



wwPDB EM Validation Summary Report ⓘ

Sep 20, 2026 – 07:03 pm BST

PDB ID : 9HD7 / pdb_00009hd7
EMDB ID : EMD-52056
Title : Cryo-EM structure of photosystem II C2S2M2L2 supercomplex from the green alga *Chlorella ohadii*
Authors : Kopecny, D.; Kouril, R.; Ardhad, R.; Skolidis, I.; Kastitis, P.
Deposited on : 2024-11-11
Resolution : 2.95 Å (reported)
Based on initial models : 8C29, 7OUI

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:

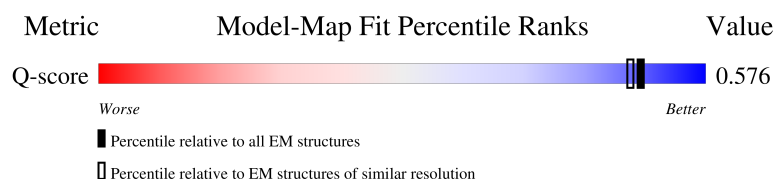
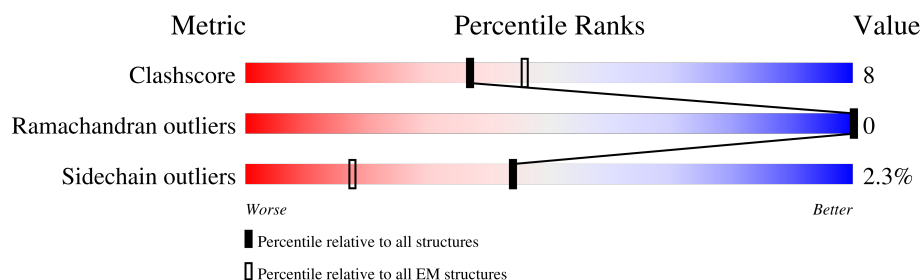
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD 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 2.95 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	13114 (2.45 - 3.45)

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

Mol	Chain	Length	Quality of chain
1	1	249	42% 71% 16% • 12%
1	11	249	49% 67% 21% • 10%
1	14	249	48% 69% 19% • 10%
1	4	249	43% 71% 15% • 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	249	
1	g	249	
2	12	247	
2	15	247	
2	2	247	
2	5	247	
2	N	247	
2	n	247	
3	3	259	
3	6	259	
4	7	140	
4	8	140	
5	13	243	
5	16	243	
6	A	353	
6	a	353	
7	B	508	
7	b	508	
8	C	473	
8	c	473	
9	D	352	
9	d	352	
10	E	83	
10	e	83	
11	F	41	

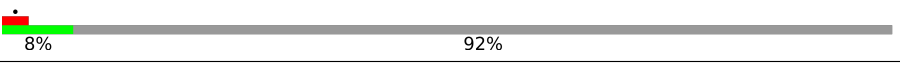
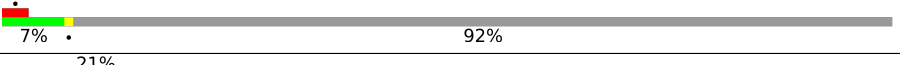
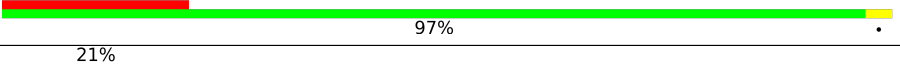
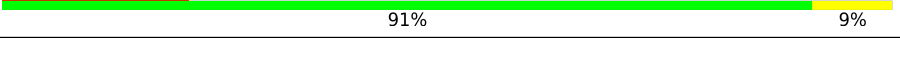
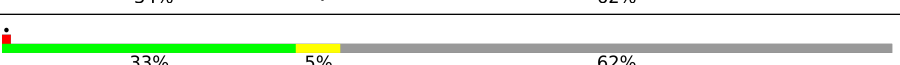
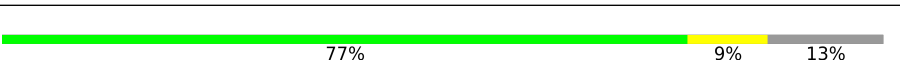
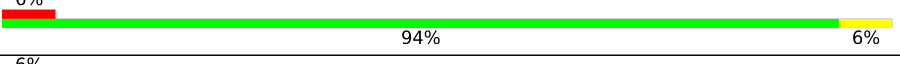
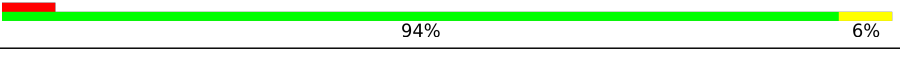
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
11	f	41	 5% 78% 12% 10%
12	H	80	 2% 72% 11% 16%
12	h	80	 2% 76% 8% 16%
13	I	38	 2% 87% 1% 11%
13	i	38	 2% 87% 1% 11%
14	J	42	 5% 76% 14% 10%
14	j	42	 2% 79% 12% 10%
15	K	42	 71% 17% 12%
15	k	42	 71% 17% 12%
16	L	38	 5% 79% 16% 2% 2%
16	l	38	 5% 74% 21% 2% 2%
17	M	34	 2% 82% 6% 12%
17	m	34	 2% 88% 12%
18	O	305	 8% 67% 10% 22%
18	o	305	 7% 66% 12% 22%
19	P	915	 19% 79%
19	p	915	 19% 79%
20	Q	203	 22% 62% 8% 29%
20	q	203	 22% 63% 8% 29%
21	R	297	 2% 67% 11% 22%
21	r	297	 2% 66% 12% 22%
22	S	293	 8% 73% 15% 12%
22	s	293	 9% 75% 13% 12%
23	T	31	 2% 94% 2% 2%
23	t	31	 2% 90% 6% 2%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
24	U	367	
24	u	367	
25	V	33	
25	v	33	
26	W	447	
26	w	447	
27	X	100	
27	x	100	
28	Y	256	
28	y	256	
29	Z	62	
29	z	62	

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
31	CLA	12	612	-	-	X	-
33	LUT	12	614	-	-	X	-

2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 112944 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Chlorophyll a-b binding protein Lhcbm-I.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	220	Total	C	N	O	S	0	0
			1673	1084	267	317	5		
1	4	220	Total	C	N	O	S	0	0
			1673	1084	267	317	5		
1	11	223	Total	C	N	O	S	0	0
			1693	1094	272	322	5		
1	14	223	Total	C	N	O	S	0	0
			1693	1094	272	322	5		
1	G	223	Total	C	N	O	S	0	0
			1693	1094	272	322	5		
1	g	223	Total	C	N	O	S	0	0
			1693	1094	272	322	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	196	Total	C	N	O	S	0	0
			1496	966	249	276	5		
2	5	196	Total	C	N	O	S	0	0
			1496	966	249	276	5		
2	12	170	Total	C	N	O	S	0	0
			1330	863	220	242	5		
2	15	170	Total	C	N	O	S	0	0
			1330	863	220	242	5		
2	N	220	Total	C	N	O	S	0	0
			1679	1085	278	311	5		
2	n	220	Total	C	N	O	S	0	0
			1679	1085	278	311	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	214	Total	C	N	O	S	0	0
			1630	1056	265	304	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	214	Total	C	N	O	S	0	0
			1630	1056	265	304	5		

- Molecule 4 is a protein called Chloroplast photosystem II 10 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	7	107	Total	C	N	O	S	0	0
			816	522	136	156	2		
4	8	107	Total	C	N	O	S	0	0
			816	522	136	156	2		

- Molecule 5 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	13	215	Total	C	N	O	S	0	0
			1645	1064	268	308	5		
5	16	215	Total	C	N	O	S	0	0
			1645	1064	268	308	5		

- Molecule 6 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	336	Total	C	N	O	S	0	0
			2632	1718	431	469	14		
6	a	336	Total	C	N	O	S	0	0
			2632	1718	431	469	14		

- Molecule 7 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	505	Total	C	N	O	S	0	0
			3963	2588	669	694	12		
7	b	505	Total	C	N	O	S	0	0
			3963	2588	669	694	12		

- Molecule 8 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	449	Total	C	N	O	S	0	0
			3491	2284	585	607	15		
8	c	449	Total	C	N	O	S	0	0
			3491	2284	585	607	15		

- Molecule 9 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	342	Total	C	N	O	S	0	0
			2730	1806	449	464	11		
9	d	342	Total	C	N	O	S	0	0
			2730	1806	449	464	11		

- Molecule 10 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	E	80	Total	C	N	O	0	0
			646	420	105	121		
10	e	80	Total	C	N	O	0	0
			646	420	105	121		

- Molecule 11 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	37	Total	C	N	O	S	0	0
			303	206	49	47	1		
11	f	37	Total	C	N	O	S	0	0
			303	206	49	47	1		

- Molecule 12 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	67	Total	C	N	O	S	0	0
			507	336	73	95	3		
12	h	67	Total	C	N	O	S	0	0
			507	336	73	95	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	34	Total	C	N	O	S	0	0
			274	187	41	45	1		
13	i	34	Total	C	N	O	S	0	0
			274	187	41	45	1		

- Molecule 14 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	J	38	Total	C	N	O	0	0
			270	182	42	46		
14	j	38	Total	C	N	O	0	0
			270	182	42	46		

- Molecule 15 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	K	37	Total	C	N	O	0	0
			295	204	43	48		
15	k	37	Total	C	N	O	0	0
			295	204	43	48		

- Molecule 16 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	L	37	Total	C	N	O	0	0
			303	203	48	52		
16	l	37	Total	C	N	O	0	0
			303	203	48	52		

- Molecule 17 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	M	30	Total	C	N	O	0	0
			228	157	33	38		
17	m	30	Total	C	N	O	0	0
			228	157	33	38		

- Molecule 18 is a protein called Chloroplast oxygen-evolving enhancer protein 1b (PsbO).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	238	Total	C	N	O	S	0	0
			1759	1106	288	357	8		
18	o	238	Total	C	N	O	S	0	0
			1759	1106	288	357	8		

- Molecule 19 is a protein called PWWP domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	188	Total	C	N	O	S	0	0
			1443	918	245	279	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
19	p	188	Total	C	N	O	S	0	0
			1443	918	245	279	1		

- Molecule 20 is a protein called Chloroplast oxygen-evolving enhancer protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	144	Total	C	N	O		0	0
			1122	701	207	214			
20	q	144	Total	C	N	O		0	0
			1122	701	207	214			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	231	Total	C	N	O	S	0	0
			1783	1132	303	342	6		
21	r	231	Total	C	N	O	S	0	0
			1783	1132	303	342	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	257	Total	C	N	O	S	0	0
			1934	1242	323	364	5		
22	s	257	Total	C	N	O	S	0	0
			1934	1242	323	364	5		

- Molecule 23 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	T	30	Total	C	N	O	S	0	0
			246	172	36	37	1		
23	t	30	Total	C	N	O	S	0	0
			246	172	36	37	1		

- Molecule 24 is a protein called Chloroplast PsbY.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	30	Total	C	N	O		0	0
			233	156	40	37			
24	u	30	Total	C	N	O		0	0
			233	156	40	37			

- Molecule 25 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	V	33	Total	C	N	O	S	0	0
			241	160	39	41	1		
25	v	33	Total	C	N	O	S	0	0
			241	160	39	41	1		

- Molecule 26 is a protein called PSII 6.1 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	W	60	Total	C	N	O	0	0
			468	301	74	93		
26	w	60	Total	C	N	O	0	0
			468	301	74	93		

- Molecule 27 is a protein called Photosystem II reaction center protein X (PsbX).

Mol	Chain	Residues	Atoms				AltConf	Trace
27	X	38	Total	C	N	O	0	0
			258	162	47	49		
27	x	38	Total	C	N	O	0	0
			258	162	47	49		

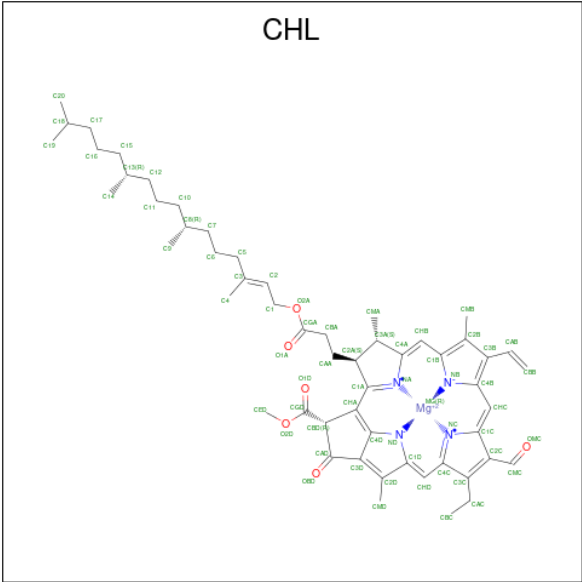
- Molecule 28 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Y	222	Total	C	N	O	S	0	0
			1694	1102	271	316	5		
28	y	222	Total	C	N	O	S	0	0
			1694	1102	271	316	5		

- Molecule 29 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	62	Total	C	N	O	S	0	0
			478	335	68	74	1		
29	z	62	Total	C	N	O	S	0	0
			478	335	68	74	1		

- Molecule 30 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
30	1	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
30	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	1	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
30	1	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	1	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	1	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
30	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
30	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	2	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	2	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
30	3	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
30	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
30	3	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
30	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	3	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	4	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
30	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	4	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
30	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	4	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	5	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	5	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	5	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
30	6	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
30	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	6	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
30	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	6	1	Total	C	Mg	N	O	0
			50	39	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
30	6	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	11	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	11	1	Total 48	C 37	Mg 1	N 4	O 6	0
30	11	1	Total 47	C 36	Mg 1	N 4	O 6	0
30	11	1	Total 46	C 35	Mg 1	N 4	O 6	0
30	11	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	11	1	Total 56	C 45	Mg 1	N 4	O 6	0
30	12	1	Total 50	C 39	Mg 1	N 4	O 6	0
30	12	1	Total 46	C 35	Mg 1	N 4	O 6	0
30	12	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	12	1	Total 50	C 39	Mg 1	N 4	O 6	0
30	12	1	Total 53	C 42	Mg 1	N 4	O 6	0
30	13	1	Total 56	C 45	Mg 1	N 4	O 6	0
30	13	1	Total 56	C 45	Mg 1	N 4	O 6	0
30	13	1	Total 61	C 50	Mg 1	N 4	O 6	0
30	13	1	Total 61	C 50	Mg 1	N 4	O 6	0
30	13	1	Total 50	C 39	Mg 1	N 4	O 6	0
30	13	1	Total 61	C 50	Mg 1	N 4	O 6	0
30	14	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	14	1	Total 48	C 37	Mg 1	N 4	O 6	0
30	14	1	Total 47	C 36	Mg 1	N 4	O 6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
30	14	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	14	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	14	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
30	15	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	15	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	15	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	15	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	15	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
30	16	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
30	16	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
30	16	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
30	16	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
30	16	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	16	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
30	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	G	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
30	G	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
30	G	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
30	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	G	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	N	1	Total	C	Mg	N	O	0
			53	42	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
30	N	1	Total 61	C 50	Mg 1	N 4	O 6	0
30	N	1	Total 61	C 50	Mg 1	N 4	O 6	0
30	N	1	Total 50	C 39	Mg 1	N 4	O 6	0
30	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	R	1	Total 56	C 45	Mg 1	N 4	O 6	0
30	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	R	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
30	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	S	1	Total 43	C 34	Mg 1	N 4	O 4	0
30	S	1	Total 49	C 38	Mg 1	N 4	O 6	0
30	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	Y	1	Total 56	C 45	Mg 1	N 4	O 6	0
30	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	Y	1	Total 44	C 35	Mg 1	N 4	O 4	0
30	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	g	1	Total 48	C 37	Mg 1	N 4	O 6	0
30	g	1	Total 50	C 39	Mg 1	N 4	O 6	0

Continued on next page...

Continued from previous page...

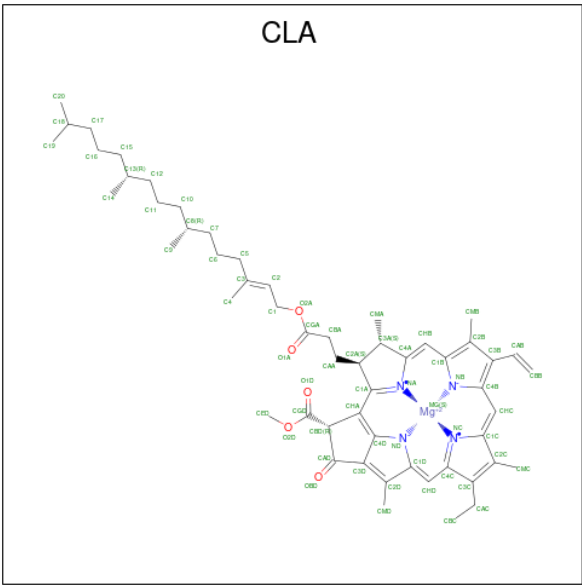
Mol	Chain	Residues	Atoms					AltConf
30	g	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
30	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	g	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	n	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
30	n	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
30	n	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
30	n	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	r	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
30	r	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	r	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	s	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	s	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
30	s	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
30	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	y	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
30	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	y	1	Total	C	Mg	N	O	0
			44	35	1	4	4	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
30	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 31 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
31	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
31	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	2	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	4	1	Total 55	C 45	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
31	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	11	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	11	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	11	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	11	1	Total 55	C 45	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
31	11	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	11	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	11	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	11	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	12	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	12	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	12	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	12	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	12	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	13	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	13	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	13	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	13	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	13	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	13	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	13	1	Total 45	C 35	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
31	14	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	14	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	14	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	14	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	14	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	14	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	14	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	14	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	15	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	15	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	15	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	15	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	15	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	16	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	16	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	16	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	16	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	16	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
31	16	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	16	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	16	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	16	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	G	1	Total 50	C 40	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
31	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	G	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	N	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	N	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	N	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	R	1	Total 48	C 38	Mg 1	N 4	O 5	0
31	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	R	1	Total 60	C 50	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
31	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	R	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	R	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	S	1	Total 42	C 34	Mg 1	N 4	O 3	0
31	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	S	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	Y	1	Total 56	C 46	Mg 1	N 4	O 5	0
31	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	Y	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
31	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	Y	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
31	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	g	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	g	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
31	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	g	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	n	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	n	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	n	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	r	1	Total 48	C 38	Mg 1	N 4	O 5	0
31	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	r	1	Total 49	C 39	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

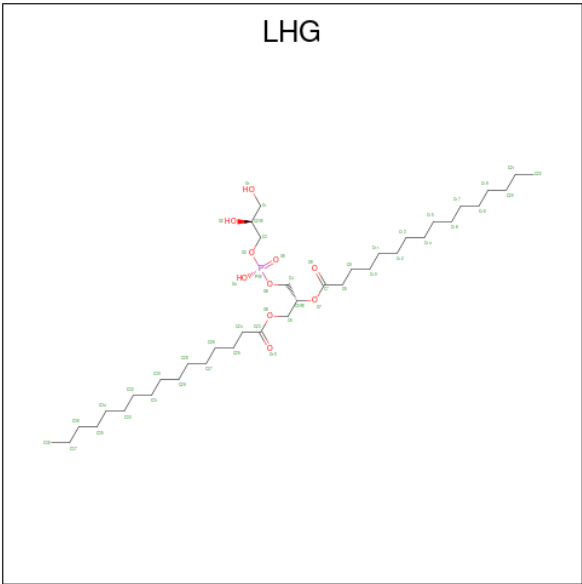
Mol	Chain	Residues	Atoms					AltConf
31	r	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	r	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	s	1	Total 42	C 34	Mg 1	N 4	O 3	0
31	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	s	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	s	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	y	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	y	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
31	y	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	y	1	Total	C	Mg	N	O	0
			56	46	1	4	5	

- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
32	1	1	Total	C	O	P	0
			43	32	10	1	
32	3	1	Total	C	O	P	0
			44	33	10	1	
32	3	1	Total	C	O	P	0
			47	36	10	1	
32	4	1	Total	C	O	P	0
			47	36	10	1	
32	6	1	Total	C	O	P	0
			44	33	10	1	
32	6	1	Total	C	O	P	0
			47	36	10	1	
32	11	1	Total	C	O	P	0
			49	38	10	1	
32	13	1	Total	C	O	P	0
			40	29	10	1	
32	14	1	Total	C	O	P	0
			49	38	10	1	

Continued on next page...

Continued from previous page...

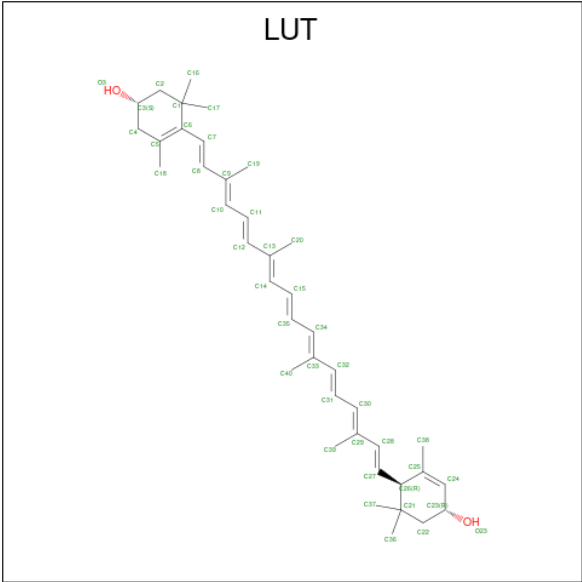
Mol	Chain	Residues	Atoms				AltConf
32	16	1	Total 40	C 29	O 10	P 1	0
32	A	1	Total 49	C 38	O 10	P 1	0
32	A	1	Total 44	C 33	O 10	P 1	0
32	A	1	Total 43	C 32	O 10	P 1	0
32	A	1	Total 49	C 38	O 10	P 1	0
32	C	1	Total 42	C 31	O 10	P 1	0
32	D	1	Total 49	C 38	O 10	P 1	0
32	D	1	Total 39	C 28	O 10	P 1	0
32	D	1	Total 49	C 38	O 10	P 1	0
32	G	1	Total 49	C 38	O 10	P 1	0
32	L	1	Total 47	C 36	O 10	P 1	0
32	N	1	Total 49	C 38	O 10	P 1	0
32	R	1	Total 44	C 33	O 10	P 1	0
32	R	1	Total 38	C 27	O 10	P 1	0
32	R	1	Total 47	C 36	O 10	P 1	0
32	S	1	Total 49	C 38	O 10	P 1	0
32	S	1	Total 45	C 34	O 10	P 1	0
32	Y	1	Total 47	C 36	O 10	P 1	0
32	Y	1	Total 49	C 38	O 10	P 1	0
32	Y	1	Total 47	C 36	O 10	P 1	0
32	a	1	Total 49	C 38	O 10	P 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
32	a	1	Total	C	O	P	0
			49	38	10	1	
32	a	1	Total	C	O	P	0
			44	33	10	1	
32	a	1	Total	C	O	P	0
			43	32	10	1	
32	c	1	Total	C	O	P	0
			42	31	10	1	
32	d	1	Total	C	O	P	0
			49	38	10	1	
32	d	1	Total	C	O	P	0
			39	28	10	1	
32	d	1	Total	C	O	P	0
			49	38	10	1	
32	g	1	Total	C	O	P	0
			49	38	10	1	
32	l	1	Total	C	O	P	0
			47	36	10	1	
32	n	1	Total	C	O	P	0
			49	38	10	1	
32	r	1	Total	C	O	P	0
			44	33	10	1	
32	r	1	Total	C	O	P	0
			38	27	10	1	
32	r	1	Total	C	O	P	0
			47	36	10	1	
32	s	1	Total	C	O	P	0
			49	38	10	1	
32	s	1	Total	C	O	P	0
			45	34	10	1	
32	y	1	Total	C	O	P	0
			47	36	10	1	
32	y	1	Total	C	O	P	0
			49	38	10	1	
32	y	1	Total	C	O	P	0
			47	36	10	1	

- Molecule 33 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
33	1	1	Total	C	O	0
			42	40	2	
33	1	1	Total	C	O	0
			42	40	2	
33	2	1	Total	C	O	0
			42	40	2	
33	2	1	Total	C	O	0
			42	40	2	
33	3	1	Total	C	O	0
			42	40	2	
33	3	1	Total	C	O	0
			42	40	2	
33	4	1	Total	C	O	0
			42	40	2	
33	4	1	Total	C	O	0
			42	40	2	
33	5	1	Total	C	O	0
			42	40	2	
33	5	1	Total	C	O	0
			42	40	2	
33	6	1	Total	C	O	0
			42	40	2	
33	6	1	Total	C	O	0
			42	40	2	
33	11	1	Total	C	O	0
			42	40	2	
33	11	1	Total	C	O	0
			42	40	2	

Continued on next page...

Continued from previous page...

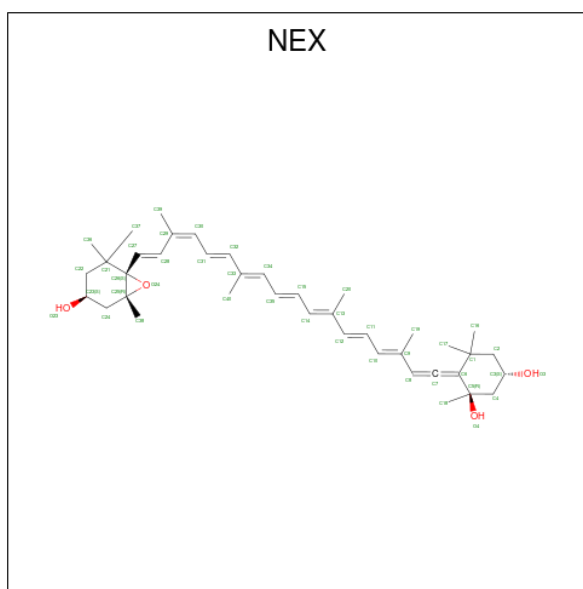
Mol	Chain	Residues	Atoms			AltConf
33	12	1	Total 42	C 40	O 2	0
33	12	1	Total 42	C 40	O 2	0
33	13	1	Total 42	C 40	O 2	0
33	13	1	Total 42	C 40	O 2	0
33	14	1	Total 42	C 40	O 2	0
33	14	1	Total 42	C 40	O 2	0
33	15	1	Total 42	C 40	O 2	0
33	15	1	Total 42	C 40	O 2	0
33	16	1	Total 42	C 40	O 2	0
33	16	1	Total 42	C 40	O 2	0
33	G	1	Total 42	C 40	O 2	0
33	G	1	Total 42	C 40	O 2	0
33	N	1	Total 42	C 40	O 2	0
33	N	1	Total 42	C 40	O 2	0
33	R	1	Total 42	C 40	O 2	0
33	S	1	Total 42	C 40	O 2	0
33	S	1	Total 42	C 40	O 2	0
33	Y	1	Total 42	C 40	O 2	0
33	Y	1	Total 42	C 40	O 2	0
33	g	1	Total 42	C 40	O 2	0
33	g	1	Total 42	C 40	O 2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
33	n	1	Total	C	O	0
			42	40	2	
33	n	1	Total	C	O	0
			42	40	2	
33	r	1	Total	C	O	0
			42	40	2	
33	s	1	Total	C	O	0
			42	40	2	
33	s	1	Total	C	O	0
			42	40	2	
33	y	1	Total	C	O	0
			42	40	2	
33	y	1	Total	C	O	0
			42	40	2	

- Molecule 34 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄).



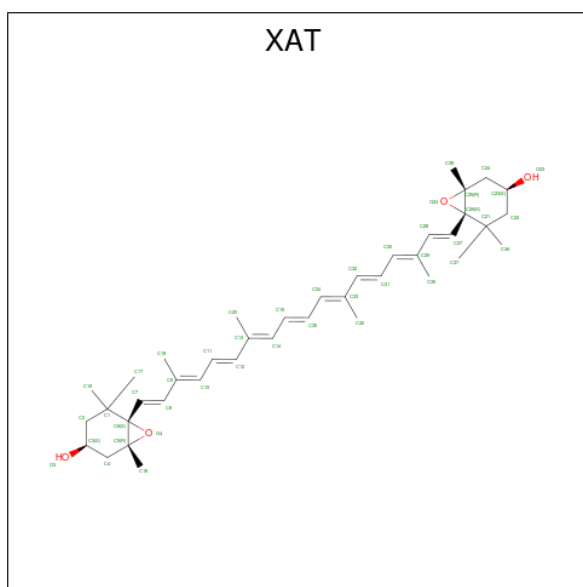
Mol	Chain	Residues	Atoms			AltConf
34	1	1	Total	C	O	0
			16	14	2	
34	2	1	Total	C	O	0
			32	30	2	
34	3	1	Total	C	O	0
			44	40	4	

Continued on next page...

Continued from previous page...

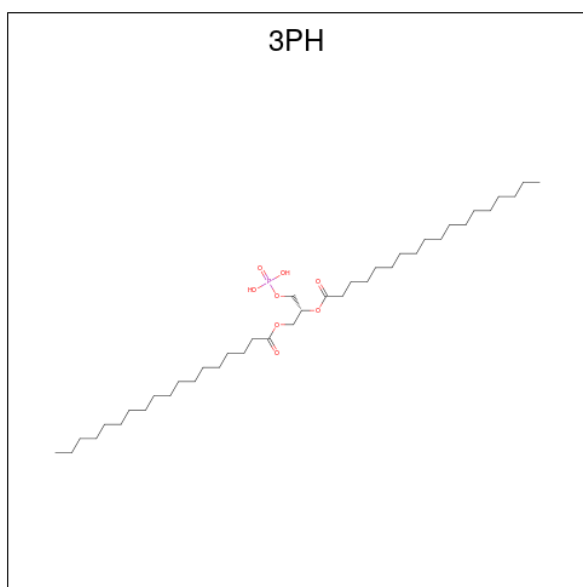
Mol	Chain	Residues	Atoms			AltConf
34	4	1	Total	C	O	0
			16	14	2	
34	5	1	Total	C	O	0
			32	30	2	
34	6	1	Total	C	O	0
			44	40	4	
34	11	1	Total	C	O	0
			16	14	2	
34	12	1	Total	C	O	0
			27	25	2	
34	13	1	Total	C	O	0
			44	40	4	
34	14	1	Total	C	O	0
			16	14	2	
34	15	1	Total	C	O	0
			27	25	2	
34	16	1	Total	C	O	0
			44	40	4	
34	G	1	Total	C	O	0
			43	39	4	
34	N	1	Total	C	O	0
			44	40	4	
34	R	1	Total	C	O	0
			44	40	4	
34	S	1	Total	C	O	0
			44	40	4	
34	Y	1	Total	C	O	0
			44	40	4	
34	g	1	Total	C	O	0
			44	40	4	
34	n	1	Total	C	O	0
			44	40	4	
34	r	1	Total	C	O	0
			44	40	4	
34	s	1	Total	C	O	0
			44	40	4	
34	y	1	Total	C	O	0
			44	40	4	

- Molecule 35 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: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



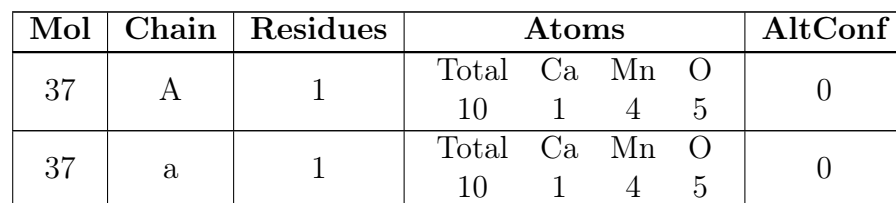
Mol	Chain	Residues	Atoms			AltConf
35	3	1	Total	C	O	0
			44	40	4	
35	6	1	Total	C	O	0
			44	40	4	
35	11	1	Total	C	O	0
			44	40	4	
35	14	1	Total	C	O	0
			44	40	4	
35	G	1	Total	C	O	0
			44	40	4	
35	R	1	Total	C	O	0
			44	40	4	
35	g	1	Total	C	O	0
			44	40	4	
35	r	1	Total	C	O	0
			44	40	4	

- Molecule 36 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).



Mol	Chain	Residues	Atoms				AltConf
36	7	1	Total	C	O	P	0
			48	39	8	1	
36	8	1	Total	C	O	P	0
			48	39	8	1	
36	B	1	Total	C	O	P	0
			48	39	8	1	
36	B	1	Total	C	O	P	0
			38	29	8	1	
36	T	1	Total	C	O	P	0
			48	39	8	1	
36	b	1	Total	C	O	P	0
			39	30	8	1	

- Molecule 37 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn₄O₅).



- # PHO

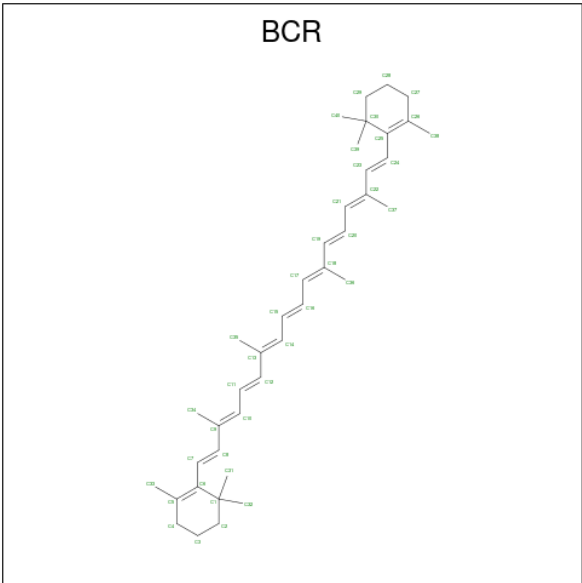
Mol	Chain	Residues	Atoms				AltConf
38	A	1	Total	C	N	O	0
			64	55	4	5	



Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
38	D	1	Total	C	N	O	0
			64	55	4	5	
38	a	1	Total	C	N	O	0
			64	55	4	5	
38	a	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 39 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



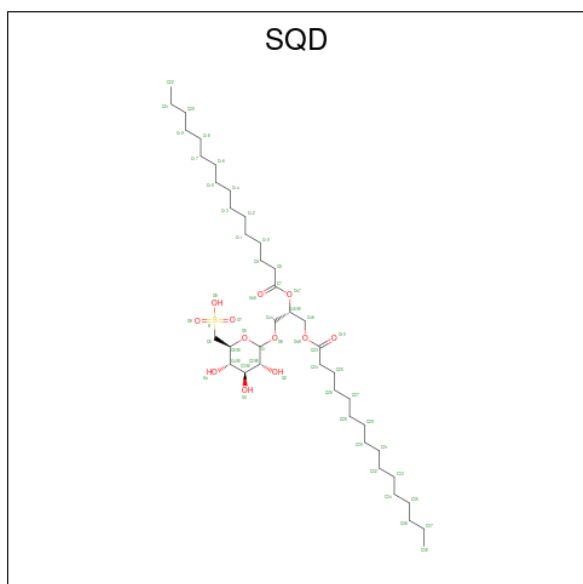
Mol	Chain	Residues	Atoms		AltConf
39	A	1	Total	C	0
			40	40	
39	B	1	Total	C	0
			40	40	
39	B	1	Total	C	0
			40	40	
39	B	1	Total	C	0
			40	40	
39	C	1	Total	C	0
			40	40	
39	C	1	Total	C	0
			40	40	
39	C	1	Total	C	0
			40	40	
39	D	1	Total	C	0
			40	40	

Continued on next page...

Continued from previous page...

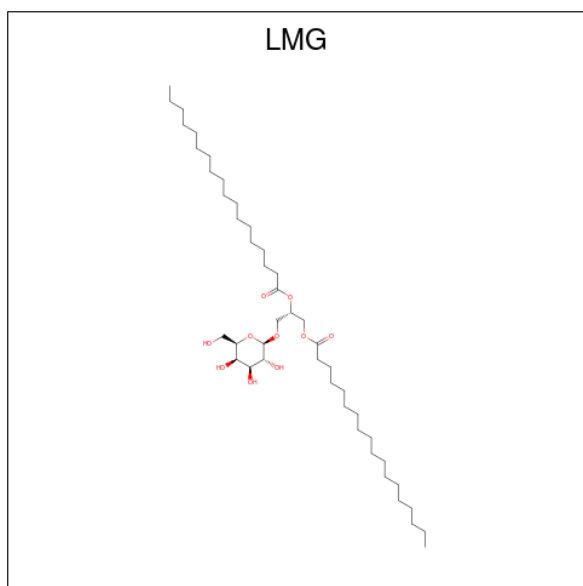
Mol	Chain	Residues	Atoms	AltConf
39	H	1	Total C 40 40	0
39	J	1	Total C 40 40	0
39	a	1	Total C 40 40	0
39	b	1	Total C 40 40	0
39	b	1	Total C 40 40	0
39	b	1	Total C 40 40	0
39	c	1	Total C 40 40	0
39	c	1	Total C 40 40	0
39	c	1	Total C 40 40	0
39	d	1	Total C 40 40	0
39	h	1	Total C 40 40	0
39	j	1	Total C 40 40	0

- Molecule 40 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
40	A	1	Total	C	O	S	0
			51	38	12	1	
40	D	1	Total	C	O	S	0
			54	41	12	1	
40	D	1	Total	C	O	S	0
			46	33	12	1	
40	L	1	Total	C	O	S	0
			50	37	12	1	
40	a	1	Total	C	O	S	0
			51	38	12	1	
40	d	1	Total	C	O	S	0
			54	41	12	1	
40	d	1	Total	C	O	S	0
			46	33	12	1	
40	l	1	Total	C	O	S	0
			50	37	12	1	

- Molecule 41 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



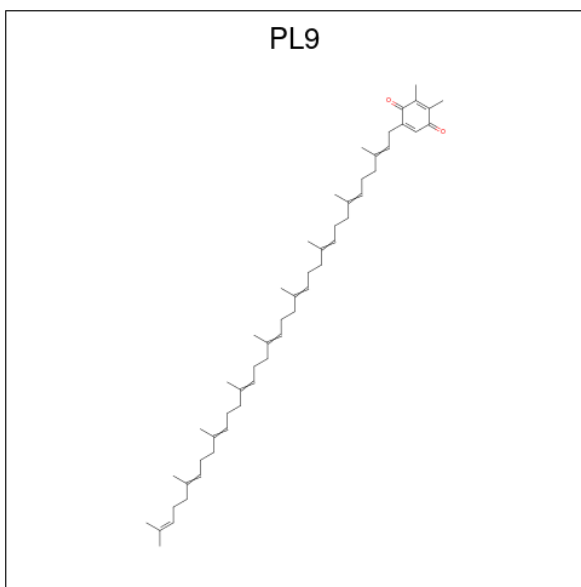
Mol	Chain	Residues	Atoms			AltConf
41	A	1	Total	C	O	0
			55	45	10	
41	B	1	Total	C	O	0
			49	39	10	
41	B	1	Total	C	O	0
			48	38	10	

Continued on next page...

Continued from previous page...

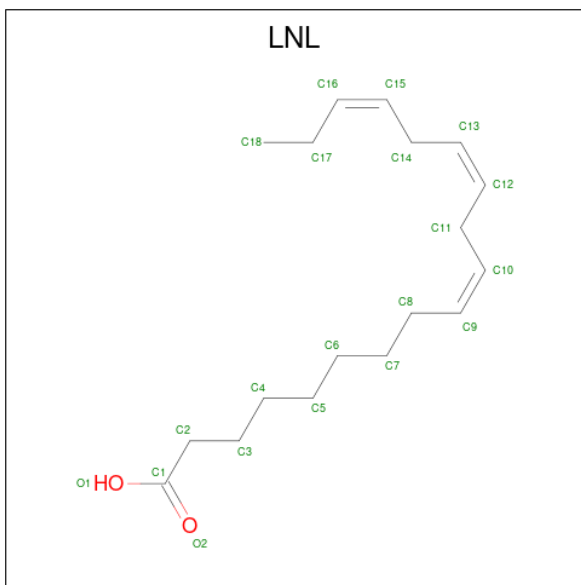
Mol	Chain	Residues	Atoms			AltConf
41	C	1	Total	C	O	0
			47	37	10	
41	C	1	Total	C	O	0
			55	45	10	
41	D	1	Total	C	O	0
			44	34	10	
41	D	1	Total	C	O	0
			48	38	10	
41	H	1	Total	C	O	0
			35	30	5	
41	J	1	Total	C	O	0
			51	41	10	
41	K	1	Total	C	O	0
			51	41	10	
41	S	1	Total	C	O	0
			42	32	10	
41	b	1	Total	C	O	0
			49	39	10	
41	b	1	Total	C	O	0
			46	36	10	
41	c	1	Total	C	O	0
			47	37	10	
41	c	1	Total	C	O	0
			55	45	10	
41	d	1	Total	C	O	0
			44	34	10	
41	d	1	Total	C	O	0
			35	30	5	
41	d	1	Total	C	O	0
			48	38	10	
41	j	1	Total	C	O	0
			51	41	10	
41	s	1	Total	C	O	0
			42	32	10	
41	v	1	Total	C	O	0
			51	41	10	
41	w	1	Total	C	O	0
			55	45	10	

- Molecule 42 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂) (labeled as "Ligand of Interest" by depositor).



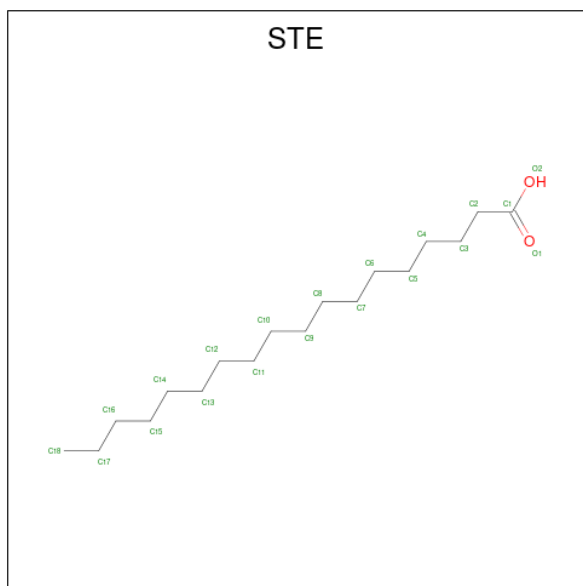
Mol	Chain	Residues	Atoms			AltConf
42	A	1	Total	C	O	0
			55	53	2	
42	D	1	Total	C	O	0
			55	53	2	
42	a	1	Total	C	O	0
			55	53	2	
42	d	1	Total	C	O	0
			55	53	2	

- Molecule 43 is ALPHA-LINOLENIC ACID (CCD ID: LNL) (formula: $C_{18}H_{30}O_2$).



Mol	Chain	Residues	Atoms			AltConf
43	A	1	Total	C	O	0
			20	18	2	
43	C	1	Total	C	O	0
			20	18	2	
43	C	1	Total	C	O	0
			20	18	2	
43	H	1	Total	C	O	0
			20	18	2	
43	I	1	Total	C	O	0
			20	18	2	
43	R	1	Total	C	O	0
			20	18	2	
43	W	1	Total	C	O	0
			20	18	2	
43	W	1	Total	C	O	0
			20	18	2	
43	X	1	Total	C	O	0
			20	18	2	
43	Y	1	Total	C	O	0
			20	18	2	
43	Y	1	Total	C	O	0
			20	18	2	
43	a	1	Total	C	O	0
			20	18	2	
43	c	1	Total	C	O	0
			20	18	2	
43	c	1	Total	C	O	0
			20	18	2	
43	h	1	Total	C	O	0
			20	18	2	
43	i	1	Total	C	O	0
			20	18	2	
43	r	1	Total	C	O	0
			20	18	2	
43	w	1	Total	C	O	0
			20	18	2	
43	x	1	Total	C	O	0
			20	18	2	
43	y	1	Total	C	O	0
			20	18	2	
43	y	1	Total	C	O	0
			20	18	2	
43	y	1	Total	C	O	0
			20	18	2	

- Molecule 44 is STEARIC ACID (CCD ID: STE) (formula: $C_{18}H_{36}O_2$).

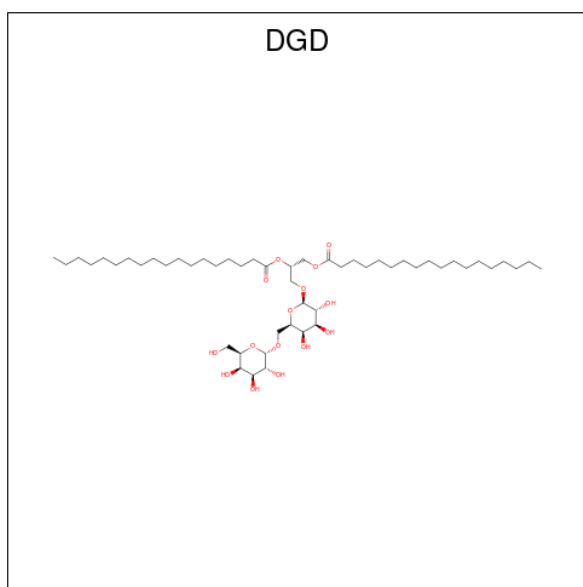


Mol	Chain	Residues	Atoms			AltConf
44	B	1	Total	C	O	0
			20	18	2	
44	b	1	Total	C	O	0
			20	18	2	

- Molecule 45 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
45	C	1	Total	Cl	0
			1	1	
45	c	1	Total	Cl	0
			1	1	

- Molecule 46 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).

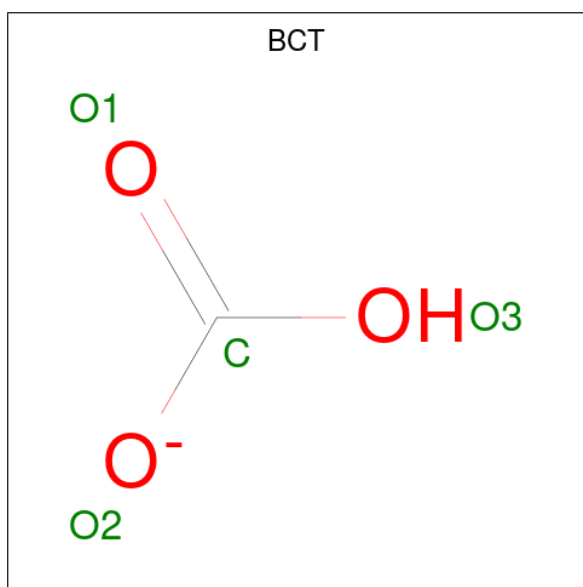


Mol	Chain	Residues	Atoms			AltConf
46	C	1	Total	C	O	0
			66	51	15	
46	C	1	Total	C	O	0
			58	43	15	
46	C	1	Total	C	O	0
			59	44	15	
46	W	1	Total	C	O	0
			46	36	10	
46	c	1	Total	C	O	0
			66	51	15	
46	c	1	Total	C	O	0
			58	43	15	
46	c	1	Total	C	O	0
			59	44	15	
46	w	1	Total	C	O	0
			40	30	10	

- Molecule 47 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

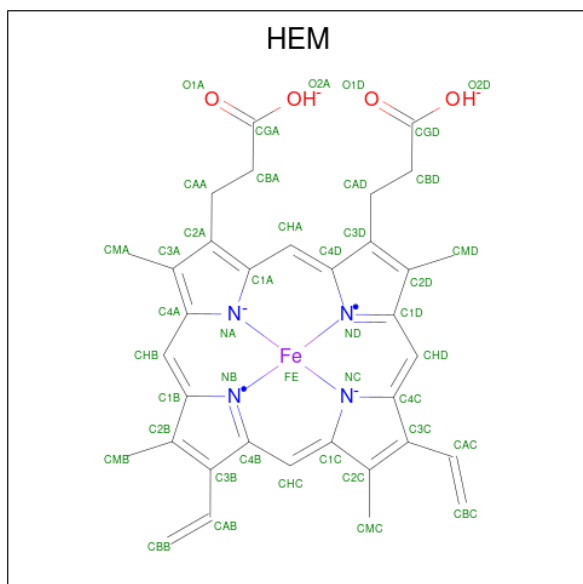
Mol	Chain	Residues	Atoms		AltConf
47	D	1	Total	Fe	0
			1	1	
47	d	1	Total	Fe	0
			1	1	

- Molecule 48 is BICARBONATE ION (CCD ID: BCT) (formula: CHO₃).



Mol	Chain	Residues	Atoms			AltConf
48	D	1	Total	C	O	0
			4	1	3	
48	d	1	Total	C	O	0
			4	1	3	

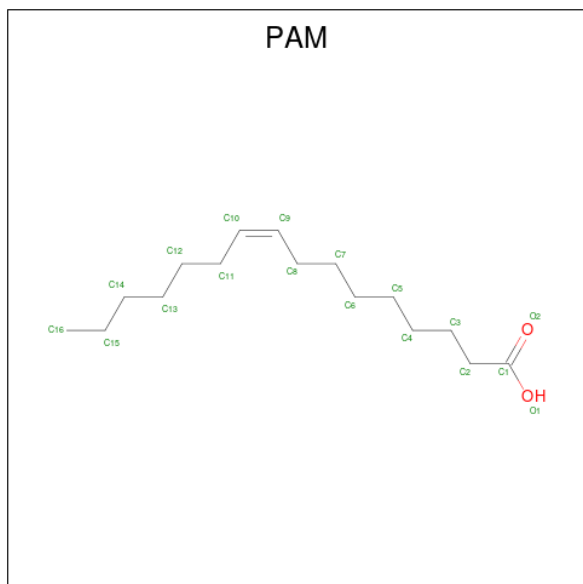
- Molecule 49 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
49	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 50 is PALMITOLEIC ACID (CCD ID: PAM) (formula: $C_{16}H_{30}O_2$).

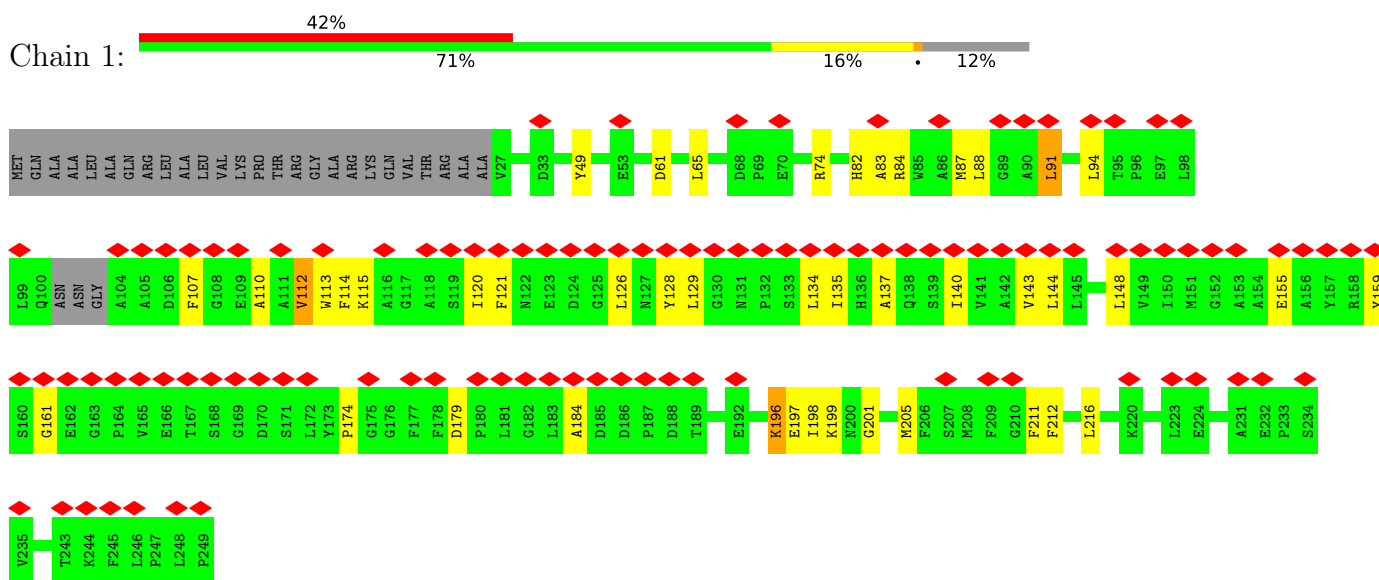


Mol	Chain	Residues	Atoms			AltConf
50	N	1	Total	C	O	0
			18	16	2	
50	n	1	Total	C	O	0
			18	16	2	

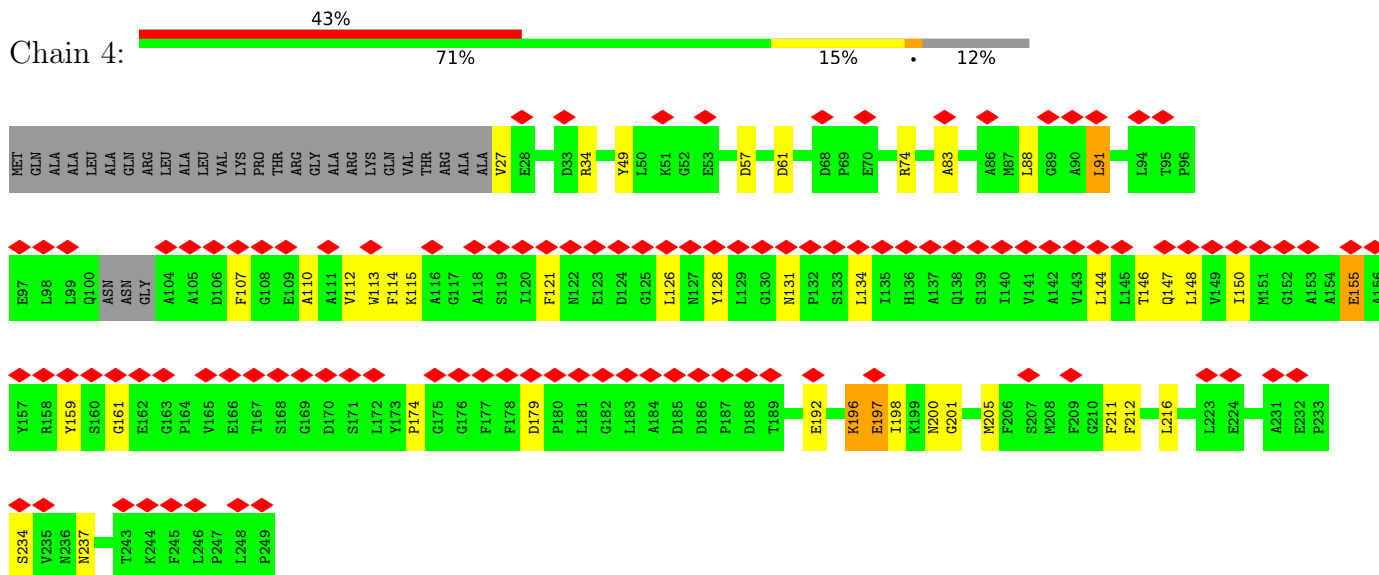
3 Residue-property plots

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.

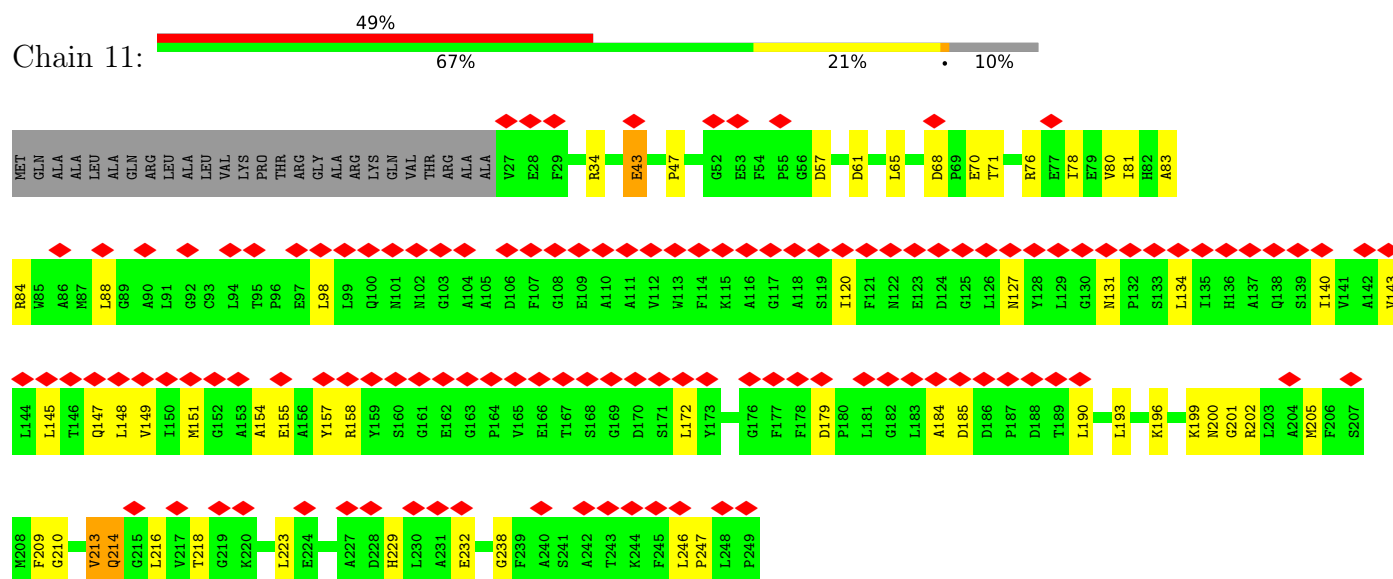
- Molecule 1: Chlorophyll a-b binding protein Lhcbm-I



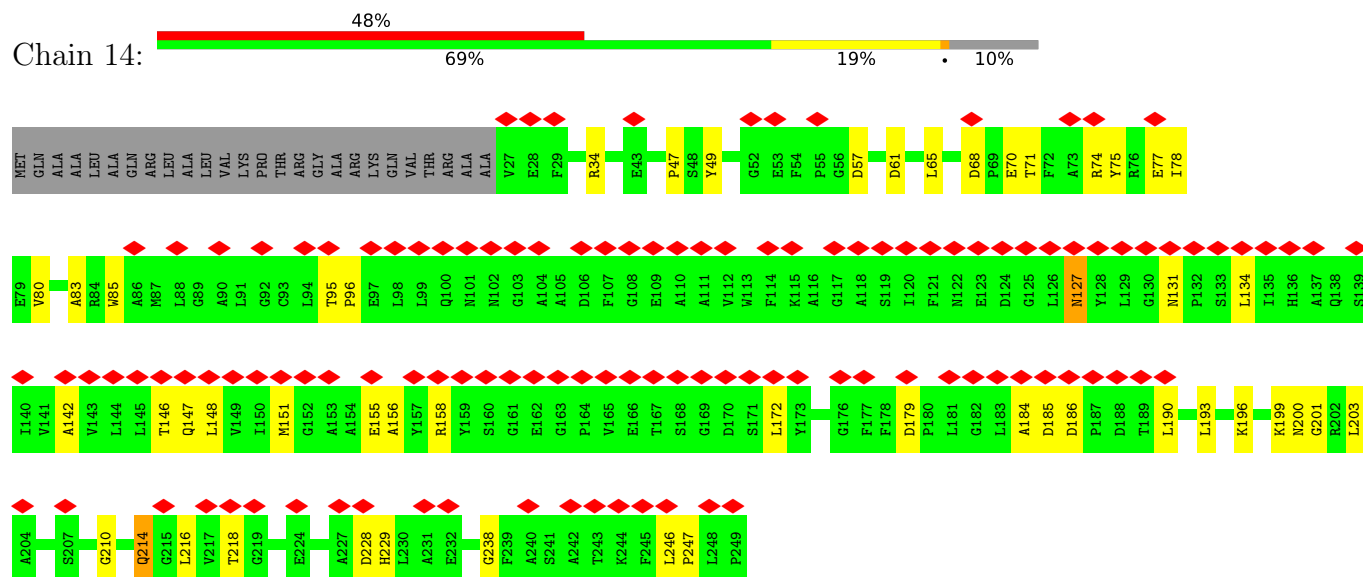
- Molecule 1: Chlorophyll a-b binding protein Lhcbm-I



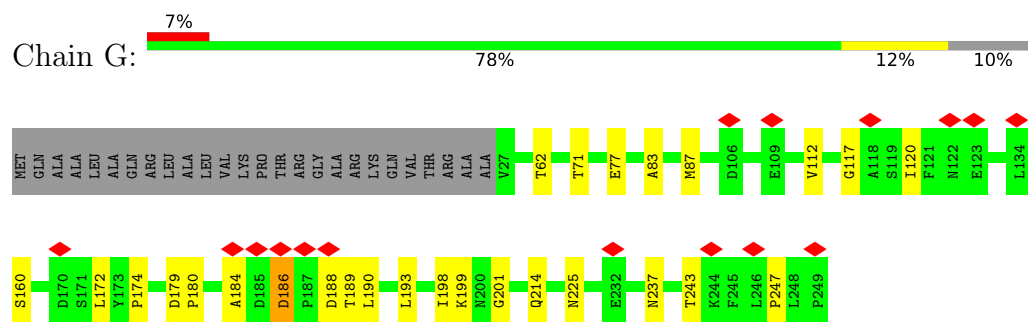
- Molecule 1: Chlorophyll a-b binding protein Lhcbm-I



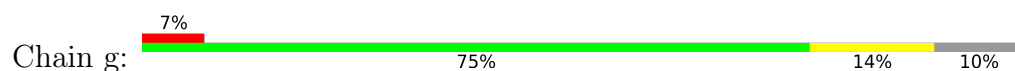
- Molecule 1: Chlorophyll a-b binding protein Lhcbm-I

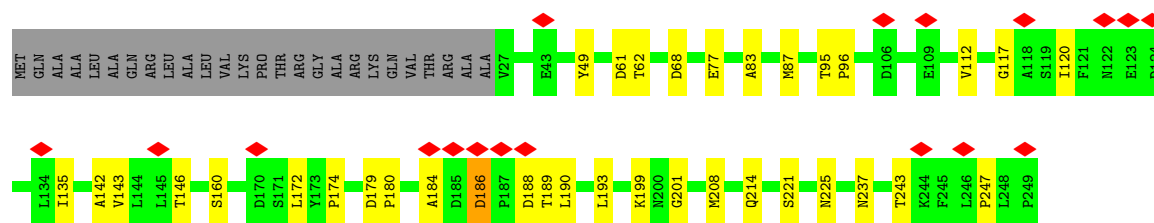


- Molecule 1: Chlorophyll a-b binding protein Lhcbm-I

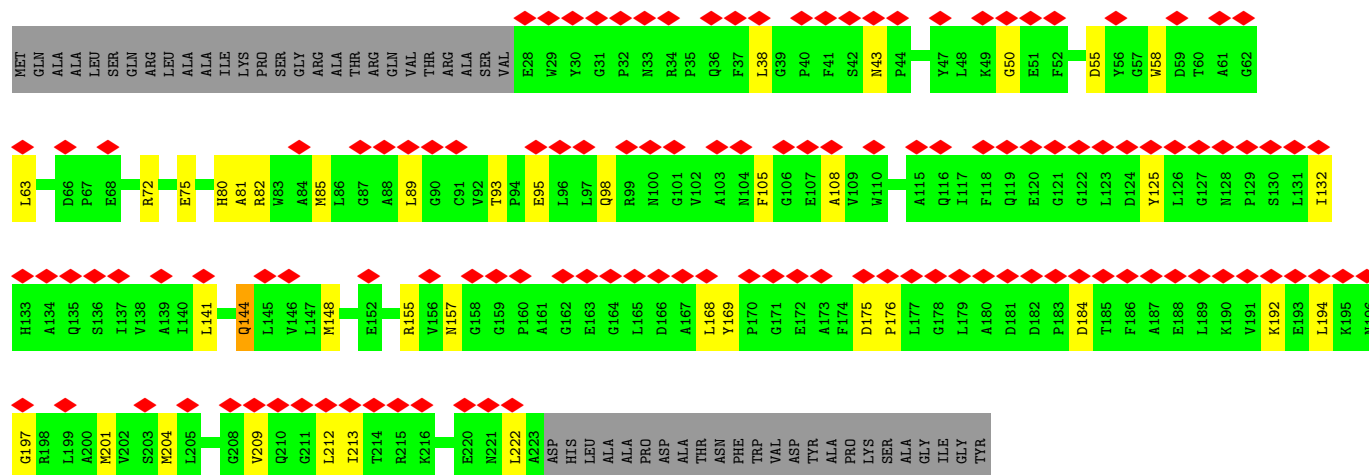


- Molecule 1: Chlorophyll a-b binding protein Lhcbm-I

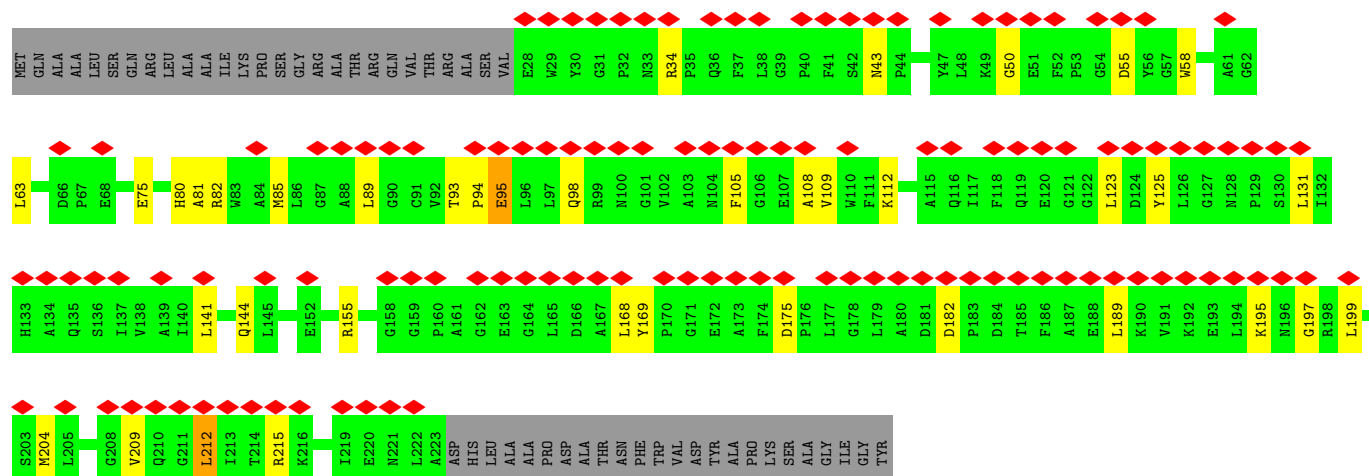




- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

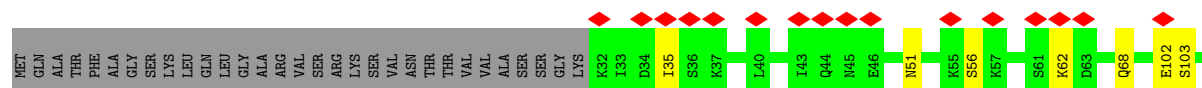


- Molecule 2: Chlorophyll a-b binding protein, chloroplastic



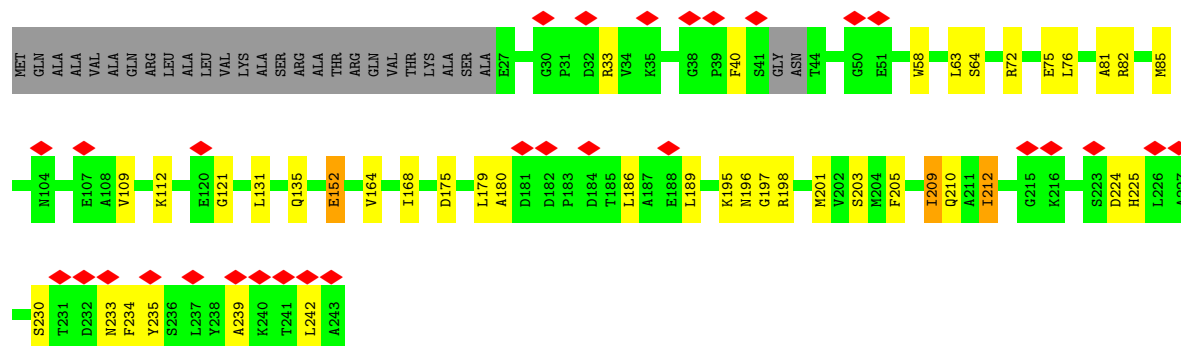
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic



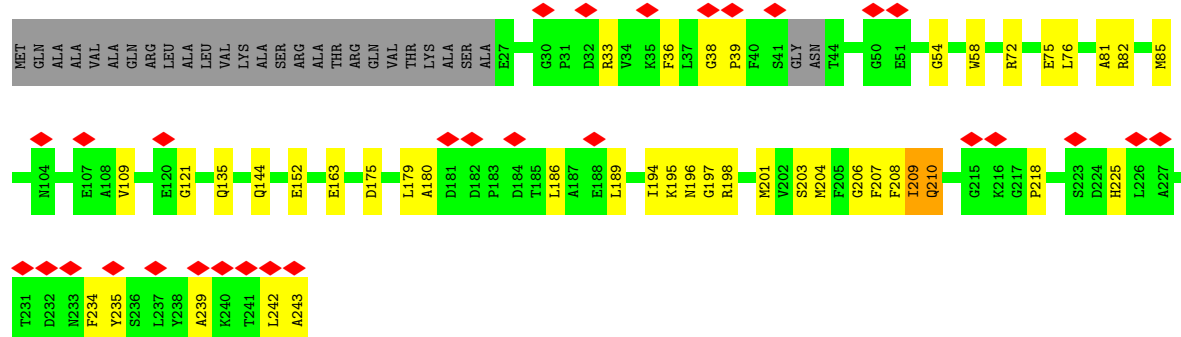




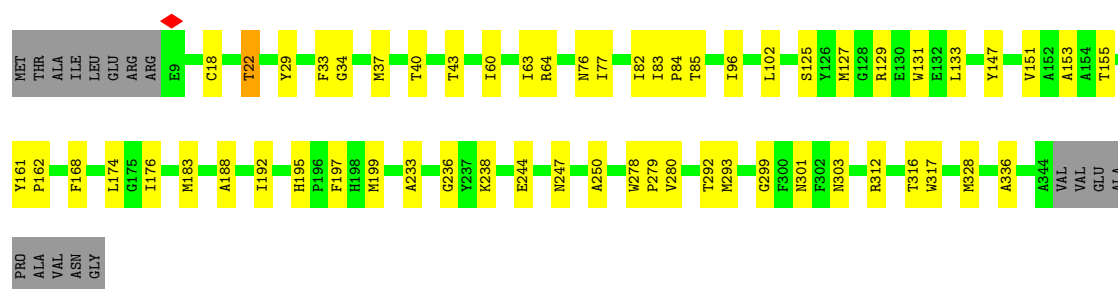
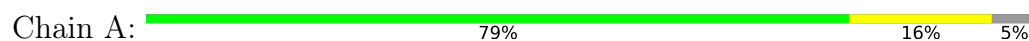
- Molecule 5: Chlorophyll a-b binding protein, chloroplastic



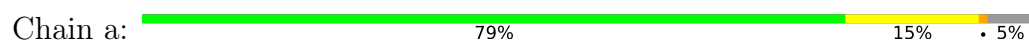
- Molecule 5: Chlorophyll a-b binding protein, chloroplastic

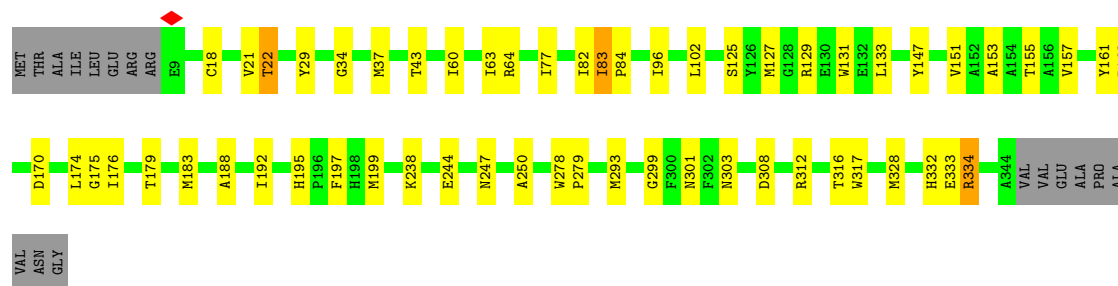


- Molecule 6: Photosystem II protein D1



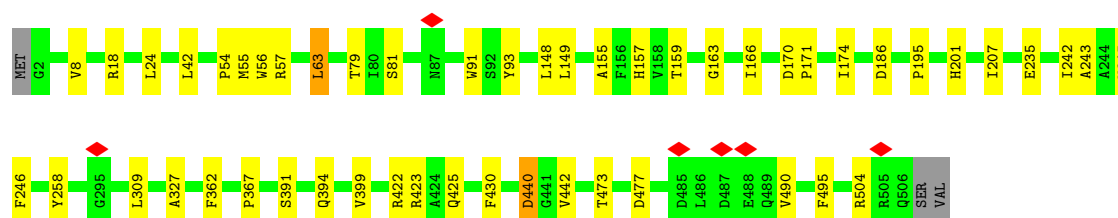
- Molecule 6: Photosystem II protein D1





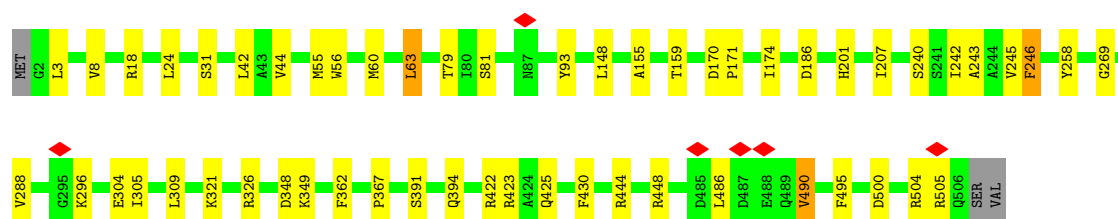
- Molecule 7: Photosystem II CP47 reaction center protein

Chain B: 89% 10%



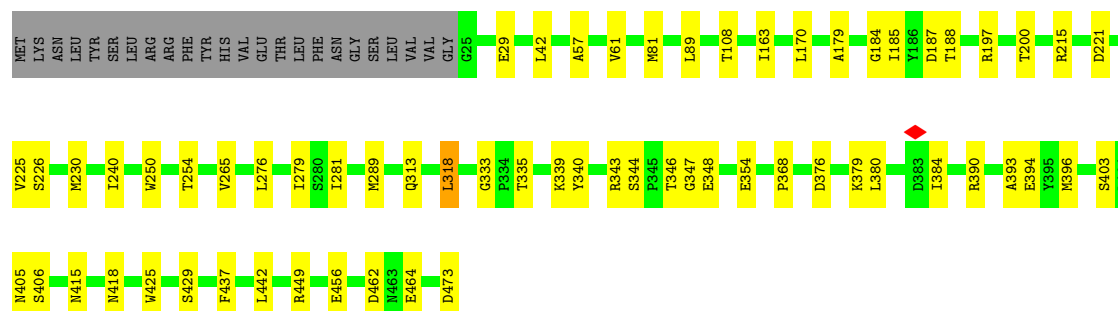
- Molecule 7: Photosystem II CP47 reaction center protein

Chain b: 89% 10%



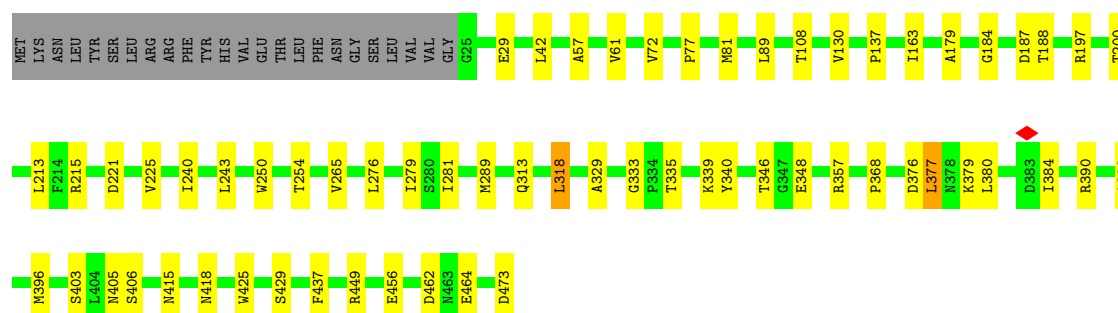
- Molecule 8: Photosystem II CP43 reaction center protein

Chain C: 81% 13% 5%

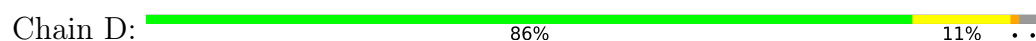


- Molecule 8: Photosystem II CP43 reaction center protein

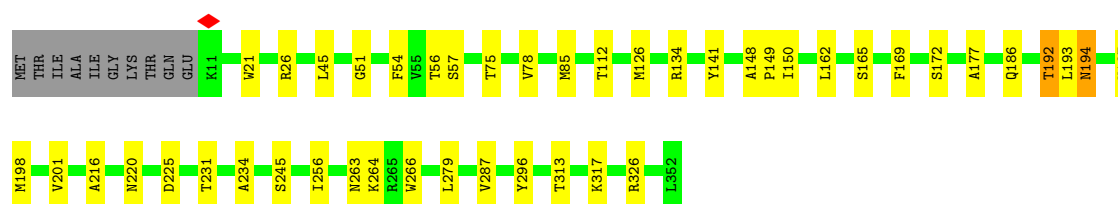
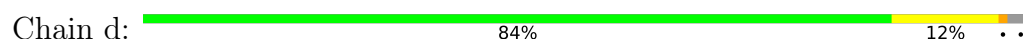
Chain c: 82% 13% 5%



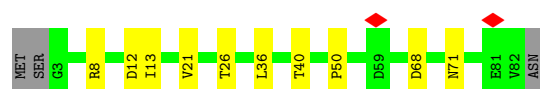
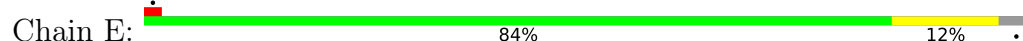
• Molecule 9: Photosystem II D2 protein



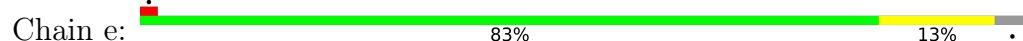
• Molecule 9: Photosystem II D2 protein



• Molecule 10: Cytochrome b559 subunit alpha

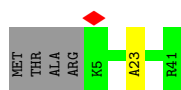


• Molecule 10: Cytochrome b559 subunit alpha

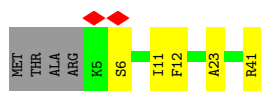
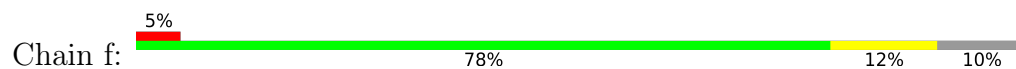


• Molecule 11: Cytochrome b559 subunit beta

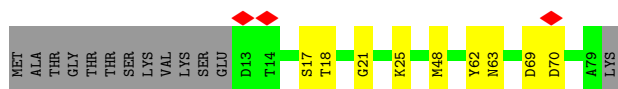




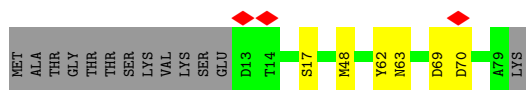
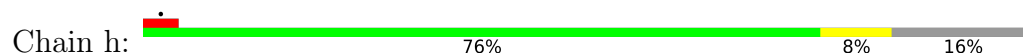
- Molecule 11: Cytochrome b559 subunit beta



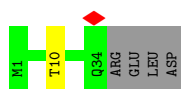
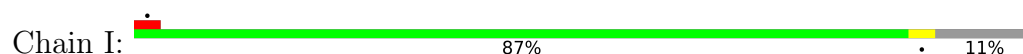
- Molecule 12: Photosystem II reaction center protein H



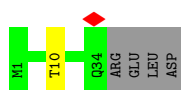
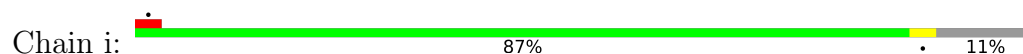
- Molecule 12: Photosystem II reaction center protein H



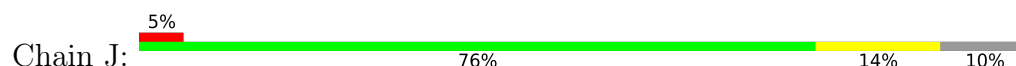
- Molecule 13: Photosystem II reaction center protein I



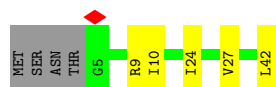
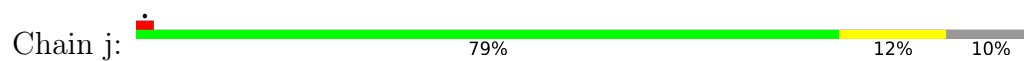
- Molecule 13: Photosystem II reaction center protein I



- Molecule 14: Photosystem II reaction center protein J



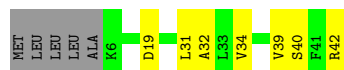
- Molecule 14: Photosystem II reaction center protein J



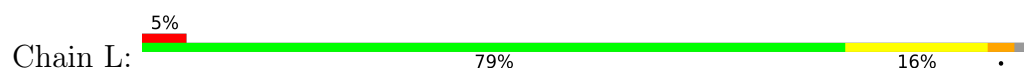
- Molecule 15: Photosystem II reaction center protein K



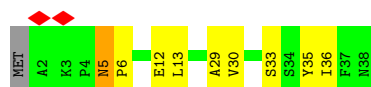
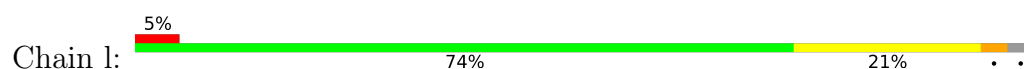
- Molecule 15: Photosystem II reaction center protein K



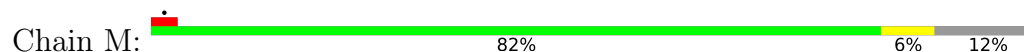
- Molecule 16: Photosystem II reaction center protein L



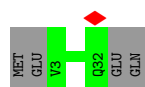
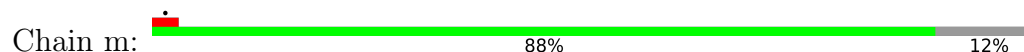
- Molecule 16: Photosystem II reaction center protein L



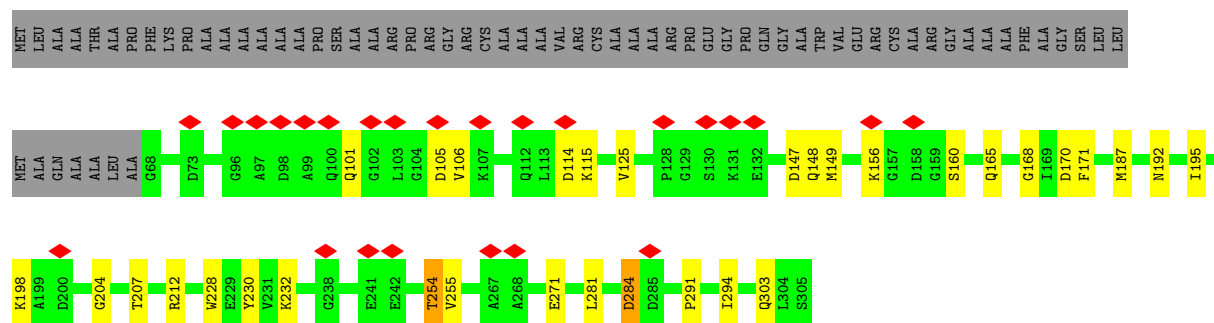
- Molecule 17: Photosystem II reaction center protein M



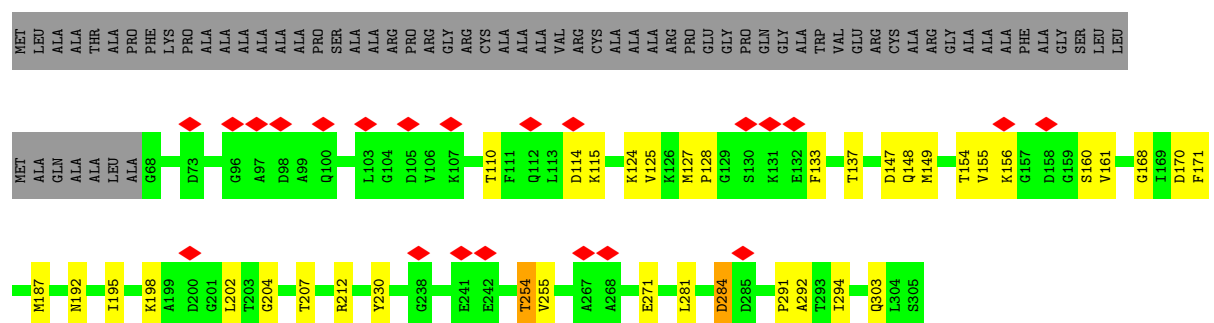
- Molecule 17: Photosystem II reaction center protein M



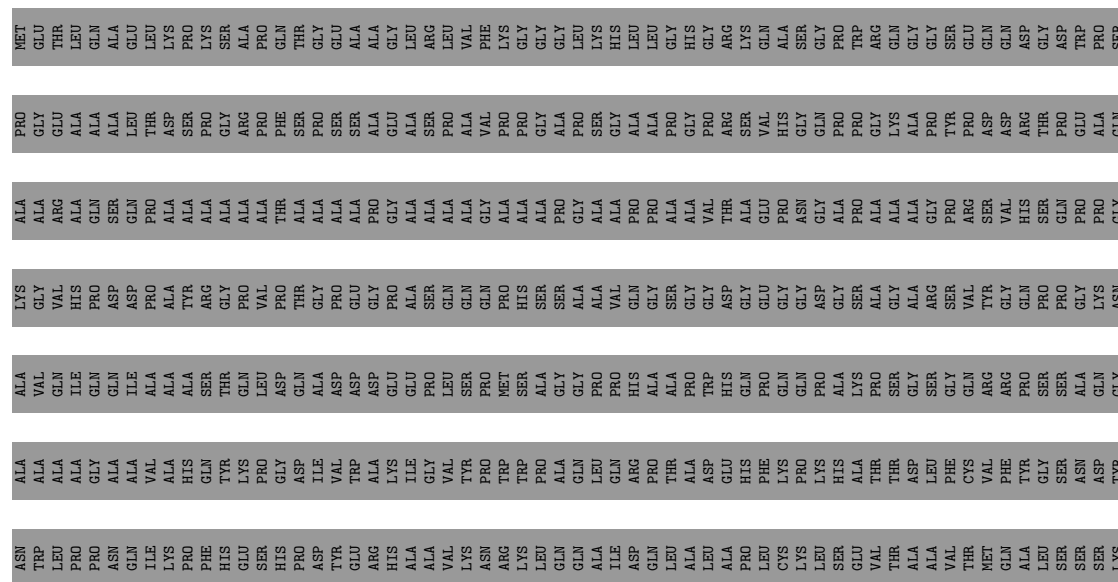
Chain O: 8% 67% 10% 22%

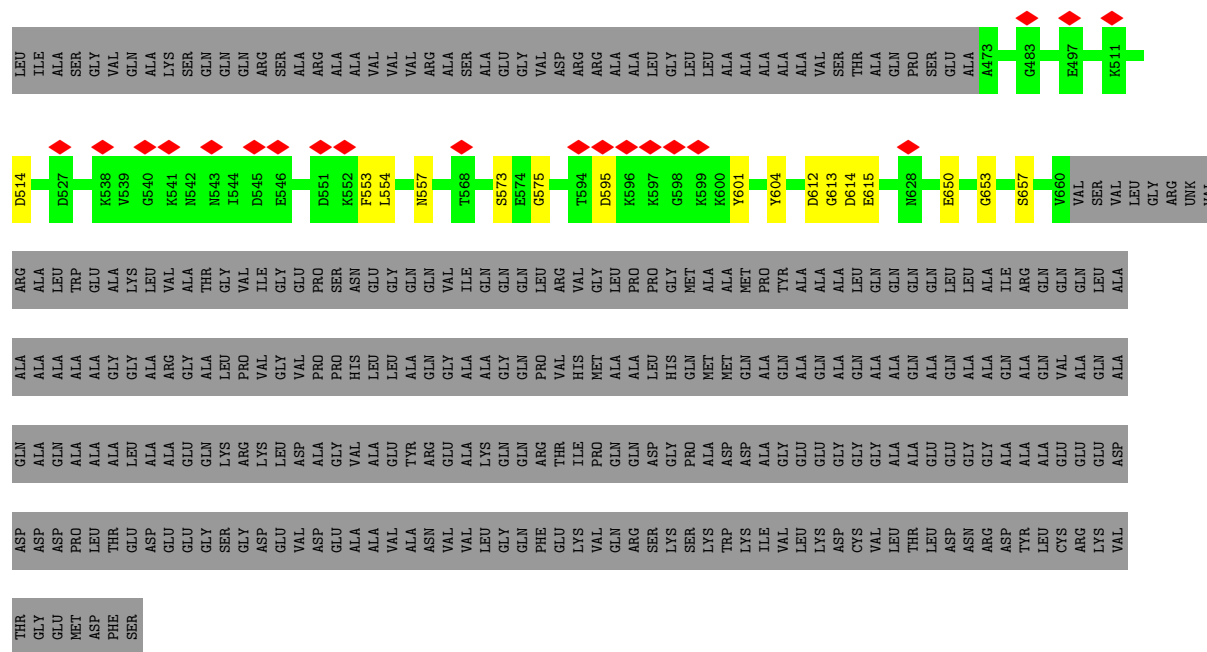


Chain o: 7% 66% 12% 22%

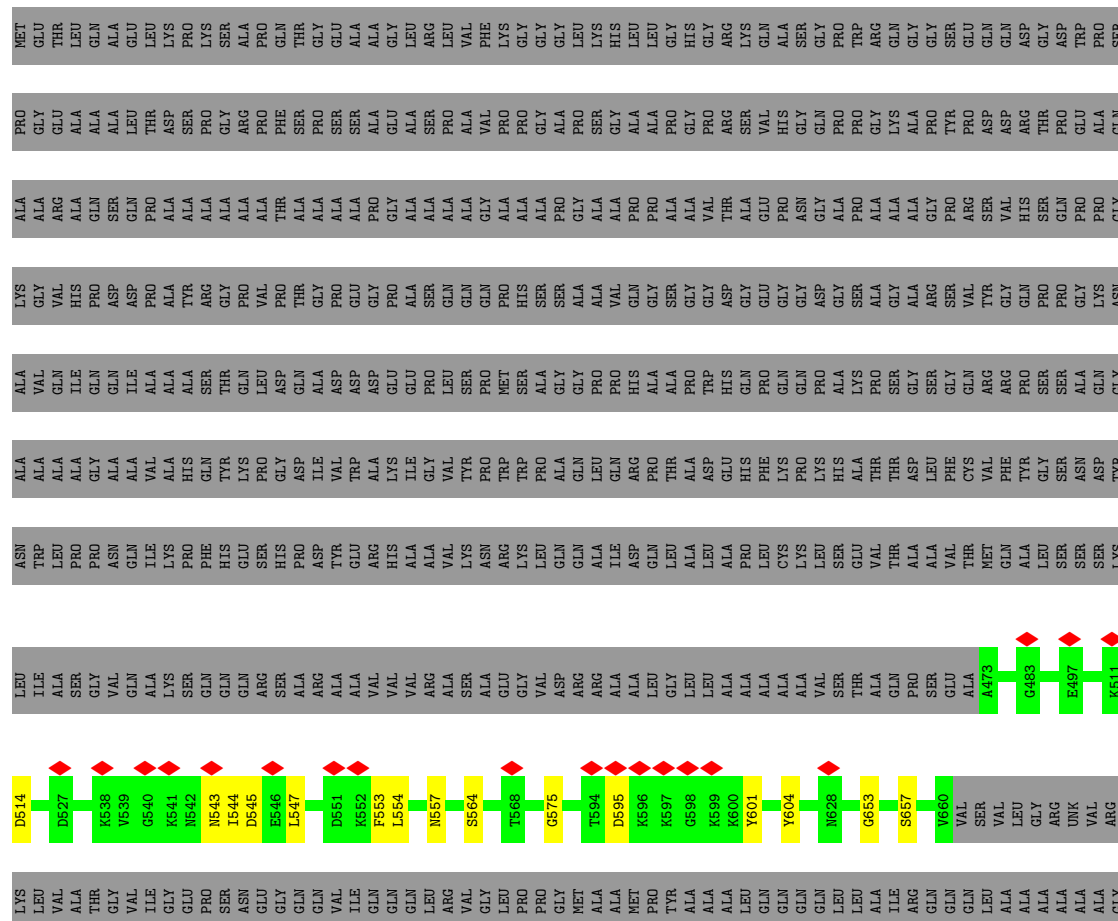


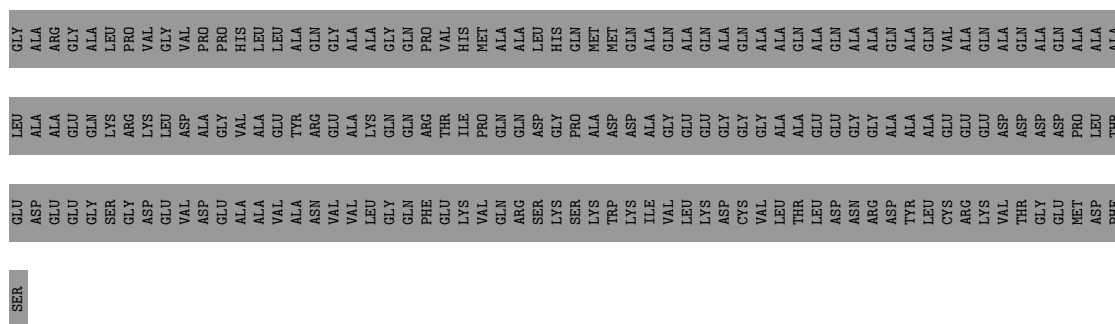
Chain P:



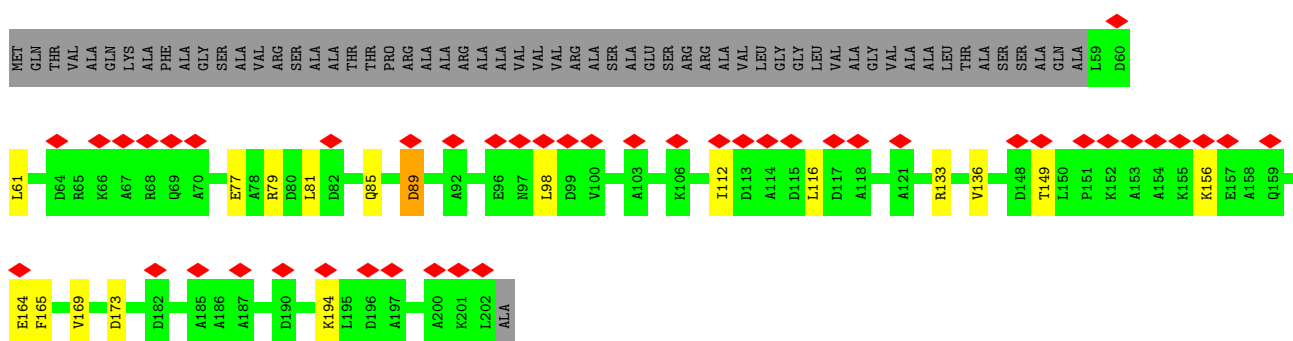


- Molecule 19: PWWP domain-containing protein

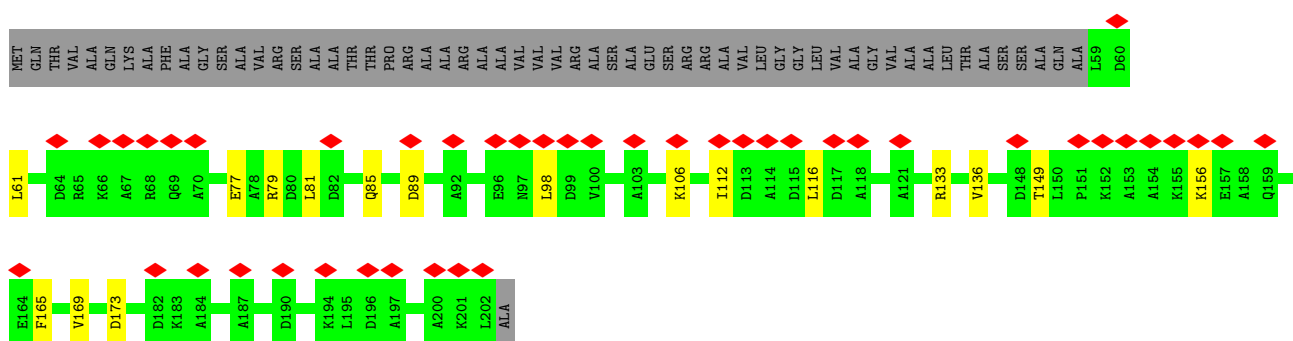




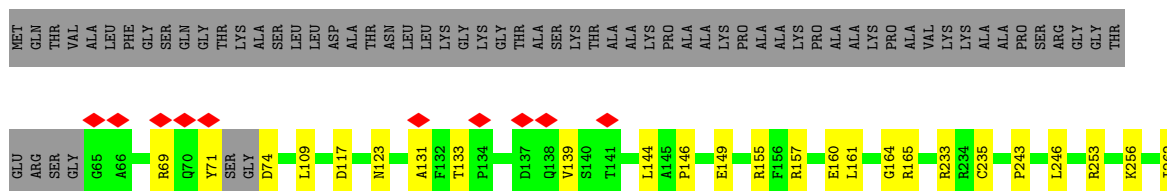
- Molecule 20: Chloroplast oxygen-evolving enhancer protein 3

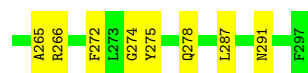


- Molecule 20: Chloroplast oxygen-evolving enhancer protein 3



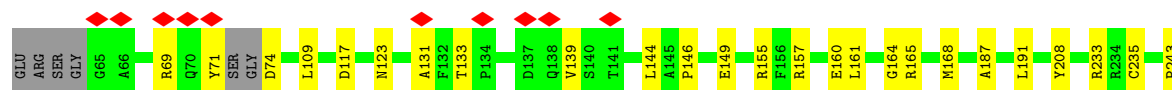
- Molecule 21: Chlorophyll a-b binding protein, chloroplastic





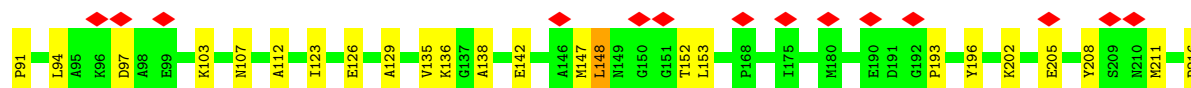
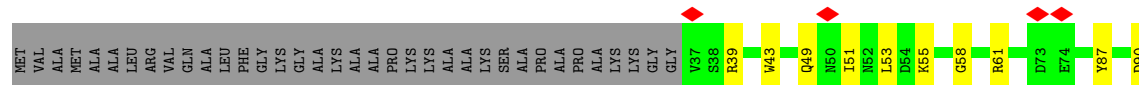
- Molecule 21: Chlorophyll a-b binding protein, chloroplastic

Chain r: 66% 12% 22%



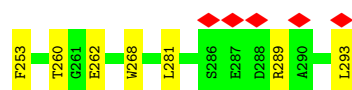
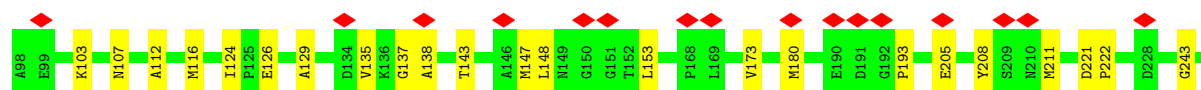
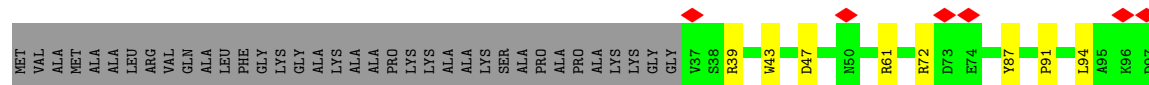
- Molecule 22: Chlorophyll a-b binding protein, chloroplastic

Chain S: 8% 73% 15% 12%



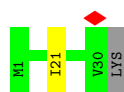
- Molecule 22: Chlorophyll a-b binding protein, chloroplastic

Chain s: 9% 75% 13% 12%



- Molecule 23: Photosystem II reaction center protein T

Chain T: 94%



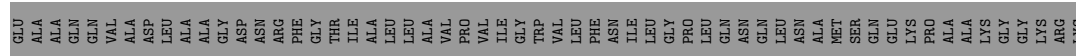
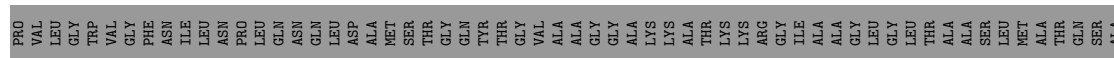
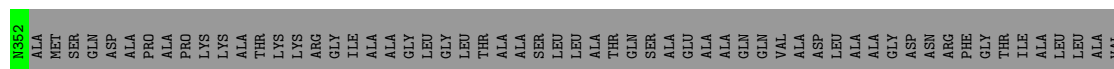
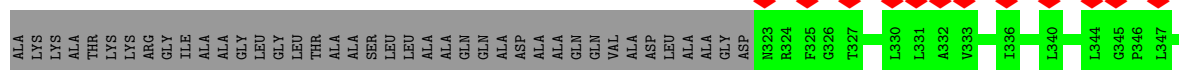
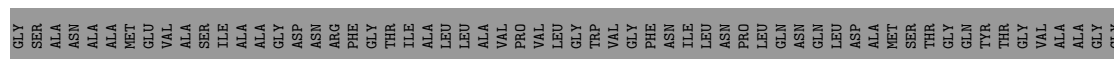
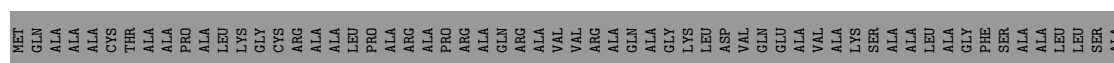
- Molecule 23: Photosystem II reaction center protein T

Chain t: 90% 6%



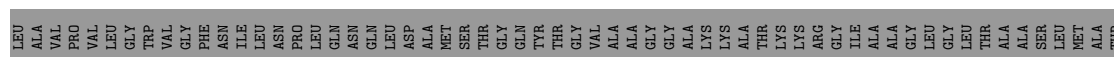
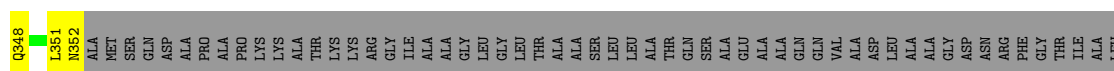
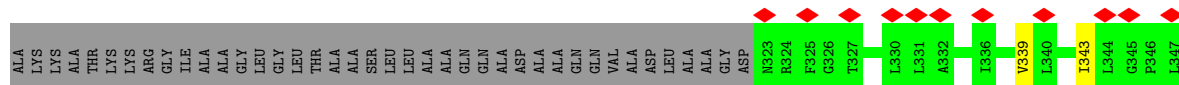
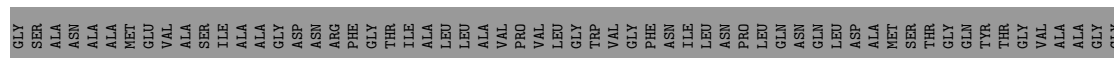
- Molecule 24: Chloroplast PsbY

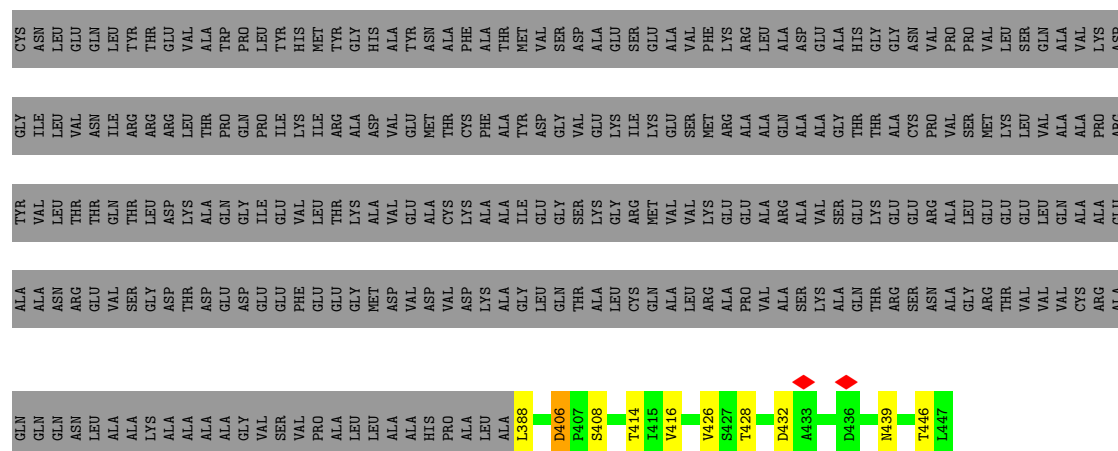
Chain U: 8% 92%



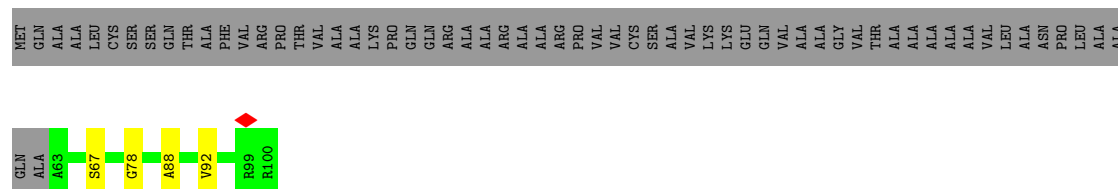
- Molecule 24: Chloroplast PsbY

Chain u: 7% 92%

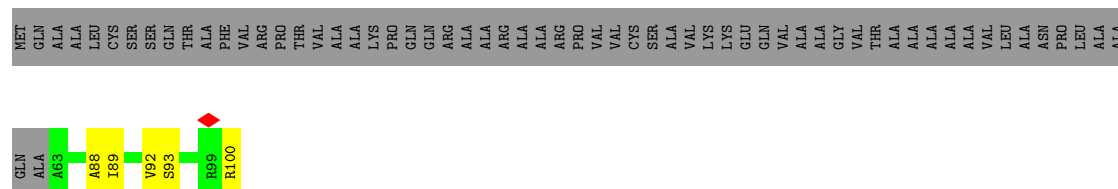




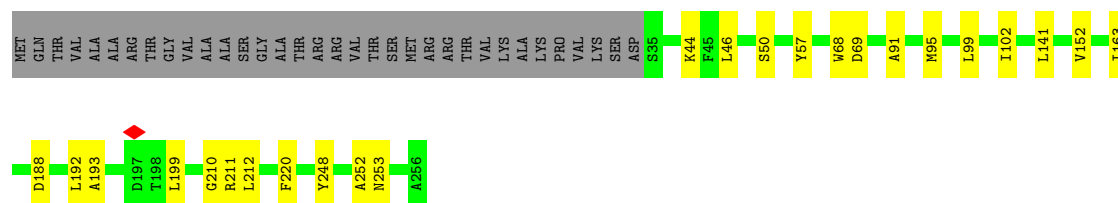
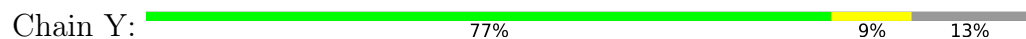
• Molecule 27: Photosystem II reaction center protein X (PsbX)



• Molecule 27: Photosystem II reaction center protein X (PsbX)

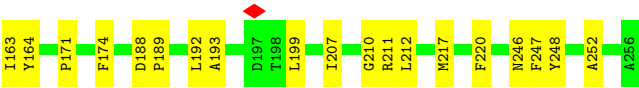
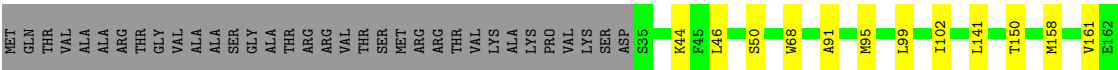


• Molecule 28: Chlorophyll a-b binding protein, chloroplastic

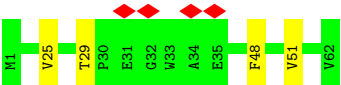
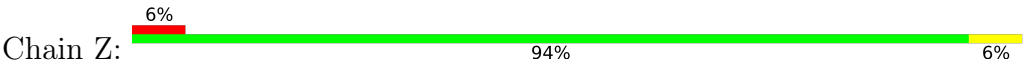


• Molecule 28: Chlorophyll a-b binding protein, chloroplastic

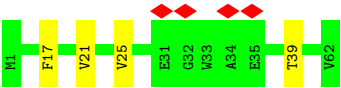




• Molecule 29: Photosystem II reaction center protein Z



• Molecule 29: Photosystem II reaction center protein Z



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	225372	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	90	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.292	Depositor
Minimum map value	-0.740	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	454.56, 454.56, 454.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.94699997, 0.94699997, 0.94699997	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NEX, BCR, DGD, 3PH, SQD, BCT, OEX, LNL, PHO, CHL, STE, FE2, PAM, XAT, CLA, LMG, LUT, LHG, CL, HEM, PL9

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.35	2/1720 (0.1%)	0.31	0/2339
1	11	0.54	5/1741 (0.3%)	0.30	0/2369
1	14	0.69	5/1741 (0.3%)	0.38	2/2369 (0.1%)
1	4	0.37	3/1720 (0.2%)	0.33	1/2339 (0.0%)
1	G	0.13	0/1741	0.25	0/2369
1	g	0.12	0/1741	0.24	0/2369
2	12	0.61	3/1362 (0.2%)	0.44	2/1844 (0.1%)
2	15	0.36	3/1362 (0.2%)	0.34	0/1844
2	2	0.15	0/1536	0.33	0/2088
2	5	0.15	0/1536	0.29	0/2088
2	N	0.14	0/1727	0.26	0/2352
2	n	0.14	0/1727	0.33	1/2352 (0.0%)
3	3	0.12	0/1675	0.24	0/2283
3	6	0.14	0/1675	0.27	0/2283
4	7	0.10	0/831	0.24	0/1122
4	8	0.10	0/831	0.24	0/1122
5	13	0.54	6/1688 (0.4%)	0.32	0/2296
5	16	0.53	5/1688 (0.3%)	0.31	0/2296
6	A	0.18	0/2714	0.34	0/3701
6	a	0.21	0/2714	0.39	1/3701 (0.0%)
7	B	0.15	0/4094	0.26	0/5576
7	b	0.15	0/4094	0.26	0/5576
8	C	0.15	0/3611	0.26	0/4921
8	c	0.15	0/3611	0.26	0/4921
9	D	0.16	0/2825	0.29	0/3849
9	d	0.17	0/2825	0.29	0/3849
10	E	0.12	0/664	0.24	0/905
10	e	0.12	0/664	0.24	0/905
11	F	0.13	0/313	0.23	0/426
11	f	0.14	0/313	0.25	0/426
12	H	0.14	0/518	0.24	0/708

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
12	h	0.14	0/518	0.24	0/708
13	I	0.17	0/282	0.28	0/382
13	i	0.17	0/282	0.28	0/382
14	J	0.12	0/276	0.25	0/377
14	j	0.12	0/276	0.24	0/377
15	K	0.18	0/305	0.37	0/420
15	k	0.18	0/305	0.38	0/420
16	L	0.18	0/311	0.29	0/422
16	l	0.18	0/311	0.28	0/422
17	M	0.16	0/231	0.27	0/316
17	m	0.15	0/231	0.28	0/316
18	O	0.11	0/1790	0.26	0/2420
18	o	0.10	0/1790	0.24	0/2420
19	P	0.09	0/1473	0.21	0/1991
19	p	0.09	0/1473	0.20	0/1991
20	Q	0.11	0/1132	0.23	0/1521
20	q	0.11	0/1132	0.24	0/1521
21	R	0.15	0/1820	0.27	0/2475
21	r	0.14	0/1820	0.24	0/2475
22	S	0.16	0/1985	0.32	0/2711
22	s	0.12	0/1985	0.28	0/2711
23	T	0.14	0/253	0.20	0/343
23	t	0.14	0/253	0.20	0/343
24	U	0.12	0/238	0.24	0/326
24	u	0.15	0/238	0.30	0/326
25	V	0.08	0/242	0.19	0/329
25	v	0.08	0/242	0.19	0/329
26	W	0.14	0/477	0.23	0/650
26	w	0.15	0/477	0.25	0/650
27	X	0.11	0/259	0.18	0/353
27	x	0.11	0/259	0.19	0/353
28	Y	0.15	0/1741	0.25	0/2367
28	y	0.15	0/1741	0.24	0/2367
29	Z	0.11	0/491	0.24	0/672
29	z	0.10	0/491	0.24	0/672
All	All	0.24	32/84132 (0.0%)	0.28	7/114446 (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
6	a	0	1

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	14	229	HIS	C-N	19.06	1.59	1.33
1	14	214	GLN	C-N	16.36	1.53	1.33
1	11	214	GLN	C-N	14.82	1.53	1.33
2	12	224	ASP	C-N	14.44	1.51	1.33
2	12	196	ASN	C-N	12.55	1.50	1.33

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	12	225	HIS	O-C-N	6.57	128.93	122.09
6	a	332	HIS	CA-CB-CG	6.53	120.33	113.80
2	n	210	GLN	CA-CB-CG	5.64	125.37	114.10
2	12	224	ASP	O-C-N	-5.61	116.17	122.12
1	14	228	ASP	CA-C-N	-5.42	113.22	120.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	a	334	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1673	0	1609	34	0
1	11	1693	0	1625	34	0
1	14	1693	0	1625	33	0
1	4	1673	0	1609	26	0
1	G	1693	0	1625	19	0
1	g	1693	0	1625	25	0
2	12	1330	0	1299	37	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	15	1330	0	1299	40	0
2	2	1496	0	1463	33	0
2	5	1496	0	1463	27	0
2	N	1679	0	1626	24	0
2	n	1679	0	1626	36	0
3	3	1630	0	1583	18	0
3	6	1630	0	1583	18	0
4	7	816	0	831	11	0
4	8	816	0	831	5	0
5	13	1645	0	1602	29	0
5	16	1645	0	1602	31	0
6	A	2632	0	2532	43	0
6	a	2632	0	2532	37	0
7	B	3963	0	3831	34	0
7	b	3963	0	3831	35	0
8	C	3491	0	3379	42	0
8	c	3491	0	3379	43	0
9	D	2730	0	2630	33	0
9	d	2730	0	2630	30	0
10	E	646	0	631	6	0
10	e	646	0	631	8	0
11	F	303	0	311	1	0
11	f	303	0	311	5	0
12	H	507	0	520	7	0
12	h	507	0	520	5	0
13	I	274	0	280	1	0
13	i	274	0	280	1	0
14	J	270	0	282	5	0
14	j	270	0	282	5	0
15	K	295	0	311	6	0
15	k	295	0	311	6	0
16	L	303	0	311	5	0
16	l	303	0	311	7	0
17	M	228	0	257	1	0
17	m	228	0	257	0	0
18	O	1759	0	1714	20	0
18	o	1759	0	1714	21	0
19	P	1443	0	1408	10	0
19	p	1443	0	1408	9	0
20	Q	1122	0	1151	12	0
20	q	1122	0	1151	11	0
21	R	1783	0	1705	21	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	r	1783	0	1705	24	0
22	S	1934	0	1878	33	0
22	s	1934	0	1878	31	0
23	T	246	0	262	2	0
23	t	246	0	262	3	0
24	U	233	0	246	0	0
24	u	233	0	246	5	0
25	V	241	0	275	1	0
25	v	241	0	275	2	0
26	W	468	0	450	7	0
26	w	468	0	450	5	0
27	X	258	0	273	2	0
27	x	258	0	273	5	0
28	Y	1694	0	1641	18	0
28	y	1694	0	1641	26	0
29	Z	478	0	513	2	0
29	z	478	0	513	2	0
30	1	311	0	240	14	0
30	11	314	0	249	9	0
30	12	250	0	183	8	0
30	13	345	0	302	14	0
30	14	318	0	255	7	0
30	15	258	0	199	16	0
30	16	345	0	302	11	0
30	2	311	0	247	13	0
30	3	365	0	351	11	0
30	4	321	0	263	19	0
30	5	315	0	253	8	0
30	6	365	0	351	15	0
30	G	329	0	280	11	0
30	N	357	0	332	19	0
30	R	173	0	154	12	0
30	S	204	0	164	8	0
30	Y	364	0	358	10	0
30	g	332	0	286	13	0
30	n	356	0	330	18	0
30	r	173	0	154	6	0
30	s	204	0	164	11	0
30	y	364	0	358	9	0
31	1	409	0	336	18	0
31	11	413	0	350	20	0
31	12	410	0	344	58	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	13	495	0	462	25	0
31	14	442	0	409	27	0
31	15	410	0	344	41	0
31	16	495	0	462	23	0
31	2	349	0	277	17	0
31	3	521	0	504	12	0
31	4	427	0	373	10	0
31	5	352	0	281	14	0
31	6	515	0	487	14	0
31	A	250	0	265	8	0
31	B	1025	0	1116	31	0
31	C	820	0	877	24	0
31	D	130	0	144	6	0
31	G	457	0	448	10	0
31	N	492	0	448	12	0
31	R	631	0	608	21	0
31	S	613	0	586	19	0
31	Y	545	0	558	23	0
31	a	185	0	193	5	0
31	b	1025	0	1116	39	0
31	c	820	0	877	26	0
31	d	195	0	216	10	0
31	g	457	0	448	10	0
31	n	492	0	448	22	0
31	r	636	0	621	25	0
31	s	613	0	586	24	0
31	y	540	0	545	23	0
32	1	43	0	59	1	0
32	11	49	0	74	3	0
32	13	40	0	53	3	0
32	14	49	0	74	3	0
32	16	40	0	53	3	0
32	3	91	0	125	3	0
32	4	47	0	67	2	0
32	6	91	0	125	5	0
32	A	185	0	268	11	0
32	C	42	0	57	4	0
32	D	137	0	196	5	0
32	G	49	0	74	2	0
32	L	47	0	67	4	0
32	N	49	0	74	2	0
32	R	129	0	174	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	S	94	0	137	7	0
32	Y	143	0	208	9	0
32	a	185	0	268	8	0
32	c	42	0	57	3	0
32	d	137	0	196	5	0
32	g	49	0	74	5	0
32	l	47	0	67	4	0
32	n	49	0	74	5	0
32	r	129	0	174	11	0
32	s	94	0	137	7	0
32	y	143	0	208	7	0
33	1	84	0	112	6	0
33	11	84	0	112	7	0
33	12	84	0	112	35	0
33	13	84	0	112	3	0
33	14	84	0	112	5	0
33	15	84	0	112	13	0
33	16	84	0	112	6	0
33	2	84	0	112	9	0
33	3	84	0	112	3	0
33	4	84	0	112	7	0
33	5	84	0	112	3	0
33	6	84	0	112	4	0
33	G	84	0	112	3	0
33	N	84	0	112	6	0
33	R	42	0	56	1	0
33	S	84	0	112	8	0
33	Y	84	0	112	4	0
33	g	84	0	112	4	0
33	n	84	0	112	8	0
33	r	42	0	56	4	0
33	s	84	0	112	10	0
33	y	84	0	112	6	0
34	1	16	0	20	0	0
34	11	16	0	20	0	0
34	12	27	0	33	2	0
34	13	44	0	56	0	0
34	14	16	0	20	0	0
34	15	27	0	33	3	0
34	16	44	0	56	0	0
34	2	32	0	39	0	0
34	3	44	0	56	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	4	16	0	20	0	0
34	5	32	0	39	0	0
34	6	44	0	56	4	0
34	G	43	0	53	1	0
34	N	44	0	56	1	0
34	R	44	0	56	1	0
34	S	44	0	56	1	0
34	Y	44	0	56	1	0
34	g	44	0	56	0	0
34	n	44	0	56	1	0
34	r	44	0	56	1	0
34	s	44	0	56	1	0
34	y	44	0	56	0	0
35	11	44	0	56	1	0
35	14	44	0	56	1	0
35	3	44	0	56	3	0
35	6	44	0	56	4	0
35	G	44	0	56	1	0
35	R	44	0	56	2	0
35	g	44	0	56	2	0
35	r	44	0	56	1	0
36	7	48	0	75	1	0
36	8	48	0	75	2	0
36	B	86	0	127	7	0
36	T	48	0	75	4	0
36	b	39	0	54	1	0
37	A	10	0	0	0	0
37	a	10	0	0	0	0
38	A	64	0	74	0	0
38	D	64	0	74	4	0
38	a	128	0	148	1	0
39	A	40	0	56	2	0
39	B	120	0	168	7	0
39	C	120	0	168	5	0
39	D	40	0	56	2	0
39	H	40	0	56	3	0
39	J	40	0	56	3	0
39	a	40	0	56	1	0
39	b	120	0	168	5	0
39	c	120	0	168	4	0
39	d	40	0	56	1	0
39	h	40	0	56	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	j	40	0	56	3	0
40	A	51	0	68	0	0
40	D	100	0	136	2	0
40	L	50	0	64	3	0
40	a	51	0	68	0	0
40	d	100	0	136	7	0
40	l	50	0	64	2	0
41	A	55	0	86	1	0
41	B	97	0	137	3	0
41	C	102	0	153	2	0
41	D	92	0	124	2	0
41	H	35	0	51	0	0
41	J	51	0	75	5	0
41	K	51	0	72	3	0
41	S	42	0	54	3	0
41	b	95	0	130	2	0
41	c	102	0	153	2	0
41	d	127	0	175	4	0
41	j	51	0	75	5	0
41	s	42	0	54	2	0
41	v	51	0	72	1	0
41	w	55	0	86	3	0
42	A	55	0	80	2	0
42	D	55	0	80	2	0
42	a	55	0	80	4	0
42	d	55	0	80	2	0
43	A	20	0	29	0	0
43	C	40	0	58	1	0
43	H	20	0	29	4	0
43	I	20	0	29	0	0
43	R	20	0	29	0	0
43	W	40	0	58	2	0
43	X	20	0	29	1	0
43	Y	40	0	58	2	0
43	a	20	0	29	0	0
43	c	40	0	58	1	0
43	h	20	0	29	2	0
43	i	20	0	29	0	0
43	r	20	0	29	0	0
43	w	20	0	29	1	0
43	x	20	0	29	1	0
43	y	60	0	87	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	B	20	0	35	1	0
44	b	20	0	35	0	0
45	C	1	0	0	0	0
45	c	1	0	0	0	0
46	C	183	0	246	9	0
46	W	46	0	64	4	0
46	c	183	0	246	8	0
46	w	40	0	52	2	0
47	D	1	0	0	0	0
47	d	1	0	0	0	0
48	D	4	0	1	0	0
48	d	4	0	0	0	0
49	F	43	0	30	2	0
49	f	43	0	30	2	0
50	N	18	0	29	1	0
50	n	18	0	29	1	0
All	All	112944	0	113167	1728	0

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

The worst 5 of 1728 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)
31:12:612:CLA:C3B	33:12:614:LUT:H183	1.22	1.54
31:12:612:CLA:CAB	33:12:614:LUT:H183	1.53	1.36
31:12:612:CLA:C3B	33:12:614:LUT:C18	2.18	1.21
31:12:612:CLA:CAB	33:12:614:LUT:C18	2.22	1.17
1:11:210:GLY:O	1:11:214:GLN:HG3	1.44	1.17

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	216/249 (87%)	210 (97%)	6 (3%)	0	100	100
1	11	221/249 (89%)	213 (96%)	8 (4%)	0	100	100
1	14	221/249 (89%)	213 (96%)	8 (4%)	0	100	100
1	4	216/249 (87%)	208 (96%)	8 (4%)	0	100	100
1	G	221/249 (89%)	217 (98%)	4 (2%)	0	100	100
1	g	221/249 (89%)	215 (97%)	6 (3%)	0	100	100
2	12	158/247 (64%)	154 (98%)	4 (2%)	0	100	100
2	15	158/247 (64%)	150 (95%)	8 (5%)	0	100	100
2	2	194/247 (78%)	187 (96%)	7 (4%)	0	100	100
2	5	194/247 (78%)	190 (98%)	4 (2%)	0	100	100
2	N	218/247 (88%)	209 (96%)	9 (4%)	0	100	100
2	n	218/247 (88%)	210 (96%)	8 (4%)	0	100	100
3	3	212/259 (82%)	204 (96%)	8 (4%)	0	100	100
3	6	212/259 (82%)	206 (97%)	6 (3%)	0	100	100
4	7	105/140 (75%)	104 (99%)	1 (1%)	0	100	100
4	8	105/140 (75%)	102 (97%)	3 (3%)	0	100	100
5	13	211/243 (87%)	205 (97%)	6 (3%)	0	100	100
5	16	211/243 (87%)	205 (97%)	6 (3%)	0	100	100
6	A	334/353 (95%)	322 (96%)	12 (4%)	0	100	100
6	a	334/353 (95%)	322 (96%)	12 (4%)	0	100	100
7	B	503/508 (99%)	488 (97%)	15 (3%)	0	100	100
7	b	503/508 (99%)	486 (97%)	17 (3%)	0	100	100
8	C	447/473 (94%)	437 (98%)	10 (2%)	0	100	100
8	c	447/473 (94%)	437 (98%)	10 (2%)	0	100	100
9	D	340/352 (97%)	330 (97%)	10 (3%)	0	100	100
9	d	340/352 (97%)	330 (97%)	10 (3%)	0	100	100
10	E	78/83 (94%)	77 (99%)	1 (1%)	0	100	100
10	e	78/83 (94%)	77 (99%)	1 (1%)	0	100	100
11	F	35/41 (85%)	35 (100%)	0	0	100	100
11	f	35/41 (85%)	35 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	H	65/80 (81%)	63 (97%)	2 (3%)	0	100	100
12	h	65/80 (81%)	63 (97%)	2 (3%)	0	100	100
13	I	32/38 (84%)	31 (97%)	1 (3%)	0	100	100
13	i	32/38 (84%)	28 (88%)	4 (12%)	0	100	100
14	J	36/42 (86%)	35 (97%)	1 (3%)	0	100	100
14	j	36/42 (86%)	35 (97%)	1 (3%)	0	100	100
15	K	35/42 (83%)	34 (97%)	1 (3%)	0	100	100
15	k	35/42 (83%)	34 (97%)	1 (3%)	0	100	100
16	L	35/38 (92%)	35 (100%)	0	0	100	100
16	l	35/38 (92%)	35 (100%)	0	0	100	100
17	M	28/34 (82%)	28 (100%)	0	0	100	100
17	m	28/34 (82%)	28 (100%)	0	0	100	100
18	O	236/305 (77%)	230 (98%)	6 (2%)	0	100	100
18	o	236/305 (77%)	229 (97%)	7 (3%)	0	100	100
19	P	186/915 (20%)	183 (98%)	3 (2%)	0	100	100
19	p	186/915 (20%)	183 (98%)	3 (2%)	0	100	100
20	Q	142/203 (70%)	139 (98%)	3 (2%)	0	100	100
20	q	142/203 (70%)	137 (96%)	5 (4%)	0	100	100
21	R	226/297 (76%)	219 (97%)	7 (3%)	0	100	100
21	r	226/297 (76%)	220 (97%)	6 (3%)	0	100	100
22	S	255/293 (87%)	248 (97%)	7 (3%)	0	100	100
22	s	255/293 (87%)	244 (96%)	11 (4%)	0	100	100
23	T	28/31 (90%)	28 (100%)	0	0	100	100
23	t	28/31 (90%)	28 (100%)	0	0	100	100
24	U	28/367 (8%)	28 (100%)	0	0	100	100
24	u	28/367 (8%)	28 (100%)	0	0	100	100
25	V	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
25	v	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
26	W	58/447 (13%)	56 (97%)	2 (3%)	0	100	100
26	w	58/447 (13%)	56 (97%)	2 (3%)	0	100	100
27	X	36/100 (36%)	36 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	x	36/100 (36%)	36 (100%)	0	0	100	100
28	Y	220/256 (86%)	217 (99%)	3 (1%)	0	100	100
28	y	220/256 (86%)	215 (98%)	5 (2%)	0	100	100
29	Z	60/62 (97%)	60 (100%)	0	0	100	100
29	z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
All	All	10460/15046 (70%)	10166 (97%)	294 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	1	170/190 (90%)	165 (97%)	5 (3%)	37	61
1	11	172/190 (90%)	166 (96%)	6 (4%)	32	57
1	14	172/190 (90%)	167 (97%)	5 (3%)	37	61
1	4	170/190 (90%)	164 (96%)	6 (4%)	32	57
1	G	172/190 (90%)	166 (96%)	6 (4%)	32	57
1	g	172/190 (90%)	167 (97%)	5 (3%)	37	61
2	12	136/187 (73%)	132 (97%)	4 (3%)	37	61
2	15	136/187 (73%)	129 (95%)	7 (5%)	21	47
2	2	150/187 (80%)	147 (98%)	3 (2%)	48	71
2	5	150/187 (80%)	143 (95%)	7 (5%)	23	49
2	N	167/187 (89%)	161 (96%)	6 (4%)	31	56
2	n	167/187 (89%)	162 (97%)	5 (3%)	36	60
3	3	165/196 (84%)	162 (98%)	3 (2%)	51	72
3	6	165/196 (84%)	162 (98%)	3 (2%)	51	72
4	7	88/113 (78%)	86 (98%)	2 (2%)	44	67
4	8	88/113 (78%)	83 (94%)	5 (6%)	18	42

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	13	168/187 (90%)	161 (96%)	7 (4%)	26	53
5	16	168/187 (90%)	162 (96%)	6 (4%)	31	56
6	A	274/287 (96%)	269 (98%)	5 (2%)	51	72
6	a	274/287 (96%)	268 (98%)	6 (2%)	45	69
7	B	403/406 (99%)	396 (98%)	7 (2%)	53	73
7	b	403/406 (99%)	395 (98%)	8 (2%)	48	71
8	C	351/373 (94%)	345 (98%)	6 (2%)	53	73
8	c	351/373 (94%)	344 (98%)	7 (2%)	48	71
9	D	277/285 (97%)	274 (99%)	3 (1%)	65	80
9	d	277/285 (97%)	272 (98%)	5 (2%)	51	72
10	E	71/74 (96%)	70 (99%)	1 (1%)	59	77
10	e	71/74 (96%)	71 (100%)	0	100	100
11	F	31/34 (91%)	31 (100%)	0	100	100
11	f	31/34 (91%)	31 (100%)	0	100	100
12	H	57/68 (84%)	55 (96%)	2 (4%)	32	57
12	h	57/68 (84%)	55 (96%)	2 (4%)	32	57
13	I	31/35 (89%)	31 (100%)	0	100	100
13	i	31/35 (89%)	31 (100%)	0	100	100
14	J	27/31 (87%)	27 (100%)	0	100	100
14	j	27/31 (87%)	27 (100%)	0	100	100
15	K	33/37 (89%)	32 (97%)	1 (3%)	36	60
15	k	33/37 (89%)	32 (97%)	1 (3%)	36	60
16	L	34/35 (97%)	32 (94%)	2 (6%)	18	41
16	l	34/35 (97%)	31 (91%)	3 (9%)	9	24
17	M	26/30 (87%)	26 (100%)	0	100	100
17	m	26/30 (87%)	26 (100%)	0	100	100
18	O	182/217 (84%)	178 (98%)	4 (2%)	45	69
18	o	182/217 (84%)	178 (98%)	4 (2%)	45	69
19	P	147/651 (23%)	145 (99%)	2 (1%)	59	77
19	p	147/651 (23%)	146 (99%)	1 (1%)	76	87
20	Q	108/143 (76%)	105 (97%)	3 (3%)	38	62

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	q	108/143 (76%)	106 (98%)	2 (2%)	50	71
21	R	182/225 (81%)	177 (97%)	5 (3%)	39	64
21	r	182/225 (81%)	178 (98%)	4 (2%)	45	69
22	S	192/212 (91%)	190 (99%)	2 (1%)	68	82
22	s	192/212 (91%)	190 (99%)	2 (1%)	68	82
23	T	26/27 (96%)	26 (100%)	0	100	100
23	t	26/27 (96%)	26 (100%)	0	100	100
24	U	25/241 (10%)	25 (100%)	0	100	100
24	u	25/241 (10%)	25 (100%)	0	100	100
25	V	27/27 (100%)	27 (100%)	0	100	100
25	v	27/27 (100%)	26 (96%)	1 (4%)	30	55
26	W	50/362 (14%)	47 (94%)	3 (6%)	17	40
26	w	50/362 (14%)	46 (92%)	4 (8%)	11	28
27	X	26/66 (39%)	25 (96%)	1 (4%)	29	55
27	x	26/66 (39%)	26 (100%)	0	100	100
28	Y	171/197 (87%)	169 (99%)	2 (1%)	63	79
28	y	171/197 (87%)	170 (99%)	1 (1%)	78	89
29	Z	52/52 (100%)	52 (100%)	0	100	100
29	z	52/52 (100%)	51 (98%)	1 (2%)	50	71
All	All	8382/11484 (73%)	8190 (98%)	192 (2%)	44	67

5 of 192 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	Q	89	ASP
7	b	505	ARG
21	R	144	LEU
6	a	21	VAL
8	c	462	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
21	R	80	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	y	234	ASN
6	a	267	ASN
28	y	209	ASN
21	r	80	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 612 ligands modelled in this entry, 4 are monoatomic - leaving 608 for Mogul analysis.

