



wwPDB EM Validation Summary Report ⓘ

Sep 9, 2026 – 06:41 pm BST

PDB ID : 7A4P / pdb_00007a4p
EMDB ID : EMD-11640
Title : Structure of small high-light grown *Chlorella ohadii* photosystem I
Authors : Caspy, I.; Nelson, N.; Nechushtai, R.; Shkolnisky, Y.; Neumann, E.
Deposited on : 2020-08-20
Resolution : 4.20 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:

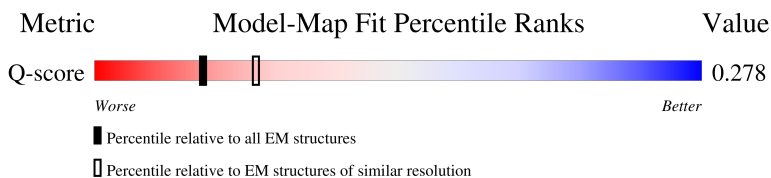
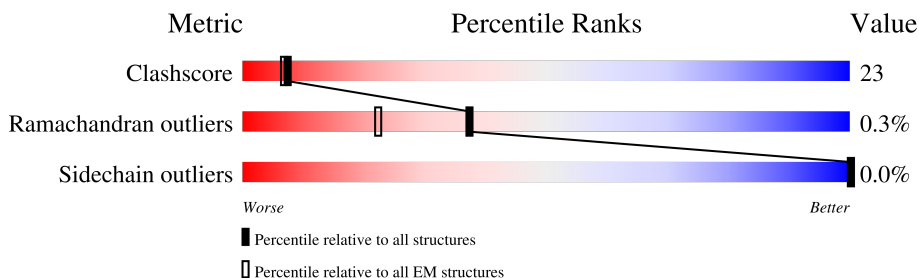
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.20 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	5410 (3.70 - 4.70)

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

Mol	Chain	Length	Quality of chain
1	A	741	
2	B	731	
3	C	80	
4	D	143	

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Mol	Chain	Length	Quality of chain
5	E	64	
6	F	165	
7	G	99	
8	J	41	
9	K	86	
10	M	31	
11	I	35	
12	L	157	
13	1	192	
13	a	192	
14	3	241	
15	4	207	
16	5	227	
17	6	231	
18	7	221	
19	8	219	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	6	601	-	-	X	-
21	CLA	6	609	-	-	X	-
21	CLA	K	1403	-	-	X	-
33	ERG	G	5002	X	-	-	-
34	RRX	J	4002	X	-	-	-
37	LUT	1	503	X	-	-	-
37	LUT	5	505	X	-	-	-
37	LUT	6	501	X	-	-	-
37	LUT	6	502	X	-	-	-
37	LUT	7	501	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
37	LUT	a	502	X	-	-	-
38	CHL	1	609	X	-	-	-
38	CHL	3	608	X	-	-	-
38	CHL	4	609	X	-	-	-
38	CHL	4	618	X	-	-	-
38	CHL	5	610	X	-	-	-
38	CHL	5	613	X	-	-	-
38	CHL	6	610	X	-	-	-
38	CHL	6	619	X	-	-	-
38	CHL	7	613	X	-	-	-
38	CHL	8	601	X	-	-	-
38	CHL	8	604	X	-	-	-
38	CHL	a	606	X	-	-	-
40	QTB	3	506	X	-	-	-
45	XAT	7	502	X	-	-	-
47	C7Z	7	504	X	-	-	-

2 Entry composition

There are 48 unique types of molecules in this entry. The entry contains 48636 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 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	4	LYS	THR	conflict	UNP W8SUA3
B	5	LEU	LYS	conflict	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 PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	140	Total	C	N	O	S	0	0
			1041	682	167	188	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 13 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1	192	Total	C	N	O	S	0	0
			1405	900	237	261	7		
13	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 14 is a protein called Glutathione reductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	3	241	Total	C	N	O	S	0	0
			1844	1194	302	337	11		

There are 10 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	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	conflict	UNP A0A2P6TQ14

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	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 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	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 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	7	221	Total	C	N	O	S	0	0
			1698	1090	294	308	6		

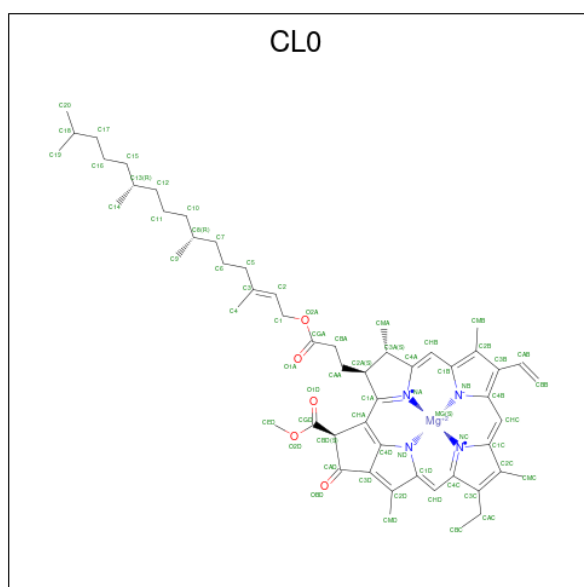
There are 10 discrepancies between the modelled and reference sequences:

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

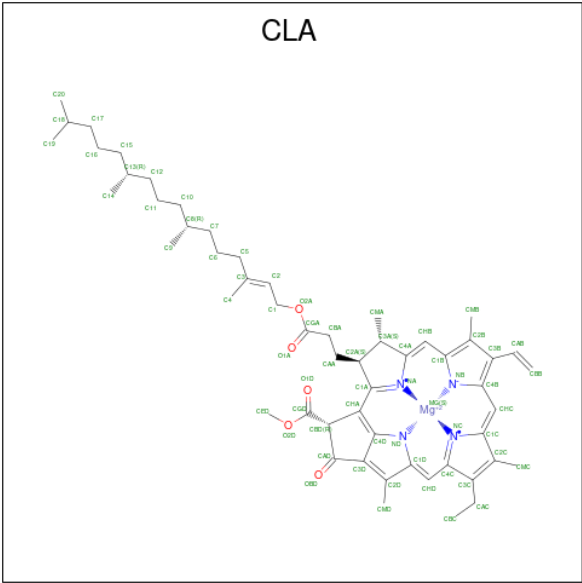
Mol	Chain	Residues	Atoms					AltConf	Trace
19	8	219	Total	C	N	O	S	0	0
			1669	1073	285	305	6		

- Molecule 20 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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

- Molecule 21 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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Mol	Chain	Residues	Atoms					AltConf
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	B	1	Total 62	C 52	Mg 1	N 4	O 5	0
21	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	B	1	Total 61	C 51	Mg 1	N 4	O 5	0
21	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
21	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
21	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 45	C 35	Mg 1	N 4	O 5	0

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

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Mol	Chain	Residues	Atoms					AltConf
21	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	1	1	Total 57	C 47	Mg 1	N 4	O 5	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	a	1	Total 58	C 48	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	a	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
21	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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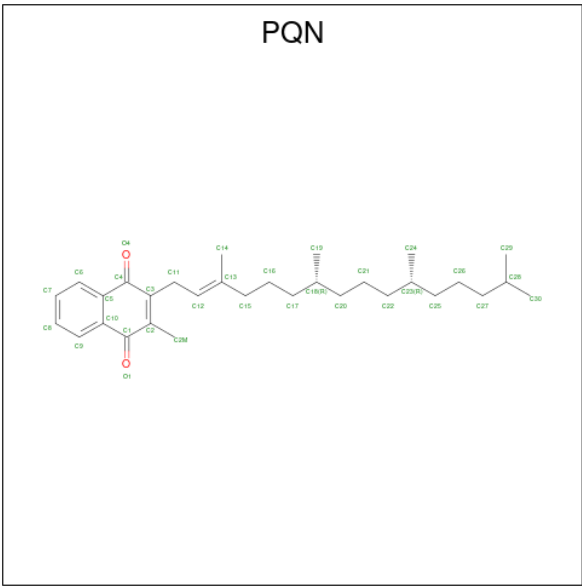
Mol	Chain	Residues	Atoms					AltConf
21	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	5	1	Total 52	C 42	Mg 1	N 4	O 5	0
21	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	6	1	Total 52	C 42	Mg 1	N 4	O 5	0
21	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	6	1	Total 52	C 42	Mg 1	N 4	O 5	0
21	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	7	1	Total 44	C 35	Mg 1	N 4	O 4	0
21	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	7	1	Total 44	C 34	Mg 1	N 4	O 5	0

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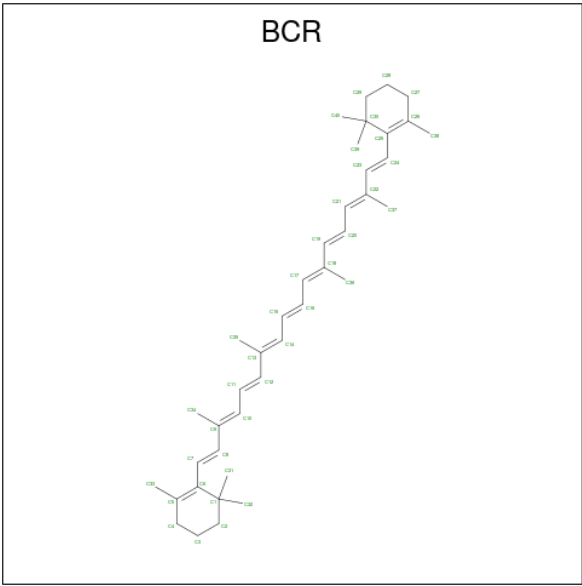
Mol	Chain	Residues	Atoms					AltConf
21	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	7	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
21	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
21	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	7	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
21	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	8	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	8	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
21	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	8	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 22 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



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

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



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

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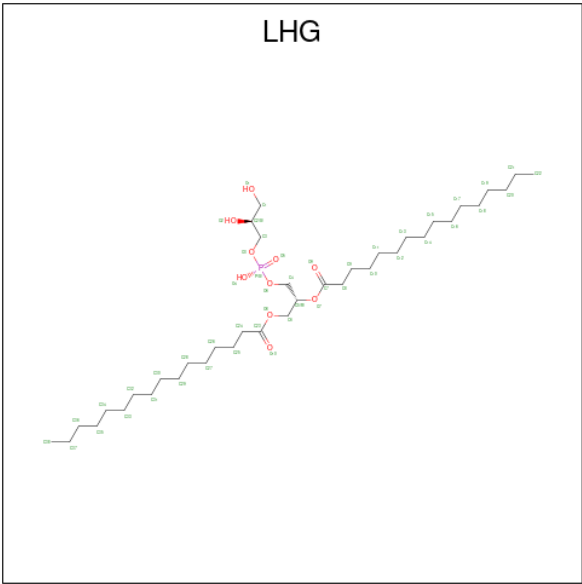
Mol	Chain	Residues	Atoms	AltConf
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	F	1	Total C 40 40	0
23	G	1	Total C 40 40	0
23	J	1	Total C 40 40	0
23	K	1	Total C 40 40	0
23	K	1	Total C 40 40	0
23	I	1	Total C 40 40	0
23	L	1	Total C 40 40	0
23	L	1	Total C 40 40	0
23	L	1	Total C 40 40	0
23	3	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms		AltConf
23	3	1	Total	C	0
			40	40	
23	3	1	Total	C	0
			40	40	
23	4	1	Total	C	0
			40	40	
23	5	1	Total	C	0
			40	40	
23	5	1	Total	C	0
			40	40	
23	6	1	Total	C	0
			40	40	
23	6	1	Total	C	0
			40	40	
23	7	1	Total	C	0
			40	40	
23	8	1	Total	C	0
			40	40	

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



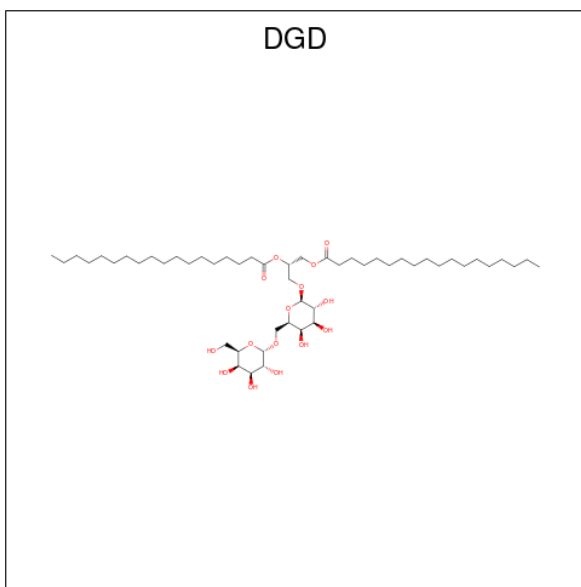
Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	P	0
			29	18	10	1	
24	A	1	Total	C	O	P	0
			49	38	10	1	

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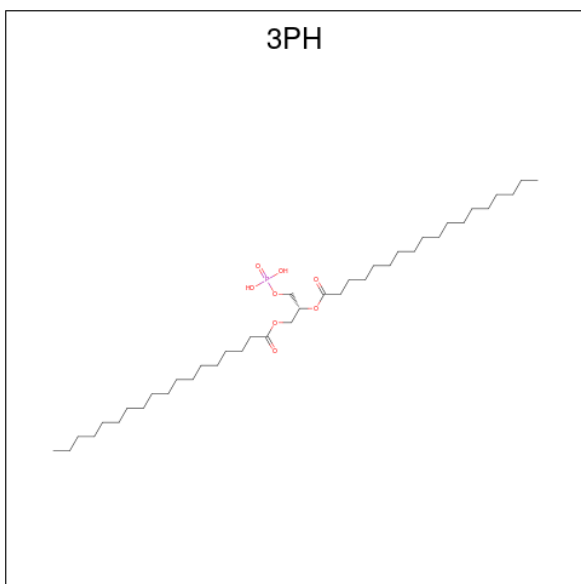
Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	P	0
			42	31	10	1	
24	B	1	Total	C	O	P	0
			49	38	10	1	
24	B	1	Total	C	O	P	0
			46	35	10	1	
24	F	1	Total	C	O	P	0
			36	25	10	1	
24	F	1	Total	C	O	P	0
			43	32	10	1	
24	1	1	Total	C	O	P	0
			35	24	10	1	
24	1	1	Total	C	O	P	0
			42	31	10	1	
24	a	1	Total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

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



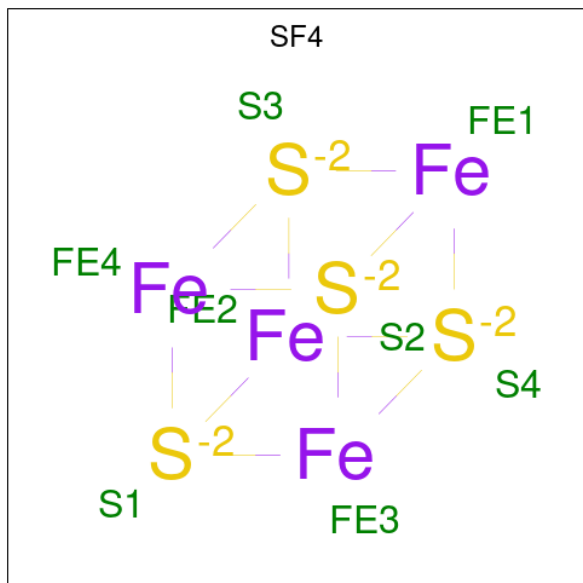
Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	C	O	0
			51	36	15	
25	B	1	Total	C	O	0
			66	51	15	
25	8	1	Total	C	O	0
			66	51	15	

- Molecule 26 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).



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

- Molecule 27 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 28 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $\text{C}_{24}\text{H}_{46}\text{O}_{11}$).



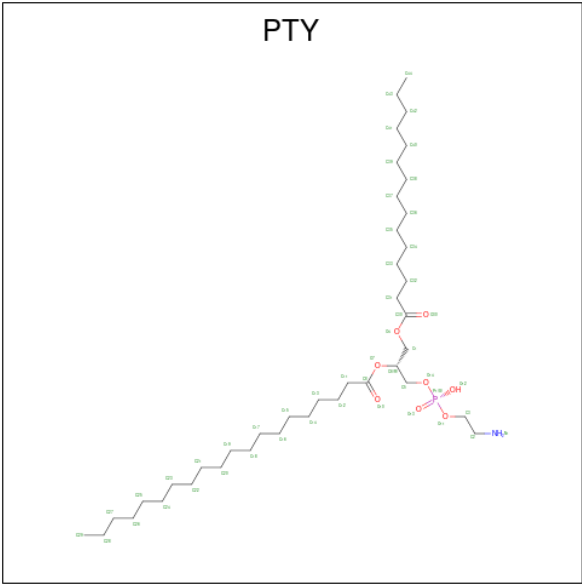
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total 35	C 24	O 11	0
28	B	1	Total 35	C 24	O 11	0
28	1	1	Total 35	C 24	O 11	0

- Molecule 29 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: $C_{44}H_{85}NO_8P$).



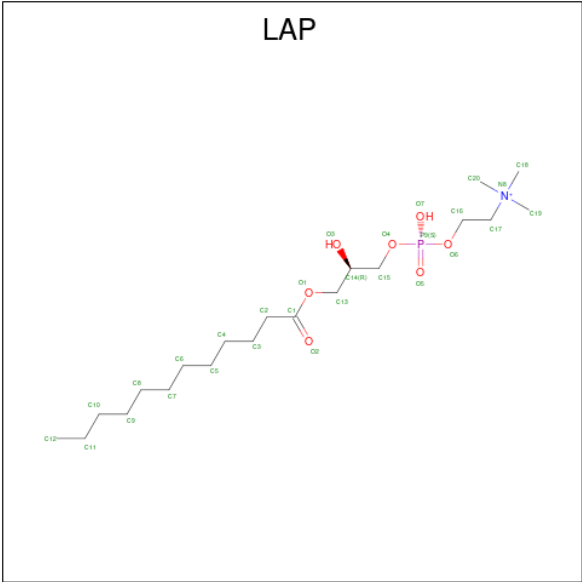
Mol	Chain	Residues	Atoms					AltConf
29	B	1	Total	C	N	O	P	0
			30	20	1	8	1	
29	6	1	Total	C	N	O	P	0
			36	26	1	8	1	

- Molecule 30 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



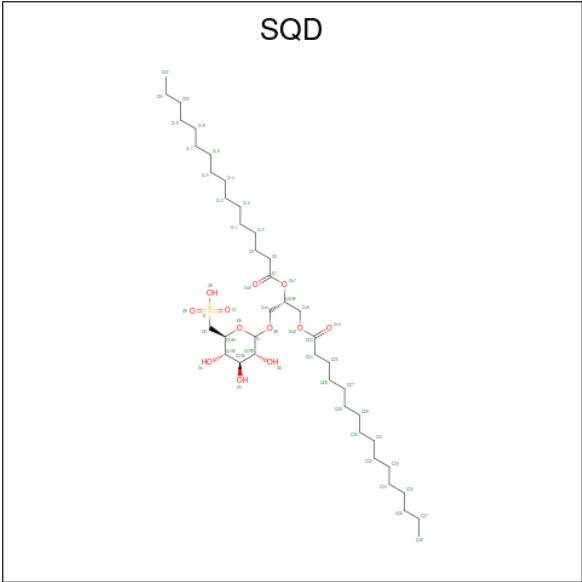
Mol	Chain	Residues	Atoms					AltConf
30	B	1	Total	C	N	O	P	0
			41	31	1	8	1	
30	3	1	Total	C	N	O	P	0
			38	28	1	8	1	
30	5	1	Total	C	N	O	P	0
			38	28	1	8	1	
30	7	1	Total	C	N	O	P	0
			33	23	1	8	1	
30	8	1	Total	C	N	O	P	0
			35	25	1	8	1	

- Molecule 31 is [2-((1-OXODODECANOXY-(2-HYDROXY-3-PROPANYL))-PHOSPHONATE-OXY)-ETHYL]-TRIMETHYLAMMONIUM (CCD ID: LAP) (formula: C₂₀H₄₃NO₇P).



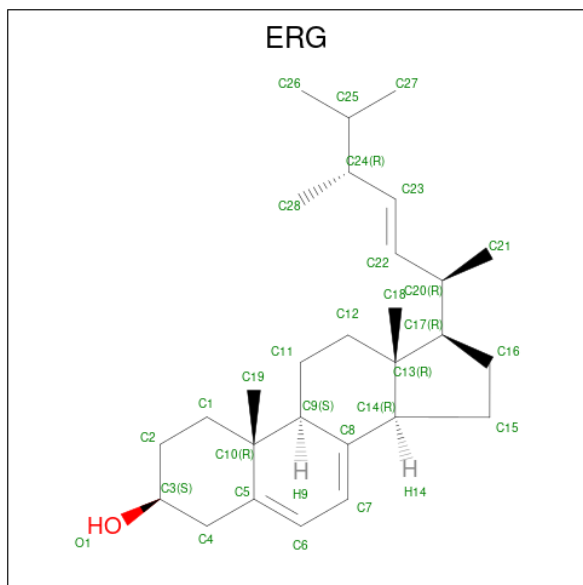
Mol	Chain	Residues	Atoms					AltConf
31	B	1	Total	C	N	O	P	0
			29	20	1	7	1	
31	F	1	Total	C	N	O	P	0
			29	20	1	7	1	
31	K	1	Total	C	N	O	P	0
			29	20	1	7	1	

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



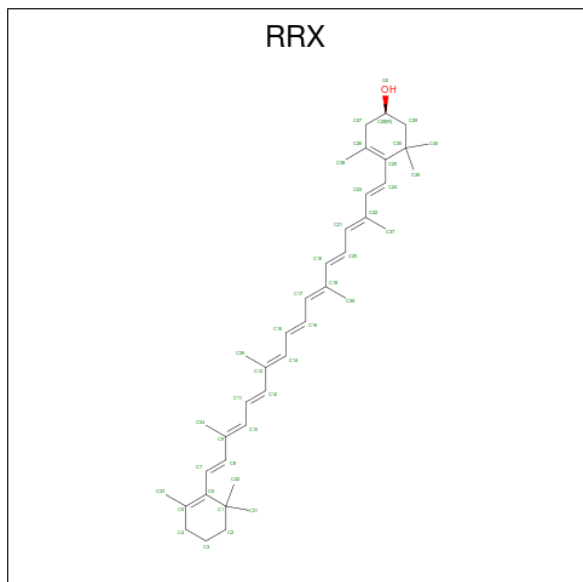
Mol	Chain	Residues	Atoms				AltConf
32	G	1	Total	C	O	S	0
			46	33	12	1	
32	7	1	Total	C	O	S	0
			39	26	12	1	

- Molecule 33 is ERGOSTEROL (CCD ID: ERG) (formula: $C_{28}H_{44}O$).



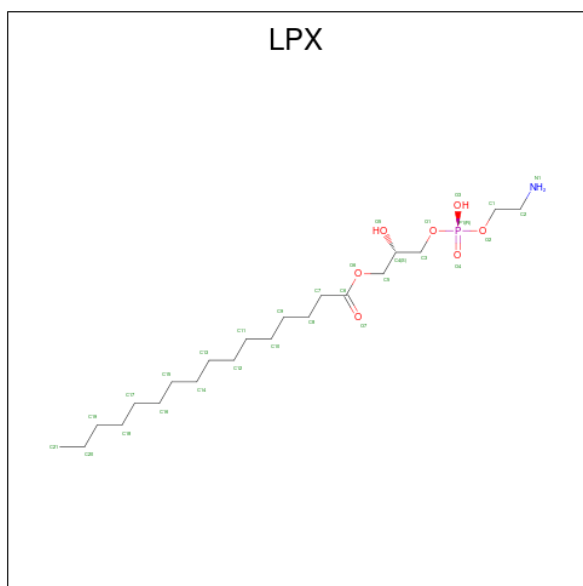
Mol	Chain	Residues	Atoms				AltConf
33	G	1	Total	C	O		0
			29	28	1		

- Molecule 34 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: $C_{40}H_{56}O$).



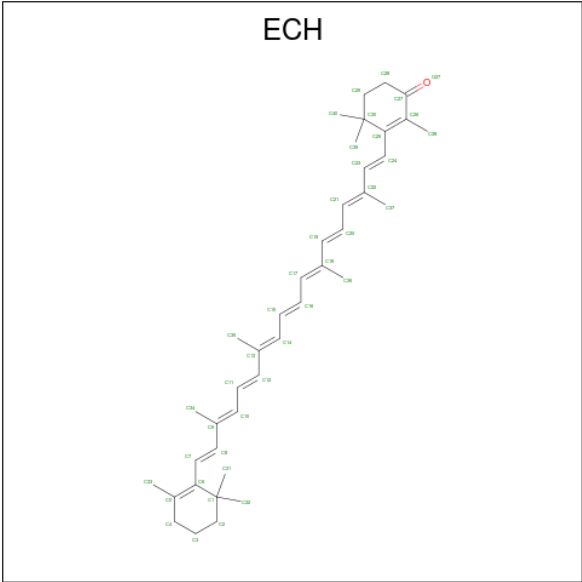
Mol	Chain	Residues	Atoms			AltConf
34	J	1	Total	C	O	0
			41	40	1	

- Molecule 35 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (CCD ID: LPX) (formula: C₂₁H₄₄NO₇P).



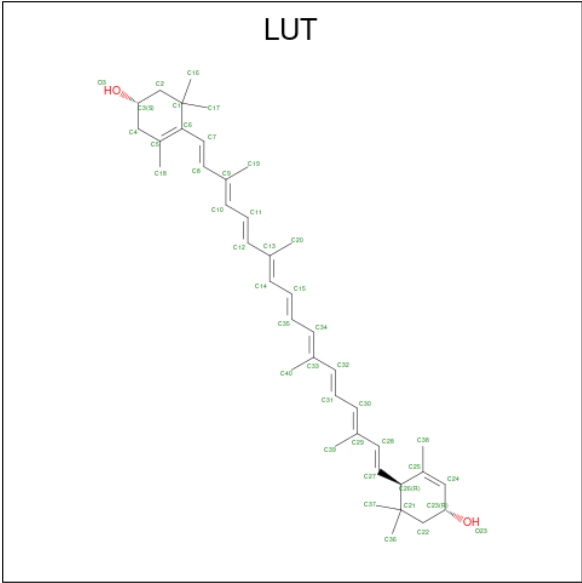
Mol	Chain	Residues	Atoms					AltConf
35	J	1	Total	C	N	O	P	0
			17	8	1	7	1	
35	a	1	Total	C	N	O	P	0
			30	21	1	7	1	

- Molecule 36 is beta,beta-caroten-4-one (CCD ID: ECH) (formula: C₄₀H₅₄O).



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

- Molecule 37 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



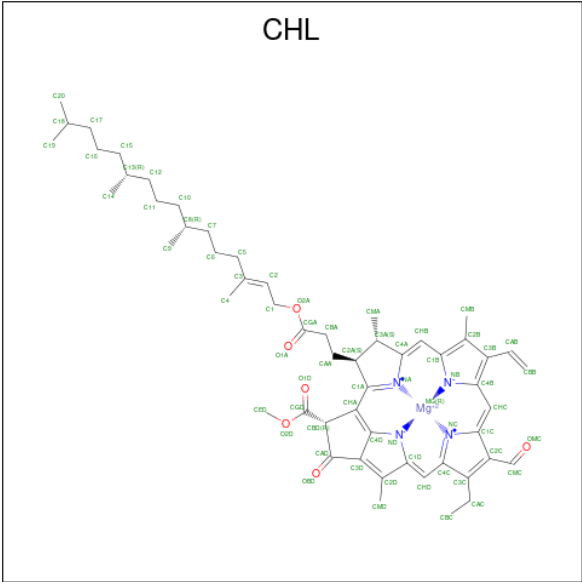
Mol	Chain	Residues	Atoms			AltConf
37	1	1	Total	C	O	0
			42	40	2	
37	1	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
37	1	1	Total	C	O	0
			42	40	2	
37	a	1	Total	C	O	0
			42	40	2	
37	a	1	Total	C	O	0
			42	40	2	
37	a	1	Total	C	O	0
			42	40	2	
37	3	1	Total	C	O	0
			42	40	2	
37	3	1	Total	C	O	0
			42	40	2	
37	4	1	Total	C	O	0
			42	40	2	
37	4	1	Total	C	O	0
			42	40	2	
37	5	1	Total	C	O	0
			42	40	2	
37	5	1	Total	C	O	0
			42	40	2	
37	5	1	Total	C	O	0
			42	40	2	
37	6	1	Total	C	O	0
			42	40	2	
37	6	1	Total	C	O	0
			42	40	2	
37	7	1	Total	C	O	0
			42	40	2	
37	8	1	Total	C	O	0
			42	40	2	
37	8	1	Total	C	O	0
			42	40	2	

- Molecule 38 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



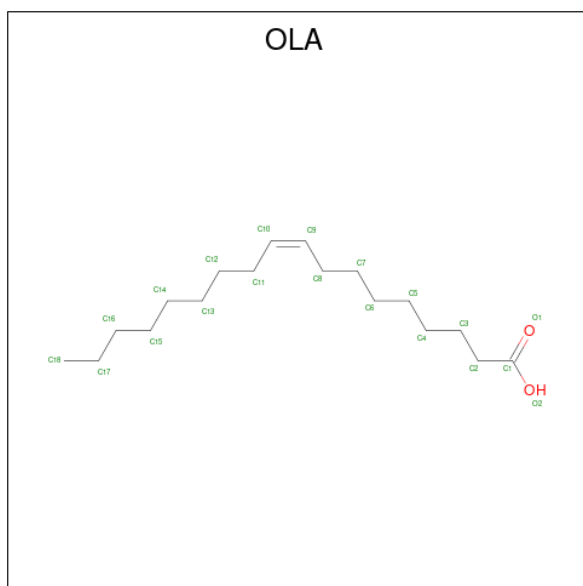
Mol	Chain	Residues	Atoms					AltConf
38	1	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
38	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	a	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
38	a	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
38	a	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
38	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
38	3	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
38	3	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
38	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	4	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
38	4	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
38	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	5	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
38	5	1	Total	C	Mg	N	O	0
			56	45	1	4	6	

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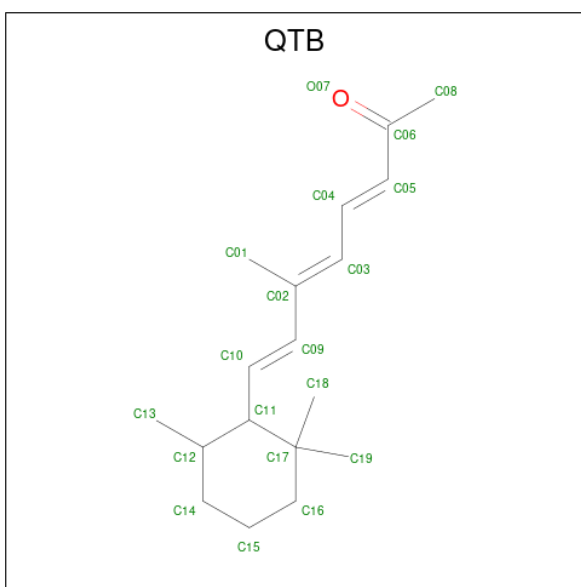
Mol	Chain	Residues	Atoms					AltConf
38	6	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
38	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
38	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
38	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	8	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
38	8	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
38	8	1	Total	C	Mg	N	O	0
			51	40	1	4	6	

- Molecule 39 is OLEIC ACID (CCD ID: OLA) (formula: $C_{18}H_{34}O_2$).



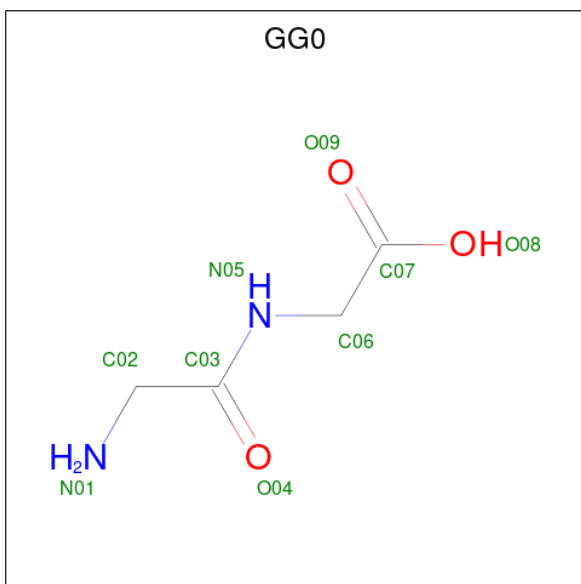
Mol	Chain	Residues	Atoms			AltConf
39	1	1	Total	C	O	0
			20	18	2	
39	8	1	Total	C	O	0
			20	18	2	

- Molecule 40 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: $C_{18}H_{28}O$).



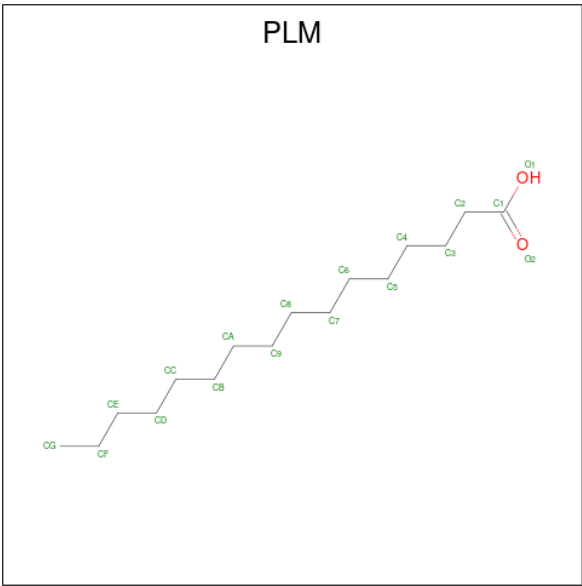
Mol	Chain	Residues	Atoms			AltConf
40	a	1	Total	C	O	0
			19	18	1	
40	3	1	Total	C	O	0
			19	18	1	

- Molecule 41 is 2-(2-azanylethanoylamino)ethanoic acid (CCD ID: GG0) (formula: $C_4H_8N_2O_3$).



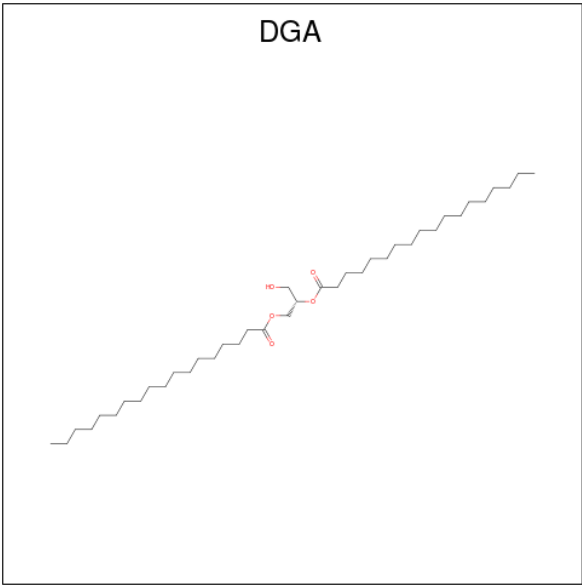
Mol	Chain	Residues	Atoms				AltConf
41	a	1	Total	C	N	O	0
			9	4	2	3	

- Molecule 42 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			AltConf
42	4	1	Total	C	O	0
			17	16	1	
42	6	1	Total	C	O	0
			18	16	2	

- Molecule 43 is DIACYL GLYCEROL (CCD ID: DGA) (formula: C₃₉H₇₆O₅).



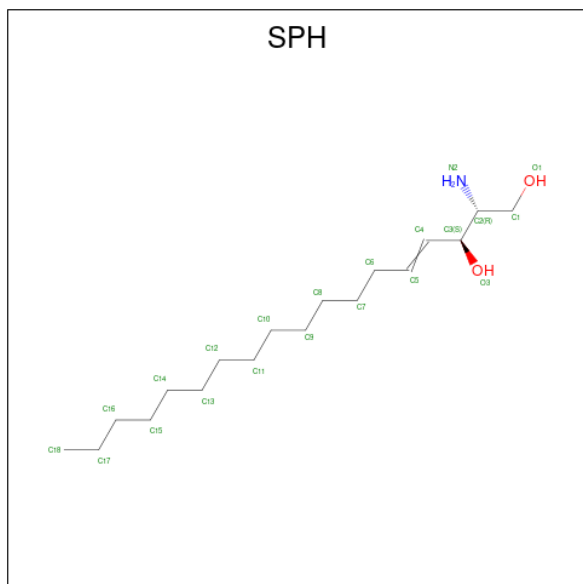
Mol	Chain	Residues	Atoms			AltConf
43	5	1	Total	C	O	0
			23	18	5	

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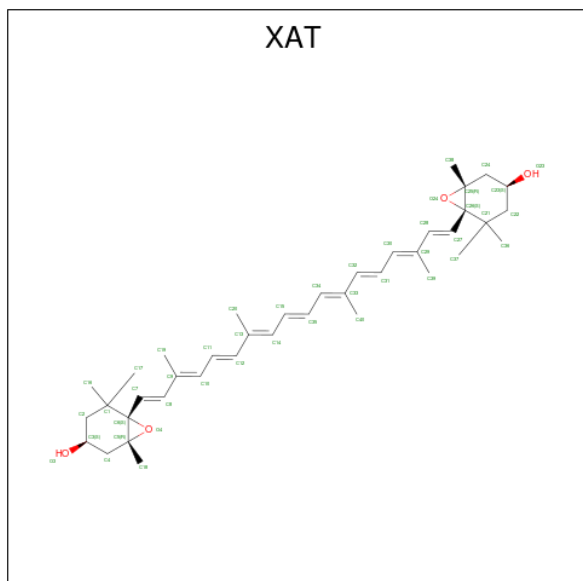
Mol	Chain	Residues	Atoms			AltConf
43	8	1	Total	C	O	0
			30	25	5	

- Molecule 44 is SPHINGOSINE (CCD ID: SPH) (formula: $C_{18}H_{37}NO_2$).



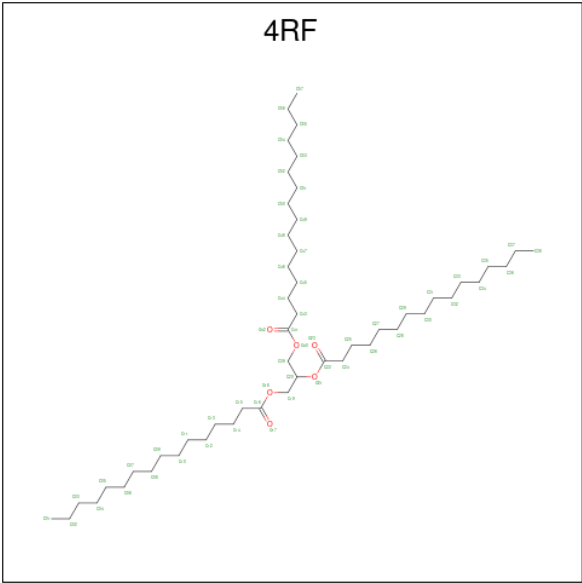
Mol	Chain	Residues	Atoms				AltConf
44	6	1	Total	C	N	O	0
			21	18	1	2	

- Molecule 45 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: $C_{40}H_{56}O_4$).



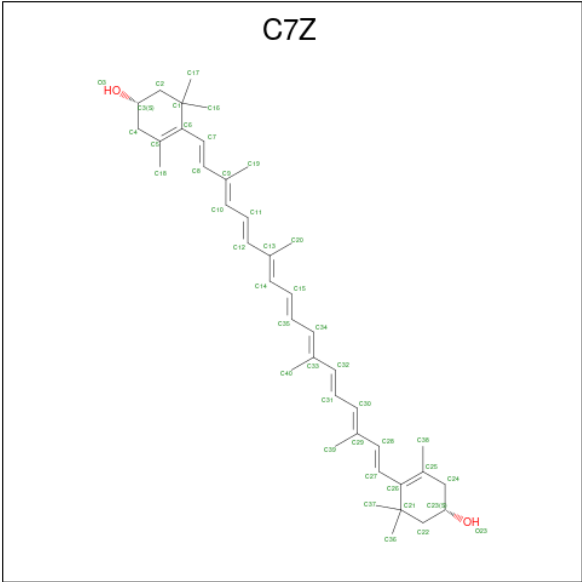
Mol	Chain	Residues	Atoms			AltConf
45	7	1	Total	C	O	0
			44	40	4	

- Molecule 46 is Tripalmitoylglycerol (CCD ID: 4RF) (formula: C₅₁H₉₈O₆).



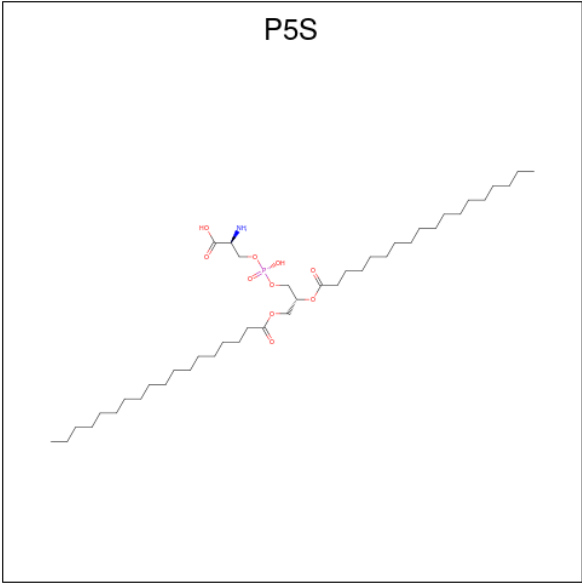
Mol	Chain	Residues	Atoms			AltConf
46	7	1	Total	C	O	0
			32	26	6	
46	8	1	Total	C	O	0
			42	36	6	
46	8	1	Total	C	O	0
			54	48	6	

- Molecule 47 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: C₄₀H₅₆O₂).



Mol	Chain	Residues	Atoms			AltConf
47	7	1	Total	C	O	0
			42	40	2	

- Molecule 48 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (CCD ID: P5S) (formula: C₄₂H₈₂NO₁₀P).



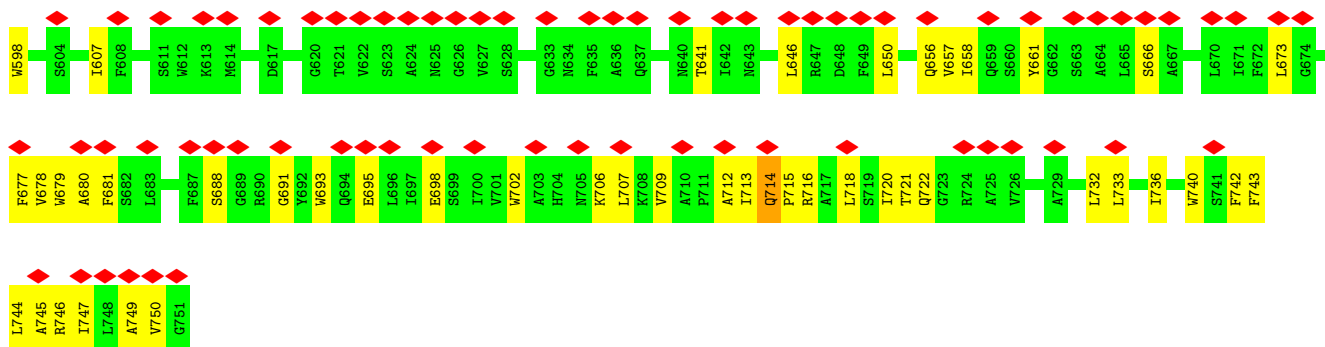
Mol	Chain	Residues	Atoms					AltConf
48	8	1	Total	C	N	O	P	0
			37	25	1	10	1	

3 Residue-property plots

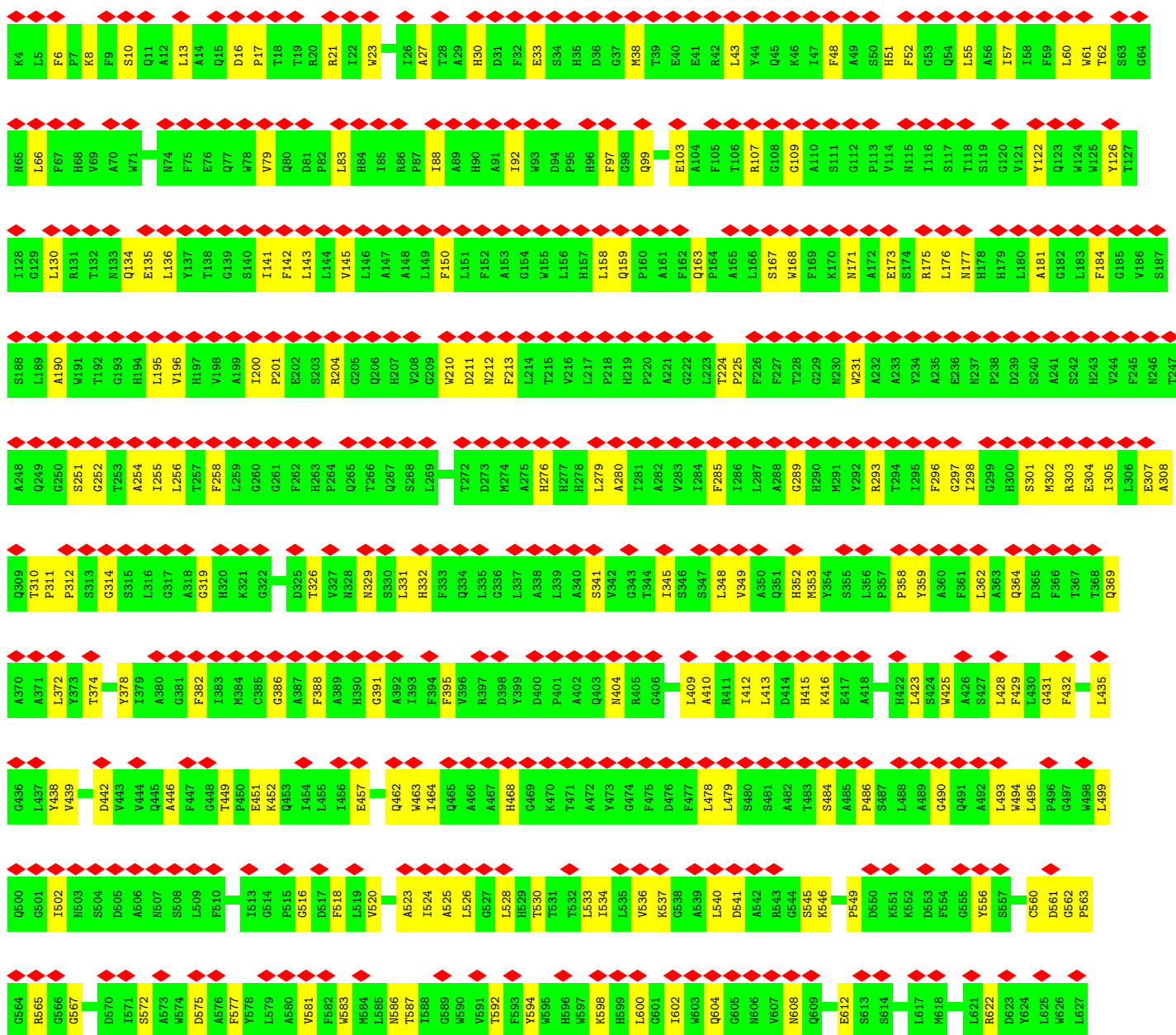
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

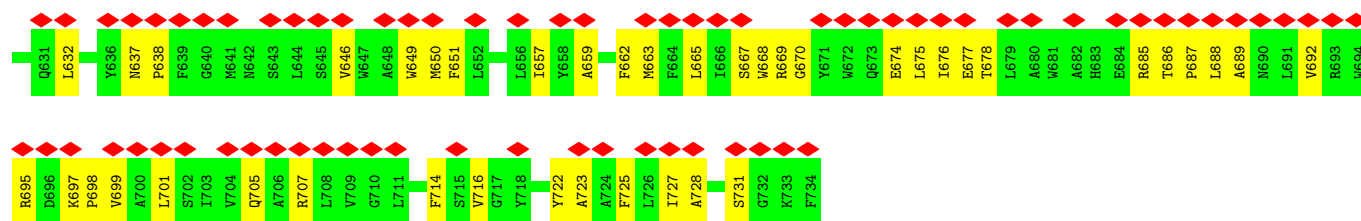
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



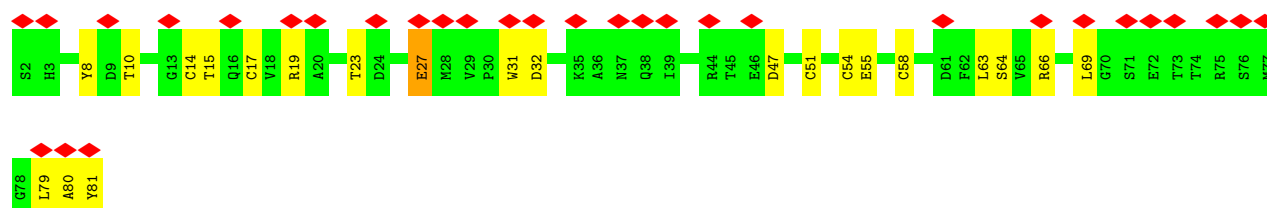
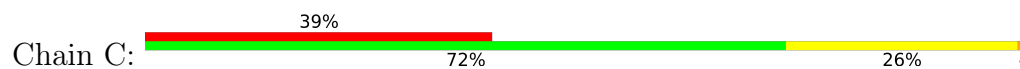


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

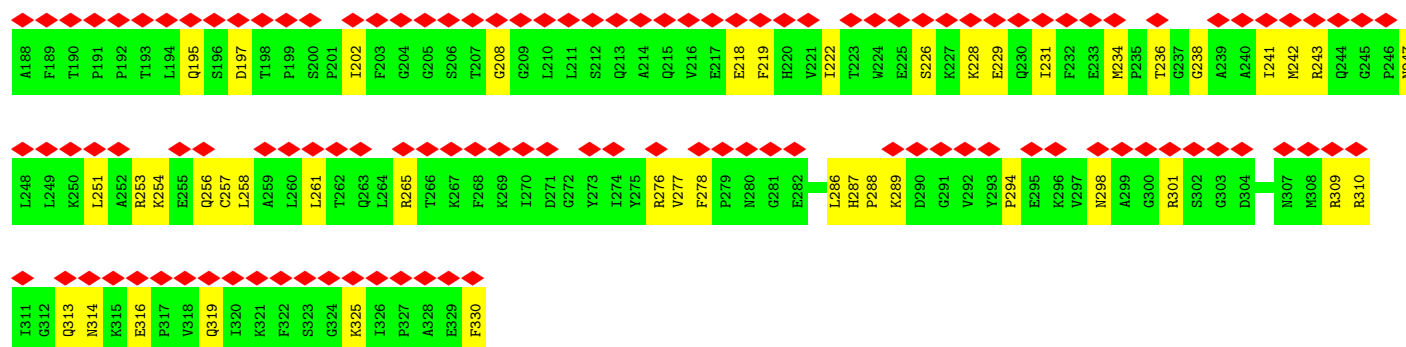
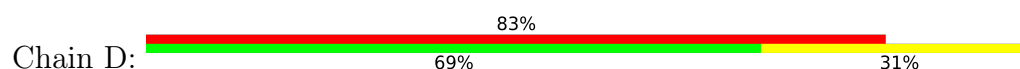




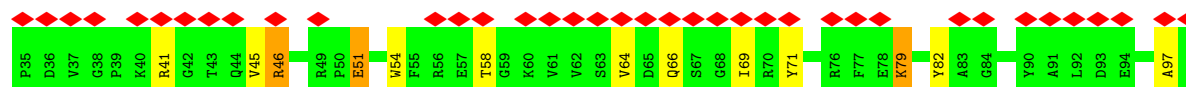
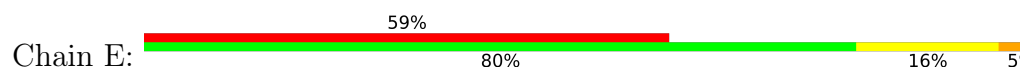
• Molecule 3: Photosystem I iron-sulfur center



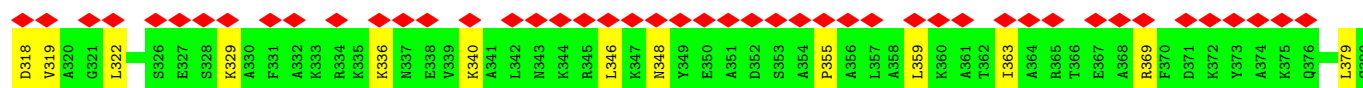
• Molecule 4: Photosystem I reaction center subunit chloroplastic

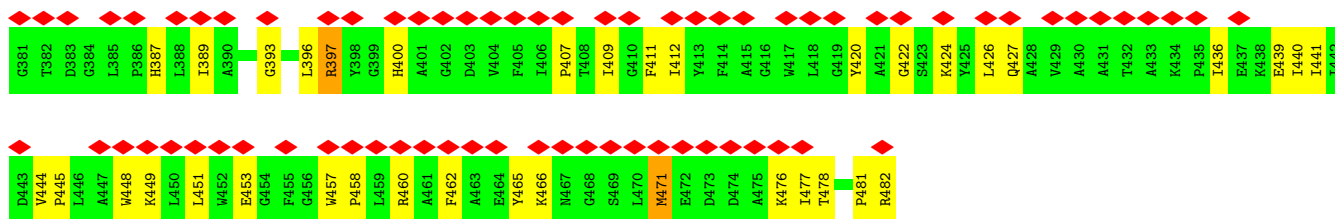


• Molecule 5: Photosystem I reaction center subunit IV



• Molecule 6: PSI-F

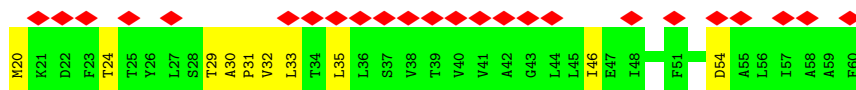
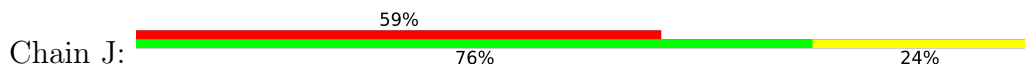




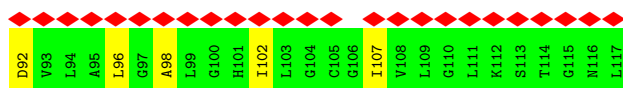
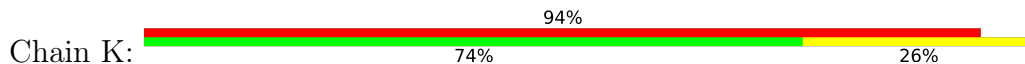
• Molecule 7: Photosystem I reaction center subunit chloroplastic



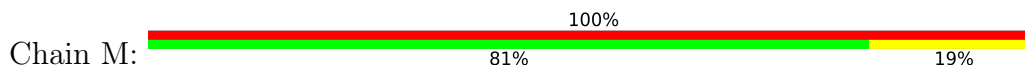
• Molecule 8: Photosystem I reaction center subunit IX



• Molecule 9: PSI-K



• Molecule 10: Photosystem I reaction center subunit XII

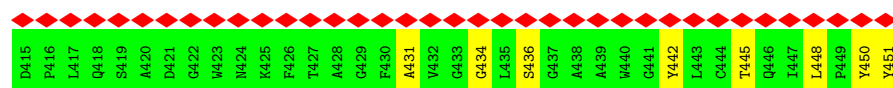
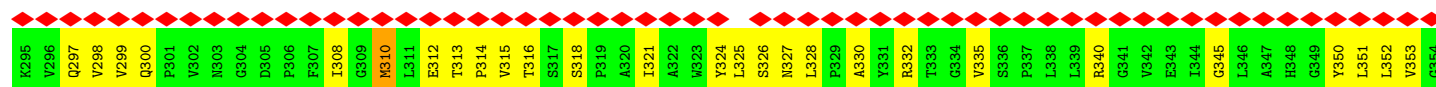
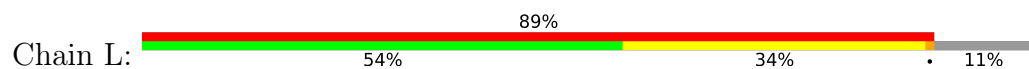


• Molecule 11: Photosystem I reaction center subunit VIII

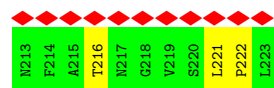
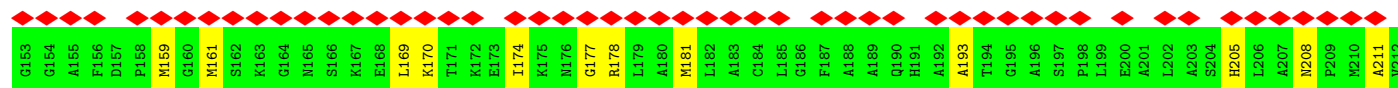
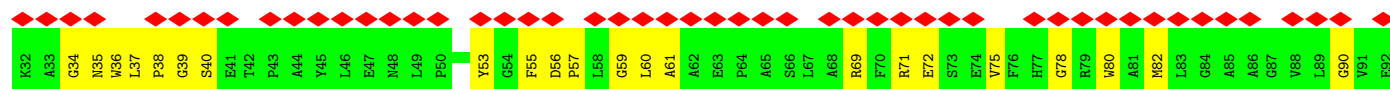
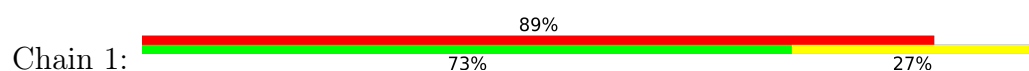




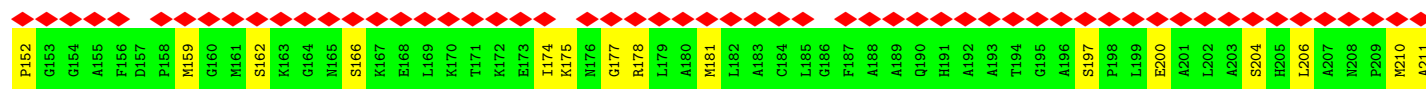
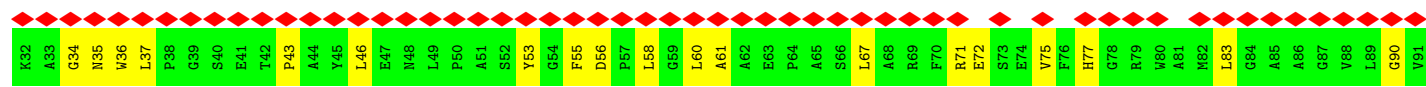
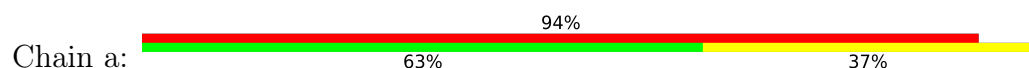
• Molecule 12: PSI subunit V

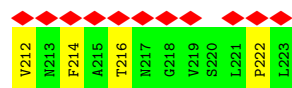


• Molecule 13: Chlorophyll a-b binding protein, chloroplastic

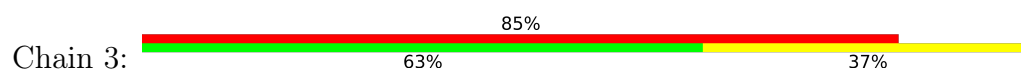


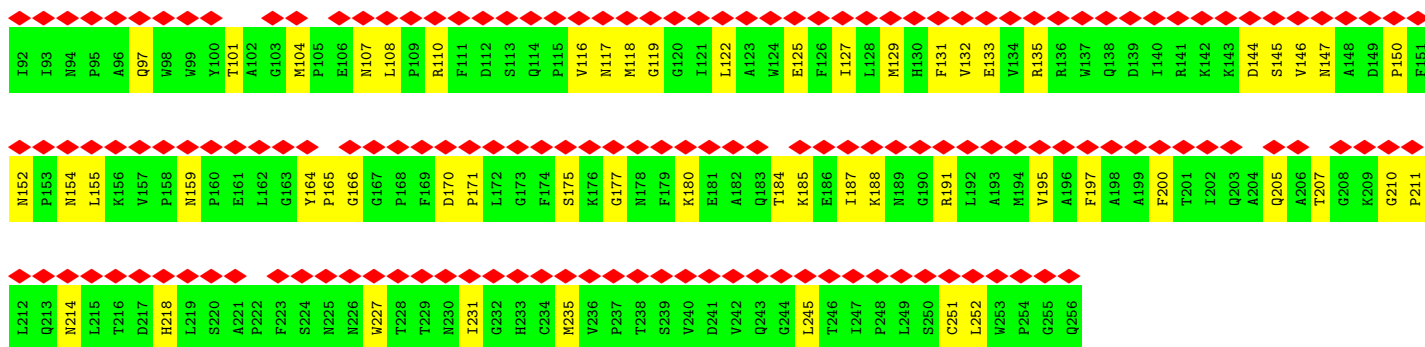
• Molecule 13: Chlorophyll a-b binding protein, chloroplastic





• Molecule 14: Glutathione reductase





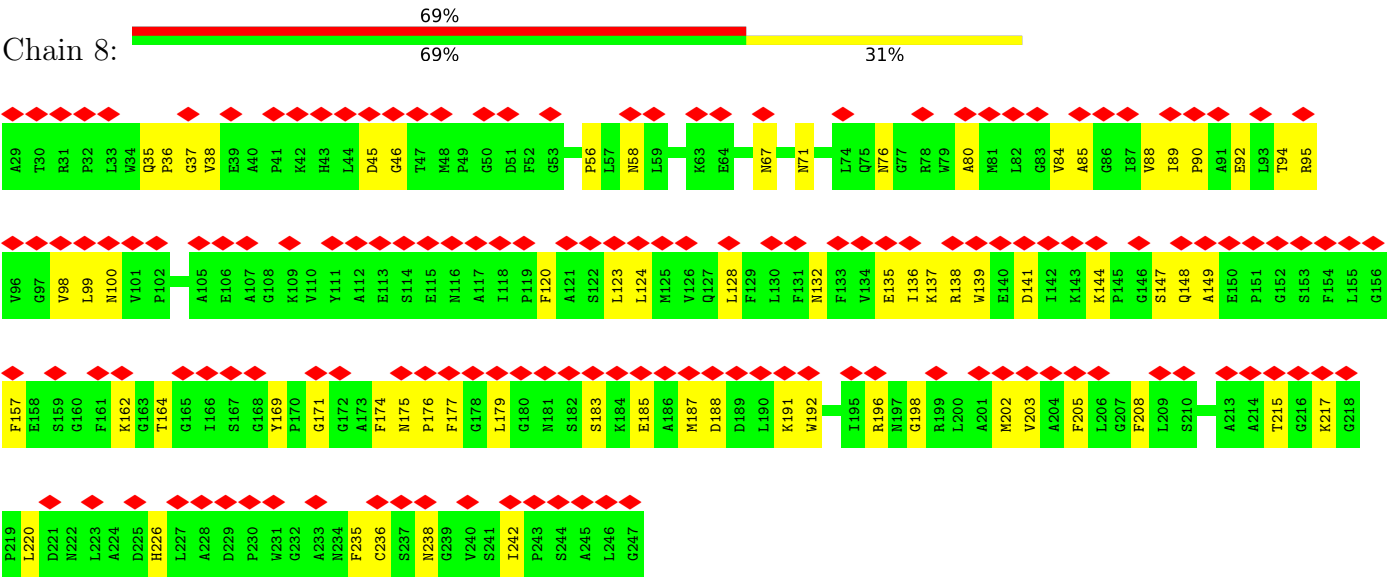
• Molecule 17: Chlorophyll a-b binding protein, chloroplastic



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	25248	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	0.034	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.01	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: PLM, BCR, ERG, XAT, OLA, LPX, DGD, QTB, 3PH, CL0, CLA, LAP, C7Z, LHG, DGA, RRX, P5S, SF4, PTY, CHL, ECH, SQD, LMT, SPH, GG0, LUT, 4RF, PCW, PQN

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	0.35	0/6022	0.44	3/8215 (0.0%)
2	B	0.35	0/6006	0.40	0/8205
3	C	0.36	0/611	0.56	1/828 (0.1%)
4	D	0.35	0/1150	0.50	0/1551
5	E	0.88	3/520 (0.6%)	0.65	4/705 (0.6%)
6	F	0.36	1/1309 (0.1%)	0.71	3/1771 (0.2%)
7	G	0.28	0/743	0.43	0/1007
8	J	0.44	0/322	0.66	0/439
9	K	0.24	0/622	0.39	0/844
10	M	0.24	0/244	0.32	0/330
11	I	0.27	0/276	0.46	0/373
12	L	0.30	0/1068	0.54	1/1462 (0.1%)
13	1	0.29	0/1443	0.45	1/1960 (0.1%)
13	a	0.29	0/1443	0.55	0/1960
14	3	0.29	0/1896	0.45	0/2573
15	4	0.29	0/1681	0.50	0/2285
16	5	0.27	0/1825	0.42	0/2483
17	6	0.31	0/1845	0.49	1/2515 (0.0%)
18	7	0.34	0/1748	0.42	0/2372
19	8	0.33	0/1717	0.45	0/2330
All	All	0.34	4/32491 (0.0%)	0.47	14/44208 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	E	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	79	LYS	CE-NZ	14.61	1.93	1.49
5	E	79	LYS	CB-CG	-7.54	1.29	1.52
6	F	471	MET	CB-CG	-6.19	1.33	1.52
5	E	51	GLU	CB-CG	-5.87	1.34	1.52

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	471	MET	CB-CG-SD	-18.14	58.27	112.70
1	A	714	GLN	CB-CA-C	-9.37	94.36	109.82
12	L	310	MET	CB-CG-SD	-8.75	86.44	112.70
17	6	200	MET	CA-CB-CG	-7.82	98.47	114.10
6	F	471	MET	CG-SD-CE	-7.31	84.81	100.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	51	GLU	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5824	0	5675	241	0
2	B	5796	0	5576	245	0
3	C	601	0	576	25	0
4	D	1124	0	1129	46	0
5	E	509	0	507	11	0
6	F	1277	0	1296	58	0
7	G	727	0	724	53	0
8	J	316	0	332	18	0
9	K	613	0	639	44	0
10	M	239	0	255	11	0
11	I	270	0	287	23	0
12	L	1041	0	1047	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	1	1405	0	1370	49	0
13	a	1405	0	1370	81	0
14	3	1844	0	1805	94	0
15	4	1631	0	1575	58	0
16	5	1769	0	1719	101	0
17	6	1787	0	1762	189	0
18	7	1698	0	1640	78	0
19	8	1669	0	1619	71	0
20	A	65	0	72	4	0
21	1	693	0	678	73	0
21	3	719	0	726	61	0
21	4	768	0	686	44	0
21	5	739	0	638	57	0
21	6	711	0	649	108	0
21	7	778	0	720	61	0
21	8	699	0	617	55	0
21	A	2621	0	2695	237	0
21	B	2583	0	2678	255	0
21	F	105	0	87	12	0
21	G	141	0	105	7	0
21	J	42	0	31	0	0
21	K	204	0	167	39	0
21	L	155	0	130	22	0
21	a	571	0	540	33	0
22	A	33	0	46	6	0
22	B	33	0	46	5	0
23	3	120	0	159	11	0
23	4	40	0	53	3	0
23	5	80	0	104	9	0
23	6	80	0	105	16	0
23	7	40	0	52	9	0
23	8	40	0	53	5	0
23	A	200	0	264	21	0
23	B	280	0	369	32	0
23	F	40	0	53	5	0
23	G	40	0	53	3	0
23	I	40	0	52	8	0
23	J	40	0	53	3	0
23	K	80	0	106	7	0
23	L	120	0	159	24	0
24	1	77	0	97	5	0
24	3	49	0	74	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	4	81	0	108	20	0
24	5	49	0	74	10	0
24	6	86	0	118	20	0
24	7	128	0	175	12	0
24	8	37	0	44	5	0
24	A	120	0	159	16	0
24	B	95	0	139	9	0
24	F	79	0	101	7	0
24	a	35	0	40	2	0
25	8	66	0	96	13	0
25	A	51	0	60	3	0
25	B	66	0	96	10	0
26	A	33	0	39	1	0
27	A	8	0	0	0	0
27	C	16	0	0	2	0
28	1	35	0	45	9	0
28	A	35	0	46	4	0
28	B	35	0	44	2	0
29	6	36	0	44	3	0
29	B	30	0	34	6	0
30	3	38	0	49	5	0
30	5	38	0	49	2	0
30	7	33	0	39	3	0
30	8	35	0	43	6	0
30	B	41	0	55	4	0
31	B	29	0	42	3	0
31	F	29	0	42	6	0
31	K	29	0	42	3	0
32	7	39	0	41	1	0
32	G	46	0	55	4	0
33	G	29	0	38	16	0
34	J	41	0	56	10	0
35	J	17	0	14	3	0
35	a	30	0	43	12	0
36	M	41	0	54	6	0
37	1	126	0	165	16	0
37	3	84	0	110	9	0
37	4	84	0	110	9	0
37	5	126	0	165	20	0
37	6	84	0	110	29	0
37	7	42	0	55	4	0
37	8	84	0	110	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	a	126	0	165	14	0
38	1	114	0	102	13	0
38	3	98	0	73	8	0
38	4	174	0	154	21	0
38	5	173	0	153	16	0
38	6	224	0	188	52	0
38	7	66	0	70	5	0
38	8	174	0	153	20	0
38	a	203	0	148	26	0
39	1	20	0	33	2	0
39	8	20	0	33	4	0
40	3	19	0	0	0	0
40	a	19	0	0	1	0
41	a	9	0	0	1	0
42	4	17	0	31	1	0
42	6	18	0	31	1	0
43	5	23	0	28	3	0
43	8	30	0	42	5	0
44	6	21	0	37	7	0
45	7	44	0	56	5	0
46	7	32	0	39	6	0
46	8	96	0	142	15	0
47	7	42	0	0	3	0
48	8	37	0	40	1	0
All	All	48636	0	48687	2256	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 23.

The worst 5 of 2256 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)
33:G:5002:ERG:O1	33:G:5002:ERG:C3	1.70	1.40
5:E:79:LYS:NZ	5:E:79:LYS:CE	1.93	1.29
21:B:1201:CLA:H72	11:I:29:TYR:CE2	1.77	1.17
17:6:135:ARG:NE	38:6:611:CHL:OMC	1.78	1.14
7:G:1317:SER:HA	33:G:5002:ERG:H7	1.13	1.11

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%)	702 (95%)	36 (5%)	1 (0%)	48	82
2	B	729/731 (100%)	682 (94%)	47 (6%)	0	100	100
3	C	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
4	D	141/143 (99%)	131 (93%)	10 (7%)	0	100	100
5	E	62/64 (97%)	56 (90%)	6 (10%)	0	100	100
6	F	163/165 (99%)	150 (92%)	13 (8%)	0	100	100
7	G	97/99 (98%)	92 (95%)	4 (4%)	1 (1%)	12	47
8	J	39/41 (95%)	39 (100%)	0	0	100	100
9	K	84/86 (98%)	78 (93%)	6 (7%)	0	100	100
10	M	29/31 (94%)	29 (100%)	0	0	100	100
11	I	33/35 (94%)	31 (94%)	2 (6%)	0	100	100
12	L	136/157 (87%)	129 (95%)	7 (5%)	0	100	100
13	1	190/192 (99%)	167 (88%)	22 (12%)	1 (0%)	24	62
13	a	190/192 (99%)	164 (86%)	25 (13%)	1 (0%)	24	62
14	3	239/241 (99%)	219 (92%)	19 (8%)	1 (0%)	30	66
15	4	205/207 (99%)	188 (92%)	16 (8%)	1 (0%)	24	62
16	5	225/227 (99%)	201 (89%)	23 (10%)	1 (0%)	30	66
17	6	229/231 (99%)	208 (91%)	19 (8%)	2 (1%)	14	49
18	7	219/221 (99%)	198 (90%)	20 (9%)	1 (0%)	24	62
19	8	217/219 (99%)	194 (89%)	21 (10%)	2 (1%)	14	49
All	All	4044/4103 (99%)	3732 (92%)	300 (7%)	12 (0%)	37	71

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	1	36	TRP

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Mol	Chain	Res	Type
17	6	46	PRO
18	7	131	PRO
19	8	45	ASP
13	a	107	VAL

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%)	70 (99%)	1 (1%)	59	70
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	L	108/122 (88%)	108 (100%)	0	100	100
13	1	134/134 (100%)	134 (100%)	0	100	100
13	a	134/134 (100%)	134 (100%)	0	100	100
14	3	186/186 (100%)	186 (100%)	0	100	100
15	4	165/165 (100%)	165 (100%)	0	100	100
16	5	183/183 (100%)	183 (100%)	0	100	100
17	6	187/187 (100%)	187 (100%)	0	100	100
18	7	176/176 (100%)	176 (100%)	0	100	100
19	8	168/168 (100%)	168 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3225/3239 (100%)	3224 (100%)	1 (0%)	100 100

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

Mol	Chain	Res	Type
7	G	1307	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
16	5	114	GLN
19	8	197	ASN
16	5	117	ASN
16	5	225	ASN
2	B	422	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

337 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	8	620	19	69,73,73	1.36	7 (10%)	83,113,113	1.91	18 (21%)
24	LHG	4	801	21	48,48,48	0.40	0	51,54,54	1.07	3 (5%)
24	LHG	4	802	-	31,31,48	0.45	0	34,37,54	1.16	2 (5%)
28	LMT	A	5008	-	36,36,36	1.12	5 (13%)	47,47,47	1.04	3 (6%)
21	CLA	B	1206	2	59,63,73	1.52	7 (11%)	71,101,113	2.09	17 (23%)
21	CLA	A	1123	-	69,73,73	1.37	7 (10%)	83,113,113	1.96	19 (22%)
21	CLA	7	606	-	59,63,73	1.48	6 (10%)	71,101,113	2.02	19 (26%)
23	BCR	6	503	-	41,41,41	1.89	5 (12%)	56,56,56	4.32	15 (26%)
38	CHL	6	611	-	55,59,74	0.95	2 (3%)	62,96,114	1.48	11 (17%)
38	CHL	a	609	13	57,61,74	0.96	3 (5%)	64,98,114	1.40	12 (18%)
21	CLA	A	1137	1	64,68,73	1.41	6 (9%)	77,107,113	2.00	22 (28%)
21	CLA	B	1204	2	69,73,73	1.40	6 (8%)	83,113,113	1.98	19 (22%)
21	CLA	4	605	-	50,54,73	1.59	6 (12%)	60,90,113	2.17	19 (31%)
21	CLA	7	612	-	64,68,73	1.49	8 (12%)	77,107,113	2.00	18 (23%)
38	CHL	4	613	-	56,60,74	0.99	2 (3%)	63,97,114	1.54	12 (19%)
21	CLA	6	605	-	50,54,73	1.59	7 (14%)	60,90,113	2.11	16 (26%)
21	CLA	5	606	-	54,58,73	1.55	6 (11%)	65,95,113	2.15	20 (30%)
21	CLA	1	615	13	50,54,73	1.60	6 (12%)	60,90,113	2.05	15 (25%)
38	CHL	6	619	17	70,74,74	0.90	3 (4%)	80,114,114	1.25	11 (13%)
21	CLA	A	1127	1	69,73,73	1.39	6 (8%)	83,113,113	1.86	16 (19%)
37	LUT	8	501	-	42,43,43	2.37	2 (4%)	51,60,60	1.83	14 (27%)
21	CLA	a	604	13	69,73,73	1.36	7 (10%)	83,113,113	2.02	21 (25%)
21	CLA	A	1108	1	69,73,73	1.38	6 (8%)	83,113,113	2.05	17 (20%)
42	PLM	4	803	-	16,16,17	0.44	0	15,15,17	0.69	0
37	LUT	a	501	-	42,43,43	2.36	1 (2%)	51,60,60	2.24	16 (31%)
21	CLA	6	601	-	64,68,73	1.42	6 (9%)	77,107,113	2.07	19 (24%)
21	CLA	6	604	-	69,73,73	1.38	6 (8%)	83,113,113	2.08	23 (27%)
21	CLA	1	602	-	49,53,73	1.61	6 (12%)	59,89,113	2.05	14 (23%)
24	LHG	B	5001	21	45,45,48	0.41	0	48,51,54	1.05	3 (6%)
38	CHL	6	610	-	60,64,74	0.90	3 (5%)	68,102,114	1.37	11 (16%)
23	BCR	K	4002	-	41,41,41	1.88	5 (12%)	56,56,56	4.14	15 (26%)
21	CLA	3	610	14	64,68,73	1.42	6 (9%)	77,107,113	1.98	18 (23%)
21	CLA	4	610	-	69,73,73	1.39	7 (10%)	83,113,113	1.97	19 (22%)
21	CLA	8	606	-	61,65,73	1.46	6 (9%)	73,103,113	2.13	19 (26%)
37	LUT	a	502	-	42,43,43	2.37	2 (4%)	51,60,60	1.99	14 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	DGD	A	5005	-	52,52,67	0.92	4 (7%)	66,66,81	1.13	5 (7%)
23	BCR	7	503	-	41,41,41	1.83	5 (12%)	56,56,56	4.31	13 (23%)
21	CLA	a	602	-	54,58,73	1.56	7 (12%)	65,95,113	2.12	18 (27%)
21	CLA	G	1602	-	50,54,73	1.61	7 (14%)	60,90,113	2.02	16 (26%)
21	CLA	6	607	24	59,63,73	1.49	7 (11%)	71,101,113	2.00	17 (23%)
21	CLA	B	1224	2	69,73,73	1.38	7 (10%)	83,113,113	1.93	18 (21%)
21	CLA	8	615	-	50,54,73	1.61	6 (12%)	60,90,113	2.08	17 (28%)
21	CLA	B	1231	2	69,73,73	1.37	6 (8%)	83,113,113	1.96	18 (21%)
21	CLA	B	1207	2	64,68,73	1.43	6 (9%)	77,107,113	1.98	19 (24%)
21	CLA	4	615	15	64,68,73	1.43	6 (9%)	77,107,113	1.99	20 (25%)
21	CLA	7	617	18	58,62,73	1.50	6 (10%)	70,100,113	2.10	18 (25%)
46	4RF	8	808	-	53,53,56	0.90	5 (9%)	56,56,59	1.04	3 (5%)
23	BCR	G	4001	-	41,41,41	1.86	4 (9%)	56,56,56	4.29	19 (33%)
23	BCR	A	4002	-	41,41,41	1.85	6 (14%)	56,56,56	4.31	16 (28%)
21	CLA	B	1217	2	60,64,73	1.45	6 (10%)	72,102,113	2.06	17 (23%)
40	QTB	3	506	-	19,19,19	2.67	6 (31%)	20,26,26	2.78	8 (40%)
38	CHL	a	606	-	60,64,74	0.91	2 (3%)	68,102,114	1.32	12 (17%)
21	CLA	A	1103	-	69,73,73	1.35	6 (8%)	83,113,113	2.02	20 (24%)
21	CLA	1	604	-	69,73,73	1.41	7 (10%)	83,113,113	1.94	19 (22%)
21	CLA	A	1120	-	53,57,73	1.54	7 (13%)	62,93,113	2.27	19 (30%)
25	DGD	8	802	-	67,67,67	1.18	7 (10%)	81,81,81	1.11	5 (6%)
21	CLA	B	1210	-	69,73,73	1.40	6 (8%)	83,113,113	2.09	17 (20%)
21	CLA	3	616	-	60,64,73	1.47	6 (10%)	72,102,113	2.00	19 (26%)
21	CLA	8	602	19	56,60,73	1.54	6 (10%)	67,97,113	2.07	18 (26%)
21	CLA	4	602	15	56,60,73	1.50	6 (10%)	67,97,113	2.13	20 (29%)
23	BCR	3	503	-	41,41,41	1.88	6 (14%)	56,56,56	4.07	18 (32%)
21	CLA	B	1208	2	64,68,73	1.43	6 (9%)	77,107,113	2.05	21 (27%)
21	CLA	4	608	15	55,59,73	1.53	7 (12%)	66,96,113	2.17	20 (30%)
37	LUT	7	501	-	42,43,43	2.37	2 (4%)	51,60,60	1.97	15 (29%)
21	CLA	7	609	-	64,68,73	1.41	6 (9%)	77,107,113	2.05	20 (25%)
21	CLA	6	612	-	54,58,73	1.54	6 (11%)	65,95,113	2.23	19 (29%)
33	ERG	G	5002	-	31,32,32	8.20	18 (58%)	47,50,50	3.19	21 (44%)
21	CLA	A	1134	1	64,68,73	1.41	6 (9%)	77,107,113	2.01	19 (24%)
22	PQN	A	2001	-	34,34,34	0.34	0	42,45,45	1.27	4 (9%)
21	CLA	A	1129	-	54,58,73	1.56	6 (11%)	65,95,113	2.19	18 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	B	1223	2	69,73,73	1.37	7 (10%)	83,113,113	1.96	19 (22%)
21	CLA	B	1220	-	64,68,73	1.44	6 (9%)	77,107,113	2.05	17 (22%)
23	BCR	A	4001	-	41,41,41	1.79	5 (12%)	56,56,56	4.02	18 (32%)
23	BCR	L	4003	-	41,41,41	1.88	4 (9%)	56,56,56	4.35	15 (26%)
21	CLA	a	608	13	59,63,73	1.47	7 (11%)	71,101,113	1.97	17 (23%)
21	CLA	5	608	-	49,53,73	1.62	7 (14%)	59,89,113	2.09	16 (27%)
24	LHG	F	5002	-	35,35,48	0.45	0	38,41,54	1.22	4 (10%)
30	PTY	7	804	-	32,32,49	1.06	4 (12%)	35,37,54	1.20	2 (5%)
21	CLA	1	603	-	69,73,73	1.33	6 (8%)	83,113,113	1.94	19 (22%)
46	4RF	8	807	-	41,41,56	1.00	6 (14%)	44,44,59	1.08	3 (6%)
24	LHG	6	801	21	48,48,48	0.40	0	51,54,54	1.12	3 (5%)
23	BCR	A	4003	-	41,41,41	1.85	5 (12%)	56,56,56	4.32	16 (28%)
23	BCR	L	4001	-	41,41,41	1.87	4 (9%)	56,56,56	4.26	18 (32%)
38	CHL	3	608	-	47,51,74	1.00	2 (4%)	52,86,114	1.48	10 (19%)
21	CLA	1	610	-	49,53,73	1.63	6 (12%)	59,89,113	2.04	14 (23%)
21	CLA	3	605	-	69,73,73	1.38	6 (8%)	83,113,113	2.02	19 (22%)
23	BCR	B	4002	-	41,41,41	1.86	4 (9%)	56,56,56	4.35	13 (23%)
21	CLA	A	1141	24	49,53,73	1.61	7 (14%)	59,89,113	2.09	14 (23%)
39	OLA	1	803	-	19,19,19	0.56	0	19,19,19	1.06	1 (5%)
23	BCR	B	4001	-	41,41,41	1.85	5 (12%)	56,56,56	4.28	16 (28%)
37	LUT	3	501	-	42,43,43	2.35	1 (2%)	51,60,60	2.08	15 (29%)
24	LHG	8	801	21	36,36,48	0.46	0	39,42,54	1.22	4 (10%)
21	CLA	A	1107	1	59,63,73	1.51	7 (11%)	71,101,113	2.08	18 (25%)
21	CLA	A	1126	1	69,73,73	1.41	6 (8%)	83,113,113	1.94	16 (19%)
21	CLA	5	601	16	64,68,73	1.41	6 (9%)	77,107,113	2.03	22 (28%)
21	CLA	7	608	18	46,50,73	1.66	6 (13%)	55,85,113	2.19	14 (25%)
21	CLA	B	1201	2	69,73,73	1.37	7 (10%)	83,113,113	1.99	23 (27%)
21	CLA	K	1401	-	50,54,73	1.60	7 (14%)	60,90,113	2.00	14 (23%)
37	LUT	5	505	-	42,43,43	2.42	2 (4%)	51,60,60	2.72	19 (37%)
21	CLA	B	1218	2	59,63,73	1.48	7 (11%)	71,101,113	2.16	20 (28%)
36	ECH	M	4001	-	42,42,42	1.19	3 (7%)	55,58,58	2.03	15 (27%)
21	CLA	1	608	13	64,68,73	1.43	7 (10%)	77,107,113	1.97	18 (23%)
23	BCR	6	504	-	41,41,41	1.86	6 (14%)	56,56,56	4.27	20 (35%)
22	PQN	B	2002	-	34,34,34	0.41	0	42,45,45	1.28	4 (9%)
21	CLA	a	601	13	64,68,73	1.42	6 (9%)	77,107,113	1.98	19 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	LHG	3	801	21	48,48,48	0.40	0	51,54,54	1.05	3 (5%)
30	PTY	5	802	-	37,37,49	0.98	4 (10%)	40,42,54	1.18	2 (5%)
21	CLA	A	1013	-	69,73,73	1.38	6 (8%)	83,113,113	1.92	20 (24%)
21	CLA	B	1023	-	69,73,73	1.37	6 (8%)	83,113,113	1.94	17 (20%)
38	CHL	4	618	15	60,64,74	0.97	3 (5%)	68,102,114	1.41	12 (17%)
23	BCR	5	504	-	41,41,41	1.85	6 (14%)	56,56,56	4.18	18 (32%)
24	LHG	B	5002	-	48,48,48	0.41	0	51,54,54	0.96	3 (5%)
21	CLA	6	606	-	56,60,73	1.50	6 (10%)	67,97,113	2.09	19 (28%)
21	CLA	6	617	17	49,53,73	1.58	6 (12%)	59,89,113	2.07	17 (28%)
21	CLA	8	603	19	69,73,73	1.38	7 (10%)	83,113,113	2.08	21 (25%)
21	CLA	4	603	15	60,64,73	1.45	6 (10%)	72,102,113	2.10	19 (26%)
24	LHG	7	802	-	35,35,48	0.45	0	38,41,54	1.15	3 (7%)
21	CLA	7	601	-	64,68,73	1.45	6 (9%)	77,107,113	1.97	20 (25%)
21	CLA	L	1502	12	64,68,73	1.42	7 (10%)	77,107,113	2.09	19 (24%)
21	CLA	A	1106	1	69,73,73	1.35	6 (8%)	83,113,113	2.02	17 (20%)
42	PLM	6	804	-	17,17,17	0.56	0	17,17,17	1.12	0
21	CLA	3	602	14	50,54,73	1.60	7 (14%)	60,90,113	2.10	16 (26%)
21	CLA	3	606	-	69,73,73	1.39	6 (8%)	83,113,113	1.92	17 (20%)
37	LUT	3	502	-	42,43,43	2.36	1 (2%)	51,60,60	2.01	12 (23%)
21	CLA	3	612	-	69,73,73	1.39	6 (8%)	83,113,113	1.86	15 (18%)
21	CLA	8	610	-	59,63,73	1.49	6 (10%)	71,101,113	2.05	18 (25%)
24	LHG	F	5001	21	42,42,48	0.42	0	45,48,54	1.13	3 (6%)
21	CLA	B	1205	-	69,73,73	1.36	6 (8%)	83,113,113	2.04	18 (21%)
37	LUT	1	501	-	42,43,43	2.40	1 (2%)	51,60,60	2.02	17 (33%)
21	CLA	a	615	13	50,54,73	1.59	6 (12%)	60,90,113	2.00	15 (25%)
24	LHG	1	802	-	41,41,48	0.42	0	44,47,54	1.07	4 (9%)
21	CLA	A	1140	-	59,63,73	1.48	8 (13%)	71,101,113	2.02	16 (22%)
38	CHL	a	613	-	50,54,74	0.92	2 (4%)	56,90,114	1.49	11 (19%)
21	CLA	7	605	18	47,52,73	1.69	6 (12%)	56,88,113	2.05	13 (23%)
21	CLA	B	1226	2	69,73,73	1.38	6 (8%)	83,113,113	1.90	14 (16%)
21	CLA	B	1237	-	69,73,73	1.38	6 (8%)	83,113,113	1.96	20 (24%)
21	CLA	B	1212	2	69,73,73	1.39	7 (10%)	83,113,113	2.04	21 (25%)
21	CLA	1	611	-	59,63,73	1.49	7 (11%)	71,101,113	2.02	20 (28%)
37	LUT	a	503	-	42,43,43	2.38	1 (2%)	51,60,60	2.19	15 (29%)
48	P5S	8	806	-	35,36,53	1.17	3 (8%)	39,43,60	1.18	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	A	1132	-	69,73,73	1.36	6 (8%)	83,113,113	2.01	20 (24%)
21	CLA	3	607	24	69,73,73	1.36	6 (8%)	83,113,113	1.95	16 (19%)
23	BCR	B	4003	-	41,41,41	1.84	5 (12%)	56,56,56	4.49	18 (32%)
23	BCR	3	504	-	41,41,41	1.85	4 (9%)	56,56,56	4.26	15 (26%)
24	LHG	A	5002	-	48,48,48	0.39	0	51,54,54	1.04	3 (5%)
31	LAP	F	5003	-	28,28,28	1.24	3 (10%)	33,35,35	0.93	1 (3%)
21	CLA	A	1135	1	69,73,73	1.36	6 (8%)	83,113,113	1.92	20 (24%)
21	CLA	B	1222	-	62,66,73	1.47	6 (9%)	74,104,113	2.03	17 (22%)
21	CLA	B	1230	2	62,66,73	1.44	6 (9%)	74,104,113	2.11	20 (27%)
38	CHL	5	613	-	60,64,74	0.90	2 (3%)	68,102,114	1.34	10 (14%)
21	CLA	A	1139	1	59,63,73	1.51	6 (10%)	71,101,113	2.03	19 (26%)
21	CLA	A	1133	1	69,73,73	1.36	6 (8%)	83,113,113	1.92	18 (21%)
21	CLA	4	616	-	54,58,73	1.54	7 (12%)	65,95,113	2.16	18 (27%)
21	CLA	8	609	19	64,68,73	1.42	6 (9%)	77,107,113	2.02	17 (22%)
23	BCR	A	4004	-	41,41,41	1.93	6 (14%)	56,56,56	4.50	15 (26%)
21	CLA	B	1229	-	69,73,73	1.36	6 (8%)	83,113,113	1.95	20 (24%)
21	CLA	8	608	19	56,60,73	1.53	6 (10%)	67,97,113	2.29	21 (31%)
32	SQD	G	5001	-	45,46,54	0.82	0	54,57,65	0.95	2 (3%)
38	CHL	3	611	-	59,63,74	0.96	3 (5%)	66,100,114	1.51	12 (18%)
23	BCR	L	4002	-	41,41,41	1.81	4 (9%)	56,56,56	4.41	17 (30%)
37	LUT	1	502	-	42,43,43	2.28	1 (2%)	51,60,60	2.05	16 (31%)
38	CHL	5	611	-	55,59,74	1.00	4 (7%)	62,96,114	1.47	12 (19%)
21	CLA	5	609	16	55,59,73	1.55	7 (12%)	66,96,113	2.14	18 (27%)
32	SQD	7	805	-	38,39,54	0.90	0	47,50,65	1.01	3 (6%)
27	SF4	C	3002	3	0,12,12	-	-	-	-	-
29	PCW	6	803	-	35,35,53	1.28	4 (11%)	41,43,61	1.13	2 (4%)
24	LHG	7	801	21	48,48,48	0.37	0	51,54,54	1.23	4 (7%)
21	CLA	7	615	18	59,63,73	1.46	6 (10%)	71,101,113	1.98	17 (23%)
41	GG0	a	805	-	7,8,8	1.37	2 (28%)	6,9,9	0.80	0
38	CHL	6	613	-	55,59,74	0.90	2 (3%)	62,96,114	1.38	11 (17%)
43	DGA	5	803	-	22,22,43	1.43	3 (13%)	24,24,45	1.38	2 (8%)
30	PTY	B	5005	-	40,40,49	0.94	4 (10%)	43,45,54	1.17	2 (4%)
21	CLA	4	606	-	54,58,73	1.53	6 (11%)	65,95,113	2.14	18 (27%)
47	C7Z	7	504	-	43,43,43	5.33	27 (62%)	58,60,60	2.76	26 (44%)
21	CLA	4	617	-	49,53,73	1.61	6 (12%)	59,89,113	2.11	17 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	G	1603	-	49,53,73	1.60	7 (14%)	59,89,113	2.01	14 (23%)
21	CLA	K	1403	9	50,54,73	1.61	7 (14%)	60,90,113	2.06	13 (21%)
39	OLA	8	809	-	19,19,19	0.56	0	19,19,19	1.07	0
21	CLA	8	605	-	49,53,73	1.65	6 (12%)	59,89,113	2.03	15 (25%)
21	CLA	B	1238	-	69,73,73	1.37	6 (8%)	83,113,113	1.93	17 (20%)
26	3PH	A	5007	-	32,32,47	1.01	4 (12%)	36,37,52	1.20	2 (5%)
28	LMT	1	804	-	36,36,36	1.18	6 (16%)	47,47,47	1.05	1 (2%)
21	CLA	A	1113	1	56,60,73	1.52	6 (10%)	67,97,113	2.15	19 (28%)
21	CLA	6	602	17	56,60,73	1.50	7 (12%)	67,97,113	2.15	19 (28%)
21	CLA	L	1503	-	49,53,73	1.65	8 (16%)	59,89,113	2.19	20 (33%)
21	CLA	8	611	-	54,58,73	1.53	6 (11%)	65,95,113	2.21	17 (26%)
21	CLA	6	615	-	69,73,73	1.38	7 (10%)	83,113,113	1.92	19 (22%)
21	CLA	4	611	-	60,64,73	1.45	6 (10%)	72,102,113	2.04	19 (26%)
24	LHG	a	801	-	34,34,48	0.47	0	37,40,54	1.31	5 (13%)
21	CLA	K	1402	-	64,68,73	1.40	7 (10%)	77,107,113	2.03	20 (25%)
38	CHL	4	609	15	70,74,74	0.86	2 (2%)	80,114,114	1.42	13 (16%)
24	LHG	7	803	-	42,42,48	0.39	0	45,48,54	1.07	2 (4%)
21	CLA	A	1124	-	59,63,73	1.52	6 (10%)	71,101,113	2.00	17 (23%)
21	CLA	1	606	-	61,65,73	1.47	7 (11%)	73,103,113	2.04	18 (24%)
23	BCR	K	4001	-	41,41,41	1.86	4 (9%)	56,56,56	4.34	17 (30%)
21	CLA	B	1232	-	49,53,73	1.63	7 (14%)	59,89,113	2.01	13 (22%)
23	BCR	I	4001	-	41,41,41	1.84	4 (9%)	56,56,56	4.21	17 (30%)
38	CHL	8	613	-	55,59,74	1.00	3 (5%)	62,96,114	1.49	10 (16%)
29	PCW	B	5004	-	29,29,53	1.32	3 (10%)	35,37,61	0.95	1 (2%)
31	LAP	K	5001	-	28,28,28	1.26	3 (10%)	33,35,35	1.06	2 (6%)
38	CHL	7	613	-	70,74,74	0.88	2 (2%)	80,114,114	1.31	14 (17%)
21	CLA	B	1215	2	64,68,73	1.42	6 (9%)	77,107,113	1.90	18 (23%)
21	CLA	3	604	-	64,68,73	1.42	6 (9%)	77,107,113	2.05	21 (27%)
21	CLA	5	616	-	50,54,73	1.61	7 (14%)	60,90,113	2.05	15 (25%)
21	CLA	4	604	15	64,68,73	1.45	7 (10%)	77,107,113	1.95	18 (23%)
21	CLA	a	603	-	69,73,73	1.38	6 (8%)	83,113,113	1.99	20 (24%)
21	CLA	7	610	-	59,63,73	1.47	6 (10%)	71,101,113	2.01	20 (28%)
21	CLA	5	618	16	56,60,73	1.52	7 (12%)	67,97,113	2.07	21 (31%)
23	BCR	5	503	-	41,41,41	1.85	5 (12%)	56,56,56	4.32	18 (32%)
21	CLA	A	1114	-	69,73,73	1.38	6 (8%)	83,113,113	2.00	22 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	DGA	8	803	-	29,29,43	1.25	2 (6%)	31,31,45	1.16	2 (6%)
21	CLA	4	607	24	59,63,73	1.48	7 (11%)	71,101,113	2.05	17 (23%)
44	SPH	6	806	-	19,20,20	0.61	0	18,21,21	1.13	1 (5%)
21	CLA	B	1236	2	57,61,73	1.54	6 (10%)	68,98,113	2.29	21 (30%)
21	CLA	5	604	-	69,73,73	1.38	6 (8%)	83,113,113	1.97	20 (24%)
21	CLA	1	605	-	69,73,73	1.36	6 (8%)	83,113,113	2.04	20 (24%)
21	CLA	J	1901	8	46,50,73	1.63	6 (13%)	55,85,113	2.15	15 (27%)
21	CLA	4	601	-	64,68,73	1.44	5 (7%)	77,107,113	2.01	18 (23%)
21	CLA	A	1122	-	69,73,73	1.38	7 (10%)	83,113,113	1.90	16 (19%)
21	CLA	5	602	16	56,60,73	1.52	6 (10%)	67,97,113	2.15	19 (28%)
21	CLA	5	614	-	50,54,73	1.58	7 (14%)	60,90,113	2.08	14 (23%)
21	CLA	6	608	-	49,53,73	1.61	6 (12%)	59,89,113	2.10	17 (28%)
23	BCR	B	4006	-	41,41,41	1.81	5 (12%)	56,56,56	4.34	15 (26%)
21	CLA	A	1102	21,1	69,73,73	1.40	6 (8%)	83,113,113	2.19	18 (21%)
21	CLA	5	605	-	50,54,73	1.64	6 (12%)	60,90,113	2.06	17 (28%)
23	BCR	B	4007	-	41,41,41	1.84	5 (12%)	56,56,56	4.14	16 (28%)
21	CLA	A	1128	1	69,73,73	1.40	6 (8%)	83,113,113	1.96	19 (22%)
21	CLA	4	612	15	66,70,73	1.39	8 (12%)	79,109,113	2.05	19 (24%)
21	CLA	A	1109	21,1	69,73,73	1.34	7 (10%)	83,113,113	2.10	21 (25%)
21	CLA	A	1119	-	69,73,73	1.38	6 (8%)	83,113,113	1.76	16 (19%)
21	CLA	7	603	18	69,73,73	1.38	6 (8%)	83,113,113	1.94	17 (20%)
34	RRX	J	4002	-	42,42,42	4.86	24 (57%)	57,58,58	2.45	20 (35%)
21	CLA	A	1130	1	60,64,73	1.44	6 (10%)	72,102,113	2.03	18 (25%)
21	CLA	6	603	-	69,73,73	1.40	7 (10%)	83,113,113	2.01	18 (21%)
21	CLA	A	1138	1	69,73,73	1.39	7 (10%)	83,113,113	2.02	18 (21%)
21	CLA	B	1221	-	69,73,73	1.39	8 (11%)	83,113,113	1.98	17 (20%)
21	CLA	B	1203	-	69,73,73	1.36	6 (8%)	83,113,113	1.93	17 (20%)
38	CHL	5	610	-	70,74,74	0.85	2 (2%)	80,114,114	1.29	13 (16%)
21	CLA	B	1022	-	69,73,73	1.40	6 (8%)	83,113,113	1.89	18 (21%)
21	CLA	5	607	24	59,63,73	1.49	6 (10%)	71,101,113	1.97	17 (23%)
21	CLA	A	1116	-	64,68,73	1.45	6 (9%)	77,107,113	2.06	19 (24%)
30	PTY	8	810	-	34,34,49	1.02	3 (8%)	37,39,54	1.33	3 (8%)
38	CHL	8	604	19	66,70,74	0.94	3 (4%)	75,109,114	1.36	10 (13%)
35	LPX	a	804	-	29,29,29	1.01	2 (6%)	31,33,33	0.92	1 (3%)
21	CLA	A	1012	-	69,73,73	1.39	6 (8%)	83,113,113	1.88	16 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	6	618	-	50,54,73	1.59	6 (12%)	60,90,113	2.13	15 (25%)
21	CLA	A	1118	1	59,63,73	1.48	6 (10%)	71,101,113	2.11	17 (23%)
46	4RF	7	807	-	31,31,56	1.16	6 (19%)	34,34,59	1.17	3 (8%)
21	CLA	F	1301	6	54,58,73	1.54	6 (11%)	65,95,113	2.24	19 (29%)
21	CLA	B	1227	2	54,58,73	1.56	6 (11%)	65,95,113	2.13	19 (29%)
21	CLA	B	1239	2	69,73,73	1.39	6 (8%)	83,113,113	1.92	18 (21%)
21	CLA	a	611	-	54,58,73	1.55	6 (11%)	65,95,113	2.12	19 (29%)
23	BCR	3	505	-	41,41,41	1.89	4 (9%)	56,56,56	4.12	17 (30%)
21	CLA	B	1234	2	60,64,73	1.50	6 (10%)	72,102,113	2.23	19 (26%)
21	CLA	8	618	-	64,68,73	1.42	6 (9%)	77,107,113	2.03	19 (24%)
21	CLA	B	1202	2	69,73,73	1.36	6 (8%)	83,113,113	1.96	17 (20%)
23	BCR	8	503	-	41,41,41	1.88	4 (9%)	56,56,56	4.25	17 (30%)
38	CHL	a	610	-	52,56,74	0.90	2 (3%)	58,92,114	1.44	12 (20%)
24	LHG	5	801	21	48,48,48	0.39	0	51,54,54	1.04	3 (5%)
38	CHL	8	601	19	65,69,74	0.97	4 (6%)	74,108,114	1.37	11 (14%)
21	CLA	F	1302	24	59,63,73	1.49	6 (10%)	71,101,113	2.17	20 (28%)
24	LHG	A	5003	-	41,41,48	0.43	0	44,47,54	1.16	3 (6%)
21	CLA	A	1105	-	61,65,73	1.47	7 (11%)	73,103,113	2.08	21 (28%)
31	LAP	B	5007	-	28,28,28	1.21	3 (10%)	33,35,35	0.96	1 (3%)
21	CLA	B	1214	2	66,70,73	1.41	6 (9%)	79,109,113	1.92	18 (22%)
35	LPX	J	5001	-	16,16,29	1.32	2 (12%)	18,20,33	1.06	2 (11%)
25	DGD	B	5003	-	67,67,67	1.18	7 (10%)	81,81,81	1.08	4 (4%)
23	BCR	F	4001	-	41,41,41	1.89	5 (12%)	56,56,56	3.99	16 (28%)
21	CLA	A	1111	-	69,73,73	1.40	6 (8%)	83,113,113	1.92	20 (24%)
21	CLA	3	603	-	69,73,73	1.38	7 (10%)	83,113,113	1.92	16 (19%)
21	CLA	B	1240	24	69,73,73	1.39	6 (8%)	83,113,113	1.97	18 (21%)
21	CLA	A	1101	1	69,73,73	1.39	6 (8%)	83,113,113	2.03	19 (22%)
21	CLA	B	1216	-	65,69,73	1.41	6 (9%)	78,108,113	1.91	18 (23%)
28	LMT	B	5006	-	36,36,36	1.18	5 (13%)	47,47,47	1.01	2 (4%)
21	CLA	3	613	-	65,69,73	1.43	6 (9%)	78,108,113	1.93	16 (20%)
37	LUT	5	502	-	42,43,43	2.35	2 (4%)	51,60,60	2.05	13 (25%)
21	CLA	A	1121	1	61,65,73	1.48	7 (11%)	73,103,113	2.17	19 (26%)
21	CLA	1	607	-	69,73,73	1.37	6 (8%)	83,113,113	1.92	18 (21%)
21	CLA	L	1501	-	54,58,73	1.53	6 (11%)	65,95,113	2.29	20 (30%)
37	LUT	4	501	-	42,43,43	2.28	1 (2%)	51,60,60	1.94	15 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	7	611	-	64,68,73	1.40	6 (9%)	77,107,113	2.12	22 (28%)
23	BCR	4	503	-	41,41,41	1.86	5 (12%)	56,56,56	4.38	12 (21%)
21	CLA	a	605	-	69,73,73	1.36	6 (8%)	83,113,113	1.94	20 (24%)
37	LUT	6	501	-	42,43,43	2.36	1 (2%)	51,60,60	2.26	15 (29%)
37	LUT	8	502	-	42,43,43	2.33	1 (2%)	51,60,60	1.91	14 (27%)
21	CLA	a	612	13	61,65,73	1.48	5 (8%)	73,103,113	1.95	19 (26%)
21	CLA	7	602	-	48,52,73	1.64	6 (12%)	56,87,113	2.13	17 (30%)
21	CLA	5	612	16	69,73,73	1.37	6 (8%)	83,113,113	1.88	14 (16%)
21	CLA	B	1235	2	69,73,73	1.39	7 (10%)	83,113,113	1.98	17 (20%)
21	CLA	3	601	-	69,73,73	1.38	6 (8%)	83,113,113	1.96	17 (20%)
23	BCR	A	4005	-	41,41,41	1.85	6 (14%)	56,56,56	4.26	15 (26%)
21	CLA	B	1209	2	69,73,73	1.37	7 (10%)	83,113,113	2.04	21 (25%)
21	CLA	6	609	17	69,73,73	1.38	6 (8%)	83,113,113	1.92	16 (19%)
37	LUT	4	502	-	42,43,43	2.33	1 (2%)	51,60,60	1.92	12 (23%)
21	CLA	B	1225	2	69,73,73	1.39	6 (8%)	83,113,113	1.86	16 (19%)
40	QTB	a	504	-	19,19,19	2.62	5 (26%)	20,26,26	2.82	10 (50%)
21	CLA	A	1117	1	69,73,73	1.38	6 (8%)	83,113,113	1.91	15 (18%)
24	LHG	1	801	-	34,34,48	0.45	0	37,40,54	1.25	4 (10%)
27	SF4	C	3003	3	0,12,12	-	-	-	-	-
37	LUT	6	502	-	42,43,43	2.32	2 (4%)	51,60,60	2.29	13 (25%)
27	SF4	A	3001	2,1	0,12,12	-	-	-	-	-
21	CLA	A	1131	1	69,73,73	1.40	6 (8%)	83,113,113	1.92	17 (20%)
21	CLA	A	1104	-	69,73,73	1.36	6 (8%)	83,113,113	1.98	20 (24%)
37	LUT	1	503	-	42,43,43	2.41	1 (2%)	51,60,60	2.31	13 (25%)
21	CLA	1	601	13	64,68,73	1.42	7 (10%)	77,107,113	1.95	17 (22%)
21	CLA	a	607	-	62,66,73	1.44	7 (11%)	74,104,113	2.14	18 (24%)
21	CLA	A	1112	-	59,63,73	1.50	7 (11%)	71,101,113	2.14	18 (25%)
21	CLA	7	604	-	69,73,73	1.38	6 (8%)	83,113,113	1.94	22 (26%)
21	CLA	5	603	-	60,64,73	1.47	7 (11%)	72,102,113	2.08	17 (23%)
21	CLA	A	1125	1	69,73,73	1.44	8 (11%)	83,113,113	2.23	21 (25%)
21	CLA	1	612	13	69,73,73	1.36	6 (8%)	83,113,113	1.91	17 (20%)
21	CLA	K	1404	9	56,60,73	1.53	8 (14%)	67,97,113	2.15	20 (29%)
21	CLA	B	1219	-	63,67,73	1.46	6 (9%)	75,105,113	1.99	16 (21%)
24	LHG	6	802	-	36,36,48	0.43	0	39,42,54	1.17	3 (7%)
21	CLA	8	607	24	50,54,73	1.60	6 (12%)	60,90,113	2.01	12 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	CHL	1	609	13	70,74,74	0.97	4 (5%)	80,114,114	1.35	14 (17%)
45	XAT	7	502	-	39,47,47	0.78	1 (2%)	54,74,74	1.98	12 (22%)
21	CLA	A	1115	1	64,68,73	1.43	7 (10%)	77,107,113	2.03	19 (24%)
21	CLA	B	1021	-	69,73,73	1.40	6 (8%)	83,113,113	1.92	18 (21%)
21	CLA	A	1136	1	69,73,73	1.37	6 (8%)	83,113,113	1.92	17 (20%)
21	CLA	7	607	24	63,67,73	1.44	6 (9%)	75,105,113	1.98	16 (21%)
23	BCR	B	4005	-	41,41,41	1.89	6 (14%)	56,56,56	4.28	20 (35%)
21	CLA	B	1211	-	59,63,73	1.50	6 (10%)	71,101,113	2.03	18 (25%)
23	BCR	B	4004	-	41,41,41	1.85	4 (9%)	56,56,56	4.36	20 (35%)
21	CLA	G	1601	-	54,58,73	1.55	6 (11%)	65,95,113	2.17	19 (29%)
21	CLA	5	617	-	54,58,73	1.56	6 (11%)	65,95,113	2.26	19 (29%)
37	LUT	5	501	-	42,43,43	2.37	1 (2%)	51,60,60	2.03	15 (29%)
30	PTY	3	802	-	37,37,49	1.00	4 (10%)	40,42,54	1.09	2 (5%)
38	CHL	1	613	-	52,56,74	1.02	3 (5%)	58,92,114	1.33	10 (17%)
24	LHG	A	5001	21	28,28,48	0.51	0	31,34,54	1.34	3 (9%)
20	CL0	A	1011	1	69,73,73	2.31	19 (27%)	83,113,113	2.54	26 (31%)
21	CLA	B	1228	2	69,73,73	1.40	9 (13%)	83,113,113	2.78	24 (28%)
21	CLA	B	1213	2	64,68,73	1.45	7 (10%)	77,107,113	2.02	20 (25%)
23	BCR	J	4001	-	41,41,41	1.84	5 (12%)	56,56,56	4.37	16 (28%)
21	CLA	A	1110	1	64,68,73	1.44	7 (10%)	77,107,113	1.97	18 (23%)
21	CLA	8	612	19	50,54,73	1.61	6 (12%)	60,90,113	2.02	14 (23%)
21	CLA	3	618	-	50,54,73	1.63	7 (14%)	60,90,113	2.05	14 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	8	620	19	-	17/39/115/115	-
24	LHG	4	801	21	-	37/53/53/53	-
24	LHG	4	802	-	-	19/36/36/53	-
28	LMT	A	5008	-	-	7/21/61/61	0/2/2/2
21	CLA	B	1206	2	-	13/27/103/115	-
21	CLA	A	1123	-	-	15/39/115/115	-
21	CLA	7	606	-	-	9/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	6	503	-	-	14/29/63/63	0/2/2/2
38	CHL	6	611	-	-	3/23/99/117	-
38	CHL	a	609	13	-	4/26/102/117	-
21	CLA	A	1137	1	-	12/33/109/115	-
21	CLA	B	1204	2	-	27/39/115/115	-
21	CLA	4	605	-	-	6/17/93/115	-
21	CLA	7	612	-	-	19/33/109/115	-
38	CHL	4	613	-	-	7/25/101/117	-
21	CLA	6	605	-	-	7/17/93/115	-
21	CLA	5	606	-	-	9/21/97/115	-
21	CLA	1	615	13	-	10/17/93/115	-
38	CHL	6	619	17	2/2/15/21	18/41/117/117	-
21	CLA	A	1127	1	-	13/39/115/115	-
37	LUT	8	501	-	-	2/29/67/67	0/2/2/2
21	CLA	a	604	13	-	19/39/115/115	-
21	CLA	A	1108	1	-	17/39/115/115	-
42	PLM	4	803	-	-	8/13/14/15	-
37	LUT	a	501	-	-	7/29/67/67	0/2/2/2
21	CLA	6	601	-	-	14/33/109/115	-
21	CLA	6	604	-	-	21/39/115/115	-
38	CHL	6	610	-	1/1/13/21	6/29/105/117	-
21	CLA	1	602	-	-	7/15/91/115	-
24	LHG	B	5001	21	-	29/50/50/53	-
23	BCR	K	4002	-	-	12/29/63/63	0/2/2/2
21	CLA	3	610	14	-	15/33/109/115	-
21	CLA	4	610	-	-	21/39/115/115	-
37	LUT	a	502	-	1/1/12/27	11/29/67/67	0/2/2/2
21	CLA	8	606	-	-	14/30/106/115	-
25	DGD	A	5005	-	-	20/40/80/95	0/2/2/2
23	BCR	7	503	-	-	16/29/63/63	0/2/2/2
21	CLA	a	602	-	-	6/21/97/115	-
21	CLA	G	1602	-	-	9/17/93/115	-
21	CLA	6	607	24	-	9/27/103/115	-
21	CLA	8	615	-	-	8/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	1224	2	-	27/39/115/115	-
21	CLA	B	1231	2	-	17/39/115/115	-
21	CLA	B	1207	2	-	21/33/109/115	-
21	CLA	4	615	15	-	14/33/109/115	-
21	CLA	7	617	18	-	13/25/101/115	-
46	4RF	8	808	-	-	25/56/56/59	-
23	BCR	G	4001	-	-	10/29/63/63	0/2/2/2
23	BCR	A	4002	-	-	11/29/63/63	0/2/2/2
21	CLA	B	1217	2	-	15/29/105/115	-
40	QTB	3	506	-	2/2/5/10	3/11/28/28	0/1/1/1
38	CHL	a	606	-	1/1/13/21	8/29/105/117	-
21	CLA	A	1103	-	-	16/39/115/115	-
21	CLA	1	604	-	-	22/39/115/115	-
21	CLA	A	1120	-	-	11/20/96/115	-
25	DGD	8	802	-	-	26/55/95/95	0/2/2/2
21	CLA	B	1210	-	-	22/39/115/115	-
21	CLA	3	616	-	-	17/29/105/115	-
21	CLA	8	602	19	-	8/24/100/115	-
21	CLA	4	602	15	-	5/24/100/115	-
23	BCR	3	503	-	-	9/29/63/63	0/2/2/2
21	CLA	B	1208	2	-	11/33/109/115	-
21	CLA	4	608	15	-	9/23/99/115	-
37	LUT	7	501	-	1/1/12/27	6/29/67/67	0/2/2/2
21	CLA	7	609	-	-	16/33/109/115	-
21	CLA	6	612	-	-	14/21/97/115	-
33	ERG	G	5002	-	4/4/11/15	10/13/71/71	0/4/4/4
21	CLA	A	1134	1	-	21/33/109/115	-
22	PQN	A	2001	-	-	9/23/43/43	0/2/2/2
21	CLA	A	1129	-	-	14/21/97/115	-
21	CLA	B	1223	2	-	14/39/115/115	-
21	CLA	B	1220	-	-	19/33/109/115	-
23	BCR	A	4001	-	-	10/29/63/63	0/2/2/2
23	BCR	L	4003	-	-	9/29/63/63	0/2/2/2
21	CLA	a	608	13	-	13/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	5	608	-	-	6/15/91/115	-
24	LHG	F	5002	-	-	28/40/40/53	-
30	PTY	7	804	-	-	17/36/36/53	-
21	CLA	1	603	-	-	23/39/115/115	-
46	4RF	8	807	-	-	23/44/44/59	-
24	LHG	6	801	21	-	29/53/53/53	-
23	BCR	A	4003	-	-	11/29/63/63	0/2/2/2
23	BCR	L	4001	-	-	13/29/63/63	0/2/2/2
38	CHL	3	608	-	1/1/10/21	3/14/90/117	-
21	CLA	1	610	-	-	4/15/91/115	-
21	CLA	3	605	-	-	16/39/115/115	-
23	BCR	B	4002	-	-	13/29/63/63	0/2/2/2
21	CLA	A	1141	24	-	10/15/91/115	-
39	OLA	1	803	-	-	8/17/17/17	-
23	BCR	B	4001	-	-	15/29/63/63	0/2/2/2
37	LUT	3	501	-	-	2/29/67/67	0/2/2/2
24	LHG	8	801	21	-	27/41/41/53	-
21	CLA	A	1107	1	-	8/27/103/115	-
21	CLA	A	1126	1	-	25/39/115/115	-
21	CLA	5	601	16	-	13/33/109/115	-
21	CLA	7	608	18	-	9/12/88/115	-
21	CLA	B	1201	2	-	17/39/115/115	-
21	CLA	K	1401	-	-	9/17/93/115	-
37	LUT	5	505	-	1/1/12/27	9/29/67/67	0/2/2/2
21	CLA	B	1218	2	-	10/27/103/115	-
36	ECH	M	4001	-	-	9/29/66/66	0/2/2/2
21	CLA	1	608	13	-	16/33/109/115	-
23	BCR	6	504	-	-	9/29/63/63	0/2/2/2
22	PQN	B	2002	-	-	5/23/43/43	0/2/2/2
21	CLA	a	601	13	-	8/33/109/115	-
24	LHG	3	801	21	-	33/53/53/53	-
30	PTY	5	802	-	-	19/41/41/53	-
21	CLA	A	1013	-	-	15/39/115/115	-
21	CLA	B	1023	-	-	19/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	CHL	4	618	15	1/1/13/21	7/29/105/117	-
23	BCR	5	504	-	-	9/29/63/63	0/2/2/2
24	LHG	B	5002	-	-	37/53/53/53	-
21	CLA	6	606	-	-	12/24/100/115	-
21	CLA	6	617	17	-	4/15/91/115	-
21	CLA	8	603	19	-	22/39/115/115	-
21	CLA	4	603	15	-	15/29/105/115	-
24	LHG	7	802	-	-	23/40/40/53	-
21	CLA	7	601	-	-	17/33/109/115	-
21	CLA	L	1502	12	-	13/33/109/115	-
21	CLA	A	1106	1	-	20/39/115/115	-
42	PLM	6	804	-	-	6/15/15/15	-
21	CLA	3	602	14	-	8/17/93/115	-
21	CLA	3	606	-	-	12/39/115/115	-
37	LUT	3	502	-	-	2/29/67/67	0/2/2/2
21	CLA	3	612	-	-	15/39/115/115	-
21	CLA	8	610	-	-	15/27/103/115	-
24	LHG	F	5001	21	-	31/47/47/53	-
21	CLA	B	1205	-	-	16/39/115/115	-
37	LUT	1	501	-	-	3/29/67/67	0/2/2/2
21	CLA	a	615	13	-	5/17/93/115	-
24	LHG	1	802	-	-	29/46/46/53	-
21	CLA	A	1140	-	-	16/27/103/115	-
38	CHL	a	613	-	-	6/17/93/117	-
21	CLA	7	605	18	-	10/13/89/115	-
21	CLA	B	1226	2	-	14/39/115/115	-
21	CLA	B	1237	-	-	17/39/115/115	-
21	CLA	B	1212	2	-	23/39/115/115	-
21	CLA	1	611	-	-	13/27/103/115	-
37	LUT	a	503	-	-	4/29/67/67	0/2/2/2
48	P5S	8	806	-	-	31/42/42/59	-
21	CLA	A	1132	-	-	19/39/115/115	-
21	CLA	3	607	24	-	10/39/115/115	-
23	BCR	B	4003	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	3	504	-	-	12/29/63/63	0/2/2/2
24	LHG	A	5002	-	-	34/53/53/53	-
31	LAP	F	5003	-	-	20/30/30/30	-
21	CLA	A	1135	1	-	22/39/115/115	-
21	CLA	B	1222	-	-	5/31/107/115	-
21	CLA	B	1230	2	-	13/31/107/115	-
38	CHL	5	613	-	1/1/13/21	5/29/105/117	-
21	CLA	A	1139	1	-	15/27/103/115	-
21	CLA	A	1133	1	-	19/39/115/115	-
21	CLA	4	616	-	-	10/21/97/115	-
21	CLA	8	609	19	-	22/33/109/115	-
23	BCR	A	4004	-	-	12/29/63/63	0/2/2/2
21	CLA	B	1229	-	-	11/39/115/115	-
21	CLA	8	608	19	-	12/24/100/115	-
32	SQD	G	5001	-	-	21/41/61/69	0/1/1/1
38	CHL	3	611	-	-	4/28/104/117	-
23	BCR	L	4002	-	-	8/29/63/63	0/2/2/2
37	LUT	1	502	-	-	2/29/67/67	0/2/2/2
38	CHL	5	611	-	-	6/23/99/117	-
21	CLA	5	609	16	-	9/23/99/115	-
32	SQD	7	805	-	-	14/34/54/69	0/1/1/1
27	SF4	C	3002	3	-	-	0/6/5/5
29	PCW	6	803	-	-	19/39/39/57	-
24	LHG	7	801	21	-	27/53/53/53	-
21	CLA	7	615	18	-	15/27/103/115	-
41	GG0	a	805	-	-	2/7/7/7	-
38	CHL	6	613	-	-	2/23/99/117	-
43	DGA	5	803	-	-	13/24/24/45	-
30	PTY	B	5005	-	-	22/44/44/53	-
47	C7Z	7	504	-	1/1/12/26	8/29/67/67	0/2/2/2
21	CLA	4	606	-	-	5/21/97/115	-
21	CLA	4	617	-	-	5/15/91/115	-
21	CLA	G	1603	-	-	6/15/91/115	-
21	CLA	K	1403	9	-	10/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	OLA	8	809	-	-	8/17/17/17	-
21	CLA	8	605	-	-	6/15/91/115	-
21	CLA	B	1238	-	-	13/39/115/115	-
26	3PH	A	5007	-	-	10/34/34/49	-
28	LMT	1	804	-	-	10/21/61/61	0/2/2/2
21	CLA	A	1113	1	-	11/24/100/115	-
21	CLA	6	602	17	-	6/24/100/115	-
21	CLA	L	1503	-	-	8/15/91/115	-
21	CLA	8	611	-	-	7/21/97/115	-
21	CLA	6	615	-	-	22/39/115/115	-
21	CLA	4	611	-	-	9/29/105/115	-
24	LHG	a	801	-	-	25/39/39/53	-
38	CHL	4	609	15	1/1/15/21	19/41/117/117	-
21	CLA	K	1402	-	-	13/33/109/115	-
24	LHG	7	803	-	-	28/47/47/53	-
21	CLA	A	1124	-	-	9/27/103/115	-
21	CLA	1	606	-	-	13/30/106/115	-
23	BCR	K	4001	-	-	12/29/63/63	0/2/2/2
21	CLA	B	1232	-	-	7/15/91/115	-
23	BCR	I	4001	-	-	10/29/63/63	0/2/2/2
38	CHL	8	613	-	-	2/23/99/117	-
29	PCW	B	5004	-	-	15/33/33/57	-
31	LAP	K	5001	-	-	19/30/30/30	-
38	CHL	7	613	-	1/1/15/21	10/41/117/117	-
21	CLA	B	1215	2	-	20/33/109/115	-
21	CLA	3	604	-	-	13/33/109/115	-
21	CLA	5	616	-	-	8/17/93/115	-
21	CLA	4	604	15	-	13/33/109/115	-
21	CLA	a	603	-	-	16/39/115/115	-
21	CLA	7	610	-	-	10/27/103/115	-
21	CLA	5	618	16	-	4/24/100/115	-
23	BCR	5	503	-	-	16/29/63/63	0/2/2/2
21	CLA	A	1114	-	-	17/39/115/115	-
43	DGA	8	803	-	-	12/31/31/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	4	607	24	-	13/27/103/115	-
44	SPH	6	806	-	-	13/21/21/21	-
21	CLA	B	1236	2	-	13/25/101/115	-
21	CLA	5	604	-	-	12/39/115/115	-
21	CLA	1	605	-	-	16/39/115/115	-
21	CLA	J	1901	8	-	5/12/88/115	-
21	CLA	4	601	-	-	8/33/109/115	-
21	CLA	A	1122	-	-	21/39/115/115	-
21	CLA	5	602	16	-	10/24/100/115	-
21	CLA	5	614	-	-	5/17/93/115	-
21	CLA	6	608	-	-	6/15/91/115	-
23	BCR	B	4006	-	-	13/29/63/63	0/2/2/2
21	CLA	A	1102	21,1	-	18/39/115/115	-
21	CLA	5	605	-	-	8/17/93/115	-
23	BCR	B	4007	-	-	10/29/63/63	0/2/2/2
21	CLA	A	1128	1	-	15/39/115/115	-
21	CLA	4	612	15	-	16/36/112/115	-
21	CLA	A	1109	21,1	-	25/39/115/115	-
34	RRX	J	4002	-	1/1/11/25	12/29/65/65	0/2/2/2
21	CLA	A	1119	-	-	17/39/115/115	-
21	CLA	7	603	18	-	21/39/115/115	-
21	CLA	A	1130	1	-	13/29/105/115	-
21	CLA	6	603	-	-	19/39/115/115	-
21	CLA	A	1138	1	-	16/39/115/115	-
21	CLA	B	1221	-	-	13/39/115/115	-
21	CLA	B	1203	-	-	19/39/115/115	-
38	CHL	5	610	-	1/1/15/21	9/41/117/117	-
21	CLA	B	1022	-	-	15/39/115/115	-
21	CLA	5	607	24	-	12/27/103/115	-
21	CLA	A	1116	-	-	16/33/109/115	-
30	PTY	8	810	-	-	19/38/38/53	-
38	CHL	8	604	19	1/1/14/21	13/37/113/117	-
35	LPX	a	804	-	-	14/31/31/31	-
21	CLA	A	1012	-	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	6	618	-	-	9/17/93/115	-
21	CLA	A	1118	1	-	17/27/103/115	-
46	4RF	7	807	-	-	20/34/34/59	-
21	CLA	F	1301	6	-	6/21/97/115	-
21	CLA	B	1227	2	-	8/21/97/115	-
21	CLA	B	1239	2	-	18/39/115/115	-
21	CLA	a	611	-	-	10/21/97/115	-
23	BCR	3	505	-	-	13/29/63/63	0/2/2/2
21	CLA	B	1234	2	-	14/29/105/115	-
21	CLA	8	618	-	-	17/33/109/115	-
21	CLA	B	1202	2	-	14/39/115/115	-
23	BCR	8	503	-	-	10/29/63/63	0/2/2/2
38	CHL	a	610	-	-	6/20/96/117	-
24	LHG	5	801	21	-	30/53/53/53	-
38	CHL	8	601	19	1/1/14/21	10/35/111/117	-
21	CLA	F	1302	24	-	12/27/103/115	-
24	LHG	A	5003	-	-	31/46/46/53	-
21	CLA	A	1105	-	-	10/30/106/115	-
31	LAP	B	5007	-	-	19/30/30/30	-
21	CLA	B	1214	2	-	21/36/112/115	-
35	LPX	J	5001	-	-	11/18/18/31	-
25	DGD	B	5003	-	-	19/55/95/95	0/2/2/2
23	BCR	F	4001	-	-	9/29/63/63	0/2/2/2
21	CLA	A	1111	-	-	25/39/115/115	-
21	CLA	3	603	-	-	21/39/115/115	-
21	CLA	B	1240	24	-	11/39/115/115	-
21	CLA	A	1101	1	-	23/39/115/115	-
21	CLA	B	1216	-	-	21/35/111/115	-
28	LMT	B	5006	-	-	10/21/61/61	0/2/2/2
21	CLA	3	613	-	-	14/35/111/115	-
37	LUT	5	502	-	-	1/29/67/67	0/2/2/2
21	CLA	A	1121	1	-	14/30/106/115	-
21	CLA	1	607	-	-	16/39/115/115	-
21	CLA	L	1501	-	-	10/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	LUT	4	501	-	-	2/29/67/67	0/2/2/2
21	CLA	7	611	-	-	10/33/109/115	-
23	BCR	4	503	-	-	15/29/63/63	0/2/2/2
21	CLA	a	605	-	-	10/39/115/115	-
37	LUT	6	501	-	1/1/12/27	7/29/67/67	0/2/2/2
37	LUT	8	502	-	-	3/29/67/67	0/2/2/2
21	CLA	a	612	13	-	10/30/106/115	-
21	CLA	7	602	-	-	9/13/90/115	-
21	CLA	5	612	16	-	22/39/115/115	-
21	CLA	B	1235	2	-	21/39/115/115	-
21	CLA	3	601	-	-	13/39/115/115	-
23	BCR	A	4005	-	-	16/29/63/63	0/2/2/2
21	CLA	B	1209	2	-	18/39/115/115	-
21	CLA	6	609	17	-	22/39/115/115	-
37	LUT	4	502	-	-	3/29/67/67	0/2/2/2
21	CLA	B	1225	2	-	12/39/115/115	-
40	QTB	a	504	-	-	6/11/28/28	0/1/1/1
21	CLA	A	1117	1	-	21/39/115/115	-
24	LHG	1	801	-	-	26/39/39/53	-
37	LUT	6	502	-	1/1/12/27	8/29/67/67	0/2/2/2
27	SF4	C	3003	3	-	-	0/6/5/5
27	SF4	A	3001	2,1	-	-	0/6/5/5
21	CLA	A	1131	1	-	23/39/115/115	-
21	CLA	A	1104	-	-	21/39/115/115	-
37	LUT	1	503	-	1/1/12/27	8/29/67/67	0/2/2/2
21	CLA	1	601	13	-	9/33/109/115	-
21	CLA	a	607	-	-	12/31/107/115	-
21	CLA	A	1112	-	-	9/27/103/115	-
21	CLA	7	604	-	-	18/39/115/115	-
21	CLA	5	603	-	-	16/29/105/115	-
21	CLA	A	1125	1	-	22/39/115/115	-
21	CLA	1	612	13	-	18/39/115/115	-
21	CLA	K	1404	9	-	11/24/100/115	-
21	CLA	B	1219	-	-	10/32/108/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LHG	6	802	-	-	27/41/41/53	-
21	CLA	8	607	24	-	6/17/93/115	-
38	CHL	1	609	13	1/1/15/21	14/41/117/117	-
45	XAT	7	502	-	3/3/12/26	1/31/93/93	0/4/4/4
21	CLA	A	1115	1	-	10/33/109/115	-
21	CLA	B	1021	-	-	25/39/115/115	-
21	CLA	A	1136	1	-	18/39/115/115	-
21	CLA	7	607	24	-	14/31/107/115	-
23	BCR	B	4005	-	-	12/29/63/63	0/2/2/2
21	CLA	B	1211	-	-	12/27/103/115	-
23	BCR	B	4004	-	-	11/29/63/63	0/2/2/2
21	CLA	G	1601	-	-	14/21/97/115	-
21	CLA	5	617	-	-	13/21/97/115	-
37	LUT	5	501	-	-	1/29/67/67	0/2/2/2
30	PTY	3	802	-	-	24/41/41/53	-
38	CHL	1	613	-	-	2/20/96/117	-
24	LHG	A	5001	21	-	20/33/33/53	-
20	CL0	A	1011	1	-	13/39/115/115	-
21	CLA	B	1228	2	-	18/39/115/115	-
21	CLA	B	1213	2	-	19/33/109/115	-
23	BCR	J	4001	-	-	13/29/63/63	0/2/2/2
21	CLA	A	1110	1	-	16/33/109/115	-
21	CLA	8	612	19	-	10/17/93/115	-
21	CLA	3	618	-	-	6/17/93/115	-

The worst 5 of 1713 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	G	5002	ERG	C1-C10	-24.25	1.08	1.54
33	G	5002	ERG	C10-C9	-22.01	1.26	1.55
47	7	504	C7Z	C25-C26	15.87	1.61	1.34
33	G	5002	ERG	C10-C5	-15.71	1.21	1.52
34	J	4002	RRX	C26-C25	15.66	1.61	1.34

The worst 5 of 4914 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J	4001	BCR	C10-C11-C12	18.04	179.50	123.22
23	A	4004	BCR	C10-C11-C12	17.82	178.83	123.22
23	A	4002	BCR	C10-C11-C12	17.72	178.51	123.22
23	4	503	BCR	C10-C11-C12	17.70	178.47	123.22
23	F	4001	BCR	C10-C11-C12	17.67	178.36	123.22

5 of 30 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
33	G	5002	ERG	C24
33	G	5002	ERG	C14
33	G	5002	ERG	C9
33	G	5002	ERG	C20
34	J	4002	RRX	C28

5 of 4534 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	1011	CL0	C2-C1-O2A-CGA
21	A	1013	CLA	CHA-CBD-CGD-O1D
21	A	1013	CLA	CHA-CBD-CGD-O2D
21	A	1013	CLA	CBD-CGD-O2D-CED
21	A	1102	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

328 monomers are involved in 1533 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	8	620	CLA	5	0
24	4	801	LHG	15	0
24	4	802	LHG	5	0
28	A	5008	LMT	4	0
21	B	1206	CLA	6	0
21	A	1123	CLA	4	0
21	7	606	CLA	5	0
23	6	503	BCR	11	0
38	6	611	CHL	19	0
38	a	609	CHL	7	0
21	A	1137	CLA	4	0
21	B	1204	CLA	10	0
21	4	605	CLA	1	0
21	7	612	CLA	9	0
38	4	613	CHL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	6	605	CLA	1	0
21	5	606	CLA	2	0
21	1	615	CLA	4	0
38	6	619	CHL	9	0
21	A	1127	CLA	7	0
37	8	501	LUT	12	0
21	a	604	CLA	4	0
21	A	1108	CLA	10	0
42	4	803	PLM	1	0
37	a	501	LUT	5	0
21	6	601	CLA	24	0
21	6	604	CLA	18	0
21	1	602	CLA	4	0
24	B	5001	LHG	7	0
38	6	610	CHL	9	0
23	K	4002	BCR	1	0
21	3	610	CLA	5	0
21	4	610	CLA	8	0
21	8	606	CLA	4	0
37	a	502	LUT	5	0
25	A	5005	DGD	3	0
23	7	503	BCR	9	0
21	a	602	CLA	2	0
21	G	1602	CLA	2	0
21	6	607	CLA	12	0
21	B	1224	CLA	6	0
21	8	615	CLA	3	0
21	B	1231	CLA	7	0
21	B	1207	CLA	9	0
21	4	615	CLA	2	0
21	7	617	CLA	6	0
46	8	808	4RF	13	0
23	G	4001	BCR	3	0
23	A	4002	BCR	4	0
21	B	1217	CLA	5	0
38	a	606	CHL	13	0
21	A	1103	CLA	11	0
21	1	604	CLA	12	0
21	A	1120	CLA	5	0
25	8	802	DGD	13	0
21	B	1210	CLA	7	0
21	3	616	CLA	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	8	602	CLA	3	0
21	4	602	CLA	1	0
23	3	503	BCR	1	0
21	B	1208	CLA	5	0
21	4	608	CLA	3	0
37	7	501	LUT	4	0
21	7	609	CLA	4	0
21	6	612	CLA	2	0
33	G	5002	ERG	16	0
21	A	1134	CLA	6	0
22	A	2001	PQN	6	0
21	A	1129	CLA	2	0
21	B	1223	CLA	3	0
21	B	1220	CLA	6	0
23	A	4001	BCR	5	0
23	L	4003	BCR	2	0
21	a	608	CLA	3	0
21	5	608	CLA	3	0
24	F	5002	LHG	3	0
30	7	804	PTY	3	0
21	1	603	CLA	8	0
46	8	807	4RF	2	0
24	6	801	LHG	16	0
23	A	4003	BCR	5	0
23	L	4001	BCR	17	0
38	3	608	CHL	1	0
21	1	610	CLA	2	0
21	3	605	CLA	6	0
23	B	4002	BCR	4	0
39	1	803	OLA	2	0
23	B	4001	BCR	5	0
37	3	501	LUT	6	0
24	8	801	LHG	5	0
21	A	1107	CLA	8	0
21	A	1126	CLA	11	0
21	5	601	CLA	5	0
21	7	608	CLA	6	0
21	B	1201	CLA	16	0
21	K	1401	CLA	3	0
37	5	505	LUT	7	0
21	B	1218	CLA	7	0
36	M	4001	ECH	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	1	608	CLA	5	0
23	6	504	BCR	5	0
22	B	2002	PQN	5	0
21	a	601	CLA	5	0
24	3	801	LHG	5	0
30	5	802	PTY	2	0
21	A	1013	CLA	8	0
21	B	1023	CLA	15	0
38	4	618	CHL	8	0
23	5	504	BCR	5	0
24	B	5002	LHG	2	0
21	6	606	CLA	2	0
21	6	617	CLA	12	0
21	8	603	CLA	4	0
21	4	603	CLA	3	0
24	7	802	LHG	1	0
21	7	601	CLA	6	0
21	L	1502	CLA	15	0
21	A	1106	CLA	9	0
42	6	804	PLM	1	0
21	3	602	CLA	2	0
21	3	606	CLA	3	0
37	3	502	LUT	3	0
21	3	612	CLA	5	0
21	8	610	CLA	6	0
24	F	5001	LHG	4	0
21	B	1205	CLA	7	0
37	1	501	LUT	5	0
21	a	615	CLA	4	0
24	1	802	LHG	2	0
21	A	1140	CLA	7	0
38	a	613	CHL	7	0
21	7	605	CLA	5	0
21	B	1226	CLA	7	0
21	B	1237	CLA	8	0
21	B	1212	CLA	10	0
21	1	611	CLA	4	0
37	a	503	LUT	4	0
48	8	806	P5S	1	0
21	A	1132	CLA	3	0
21	3	607	CLA	7	0
23	B	4003	BCR	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	3	504	BCR	9	0
24	A	5002	LHG	8	0
31	F	5003	LAP	6	0
21	A	1135	CLA	5	0
21	B	1222	CLA	5	0
21	B	1230	CLA	4	0
38	5	613	CHL	2	0
21	A	1139	CLA	2	0
21	A	1133	CLA	9	0
21	4	616	CLA	2	0
21	8	609	CLA	6	0
23	A	4004	BCR	6	0
21	B	1229	CLA	4	0
21	8	608	CLA	5	0
32	G	5001	SQD	4	0
38	3	611	CHL	7	0
23	L	4002	BCR	5	0
37	1	502	LUT	3	0
38	5	611	CHL	4	0
21	5	609	CLA	9	0
32	7	805	SQD	1	0
27	C	3002	SF4	1	0
29	6	803	PCW	3	0
24	7	801	LHG	6	0
21	7	615	CLA	1	0
41	a	805	GG0	1	0
38	6	613	CHL	19	0
43	5	803	DGA	3	0
30	B	5005	PTY	4	0
21	4	606	CLA	3	0
47	7	504	C7Z	3	0
21	4	617	CLA	1	0
21	G	1603	CLA	5	0
21	K	1403	CLA	28	0
39	8	809	OLA	4	0
21	8	605	CLA	4	0
21	B	1238	CLA	5	0
26	A	5007	3PH	1	0
28	1	804	LMT	9	0
21	A	1113	CLA	4	0
21	6	602	CLA	5	0
21	L	1503	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	8	611	CLA	3	0
21	6	615	CLA	3	0
24	a	801	LHG	2	0
21	K	1402	CLA	6	0
38	4	609	CHL	9	0
24	7	803	LHG	5	0
21	A	1124	CLA	5	0
21	1	606	CLA	2	0
23	K	4001	BCR	6	0
21	B	1232	CLA	3	0
23	I	4001	BCR	8	0
38	8	613	CHL	3	0
29	B	5004	PCW	6	0
31	K	5001	LAP	3	0
38	7	613	CHL	5	0
21	B	1215	CLA	5	0
21	3	604	CLA	3	0
21	5	616	CLA	2	0
21	4	604	CLA	5	0
21	a	603	CLA	2	0
21	7	610	CLA	4	0
21	5	618	CLA	7	0
23	5	503	BCR	4	0
21	A	1114	CLA	6	0
43	8	803	DGA	5	0
21	4	607	CLA	5	0
44	6	806	SPH	7	0
21	B	1236	CLA	5	0
21	5	604	CLA	10	0
21	1	605	CLA	8	0
21	4	601	CLA	8	0
21	A	1122	CLA	3	0
21	5	602	CLA	1	0
23	B	4006	BCR	1	0
21	A	1102	CLA	6	0
21	5	605	CLA	2	0
23	B	4007	BCR	3	0
21	A	1128	CLA	3	0
21	4	612	CLA	5	0
21	A	1109	CLA	13	0
21	A	1119	CLA	4	0
21	7	603	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	J	4002	RRX	10	0
21	A	1130	CLA	8	0
21	6	603	CLA	6	0
21	A	1138	CLA	8	0
21	B	1221	CLA	8	0
21	B	1203	CLA	6	0
38	5	610	CHL	10	0
21	B	1022	CLA	4	0
21	5	607	CLA	3	0
21	A	1116	CLA	6	0
30	8	810	PTY	6	0
38	8	604	CHL	9	0
35	a	804	LPX	12	0
21	A	1012	CLA	11	0
21	6	618	CLA	4	0
21	A	1118	CLA	5	0
46	7	807	4RF	6	0
21	F	1301	CLA	5	0
21	B	1227	CLA	3	0
21	B	1239	CLA	8	0
21	a	611	CLA	2	0
23	3	505	BCR	1	0
21	B	1234	CLA	10	0
21	8	618	CLA	7	0
21	B	1202	CLA	6	0
23	8	503	BCR	5	0
38	a	610	CHL	2	0
24	5	801	LHG	10	0
38	8	601	CHL	8	0
21	F	1302	CLA	7	0
24	A	5003	LHG	7	0
21	A	1105	CLA	3	0
31	B	5007	LAP	3	0
21	B	1214	CLA	4	0
35	J	5001	LPX	3	0
25	B	5003	DGD	10	0
23	F	4001	BCR	5	0
21	A	1111	CLA	10	0
21	3	603	CLA	8	0
21	B	1240	CLA	5	0
21	A	1101	CLA	7	0
21	B	1216	CLA	5	0

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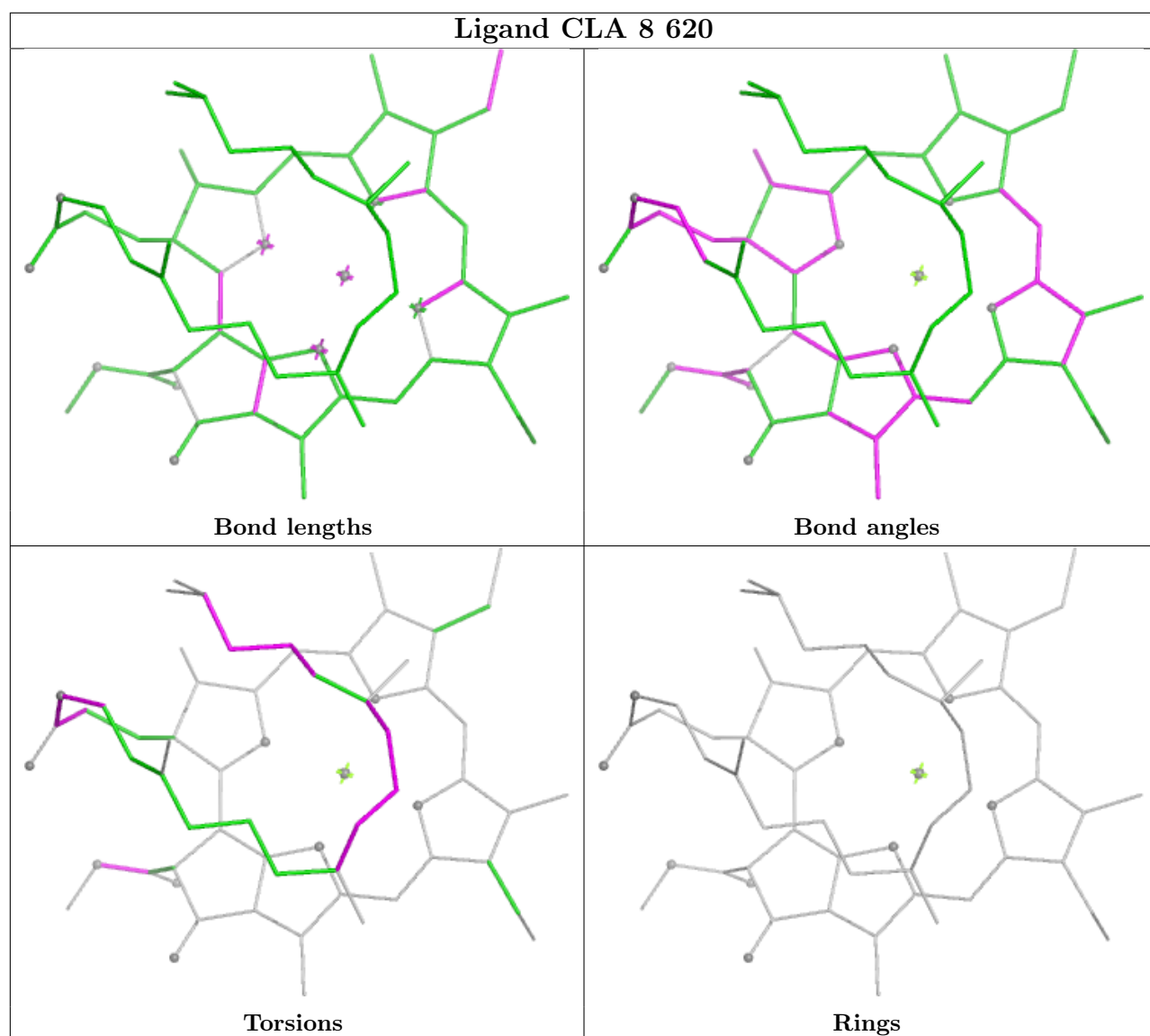
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	B	5006	LMT	2	0
21	3	613	CLA	4	0
37	5	502	LUT	5	0
21	A	1121	CLA	7	0
21	1	607	CLA	14	0
21	L	1501	CLA	3	0
37	4	501	LUT	5	0
21	7	611	CLA	5	0
23	4	503	BCR	3	0
21	a	605	CLA	6	0
37	6	501	LUT	16	0
37	8	502	LUT	5	0
21	a	612	CLA	6	0
21	7	602	CLA	2	0
21	5	612	CLA	9	0
21	B	1235	CLA	8	0
21	3	601	CLA	12	0
23	A	4005	BCR	3	0
21	B	1209	CLA	11	0
21	6	609	CLA	23	0
37	4	502	LUT	4	0
21	B	1225	CLA	6	0
40	a	504	QTB	1	0
21	A	1117	CLA	5	0
24	1	801	LHG	3	0
27	C	3003	SF4	1	0
37	6	502	LUT	13	0
21	A	1131	CLA	11	0
21	A	1104	CLA	6	0
37	1	503	LUT	8	0
21	1	601	CLA	5	0
21	a	607	CLA	1	0
21	A	1112	CLA	1	0
21	7	604	CLA	7	0
21	5	603	CLA	4	0
21	A	1125	CLA	8	0
21	1	612	CLA	9	0
21	K	1404	CLA	2	0
21	B	1219	CLA	4	0
24	6	802	LHG	4	0
21	8	607	CLA	2	0
38	1	609	CHL	8	0

