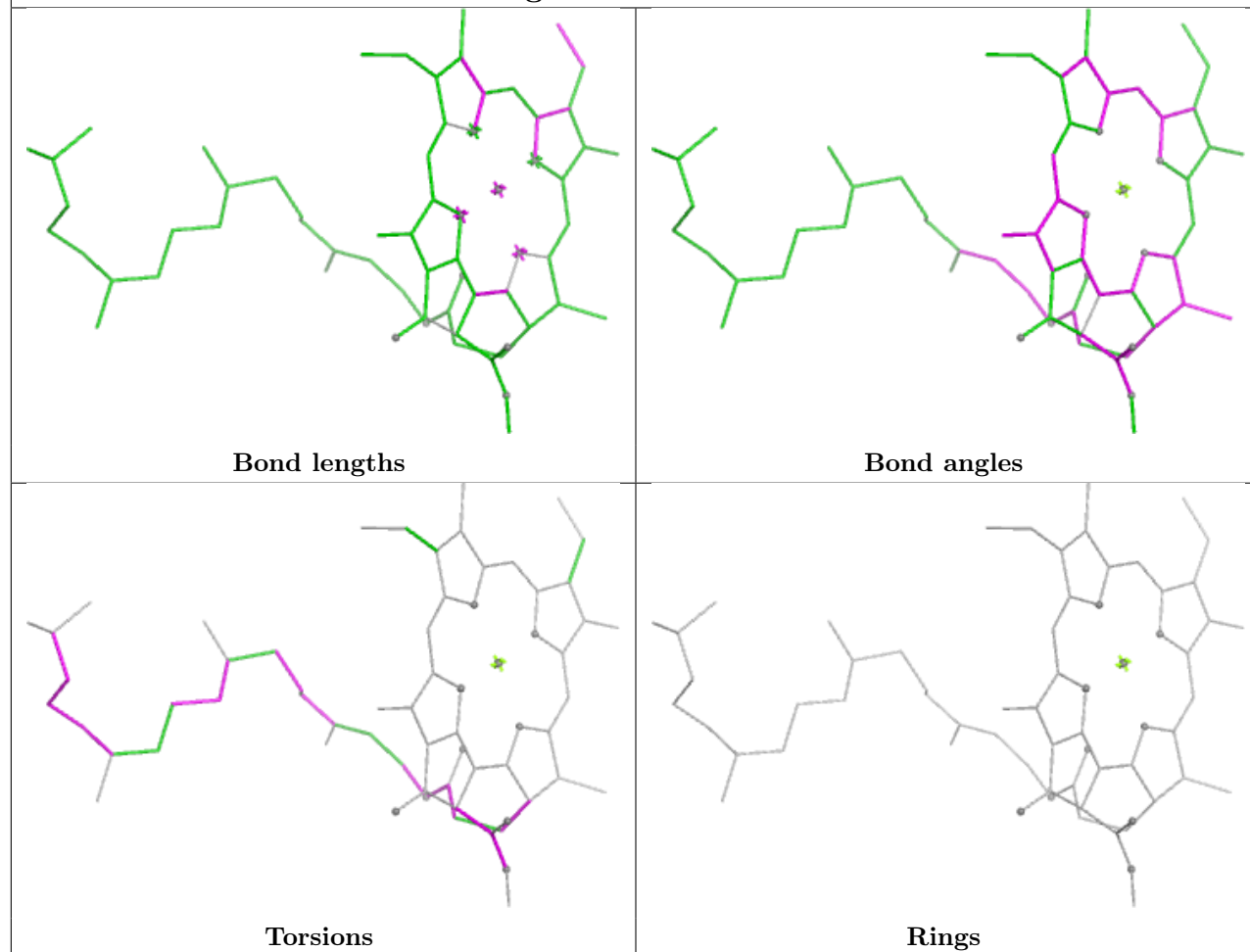
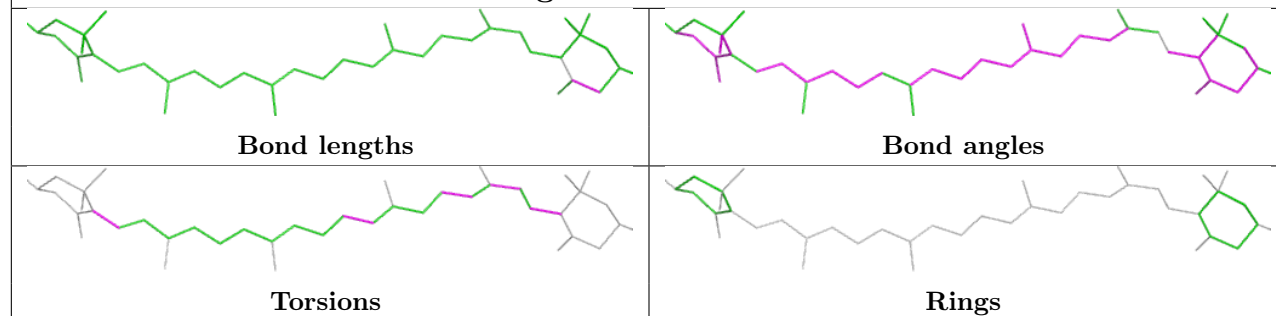
Ligand CLA 3 618



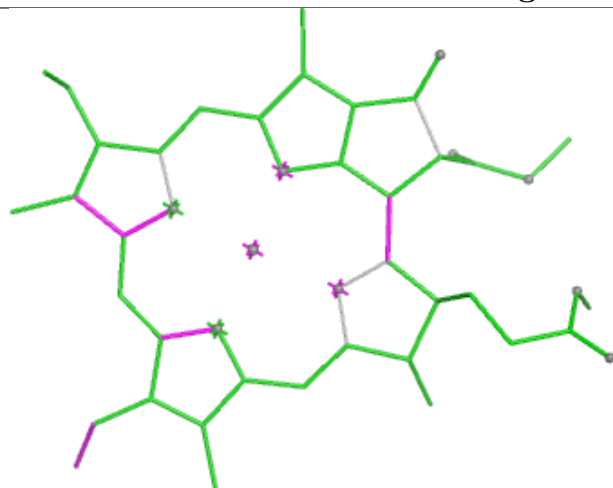




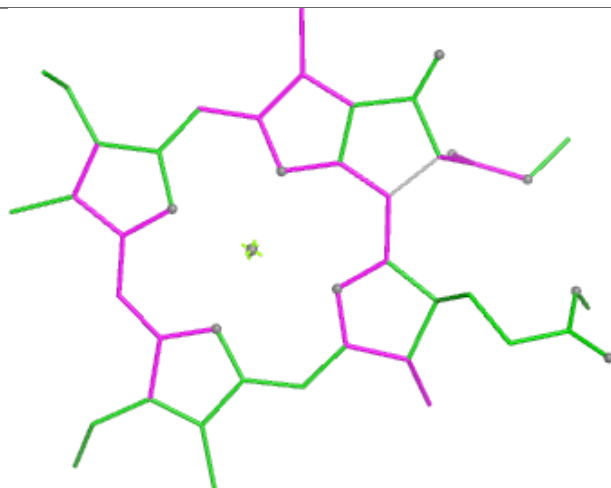


Ligand CLA 9 612**Ligand LUT 6 502**

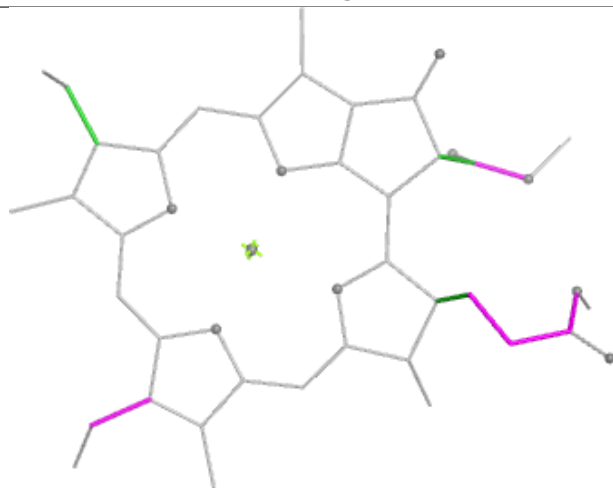
Ligand CLA 9 609



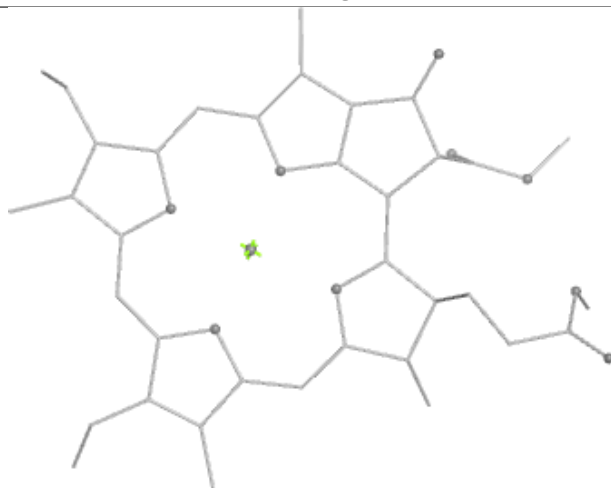
Bond lengths



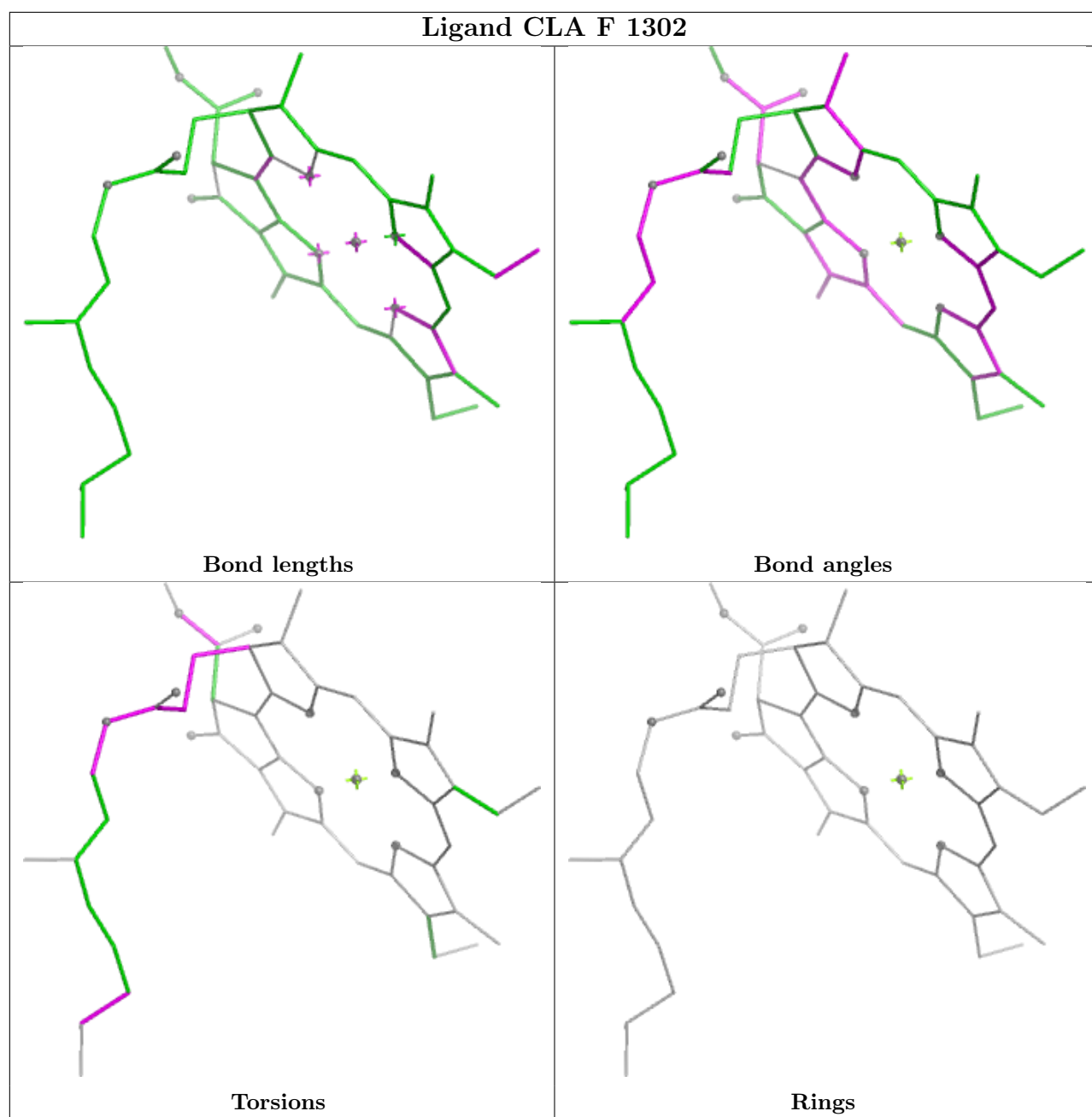
Bond angles

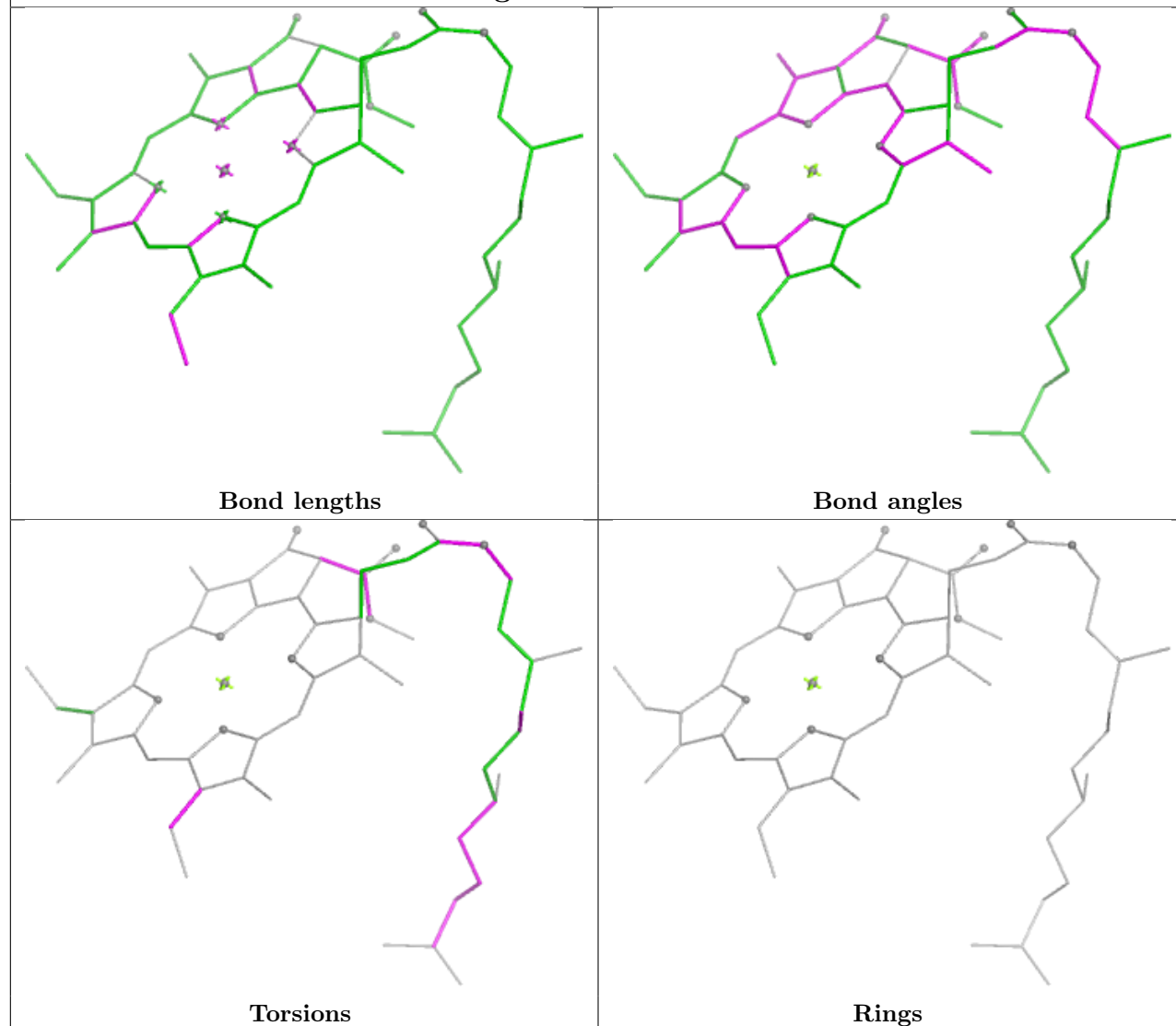
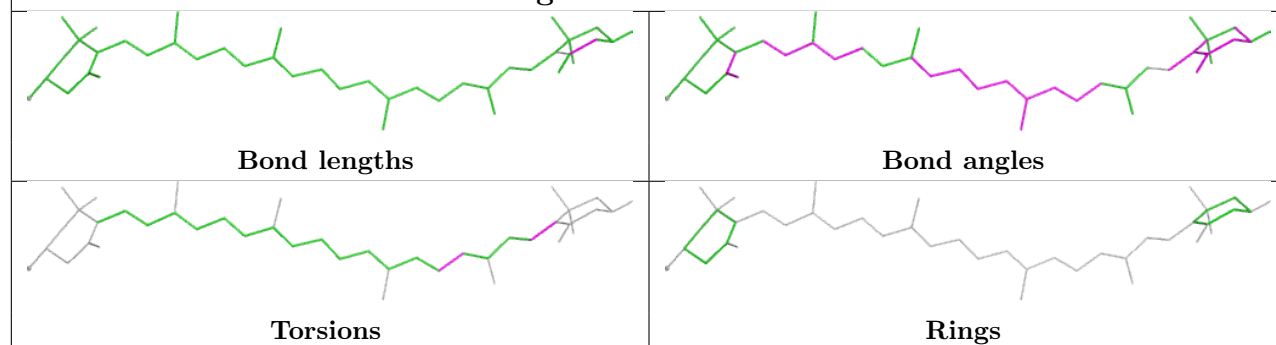


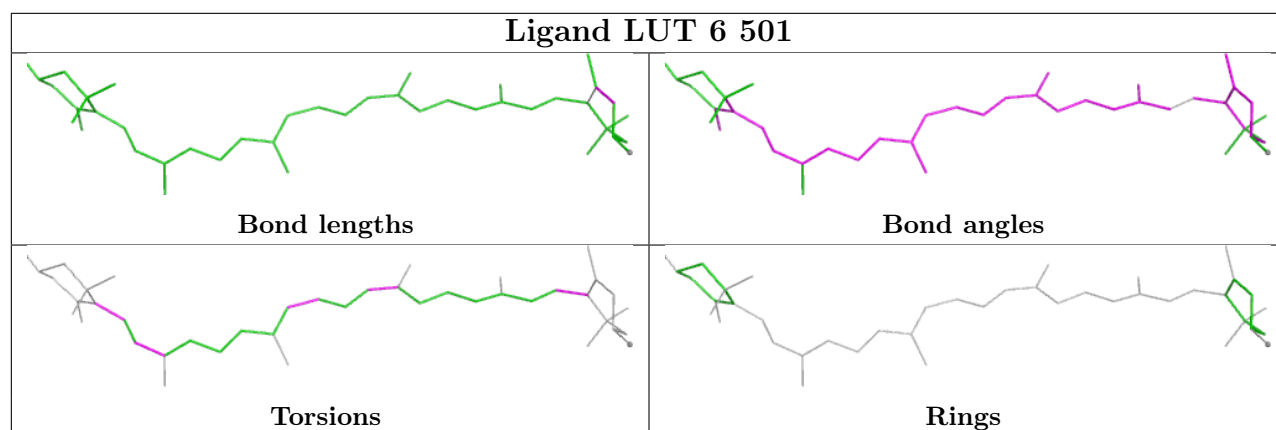
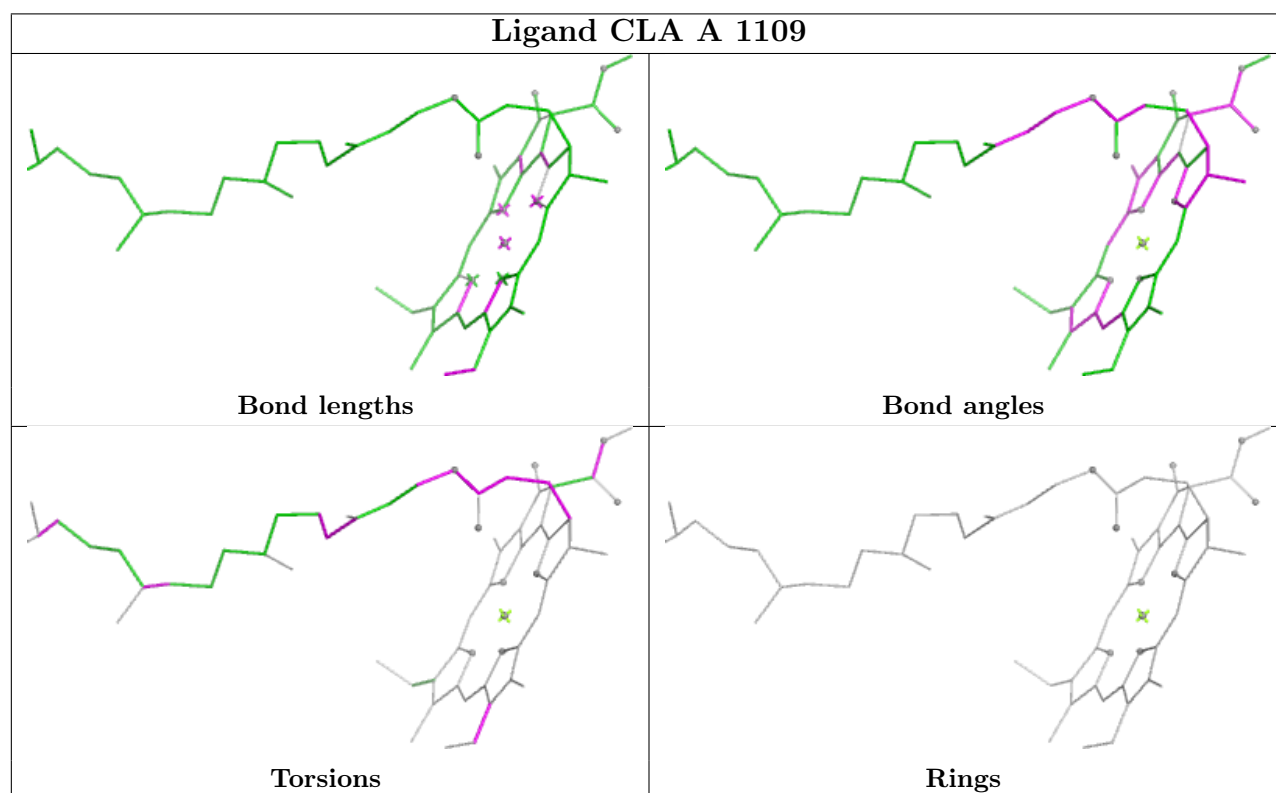
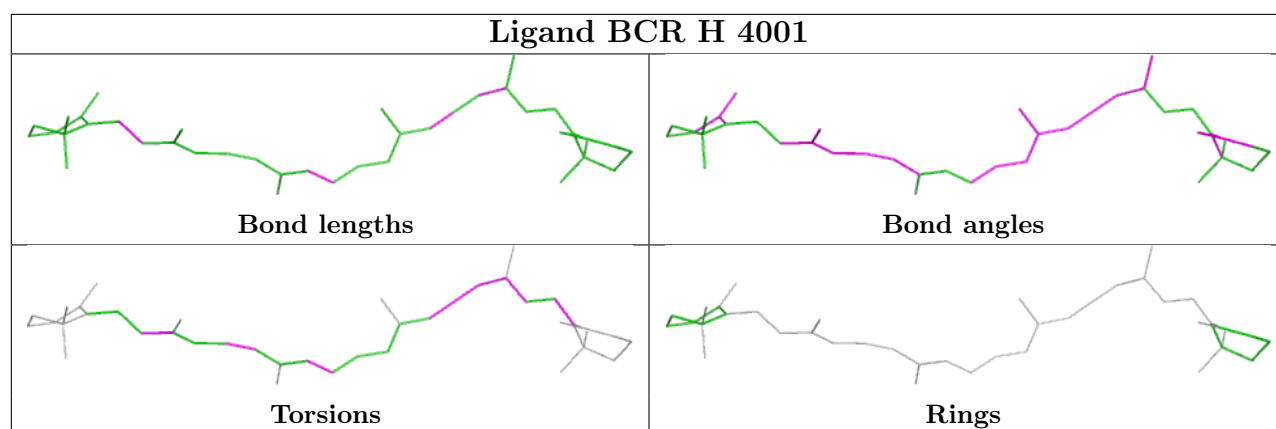
Torsions

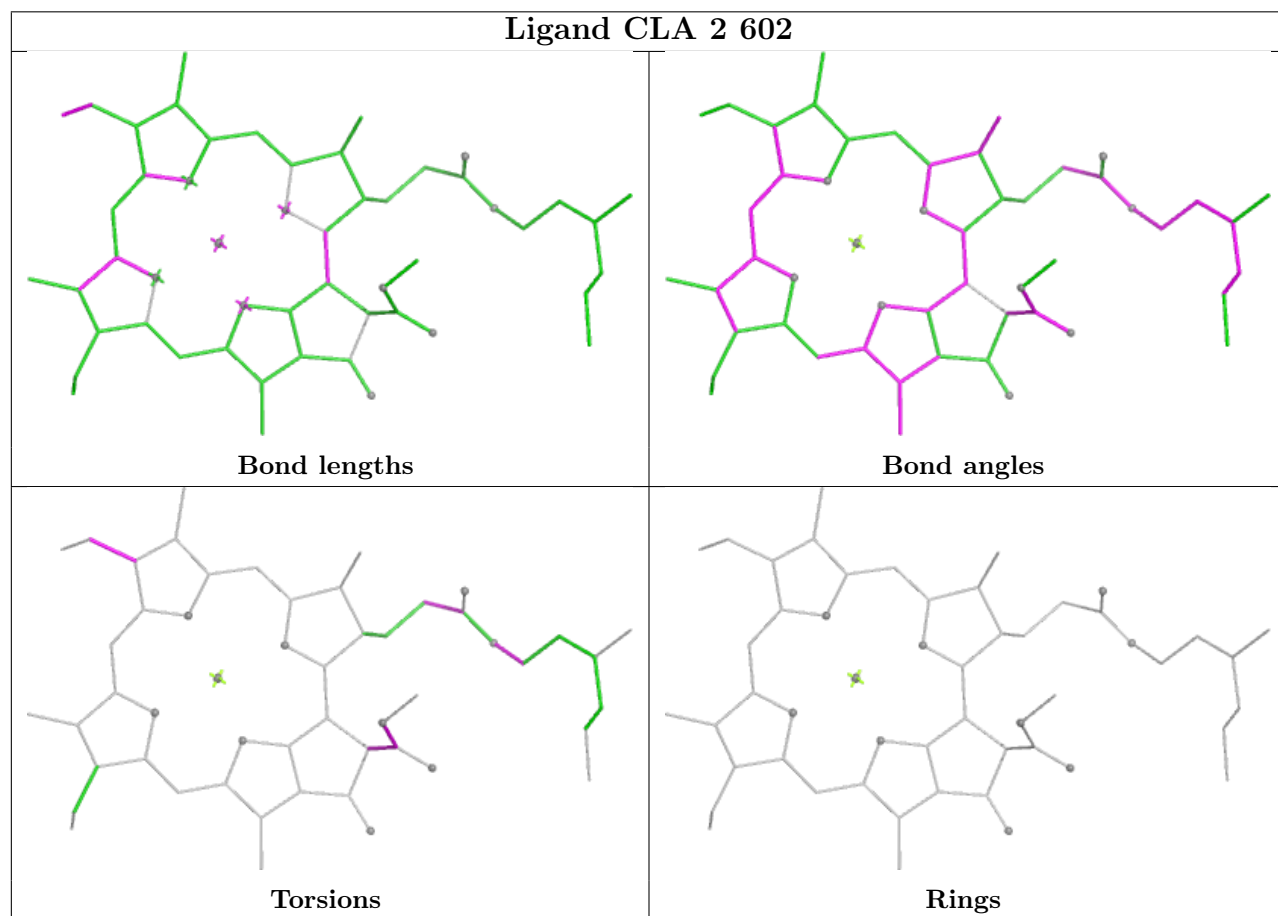
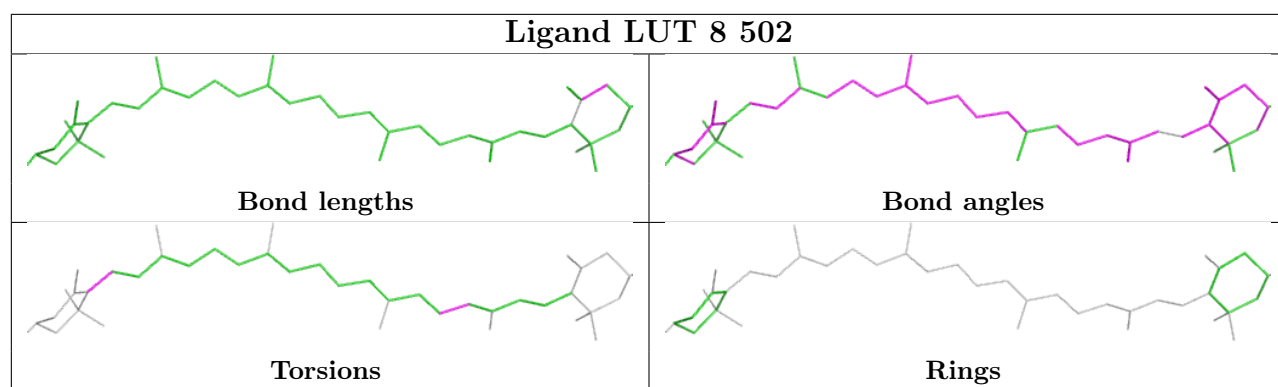


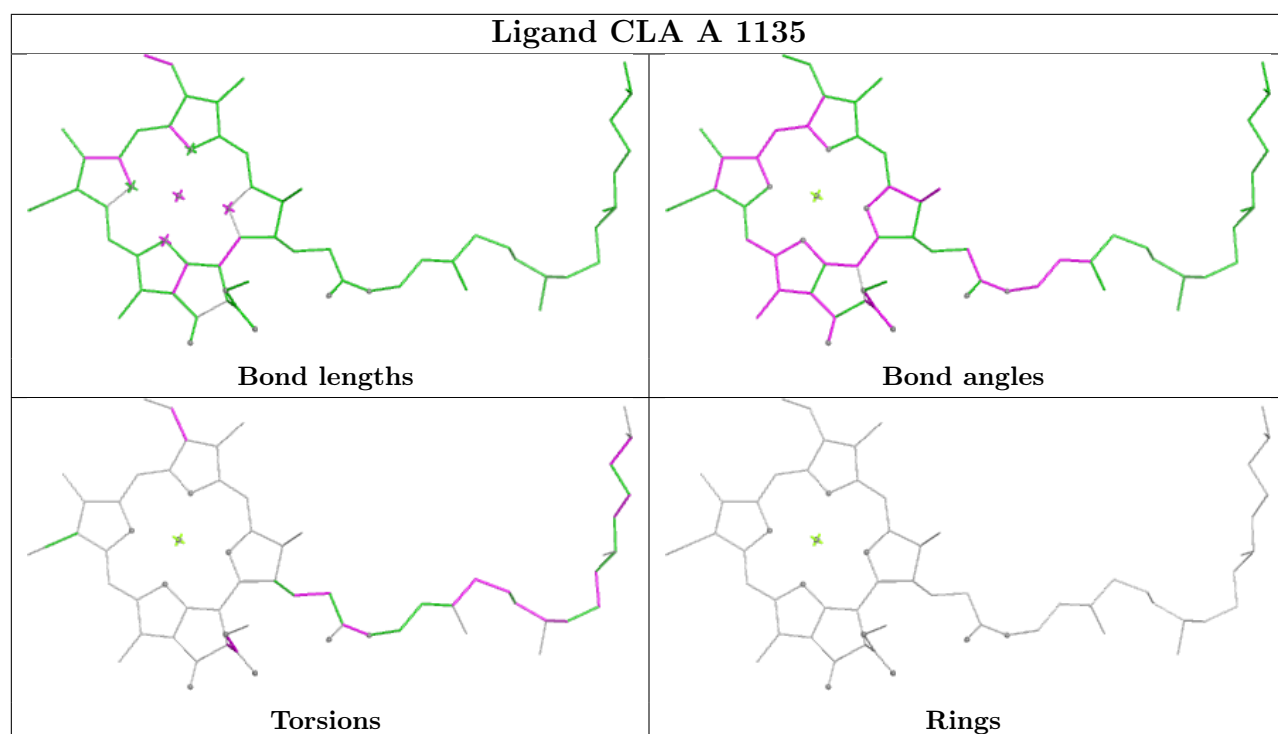
Rings

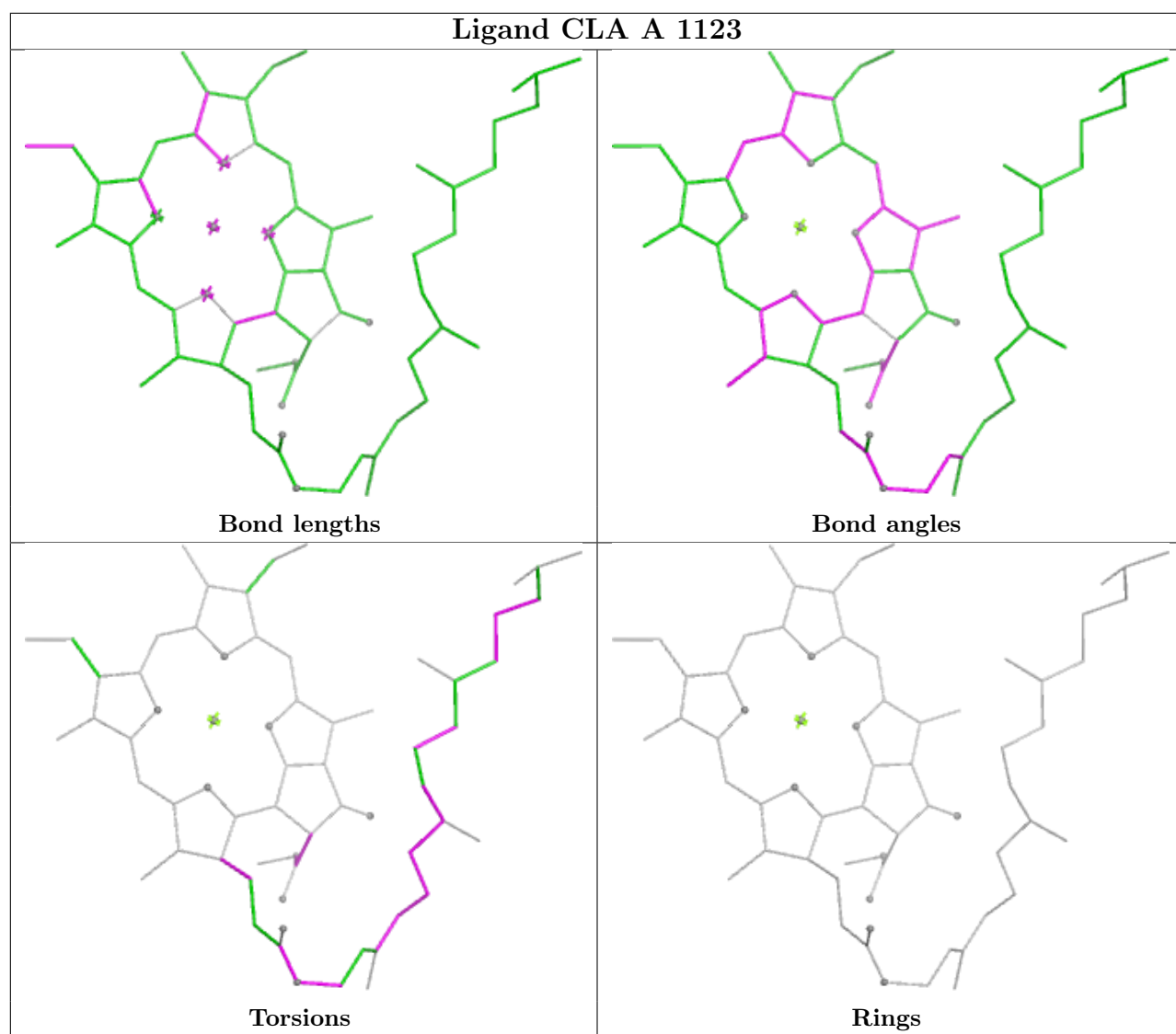


Ligand CLA 9 605**Ligand LUT 2 502**

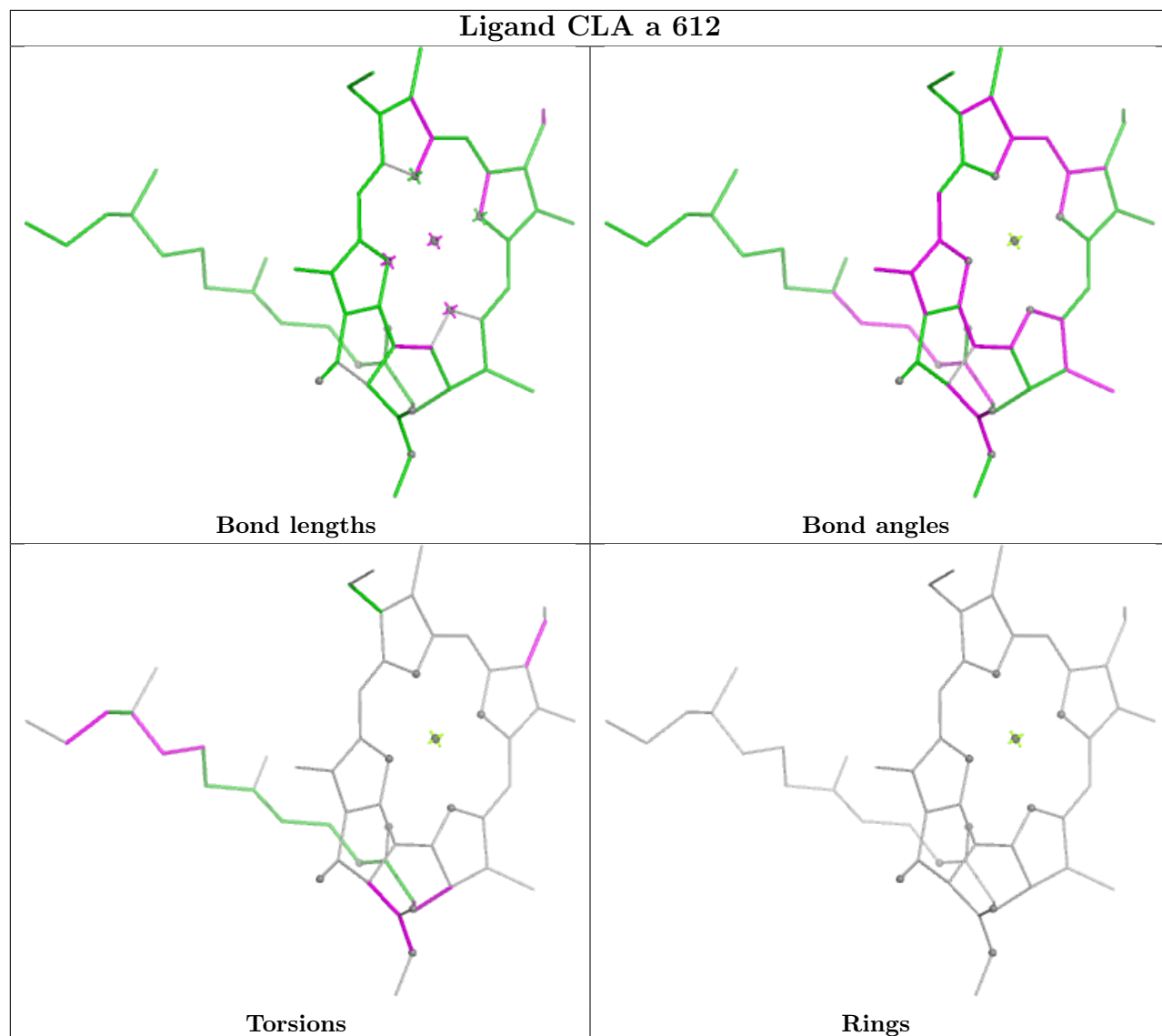




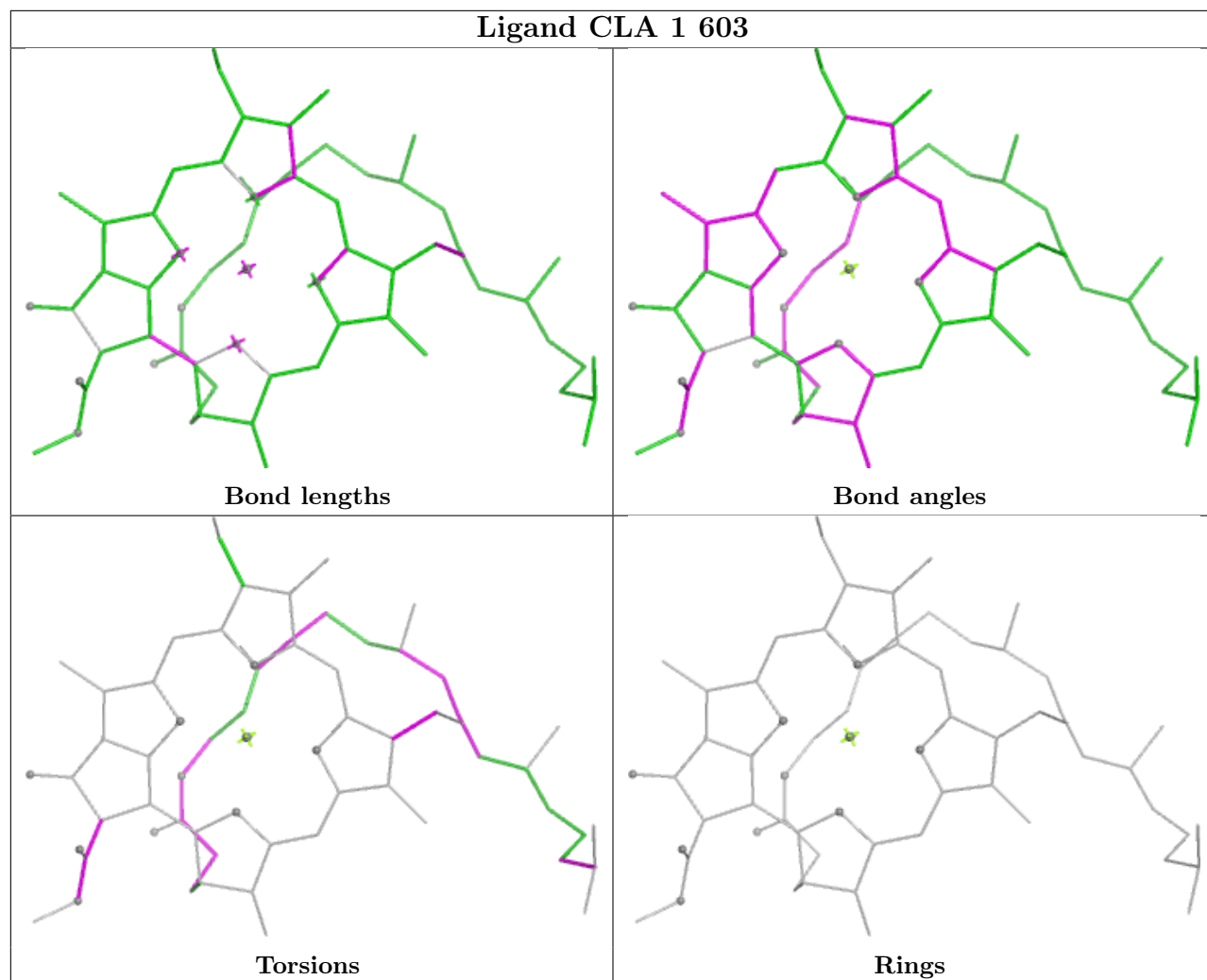


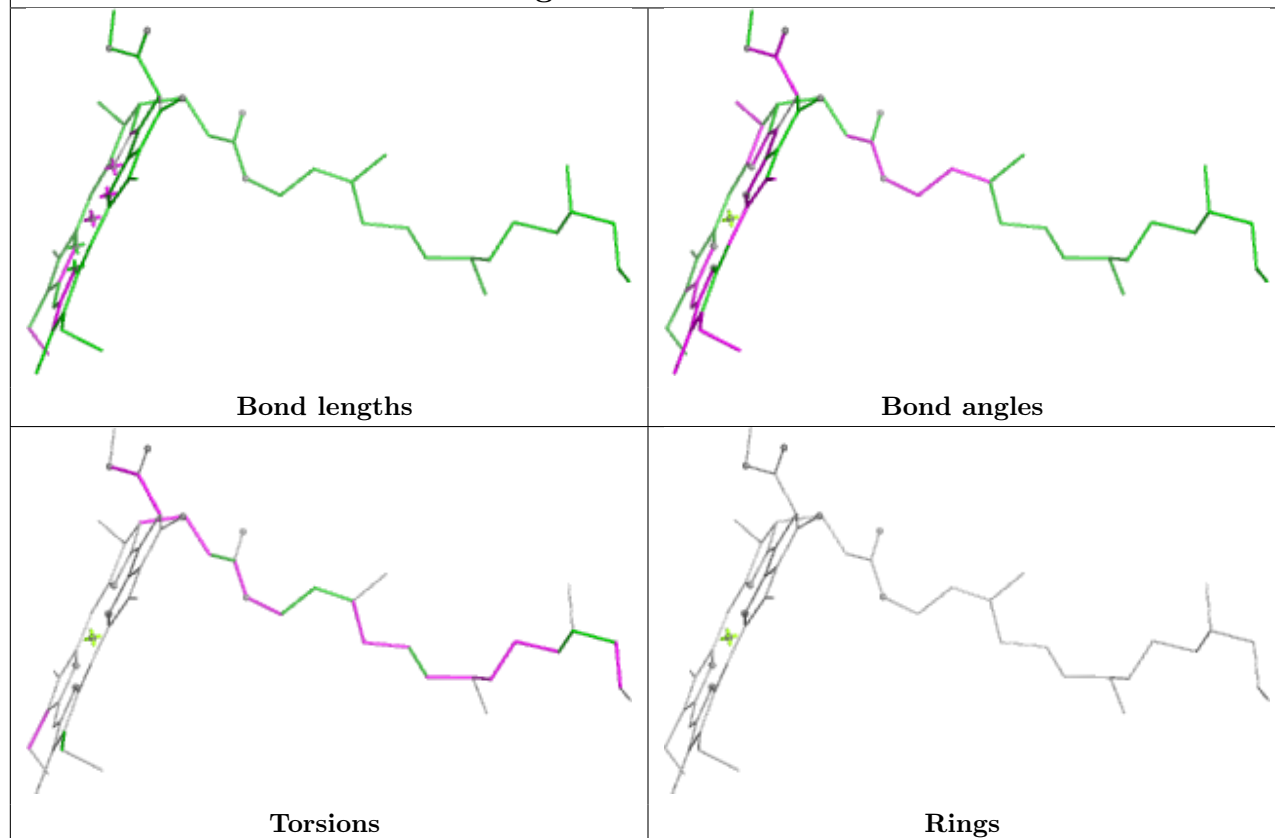
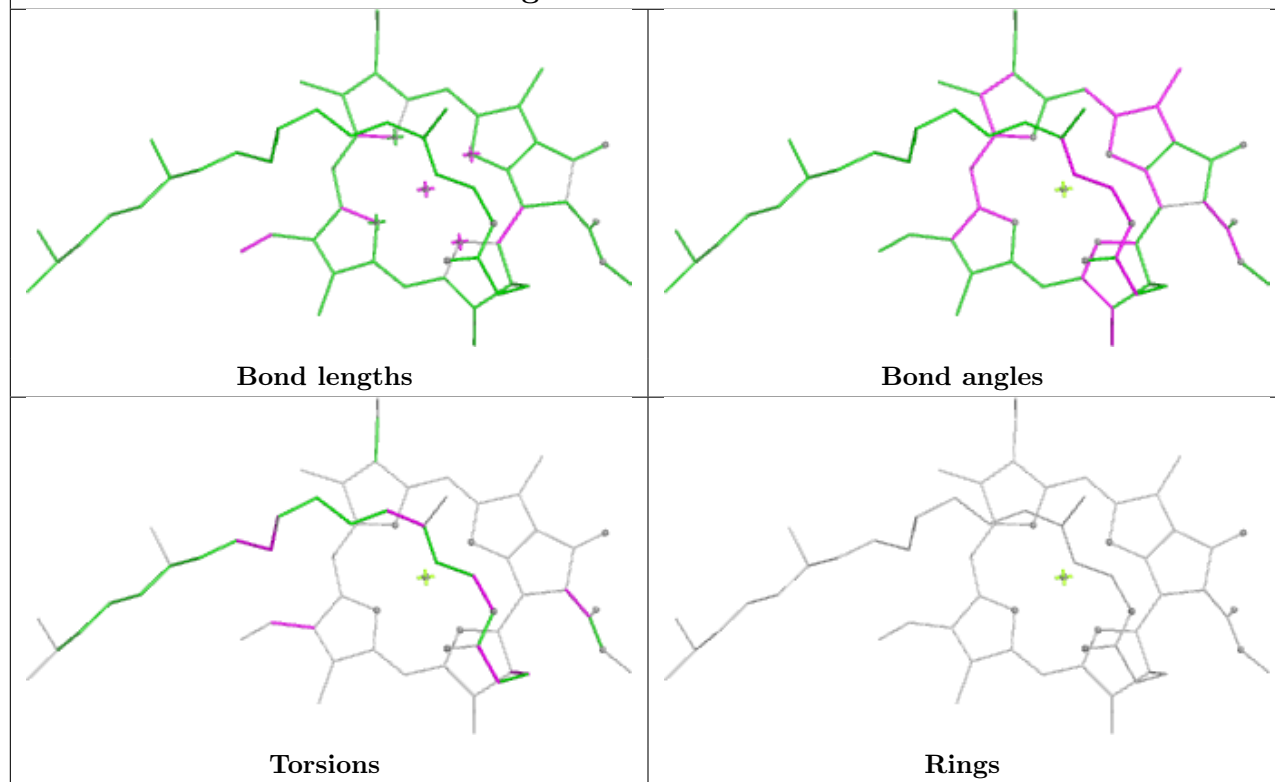


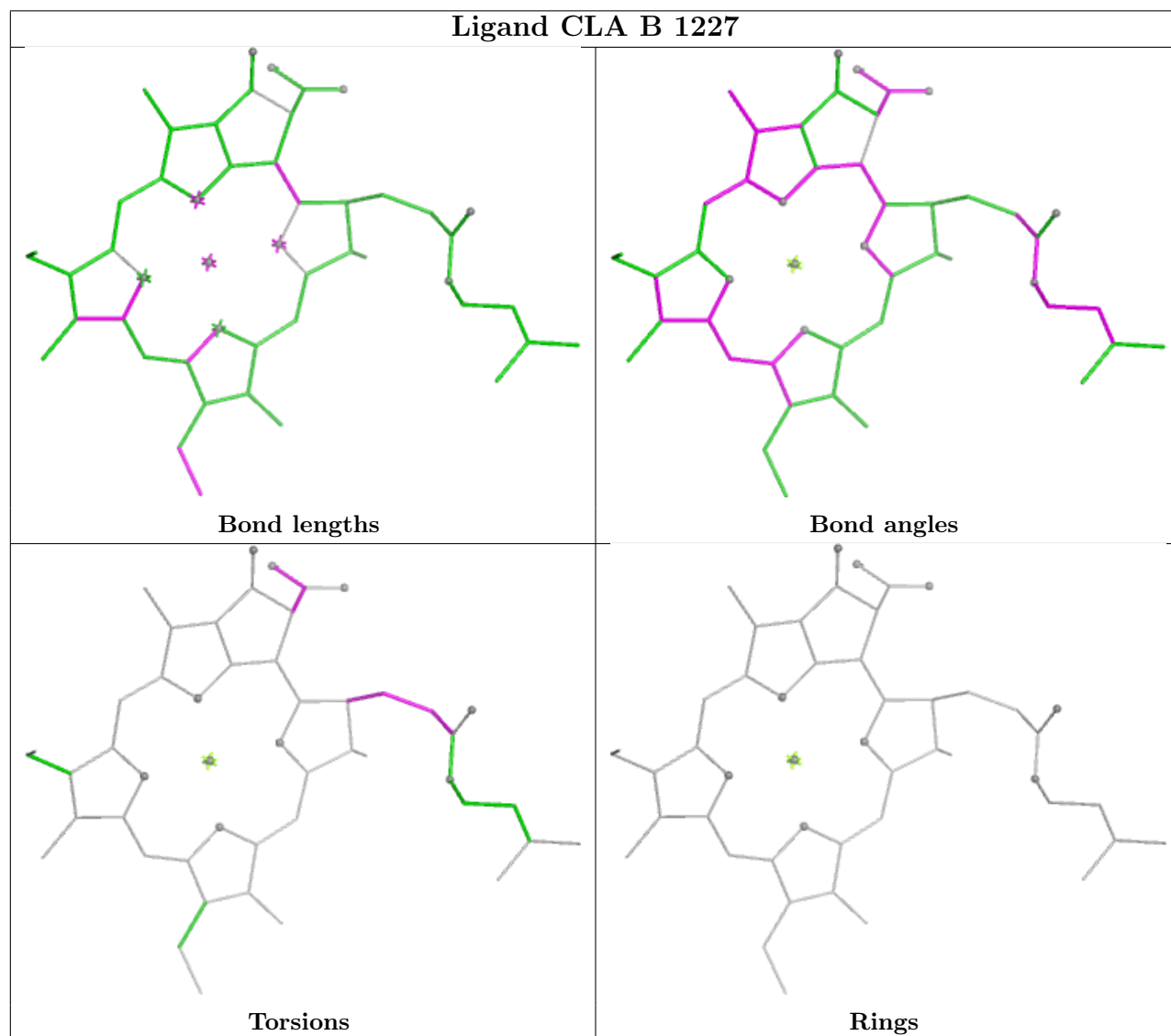
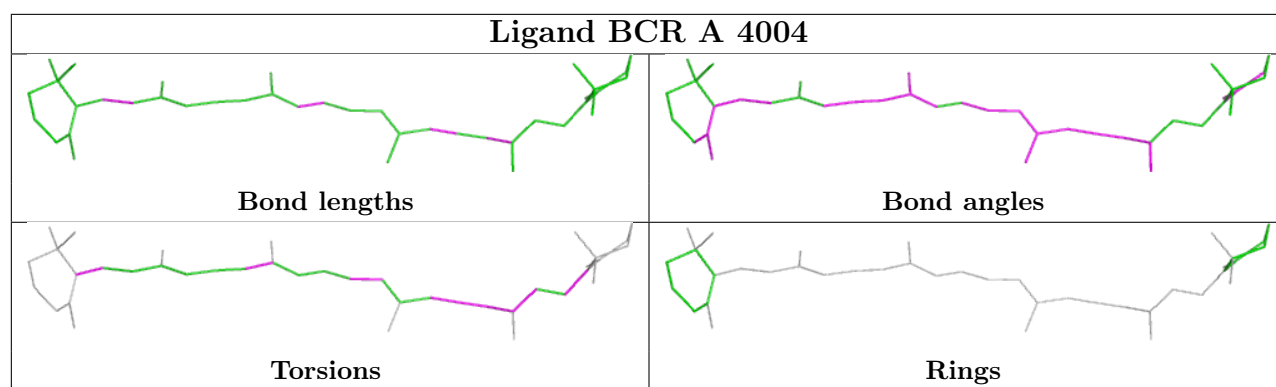
Ligand CLA a 612

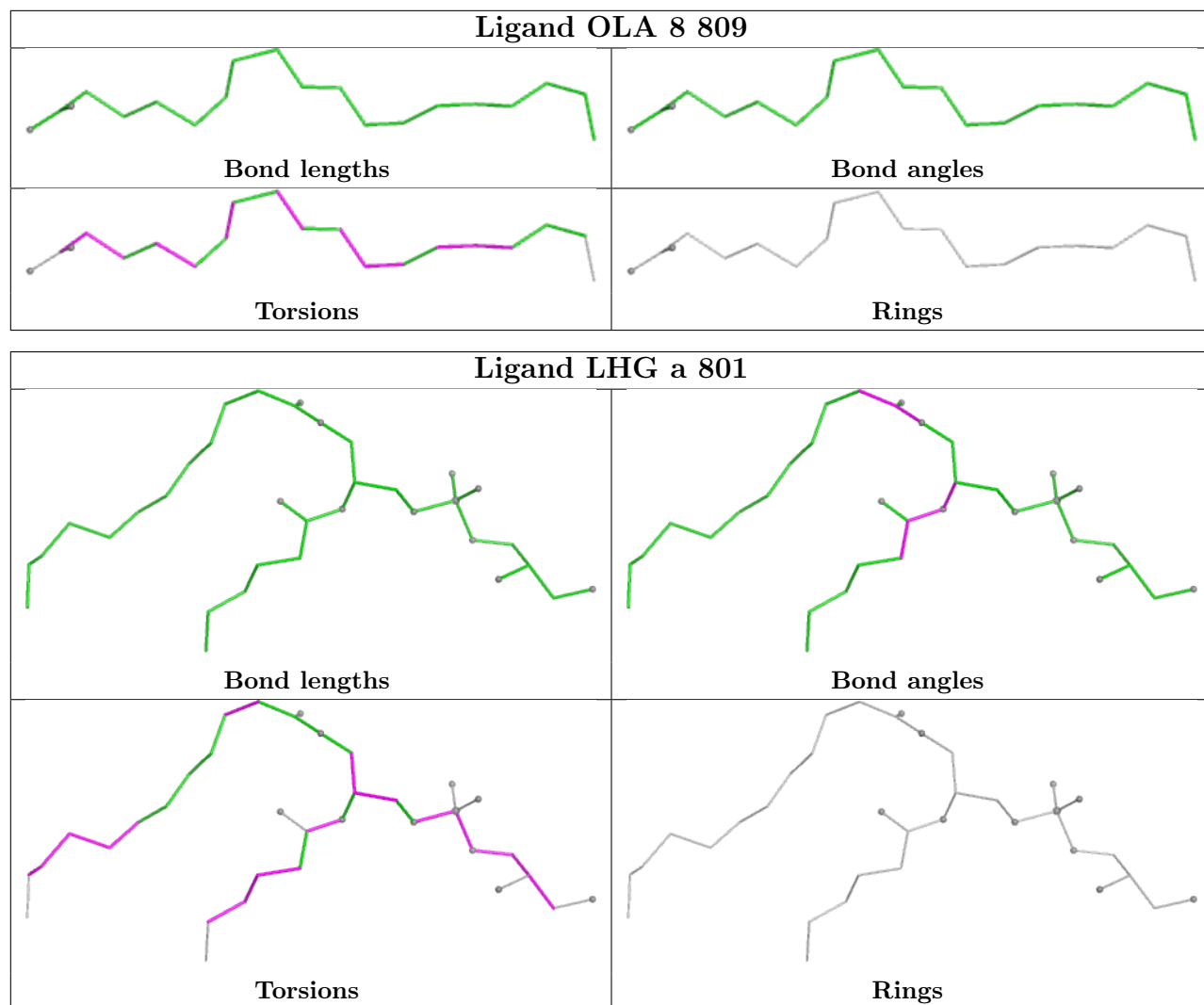


Ligand CLA 1 603

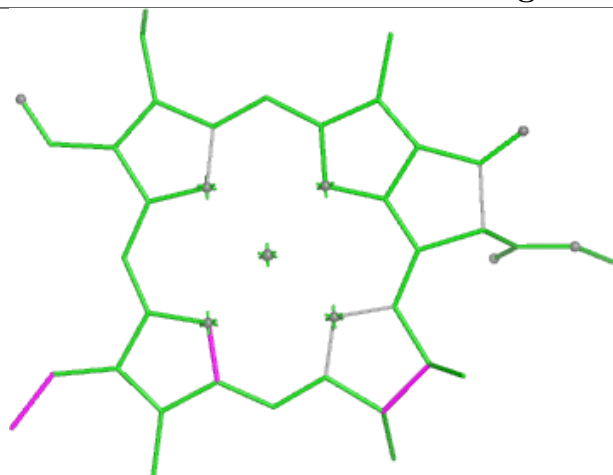


Ligand CLA 4 612**Ligand CLA A 1138**

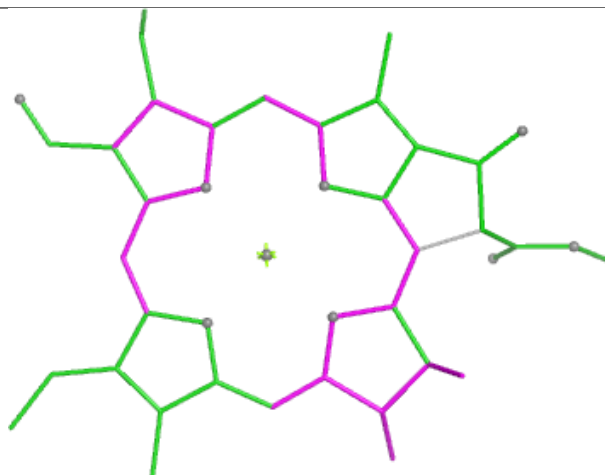




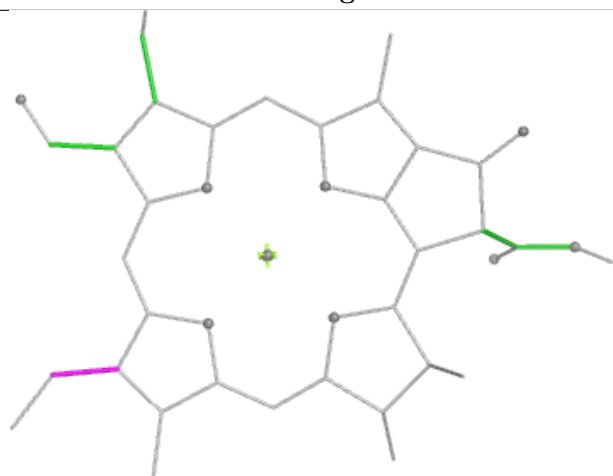
Ligand CHL 9 613



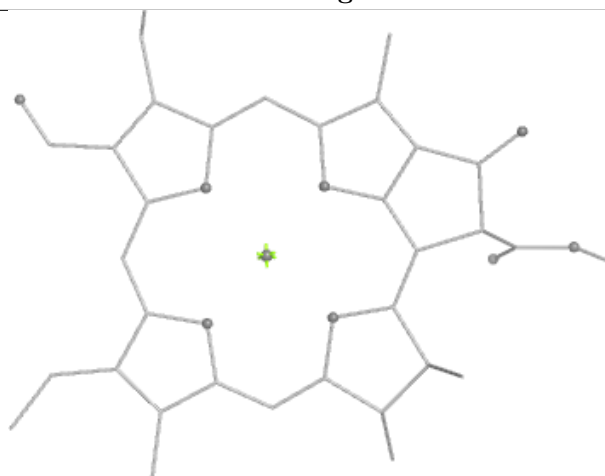
Bond lengths



Bond angles

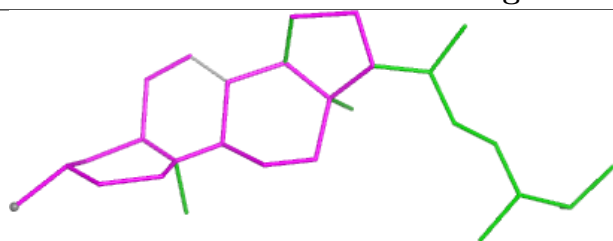


Torsions

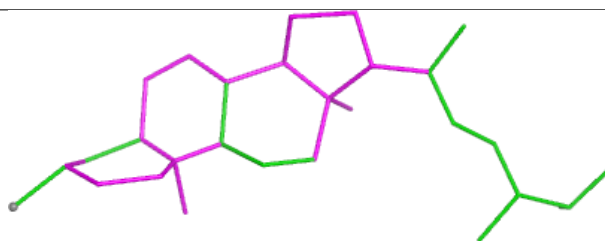


Rings

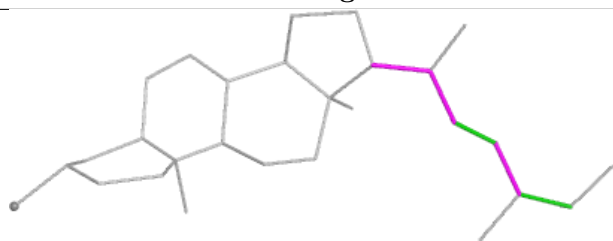
Ligand ERG G 5002



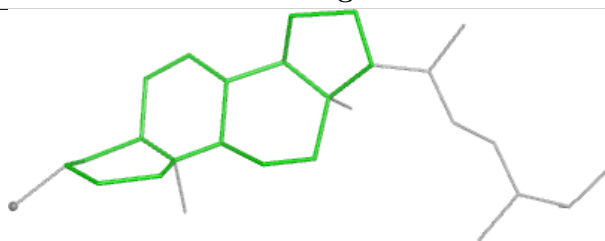
Bond lengths



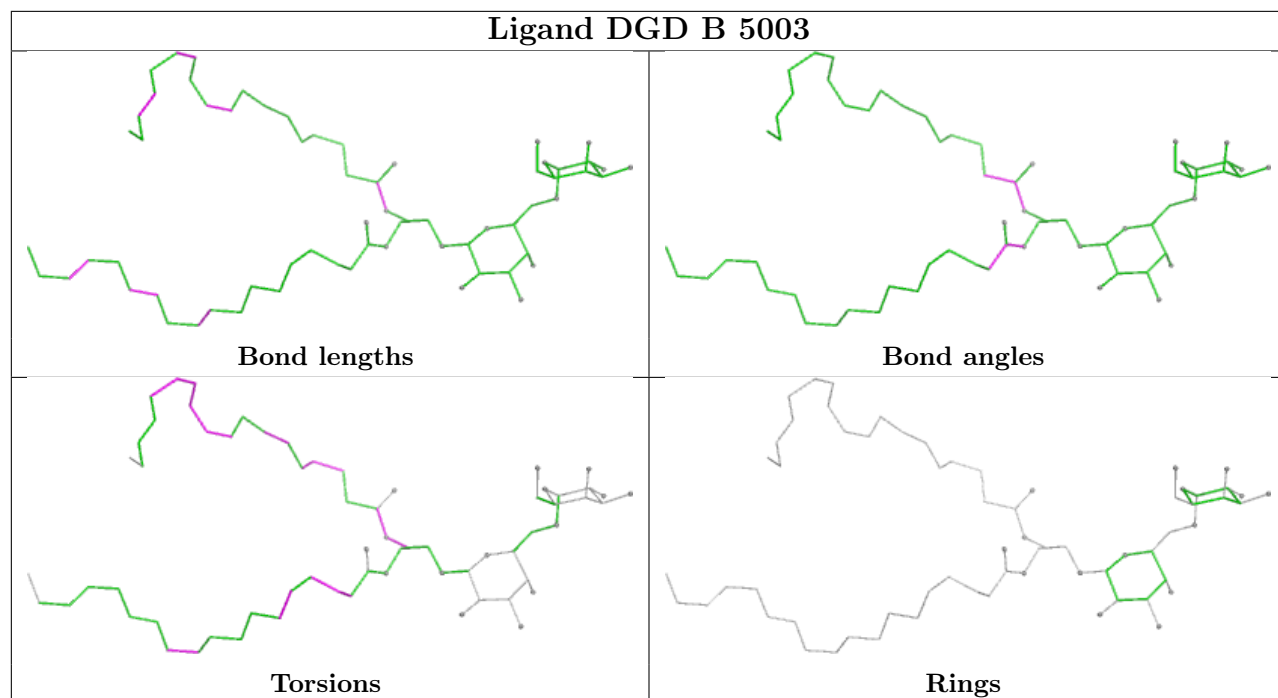
Bond angles



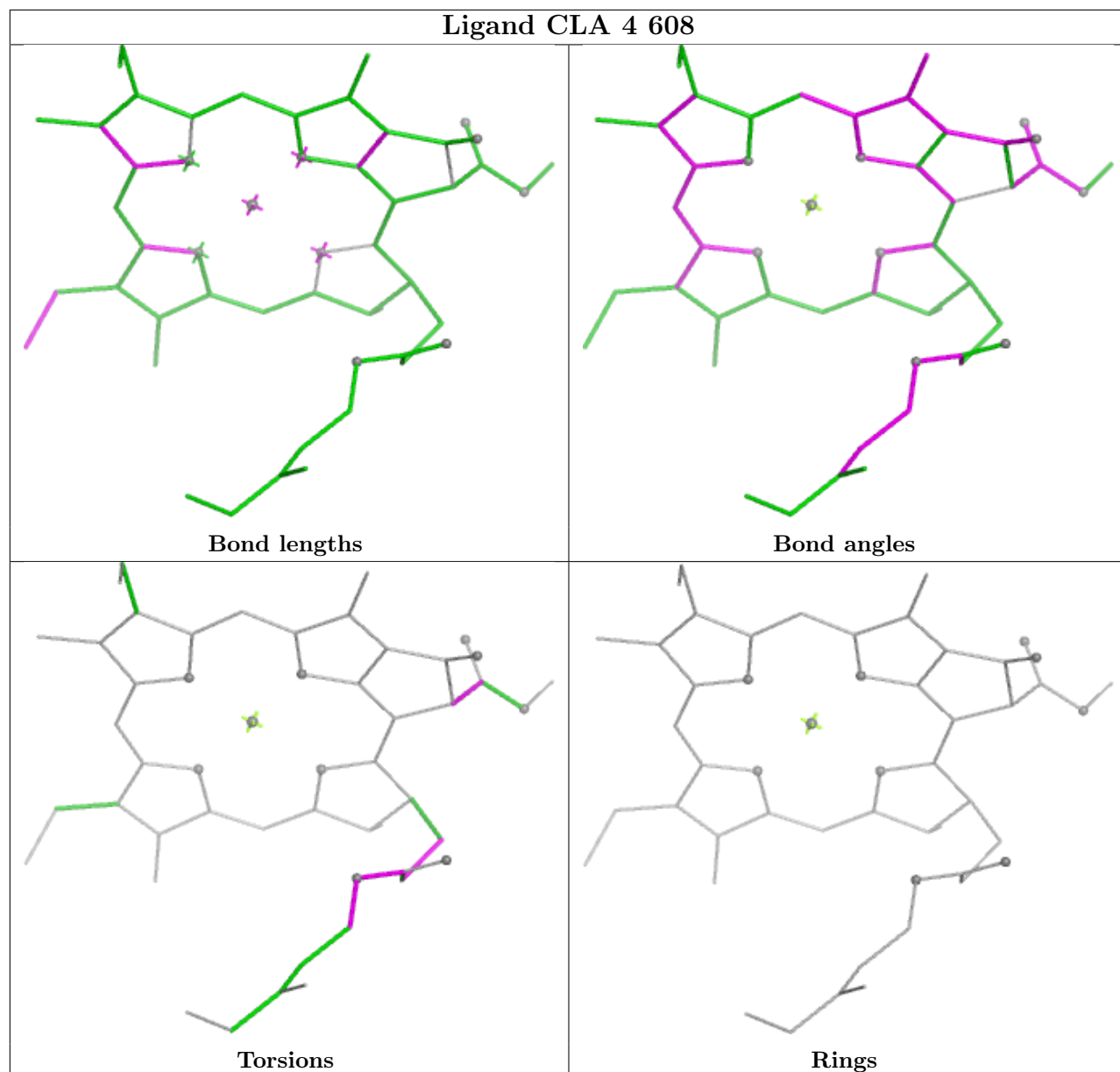
Torsions

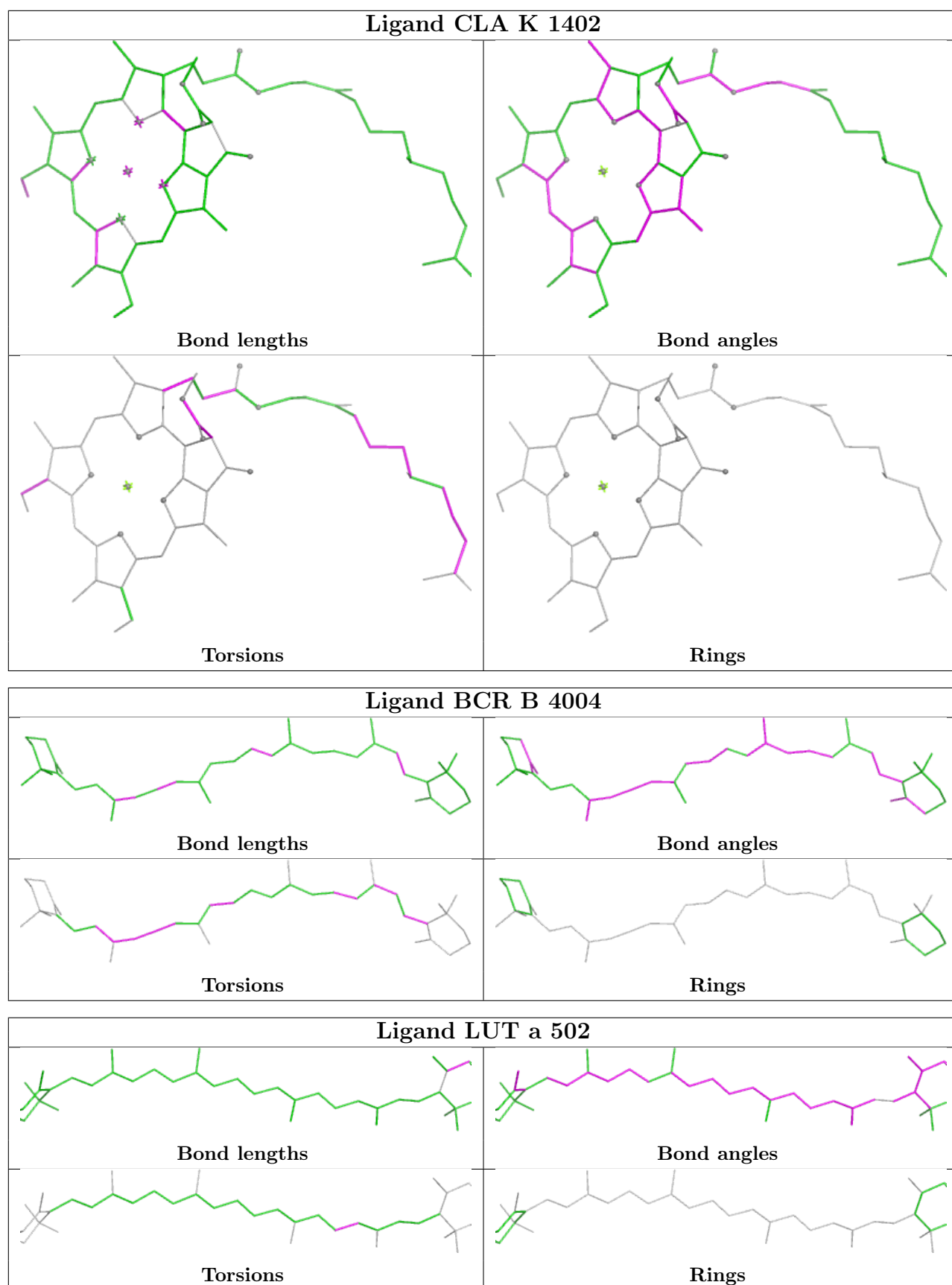


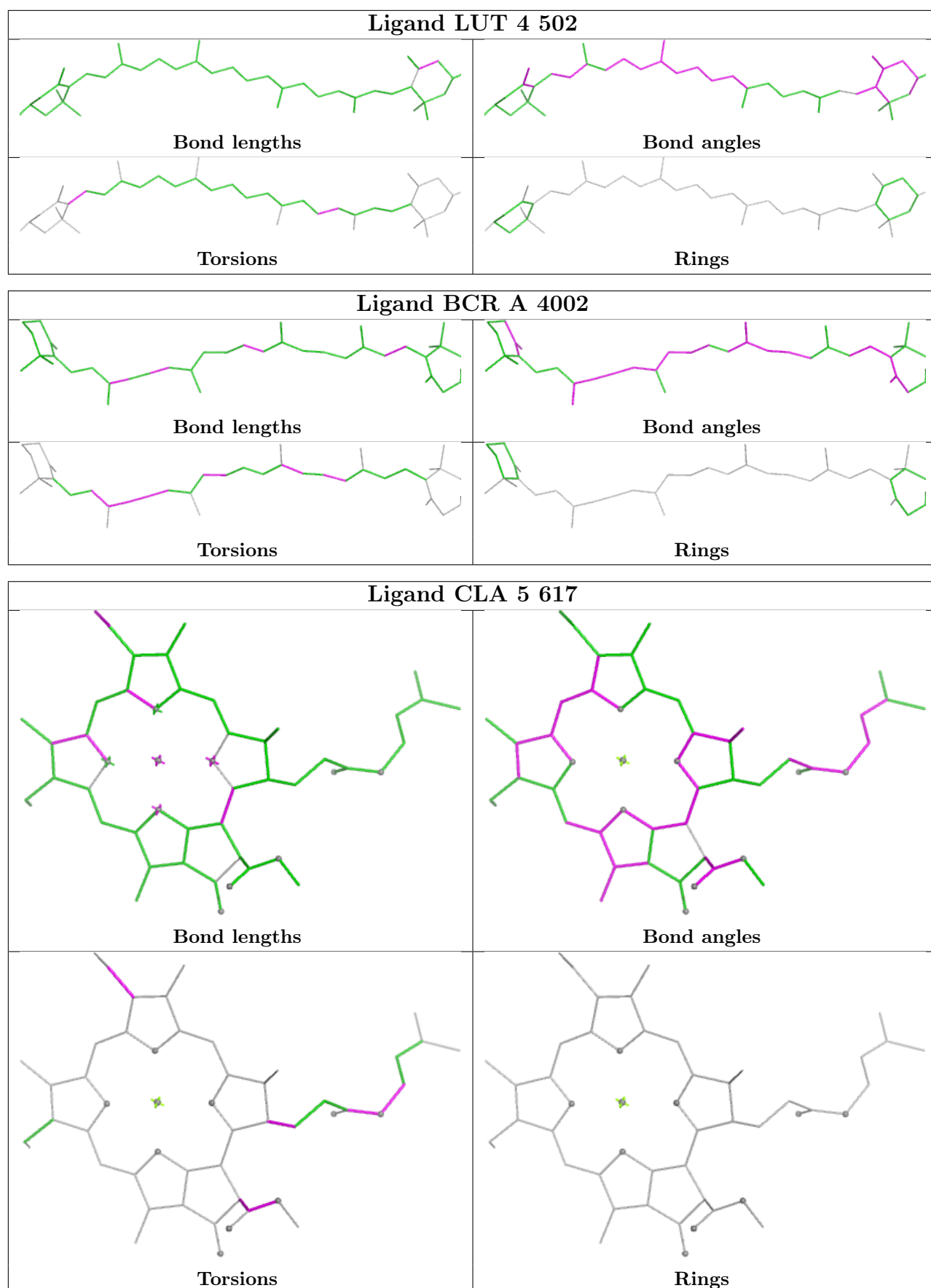
Rings

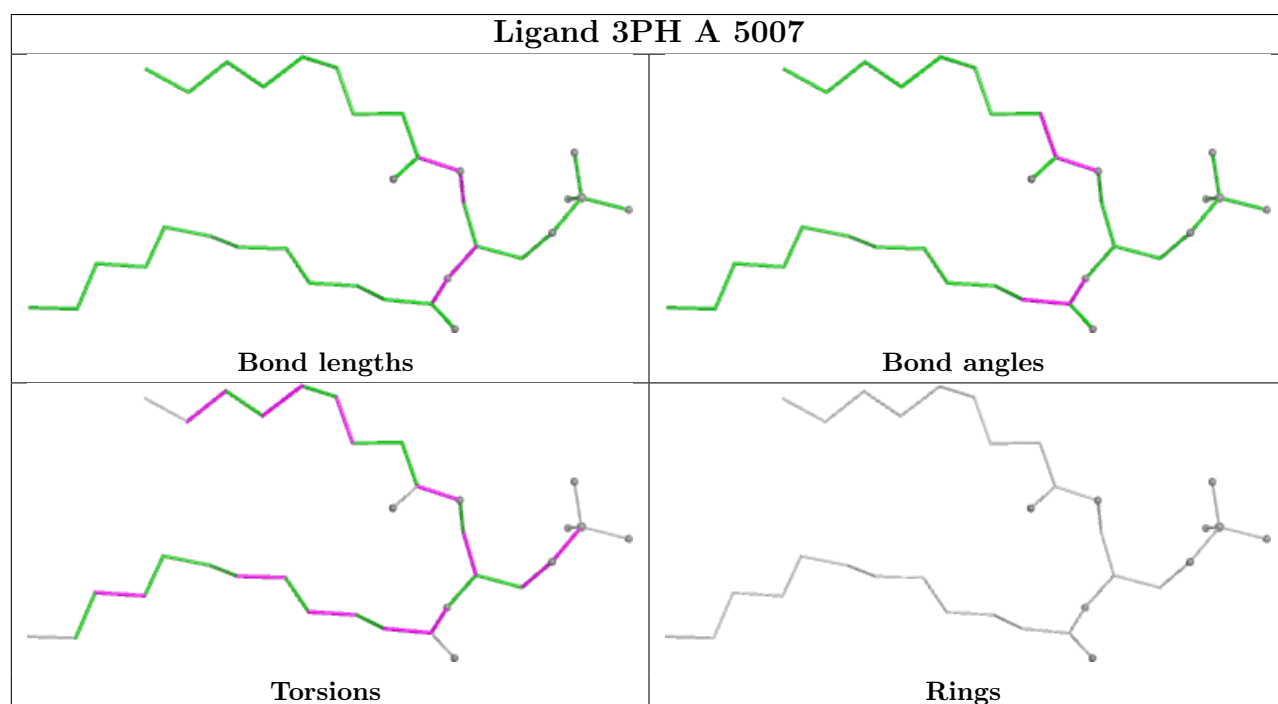
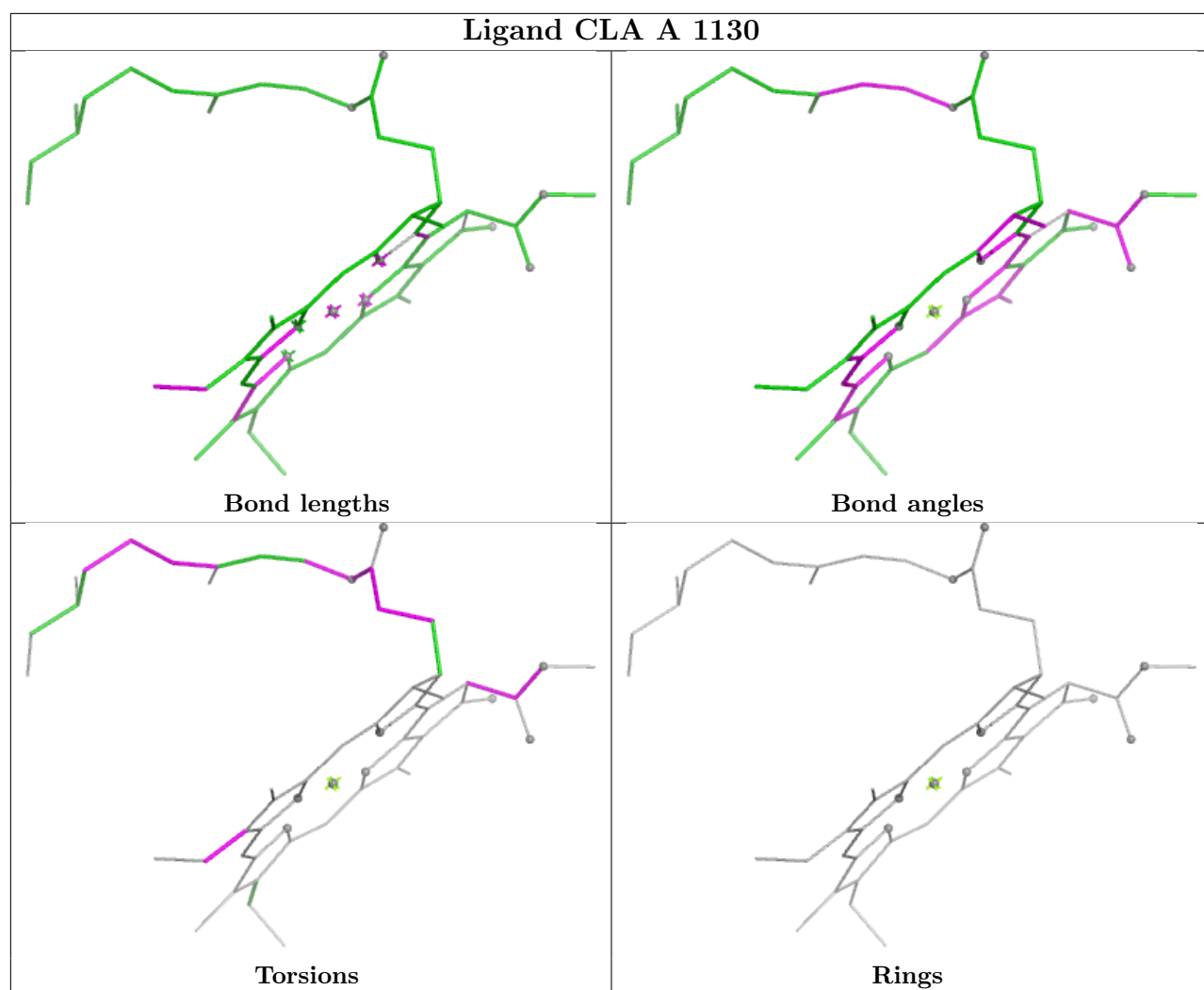


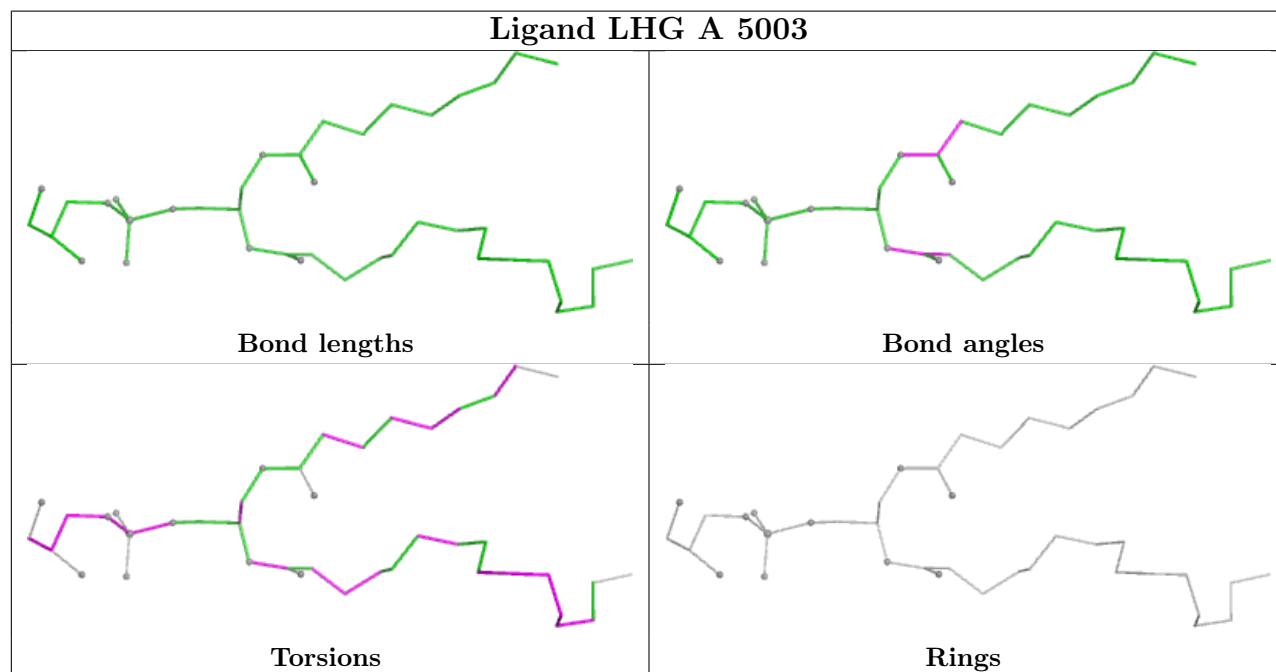
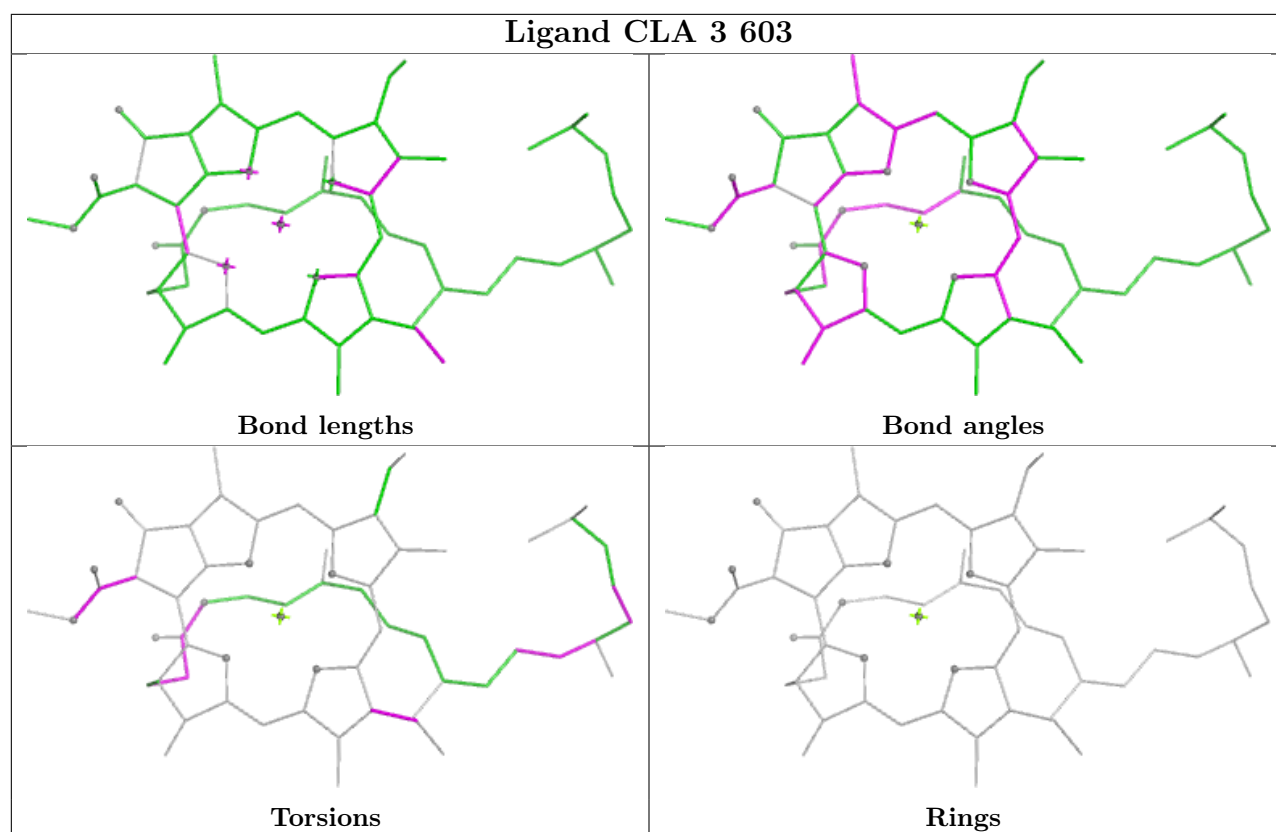
Ligand CLA 4 608

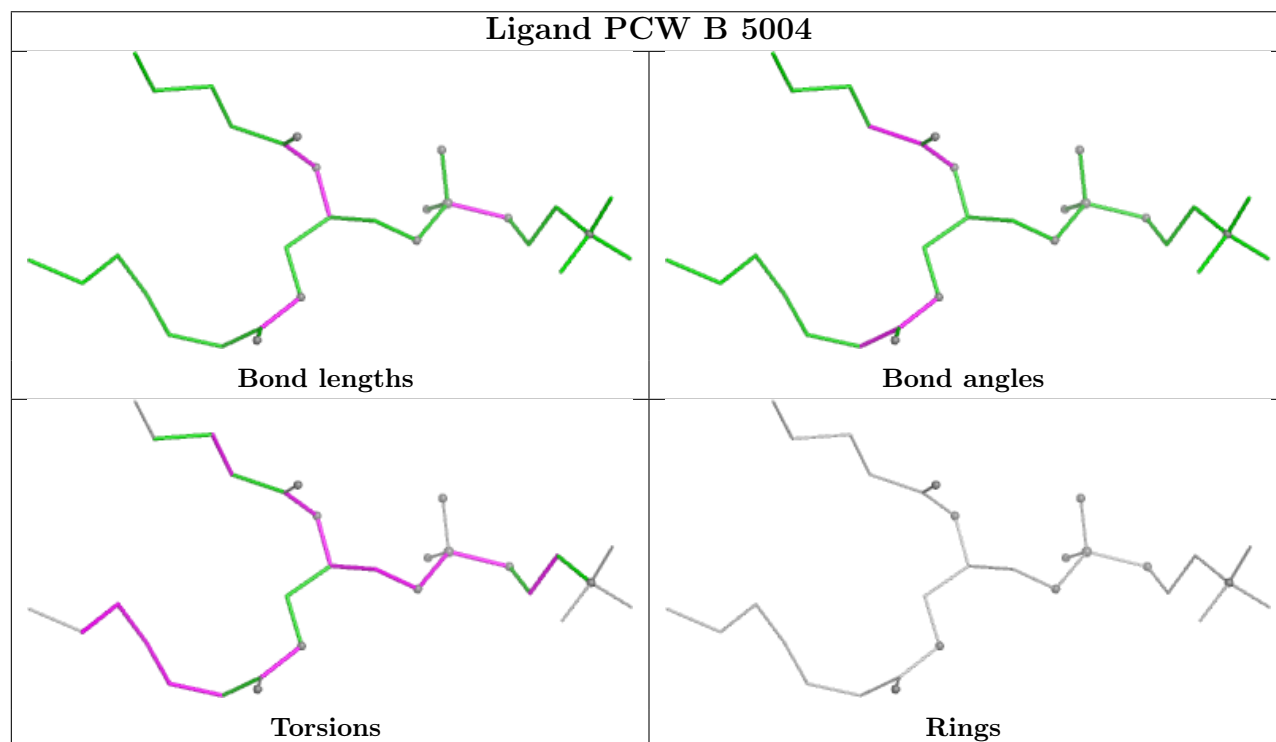
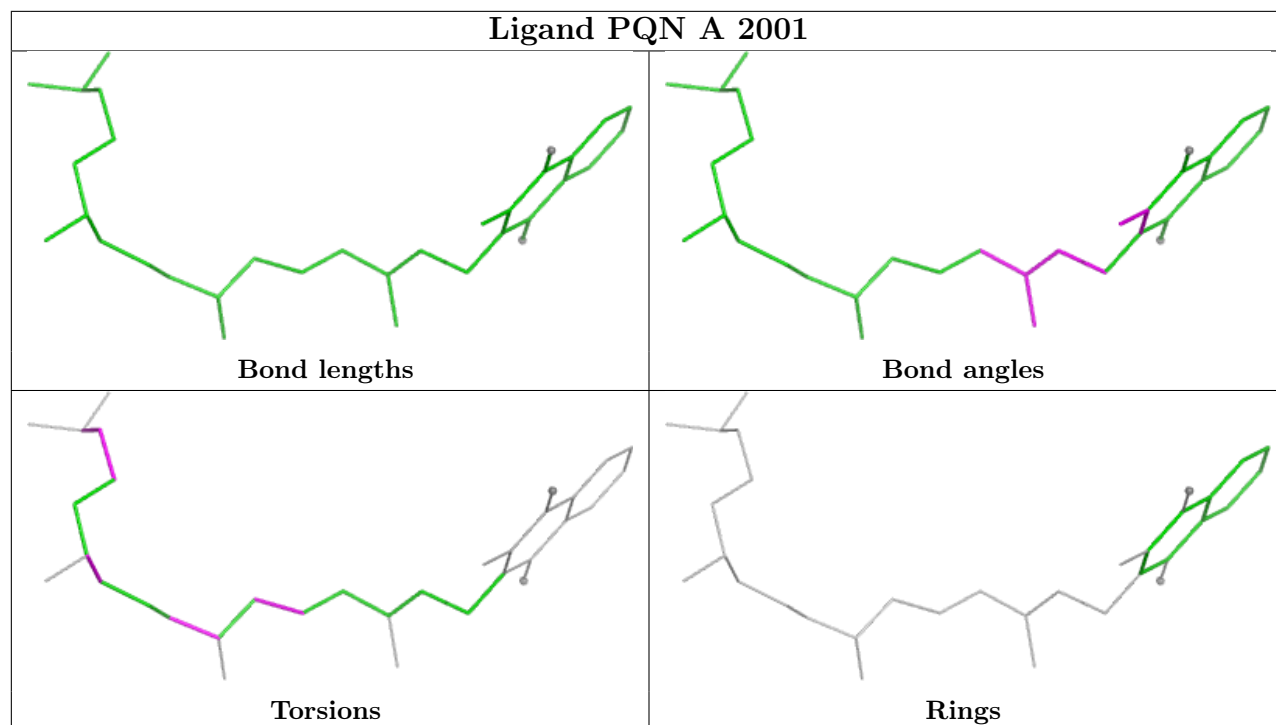