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	$\# Z > 2$
31	CLA	11	604	-	50,54,73	1.41	7 (14%)	60,90,113	1.83	7 (11%)
31	CLA	Y	610	28	69,73,73	1.23	8 (11%)	83,113,113	1.69	12 (14%)
31	CLA	A	406	6	59,63,73	1.33	7 (11%)	71,101,113	1.73	9 (12%)
33	LUT	1	616	-	42,43,43	0.36	0	51,60,60	0.35	0
43	LNL	A	412	-	19,19,19	0.44	0	18,19,19	0.49	0
31	CLA	S	604	-	69,73,73	1.23	7 (10%)	83,113,113	1.59	10 (12%)
34	NEX	1	618	-	13,17,46	0.37	0	19,29,70	0.49	0
30	CHL	15	607	-	54,58,74	1.47	7 (12%)	59,94,114	2.09	13 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	BCT	d	403	47	2,3,3	0.88	0	2,3,3	3.17	2 (100%)
31	CLA	G	613	1	69,73,73	1.23	8 (11%)	83,113,113	1.64	10 (12%)
39	BCR	J	101	-	41,41,41	0.21	0	56,56,56	0.47	0
40	SQD	d	412	-	53,54,54	0.17	0	62,65,65	0.21	0
40	SQD	D	413	-	45,46,54	0.19	0	54,57,65	0.21	0
34	NEX	Y	623	-	38,46,46	0.47	1 (2%)	50,70,70	0.40	0
30	CHL	6	605	3	70,74,74	1.33	7 (10%)	80,114,114	1.90	14 (17%)
30	CHL	2	607	-	60,64,74	1.43	8 (13%)	68,102,114	1.95	11 (16%)
31	CLA	6	603	3	59,63,73	1.33	7 (11%)	71,101,113	1.83	8 (11%)
41	LMG	j	102	-	51,51,55	0.18	0	59,59,63	0.17	0
31	CLA	G	604	-	54,58,73	1.39	8 (14%)	65,95,113	1.79	9 (13%)
33	LUT	R	615	-	42,43,43	0.38	0	51,60,60	0.38	0
31	CLA	b	605	7	69,73,73	1.23	8 (11%)	83,113,113	1.70	10 (12%)
34	NEX	n	619	-	38,46,46	0.43	1 (2%)	50,70,70	0.39	0
31	CLA	16	615	-	49,53,73	1.42	7 (14%)	59,89,113	1.72	10 (16%)
43	LNL	a	412	-	19,19,19	0.44	0	18,19,19	0.48	0
30	CHL	R	607	-	55,59,74	1.47	7 (12%)	62,96,114	2.01	14 (22%)
35	XAT	11	619	-	39,47,47	0.09	0	54,74,74	0.46	0
41	LMG	B	621	-	49,49,55	0.19	0	57,57,63	0.19	0
38	PHO	a	405	-	58,69,69	0.92	1 (1%)	56,99,99	1.00	5 (8%)
31	CLA	C	502	8	69,73,73	1.22	8 (11%)	83,113,113	1.62	10 (12%)
32	LHG	a	411	-	48,48,48	1.35	8 (16%)	51,54,54	0.73	2 (3%)
30	CHL	12	605	-	50,54,74	1.54	7 (14%)	56,90,114	2.16	9 (16%)
34	NEX	s	620	-	38,46,46	0.45	1 (2%)	50,70,70	0.46	0
35	XAT	G	619	-	39,47,47	0.10	0	54,74,74	0.43	0
50	PAM	n	620	-	17,17,17	0.45	0	17,17,17	0.49	0
31	CLA	C	506	8	69,73,73	1.23	7 (10%)	83,113,113	1.69	10 (12%)
30	CHL	Y	609	28	70,74,74	1.31	7 (10%)	80,114,114	1.82	12 (15%)
31	CLA	B	612	7	69,73,73	1.24	8 (11%)	83,113,113	1.78	10 (12%)
31	CLA	B	602	7	69,73,73	1.23	7 (10%)	83,113,113	1.65	12 (14%)
31	CLA	Y	615	28	60,64,73	1.33	8 (13%)	72,102,113	1.74	11 (15%)
31	CLA	C	509	8	64,68,73	1.31	8 (12%)	77,107,113	1.73	13 (16%)
33	LUT	16	617	-	42,43,43	0.38	0	51,60,60	0.54	1 (1%)
30	CHL	y	607	-	70,74,74	1.31	7 (10%)	80,114,114	1.84	15 (18%)
32	LHG	3	617	-	46,46,48	1.39	8 (17%)	49,52,54	0.75	2 (4%)
30	CHL	16	605	5	60,64,74	1.42	7 (11%)	68,102,114	1.97	15 (22%)
33	LUT	S	619	-	42,43,43	0.35	0	51,60,60	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	B	613	7	69,73,73	1.22	8 (11%)	83,113,113	1.78	10 (12%)
34	NEX	15	616	-	24,28,46	0.36	0	32,42,70	0.58	0
30	CHL	13	601	5	60,64,74	1.45	7 (11%)	68,102,114	1.96	15 (22%)
38	PHO	a	406	-	58,69,69	0.96	1 (1%)	56,99,99	1.03	5 (8%)
31	CLA	B	608	7	69,73,73	1.23	8 (11%)	83,113,113	1.59	11 (13%)
50	PAM	N	621	-	17,17,17	0.46	0	17,17,17	0.46	0
31	CLA	D	404	9	69,73,73	1.22	8 (11%)	83,113,113	1.69	11 (13%)
31	CLA	16	613	5	54,58,73	1.39	7 (12%)	65,95,113	1.86	8 (12%)
43	LNL	h	101	-	19,19,19	0.44	0	18,19,19	0.49	0
46	DGD	c	518	-	59,59,67	0.18	0	73,73,81	0.17	0
42	PL9	d	407	-	55,55,55	0.09	0	68,69,69	0.18	0
30	CHL	14	606	-	51,55,74	1.50	7 (13%)	57,91,114	1.95	11 (19%)
49	HEM	F	101	10,11	50,50,50	0.53	0	66,82,82	0.44	0
31	CLA	b	611	7	69,73,73	1.24	7 (10%)	83,113,113	1.64	11 (13%)
43	LNL	x	201	-	19,19,19	0.42	0	18,19,19	0.47	0
31	CLA	R	603	21	69,73,73	1.24	8 (11%)	83,113,113	1.74	11 (13%)
30	CHL	14	609	1	60,64,74	1.45	7 (11%)	68,102,114	1.97	15 (22%)
31	CLA	Y	611	32	69,73,73	1.24	8 (11%)	83,113,113	1.67	12 (14%)
43	LNL	X	201	-	19,19,19	0.43	0	18,19,19	0.49	0
34	NEX	11	618	-	13,17,46	0.36	0	19,29,70	0.48	0
30	CHL	N	608	-	54,58,74	1.44	6 (11%)	59,94,114	2.05	15 (25%)
39	BCR	C	515	-	41,41,41	0.11	0	56,56,56	0.23	0
30	CHL	13	609	5	65,69,74	1.40	7 (10%)	74,108,114	1.78	11 (14%)
31	CLA	s	609	22	59,63,73	1.35	7 (11%)	71,101,113	1.67	8 (11%)
49	HEM	f	101	10,11	50,50,50	0.53	0	66,82,82	0.44	0
30	CHL	6	606	-	60,64,74	1.43	7 (11%)	68,102,114	1.88	10 (14%)
46	DGD	C	517	-	67,67,67	0.17	0	81,81,81	0.18	0
39	BCR	H	103	-	41,41,41	0.13	0	56,56,56	0.33	0
30	CHL	5	605	2	50,54,74	1.53	8 (16%)	56,90,114	1.92	10 (17%)
30	CHL	11	608	-	55,59,74	1.49	8 (14%)	62,96,114	1.99	14 (22%)
31	CLA	15	610	-	49,53,73	1.42	7 (14%)	59,89,113	1.83	9 (15%)
31	CLA	15	612	2	54,58,73	1.40	8 (14%)	65,95,113	1.75	9 (13%)
31	CLA	B	615	7	69,73,73	1.25	8 (11%)	83,113,113	1.72	13 (15%)
32	LHG	Y	618	-	46,46,48	1.42	8 (17%)	49,52,54	0.75	2 (4%)
32	LHG	l	102	-	46,46,48	1.30	8 (17%)	49,52,54	0.77	2 (4%)
30	CHL	s	601	22	50,54,74	1.52	7 (14%)	56,90,114	2.06	13 (23%)
33	LUT	2	615	-	42,43,43	0.37	0	51,60,60	0.31	0
39	BCR	A	407	-	41,41,41	0.11	0	56,56,56	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	y	602	28	64,68,73	1.29	8 (12%)	77,107,113	1.70	10 (12%)
37	OEX	a	402	6,8	0,14,14	-	-	-		
31	CLA	y	614	28	53,57,73	1.38	8 (15%)	62,93,113	1.87	10 (16%)
30	CHL	11	606	-	51,55,74	1.50	7 (13%)	57,91,114	1.96	13 (22%)
31	CLA	3	610	3	64,68,73	1.28	7 (10%)	77,107,113	1.68	11 (14%)
31	CLA	15	602	2	64,68,73	1.30	7 (10%)	77,107,113	1.64	11 (14%)
39	BCR	j	101	-	41,41,41	0.20	0	56,56,56	0.47	0
31	CLA	4	614	1	50,54,73	1.41	7 (14%)	60,90,113	1.85	10 (16%)
31	CLA	14	610	1	69,73,73	1.24	6 (8%)	83,113,113	1.72	12 (14%)
31	CLA	A	402	6	69,73,73	1.24	8 (11%)	83,113,113	1.69	11 (13%)
31	CLA	R	612	21	54,58,73	1.41	7 (12%)	65,95,113	1.61	9 (13%)
31	CLA	S	609	22	59,63,73	1.34	7 (11%)	71,101,113	1.78	10 (14%)
30	CHL	1	601	1	65,69,74	1.37	7 (10%)	74,108,114	1.90	16 (21%)
32	LHG	n	616	31	48,48,48	1.32	7 (14%)	51,54,54	0.77	2 (3%)
31	CLA	S	605	22	54,58,73	1.39	7 (12%)	65,95,113	1.72	9 (13%)
43	LNL	c	523	-	19,19,19	0.43	0	18,19,19	0.49	0
31	CLA	N	612	2	49,53,73	1.43	7 (14%)	59,89,113	1.89	9 (15%)
41	LMG	b	620	-	49,49,55	0.19	0	57,57,63	0.16	0
30	CHL	Y	607	-	70,74,74	1.31	7 (10%)	80,114,114	1.84	15 (18%)
31	CLA	S	614	22	69,73,73	1.23	7 (10%)	83,113,113	1.63	11 (13%)
30	CHL	N	601	2	57,61,74	1.46	7 (12%)	64,98,114	1.93	11 (17%)
31	CLA	16	610	5	69,73,73	1.23	7 (10%)	83,113,113	1.70	11 (13%)
31	CLA	A	404	-	69,73,73	1.23	8 (11%)	83,113,113	1.58	12 (14%)
33	LUT	6	618	-	42,43,43	0.43	1 (2%)	51,60,60	0.43	0
31	CLA	6	604	-	69,73,73	1.24	8 (11%)	83,113,113	1.65	12 (14%)
41	LMG	D	414	-	48,48,55	0.19	0	56,56,63	0.15	0
31	CLA	1	612	1	50,54,73	1.41	7 (14%)	60,90,113	1.76	7 (11%)
42	PL9	D	407	-	55,55,55	0.09	0	68,69,69	0.18	0
36	3PH	B	620	-	47,47,47	0.27	0	51,52,52	0.29	0
43	LNL	c	524	-	19,19,19	0.44	0	18,19,19	0.50	0
31	CLA	s	604	-	69,73,73	1.23	7 (10%)	83,113,113	1.58	9 (10%)
31	CLA	r	614	-	59,63,73	1.32	8 (13%)	71,101,113	1.73	10 (14%)
30	CHL	3	609	3	70,74,74	1.34	8 (11%)	80,114,114	1.80	12 (15%)
31	CLA	r	603	21	69,73,73	1.25	8 (11%)	83,113,113	1.73	11 (13%)
31	CLA	c	505	-	59,63,73	1.32	8 (13%)	71,101,113	1.74	10 (14%)
31	CLA	R	613	21	64,68,73	1.29	8 (12%)	77,107,113	1.79	12 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	c	513	8	59,63,73	1.34	8 (13%)	71,101,113	1.77	10 (14%)
32	LHG	R	618	31	37,37,48	1.44	7 (18%)	40,43,54	0.86	2 (5%)
31	CLA	a	404	-	69,73,73	1.23	8 (11%)	83,113,113	1.59	12 (14%)
31	CLA	r	601	21	53,57,73	1.37	7 (13%)	62,93,113	1.71	8 (12%)
31	CLA	1	602	1	64,68,73	1.28	8 (12%)	77,107,113	1.71	13 (16%)
41	LMG	B	622	-	48,48,55	0.18	0	56,56,63	0.20	0
31	CLA	y	612	28	69,73,73	1.25	8 (11%)	83,113,113	1.64	13 (15%)
31	CLA	13	615	5	49,53,73	1.41	7 (14%)	59,89,113	1.84	6 (10%)
34	NEX	3	621	-	38,46,46	0.45	1 (2%)	50,70,70	0.34	0
31	CLA	r	613	21	69,73,73	1.24	8 (11%)	83,113,113	1.74	11 (13%)
34	NEX	r	617	-	38,46,46	0.40	1 (2%)	50,70,70	0.45	0
31	CLA	D	405	9	69,73,73	1.23	8 (11%)	83,113,113	1.59	11 (13%)
30	CHL	y	606	-	70,74,74	1.32	7 (10%)	80,114,114	1.82	13 (16%)
31	CLA	1	610	1	59,63,73	1.33	7 (11%)	71,101,113	1.65	11 (15%)
33	LUT	4	616	-	42,43,43	0.39	1 (2%)	51,60,60	0.39	0
31	CLA	S	611	32	69,73,73	1.25	8 (11%)	83,113,113	1.71	13 (15%)
30	CHL	15	606	-	55,59,74	1.49	7 (12%)	62,96,114	2.02	13 (20%)
36	3PH	T	101	-	47,47,47	0.28	0	51,52,52	0.29	0
31	CLA	y	615	28	60,64,73	1.32	8 (13%)	72,102,113	1.74	11 (15%)
31	CLA	R	602	21	69,73,73	1.26	8 (11%)	83,113,113	1.68	12 (14%)
31	CLA	16	604	-	59,63,73	1.33	8 (13%)	71,101,113	1.69	10 (14%)
31	CLA	11	603	1	59,63,73	1.33	7 (11%)	71,101,113	1.69	10 (14%)
30	CHL	5	608	-	54,58,74	1.46	7 (12%)	59,94,114	2.00	11 (18%)
30	CHL	11	601	1	70,74,74	1.33	7 (10%)	80,114,114	1.79	15 (18%)
31	CLA	y	610	28	69,73,73	1.23	8 (11%)	83,113,113	1.69	12 (14%)
31	CLA	r	602	21	69,73,73	1.26	8 (11%)	83,113,113	1.69	12 (14%)
41	LMG	d	415	-	48,48,55	0.19	0	56,56,63	0.15	0
31	CLA	3	613	3	59,63,73	1.32	8 (13%)	71,101,113	1.73	9 (12%)
31	CLA	G	603	1	59,63,73	1.34	8 (13%)	71,101,113	1.81	9 (12%)
31	CLA	g	610	1	69,73,73	1.23	7 (10%)	83,113,113	1.68	12 (14%)
46	DGD	w	502	-	40,40,67	0.21	0	48,48,81	0.22	0
31	CLA	C	504	8	69,73,73	1.24	8 (11%)	83,113,113	1.71	13 (15%)
30	CHL	3	608	-	54,58,74	1.45	6 (11%)	59,94,114	2.03	14 (23%)
33	LUT	14	616	-	42,43,43	0.30	0	51,60,60	0.41	1 (1%)
31	CLA	b	610	-	69,73,73	1.22	8 (11%)	83,113,113	1.69	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CHL	3	601	3	65,69,74	1.37	7 (10%)	74,108,114	1.79	13 (17%)
30	CHL	r	606	21	70,74,74	1.29	7 (10%)	80,114,114	1.82	16 (20%)
30	CHL	5	609	2	70,74,74	1.34	7 (10%)	80,114,114	1.76	11 (13%)
31	CLA	C	505	-	59,63,73	1.32	8 (13%)	71,101,113	1.73	10 (14%)
43	LNL	C	524	-	19,19,19	0.44	0	18,19,19	0.50	0
42	PL9	a	410	-	55,55,55	0.09	0	68,69,69	0.18	0
31	CLA	3	612	3	69,73,73	1.25	7 (10%)	83,113,113	1.68	12 (14%)
39	BCR	B	619	-	41,41,41	0.12	0	56,56,56	0.24	0
32	LHG	6	616	31	43,43,48	1.43	8 (18%)	46,49,54	0.79	2 (4%)
43	LNL	I	101	-	19,19,19	0.43	0	18,19,19	0.50	0
39	BCR	b	618	-	41,41,41	0.14	0	56,56,56	0.24	0
33	LUT	5	614	-	42,43,43	0.35	0	51,60,60	0.42	0
32	LHG	D	409	-	38,38,48	1.39	8 (21%)	41,44,54	0.79	2 (4%)
31	CLA	6	613	3	59,63,73	1.33	7 (11%)	71,101,113	1.69	8 (11%)
33	LUT	Y	621	-	42,43,43	0.39	0	51,60,60	0.49	0
31	CLA	Y	612	28	69,73,73	1.25	8 (11%)	83,113,113	1.64	13 (15%)
30	CHL	y	609	28	70,74,74	1.32	7 (10%)	80,114,114	1.84	15 (18%)
31	CLA	3	602	3	64,68,73	1.29	8 (12%)	77,107,113	1.66	12 (15%)
31	CLA	12	602	2	64,68,73	1.30	7 (10%)	77,107,113	1.66	12 (15%)
32	LHG	d	413	-	48,48,48	1.43	8 (16%)	51,54,54	0.75	2 (3%)
31	CLA	c	509	8	64,68,73	1.30	8 (12%)	77,107,113	1.73	13 (16%)
31	CLA	Y	603	28	64,68,73	1.28	8 (12%)	77,107,113	1.78	12 (15%)
30	CHL	g	608	-	56,60,74	1.47	8 (14%)	63,97,114	1.95	12 (19%)
31	CLA	14	612	1	47,51,73	1.43	7 (14%)	56,86,113	1.78	7 (12%)
31	CLA	5	612	-	50,54,73	1.42	7 (14%)	60,90,113	1.82	8 (13%)
31	CLA	5	610	2	54,58,73	1.39	7 (12%)	65,95,113	1.71	12 (18%)
31	CLA	C	503	8	69,73,73	1.22	8 (11%)	83,113,113	1.72	11 (13%)
30	CHL	Y	606	-	70,74,74	1.32	7 (10%)	80,114,114	1.82	14 (17%)
31	CLA	15	613	2	49,53,73	1.44	8 (16%)	59,89,113	1.76	8 (13%)
31	CLA	B	604	7	69,73,73	1.24	8 (11%)	83,113,113	1.69	13 (15%)
31	CLA	g	612	1	47,51,73	1.42	8 (17%)	56,86,113	1.85	7 (12%)
30	CHL	12	608	2	57,61,74	1.48	8 (14%)	64,98,114	1.90	14 (21%)
30	CHL	S	608	-	53,57,74	1.46	6 (11%)	59,93,114	2.07	11 (18%)
32	LHG	y	617	-	46,46,48	1.44	8 (17%)	49,52,54	0.73	2 (4%)
31	CLA	11	610	1	59,63,73	1.33	6 (10%)	71,101,113	1.83	13 (18%)
32	LHG	c	521	-	41,41,48	1.46	8 (19%)	44,47,54	0.78	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	NEX	N	619	-	38,46,46	0.42	1 (2%)	50,70,70	0.40	0
33	LUT	15	614	-	42,43,43	0.38	0	51,60,60	0.49	0
31	CLA	c	504	8	69,73,73	1.24	8 (11%)	83,113,113	1.71	12 (14%)
30	CHL	13	605	5	60,64,74	1.43	7 (11%)	68,102,114	1.99	16 (23%)
30	CHL	g	606	-	54,58,74	1.45	6 (11%)	59,94,114	1.95	11 (18%)
31	CLA	y	611	32	69,73,73	1.24	8 (11%)	83,113,113	1.65	12 (14%)
32	LHG	16	616	31	39,39,48	1.51	8 (20%)	42,45,54	0.81	2 (4%)
31	CLA	4	602	1	64,68,73	1.28	7 (10%)	77,107,113	1.70	12 (15%)
30	CHL	n	608	-	54,58,74	1.43	6 (11%)	59,94,114	2.08	13 (22%)
31	CLA	Y	613	28	69,73,73	1.23	7 (10%)	83,113,113	1.60	10 (12%)
32	LHG	Y	617	-	46,46,48	1.44	8 (17%)	49,52,54	0.76	2 (4%)
41	LMG	v	101	-	51,51,55	0.19	0	59,59,63	0.16	0
31	CLA	N	611	32	64,68,73	1.31	8 (12%)	77,107,113	1.72	9 (11%)
43	LNL	y	619	-	19,19,19	0.43	0	18,19,19	0.50	0
30	CHL	3	606	-	60,64,74	1.43	7 (11%)	68,102,114	1.87	9 (13%)
31	CLA	C	511	8	69,73,73	1.22	8 (11%)	83,113,113	1.73	12 (14%)
30	CHL	n	605	2	65,69,74	1.36	7 (10%)	74,108,114	1.84	15 (20%)
31	CLA	G	611	32	69,73,73	1.24	7 (10%)	83,113,113	1.63	8 (9%)
31	CLA	A	403	-	69,73,73	1.23	8 (11%)	83,113,113	1.61	13 (15%)
34	NEX	12	616	-	24,28,46	0.36	0	32,42,70	0.56	0
31	CLA	r	611	21	53,57,73	1.38	8 (15%)	62,93,113	1.83	6 (9%)
31	CLA	6	612	3	59,63,73	1.35	7 (11%)	71,101,113	1.77	11 (15%)
39	BCR	b	617	-	41,41,41	0.14	0	56,56,56	0.26	0
48	BCT	D	403	47	2,3,3	0.88	0	2,3,3	3.15	2 (100%)
33	LUT	11	616	-	42,43,43	0.33	0	51,60,60	0.47	1 (1%)
30	CHL	2	609	2	70,74,74	1.35	7 (10%)	80,114,114	1.75	12 (15%)
43	LNL	Y	619	-	19,19,19	0.43	0	18,19,19	0.50	0
30	CHL	15	601	2	54,58,74	1.46	7 (12%)	59,94,114	2.05	12 (20%)
43	LNL	W	502	-	19,19,19	0.44	0	18,19,19	0.52	0
43	LNL	C	523	-	19,19,19	0.43	0	18,19,19	0.50	0
31	CLA	16	614	5	49,53,73	1.41	7 (14%)	59,89,113	1.82	10 (16%)
38	PHO	D	402	-	58,69,69	0.96	1 (1%)	56,99,99	1.02	5 (8%)
39	BCR	b	619	-	41,41,41	0.12	0	56,56,56	0.25	0
31	CLA	n	612	2	49,53,73	1.42	8 (16%)	59,89,113	1.89	9 (15%)
31	CLA	16	603	5	64,68,73	1.28	7 (10%)	77,107,113	1.68	11 (14%)
44	STE	b	622	-	19,19,19	0.60	0	19,19,19	0.99	2 (10%)
41	LMG	d	411	-	34,34,55	0.21	0	36,36,63	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	LNL	R	620	-	19,19,19	0.44	0	18,19,19	0.51	0
30	CHL	n	601	2	56,60,74	1.47	7 (12%)	63,97,114	2.06	14 (22%)
31	CLA	15	604	-	59,63,73	1.34	7 (11%)	71,101,113	1.64	9 (12%)
31	CLA	C	510	8	69,73,73	1.24	8 (11%)	83,113,113	1.79	8 (9%)
31	CLA	R	610	32	64,68,73	1.28	7 (10%)	77,107,113	1.65	11 (14%)
34	NEX	5	616	-	29,33,46	0.48	1 (3%)	38,48,70	0.50	0
41	LMG	b	621	-	46,46,55	0.18	0	54,54,63	0.16	0
30	CHL	N	607	-	70,74,74	1.31	7 (10%)	80,114,114	1.80	13 (16%)
30	CHL	12	606	-	55,59,74	1.49	7 (12%)	62,96,114	2.06	12 (19%)
39	BCR	C	516	-	41,41,41	0.12	0	56,56,56	0.31	0
32	LHG	A	413	-	43,43,48	1.39	8 (18%)	46,49,54	0.83	2 (4%)
31	CLA	R	608	21	69,73,73	1.23	8 (11%)	83,113,113	1.62	13 (15%)
31	CLA	n	611	32	64,68,73	1.30	7 (10%)	77,107,113	1.72	9 (11%)
30	CHL	6	601	3	65,69,74	1.38	8 (12%)	74,108,114	1.83	13 (17%)
31	CLA	C	508	-	69,73,73	1.24	7 (10%)	83,113,113	1.51	12 (14%)
33	LUT	13	617	-	42,43,43	0.37	0	51,60,60	0.54	1 (1%)
30	CHL	16	601	5	60,64,74	1.45	8 (13%)	68,102,114	1.96	13 (19%)
30	CHL	r	607	-	55,59,74	1.47	7 (12%)	62,96,114	2.02	14 (22%)
30	CHL	g	605	1	52,56,74	1.48	7 (13%)	58,92,114	2.02	12 (20%)
30	CHL	4	609	1	70,74,74	1.34	8 (11%)	80,114,114	1.75	14 (17%)
32	LHG	y	616	31	48,48,48	1.27	6 (12%)	51,54,54	0.79	2 (3%)
33	LUT	1	617	-	42,43,43	0.37	0	51,60,60	0.30	0
43	LNL	H	101	-	19,19,19	0.43	0	18,19,19	0.49	0
31	CLA	g	603	1	59,63,73	1.33	8 (13%)	71,101,113	1.81	9 (12%)
31	CLA	15	611	2	49,53,73	1.44	7 (14%)	59,89,113	1.80	8 (13%)
34	NEX	2	616	-	29,33,46	0.48	1 (3%)	38,48,70	0.50	0
43	LNL	w	503	-	19,19,19	0.44	0	18,19,19	0.52	0
30	CHL	15	605	-	50,54,74	1.54	7 (14%)	56,90,114	2.20	9 (16%)
31	CLA	13	612	5	49,53,73	1.45	7 (14%)	59,89,113	1.82	8 (13%)
30	CHL	16	606	-	65,69,74	1.37	7 (10%)	74,108,114	1.80	12 (16%)
32	LHG	D	412	-	48,48,48	1.43	8 (16%)	51,54,54	0.74	2 (3%)
31	CLA	r	609	21	69,73,73	1.24	7 (10%)	83,113,113	1.66	10 (12%)
30	CHL	G	606	-	51,55,74	1.48	6 (11%)	57,91,114	1.98	11 (19%)
31	CLA	a	403	6	69,73,73	1.24	8 (11%)	83,113,113	1.69	12 (14%)
39	BCR	a	408	-	41,41,41	0.11	0	56,56,56	0.24	0
31	CLA	G	612	1	47,51,73	1.42	7 (14%)	56,86,113	1.86	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	11	611	32	54,58,73	1.40	7 (12%)	65,95,113	1.76	8 (12%)
41	LMG	C	522	-	55,55,55	0.18	0	63,63,63	0.16	0
30	CHL	12	601	2	54,58,74	1.47	7 (12%)	59,94,114	2.05	12 (20%)
31	CLA	B	607	-	69,73,73	1.22	8 (11%)	83,113,113	1.69	9 (10%)
30	CHL	G	607	-	54,58,74	1.46	6 (11%)	59,94,114	2.05	11 (18%)
32	LHG	R	619	-	46,46,48	1.39	8 (17%)	49,52,54	0.78	2 (4%)
30	CHL	R	605	21	60,64,74	1.41	7 (11%)	68,102,114	1.96	13 (19%)
30	CHL	13	606	-	65,69,74	1.37	7 (10%)	74,108,114	1.80	12 (16%)
31	CLA	2	613	2	51,55,73	1.38	7 (13%)	61,91,113	1.67	9 (14%)
37	OEX	A	401	6,8	0,14,14	-	-	-	-	-
33	LUT	g	617	-	42,43,43	0.45	1 (2%)	51,60,60	0.44	1 (1%)
30	CHL	2	601	2	51,55,74	1.49	7 (13%)	57,91,114	1.77	11 (19%)
31	CLA	4	612	1	50,54,73	1.45	7 (14%)	60,90,113	1.65	8 (13%)
31	CLA	y	604	-	59,63,73	1.33	7 (11%)	71,101,113	1.78	10 (14%)
33	LUT	G	616	-	42,43,43	0.38	0	51,60,60	0.40	0
30	CHL	3	607	-	70,74,74	1.31	7 (10%)	80,114,114	1.86	14 (17%)
30	CHL	S	607	-	47,51,74	1.44	6 (12%)	52,86,114	2.21	11 (21%)
31	CLA	12	613	2	49,53,73	1.42	7 (14%)	59,89,113	1.80	8 (13%)
31	CLA	C	512	8	69,73,73	1.23	8 (11%)	83,113,113	1.68	11 (13%)
31	CLA	y	603	28	64,68,73	1.28	8 (12%)	77,107,113	1.76	12 (15%)
31	CLA	B	614	7	69,73,73	1.24	7 (10%)	83,113,113	1.68	11 (13%)
31	CLA	B	603	7	69,73,73	1.24	8 (11%)	83,113,113	1.68	11 (13%)
30	CHL	G	601	1	70,74,74	1.32	7 (10%)	80,114,114	1.77	13 (16%)
31	CLA	b	612	7	69,73,73	1.25	8 (11%)	83,113,113	1.76	8 (9%)
39	BCR	h	102	-	41,41,41	0.13	0	56,56,56	0.33	0
30	CHL	N	605	2	65,69,74	1.36	7 (10%)	74,108,114	1.79	13 (17%)
31	CLA	N	614	2	49,53,73	1.42	8 (16%)	59,89,113	1.75	9 (15%)
31	CLA	14	613	1	59,63,73	1.33	7 (11%)	71,101,113	1.72	10 (14%)
40	SQD	l	101	-	49,50,54	0.18	0	58,61,65	0.20	0
31	CLA	B	601	-	59,63,73	1.32	8 (13%)	71,101,113	1.74	9 (12%)
30	CHL	n	607	-	70,74,74	1.30	7 (10%)	80,114,114	1.77	12 (15%)
31	CLA	N	615	2	51,55,73	1.38	7 (13%)	61,91,113	1.91	9 (14%)
31	CLA	r	604	-	52,56,73	1.39	7 (13%)	62,92,113	1.79	10 (16%)
32	LHG	s	617	31	44,44,48	1.36	7 (15%)	47,50,54	0.72	2 (4%)
31	CLA	1	613	1	59,63,73	1.33	7 (11%)	71,101,113	1.73	10 (14%)
32	LHG	S	621	-	48,48,48	1.36	8 (16%)	51,54,54	0.77	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	3PH	b	623	-	38,38,47	0.29	0	42,43,52	0.33	0
31	CLA	2	602	2	59,63,73	1.34	8 (13%)	71,101,113	1.74	12 (16%)
31	CLA	c	512	8	69,73,73	1.23	8 (11%)	83,113,113	1.69	11 (13%)
33	LUT	s	619	-	42,43,43	0.33	0	51,60,60	0.42	1 (1%)
31	CLA	R	611	21	53,57,73	1.38	8 (15%)	62,93,113	1.81	7 (11%)
31	CLA	13	611	32	69,73,73	1.24	7 (10%)	83,113,113	1.65	11 (13%)
33	LUT	S	618	-	42,43,43	0.36	0	51,60,60	0.43	0
31	CLA	b	615	7	69,73,73	1.25	8 (11%)	83,113,113	1.70	12 (14%)
41	LMG	D	410	-	44,44,55	0.19	0	52,52,63	0.17	0
31	CLA	5	603	2	59,63,73	1.33	7 (11%)	71,101,113	1.84	8 (11%)
32	LHG	Y	616	31	48,48,48	1.28	6 (12%)	51,54,54	0.79	2 (3%)
31	CLA	2	610	2	54,58,73	1.38	7 (12%)	65,95,113	1.78	11 (16%)
31	CLA	3	615	3	50,54,73	1.40	8 (16%)	60,90,113	1.88	10 (16%)
32	LHG	A	415	-	48,48,48	1.40	8 (16%)	51,54,54	0.75	2 (3%)
31	CLA	d	405	9	69,73,73	1.23	7 (10%)	83,113,113	1.59	12 (14%)
33	LUT	y	623	-	42,43,43	0.43	1 (2%)	51,60,60	0.40	0
35	XAT	14	619	-	39,47,47	0.10	0	54,74,74	0.44	0
31	CLA	B	611	7	69,73,73	1.24	8 (11%)	83,113,113	1.65	11 (13%)
31	CLA	13	602	5	69,73,73	1.25	7 (10%)	83,113,113	1.66	11 (13%)
43	LNL	W	503	-	19,19,19	0.42	0	18,19,19	0.49	0
41	LMG	w	501	-	55,55,55	0.17	0	63,63,63	0.17	0
30	CHL	Y	605	28	60,64,74	1.41	7 (11%)	68,102,114	1.96	13 (19%)
31	CLA	S	602	22	69,73,73	1.25	8 (11%)	83,113,113	1.68	11 (13%)
30	CHL	2	606	-	50,54,74	1.53	8 (16%)	56,90,114	2.04	11 (19%)
31	CLA	12	609	2	59,63,73	1.33	7 (11%)	71,101,113	1.69	8 (11%)
31	CLA	2	612	-	50,54,73	1.42	8 (16%)	60,90,113	1.82	8 (13%)
33	LUT	N	617	-	42,43,43	0.37	0	51,60,60	0.34	0
32	LHG	g	615	31	48,48,48	1.30	6 (12%)	51,54,54	0.70	2 (3%)
30	CHL	14	601	1	70,74,74	1.32	7 (10%)	80,114,114	1.78	15 (18%)
31	CLA	Y	604	-	59,63,73	1.33	8 (13%)	71,101,113	1.77	9 (12%)
41	LMG	J	102	-	51,51,55	0.18	0	59,59,63	0.17	0
31	CLA	N	613	2	59,63,73	1.34	8 (13%)	71,101,113	1.77	7 (9%)
30	CHL	R	606	21	70,74,74	1.29	7 (10%)	80,114,114	1.83	17 (21%)
31	CLA	n	602	2	69,73,73	1.25	8 (11%)	83,113,113	1.68	10 (12%)
41	LMG	K	102	-	51,51,55	0.20	0	59,59,63	0.15	0
46	DGD	C	519	-	60,60,67	0.18	0	74,74,81	0.19	0
30	CHL	13	608	-	54,58,74	1.44	6 (11%)	59,94,114	2.04	15 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	3	611	32	69,73,73	1.24	7 (10%)	83,113,113	1.57	12 (14%)
30	CHL	4	608	-	54,58,74	1.47	7 (12%)	59,94,114	1.99	13 (22%)
30	CHL	11	605	-	52,56,74	1.48	6 (11%)	58,92,114	1.84	13 (22%)
30	CHL	1	608	-	54,58,74	1.47	6 (11%)	59,94,114	1.98	13 (22%)
30	CHL	3	605	3	70,74,74	1.33	7 (10%)	80,114,114	1.88	15 (18%)
31	CLA	S	613	22	53,57,73	1.38	8 (15%)	62,93,113	1.79	10 (16%)
31	CLA	s	610	22	69,73,73	1.23	7 (10%)	83,113,113	1.66	10 (12%)
39	BCR	d	406	-	41,41,41	0.13	0	56,56,56	0.21	0
30	CHL	6	608	-	54,58,74	1.45	6 (11%)	59,94,114	2.03	14 (23%)
31	CLA	g	614	1	53,57,73	1.38	7 (13%)	62,93,113	1.77	7 (11%)
31	CLA	b	602	7	69,73,73	1.23	7 (10%)	83,113,113	1.65	12 (14%)
31	CLA	16	611	32	69,73,73	1.24	7 (10%)	83,113,113	1.63	11 (13%)
31	CLA	b	608	7	69,73,73	1.23	8 (11%)	83,113,113	1.60	12 (14%)
33	LUT	s	618	-	42,43,43	0.35	0	51,60,60	0.51	0
41	LMG	H	102	-	34,34,55	0.21	0	36,36,63	0.18	0
39	BCR	c	516	-	41,41,41	0.12	0	56,56,56	0.32	0
31	CLA	n	613	2	59,63,73	1.39	6 (10%)	71,101,113	1.62	9 (12%)
31	CLA	11	612	1	47,51,73	1.43	7 (14%)	56,86,113	1.76	7 (12%)
31	CLA	B	606	7	69,73,73	1.23	7 (10%)	83,113,113	1.57	11 (13%)
30	CHL	14	605	1	52,56,74	1.49	6 (11%)	58,92,114	2.01	13 (22%)
31	CLA	1	614	1	50,54,73	1.41	7 (14%)	60,90,113	1.87	10 (16%)
31	CLA	B	605	7	69,73,73	1.24	7 (10%)	83,113,113	1.69	10 (12%)
31	CLA	B	609	7	69,73,73	1.24	8 (11%)	83,113,113	1.66	10 (12%)
31	CLA	N	610	2	64,68,73	1.28	7 (10%)	77,107,113	1.70	9 (11%)
31	CLA	Y	614	28	53,57,73	1.38	8 (15%)	62,93,113	1.86	10 (16%)
31	CLA	b	601	-	59,63,73	1.32	8 (13%)	71,101,113	1.74	9 (12%)
31	CLA	S	612	22	49,53,73	1.55	8 (16%)	59,89,113	1.58	6 (10%)
30	CHL	S	601	22	50,54,74	1.52	7 (14%)	56,90,114	2.06	13 (23%)
32	LHG	L	102	-	46,46,48	1.31	8 (17%)	49,52,54	0.77	2 (4%)
40	SQD	L	101	-	49,50,54	0.18	0	58,61,65	0.22	0
43	LNL	y	621	-	19,19,19	0.43	0	18,19,19	0.50	0
46	DGD	C	518	-	59,59,67	0.18	0	73,73,81	0.17	0
31	CLA	12	604	-	59,63,73	1.33	7 (11%)	71,101,113	1.62	11 (15%)
31	CLA	N	602	2	69,73,73	1.23	8 (11%)	83,113,113	1.69	9 (10%)
31	CLA	b	613	7	69,73,73	1.23	8 (11%)	83,113,113	1.78	10 (12%)
30	CHL	1	606	-	51,55,74	1.47	7 (13%)	57,91,114	2.07	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	LMG	C	520	-	47,47,55	0.19	0	55,55,63	0.16	0
31	CLA	g	611	32	69,73,73	1.23	7 (10%)	83,113,113	1.63	9 (10%)
30	CHL	S	606	22	70,74,74	1.34	7 (10%)	80,114,114	1.81	14 (17%)
30	CHL	12	607	-	54,58,74	1.47	6 (11%)	59,94,114	2.06	11 (18%)
31	CLA	13	613	5	54,58,73	1.38	7 (12%)	65,95,113	1.84	8 (12%)
32	LHG	r	621	-	43,43,48	1.48	8 (18%)	46,49,54	0.81	2 (4%)
33	LUT	12	615	-	42,43,43	0.36	0	51,60,60	0.33	0
30	CHL	16	608	-	54,58,74	1.44	6 (11%)	59,94,114	2.04	15 (25%)
30	CHL	11	607	-	50,54,74	1.53	7 (14%)	56,90,114	1.98	14 (25%)
30	CHL	N	606	-	65,69,74	1.38	7 (10%)	74,108,114	1.89	12 (16%)
34	NEX	g	618	-	38,46,46	0.39	1 (2%)	50,70,70	0.48	0
41	LMG	S	616	-	42,42,55	0.19	0	50,50,63	0.18	0
46	DGD	c	517	-	67,67,67	0.18	0	81,81,81	0.18	0
31	CLA	b	607	-	69,73,73	1.22	8 (11%)	83,113,113	1.68	10 (12%)
30	CHL	N	609	2	70,74,74	1.32	7 (10%)	80,114,114	1.82	15 (18%)
43	LNL	i	101	-	19,19,19	0.44	0	18,19,19	0.50	0
32	LHG	a	413	-	43,43,48	1.39	7 (16%)	46,49,54	0.83	2 (4%)
31	CLA	1	611	32	54,58,73	1.41	9 (16%)	65,95,113	1.76	9 (13%)
31	CLA	5	604	-	54,58,73	1.41	8 (14%)	65,95,113	1.74	10 (15%)
34	NEX	16	619	-	38,46,46	0.44	1 (2%)	50,70,70	0.39	0
34	NEX	6	621	-	38,46,46	0.46	1 (2%)	50,70,70	0.35	0
30	CHL	4	601	1	65,69,74	1.37	7 (10%)	74,108,114	1.89	16 (21%)
31	CLA	s	614	22	69,73,73	1.24	7 (10%)	83,113,113	1.62	13 (15%)
30	CHL	16	609	5	65,69,74	1.39	7 (10%)	74,108,114	1.86	13 (17%)
31	CLA	n	604	-	59,63,73	1.33	7 (11%)	71,101,113	1.76	10 (14%)
32	LHG	d	409	-	38,38,48	1.40	8 (21%)	41,44,54	0.79	2 (4%)
30	CHL	16	607	-	65,69,74	1.37	8 (12%)	74,108,114	1.94	11 (14%)
31	CLA	S	610	22	69,73,73	1.23	8 (11%)	83,113,113	1.63	12 (14%)
31	CLA	R	601	21	53,57,73	1.37	7 (13%)	62,93,113	1.69	10 (16%)
31	CLA	6	611	32	69,73,73	1.23	7 (10%)	83,113,113	1.56	12 (14%)
39	BCR	C	526	-	41,41,41	0.12	0	56,56,56	0.22	0
35	XAT	r	616	-	39,47,47	0.11	0	54,74,74	0.83	3 (5%)
30	CHL	G	609	1	70,74,74	1.33	7 (10%)	80,114,114	1.81	15 (18%)
31	CLA	5	611	-	50,54,73	1.40	7 (14%)	60,90,113	1.75	8 (13%)
31	CLA	s	613	22	53,57,73	1.38	8 (15%)	62,93,113	1.78	9 (14%)
40	SQD	D	411	-	53,54,54	0.18	0	62,65,65	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LUT	3	618	-	42,43,43	0.42	1 (2%)	51,60,60	0.44	0
30	CHL	s	608	-	53,57,74	1.47	6 (11%)	59,93,114	2.08	12 (20%)
31	CLA	c	511	8	69,73,73	1.22	8 (11%)	83,113,113	1.74	12 (14%)
33	LUT	2	614	-	42,43,43	0.32	0	51,60,60	0.29	0
31	CLA	c	514	8	69,73,73	1.23	7 (10%)	83,113,113	1.58	12 (14%)
30	CHL	Y	608	-	48,52,74	1.41	5 (10%)	53,87,114	2.04	9 (16%)
31	CLA	14	604	-	59,63,73	1.34	7 (11%)	71,101,113	1.72	8 (11%)
32	LHG	a	414	-	42,42,48	1.45	8 (19%)	45,48,54	0.78	2 (4%)
32	LHG	A	414	-	42,42,48	1.46	8 (19%)	45,48,54	0.79	2 (4%)
43	LNL	y	620	-	19,19,19	0.42	0	18,19,19	0.48	0
30	CHL	s	606	22	70,74,74	1.34	7 (10%)	80,114,114	1.80	12 (15%)
30	CHL	y	601	28	70,74,74	1.30	7 (10%)	80,114,114	1.86	13 (16%)
31	CLA	13	604	-	59,63,73	1.33	8 (13%)	71,101,113	1.70	9 (12%)
31	CLA	15	609	2	59,63,73	1.34	7 (11%)	71,101,113	1.78	13 (18%)
31	CLA	16	612	5	49,53,73	1.44	7 (14%)	59,89,113	1.82	8 (13%)
31	CLA	s	612	22	49,53,73	1.44	8 (16%)	59,89,113	1.85	9 (15%)
38	PHO	A	405	-	58,69,69	0.93	1 (1%)	56,99,99	1.00	5 (8%)
31	CLA	1	604	-	54,58,73	1.40	7 (12%)	65,95,113	1.83	12 (18%)
32	LHG	y	618	-	46,46,48	1.41	8 (17%)	49,52,54	0.74	2 (4%)
33	LUT	5	615	-	42,43,43	0.37	0	51,60,60	0.32	0
44	STE	B	623	-	19,19,19	0.58	0	19,19,19	1.01	2 (10%)
30	CHL	5	601	2	55,59,74	1.50	8 (14%)	62,96,114	1.95	14 (22%)
30	CHL	13	607	-	65,69,74	1.37	7 (10%)	74,108,114	1.91	13 (17%)
31	CLA	4	610	1	69,73,73	1.30	8 (11%)	83,113,113	1.43	11 (13%)
31	CLA	4	613	1	59,63,73	1.32	7 (11%)	71,101,113	1.68	11 (15%)
39	BCR	B	618	-	41,41,41	0.14	0	56,56,56	0.24	0
30	CHL	n	609	2	70,74,74	1.32	7 (10%)	80,114,114	1.83	13 (16%)
31	CLA	d	404	9	69,73,73	1.23	8 (11%)	83,113,113	1.67	12 (14%)
31	CLA	s	602	22	69,73,73	1.25	8 (11%)	83,113,113	1.65	9 (10%)
30	CHL	2	605	2	50,54,74	1.53	8 (16%)	56,90,114	1.92	10 (17%)
30	CHL	5	607	-	60,64,74	1.43	8 (13%)	68,102,114	1.94	12 (17%)
32	LHG	3	616	31	43,43,48	1.42	8 (18%)	46,49,54	0.78	2 (4%)
31	CLA	C	507	8	69,73,73	1.24	8 (11%)	83,113,113	1.65	11 (13%)
33	LUT	4	617	-	42,43,43	0.37	0	51,60,60	0.31	0
42	PL9	A	410	-	55,55,55	0.08	0	68,69,69	0.18	0
32	LHG	D	408	-	48,48,48	1.30	7 (14%)	51,54,54	0.72	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	12	612	2	54,58,73	1.39	7 (12%)	65,95,113	1.78	10 (15%)
33	LUT	Y	622	-	42,43,43	0.43	1 (2%)	51,60,60	0.40	0
31	CLA	14	614	1	53,57,73	1.38	7 (13%)	62,93,113	1.83	8 (12%)
36	3PH	B	624	-	37,37,47	0.30	0	41,42,52	0.33	0
41	LMG	s	616	-	42,42,55	0.19	0	50,50,63	0.18	0
32	LHG	S	617	31	44,44,48	1.38	8 (18%)	47,50,54	0.77	2 (4%)
31	CLA	14	603	1	59,63,73	1.33	7 (11%)	71,101,113	1.70	11 (15%)
31	CLA	r	608	21	69,73,73	1.23	8 (11%)	83,113,113	1.61	12 (14%)
33	LUT	n	617	-	42,43,43	0.37	0	51,60,60	0.35	0
32	LHG	11	615	31	48,48,48	1.38	8 (16%)	51,54,54	0.74	2 (3%)
31	CLA	C	513	8	59,63,73	1.33	8 (13%)	71,101,113	1.76	10 (14%)
30	CHL	4	606	-	51,55,74	1.48	7 (13%)	57,91,114	2.11	11 (19%)
32	LHG	a	401	-	48,48,48	1.40	8 (16%)	51,54,54	0.72	2 (3%)
31	CLA	g	604	-	54,58,73	1.40	8 (14%)	65,95,113	1.80	10 (15%)
40	SQD	A	408	-	50,51,54	0.19	0	59,62,65	0.26	0
31	CLA	b	604	7	69,73,73	1.24	8 (11%)	83,113,113	1.68	11 (13%)
32	LHG	R	621	-	43,43,48	1.46	8 (18%)	46,49,54	0.79	2 (4%)
31	CLA	b	606	7	69,73,73	1.24	8 (11%)	83,113,113	1.58	11 (13%)
32	LHG	4	615	31	46,46,48	1.40	8 (17%)	49,52,54	0.71	2 (4%)
36	3PH	8	201	-	47,47,47	0.30	0	51,52,52	0.41	0
30	CHL	4	605	1	50,54,74	1.54	8 (16%)	56,90,114	2.05	12 (21%)
32	LHG	N	616	31	48,48,48	1.30	7 (14%)	51,54,54	0.78	2 (3%)
31	CLA	3	604	-	69,73,73	1.25	8 (11%)	83,113,113	1.64	12 (14%)
35	XAT	g	619	-	39,47,47	0.10	0	54,74,74	0.44	0
31	CLA	d	402	-	69,73,73	1.23	8 (11%)	83,113,113	1.58	14 (16%)
31	CLA	11	602	1	64,68,73	1.29	7 (10%)	77,107,113	1.73	14 (18%)
31	CLA	12	603	2	59,63,73	1.33	7 (11%)	71,101,113	1.78	9 (12%)
31	CLA	B	610	-	69,73,73	1.22	8 (11%)	83,113,113	1.70	13 (15%)
31	CLA	c	503	8	69,73,73	1.22	8 (11%)	83,113,113	1.72	11 (13%)
31	CLA	c	502	8	69,73,73	1.22	8 (11%)	83,113,113	1.62	10 (12%)
31	CLA	11	613	1	59,63,73	1.33	7 (11%)	71,101,113	1.72	10 (14%)
31	CLA	15	603	2	59,63,73	1.33	7 (11%)	71,101,113	1.83	11 (15%)
30	CHL	r	605	21	60,64,74	1.42	7 (11%)	68,102,114	1.95	13 (19%)
31	CLA	13	614	5	49,53,73	1.41	7 (14%)	59,89,113	1.83	10 (16%)
34	NEX	y	624	-	38,46,46	0.45	1 (2%)	50,70,70	0.65	1 (2%)
30	CHL	6	607	-	70,74,74	1.31	7 (10%)	80,114,114	1.85	14 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	BCR	D	406	-	41,41,41	0.13	0	56,56,56	0.21	0
31	CLA	14	602	1	64,68,73	1.29	7 (10%)	77,107,113	1.73	12 (15%)
30	CHL	5	606	-	50,54,74	1.53	8 (16%)	56,90,114	2.04	10 (17%)
31	CLA	4	603	1	59,63,73	1.33	8 (13%)	71,101,113	1.78	11 (15%)
33	LUT	16	618	-	42,43,43	0.41	1 (2%)	51,60,60	0.37	0
43	LNL	r	620	-	19,19,19	0.44	0	18,19,19	0.51	0
31	CLA	N	604	-	59,63,73	1.33	8 (13%)	71,101,113	1.77	10 (14%)
33	LUT	15	615	-	42,43,43	0.34	0	51,60,60	0.31	0
35	XAT	R	616	-	39,47,47	0.12	0	54,74,74	0.82	3 (5%)
41	LMG	c	520	-	47,47,55	0.19	0	55,55,63	0.17	0
39	BCR	c	526	-	41,41,41	0.12	0	56,56,56	0.22	0
31	CLA	N	603	2	64,68,73	1.28	8 (12%)	77,107,113	1.74	10 (12%)
30	CHL	y	605	28	60,64,74	1.43	7 (11%)	68,102,114	1.80	13 (19%)
31	CLA	12	610	-	49,53,73	1.42	7 (14%)	59,89,113	1.82	9 (15%)
31	CLA	4	611	32	54,58,73	1.41	8 (14%)	65,95,113	1.79	10 (15%)
35	XAT	3	620	-	39,47,47	0.13	0	54,74,74	0.73	1 (1%)
34	NEX	14	618	-	13,17,46	0.38	0	19,29,70	0.48	0
32	LHG	d	408	-	48,48,48	1.28	7 (14%)	51,54,54	0.73	2 (3%)
32	LHG	13	616	31	39,39,48	1.50	8 (20%)	42,45,54	0.81	2 (4%)
33	LUT	13	618	-	42,43,43	0.40	1 (2%)	51,60,60	0.36	0
30	CHL	1	605	1	50,54,74	1.54	8 (16%)	56,90,114	2.05	12 (21%)
30	CHL	6	609	3	70,74,74	1.33	7 (10%)	80,114,114	1.80	14 (17%)
31	CLA	2	604	-	54,58,73	1.42	9 (16%)	65,95,113	1.76	10 (15%)
31	CLA	n	614	2	49,53,73	1.42	8 (16%)	59,89,113	1.81	8 (13%)
33	LUT	G	617	-	42,43,43	0.45	1 (2%)	51,60,60	0.44	1 (1%)
36	3PH	7	201	-	47,47,47	0.28	0	51,52,52	0.31	0
32	LHG	A	411	-	48,48,48	1.37	8 (16%)	51,54,54	0.74	2 (3%)
30	CHL	14	608	-	55,59,74	1.50	8 (14%)	62,96,114	1.93	13 (20%)
31	CLA	C	514	8	69,73,73	1.23	7 (10%)	83,113,113	1.55	10 (12%)
39	BCR	c	515	-	41,41,41	0.11	0	56,56,56	0.23	0
31	CLA	5	613	2	54,58,73	1.38	7 (12%)	65,95,113	1.67	9 (13%)
31	CLA	13	610	5	69,73,73	1.23	6 (8%)	83,113,113	1.69	11 (13%)
33	LUT	3	619	-	42,43,43	0.40	1 (2%)	51,60,60	0.42	0
31	CLA	2	611	-	50,54,73	1.41	7 (14%)	60,90,113	1.80	9 (15%)
32	LHG	G	615	31	48,48,48	1.33	8 (16%)	51,54,54	0.73	2 (3%)
33	LUT	n	618	-	42,43,43	0.40	1 (2%)	51,60,60	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	S	615	22	51,55,73	1.39	7 (13%)	61,91,113	1.87	7 (11%)
43	LNL	Y	620	-	19,19,19	0.43	0	18,19,19	0.48	0
31	CLA	6	610	3	64,68,73	1.28	7 (10%)	77,107,113	1.66	12 (15%)
41	LMG	c	522	-	55,55,55	0.18	0	63,63,63	0.16	0
31	CLA	5	602	2	59,63,73	1.34	8 (13%)	71,101,113	1.68	10 (14%)
32	LHG	6	617	-	46,46,48	1.36	8 (17%)	49,52,54	0.75	2 (4%)
31	CLA	R	614	-	59,63,73	1.32	8 (13%)	71,101,113	1.78	11 (15%)
46	DGD	W	501	-	46,46,67	0.20	0	54,54,81	0.31	0
30	CHL	4	607	-	55,59,74	1.49	7 (12%)	62,96,114	1.94	10 (16%)
31	CLA	n	615	2	51,55,73	1.39	8 (15%)	61,91,113	1.89	10 (16%)
31	CLA	13	603	5	64,68,73	1.28	7 (10%)	77,107,113	1.75	11 (14%)
32	LHG	14	615	31	48,48,48	1.39	8 (16%)	51,54,54	0.73	2 (3%)
33	LUT	6	619	-	42,43,43	0.41	1 (2%)	51,60,60	0.41	0
31	CLA	1	603	1	51,55,73	1.38	7 (13%)	61,91,113	1.87	8 (13%)
31	CLA	G	614	1	53,57,73	1.39	7 (13%)	62,93,113	1.77	6 (9%)
31	CLA	6	602	3	64,68,73	1.28	8 (12%)	77,107,113	1.67	12 (15%)
32	LHG	C	521	-	41,41,48	1.45	8 (19%)	44,47,54	0.78	2 (4%)
30	CHL	15	608	2	65,69,74	1.40	7 (10%)	74,108,114	1.72	13 (17%)
31	CLA	S	603	22	46,50,73	1.41	7 (15%)	55,85,113	1.94	8 (14%)
34	NEX	4	618	-	13,17,46	0.35	0	19,29,70	0.49	0
31	CLA	b	616	7	64,68,73	1.28	8 (12%)	77,107,113	1.77	11 (14%)
30	CHL	2	608	-	54,58,74	1.46	7 (12%)	59,94,114	2.03	12 (20%)
31	CLA	6	615	3	54,58,73	1.39	6 (11%)	65,95,113	1.88	11 (16%)
40	SQD	d	414	-	45,46,54	0.19	0	54,57,65	0.23	0
30	CHL	g	607	-	54,58,74	1.46	6 (11%)	59,94,114	2.03	10 (16%)
31	CLA	n	603	2	64,68,73	1.28	8 (12%)	77,107,113	1.79	10 (12%)
30	CHL	s	607	-	47,51,74	1.44	6 (12%)	52,86,114	2.22	12 (23%)
33	LUT	r	615	-	42,43,43	0.39	0	51,60,60	0.36	0
30	CHL	g	609	1	70,74,74	1.33	7 (10%)	80,114,114	1.82	14 (17%)
31	CLA	11	614	1	53,57,73	1.38	7 (13%)	62,93,113	1.83	8 (12%)
31	CLA	R	609	21	69,73,73	1.23	7 (10%)	83,113,113	1.61	9 (10%)
31	CLA	c	510	8	69,73,73	1.23	7 (10%)	83,113,113	1.78	8 (9%)
31	CLA	b	614	7	69,73,73	1.24	8 (11%)	83,113,113	1.68	12 (14%)
31	CLA	b	603	7	69,73,73	1.24	8 (11%)	83,113,113	1.68	11 (13%)
32	LHG	r	619	-	46,46,48	1.40	8 (17%)	49,52,54	0.76	2 (4%)
31	CLA	y	613	28	69,73,73	1.22	7 (10%)	83,113,113	1.61	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LUT	11	617	-	42,43,43	0.43	1 (2%)	51,60,60	0.41	0
31	CLA	s	605	22	54,58,73	1.38	7 (12%)	65,95,113	1.73	9 (13%)
31	CLA	3	614	3	54,58,73	1.40	7 (12%)	65,95,113	1.76	9 (13%)
31	CLA	14	611	32	64,68,73	1.30	7 (10%)	77,107,113	1.69	11 (14%)
31	CLA	3	603	3	59,63,73	1.33	7 (11%)	71,101,113	1.80	8 (11%)
32	LHG	1	615	31	42,42,48	1.44	8 (19%)	45,48,54	0.76	2 (4%)
30	CHL	g	601	1	70,74,74	1.32	7 (10%)	80,114,114	1.77	15 (18%)
31	CLA	16	602	5	69,73,73	1.25	8 (11%)	83,113,113	1.70	12 (14%)
31	CLA	r	610	32	64,68,73	1.29	8 (12%)	77,107,113	1.74	10 (12%)
31	CLA	r	612	21	54,58,73	1.38	8 (14%)	65,95,113	1.78	11 (16%)
31	CLA	G	602	1	69,73,73	1.23	7 (10%)	83,113,113	1.58	12 (14%)
41	LMG	d	410	-	44,44,55	0.19	0	52,52,63	0.19	0
30	CHL	y	608	-	48,52,74	1.41	5 (10%)	53,87,114	2.05	10 (18%)
30	CHL	G	605	1	52,56,74	1.47	6 (11%)	58,92,114	2.03	12 (20%)
30	CHL	1	609	1	60,64,74	1.45	8 (13%)	68,102,114	1.88	14 (20%)
34	NEX	R	617	-	38,46,46	0.41	1 (2%)	50,70,70	0.46	0
31	CLA	6	614	3	54,58,73	1.40	7 (12%)	65,95,113	1.81	11 (16%)
30	CHL	Y	601	28	70,74,74	1.30	7 (10%)	80,114,114	1.86	12 (15%)
31	CLA	s	615	22	51,55,73	1.39	7 (13%)	61,91,113	1.87	8 (13%)
33	LUT	14	617	-	42,43,43	0.43	1 (2%)	51,60,60	0.39	0
34	NEX	G	618	-	38,45,46	0.75	2 (5%)	48,67,70	0.51	0
34	NEX	S	620	-	38,46,46	0.46	1 (2%)	50,70,70	0.49	0
39	BCR	B	617	-	41,41,41	0.14	0	56,56,56	0.25	0
30	CHL	n	606	-	65,69,74	1.37	7 (10%)	74,108,114	1.90	14 (18%)
31	CLA	12	611	2	49,53,73	1.45	8 (16%)	59,89,113	1.80	8 (13%)
31	CLA	G	610	1	69,73,73	1.23	6 (8%)	83,113,113	1.70	12 (14%)
31	CLA	R	604	-	52,56,73	1.39	8 (15%)	62,92,113	1.78	10 (16%)
31	CLA	g	602	1	69,73,73	1.24	8 (11%)	83,113,113	1.67	11 (13%)
33	LUT	12	614	-	42,43,43	0.38	0	51,60,60	0.46	0
33	LUT	g	616	-	42,43,43	0.38	0	51,60,60	0.39	0
31	CLA	c	507	8	69,73,73	1.24	8 (11%)	83,113,113	1.63	11 (13%)
33	LUT	N	618	-	42,43,43	0.39	1 (2%)	51,60,60	0.36	0
35	XAT	6	620	-	39,47,47	0.13	0	54,74,74	0.75	1 (1%)
30	CHL	G	608	-	56,60,74	1.47	7 (12%)	63,97,114	1.95	11 (17%)
31	CLA	B	616	7	64,68,73	1.27	8 (12%)	77,107,113	1.78	12 (15%)
33	LUT	y	622	-	42,43,43	0.39	0	51,60,60	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CHL	14	607	-	54,58,74	1.47	7 (12%)	59,94,114	1.91	13 (22%)
46	DGD	c	519	-	60,60,67	0.18	0	74,74,81	0.19	0
31	CLA	s	603	22	46,50,73	1.43	8 (17%)	55,85,113	1.92	8 (14%)
31	CLA	b	609	7	69,73,73	1.24	8 (11%)	83,113,113	1.67	11 (13%)
32	LHG	s	621	-	48,48,48	1.35	8 (16%)	51,54,54	0.78	2 (3%)
41	LMG	A	409	-	55,55,55	0.17	0	63,63,63	0.16	0
31	CLA	2	603	2	59,63,73	1.34	7 (11%)	71,101,113	1.86	8 (11%)
31	CLA	a	407	6	59,63,73	1.33	7 (11%)	71,101,113	1.72	9 (12%)
31	CLA	Y	602	28	69,73,73	1.24	8 (11%)	83,113,113	1.67	11 (13%)
31	CLA	g	613	1	69,73,73	1.23	8 (11%)	83,113,113	1.63	10 (12%)
31	CLA	c	508	-	69,73,73	1.23	8 (11%)	83,113,113	1.82	10 (12%)
30	CHL	11	609	1	60,64,74	1.45	7 (11%)	68,102,114	1.96	12 (17%)
31	CLA	c	506	8	69,73,73	1.23	7 (10%)	83,113,113	1.69	11 (13%)
31	CLA	s	611	32	69,73,73	1.25	8 (11%)	83,113,113	1.72	13 (15%)
32	LHG	r	618	31	37,37,48	1.42	7 (18%)	40,43,54	0.87	2 (5%)
34	NEX	13	619	-	38,46,46	0.42	1 (2%)	50,70,70	0.40	0
30	CHL	1	607	-	55,59,74	1.50	8 (14%)	62,96,114	2.01	13 (20%)
31	CLA	n	610	2	64,68,73	1.28	7 (10%)	77,107,113	1.73	12 (15%)
40	SQD	a	409	-	50,51,54	0.19	0	59,62,65	0.26	0
31	CLA	4	604	-	54,58,73	1.40	7 (12%)	65,95,113	1.88	8 (12%)

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
31	CLA	11	604	-	-	10/17/93/115	-
31	CLA	Y	610	28	-	9/39/115/115	-
31	CLA	A	406	6	-	9/27/103/115	-
33	LUT	1	616	-	-	0/29/67/67	0/2/2/2
43	LNL	A	412	-	-	0/17/17/17	-
31	CLA	S	604	-	-	20/39/115/115	-
34	NEX	1	618	-	-	0/6/37/83	0/2/2/3
30	CHL	15	607	-	-	12/22/98/117	-
31	CLA	G	613	1	-	16/39/115/115	-
39	BCR	J	101	-	-	6/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	SQD	d	412	-	-	12/49/69/69	0/1/1/1
40	SQD	D	413	-	-	8/41/61/69	0/1/1/1
34	NEX	Y	623	-	-	2/27/83/83	0/3/3/3
30	CHL	6	605	3	-	14/41/117/117	-
30	CHL	2	607	-	-	10/29/105/117	-
31	CLA	6	603	3	-	9/27/103/115	-
41	LMG	j	102	-	-	10/46/66/70	0/1/1/1
31	CLA	G	604	-	-	9/21/97/115	-
33	LUT	R	615	-	-	0/29/67/67	0/2/2/2
31	CLA	b	605	7	-	13/39/115/115	-
34	NEX	n	619	-	-	2/27/83/83	0/3/3/3
31	CLA	16	615	-	-	6/15/91/115	-
43	LNL	a	412	-	-	5/17/17/17	-
30	CHL	R	607	-	-	11/23/99/117	-
35	XAT	11	619	-	-	0/31/93/93	0/4/4/4
41	LMG	B	621	-	-	7/44/64/70	0/1/1/1
38	PHO	a	405	-	-	7/37/103/103	0/5/6/6
31	CLA	C	502	8	-	14/39/115/115	-
32	LHG	a	411	-	-	15/53/53/53	-
30	CHL	12	605	-	-	10/17/93/117	-
34	NEX	s	620	-	-	2/27/83/83	0/3/3/3
35	XAT	G	619	-	-	0/31/93/93	0/4/4/4
50	PAM	n	620	-	-	2/15/15/15	-
31	CLA	C	506	8	-	11/39/115/115	-
30	CHL	Y	609	28	-	18/41/117/117	-
31	CLA	B	612	7	-	16/39/115/115	-
31	CLA	B	602	7	-	10/39/115/115	-
31	CLA	Y	615	28	-	15/29/105/115	-
31	CLA	C	509	8	-	12/33/109/115	-
33	LUT	16	617	-	-	1/29/67/67	0/2/2/2
30	CHL	y	607	-	-	17/41/117/117	-
32	LHG	3	617	-	-	31/51/51/53	-
30	CHL	16	605	5	-	11/29/105/117	-
33	LUT	S	619	-	-	0/29/67/67	0/2/2/2
31	CLA	B	613	7	-	23/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	NEX	15	616	-	-	2/19/50/83	0/2/2/3
30	CHL	13	601	5	-	15/29/105/117	-
38	PHO	a	406	-	-	5/37/103/103	0/5/6/6
31	CLA	B	608	7	-	16/39/115/115	-
50	PAM	N	621	-	-	3/15/15/15	-
31	CLA	D	404	9	-	16/39/115/115	-
31	CLA	16	613	5	-	9/21/97/115	-
43	LNL	h	101	-	-	3/17/17/17	-
46	DGD	c	518	-	-	5/47/87/95	0/2/2/2
42	PL9	d	407	-	-	12/53/73/73	0/1/1/1
30	CHL	14	606	-	-	7/19/95/117	-
49	HEM	F	101	10,11	-	6/14/54/54	-
31	CLA	b	611	7	-	15/39/115/115	-
43	LNL	x	201	-	-	6/17/17/17	-
31	CLA	R	603	21	-	20/39/115/115	-
30	CHL	14	609	1	-	18/29/105/117	-
31	CLA	Y	611	32	-	10/39/115/115	-
43	LNL	X	201	-	-	5/17/17/17	-
34	NEX	11	618	-	-	0/6/37/83	0/2/2/3
30	CHL	N	608	-	-	12/22/98/117	-
39	BCR	C	515	-	-	2/29/63/63	0/2/2/2
30	CHL	13	609	5	-	16/35/111/117	-
31	CLA	s	609	22	-	10/27/103/115	-
49	HEM	f	101	10,11	-	6/14/54/54	-
30	CHL	6	606	-	-	12/29/105/117	-
46	DGD	C	517	-	-	17/55/95/95	0/2/2/2
39	BCR	H	103	-	-	2/29/63/63	0/2/2/2
30	CHL	5	605	2	-	10/17/93/117	-
30	CHL	11	608	-	-	13/23/99/117	-
31	CLA	15	610	-	-	4/15/91/115	-
31	CLA	15	612	2	-	10/21/97/115	-
31	CLA	B	615	7	-	11/39/115/115	-
32	LHG	Y	618	-	-	30/51/51/53	-
32	LHG	l	102	-	-	21/51/51/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	s	601	22	-	9/17/93/117	-
33	LUT	2	615	-	-	1/29/67/67	0/2/2/2
39	BCR	A	407	-	-	1/29/63/63	0/2/2/2
31	CLA	y	602	28	-	12/33/109/115	-
31	CLA	y	614	28	-	6/20/96/115	-
30	CHL	11	606	-	-	8/19/95/117	-
31	CLA	3	610	3	-	20/33/109/115	-
31	CLA	15	602	2	-	19/33/109/115	-
39	BCR	j	101	-	-	6/29/63/63	0/2/2/2
31	CLA	4	614	1	-	7/17/93/115	-
31	CLA	14	610	1	-	20/39/115/115	-
31	CLA	A	402	6	-	12/39/115/115	-
31	CLA	R	612	21	-	8/21/97/115	-
31	CLA	S	609	22	-	6/27/103/115	-
30	CHL	1	601	1	-	15/35/111/117	-
32	LHG	n	616	31	-	29/53/53/53	-
31	CLA	S	605	22	-	9/21/97/115	-
43	LNL	c	523	-	-	4/17/17/17	-
31	CLA	N	612	2	-	8/15/91/115	-
41	LMG	b	620	-	-	4/44/64/70	0/1/1/1
30	CHL	Y	607	-	-	18/41/117/117	-
31	CLA	S	614	22	-	13/39/115/115	-
30	CHL	N	601	2	-	13/26/102/117	-
31	CLA	16	610	5	-	11/39/115/115	-
31	CLA	A	404	-	-	18/39/115/115	-
33	LUT	6	618	-	-	0/29/67/67	0/2/2/2
31	CLA	6	604	-	-	21/39/115/115	-
41	LMG	D	414	-	-	12/43/63/70	0/1/1/1
31	CLA	1	612	1	-	7/17/93/115	-
42	PL9	D	407	-	-	12/53/73/73	0/1/1/1
36	3PH	B	620	-	-	10/49/49/49	-
43	LNL	c	524	-	-	4/17/17/17	-
31	CLA	s	604	-	-	18/39/115/115	-
31	CLA	r	614	-	-	13/27/103/115	-
30	CHL	3	609	3	-	14/41/117/117	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	r	603	21	-	15/39/115/115	-
31	CLA	c	505	-	-	12/27/103/115	-
31	CLA	R	613	21	-	12/33/109/115	-
31	CLA	c	513	8	-	8/27/103/115	-
32	LHG	R	618	31	-	14/42/42/53	-
31	CLA	a	404	-	-	18/39/115/115	-
31	CLA	r	601	21	-	10/20/96/115	-
31	CLA	1	602	1	-	14/33/109/115	-
41	LMG	B	622	-	-	6/43/63/70	0/1/1/1
31	CLA	y	612	28	-	18/39/115/115	-
31	CLA	13	615	5	-	4/15/91/115	-
34	NEX	3	621	-	-	2/27/83/83	0/3/3/3
31	CLA	r	613	21	-	12/39/115/115	-
34	NEX	r	617	-	-	3/27/83/83	0/3/3/3
31	CLA	D	405	9	-	16/39/115/115	-
30	CHL	y	606	-	-	17/41/117/117	-
31	CLA	1	610	1	-	8/27/103/115	-
33	LUT	4	616	-	-	0/29/67/67	0/2/2/2
31	CLA	S	611	32	-	15/39/115/115	-
30	CHL	15	606	-	-	8/23/99/117	-
36	3PH	T	101	-	-	10/49/49/49	-
31	CLA	y	615	28	-	18/29/105/115	-
31	CLA	R	602	21	-	15/39/115/115	-
31	CLA	16	604	-	-	8/27/103/115	-
31	CLA	11	603	1	-	9/27/103/115	-
30	CHL	5	608	-	-	9/22/98/117	-
30	CHL	11	601	1	-	15/41/117/117	-
31	CLA	y	610	28	-	9/39/115/115	-
31	CLA	r	602	21	-	12/39/115/115	-
41	LMG	d	415	-	-	12/43/63/70	0/1/1/1
31	CLA	3	613	3	-	13/27/103/115	-
31	CLA	G	603	1	-	14/27/103/115	-
31	CLA	g	610	1	-	9/39/115/115	-
46	DGD	w	502	-	-	8/35/55/95	0/1/1/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	C	504	8	-	11/39/115/115	-
30	CHL	3	608	-	-	9/22/98/117	-
33	LUT	14	616	-	-	0/29/67/67	0/2/2/2
31	CLA	b	610	-	-	17/39/115/115	-
30	CHL	3	601	3	-	14/35/111/117	-
30	CHL	r	606	21	-	20/41/117/117	-
30	CHL	5	609	2	-	14/41/117/117	-
31	CLA	C	505	-	-	8/27/103/115	-
43	LNL	C	524	-	-	4/17/17/17	-
42	PL9	a	410	-	-	9/53/73/73	0/1/1/1
31	CLA	3	612	3	-	17/39/115/115	-
39	BCR	B	619	-	-	1/29/63/63	0/2/2/2
32	LHG	6	616	31	-	16/48/48/53	-
43	LNL	I	101	-	-	4/17/17/17	-
39	BCR	b	618	-	-	0/29/63/63	0/2/2/2
33	LUT	5	614	-	-	4/29/67/67	0/2/2/2
32	LHG	D	409	-	-	11/43/43/53	-
31	CLA	6	613	3	-	11/27/103/115	-
33	LUT	Y	621	-	-	2/29/67/67	0/2/2/2
31	CLA	Y	612	28	-	16/39/115/115	-
30	CHL	y	609	28	-	18/41/117/117	-
31	CLA	3	602	3	-	13/33/109/115	-
31	CLA	12	602	2	-	16/33/109/115	-
32	LHG	d	413	-	-	17/53/53/53	-
31	CLA	c	509	8	-	12/33/109/115	-
31	CLA	Y	603	28	-	11/33/109/115	-
30	CHL	g	608	-	-	10/25/101/117	-
31	CLA	14	612	1	-	6/13/89/115	-
31	CLA	5	612	-	-	9/17/93/115	-
31	CLA	5	610	2	-	12/21/97/115	-
31	CLA	C	503	8	-	8/39/115/115	-
30	CHL	Y	606	-	-	18/41/117/117	-
31	CLA	15	613	2	-	7/15/91/115	-
31	CLA	B	604	7	-	11/39/115/115	-
31	CLA	g	612	1	-	3/13/89/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	12	608	2	-	14/26/102/117	-
30	CHL	S	608	-	-	10/21/97/117	-
32	LHG	y	617	-	-	26/51/51/53	-
31	CLA	11	610	1	-	10/27/103/115	-
32	LHG	c	521	-	-	19/46/46/53	-
34	NEX	N	619	-	-	2/27/83/83	0/3/3/3
33	LUT	15	614	-	-	5/29/67/67	0/2/2/2
31	CLA	c	504	8	-	11/39/115/115	-
30	CHL	13	605	5	-	12/29/105/117	-
30	CHL	g	606	-	-	6/22/98/117	-
31	CLA	y	611	32	-	10/39/115/115	-
32	LHG	16	616	31	-	26/44/44/53	-
31	CLA	4	602	1	-	13/33/109/115	-
30	CHL	n	608	-	-	15/22/98/117	-
31	CLA	Y	613	28	-	11/39/115/115	-
32	LHG	Y	617	-	-	25/51/51/53	-
41	LMG	v	101	-	-	11/46/66/70	0/1/1/1
31	CLA	N	611	32	-	10/33/109/115	-
43	LNL	y	619	-	-	5/17/17/17	-
30	CHL	3	606	-	-	10/29/105/117	-
31	CLA	C	511	8	-	14/39/115/115	-
30	CHL	n	605	2	-	16/35/111/117	-
31	CLA	G	611	32	-	11/39/115/115	-
31	CLA	A	403	-	-	17/39/115/115	-
34	NEX	12	616	-	-	2/19/50/83	0/2/2/3
31	CLA	r	611	21	-	8/20/96/115	-
31	CLA	6	612	3	-	12/27/103/115	-
39	BCR	b	617	-	-	2/29/63/63	0/2/2/2
33	LUT	11	616	-	-	1/29/67/67	0/2/2/2
30	CHL	2	609	2	-	24/41/117/117	-
43	LNL	Y	619	-	-	3/17/17/17	-
30	CHL	15	601	2	-	9/22/98/117	-
43	LNL	W	502	-	-	4/17/17/17	-
43	LNL	C	523	-	-	4/17/17/17	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	16	614	5	-	8/15/91/115	-
38	PHO	D	402	-	-	9/37/103/103	0/5/6/6
39	BCR	b	619	-	-	2/29/63/63	0/2/2/2
31	CLA	n	612	2	-	6/15/91/115	-
31	CLA	16	603	5	-	12/33/109/115	-
44	STE	b	622	-	-	9/17/17/17	-
41	LMG	d	411	-	-	4/36/36/70	-
43	LNL	R	620	-	-	6/17/17/17	-
30	CHL	n	601	2	-	13/25/101/117	-
31	CLA	15	604	-	-	7/27/103/115	-
31	CLA	C	510	8	-	13/39/115/115	-
31	CLA	R	610	32	-	18/33/109/115	-
34	NEX	5	616	-	-	2/25/56/83	0/2/2/3
41	LMG	b	621	-	-	7/41/61/70	0/1/1/1
30	CHL	N	607	-	-	17/41/117/117	-
30	CHL	12	606	-	-	6/23/99/117	-
39	BCR	C	516	-	-	4/29/63/63	0/2/2/2
32	LHG	A	413	-	-	12/48/48/53	-
31	CLA	R	608	21	-	9/39/115/115	-
31	CLA	n	611	32	-	10/33/109/115	-
30	CHL	6	601	3	-	15/35/111/117	-
31	CLA	C	508	-	-	18/39/115/115	-
33	LUT	13	617	-	-	2/29/67/67	0/2/2/2
30	CHL	16	601	5	-	14/29/105/117	-
30	CHL	r	607	-	-	7/23/99/117	-
30	CHL	g	605	1	-	9/20/96/117	-
30	CHL	4	609	1	-	25/41/117/117	-
32	LHG	y	616	31	-	18/53/53/53	-
33	LUT	1	617	-	-	0/29/67/67	0/2/2/2
43	LNL	H	101	-	-	3/17/17/17	-
31	CLA	g	603	1	-	15/27/103/115	-
31	CLA	15	611	2	-	6/15/91/115	-
34	NEX	2	616	-	-	2/25/56/83	0/2/2/3
43	LNL	w	503	-	-	4/17/17/17	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	15	605	-	-	10/17/93/117	-
31	CLA	13	612	5	-	2/15/91/115	-
30	CHL	16	606	-	-	17/35/111/117	-
32	LHG	D	412	-	-	21/53/53/53	-
31	CLA	r	609	21	-	17/39/115/115	-
30	CHL	G	606	-	-	4/19/95/117	-
31	CLA	a	403	6	-	12/39/115/115	-
39	BCR	a	408	-	-	1/29/63/63	0/2/2/2
31	CLA	G	612	1	-	3/13/89/115	-
31	CLA	11	611	32	-	8/21/97/115	-
41	LMG	C	522	-	-	4/50/70/70	0/1/1/1
30	CHL	12	601	2	-	9/22/98/117	-
31	CLA	B	607	-	-	10/39/115/115	-
30	CHL	G	607	-	-	9/22/98/117	-
32	LHG	R	619	-	-	13/51/51/53	-
30	CHL	R	605	21	-	11/29/105/117	-
30	CHL	13	606	-	-	15/35/111/117	-
31	CLA	2	613	2	-	7/18/94/115	-
33	LUT	g	617	-	-	0/29/67/67	0/2/2/2
30	CHL	2	601	2	-	6/19/95/117	-
31	CLA	4	612	1	-	7/17/93/115	-
31	CLA	y	604	-	-	10/27/103/115	-
33	LUT	G	616	-	-	2/29/67/67	0/2/2/2
30	CHL	3	607	-	-	20/41/117/117	-
30	CHL	S	607	-	-	6/14/90/117	-
31	CLA	12	613	2	-	7/15/91/115	-
31	CLA	C	512	8	-	19/39/115/115	-
31	CLA	y	603	28	-	13/33/109/115	-
31	CLA	B	614	7	-	20/39/115/115	-
31	CLA	B	603	7	-	13/39/115/115	-
30	CHL	G	601	1	-	14/41/117/117	-
31	CLA	b	612	7	-	18/39/115/115	-
39	BCR	h	102	-	-	2/29/63/63	0/2/2/2
30	CHL	N	605	2	-	14/35/111/117	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	N	614	2	-	5/15/91/115	-
31	CLA	14	613	1	-	13/27/103/115	-
40	SQD	l	101	-	-	9/45/65/69	0/1/1/1
31	CLA	B	601	-	-	12/27/103/115	-
30	CHL	n	607	-	-	20/41/117/117	-
31	CLA	N	615	2	-	5/18/94/115	-
31	CLA	r	604	-	-	6/19/95/115	-
32	LHG	s	617	31	-	21/49/49/53	-
31	CLA	1	613	1	-	9/27/103/115	-
32	LHG	S	621	-	-	22/53/53/53	-
36	3PH	b	623	-	-	5/40/40/49	-
31	CLA	2	602	2	-	16/27/103/115	-
31	CLA	c	512	8	-	18/39/115/115	-
33	LUT	s	619	-	-	0/29/67/67	0/2/2/2
31	CLA	R	611	21	-	7/20/96/115	-
31	CLA	13	611	32	-	12/39/115/115	-
33	LUT	S	618	-	-	1/29/67/67	0/2/2/2
31	CLA	b	615	7	-	12/39/115/115	-
41	LMG	D	410	-	-	6/39/59/70	0/1/1/1
31	CLA	5	603	2	-	9/27/103/115	-
32	LHG	Y	616	31	-	14/53/53/53	-
31	CLA	2	610	2	-	8/21/97/115	-
31	CLA	3	615	3	-	5/17/93/115	-
32	LHG	A	415	-	-	13/53/53/53	-
31	CLA	d	405	9	-	16/39/115/115	-
33	LUT	y	623	-	-	1/29/67/67	0/2/2/2
35	XAT	14	619	-	-	0/31/93/93	0/4/4/4
31	CLA	B	611	7	-	15/39/115/115	-
31	CLA	13	602	5	-	21/39/115/115	-
43	LNL	W	503	-	-	3/17/17/17	-
41	LMG	w	501	-	-	6/50/70/70	0/1/1/1
30	CHL	Y	605	28	-	13/29/105/117	-
31	CLA	S	602	22	-	14/39/115/115	-
30	CHL	2	606	-	-	10/17/93/117	-
31	CLA	12	609	2	-	16/27/103/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	2	612	-	-	6/17/93/115	-
33	LUT	N	617	-	-	0/29/67/67	0/2/2/2
32	LHG	g	615	31	-	23/53/53/53	-
30	CHL	14	601	1	-	20/41/117/117	-
31	CLA	Y	604	-	-	12/27/103/115	-
41	LMG	J	102	-	-	10/46/66/70	0/1/1/1
31	CLA	N	613	2	-	15/27/103/115	-
30	CHL	R	606	21	-	21/41/117/117	-
31	CLA	n	602	2	-	20/39/115/115	-
41	LMG	K	102	-	-	12/46/66/70	0/1/1/1
46	DGD	C	519	-	-	8/48/88/95	0/2/2/2
30	CHL	13	608	-	-	7/22/98/117	-
31	CLA	3	611	32	-	12/39/115/115	-
30	CHL	4	608	-	-	12/22/98/117	-
30	CHL	11	605	-	-	9/20/96/117	-
30	CHL	1	608	-	-	14/22/98/117	-
30	CHL	3	605	3	-	16/41/117/117	-
31	CLA	S	613	22	-	6/20/96/115	-
31	CLA	s	610	22	-	15/39/115/115	-
39	BCR	d	406	-	-	3/29/63/63	0/2/2/2
30	CHL	6	608	-	-	10/22/98/117	-
31	CLA	g	614	1	-	5/20/96/115	-
31	CLA	b	602	7	-	10/39/115/115	-
31	CLA	16	611	32	-	13/39/115/115	-
31	CLA	b	608	7	-	16/39/115/115	-
33	LUT	s	618	-	-	2/29/67/67	0/2/2/2
41	LMG	H	102	-	-	2/36/36/70	-
39	BCR	c	516	-	-	4/29/63/63	0/2/2/2
31	CLA	n	613	2	-	10/27/103/115	-
31	CLA	11	612	1	-	7/13/89/115	-
31	CLA	B	606	7	-	18/39/115/115	-
30	CHL	14	605	1	-	11/20/96/117	-
31	CLA	1	614	1	-	7/17/93/115	-
31	CLA	B	605	7	-	13/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	B	609	7	-	20/39/115/115	-
31	CLA	N	610	2	-	5/33/109/115	-
31	CLA	Y	614	28	-	5/20/96/115	-
31	CLA	b	601	-	-	10/27/103/115	-
31	CLA	S	612	22	-	6/15/91/115	-
30	CHL	S	601	22	-	9/17/93/117	-
32	LHG	L	102	-	-	22/51/51/53	-
40	SQD	L	101	-	-	13/45/65/69	0/1/1/1
43	LNL	y	621	-	-	3/17/17/17	-
46	DGD	C	518	-	-	5/47/87/95	0/2/2/2
31	CLA	12	604	-	-	9/27/103/115	-
31	CLA	N	602	2	-	18/39/115/115	-
31	CLA	b	613	7	-	20/39/115/115	-
30	CHL	1	606	-	-	10/19/95/117	-
41	LMG	C	520	-	-	9/42/62/70	0/1/1/1
31	CLA	g	611	32	-	13/39/115/115	-
30	CHL	S	606	22	-	21/41/117/117	-
30	CHL	12	607	-	-	13/22/98/117	-
31	CLA	13	613	5	-	8/21/97/115	-
32	LHG	r	621	-	-	20/48/48/53	-
33	LUT	12	615	-	-	1/29/67/67	0/2/2/2
30	CHL	16	608	-	-	7/22/98/117	-
30	CHL	11	607	-	-	12/17/93/117	-
30	CHL	N	606	-	-	16/35/111/117	-
34	NEX	g	618	-	-	2/27/83/83	0/3/3/3
41	LMG	S	616	-	-	4/37/57/70	0/1/1/1
46	DGD	c	517	-	-	17/55/95/95	0/2/2/2
31	CLA	b	607	-	-	17/39/115/115	-
30	CHL	N	609	2	-	22/41/117/117	-
43	LNL	i	101	-	-	4/17/17/17	-
32	LHG	a	413	-	-	13/48/48/53	-
31	CLA	1	611	32	-	8/21/97/115	-
31	CLA	5	604	-	-	11/21/97/115	-
34	NEX	16	619	-	-	2/27/83/83	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	NEX	6	621	-	-	2/27/83/83	0/3/3/3
30	CHL	4	601	1	-	15/35/111/117	-
31	CLA	s	614	22	-	17/39/115/115	-
30	CHL	16	609	5	-	15/35/111/117	-
31	CLA	n	604	-	-	15/27/103/115	-
32	LHG	d	409	-	-	16/43/43/53	-
30	CHL	16	607	-	-	19/35/111/117	-
31	CLA	S	610	22	-	17/39/115/115	-
31	CLA	R	601	21	-	8/20/96/115	-
31	CLA	6	611	32	-	13/39/115/115	-
39	BCR	C	526	-	-	1/29/63/63	0/2/2/2
35	XAT	r	616	-	-	0/31/93/93	0/4/4/4
30	CHL	G	609	1	-	12/41/117/117	-
31	CLA	5	611	-	-	6/17/93/115	-
31	CLA	s	613	22	-	6/20/96/115	-
40	SQD	D	411	-	-	11/49/69/69	0/1/1/1
33	LUT	3	618	-	-	0/29/67/67	0/2/2/2
30	CHL	s	608	-	-	7/21/97/117	-
31	CLA	c	511	8	-	15/39/115/115	-
33	LUT	2	614	-	-	0/29/67/67	0/2/2/2
31	CLA	c	514	8	-	16/39/115/115	-
30	CHL	Y	608	-	-	6/15/91/117	-
31	CLA	14	604	-	-	14/27/103/115	-
32	LHG	a	414	-	-	21/47/47/53	-
32	LHG	A	414	-	-	22/47/47/53	-
43	LNL	y	620	-	-	5/17/17/17	-
30	CHL	s	606	22	-	23/41/117/117	-
30	CHL	y	601	28	-	14/41/117/117	-
31	CLA	13	604	-	-	12/27/103/115	-
31	CLA	15	609	2	-	13/27/103/115	-
31	CLA	16	612	5	-	3/15/91/115	-
31	CLA	s	612	22	-	3/15/91/115	-
38	PHO	A	405	-	-	8/37/103/103	0/5/6/6
31	CLA	1	604	-	-	7/21/97/115	-
32	LHG	y	618	-	-	28/51/51/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LUT	5	615	-	-	2/29/67/67	0/2/2/2
44	STE	B	623	-	-	6/17/17/17	-
30	CHL	5	601	2	-	11/23/99/117	-
30	CHL	13	607	-	-	16/35/111/117	-
31	CLA	4	610	1	-	16/39/115/115	-
31	CLA	4	613	1	-	8/27/103/115	-
39	BCR	B	618	-	-	0/29/63/63	0/2/2/2
30	CHL	n	609	2	-	16/41/117/117	-
31	CLA	d	404	9	-	16/39/115/115	-
31	CLA	s	602	22	-	14/39/115/115	-
30	CHL	2	605	2	-	11/17/93/117	-
30	CHL	5	607	-	-	8/29/105/117	-
32	LHG	3	616	31	-	12/48/48/53	-
31	CLA	C	507	8	-	21/39/115/115	-
33	LUT	4	617	-	-	0/29/67/67	0/2/2/2
42	PL9	A	410	-	-	9/53/73/73	0/1/1/1
32	LHG	D	408	-	-	16/53/53/53	-
31	CLA	12	612	2	-	12/21/97/115	-
33	LUT	Y	622	-	-	1/29/67/67	0/2/2/2
31	CLA	14	614	1	-	9/20/96/115	-
36	3PH	B	624	-	-	6/39/39/49	-
41	LMG	s	616	-	-	10/37/57/70	0/1/1/1
32	LHG	S	617	31	-	24/49/49/53	-
31	CLA	14	603	1	-	11/27/103/115	-
31	CLA	r	608	21	-	7/39/115/115	-
33	LUT	n	617	-	-	0/29/67/67	0/2/2/2
32	LHG	11	615	31	-	18/53/53/53	-
31	CLA	C	513	8	-	8/27/103/115	-
30	CHL	4	606	-	-	7/19/95/117	-
32	LHG	a	401	-	-	12/53/53/53	-
31	CLA	g	604	-	-	10/21/97/115	-
40	SQD	A	408	-	-	7/46/66/69	0/1/1/1
31	CLA	b	604	7	-	14/39/115/115	-
32	LHG	R	621	-	-	16/48/48/53	-
31	CLA	b	606	7	-	16/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LHG	4	615	31	-	13/51/51/53	-
36	3PH	8	201	-	-	6/49/49/49	-
30	CHL	4	605	1	-	6/17/93/117	-
32	LHG	N	616	31	-	23/53/53/53	-
31	CLA	3	604	-	-	20/39/115/115	-
35	XAT	g	619	-	-	0/31/93/93	0/4/4/4
31	CLA	d	402	-	-	17/39/115/115	-
31	CLA	11	602	1	-	14/33/109/115	-
31	CLA	12	603	2	-	11/27/103/115	-
31	CLA	B	610	-	-	17/39/115/115	-
31	CLA	c	503	8	-	11/39/115/115	-
31	CLA	c	502	8	-	16/39/115/115	-
31	CLA	11	613	1	-	13/27/103/115	-
31	CLA	15	603	2	-	8/27/103/115	-
30	CHL	r	605	21	-	15/29/105/117	-
31	CLA	13	614	5	-	8/15/91/115	-
34	NEX	y	624	-	-	4/27/83/83	0/3/3/3
30	CHL	6	607	-	-	20/41/117/117	-
39	BCR	D	406	-	-	3/29/63/63	0/2/2/2
31	CLA	14	602	1	-	12/33/109/115	-
30	CHL	5	606	-	-	11/17/93/117	-
31	CLA	4	603	1	-	5/27/103/115	-
33	LUT	16	618	-	-	0/29/67/67	0/2/2/2
43	LNL	r	620	-	-	8/17/17/17	-
31	CLA	N	604	-	-	15/27/103/115	-
33	LUT	15	615	-	-	1/29/67/67	0/2/2/2
35	XAT	R	616	-	-	0/31/93/93	0/4/4/4
41	LMG	c	520	-	-	9/42/62/70	0/1/1/1
39	BCR	c	526	-	-	2/29/63/63	0/2/2/2
31	CLA	N	603	2	-	11/33/109/115	-
30	CHL	y	605	28	-	8/29/105/117	-
31	CLA	12	610	-	-	5/15/91/115	-
31	CLA	4	611	32	-	6/21/97/115	-
35	XAT	3	620	-	-	0/31/93/93	0/4/4/4
34	NEX	14	618	-	-	0/6/37/83	0/2/2/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LHG	d	408	-	-	19/53/53/53	-
32	LHG	13	616	31	-	25/44/44/53	-
33	LUT	13	618	-	-	0/29/67/67	0/2/2/2
30	CHL	1	605	1	-	7/17/93/117	-
30	CHL	6	609	3	-	15/41/117/117	-
31	CLA	2	604	-	-	10/21/97/115	-
31	CLA	n	614	2	-	9/15/91/115	-
33	LUT	G	617	-	-	0/29/67/67	0/2/2/2
36	3PH	7	201	-	-	5/49/49/49	-
32	LHG	A	411	-	-	20/53/53/53	-
30	CHL	14	608	-	-	16/23/99/117	-
31	CLA	C	514	8	-	16/39/115/115	-
39	BCR	c	515	-	-	2/29/63/63	0/2/2/2
31	CLA	5	613	2	-	8/21/97/115	-
31	CLA	13	610	5	-	11/39/115/115	-
33	LUT	3	619	-	-	0/29/67/67	0/2/2/2
31	CLA	2	611	-	-	10/17/93/115	-
32	LHG	G	615	31	-	21/53/53/53	-
33	LUT	n	618	-	-	0/29/67/67	0/2/2/2
31	CLA	S	615	22	-	7/18/94/115	-
43	LNL	Y	620	-	-	5/17/17/17	-
31	CLA	6	610	3	-	15/33/109/115	-
41	LMG	c	522	-	-	4/50/70/70	0/1/1/1
31	CLA	5	602	2	-	16/27/103/115	-
32	LHG	6	617	-	-	27/51/51/53	-
31	CLA	R	614	-	-	10/27/103/115	-
46	DGD	W	501	-	-	9/41/61/95	0/1/1/2
30	CHL	4	607	-	-	10/23/99/117	-
31	CLA	n	615	2	-	5/18/94/115	-
31	CLA	13	603	5	-	13/33/109/115	-
32	LHG	14	615	31	-	25/53/53/53	-
33	LUT	6	619	-	-	0/29/67/67	0/2/2/2
31	CLA	1	603	1	-	3/18/94/115	-
31	CLA	G	614	1	-	5/20/96/115	-
31	CLA	6	602	3	-	11/33/109/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LHG	C	521	-	-	18/46/46/53	-
30	CHL	15	608	2	-	12/35/111/117	-
31	CLA	S	603	22	-	8/12/88/115	-
34	NEX	4	618	-	-	0/6/37/83	0/2/2/3
31	CLA	b	616	7	-	16/33/109/115	-
30	CHL	2	608	-	-	7/22/98/117	-
31	CLA	6	615	3	-	11/21/97/115	-
40	SQD	d	414	-	-	7/41/61/69	0/1/1/1
30	CHL	g	607	-	-	10/22/98/117	-
31	CLA	n	603	2	-	14/33/109/115	-
30	CHL	s	607	-	-	9/14/90/117	-
33	LUT	r	615	-	-	0/29/67/67	0/2/2/2
30	CHL	g	609	1	-	14/41/117/117	-
31	CLA	11	614	1	-	11/20/96/115	-
31	CLA	R	609	21	-	18/39/115/115	-
31	CLA	c	510	8	-	13/39/115/115	-
31	CLA	b	614	7	-	19/39/115/115	-
31	CLA	b	603	7	-	14/39/115/115	-
32	LHG	r	619	-	-	19/51/51/53	-
31	CLA	y	613	28	-	13/39/115/115	-
33	LUT	11	617	-	-	0/29/67/67	0/2/2/2
31	CLA	s	605	22	-	7/21/97/115	-
31	CLA	3	614	3	-	9/21/97/115	-
31	CLA	14	611	32	-	13/33/109/115	-
31	CLA	3	603	3	-	10/27/103/115	-
32	LHG	1	615	31	-	14/47/47/53	-
30	CHL	g	601	1	-	17/41/117/117	-
31	CLA	16	602	5	-	15/39/115/115	-
31	CLA	r	610	32	-	9/33/109/115	-
31	CLA	r	612	21	-	7/21/97/115	-
31	CLA	G	602	1	-	15/39/115/115	-
41	LMG	d	410	-	-	8/39/59/70	0/1/1/1
30	CHL	y	608	-	-	7/15/91/117	-
30	CHL	G	605	1	-	9/20/96/117	-
30	CHL	1	609	1	-	15/29/105/117	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	NEX	R	617	-	-	3/27/83/83	0/3/3/3
31	CLA	6	614	3	-	11/21/97/115	-
30	CHL	Y	601	28	-	14/41/117/117	-
31	CLA	s	615	22	-	8/18/94/115	-
33	LUT	14	617	-	-	0/29/67/67	0/2/2/2
34	NEX	G	618	-	-	2/27/79/83	0/3/3/3
34	NEX	S	620	-	-	2/27/83/83	0/3/3/3
39	BCR	B	617	-	-	2/29/63/63	0/2/2/2
30	CHL	n	606	-	-	17/35/111/117	-
31	CLA	12	611	2	-	6/15/91/115	-
31	CLA	G	610	1	-	7/39/115/115	-
31	CLA	R	604	-	-	6/19/95/115	-
31	CLA	g	602	1	-	15/39/115/115	-
33	LUT	12	614	-	-	5/29/67/67	0/2/2/2
33	LUT	g	616	-	-	2/29/67/67	0/2/2/2
31	CLA	c	507	8	-	22/39/115/115	-
33	LUT	N	618	-	-	0/29/67/67	0/2/2/2
35	XAT	6	620	-	-	0/31/93/93	0/4/4/4
30	CHL	G	608	-	-	12/25/101/117	-
31	CLA	B	616	7	-	16/33/109/115	-
33	LUT	y	622	-	-	2/29/67/67	0/2/2/2
30	CHL	14	607	-	-	9/22/98/117	-
46	DGD	c	519	-	-	8/48/88/95	0/2/2/2
31	CLA	s	603	22	-	7/12/88/115	-
31	CLA	b	609	7	-	21/39/115/115	-
32	LHG	s	621	-	-	18/53/53/53	-
41	LMG	A	409	-	-	6/50/70/70	0/1/1/1
31	CLA	2	603	2	-	10/27/103/115	-
31	CLA	a	407	6	-	10/27/103/115	-
31	CLA	Y	602	28	-	14/39/115/115	-
31	CLA	g	613	1	-	12/39/115/115	-
31	CLA	c	508	-	-	18/39/115/115	-
30	CHL	11	609	1	-	22/29/105/117	-
31	CLA	c	506	8	-	11/39/115/115	-
31	CLA	s	611	32	-	17/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LHG	r	618	31	-	17/42/42/53	-
34	NEX	13	619	-	-	2/27/83/83	0/3/3/3
30	CHL	1	607	-	-	9/23/99/117	-
31	CLA	n	610	2	-	13/33/109/115	-
40	SQD	a	409	-	-	7/46/66/69	0/1/1/1
31	CLA	4	604	-	-	11/21/97/115	-

The worst 5 of 3223 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	a	406	PHO	C1D-C2D	5.77	1.46	1.39
38	A	405	PHO	C1D-C2D	5.67	1.45	1.39
38	D	402	PHO	C1D-C2D	5.66	1.45	1.39
38	a	405	PHO	C1D-C2D	5.65	1.45	1.39
31	4	610	CLA	MG-NA	5.50	2.19	2.06

The worst 5 of 4364 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	15	605	CHL	C4A-NA-C1A	11.53	111.89	106.71
31	c	510	CLA	C4A-NA-C1A	11.50	111.88	106.71
31	C	510	CLA	C4A-NA-C1A	11.47	111.86	106.71
31	B	613	CLA	C4A-NA-C1A	11.42	111.84	106.71
31	b	613	CLA	C4A-NA-C1A	11.38	111.82	106.71

There are no chirality outliers.

5 of 6244 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	1	601	CHL	C3C-C2C-CMC-OMC
30	1	605	CHL	CHA-CBD-CGD-O1D
30	1	606	CHL	C2B-C3B-CAB-CBB
30	1	606	CHL	C4B-C3B-CAB-CBB
30	1	606	CHL	C1C-C2C-CMC-OMC

There are no ring outliers.

521 monomers are involved in 1093 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	11	604	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	Y	610	CLA	2	0
31	A	406	CLA	1	0
33	1	616	LUT	4	0
31	S	604	CLA	4	0
30	15	607	CHL	2	0
31	G	613	CLA	1	0
39	J	101	BCR	3	0
40	d	412	SQD	3	0
34	Y	623	NEX	1	0
30	6	605	CHL	5	0
31	6	603	CLA	1	0
41	j	102	LMG	5	0
31	G	604	CLA	2	0
33	R	615	LUT	1	0
31	b	605	CLA	4	0
34	n	619	NEX	1	0
31	16	615	CLA	4	0
30	R	607	CHL	2	0
35	11	619	XAT	1	0
41	B	621	LMG	2	0
31	C	502	CLA	3	0
32	a	411	LHG	1	0
30	12	605	CHL	4	0
34	s	620	NEX	1	0
35	G	619	XAT	1	0
50	n	620	PAM	1	0
31	C	506	CLA	3	0
30	Y	609	CHL	1	0
31	B	612	CLA	4	0
31	B	602	CLA	3	0
31	Y	615	CLA	2	0
31	C	509	CLA	2	0
33	16	617	LUT	2	0
30	y	607	CHL	4	0
32	3	617	LHG	2	0
30	16	605	CHL	3	0
33	S	619	LUT	4	0
31	B	613	CLA	3	0
34	15	616	NEX	3	0
30	13	601	CHL	2	0
38	a	406	PHO	1	0
31	B	608	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	N	621	PAM	1	0
31	D	404	CLA	4	0
31	16	613	CLA	3	0
43	h	101	LNL	2	0
46	c	518	DGD	5	0
42	d	407	PL9	2	0
30	14	606	CHL	1	0
49	F	101	HEM	2	0
31	b	611	CLA	3	0
43	x	201	LNL	1	0
31	R	603	CLA	6	0
30	14	609	CHL	2	0
31	Y	611	CLA	4	0
43	X	201	LNL	1	0
30	N	608	CHL	4	0
39	C	515	BCR	2	0
30	13	609	CHL	4	0
31	s	609	CLA	2	0
49	f	101	HEM	2	0
30	6	606	CHL	1	0
46	C	517	DGD	2	0
39	H	103	BCR	3	0
30	5	605	CHL	2	0
30	11	608	CHL	3	0
31	15	612	CLA	8	0
31	B	615	CLA	3	0
32	Y	618	LHG	4	0
32	l	102	LHG	4	0
33	2	615	LUT	4	0
39	A	407	BCR	2	0
31	y	602	CLA	2	0
31	y	614	CLA	2	0
30	11	606	CHL	1	0
31	3	610	CLA	2	0
31	15	602	CLA	6	0
39	j	101	BCR	3	0
31	14	610	CLA	5	0
31	A	402	CLA	4	0
31	R	612	CLA	1	0
31	S	609	CLA	1	0
30	1	601	CHL	3	0
32	n	616	LHG	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	c	523	LNL	1	0
41	b	620	LMG	1	0
30	Y	607	CHL	4	0
31	S	614	CLA	2	0
30	N	601	CHL	1	0
31	16	610	CLA	3	0
31	A	404	CLA	1	0
33	6	618	LUT	3	0
31	6	604	CLA	1	0
41	D	414	LMG	1	0
31	1	612	CLA	1	0
42	D	407	PL9	2	0
36	B	620	3PH	5	0
31	s	604	CLA	9	0
31	r	614	CLA	3	0
30	3	609	CHL	1	0
31	r	603	CLA	3	0
31	c	505	CLA	2	0
31	R	613	CLA	3	0
31	c	513	CLA	2	0
32	R	618	LHG	2	0
31	r	601	CLA	2	0
31	1	602	CLA	2	0
41	B	622	LMG	1	0
31	y	612	CLA	5	0
31	13	615	CLA	1	0
34	3	621	NEX	3	0
31	r	613	CLA	2	0
34	r	617	NEX	1	0
31	D	405	CLA	2	0
31	1	610	CLA	8	0
33	4	616	LUT	5	0
31	S	611	CLA	3	0
30	15	606	CHL	1	0
36	T	101	3PH	4	0
31	y	615	CLA	2	0
31	R	602	CLA	5	0
31	16	604	CLA	1	0
31	11	603	CLA	4	0
30	5	608	CHL	3	0
30	11	601	CHL	1	0
31	y	610	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	r	602	CLA	5	0
41	d	415	LMG	1	0
31	3	613	CLA	1	0
31	g	610	CLA	2	0
46	w	502	DGD	2	0
31	C	504	CLA	4	0
30	3	608	CHL	1	0
33	14	616	LUT	4	0
31	b	610	CLA	6	0
30	3	601	CHL	1	0
30	r	606	CHL	3	0
30	5	609	CHL	2	0
31	C	505	CLA	3	0
42	a	410	PL9	4	0
31	3	612	CLA	3	0
39	B	619	BCR	1	0
32	6	616	LHG	2	0
39	b	618	BCR	1	0
33	5	614	LUT	2	0
32	D	409	LHG	2	0
31	6	613	CLA	3	0
33	Y	621	LUT	3	0
31	Y	612	CLA	4	0
30	y	609	CHL	1	0
31	3	602	CLA	2	0
31	12	602	CLA	7	0
32	d	413	LHG	1	0
31	c	509	CLA	2	0
31	Y	603	CLA	1	0
30	g	608	CHL	4	0
31	14	612	CLA	3	0
31	5	610	CLA	3	0
31	C	503	CLA	1	0
30	Y	606	CHL	4	0
31	15	613	CLA	4	0
31	B	604	CLA	3	0
30	12	608	CHL	1	0
30	S	608	CHL	4	0
31	11	610	CLA	3	0
32	c	521	LHG	3	0
34	N	619	NEX	1	0
33	15	614	LUT	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	c	504	CLA	3	0
30	13	605	CHL	2	0
30	g	606	CHL	2	0
31	y	611	CLA	4	0
32	16	616	LHG	3	0
31	4	602	CLA	1	0
30	n	608	CHL	2	0
31	Y	613	CLA	3	0
41	v	101	LMG	1	0
31	N	611	CLA	1	0
43	y	619	LNL	3	0
30	3	606	CHL	2	0
31	C	511	CLA	2	0
30	n	605	CHL	3	0
31	G	611	CLA	1	0
31	A	403	CLA	3	0
34	12	616	NEX	2	0
31	r	611	CLA	2	0
39	b	617	BCR	3	0
33	11	616	LUT	5	0
30	2	609	CHL	7	0
43	Y	619	LNL	1	0
43	W	502	LNL	1	0
43	C	523	LNL	1	0
31	16	614	CLA	2	0
38	D	402	PHO	4	0
39	b	619	BCR	1	0
31	n	612	CLA	2	0
31	16	603	CLA	5	0
41	d	411	LMG	2	0
30	n	601	CHL	2	0
31	15	604	CLA	7	0
31	C	510	CLA	1	0
31	R	610	CLA	2	0
41	b	621	LMG	1	0
30	N	607	CHL	8	0
30	12	606	CHL	1	0
32	A	413	LHG	2	0
31	R	608	CLA	2	0
31	n	611	CLA	3	0
33	13	617	LUT	2	0
30	16	601	CHL	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	r	607	CHL	1	0
30	g	605	CHL	1	0
30	4	609	CHL	4	0
32	y	616	LHG	5	0
33	l	617	LUT	2	0
43	H	101	LNL	4	0
31	g	603	CLA	2	0
31	15	611	CLA	4	0
43	w	503	LNL	1	0
30	15	605	CHL	3	0
30	16	606	CHL	1	0
31	r	609	CLA	4	0
30	G	606	CHL	1	0
31	a	403	CLA	5	0
39	a	408	BCR	1	0
31	11	611	CLA	1	0
41	C	522	LMG	1	0
31	B	607	CLA	1	0
30	G	607	CHL	2	0
32	R	619	LHG	4	0
30	R	605	CHL	3	0
30	13	606	CHL	2	0
31	2	613	CLA	4	0
33	g	617	LUT	1	0
31	4	612	CLA	1	0
33	G	616	LUT	3	0
30	3	607	CHL	3	0
30	S	607	CHL	1	0
31	C	512	CLA	4	0
31	y	603	CLA	1	0
31	B	614	CLA	2	0
31	B	603	CLA	1	0
30	G	601	CHL	1	0
31	b	612	CLA	4	0
39	h	102	BCR	4	0
30	N	605	CHL	2	0
31	14	613	CLA	3	0
40	l	101	SQD	2	0
31	B	601	CLA	2	0
30	n	607	CHL	8	0
31	N	615	CLA	1	0
32	s	617	LHG	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	1	613	CLA	1	0
32	S	621	LHG	3	0
36	b	623	3PH	1	0
31	2	602	CLA	2	0
31	c	512	CLA	3	0
33	s	619	LUT	3	0
31	13	611	CLA	1	0
33	S	618	LUT	4	0
31	b	615	CLA	4	0
41	D	410	LMG	1	0
31	5	603	CLA	2	0
32	Y	616	LHG	5	0
31	2	610	CLA	2	0
32	A	415	LHG	2	0
31	d	405	CLA	2	0
33	y	623	LUT	2	0
35	14	619	XAT	1	0
31	B	611	CLA	1	0
31	13	602	CLA	5	0
43	W	503	LNL	1	0
41	w	501	LMG	3	0
30	Y	605	CHL	1	0
31	S	602	CLA	1	0
31	12	609	CLA	13	0
31	2	612	CLA	1	0
33	N	617	LUT	5	0
32	g	615	LHG	5	0
30	14	601	CHL	3	0
41	J	102	LMG	5	0
31	N	613	CLA	2	0
30	R	606	CHL	7	0
31	n	602	CLA	4	0
41	K	102	LMG	3	0
46	C	519	DGD	3	0
30	13	608	CHL	2	0
30	4	608	CHL	5	0
30	11	605	CHL	1	0
30	1	608	CHL	4	0
30	3	605	CHL	4	0
31	S	613	CLA	1	0
31	s	610	CLA	3	0
39	d	406	BCR	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	6	608	CHL	4	0
31	b	602	CLA	4	0
31	16	611	CLA	2	0
31	b	608	CLA	1	0
33	s	618	LUT	7	0
31	n	613	CLA	4	0
31	11	612	CLA	3	0
31	B	606	CLA	3	0
31	B	605	CLA	2	0
31	B	609	CLA	2	0
31	N	610	CLA	3	0
31	Y	614	CLA	2	0
31	b	601	CLA	2	0
31	S	612	CLA	2	0
32	L	102	LHG	4	0
40	L	101	SQD	3	0
43	y	621	LNL	1	0
46	C	518	DGD	6	0
31	12	604	CLA	5	0
31	N	602	CLA	2	0
31	b	613	CLA	3	0
30	1	606	CHL	2	0
41	C	520	LMG	1	0
30	S	606	CHL	4	0
30	12	607	CHL	2	0
31	13	613	CLA	2	0
32	r	621	LHG	4	0
33	12	615	LUT	2	0
30	16	608	CHL	2	0
30	11	607	CHL	1	0
30	N	606	CHL	3	0
41	S	616	LMG	3	0
46	c	517	DGD	2	0
31	b	607	CLA	3	0
30	N	609	CHL	1	0
32	a	413	LHG	2	0
31	1	611	CLA	1	0
31	5	604	CLA	2	0
34	6	621	NEX	4	0
30	4	601	CHL	4	0
31	s	614	CLA	1	0
30	16	609	CHL	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	n	604	CLA	2	0
32	d	409	LHG	1	0
30	16	607	CHL	2	0
31	S	610	CLA	4	0
31	R	601	CLA	1	0
31	6	611	CLA	1	0
39	C	526	BCR	3	0
35	r	616	XAT	1	0
30	G	609	CHL	2	0
31	5	611	CLA	2	0
31	s	613	CLA	1	0
40	D	411	SQD	2	0
33	3	618	LUT	2	0
30	s	608	CHL	5	0
31	c	511	CLA	1	0
33	2	614	LUT	5	0
31	c	514	CLA	3	0
31	14	604	CLA	1	0
32	a	414	LHG	3	0
32	A	414	LHG	5	0
30	s	606	CHL	7	0
30	y	601	CHL	3	0
31	13	604	CLA	1	0
31	s	612	CLA	2	0
31	1	604	CLA	3	0
32	y	618	LHG	2	0
33	5	615	LUT	1	0
44	B	623	STE	1	0
30	13	607	CHL	3	0
31	4	610	CLA	3	0
31	4	613	CLA	2	0
39	B	618	BCR	3	0
30	n	609	CHL	1	0
31	d	404	CLA	3	0
31	s	602	CLA	2	0
30	2	605	CHL	1	0
30	5	607	CHL	1	0
32	3	616	LHG	1	0
31	C	507	CLA	1	0
33	4	617	LUT	2	0
42	A	410	PL9	2	0
32	D	408	LHG	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	12	612	CLA	27	0
33	Y	622	LUT	1	0
36	B	624	3PH	2	0
41	s	616	LMG	2	0
32	S	617	LHG	4	0
31	14	603	CLA	6	0
31	r	608	CLA	3	0
33	n	617	LUT	7	0
32	11	615	LHG	3	0
31	C	513	CLA	1	0
30	4	606	CHL	4	0
32	a	401	LHG	2	0
31	g	604	CLA	2	0
31	b	604	CLA	4	0
32	R	621	LHG	3	0
31	b	606	CLA	1	0
32	4	615	LHG	2	0
36	8	201	3PH	2	0
30	4	605	CHL	1	0
32	N	616	LHG	2	0
31	3	604	CLA	1	0
35	g	619	XAT	2	0
31	d	402	CLA	5	0
31	11	602	CLA	5	0
31	12	603	CLA	3	0
31	B	610	CLA	4	0
31	c	503	CLA	2	0
31	c	502	CLA	4	0
31	11	613	CLA	3	0
31	15	603	CLA	12	0
30	r	605	CHL	2	0
31	13	614	CLA	4	0
30	6	607	CHL	5	0
39	D	406	BCR	2	0
31	14	602	CLA	7	0
31	4	603	CLA	1	0
33	16	618	LUT	4	0
31	N	604	CLA	3	0
33	15	615	LUT	4	0
35	R	616	XAT	2	0
41	c	520	LMG	1	0
39	c	526	BCR	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	y	605	CHL	2	0
35	3	620	XAT	3	0
32	d	408	LHG	3	0
32	13	616	LHG	3	0
33	13	618	LUT	1	0
30	1	605	CHL	1	0
30	6	609	CHL	1	0
31	2	604	CLA	3	0
31	n	614	CLA	1	0
36	7	201	3PH	1	0
32	A	411	LHG	2	0
30	14	608	CHL	1	0
31	C	514	CLA	2	0
39	c	515	BCR	1	0
31	5	613	CLA	3	0
31	13	610	CLA	3	0
33	3	619	LUT	1	0
32	G	615	LHG	2	0
33	n	618	LUT	1	0
31	S	615	CLA	1	0
43	Y	620	LNL	1	0
31	6	610	CLA	4	0
41	c	522	LMG	1	0
31	5	602	CLA	2	0
32	6	617	LHG	3	0
31	R	614	CLA	2	0
46	W	501	DGD	4	0
30	4	607	CHL	2	0
31	n	615	CLA	2	0
31	13	603	CLA	8	0
32	14	615	LHG	3	0
33	6	619	LUT	1	0
31	1	603	CLA	2	0
32	C	521	LHG	4	0
30	15	608	CHL	10	0
31	S	603	CLA	2	0
31	b	616	CLA	3	0
30	2	608	CHL	5	0
31	6	615	CLA	3	0
40	d	414	SQD	4	0
30	g	607	CHL	2	0
31	n	603	CLA	1	0

Continued on next page...

Continued from previous page...

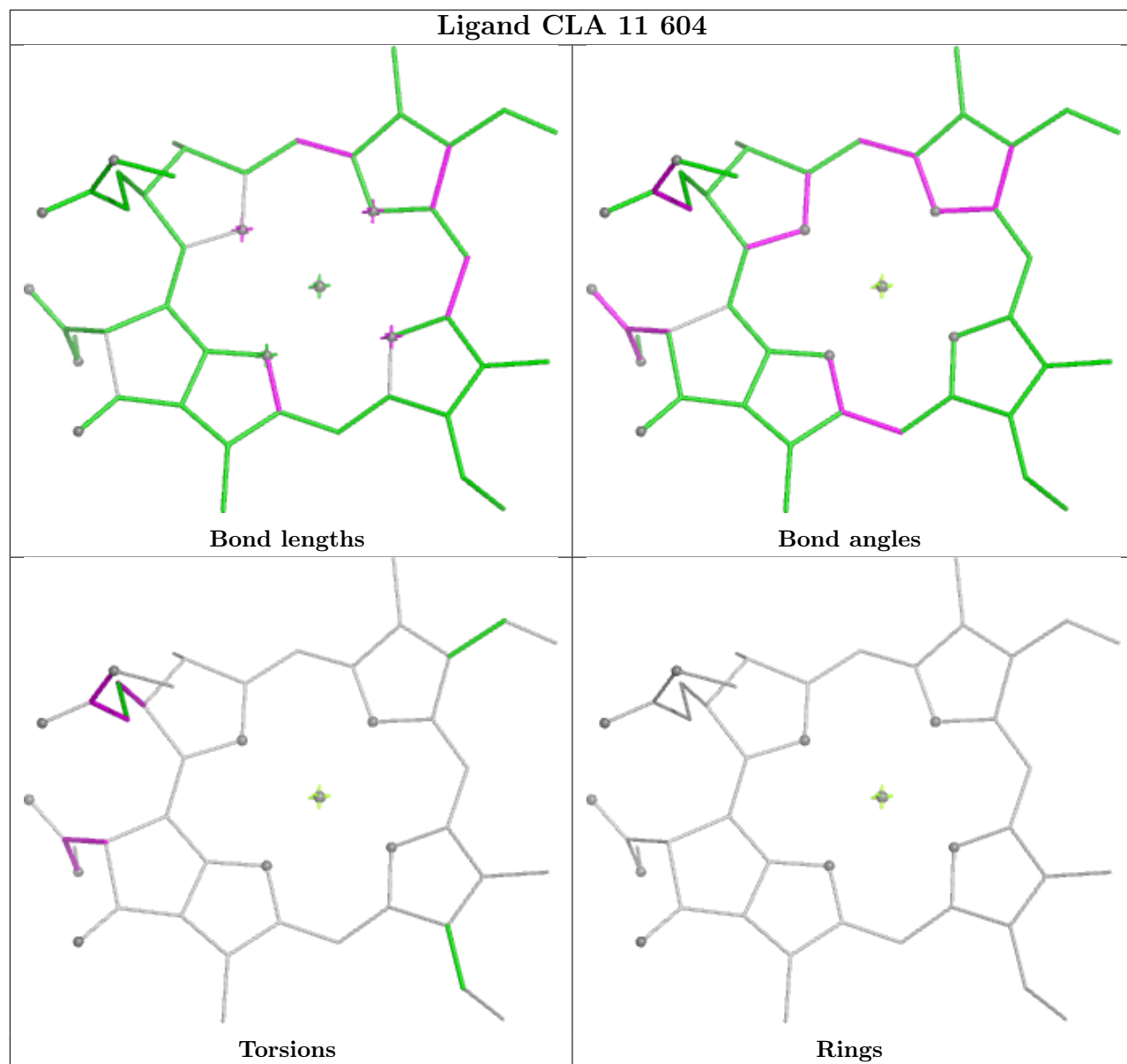
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	s	607	CHL	1	0
33	r	615	LUT	4	0
30	g	609	CHL	3	0
31	R	609	CLA	1	0
31	c	510	CLA	1	0
31	b	614	CLA	2	0
32	r	619	LHG	4	0
31	y	613	CLA	5	0
33	11	617	LUT	2	0
31	3	614	CLA	3	0
31	14	611	CLA	3	0
32	1	615	LHG	1	0
30	g	601	CHL	1	0
31	16	602	CLA	3	0
31	r	610	CLA	4	0
31	r	612	CLA	1	0
31	G	602	CLA	2	0
41	d	410	LMG	1	0
30	G	605	CHL	1	0
30	1	609	CHL	2	0
34	R	617	NEX	1	0
31	6	614	CLA	1	0
30	Y	601	CHL	1	0
31	s	615	CLA	2	0
33	14	617	LUT	1	0
34	G	618	NEX	1	0
34	S	620	NEX	1	0
39	B	617	BCR	3	0
30	n	606	CHL	2	0
31	12	611	CLA	5	0
31	G	610	CLA	4	0
31	R	604	CLA	1	0
31	g	602	CLA	1	0
33	12	614	LUT	33	0
33	g	616	LUT	3	0
31	c	507	CLA	3	0
33	N	618	LUT	1	0
35	6	620	XAT	4	0
30	G	608	CHL	4	0
31	B	616	CLA	2	0
33	y	622	LUT	4	0
30	14	607	CHL	1	0

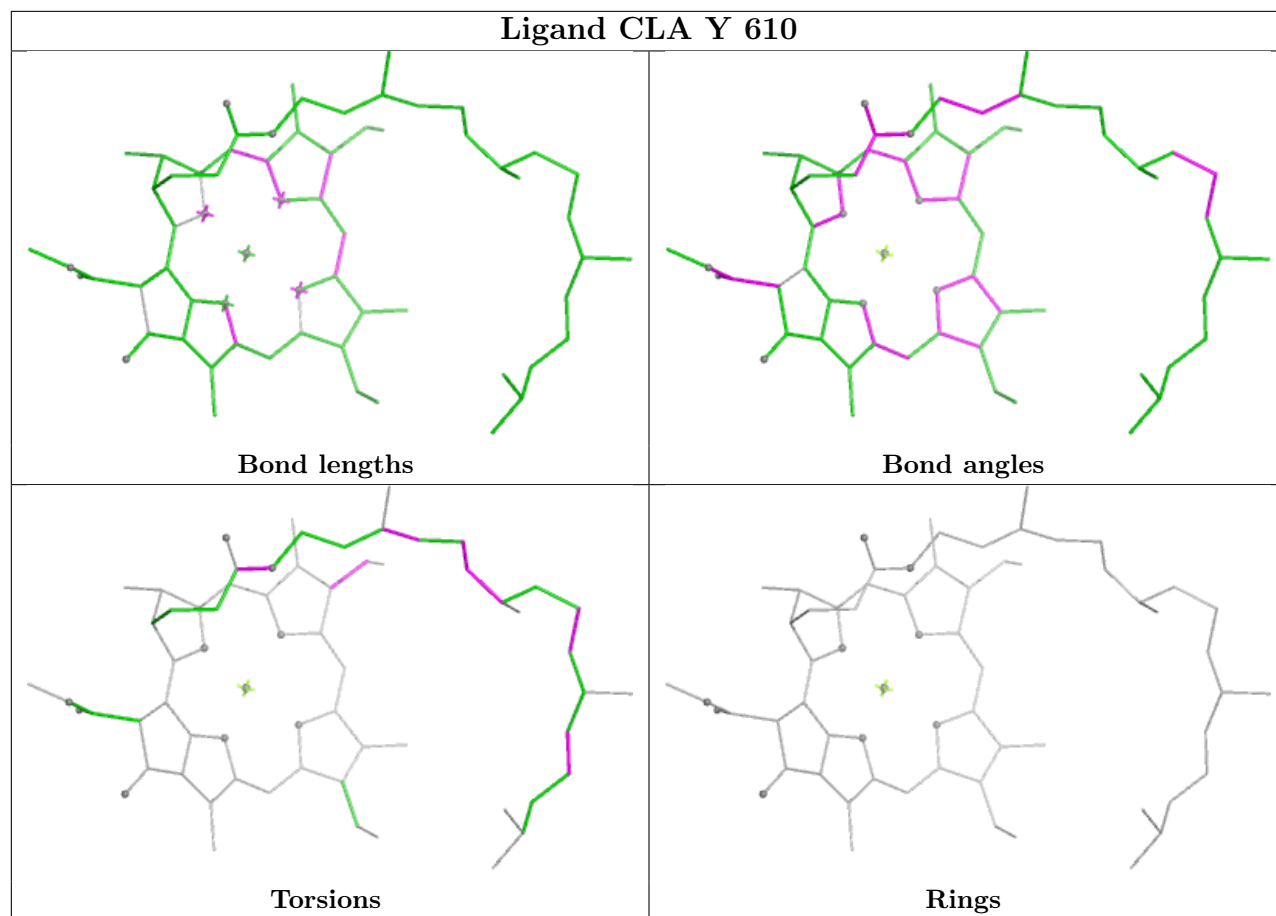
Continued on next page...

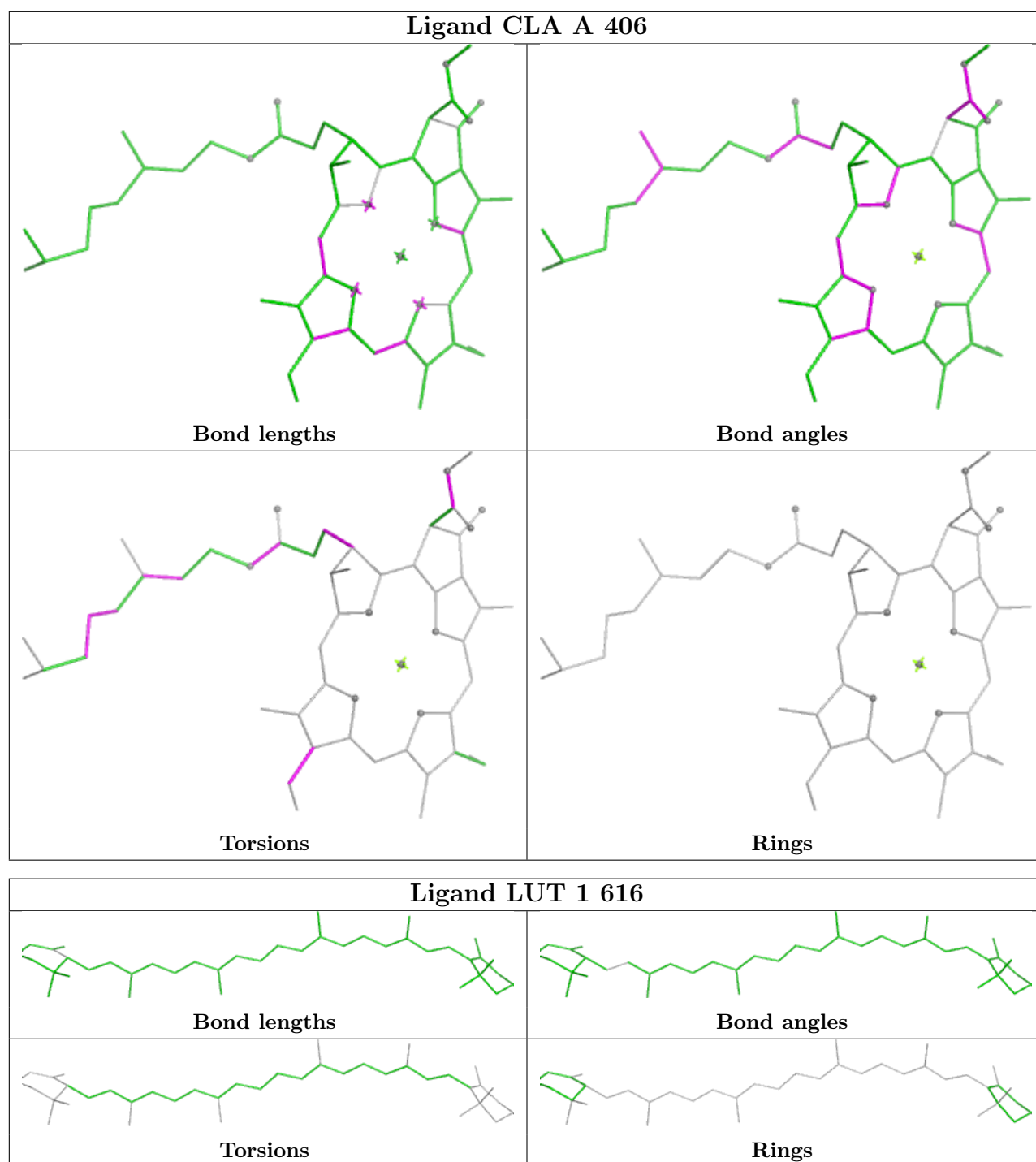
Continued from previous page...

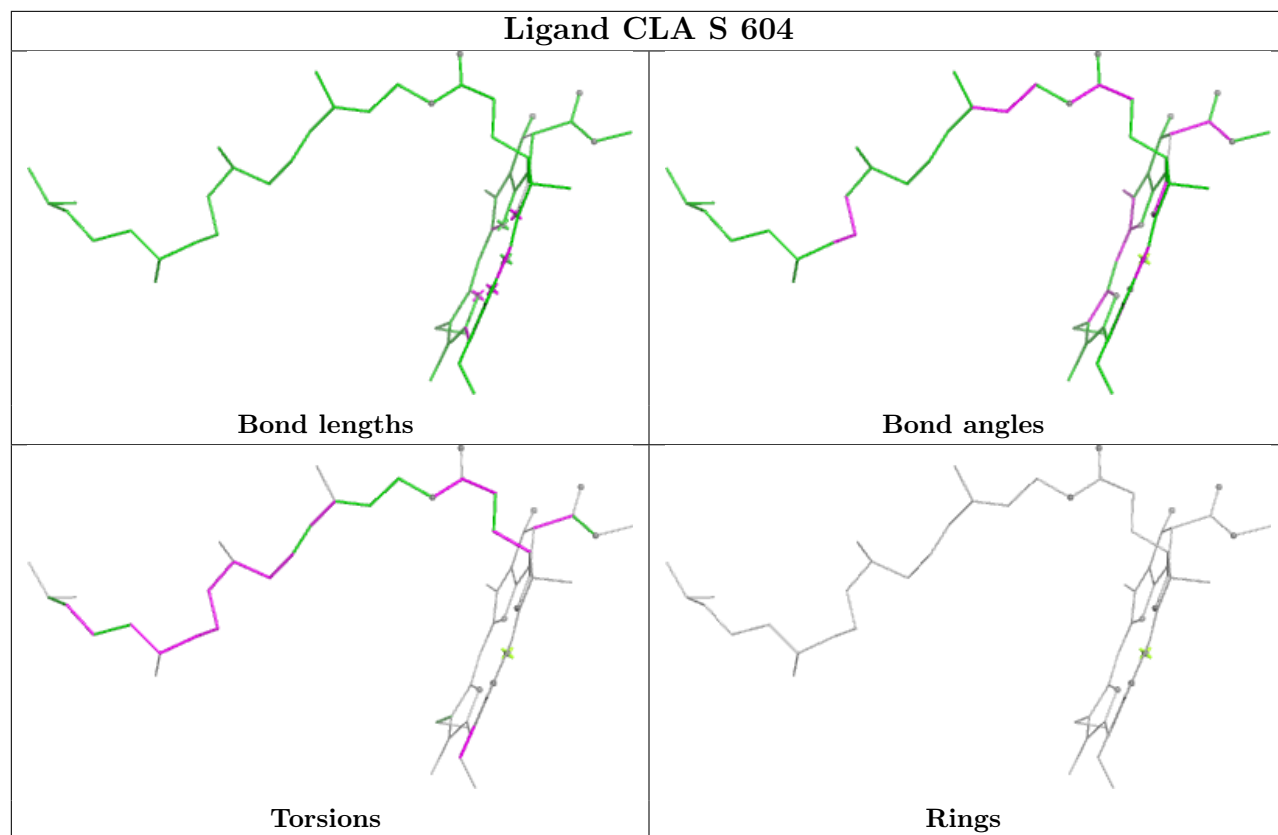
Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	c	519	DGD	3	0
31	s	603	CLA	1	0
31	b	609	CLA	2	0
32	s	621	LHG	4	0
41	A	409	LMG	1	0
31	2	603	CLA	5	0
31	Y	602	CLA	5	0
31	g	613	CLA	3	0
31	c	508	CLA	1	0
30	11	609	CHL	2	0
31	c	506	CLA	4	0
31	s	611	CLA	4	0
32	r	618	LHG	3	0
30	1	607	CHL	3	0
31	n	610	CLA	4	0
31	4	604	CLA	2	0

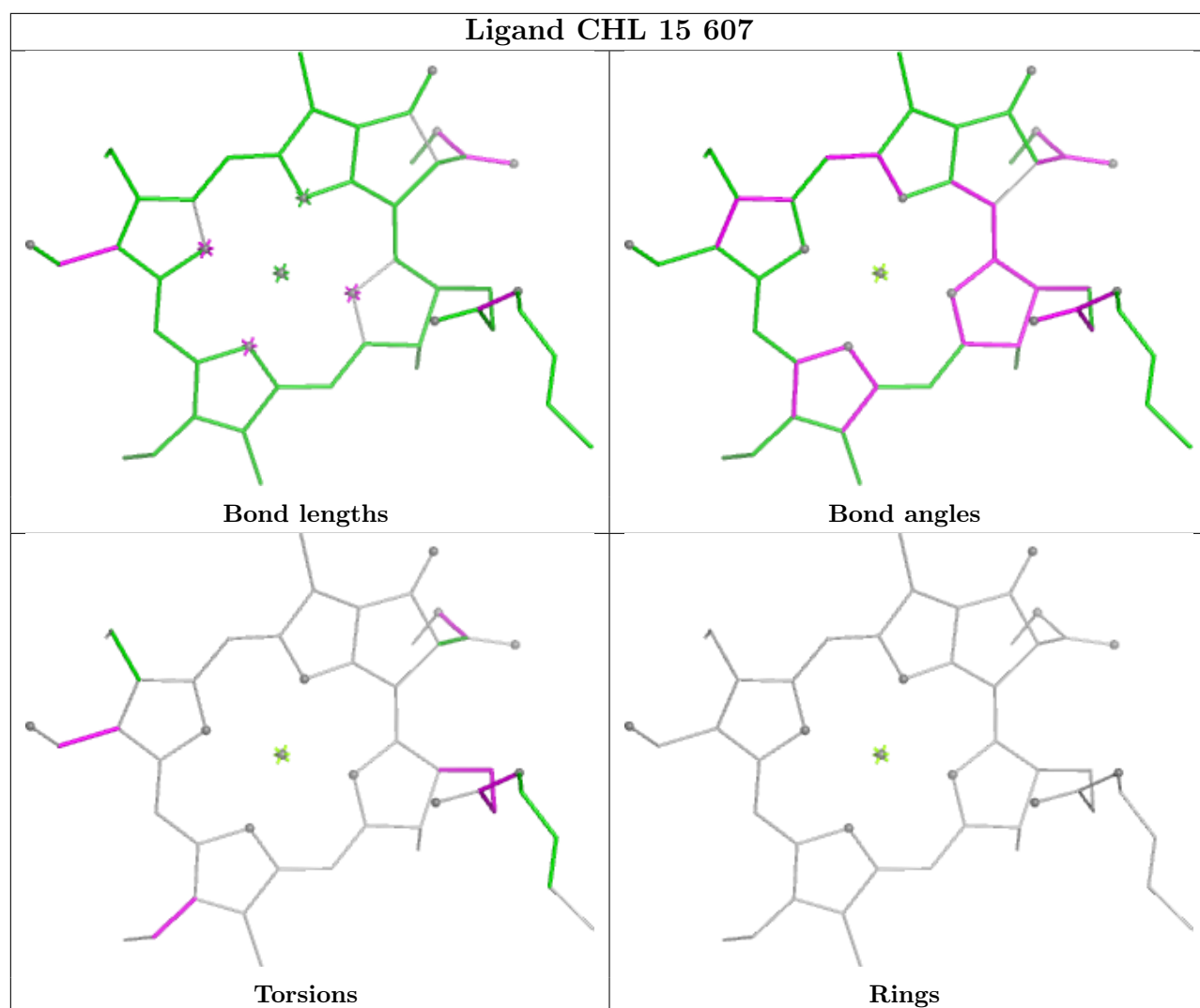
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

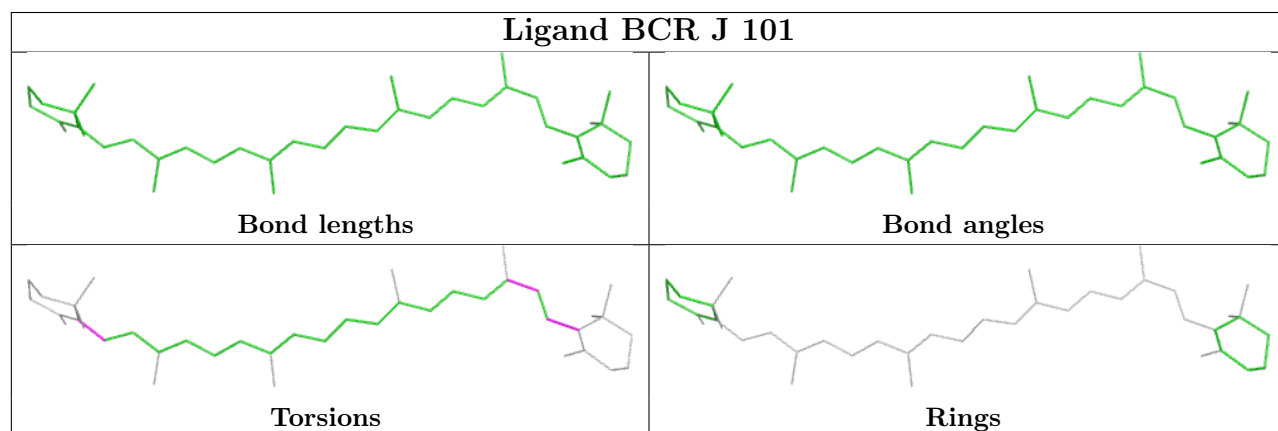
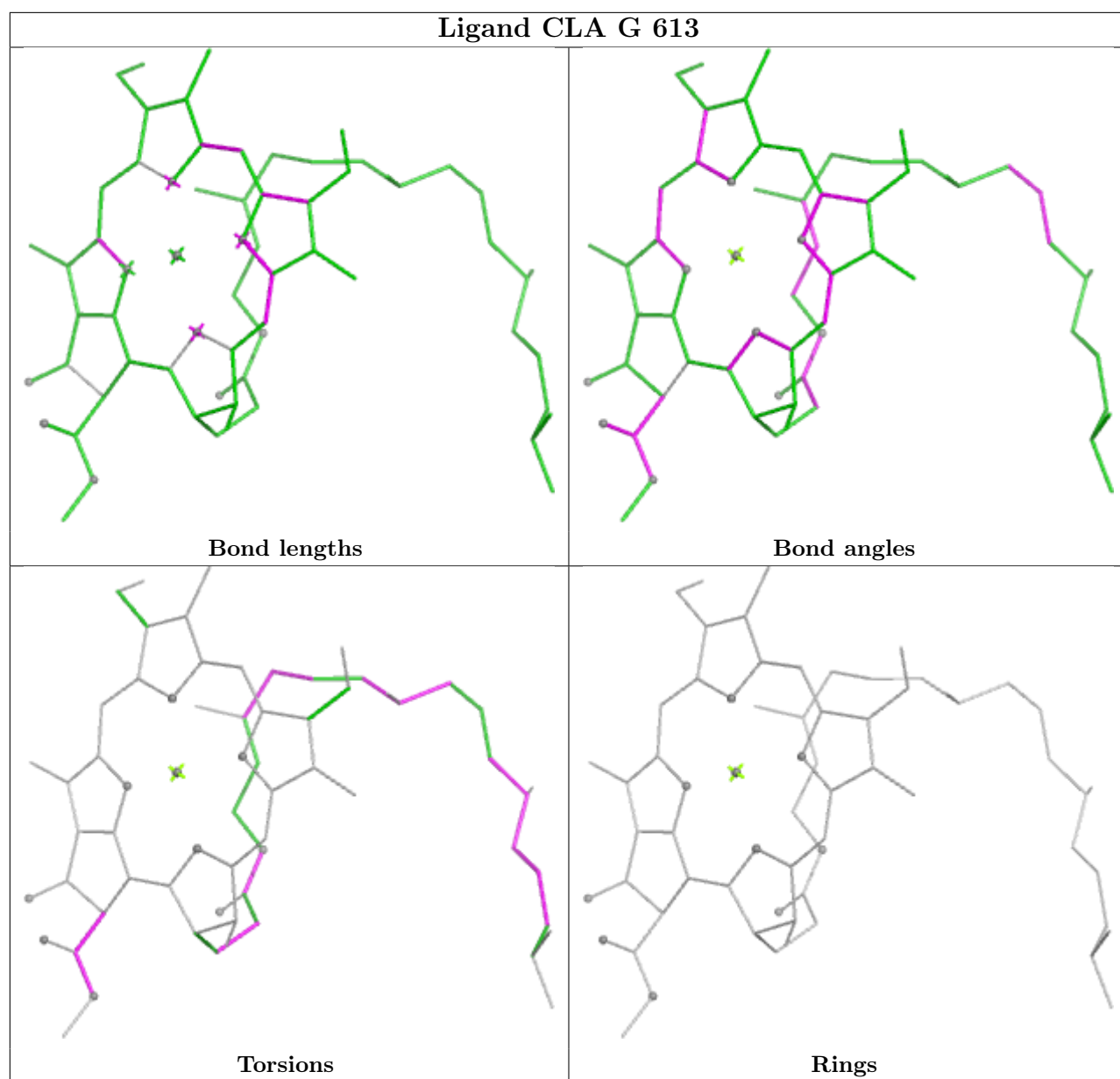


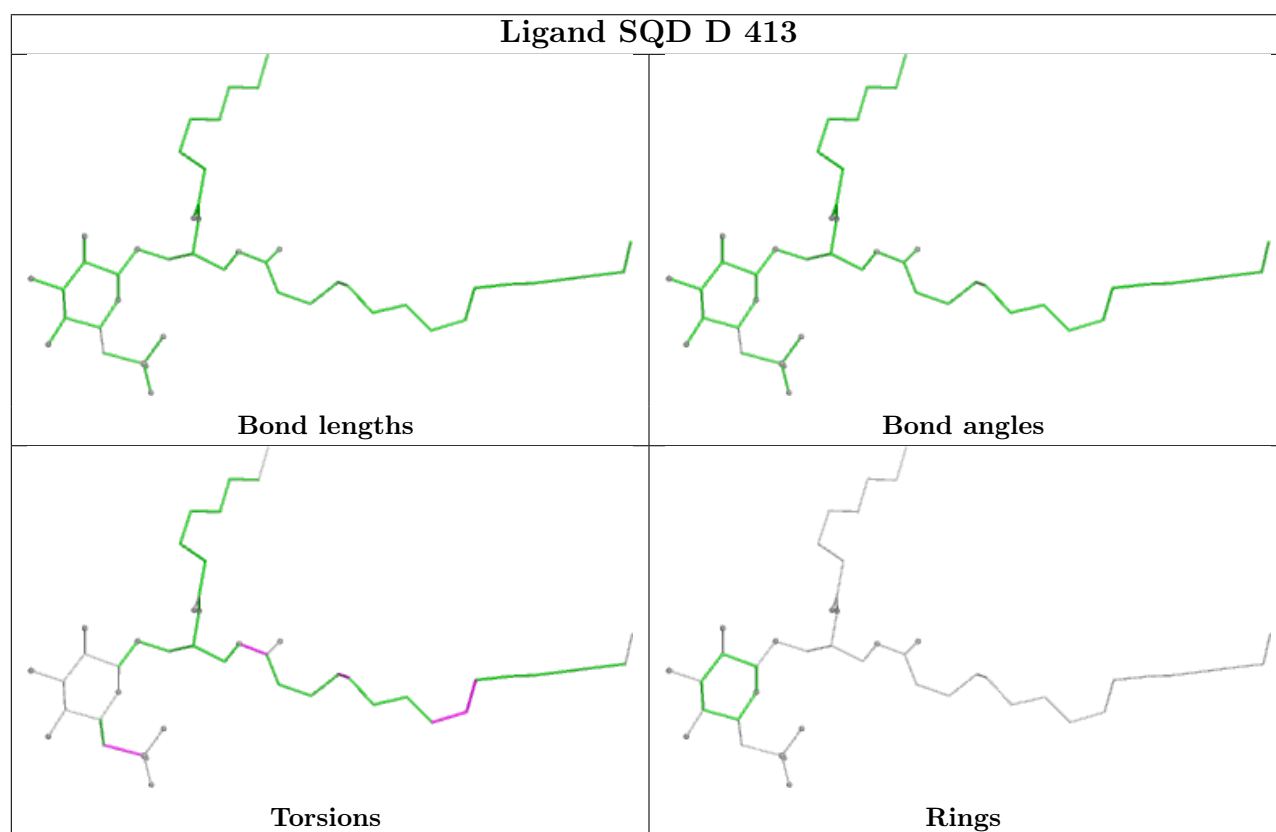
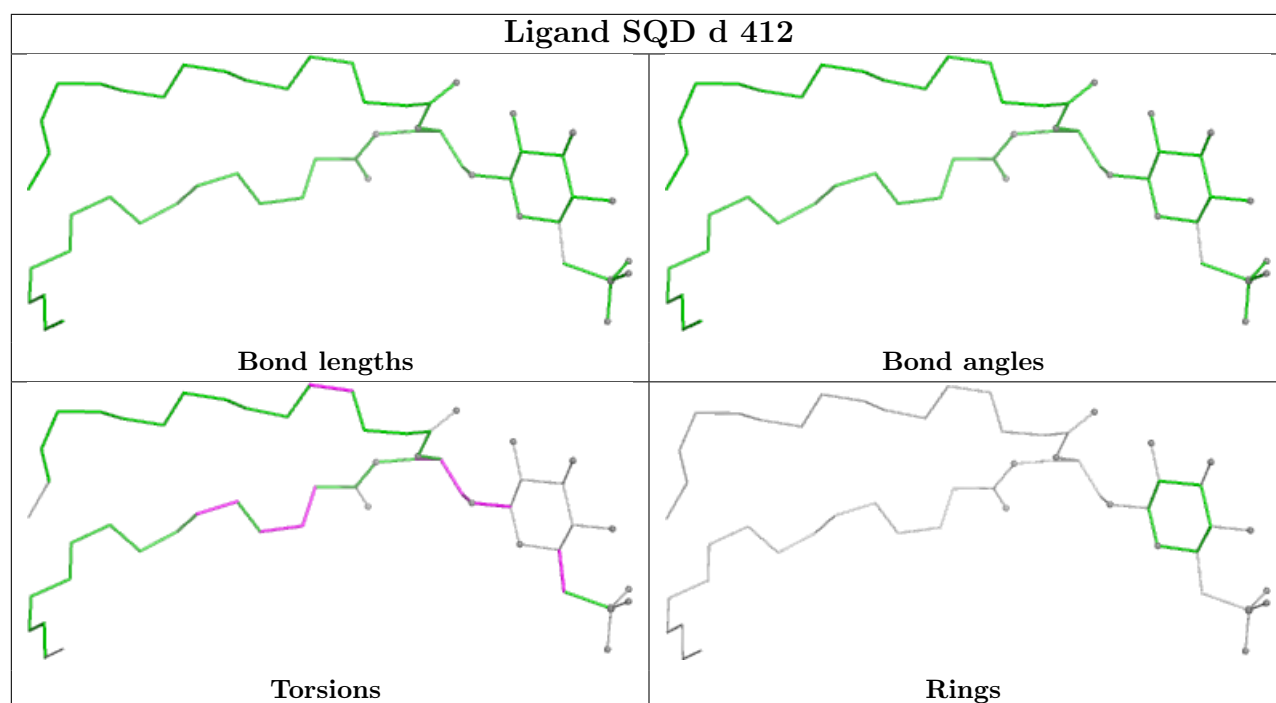


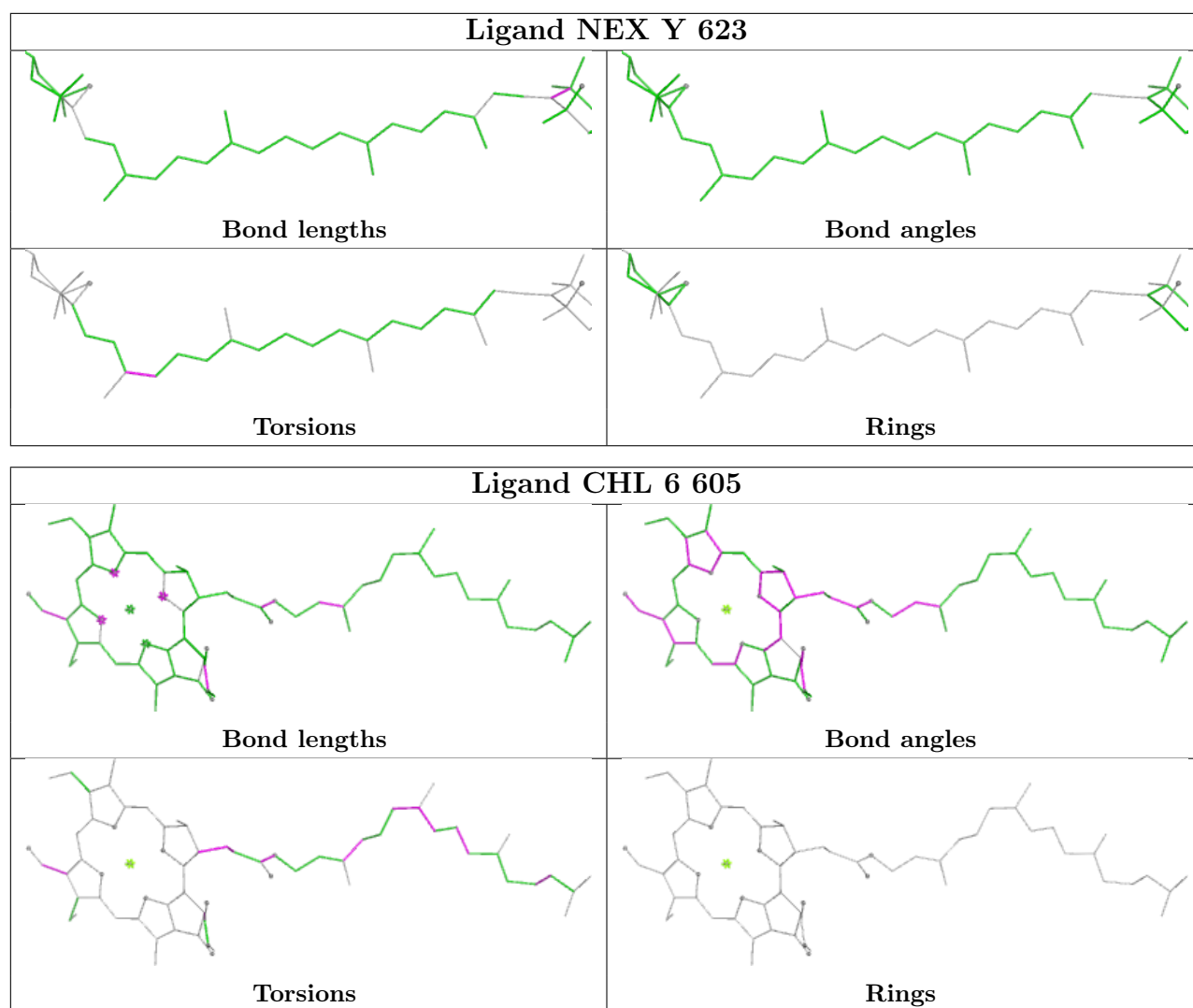


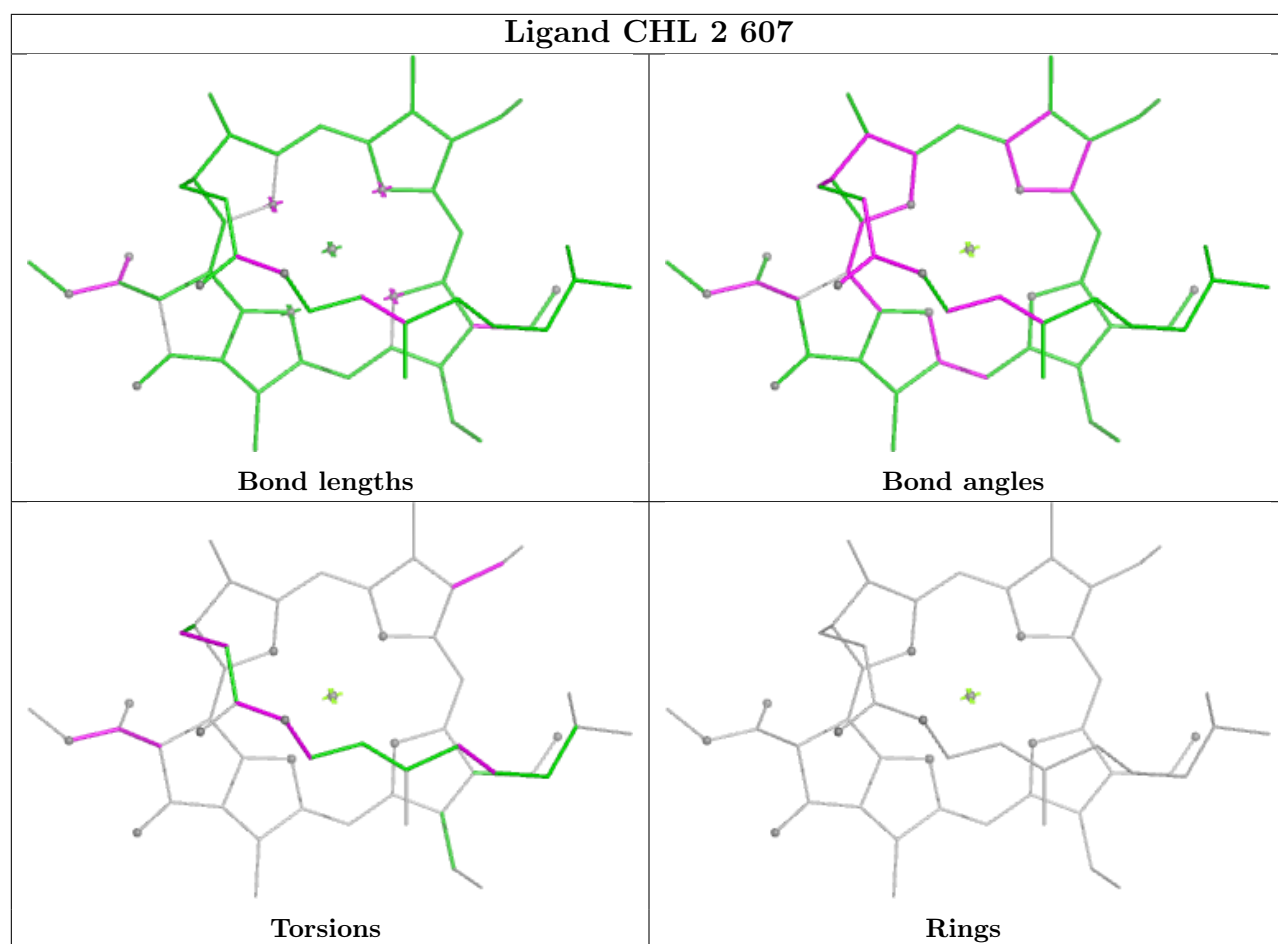


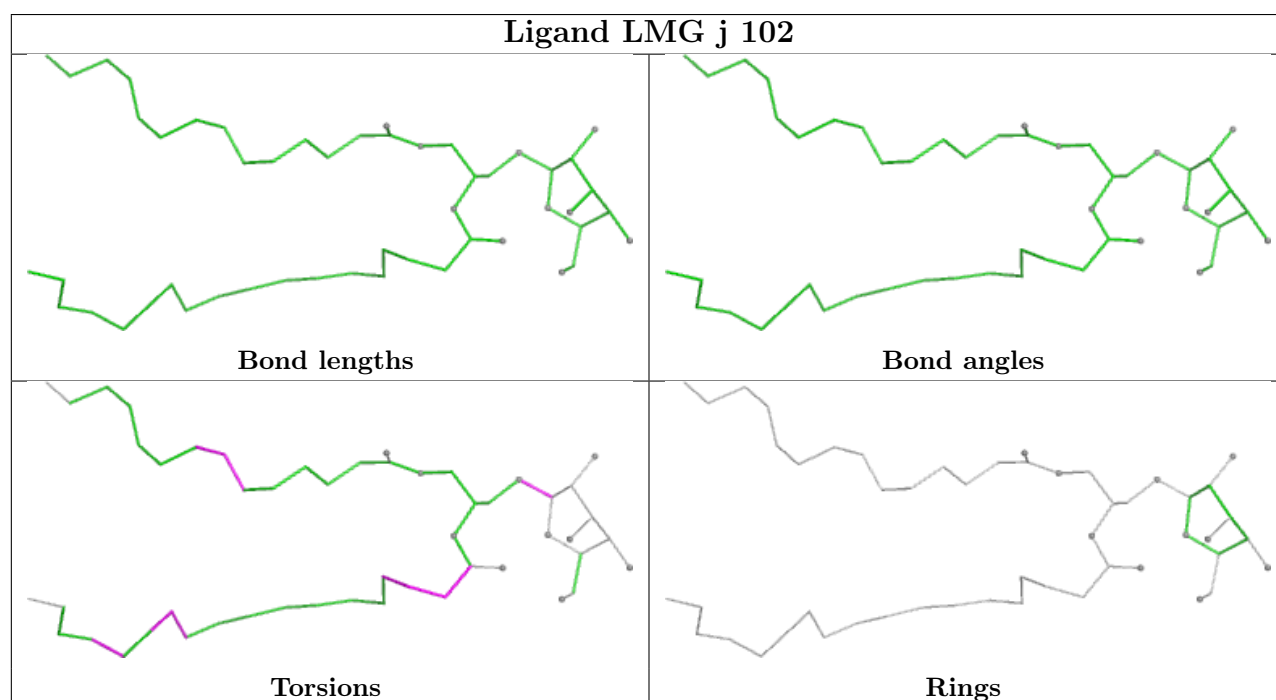
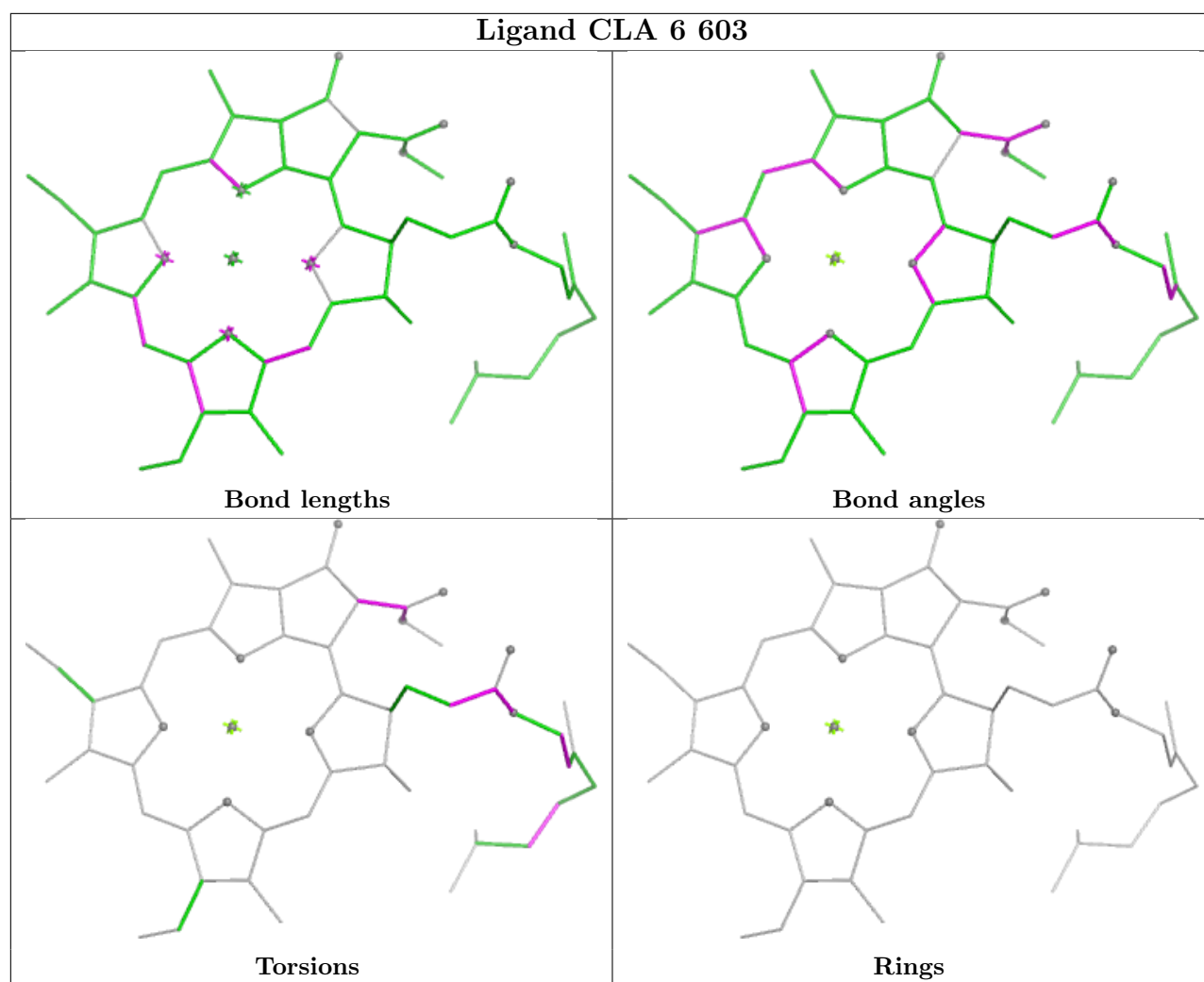


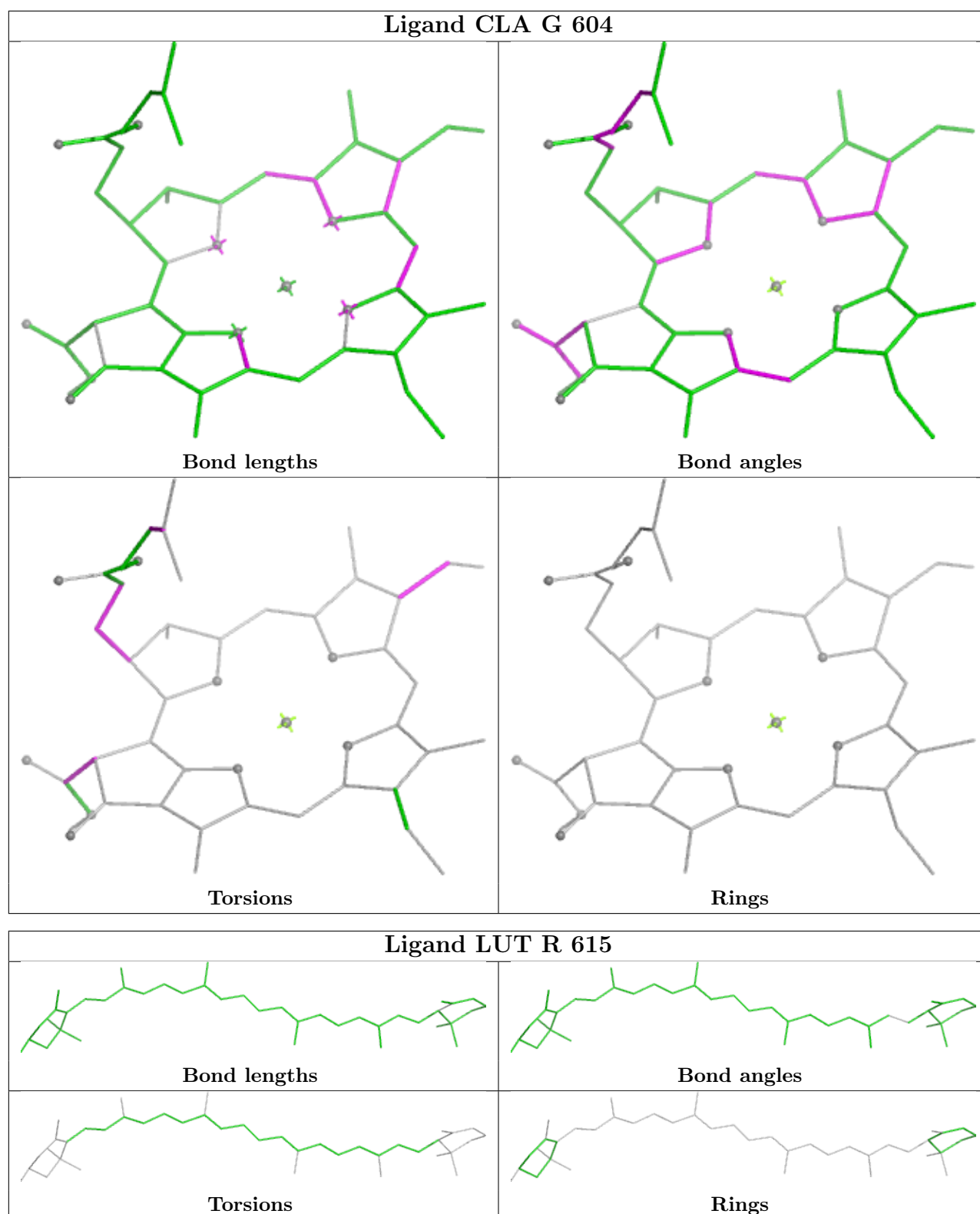


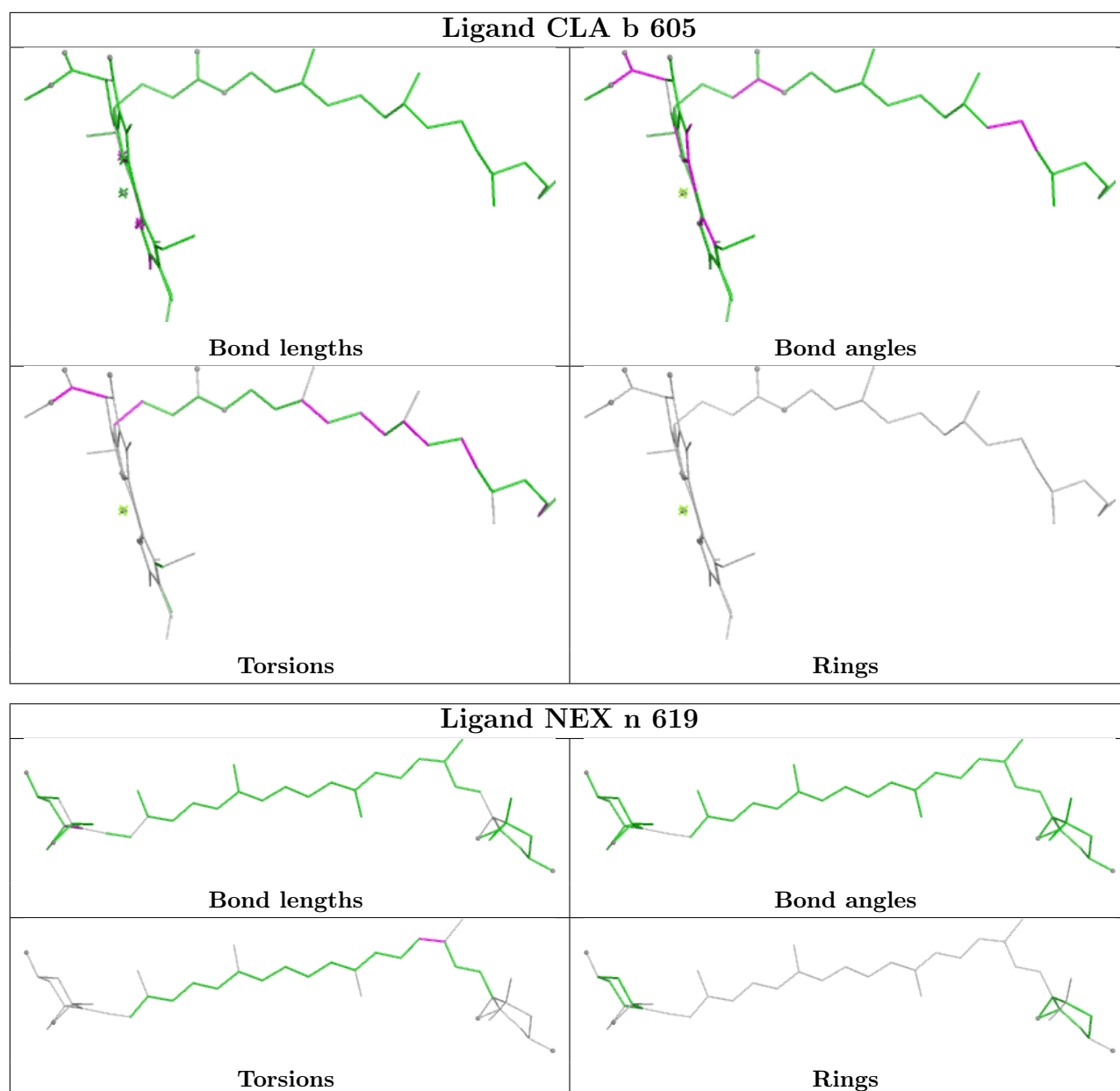


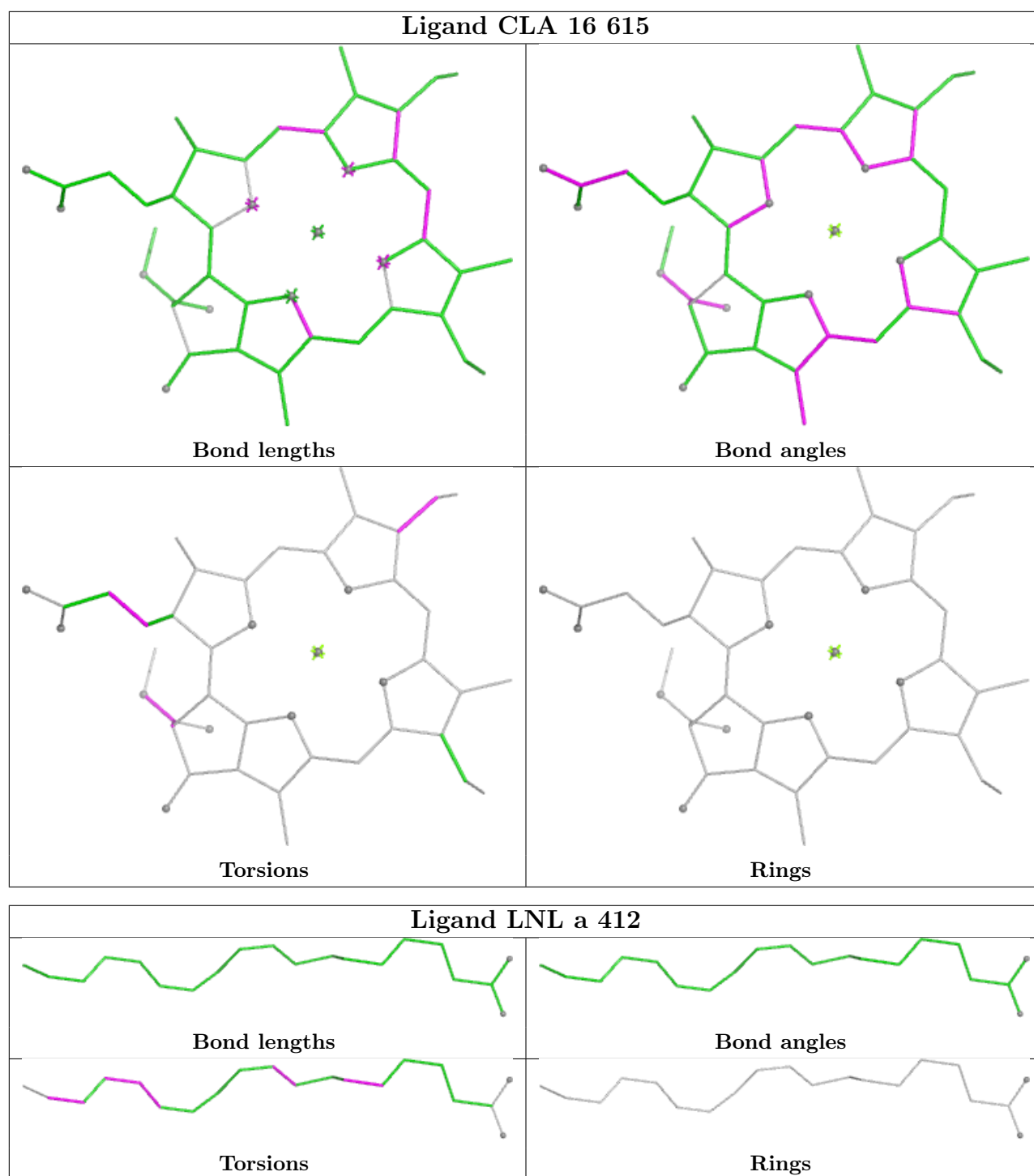


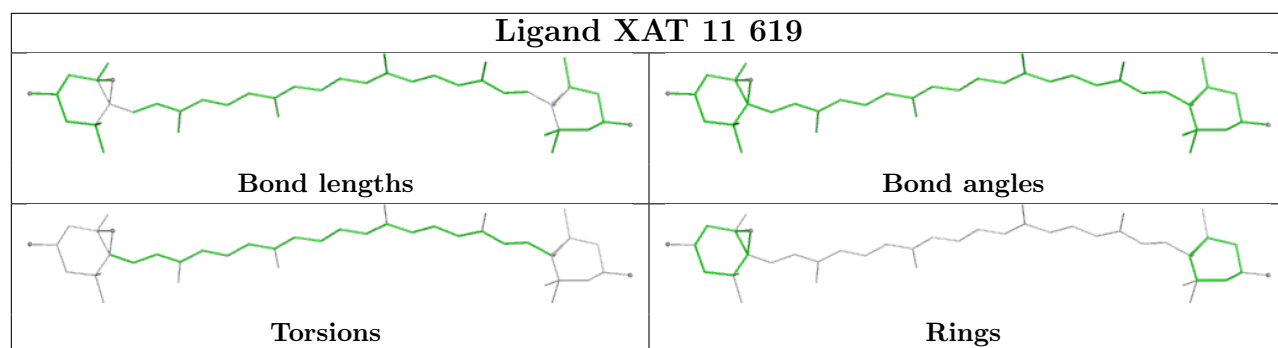
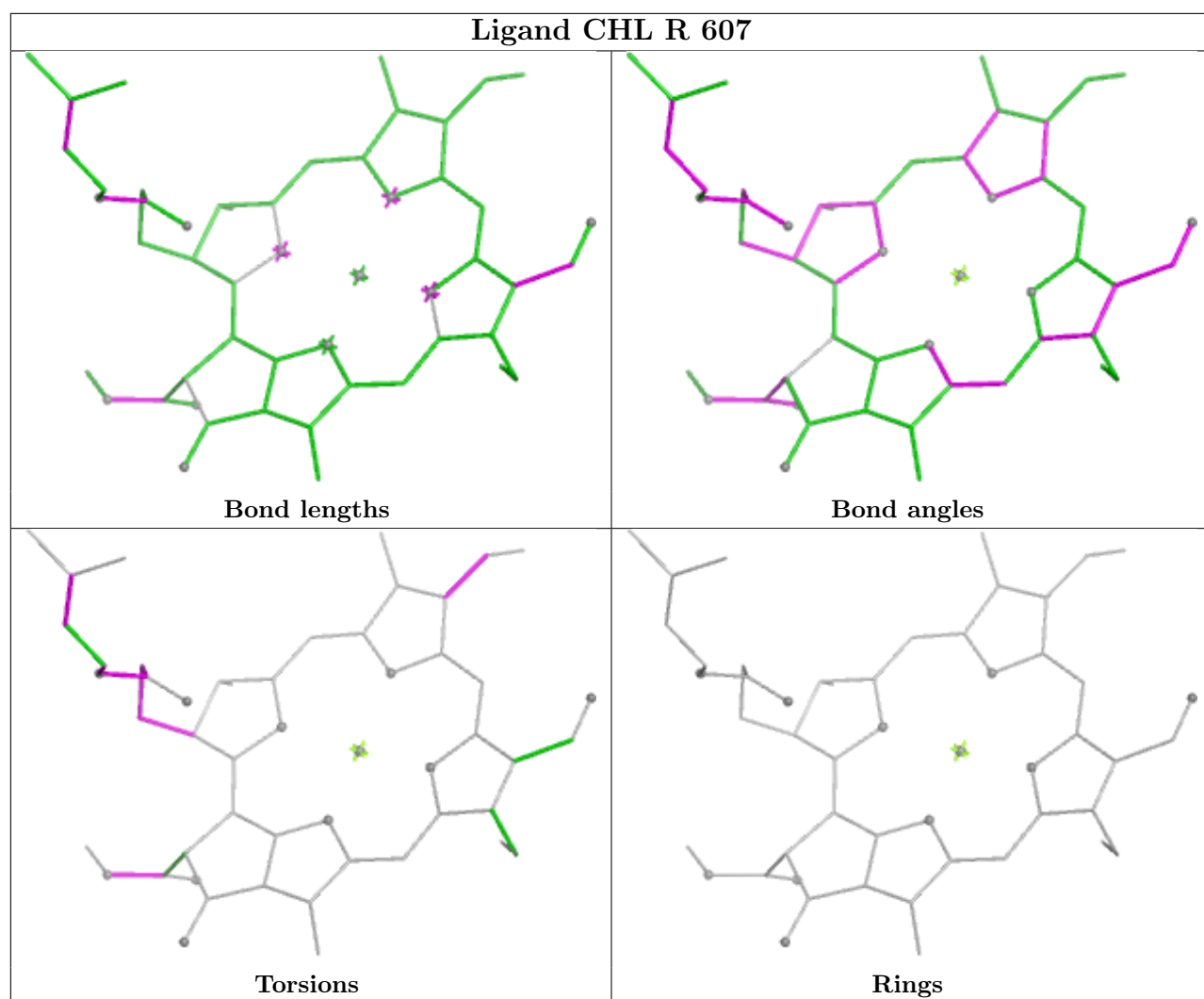