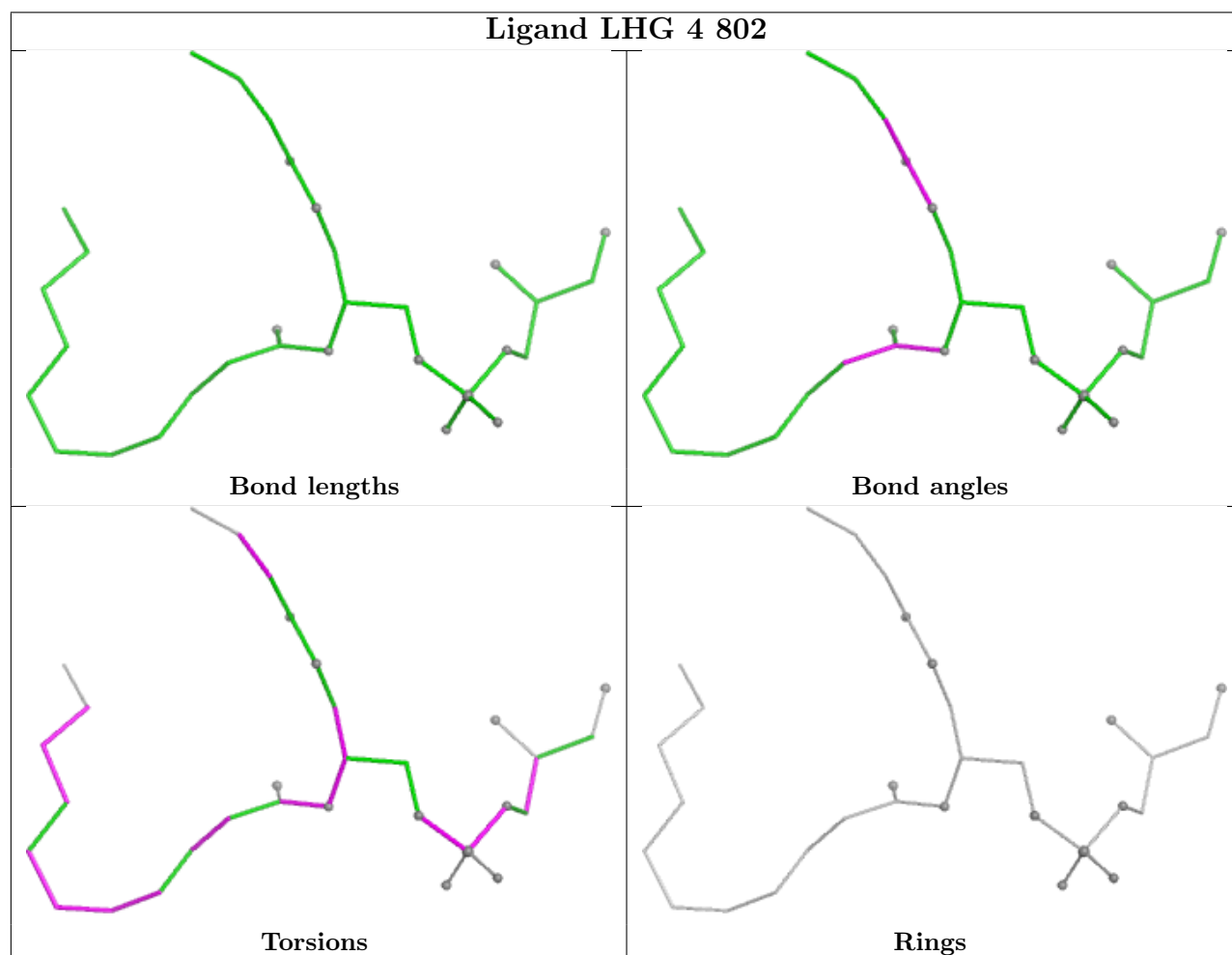
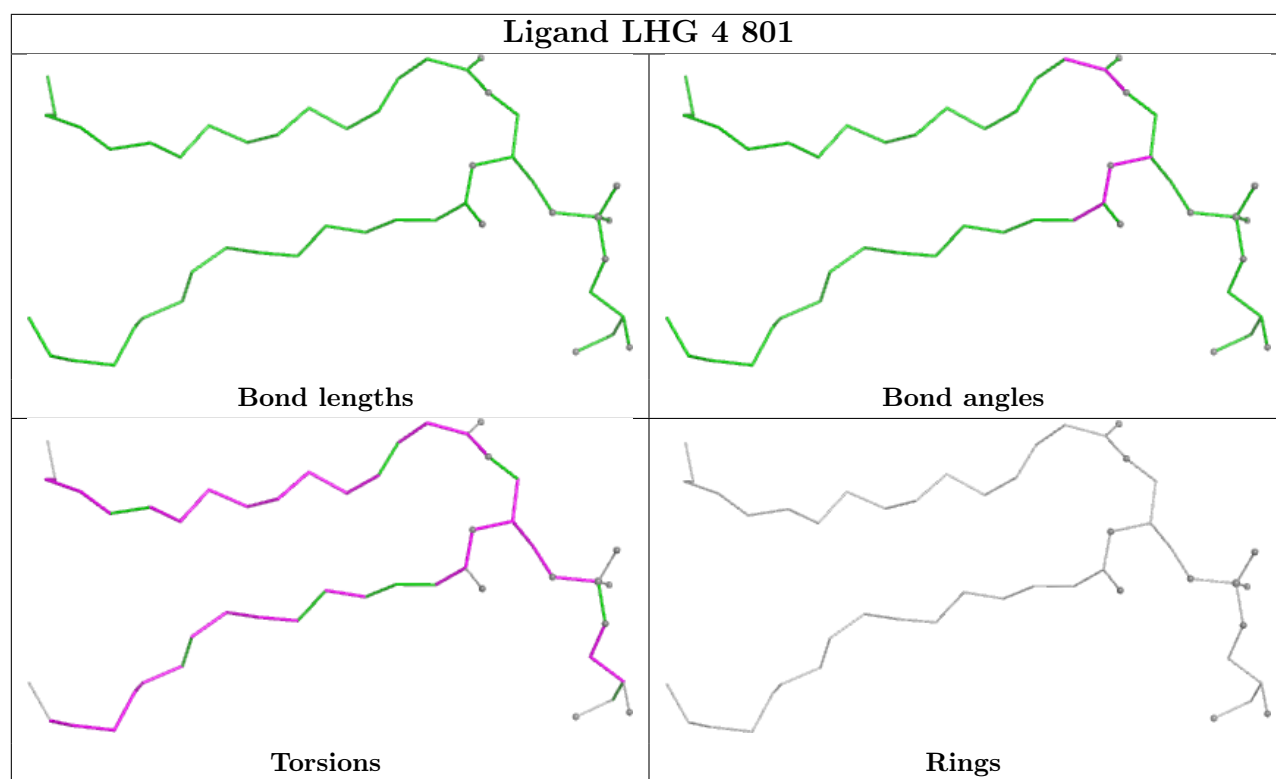
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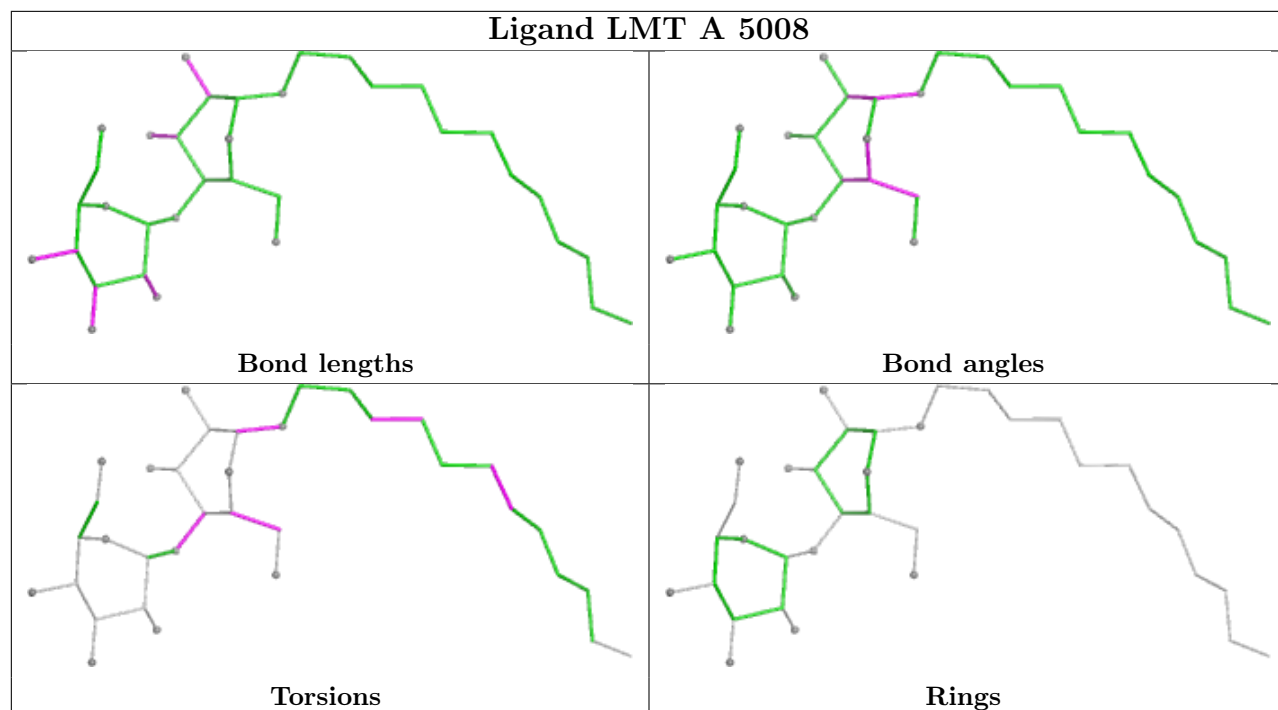
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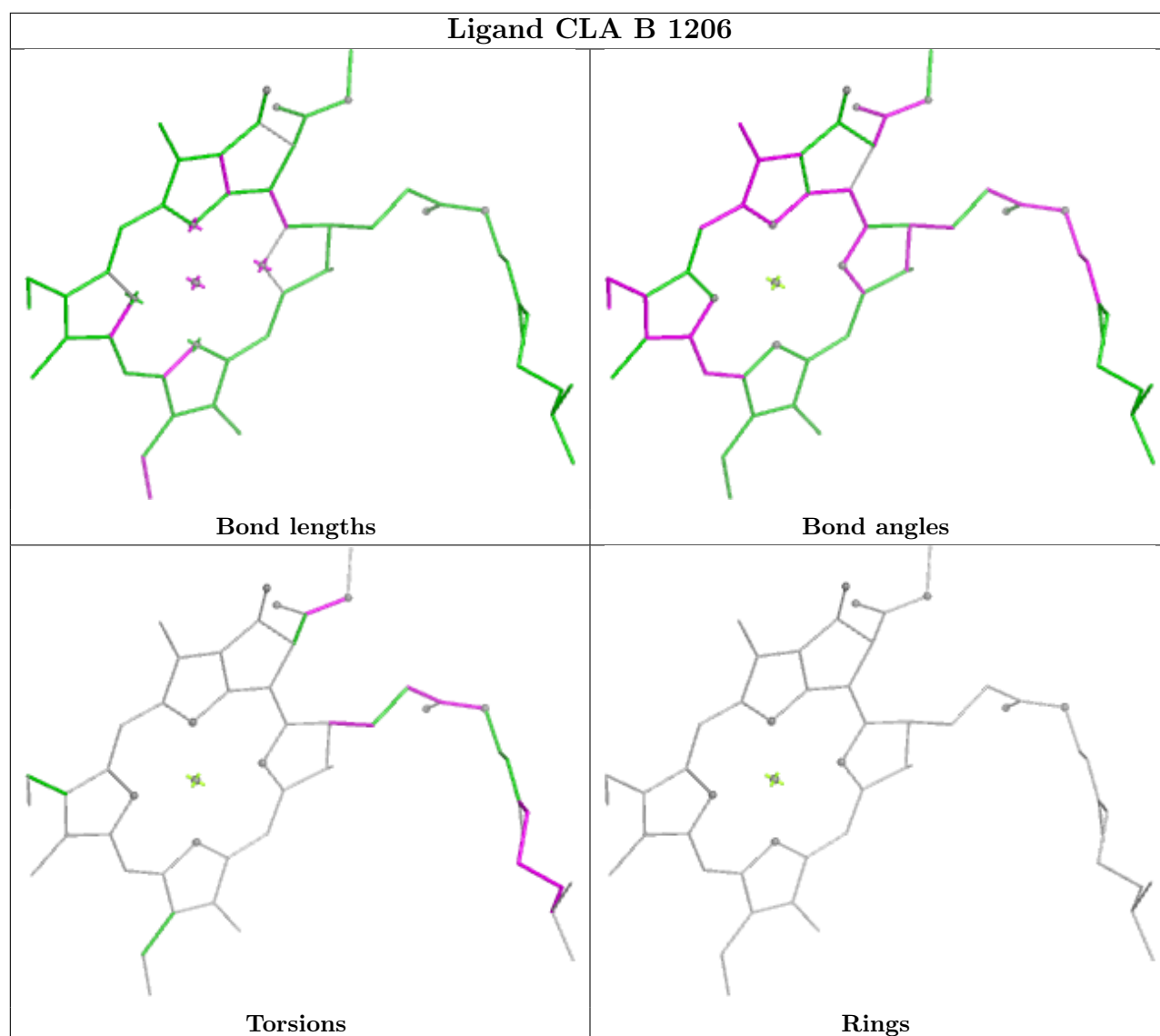
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	7	502	XAT	5	0
21	A	1115	CLA	5	0
21	B	1021	CLA	10	0
21	A	1136	CLA	10	0
23	B	4005	BCR	4	0
21	B	1211	CLA	4	0
23	B	4004	BCR	9	0
21	5	617	CLA	5	0
37	5	501	LUT	8	0
30	3	802	PTY	5	0
38	1	613	CHL	5	0
24	A	5001	LHG	1	0
20	A	1011	CL0	4	0
21	B	1228	CLA	9	0
21	B	1213	CLA	5	0
23	J	4001	BCR	3	0
21	A	1110	CLA	2	0
21	8	612	CLA	4	0
21	3	618	CLA	1	0

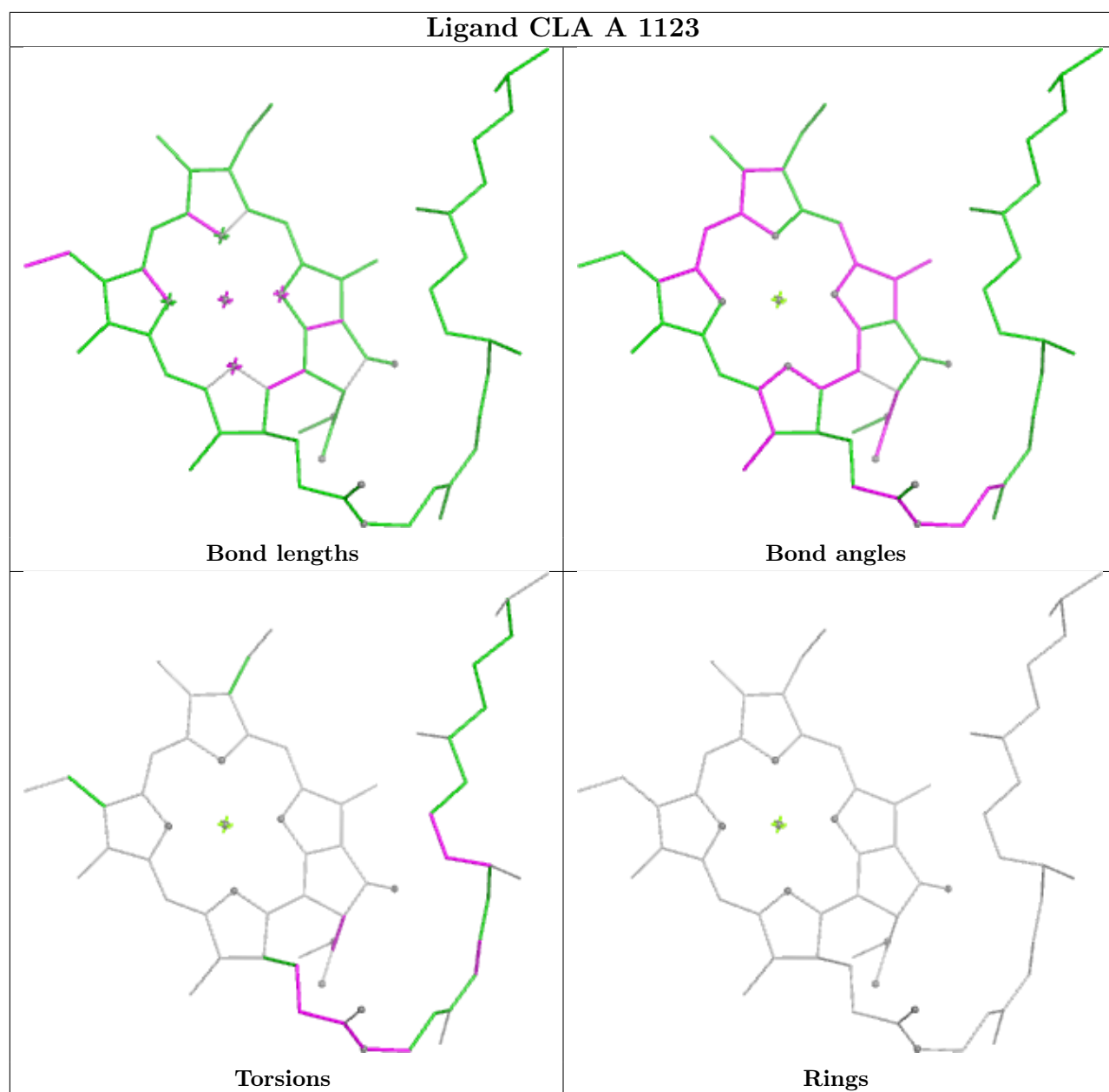
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

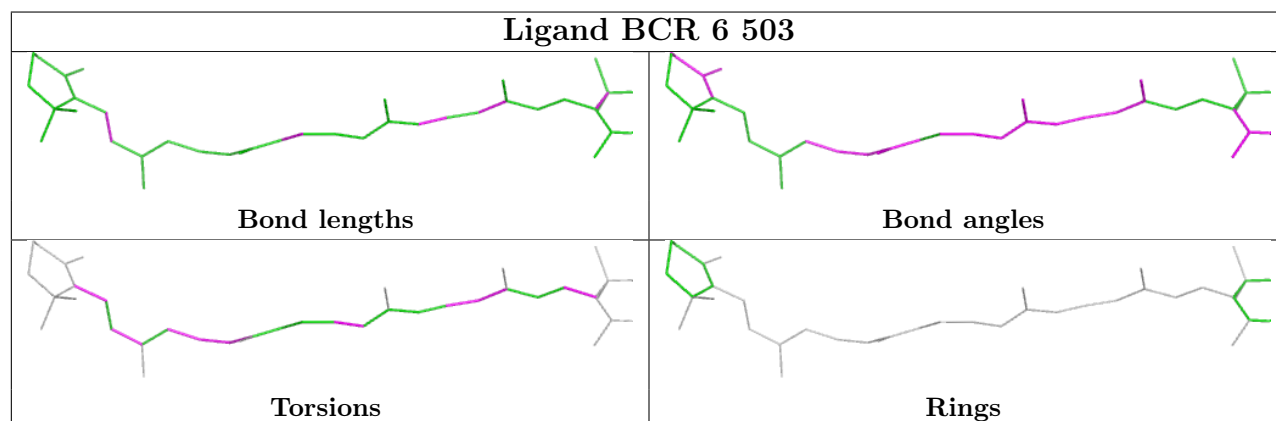
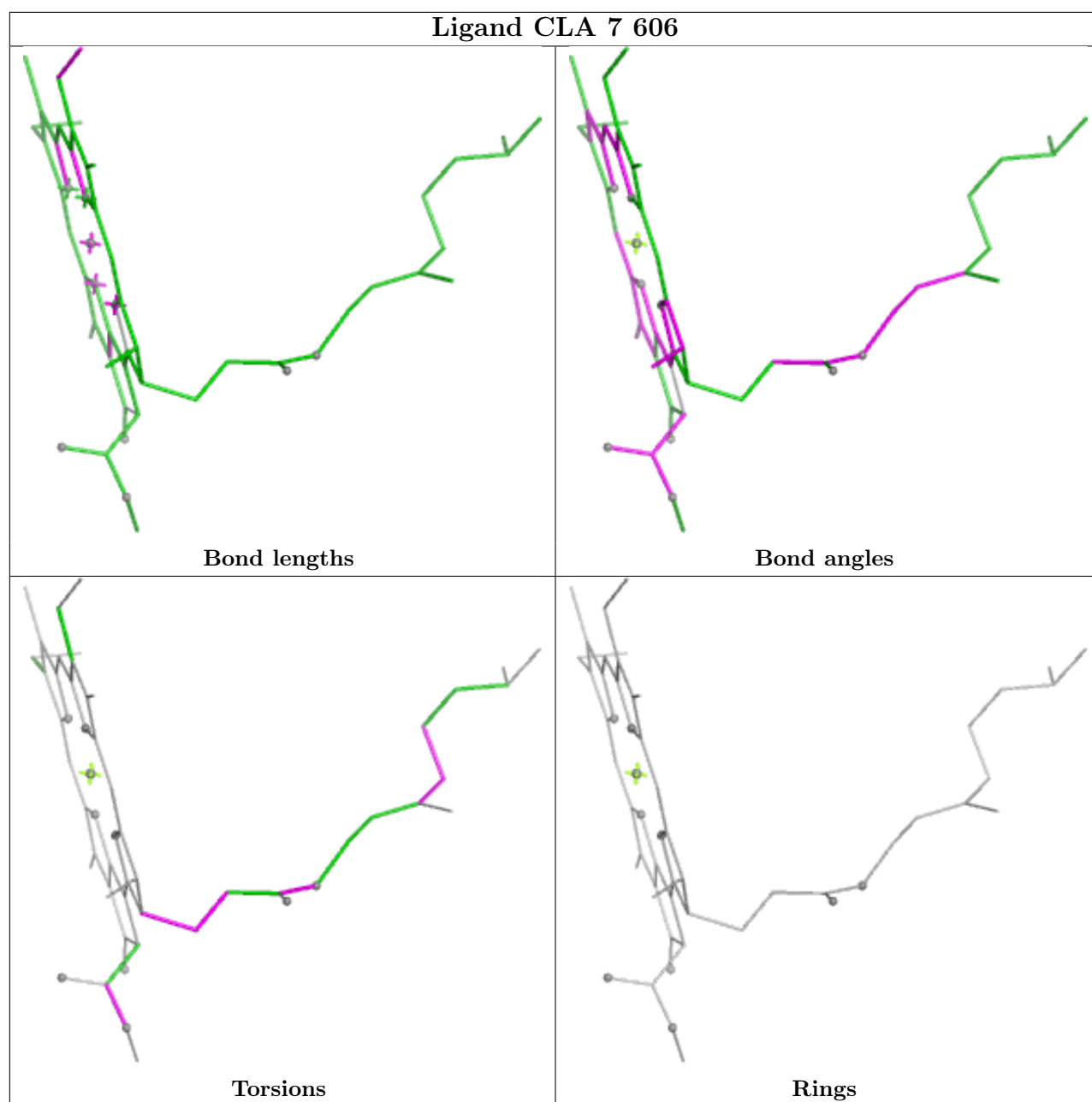




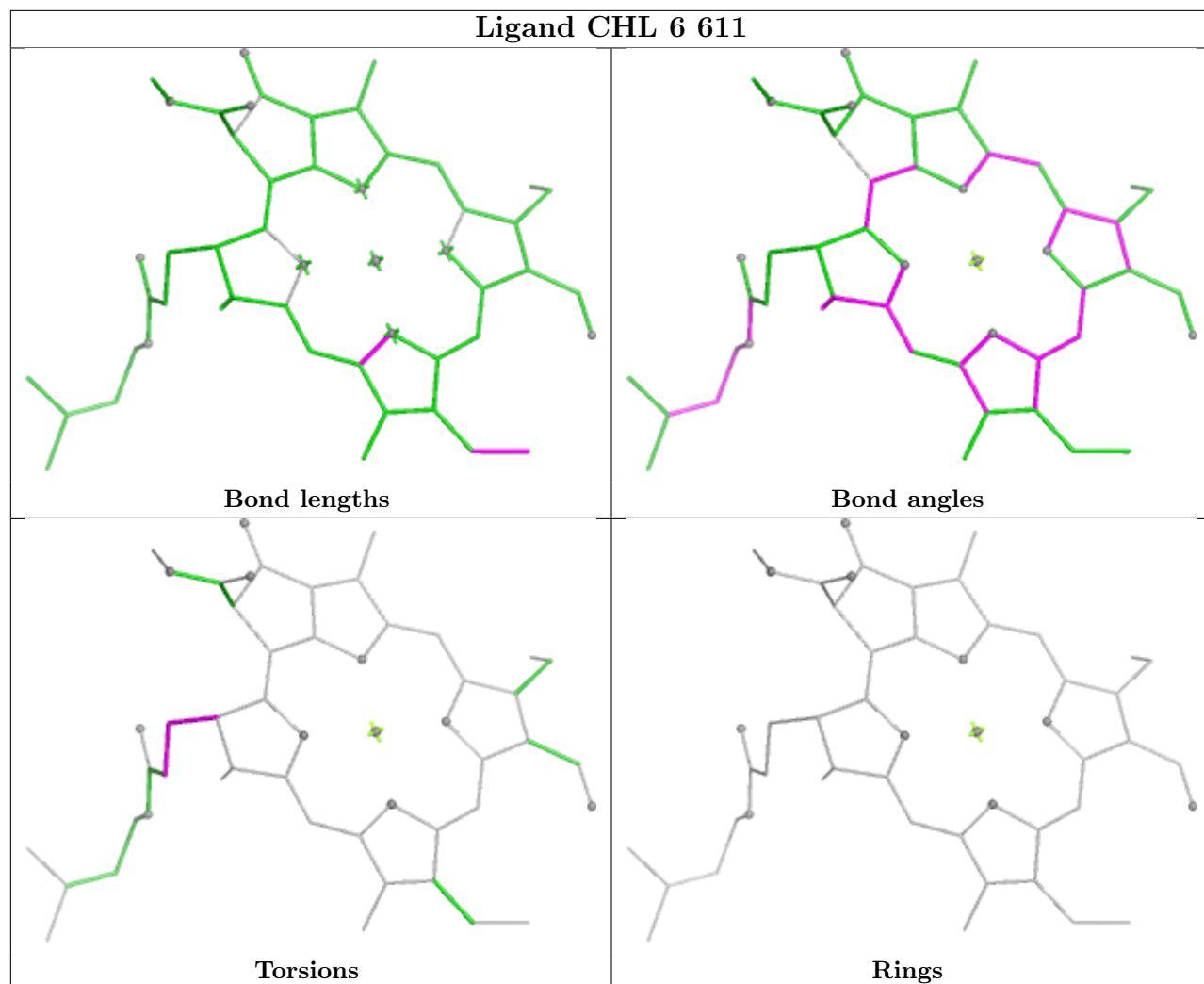


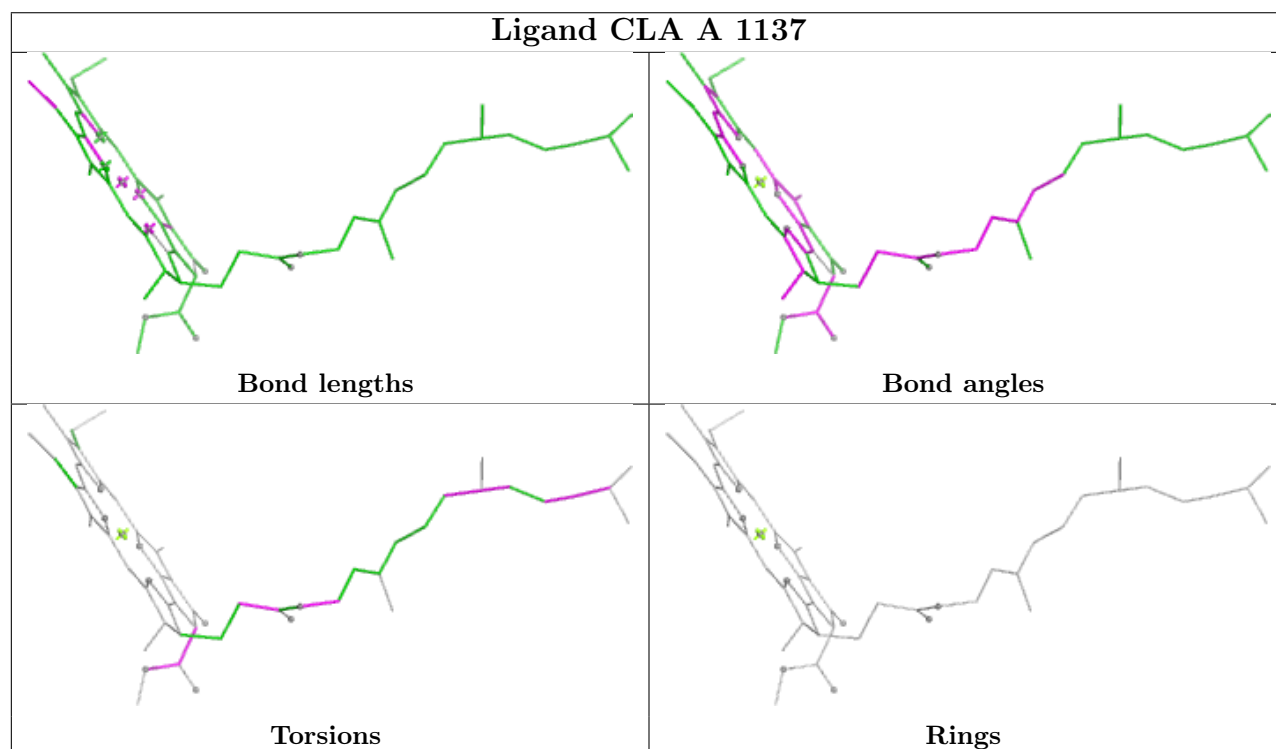
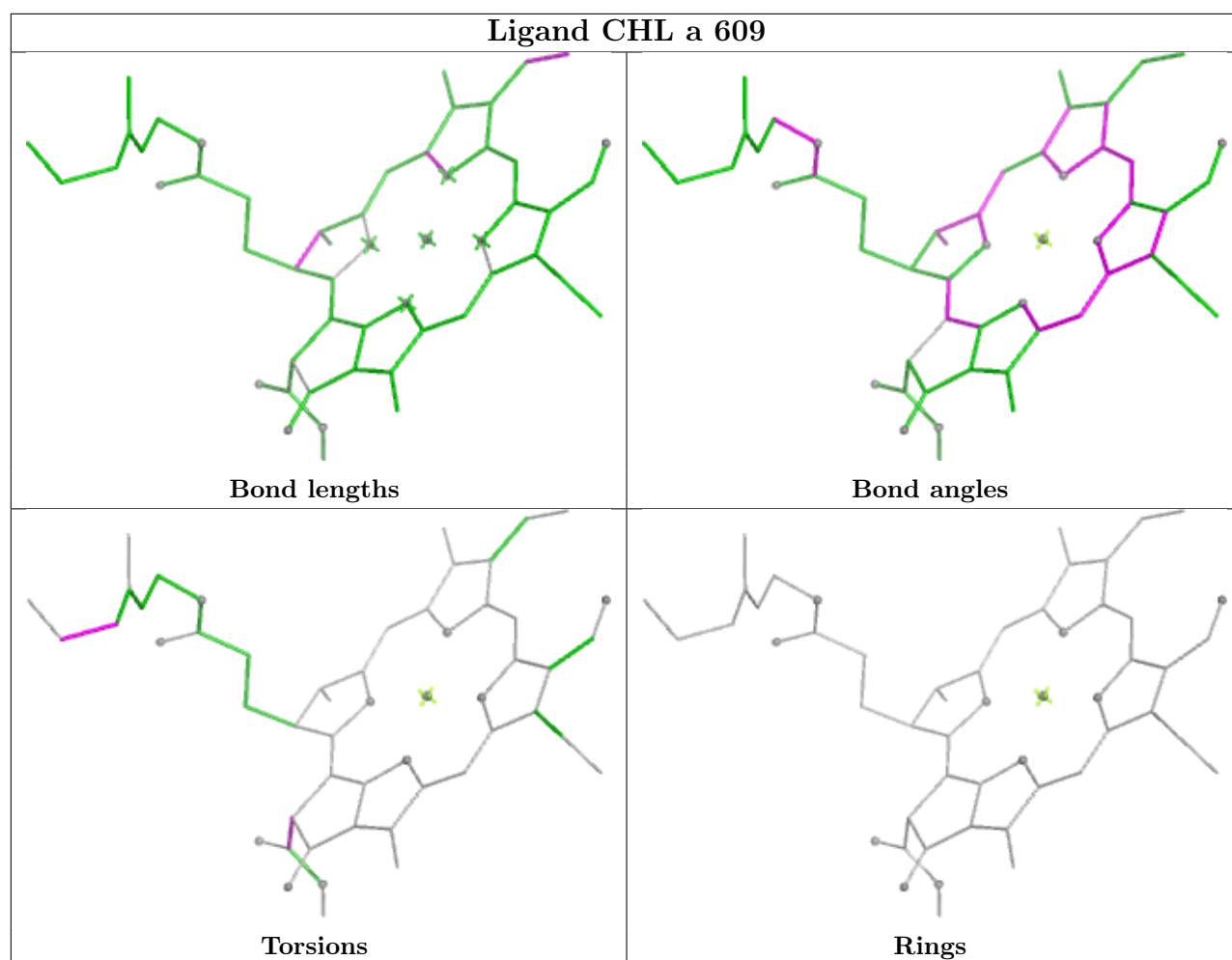


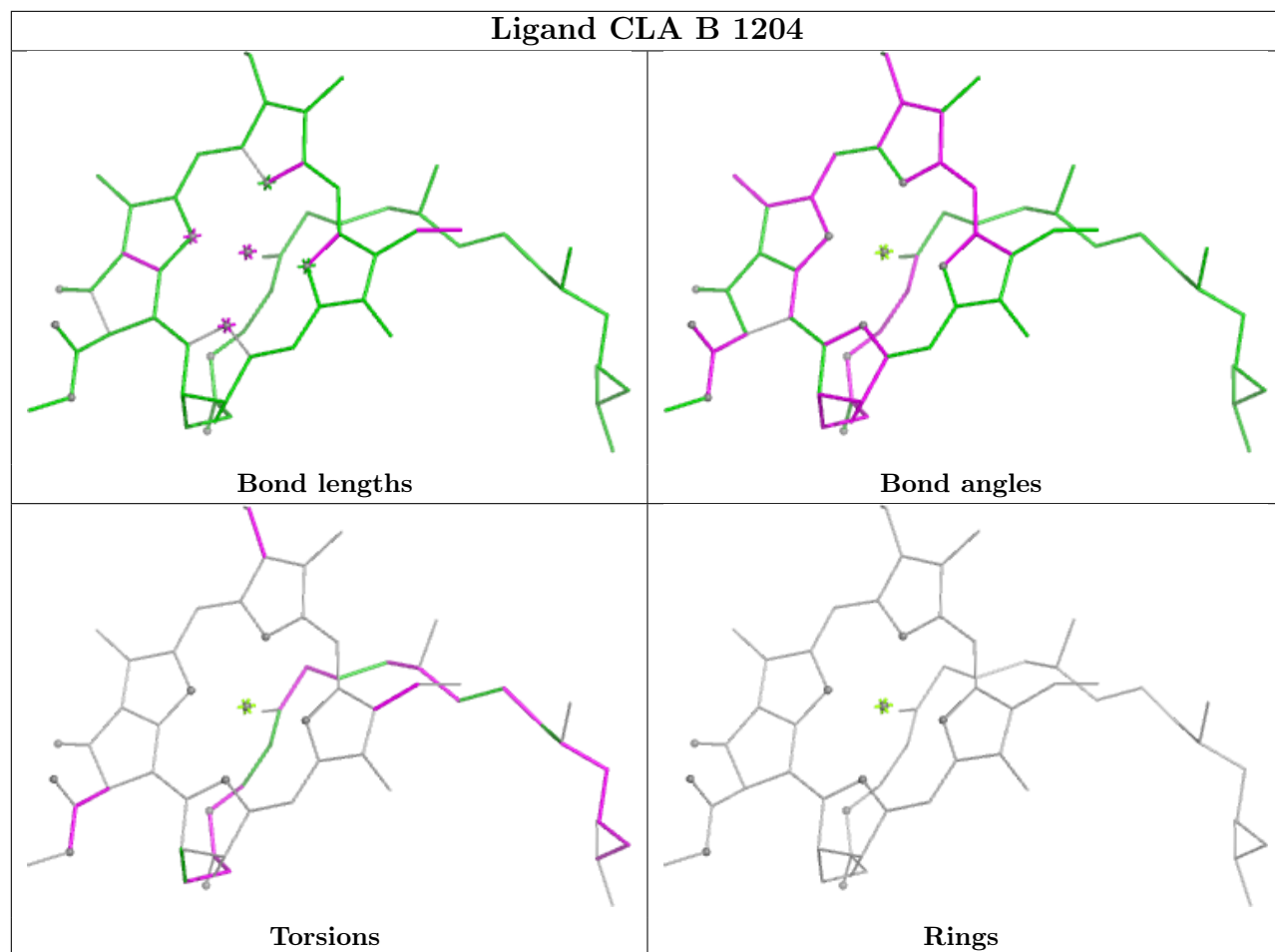




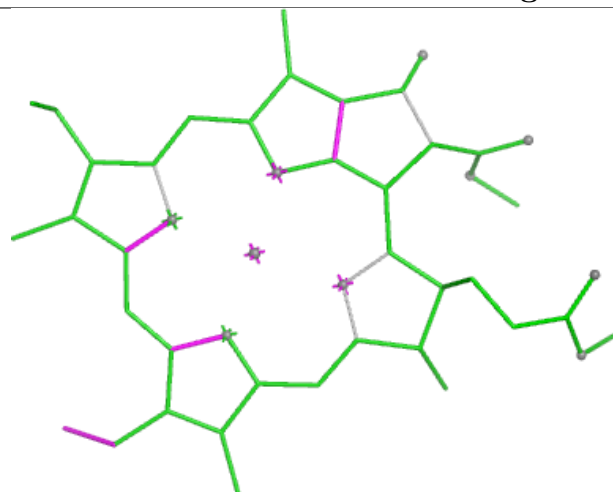
Ligand CHL 6 611



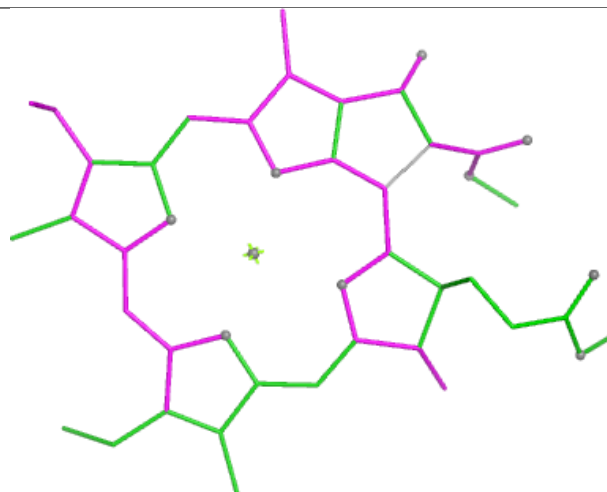




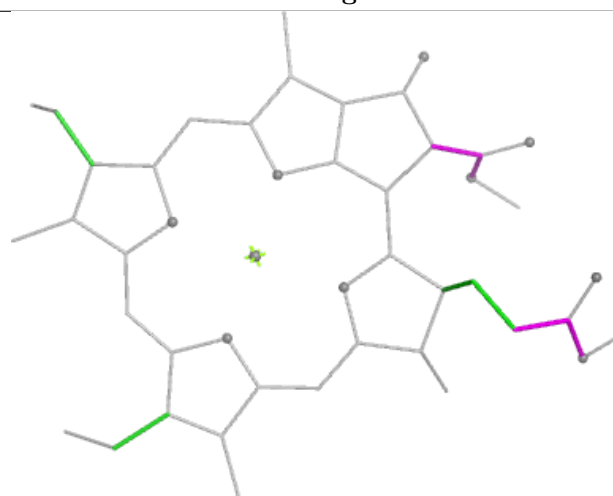
Ligand CLA 4 605



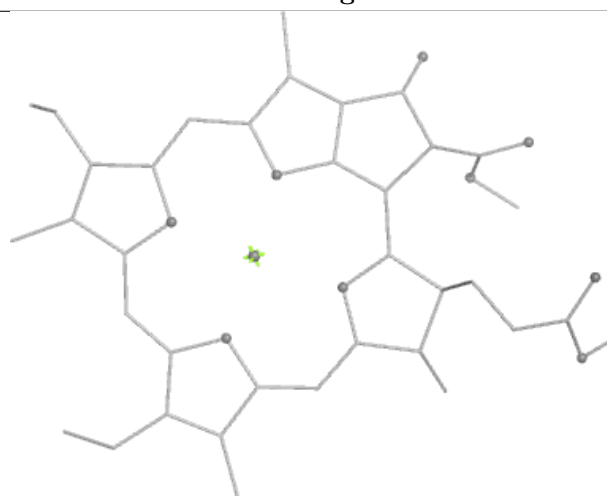
Bond lengths



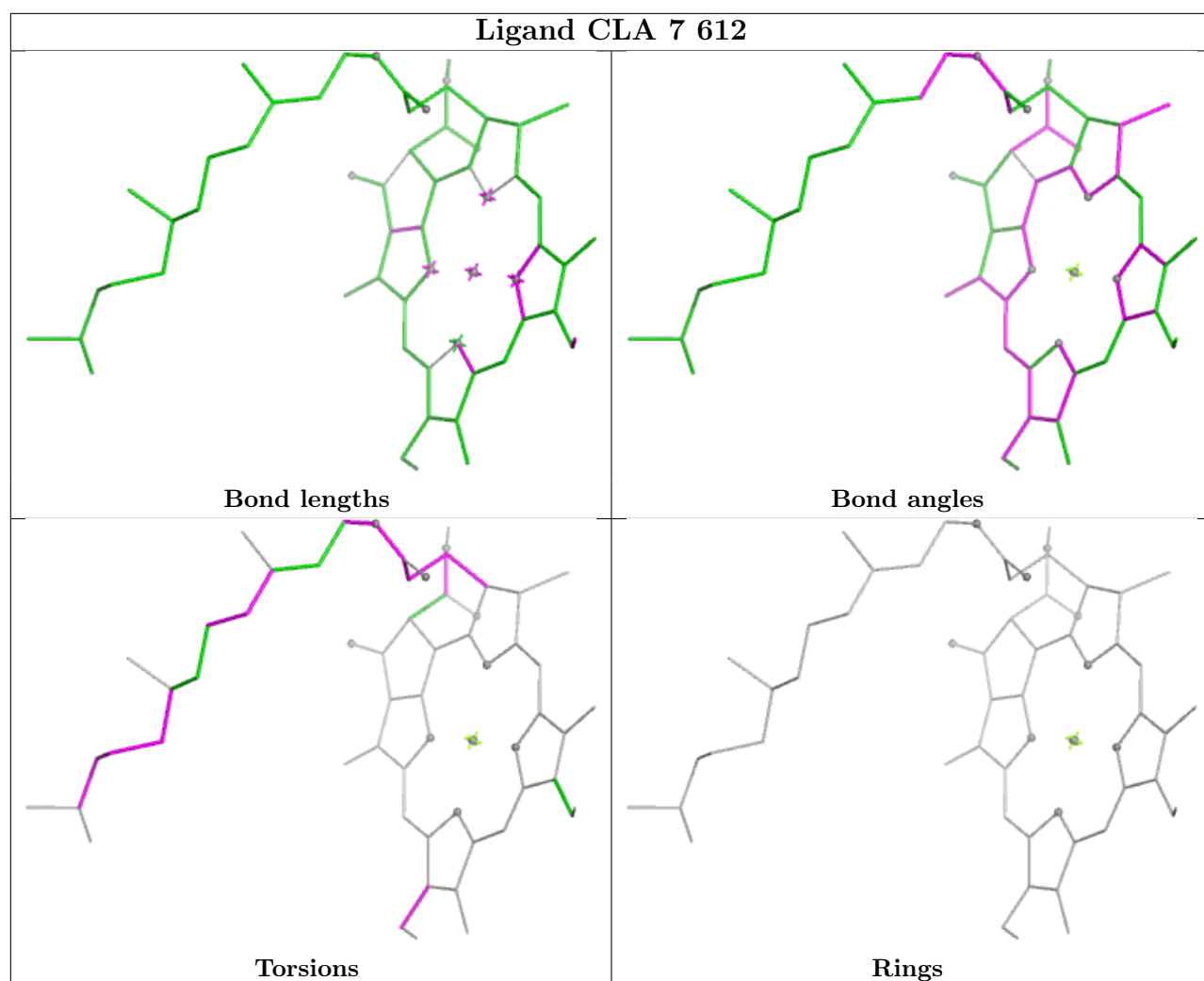
Bond angles



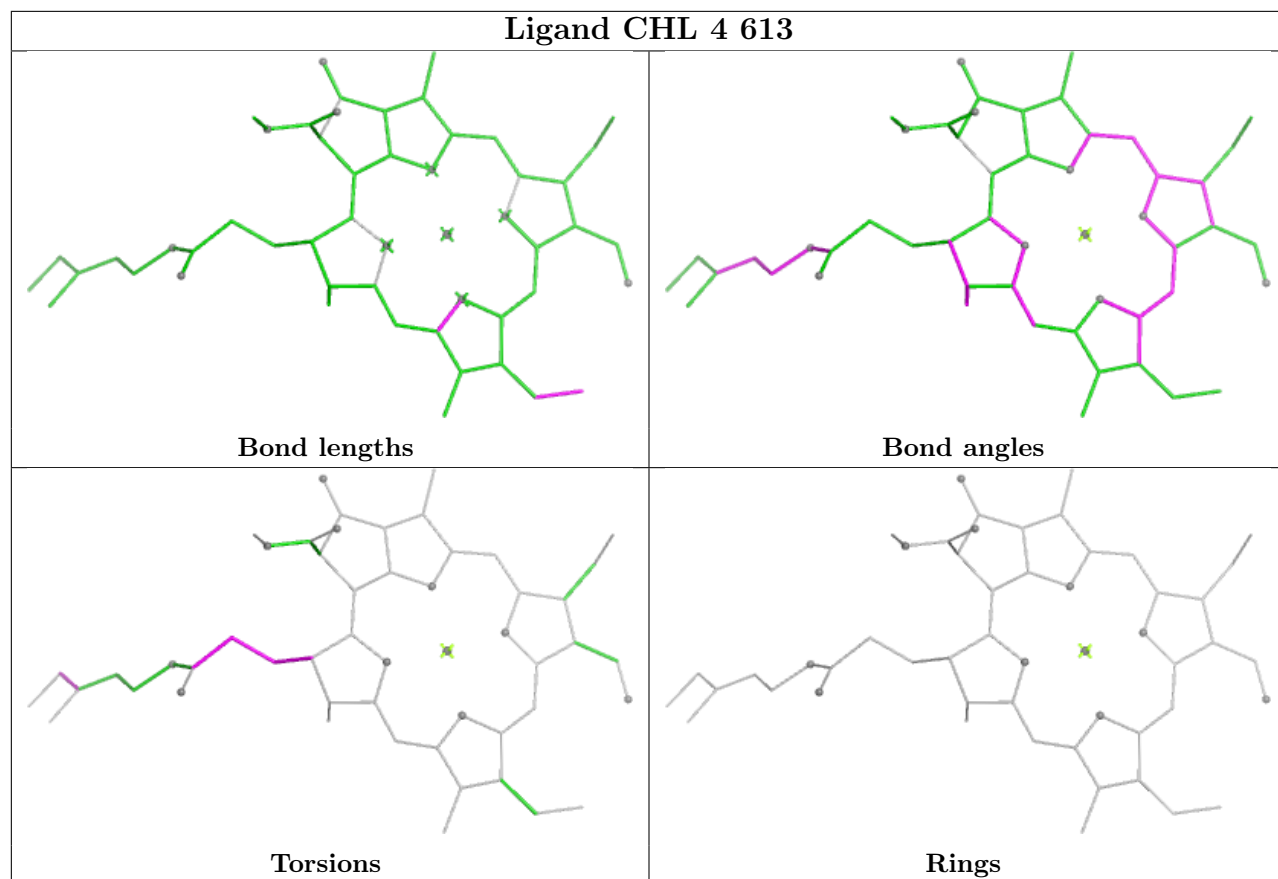
Torsions



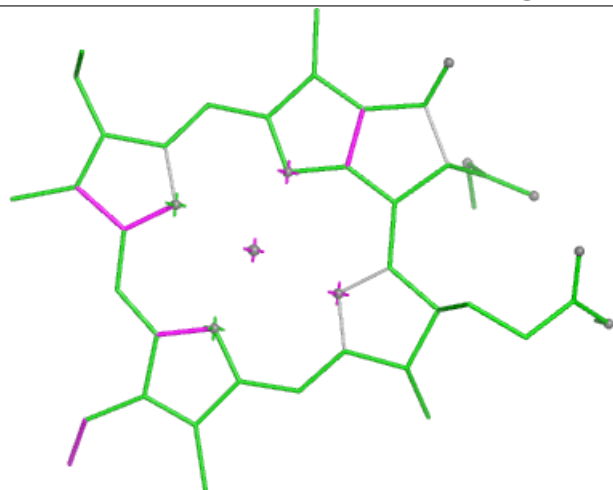
Rings



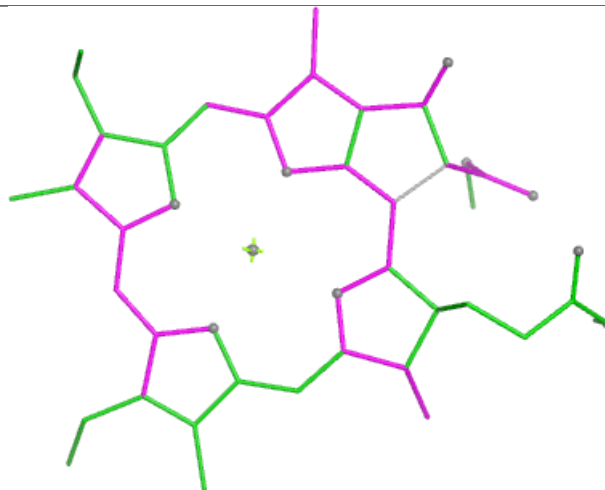
Ligand CHL 4 613



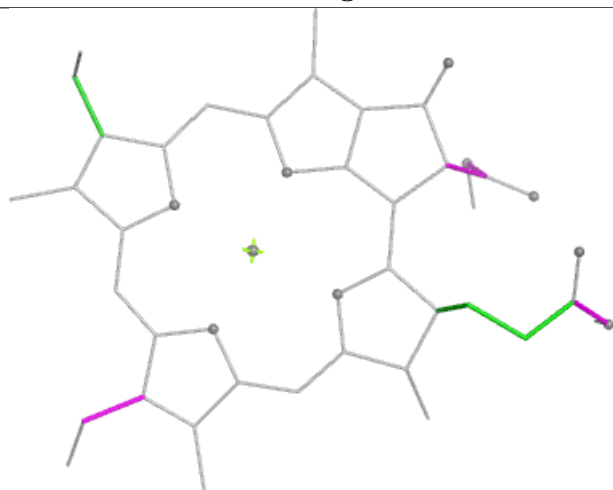
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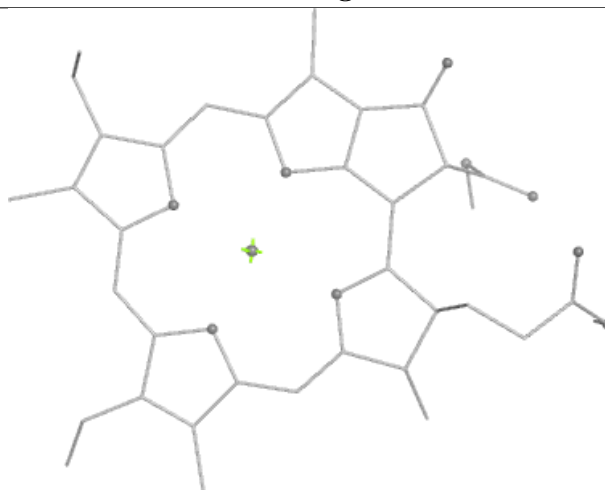
Bond lengths



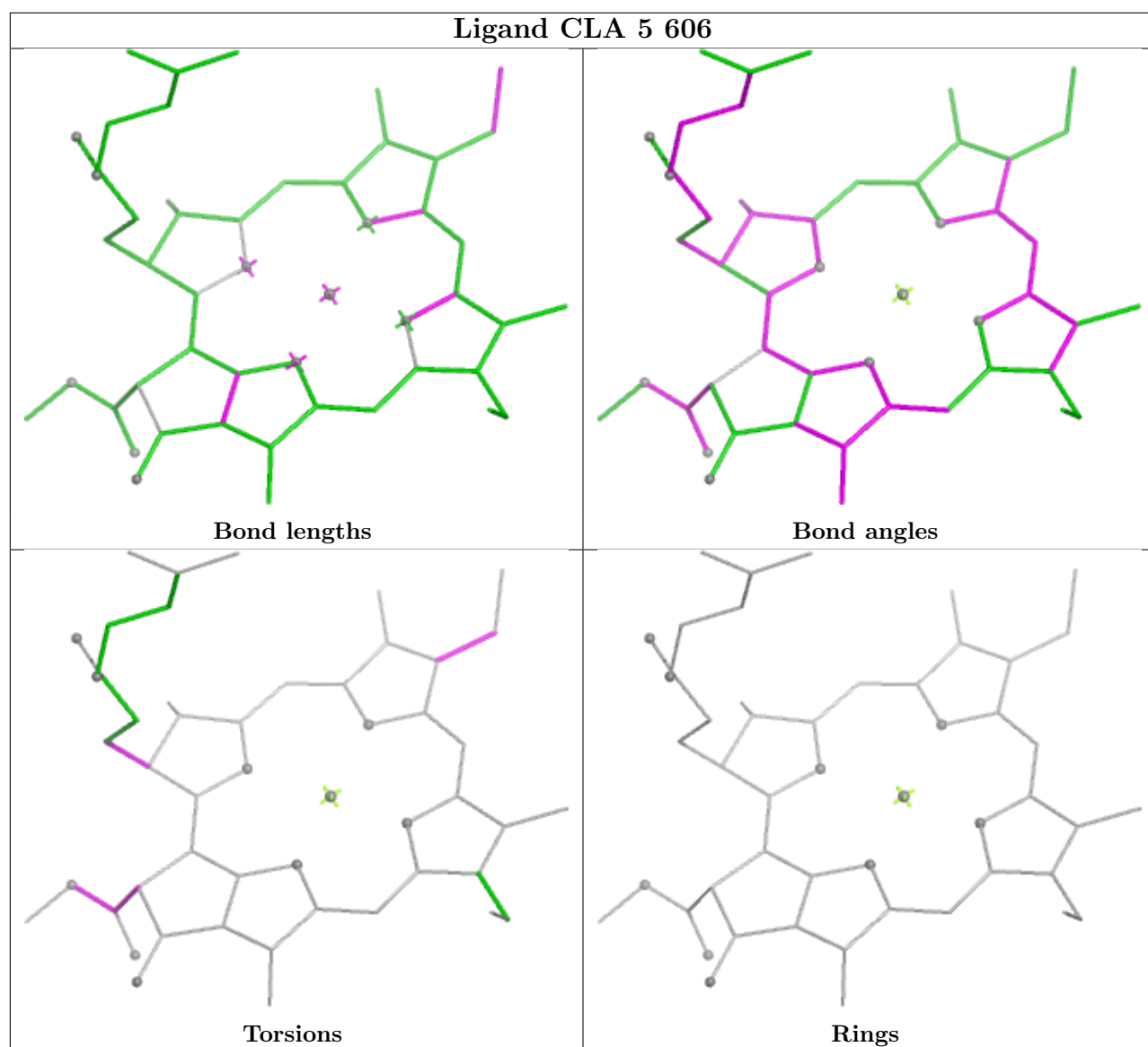
Bond angles



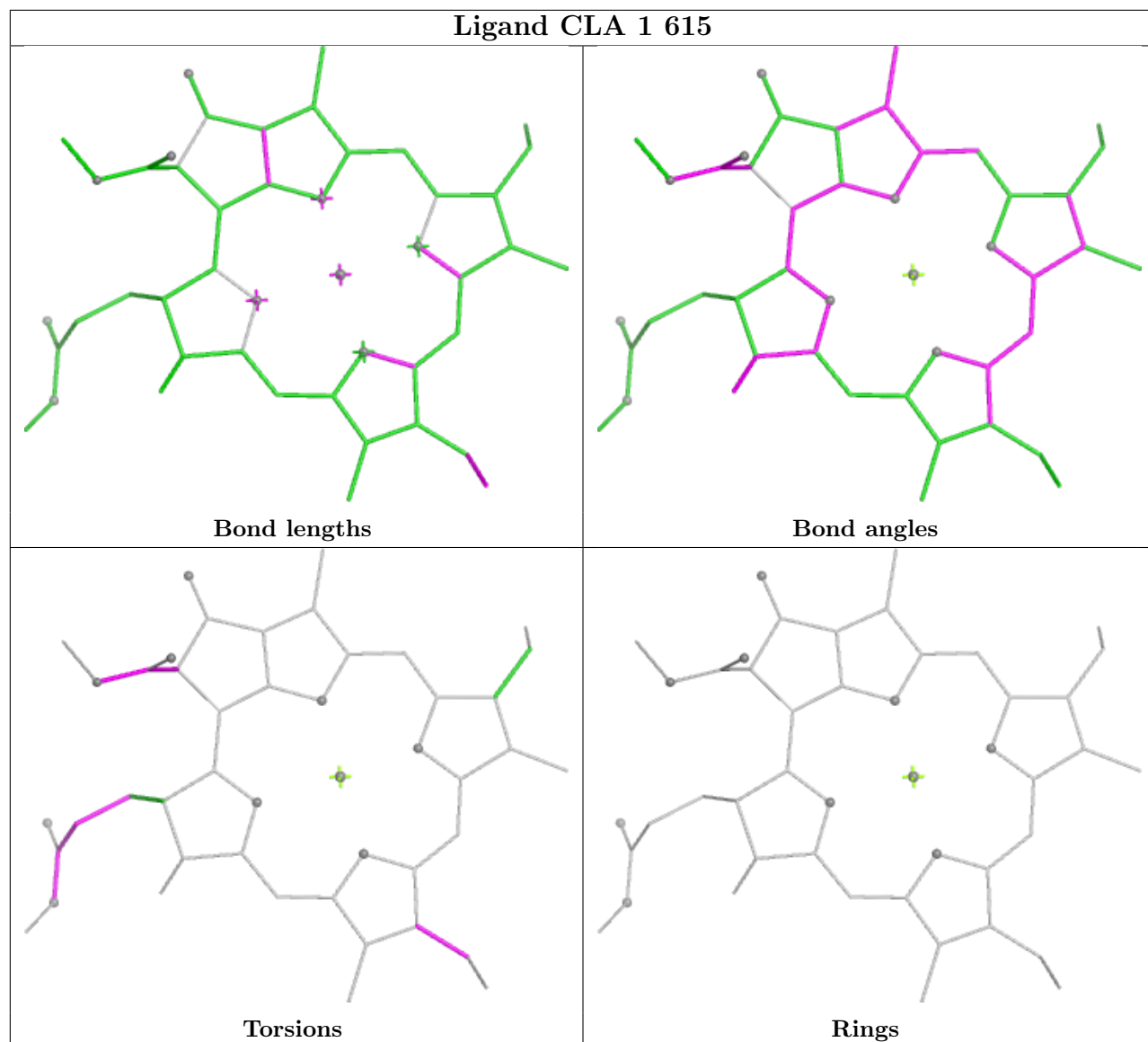
Torsions

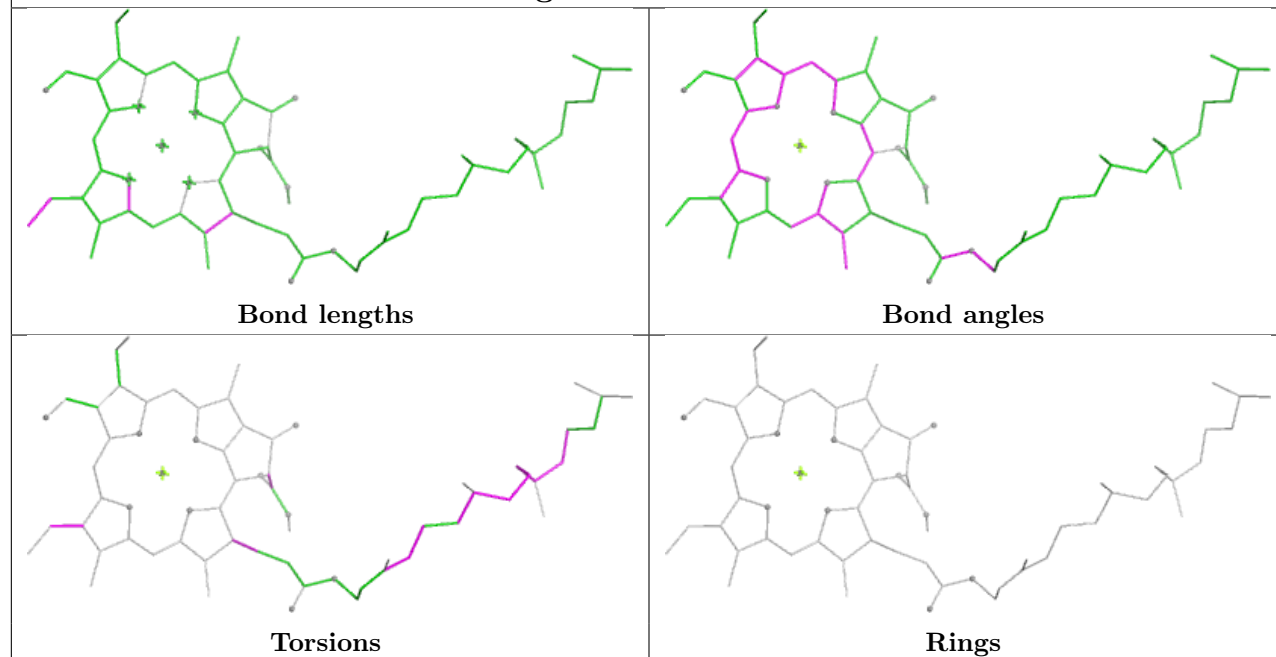
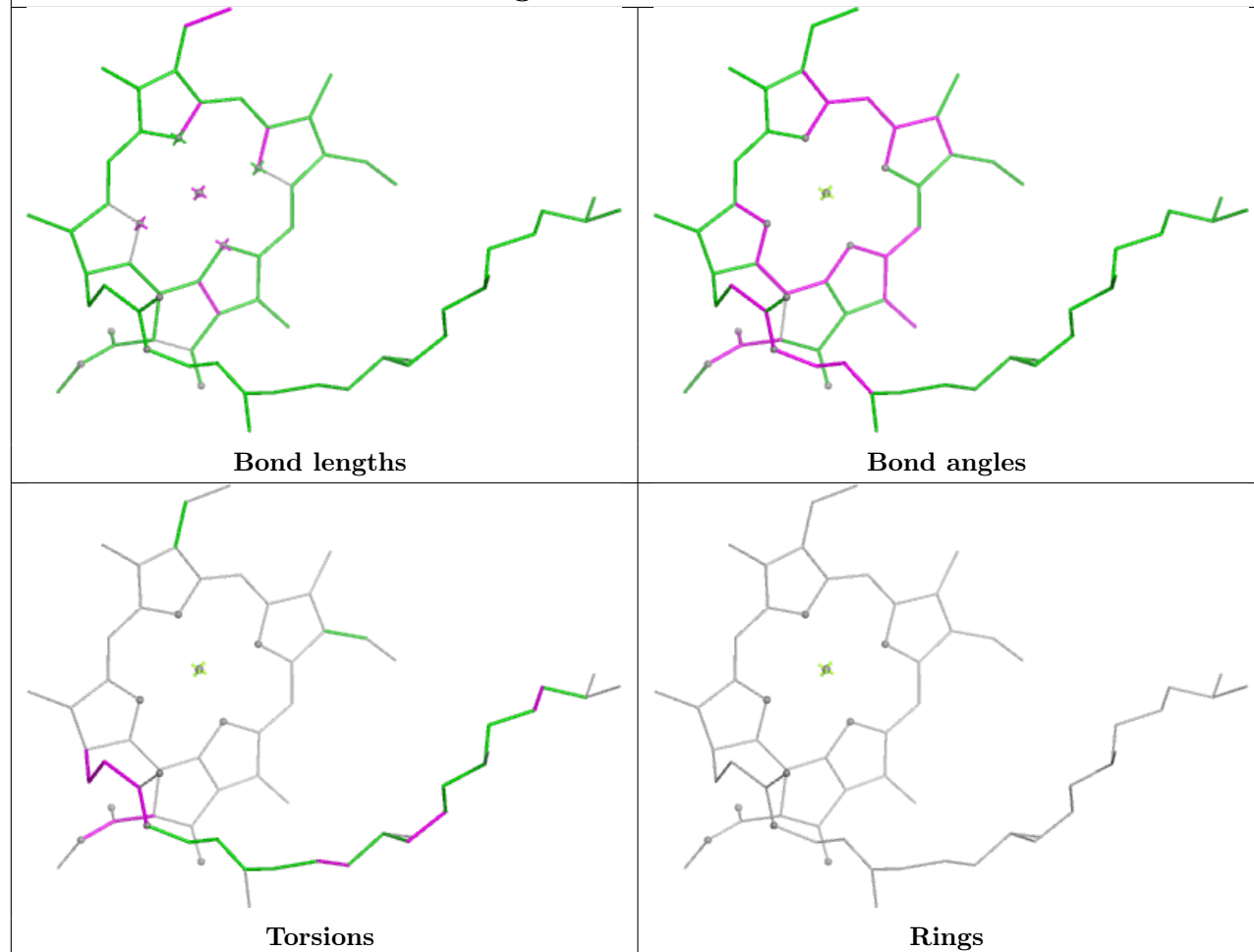


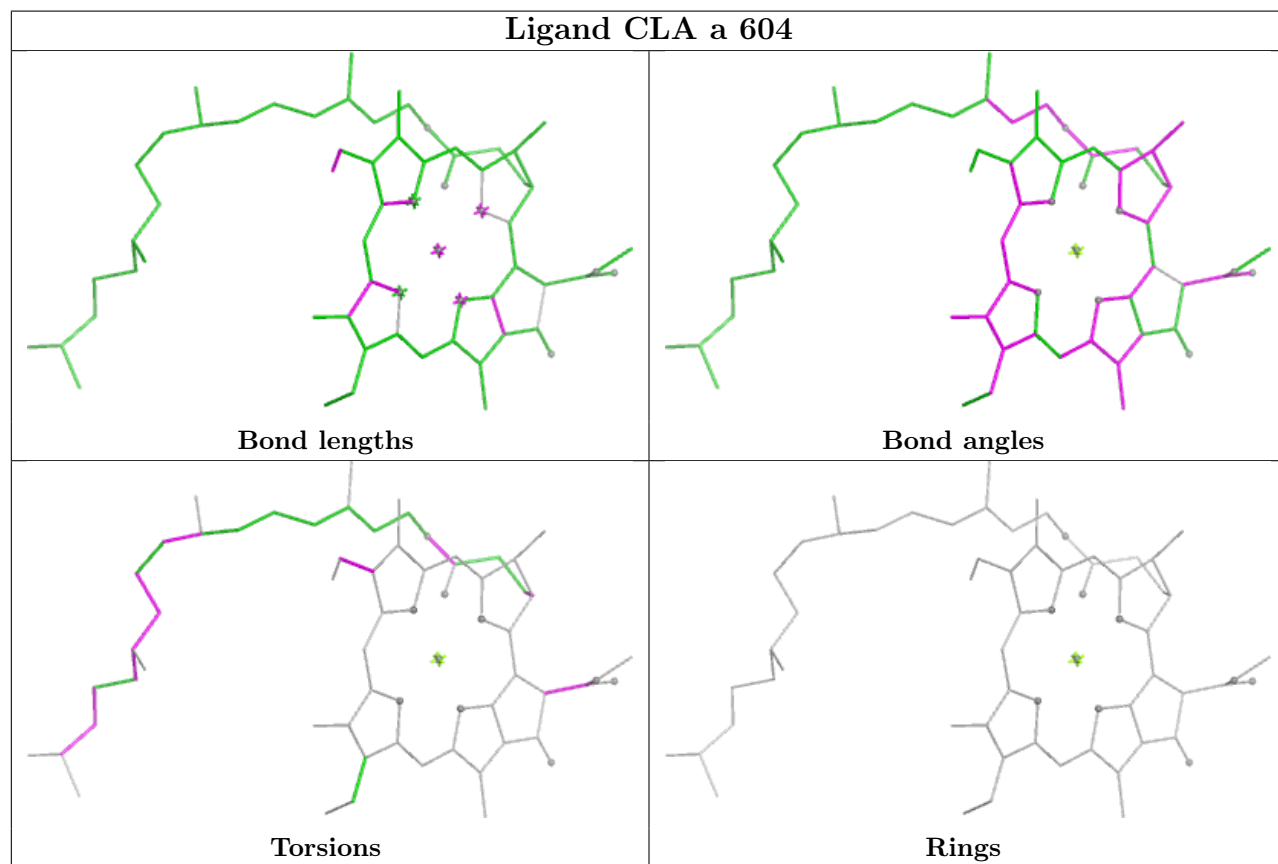
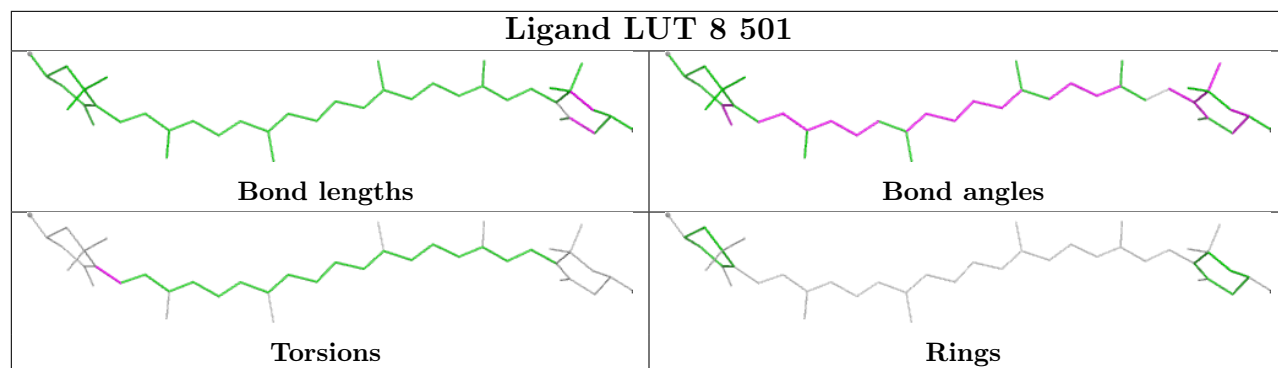
Rings

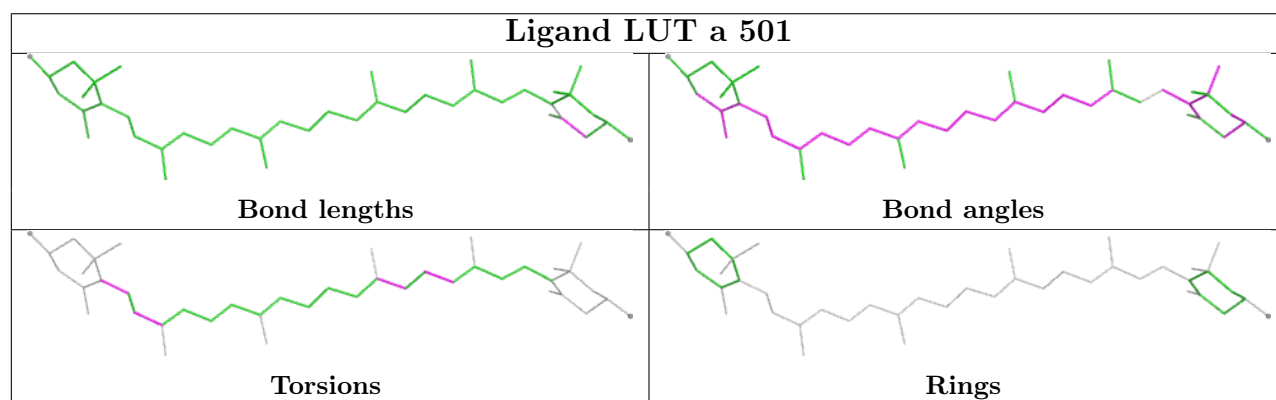
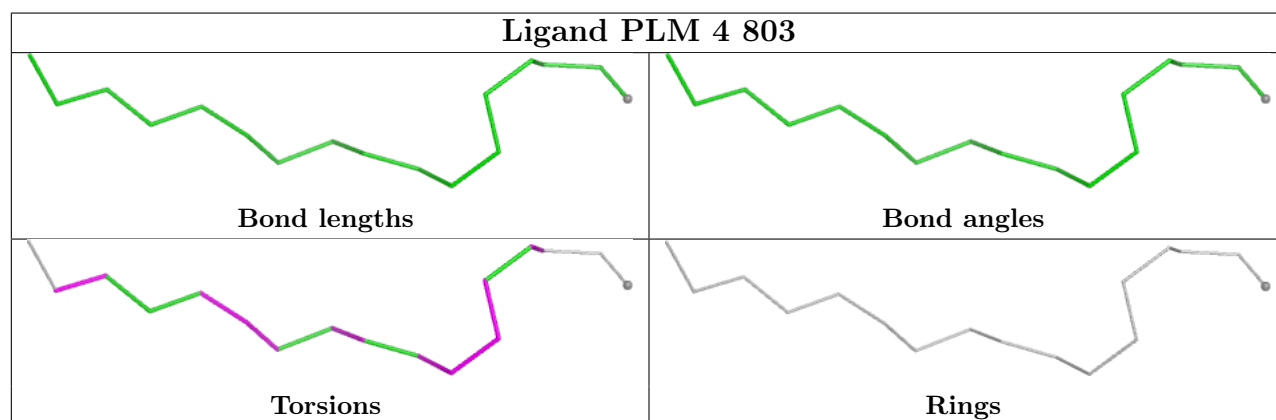
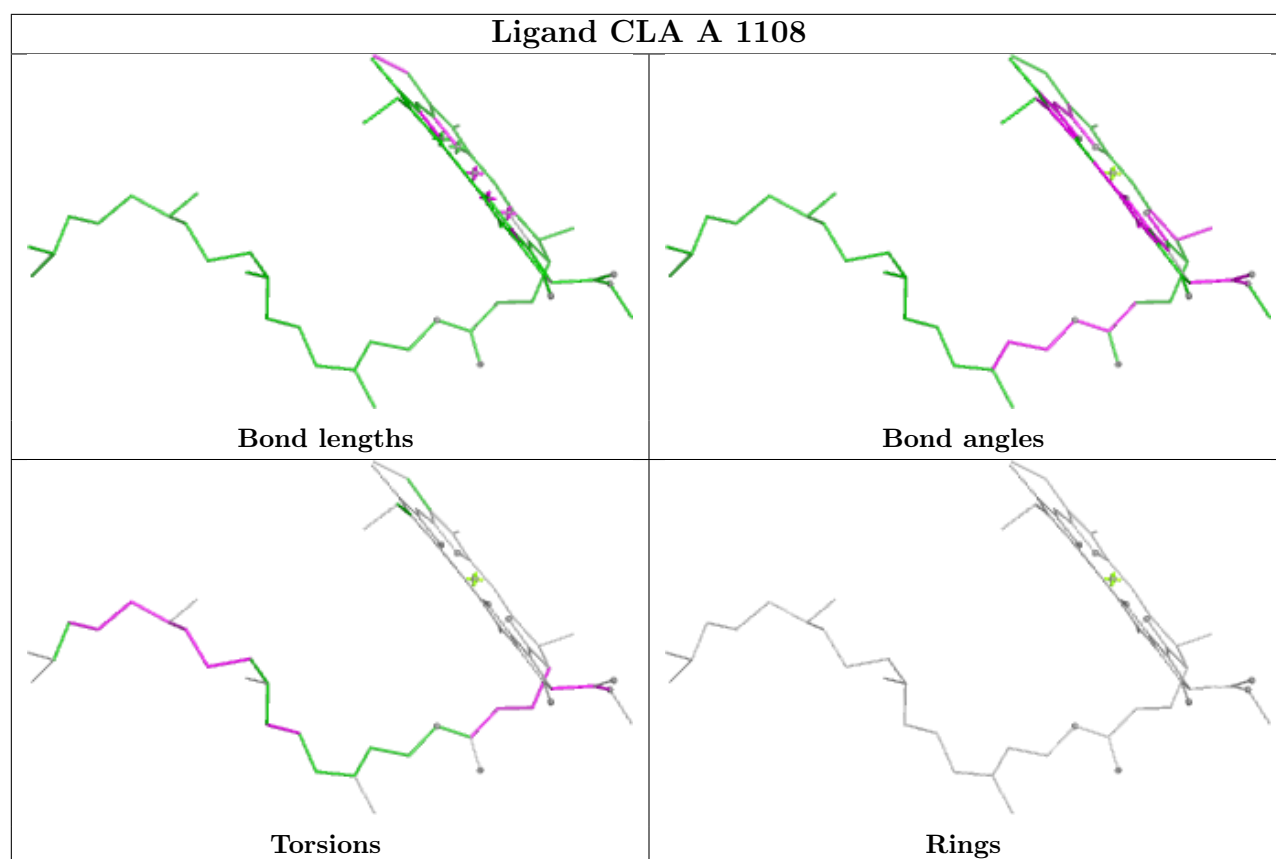


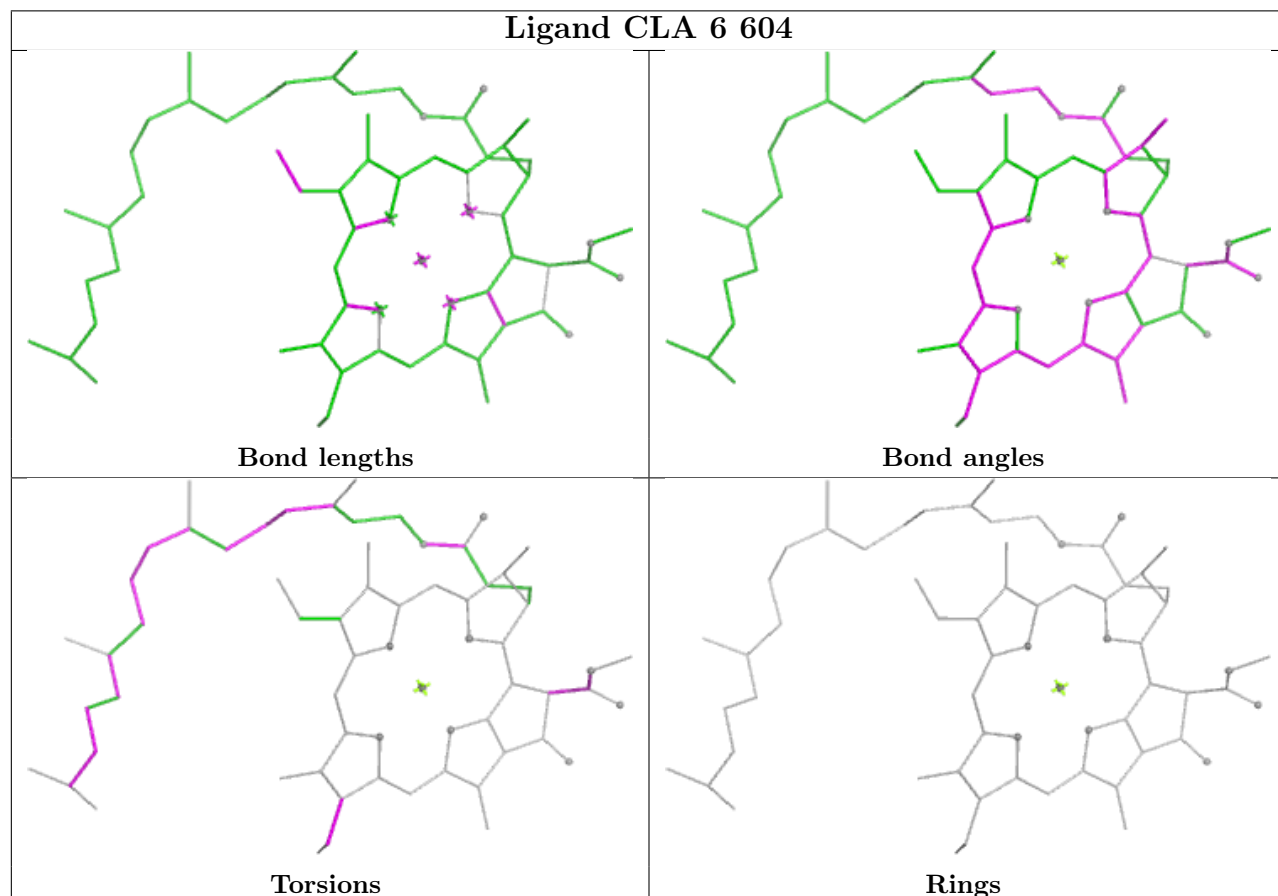
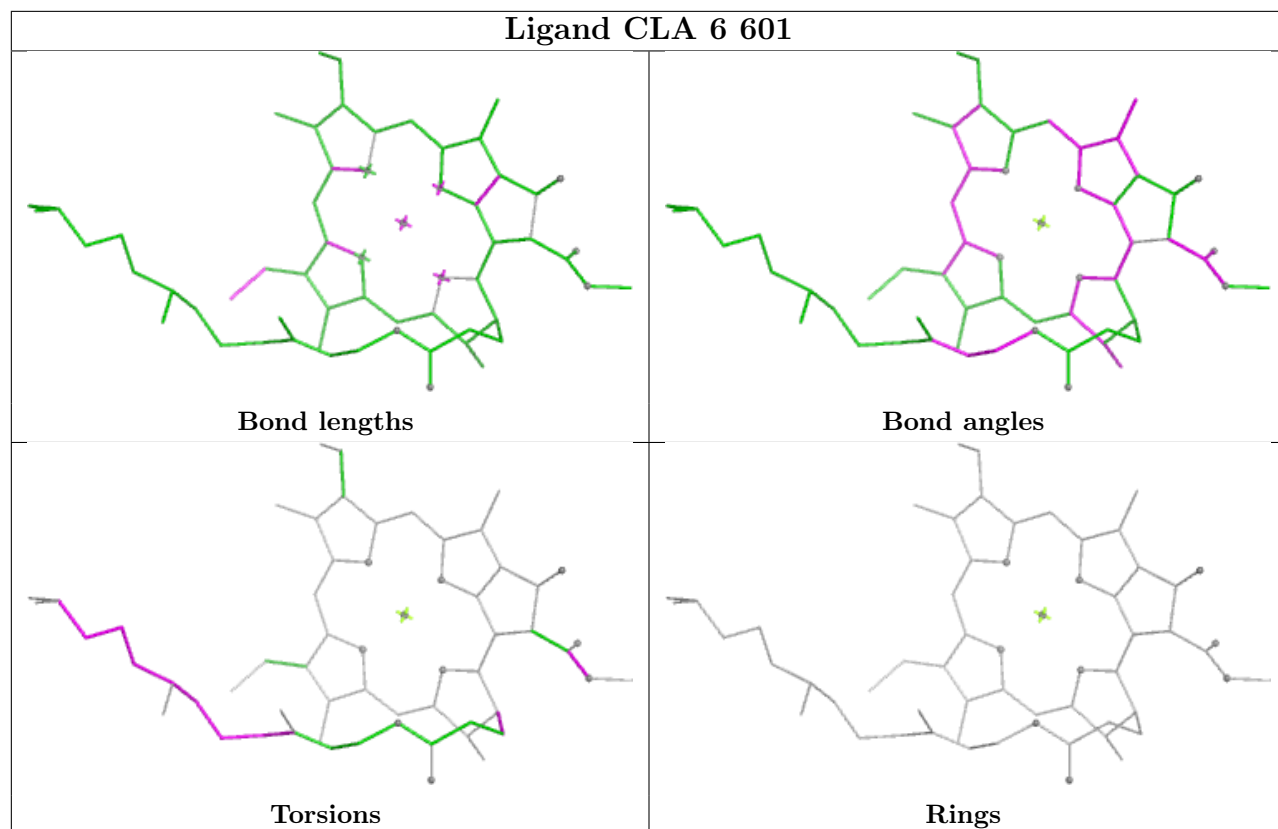
Ligand CLA 1 615



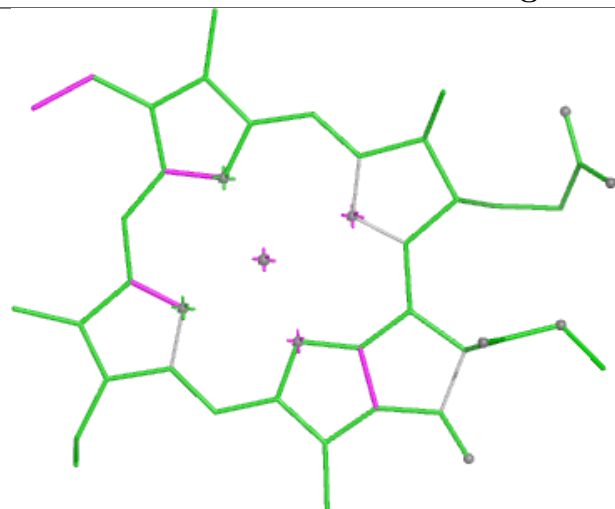
Ligand CHL 6 619**Ligand CLA A 1127**



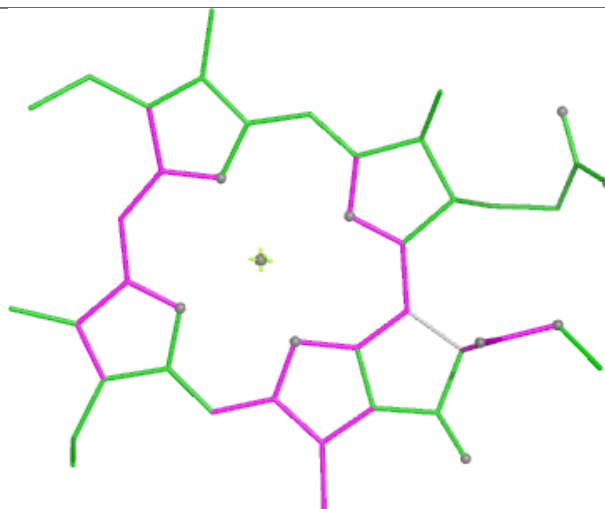




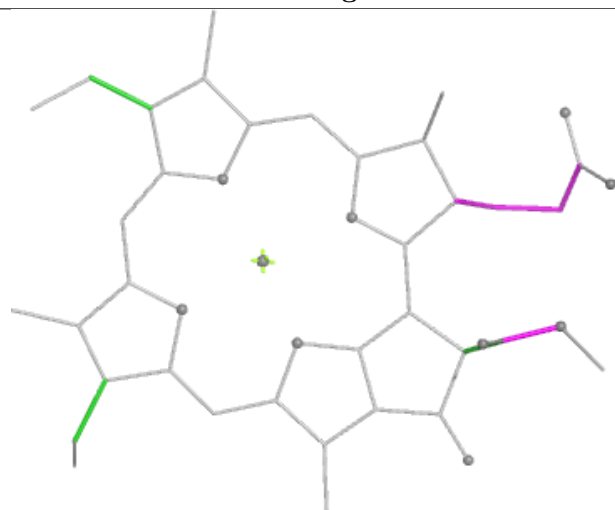
Ligand CLA 1 602



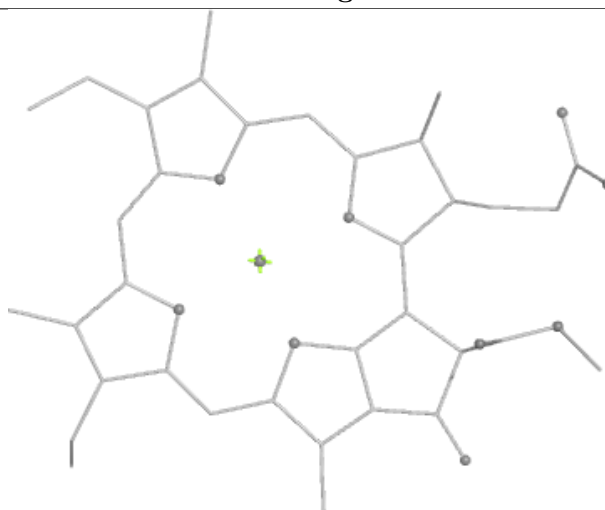
Bond lengths



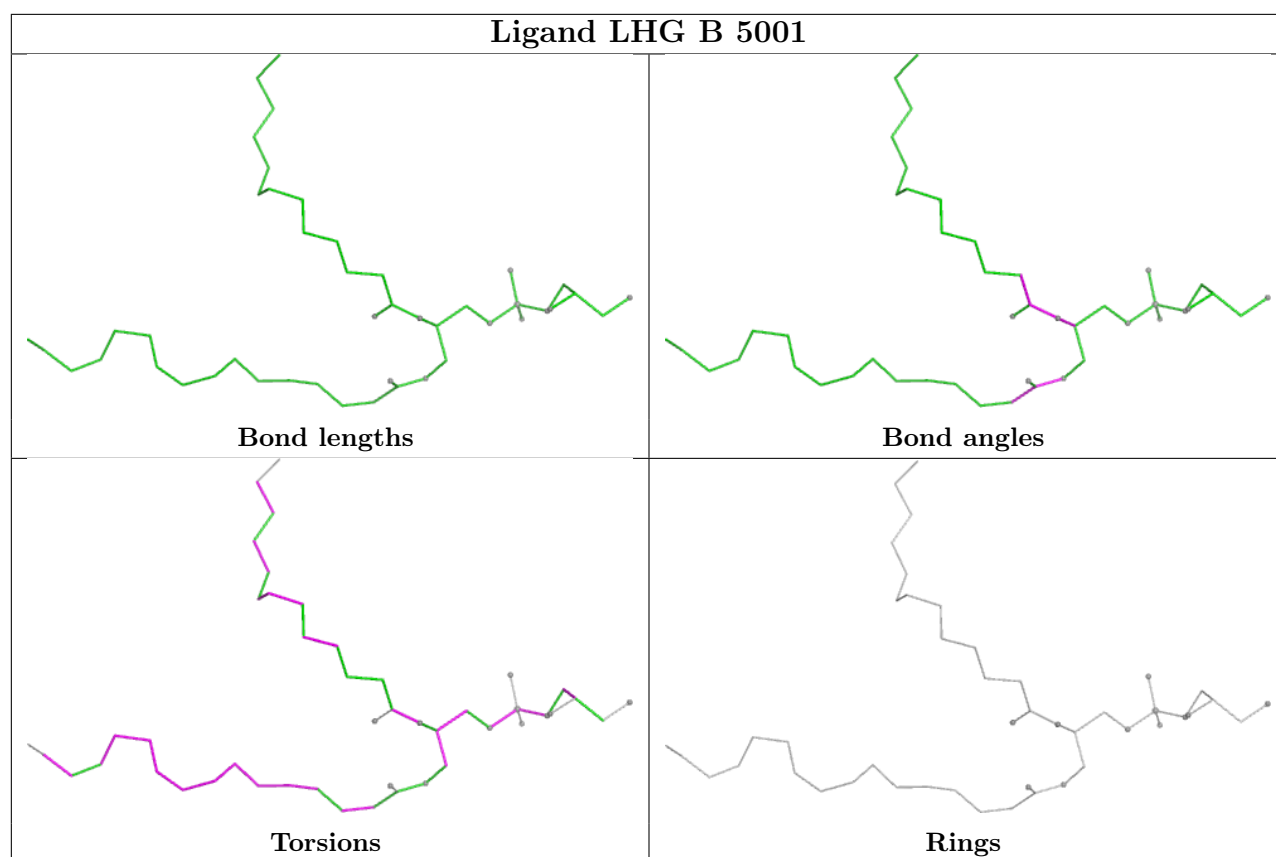
Bond angles

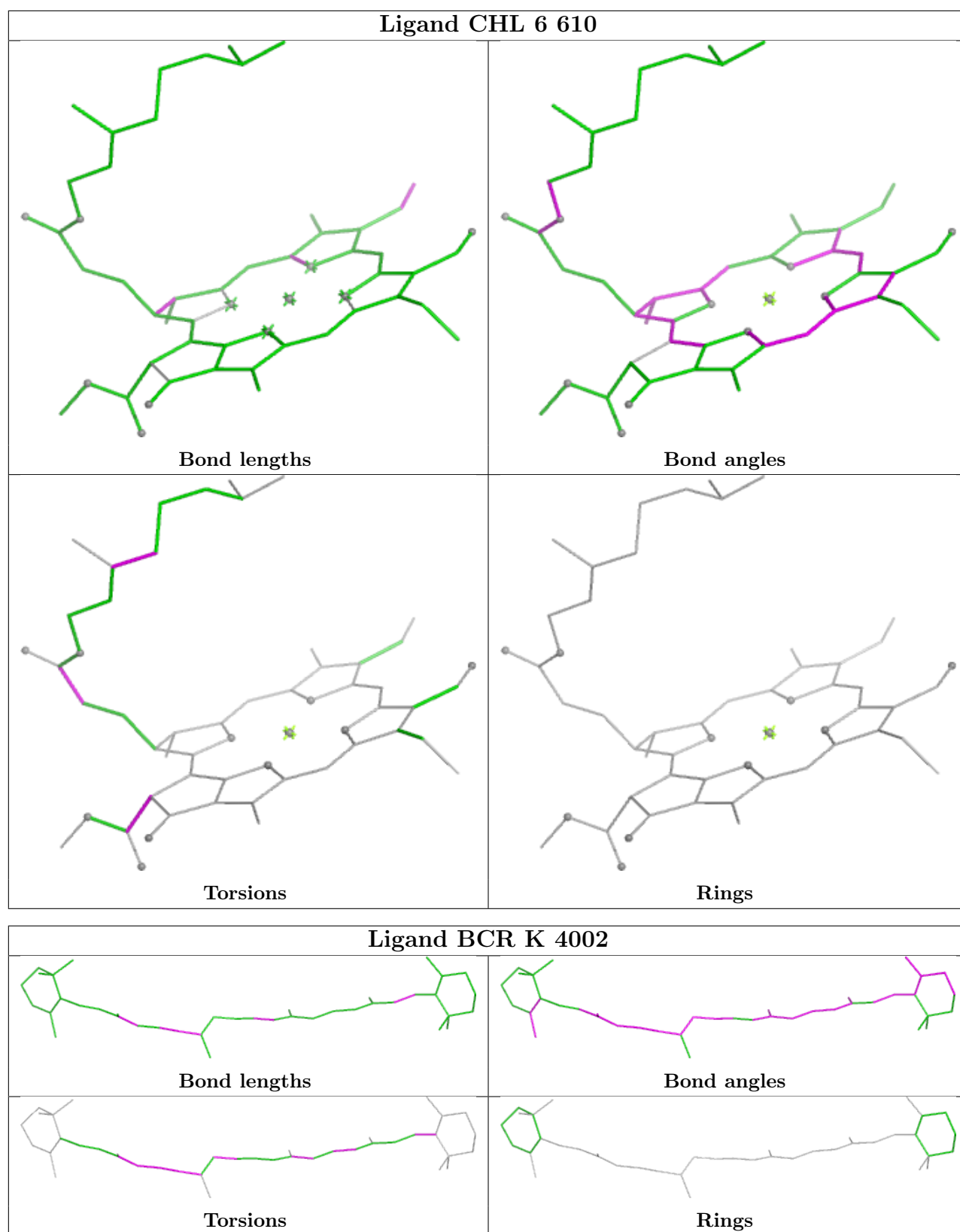


Torsions

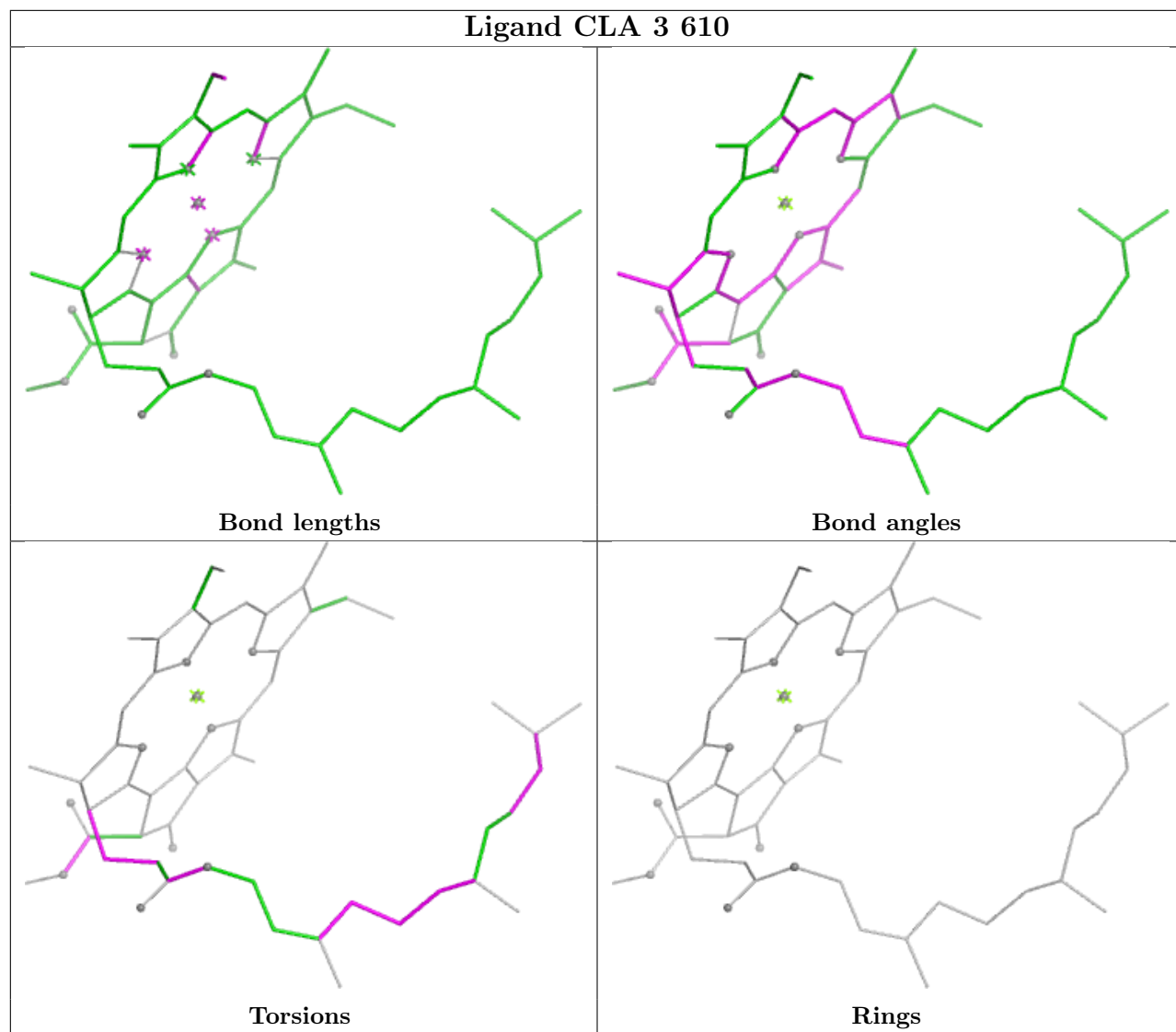


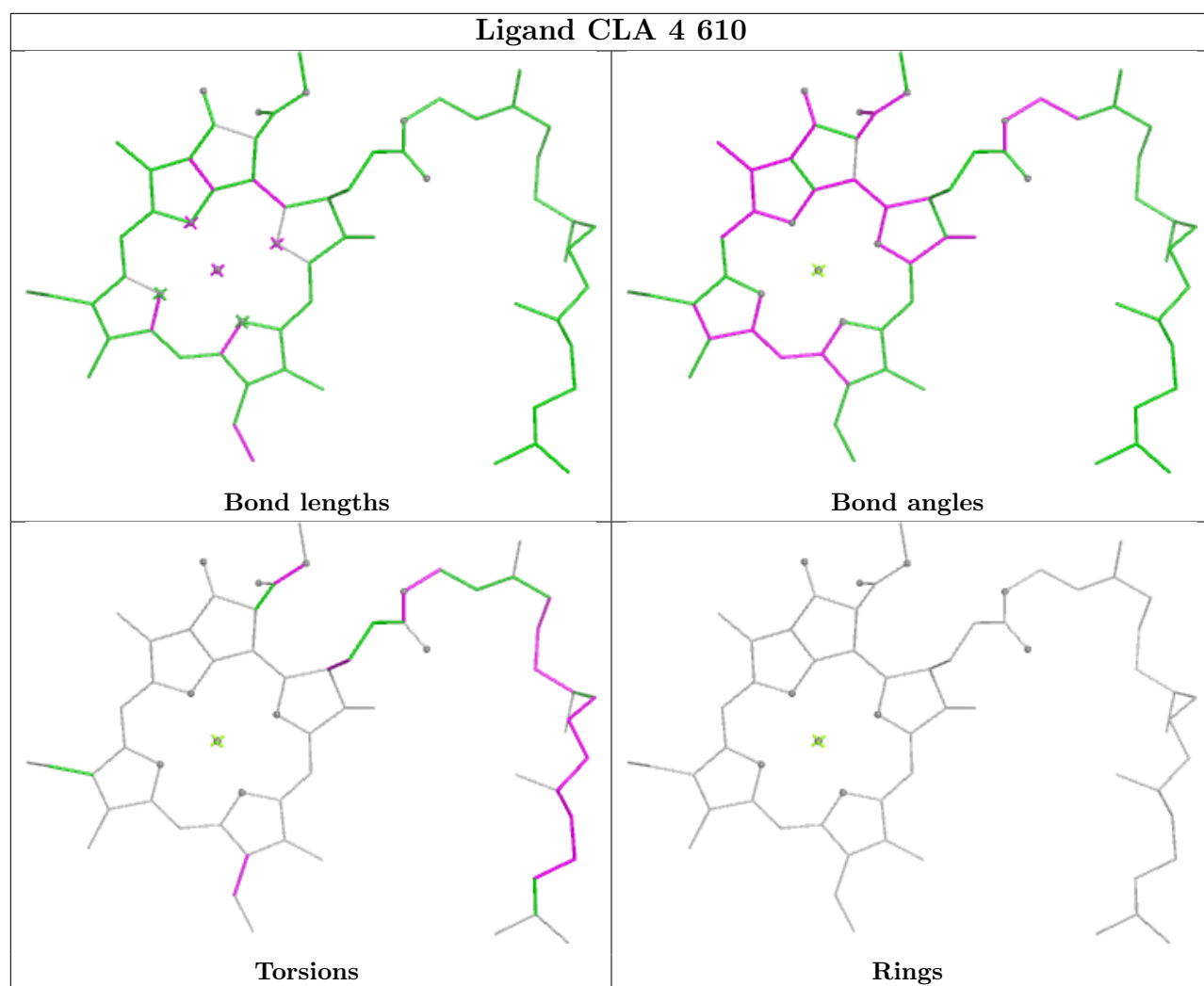
Rings

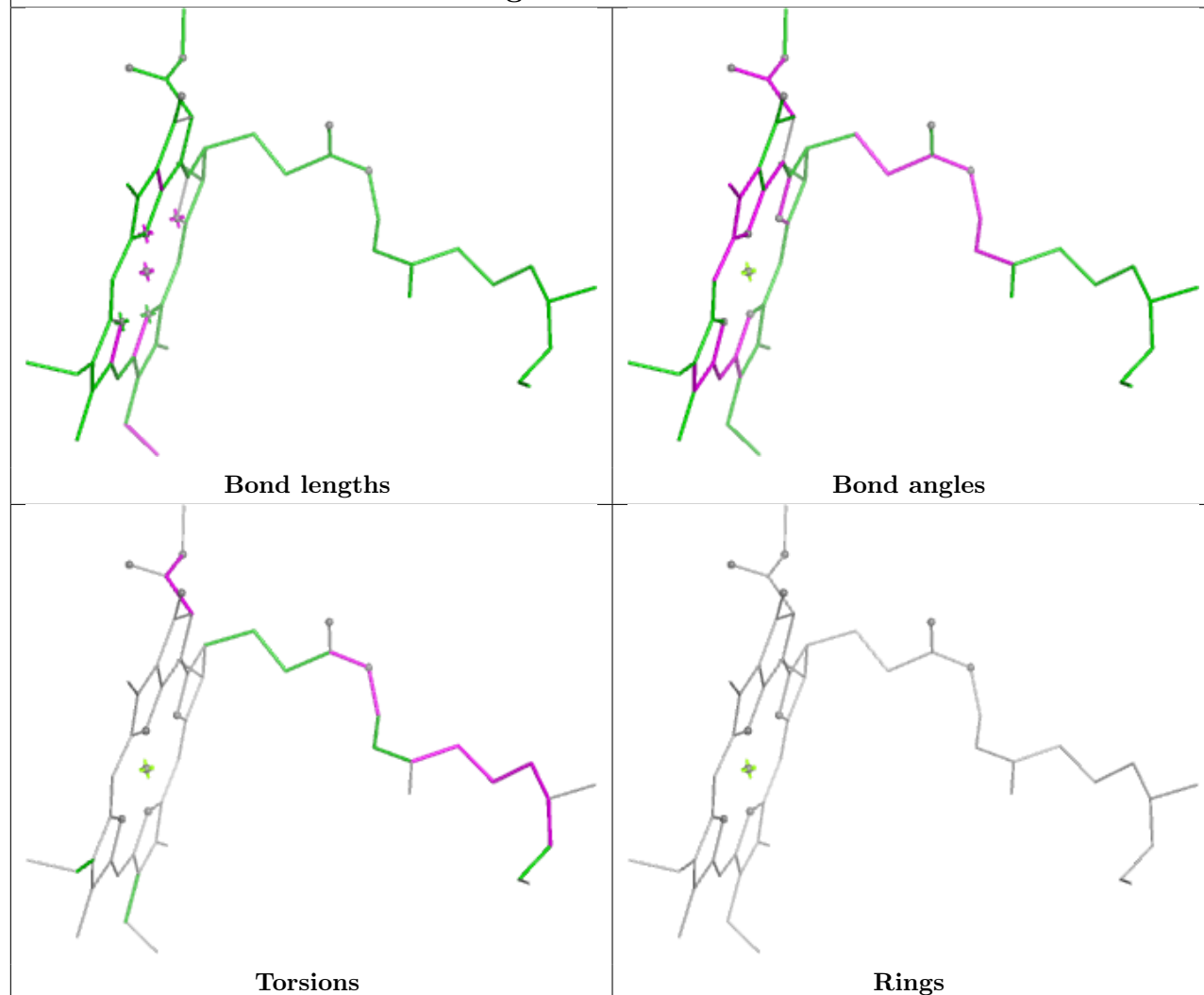
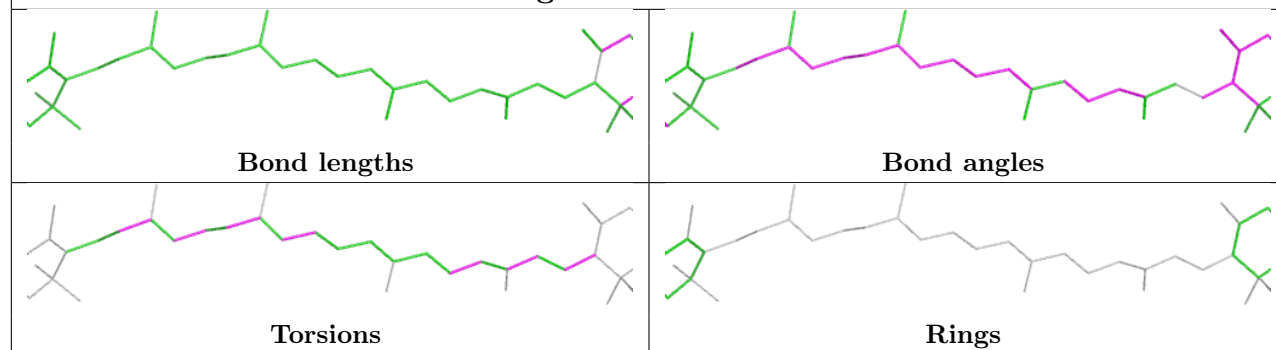


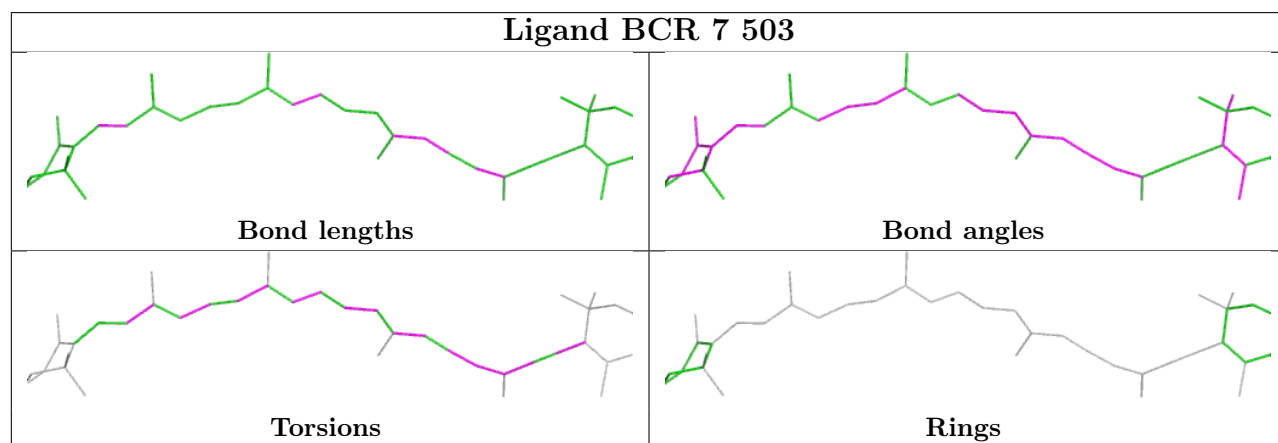
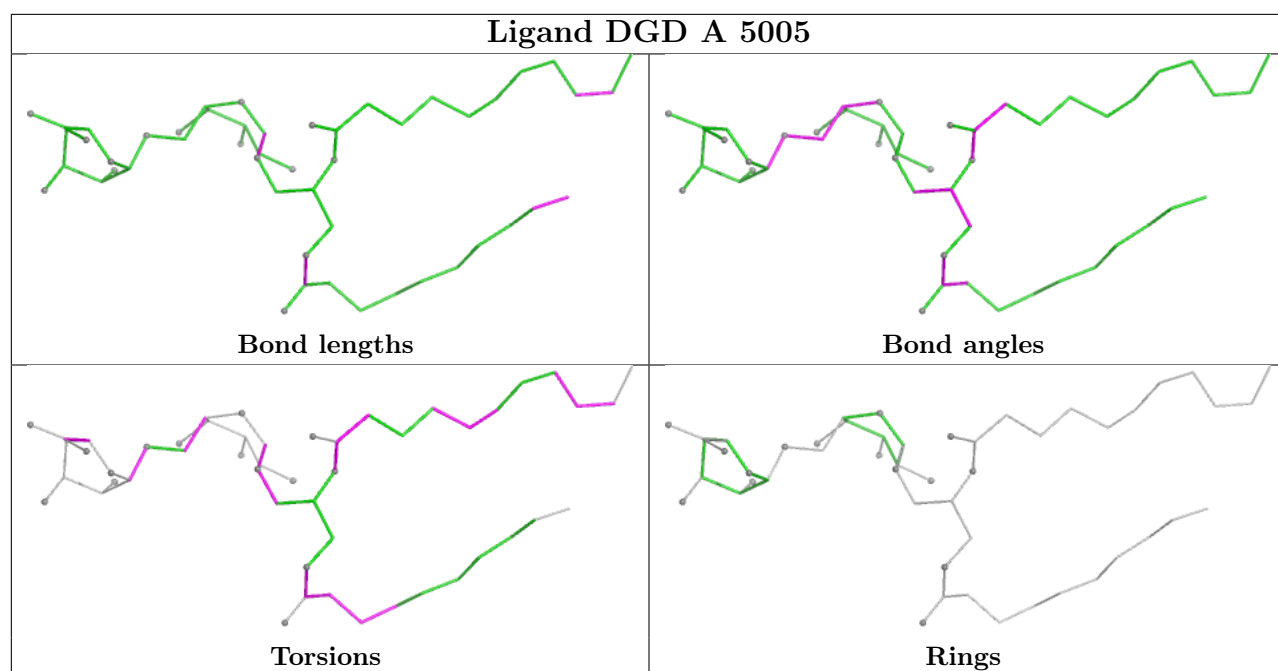


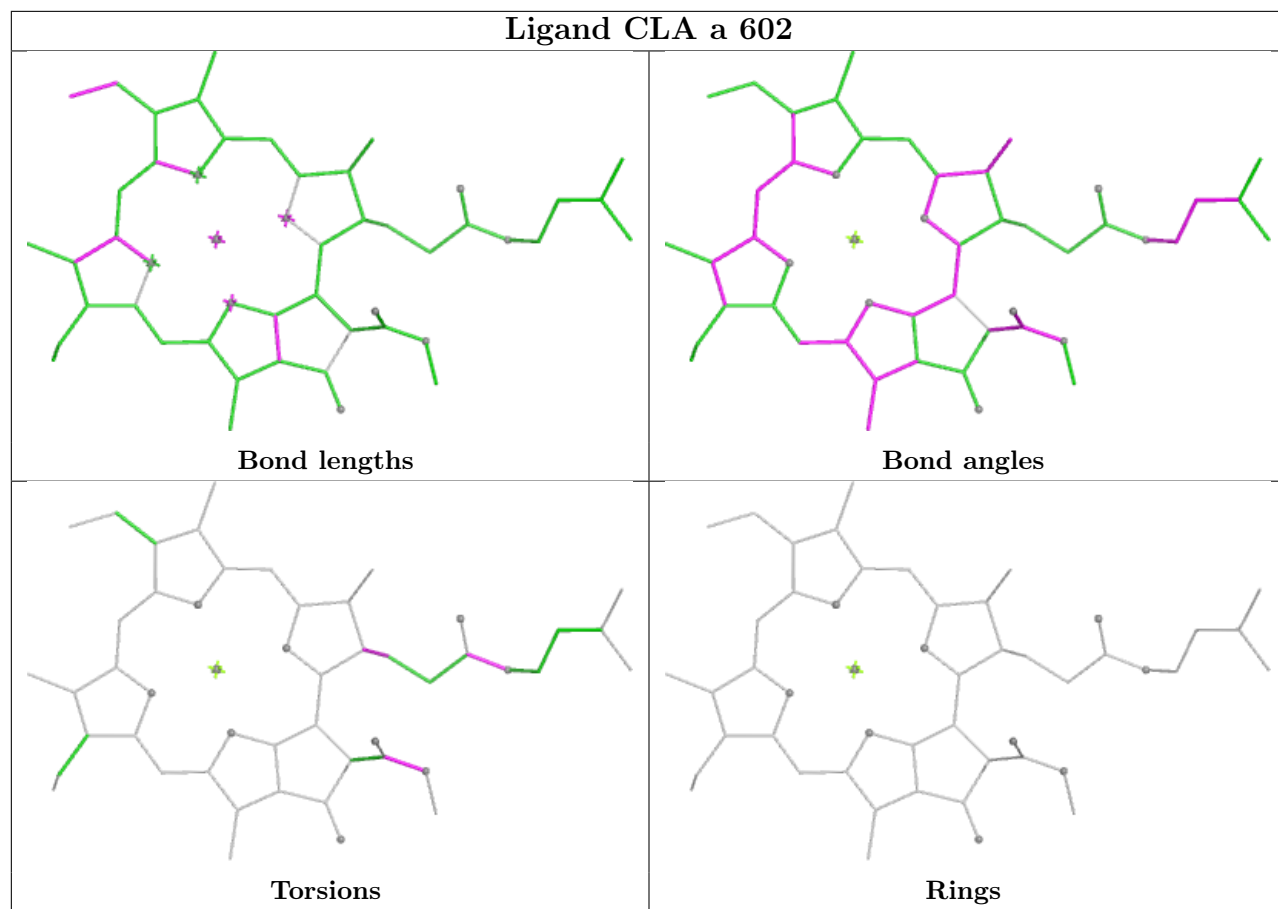
Ligand CLA 3 610

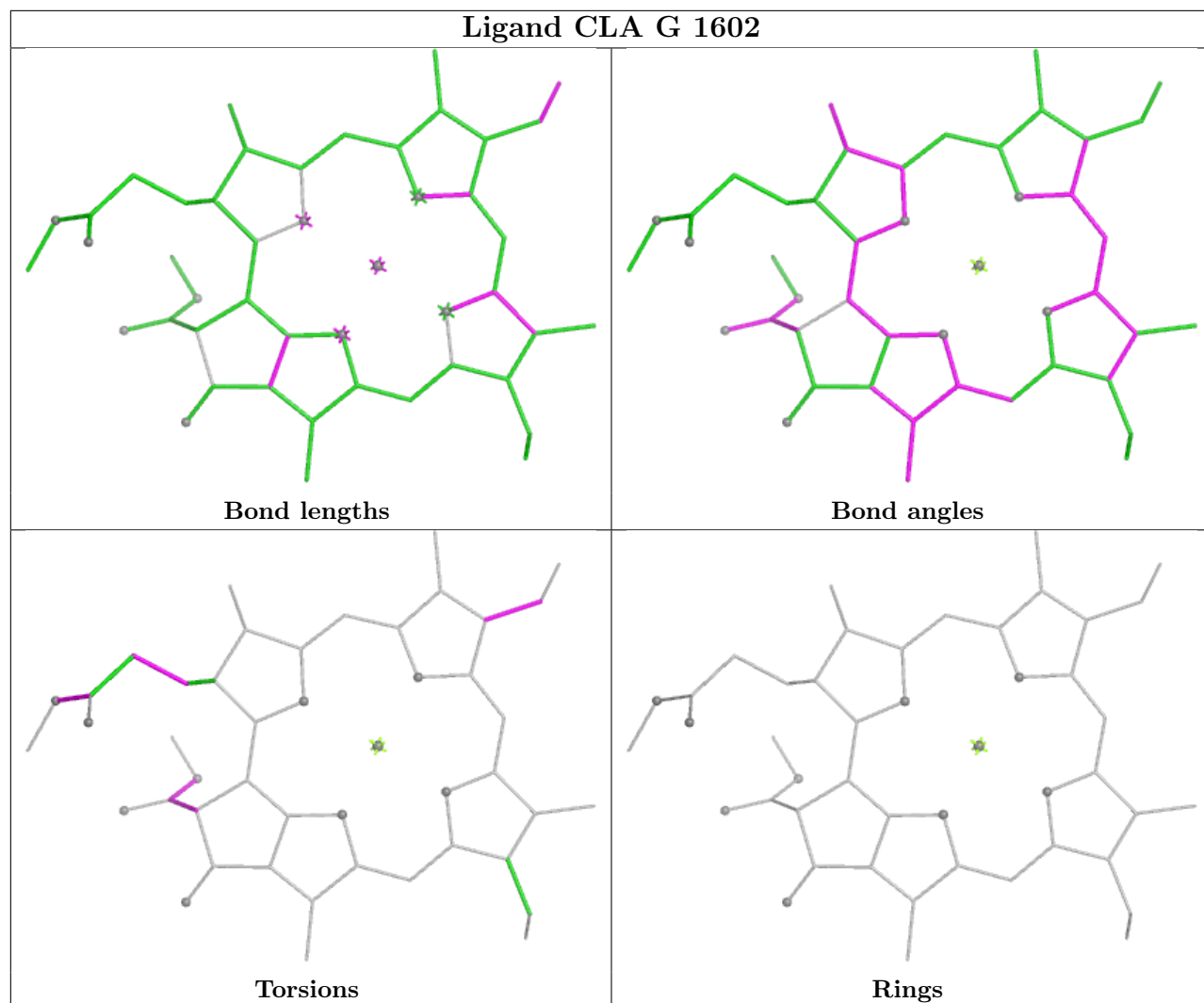




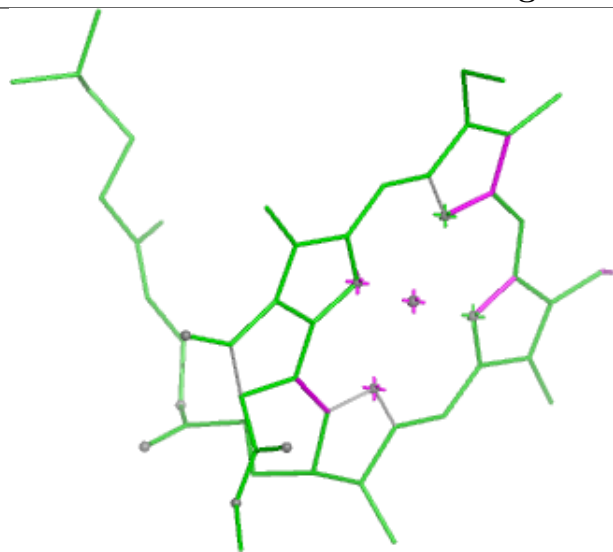
Ligand CLA 8 606**Ligand LUT a 502**



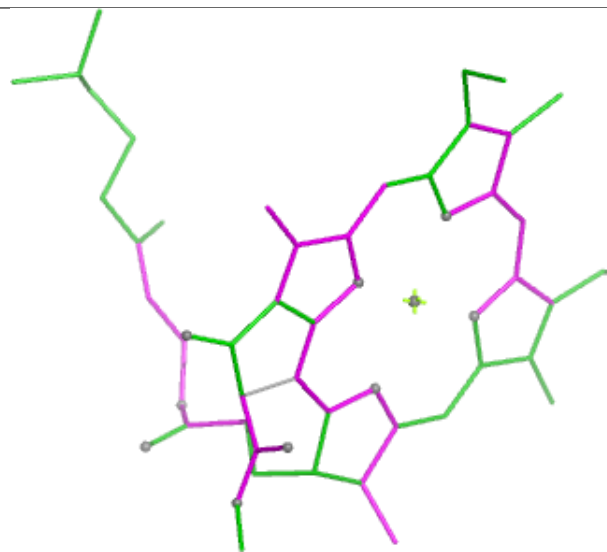




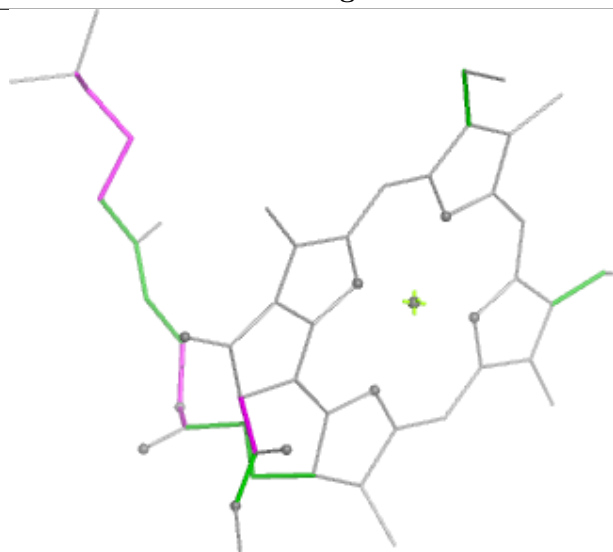
Ligand CLA 6 607



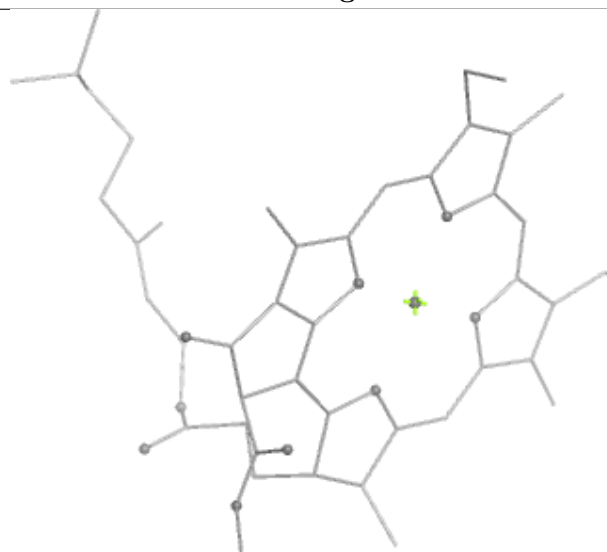
Bond lengths



Bond angles

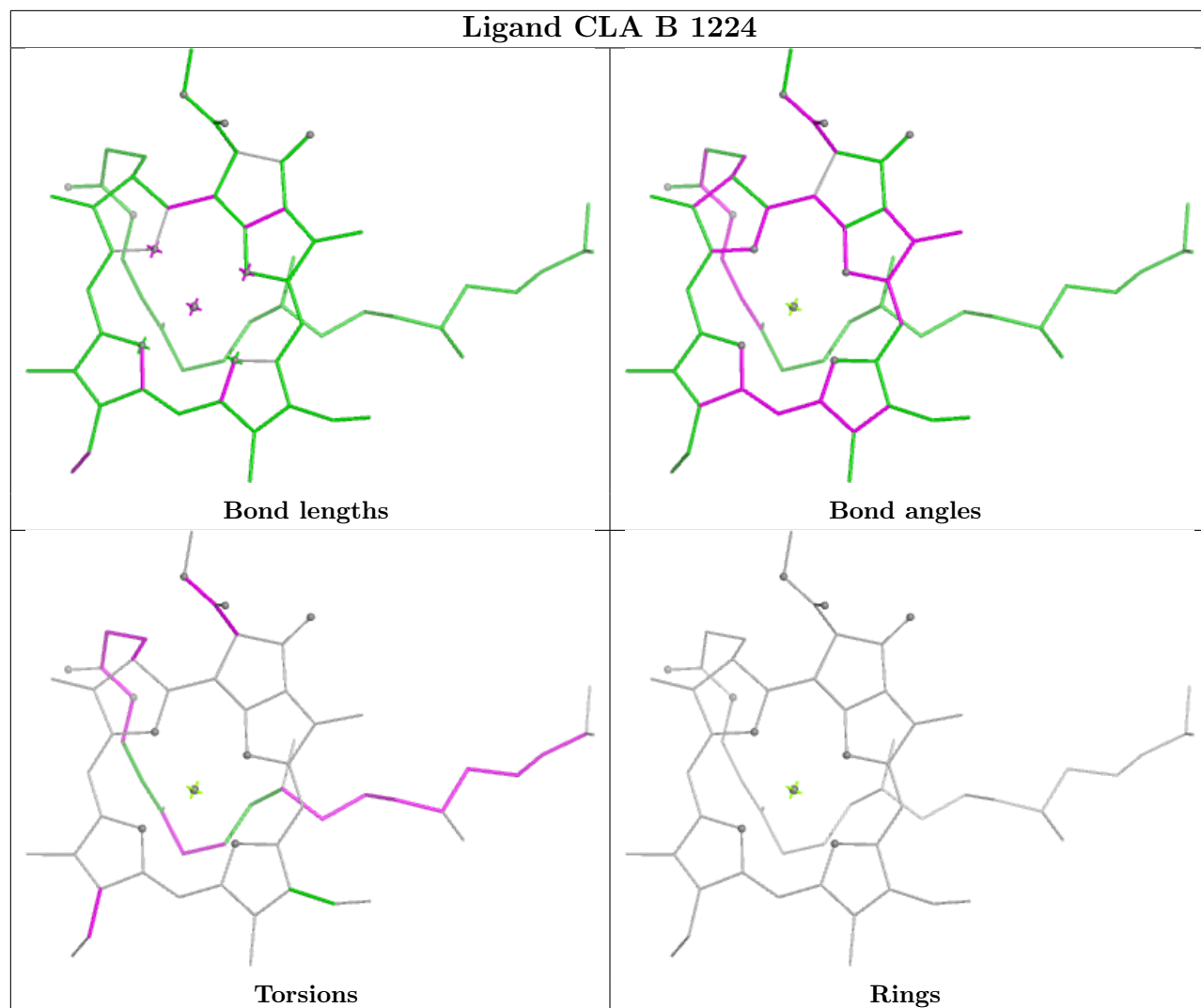


Torsions

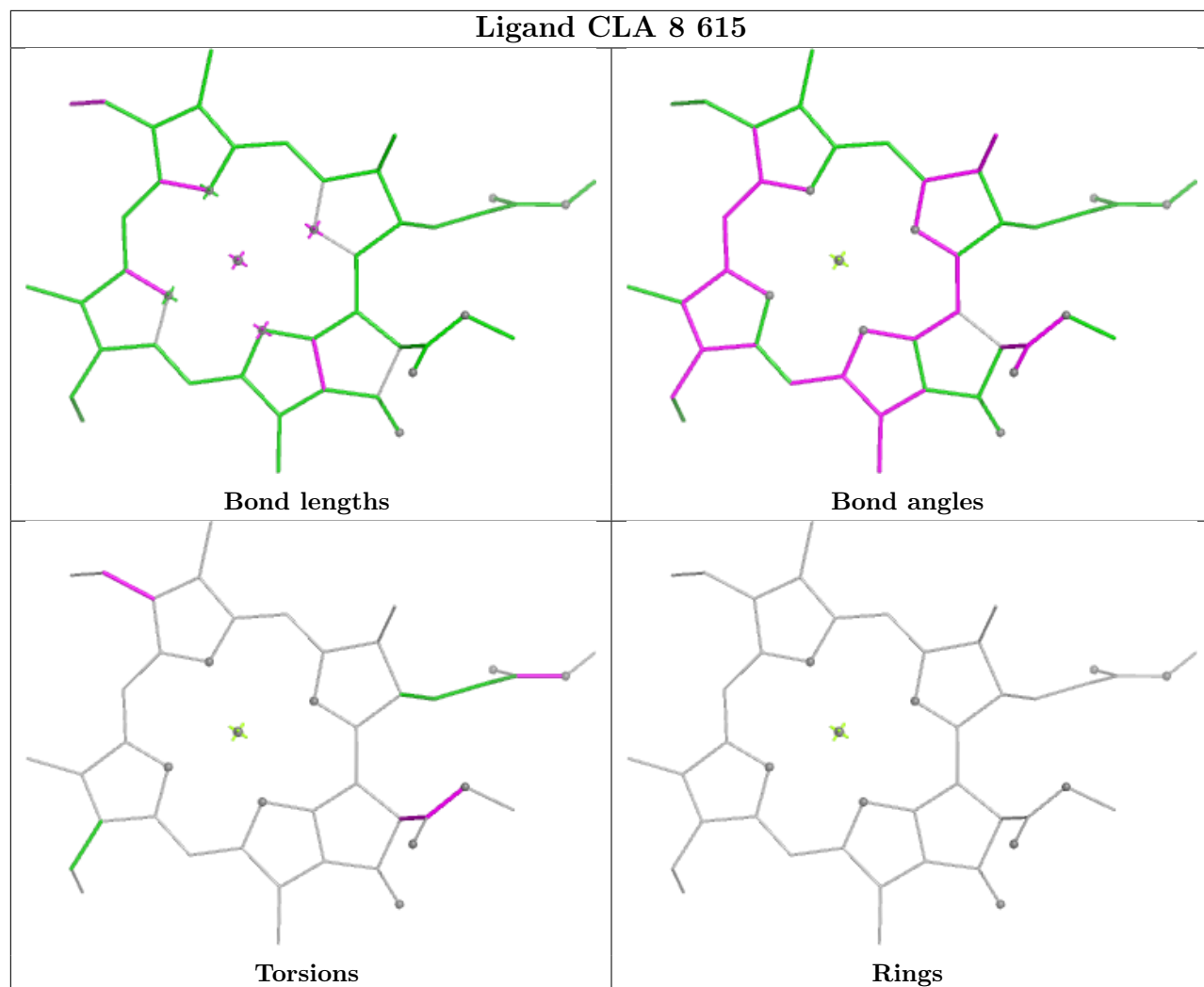


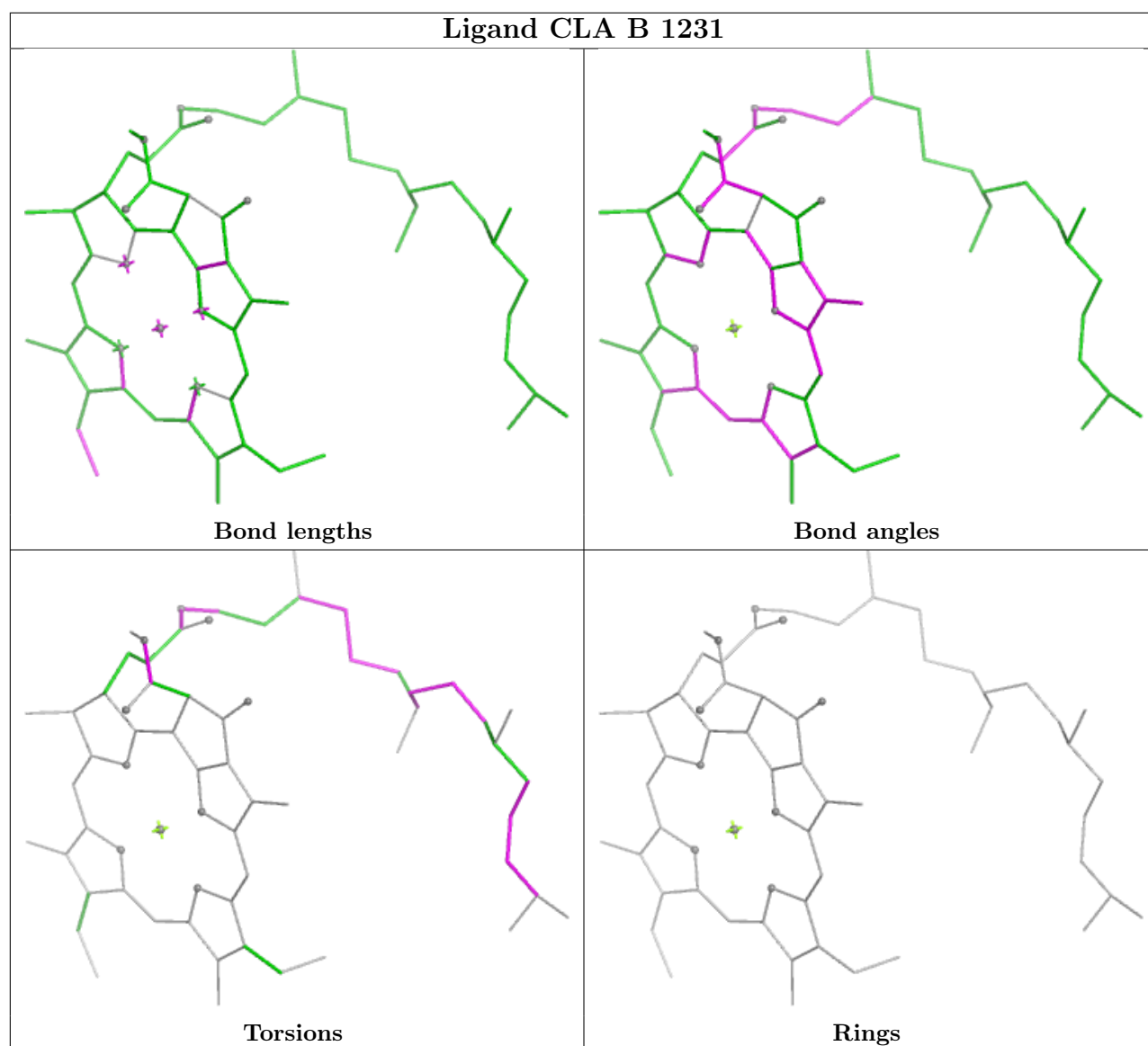
Rings

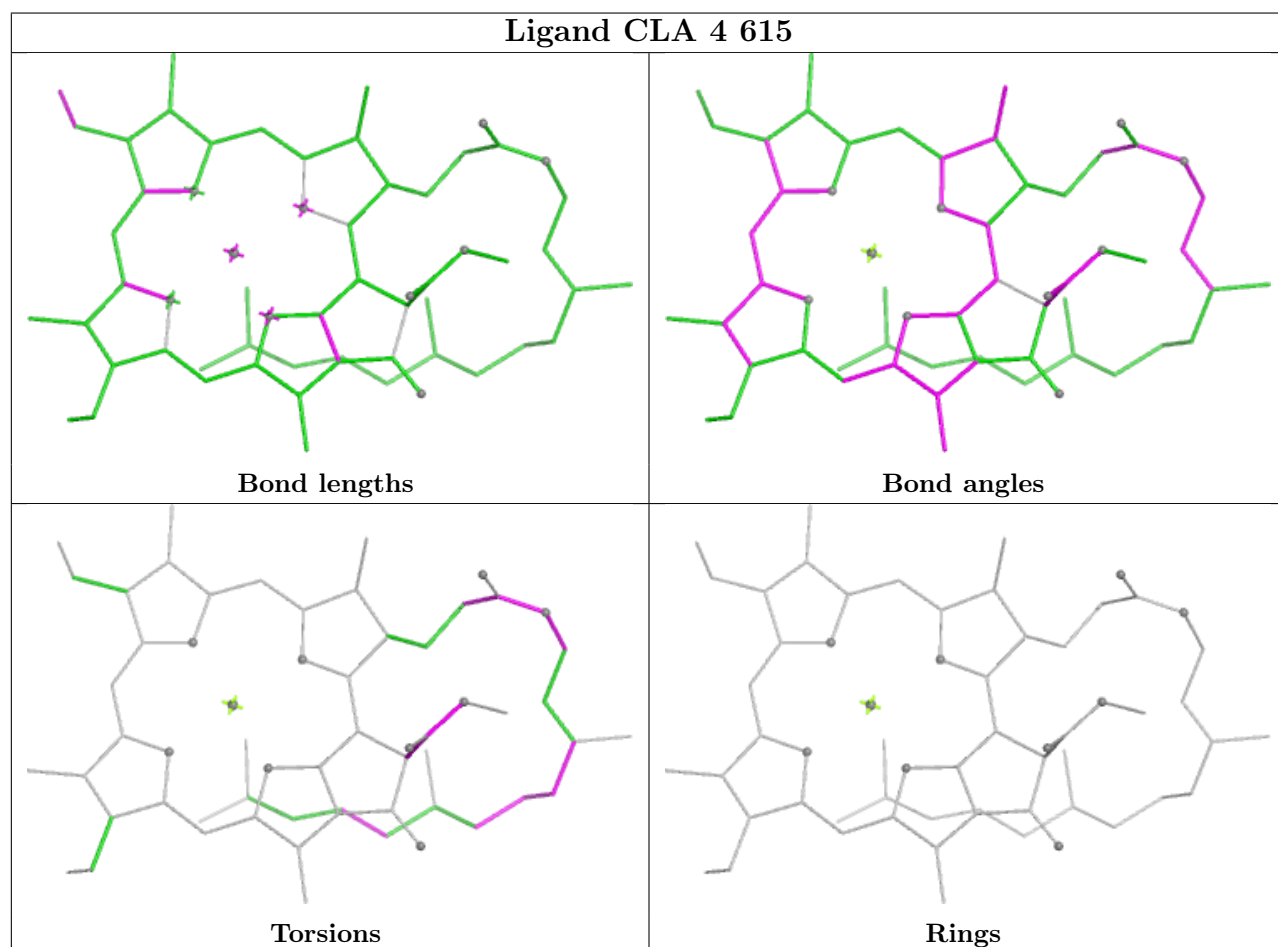
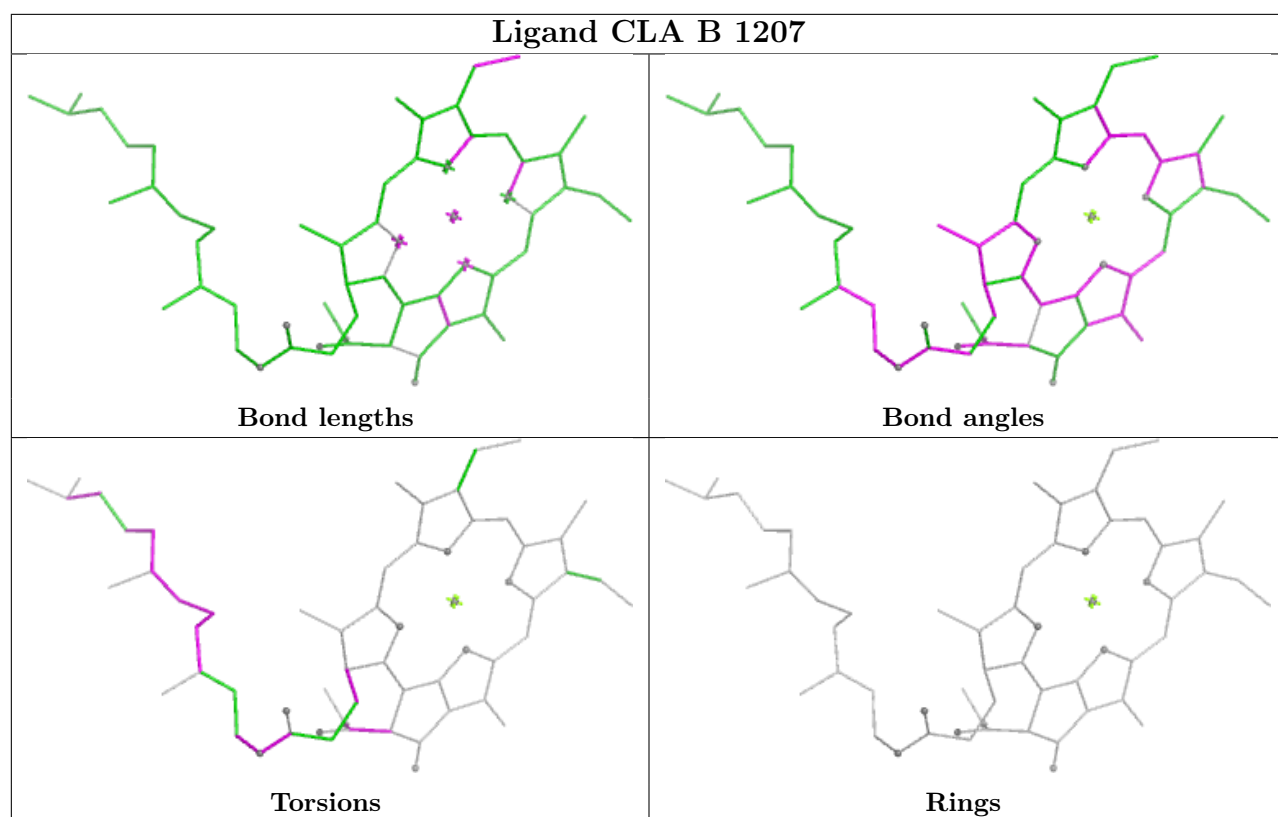
Ligand CLA B 1224

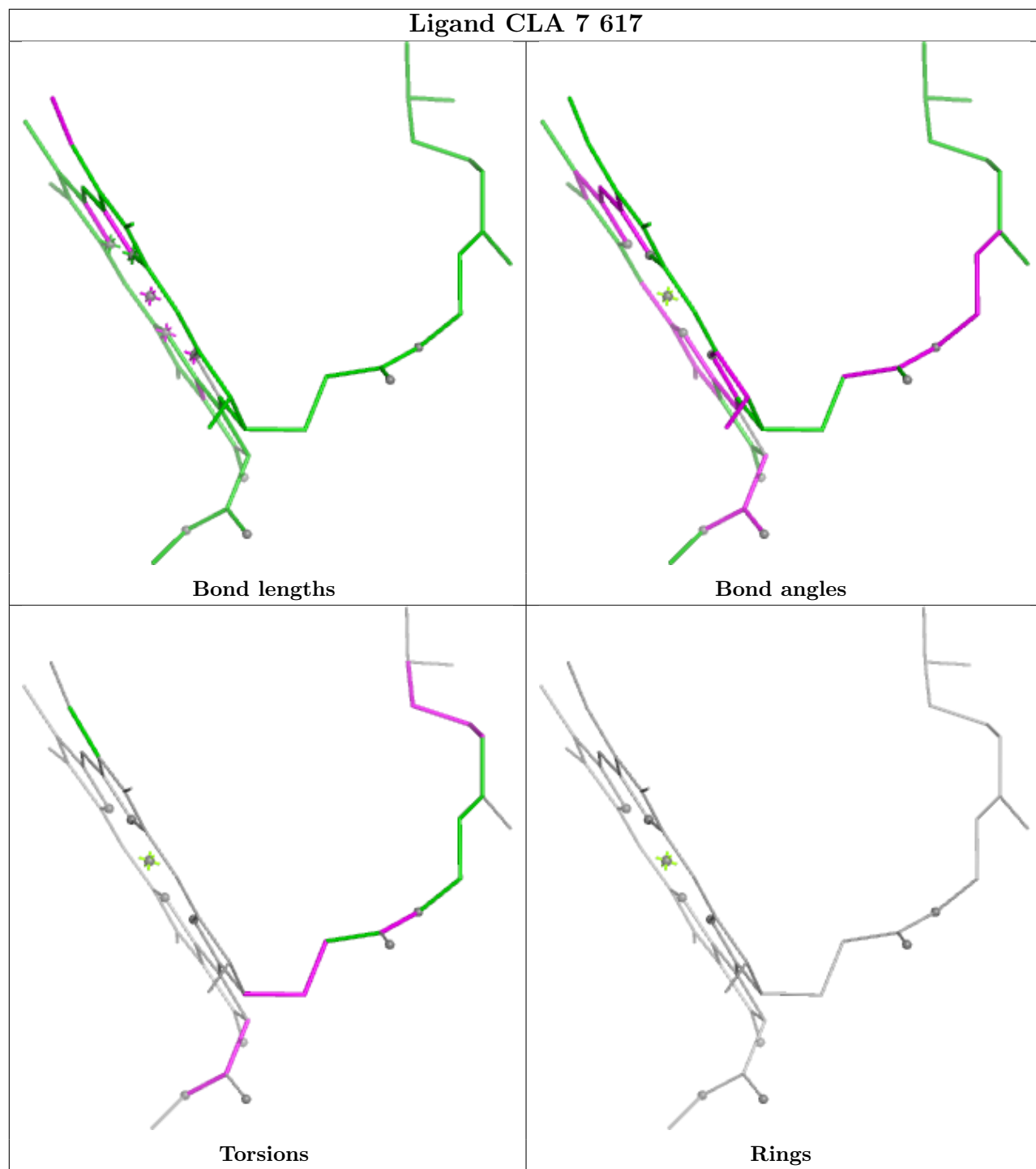


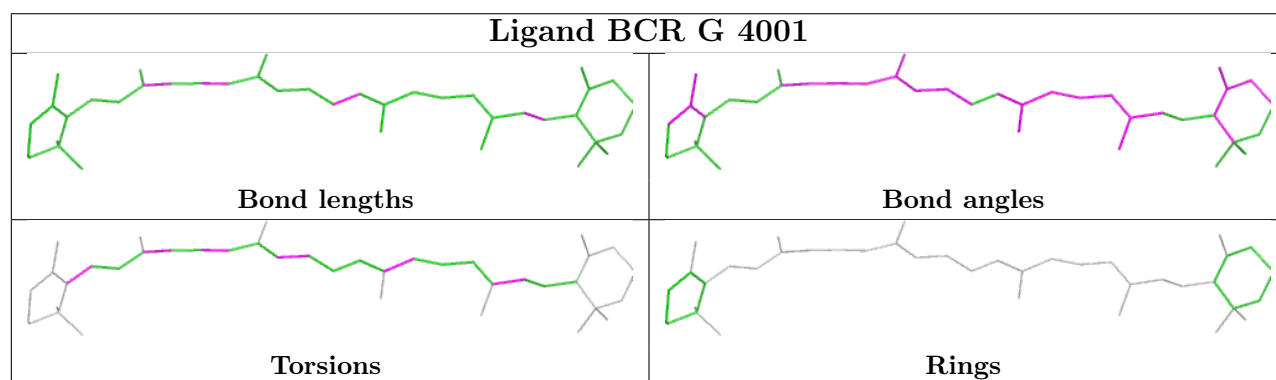
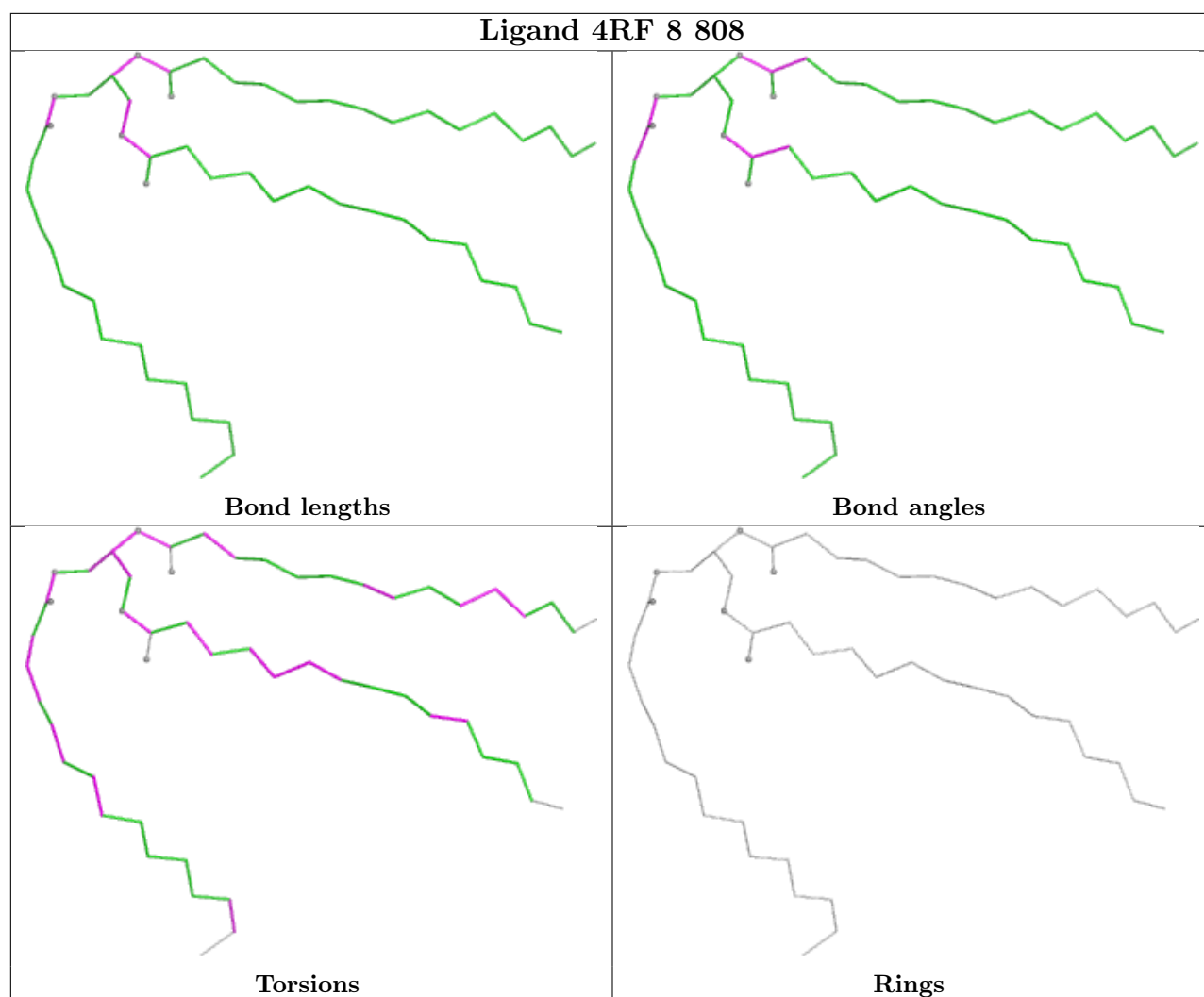
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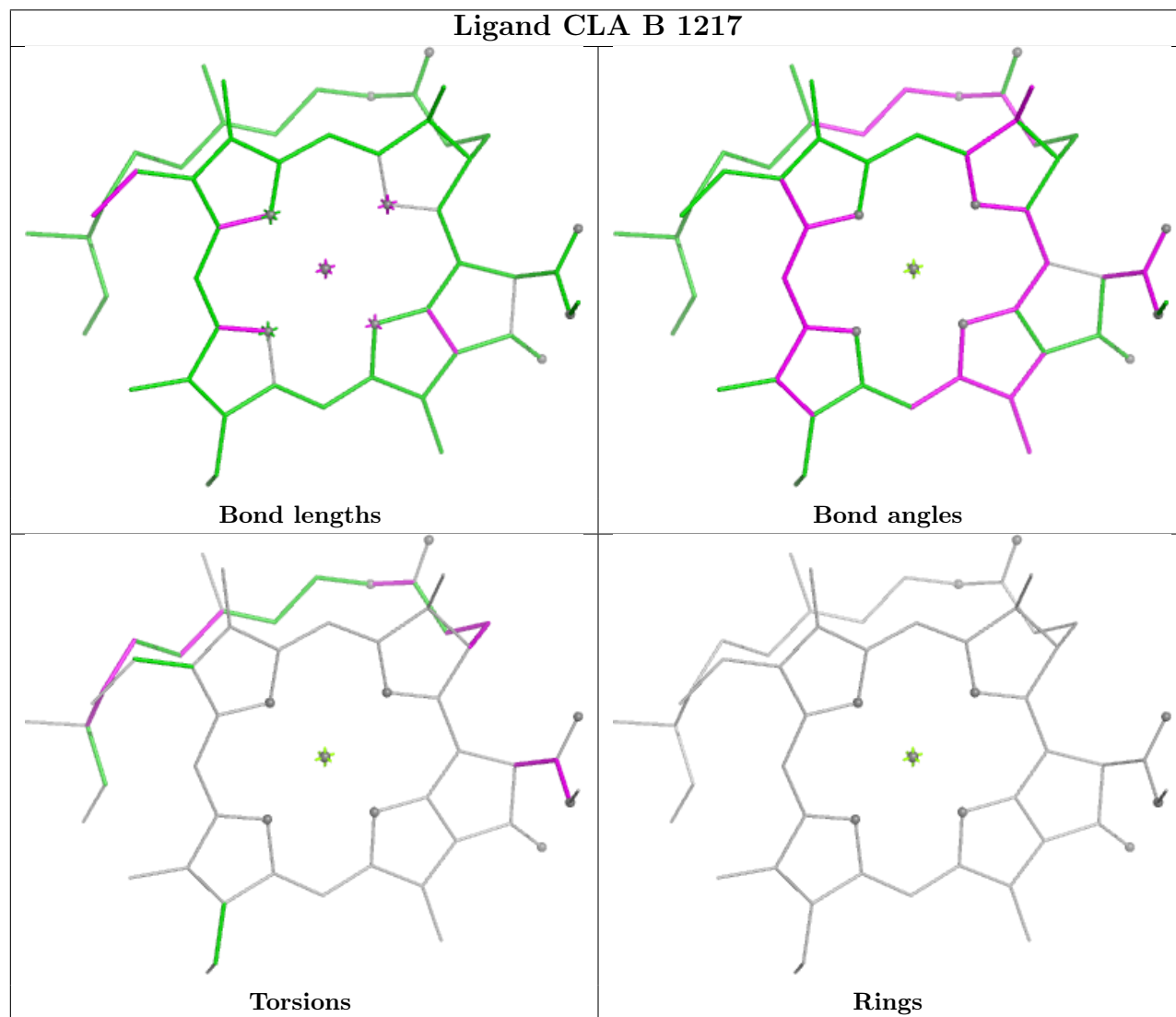
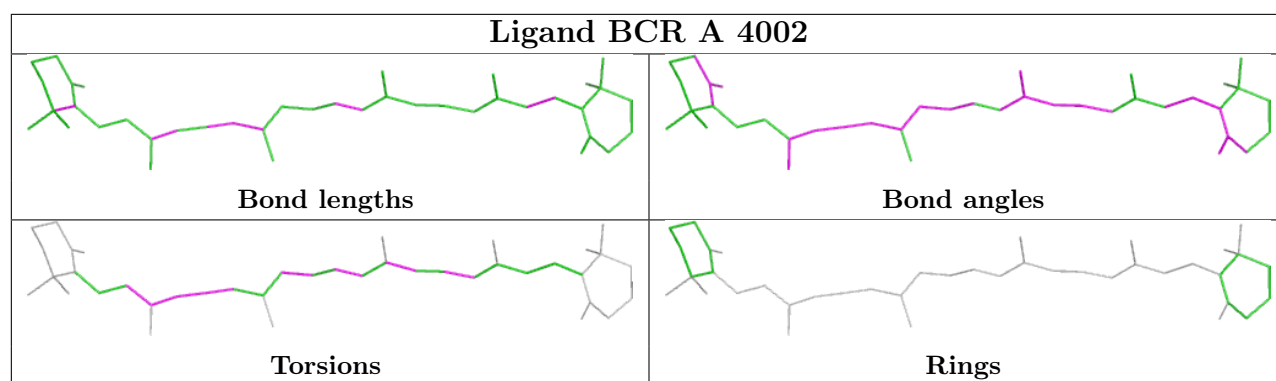