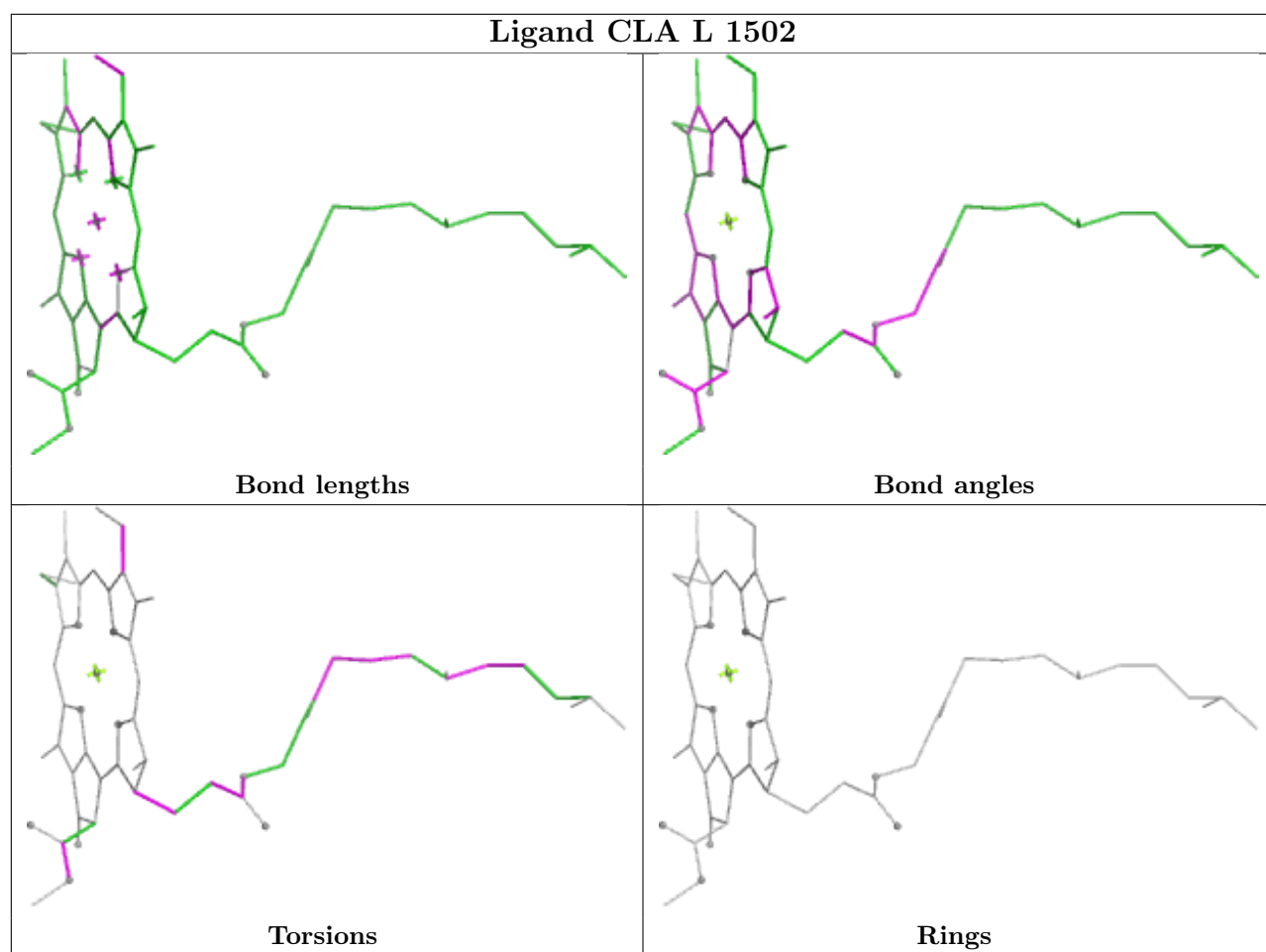


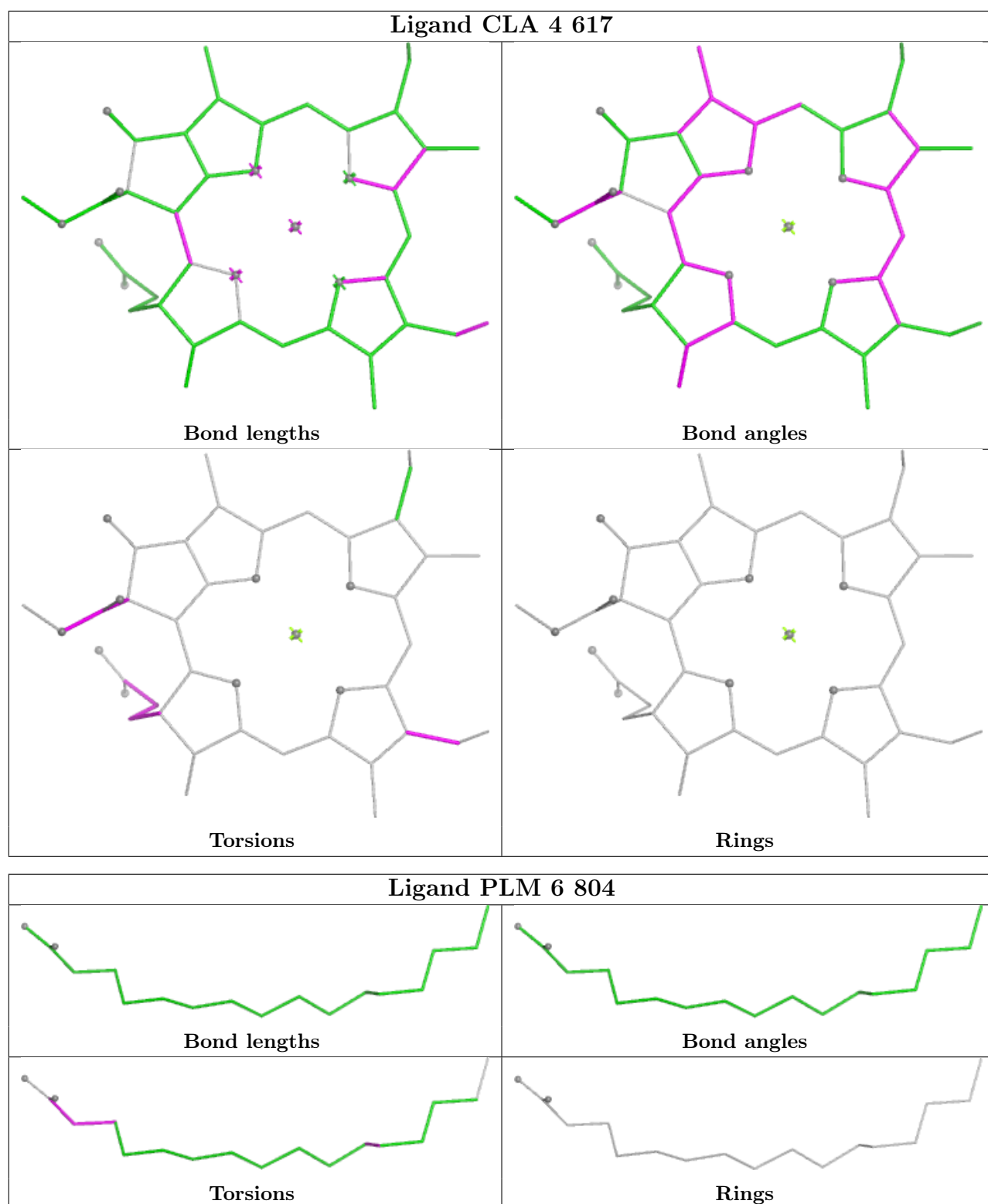


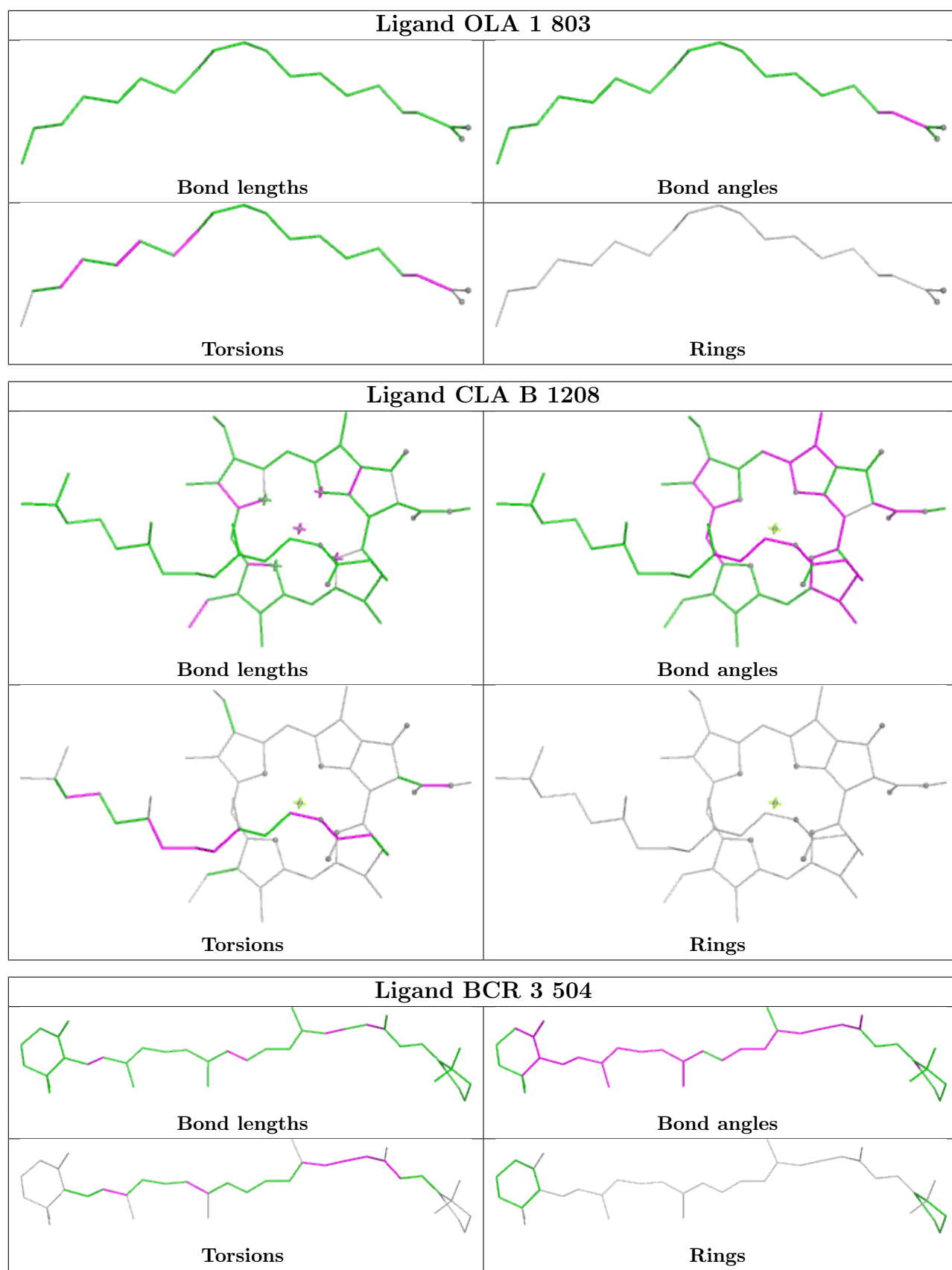




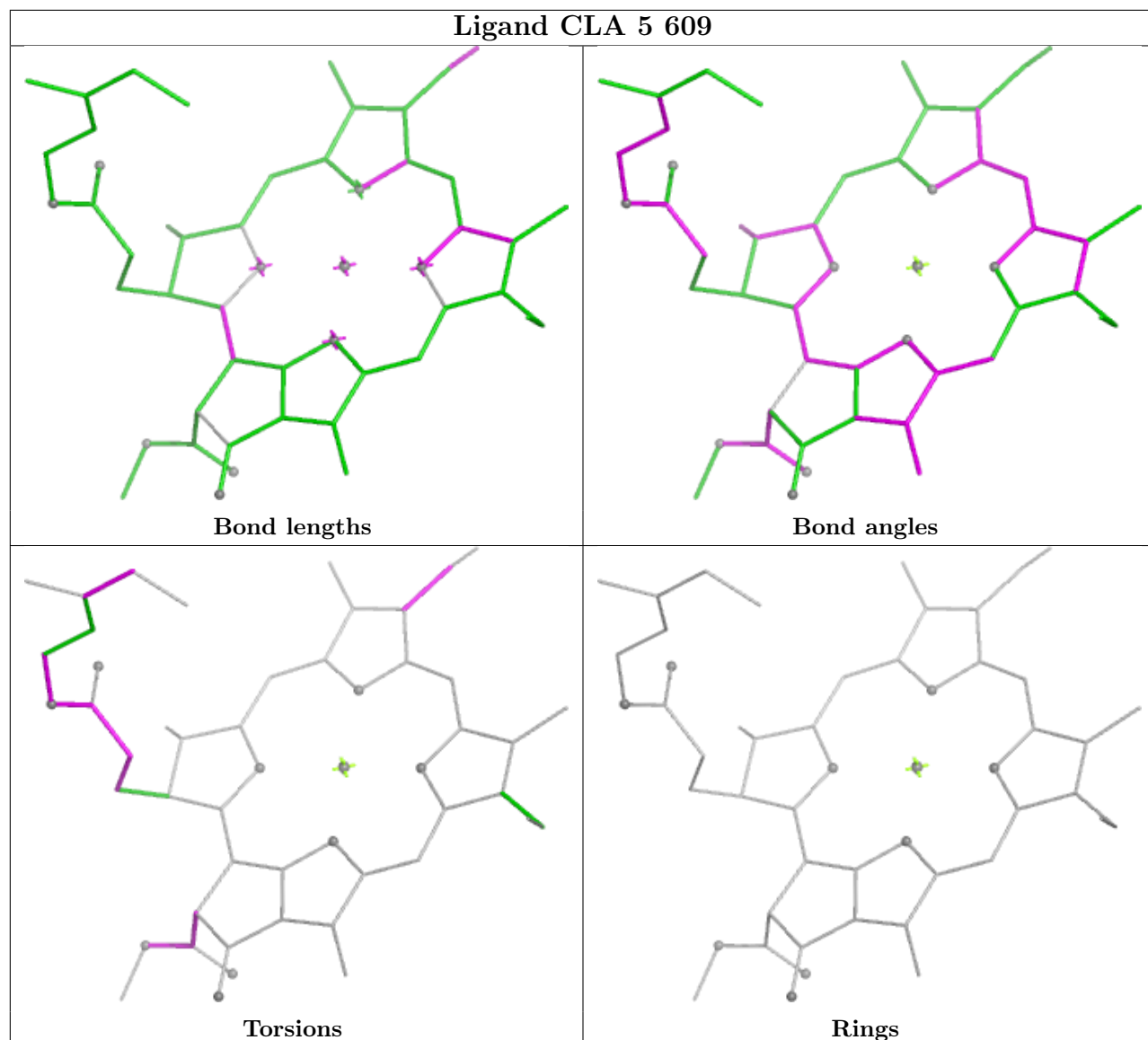


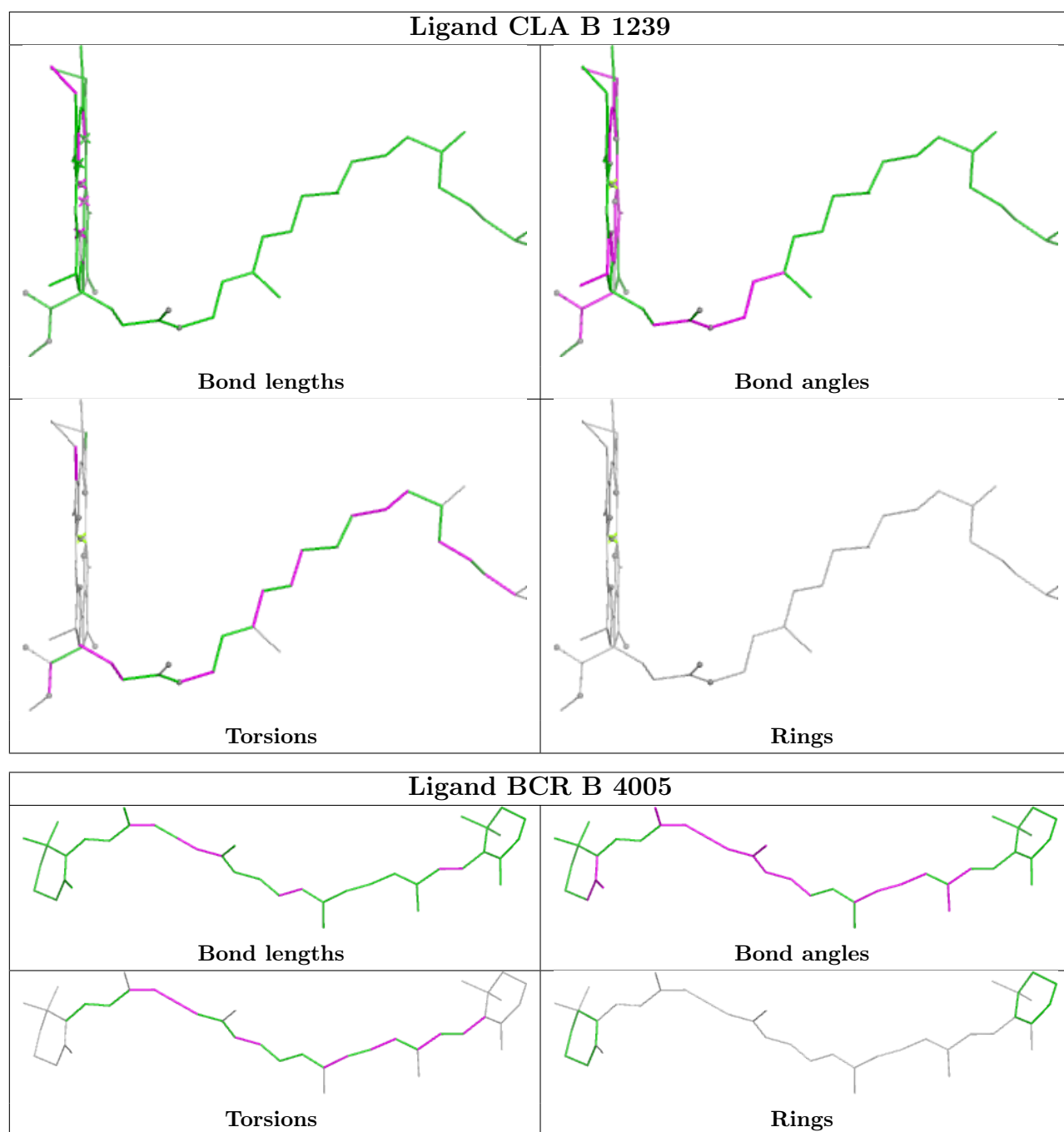


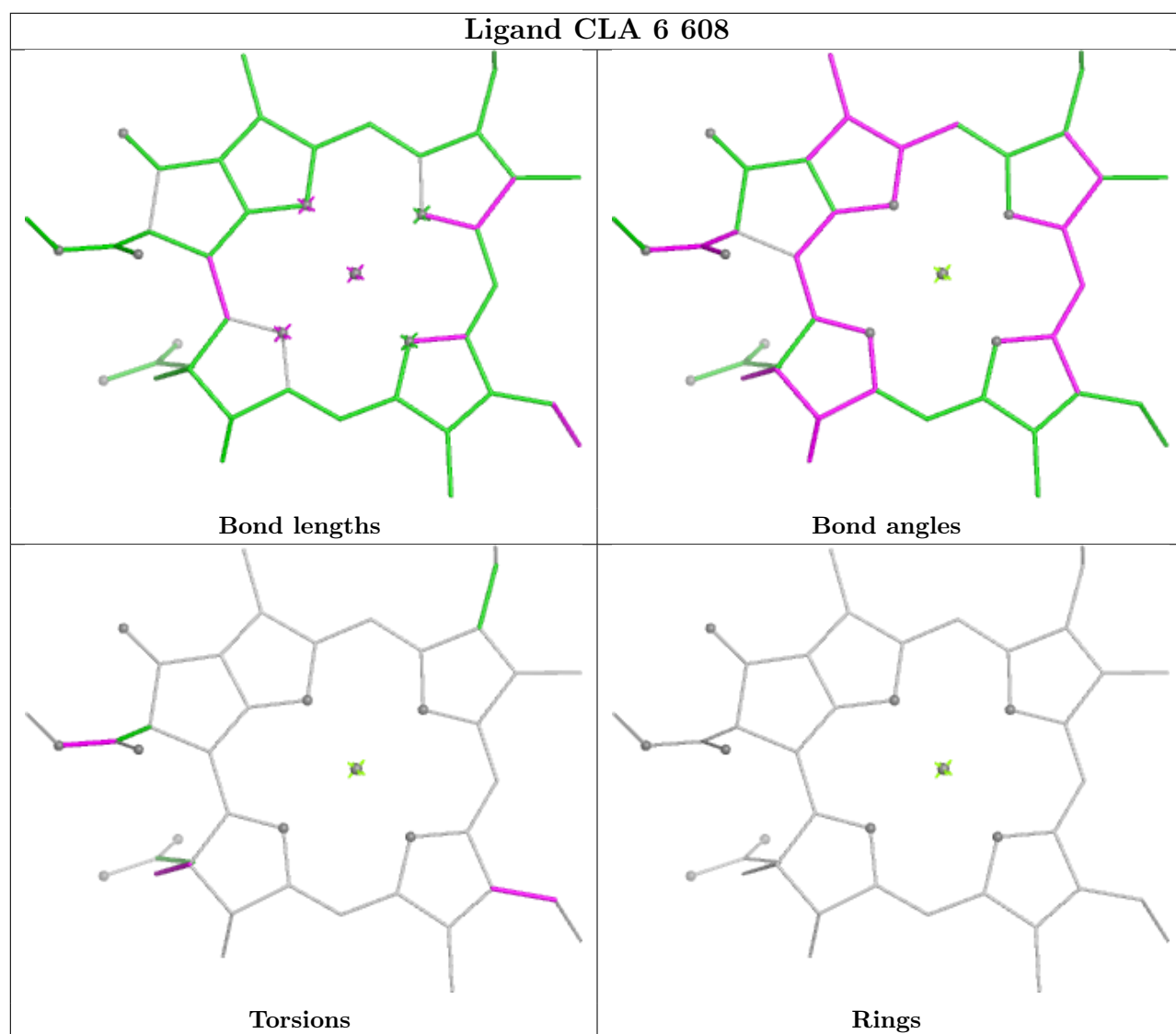


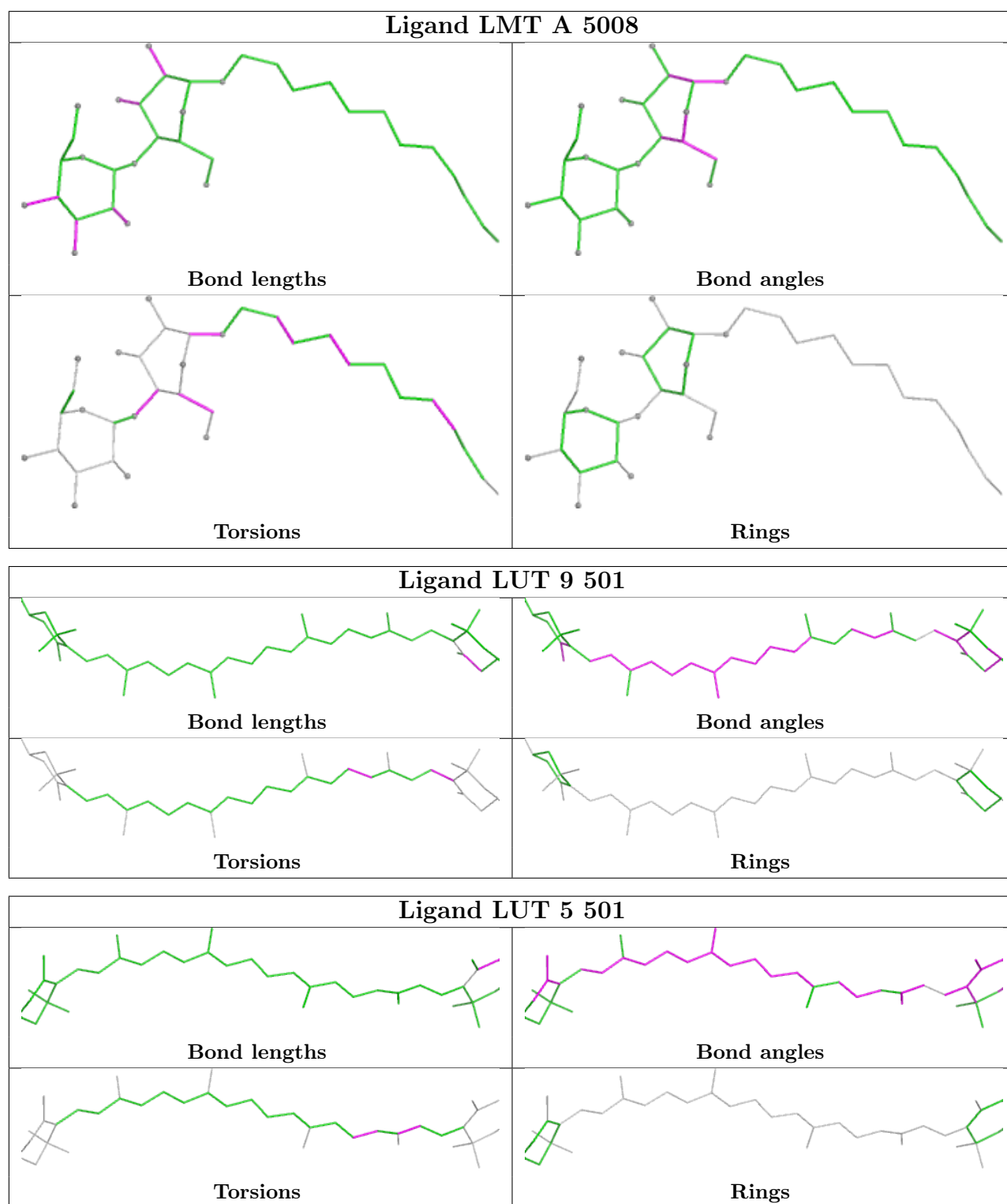


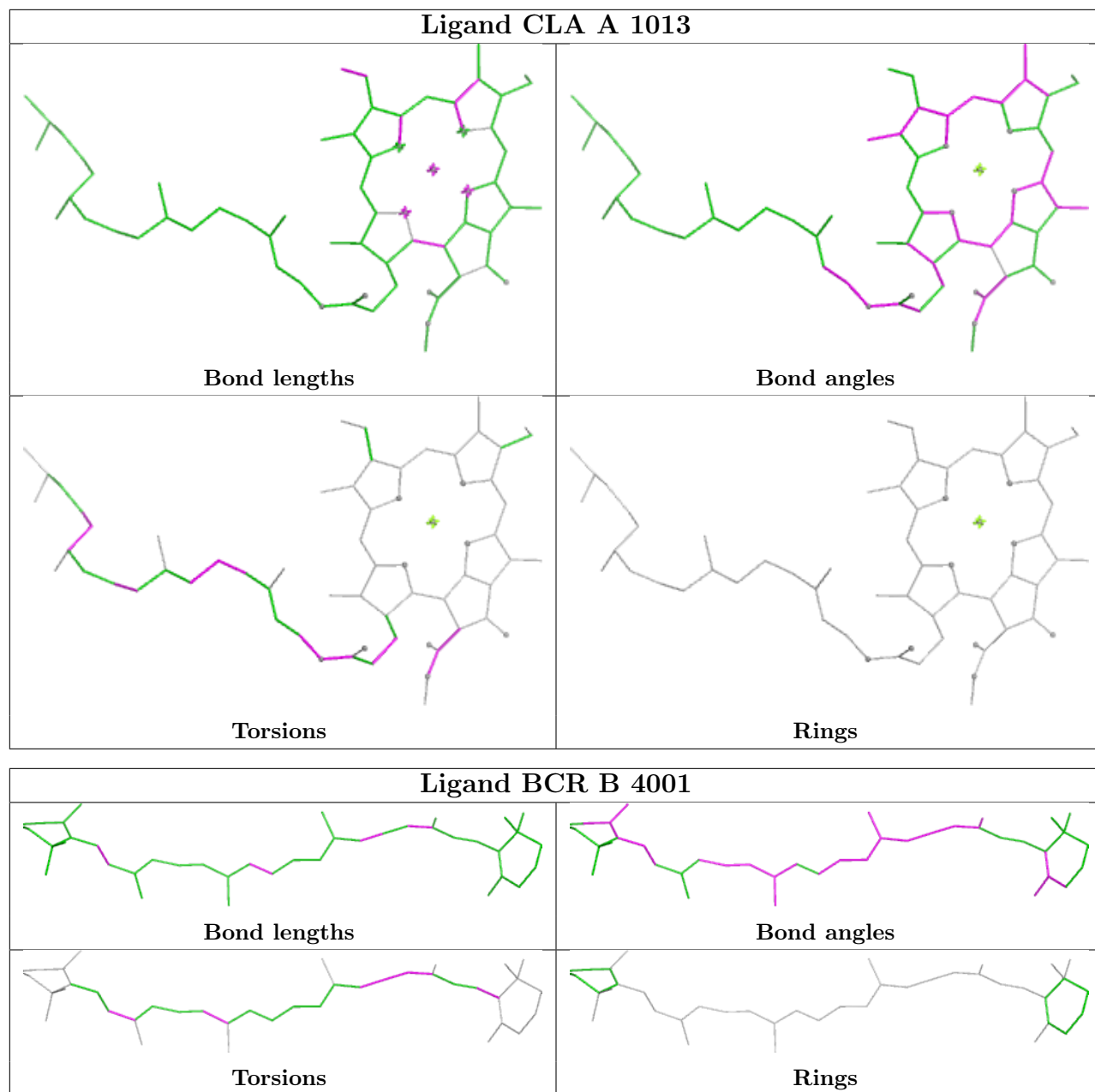
Ligand CLA 5 609

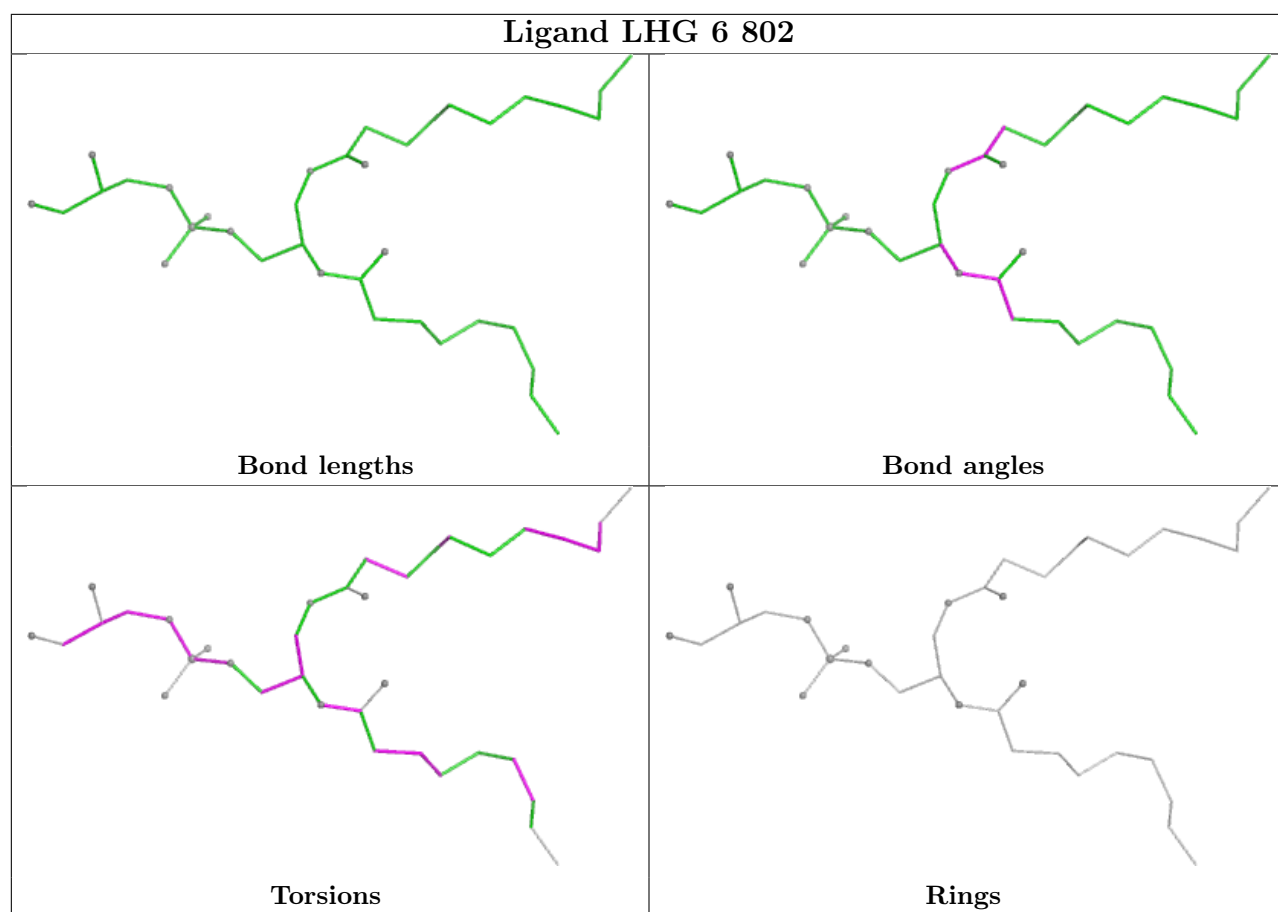


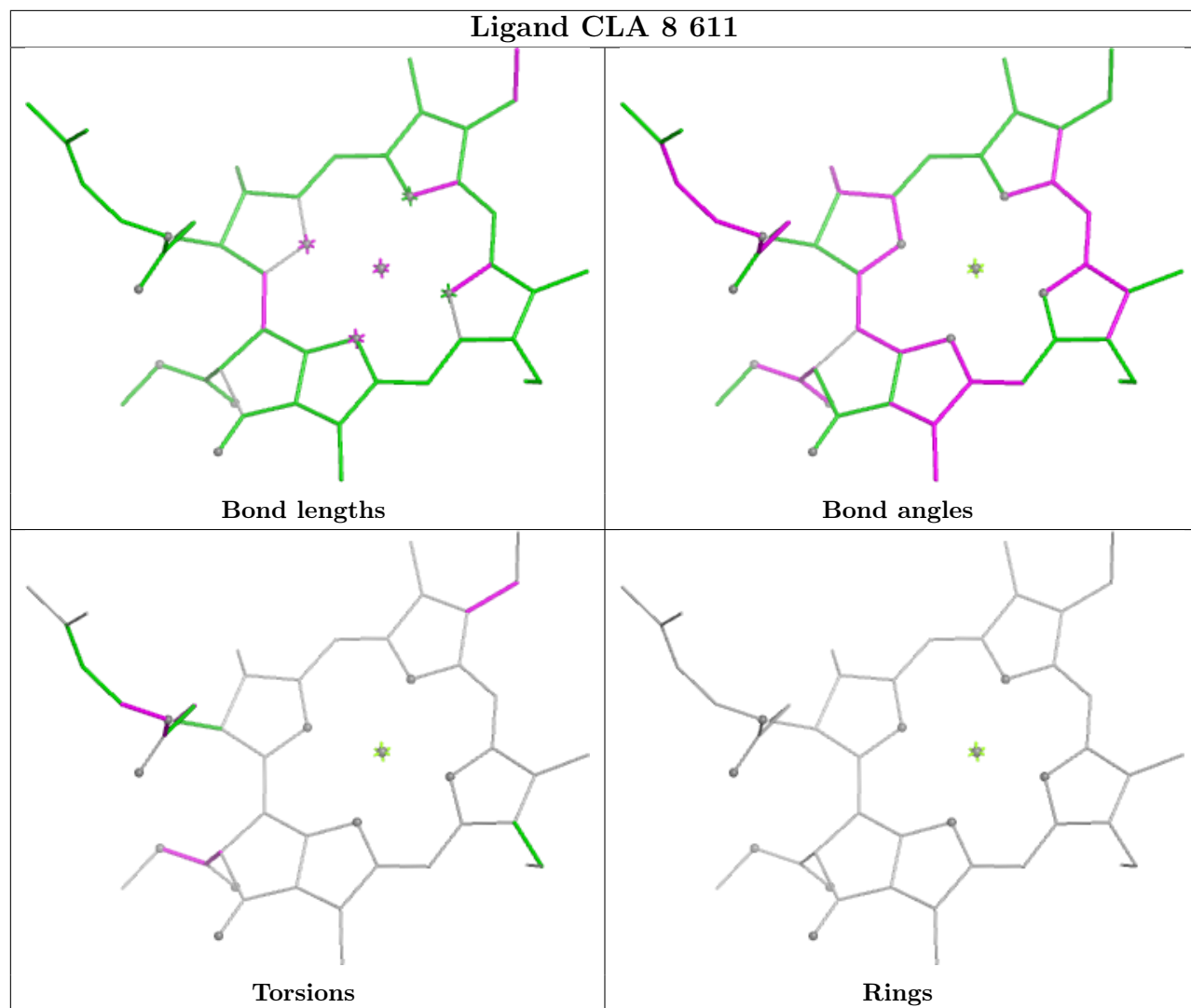


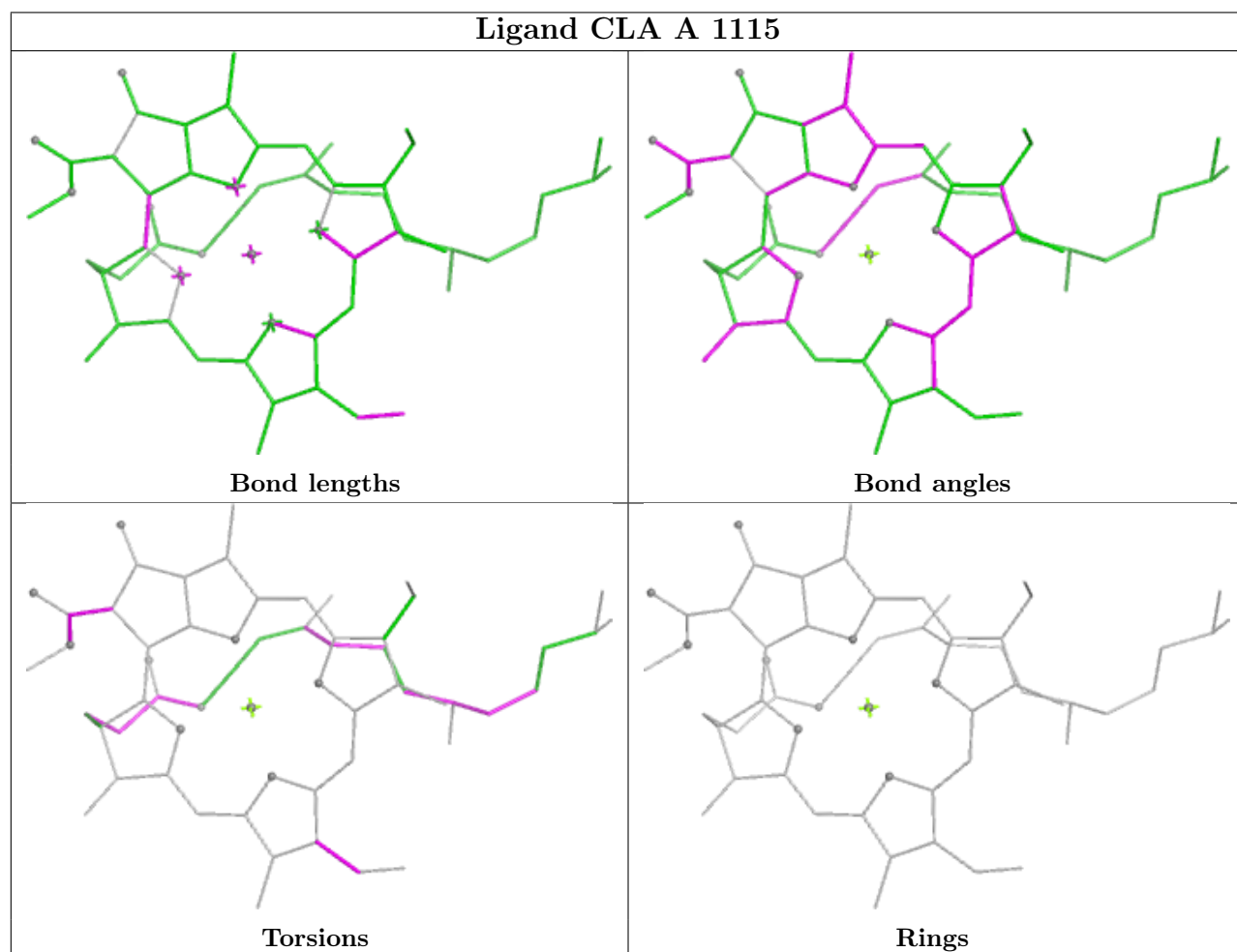
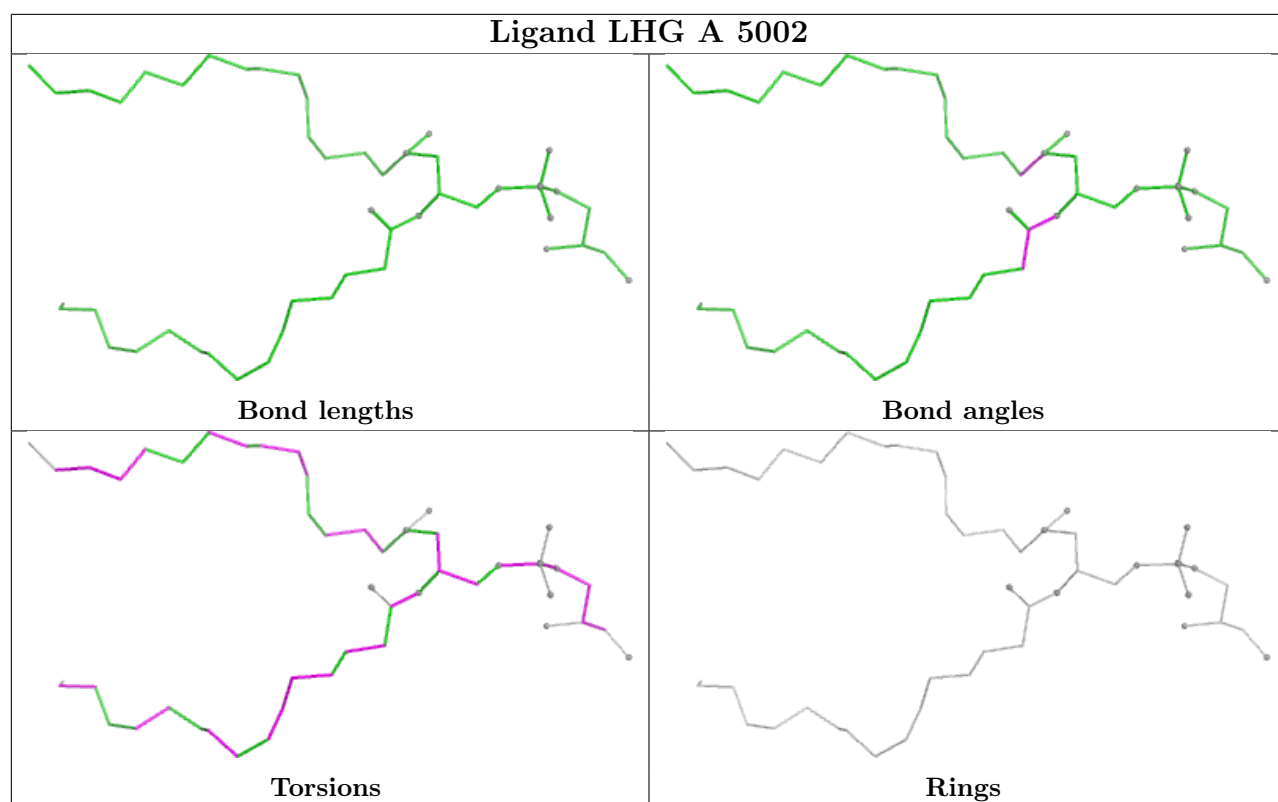


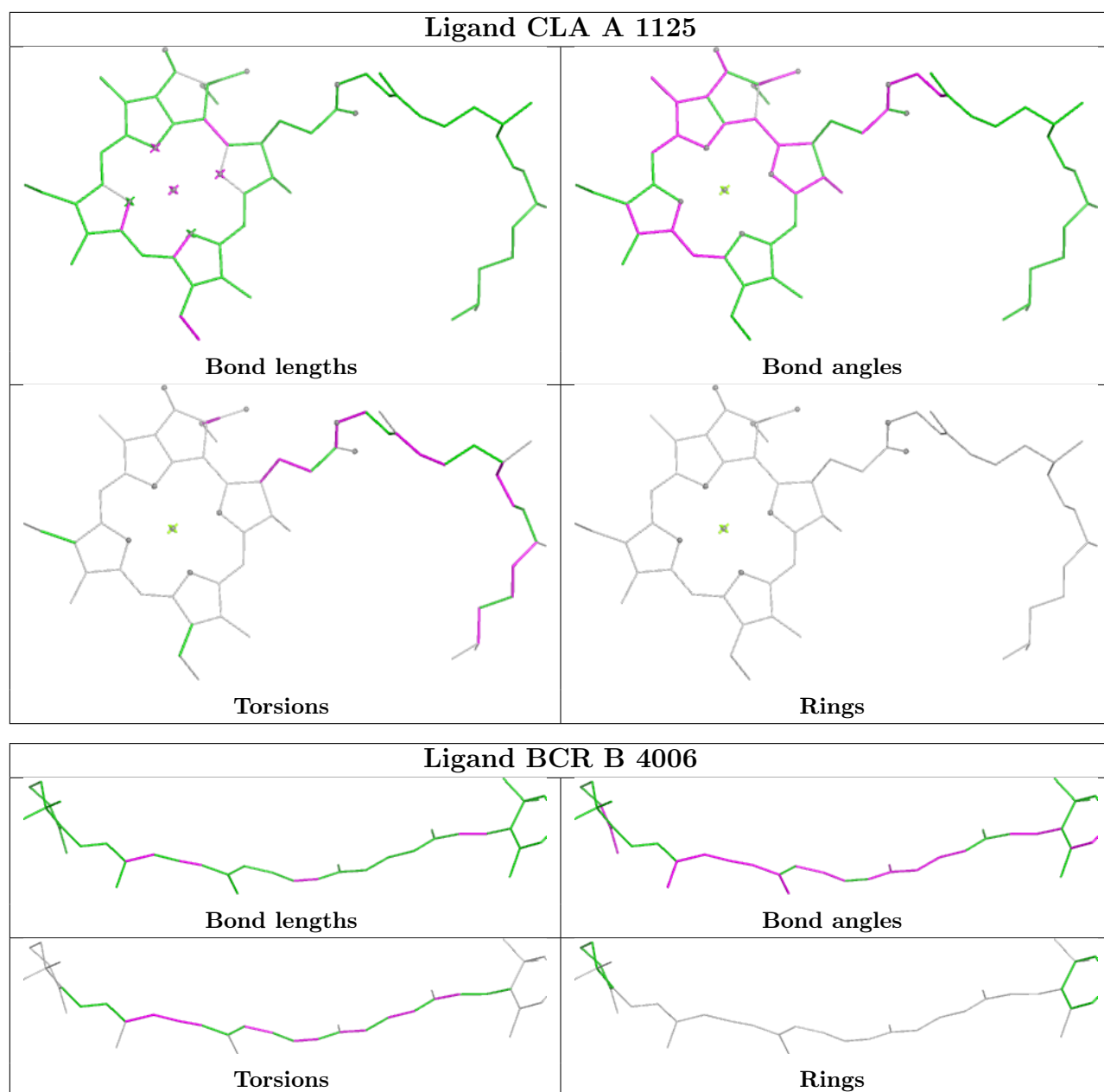


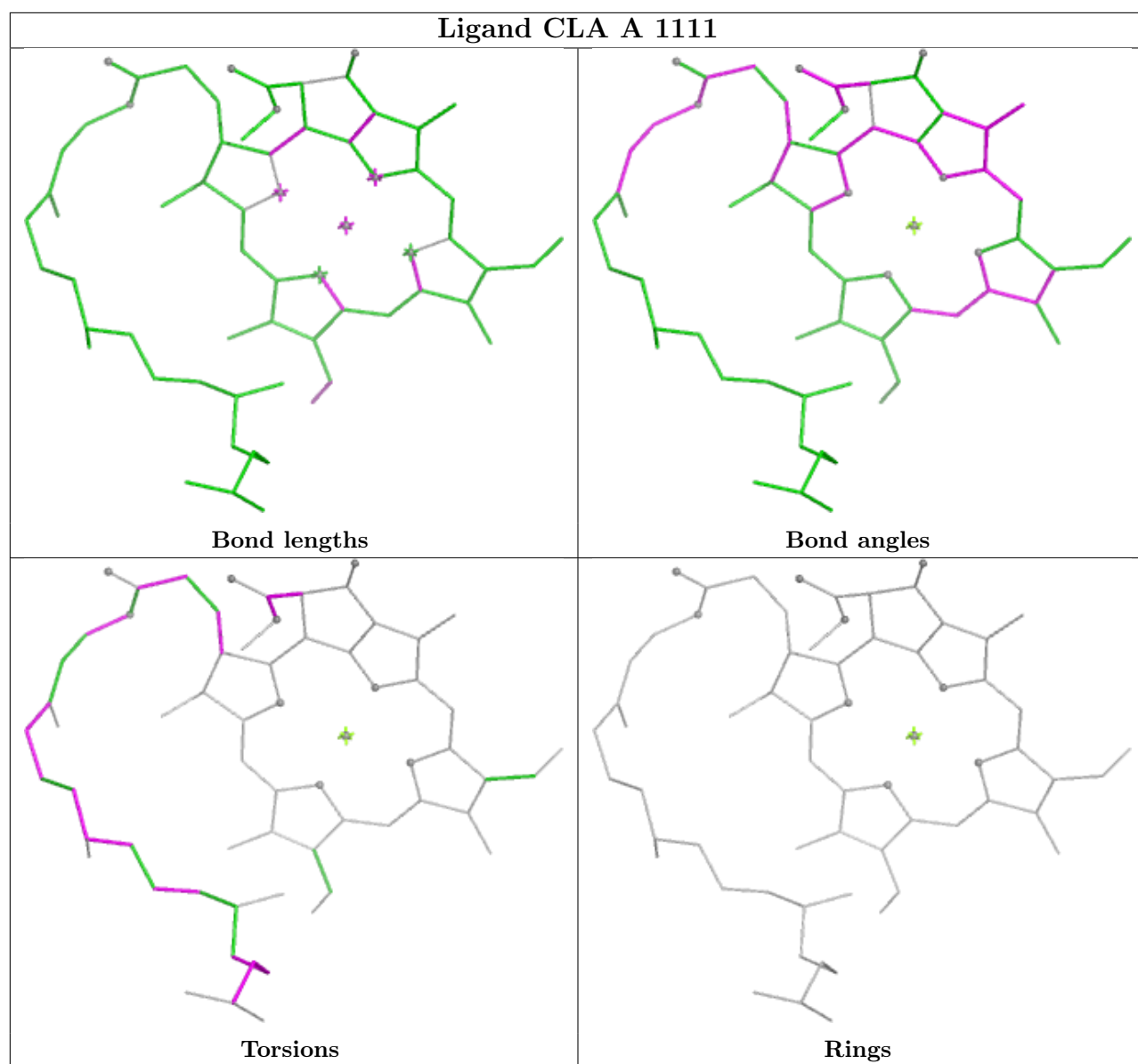




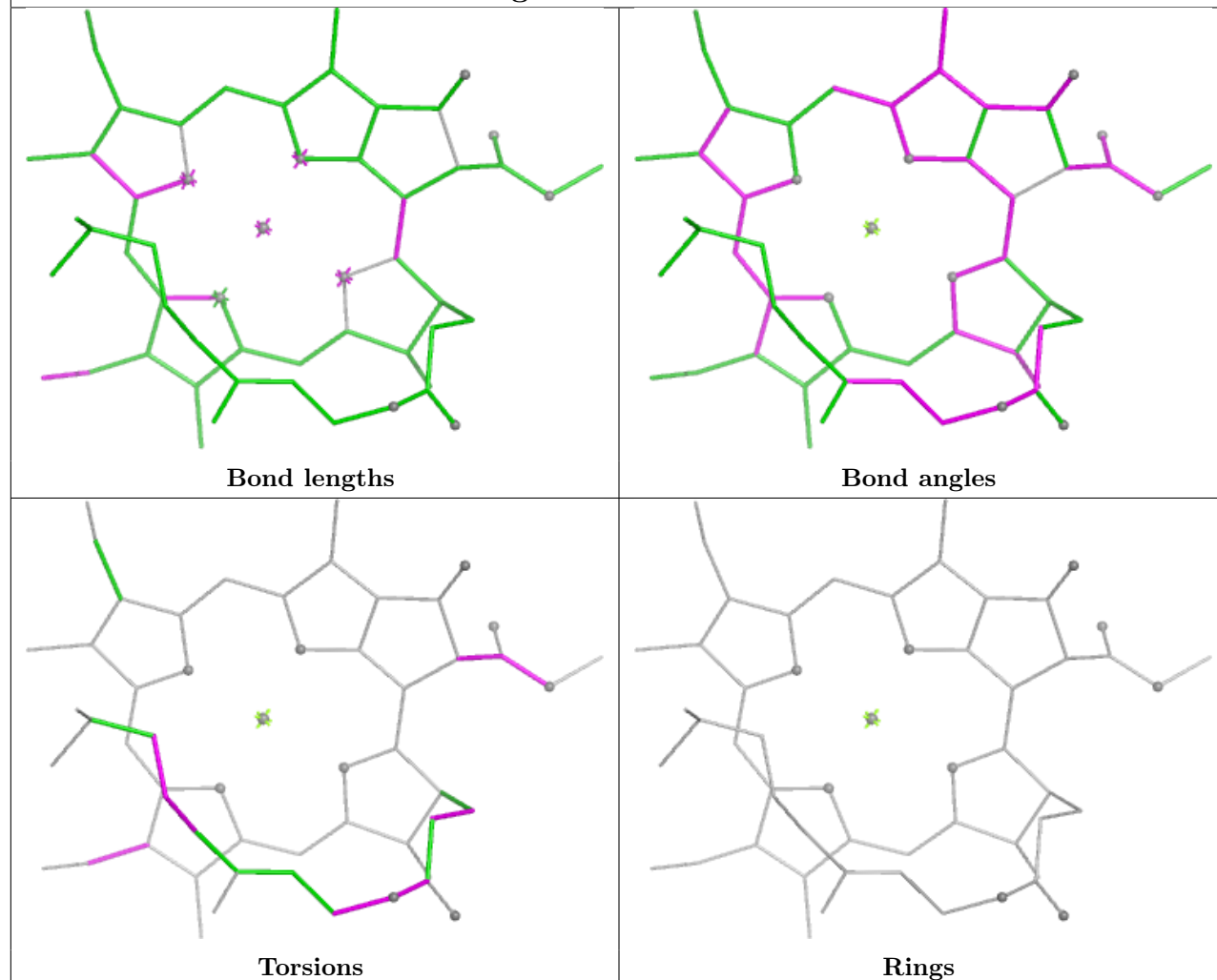




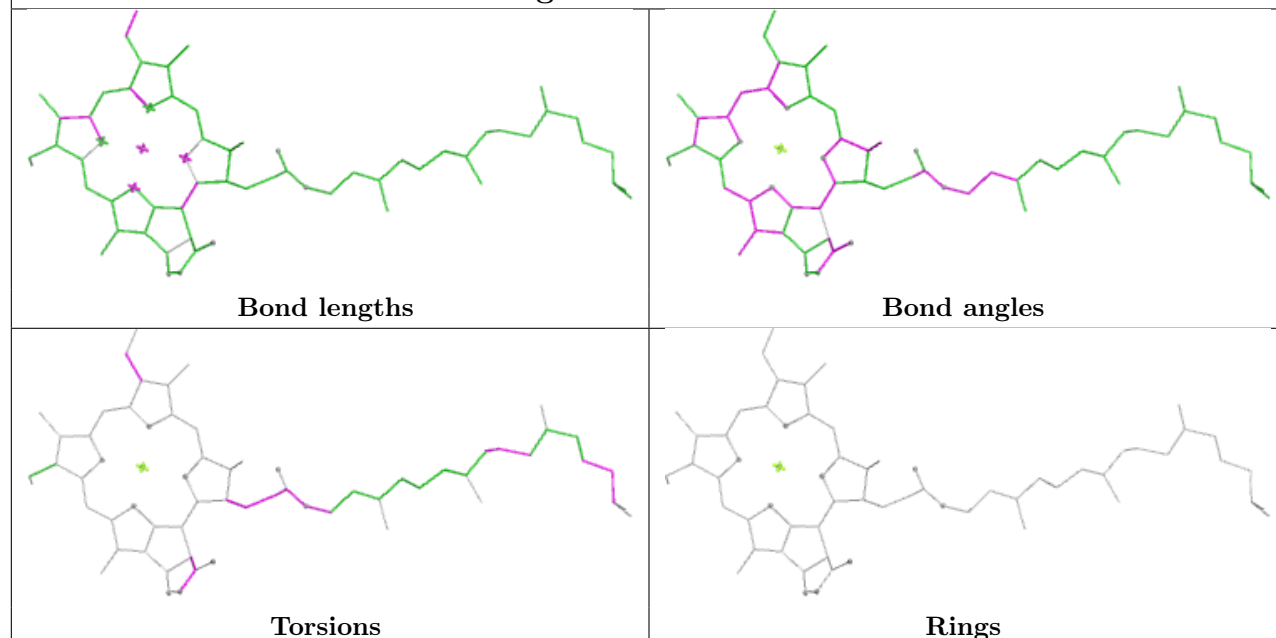


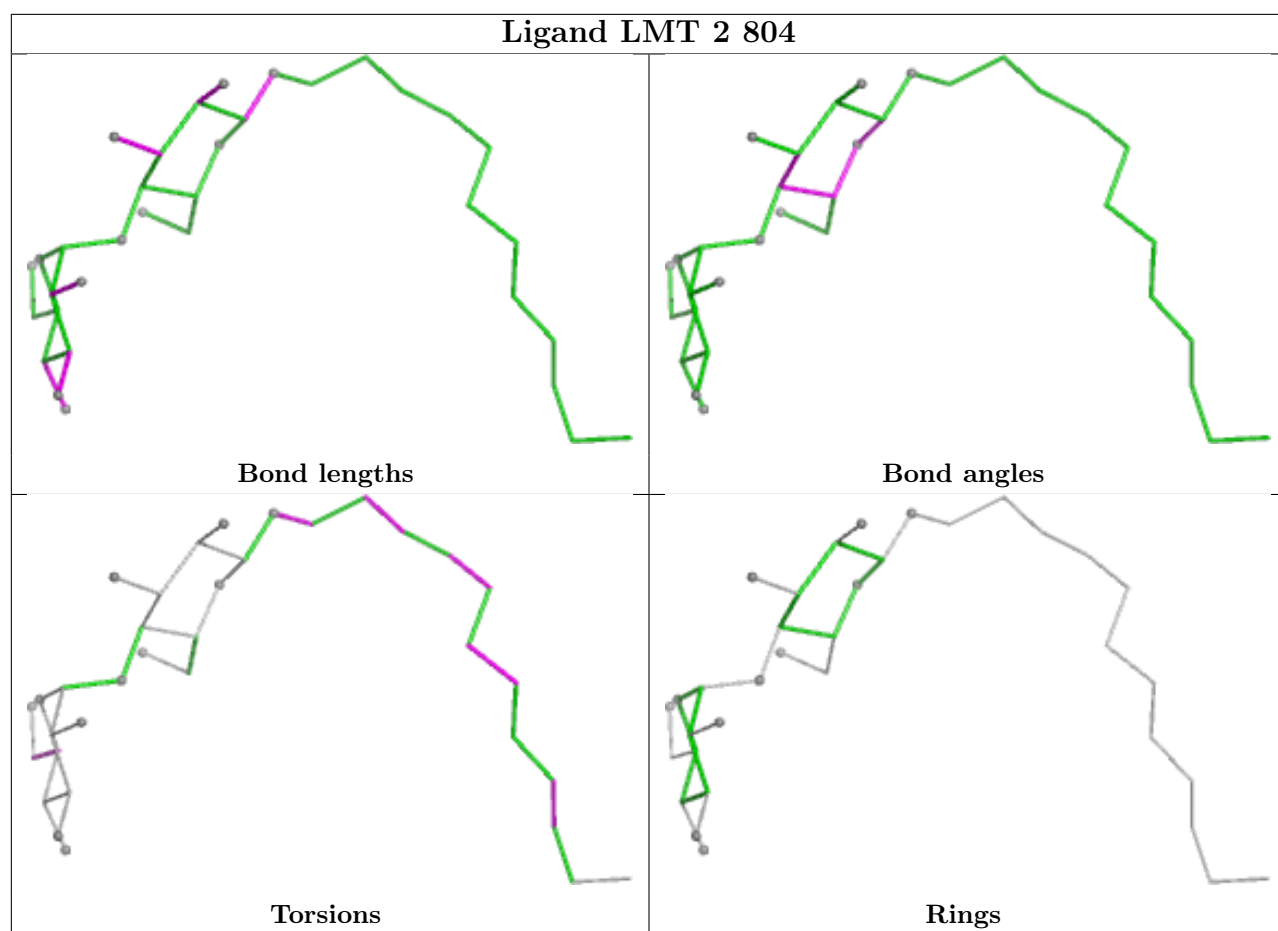


Ligand CLA 5 607

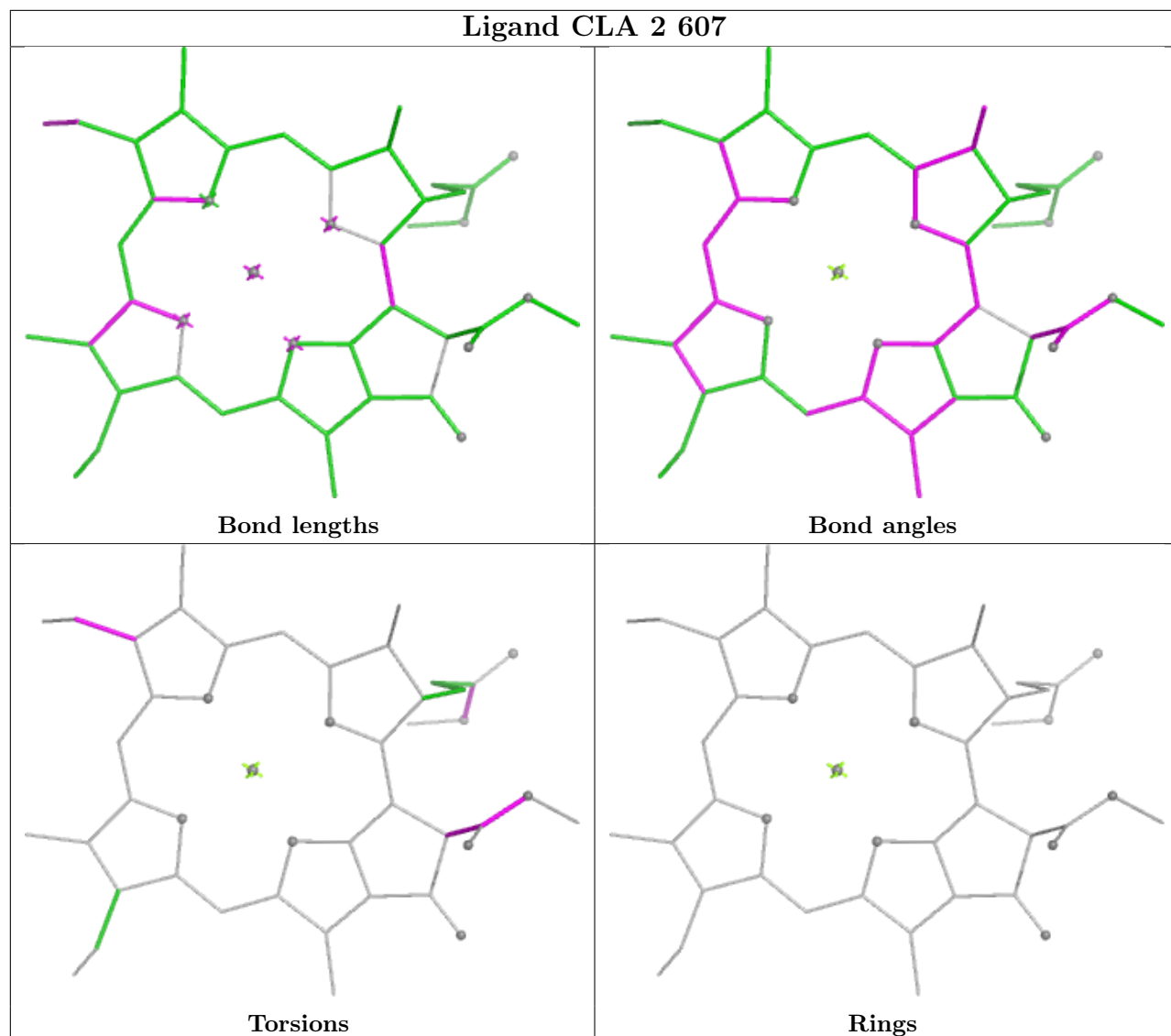


Ligand CLA 6 615

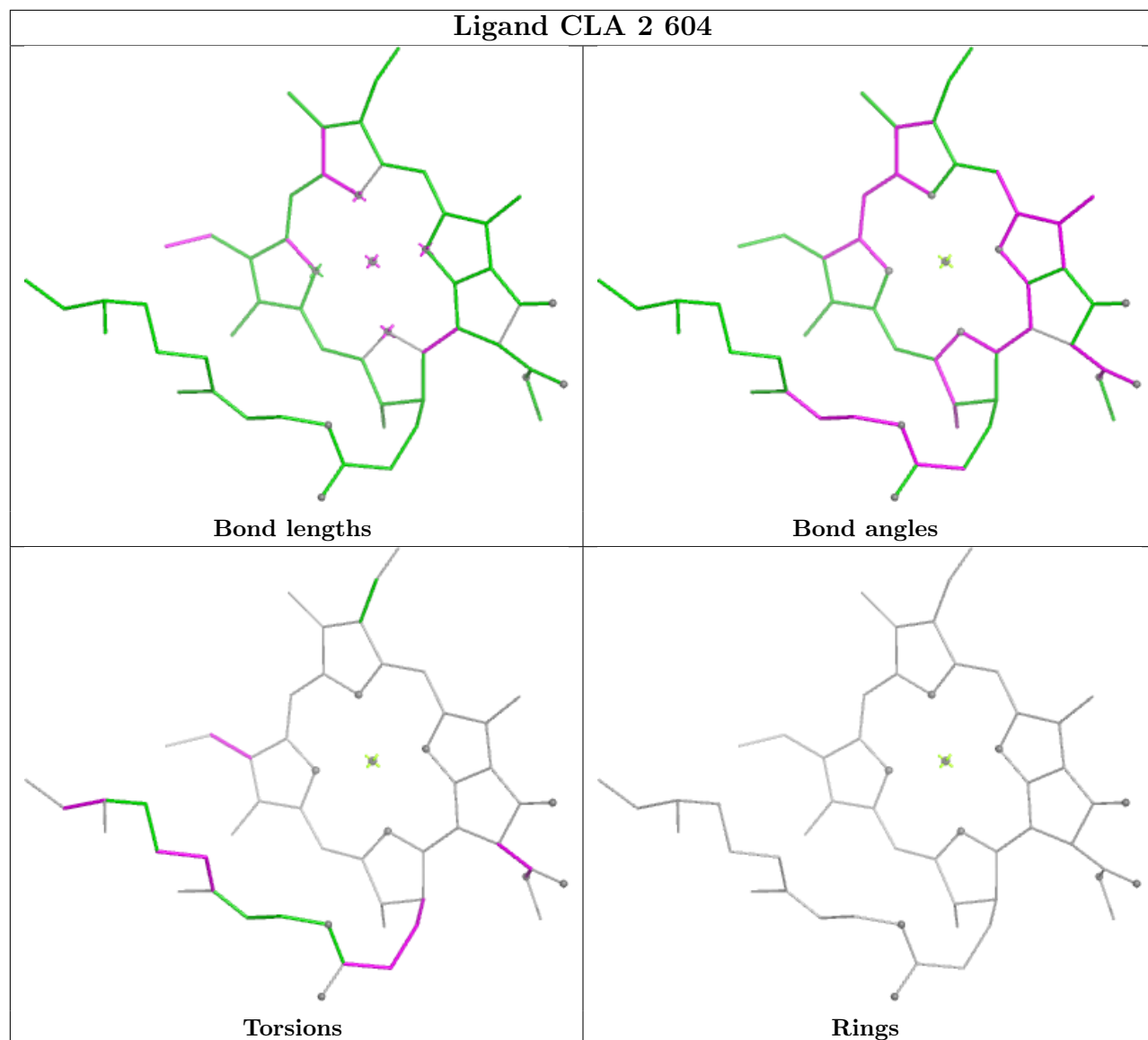


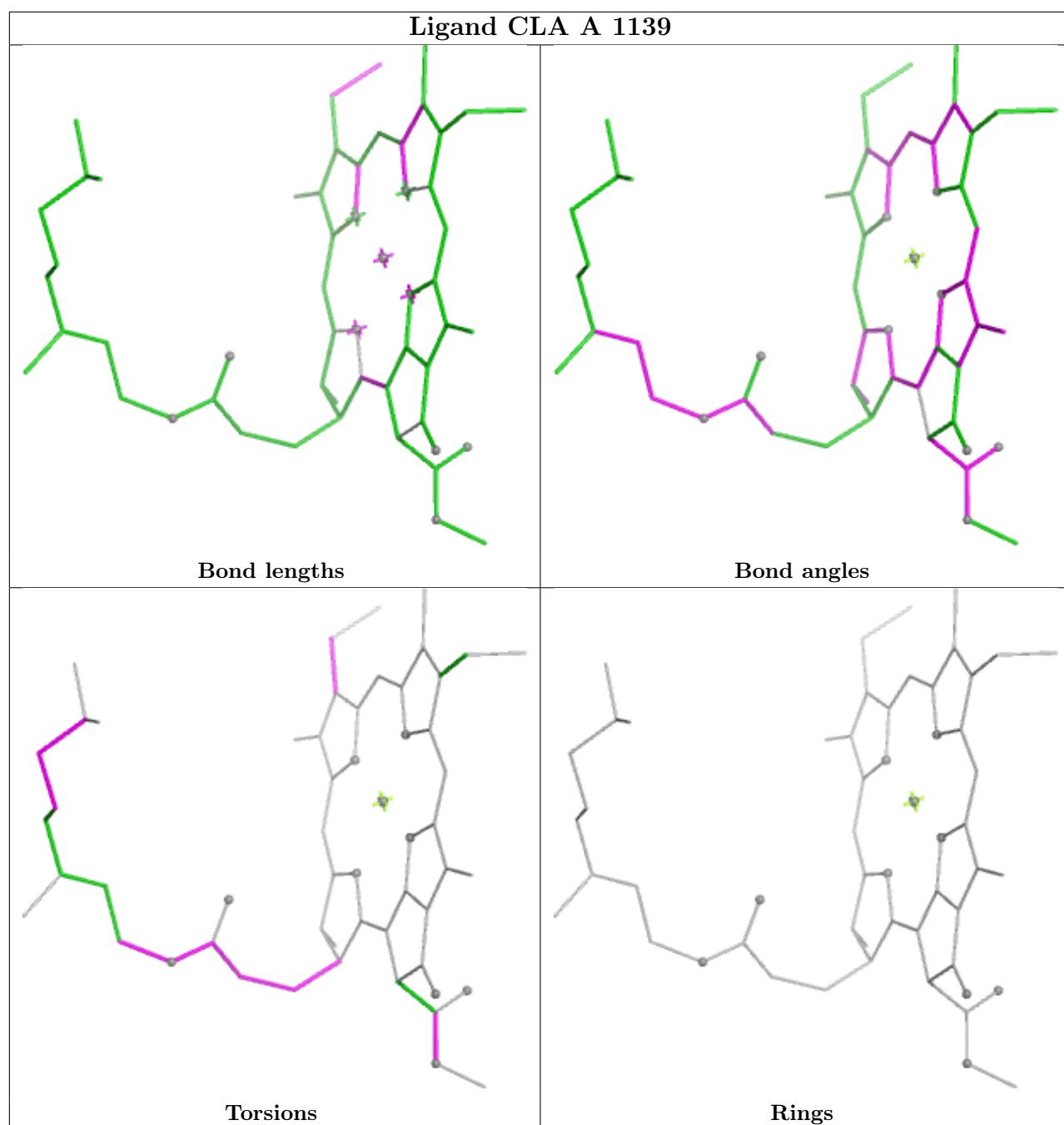


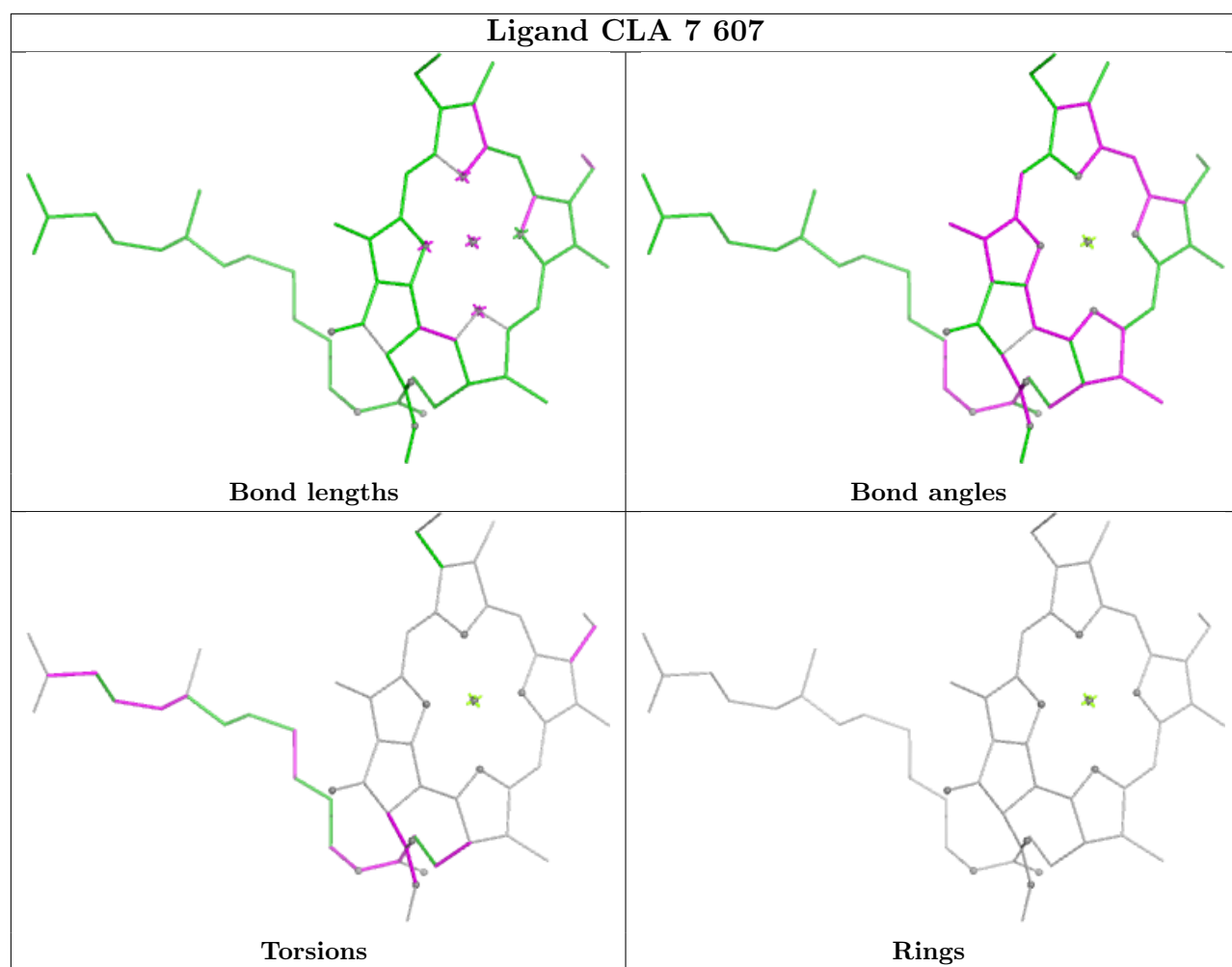
Ligand CLA 2 607

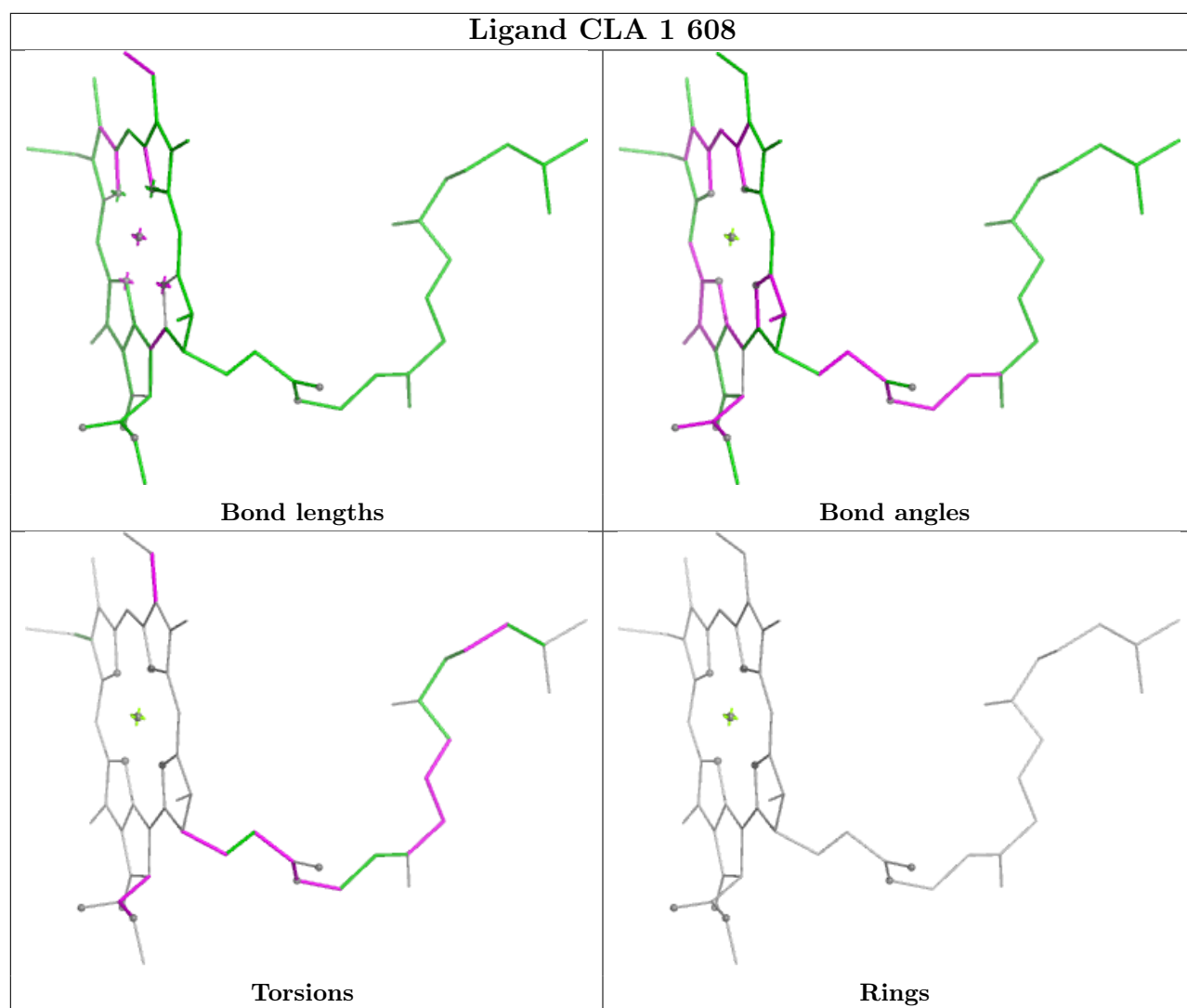


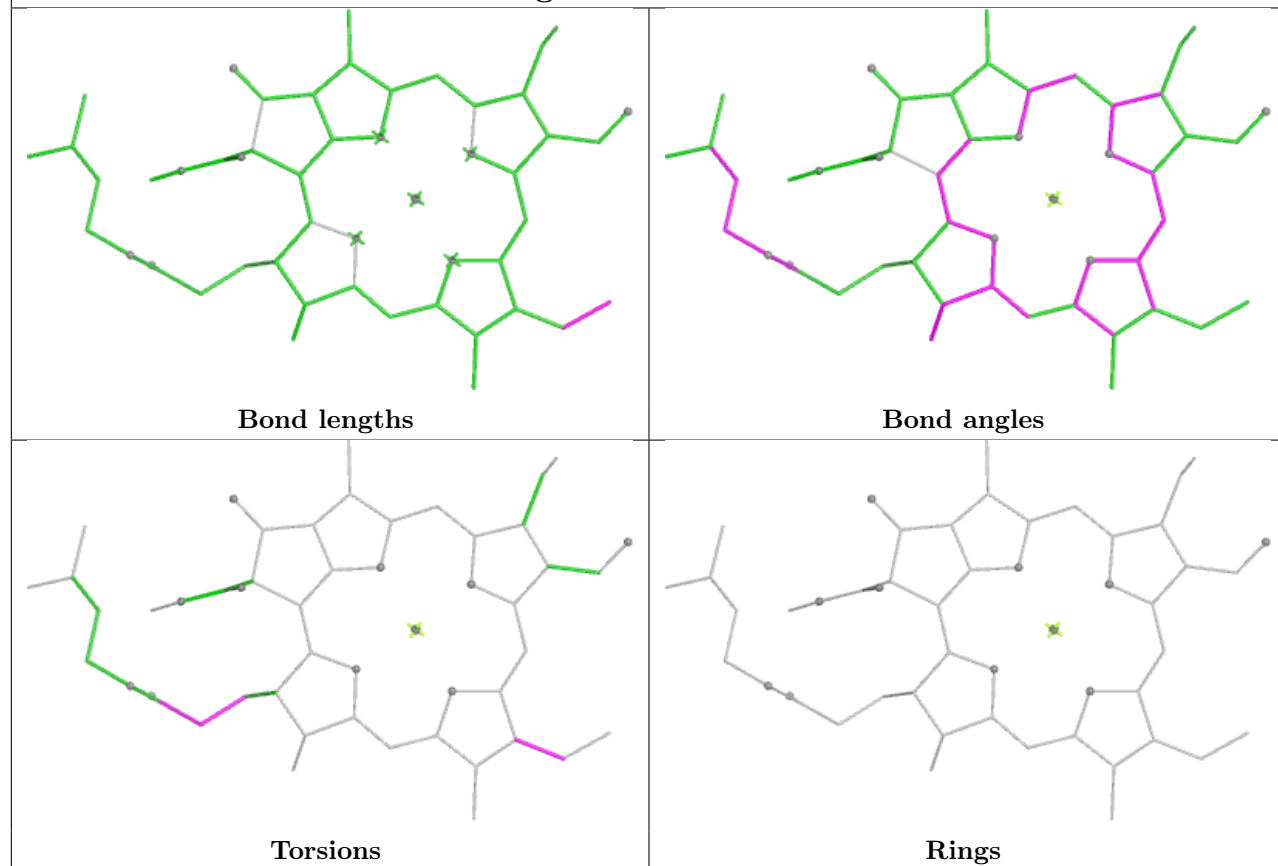
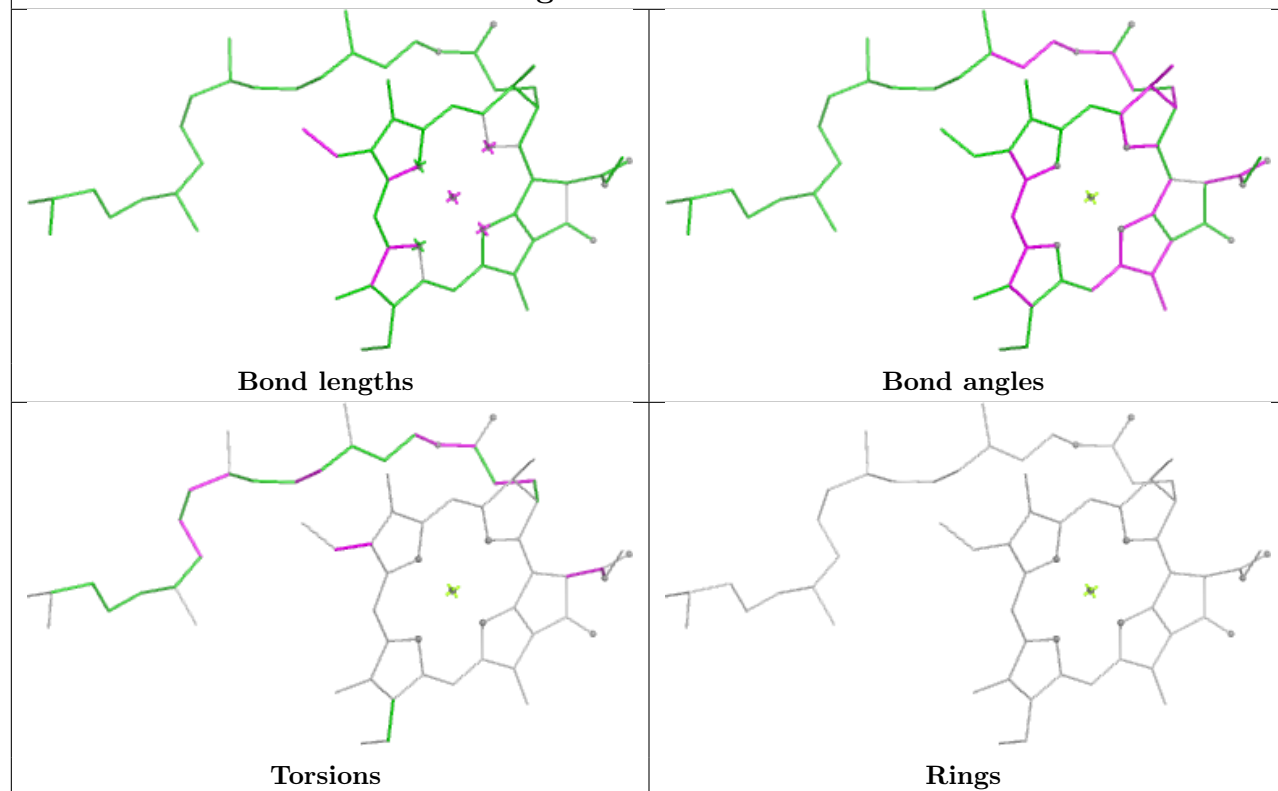
Ligand CLA 2 604

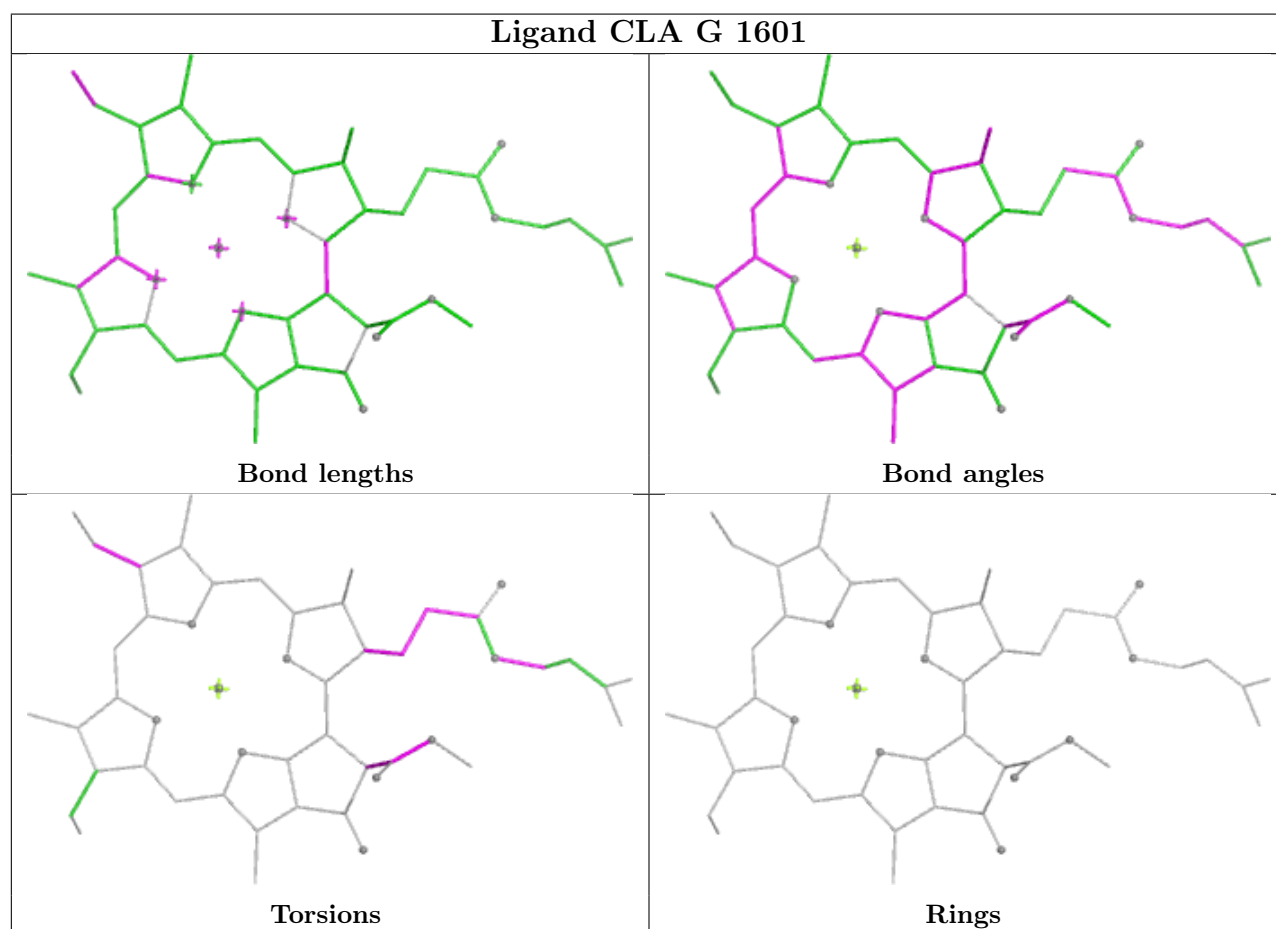
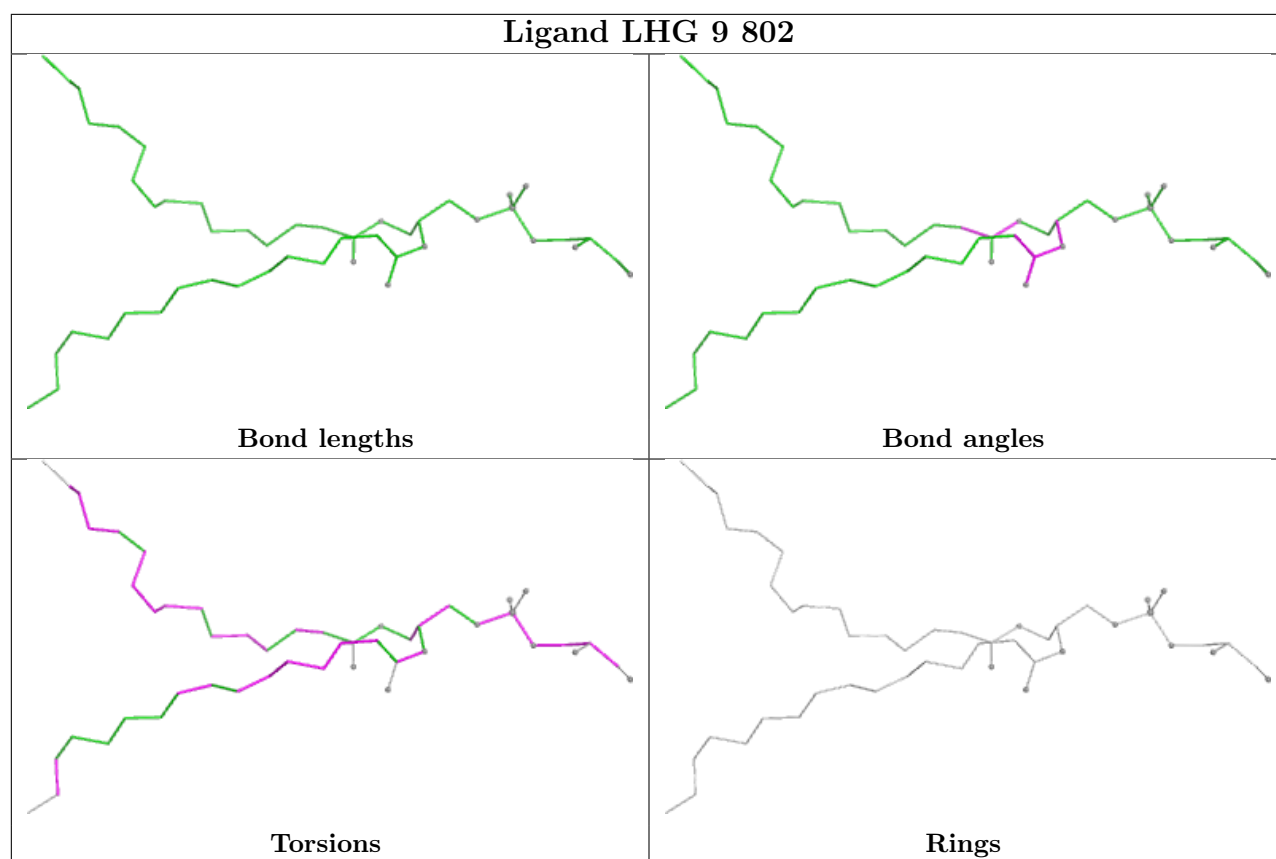


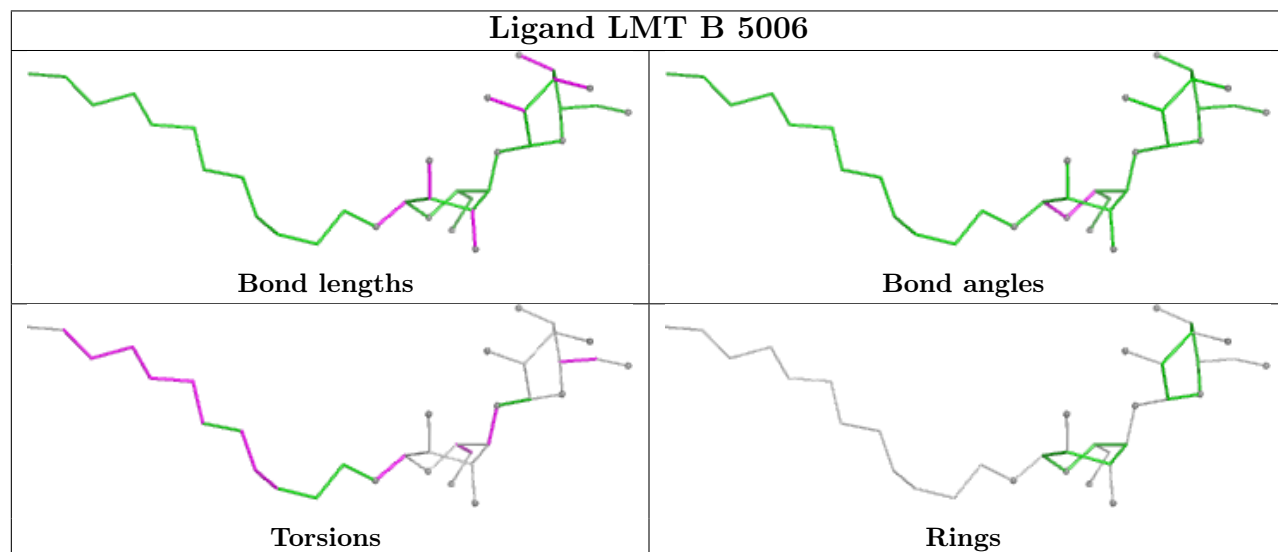
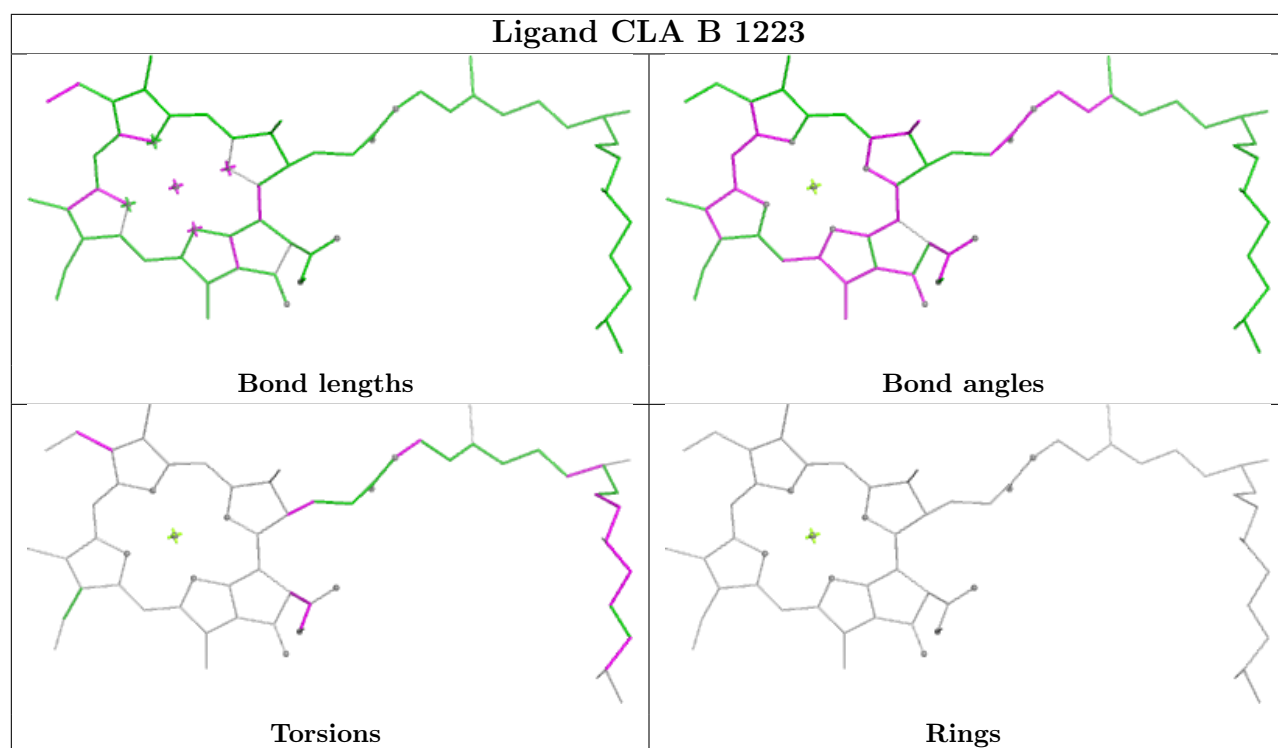