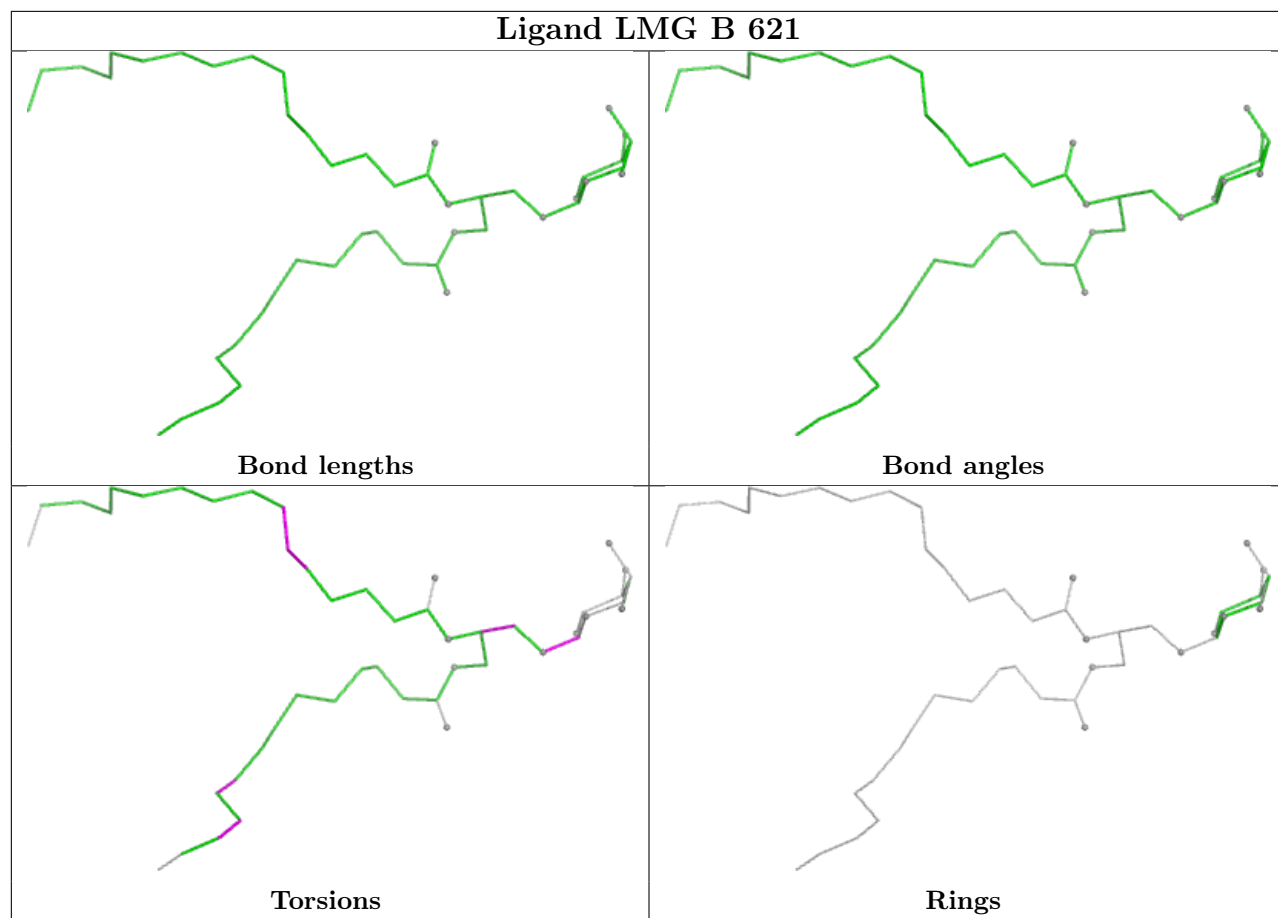


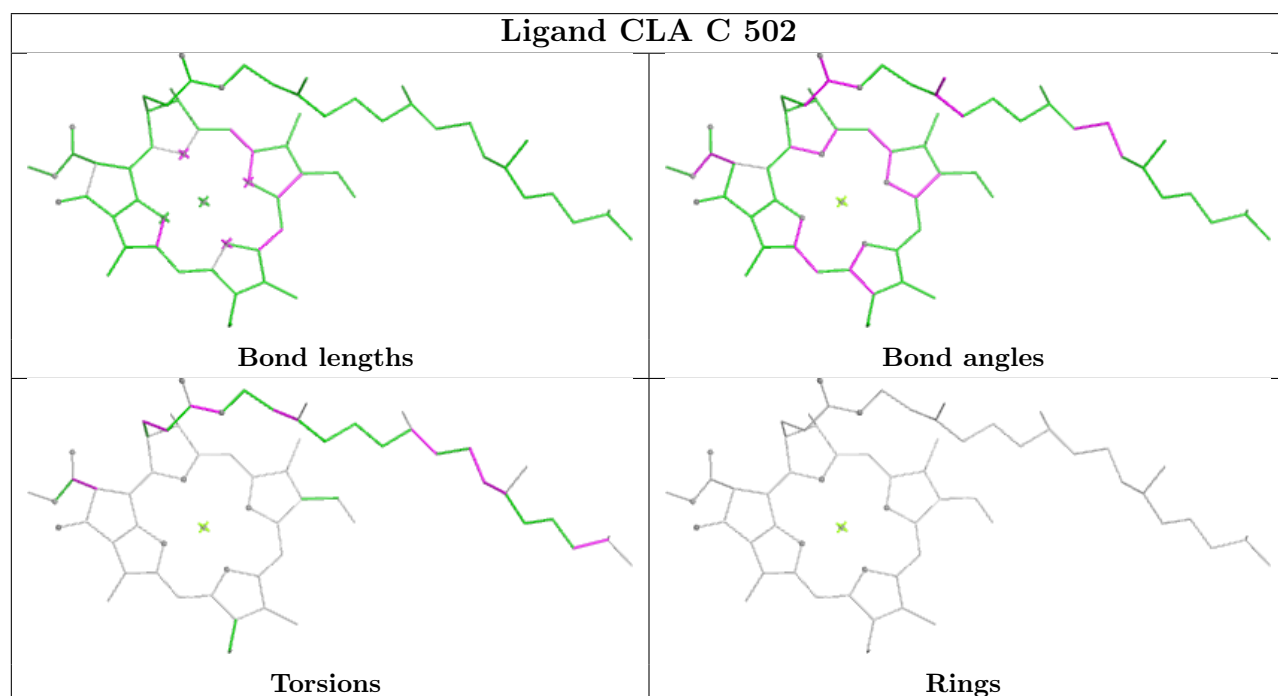
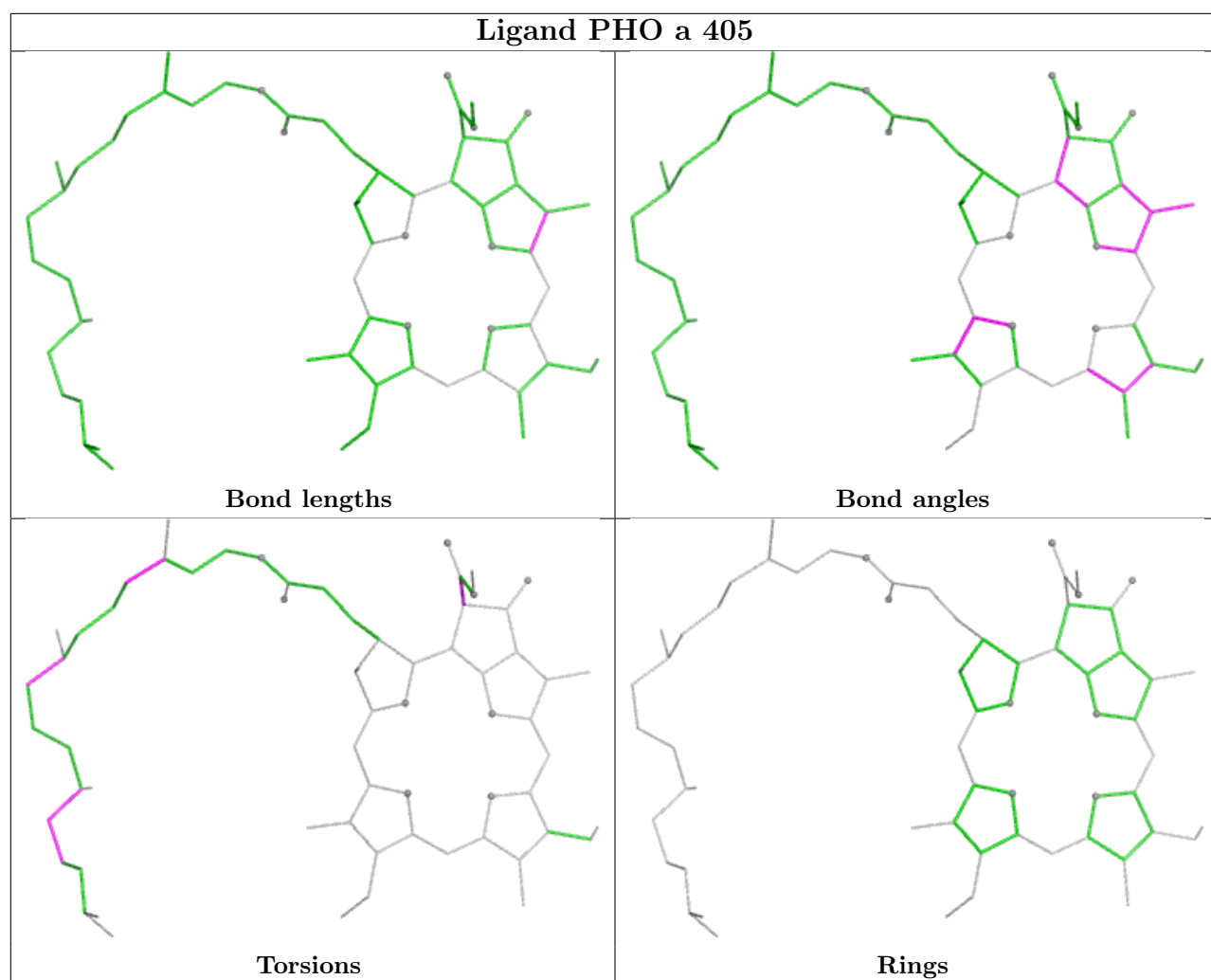


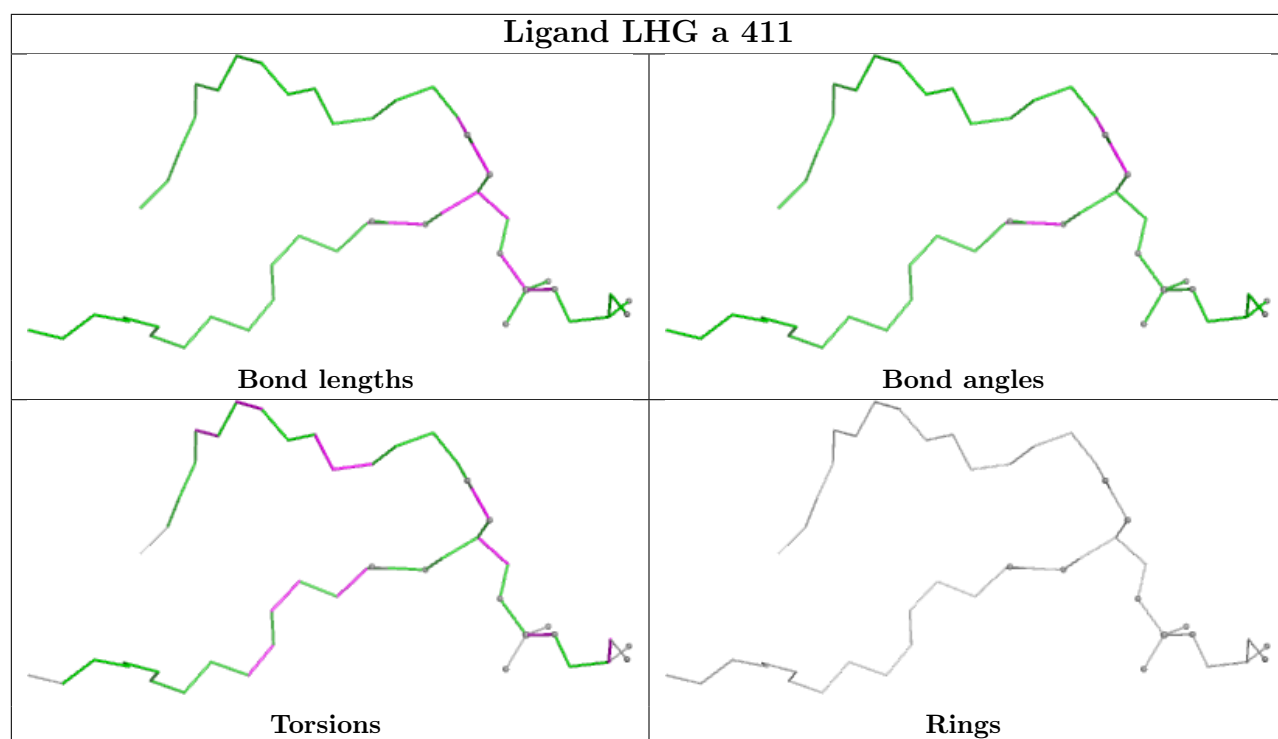


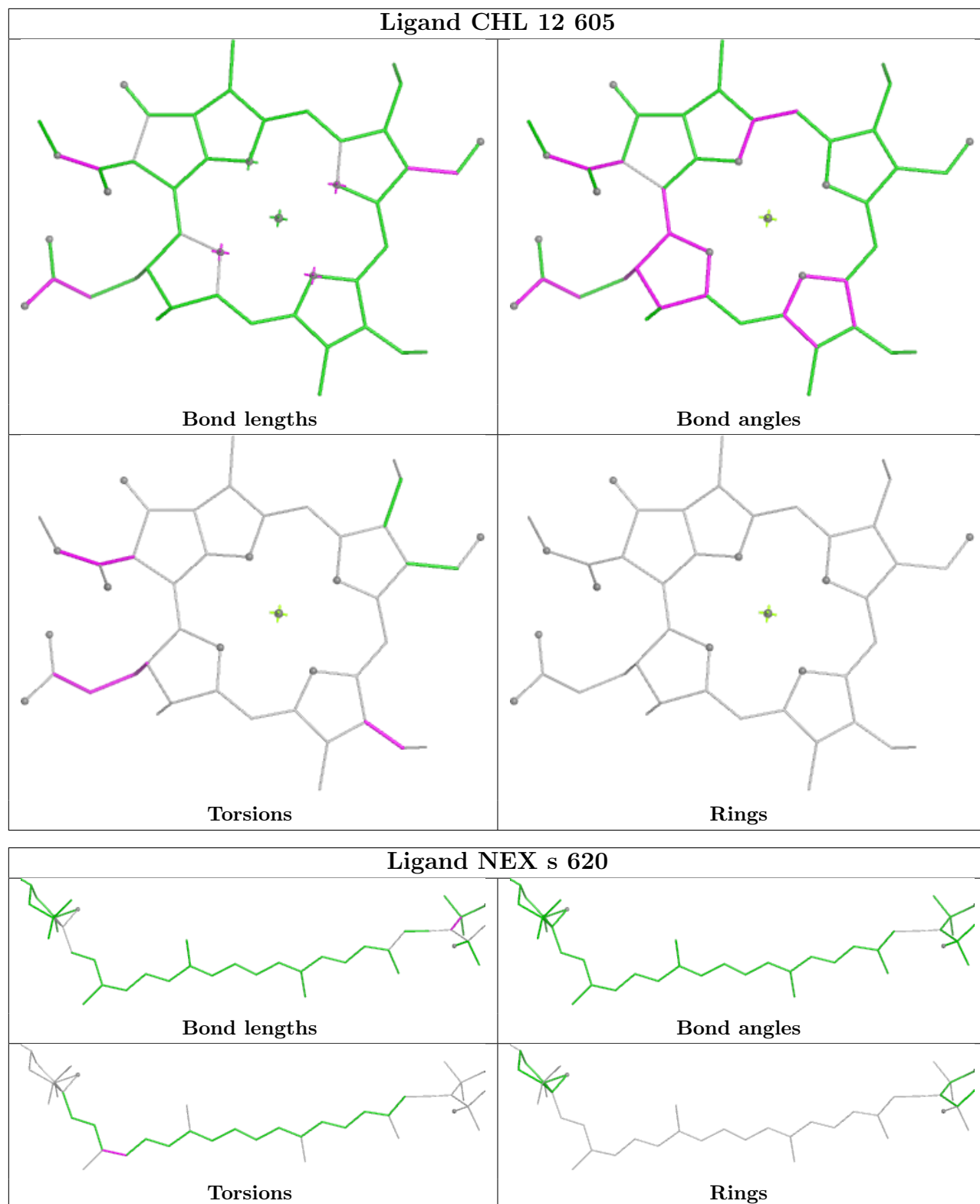


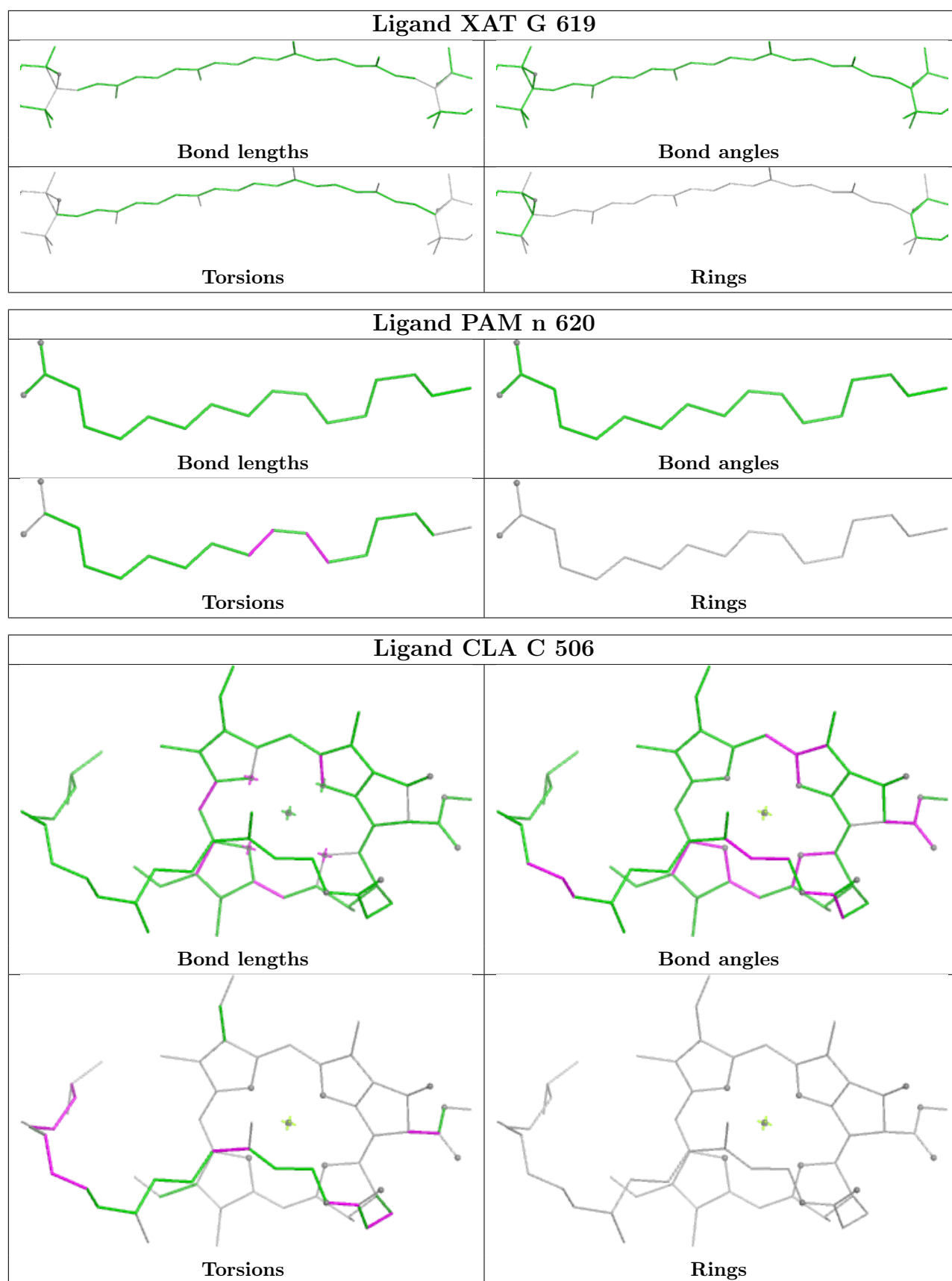


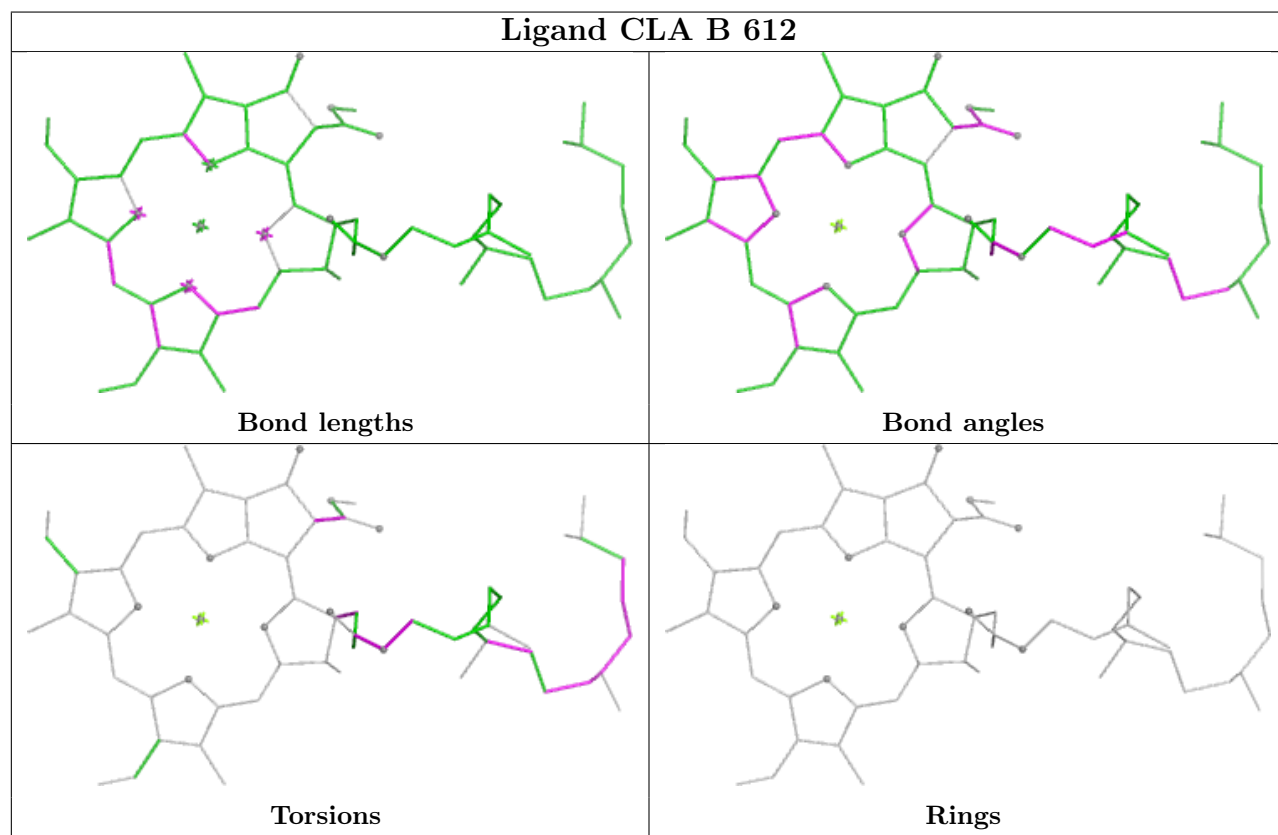
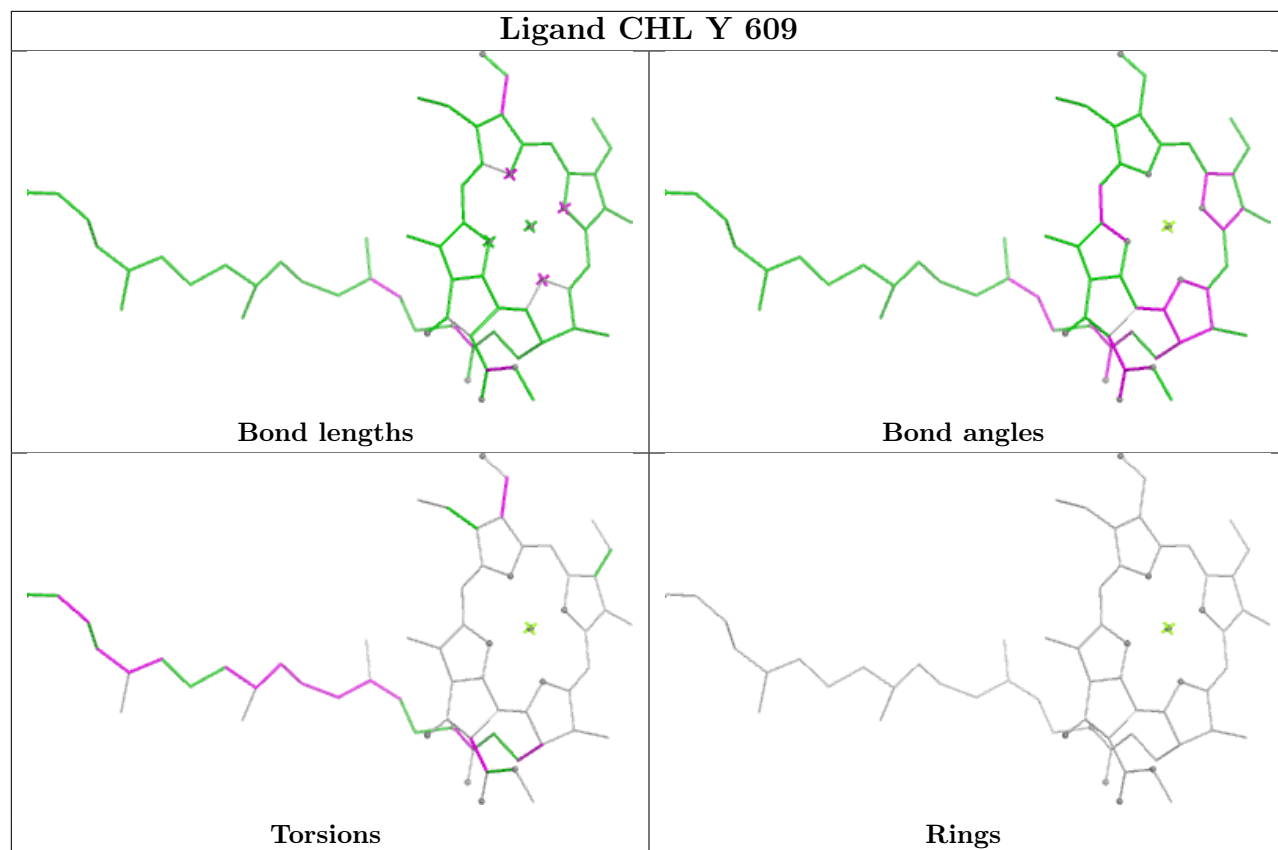


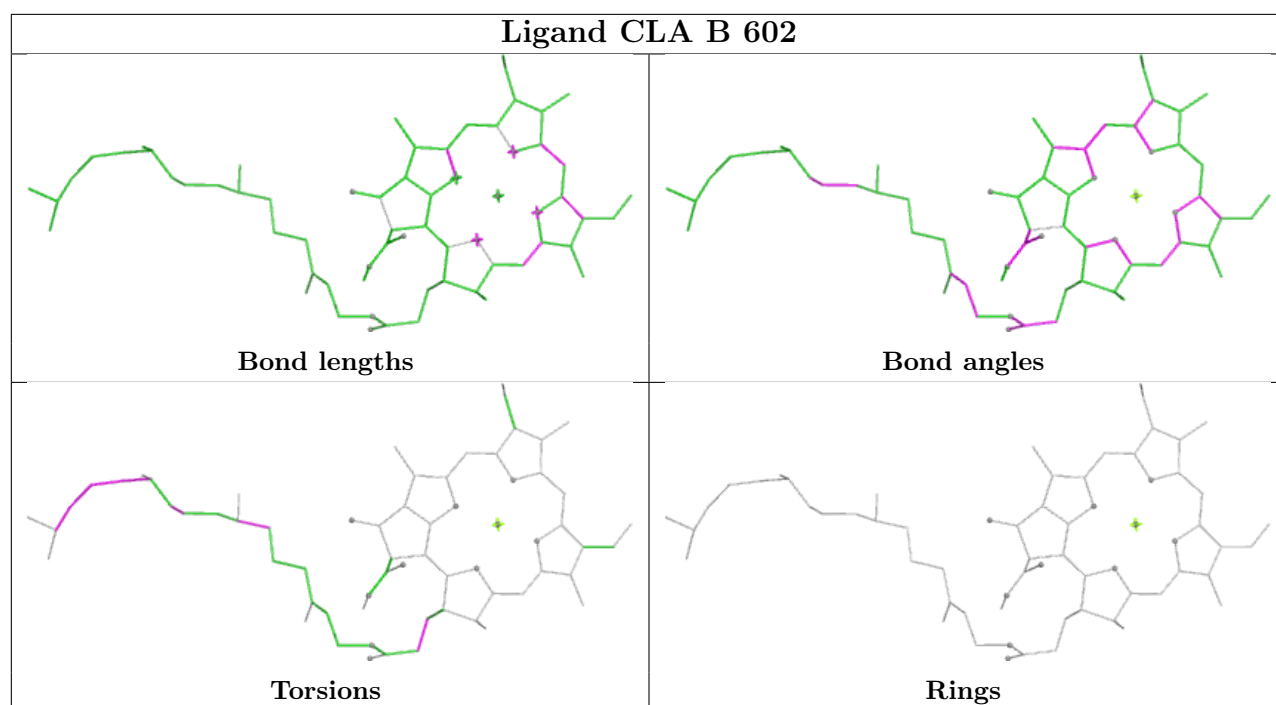


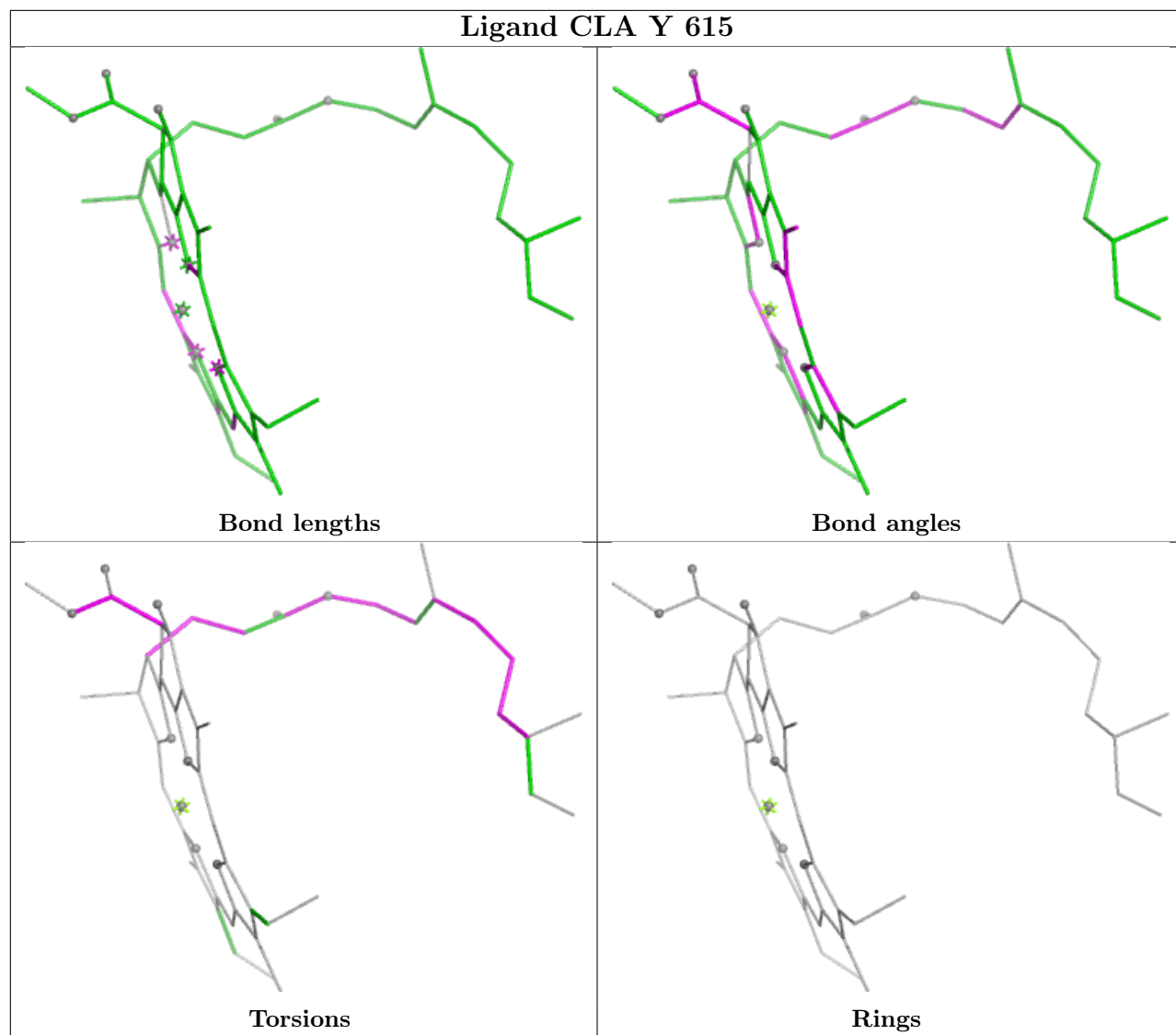


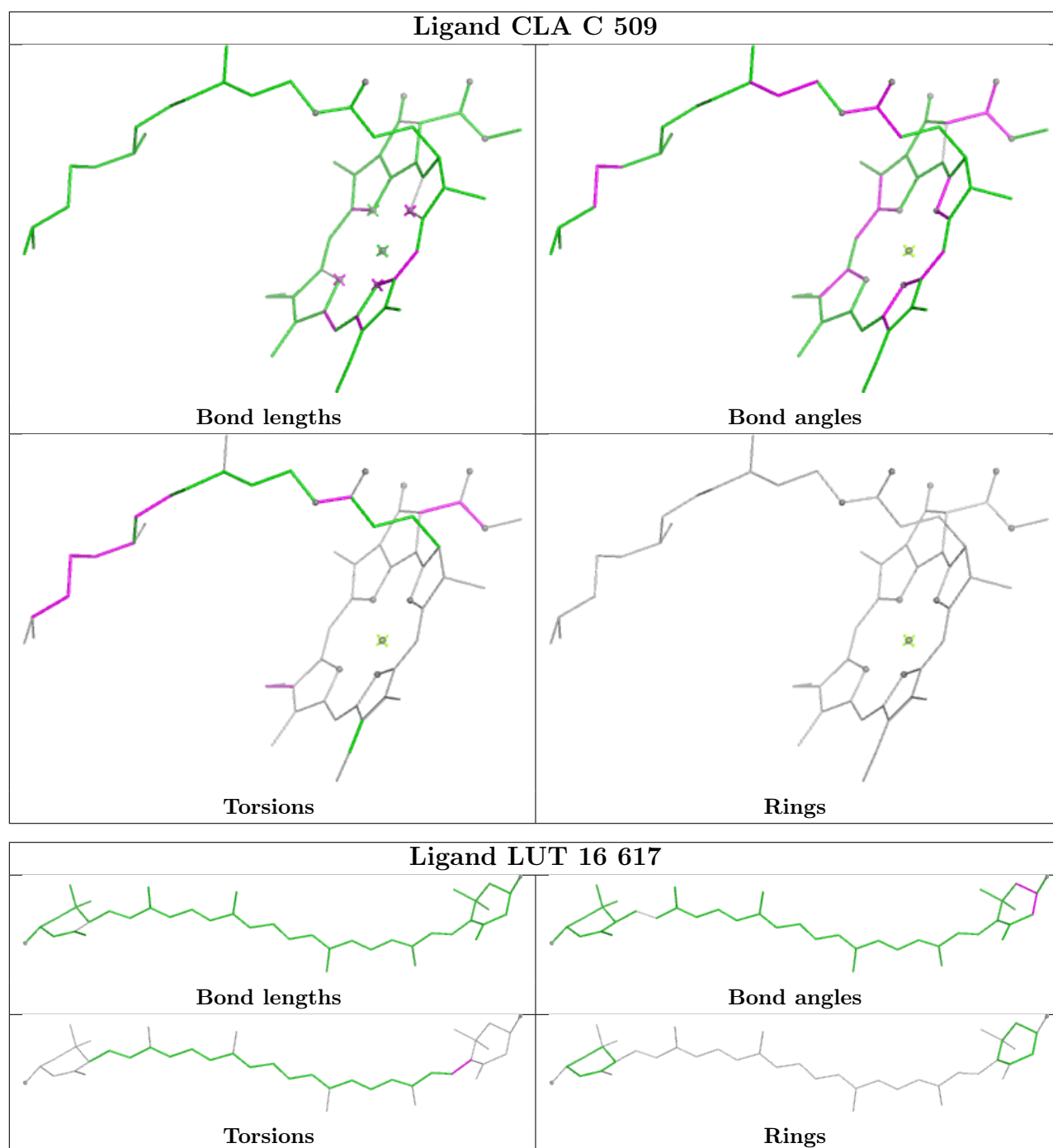




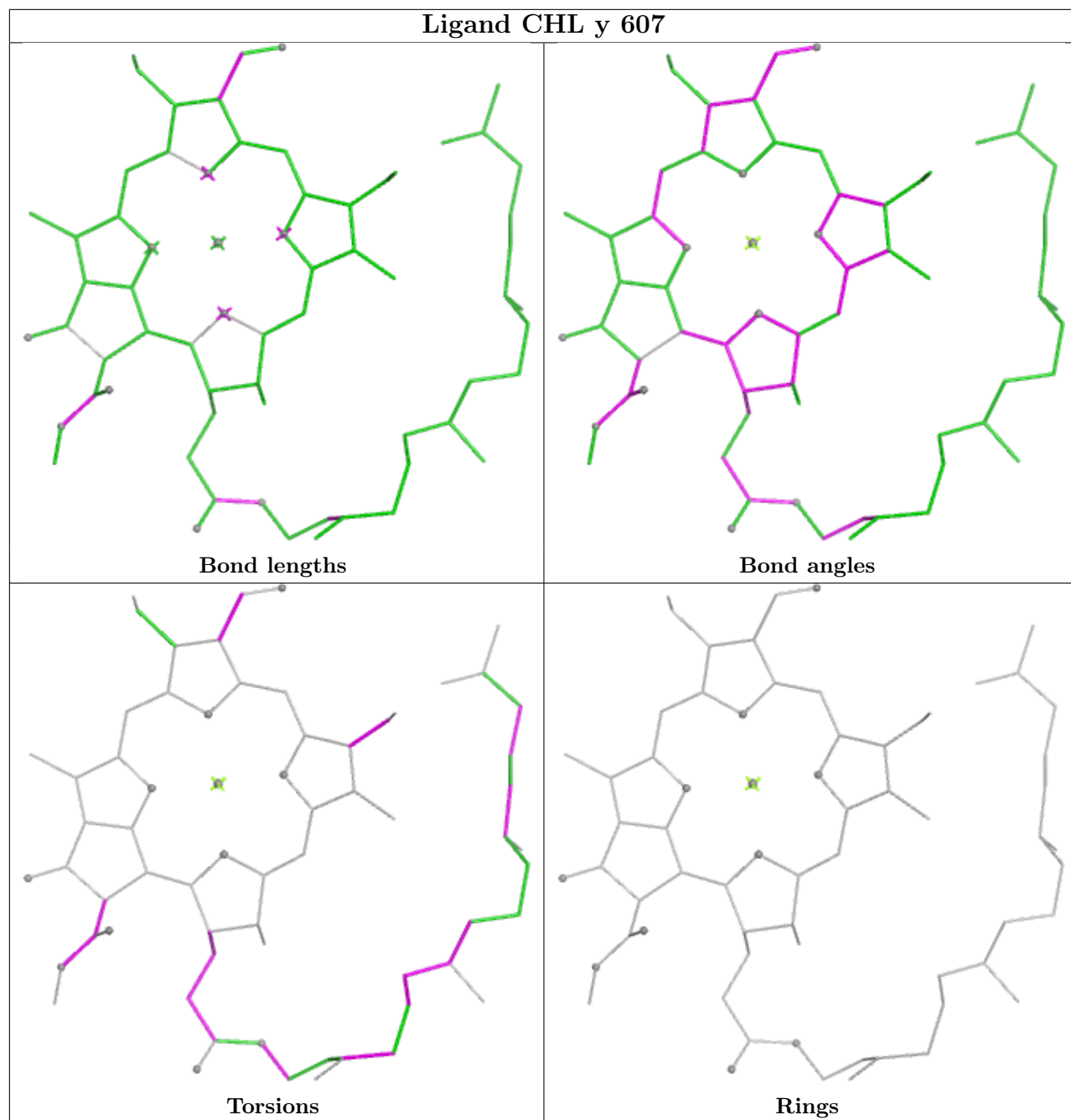


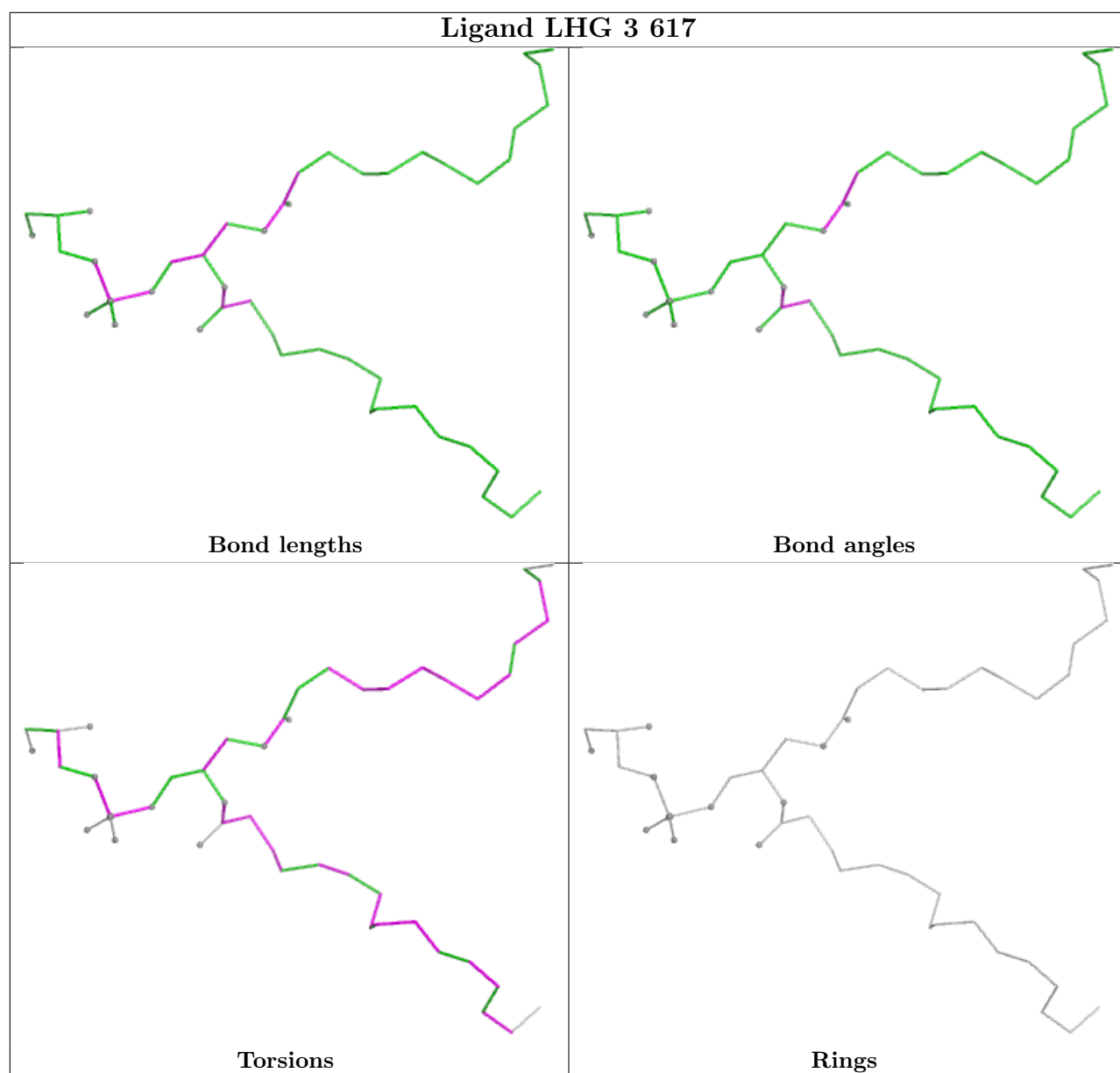


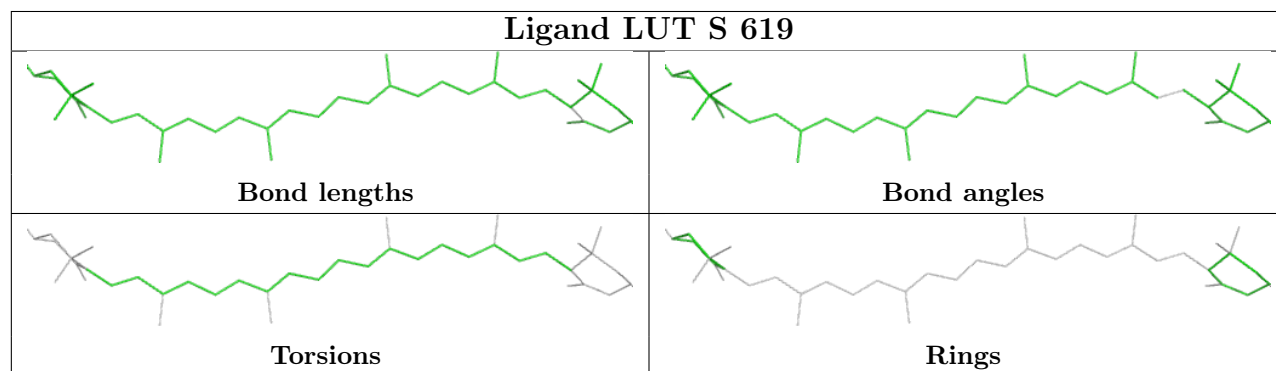
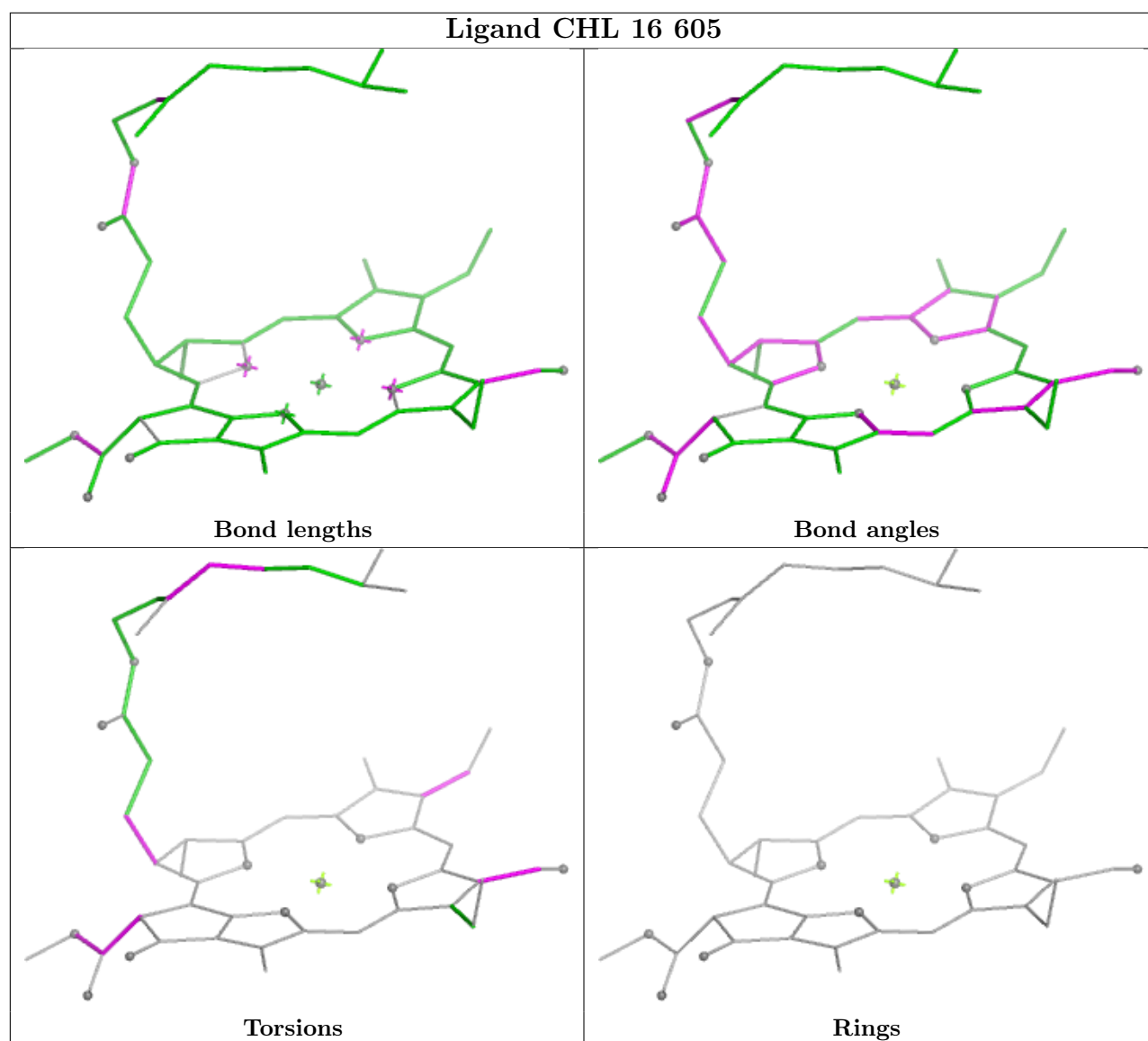


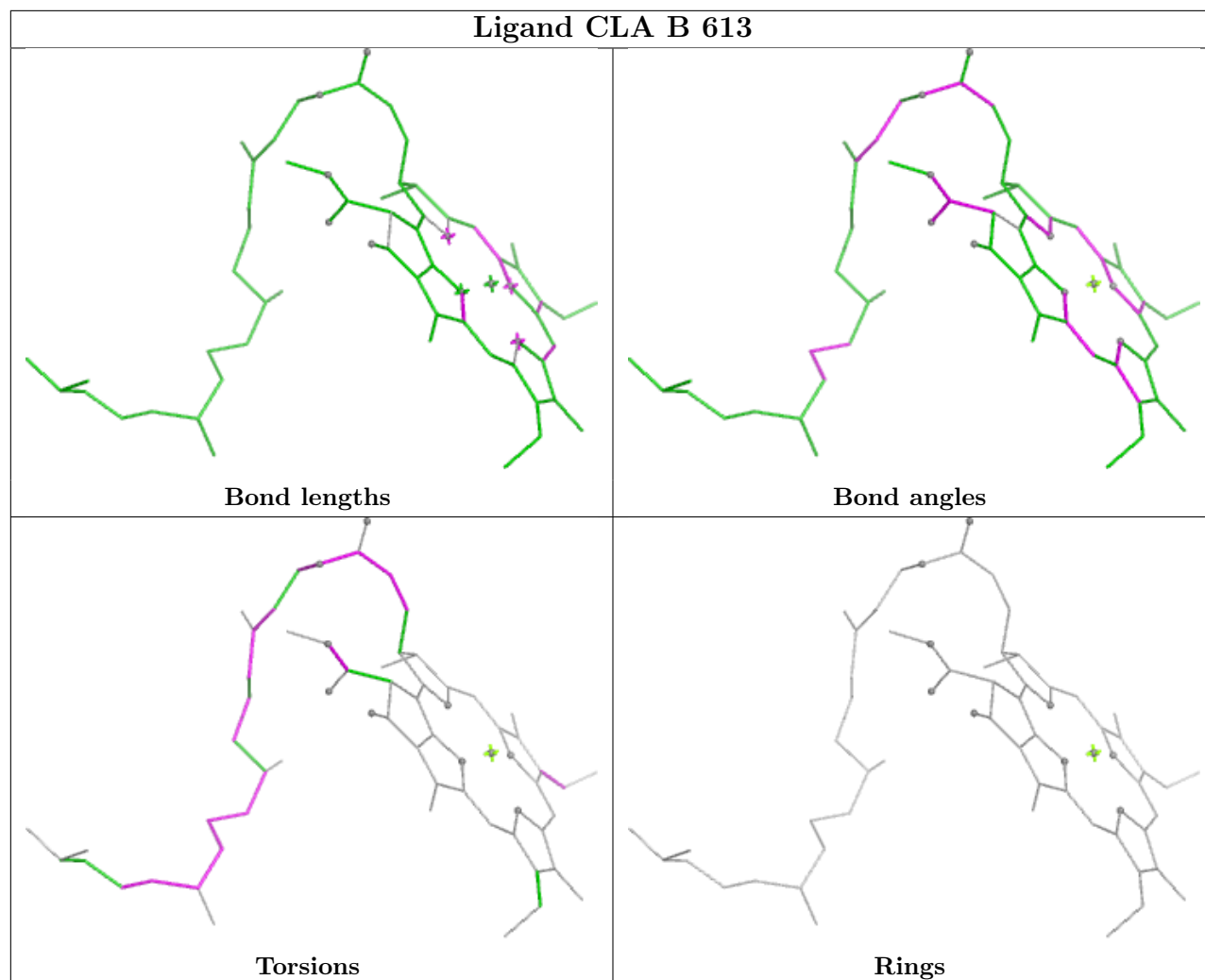
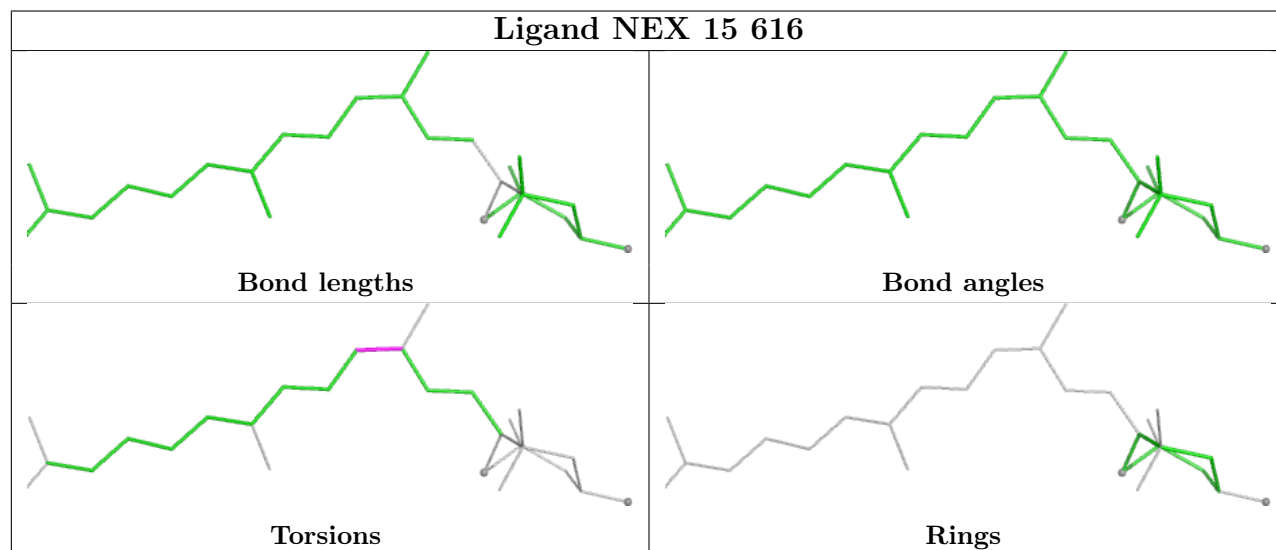


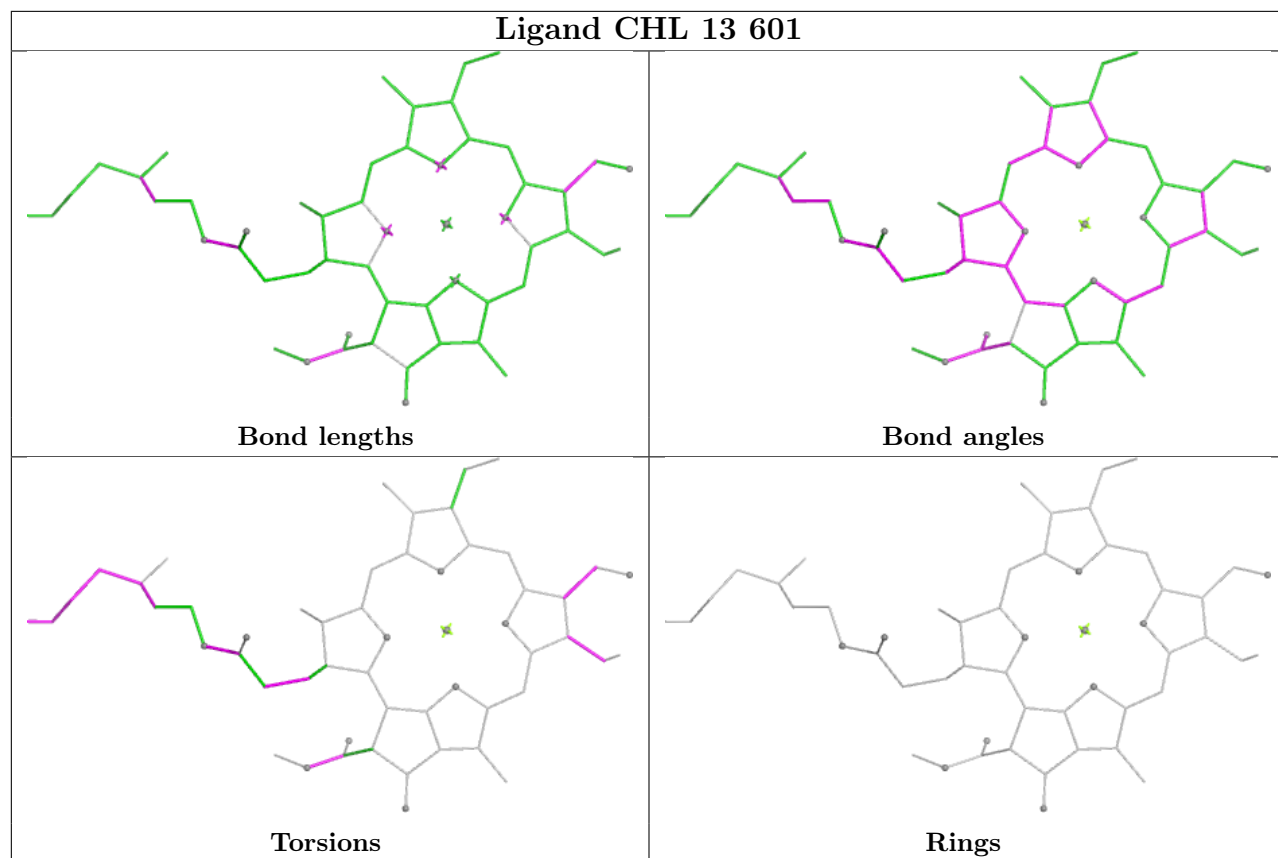
Ligand CHL y 607

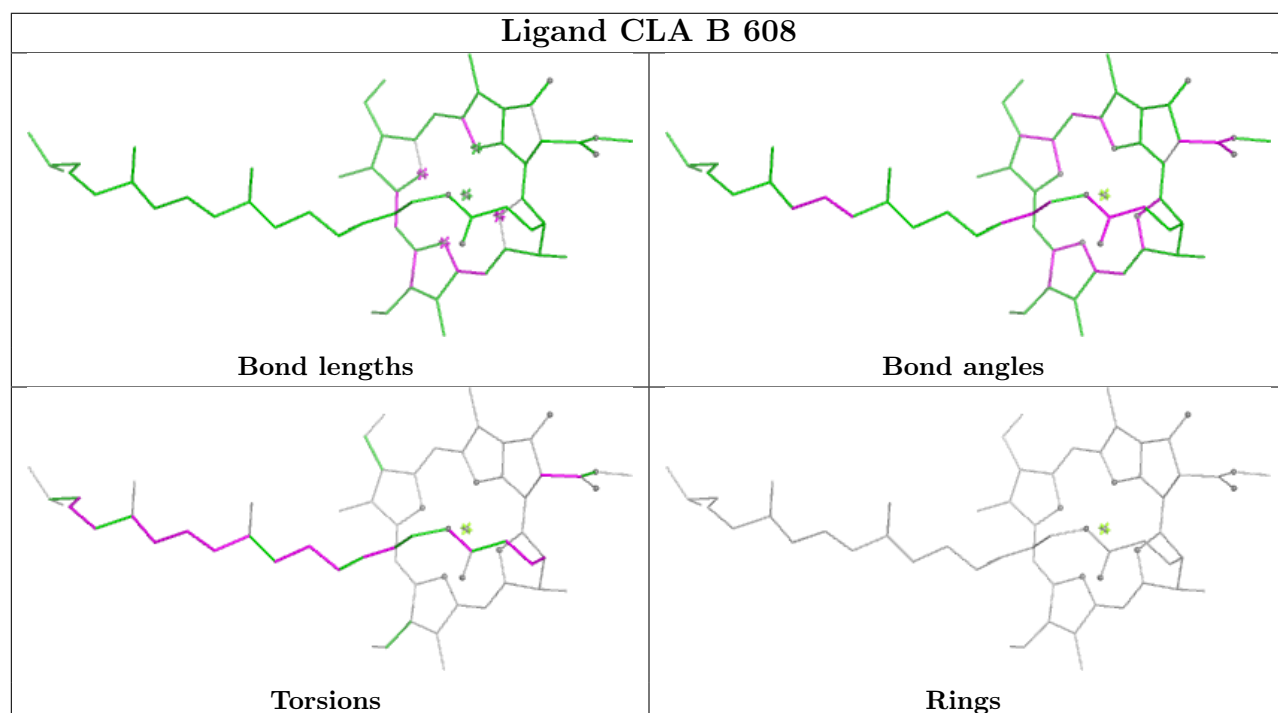
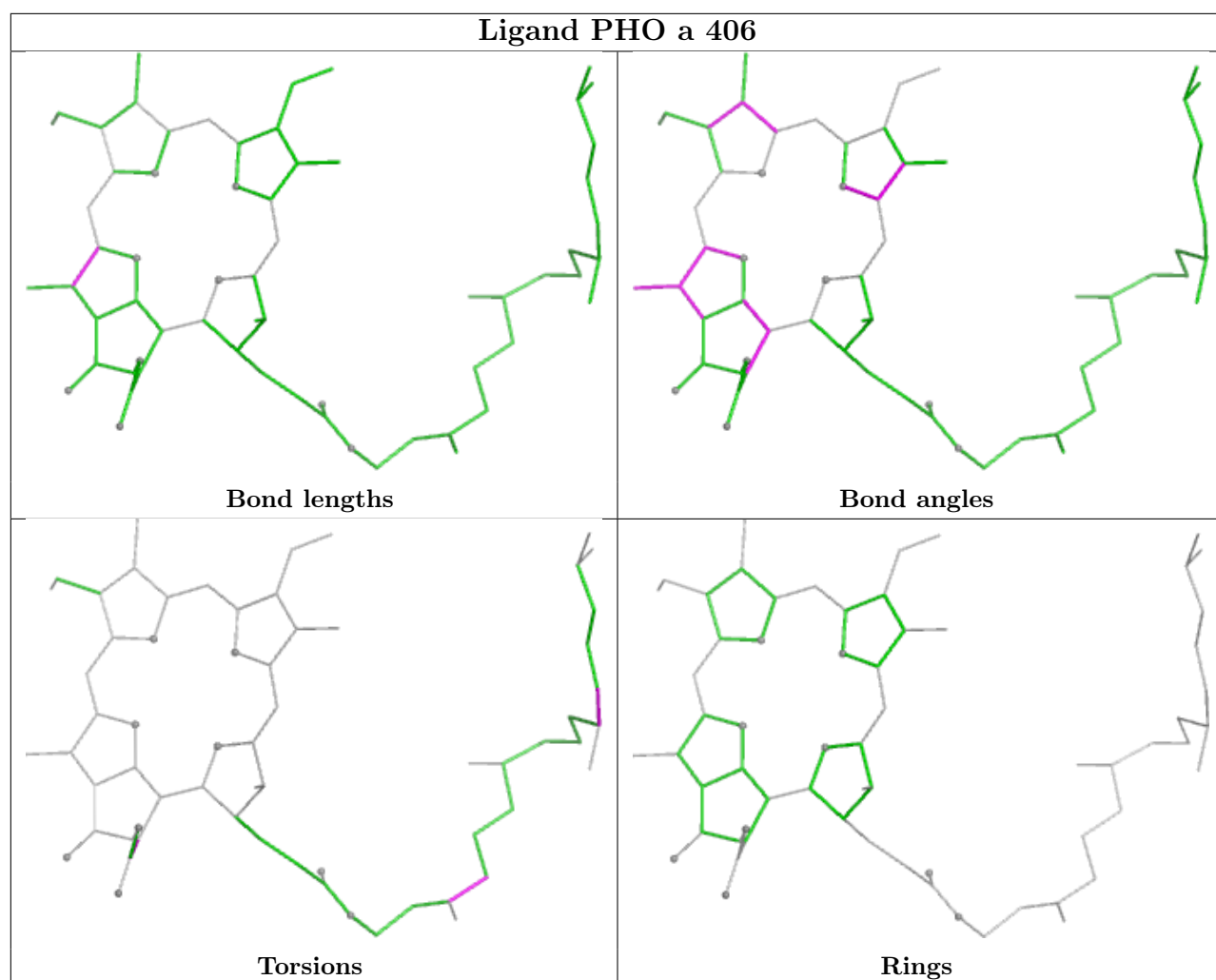


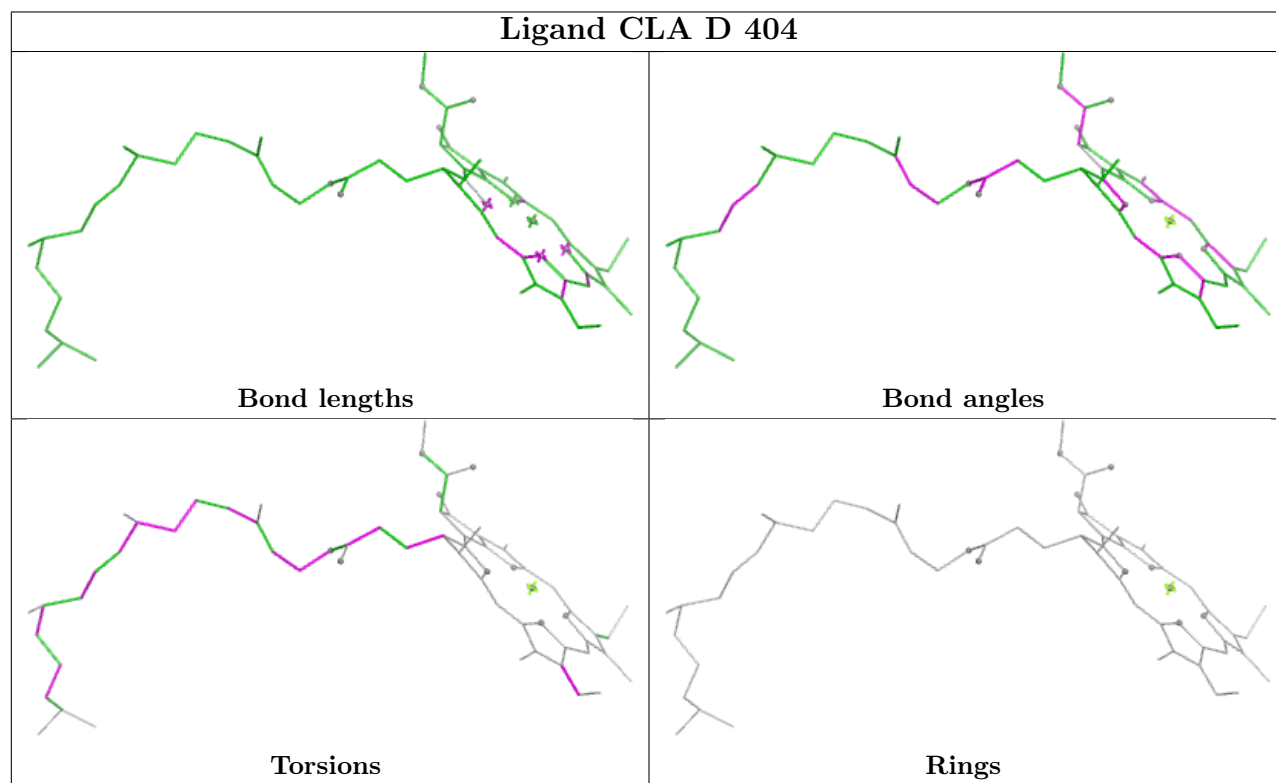
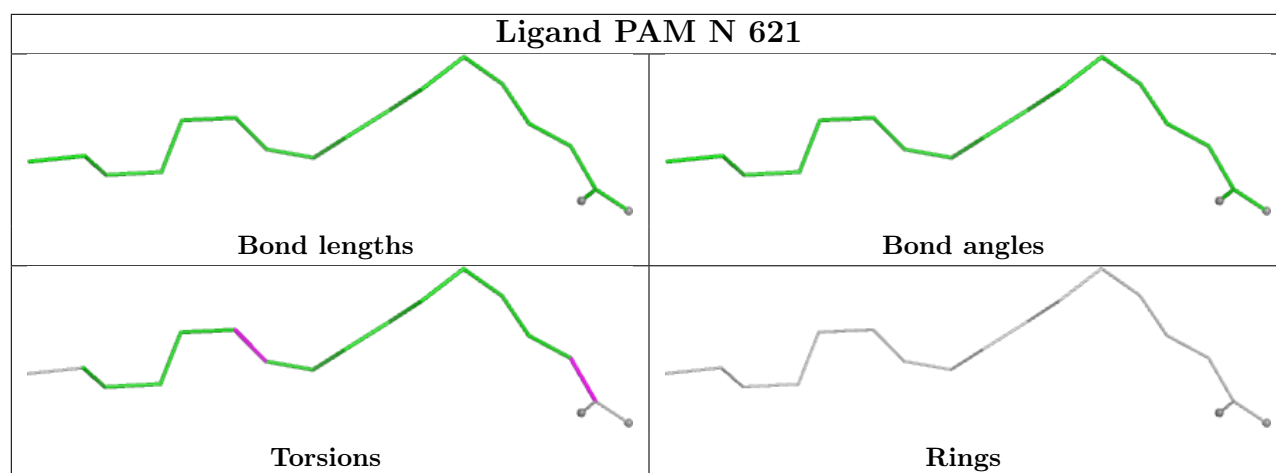


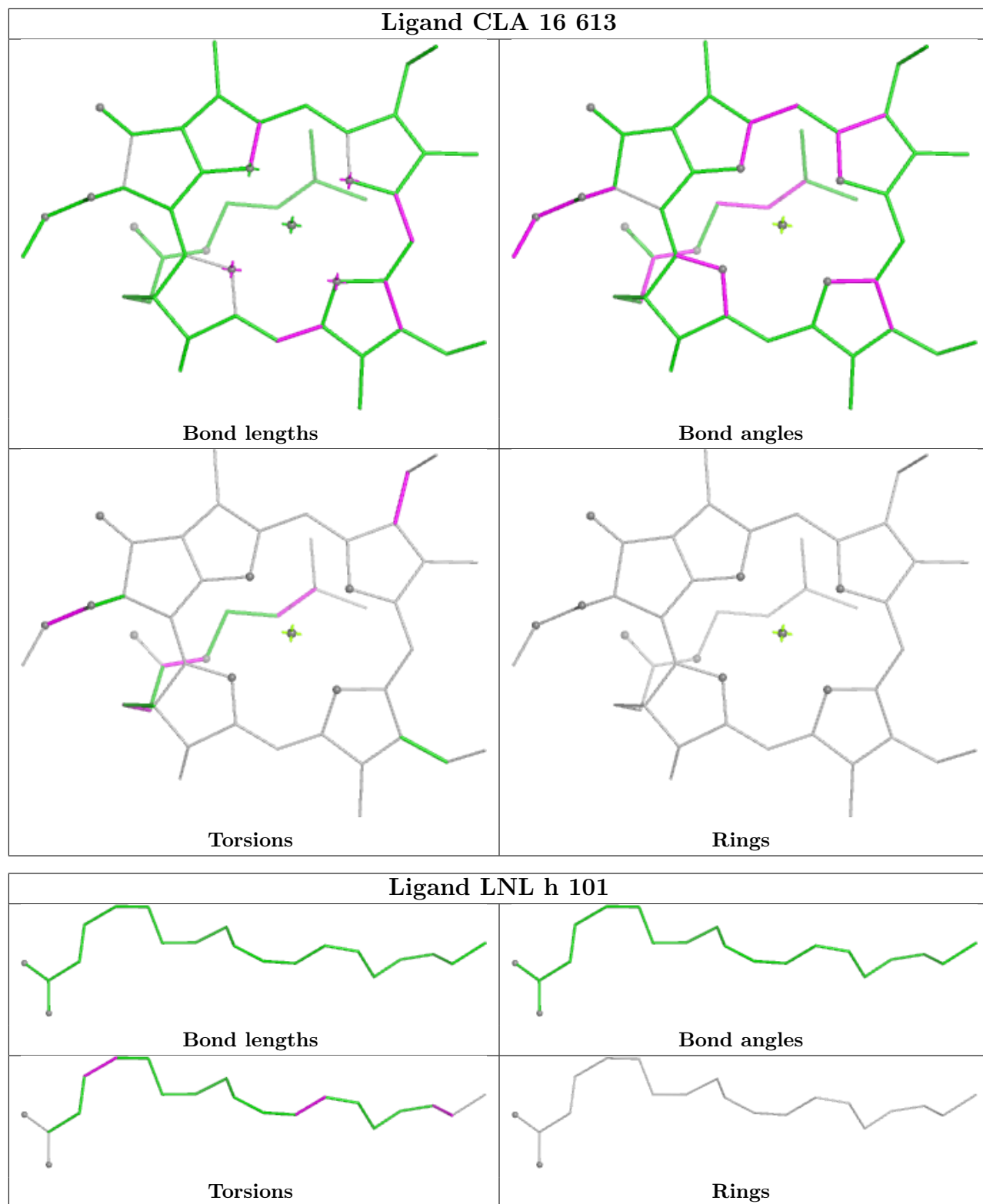


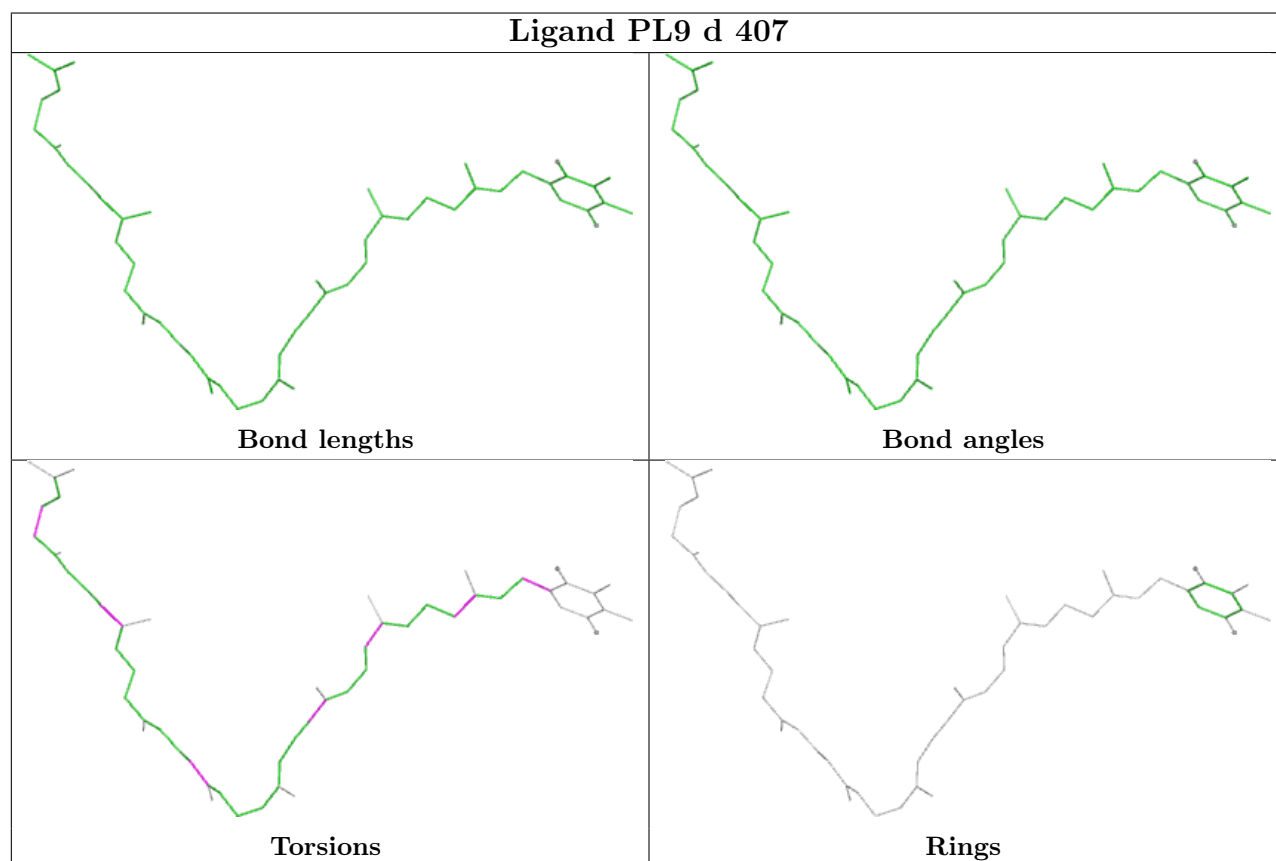
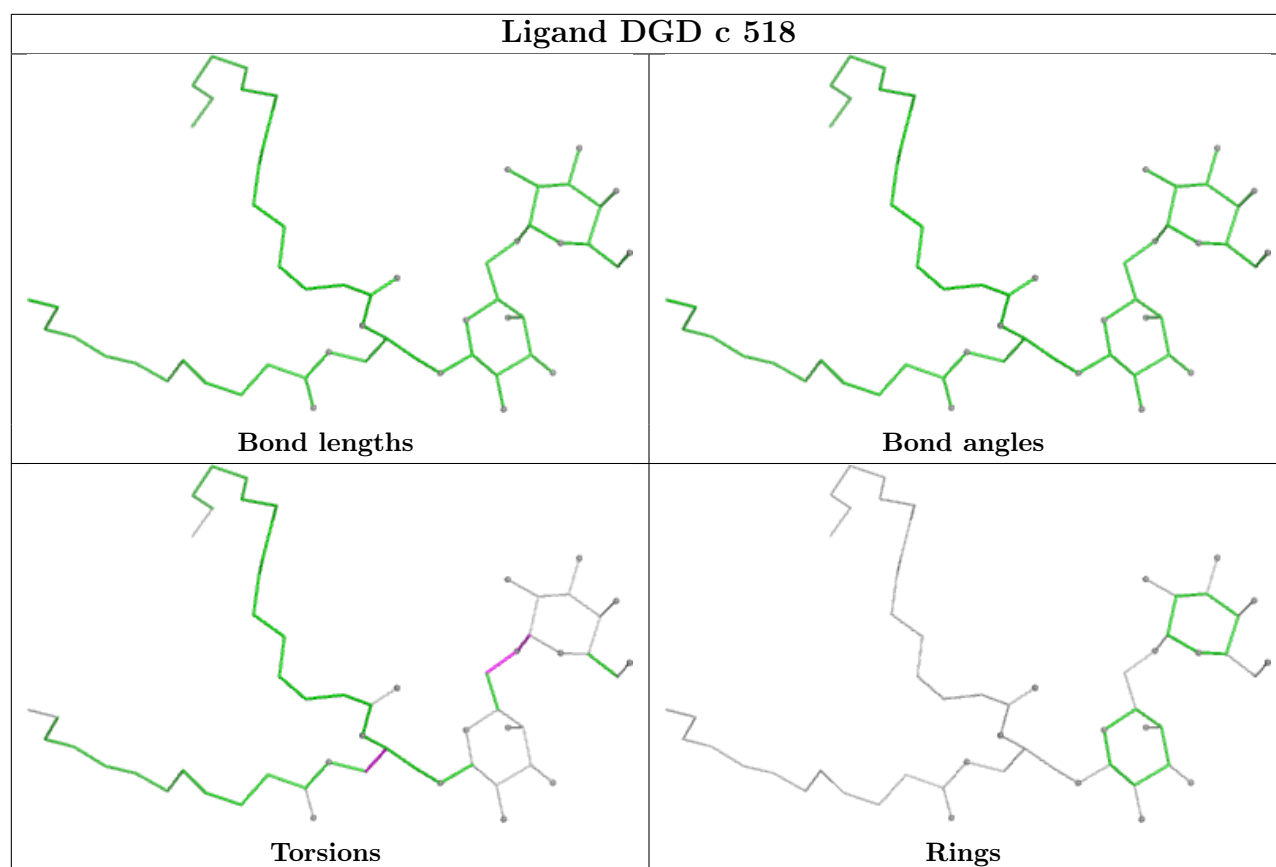
Ligand CLA B 613**Ligand NEX 15 616**

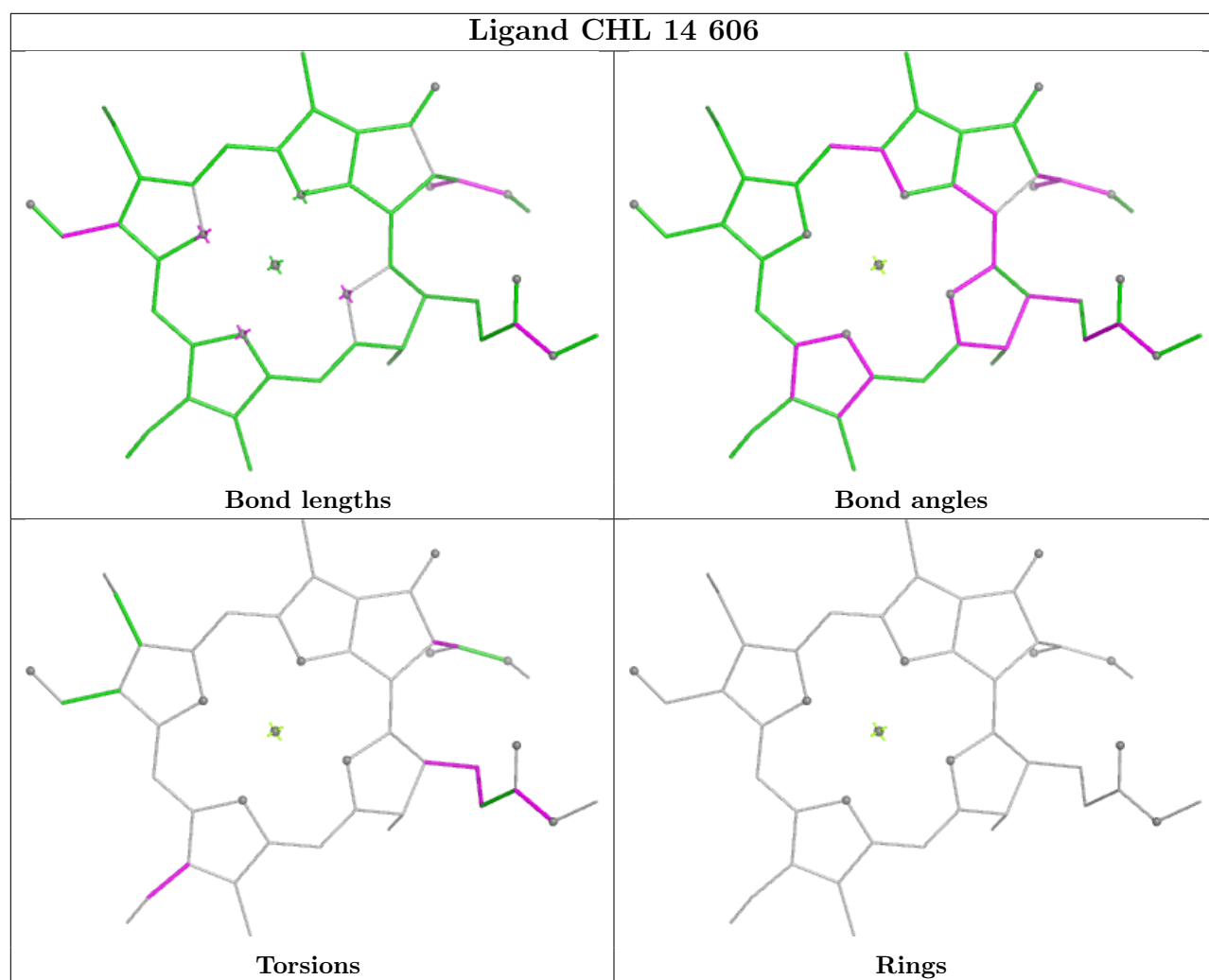


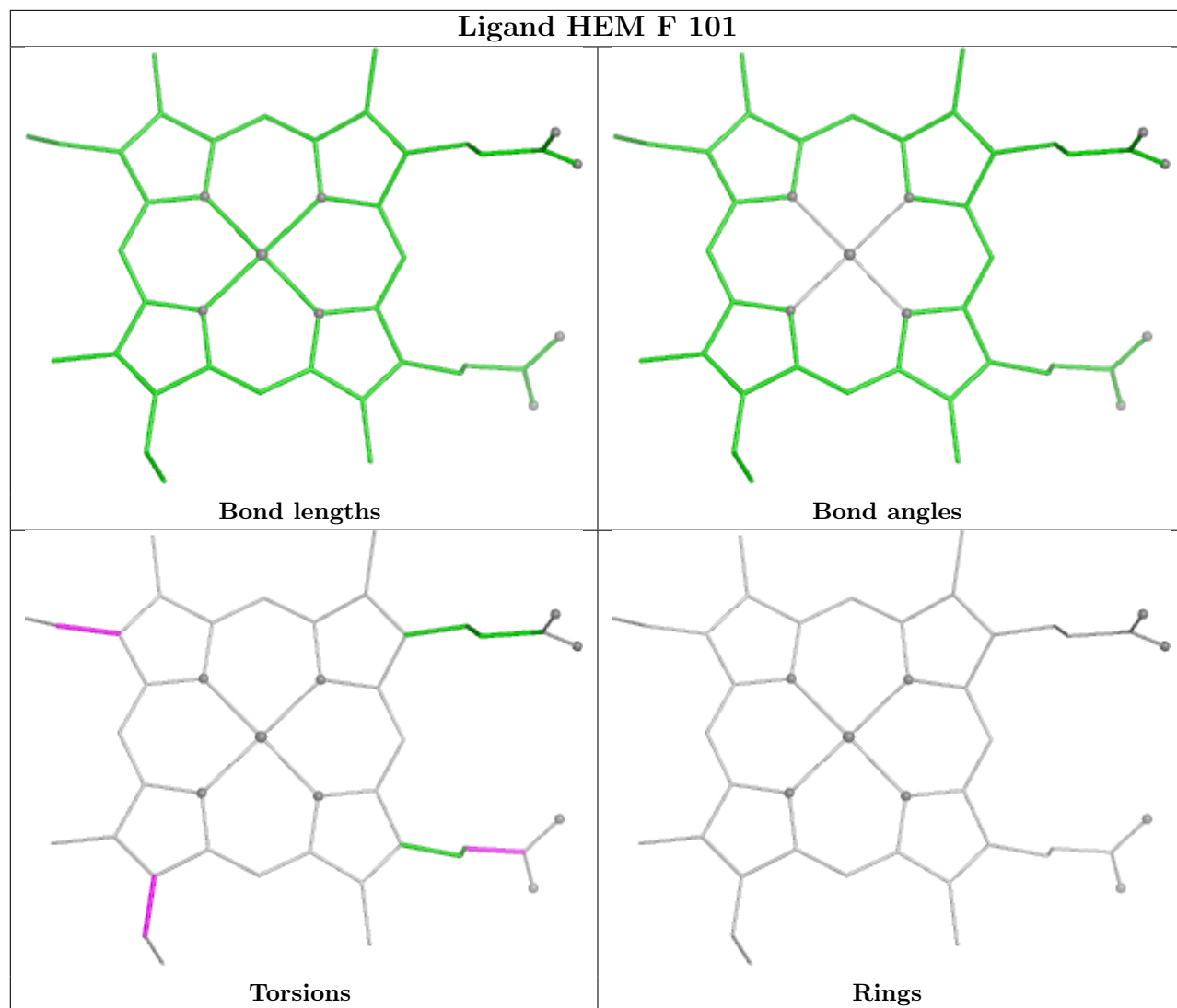


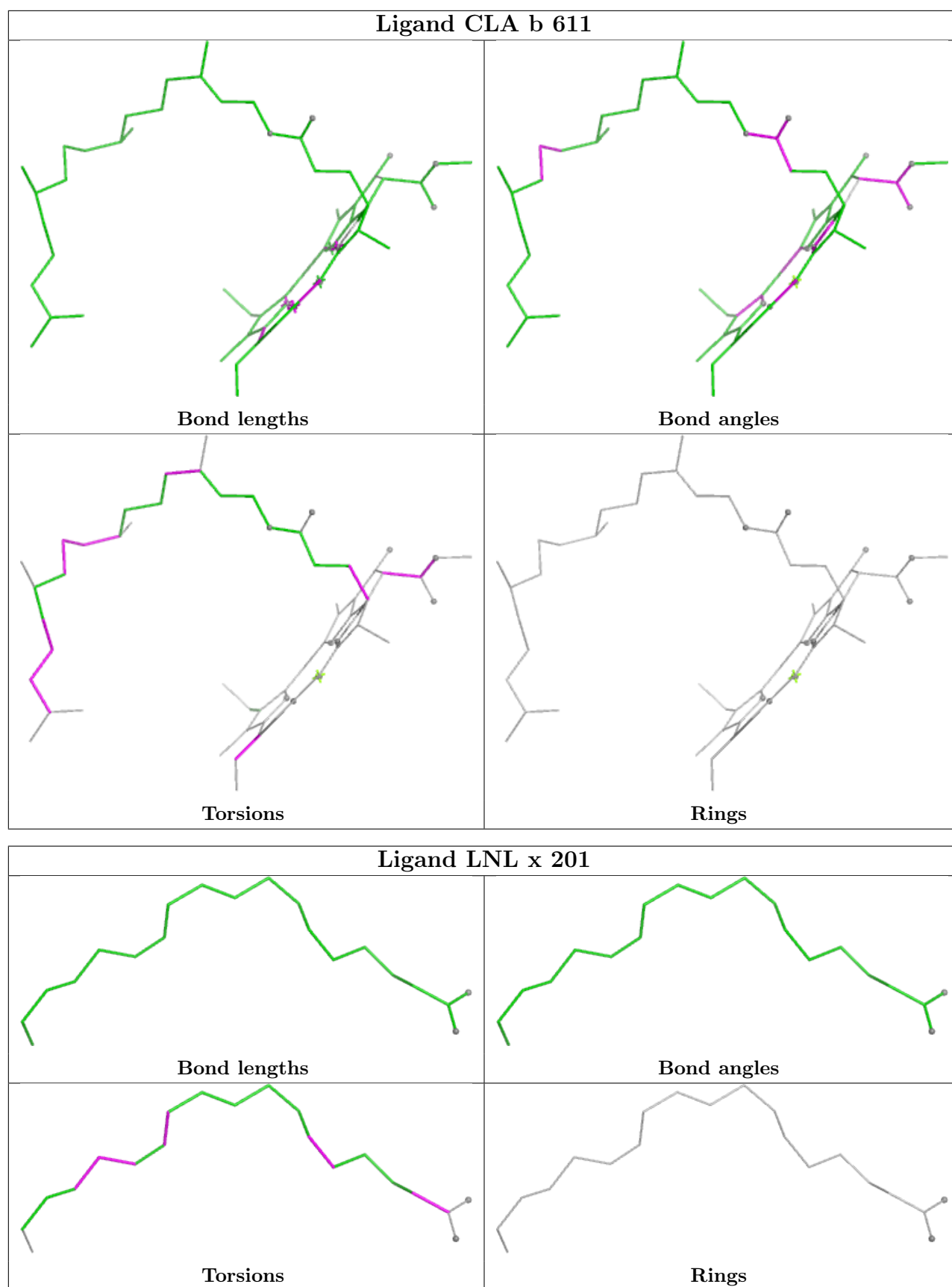




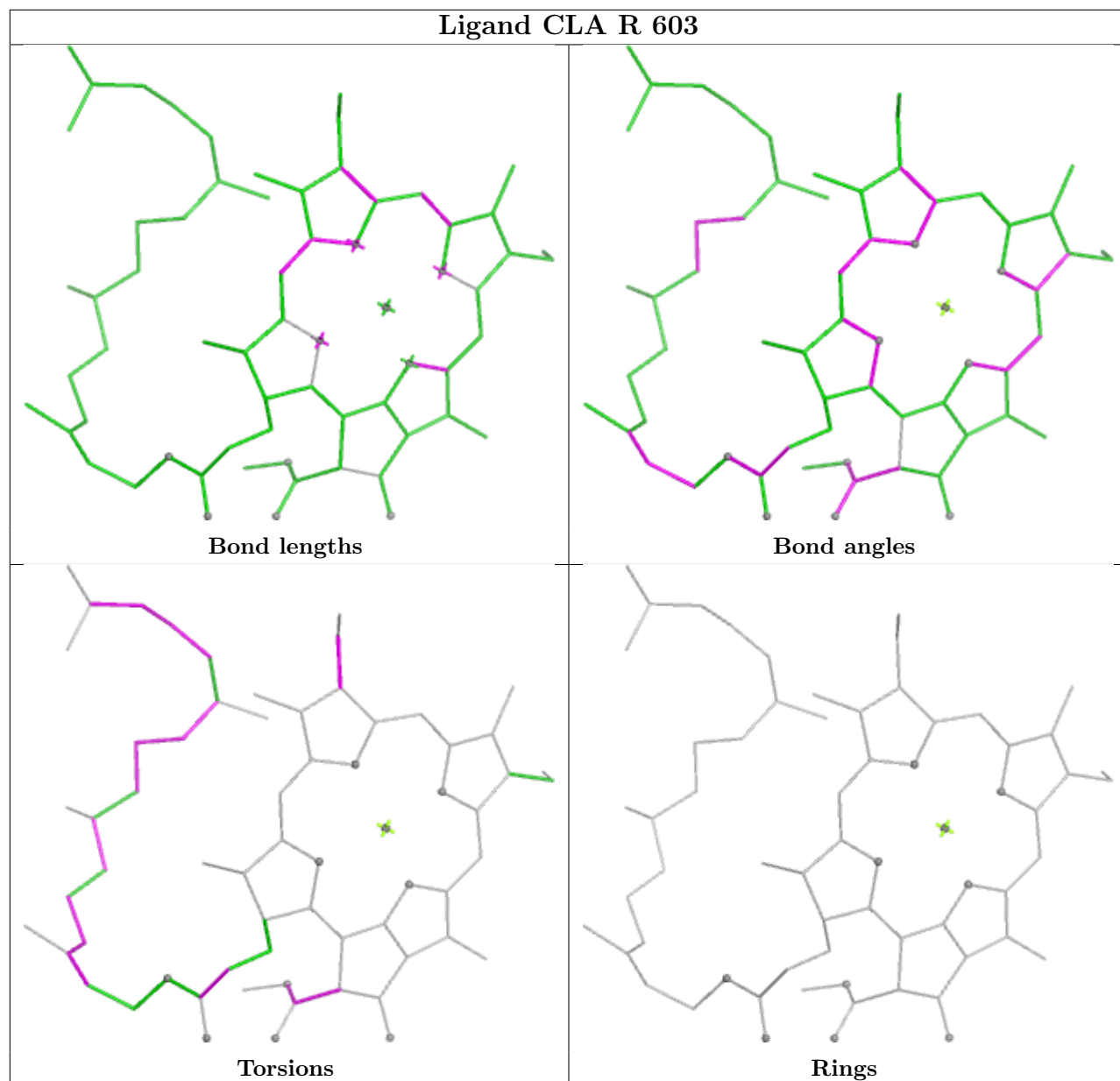


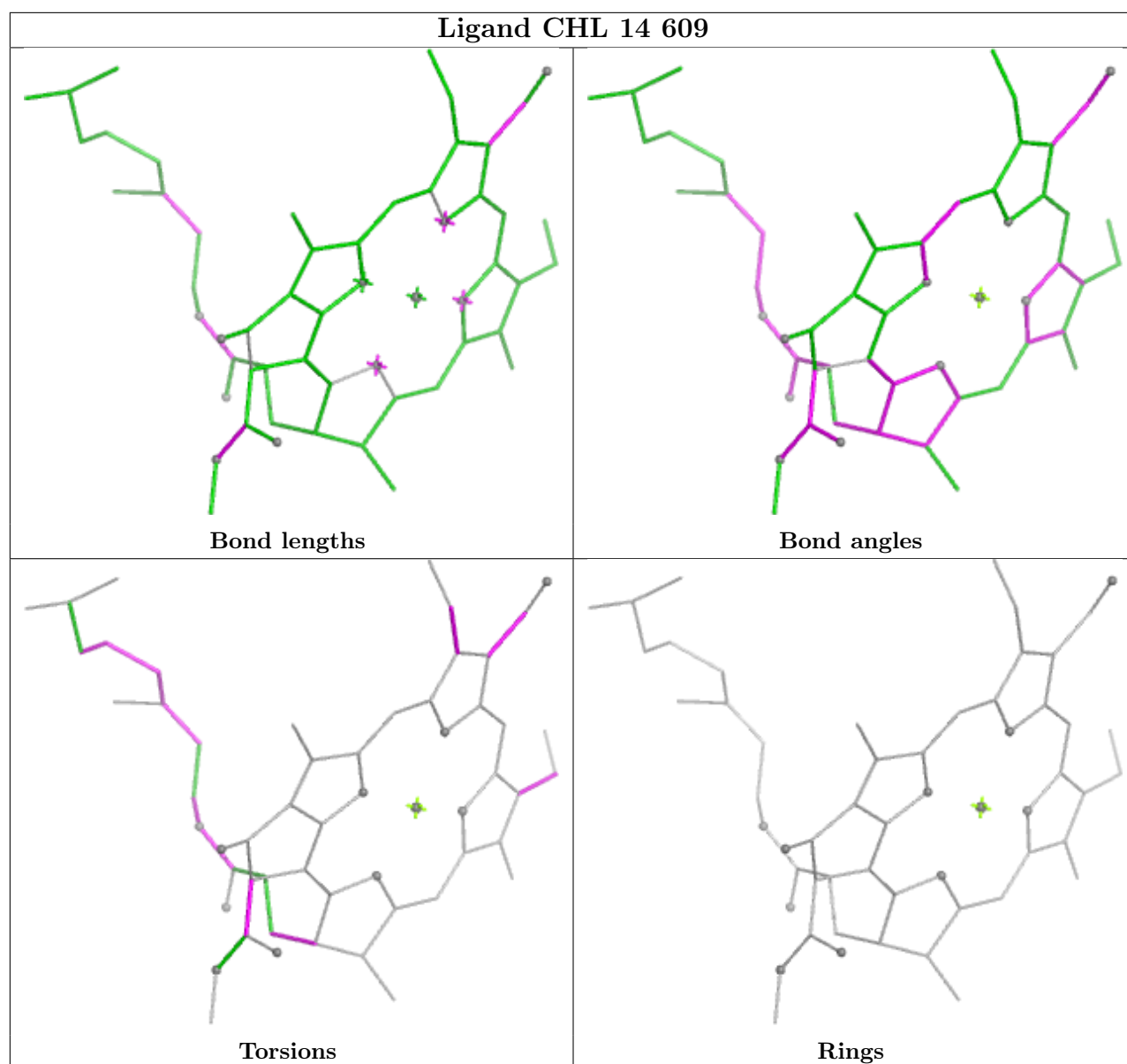


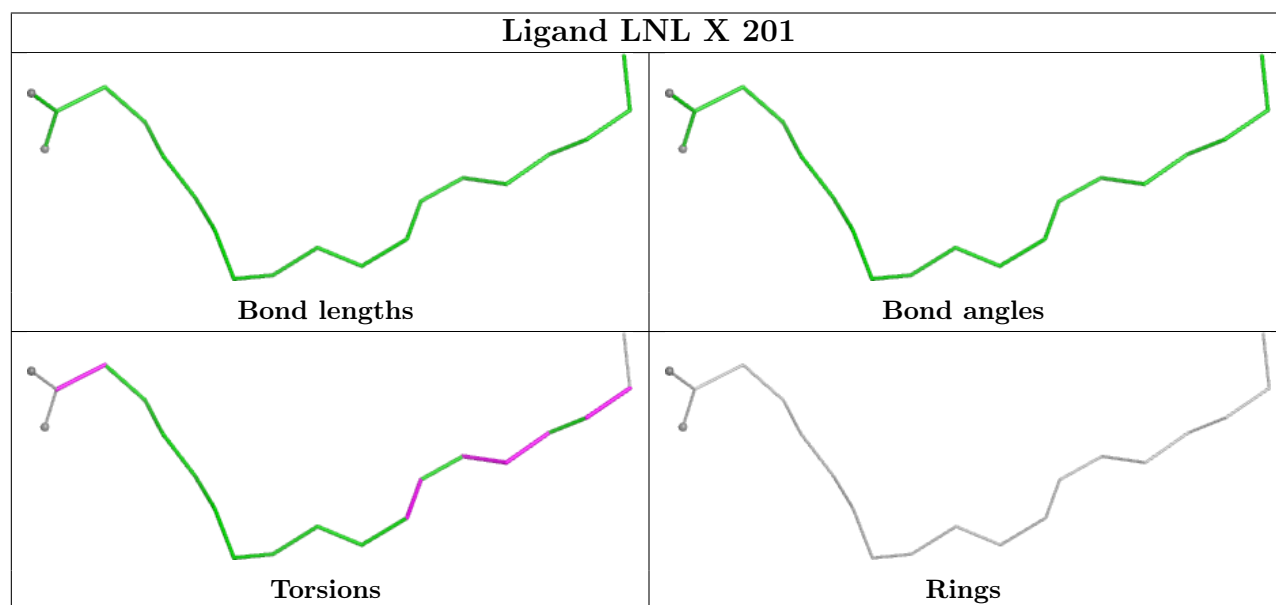
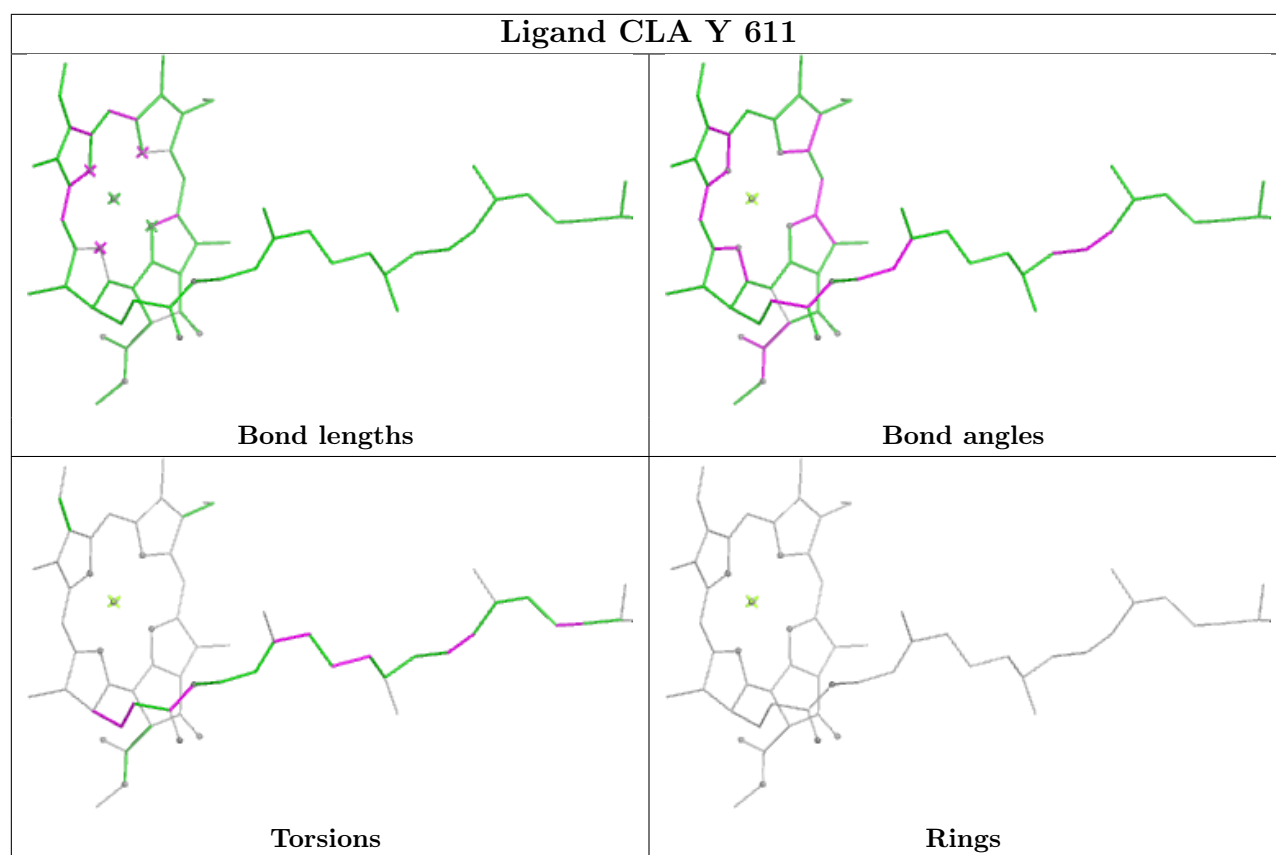


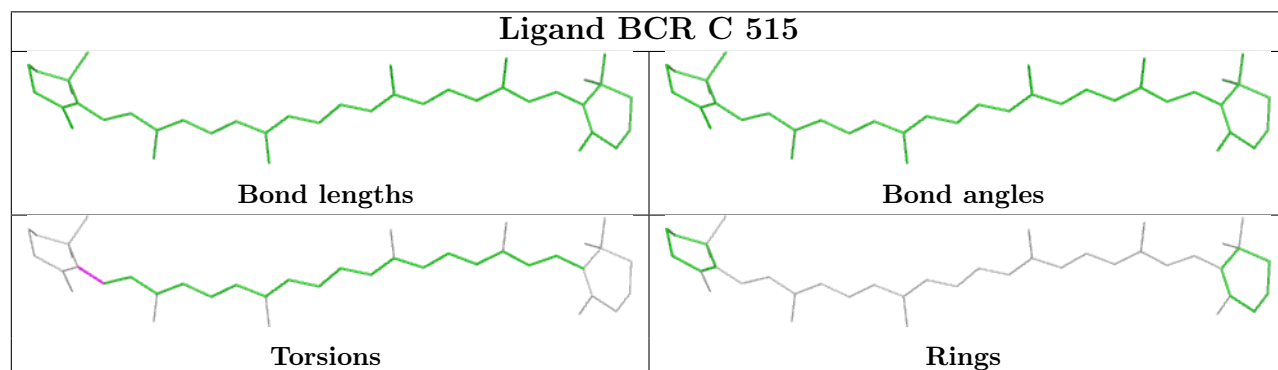
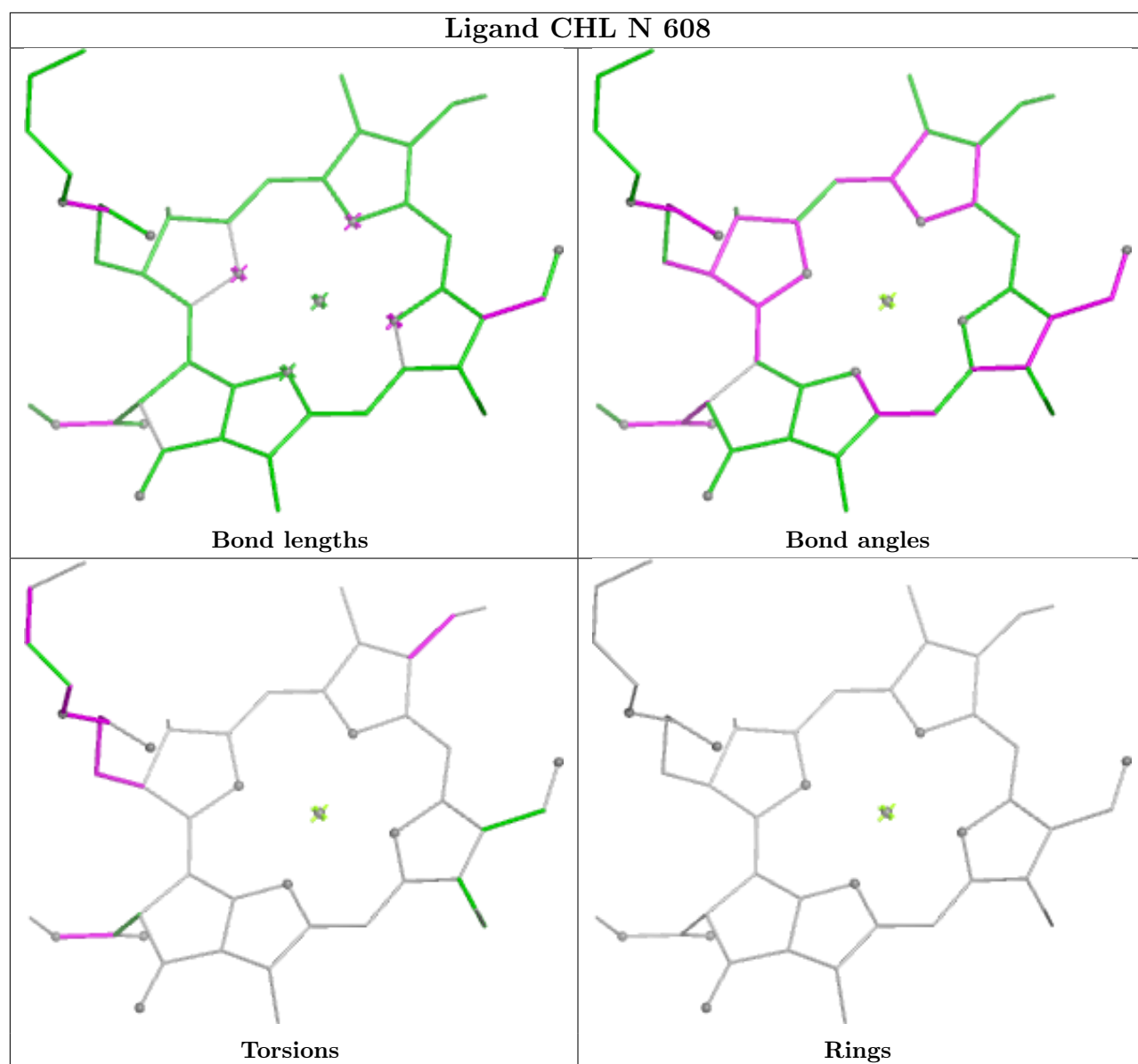


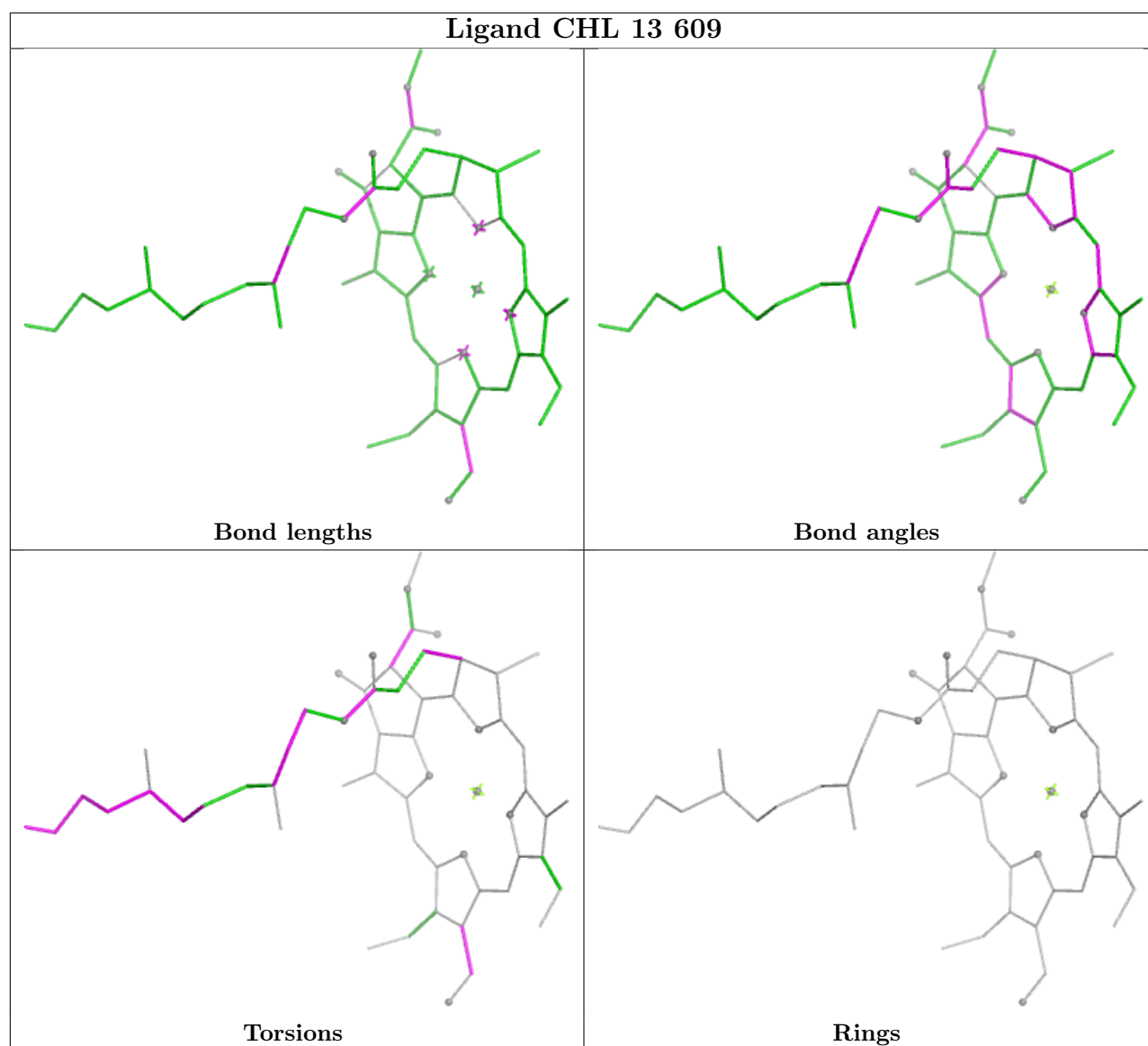
Ligand CLA R 603



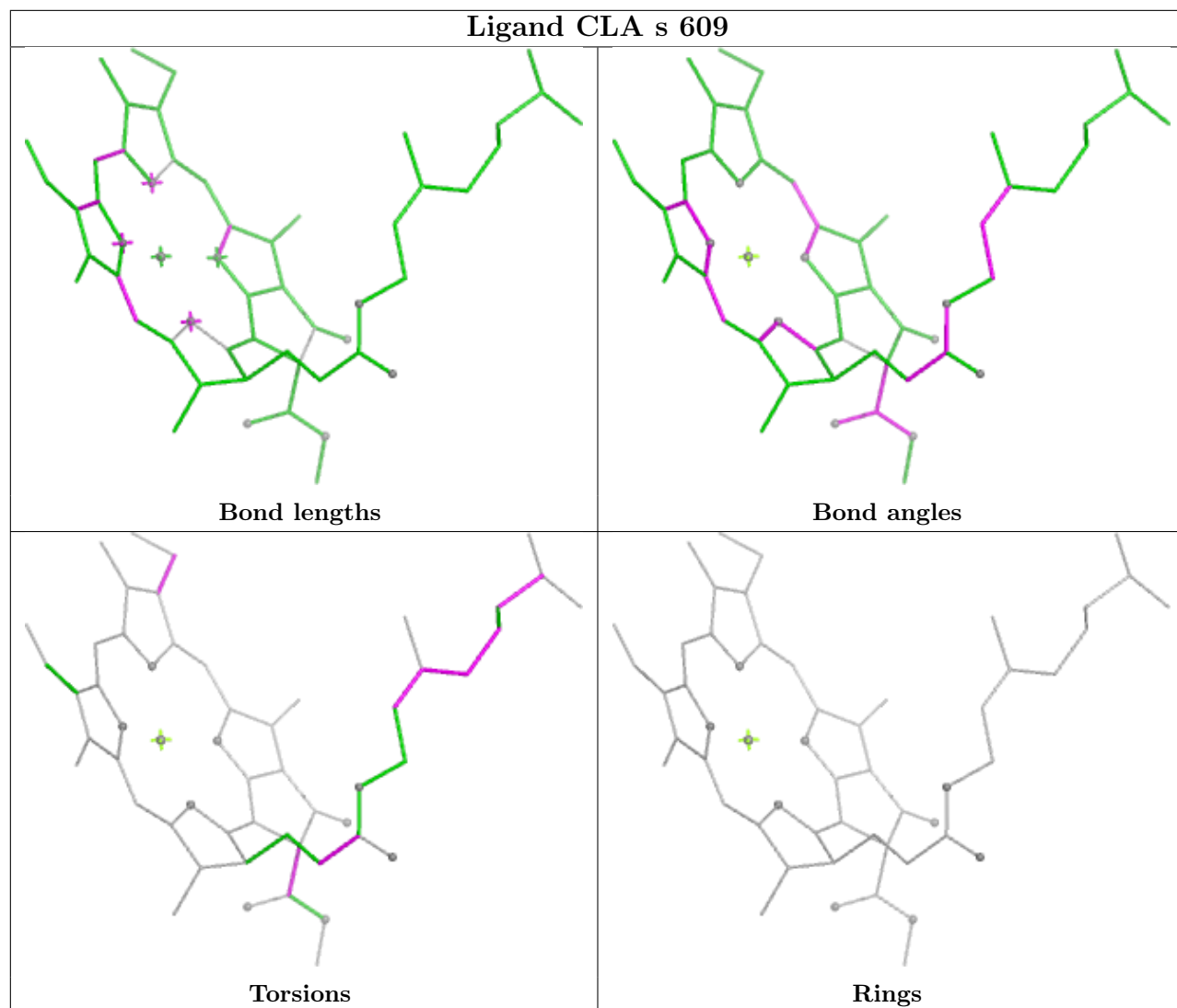




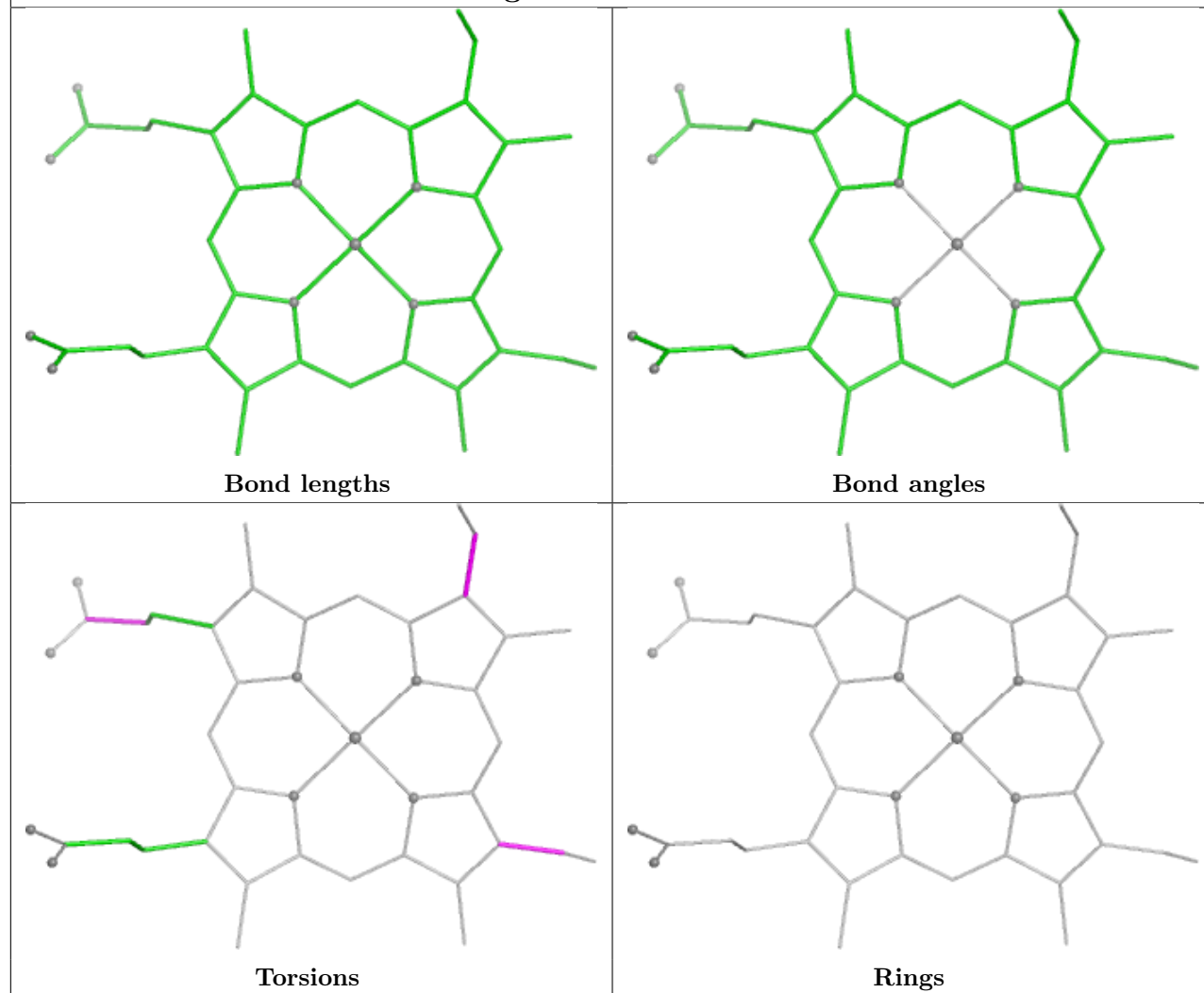


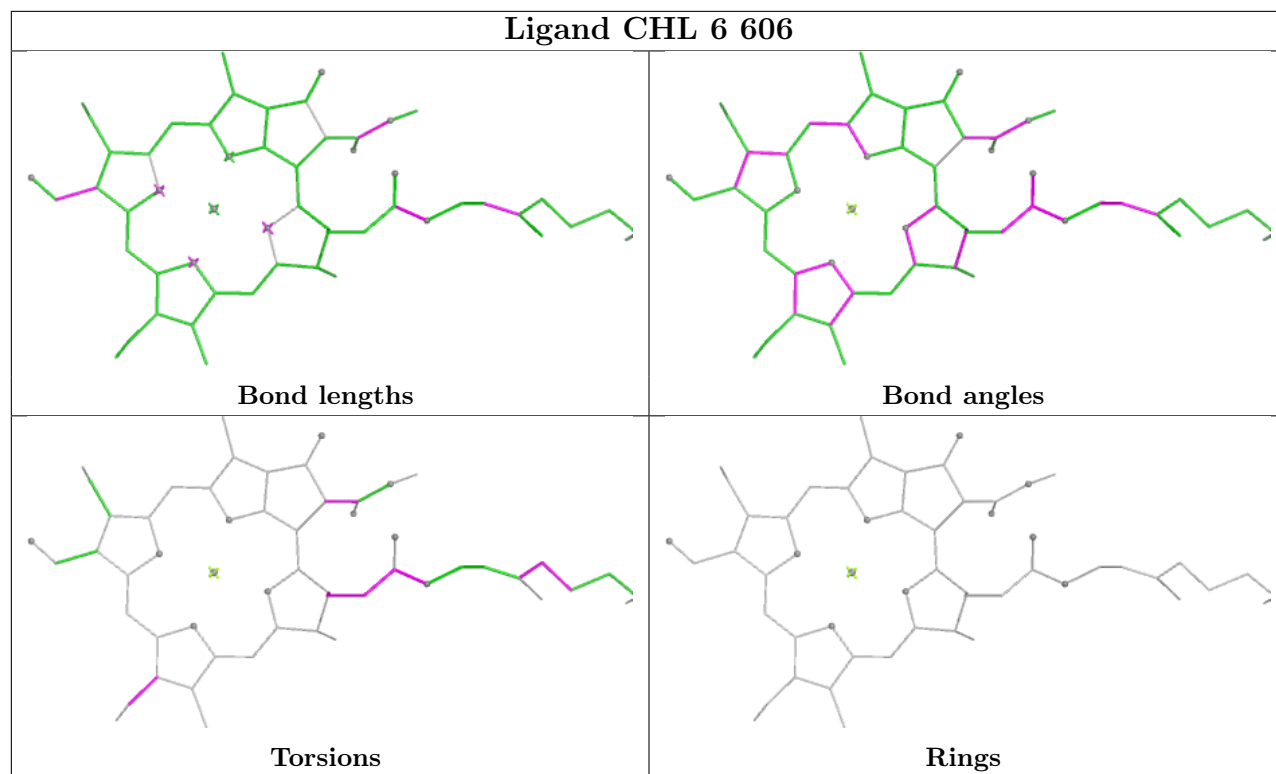
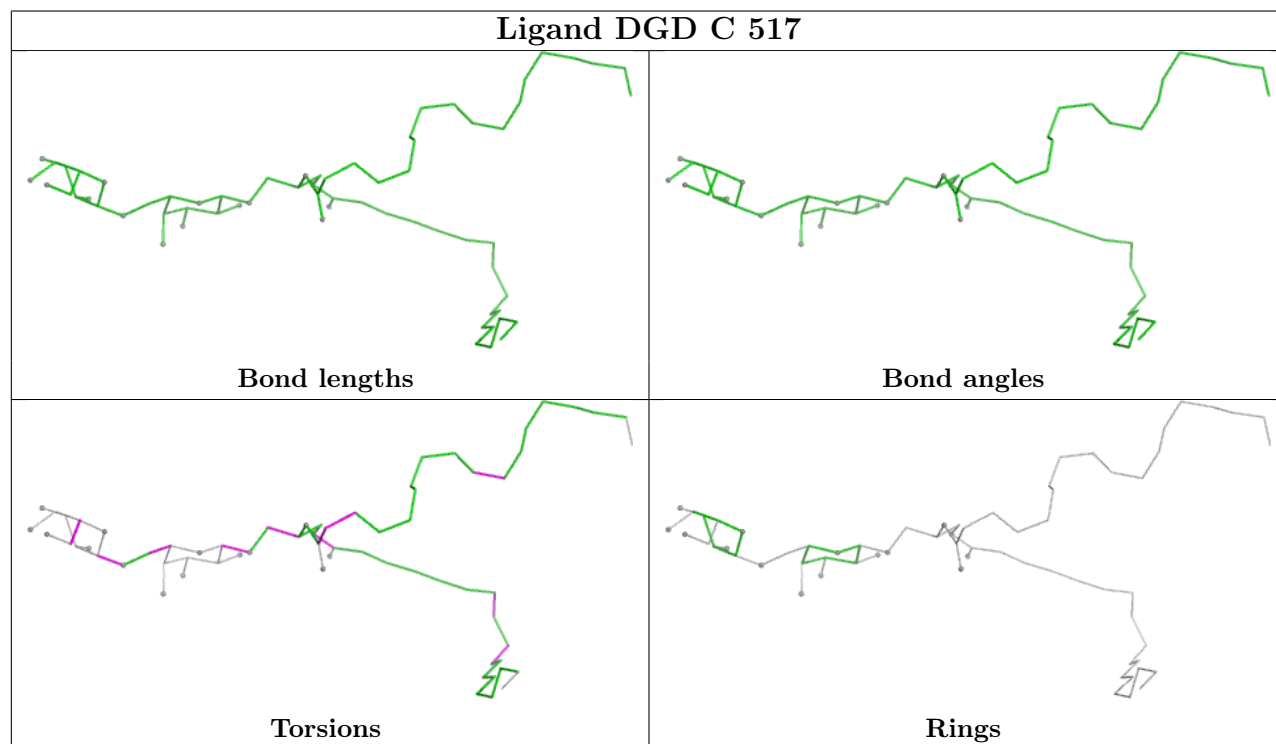


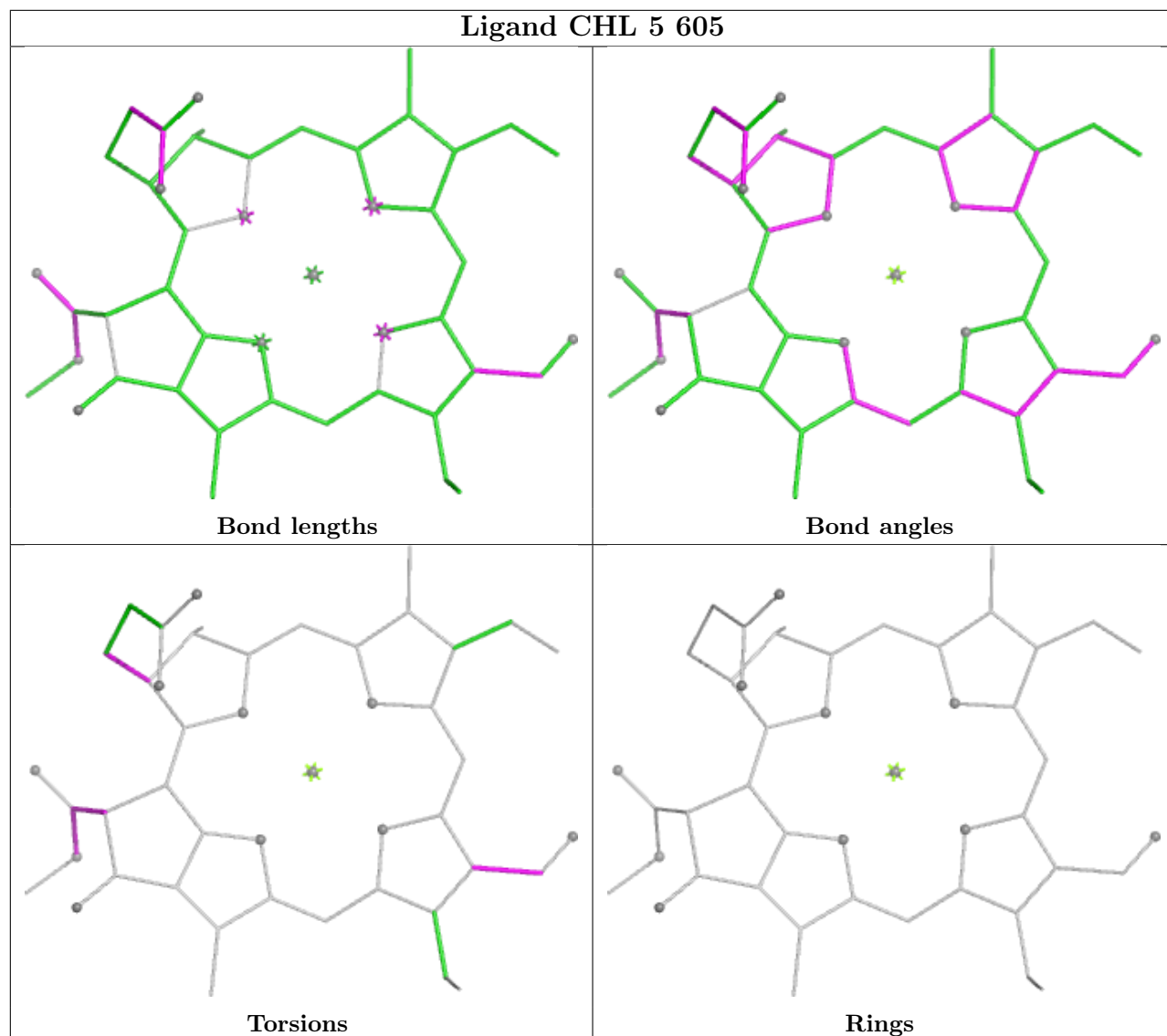
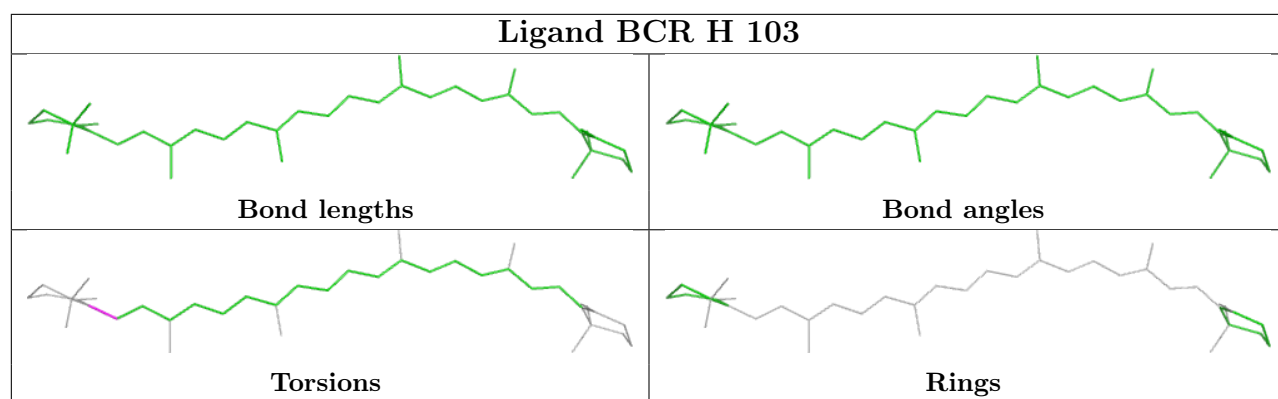
Ligand CLA s 609



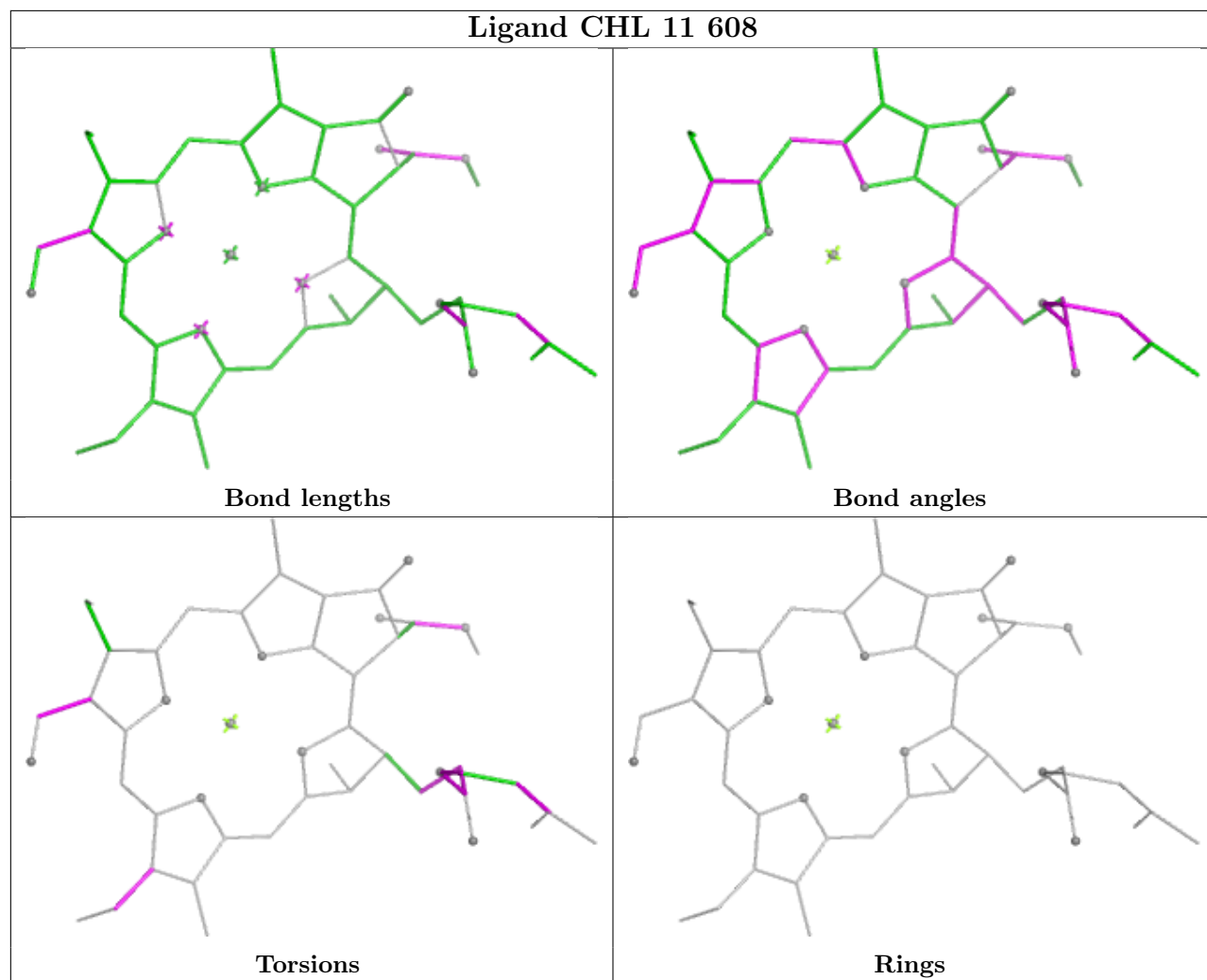
Ligand HEM f 101

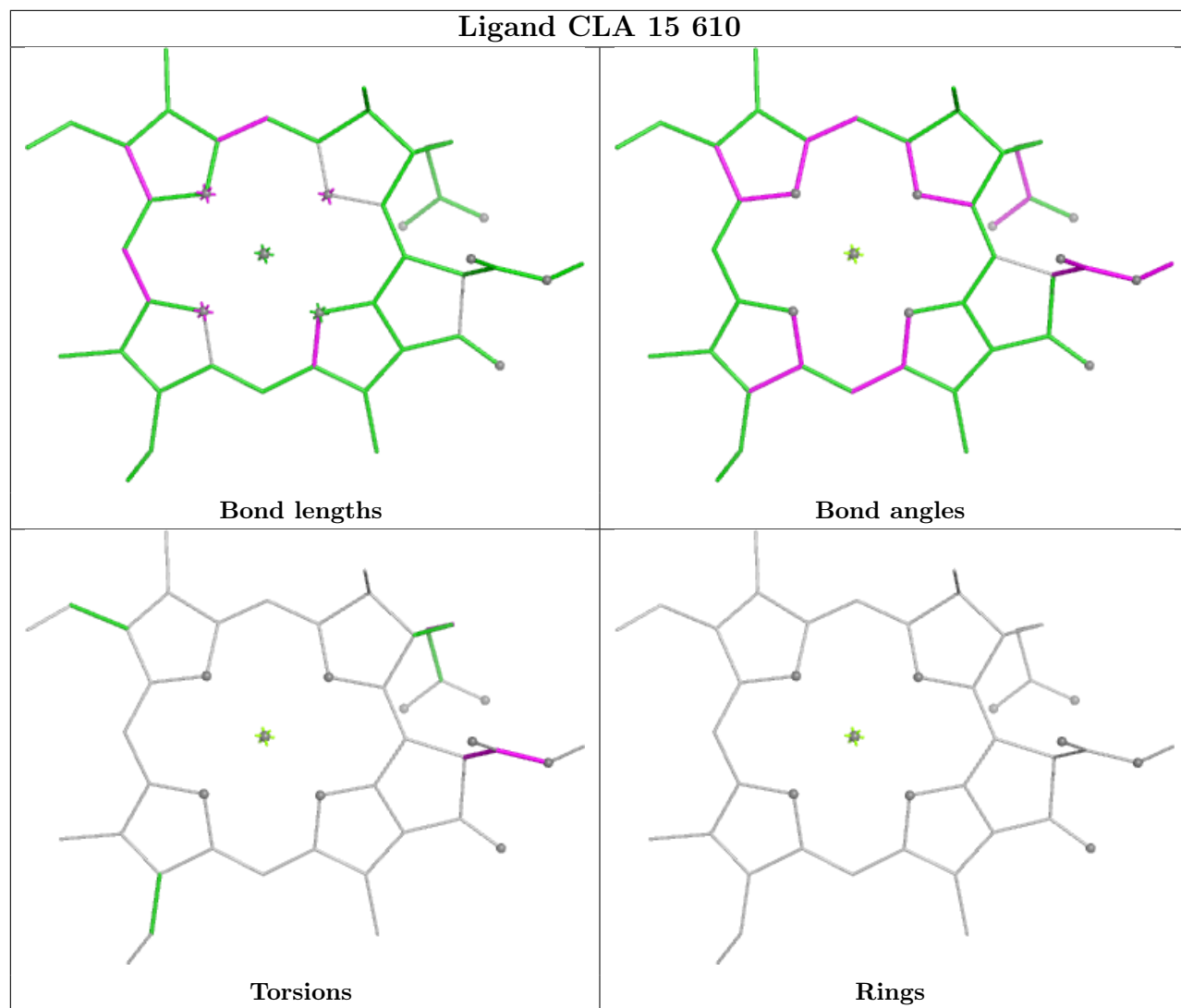


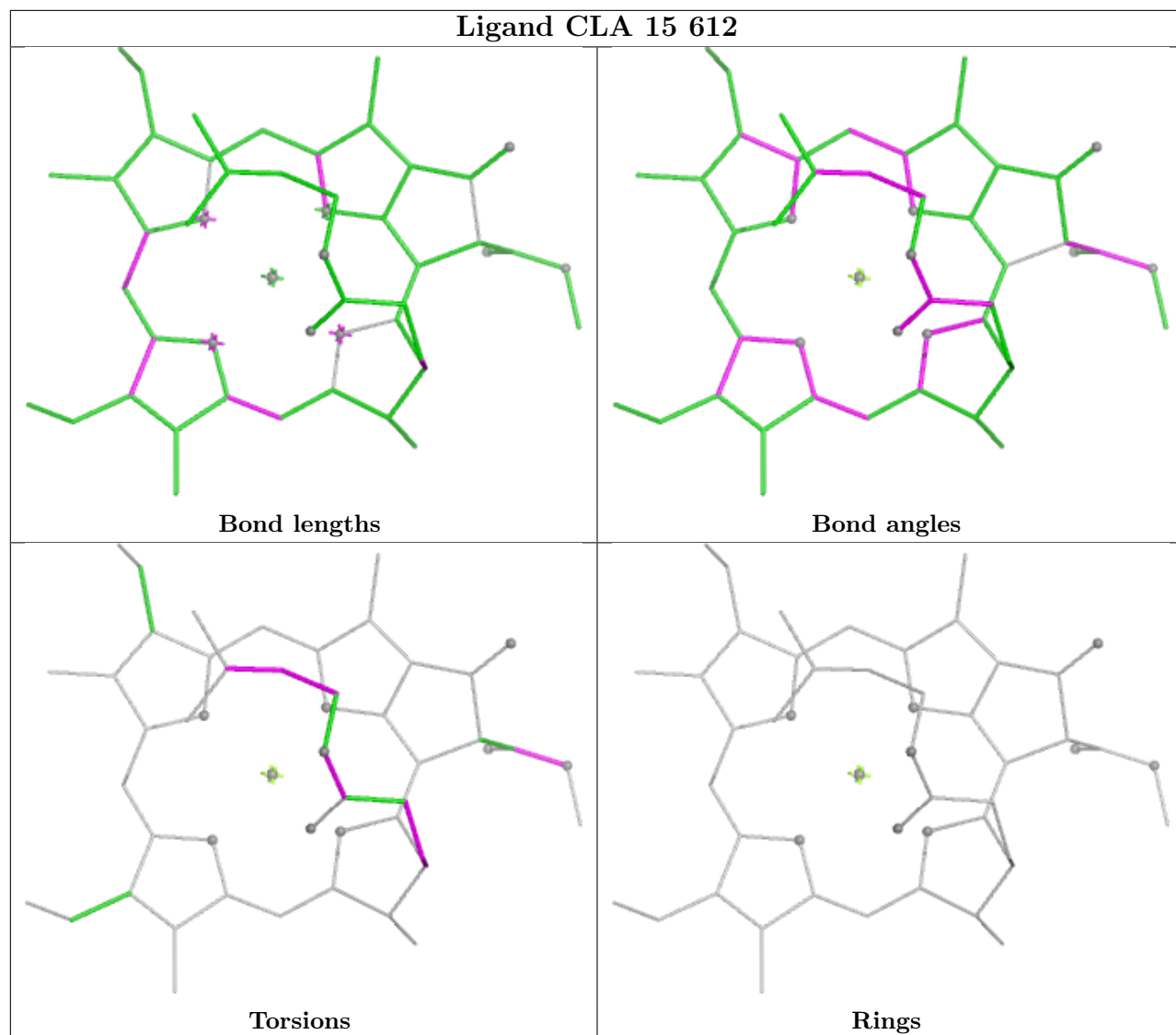
Ligand CHL 6 606**Ligand DGD C 517**

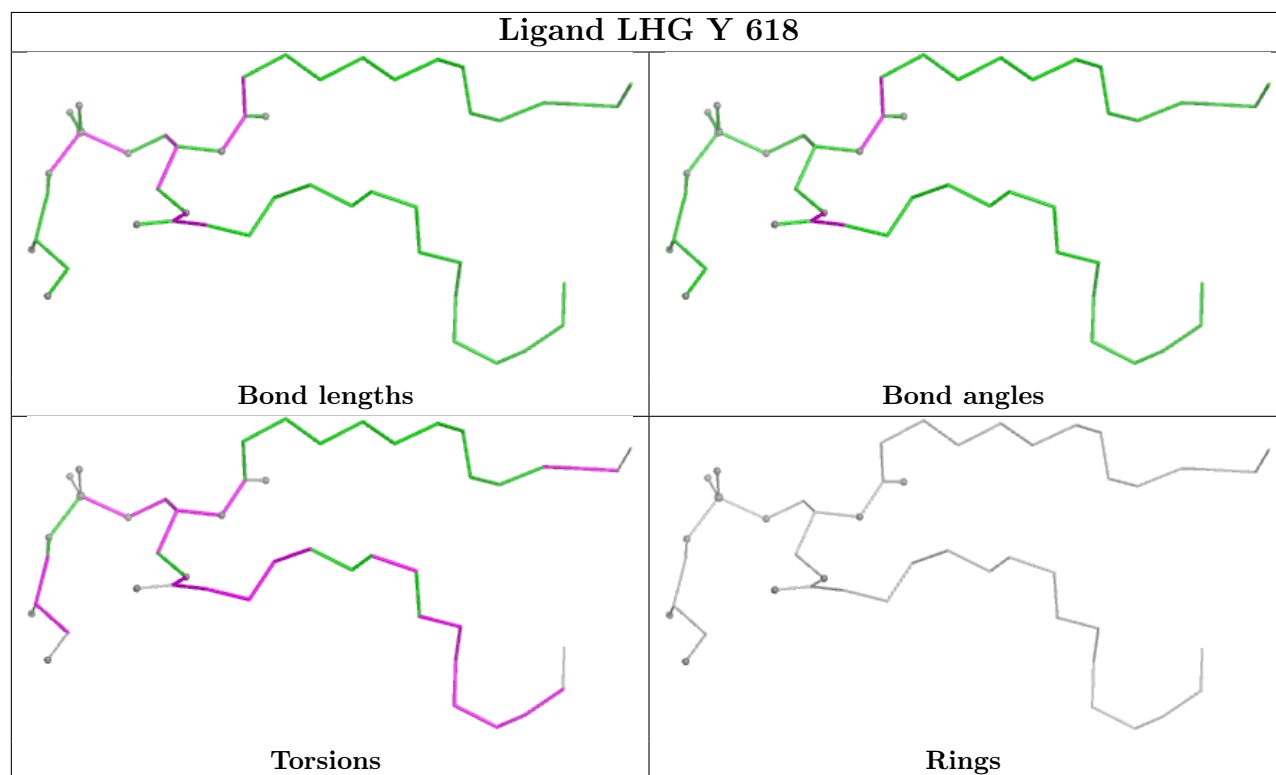
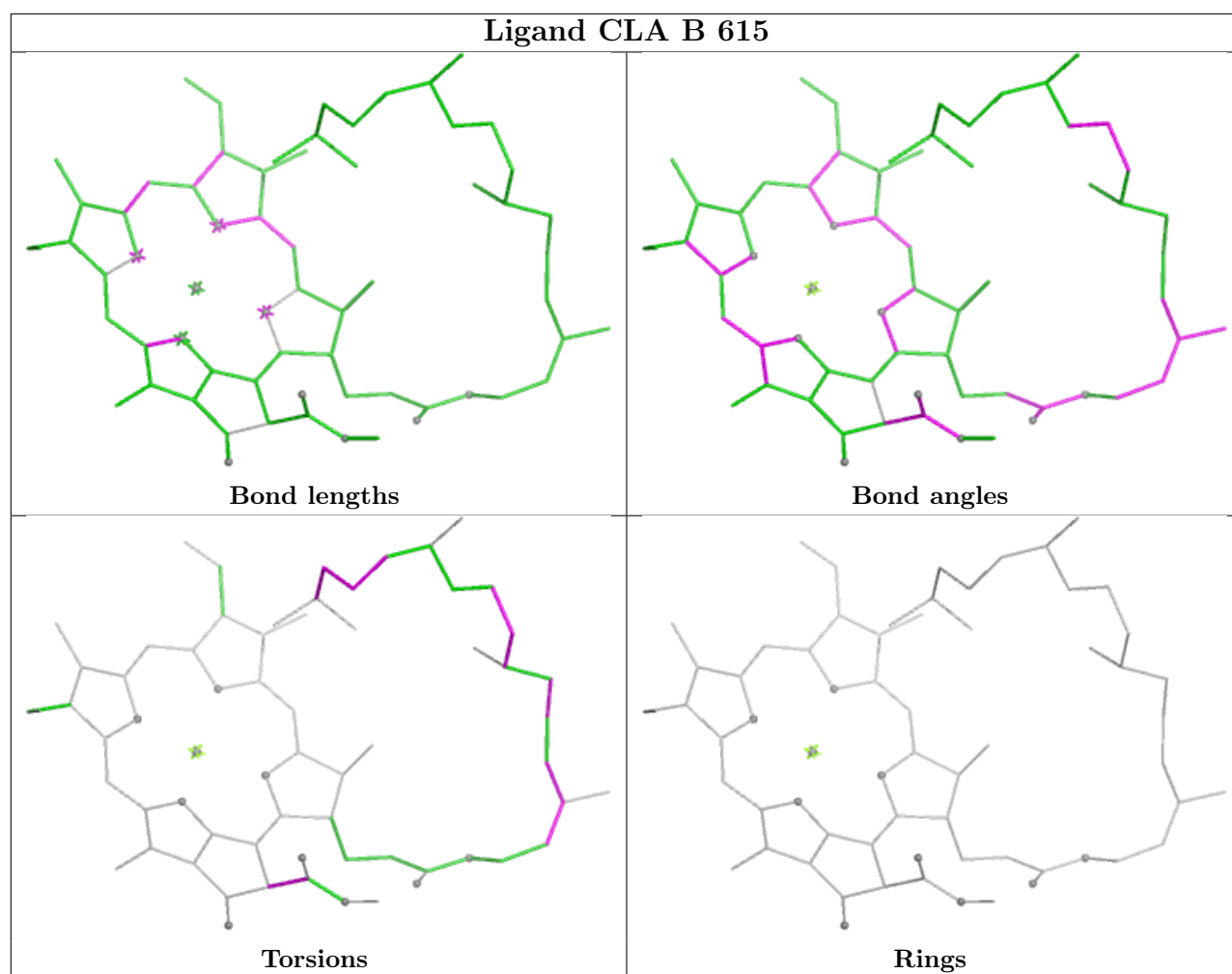


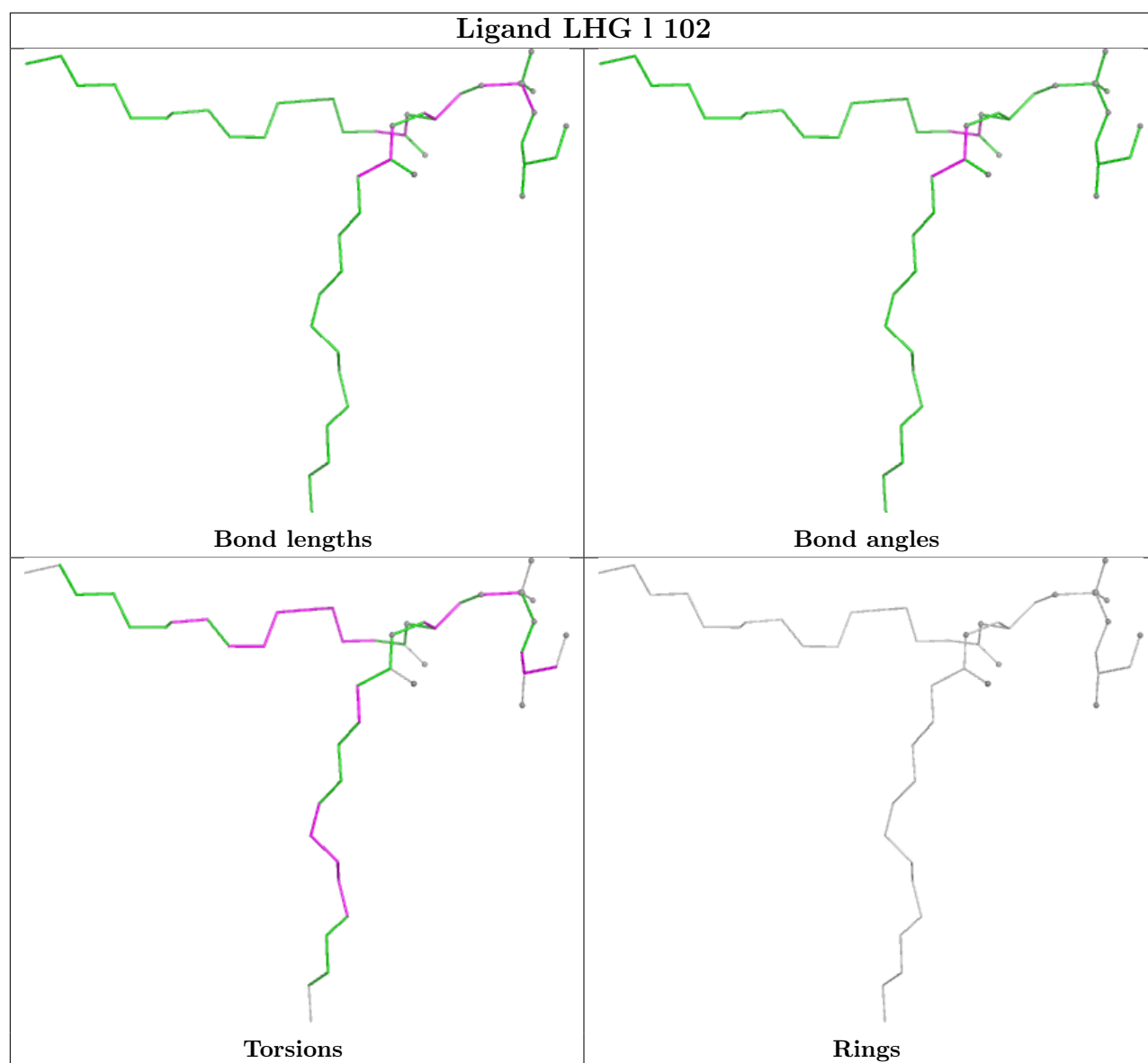
Ligand CHL 11 608



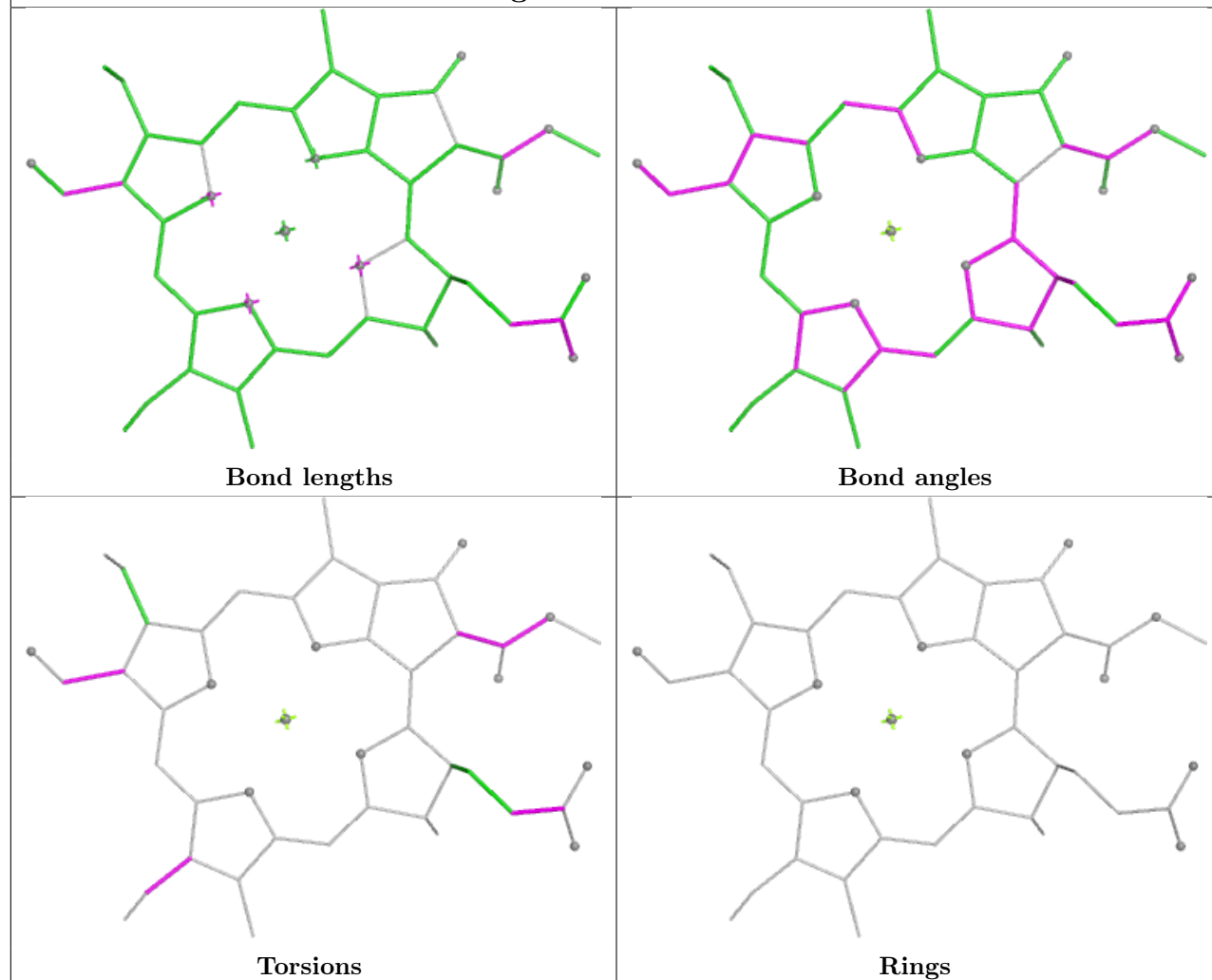




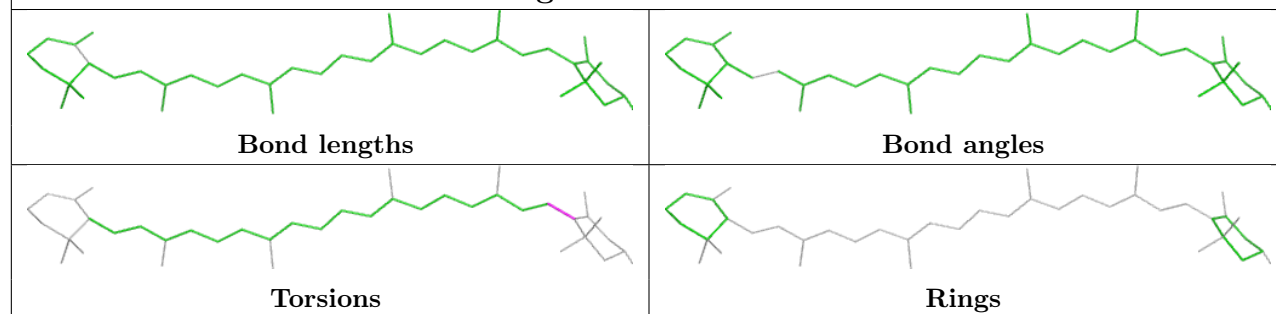


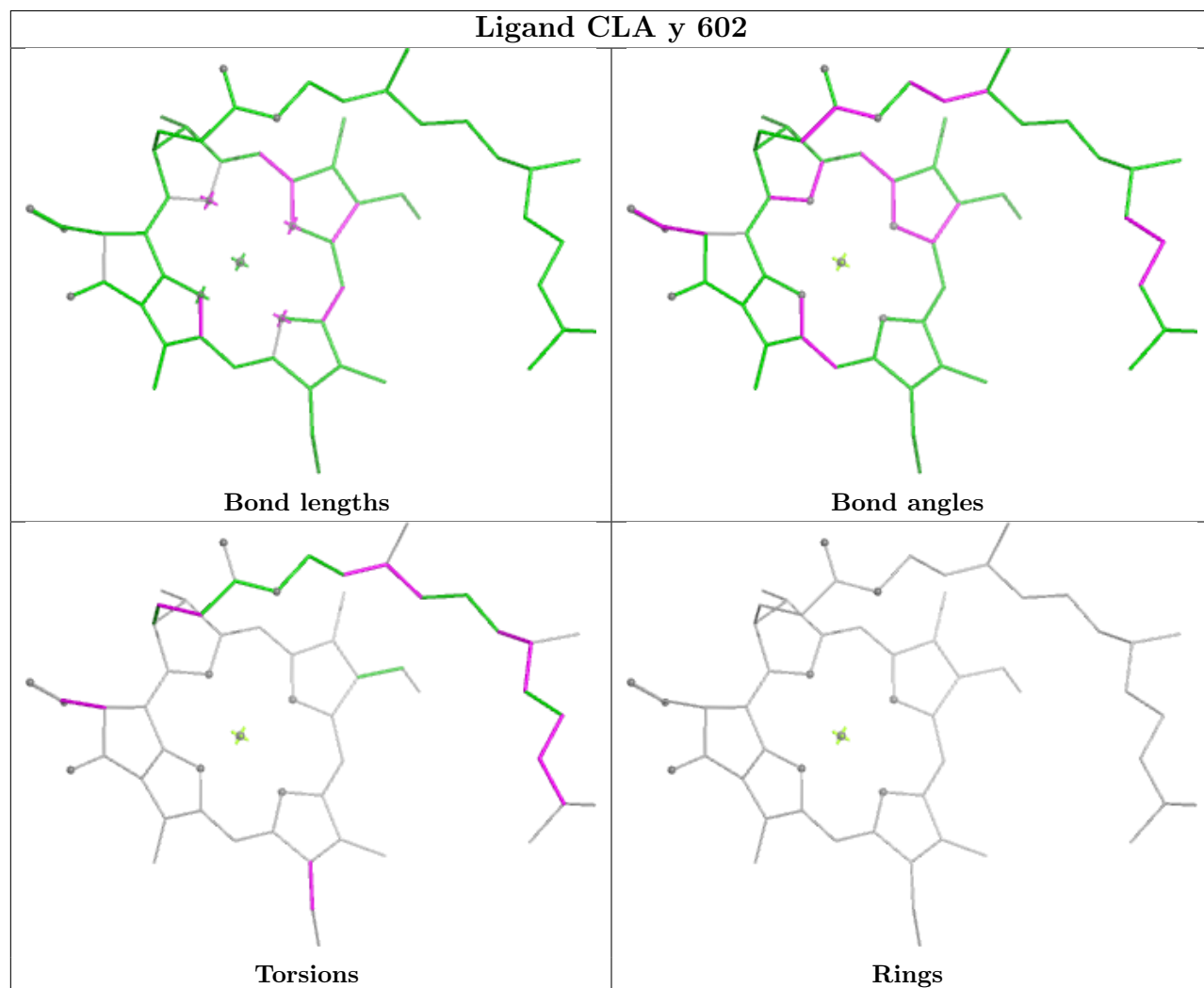
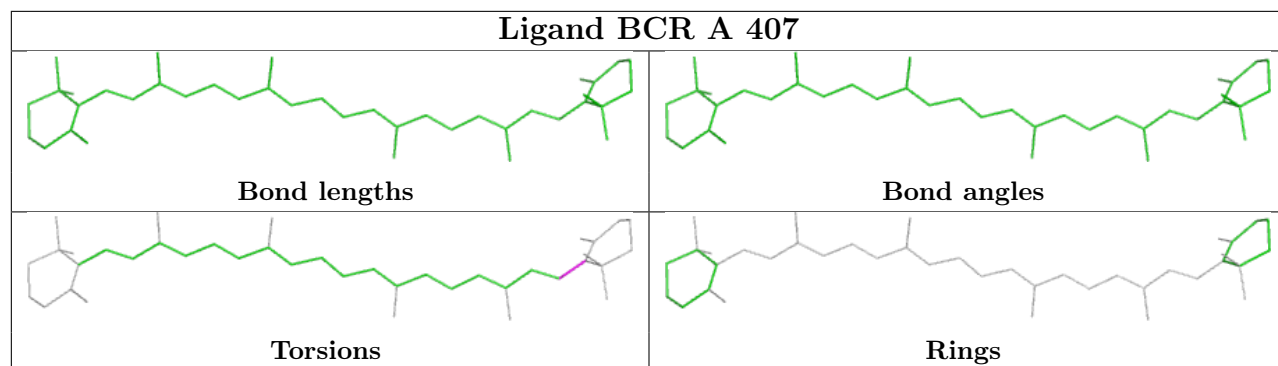