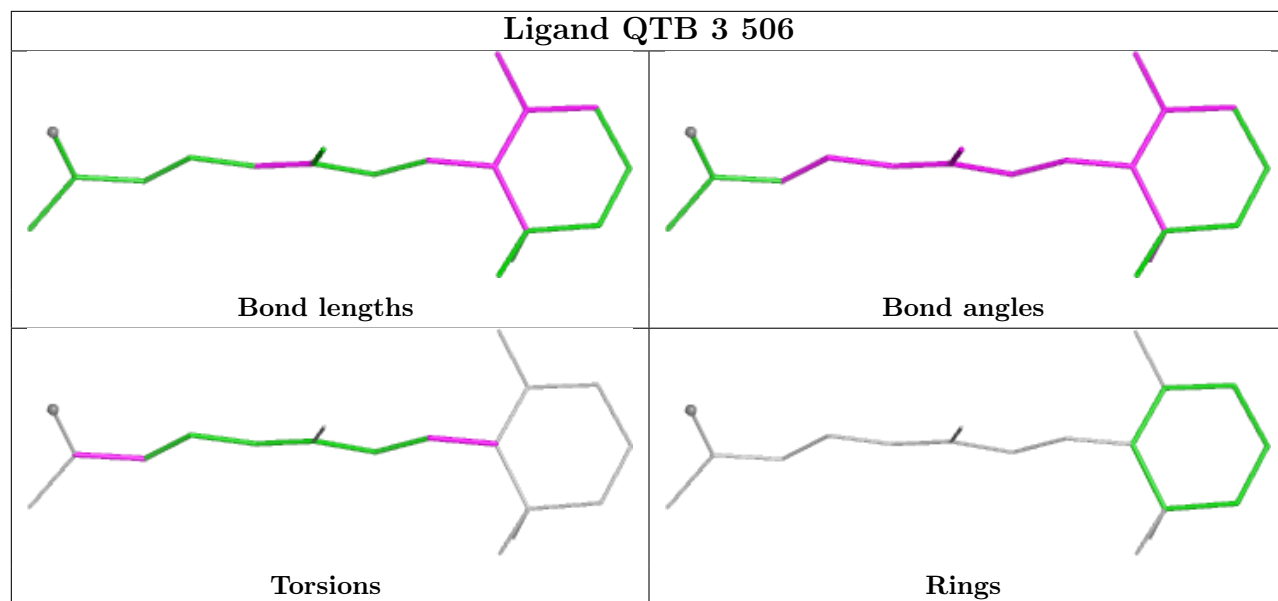




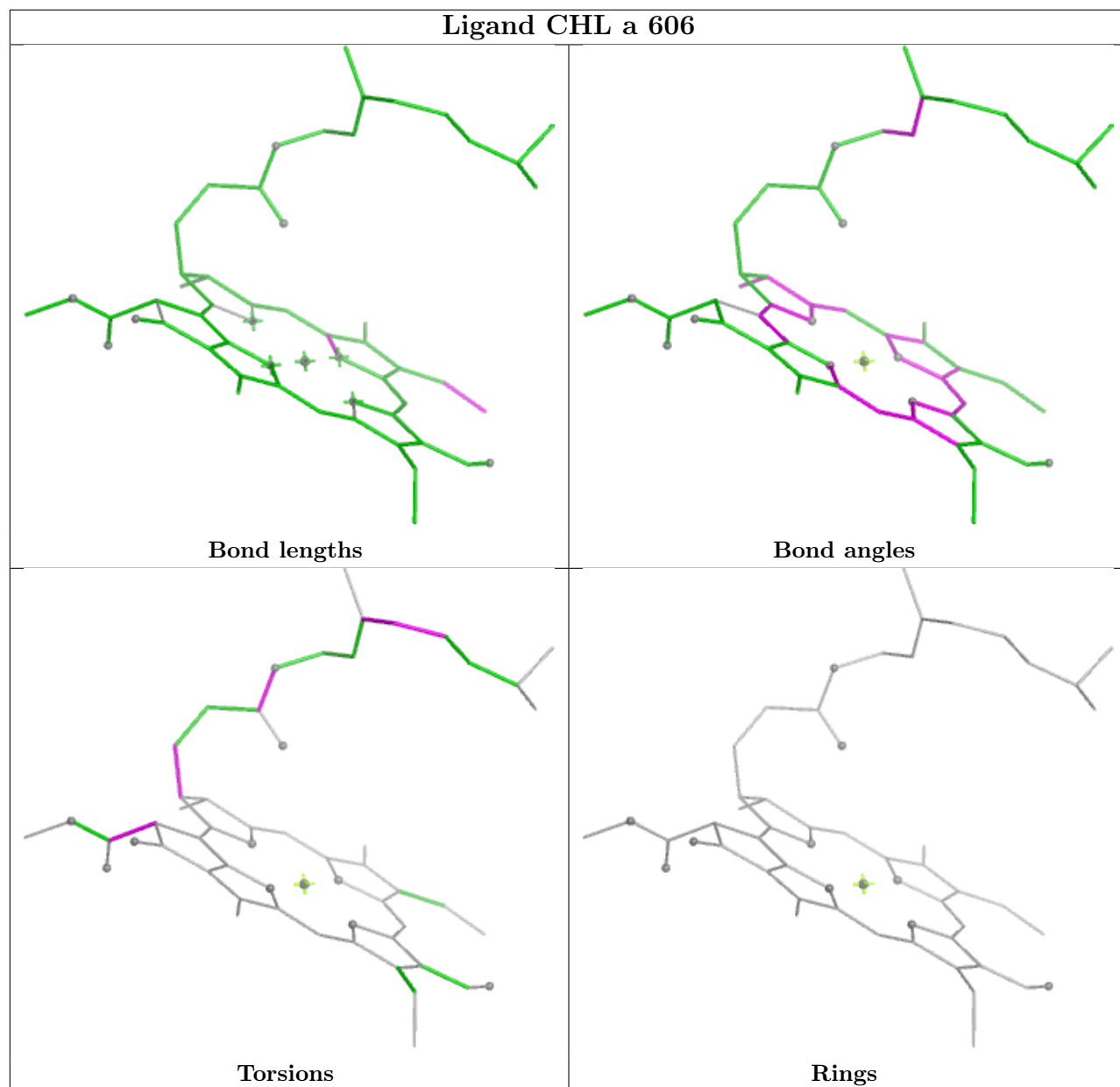


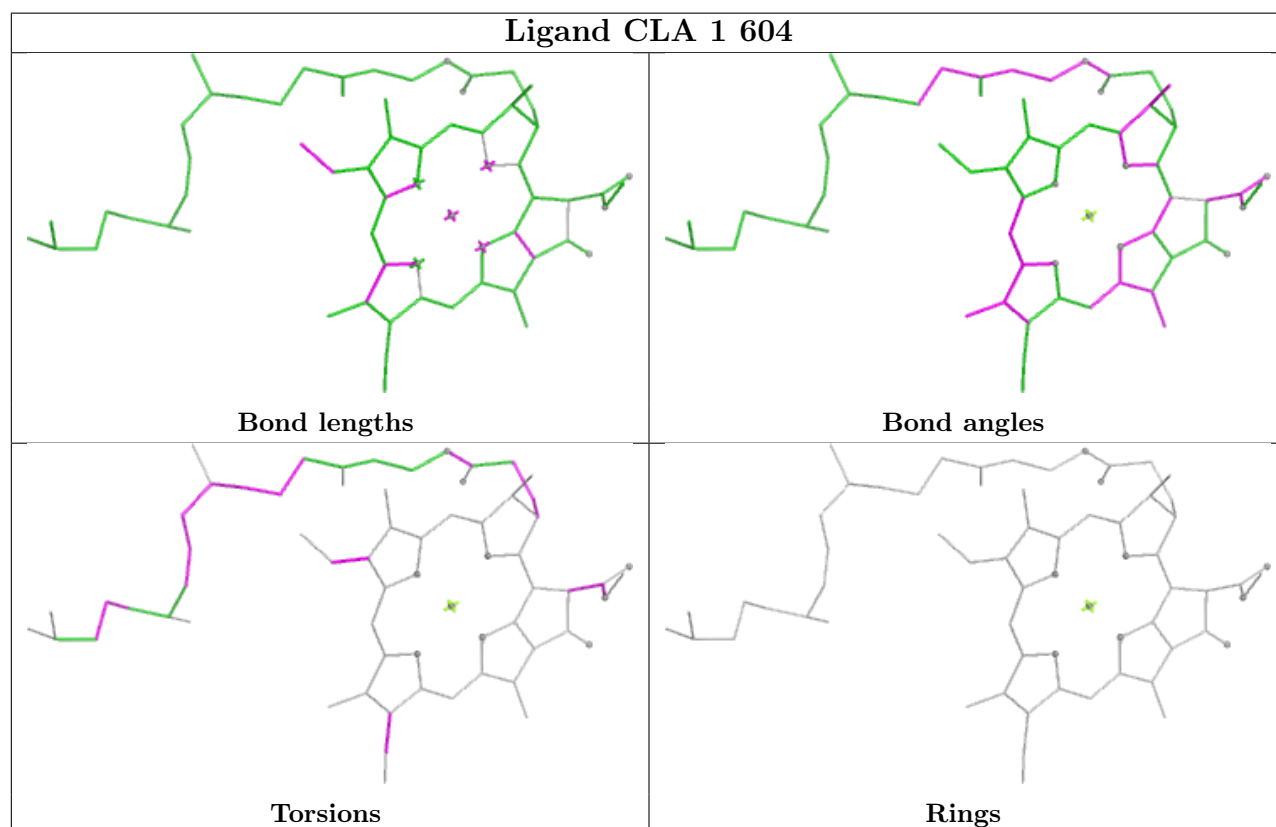
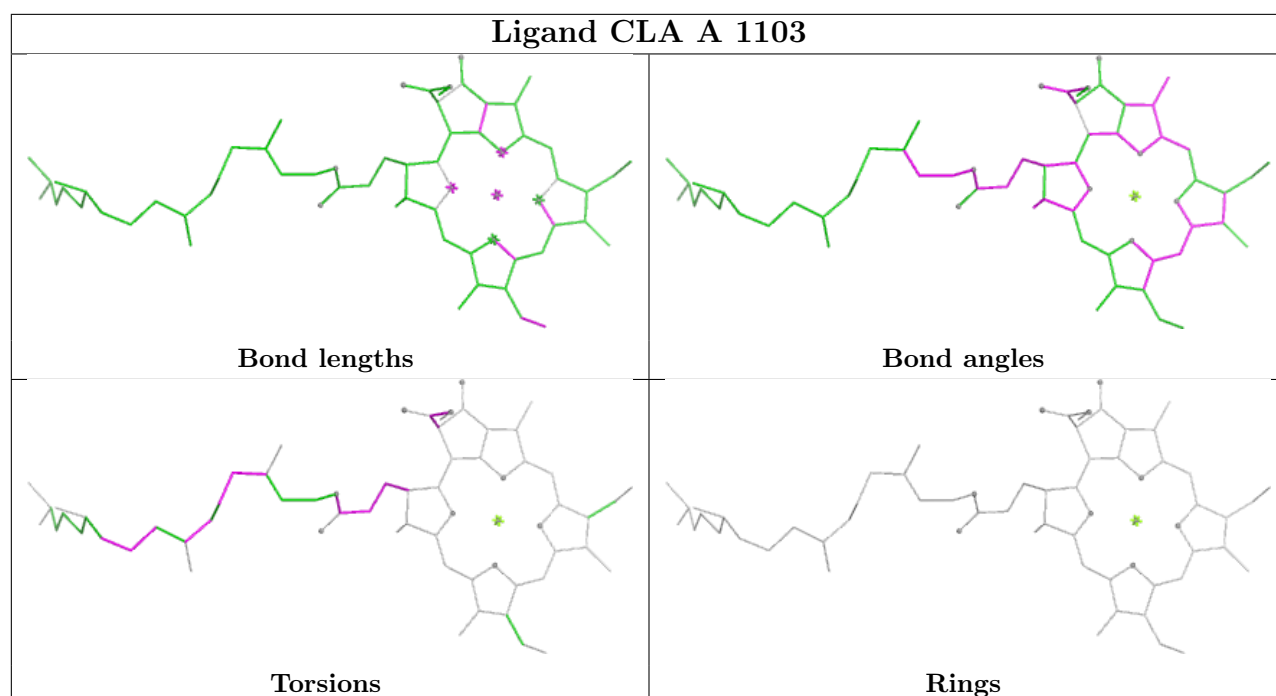


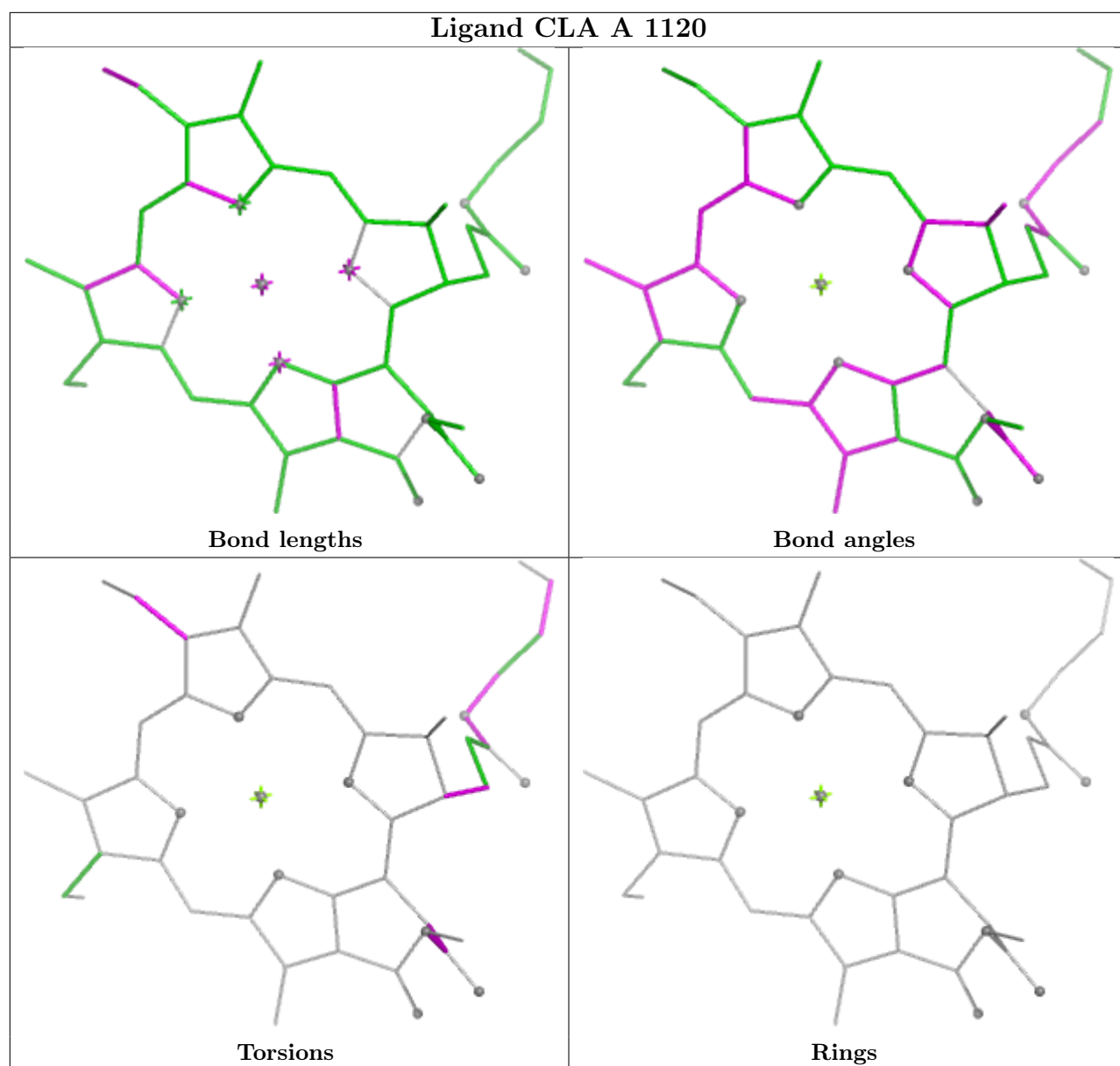


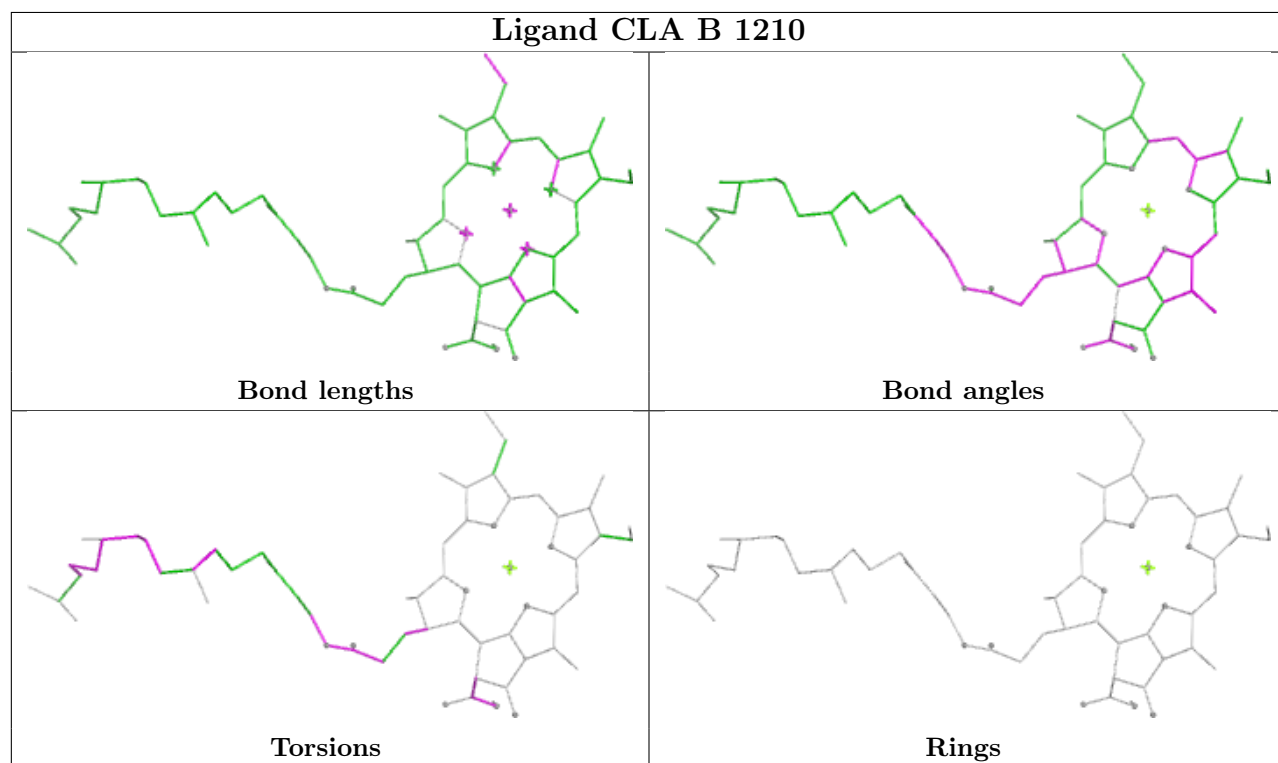
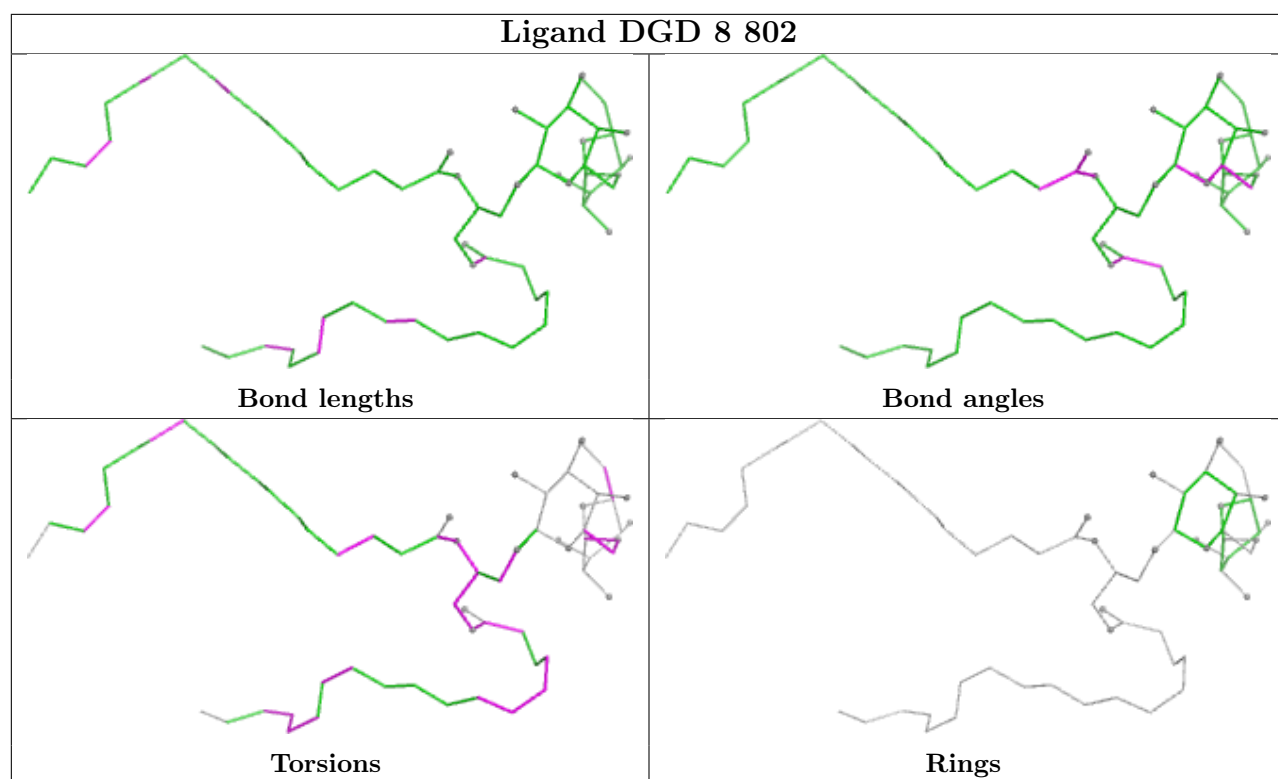


Ligand CHL a 606

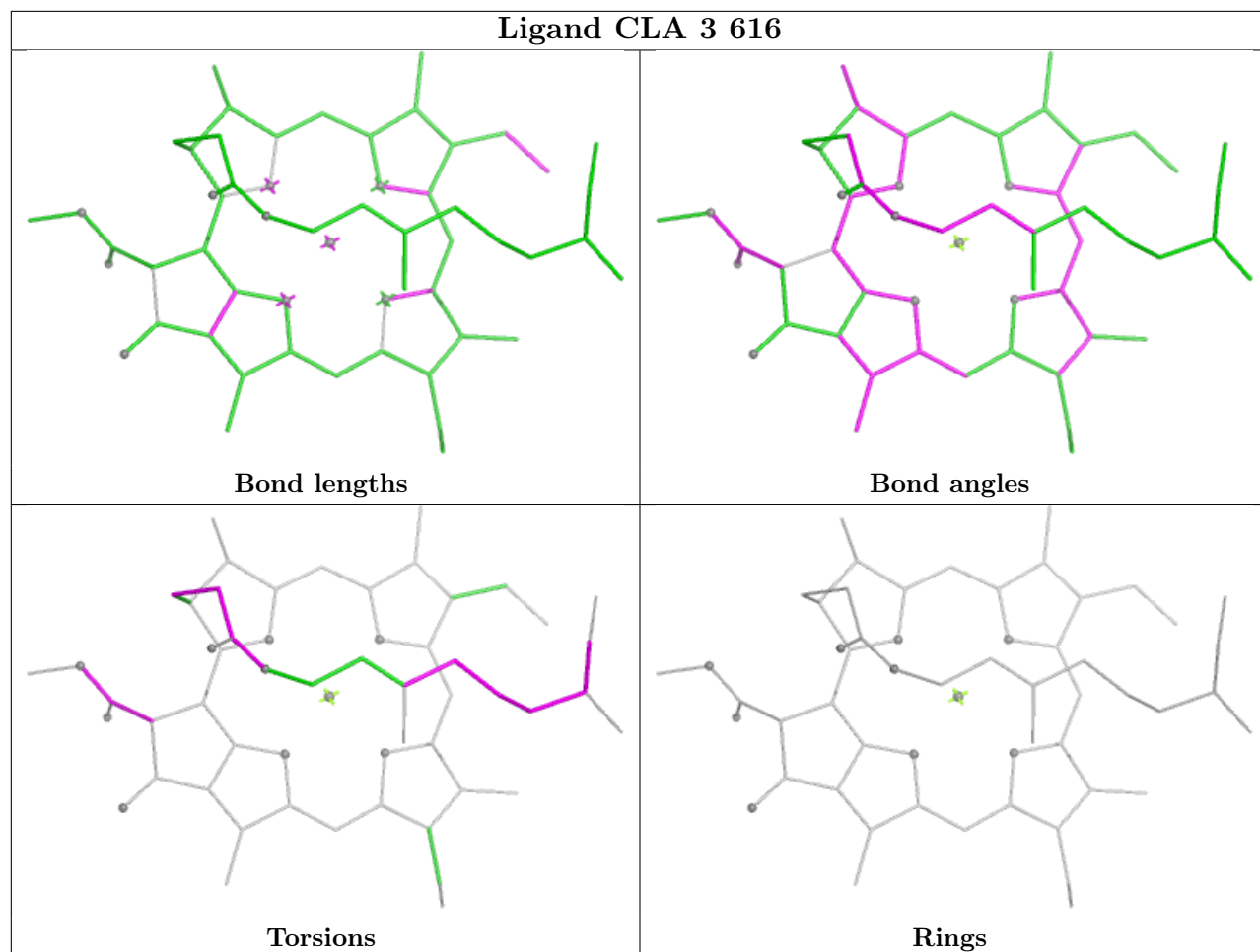


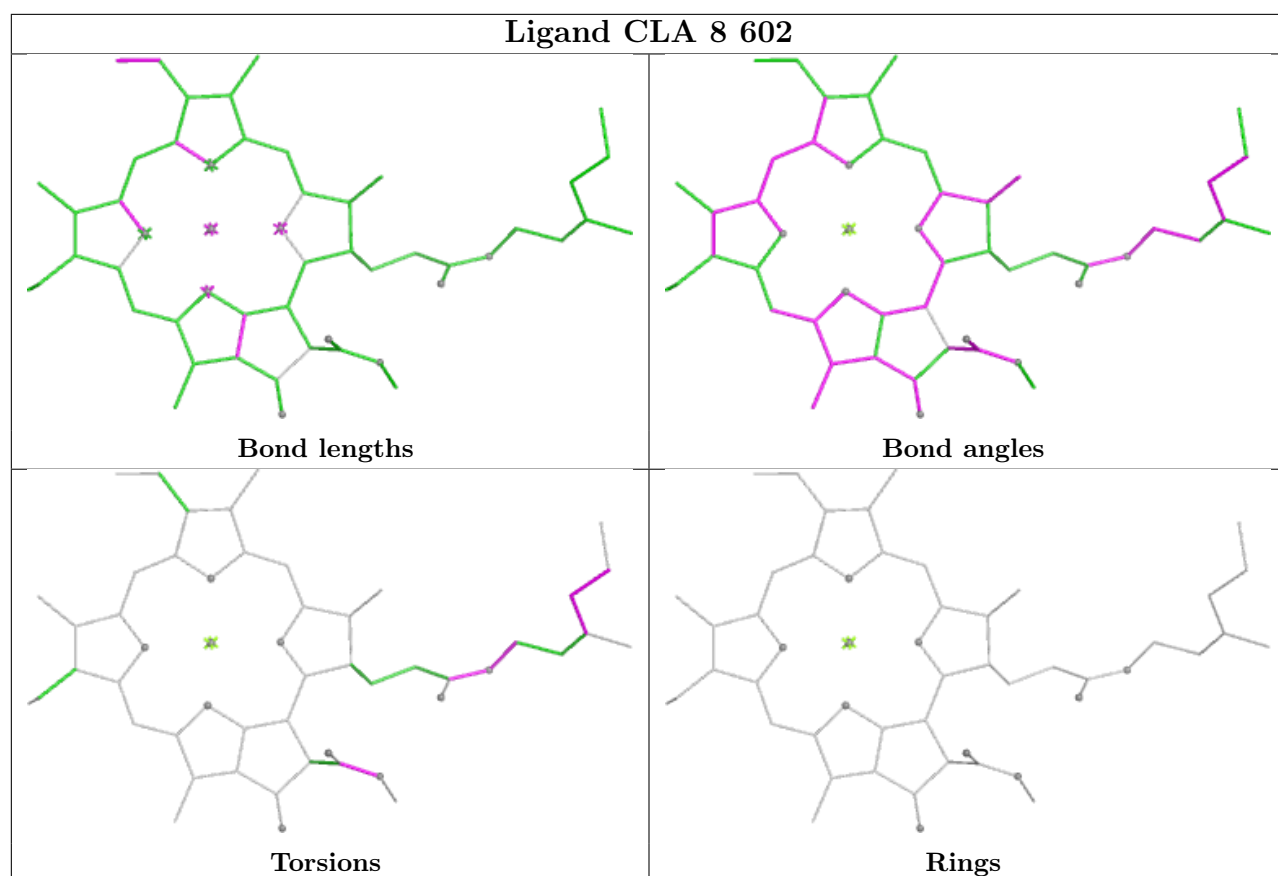




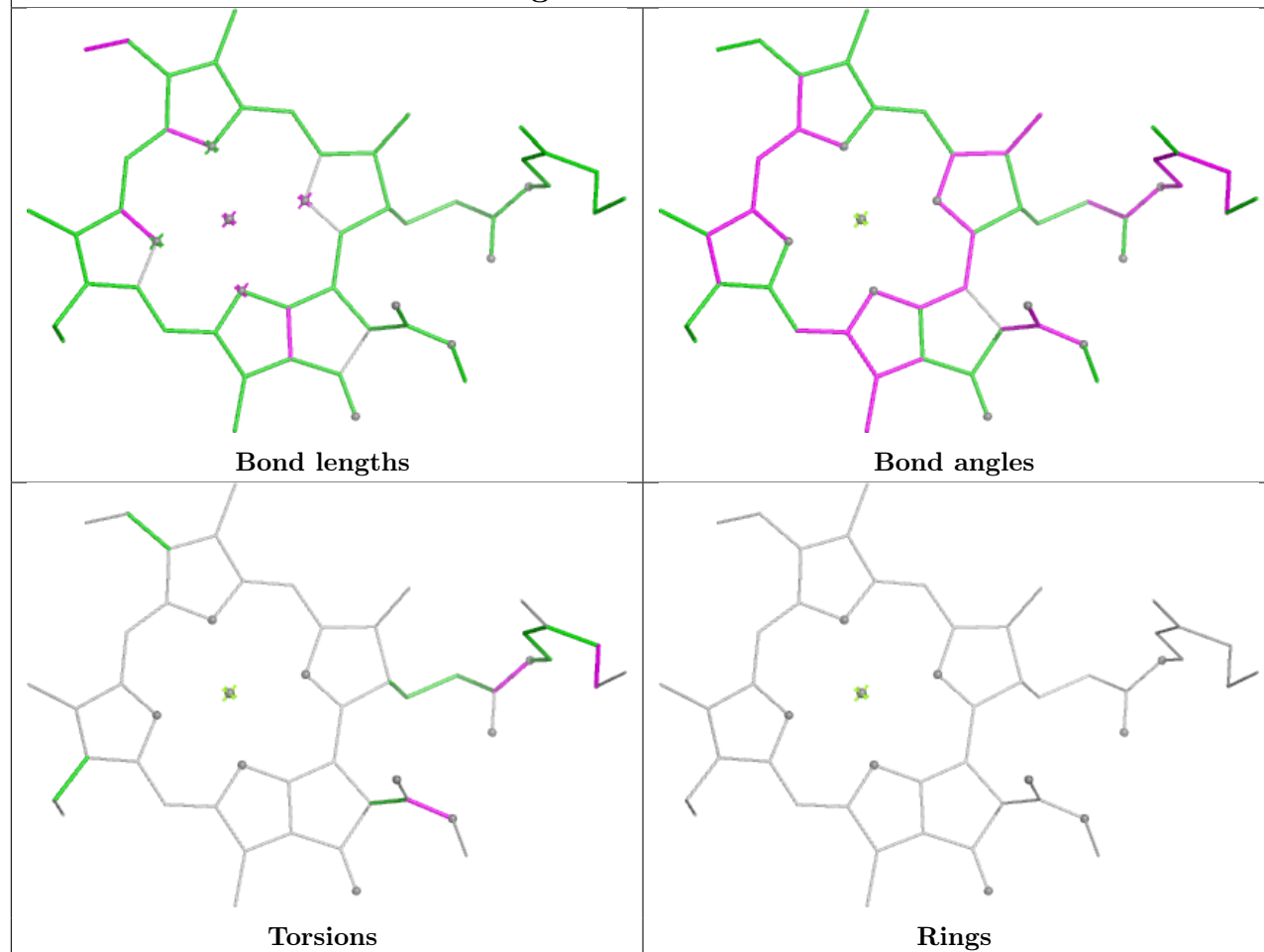


Ligand CLA 3 616

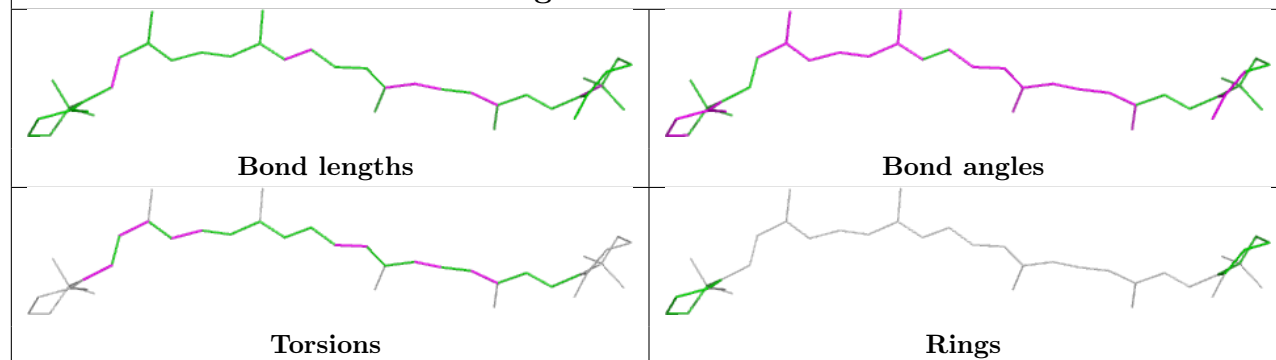


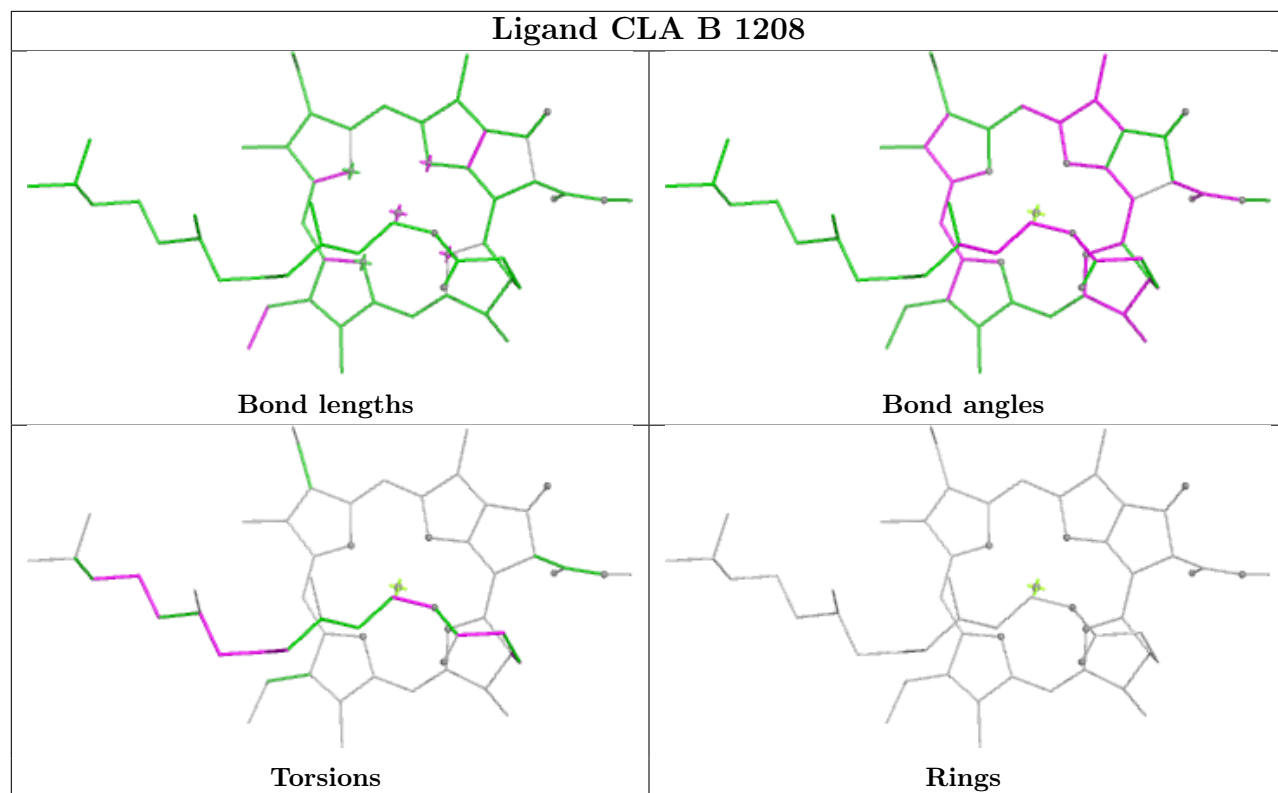


Ligand CLA 4 602

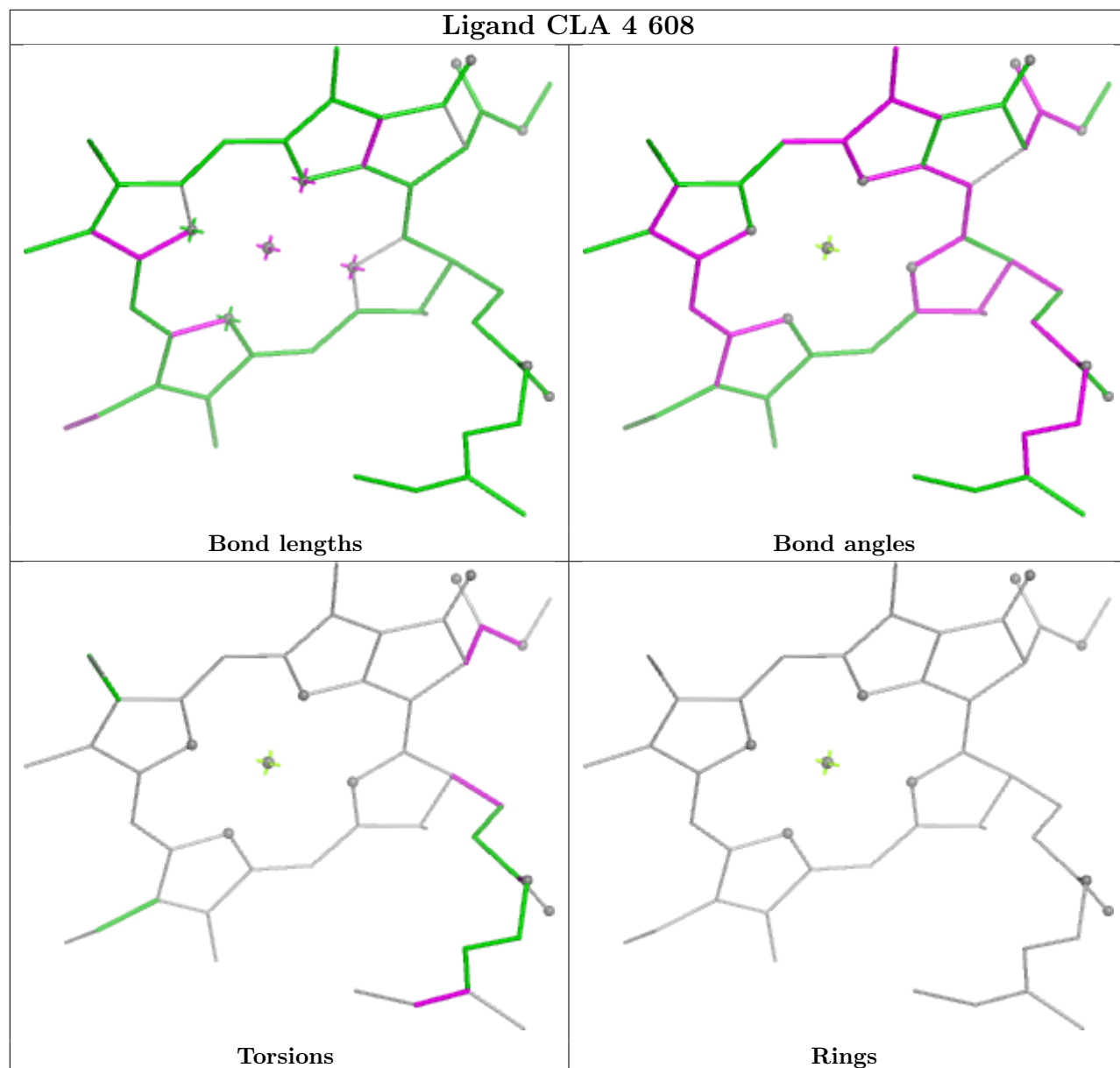


Ligand BCR 3 503

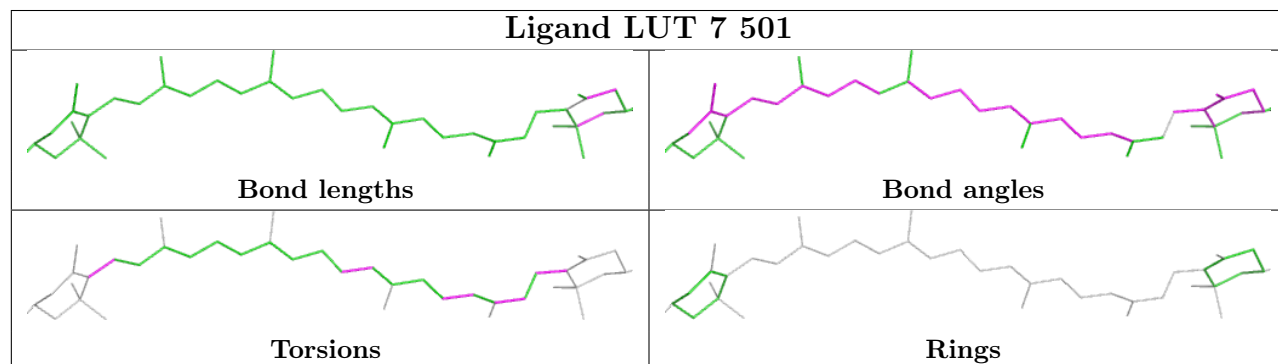


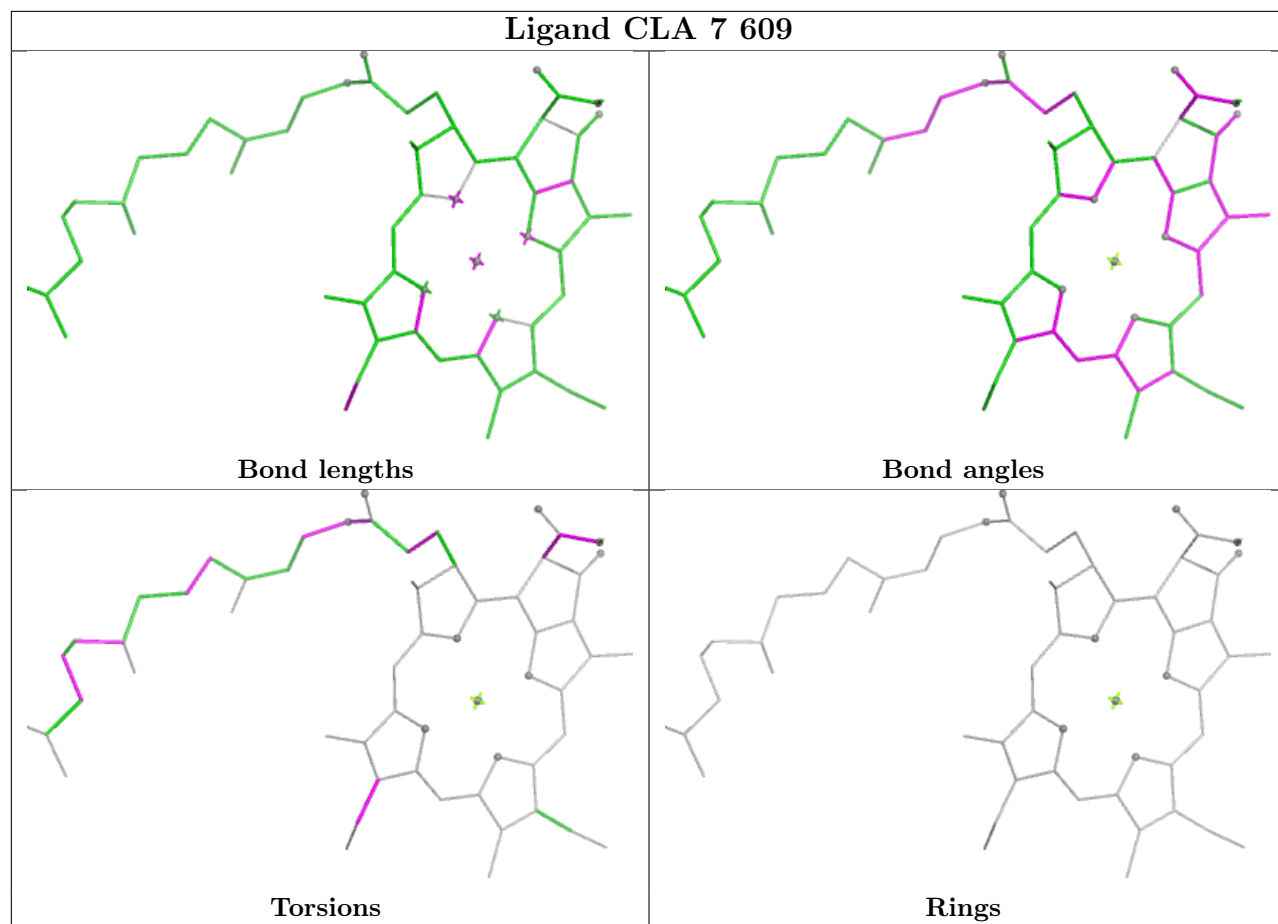


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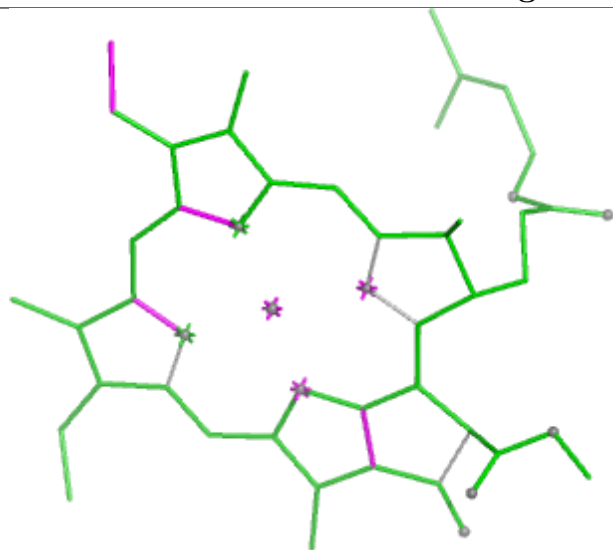


Ligand LUT 7 501

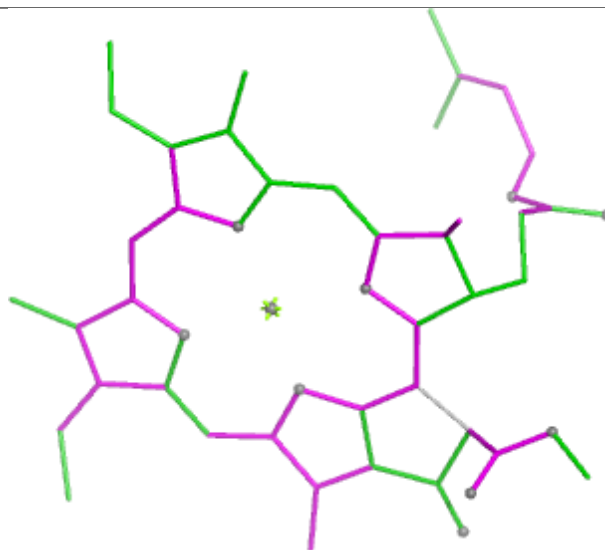




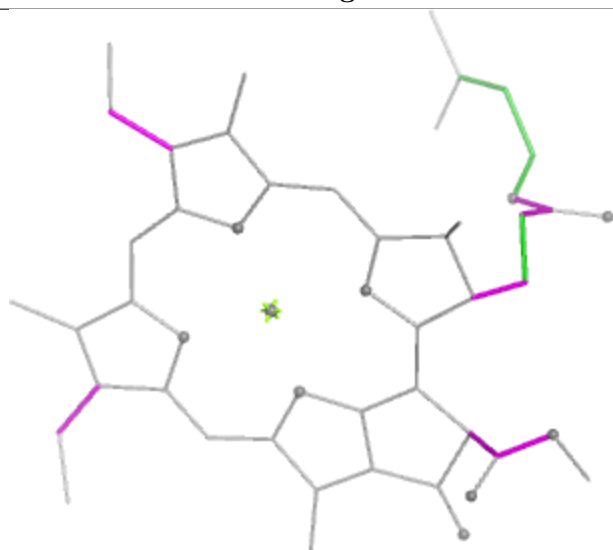
Ligand CLA 6 612



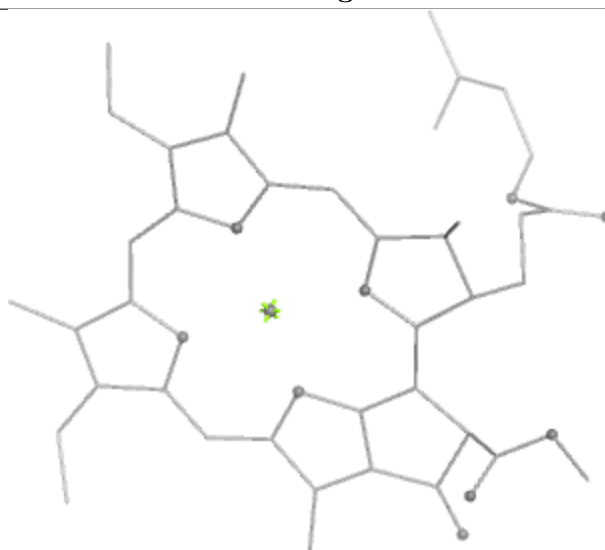
Bond lengths



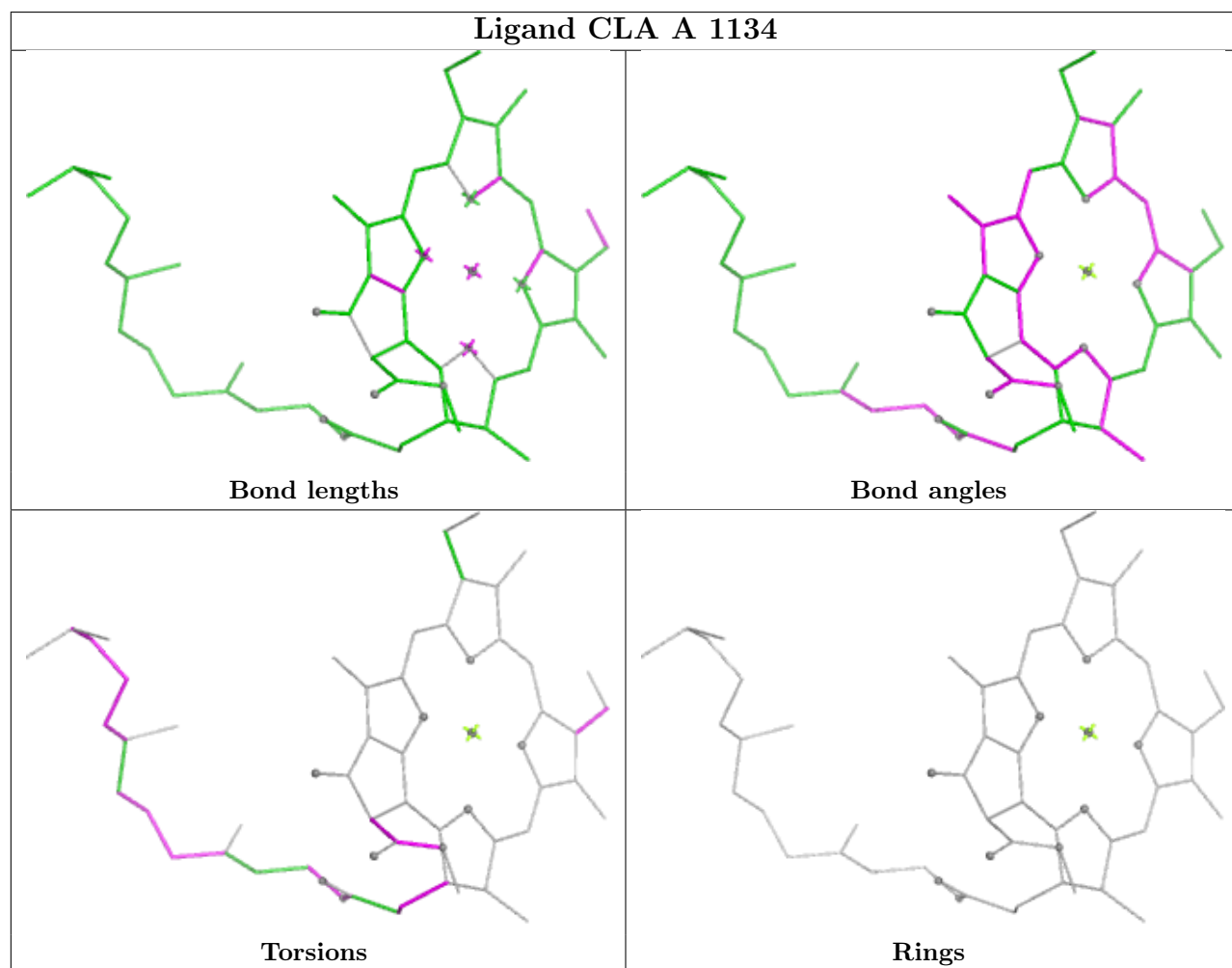
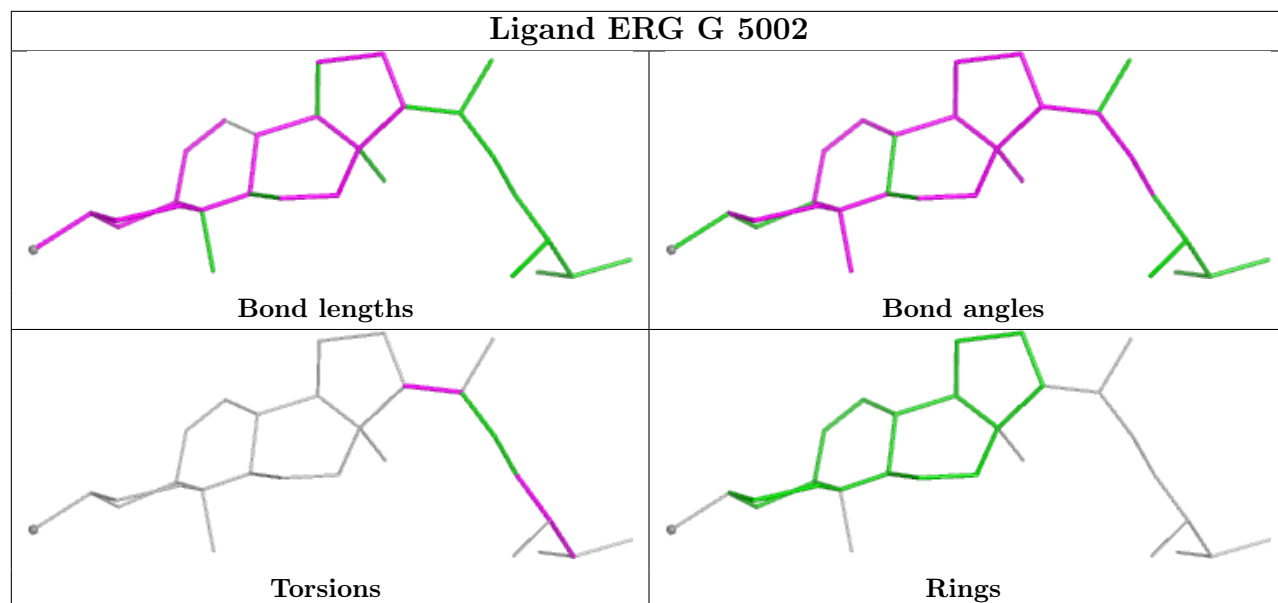
Bond angles

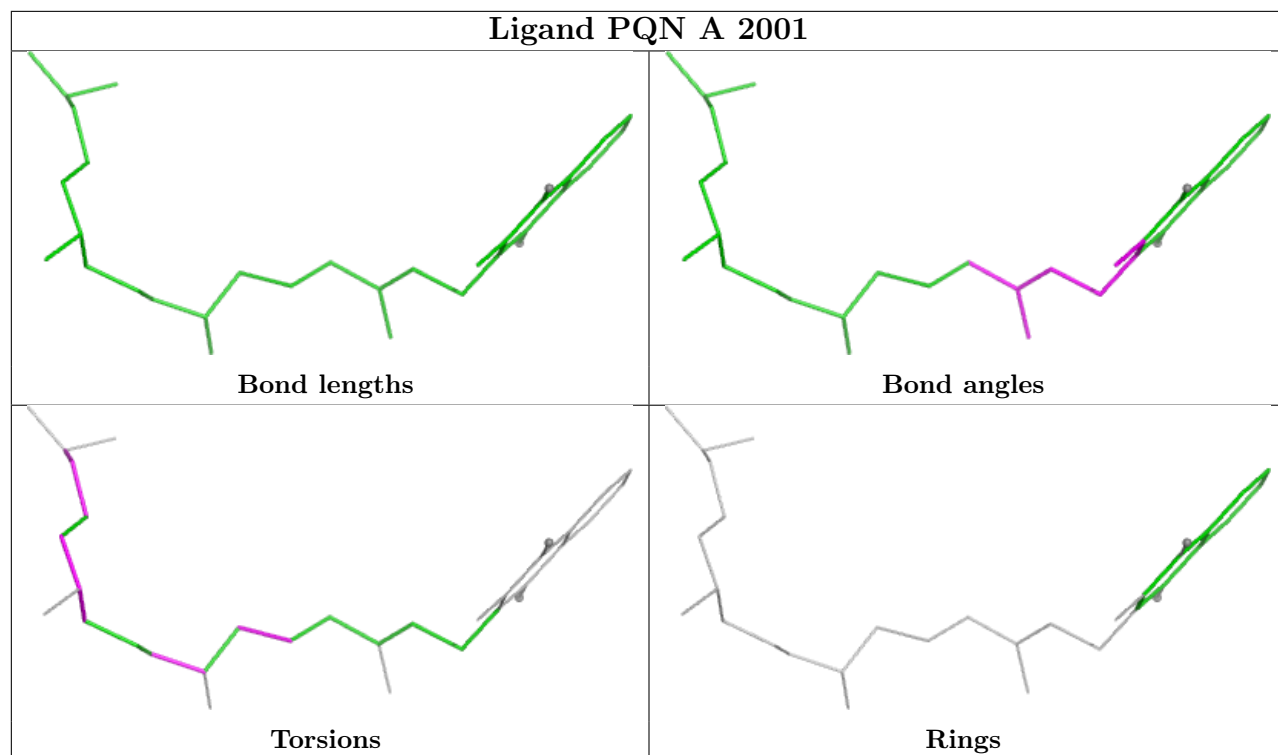


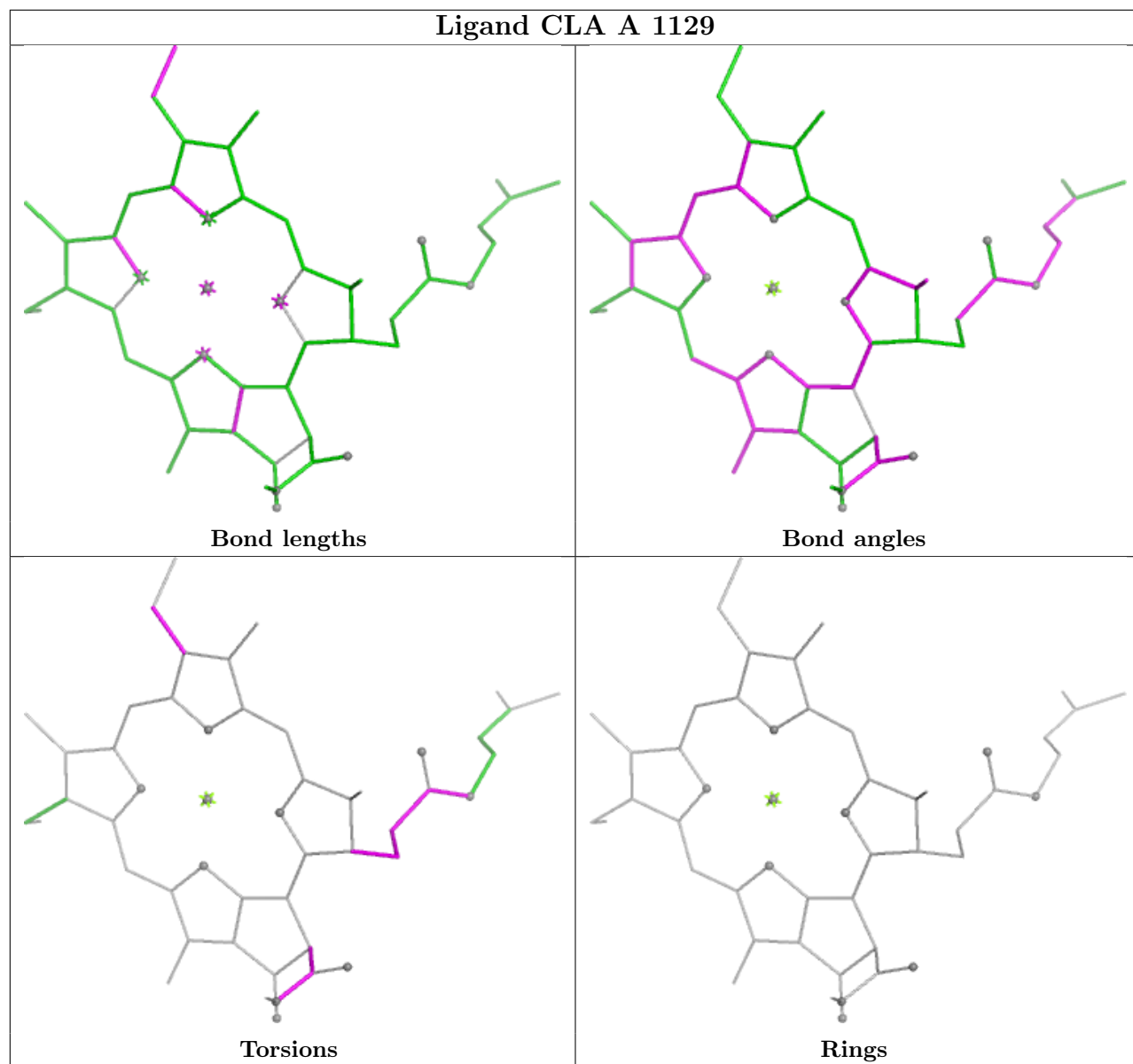
Torsions

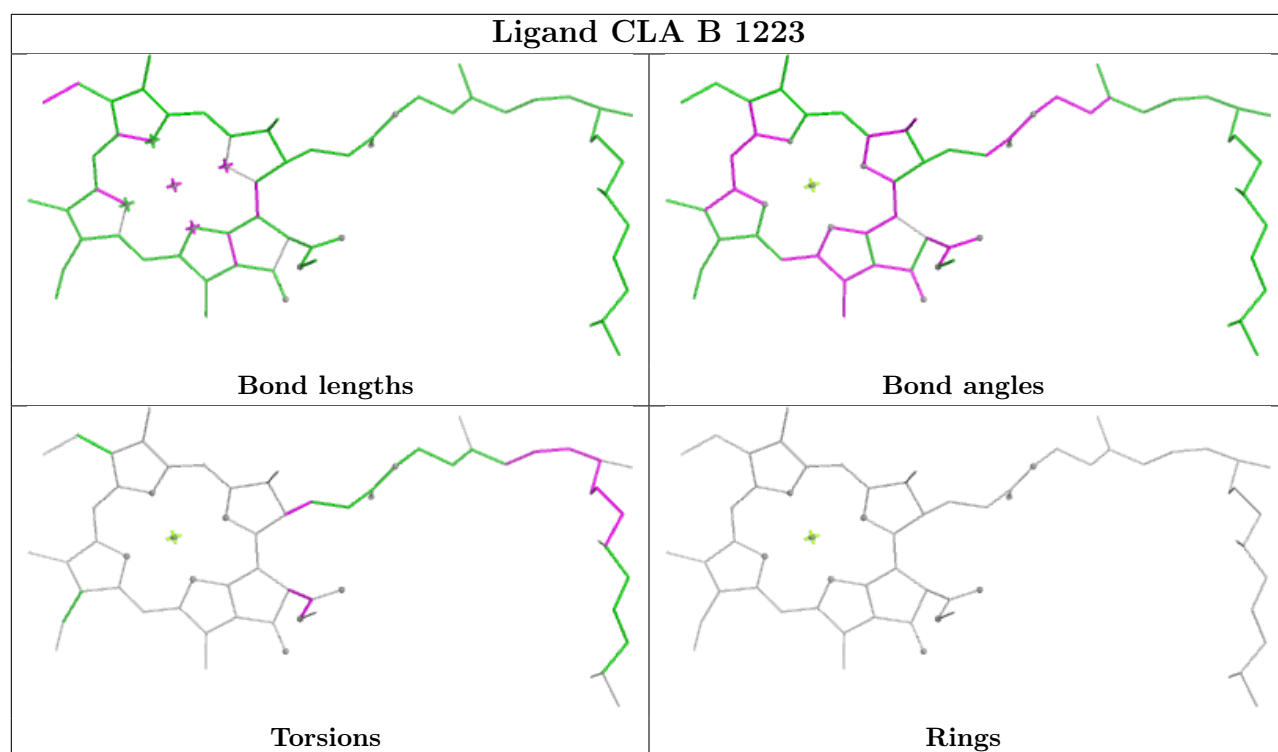


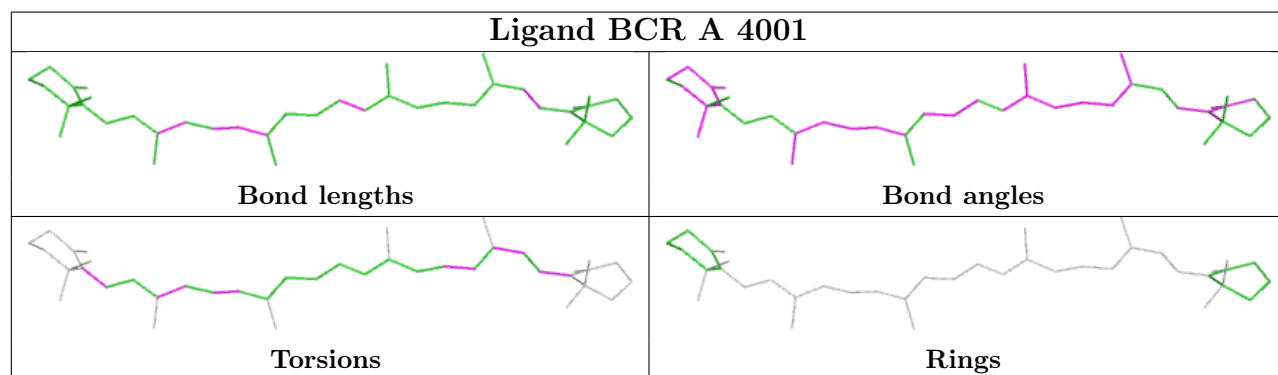
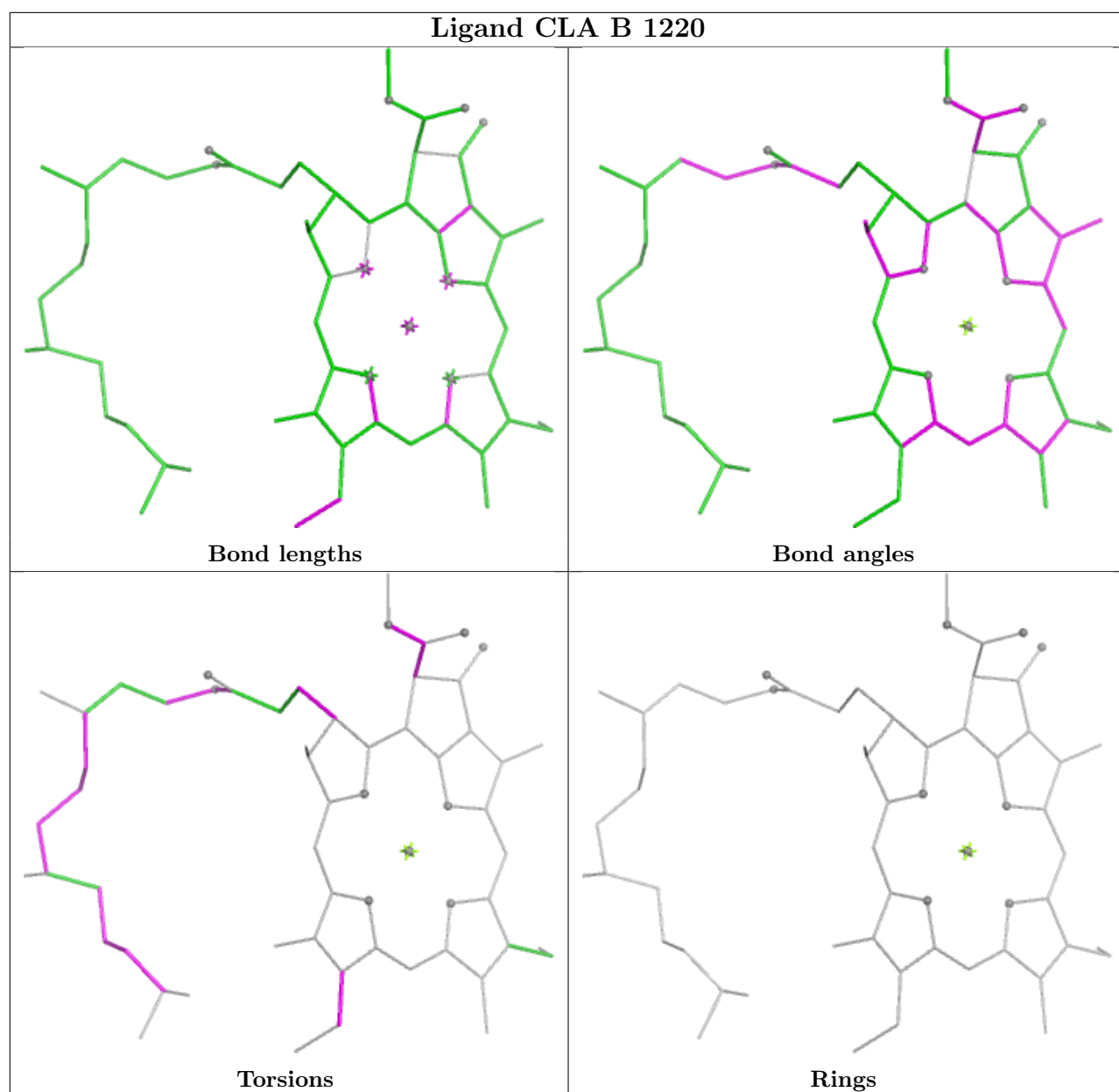
Rings

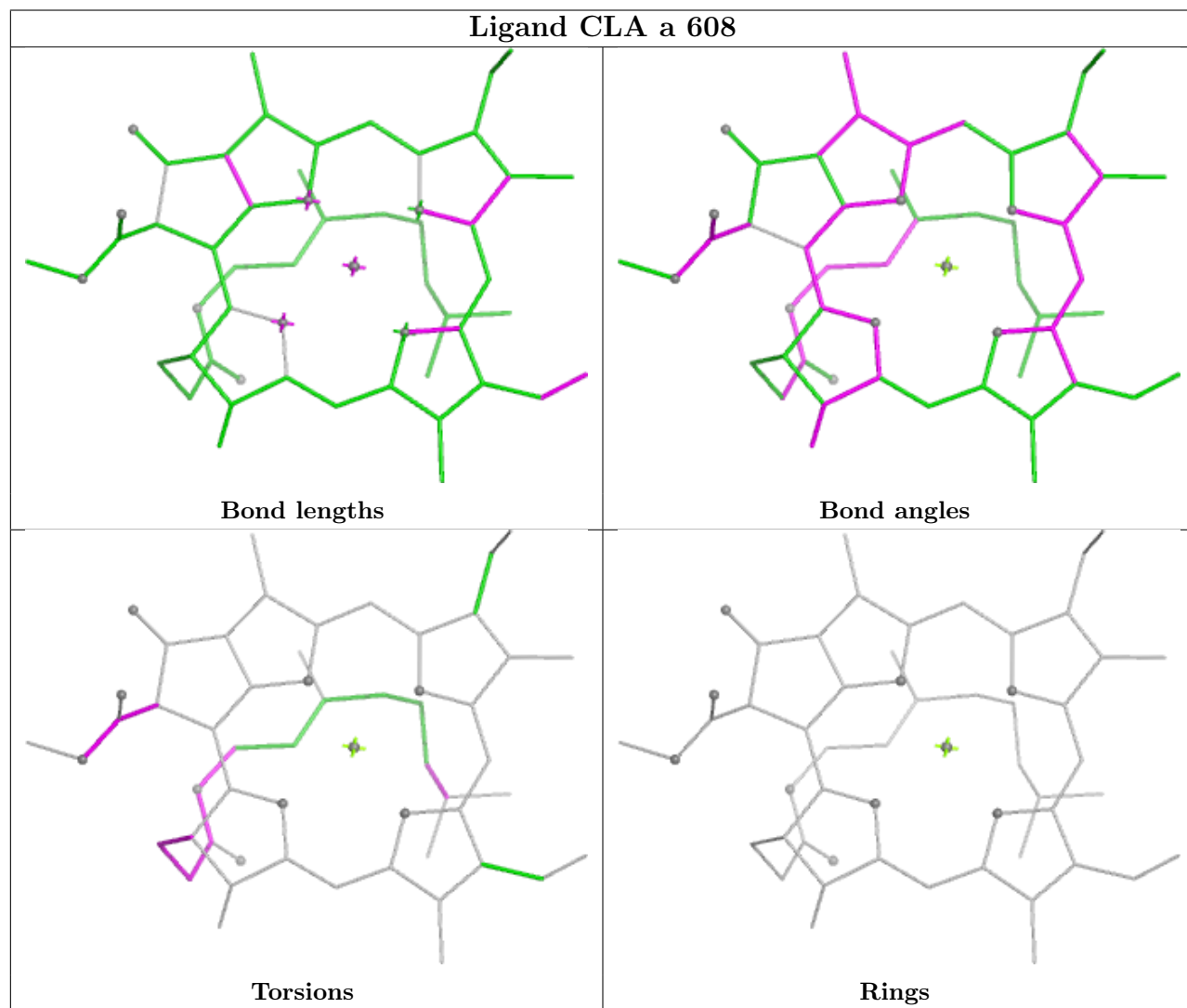
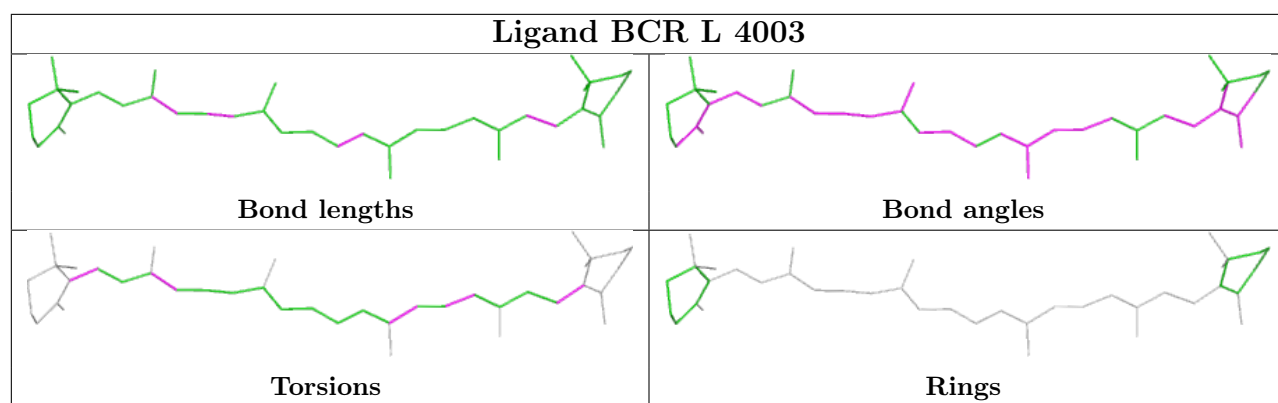




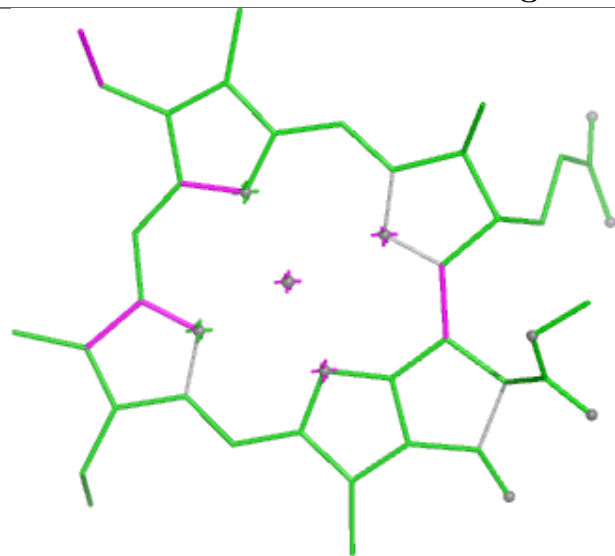




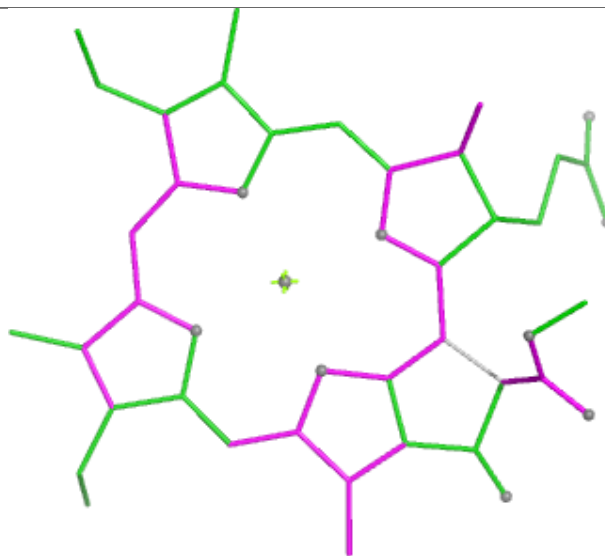




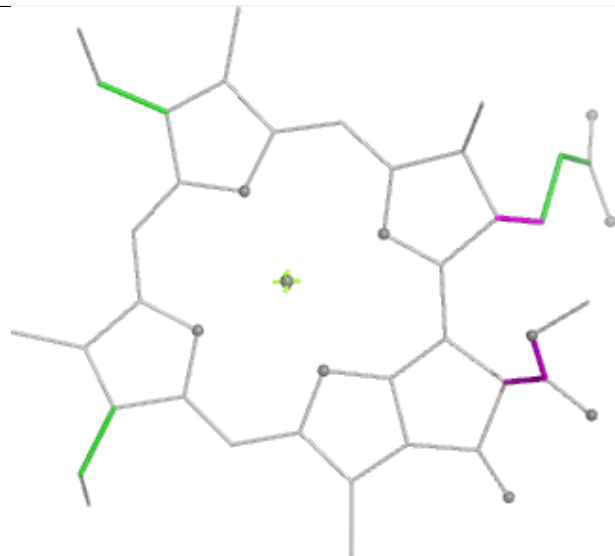
Ligand CLA 5 608



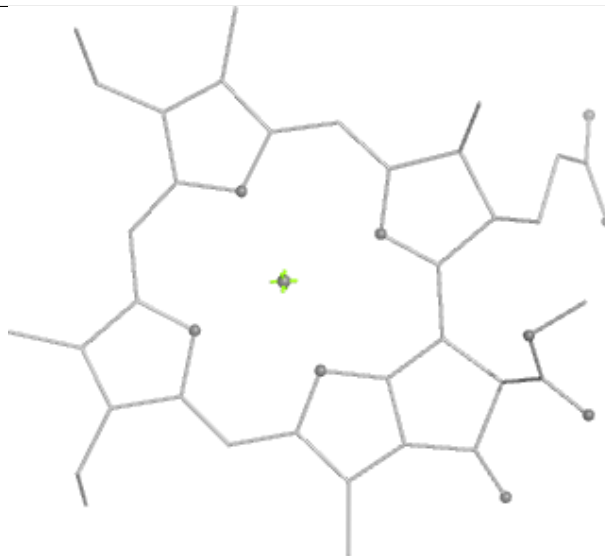
Bond lengths



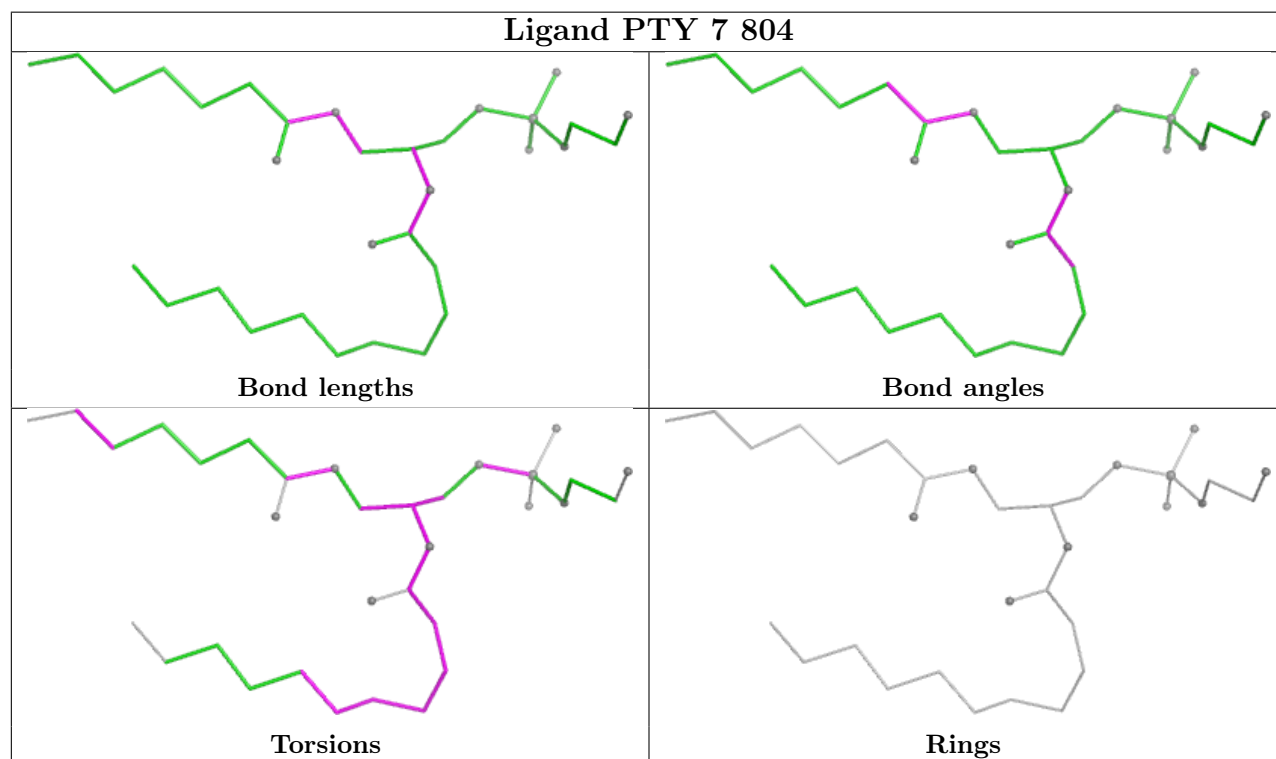
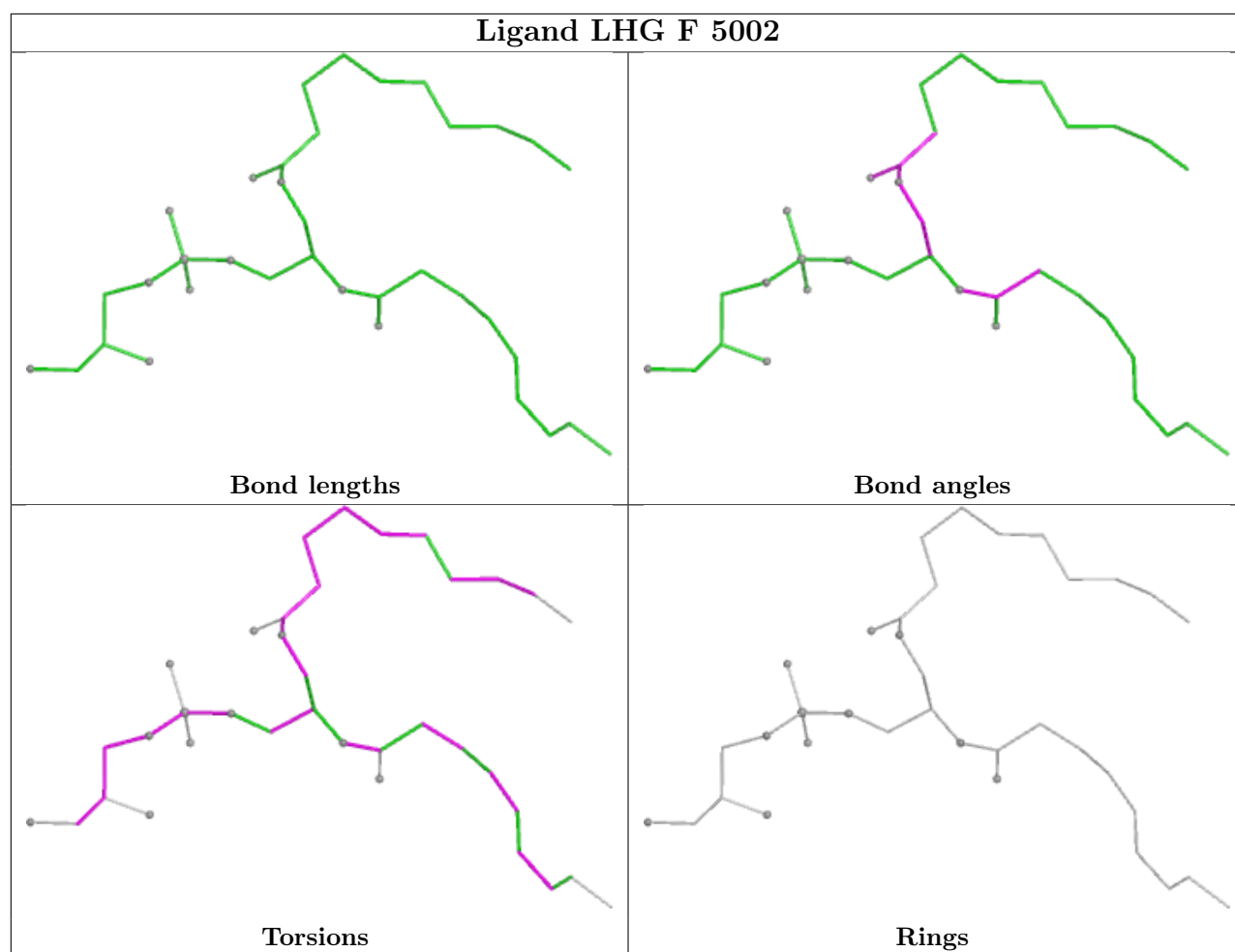
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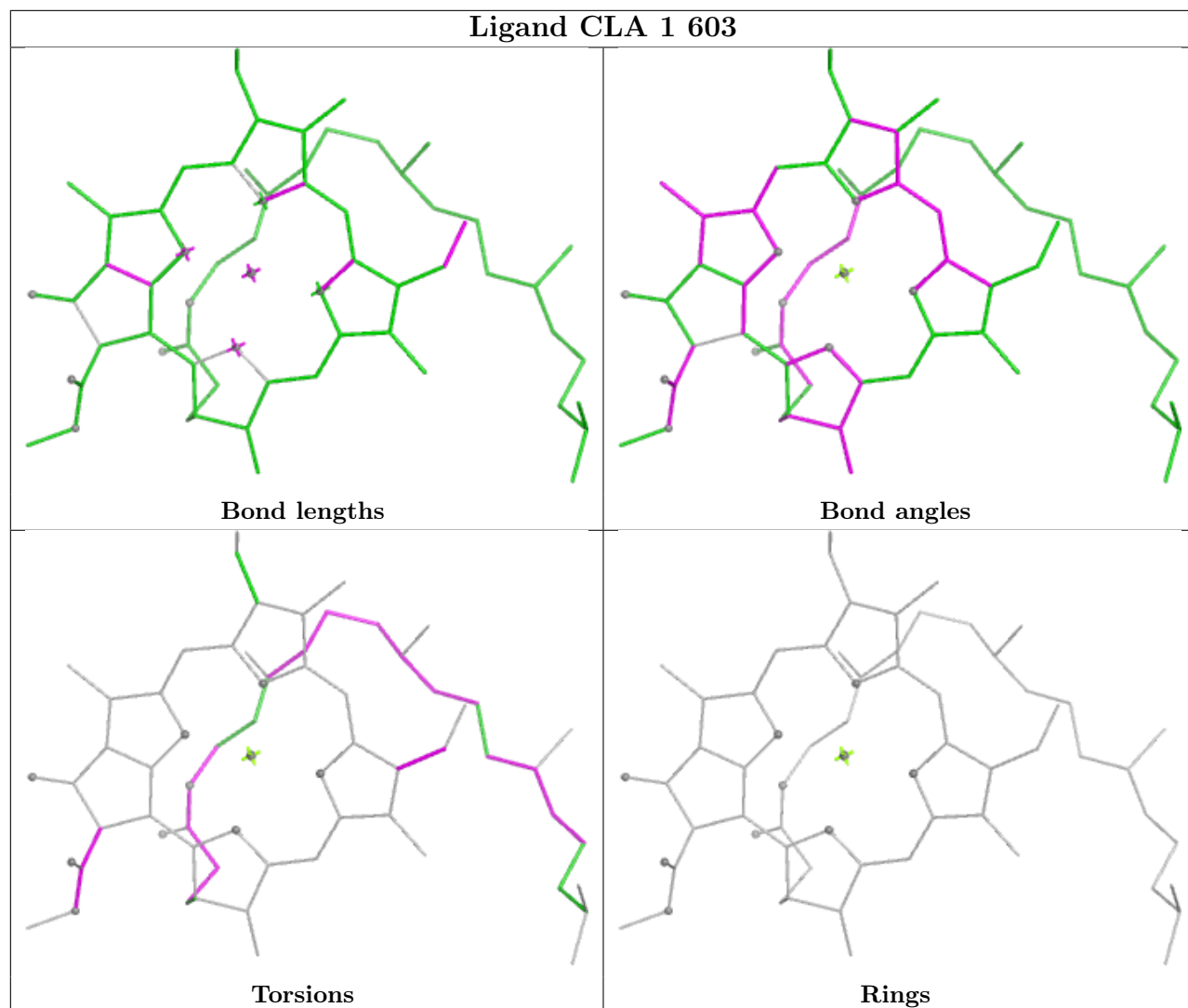
Torsions

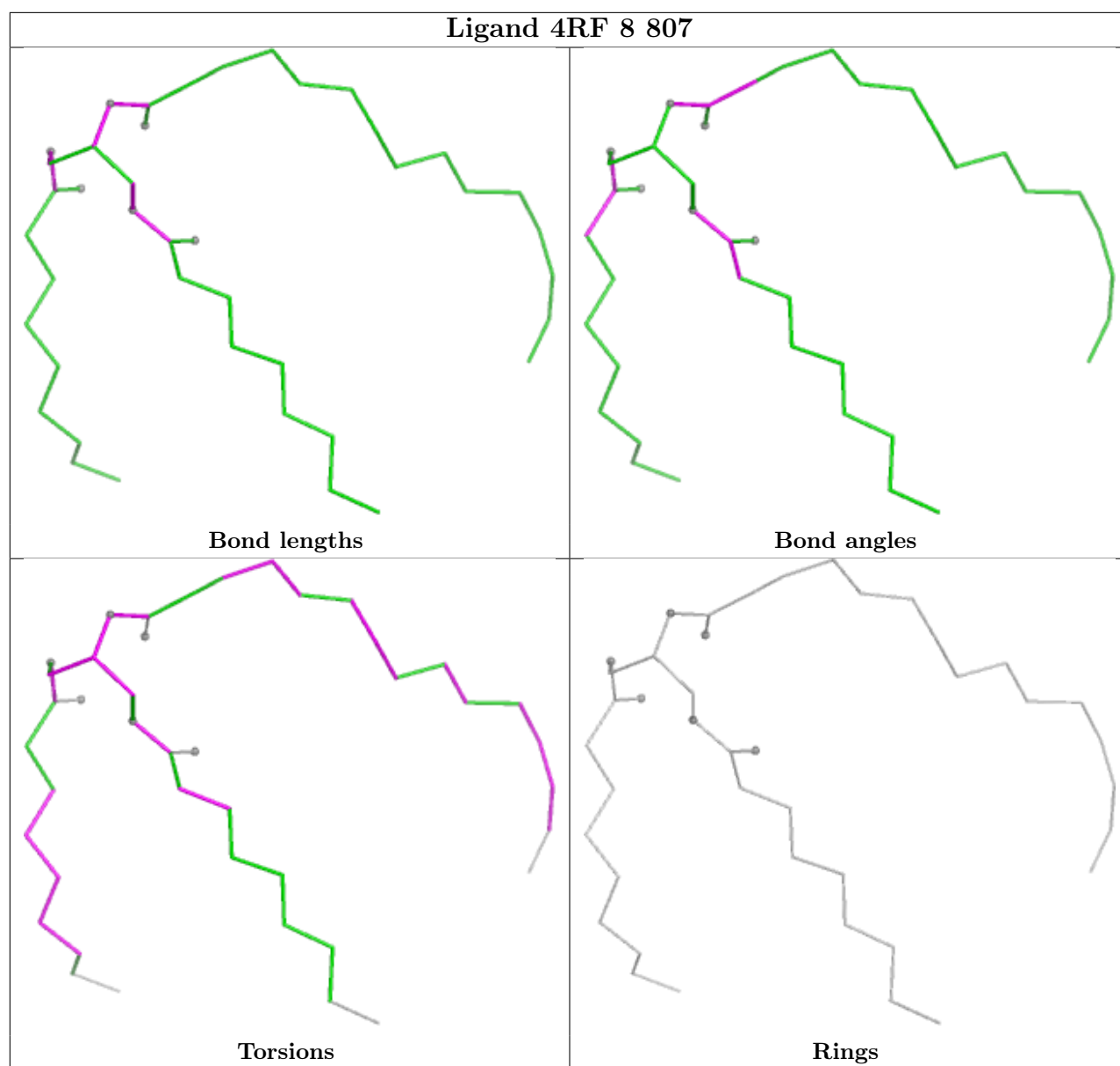


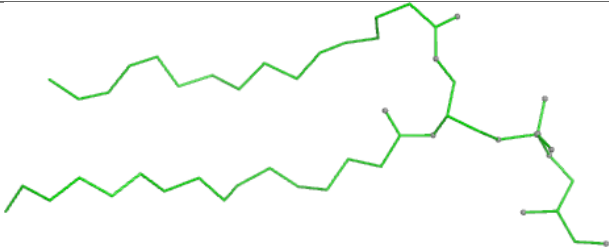
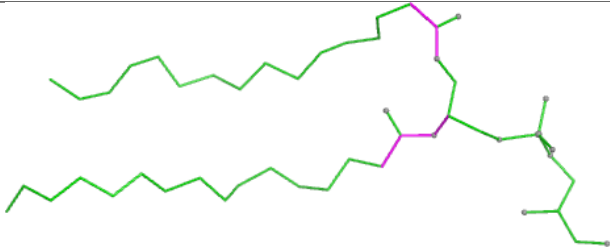
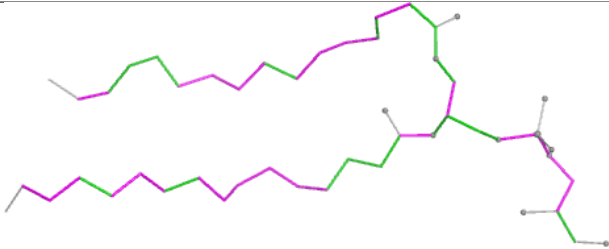
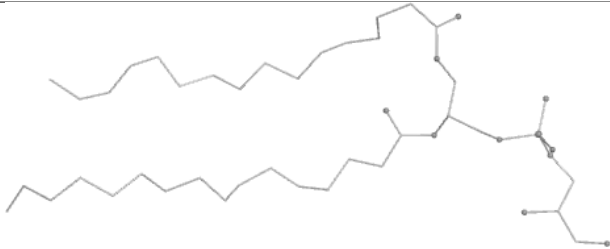
Rings

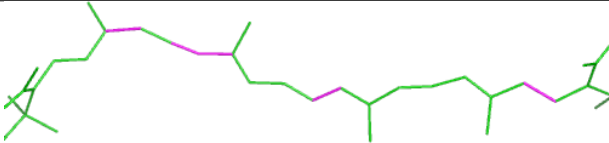
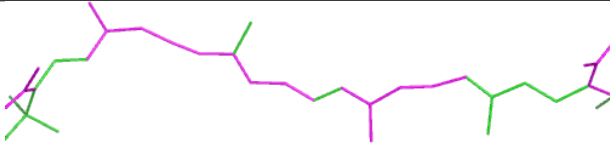
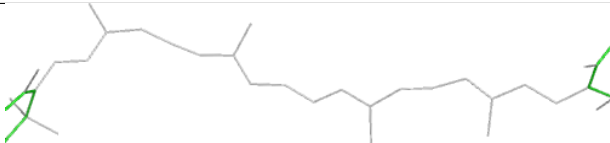


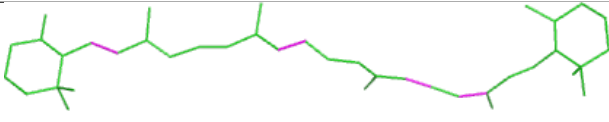
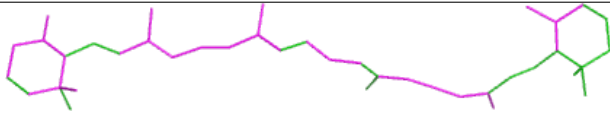
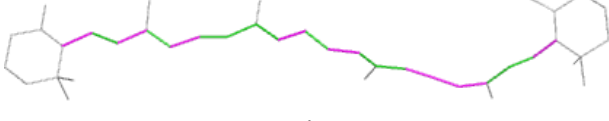
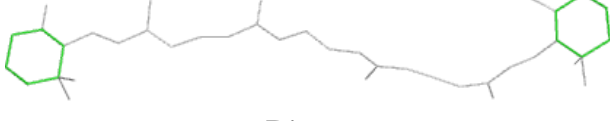
Ligand CLA 1 603



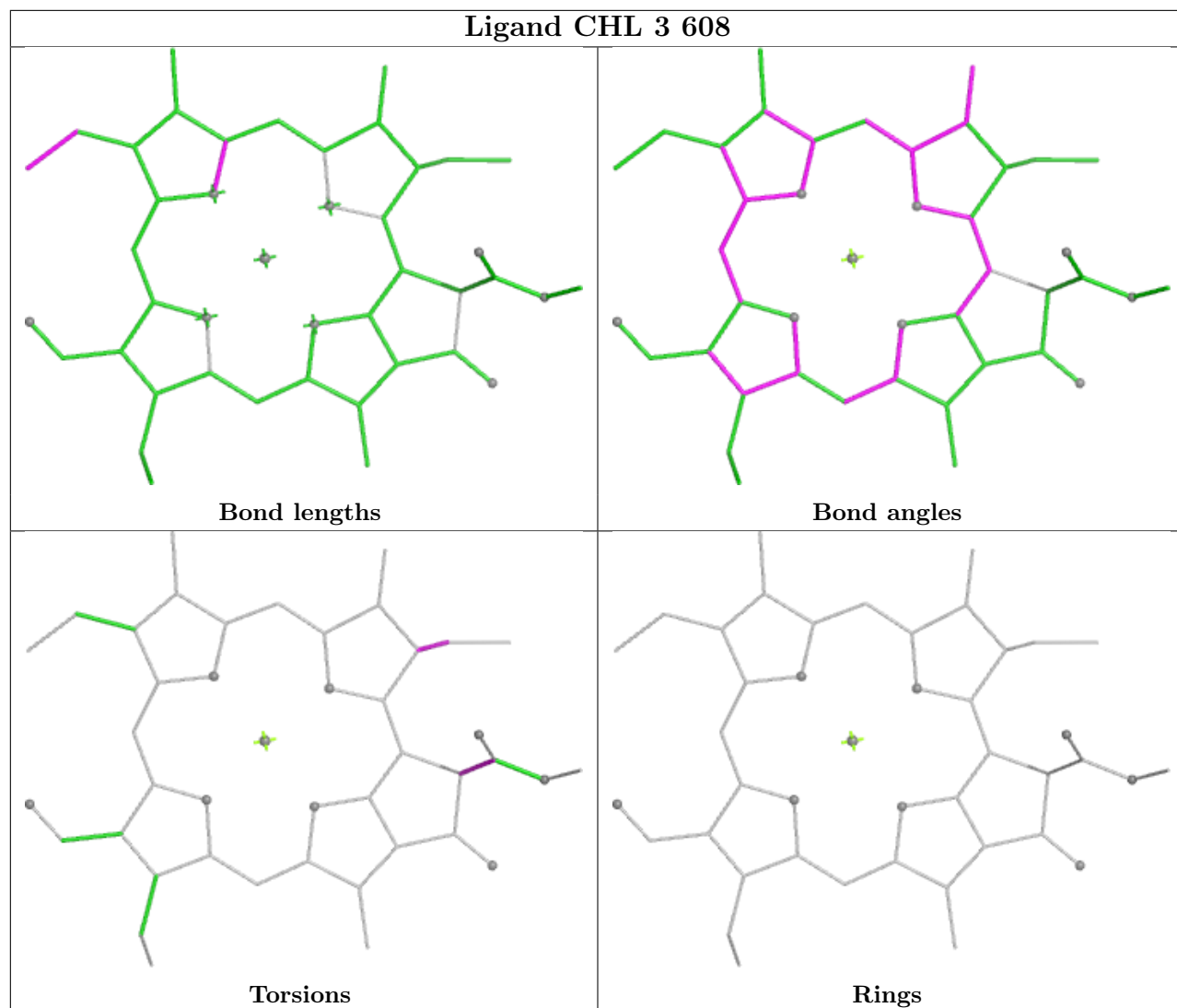


Ligand LHG 6 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

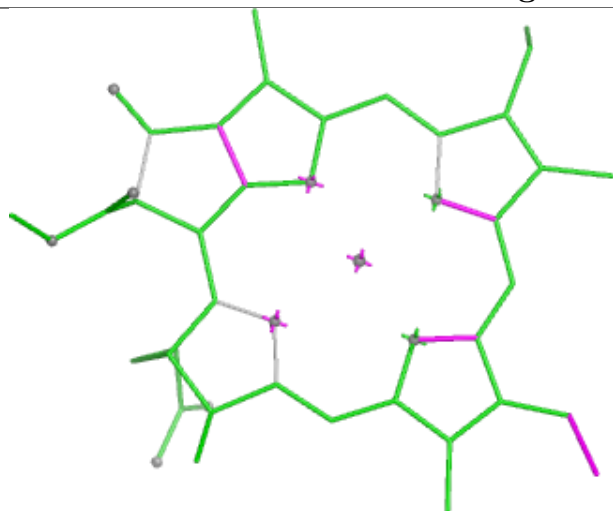
Ligand BCR A 4003	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR L 4001	
	
Bond lengths	Bond angles
	
Torsions	Rings

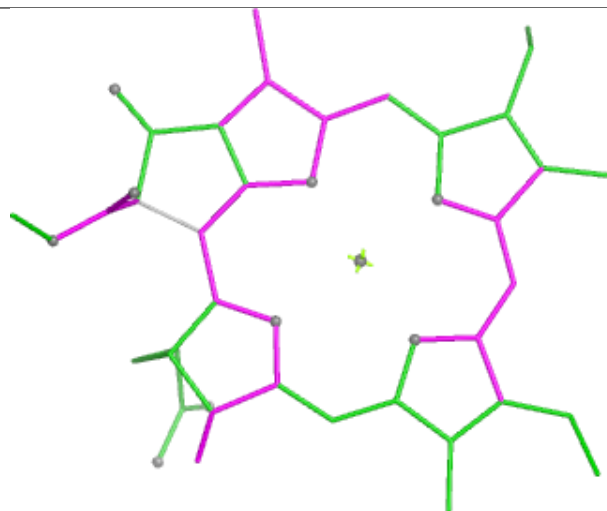
Ligand CHL 3 608



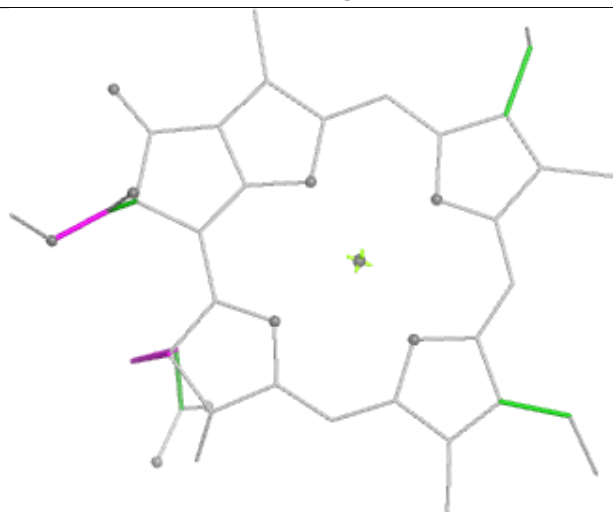
Ligand CLA 1 610



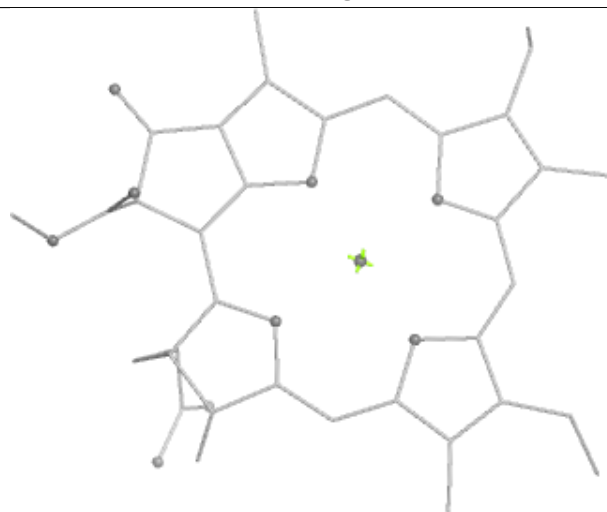
Bond lengths



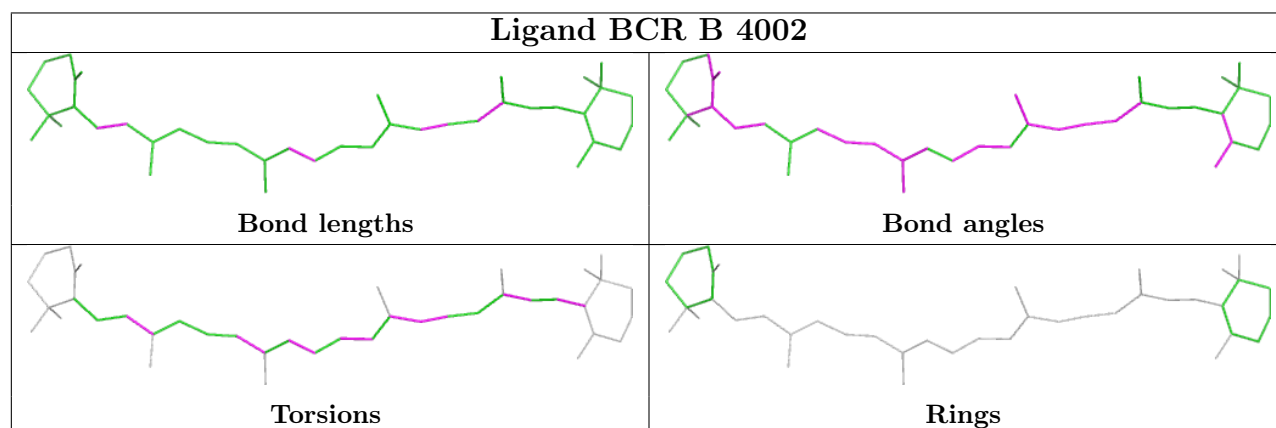
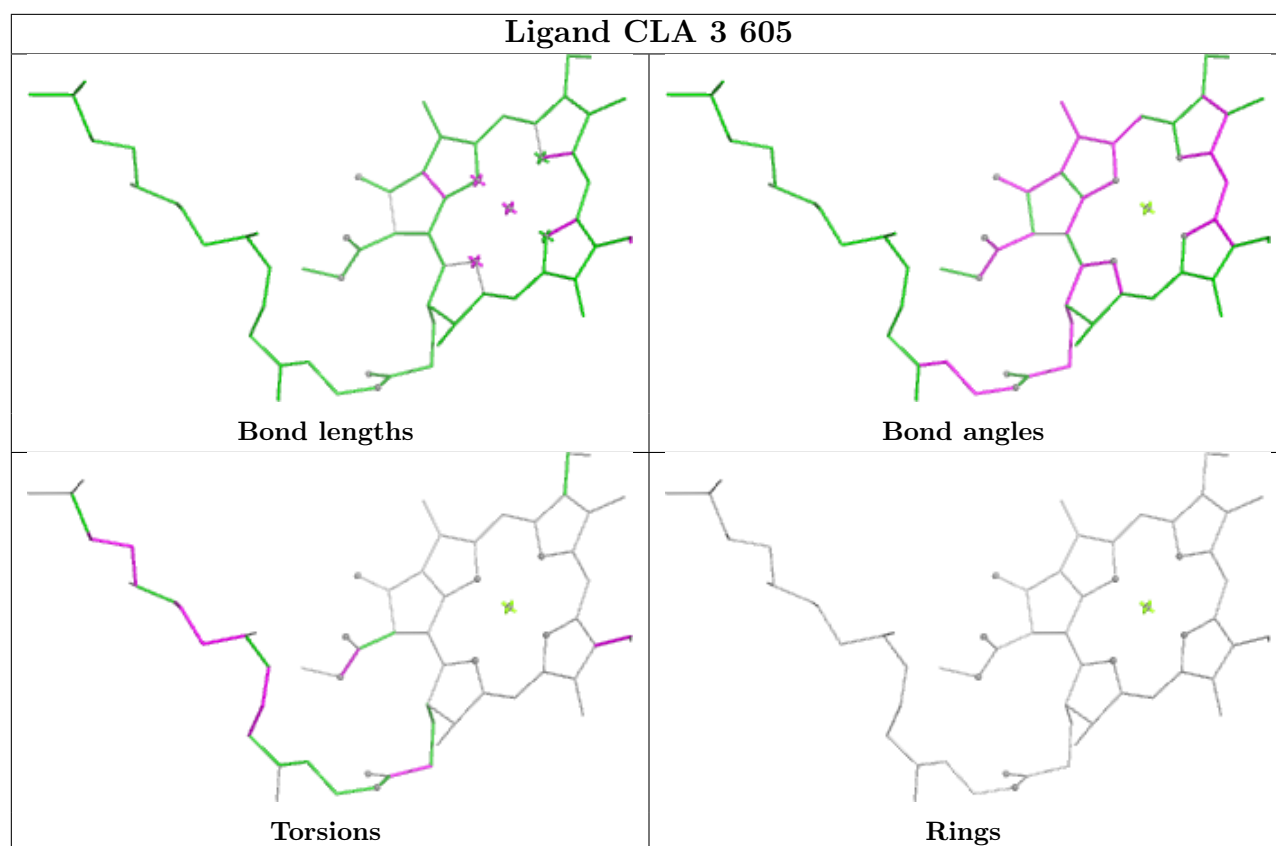
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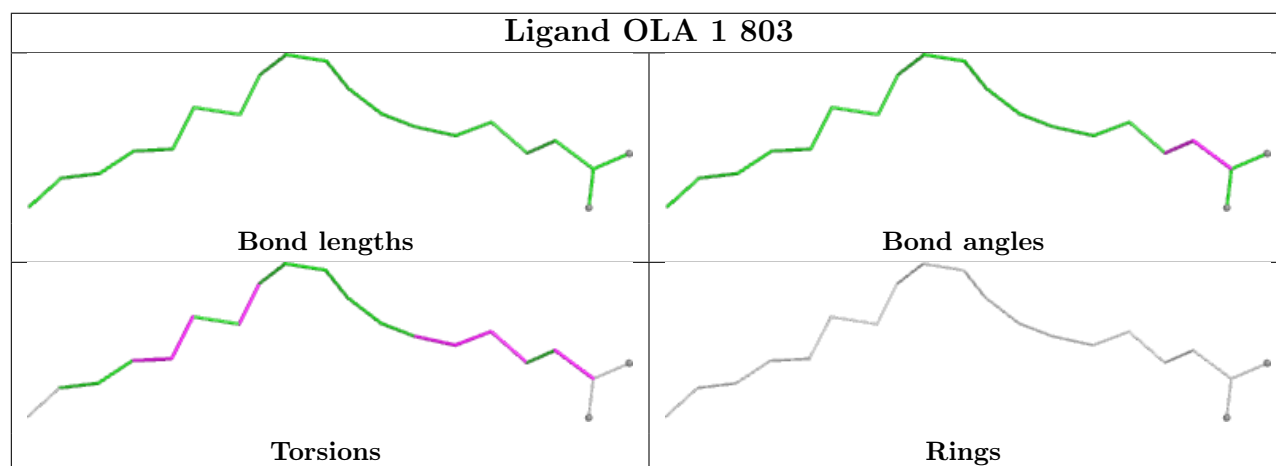
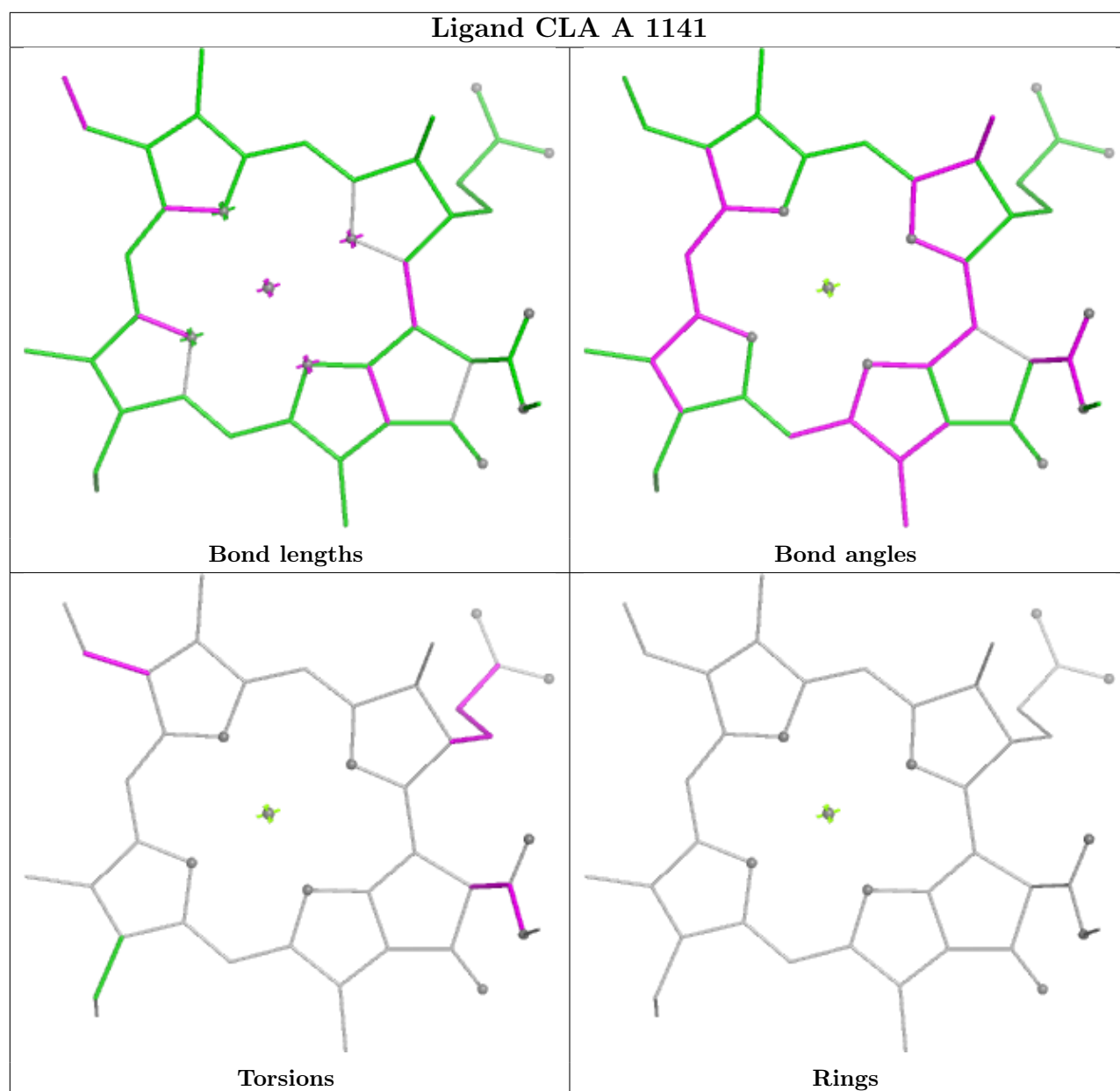


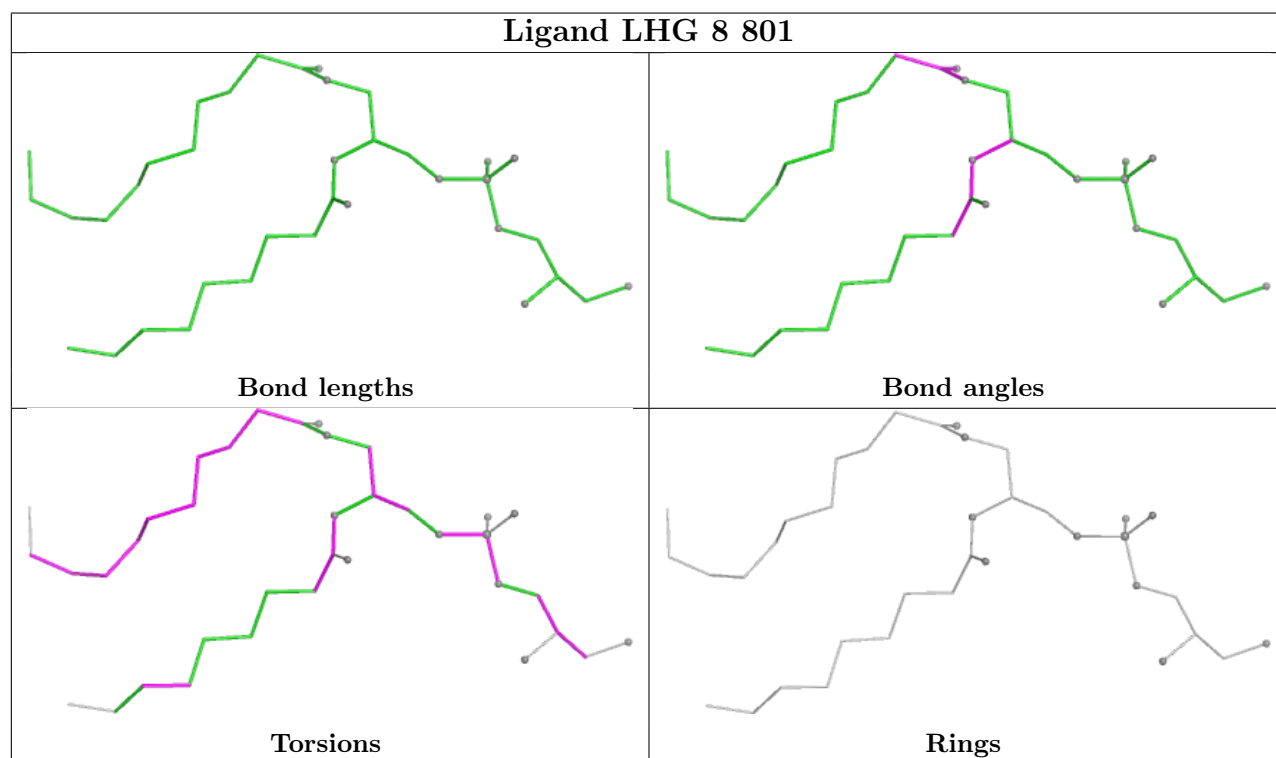
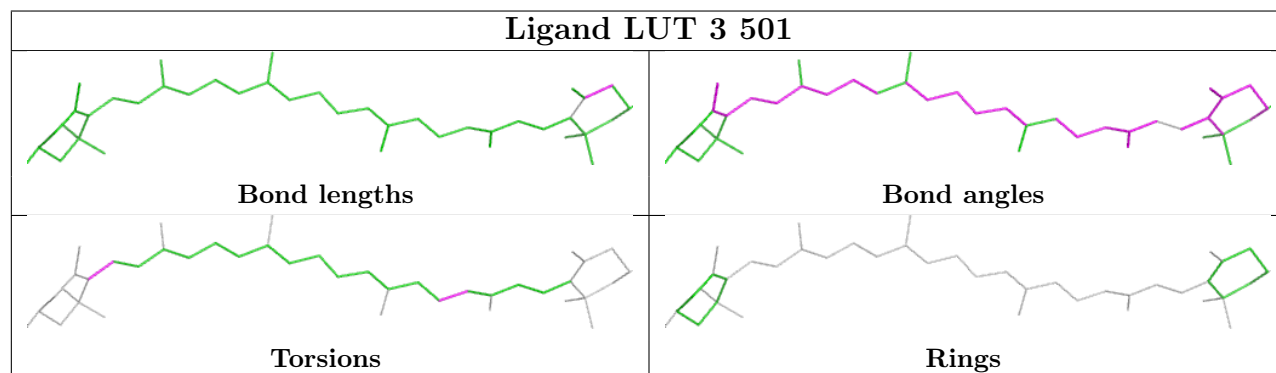
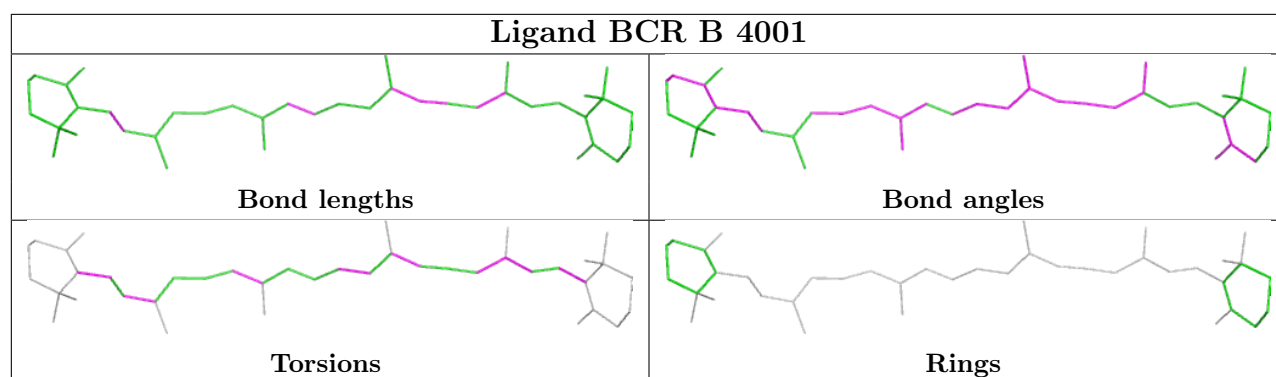
Torsions



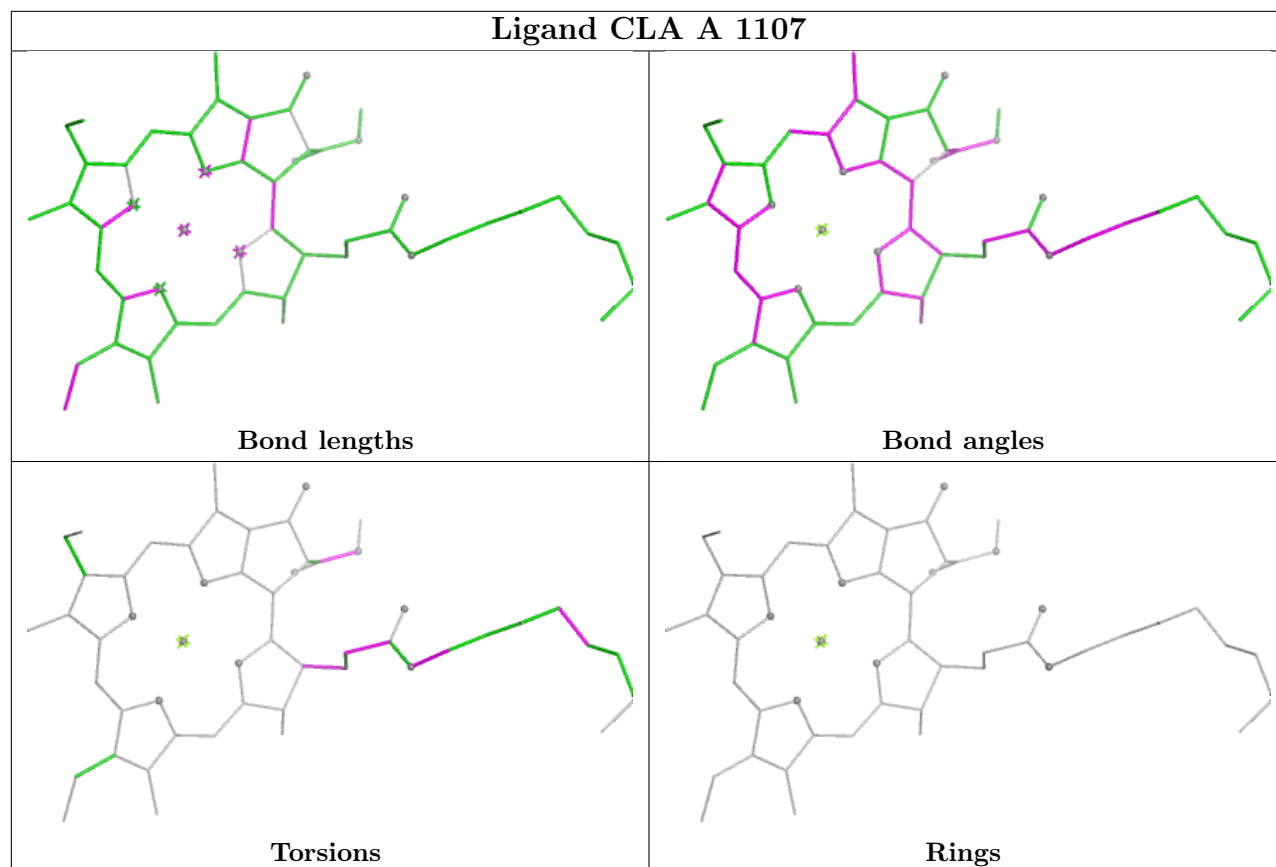
Rings

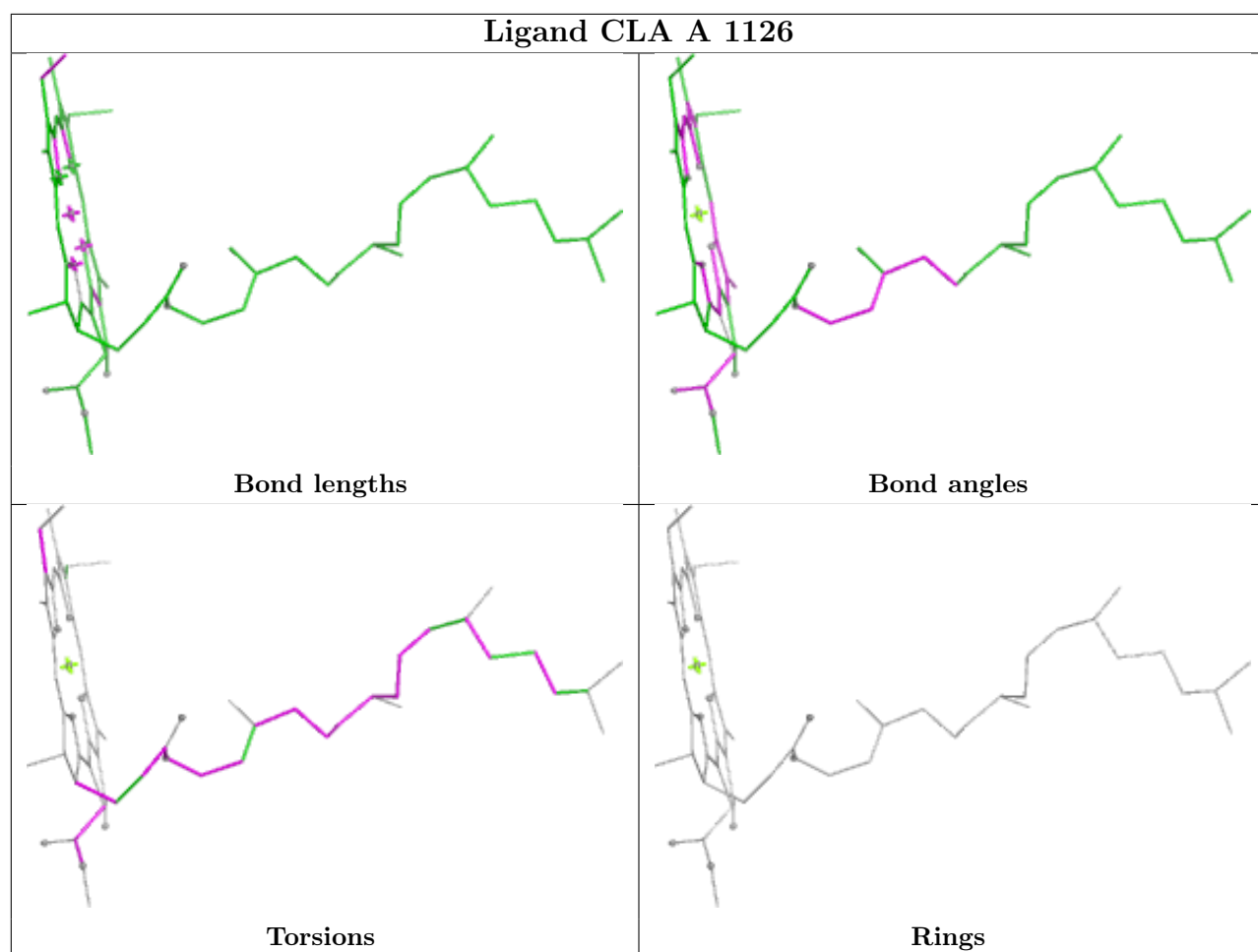


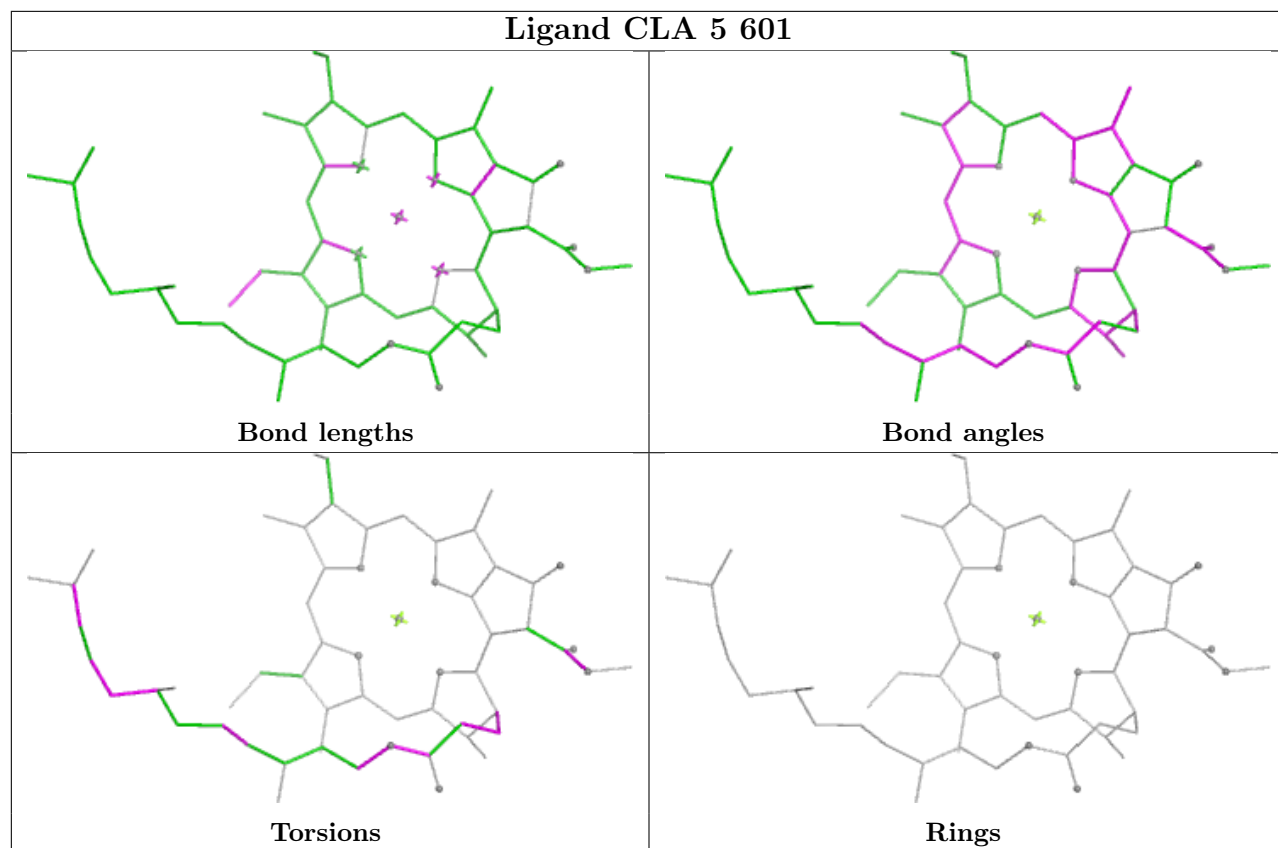




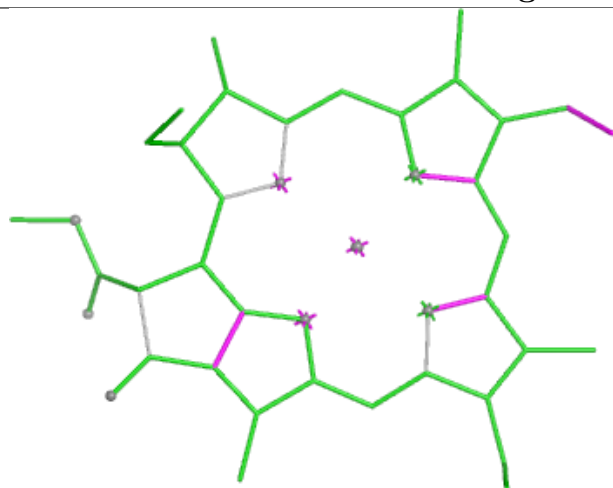
Ligand CLA A 1107



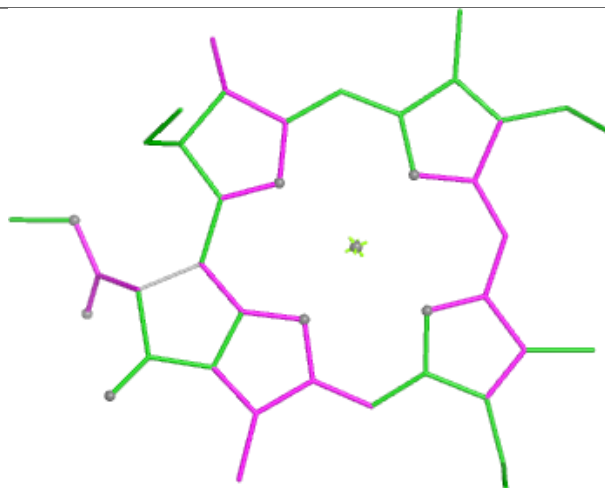




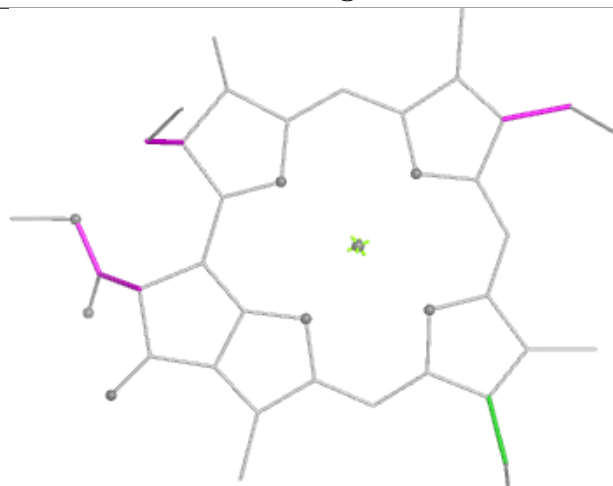
Ligand CLA 7 608



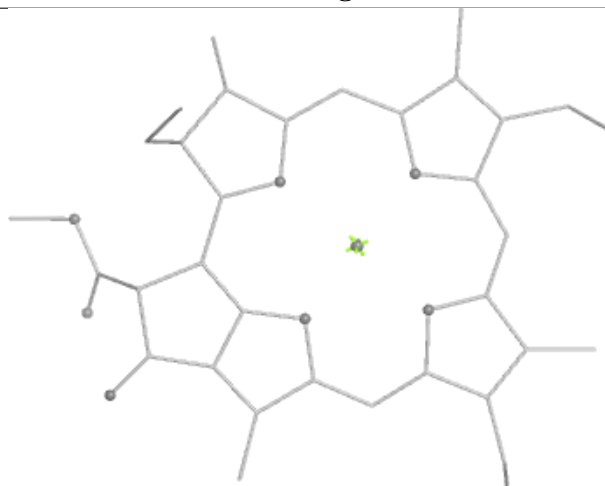
Bond lengths



Bond angles

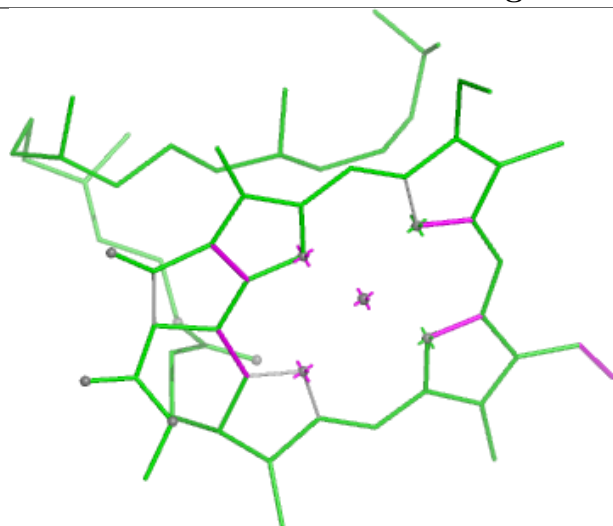


Torsions

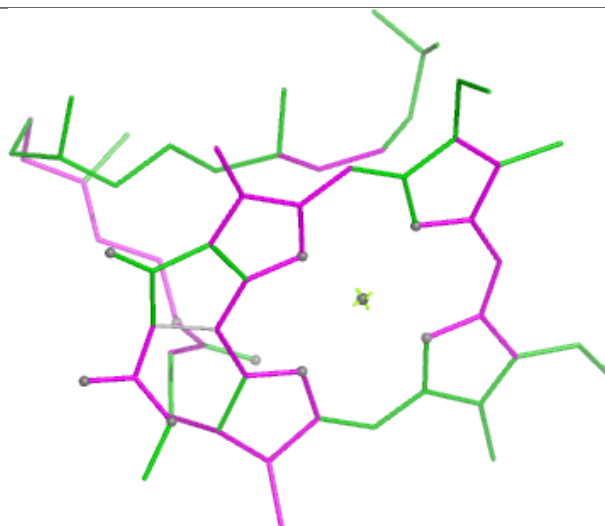


Rings

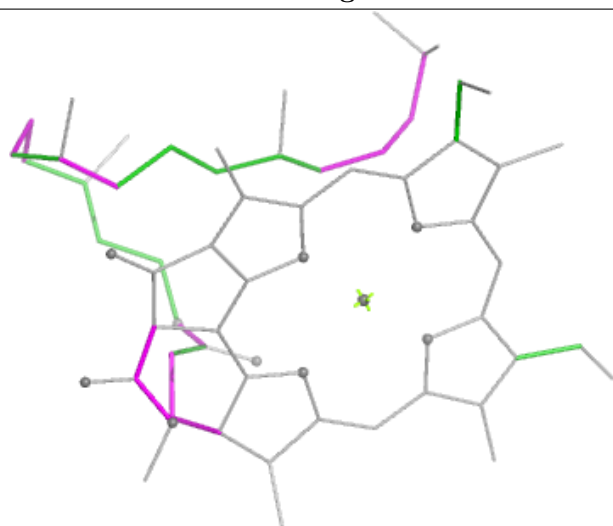
Ligand CLA B 1201



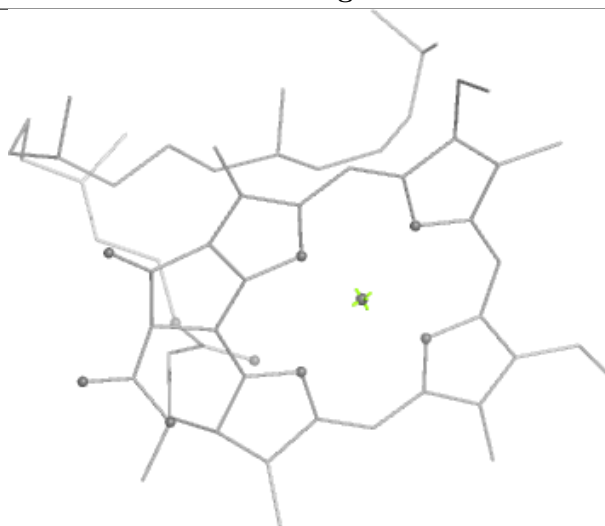
Bond lengths



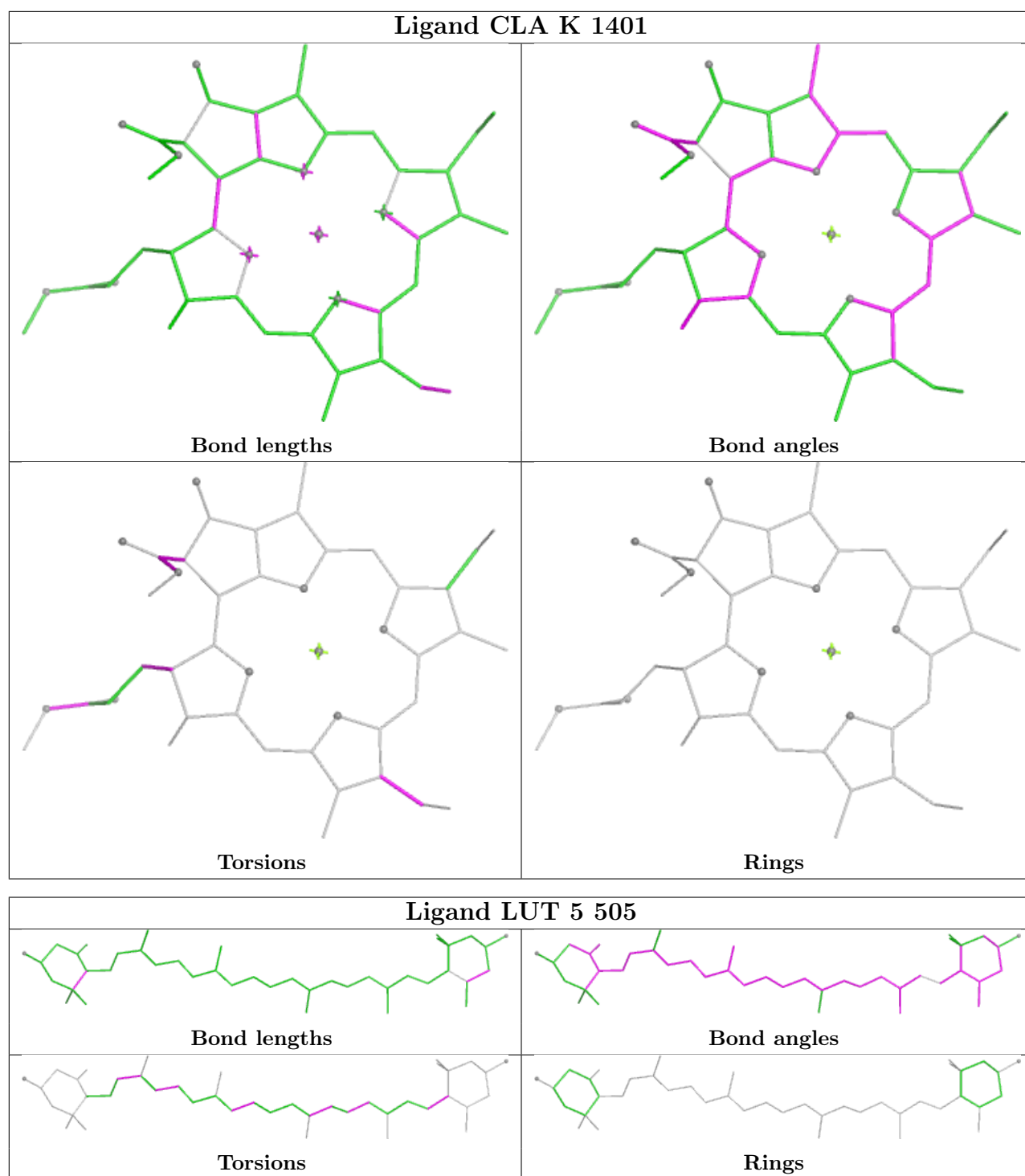
Bond angles

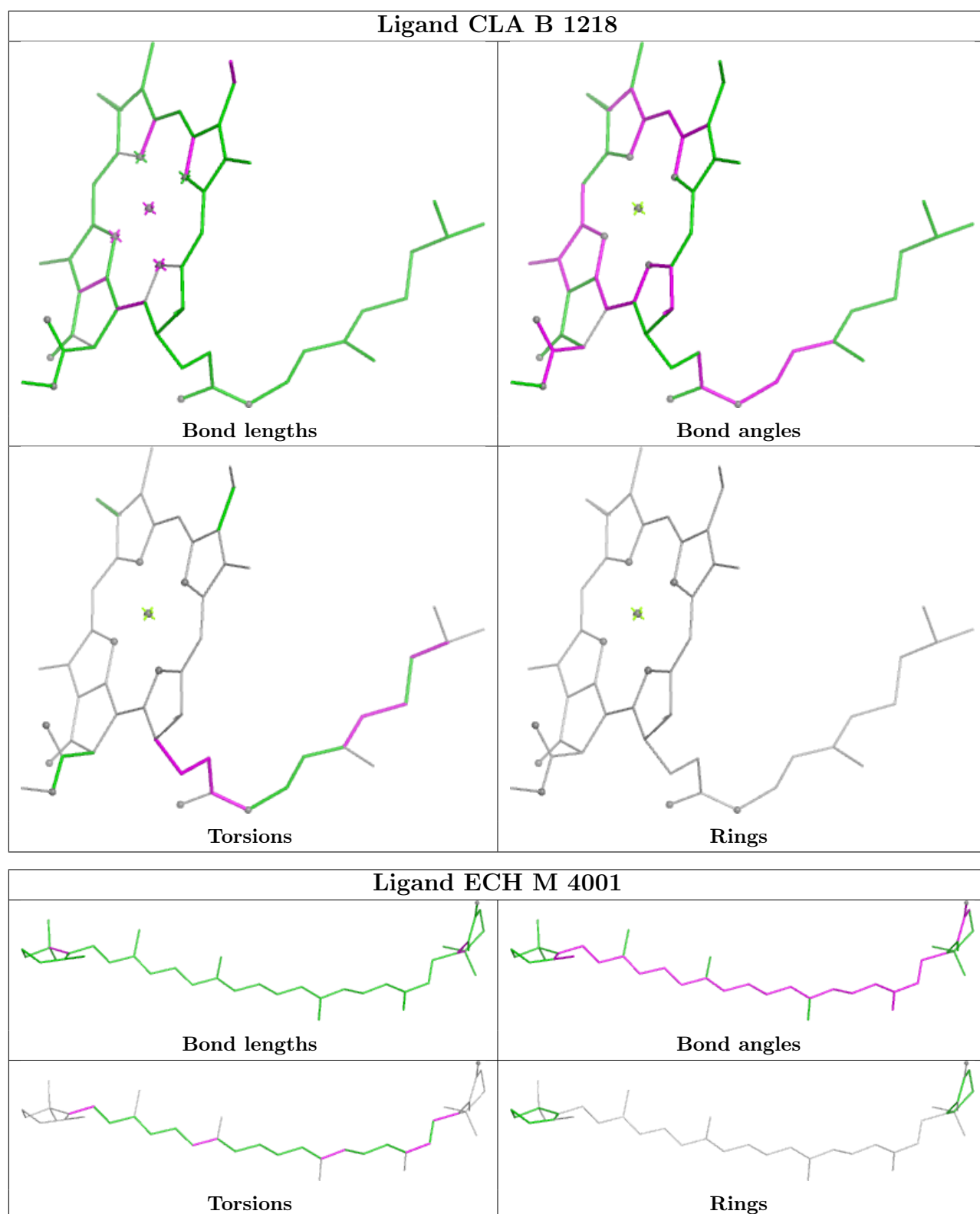


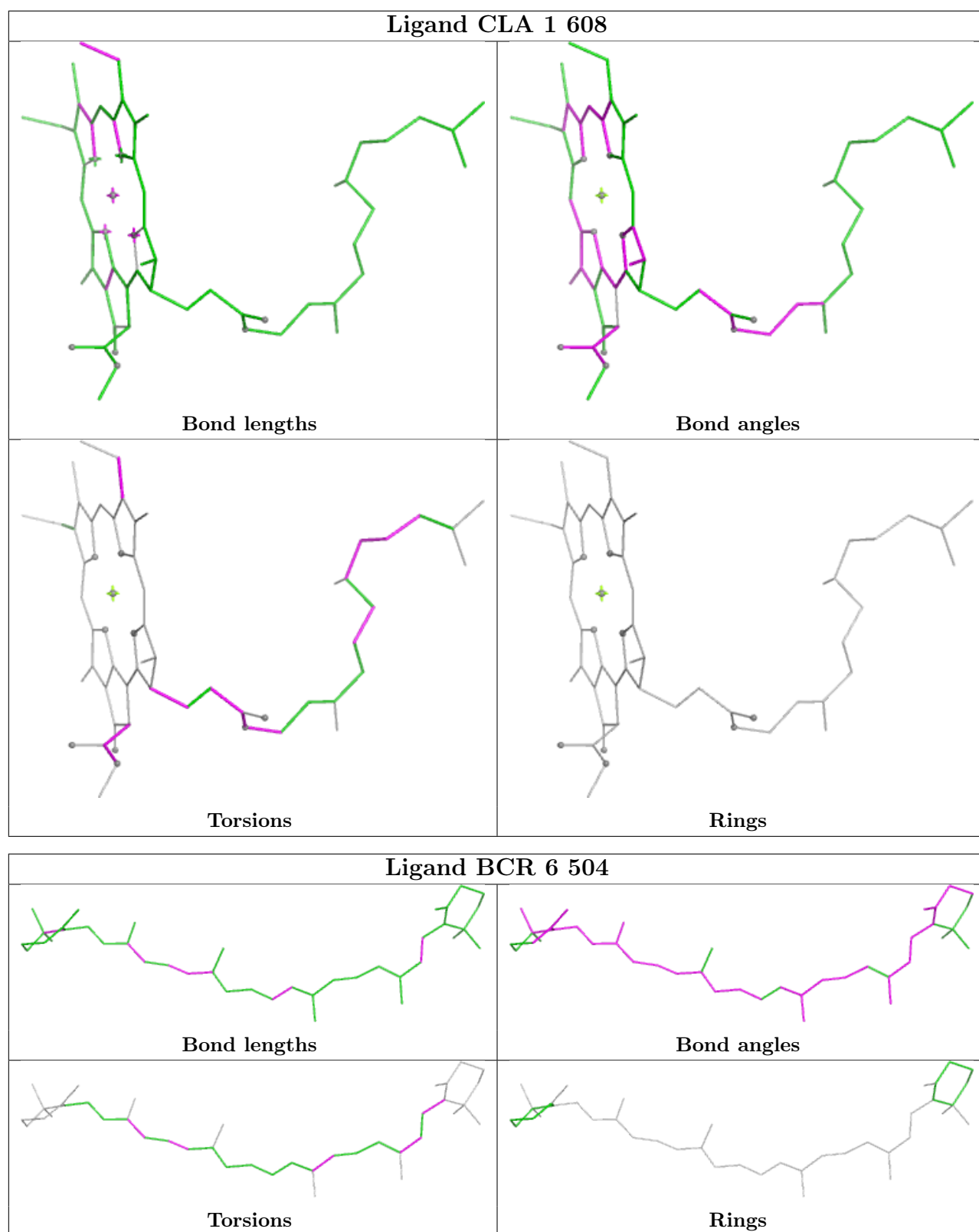
Torsions

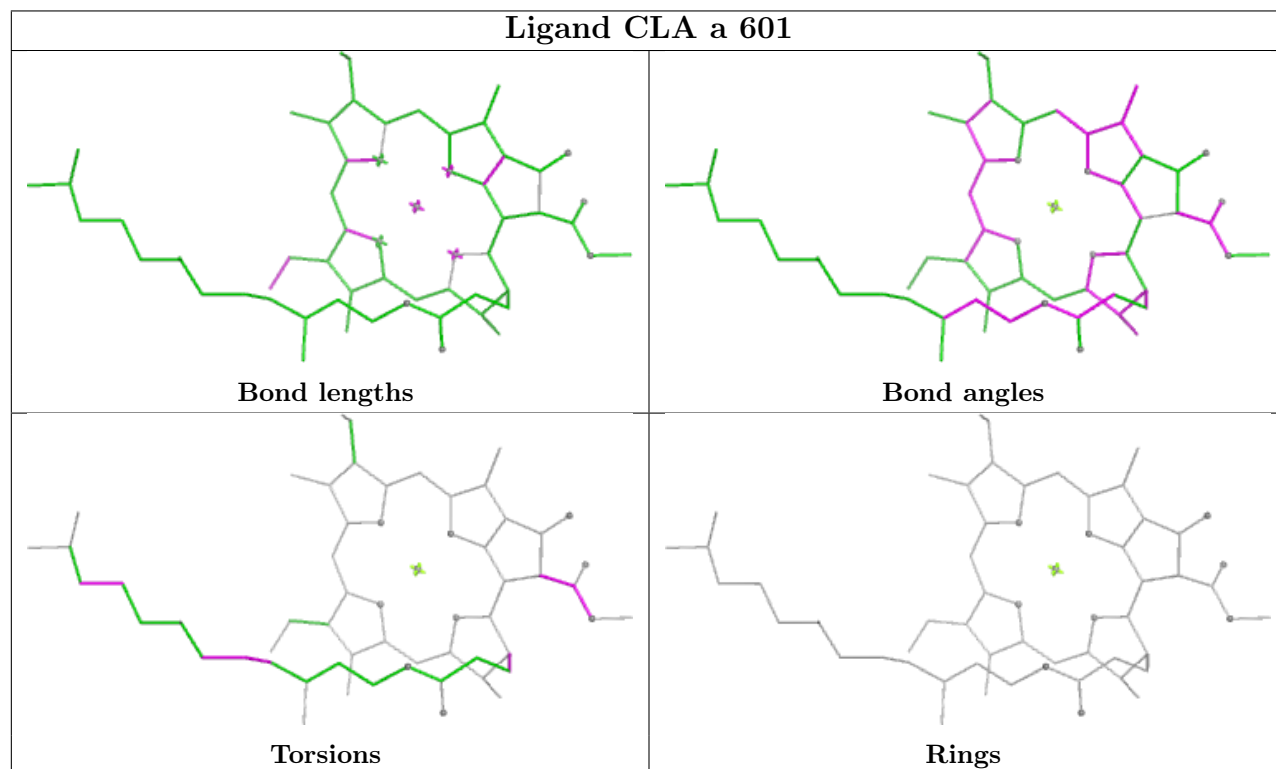
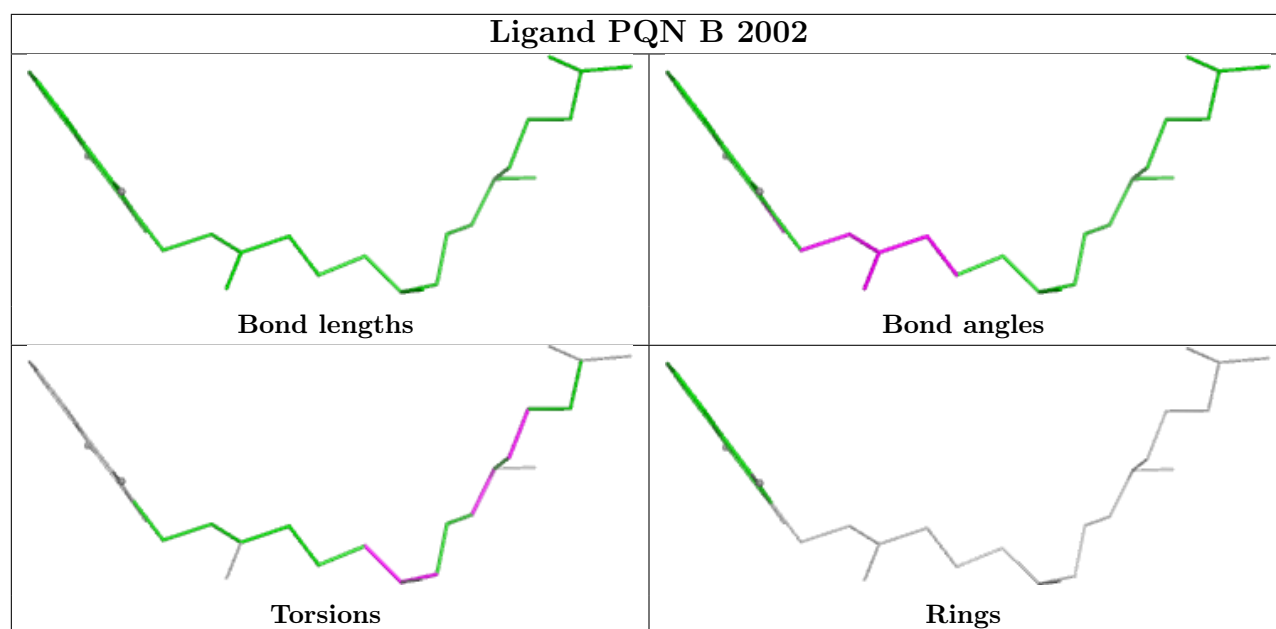