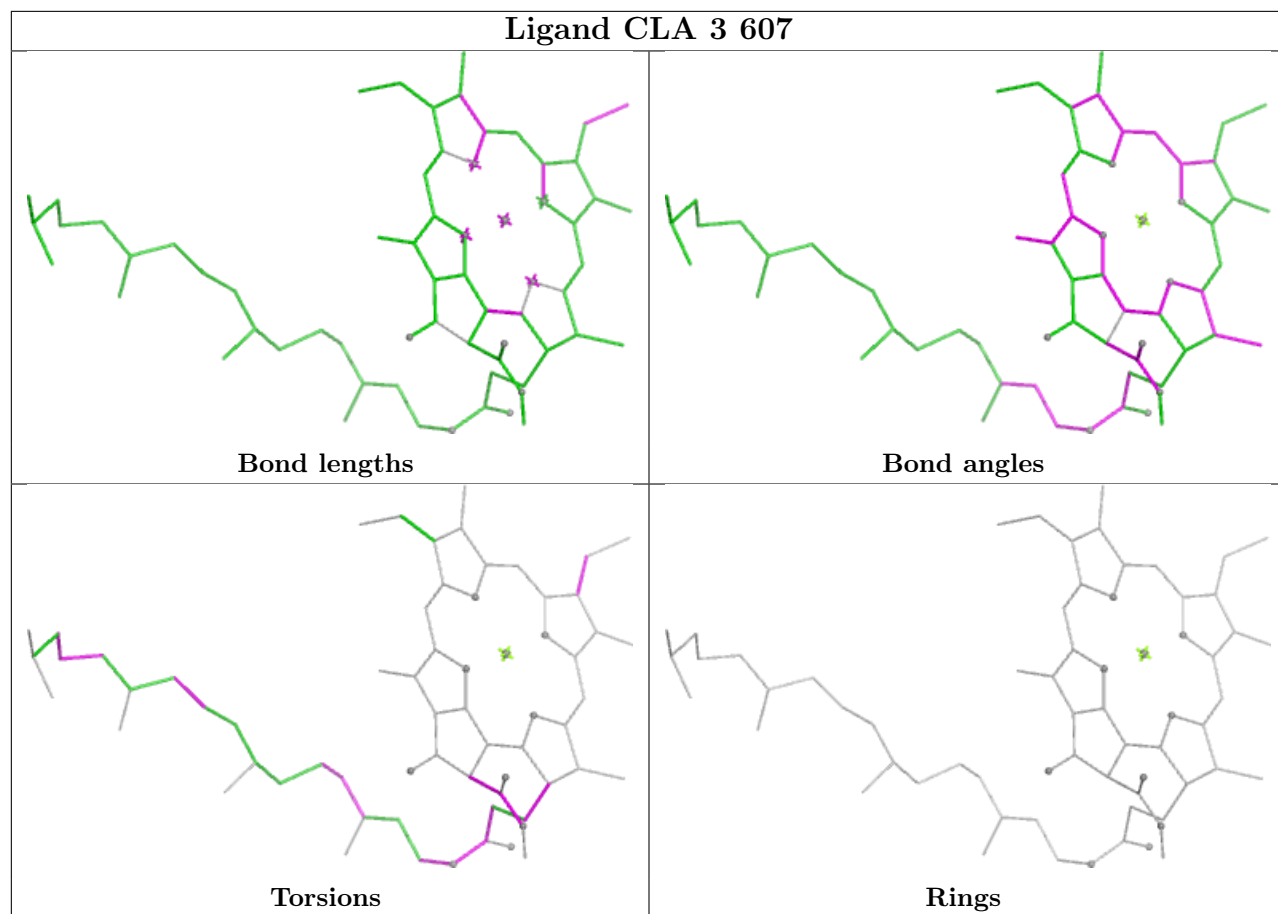




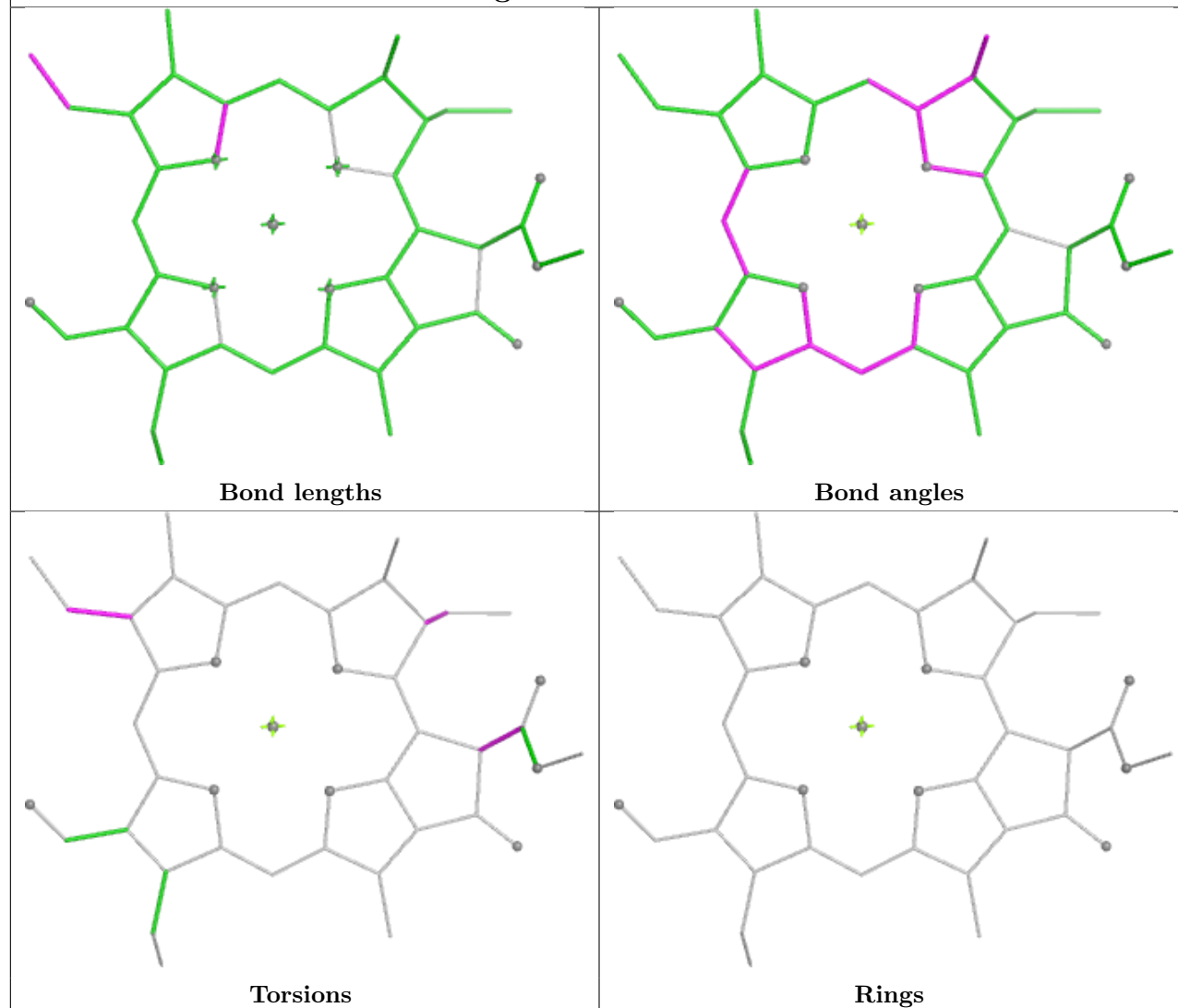
Ligand CHL 9 610**Ligand CLA 7 604**

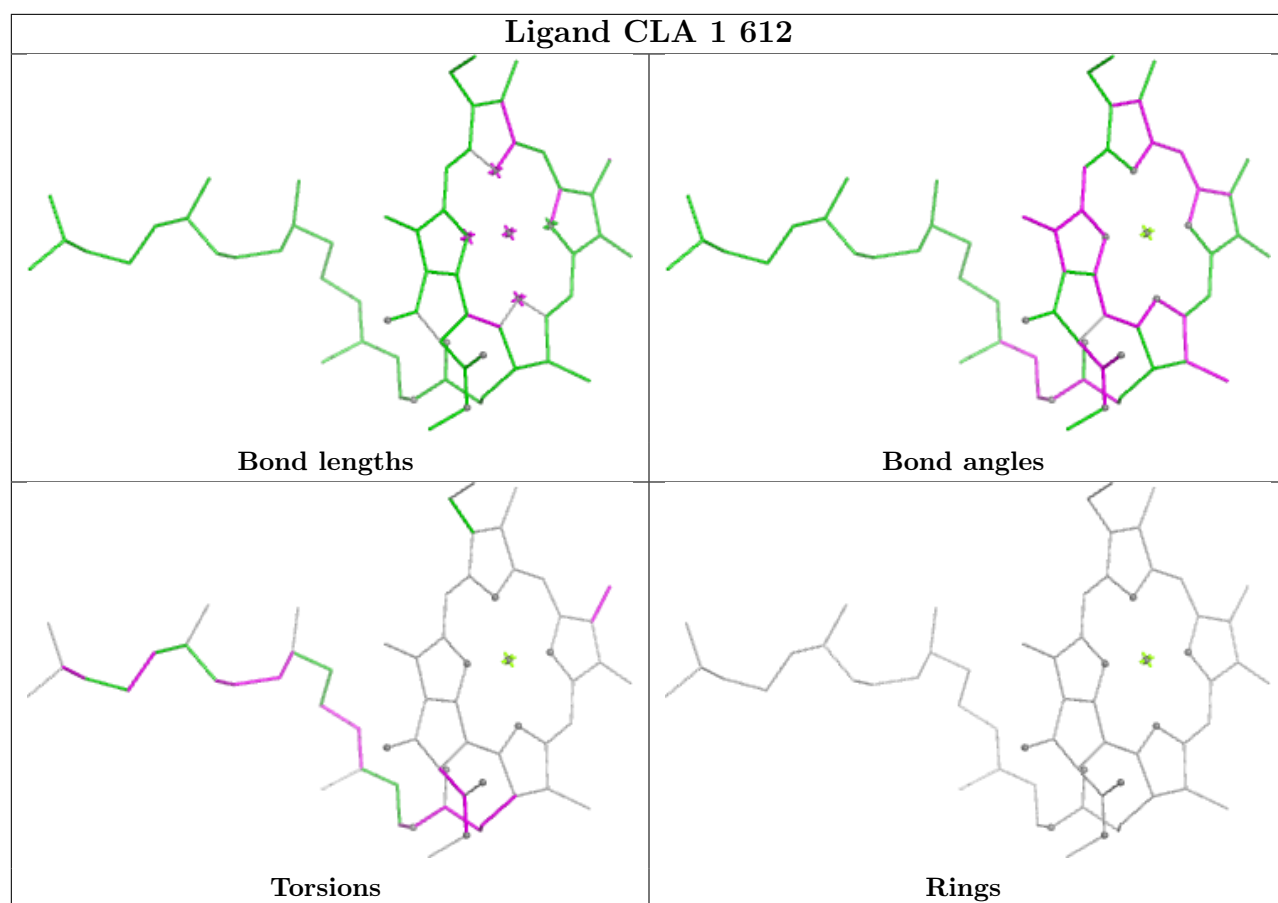




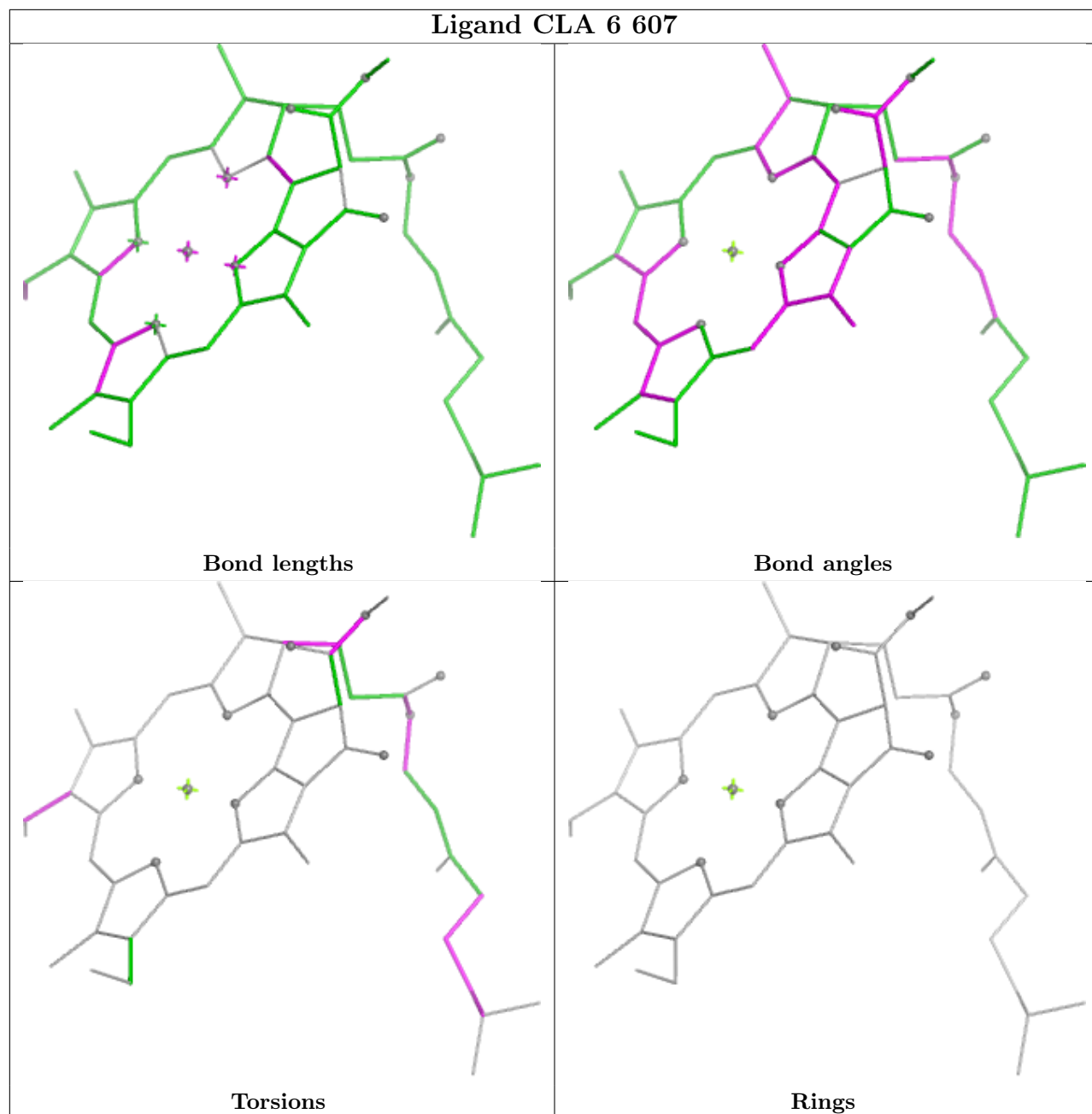


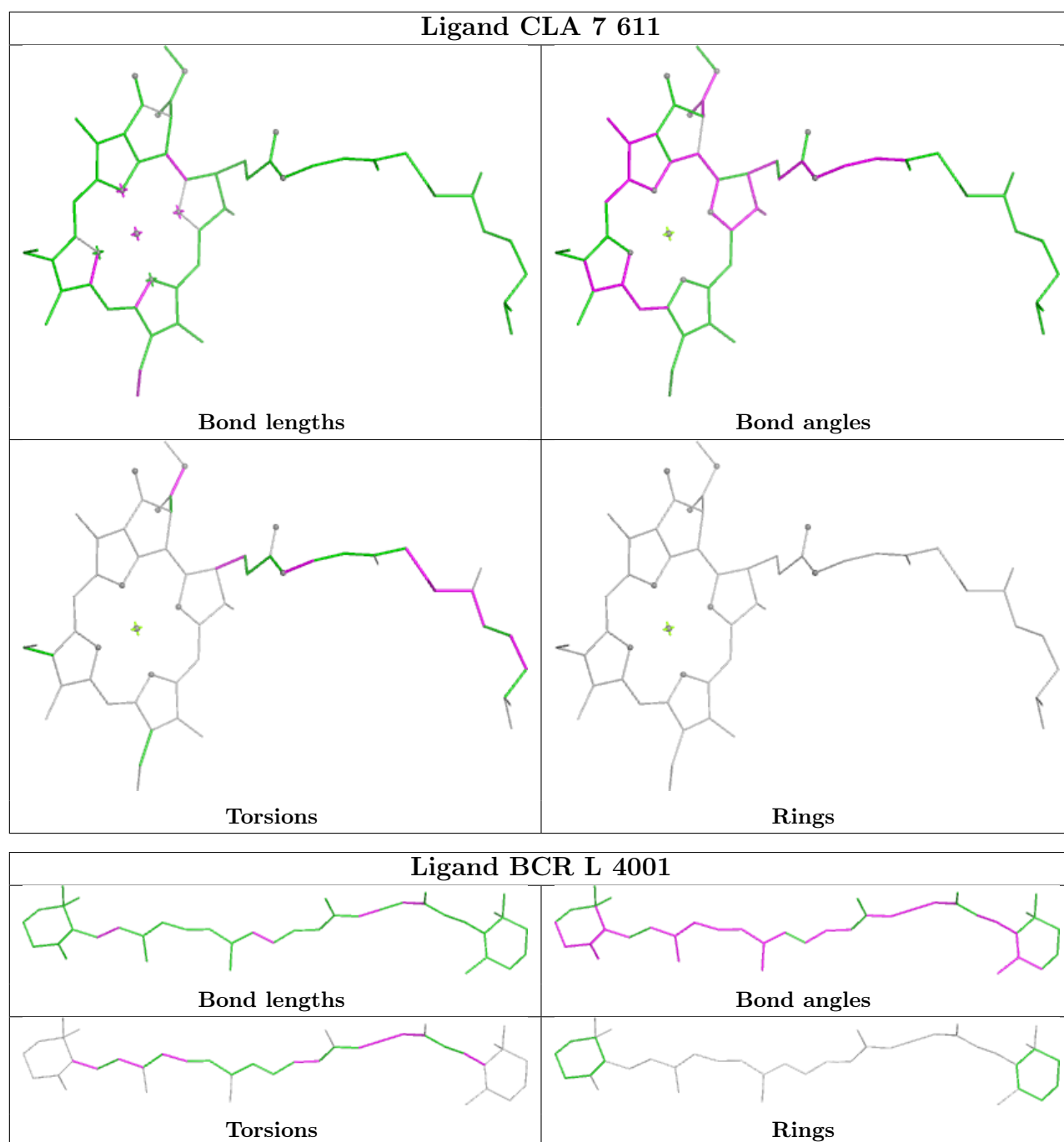
Ligand CHL 3 608



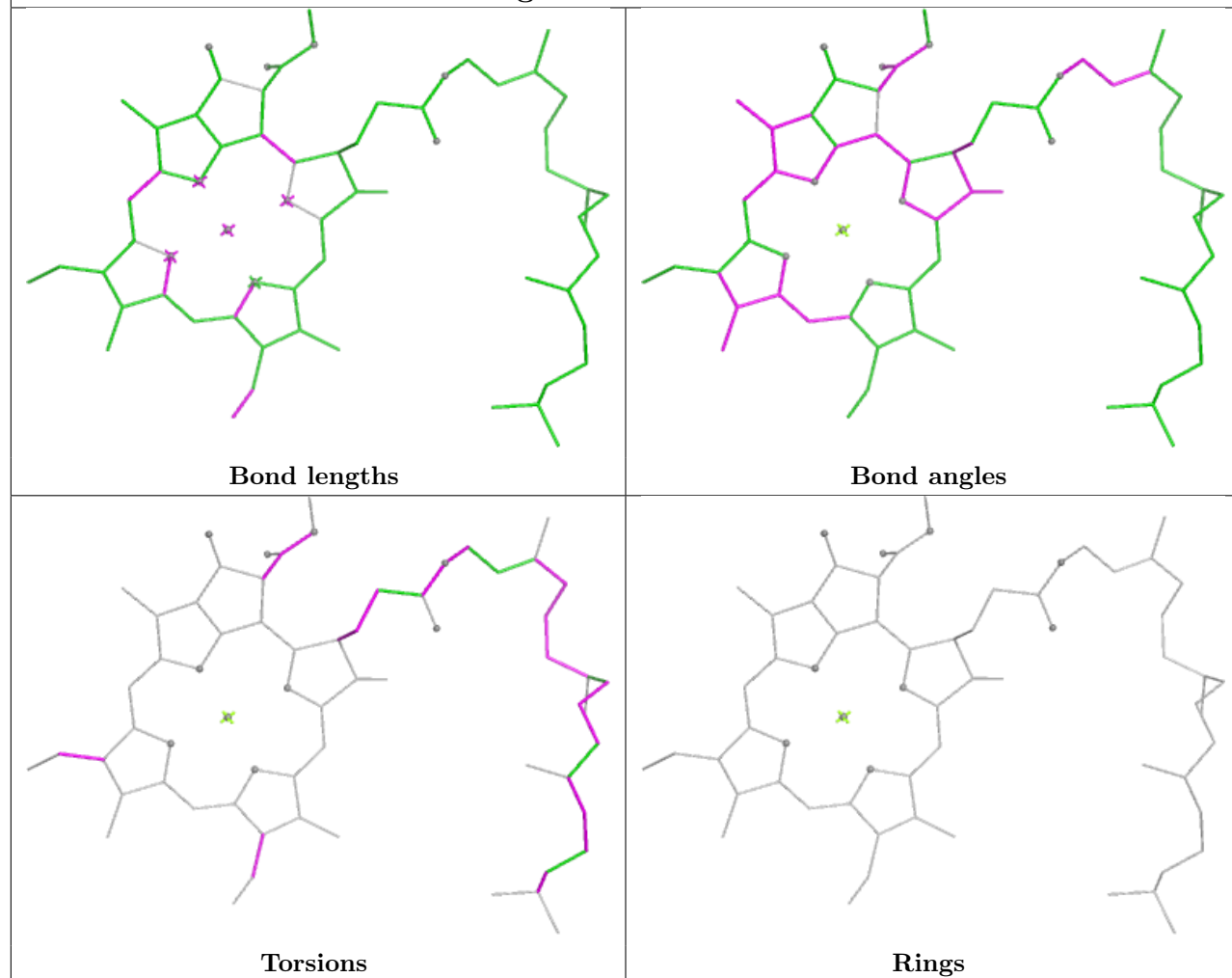


Ligand CLA 6 607

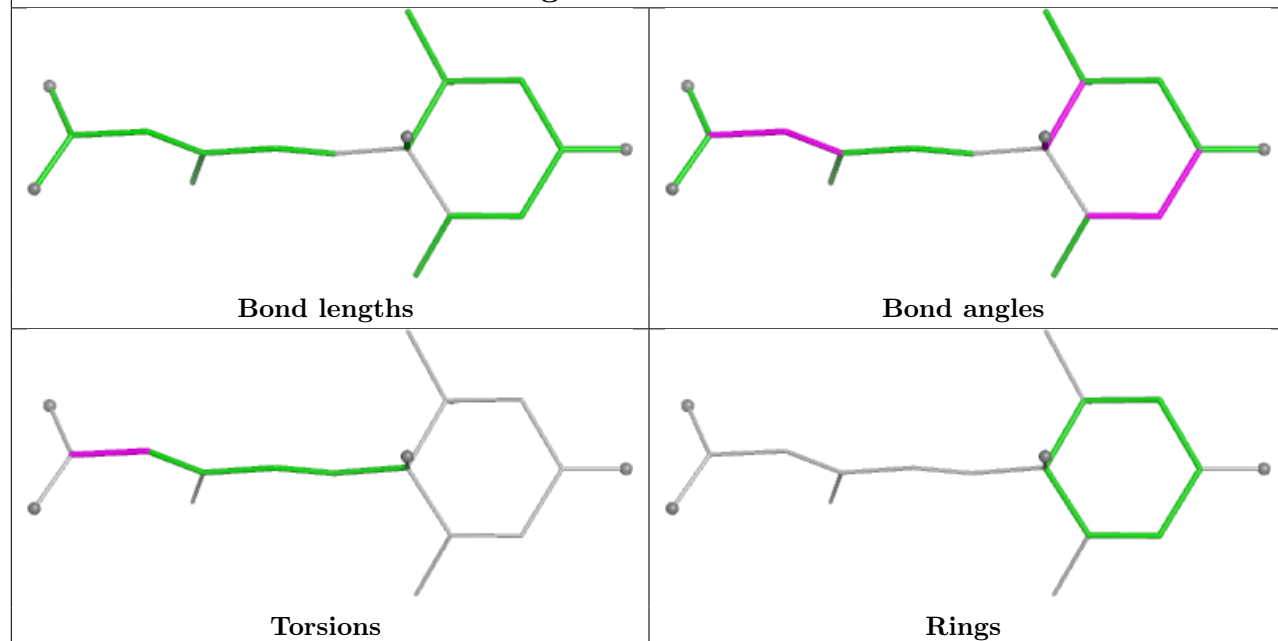


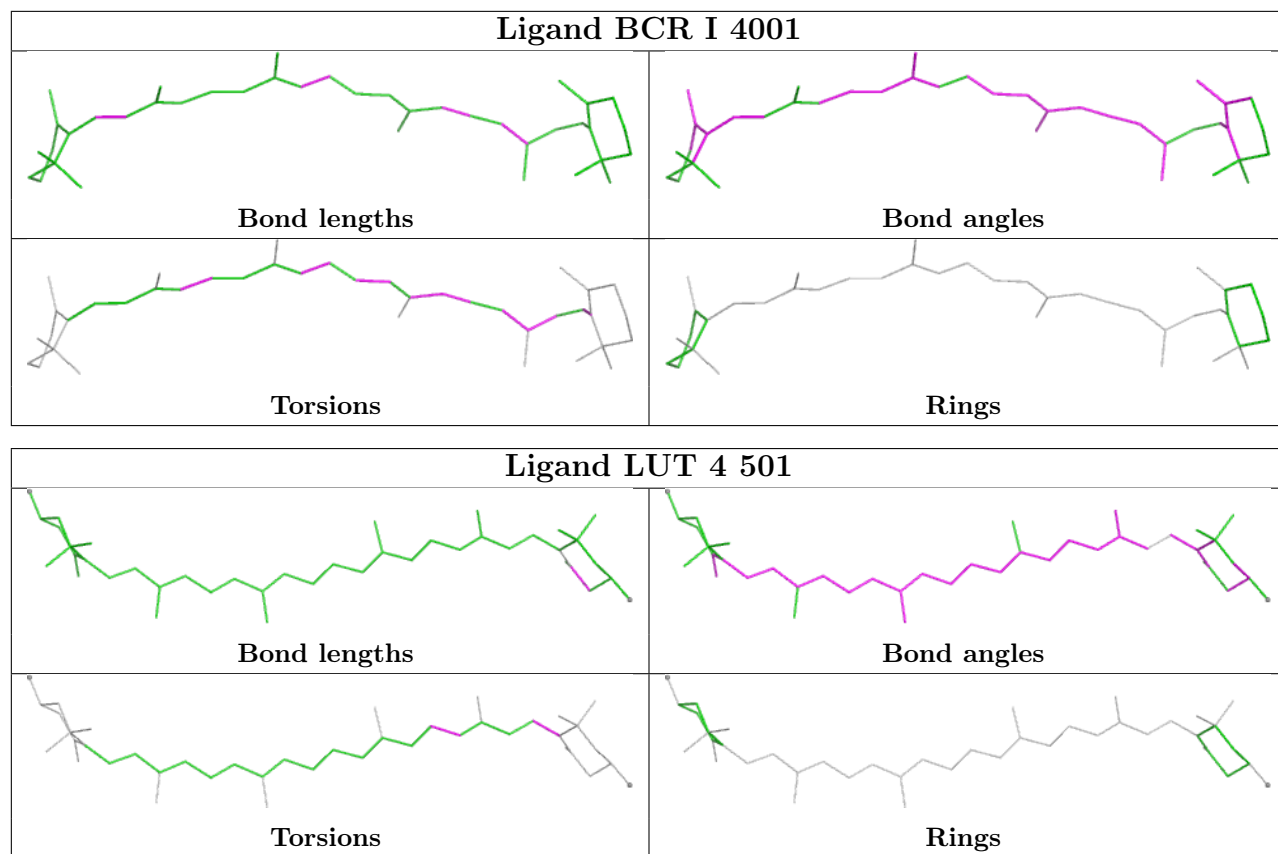


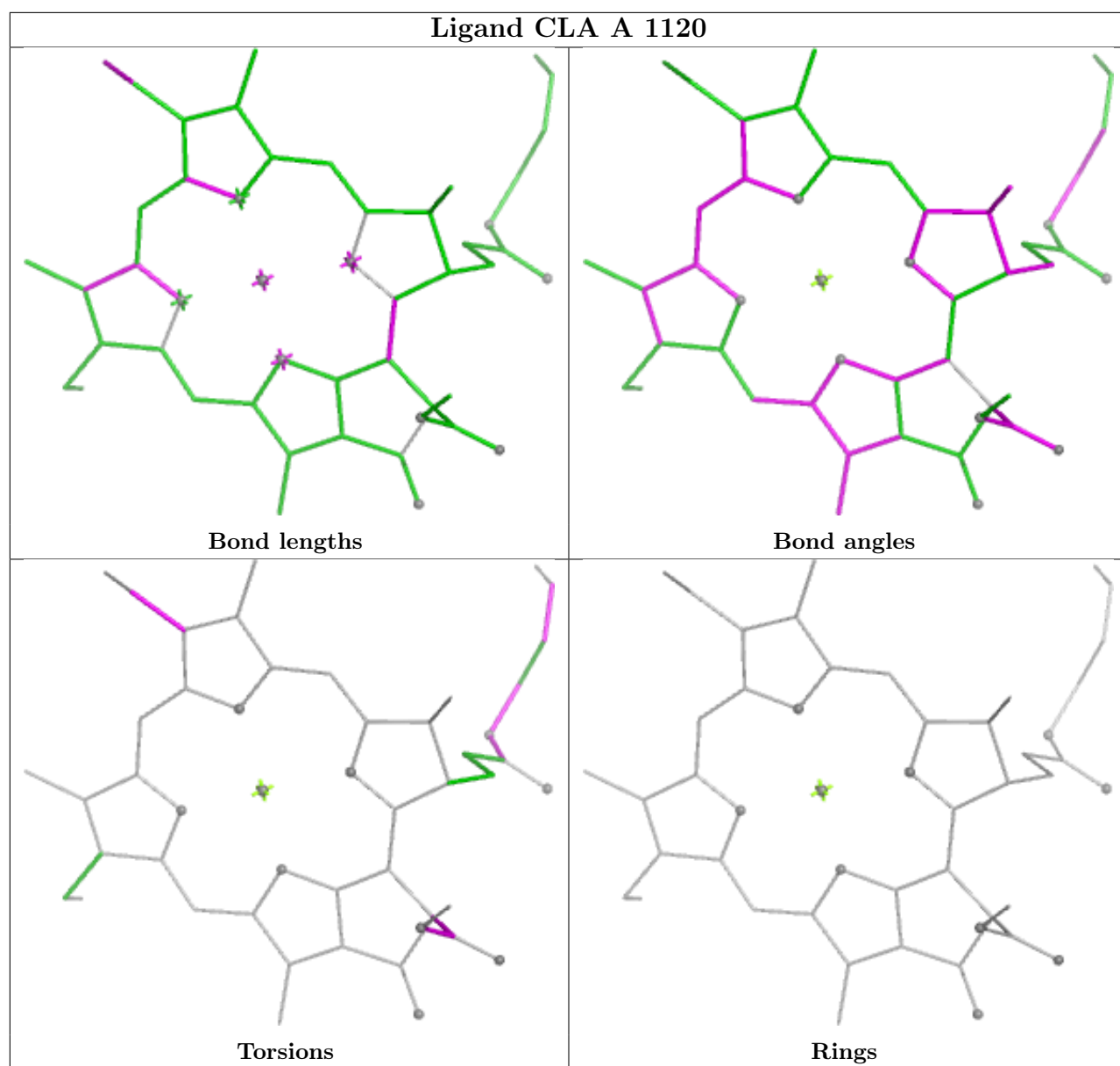
Ligand CLA 4 610

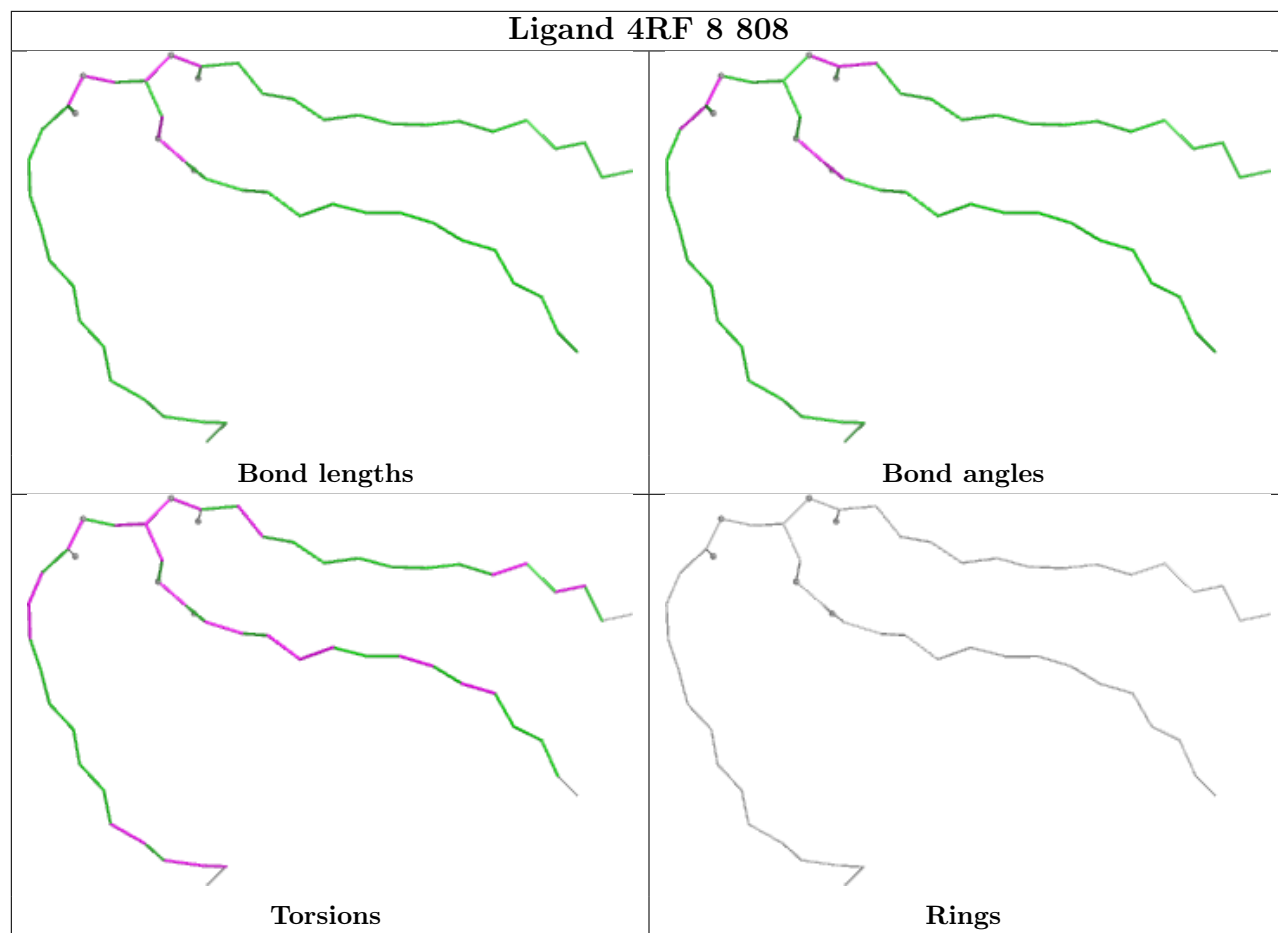


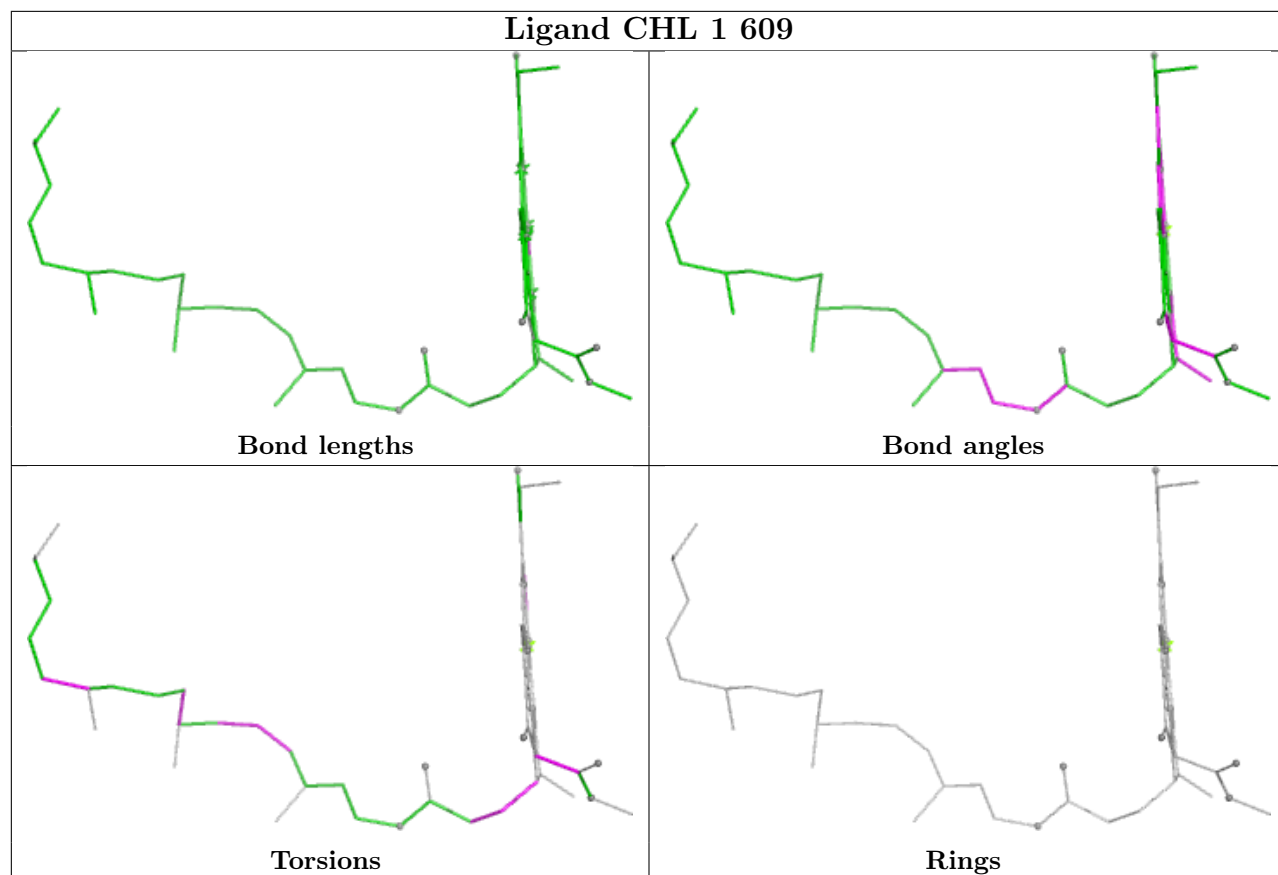
Ligand A8S 9 504



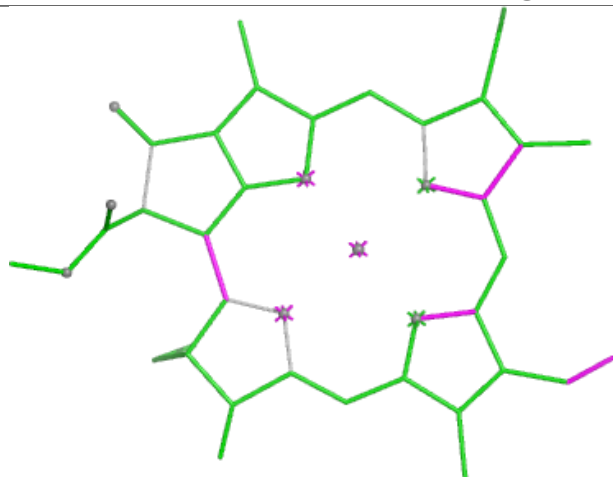




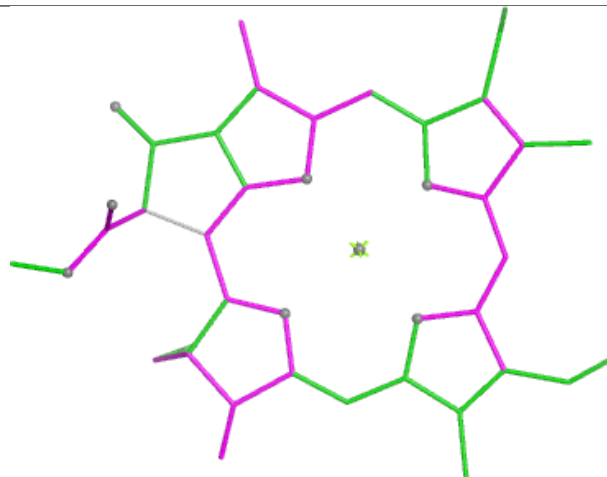




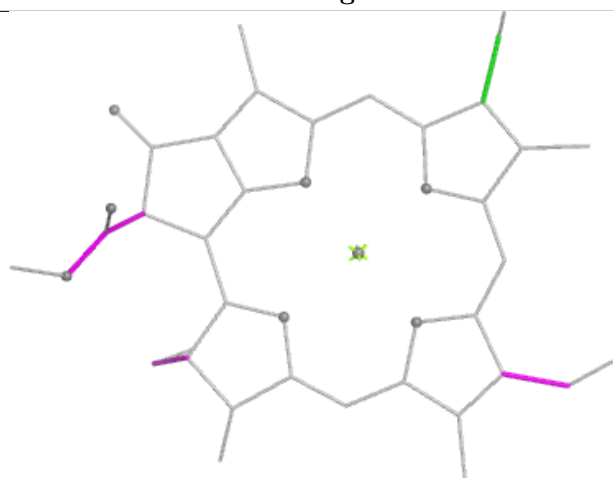
Ligand CLA 7 608



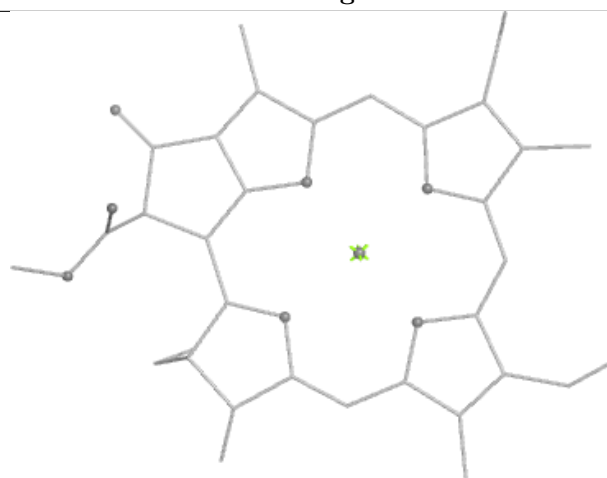
Bond lengths



Bond angles

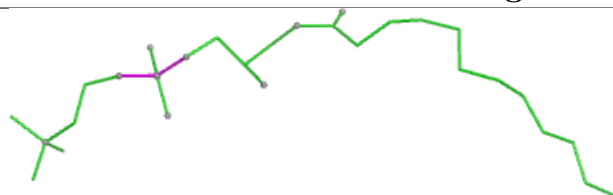


Torsions

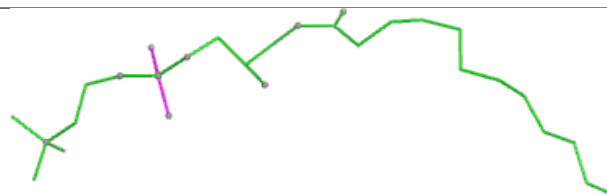


Rings

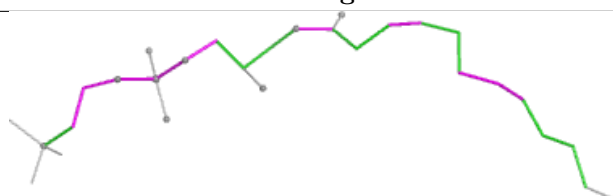
Ligand LAP K 5001



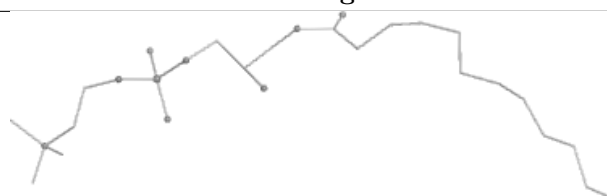
Bond lengths



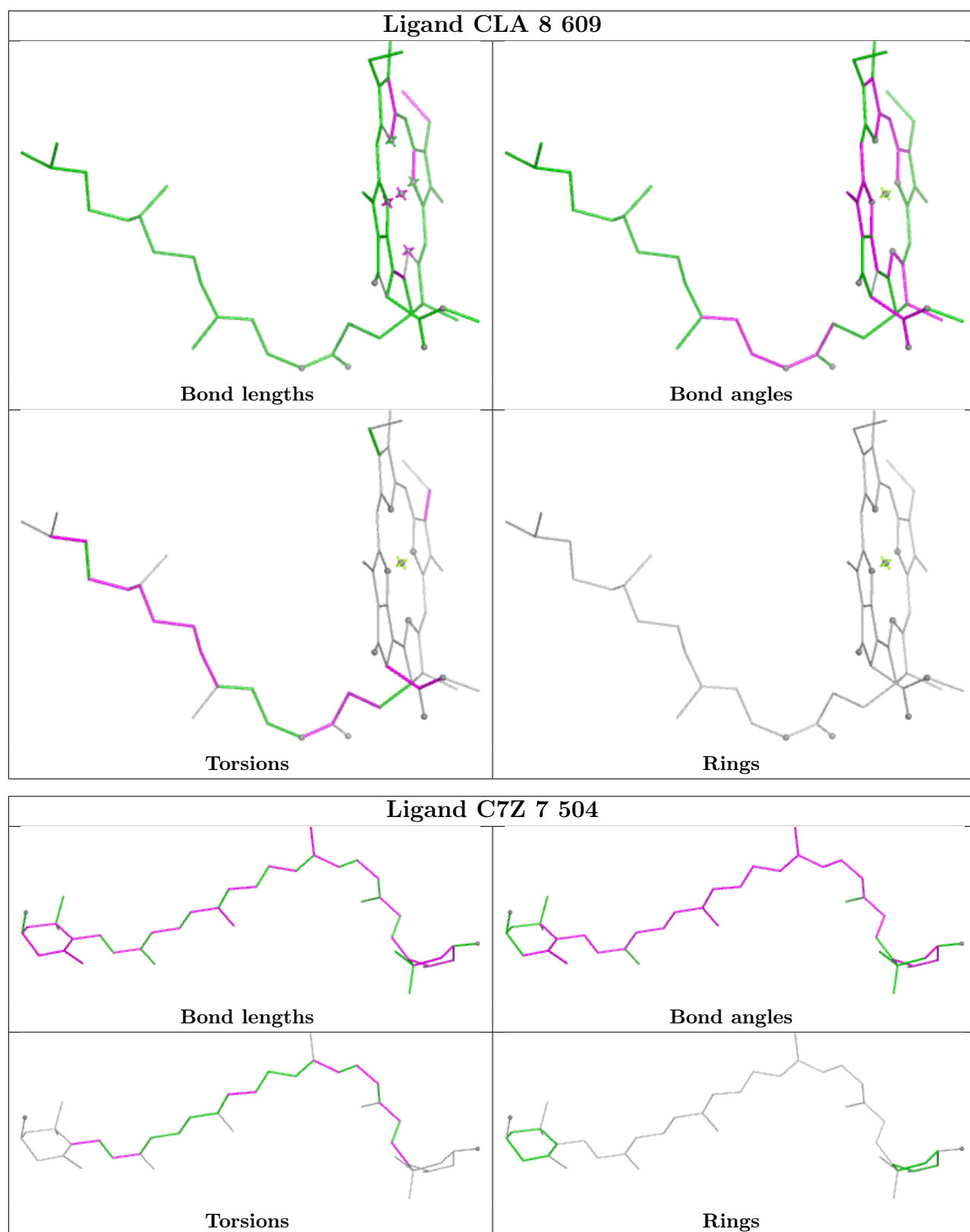
Bond angles

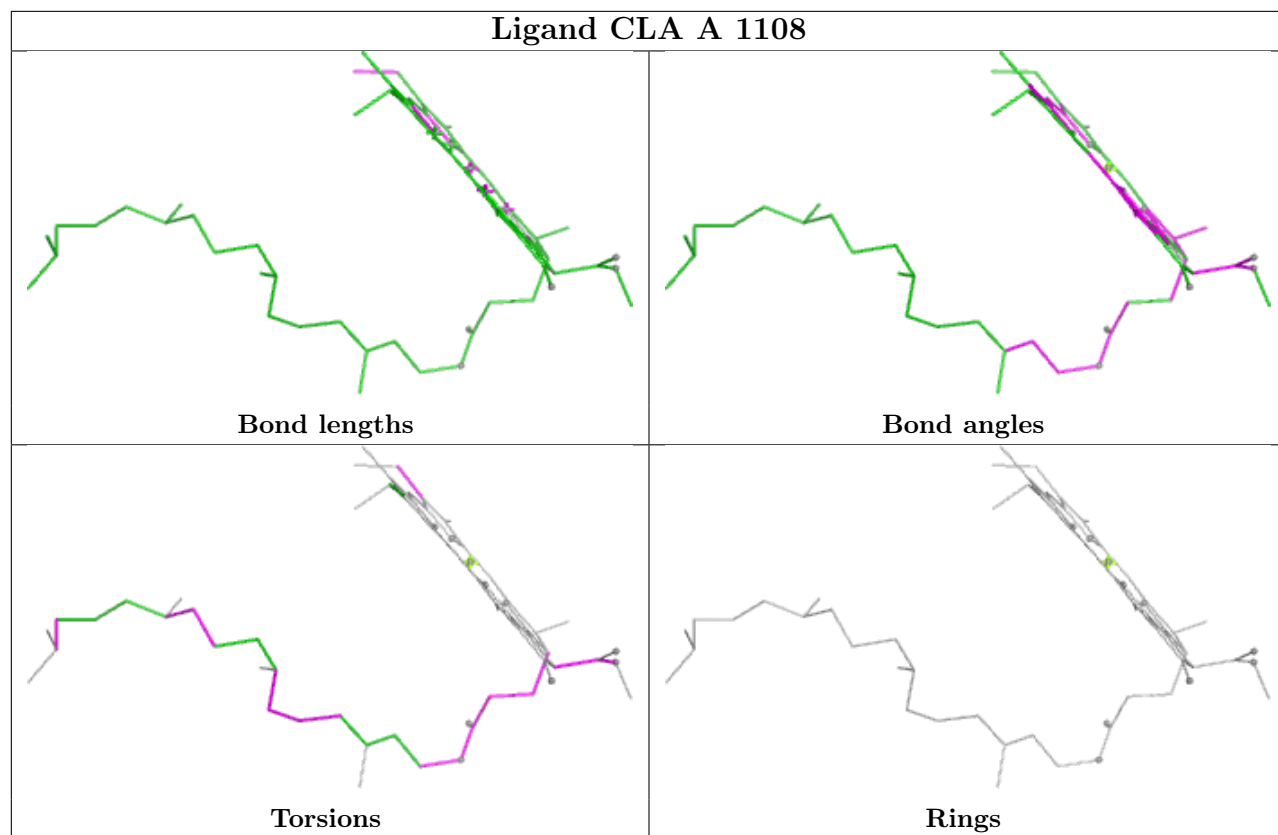


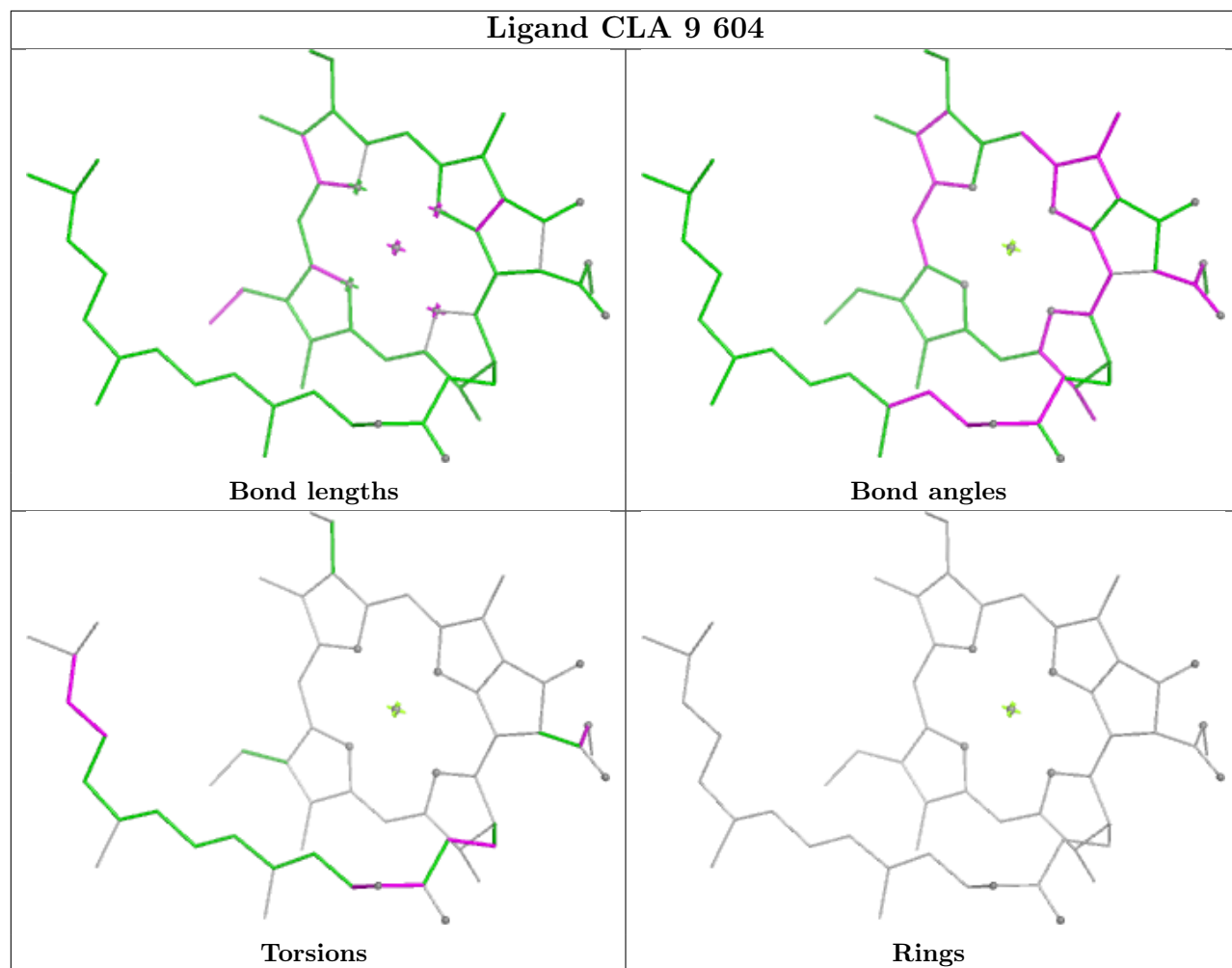
Torsions

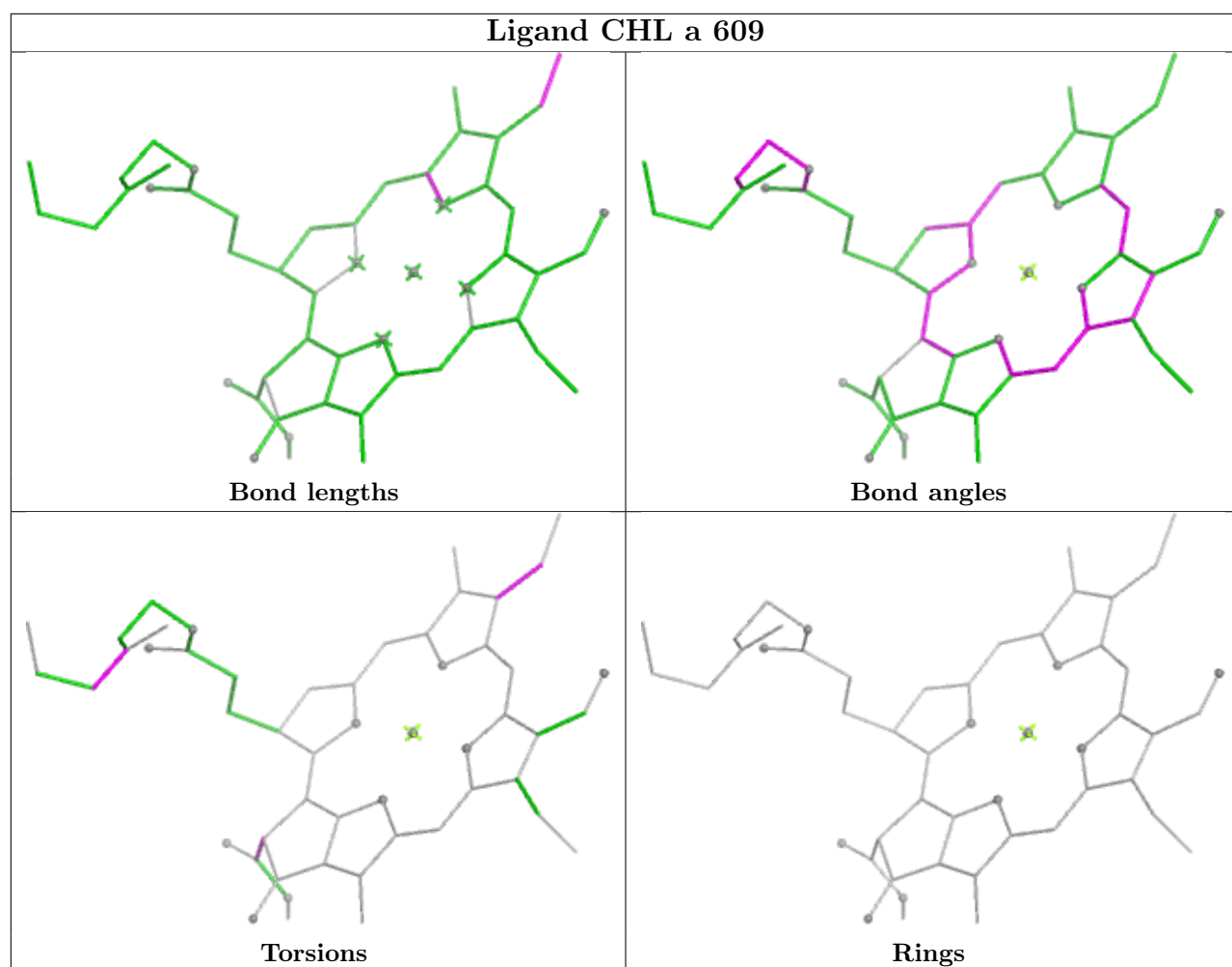


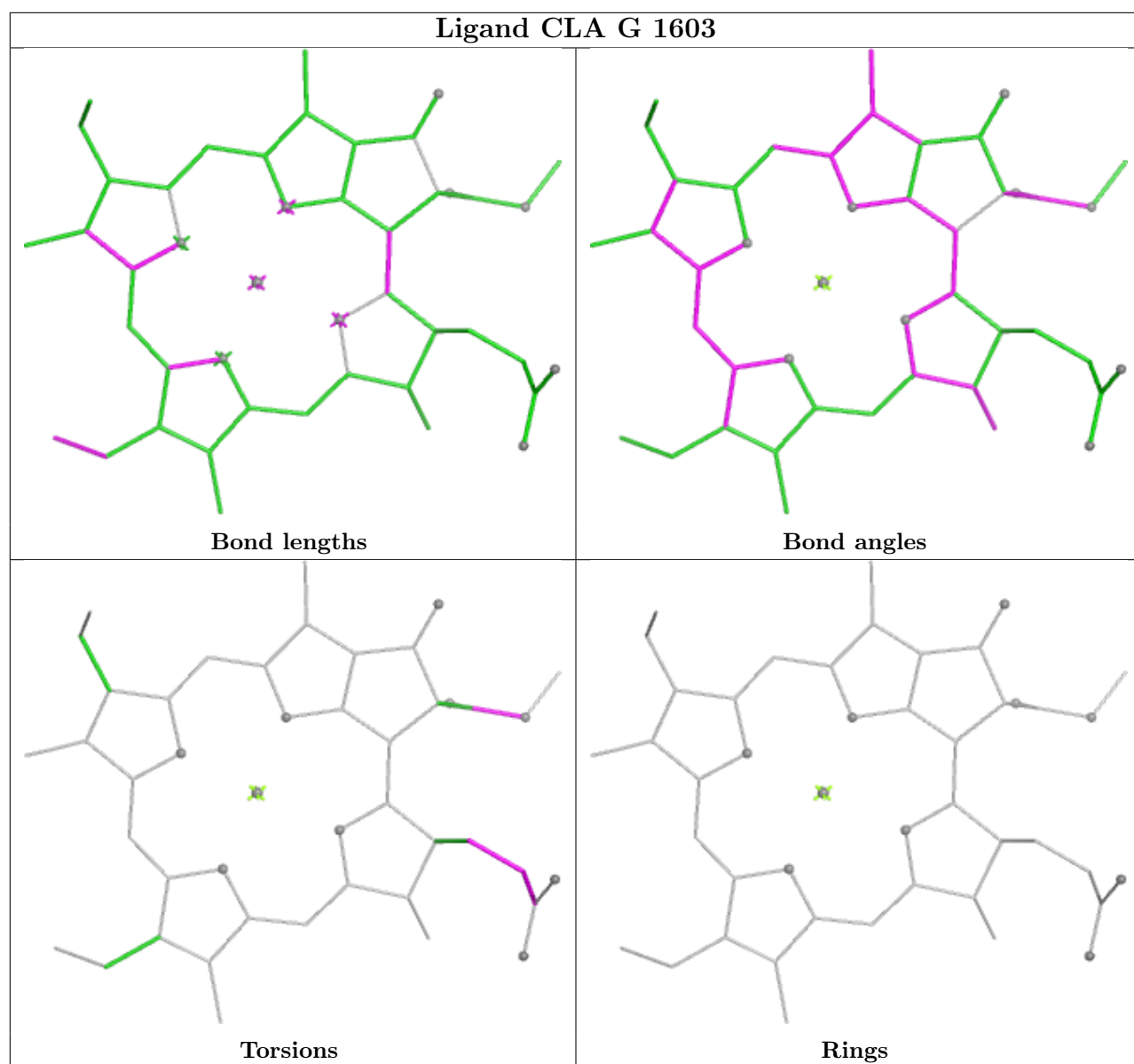
Rings



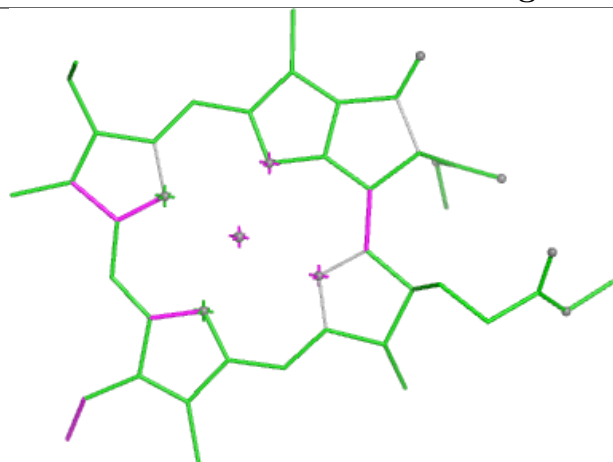




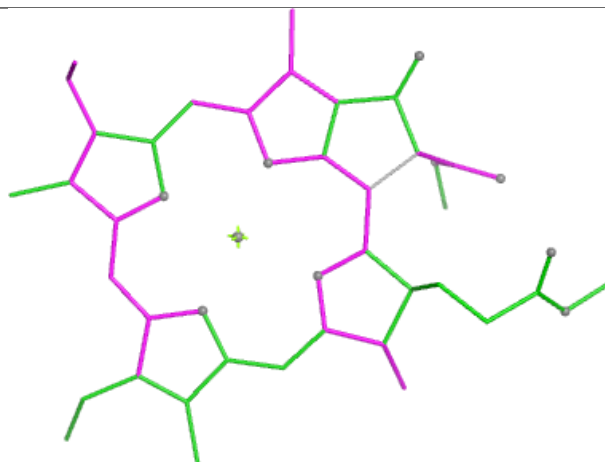




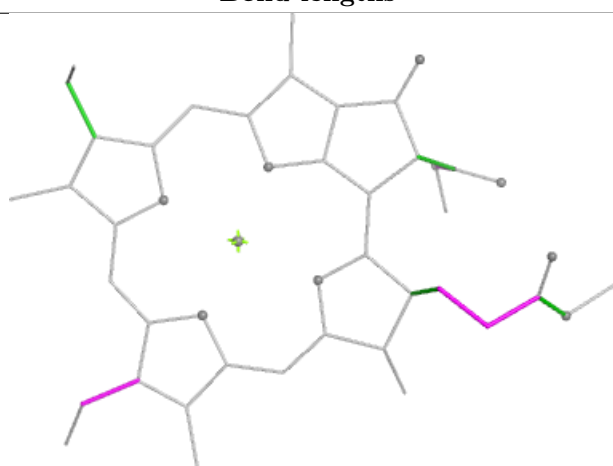
Ligand CLA 6 605



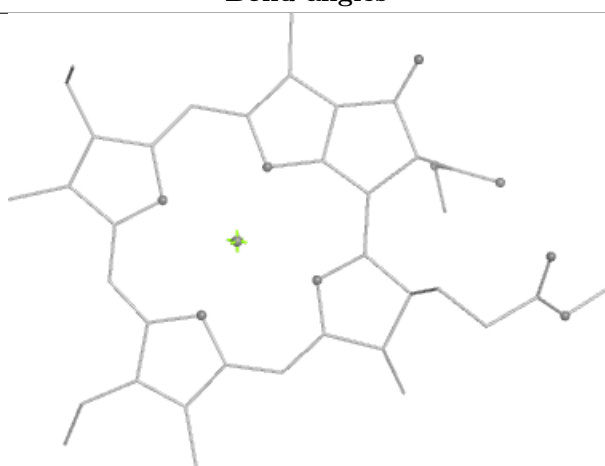
Bond lengths



Bond angles

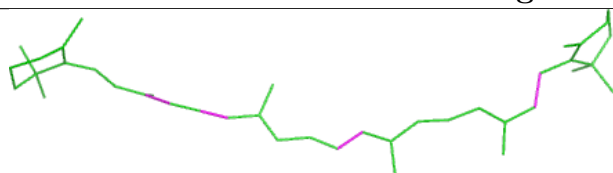


Torsions

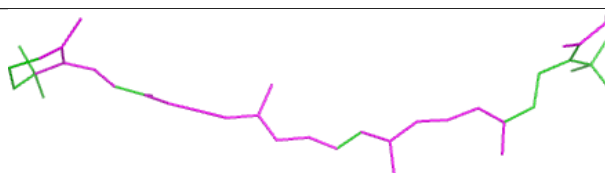


Rings

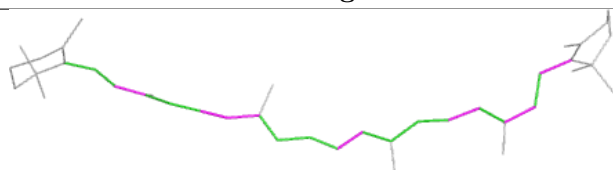
Ligand BCR 5 504



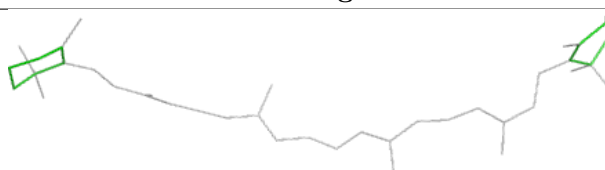
Bond lengths



Bond angles

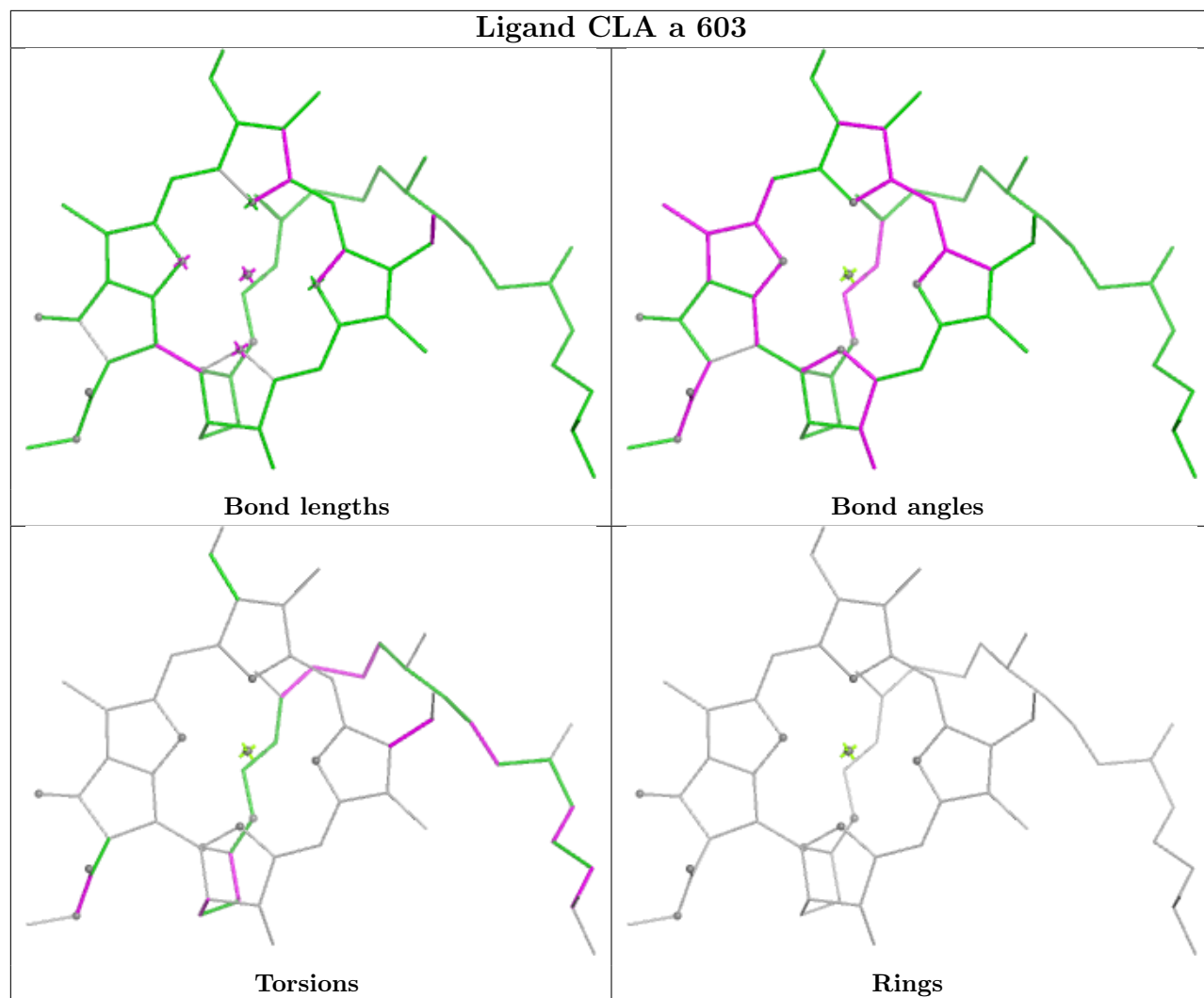


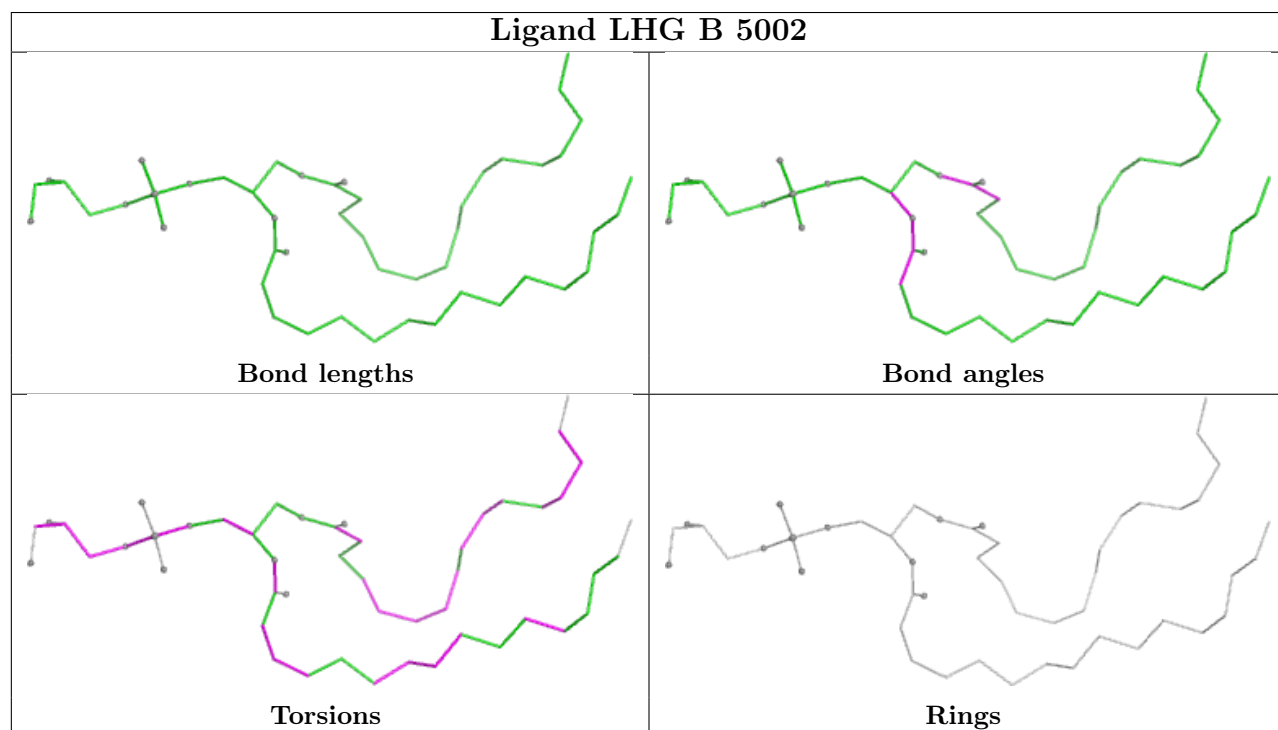
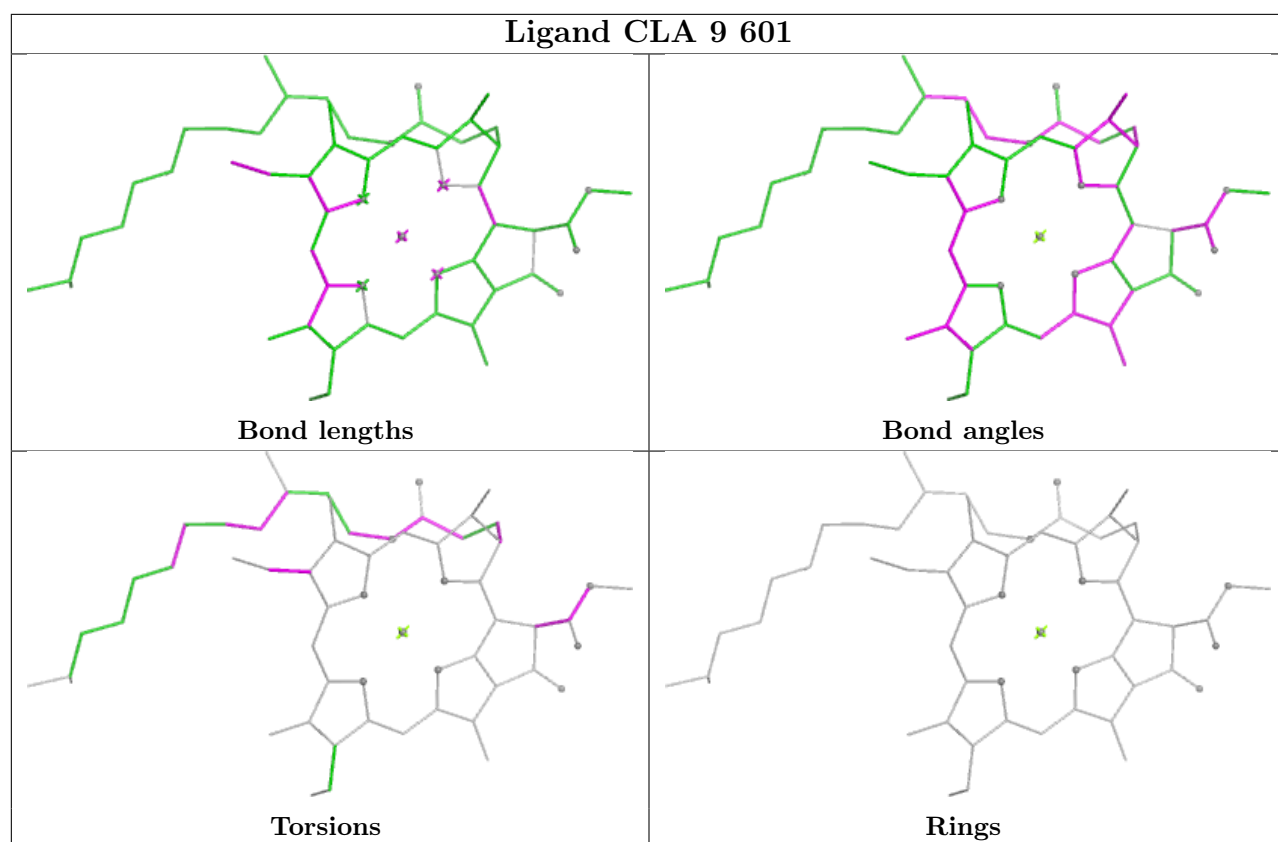
Torsions

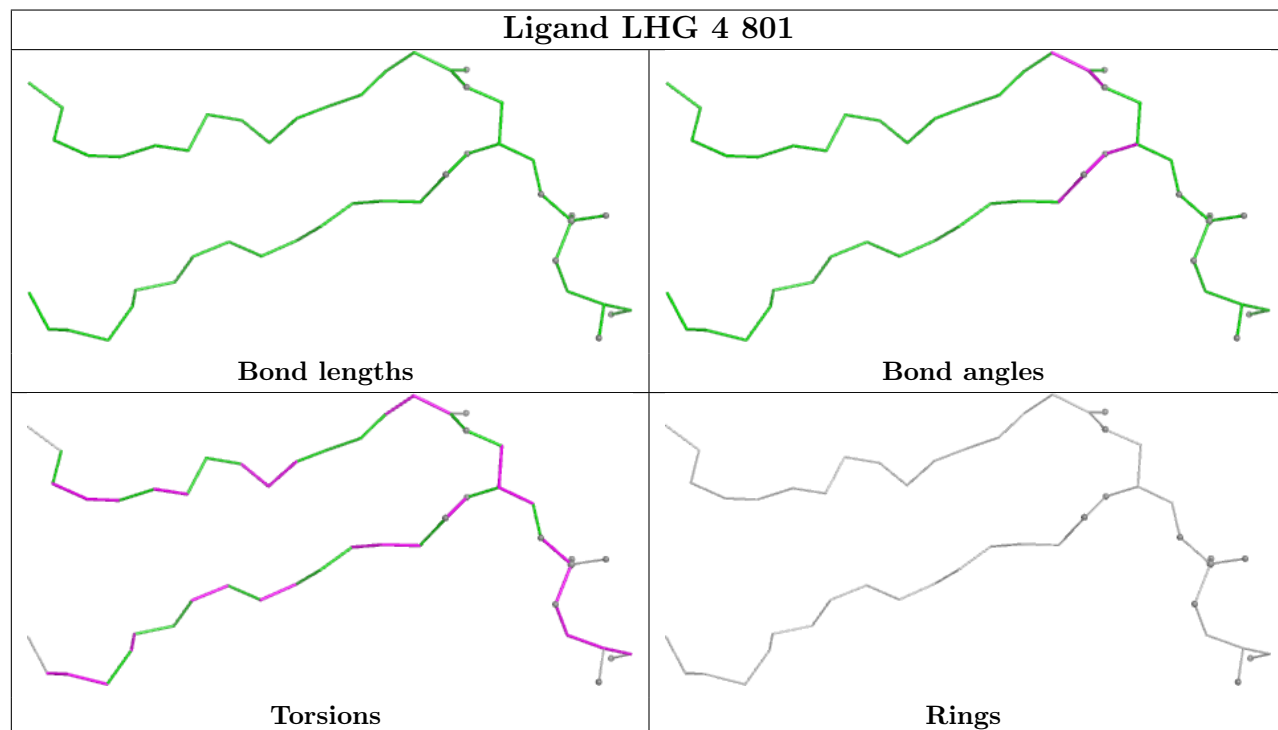
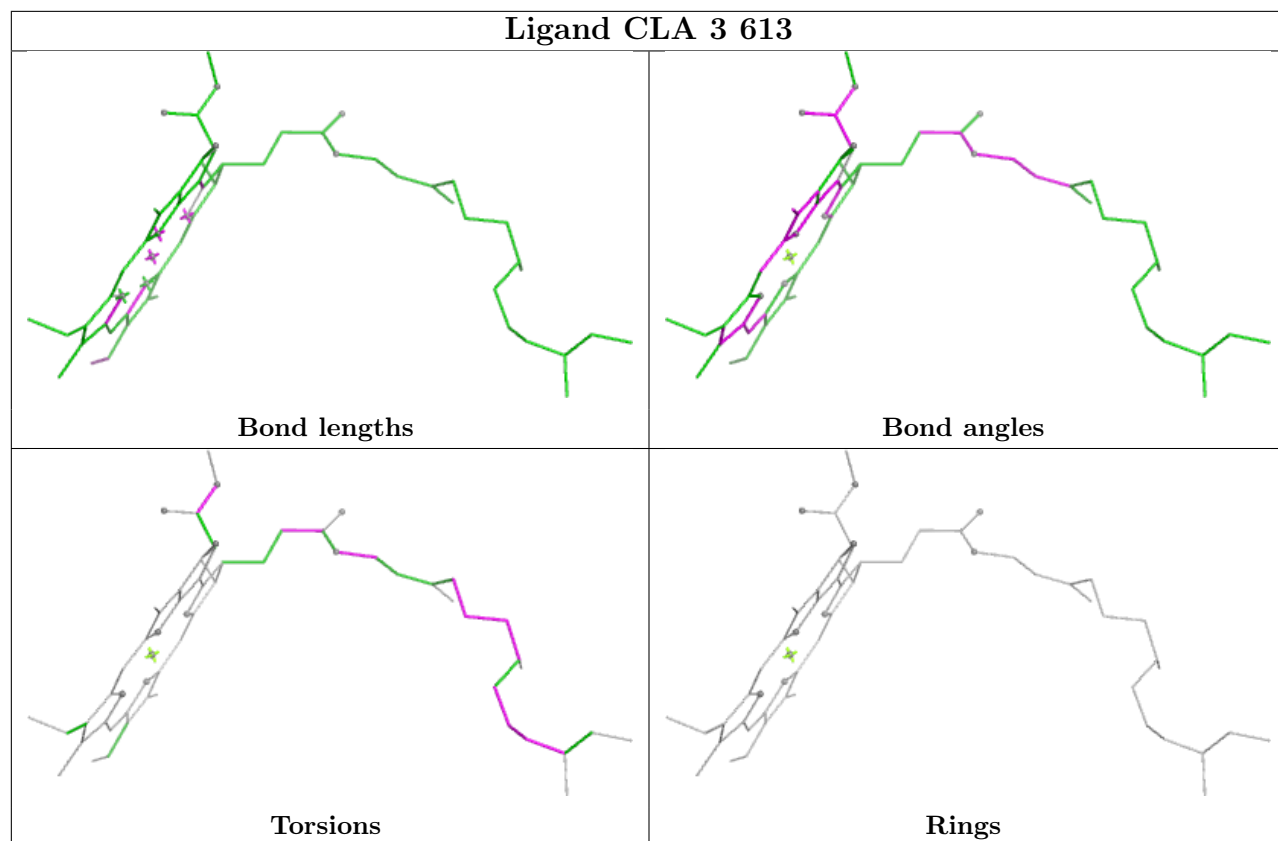


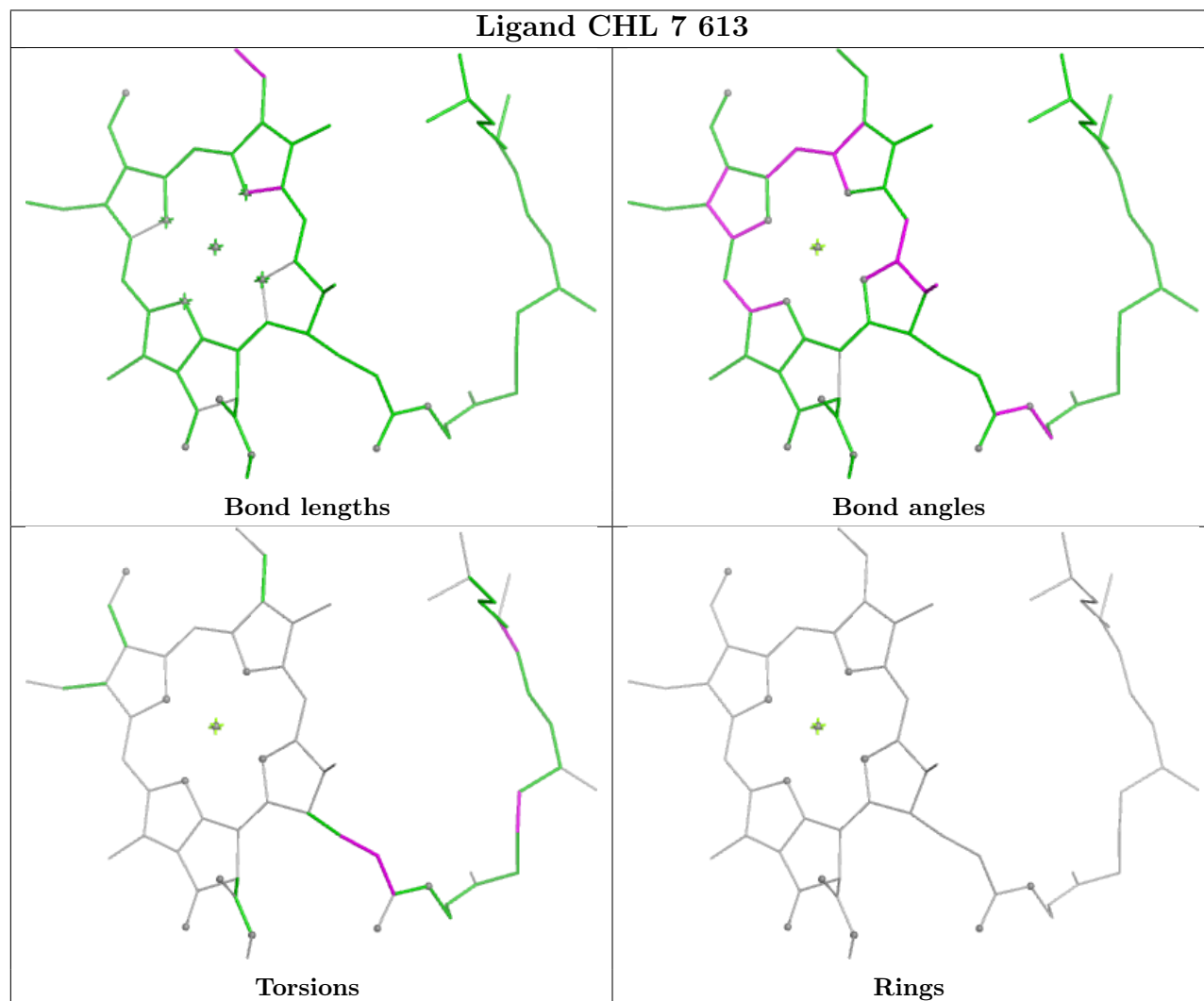
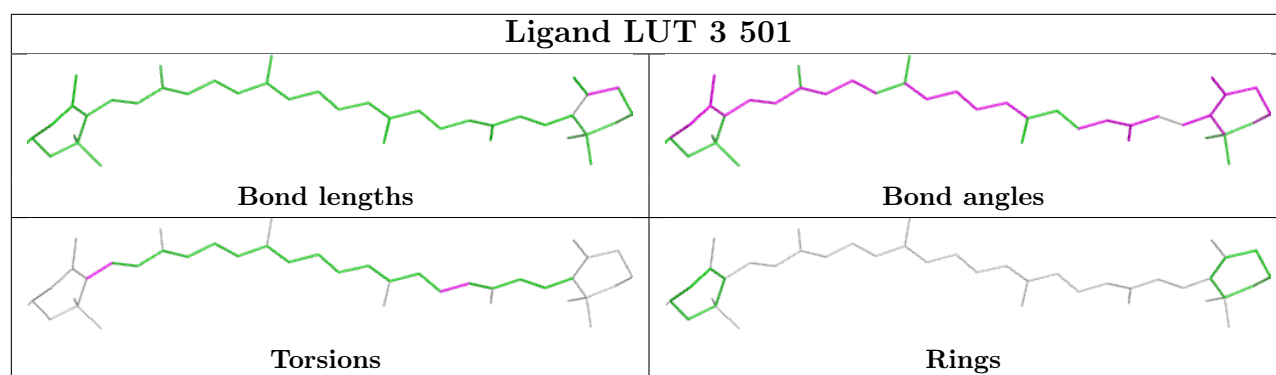
Rings

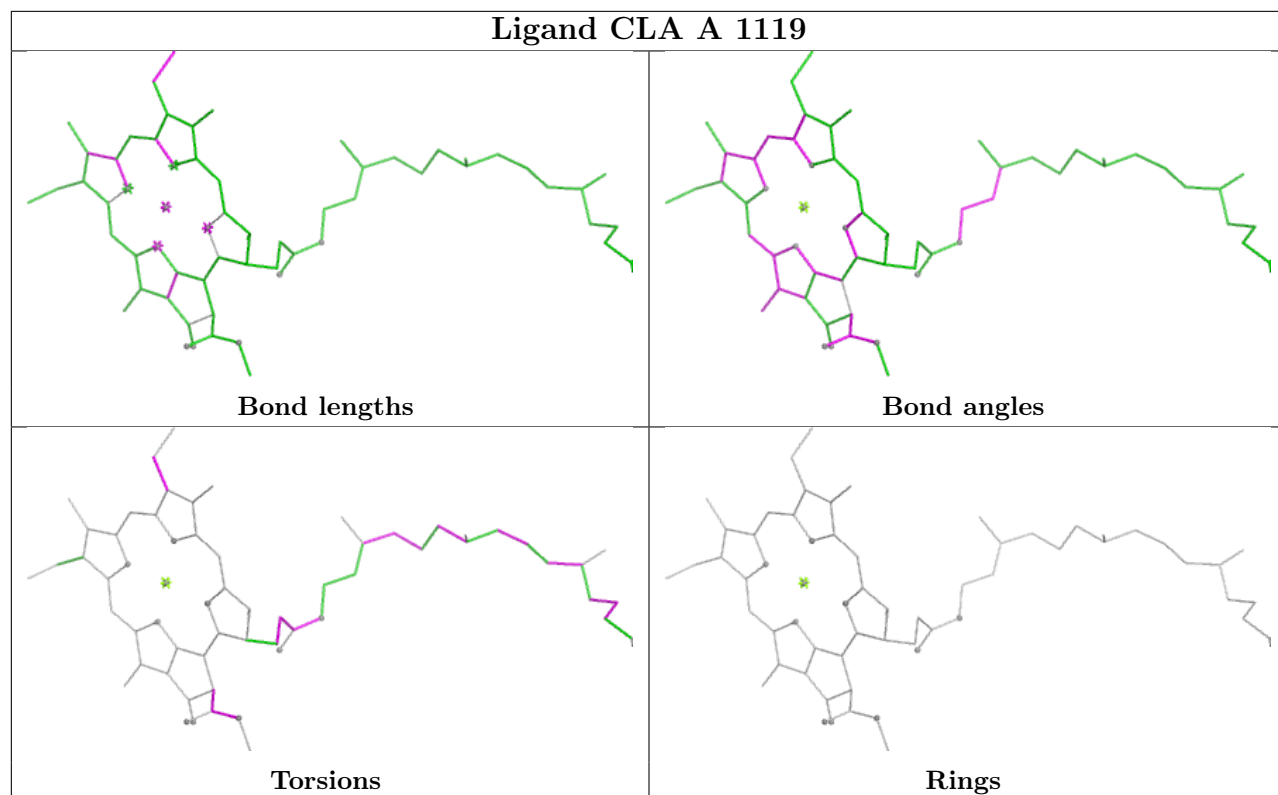
Ligand CLA a 603

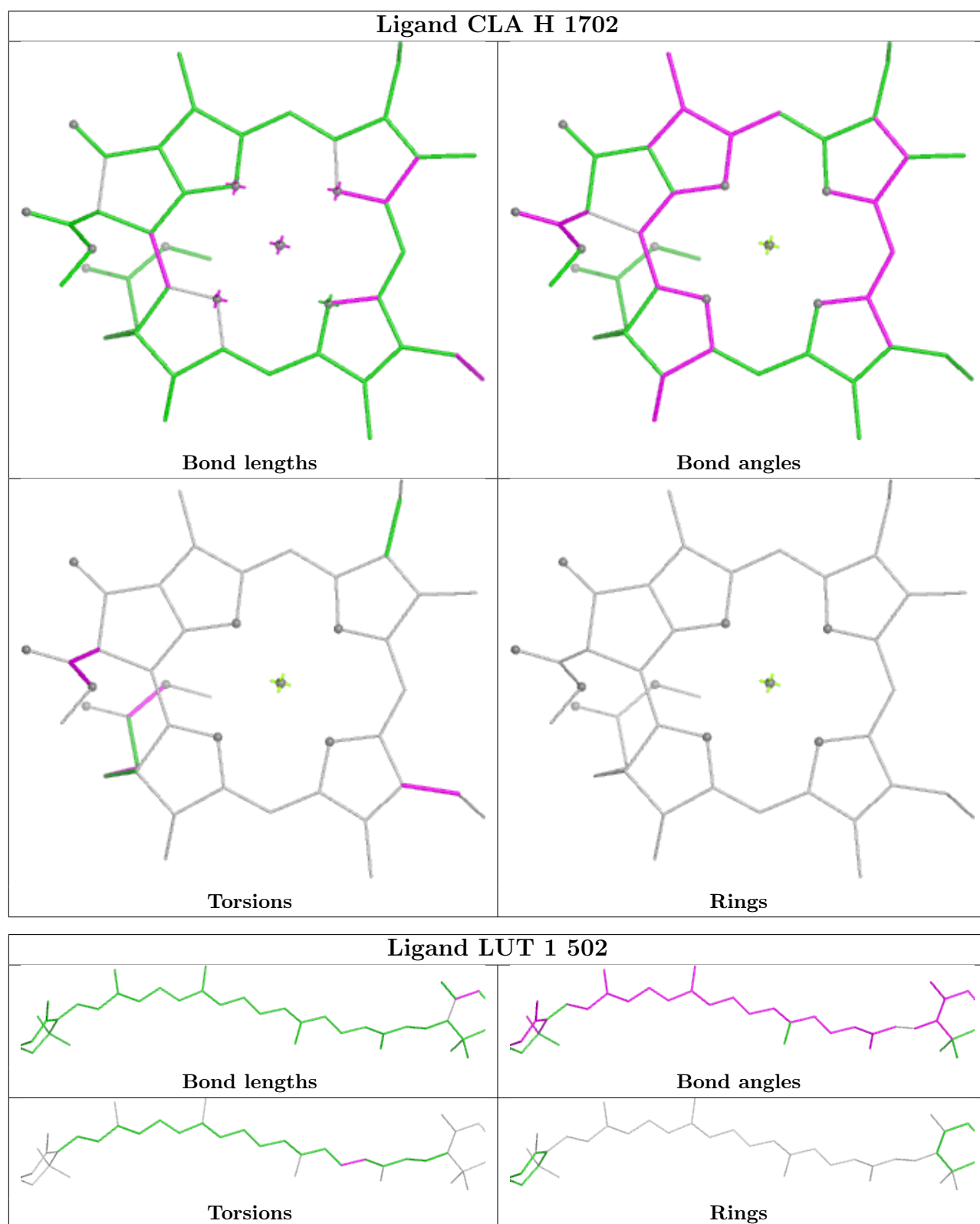


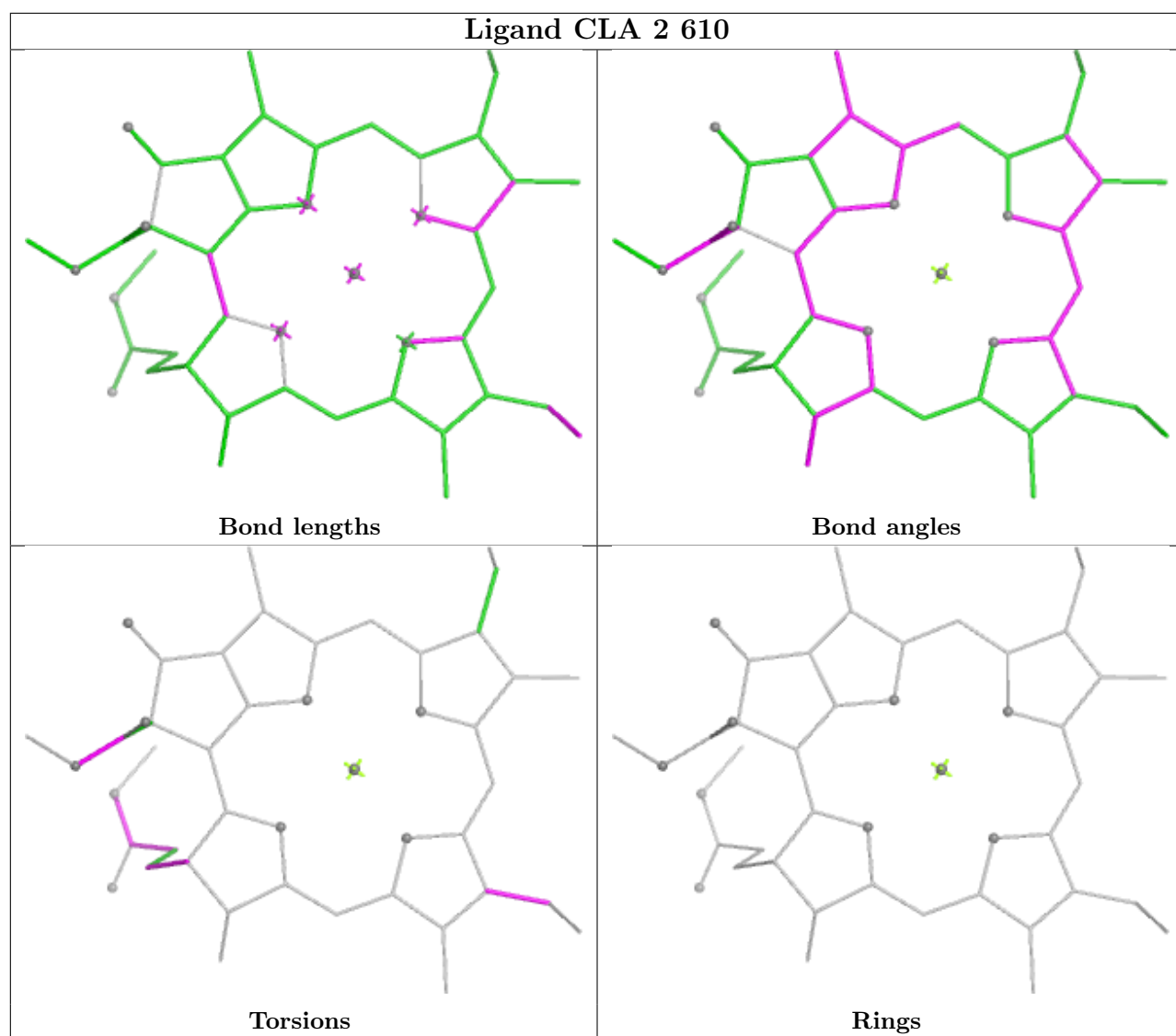


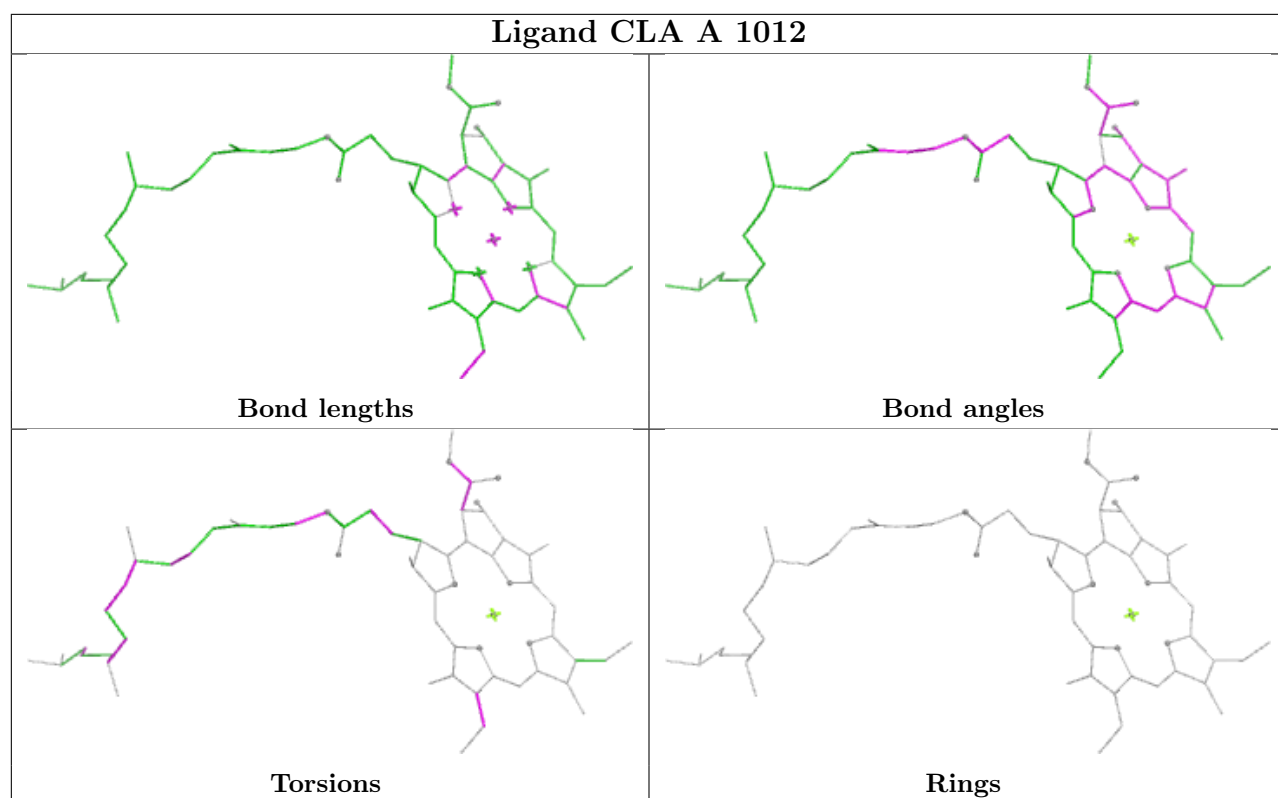




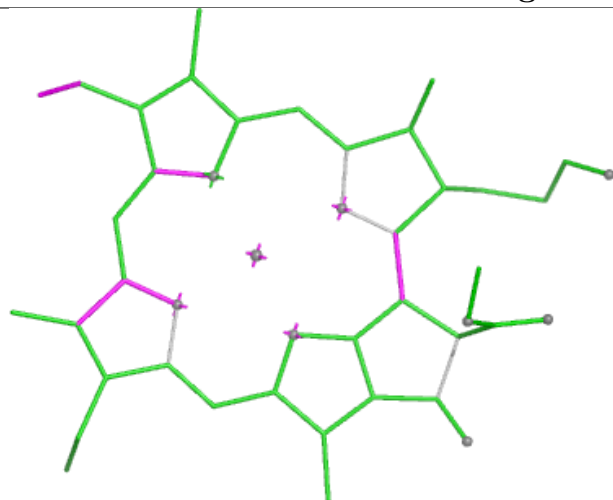




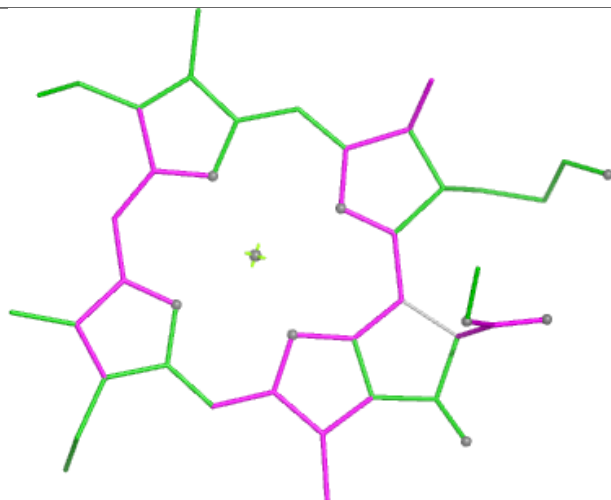




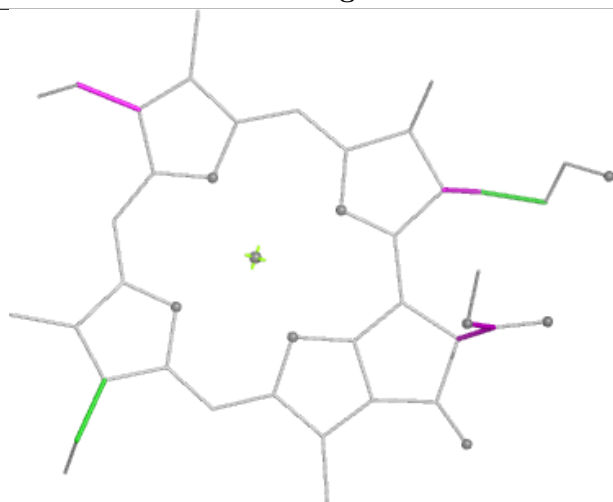
Ligand CLA 7 602



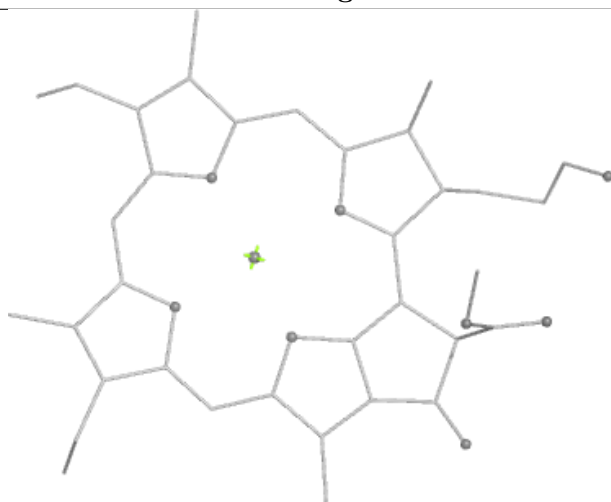
Bond lengths



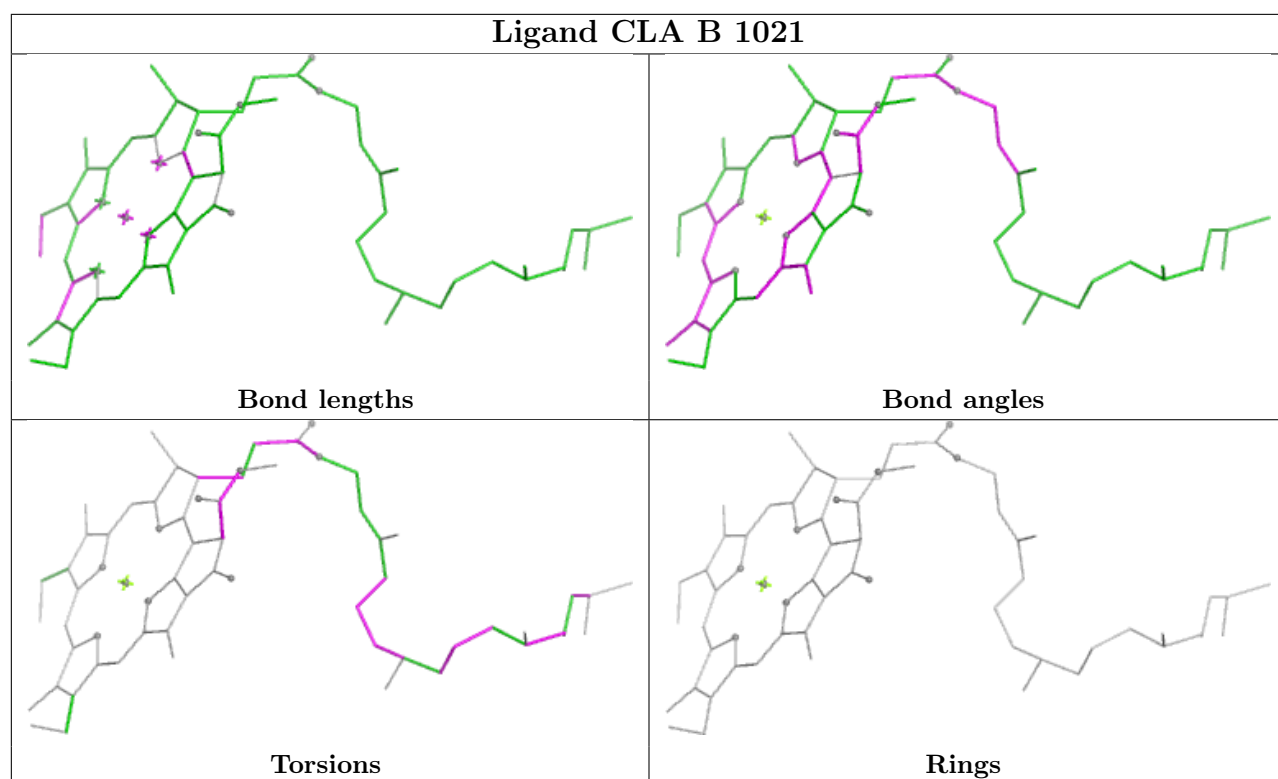
Bond angles

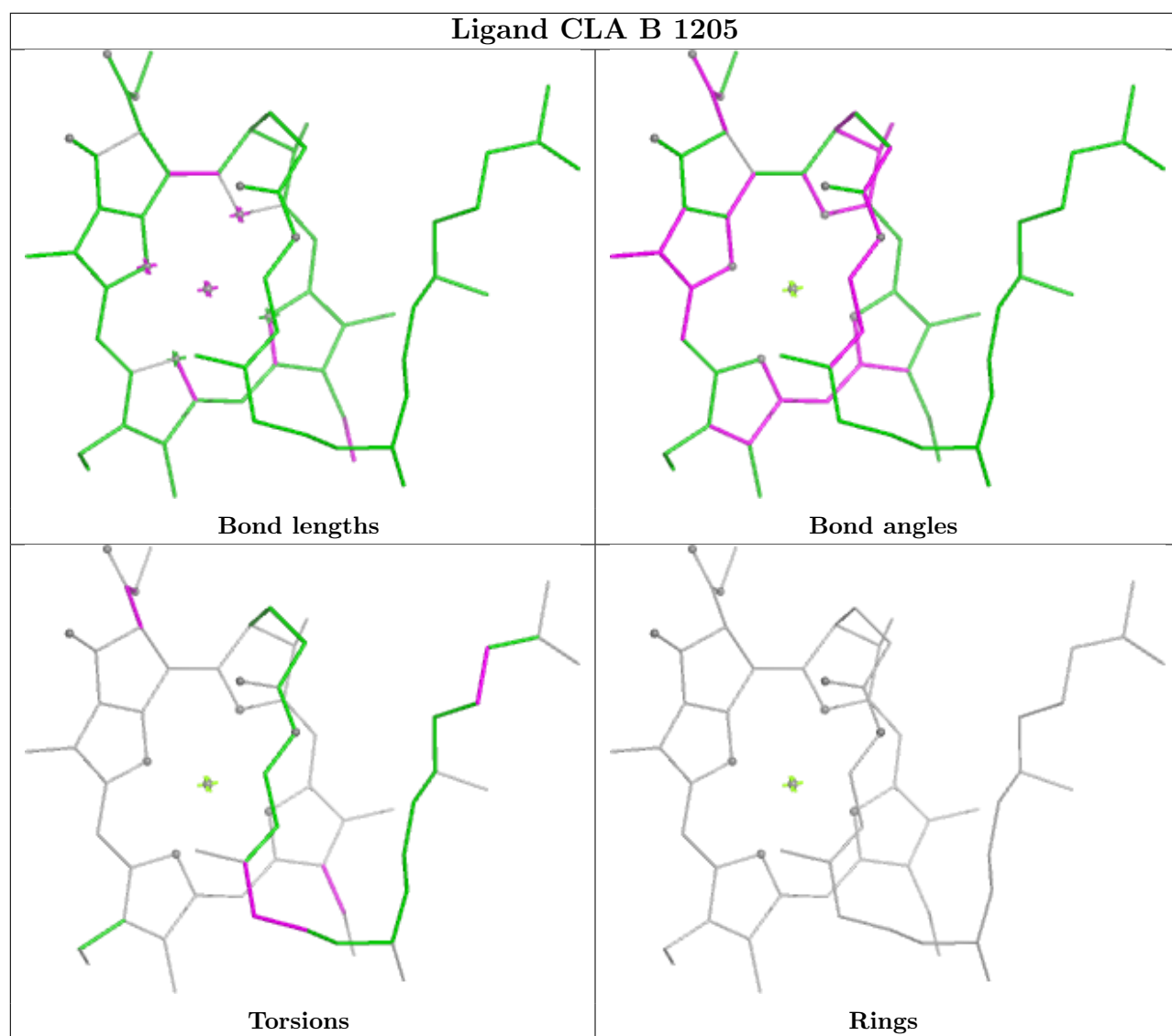


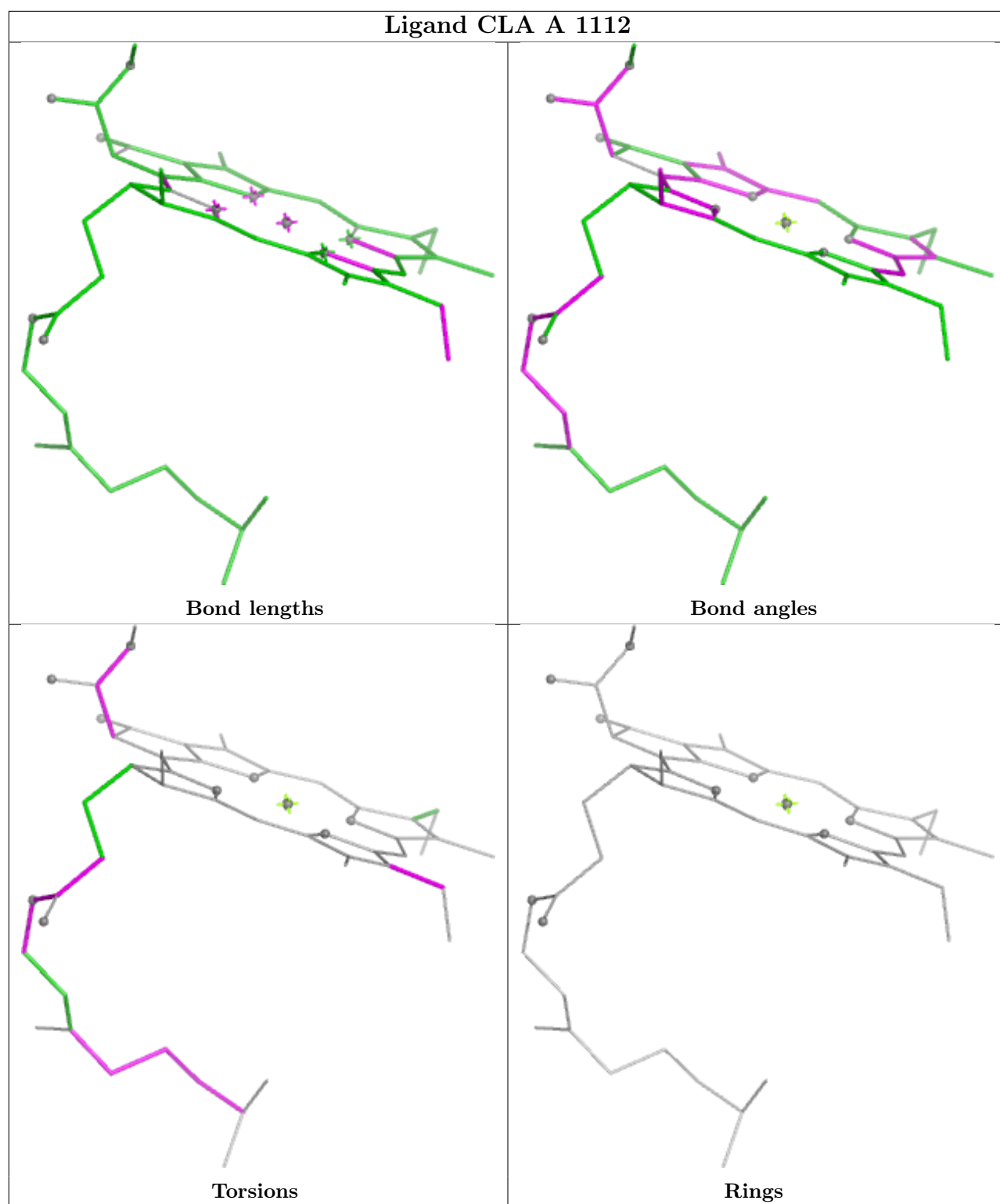
Torsions

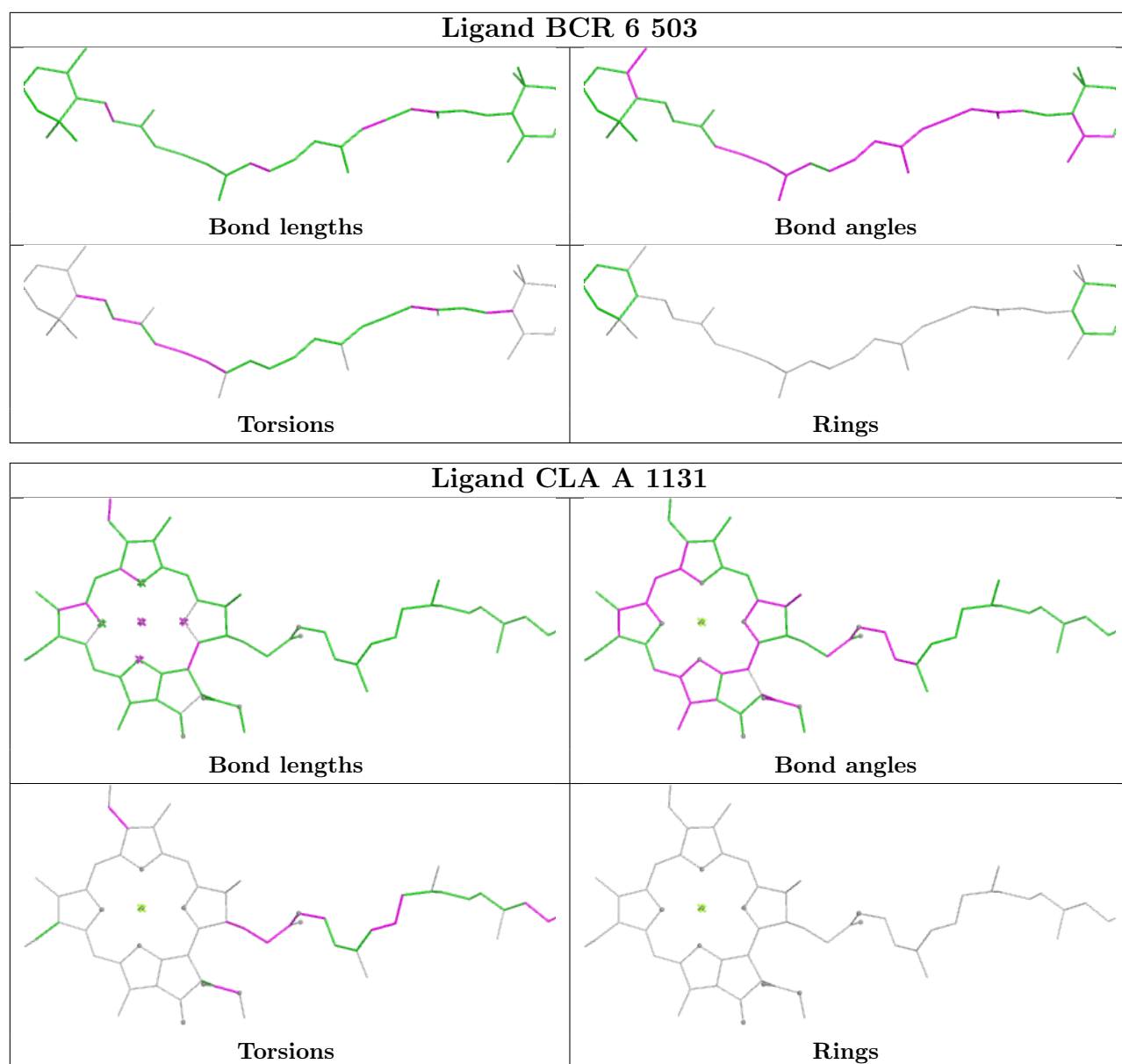


Rings

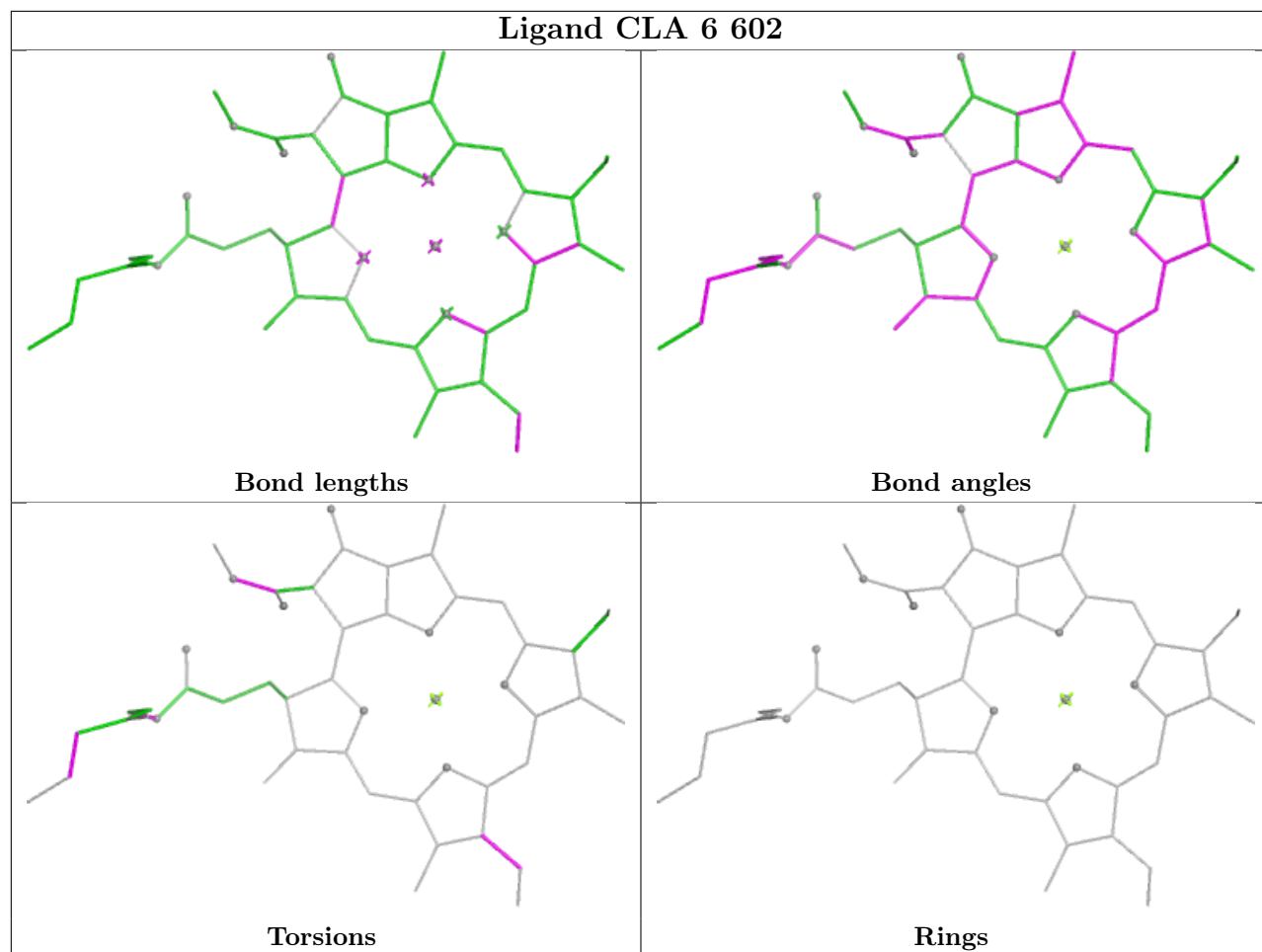




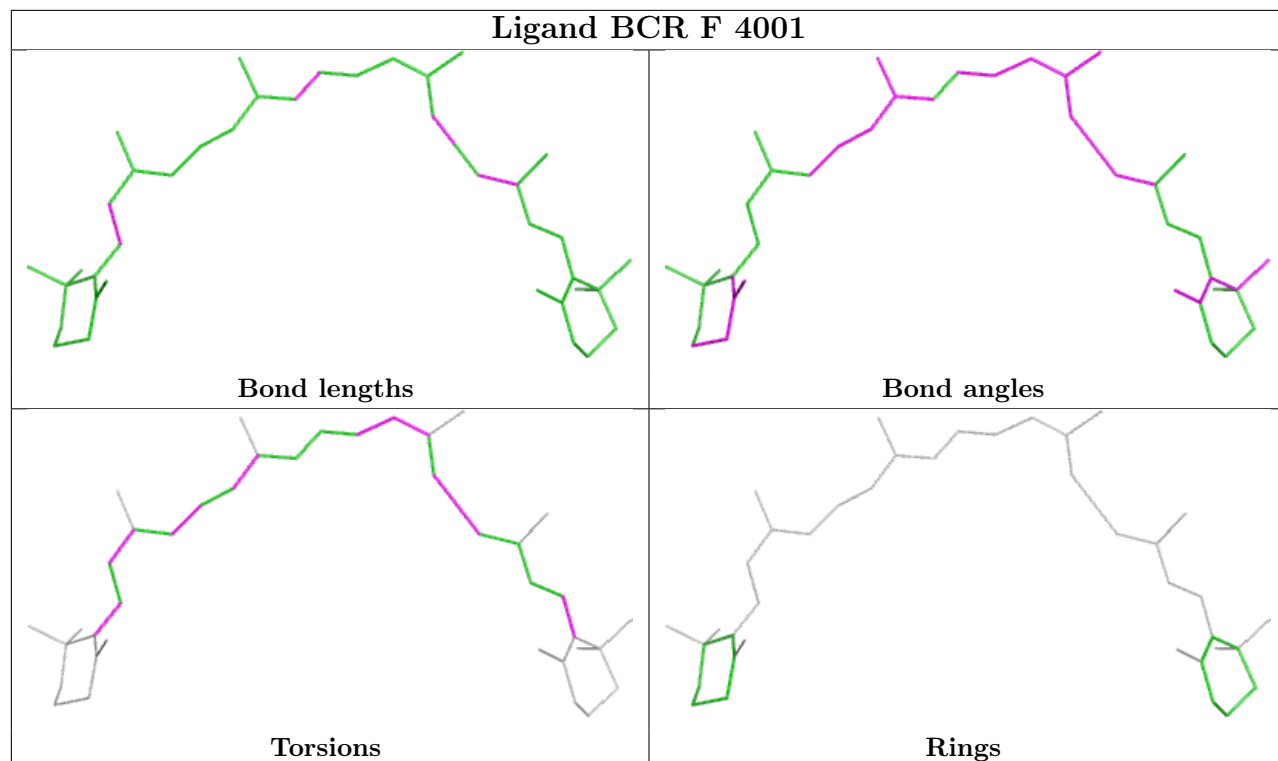


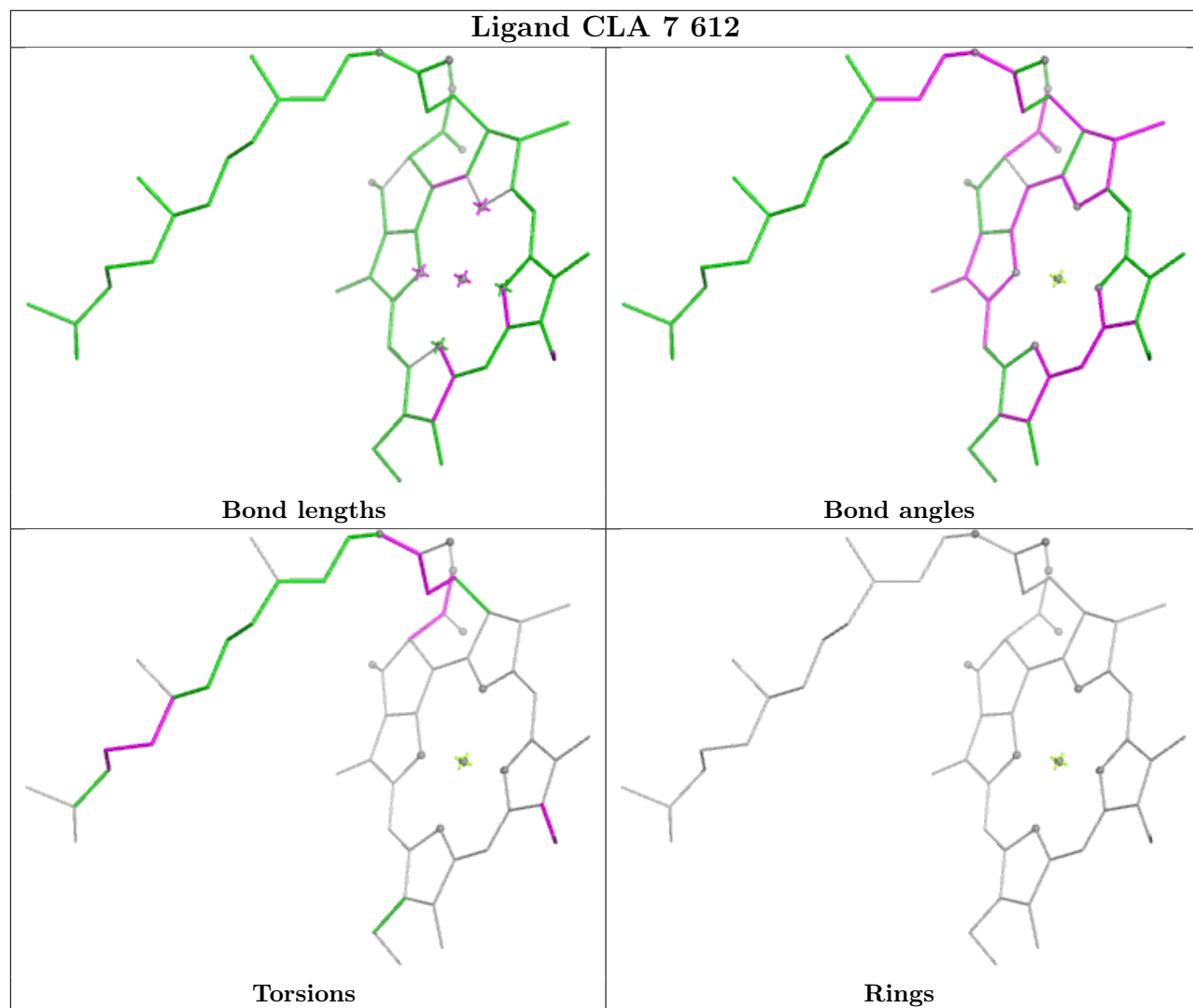
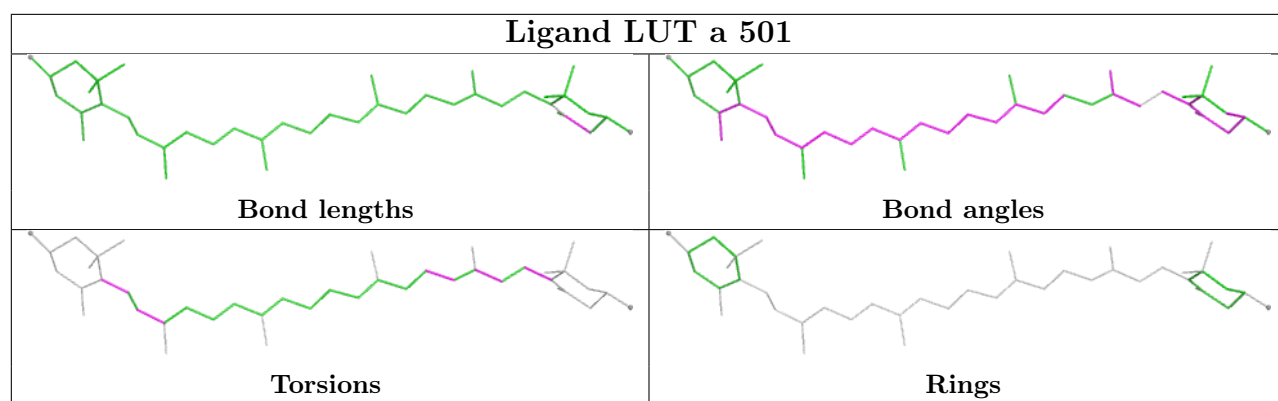


Ligand CLA 6 602

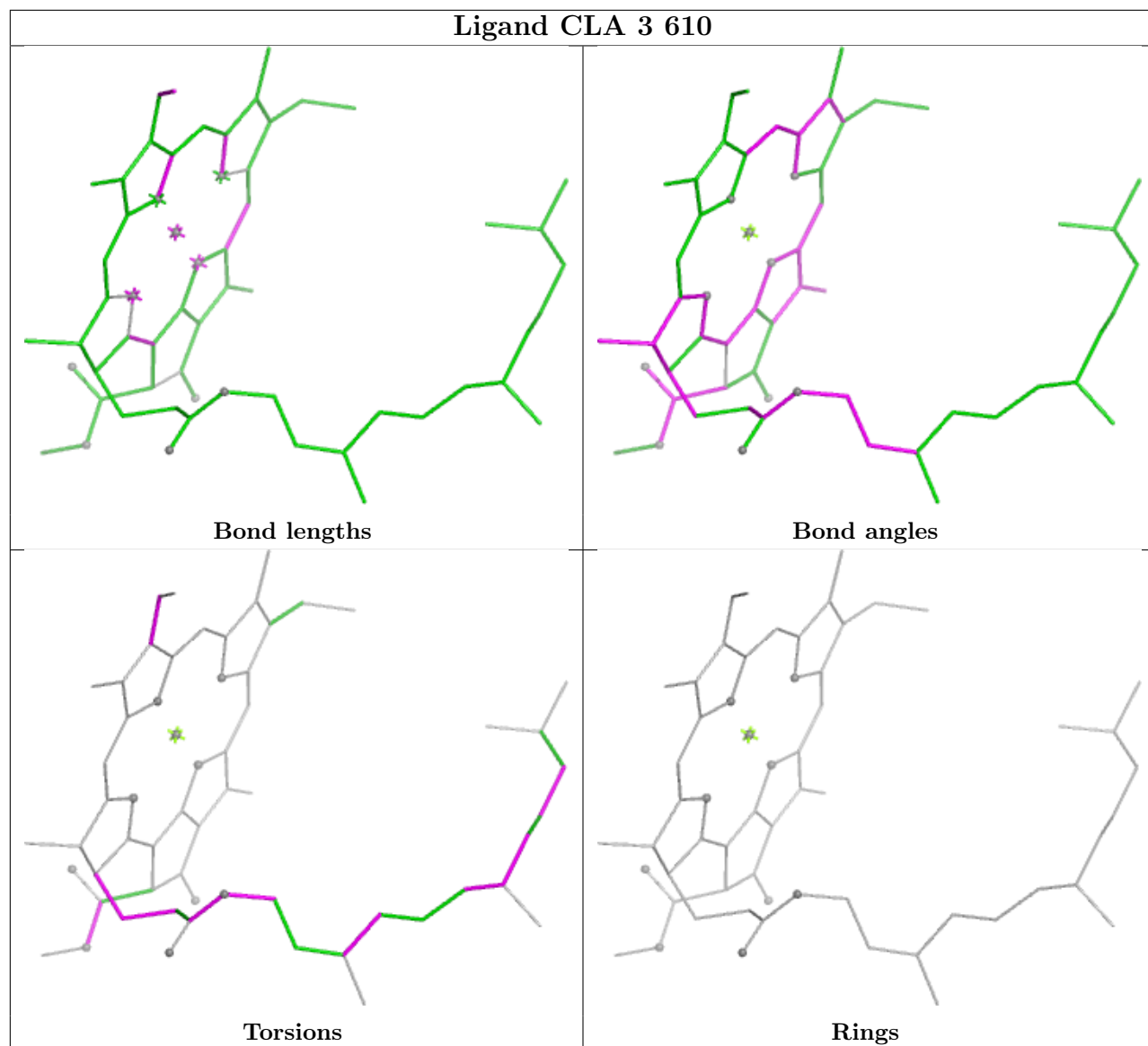


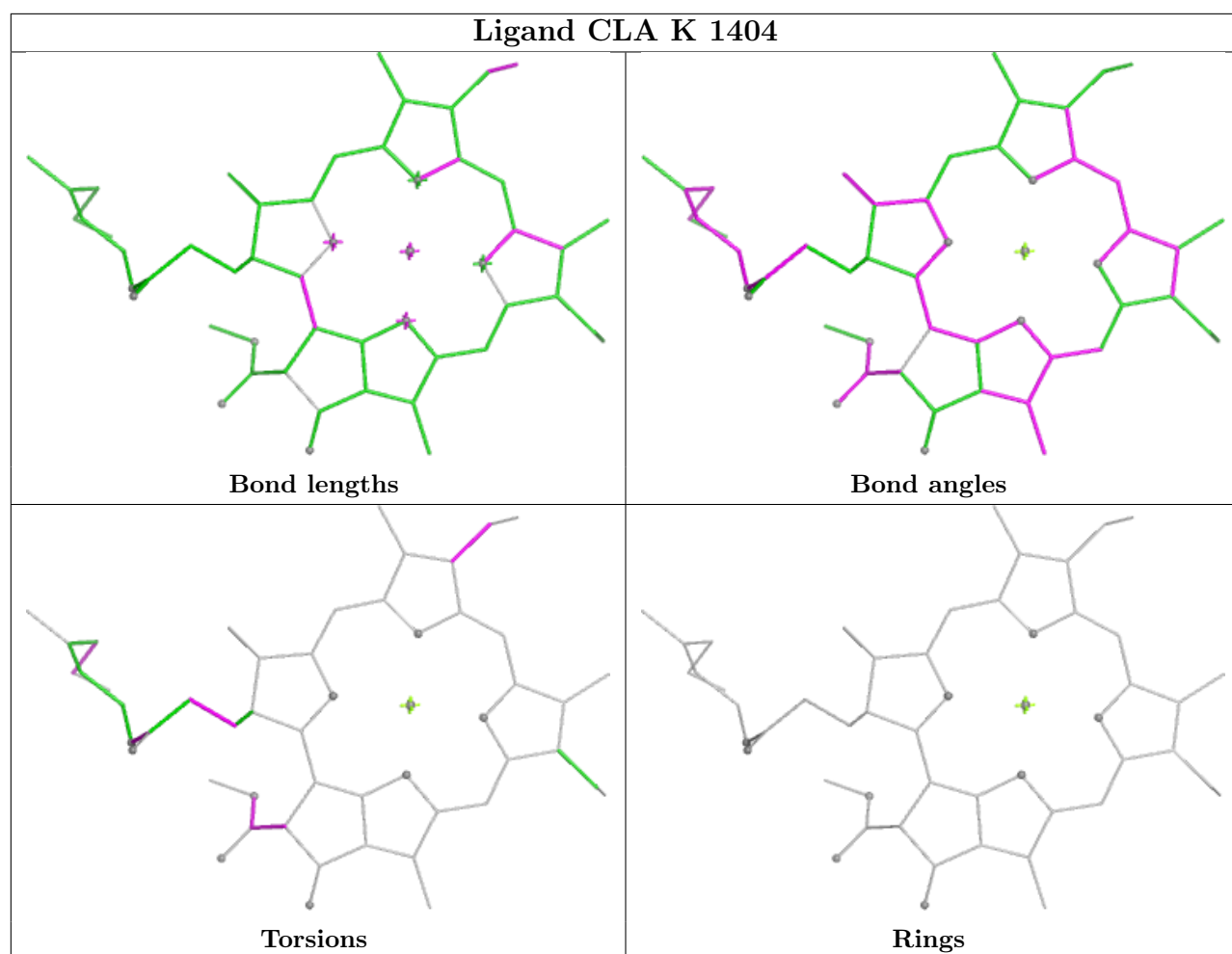
Ligand BCR F 4001

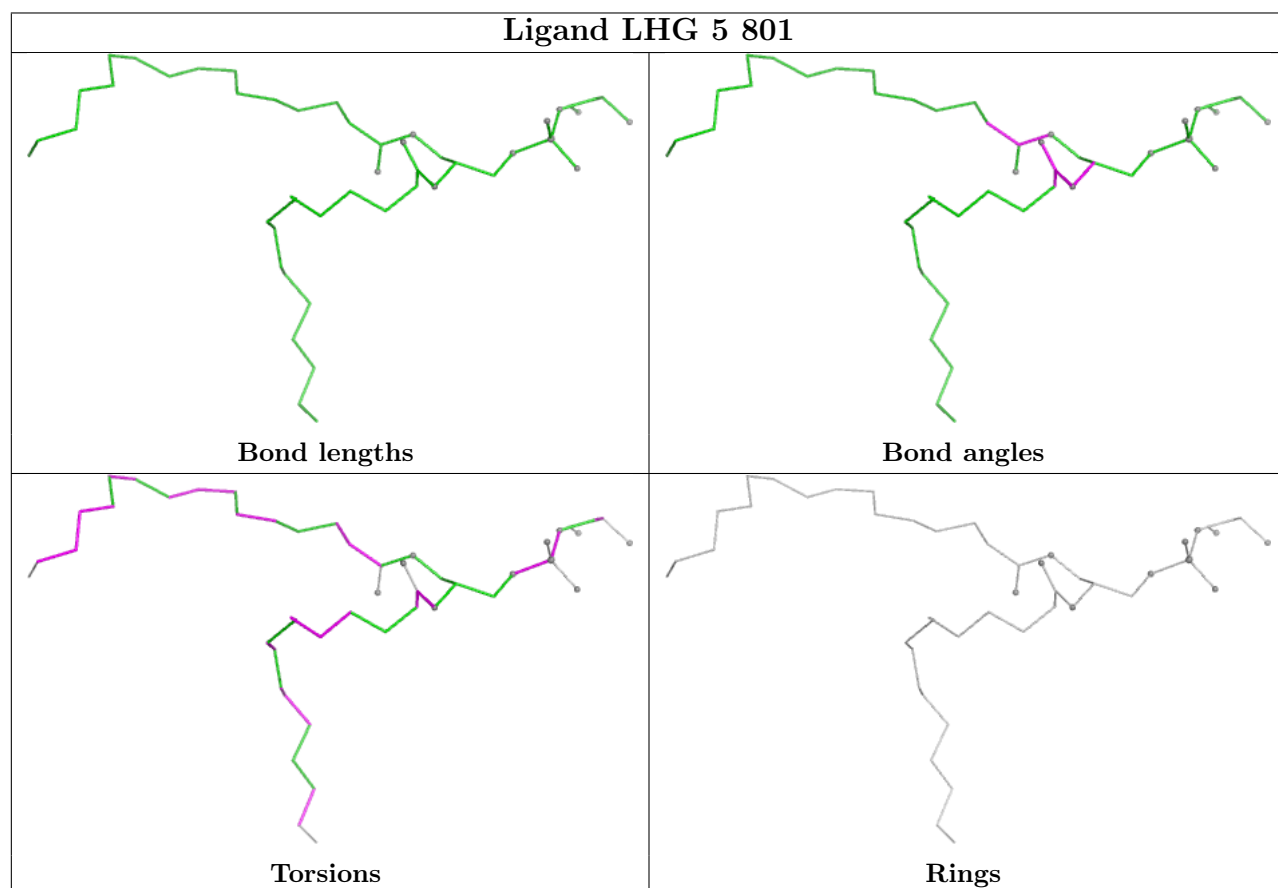
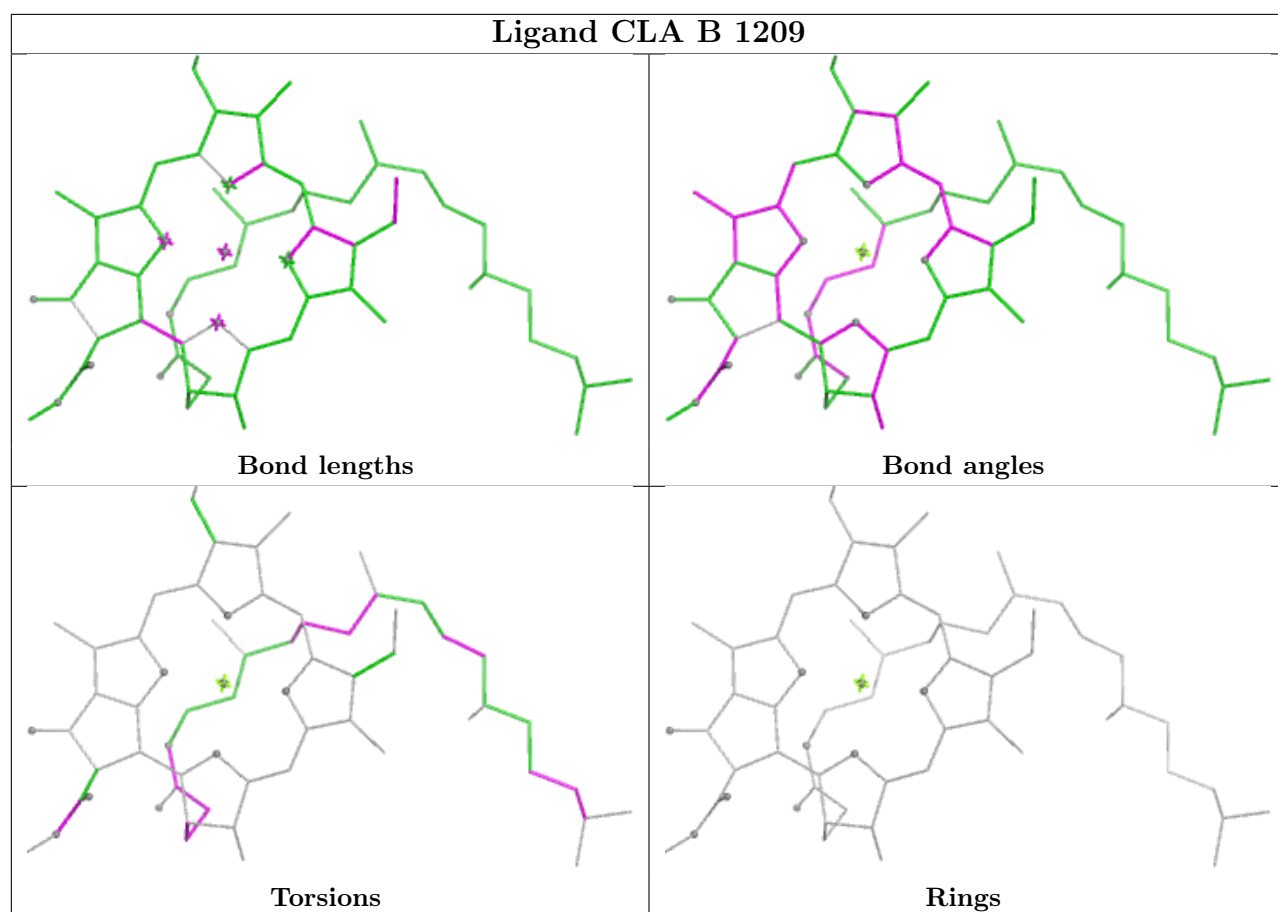


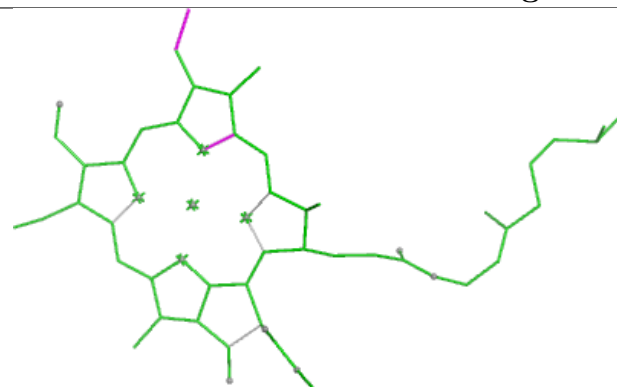
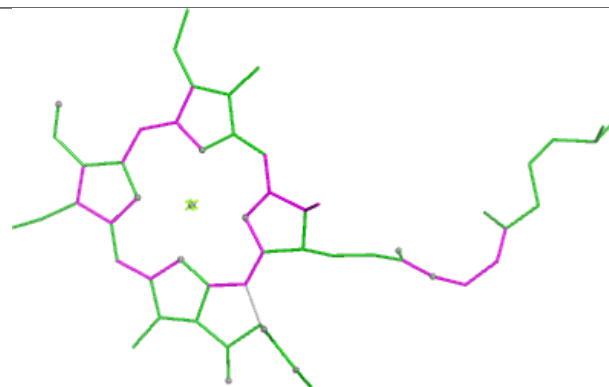
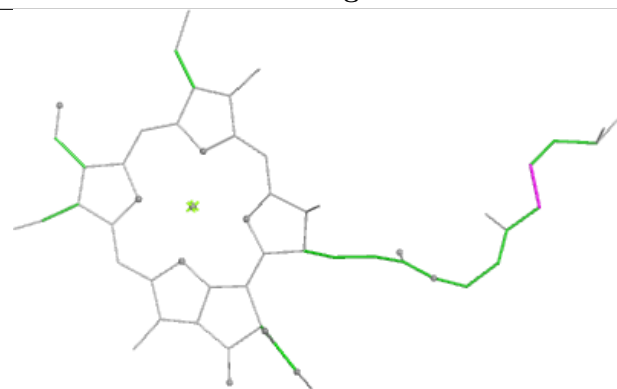