Ligand CHL s 601

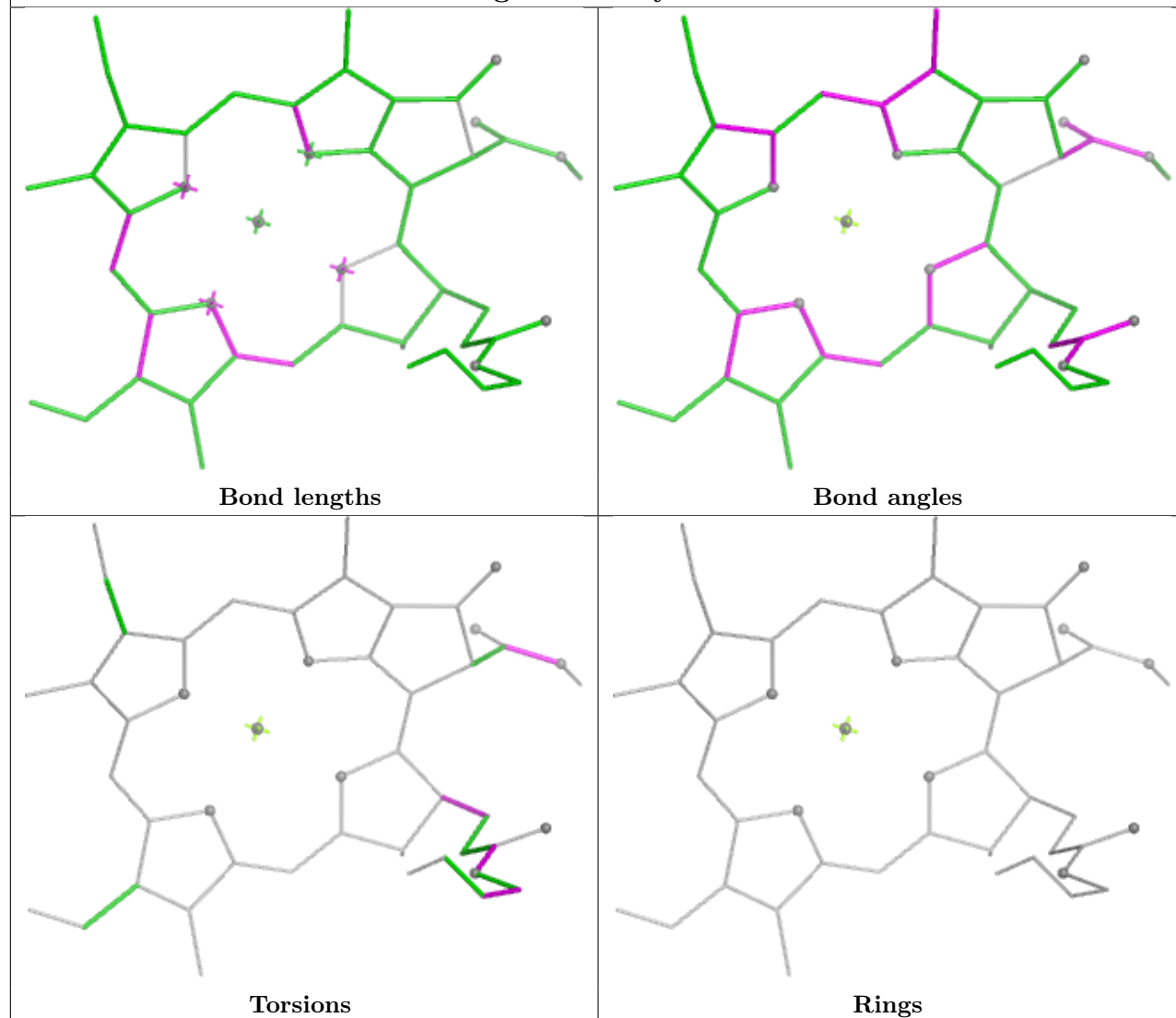


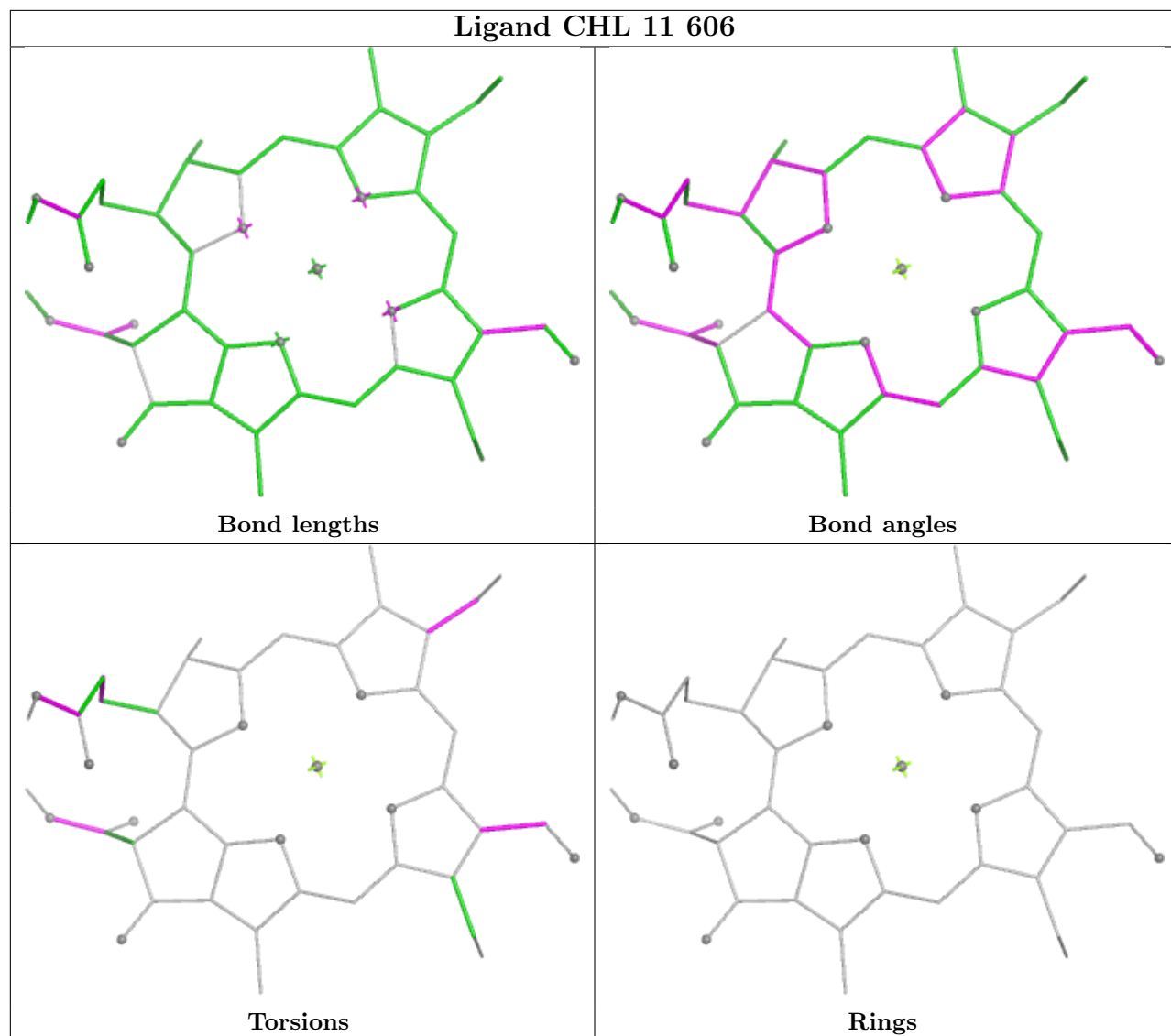
Ligand LUT 2 615

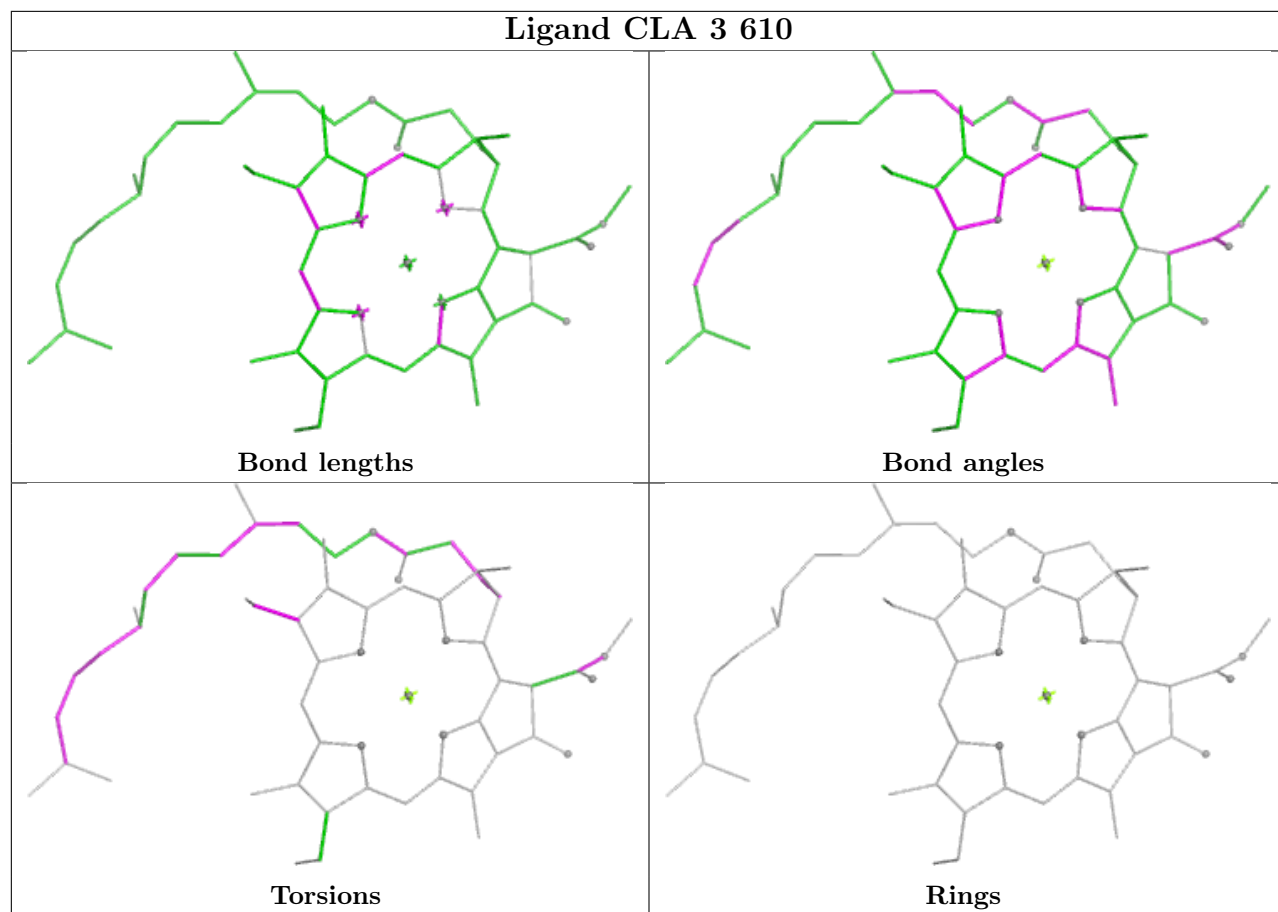


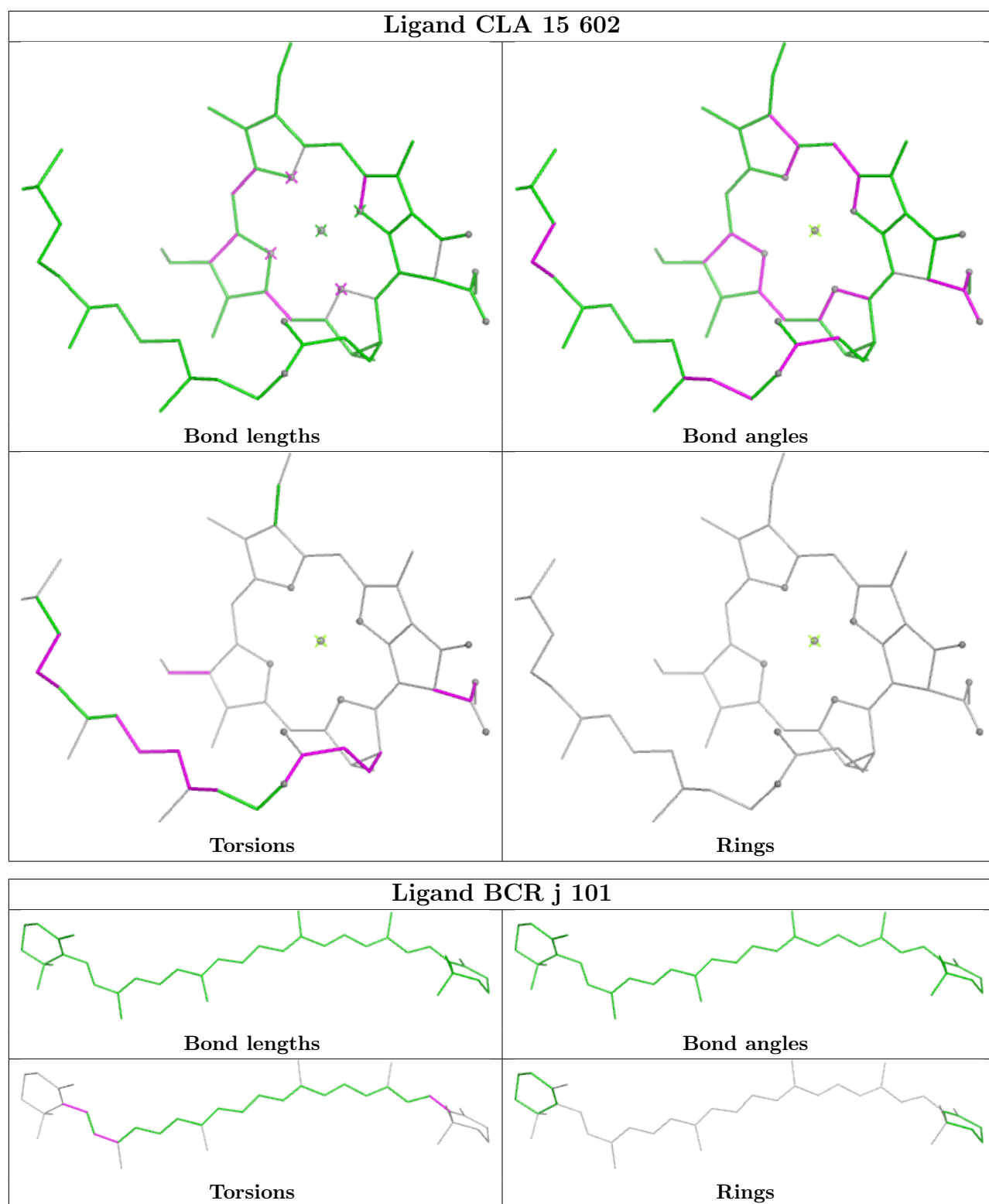


Ligand CLA y 614

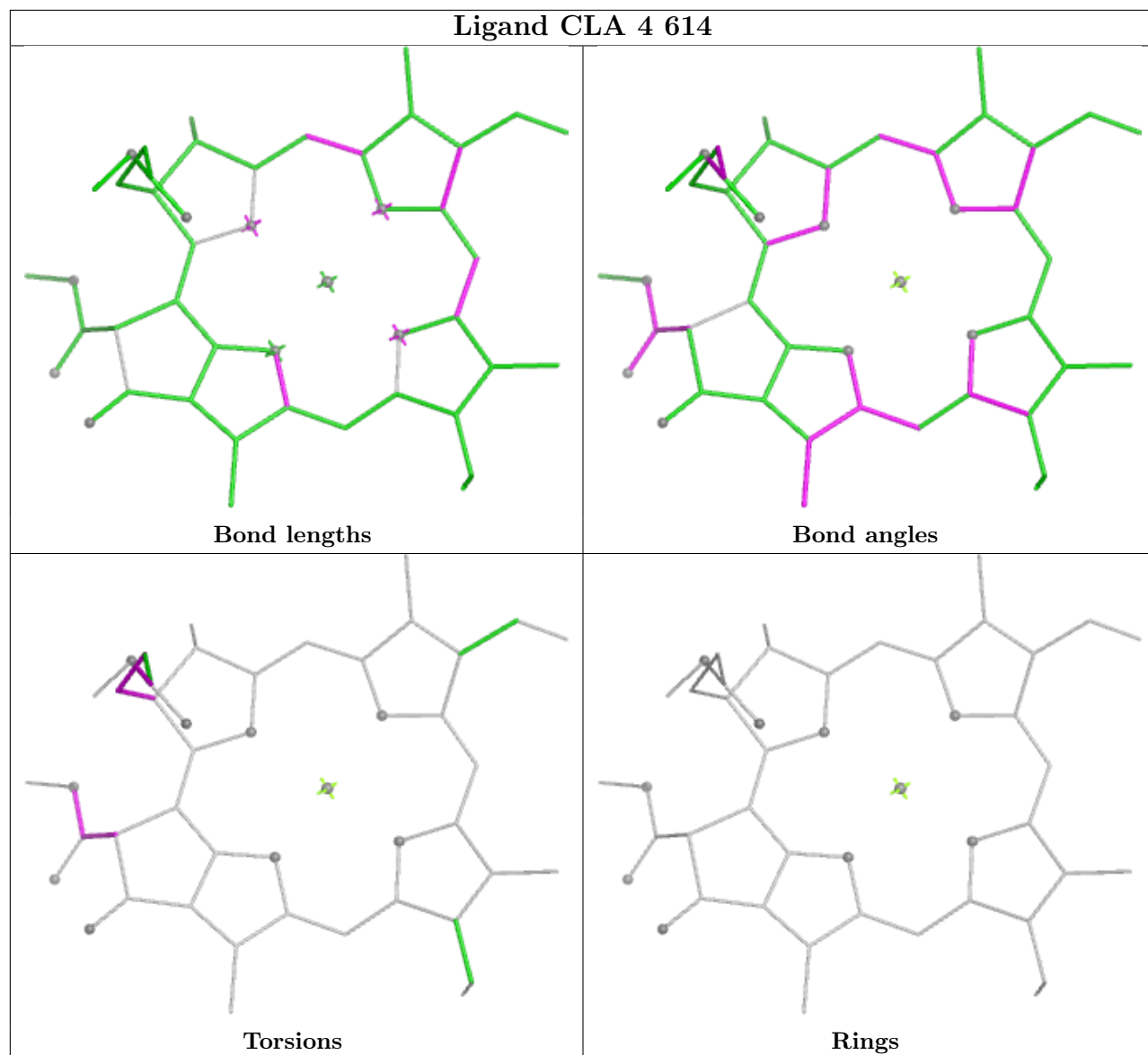


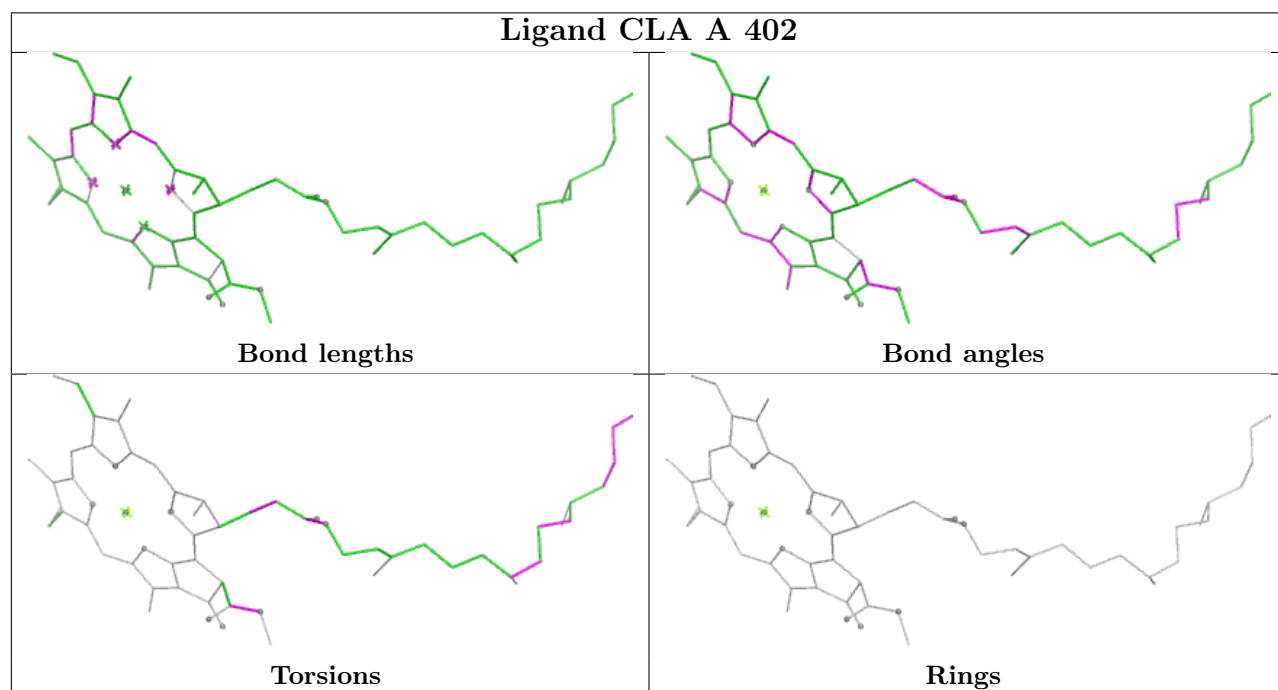
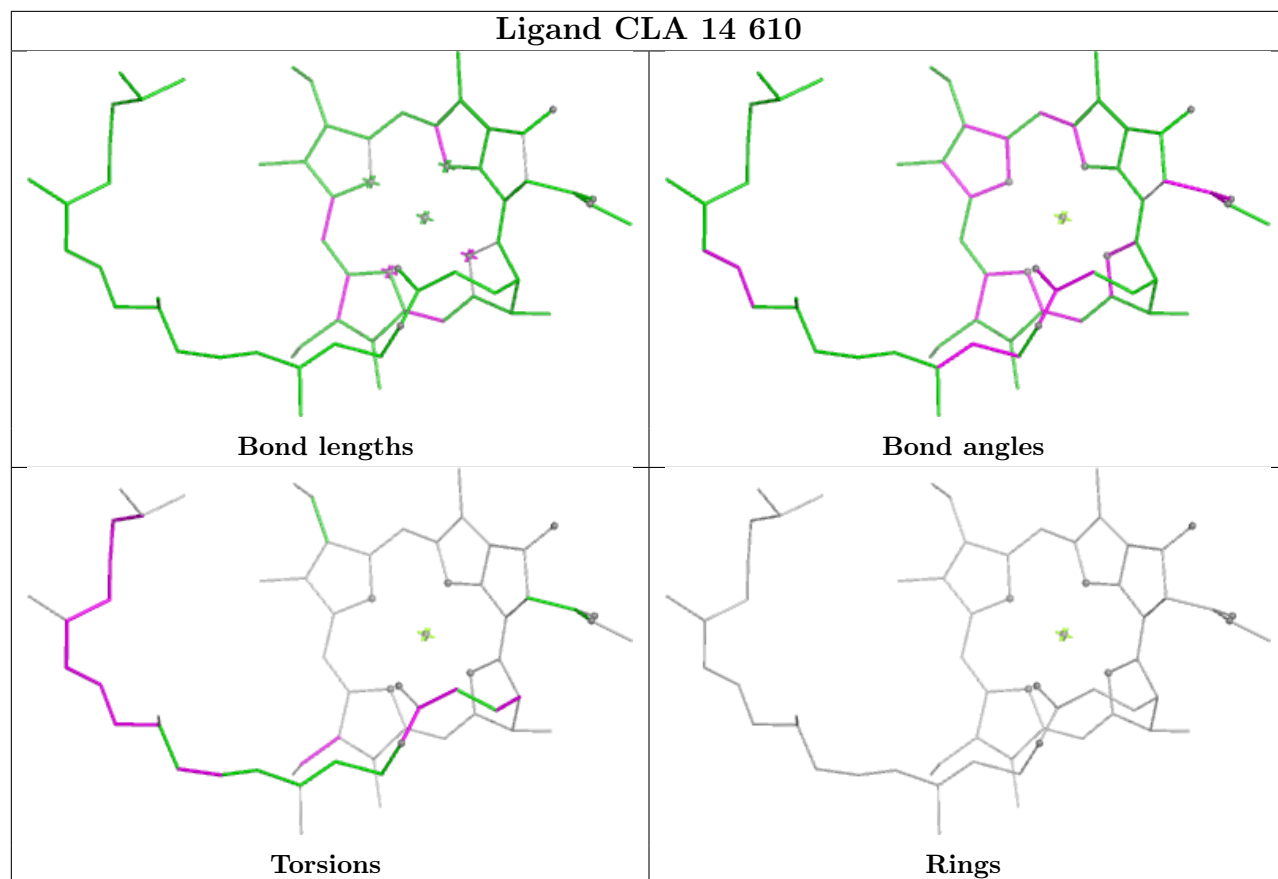


Ligand CLA 3 610

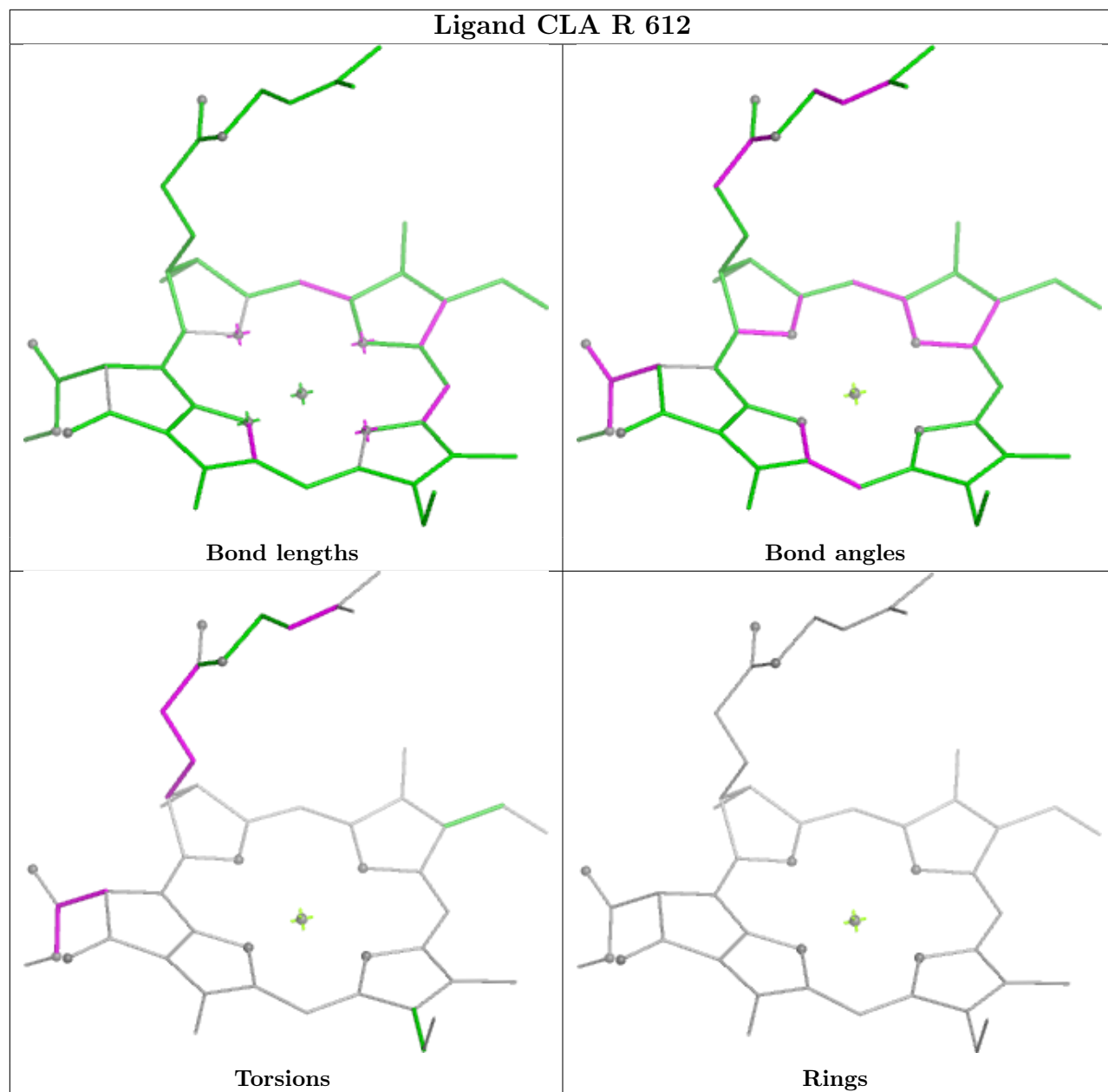


Ligand CLA 4 614

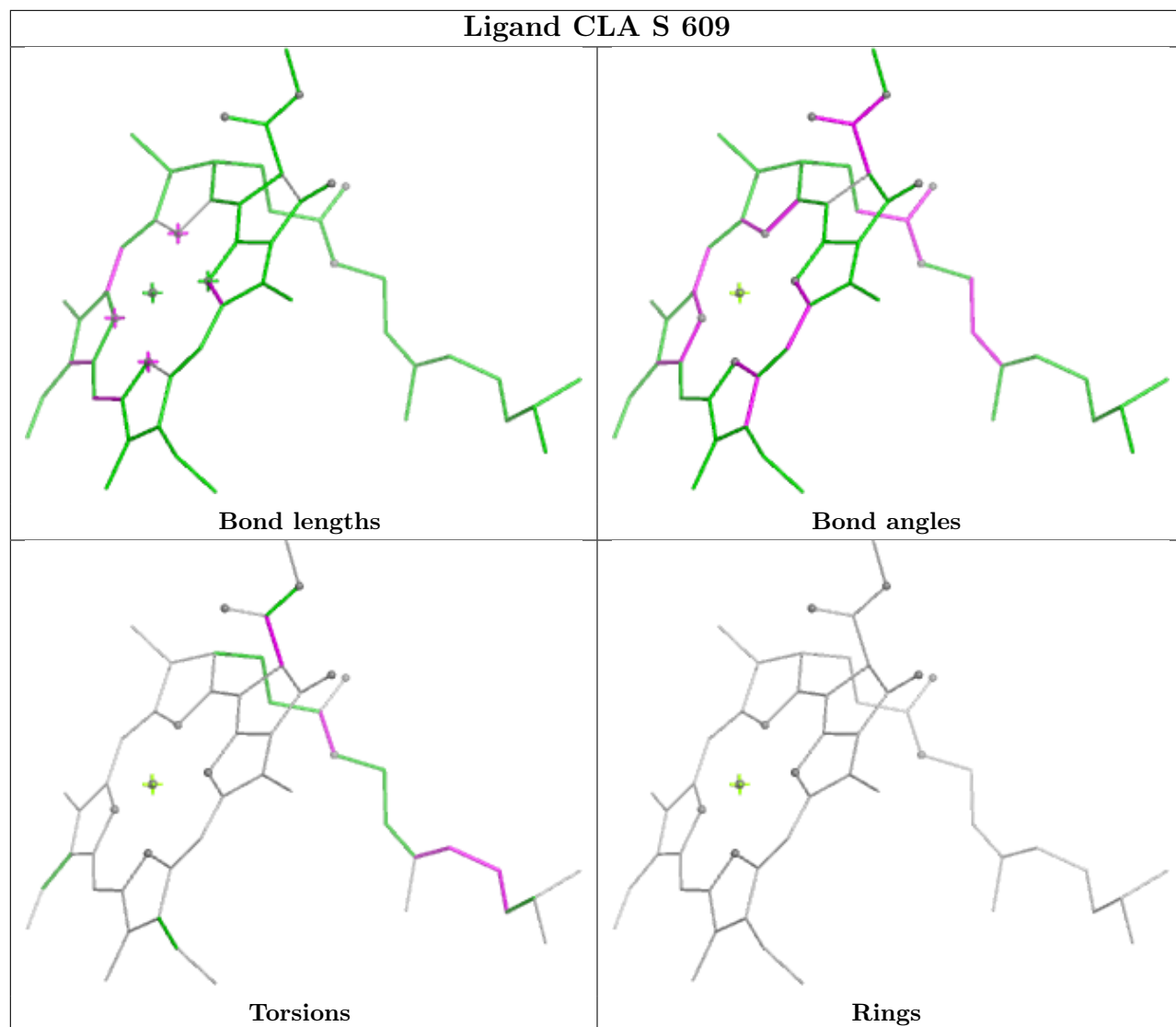


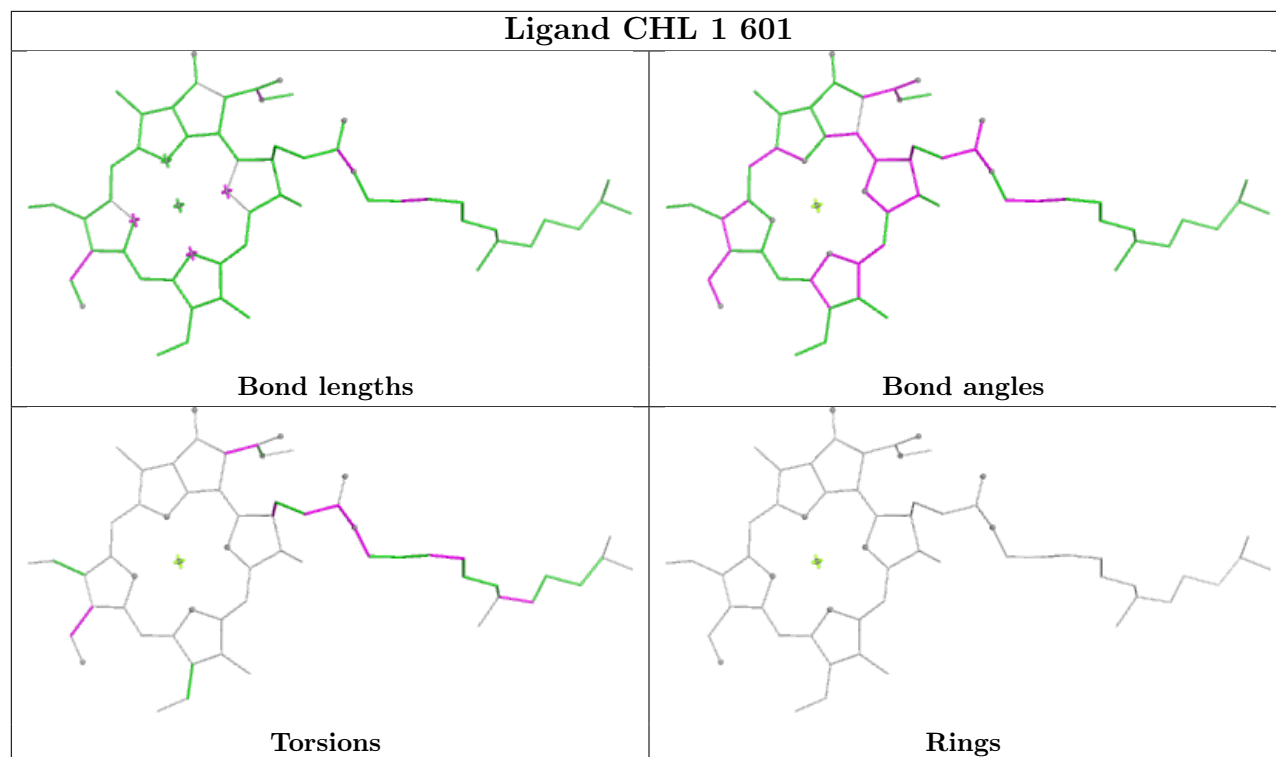
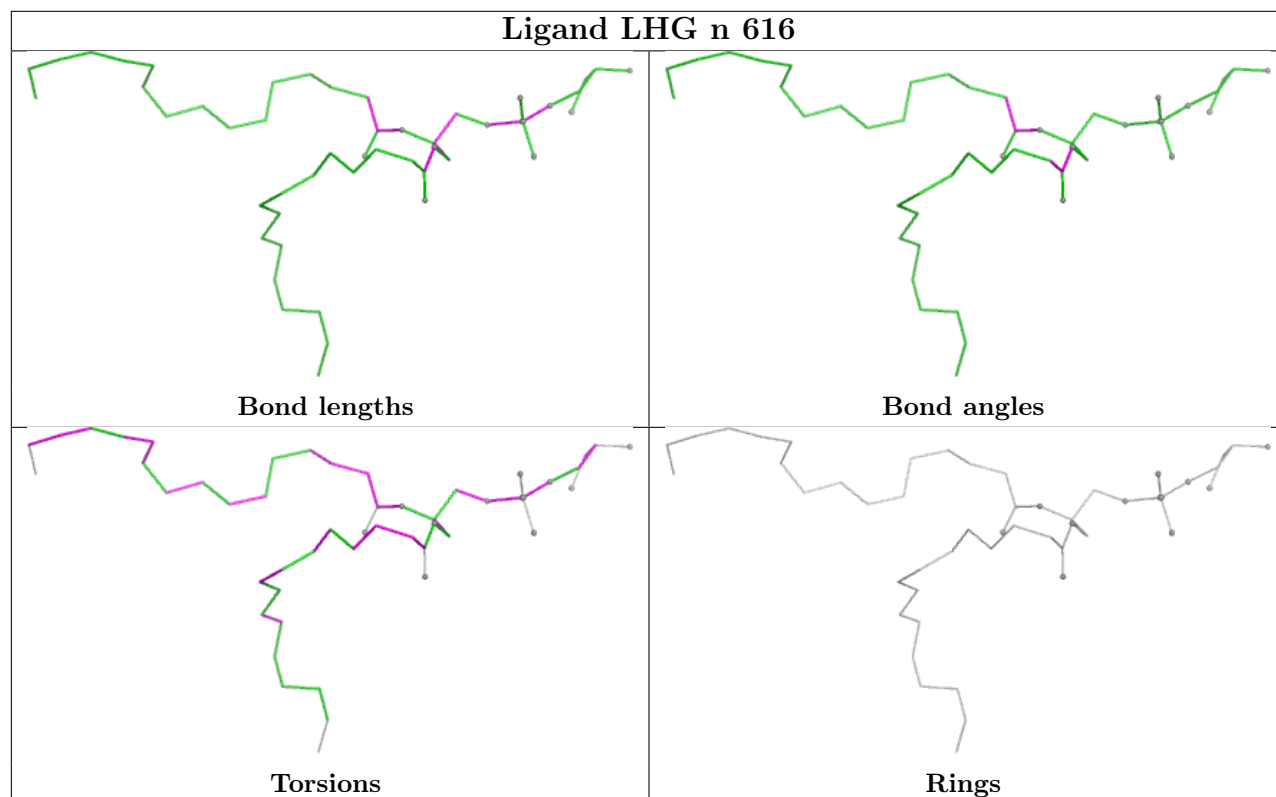


Ligand CLA R 612

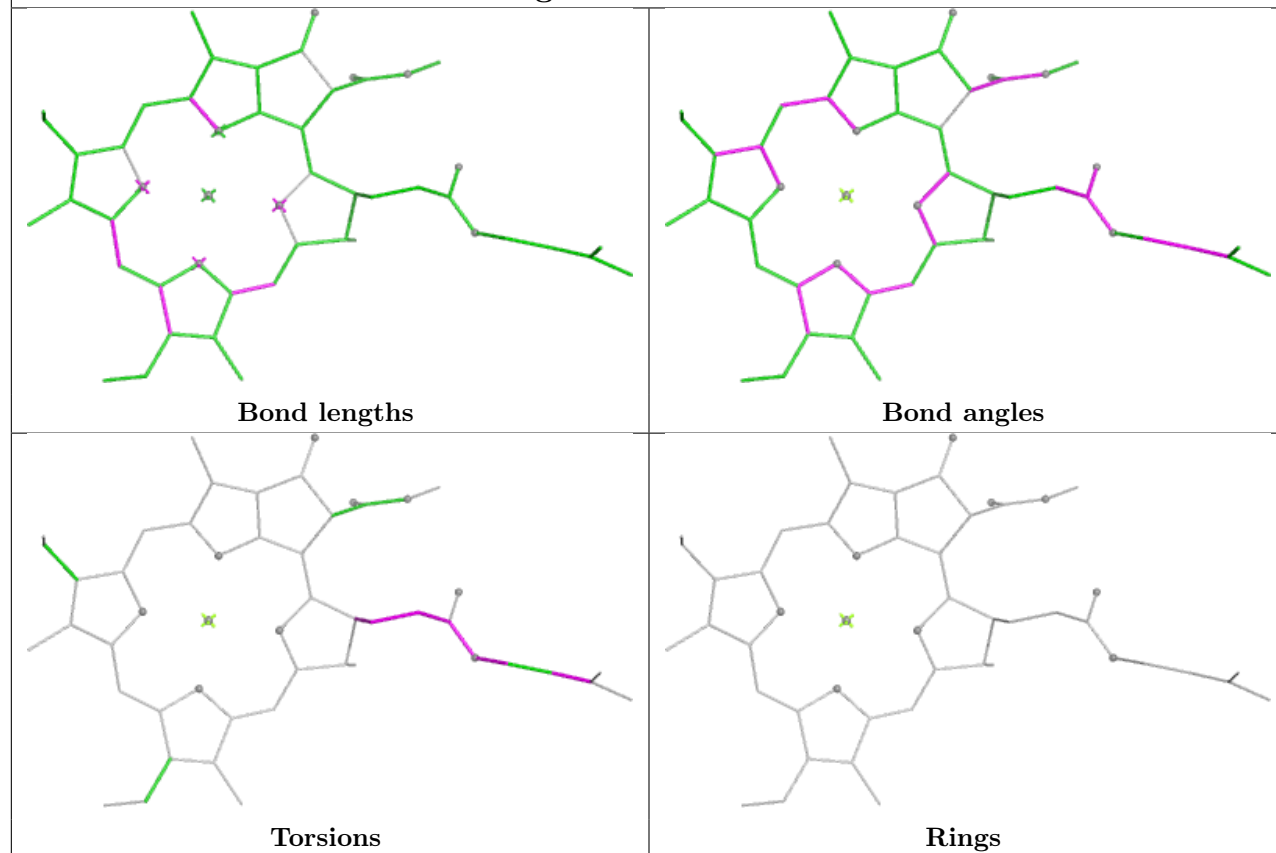


Ligand CLA S 609

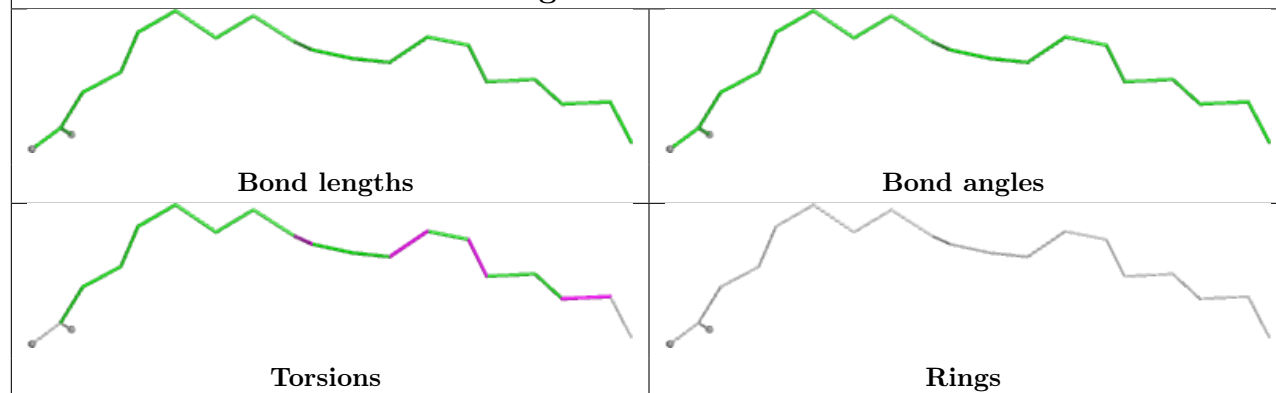


Ligand CHL 1 601**Ligand LHG n 616**

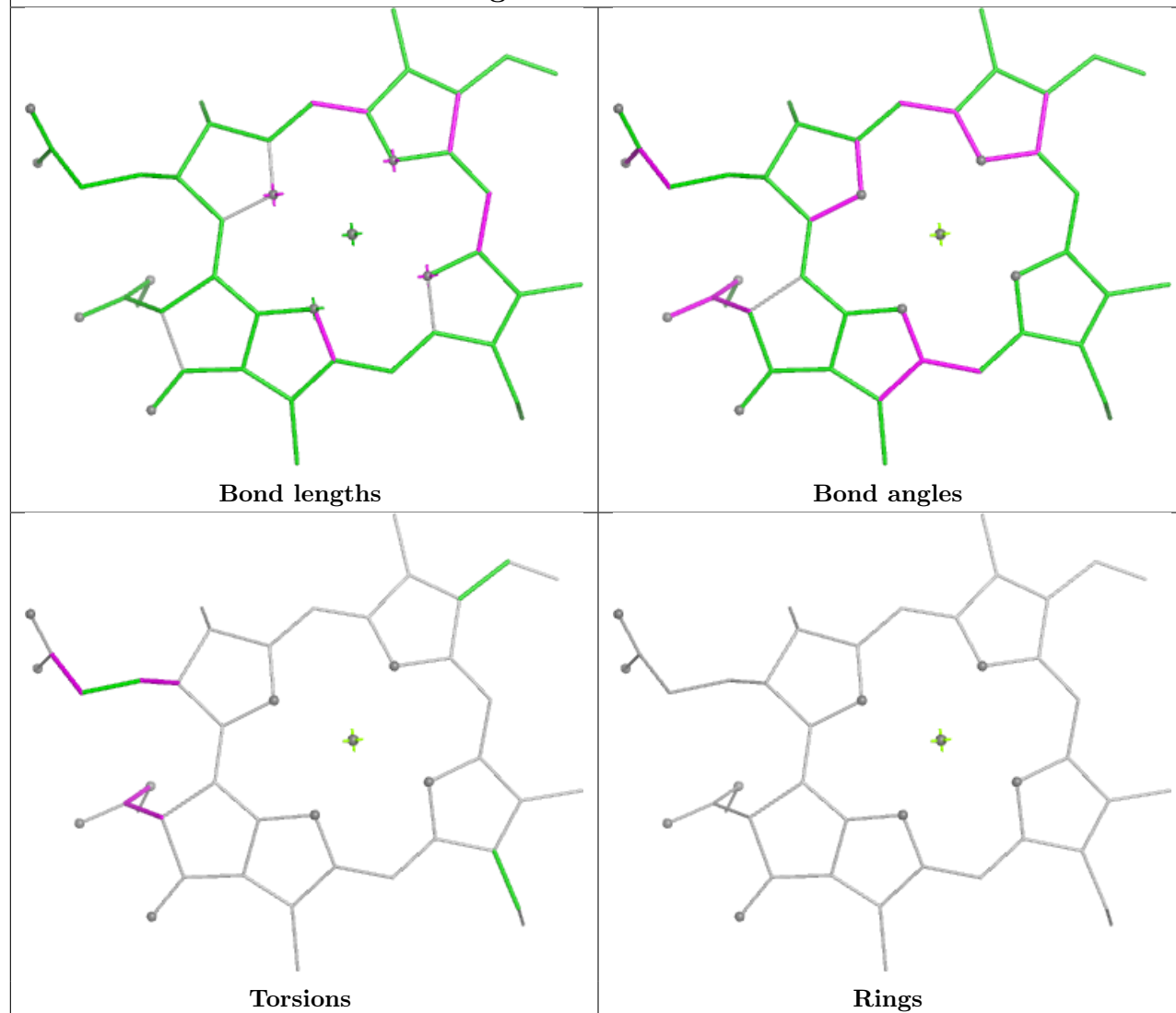
Ligand CLA S 605

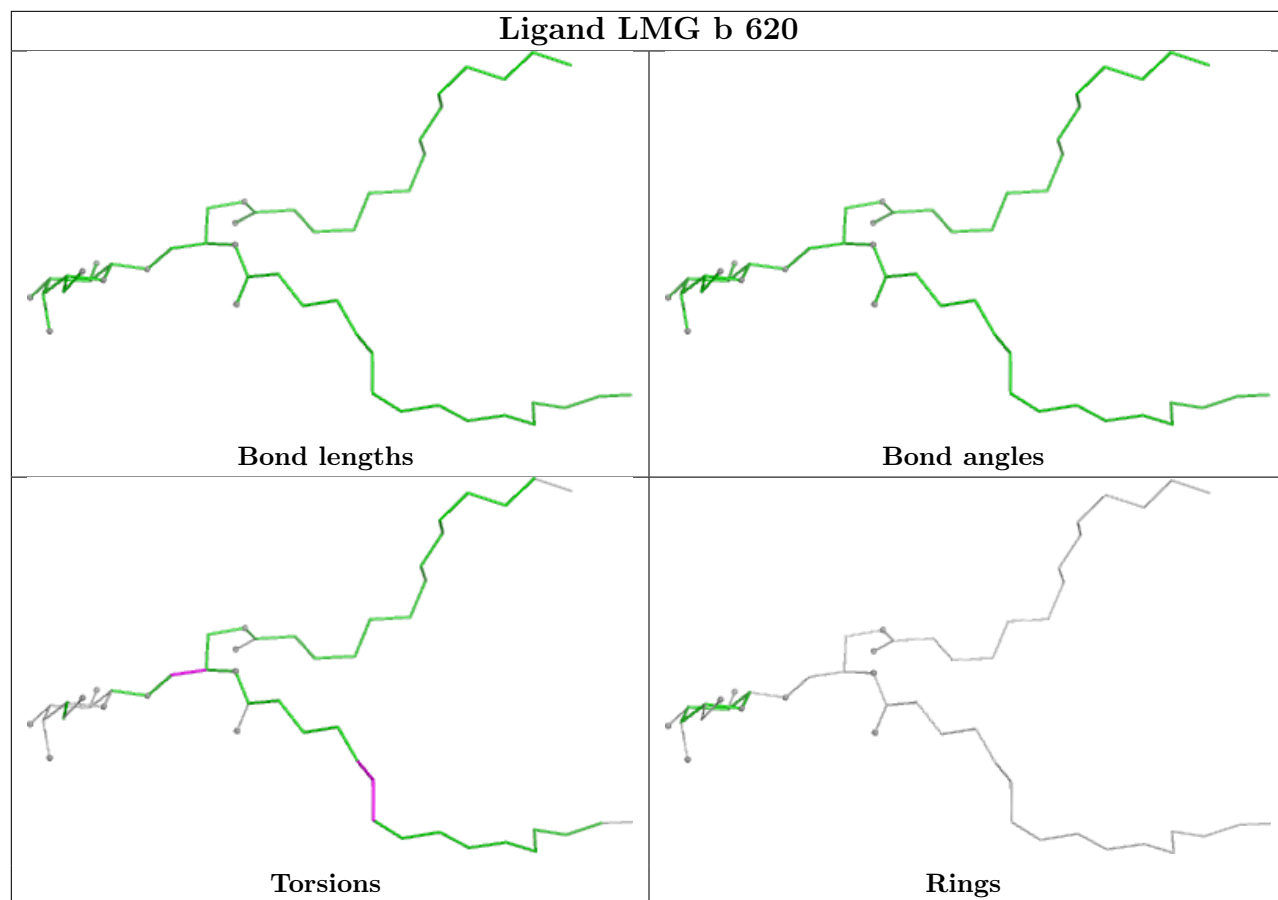


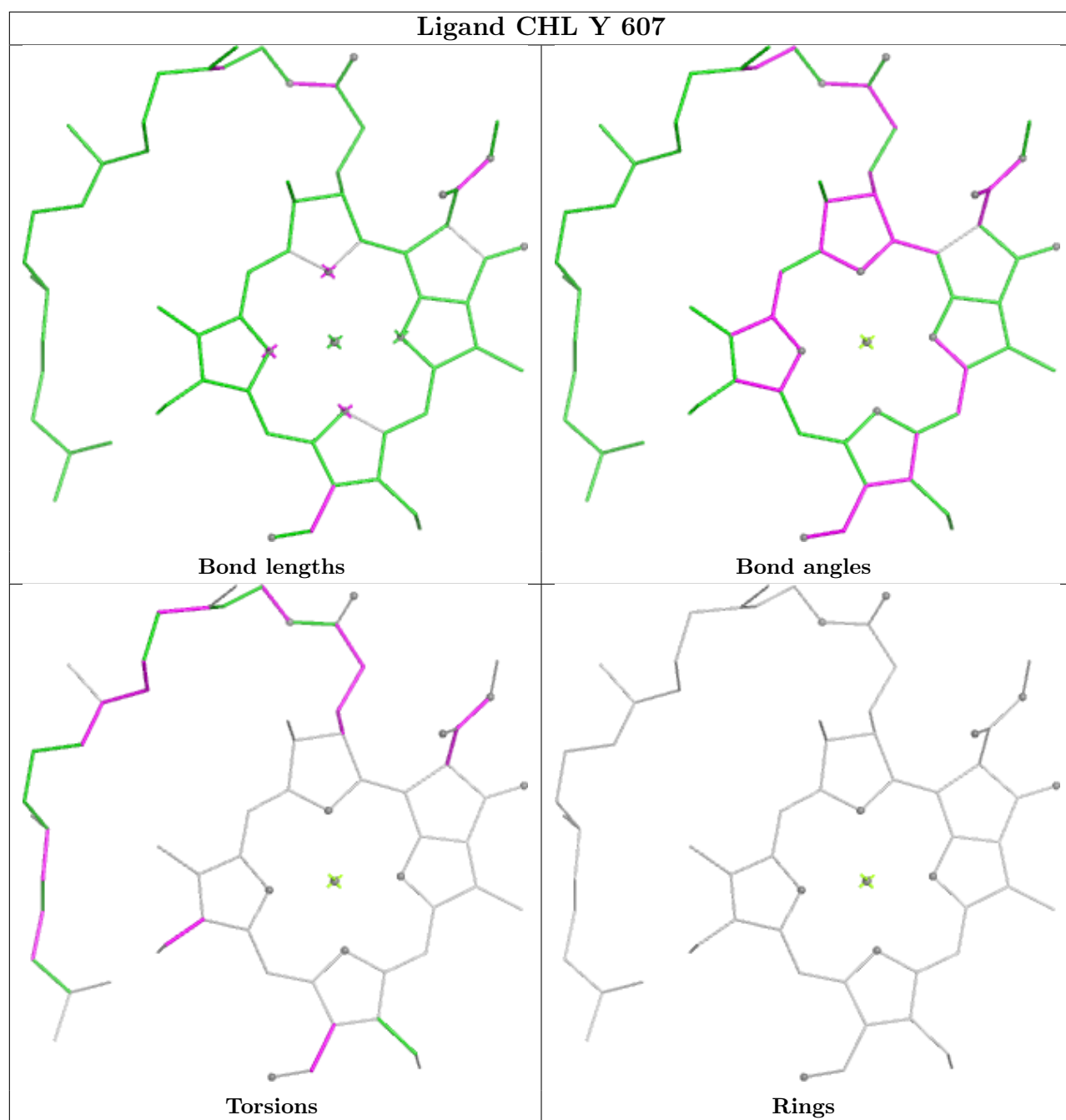
Ligand LNL c 523



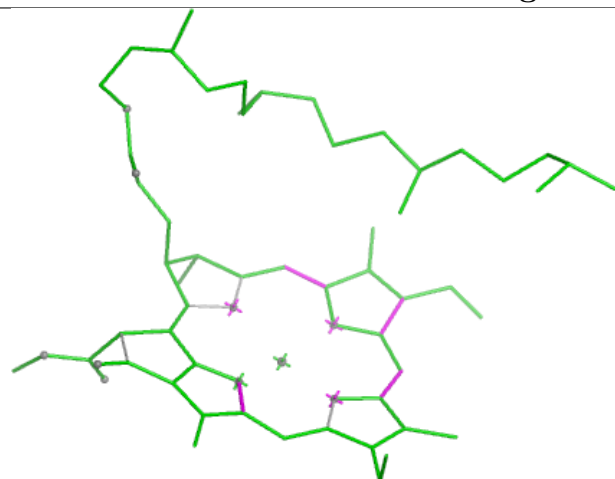
Ligand CLA N 612



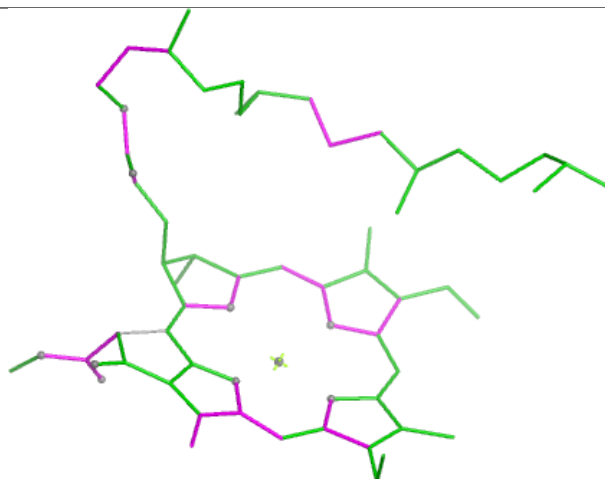




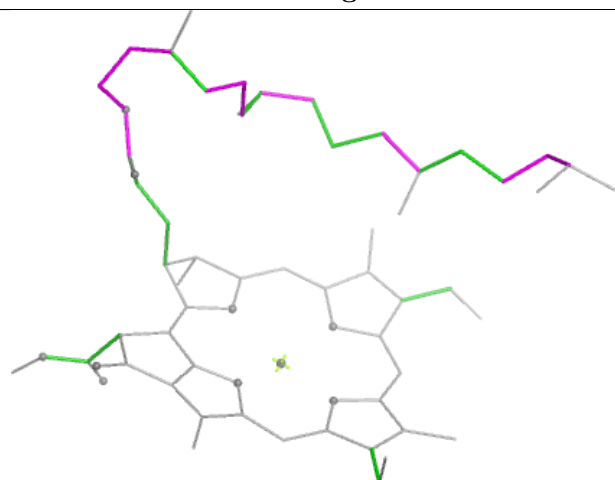
Ligand CLA S 614



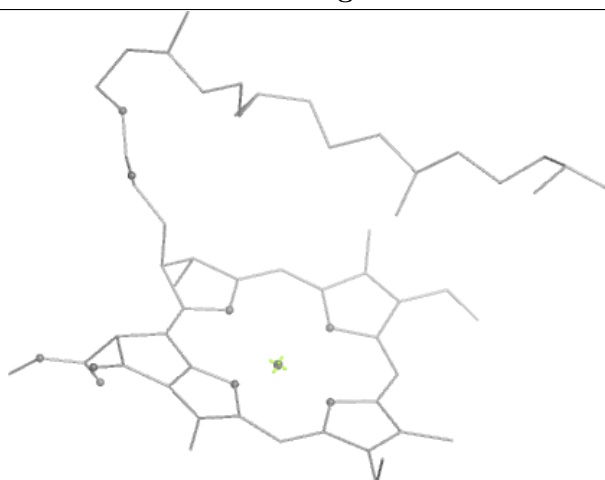
Bond lengths



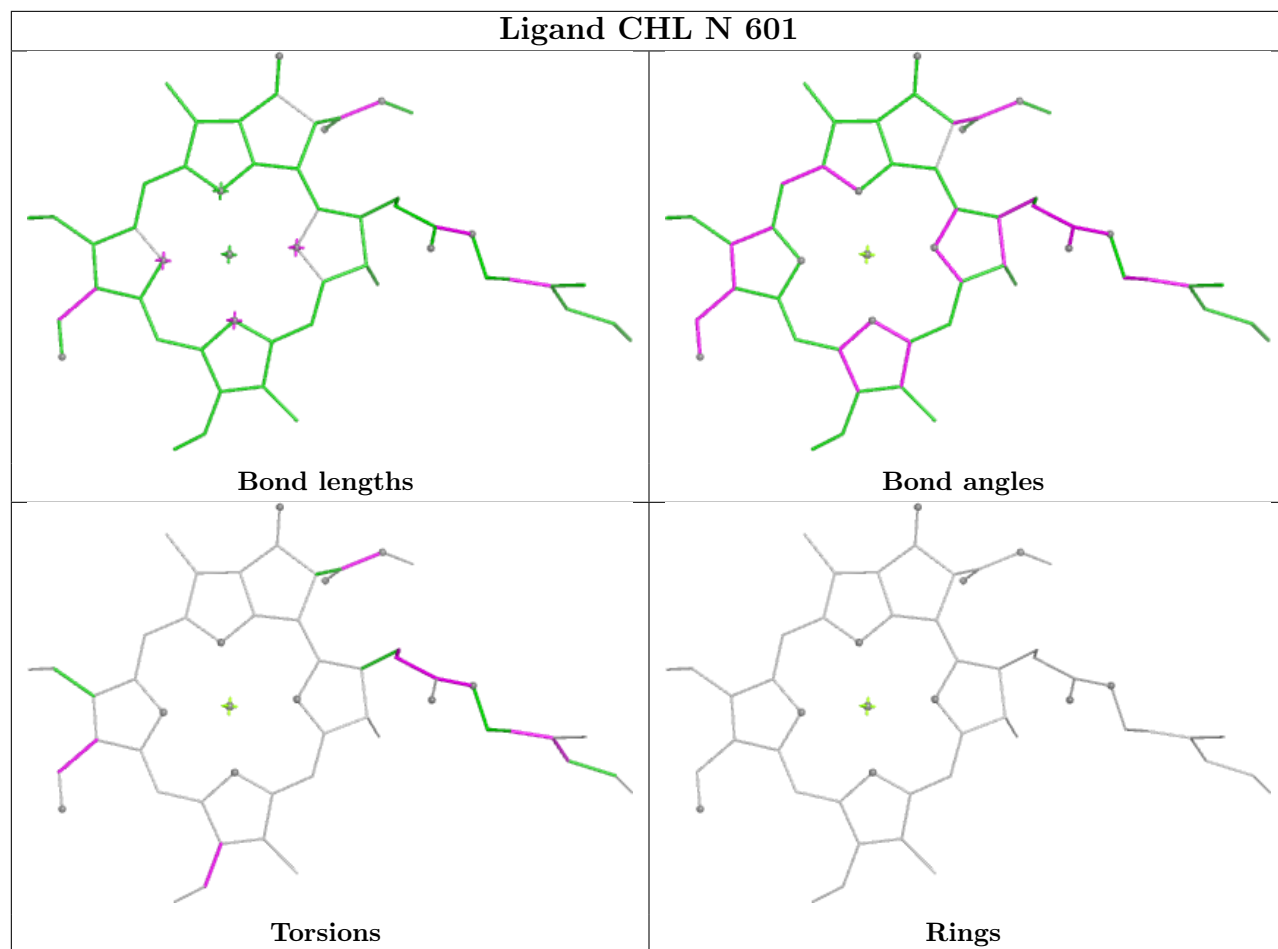
Bond angles

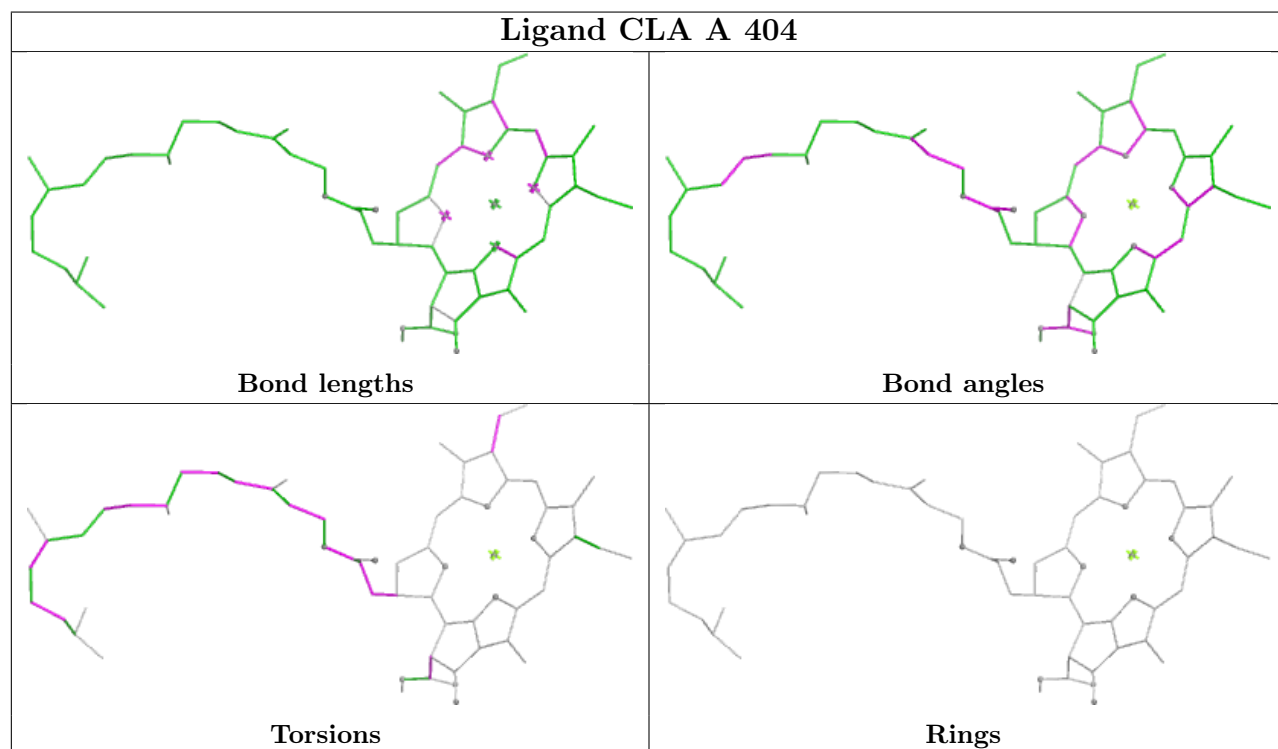
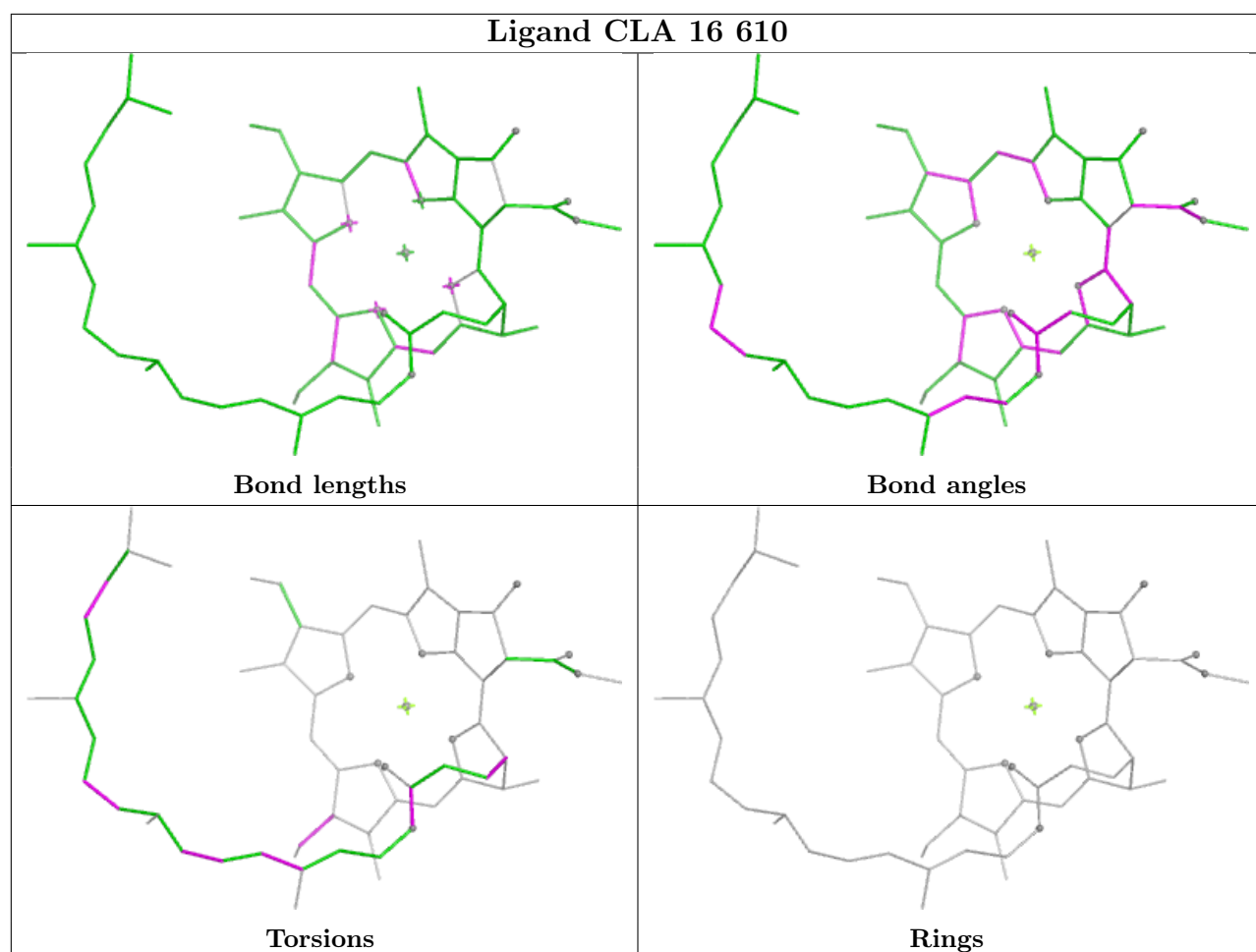


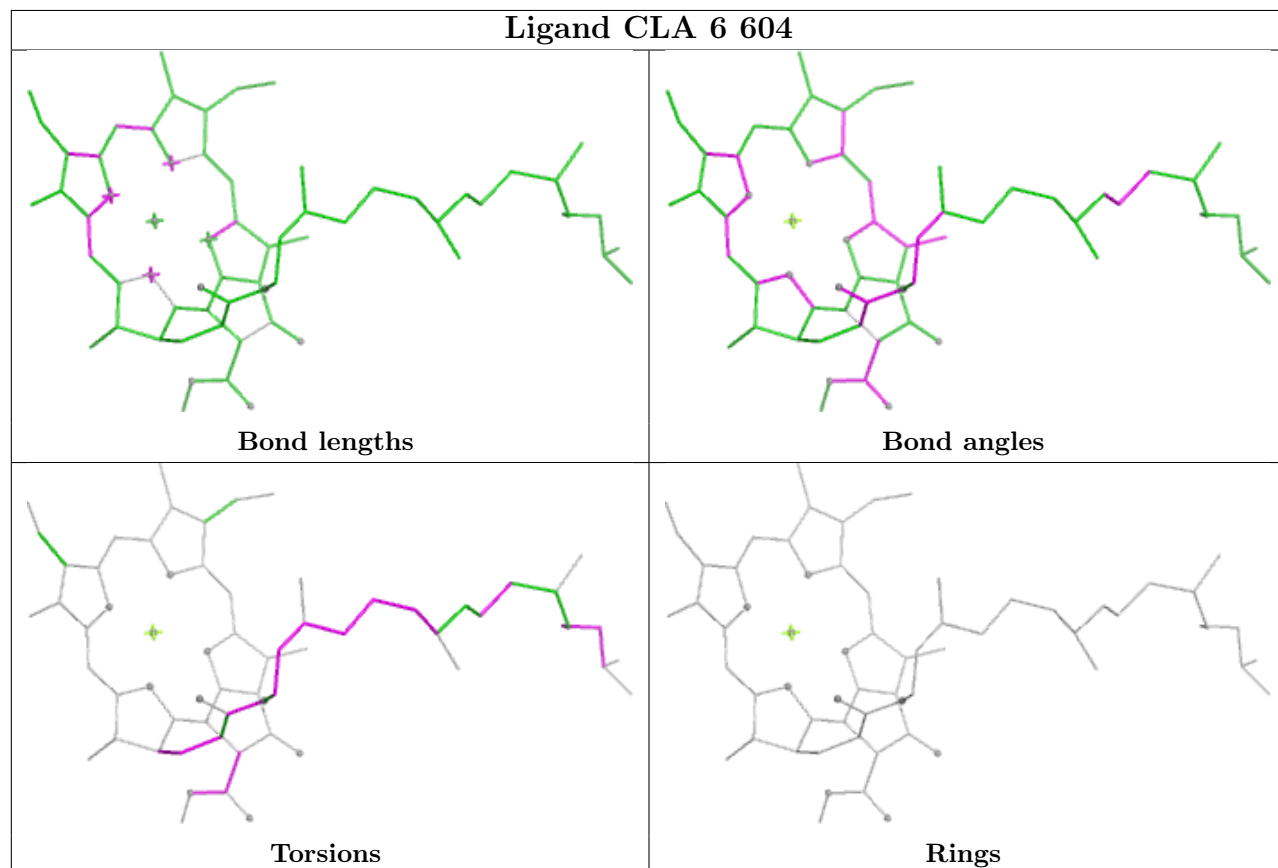
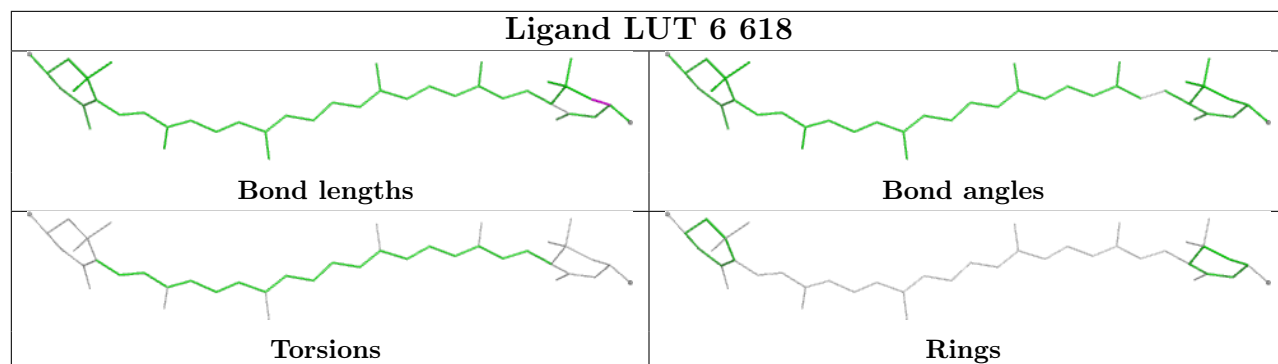
Torsions

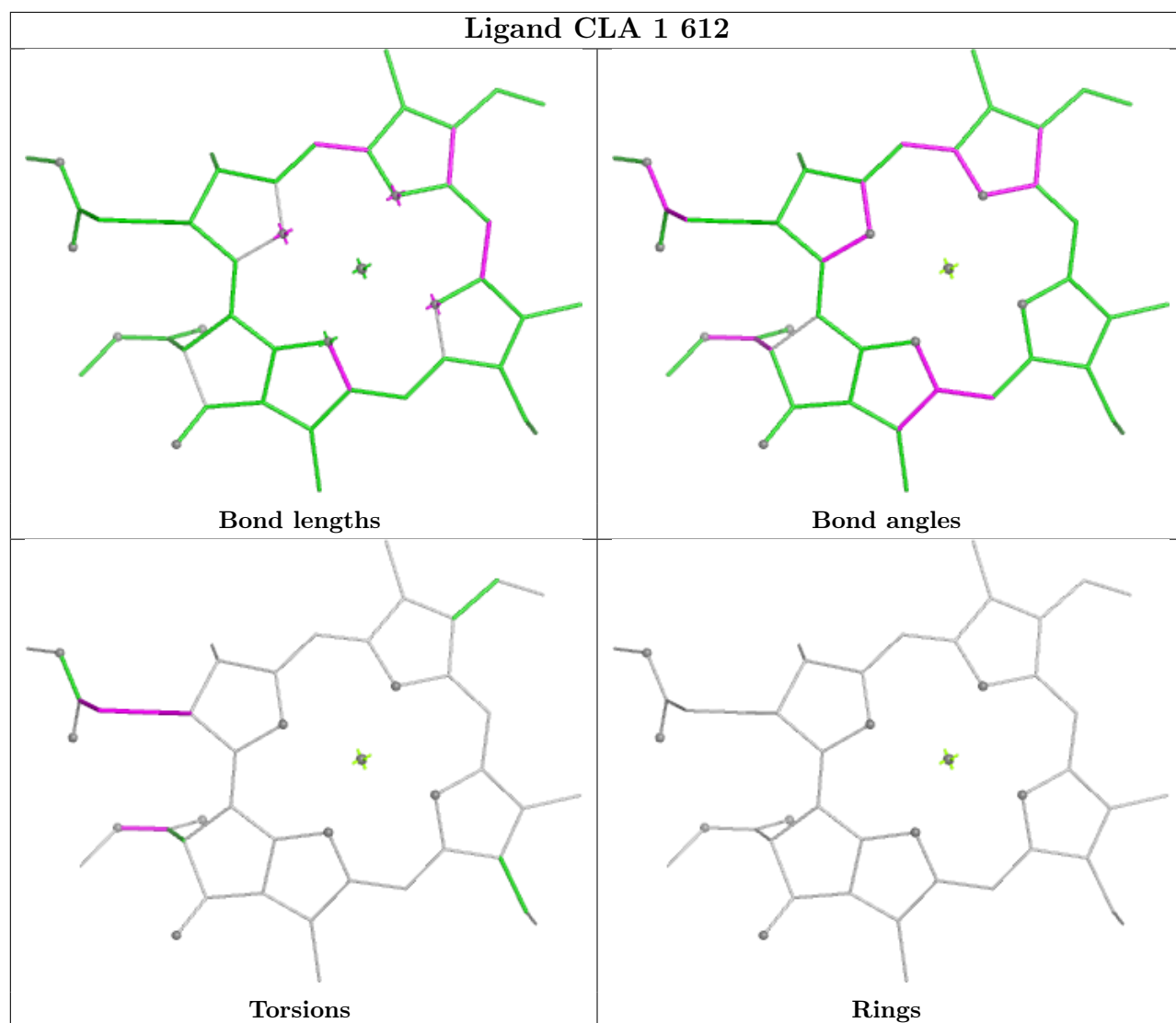
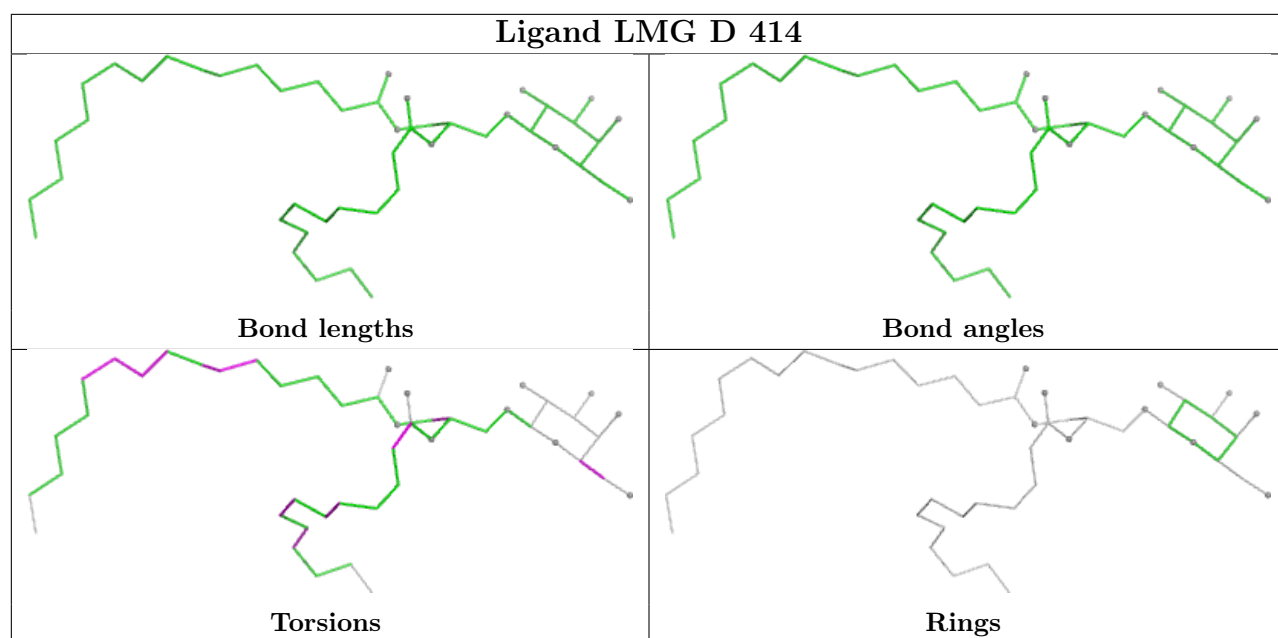


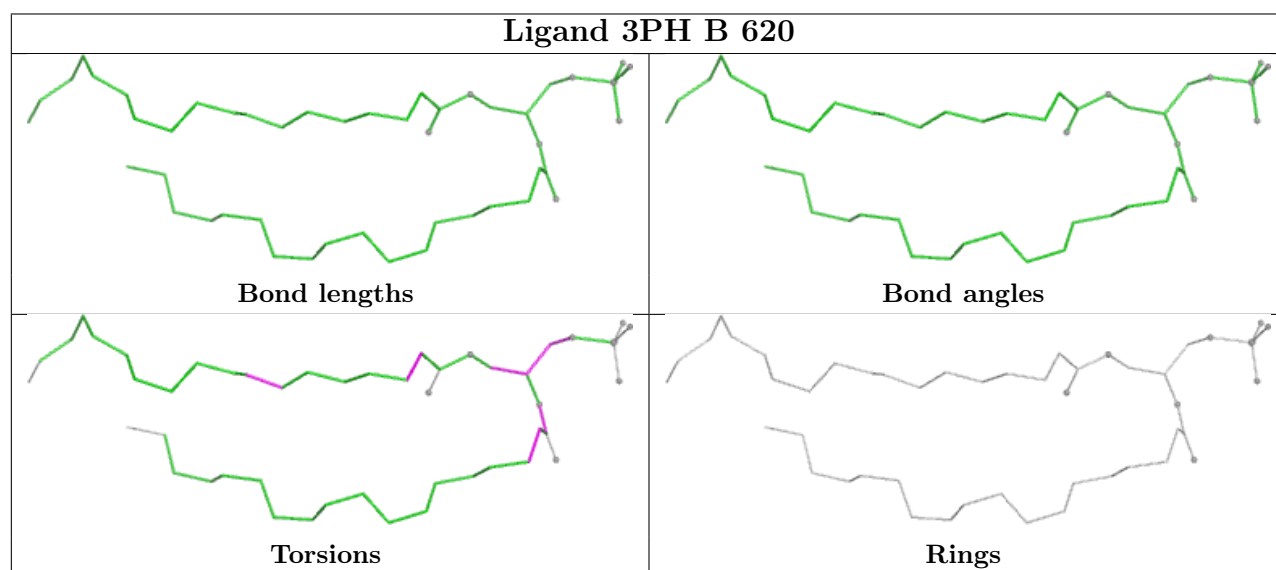
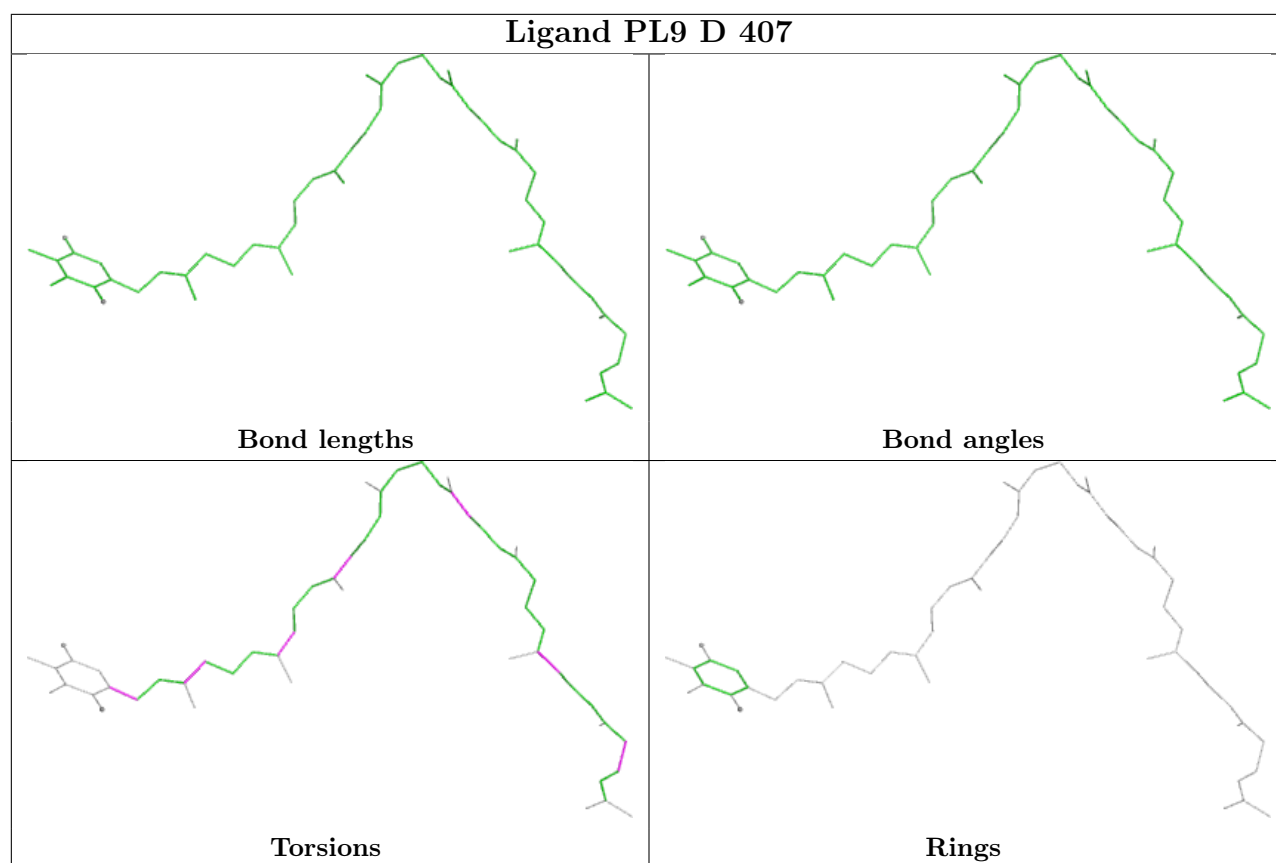
Rings

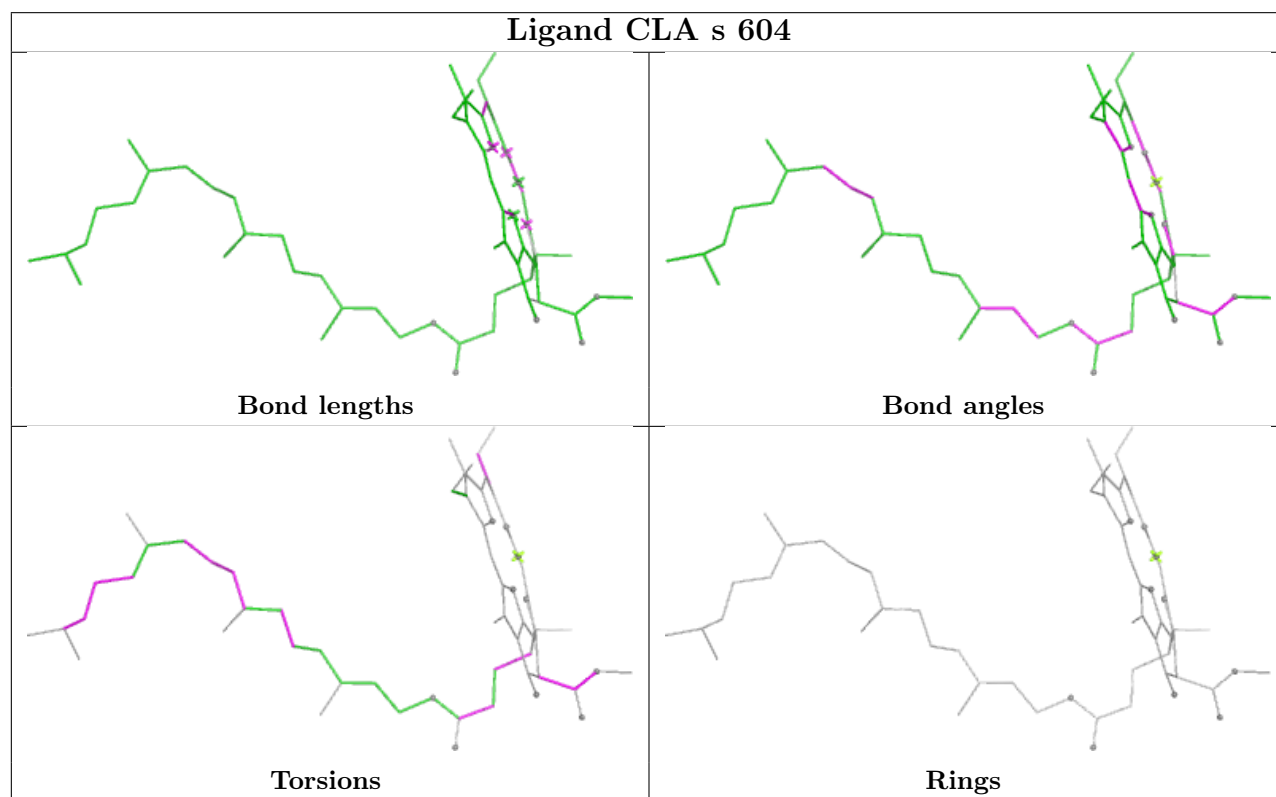
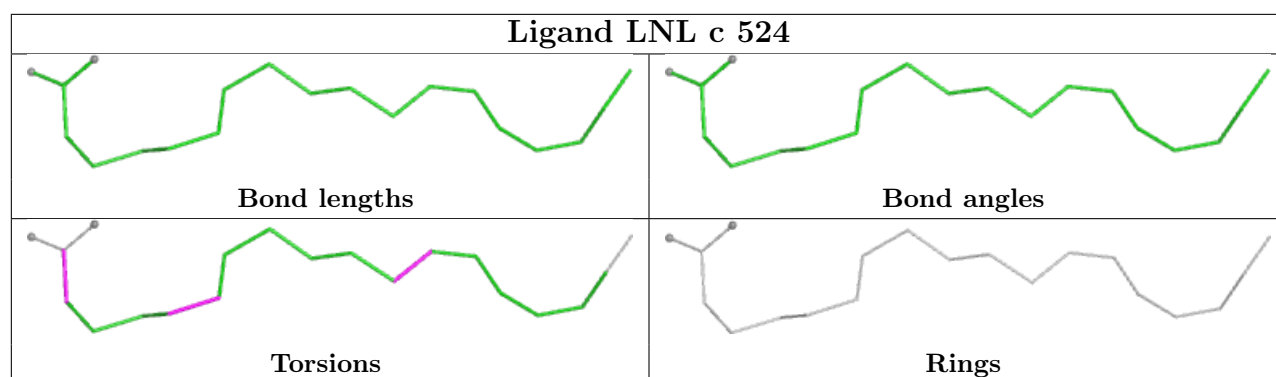




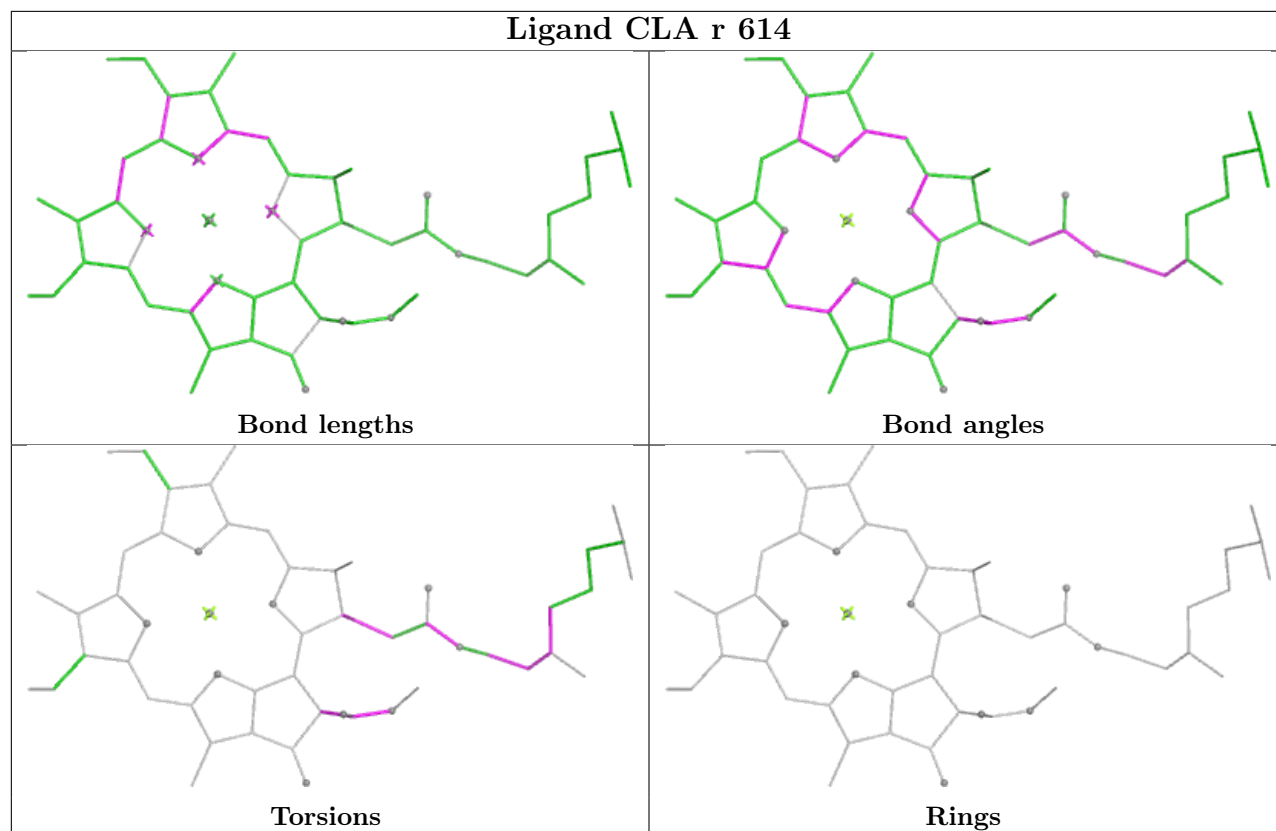




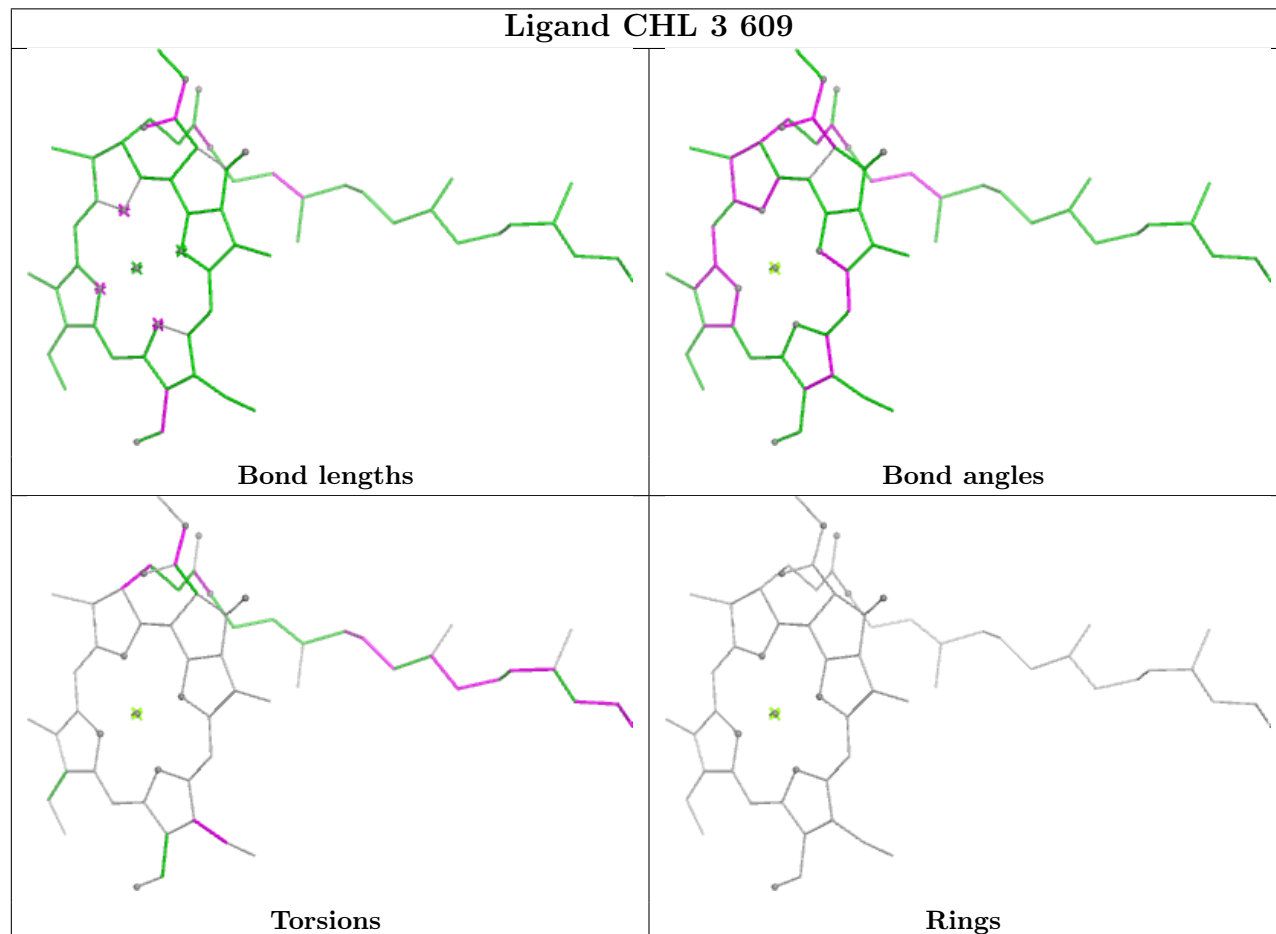




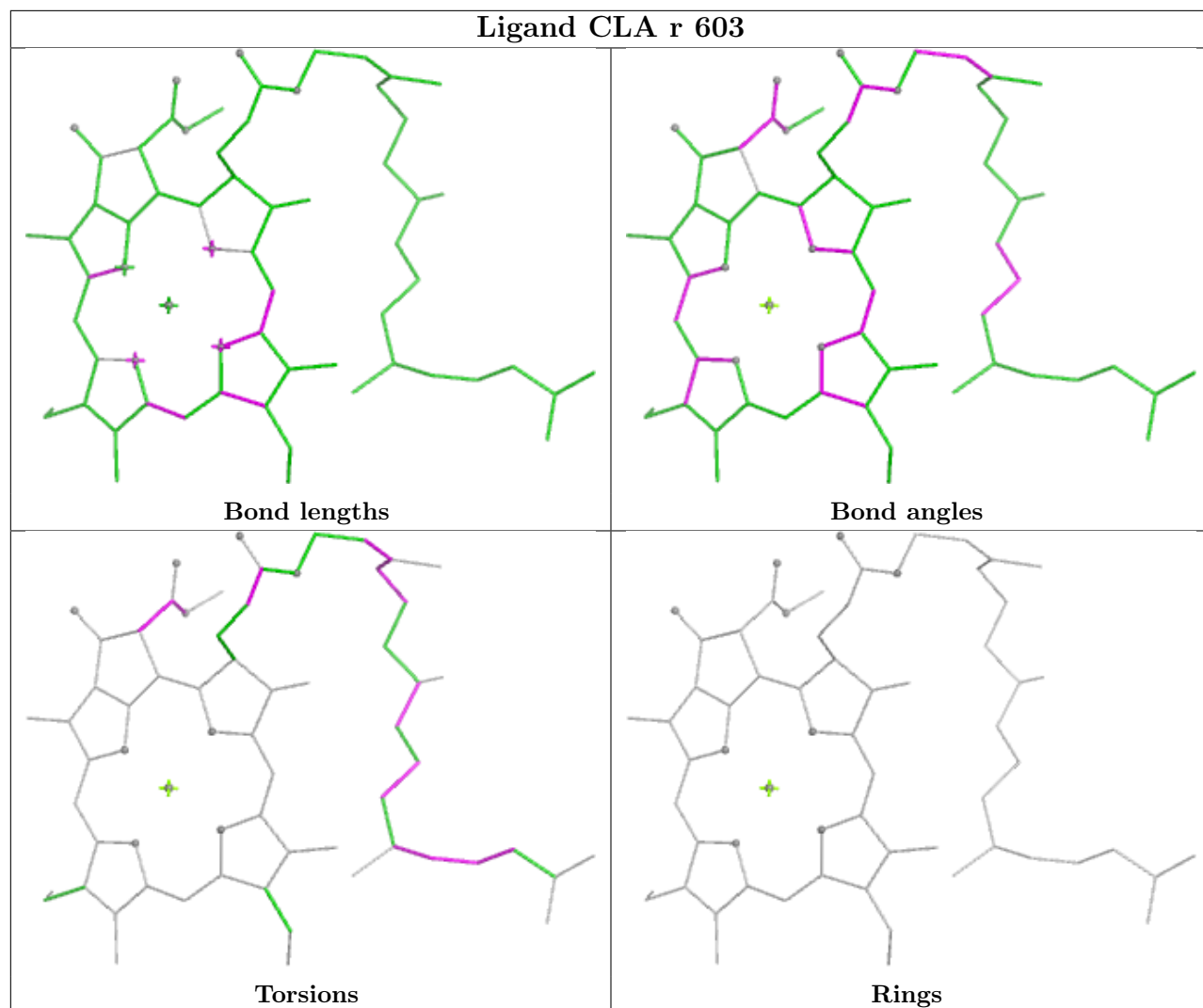
Ligand CLA r 614

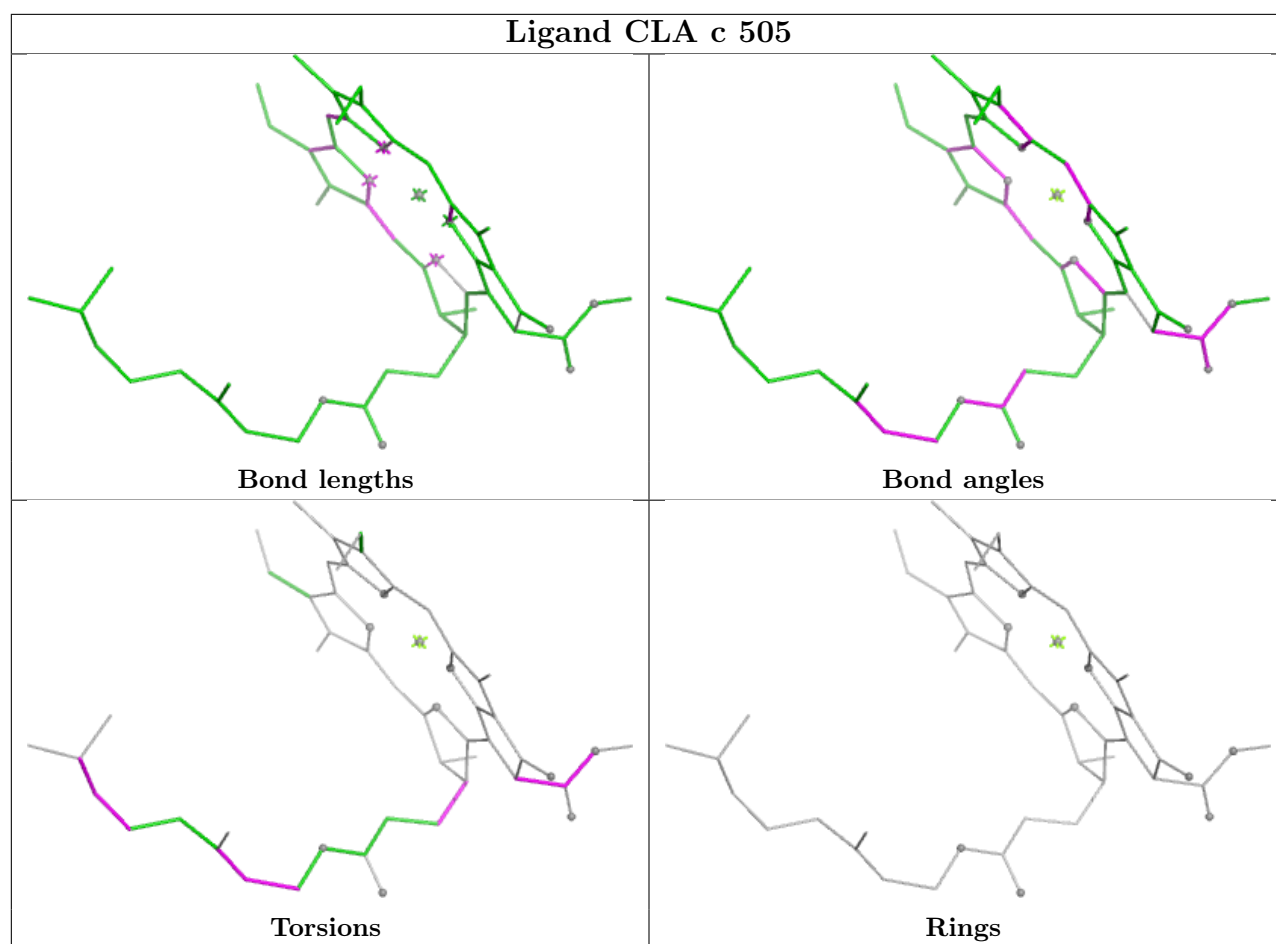


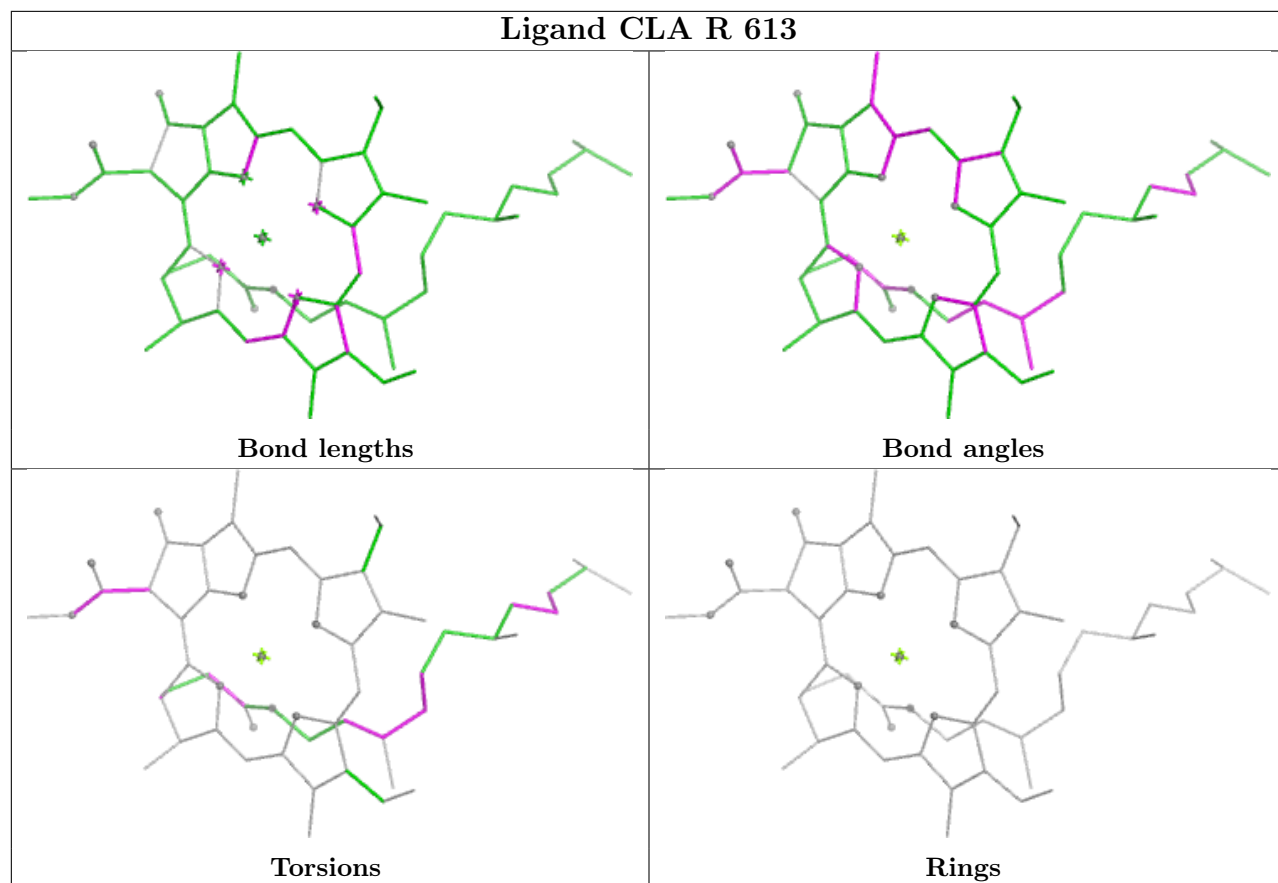
Ligand CHL 3 609



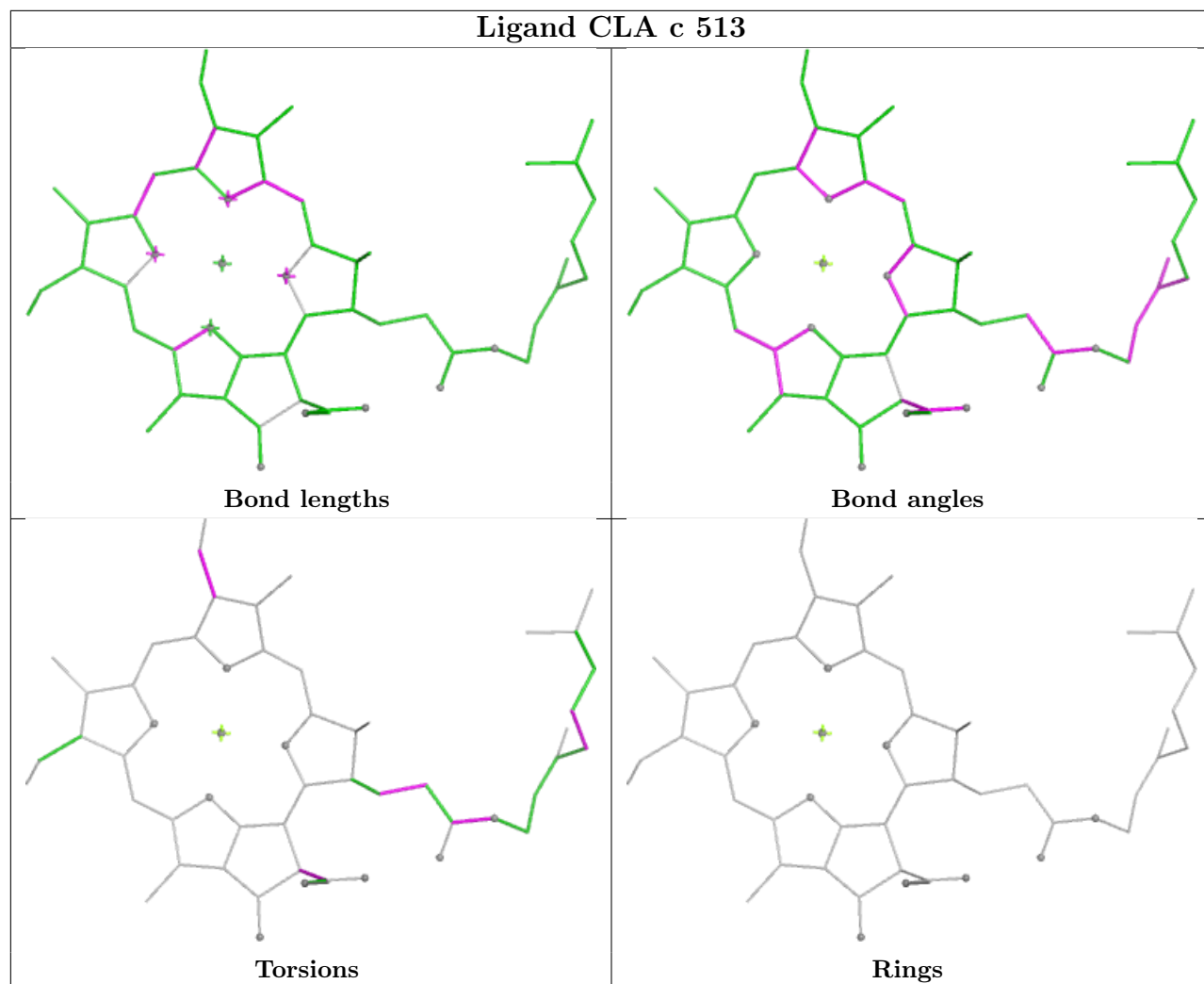
Ligand CLA r 603



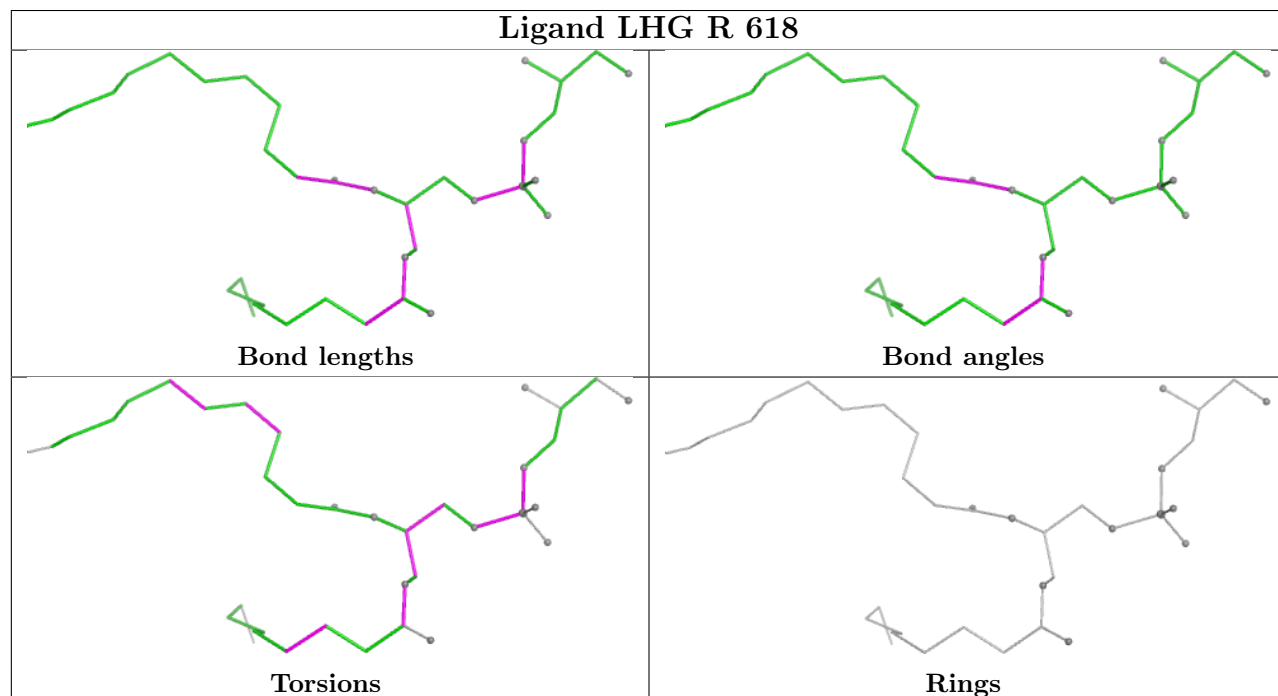


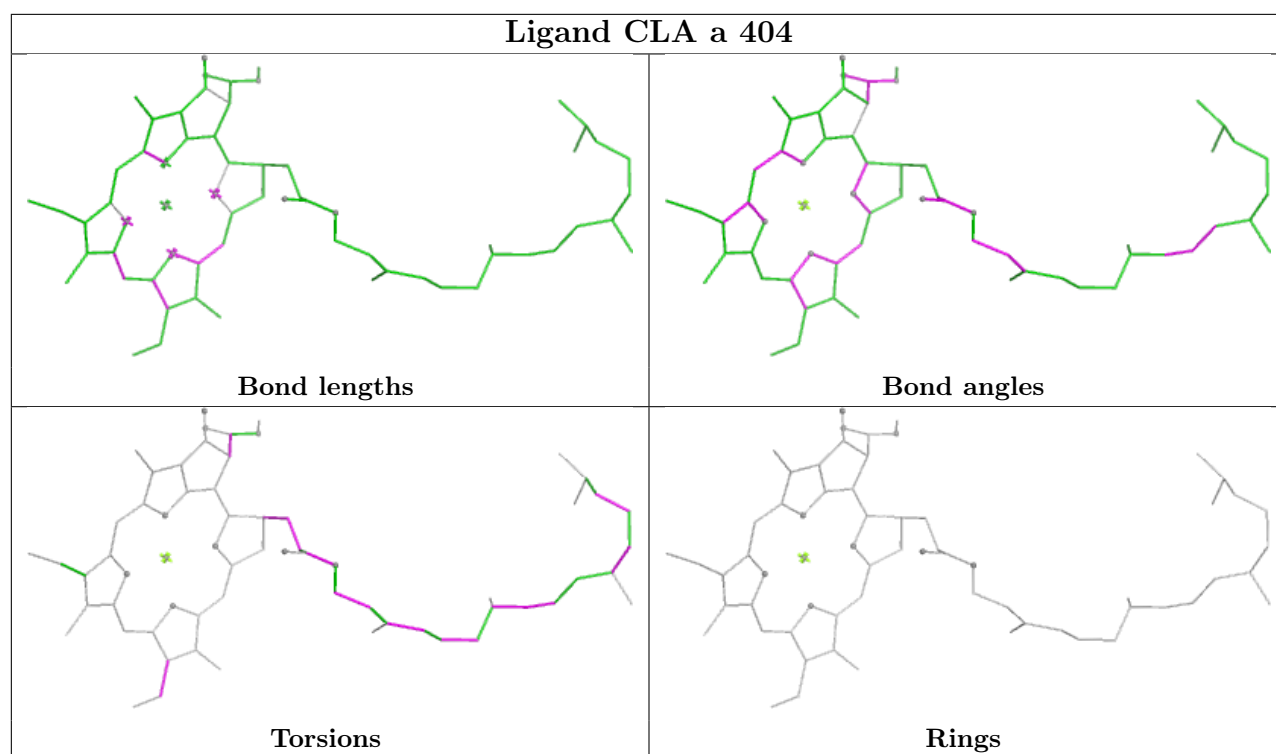


Ligand CLA c 513

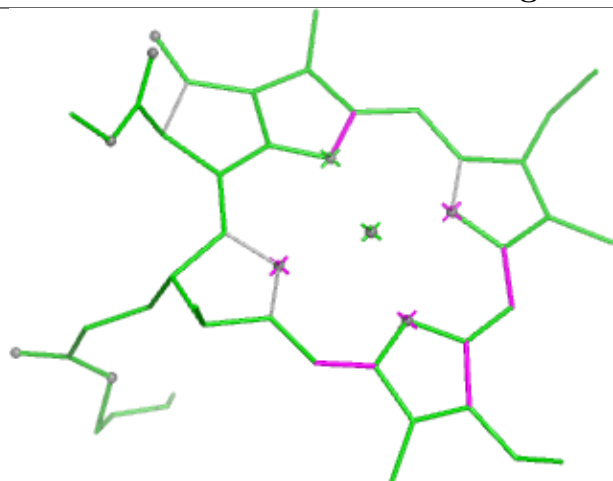


Ligand LHG R 618

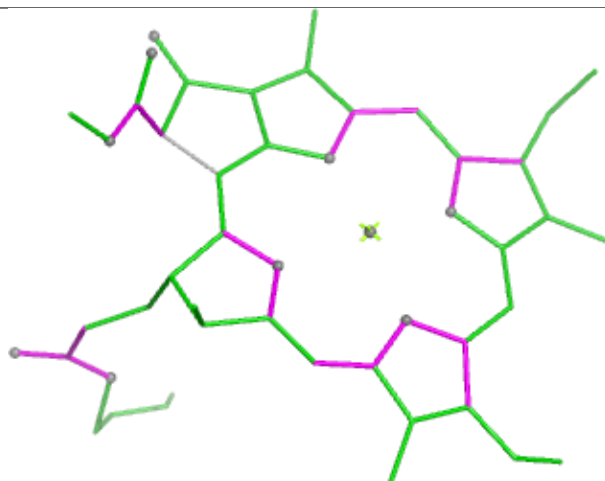




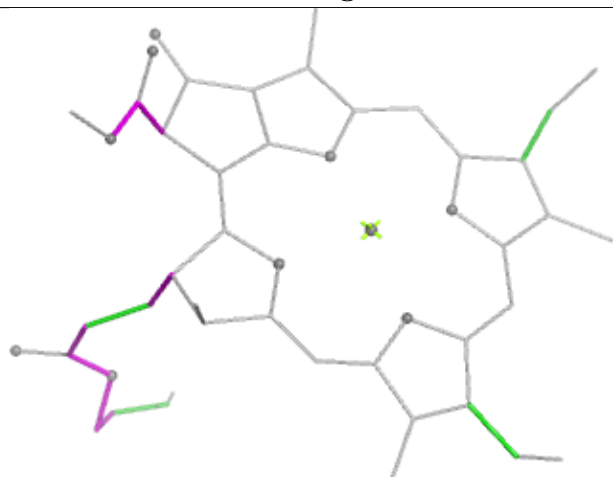
Ligand CLA r 601



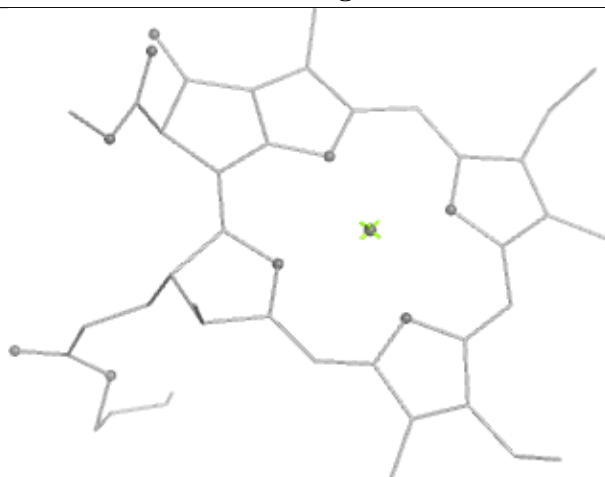
Bond lengths



Bond angles

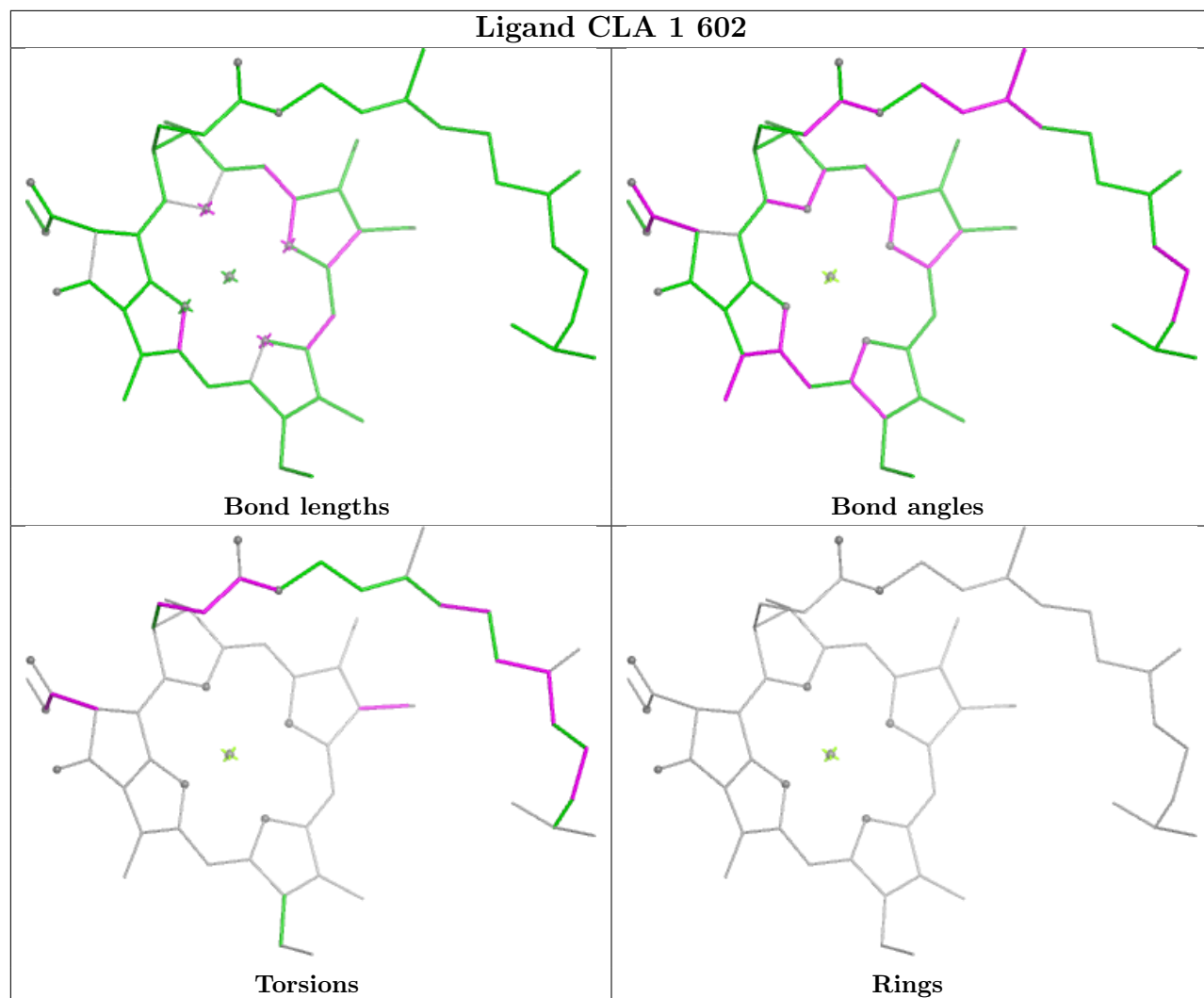


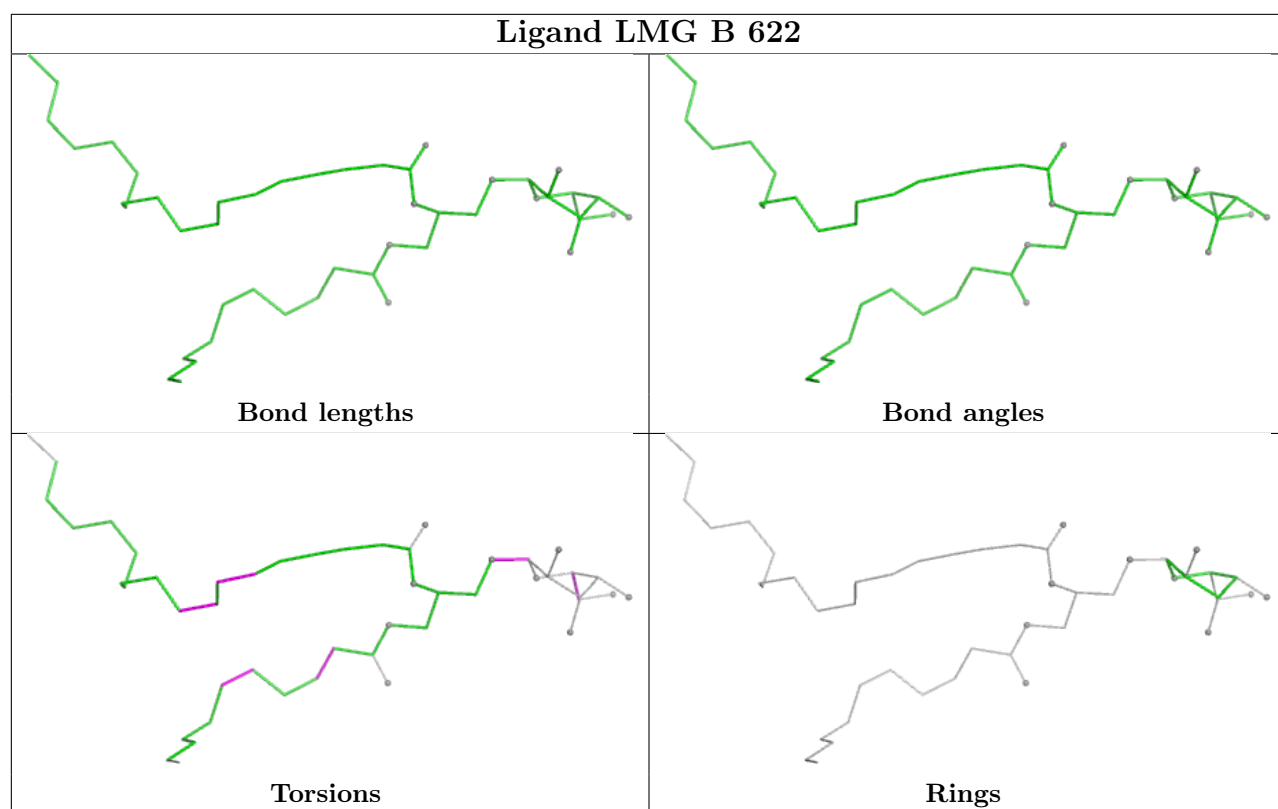
Torsions



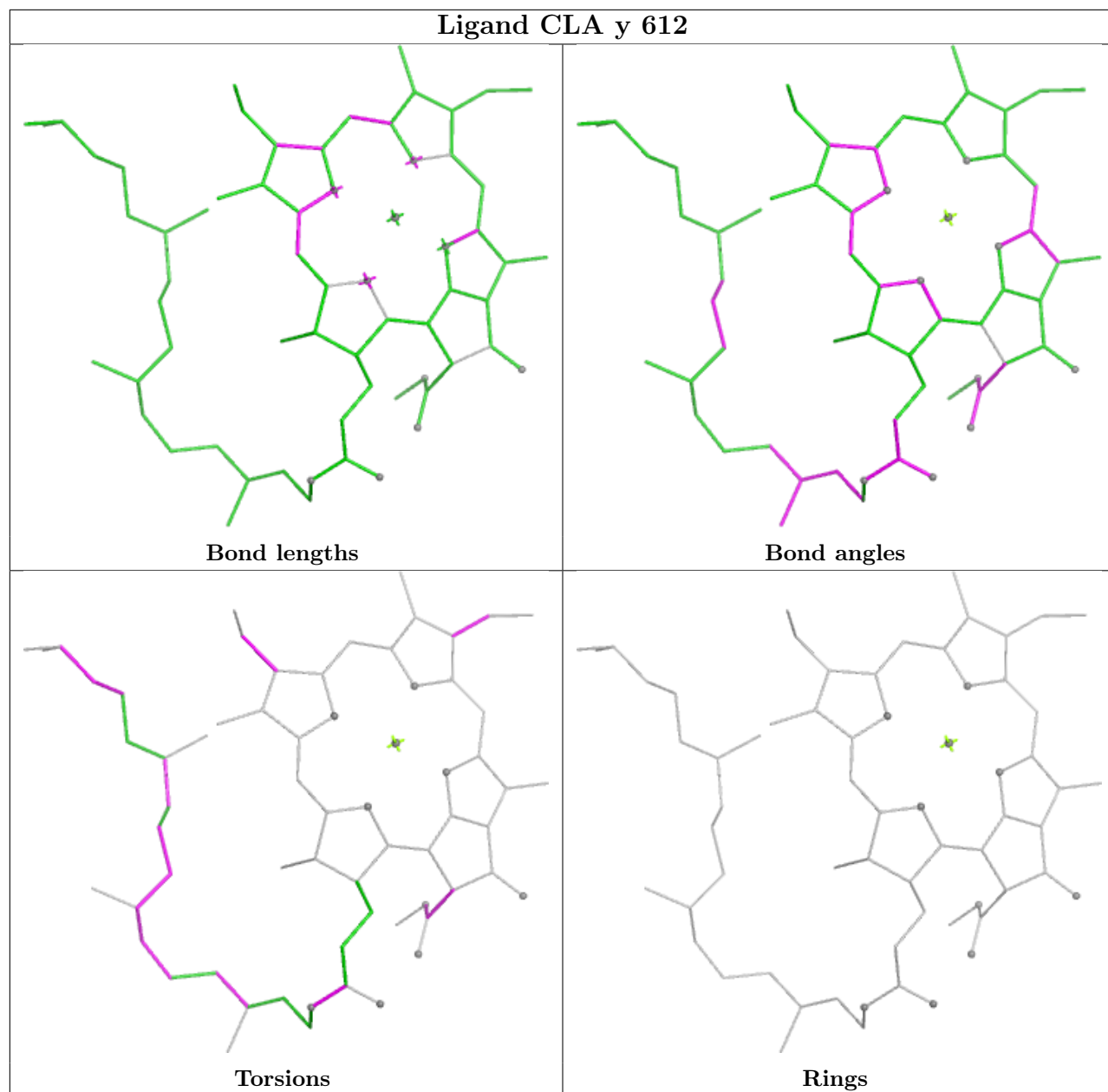
Rings

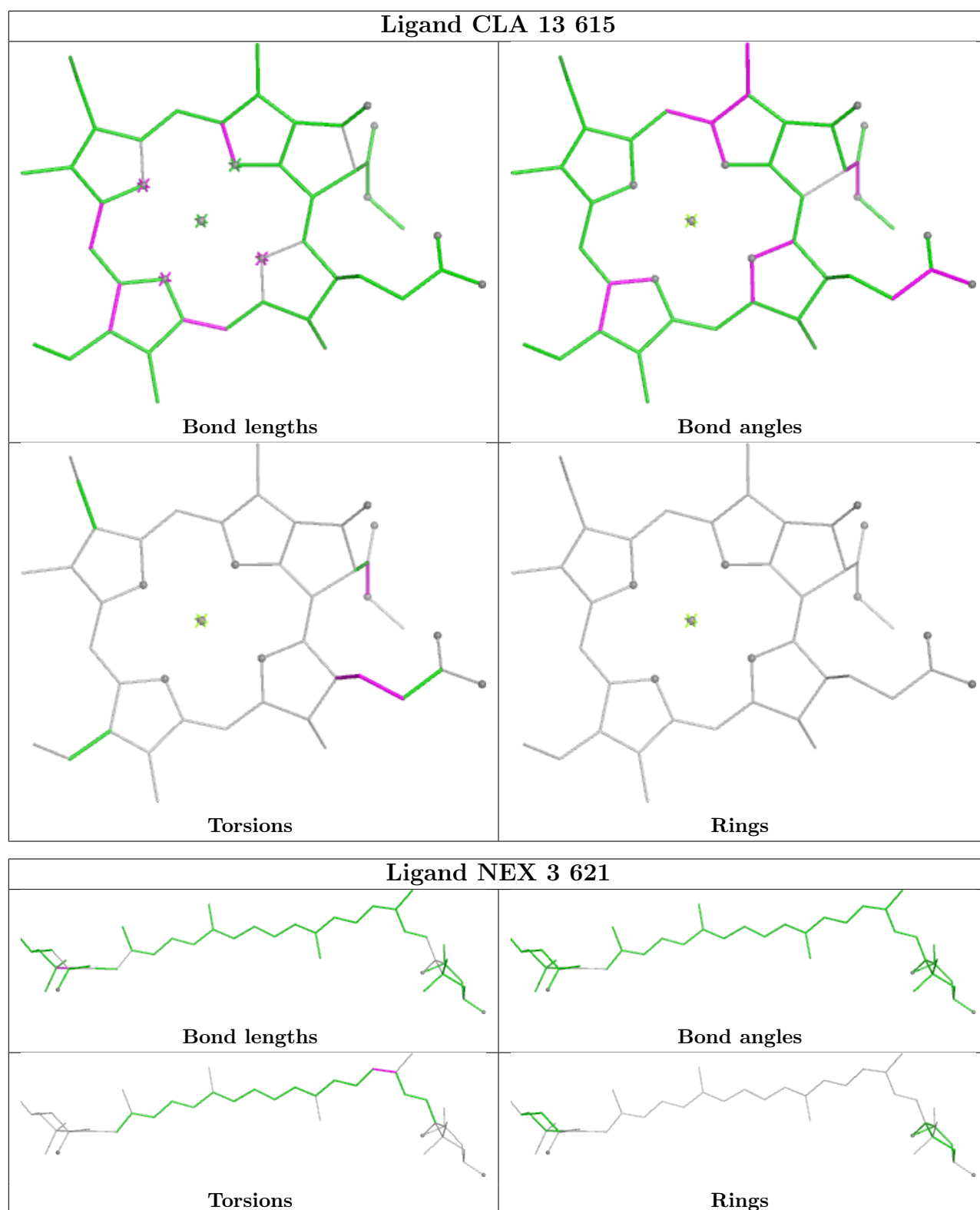
Ligand CLA 1 602

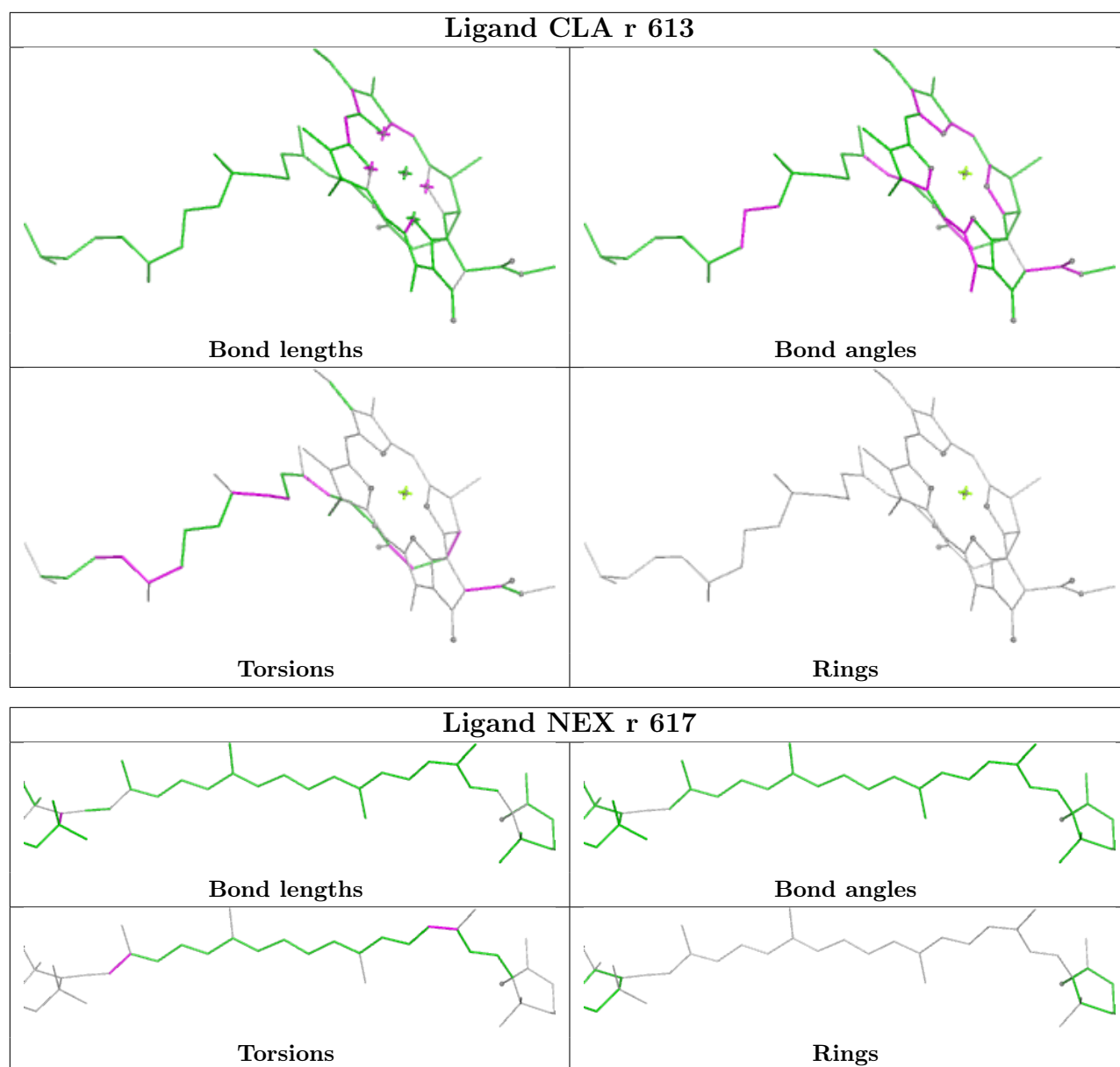


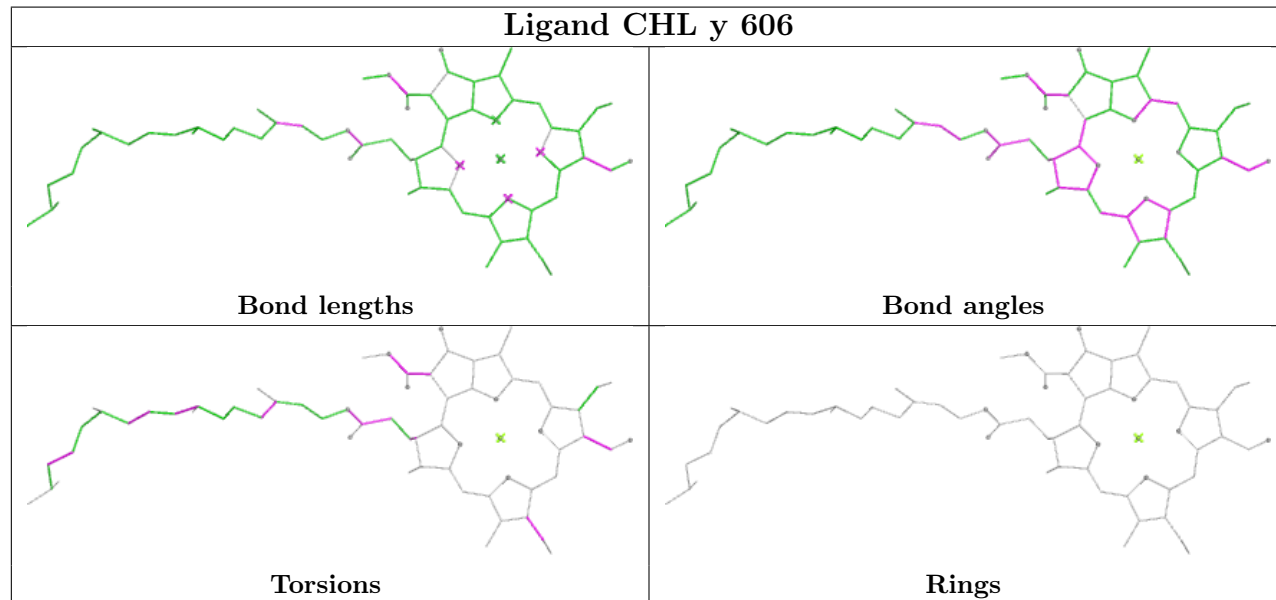
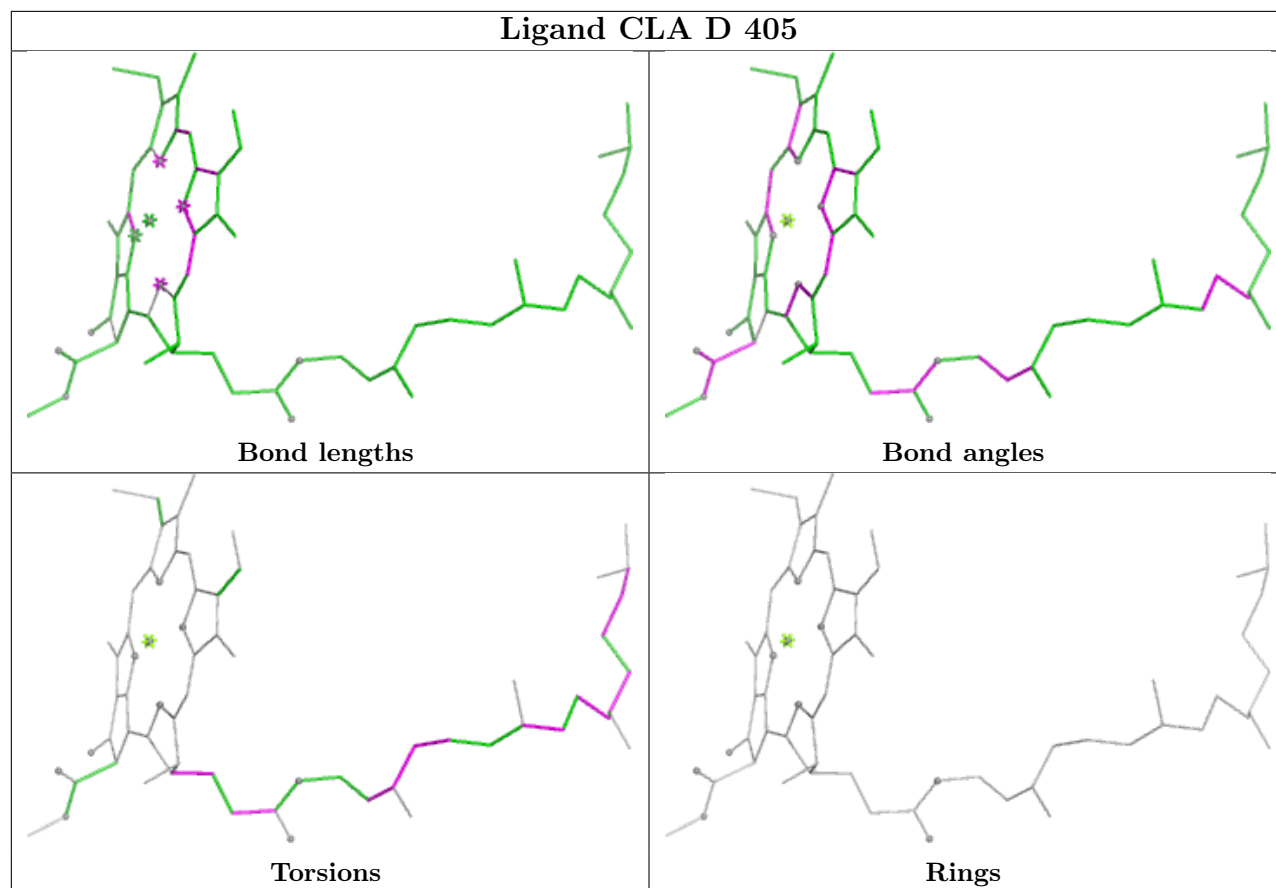