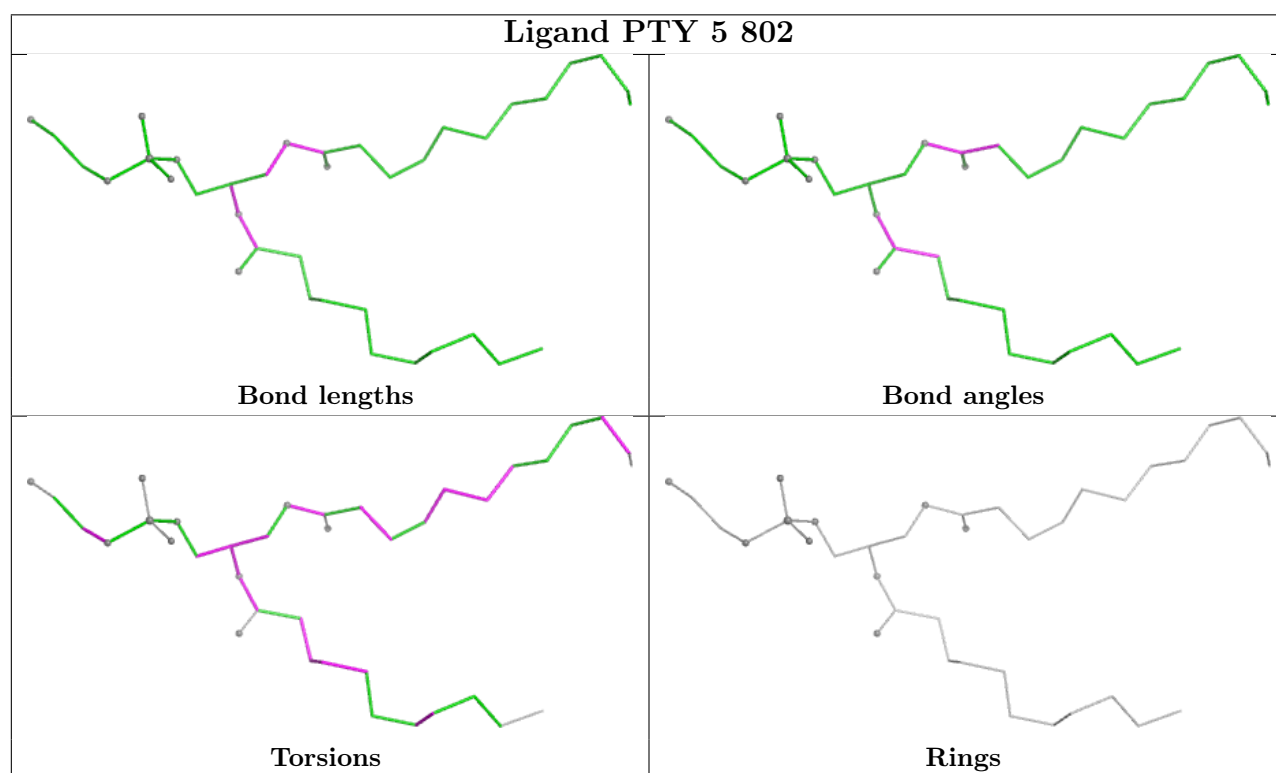
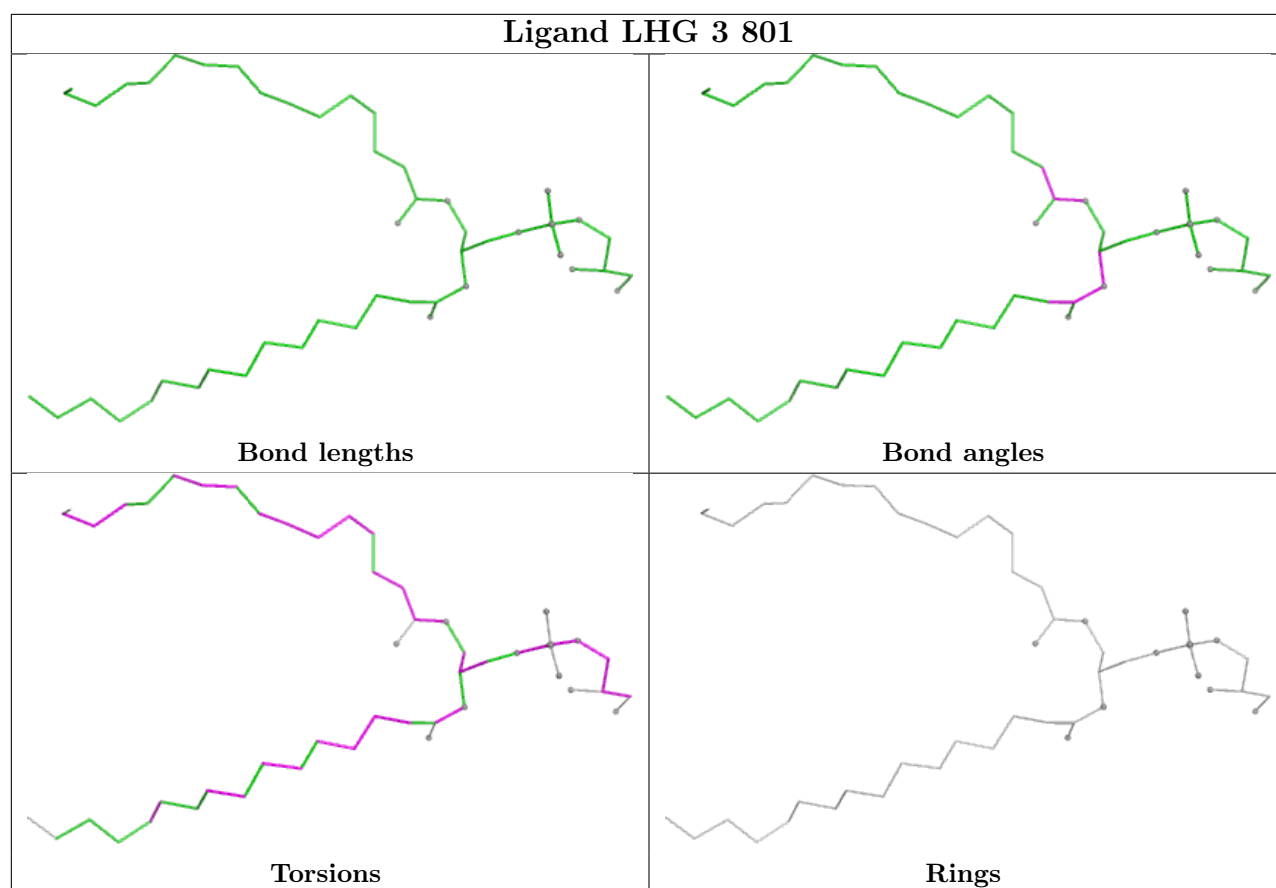
Rings

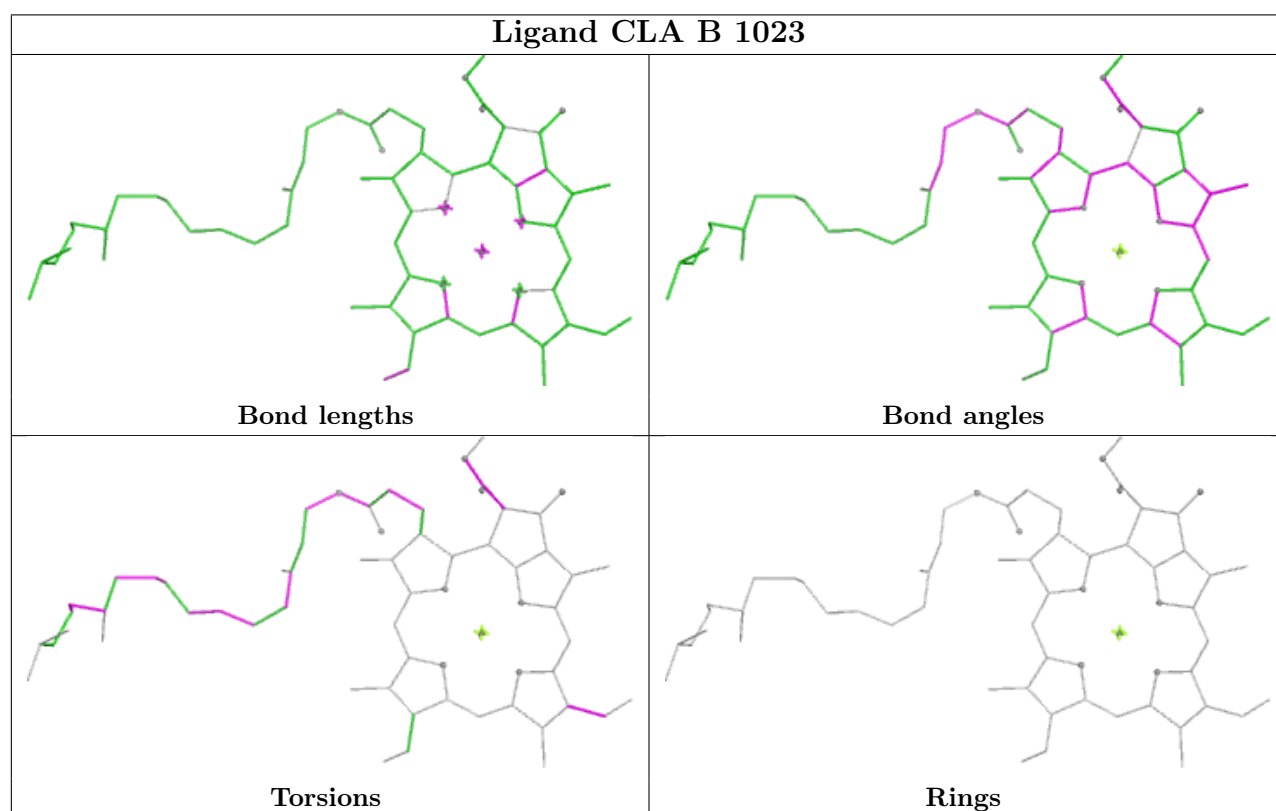
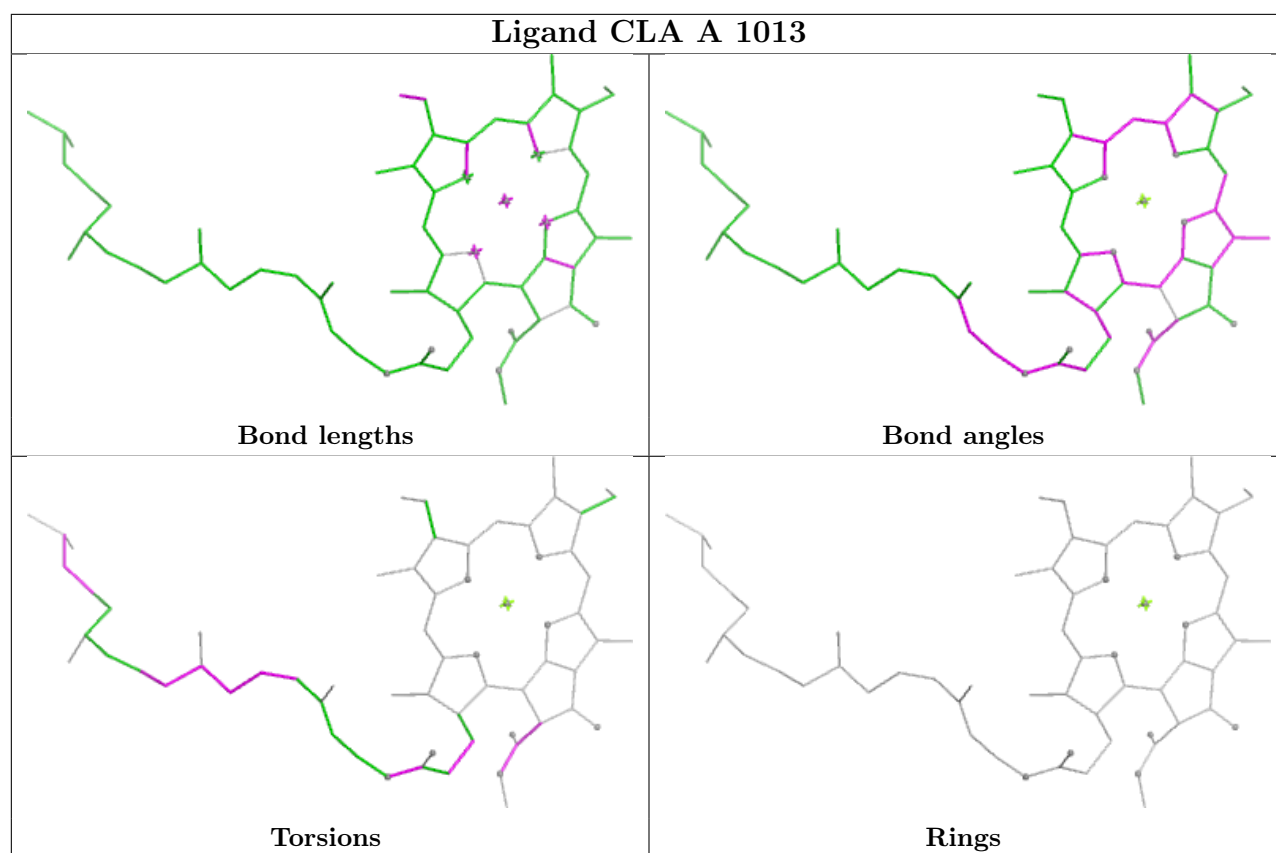




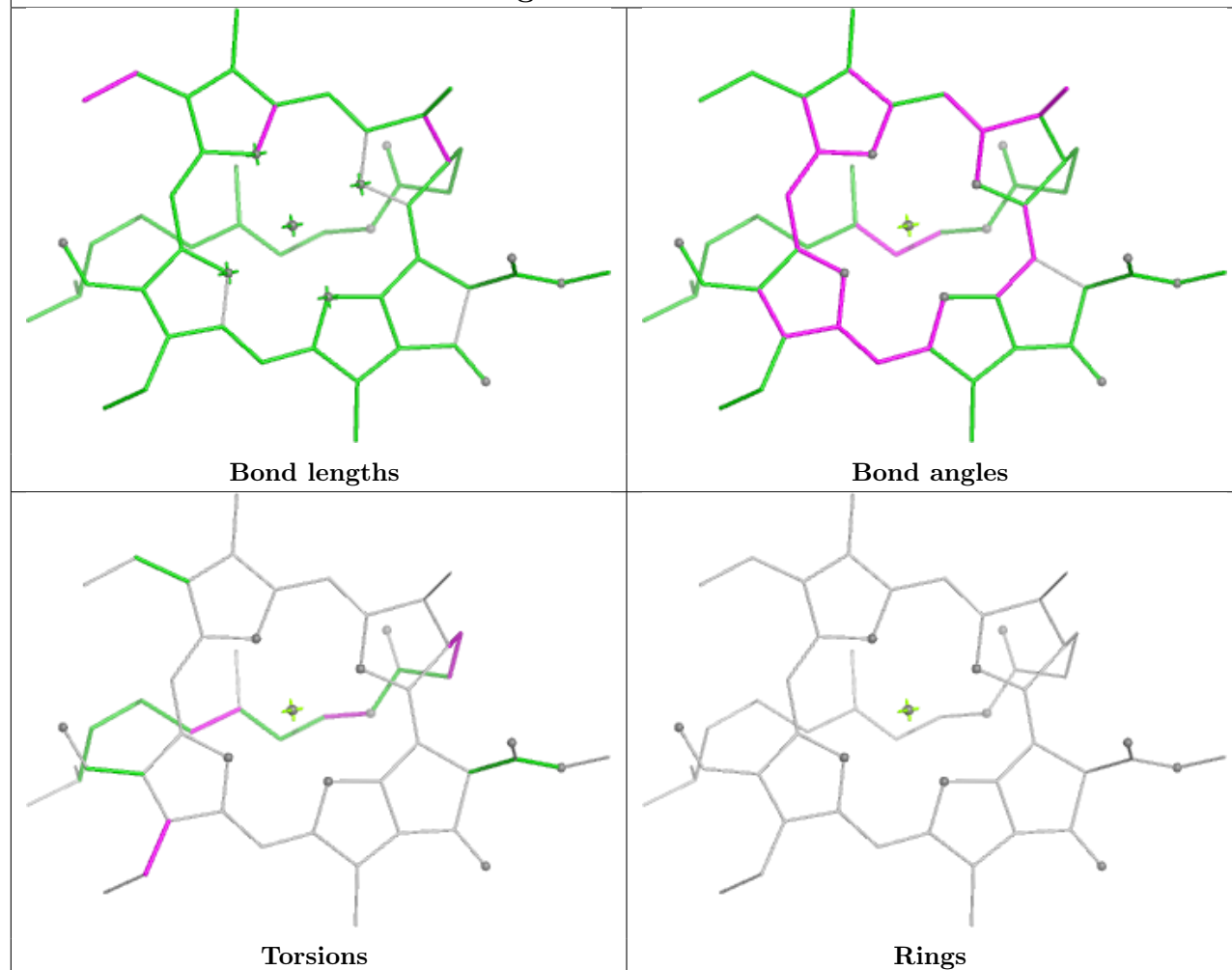




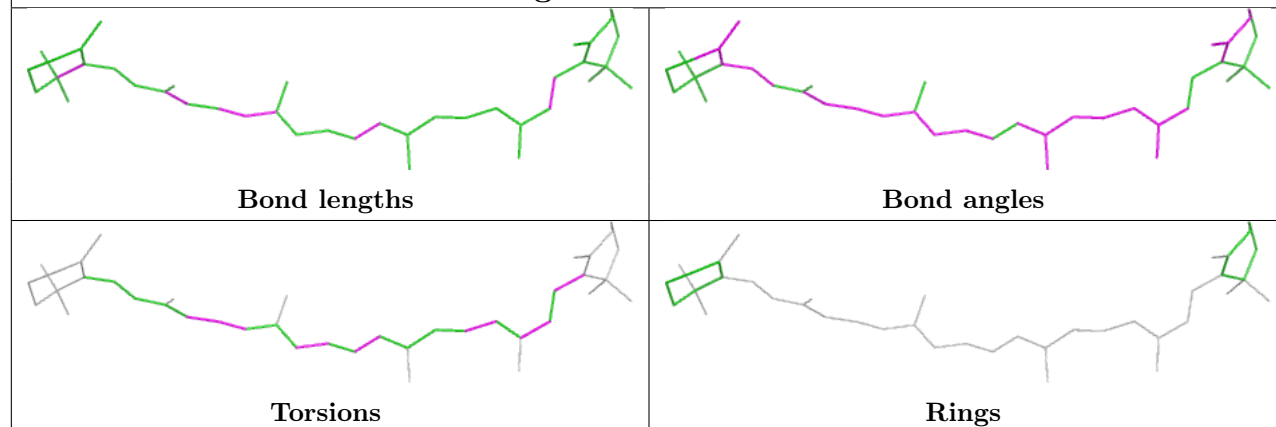


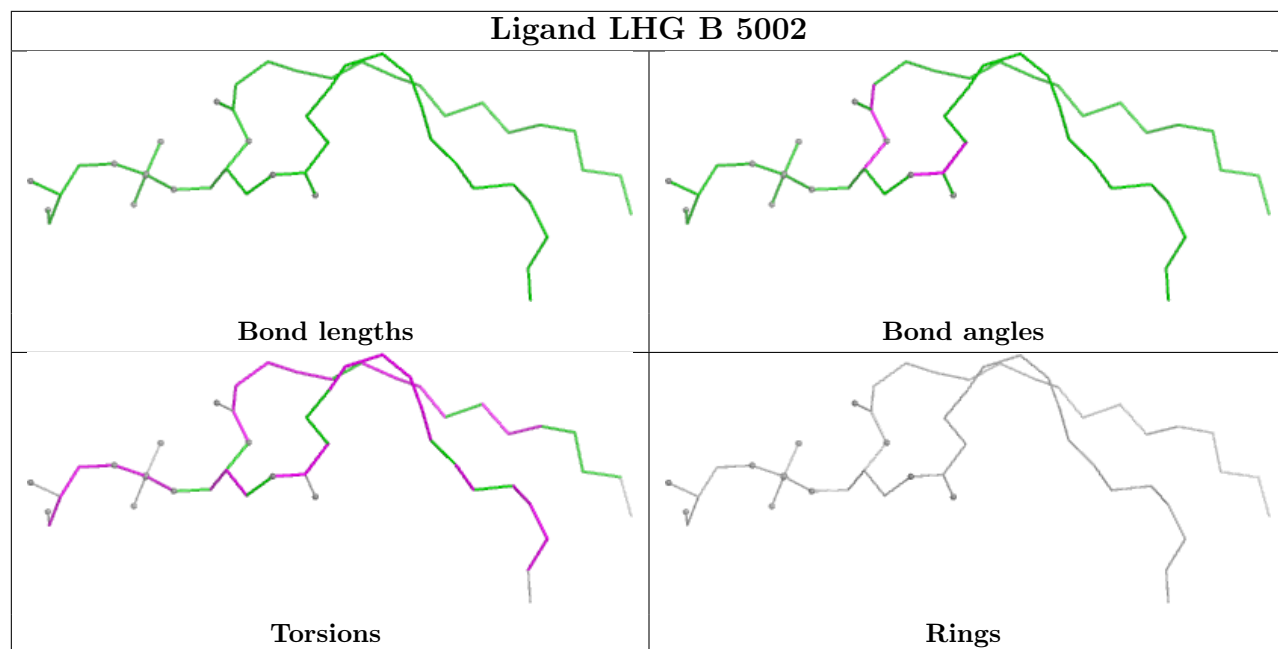


Ligand CHL 4 618

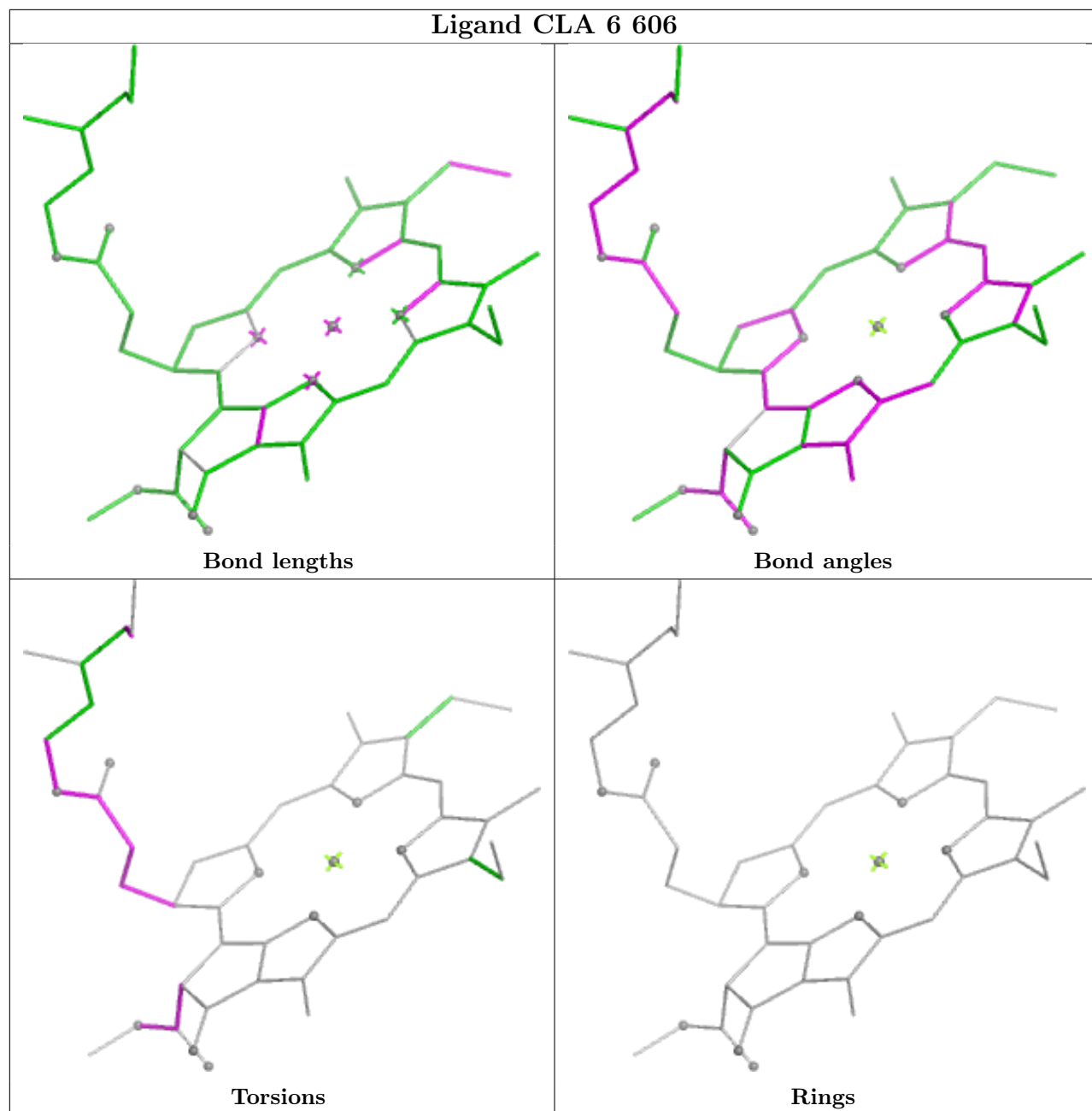


Ligand BCR 5 504

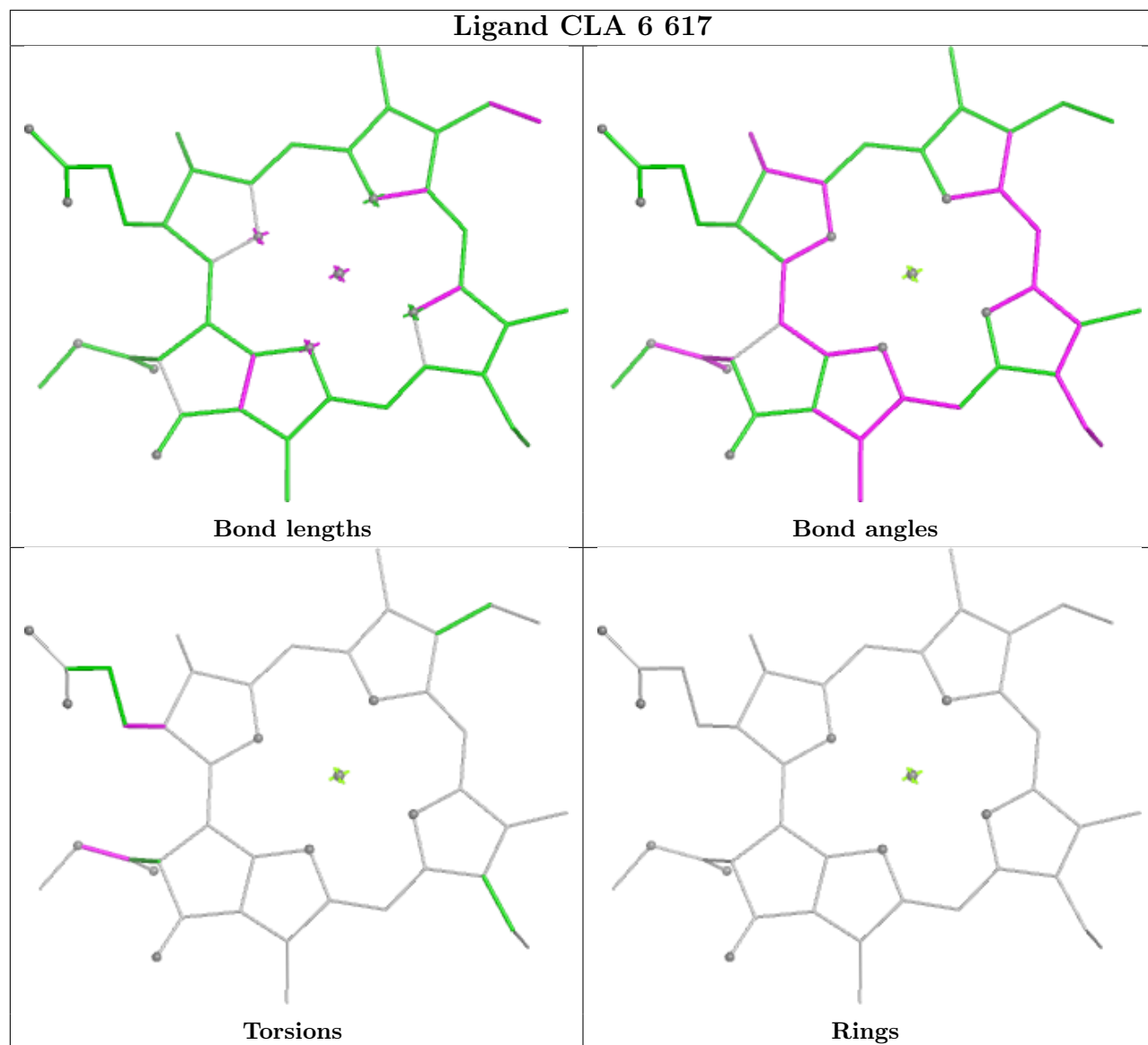




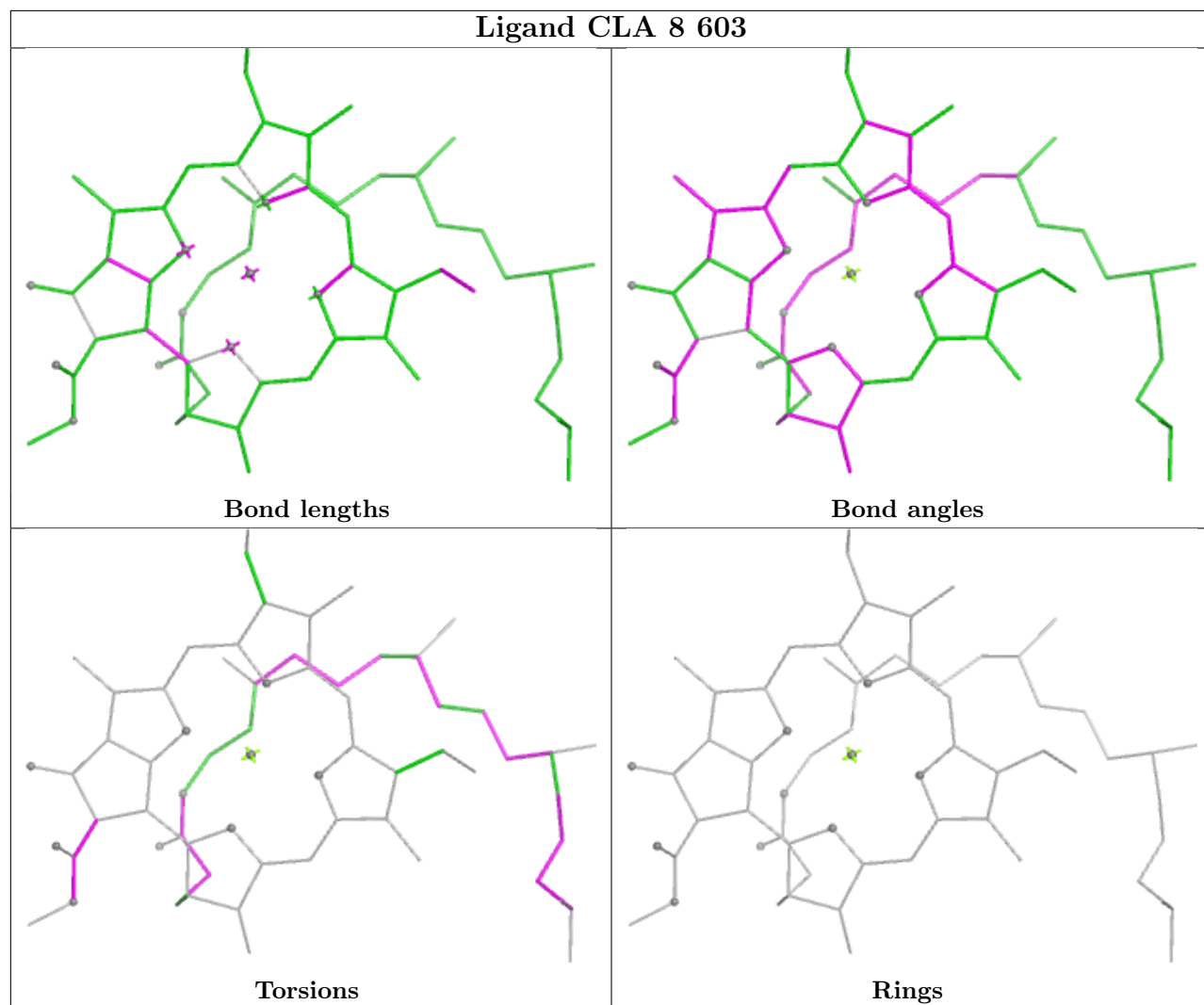
Ligand CLA 6 606



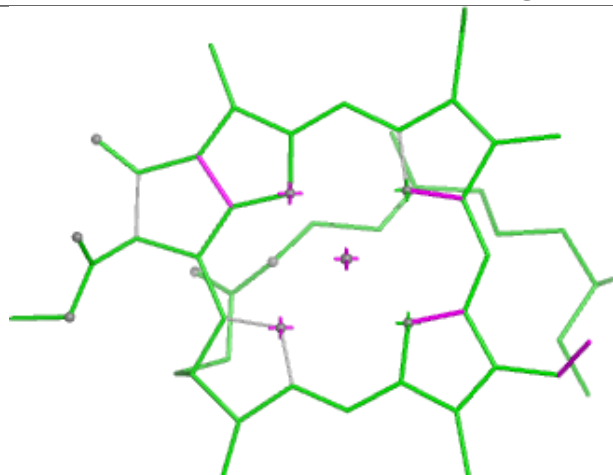
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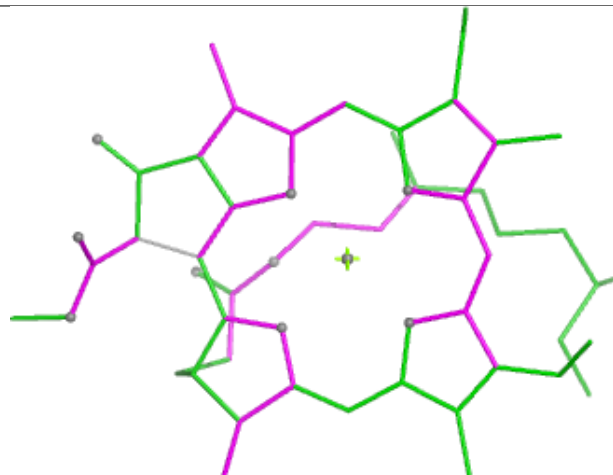
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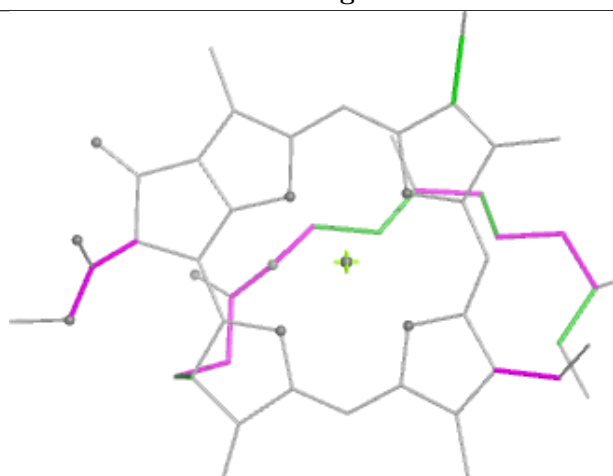
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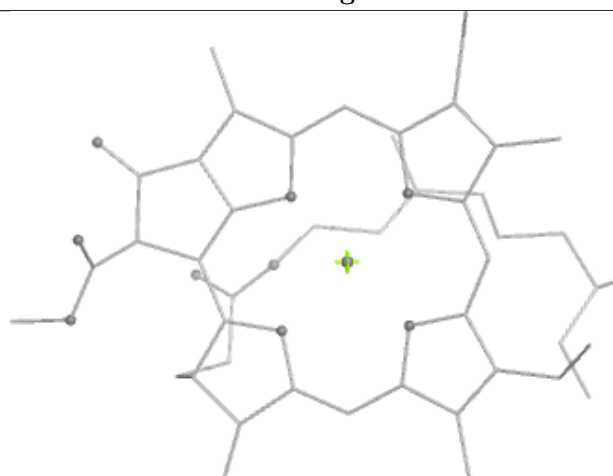
Bond lengths



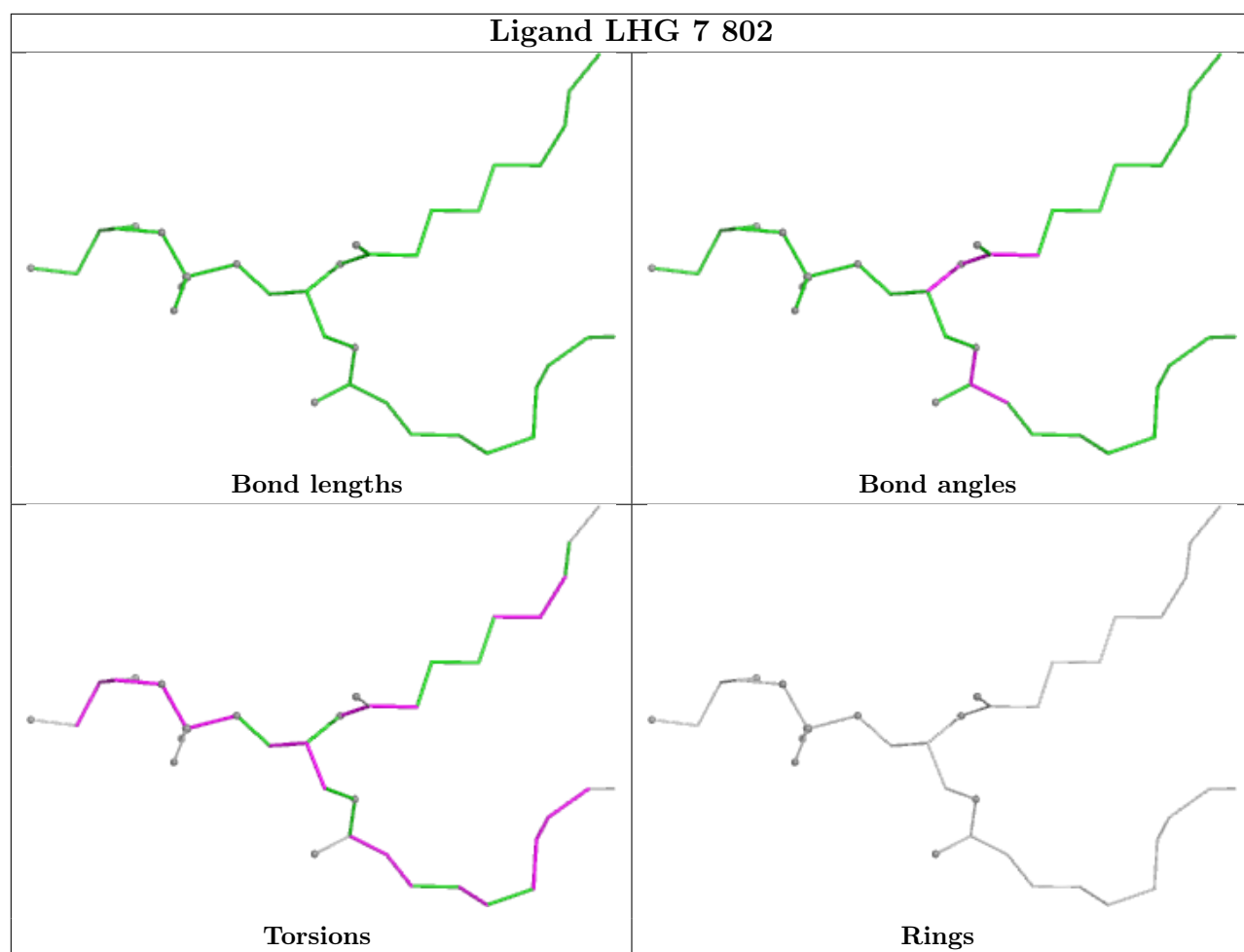
Bond angles

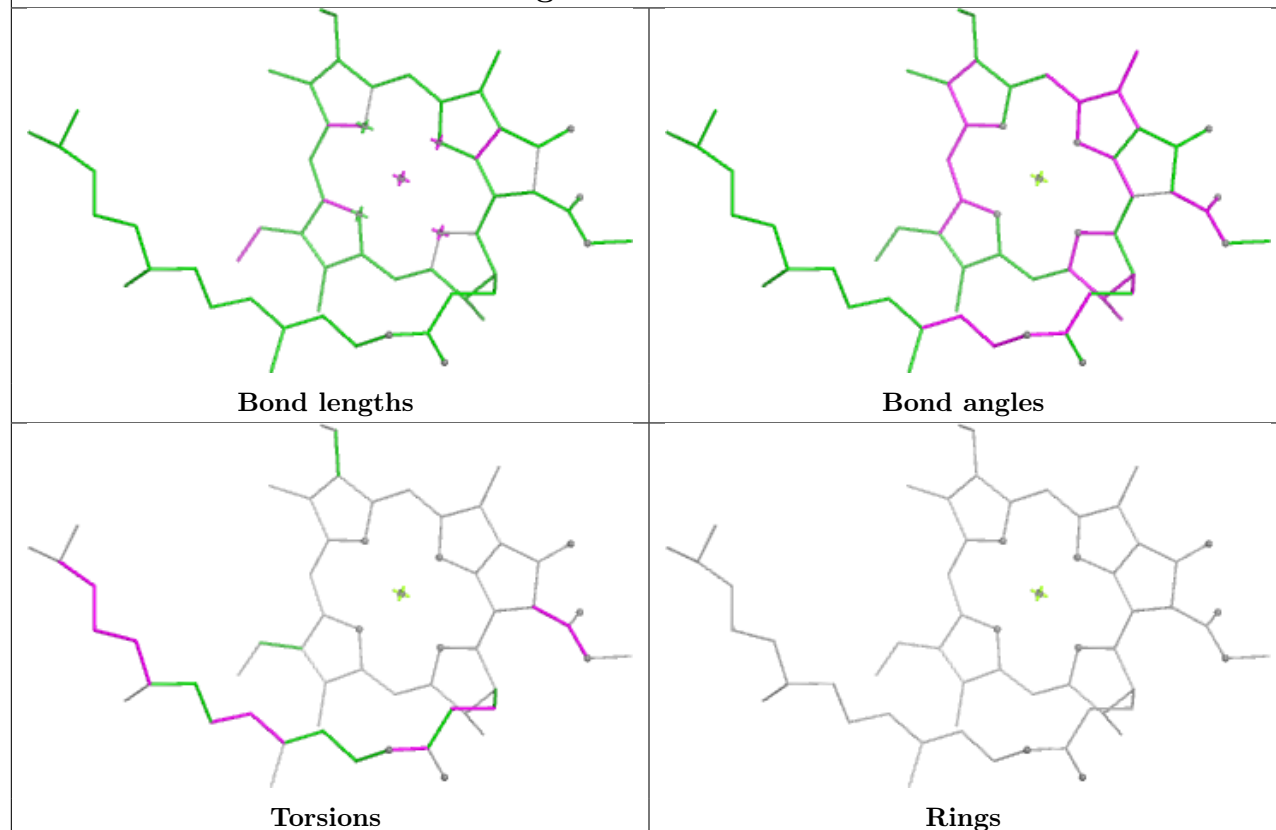
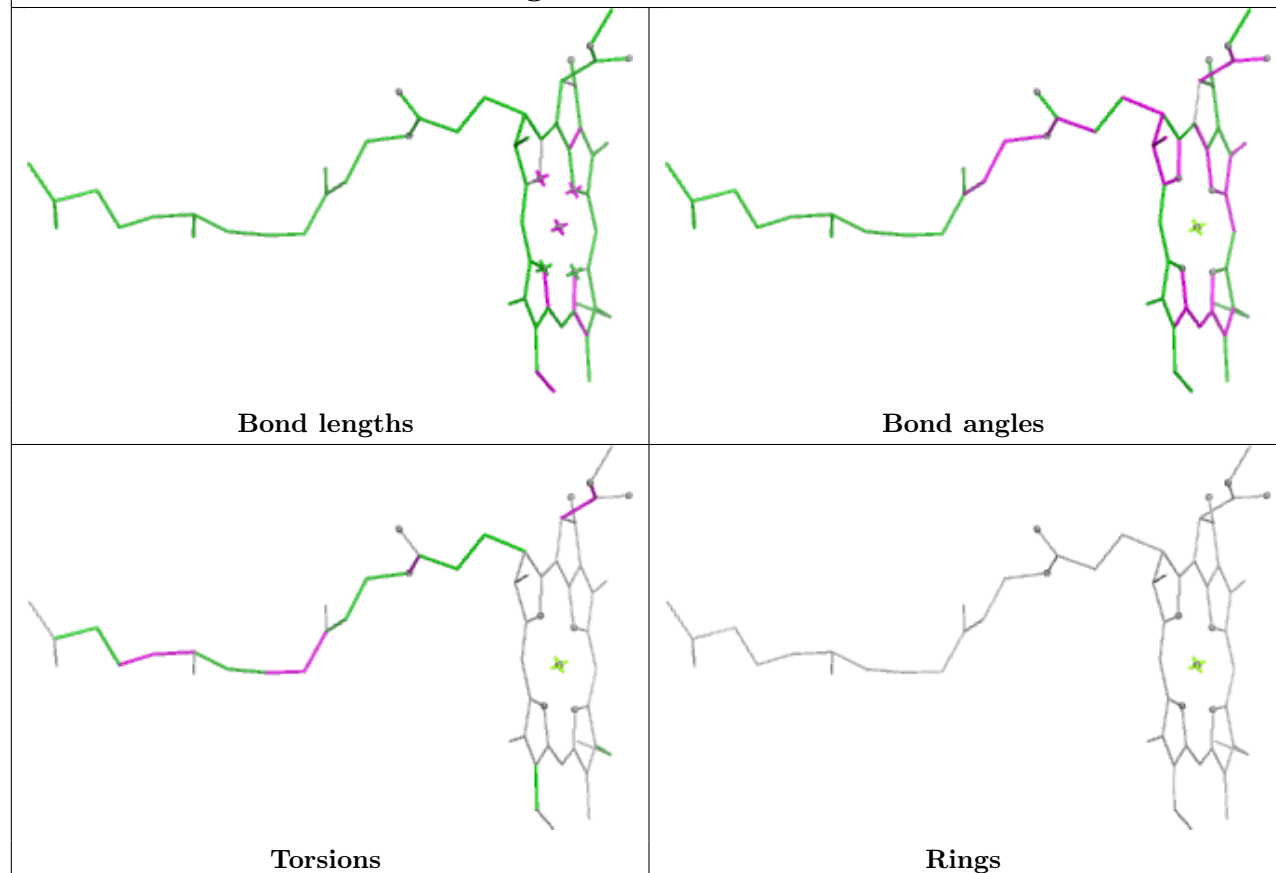


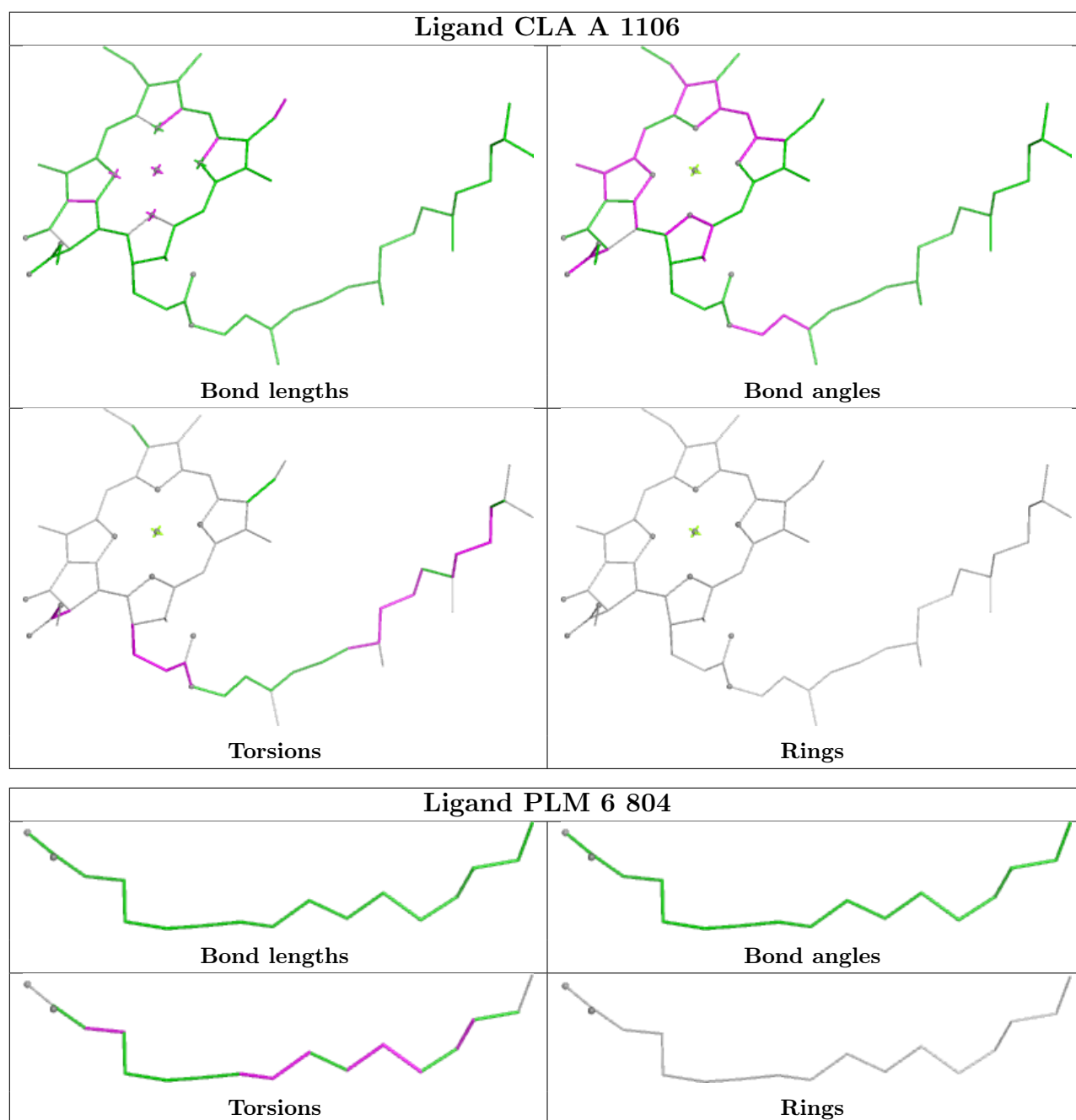
Torsions



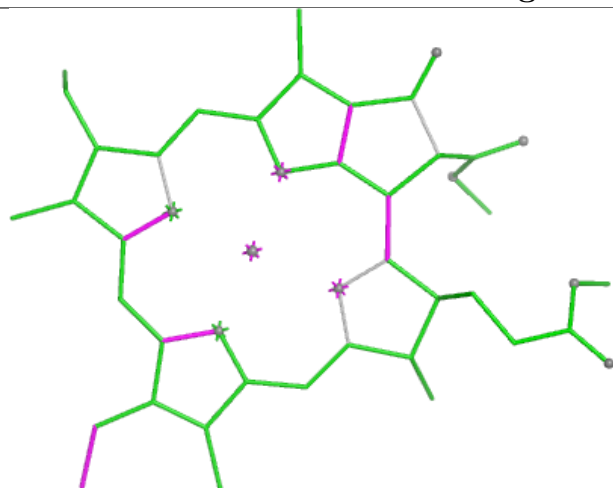
Rings



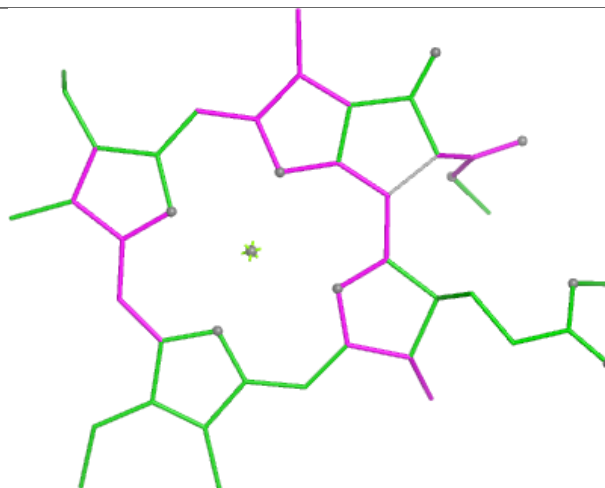
Ligand CLA 7 601**Ligand CLA L 1502**



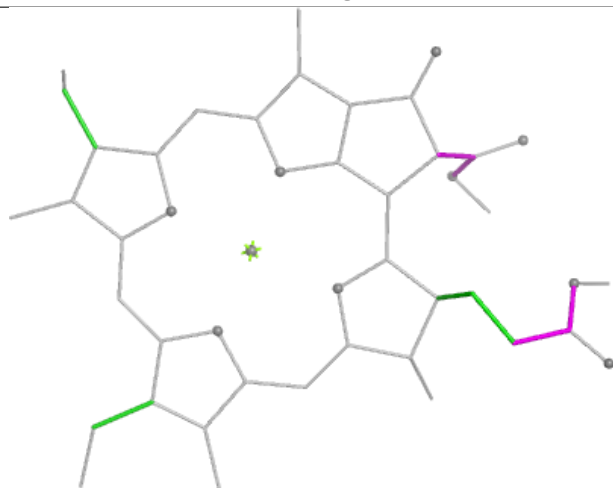
Ligand CLA 3 602



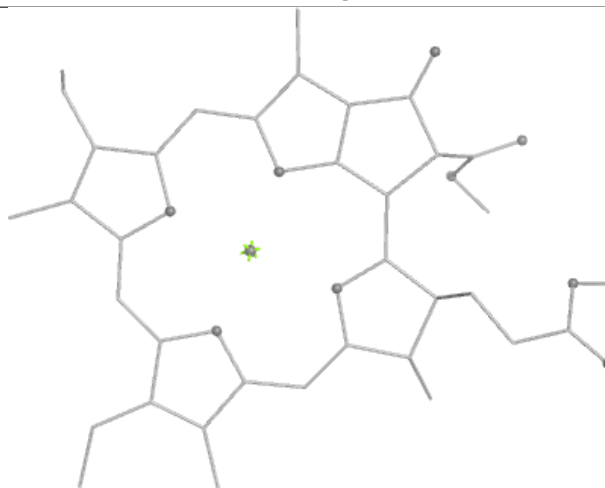
Bond lengths



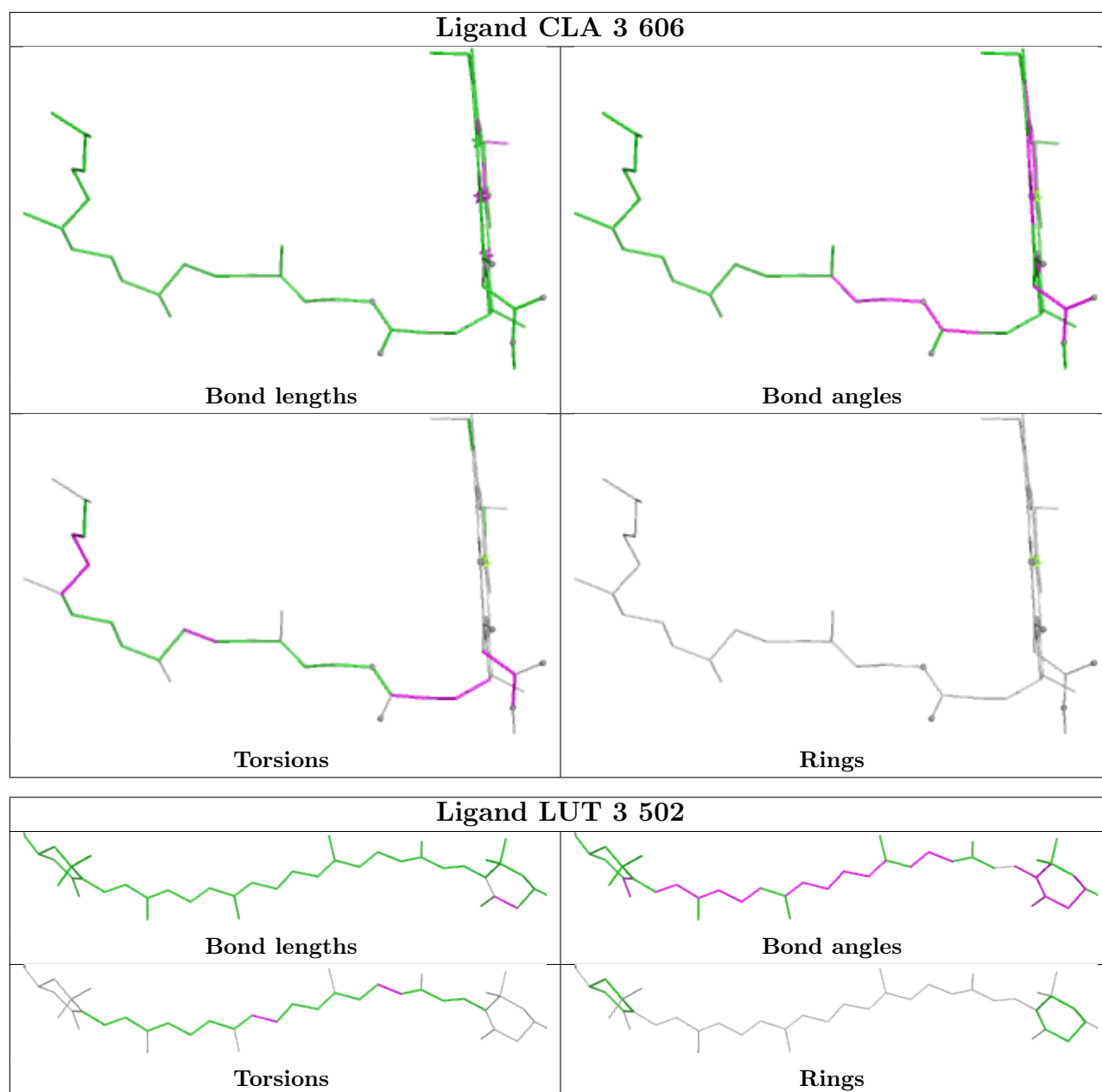
Bond angles

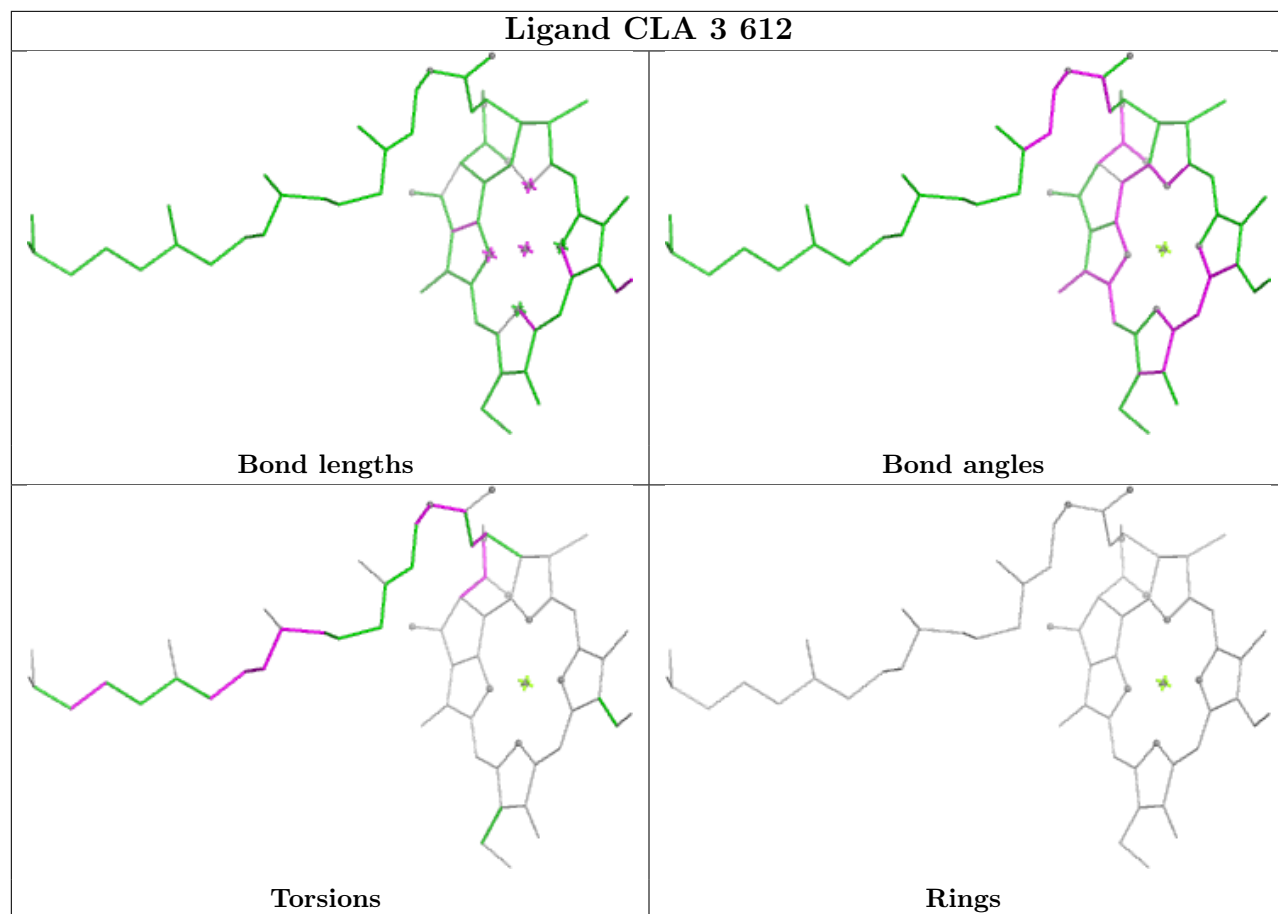


Torsions

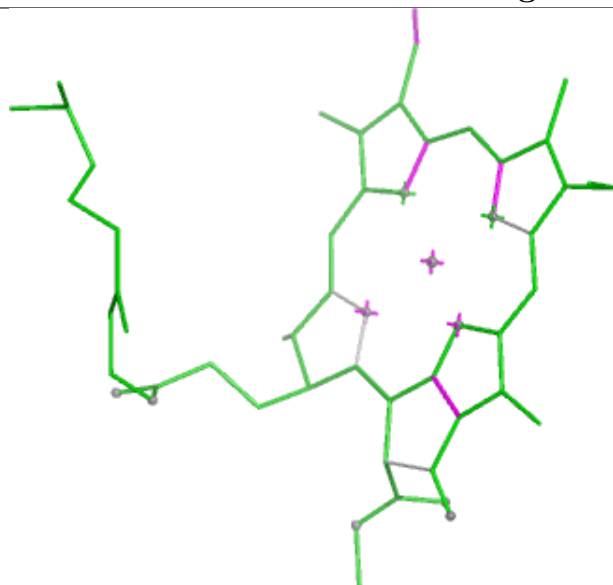


Rings

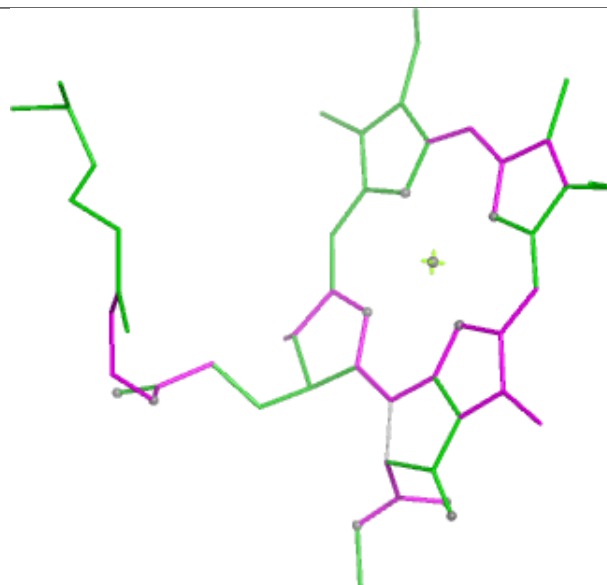




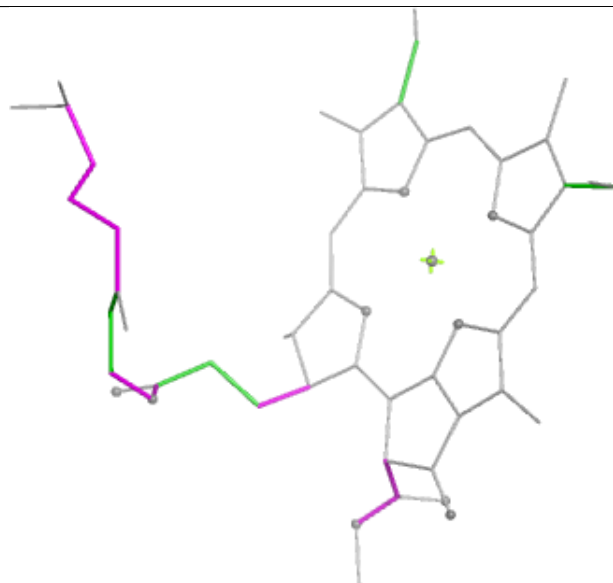
Ligand CLA 8 610



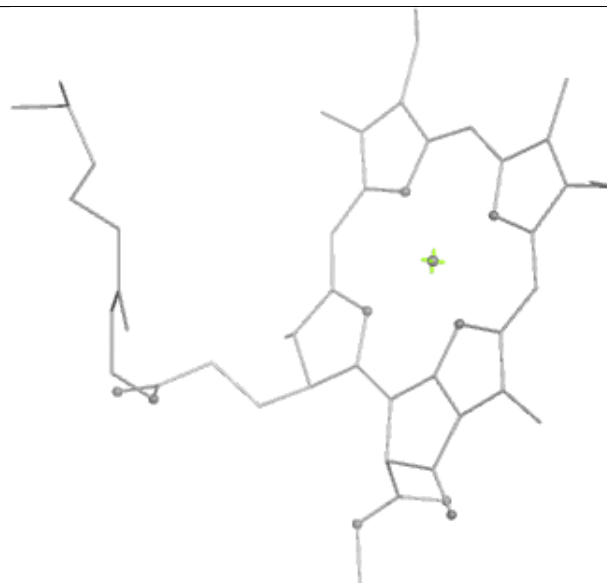
Bond lengths



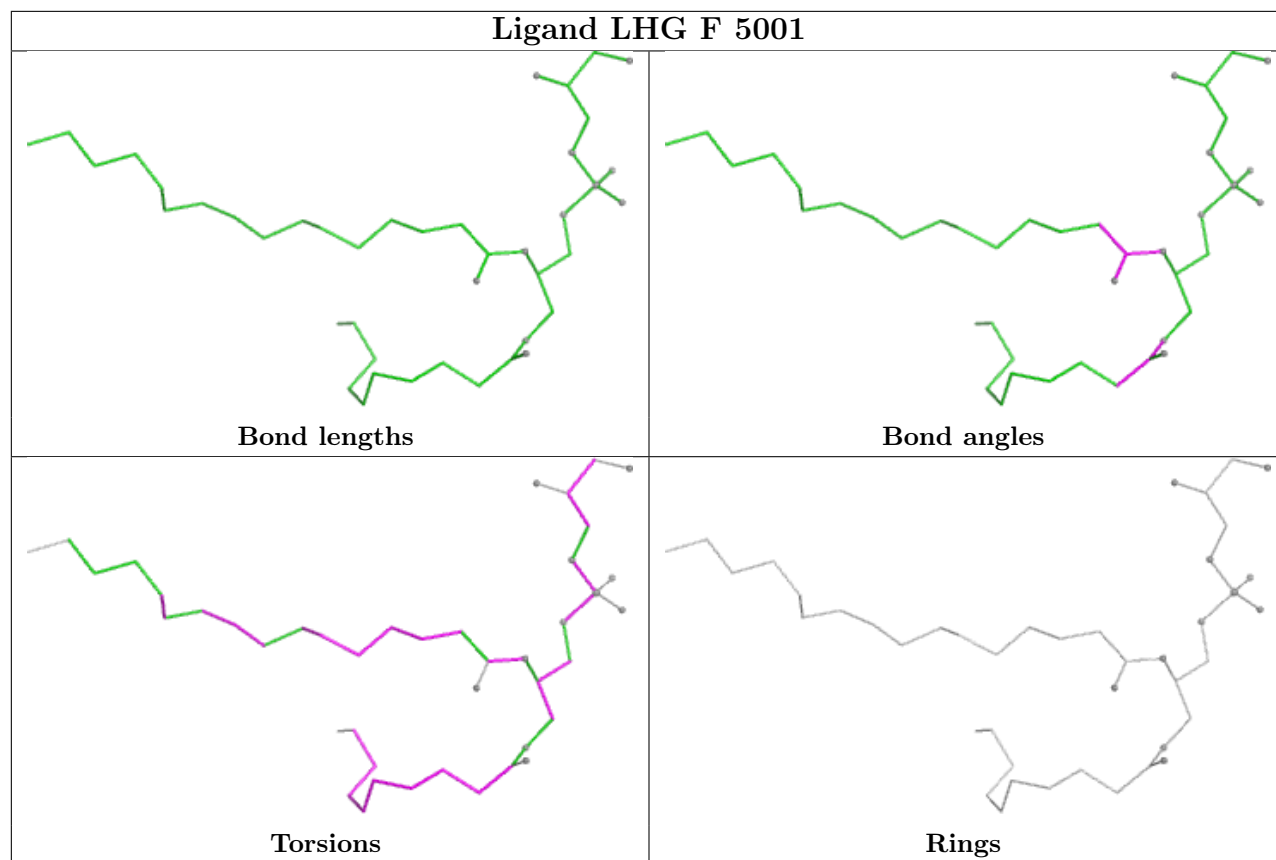
Bond angles



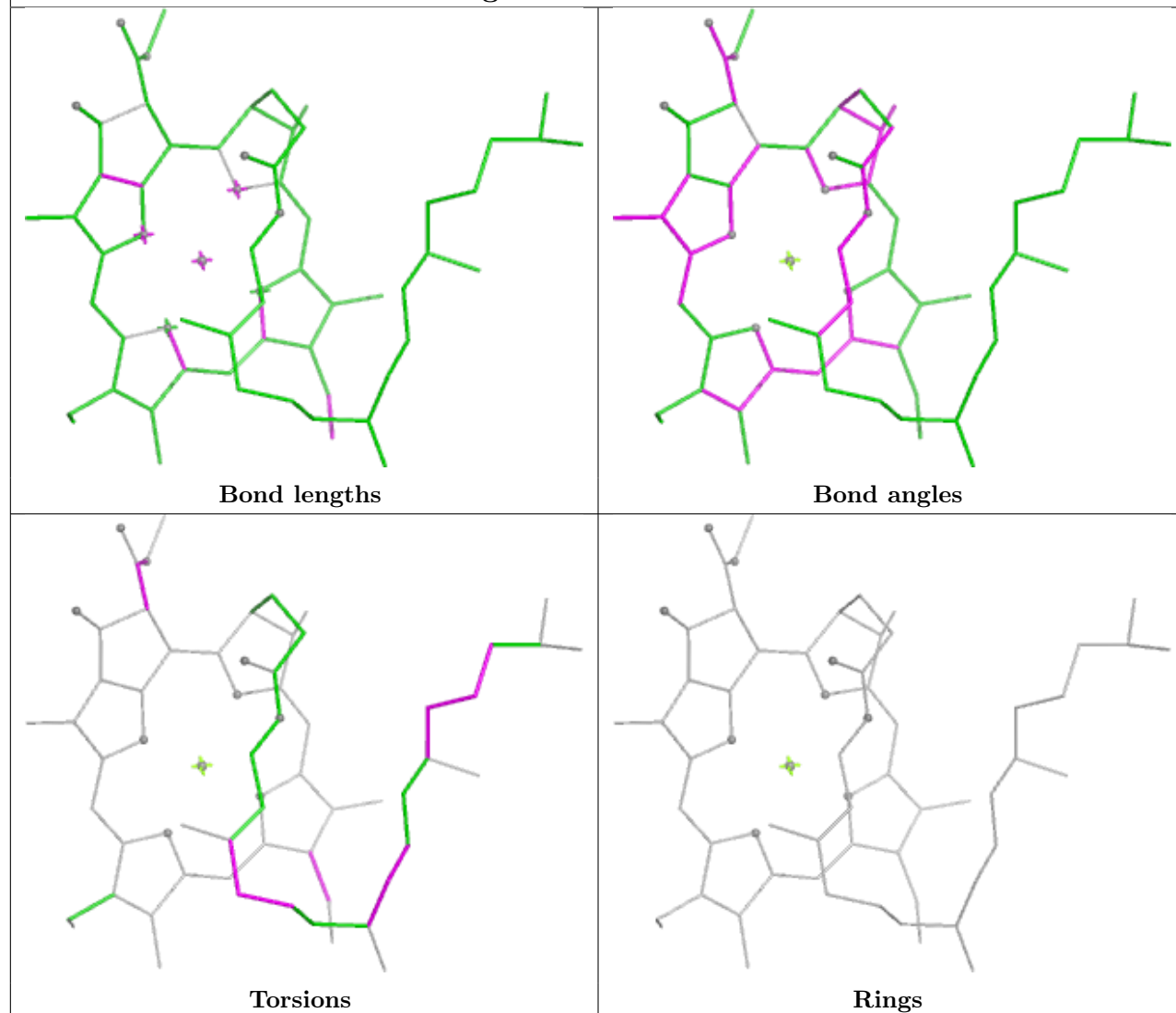
Torsions



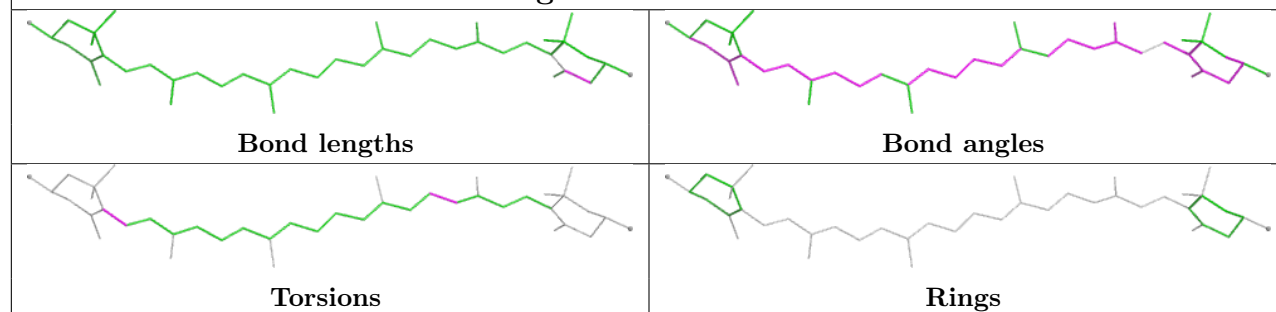
Rings



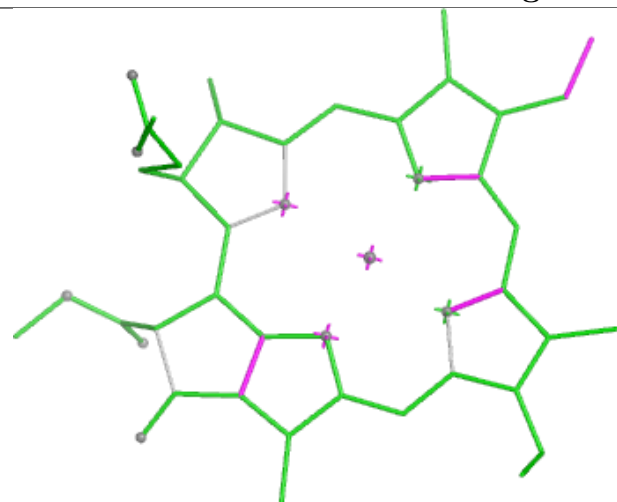
Ligand CLA B 1205



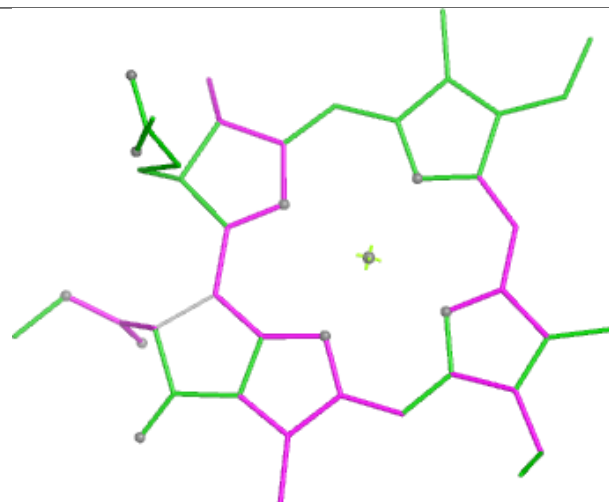
Ligand LUT 1 501



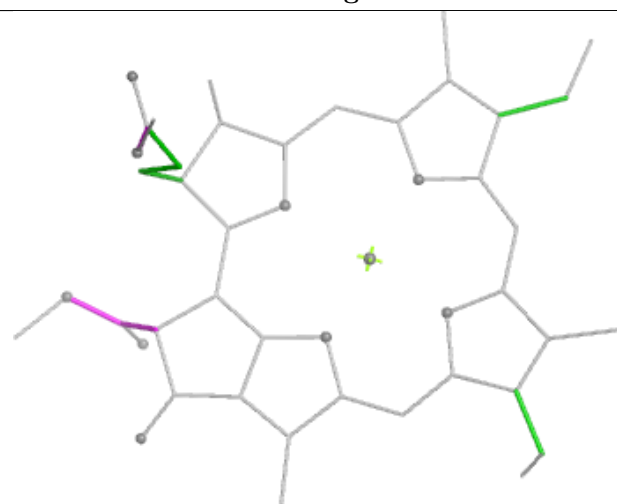
Ligand CLA a 615



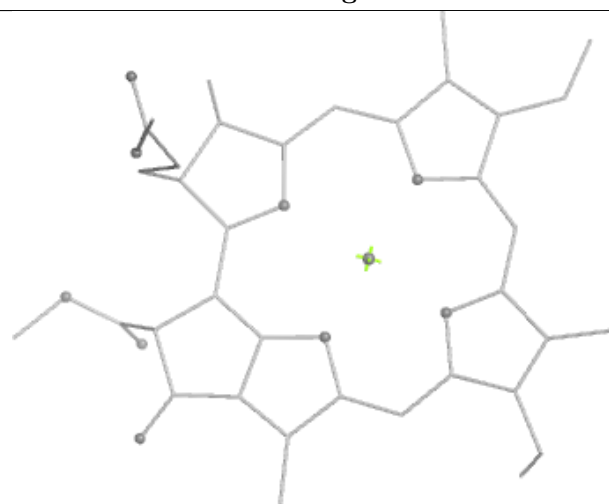
Bond lengths



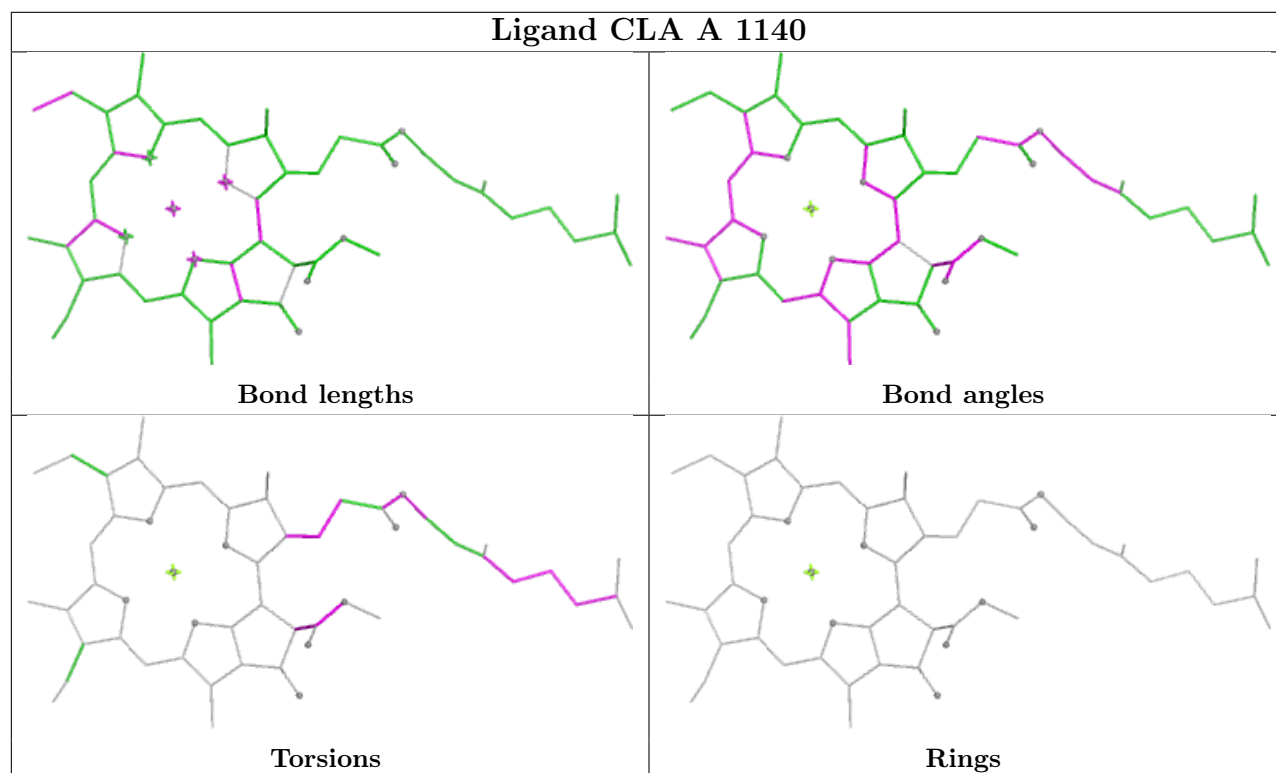
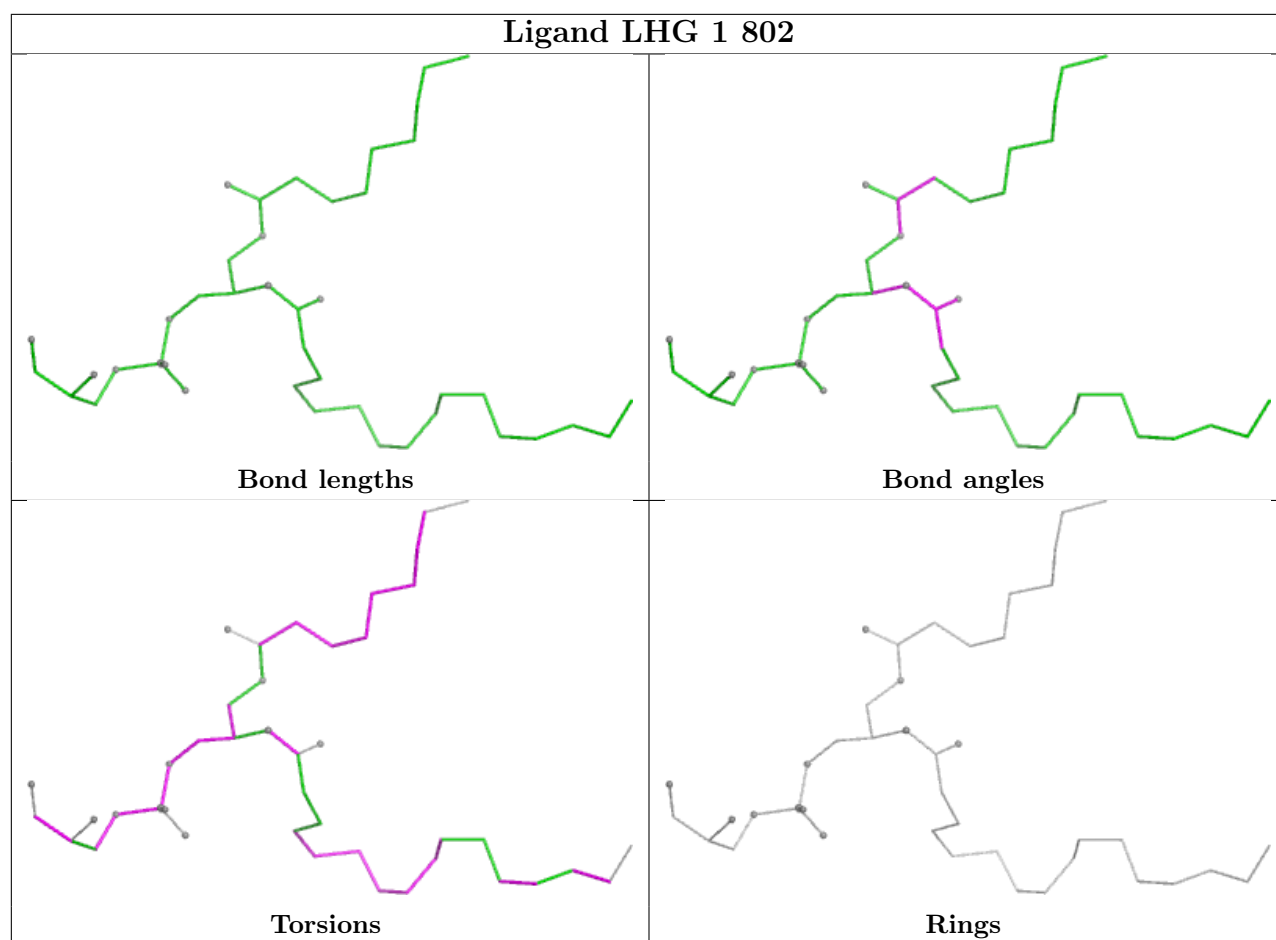
Bond angles



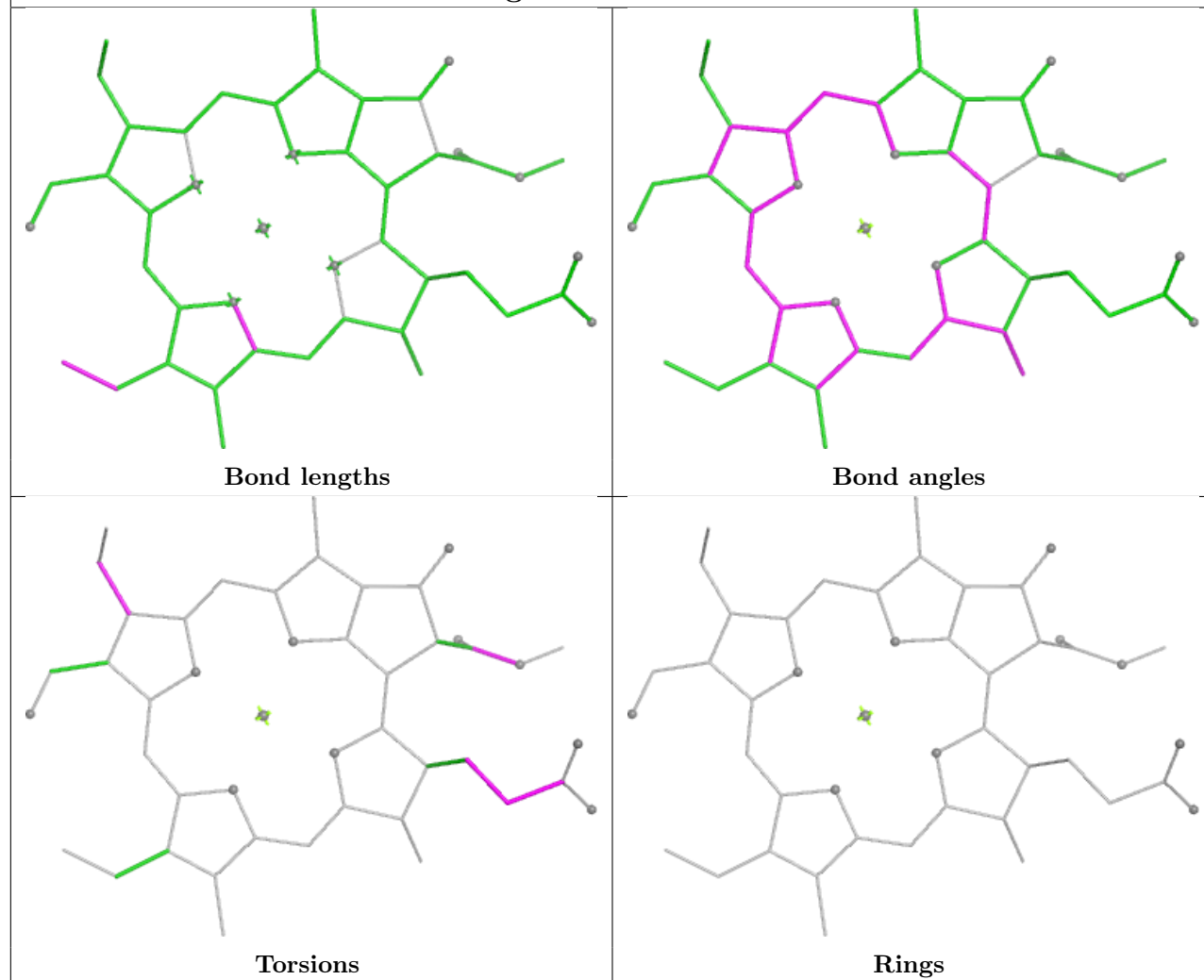
Torsions



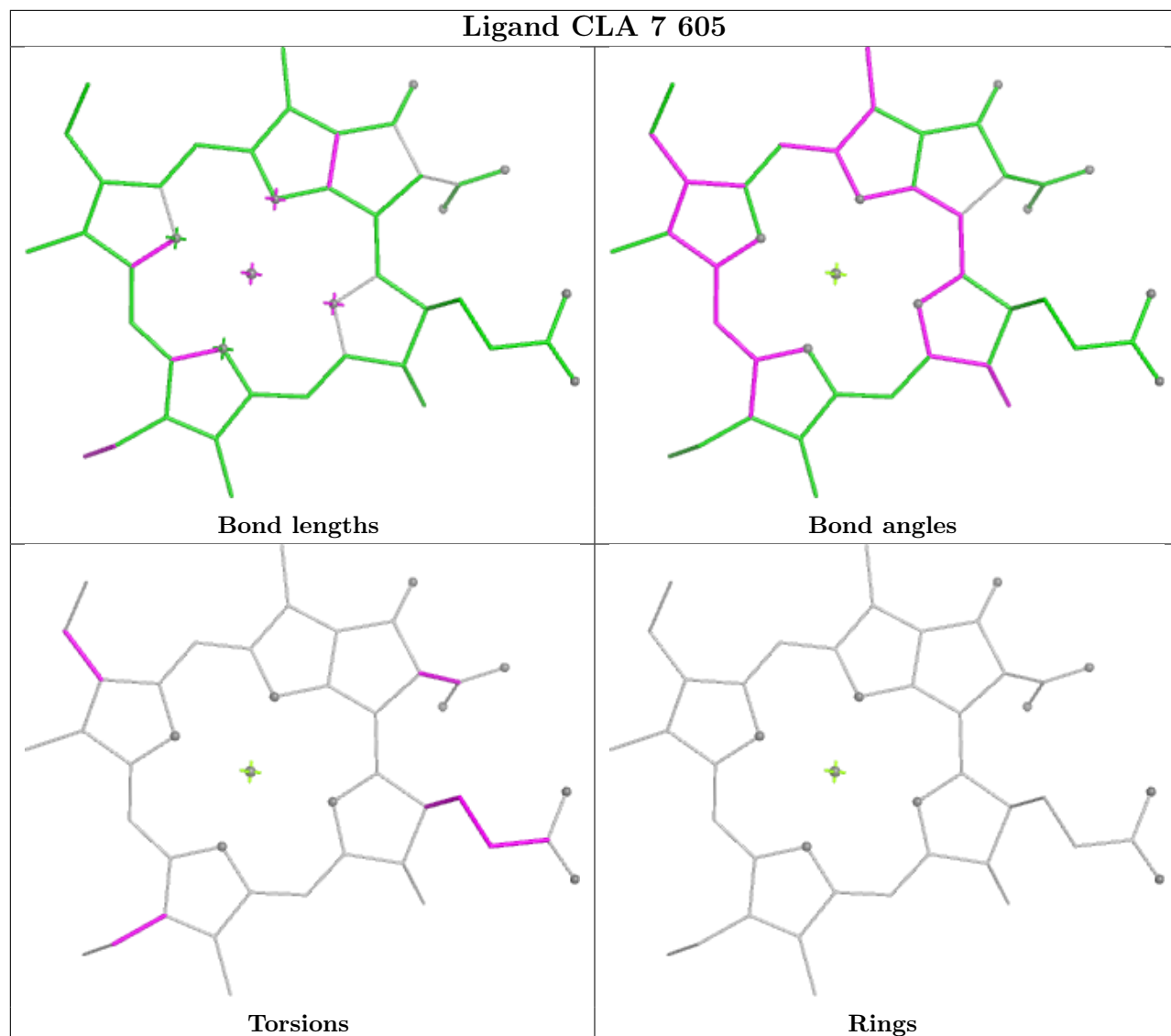
Rings

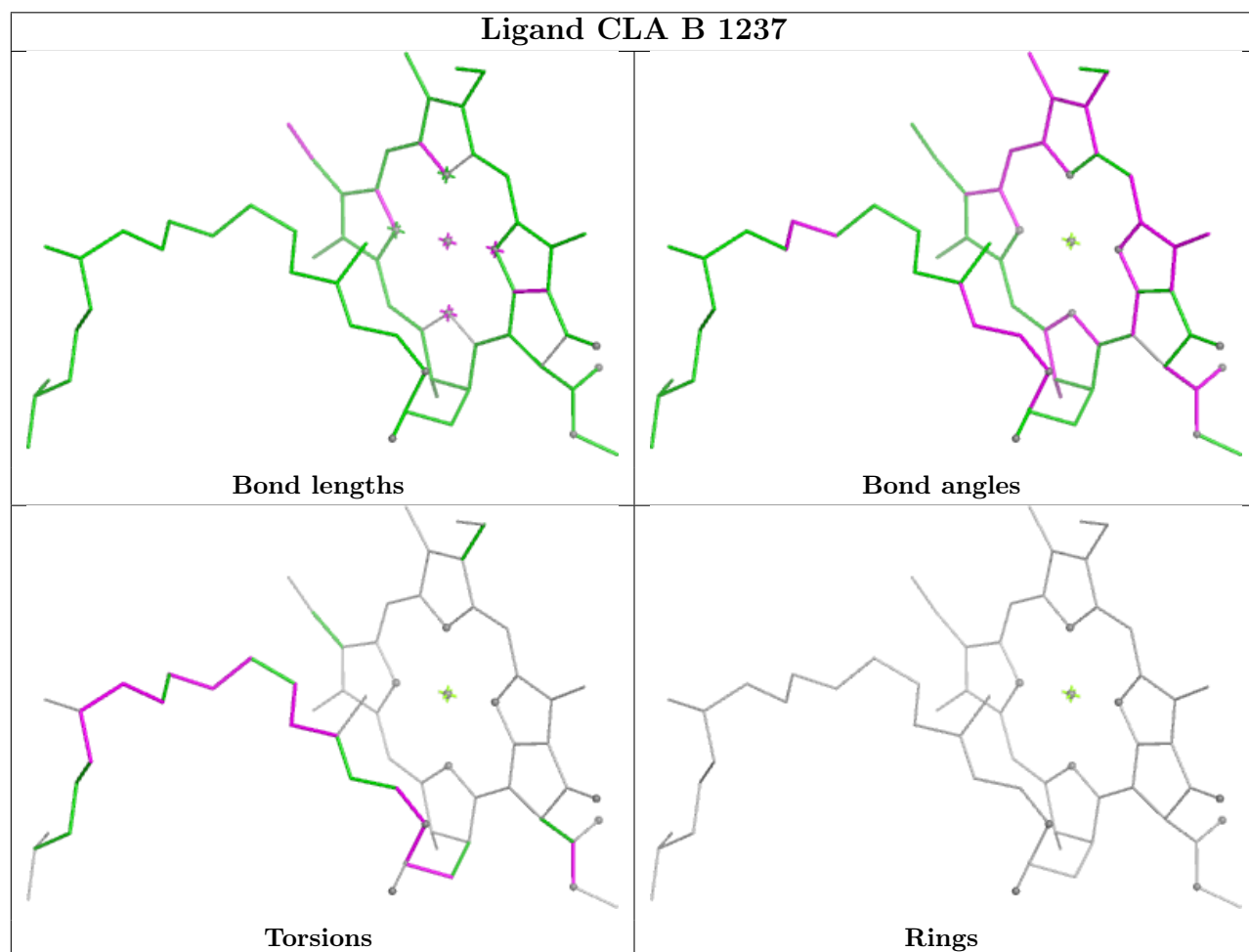
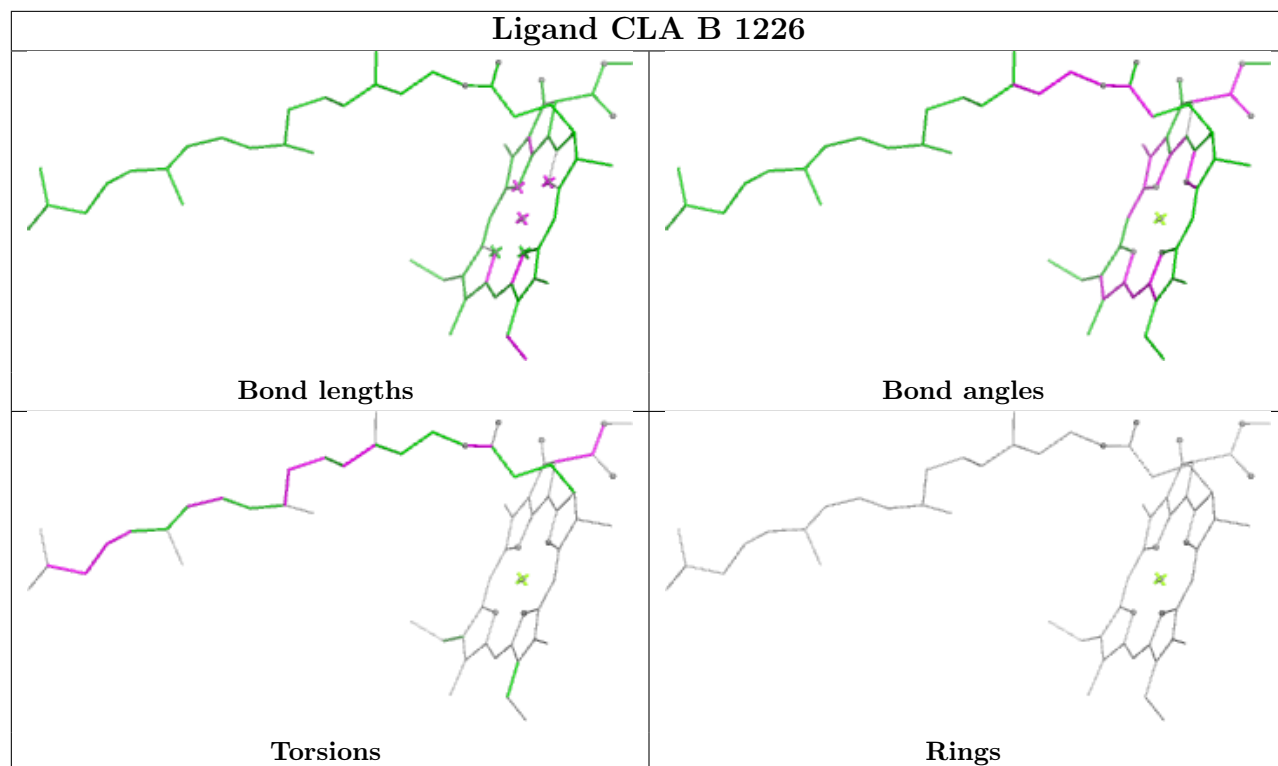


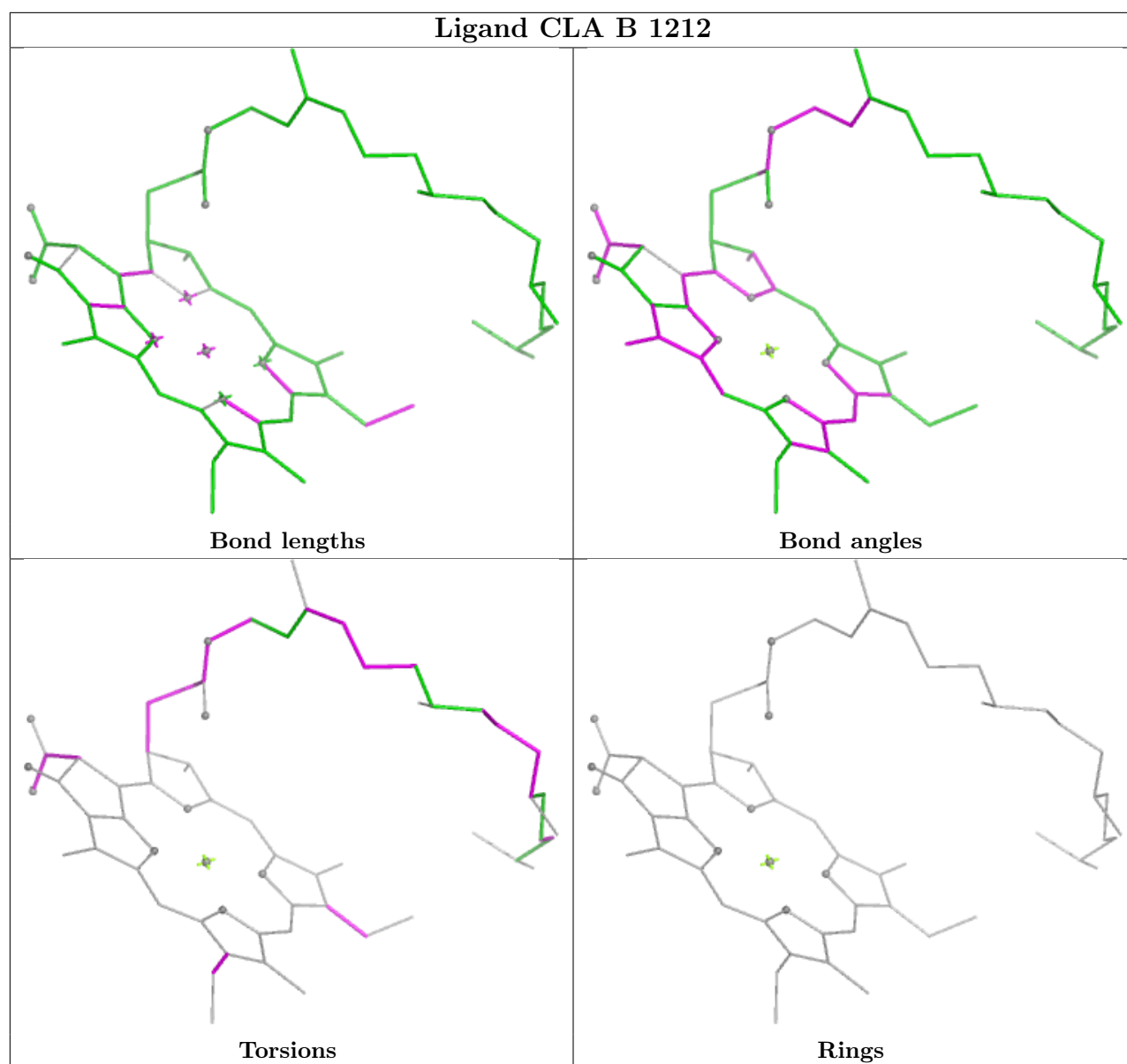
Ligand CHL a 613

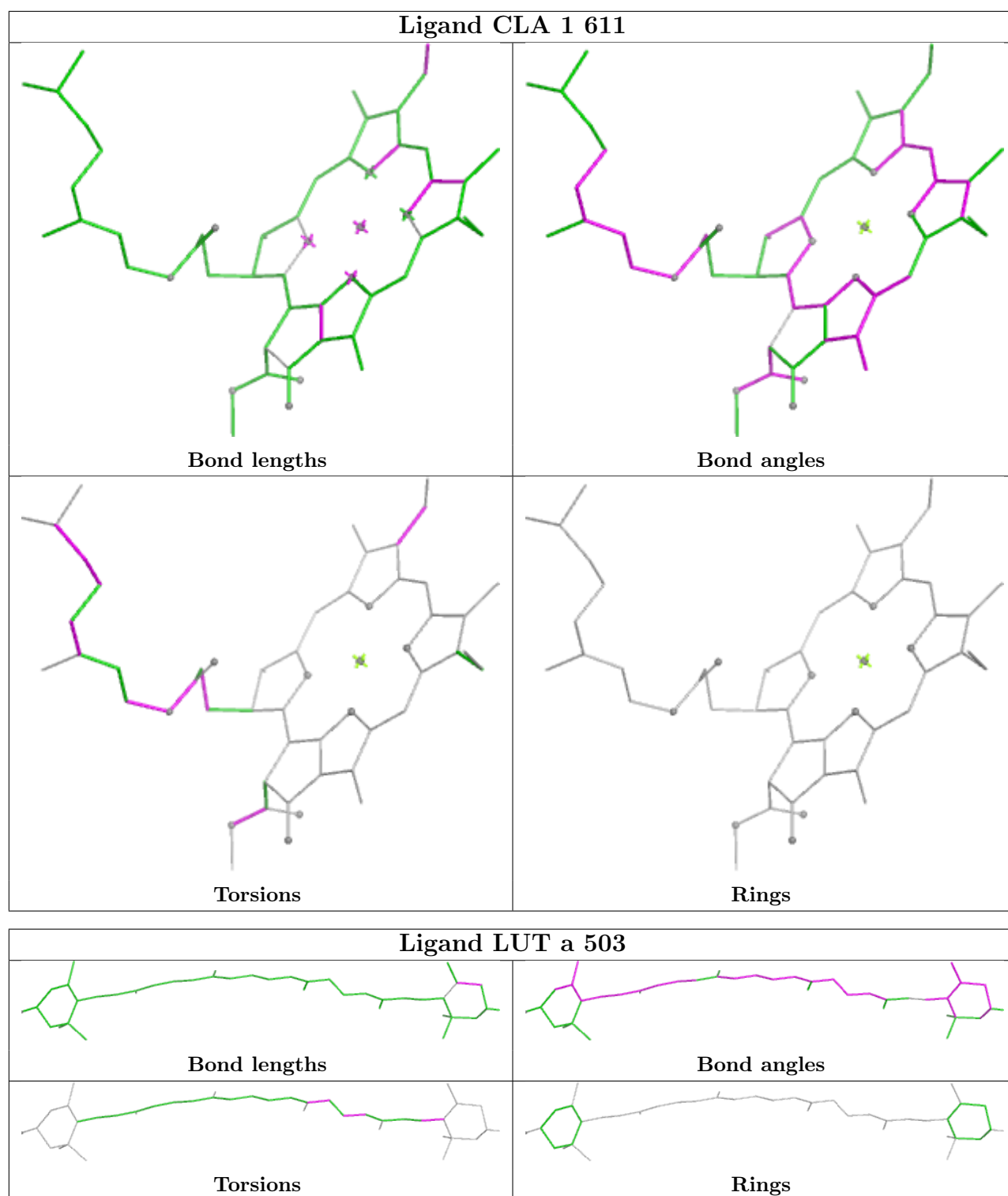


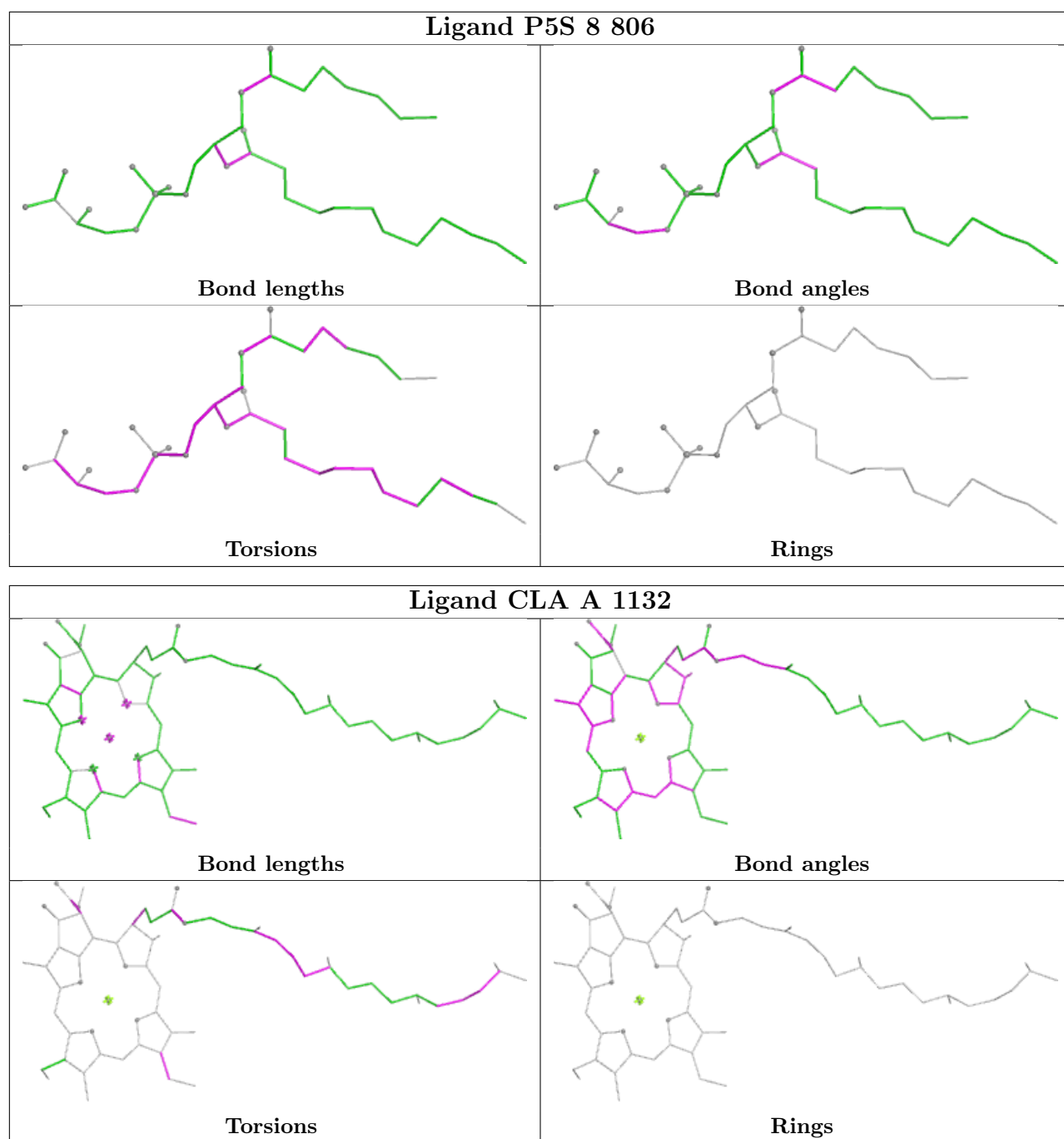
Ligand CLA 7 605

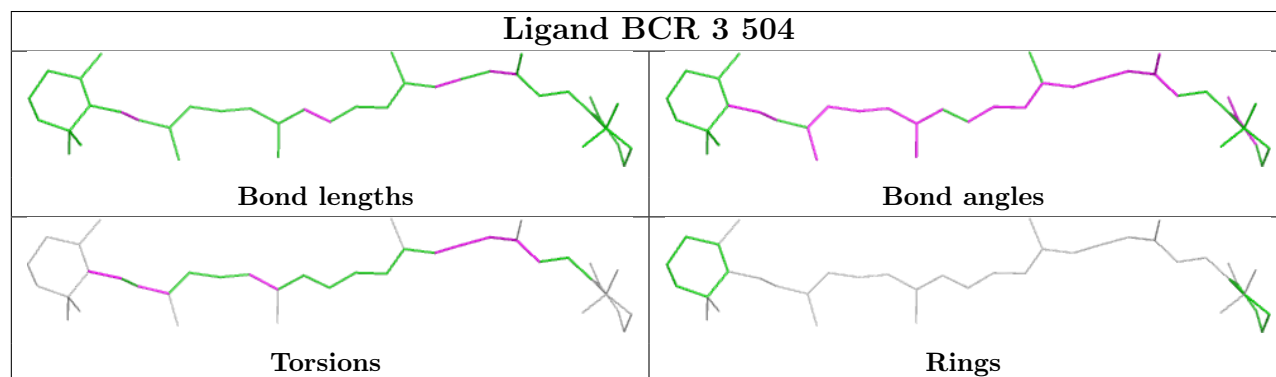
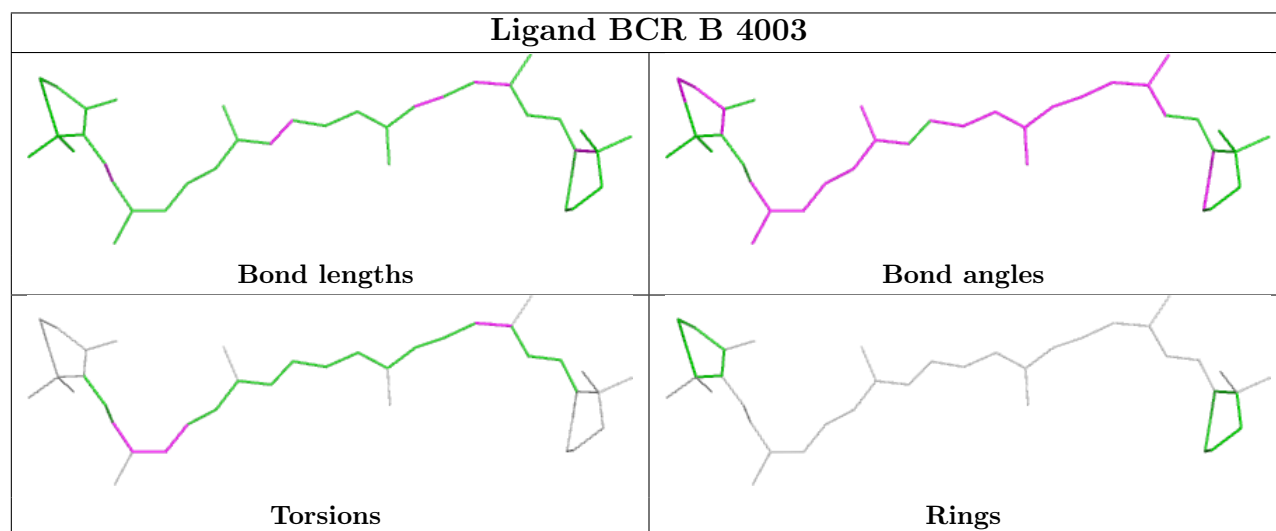
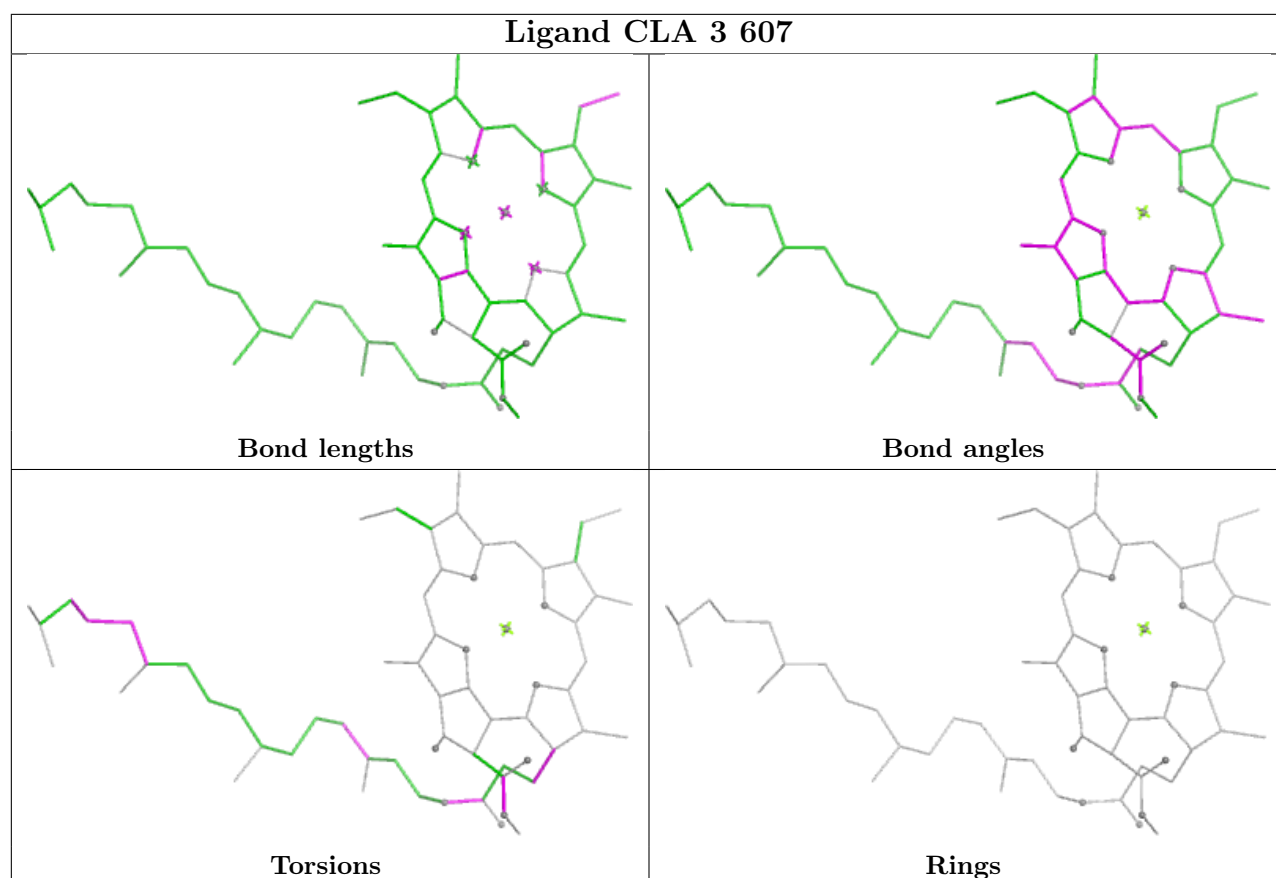


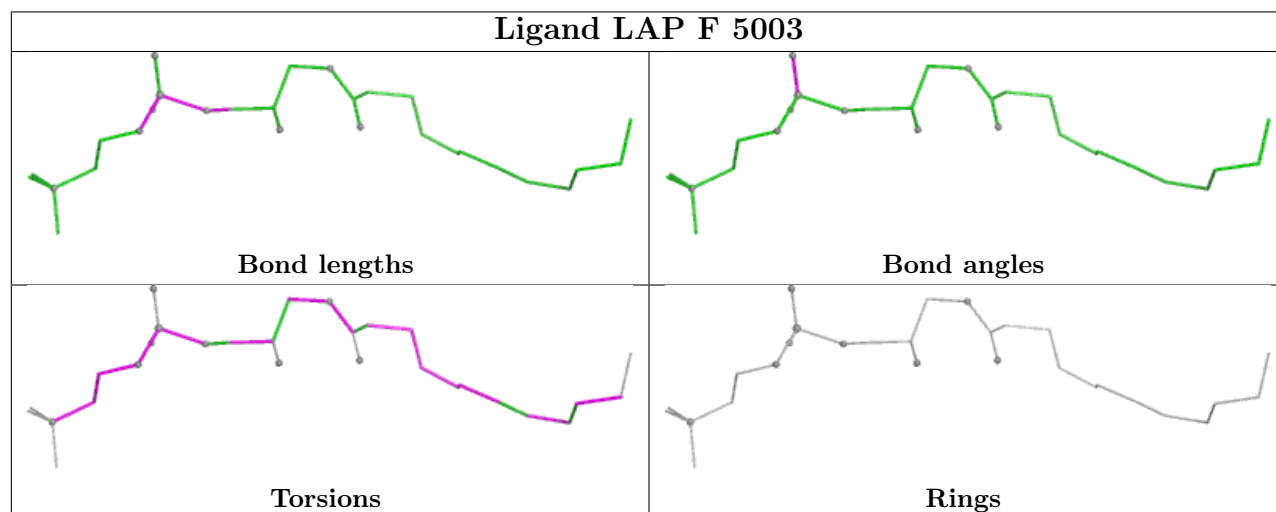
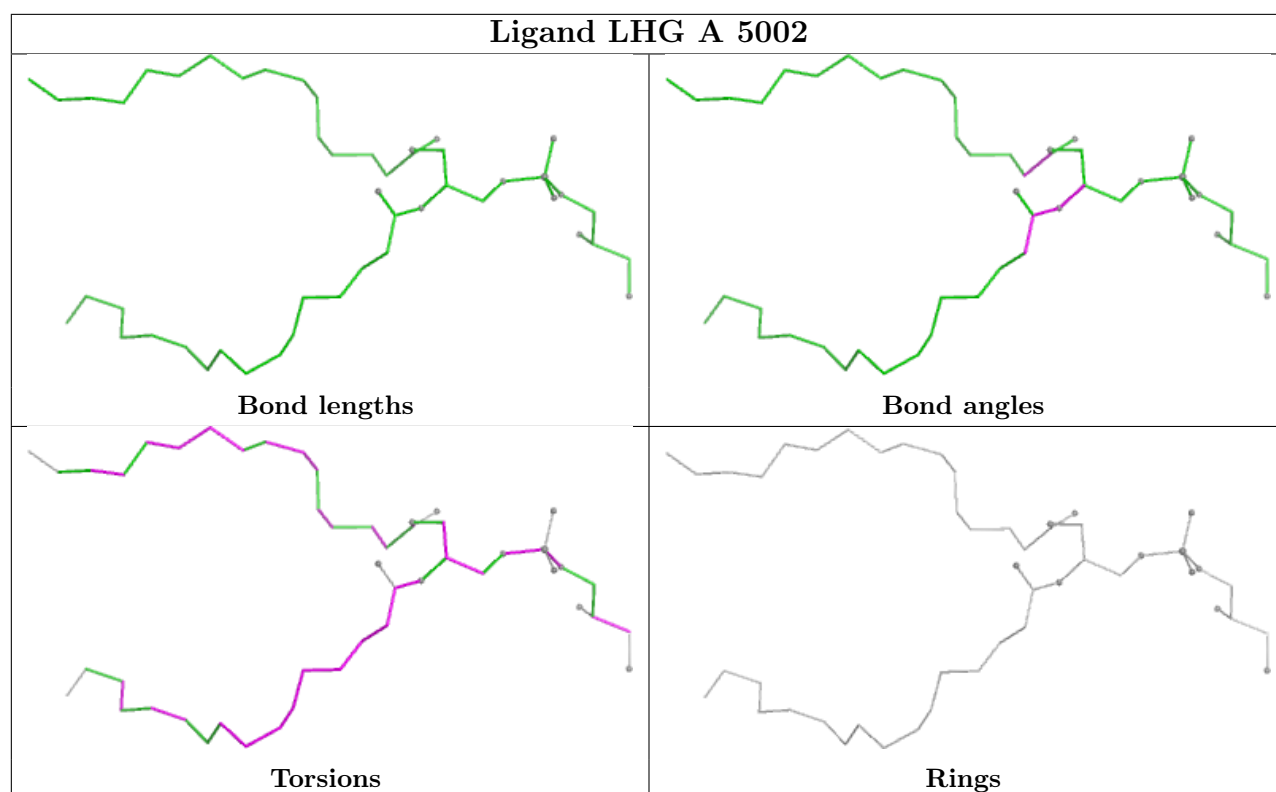


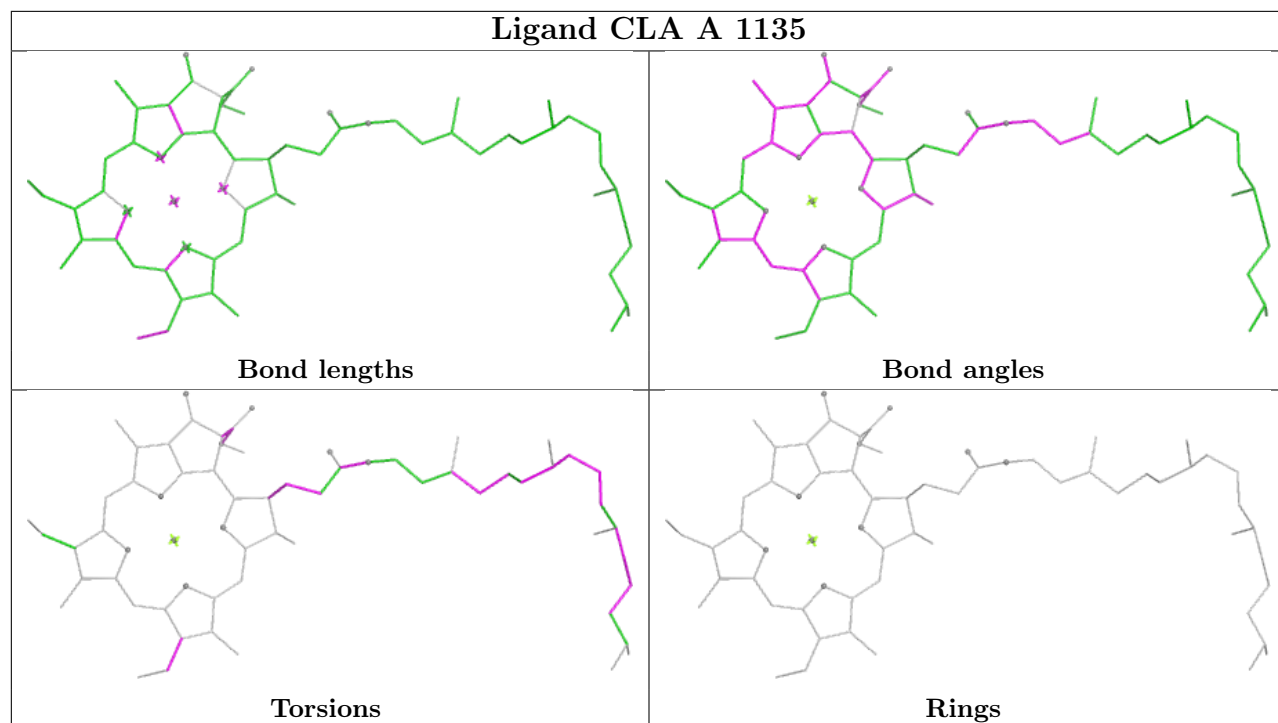
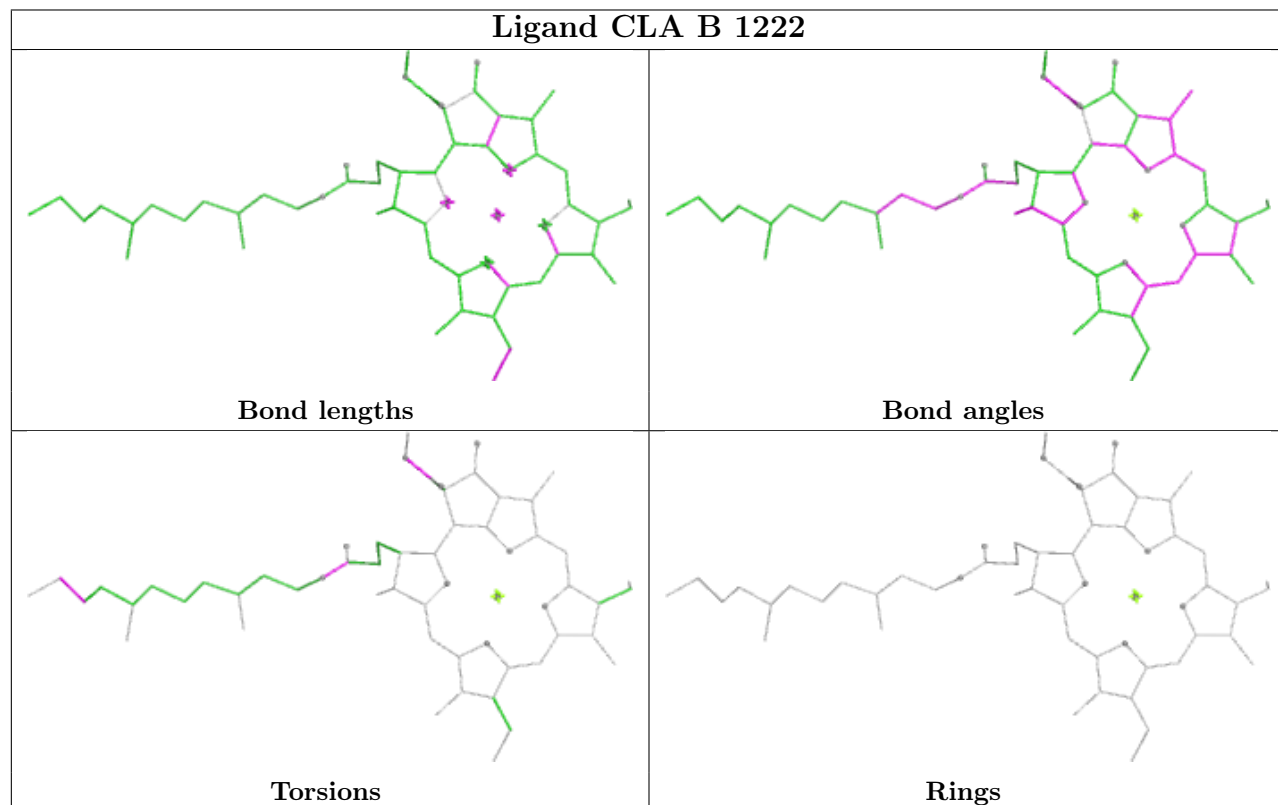


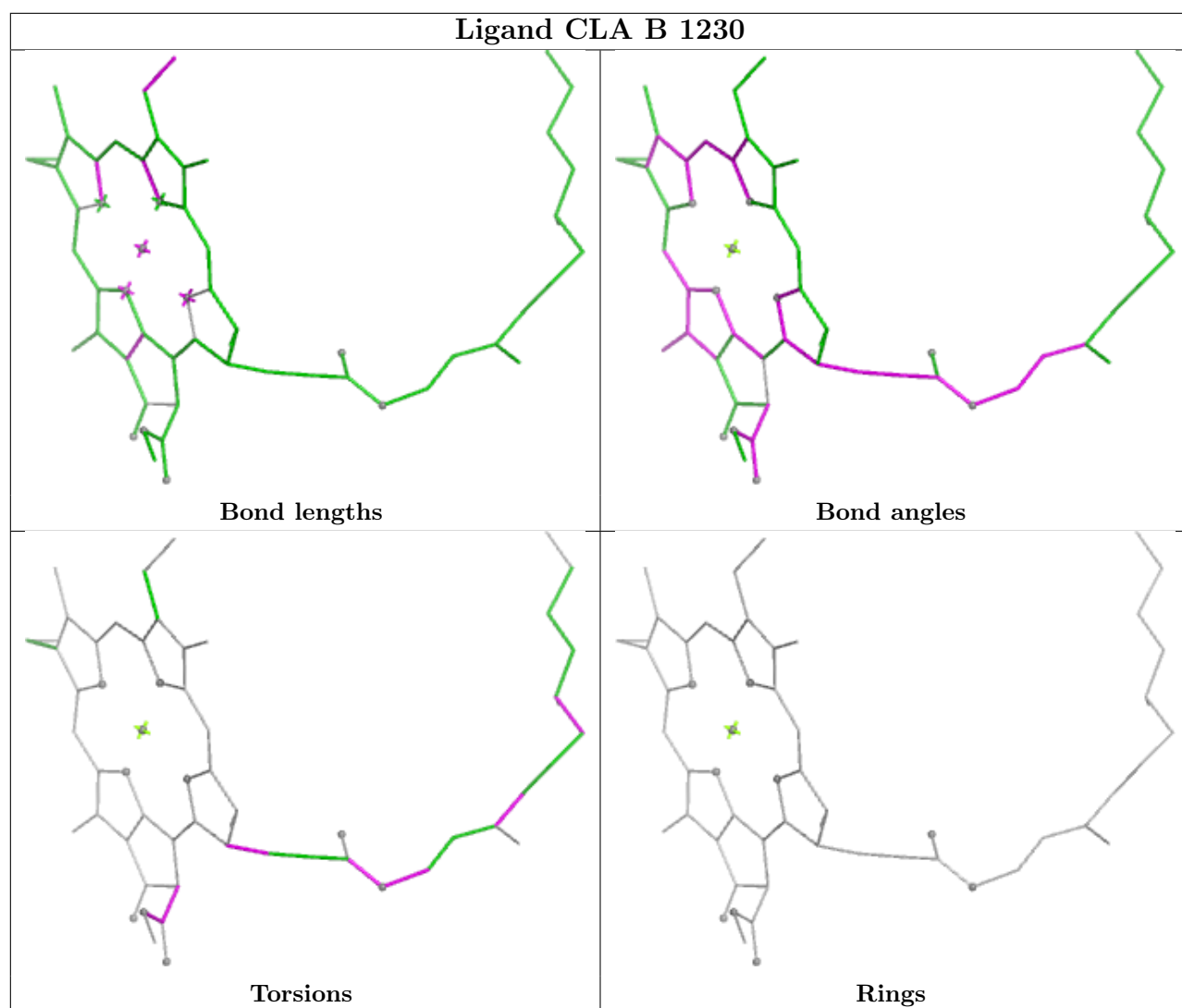


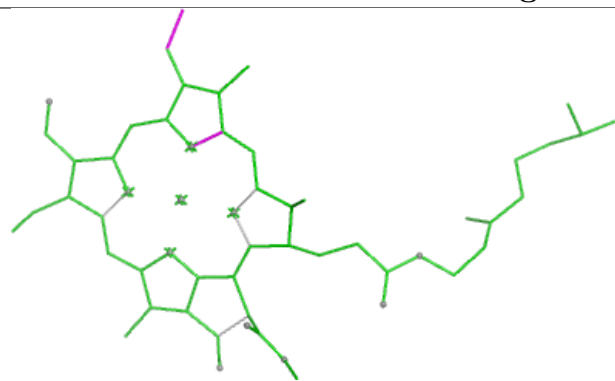
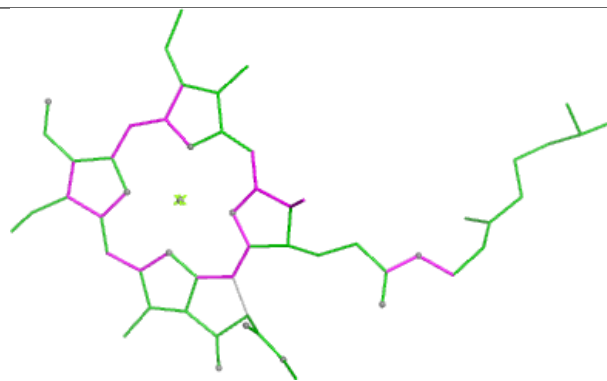
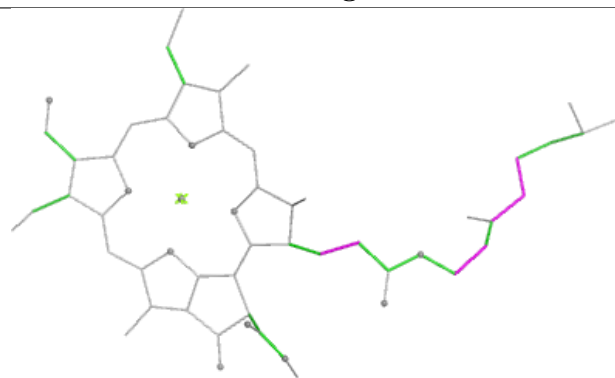
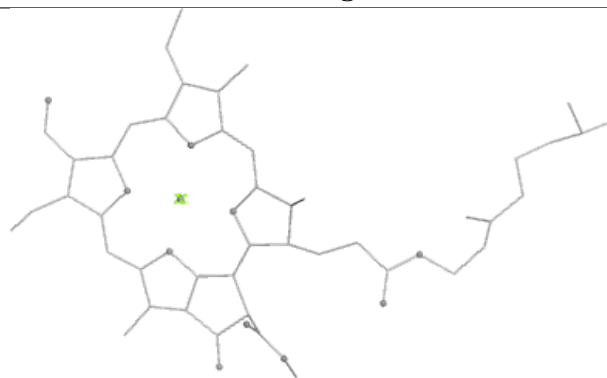