Ligand CLA 3 610

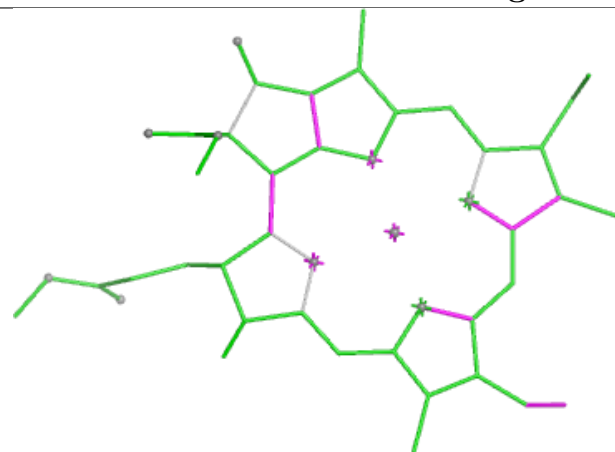




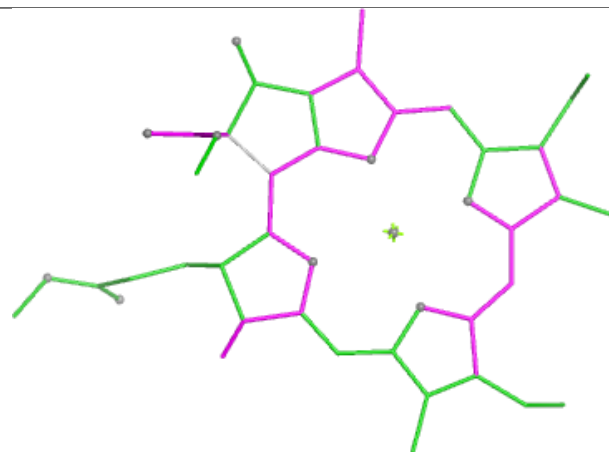


Ligand CHL 5 613**Bond lengths****Bond angles****Torsions****Rings**

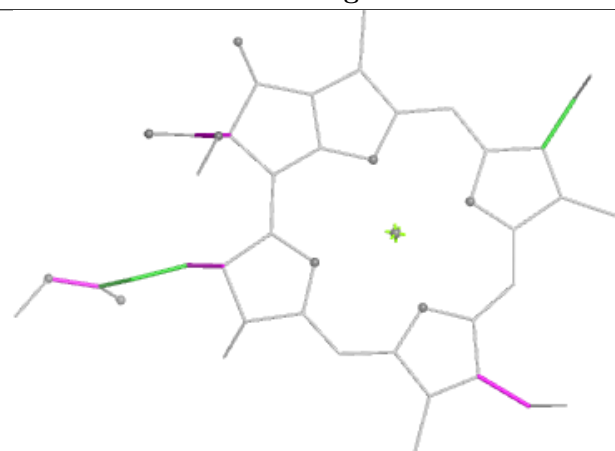
Ligand CLA K 1401



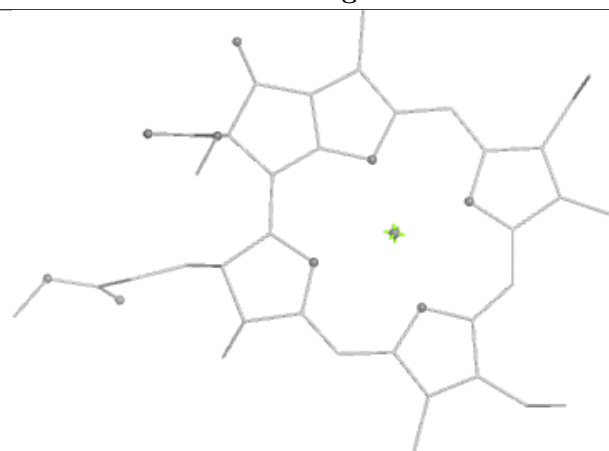
Bond lengths



Bond angles

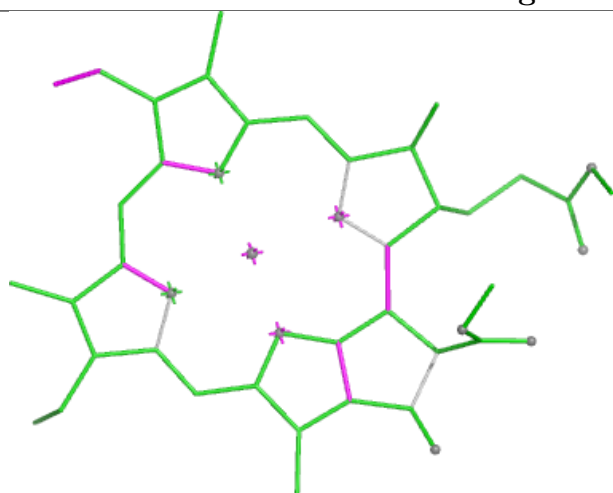


Torsions

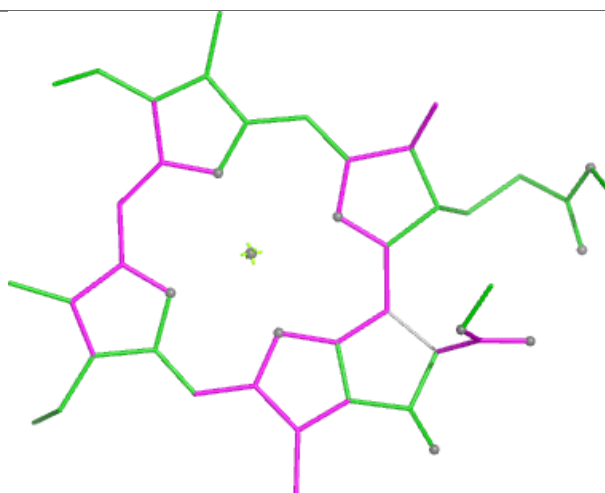


Rings

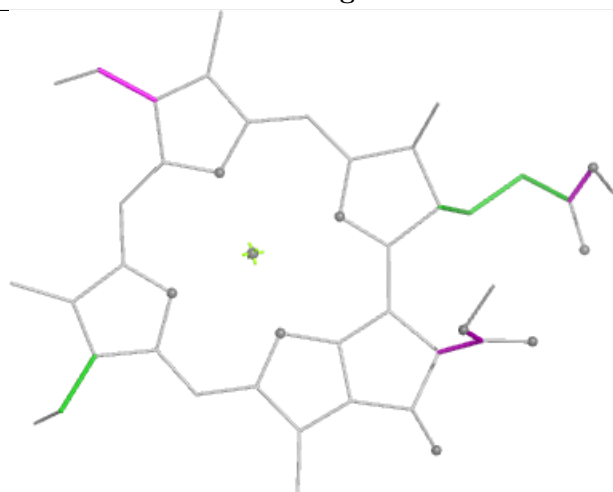
Ligand CLA 5 605



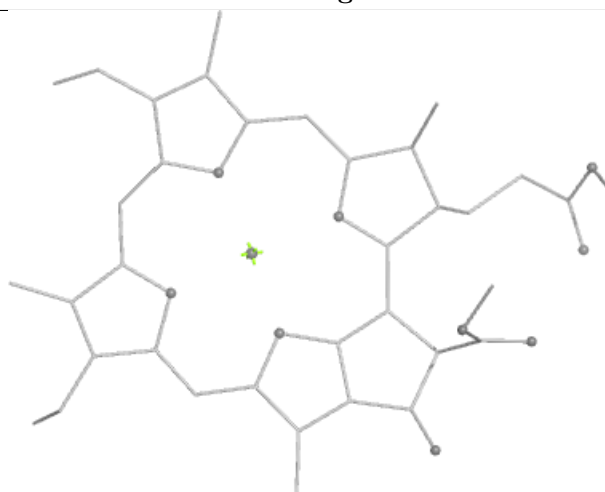
Bond lengths



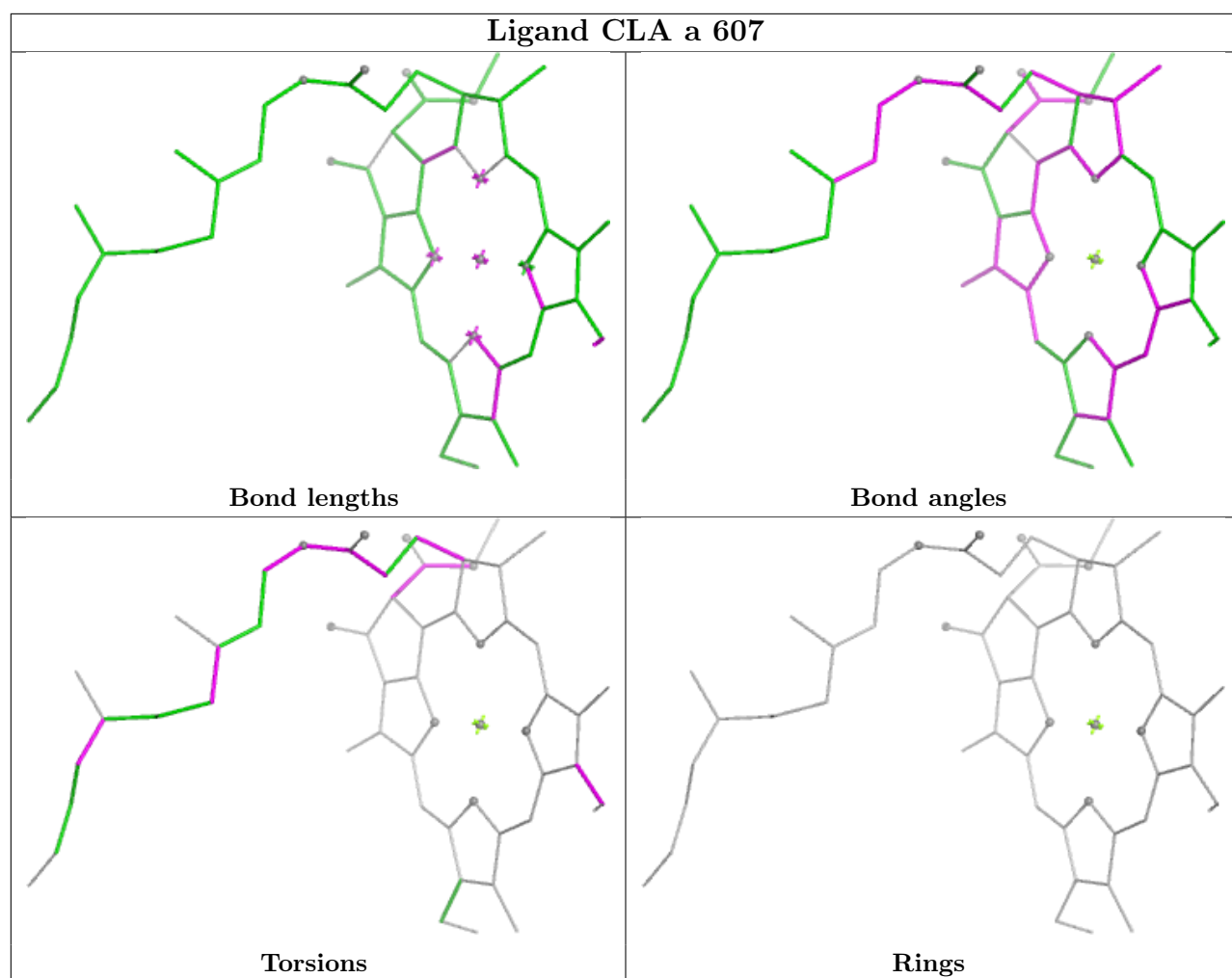
Bond angles



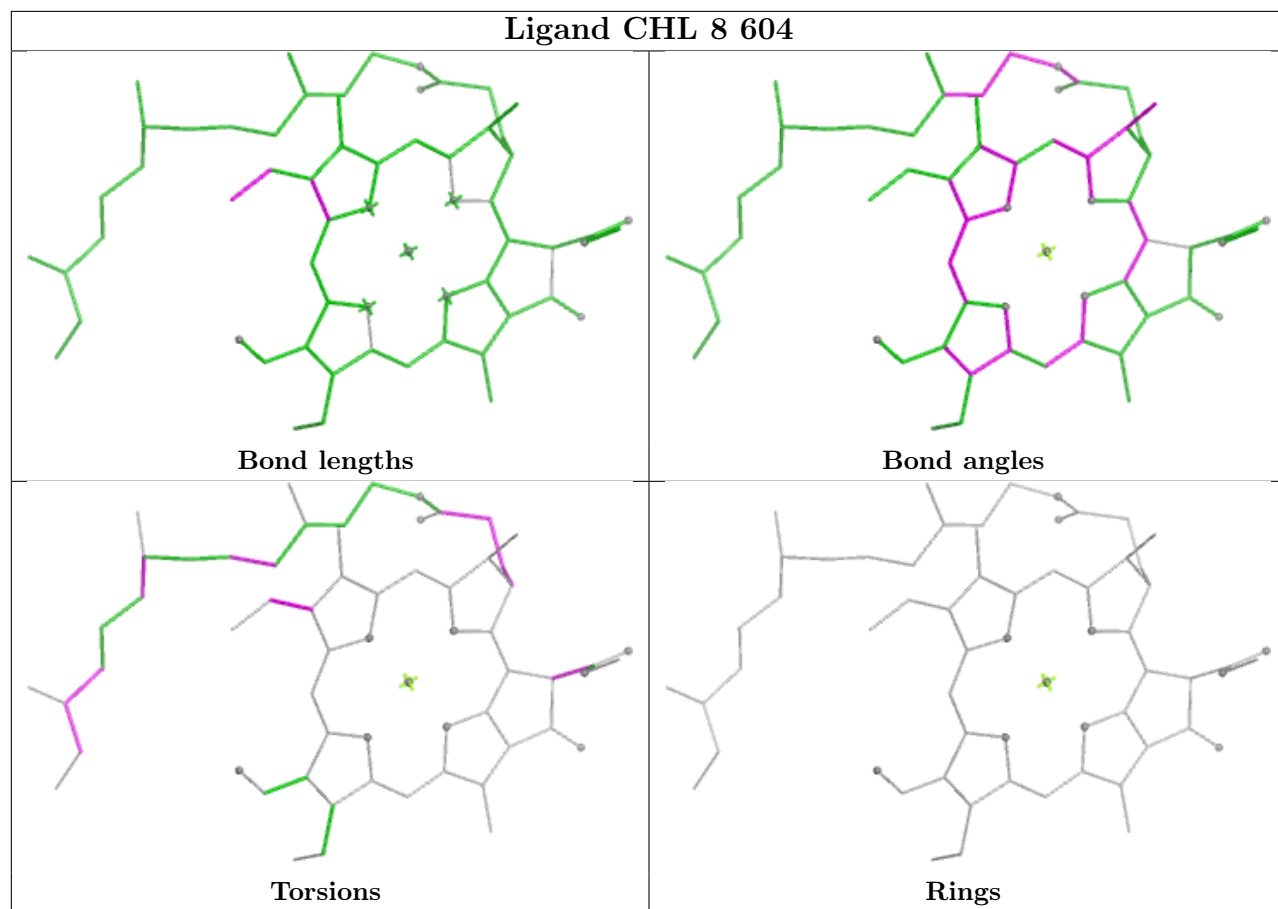
Torsions



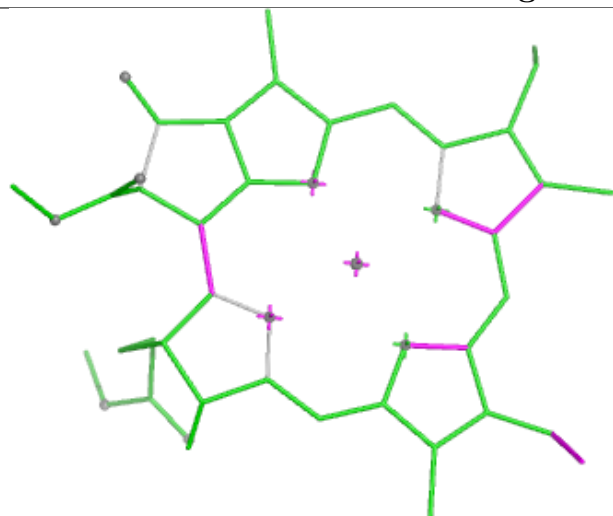
Rings



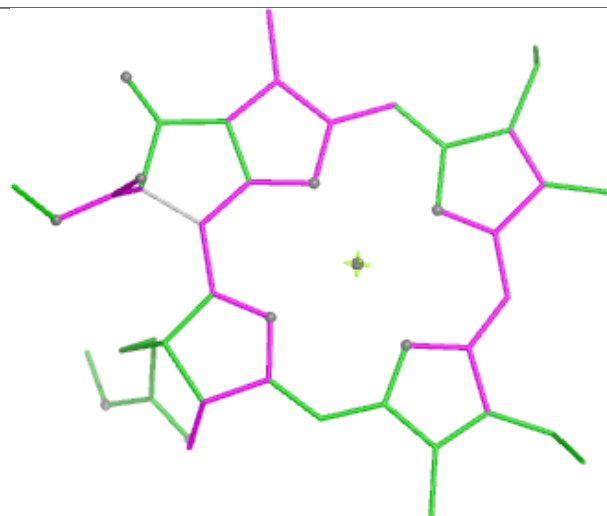
Ligand CHL 8 604



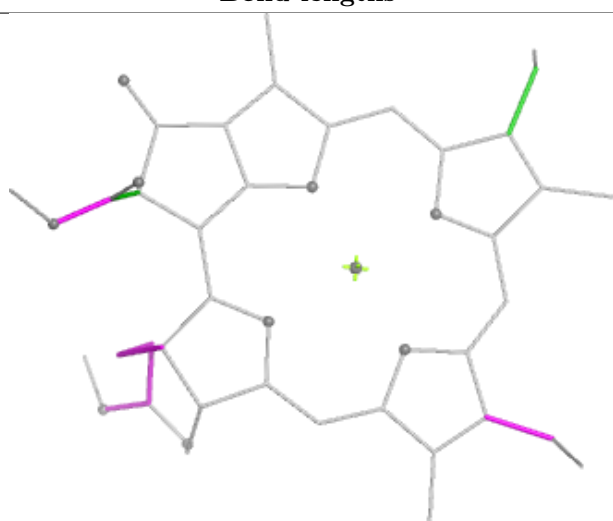
Ligand CLA 2 606



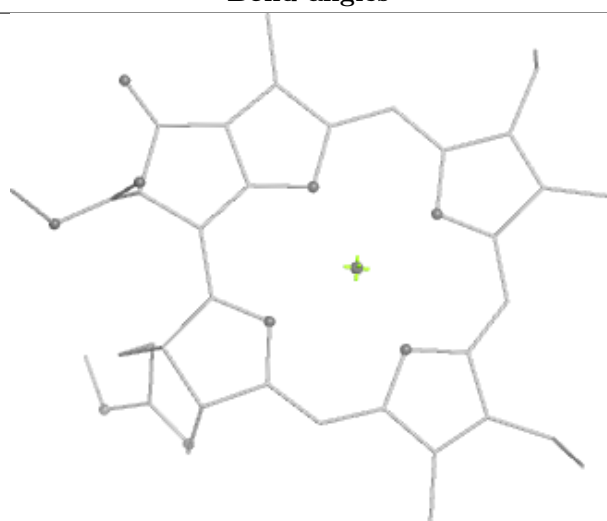
Bond lengths



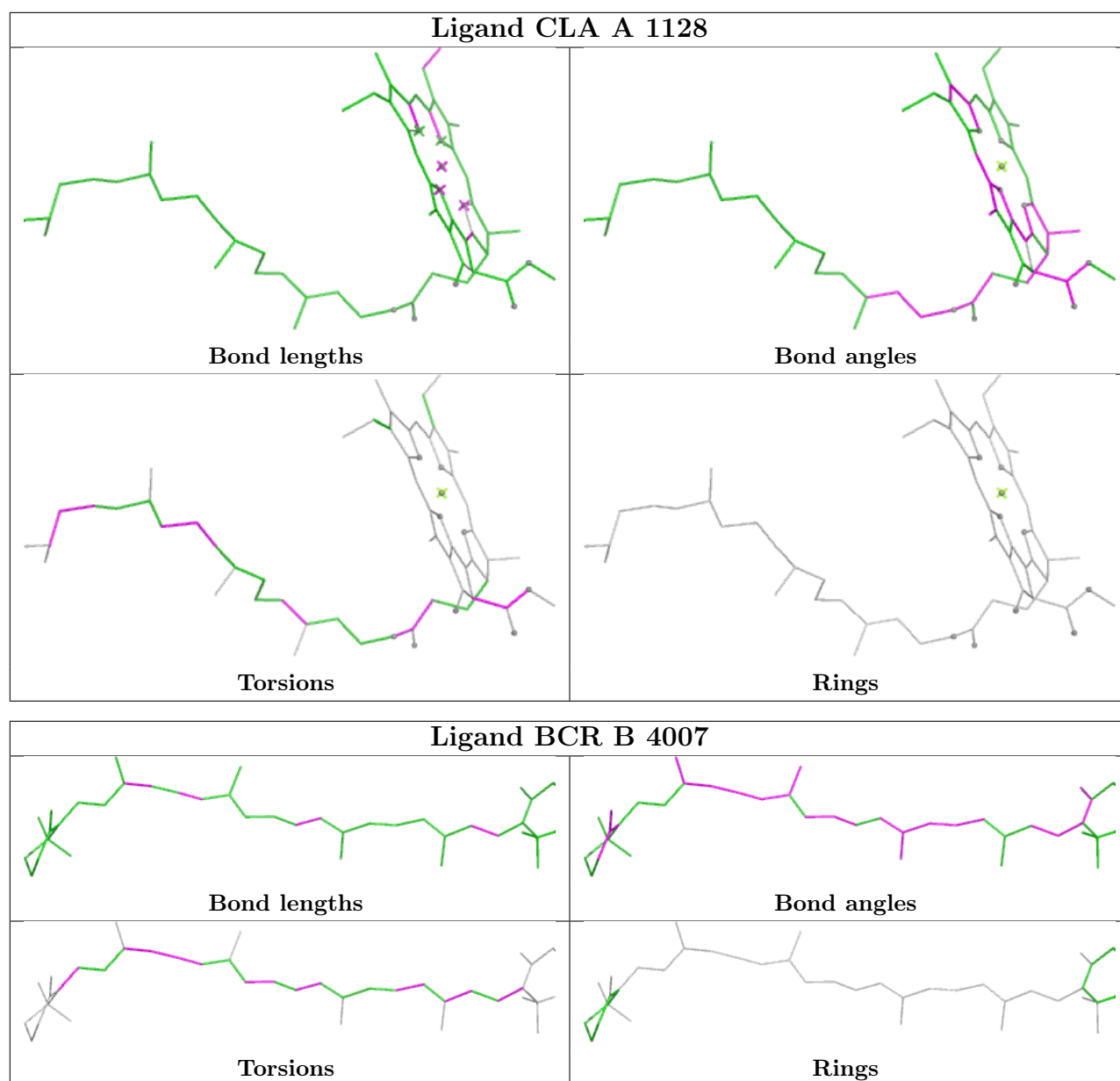
Bond angles

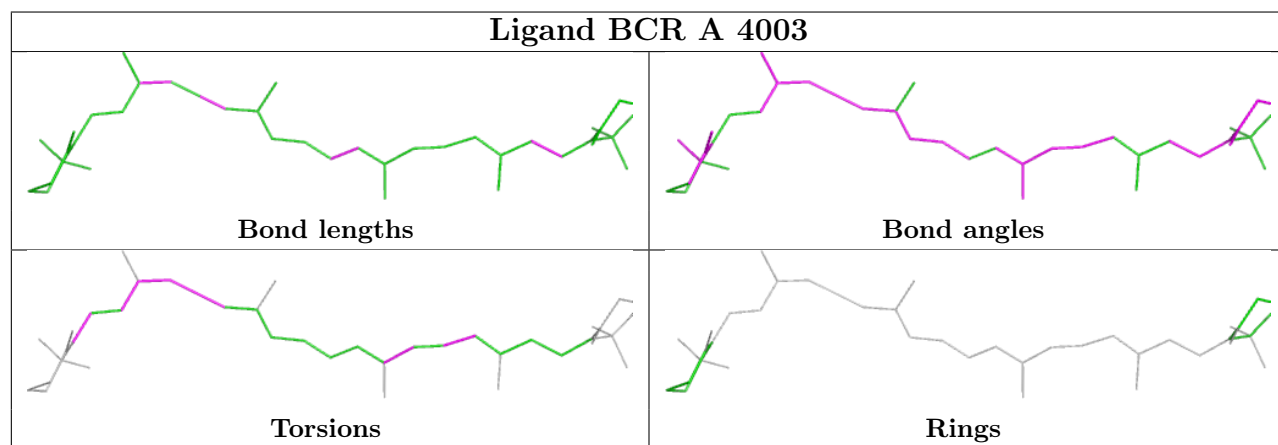
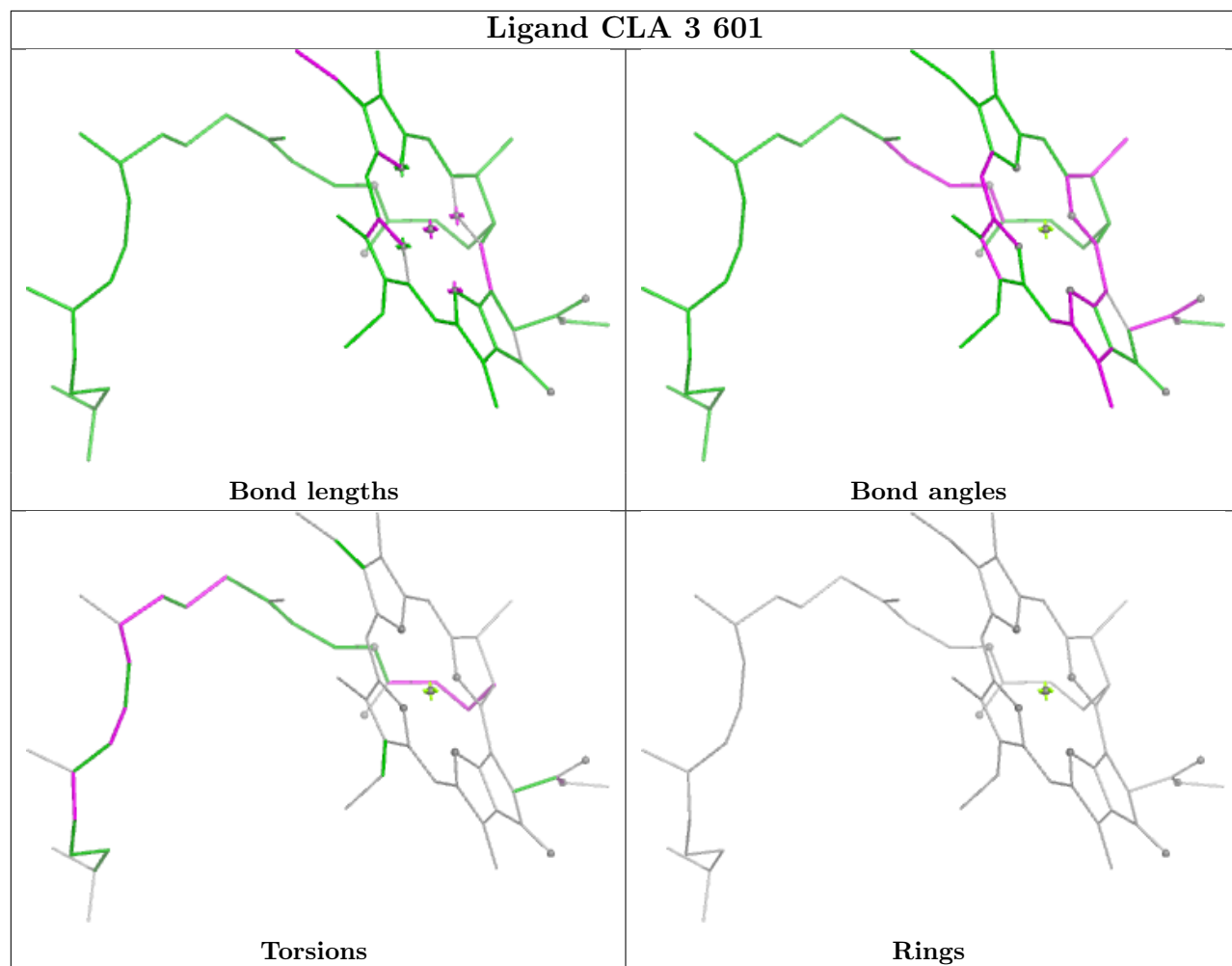


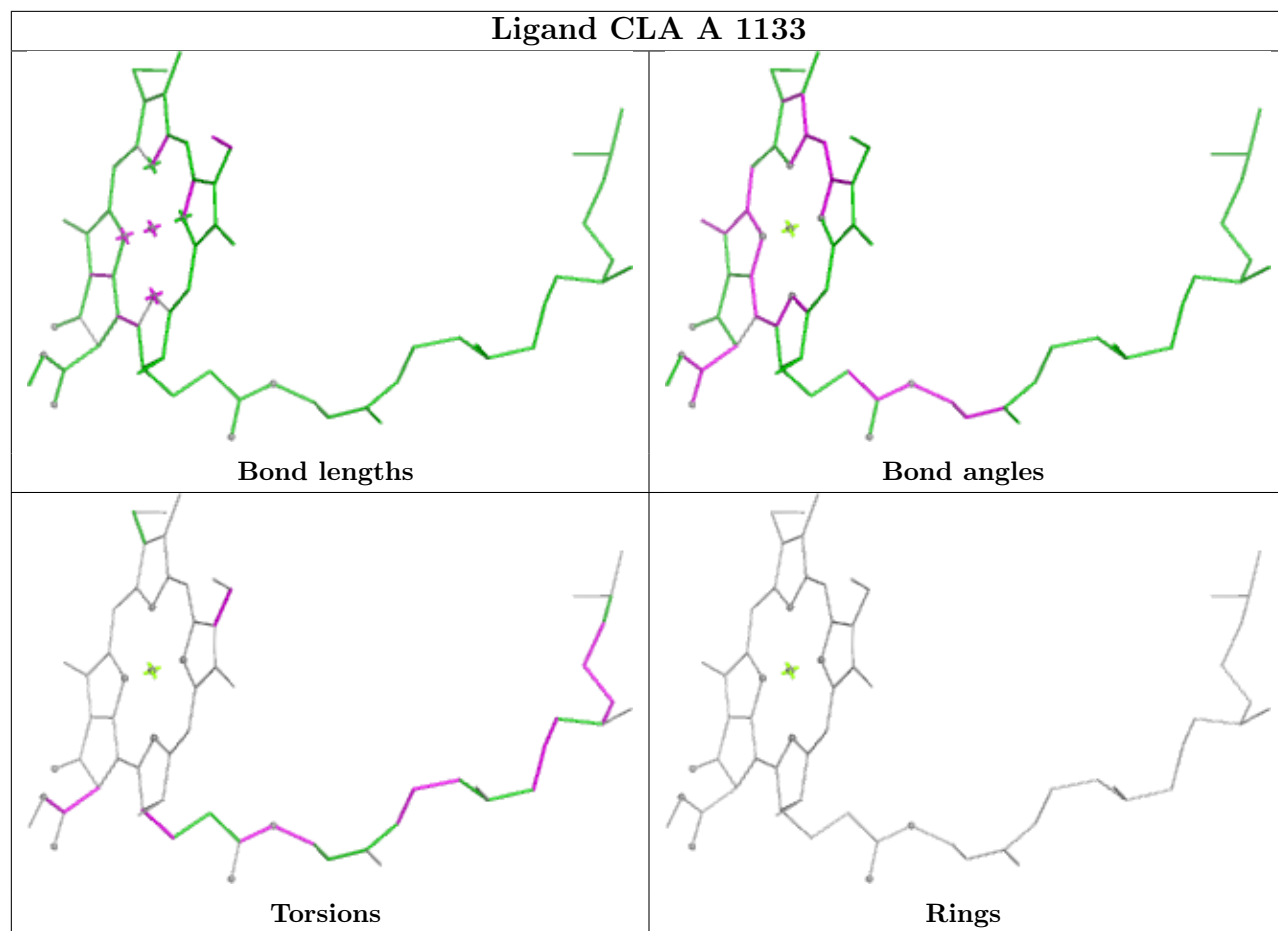
Torsions



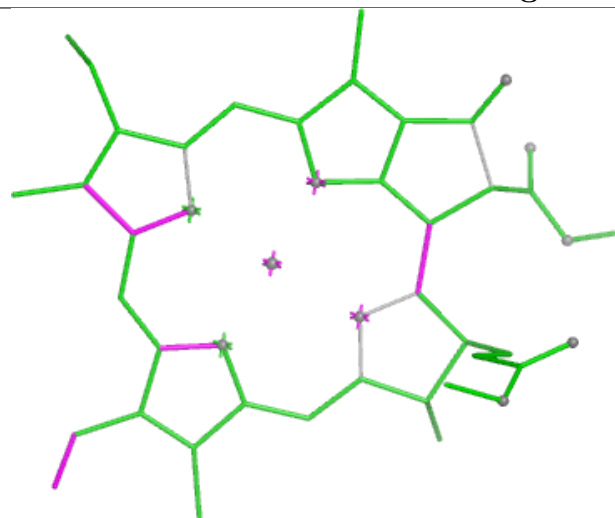
Rings



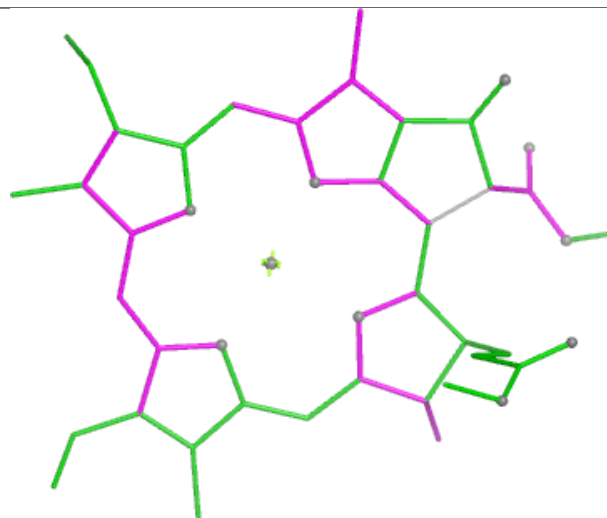




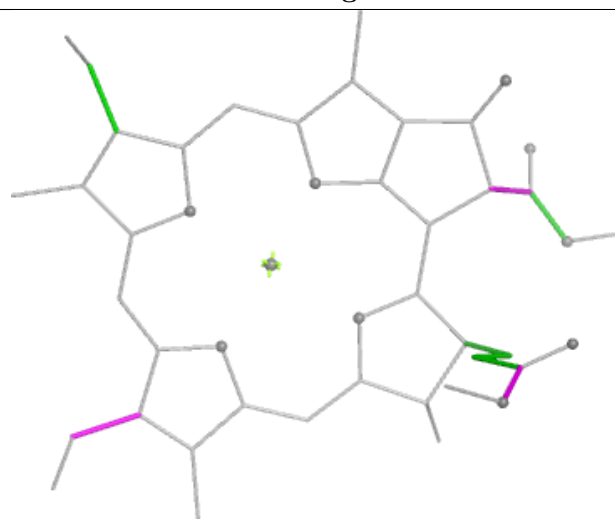
Ligand CLA 8 607



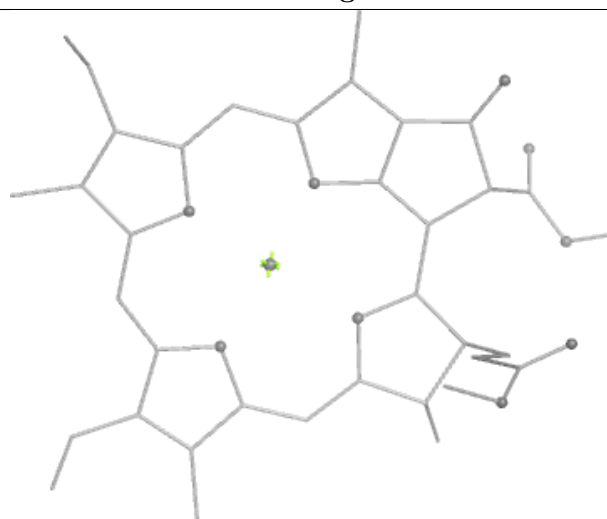
Bond lengths



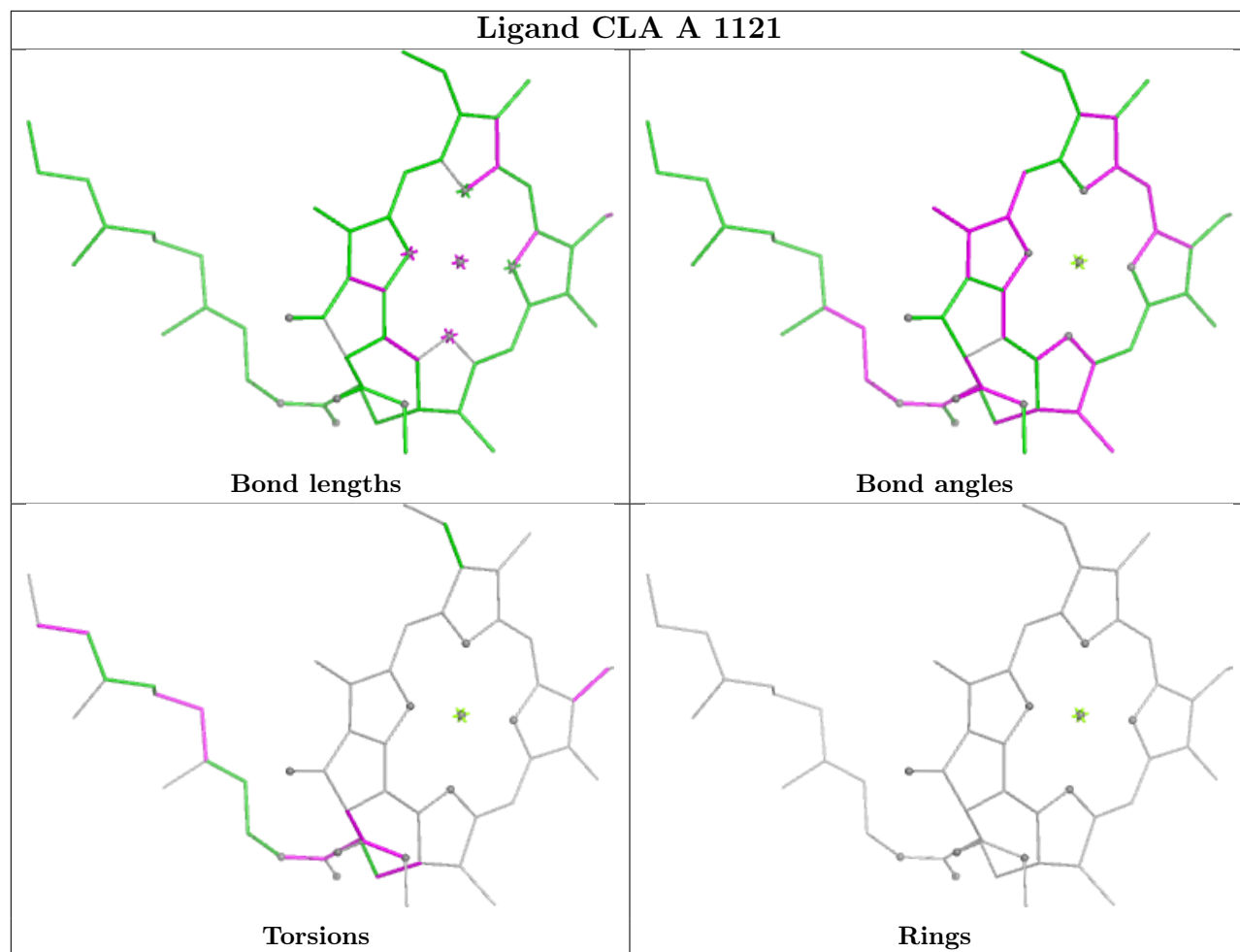
Bond angles



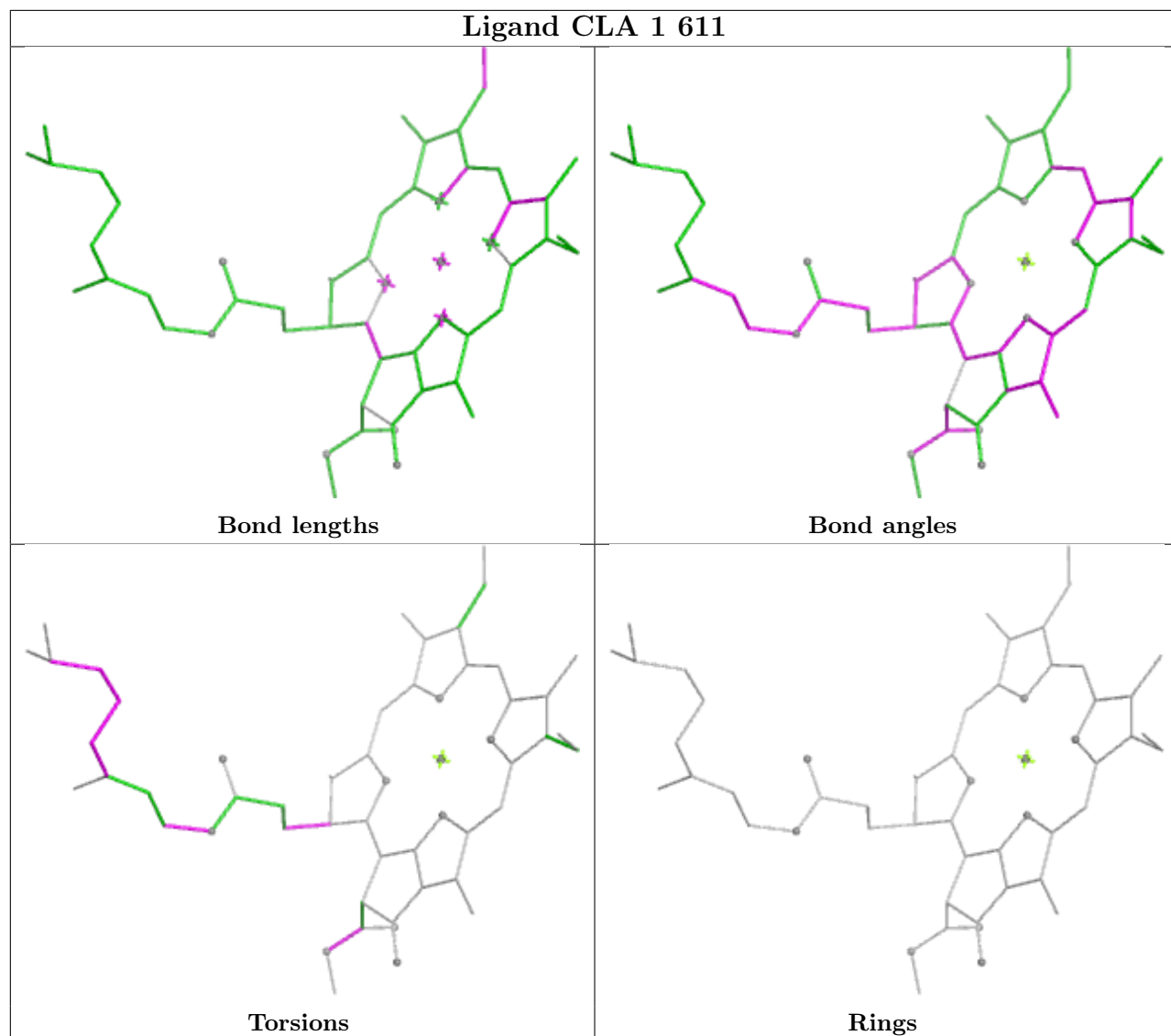
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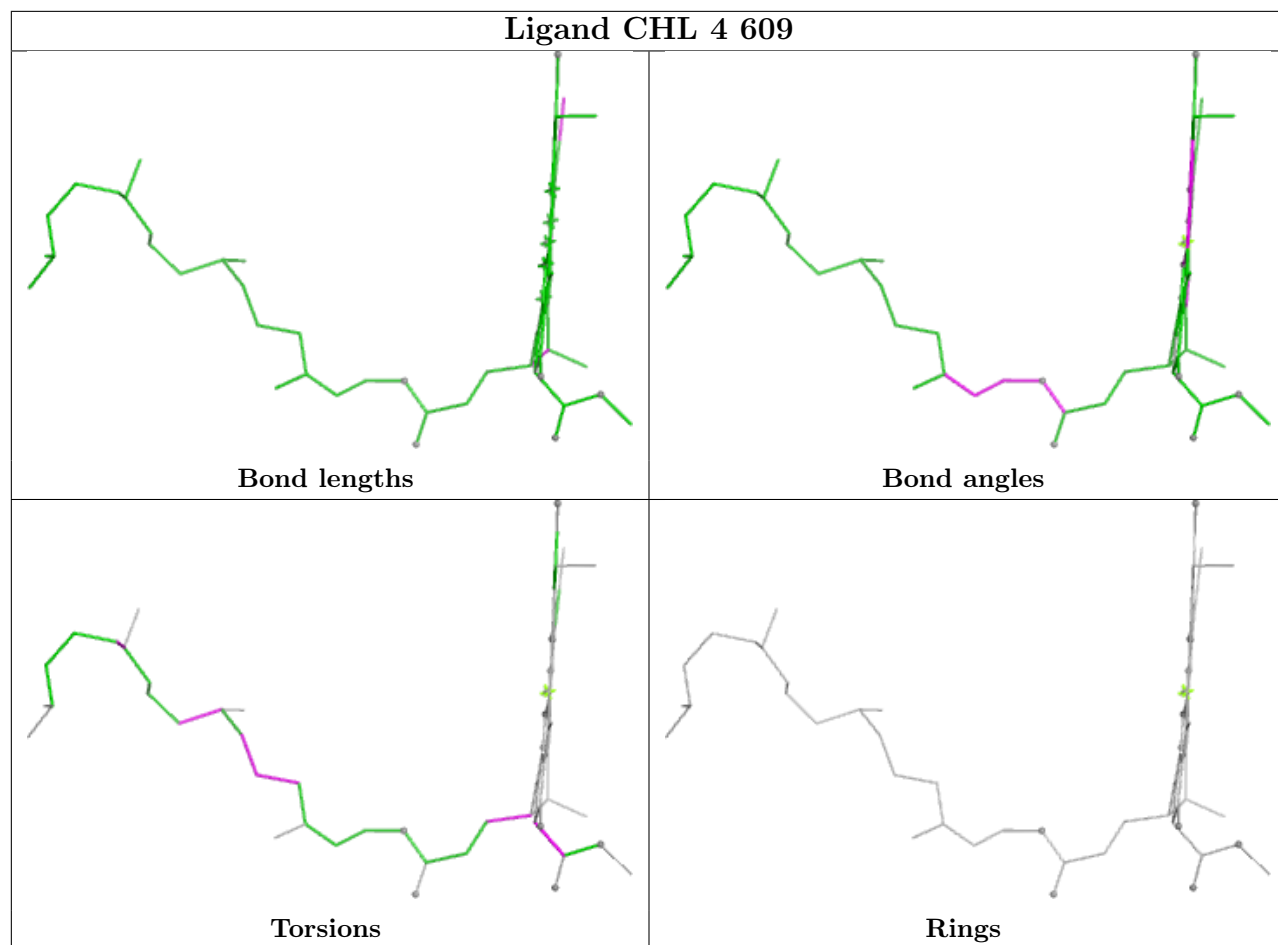


Rings

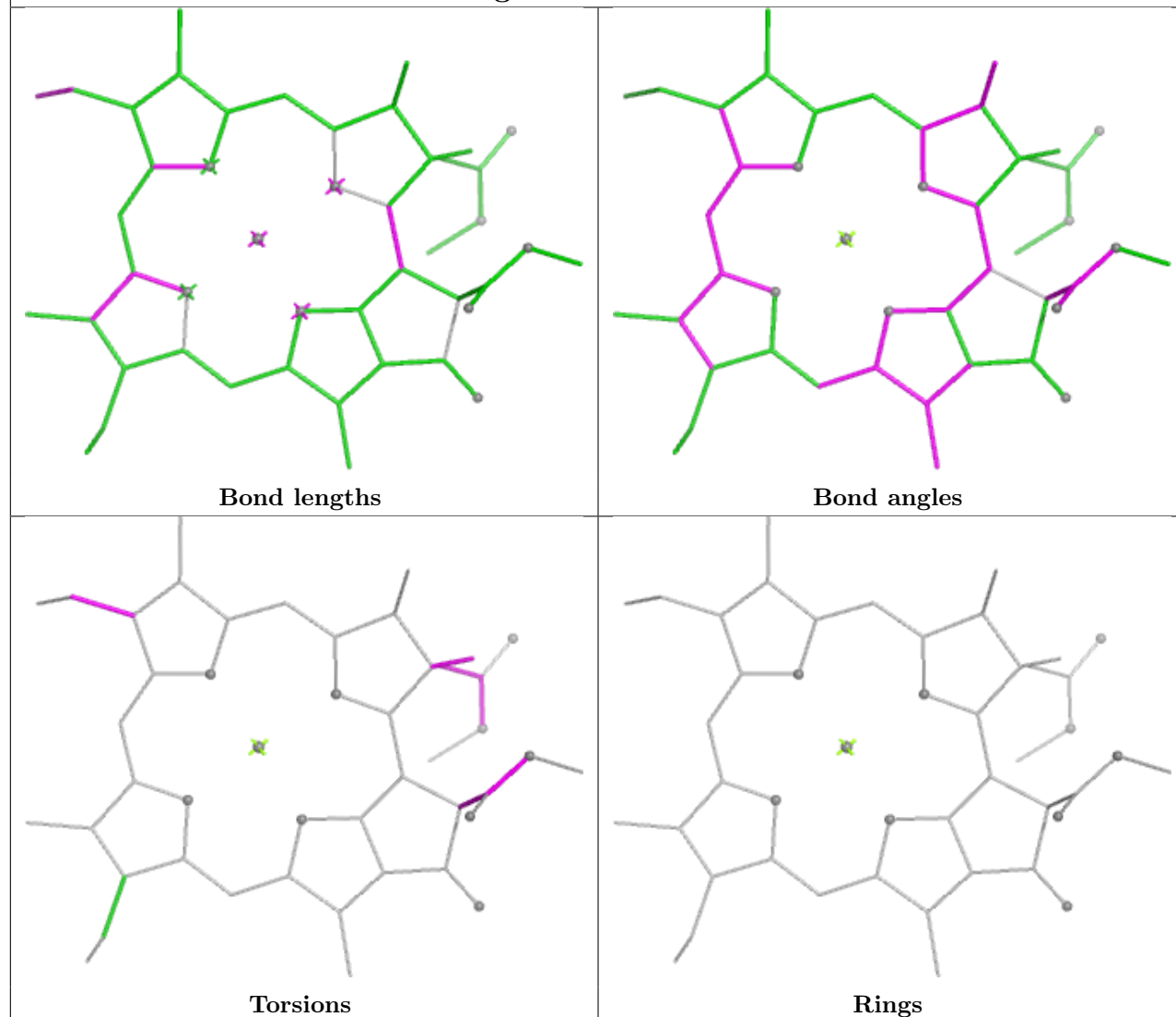


Ligand CLA 1 611

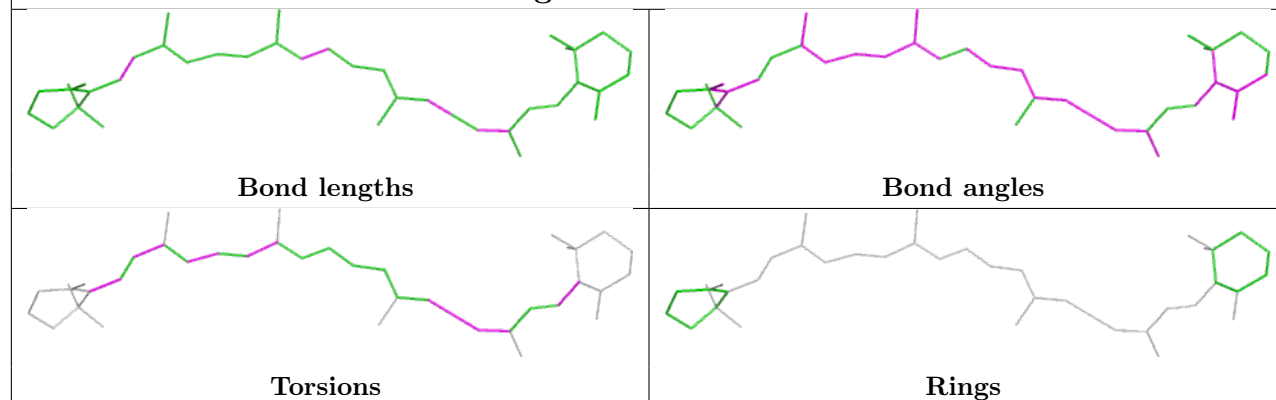




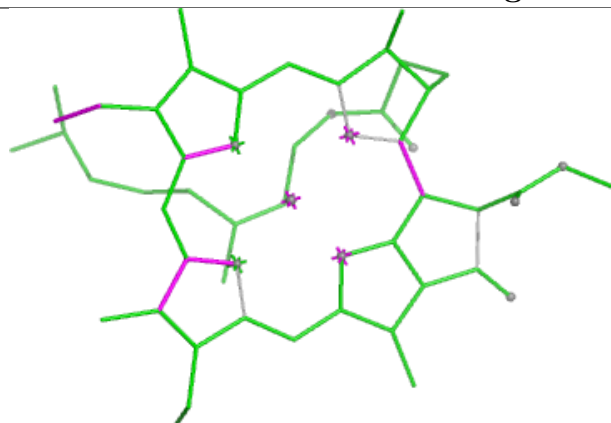
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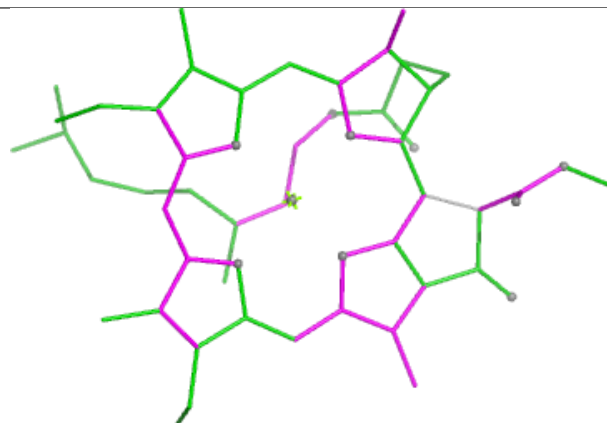
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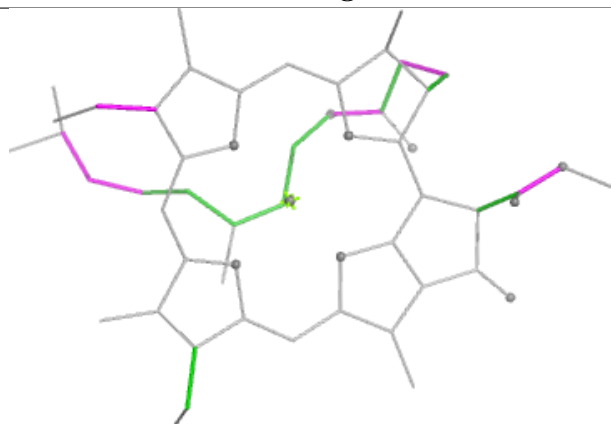
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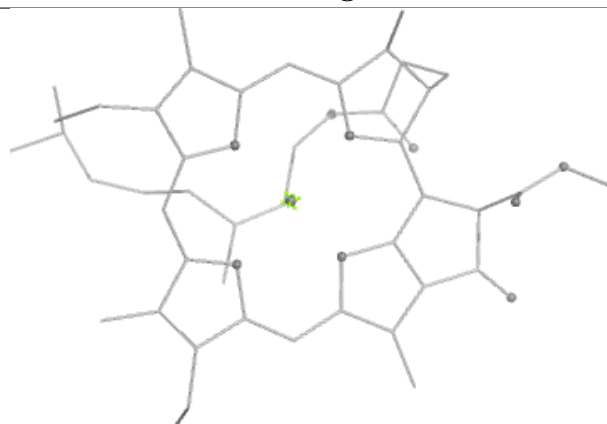
Bond lengths



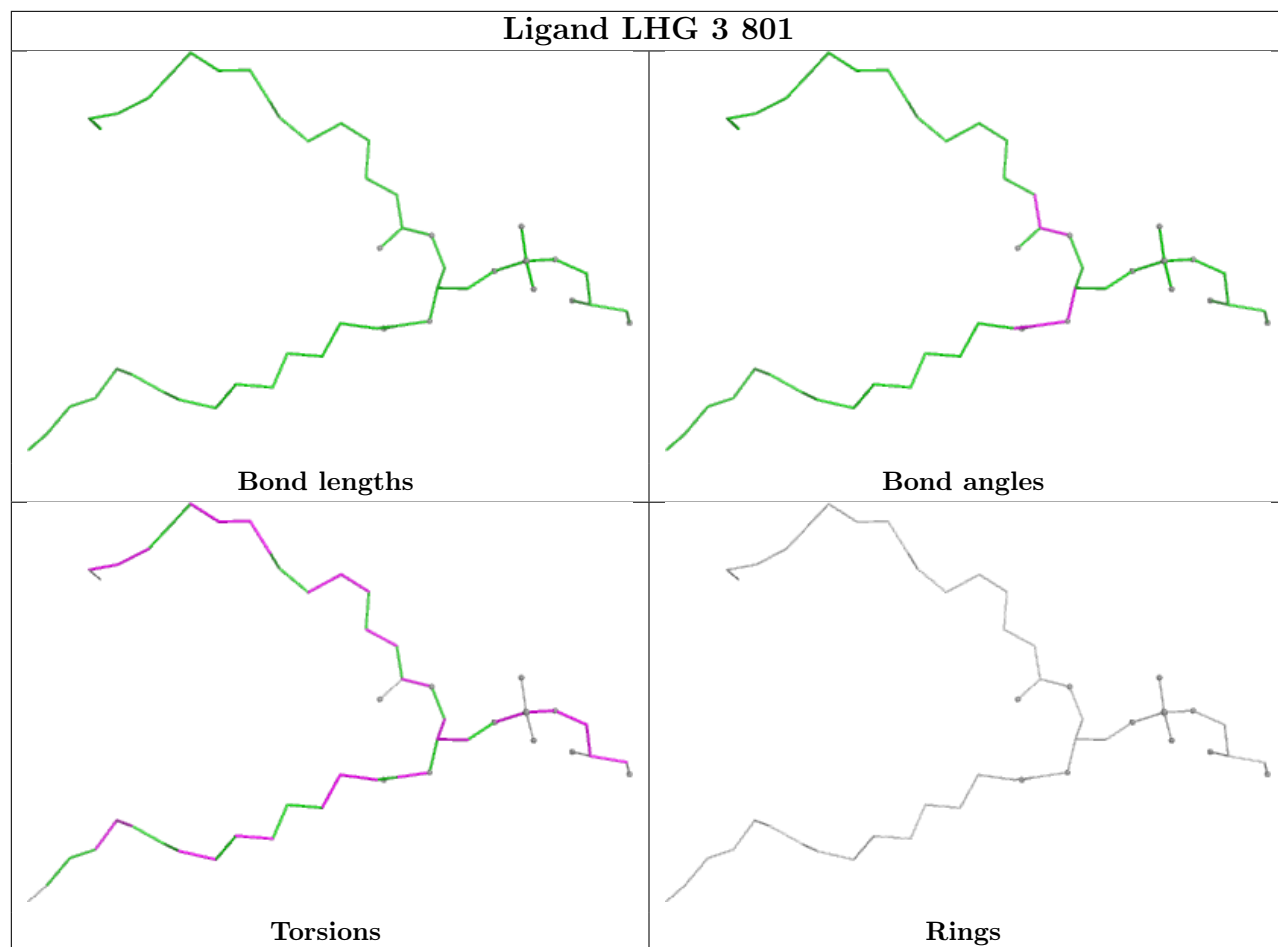
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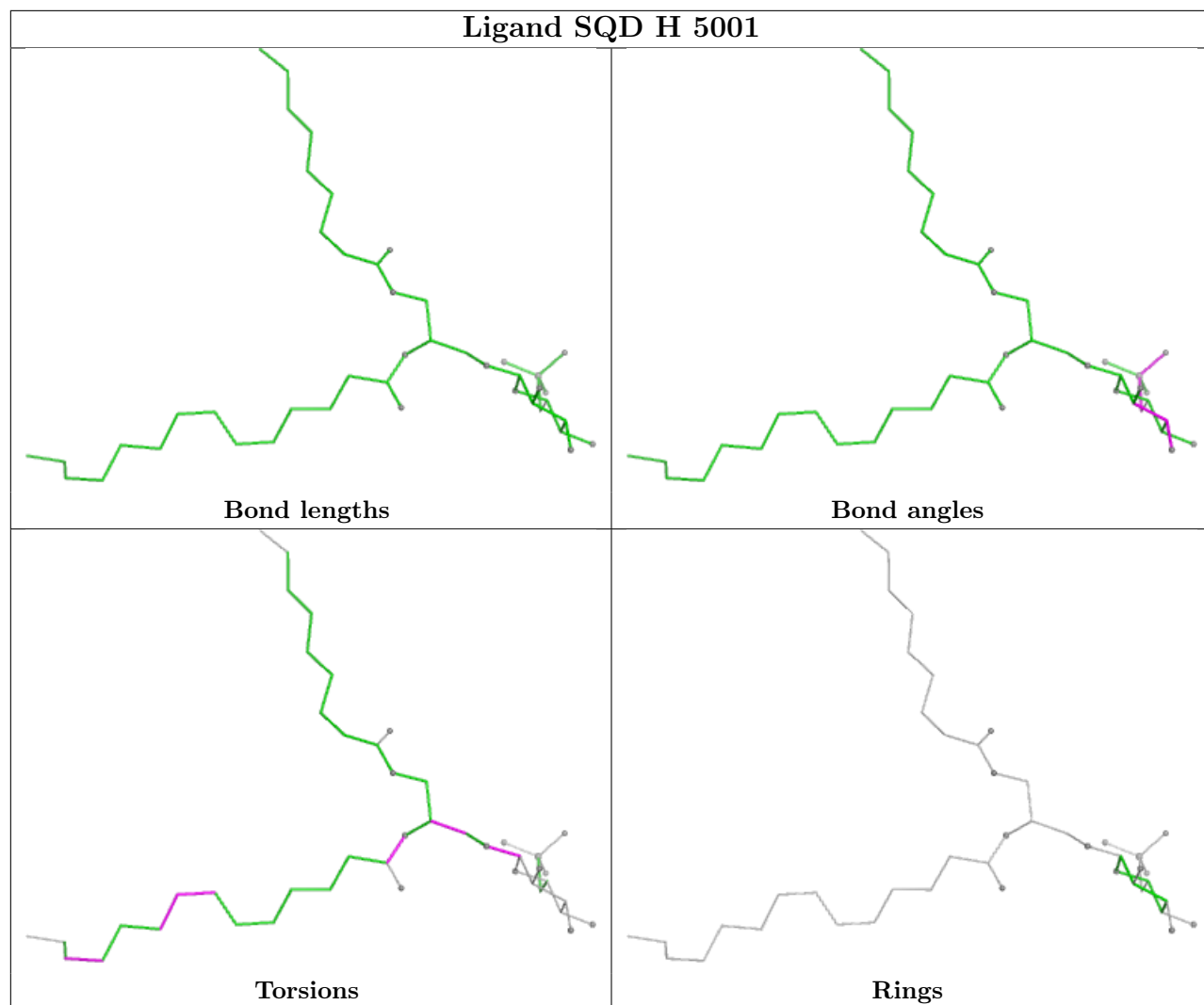


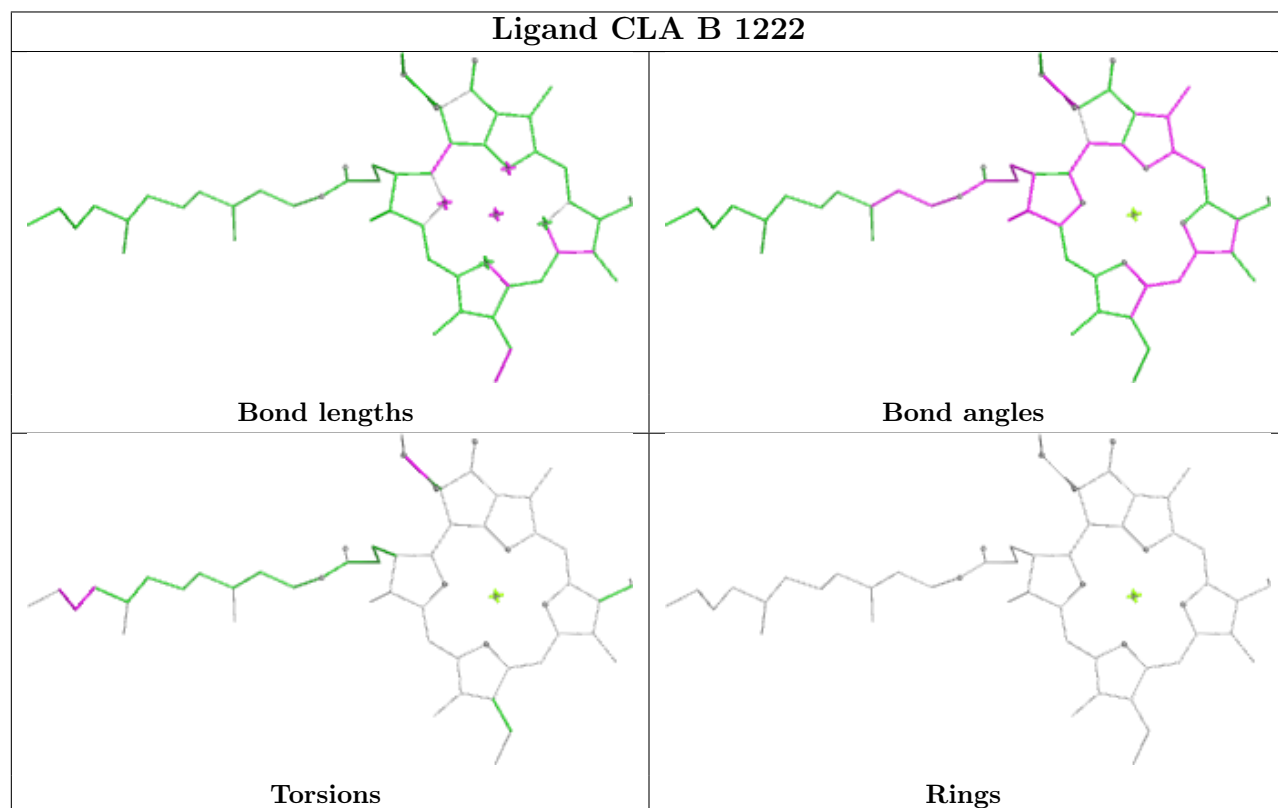
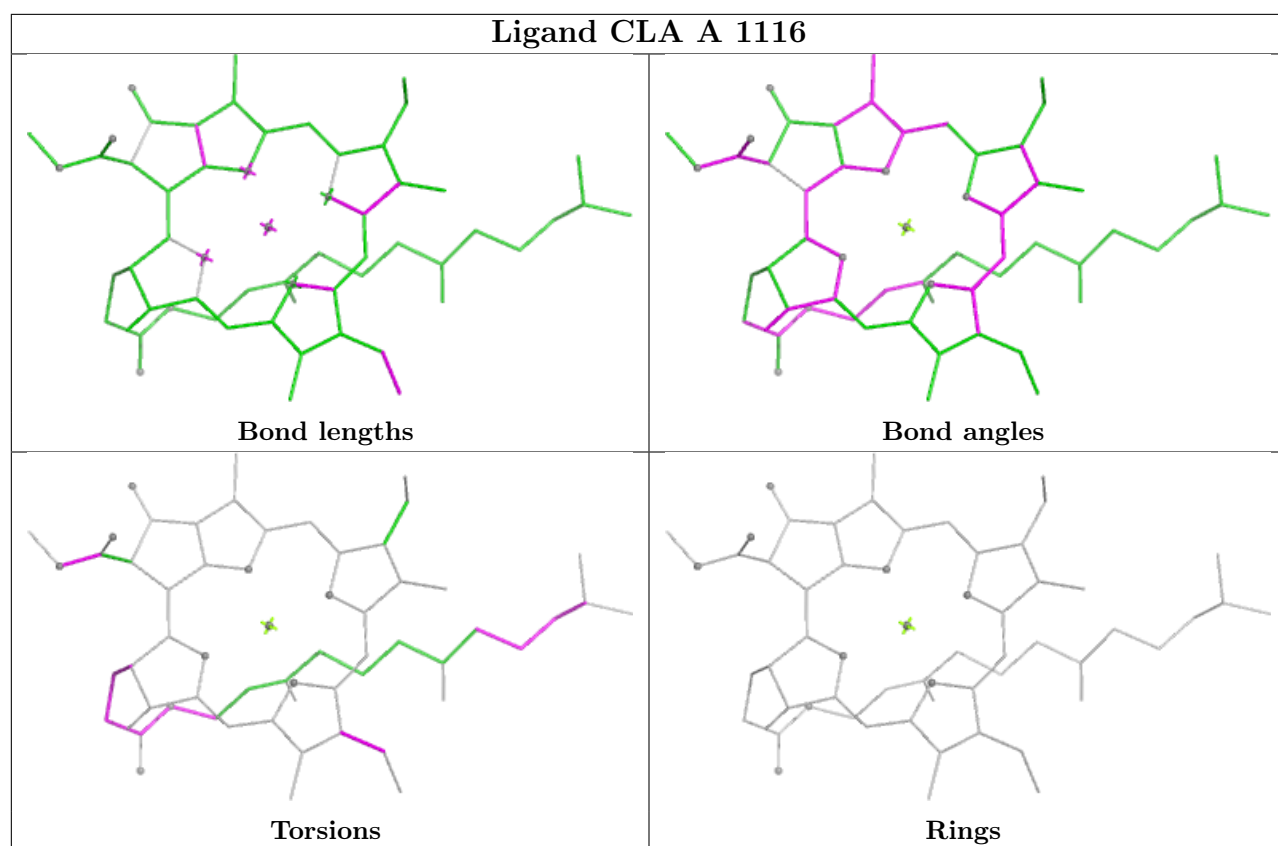
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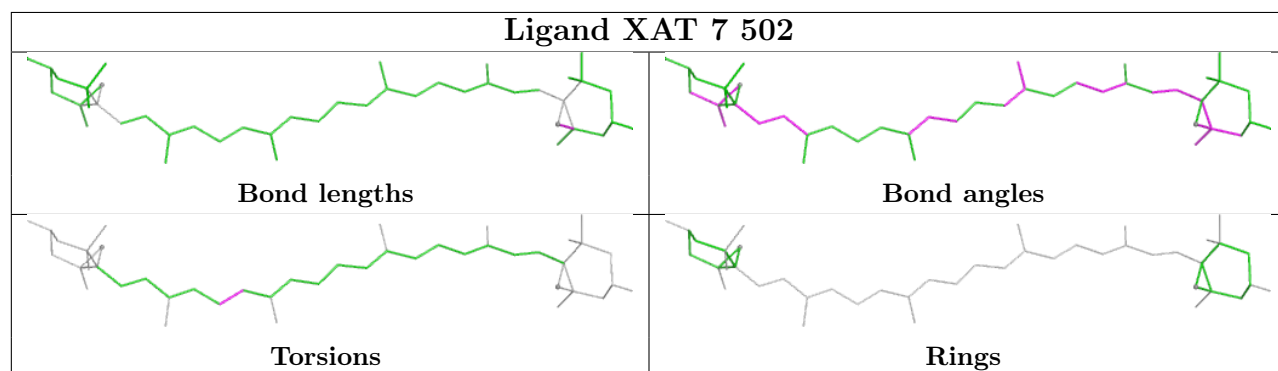
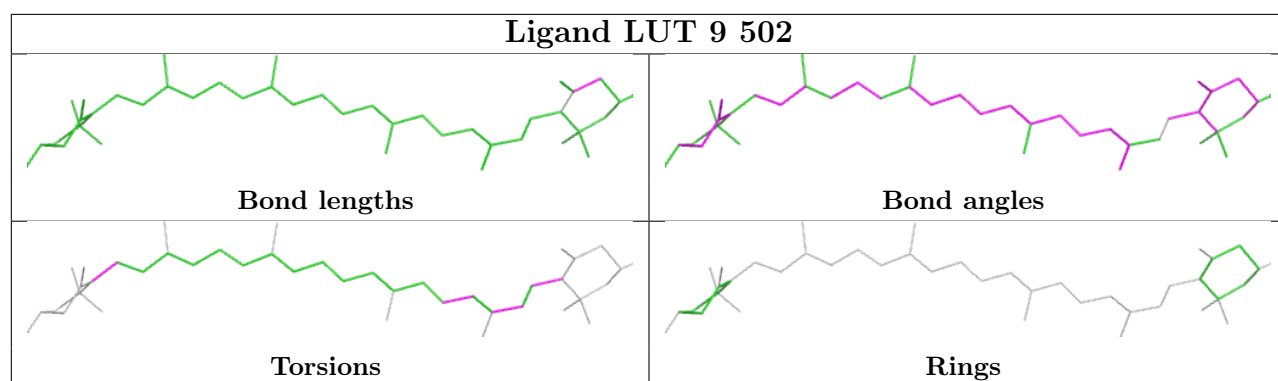
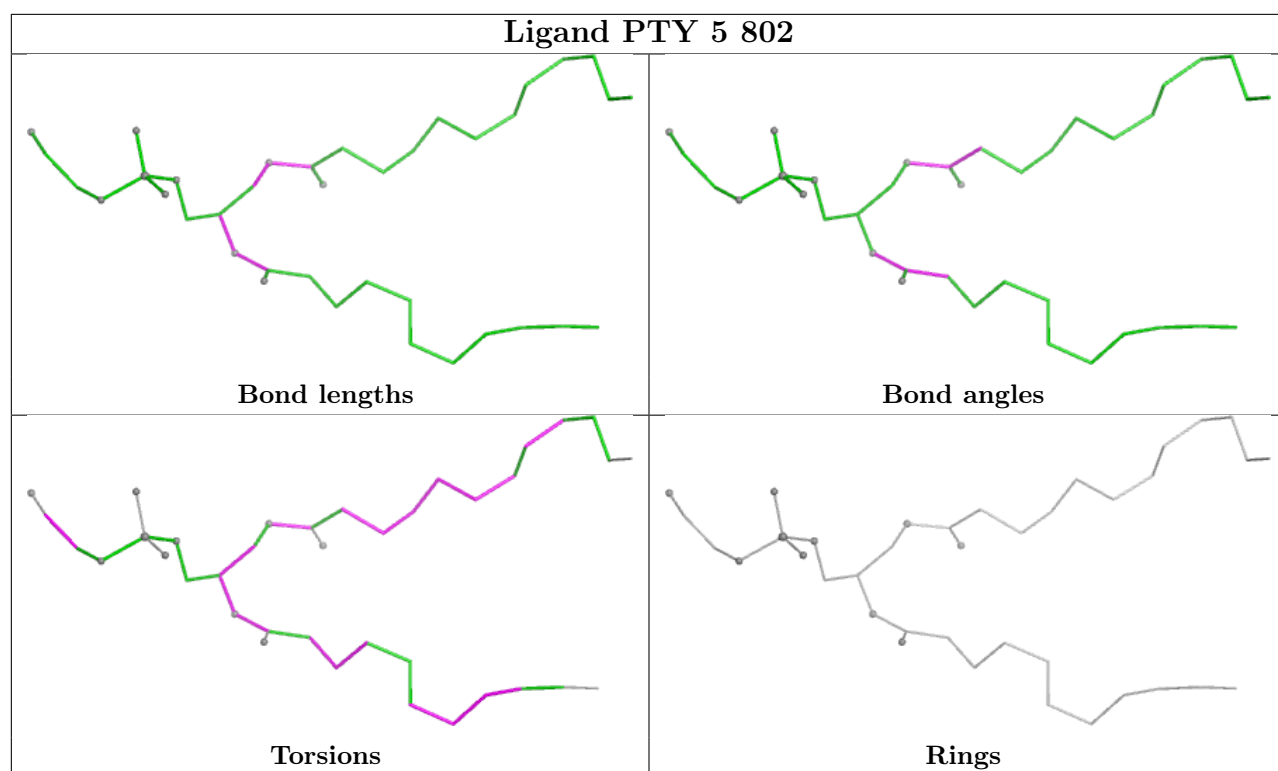


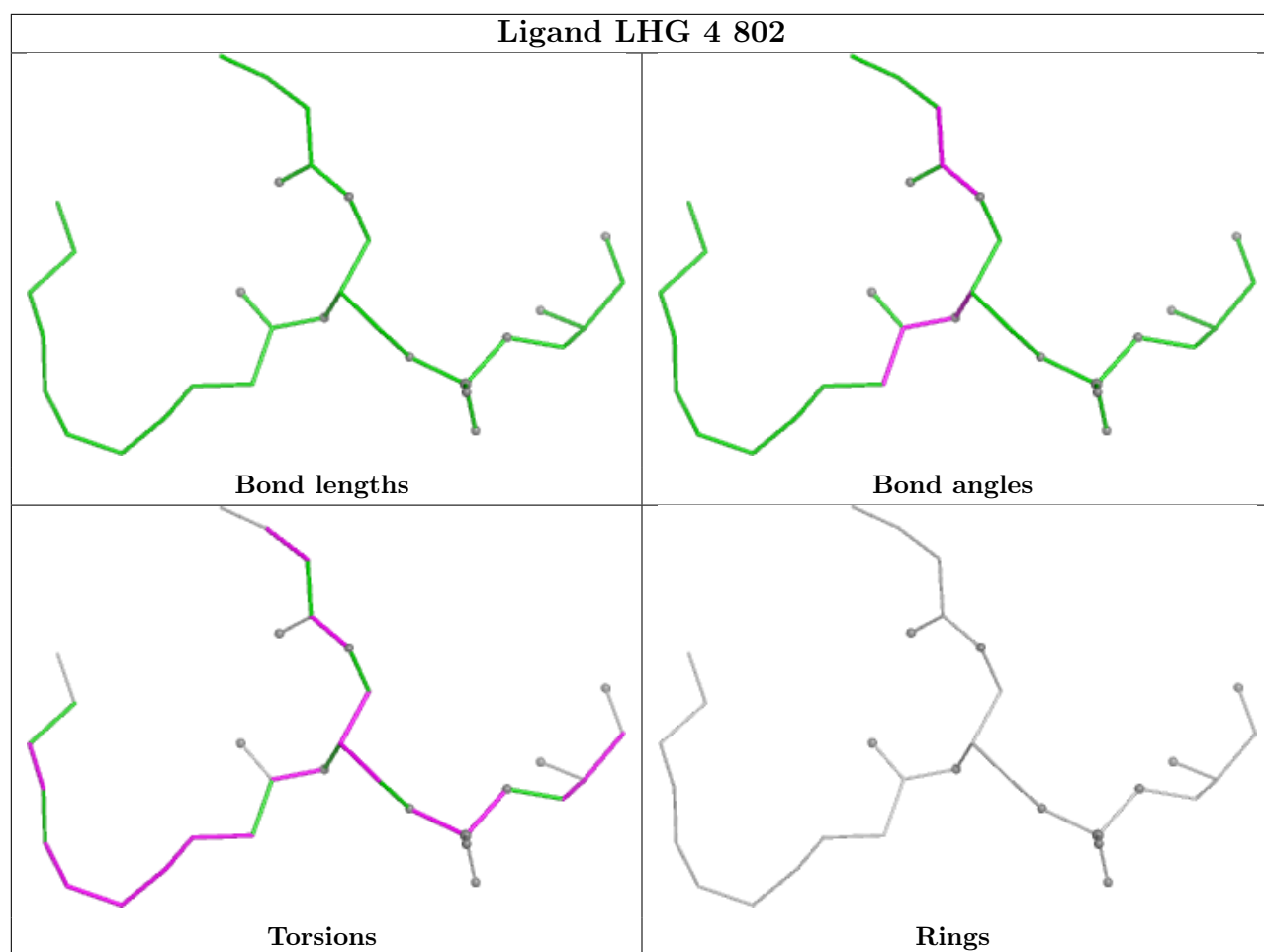
Rings



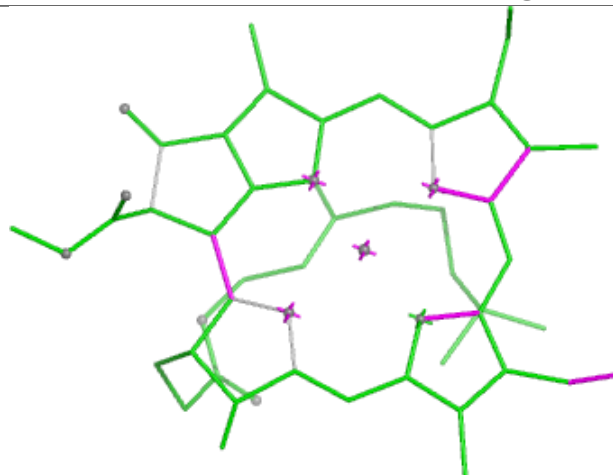




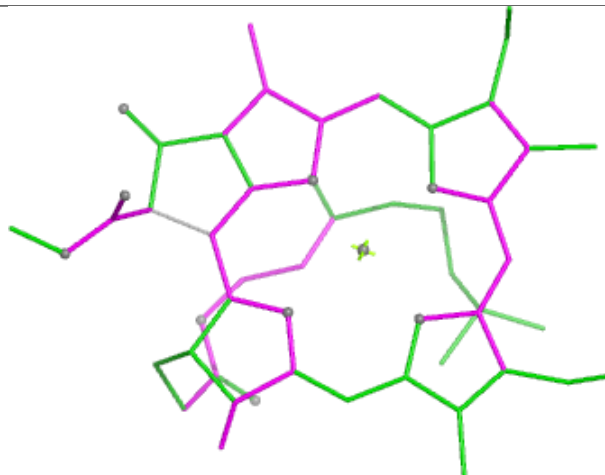




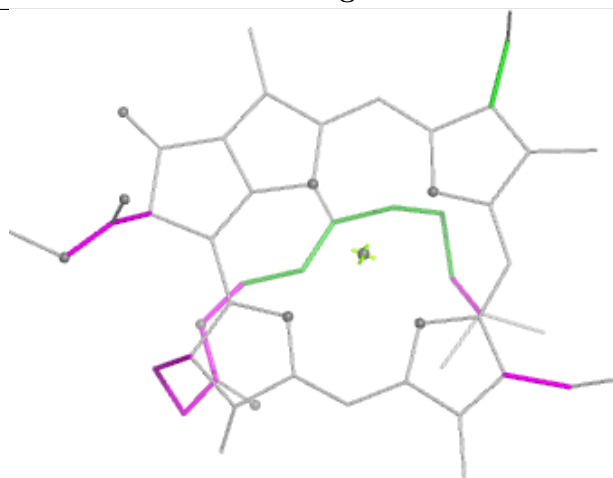
Ligand CLA a 608



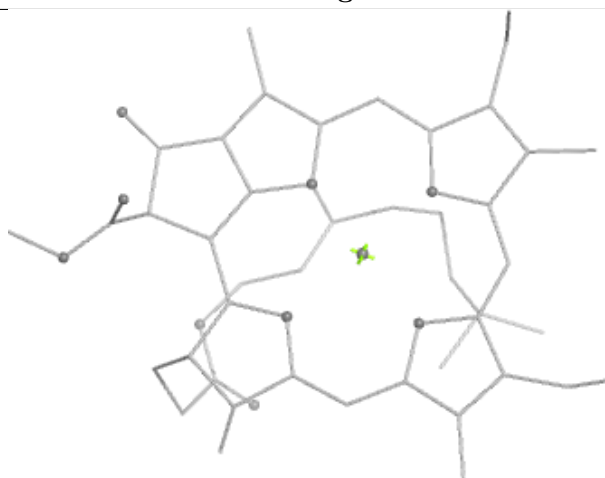
Bond lengths



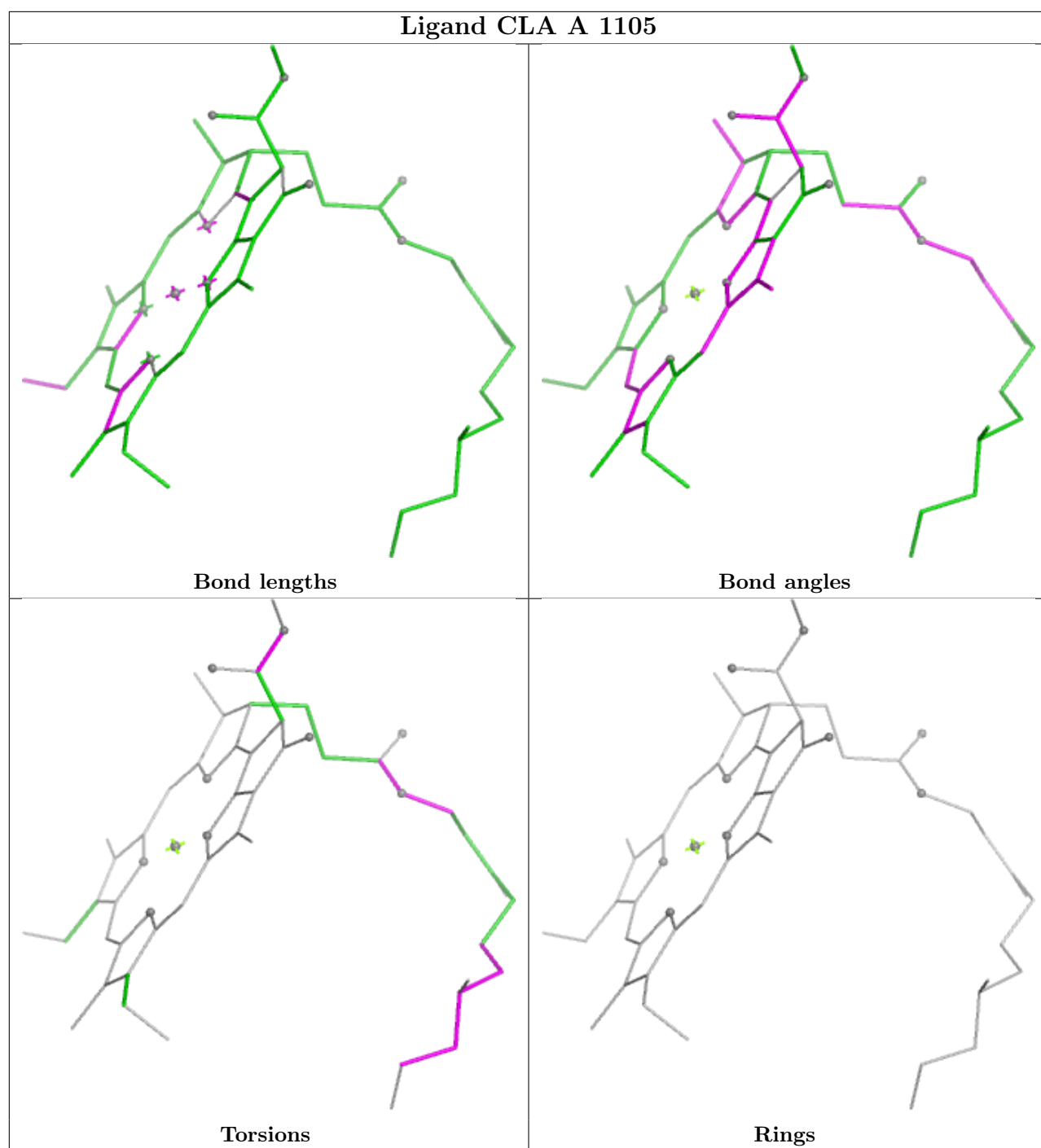
Bond angles



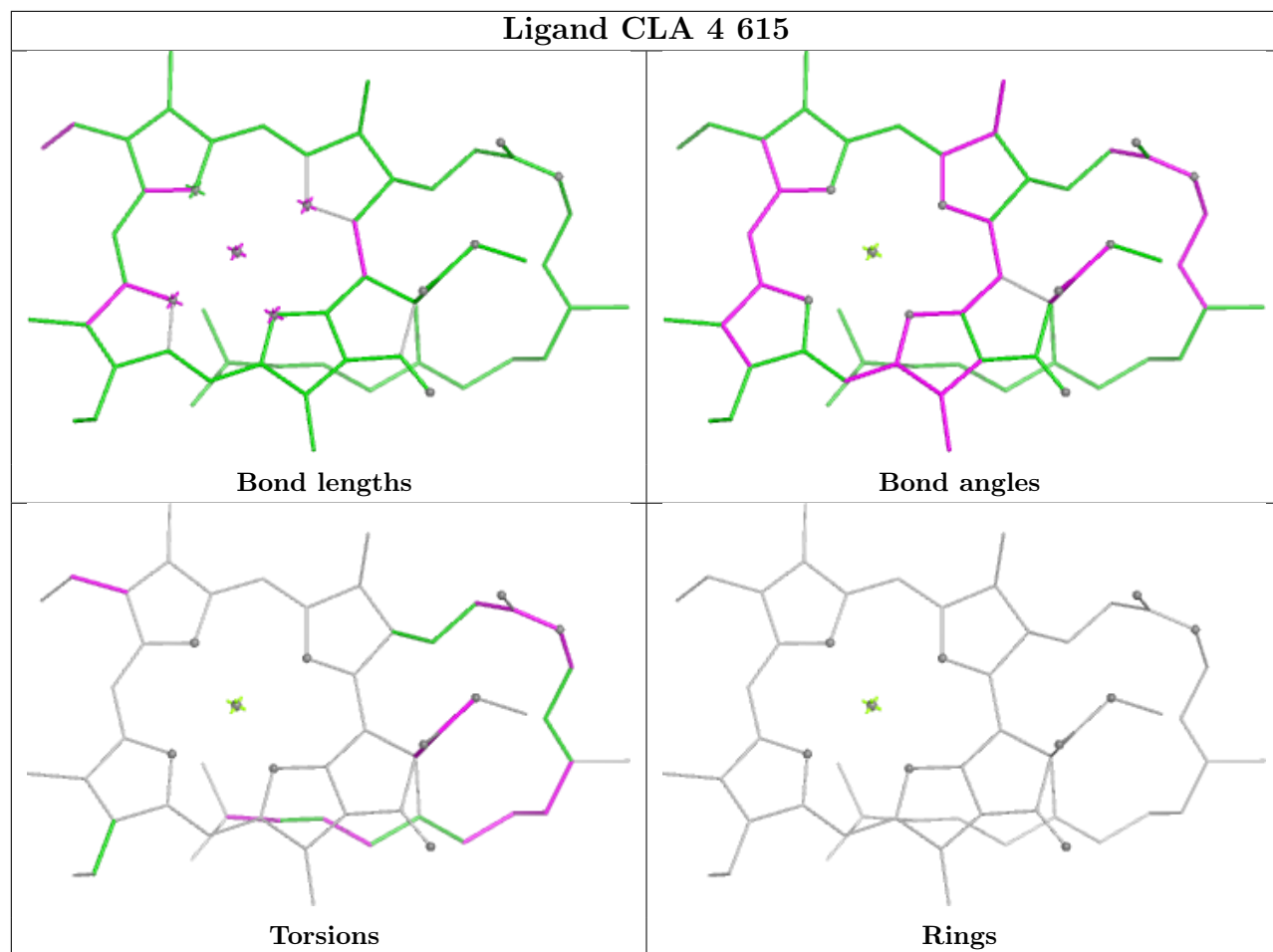
Torsions



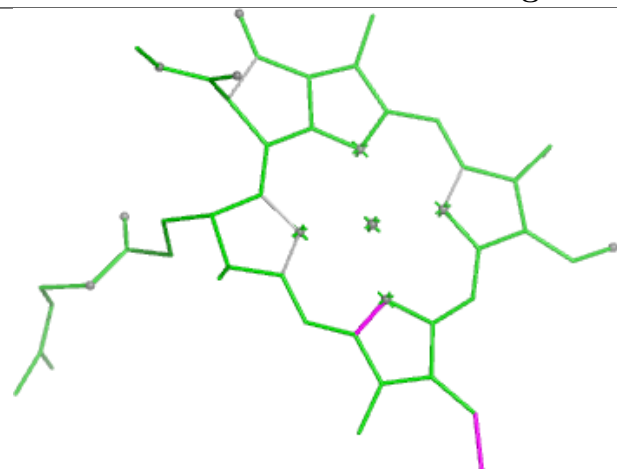
Rings



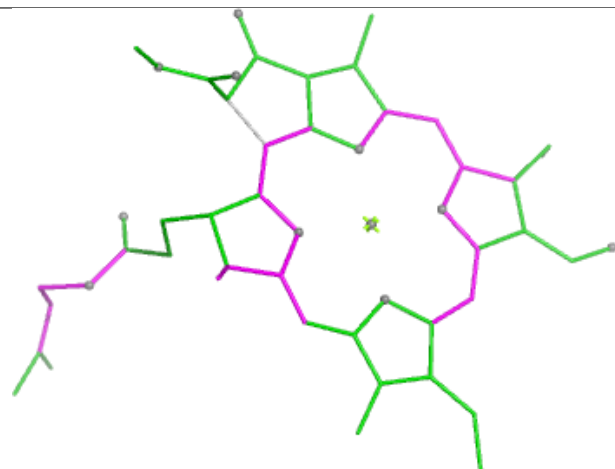
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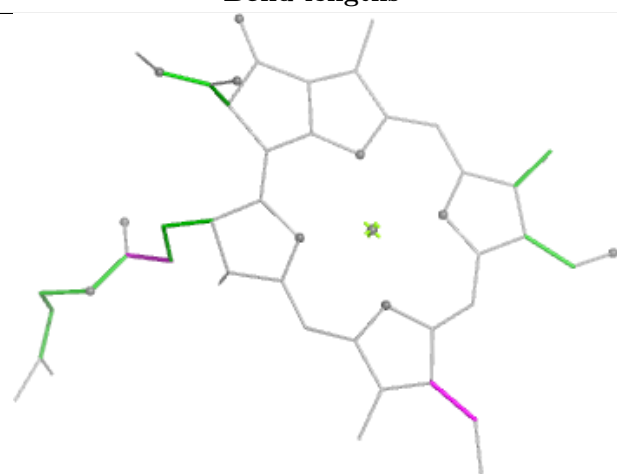
Ligand CHL 5 611



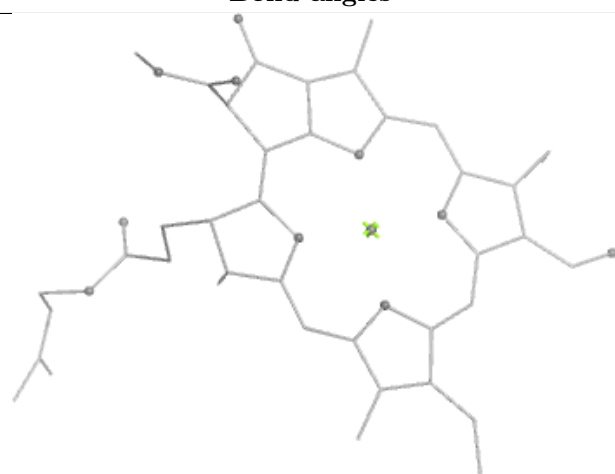
Bond lengths



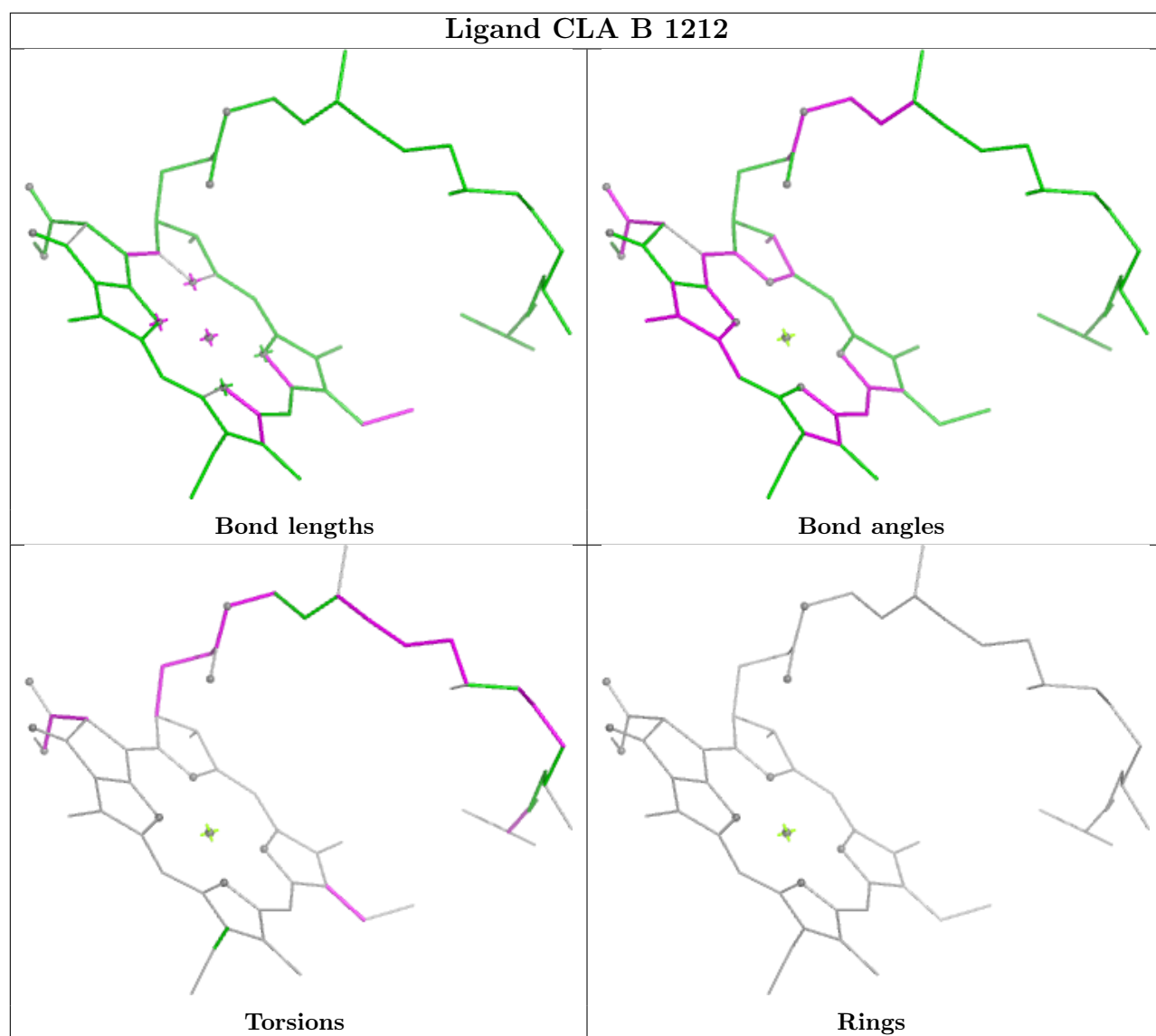
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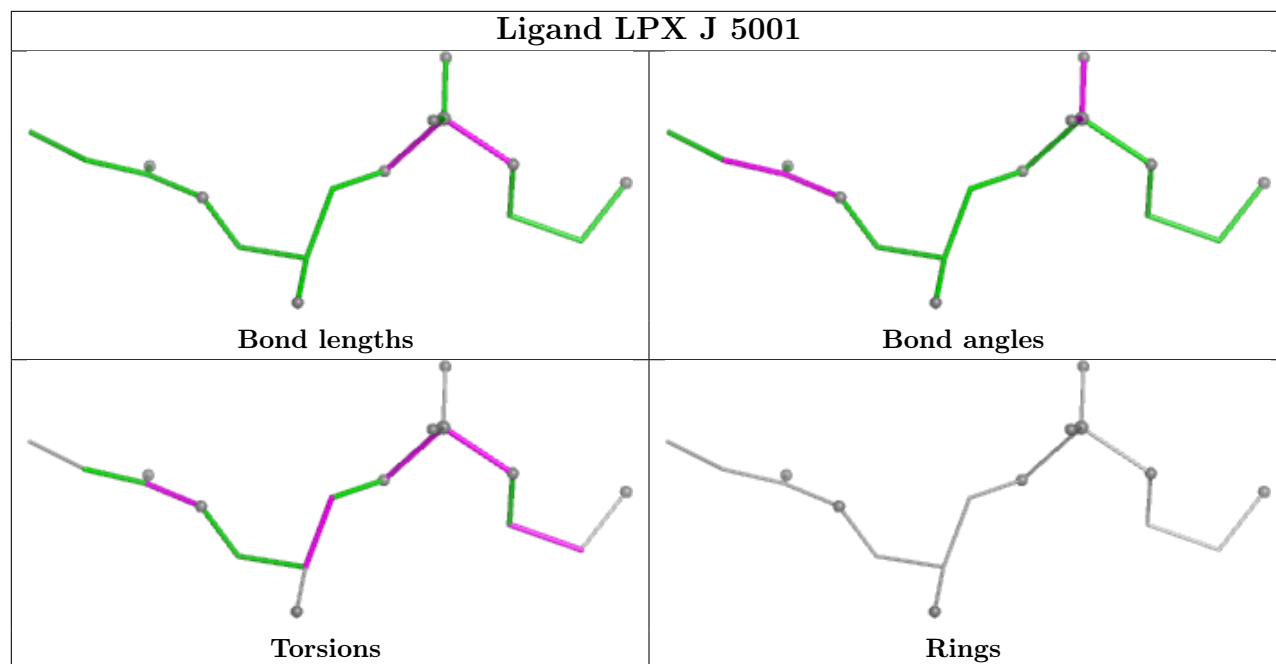


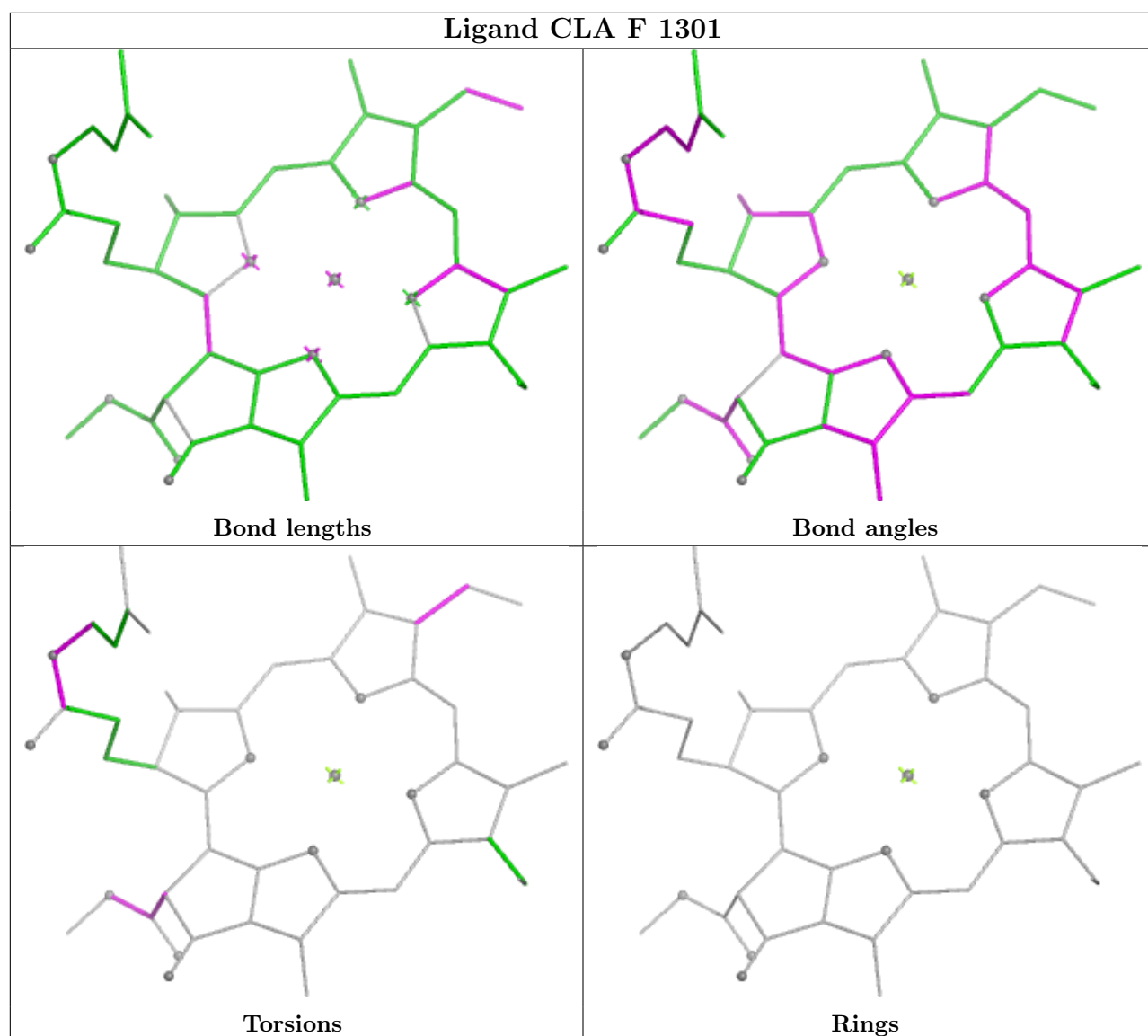
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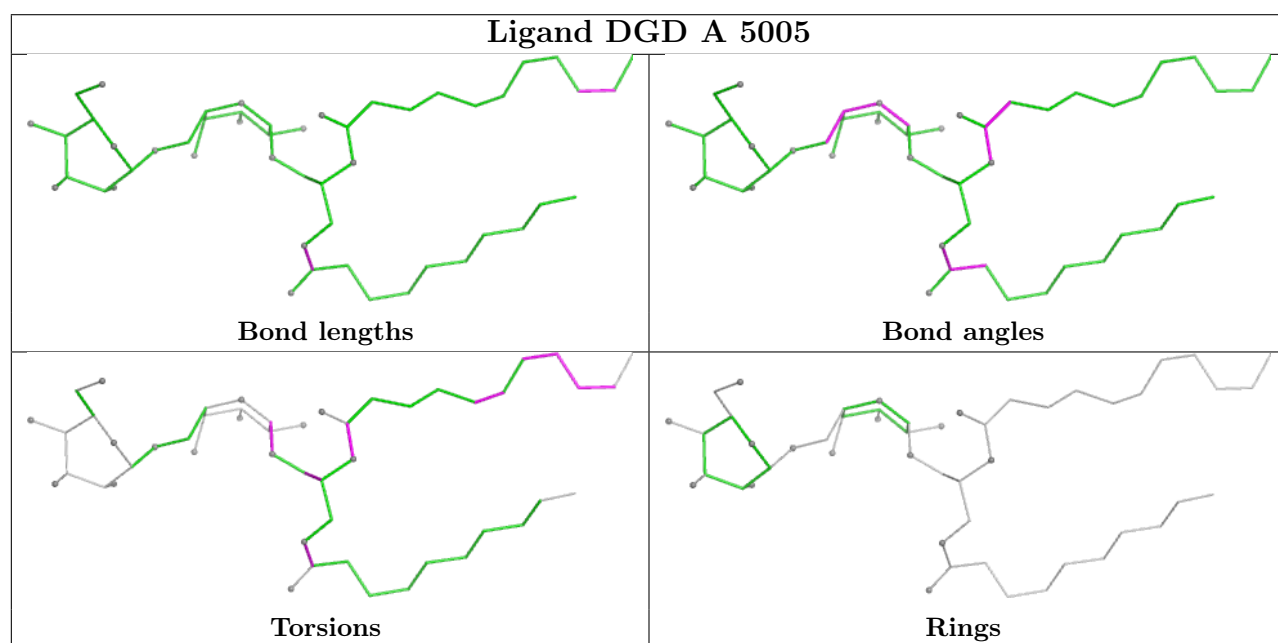
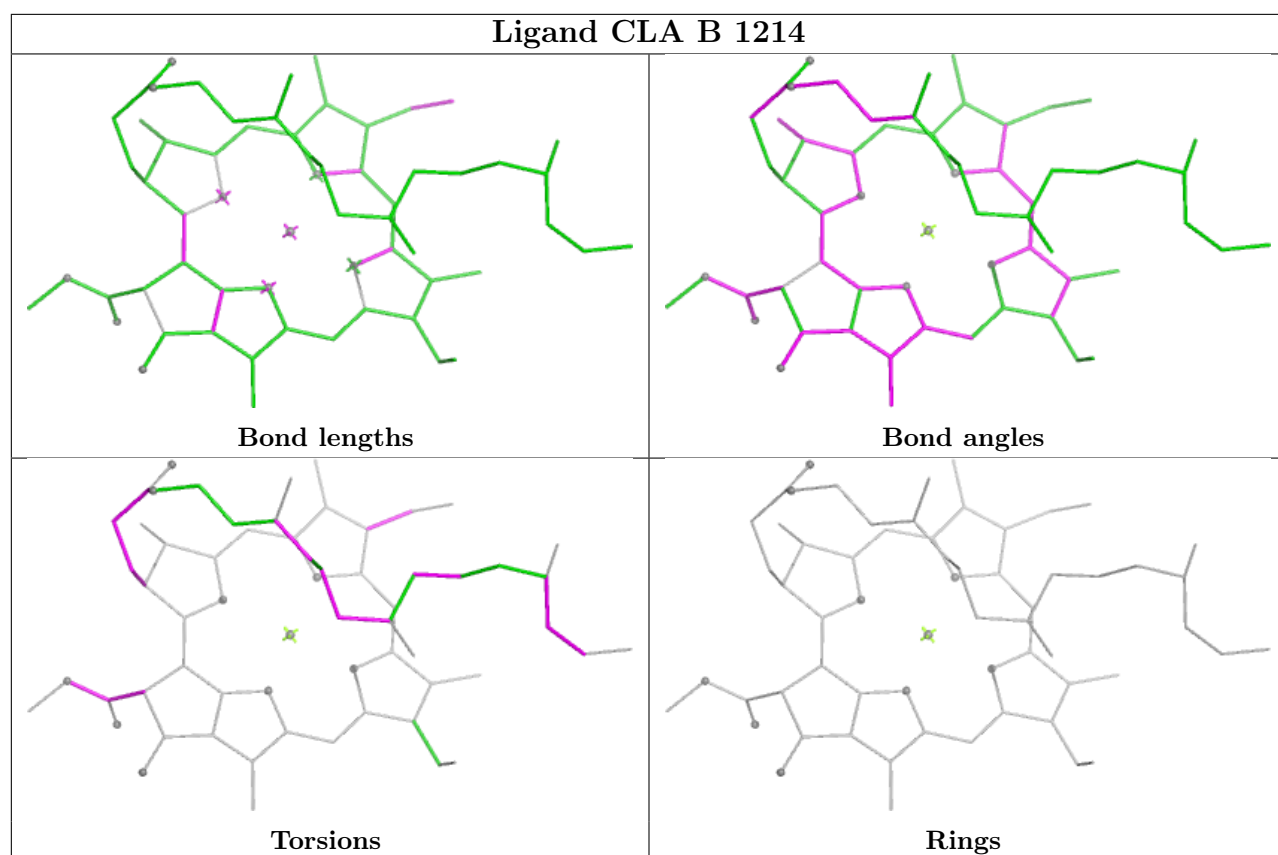


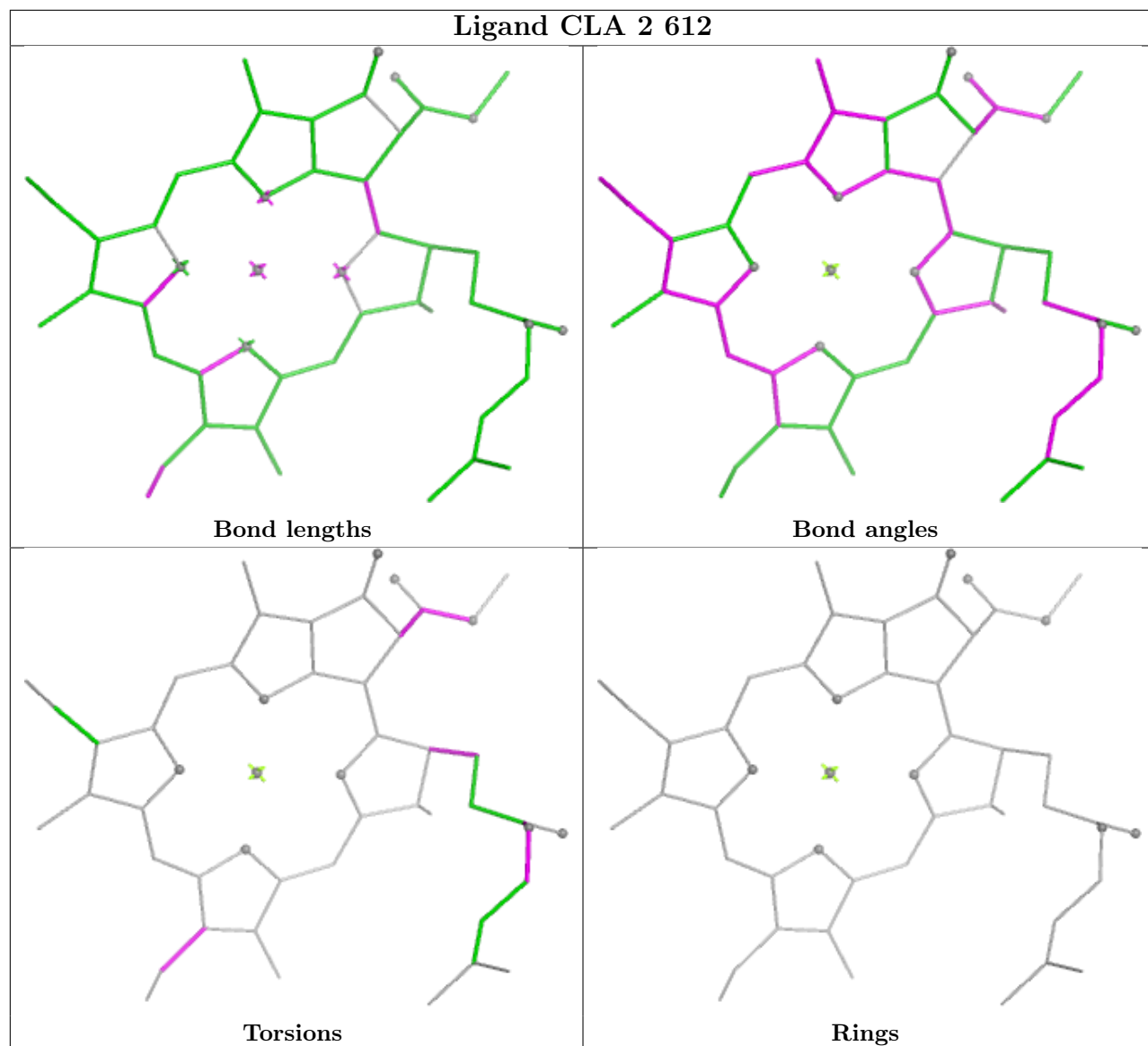
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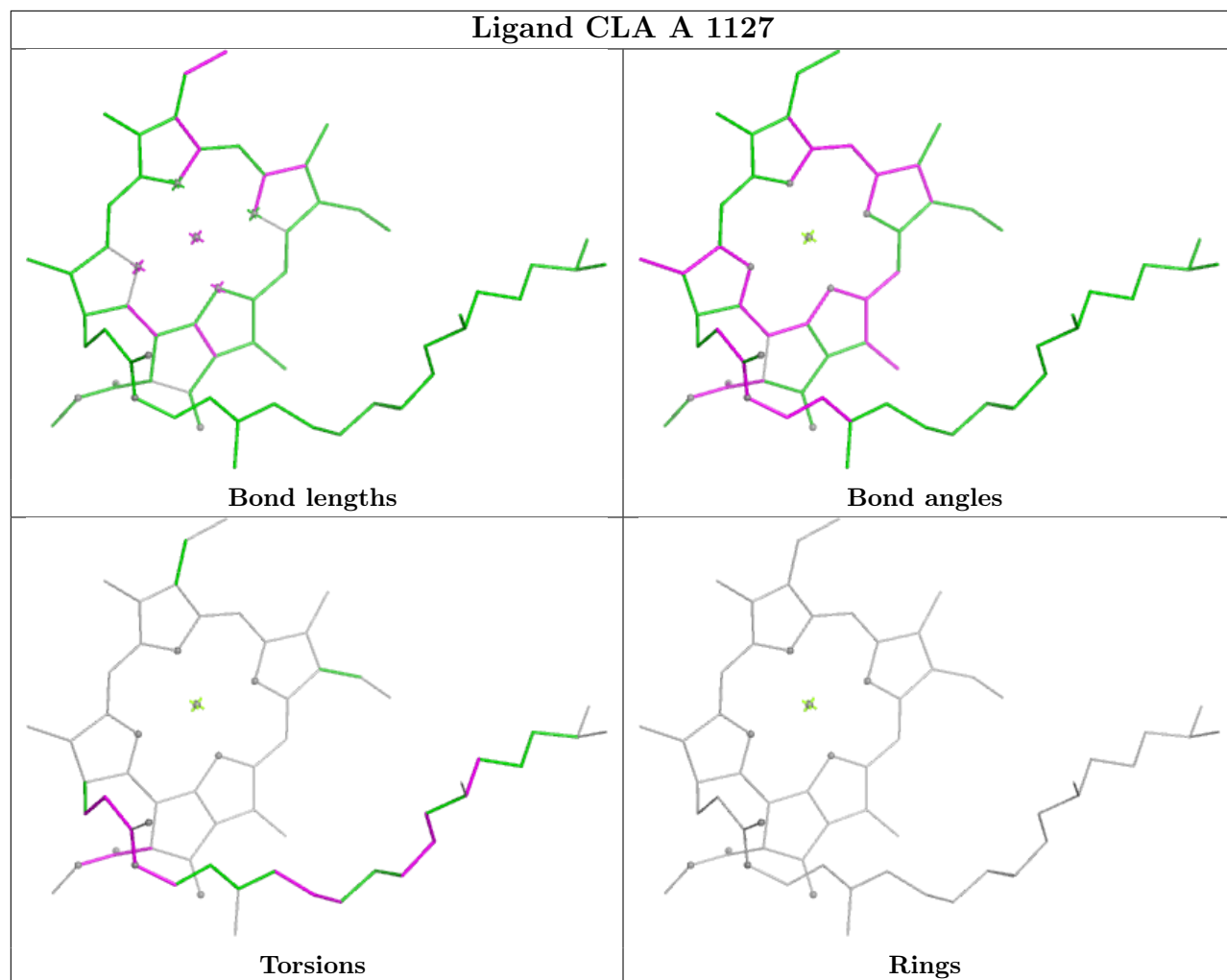