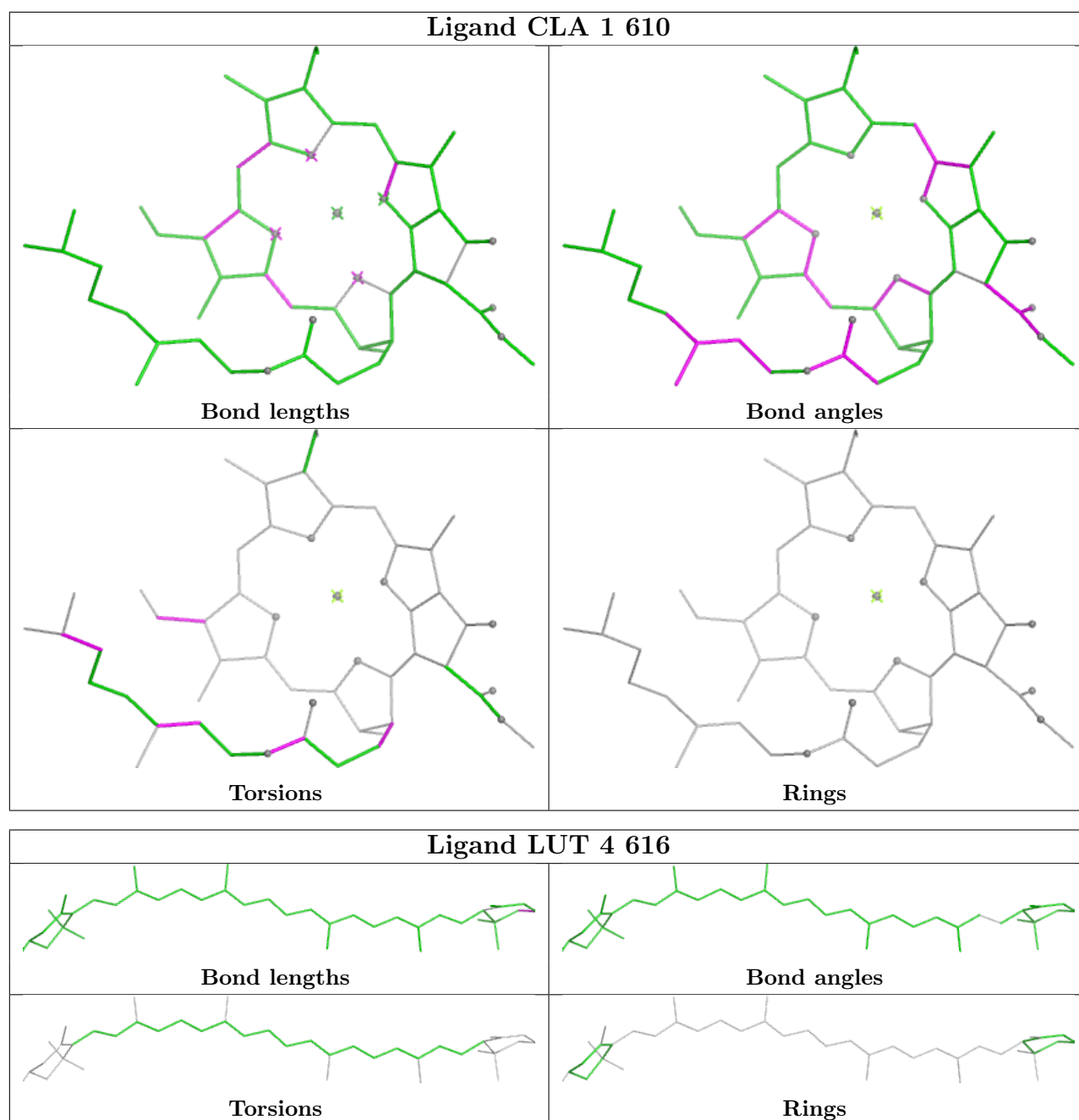
Ligand CLA y 612

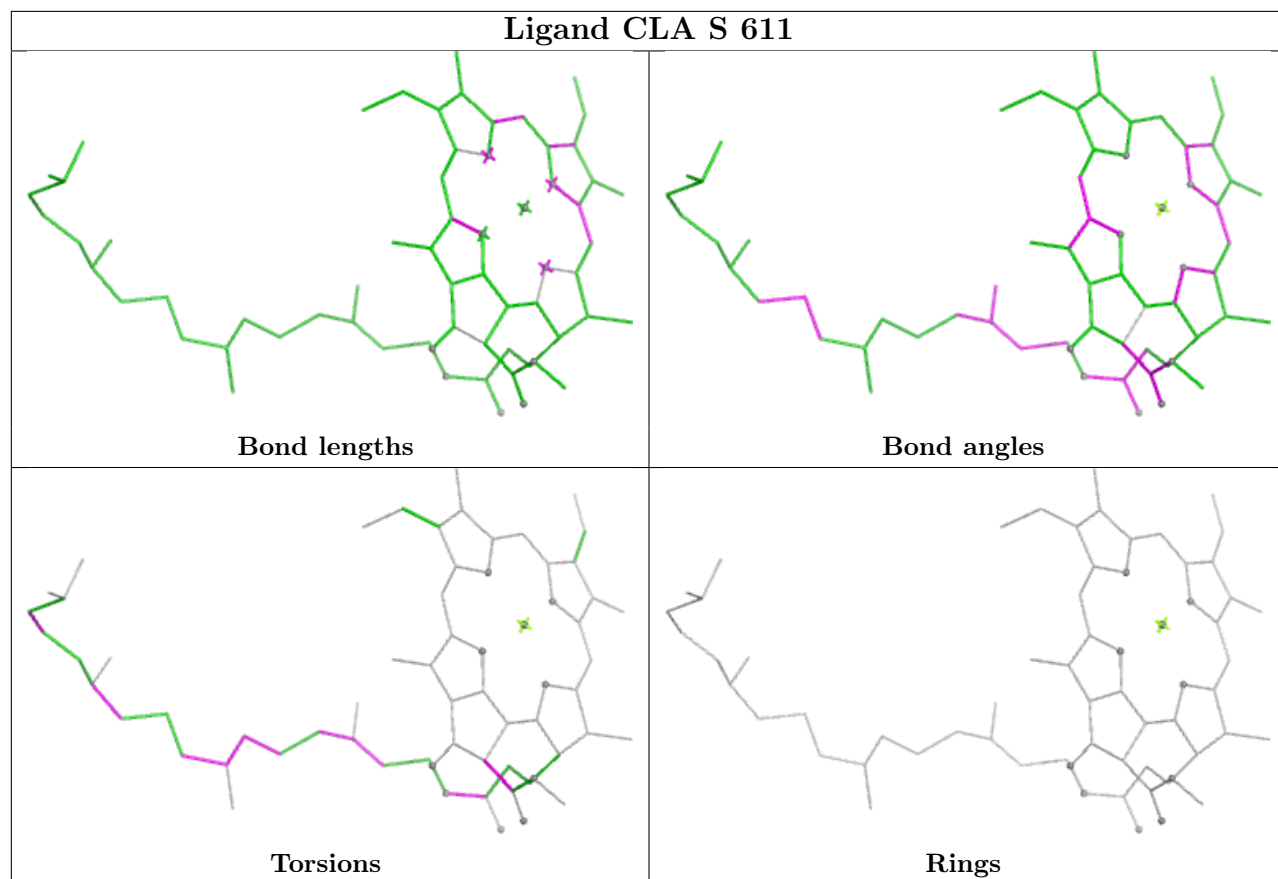


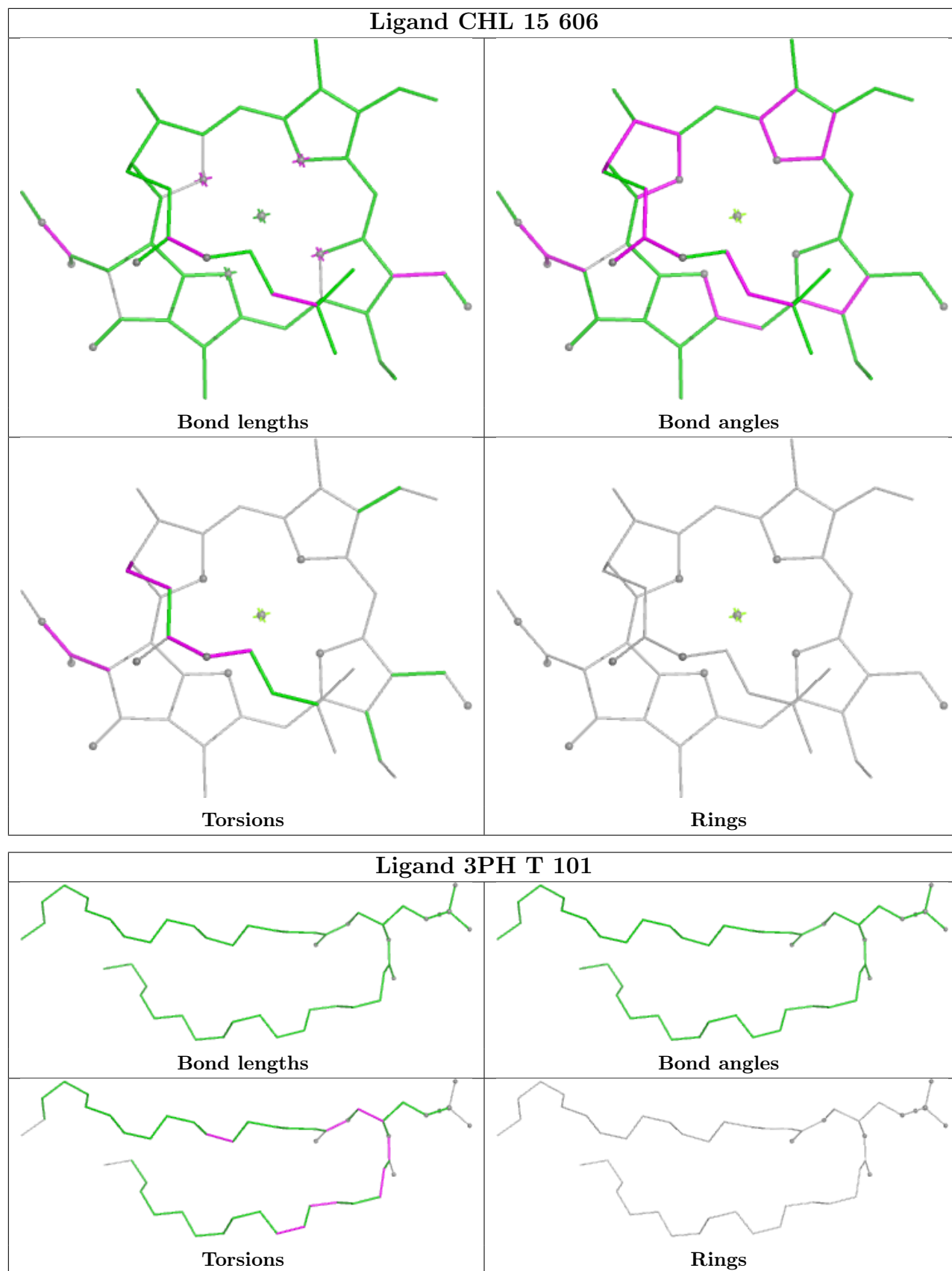


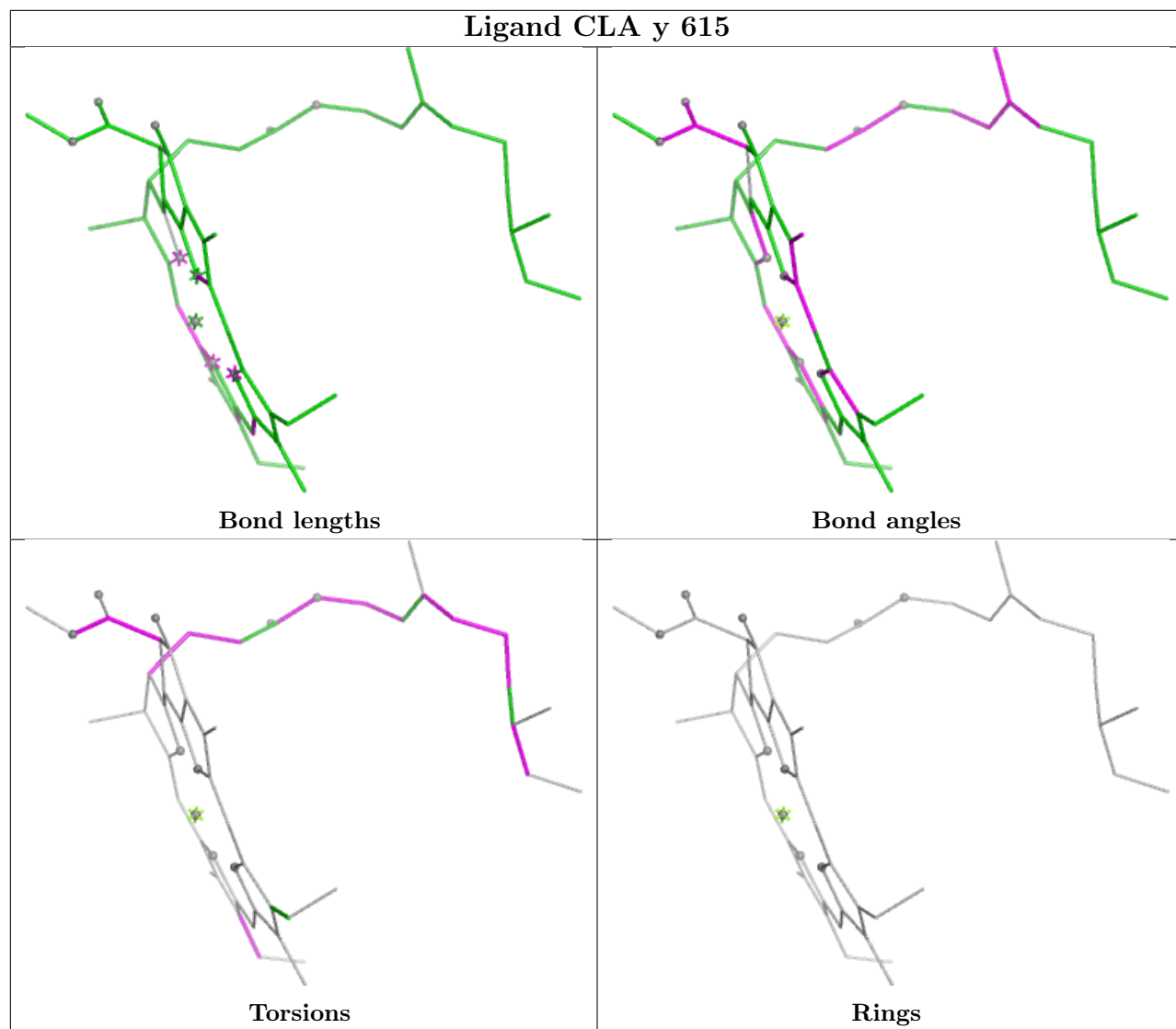


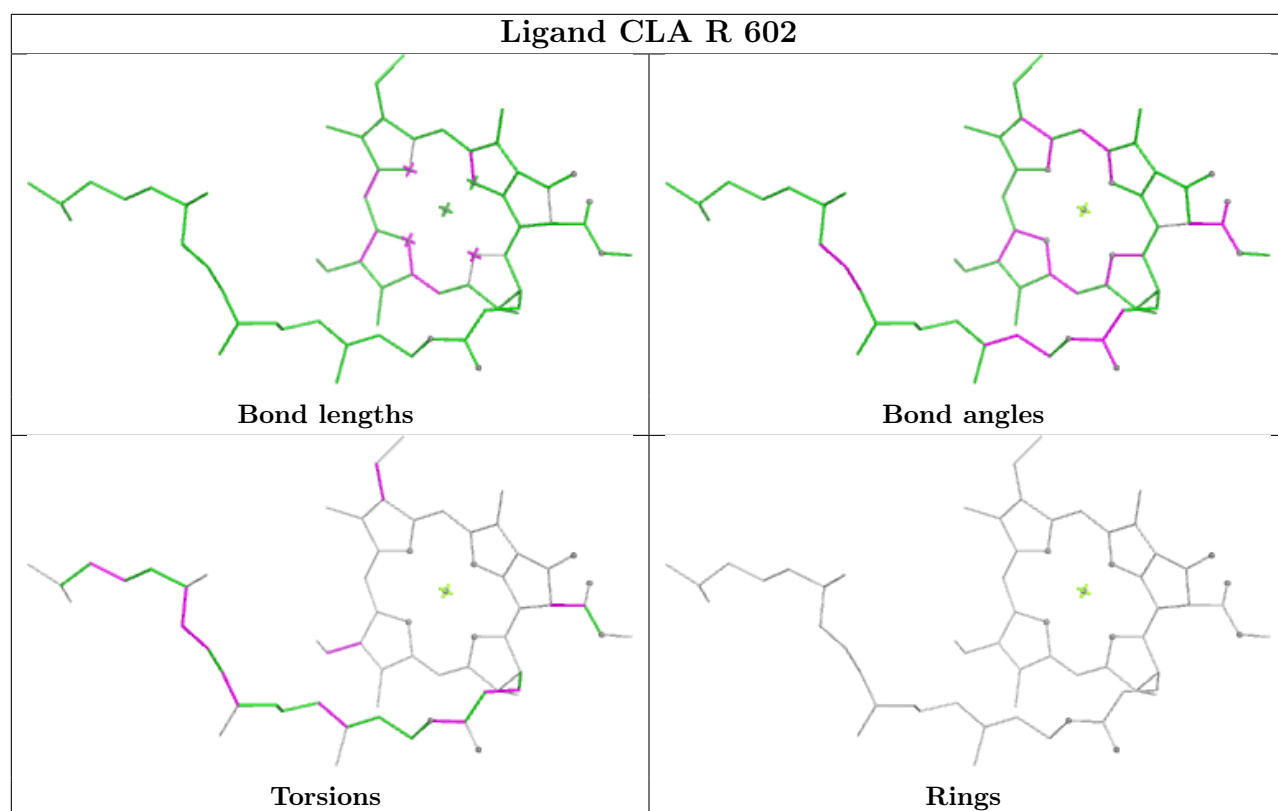


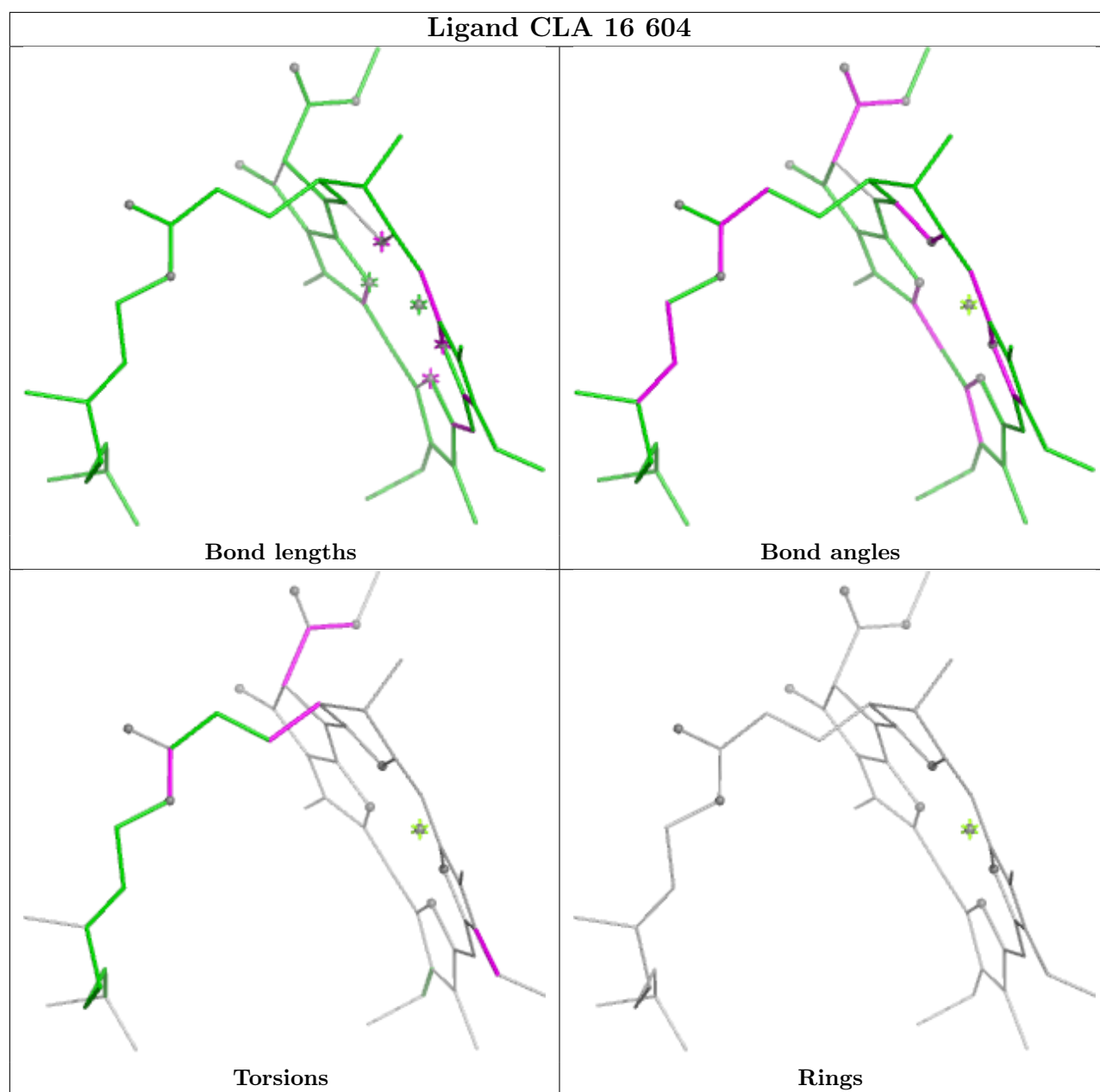


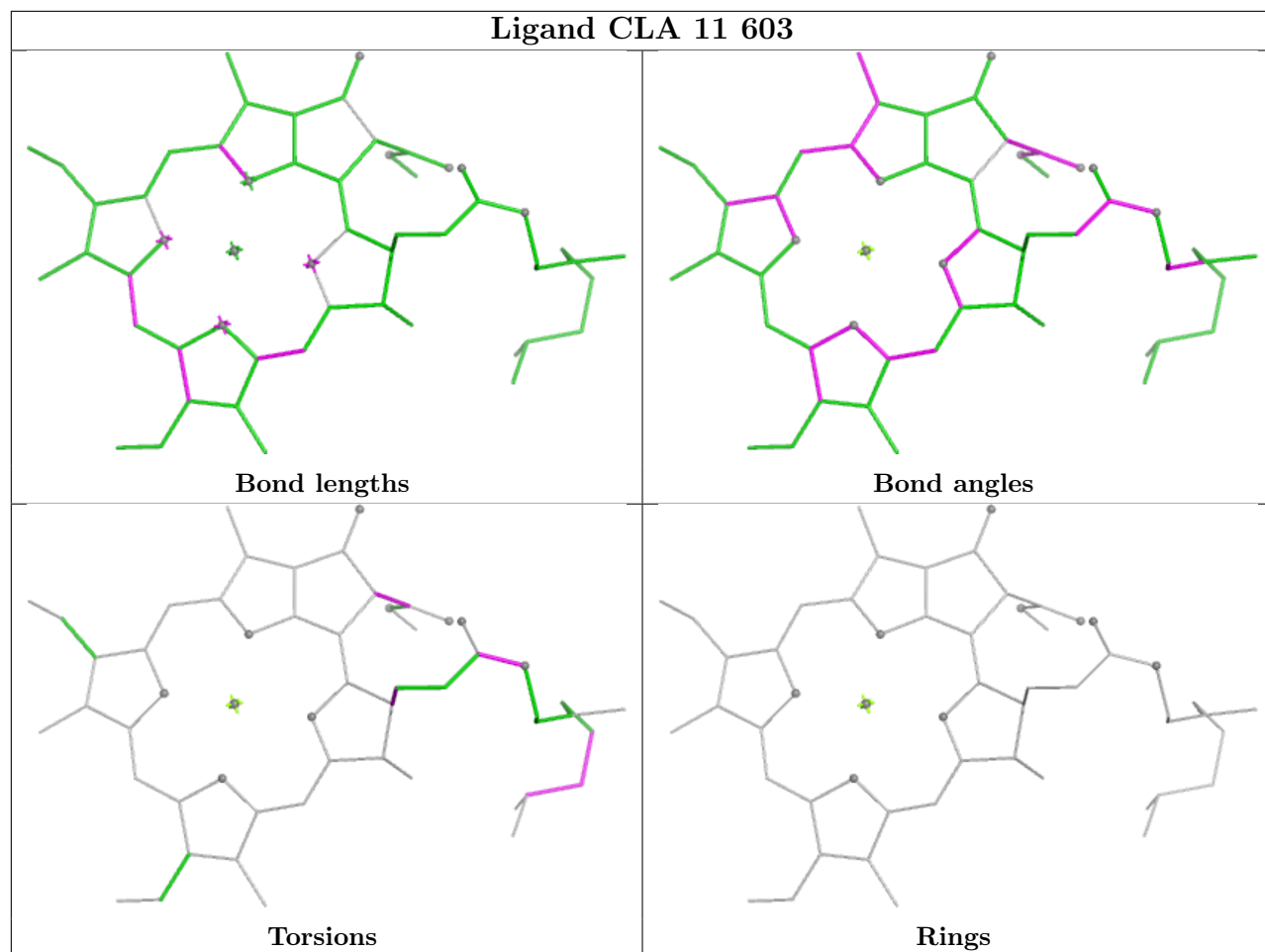




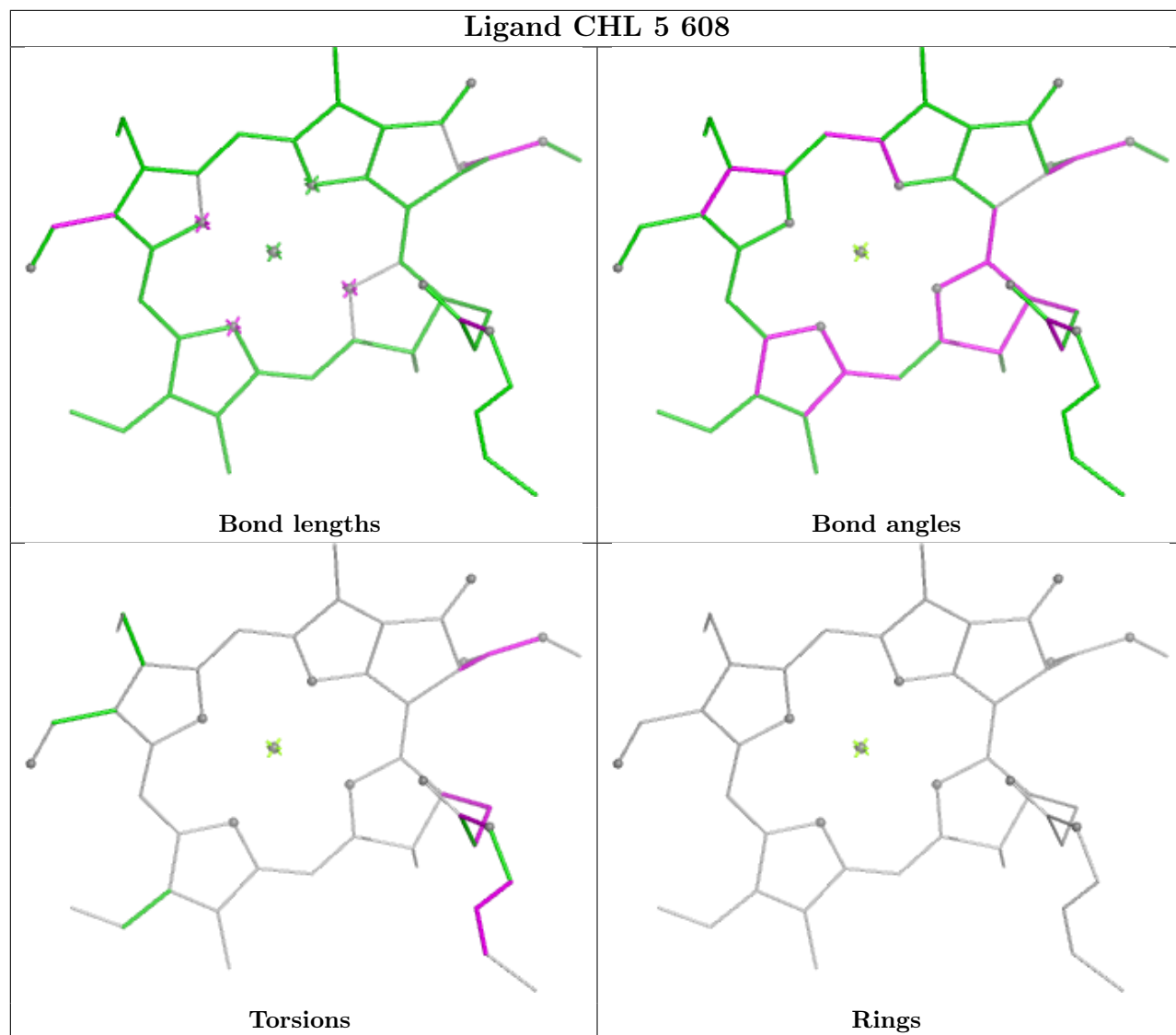


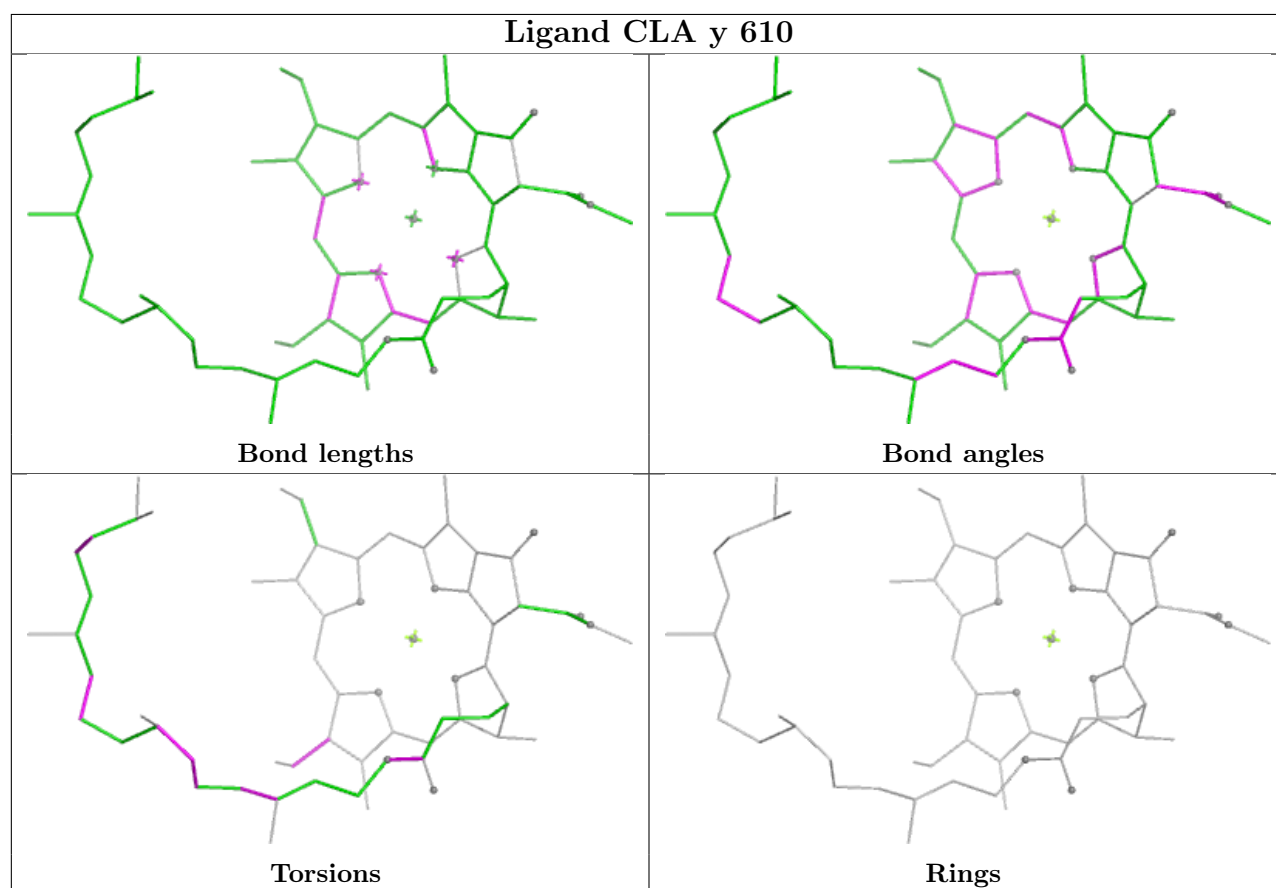
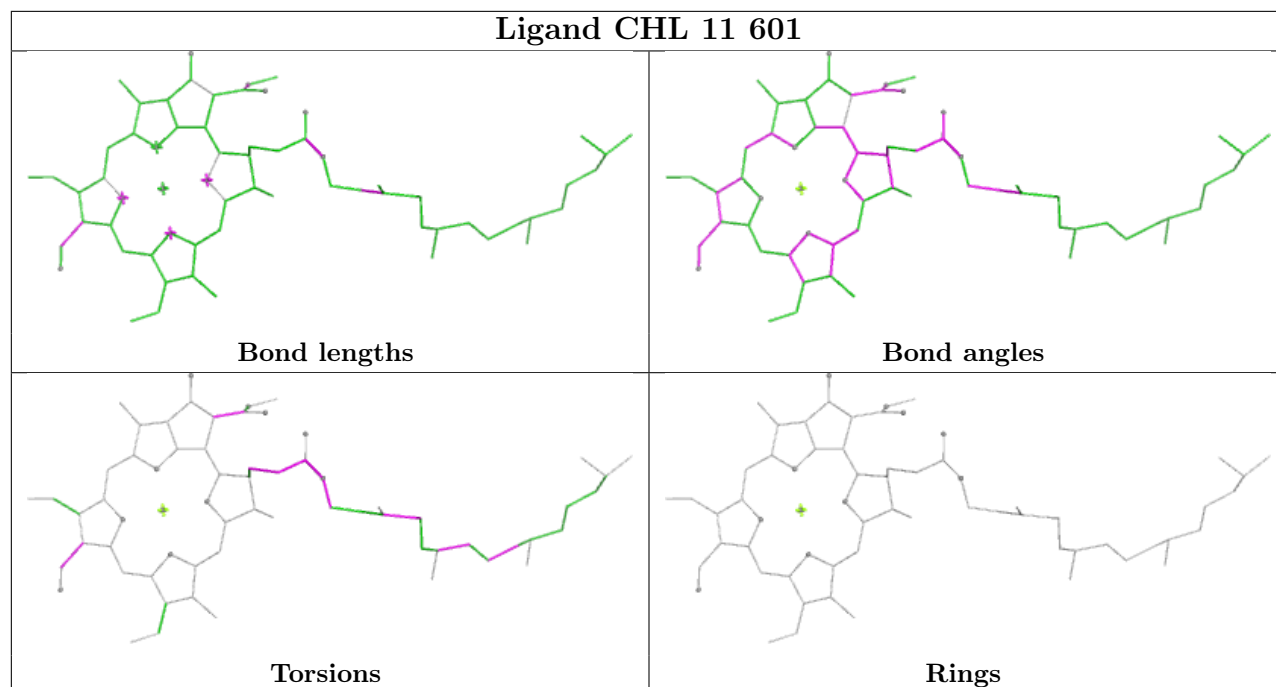


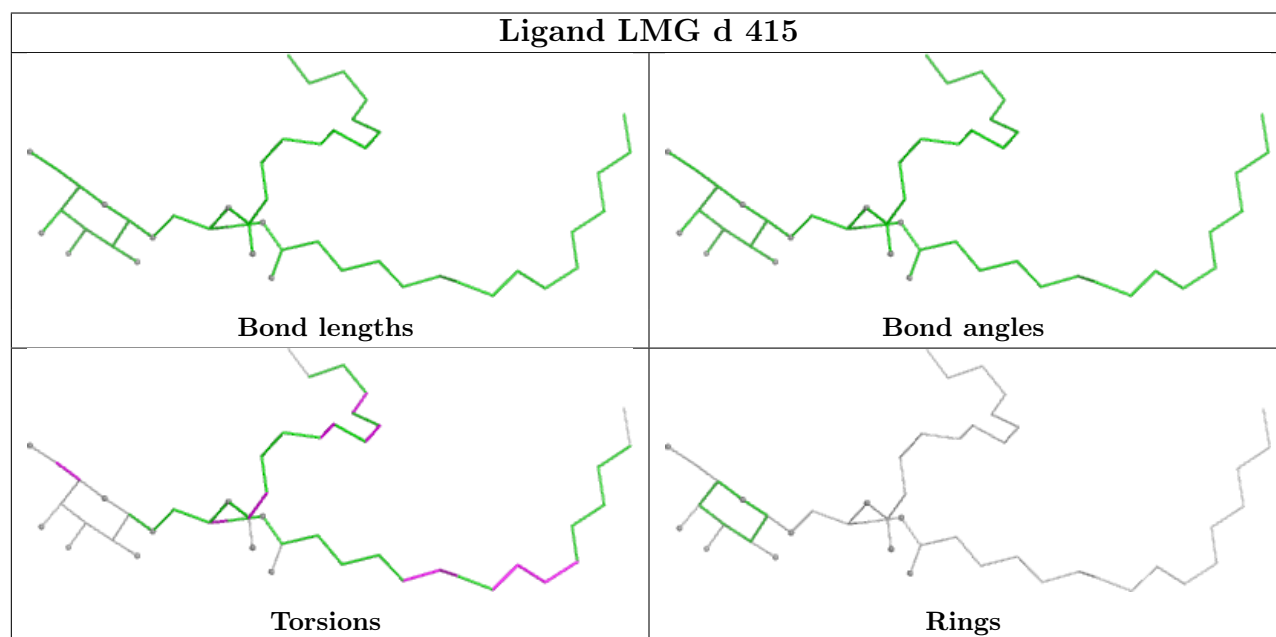
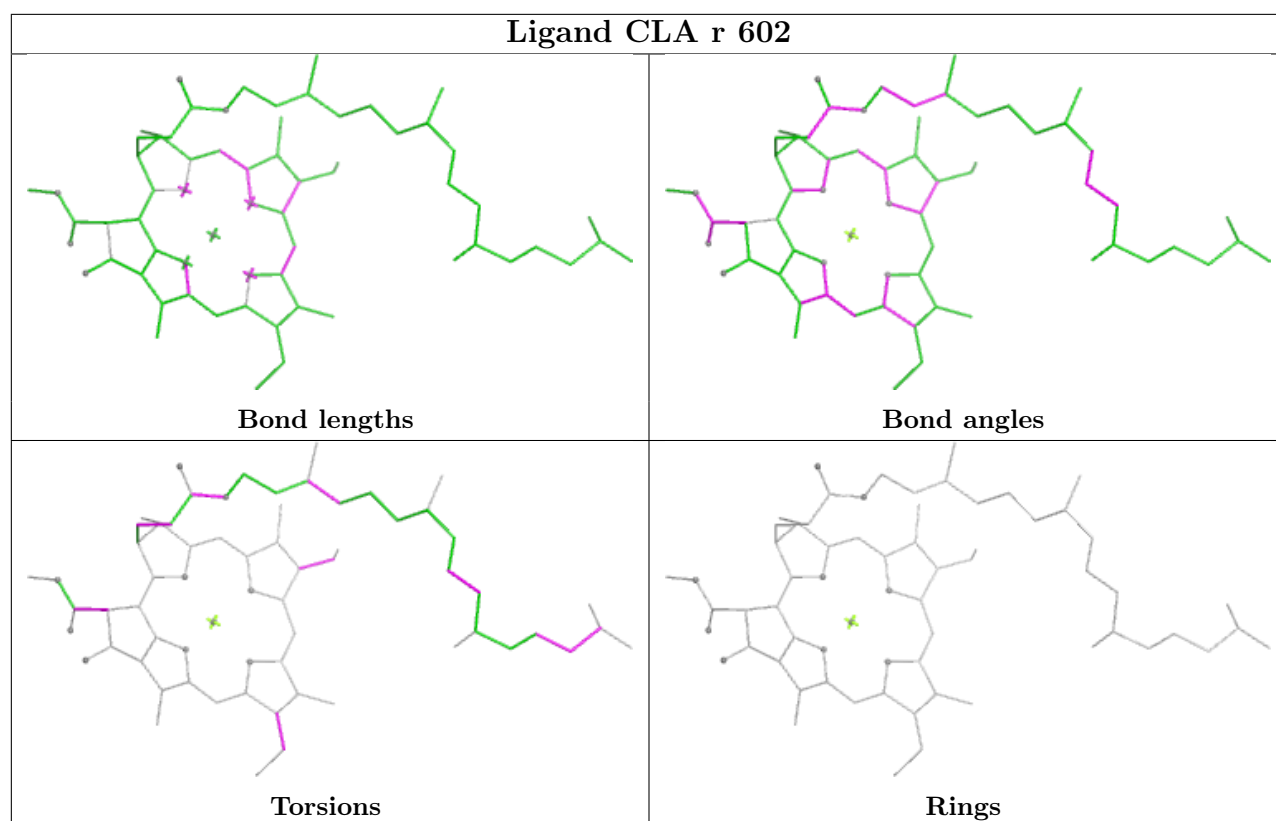


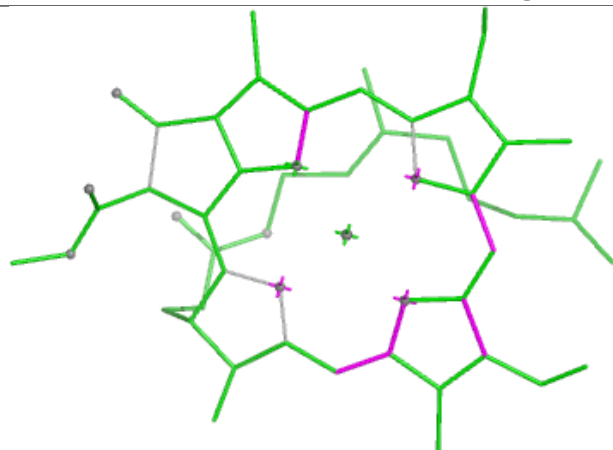


Ligand CHL 5 608

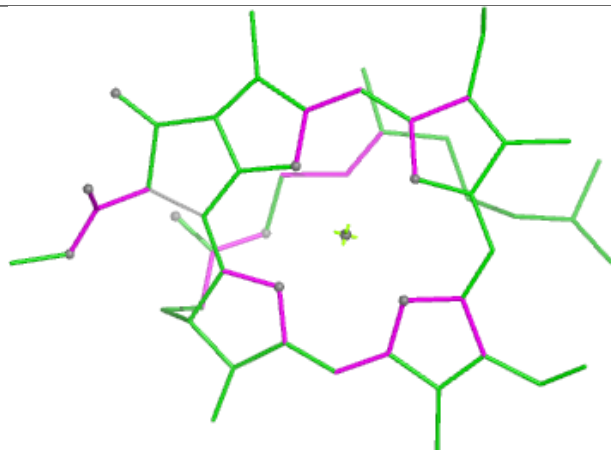




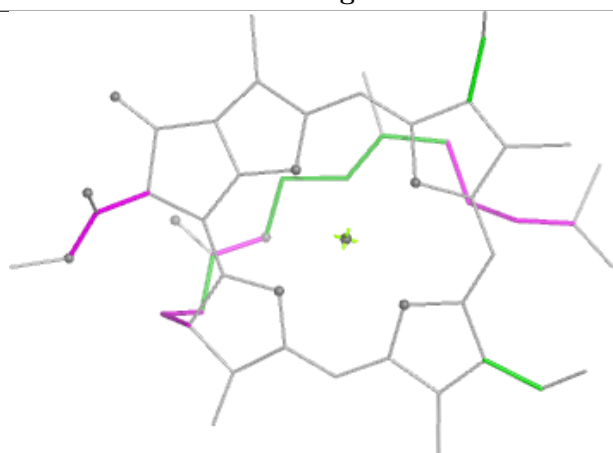


Ligand CLA 3 613

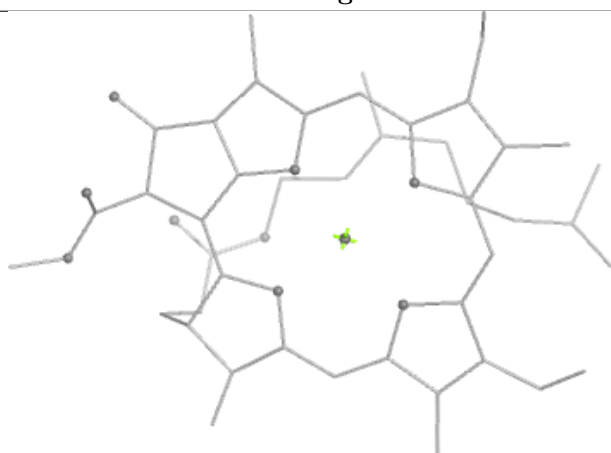
Bond lengths



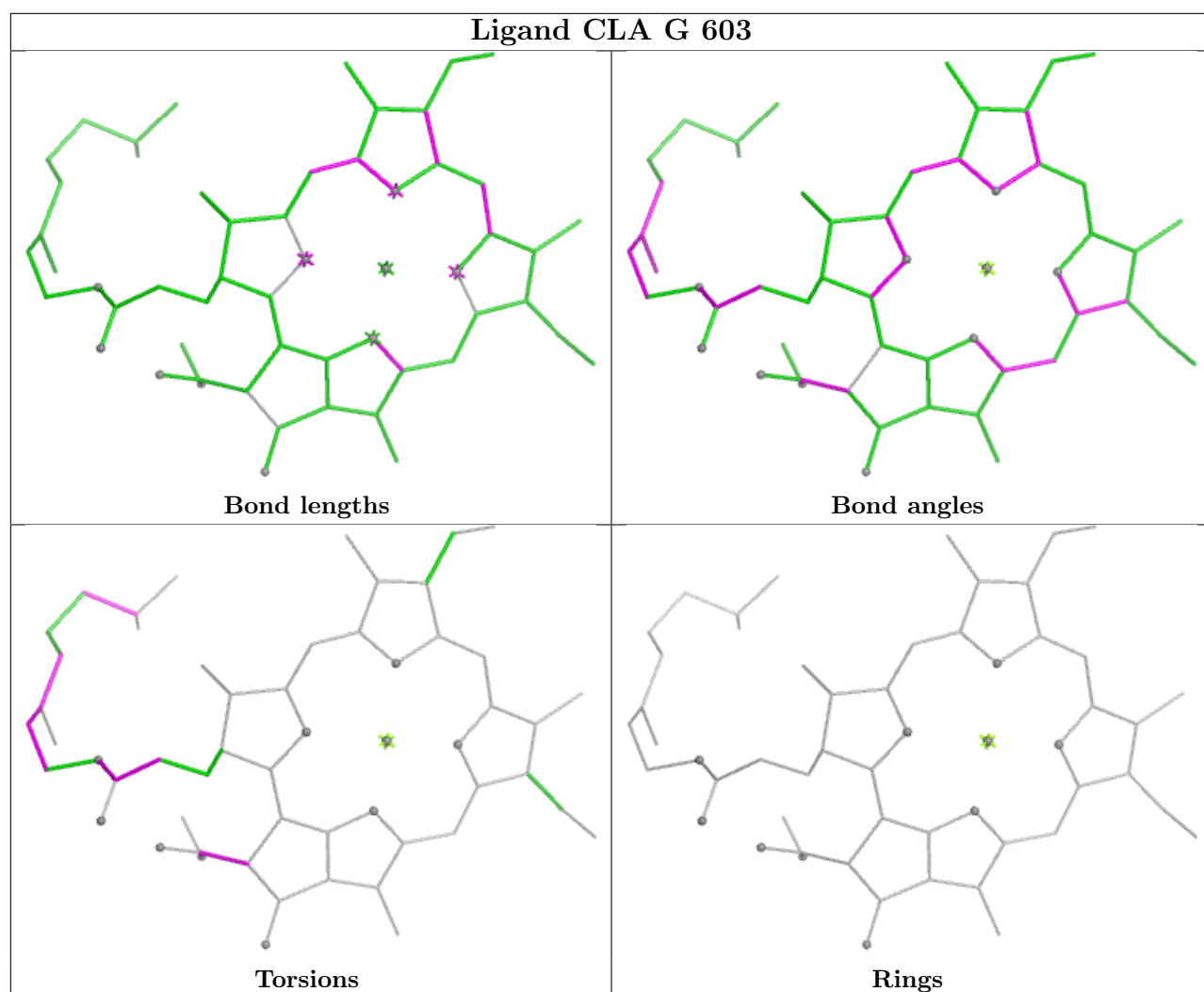
Bond angles

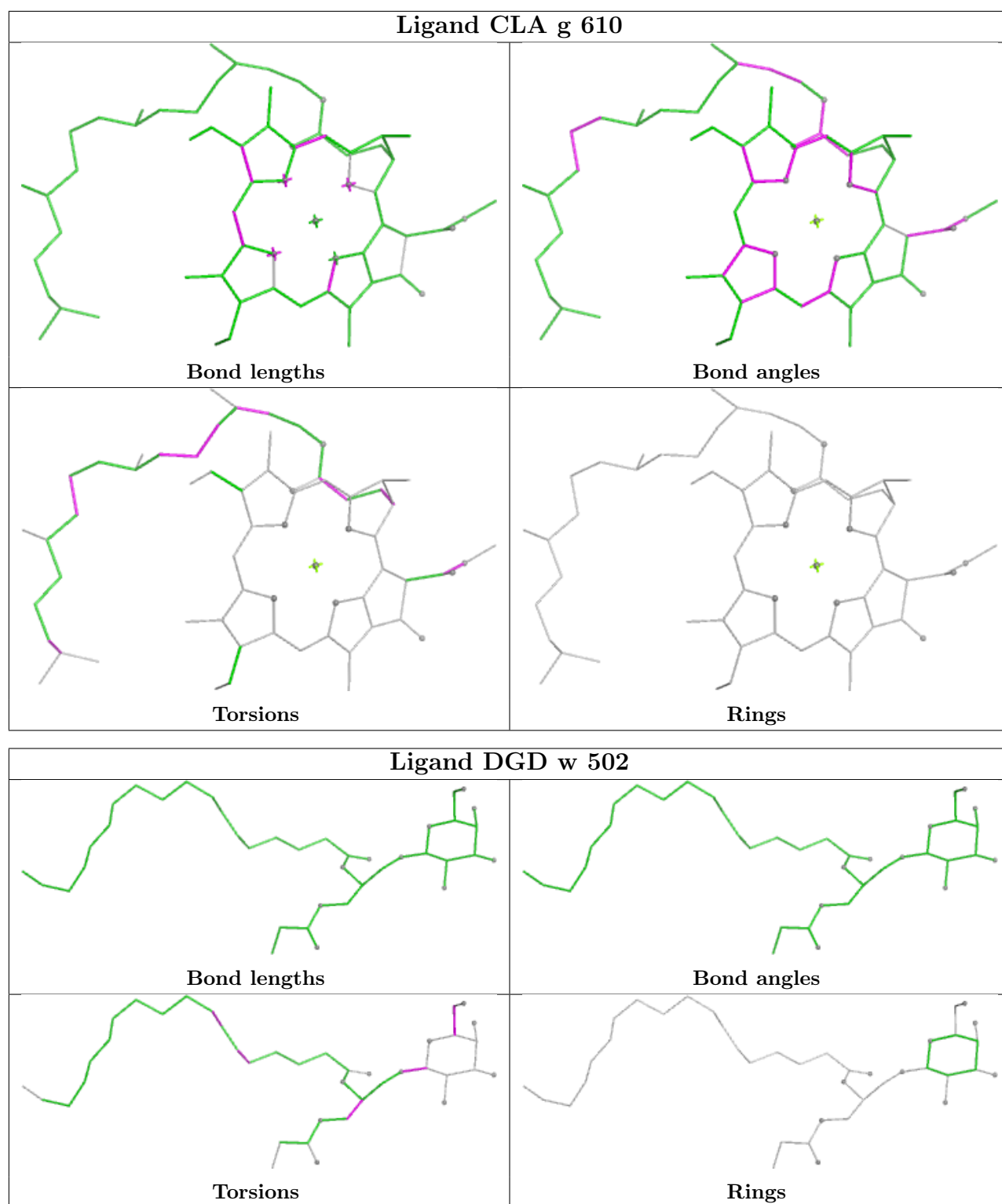


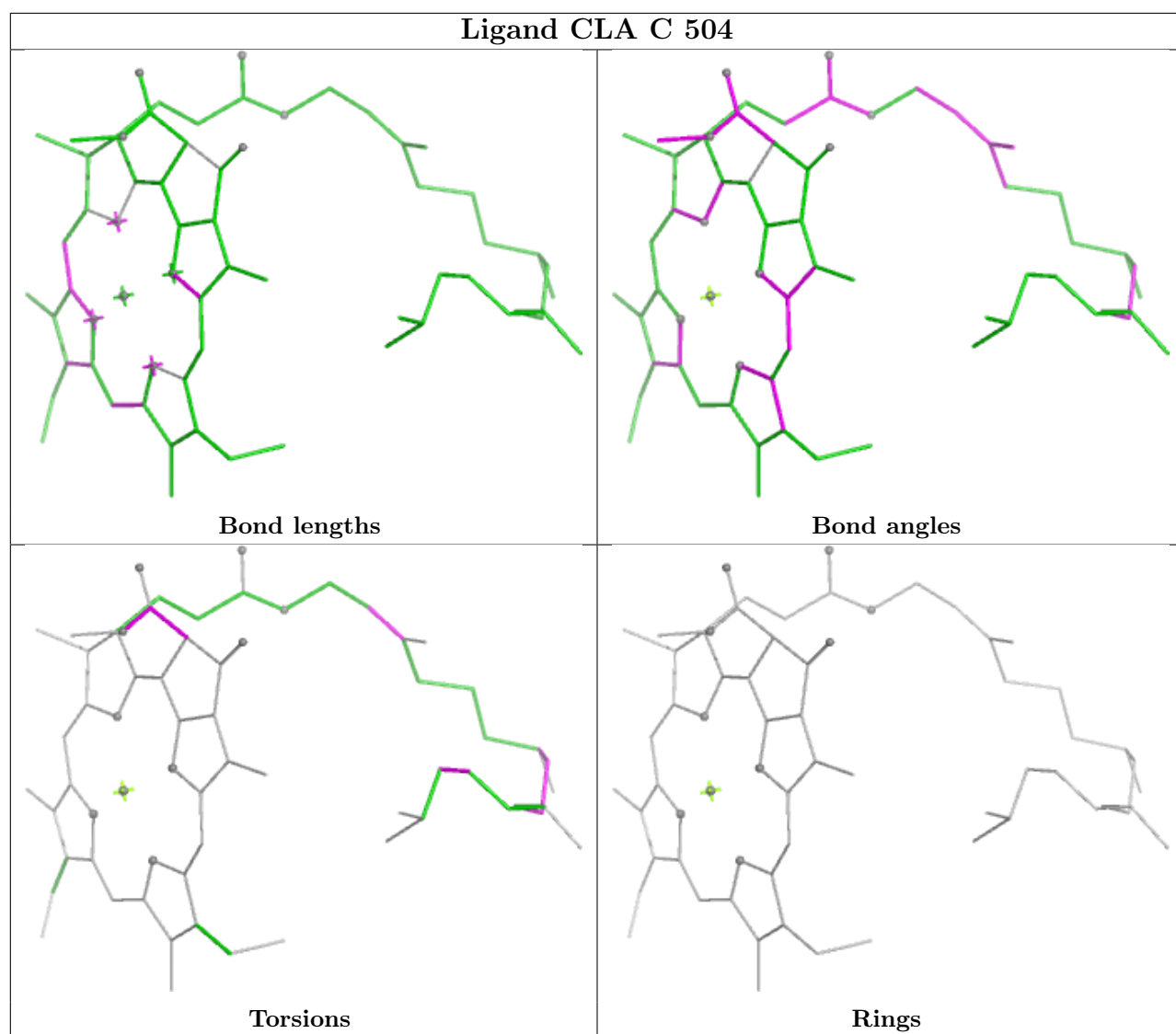
Torsions



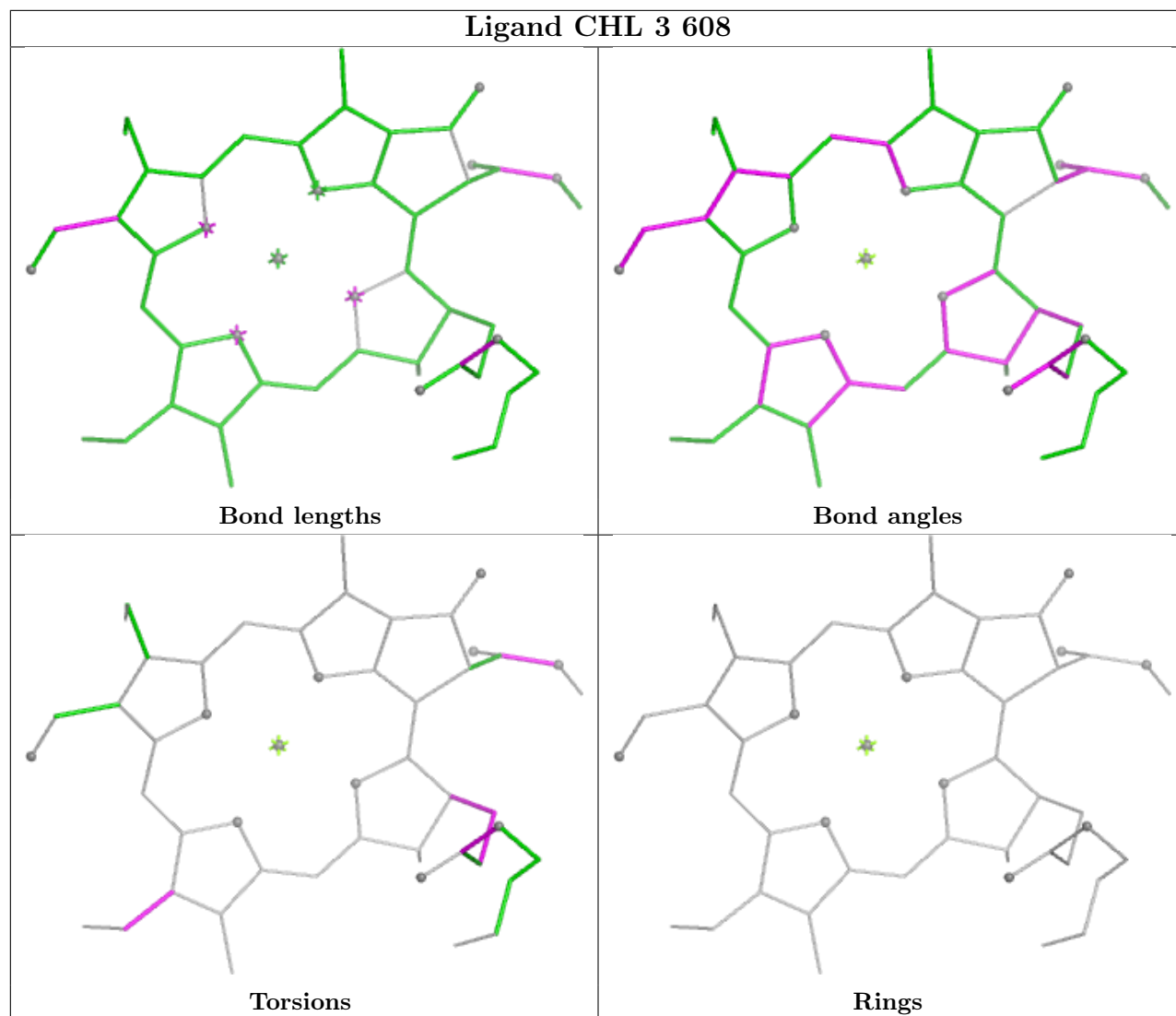
Rings



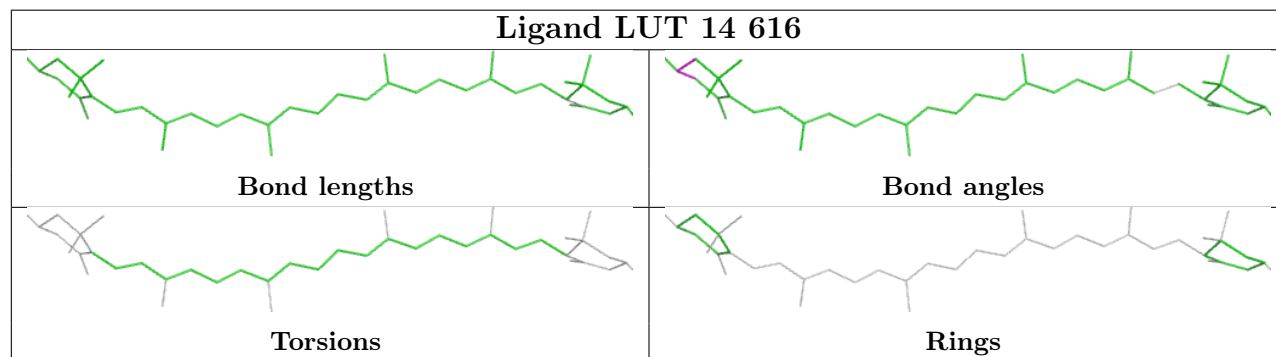


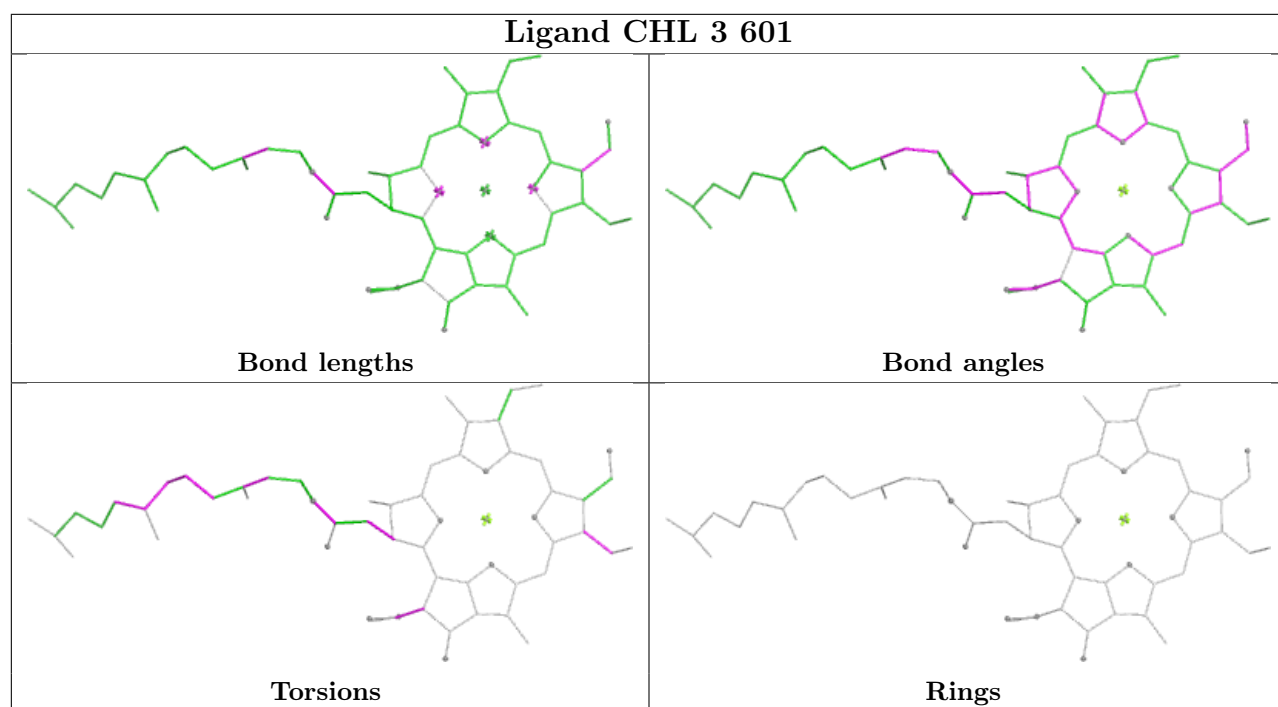
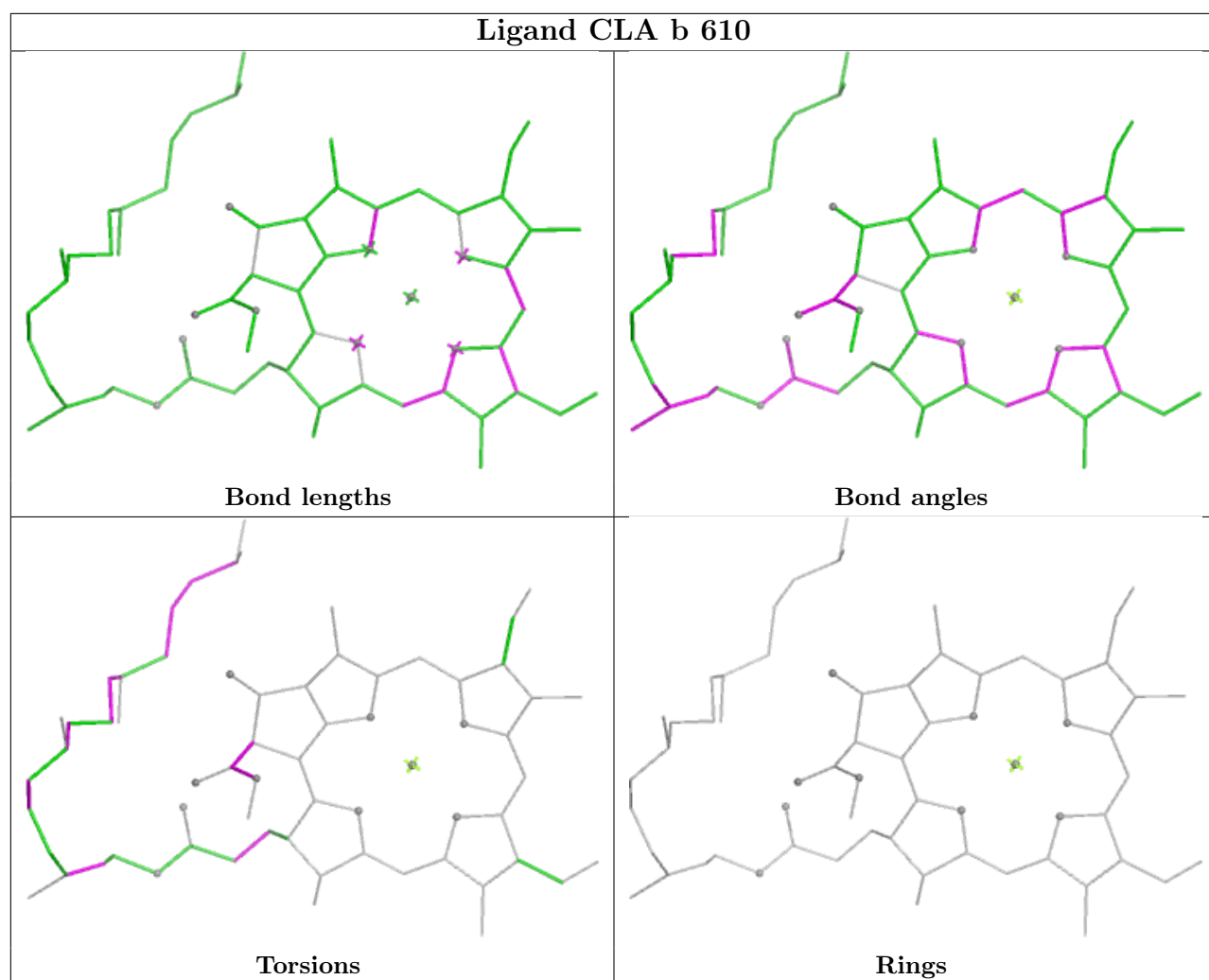


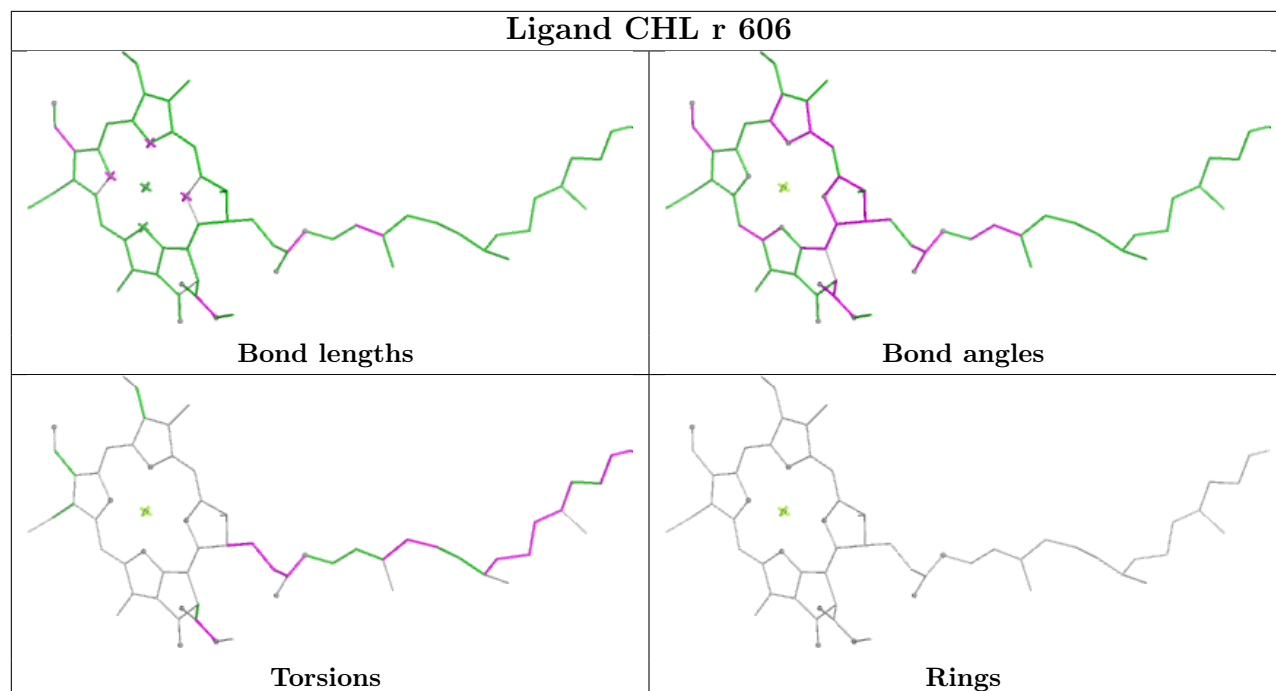
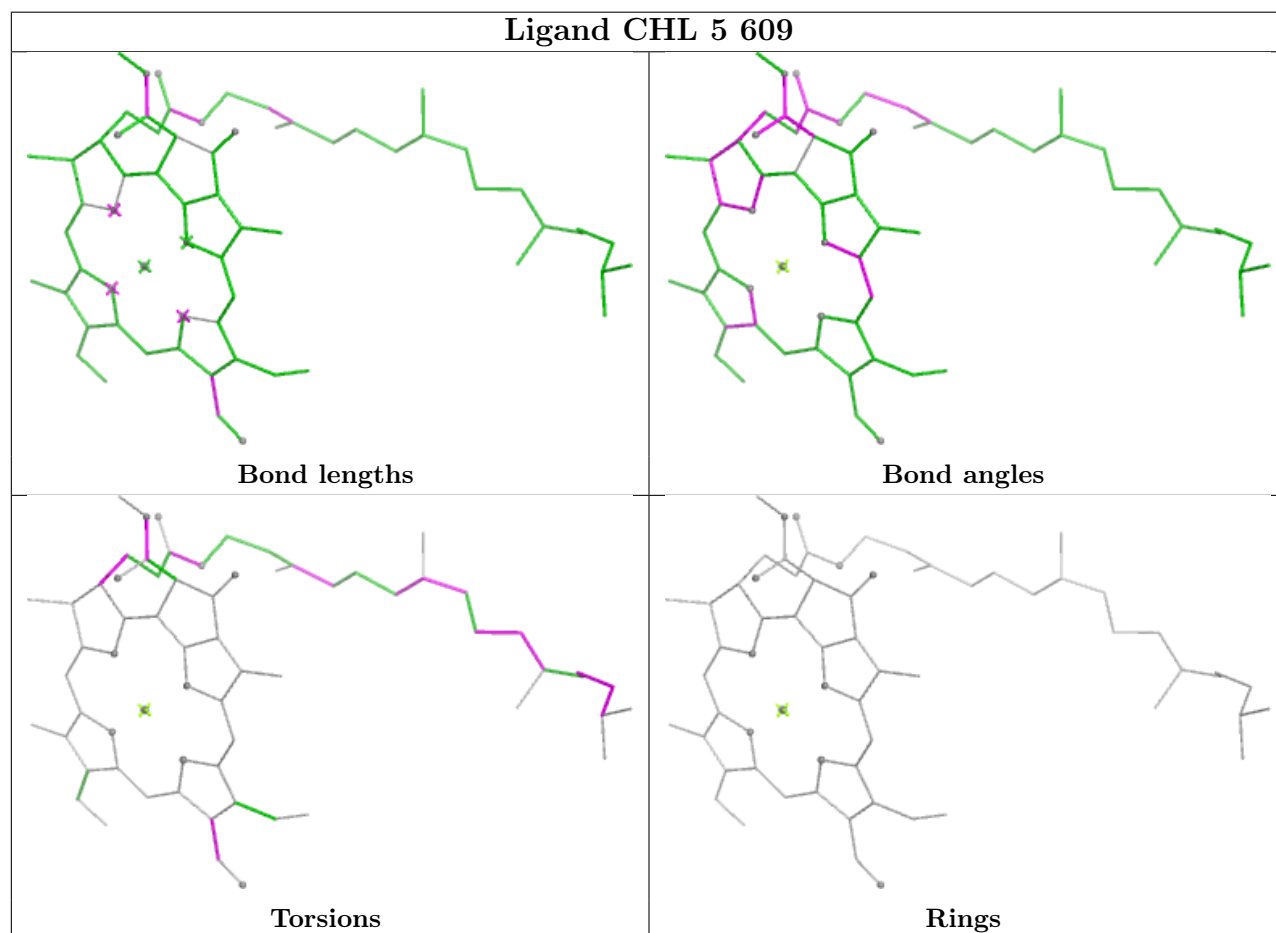
Ligand CHL 3 608

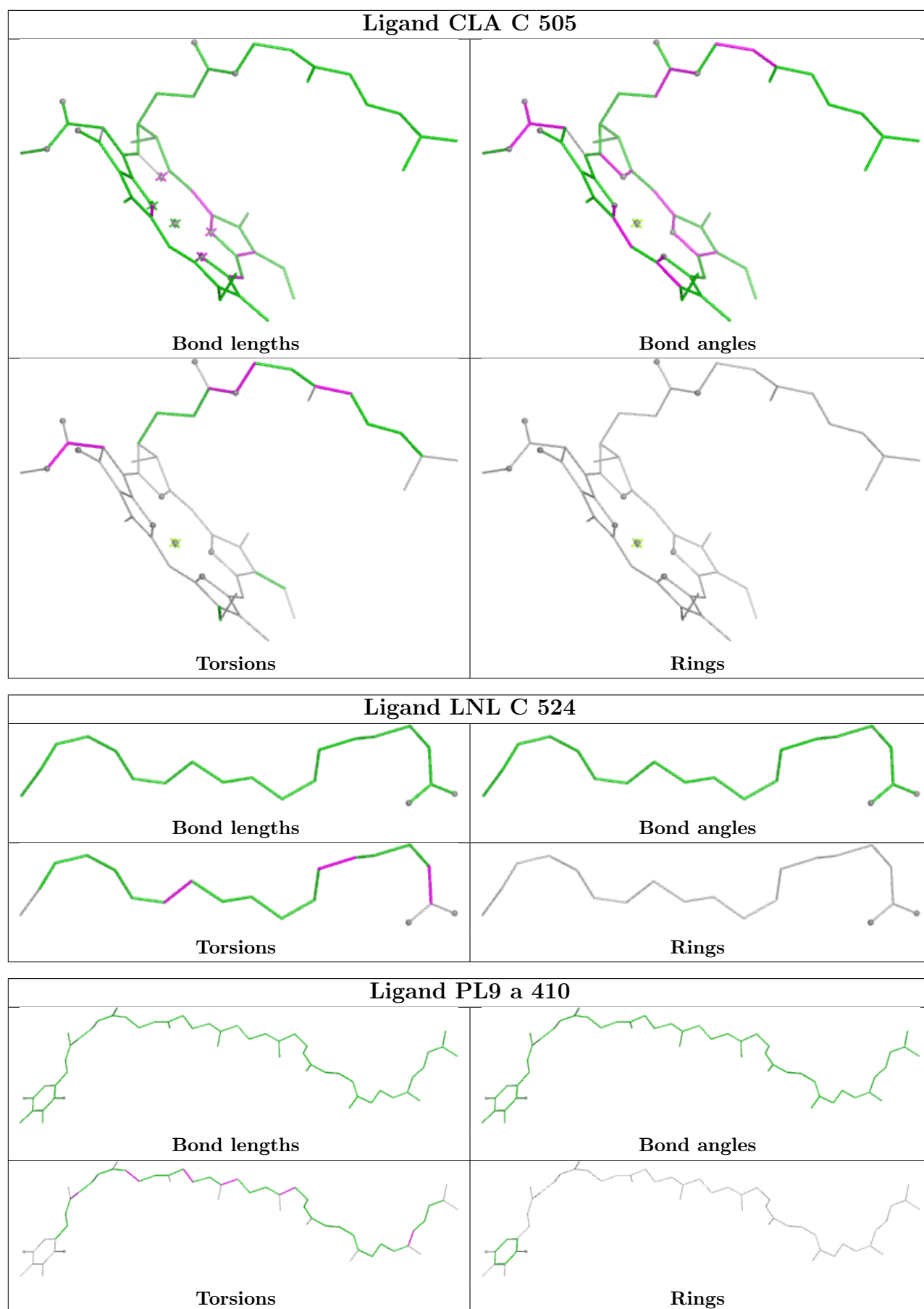


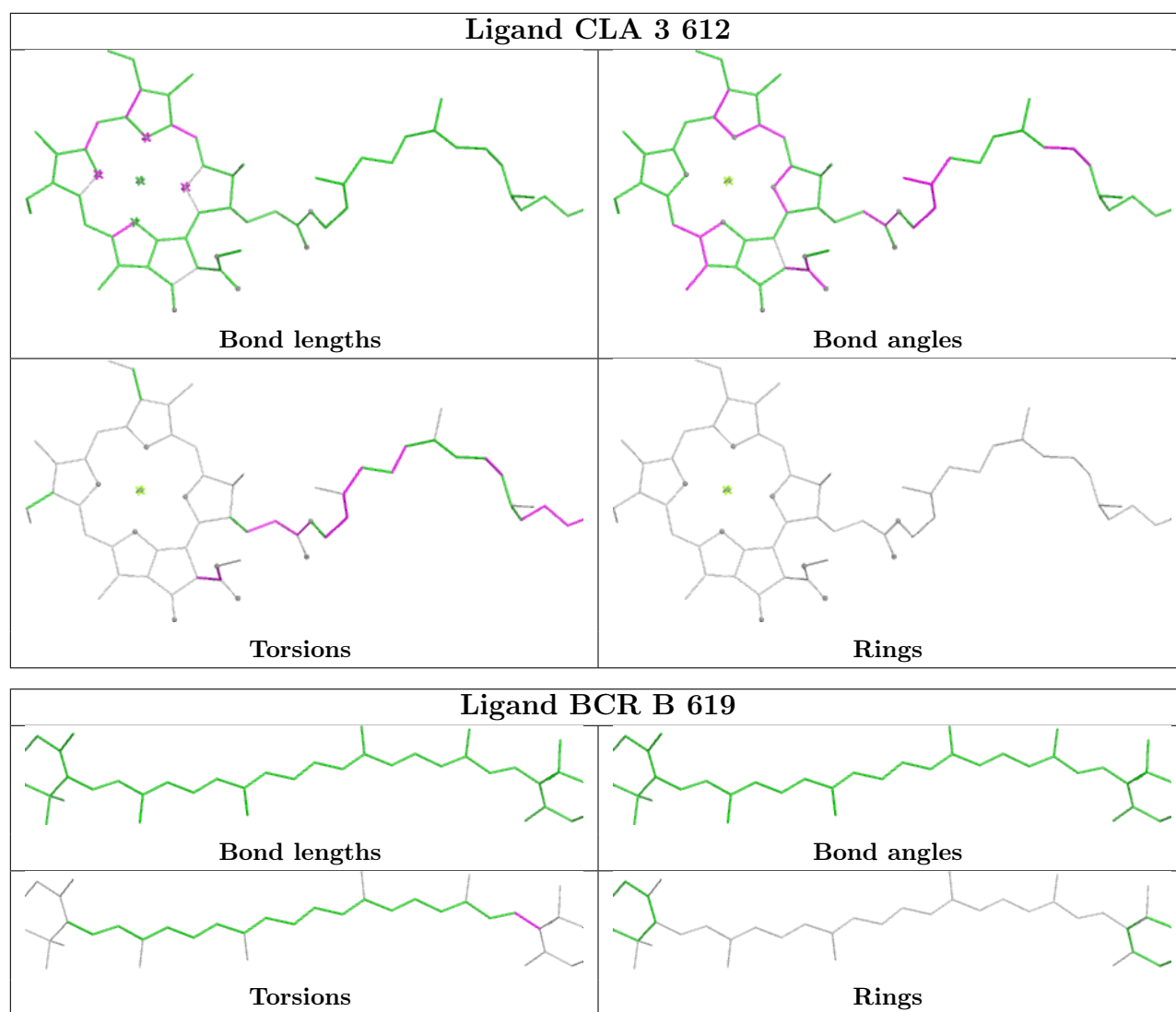
Ligand LUT 14 616

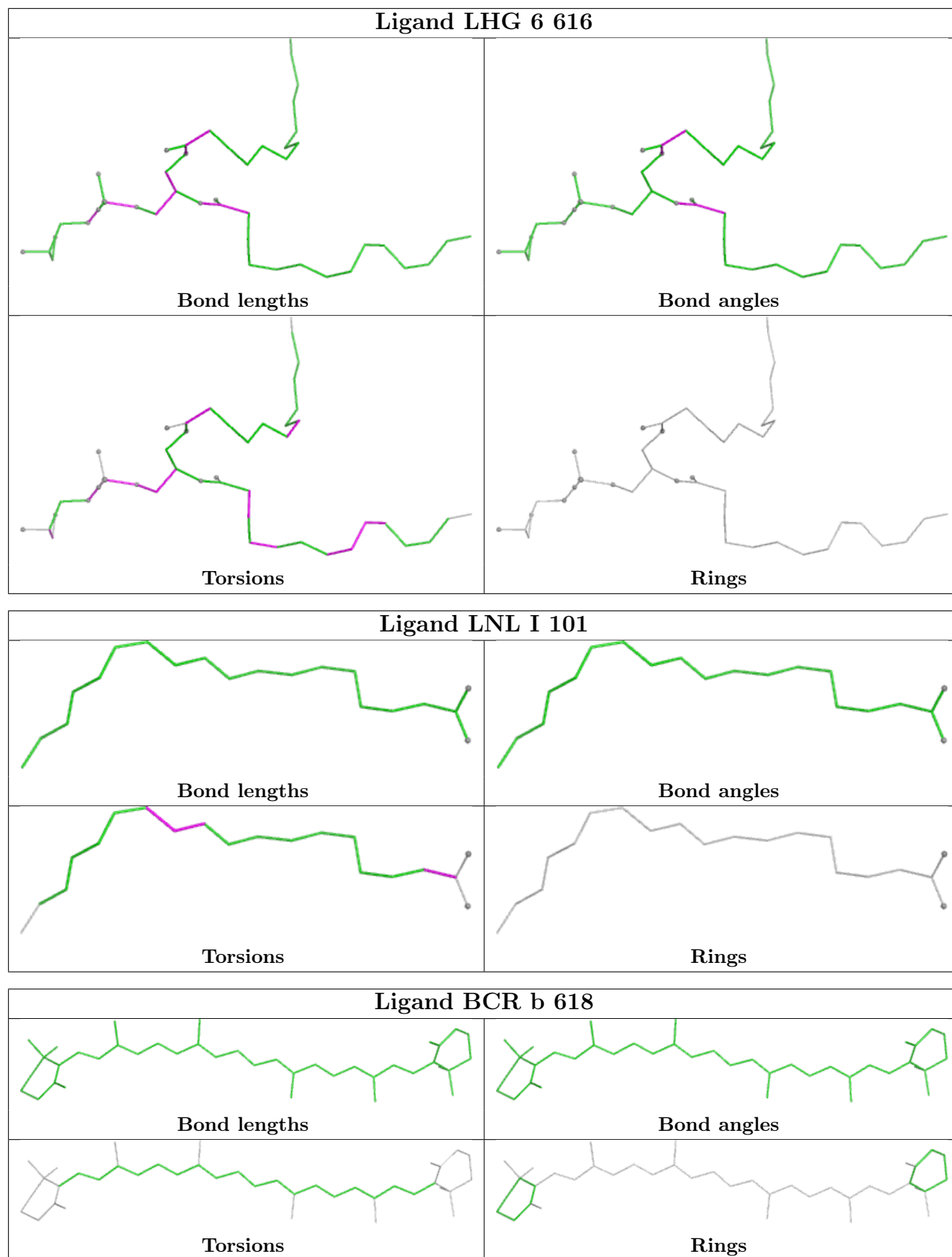


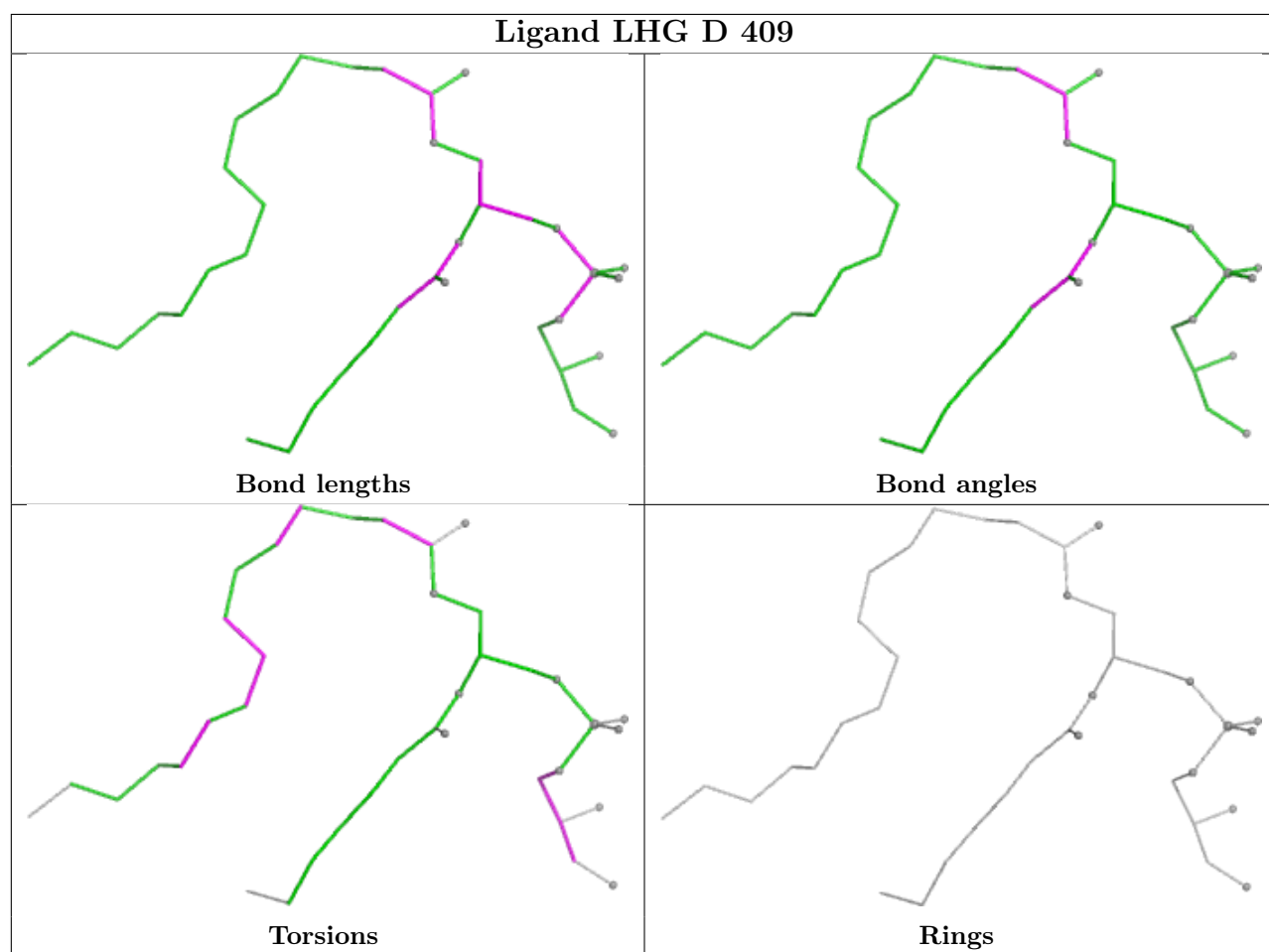
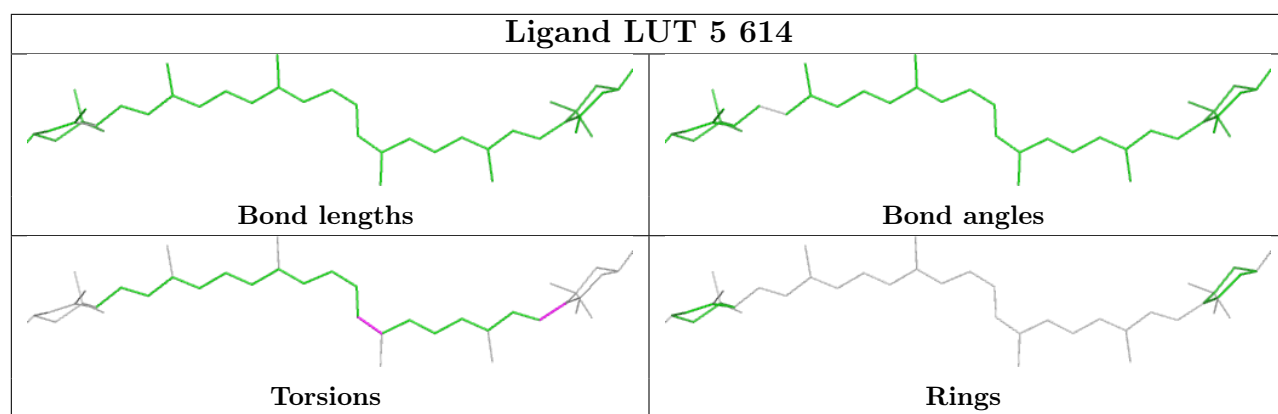


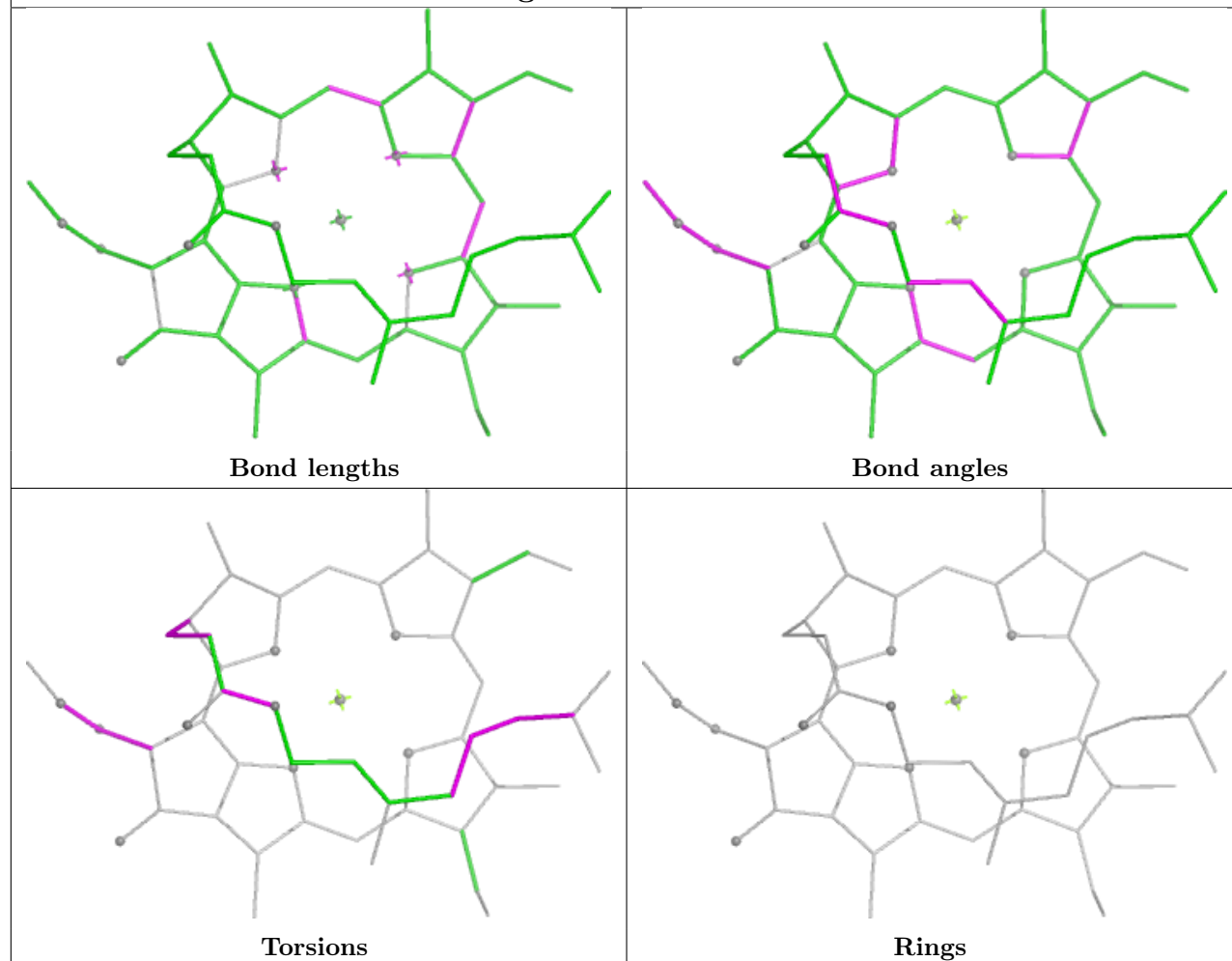
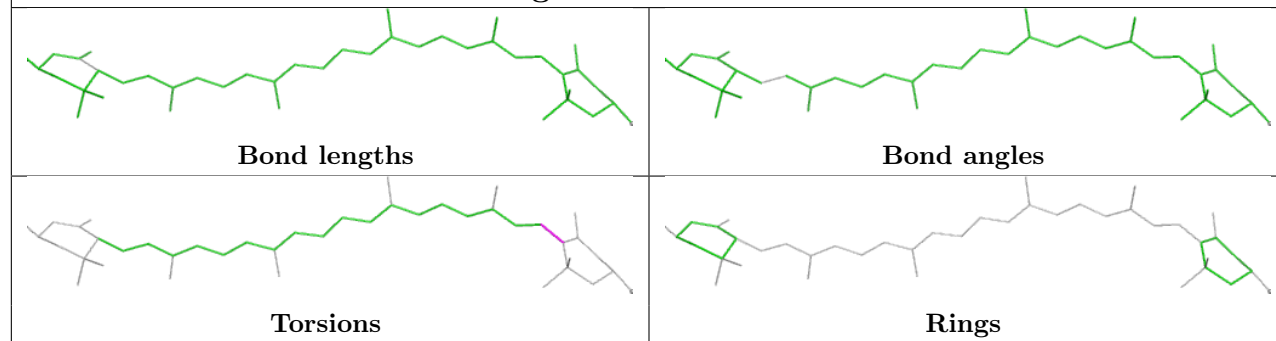
Ligand CHL r 606**Ligand CHL 5 609**

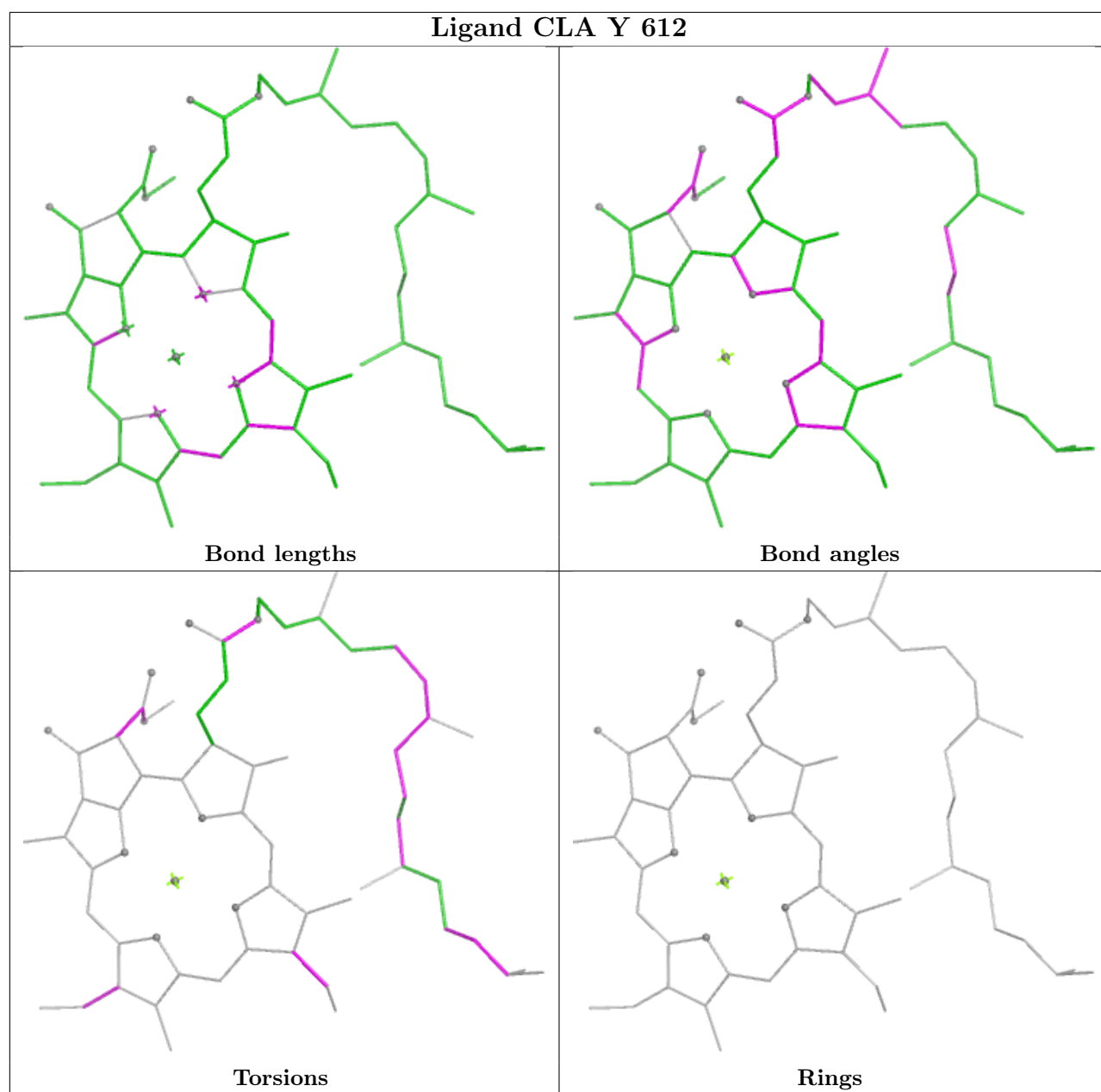




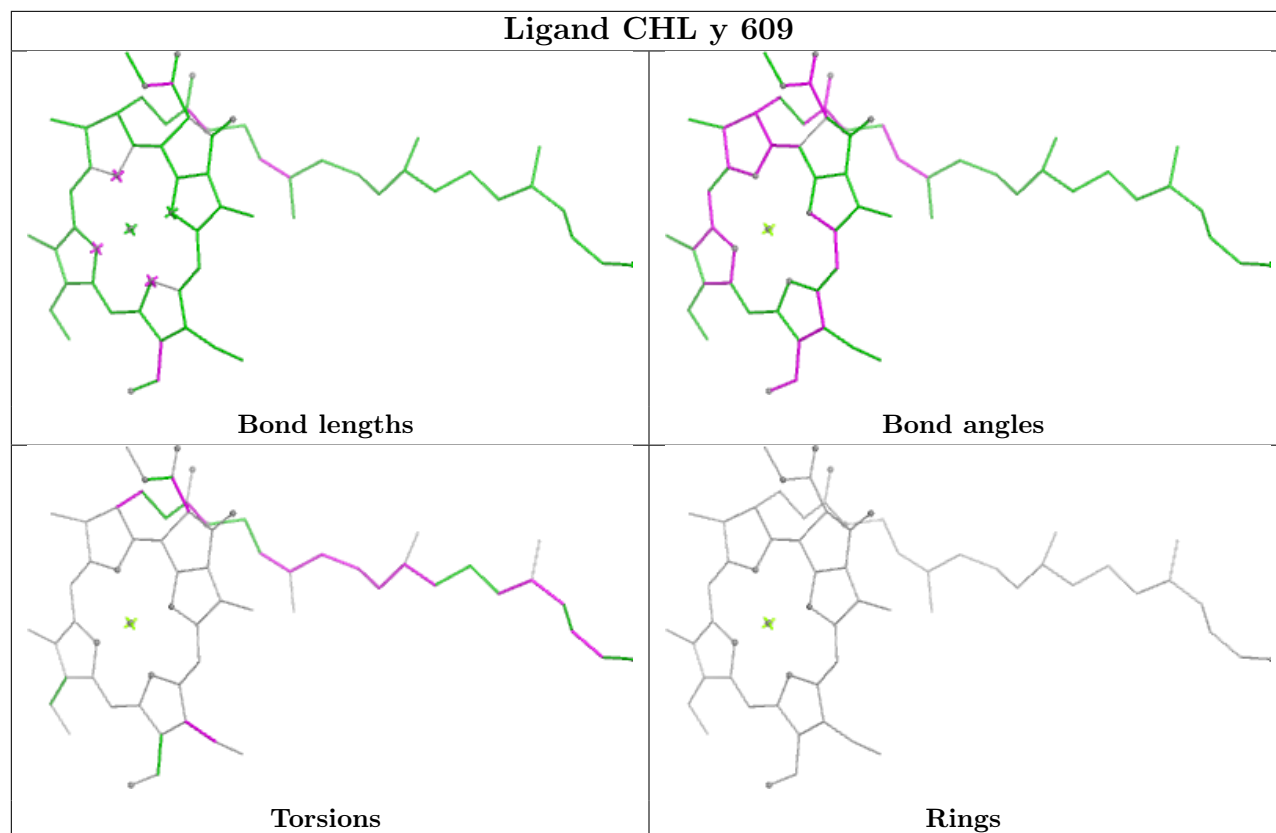




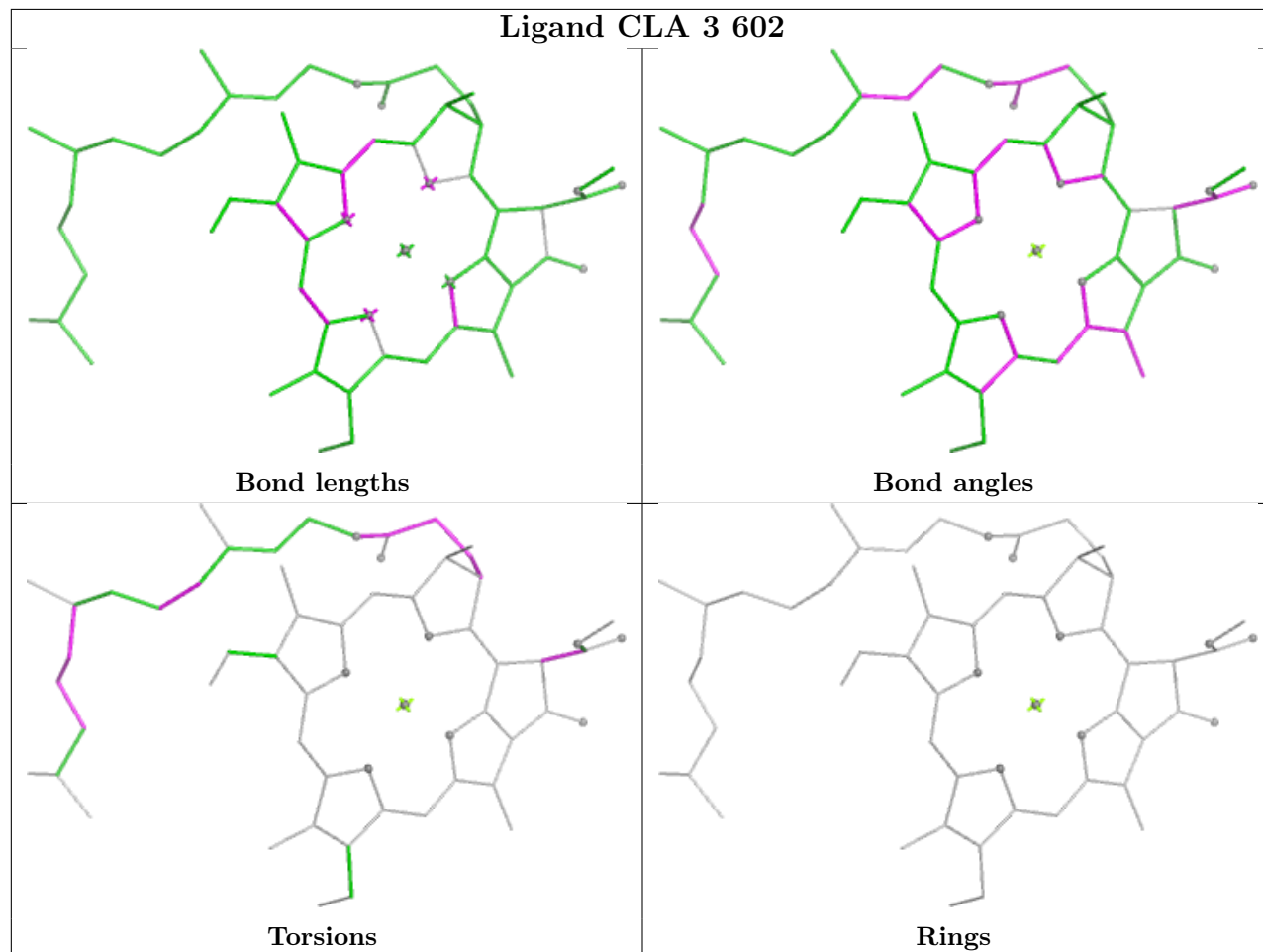
Ligand CLA 6 613**Ligand LUT Y 621**

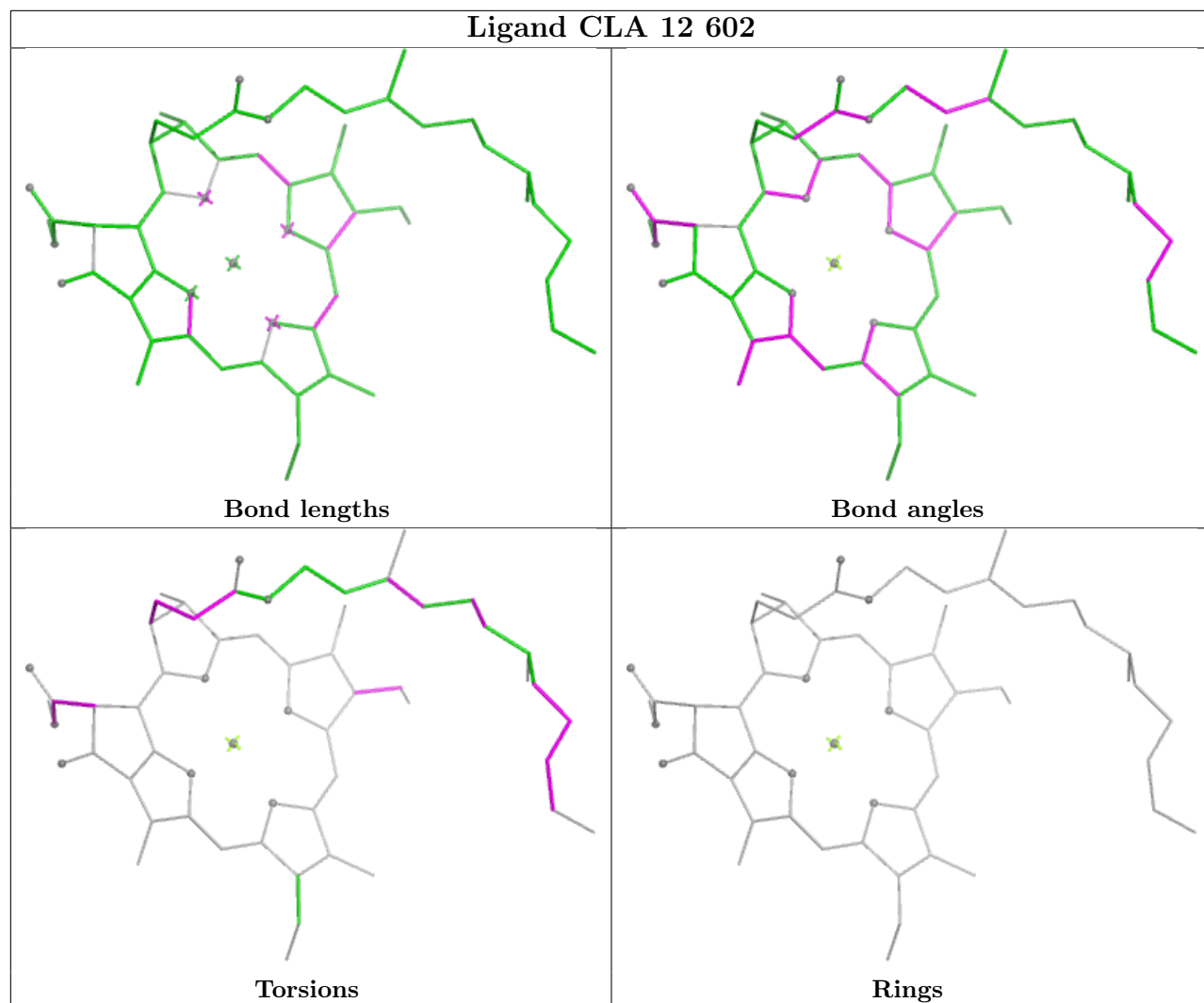


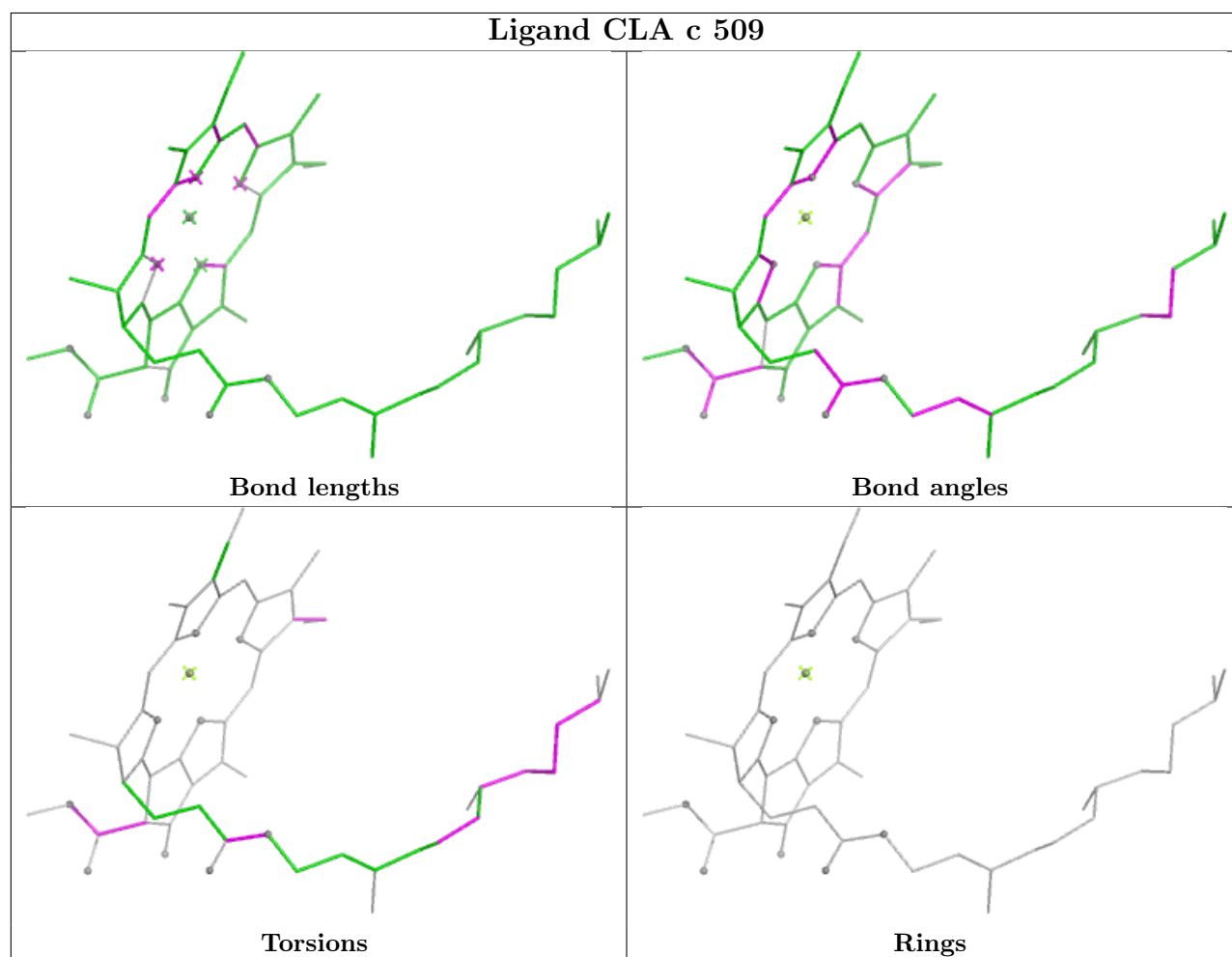
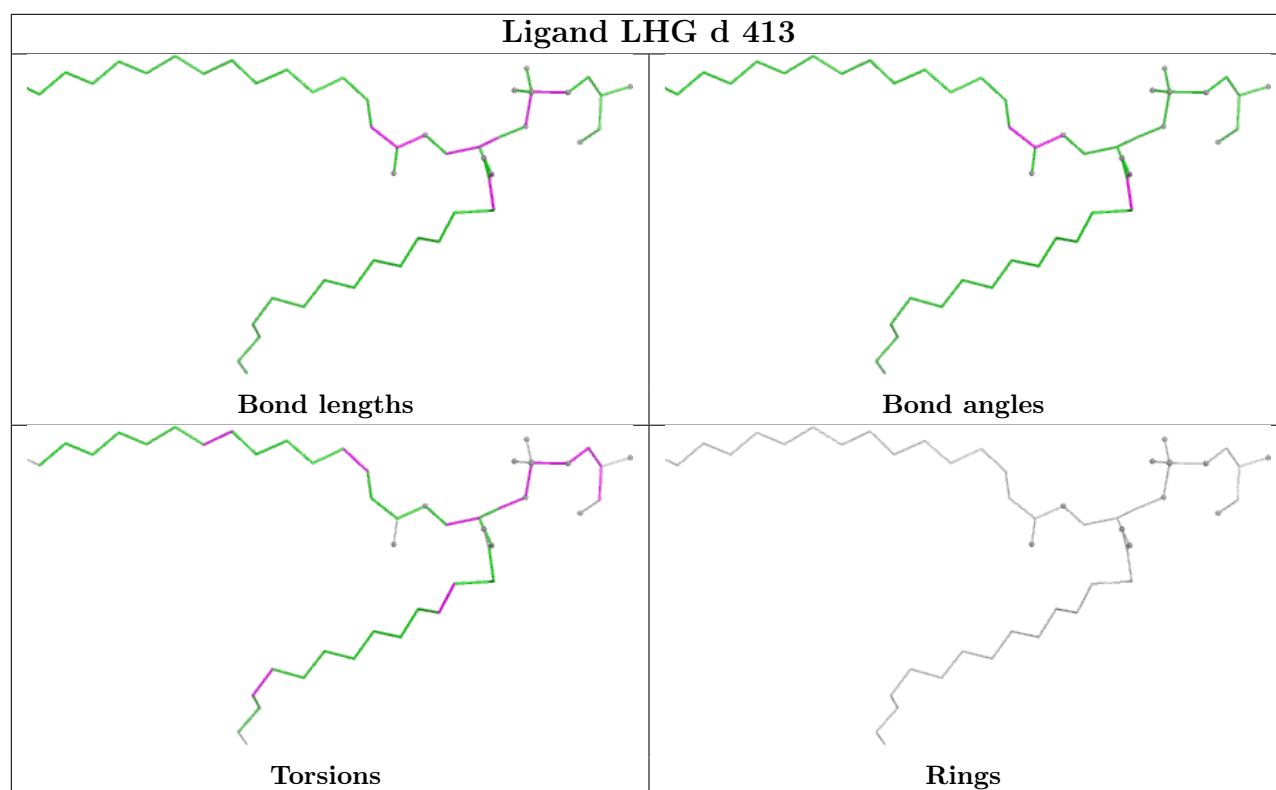
Ligand CHL y 609



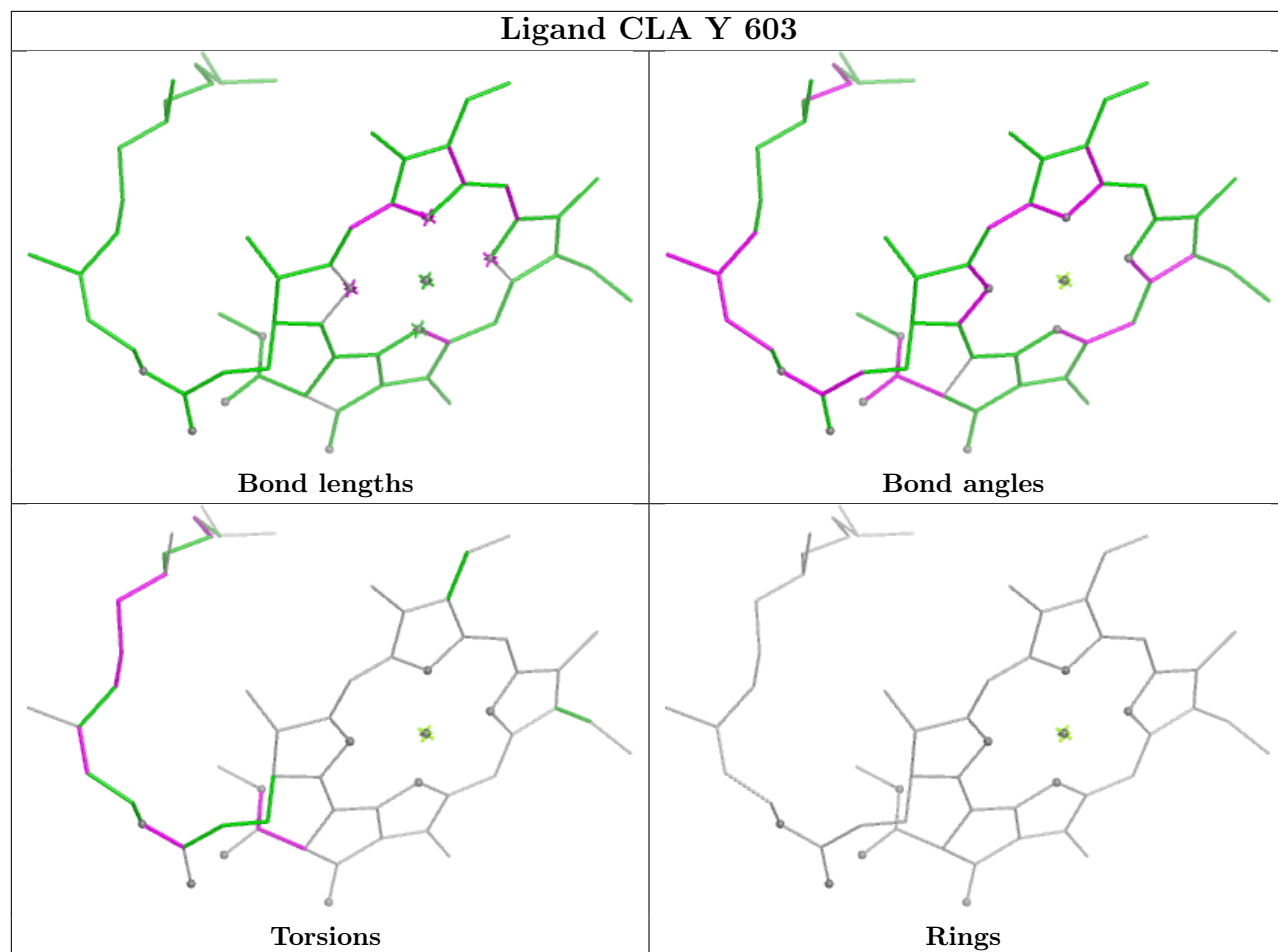
Ligand CLA 3 602

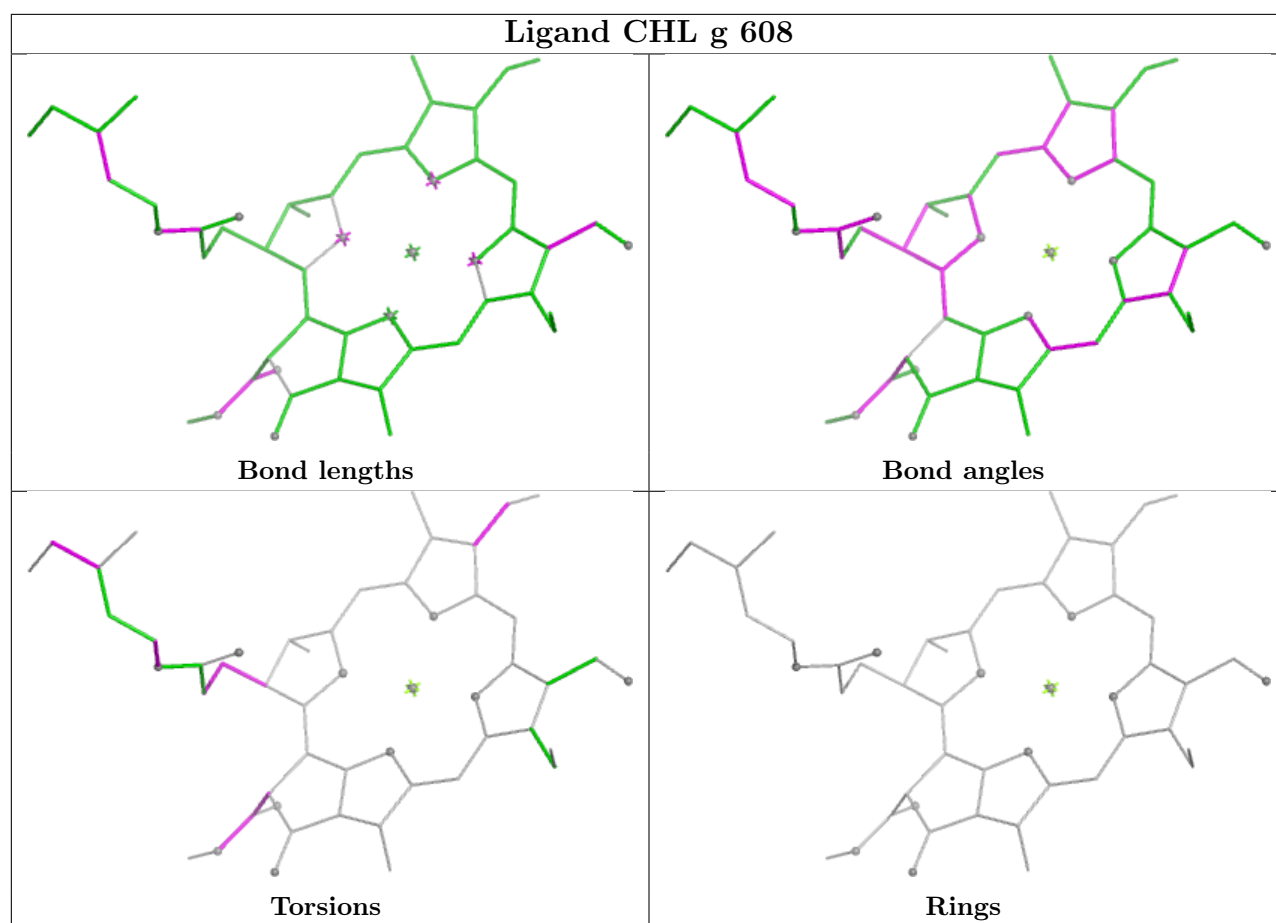


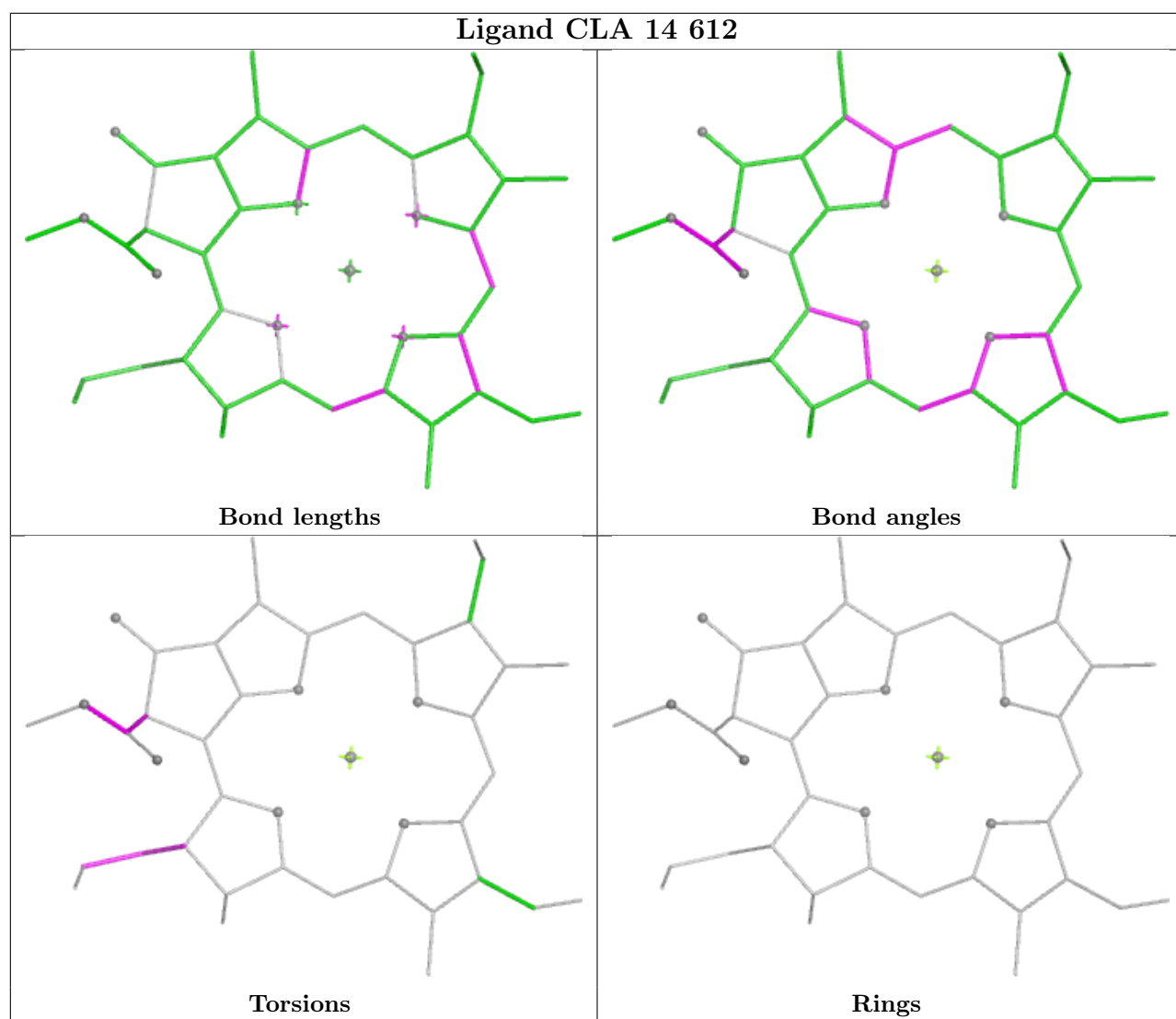




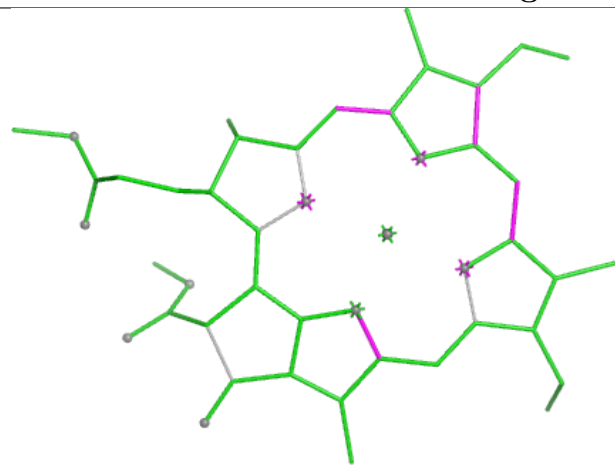
Ligand CLA Y 603



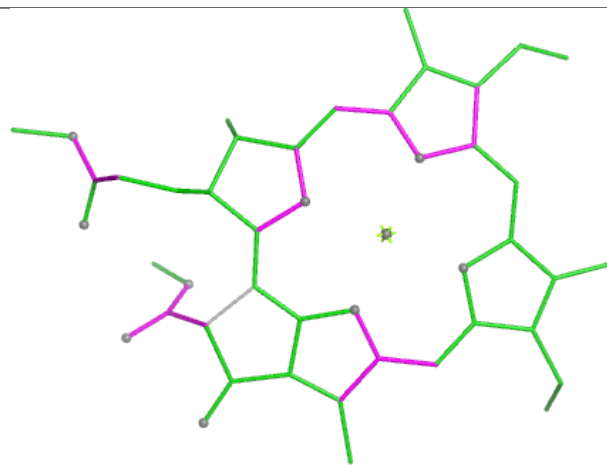




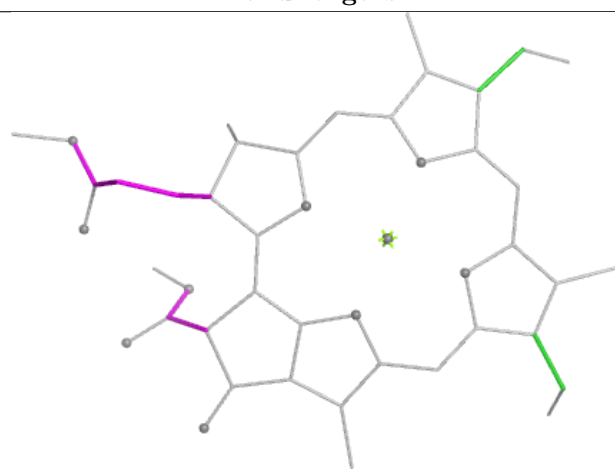
Ligand CLA 5 612



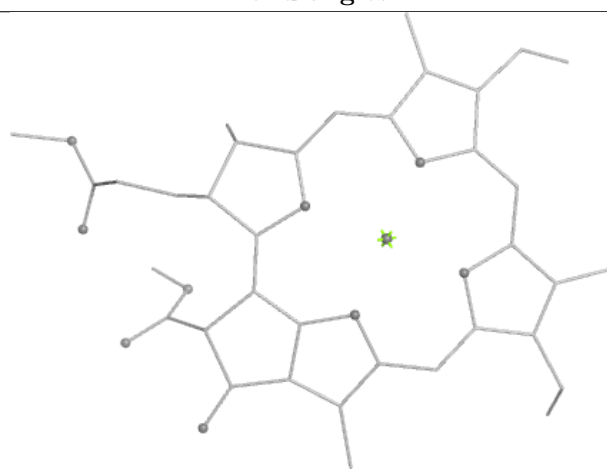
Bond lengths



Bond angles

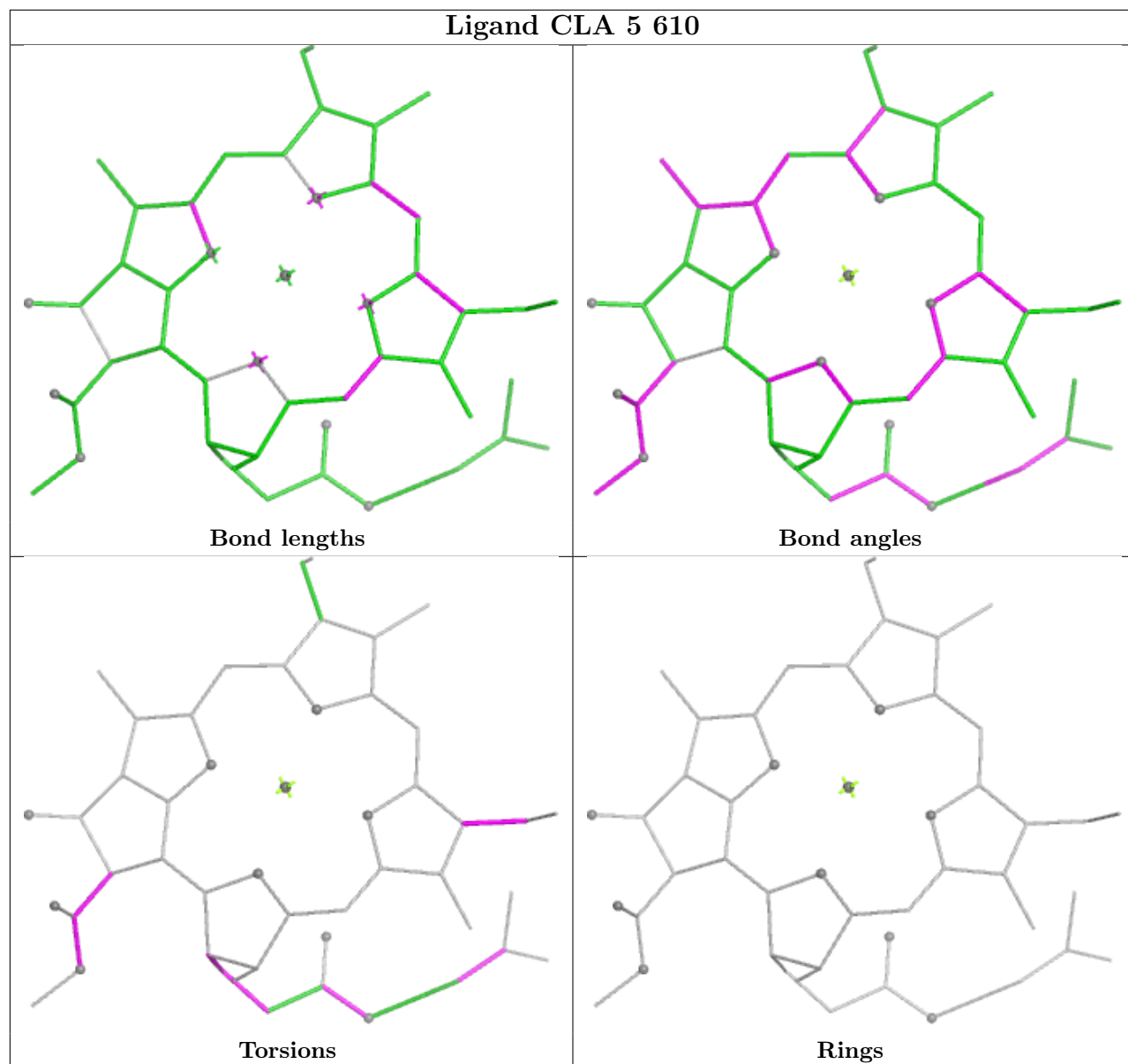


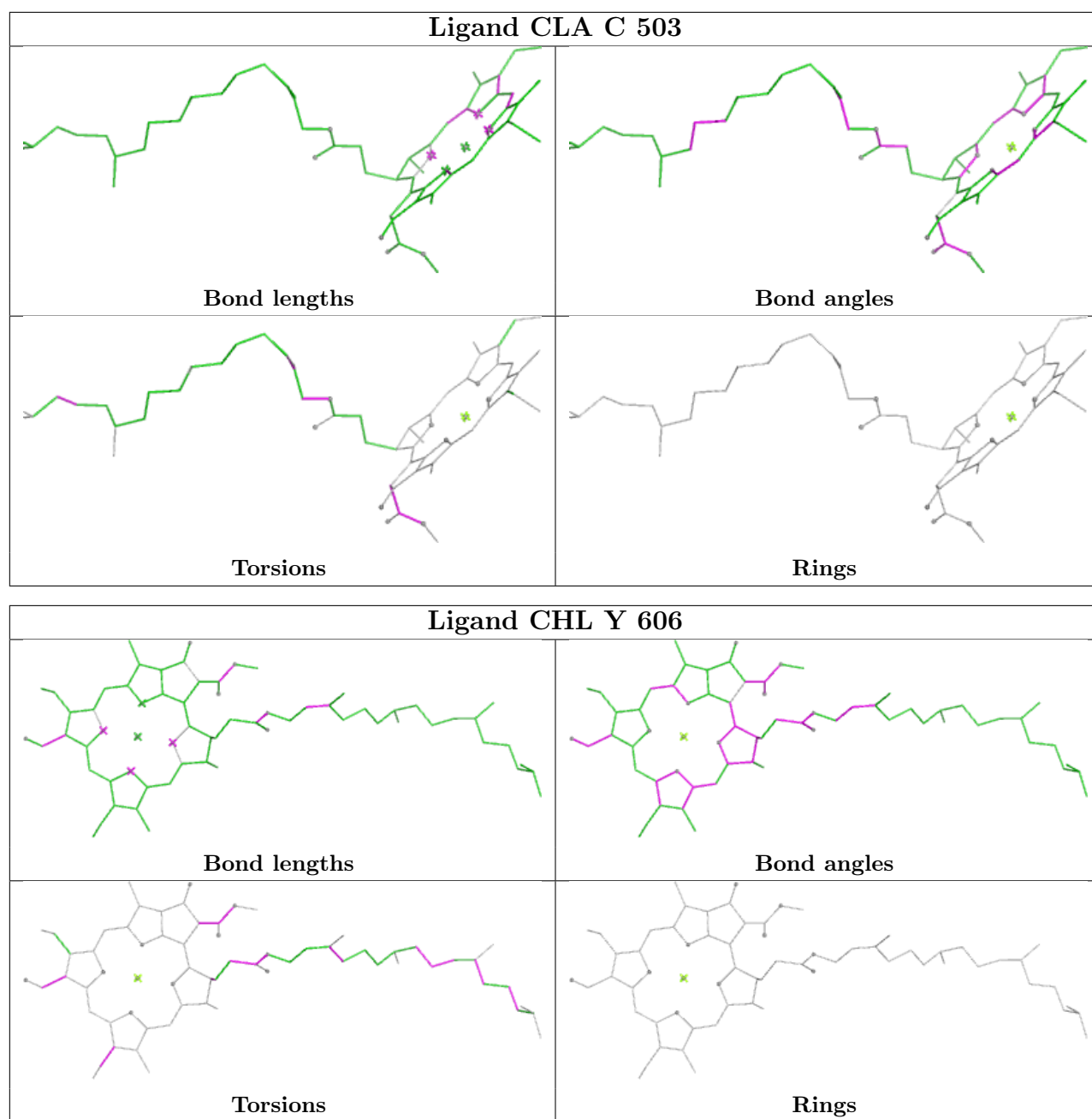
Torsions

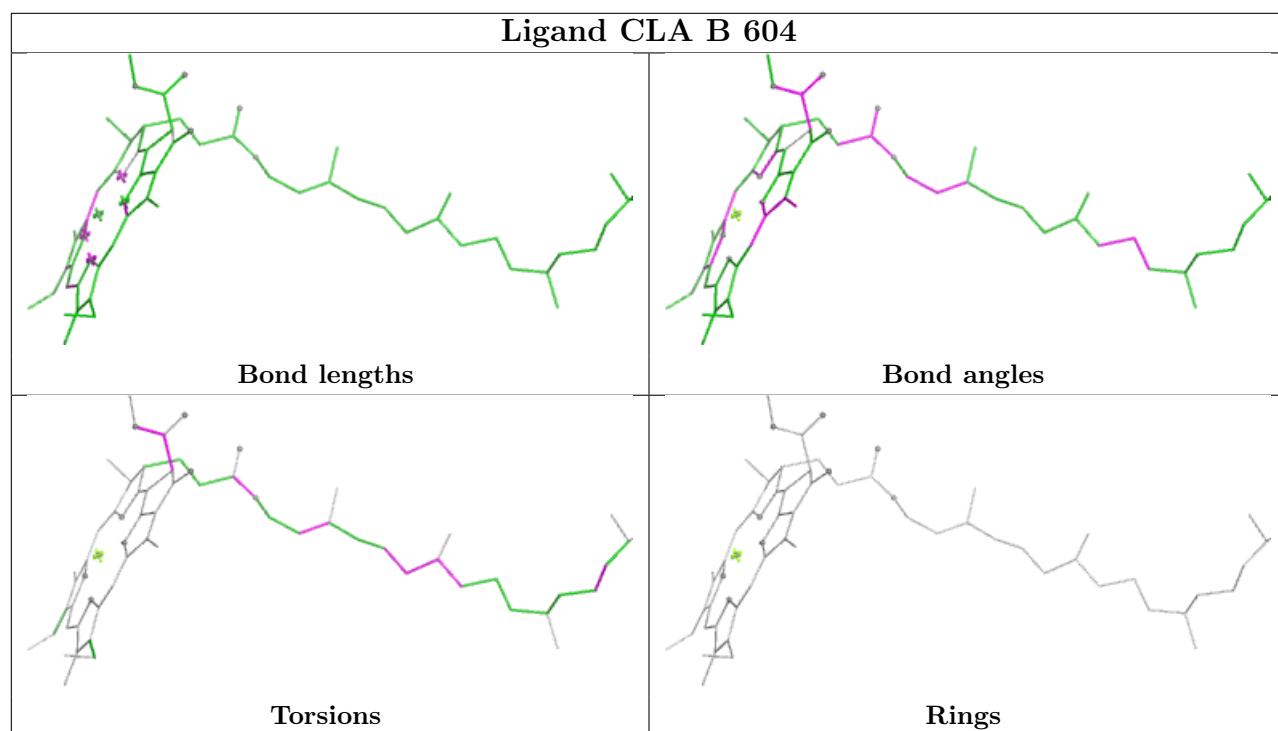
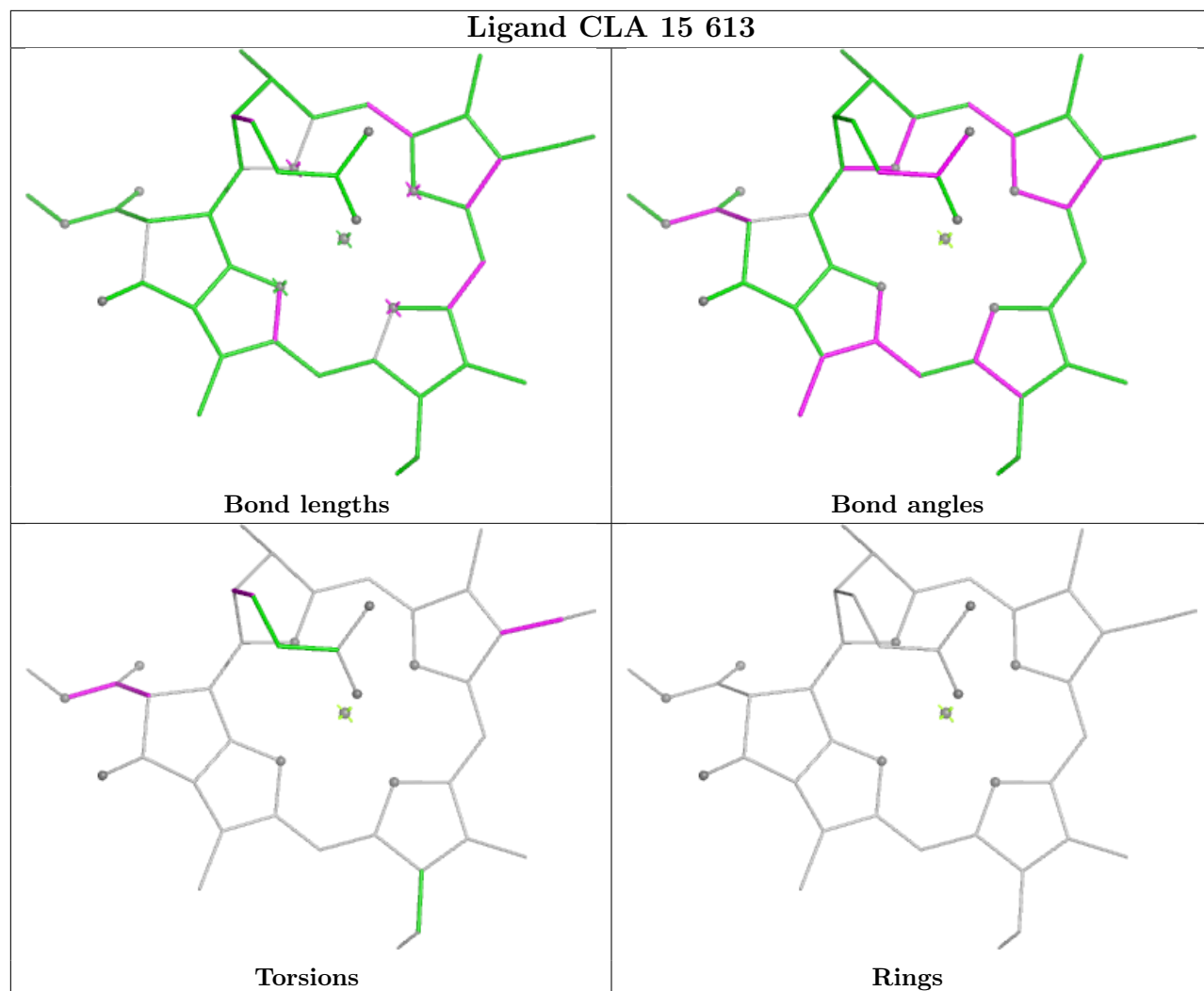