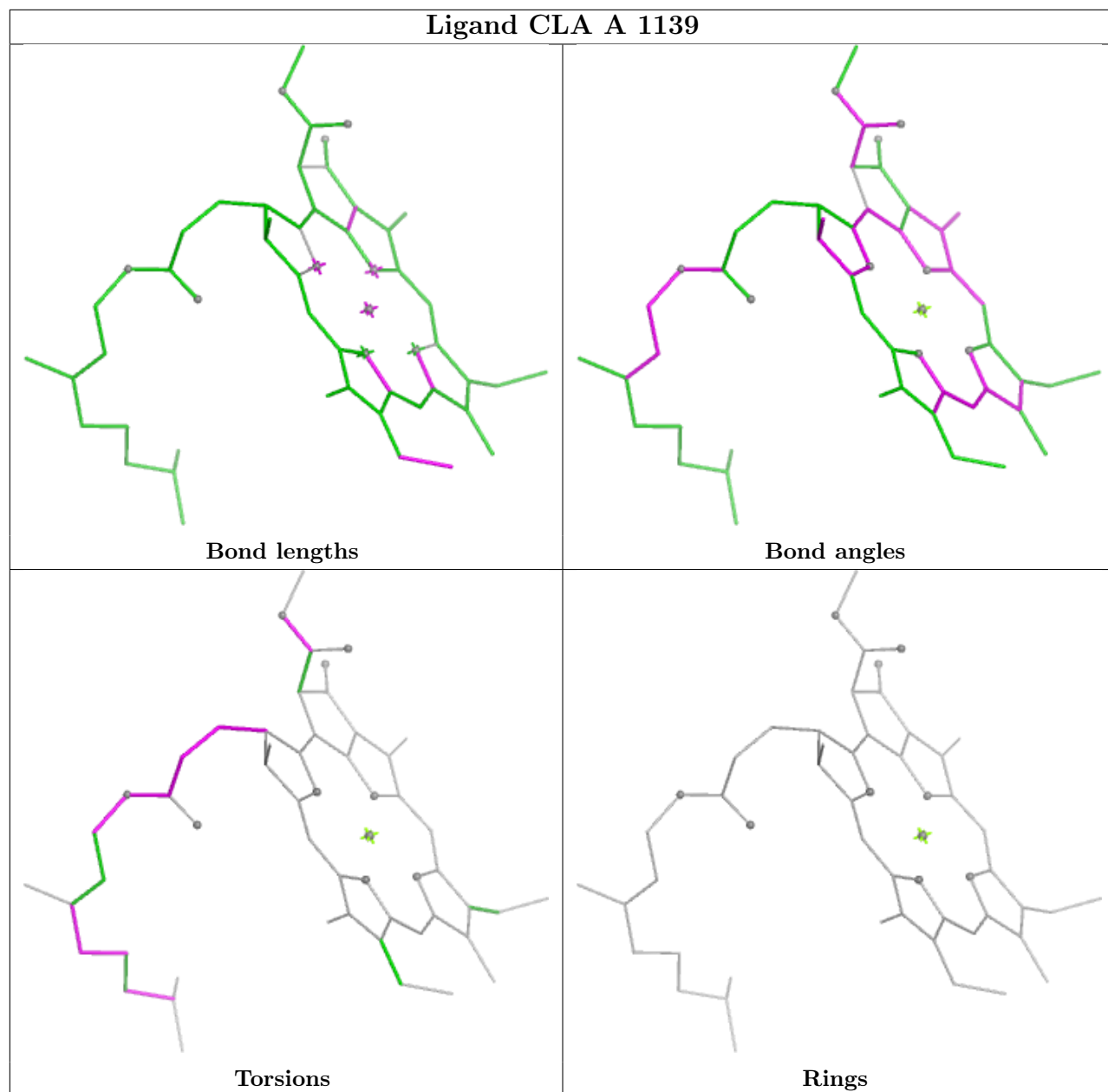


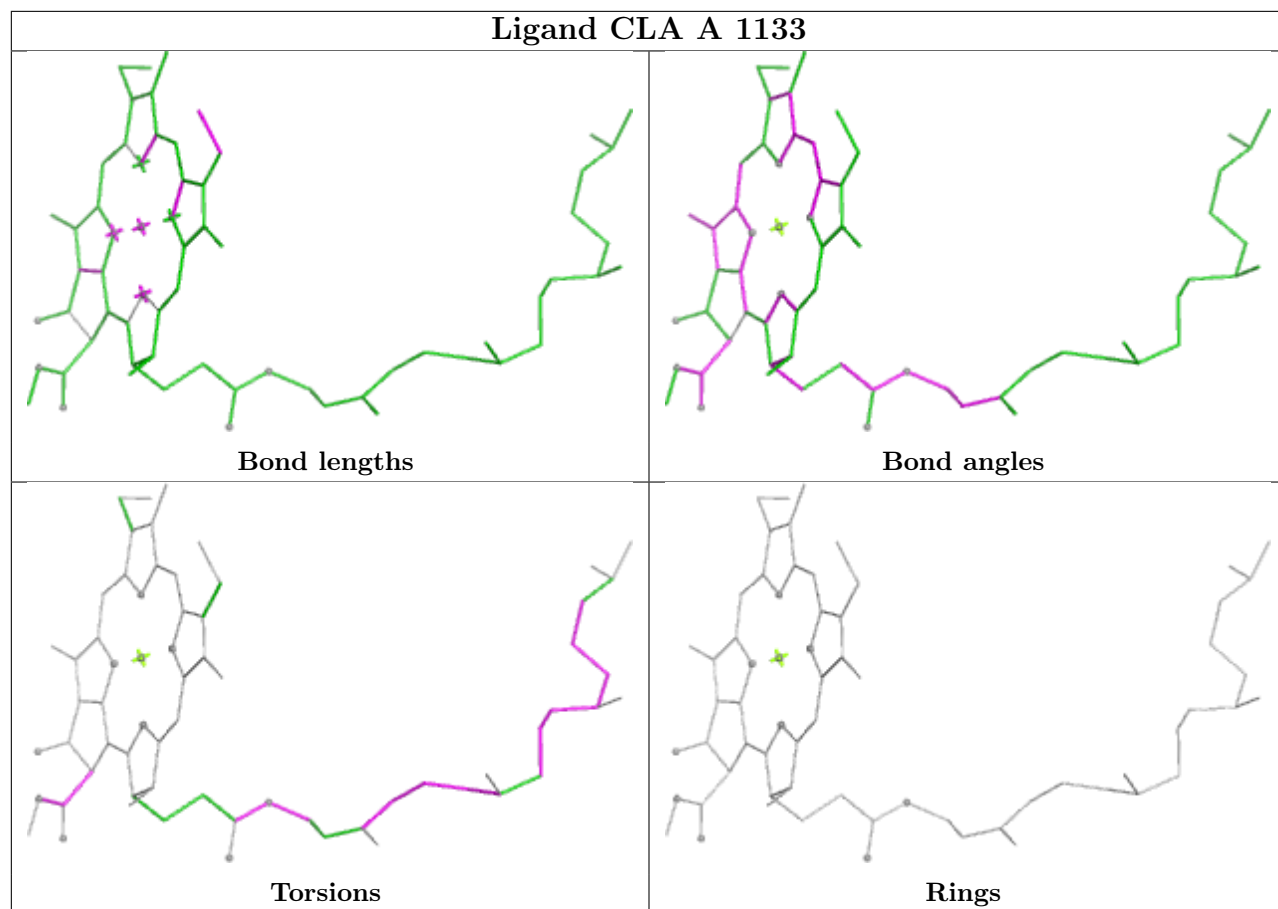


Ligand CLA A 1135**Ligand CLA B 1222**

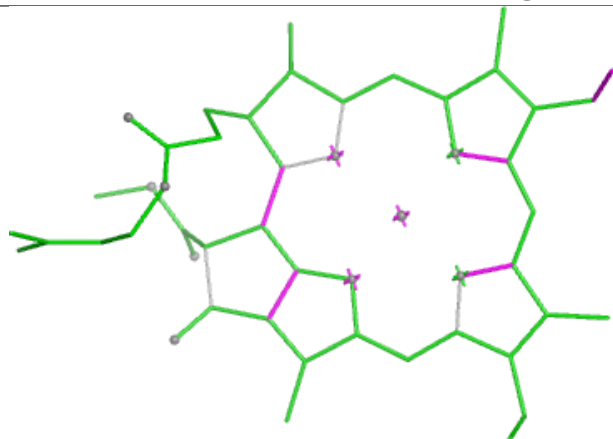


Ligand CHL 5 613**Bond lengths****Bond angles****Torsions****Rings**

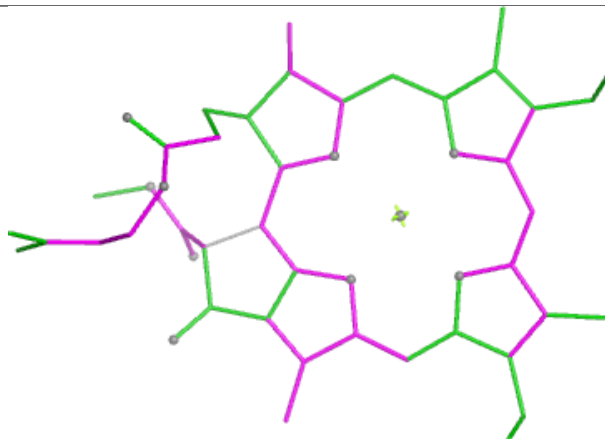




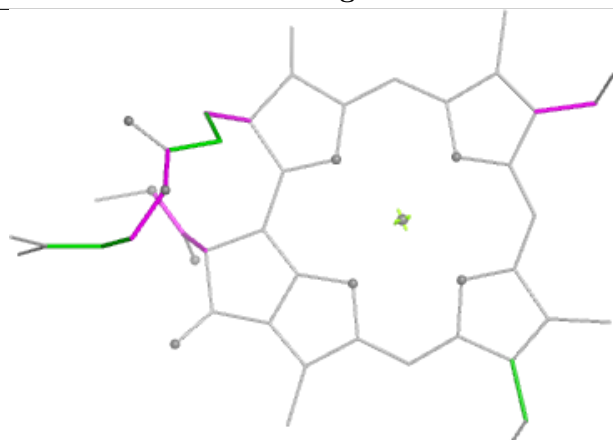
Ligand CLA 4 616



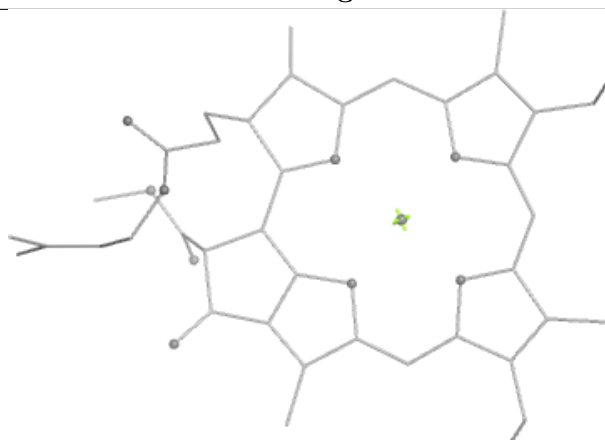
Bond lengths



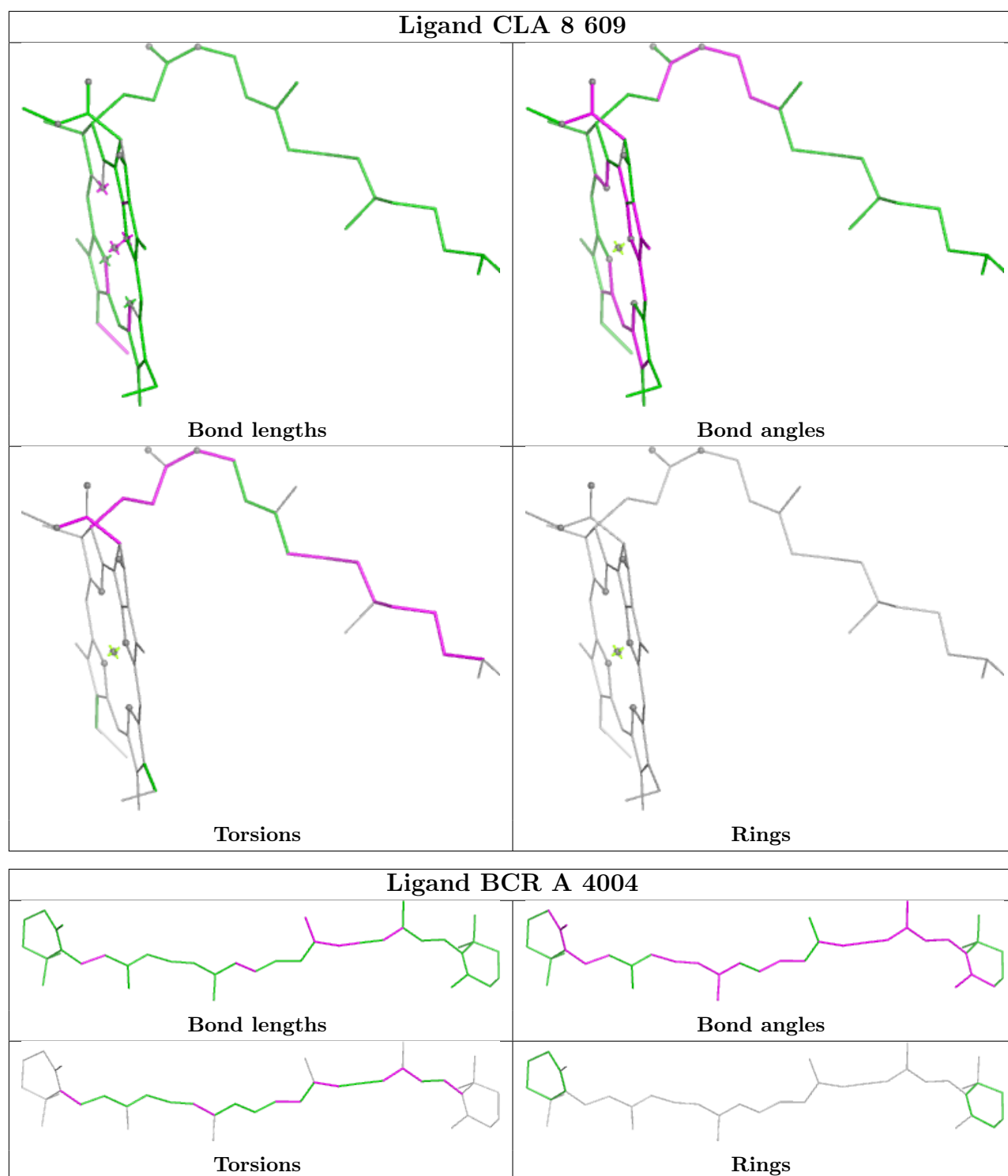
Bond angles

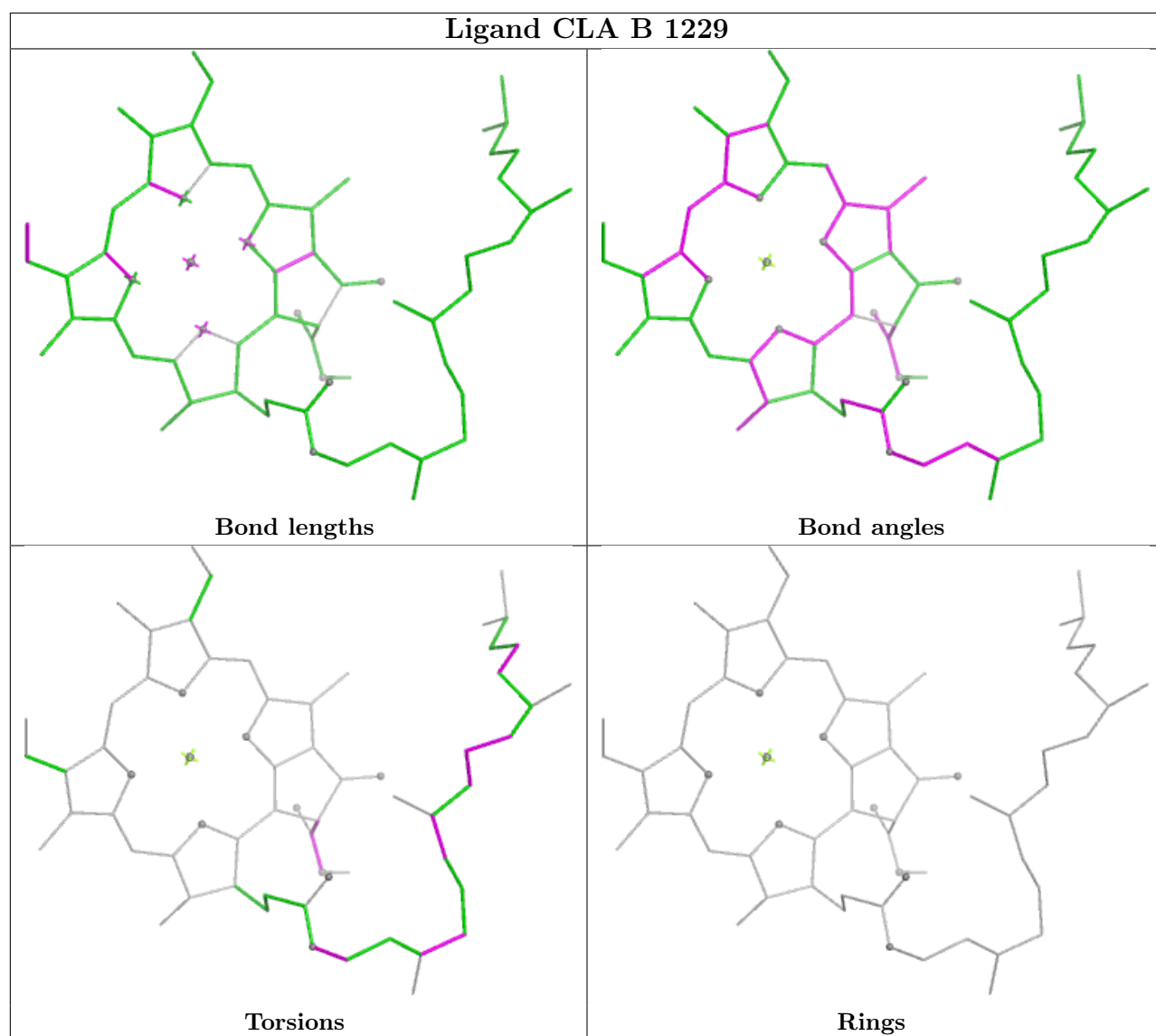


Torsions

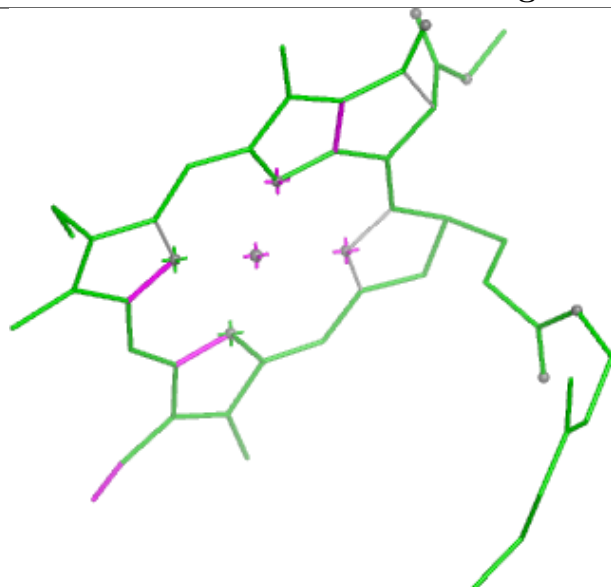


Rings

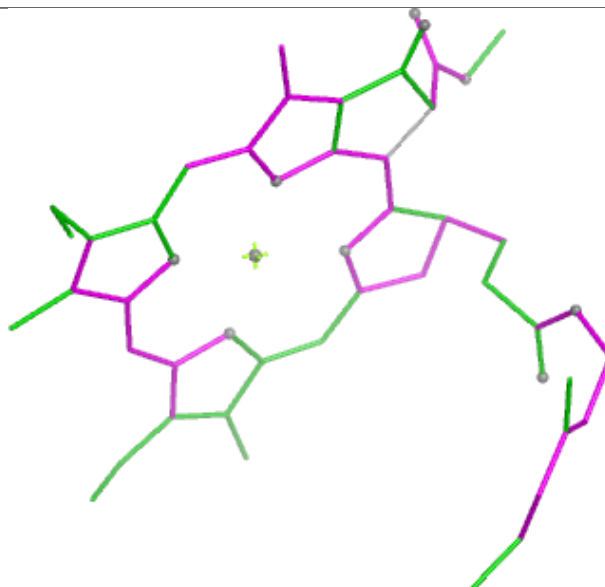




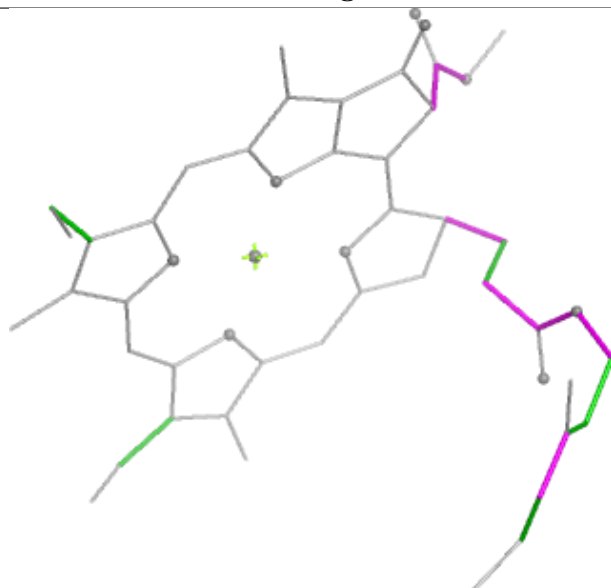
Ligand CLA 8 608



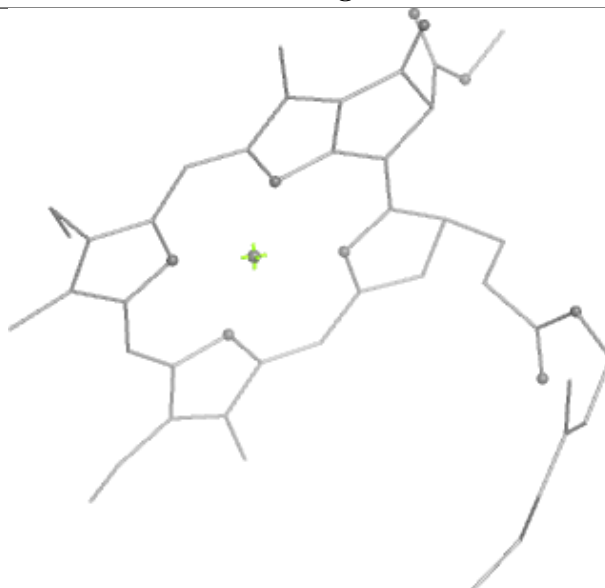
Bond lengths



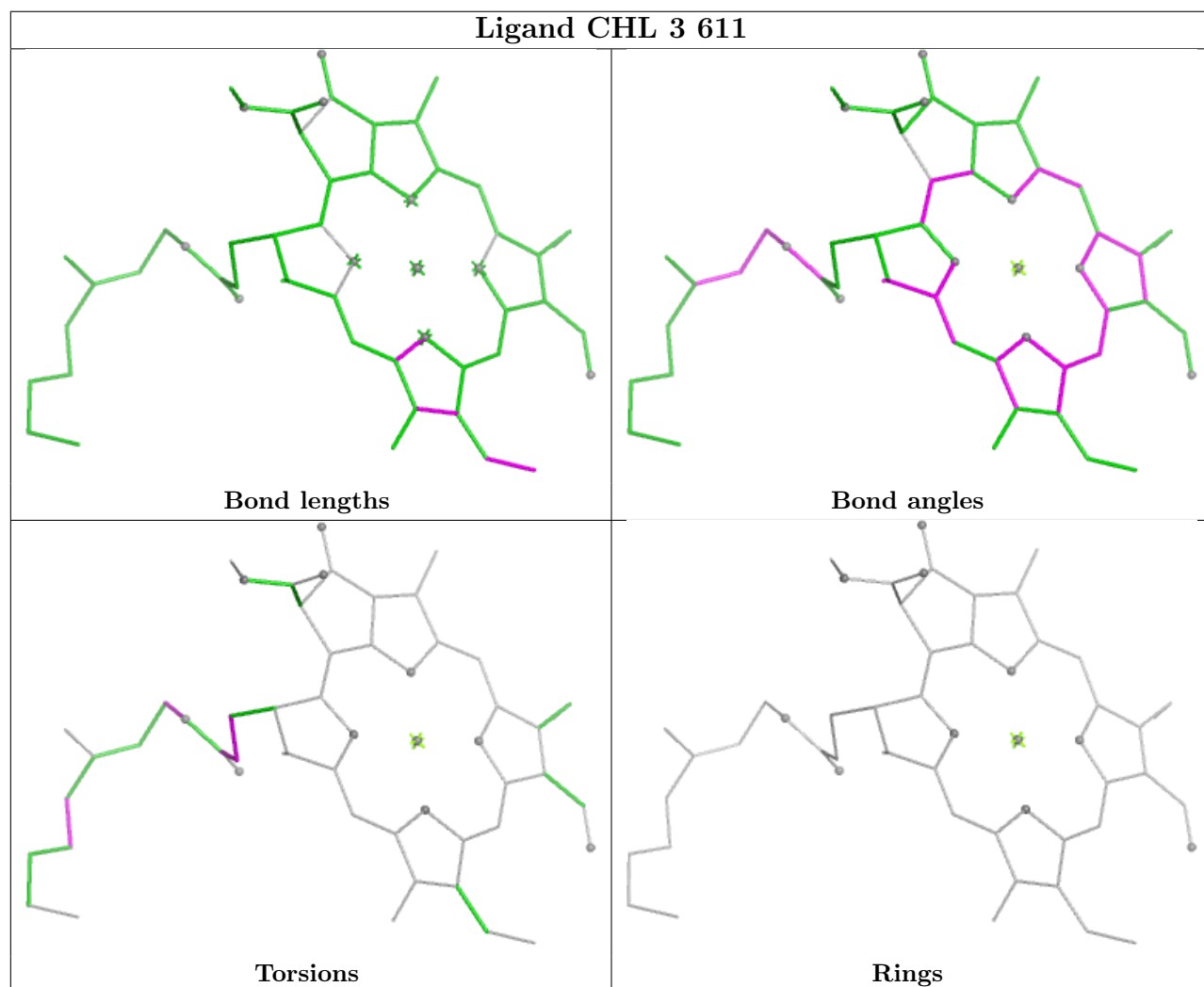
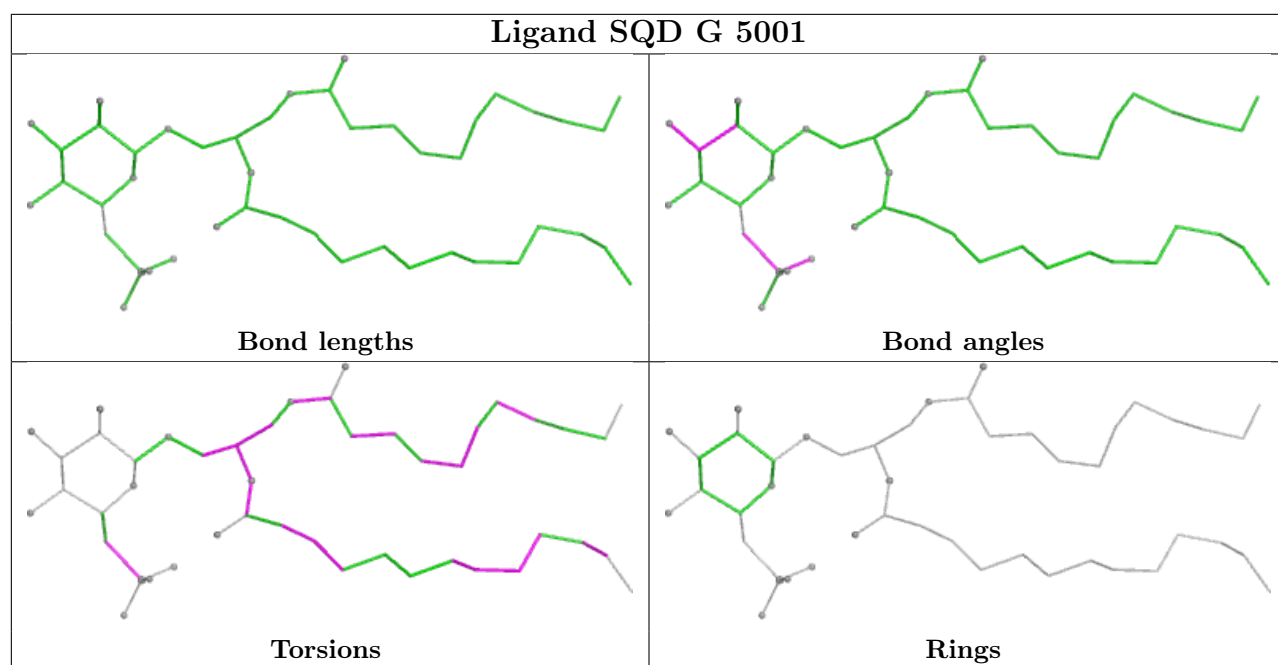
Bond angles

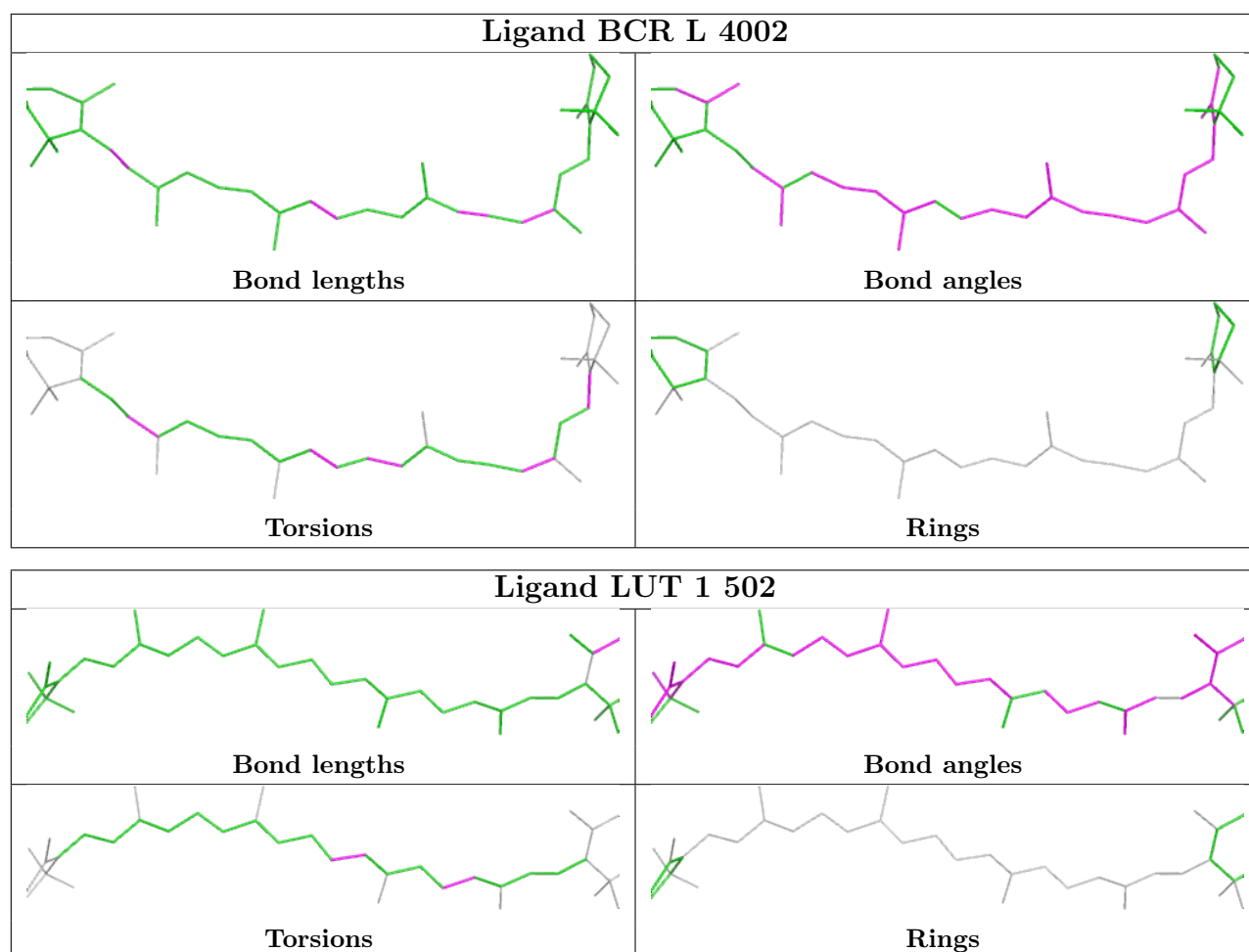


Torsions

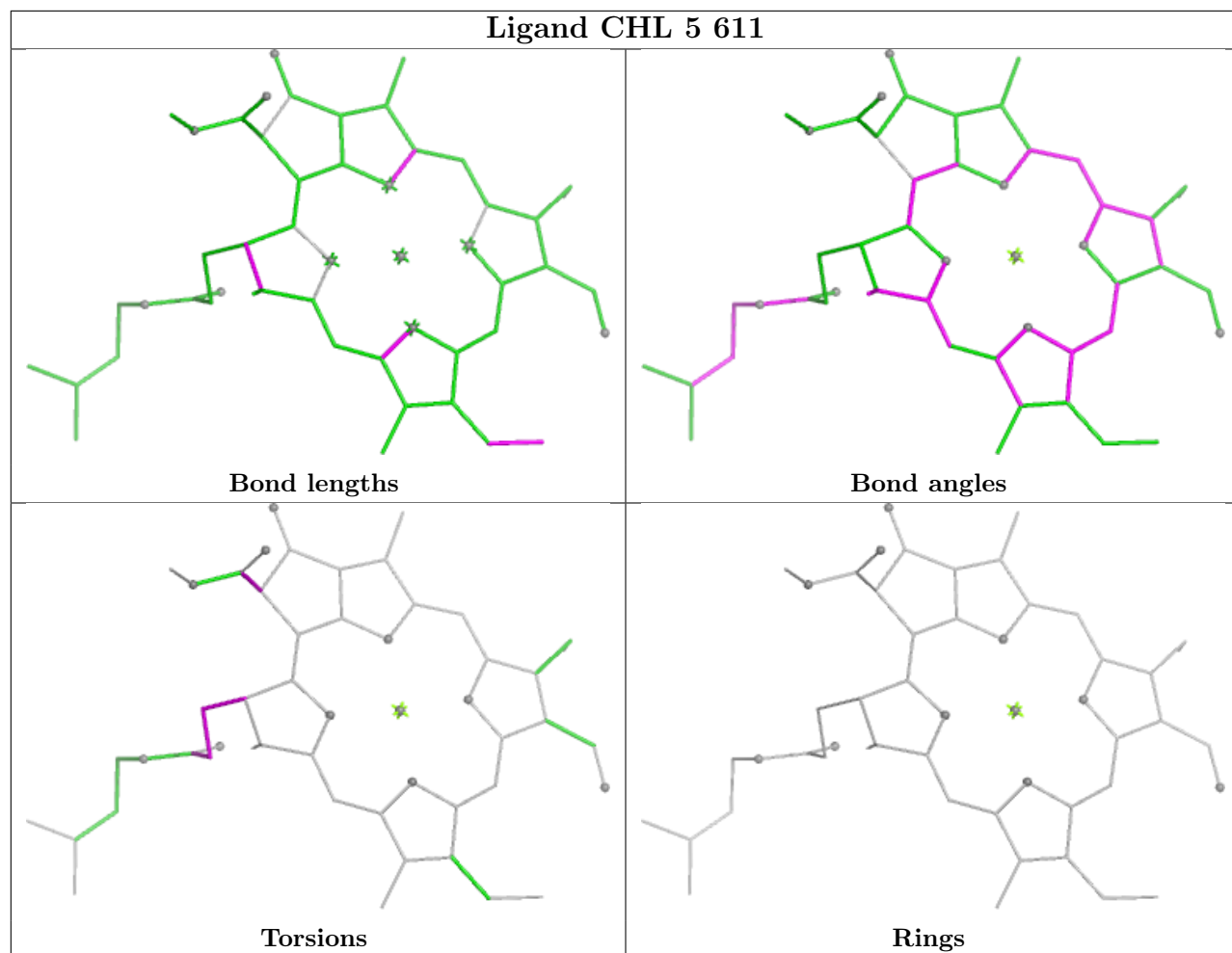


Rings

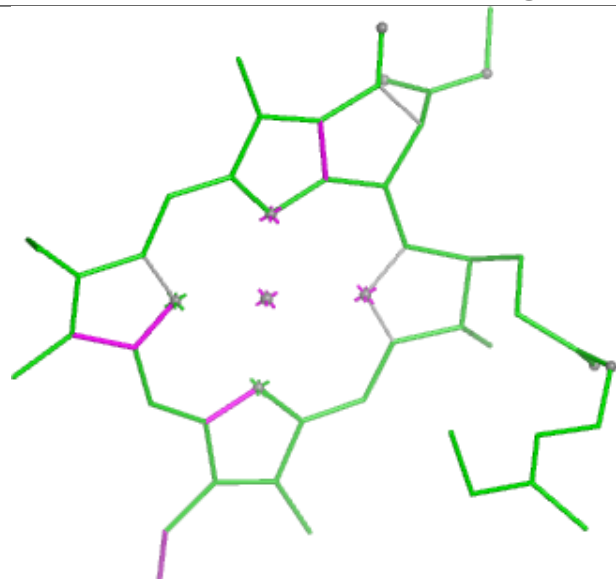




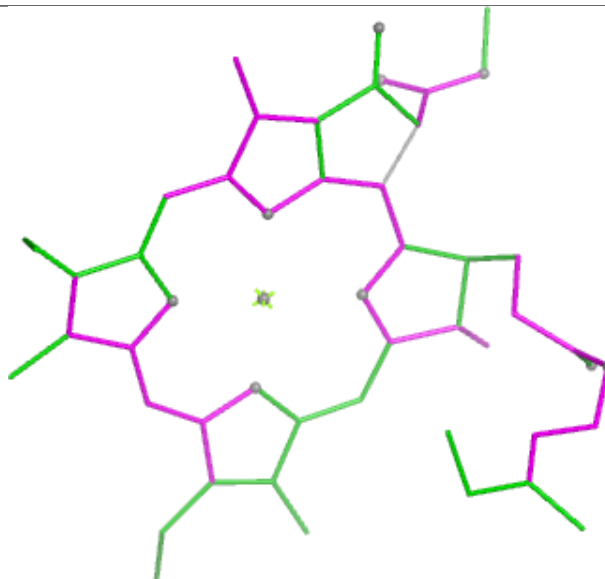
Ligand CHL 5 611



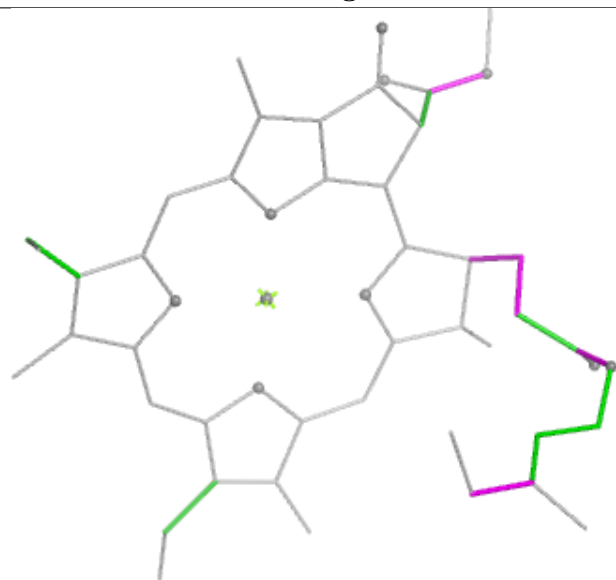
Ligand CLA 5 609



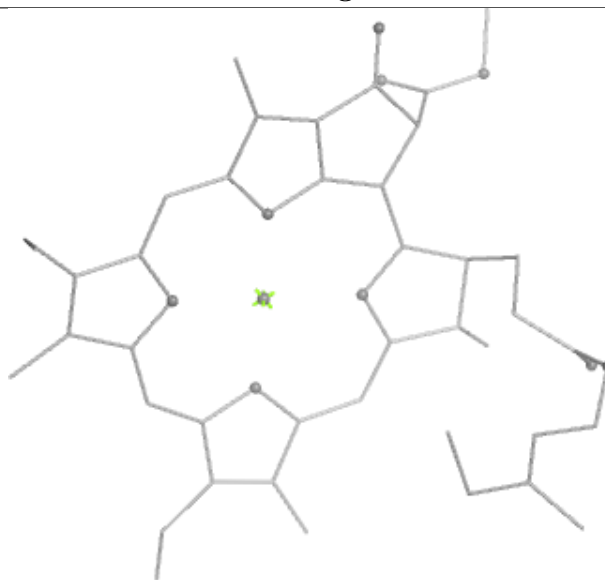
Bond lengths



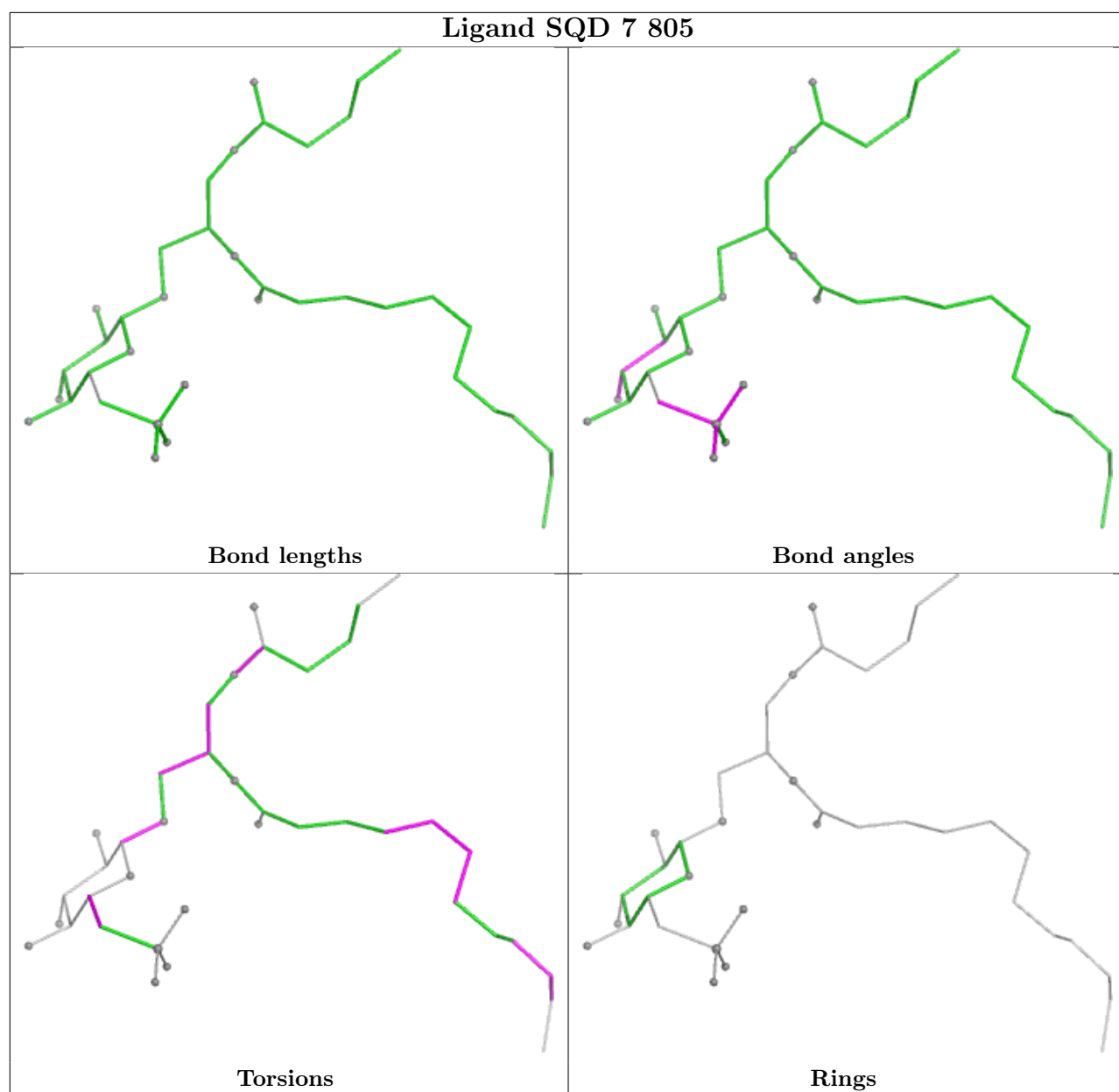
Bond angles

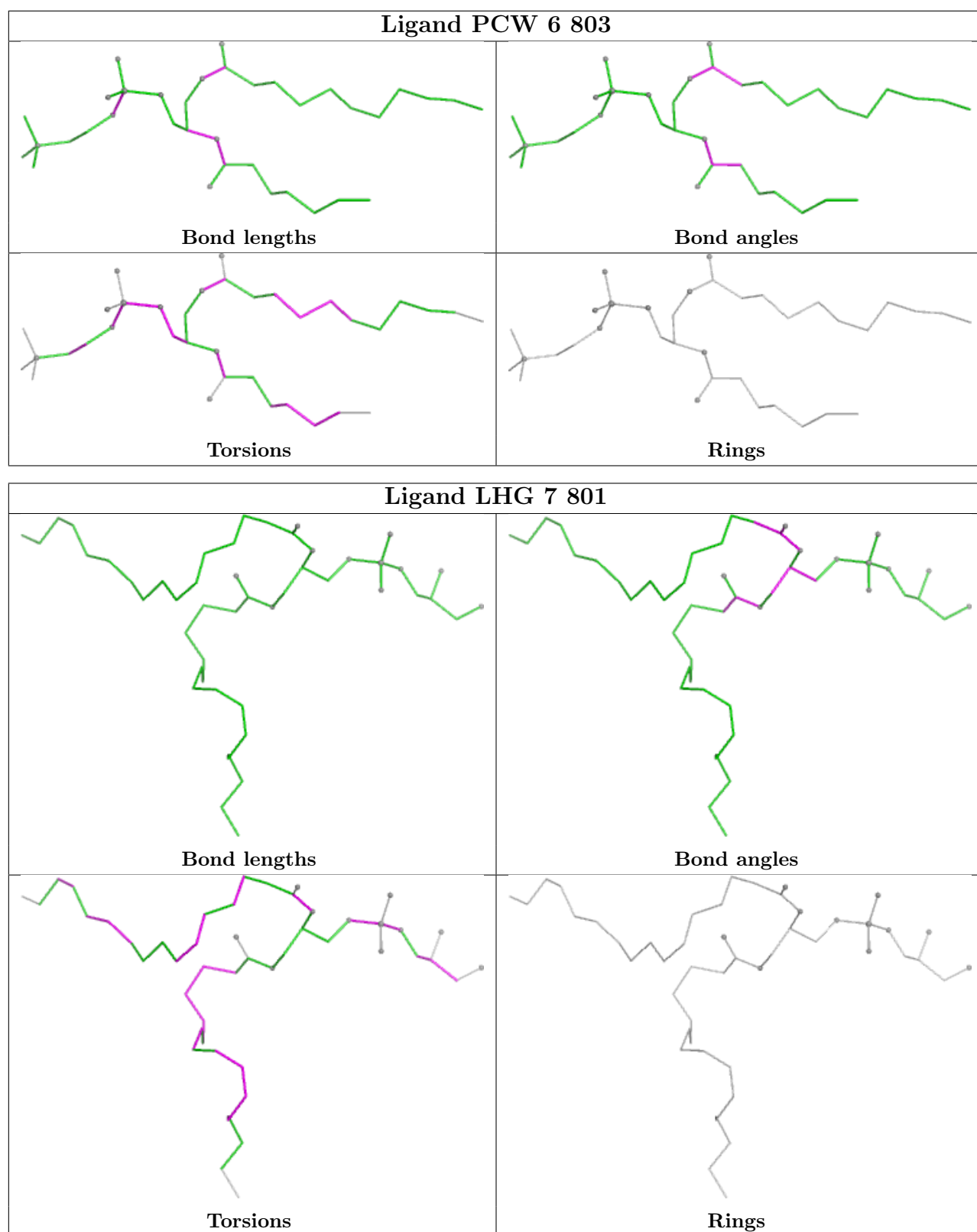


Torsions

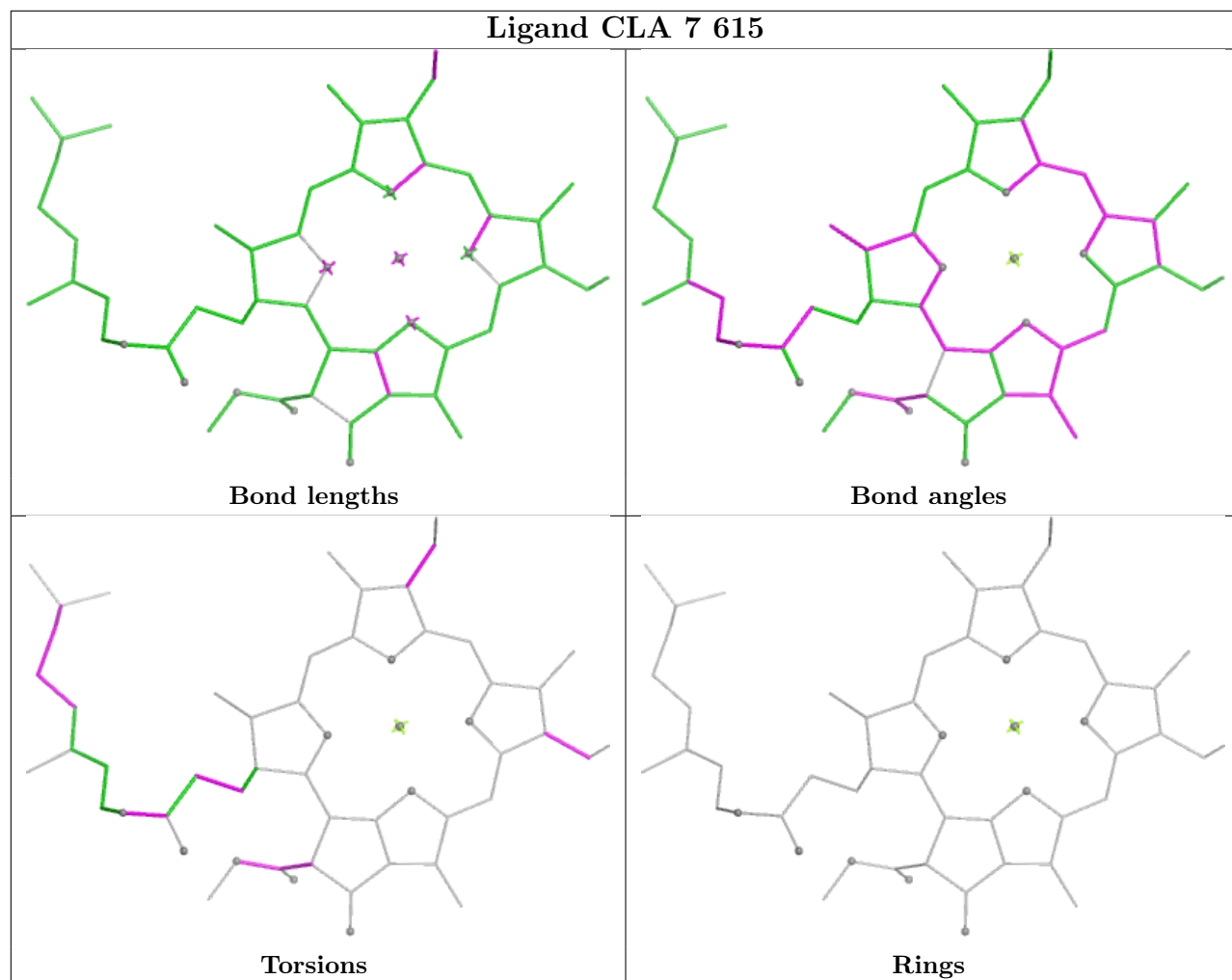


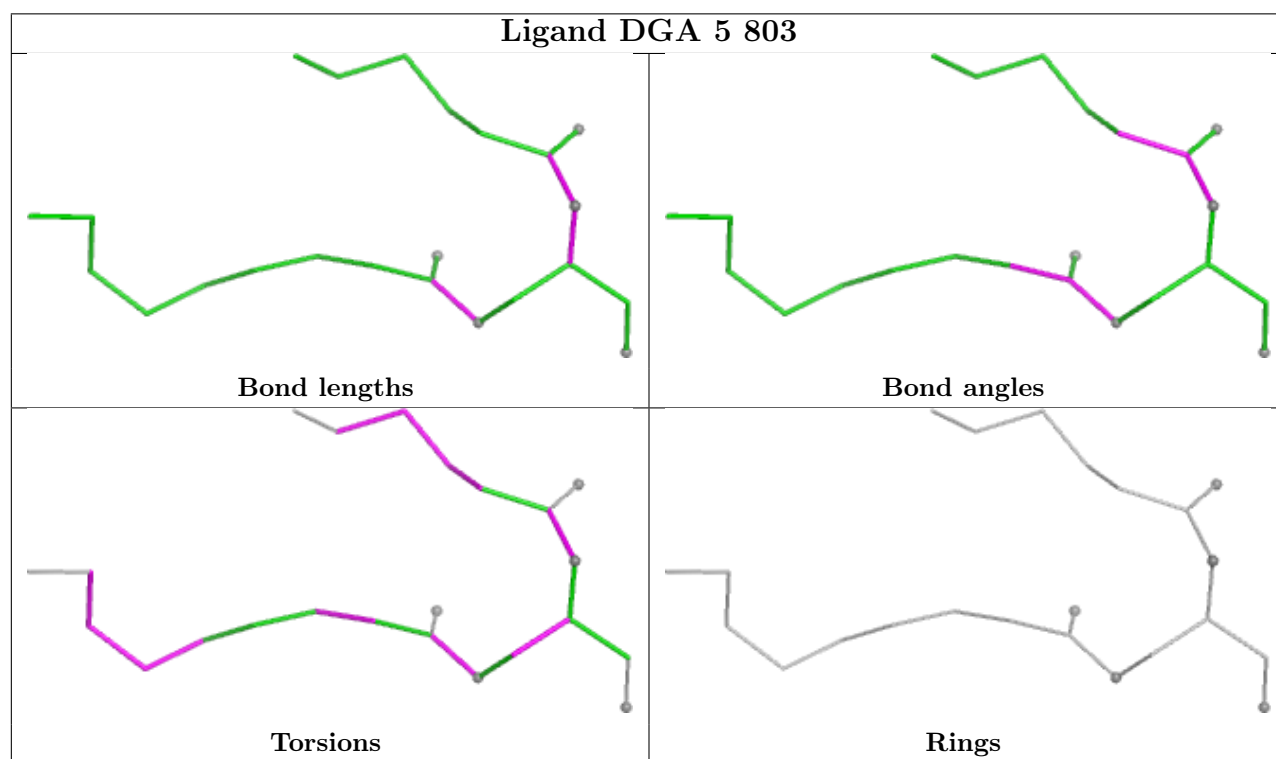
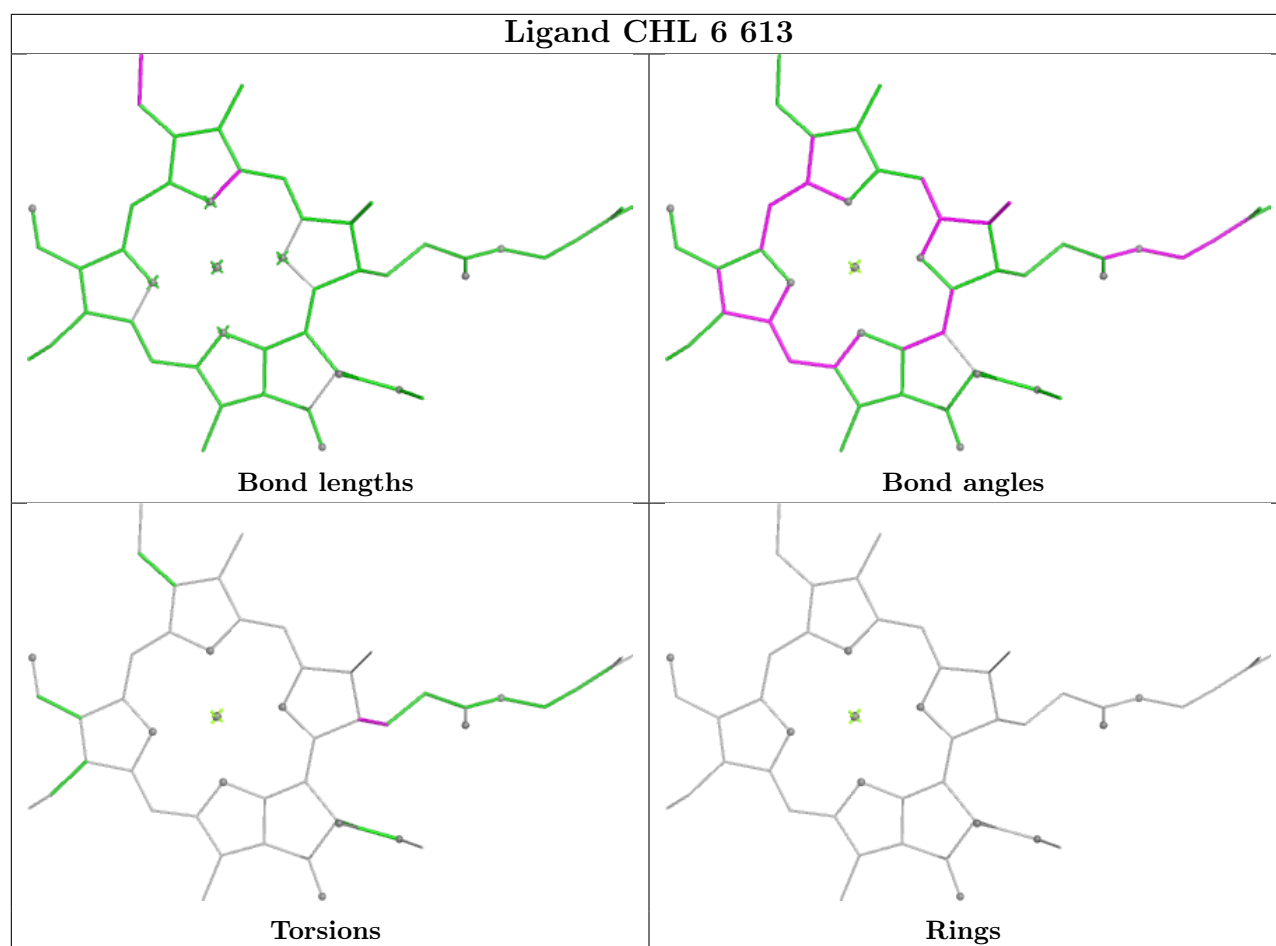
Rings

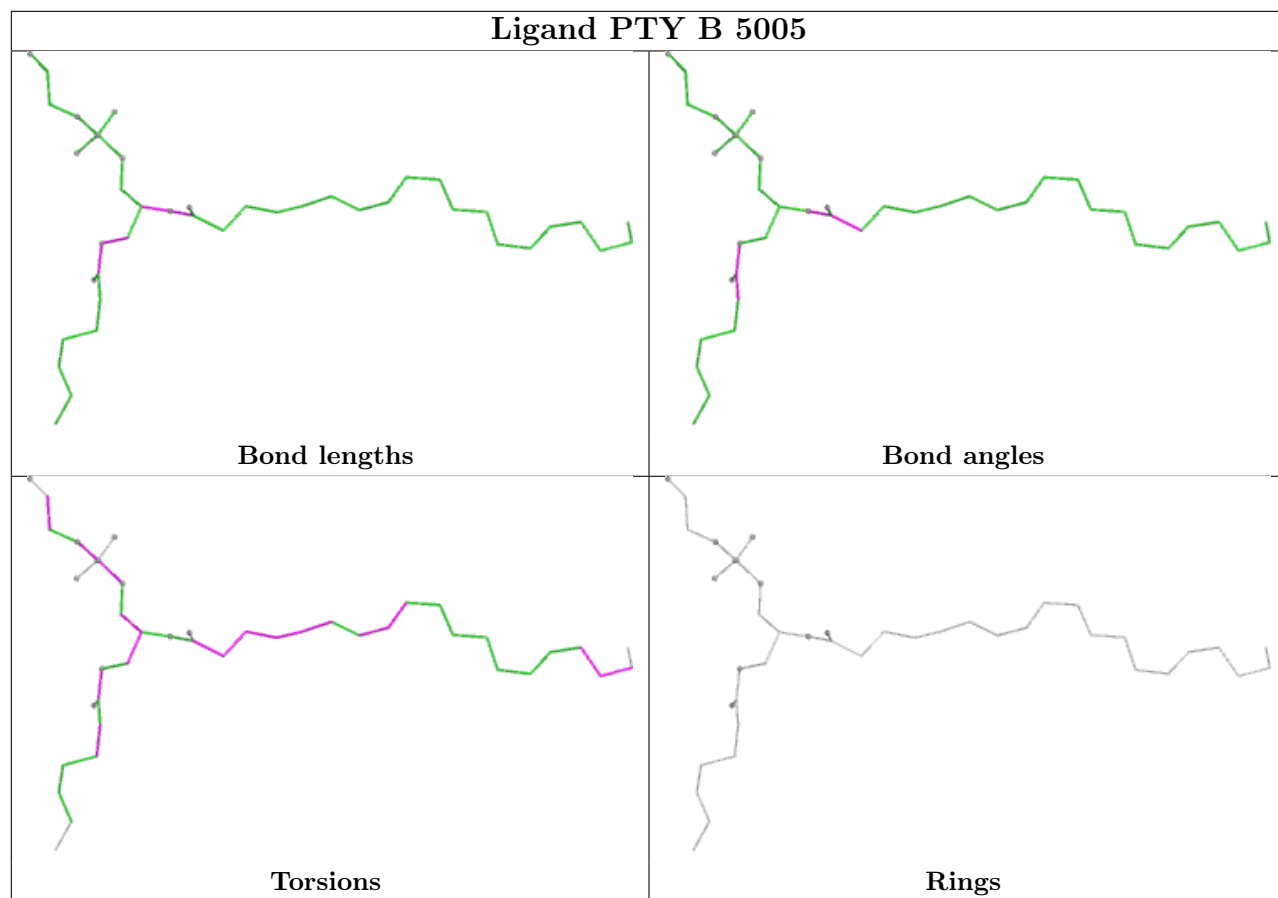


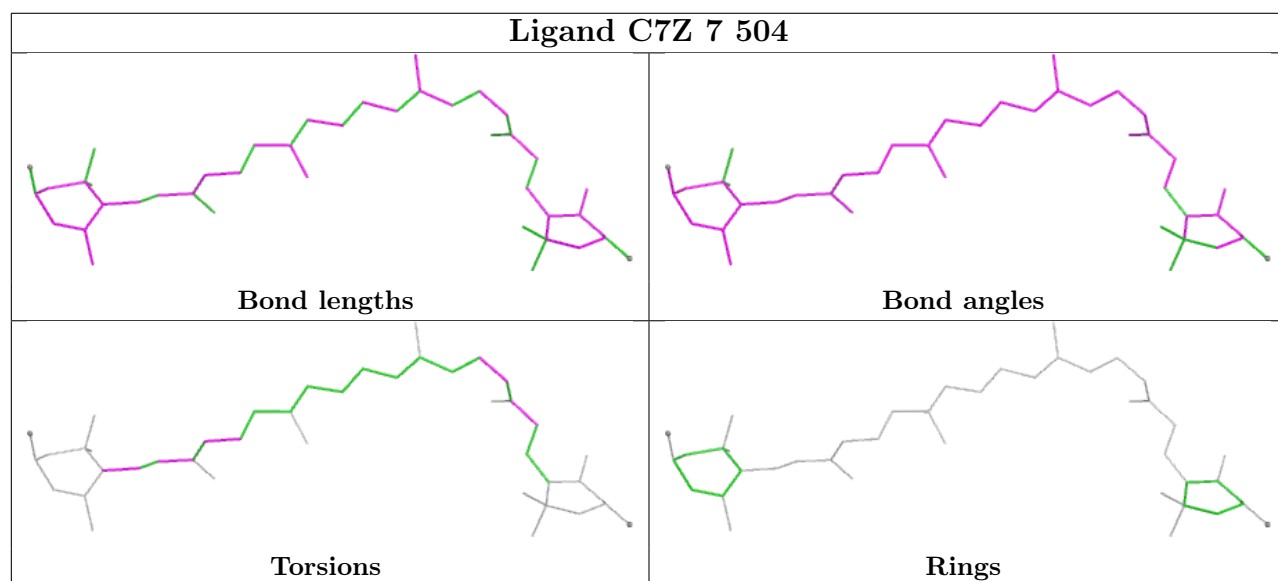
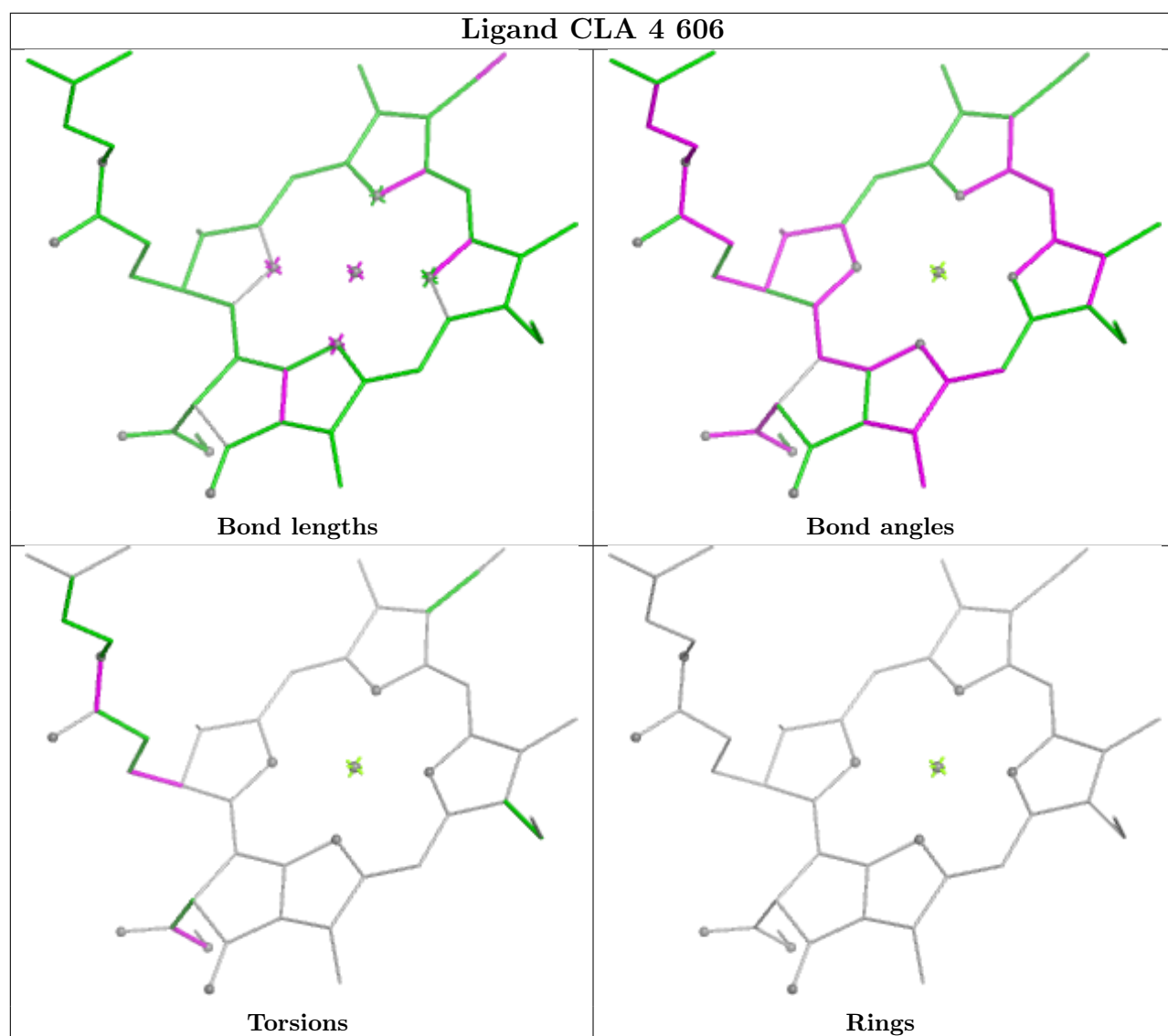


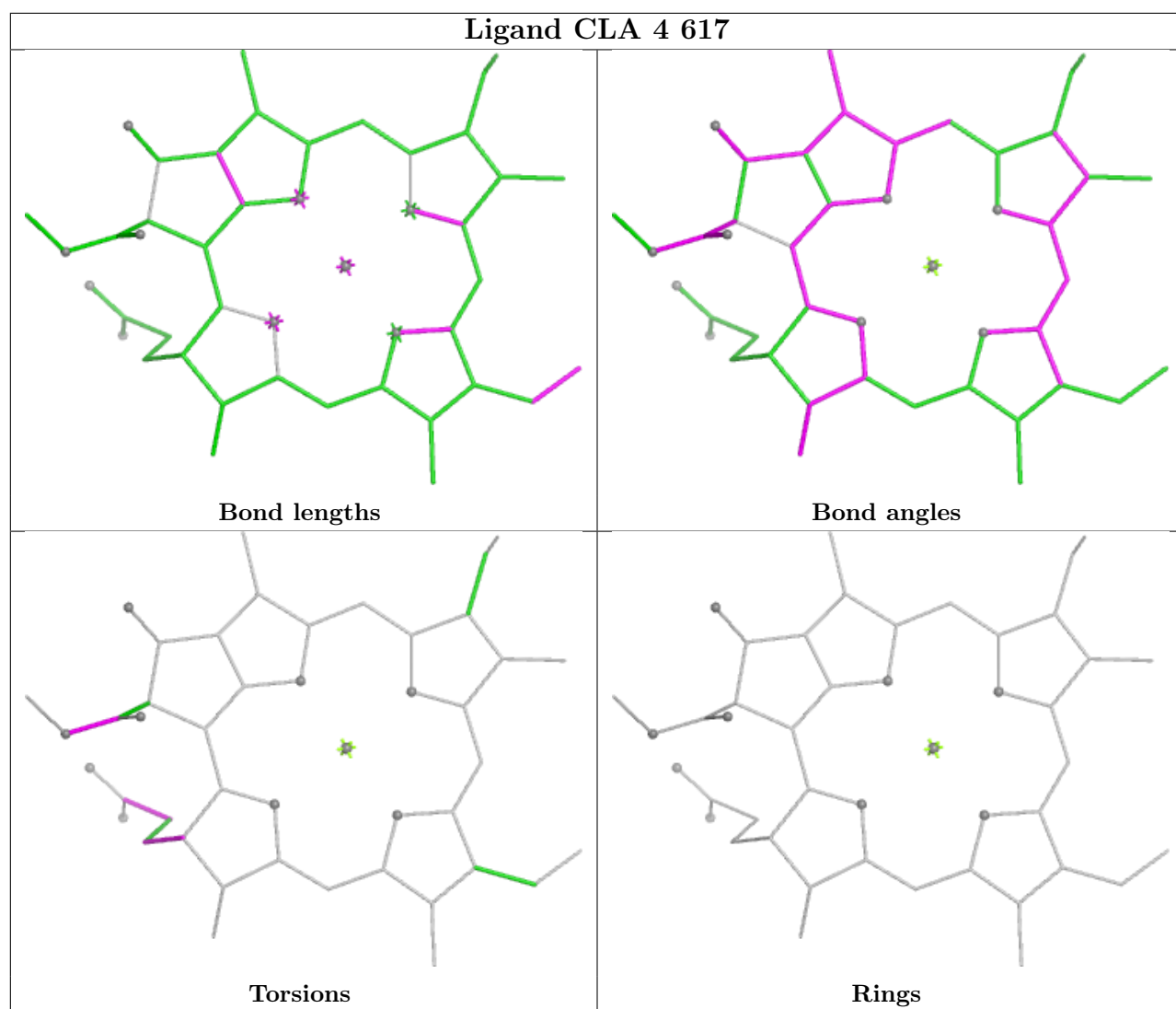
Ligand CLA 7 615

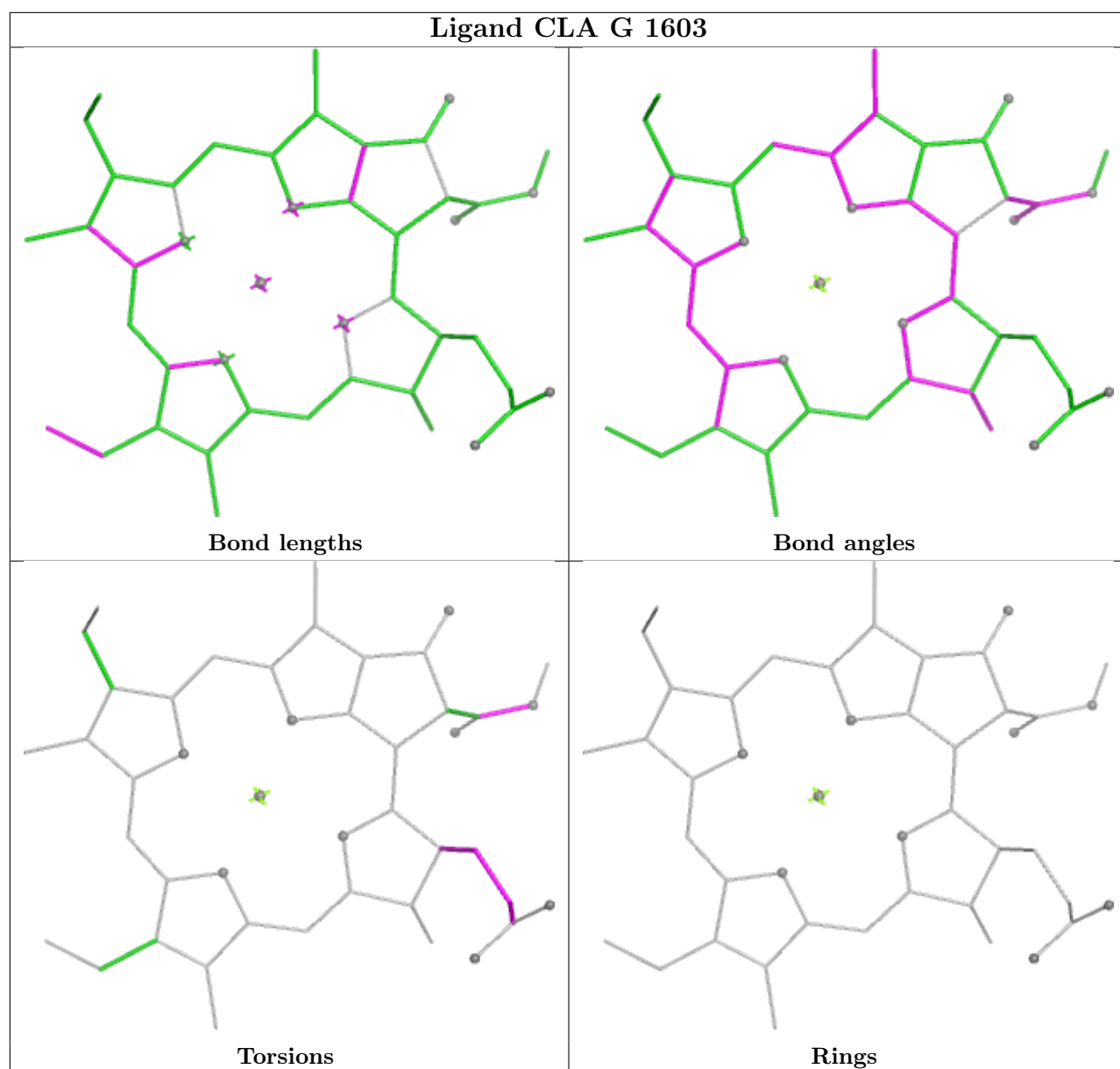


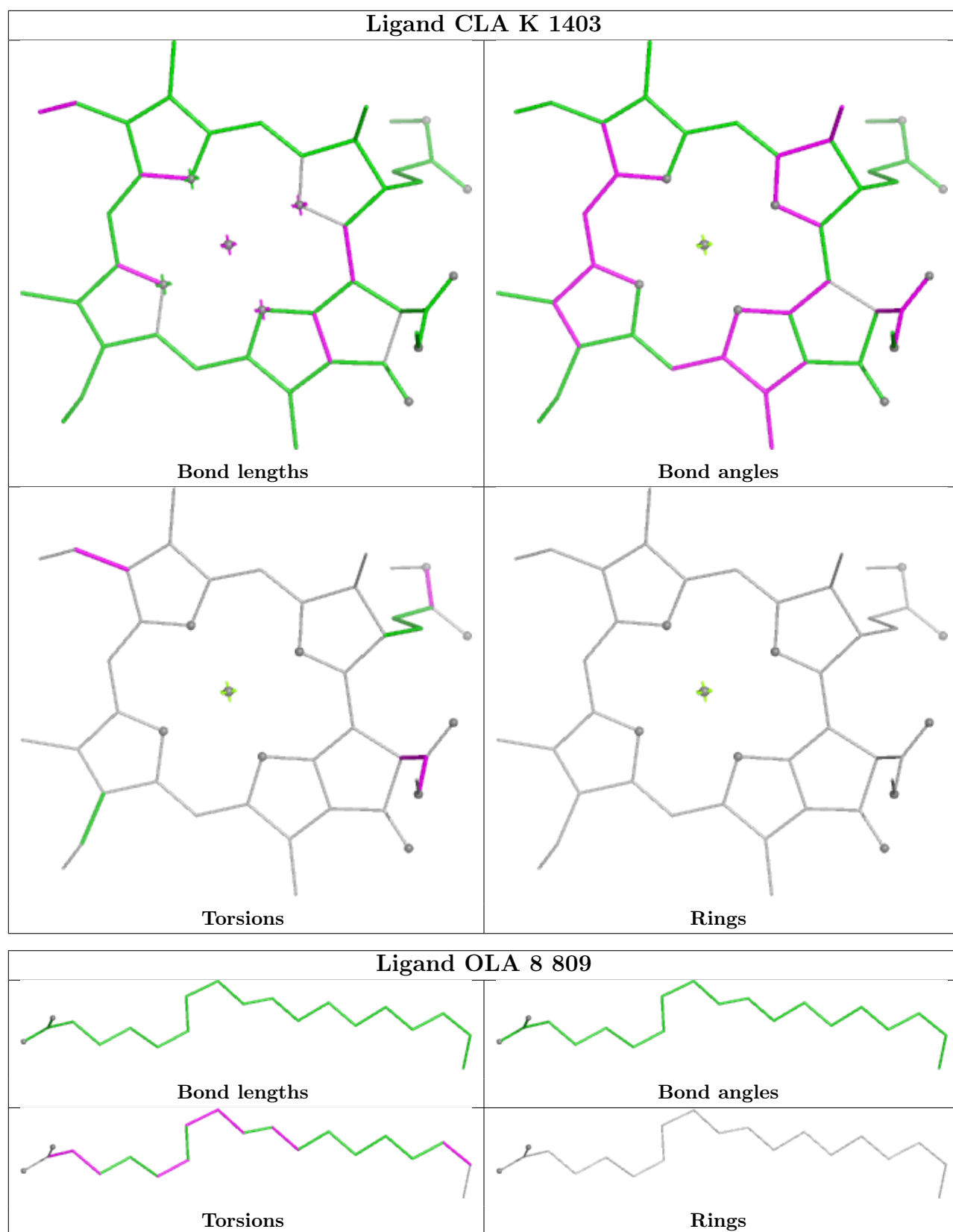




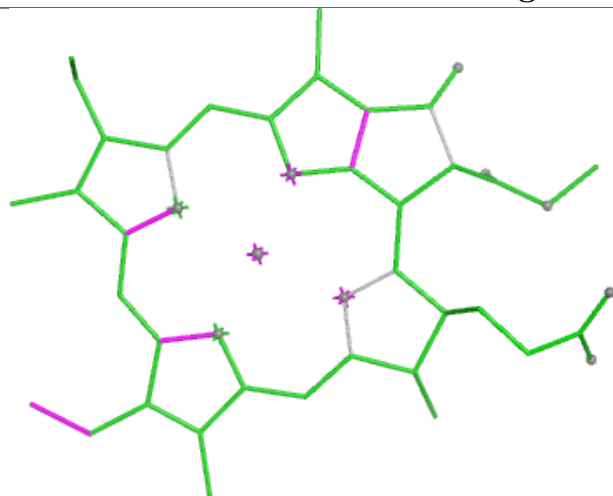




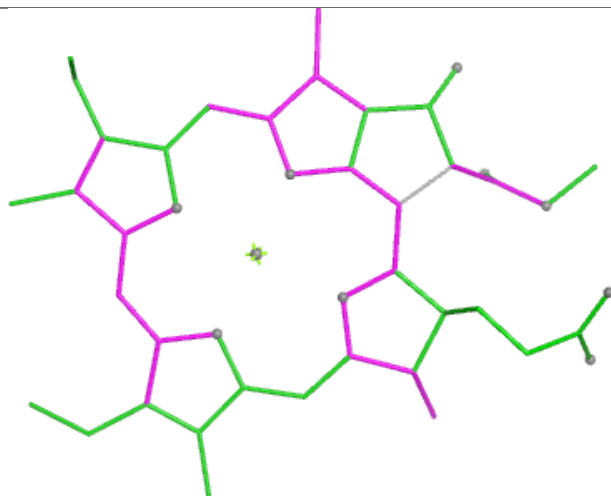




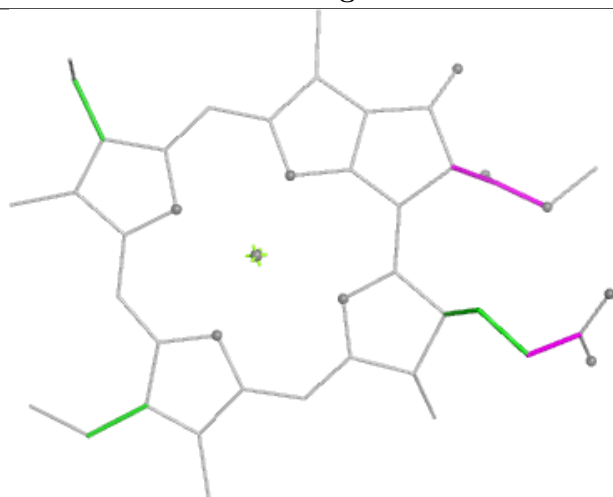
Ligand CLA 8 605



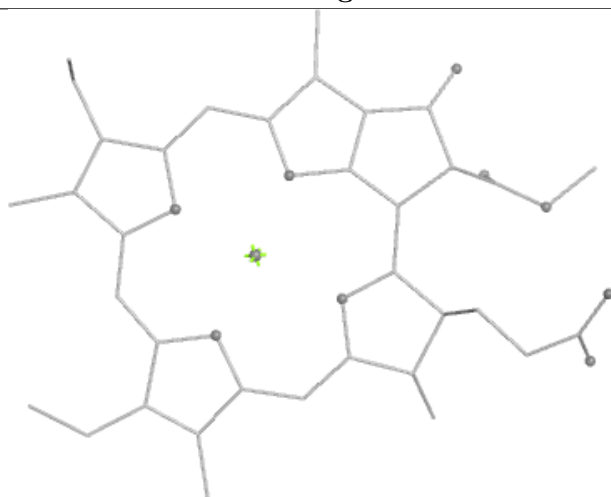
Bond lengths



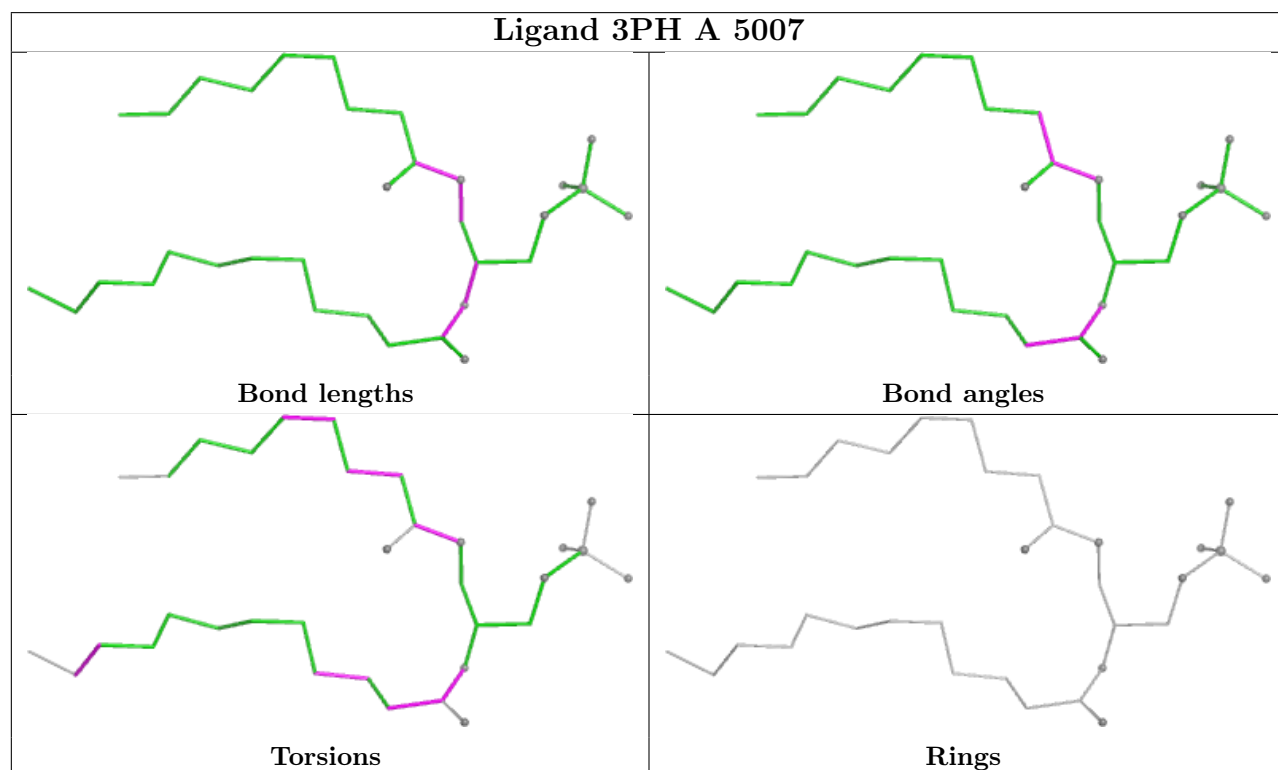
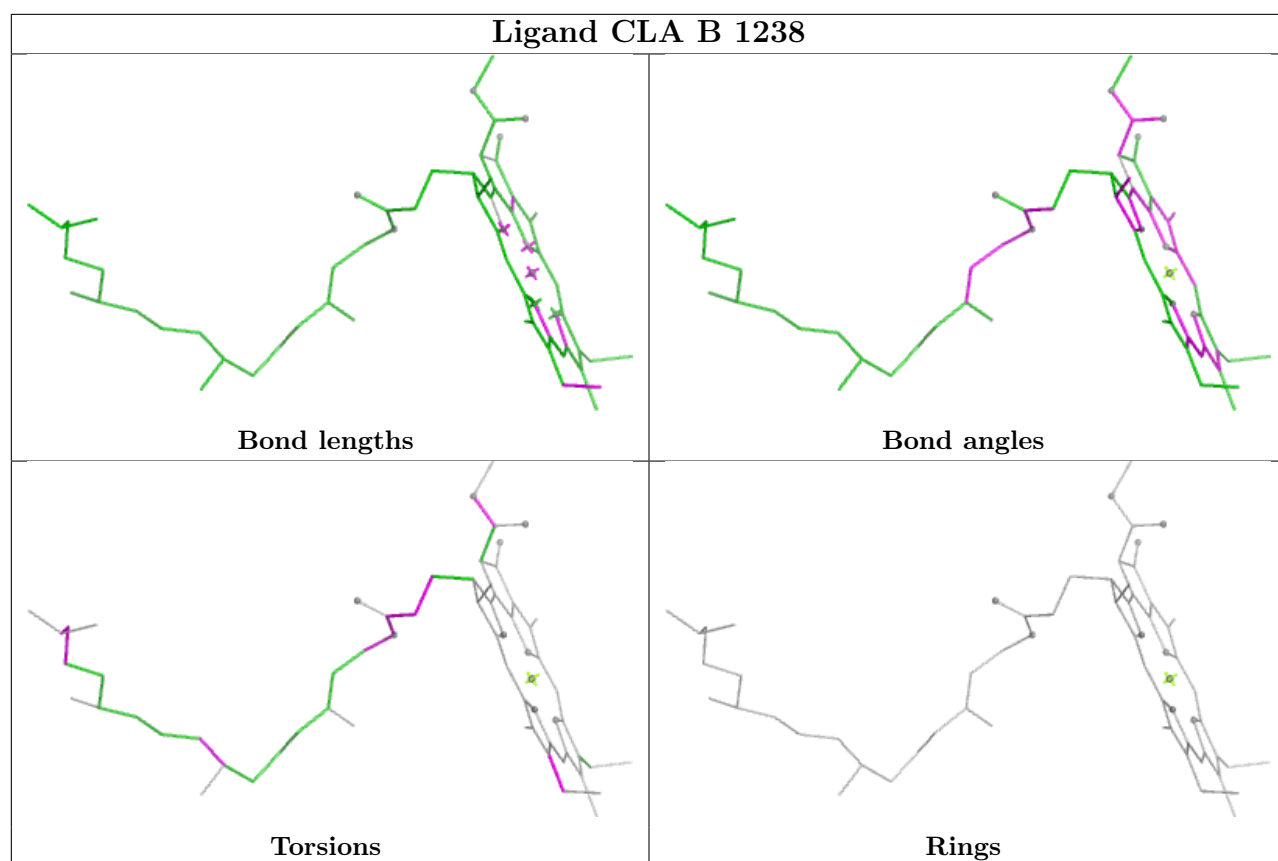
Bond angles

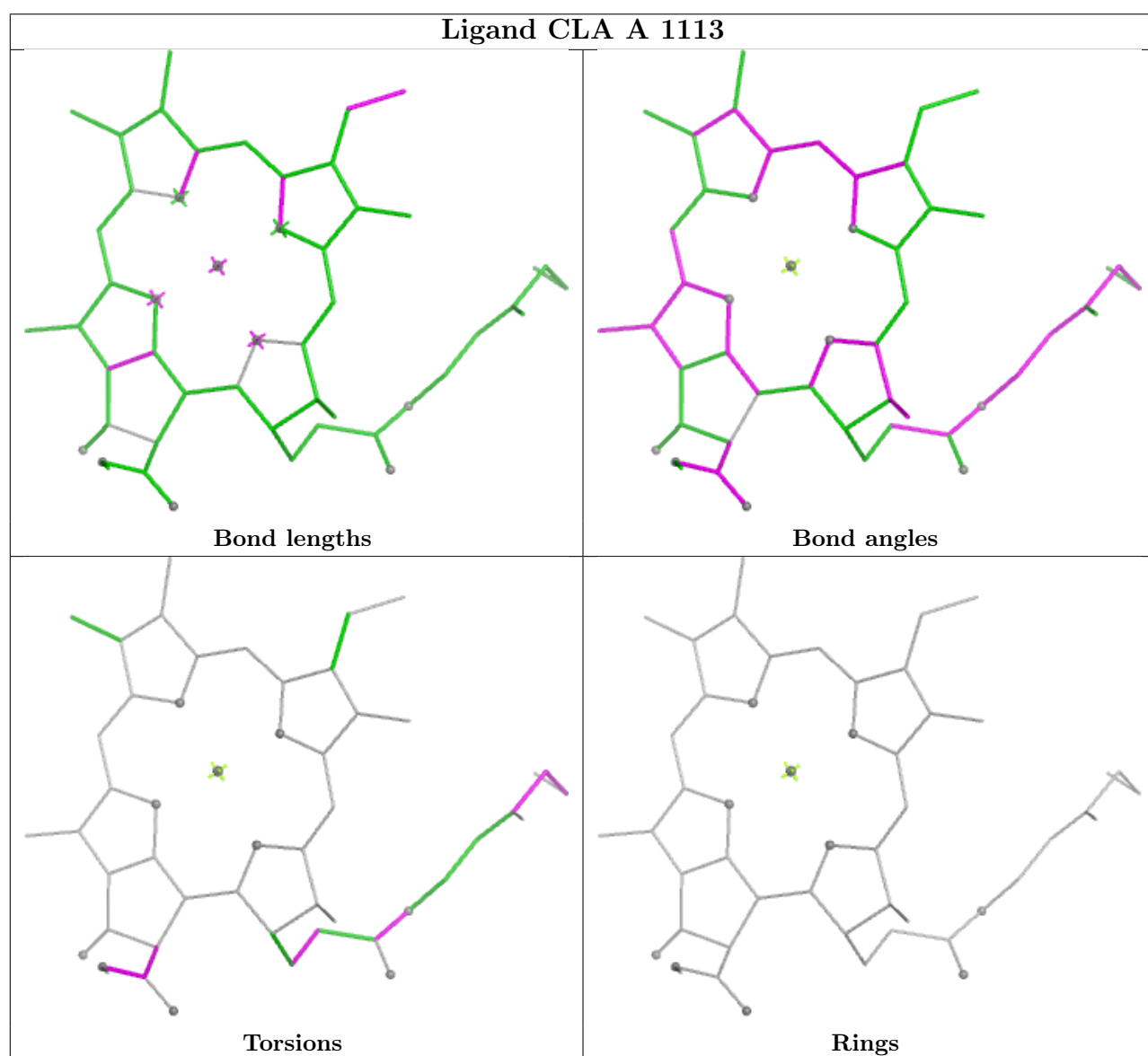
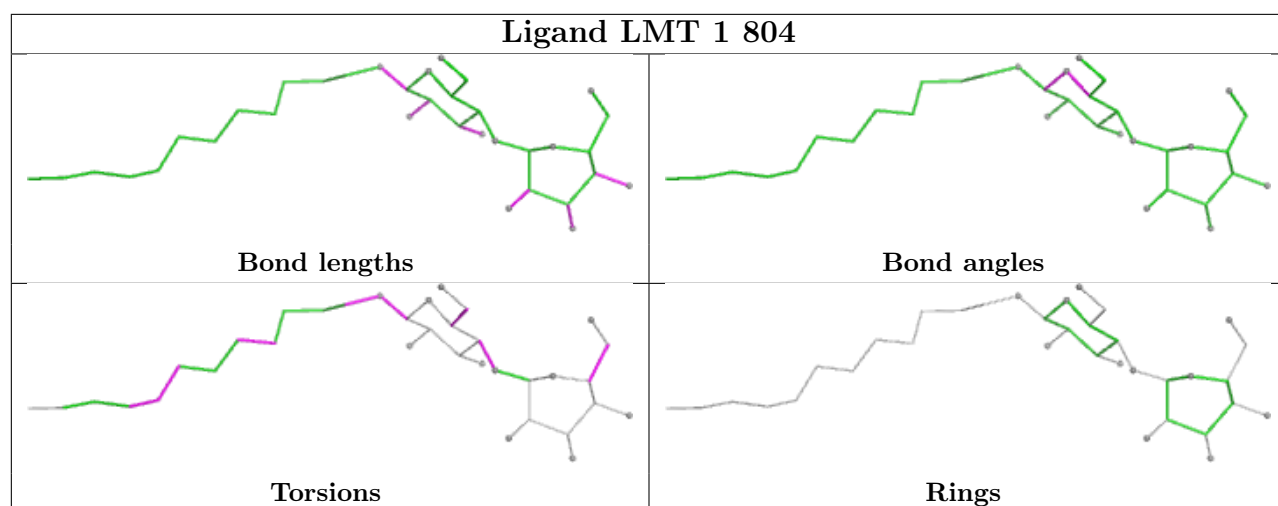


Torsions

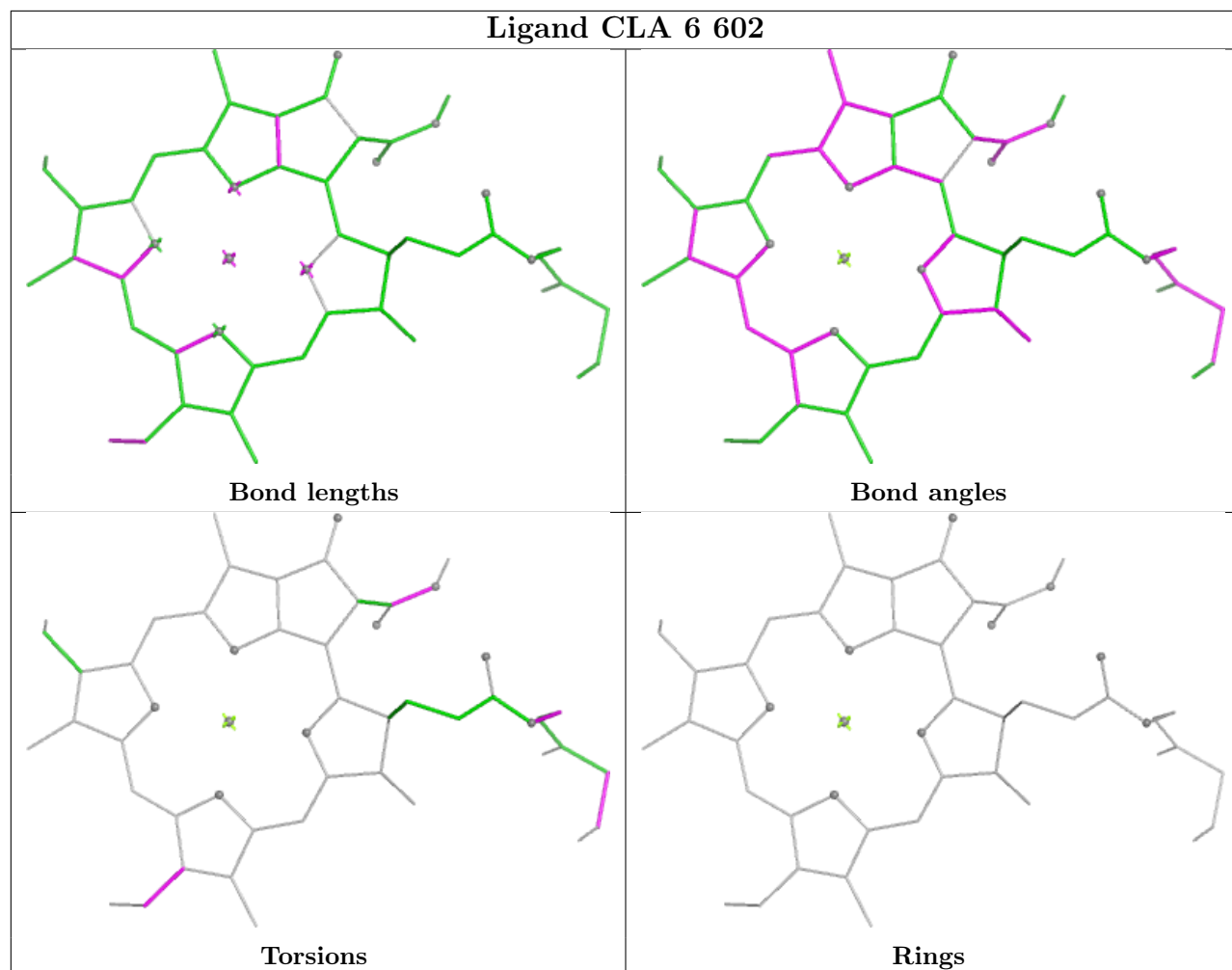


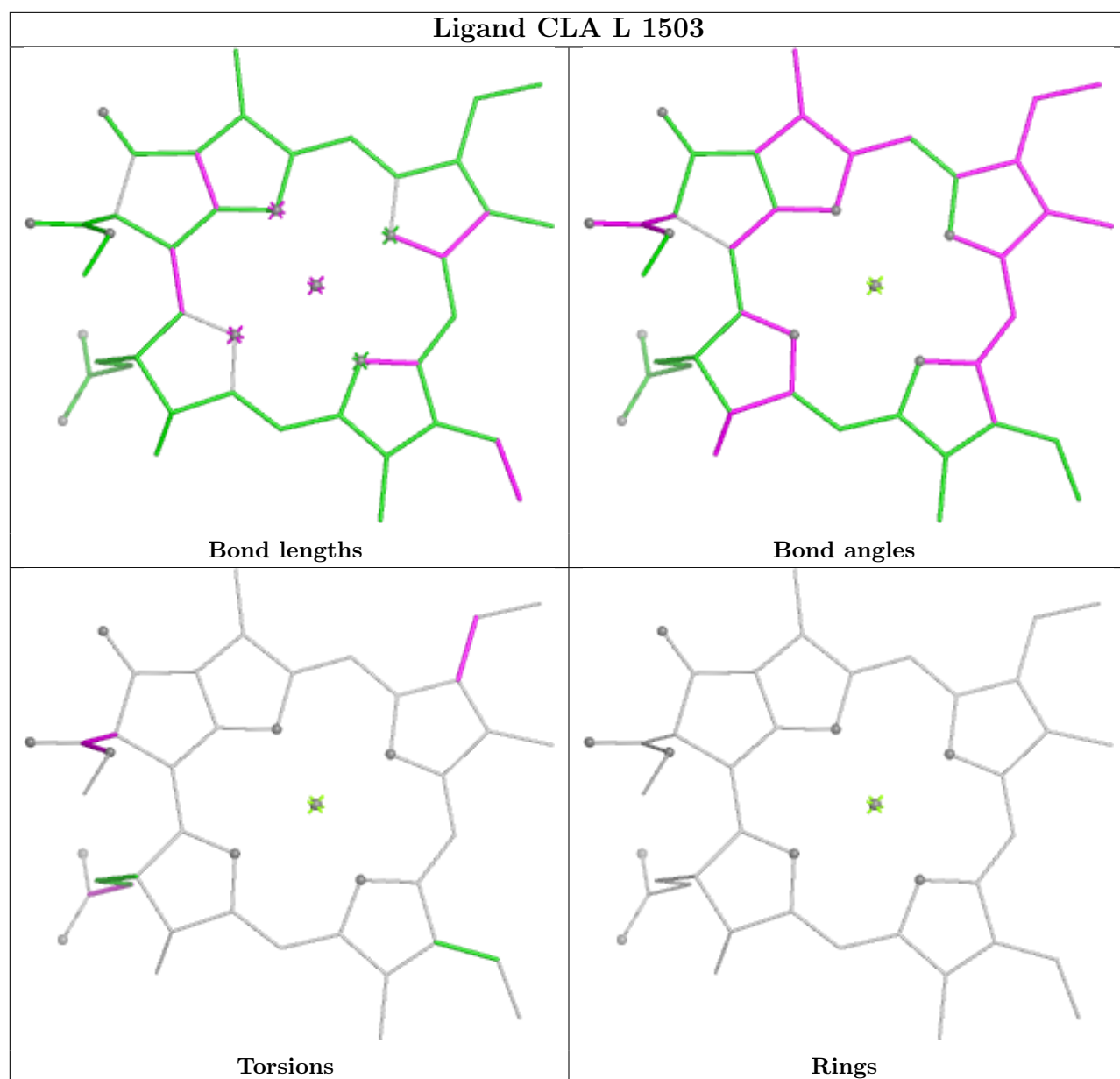
Rings



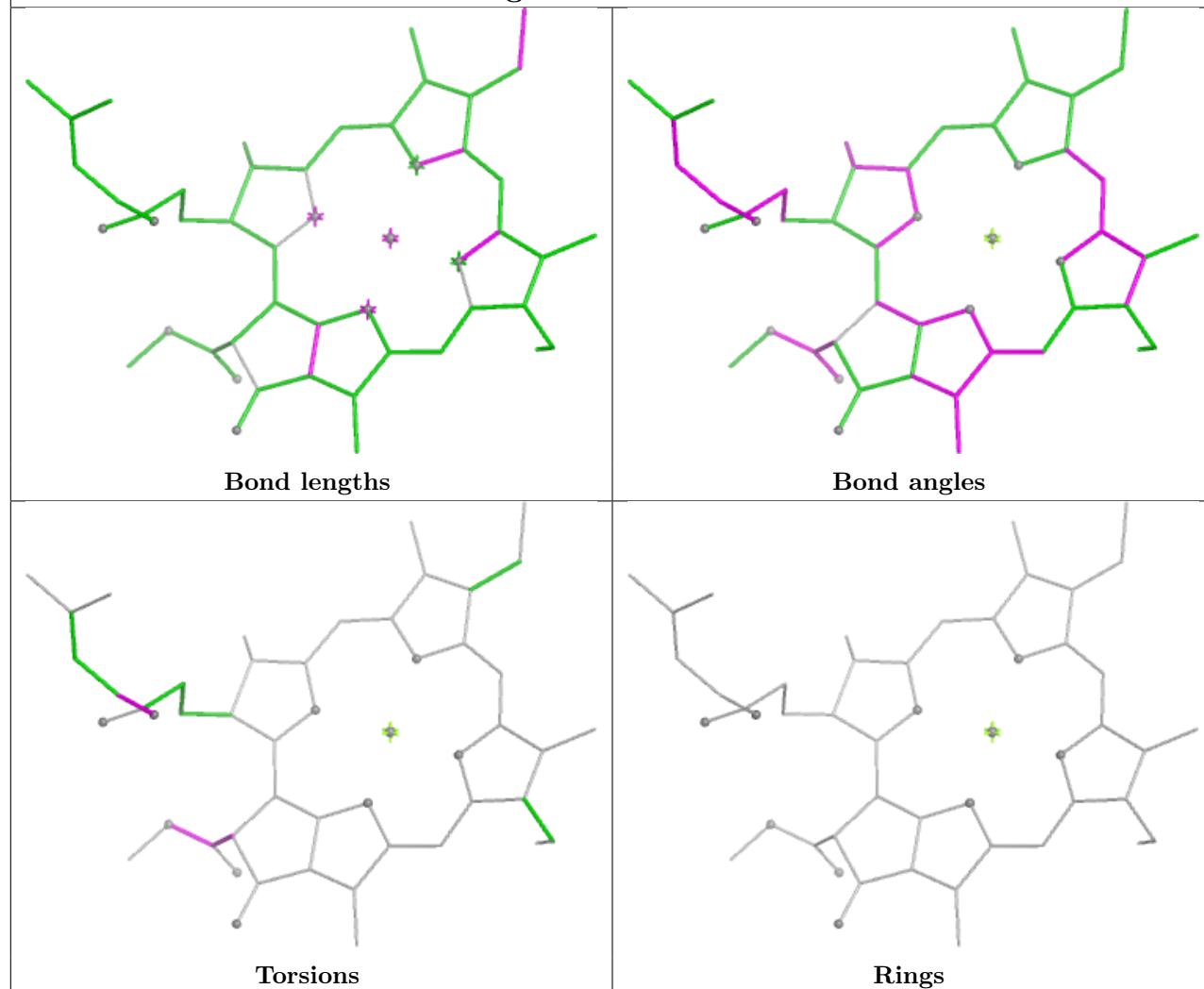


Ligand CLA 6 602

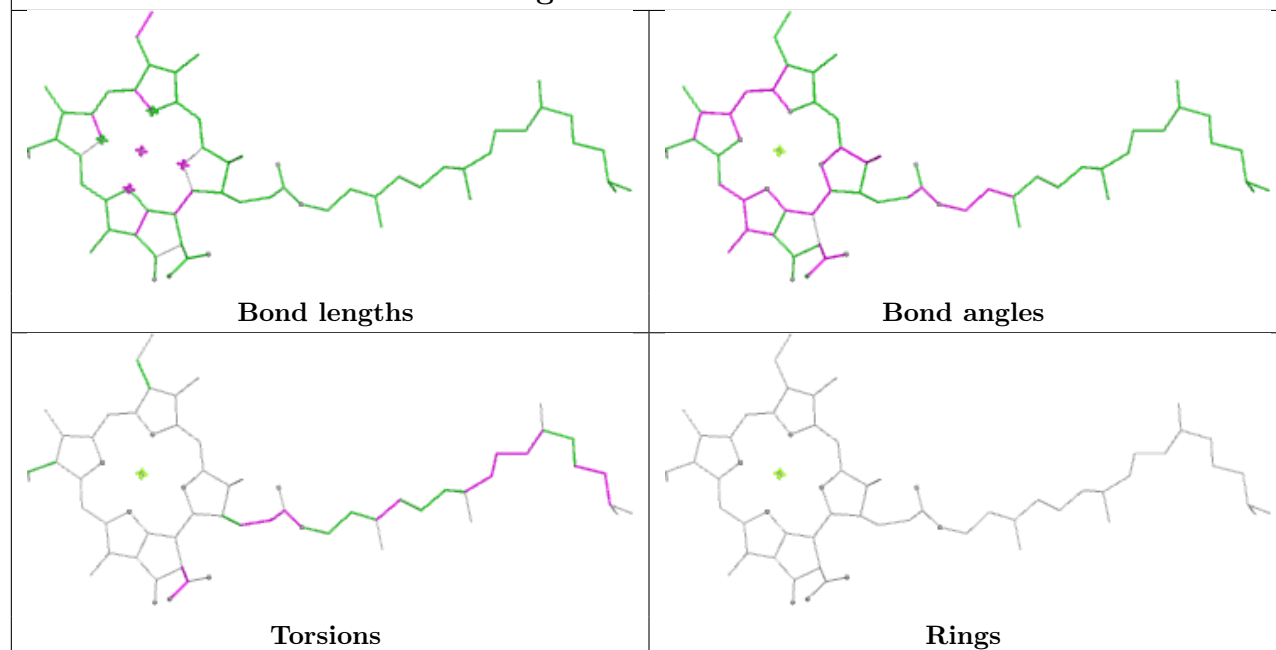




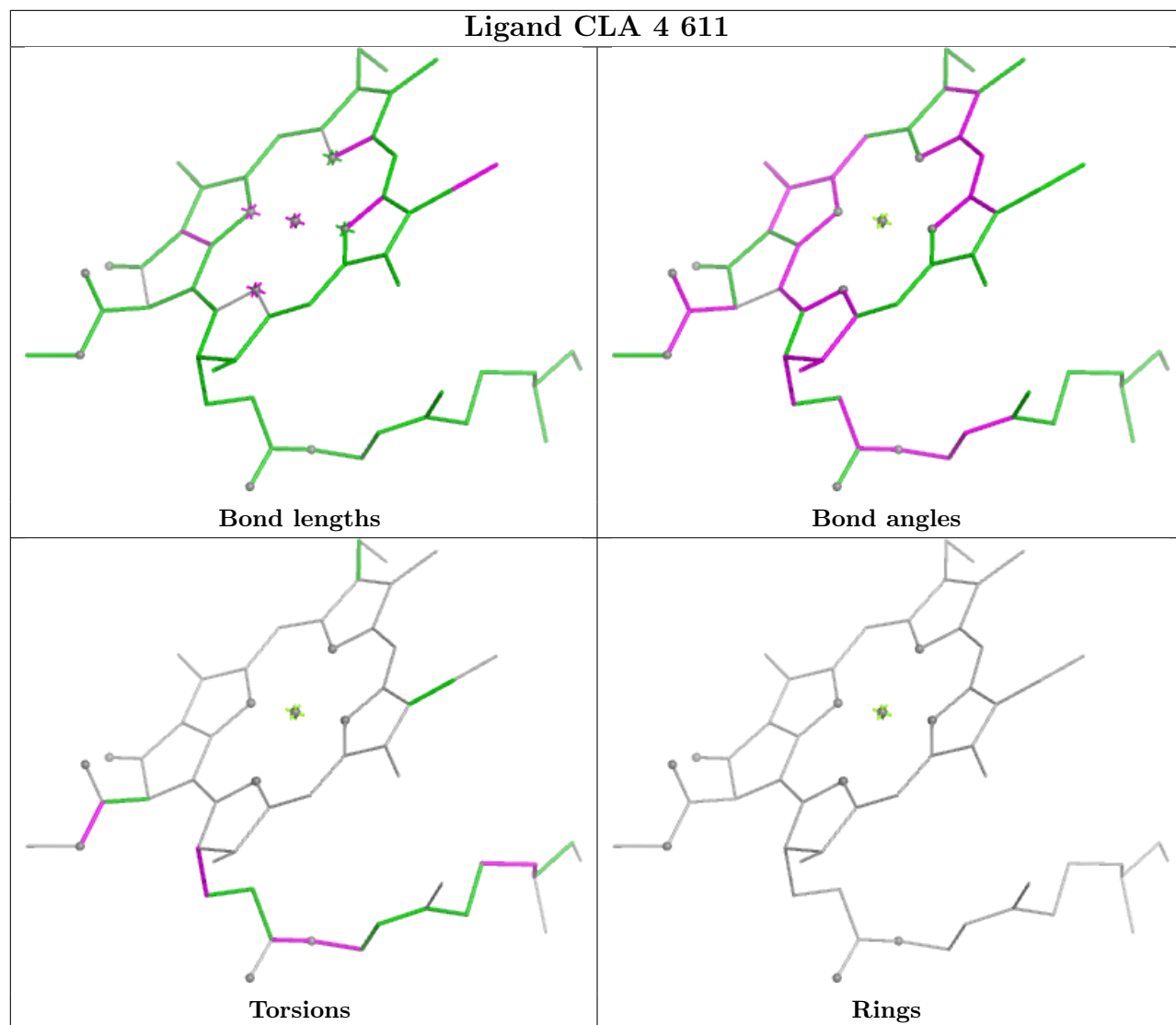
Ligand CLA 8 611

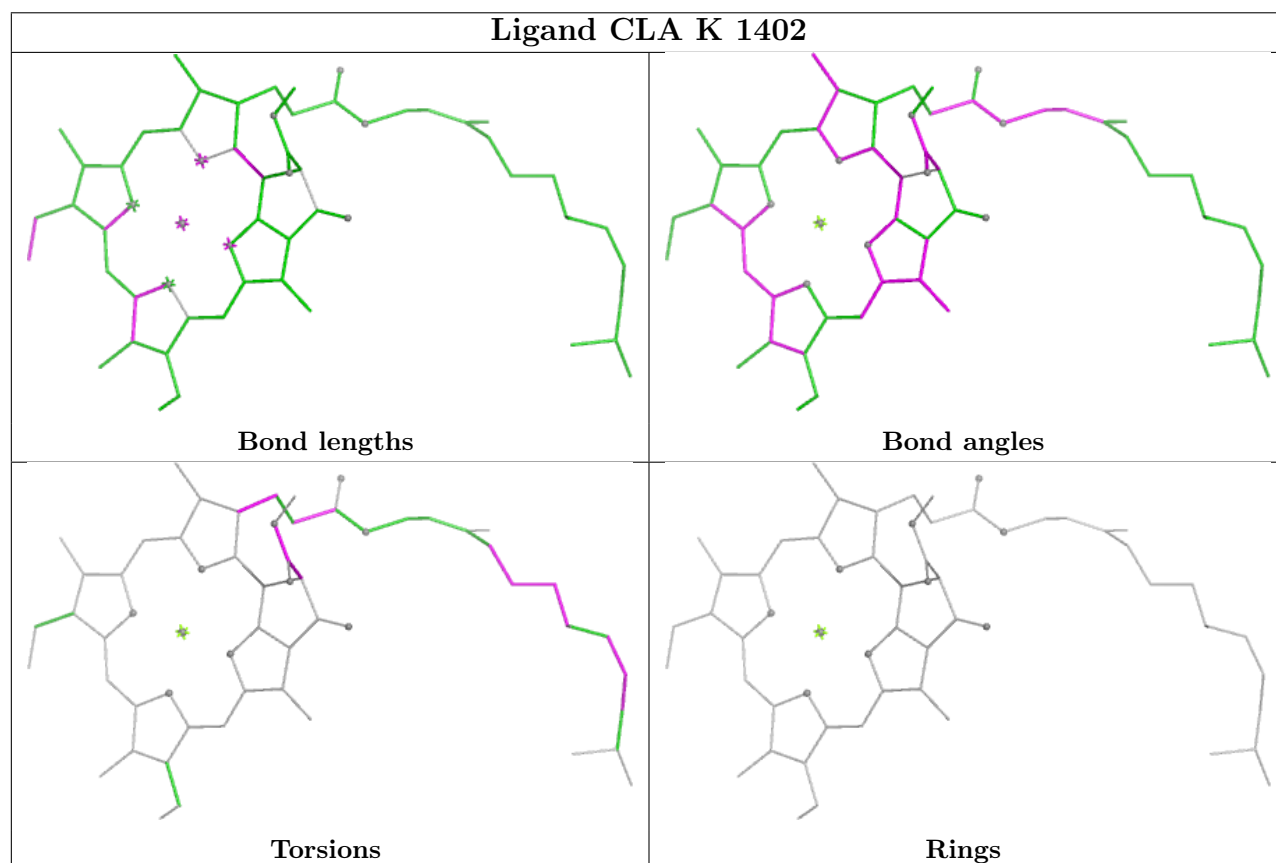
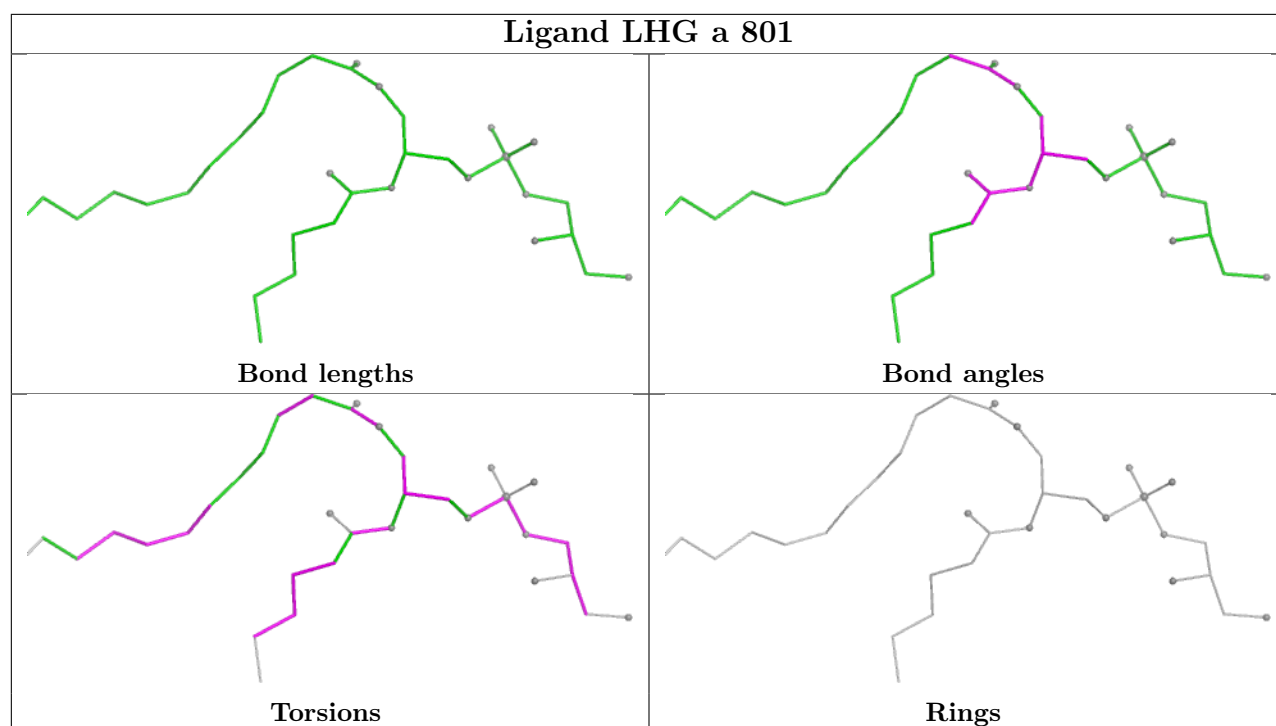


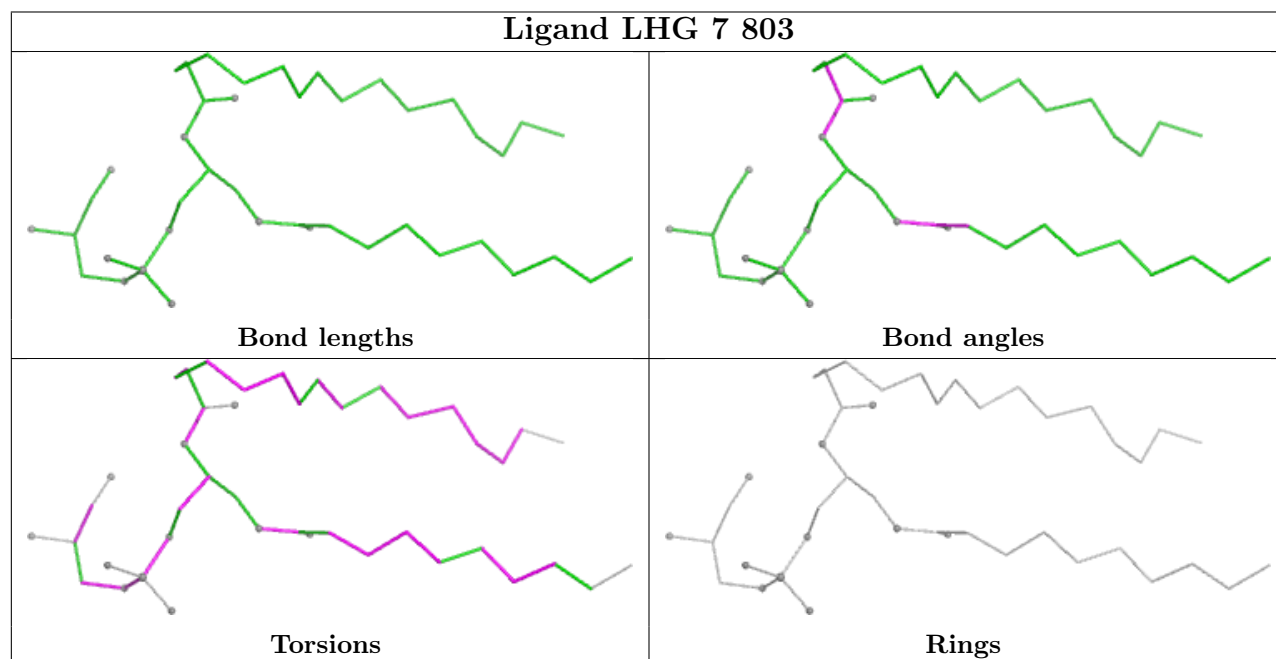
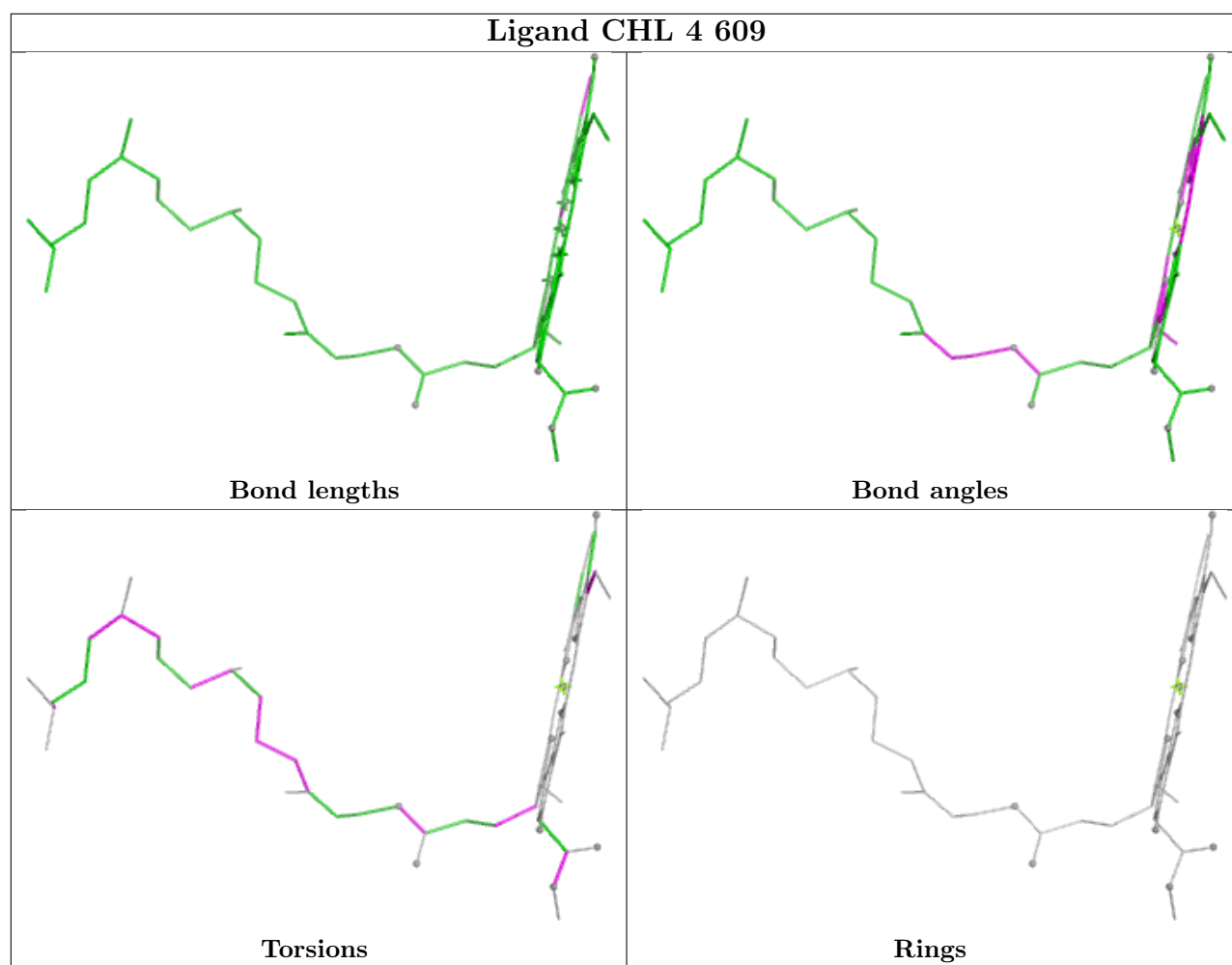
Ligand CLA 6 615

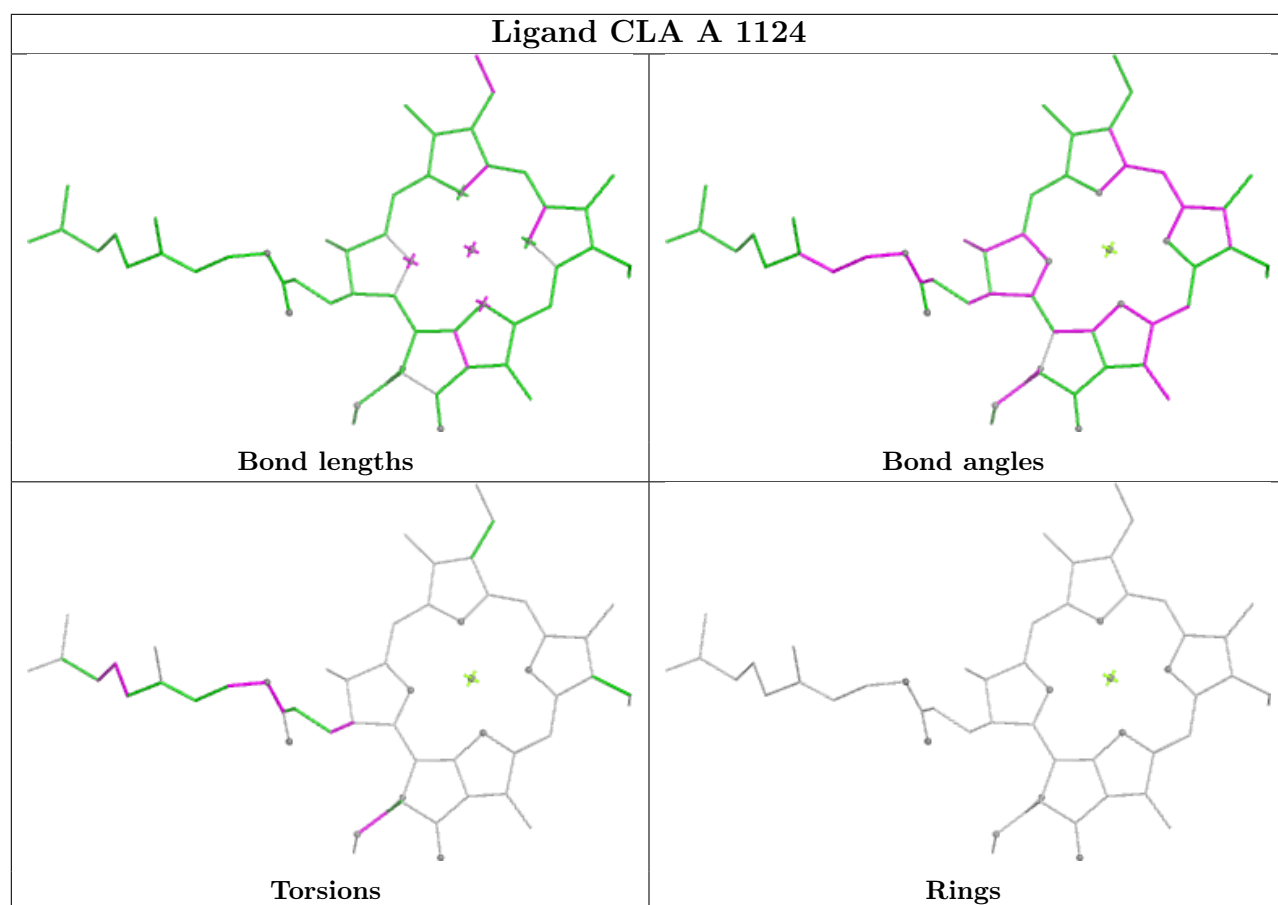


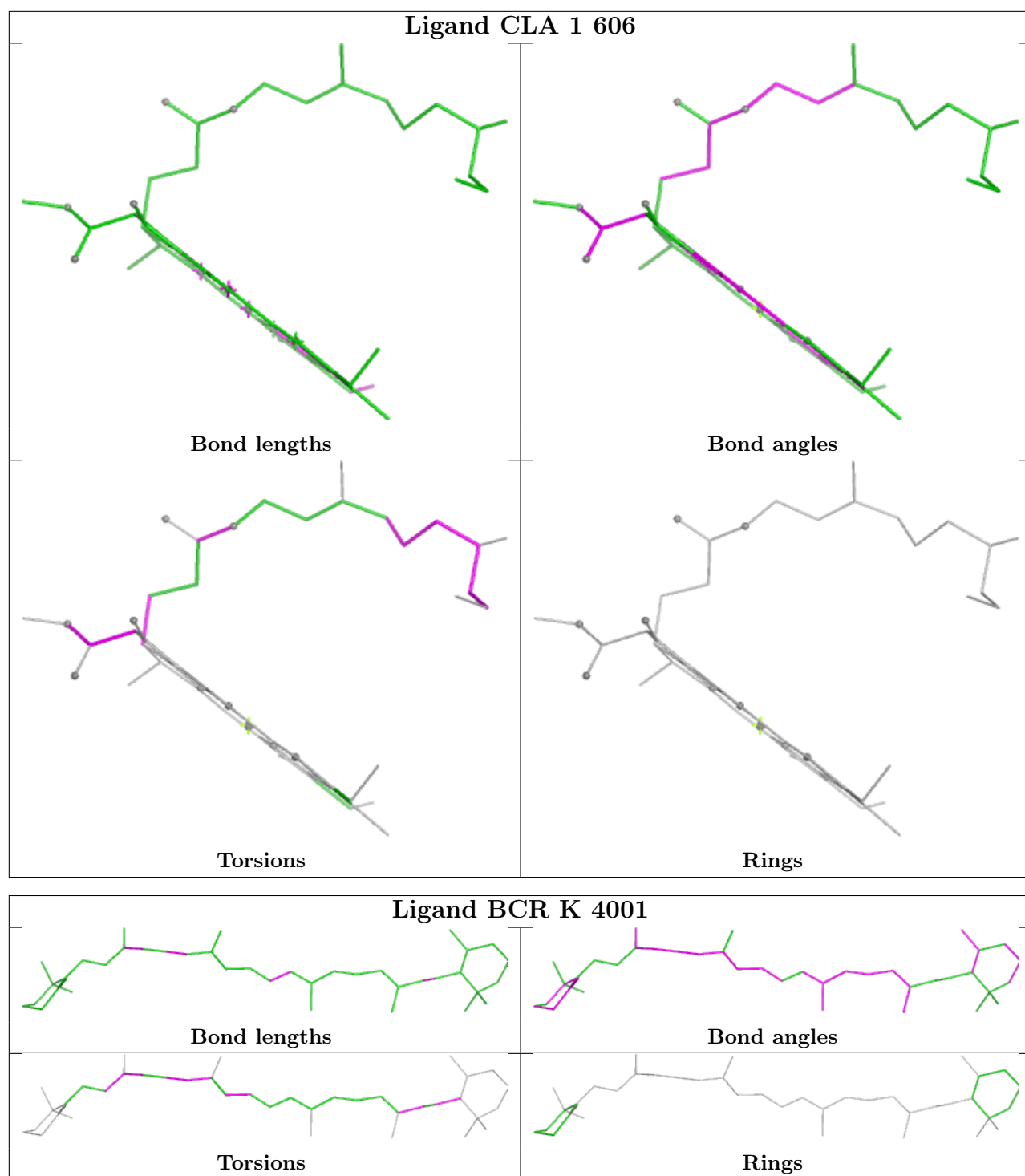
Ligand CLA 4 611

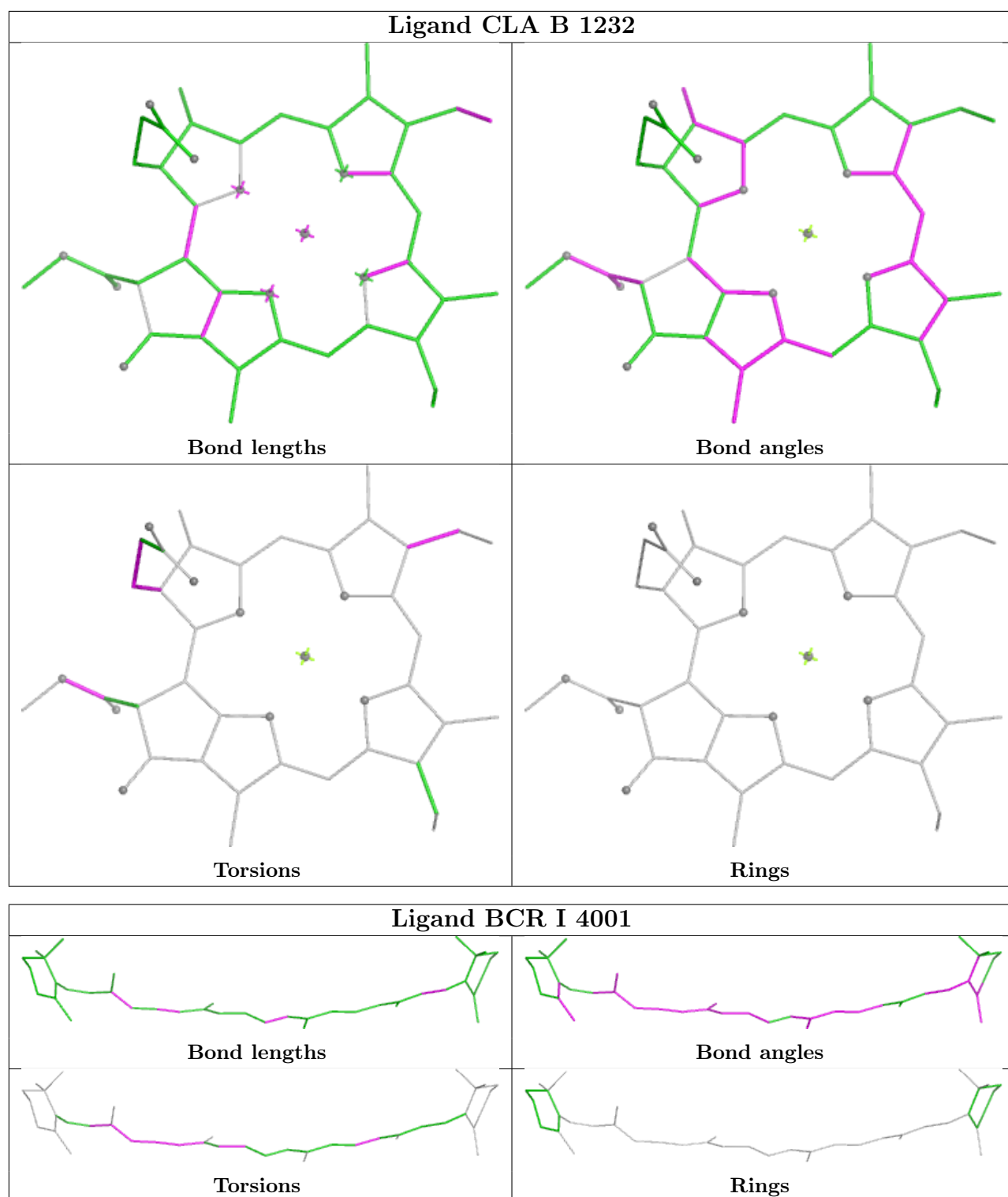


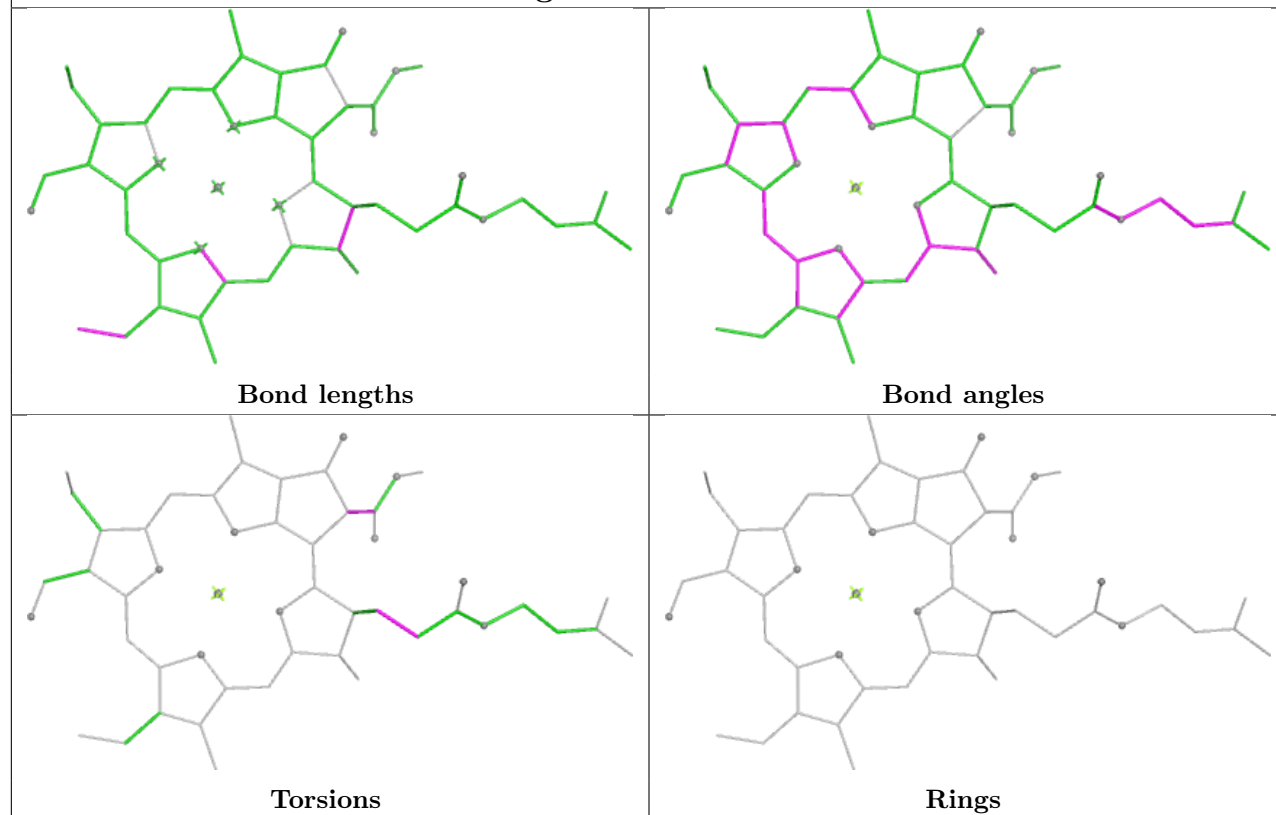
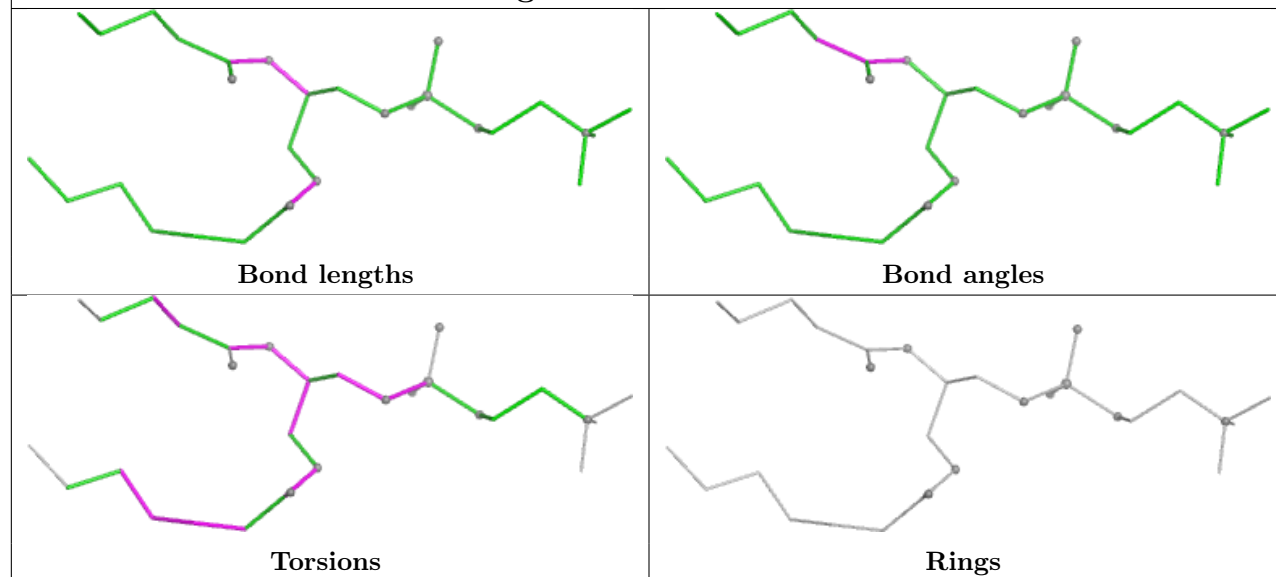


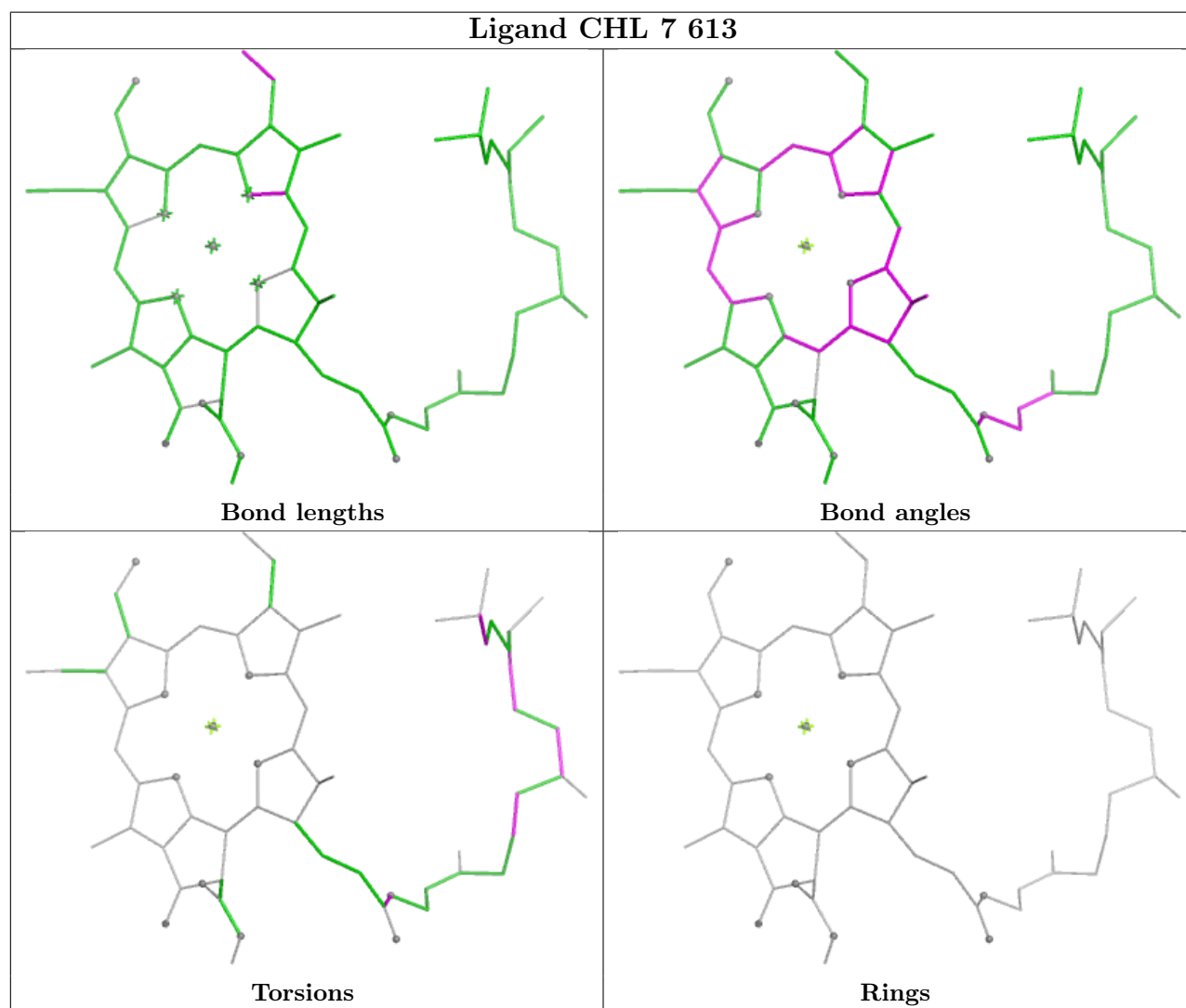
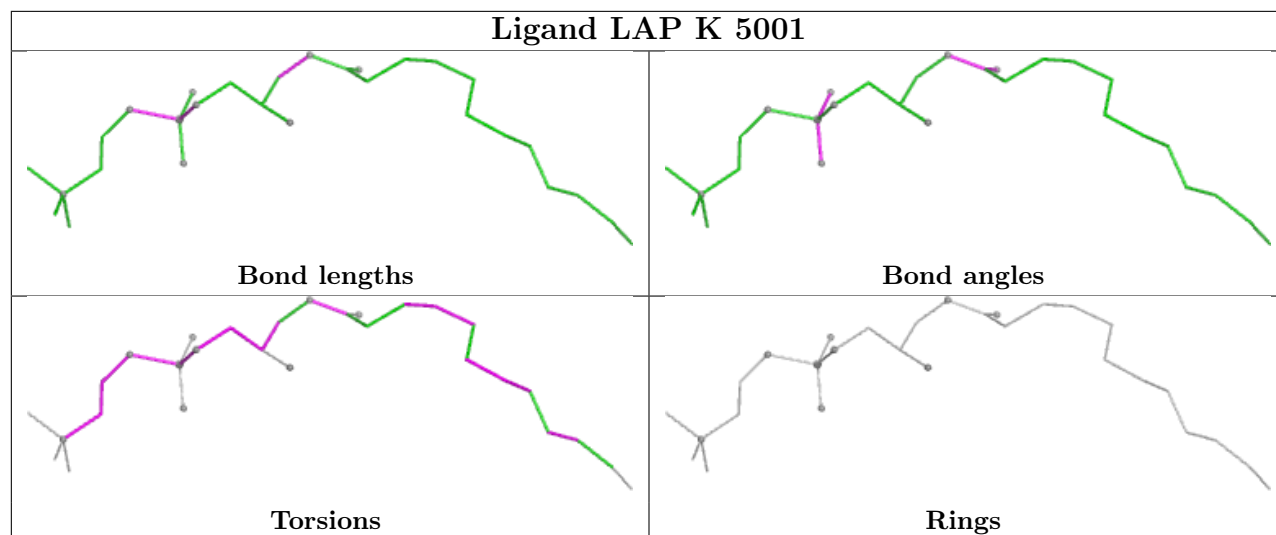