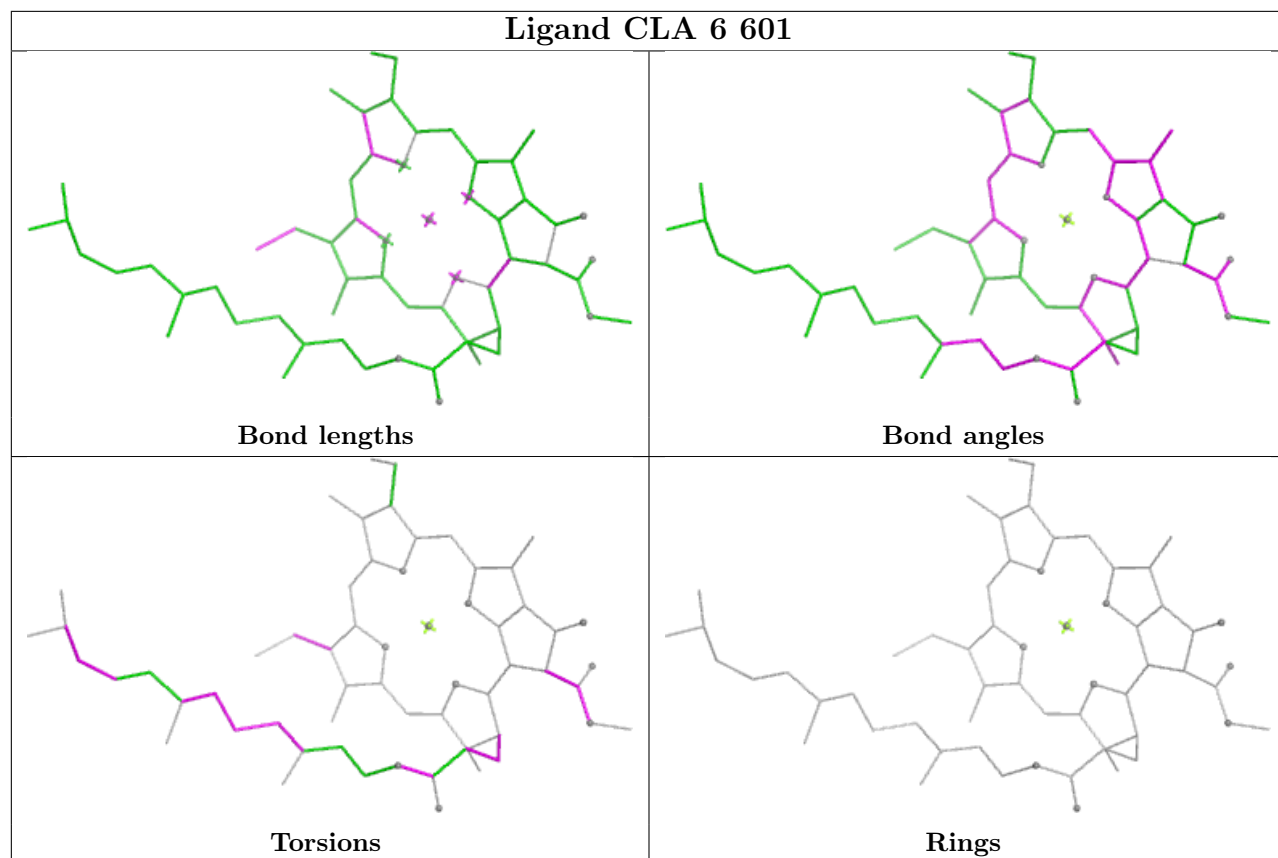




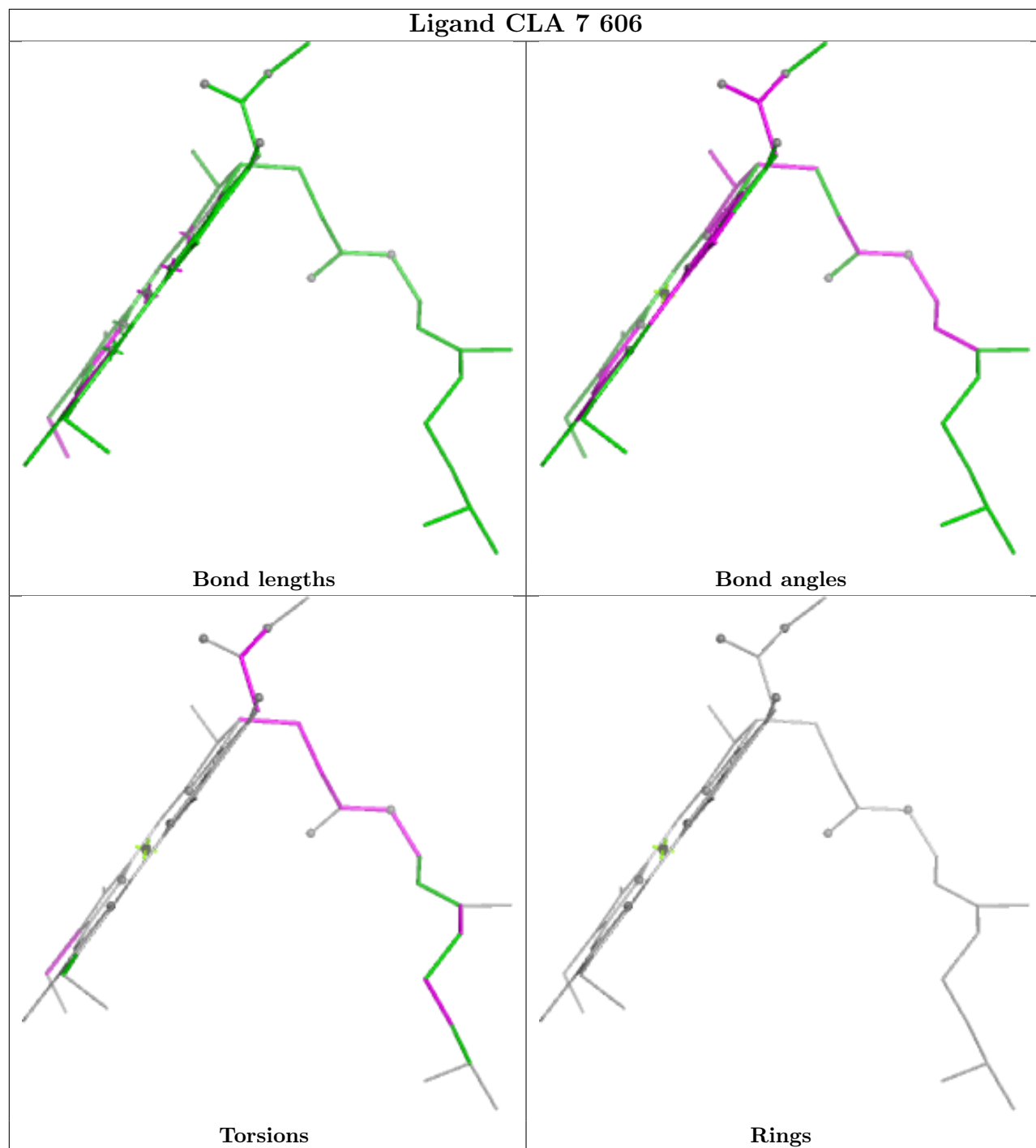




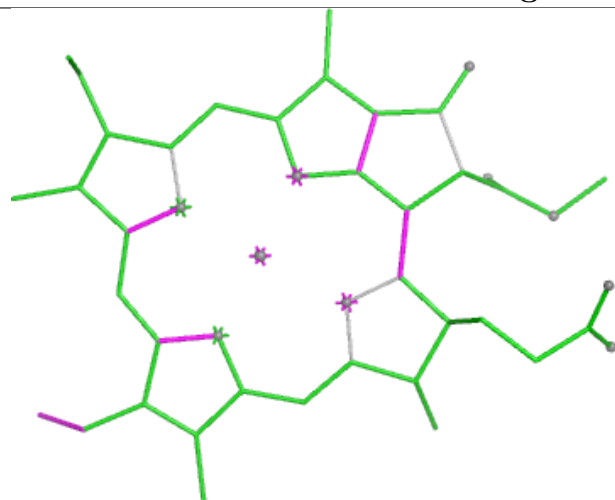




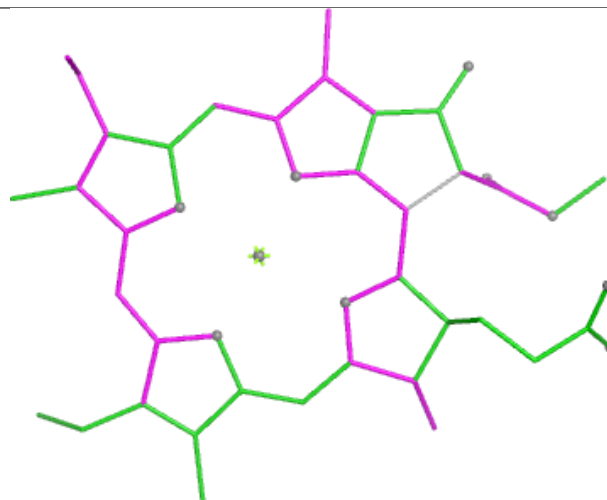
Ligand CLA 7 606



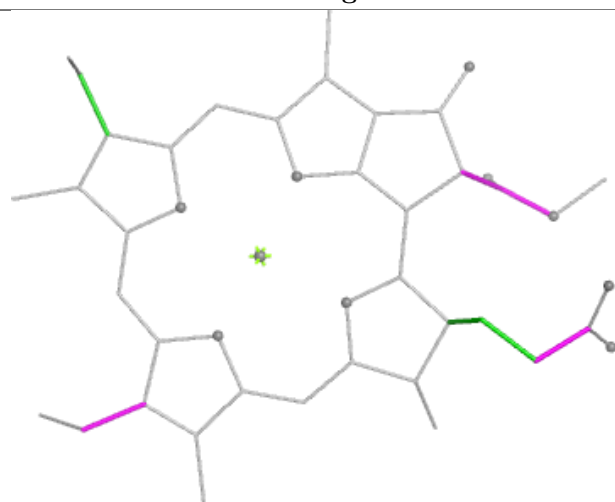
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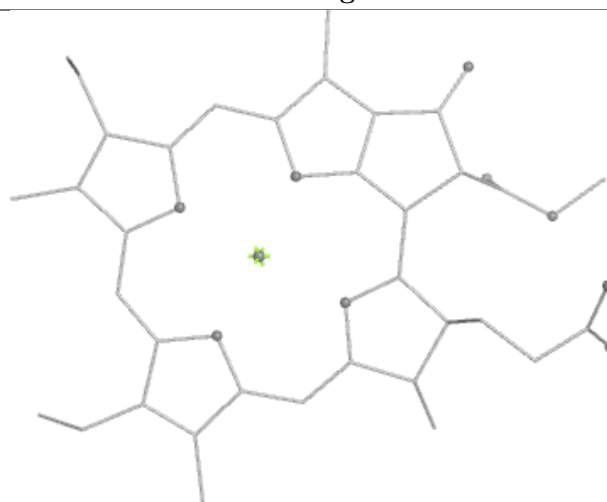
Bond lengths



Bond angles

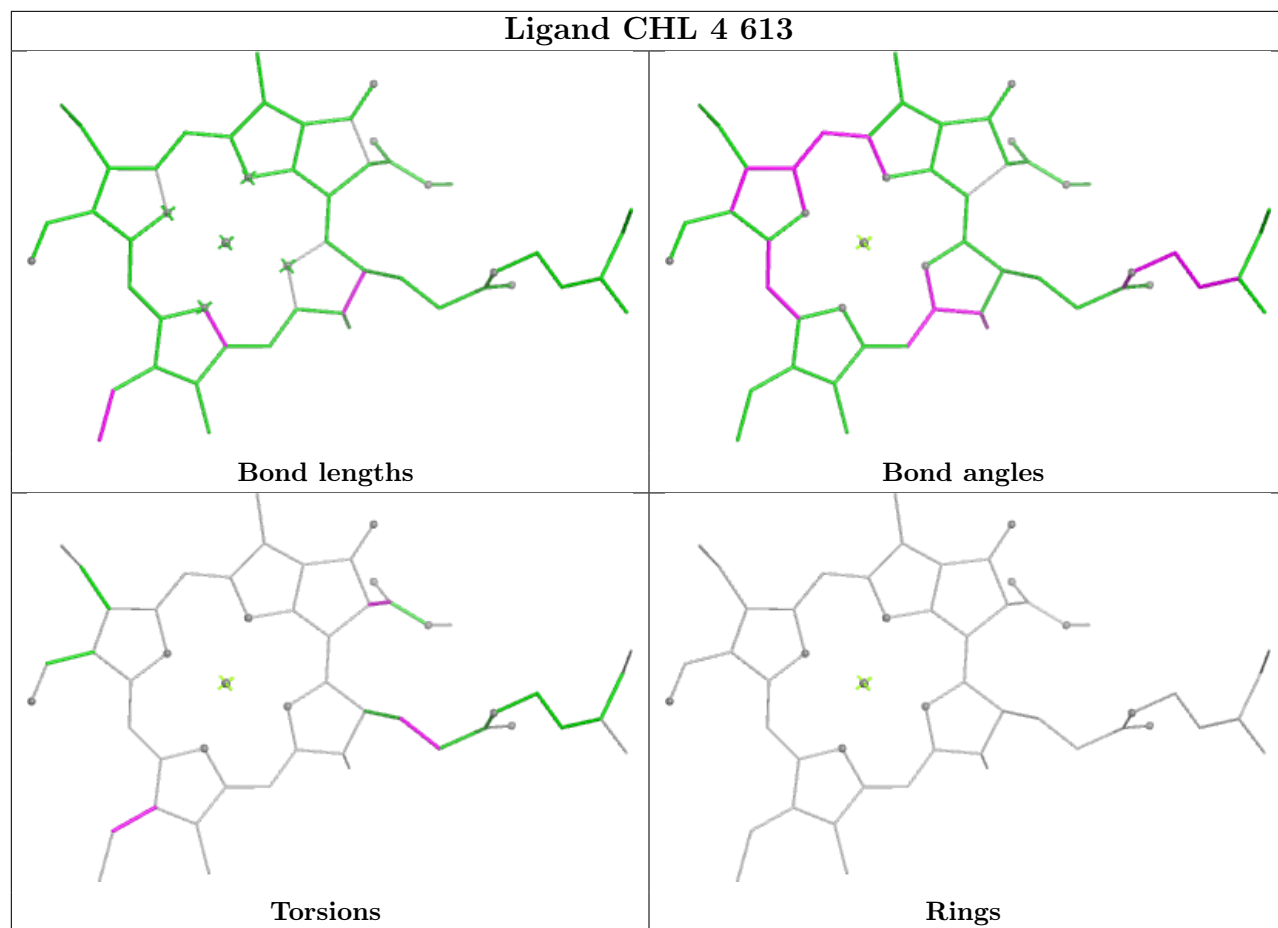


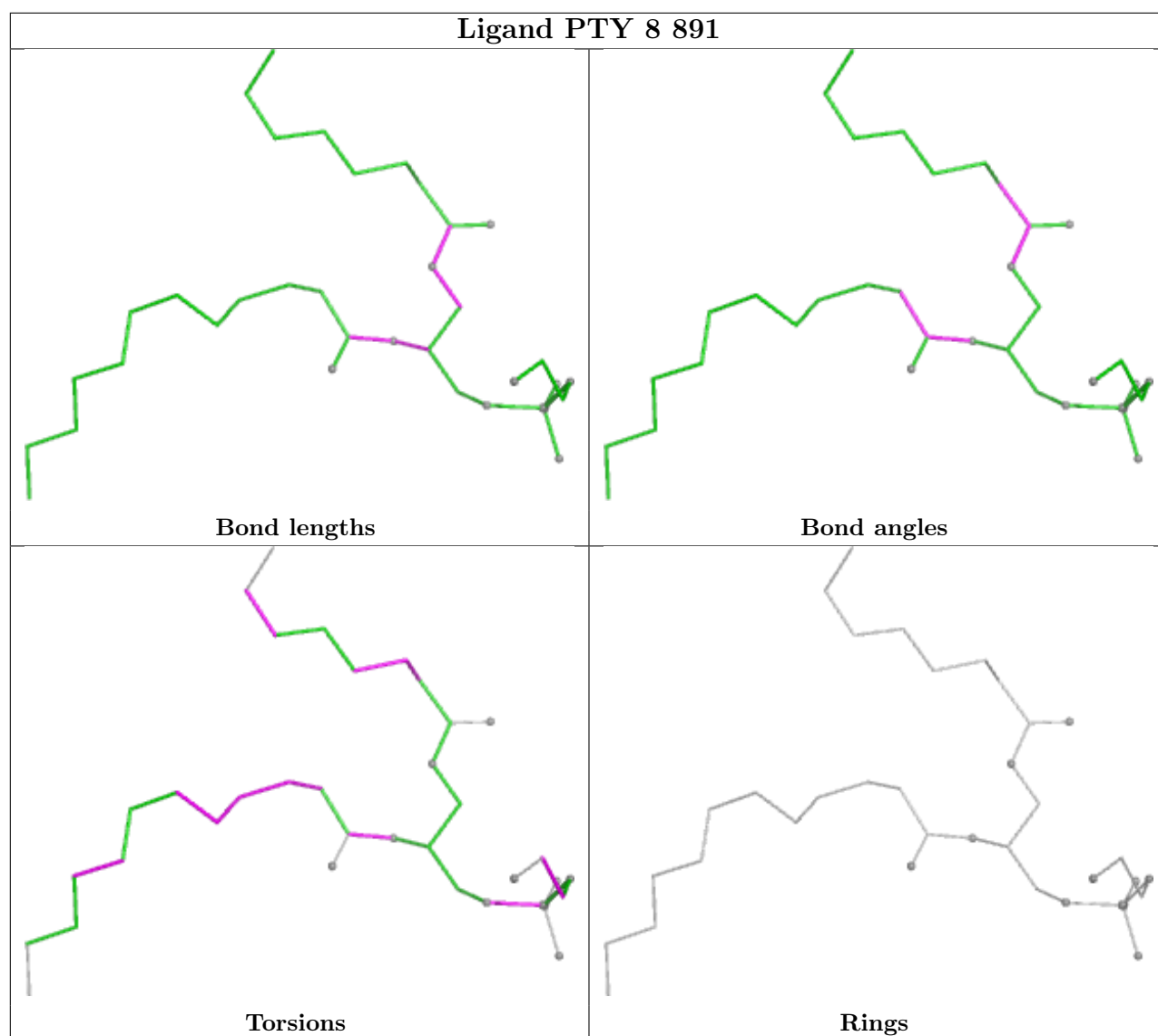
Torsions

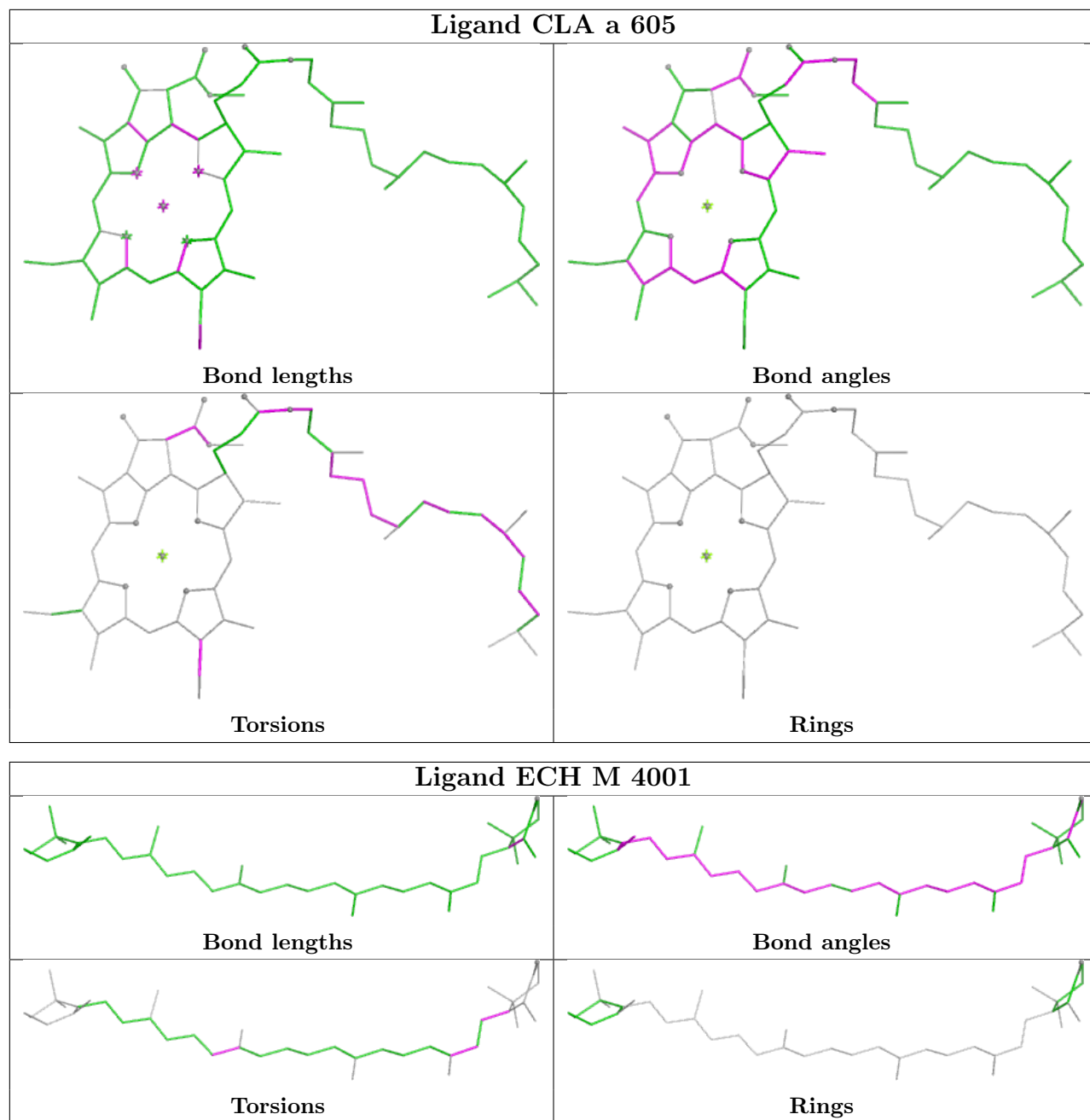


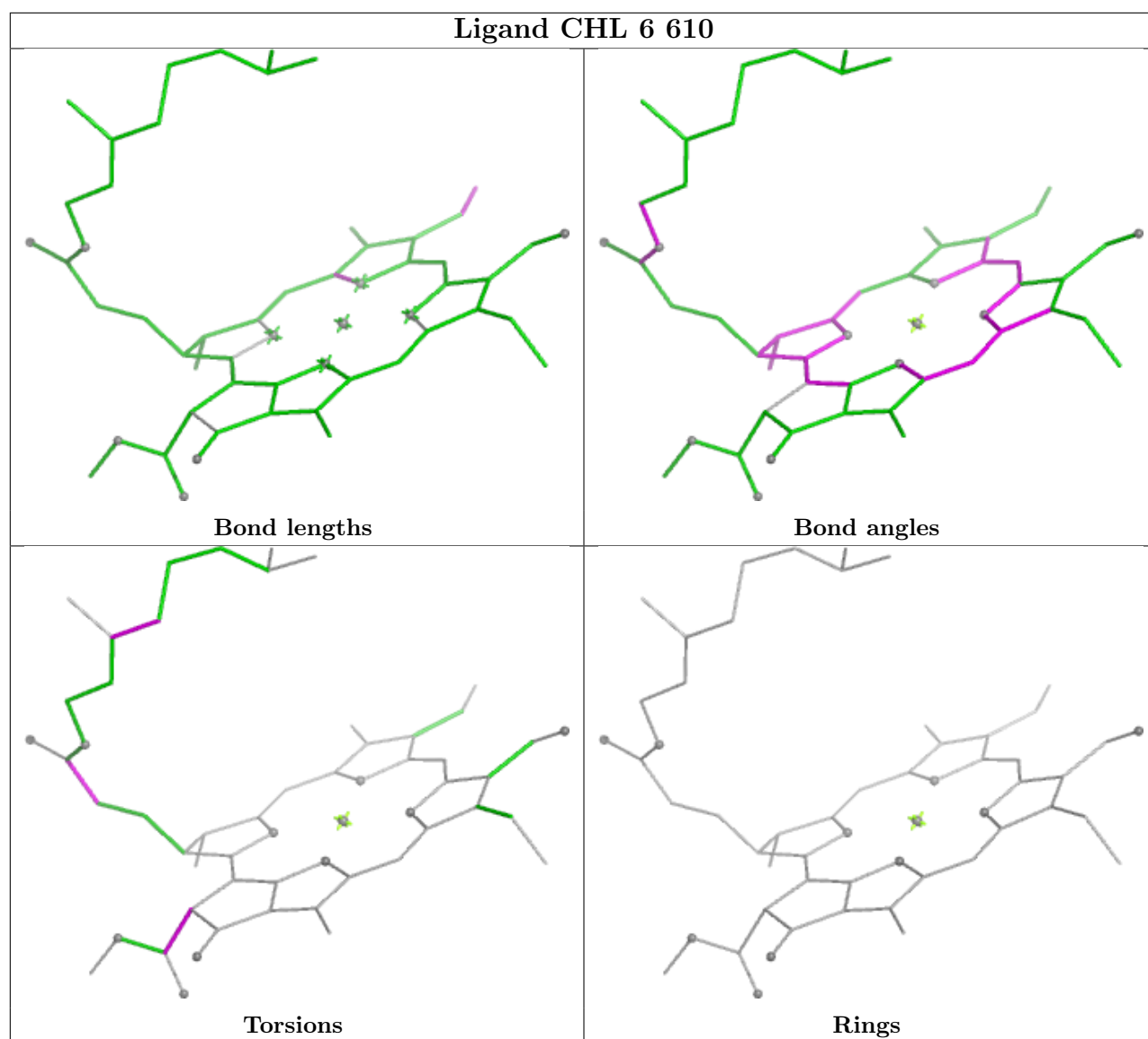
Rings

Ligand CHL 4 613

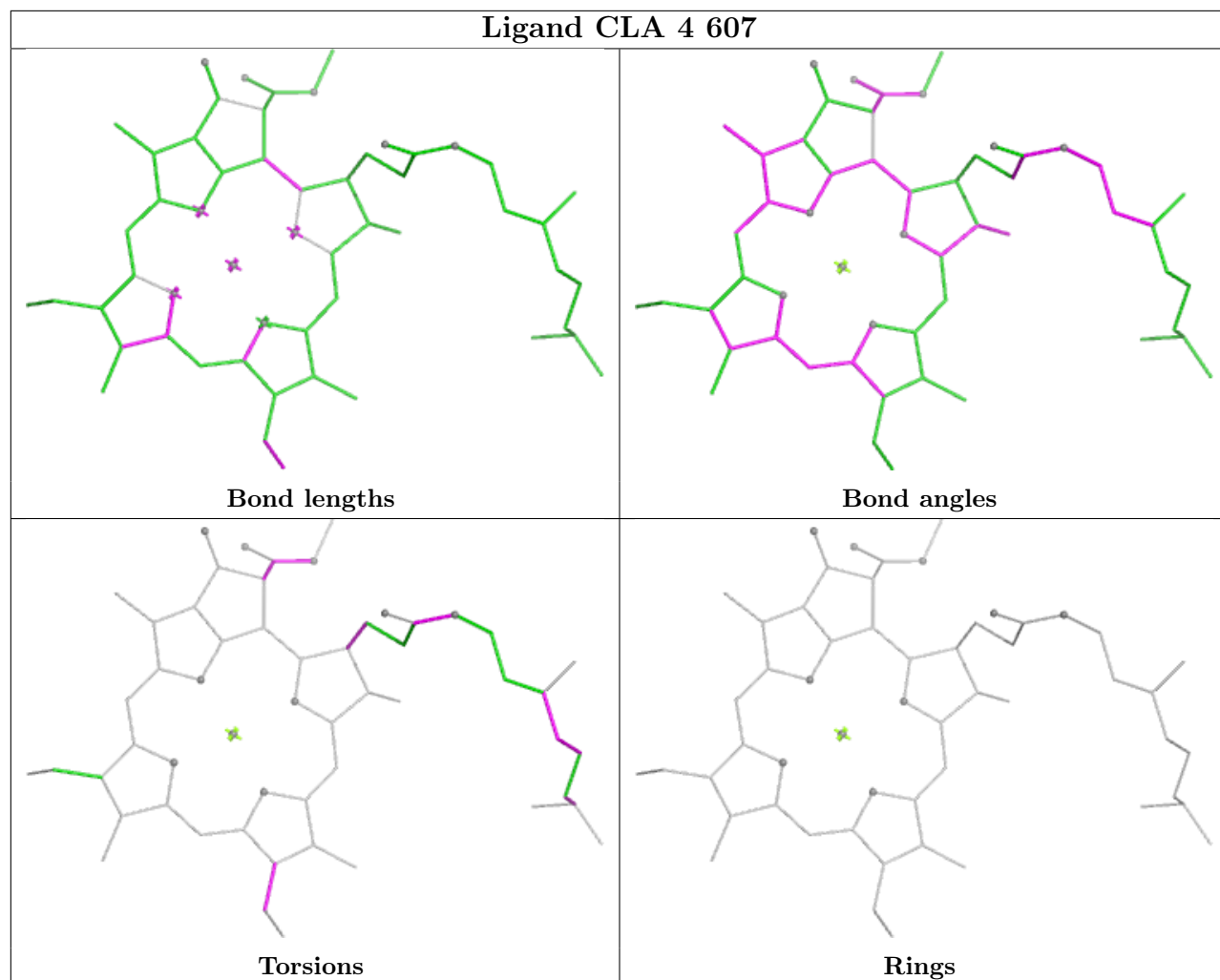




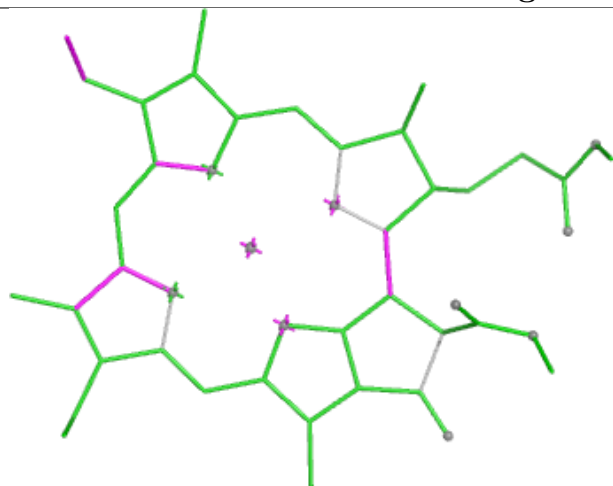




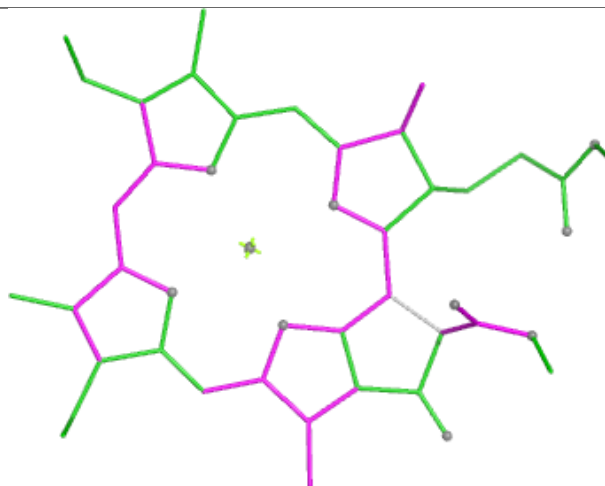
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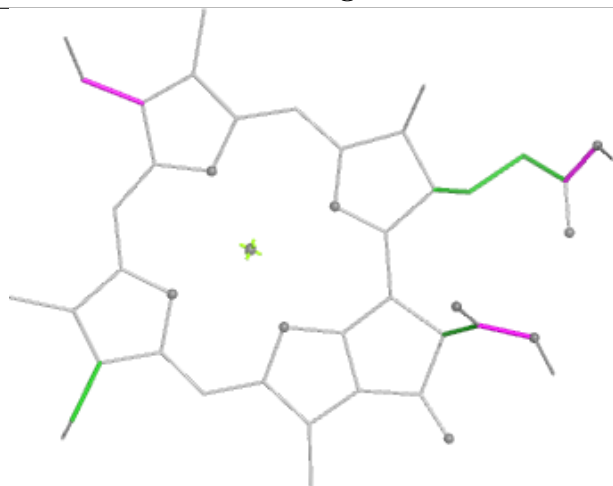
Ligand CLA 9 602



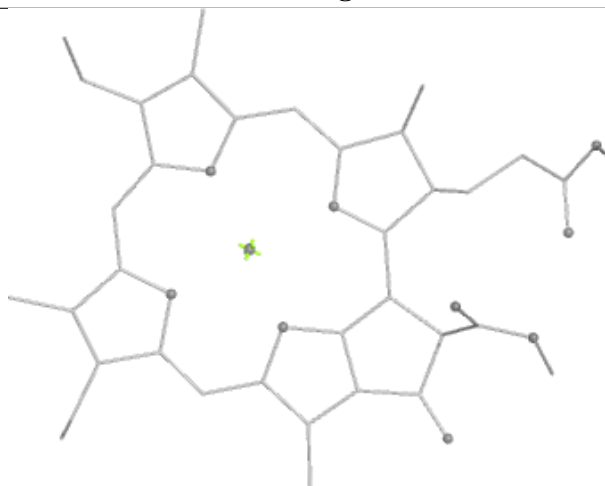
Bond lengths



Bond angles

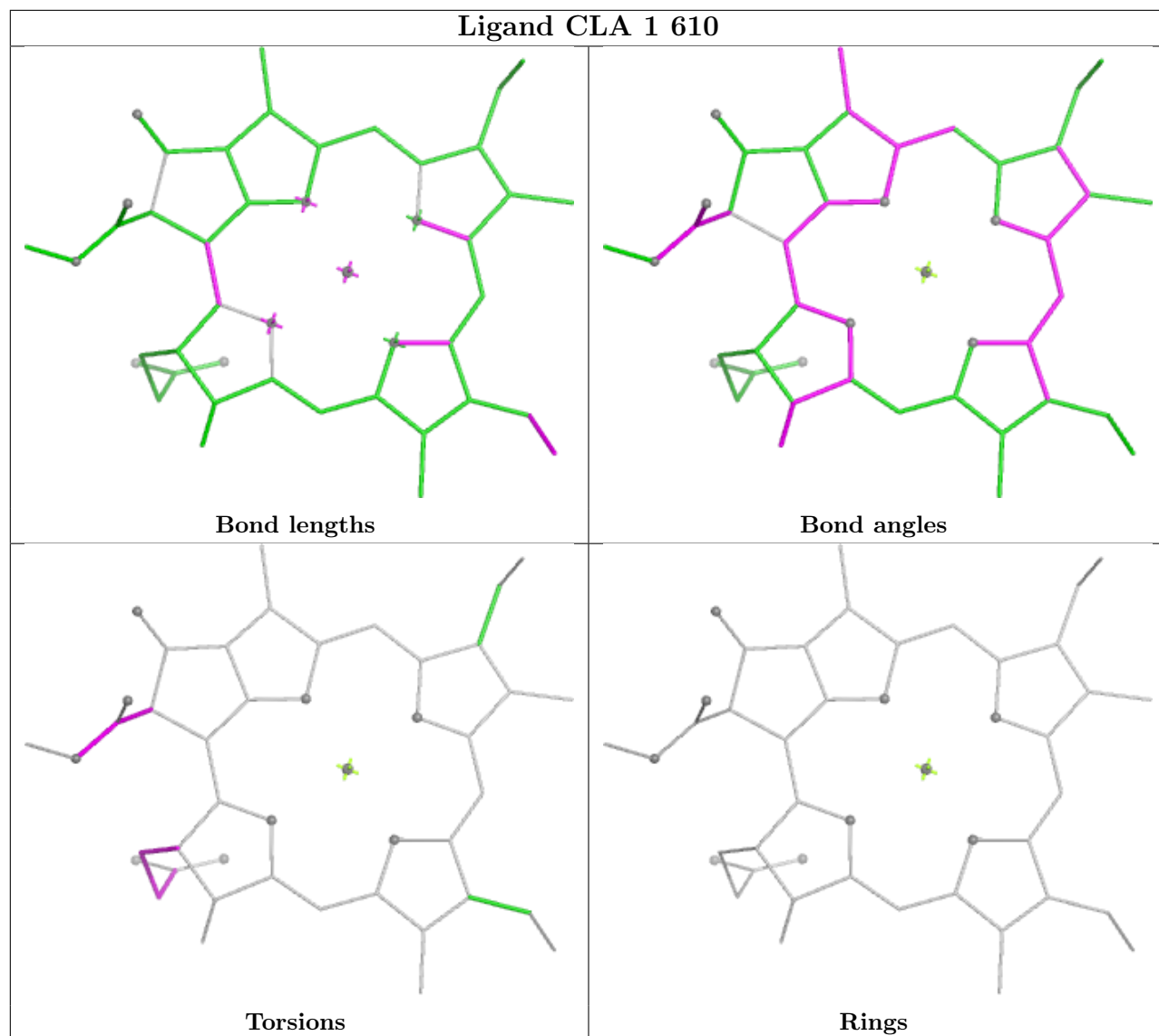


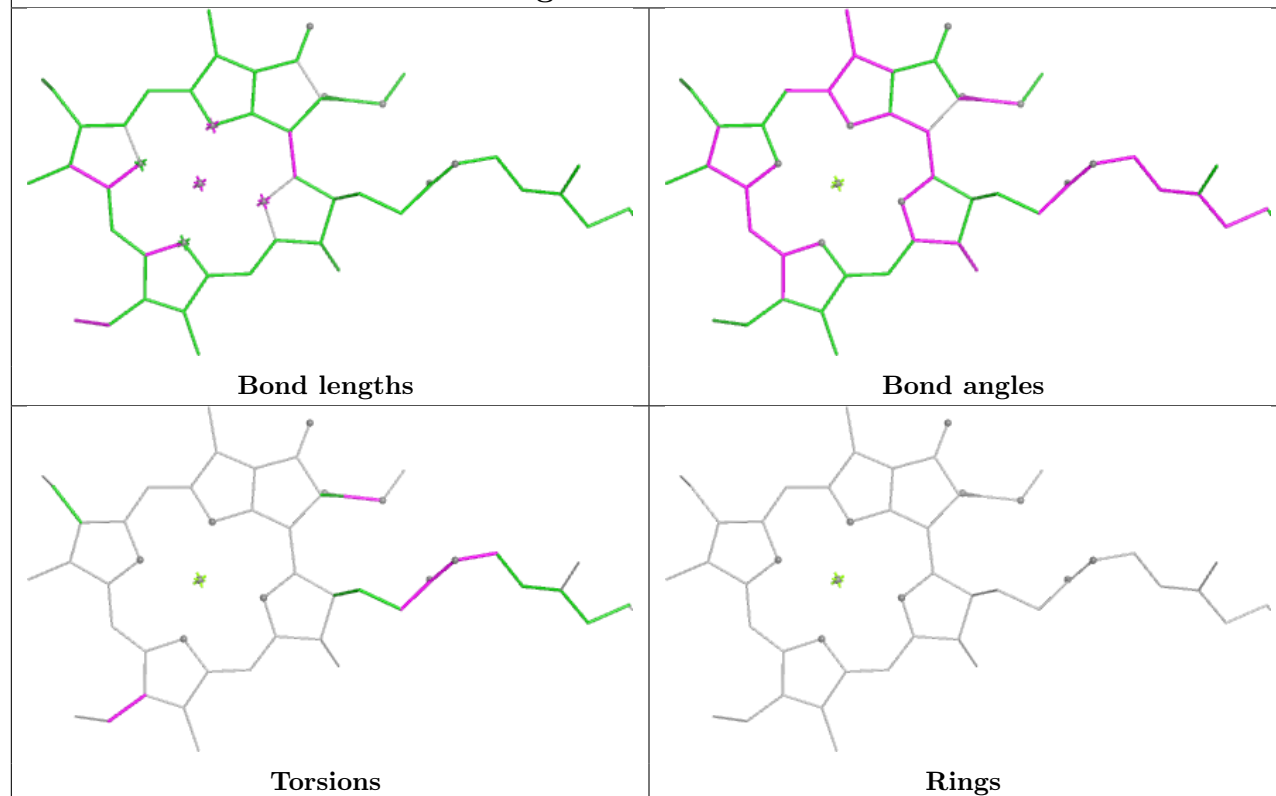
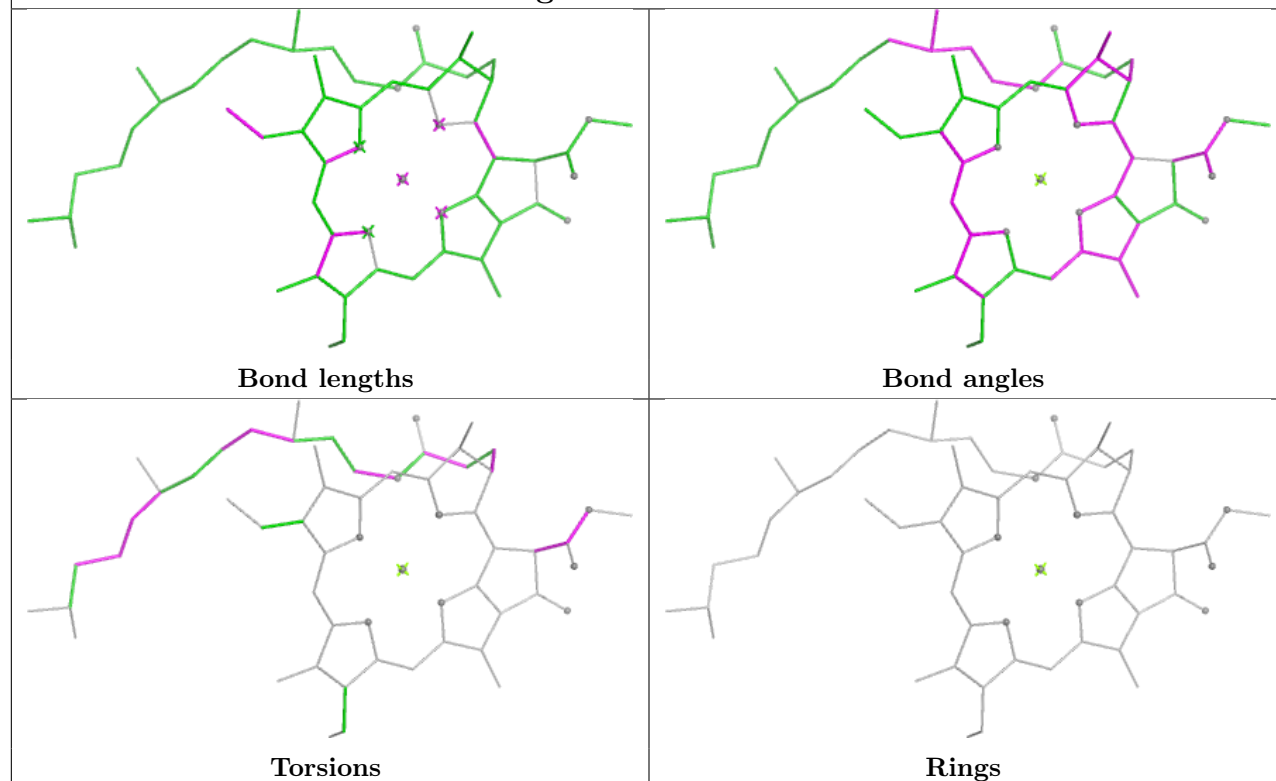
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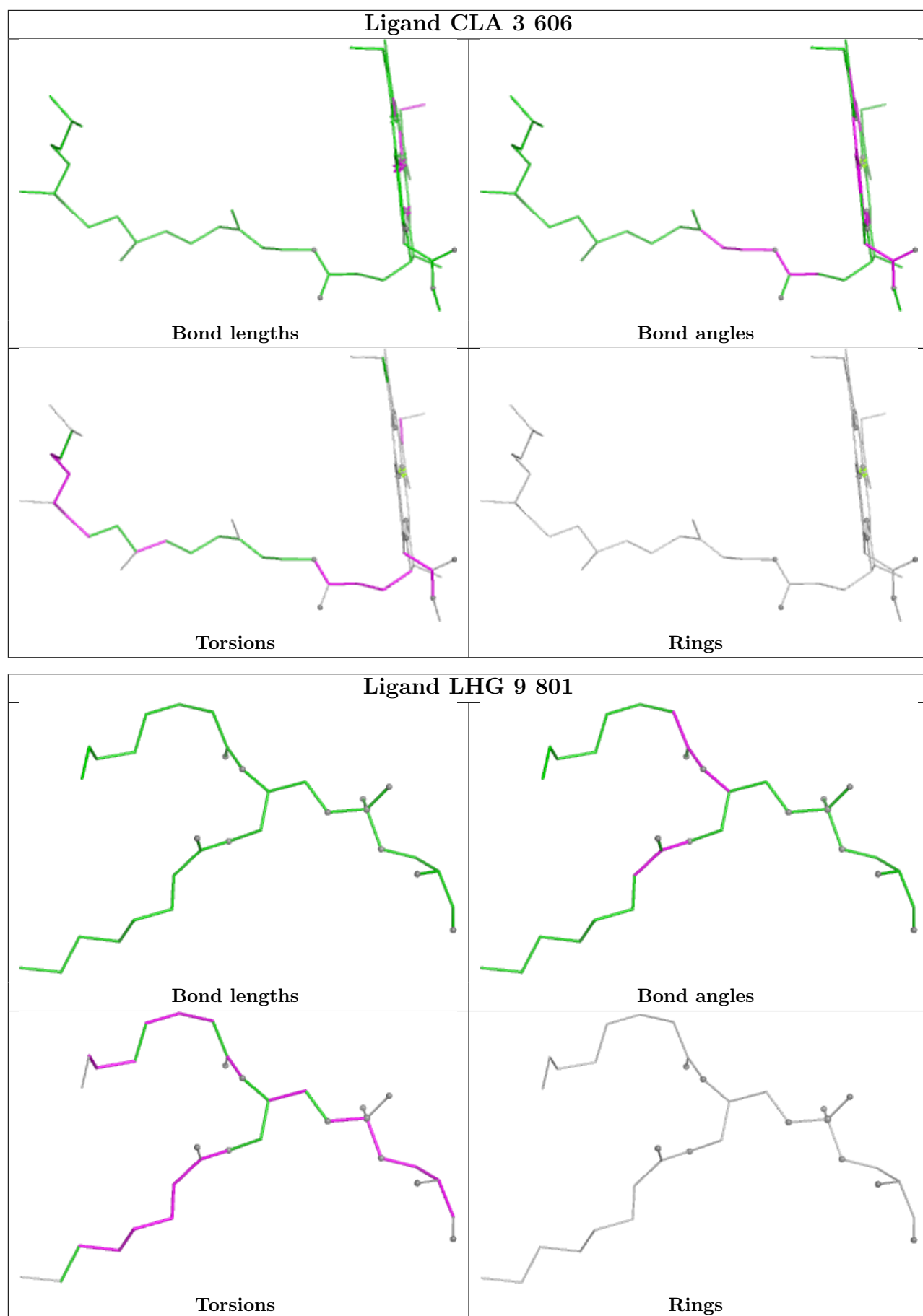


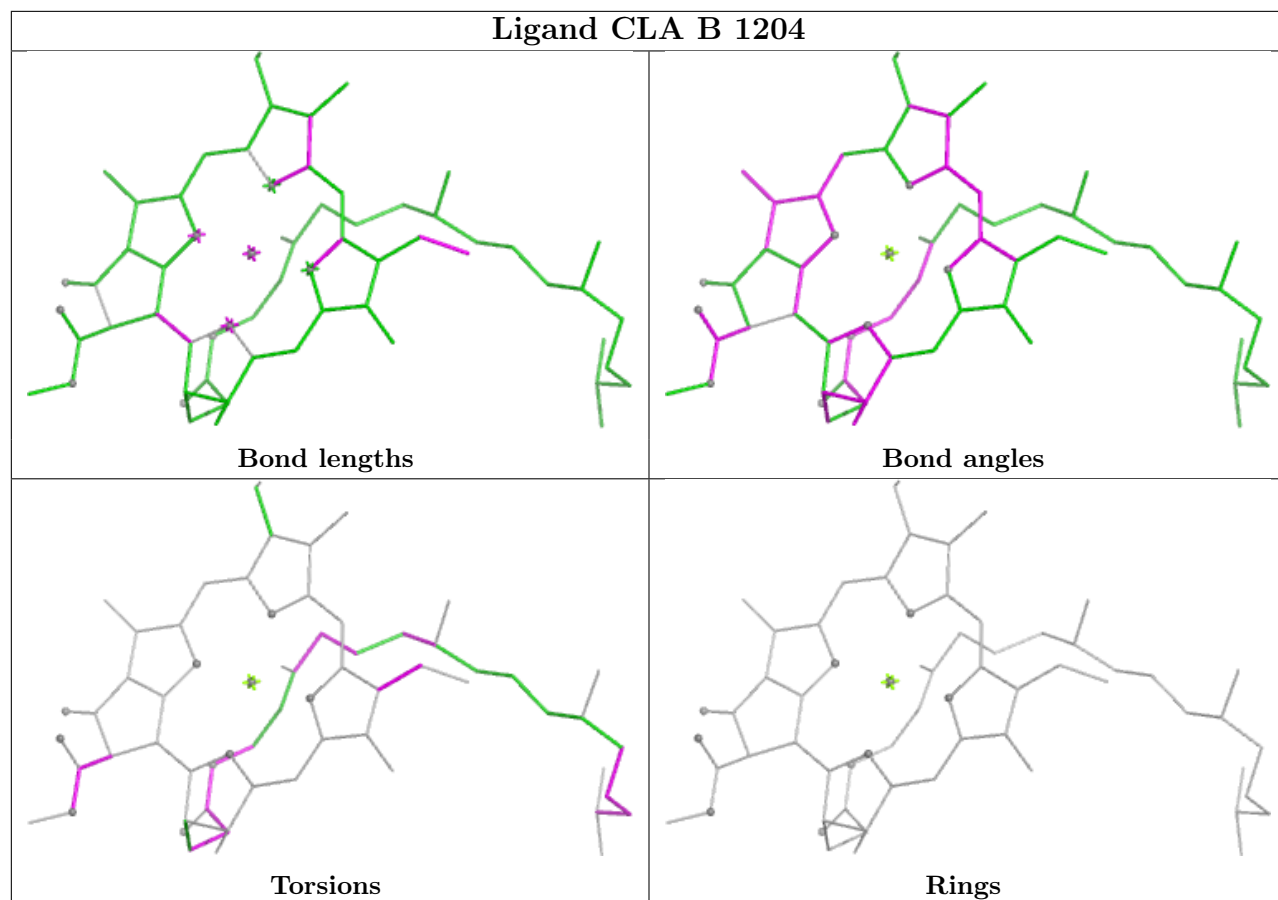
Rings

Ligand CLA 1 610

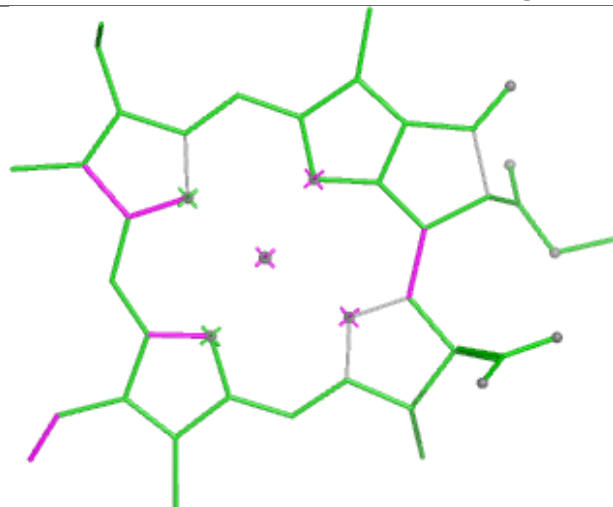


Ligand CLA 5 602**Ligand CLA 2 601**

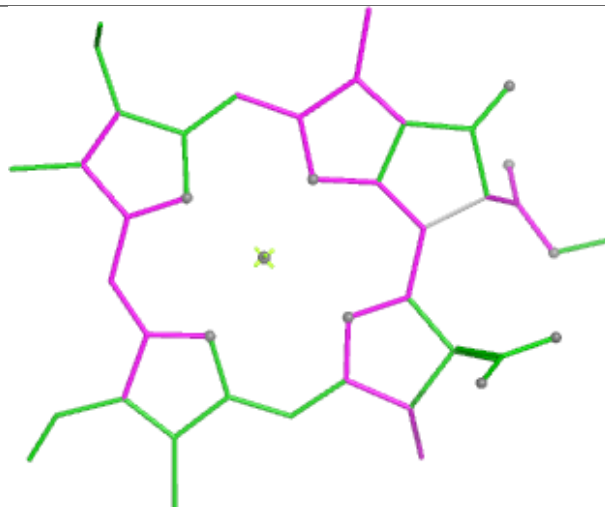




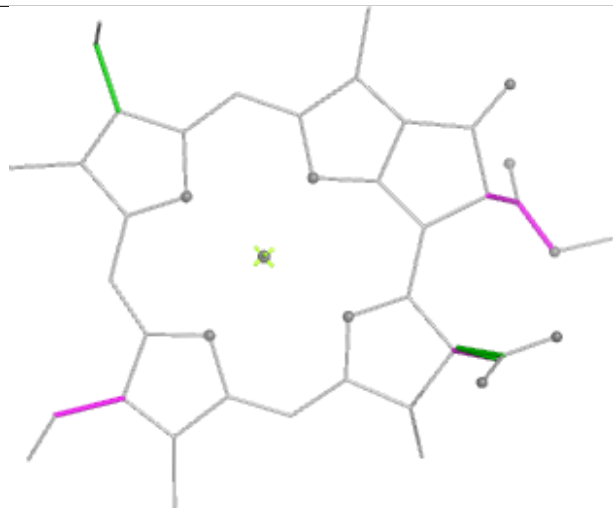
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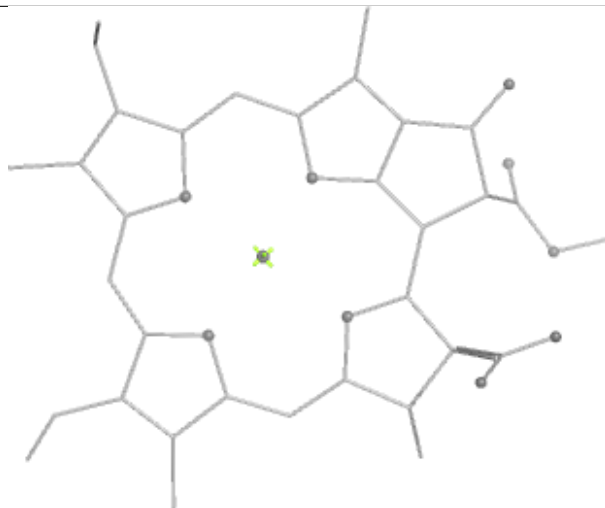
Bond lengths



Bond angles

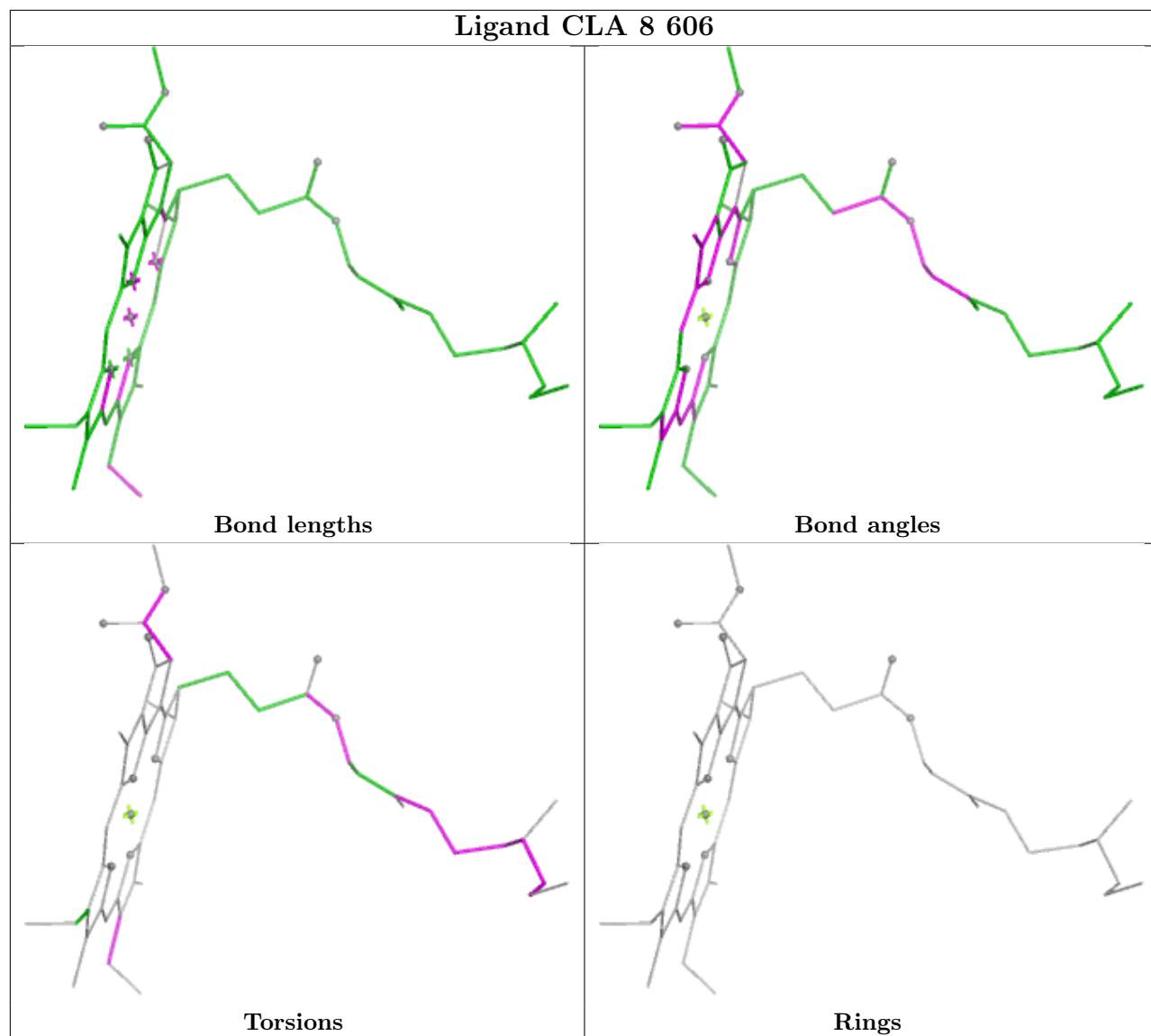


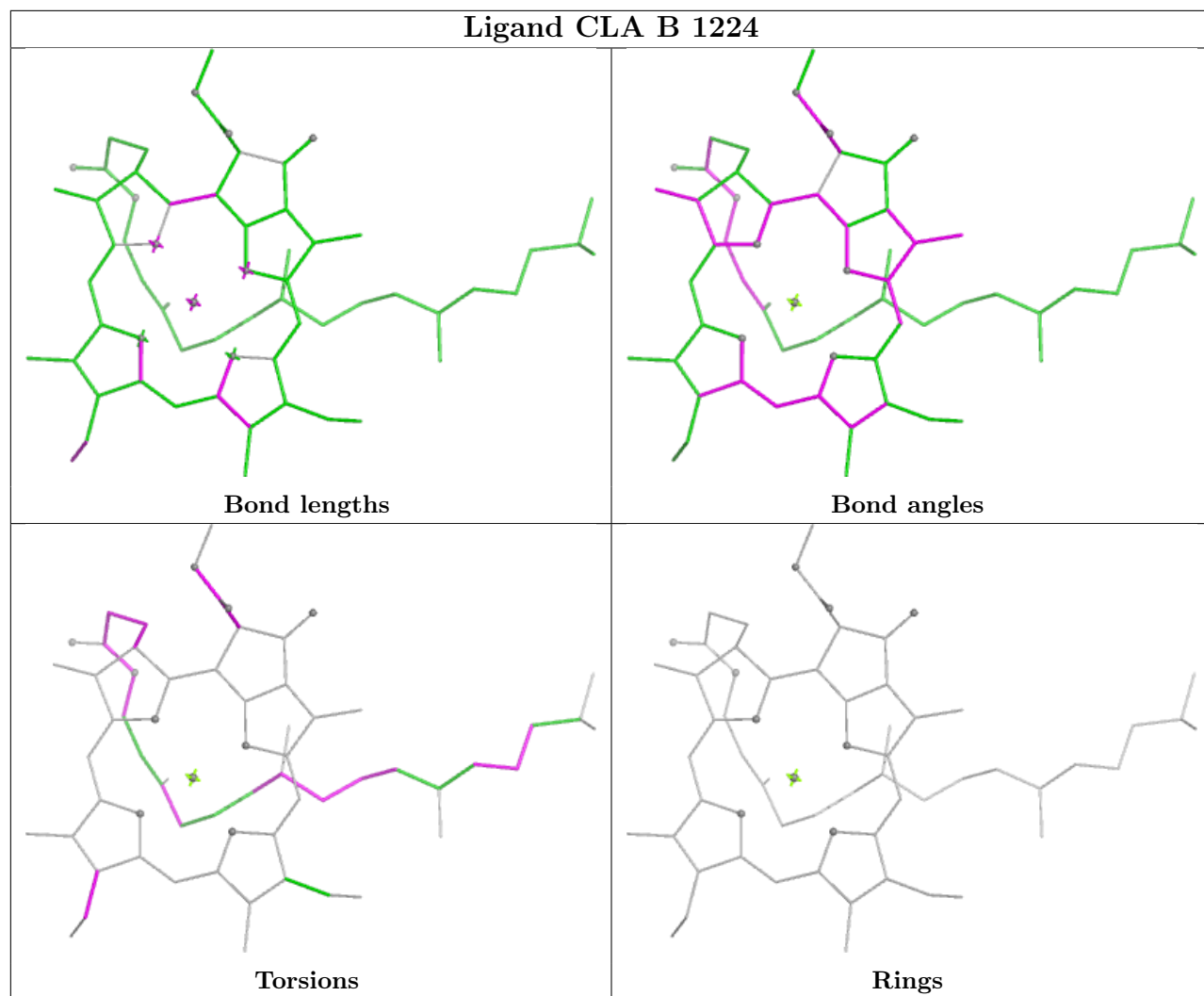
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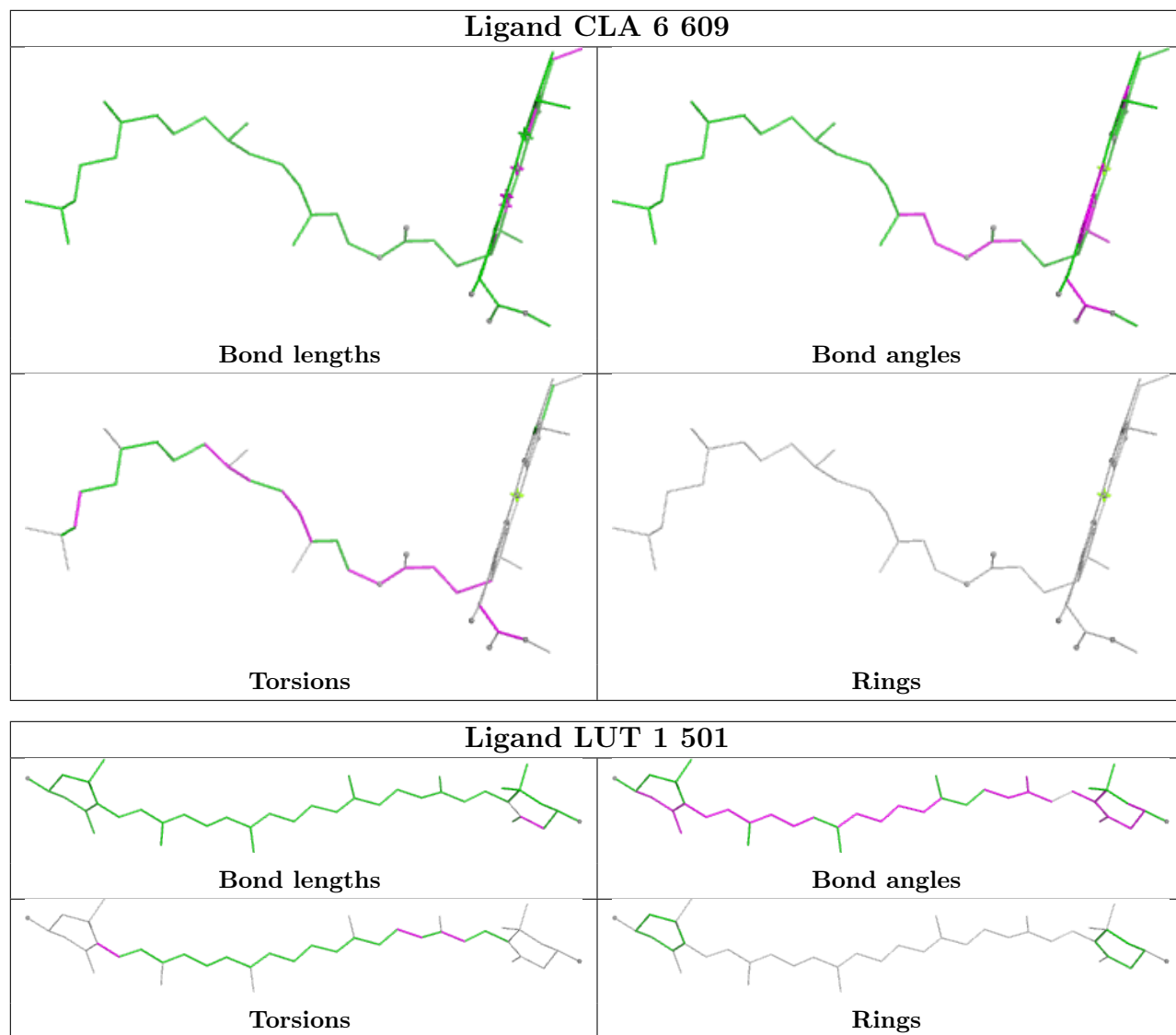


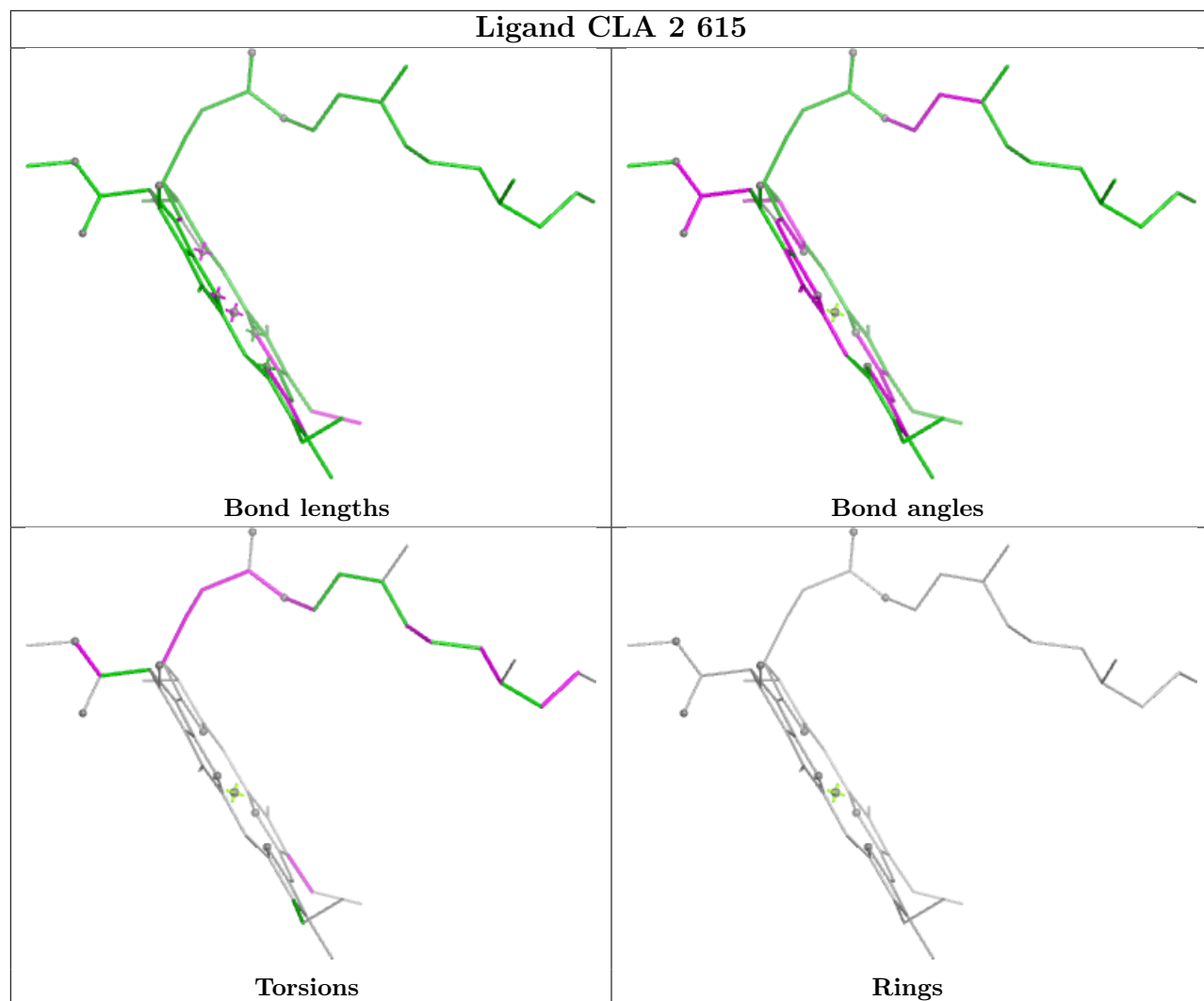
Rings

Ligand CLA 8 606

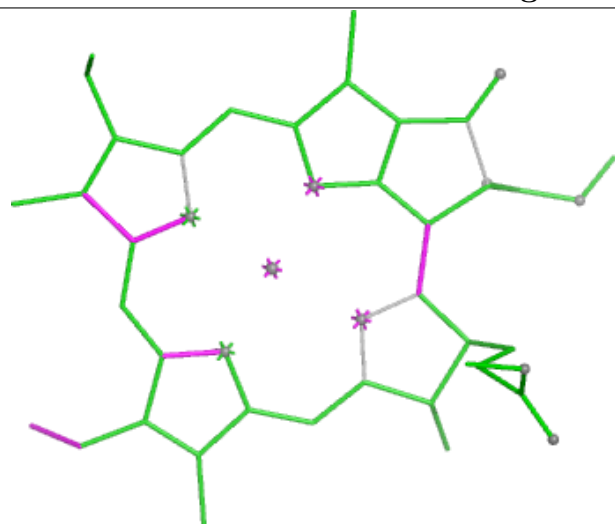




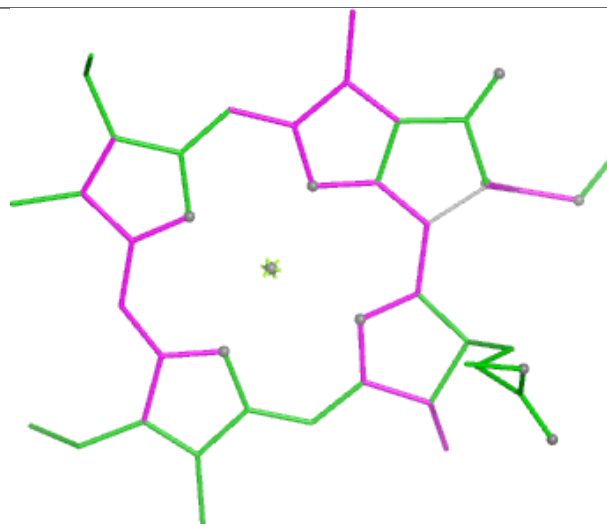




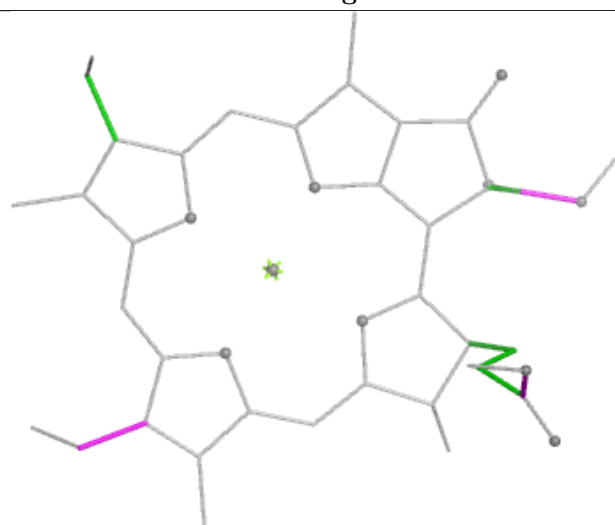
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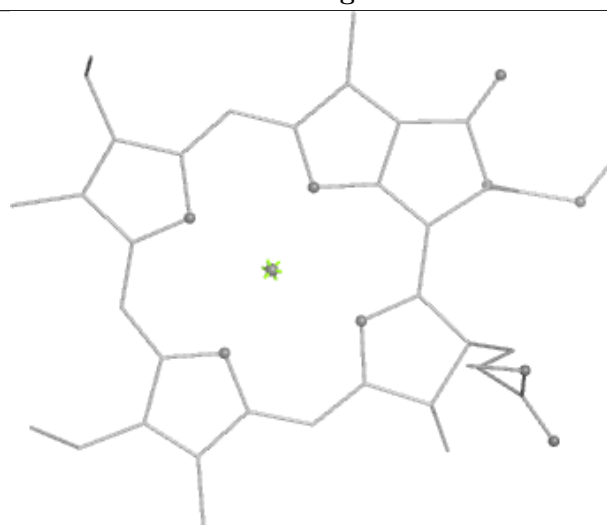
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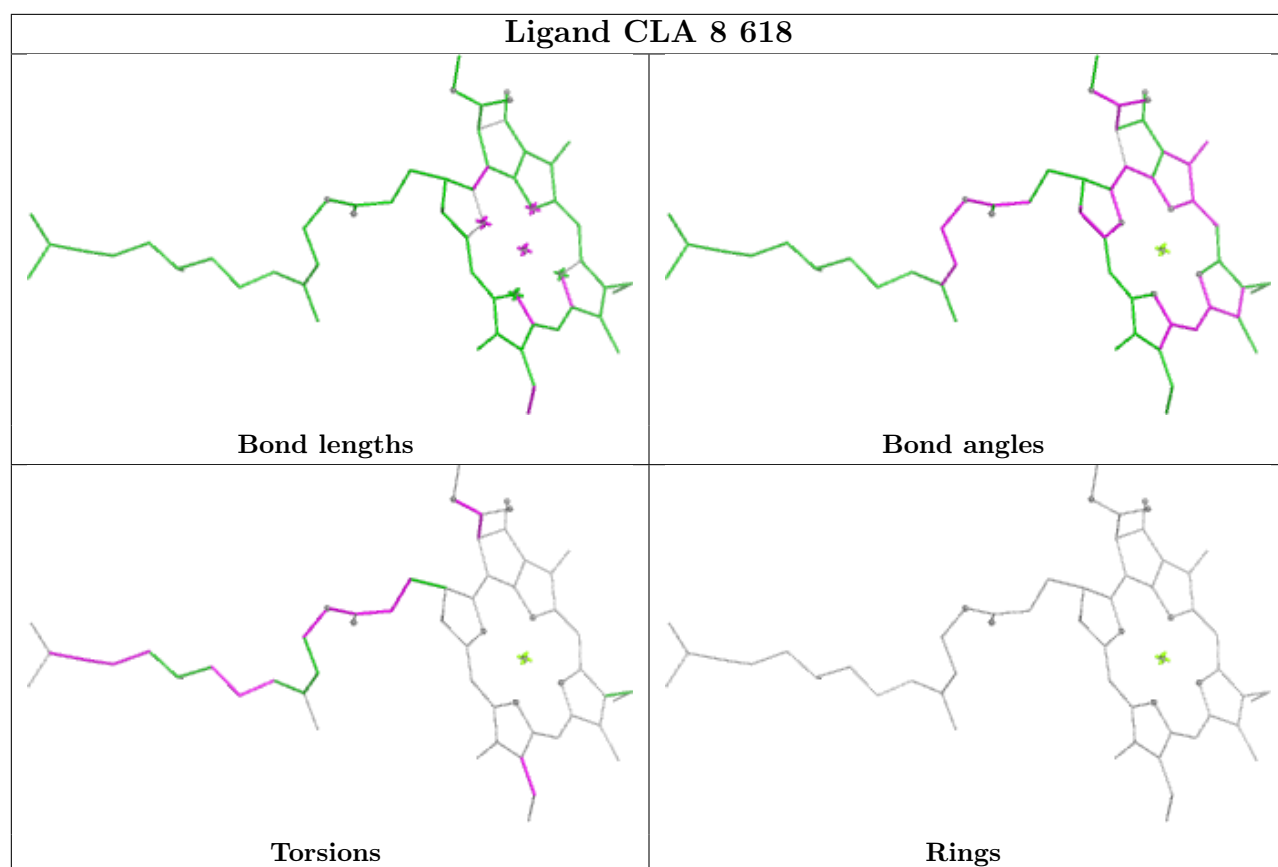
Bond angles



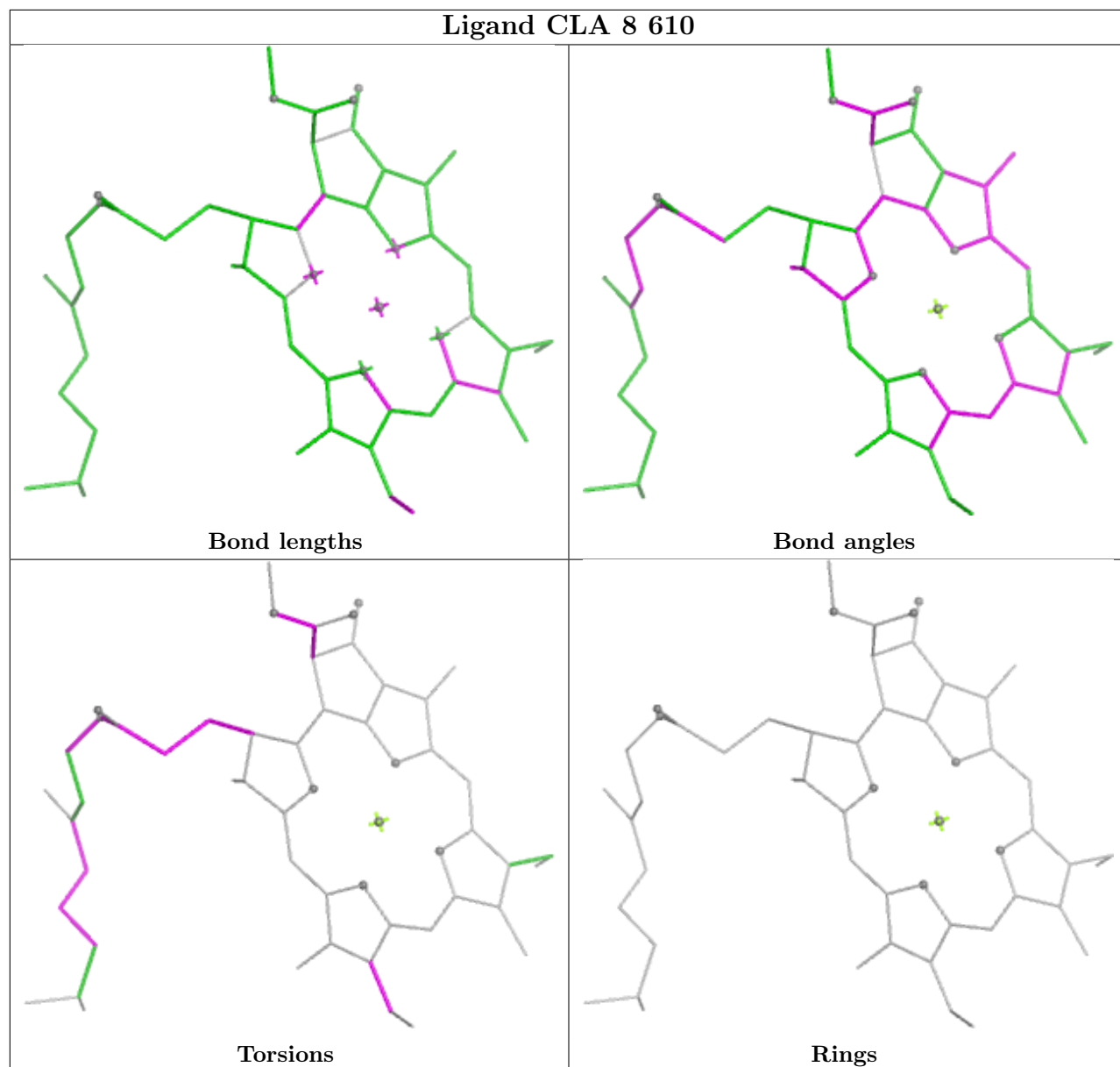
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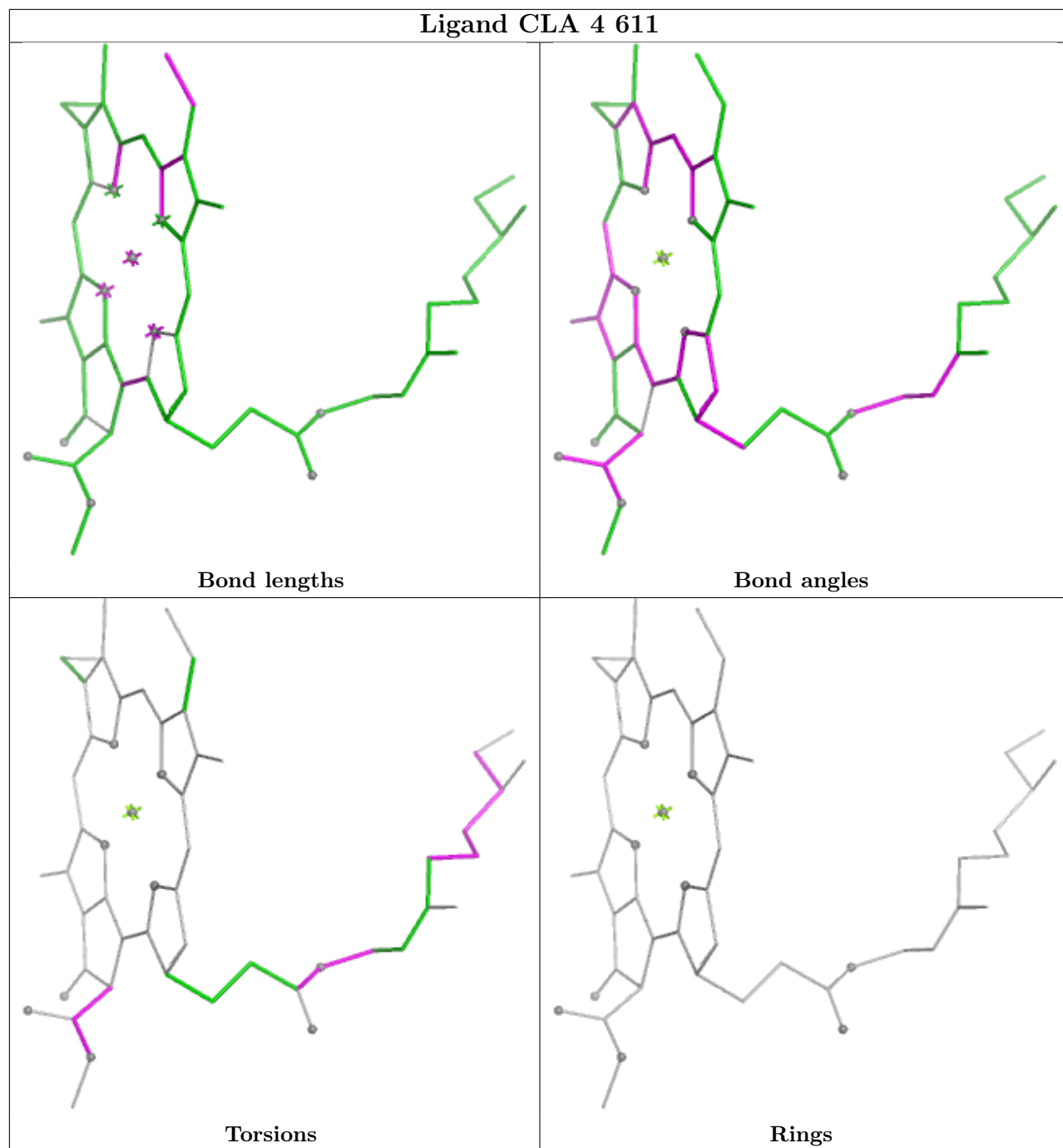
Rings



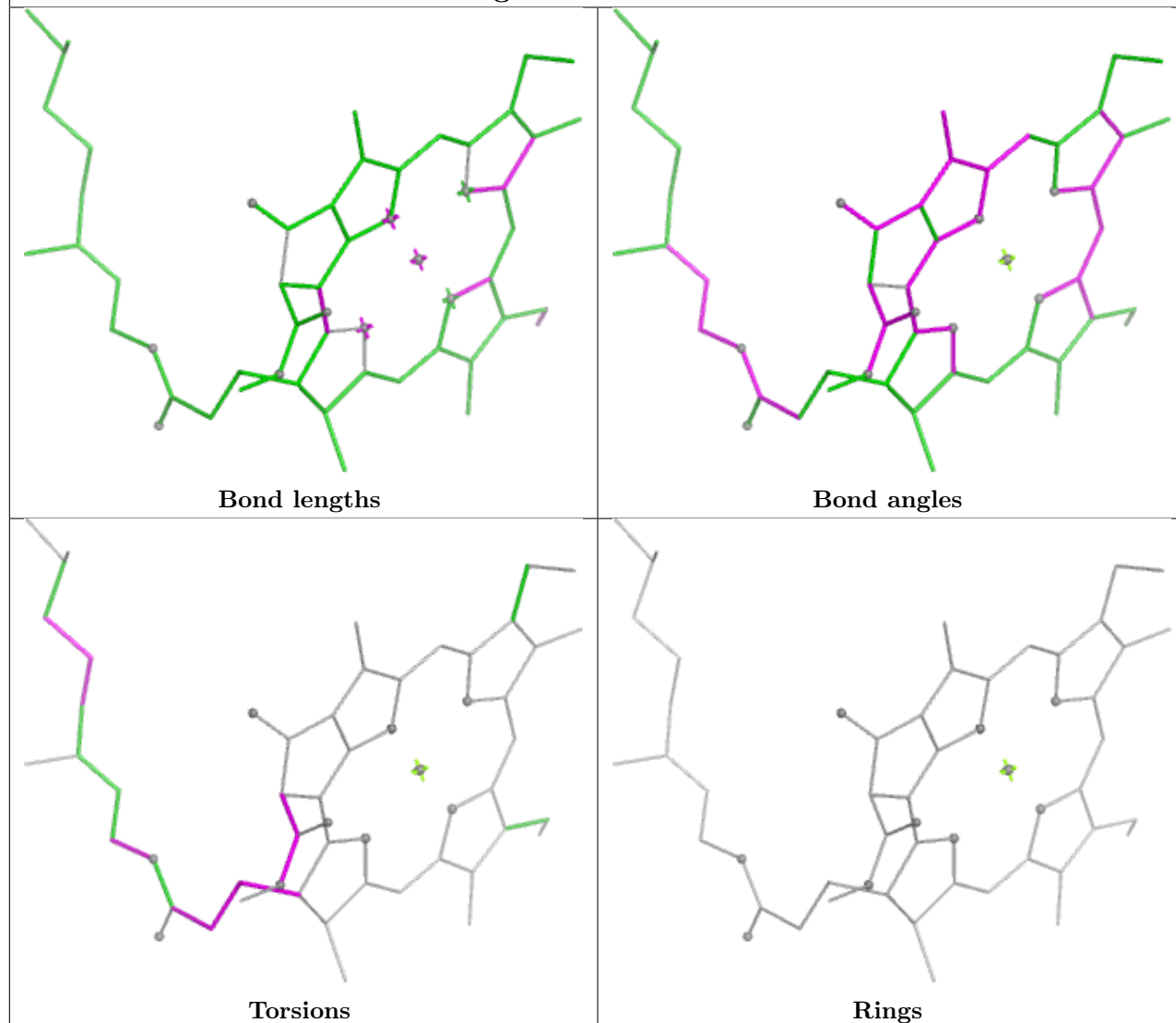
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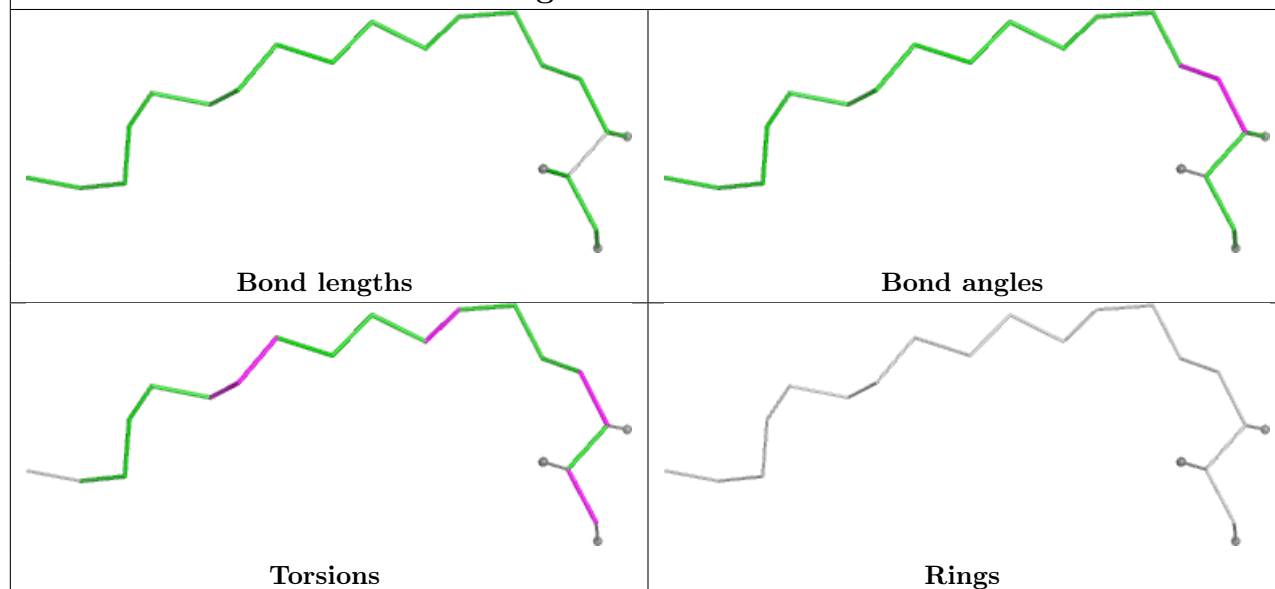
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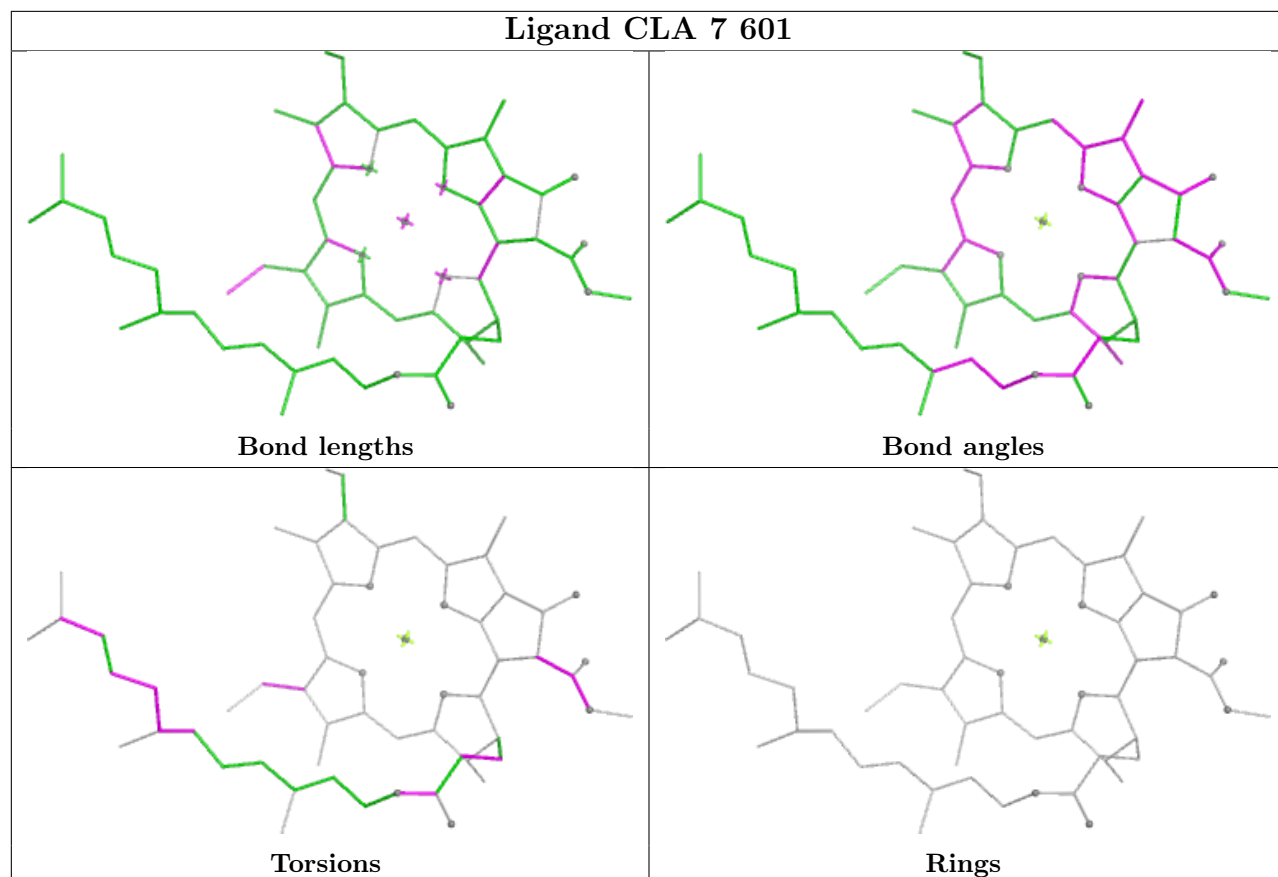
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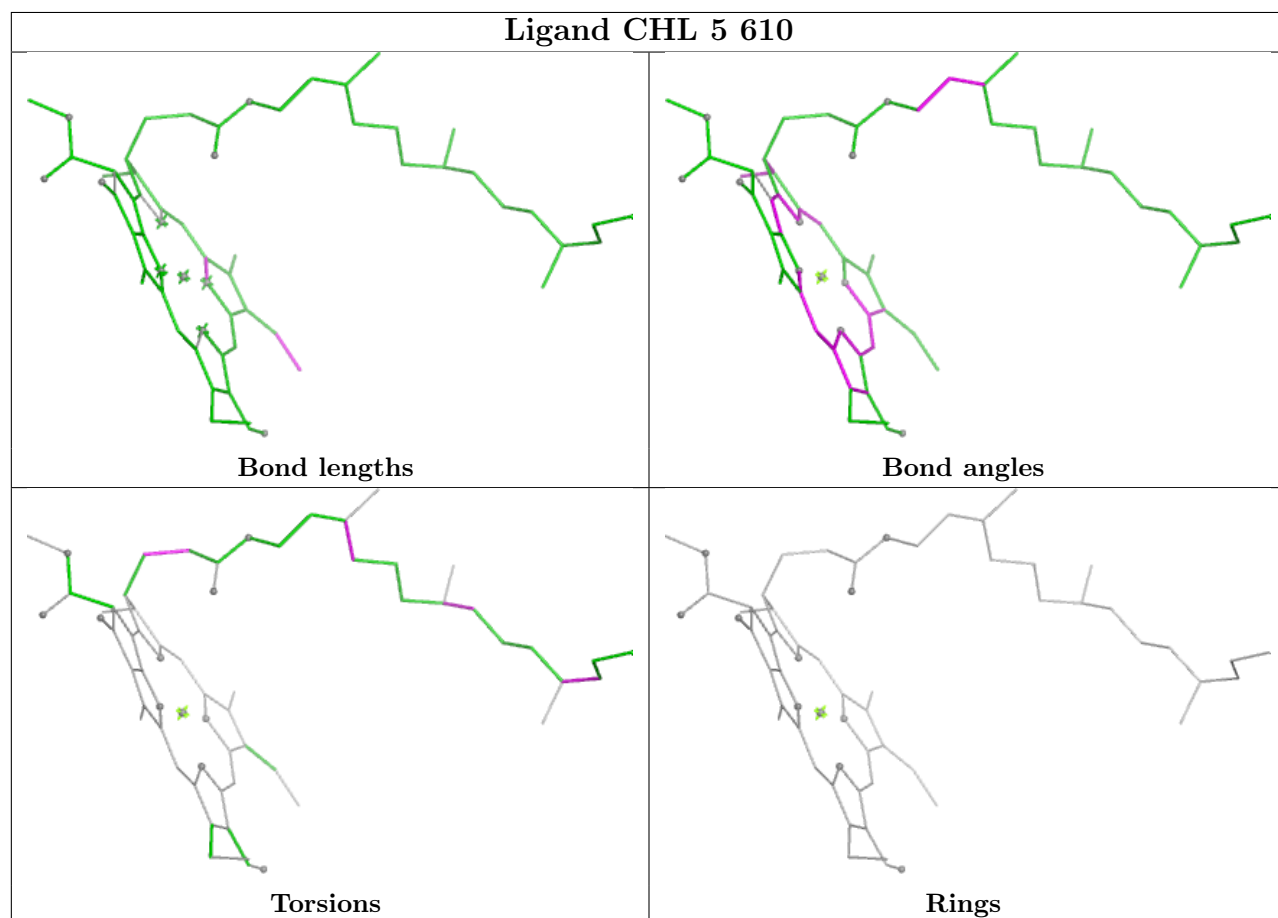
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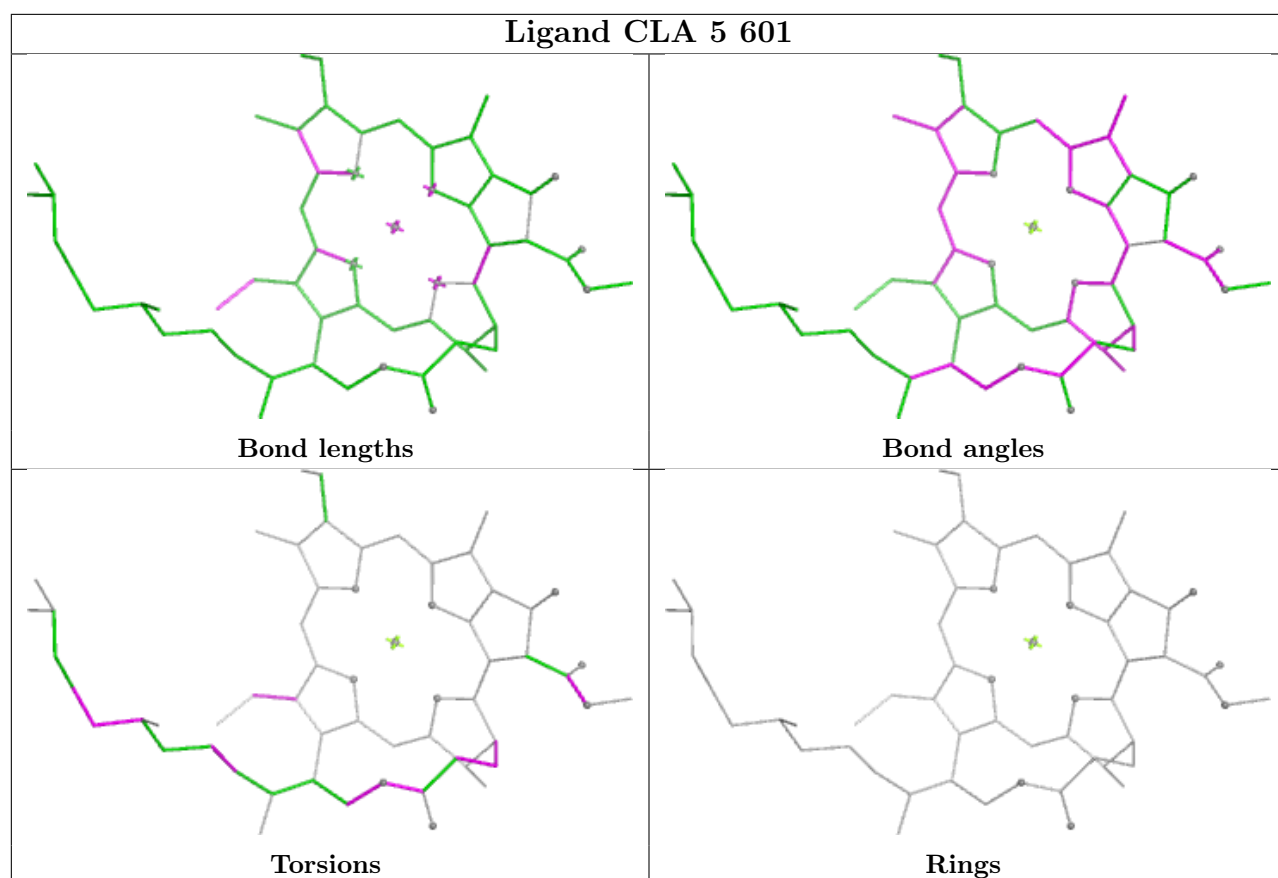


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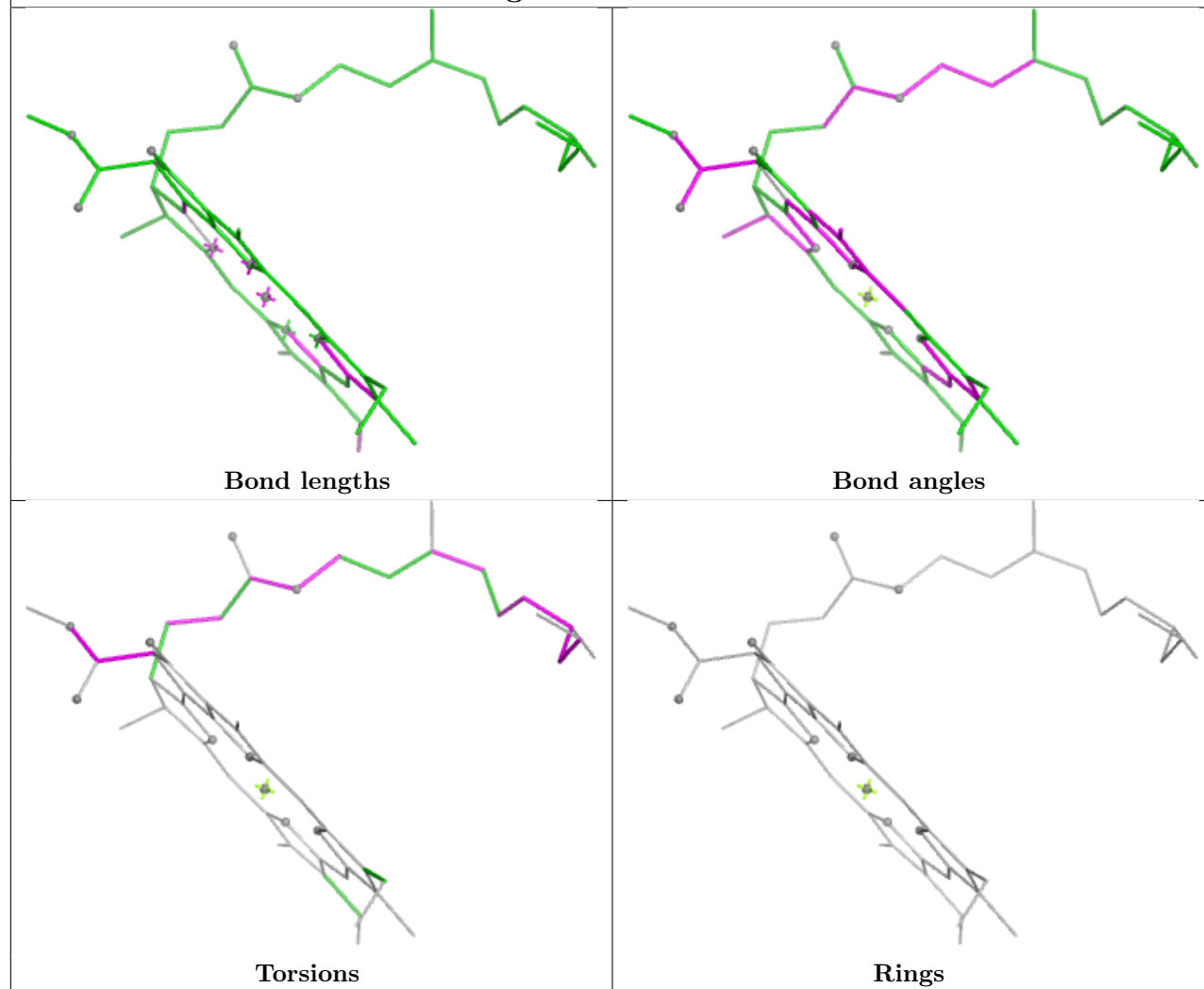


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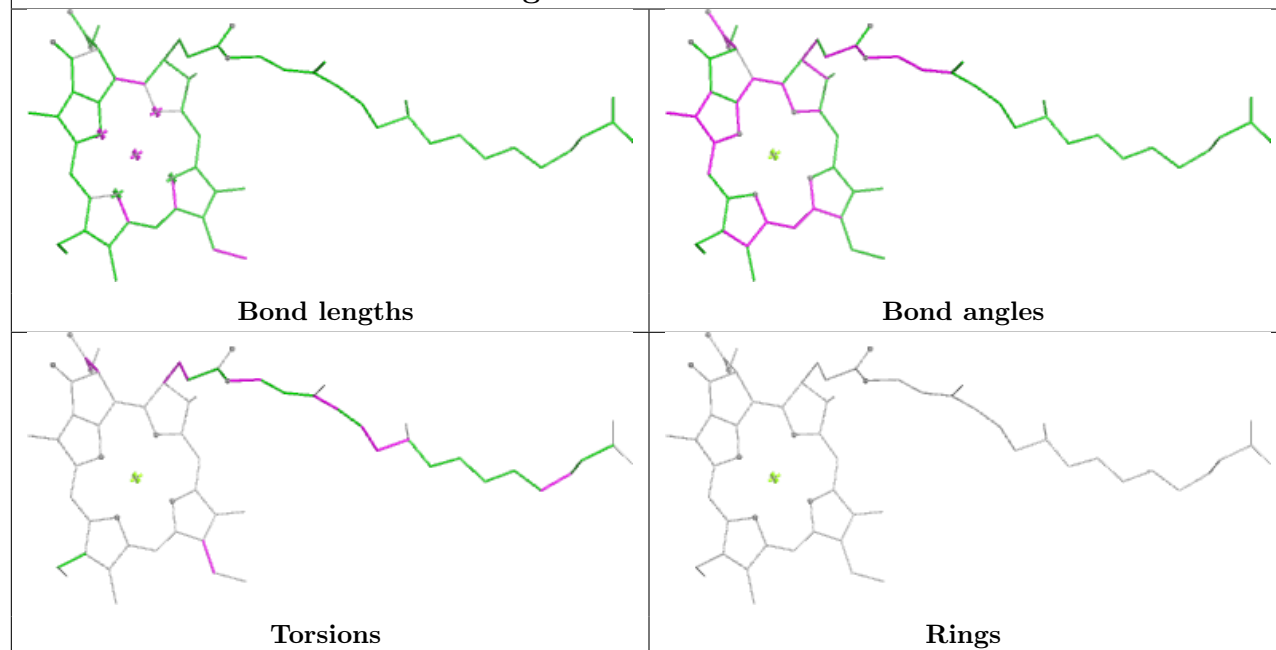


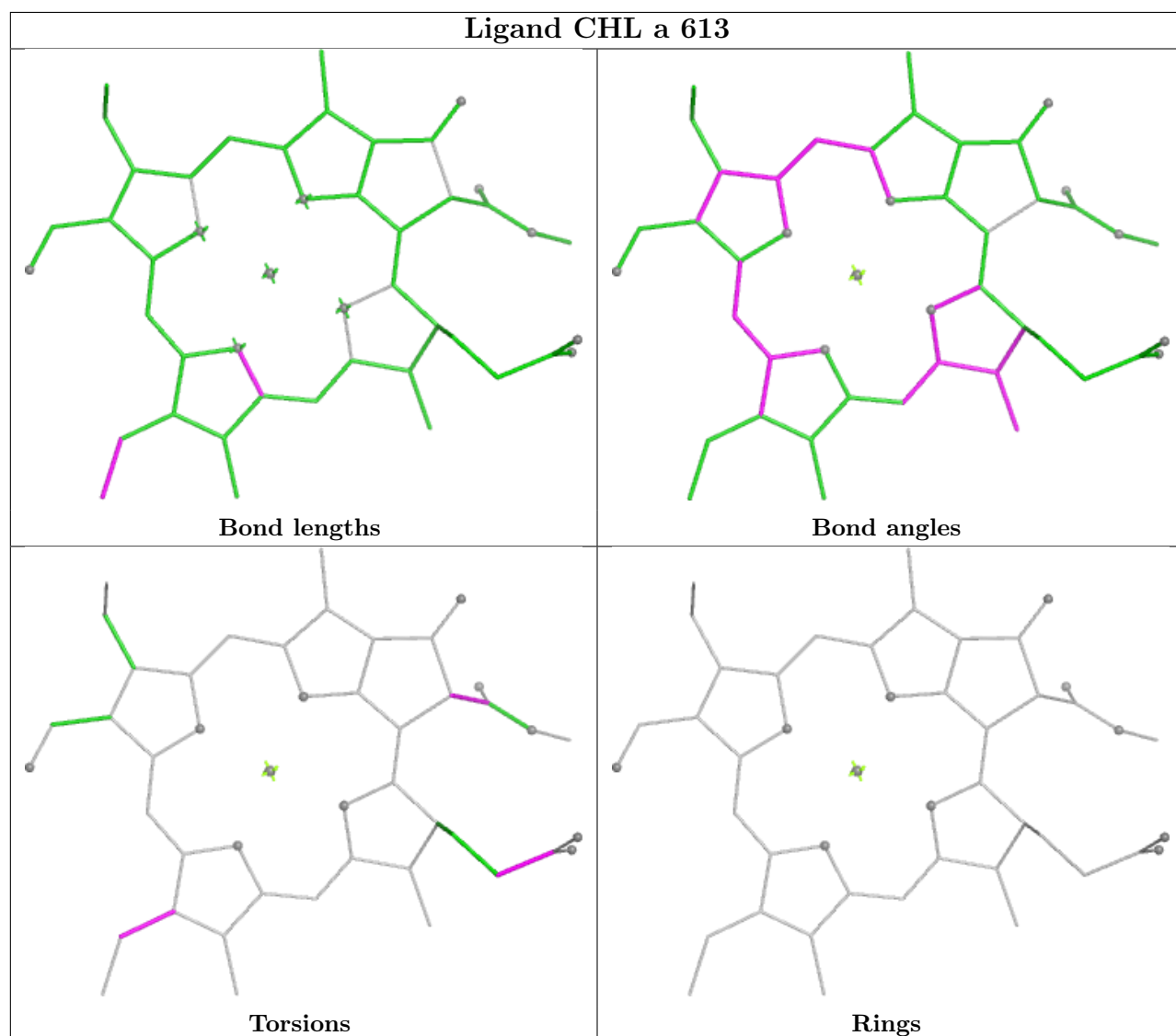
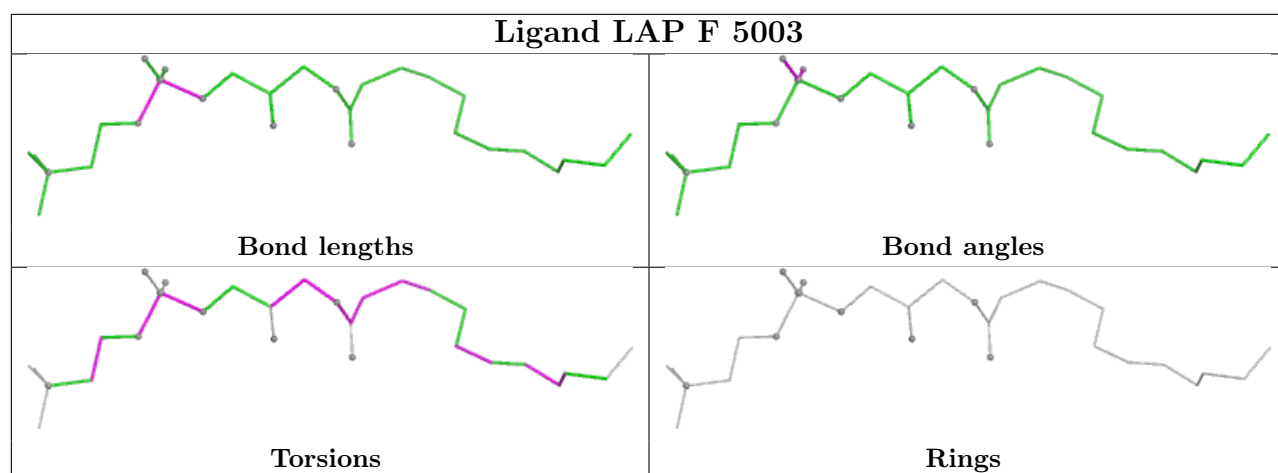


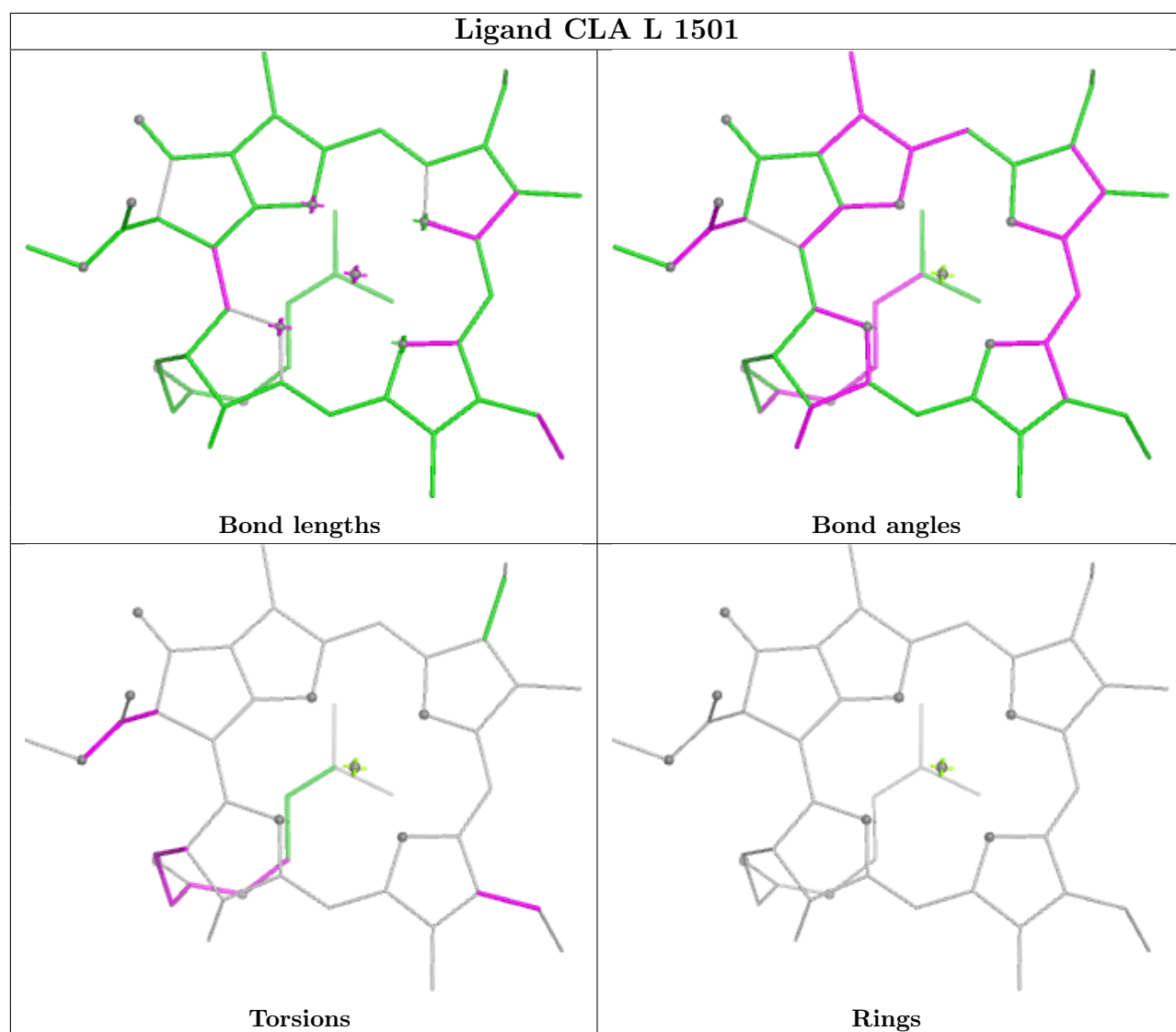
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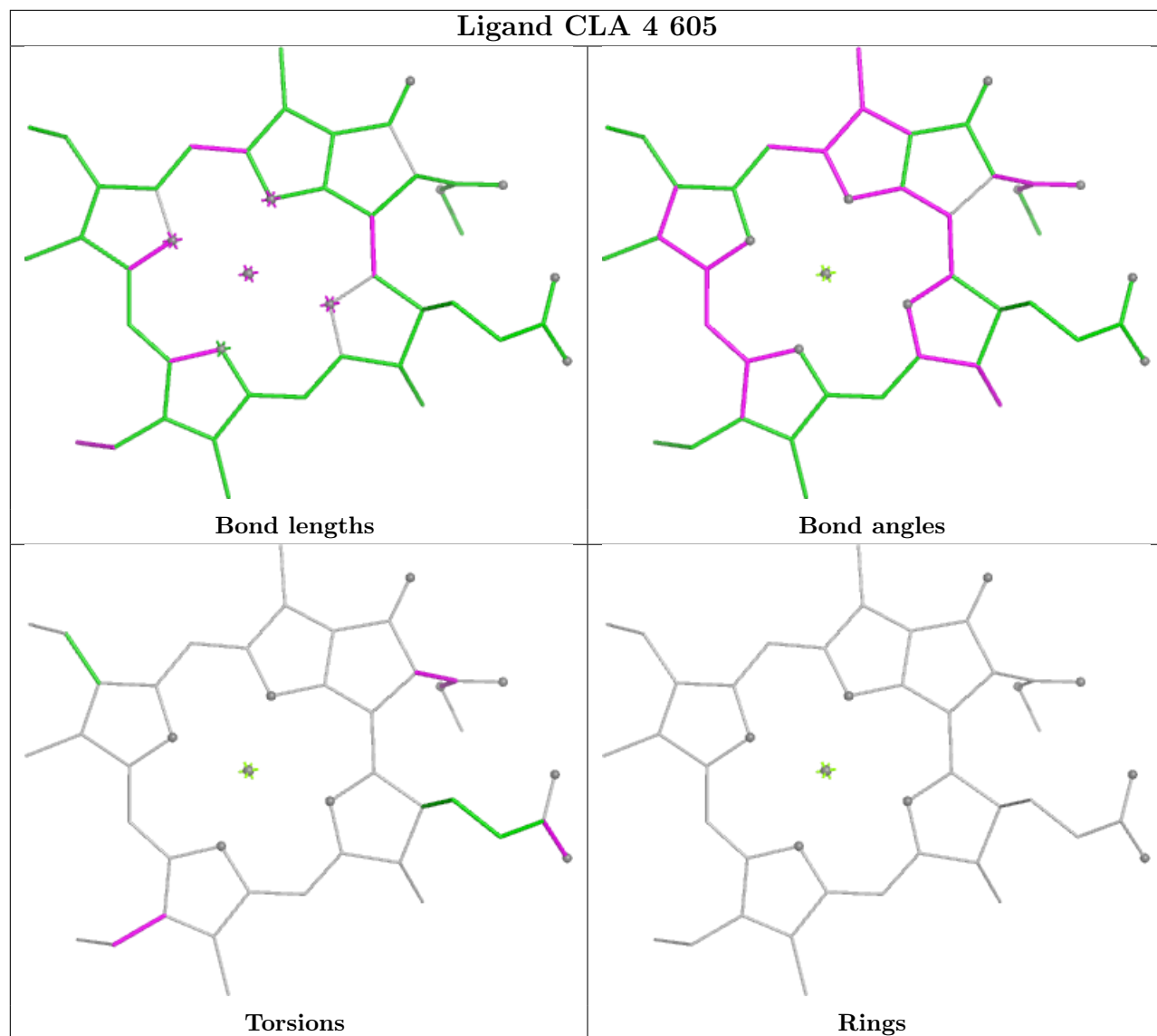
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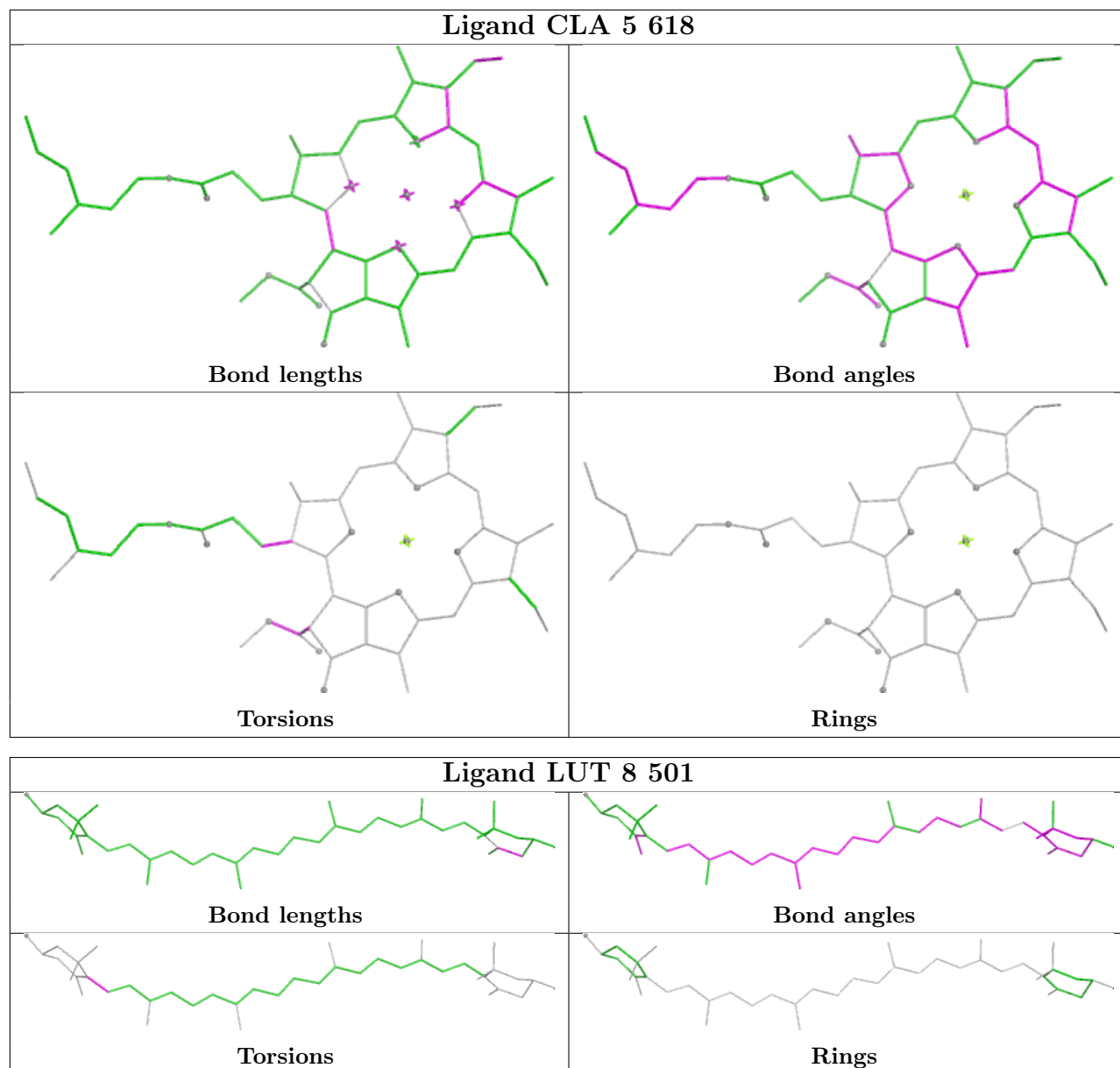