Rings

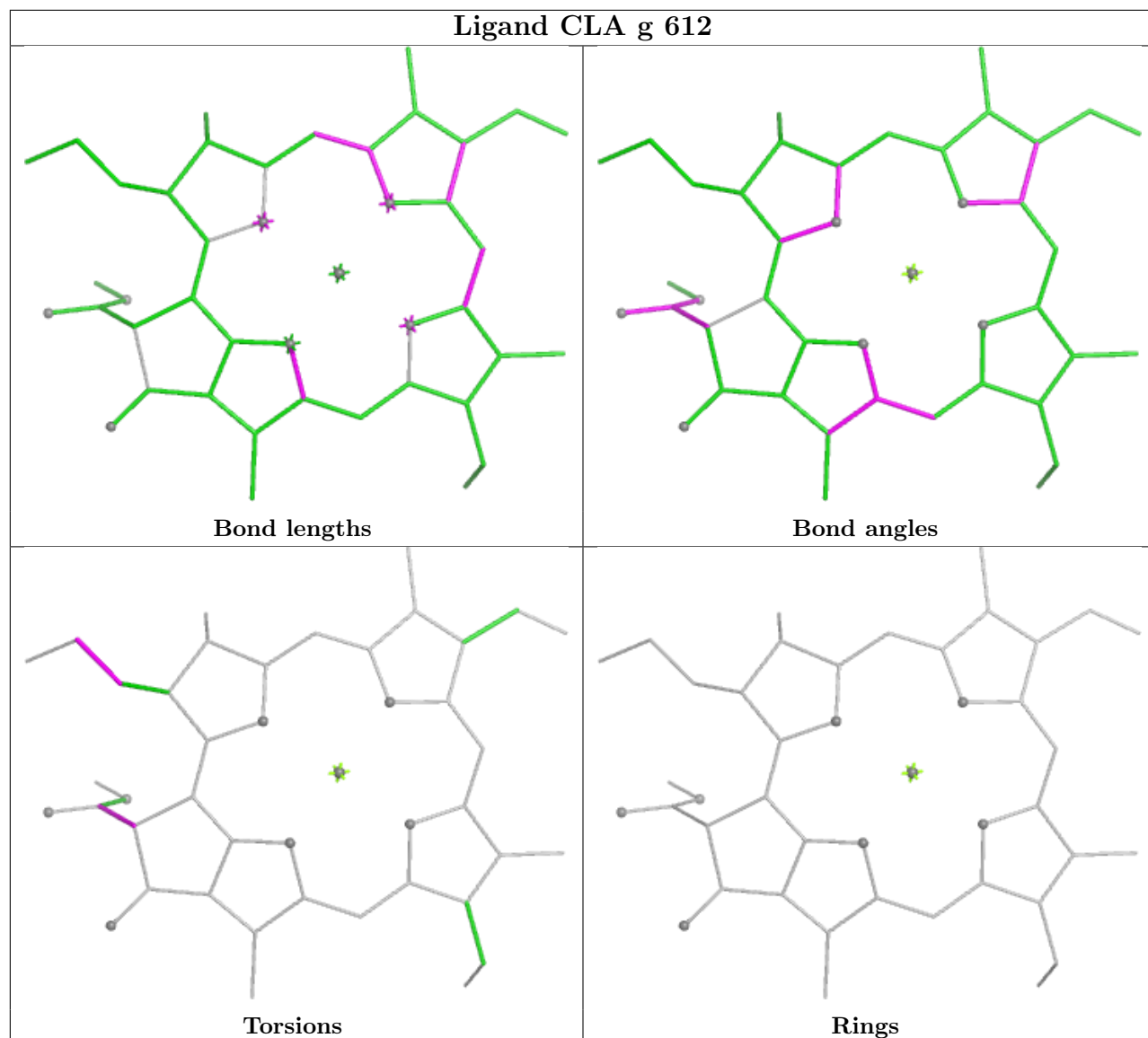
Ligand CLA 5 610

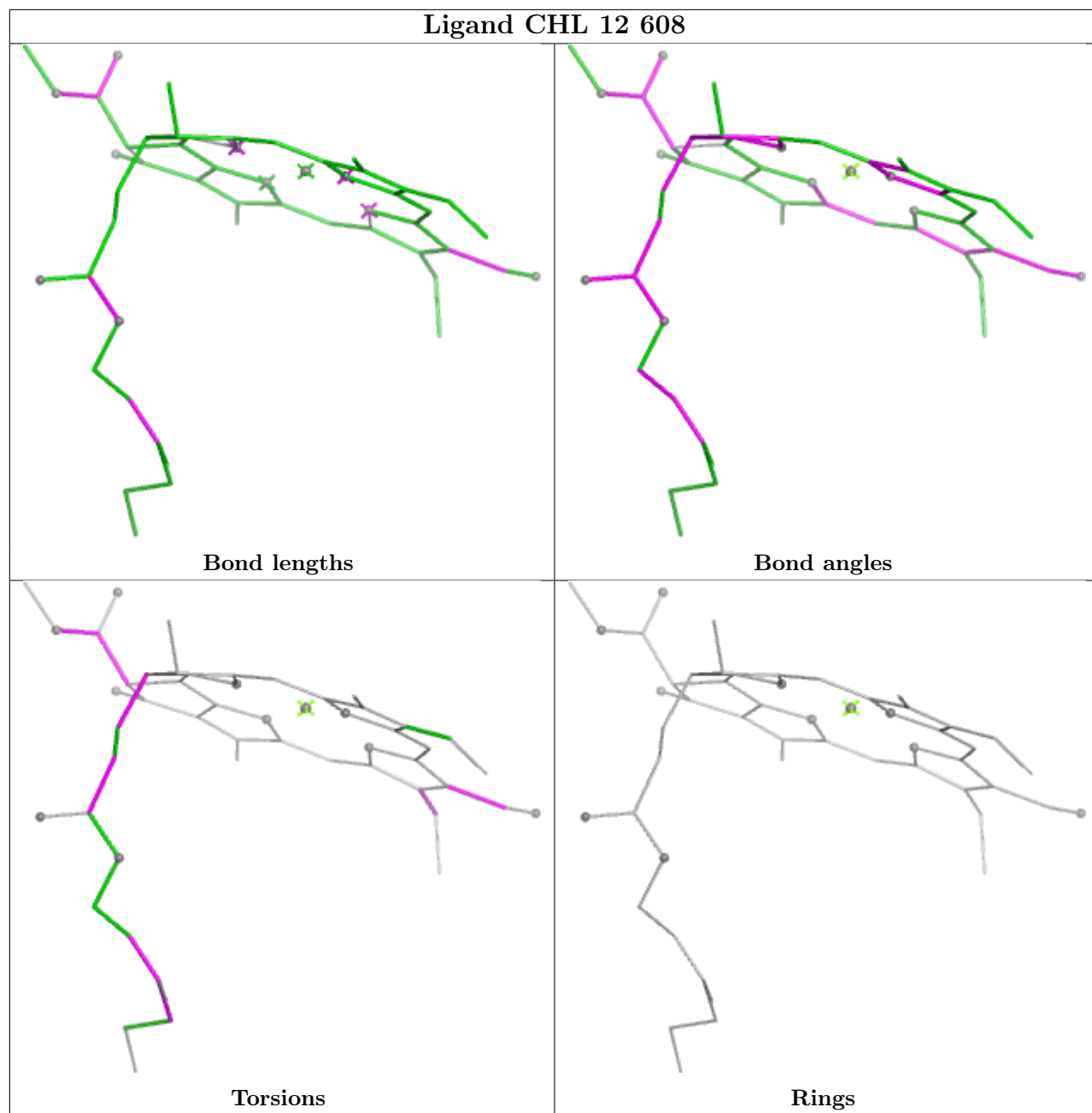




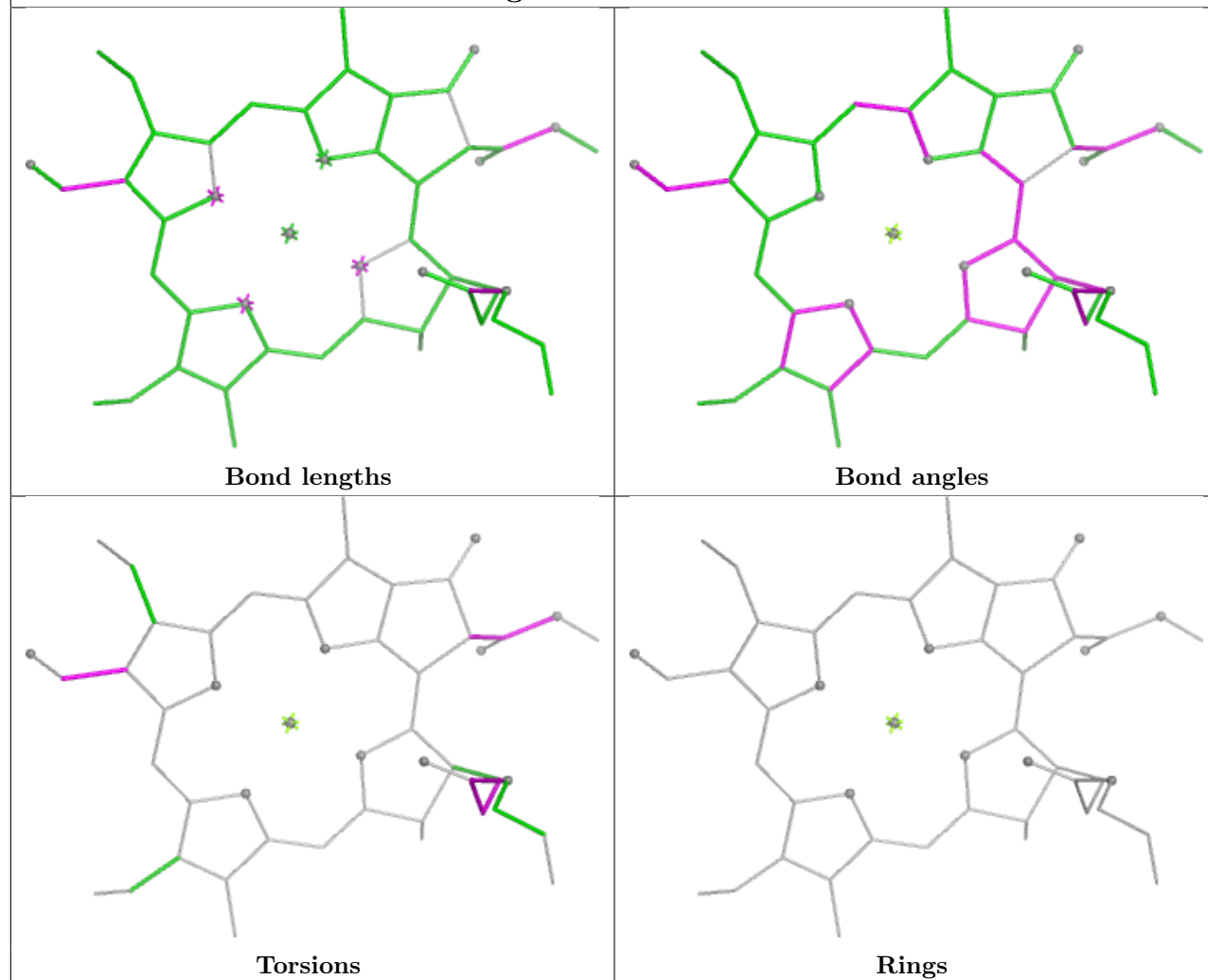


Ligand CLA g 612

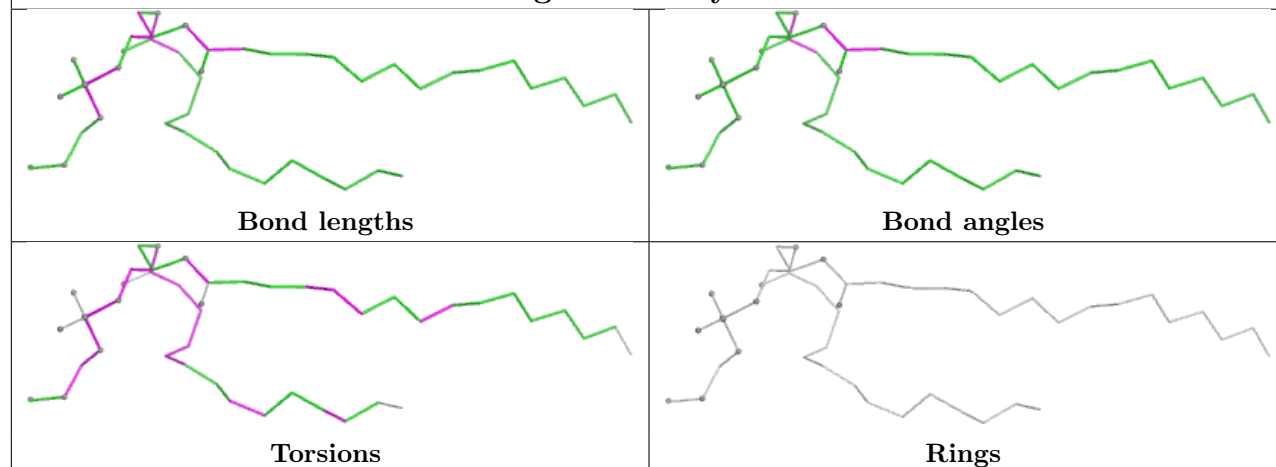




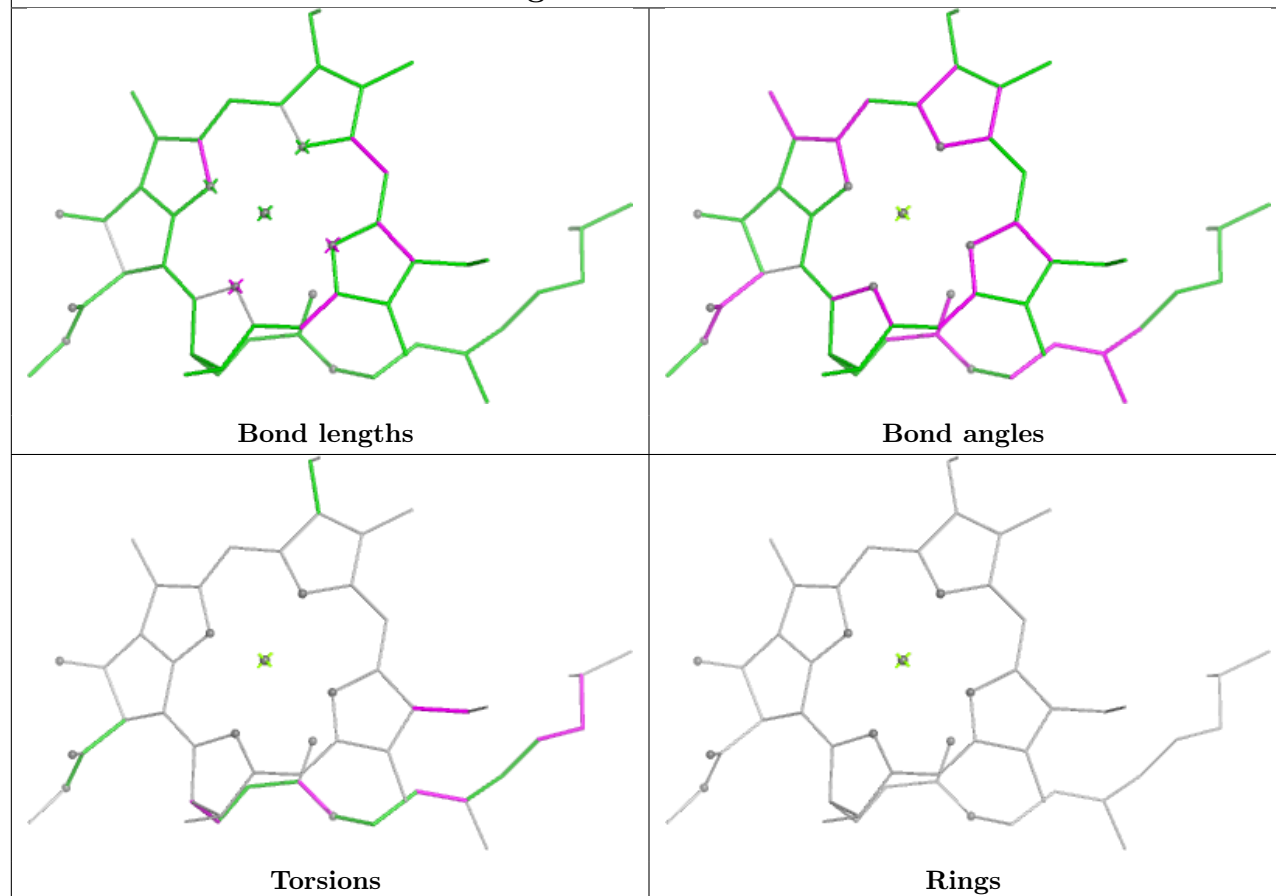
Ligand CHL S 608



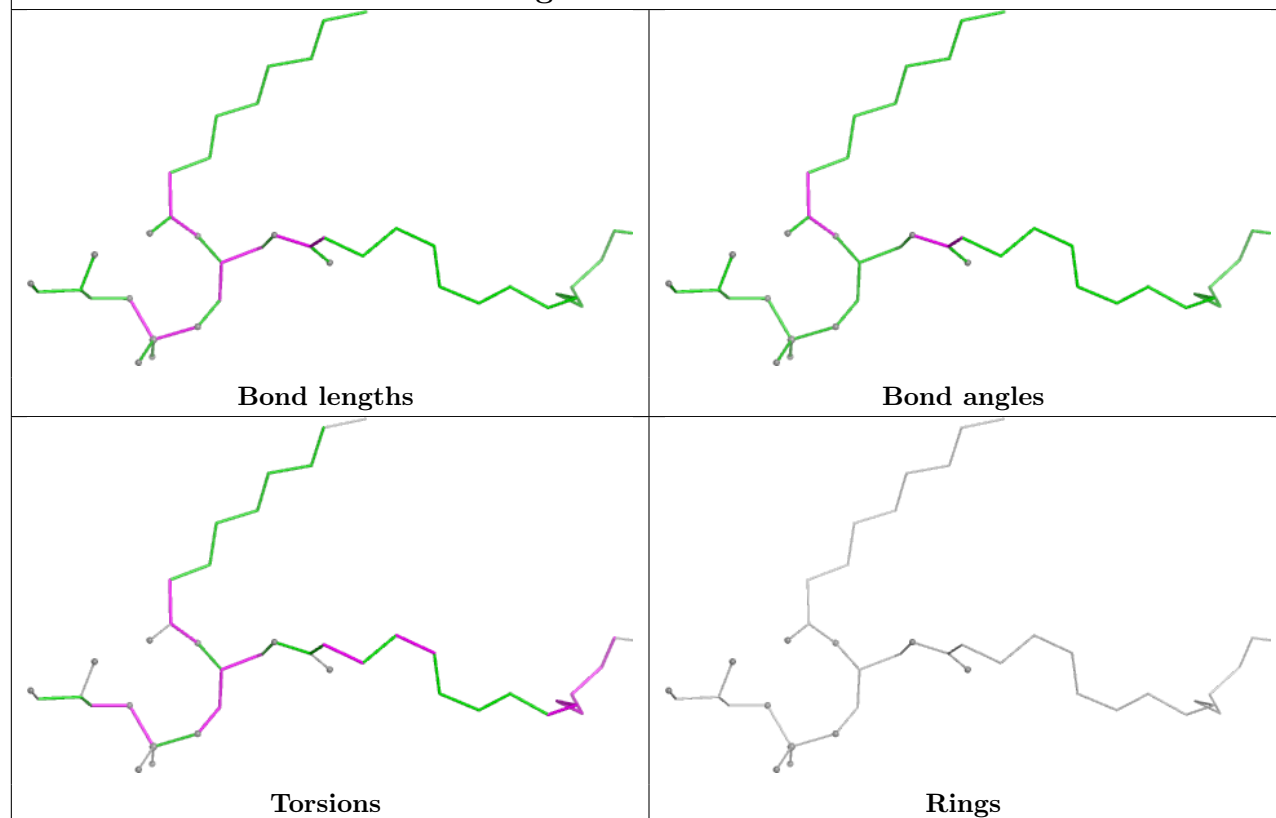
Ligand LHG y 617

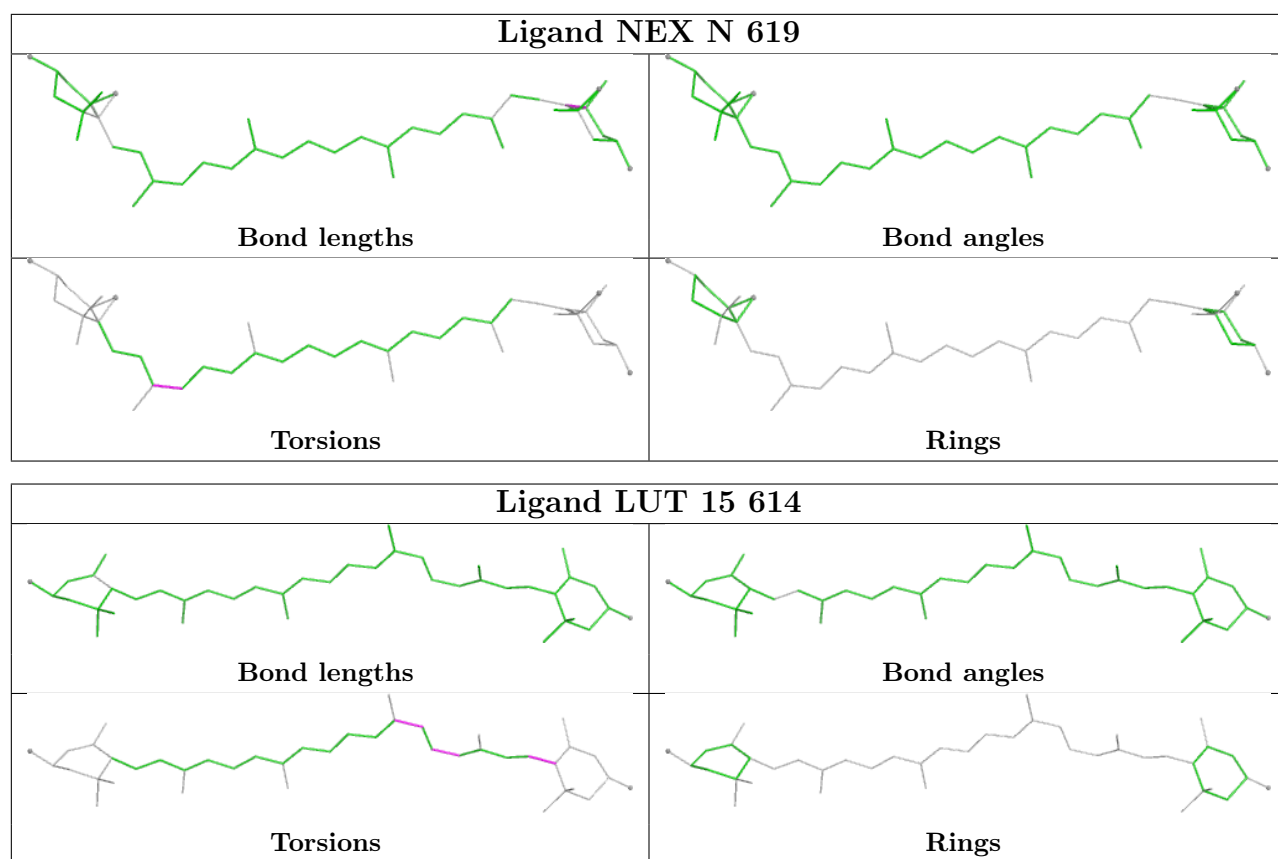


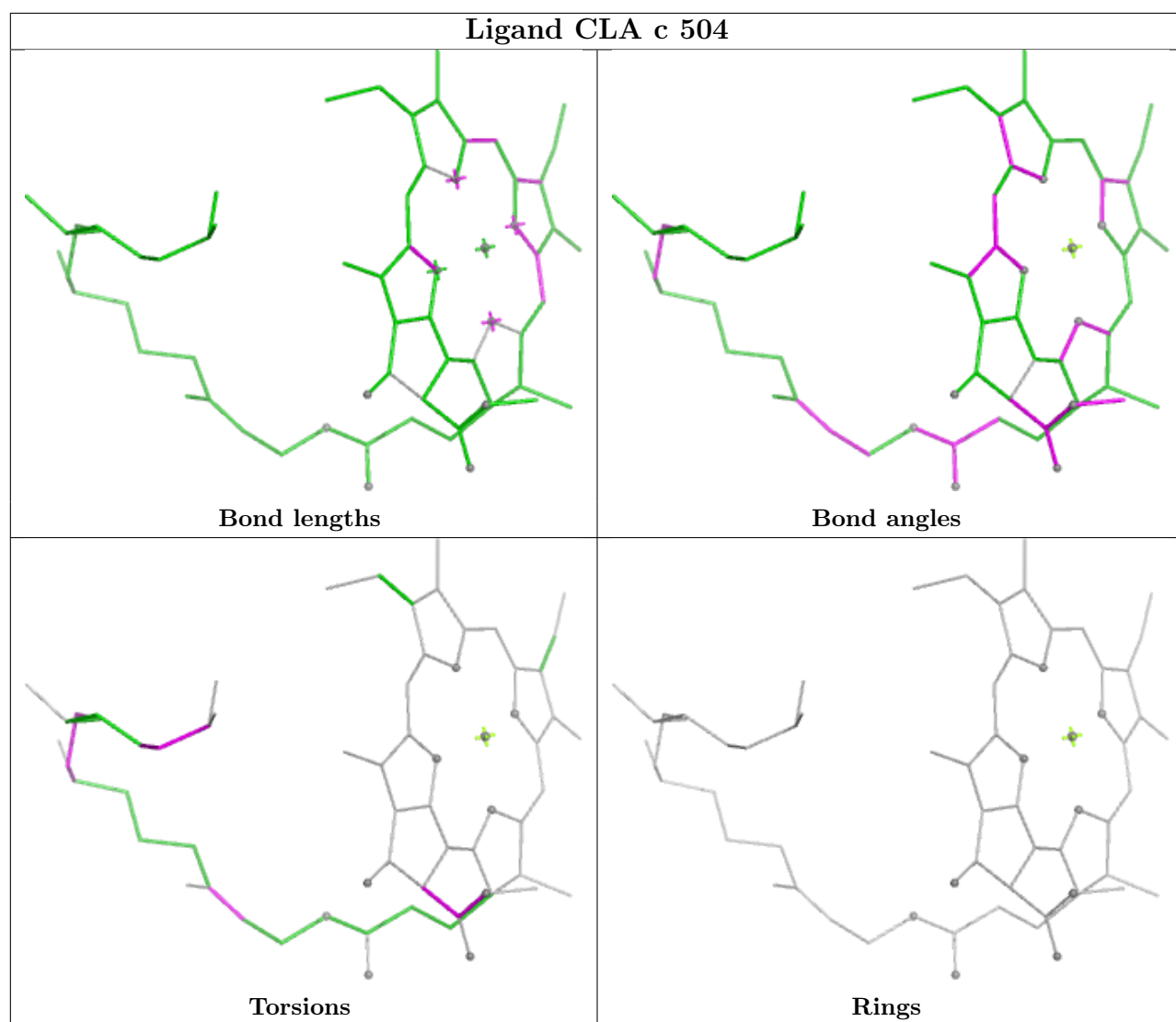
Ligand CLA 11 610

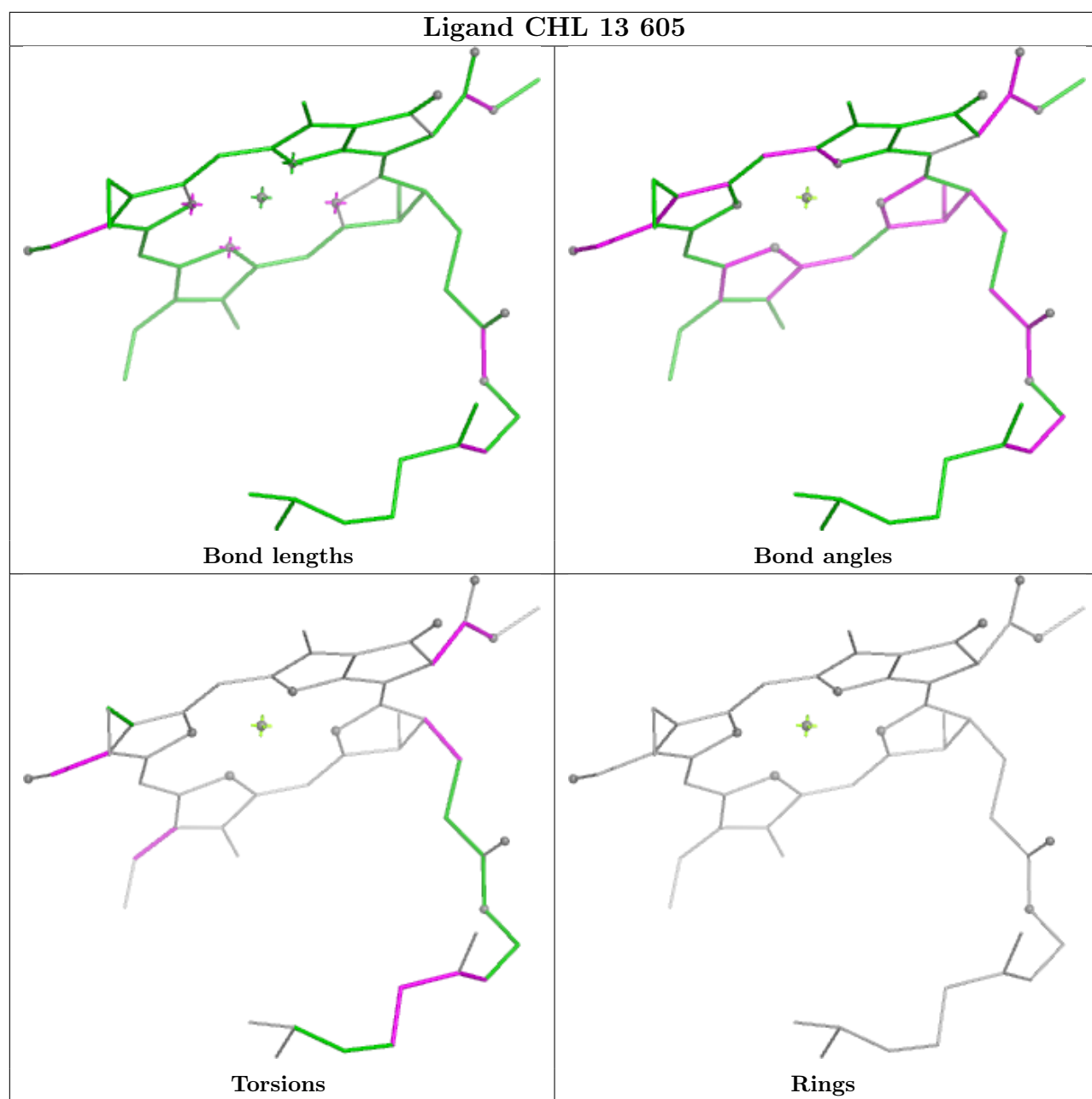


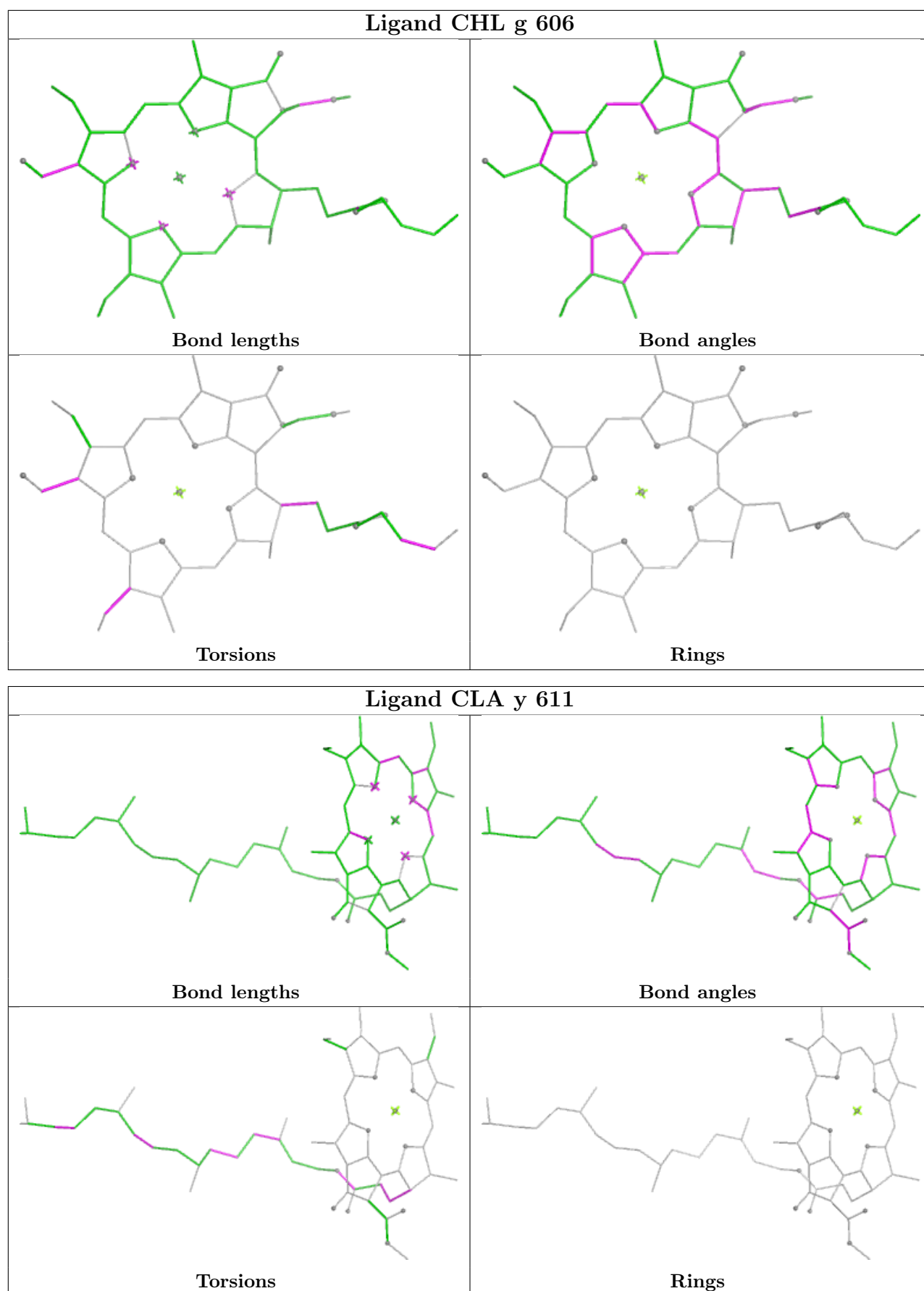
Ligand LHG c 521

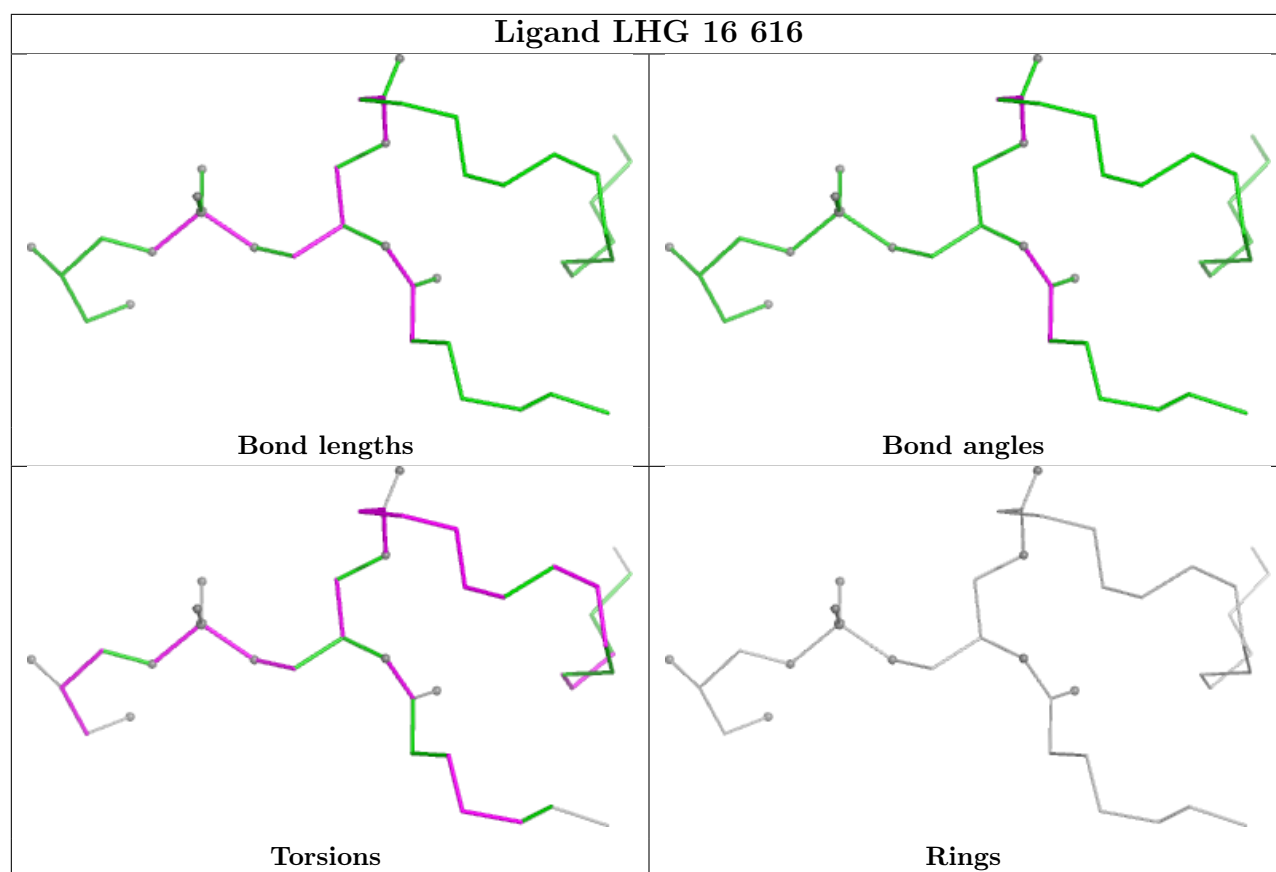




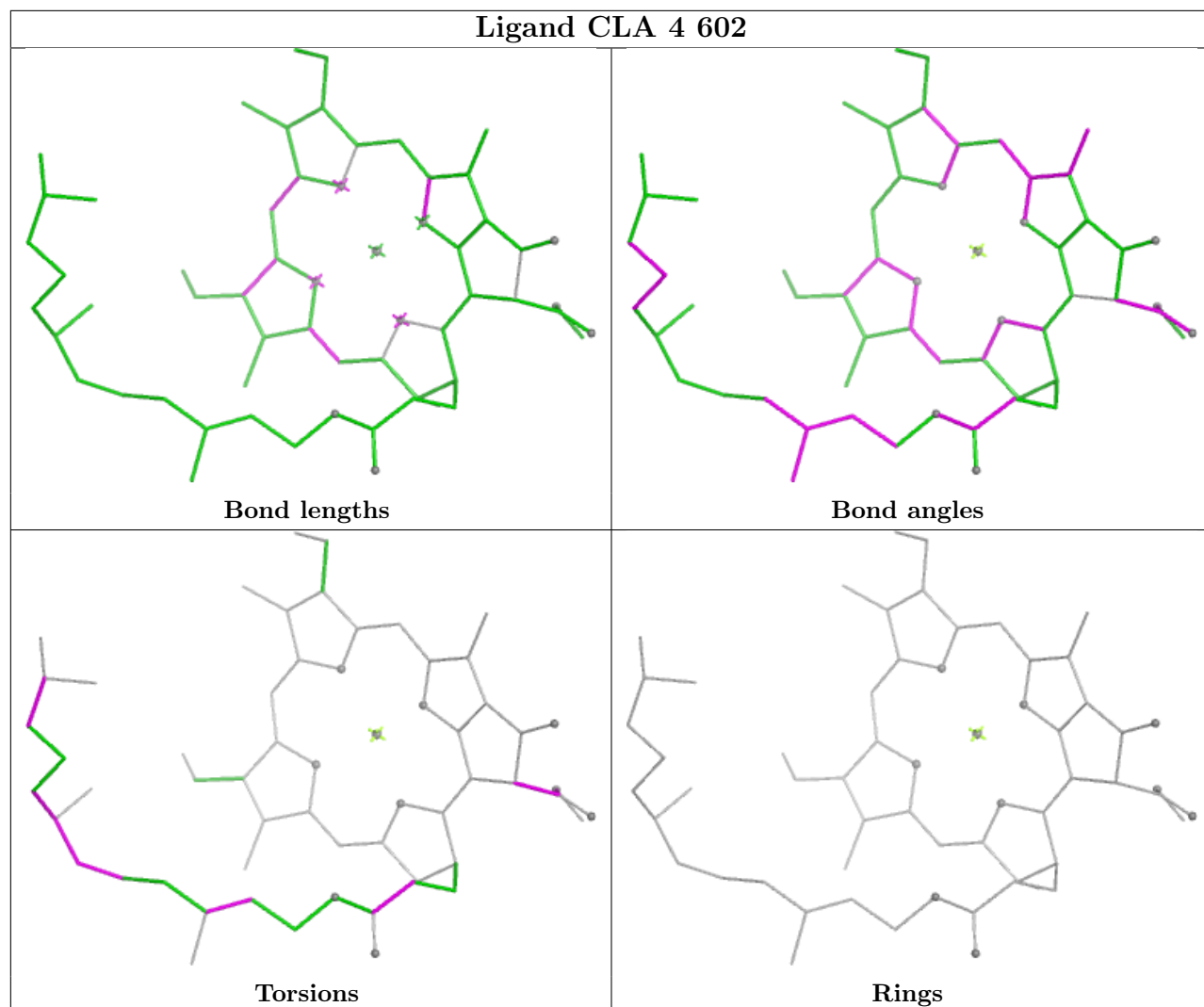




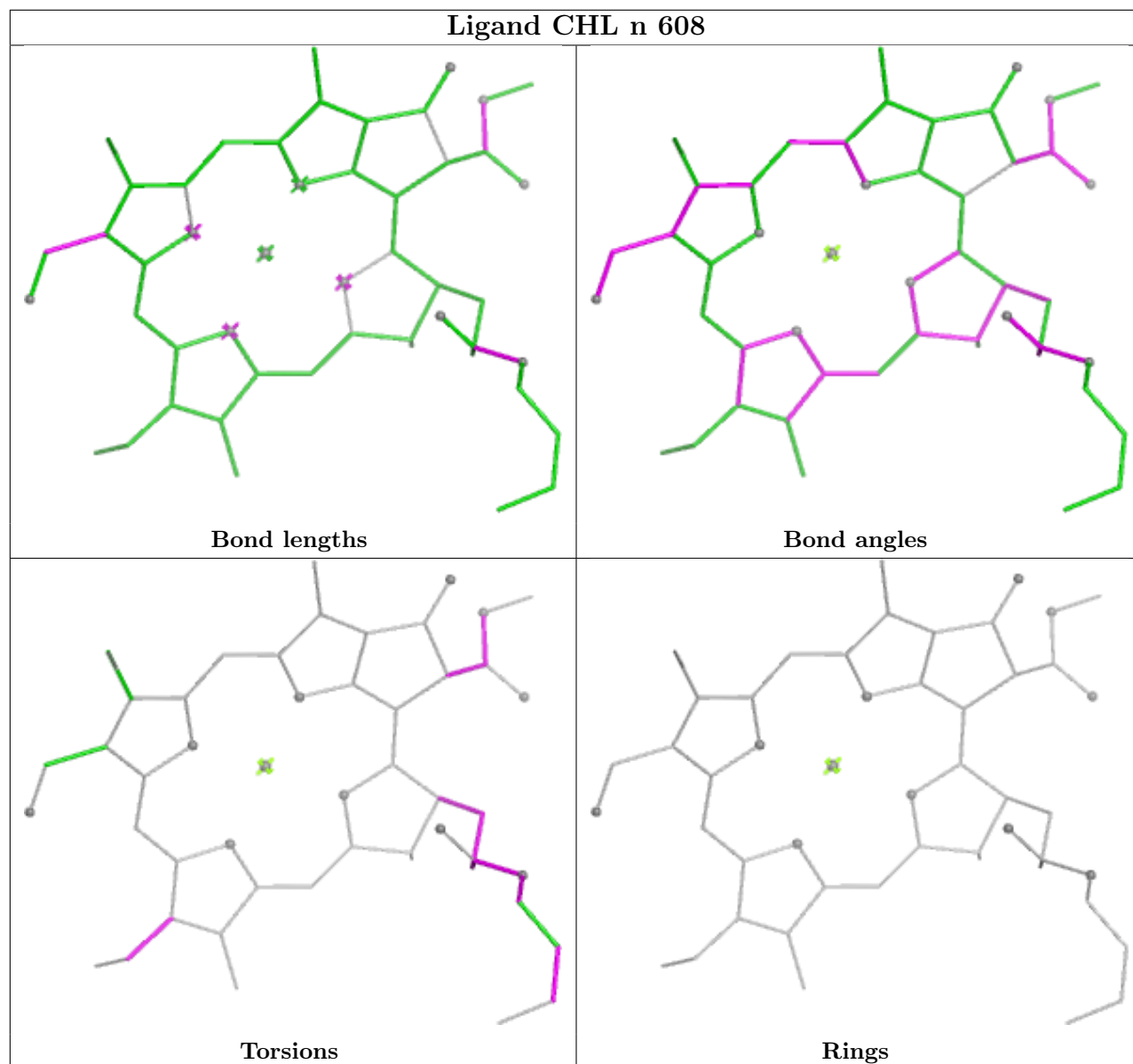




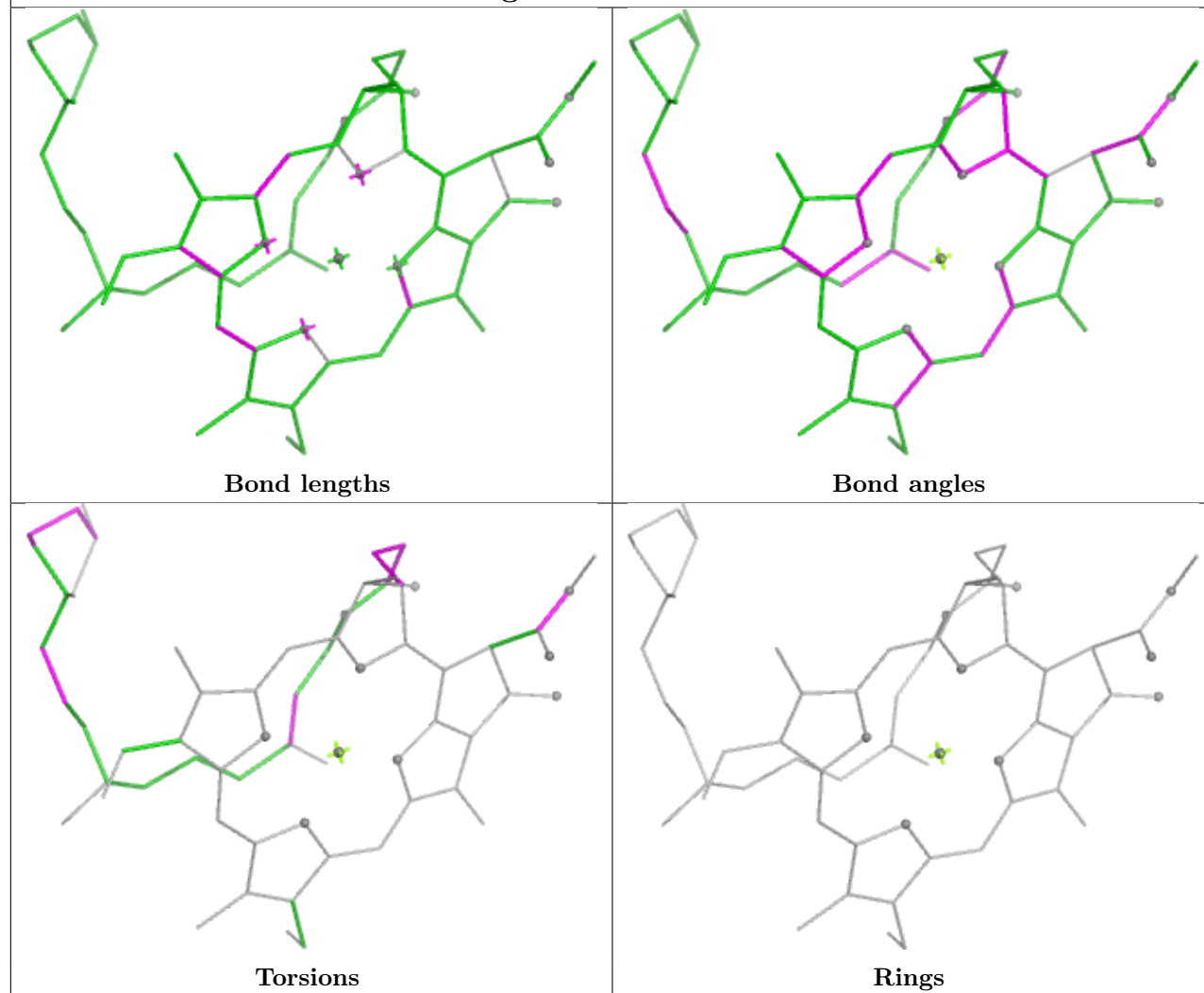
Ligand CLA 4 602



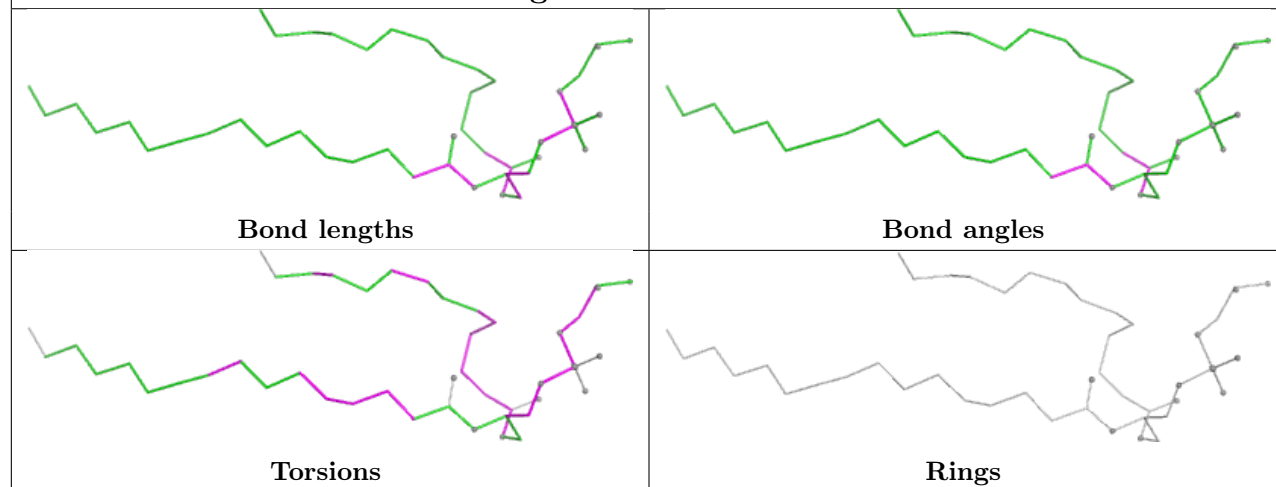
Ligand CHL n 608

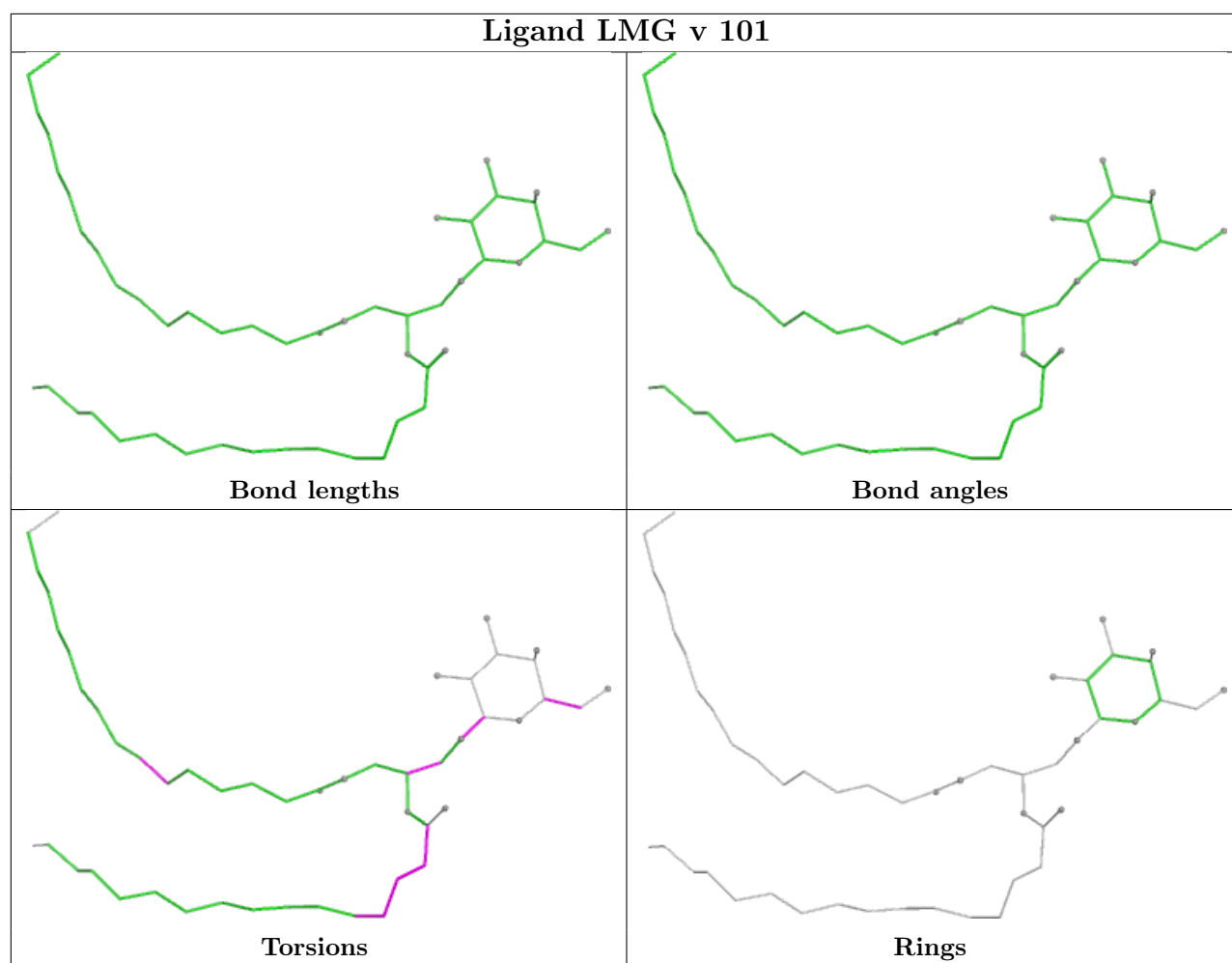


Ligand CLA Y 613

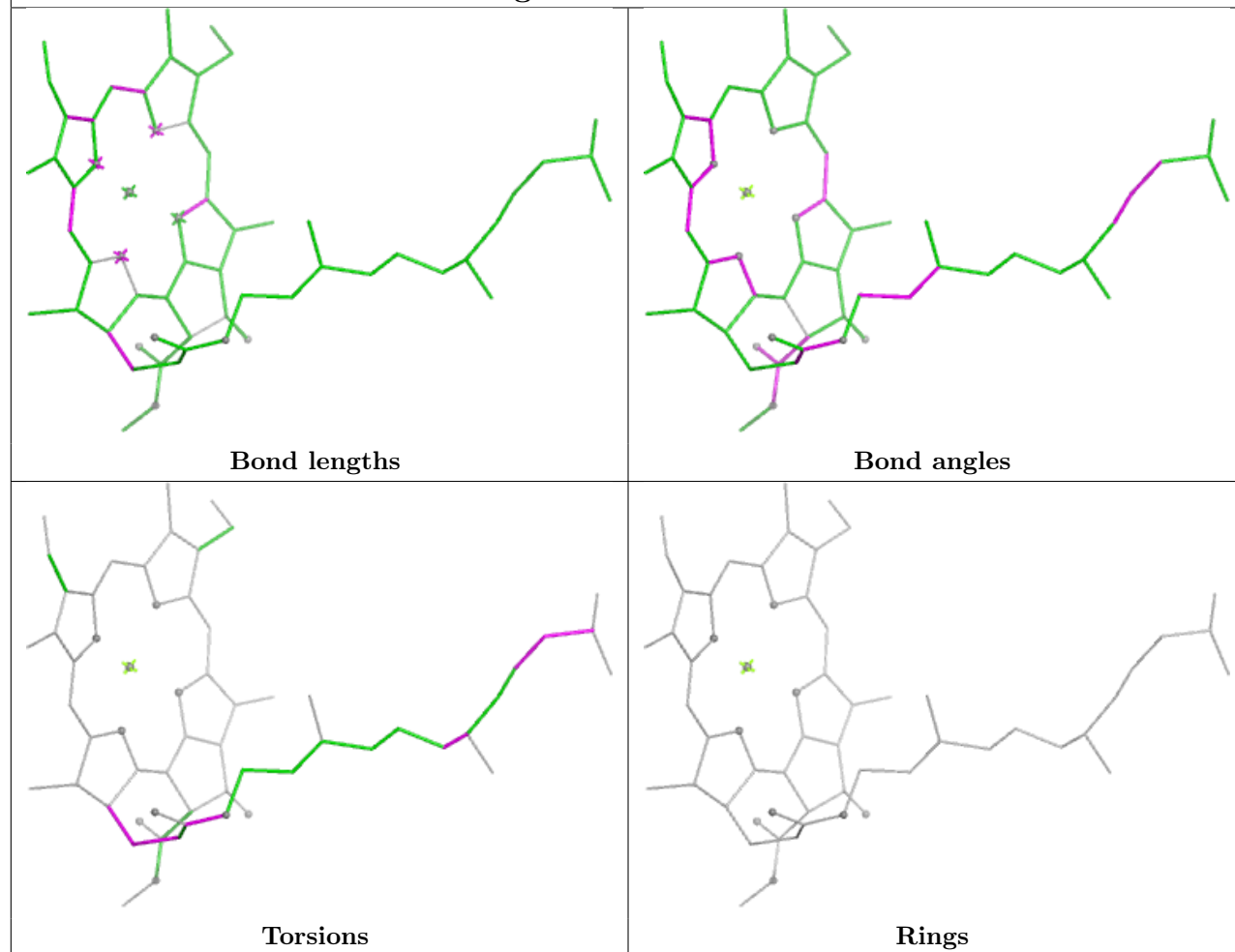


Ligand LHG Y 617

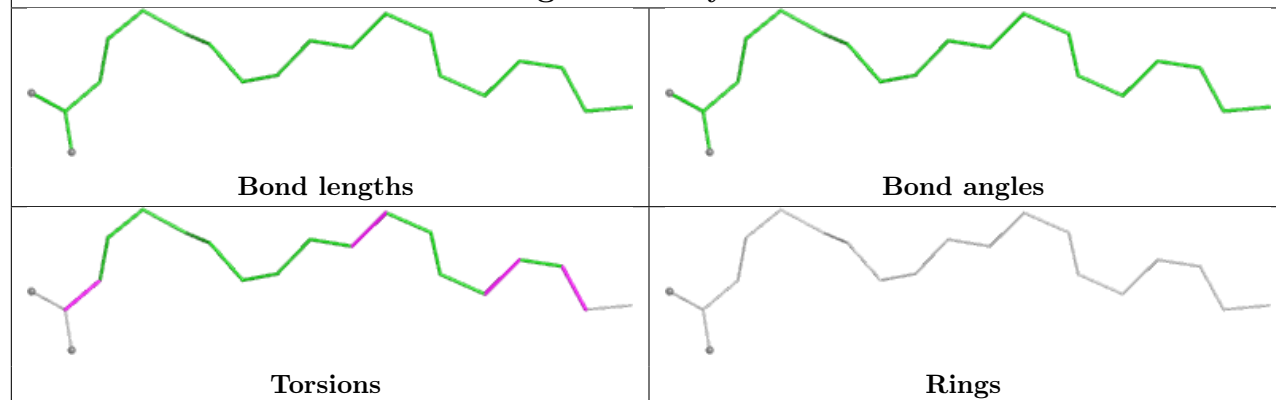


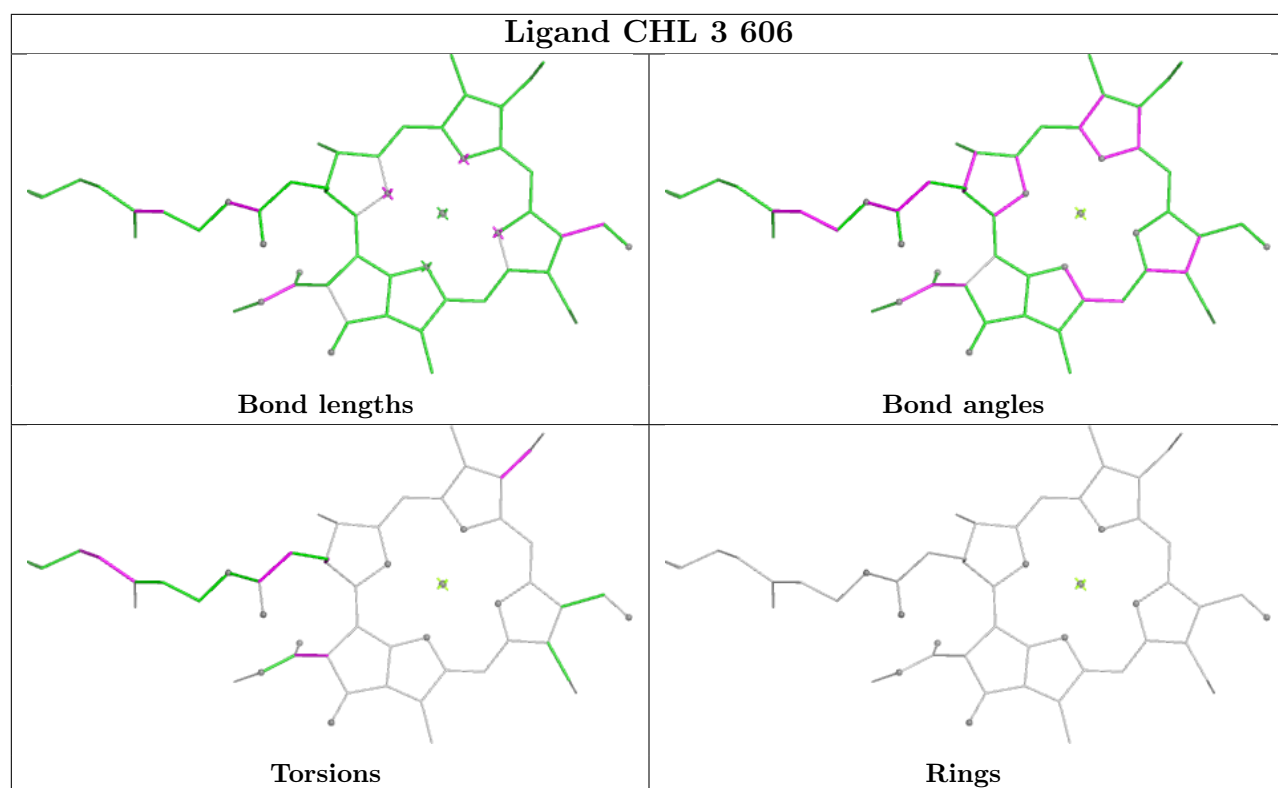


Ligand CLA N 611

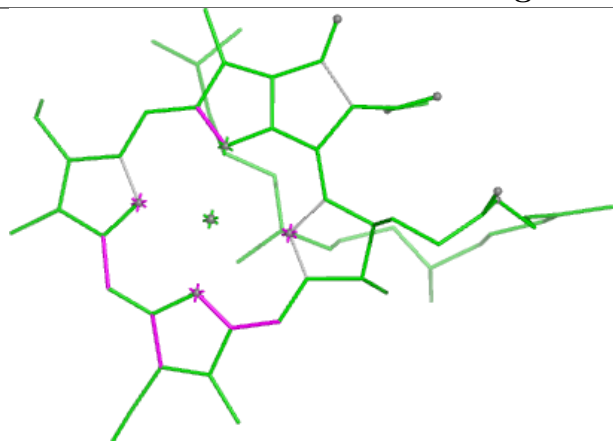


Ligand LNL y 619

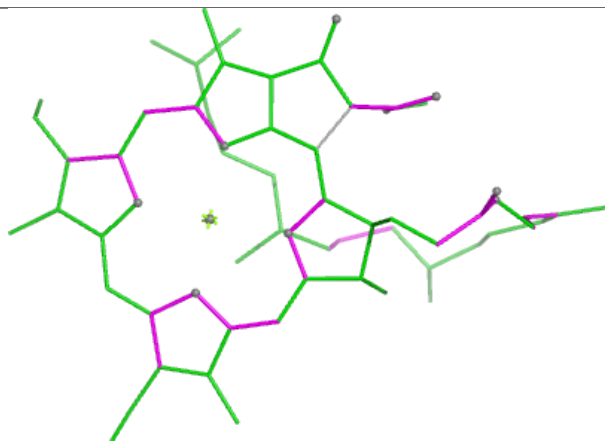




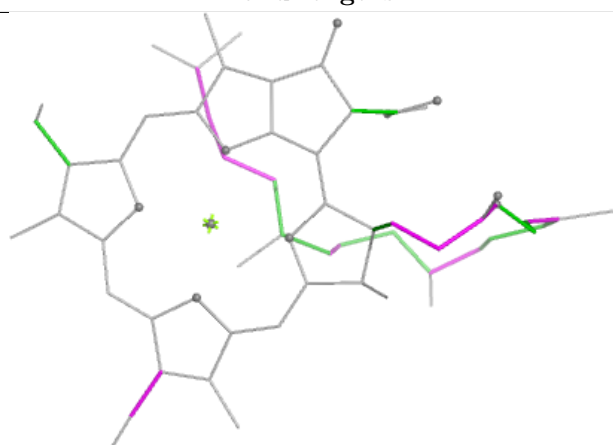
Ligand CLA C 511



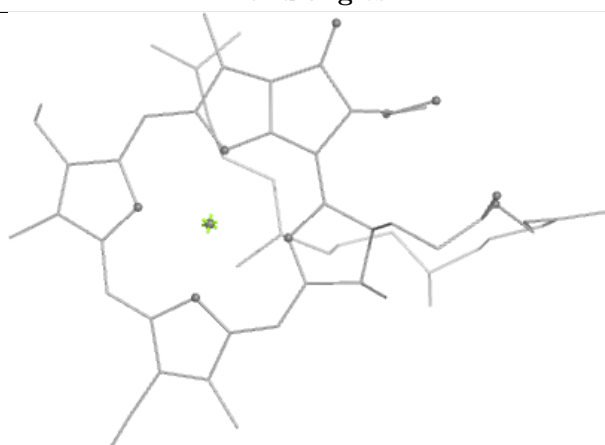
Bond lengths



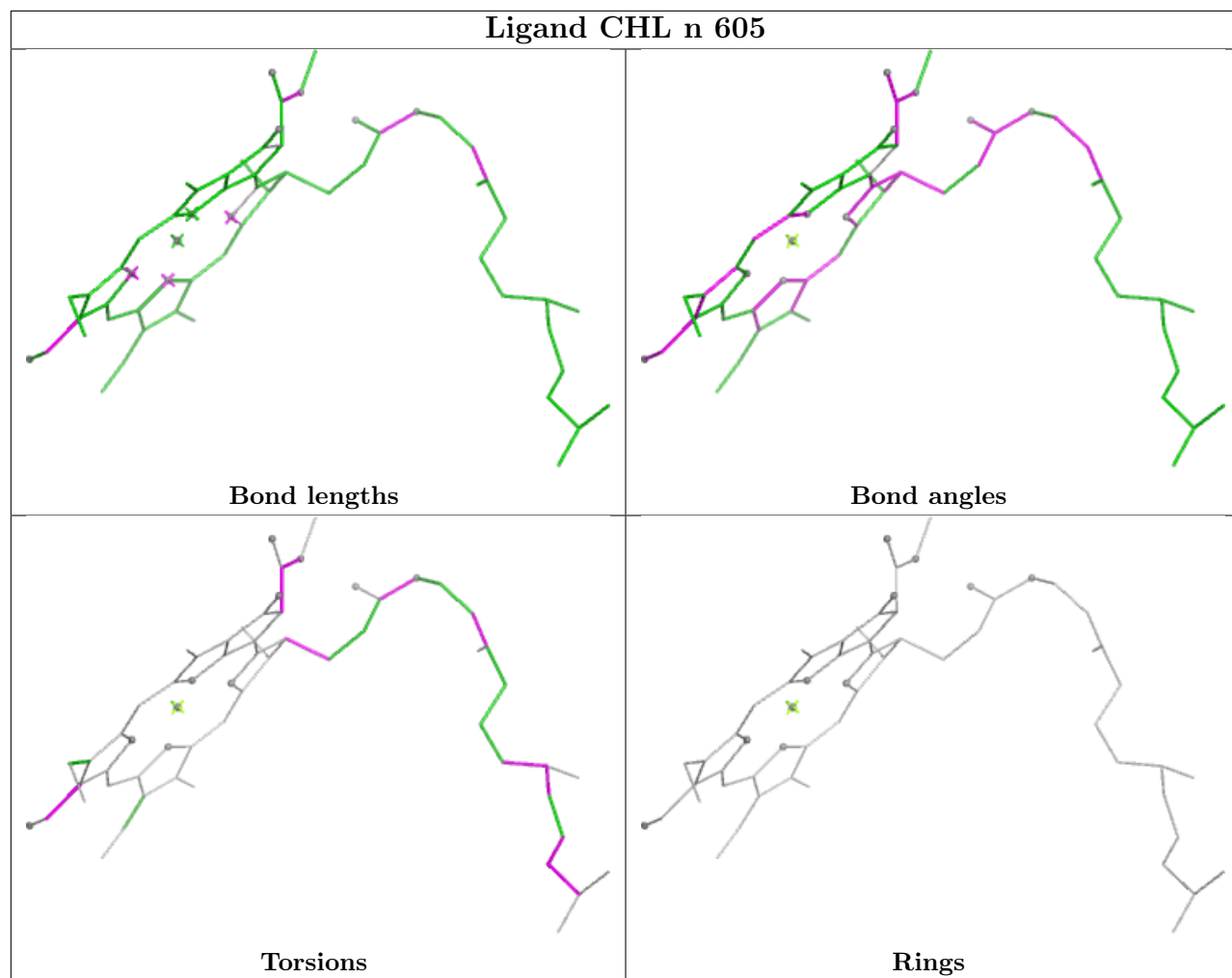
Bond angles

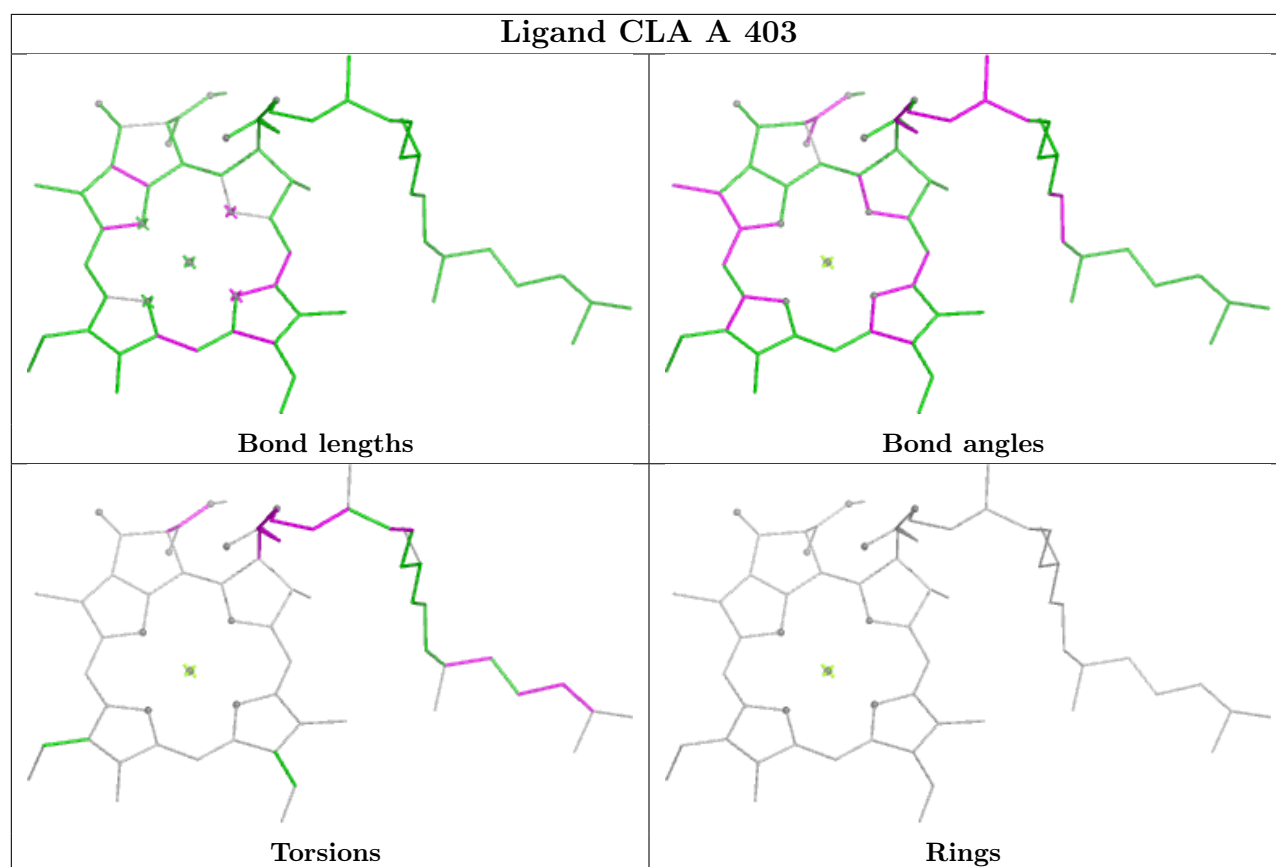
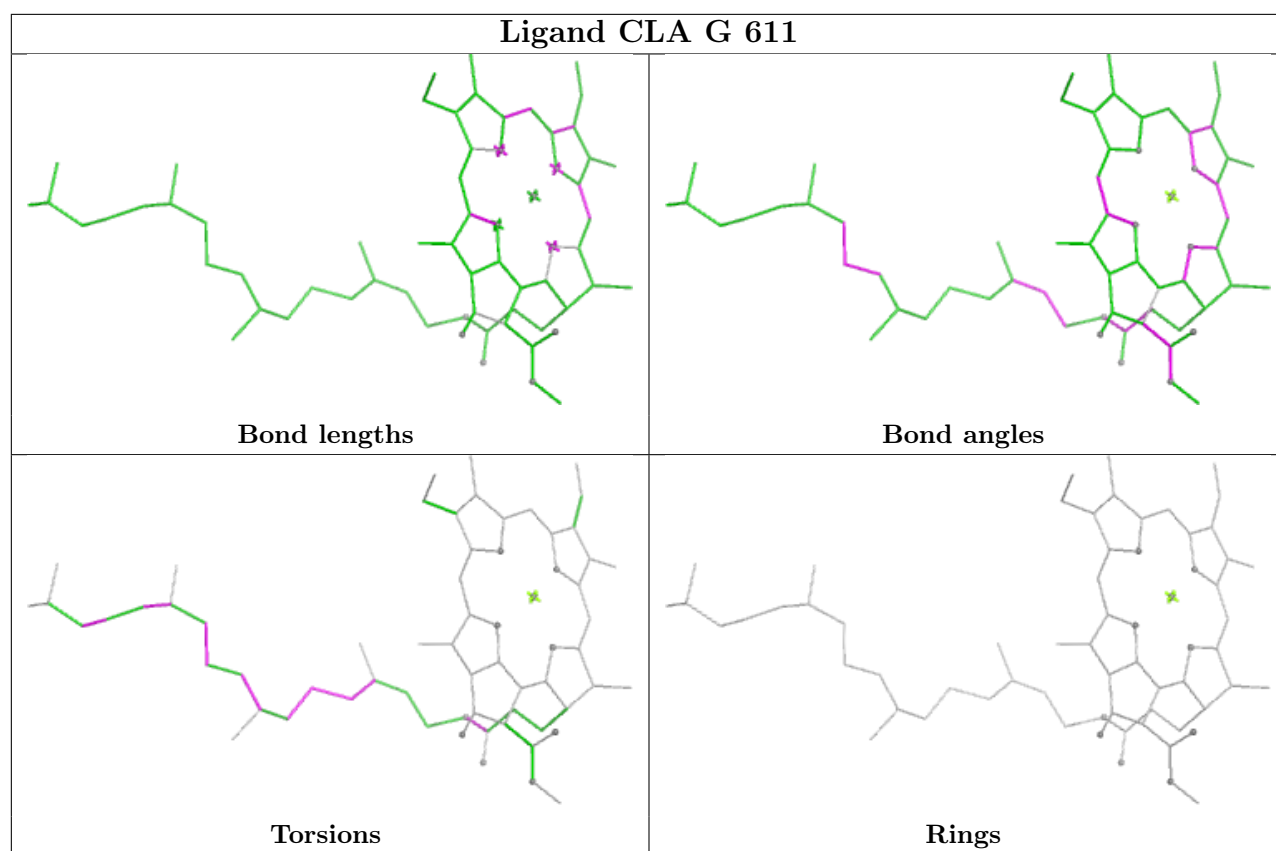


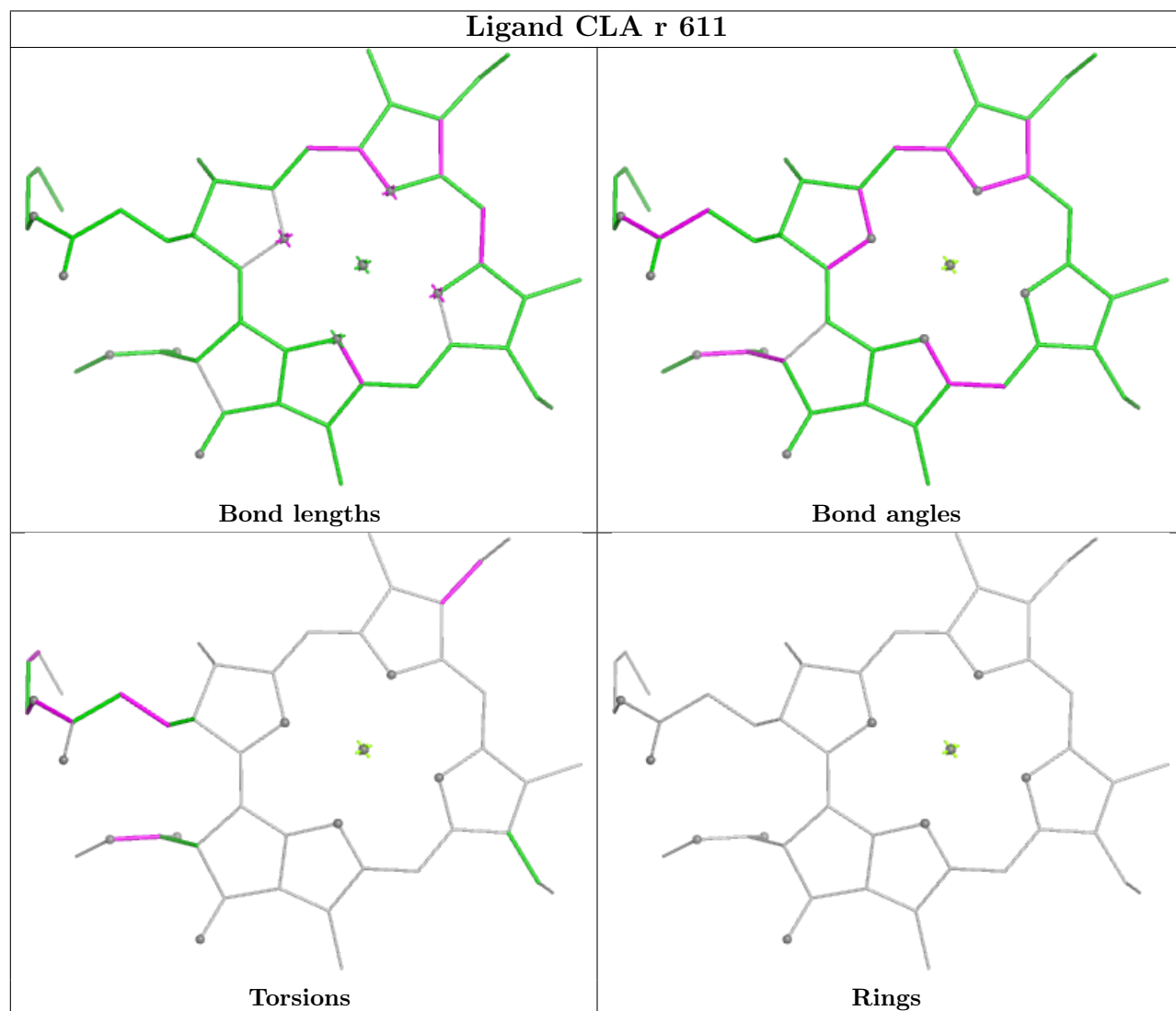
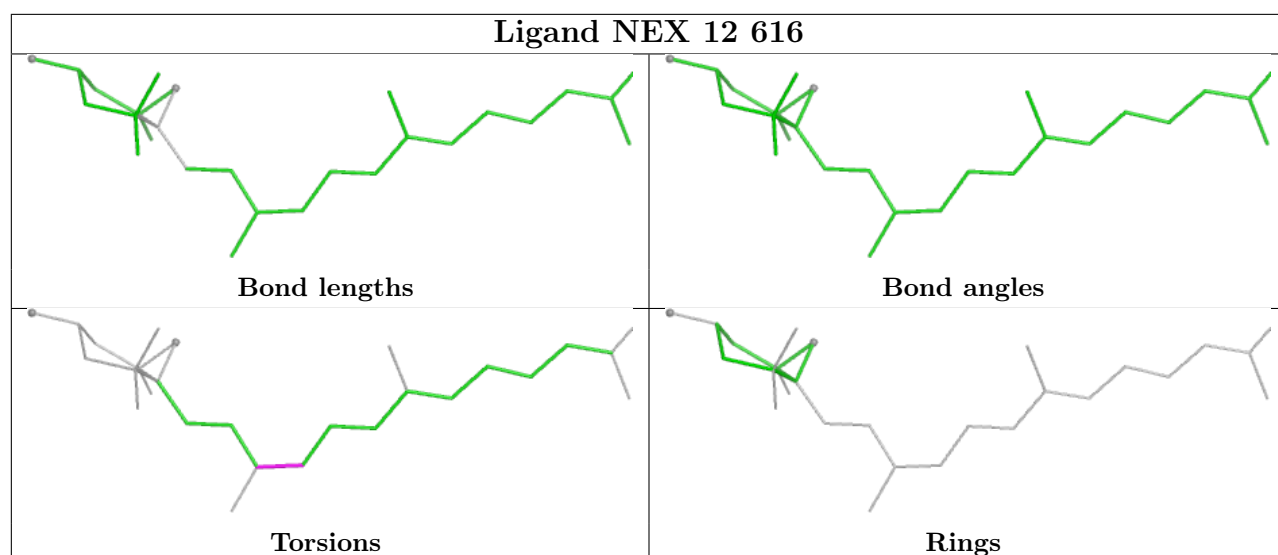
Torsions

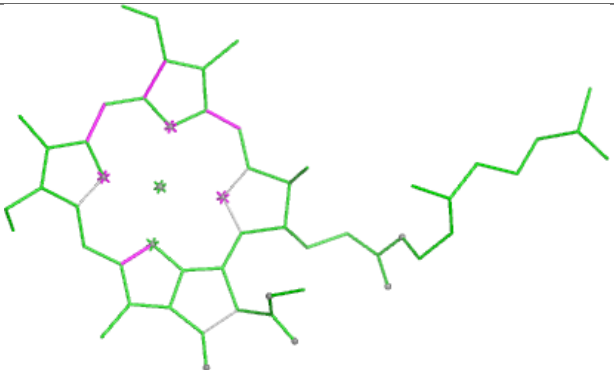
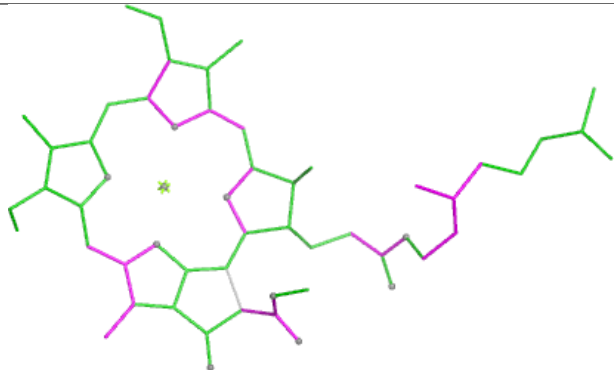
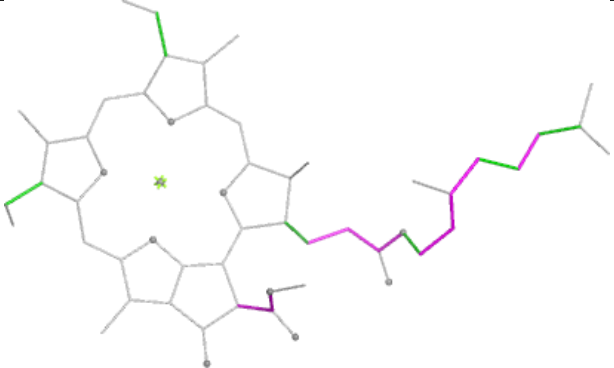
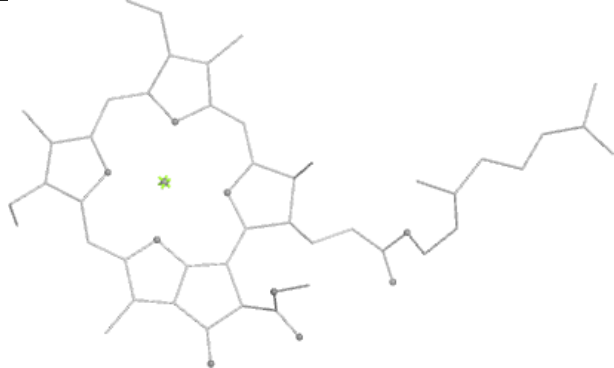


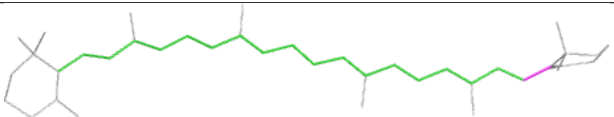
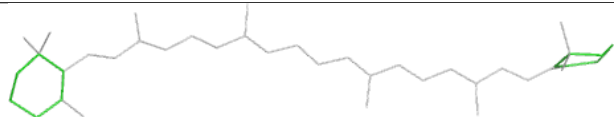
Rings



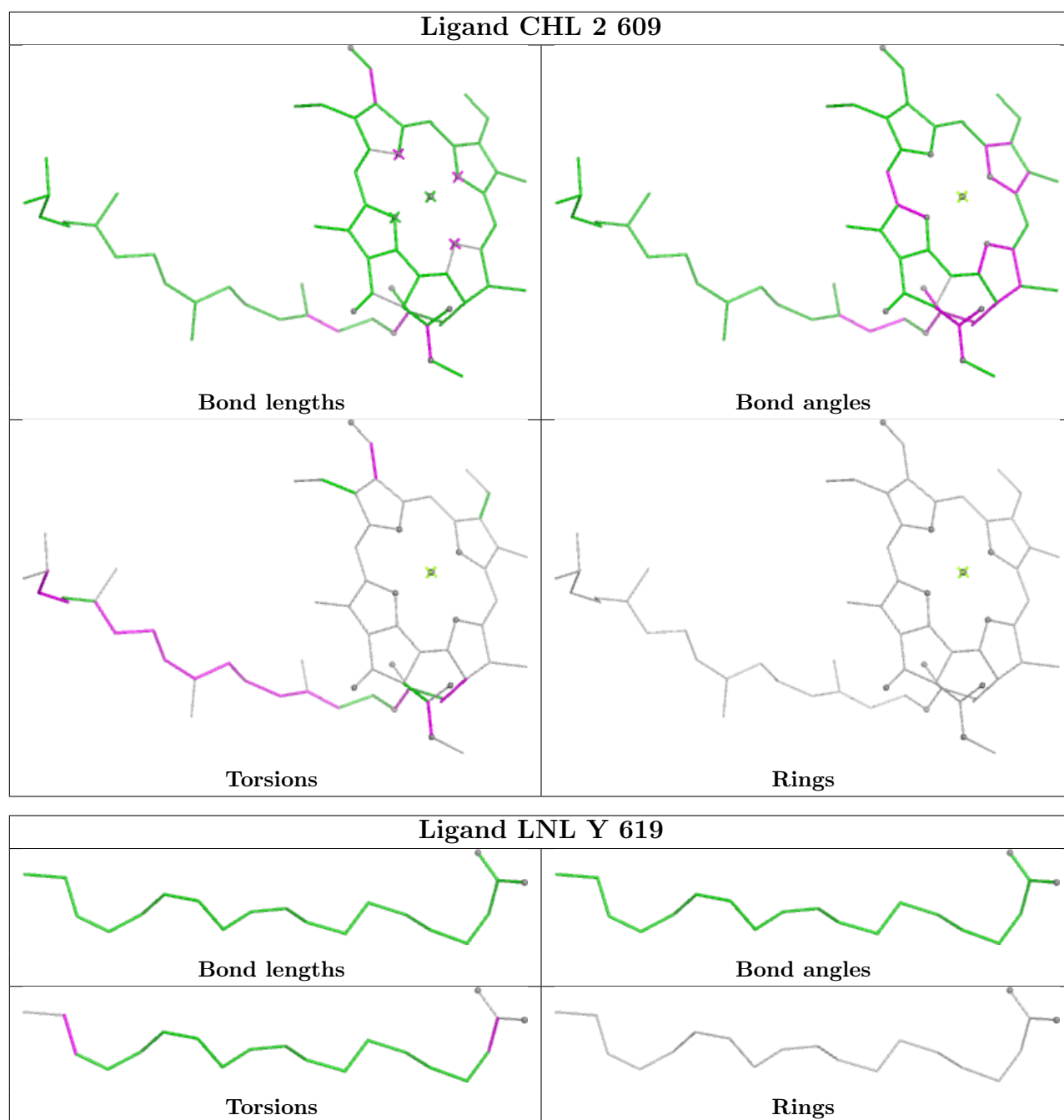


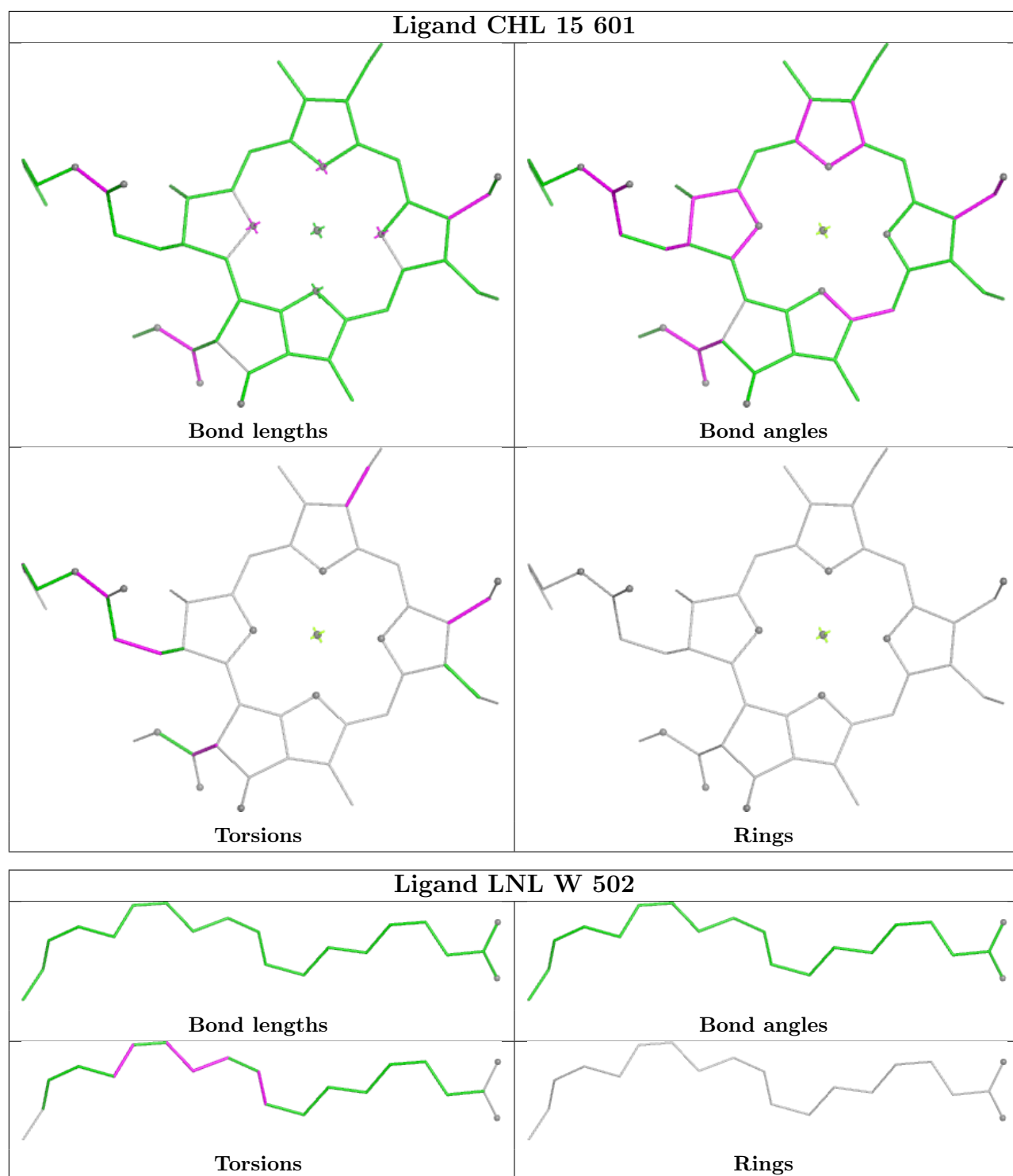


Ligand CLA 6 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

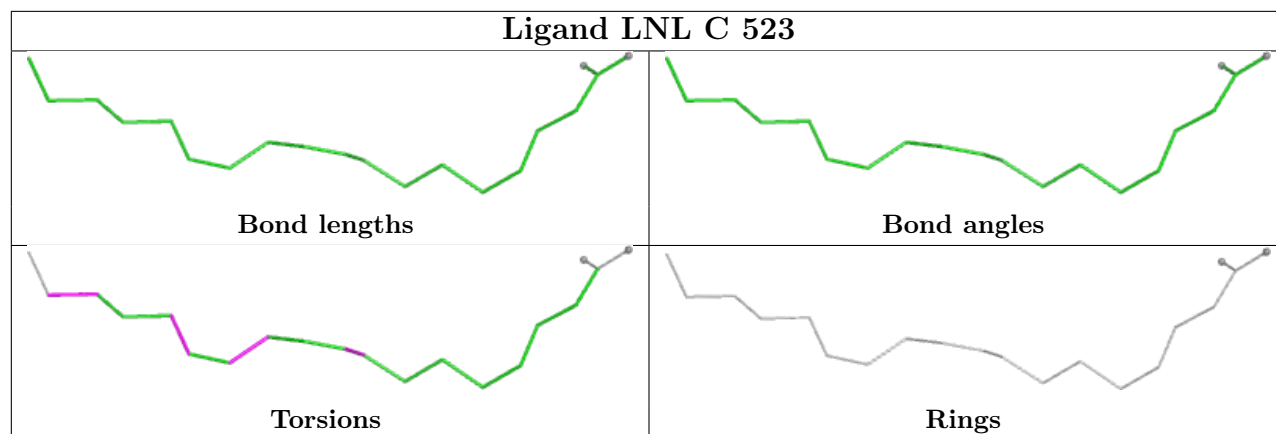
Ligand BCR b 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 11 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

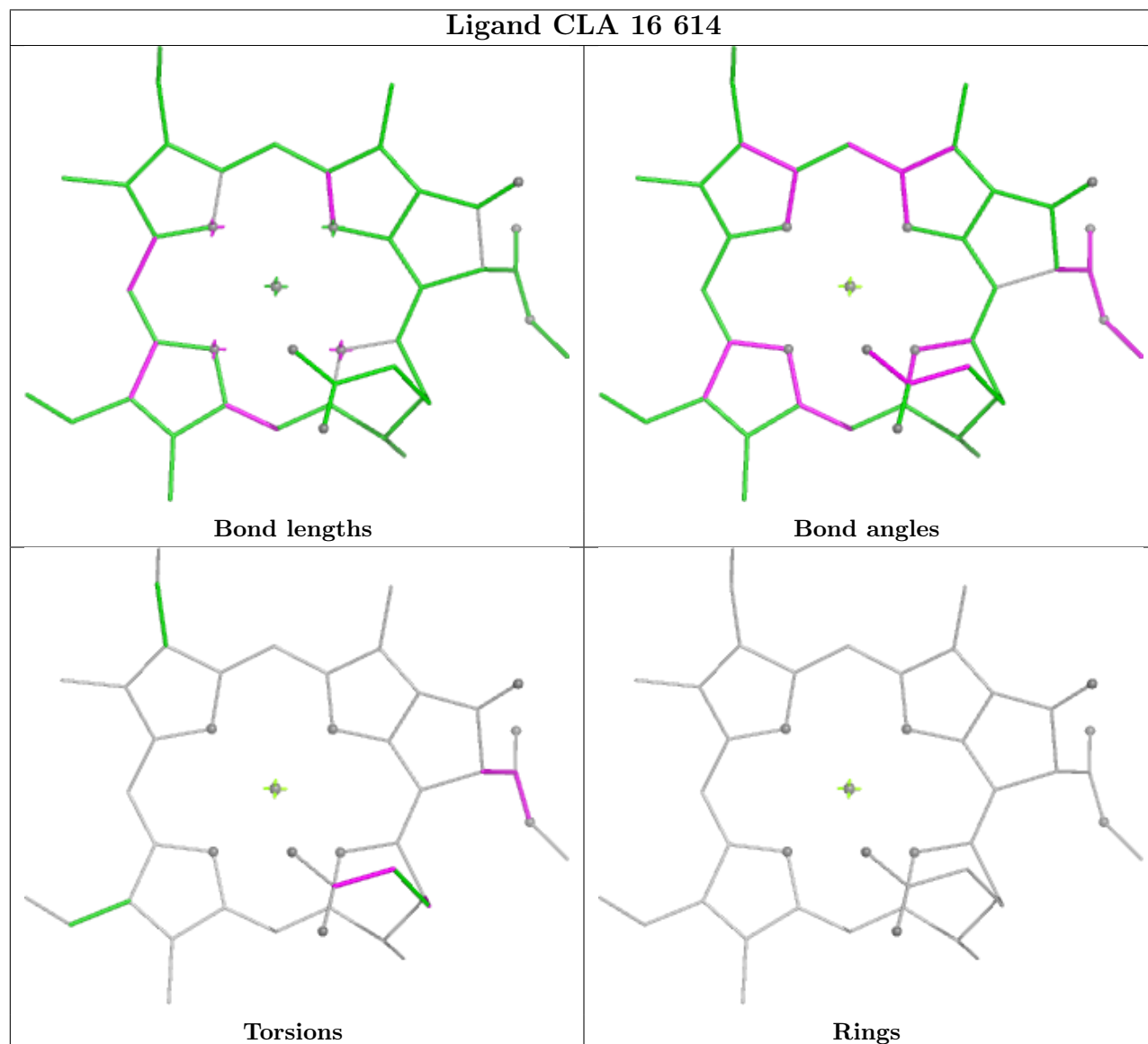


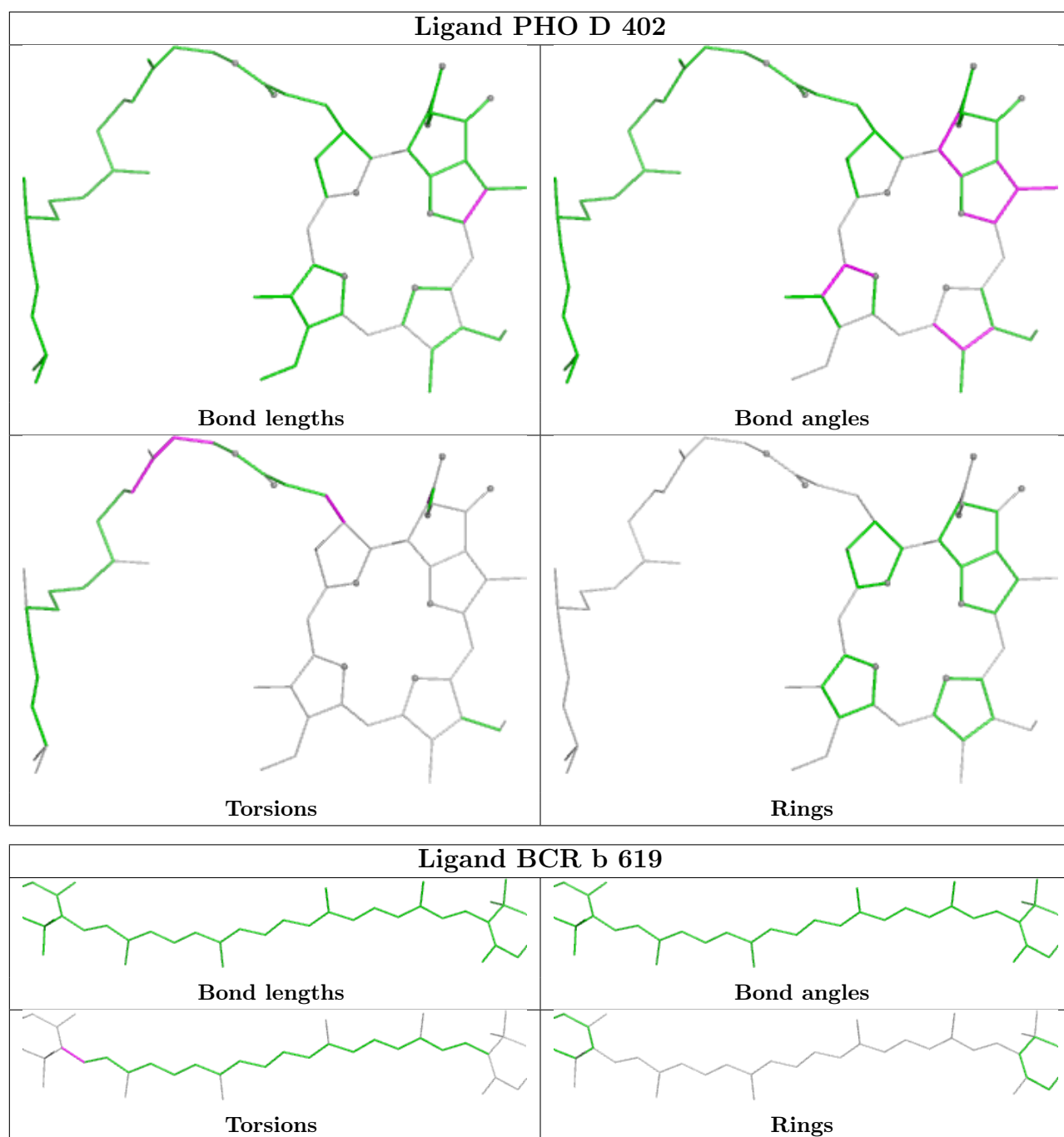


Ligand LNL C 523

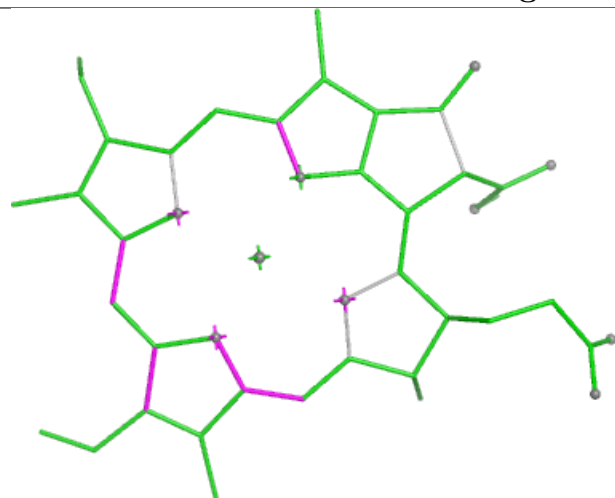


Ligand CLA 16 614

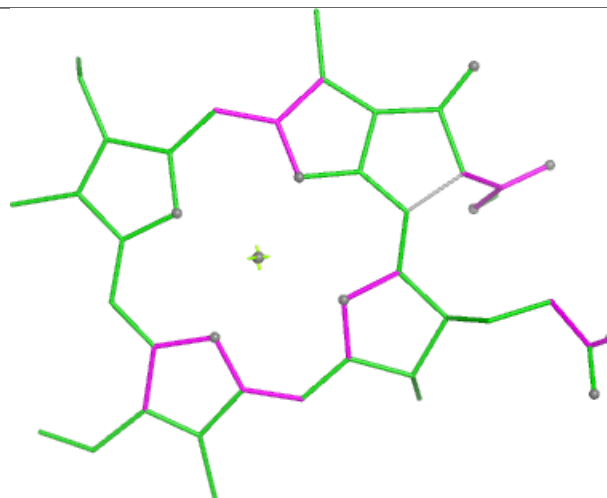




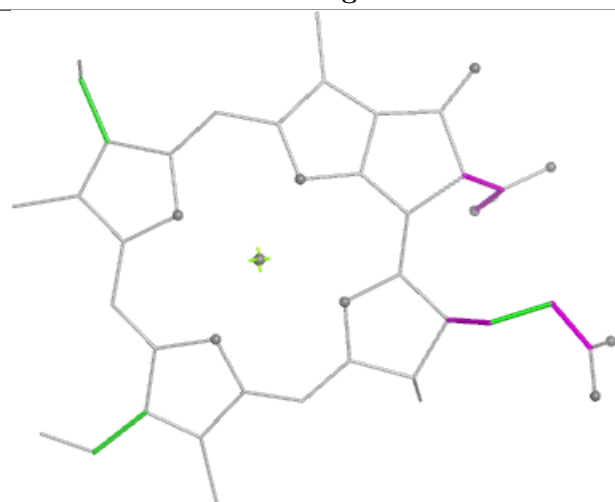
Ligand CLA n 612



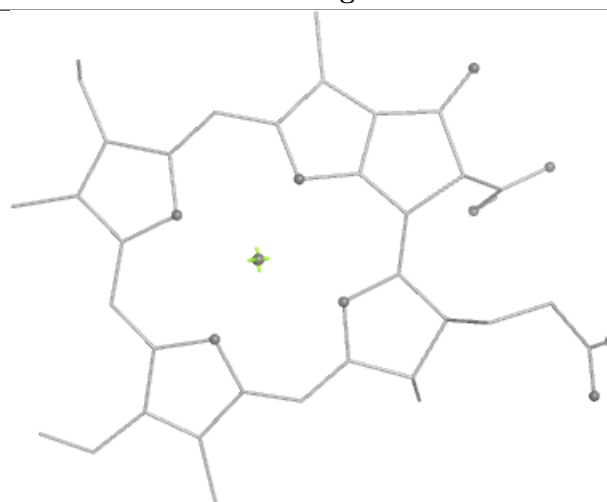
Bond lengths



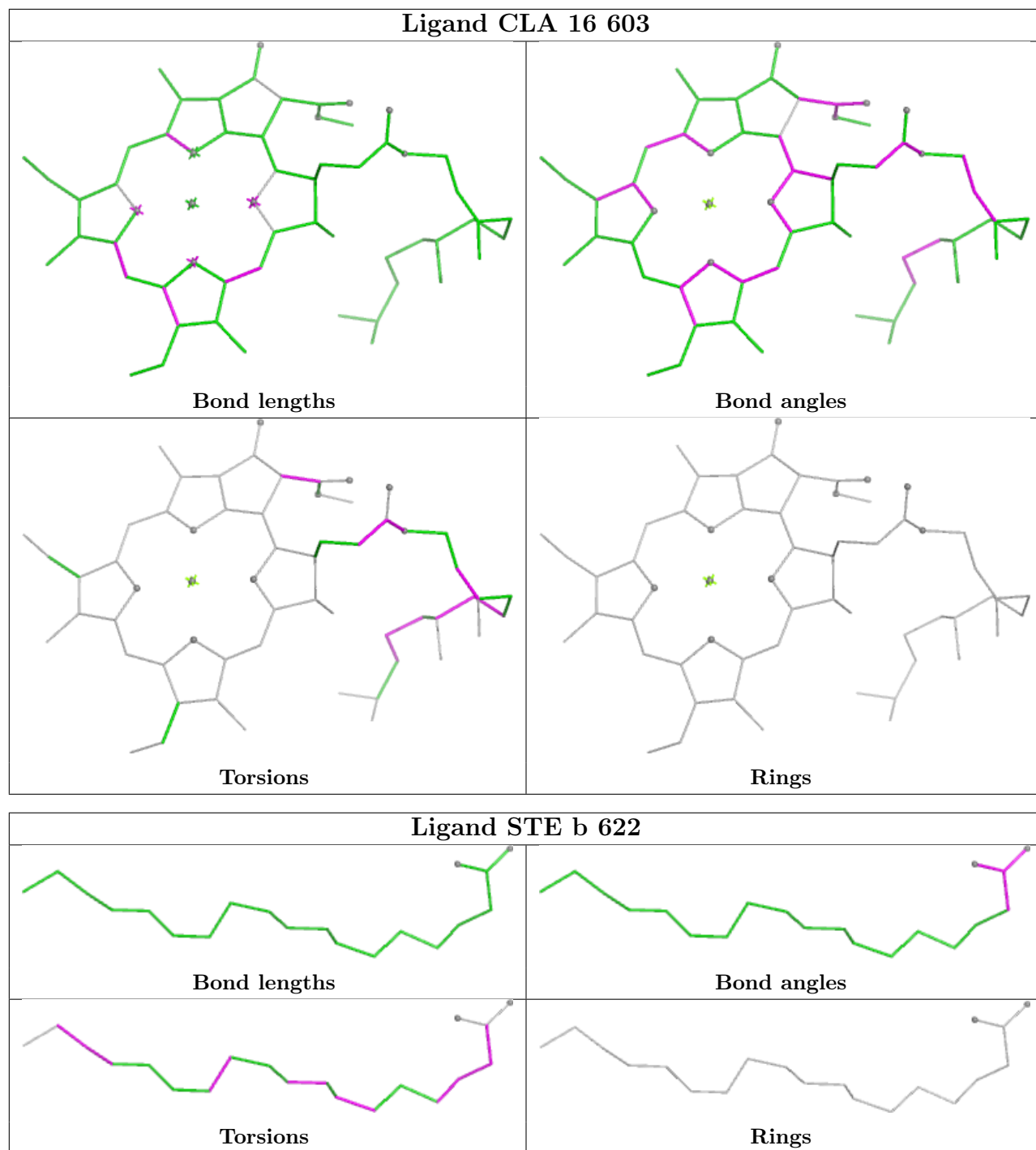
Bond angles

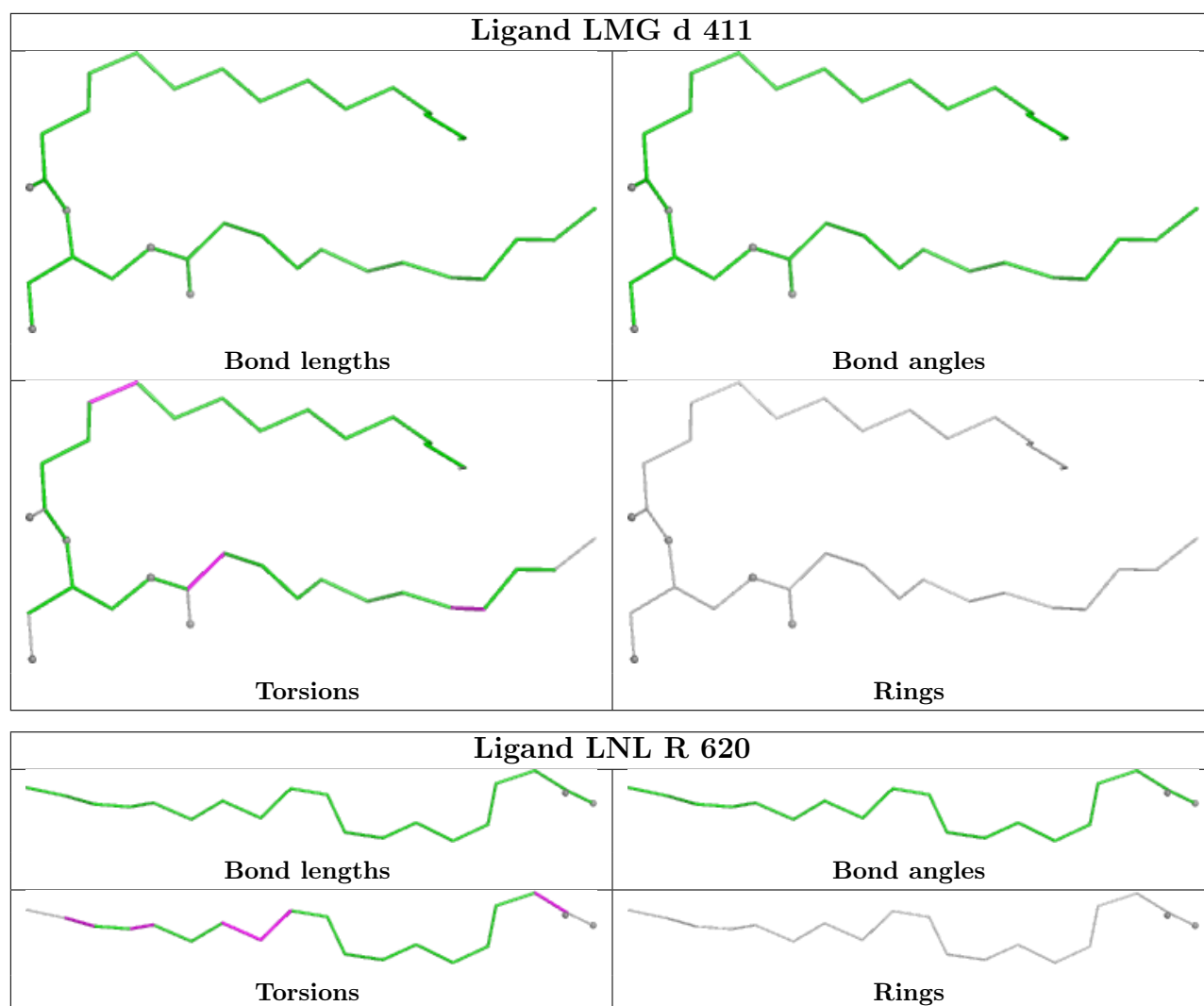


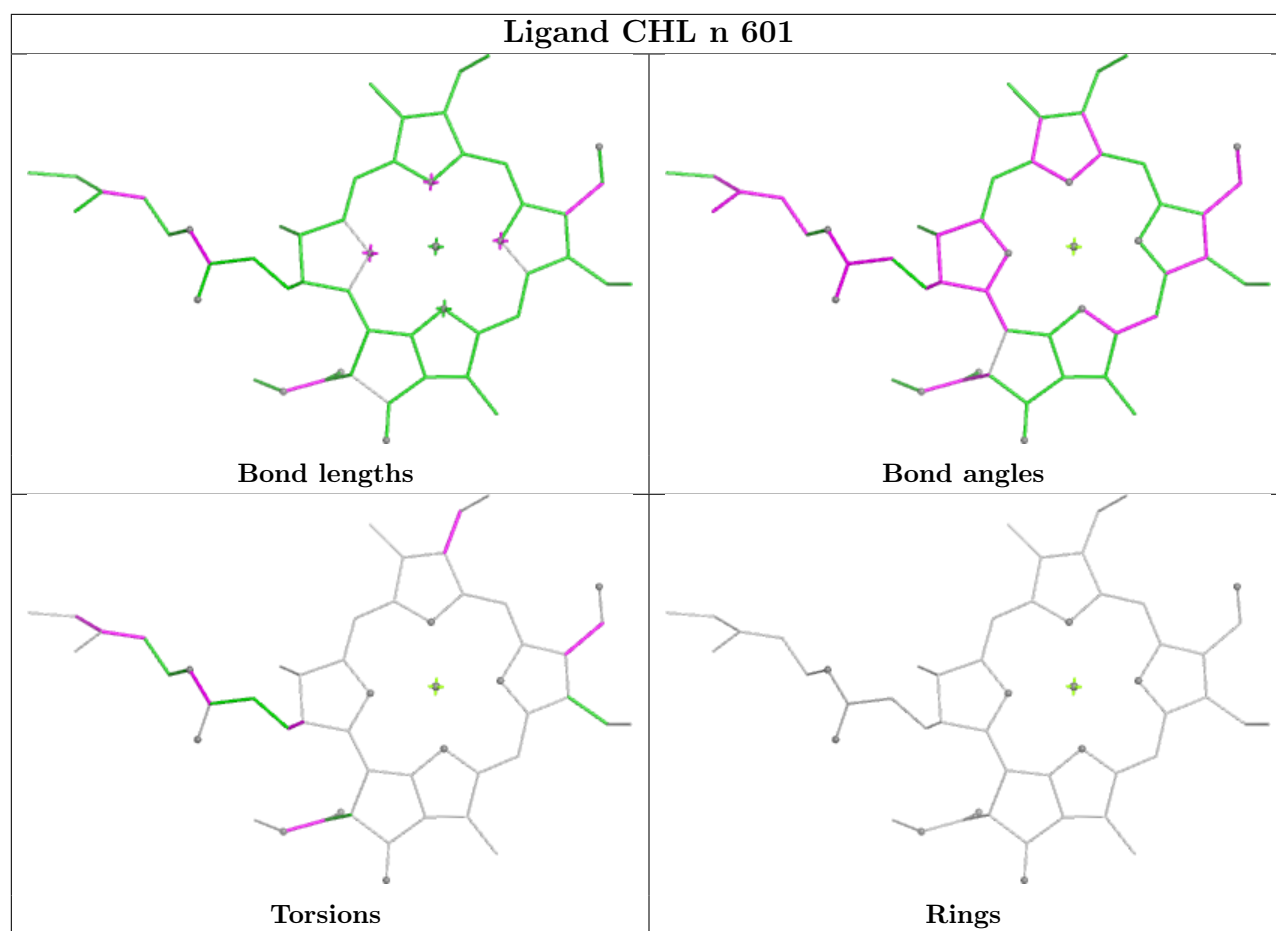
Torsions

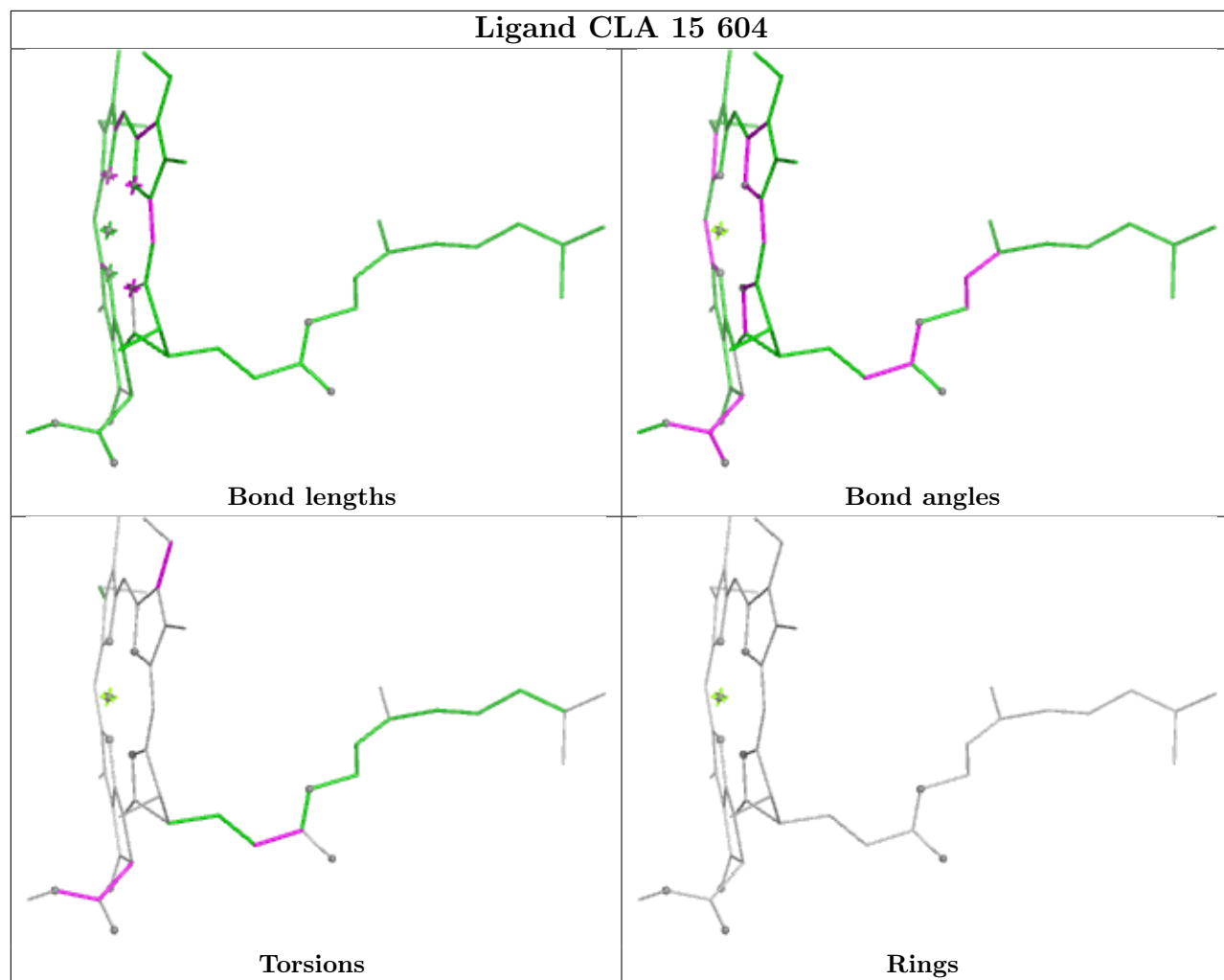


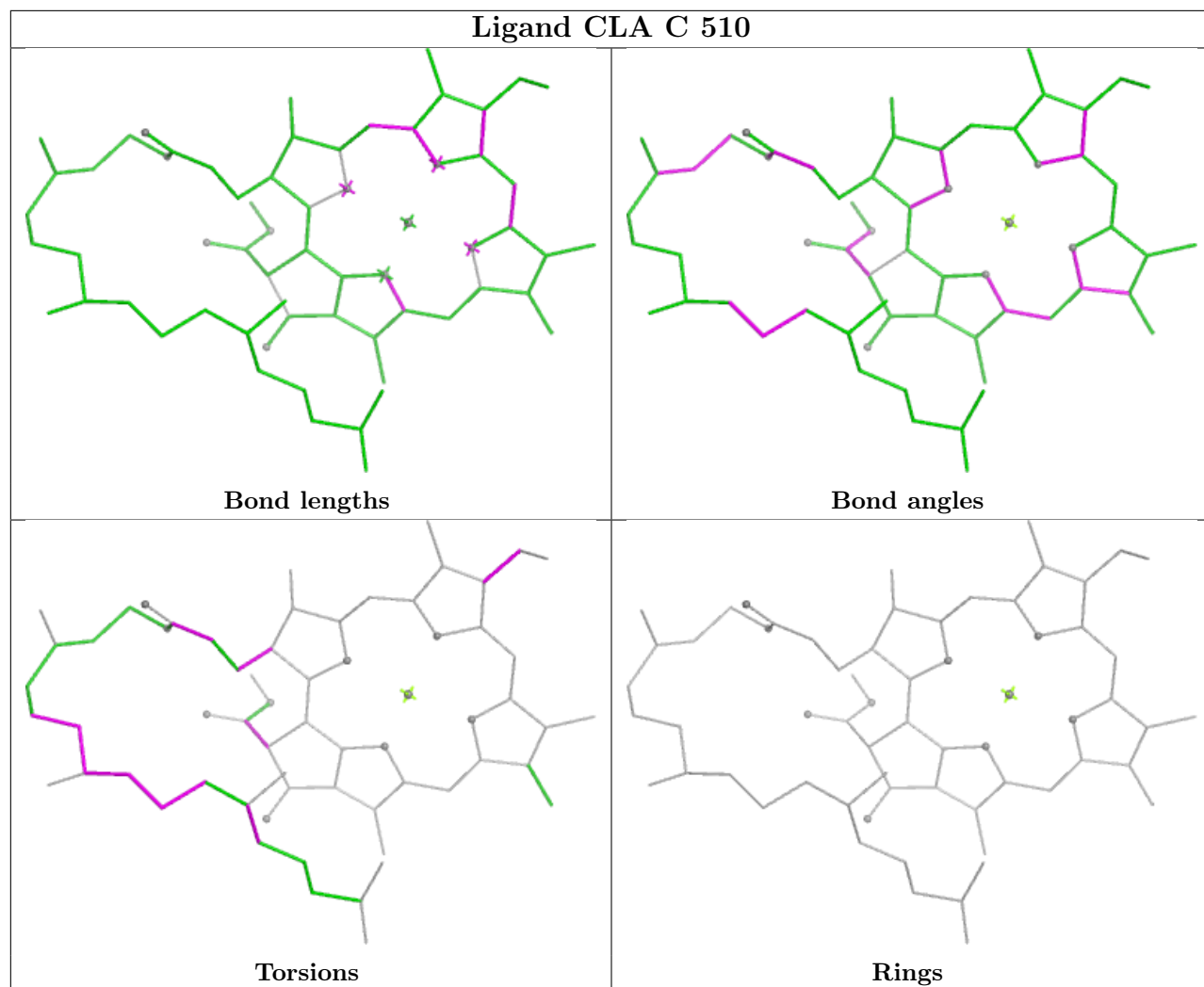
Rings

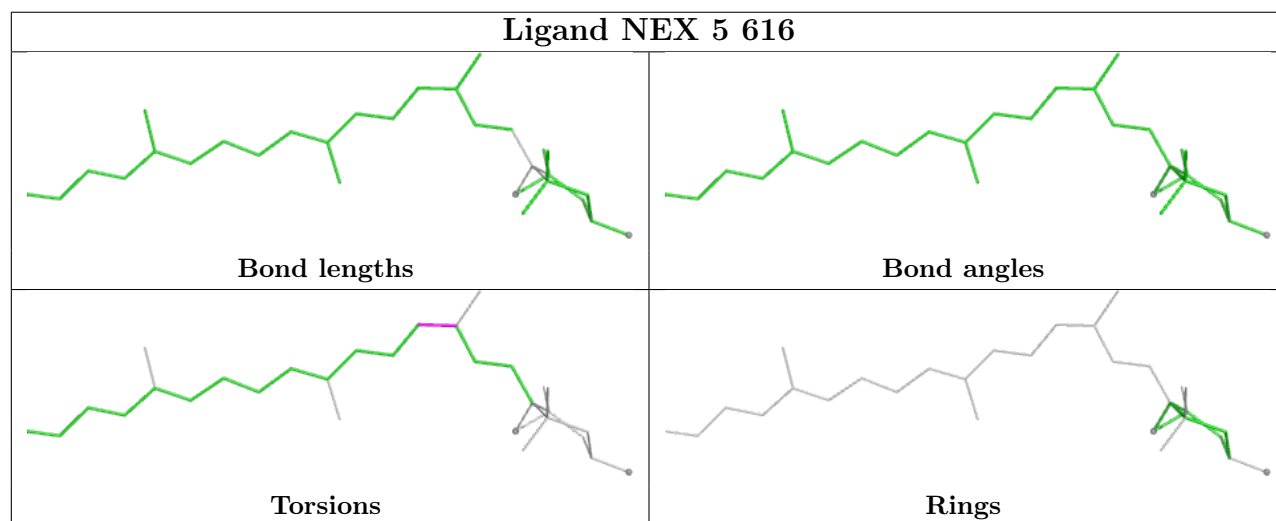
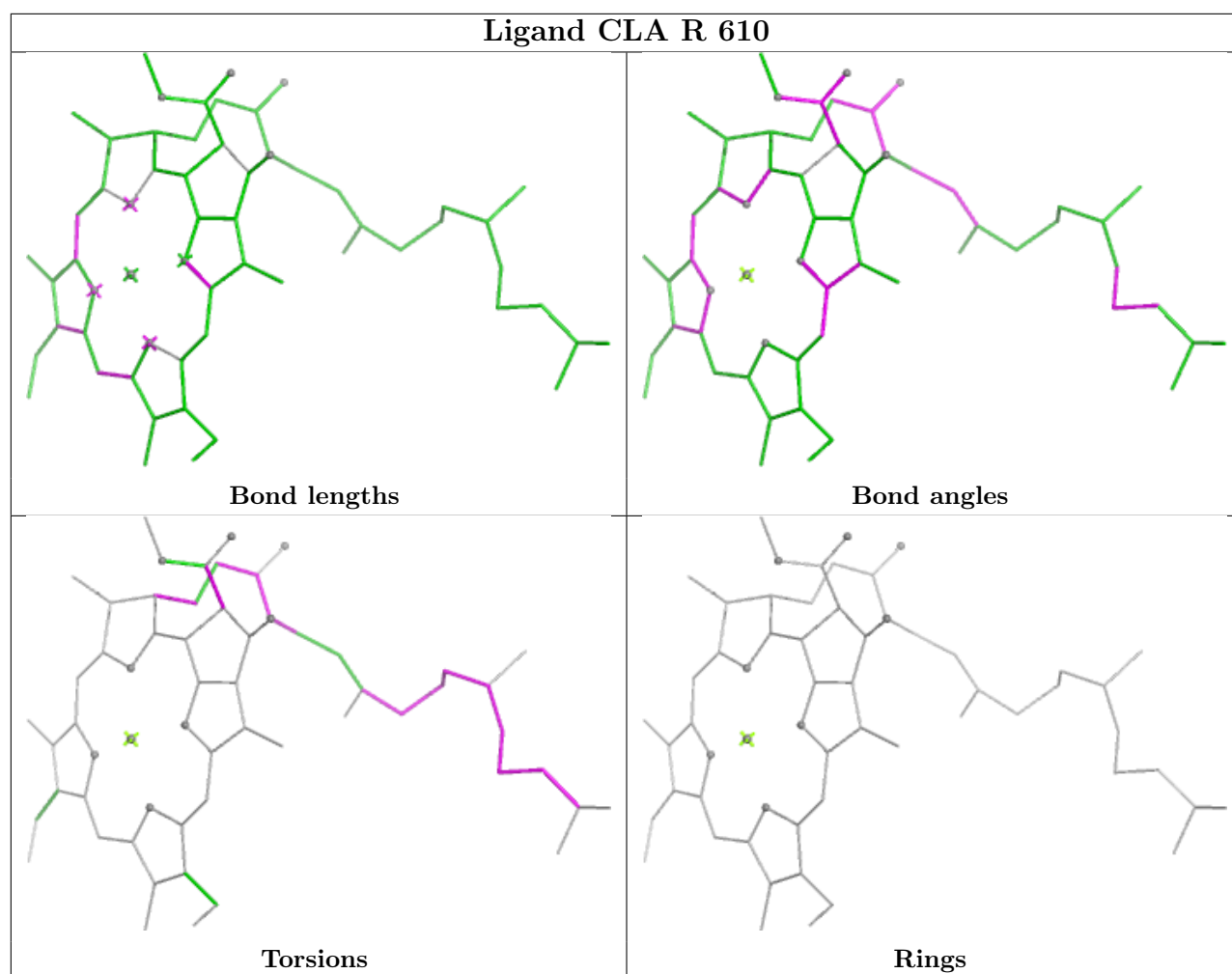


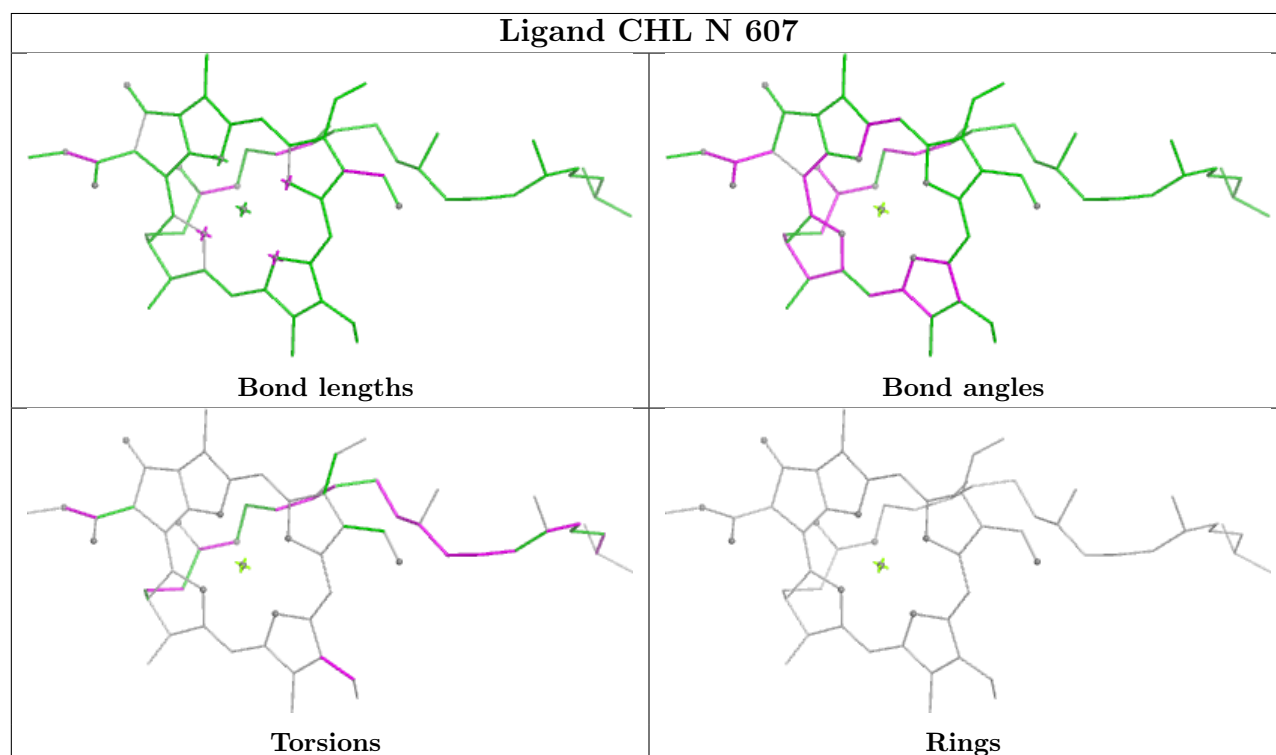
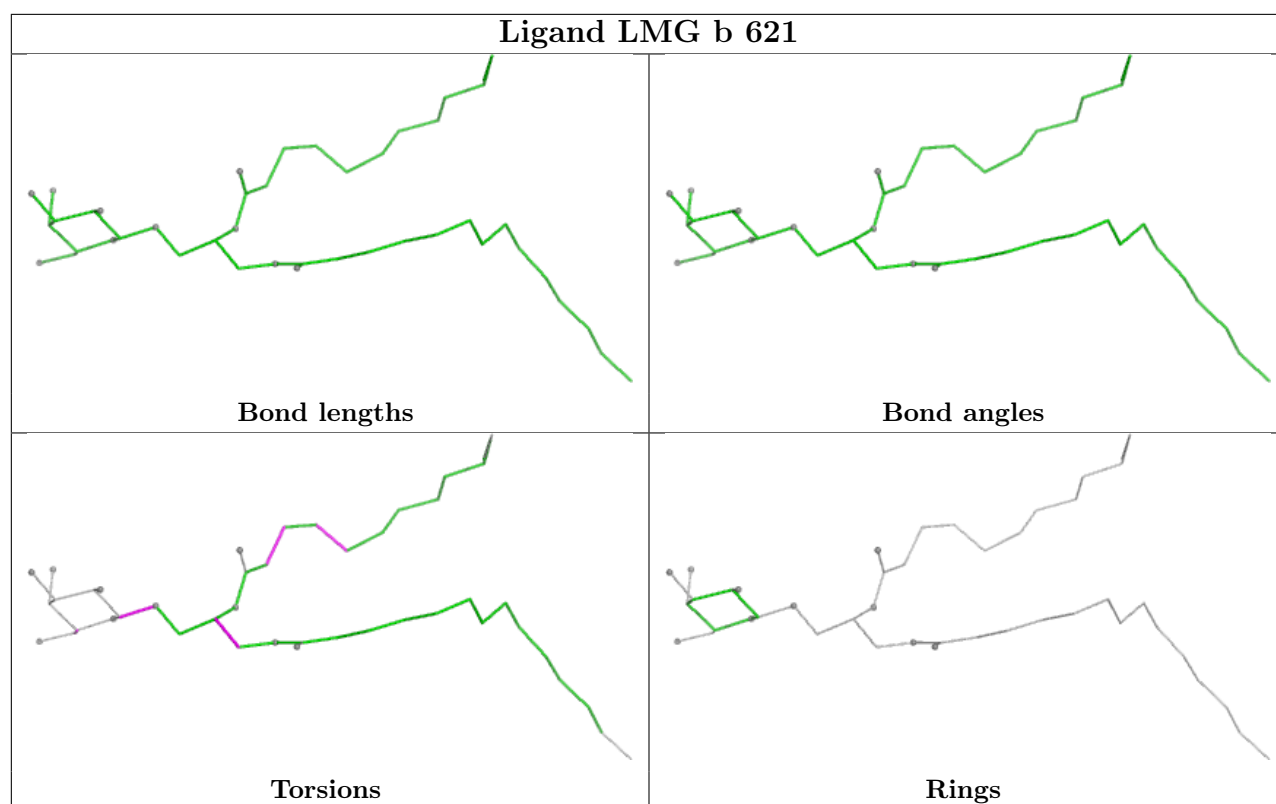


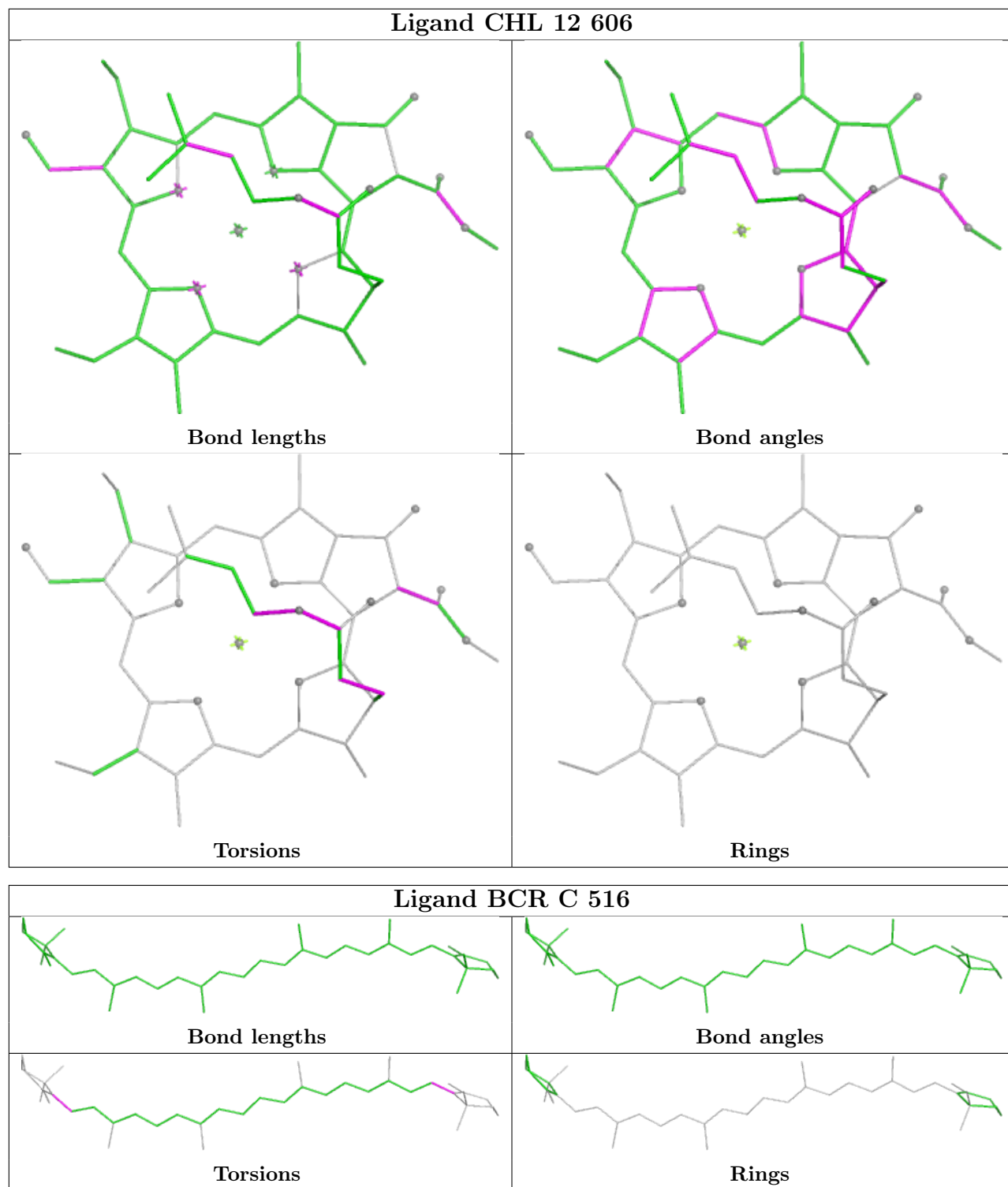


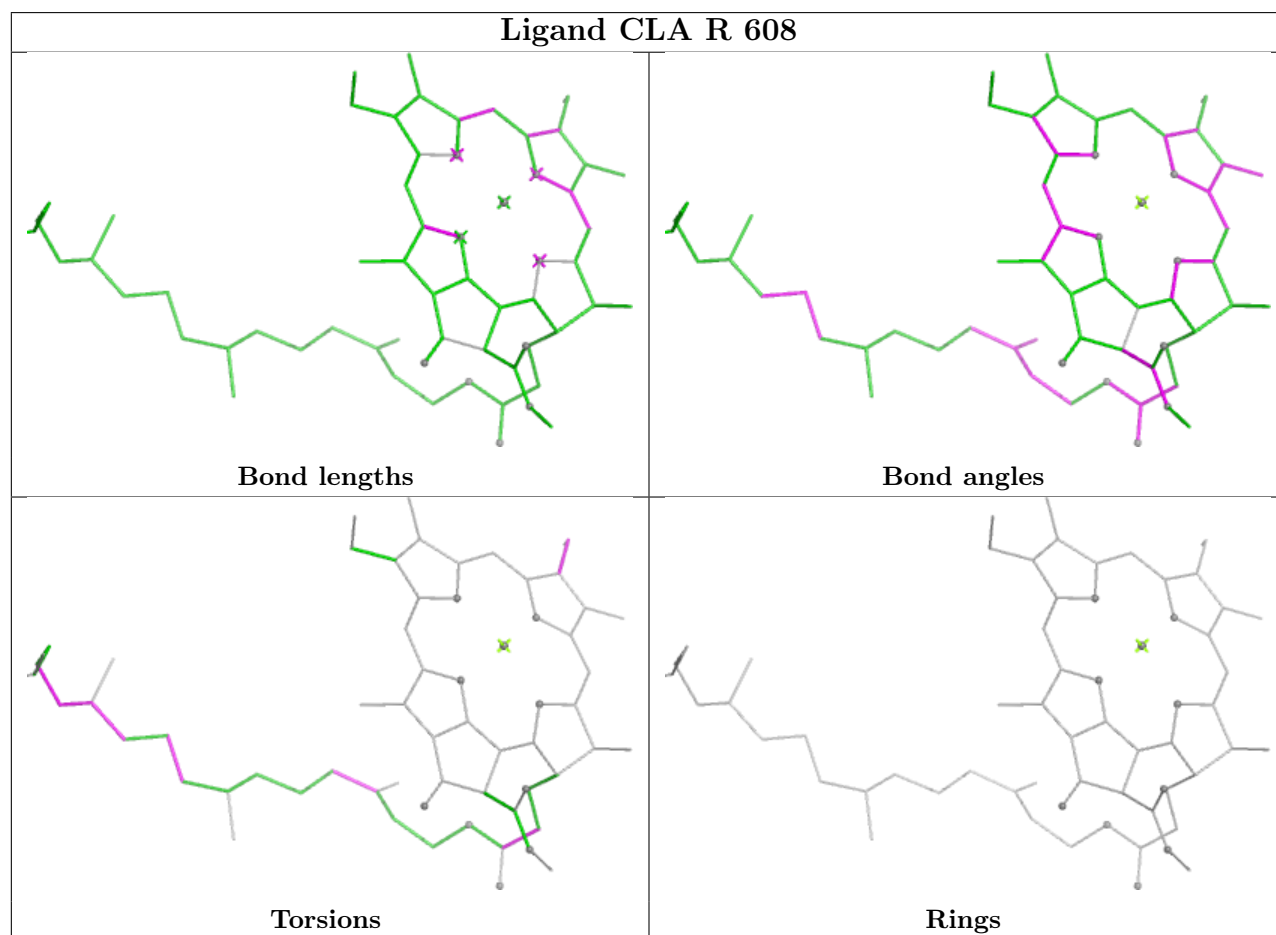
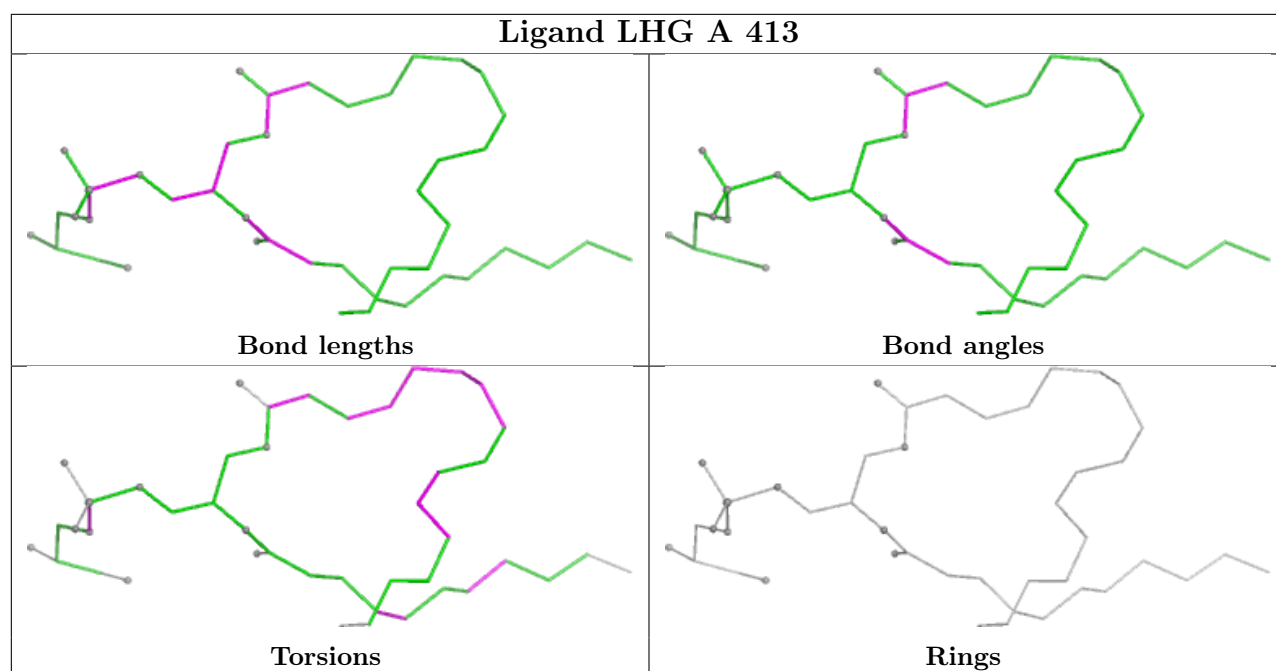




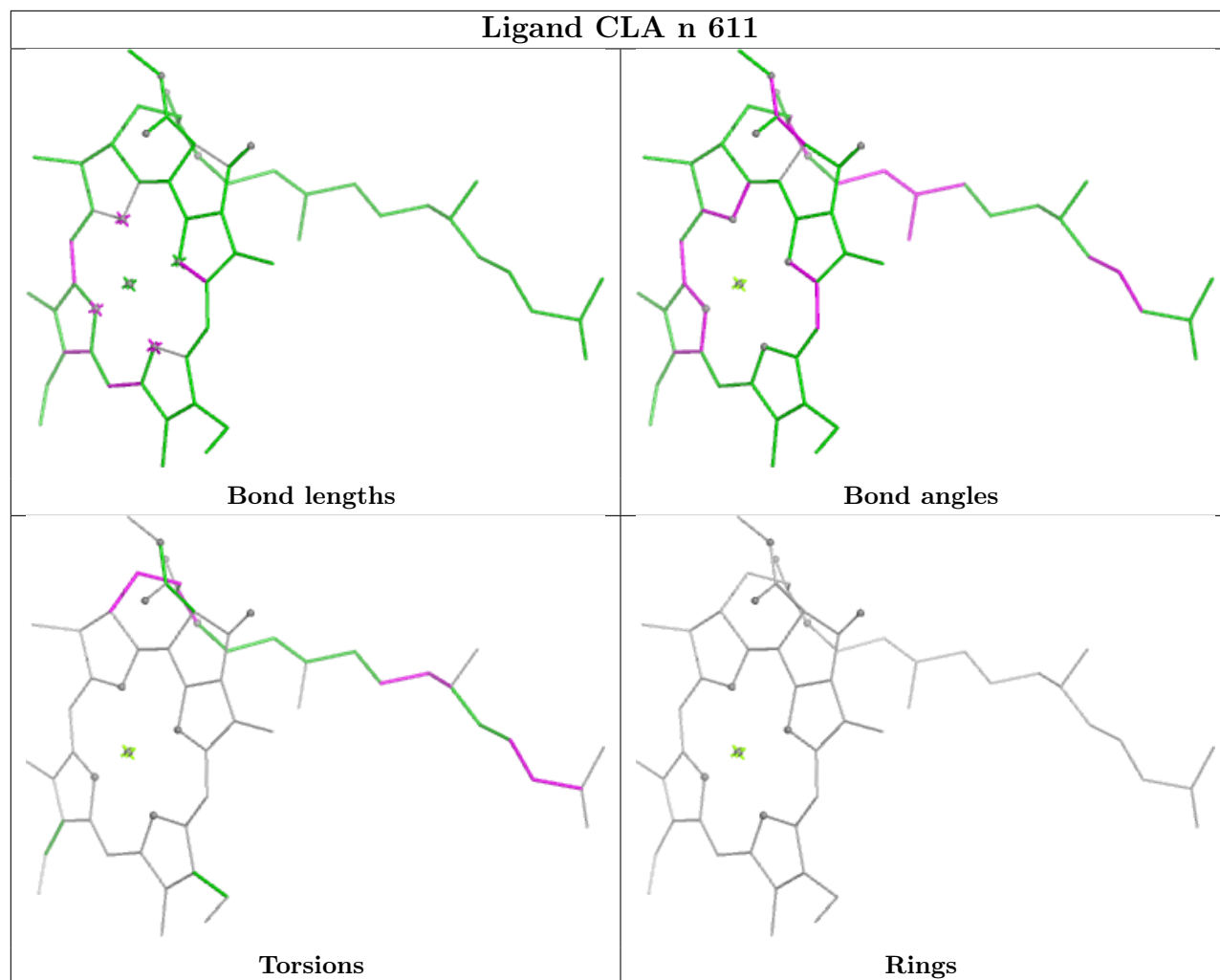




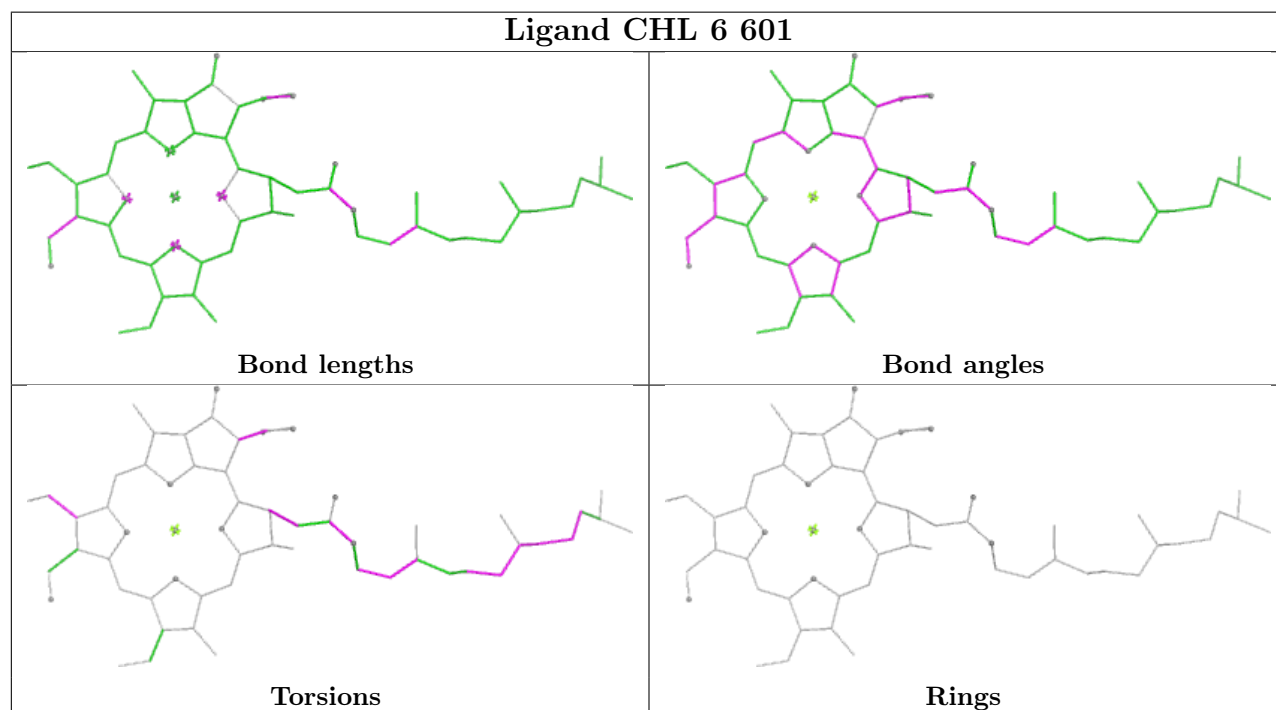


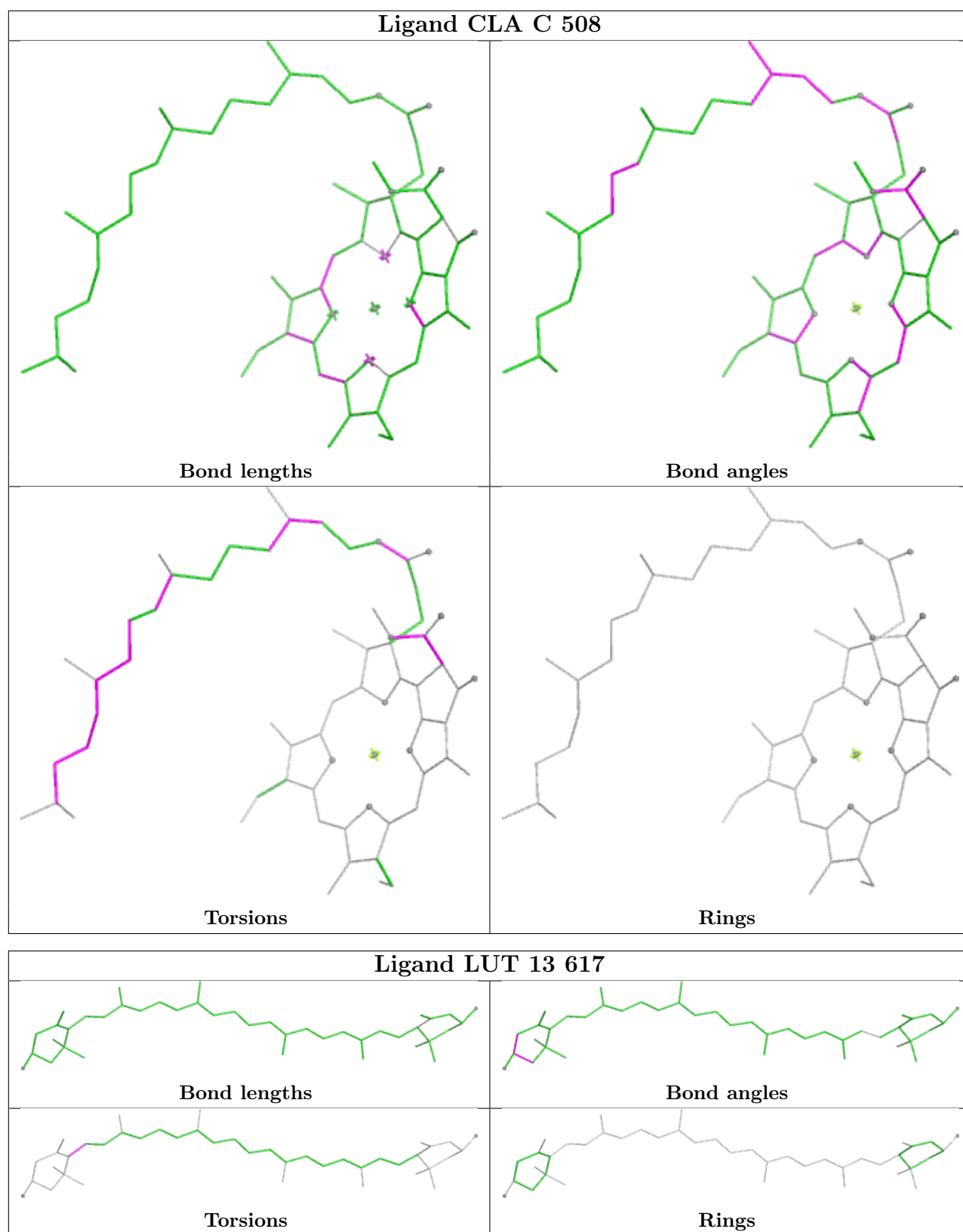


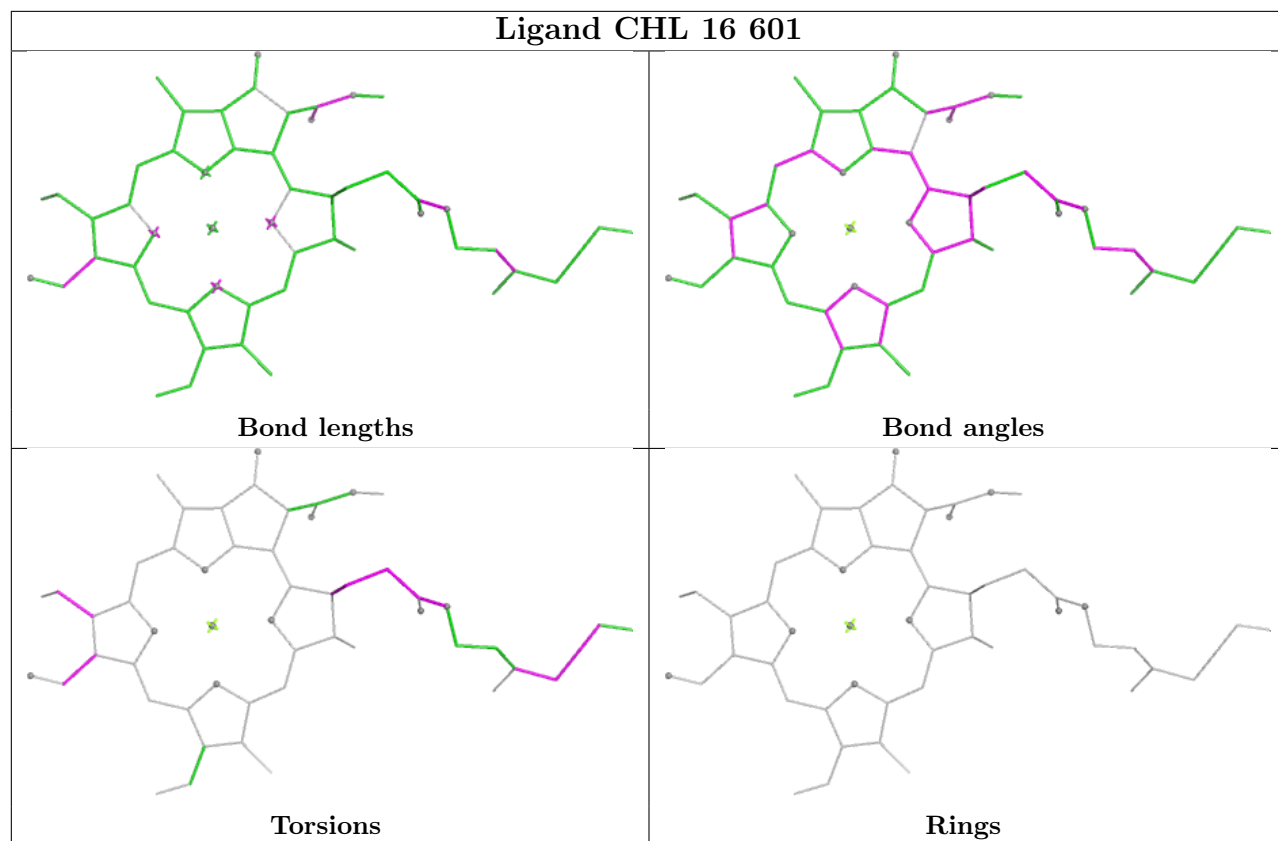
Ligand CLA n 611



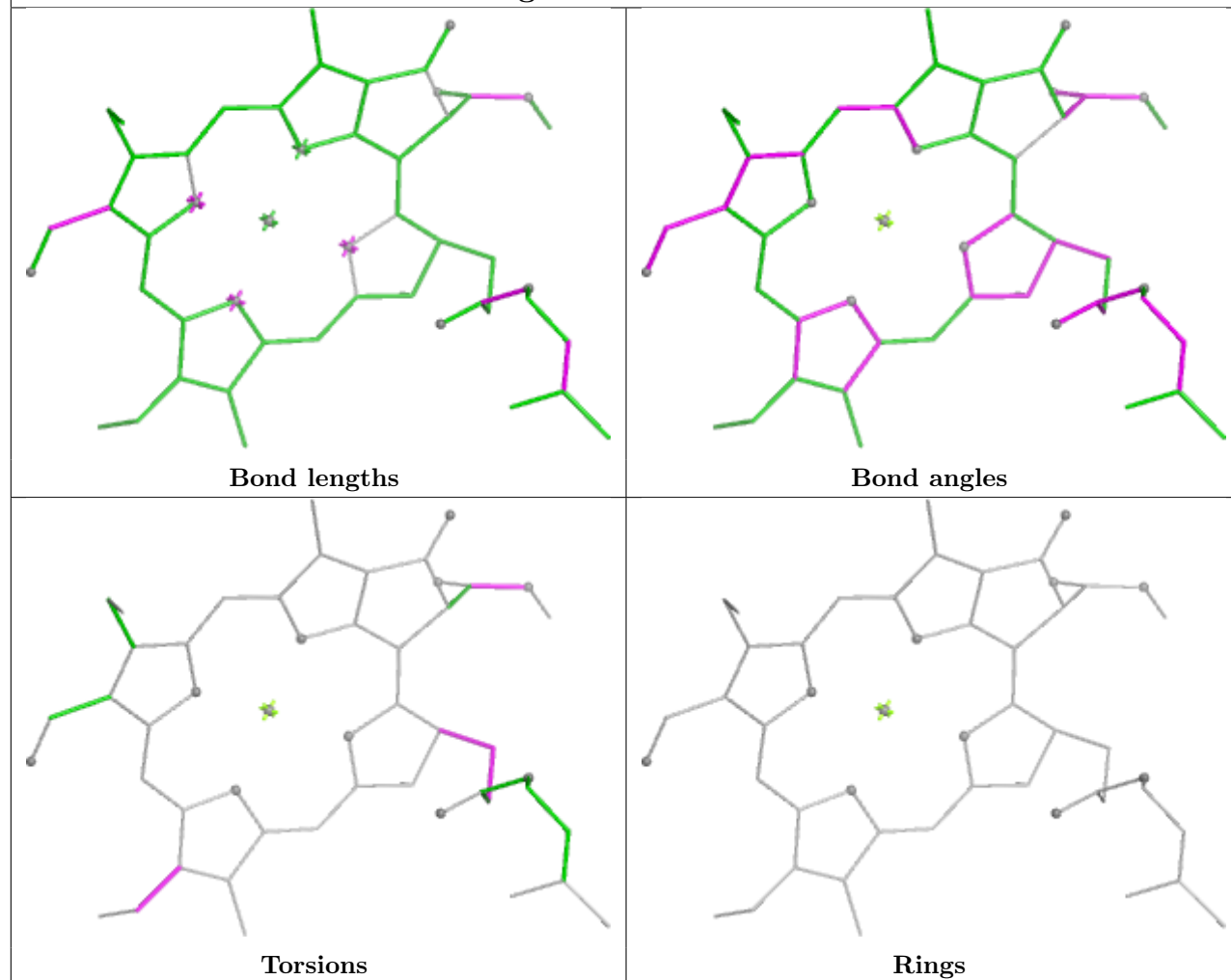
Ligand CHL 6 601



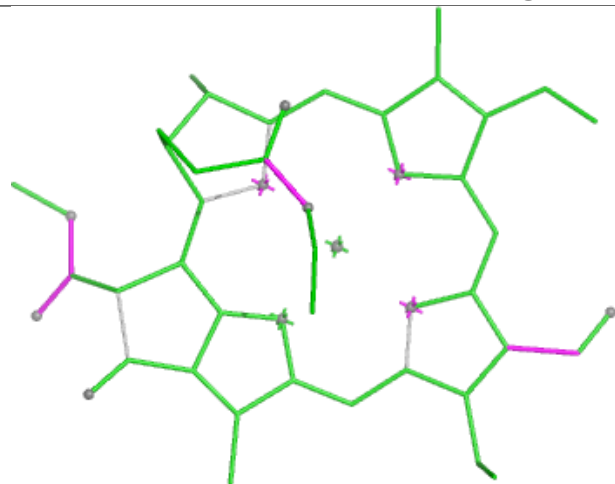




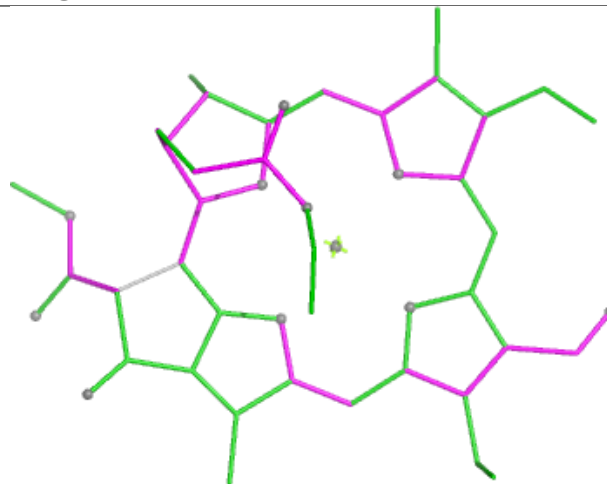
Ligand CHL r 607



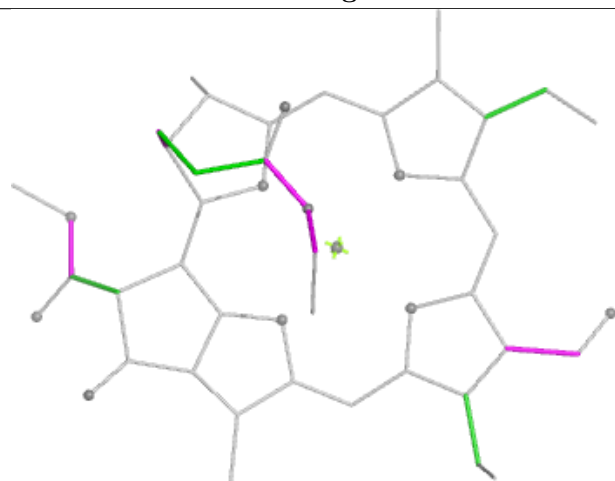
Ligand CHL g 605



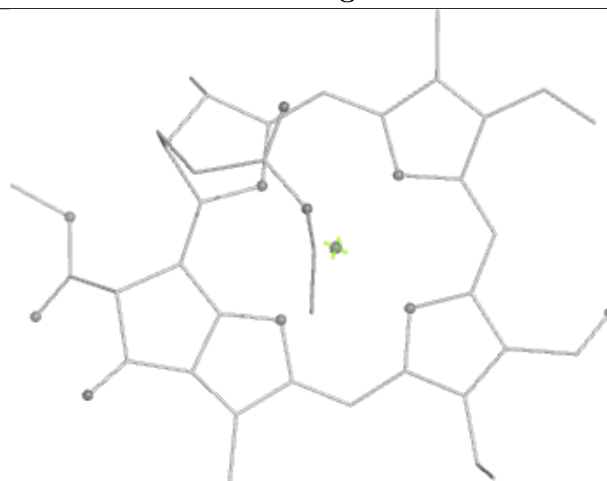
Bond lengths



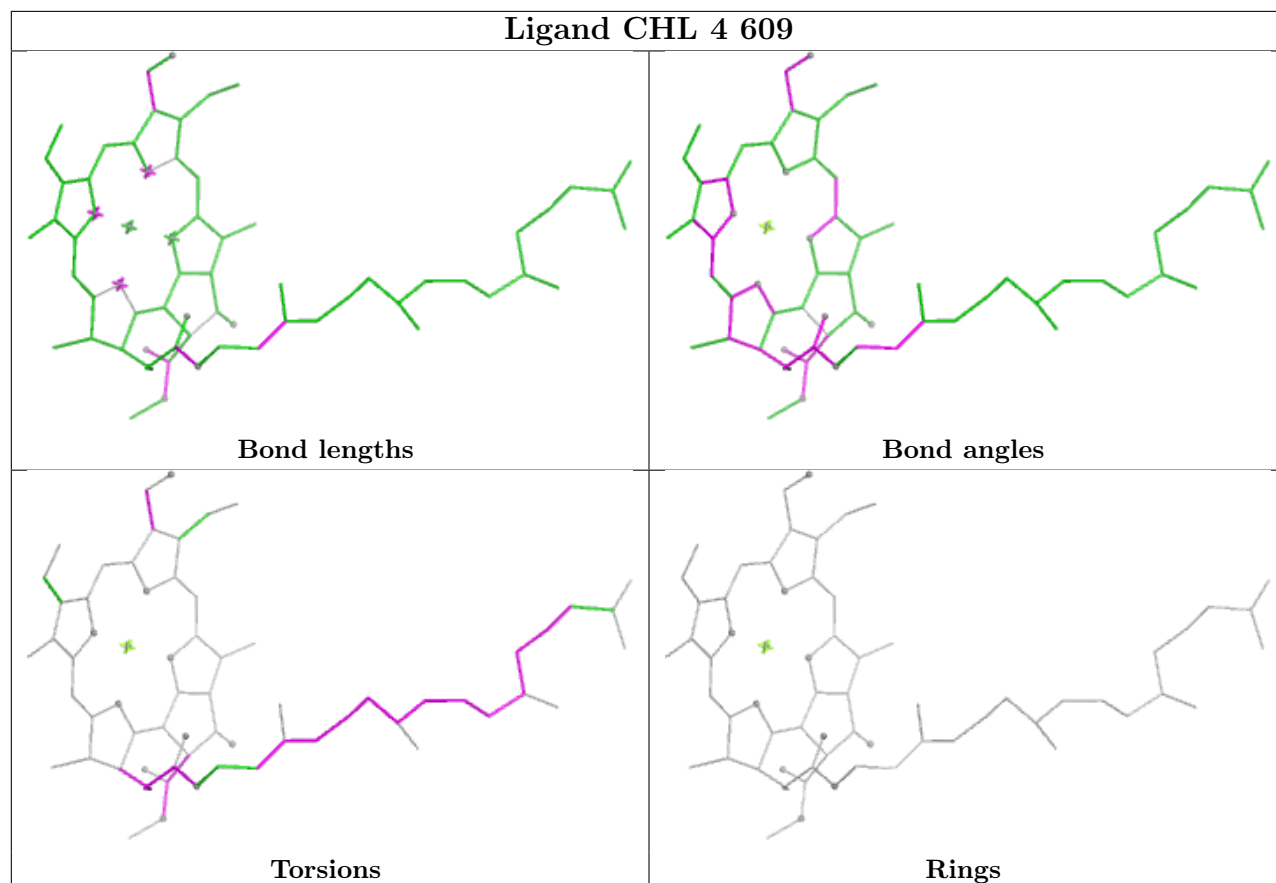
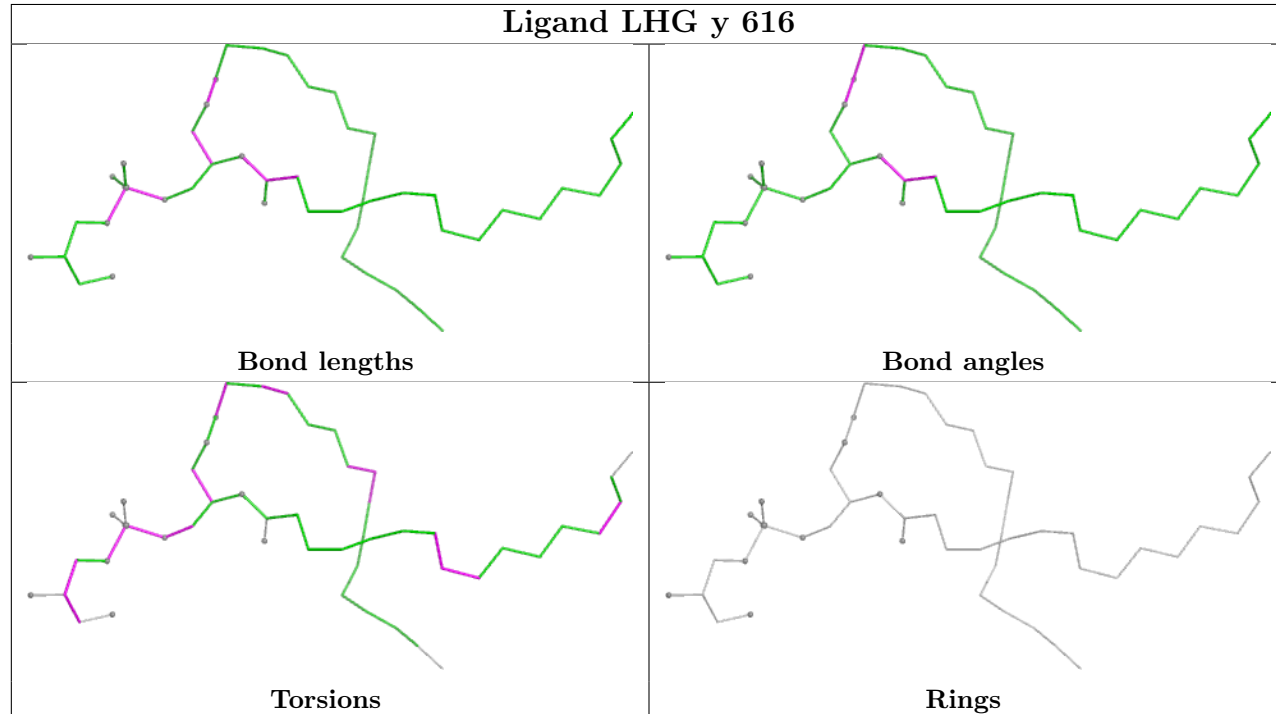
Bond angles