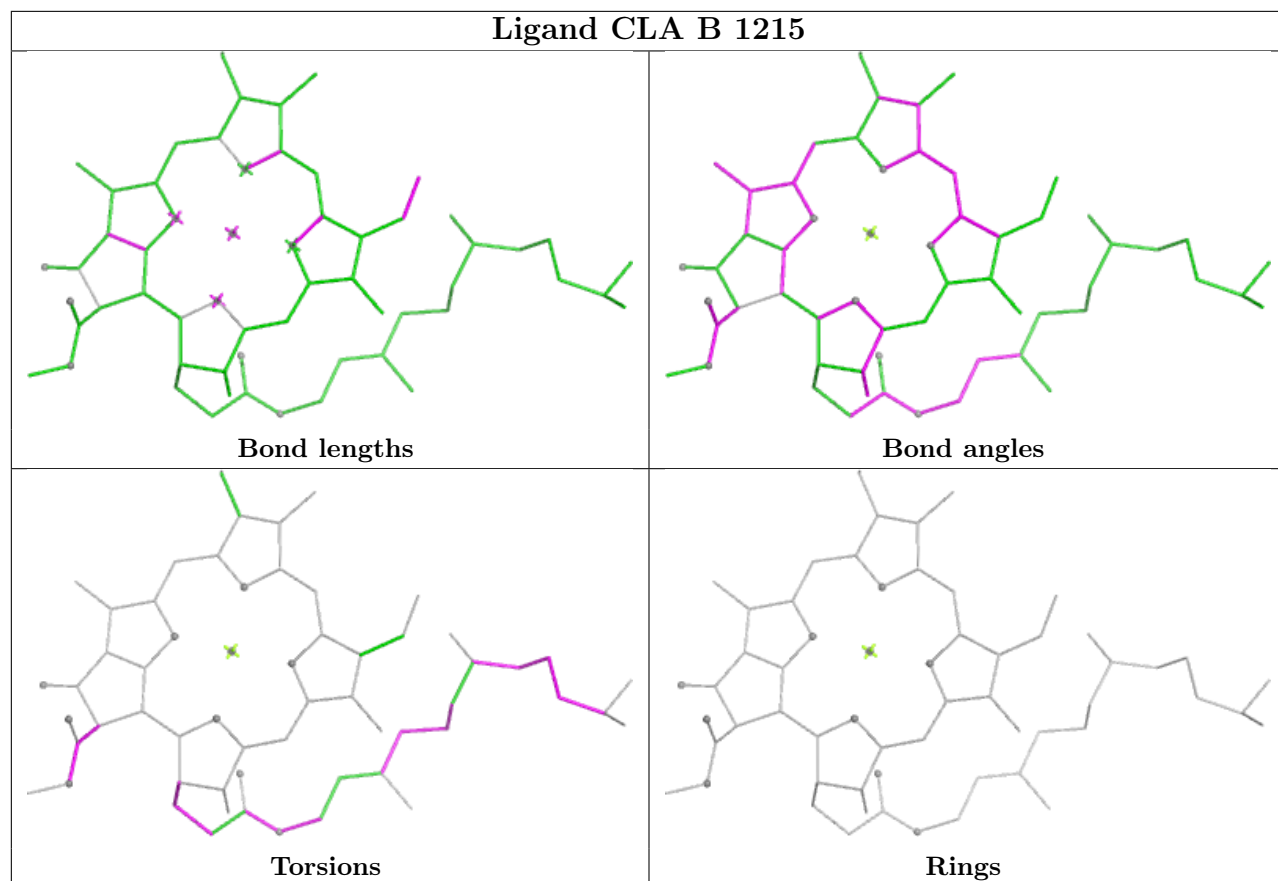




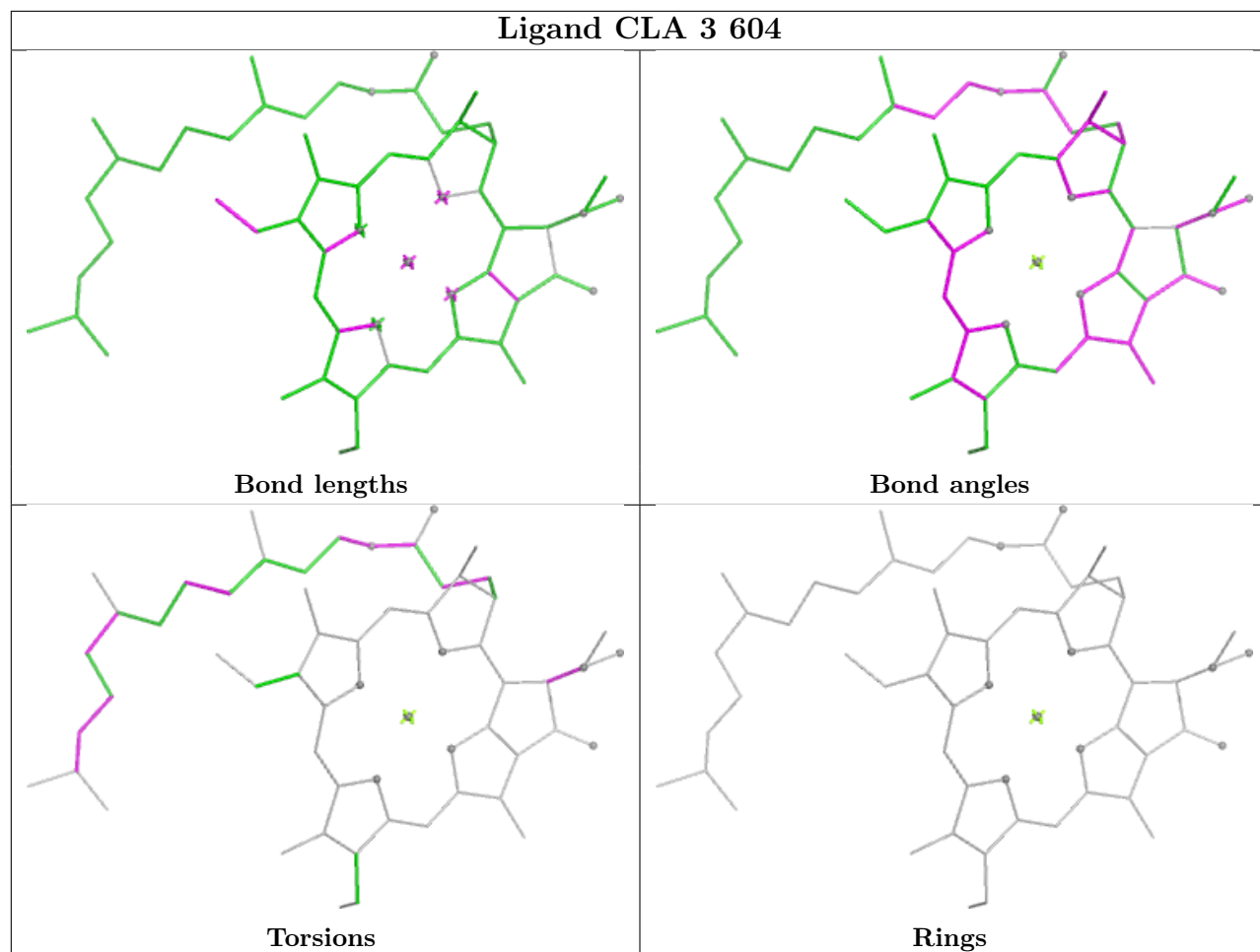


Ligand CHL 8 613**Ligand PCW B 5004**

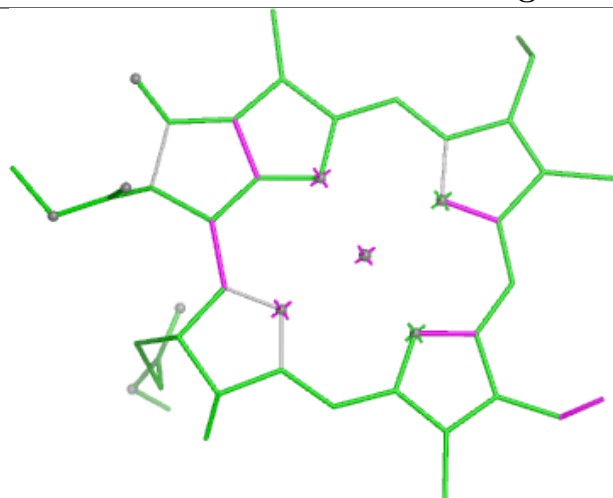




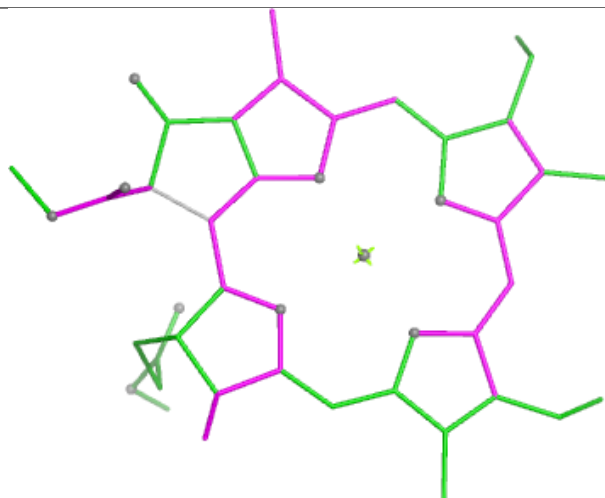
Ligand CLA 3 604



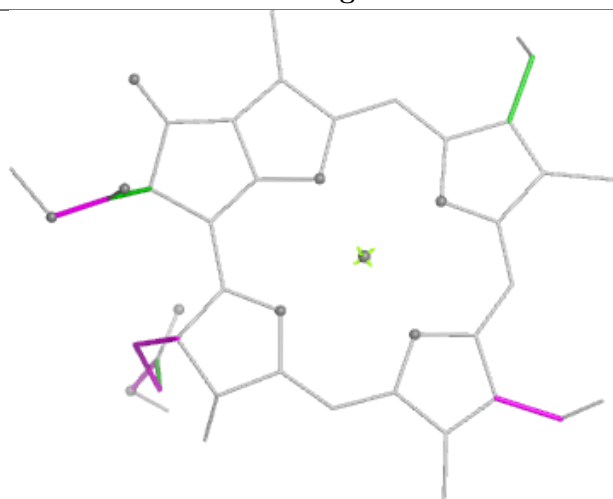
Ligand CLA 5 616



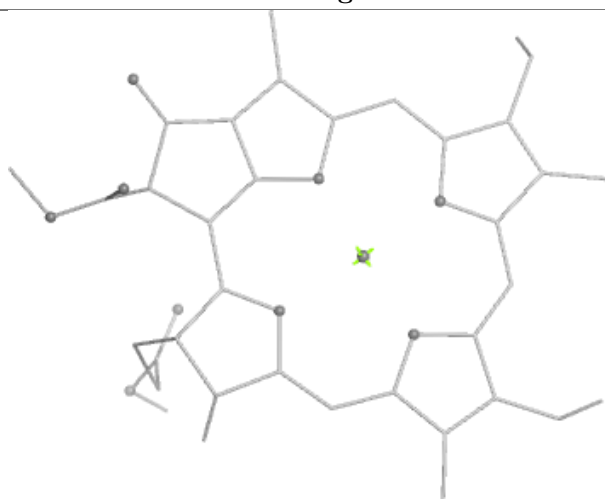
Bond lengths



Bond angles

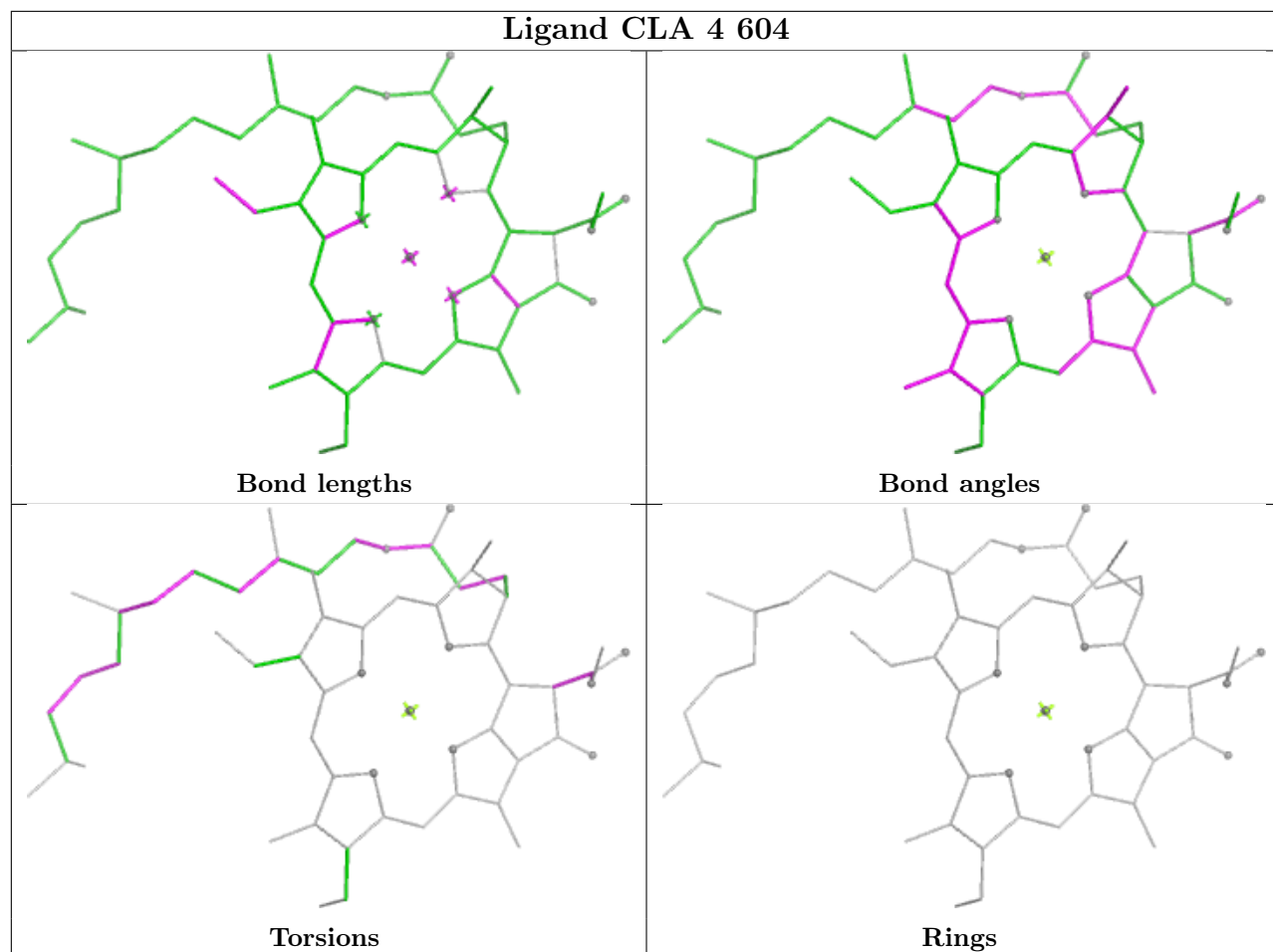


Torsions

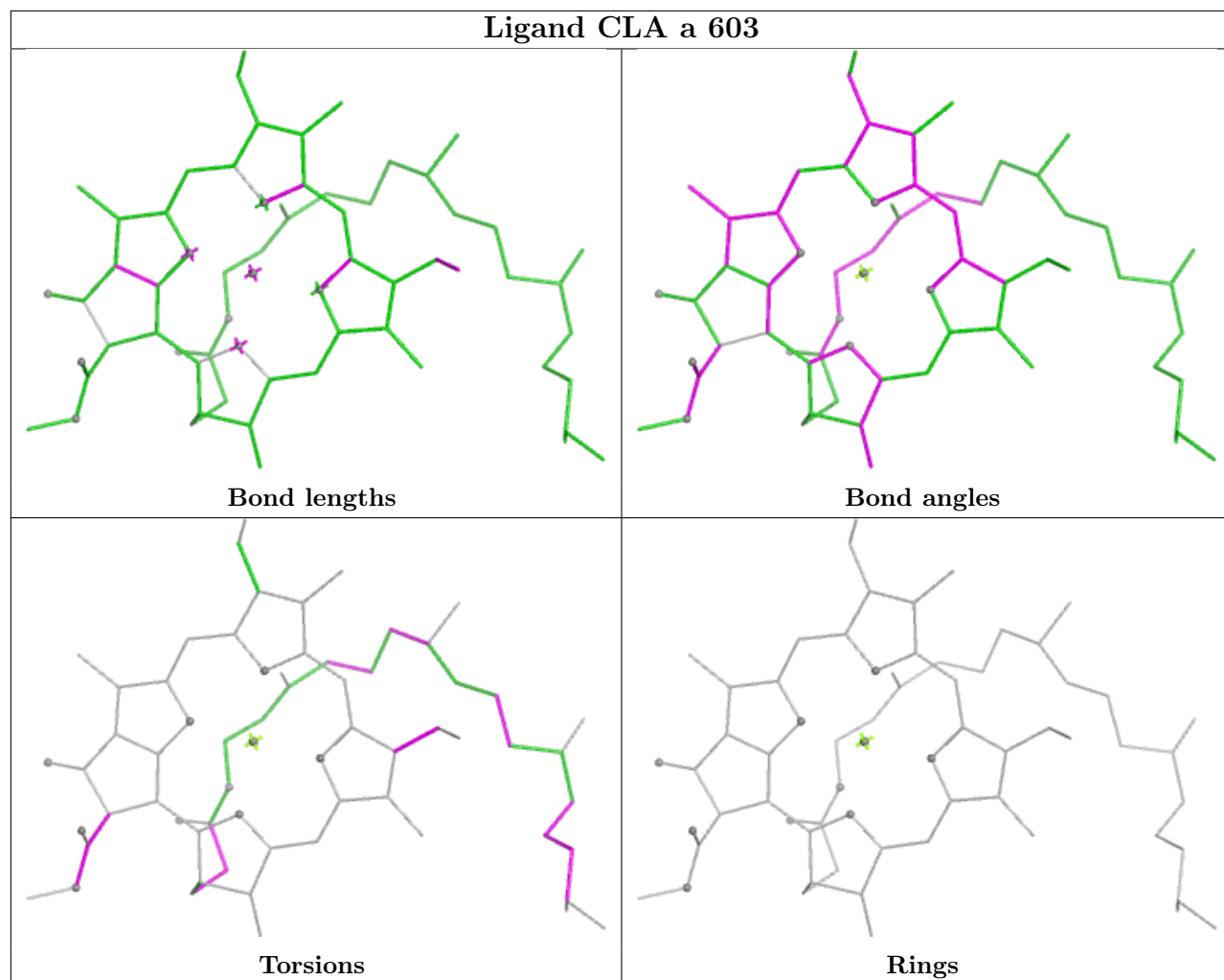


Rings

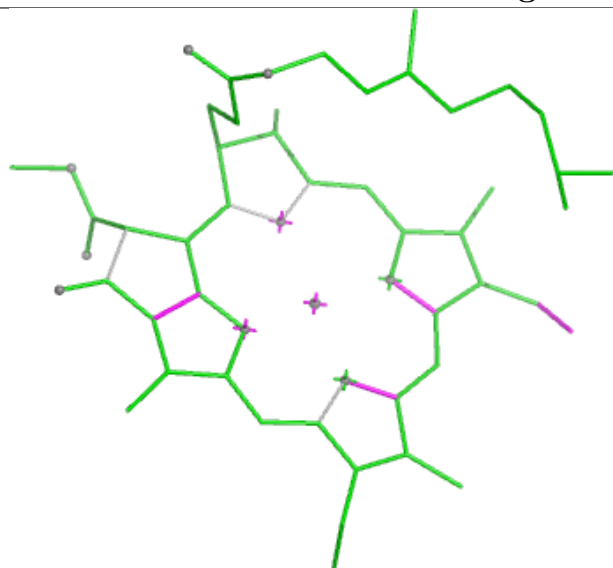
Ligand CLA 4 604



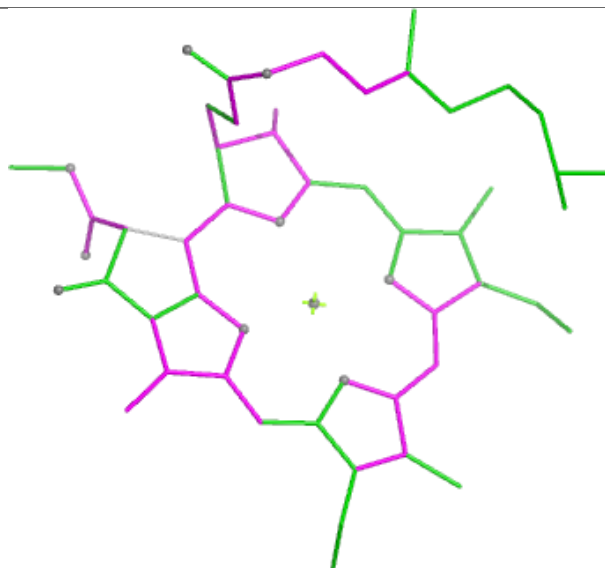
Ligand CLA a 603



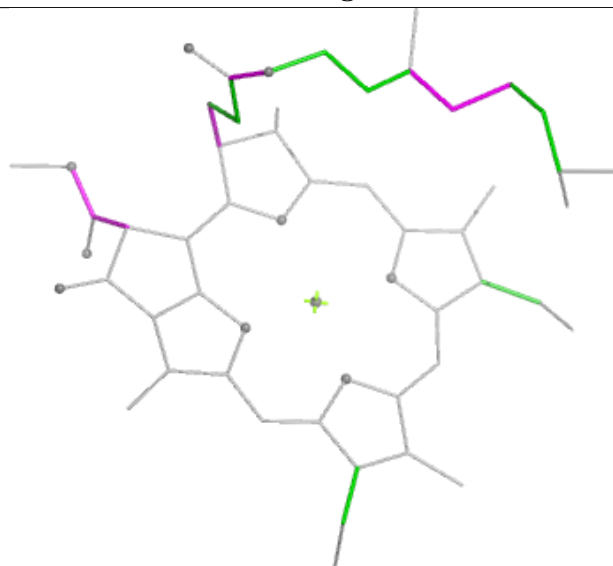
Ligand CLA 7 610



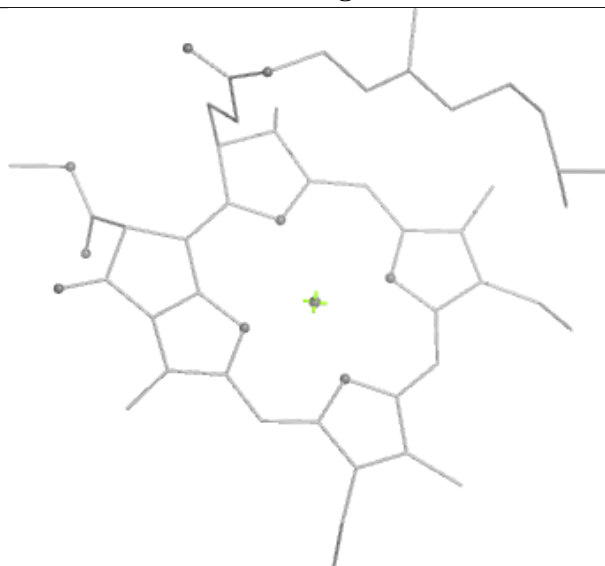
Bond lengths



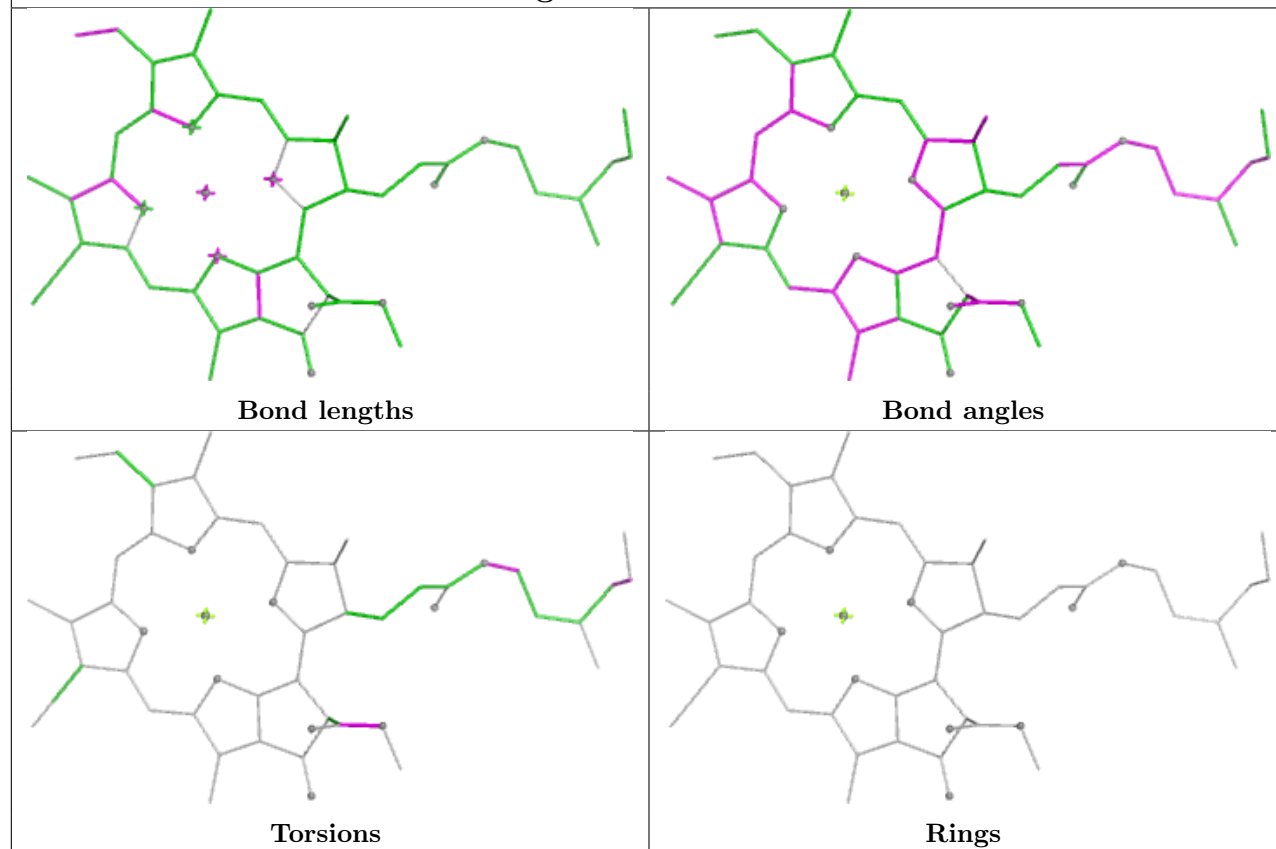
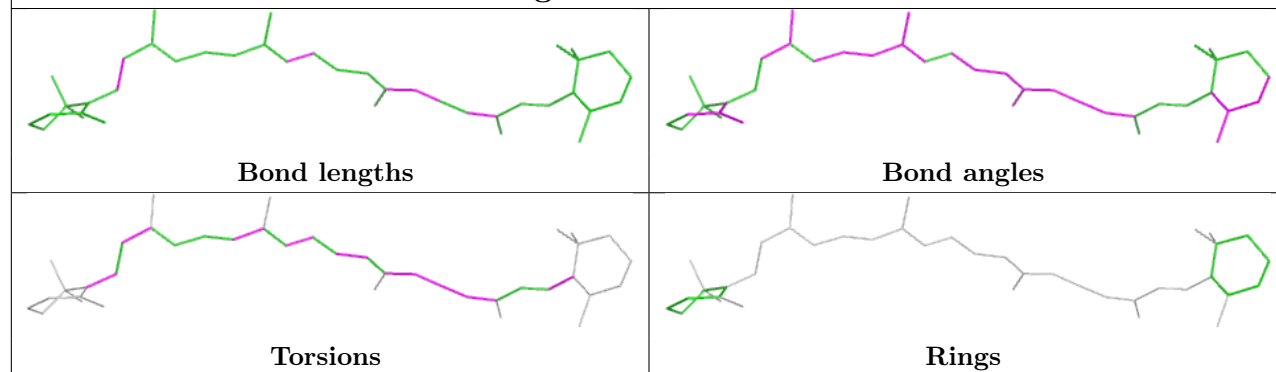
Bond angles

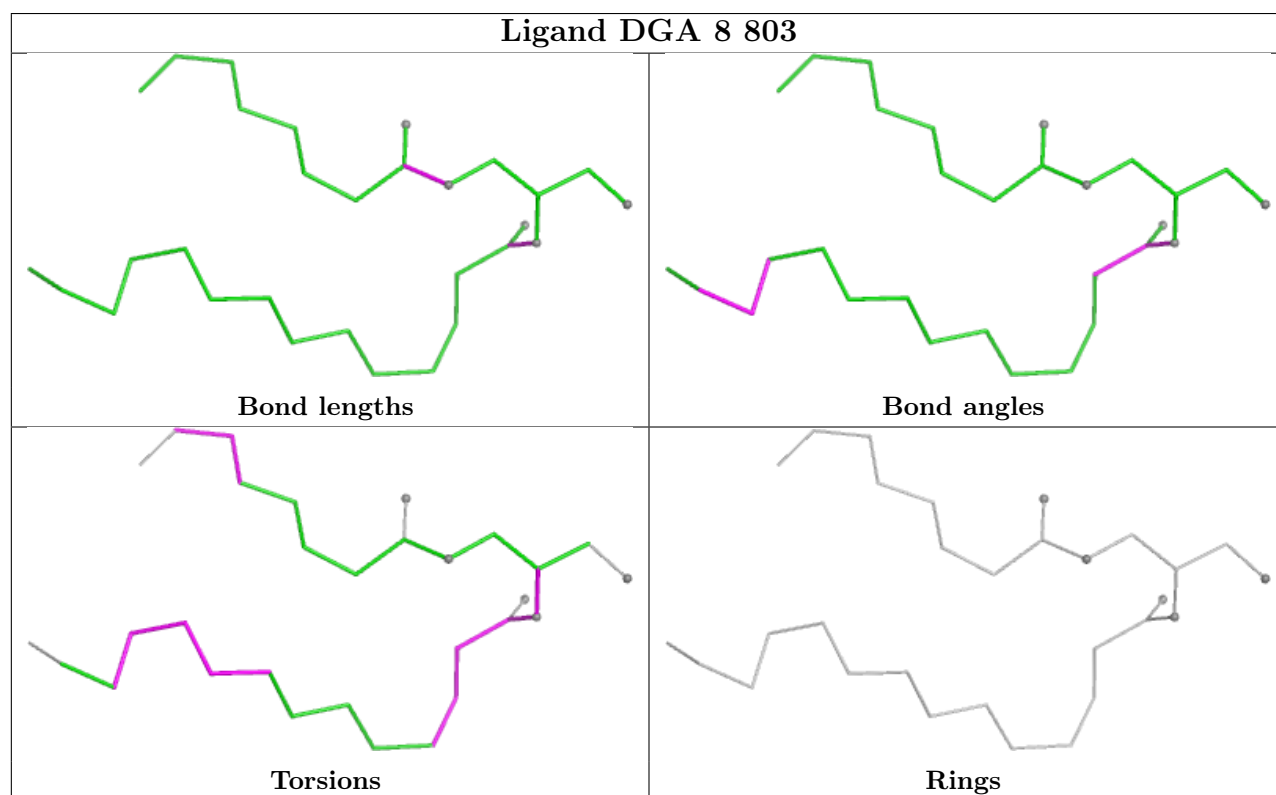
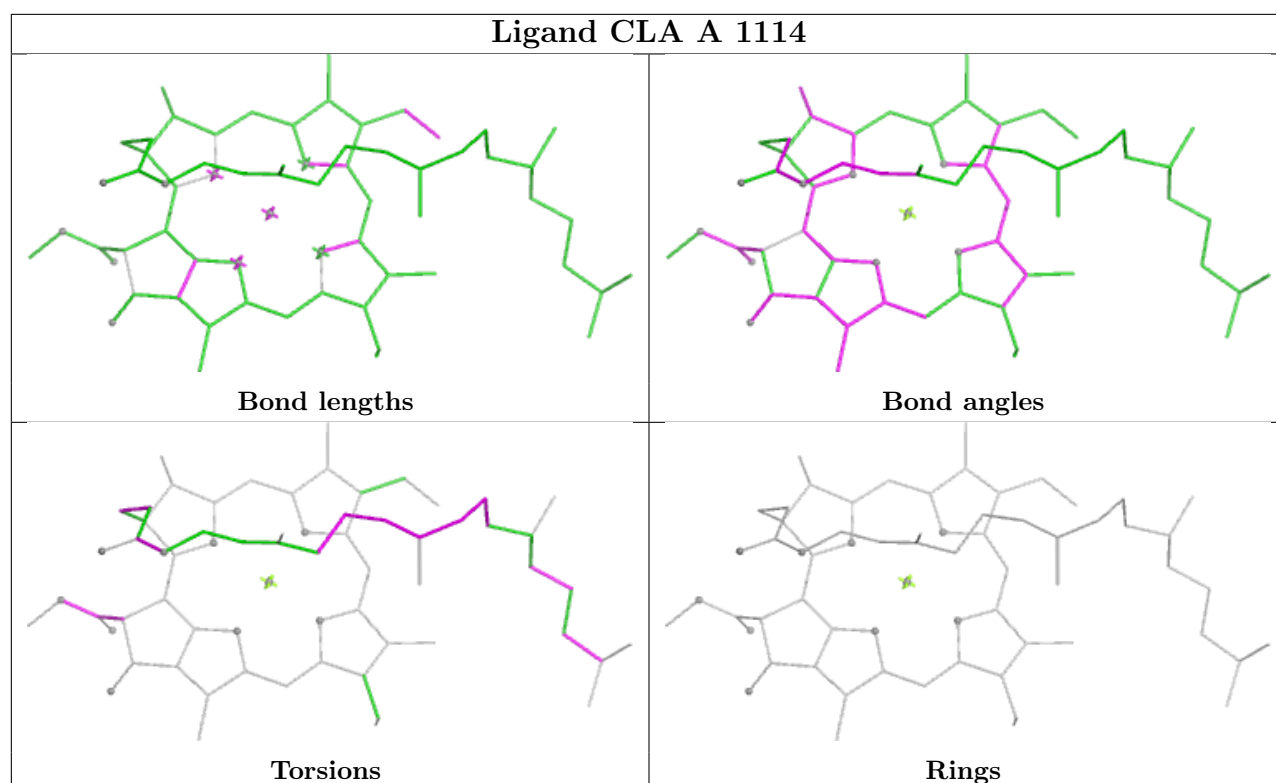


Torsions

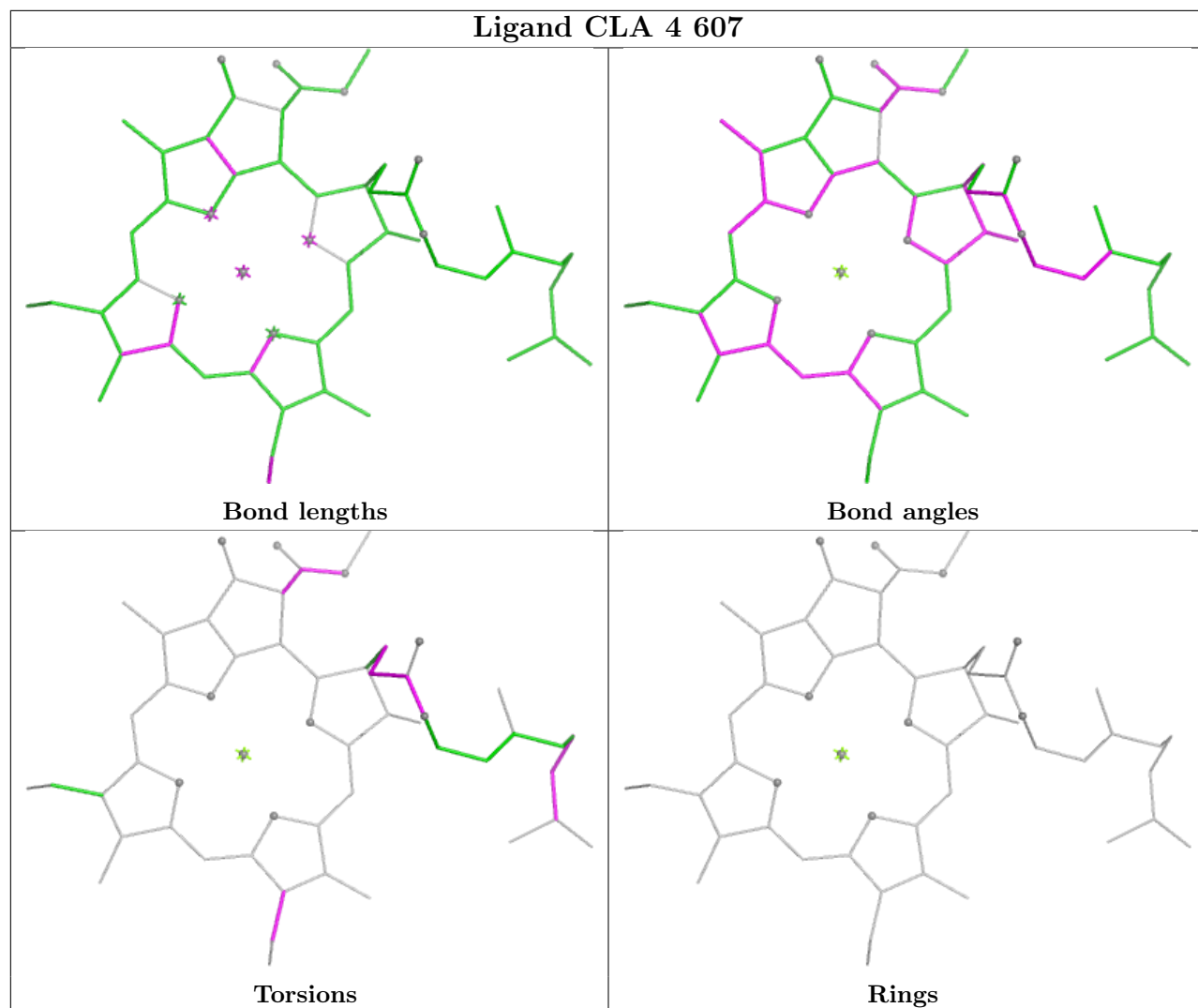


Rings

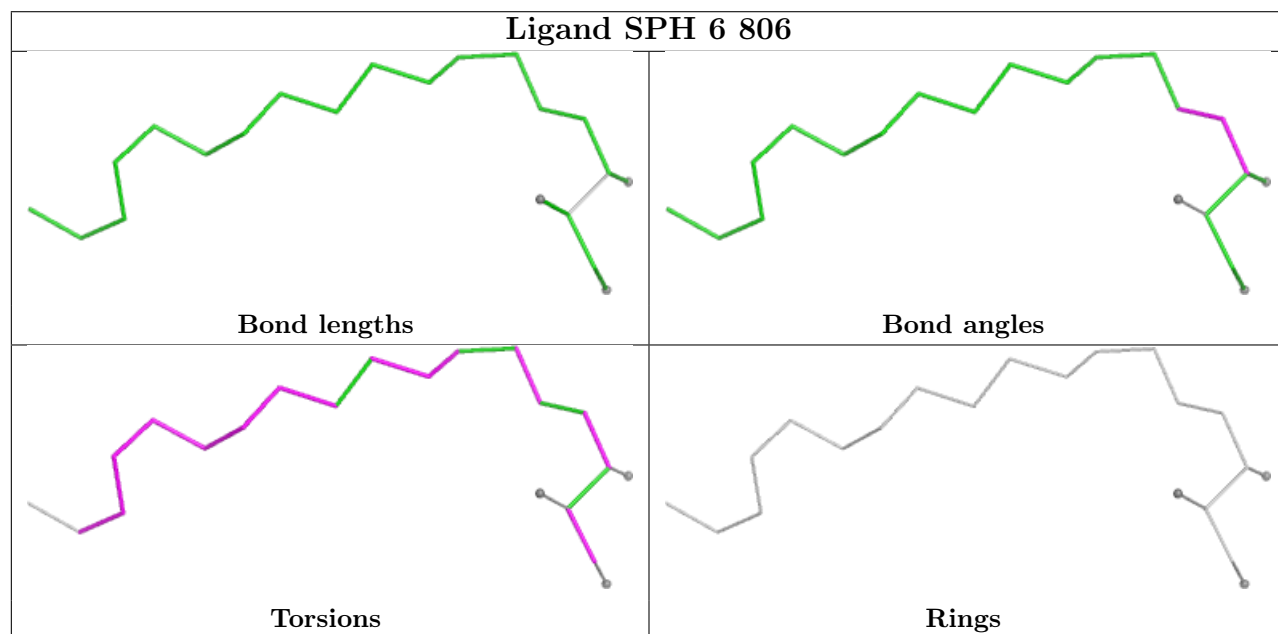
Ligand CLA 5 618**Ligand BCR 5 503**

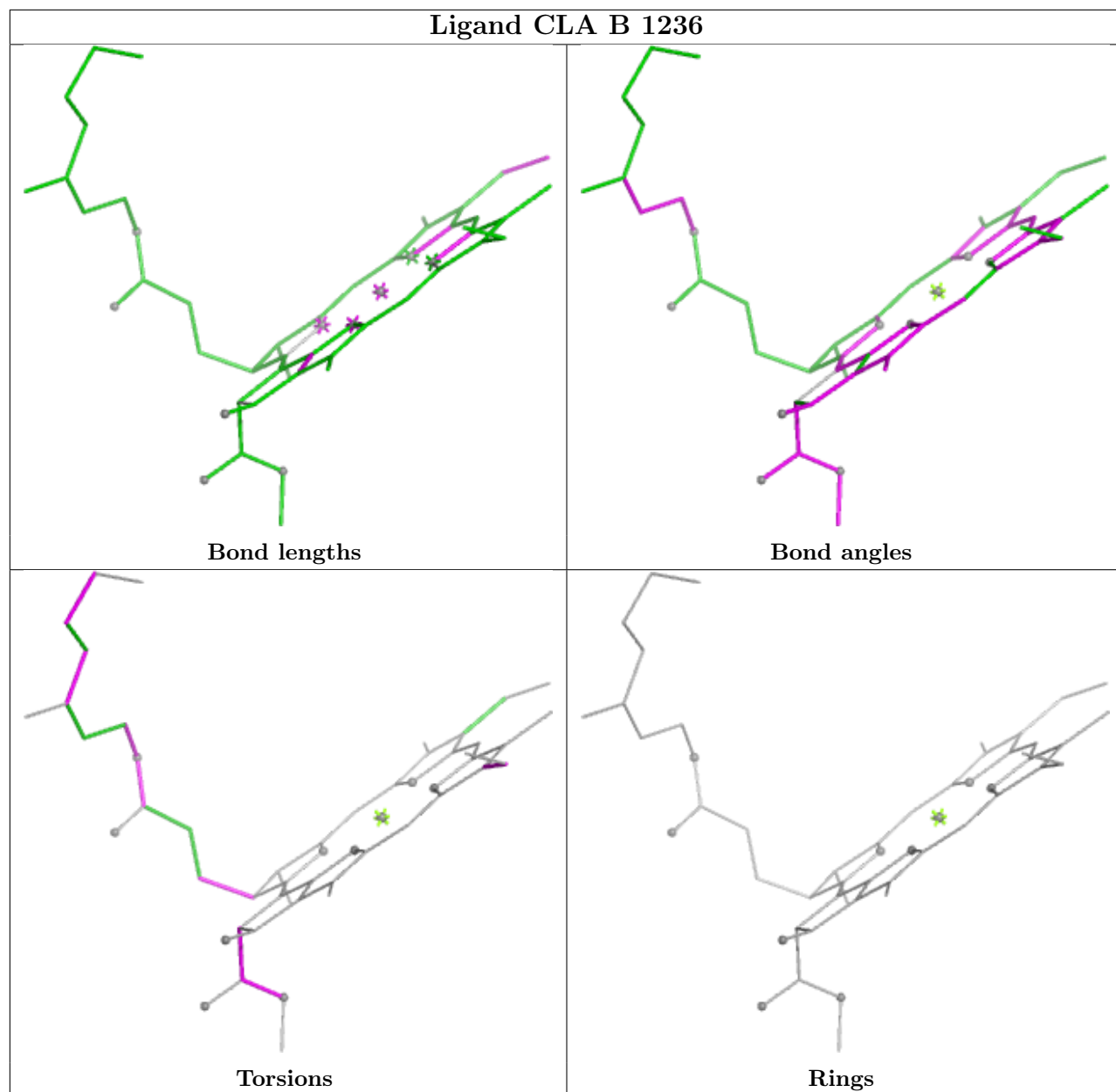


Ligand CLA 4 607

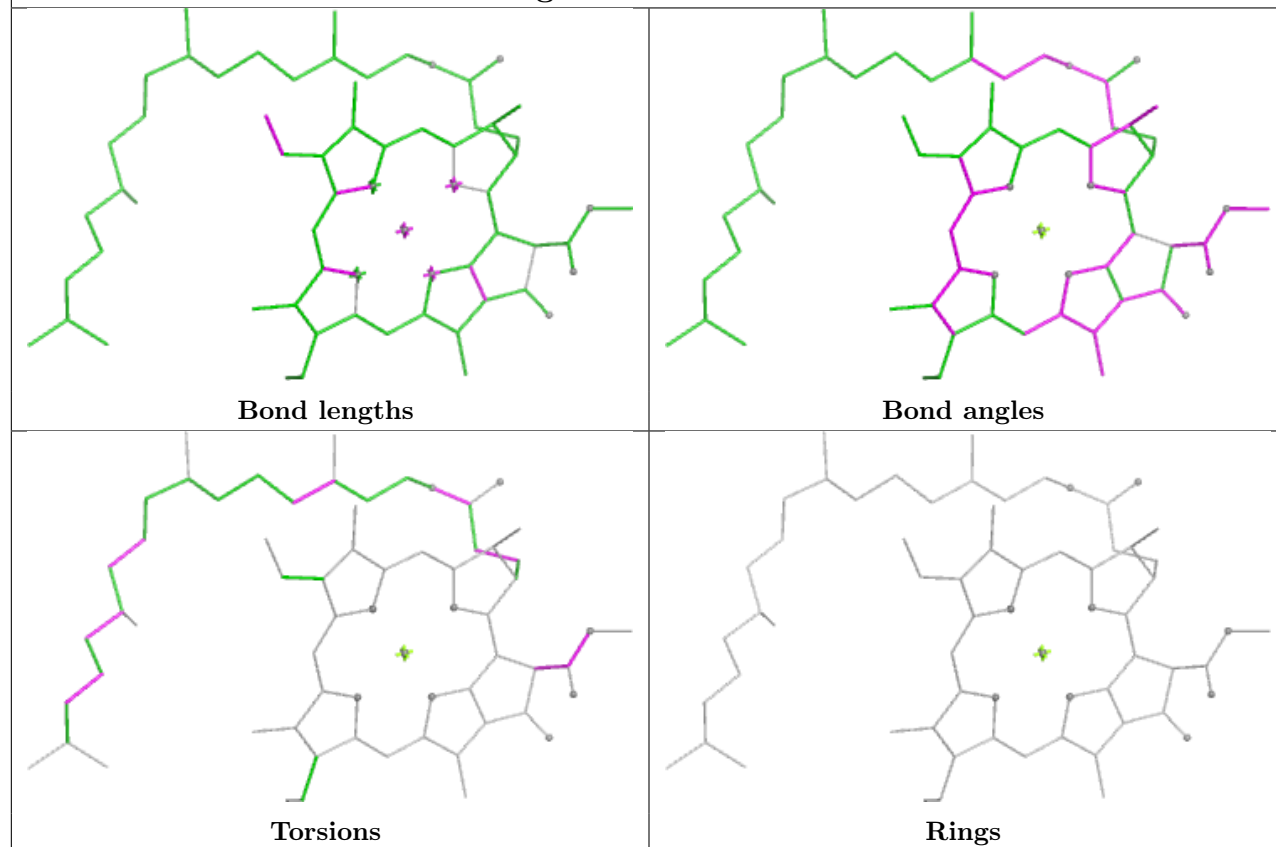


Ligand SPH 6 806

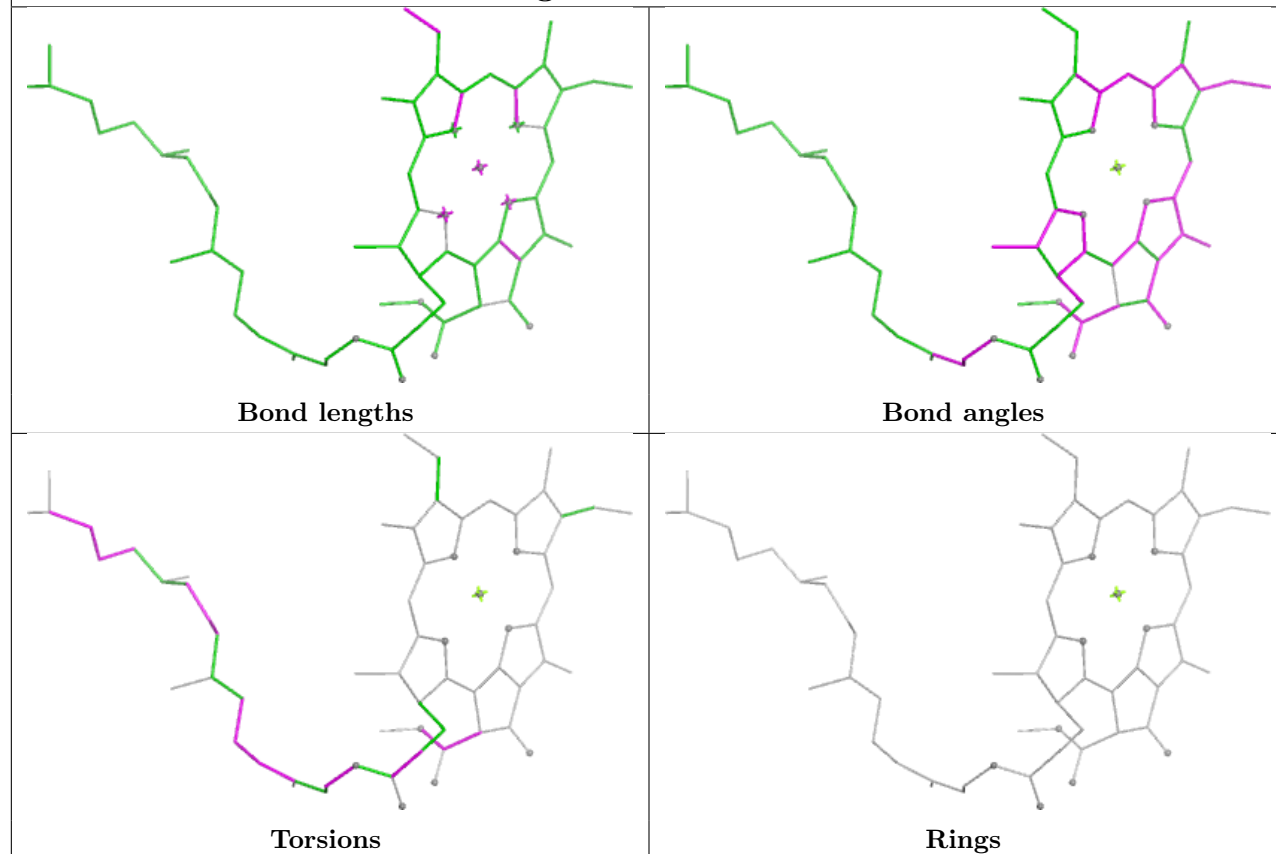


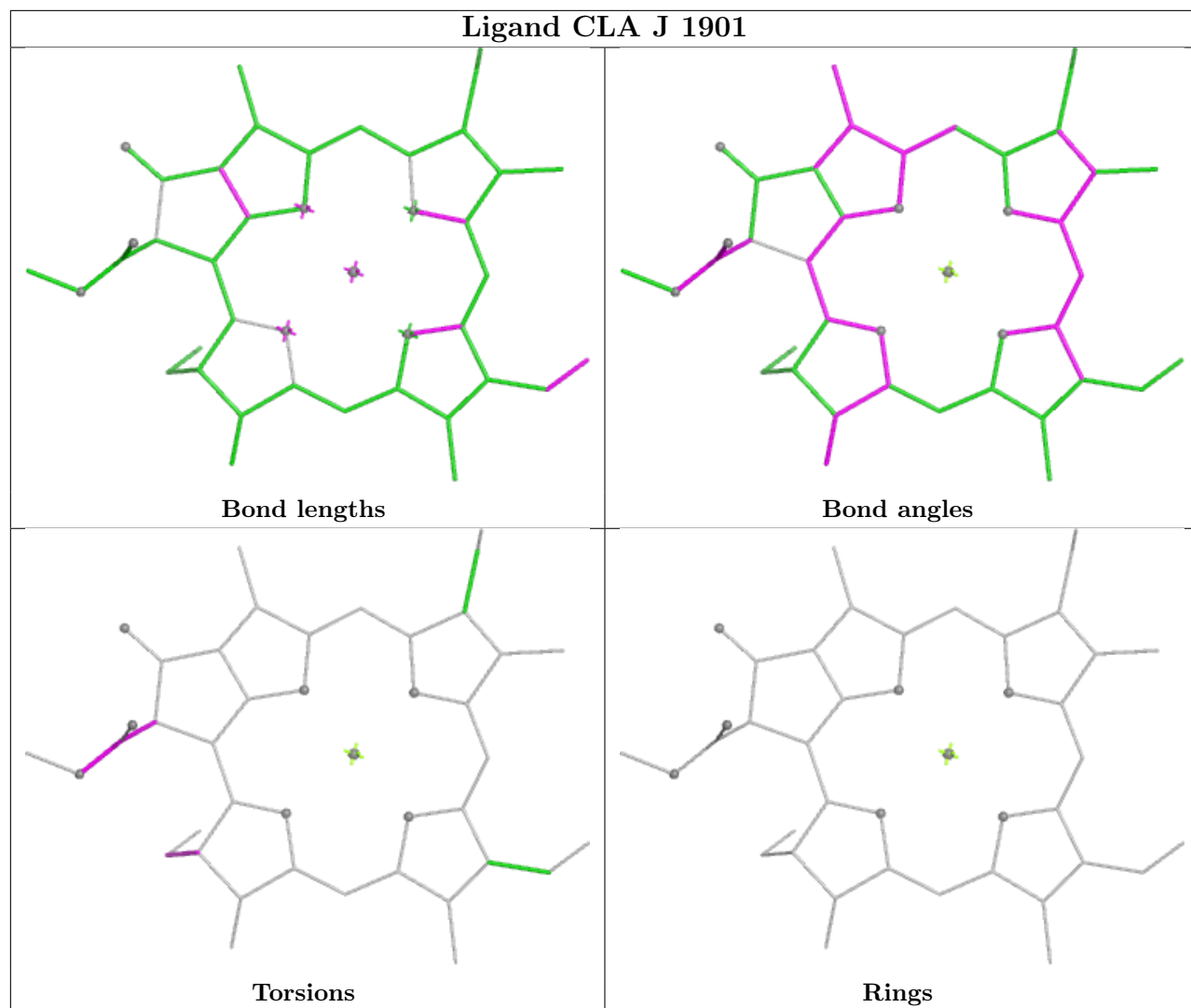


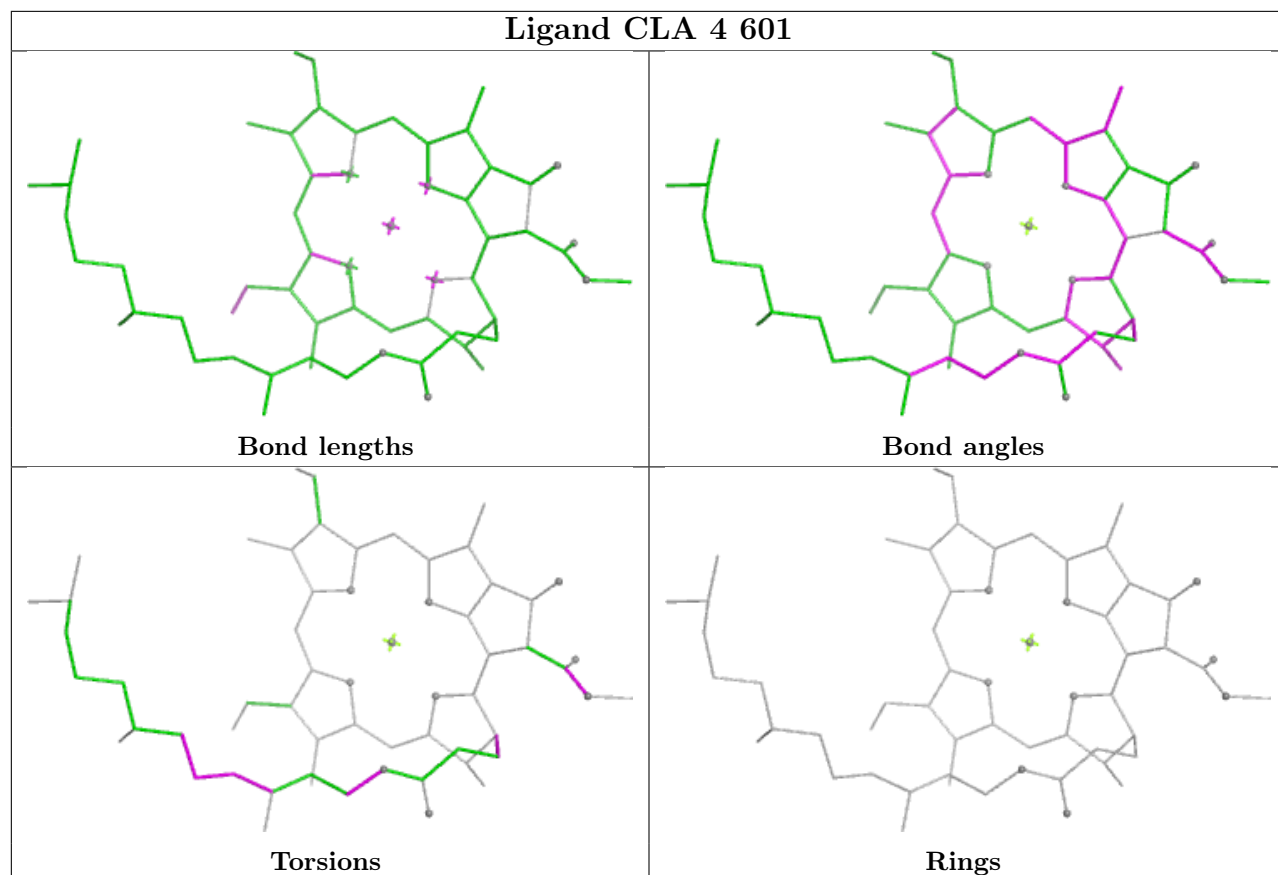
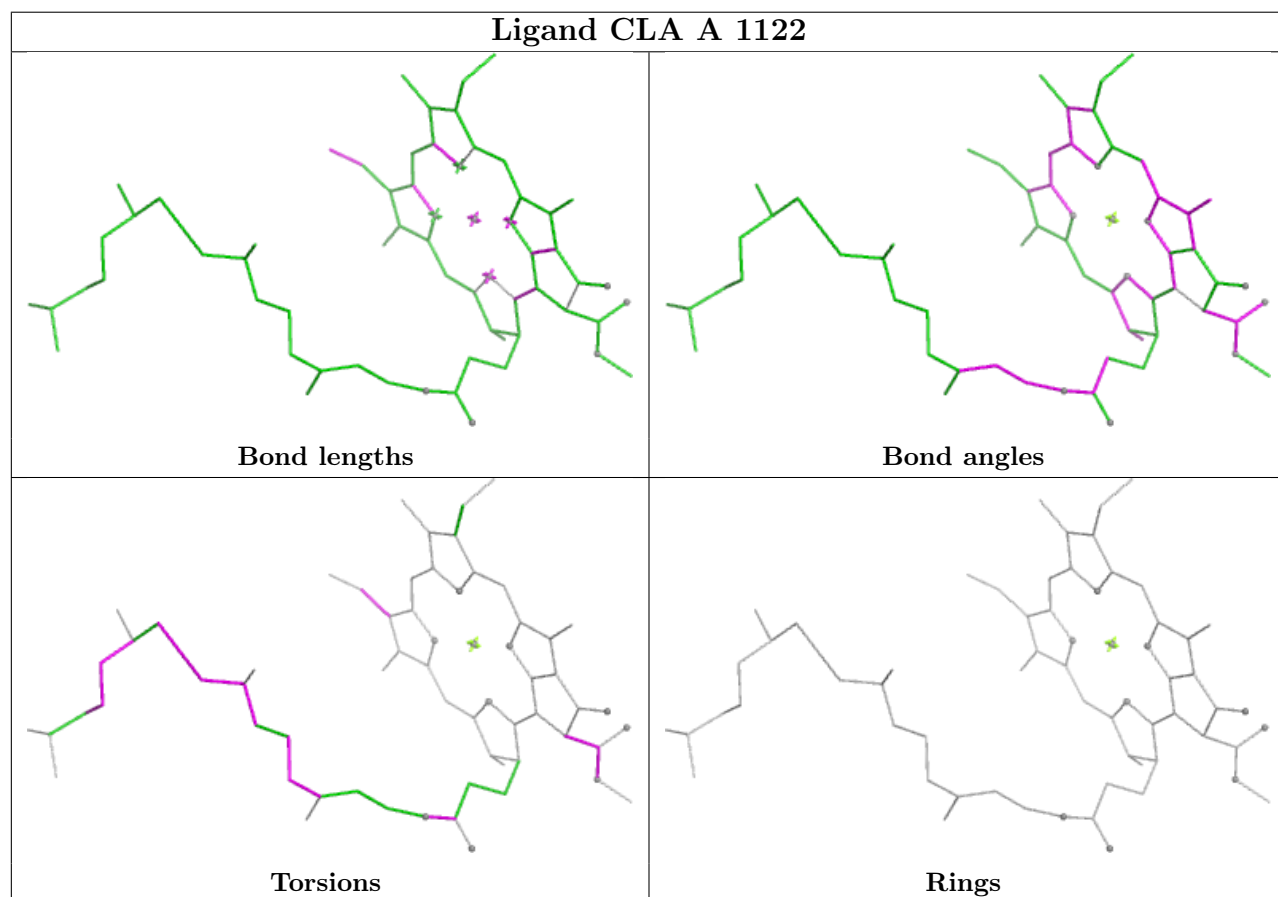
Ligand CLA 5 604

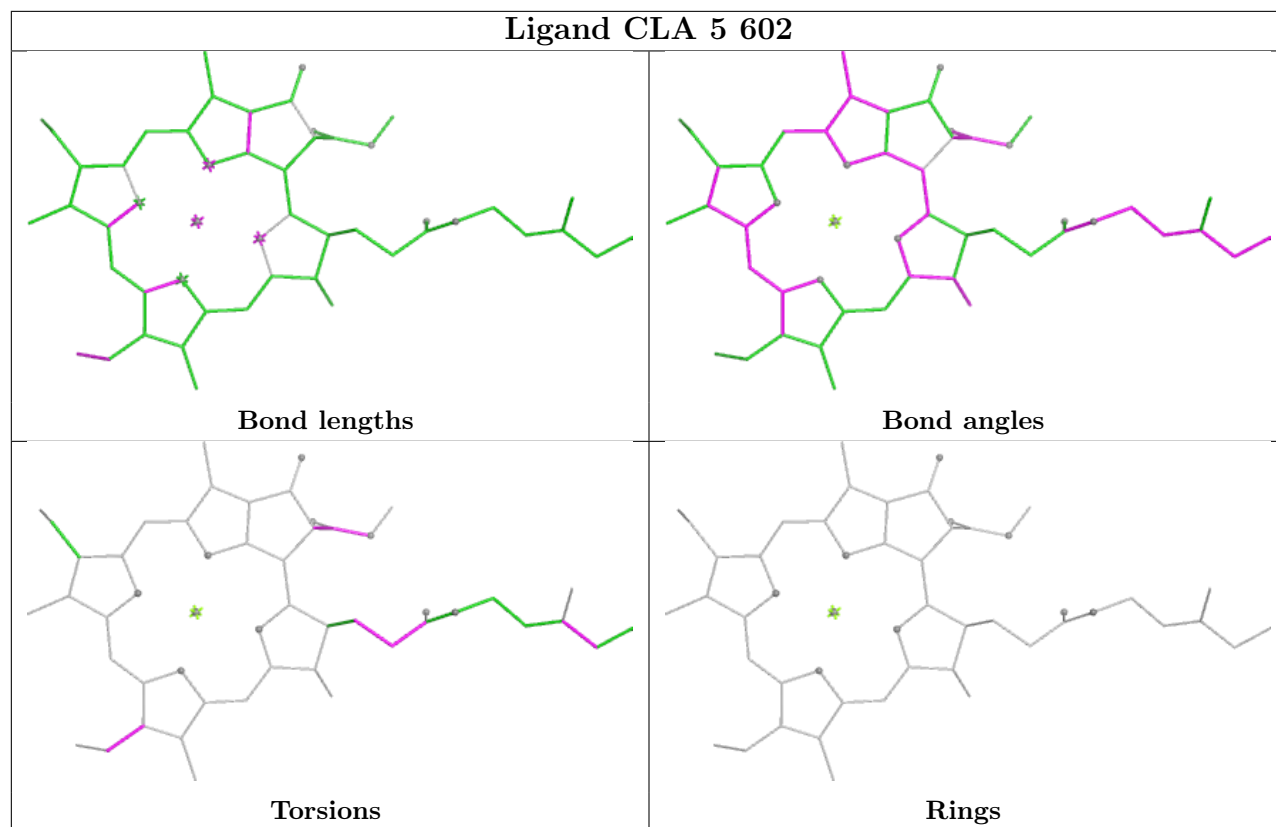


Ligand CLA 1 605

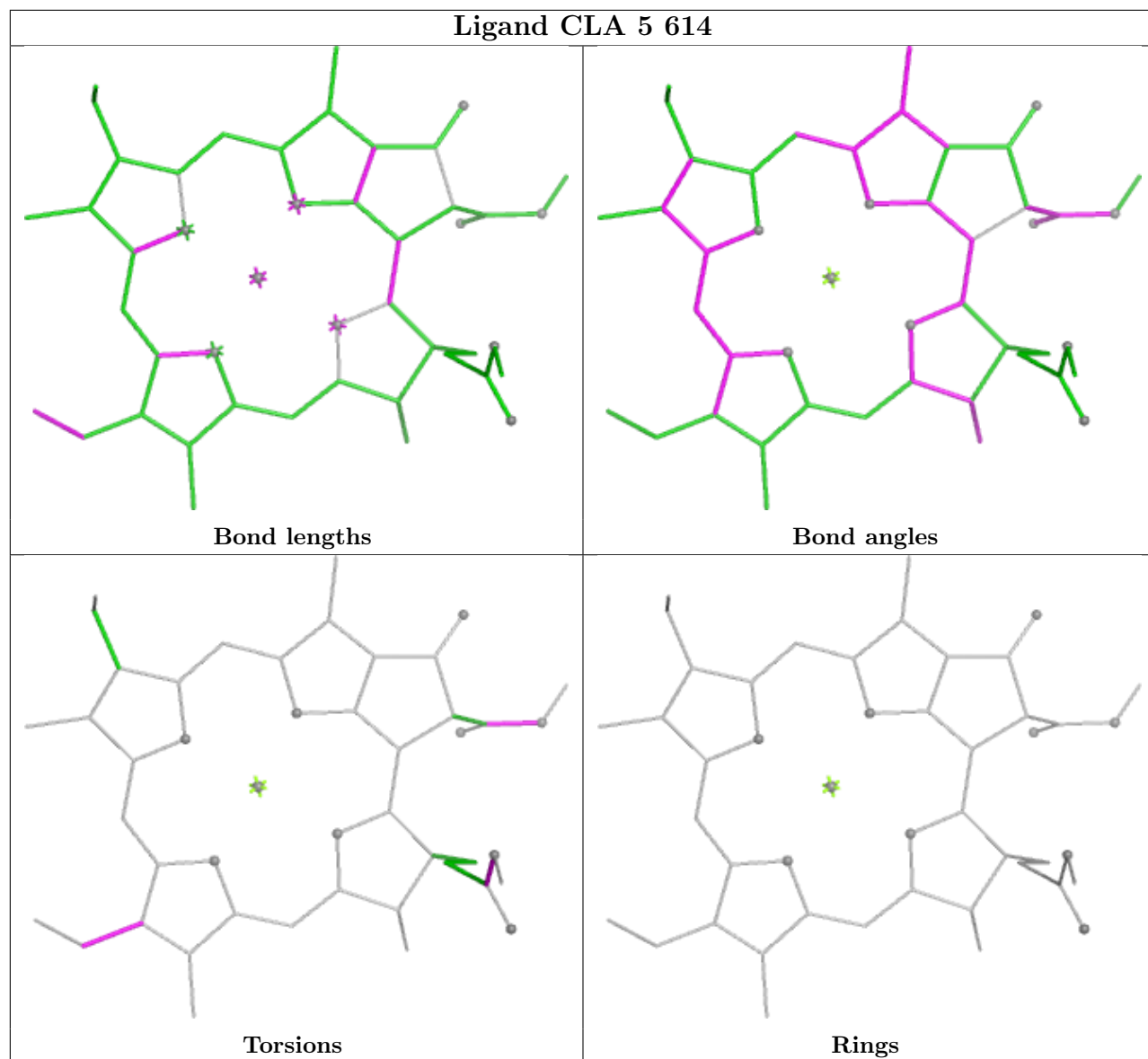




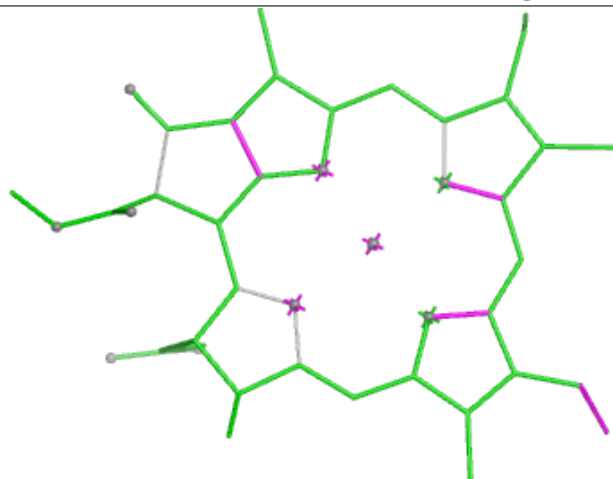
Ligand CLA 4 601**Ligand CLA A 1122**



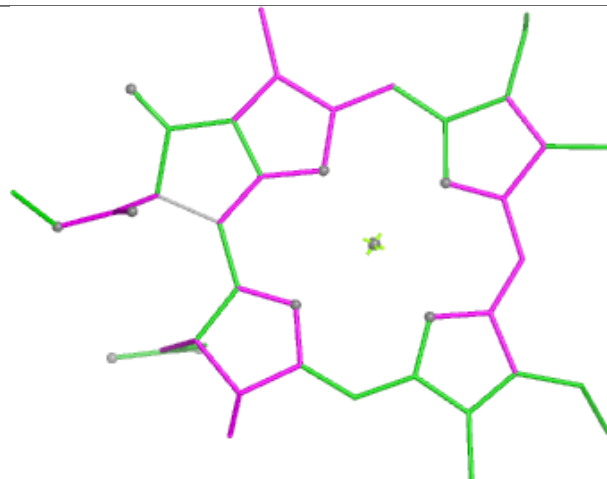
Ligand CLA 5 614



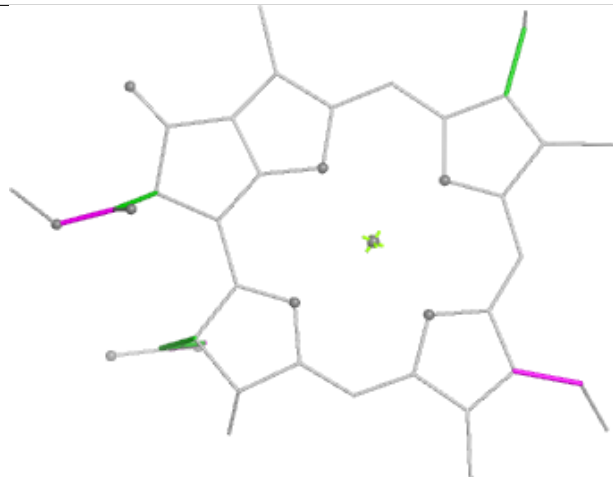
Ligand CLA 6 608



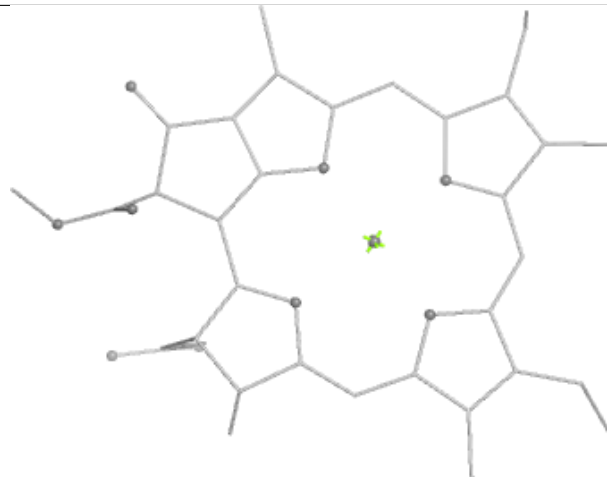
Bond lengths



Bond angles

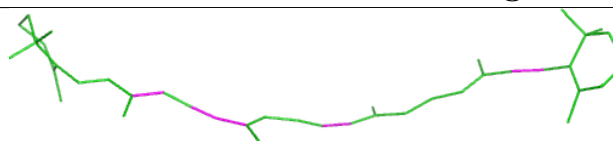


Torsions

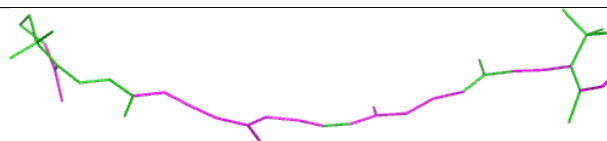


Rings

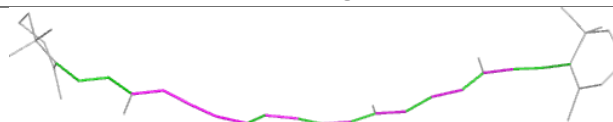
Ligand BCR B 4006



Bond lengths



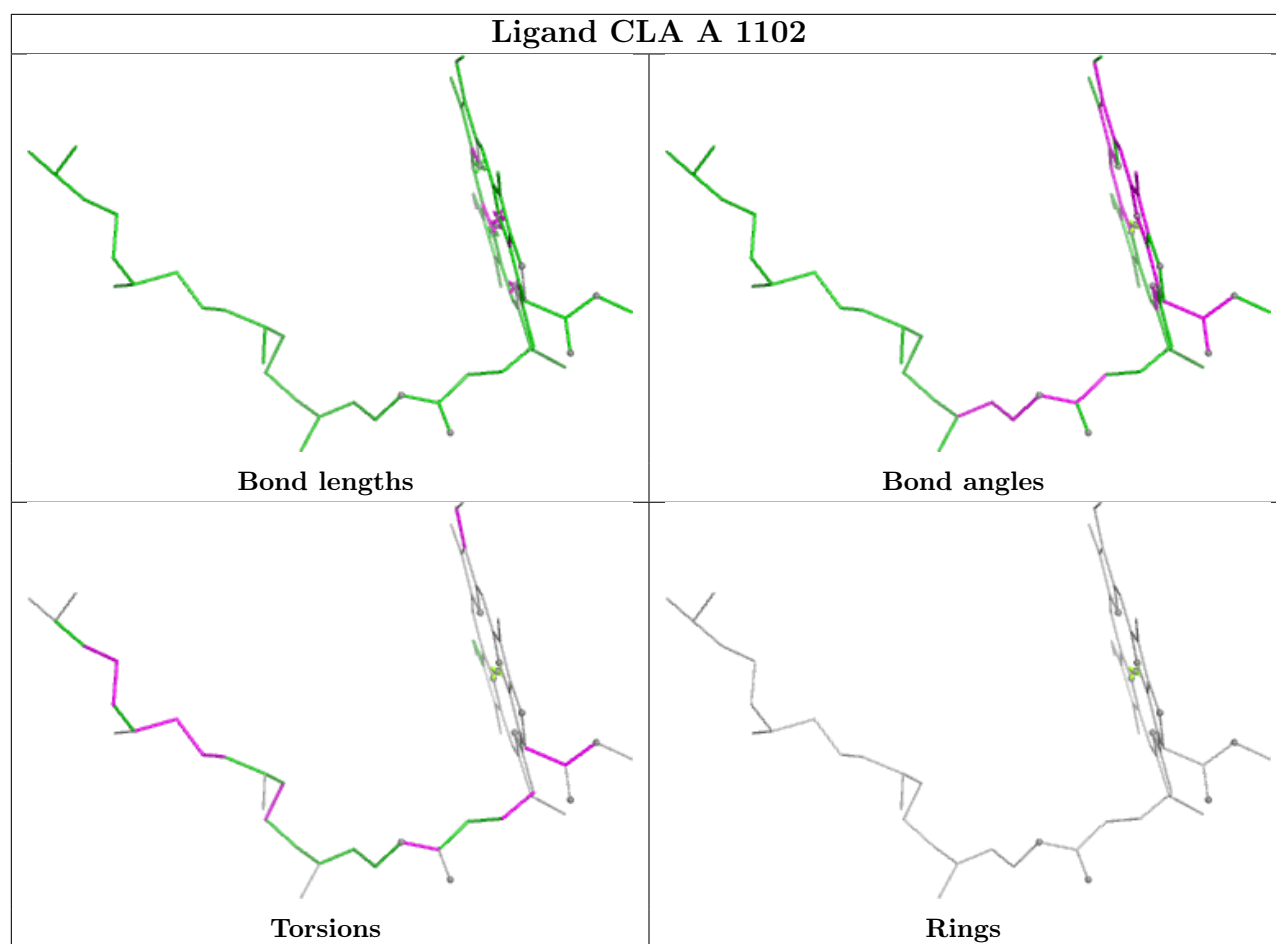
Bond angles



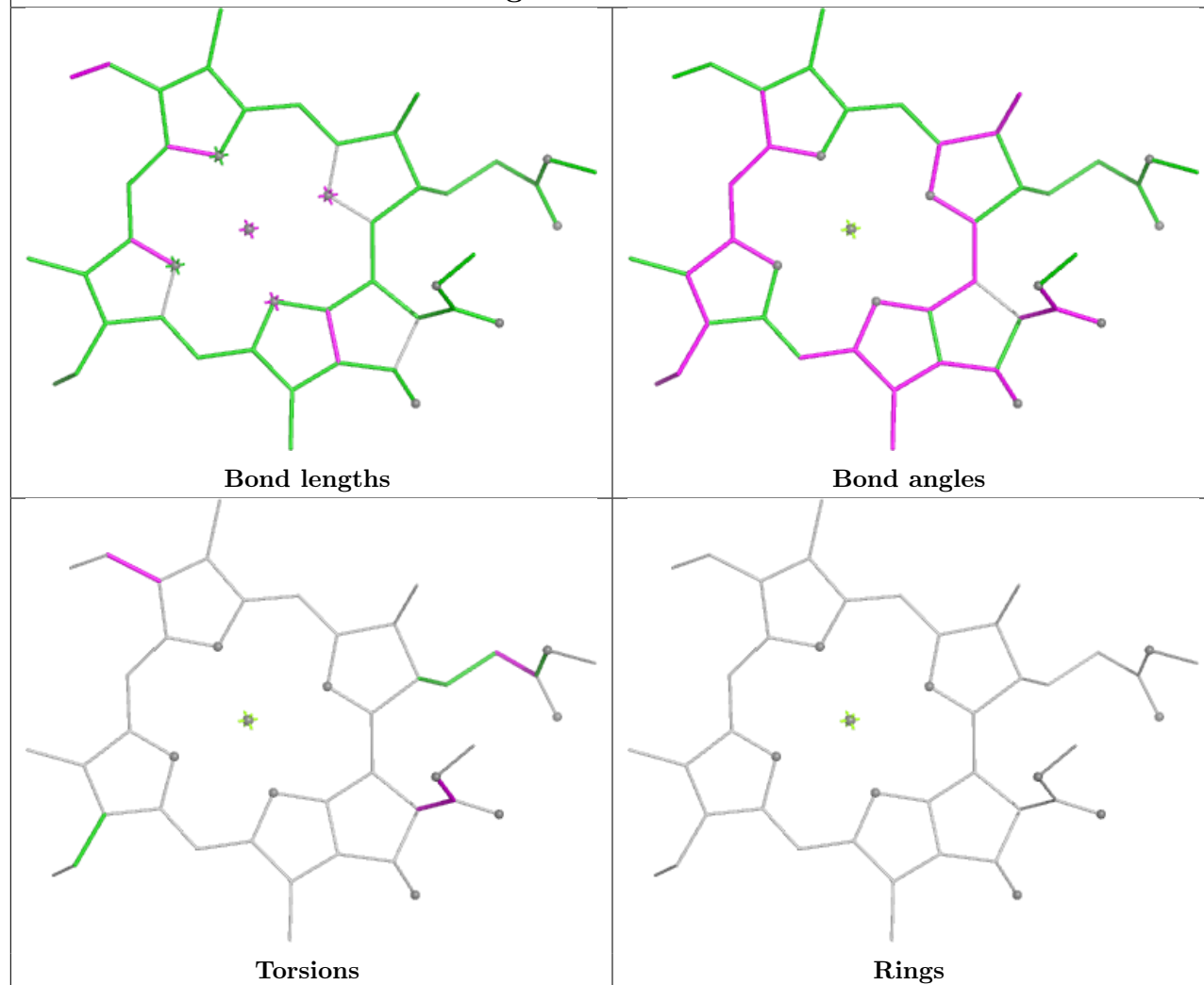
Torsions



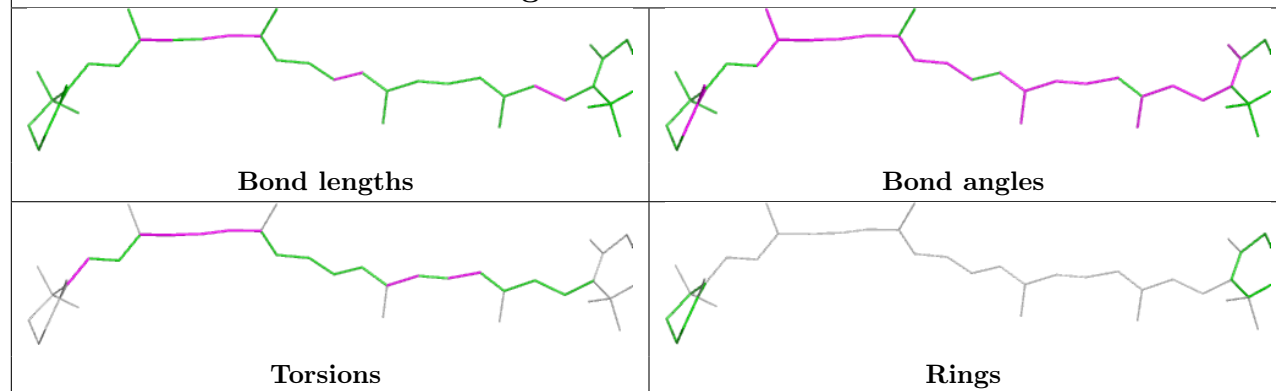
Rings

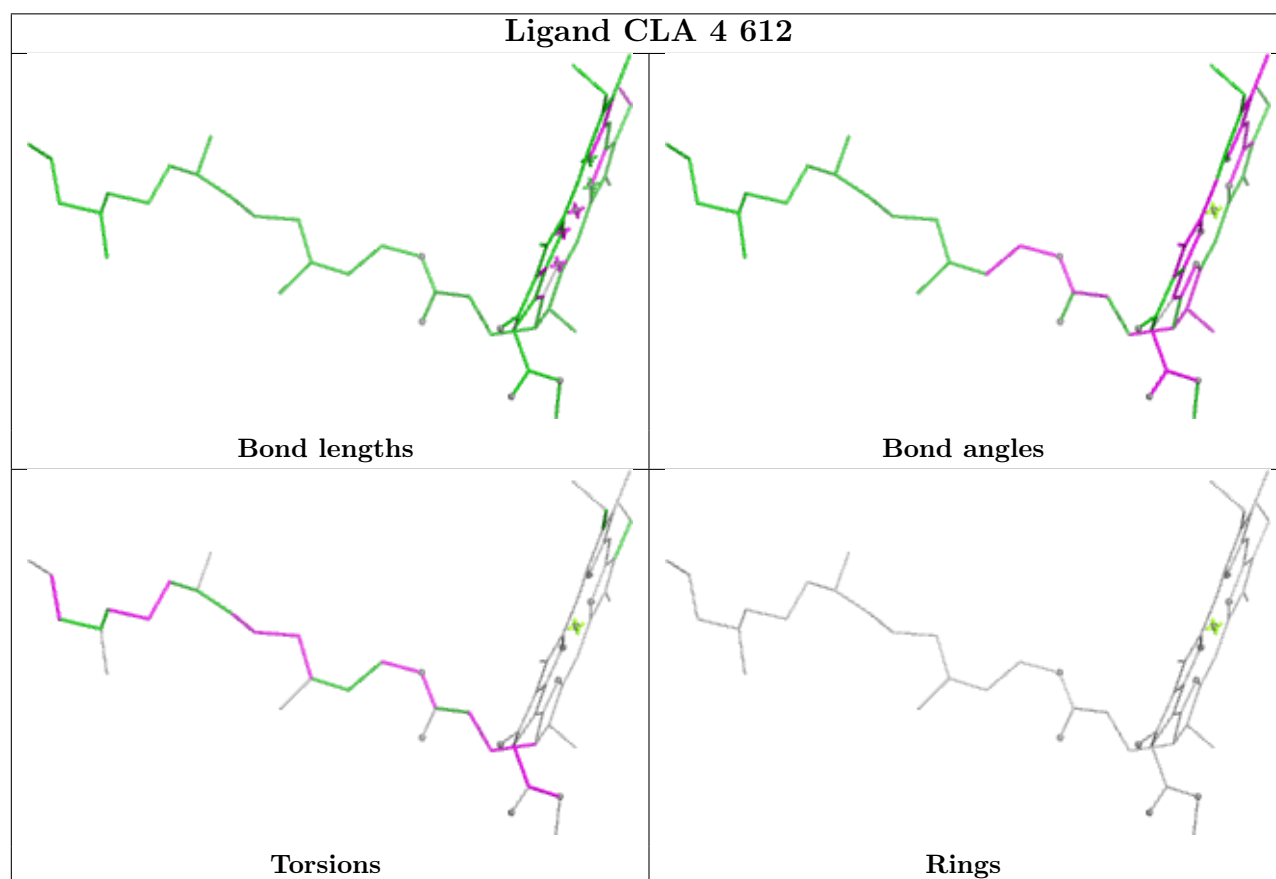
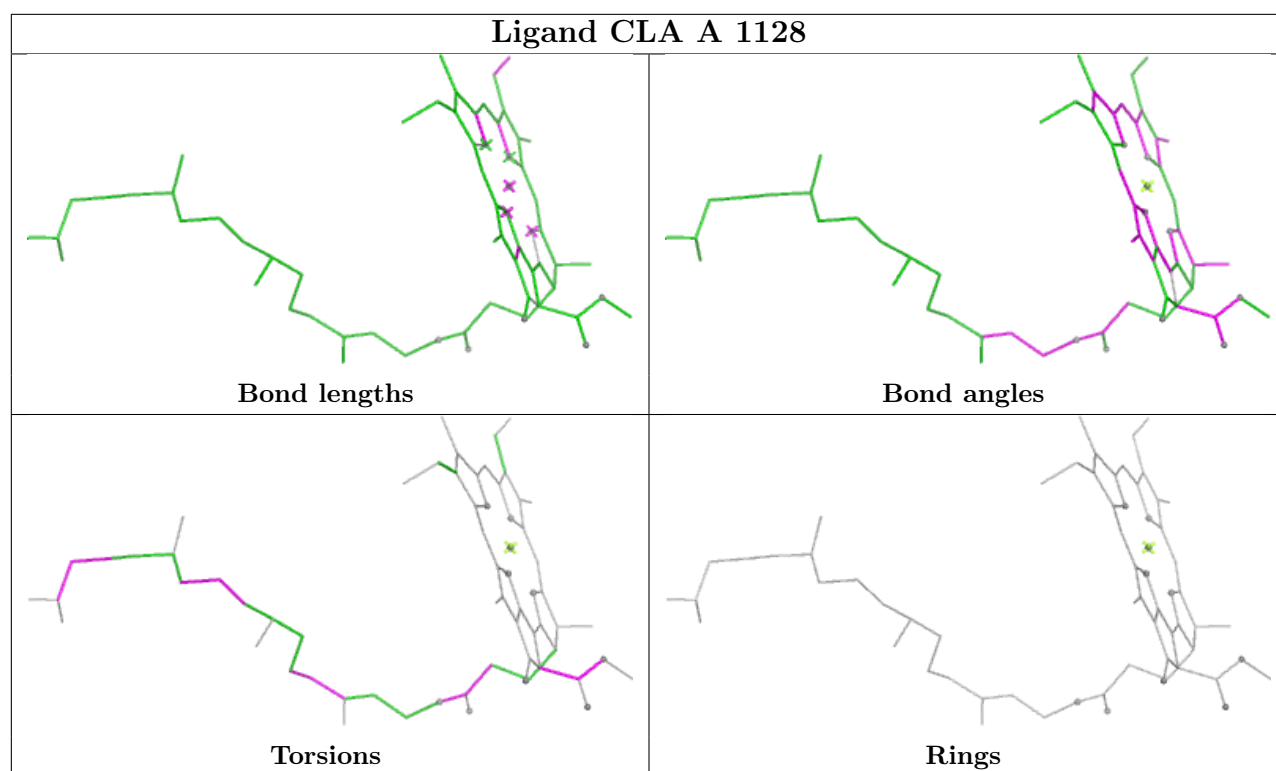


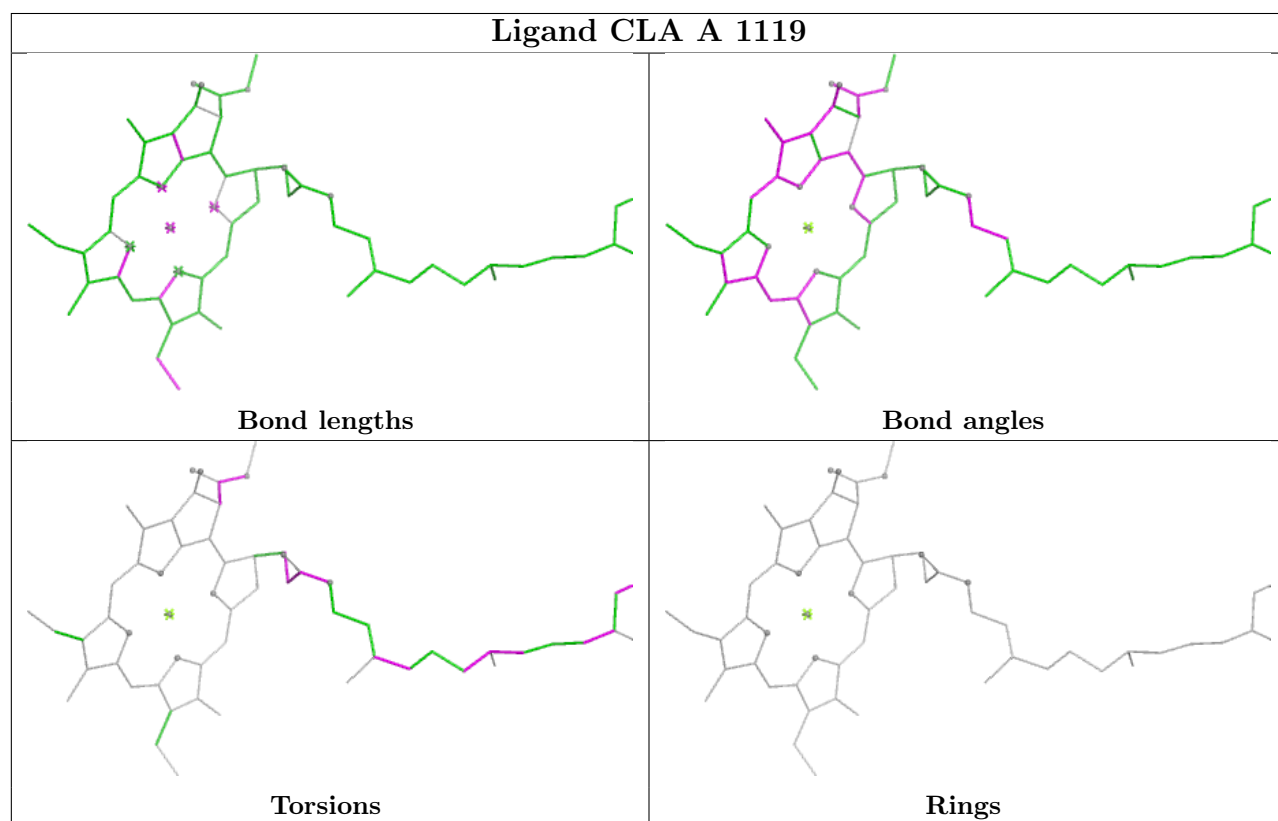
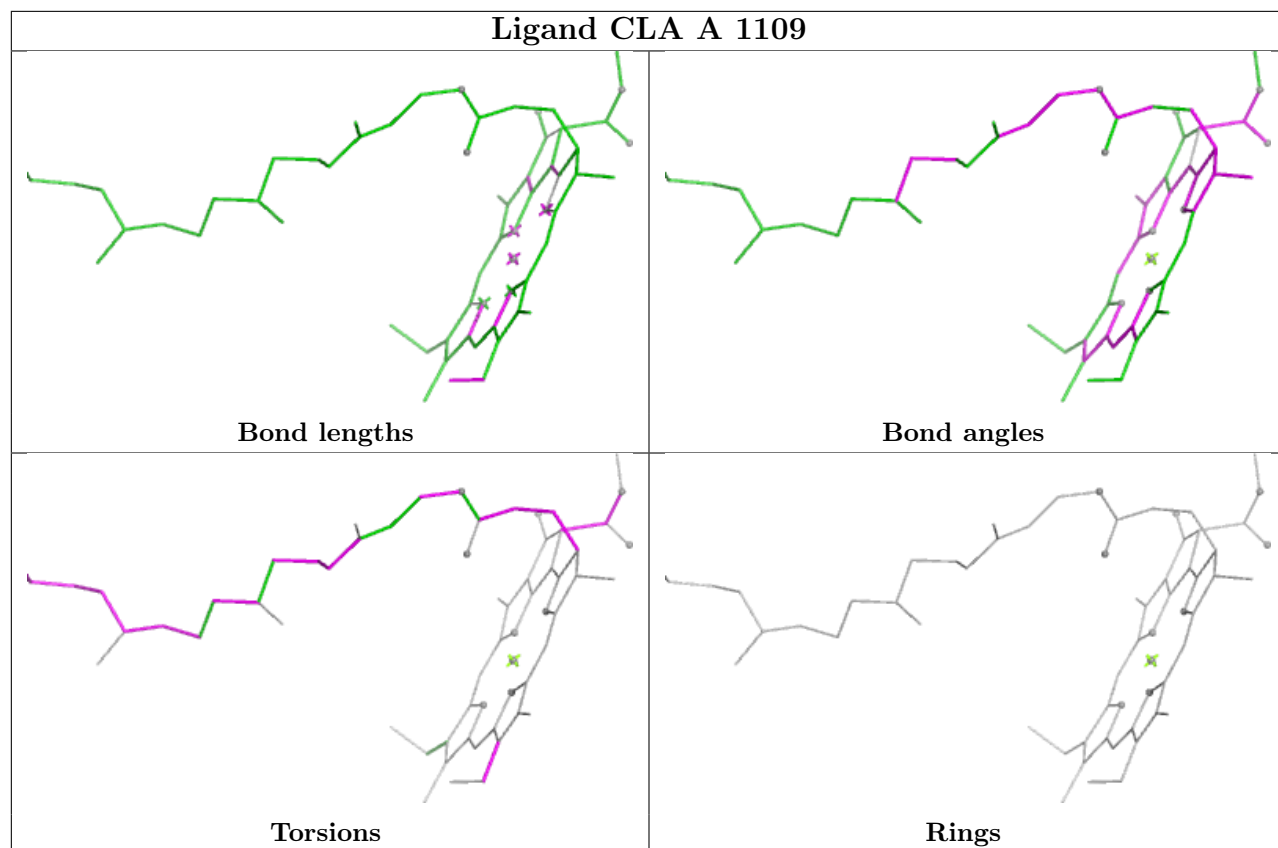
Ligand CLA 5 605

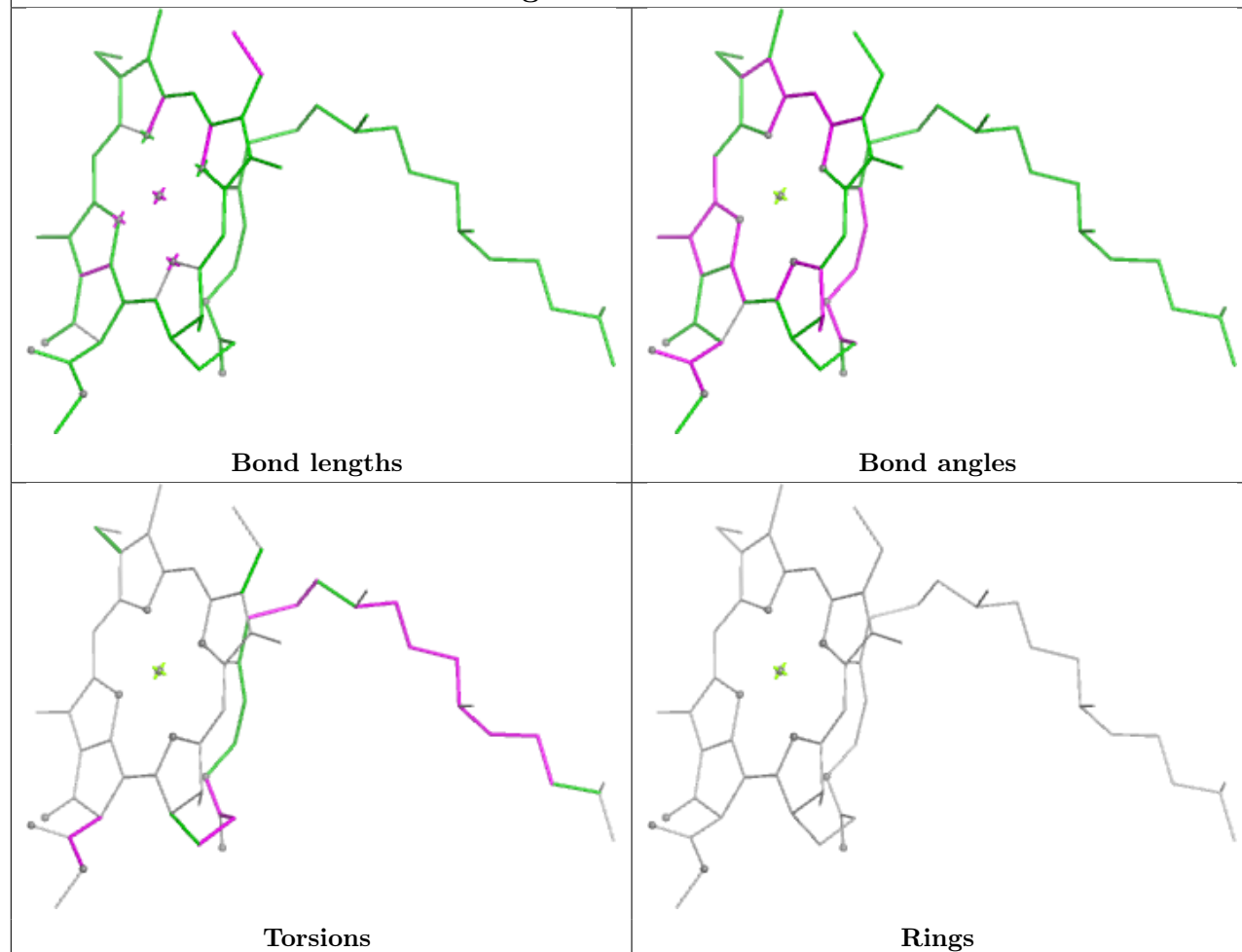
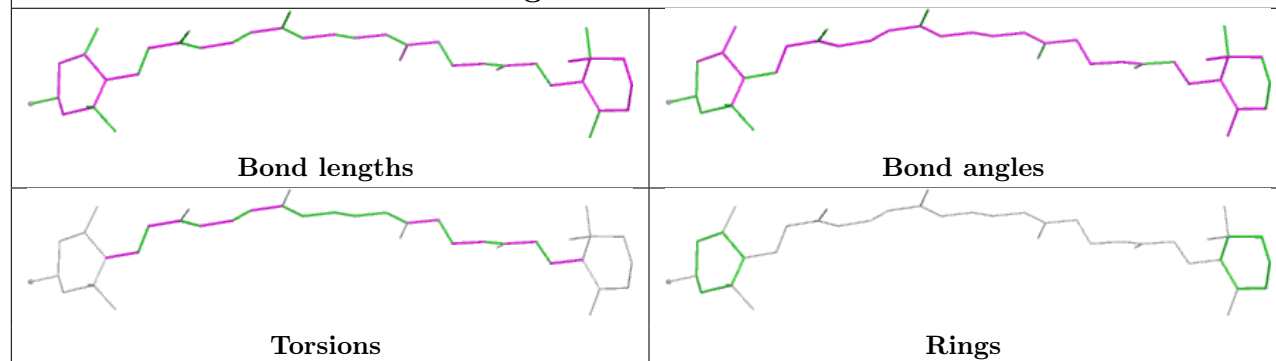


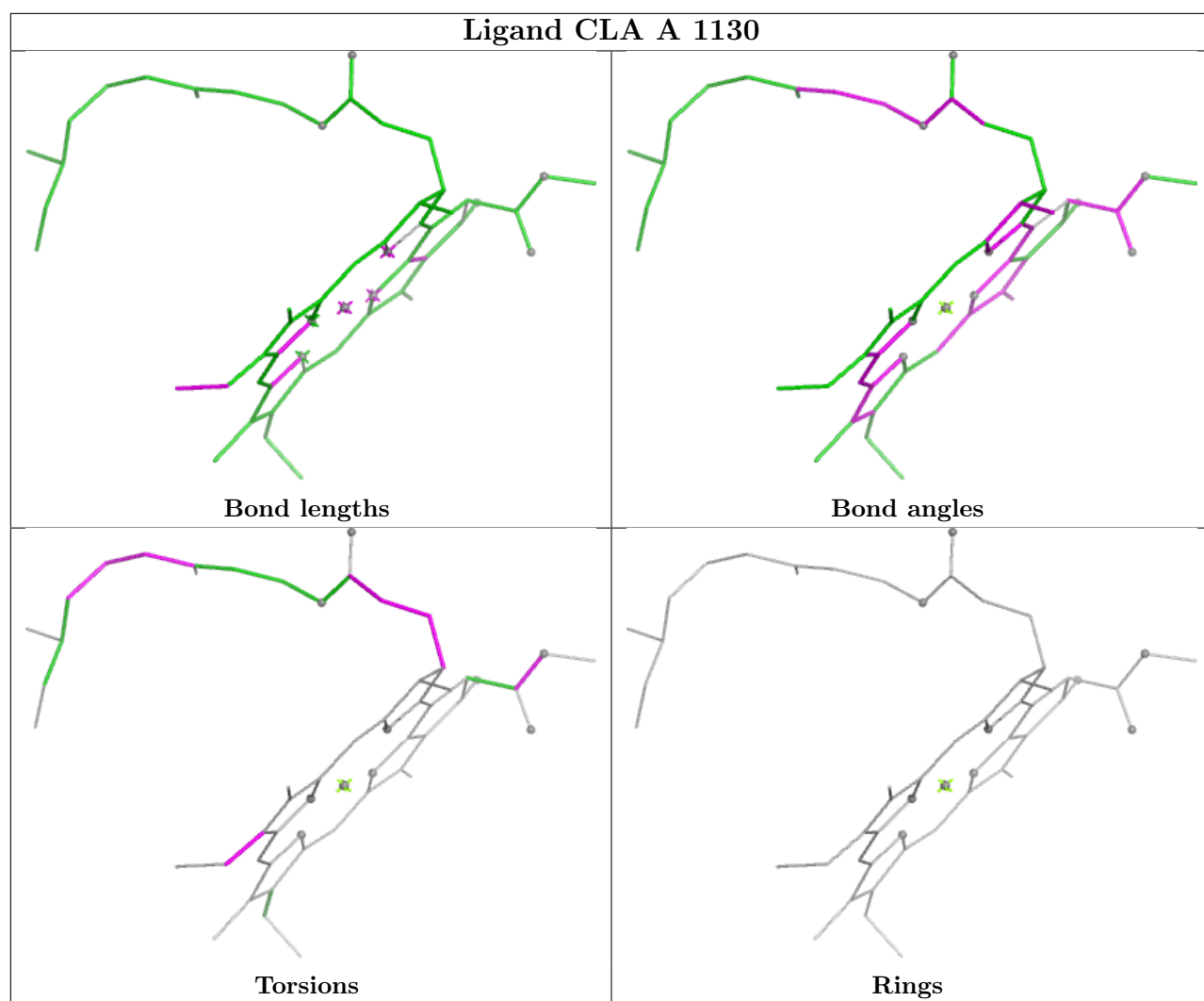
Ligand BCR B 4007



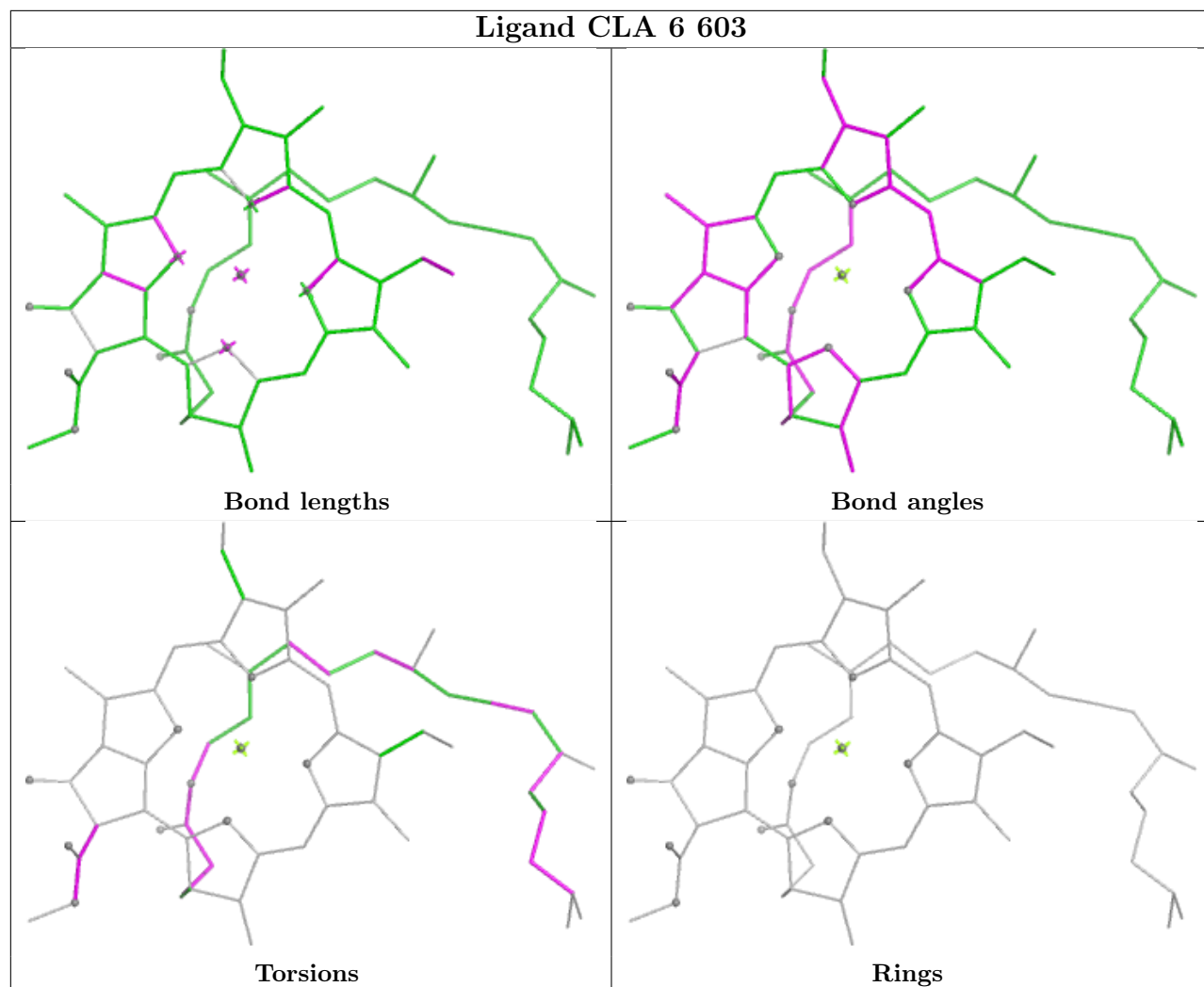


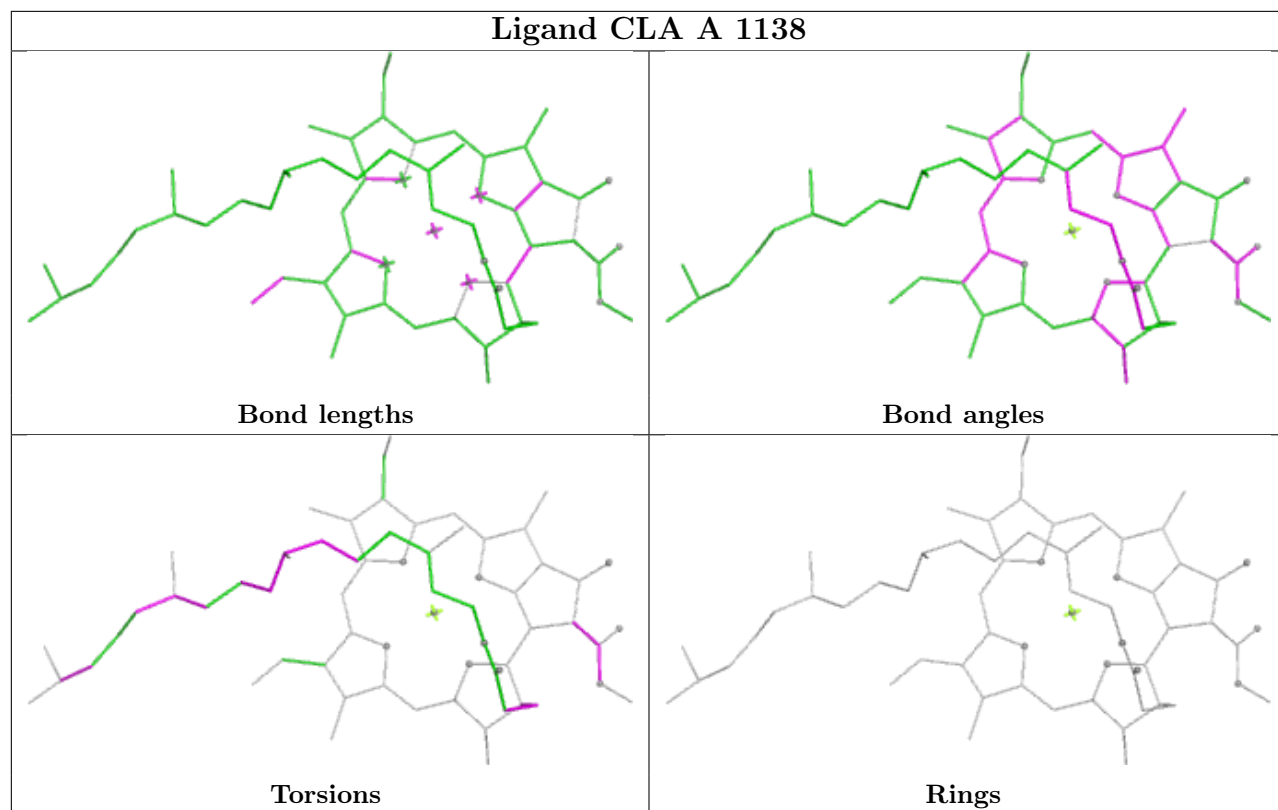


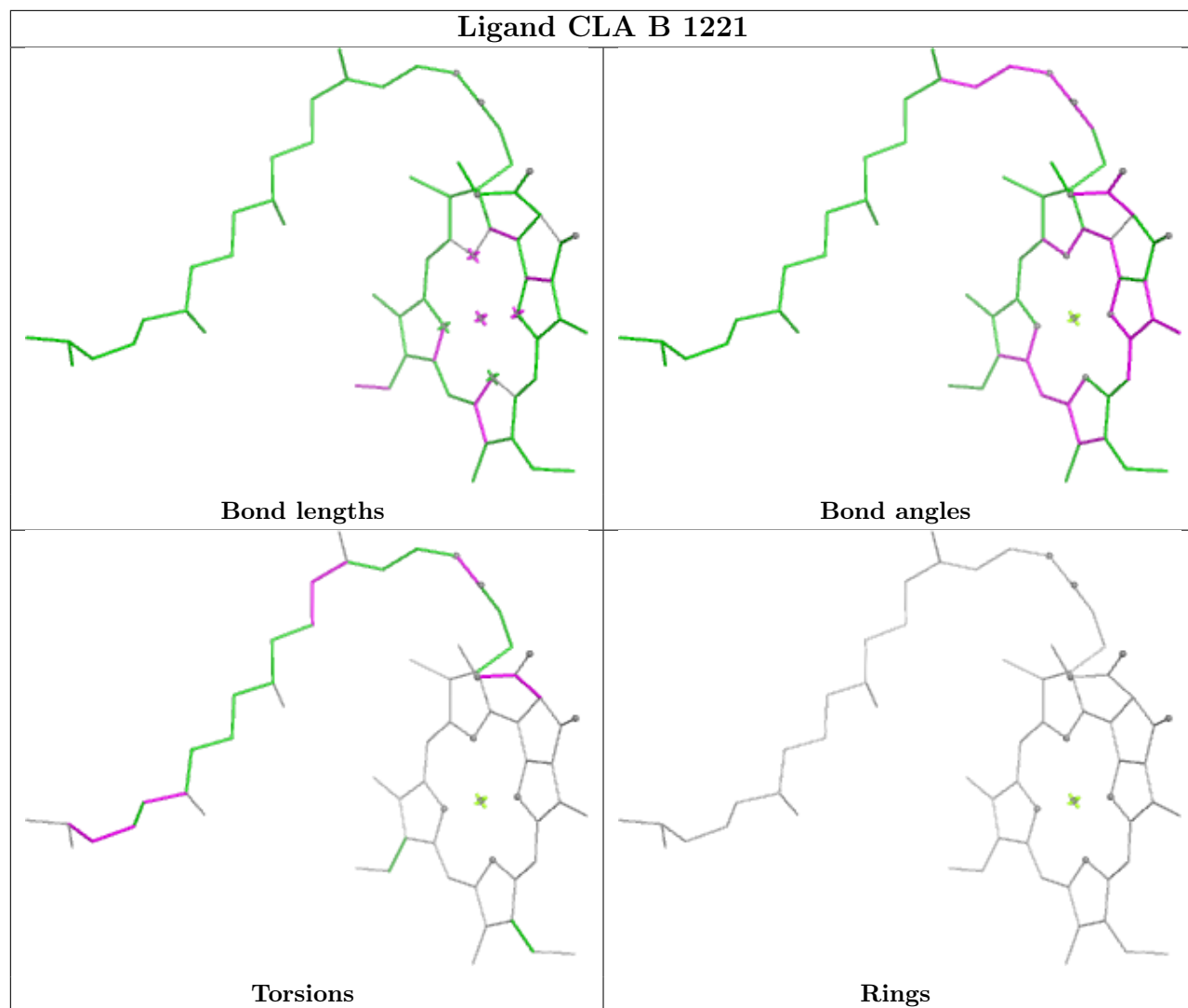
Ligand CLA 7 603**Ligand RRX J 4002**

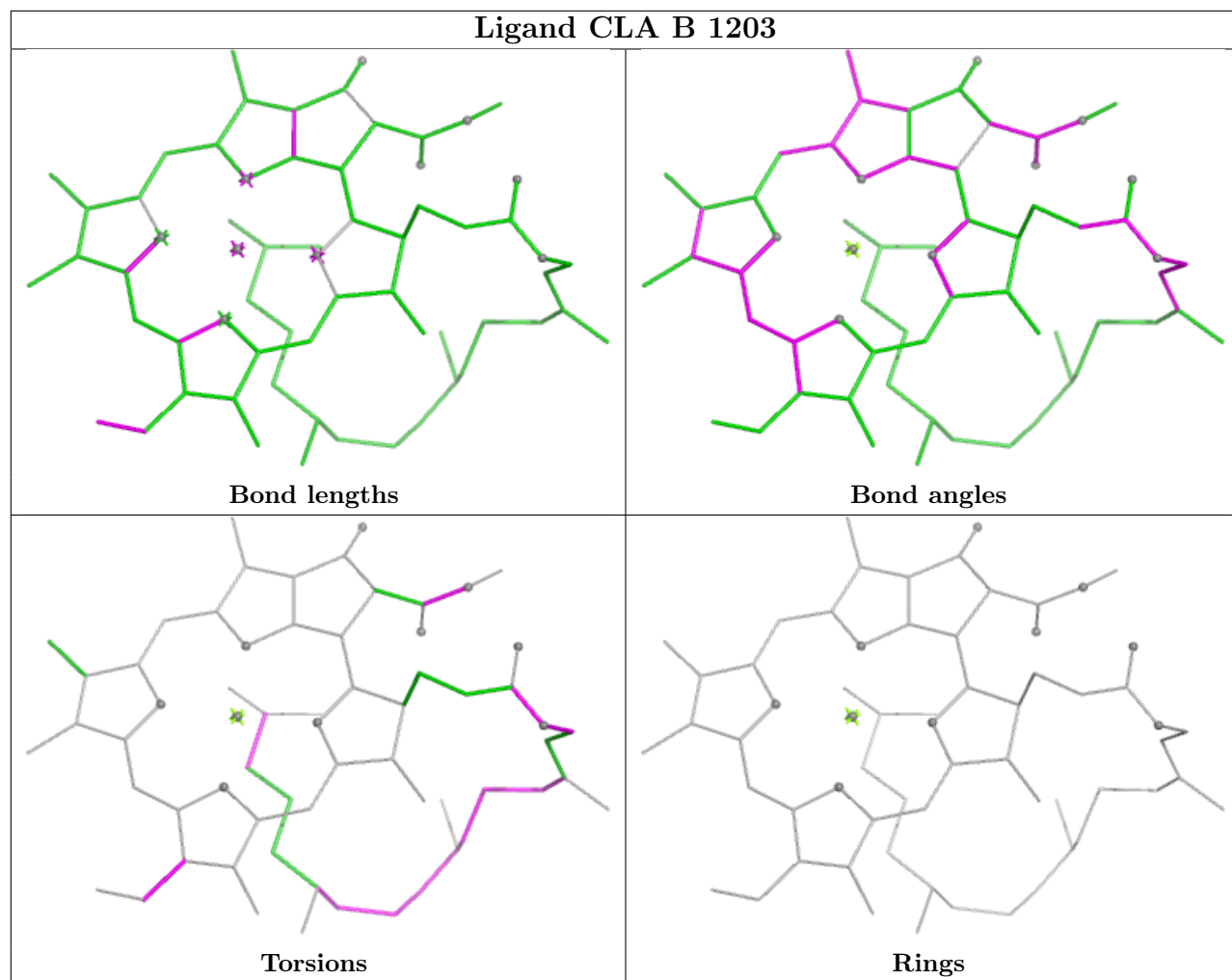


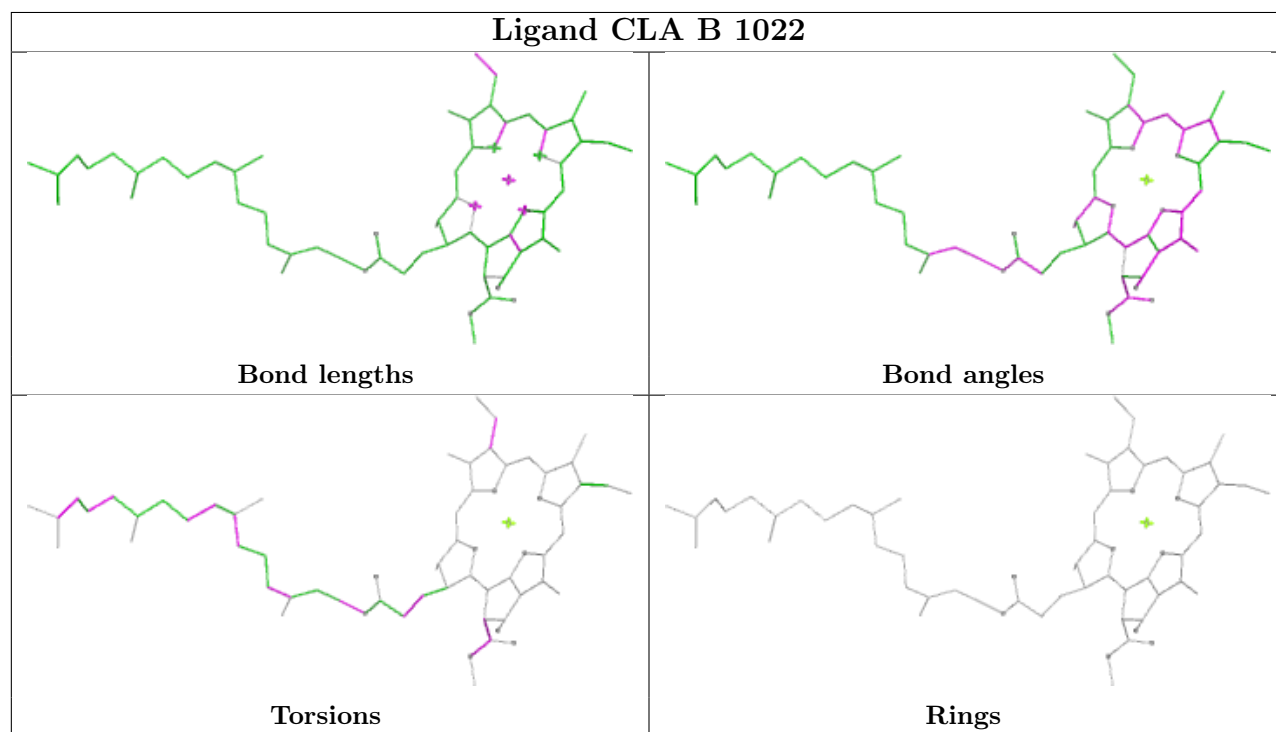
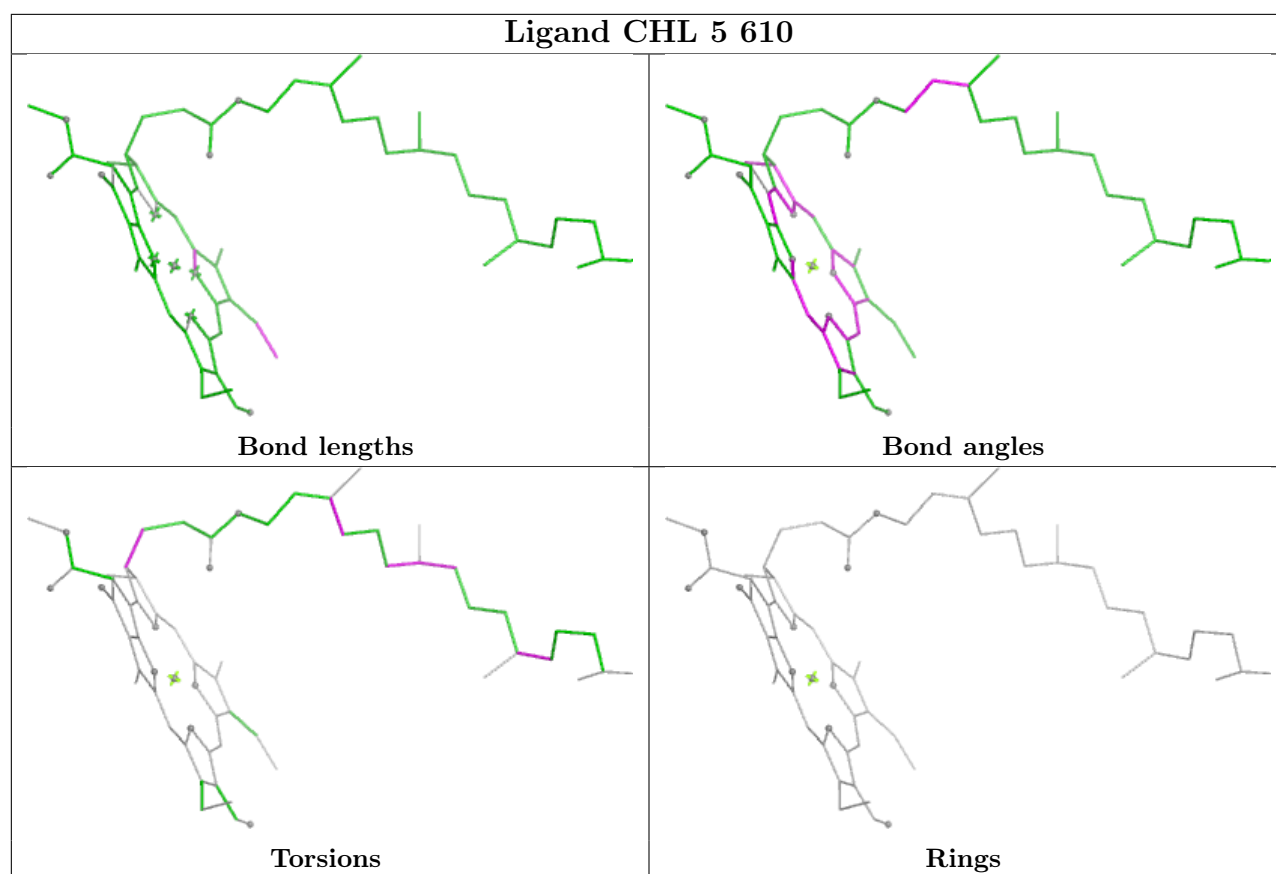
Ligand CLA 6 603



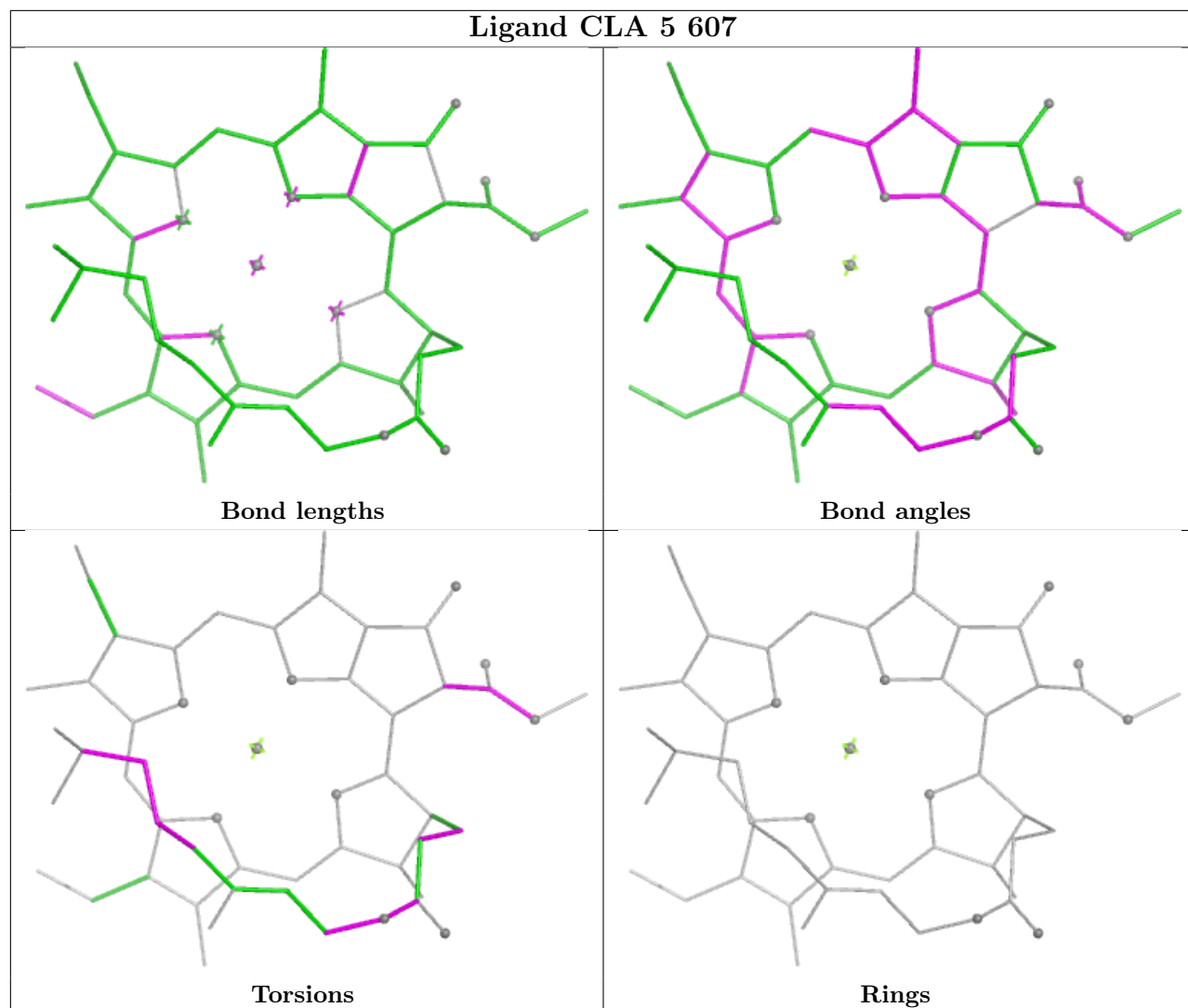


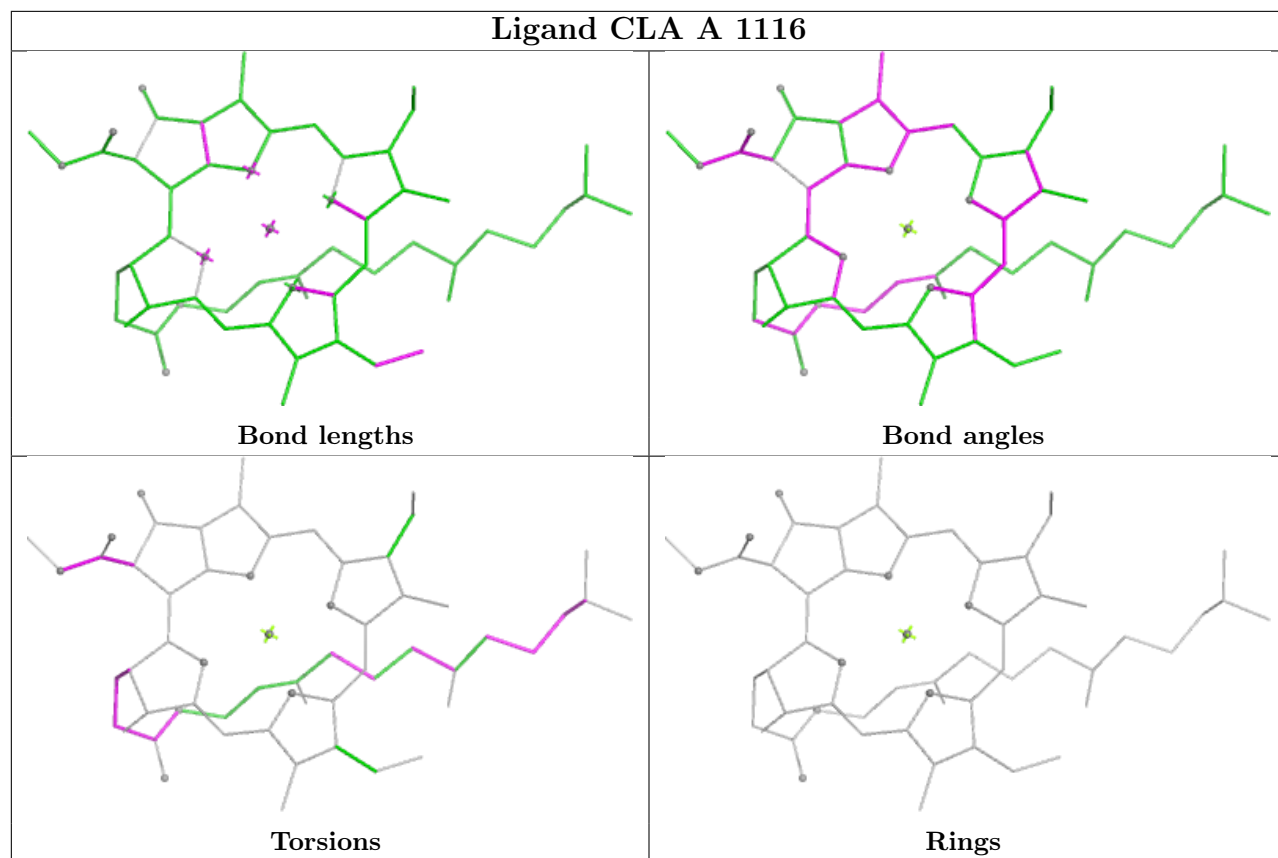


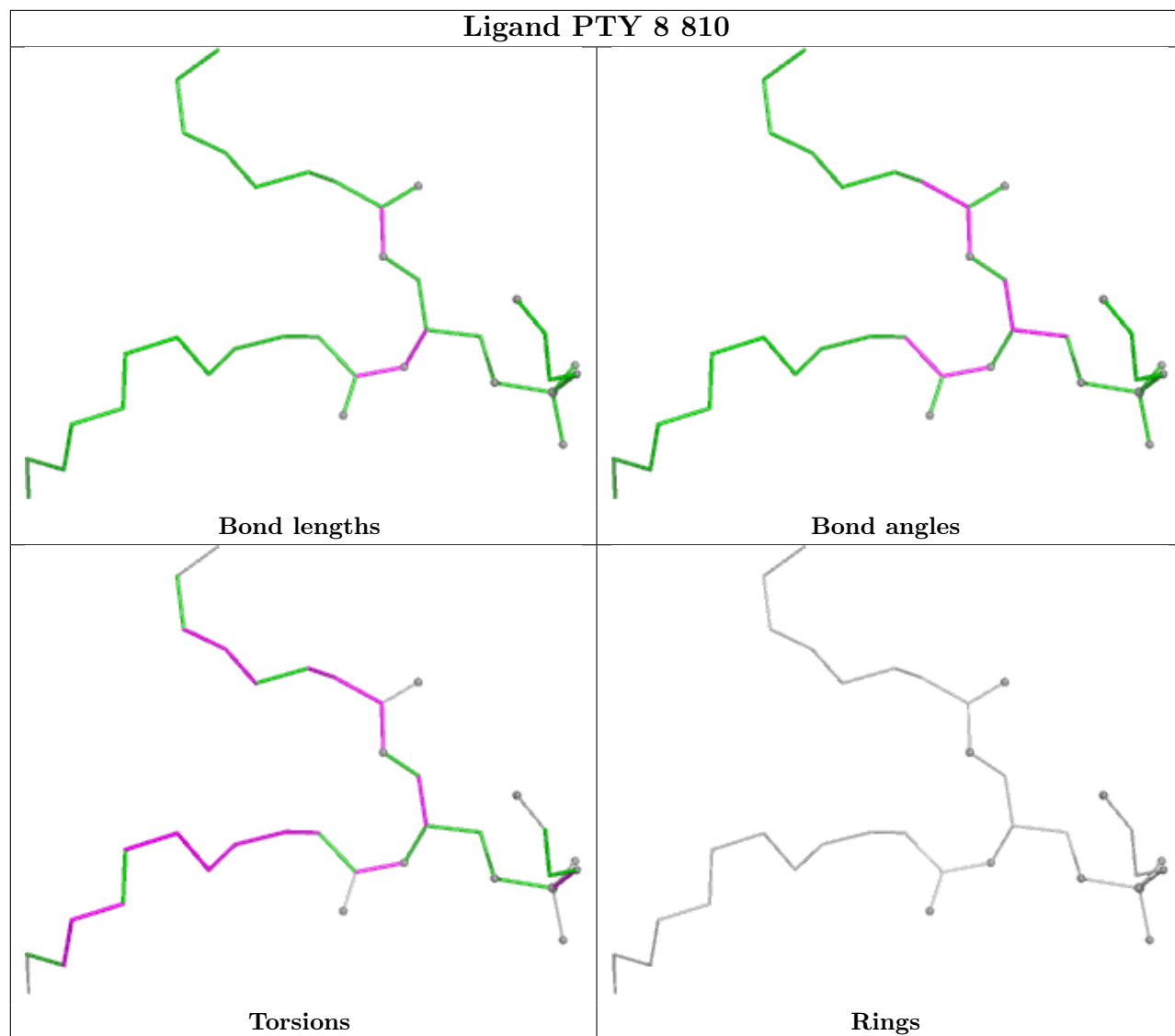


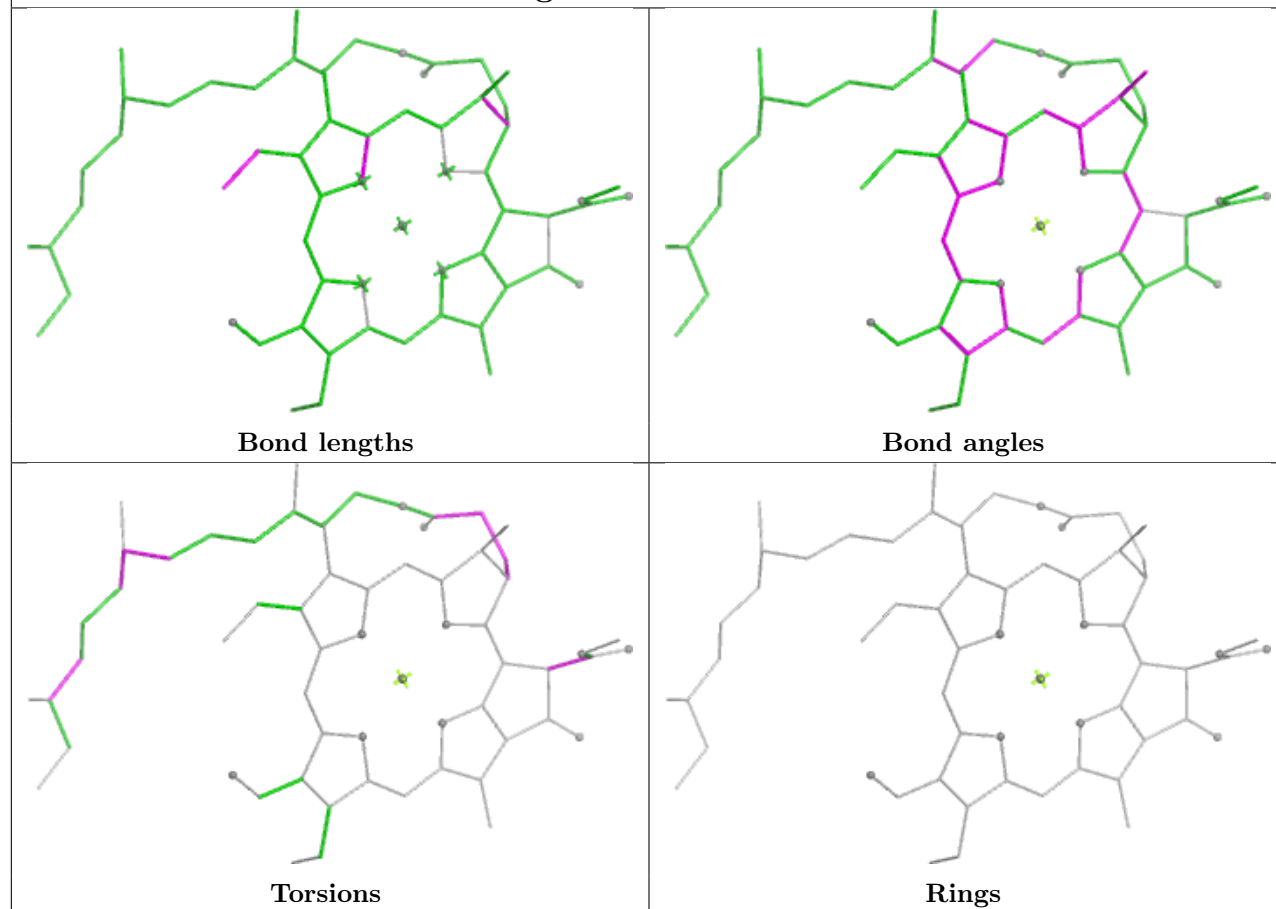
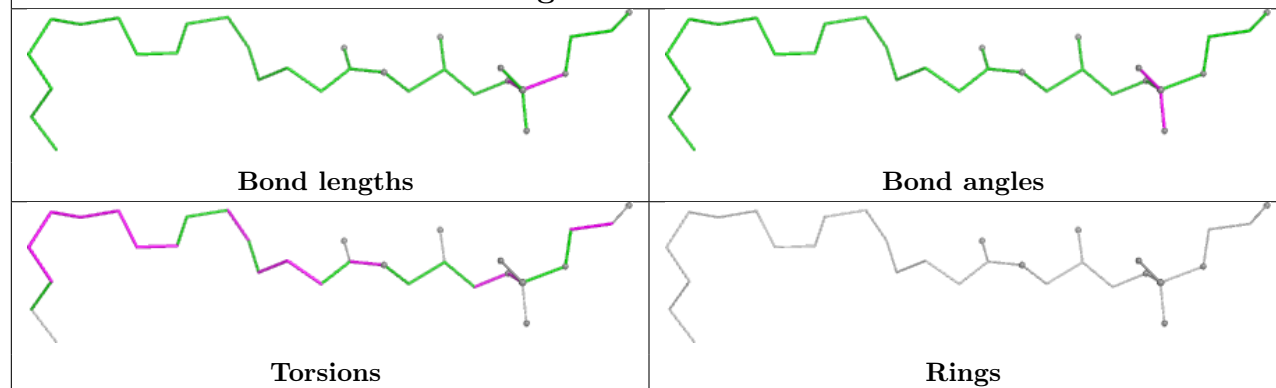