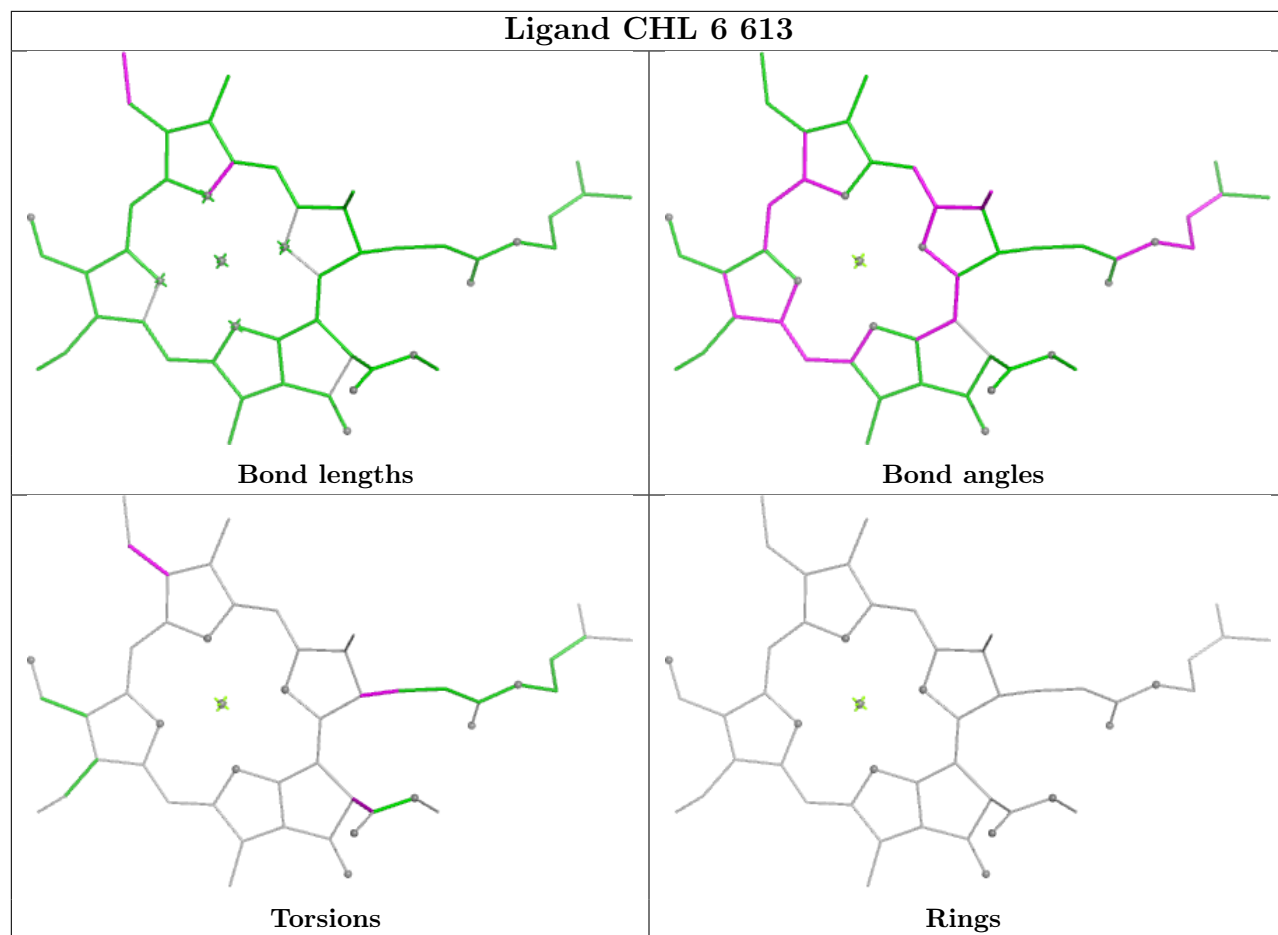


Ligand CLA 4 605

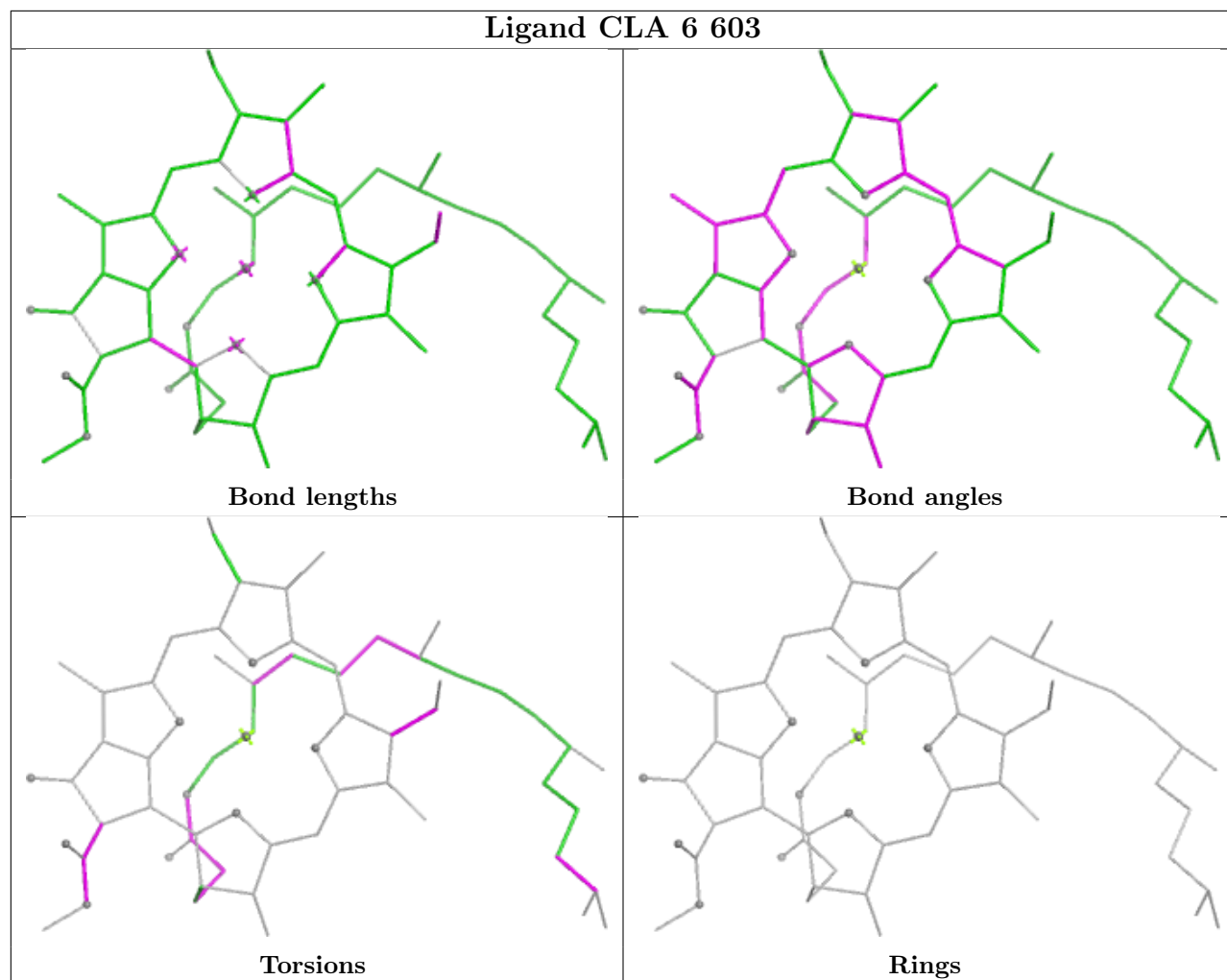


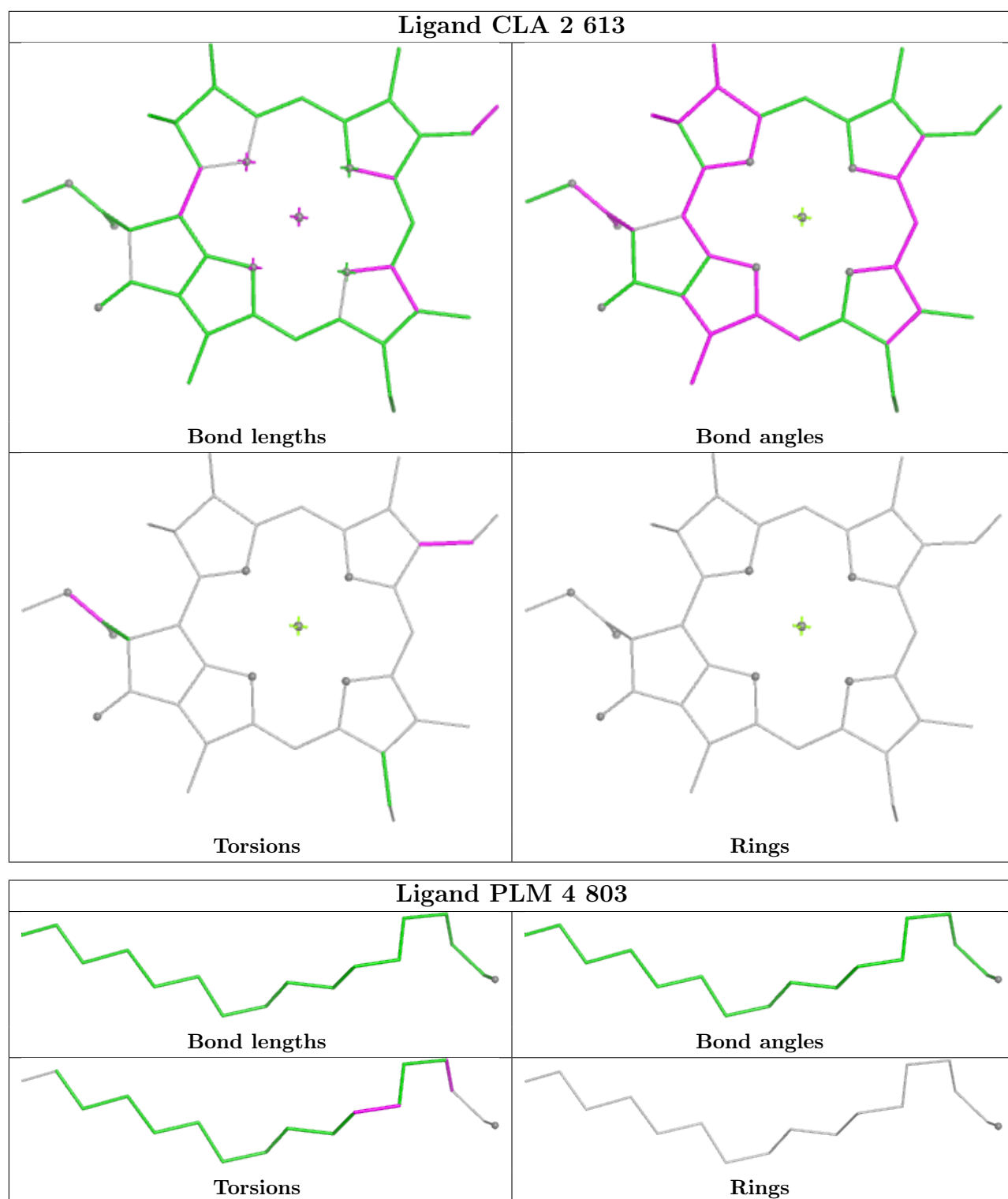


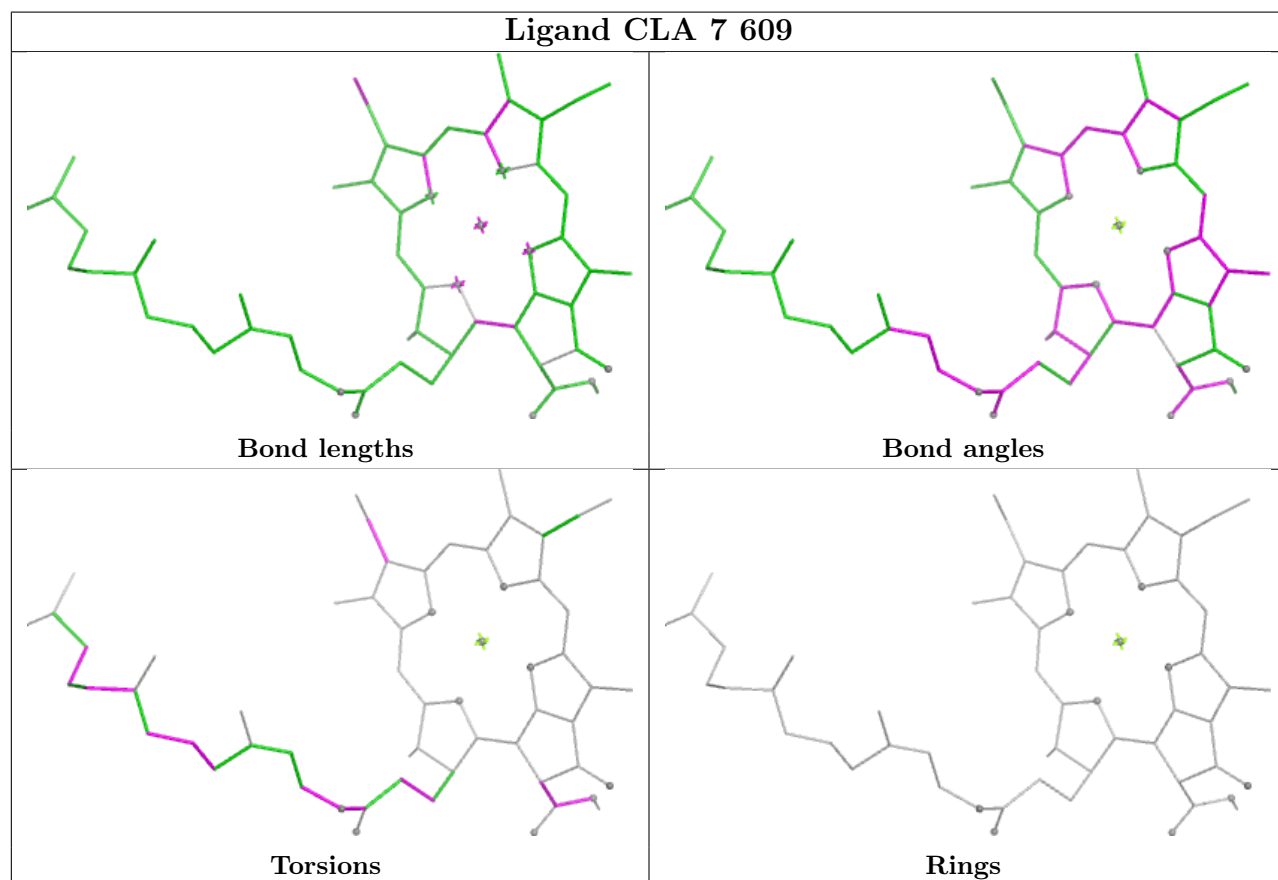
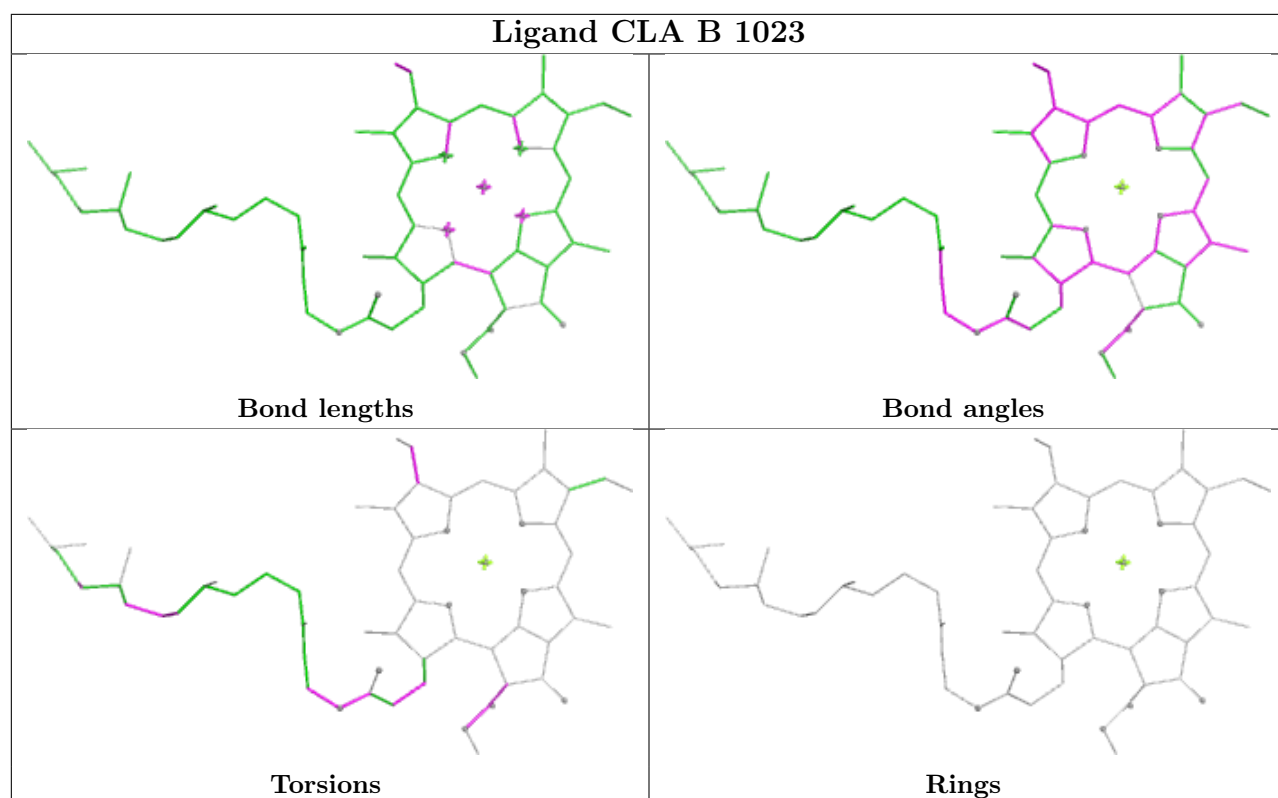
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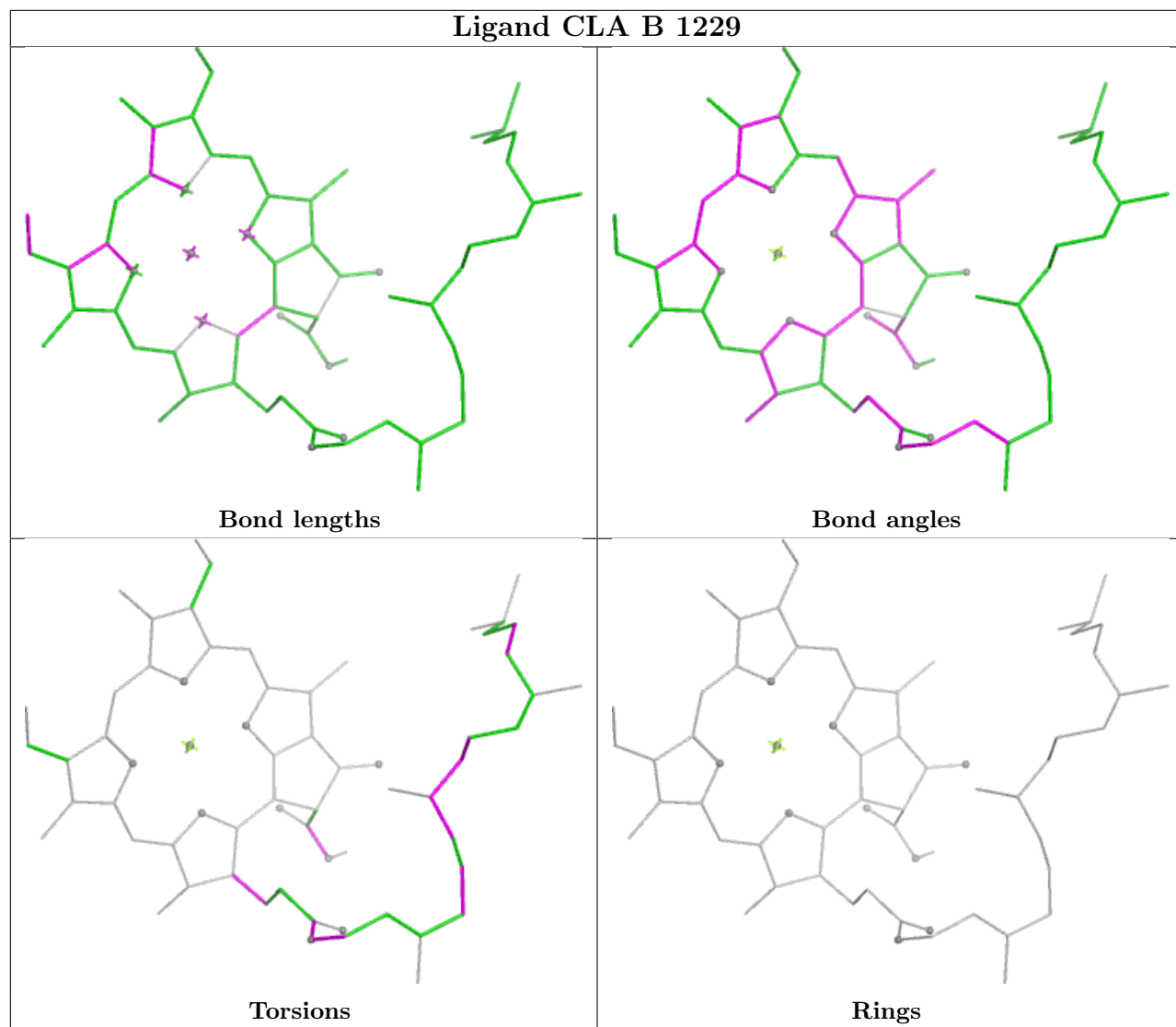


Ligand CLA 6 603

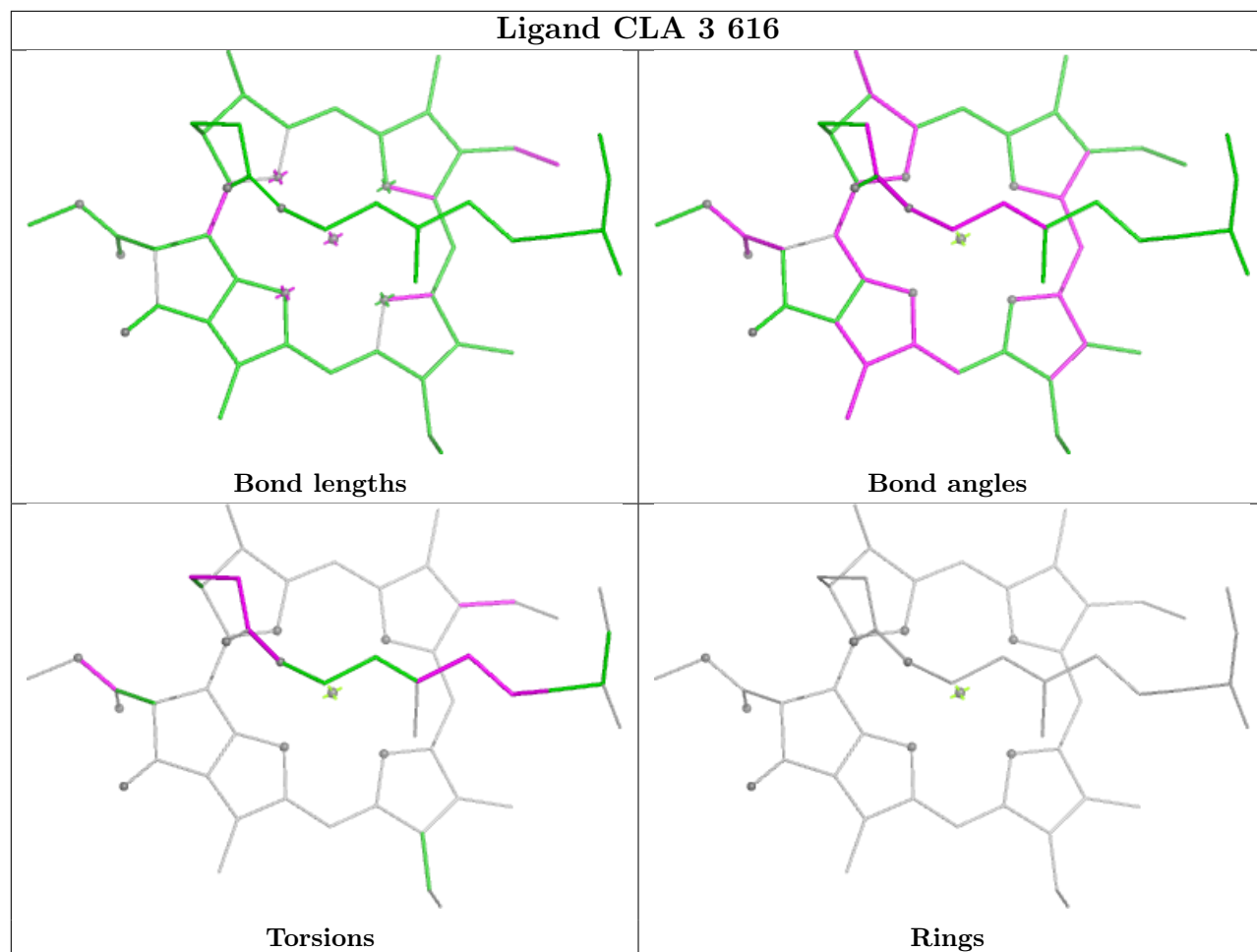


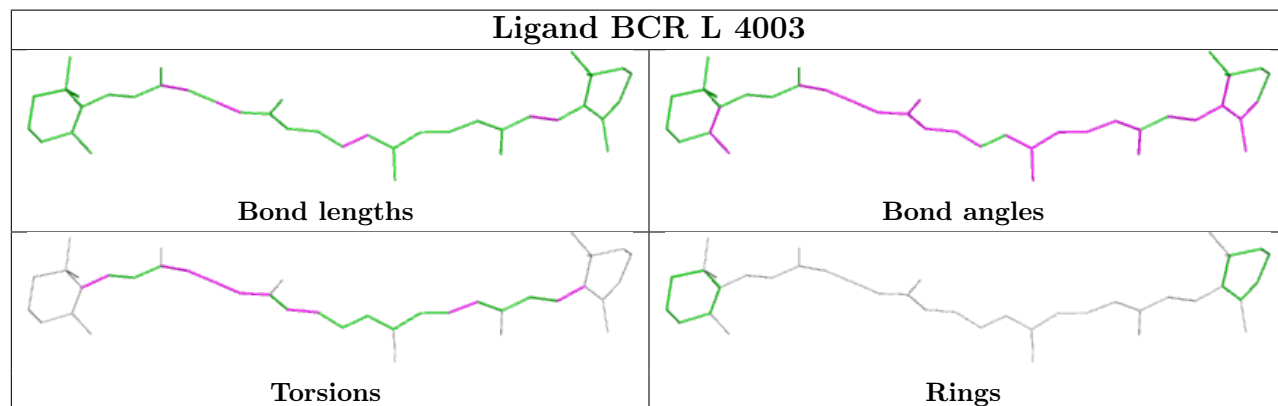
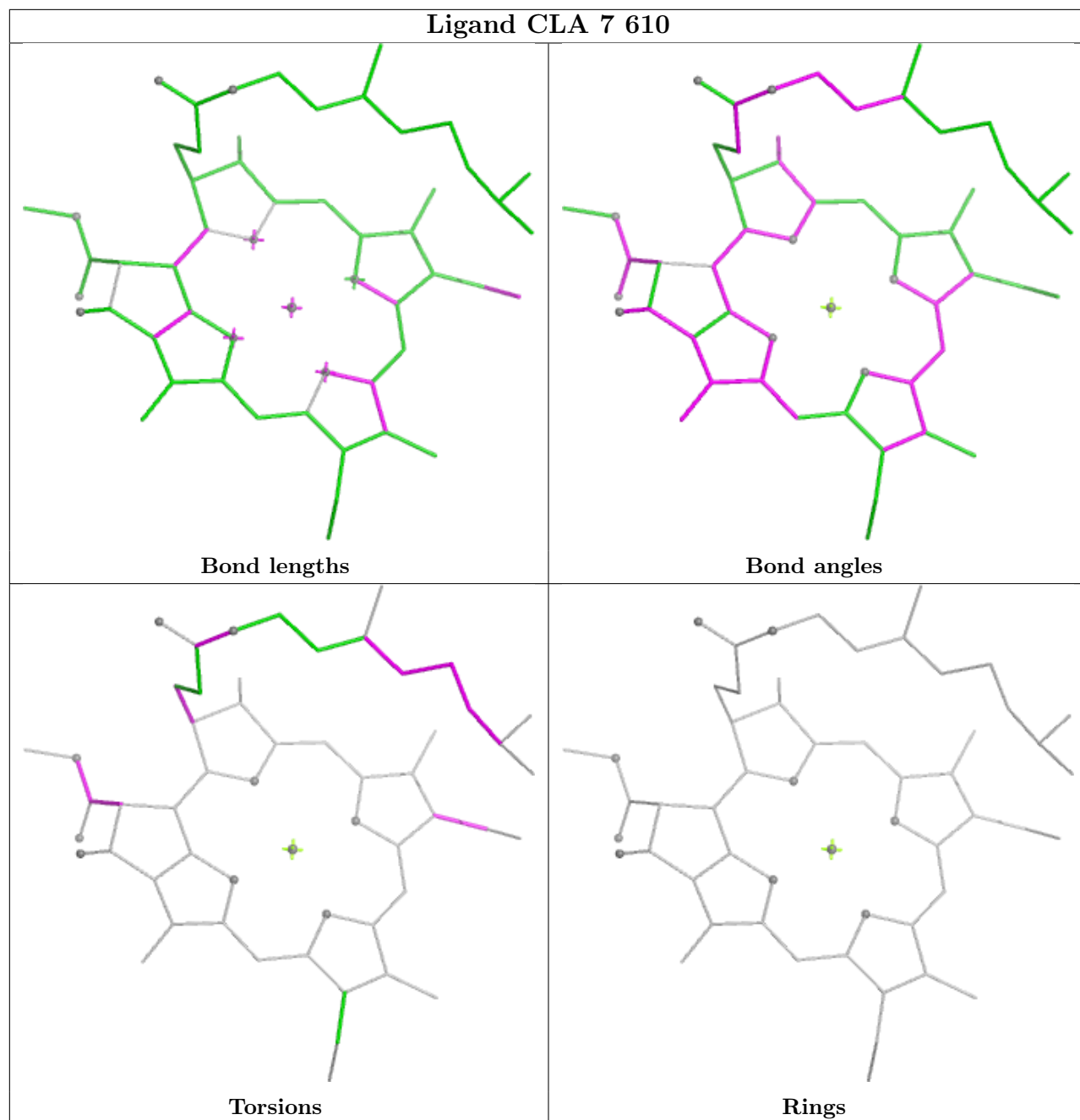


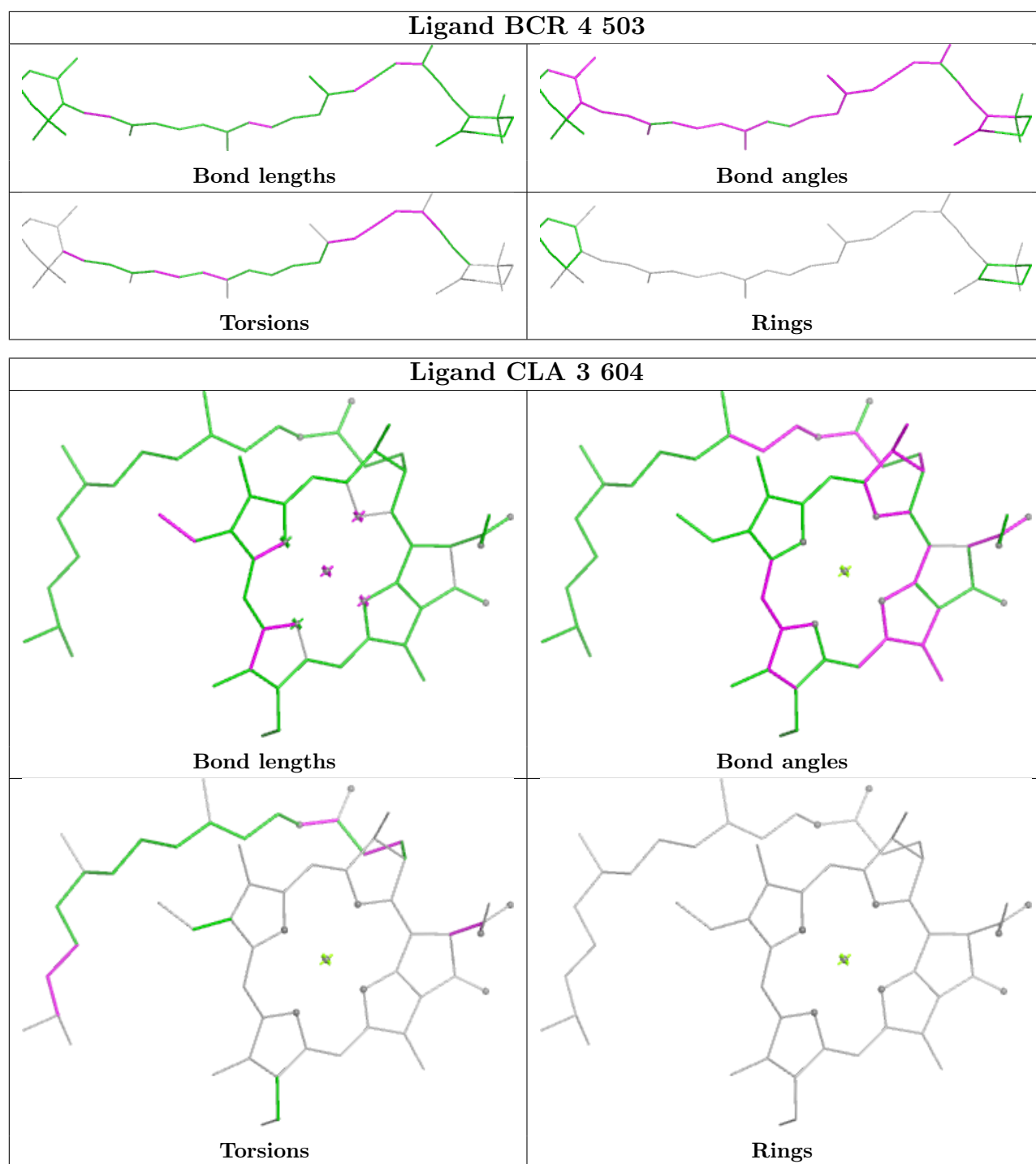


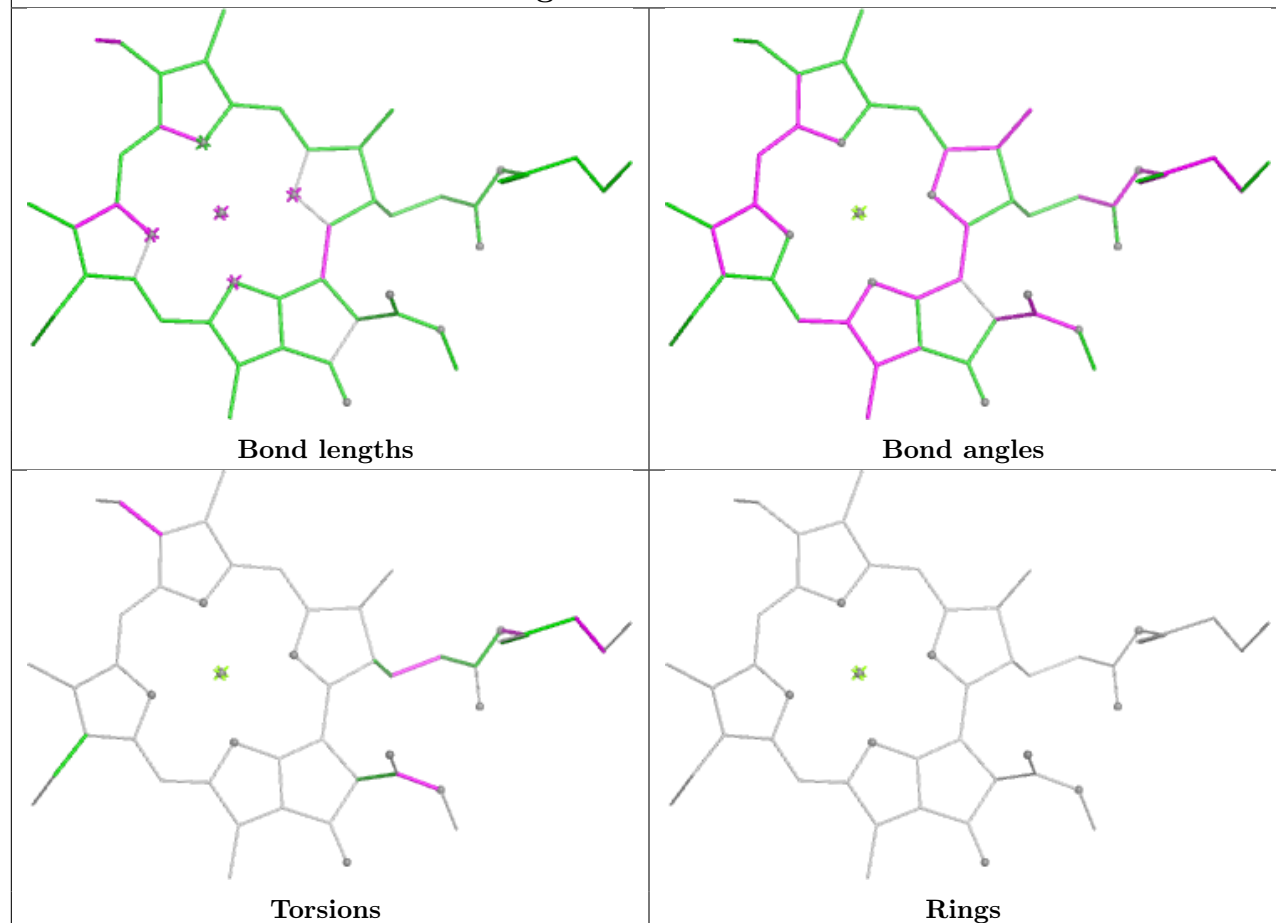
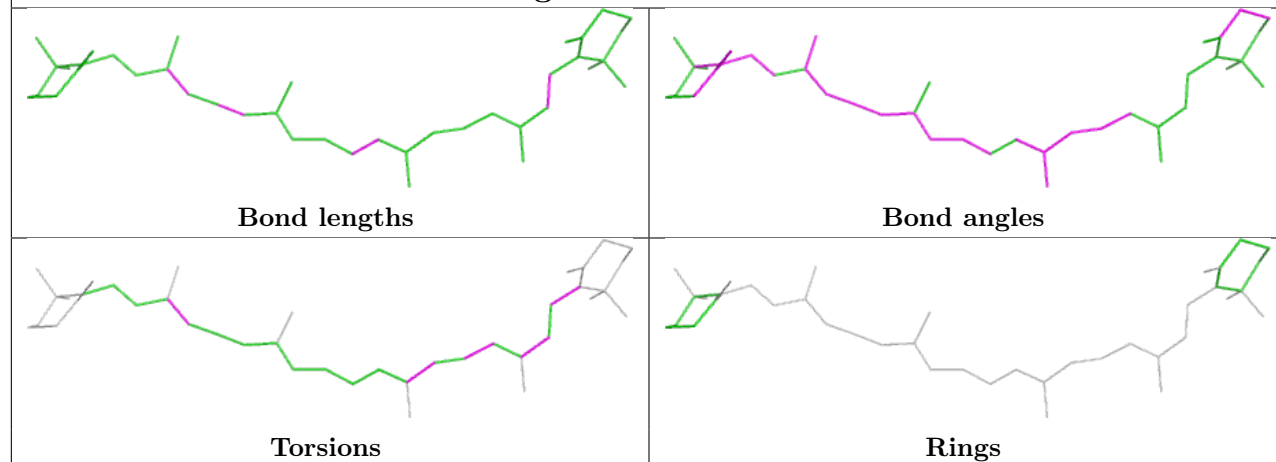


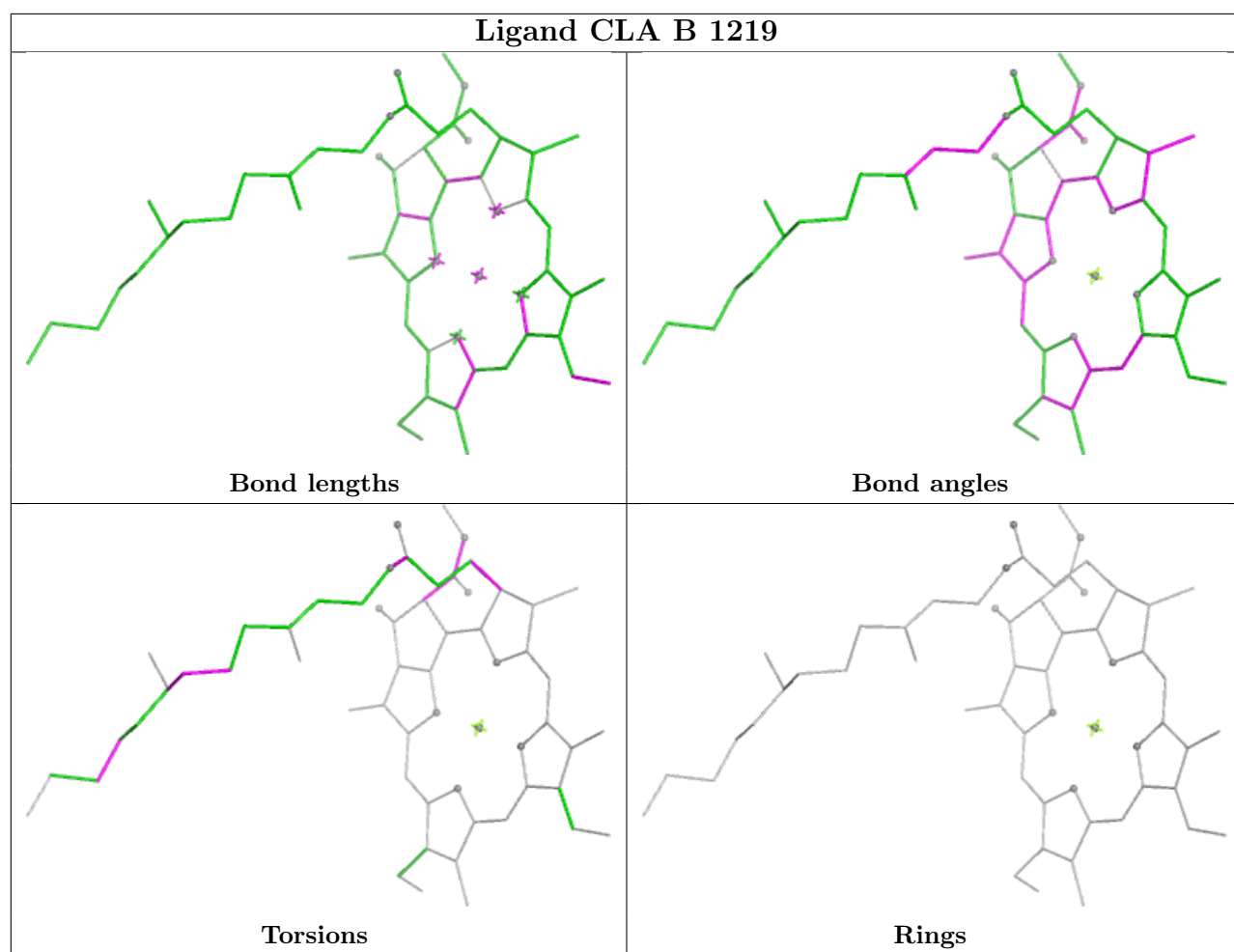
Ligand CLA 3 616

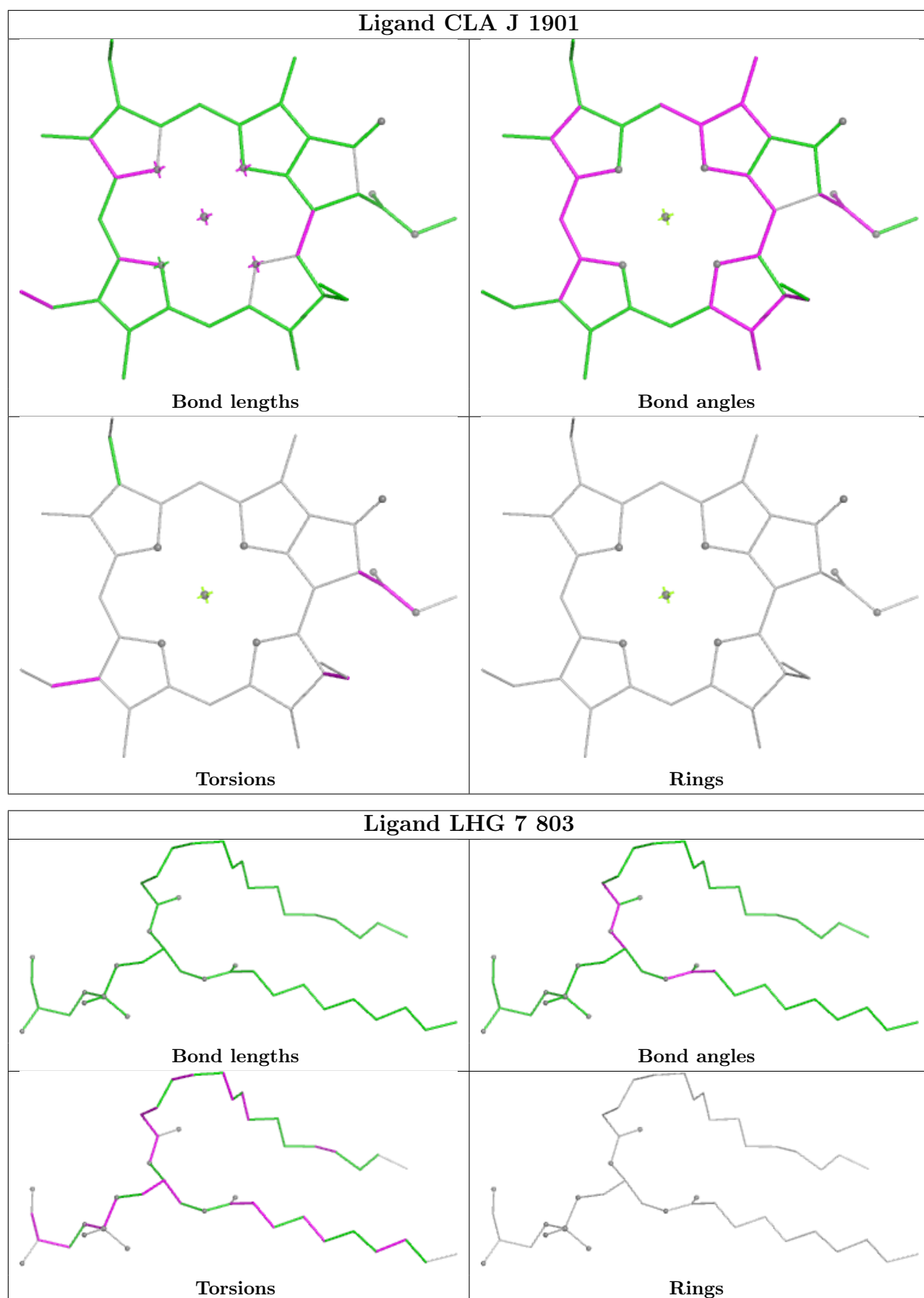




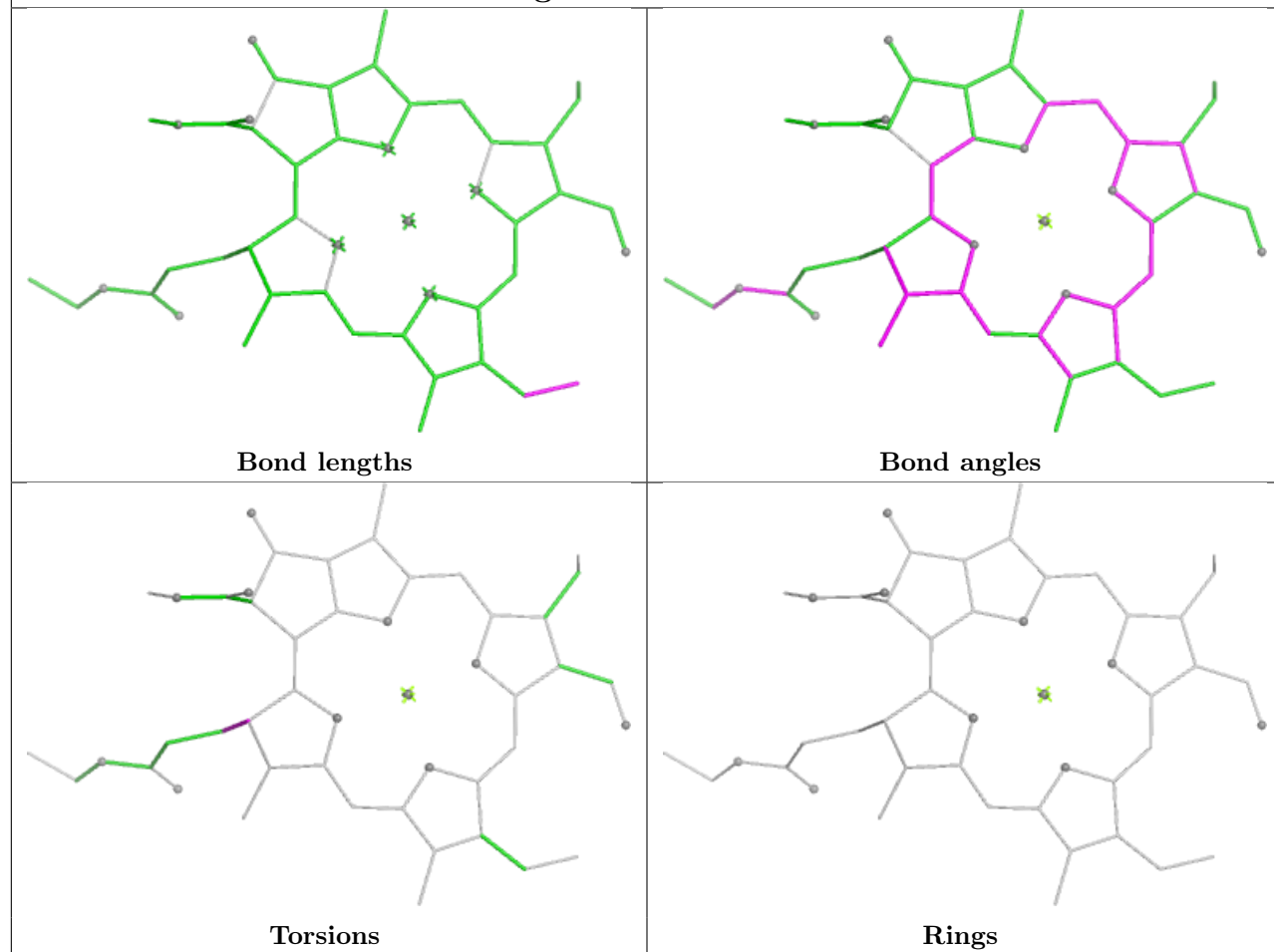


Ligand CLA 4 602**Ligand BCR 6 504**

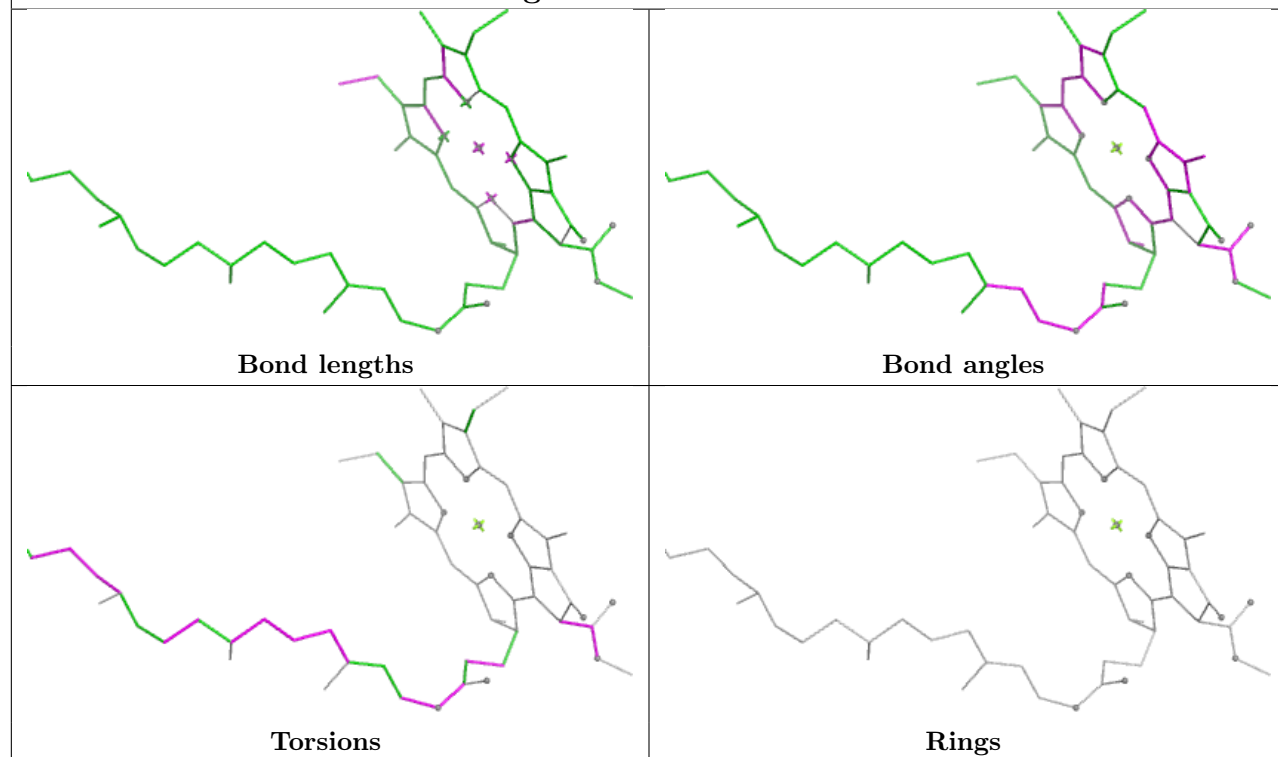




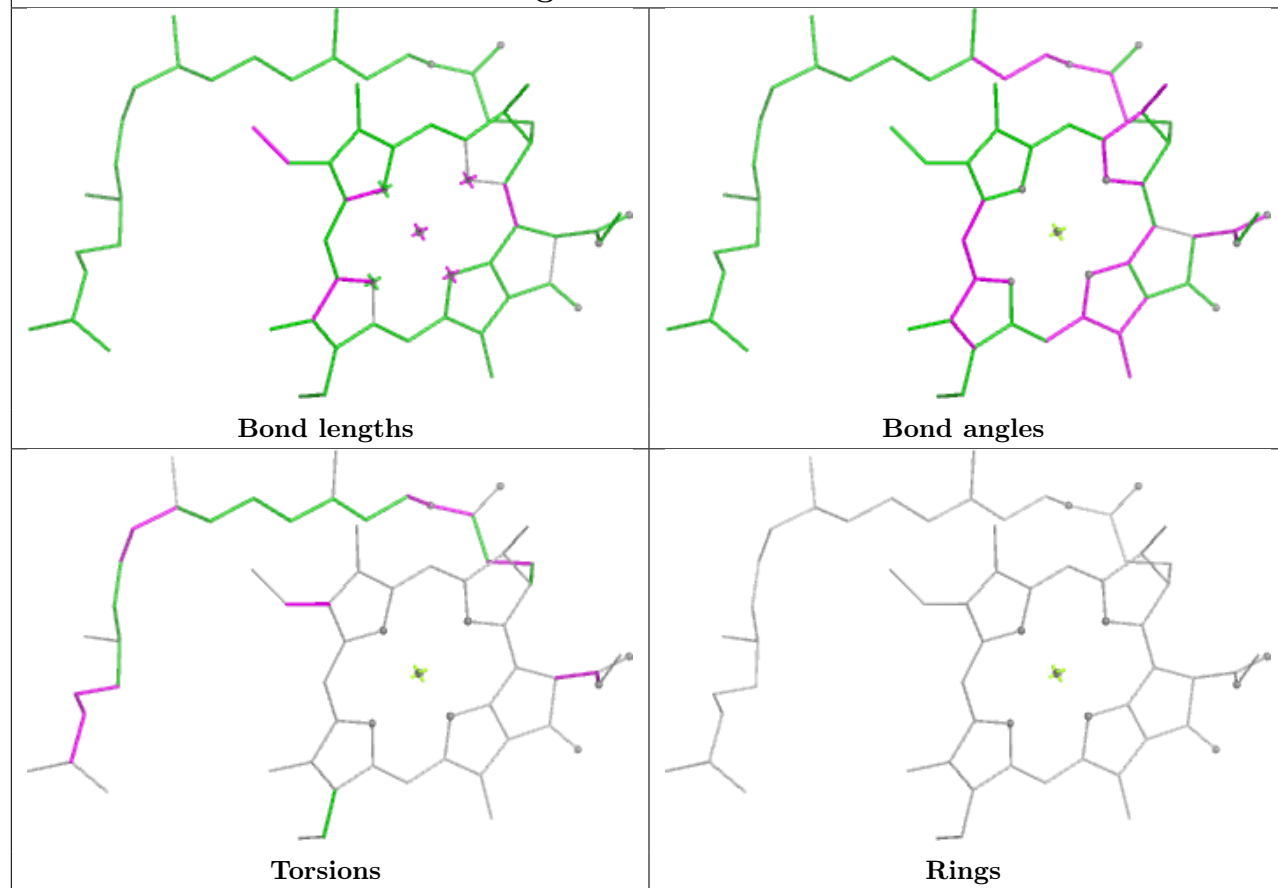
Ligand CHL a 610



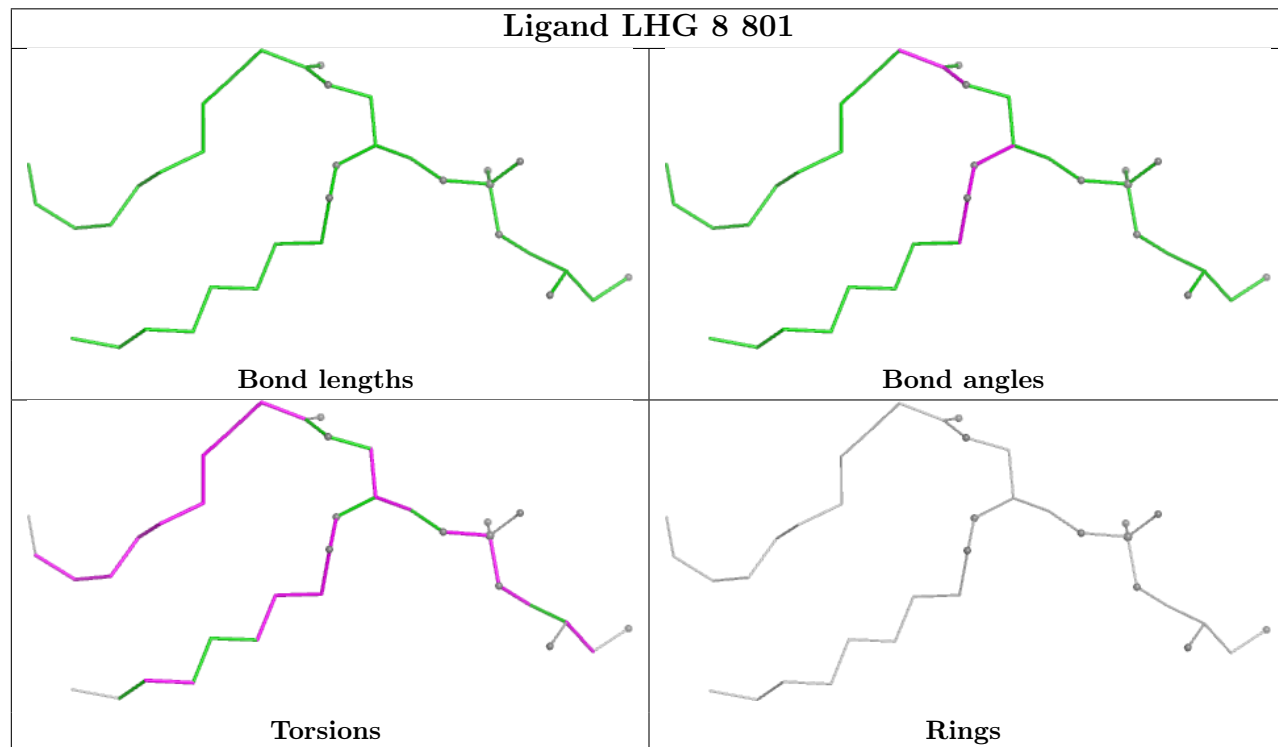
Ligand CLA B 1228

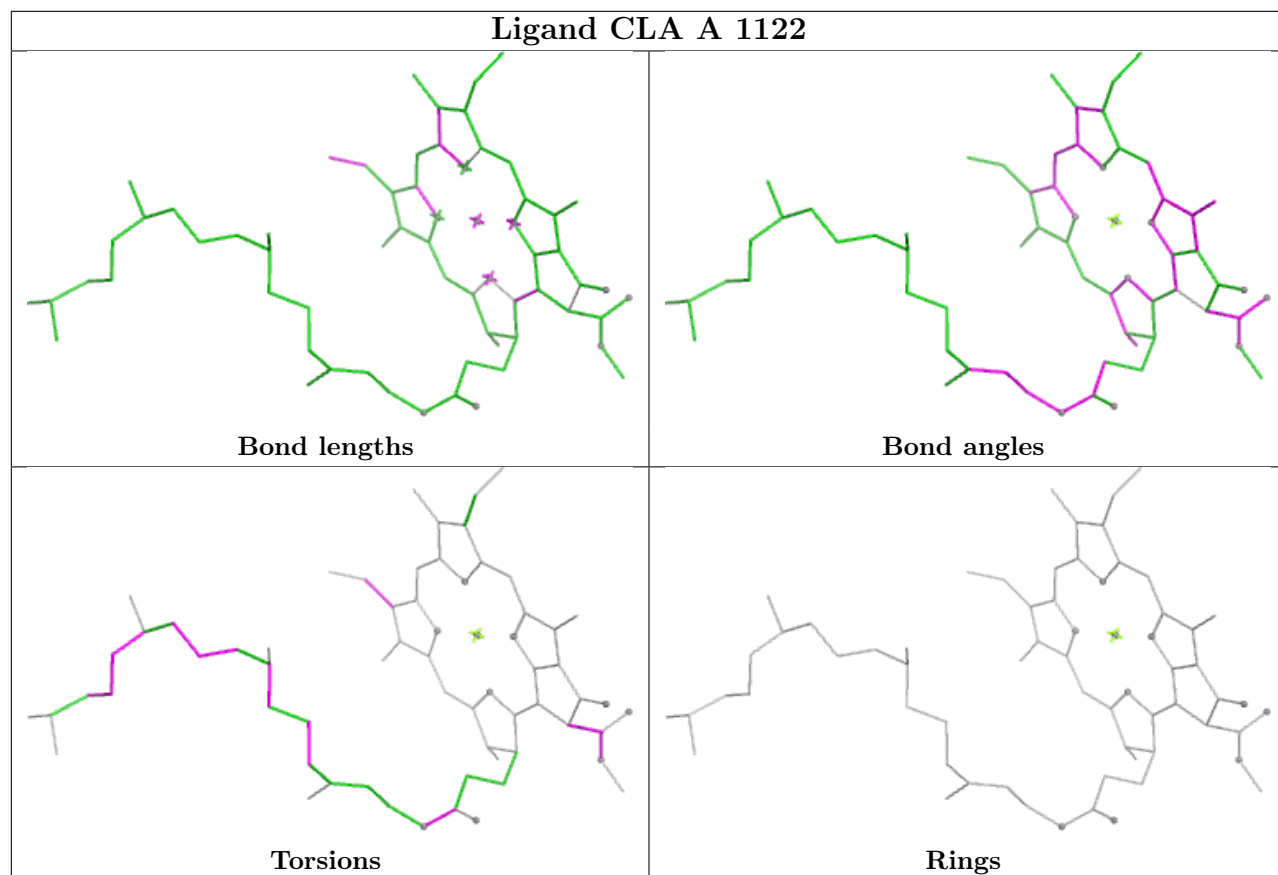


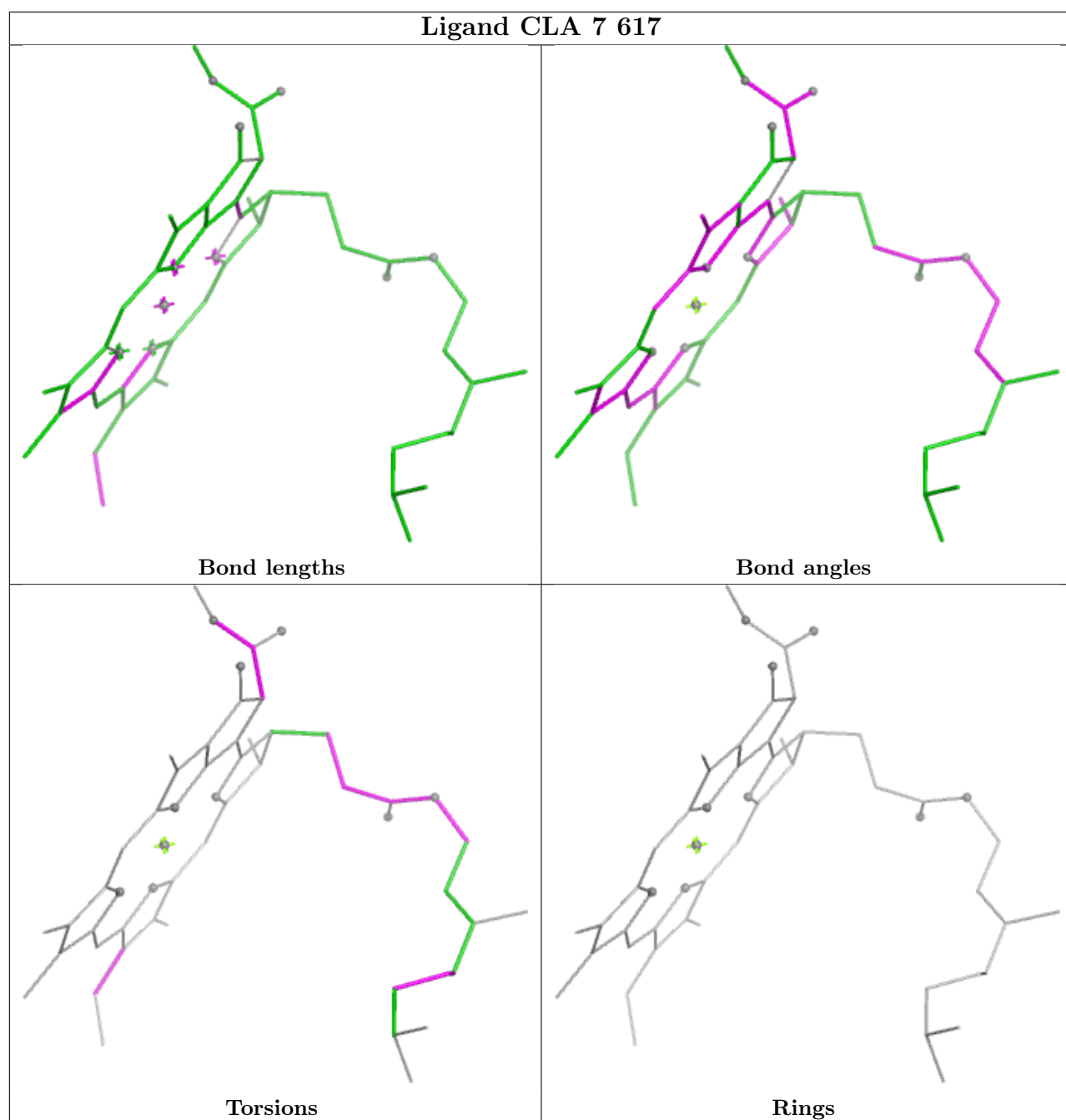
Ligand CLA 6 604

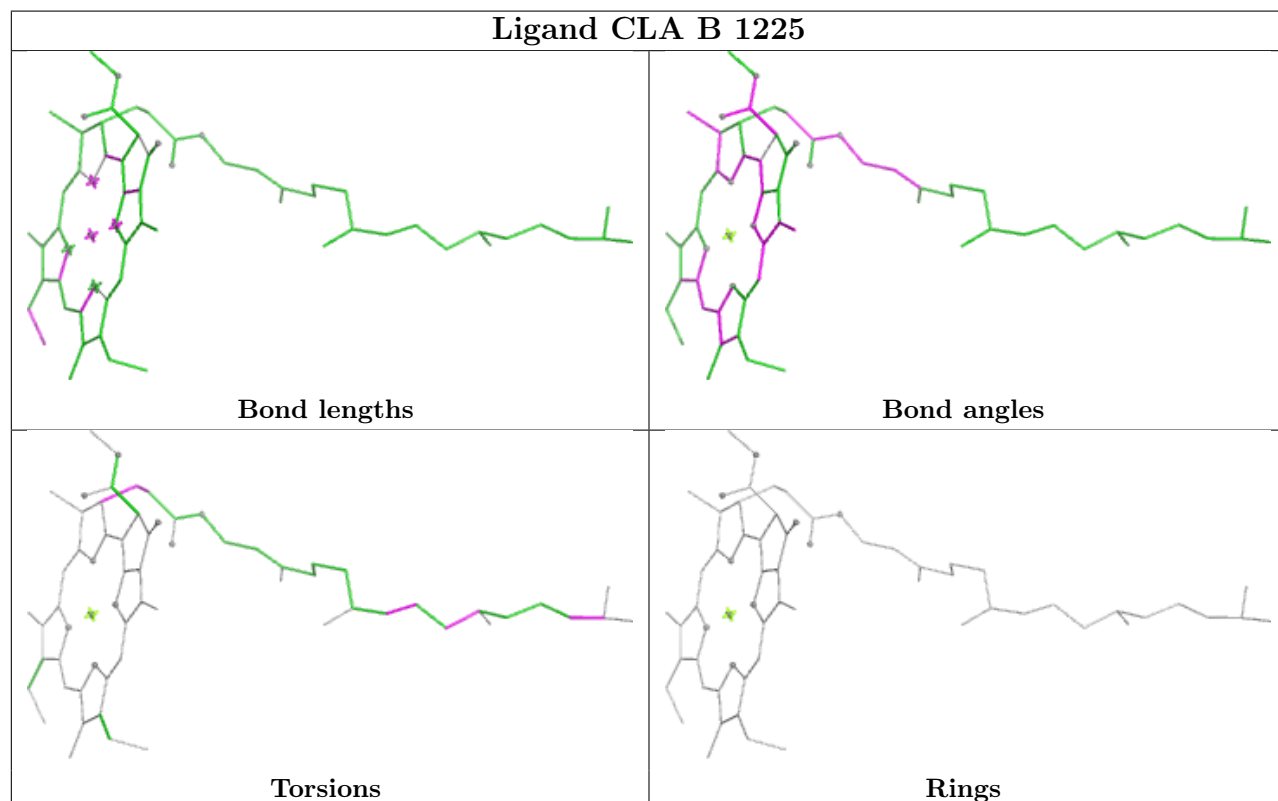
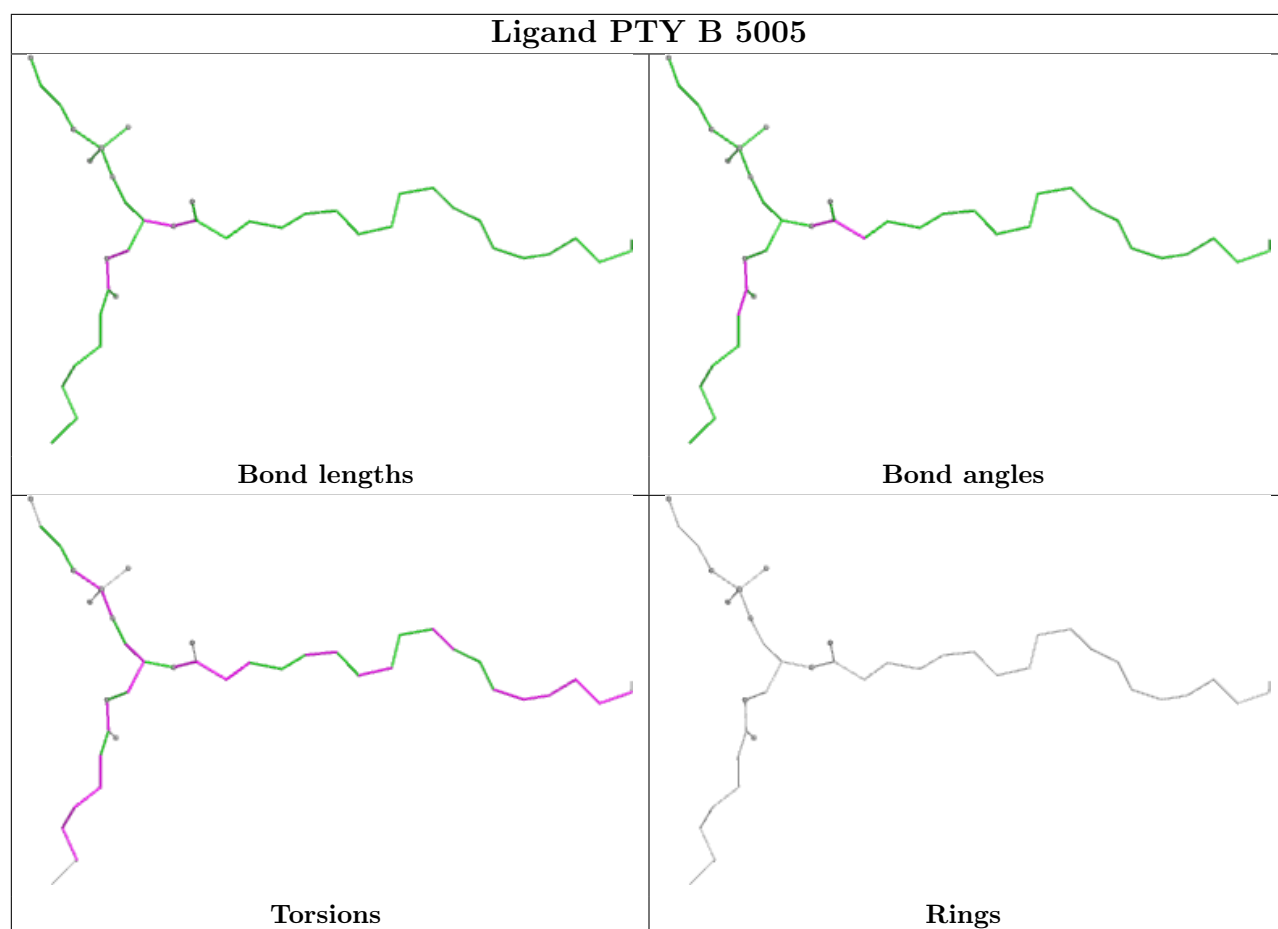


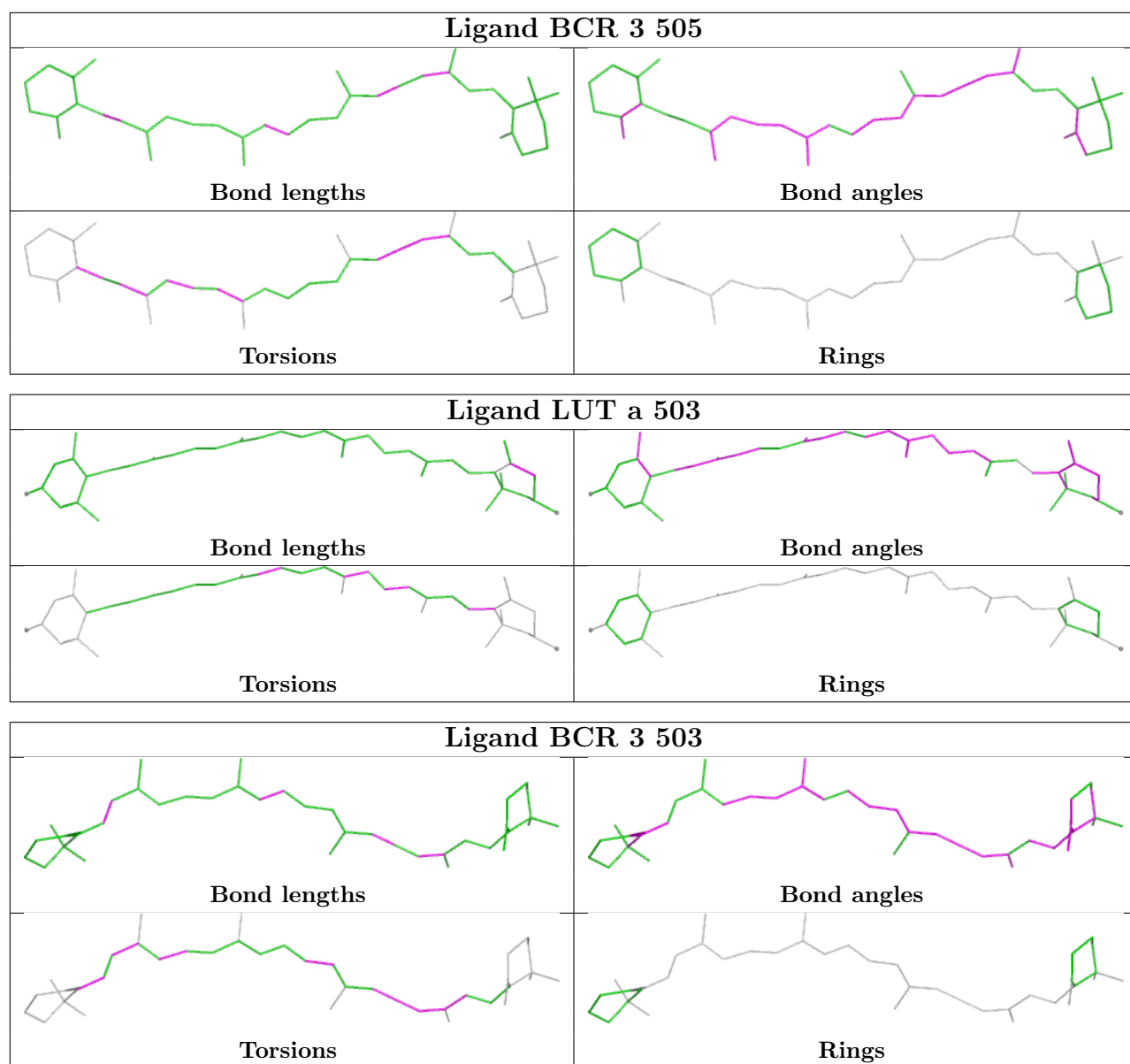
Ligand LHG 8 801



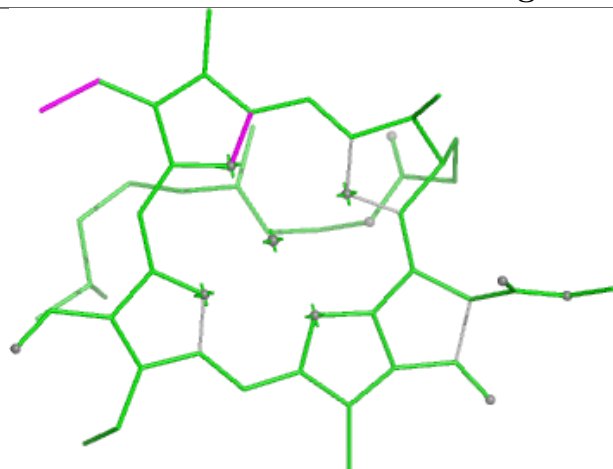




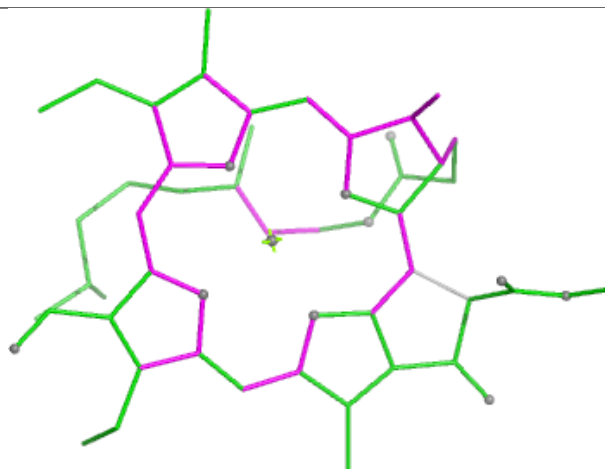




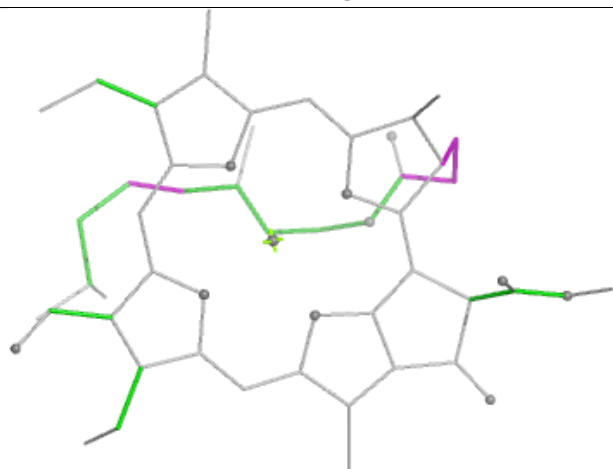
Ligand CHL 4 618



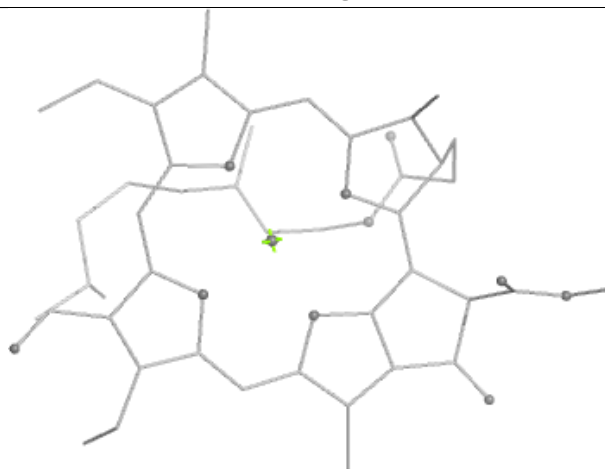
Bond lengths



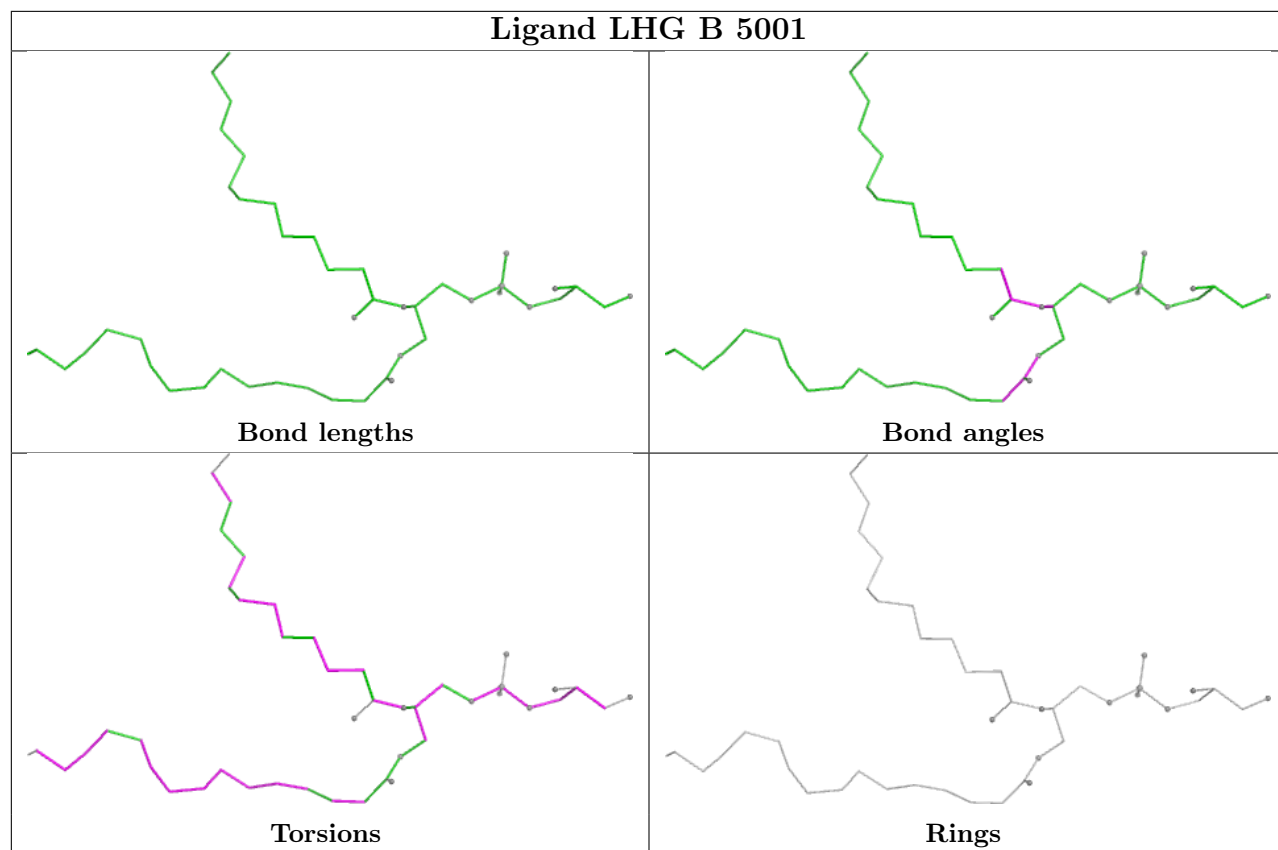
Bond angles



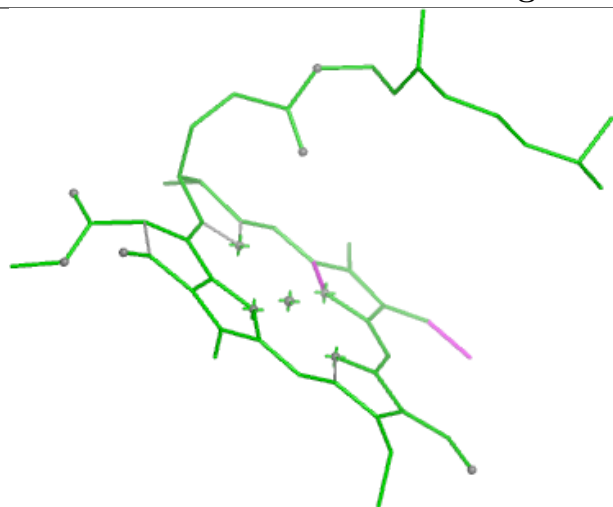
Torsions



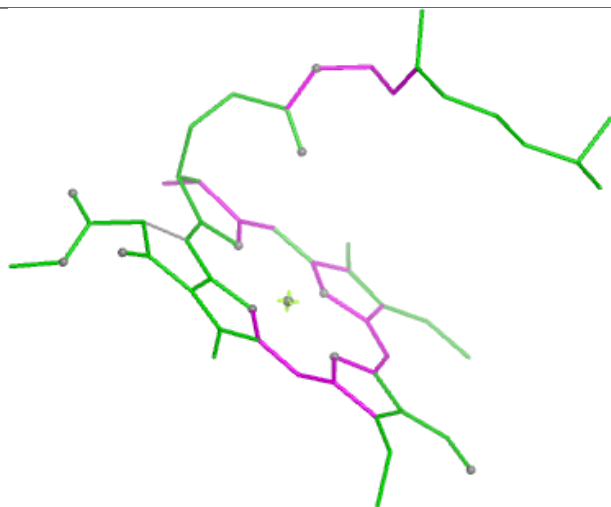
Rings



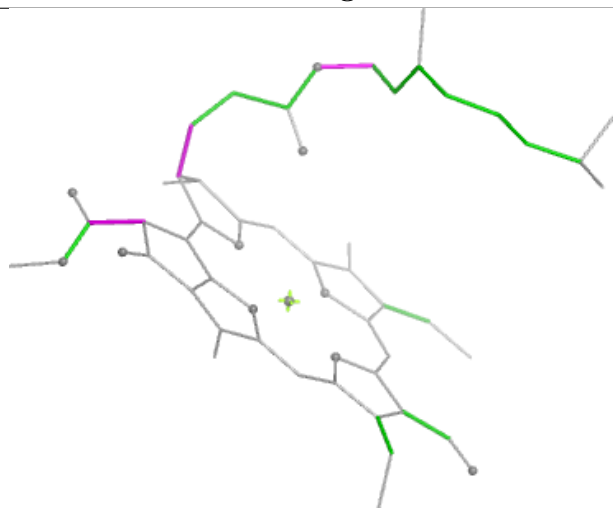
Ligand CHL a 606



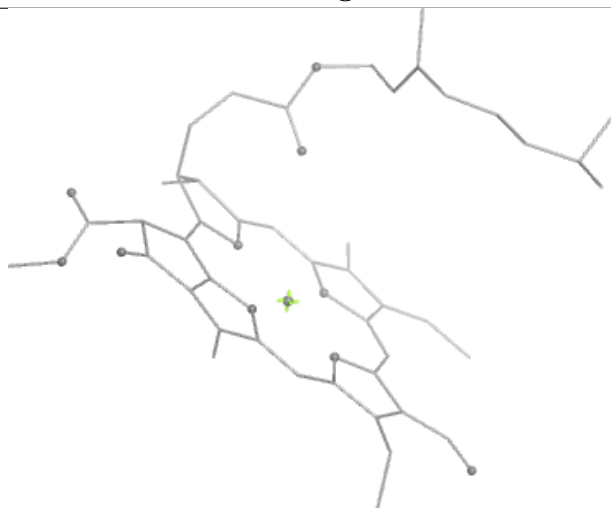
Bond lengths



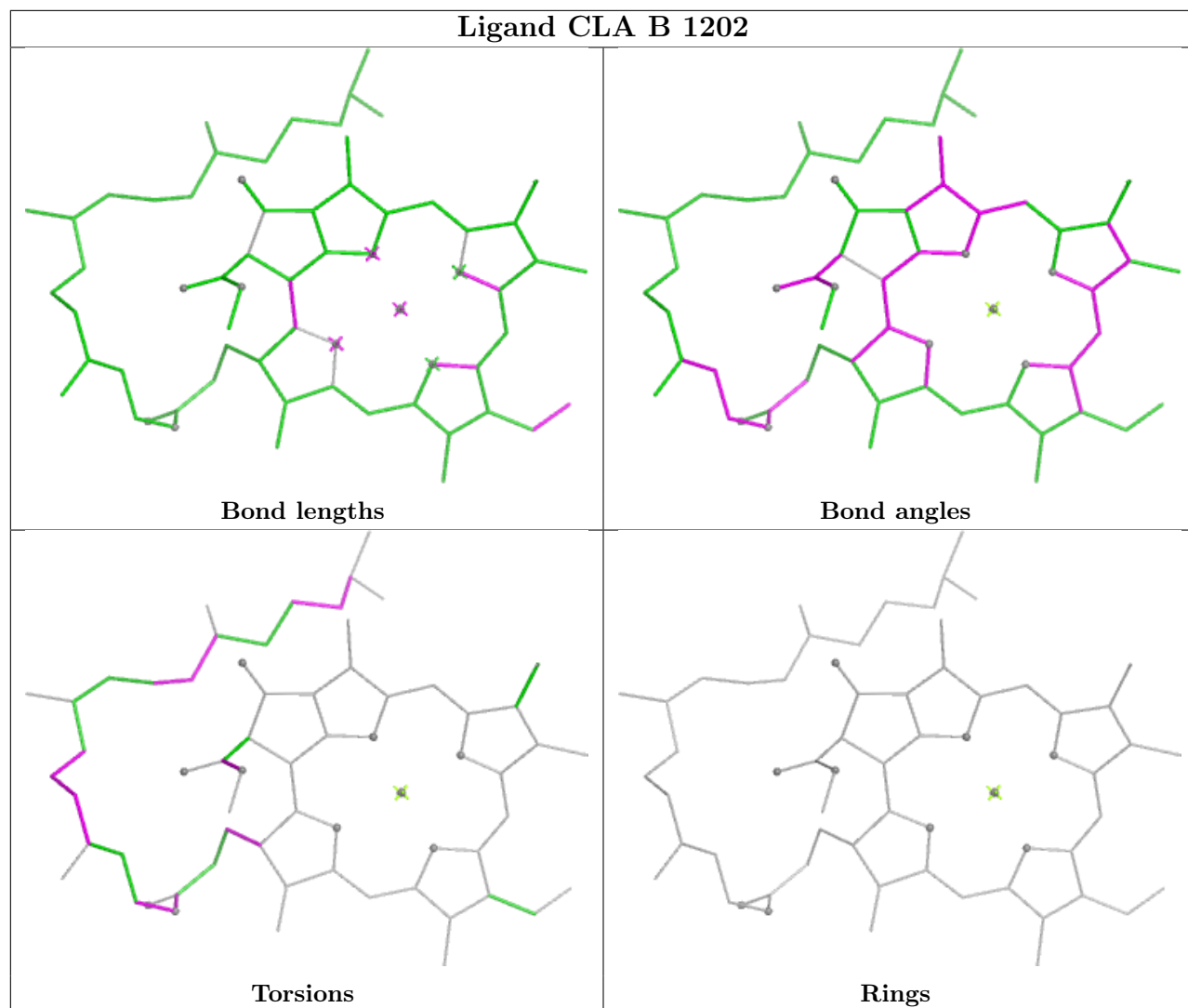
Bond angles



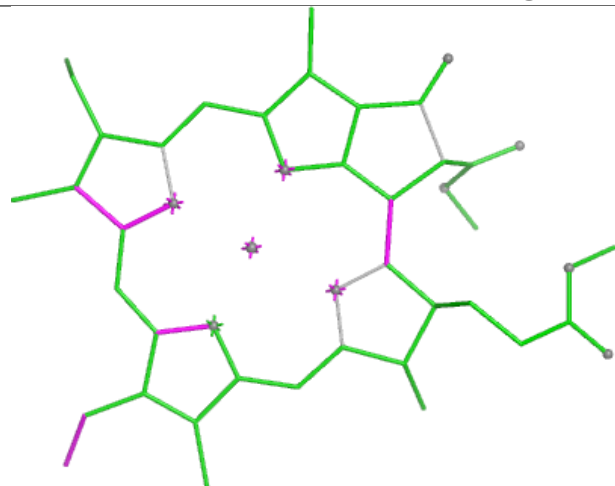
Torsions



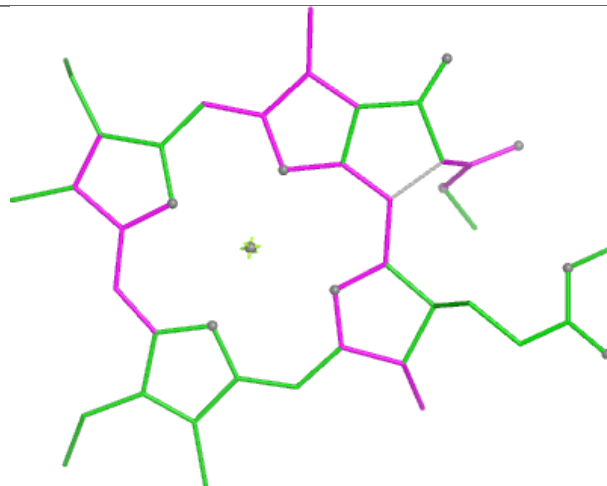
Rings



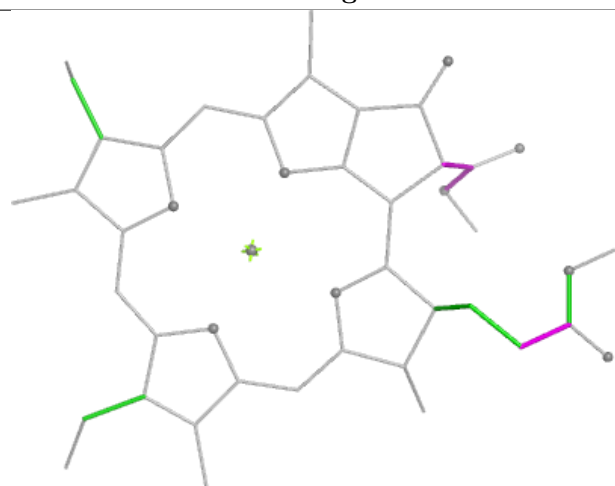
Ligand CLA 3 602



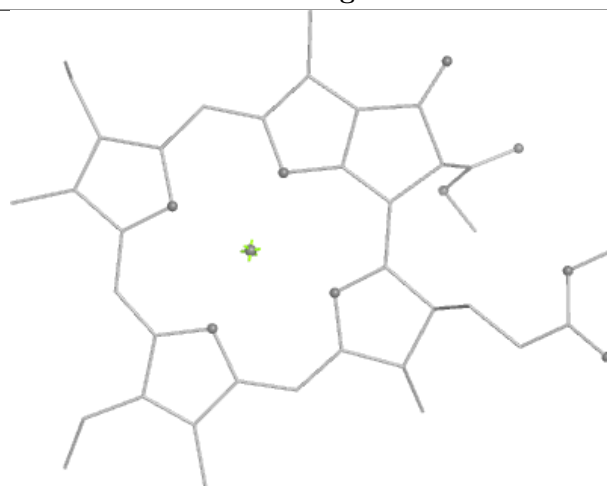
Bond lengths



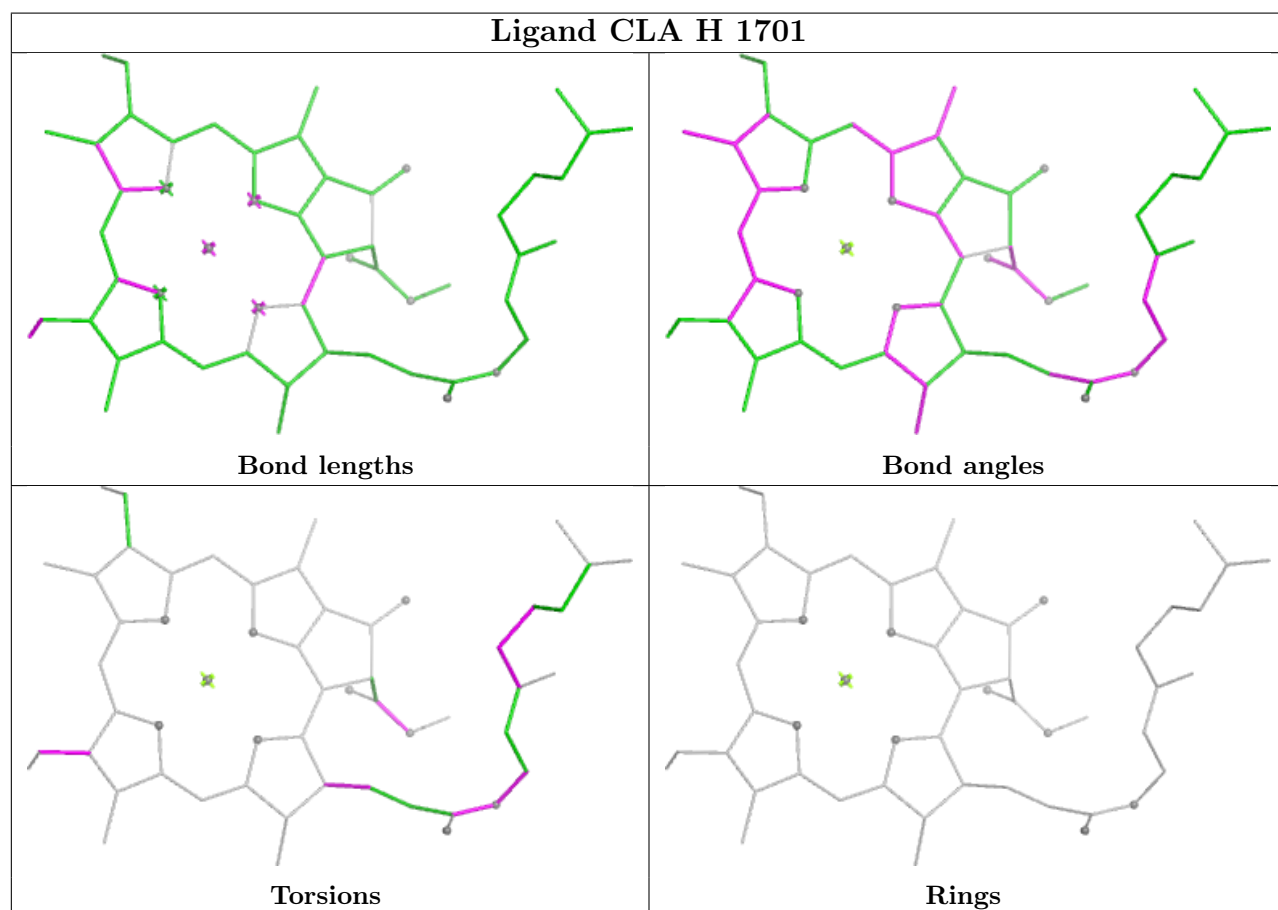
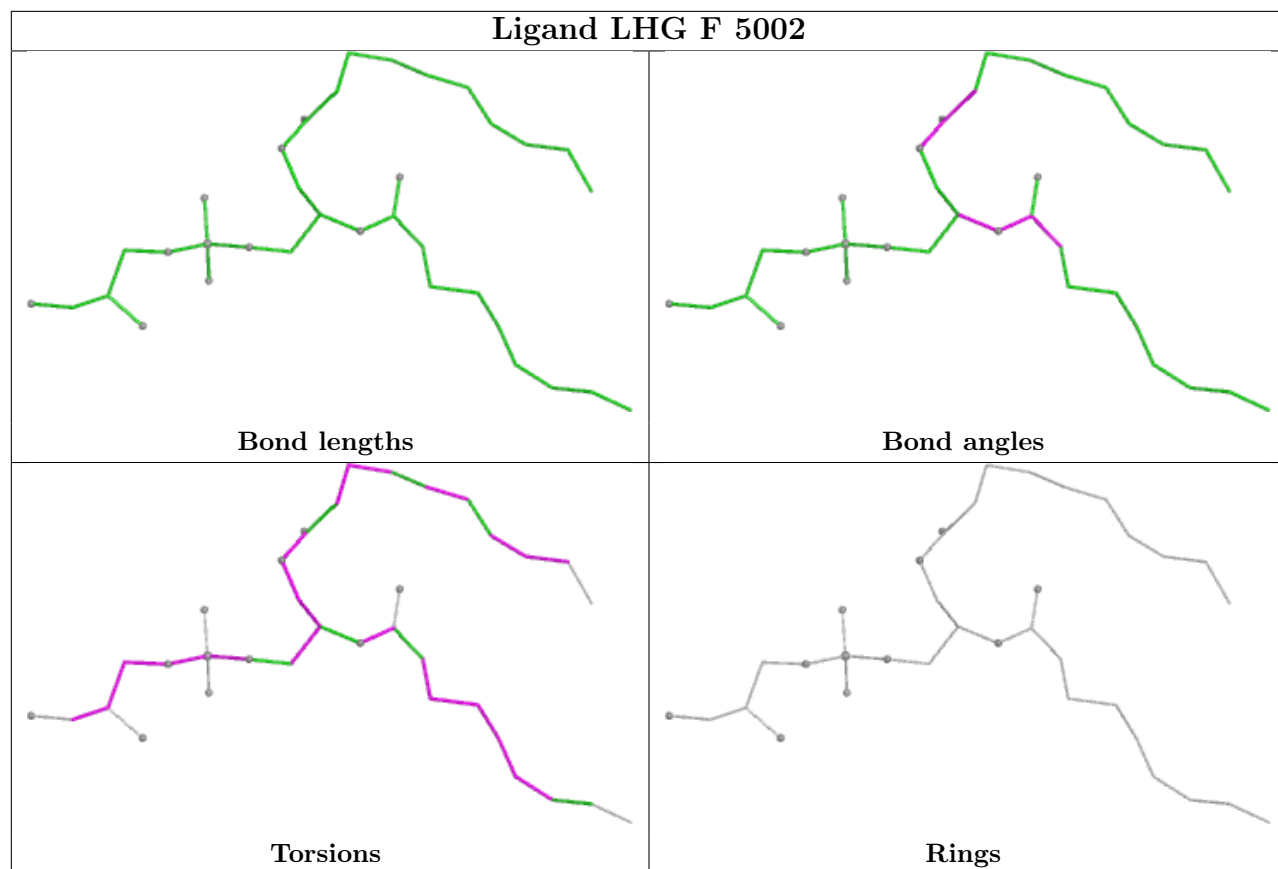
Bond angles

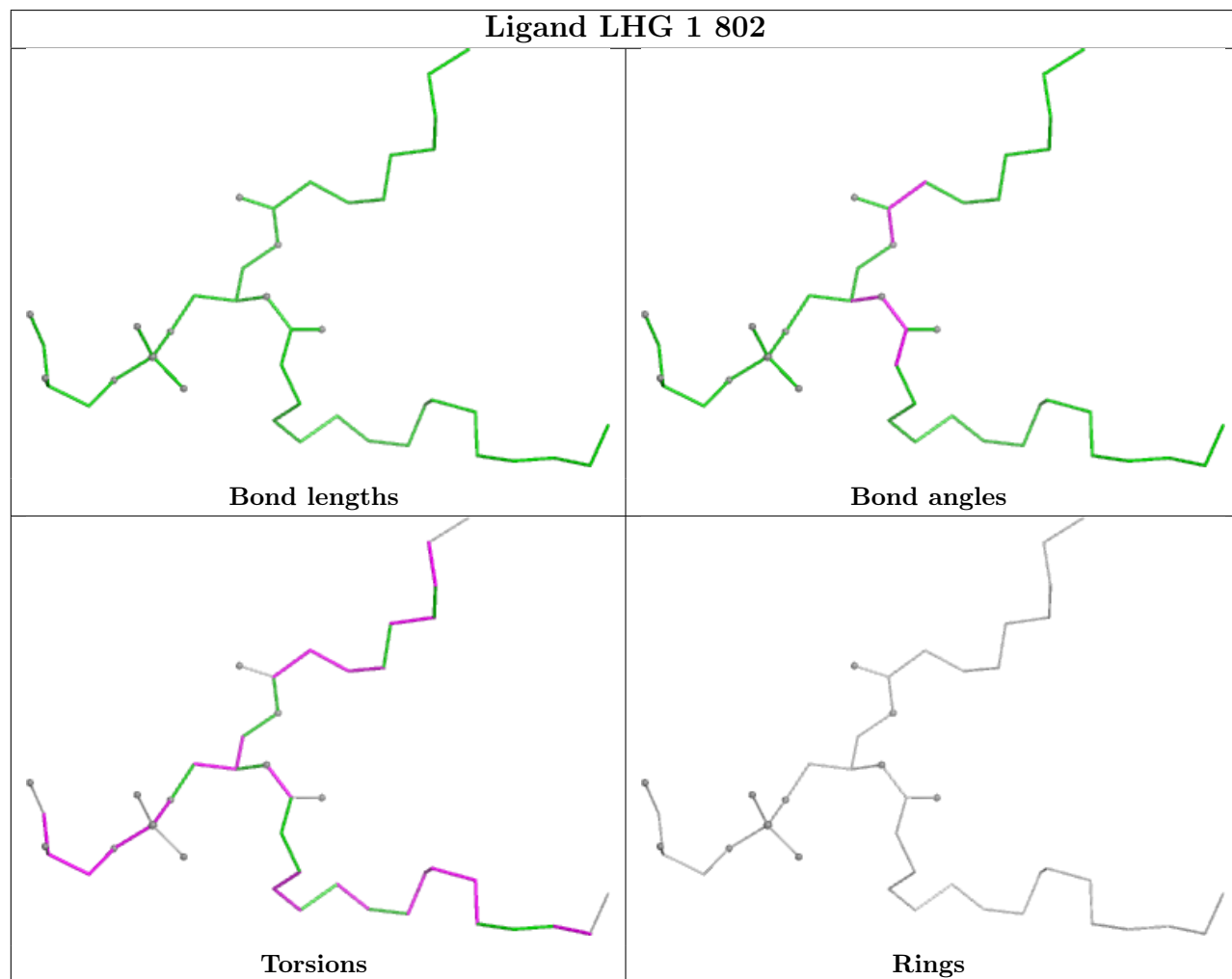
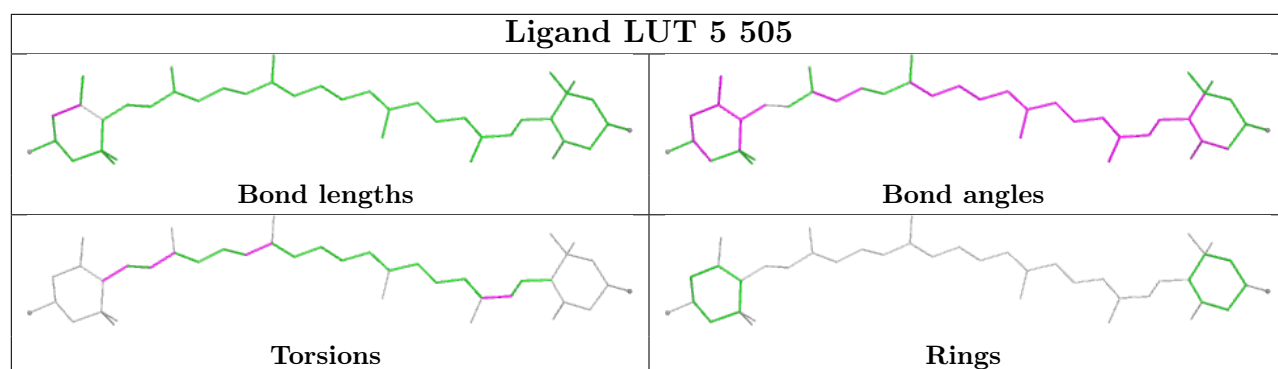