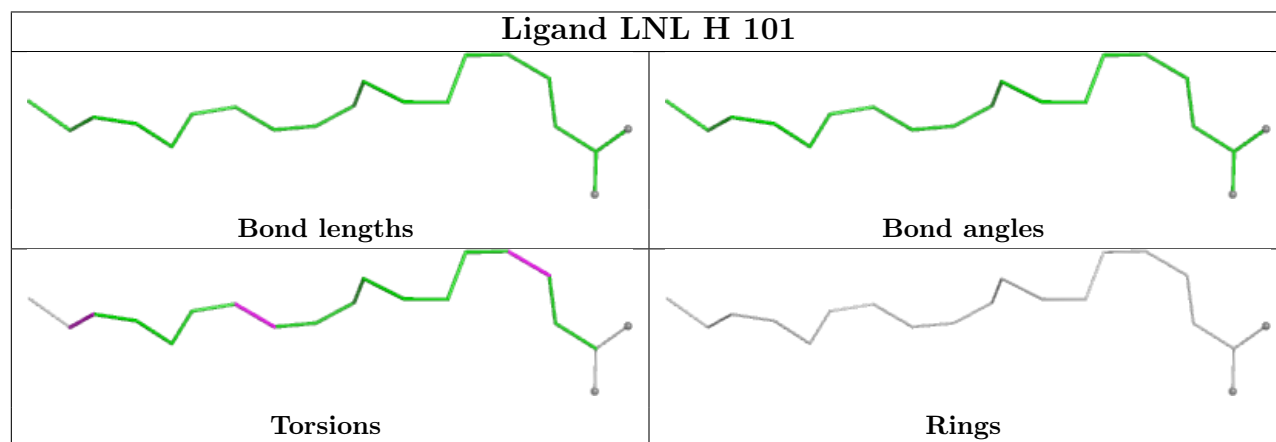
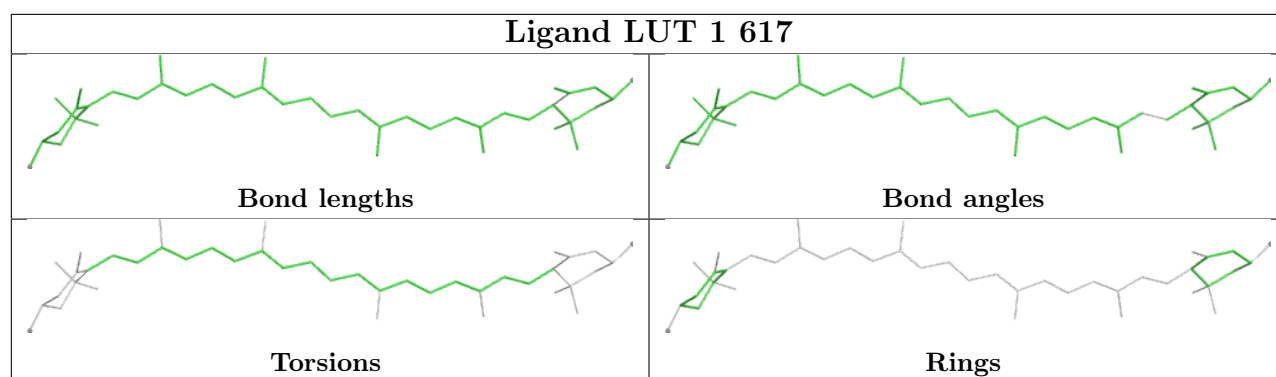


Torsions

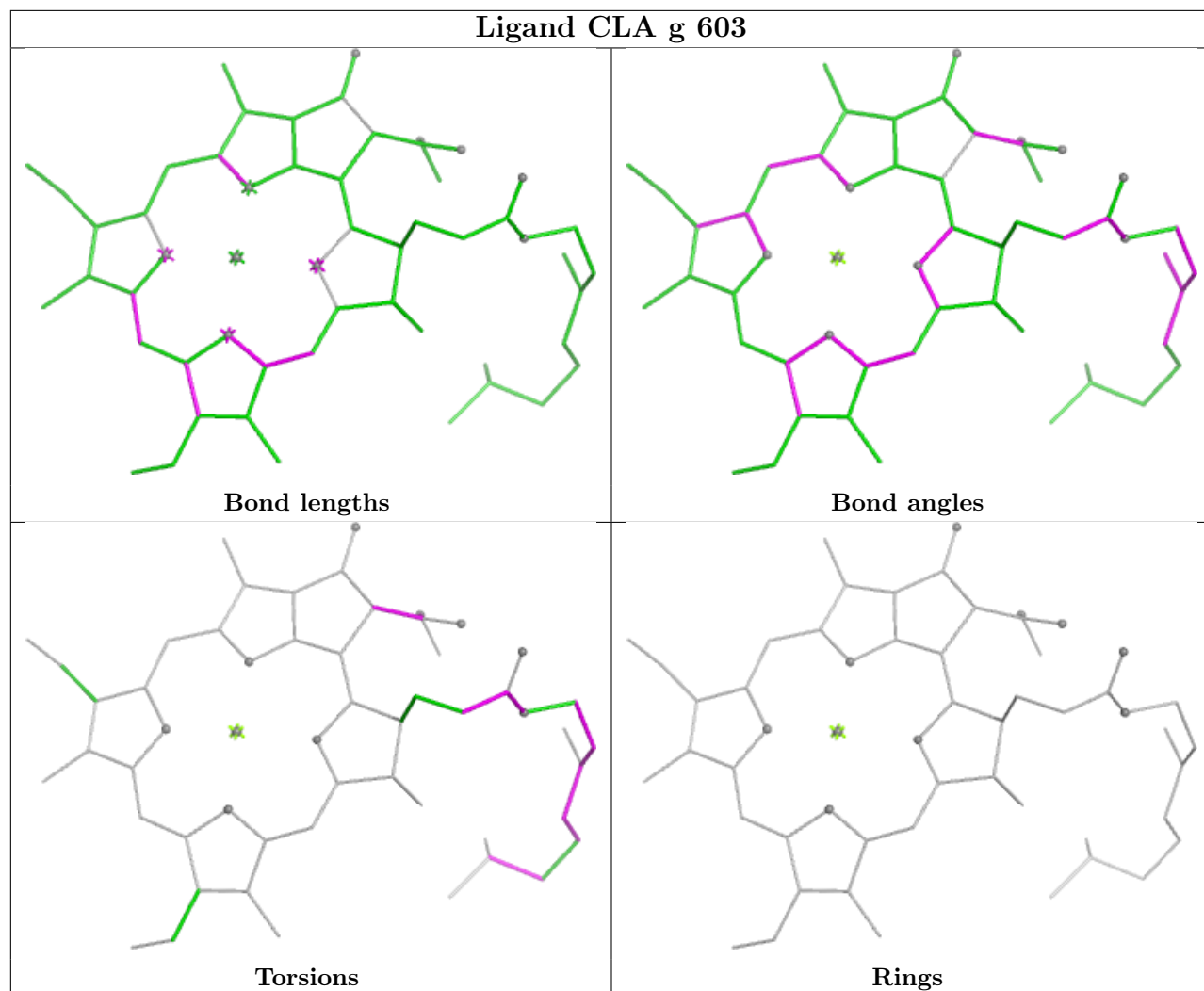


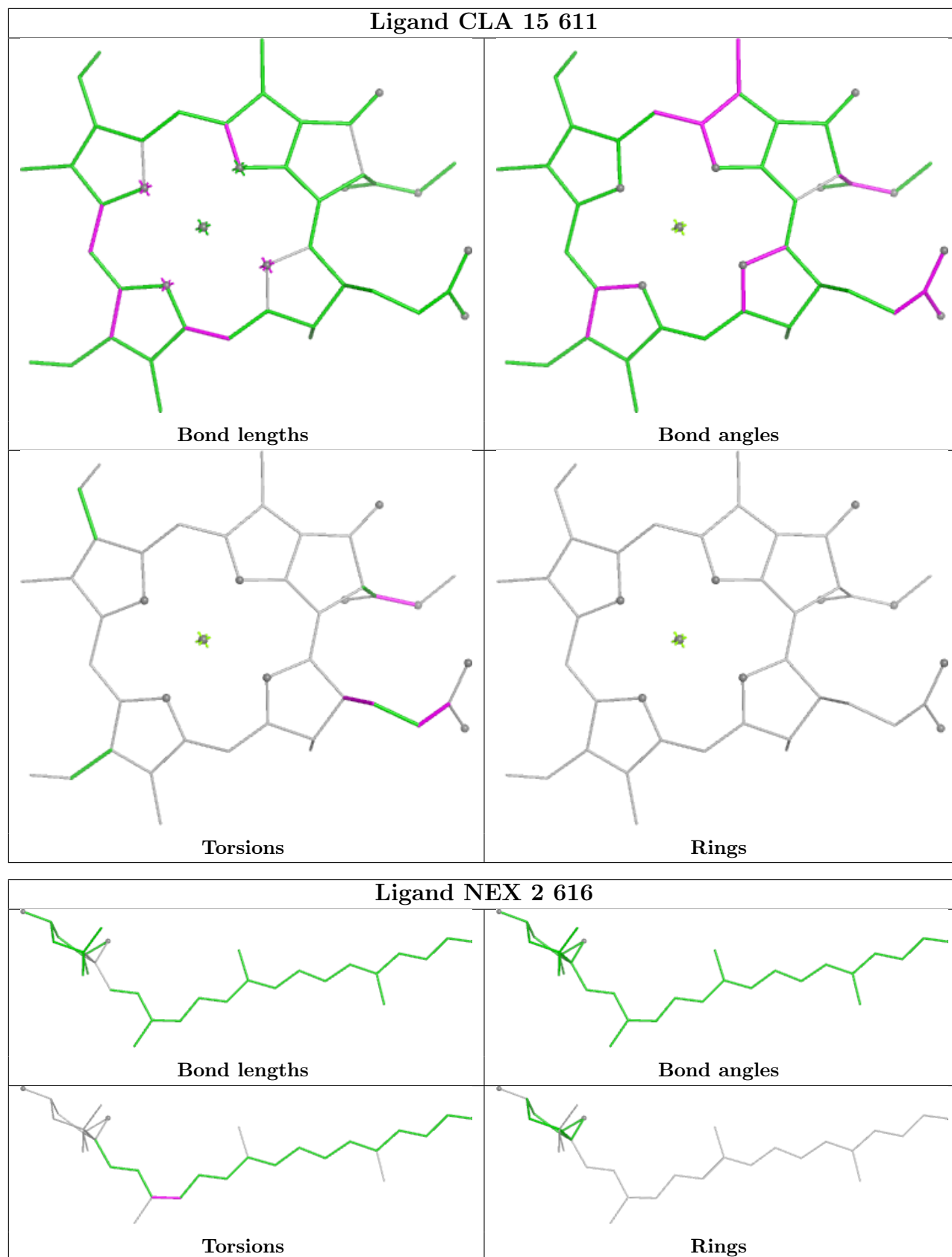
Rings

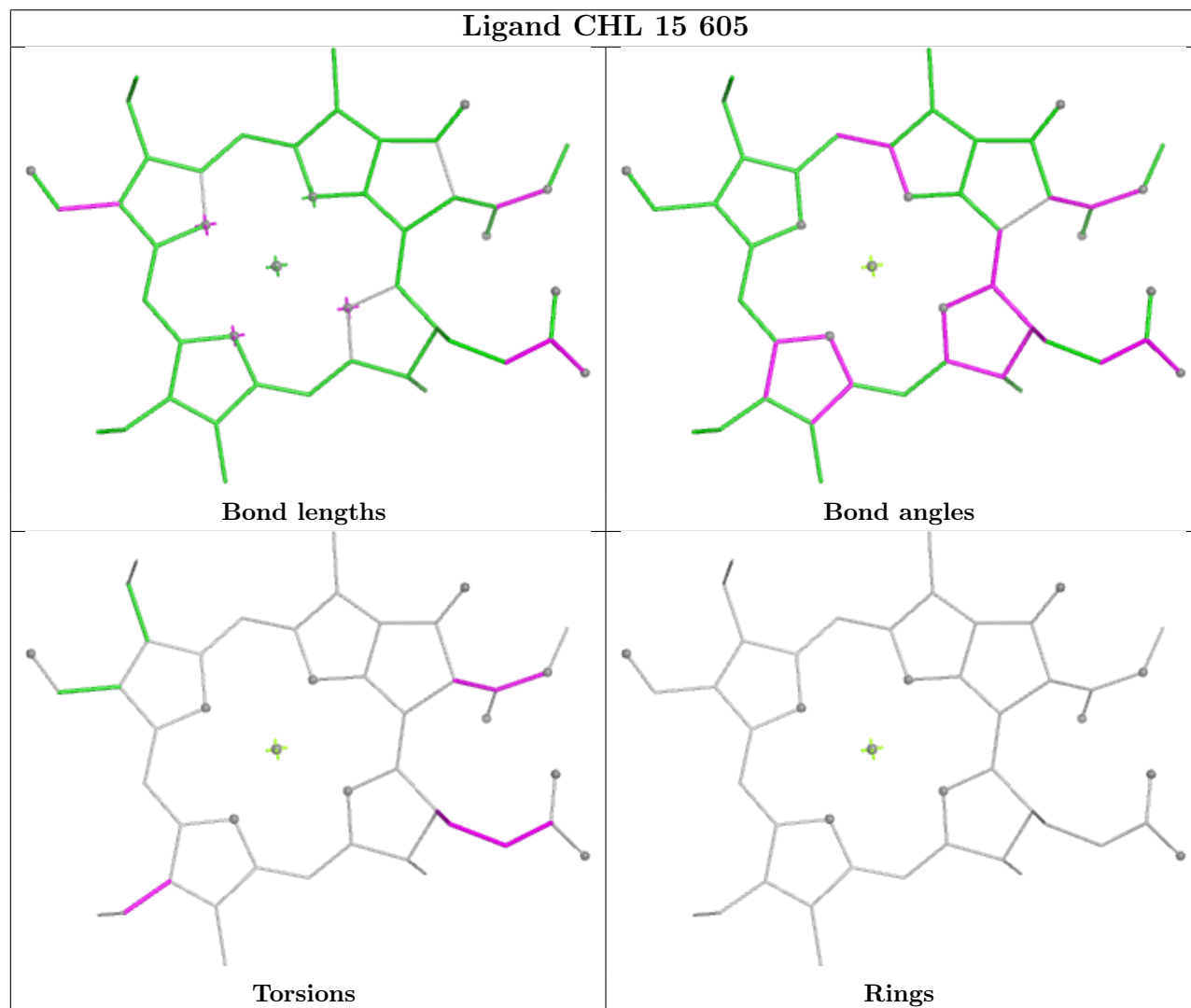
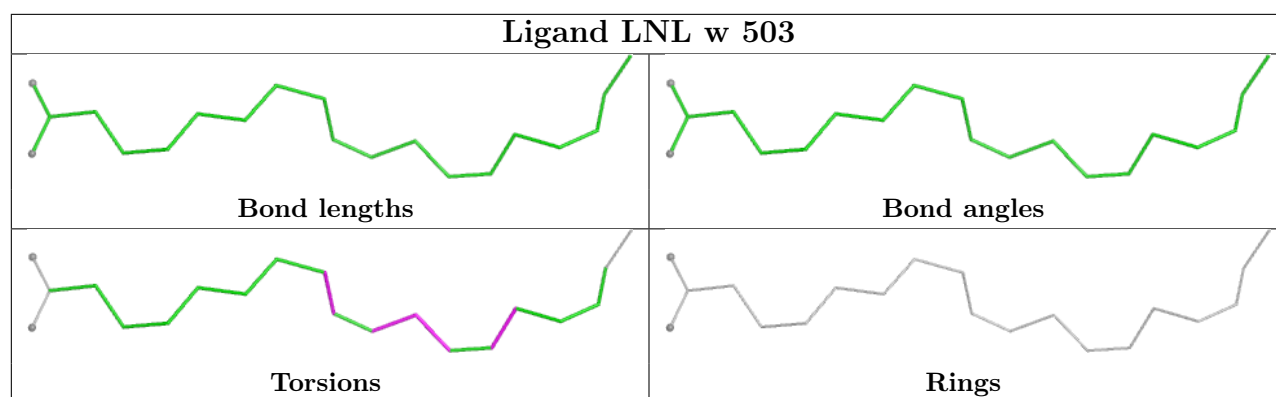
Ligand CHL 4 609**Ligand LHG y 616**

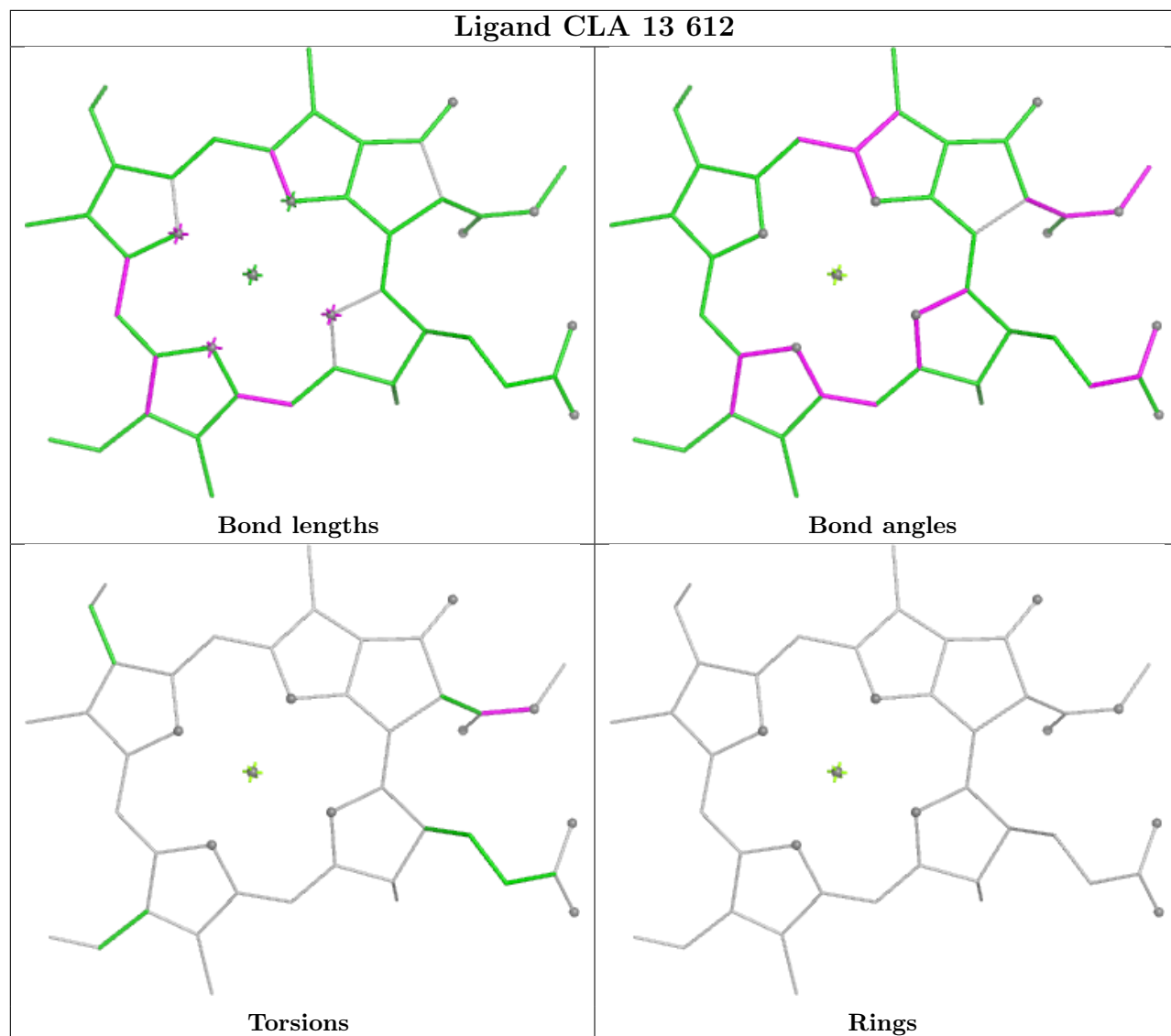


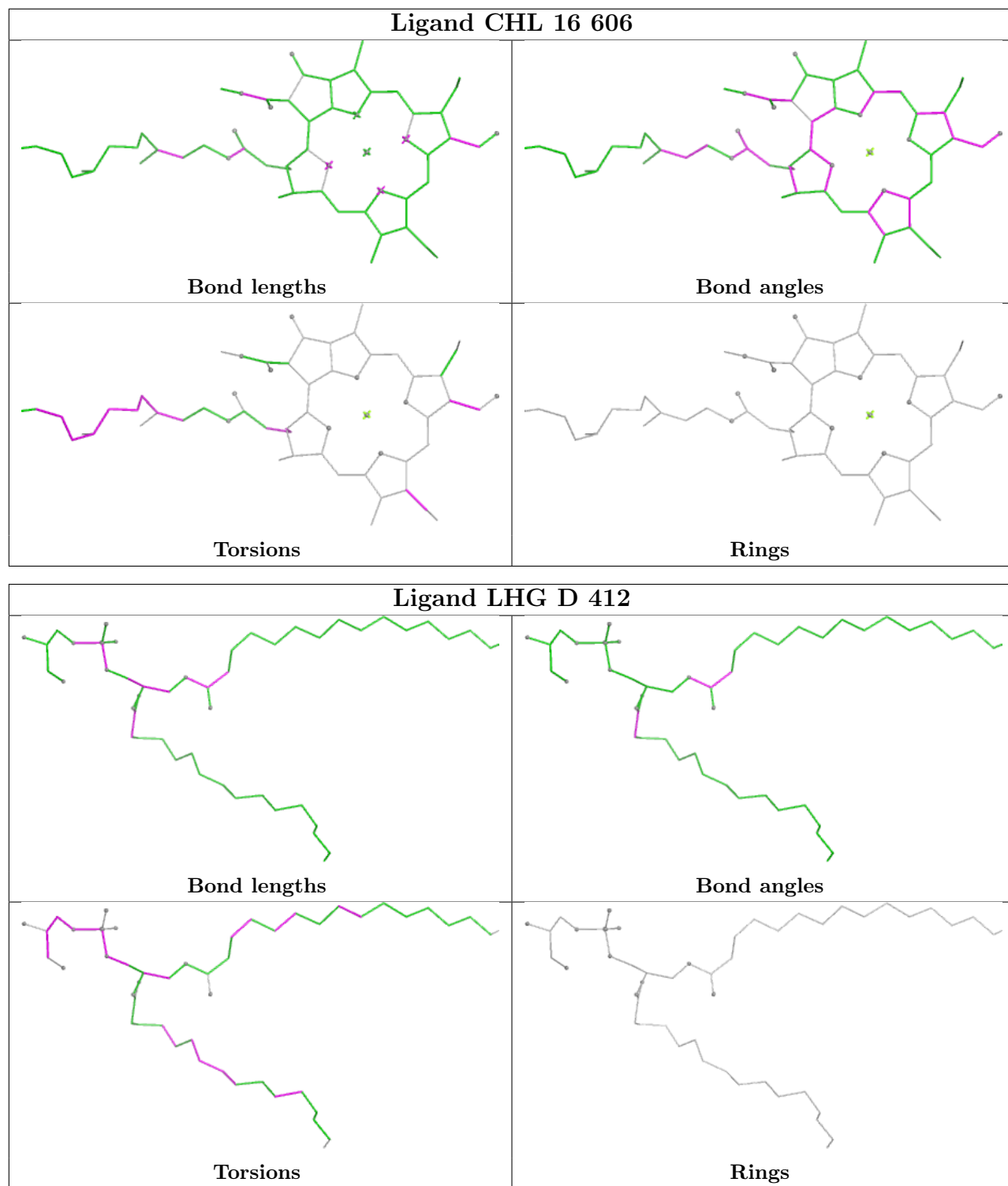
Ligand CLA g 603



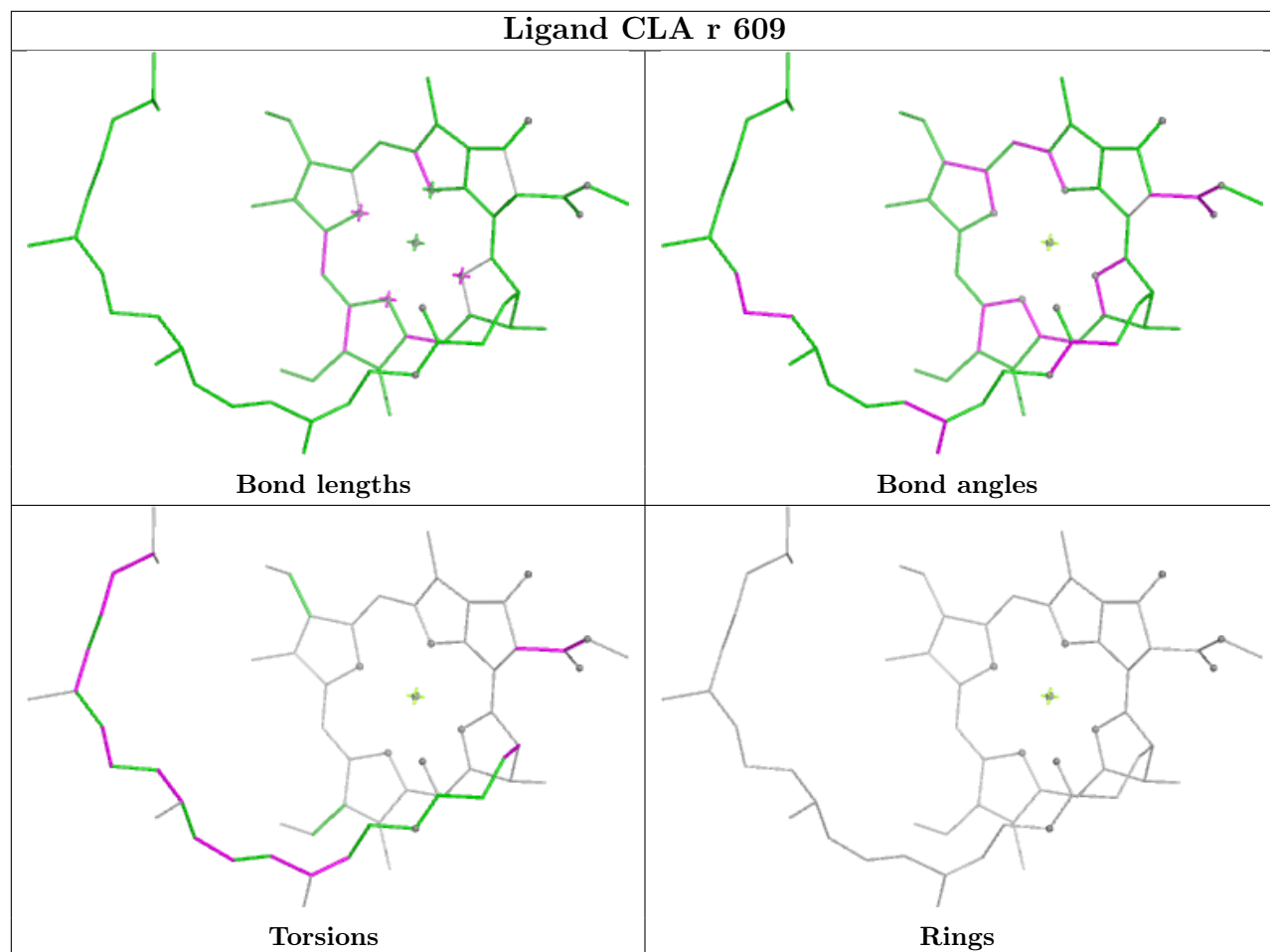


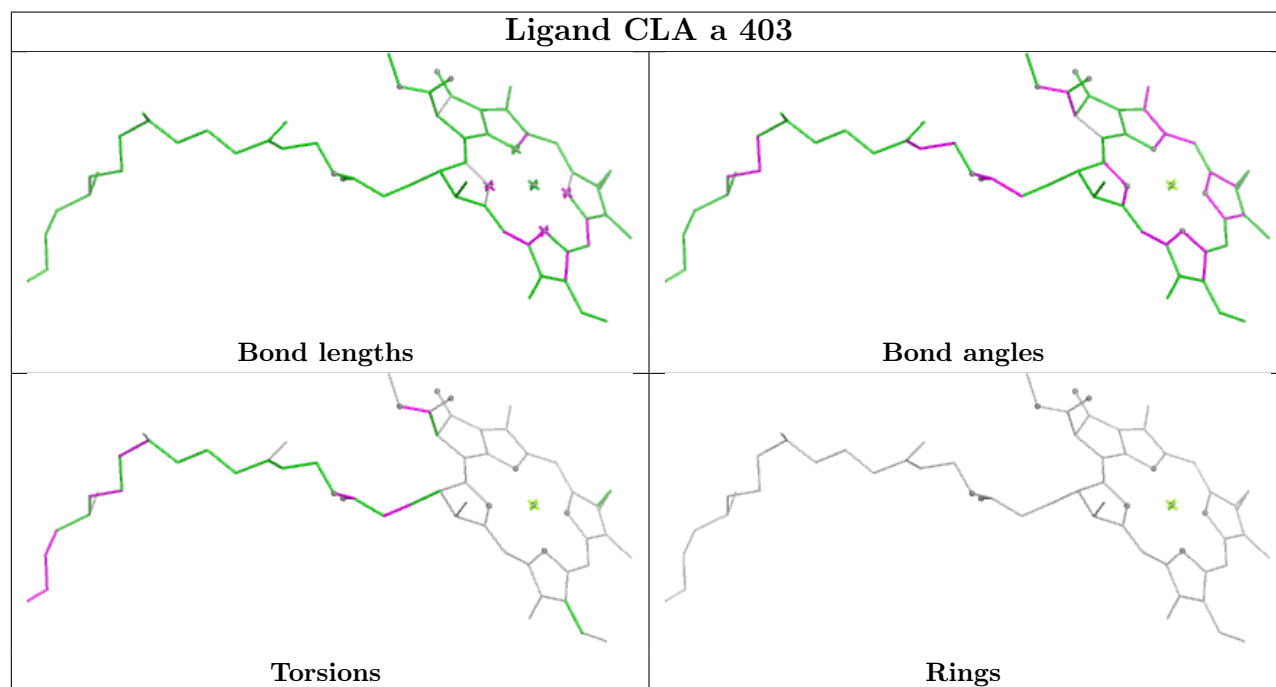
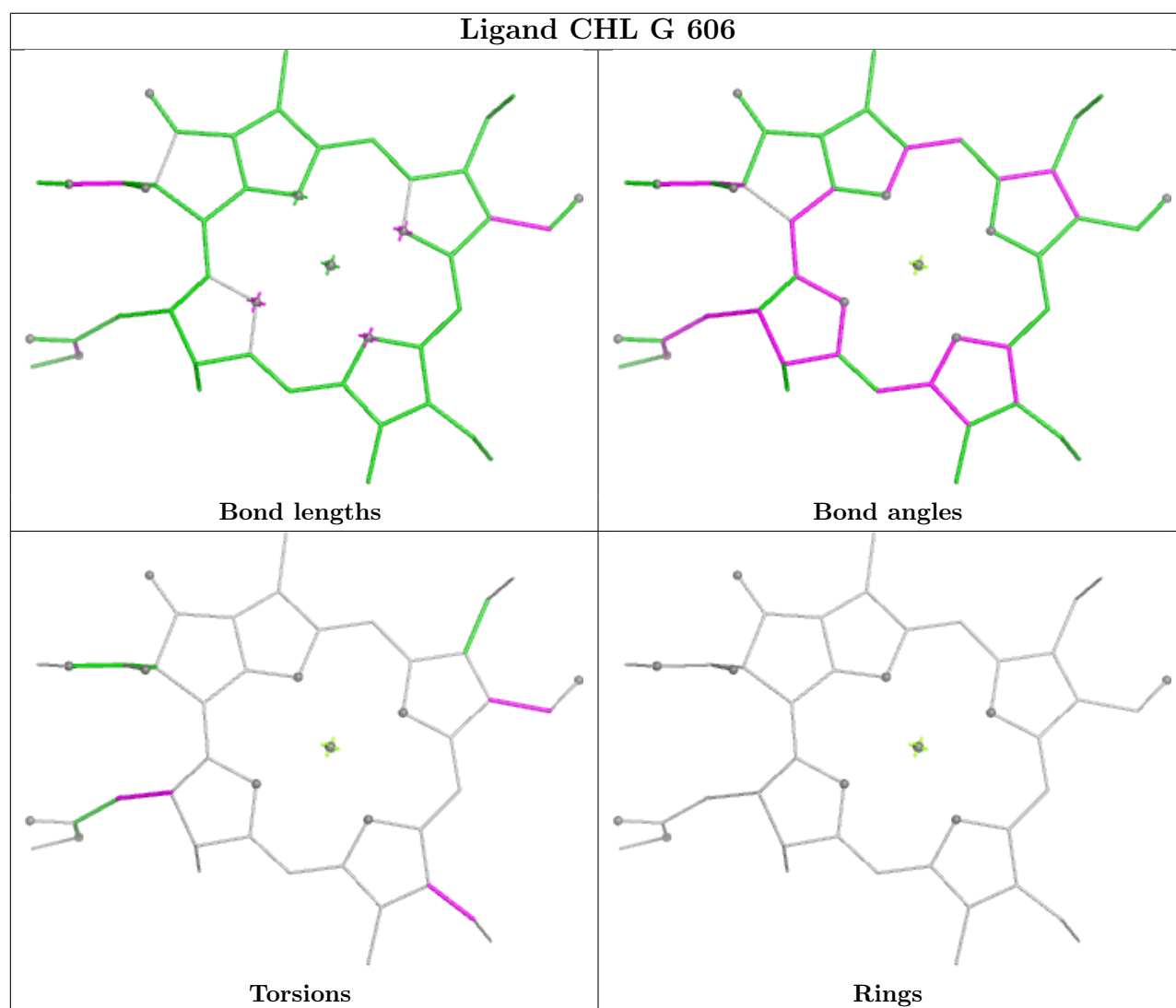


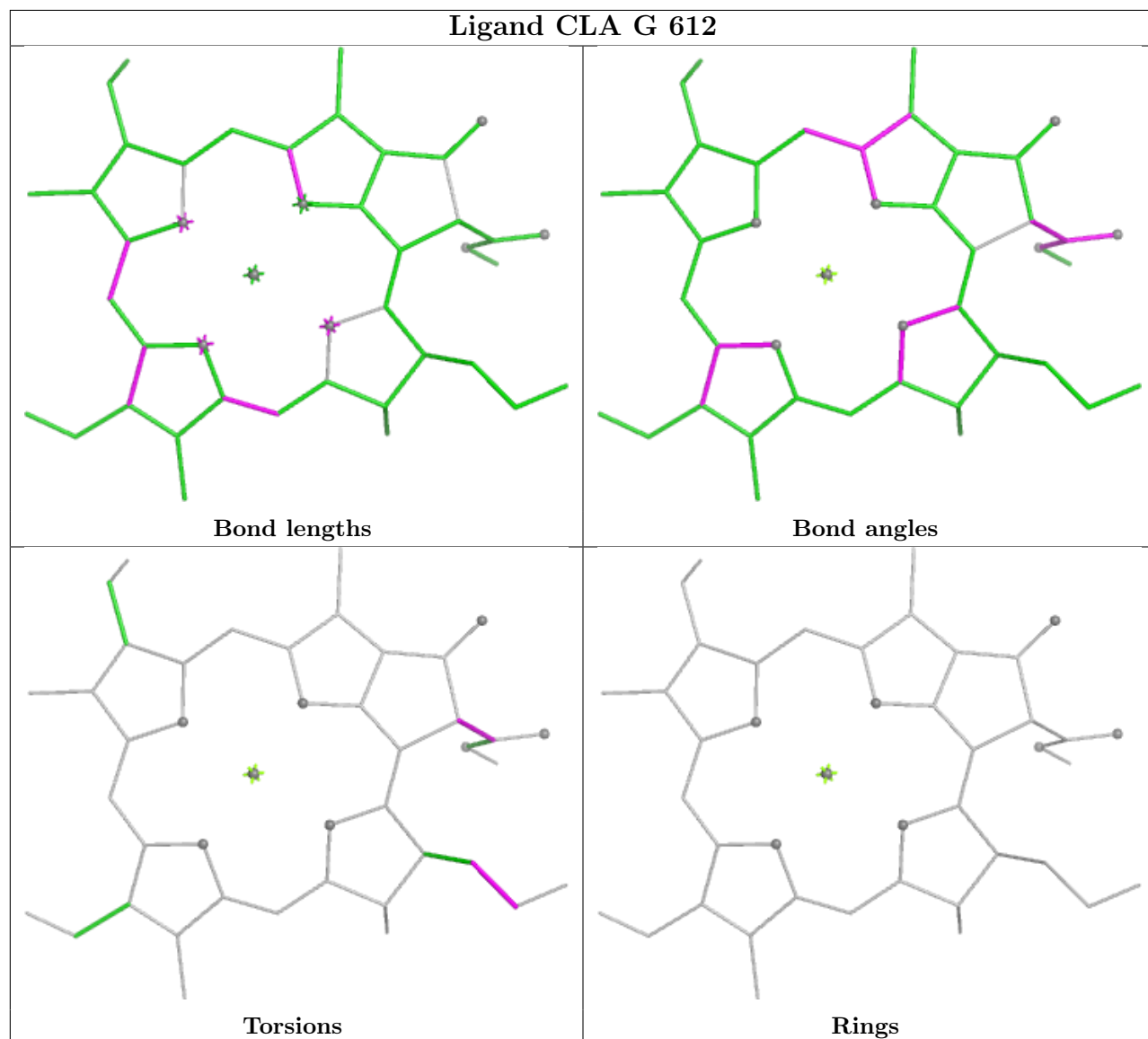
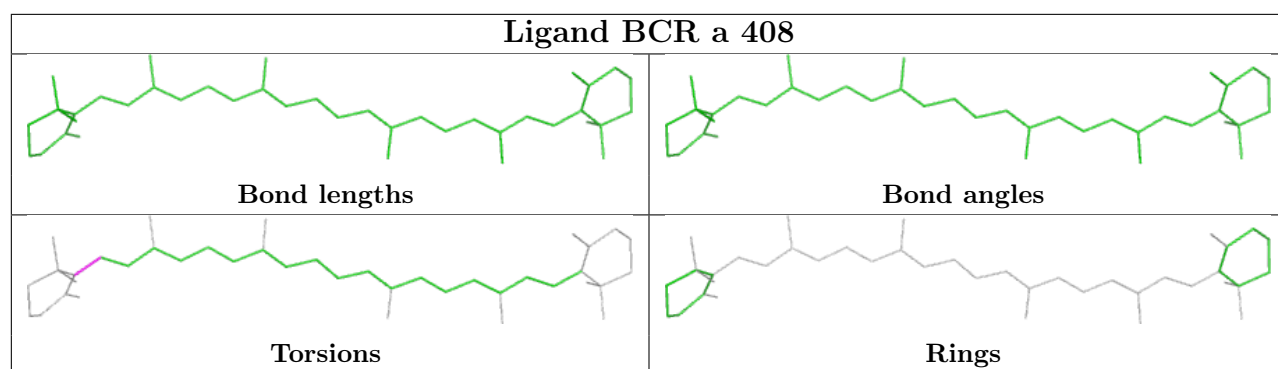


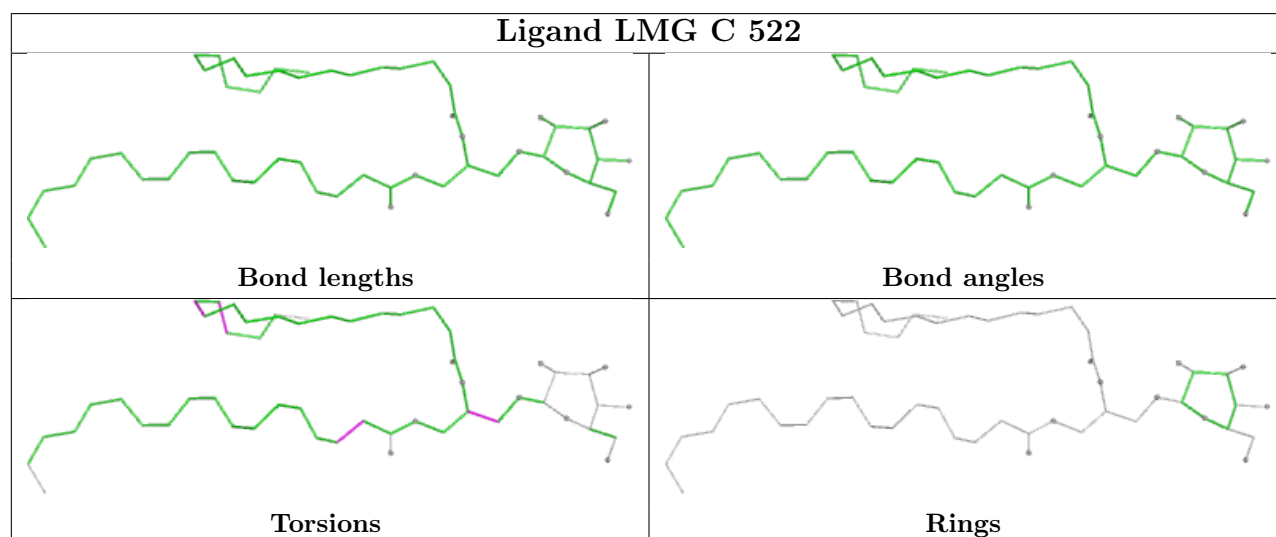
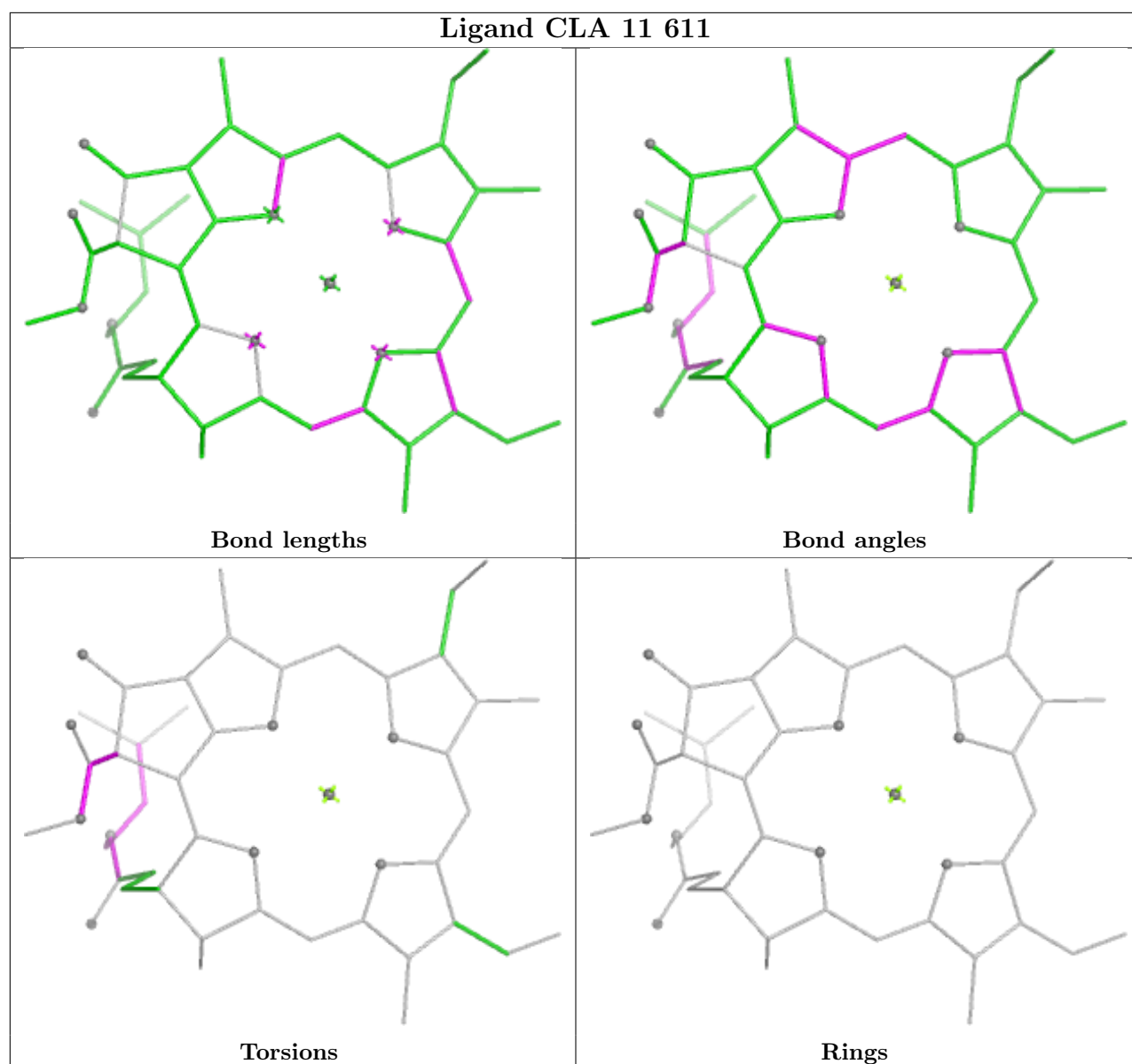


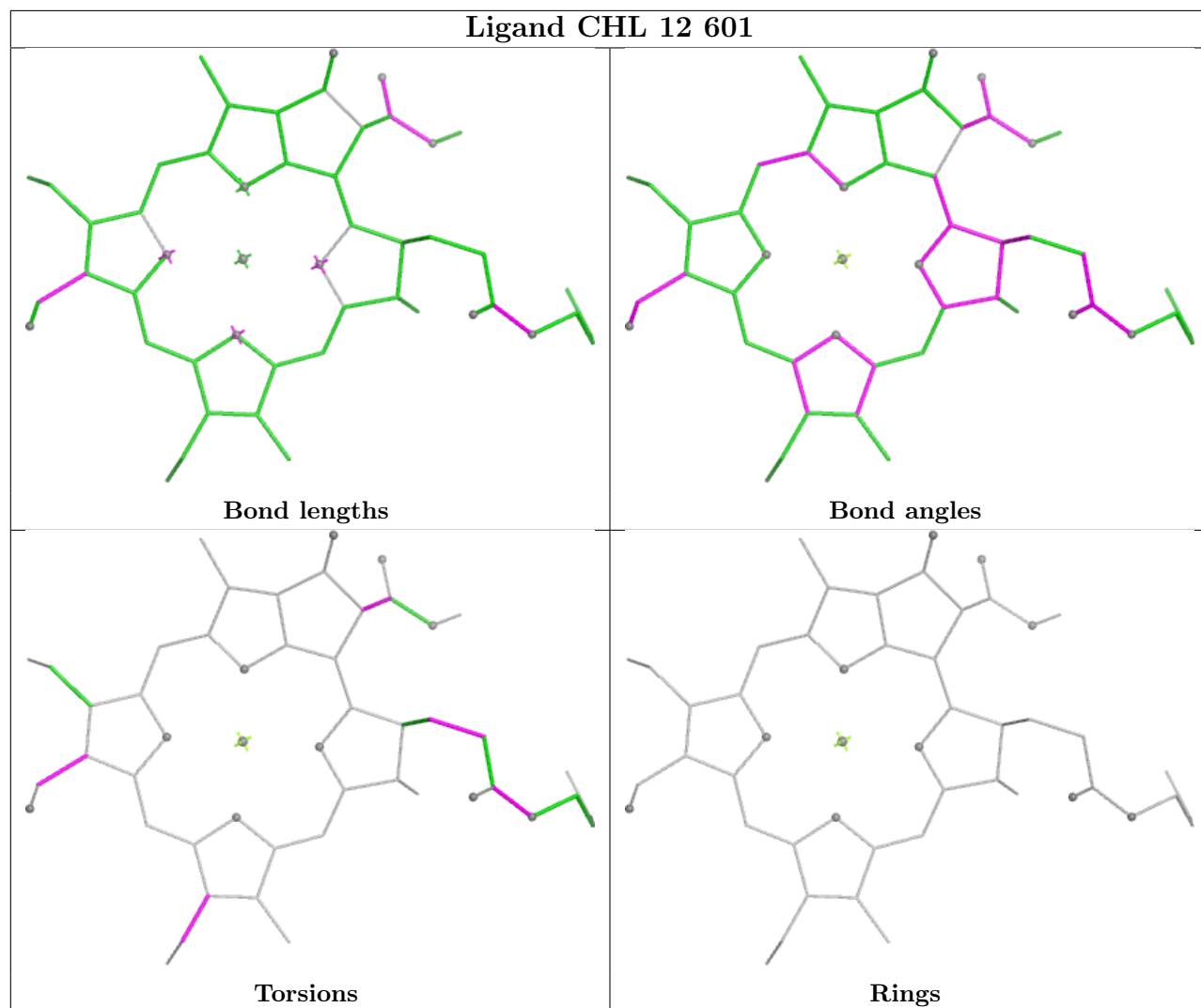
Ligand CLA r 609

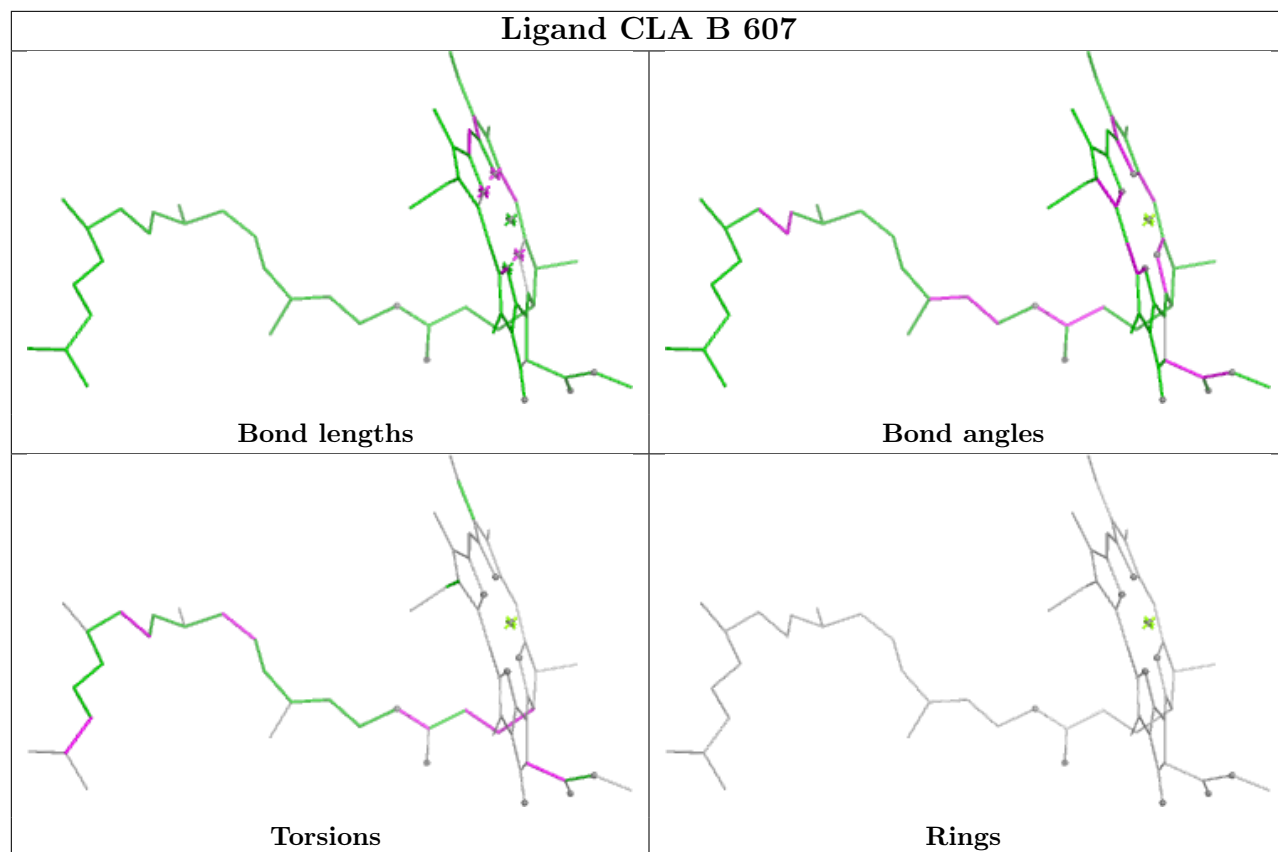




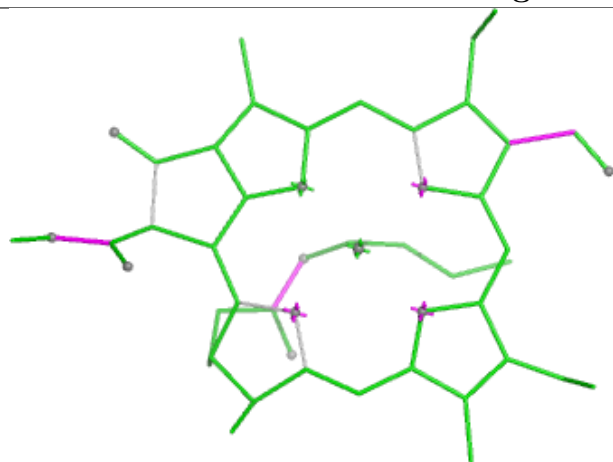




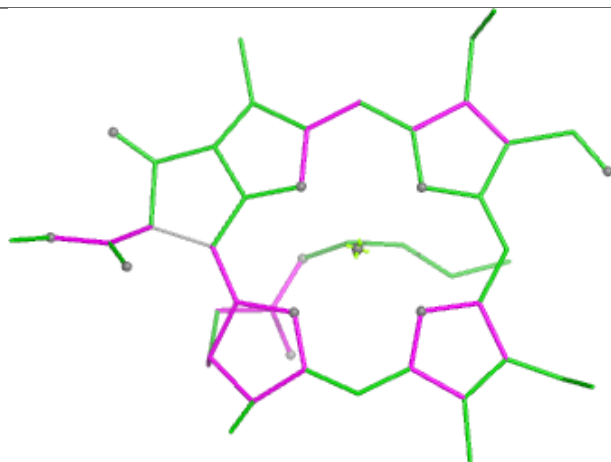




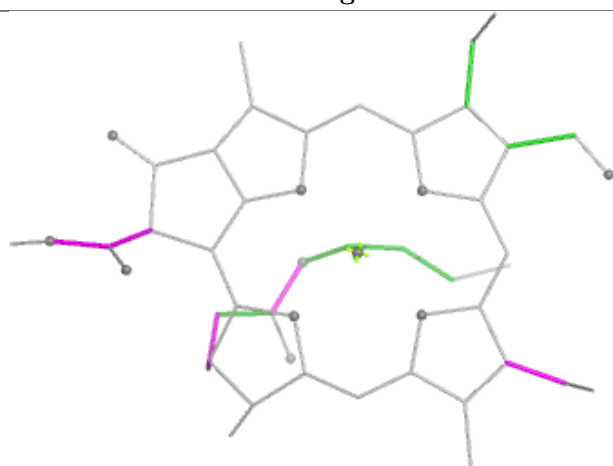
Ligand CHL G 607



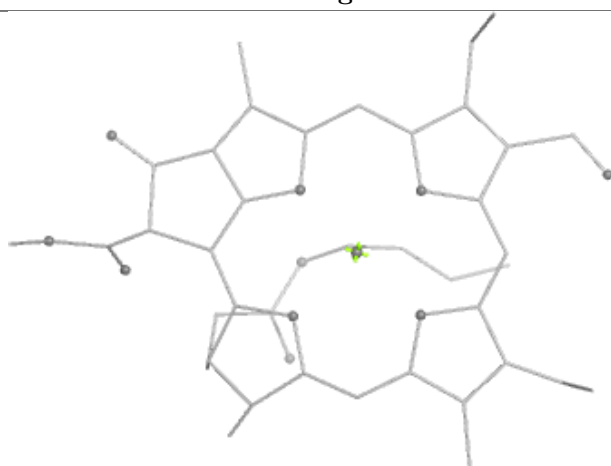
Bond lengths



Bond angles

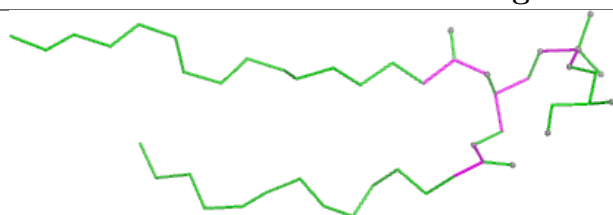


Torsions

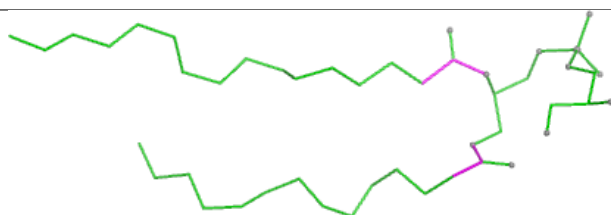


Rings

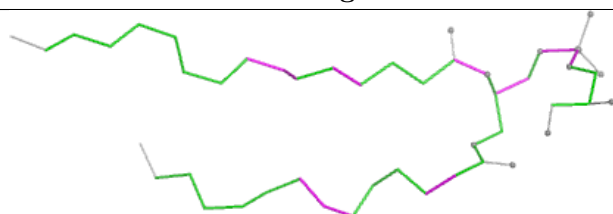
Ligand LHG R 619



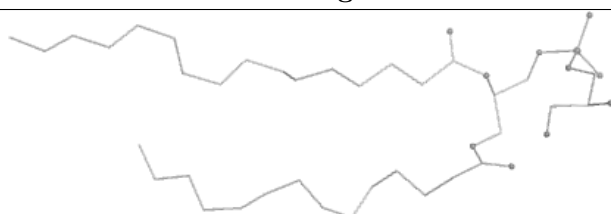
Bond lengths



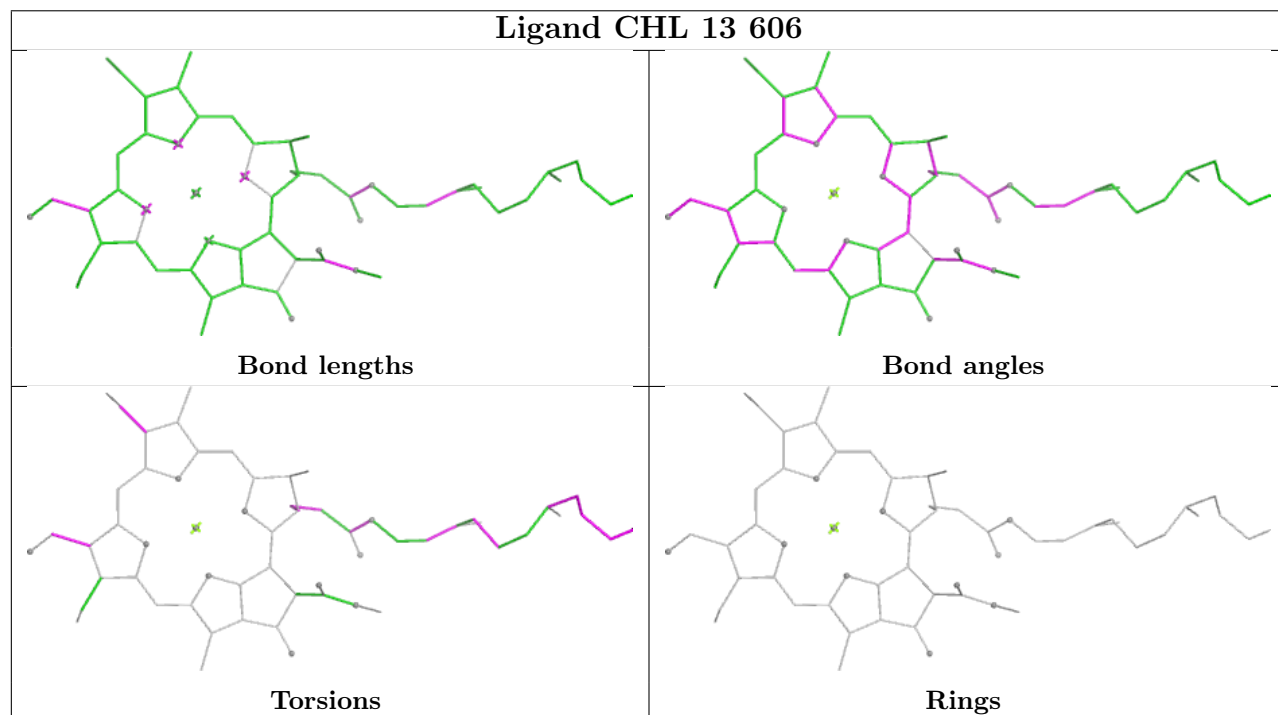
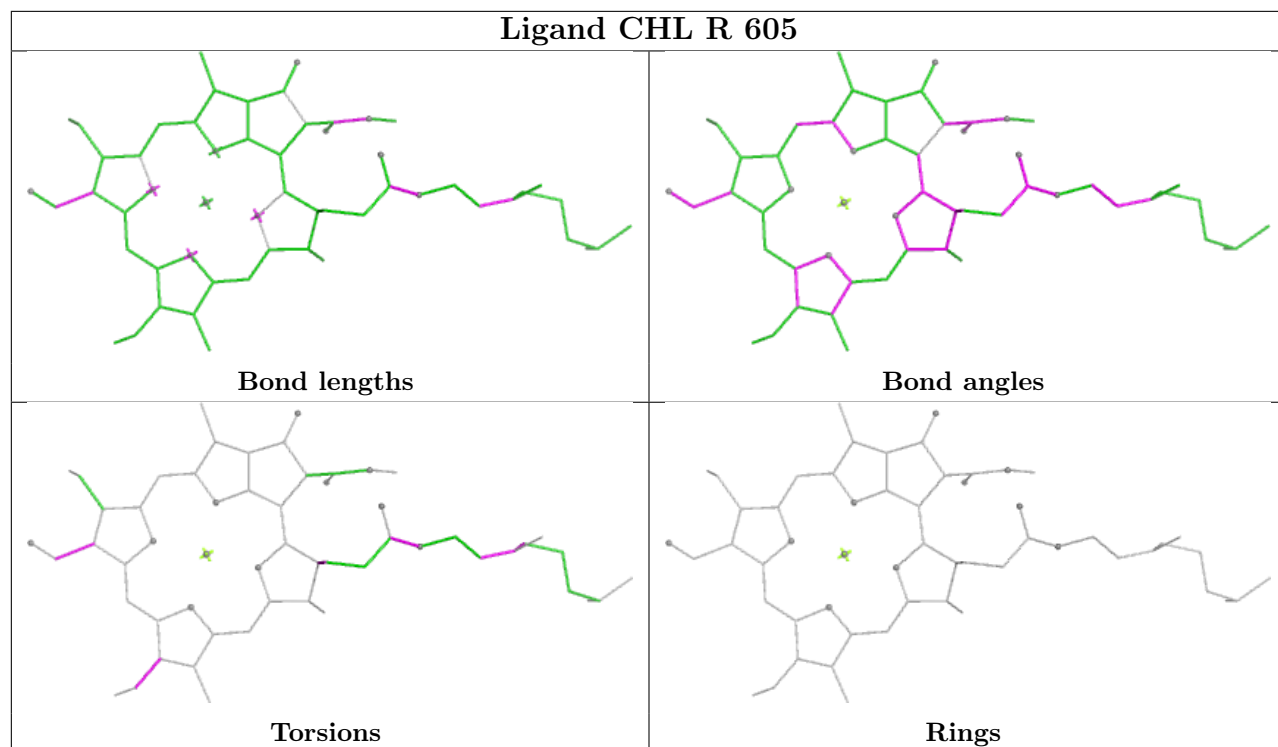
Bond angles



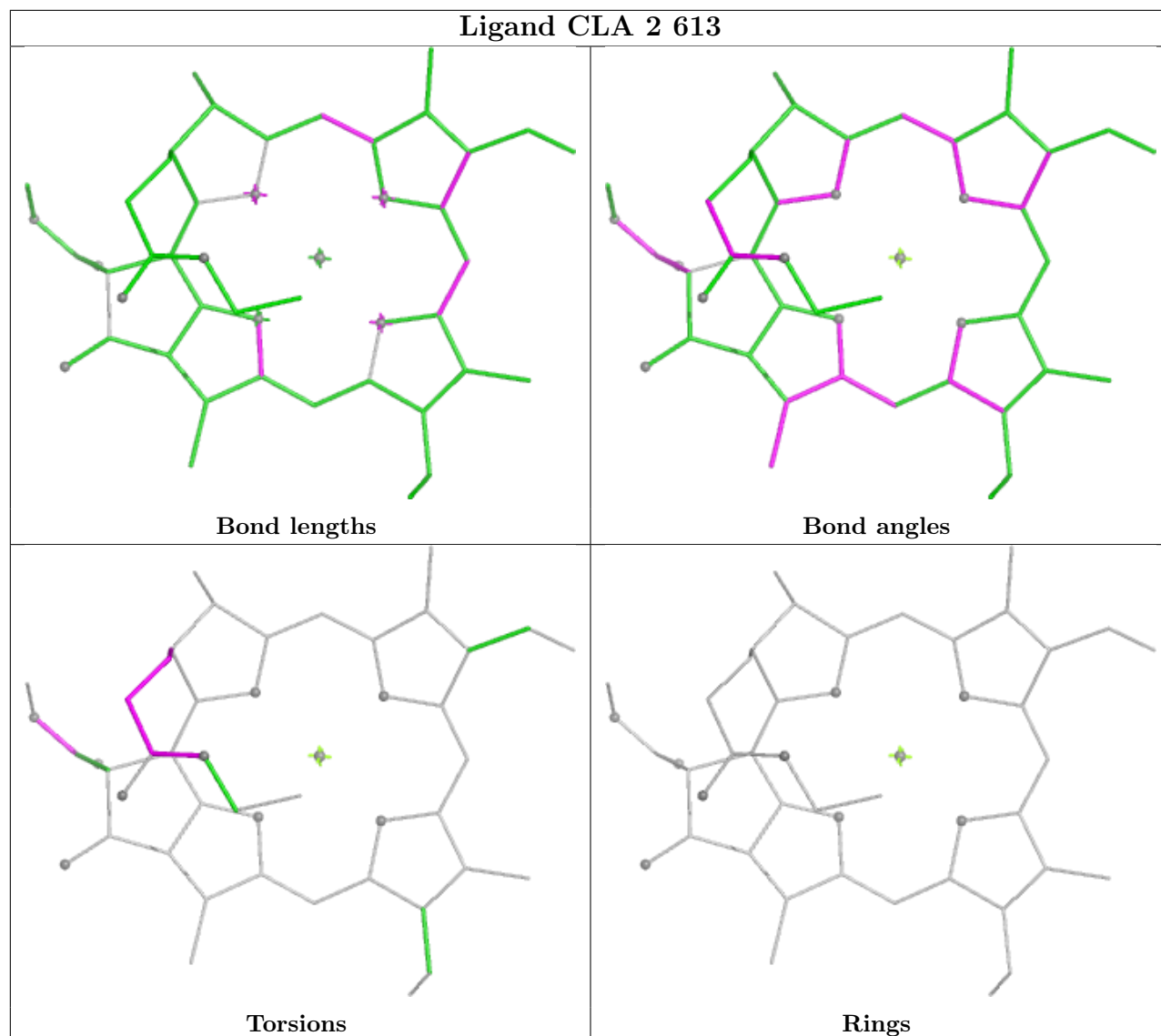
Torsions



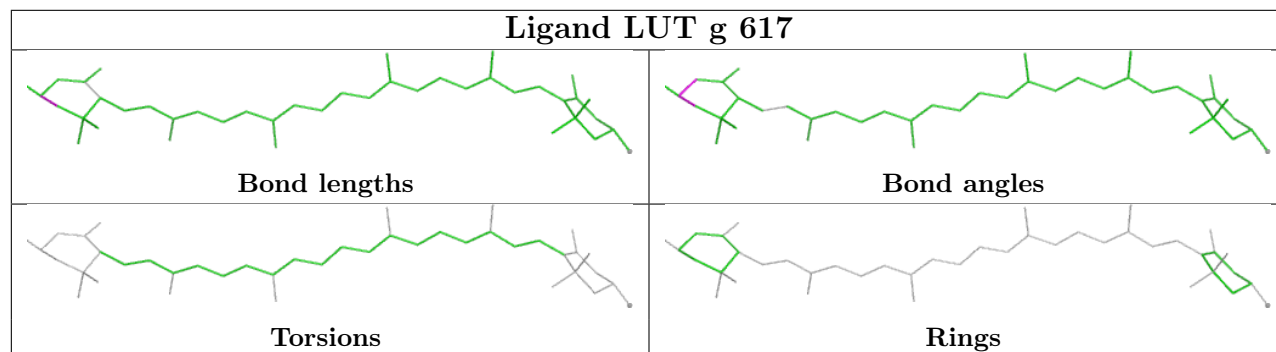
Rings



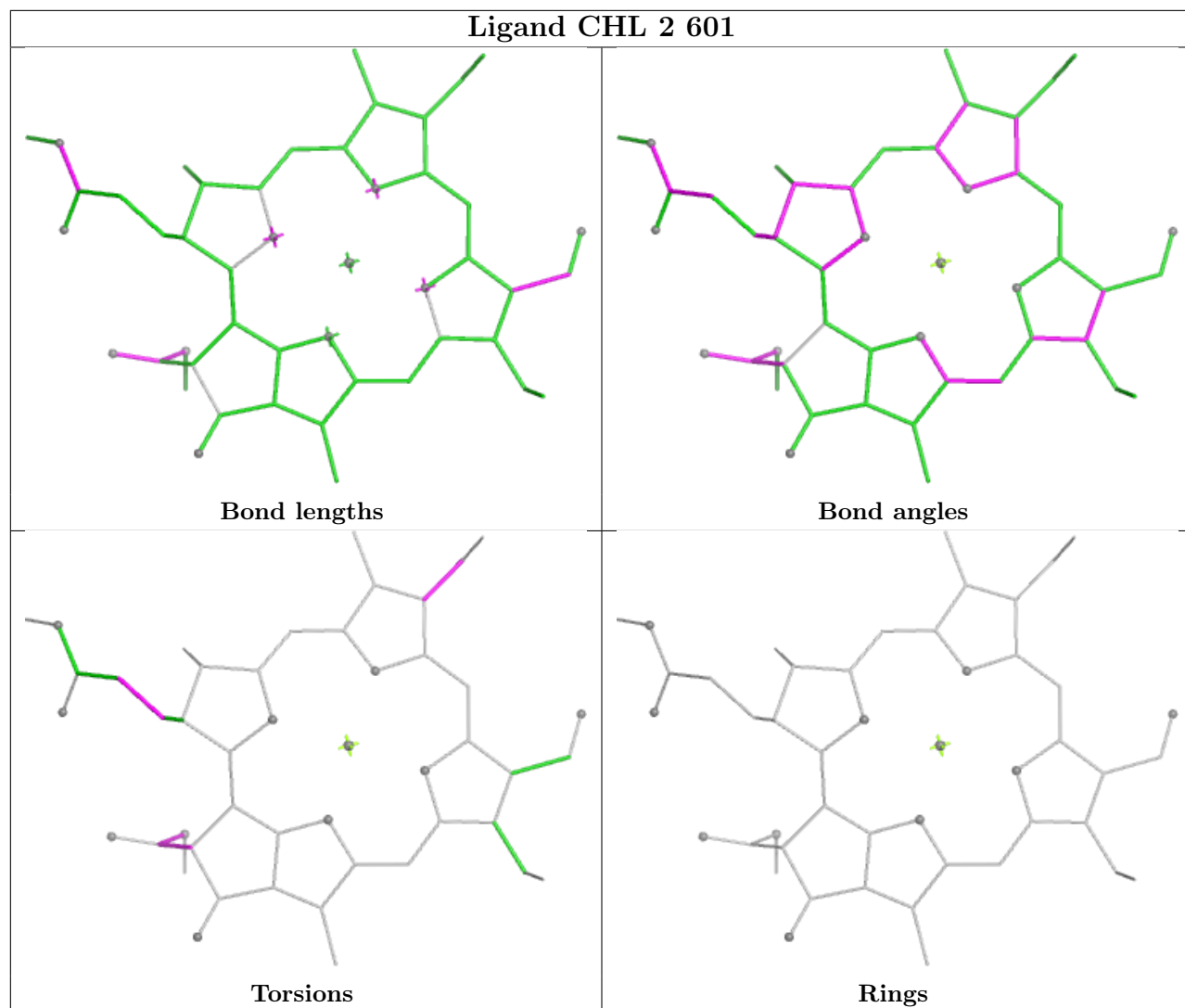
Ligand CLA 2 613



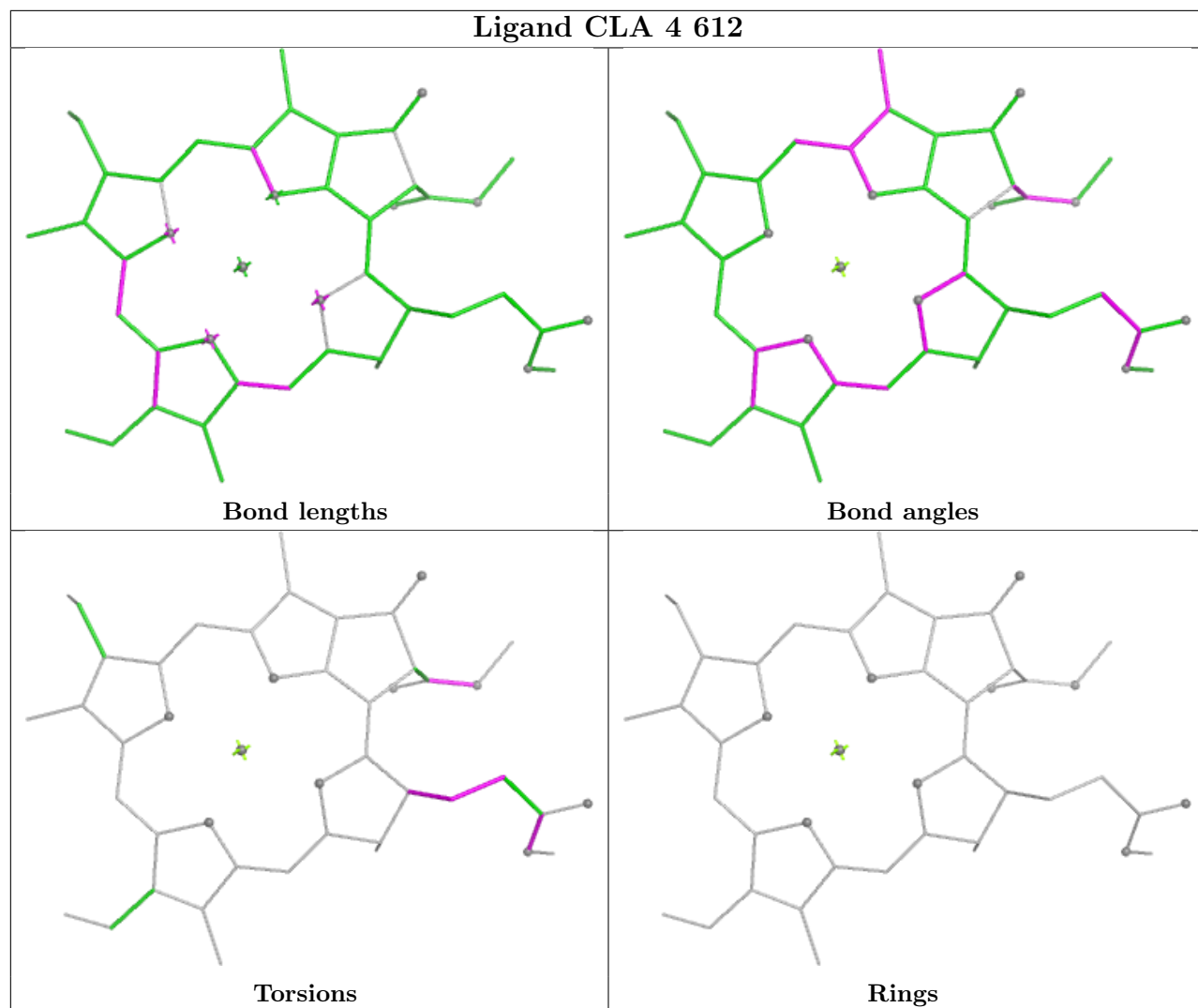
Ligand LUT g 617



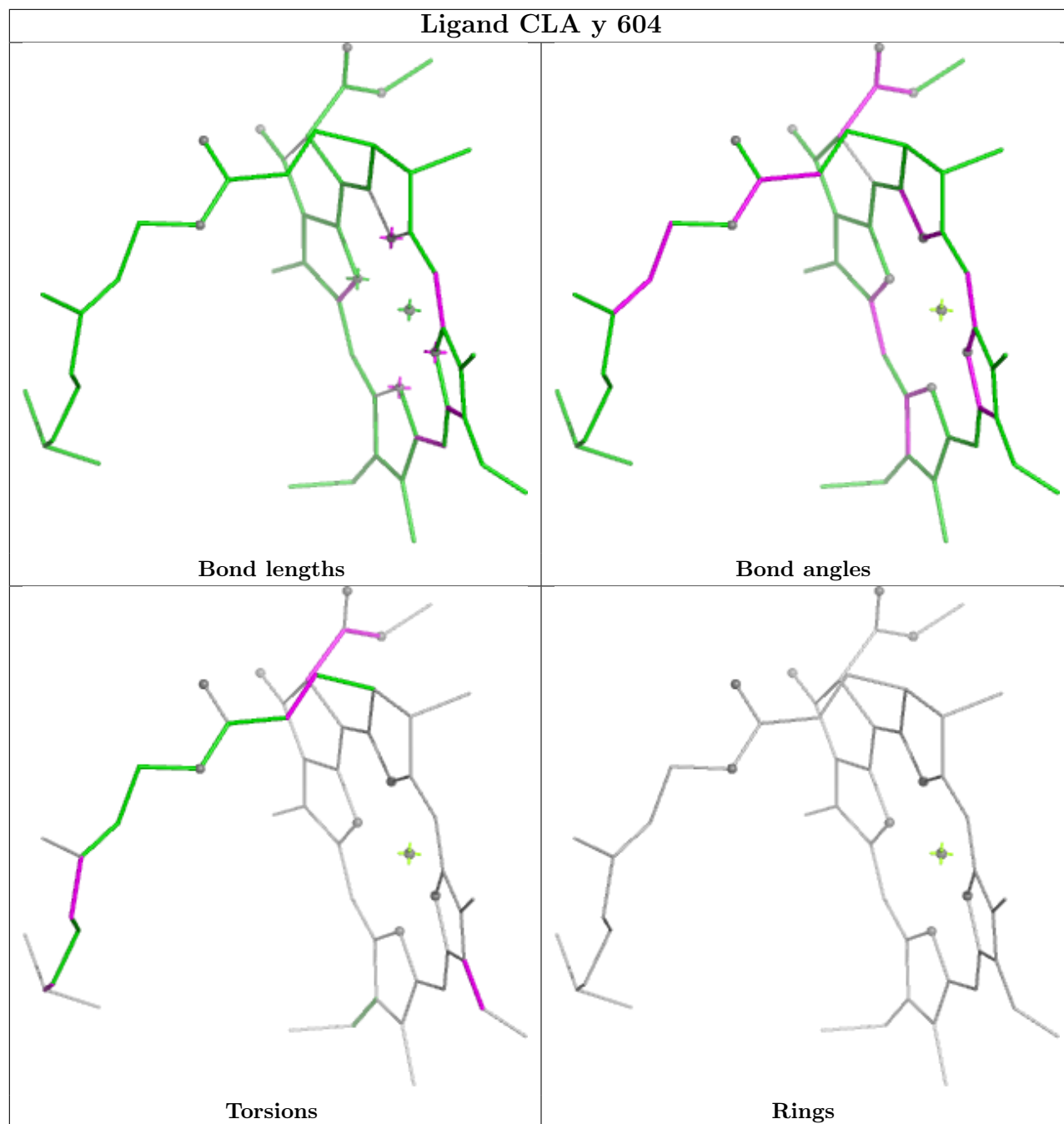
Ligand CHL 2 601



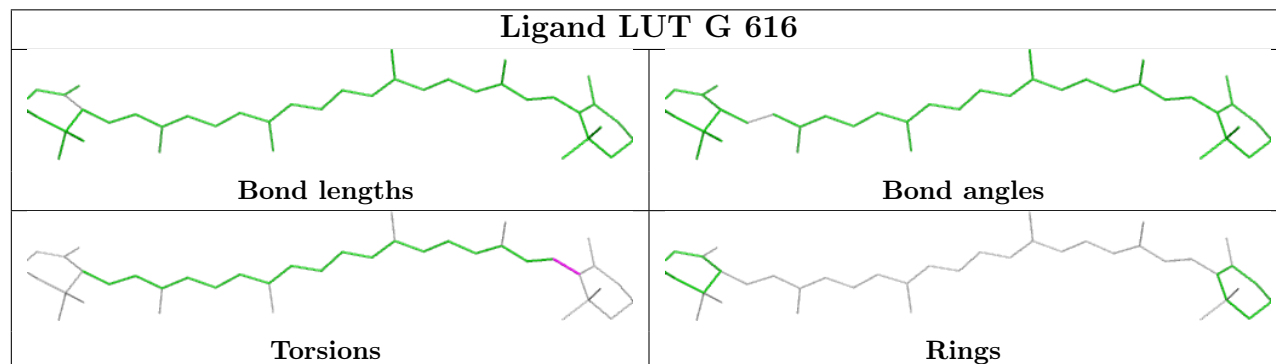
Ligand CLA 4 612



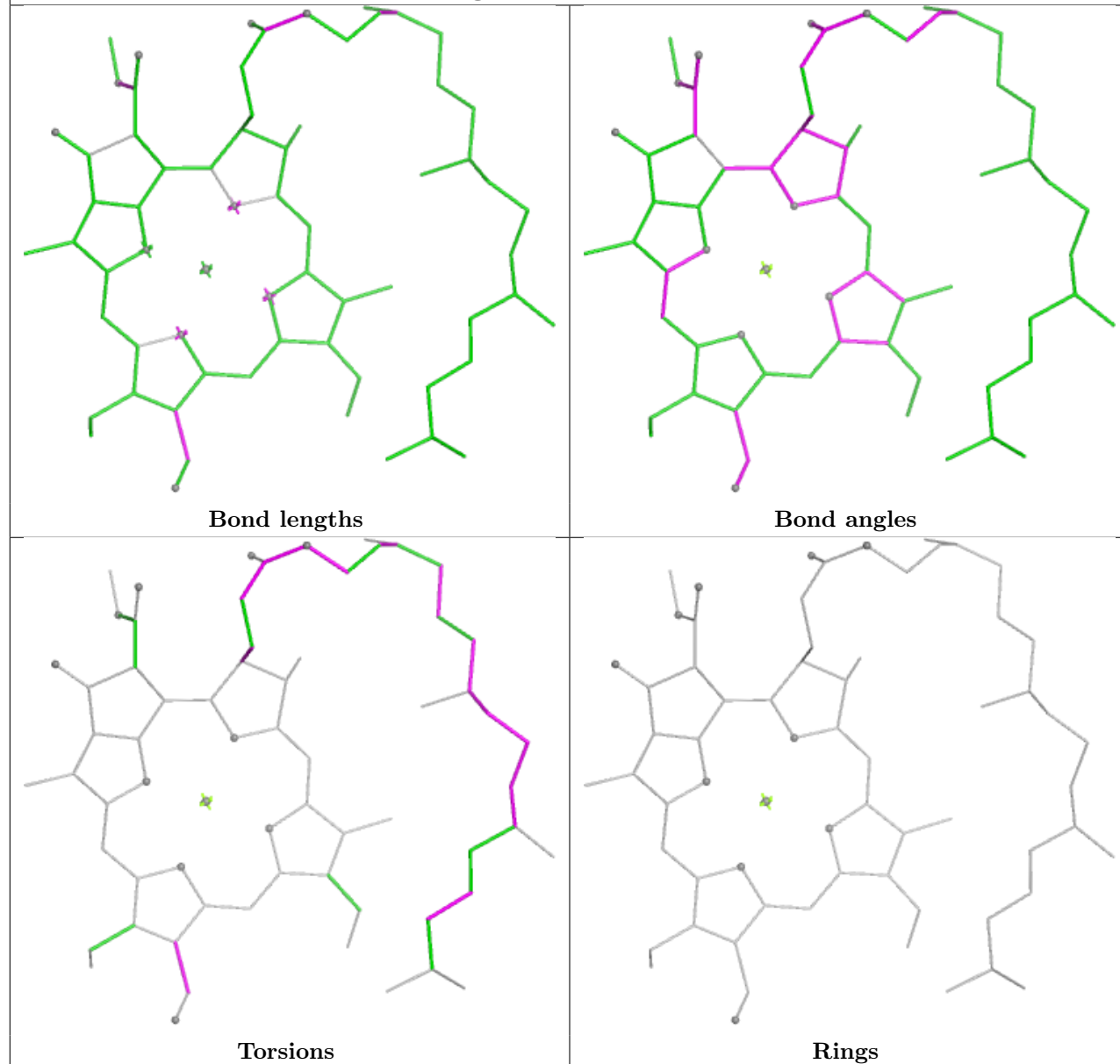
Ligand CLA y 604



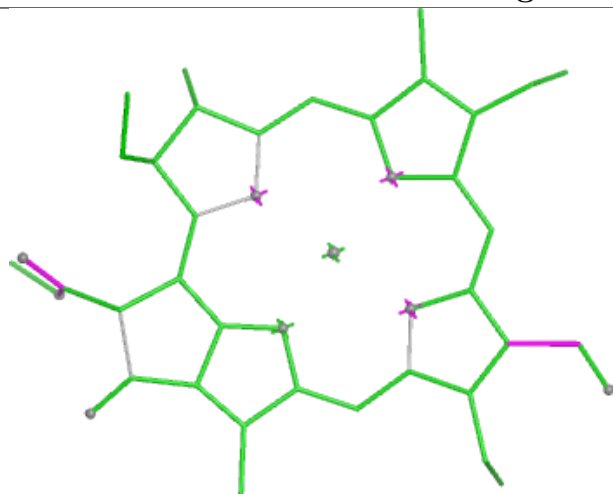
Ligand LUT G 616



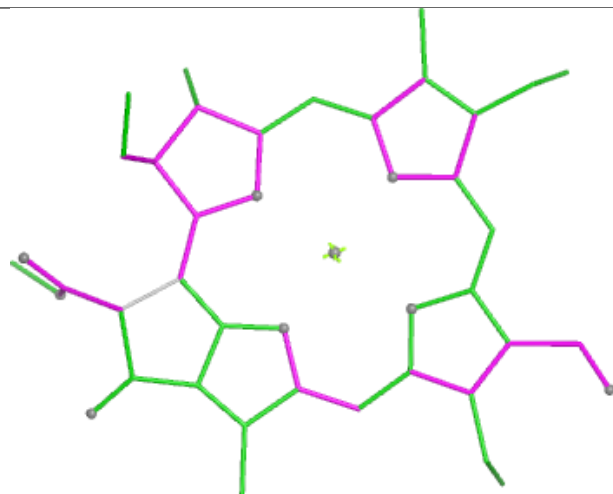
Ligand CHL 3 607



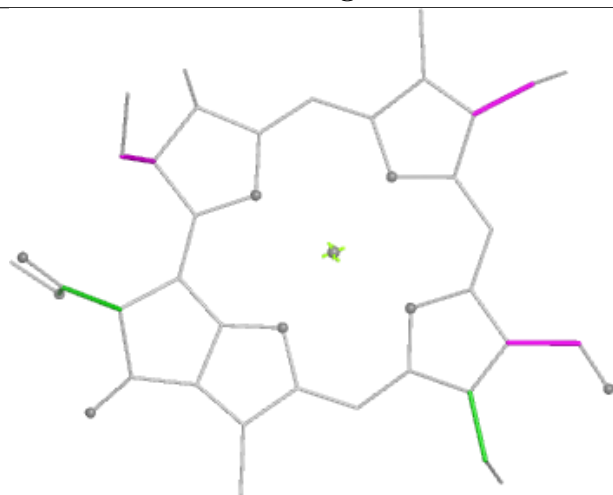
Ligand CHL S 607



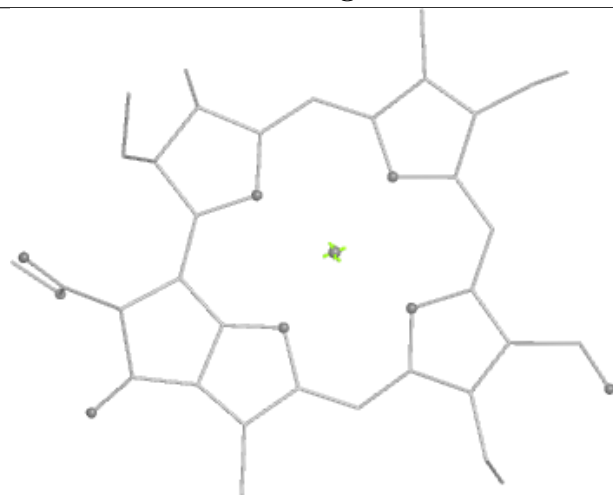
Bond lengths



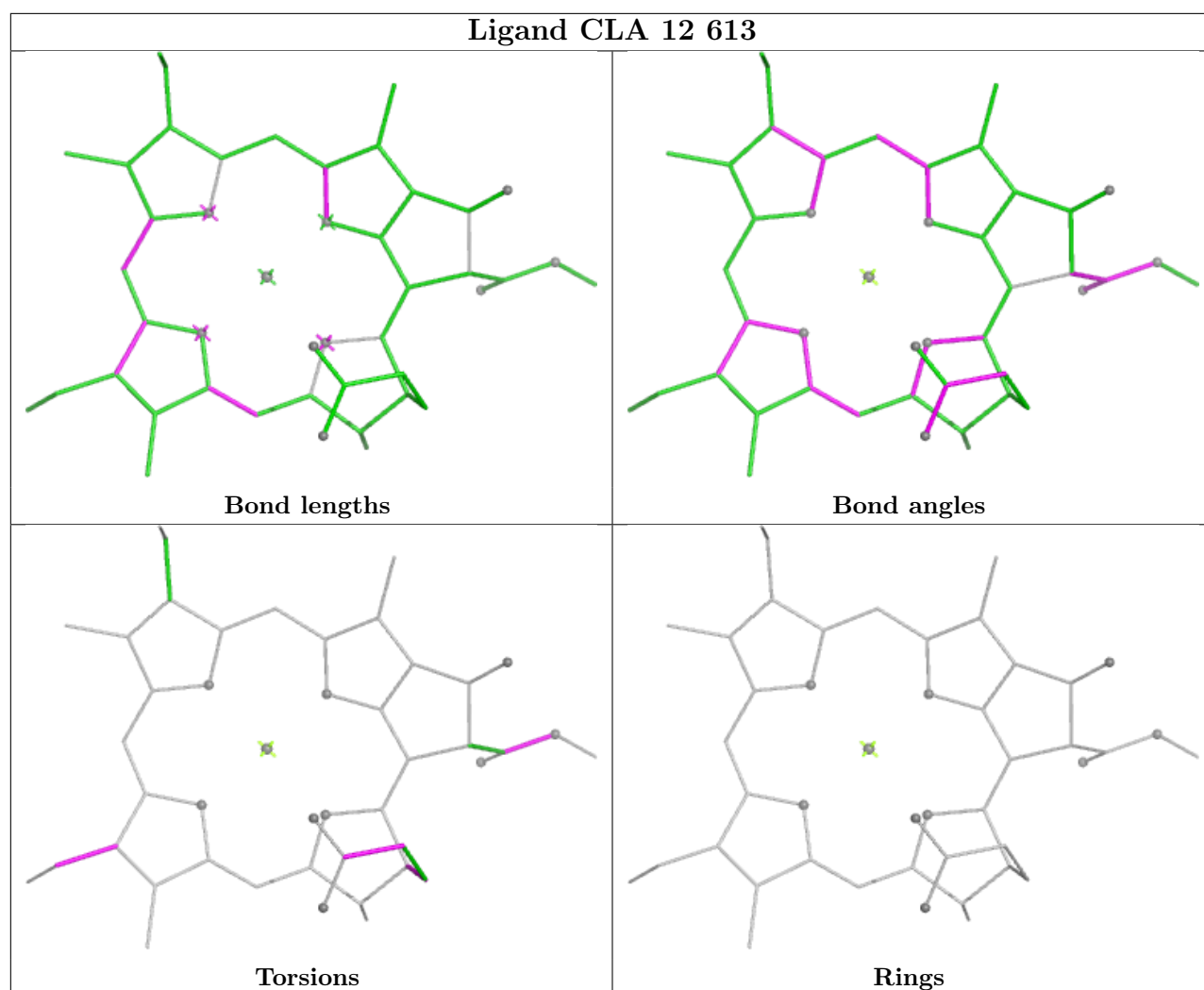
Bond angles

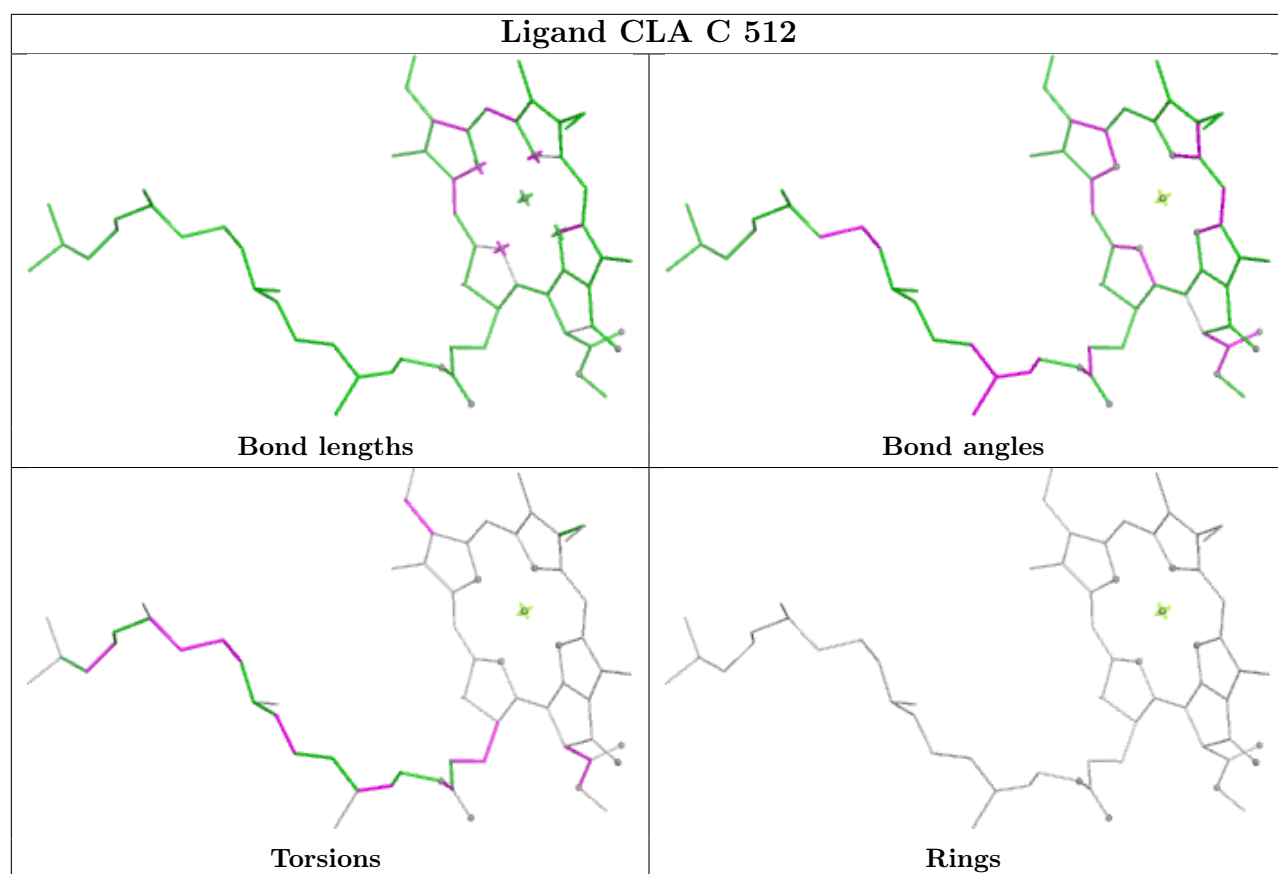


Torsions

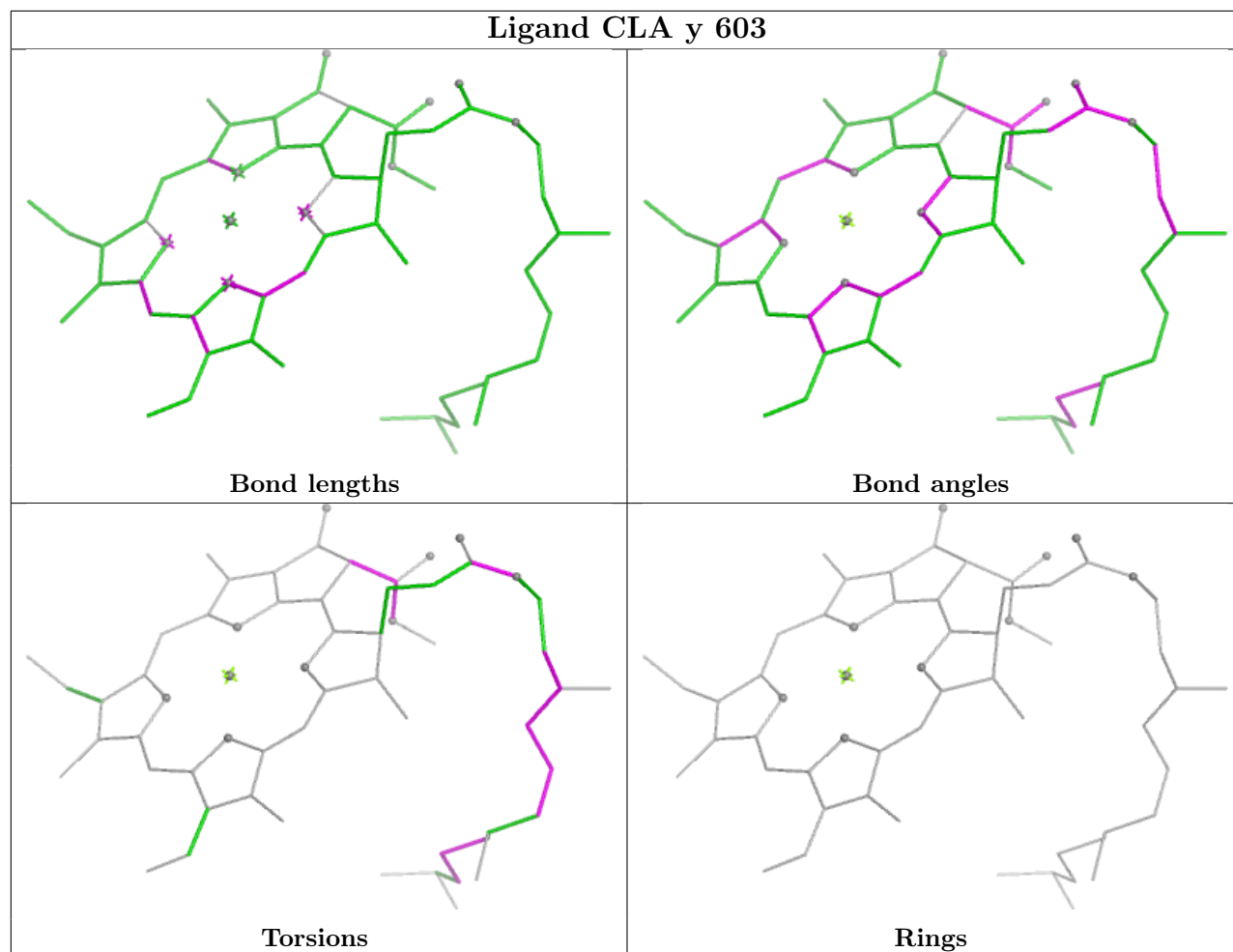


Rings

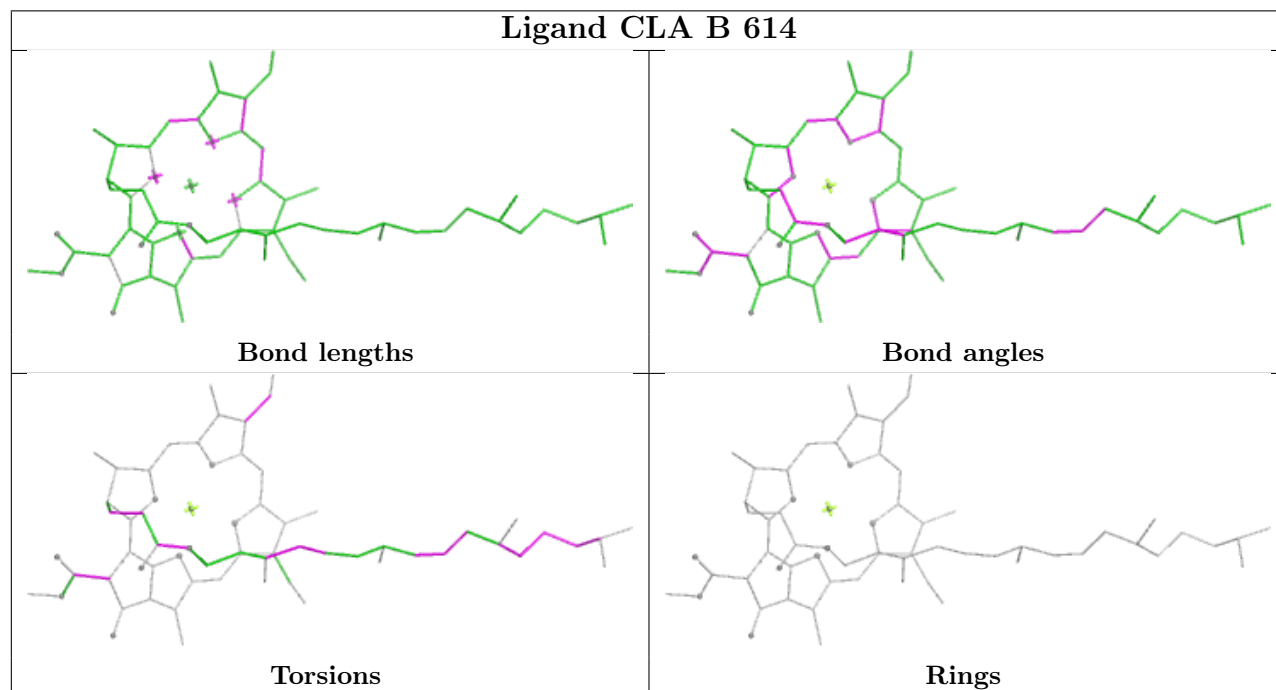


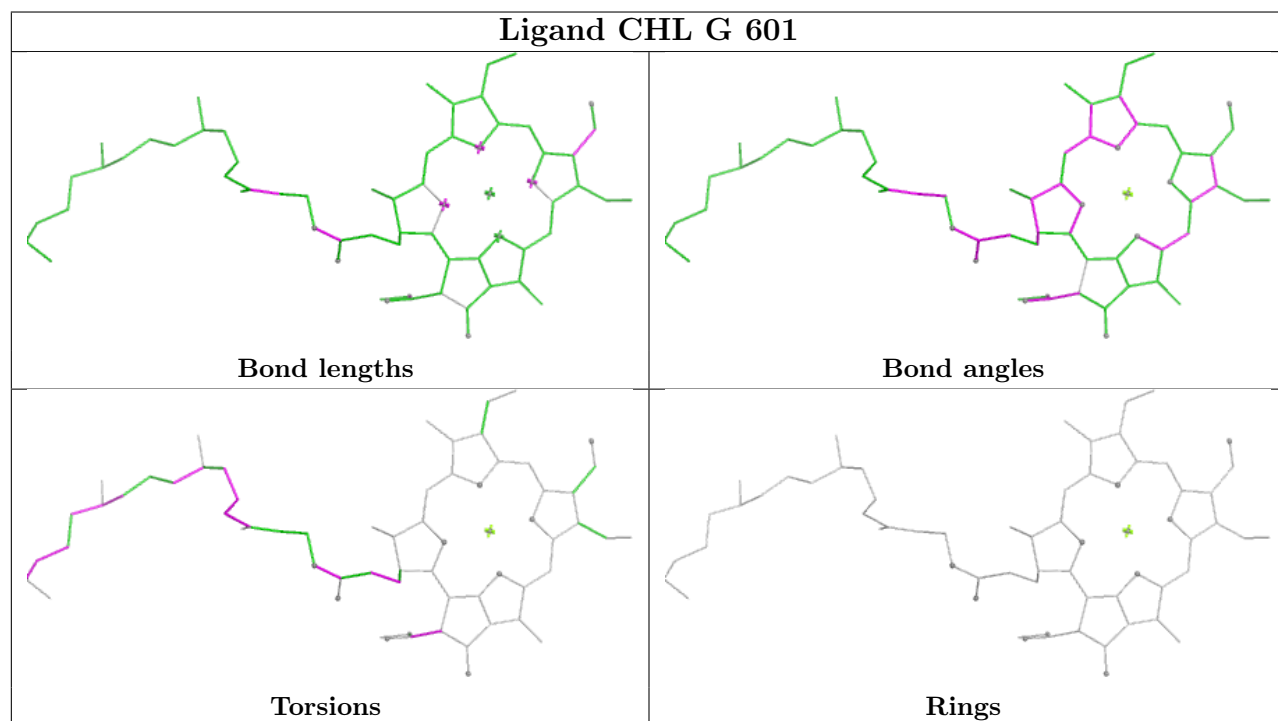
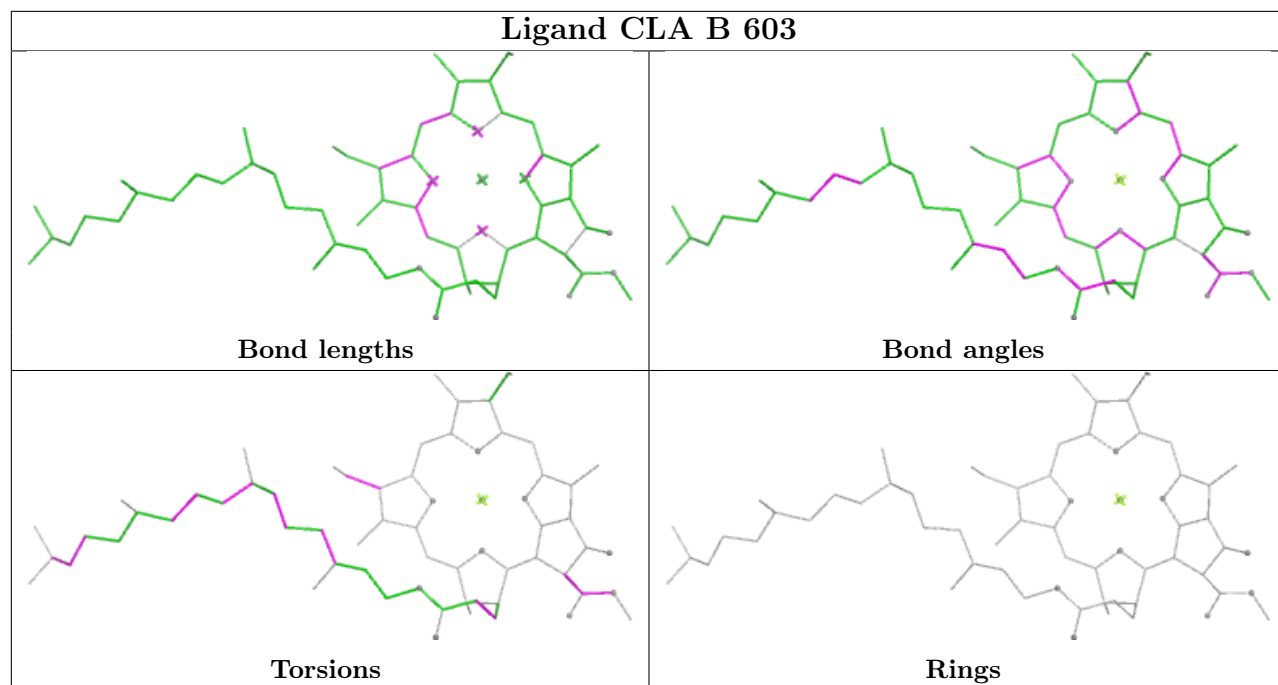


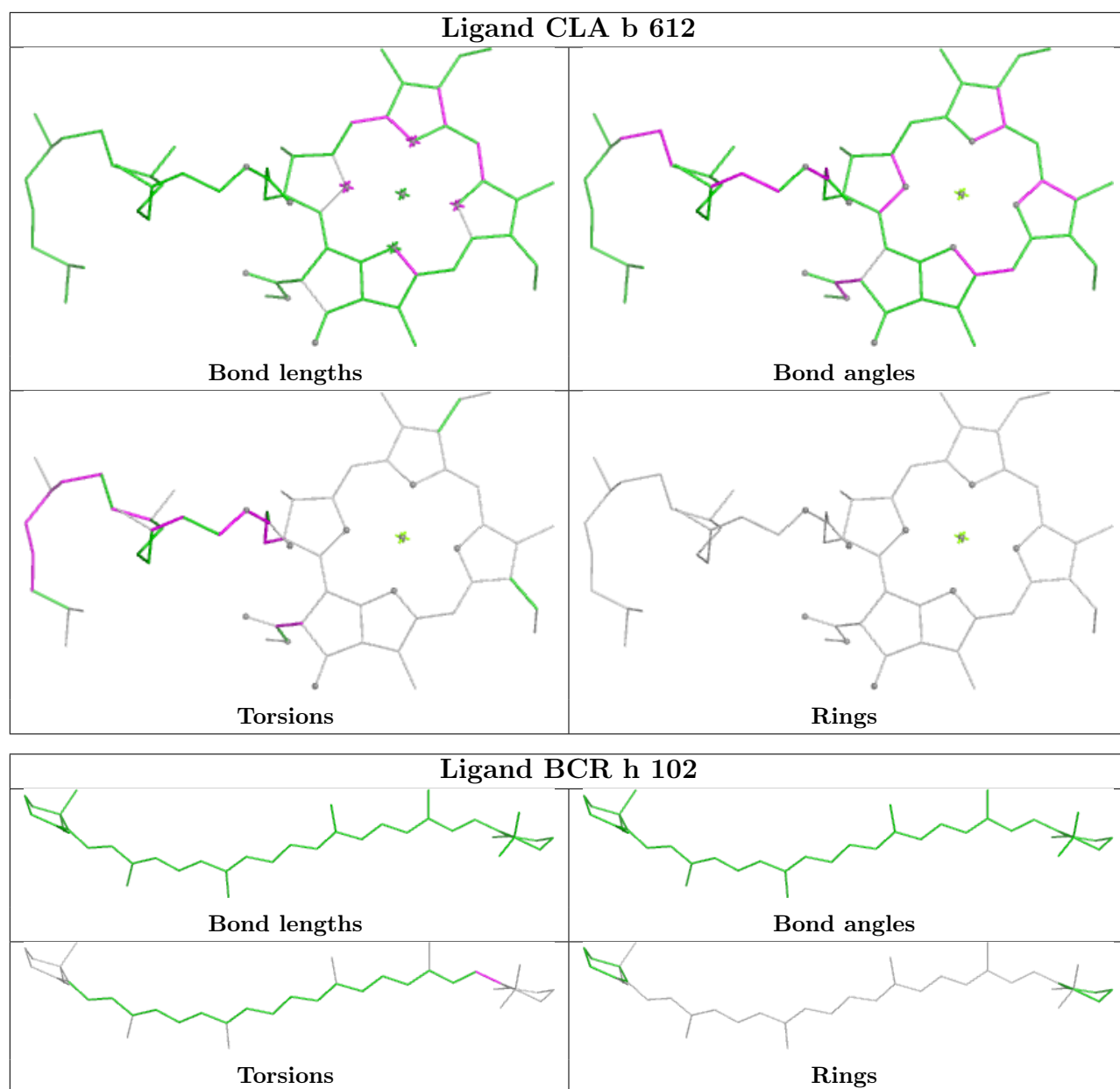
Ligand CLA y 603

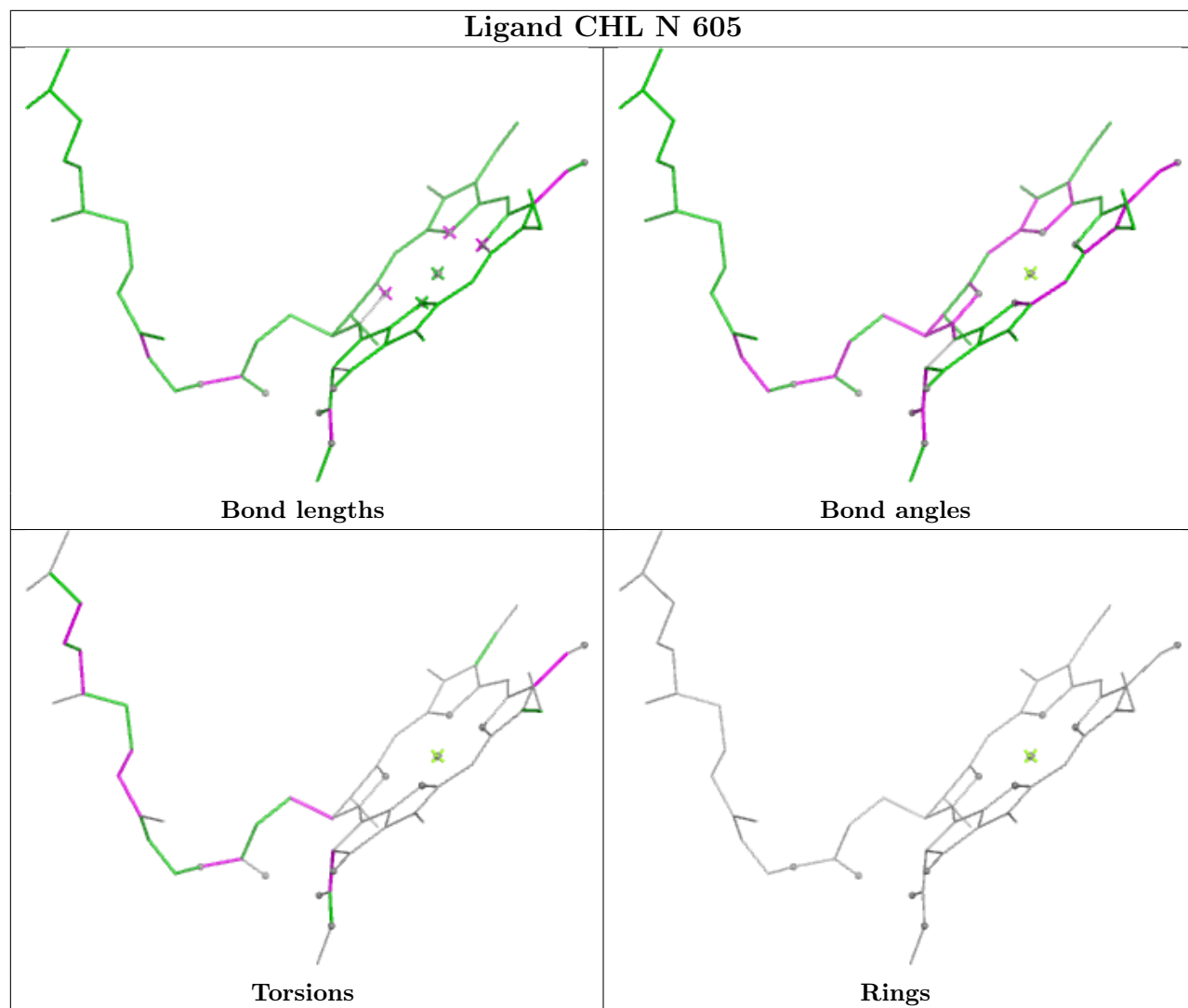


Ligand CLA B 614

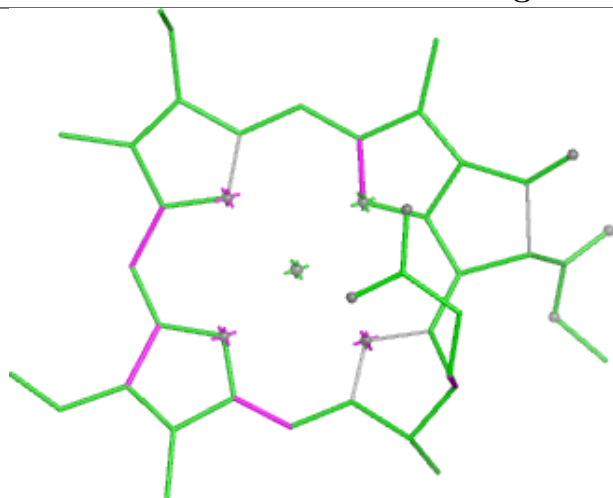




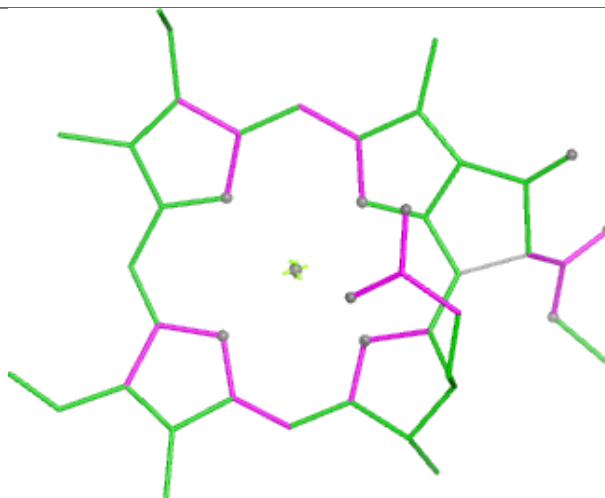




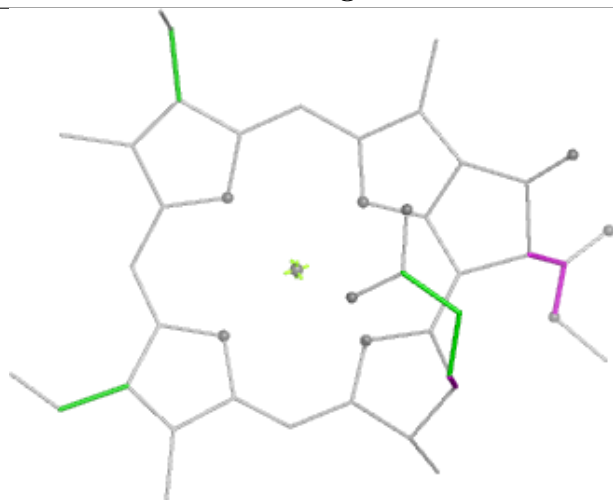
Ligand CLA N 614



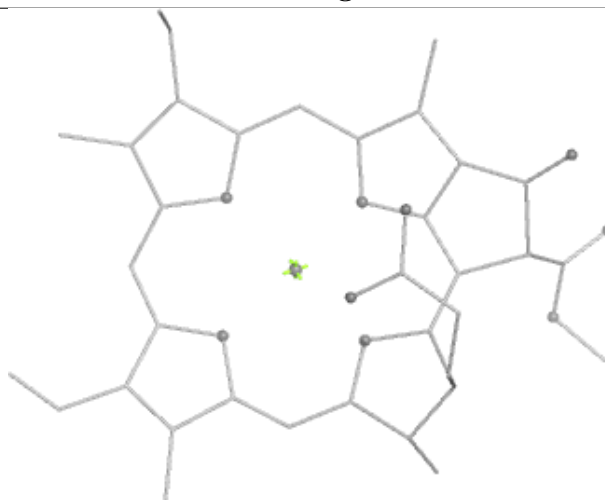
Bond lengths



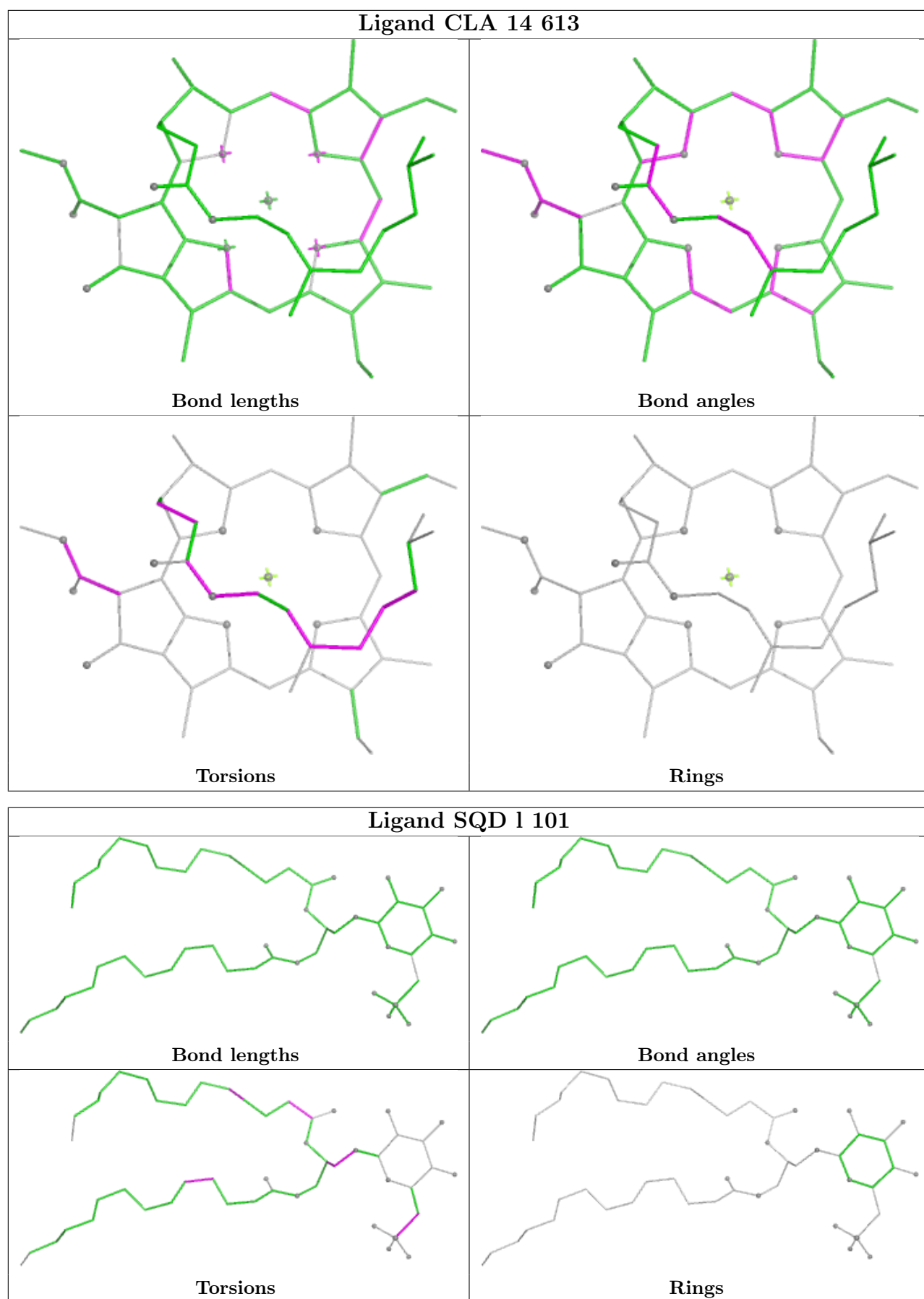
Bond angles

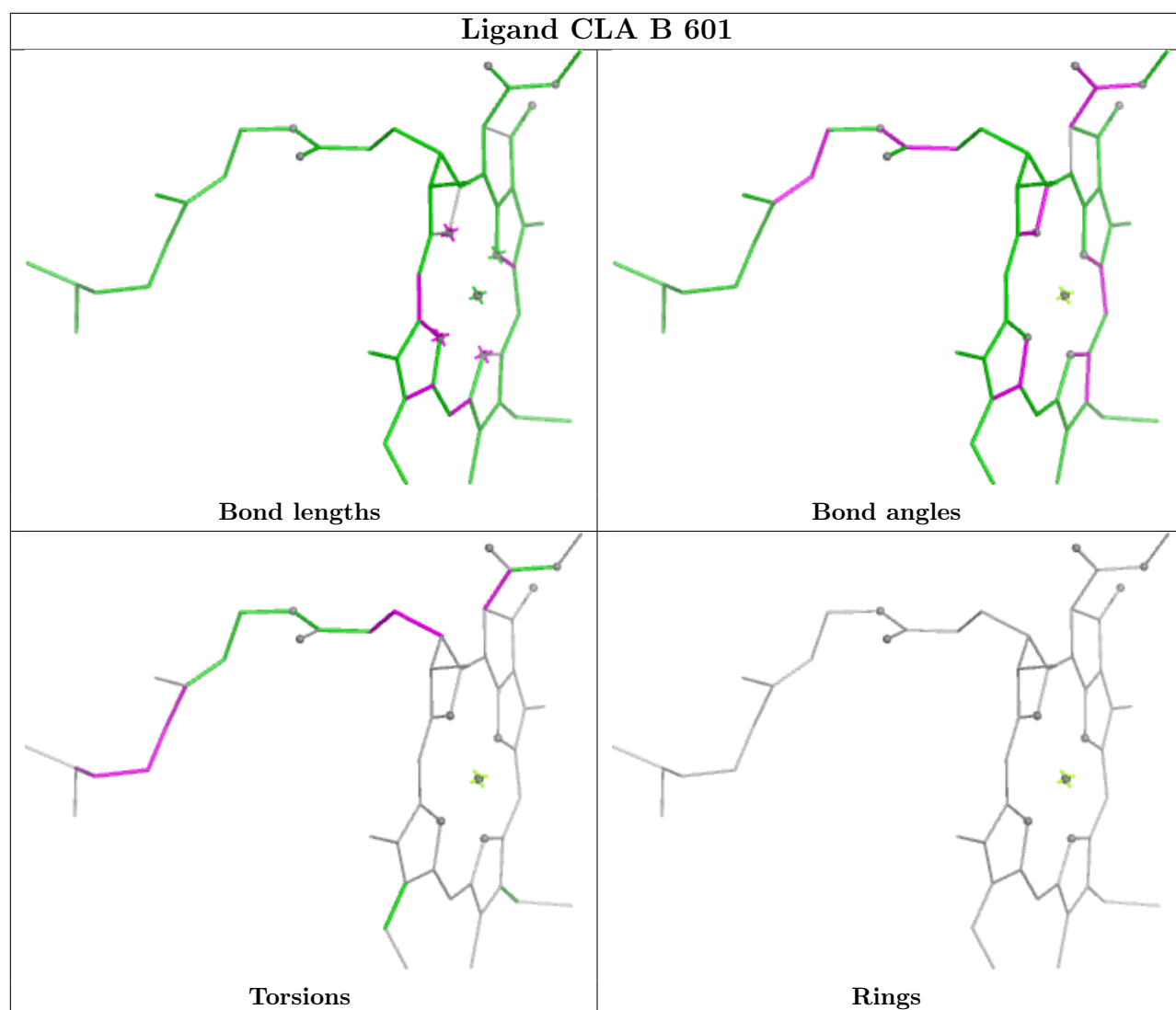


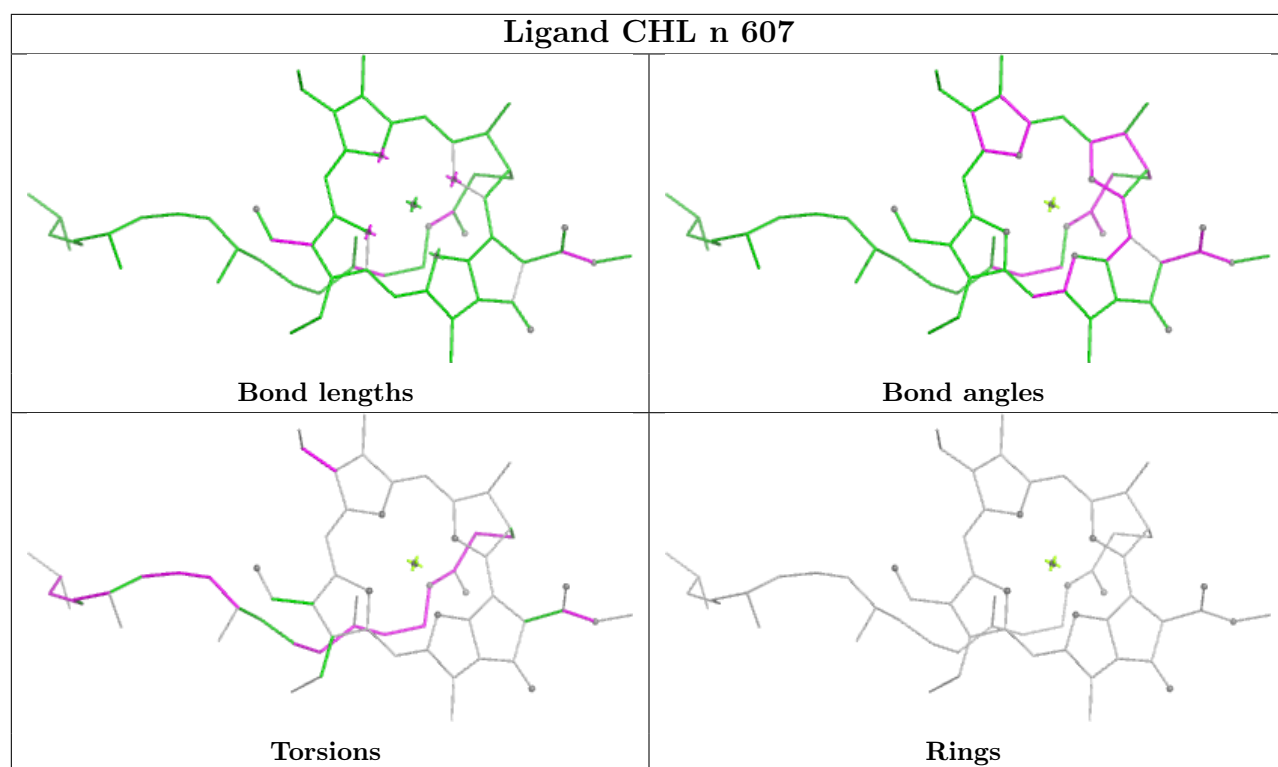
Torsions



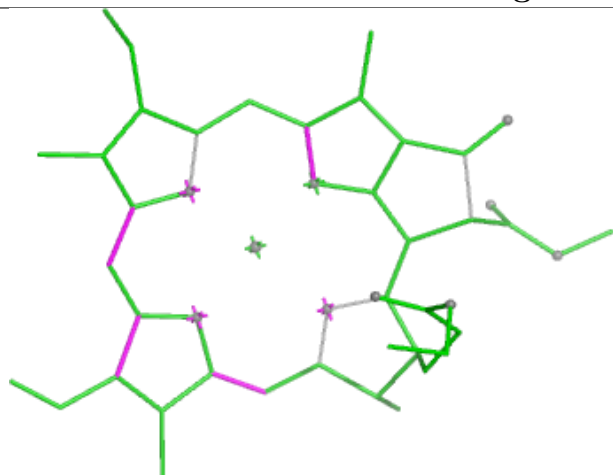
Rings



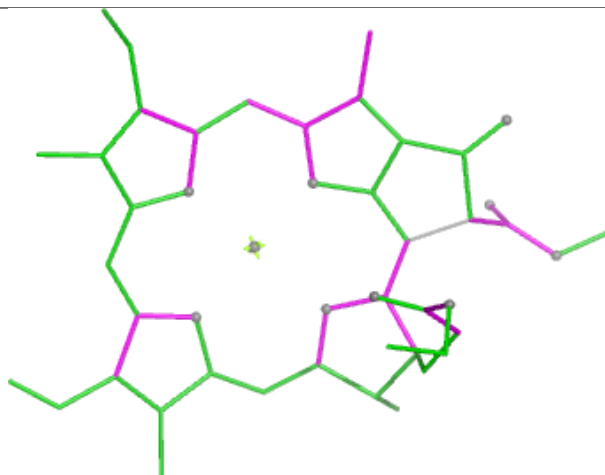




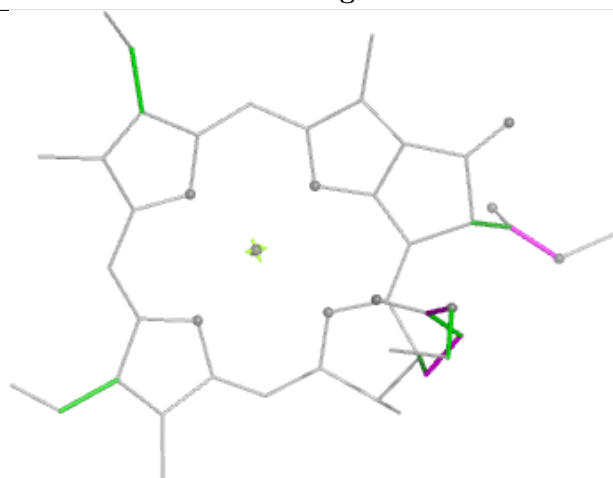
Ligand CLA N 615



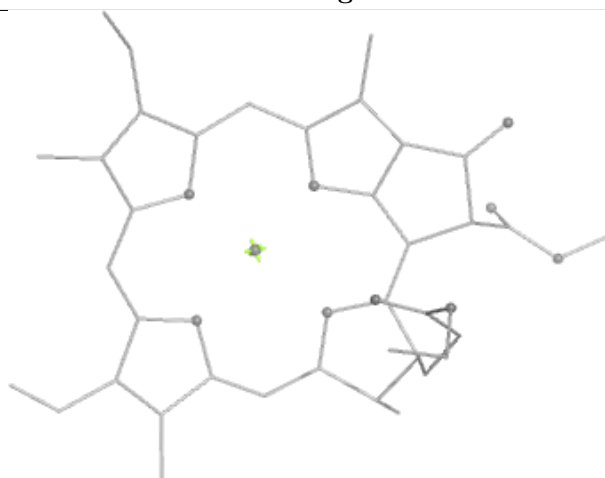
Bond lengths



Bond angles

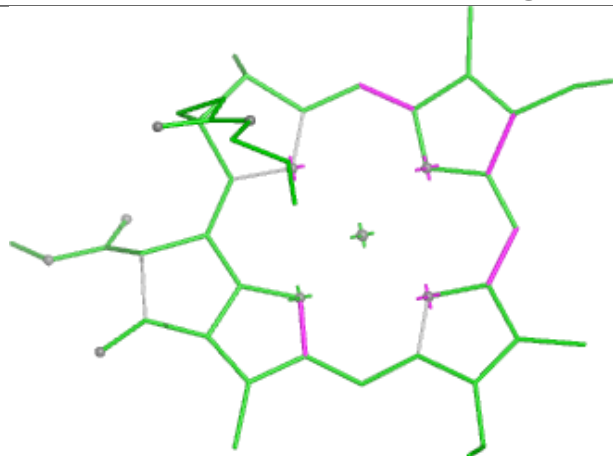


Torsions

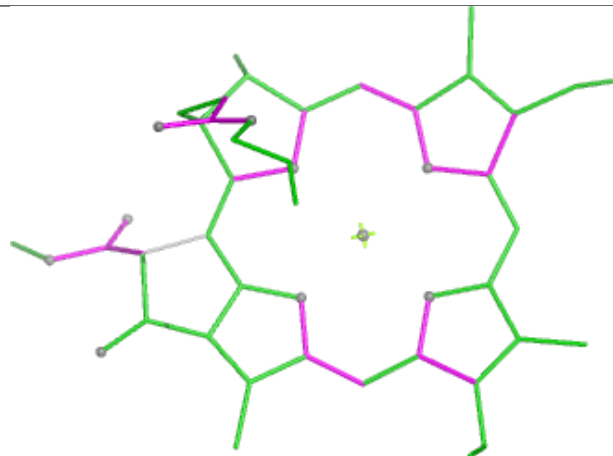


Rings

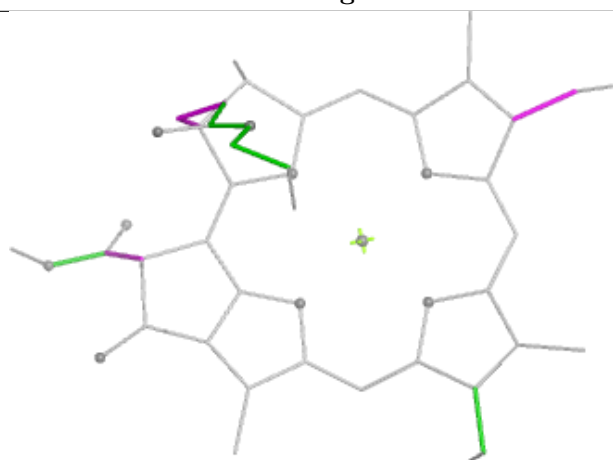
Ligand CLA r 604



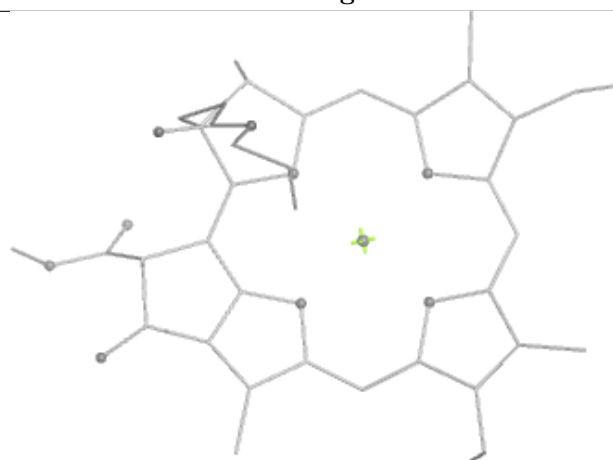
Bond lengths



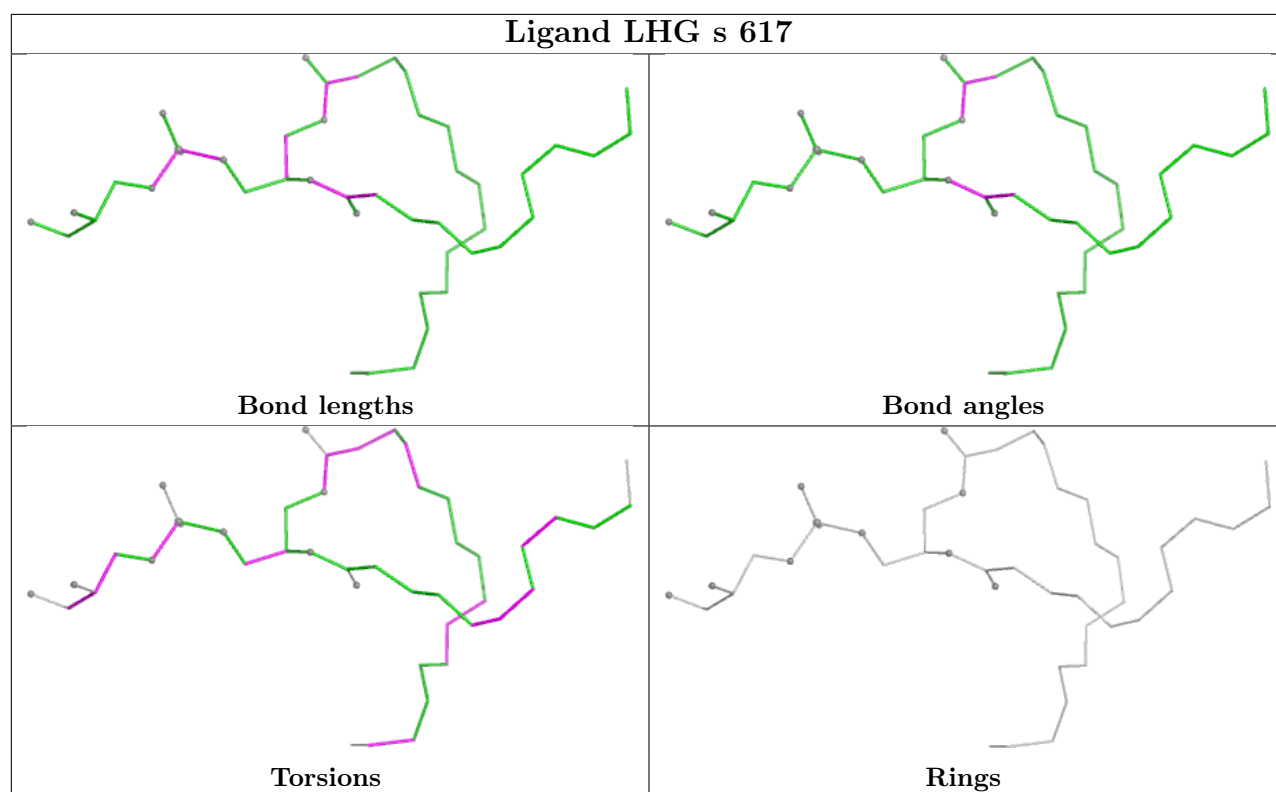
Bond angles



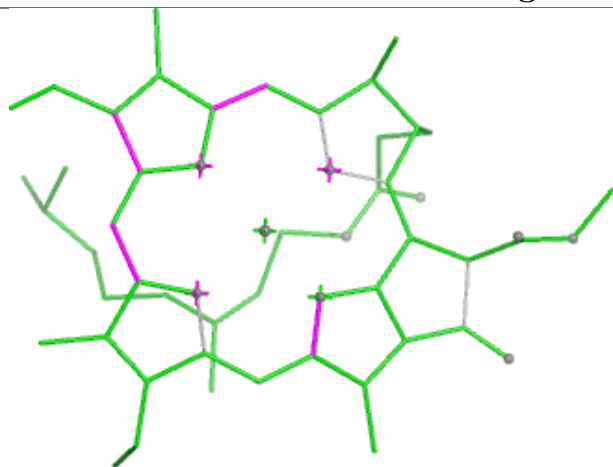
Torsions



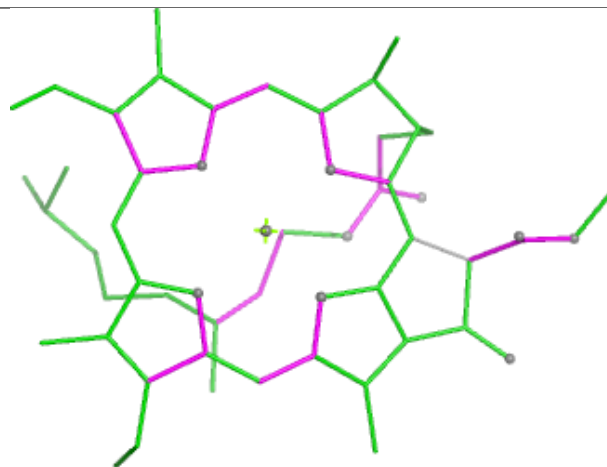
Rings



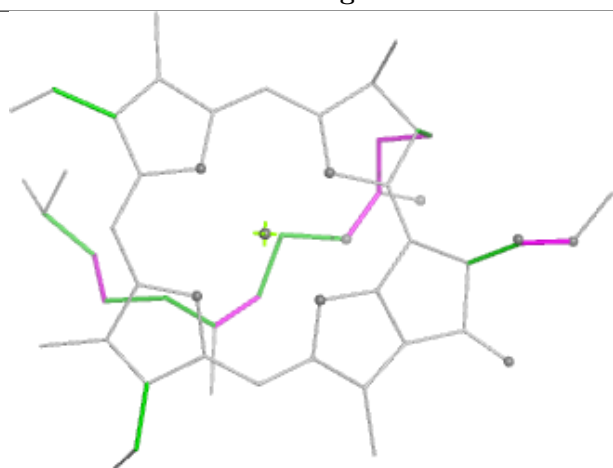
Ligand CLA 1 613



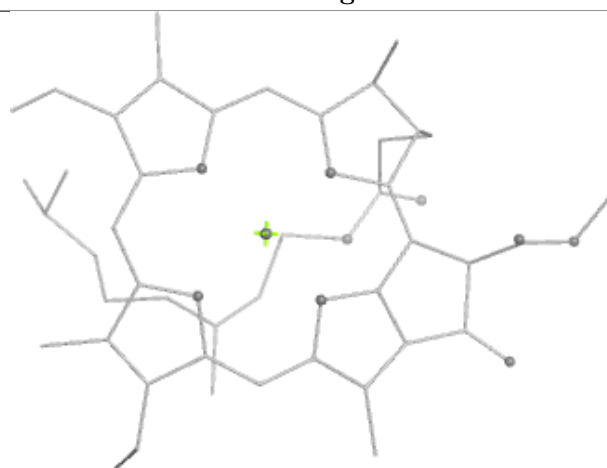
Bond lengths



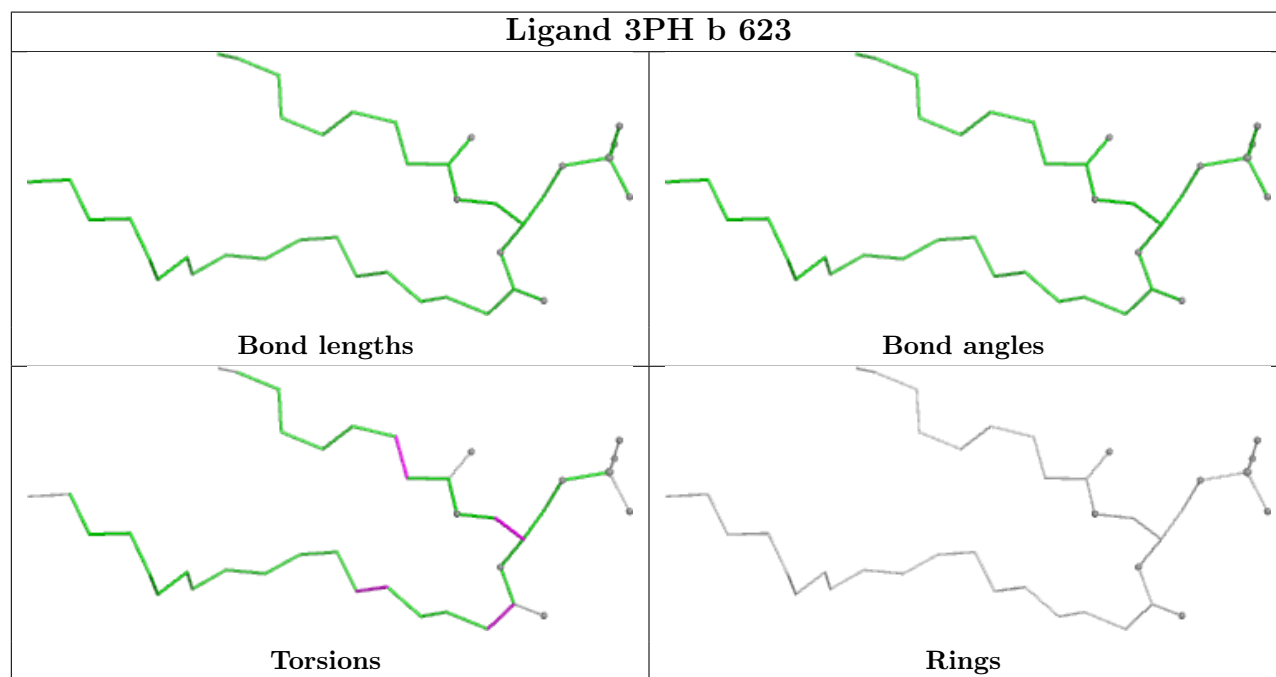
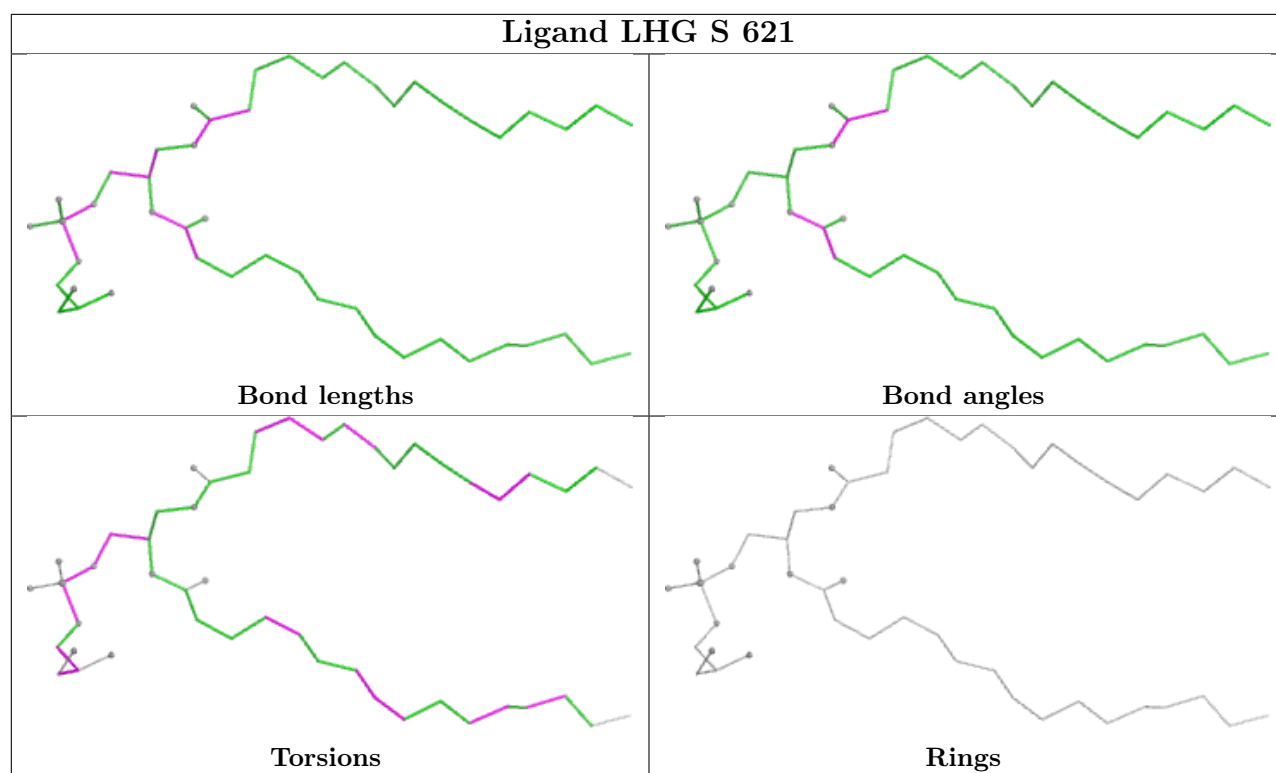
Bond angles



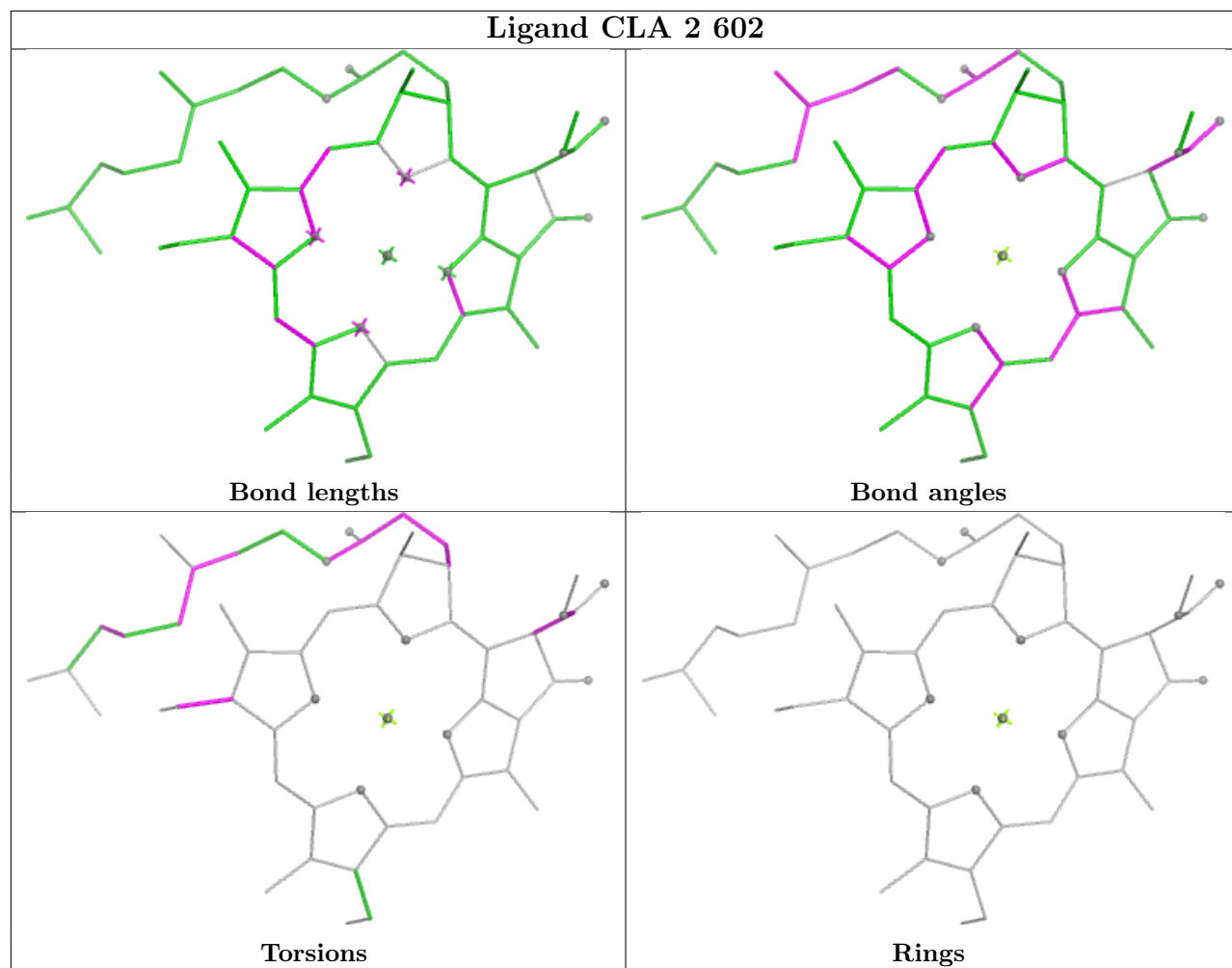
Torsions

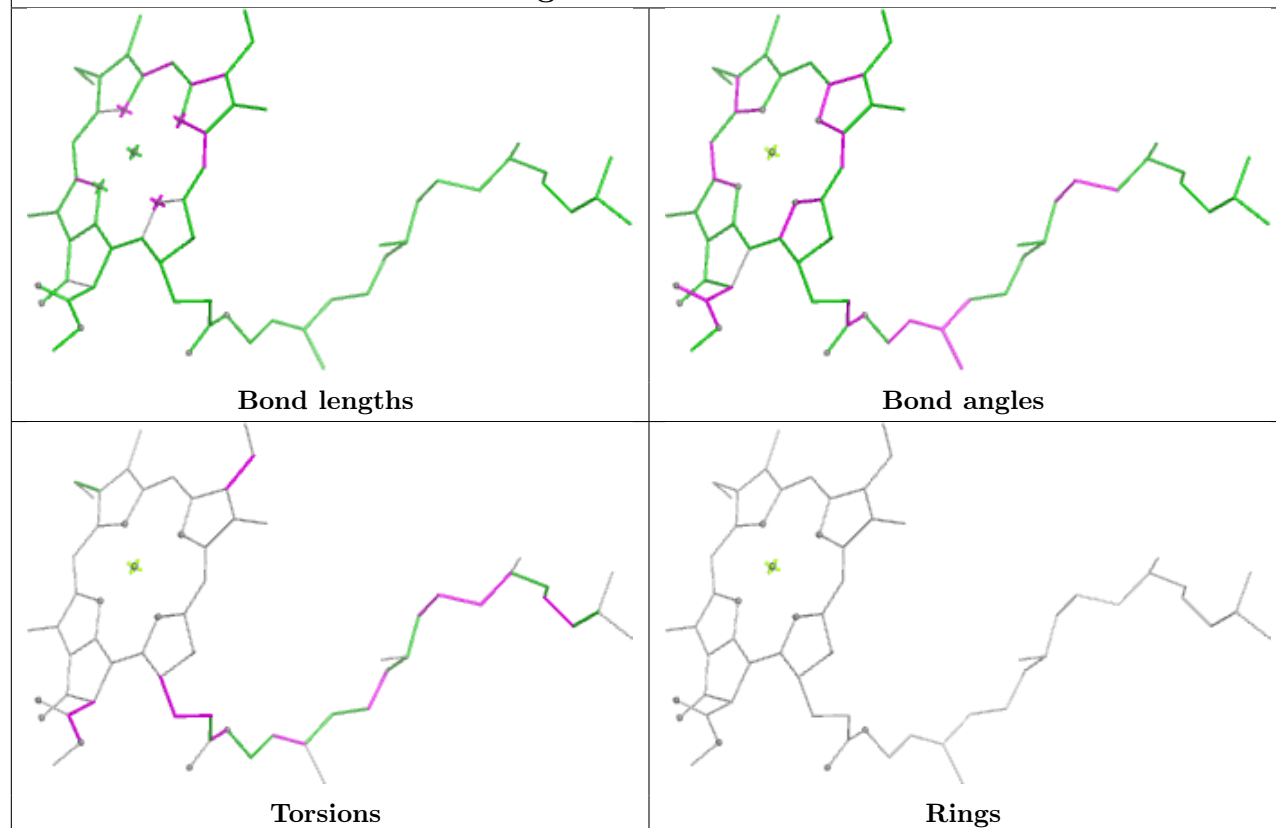
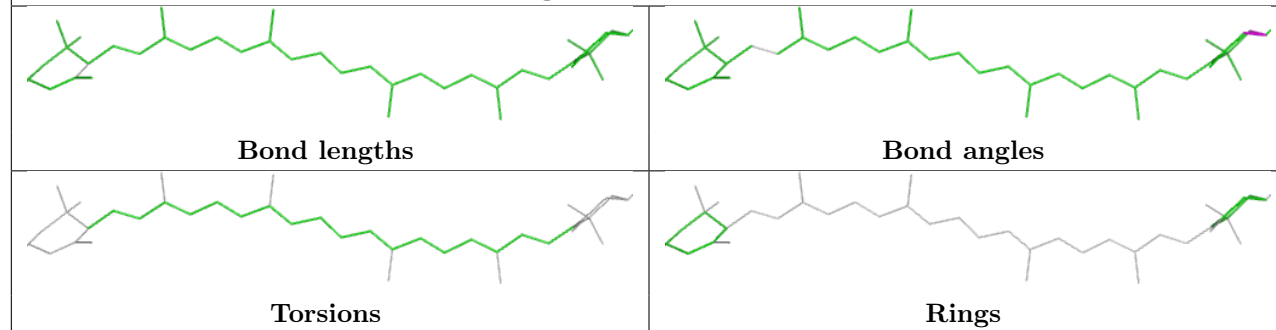