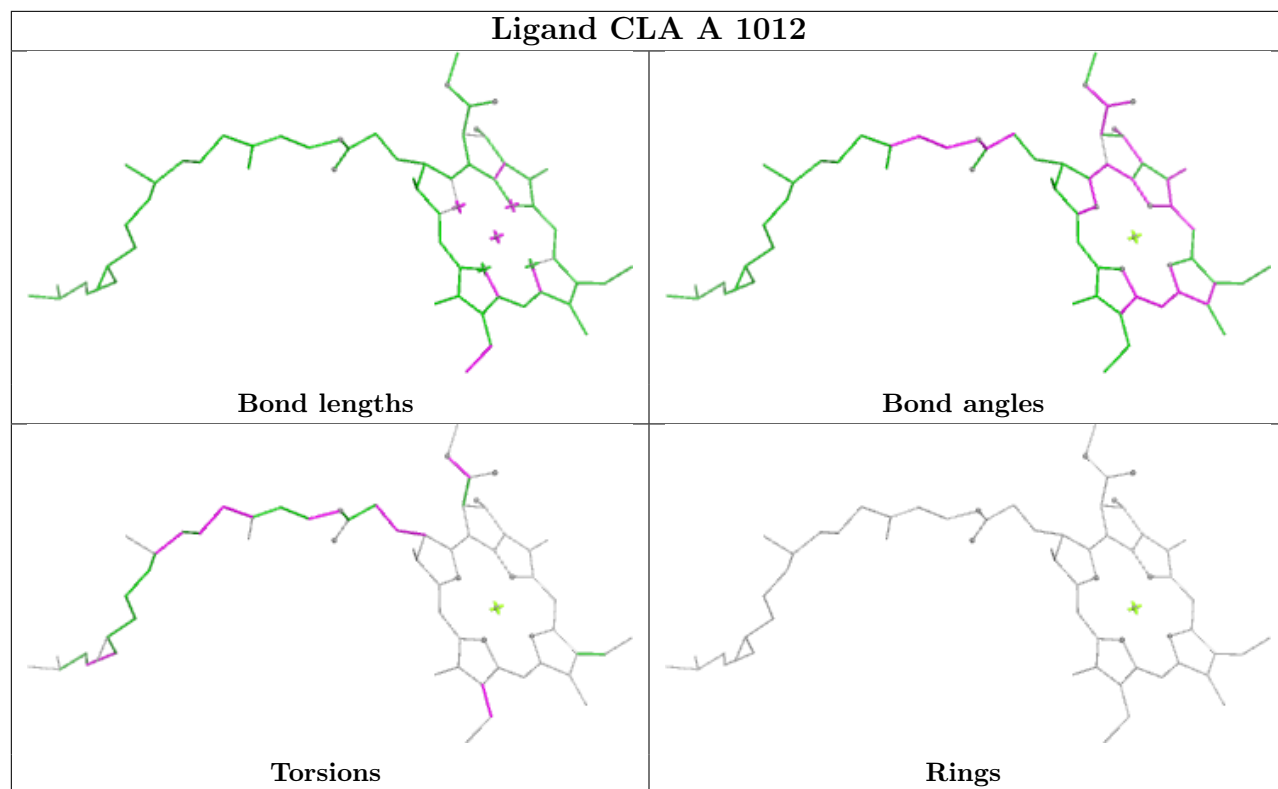
Ligand CLA 5 607



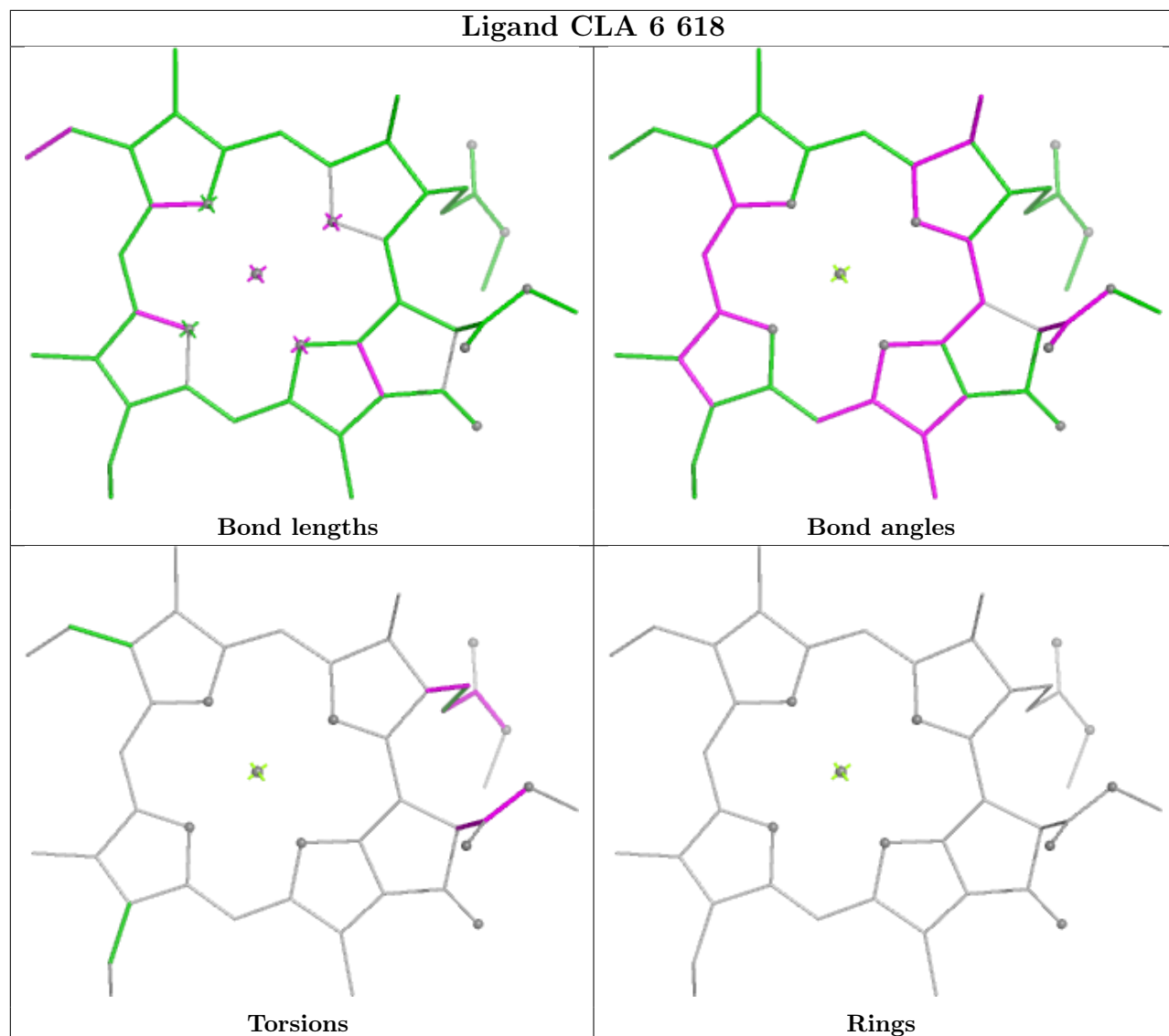


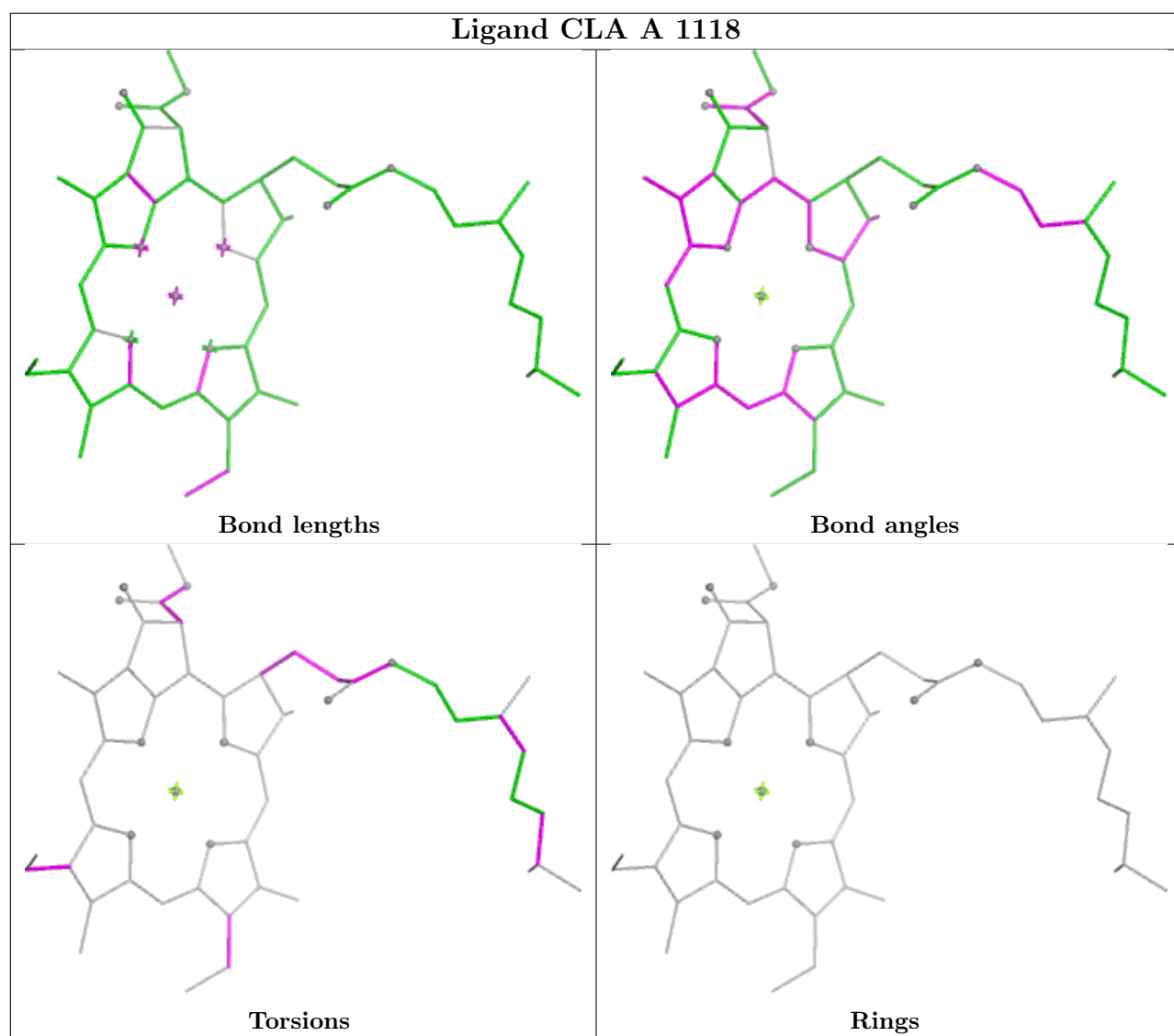


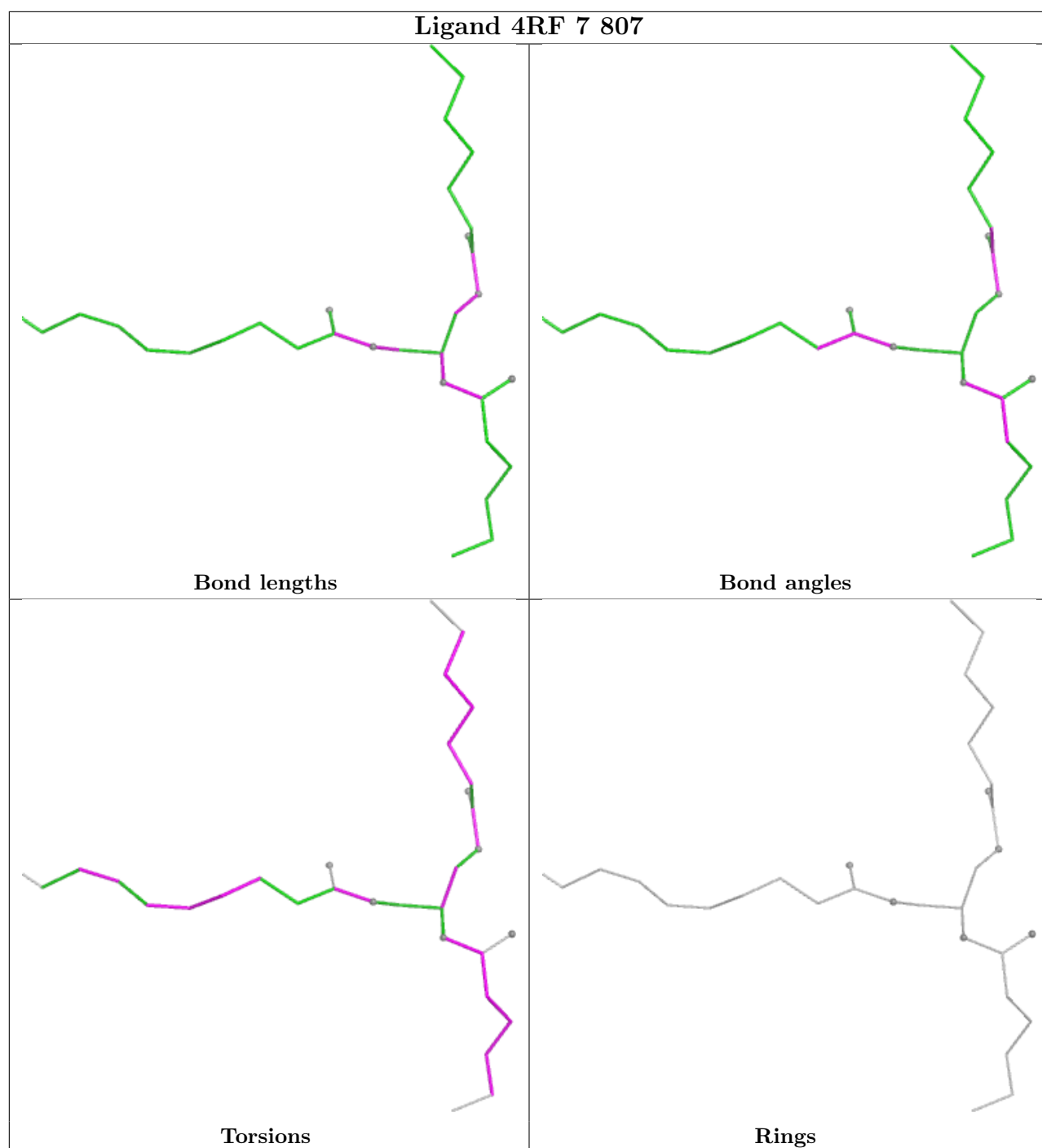
Ligand CHL 8 604**Ligand LPX a 804**

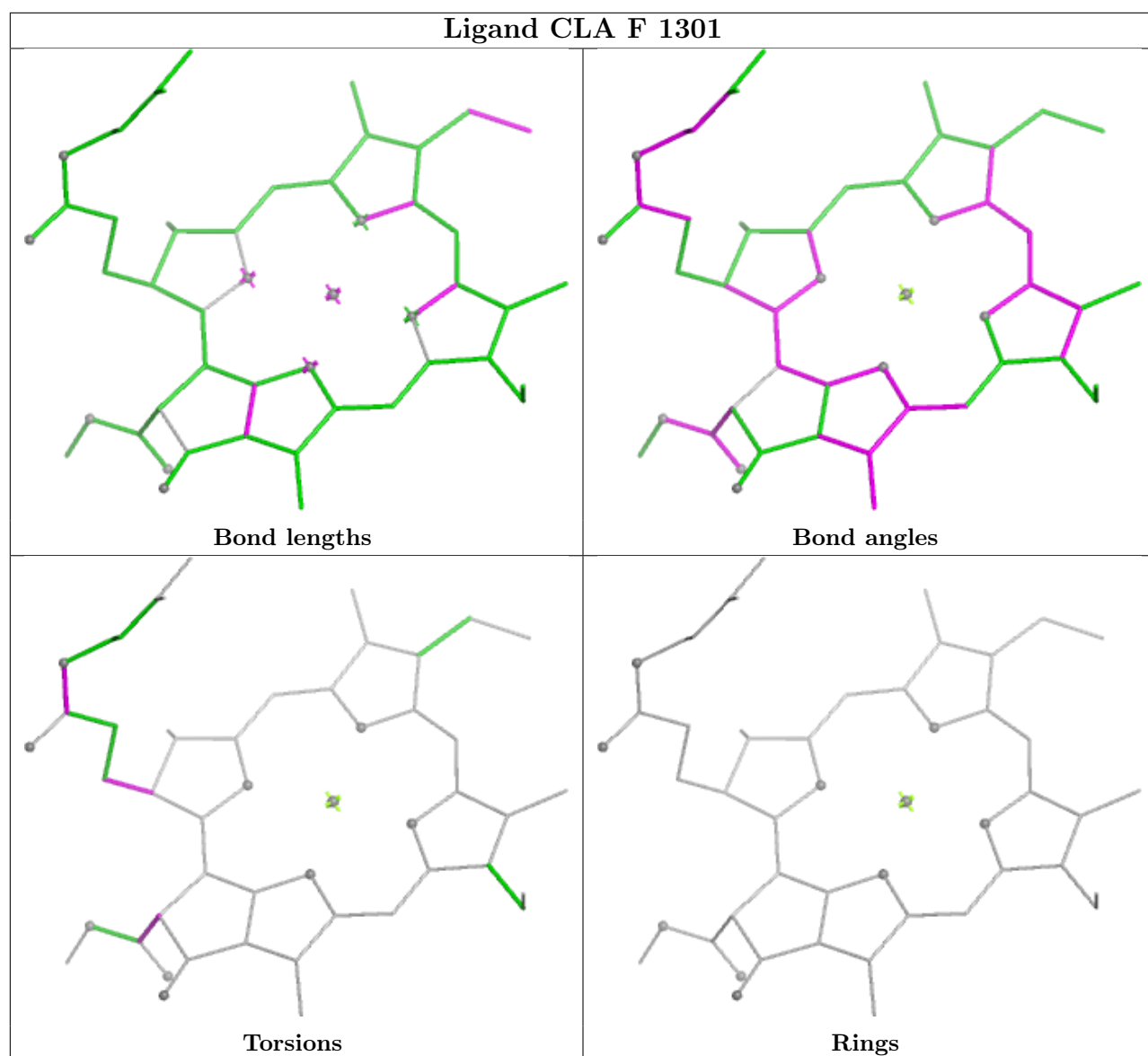


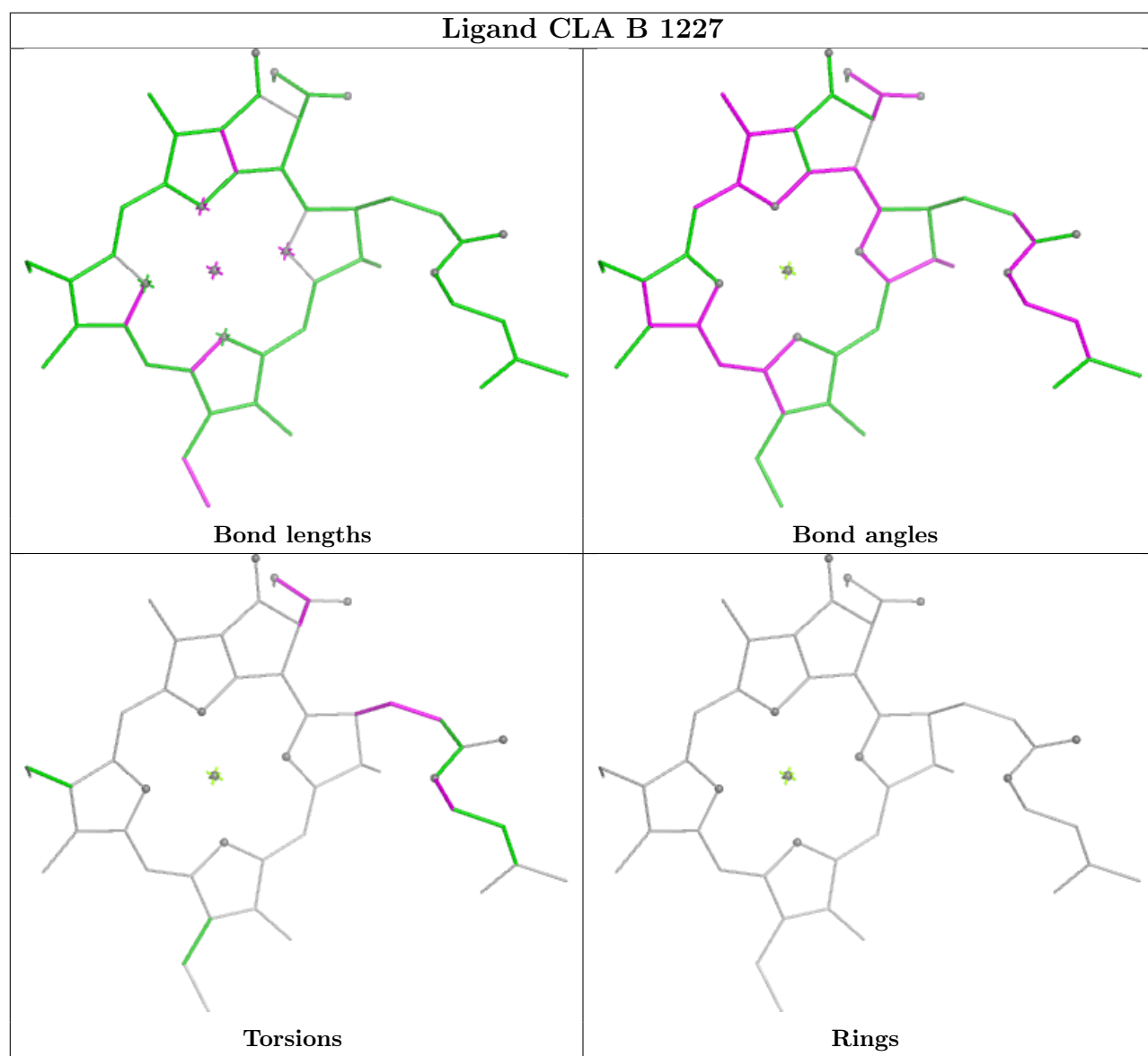
Ligand CLA 6 618

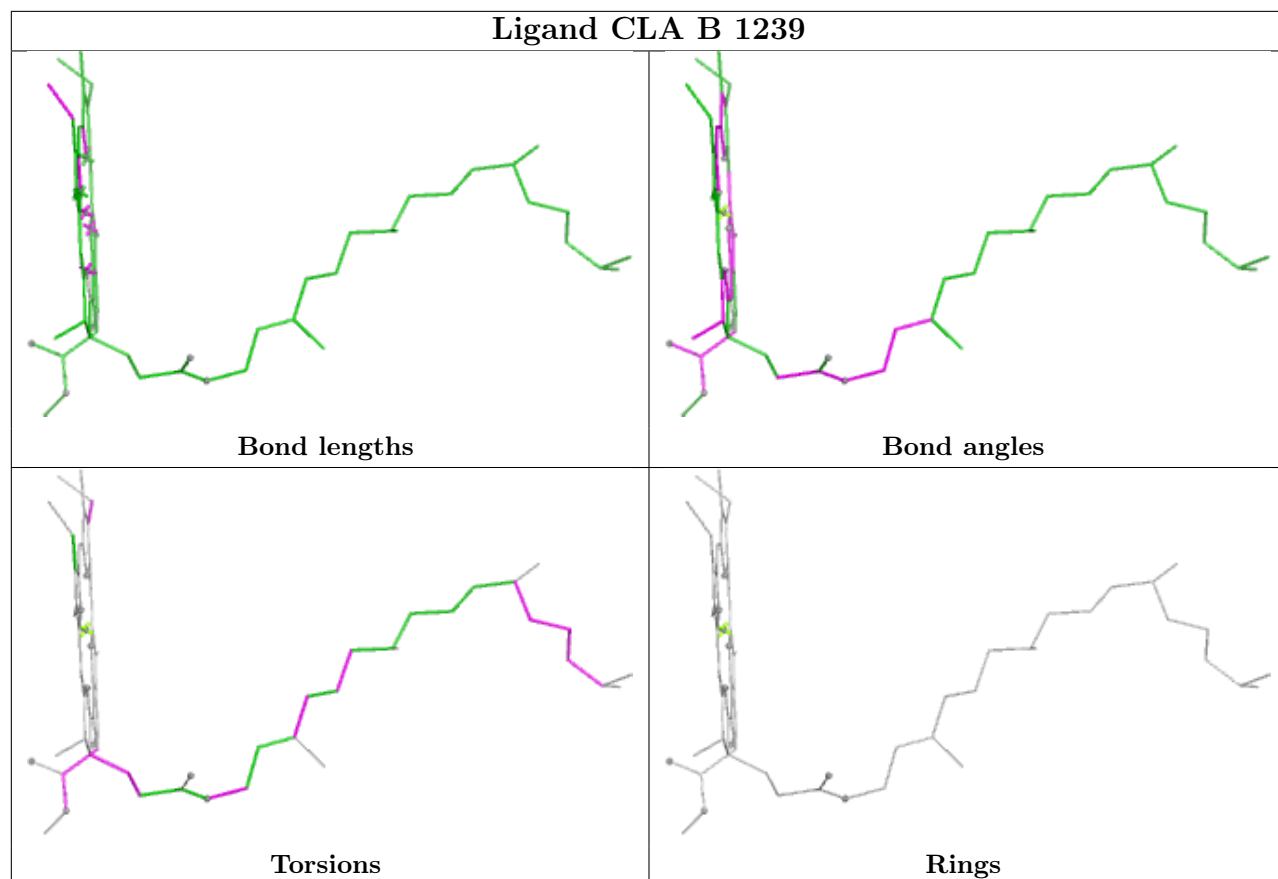




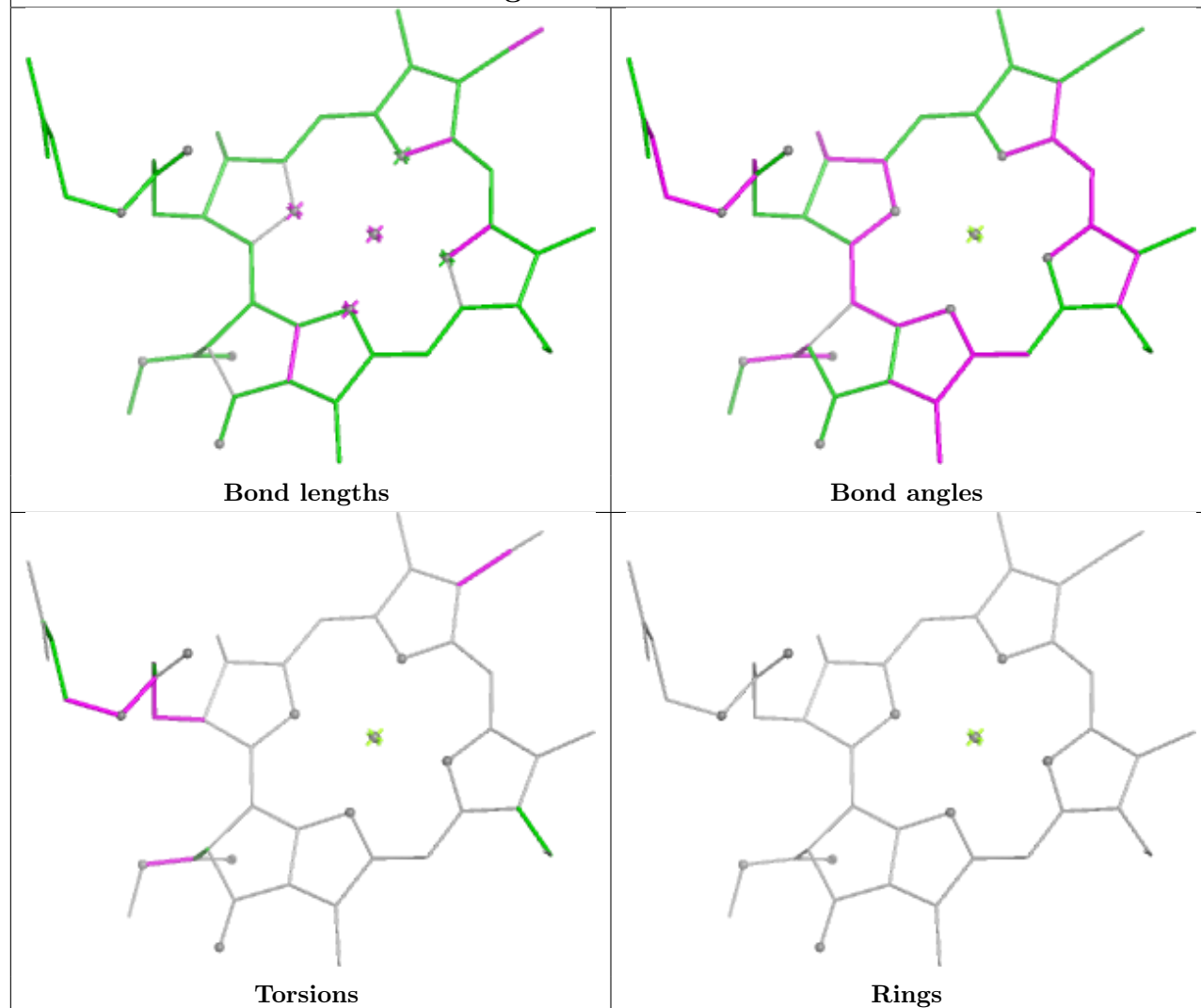




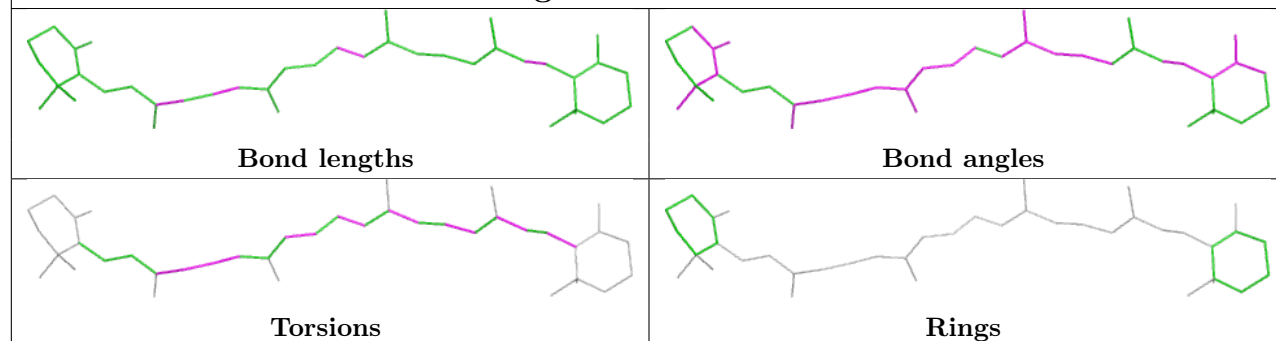


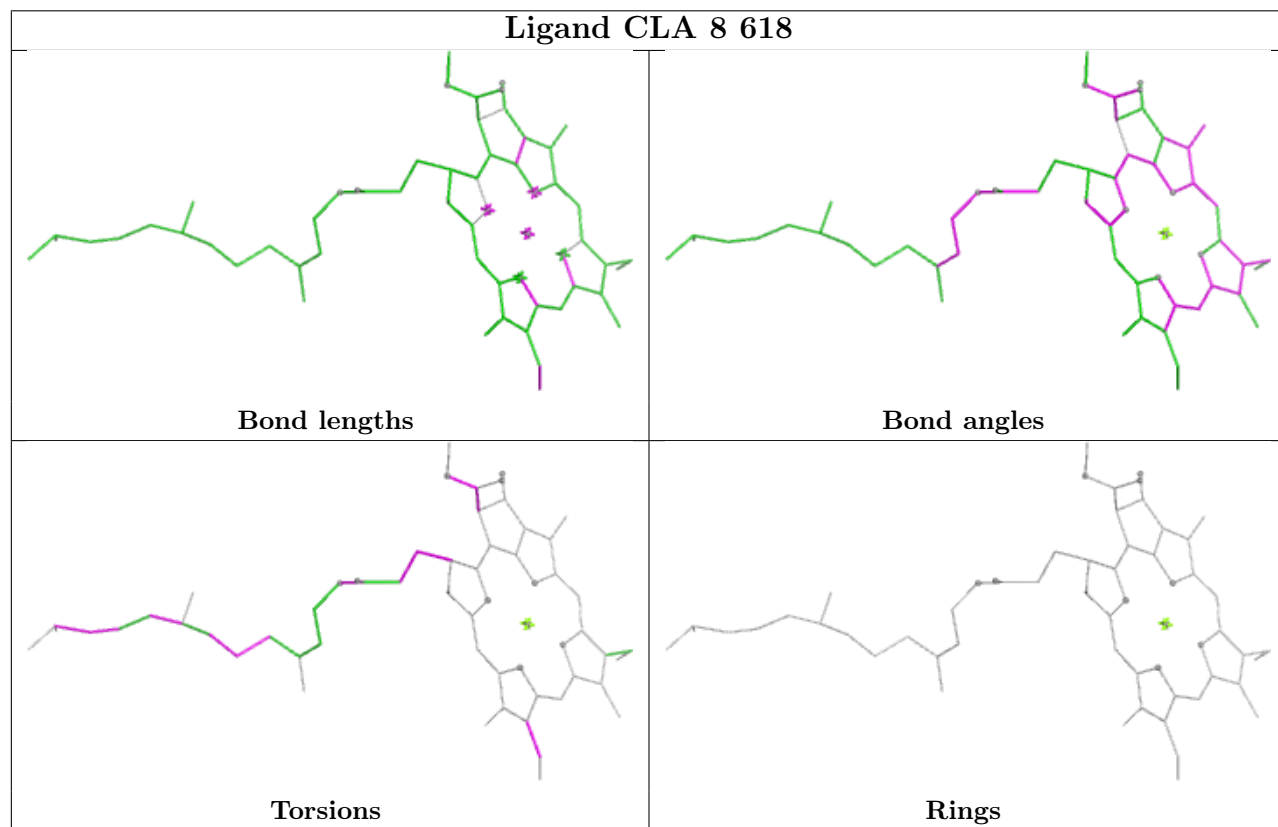
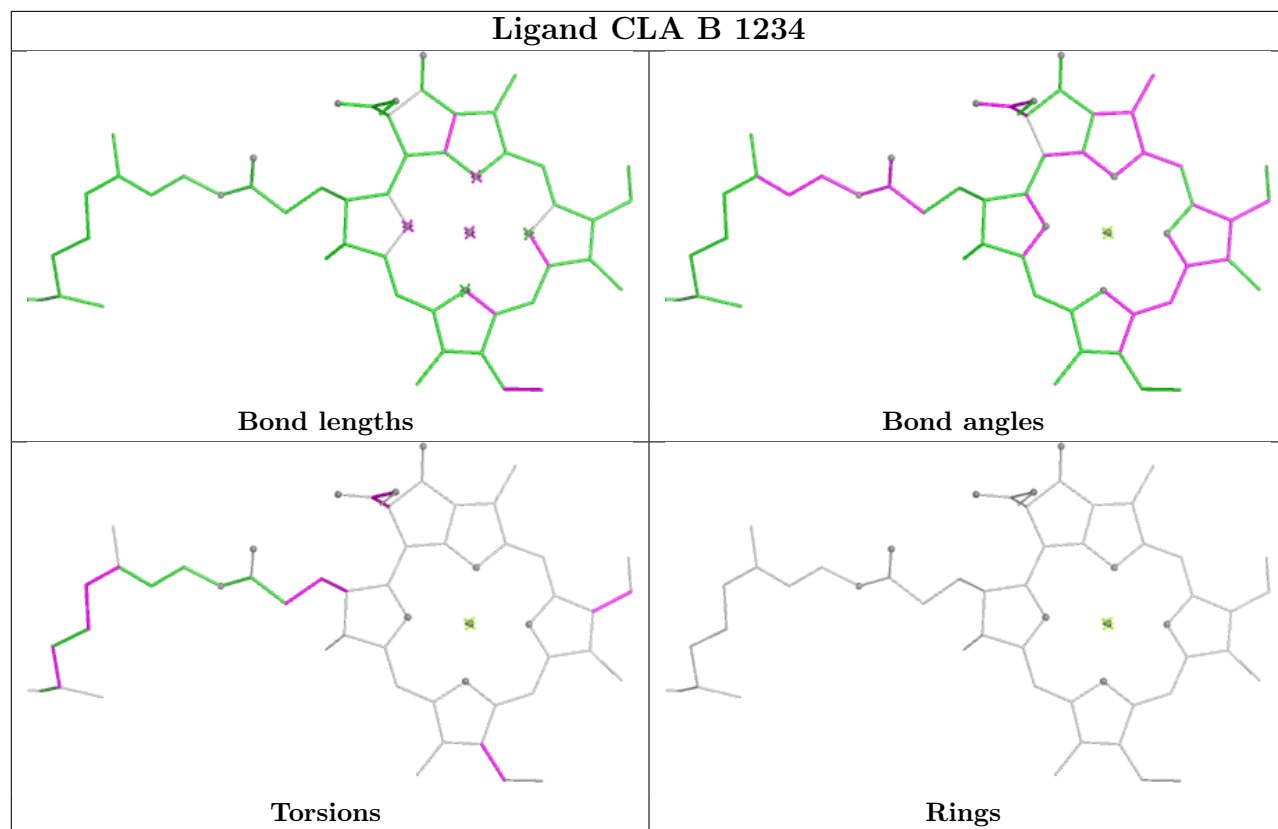


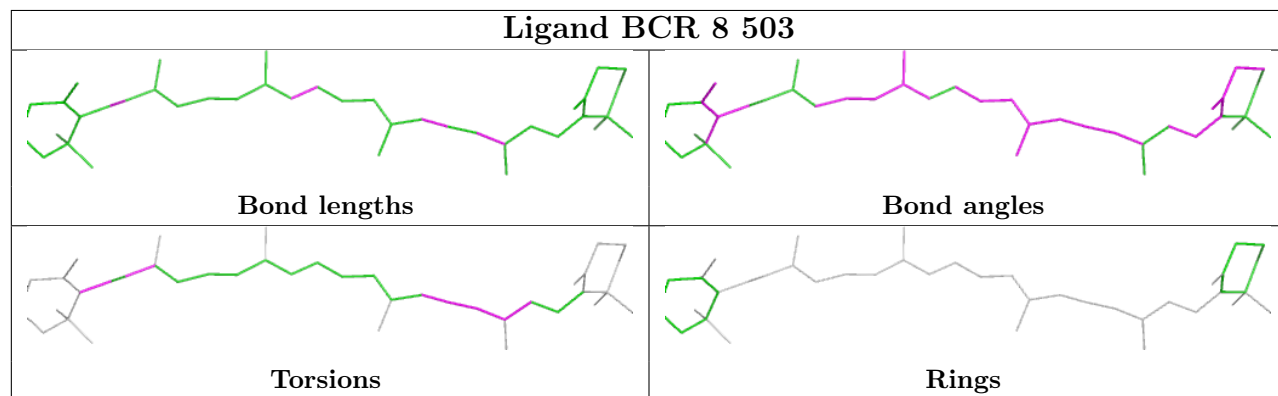
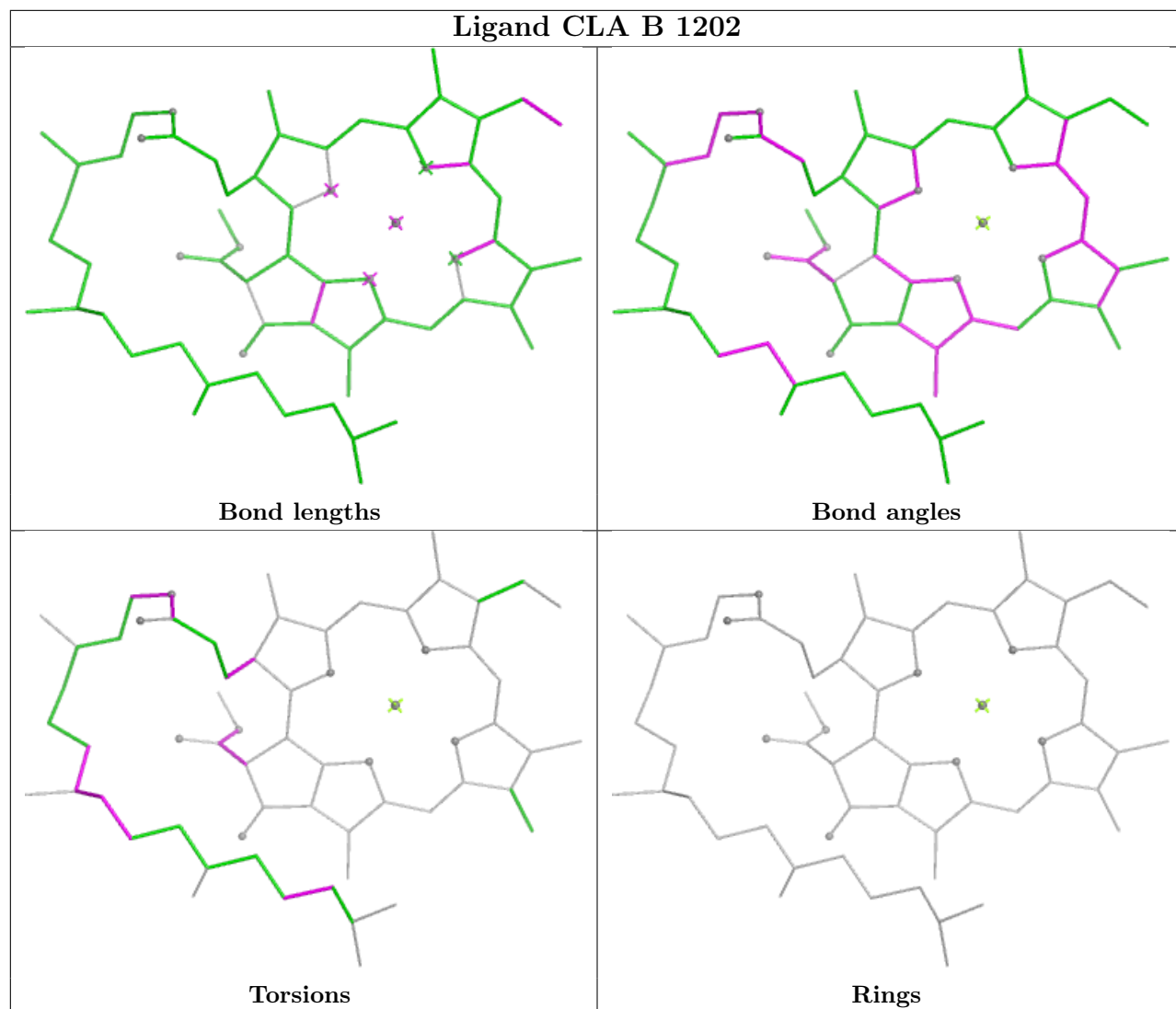
Ligand CLA a 611



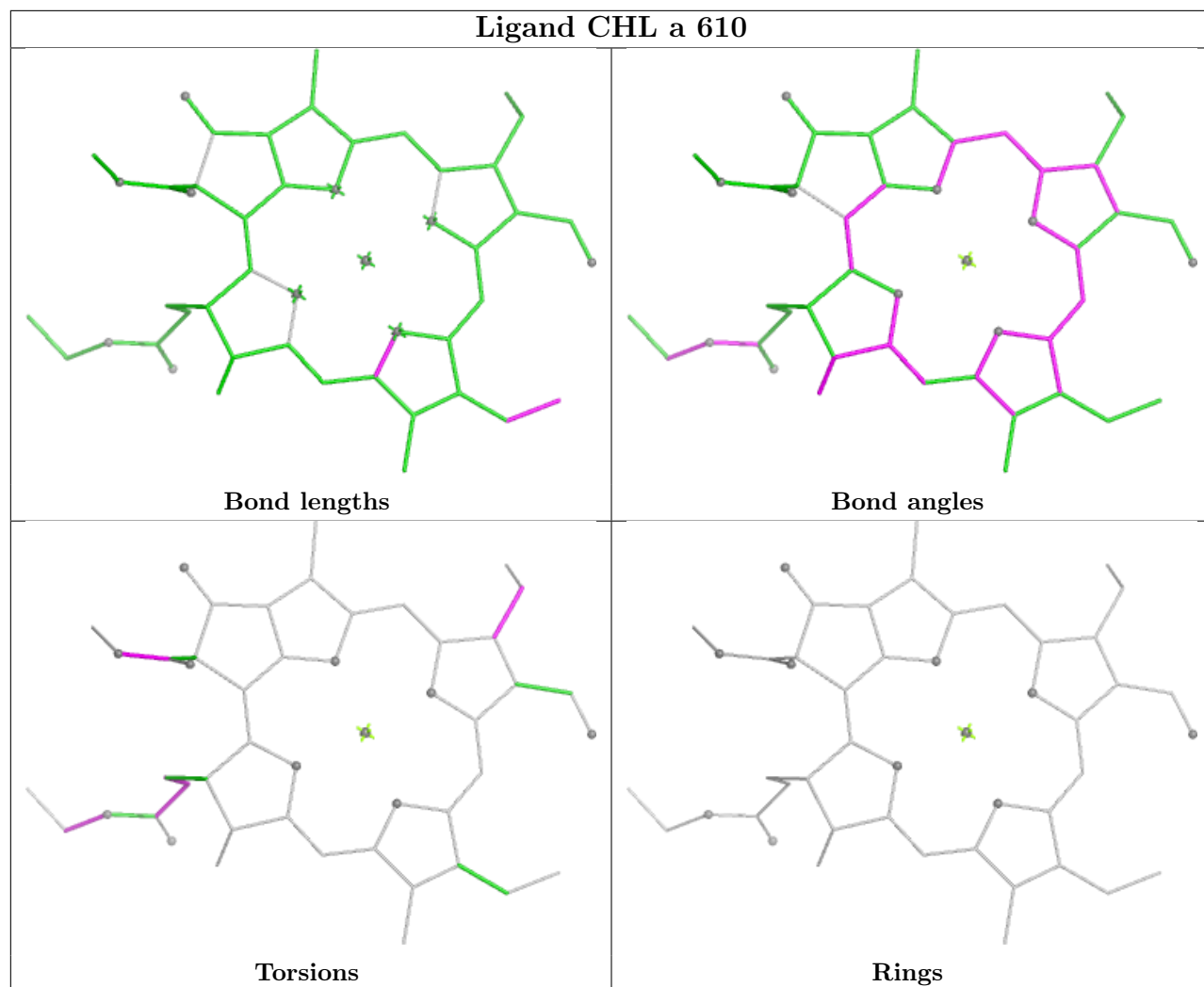
Ligand BCR 3 505

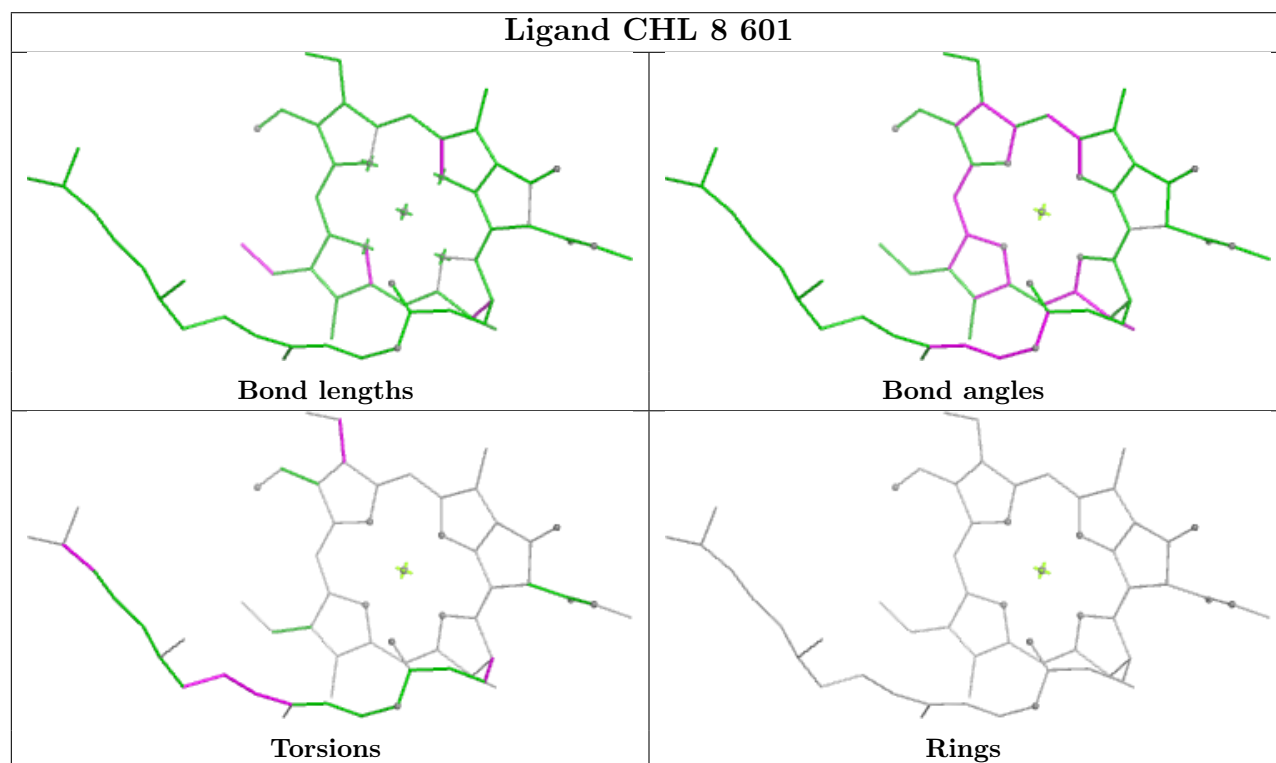
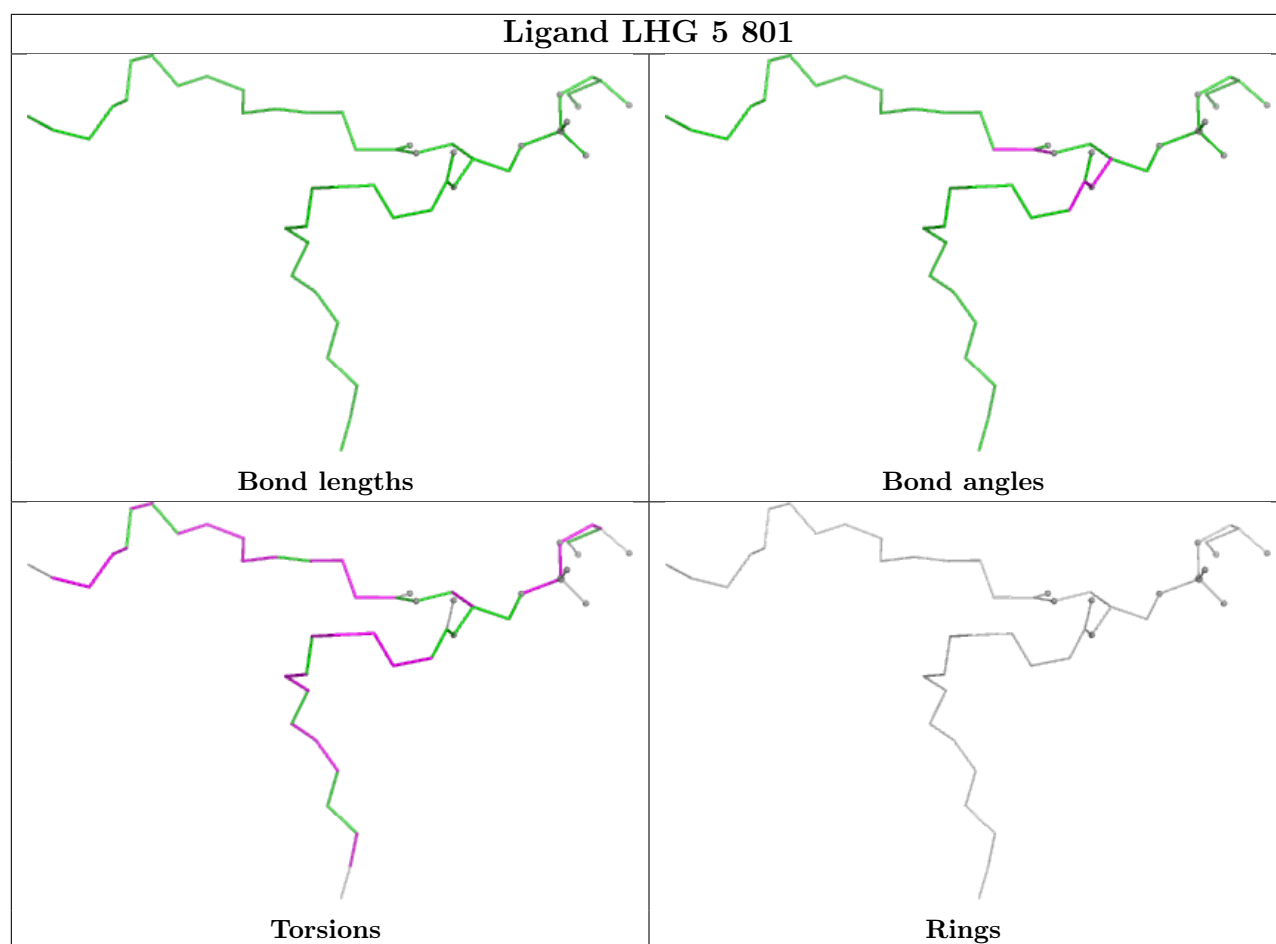


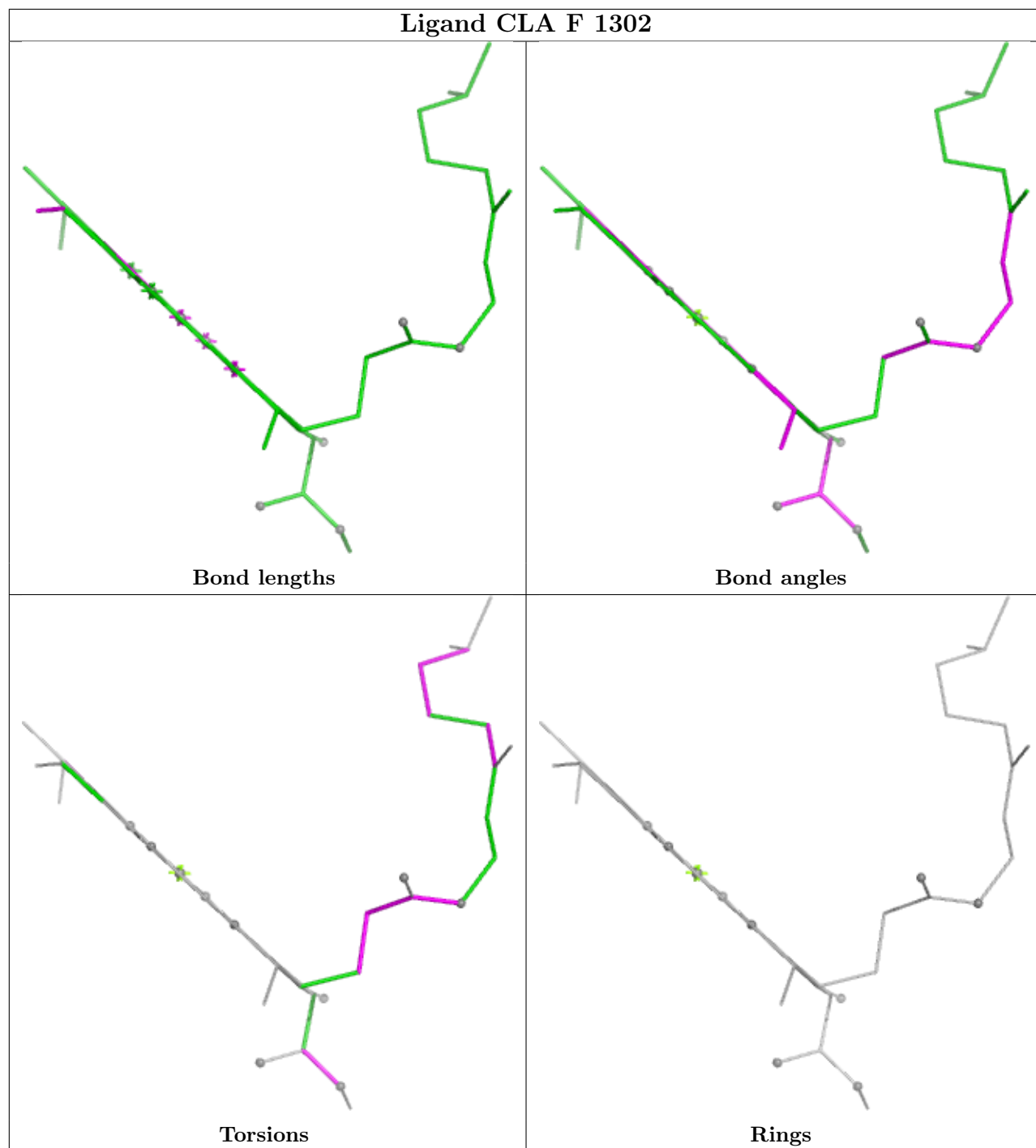


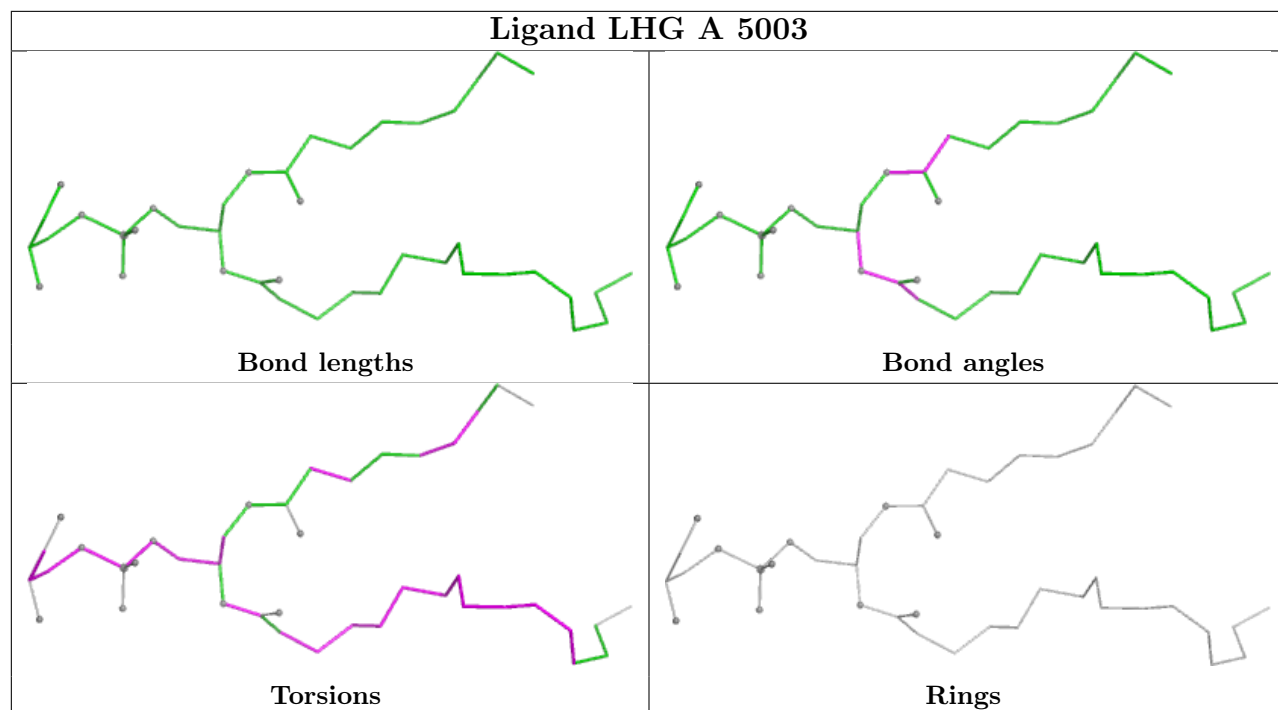


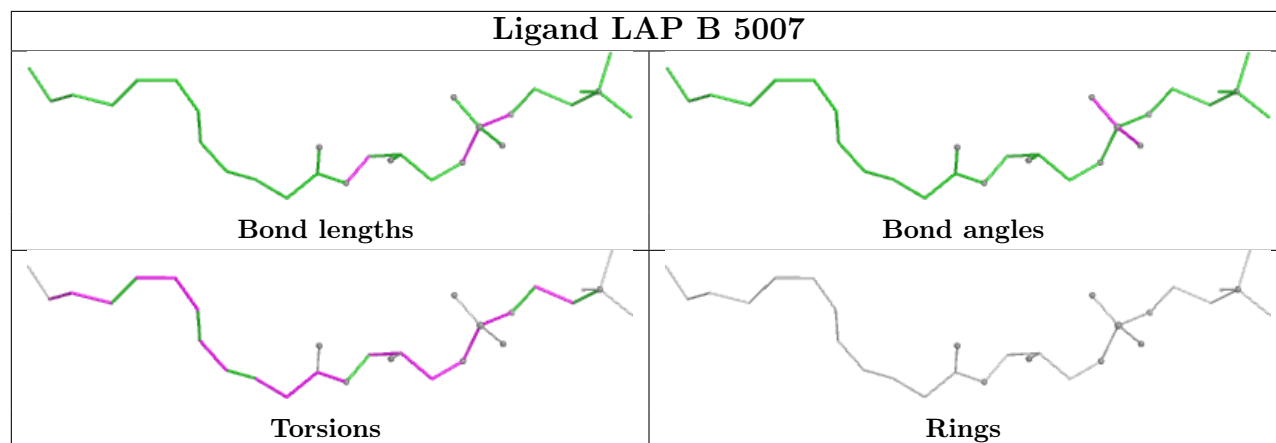
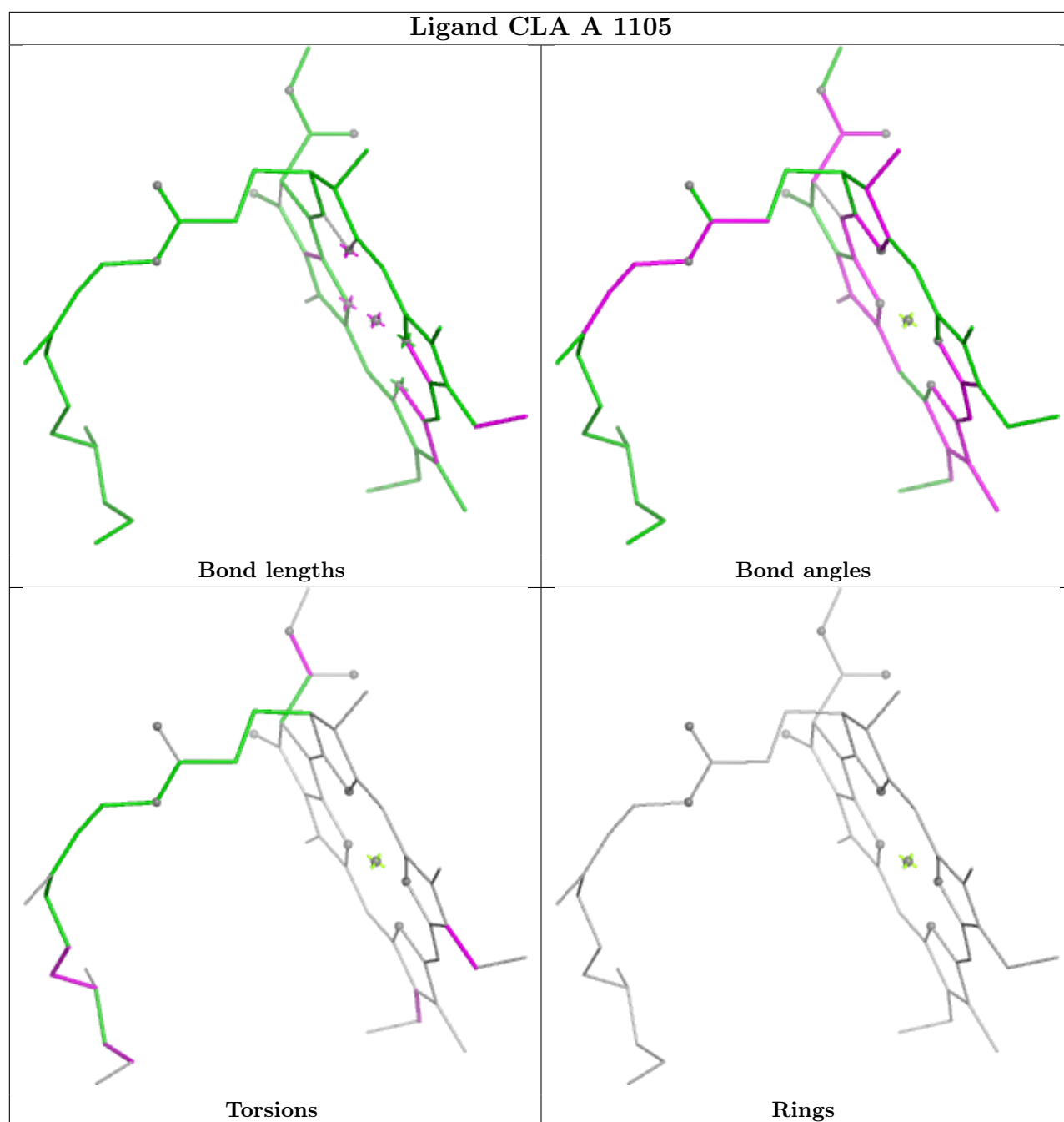
Ligand CHL a 610



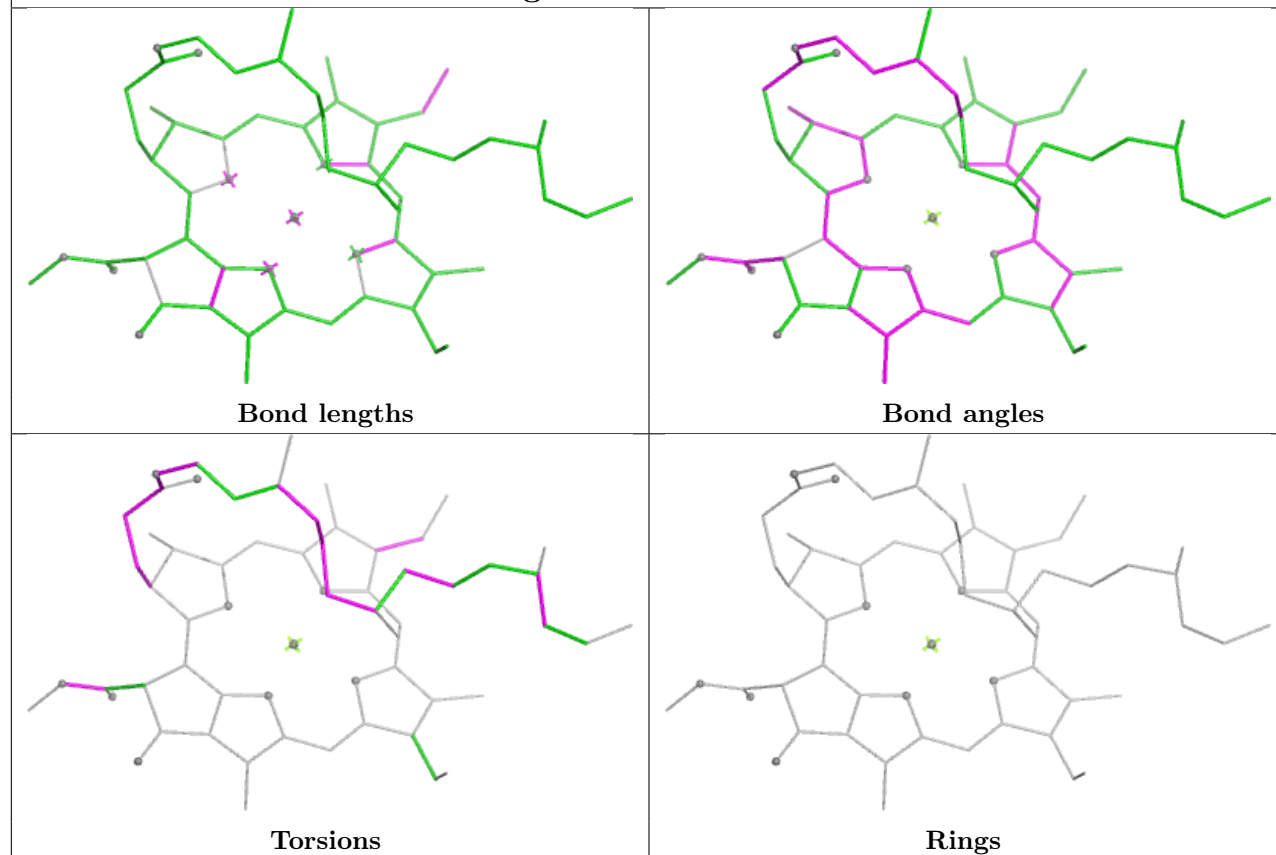




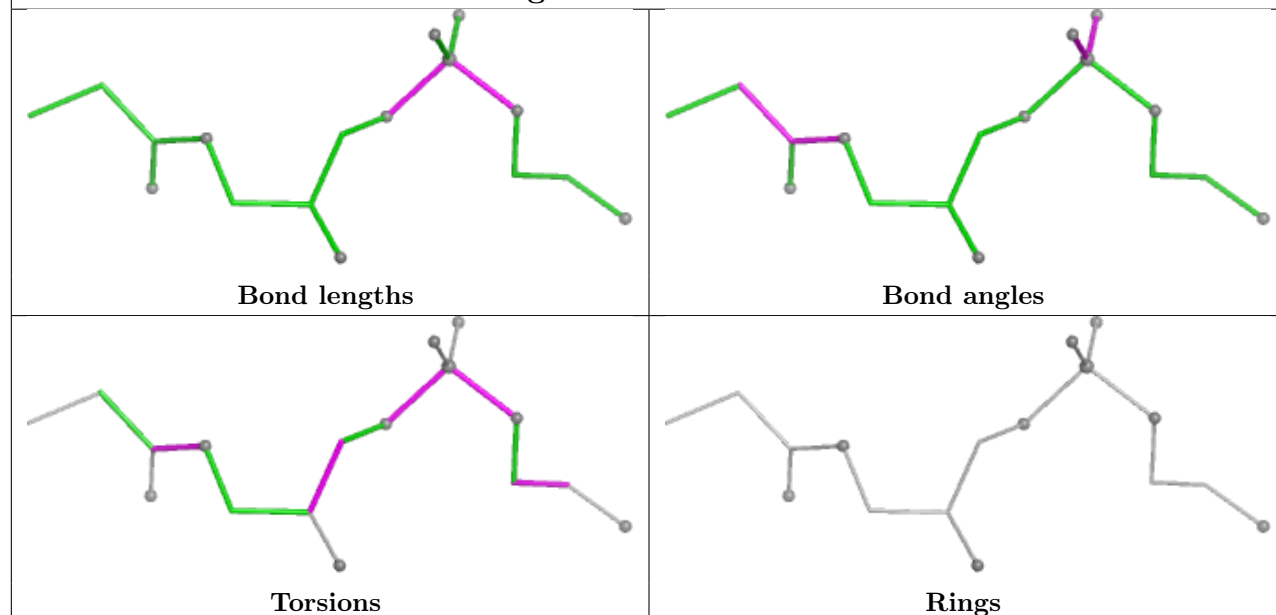


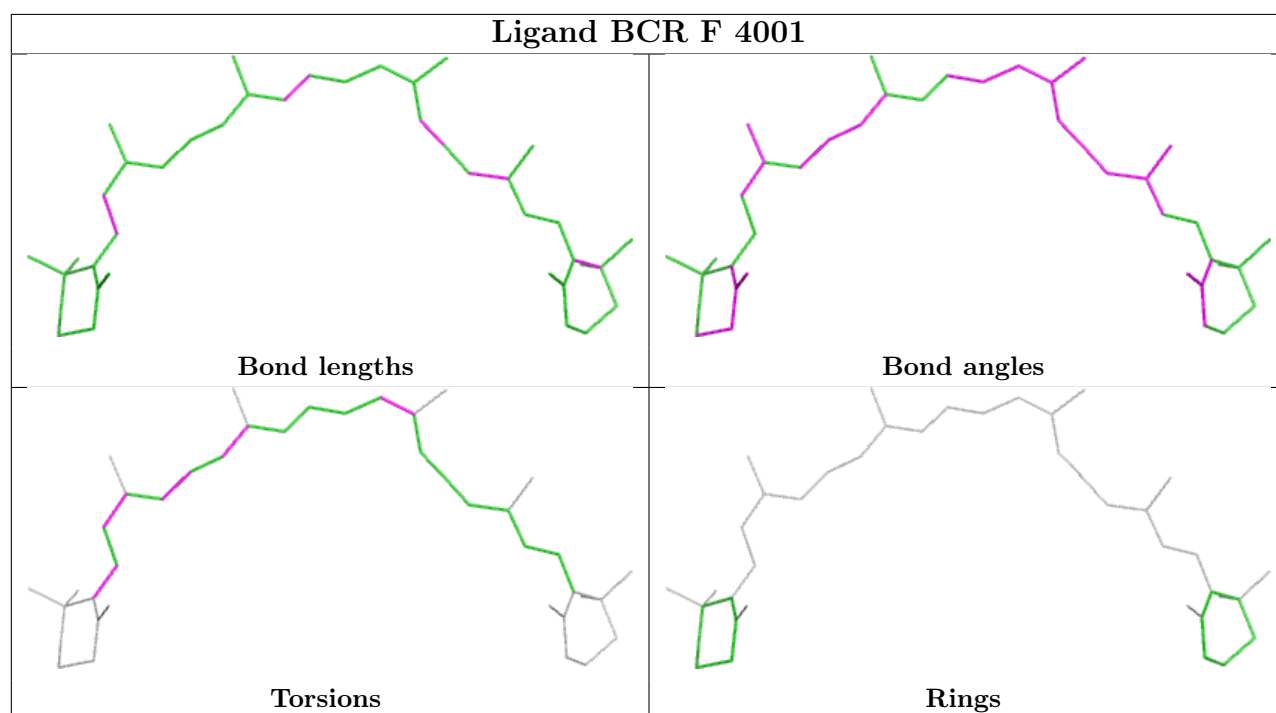
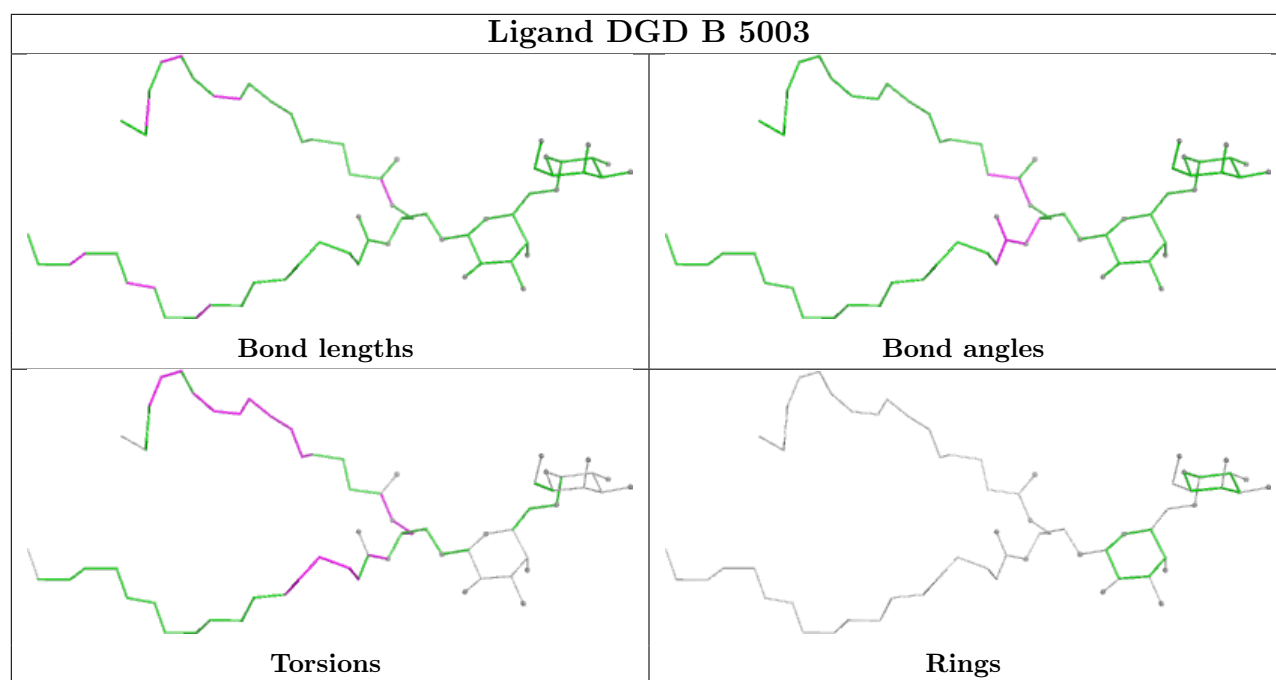


Ligand CLA B 1214

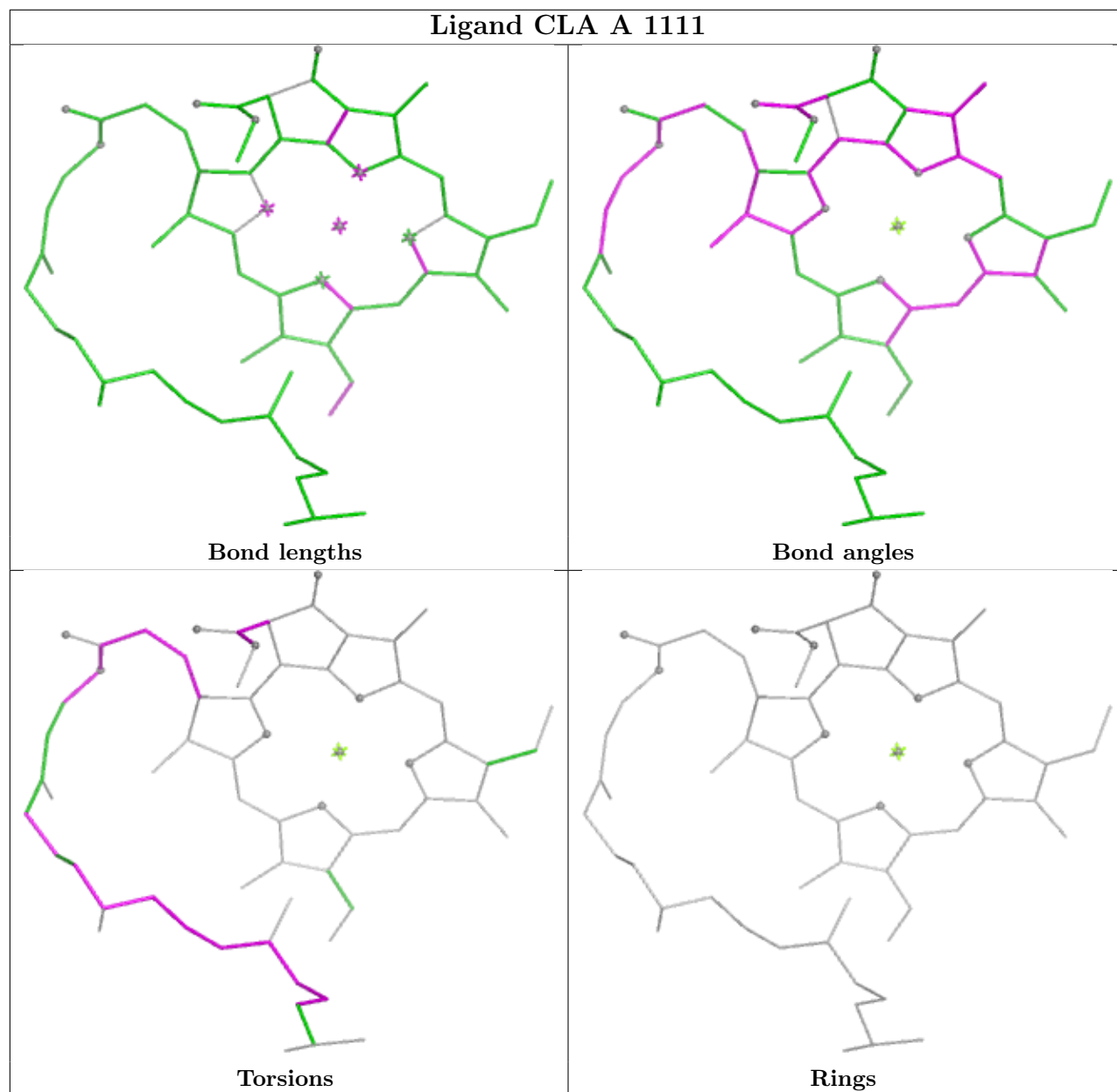


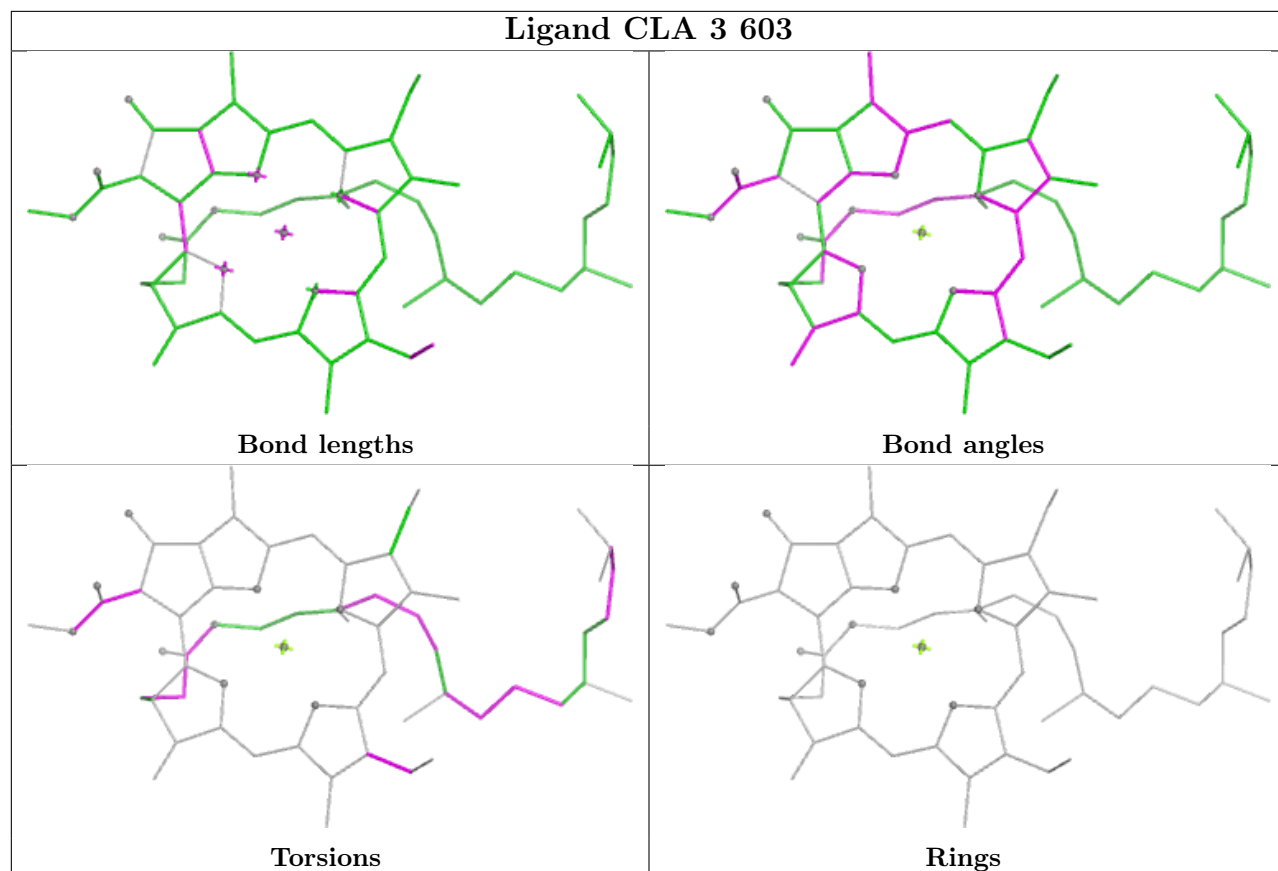
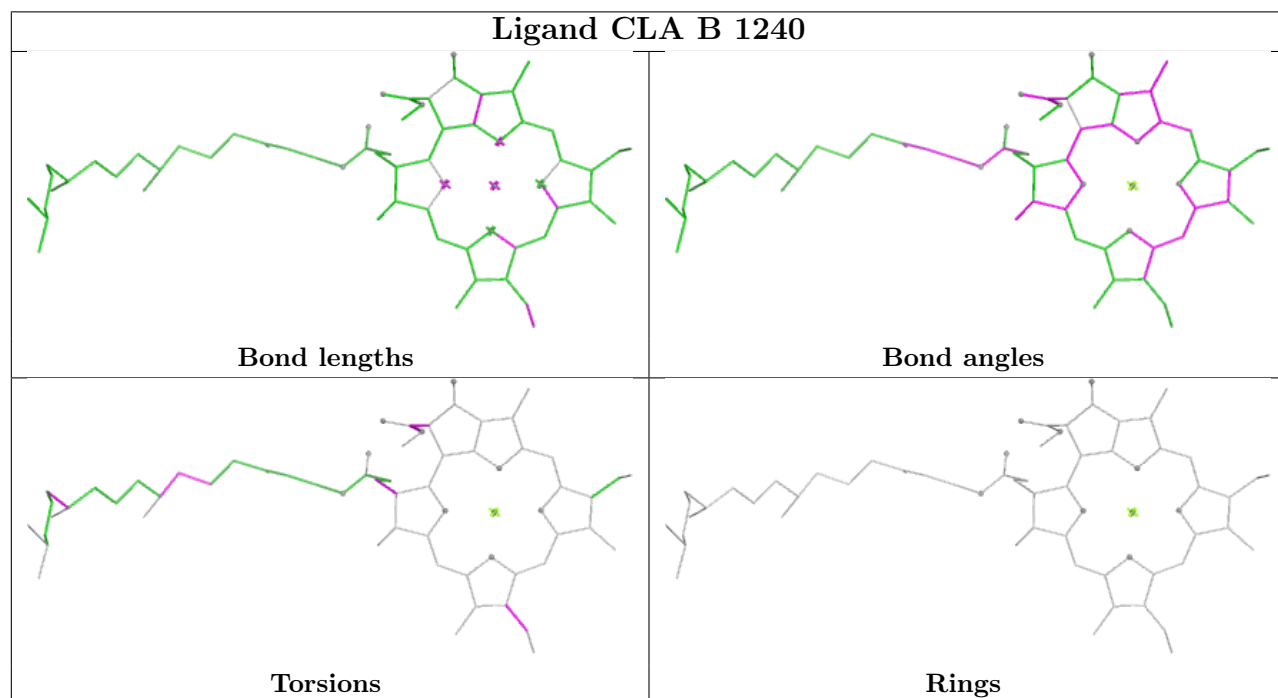
Ligand LPX J 5001

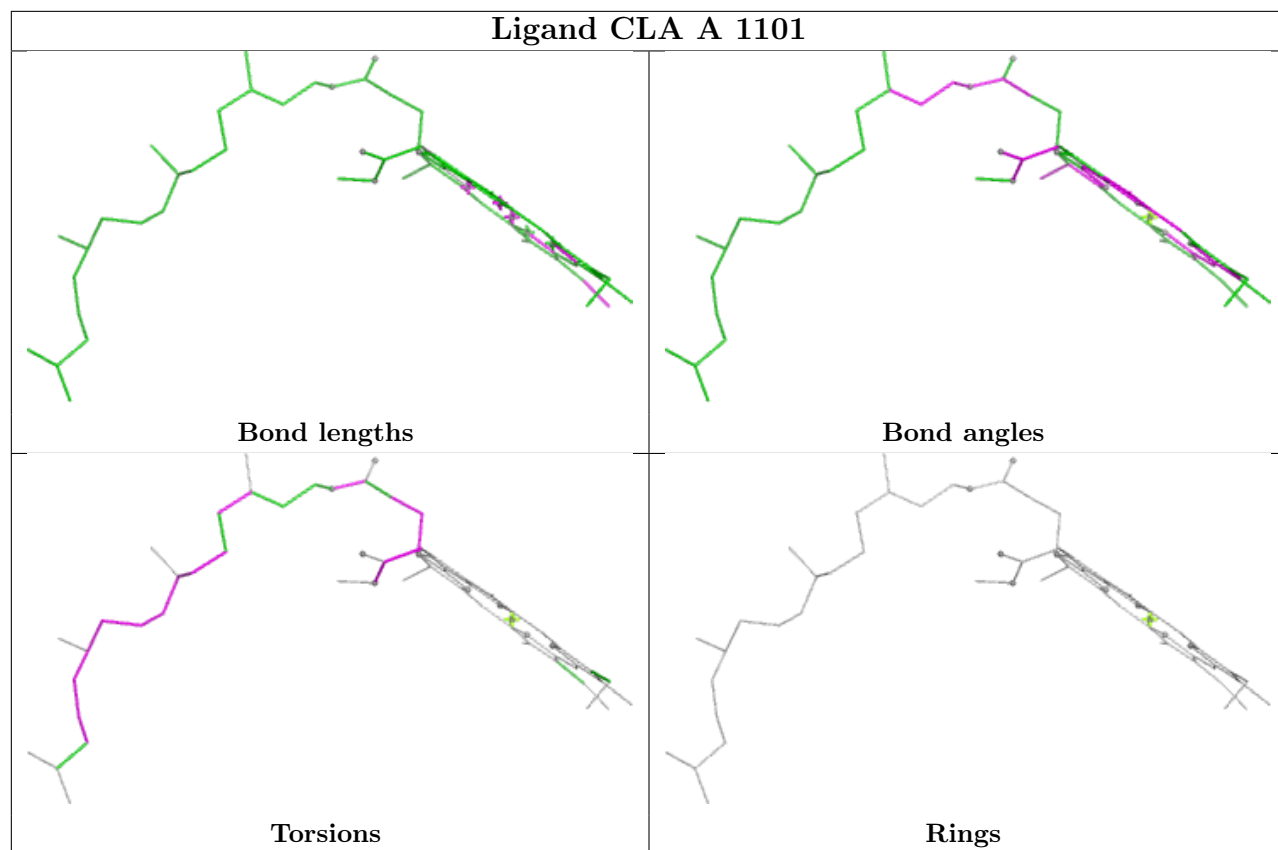


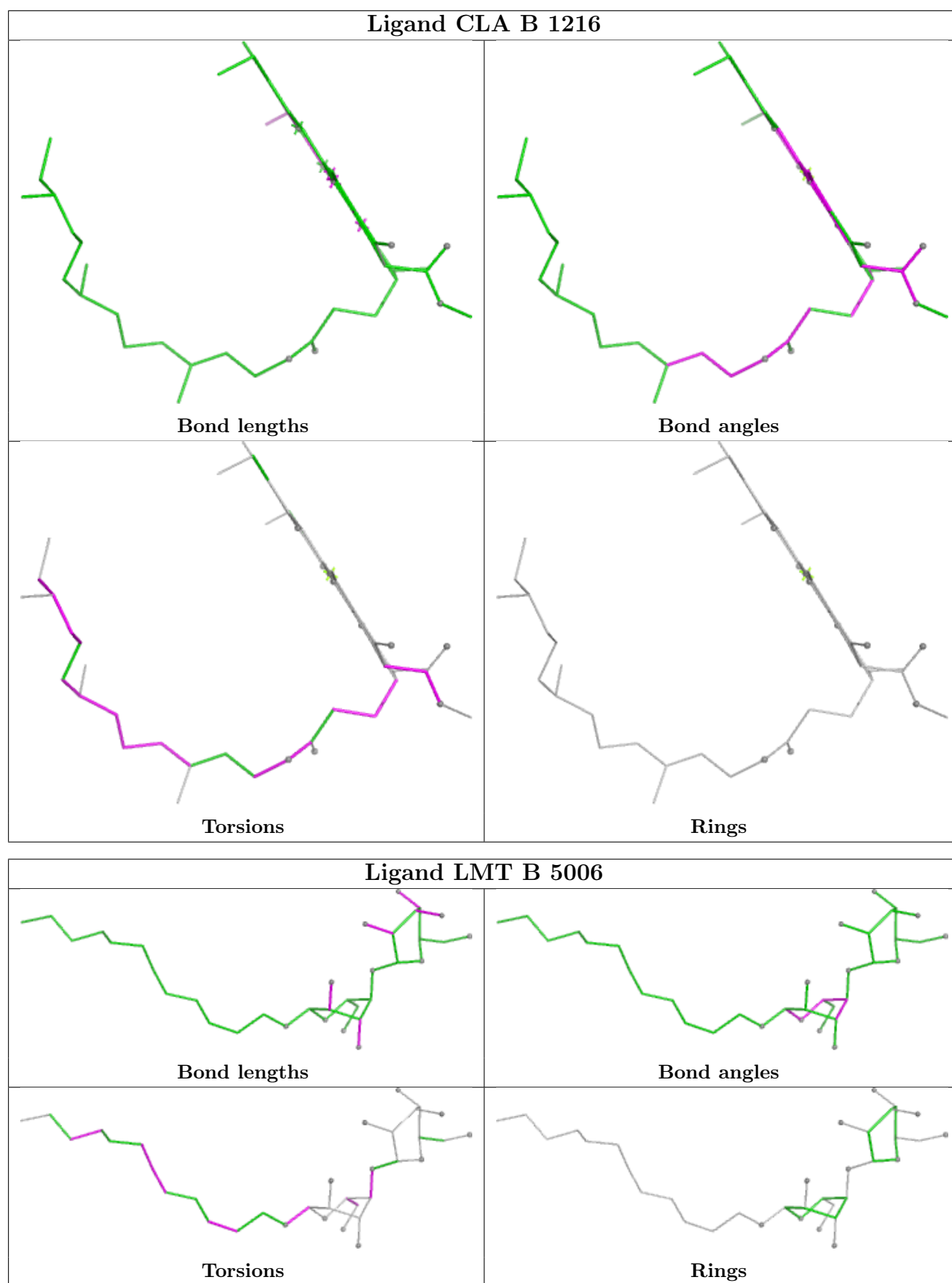


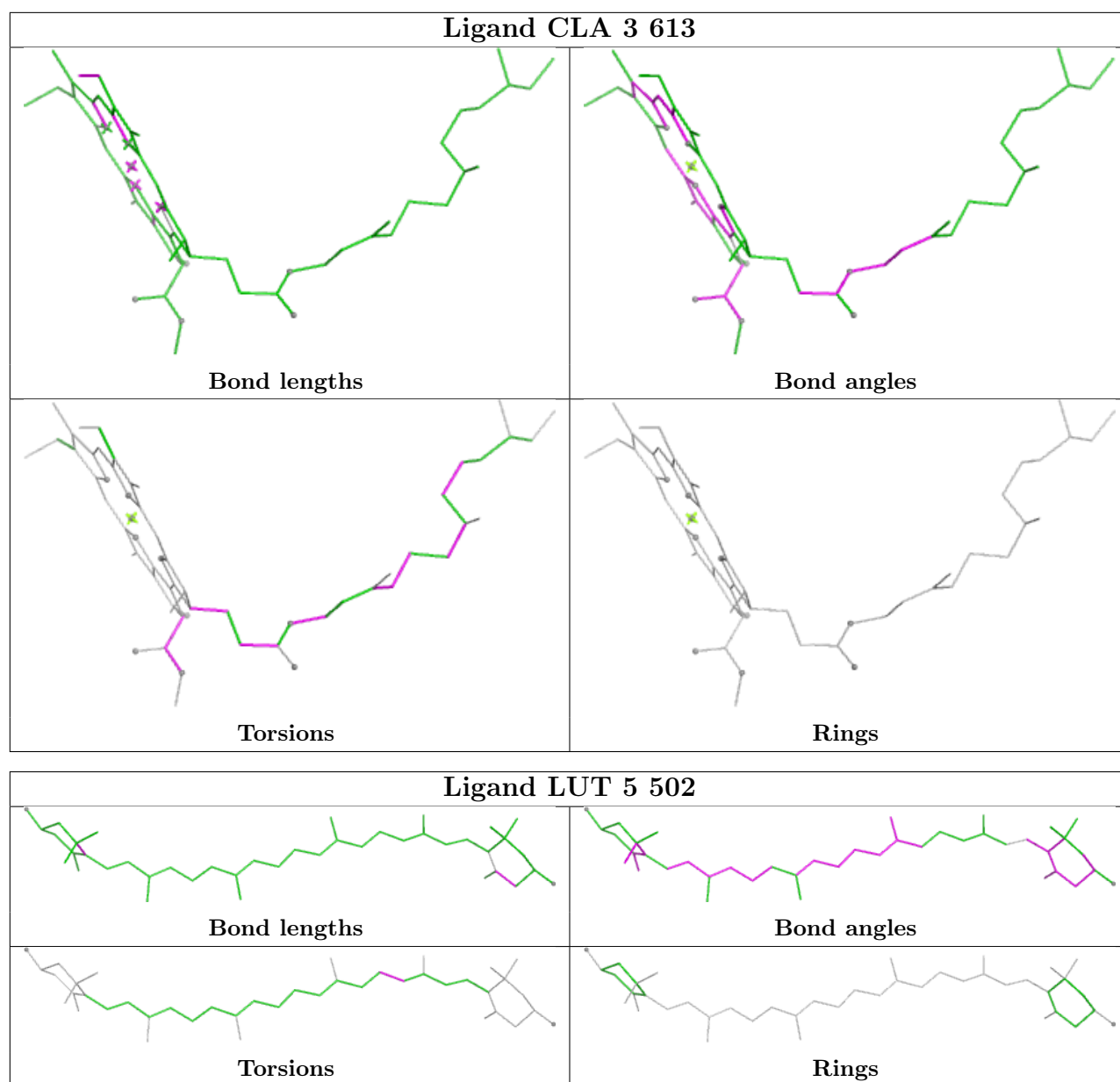
Ligand CLA A 1111

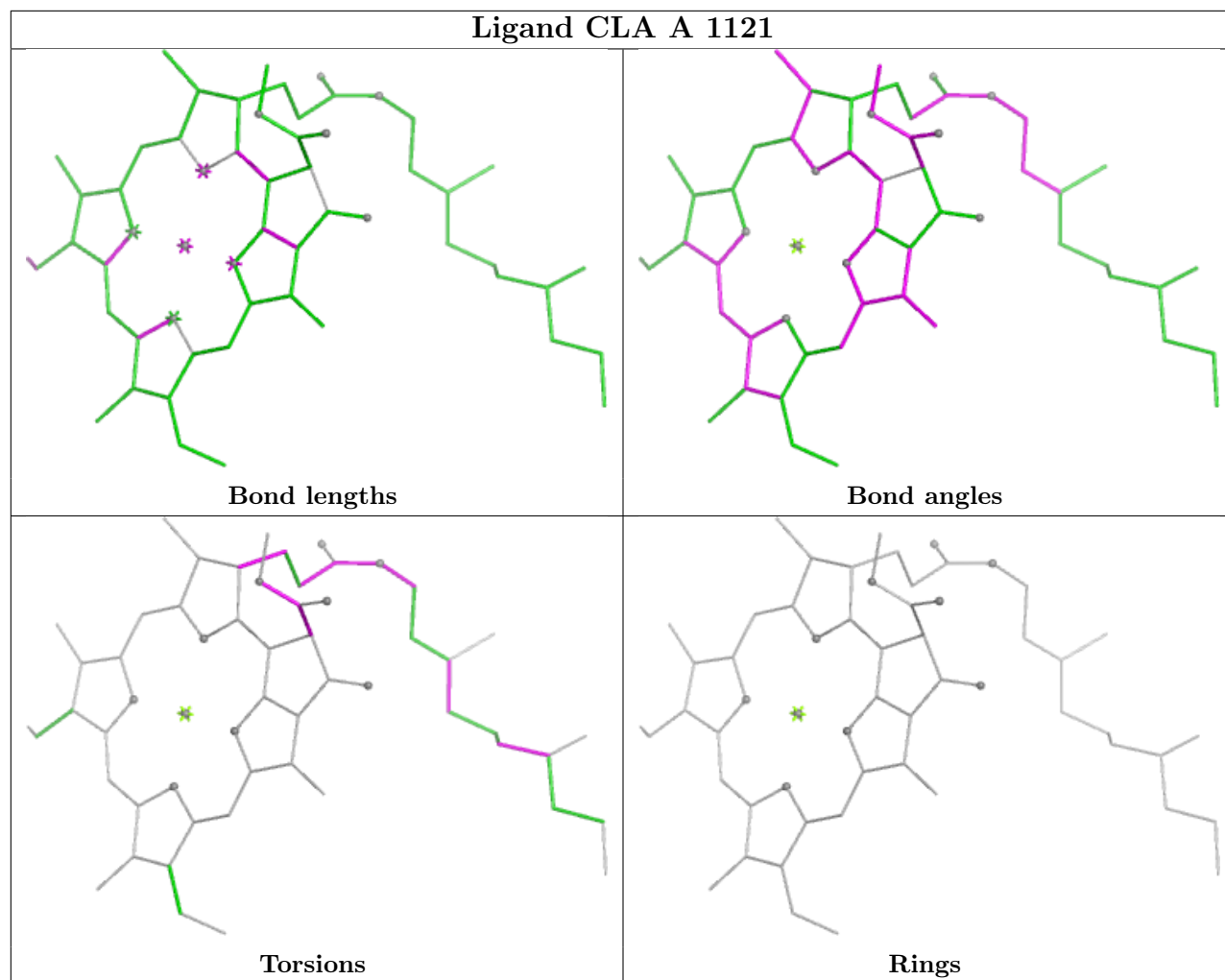


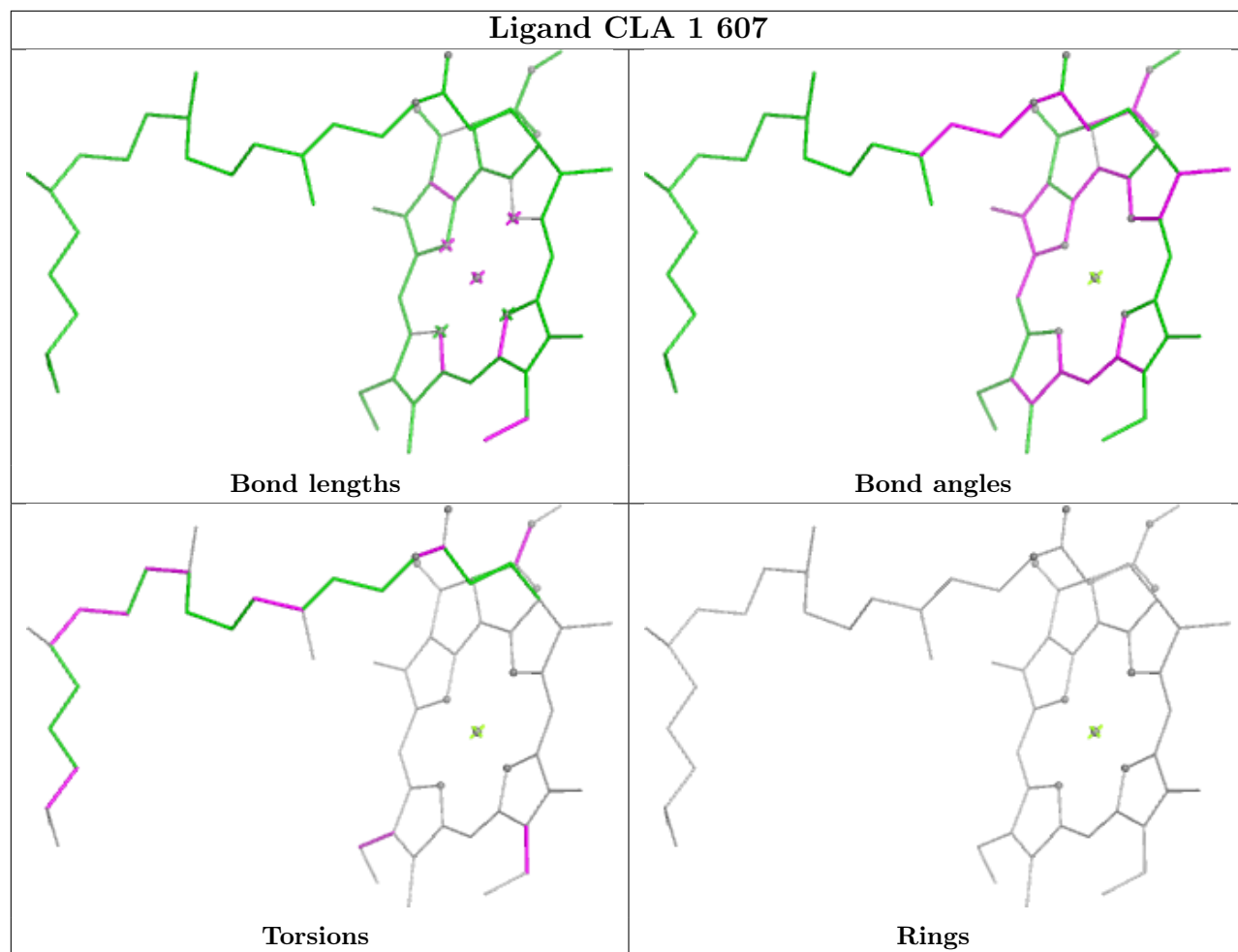
Ligand CLA 3 603**Ligand CLA B 1240**

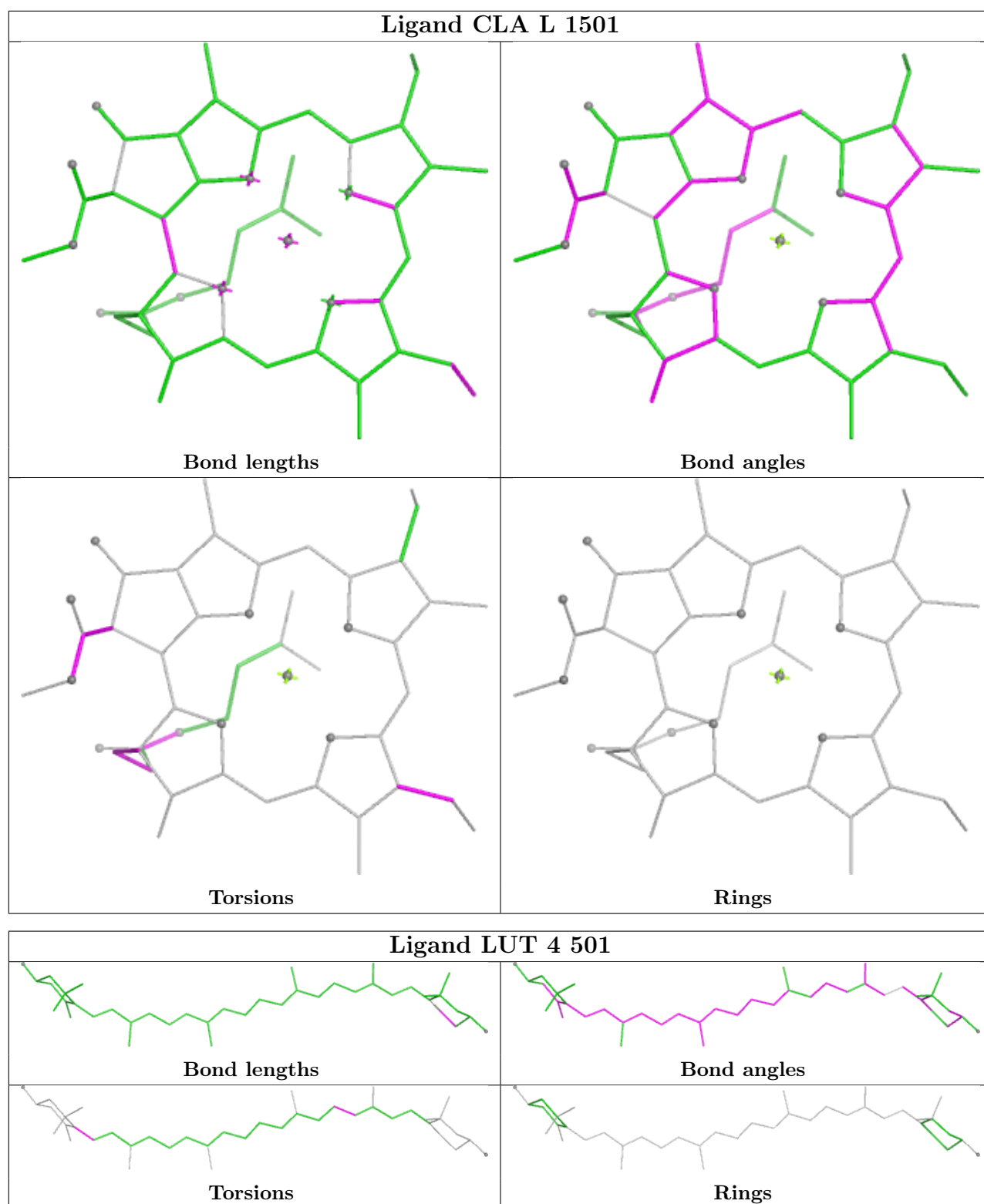


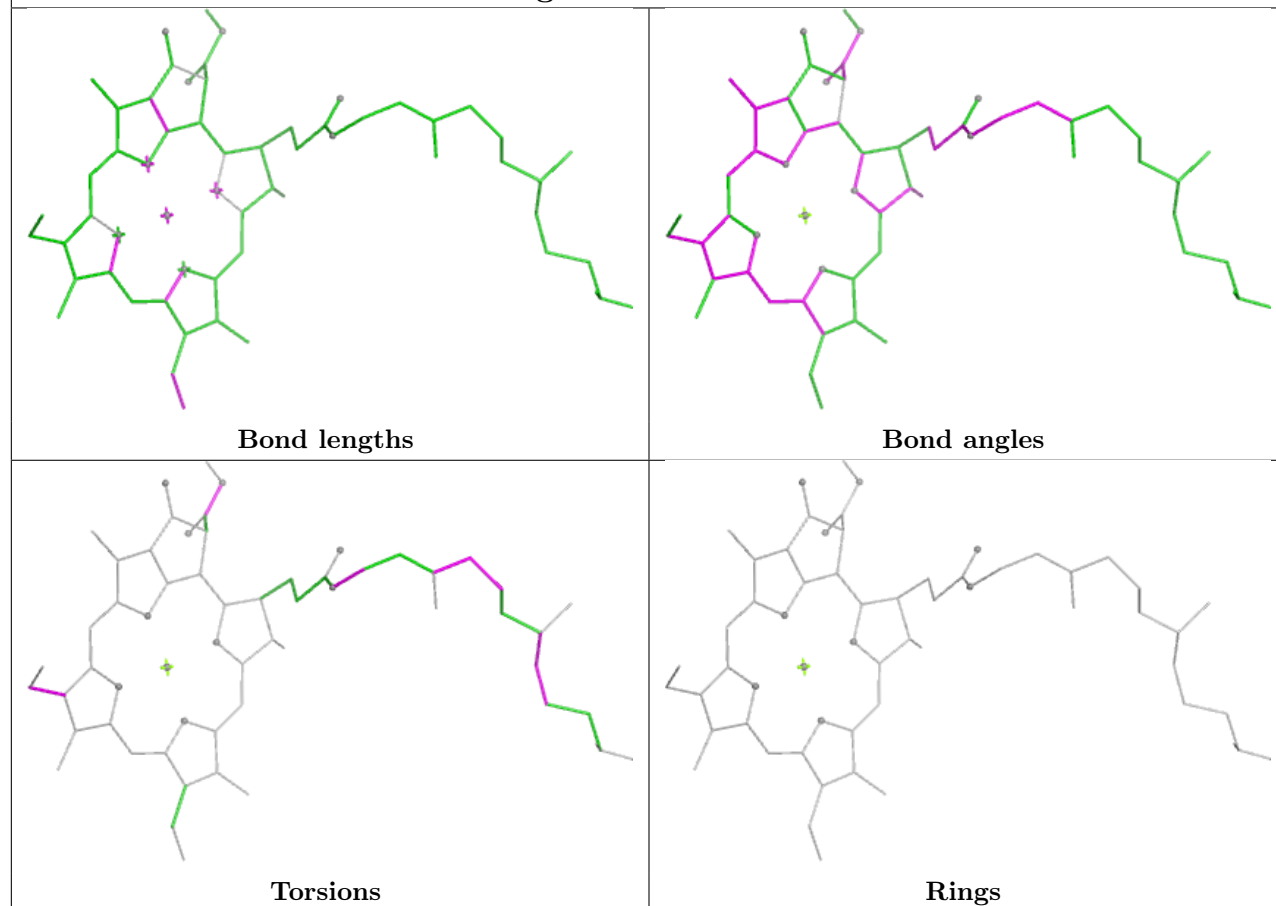
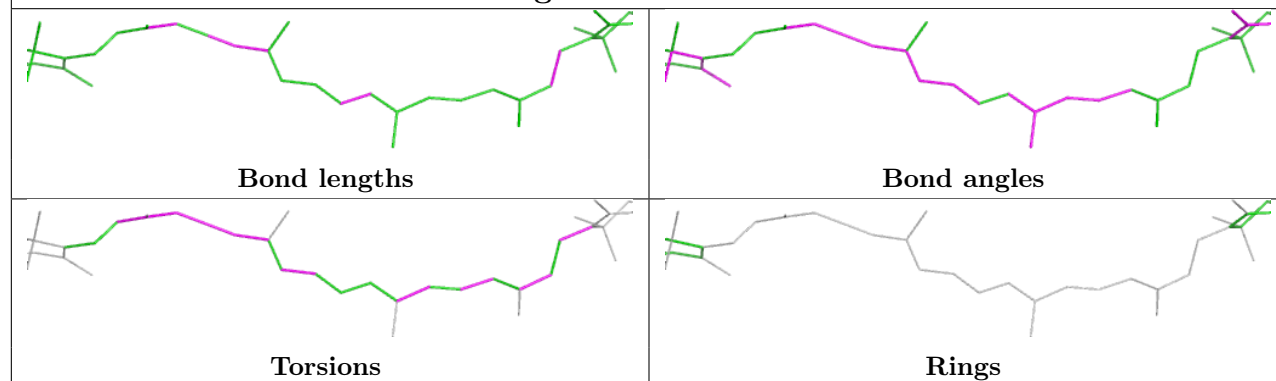


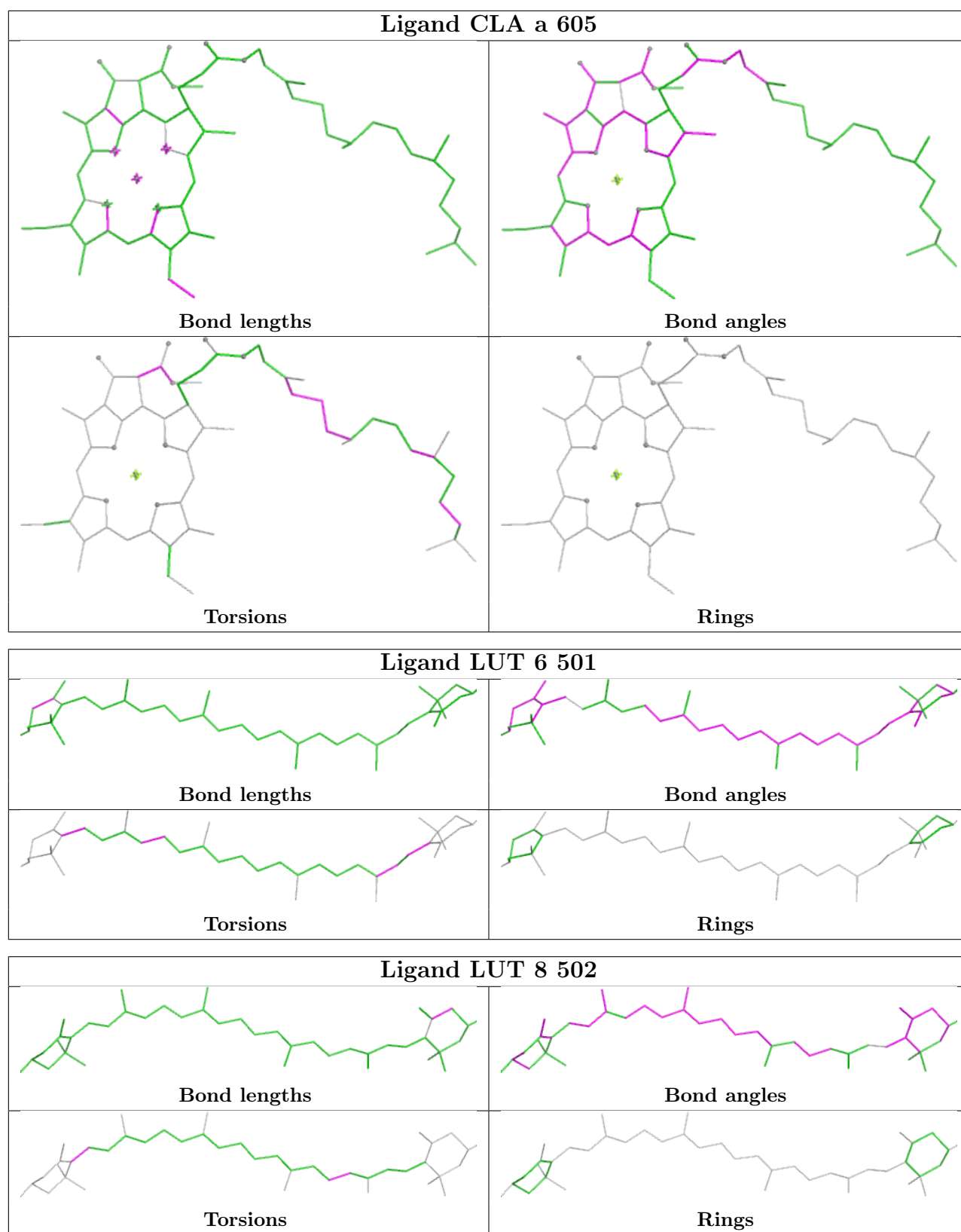


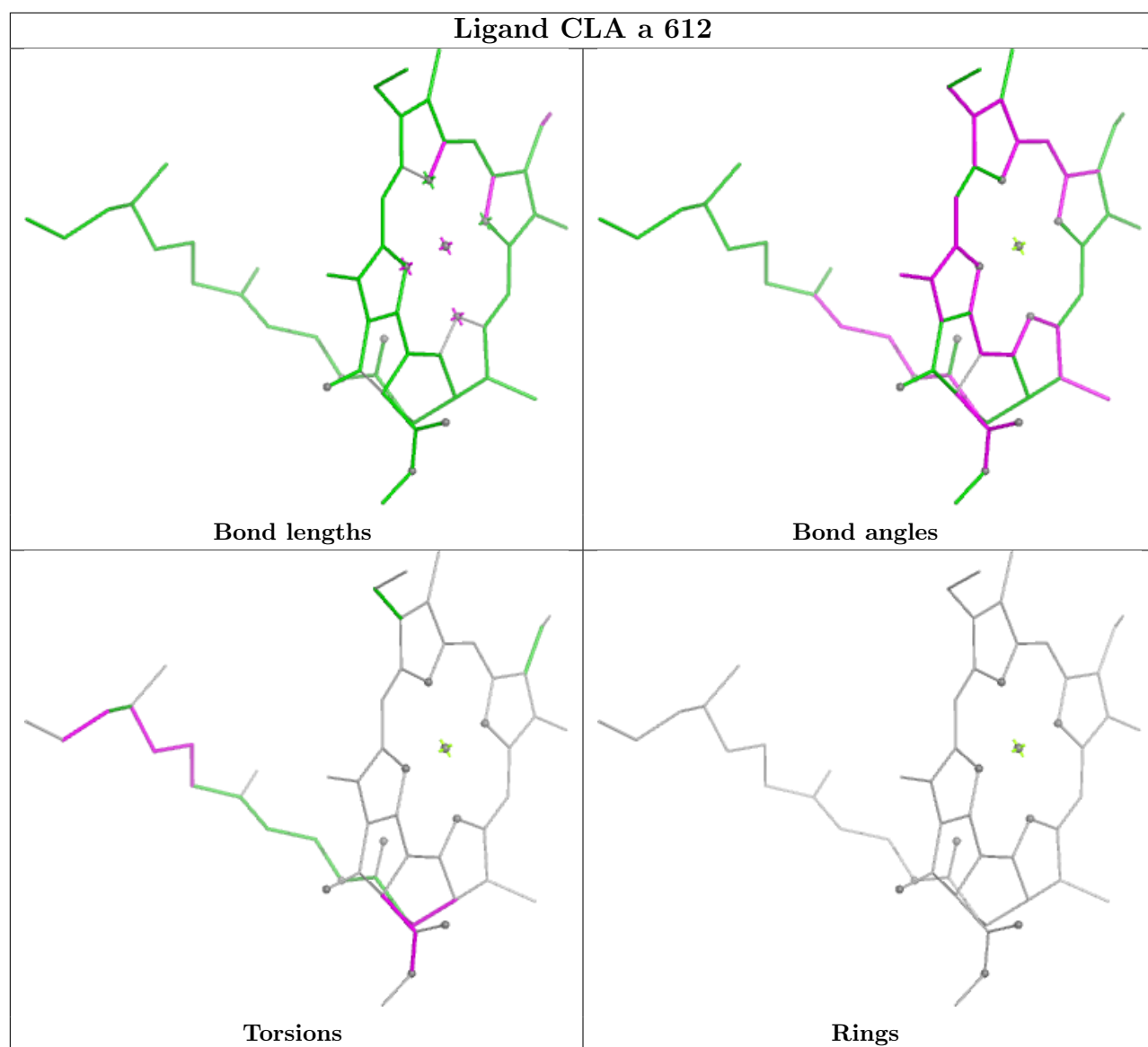




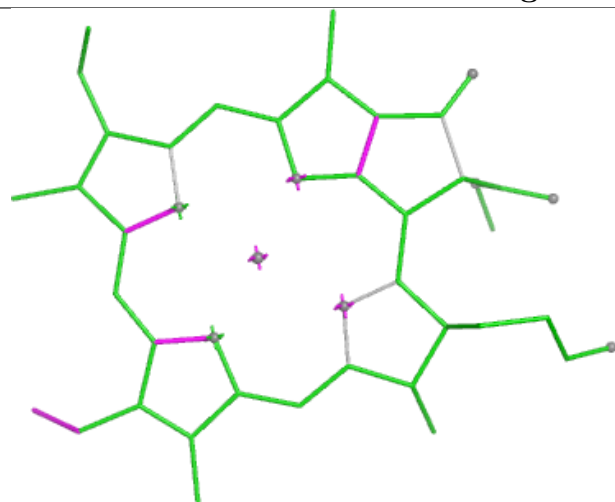


Ligand CLA 7 611**Ligand BCR 4 503**

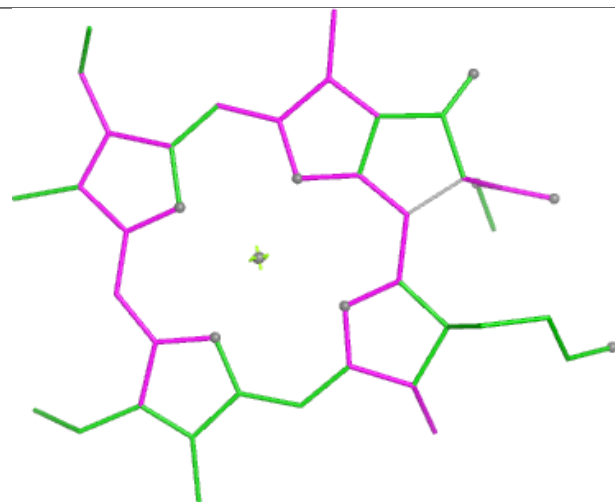




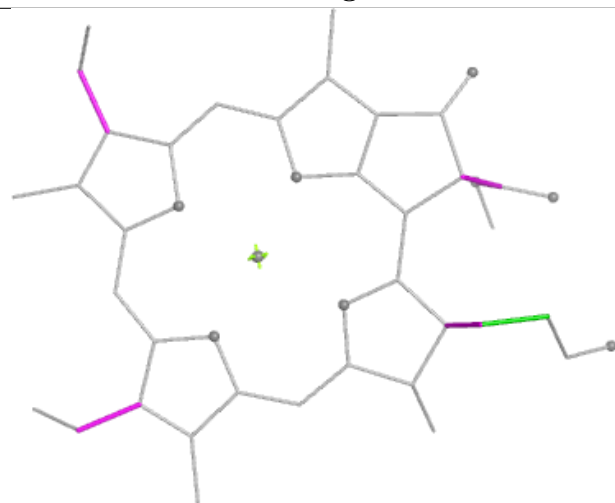
Ligand CLA 7 602



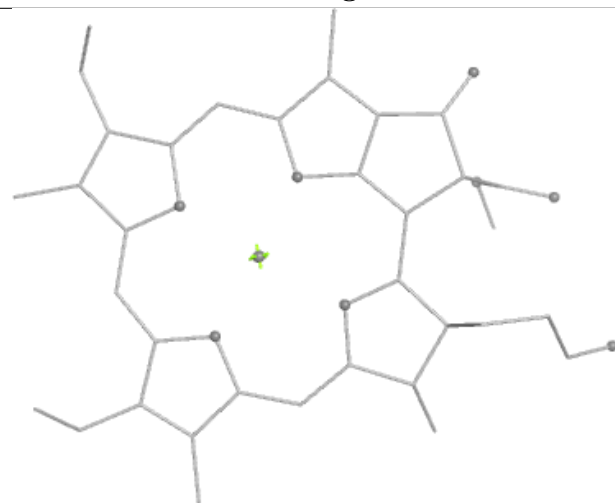
Bond lengths



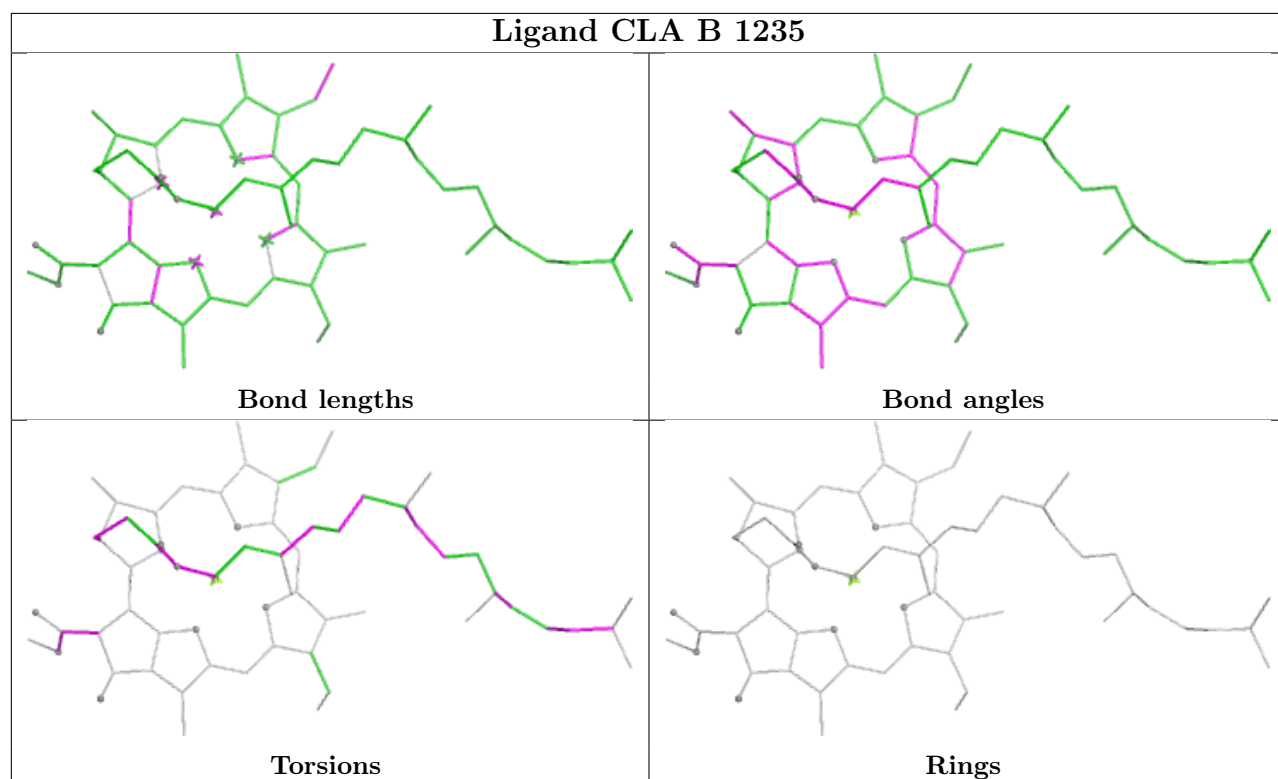
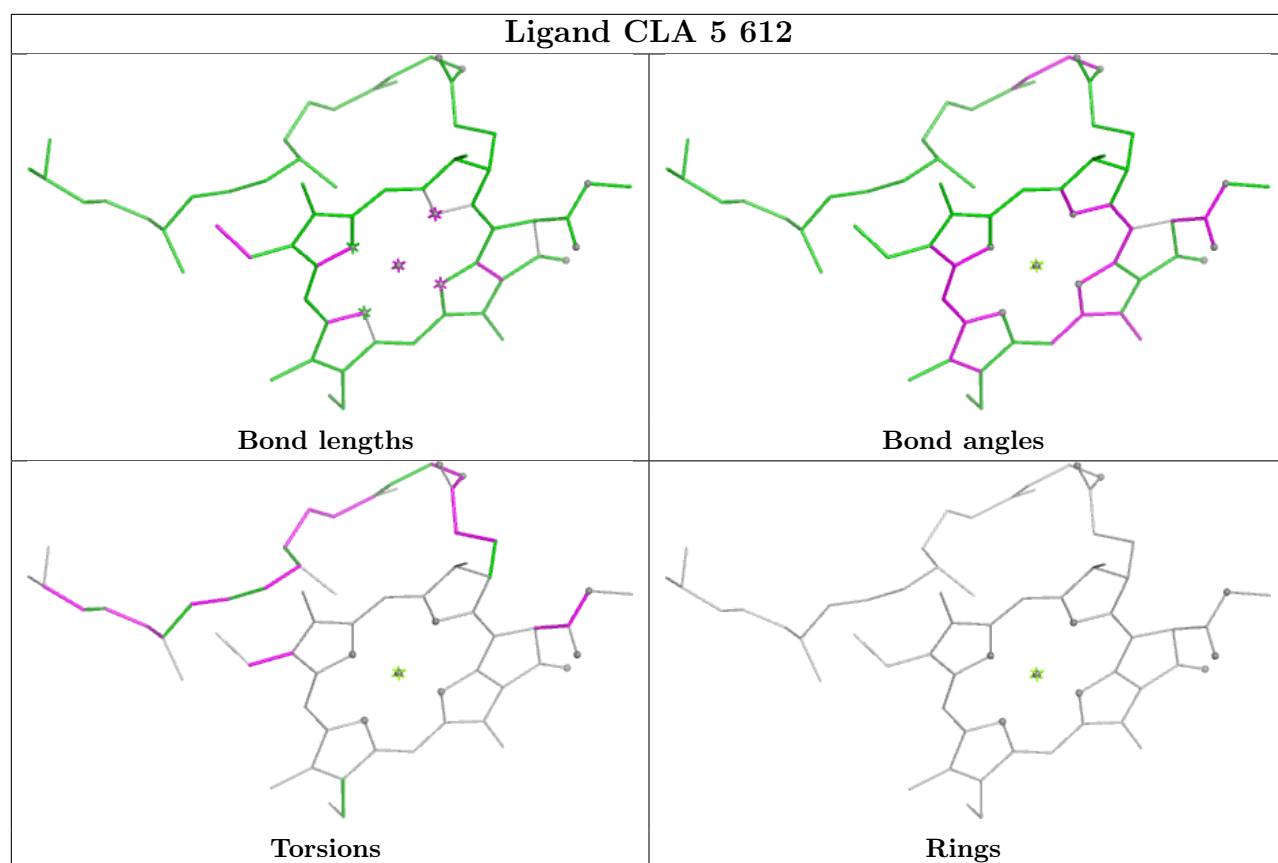
Bond angles

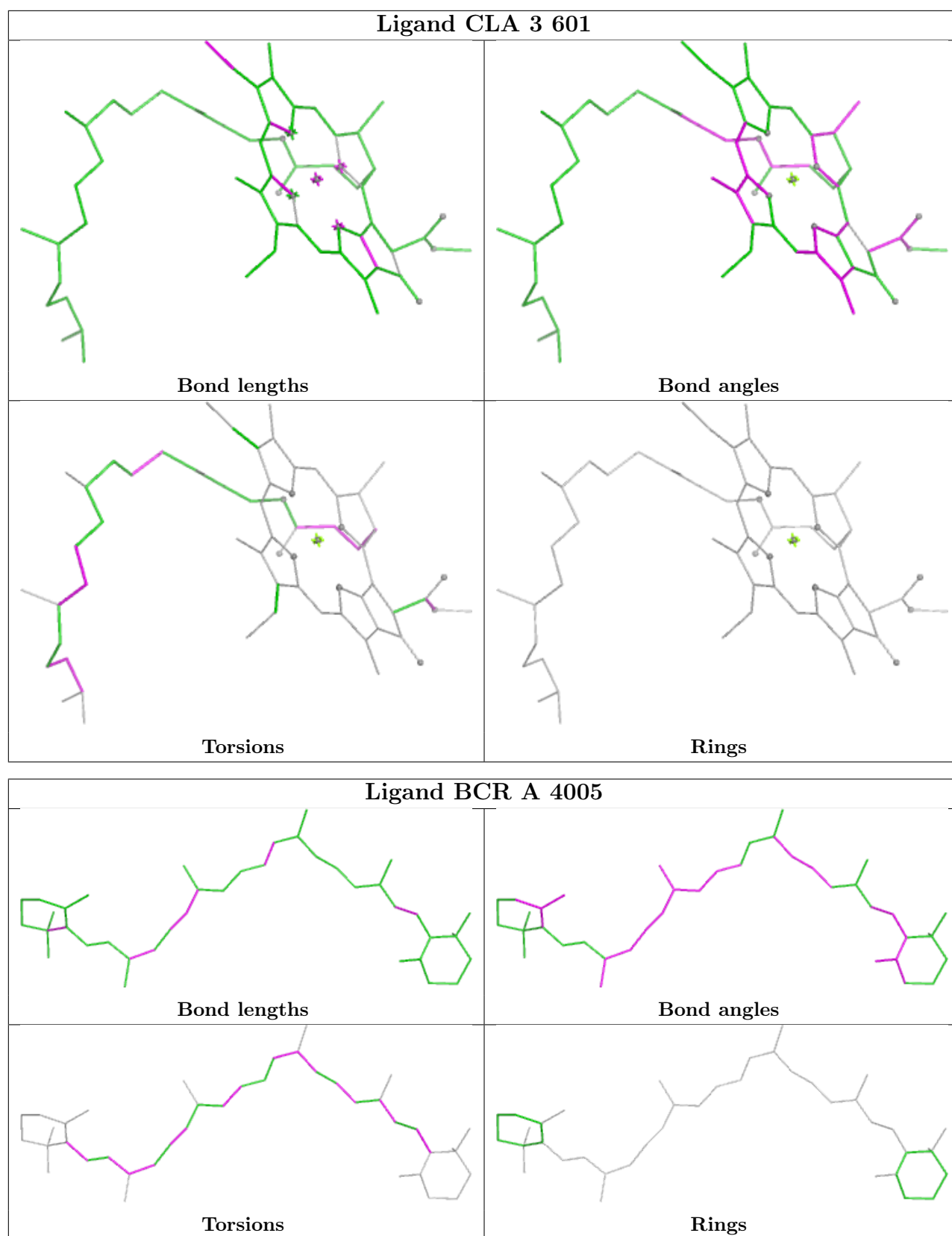


Torsions

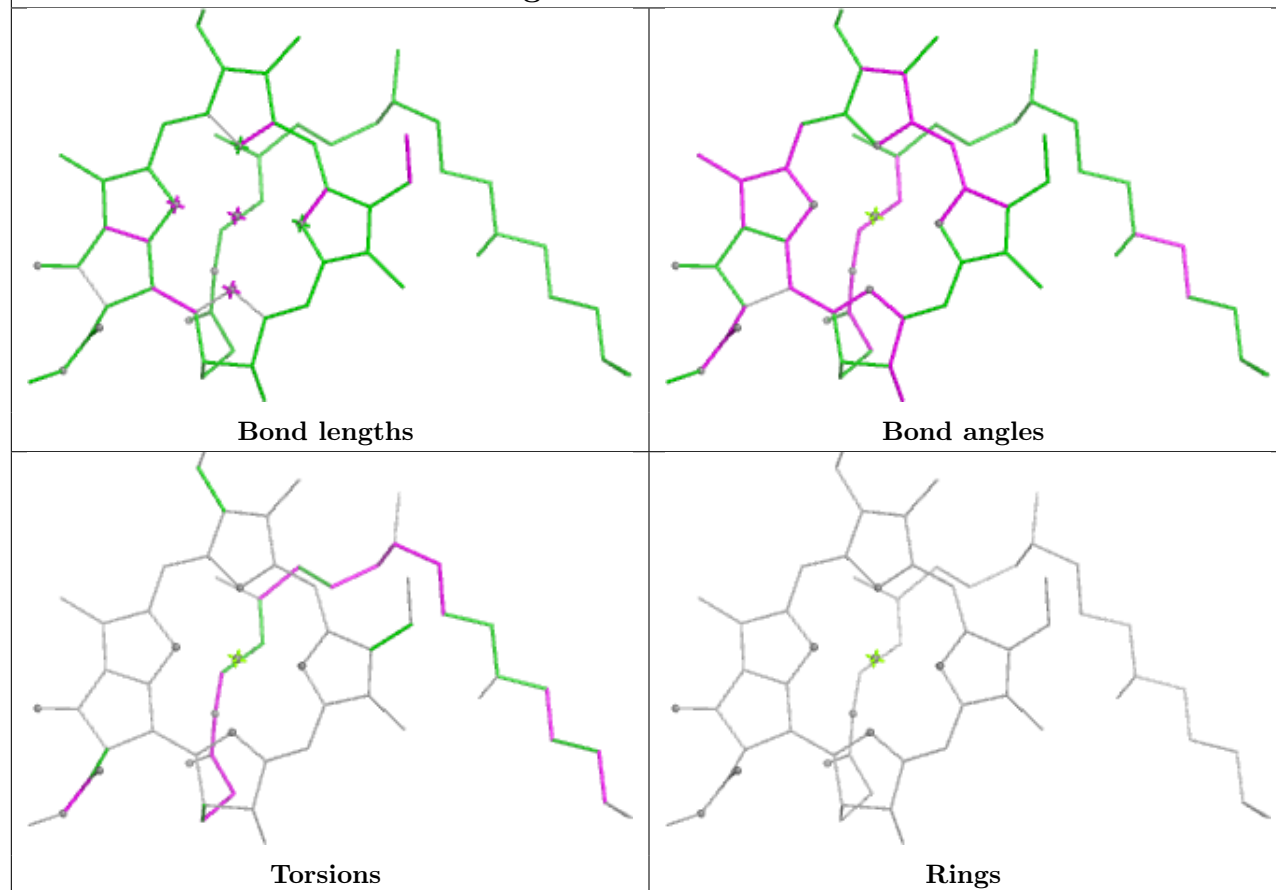


Rings

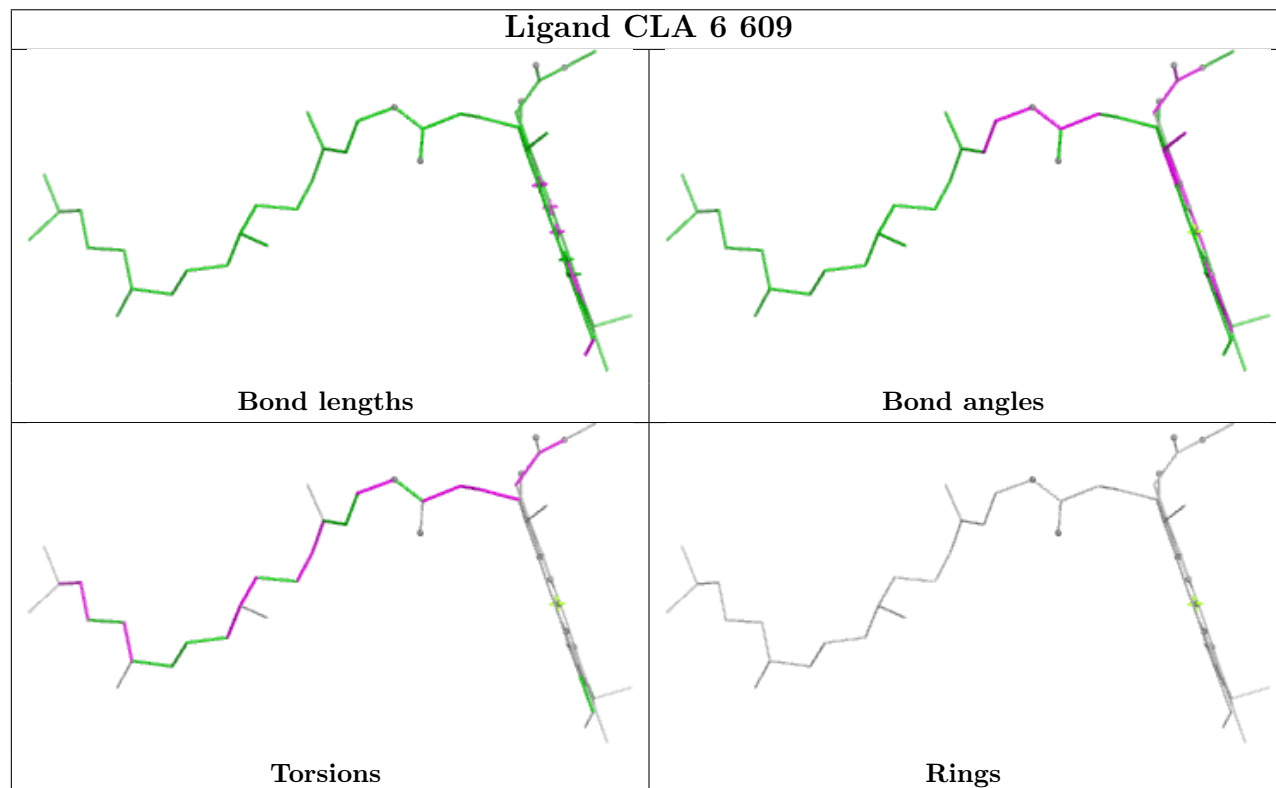


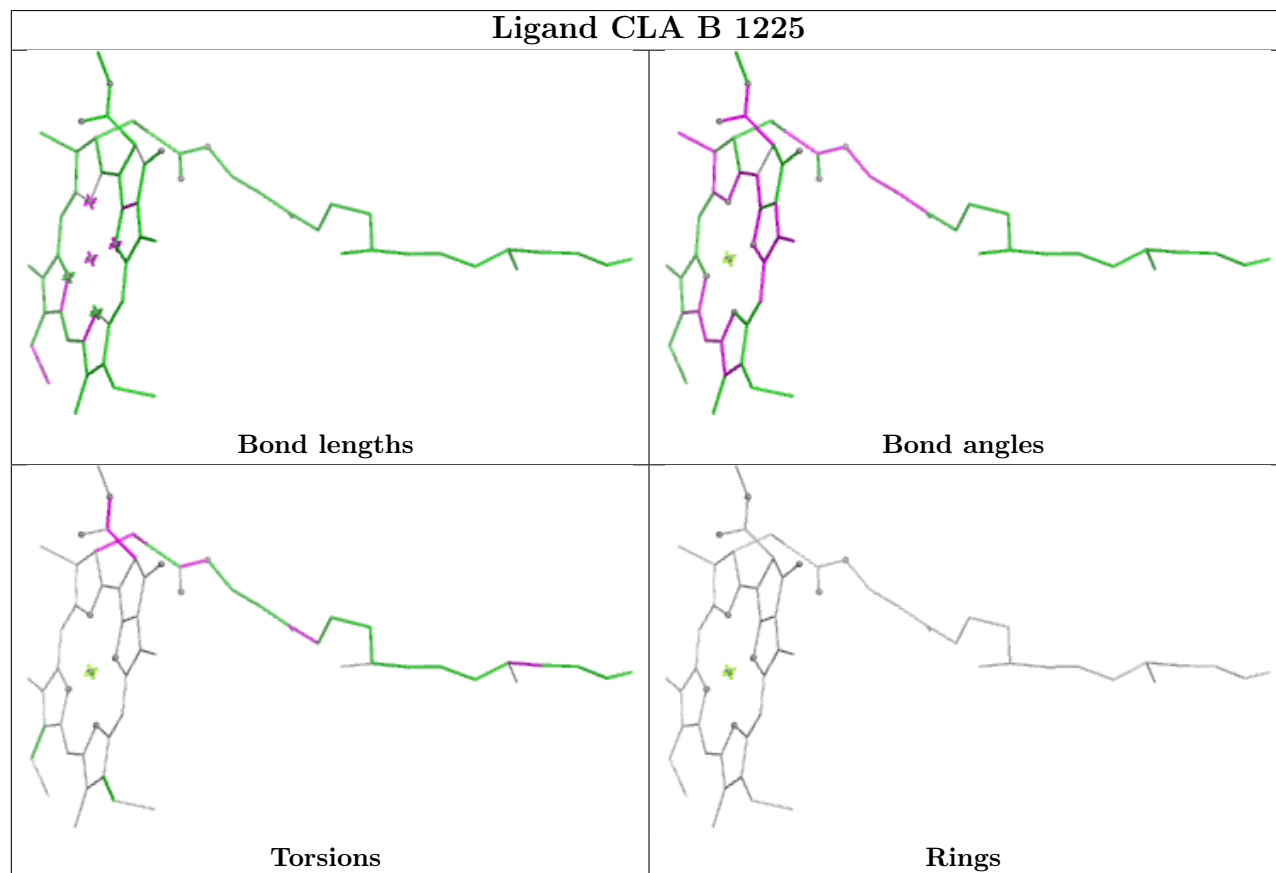
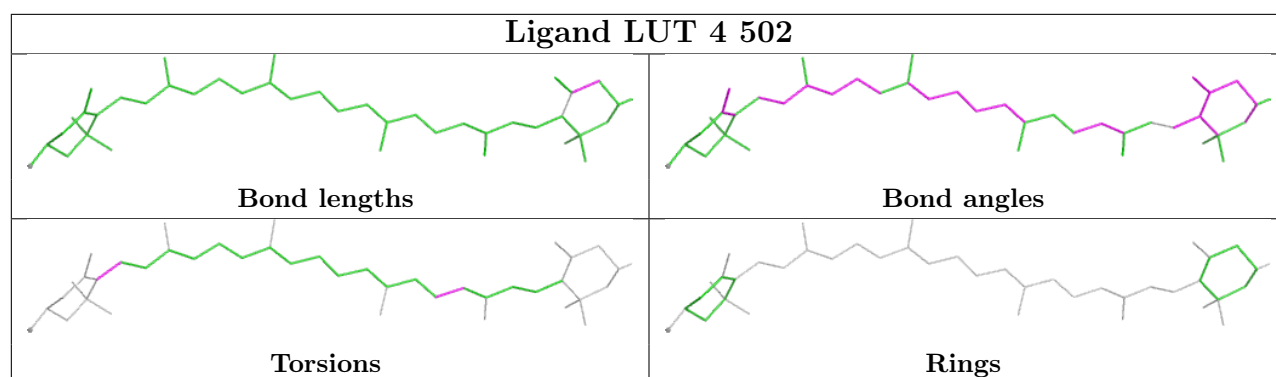


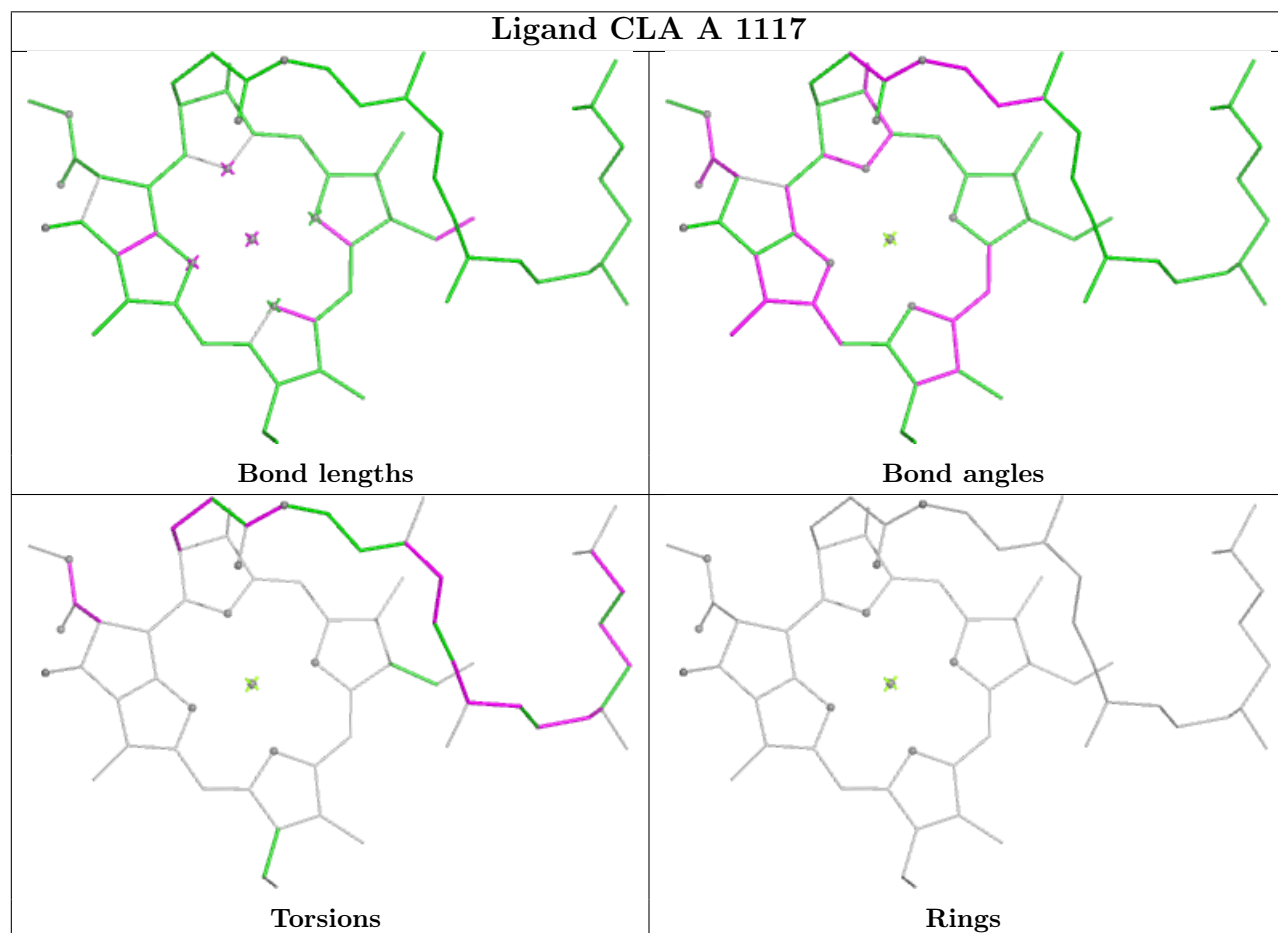
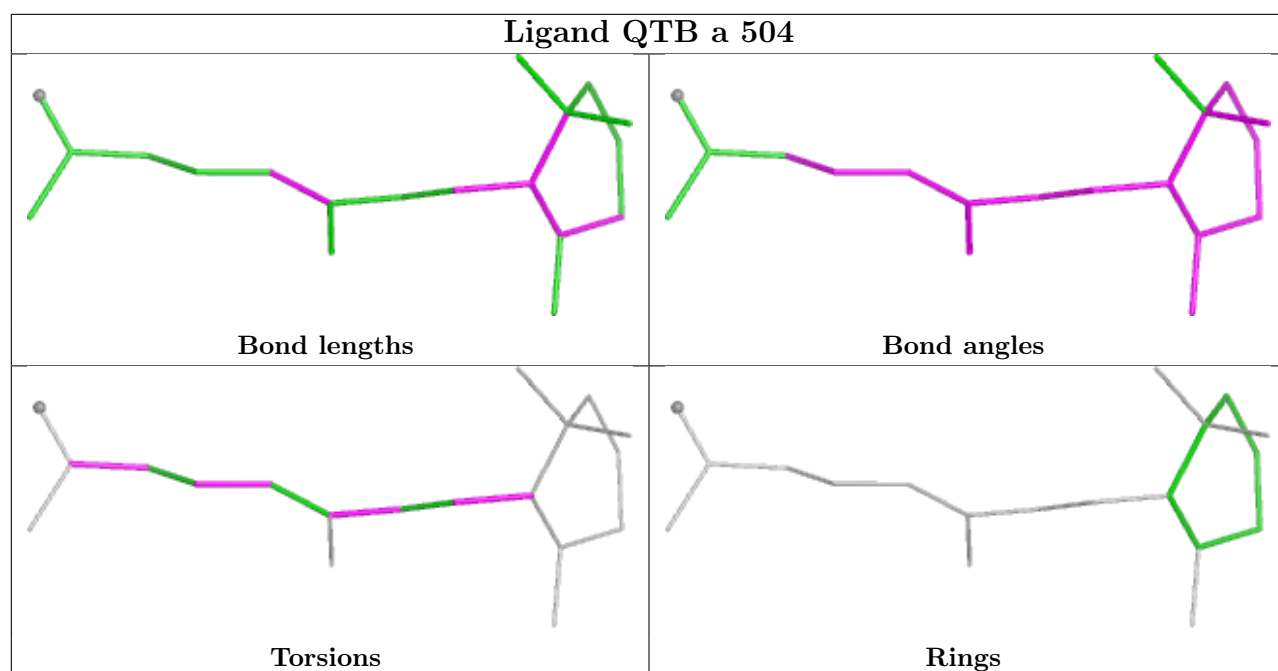
Ligand CLA B 1209

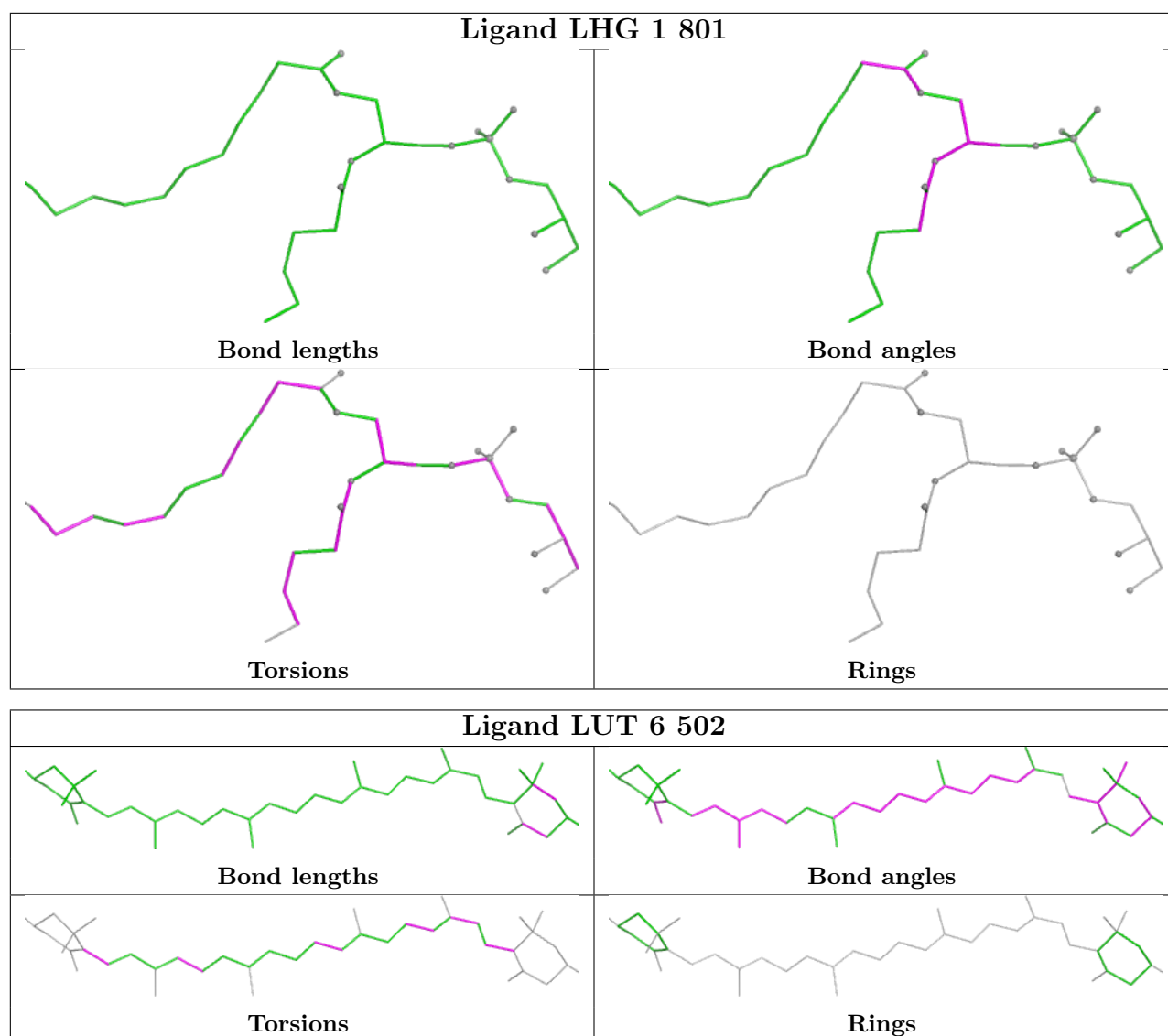


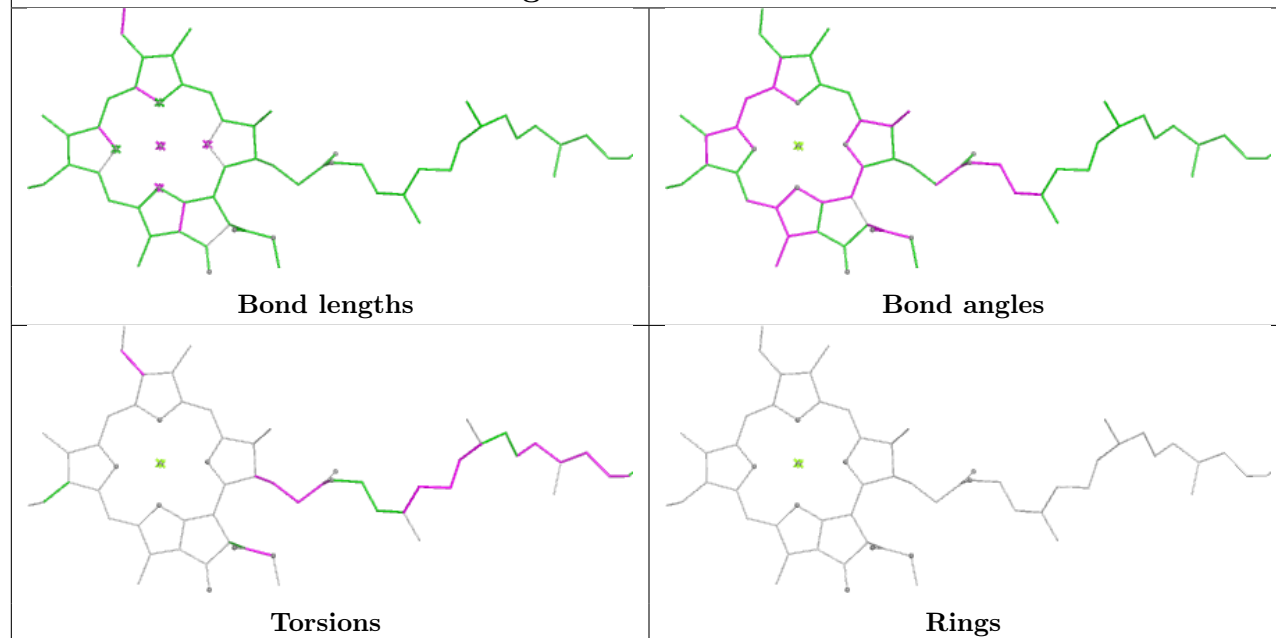
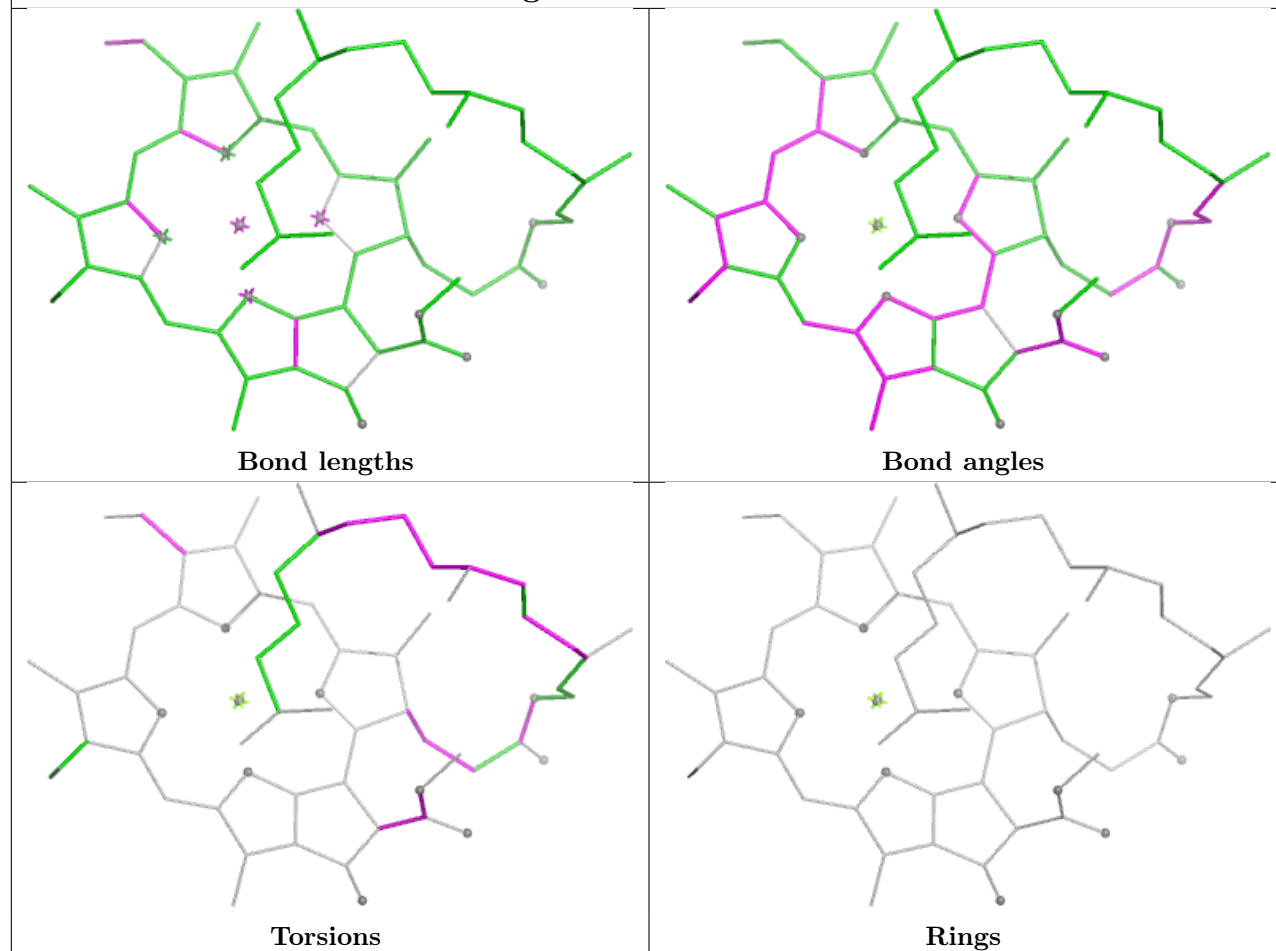
Ligand CLA 6 609