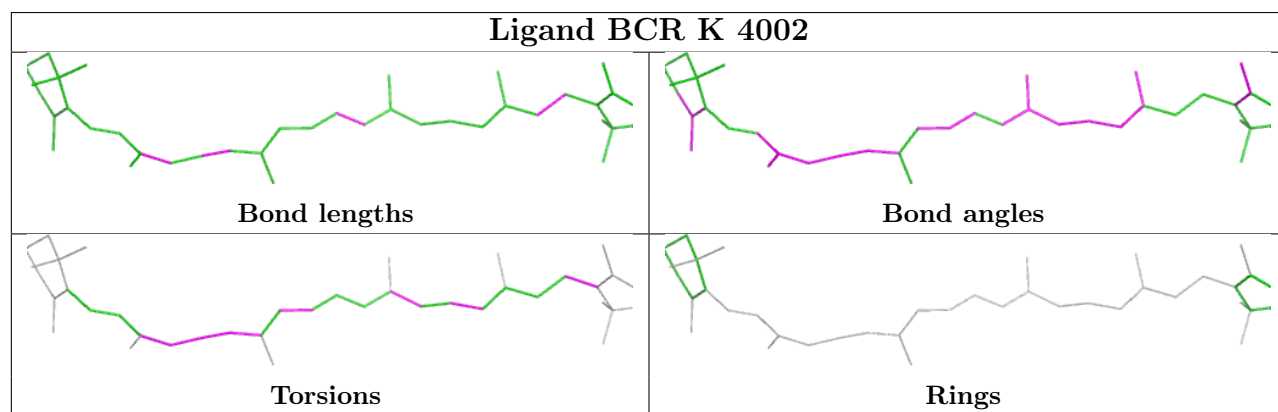
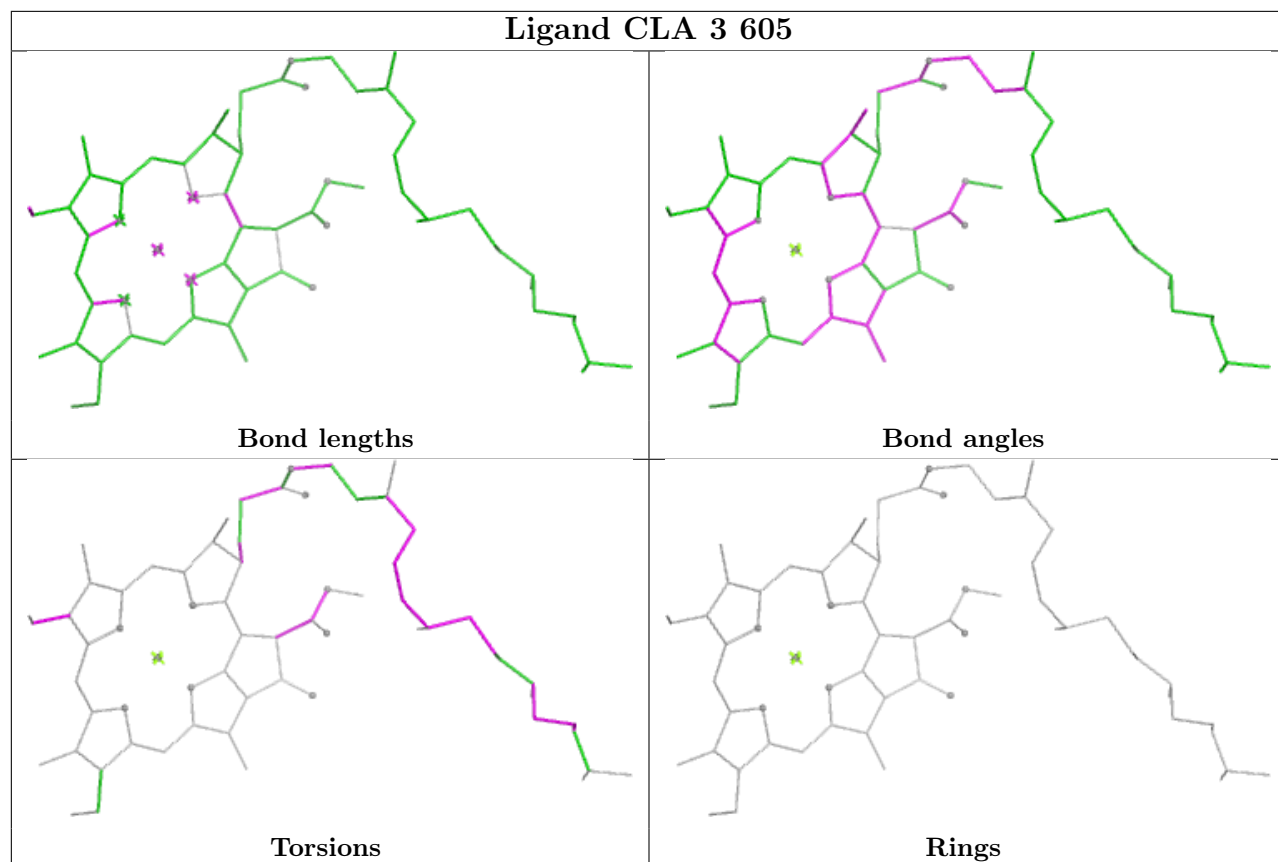
Torsions

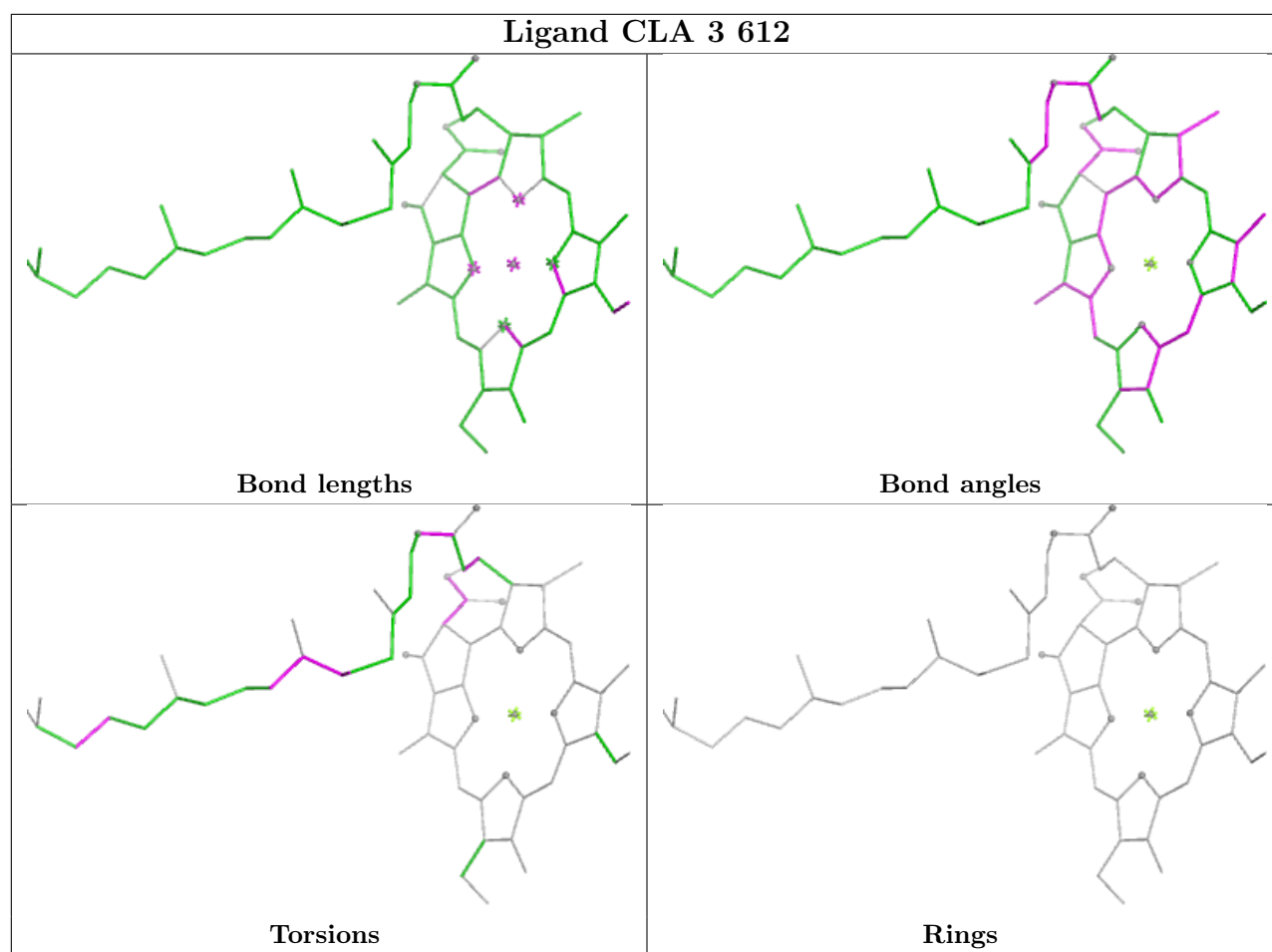


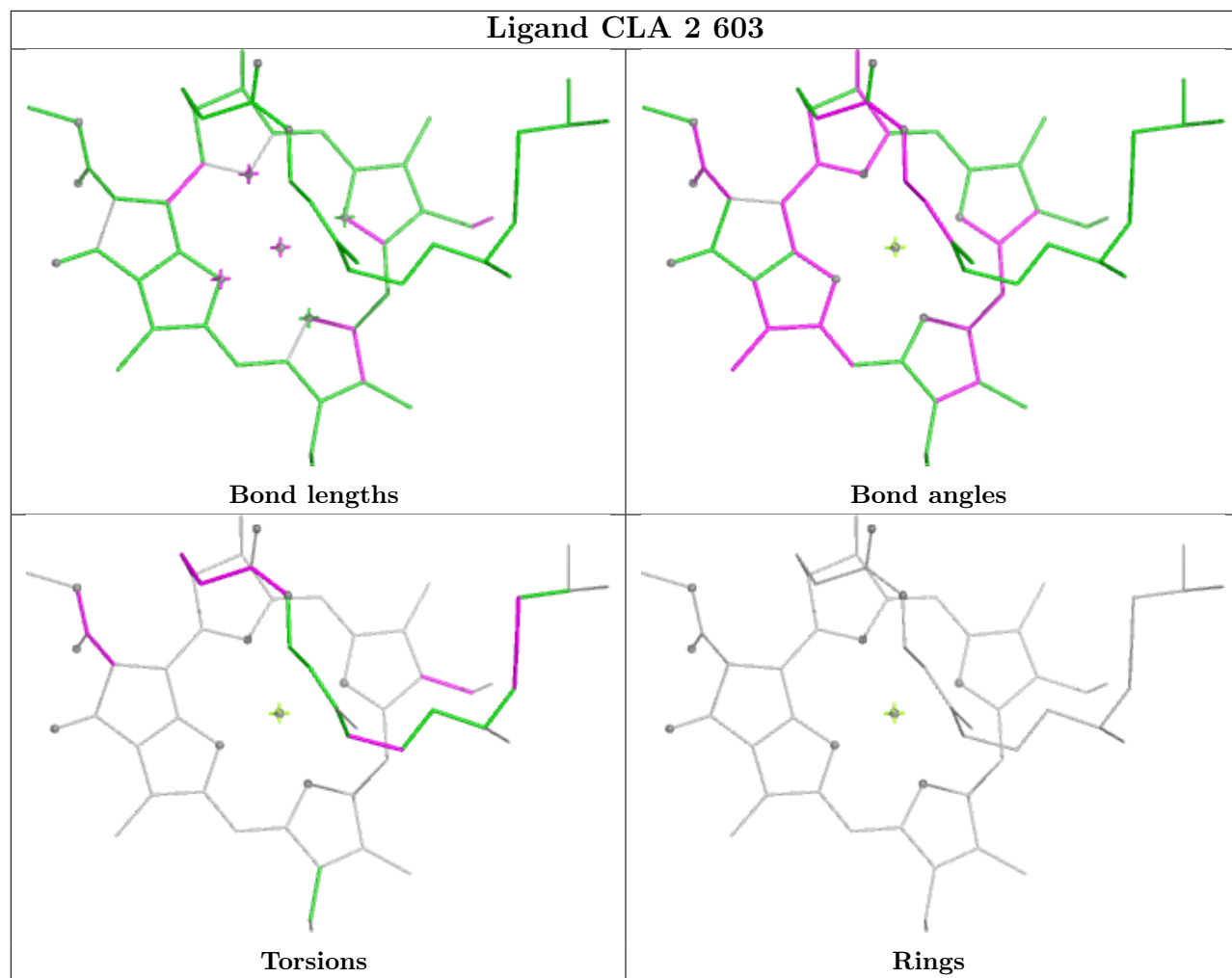
Rings

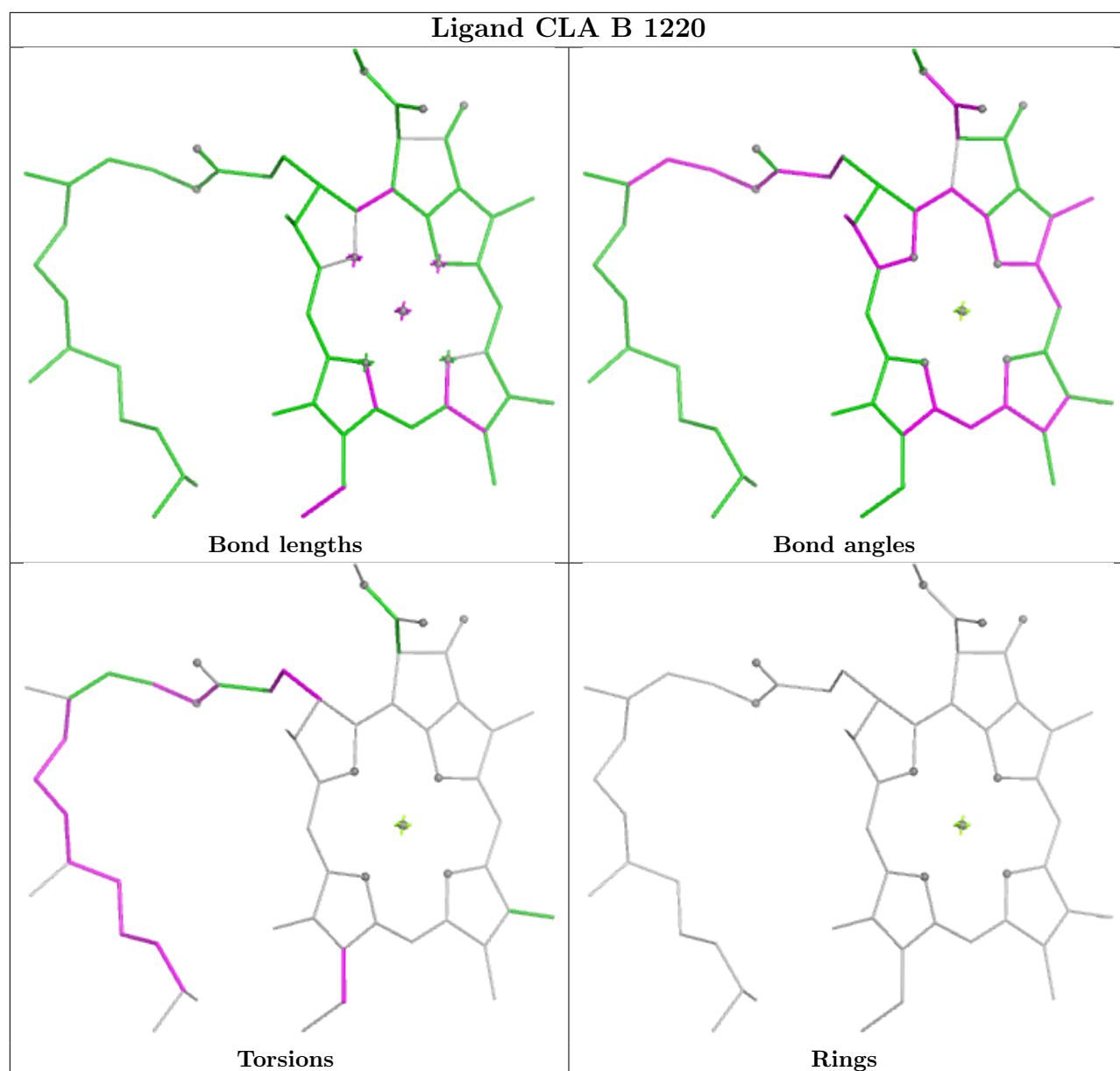


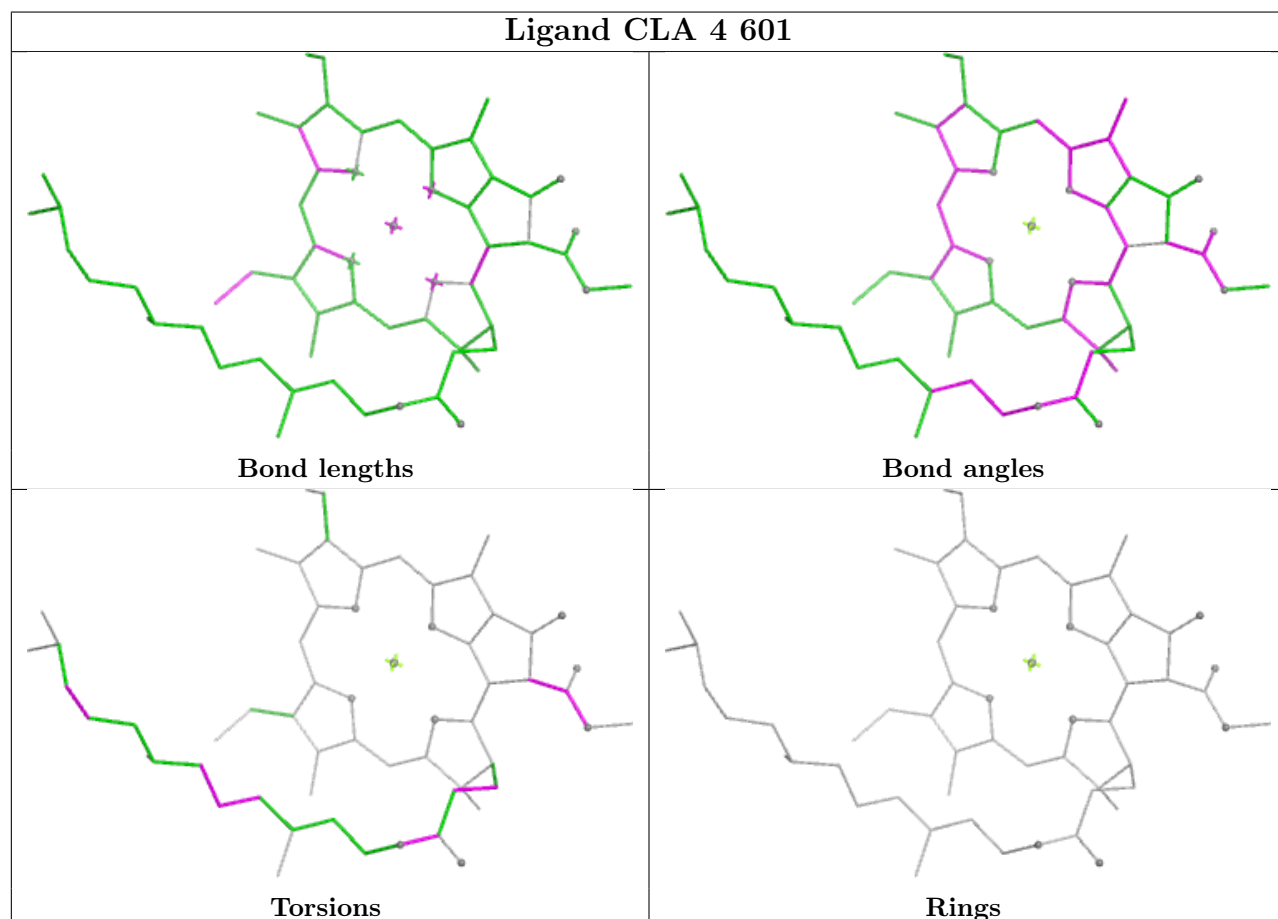
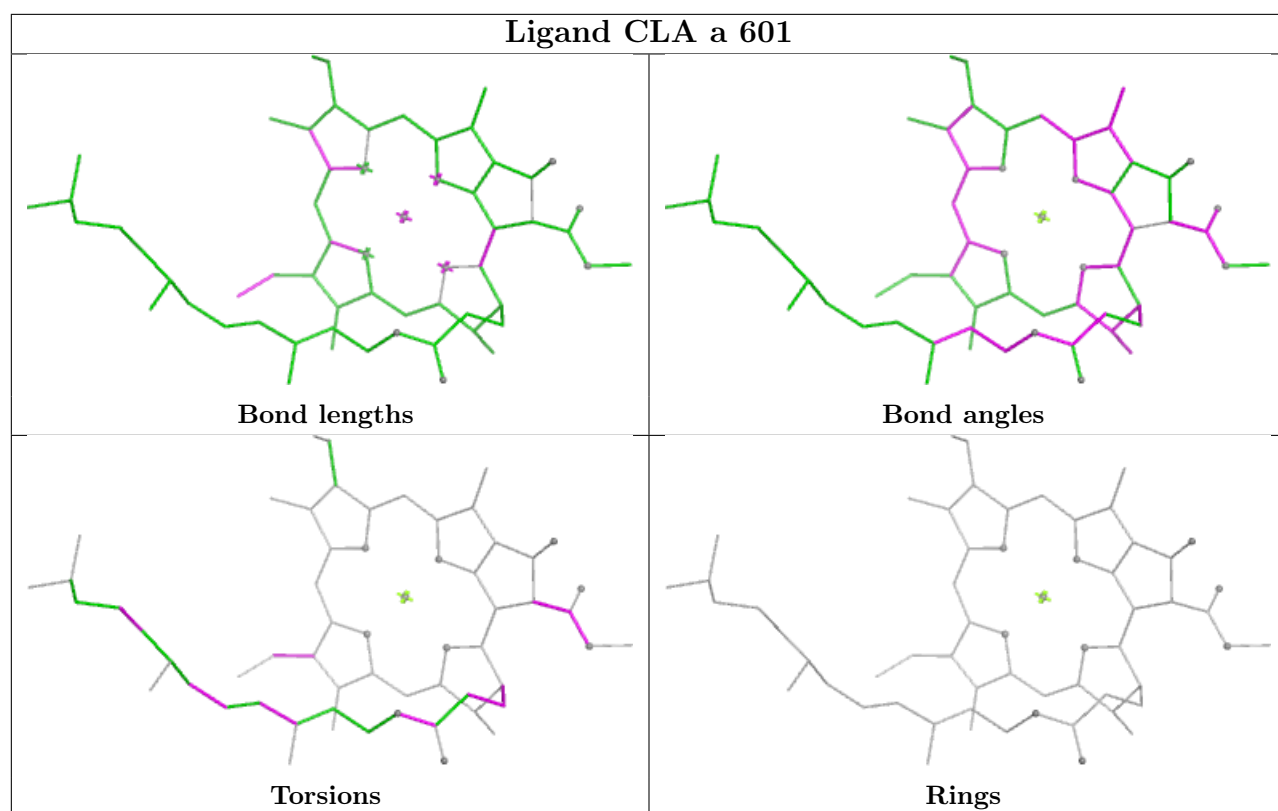


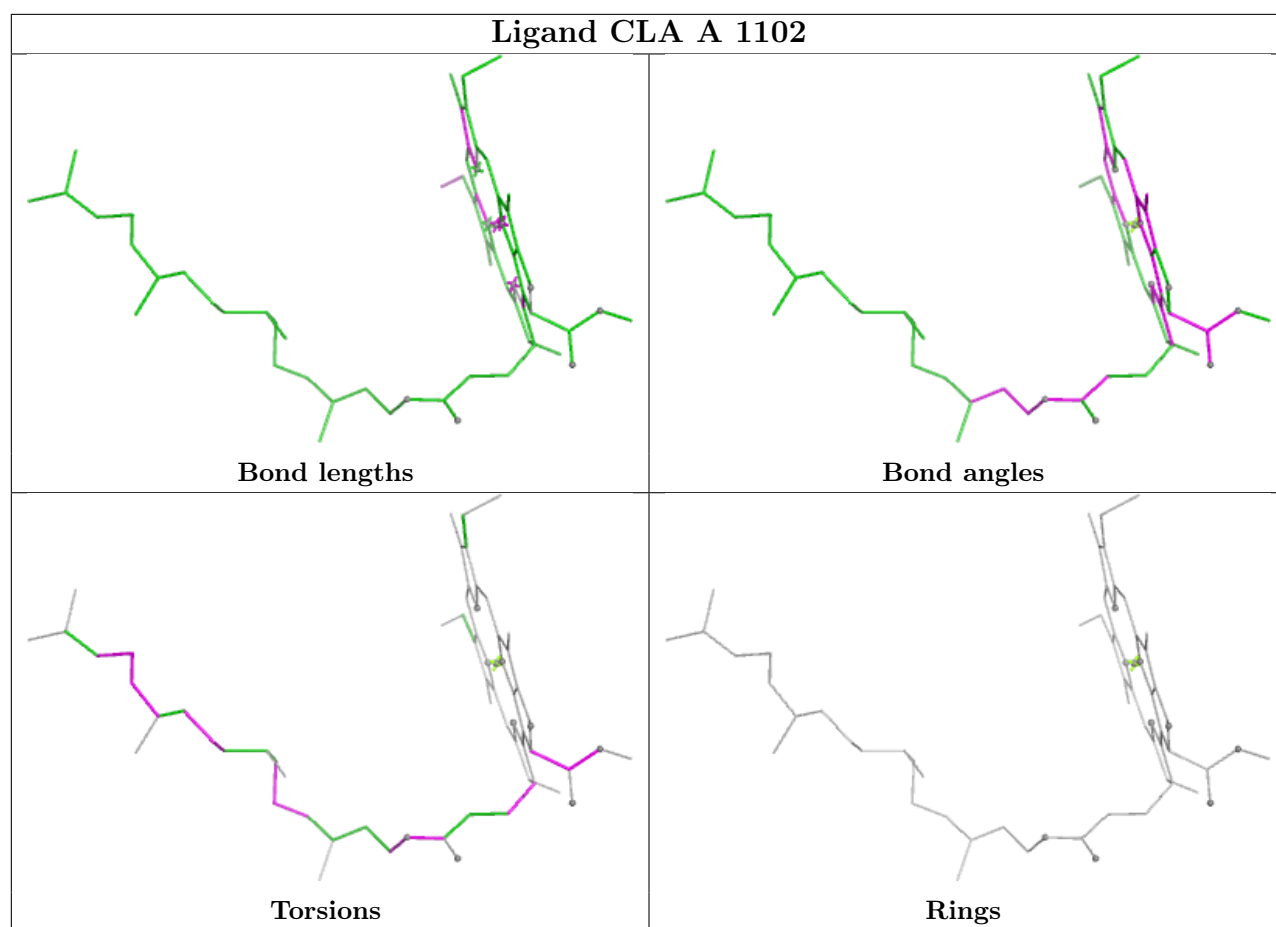


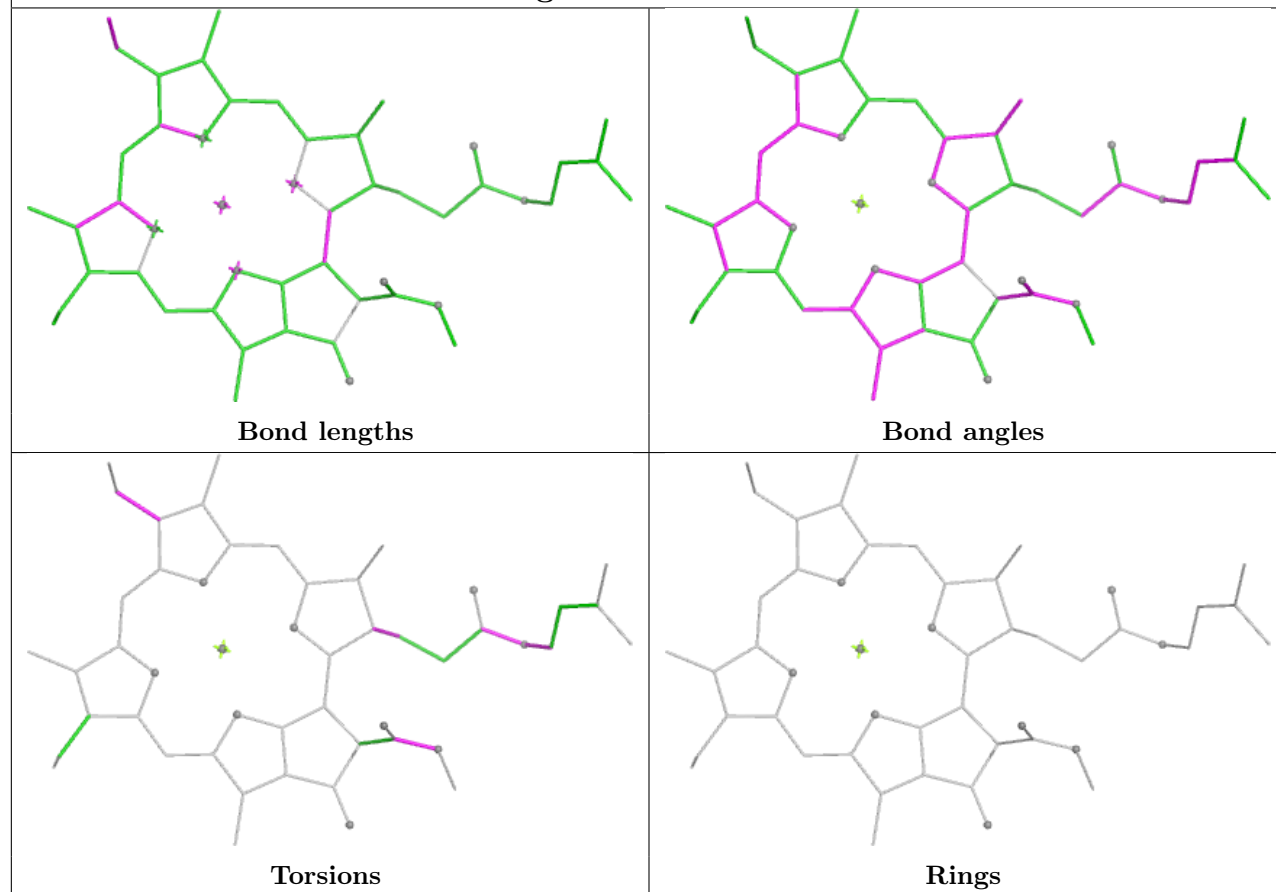
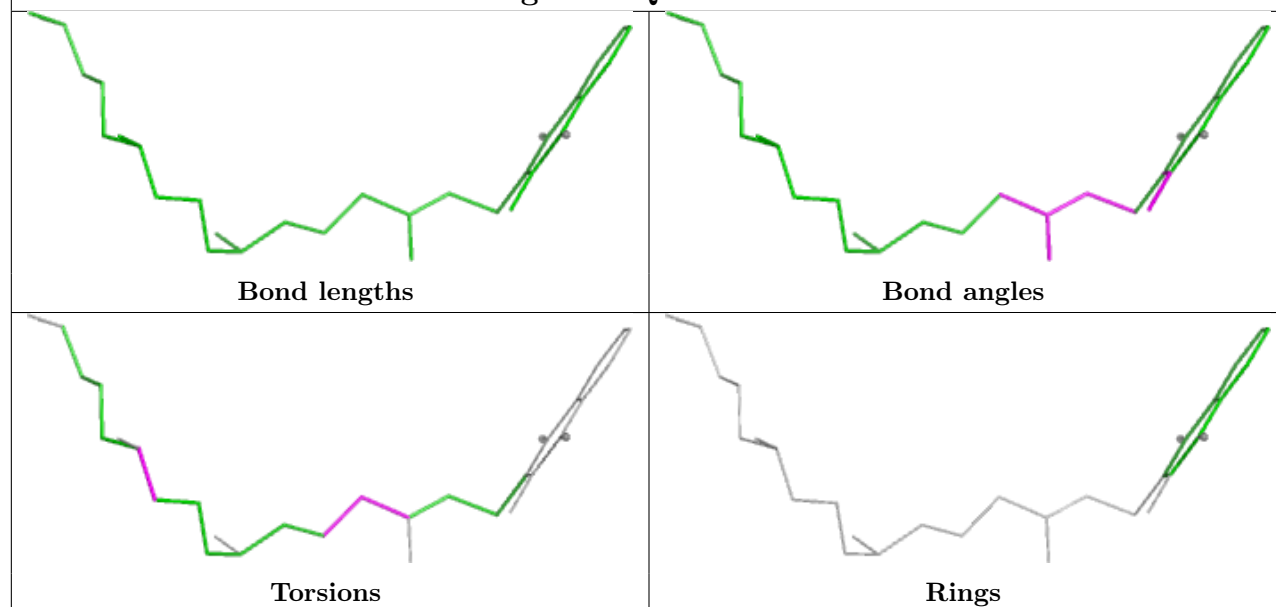




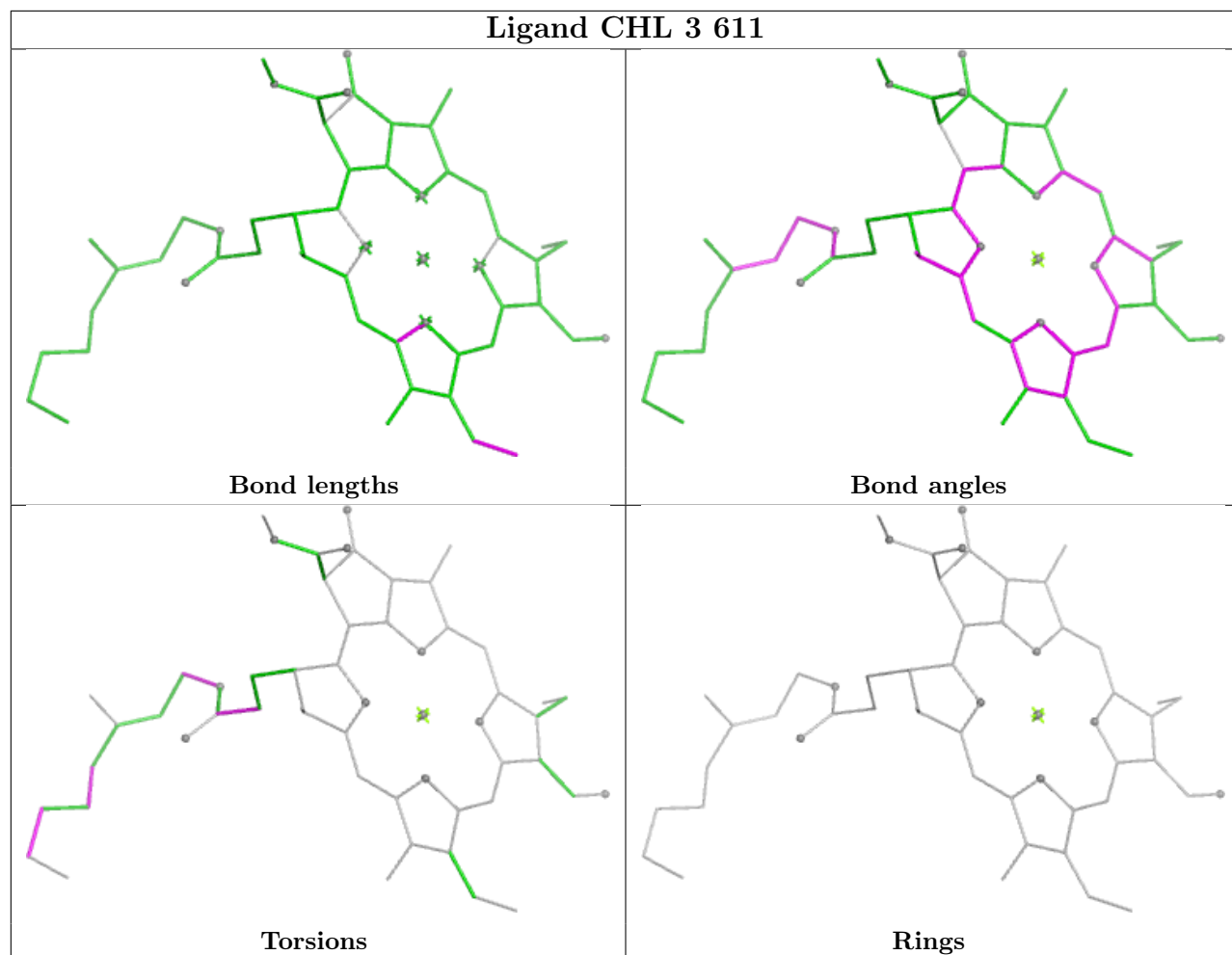




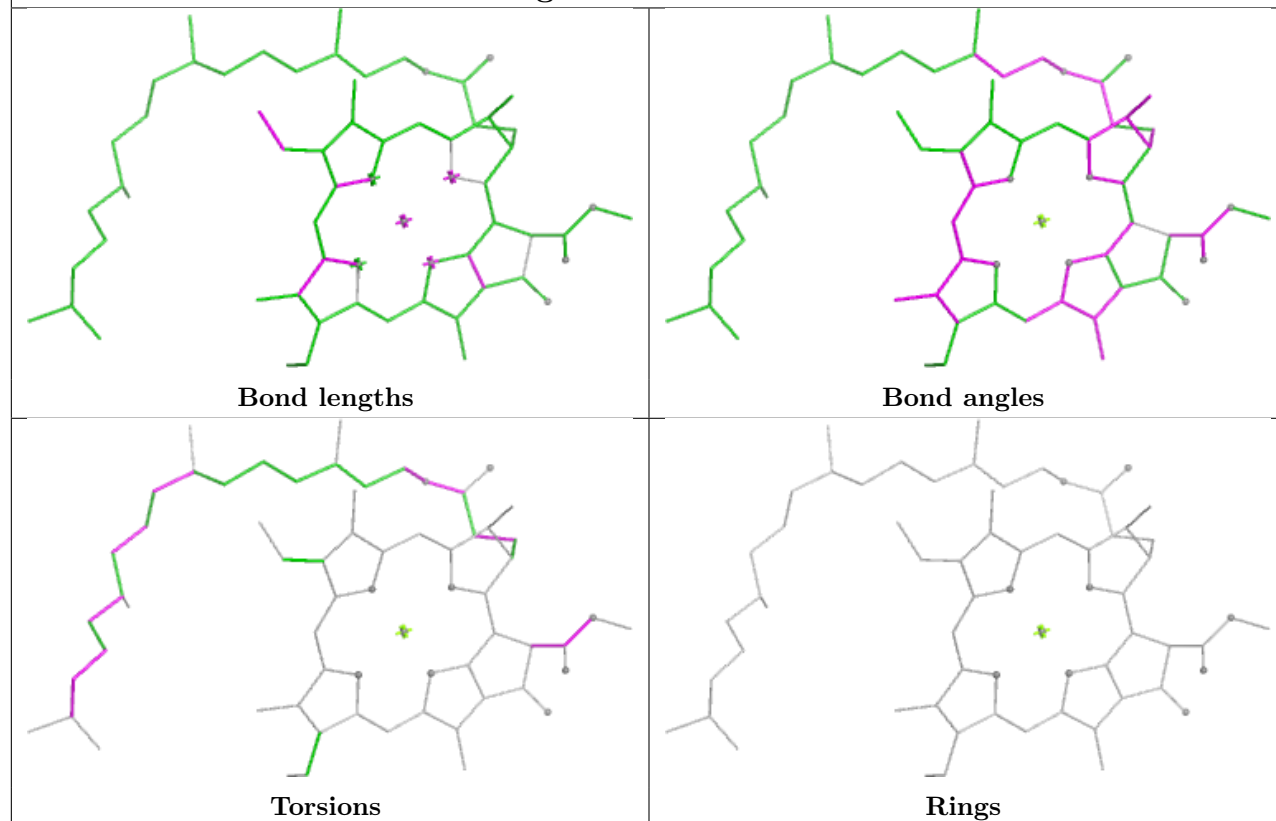


Ligand CLA a 602**Ligand PQN B 2002**

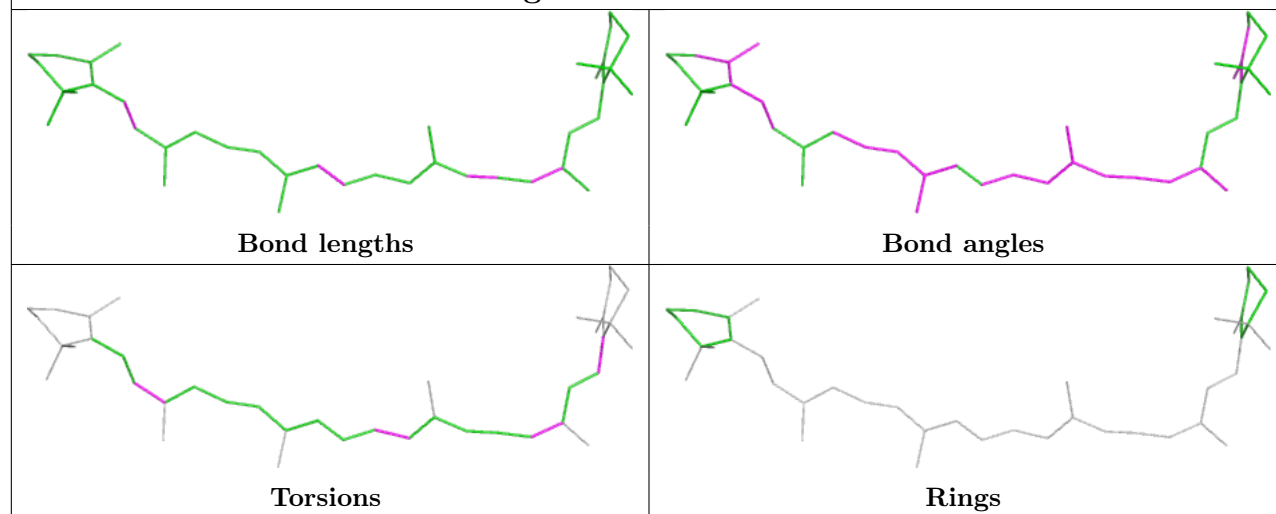
Ligand CHL 3 611

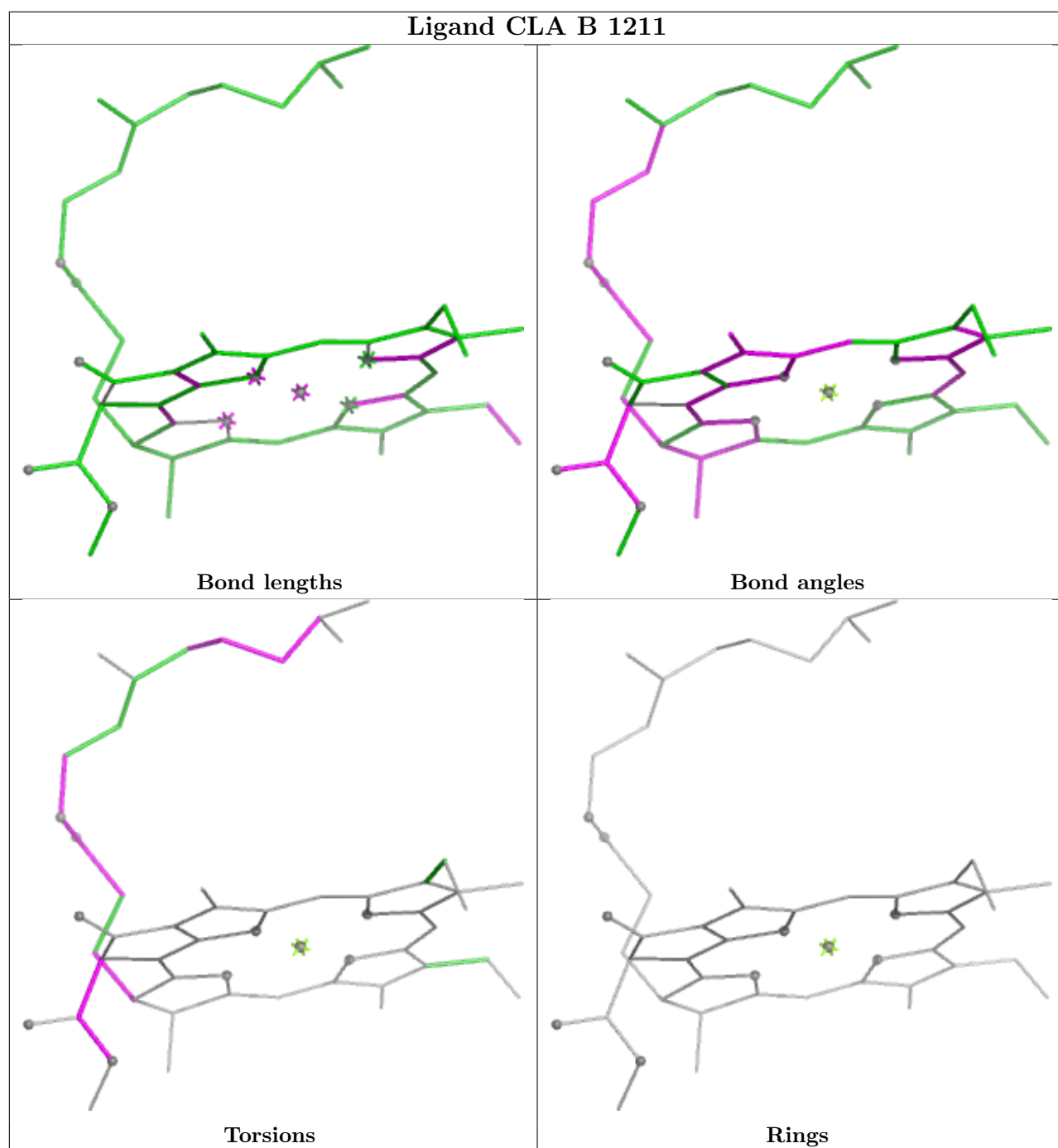


Ligand CLA 5 604

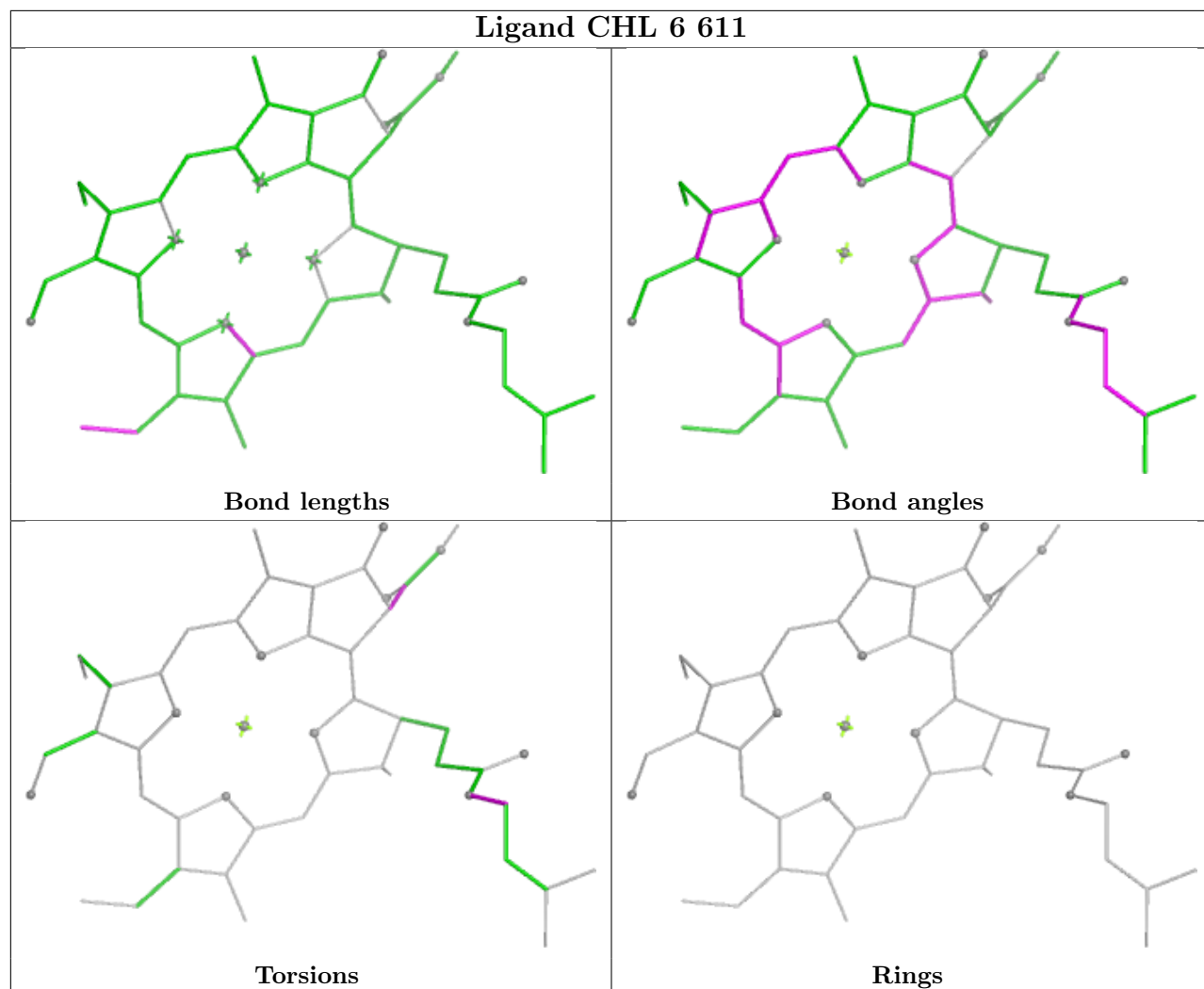


Ligand BCR L 4002

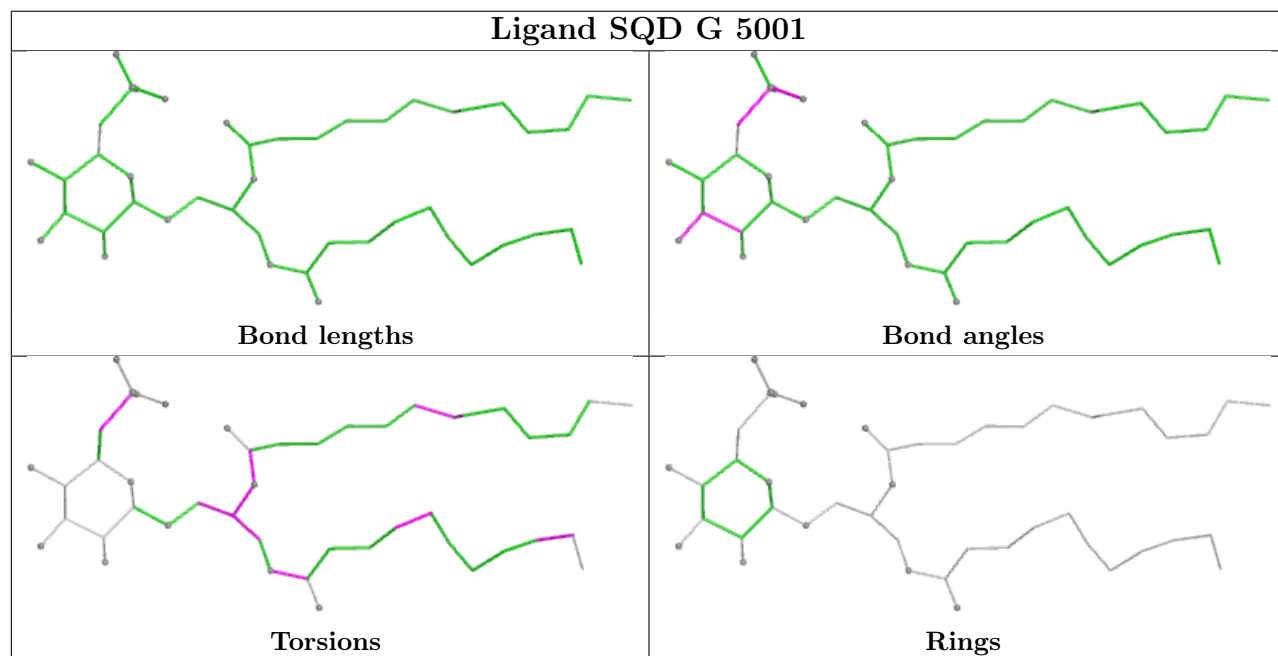


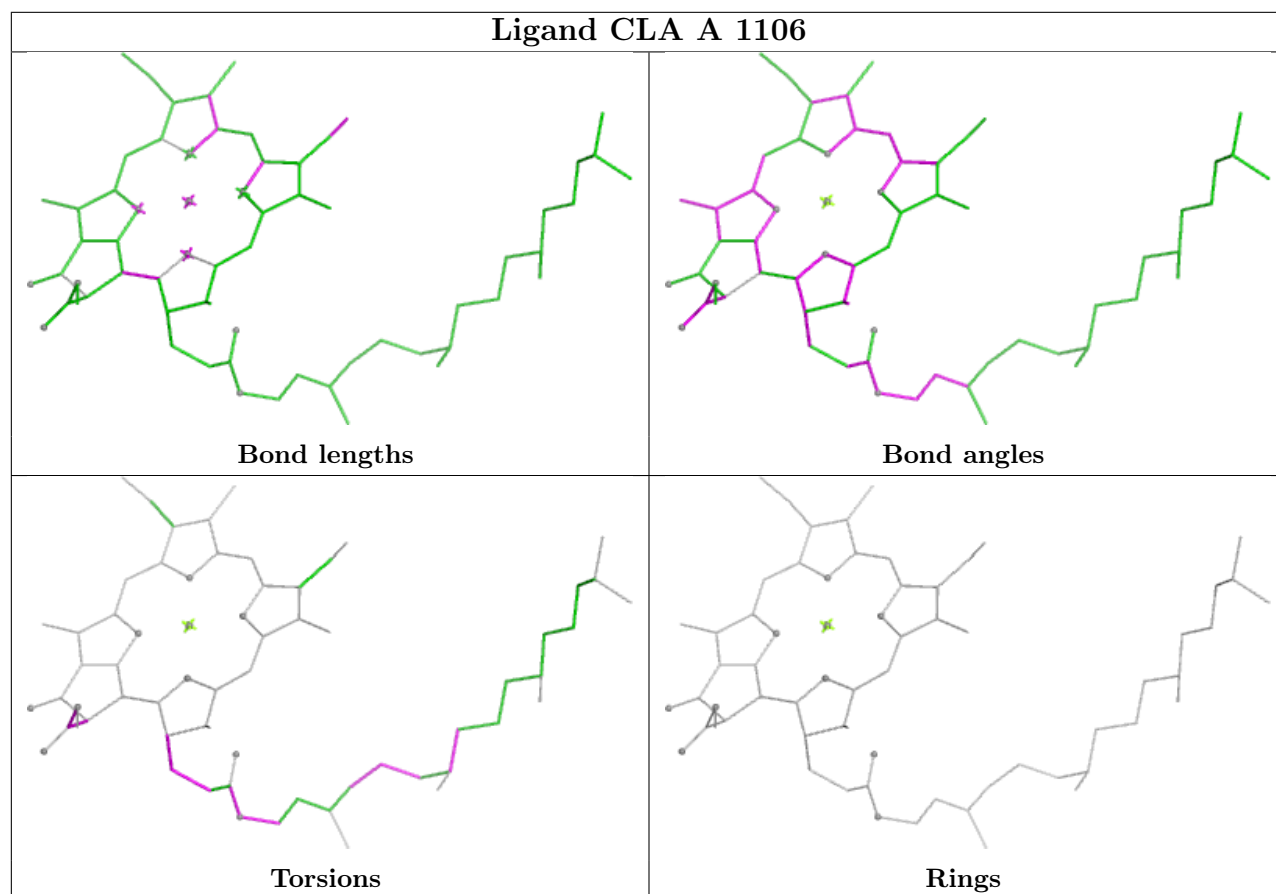
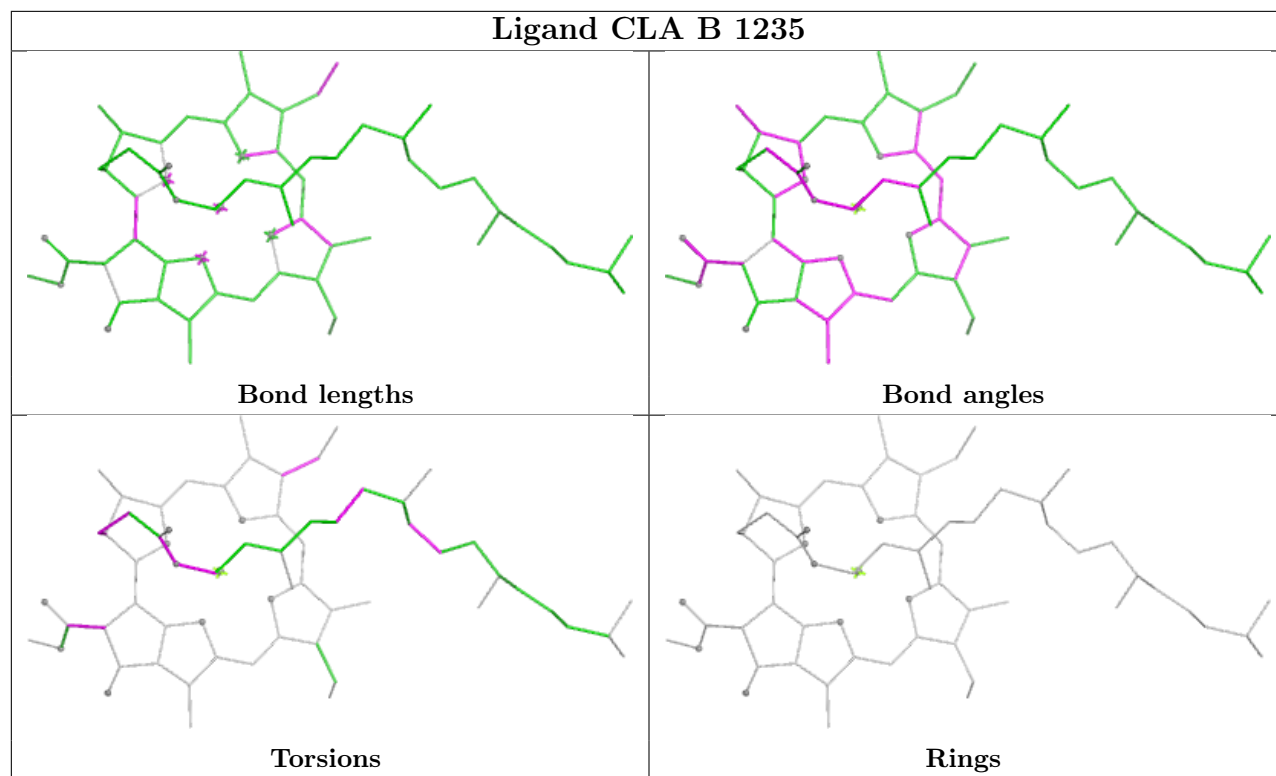


Ligand CHL 6 611

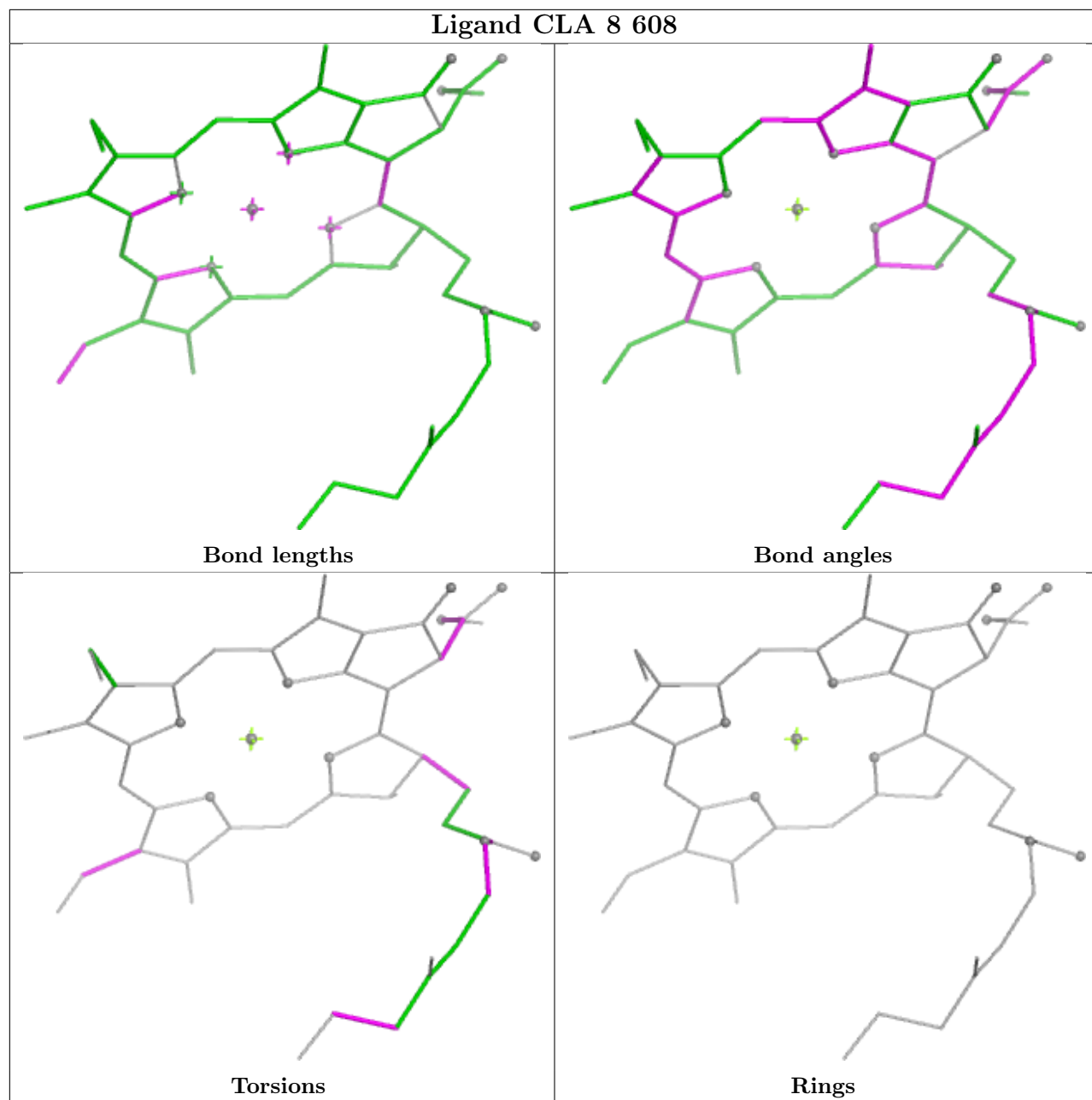


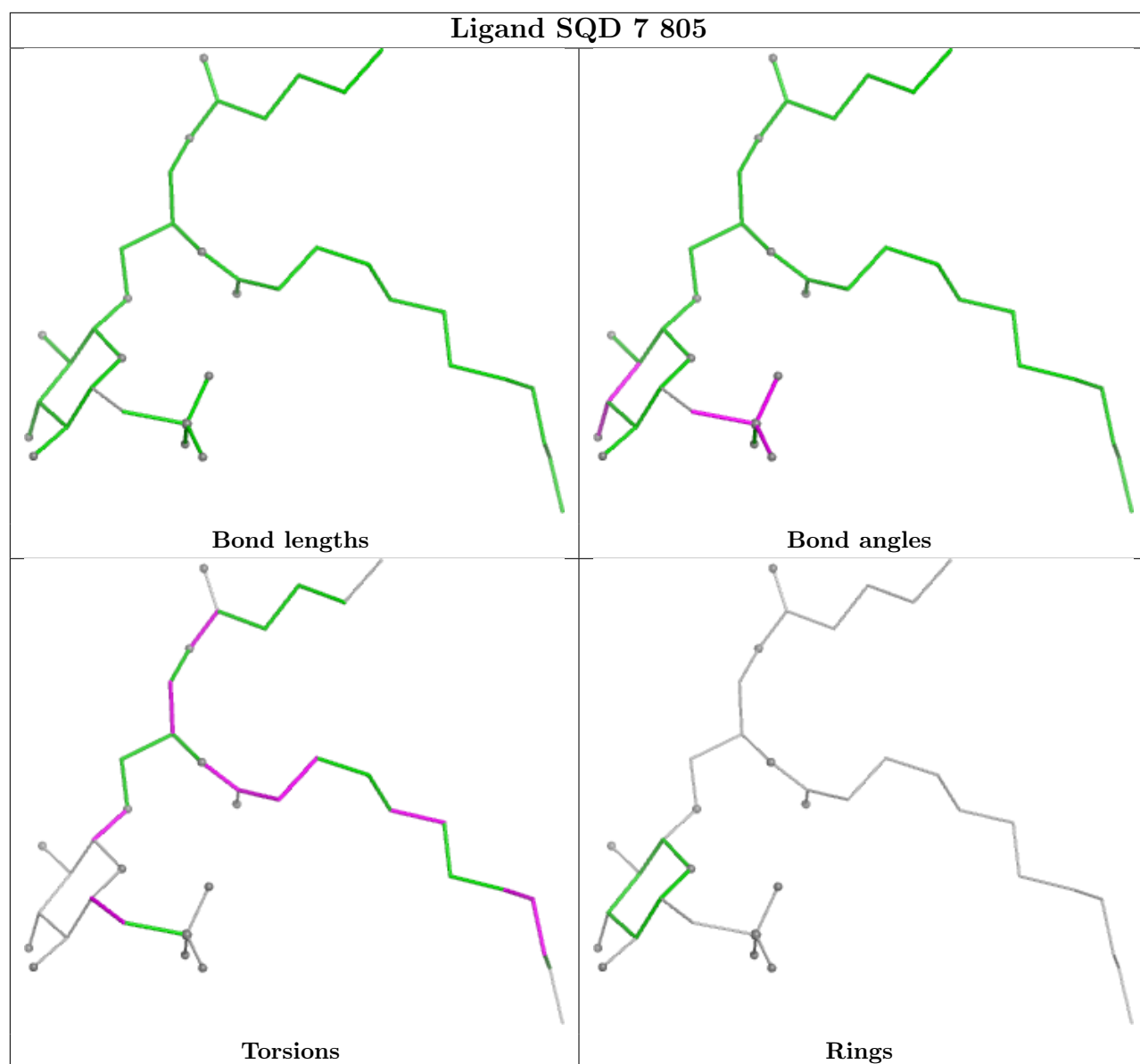
Ligand SQD G 5001

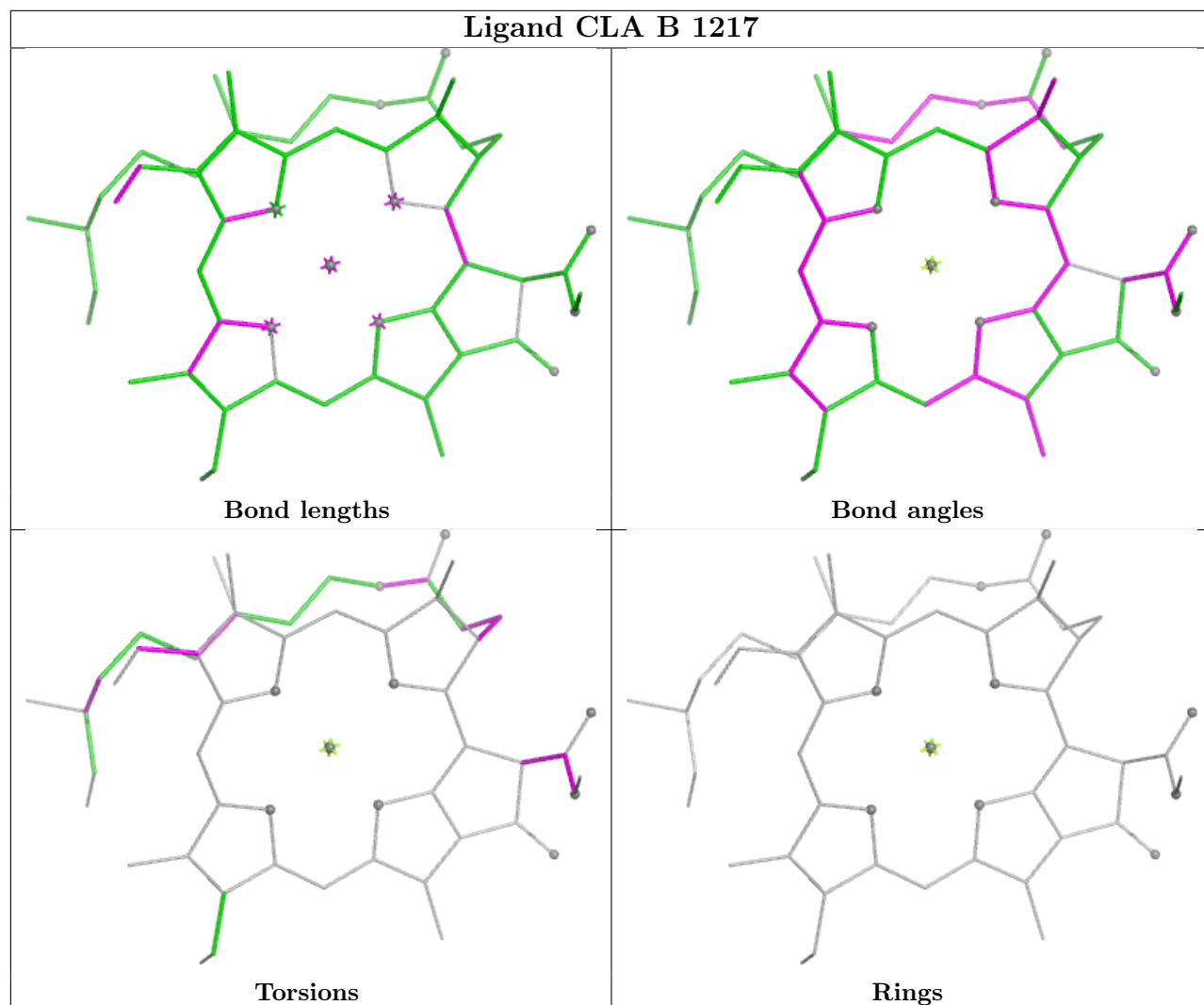


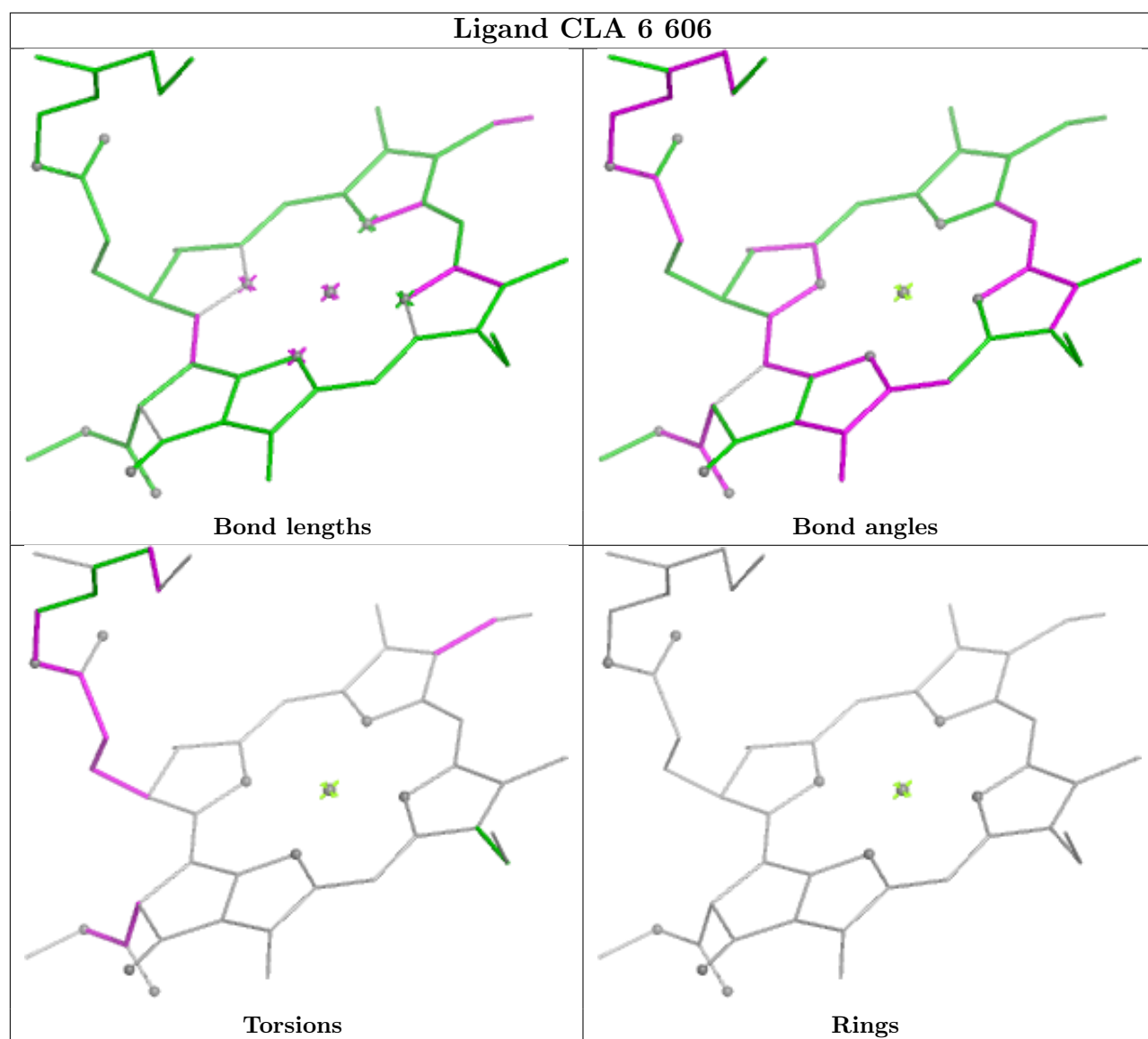


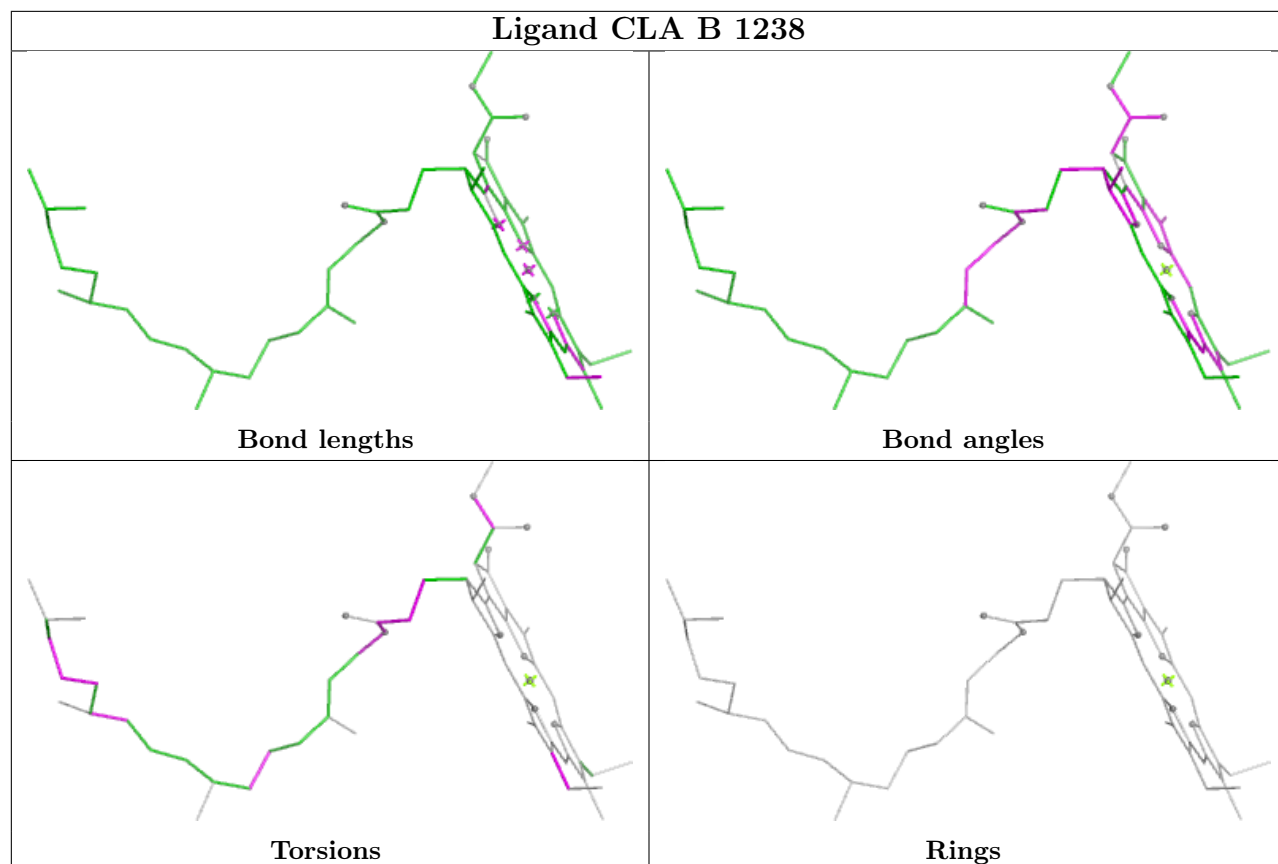
Ligand CLA 8 608



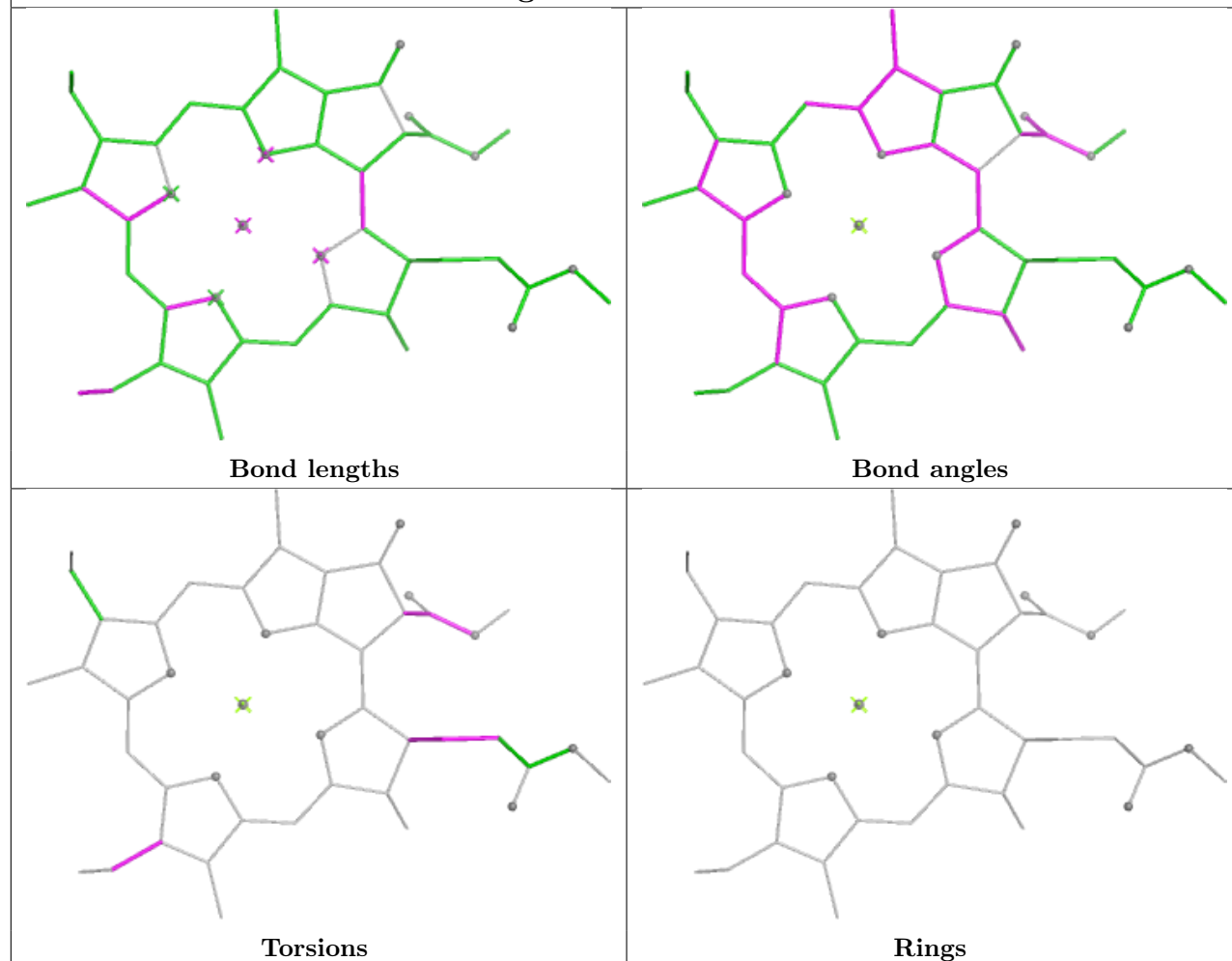




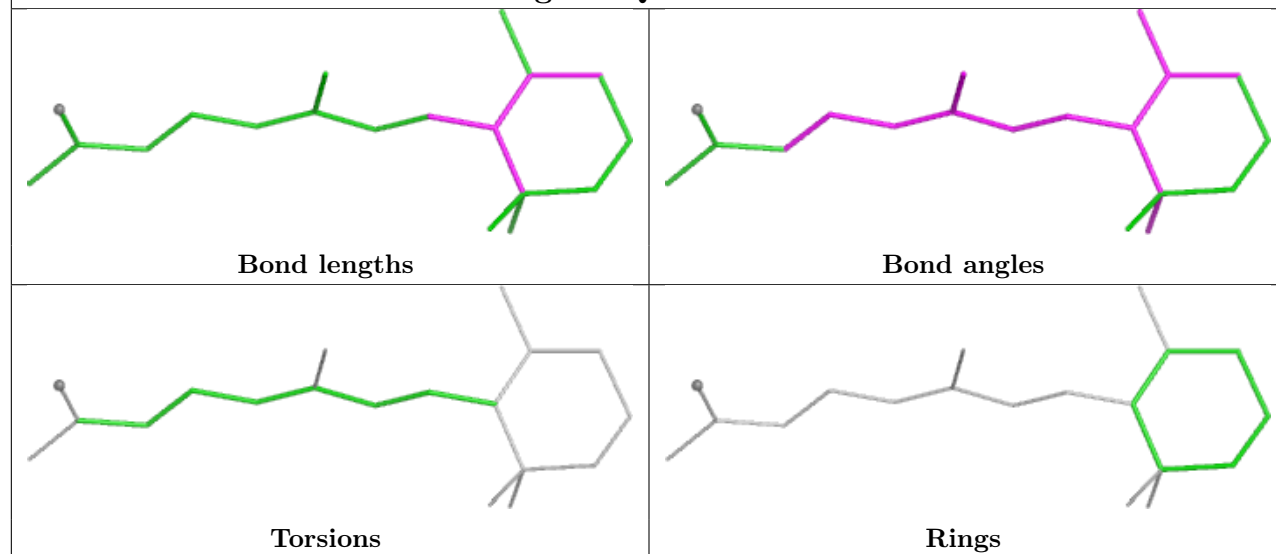


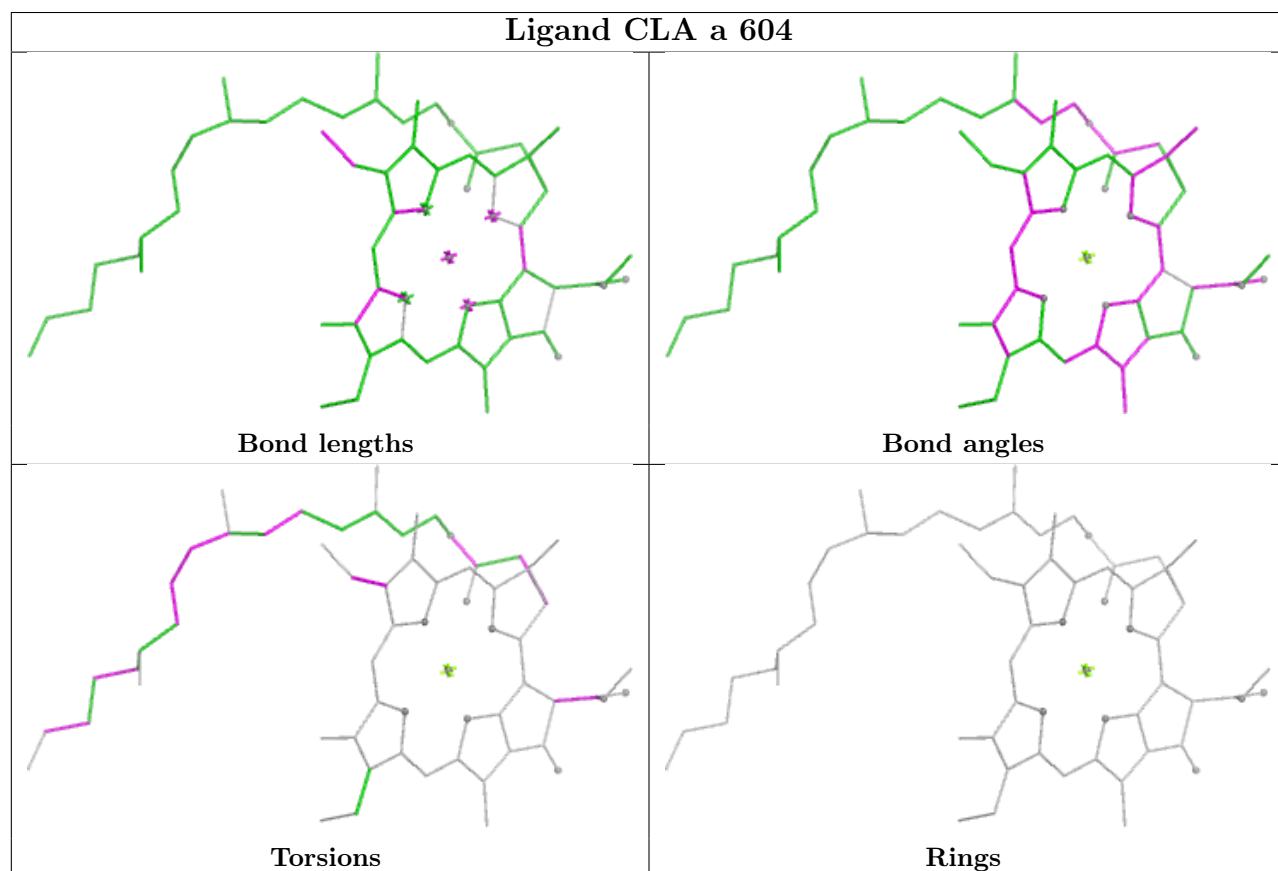
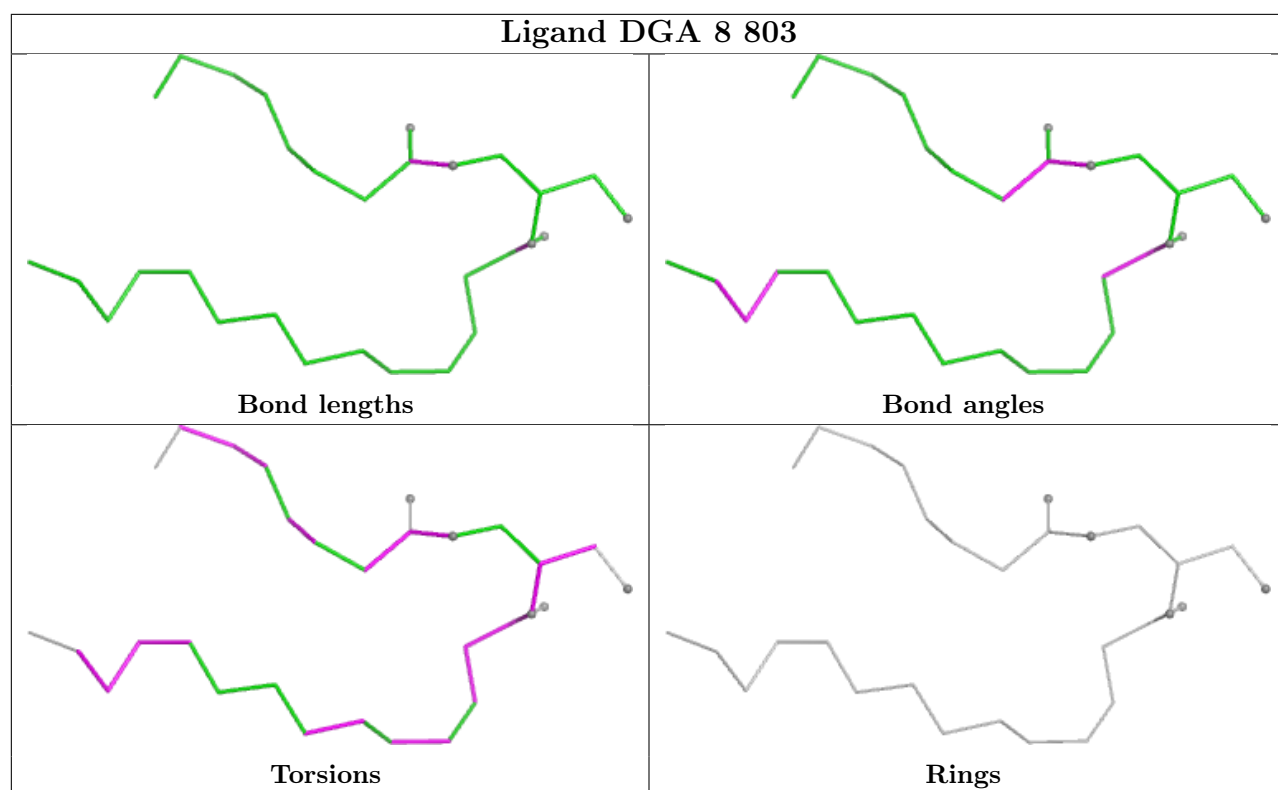


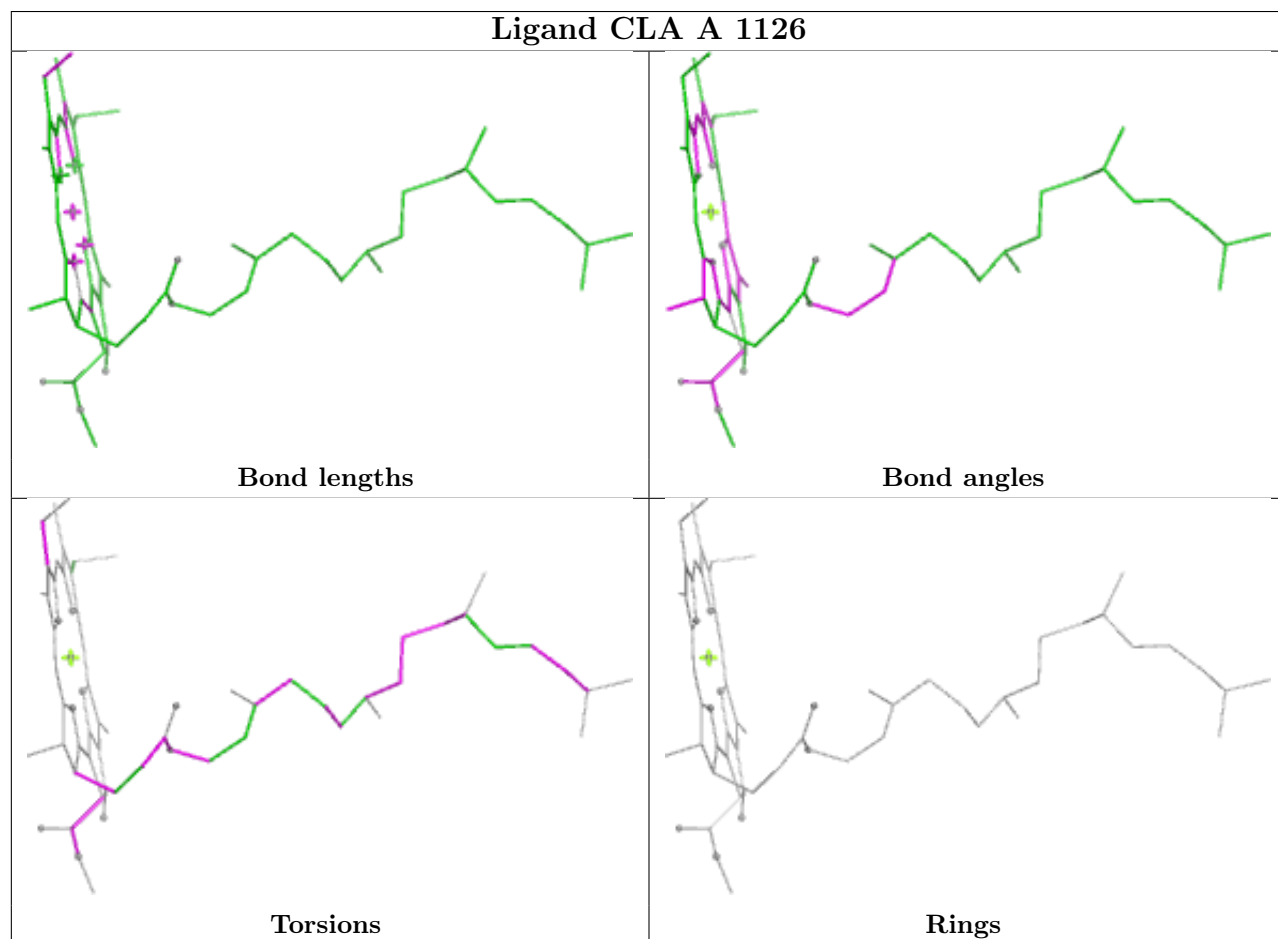
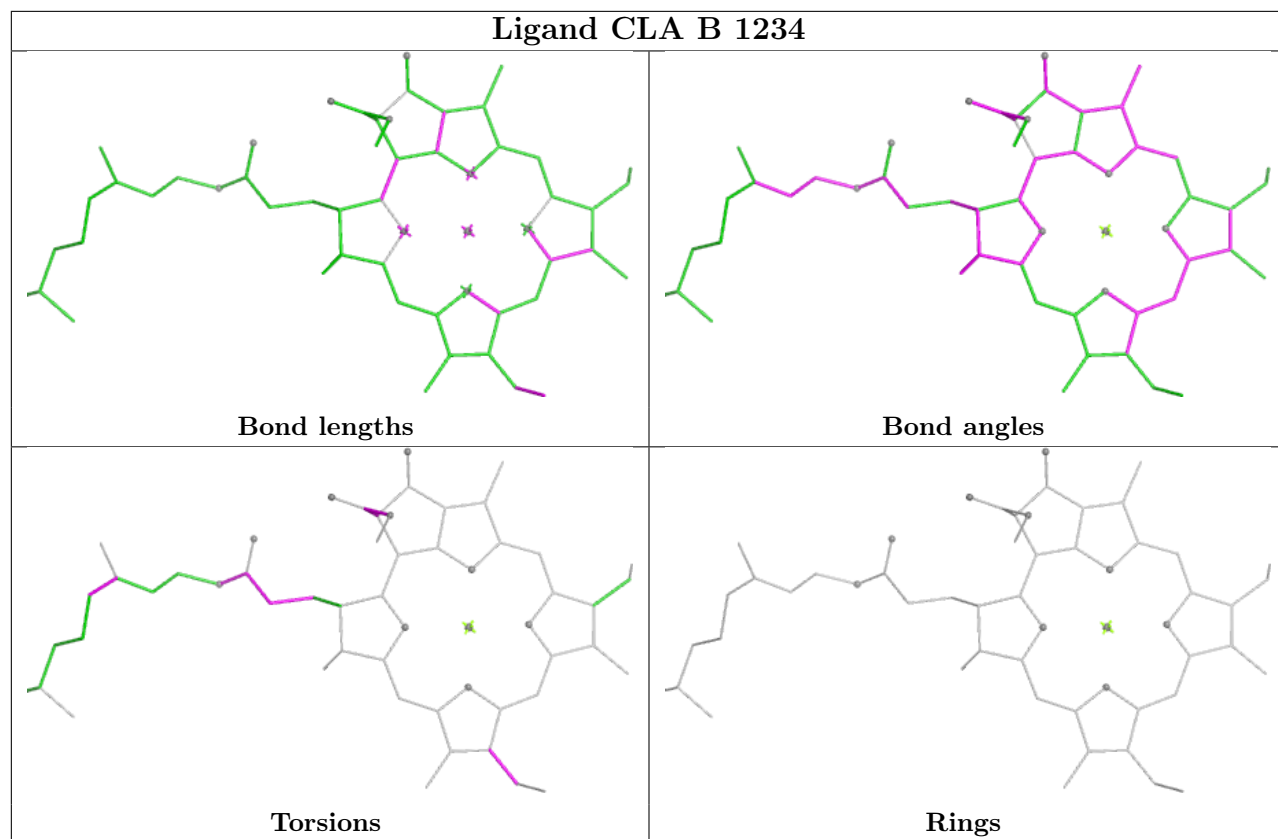
Ligand CLA 8 615

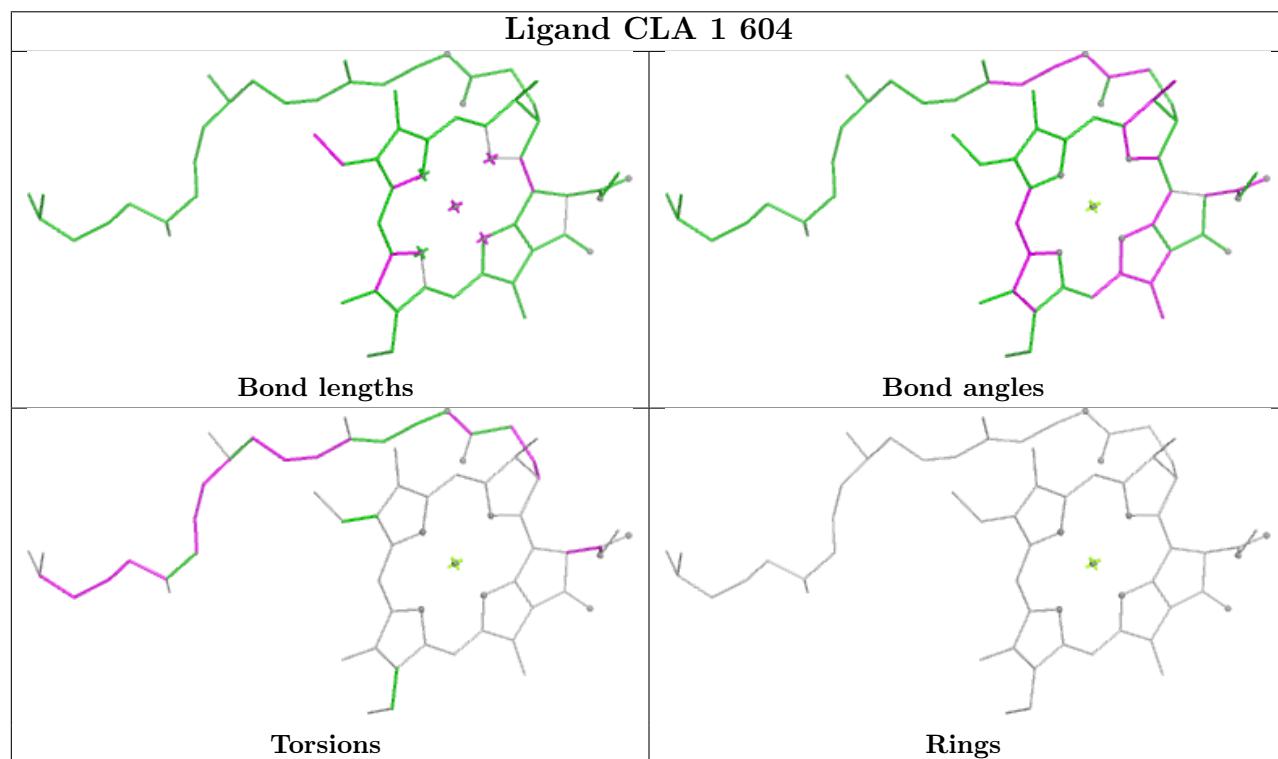
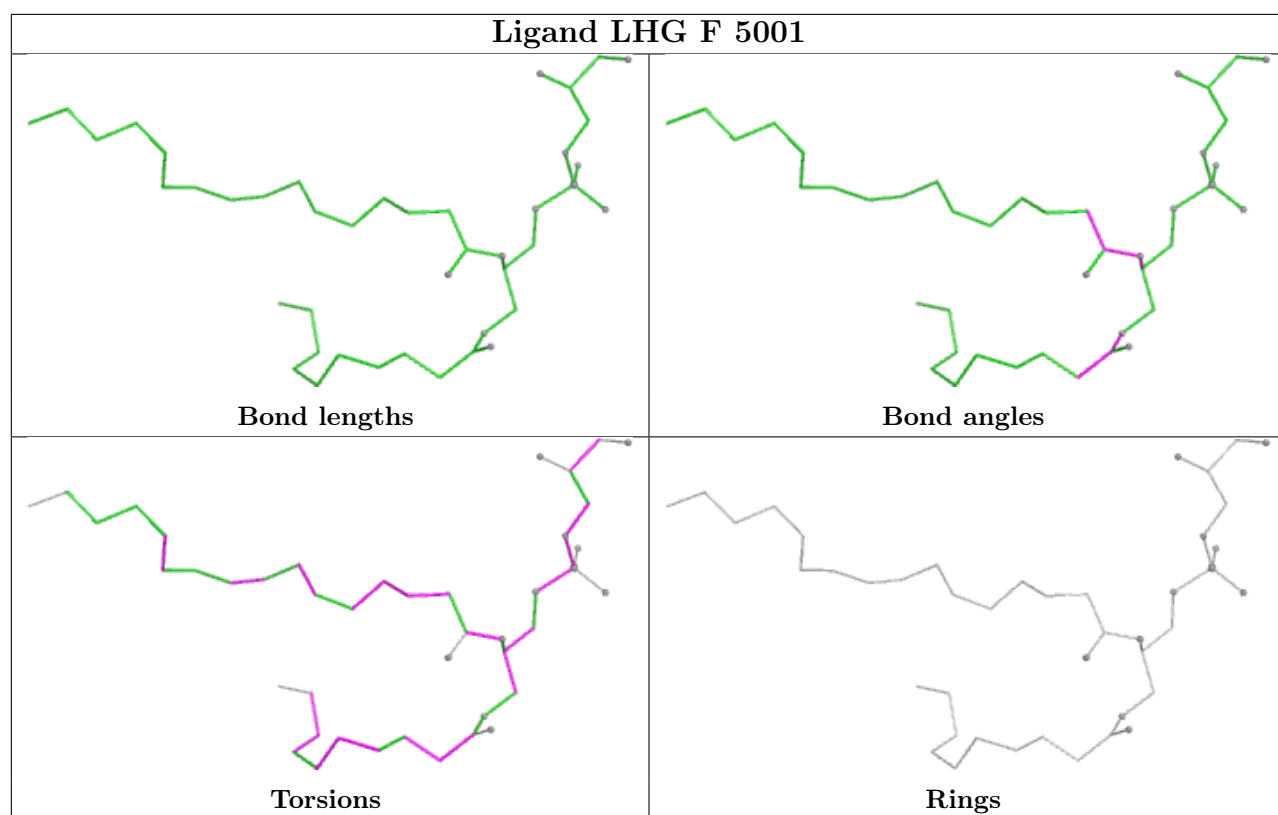


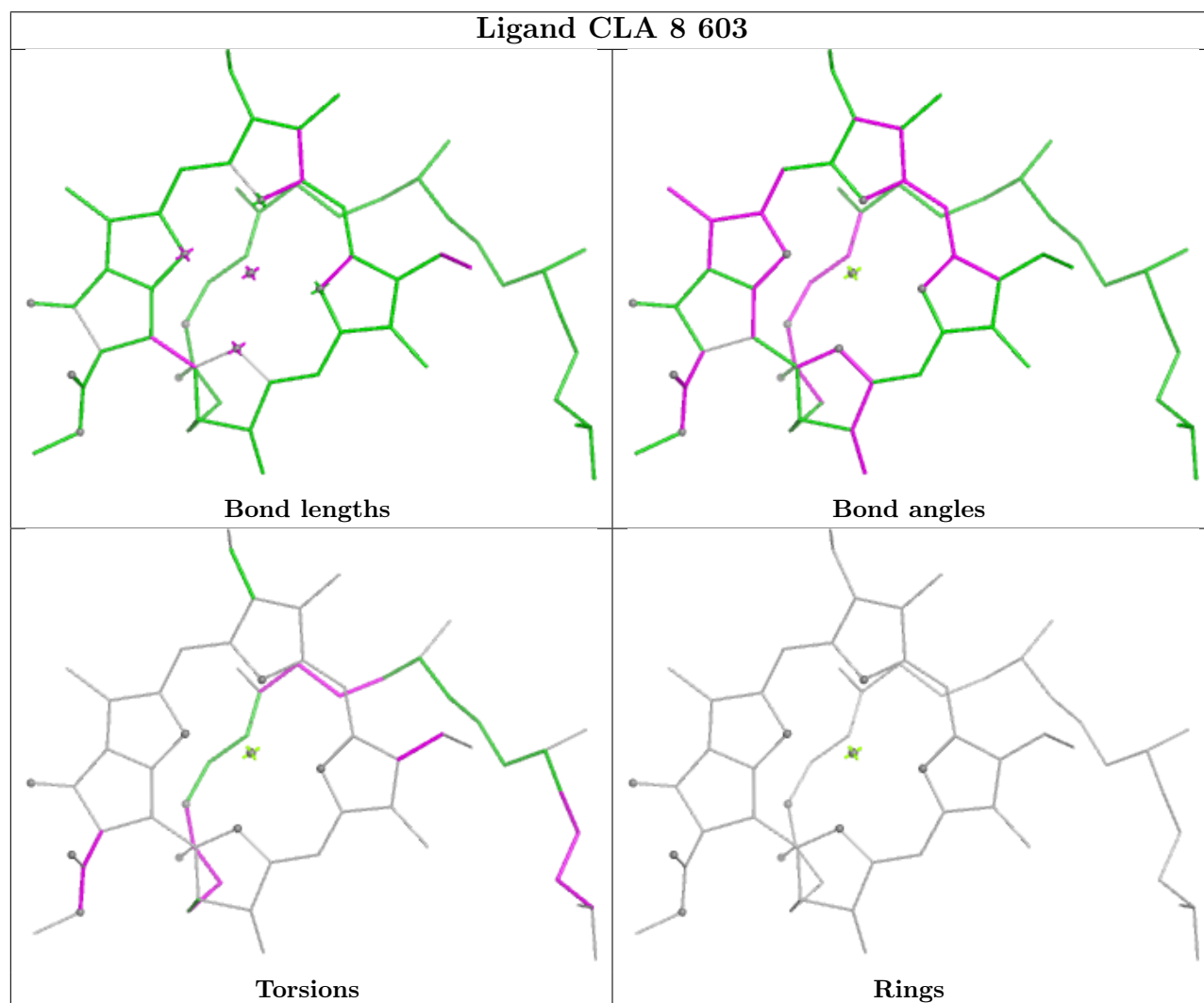
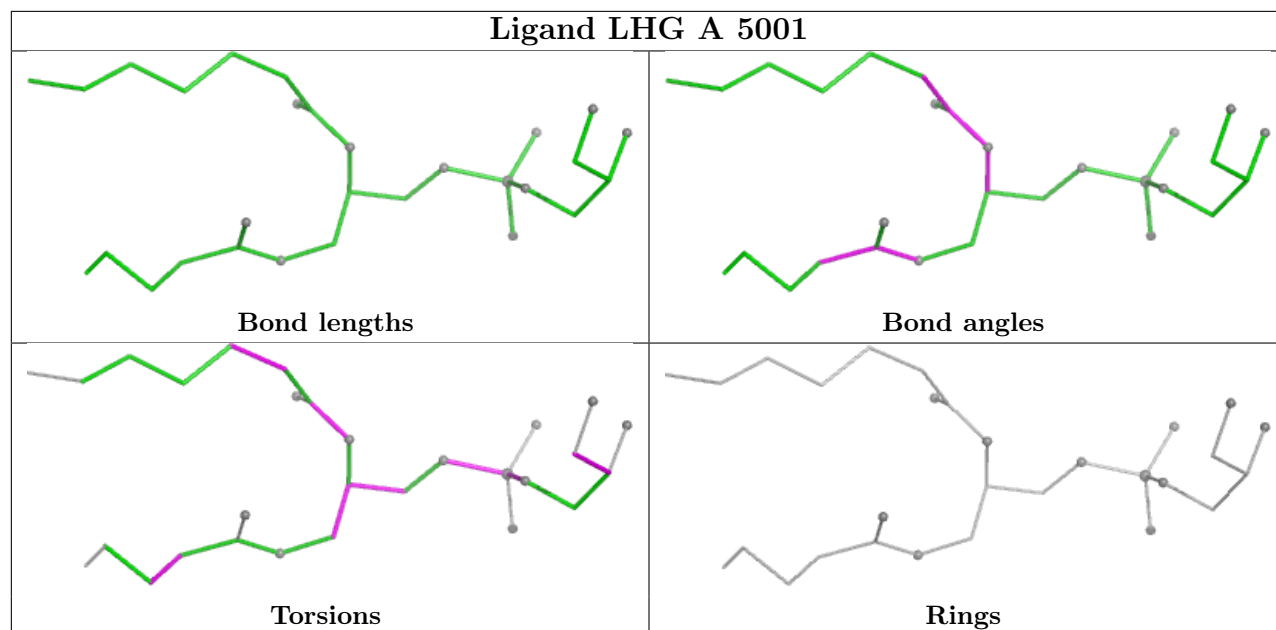
Ligand QTB 3 506

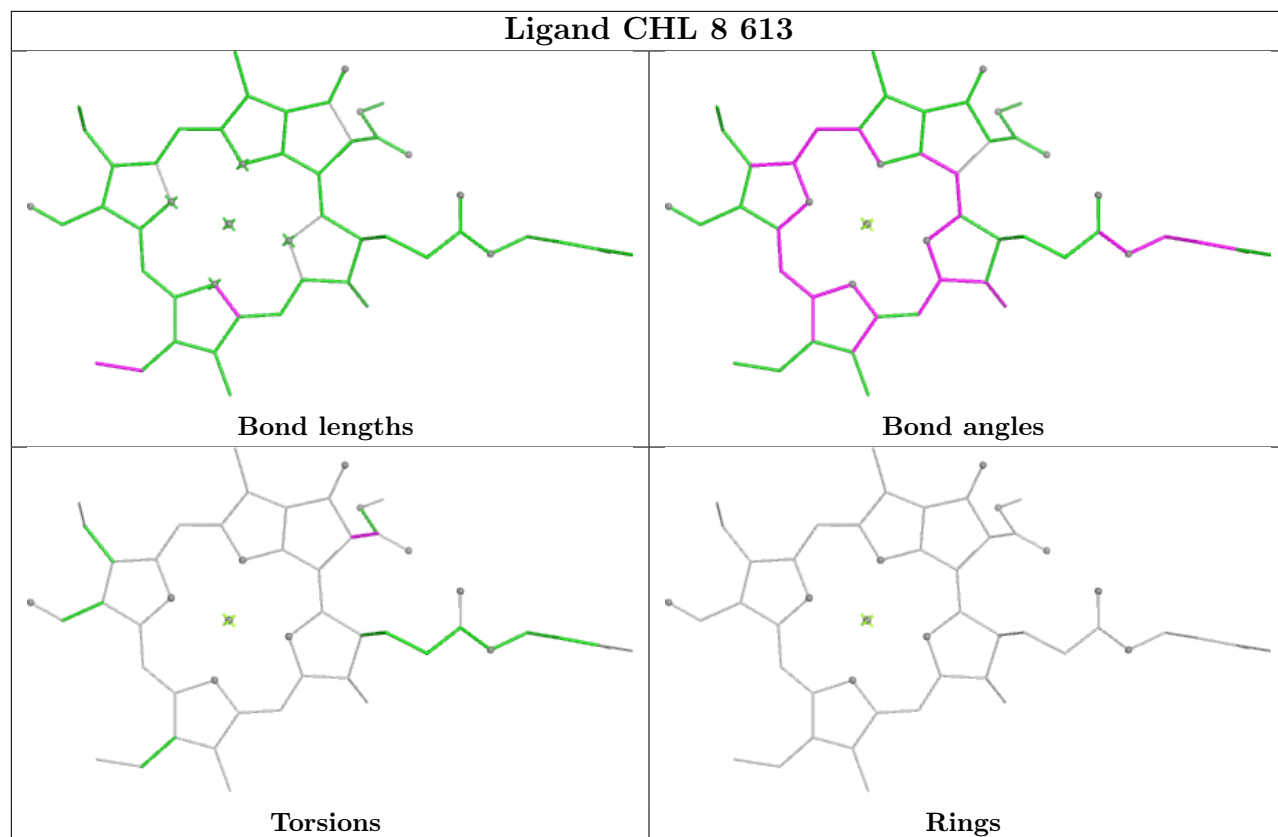
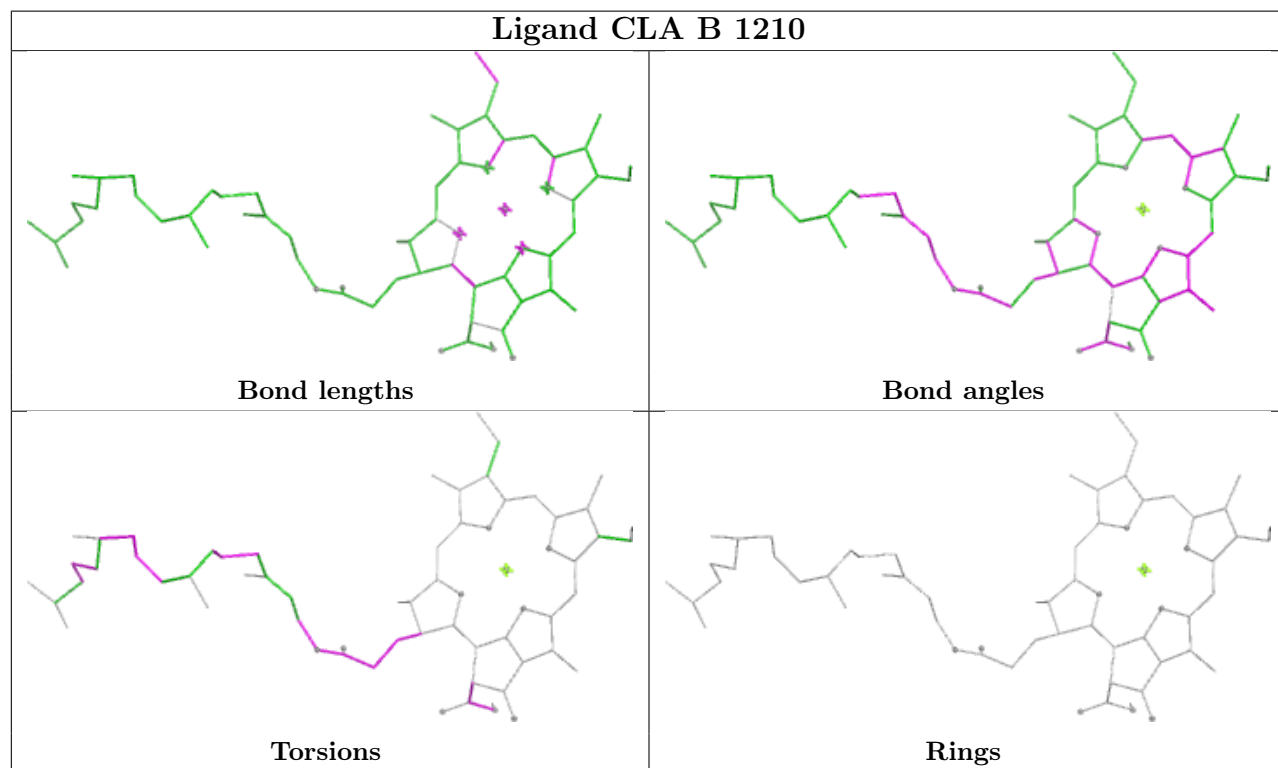