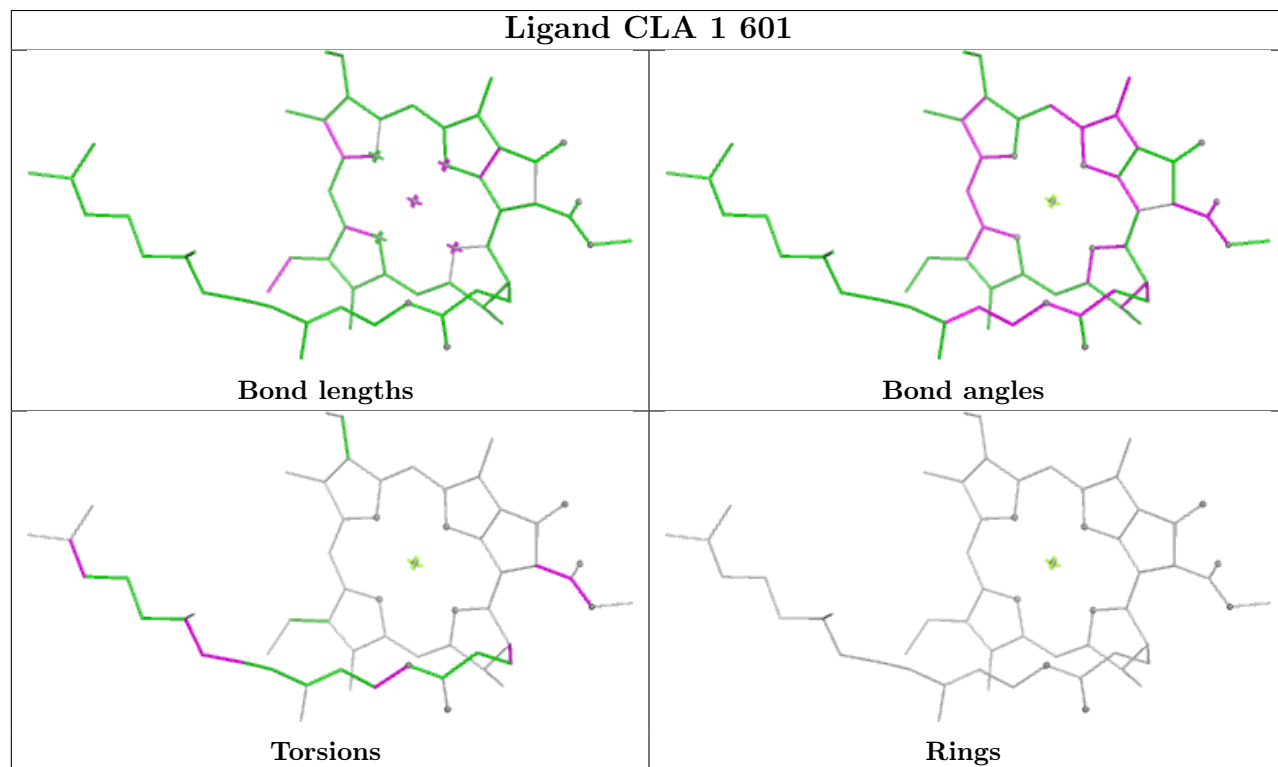
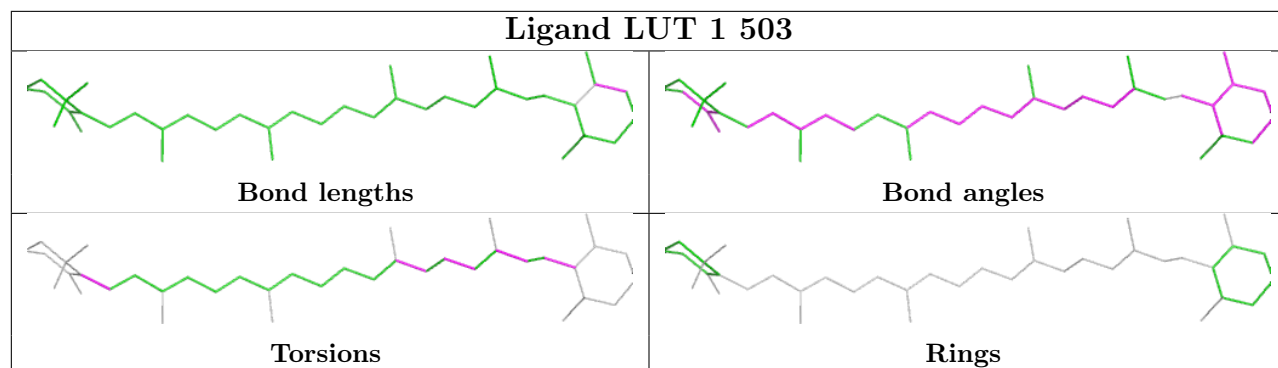


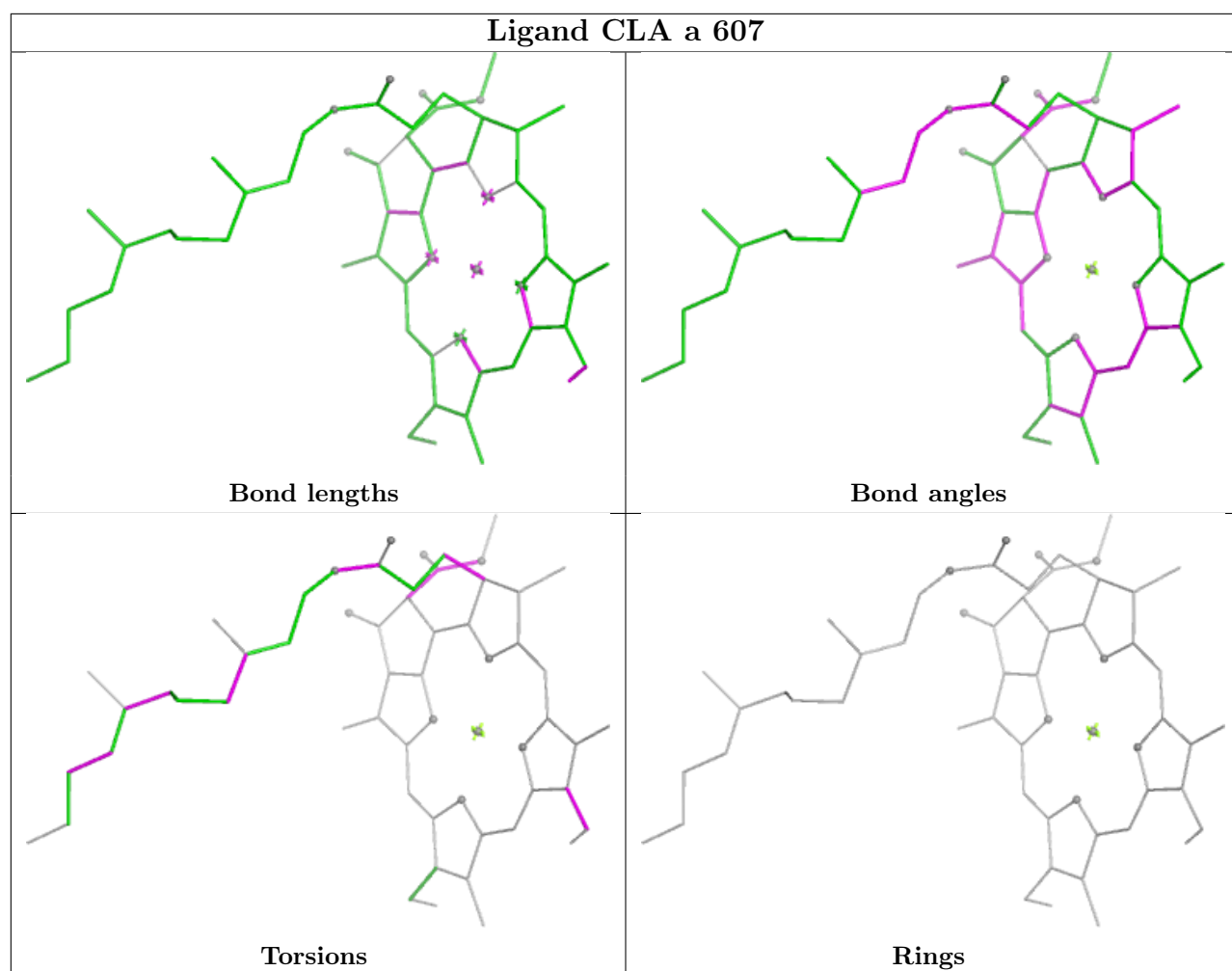


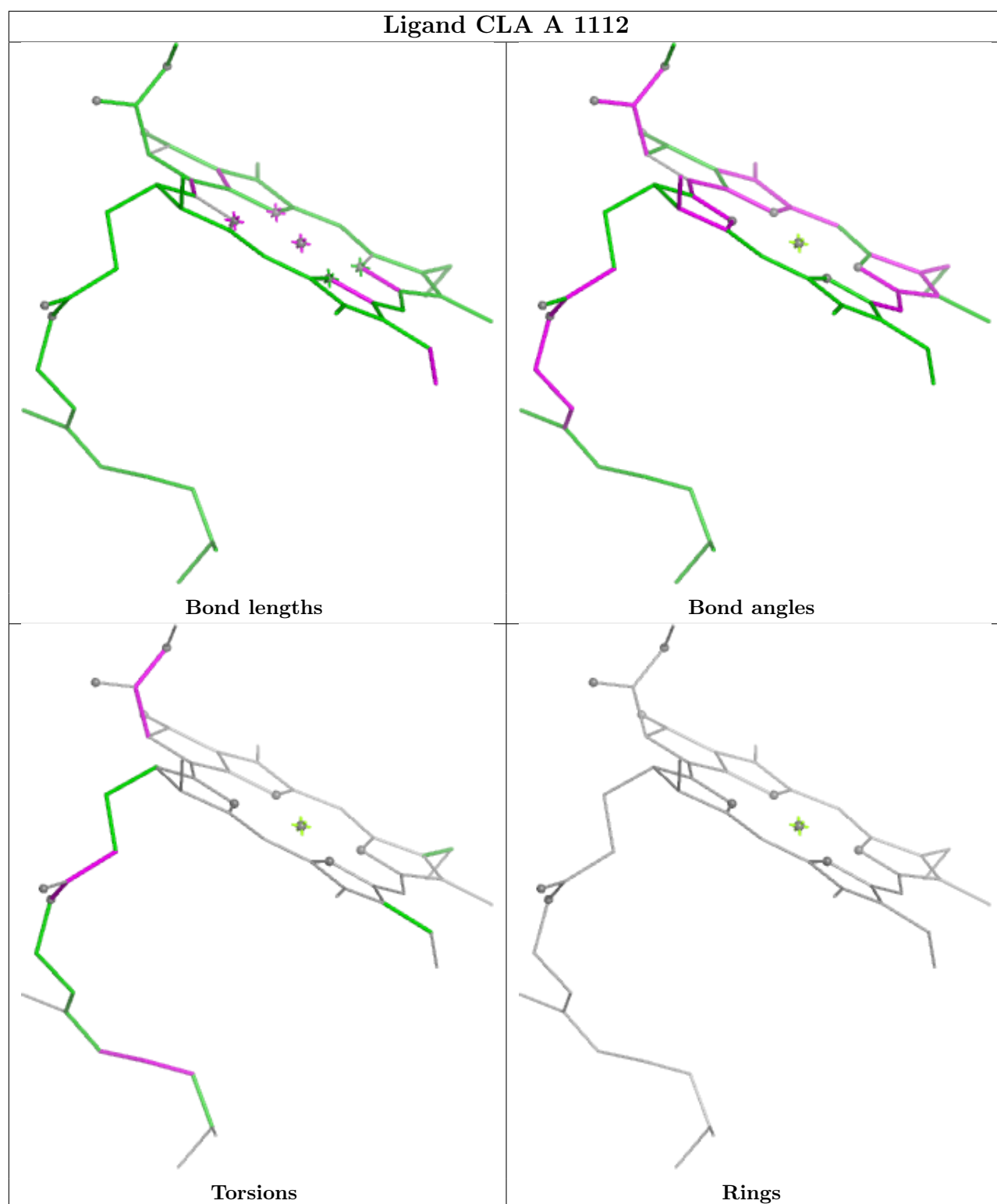


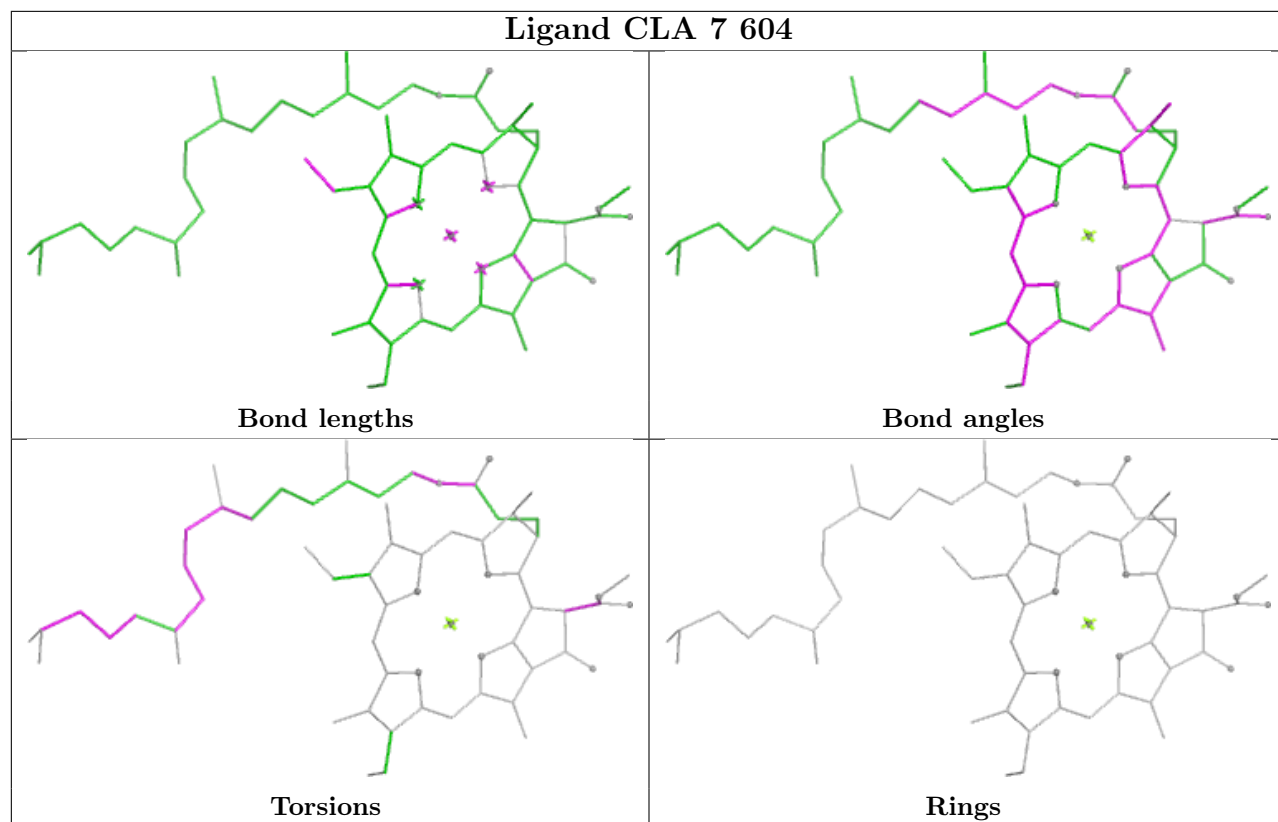


Ligand CLA A 1131**Ligand CLA A 1104**

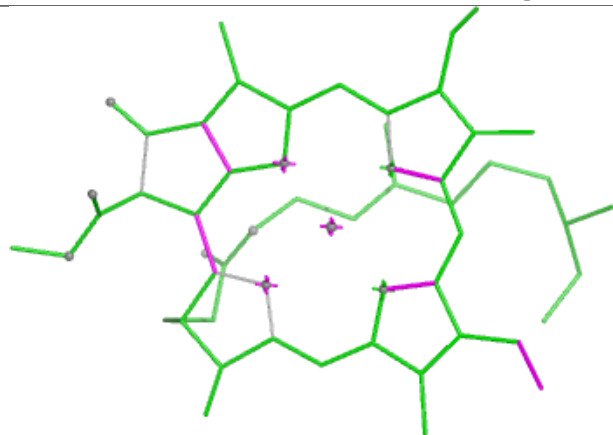




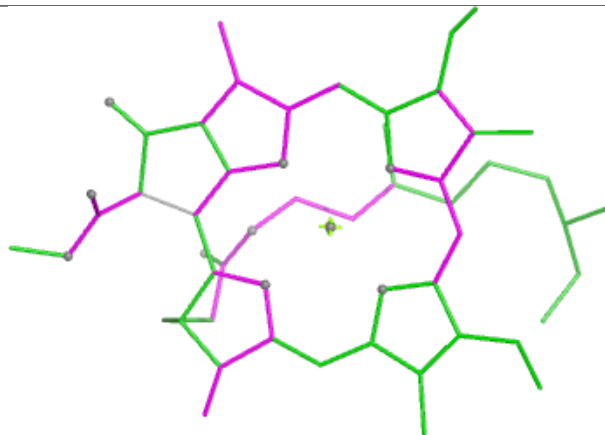




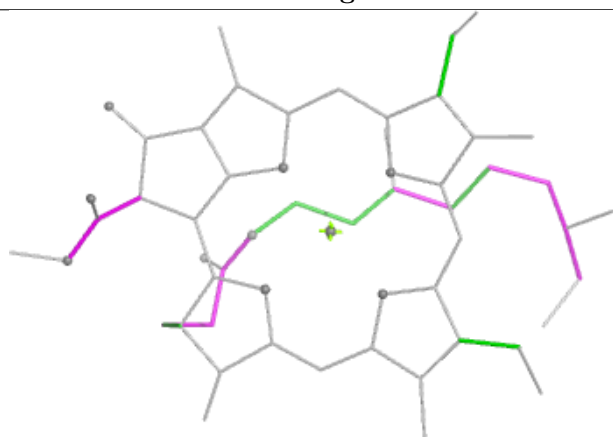
Ligand CLA 5 603



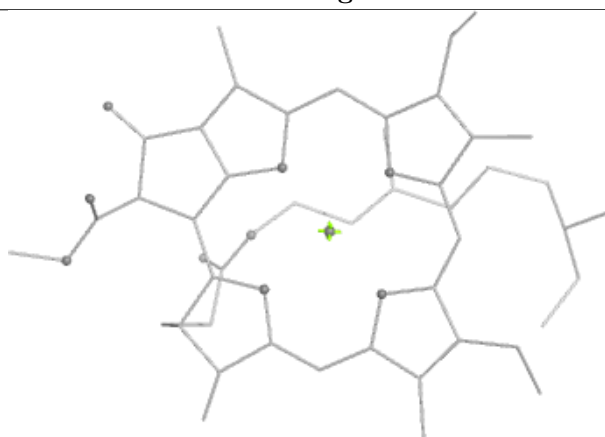
Bond lengths



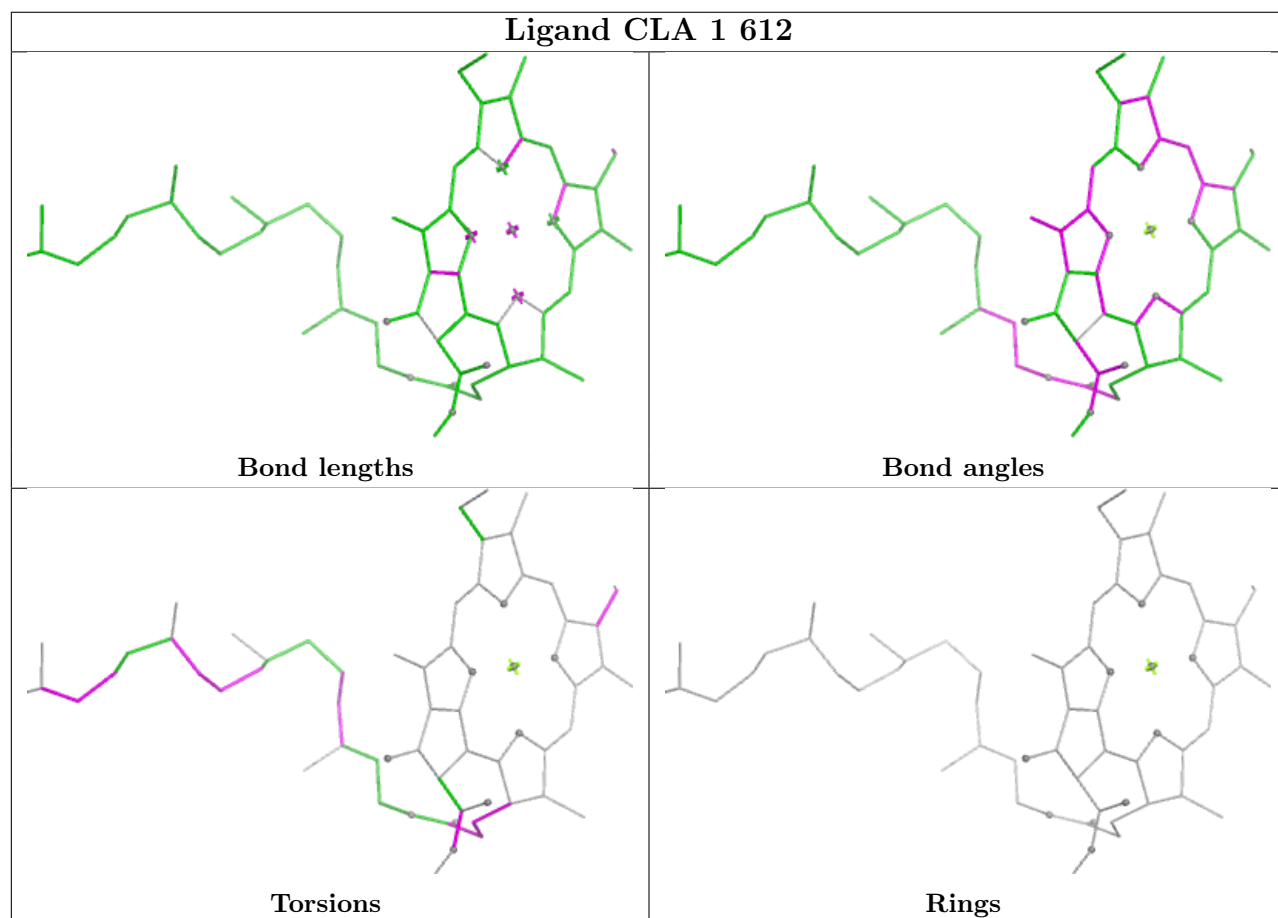
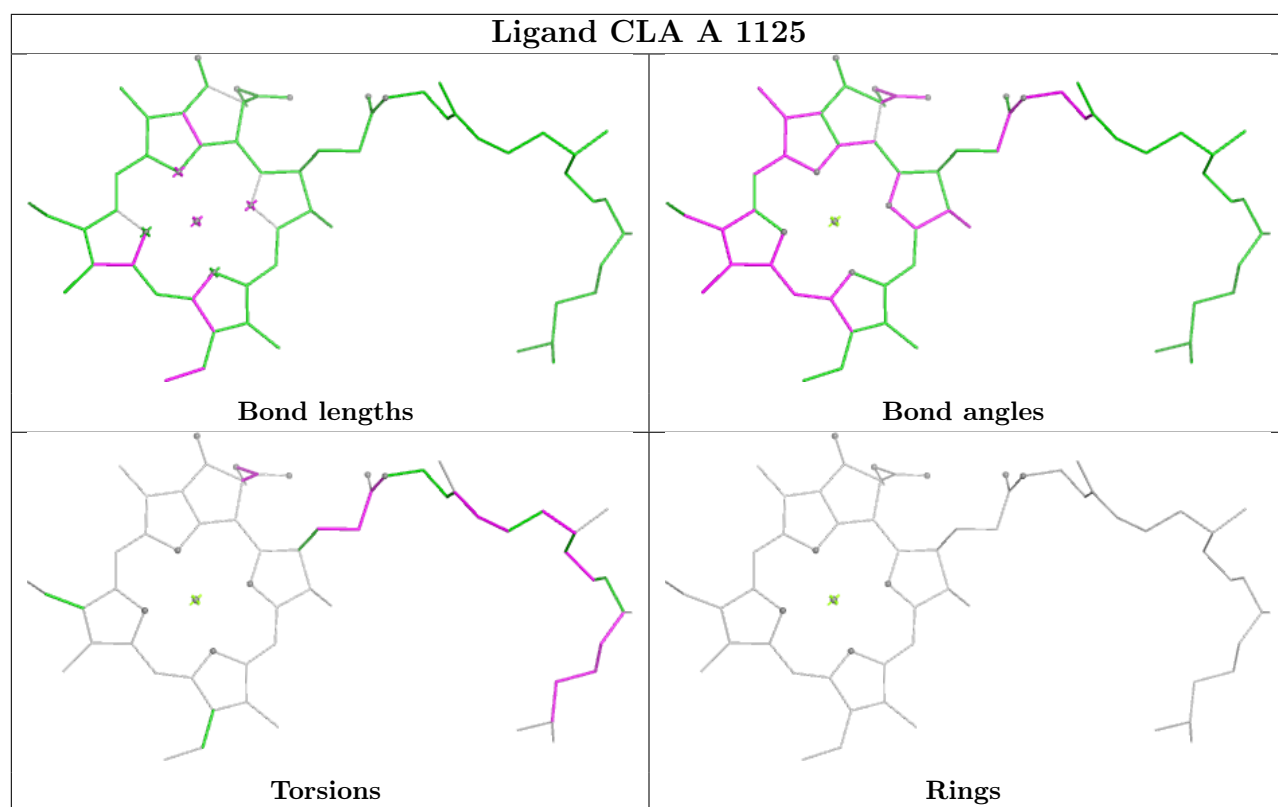
Bond angles

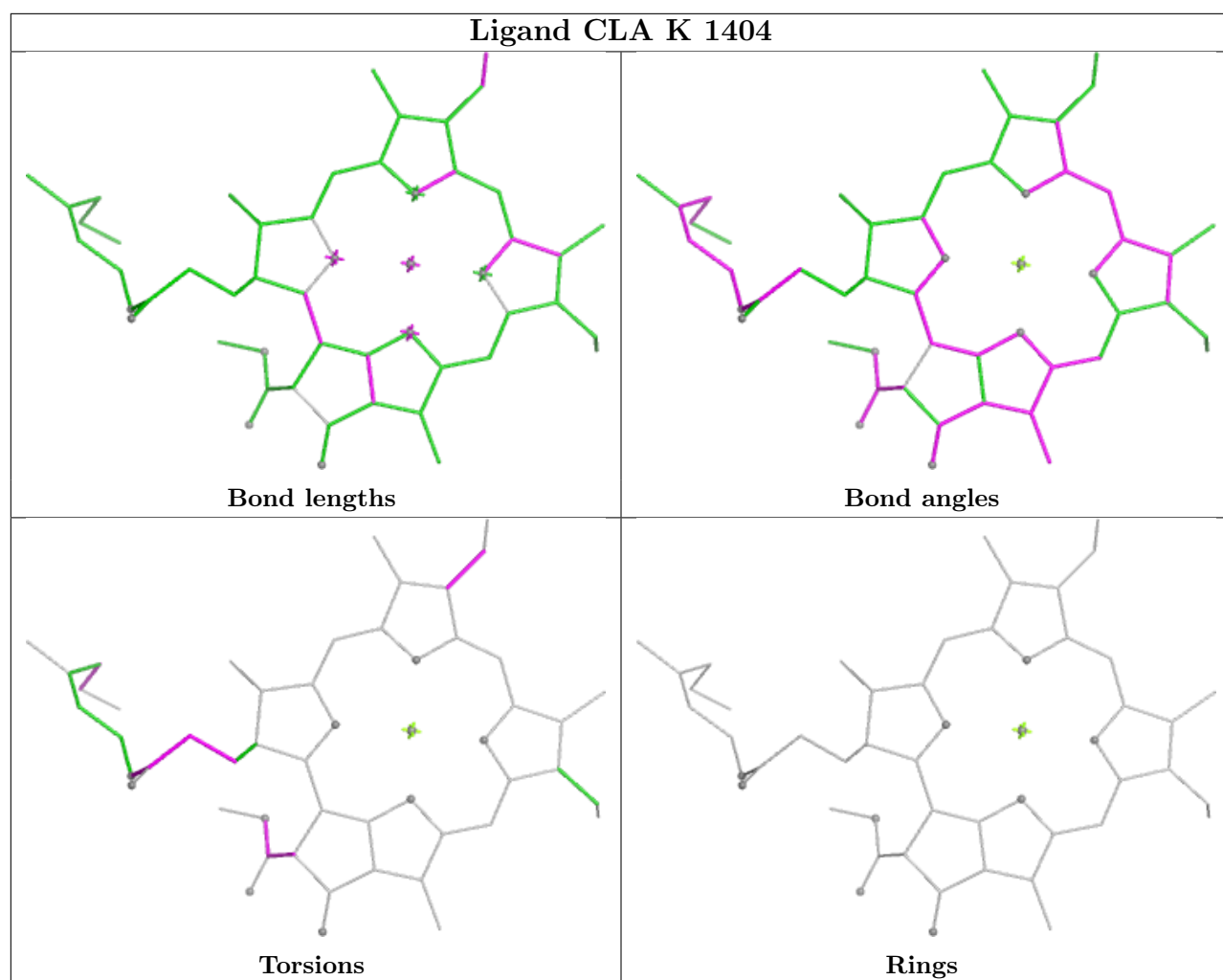


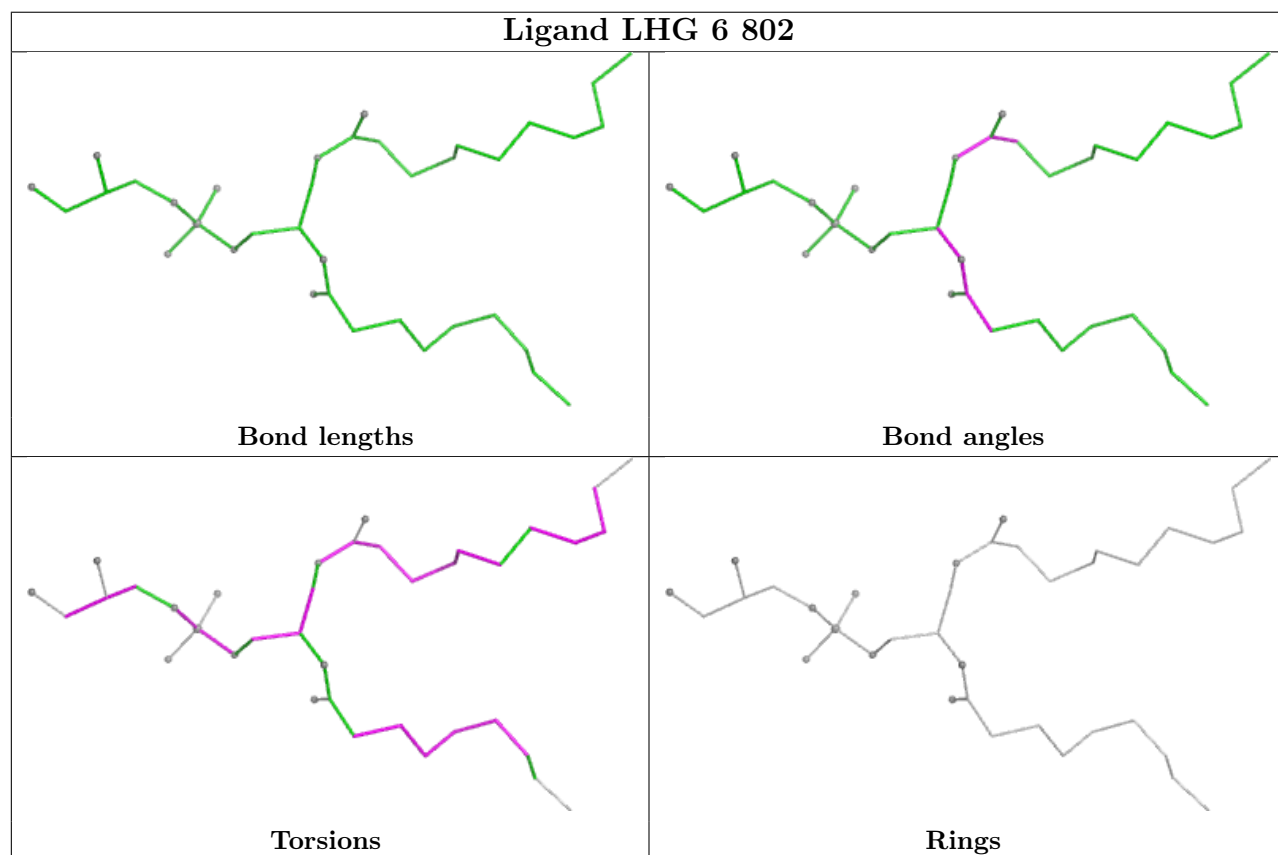
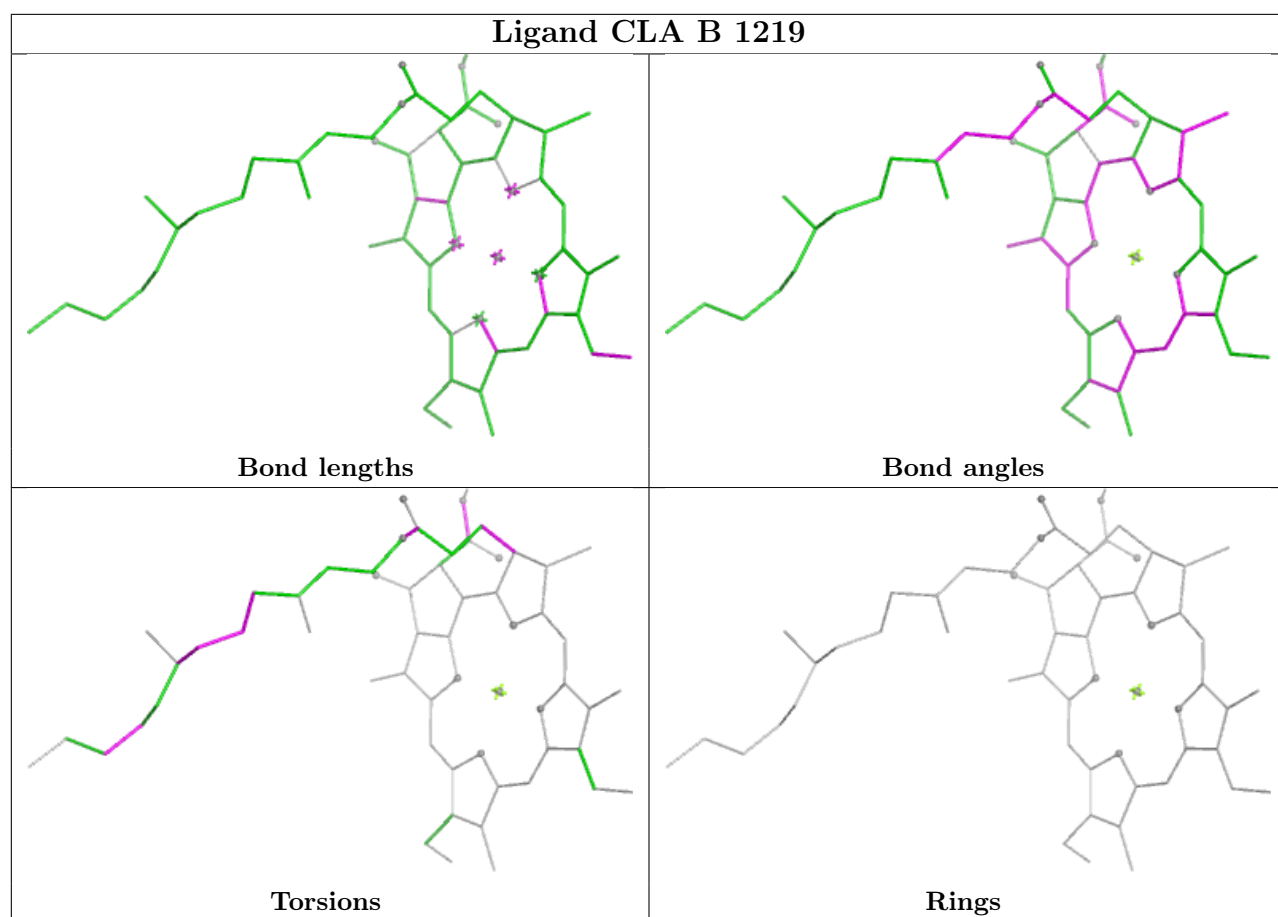
Torsions



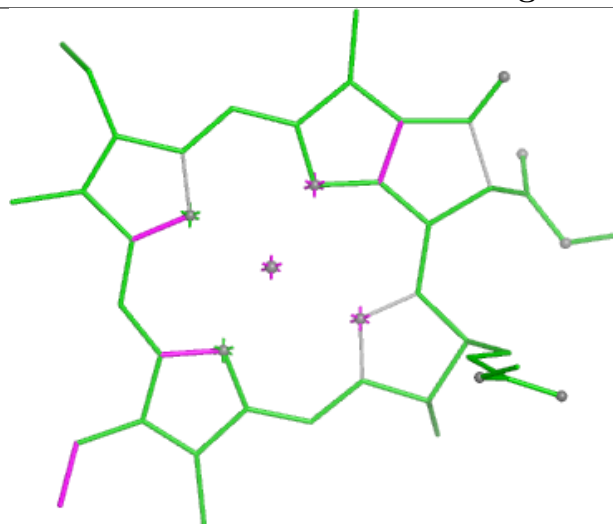
Rings



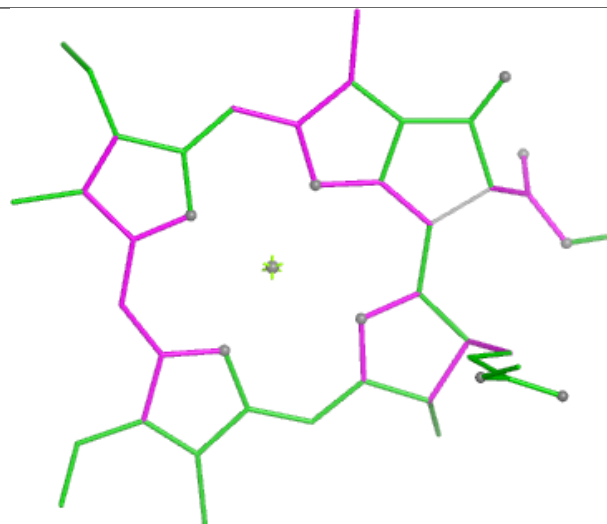




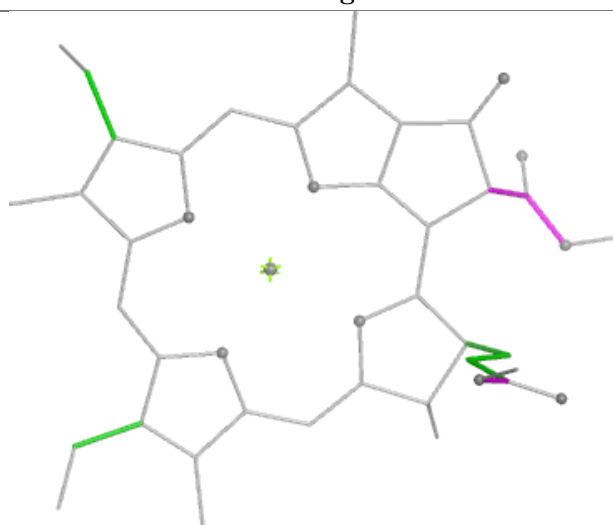
Ligand CLA 8 607



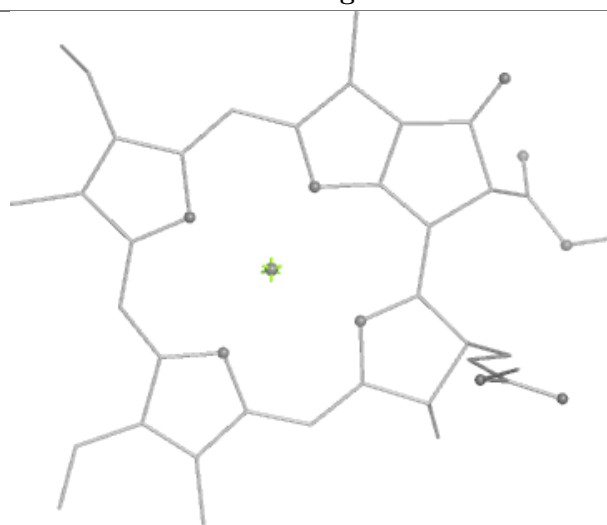
Bond lengths



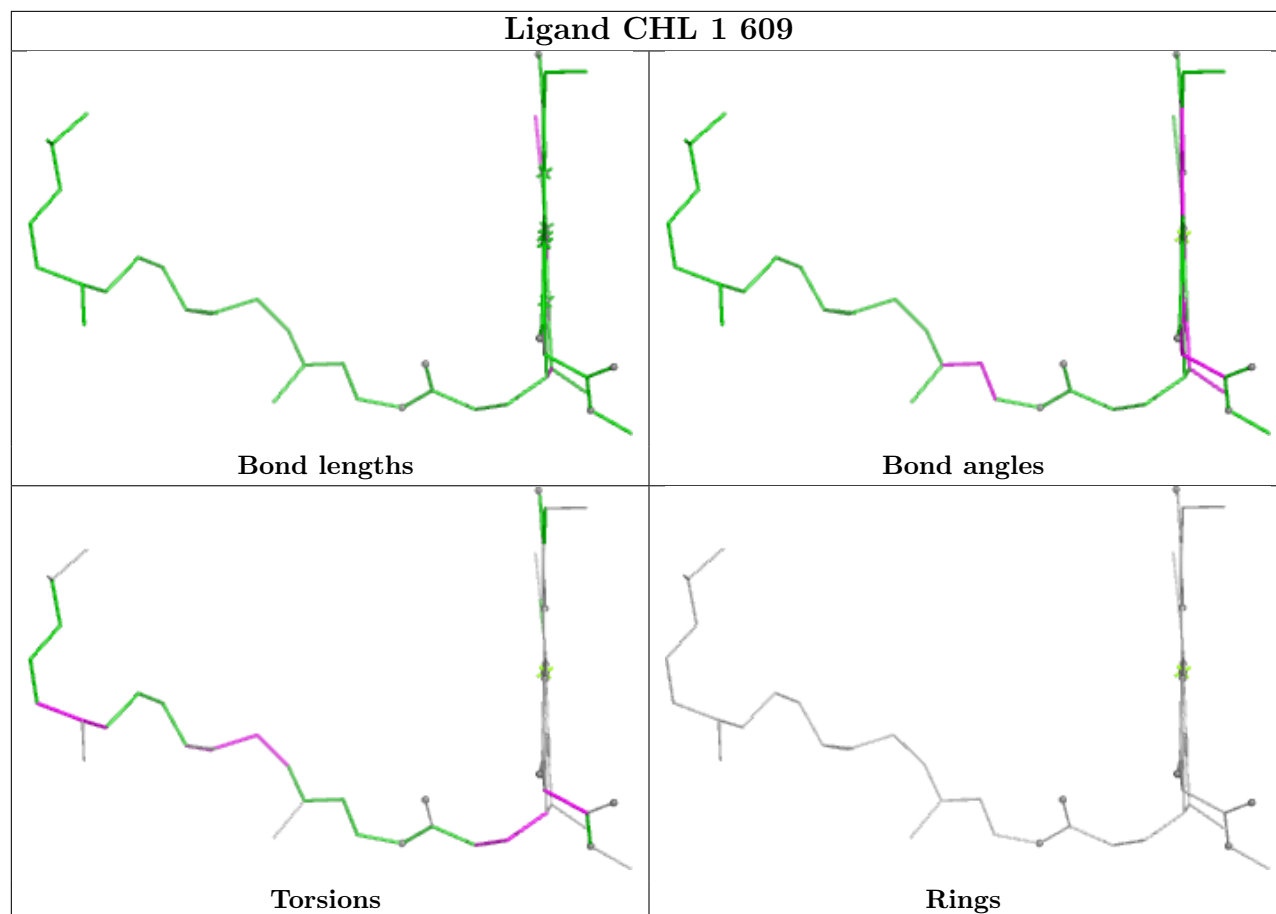
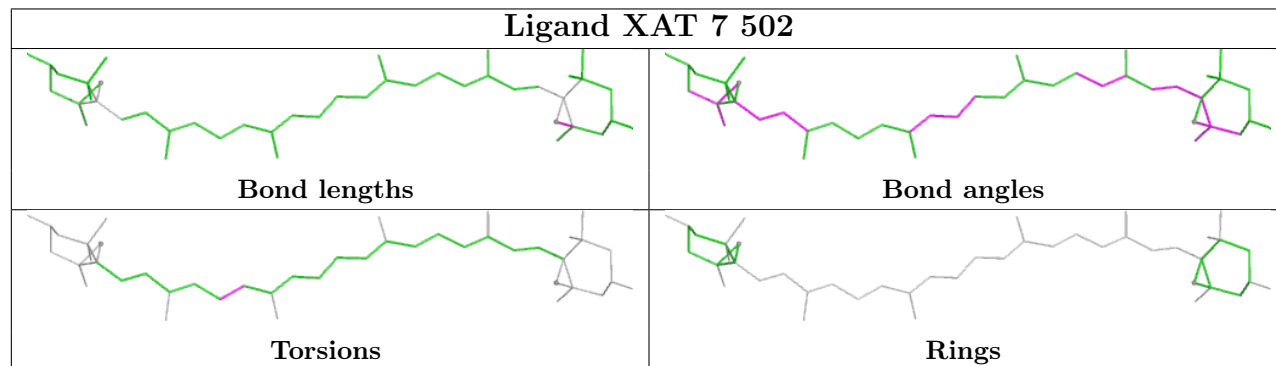
Bond angles

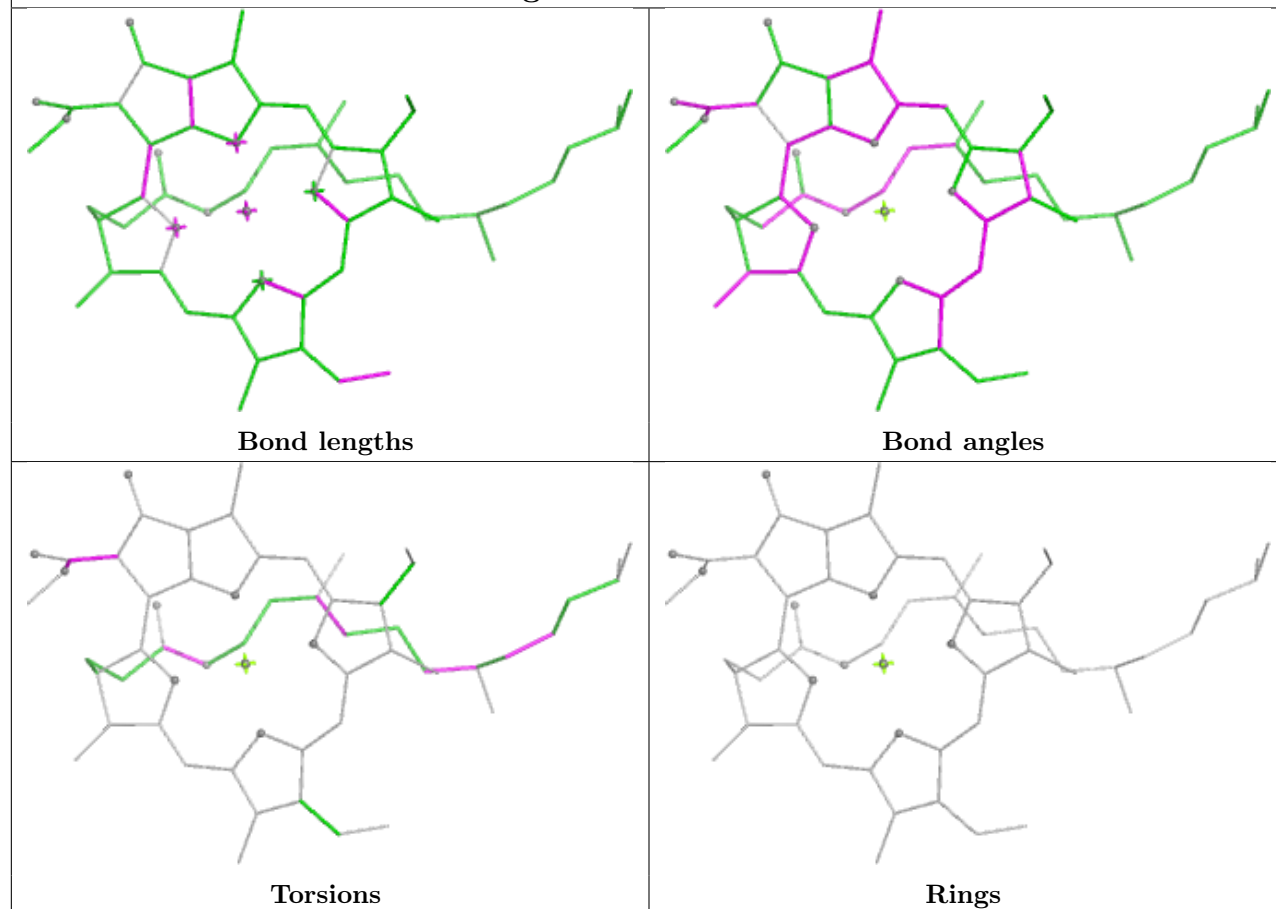
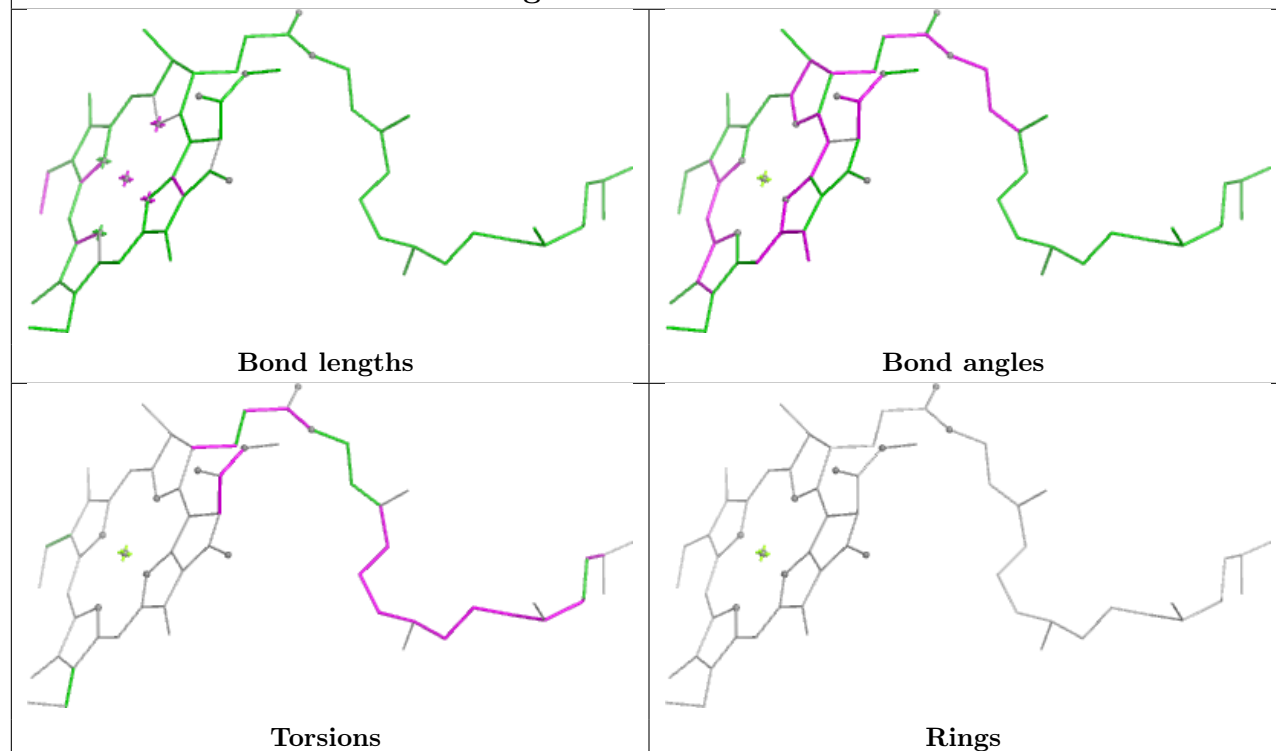


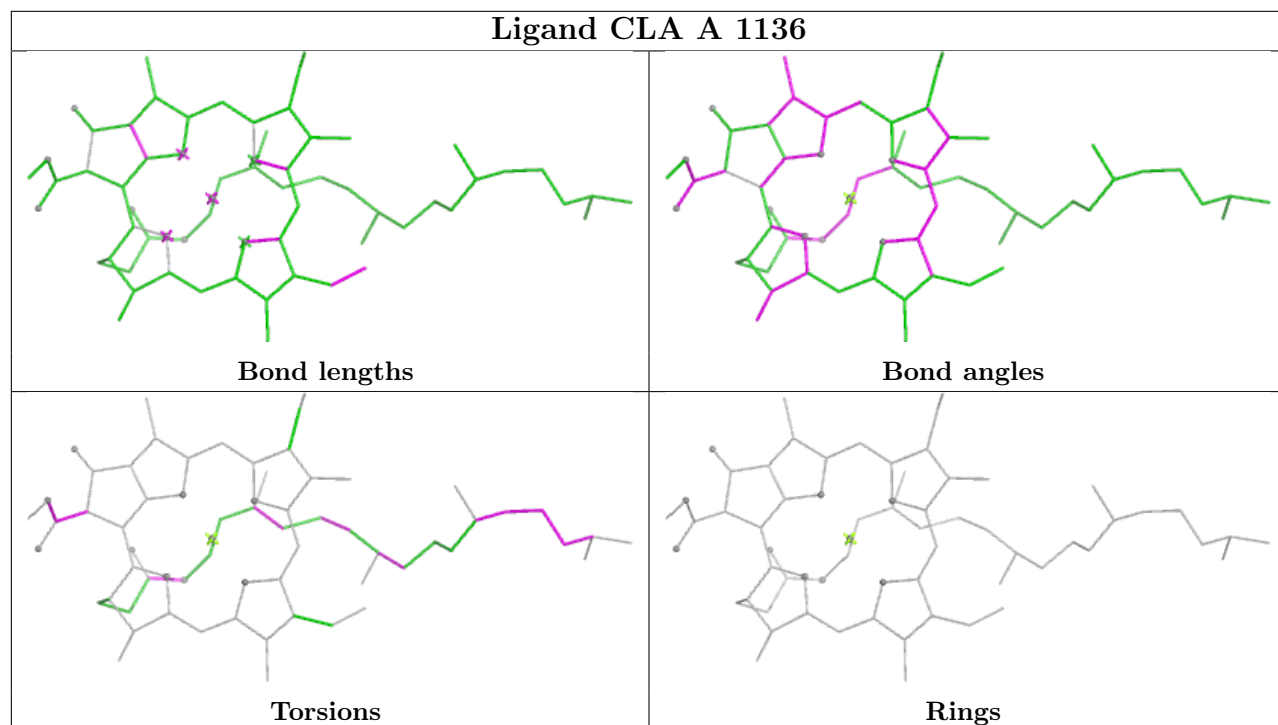
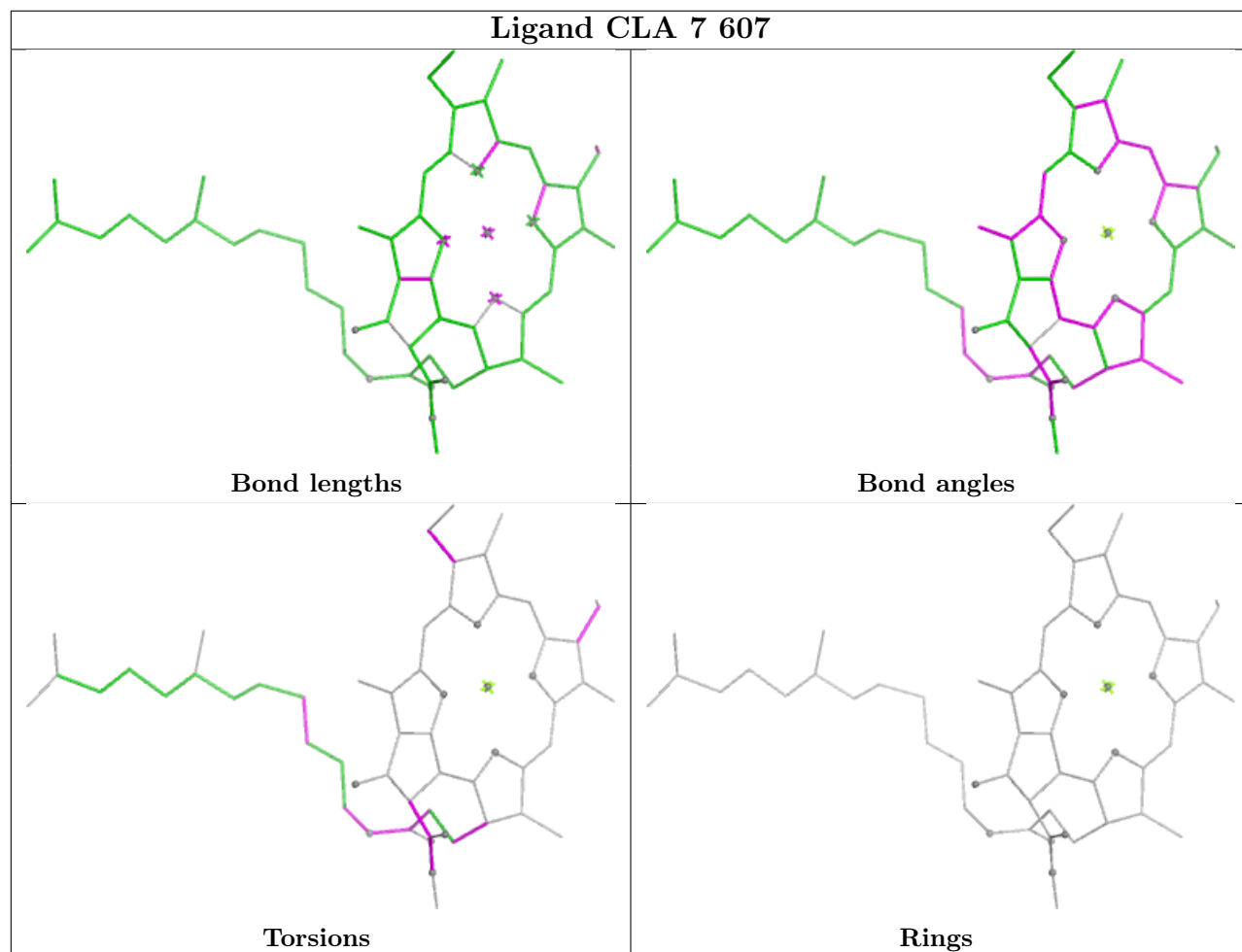
Torsions

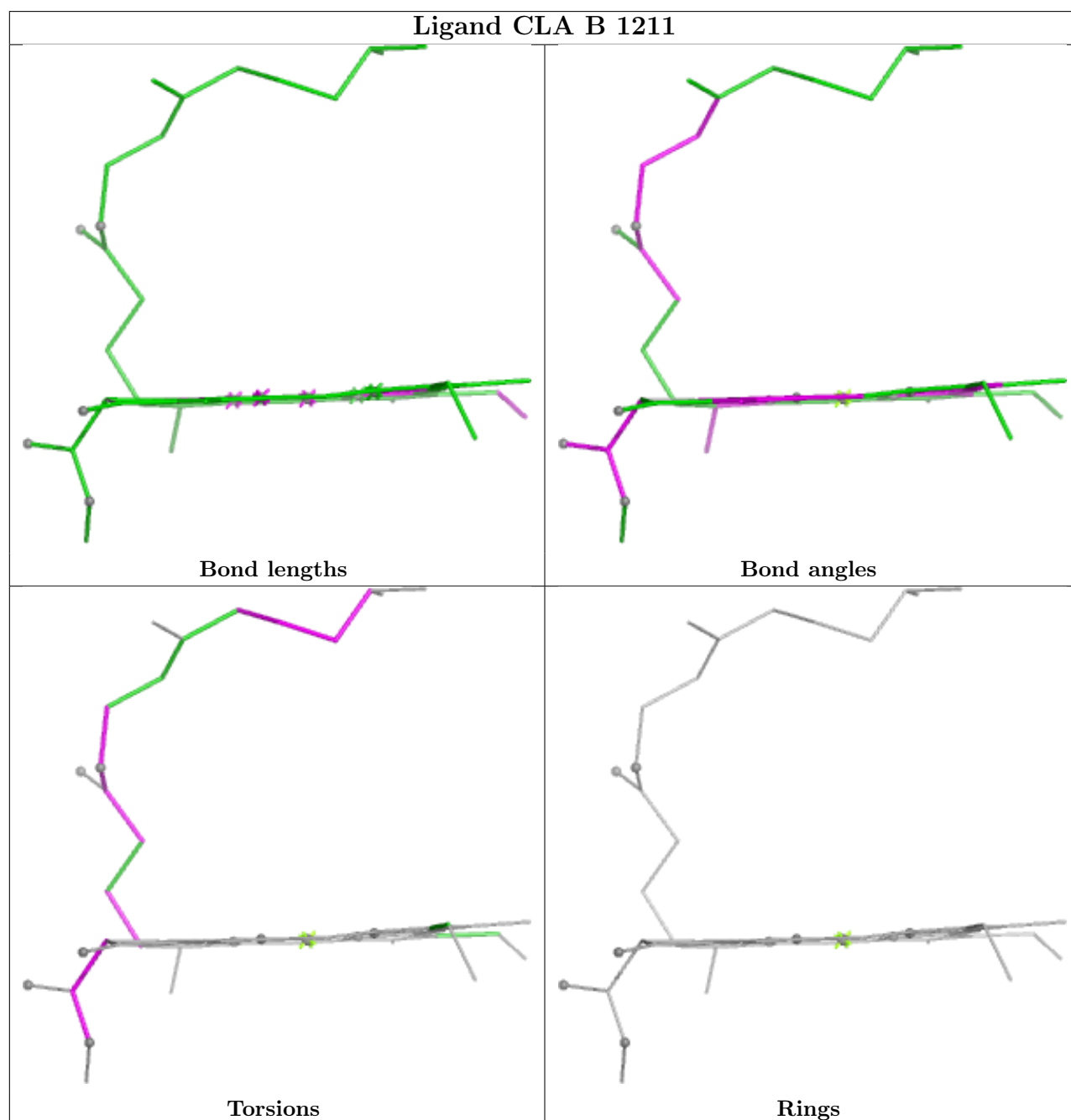
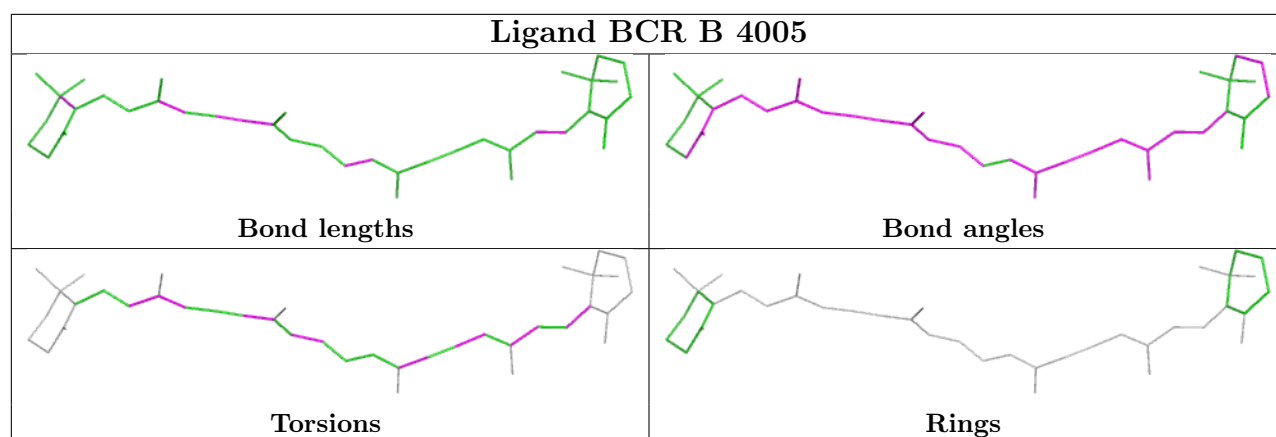


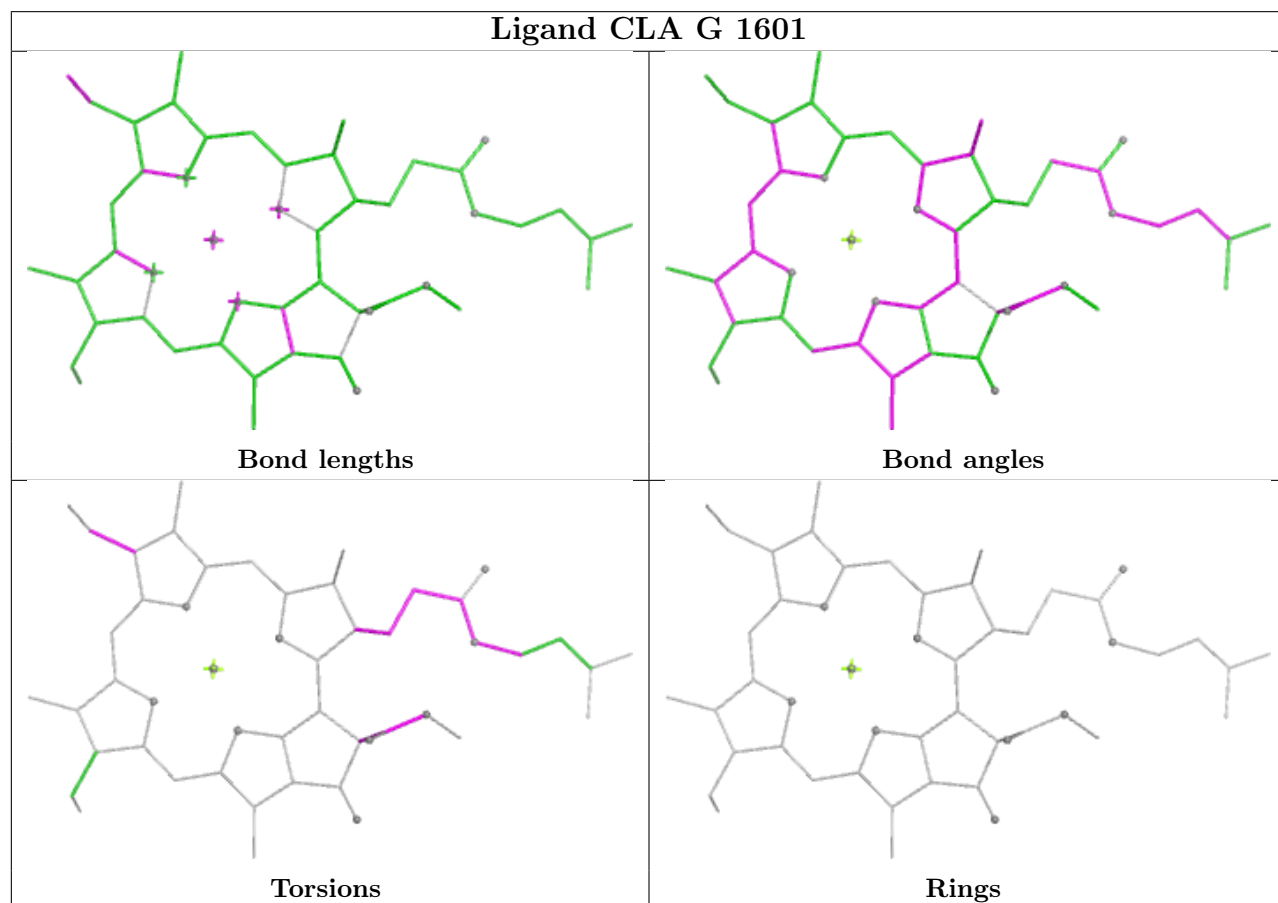
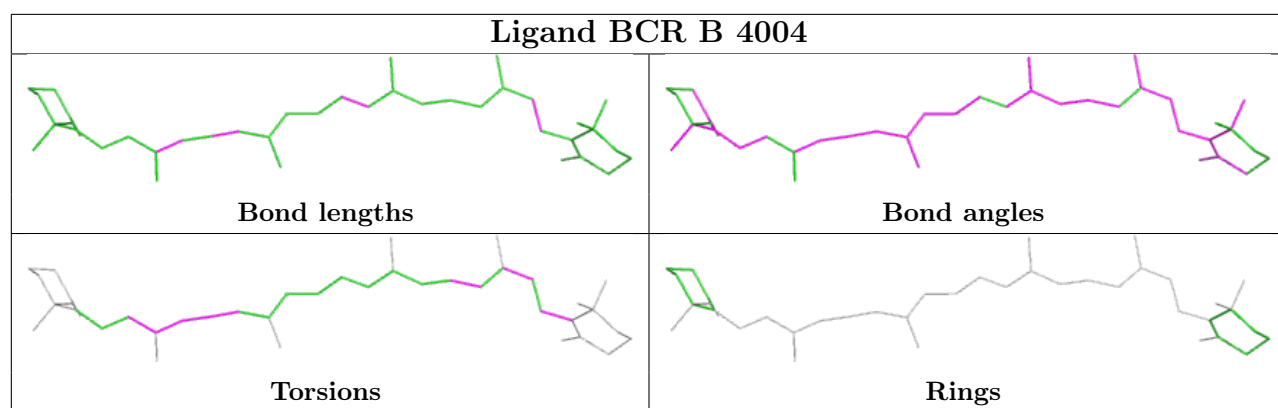
Rings

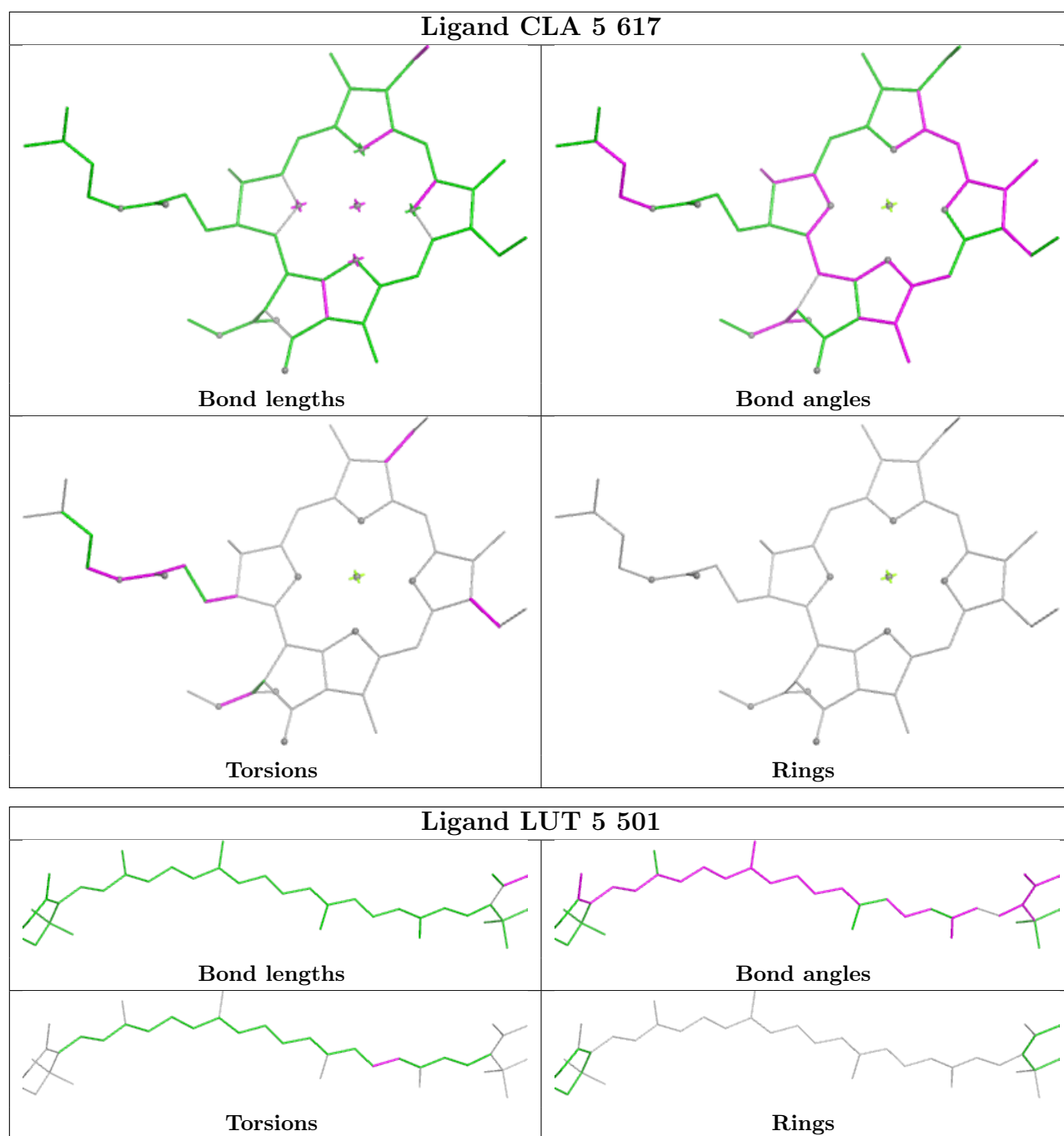
Ligand CHL 1 609**Ligand XAT 7 502**

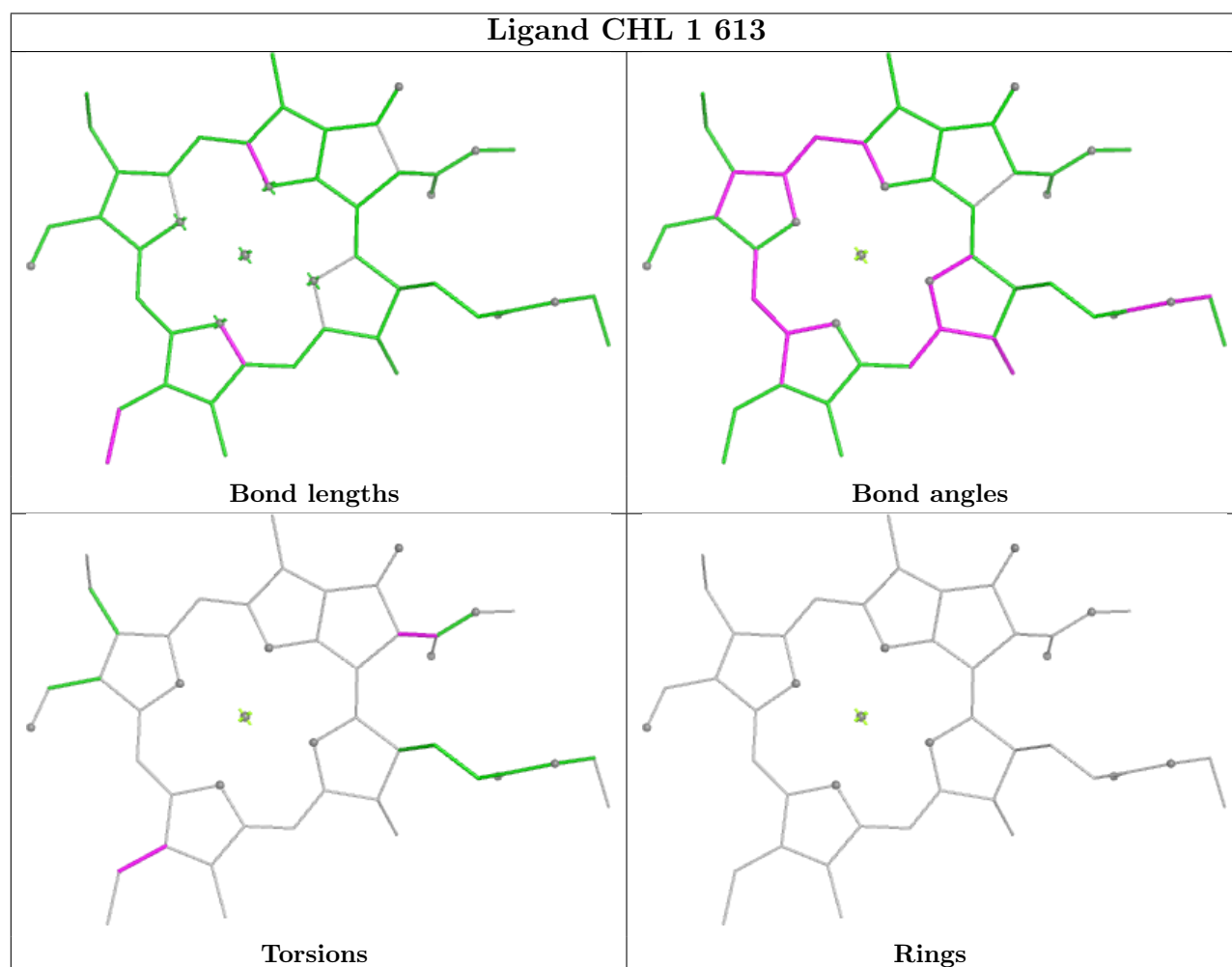
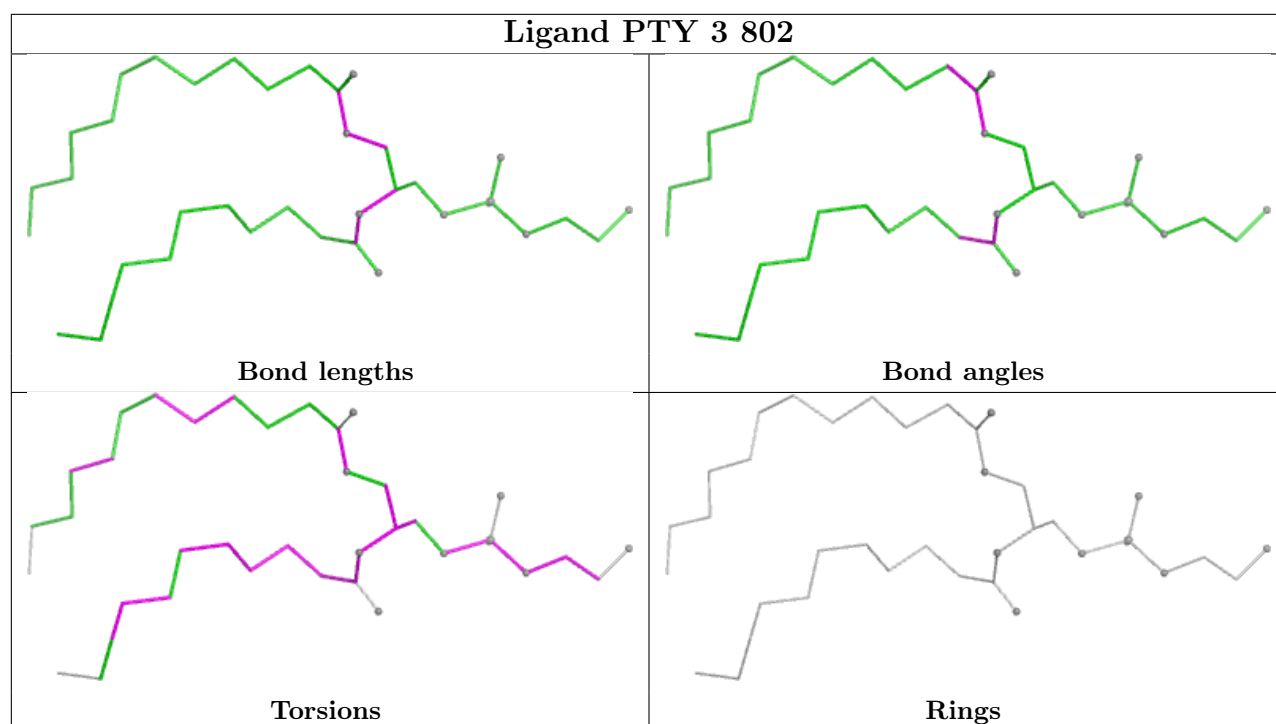
Ligand CLA A 1115**Ligand CLA B 1021**

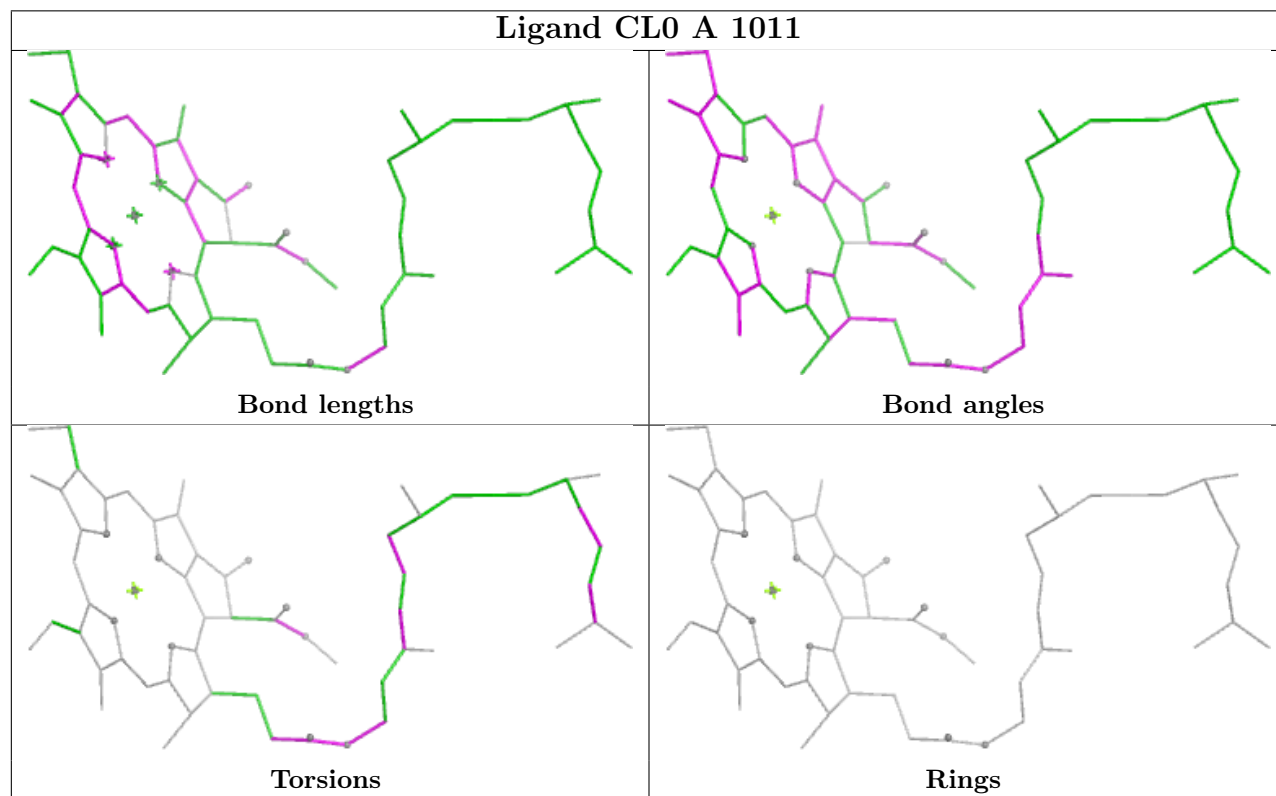
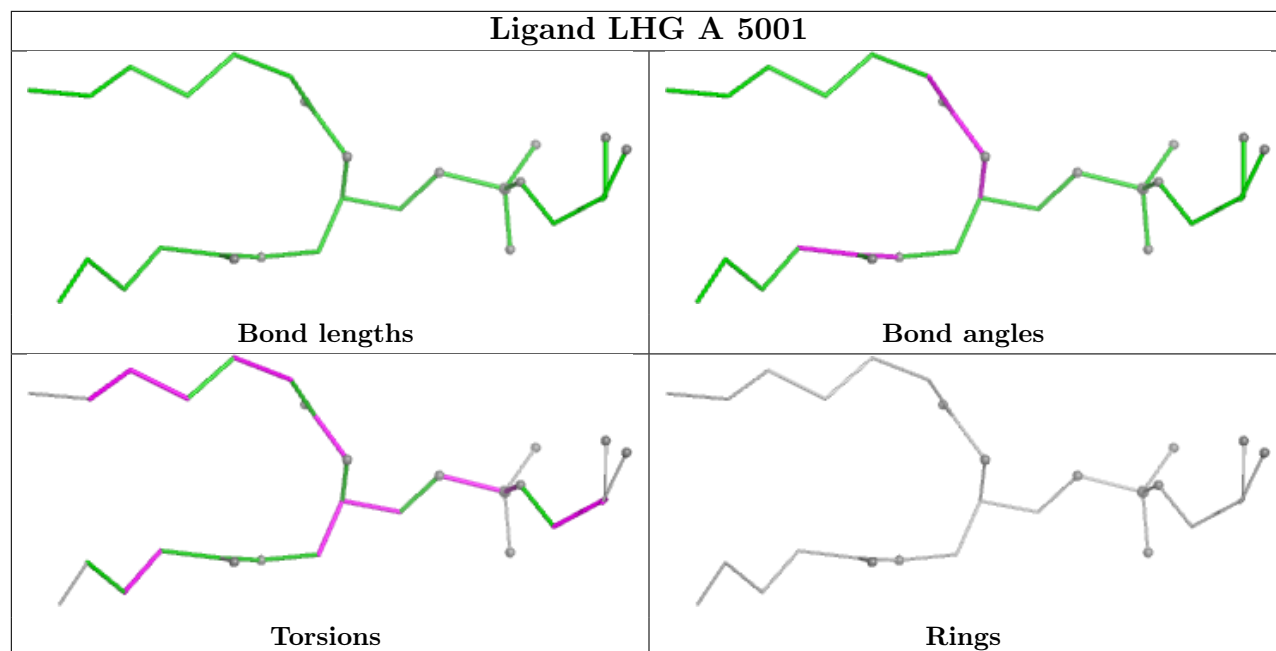
Ligand CLA A 1136**Ligand CLA 7 607**

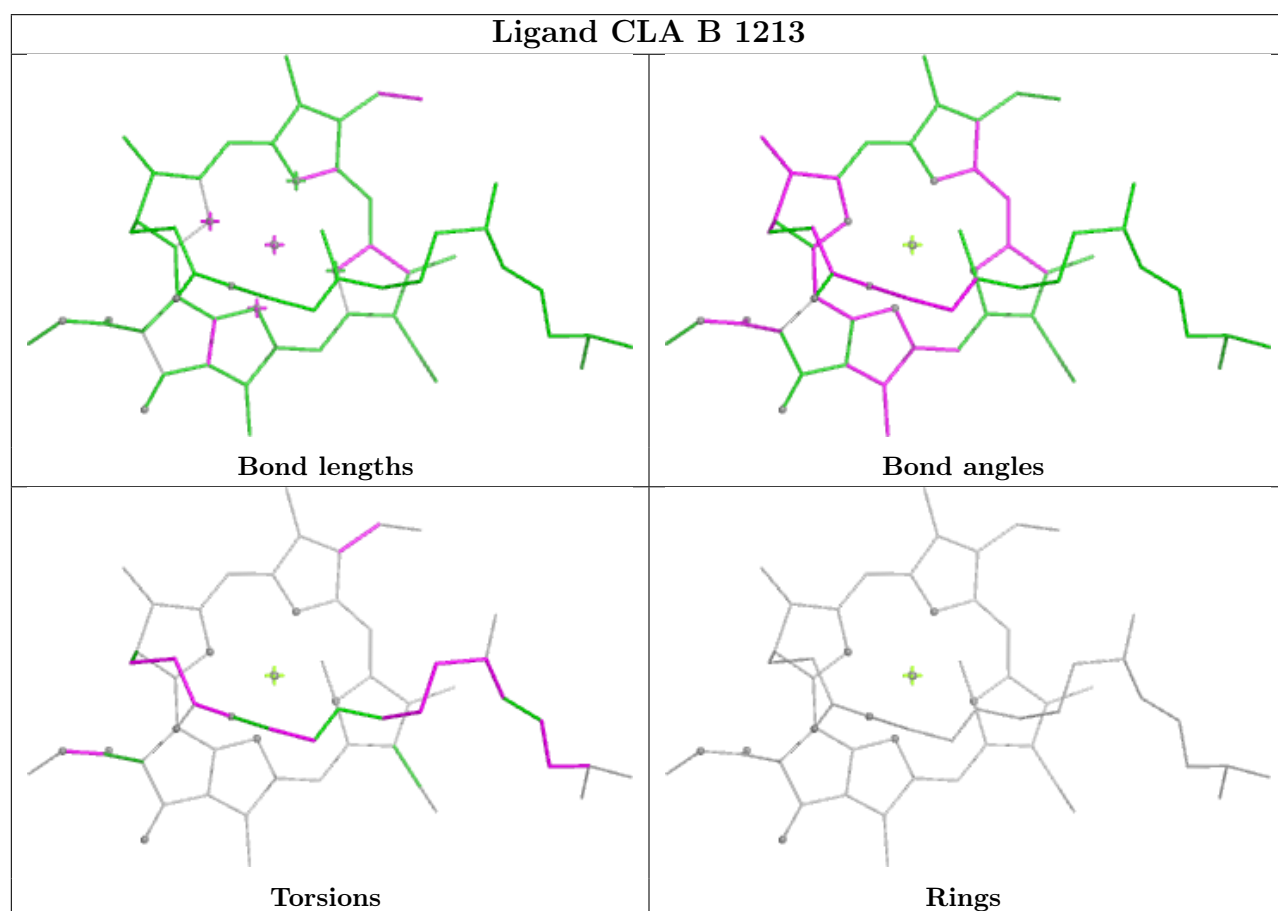
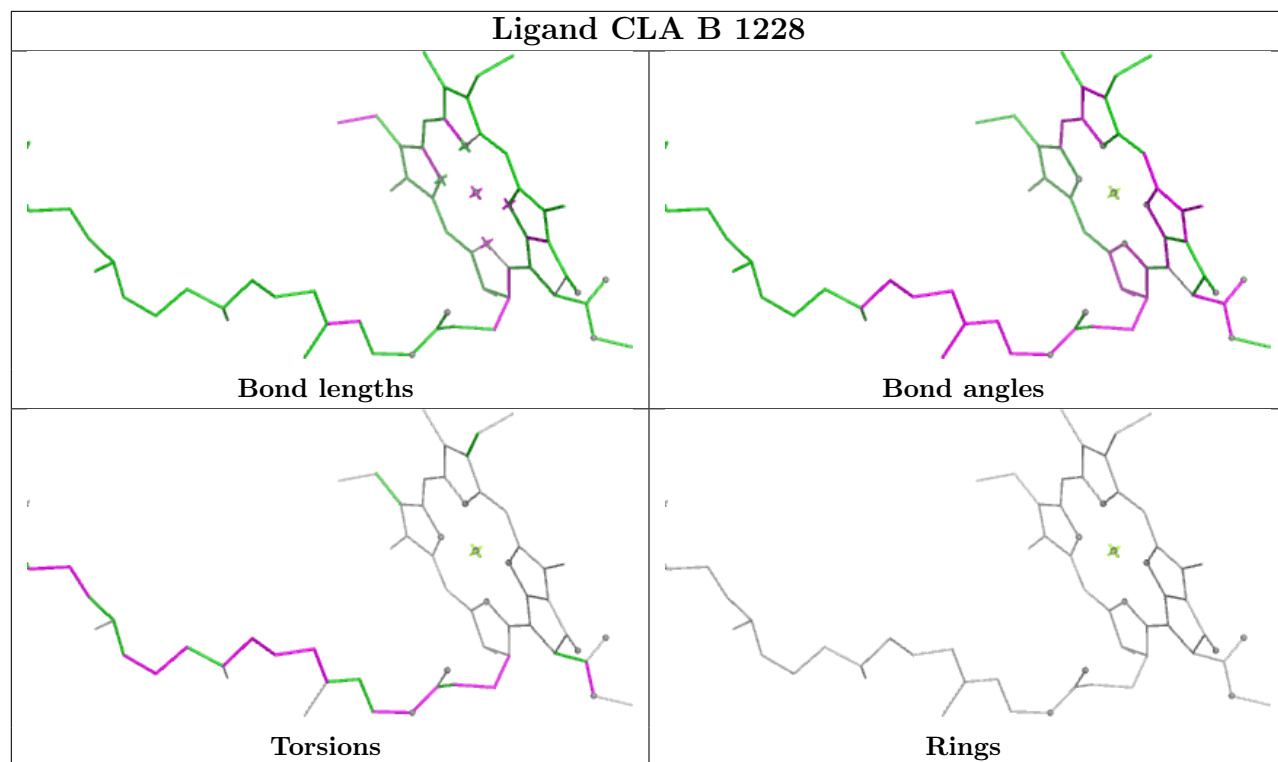


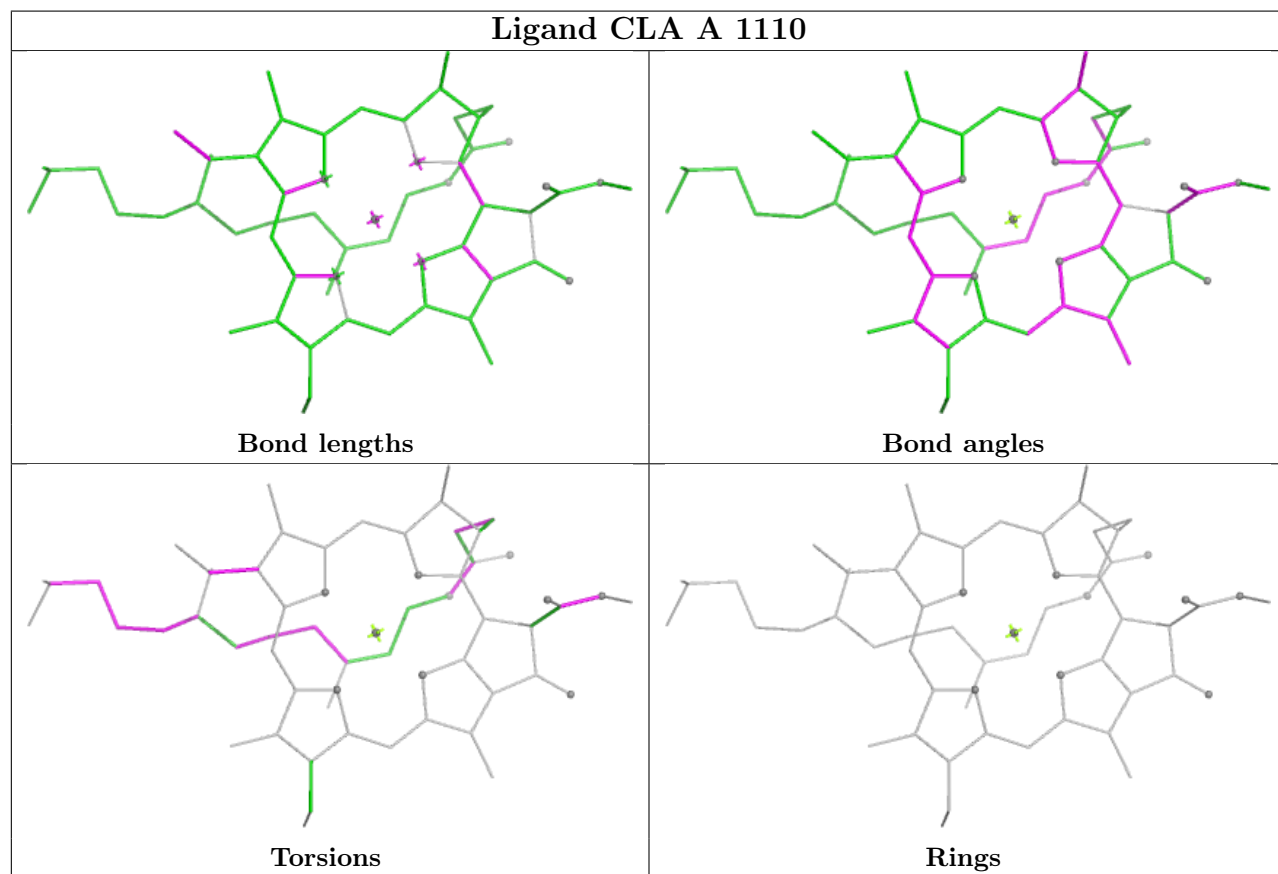
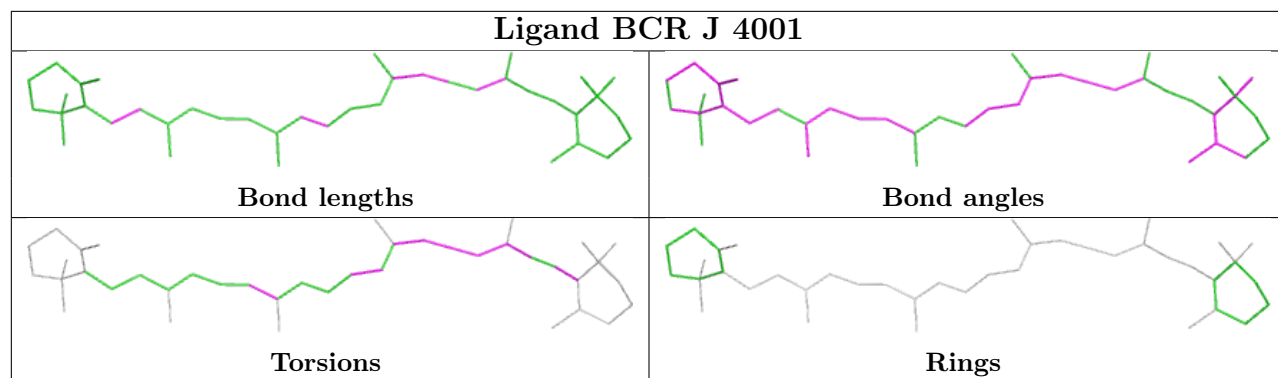




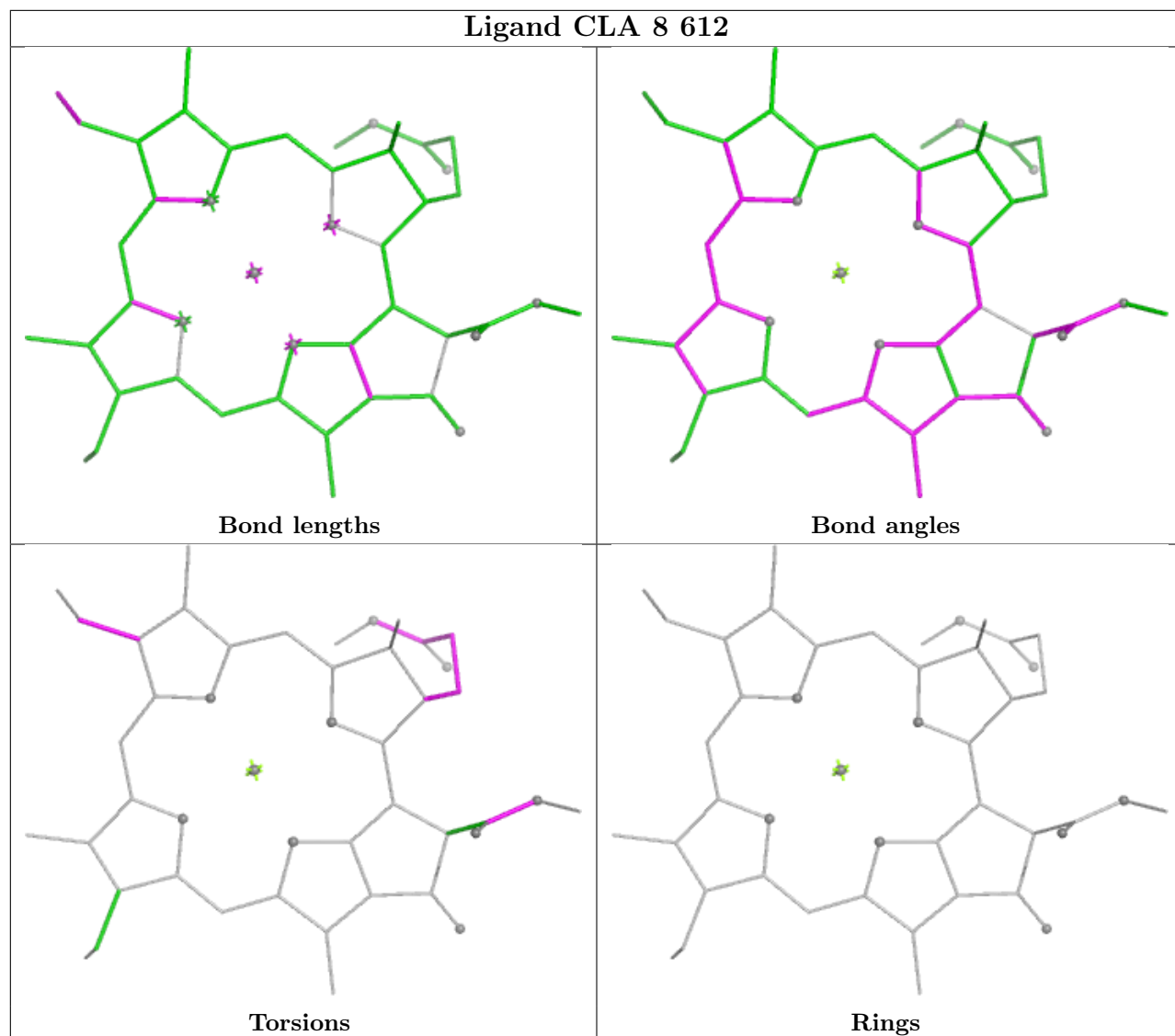


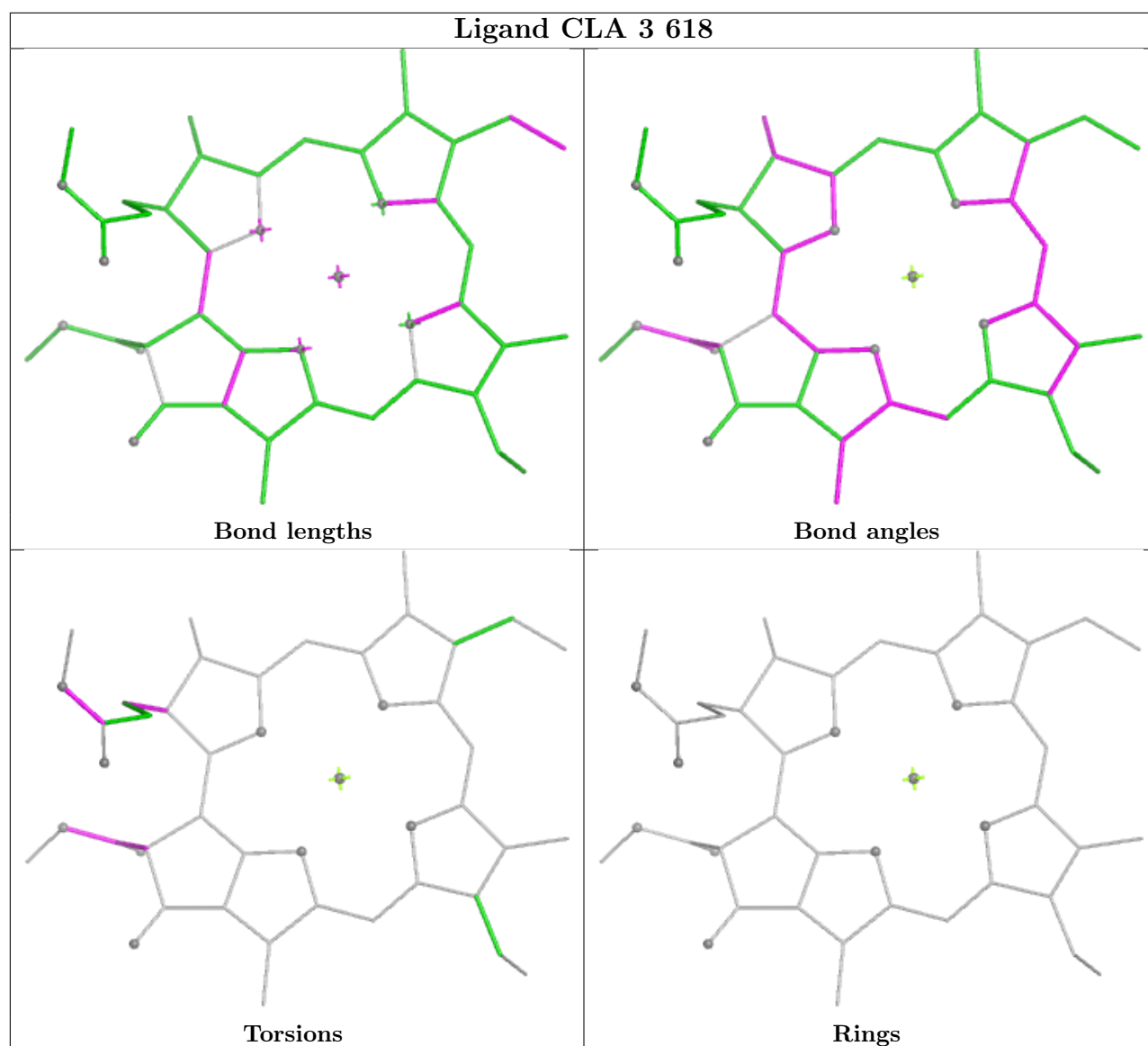






Ligand CLA 8 612





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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

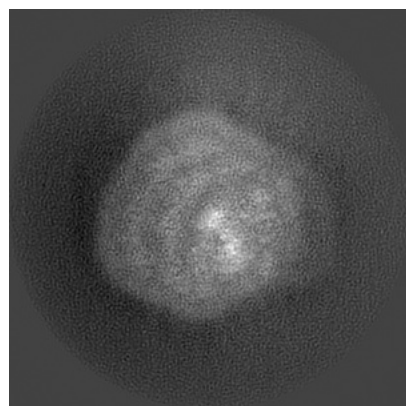
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11640. These allow visual inspection of the internal detail of the map and identification of artifacts.

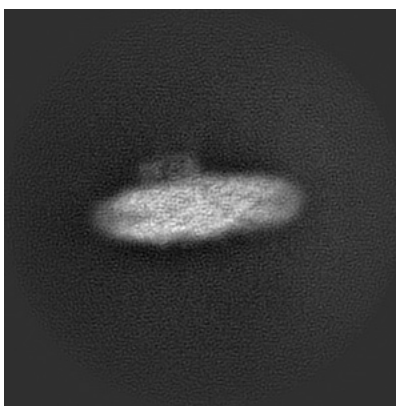
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

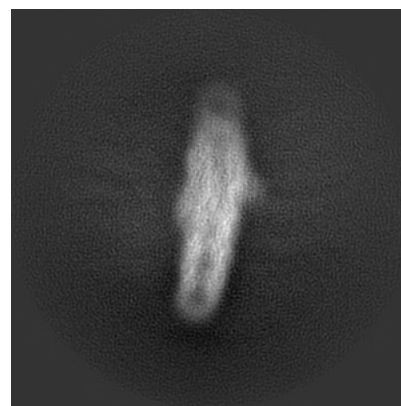
6.1.1 Primary map



X

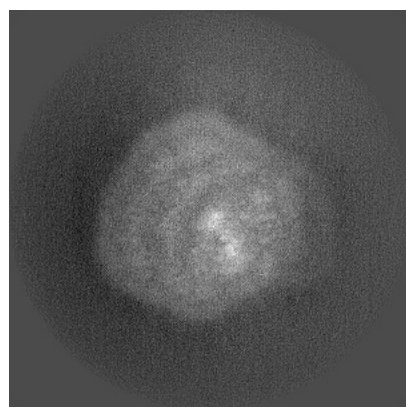


Y

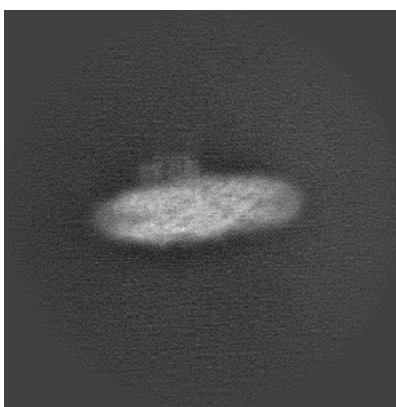


Z

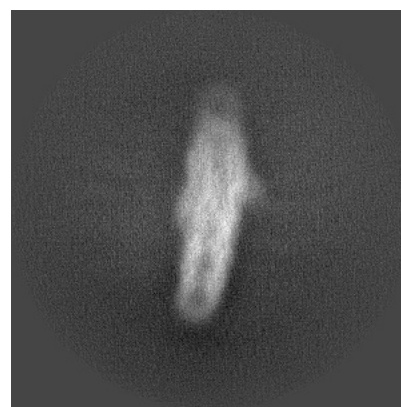
6.1.2 Raw map



X



Y

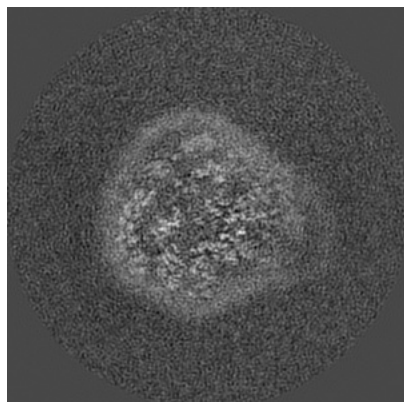


Z

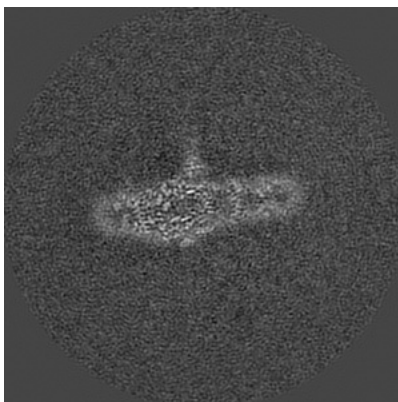
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

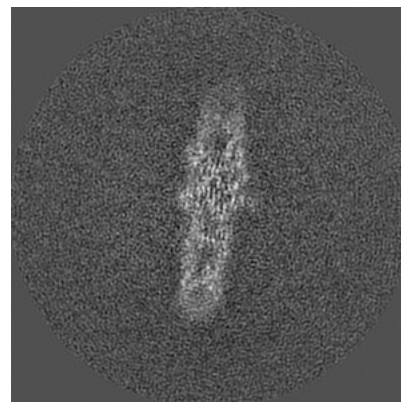
6.2.1 Primary map



X Index: 256

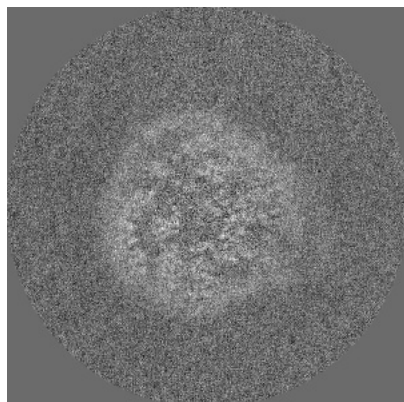


Y Index: 256

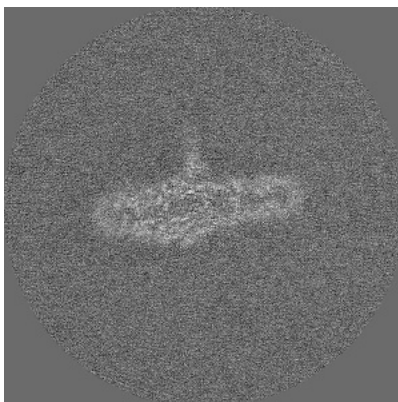


Z Index: 256

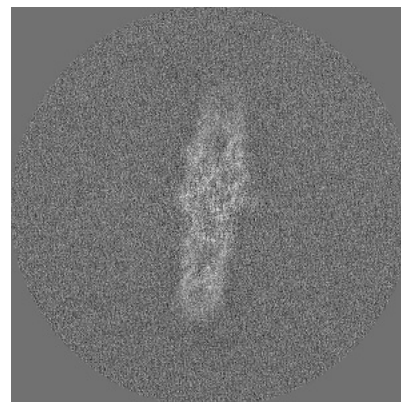
6.2.2 Raw map



X Index: 256



Y Index: 256

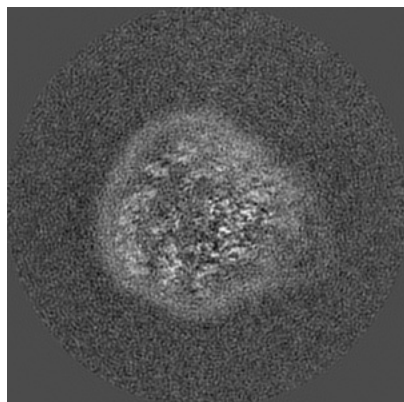


Z Index: 256

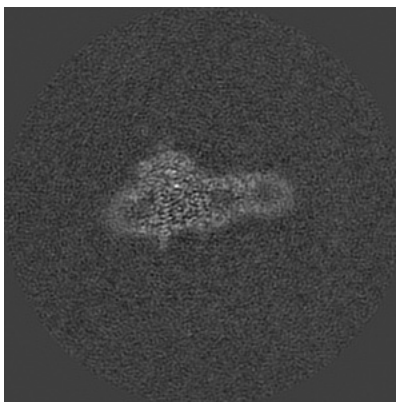
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

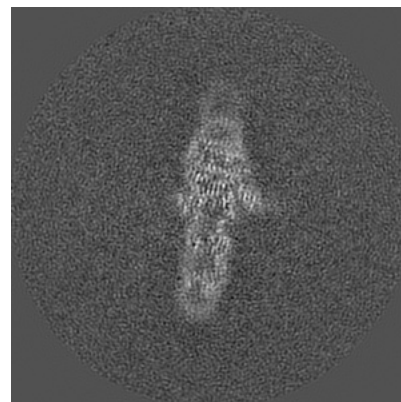
6.3.1 Primary map



X Index: 254

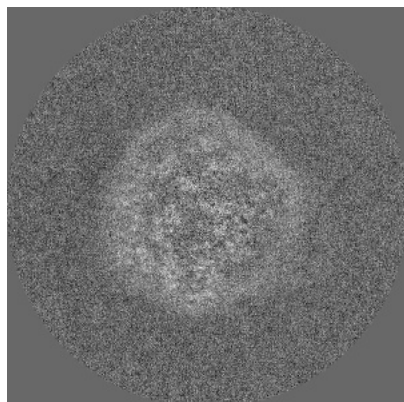


Y Index: 284

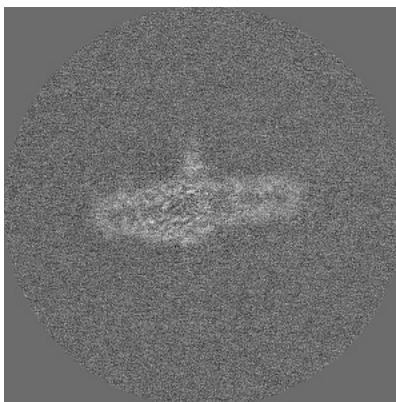


Z Index: 247

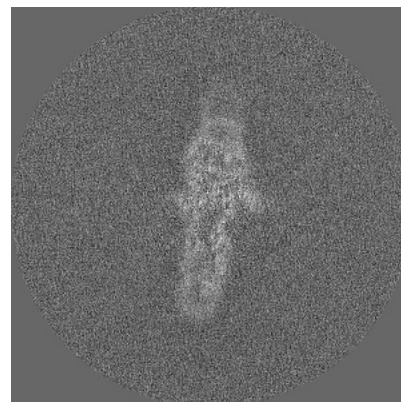
6.3.2 Raw map



X Index: 259



Y Index: 257

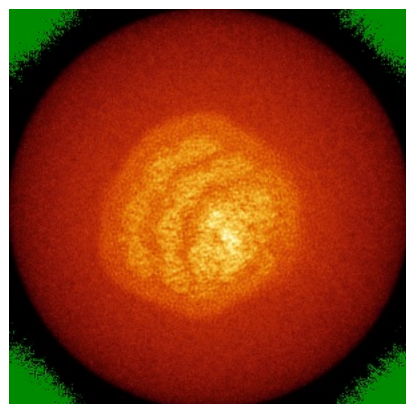


Z Index: 248

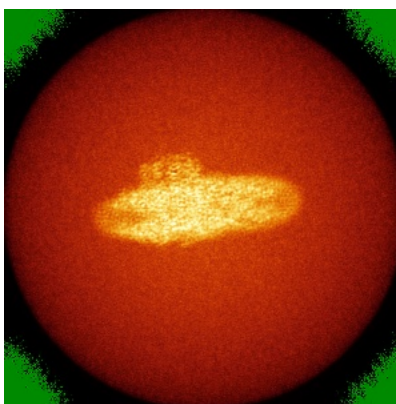
The images above show the largest variance slices of the map in three orthogonal directions.

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

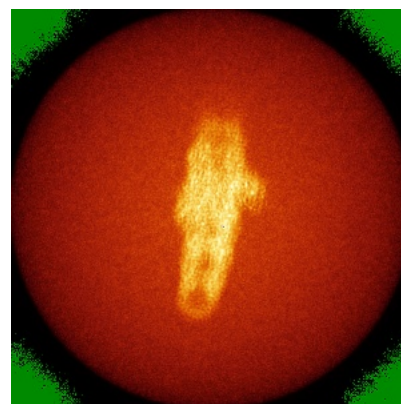
6.4.1 Primary map



X

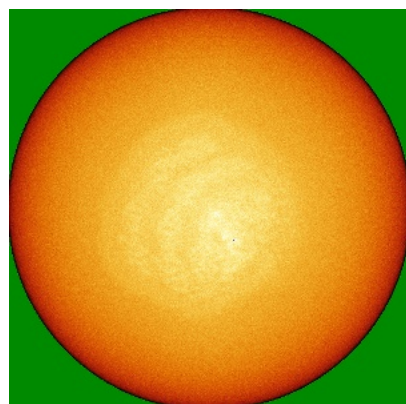


Y

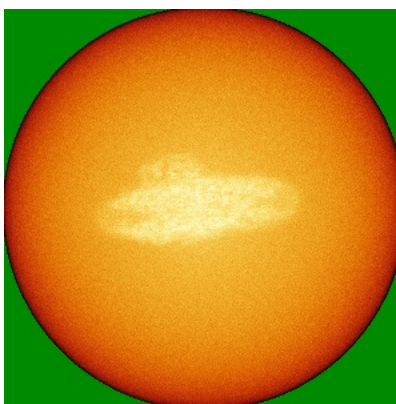


Z

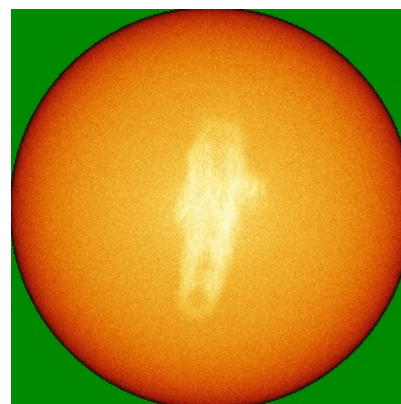
6.4.2 Raw map



X



Y

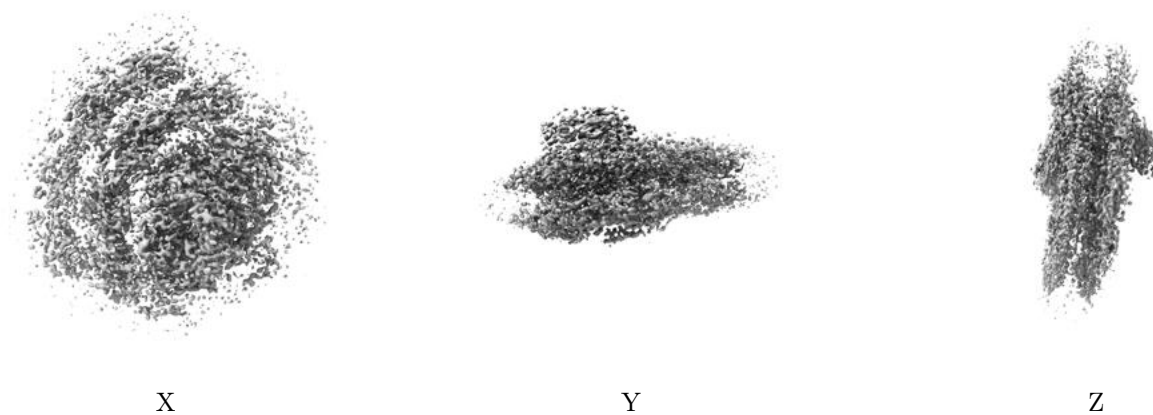


Z

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.

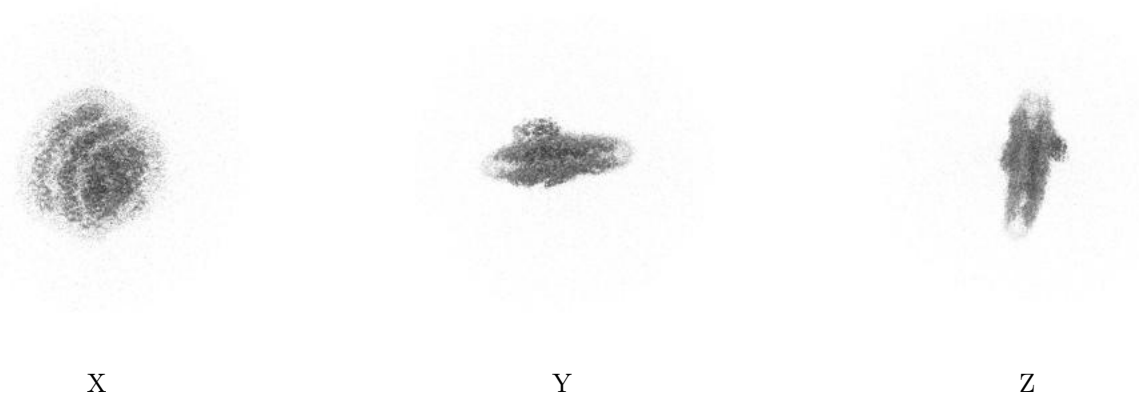
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

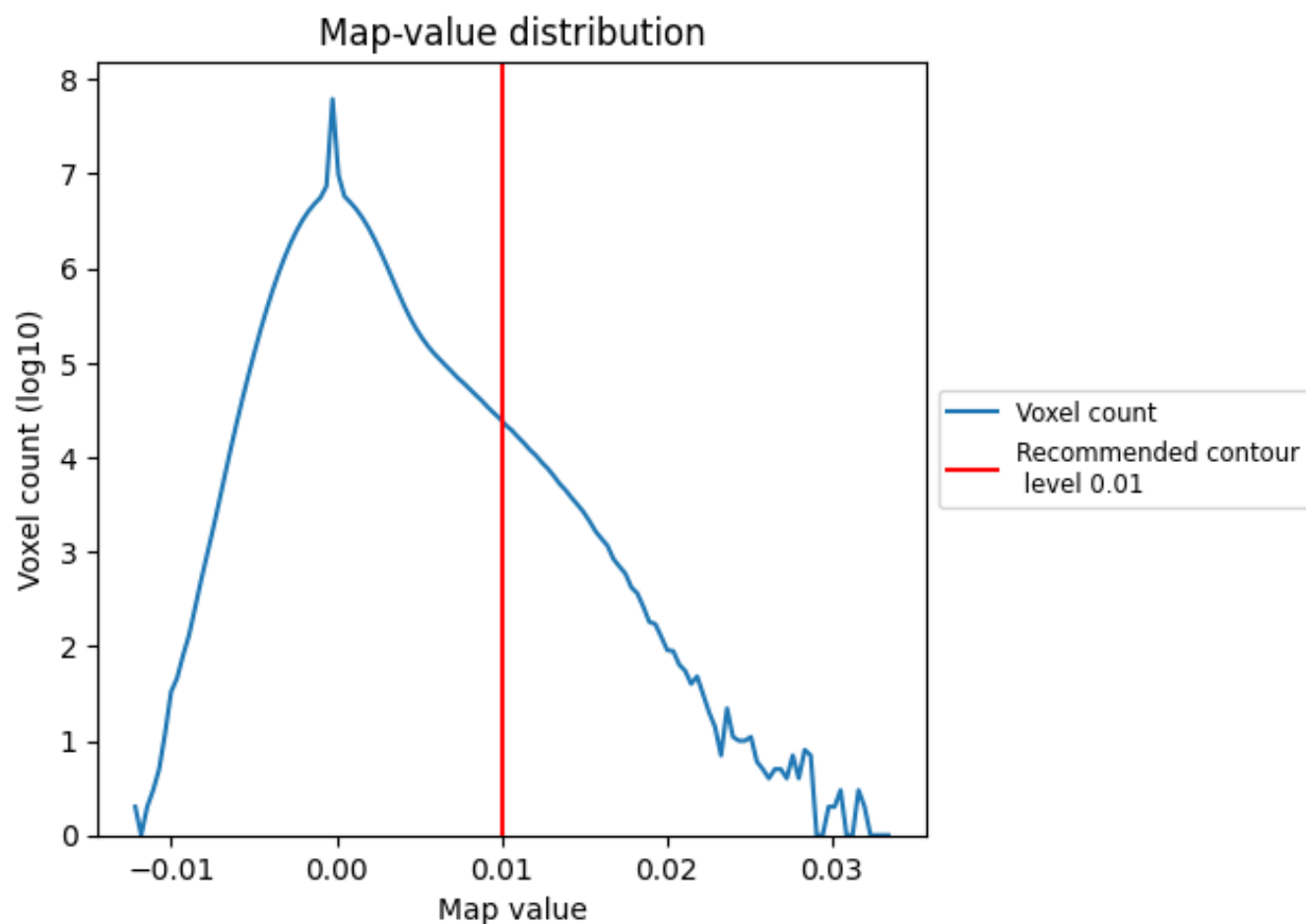
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

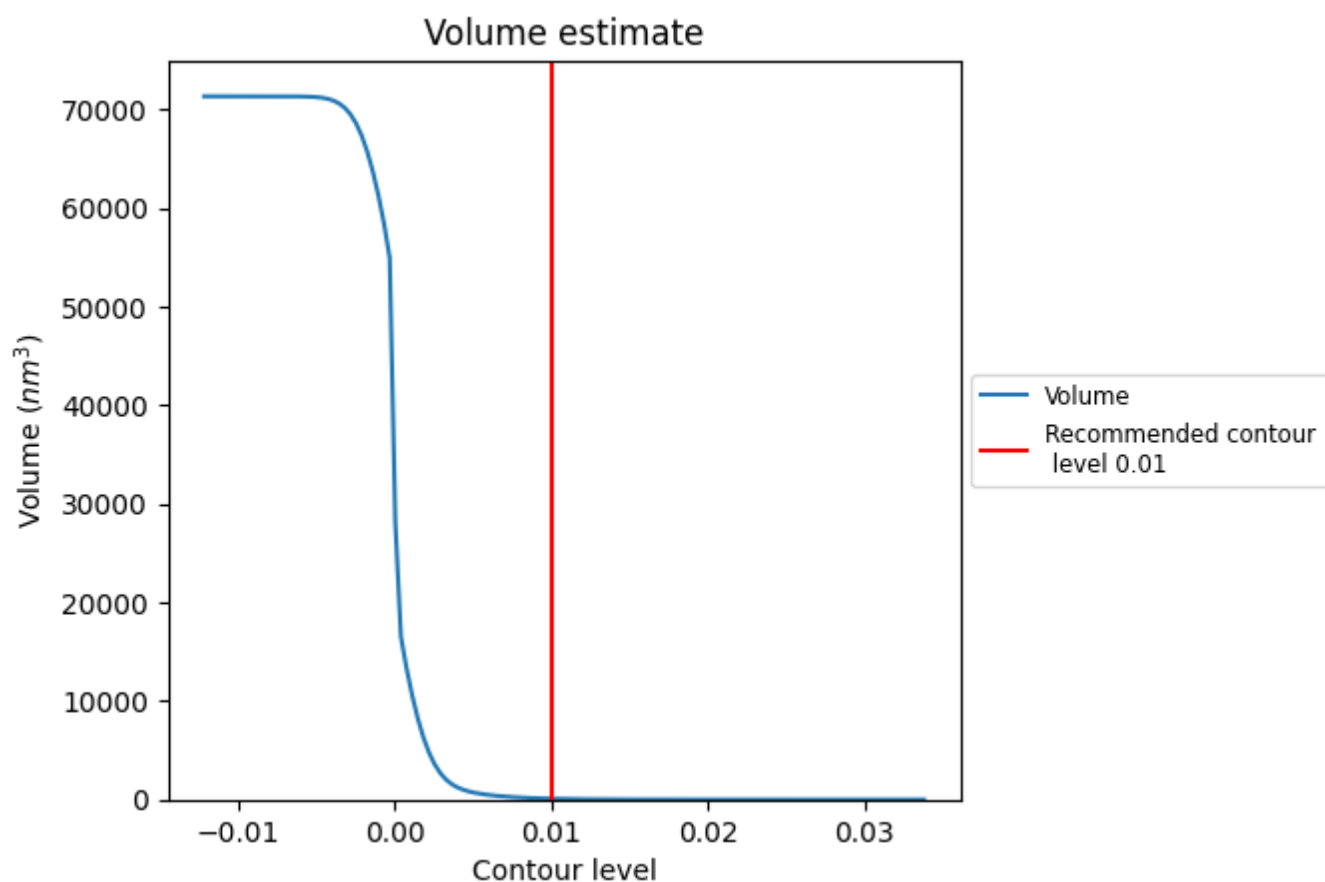
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

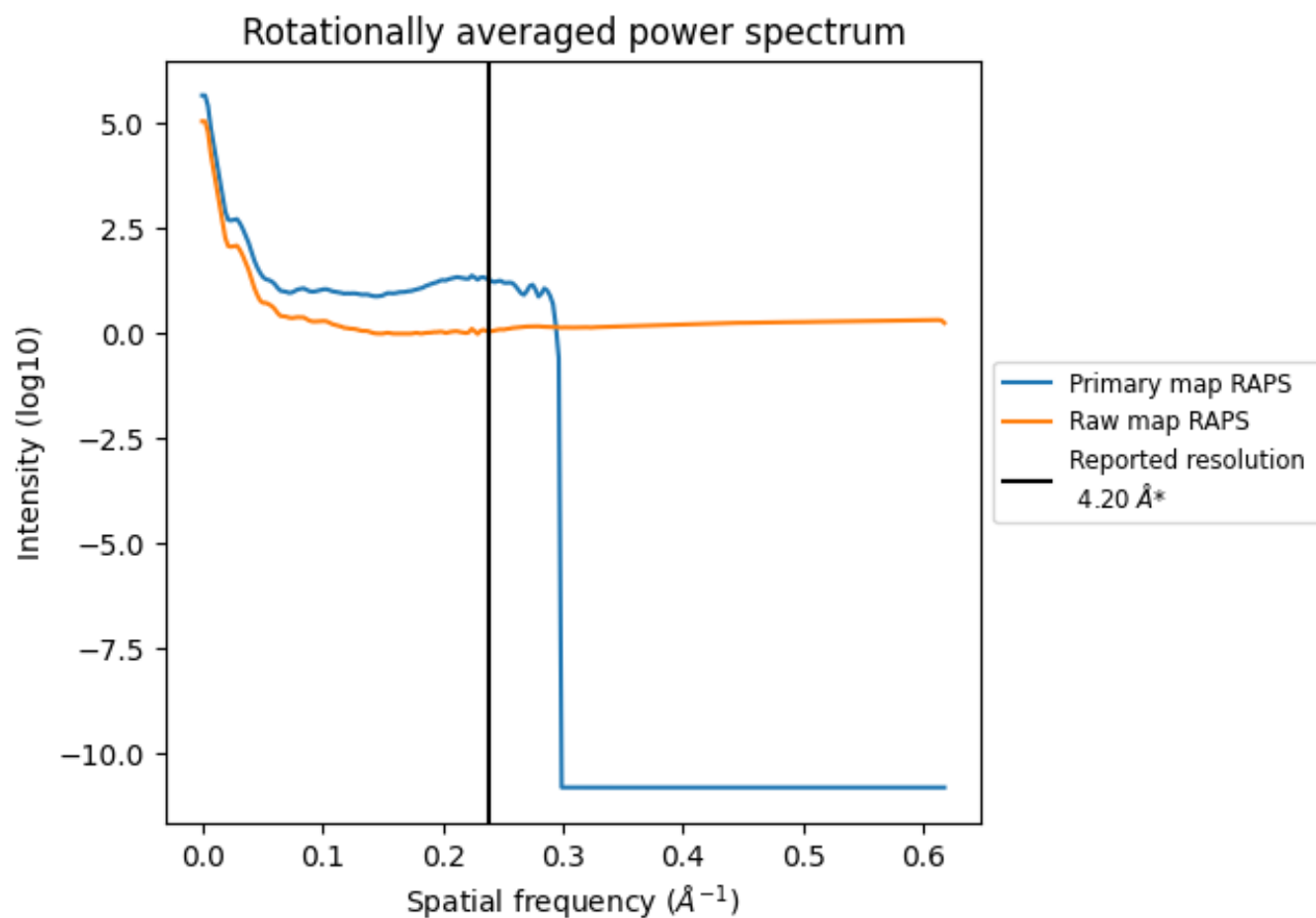
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 88 nm³; this corresponds to an approximate mass of 79 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

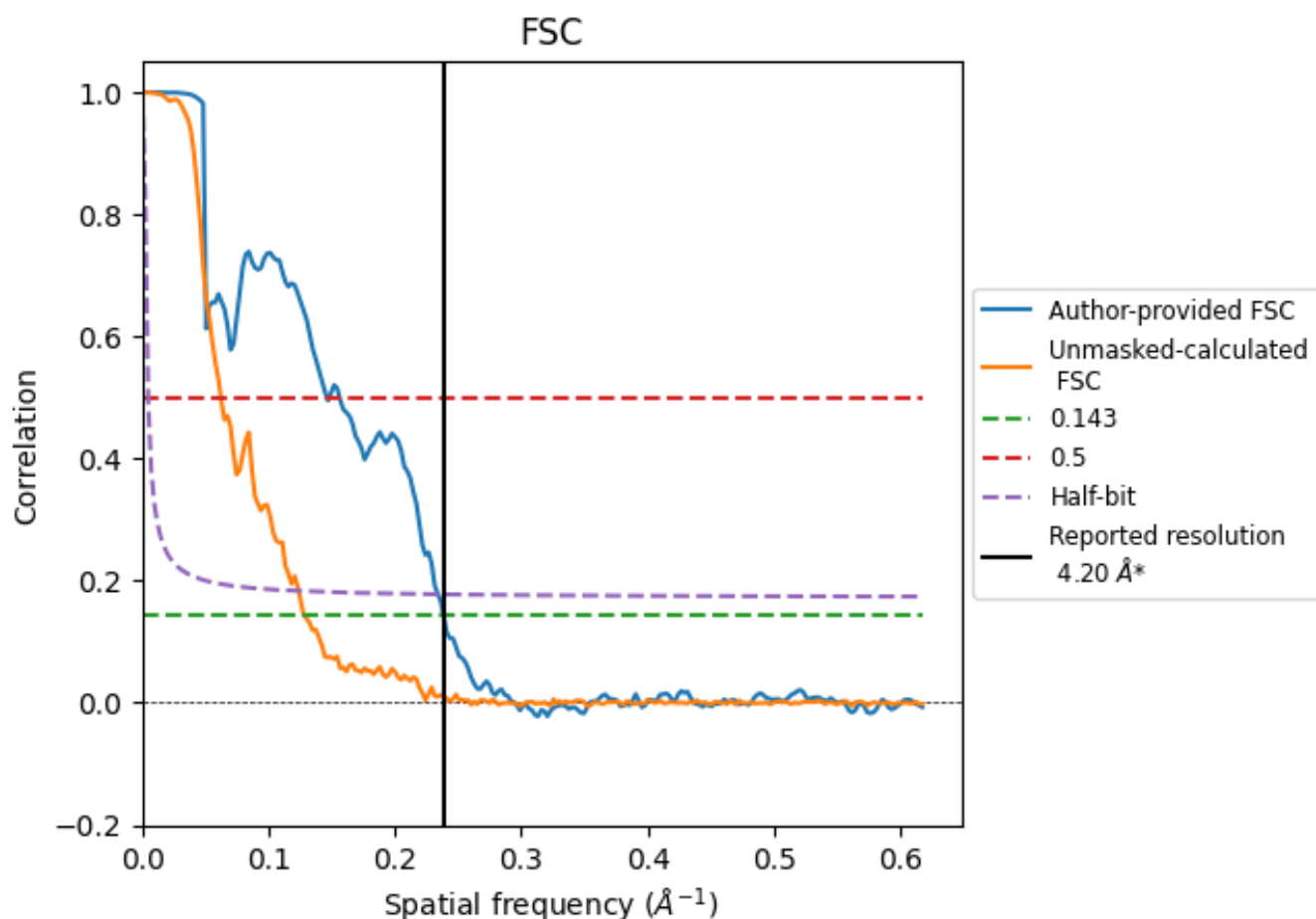


*Reported resolution corresponds to spatial frequency of 0.238 $\text{\AA}^{-1}$

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 0.238 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

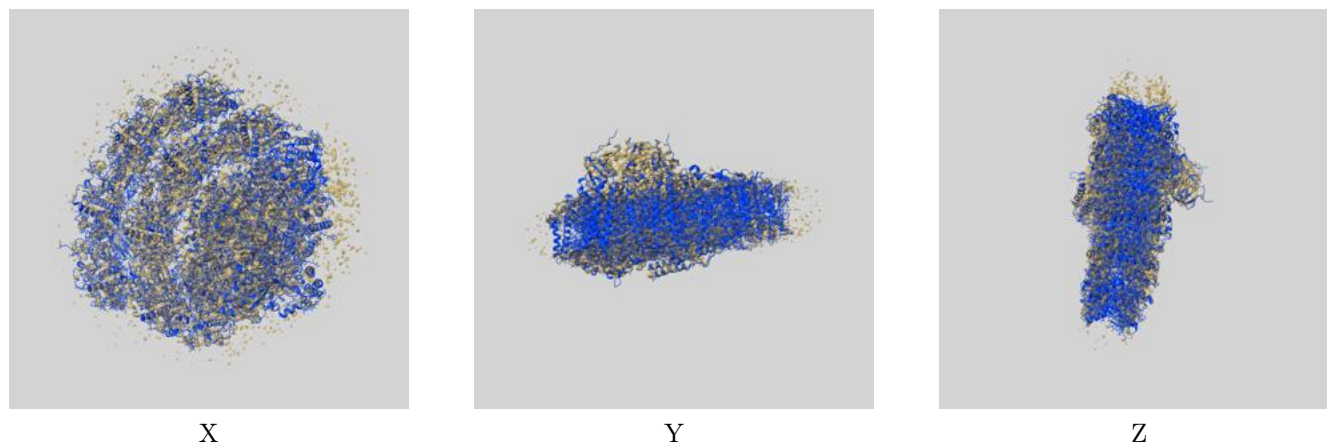
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.19	6.84	4.27
Unmasked-calculated*	7.81	16.08	8.08

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.81 differs from the reported value 4.2 by more than 10 %

9 Map-model fit [i](#)

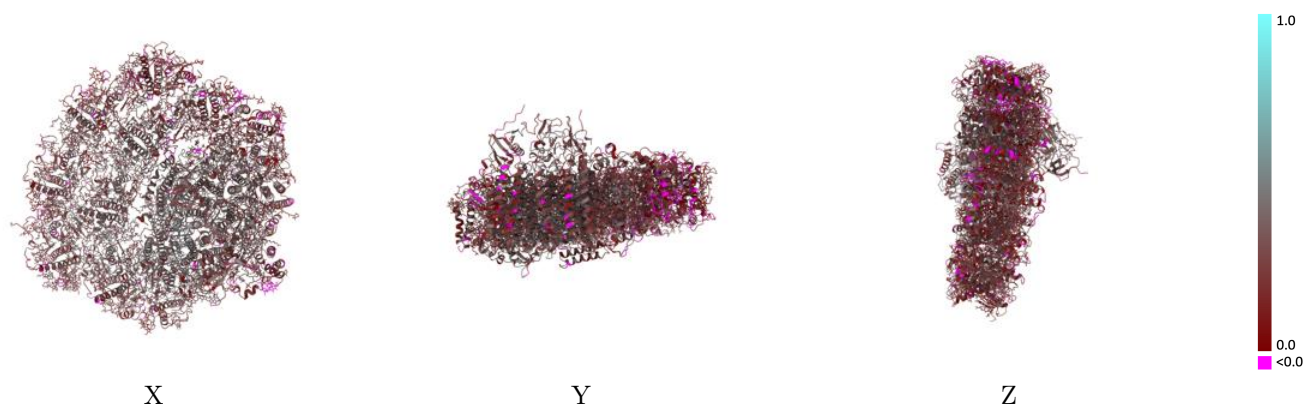
This section contains information regarding the fit between EMDB map EMD-11640 and PDB model 7A4P. Per-residue inclusion information can be found in section [3](#) on page [42](#).

9.1 Map-model overlay [i](#)



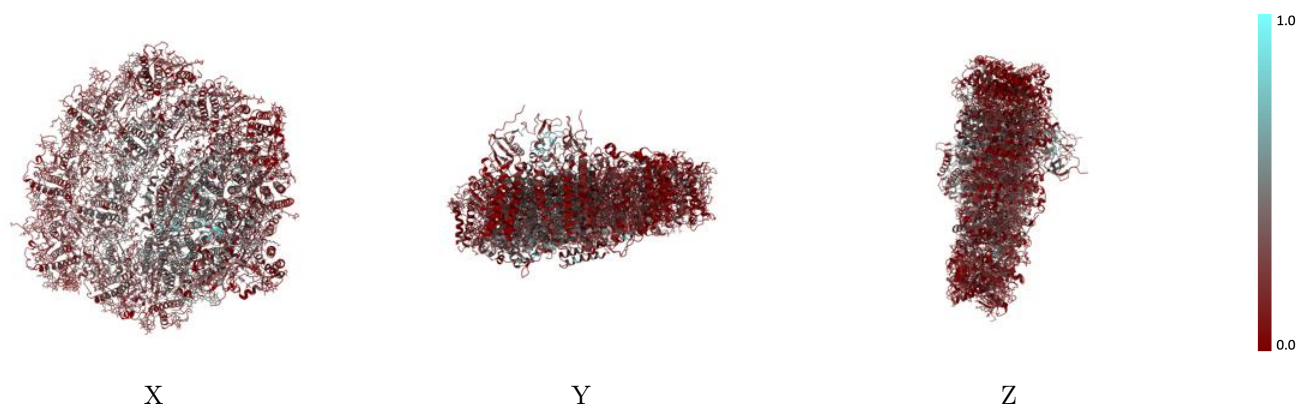
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



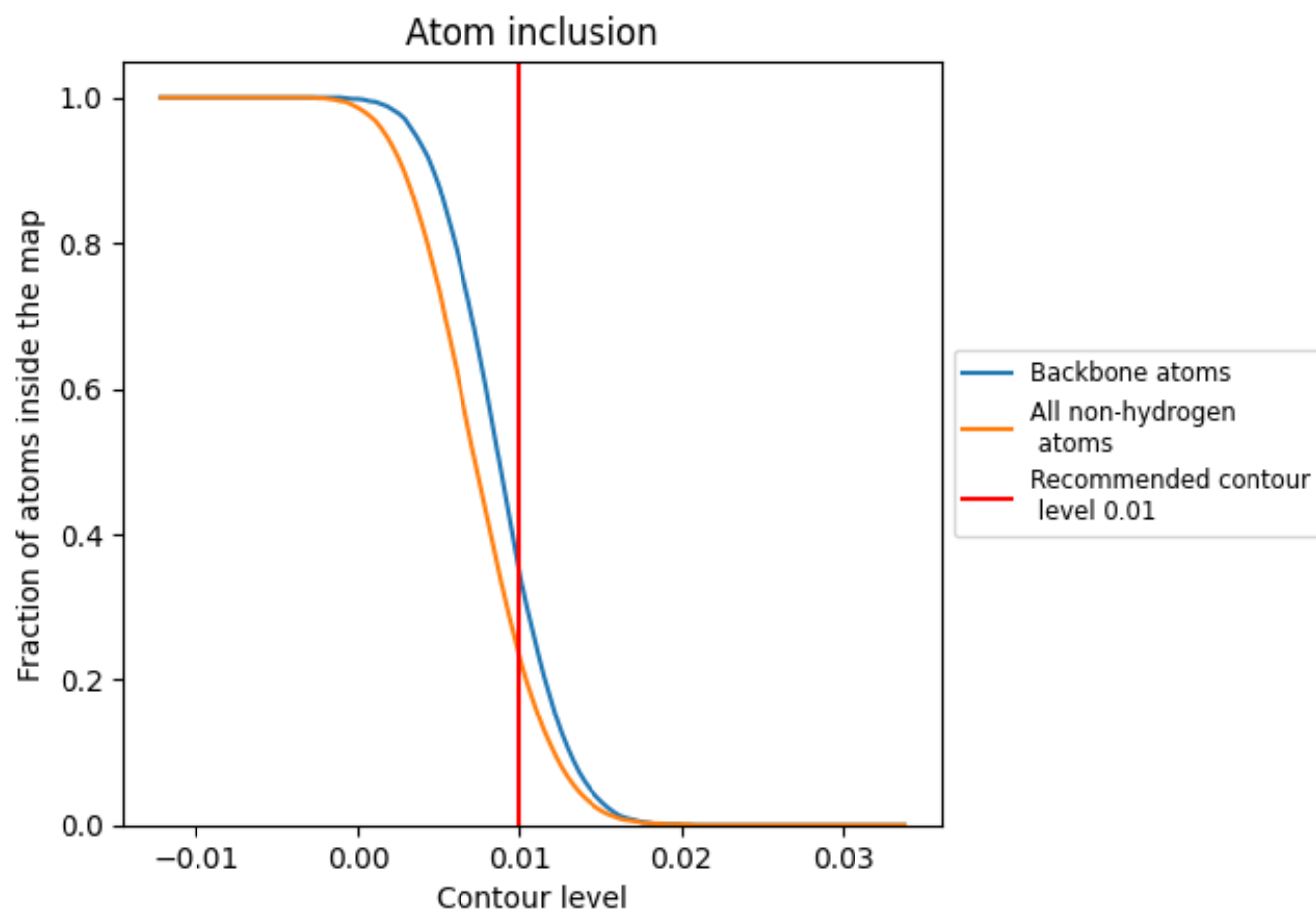
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 35% of all backbone atoms, 23% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2310	0.2780
1	0.1750	0.2150
3	0.2010	0.2770
4	0.1770	0.2250
5	0.1120	0.2330
6	0.1120	0.2290
7	0.2870	0.2990
8	0.2740	0.2880
A	0.3560	0.3500
B	0.2600	0.3140
C	0.4480	0.3400
D	0.2230	0.2740
E	0.3190	0.2800
F	0.2750	0.2970
G	0.0350	0.1850
I	0.0870	0.2110
J	0.2980	0.3560
K	0.0940	0.2190
L	0.0510	0.1760
M	0.0290	0.1970
a	0.1460	0.1790

1.0

0.0

<0.0