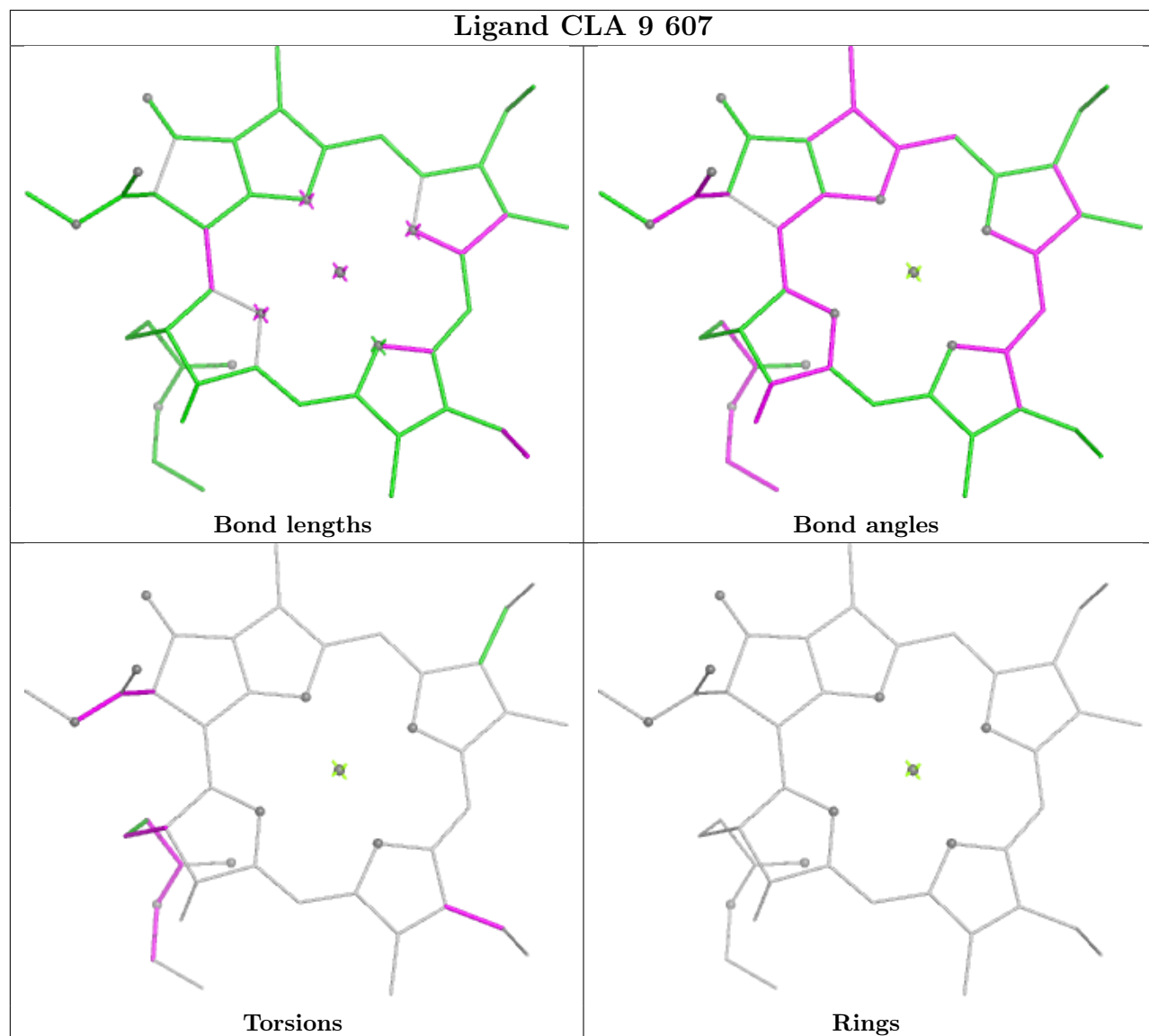


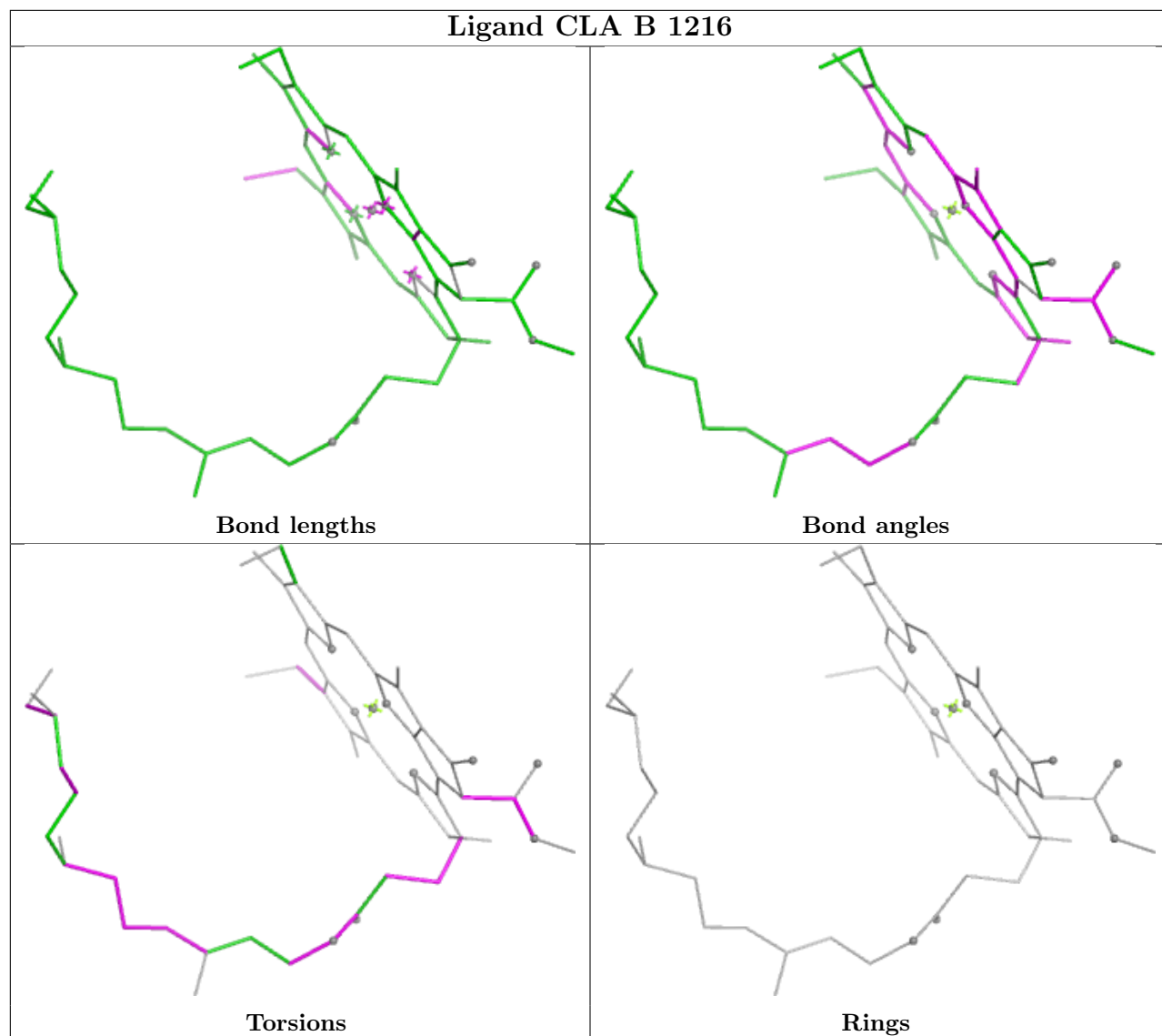


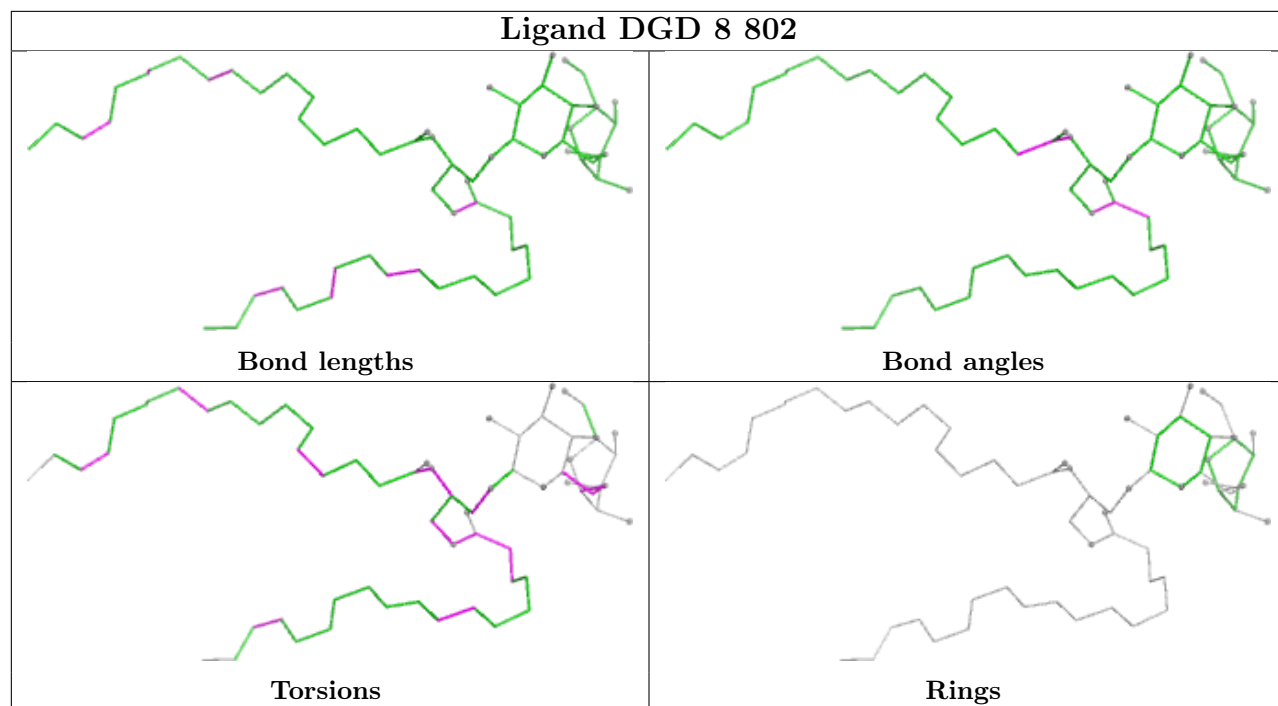


Ligand CHL 8 613**Ligand CLA B 1210**

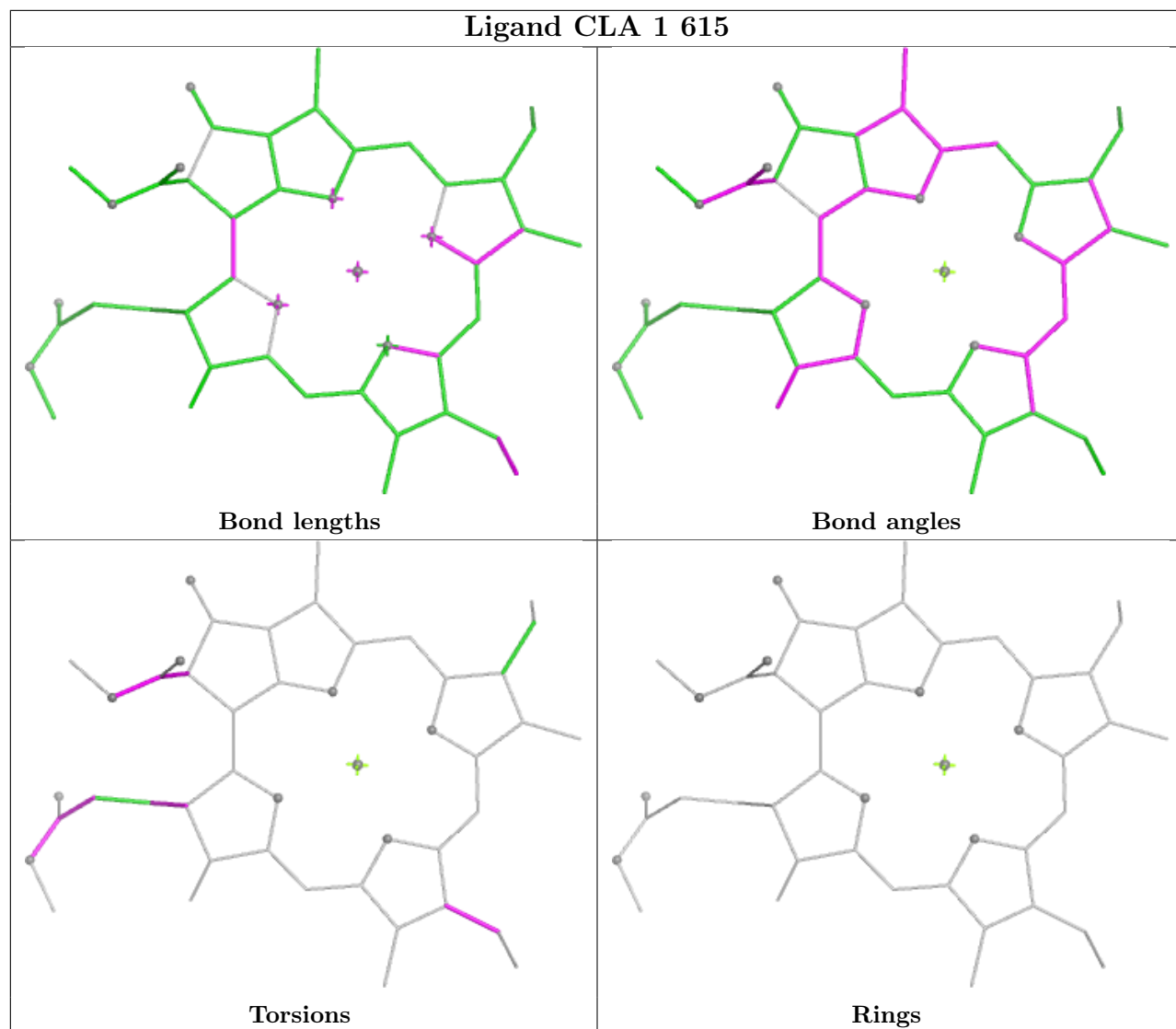
Ligand CLA 9 607

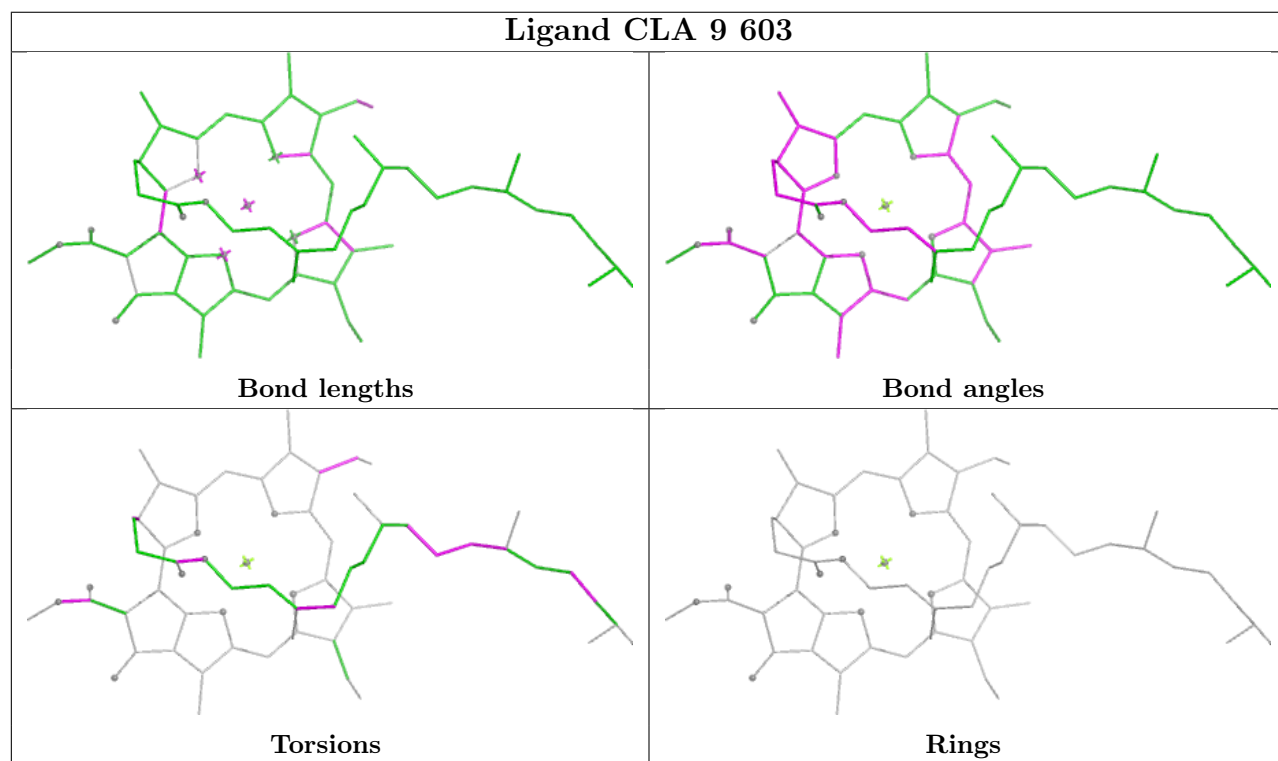
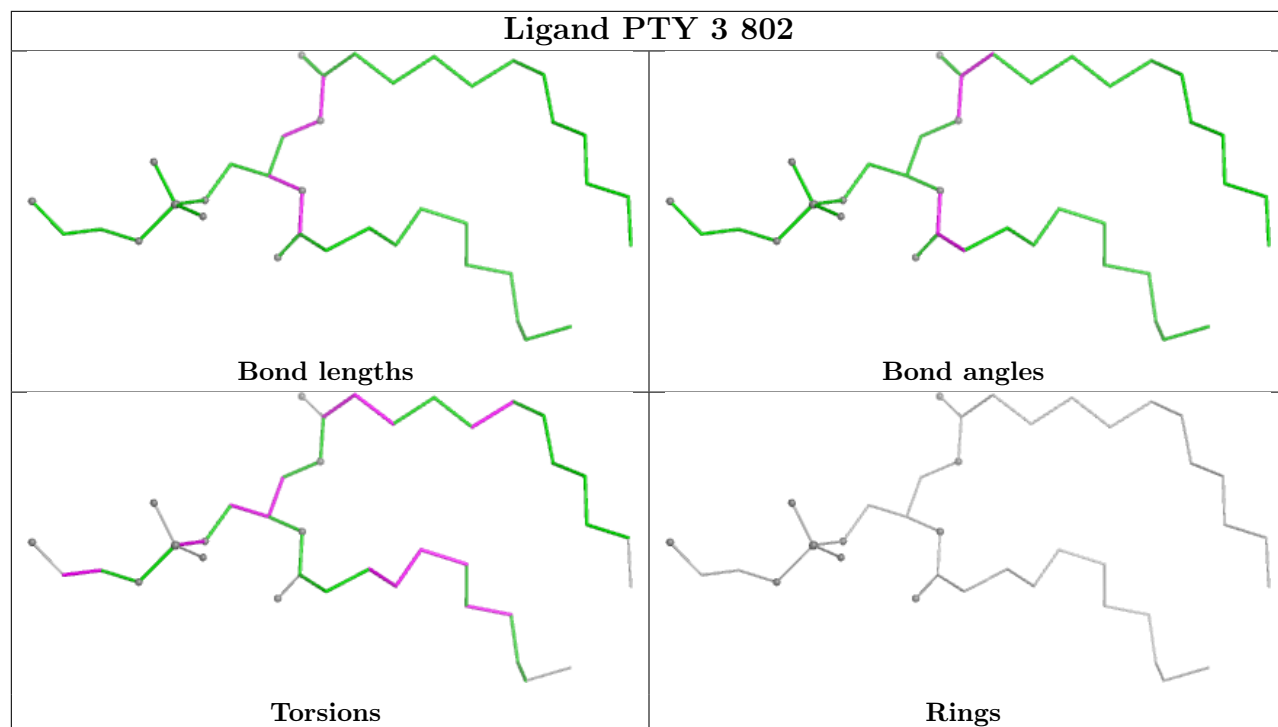


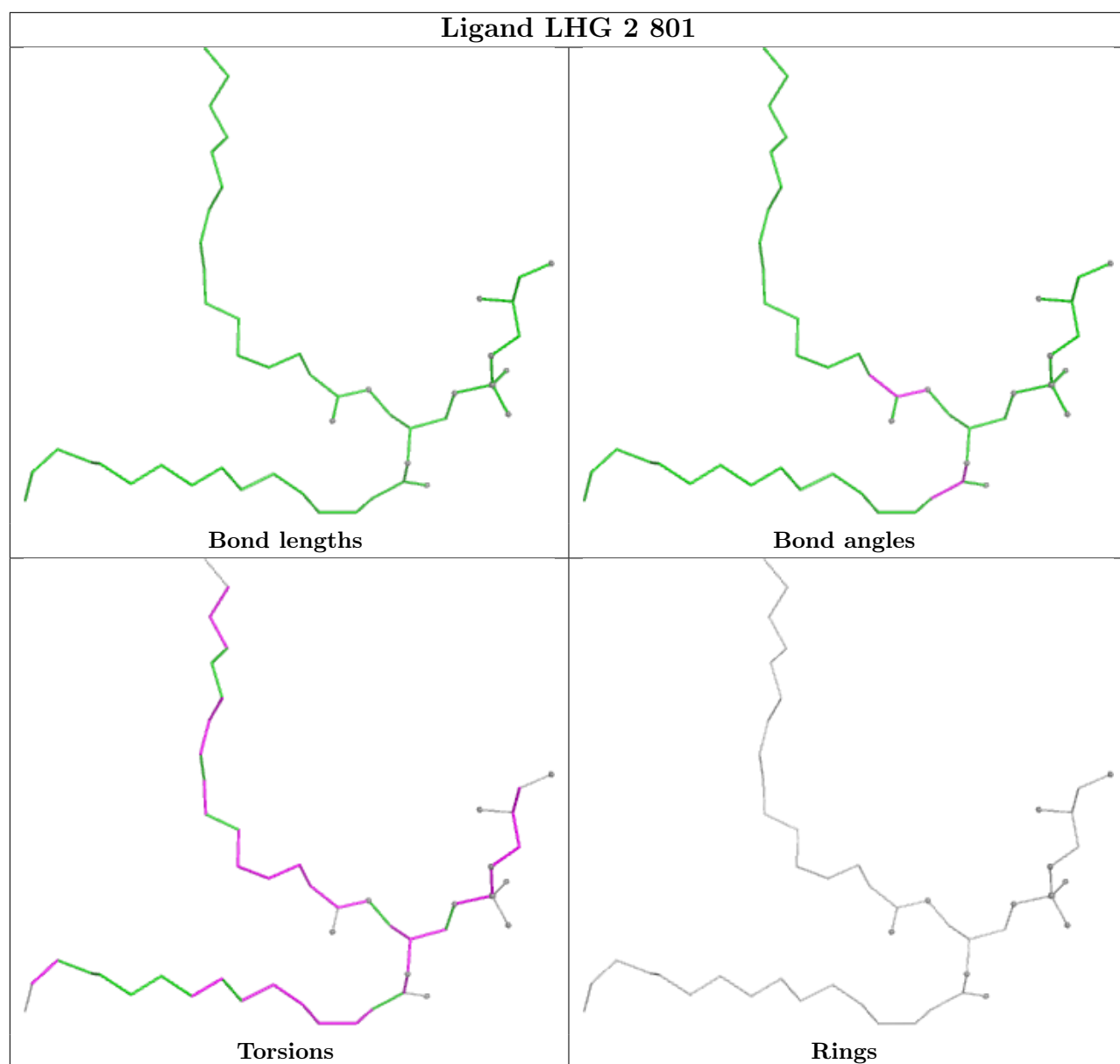


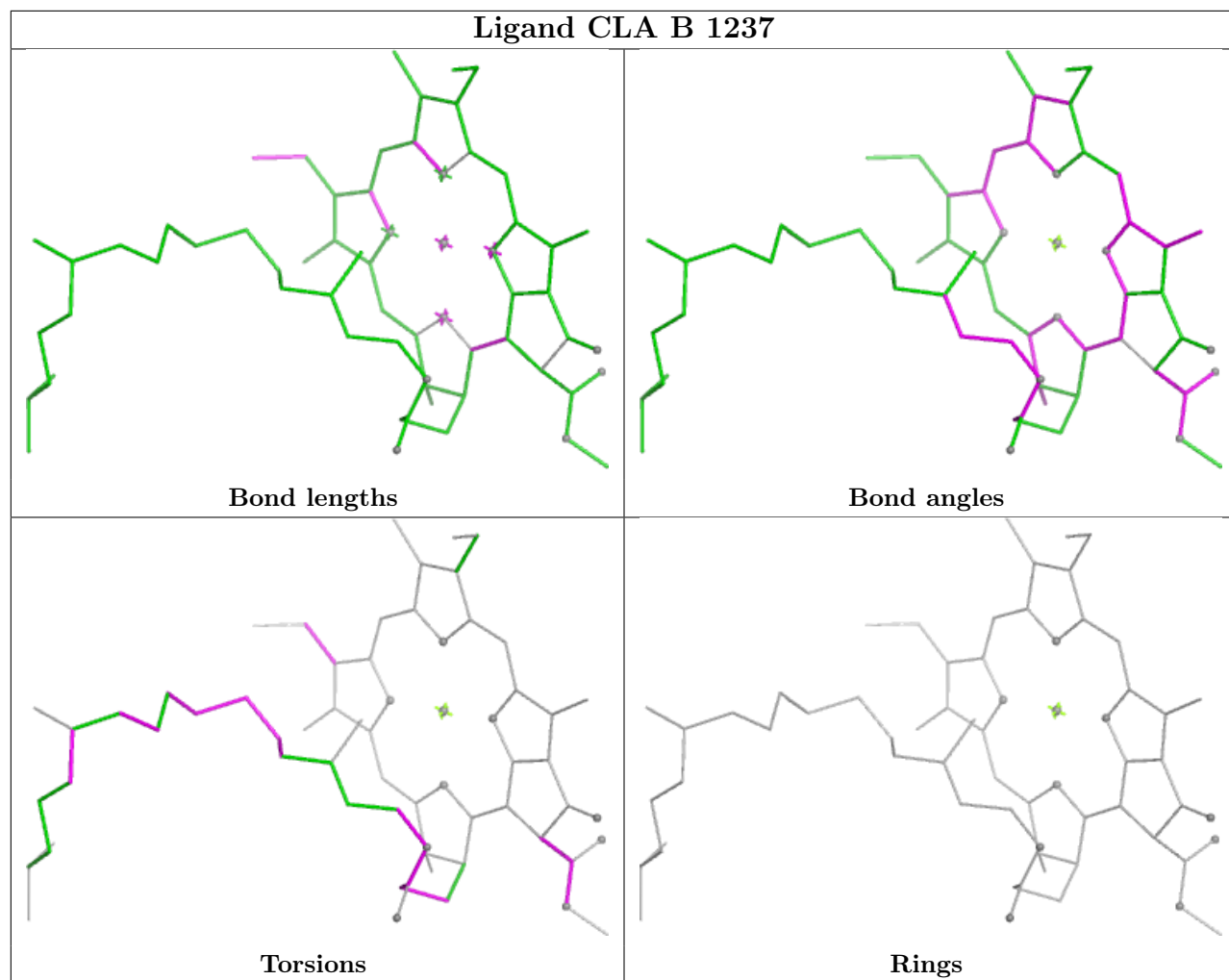


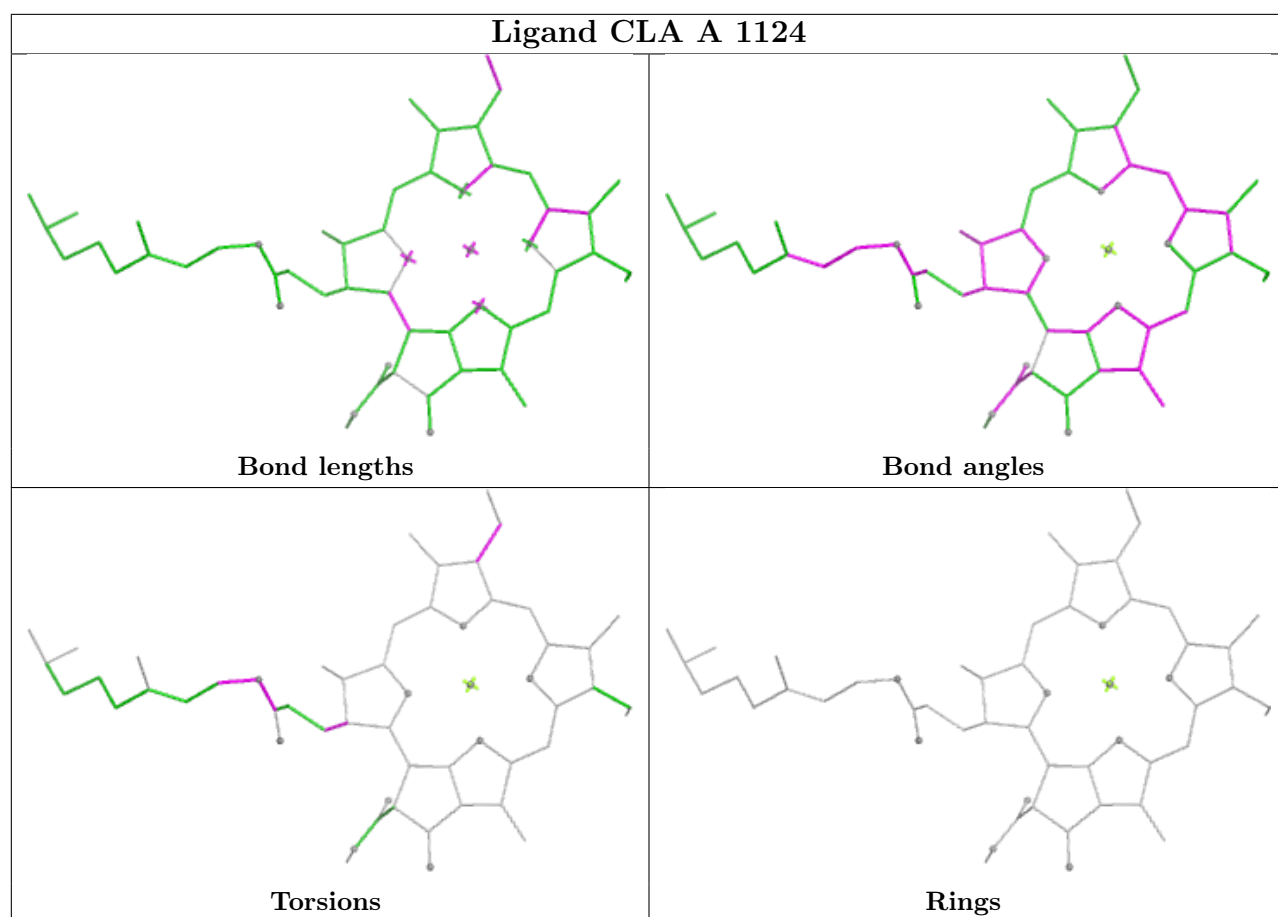
Ligand CLA 1 615

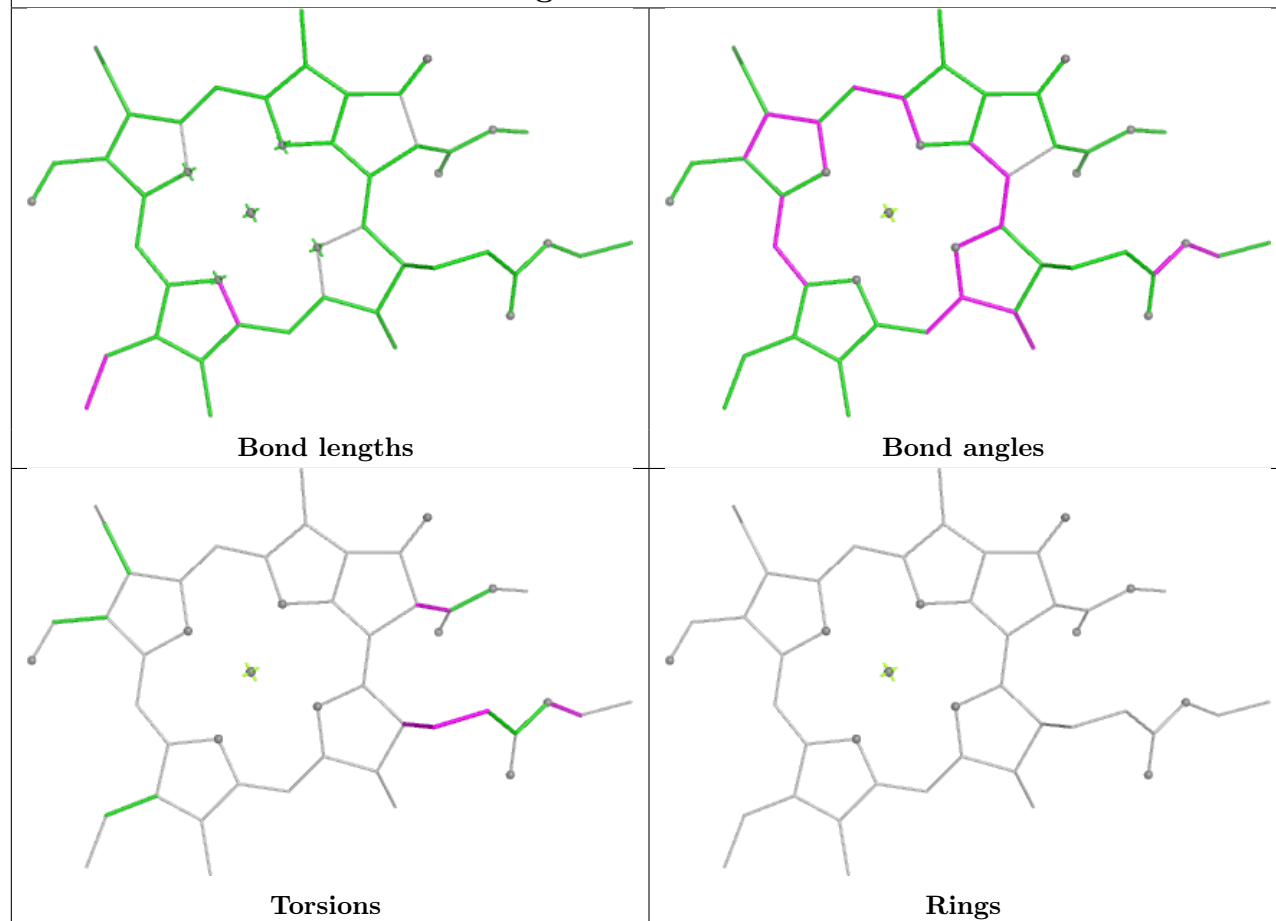
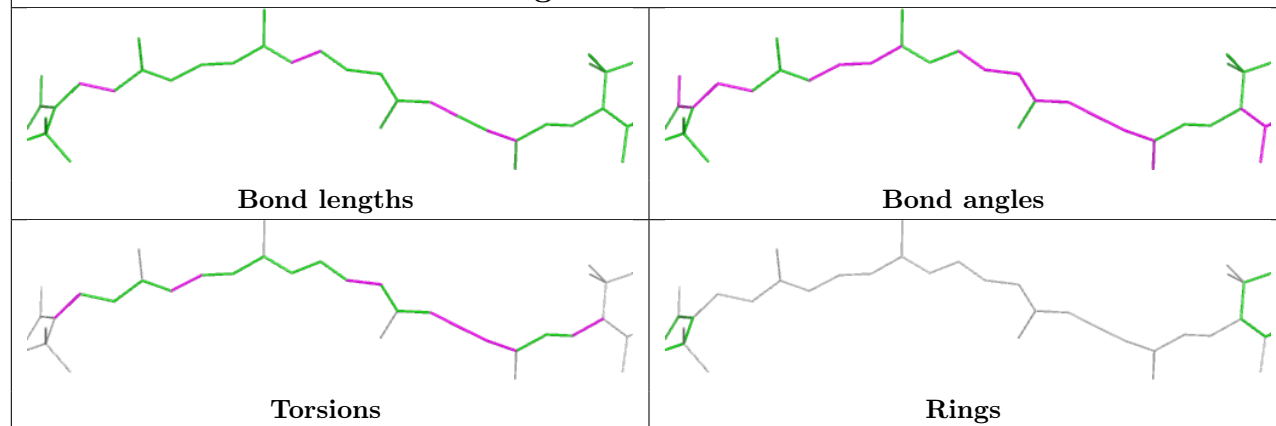




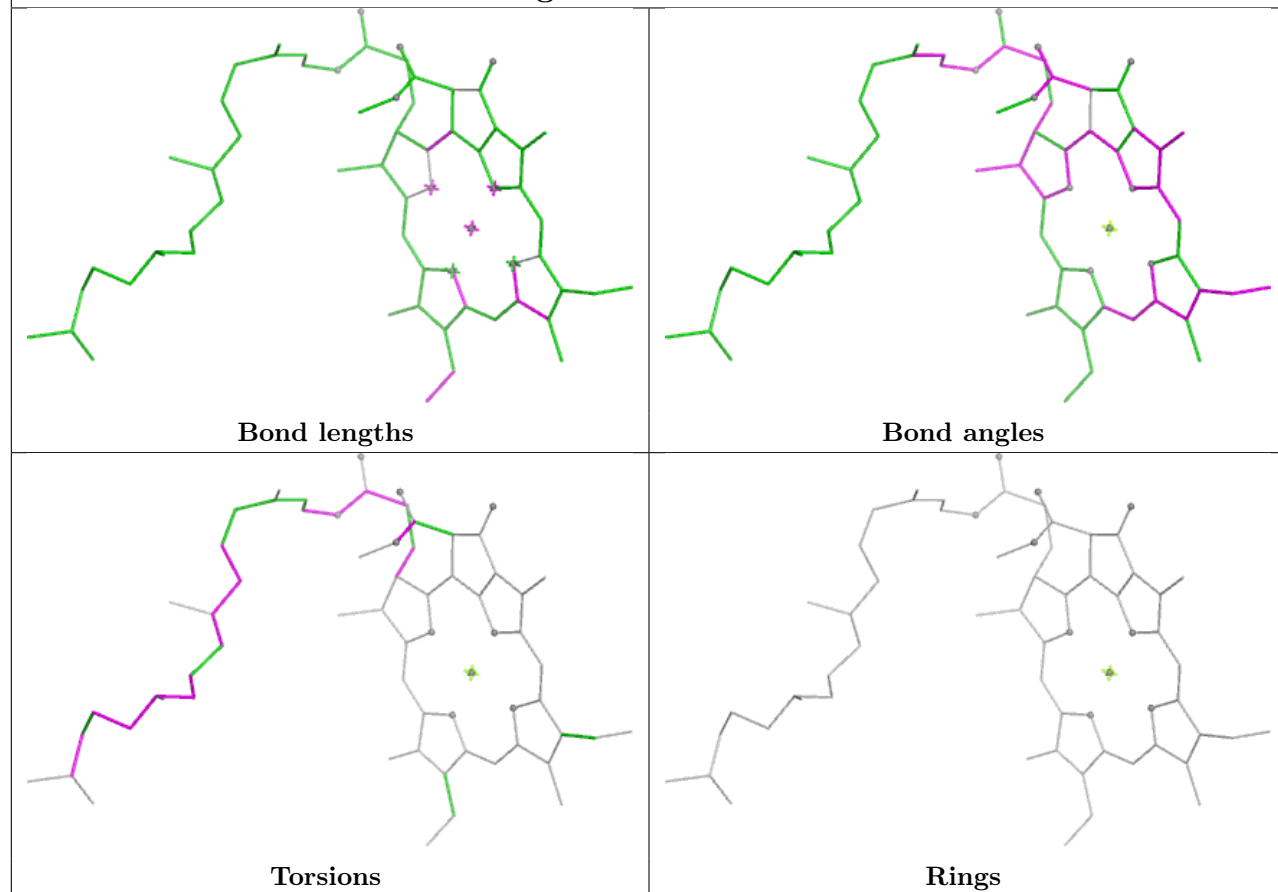




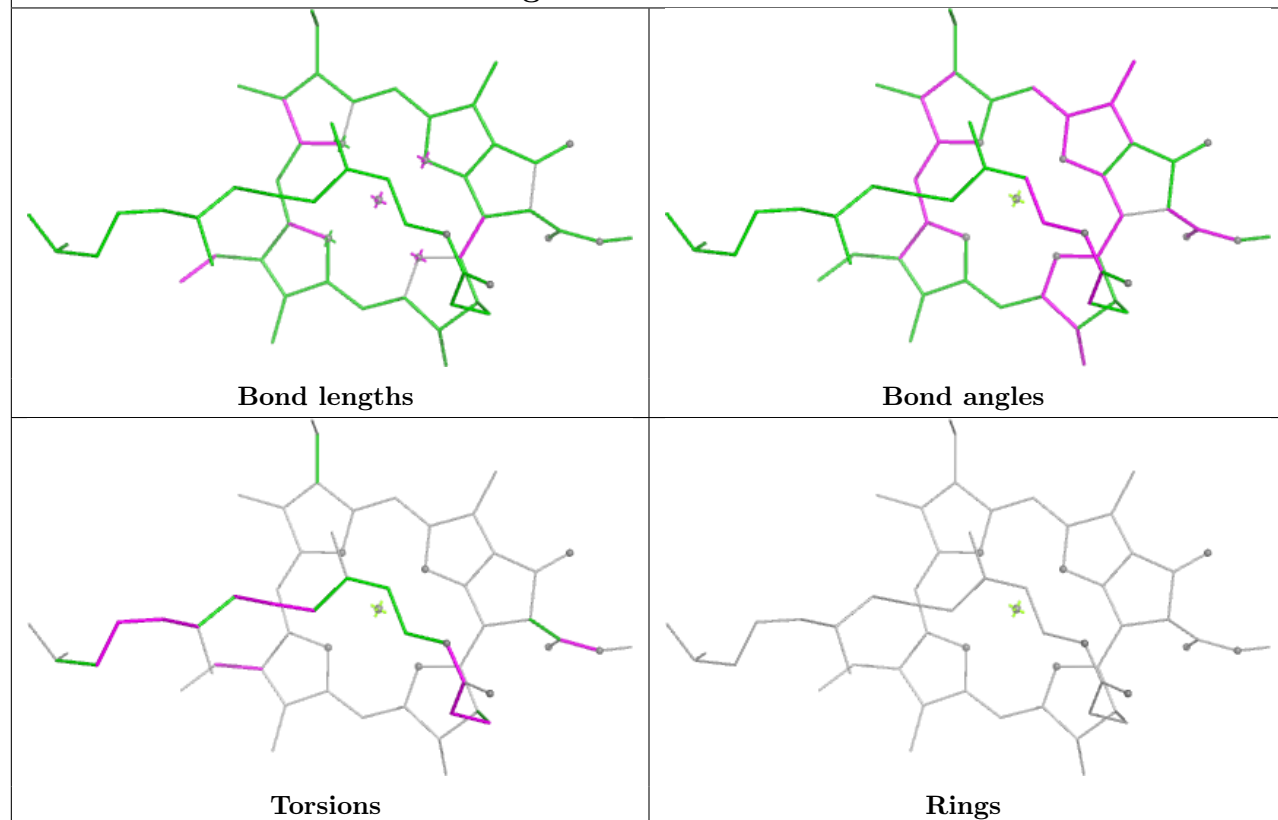


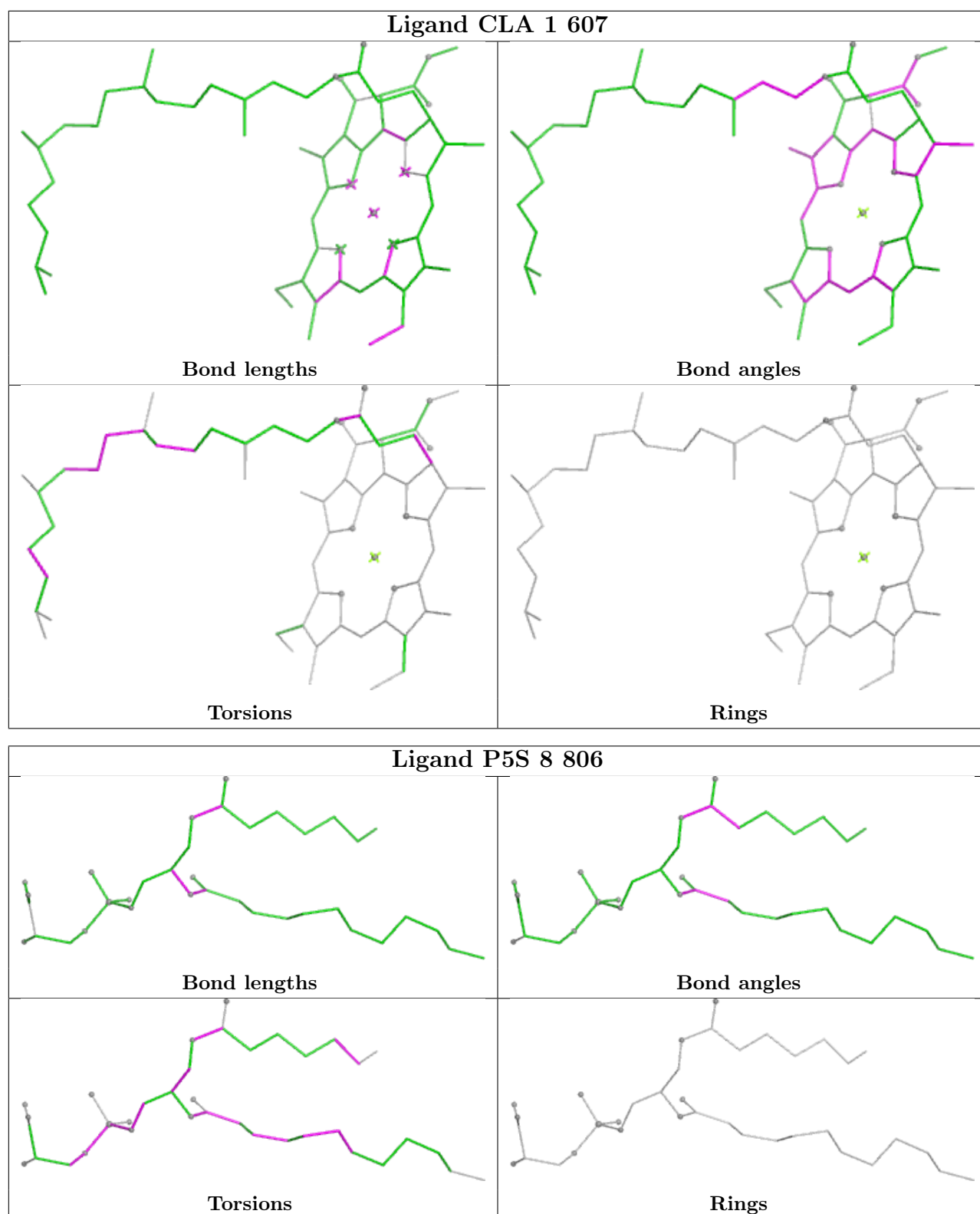
Ligand CHL 1 613**Ligand BCR 7 503**

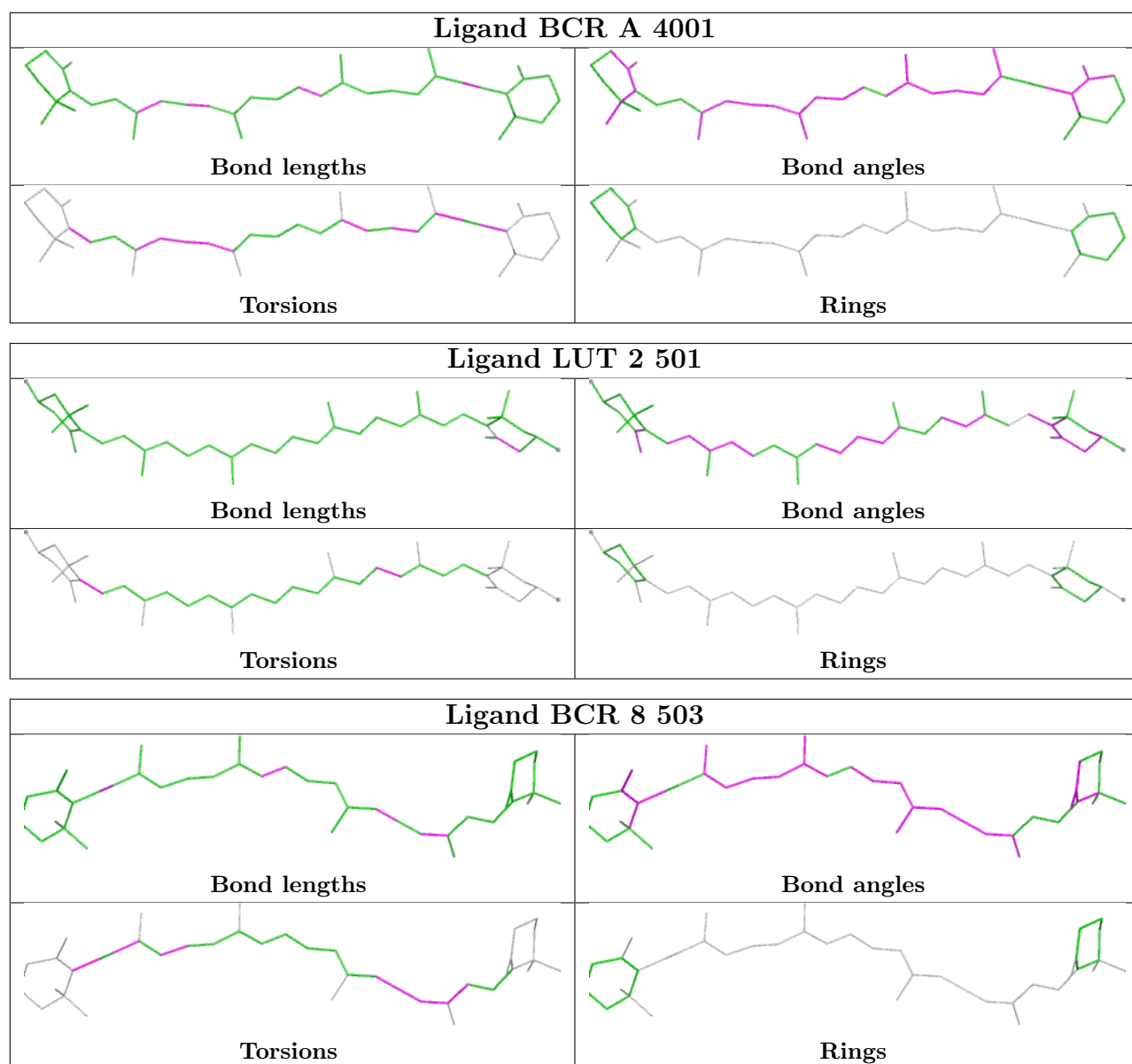
Ligand CLA 1 605



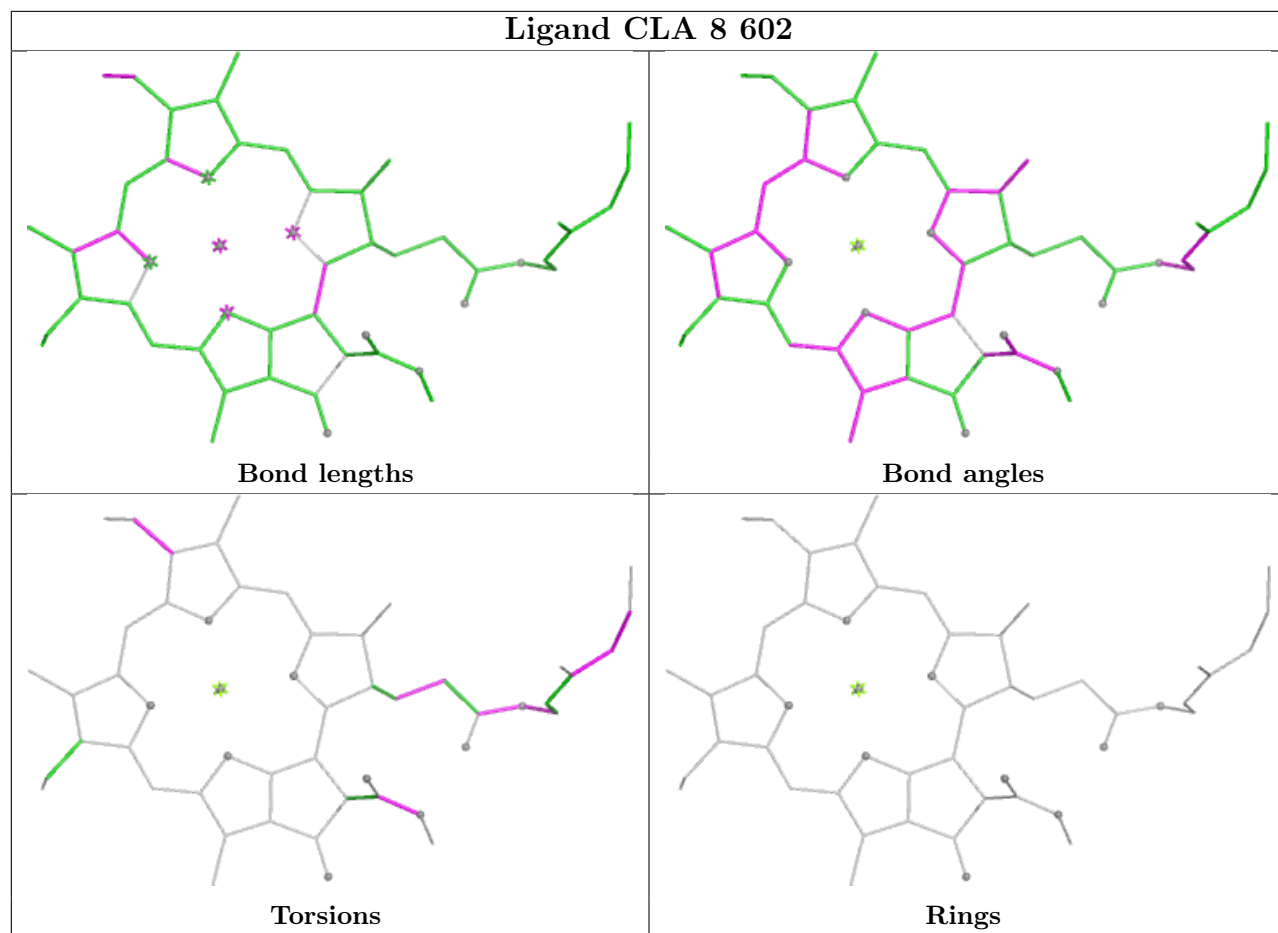
Ligand CLA A 1110



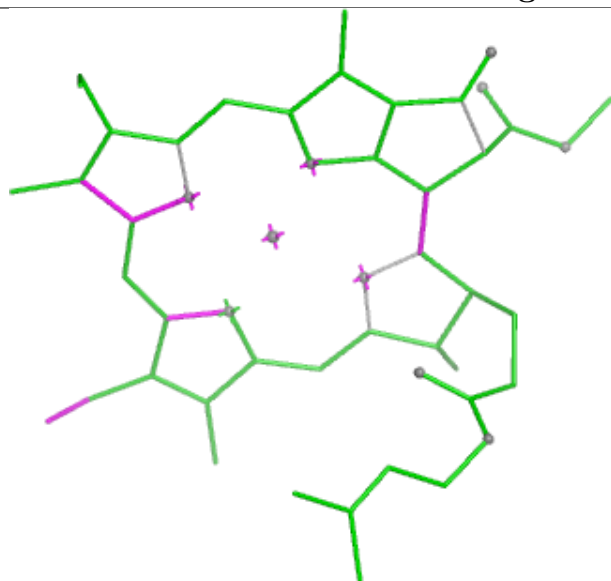




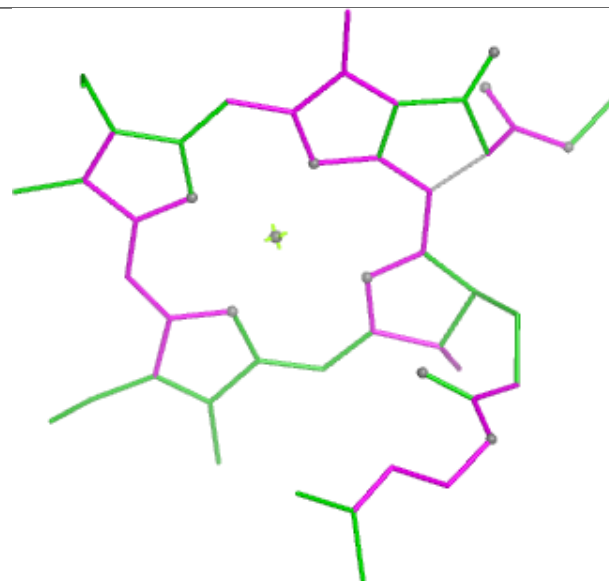
Ligand CLA 8 602



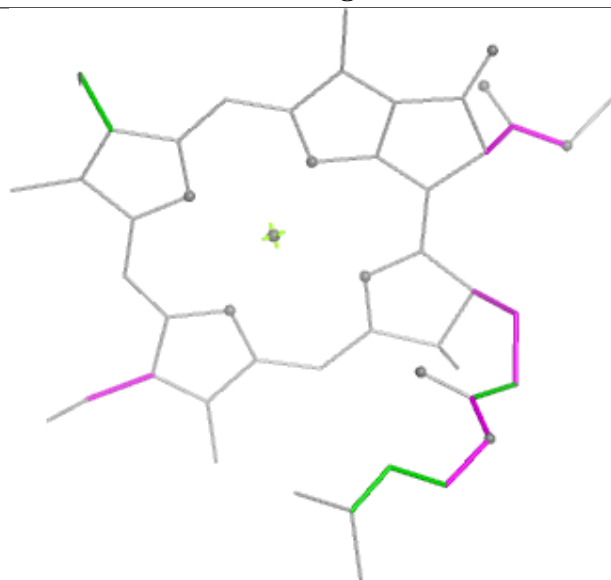
Ligand CLA 2 621



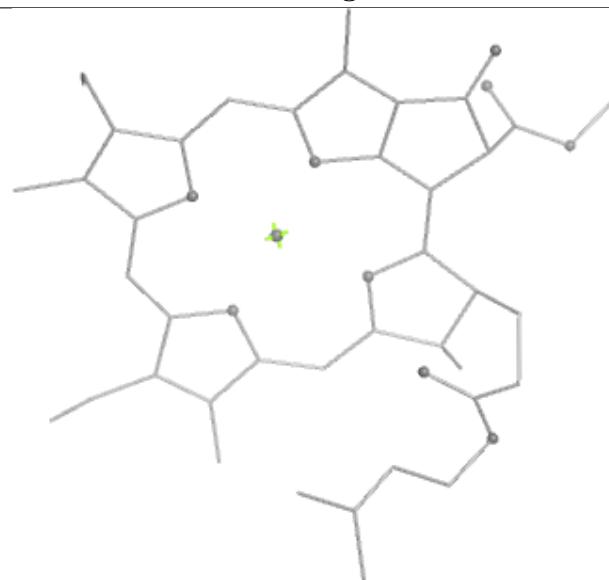
Bond lengths



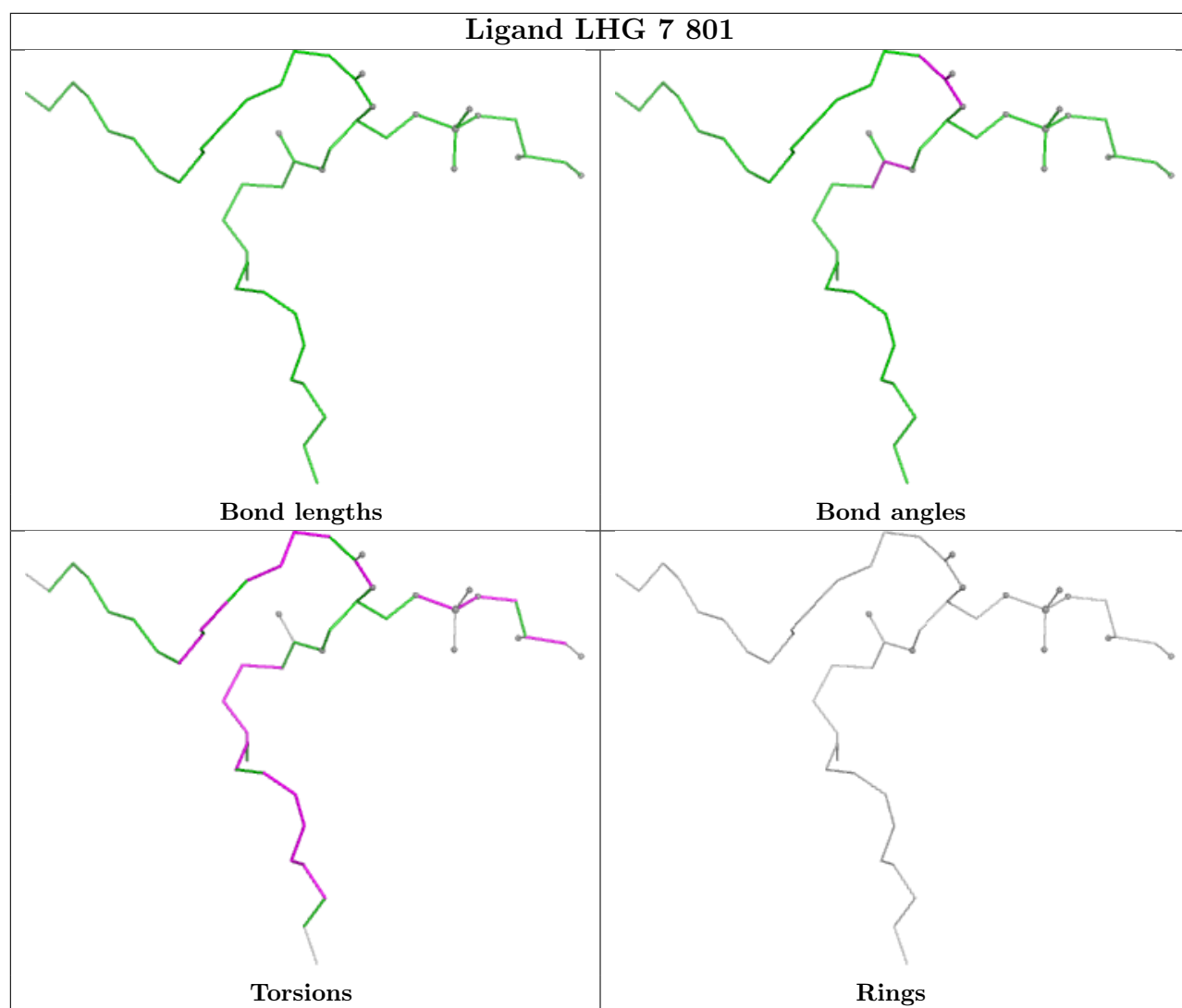
Bond angles

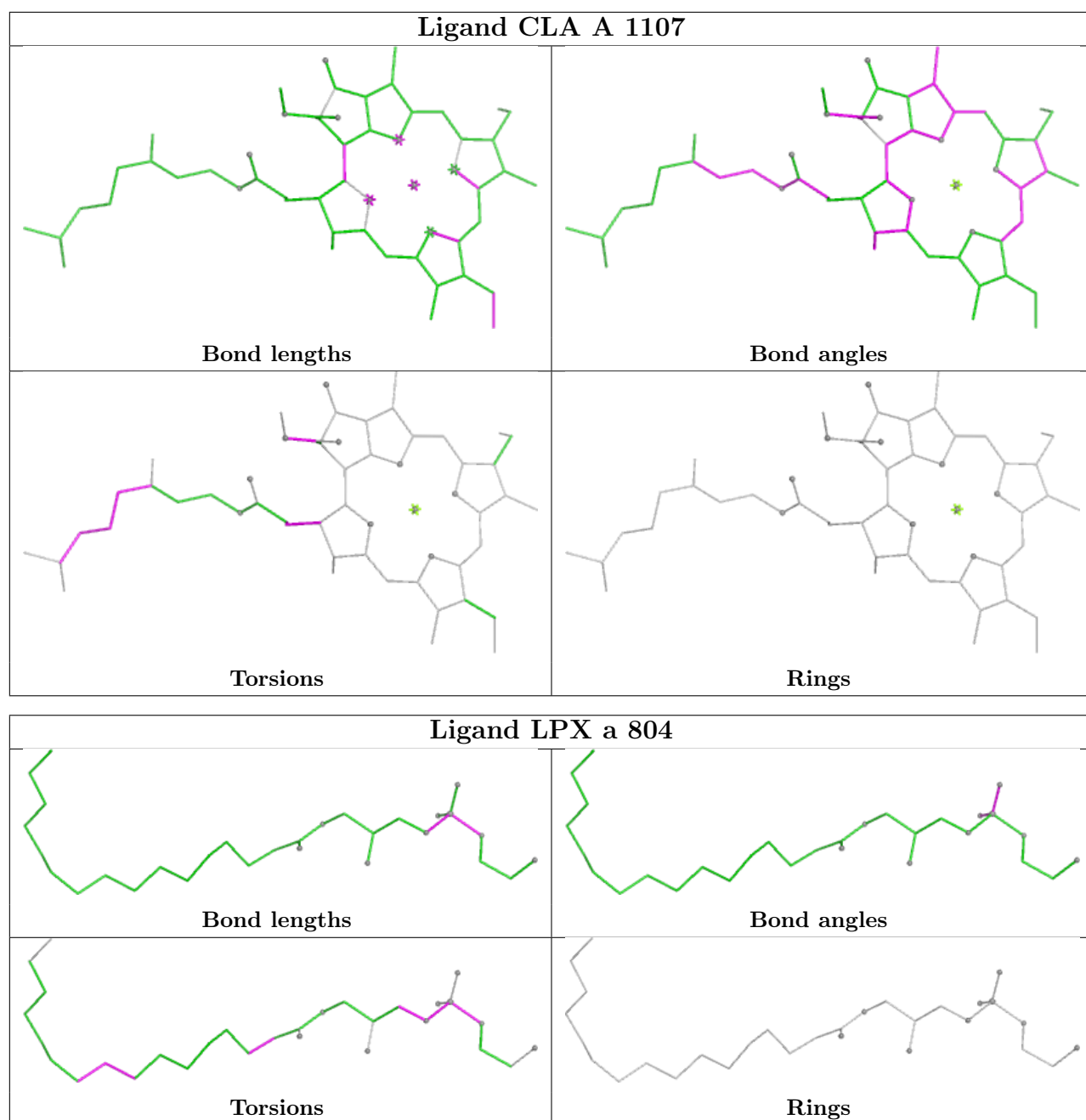


Torsions

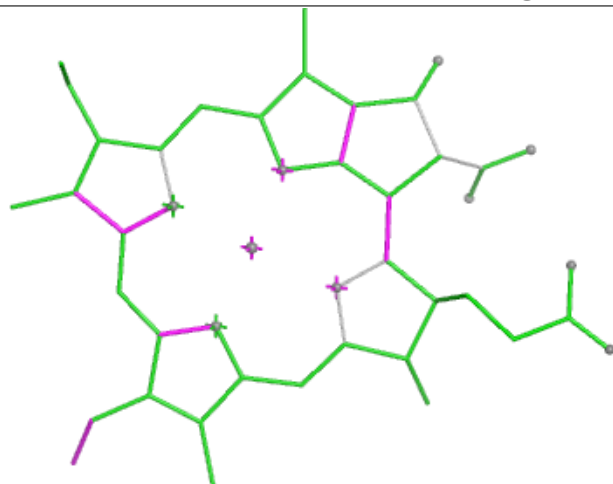


Rings

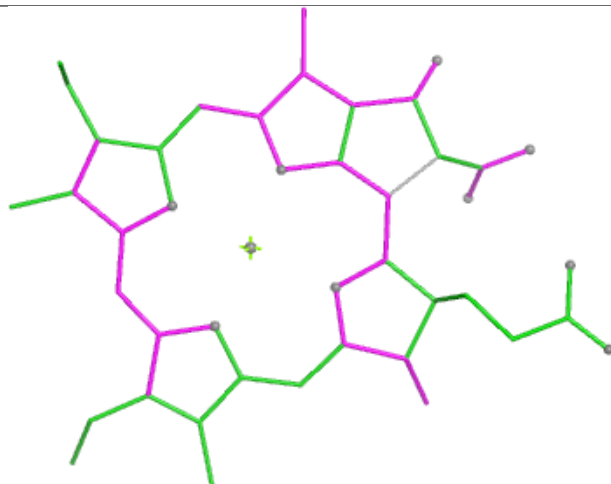




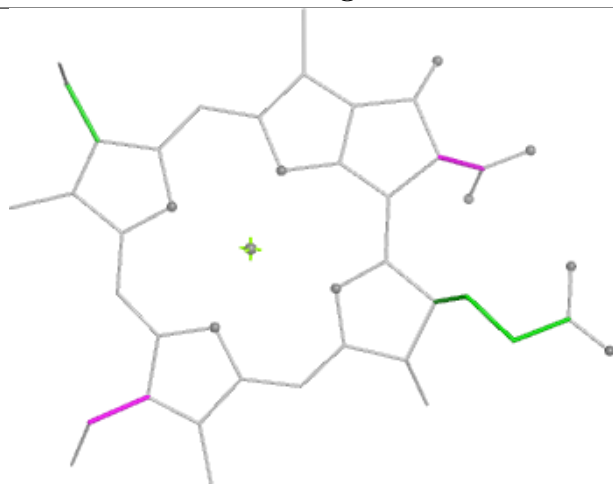
Ligand CLA 7 605



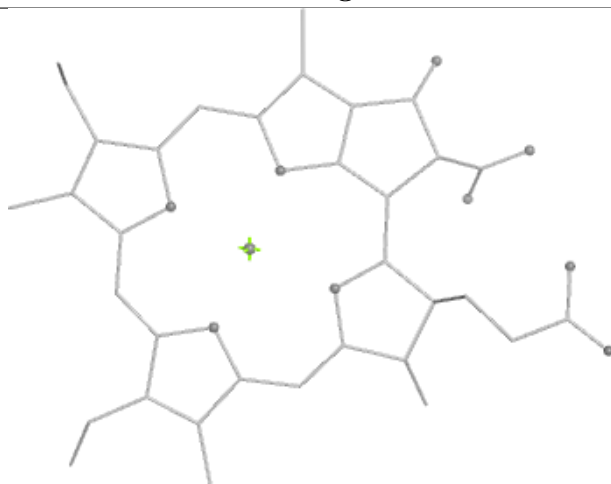
Bond lengths



Bond angles

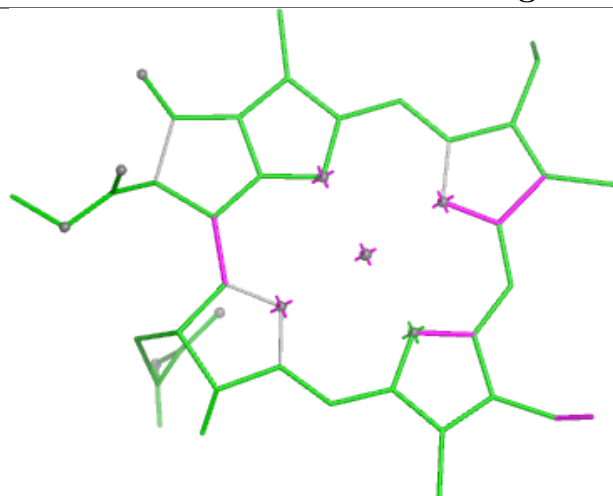


Torsions

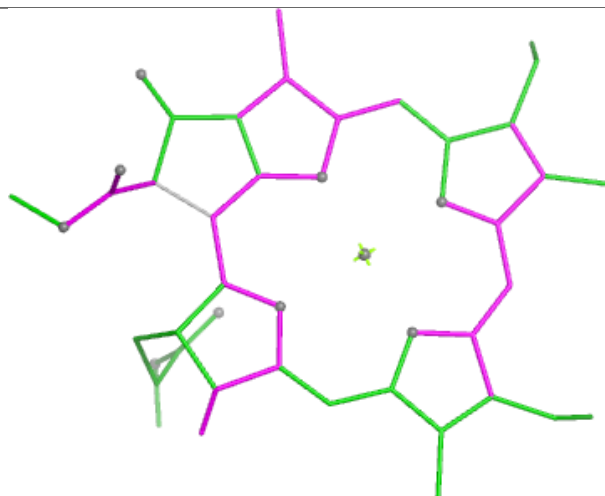


Rings

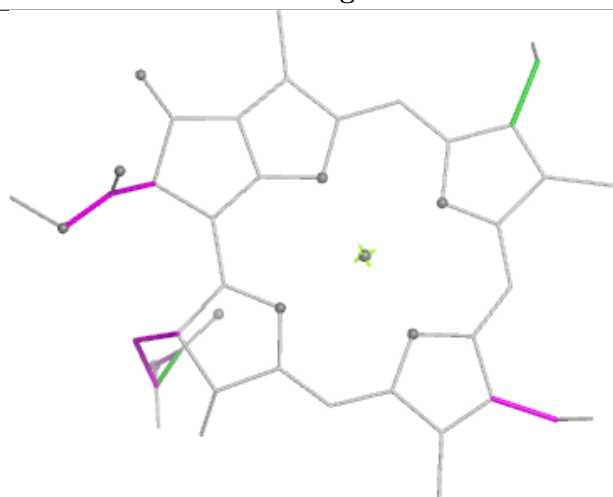
Ligand CLA 5 616



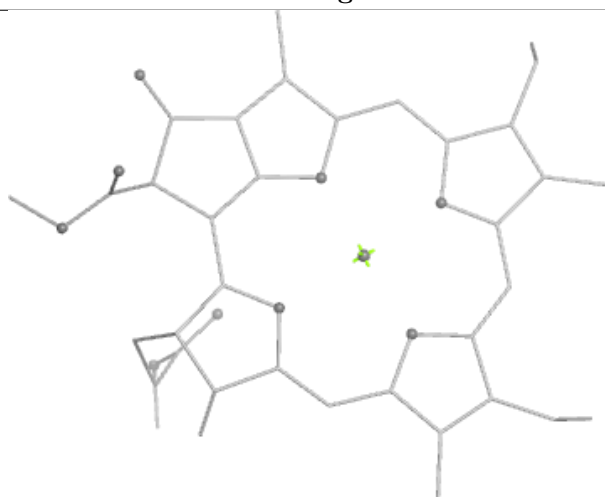
Bond lengths



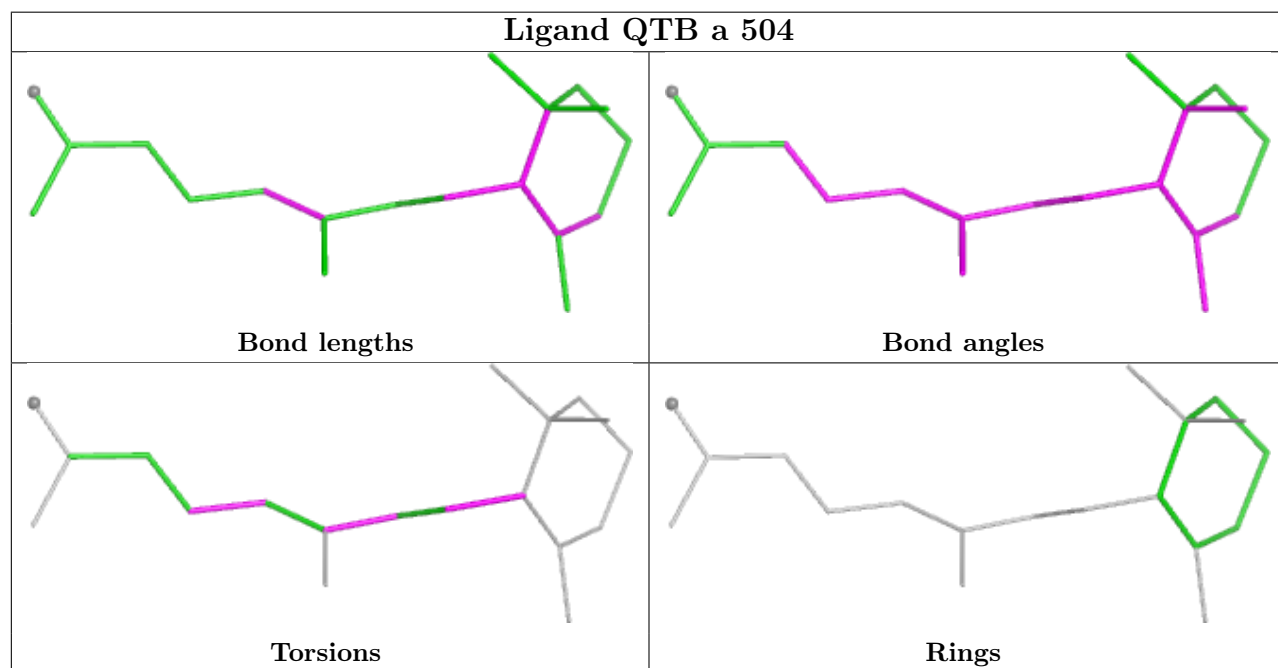
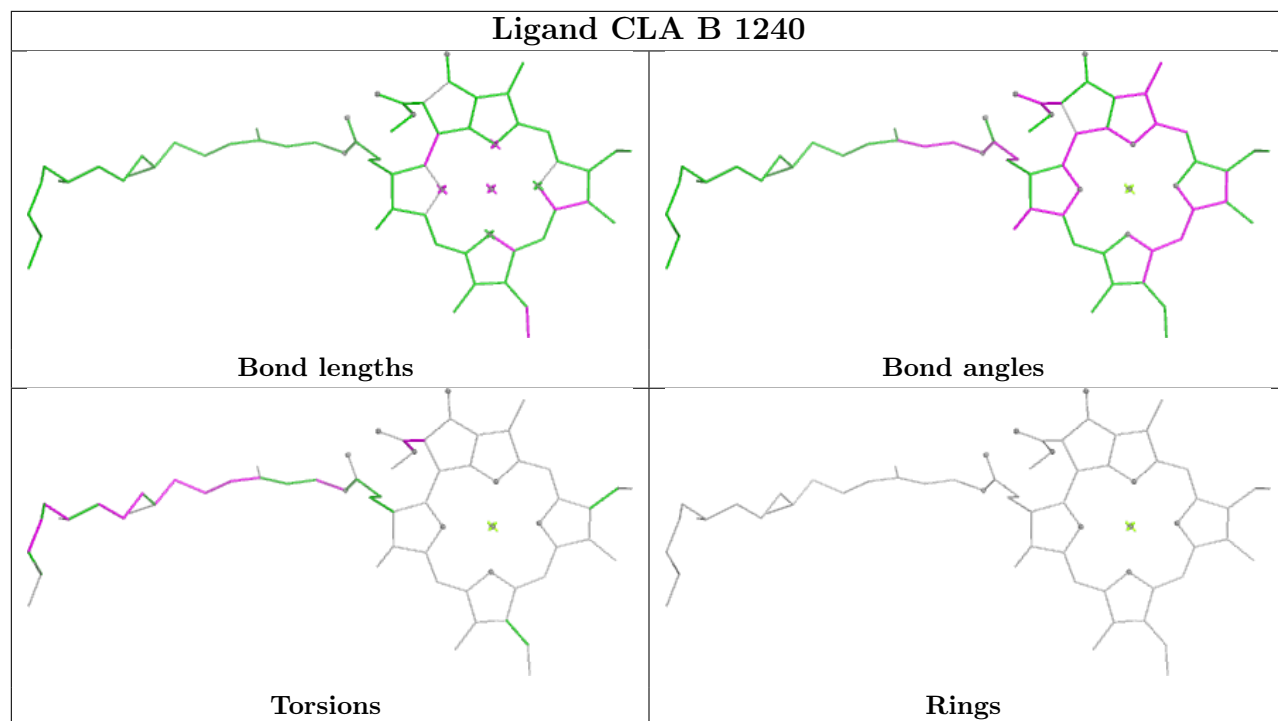
Bond angles



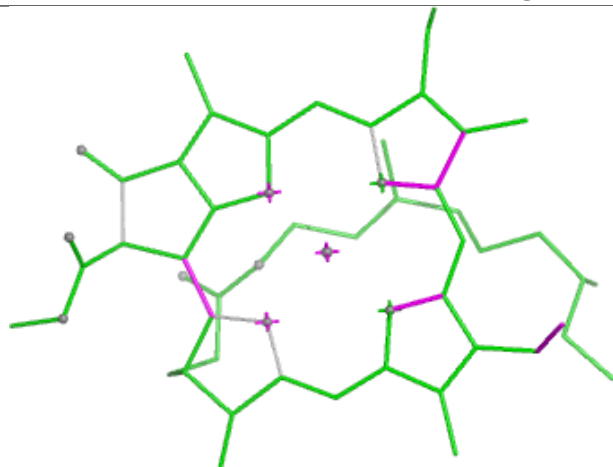
Torsions



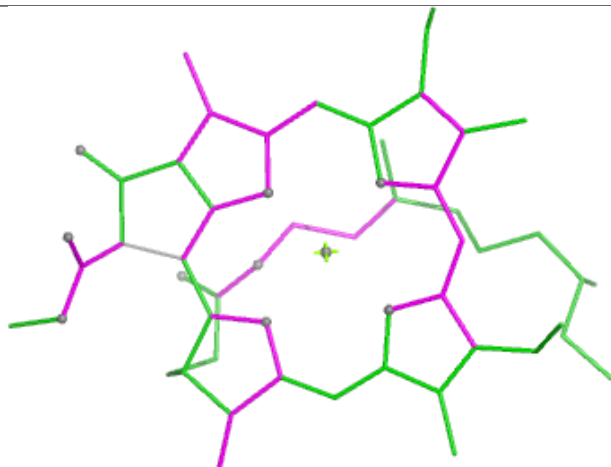
Rings



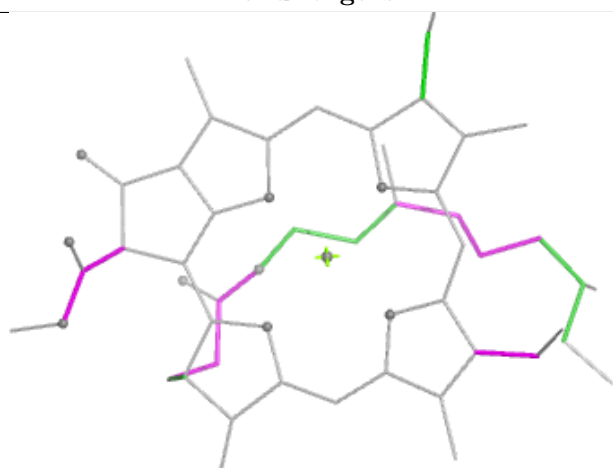
Ligand CLA 4 603



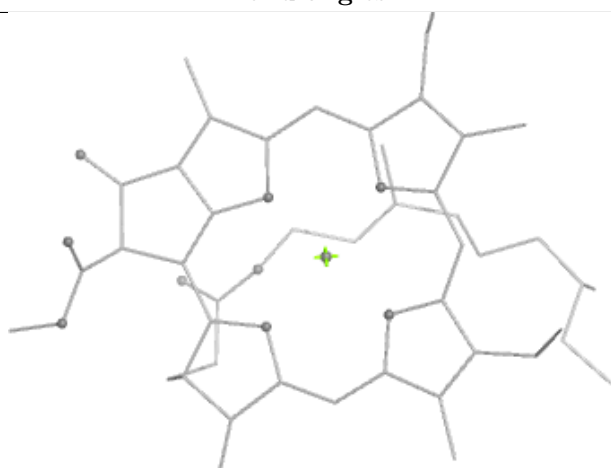
Bond lengths



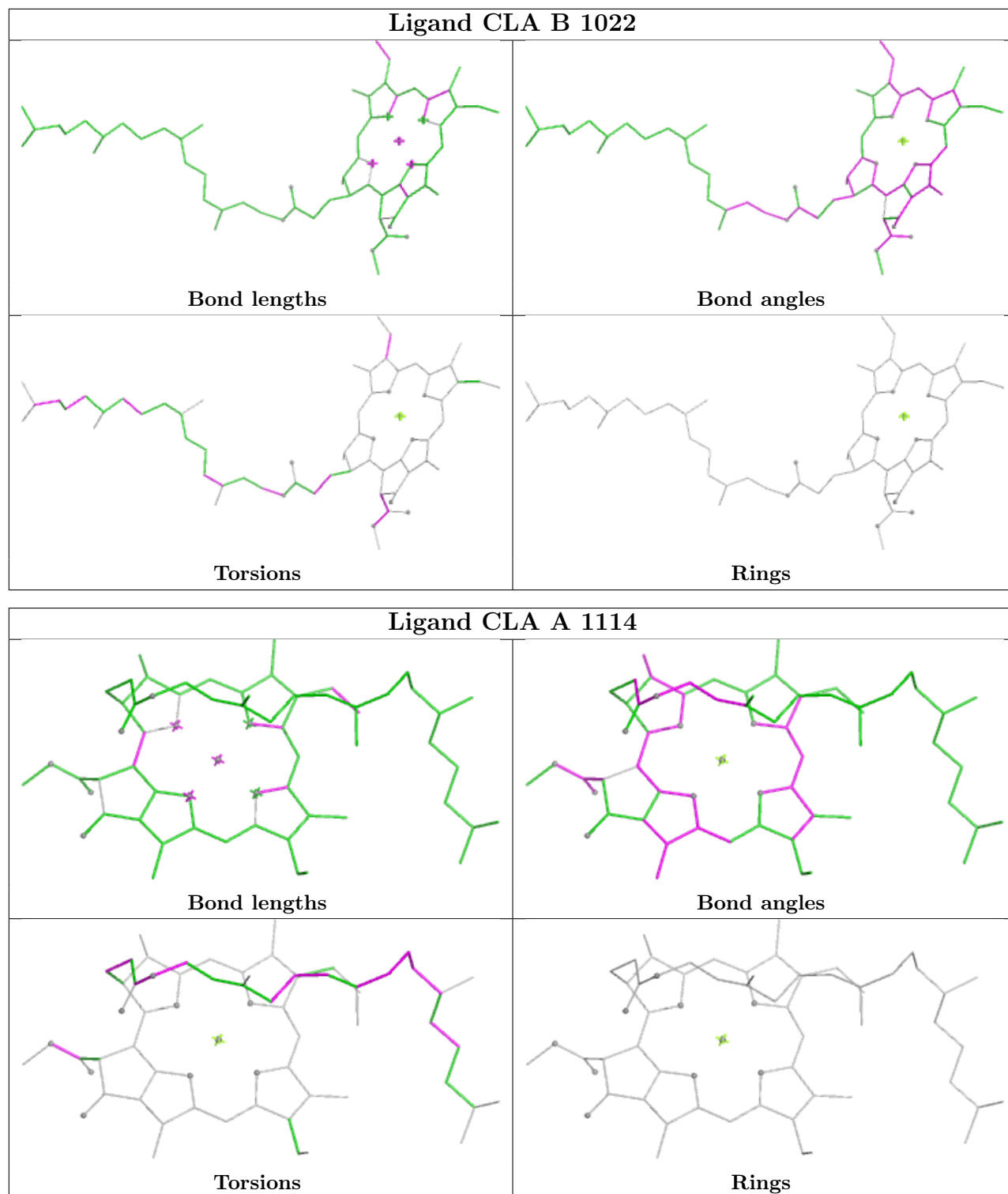
Bond angles



Torsions



Rings



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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

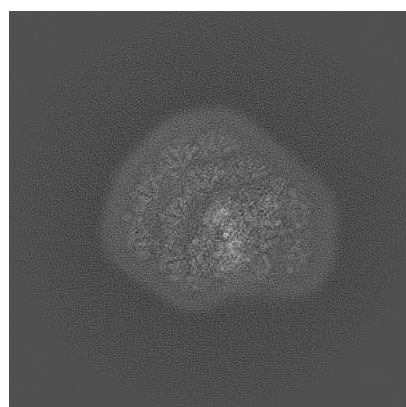
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11589. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

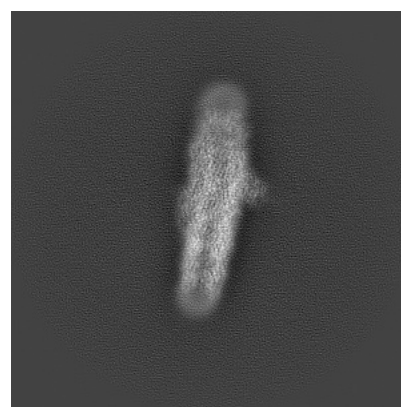
6.1.1 Primary map



X



Y

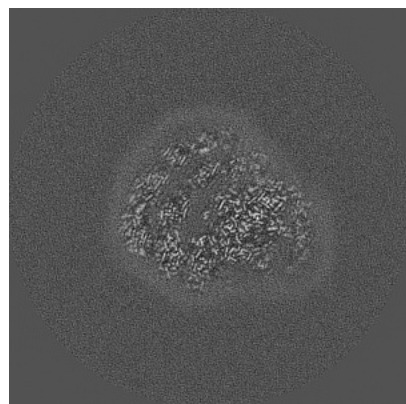


Z

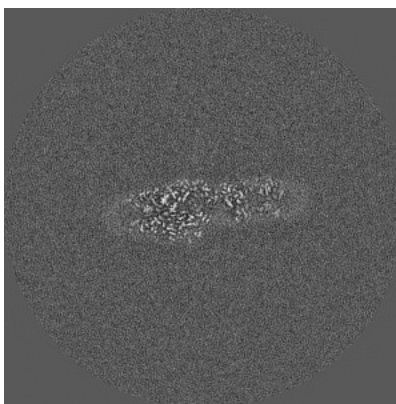
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

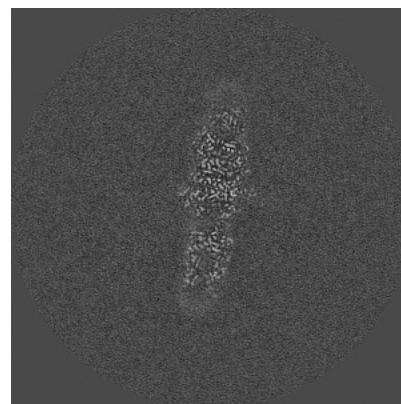
6.2.1 Primary map



X Index: 256



Y Index: 256

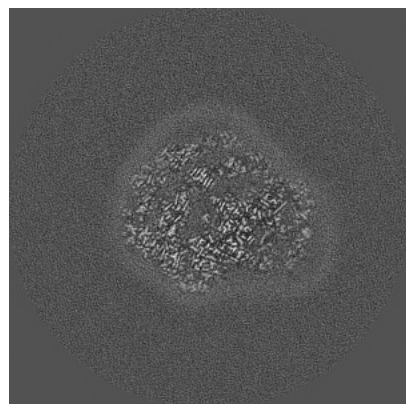


Z Index: 256

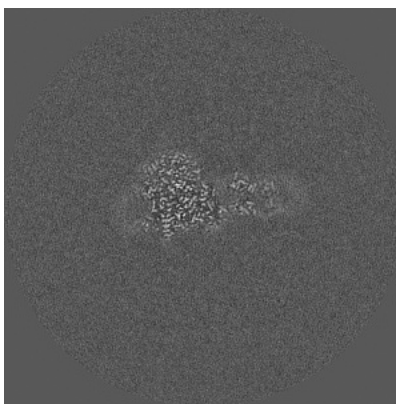
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

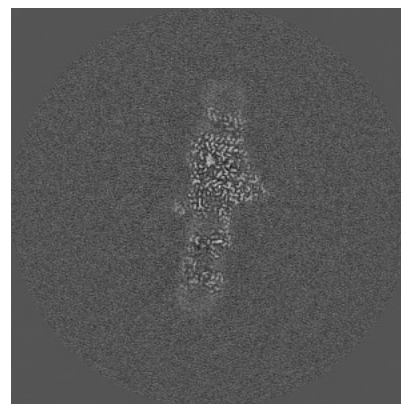
6.3.1 Primary map



X Index: 261



Y Index: 285

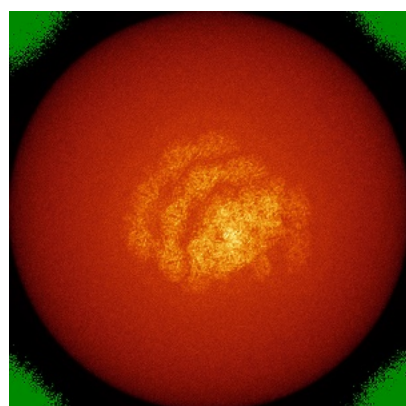


Z Index: 238

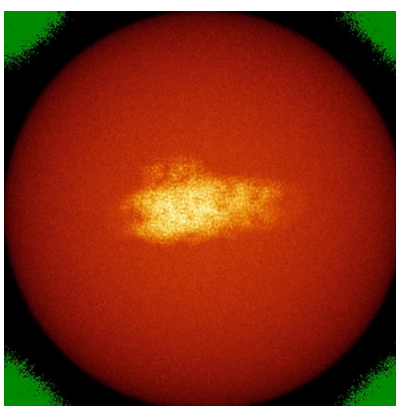
The images above show the largest variance slices of the map in three orthogonal directions.

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

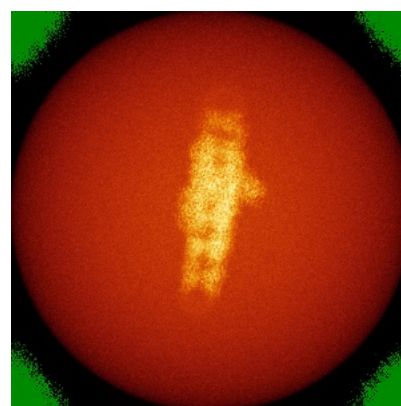
6.4.1 Primary map



X



Y

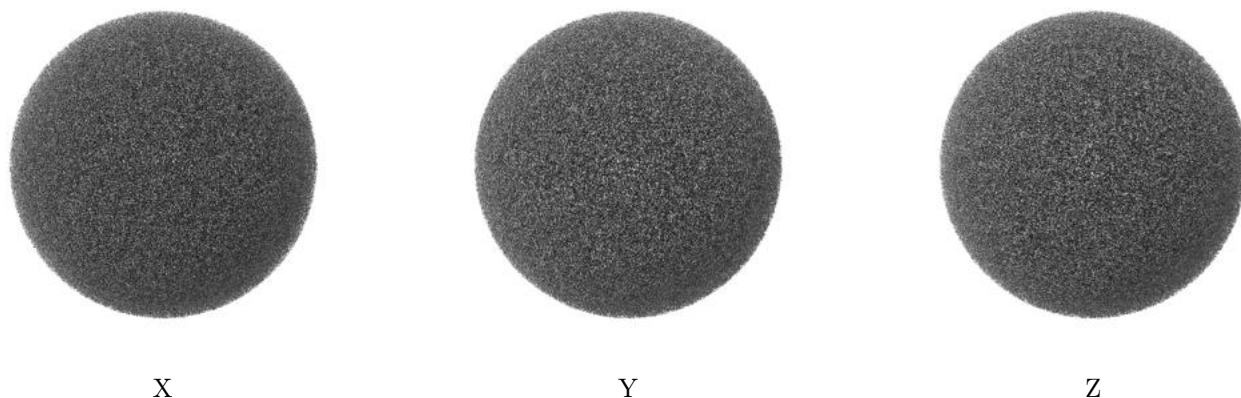


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

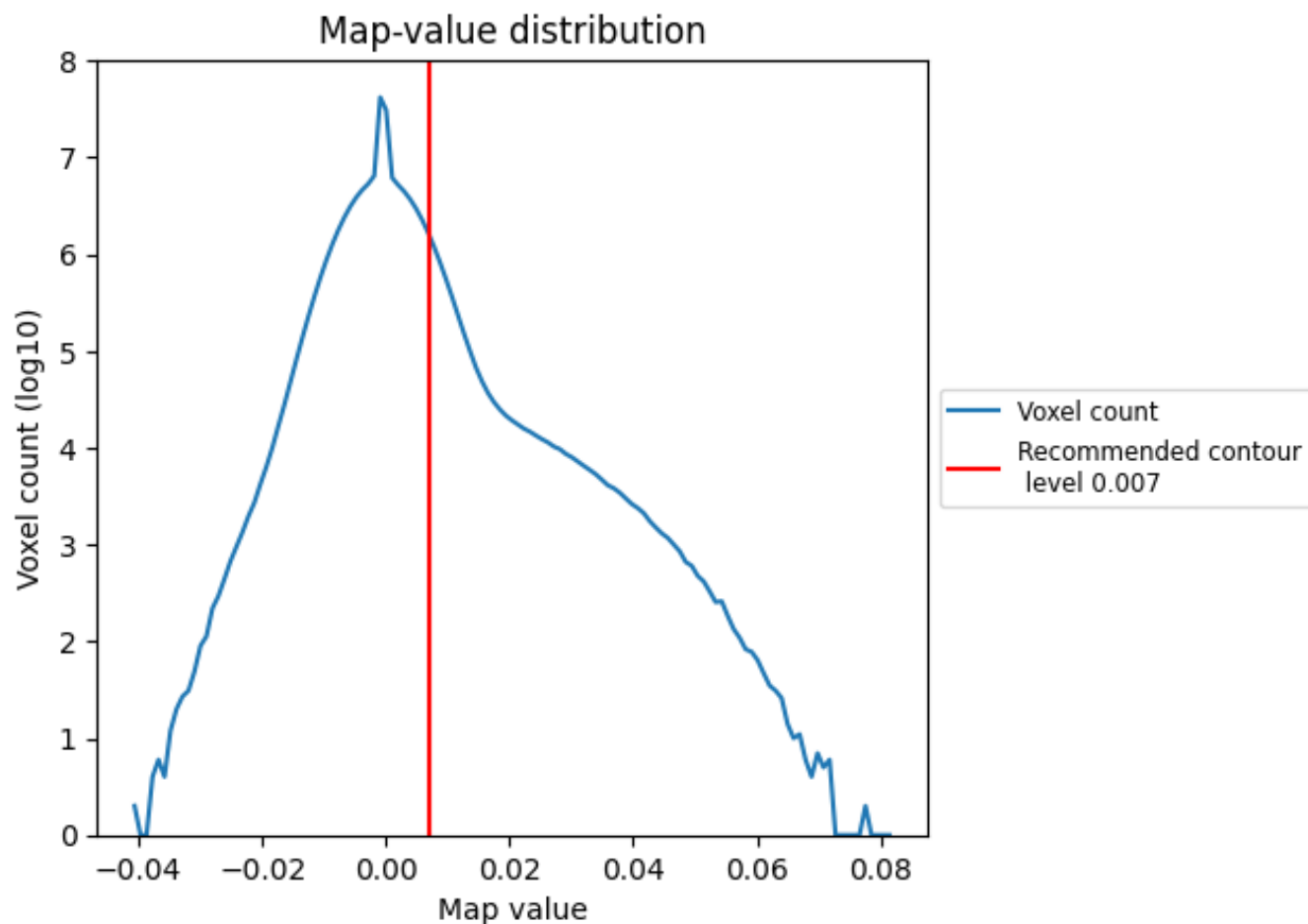
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

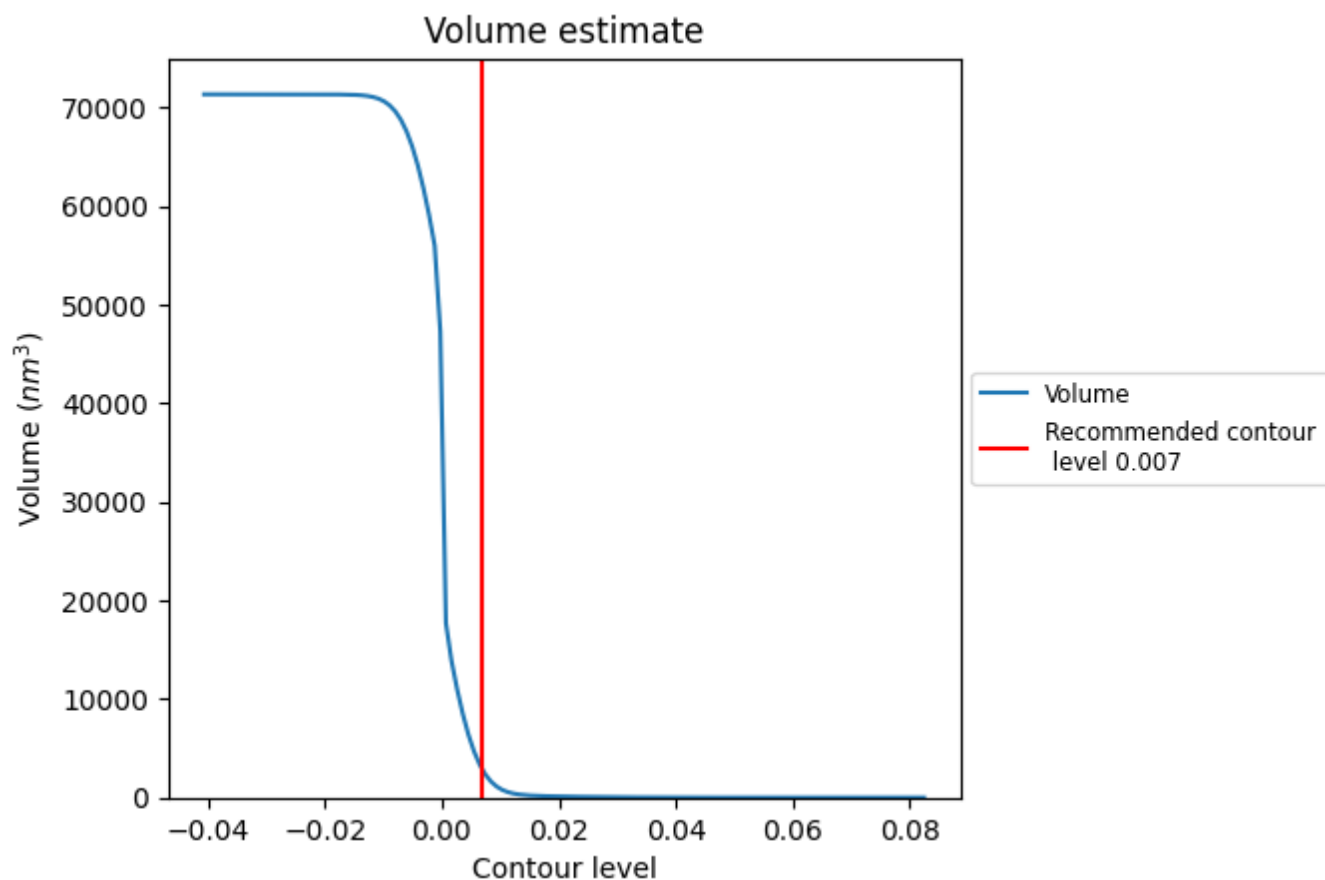
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

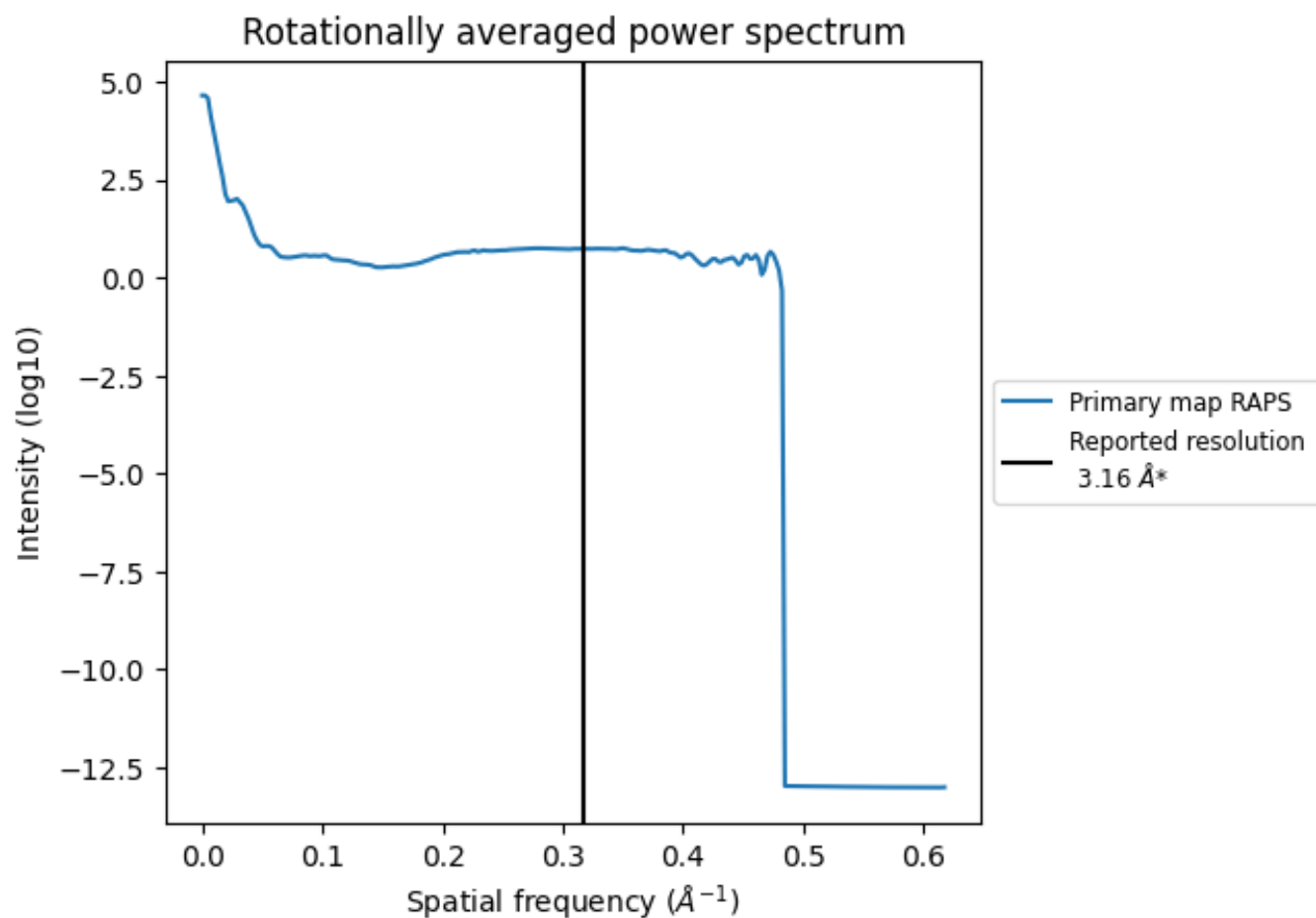
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2795 nm³; this corresponds to an approximate mass of 2525 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

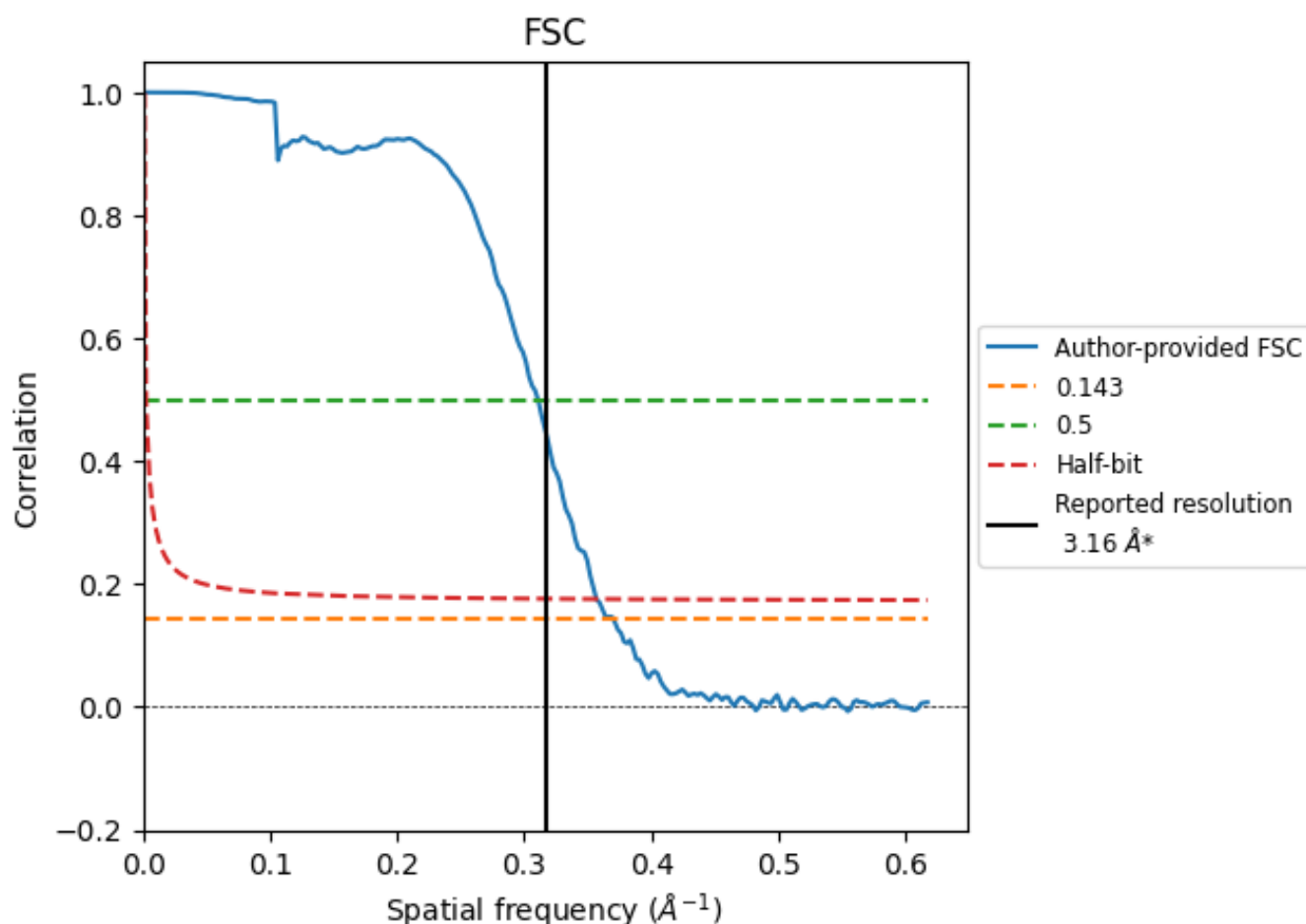


*Reported resolution corresponds to spatial frequency of 0.316 Å⁻¹

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 0.316 Å⁻¹

8.2 Resolution estimates [i](#)

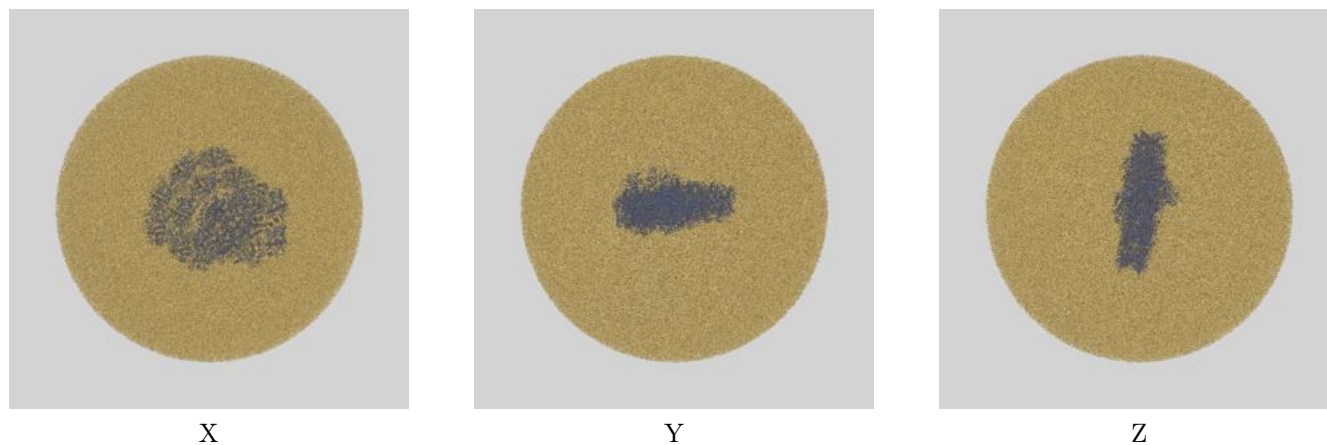
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.16	-	-
Author-provided FSC curve	2.70	3.22	2.80
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 2.70 differs from the reported value 3.16 by more than 10 %

9 Map-model fit [i](#)

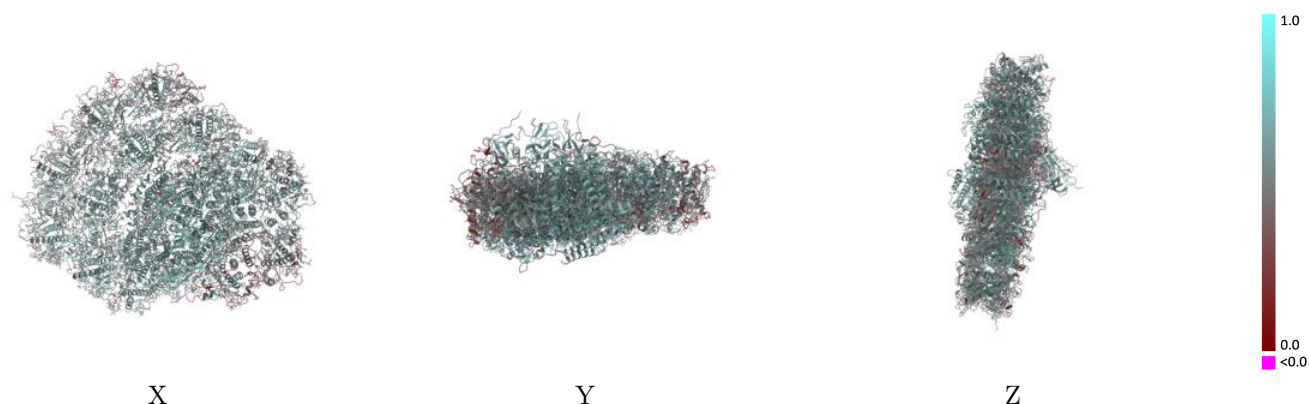
This section contains information regarding the fit between EMDB map EMD-11589 and PDB model 6ZZY. Per-residue inclusion information can be found in section [3](#) on page [46](#).

9.1 Map-model overlay [i](#)



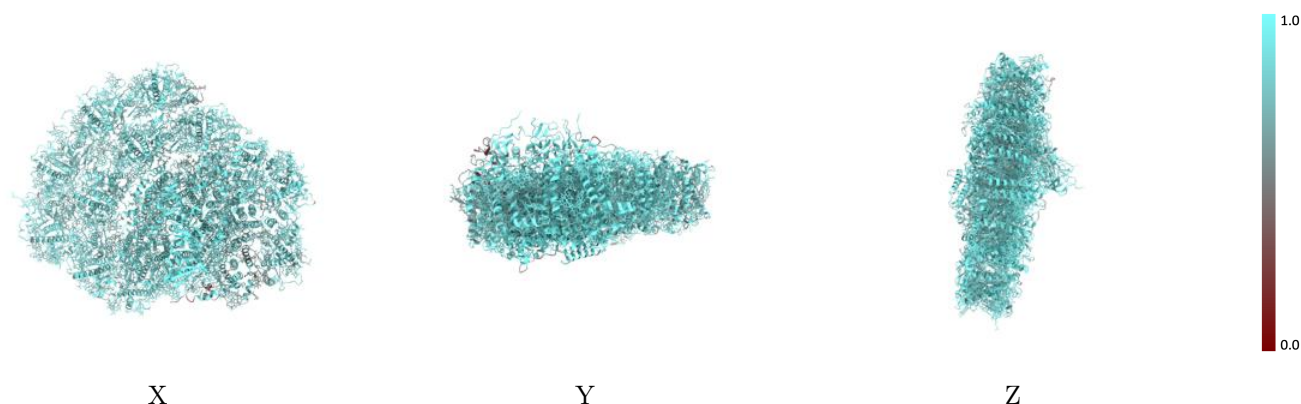
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



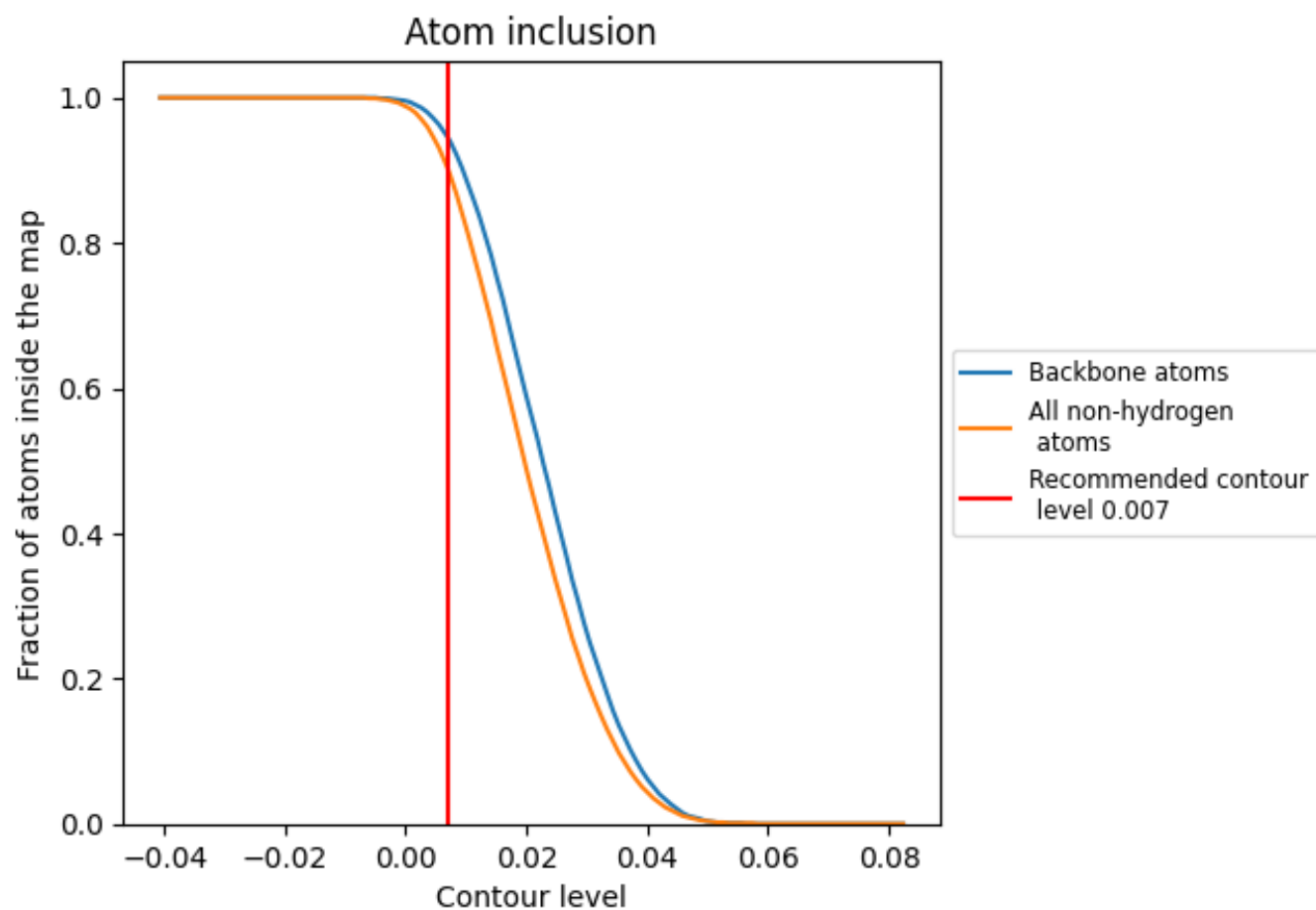
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.007).

9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 90% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9020	 0.5610
1	 0.8850	 0.5400
2	 0.8000	 0.4480
3	 0.9190	 0.5830
4	 0.8810	 0.5090
5	 0.8870	 0.5350
6	 0.8780	 0.5150
7	 0.9170	 0.5720
8	 0.9150	 0.5740
9	 0.8750	 0.5300
A	 0.9510	 0.6240
B	 0.9500	 0.6240
C	 0.9780	 0.6340
D	 0.9150	 0.5590
E	 0.9110	 0.5560
F	 0.9200	 0.5790
G	 0.8790	 0.5390
H	 0.6450	 0.3690
I	 0.8740	 0.5420
J	 0.9400	 0.5980
K	 0.8670	 0.5190
L	 0.8300	 0.4810
M	 0.9240	 0.5900
a	 0.8340	 0.4620