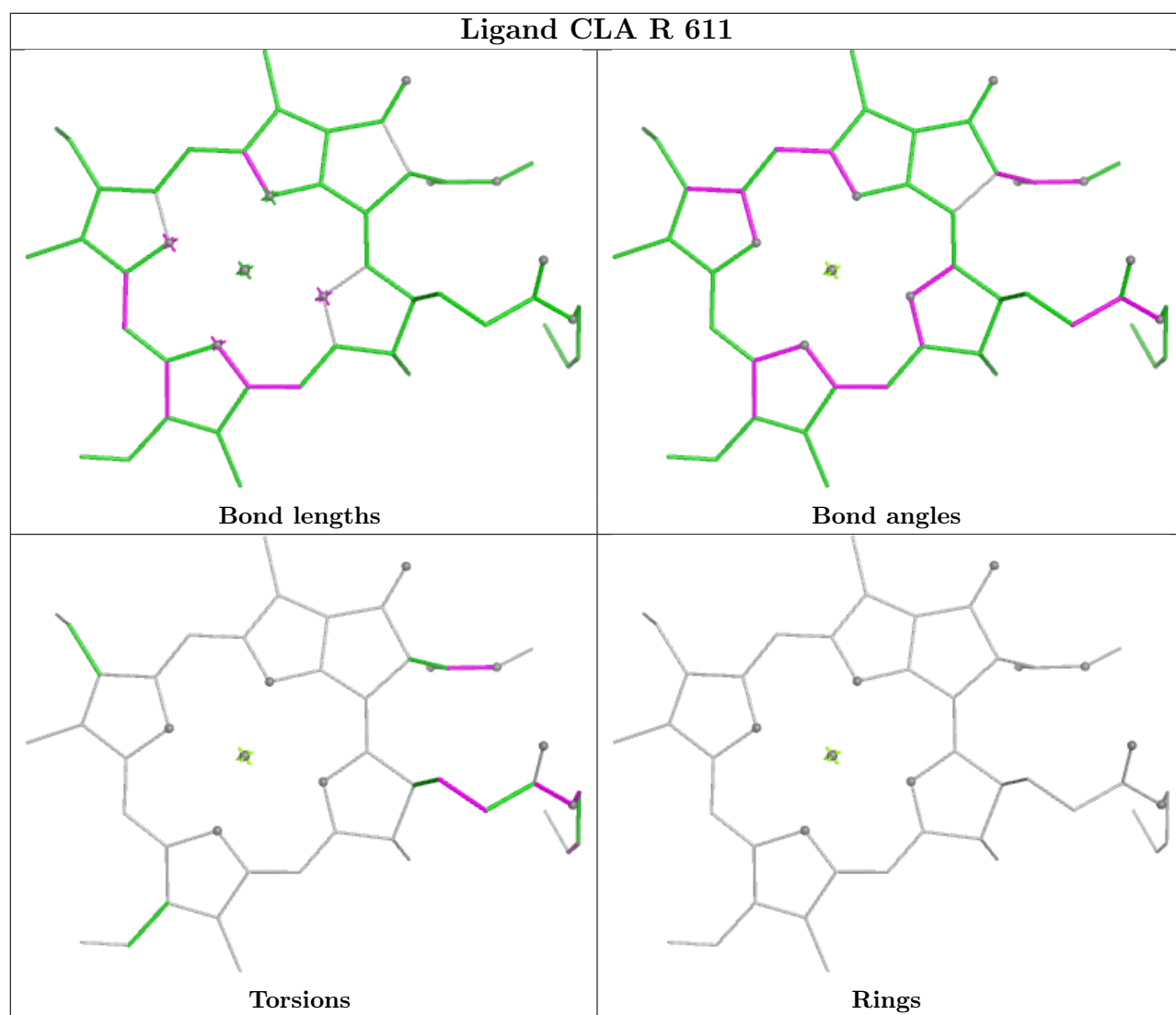
Rings

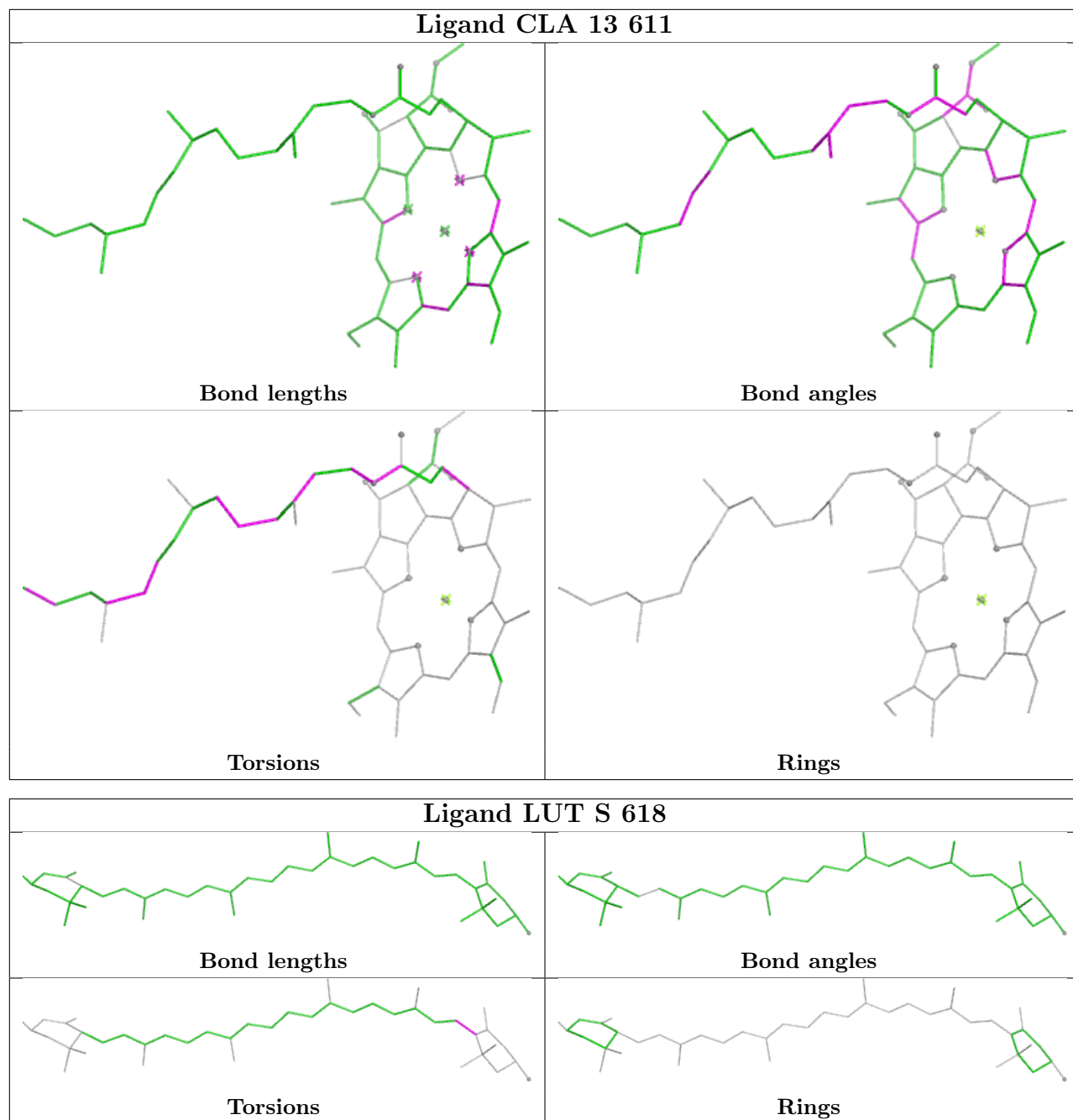


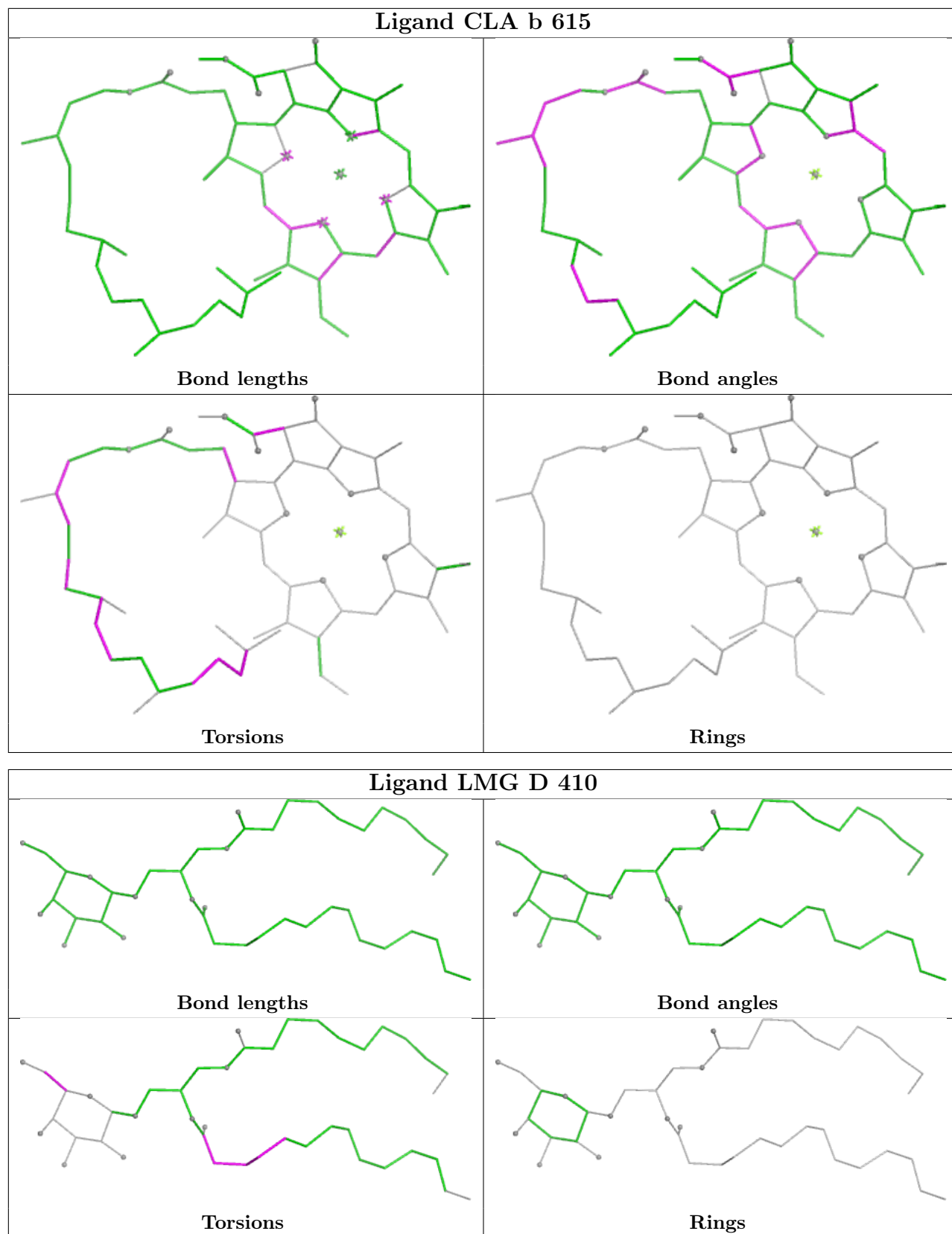
Ligand CLA 2 602



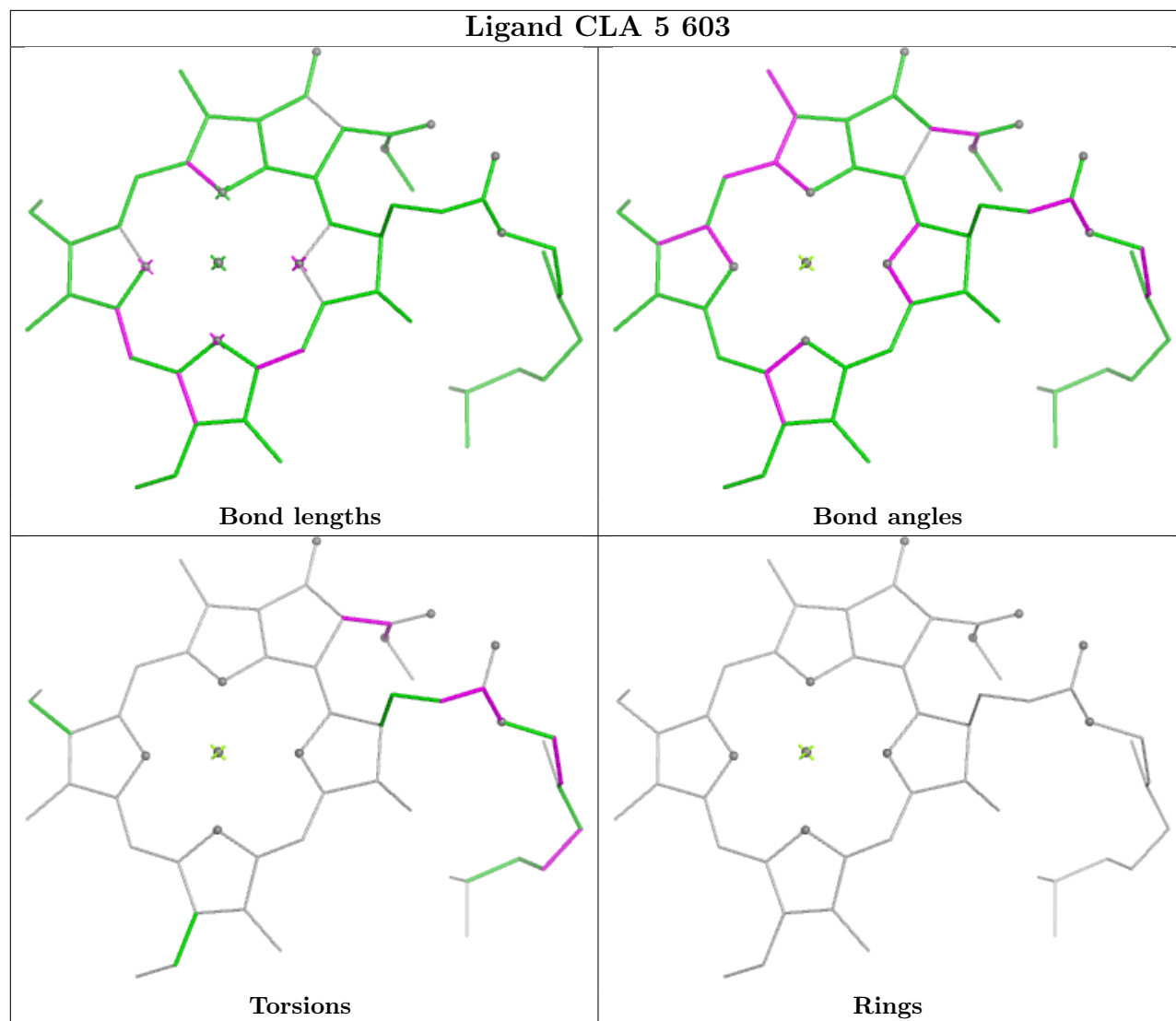
Ligand CLA c 512**Ligand LUT s 619**

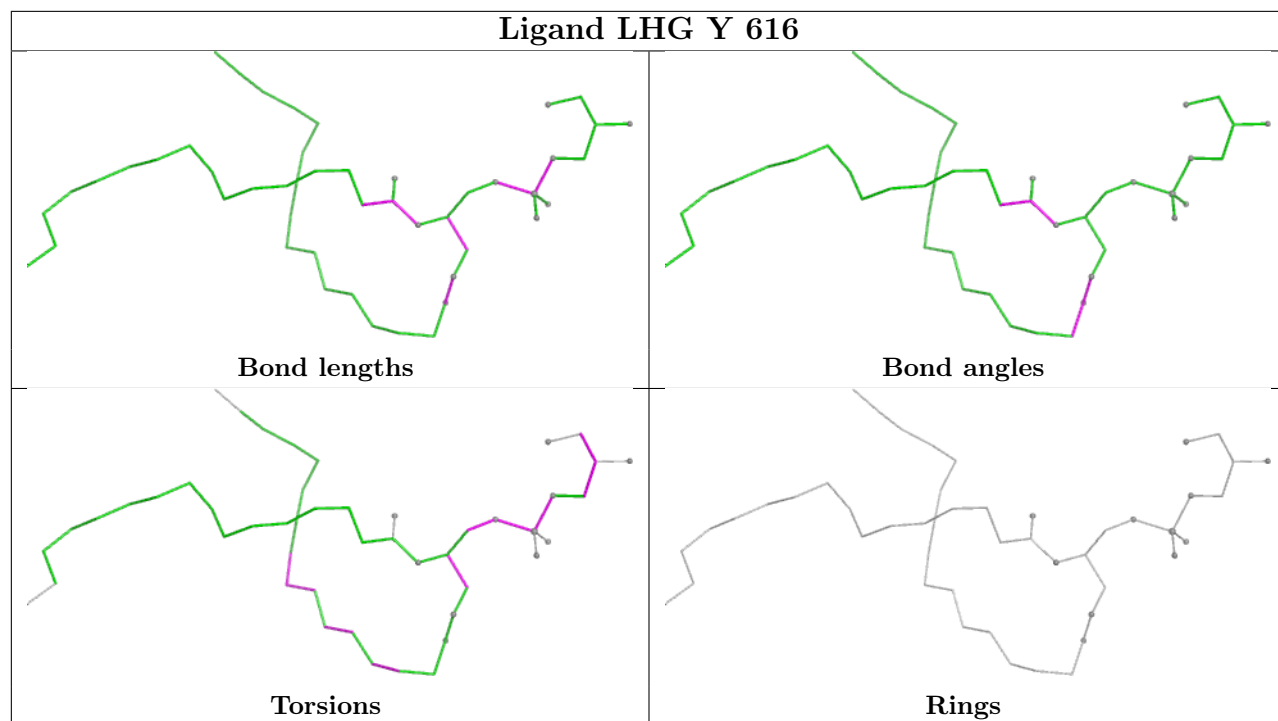




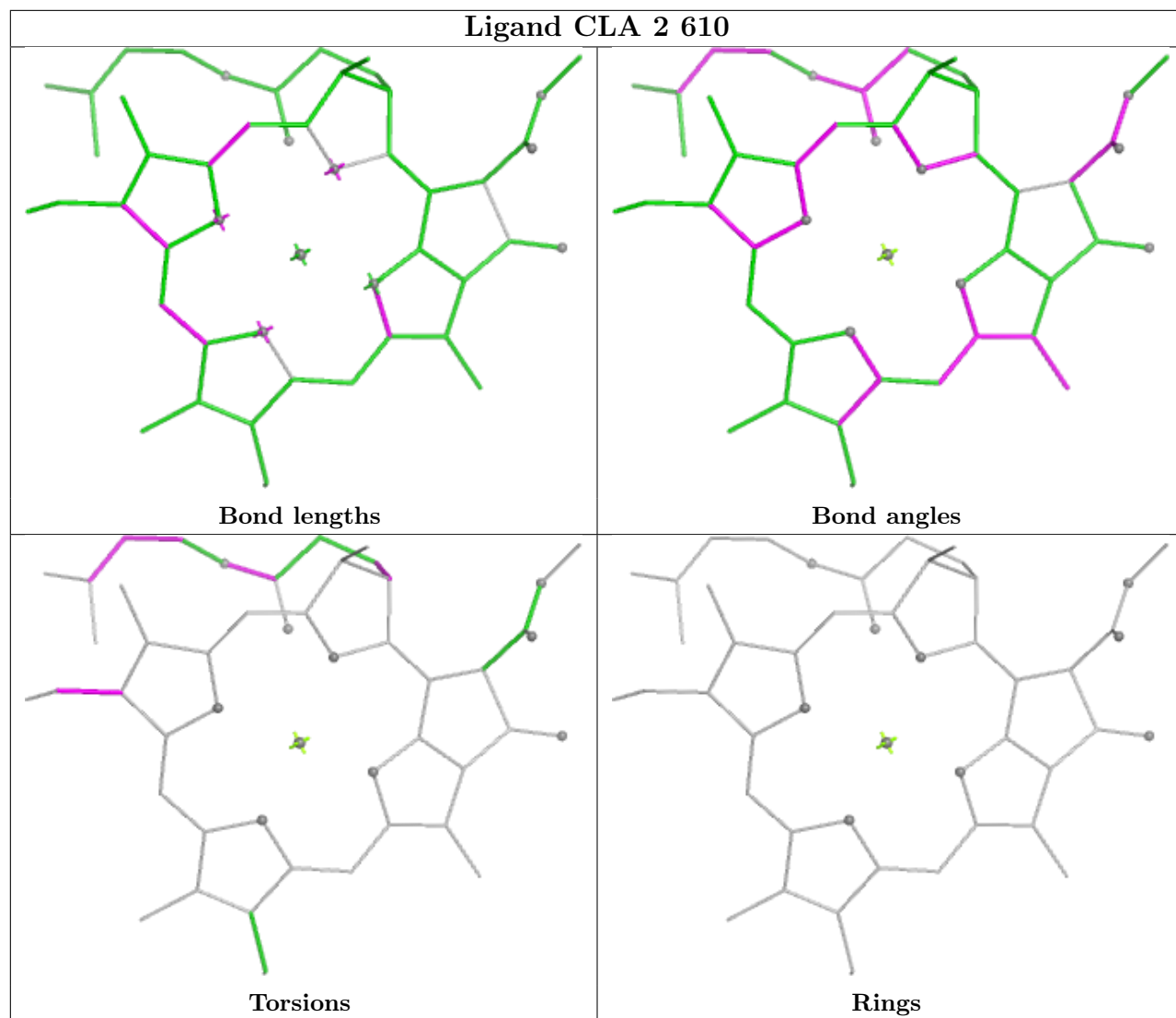


Ligand CLA 5 603

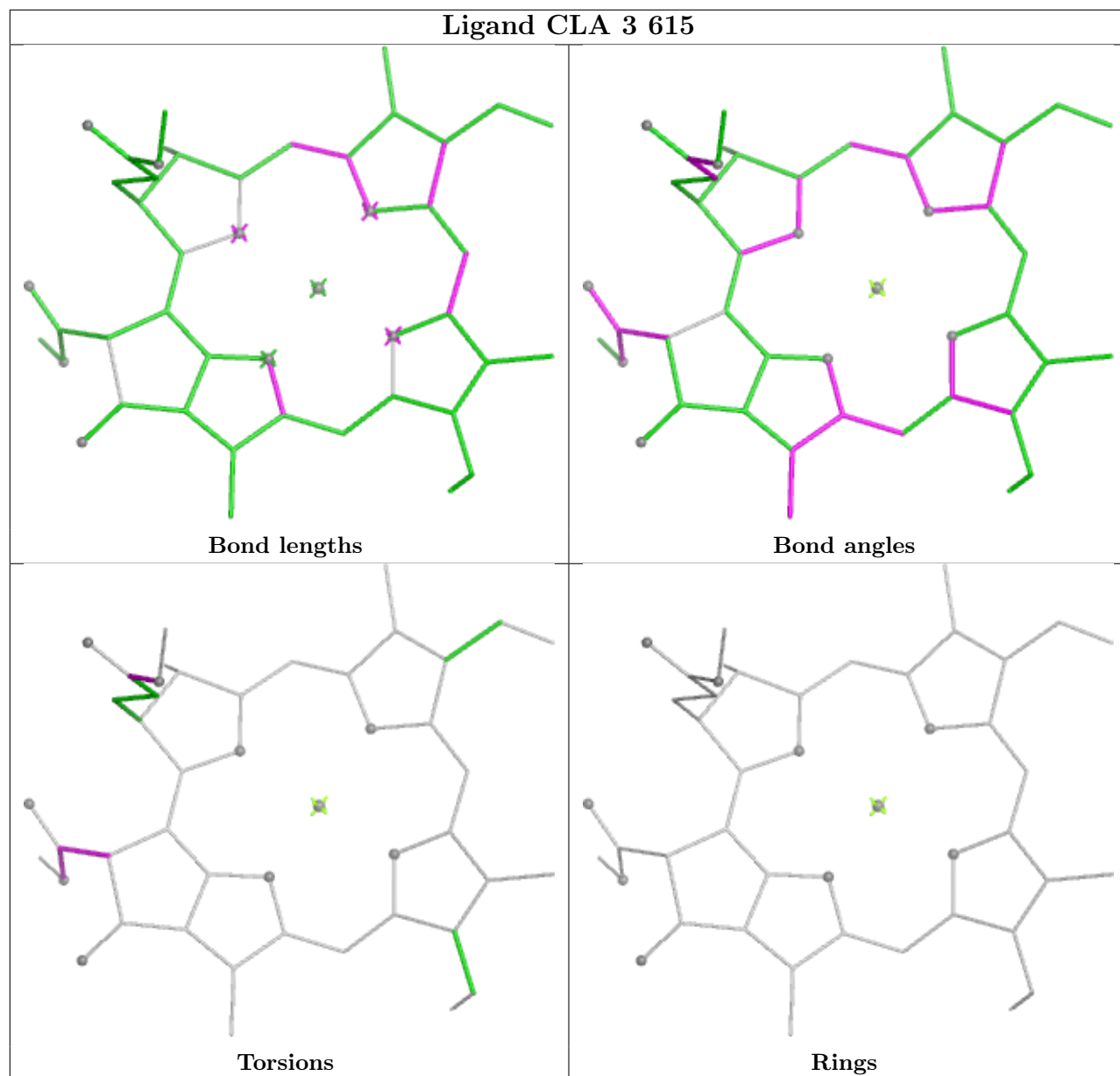


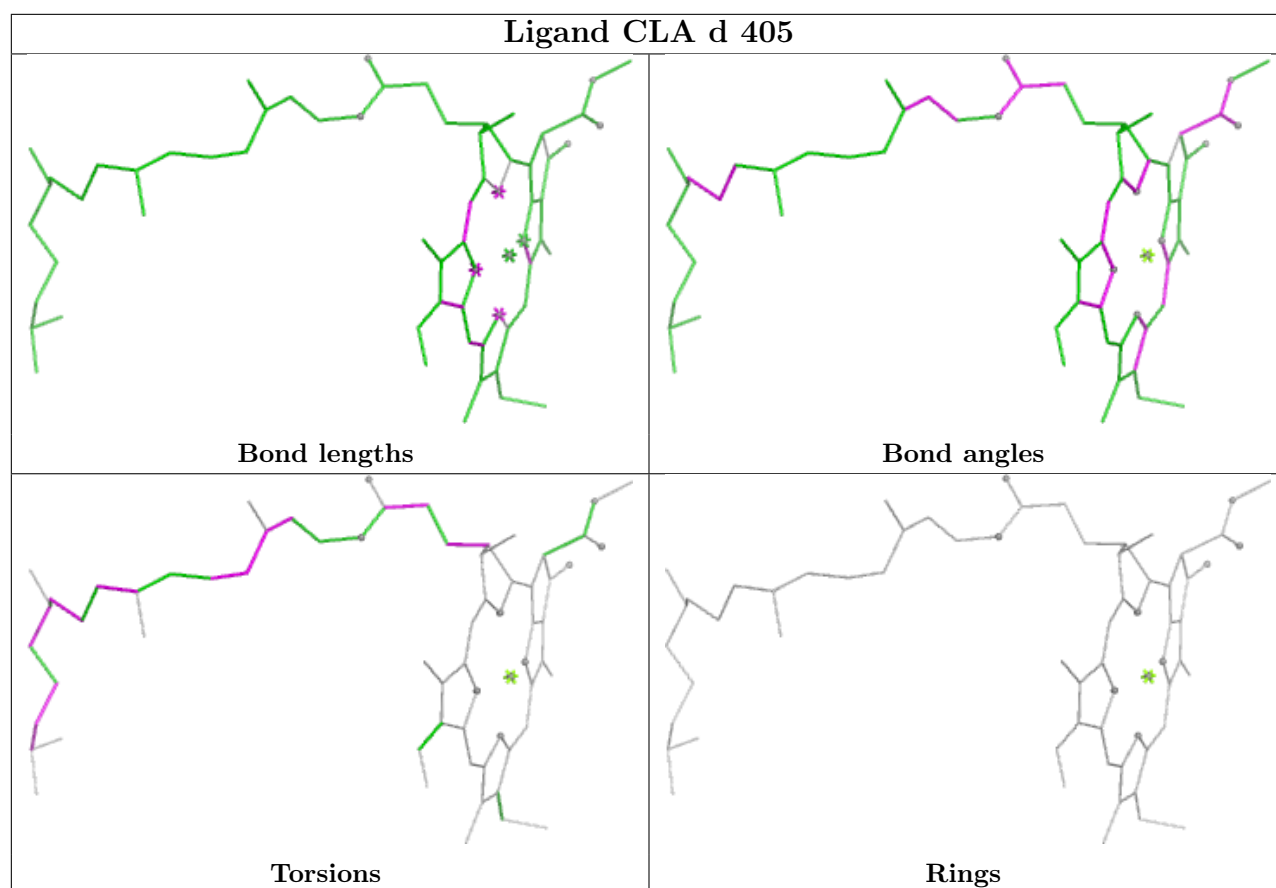
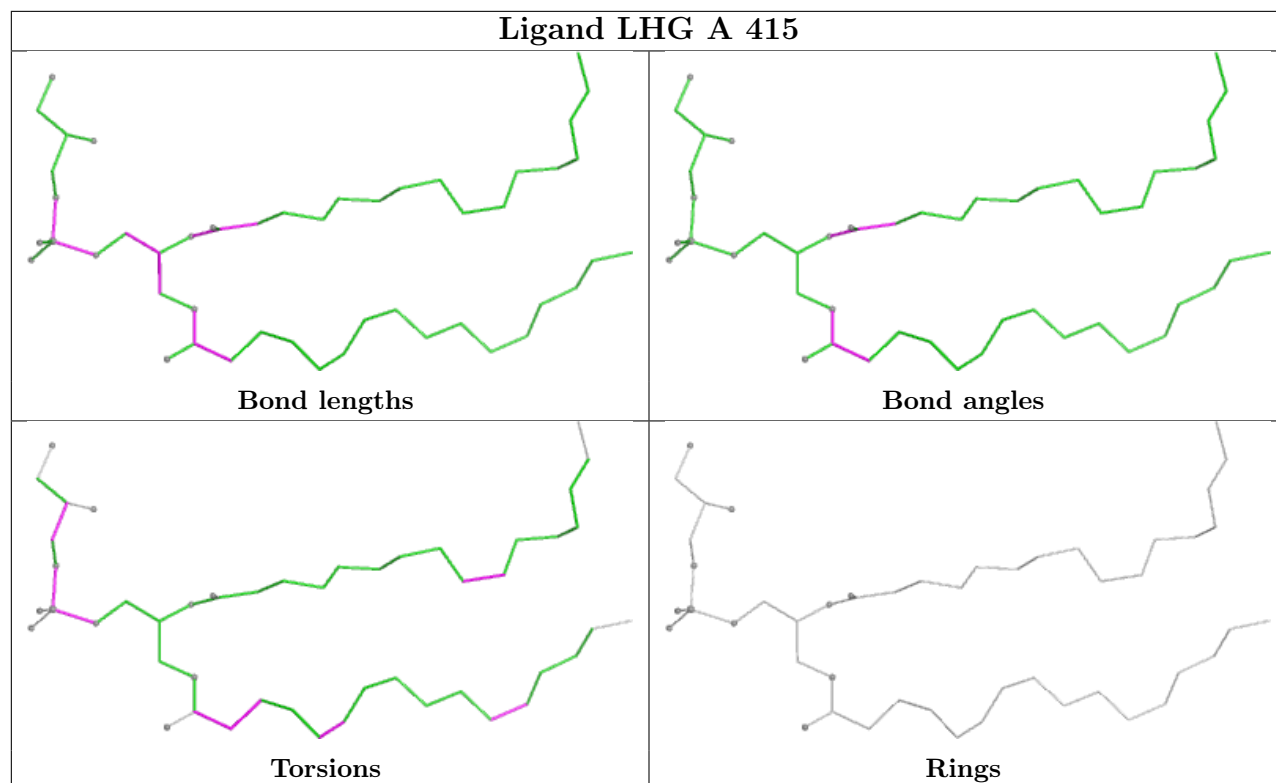


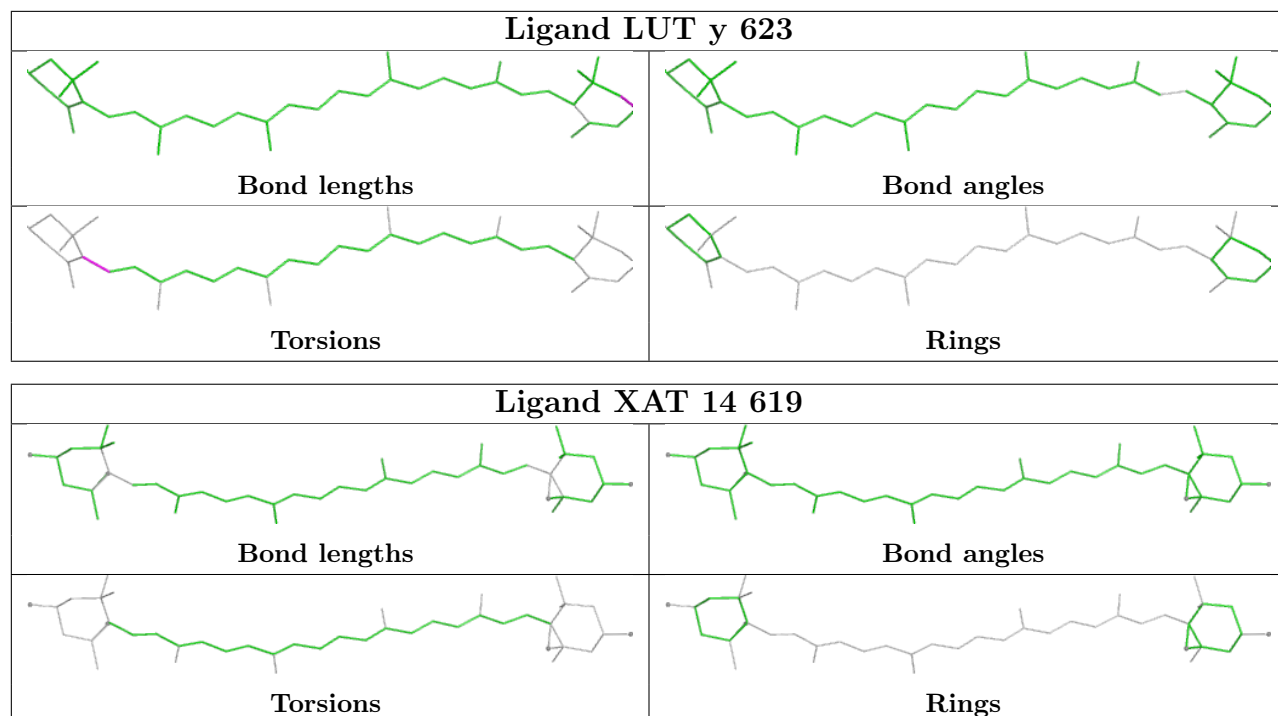
Ligand CLA 2 610

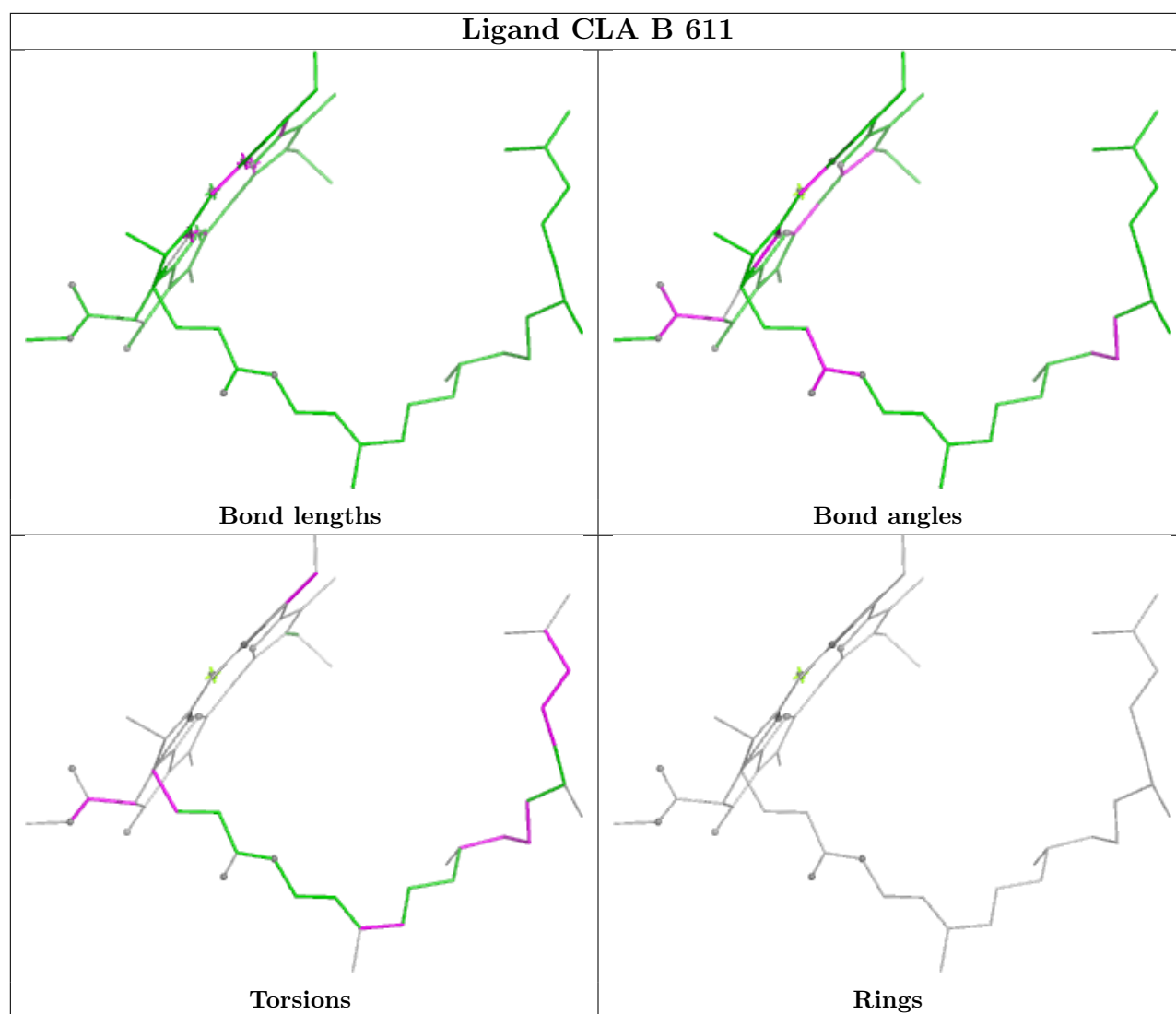


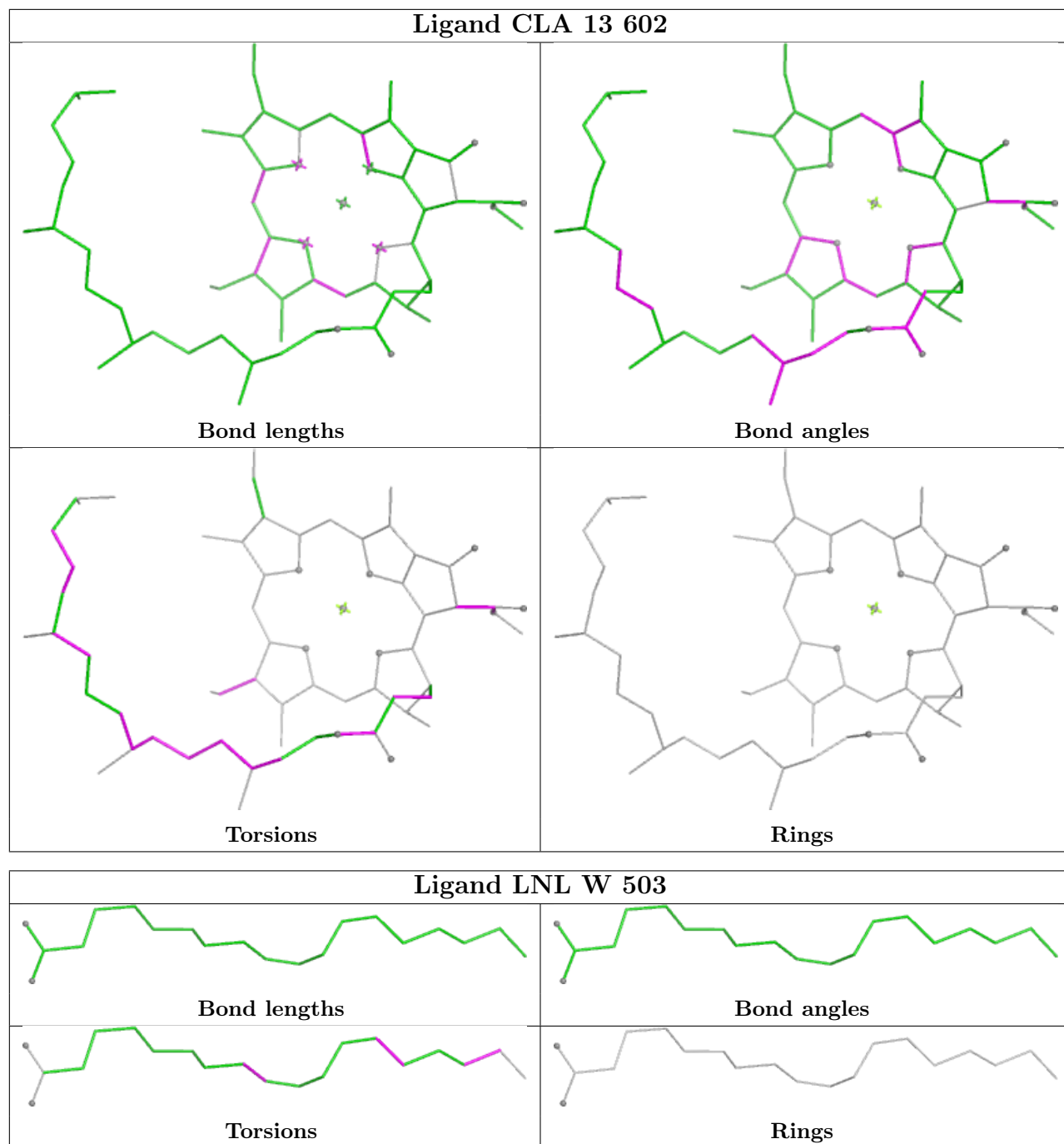
Ligand CLA 3 615

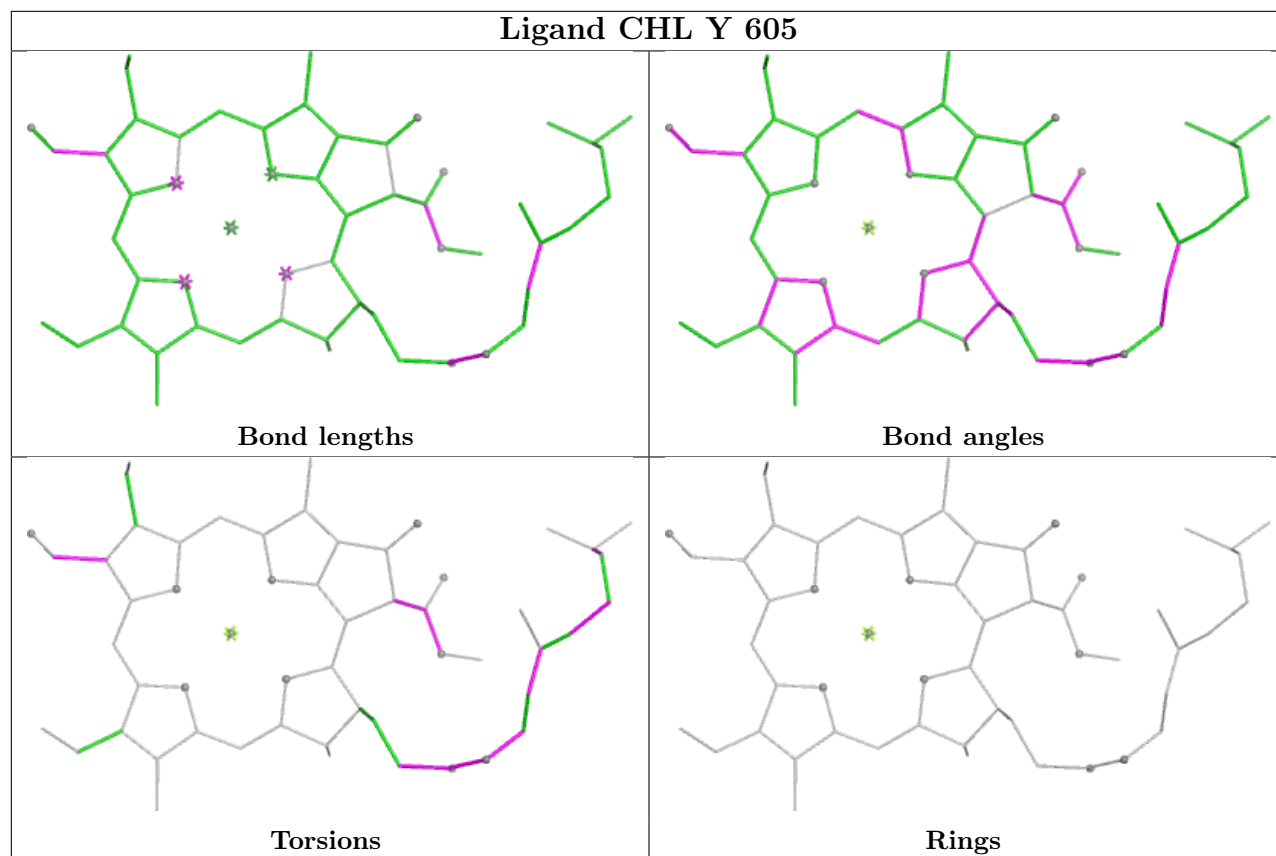
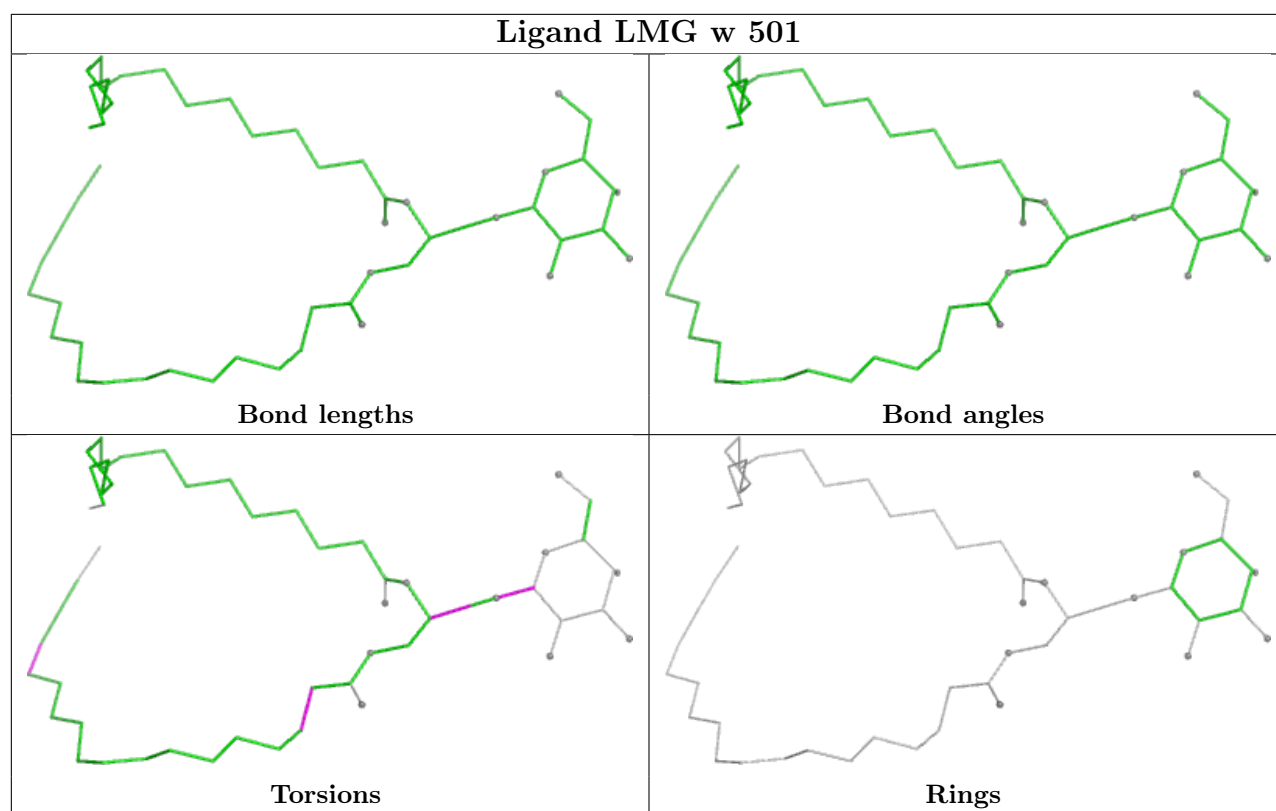


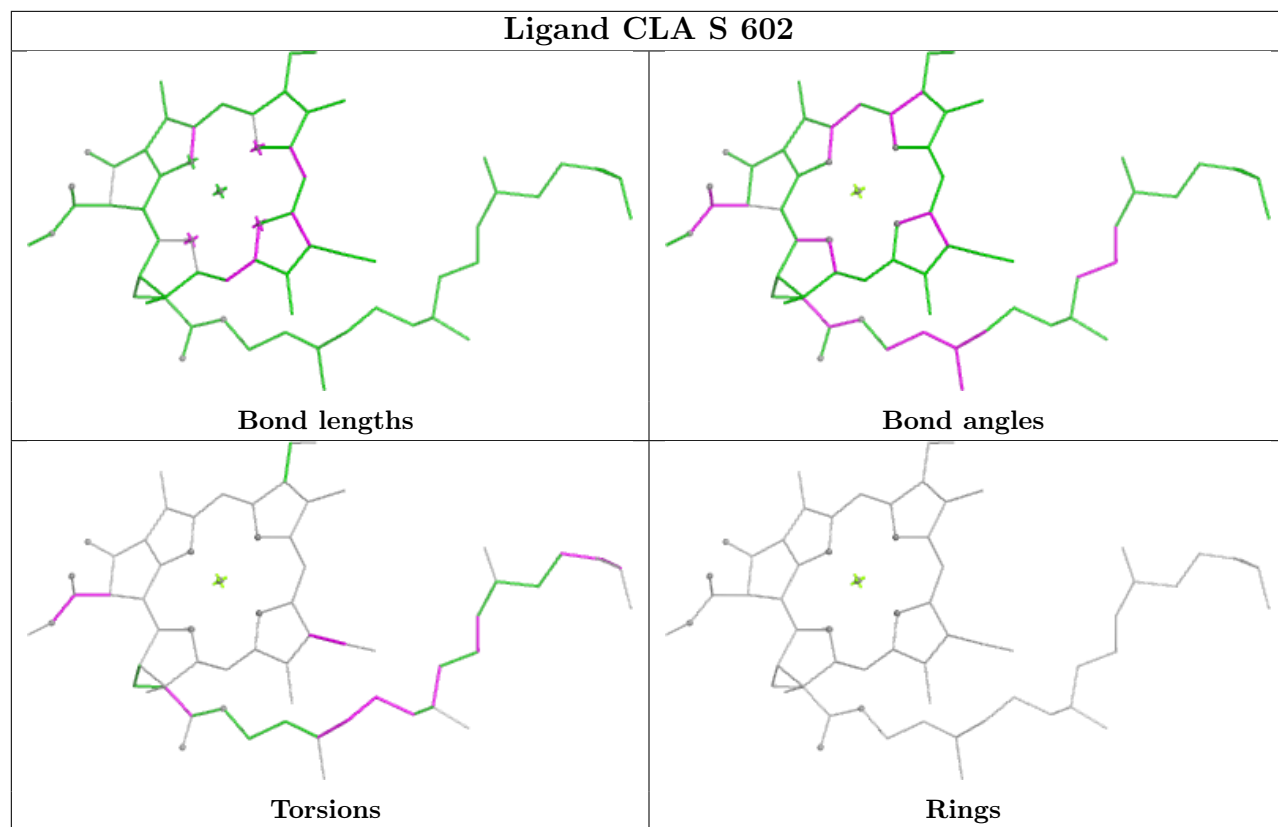




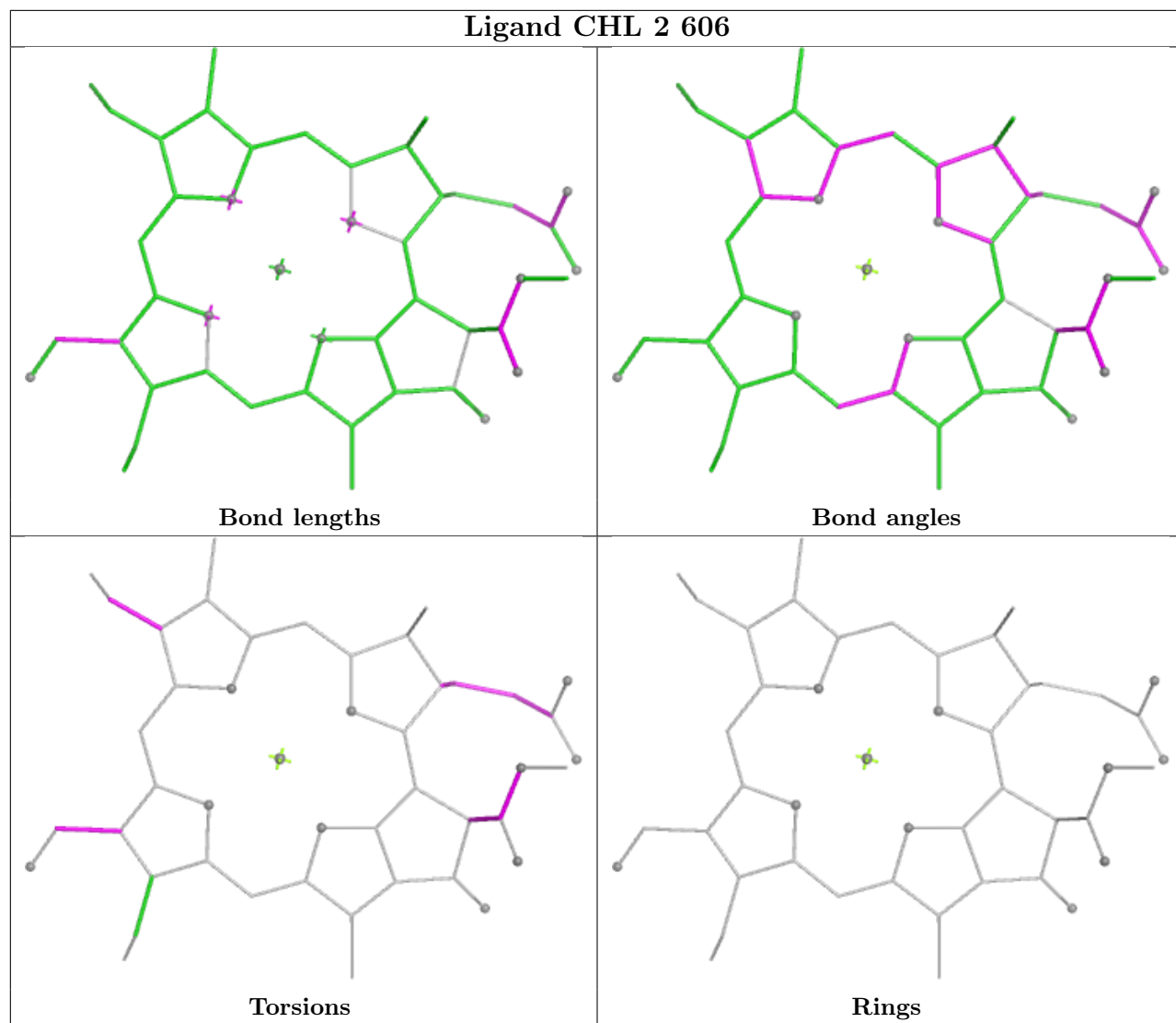


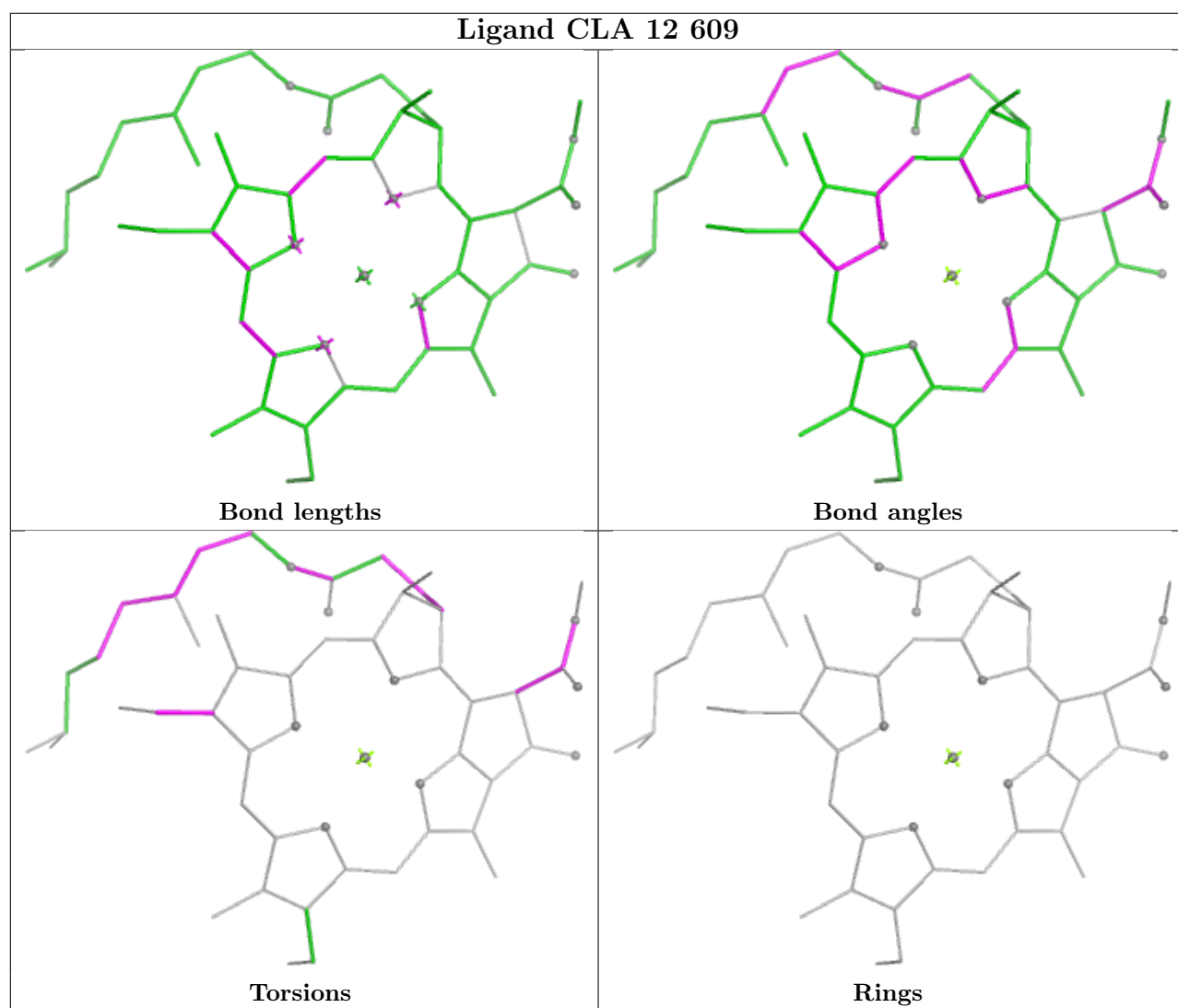




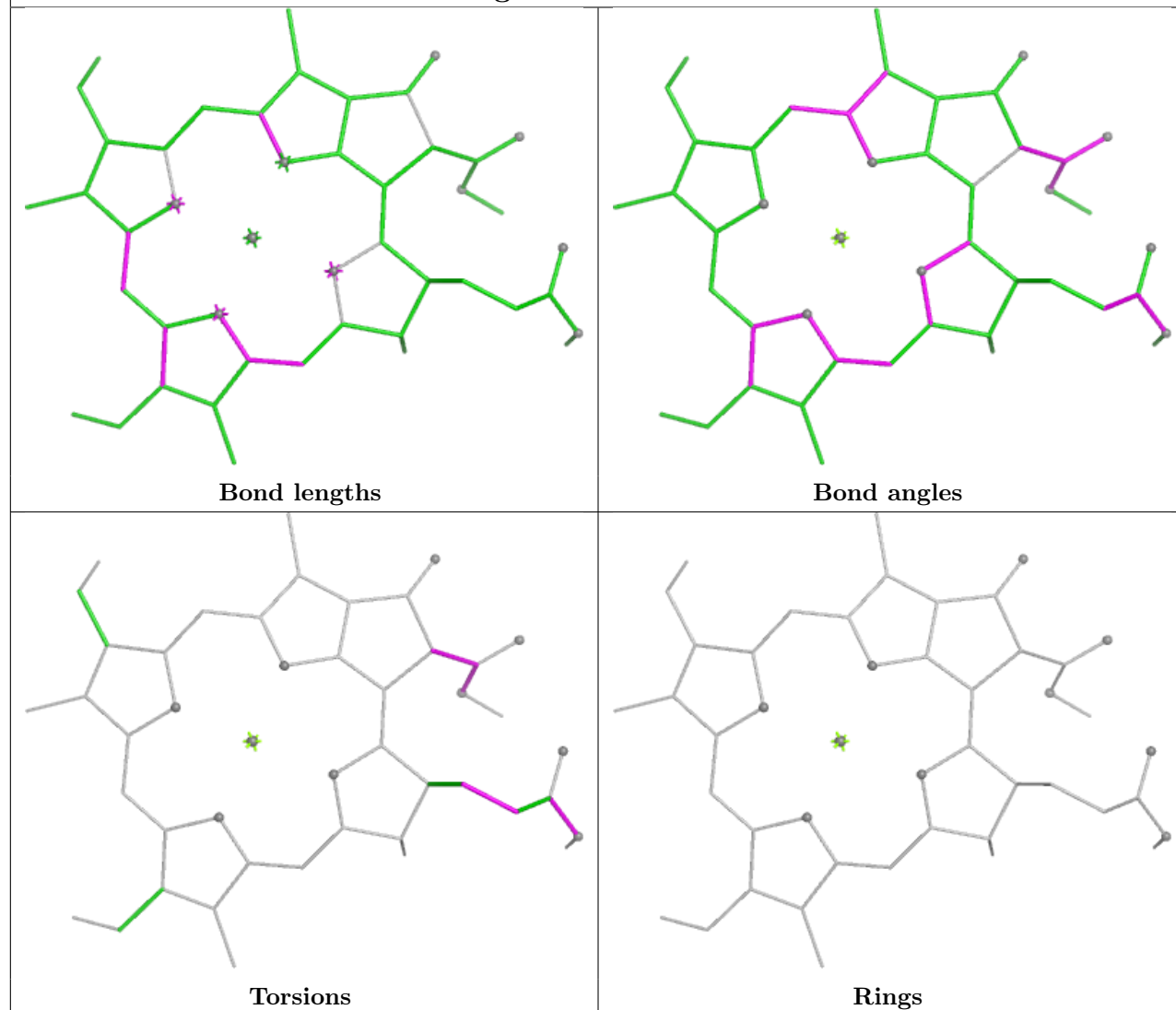


Ligand CHL 2 606

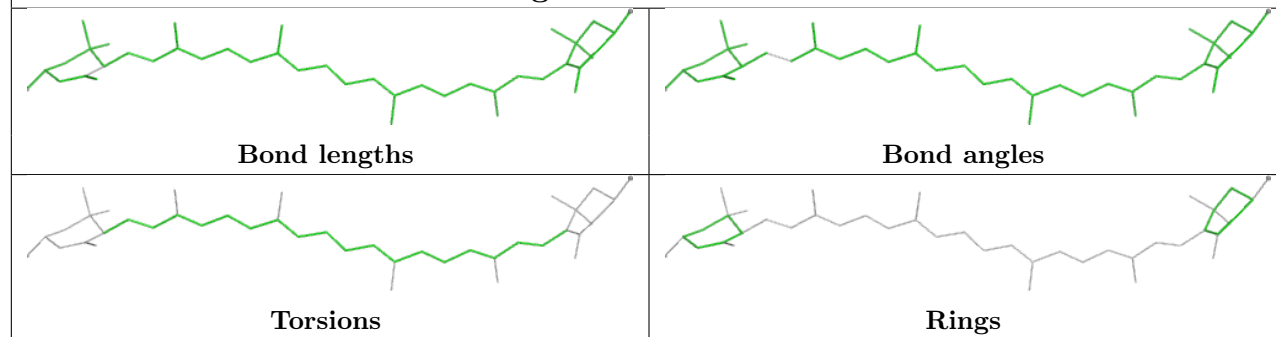


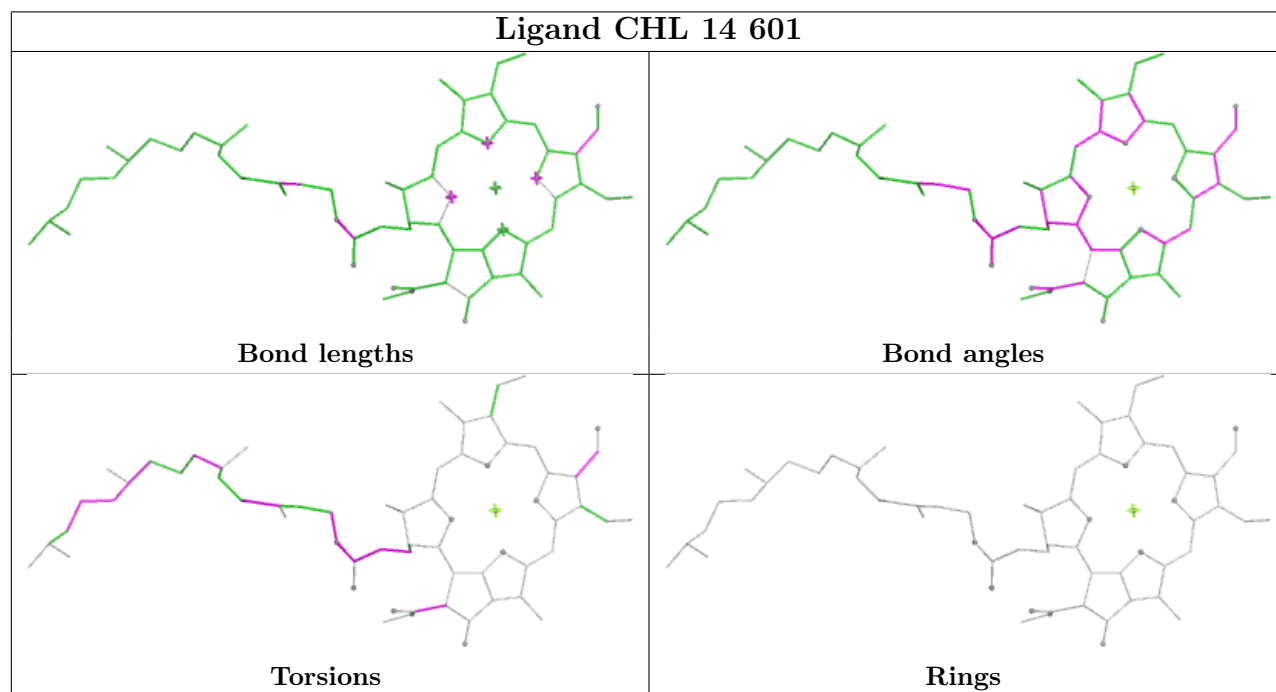
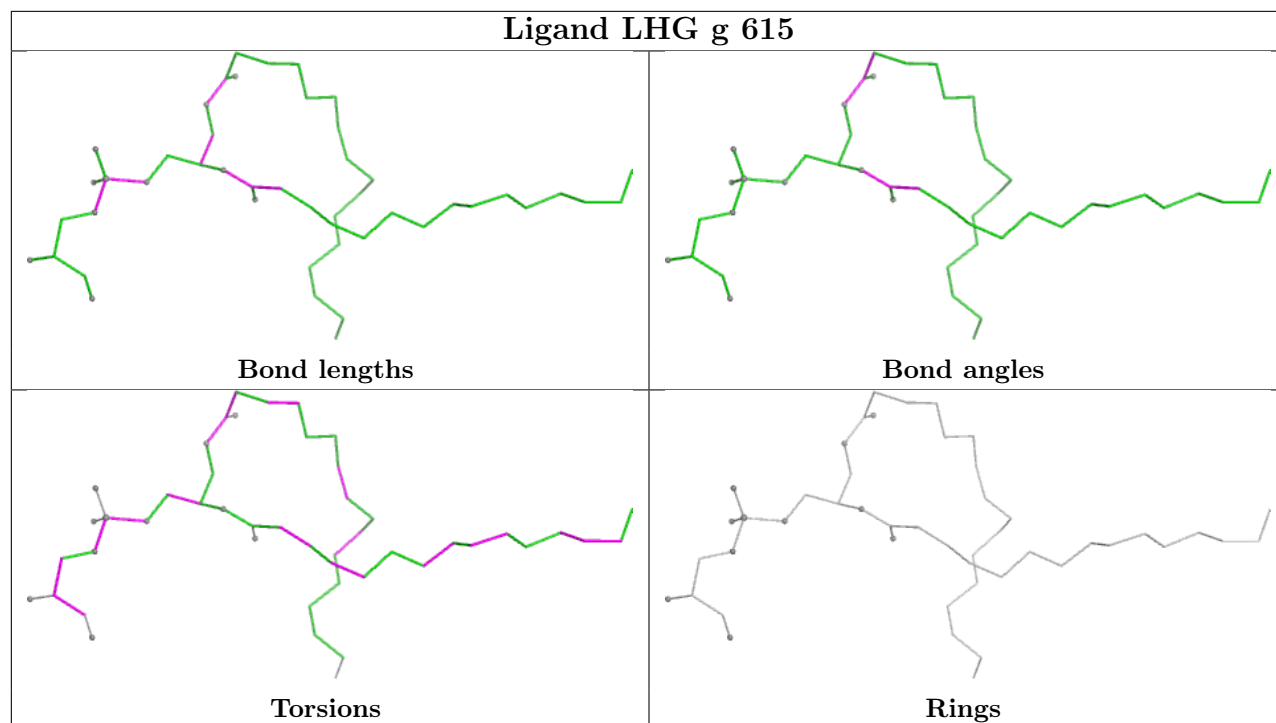


Ligand CLA 2 612

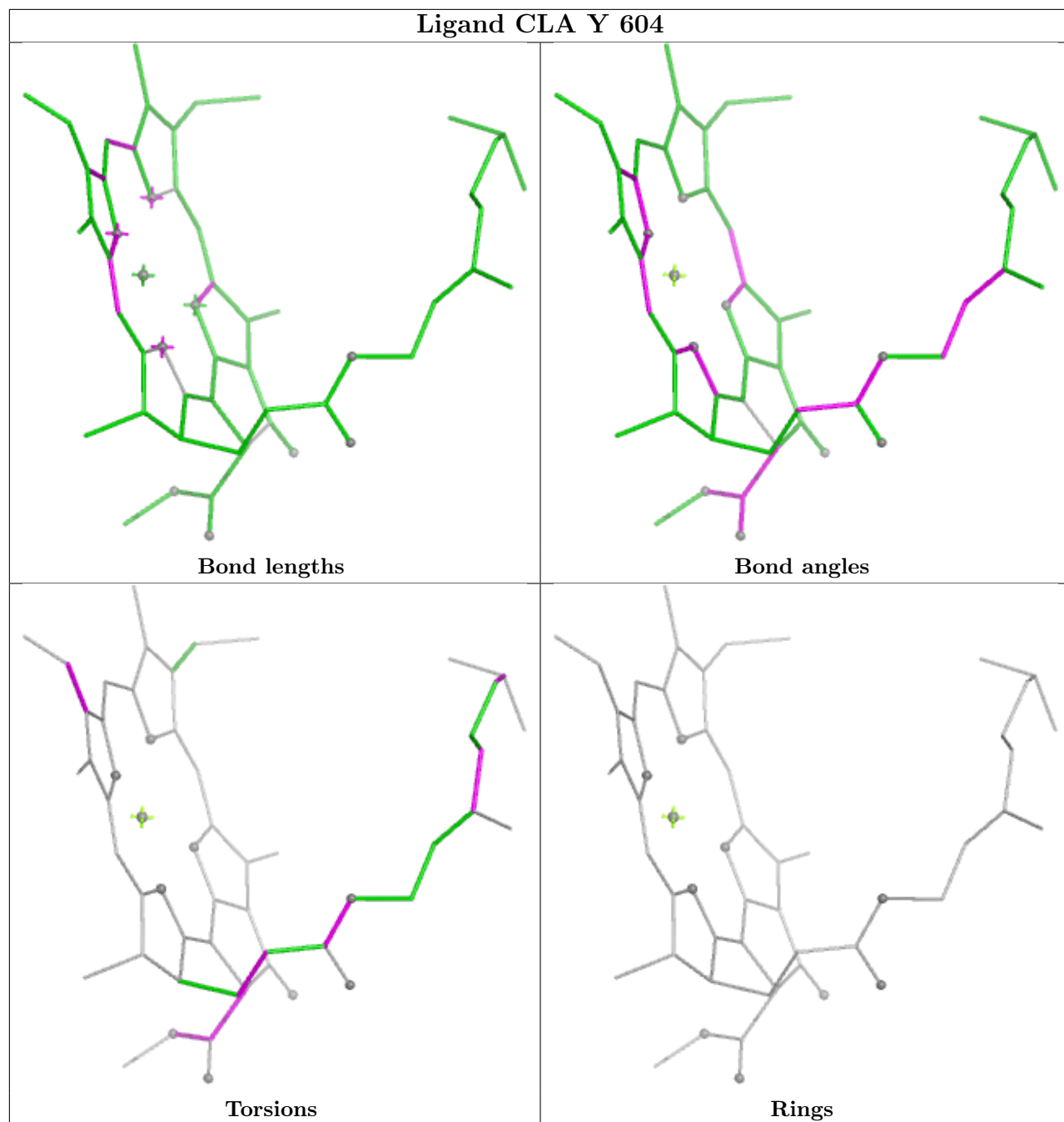


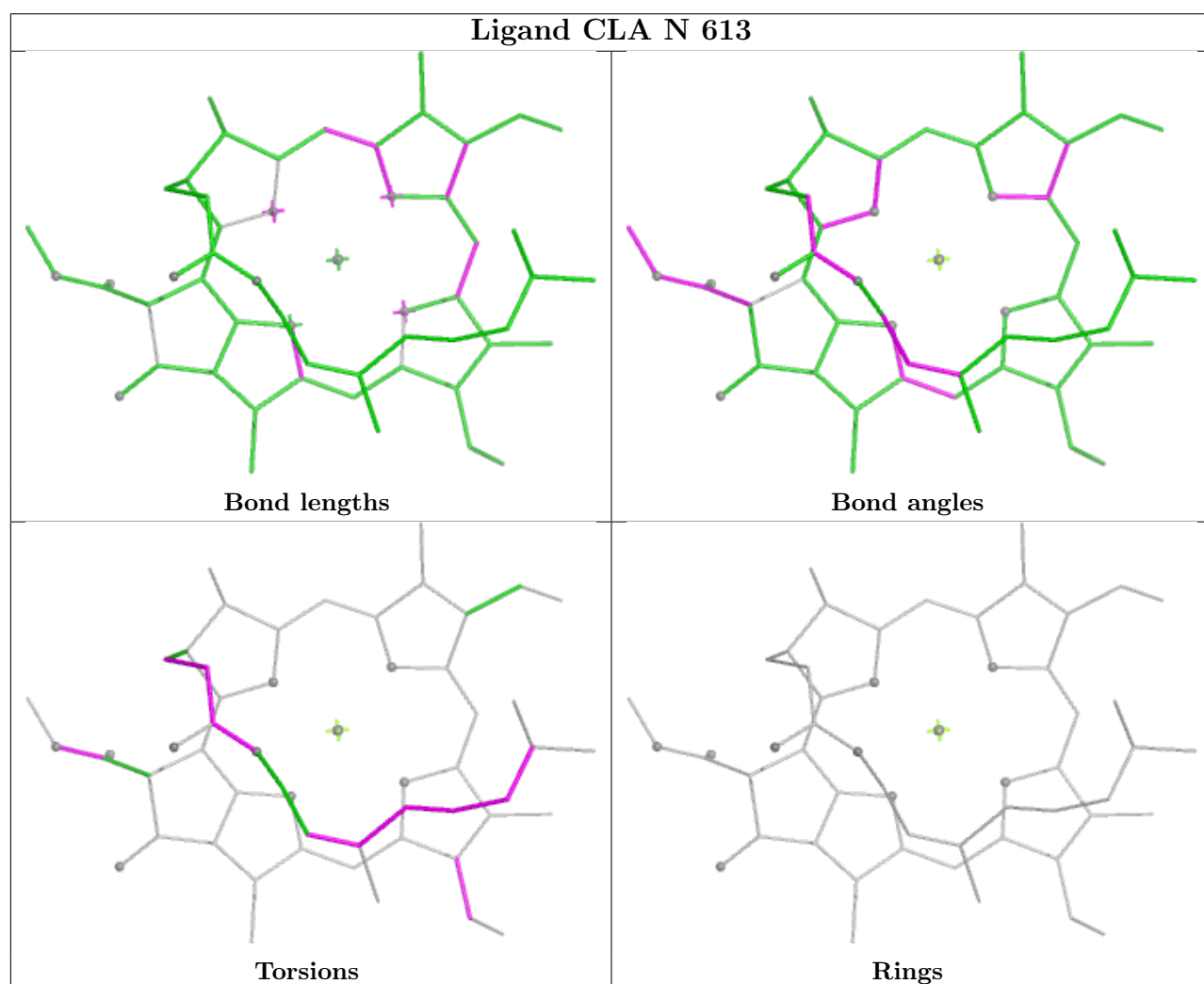
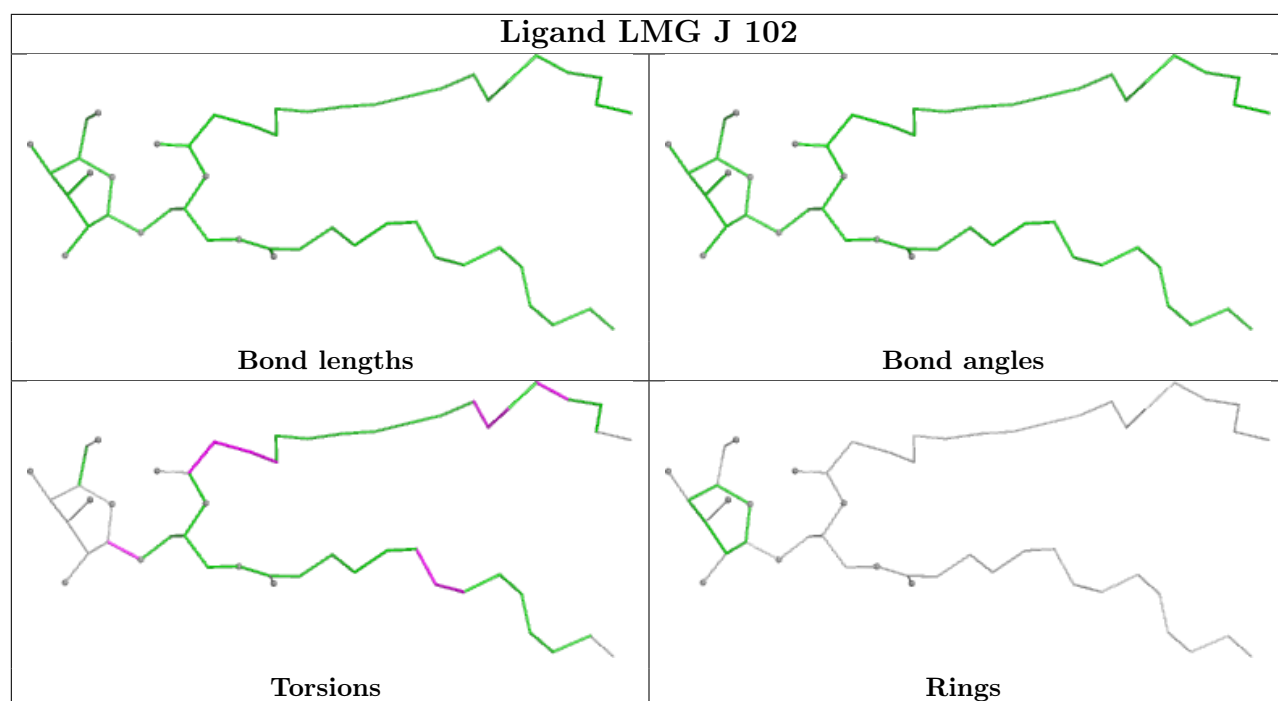
Ligand LUT N 617

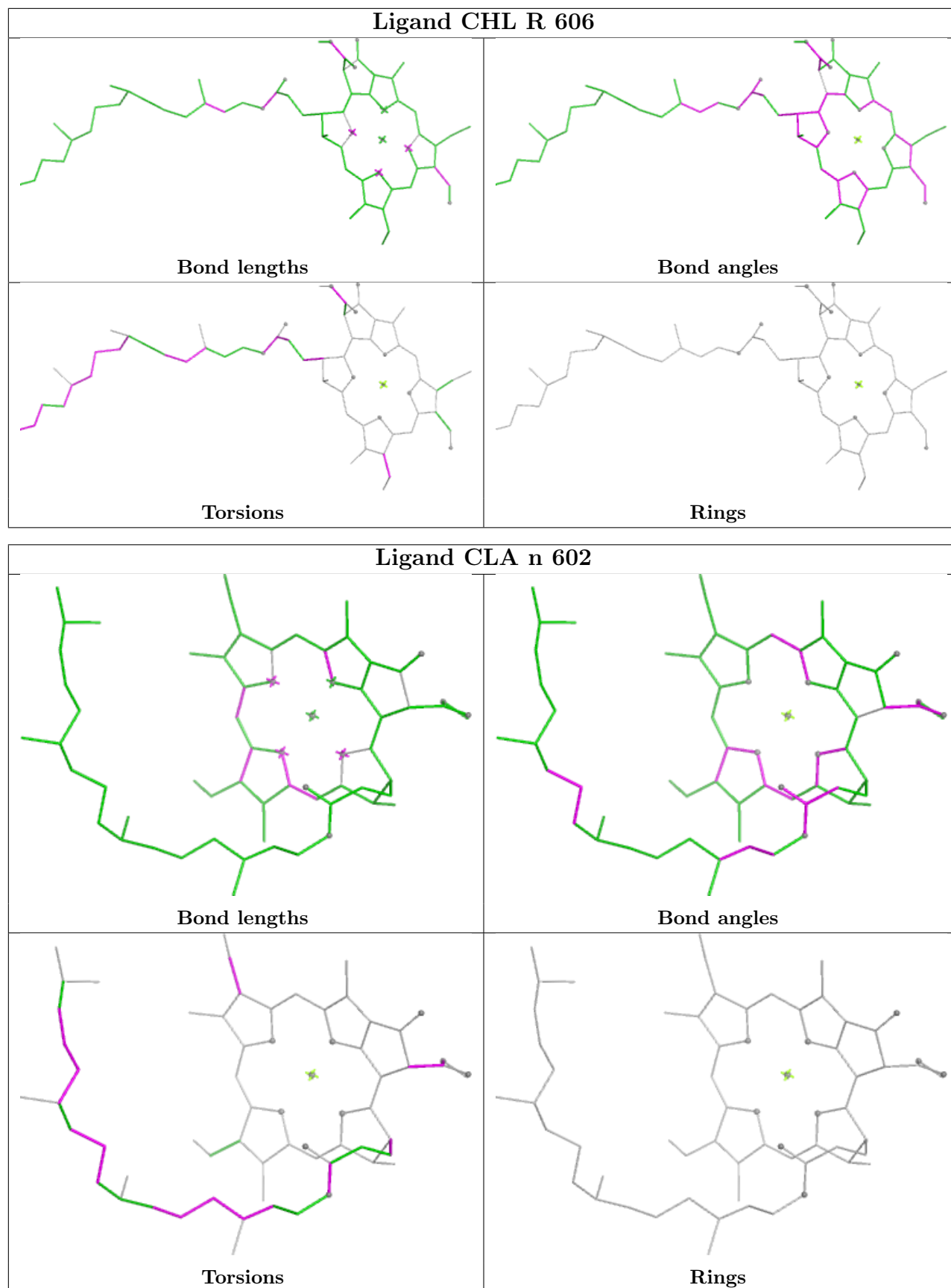


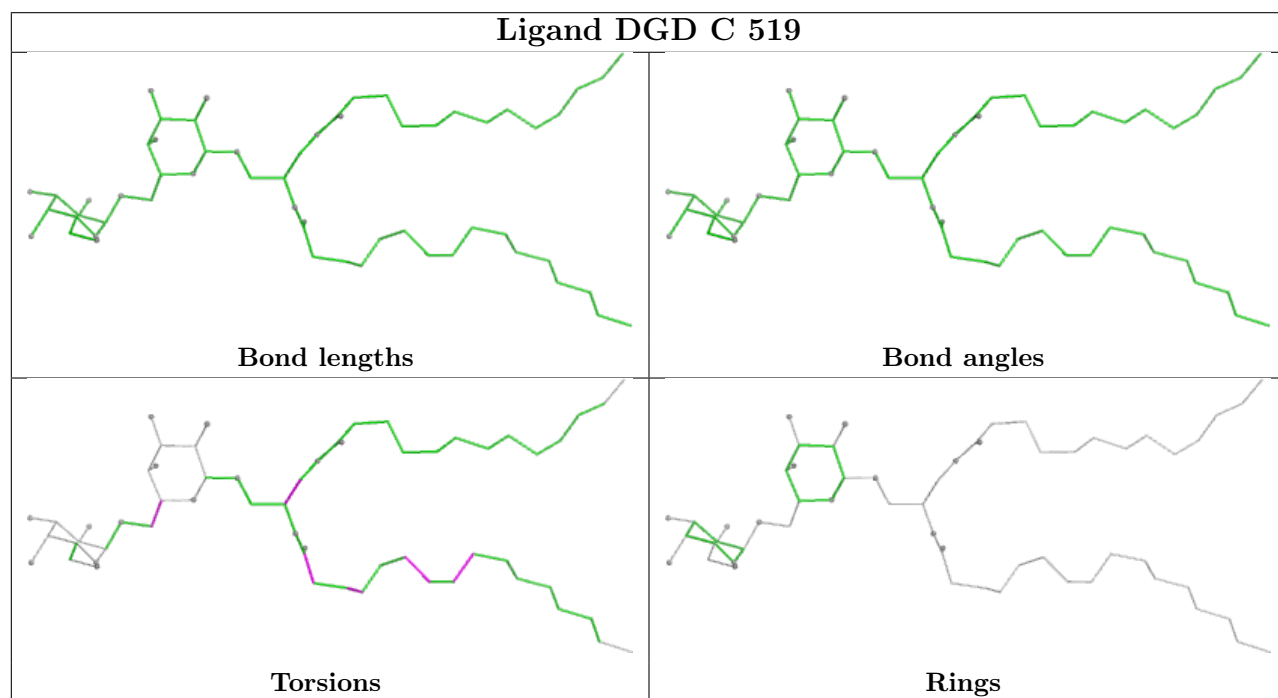
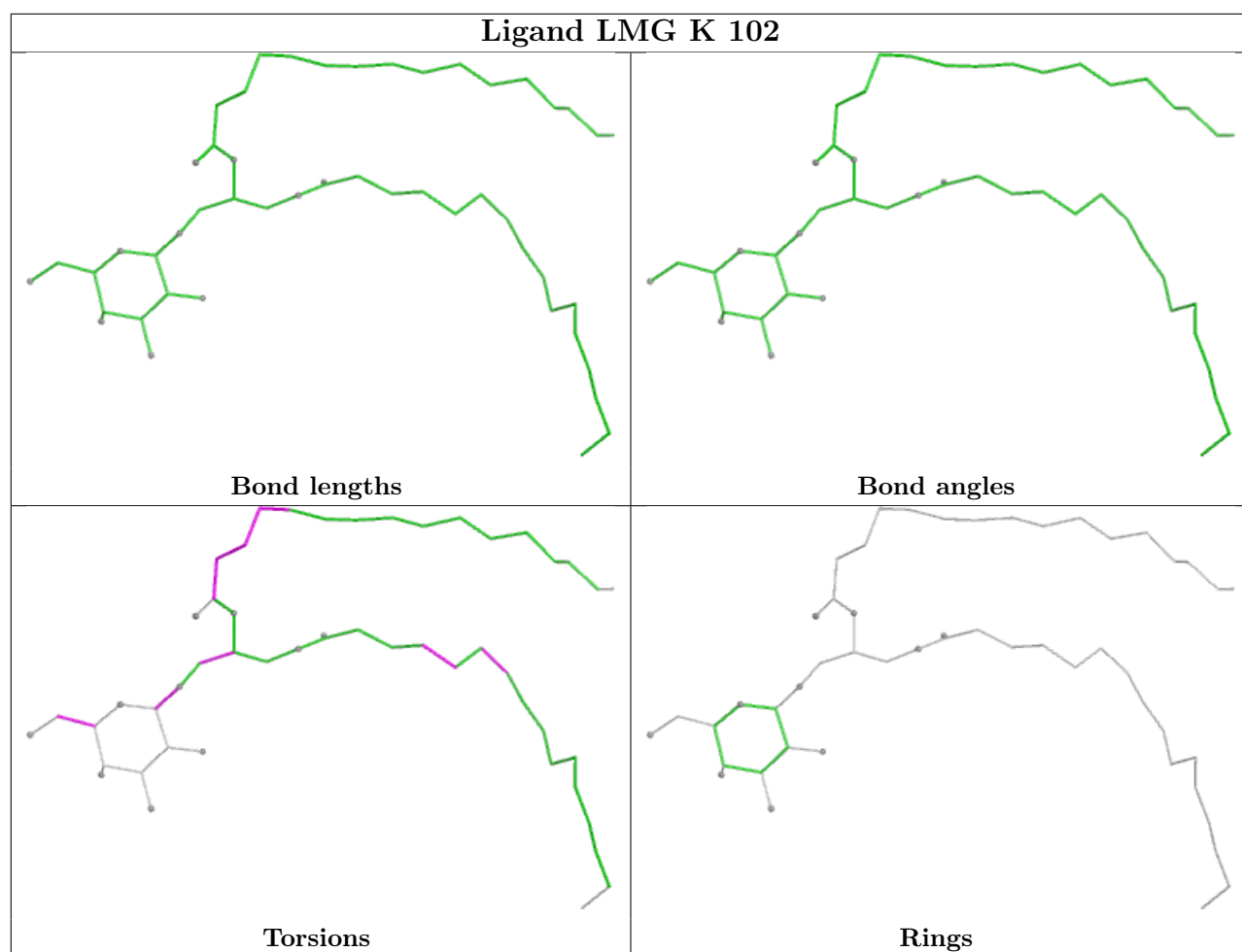


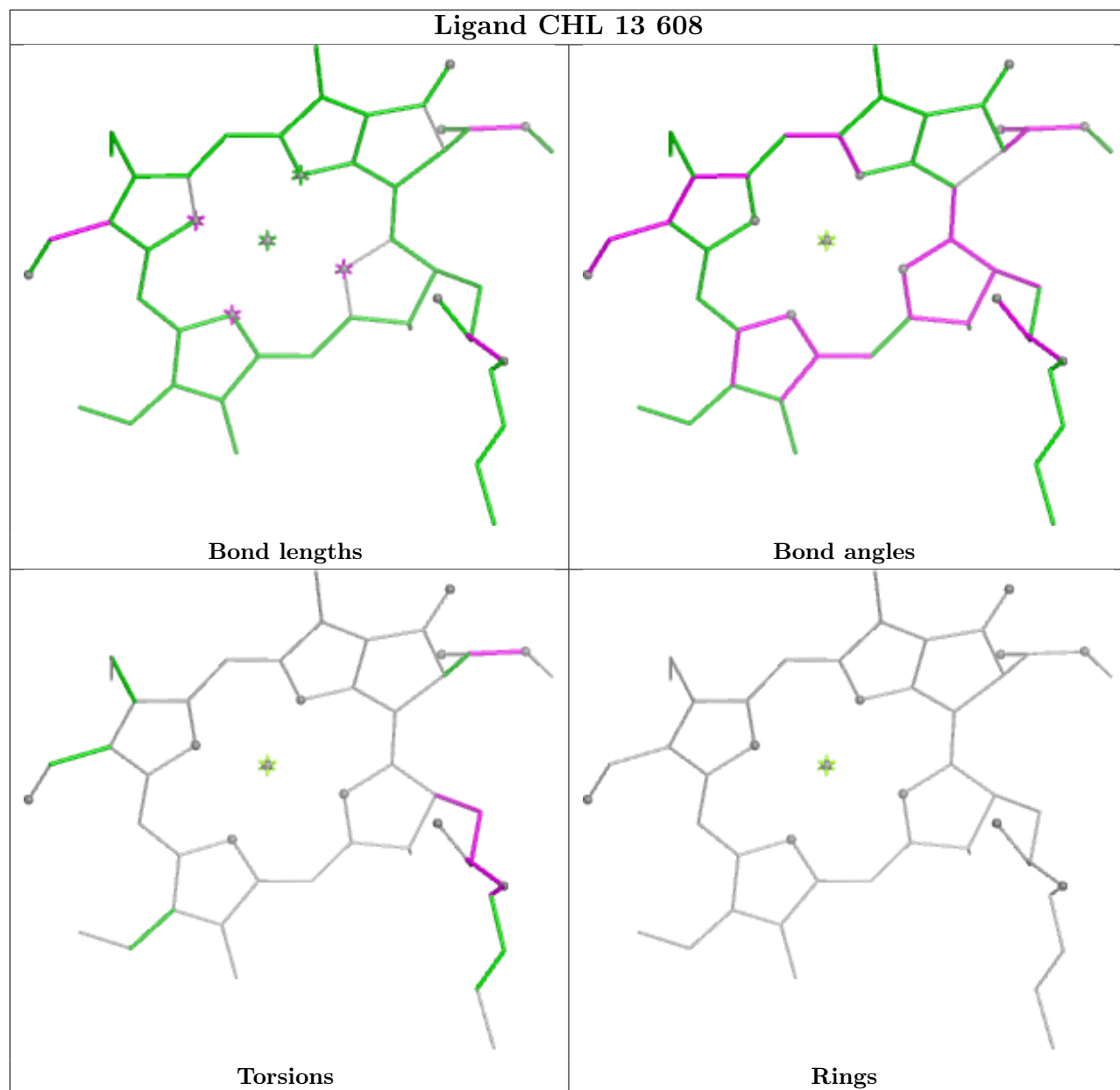
Ligand CLA Y 604

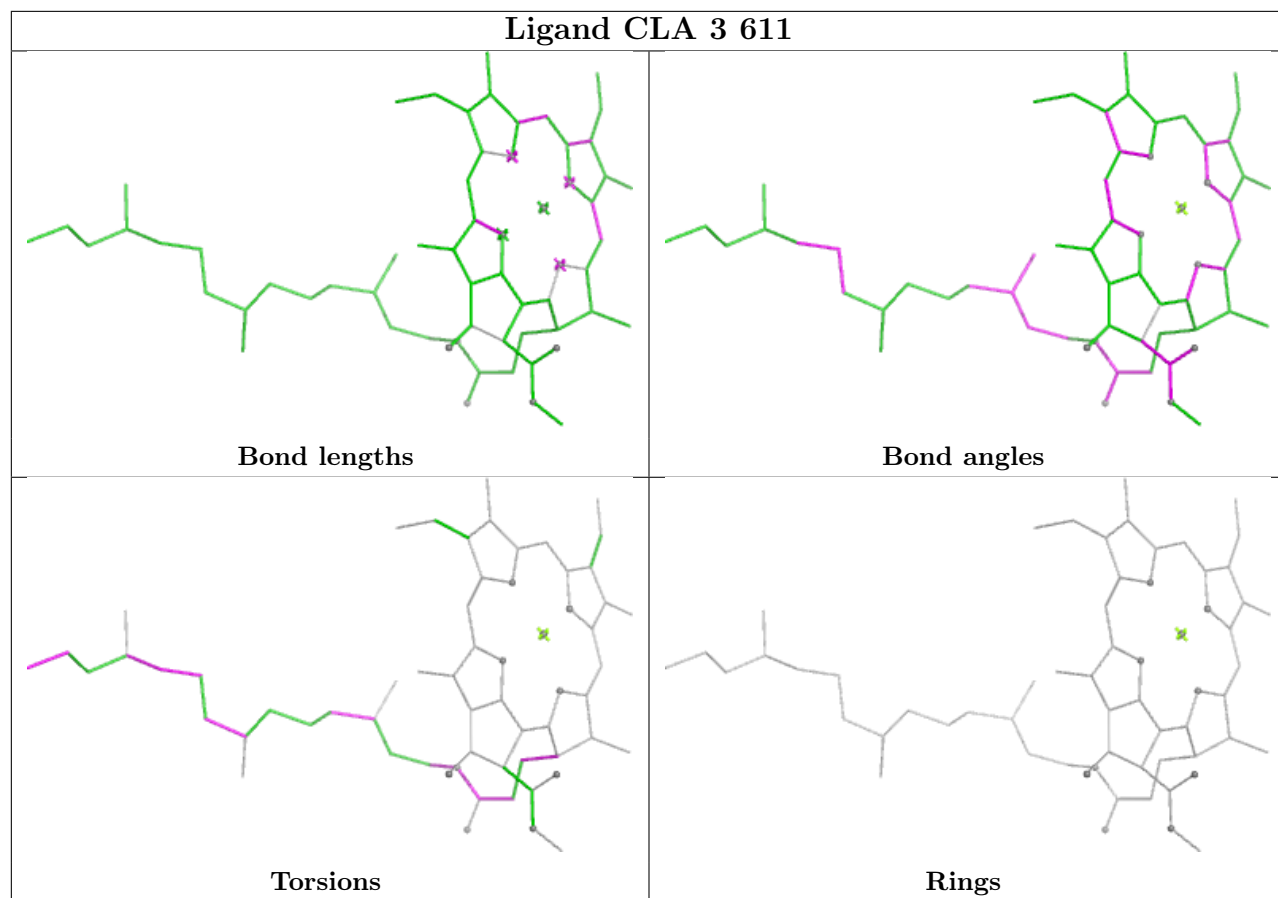




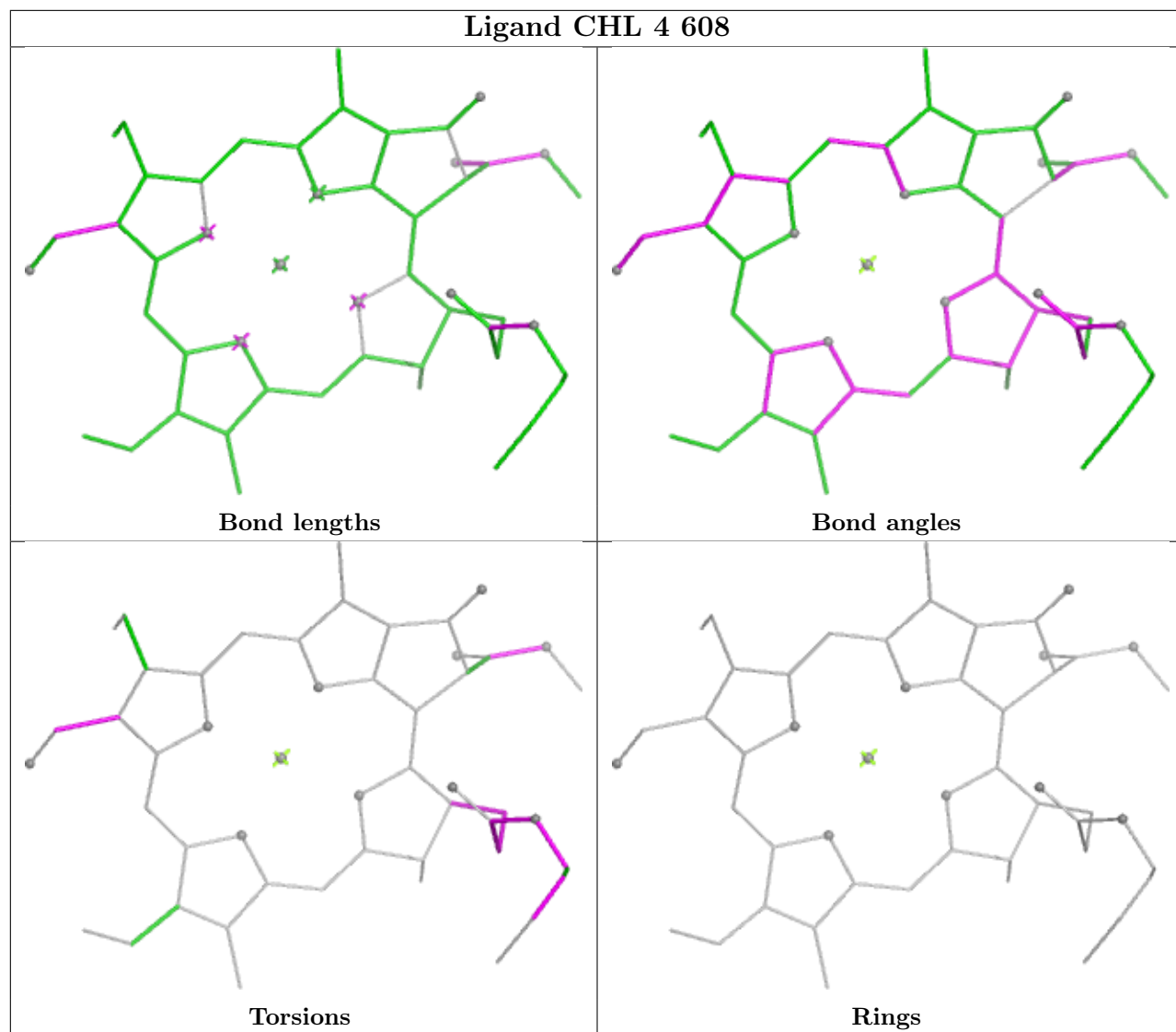


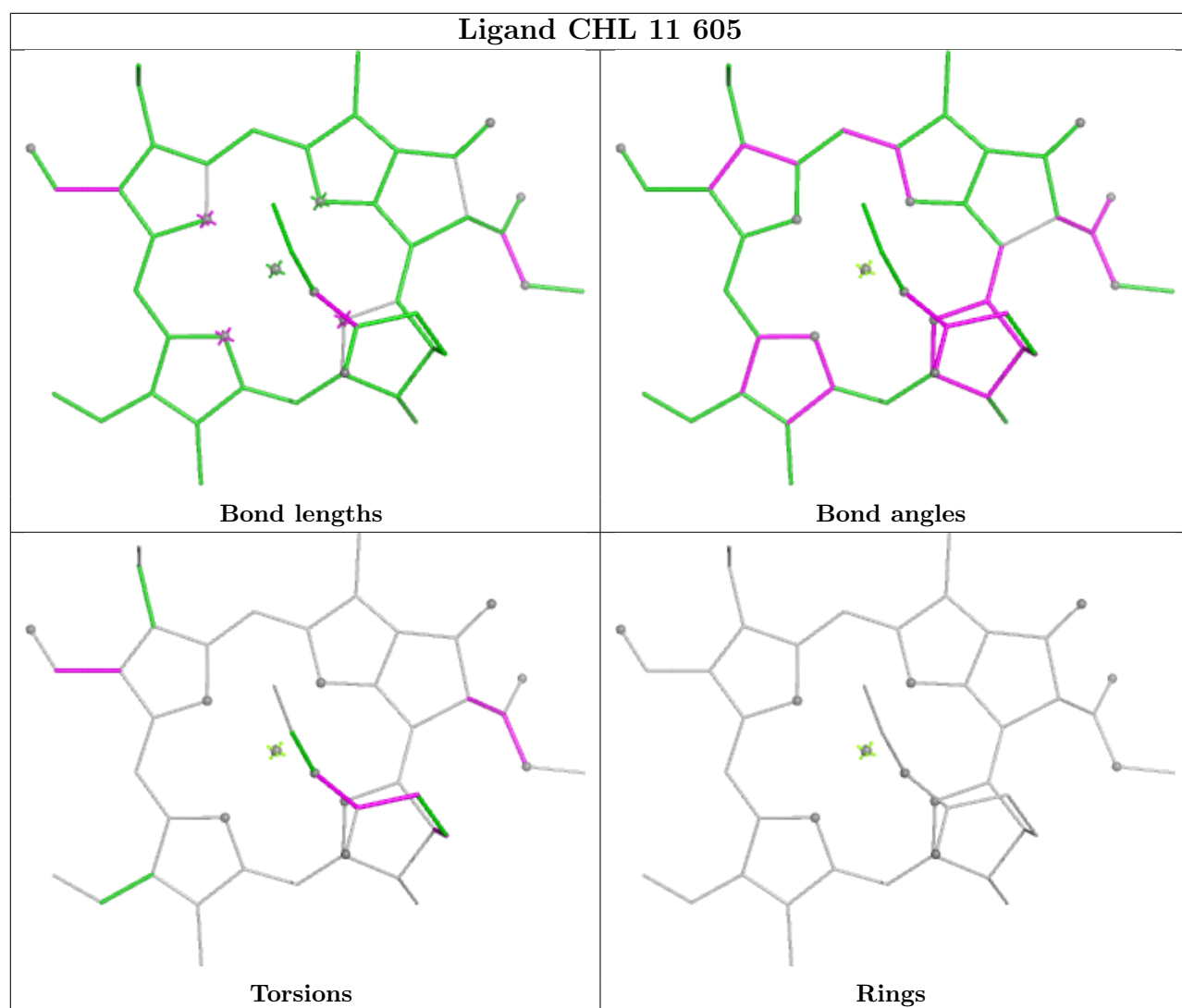




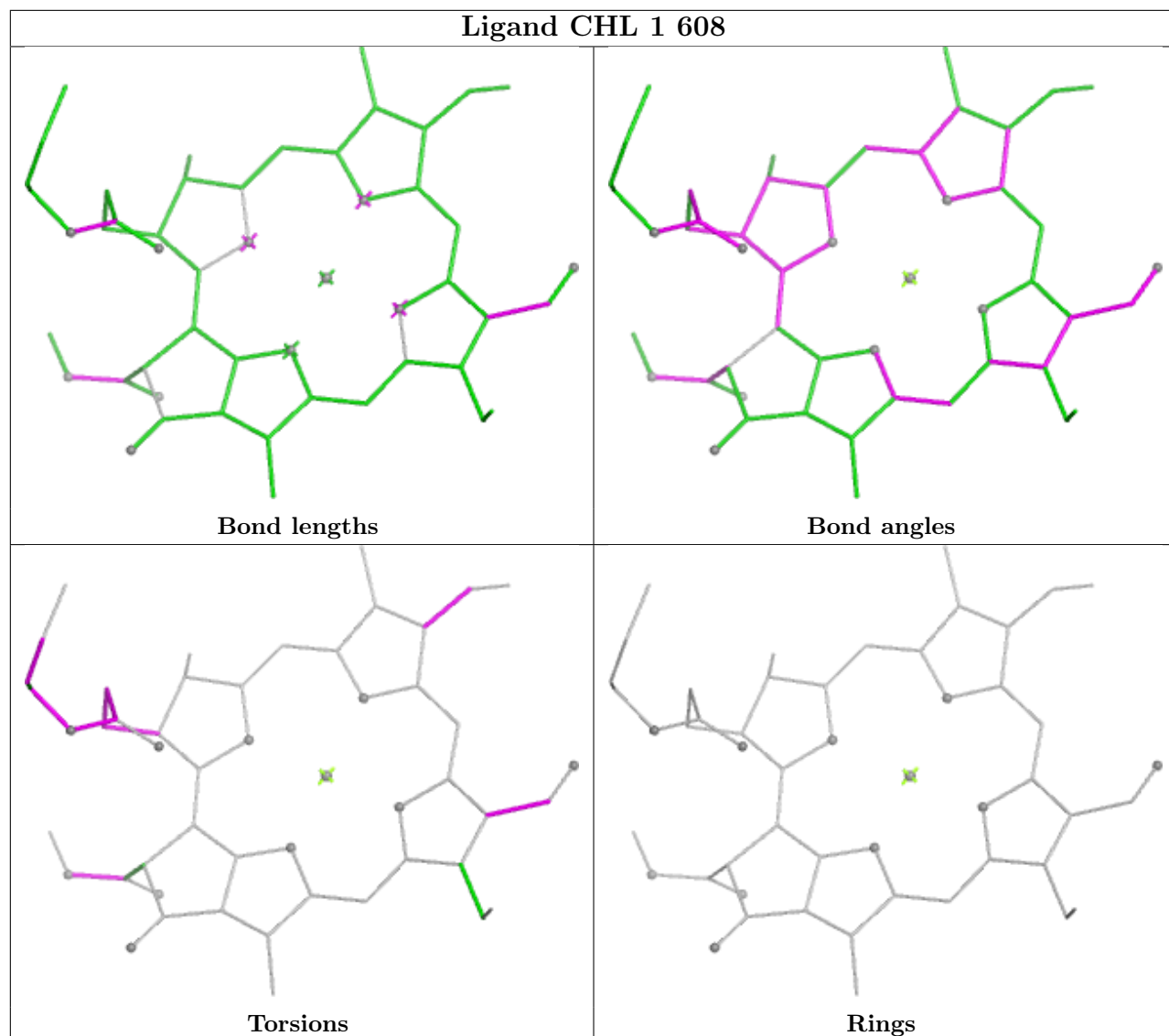


Ligand CHL 4 608

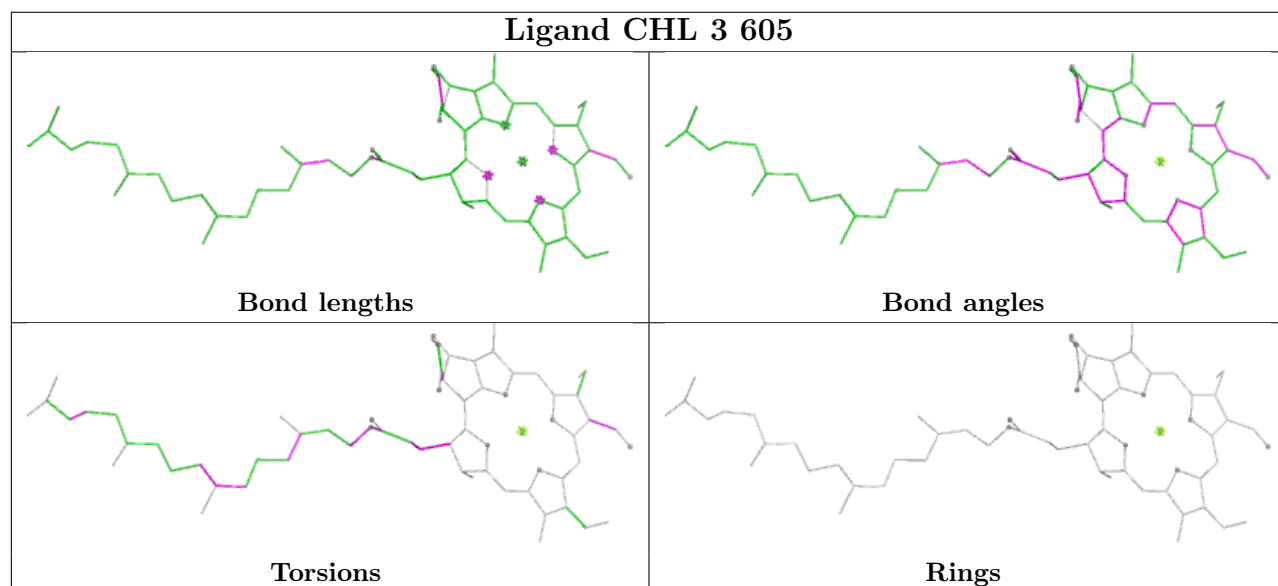




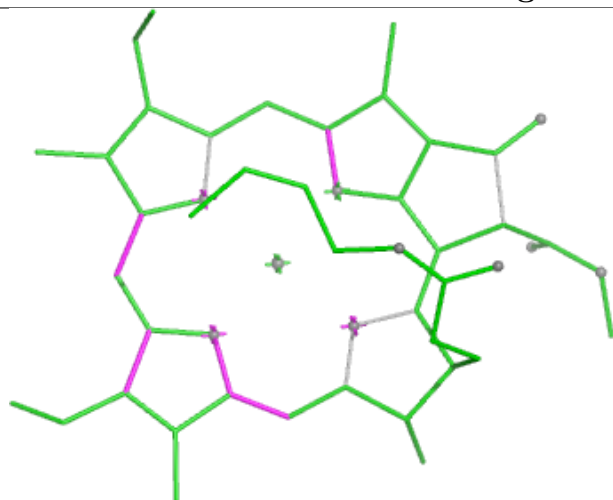
Ligand CHL 1 608



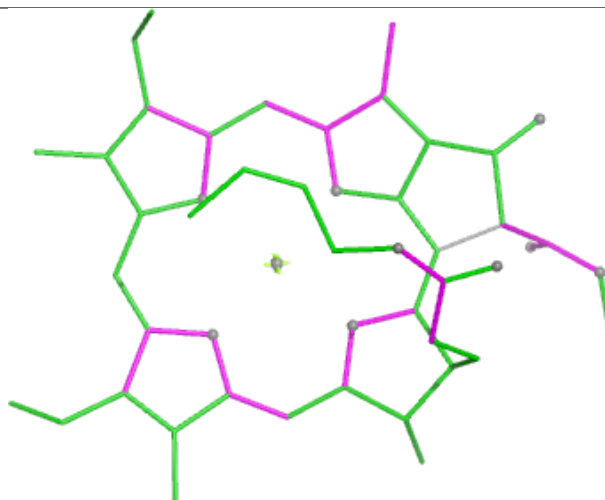
Ligand CHL 3 605



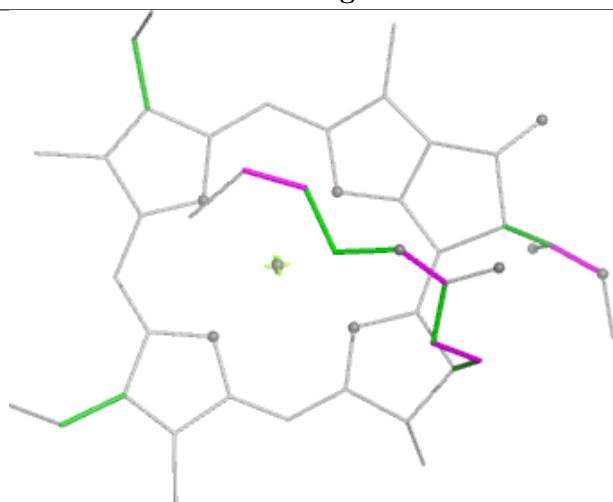
Ligand CLA S 613



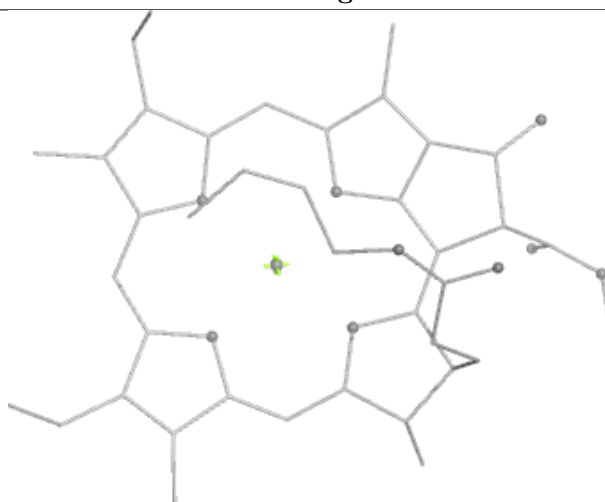
Bond lengths



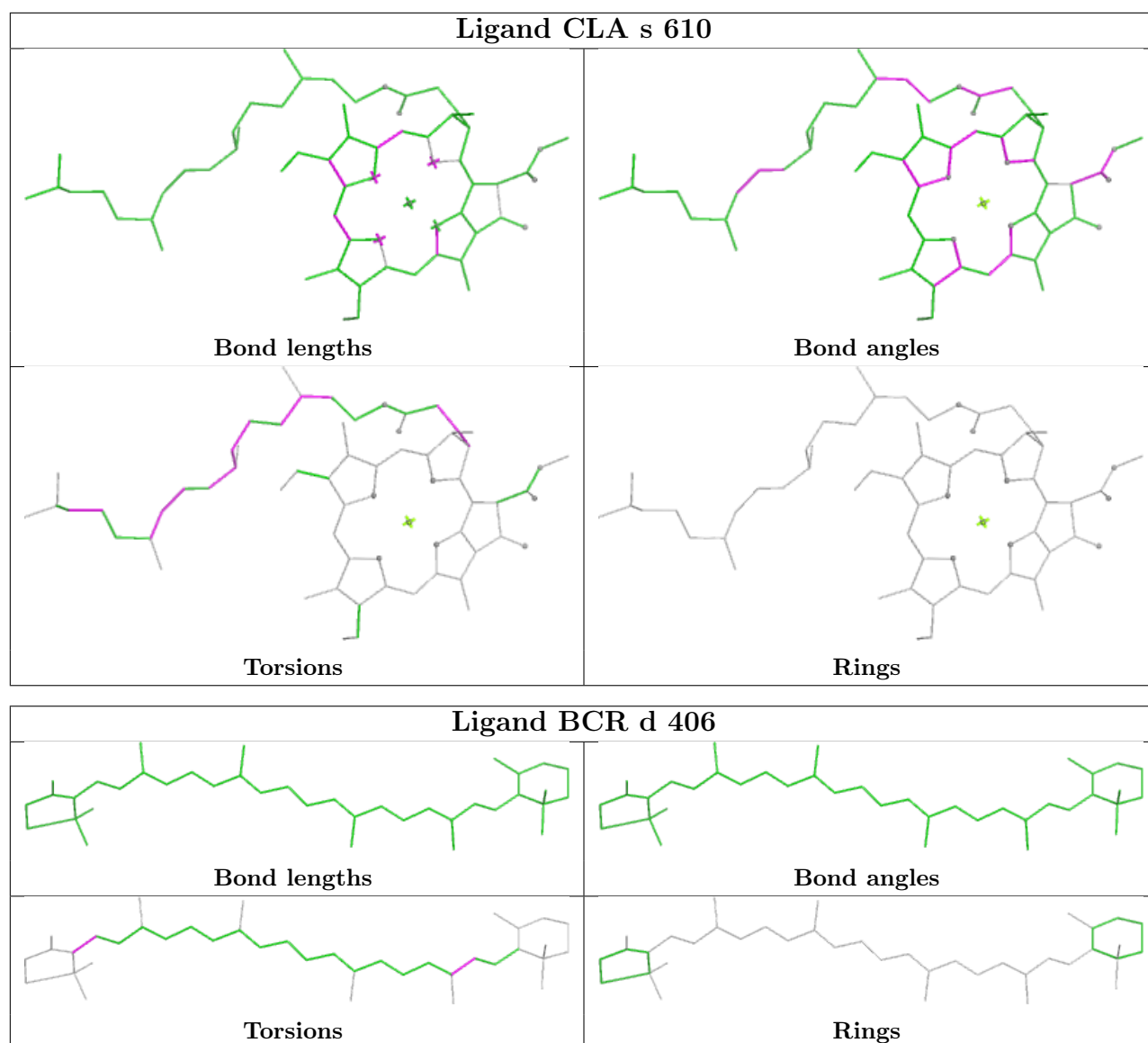
Bond angles



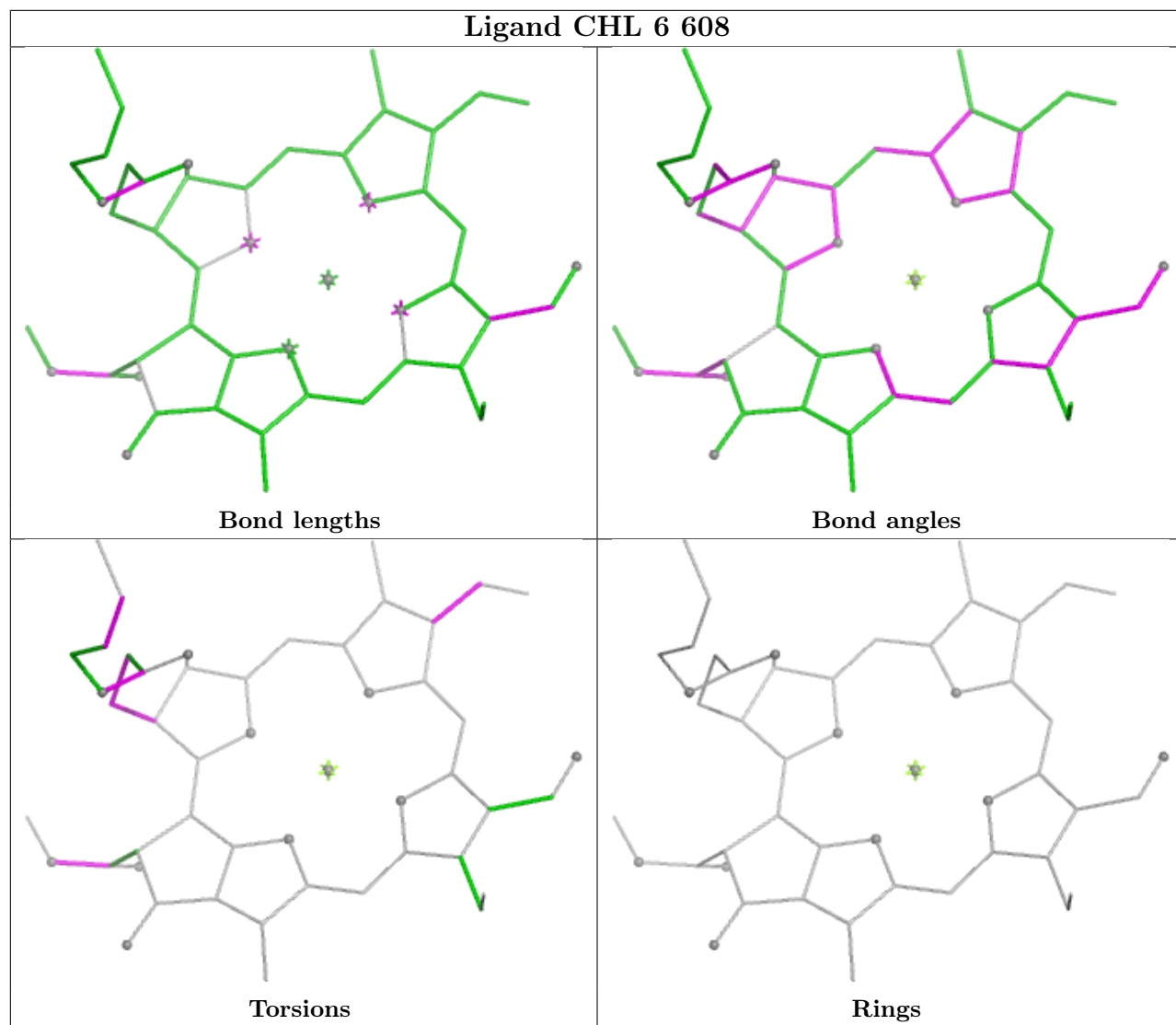
Torsions



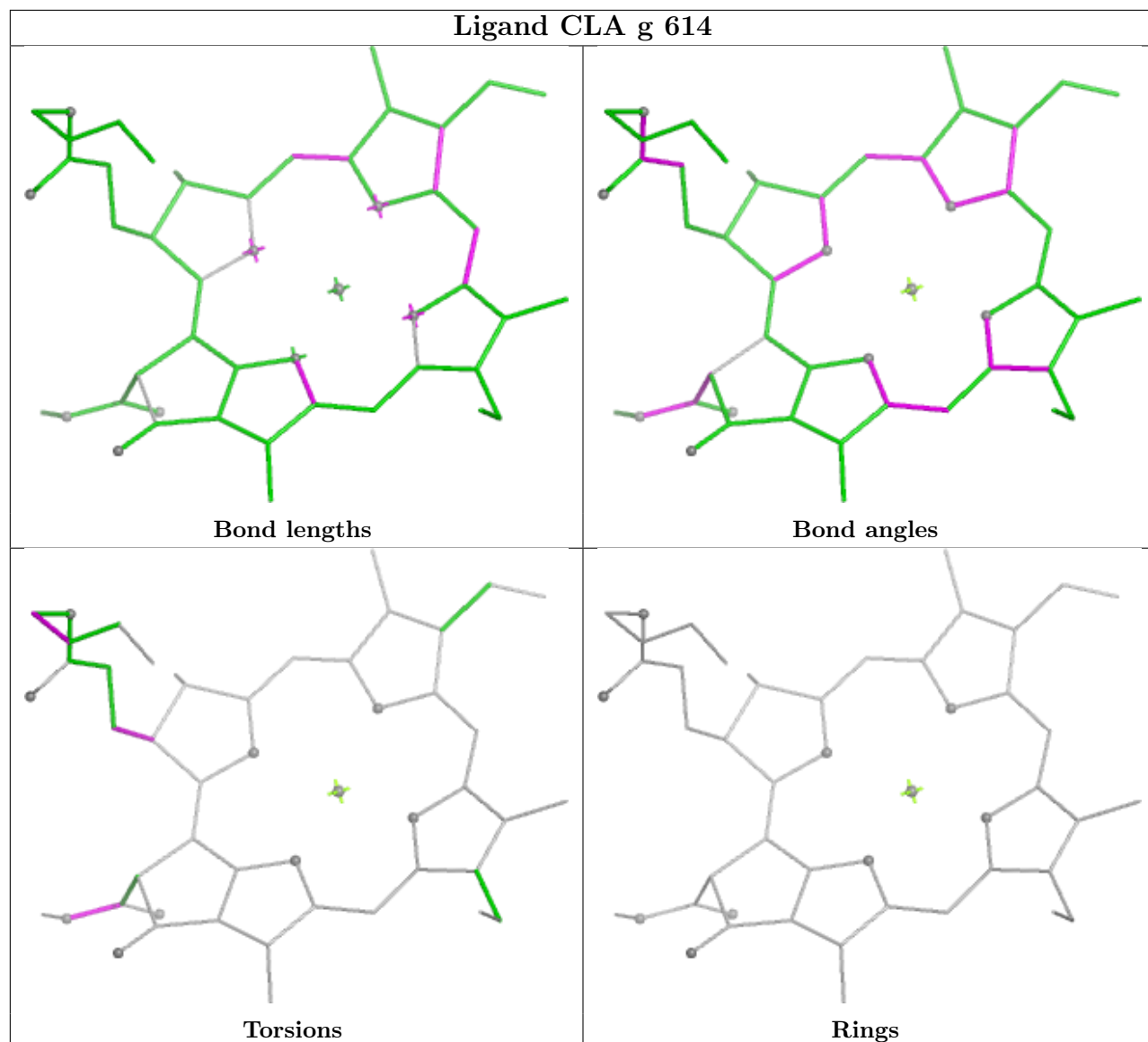
Rings

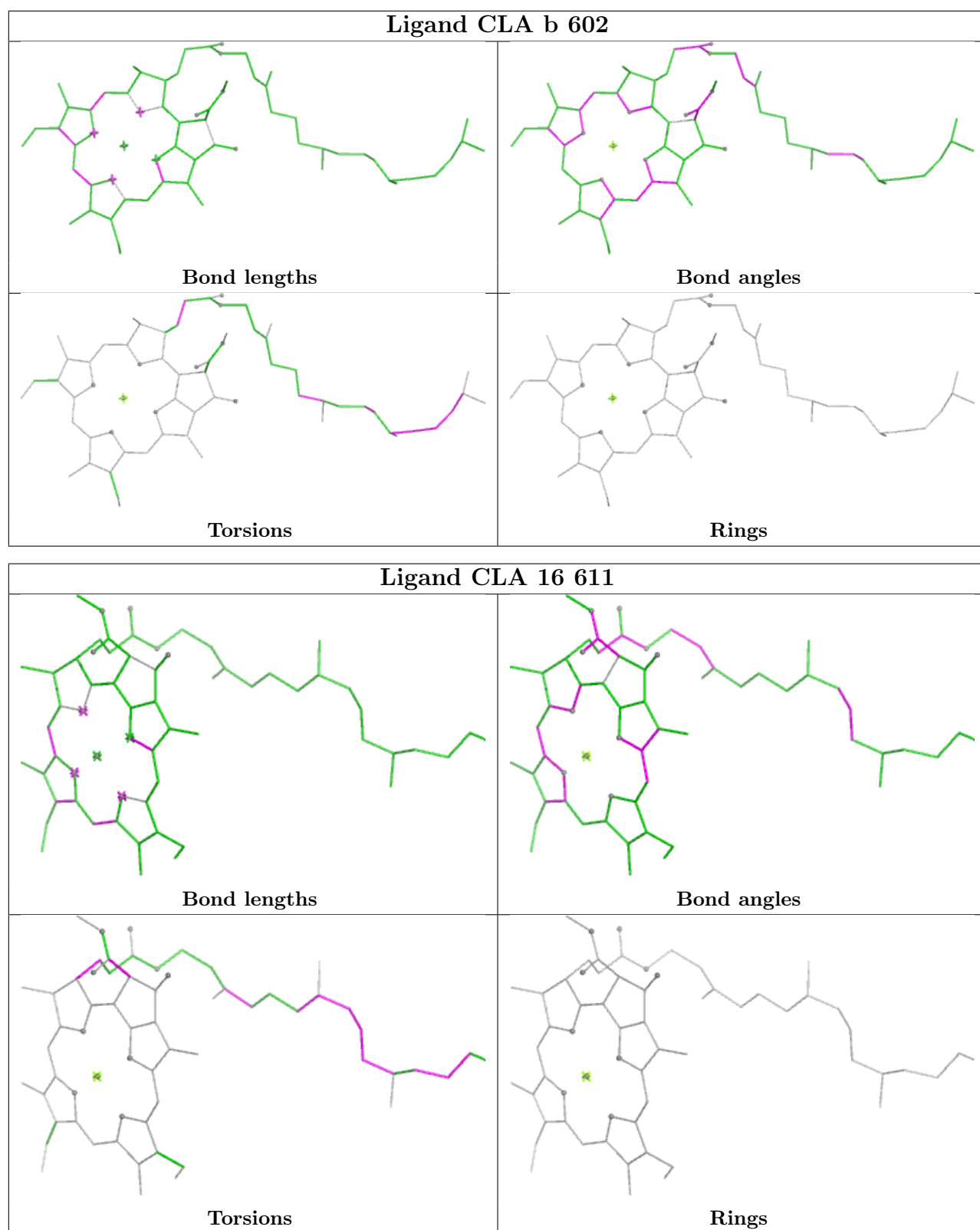


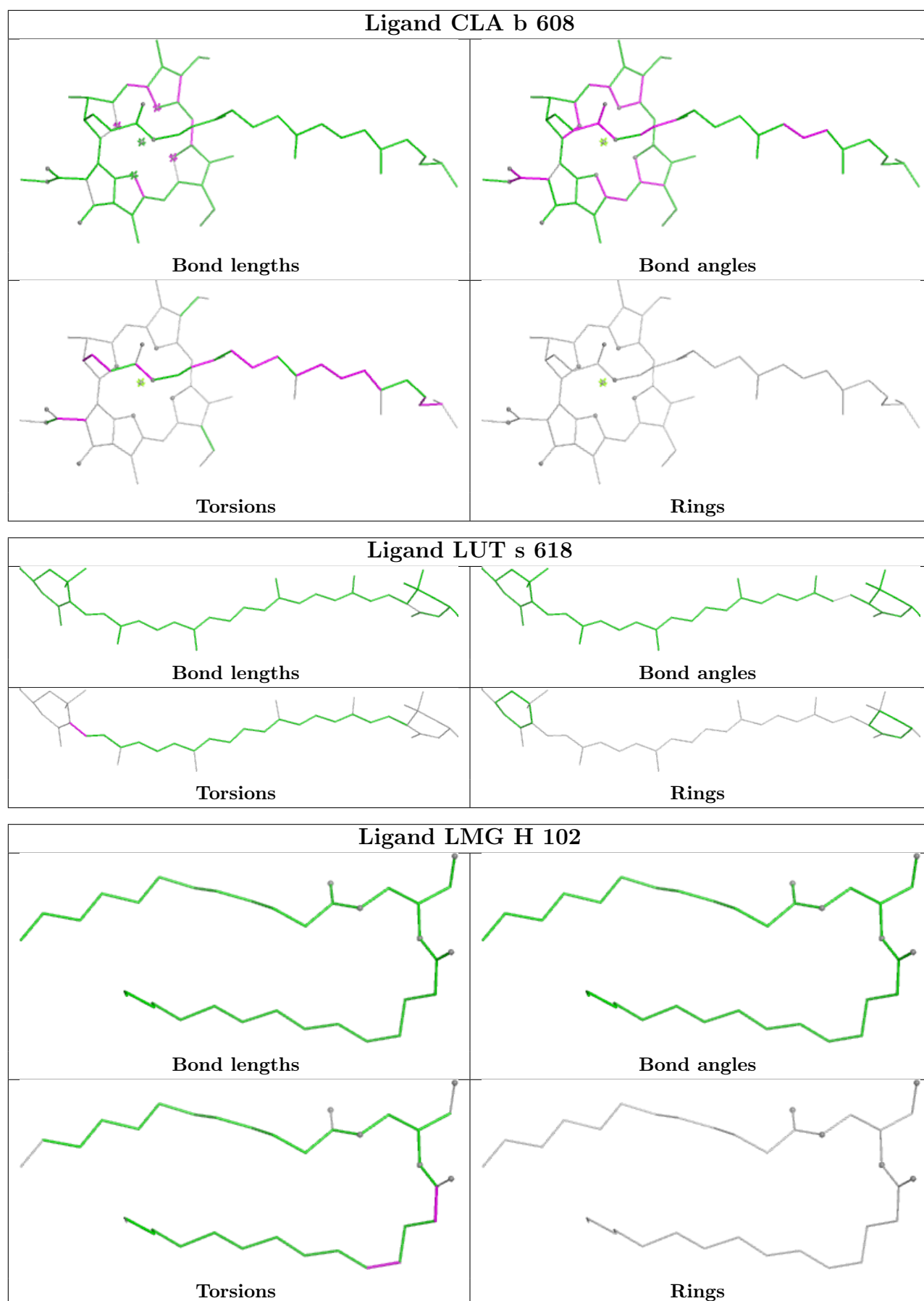
Ligand CHL 6 608

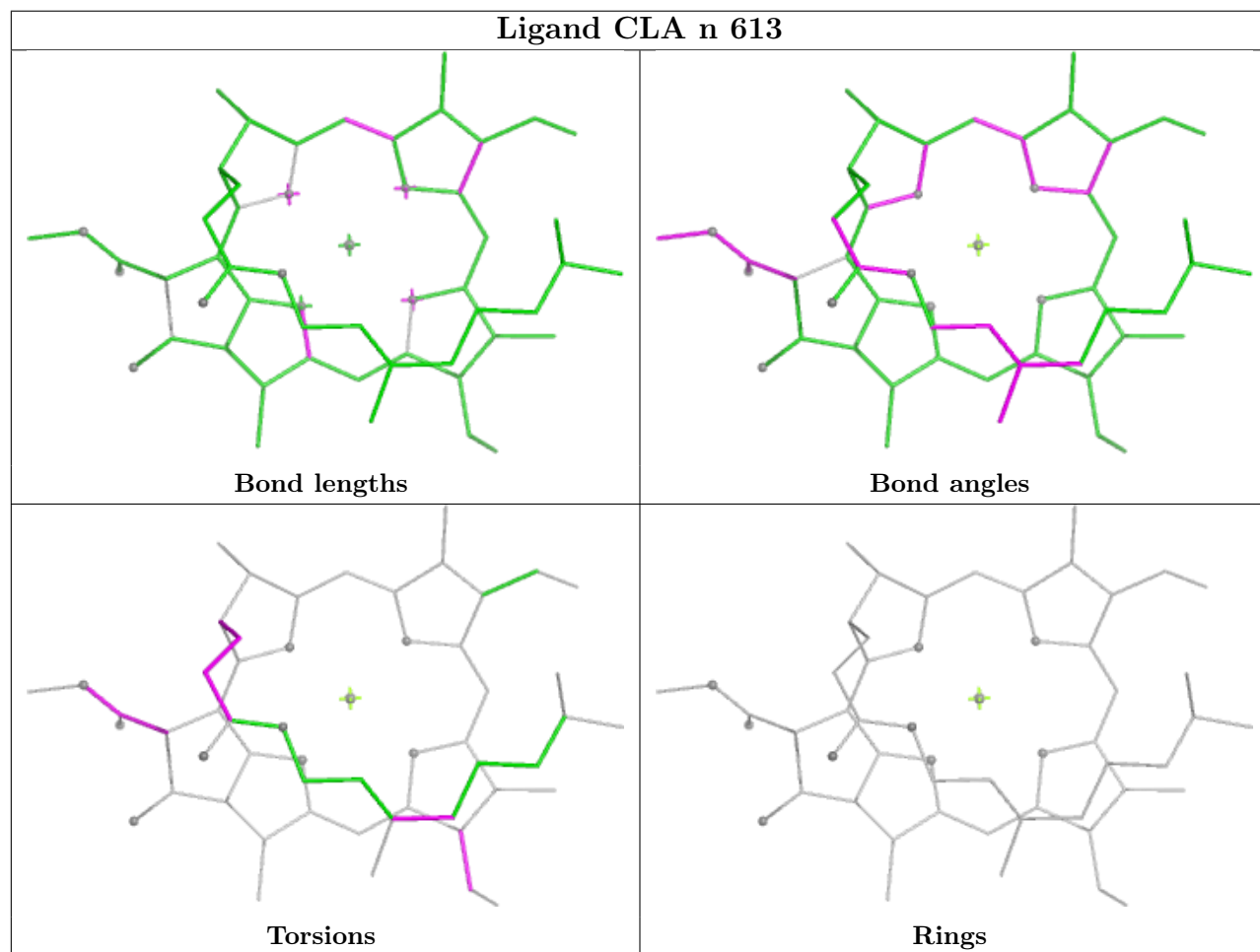
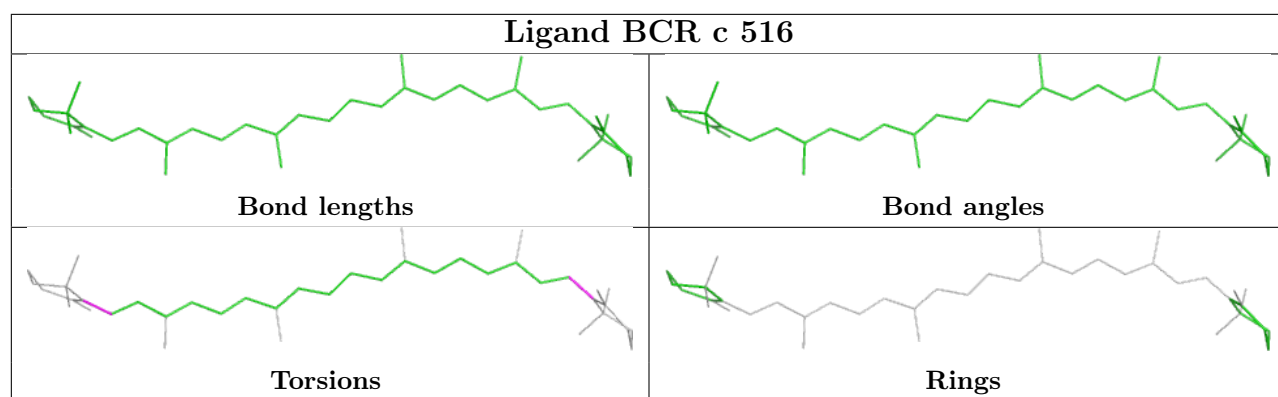


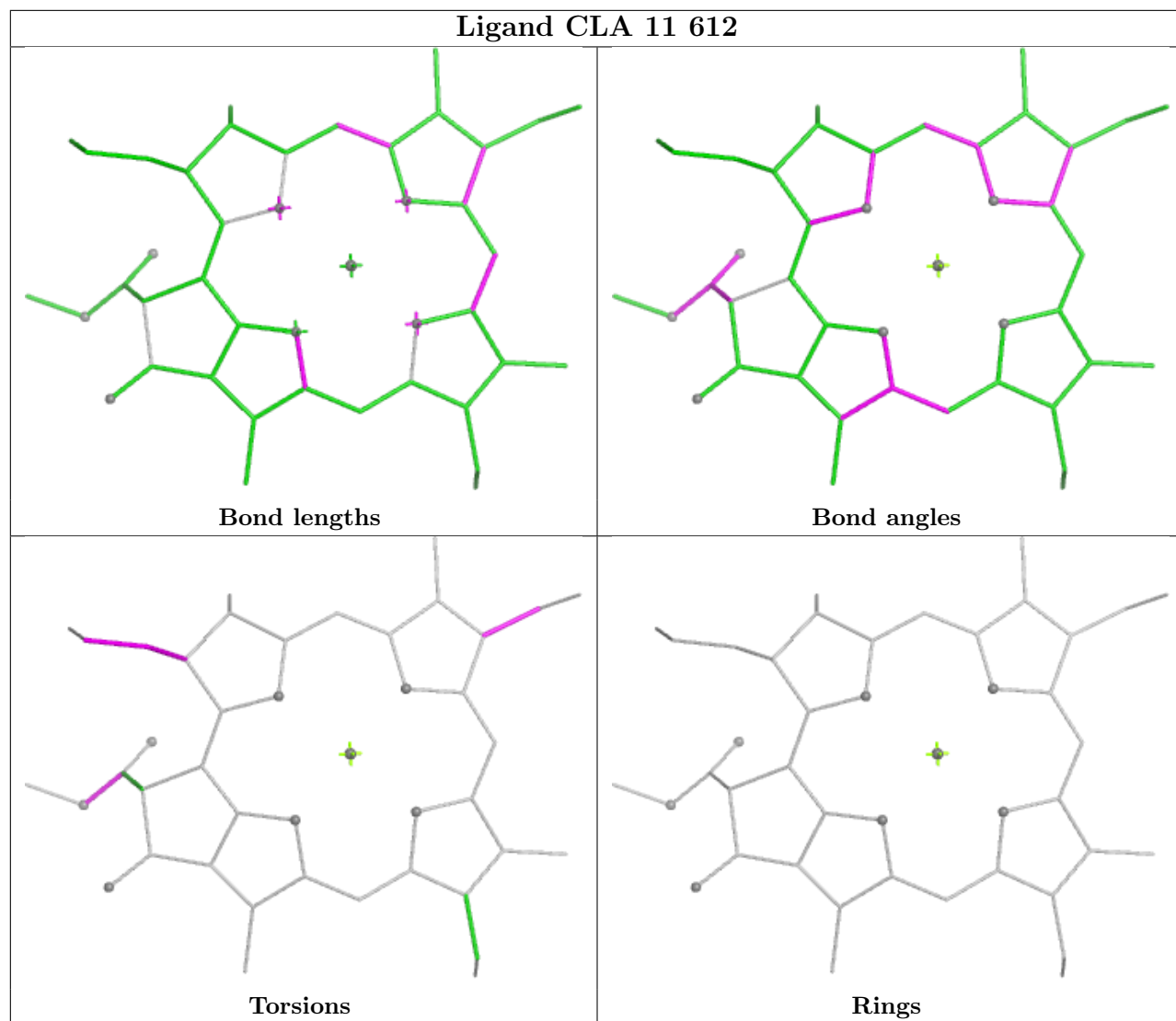
Ligand CLA g 614

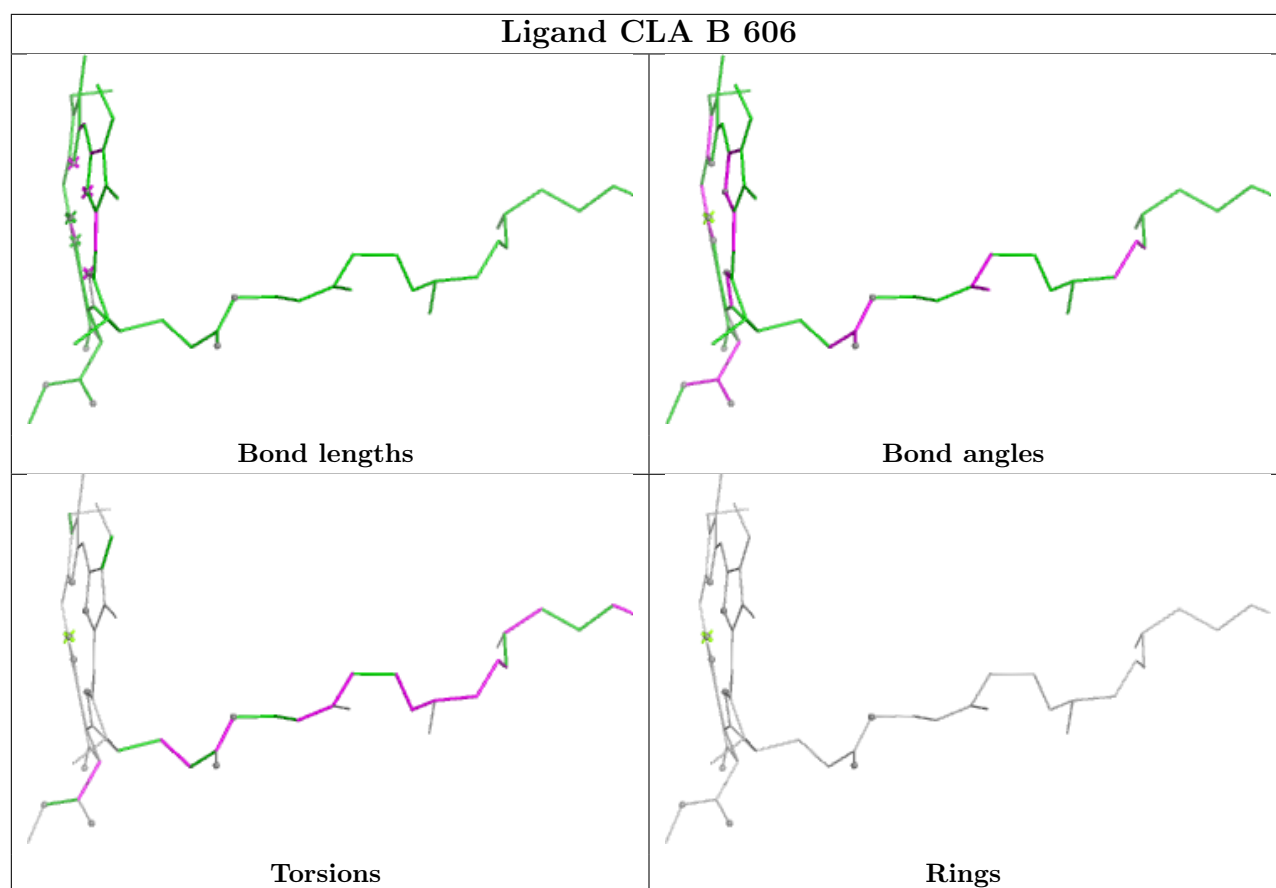


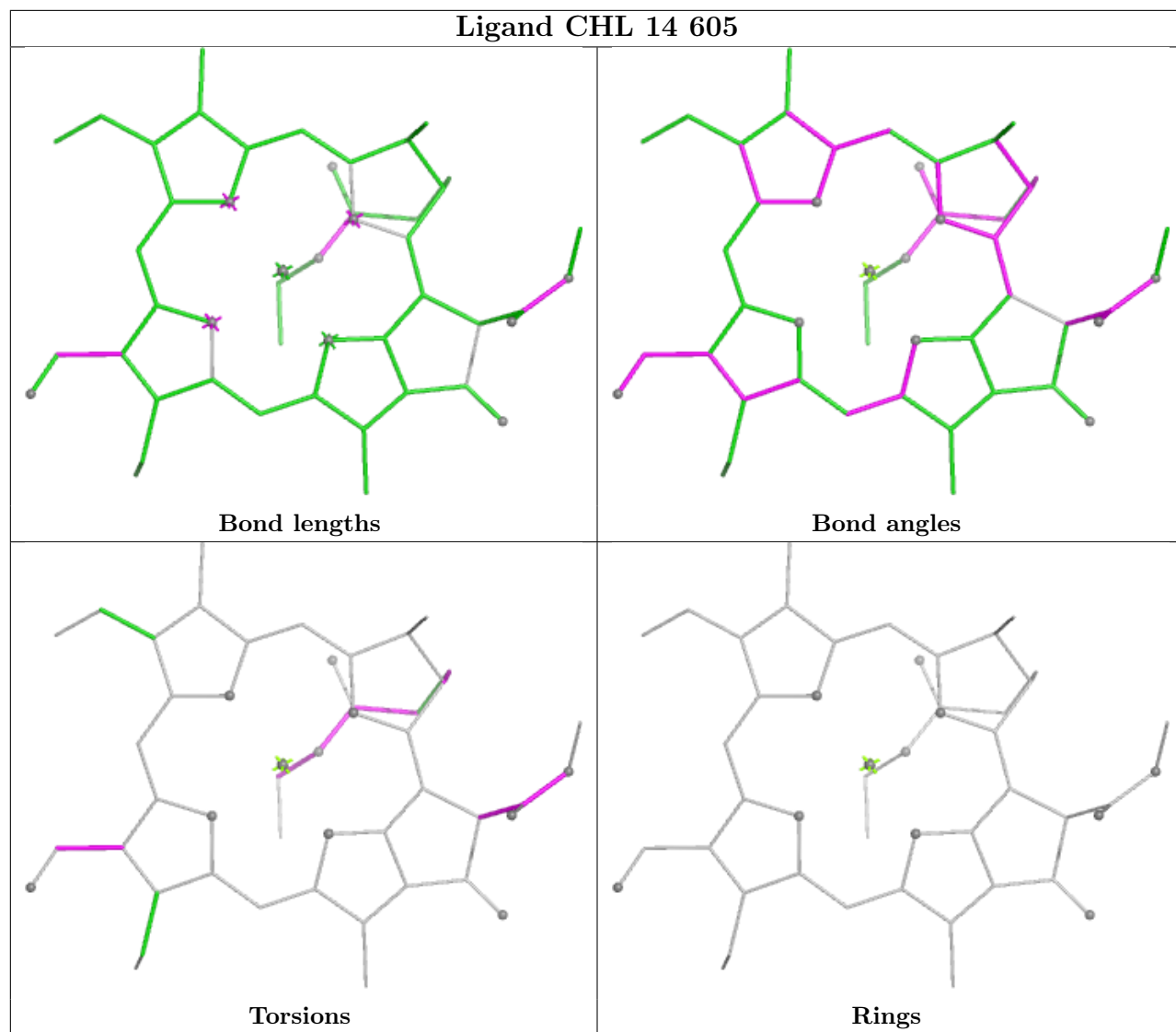




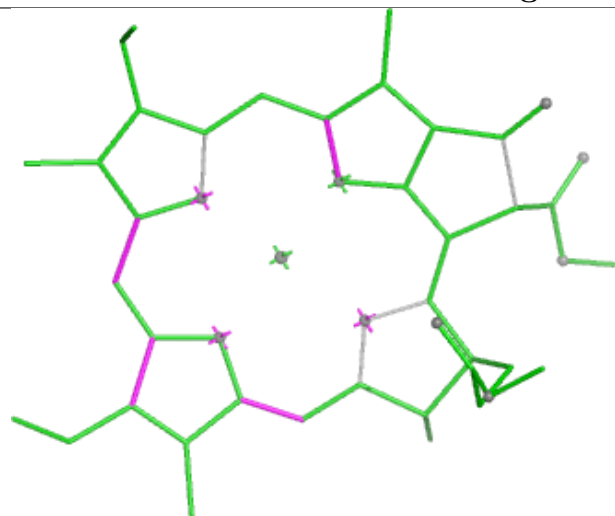




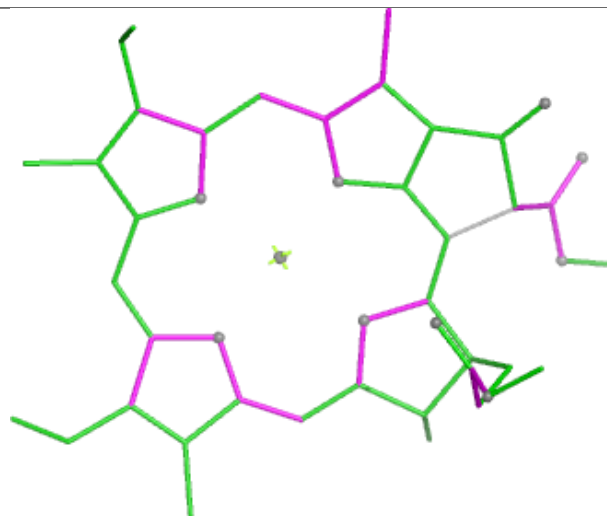




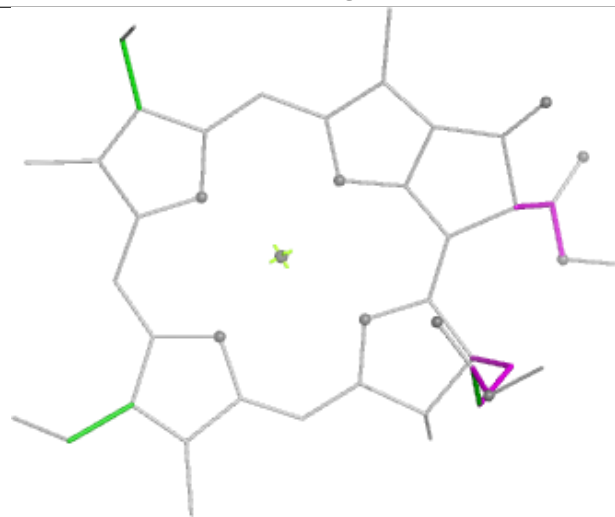
Ligand CLA 1 614



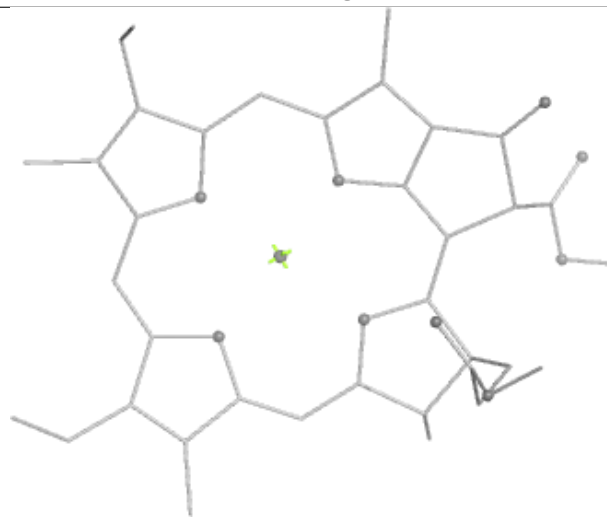
Bond lengths



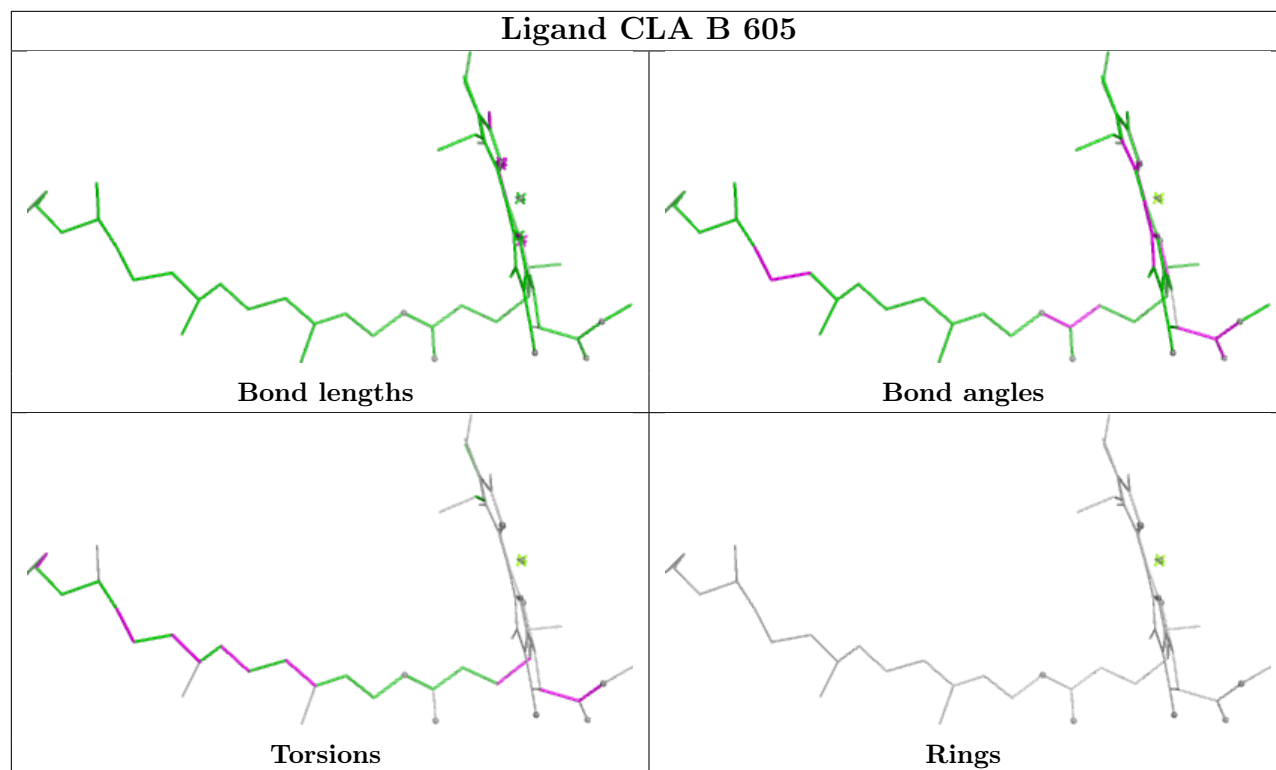
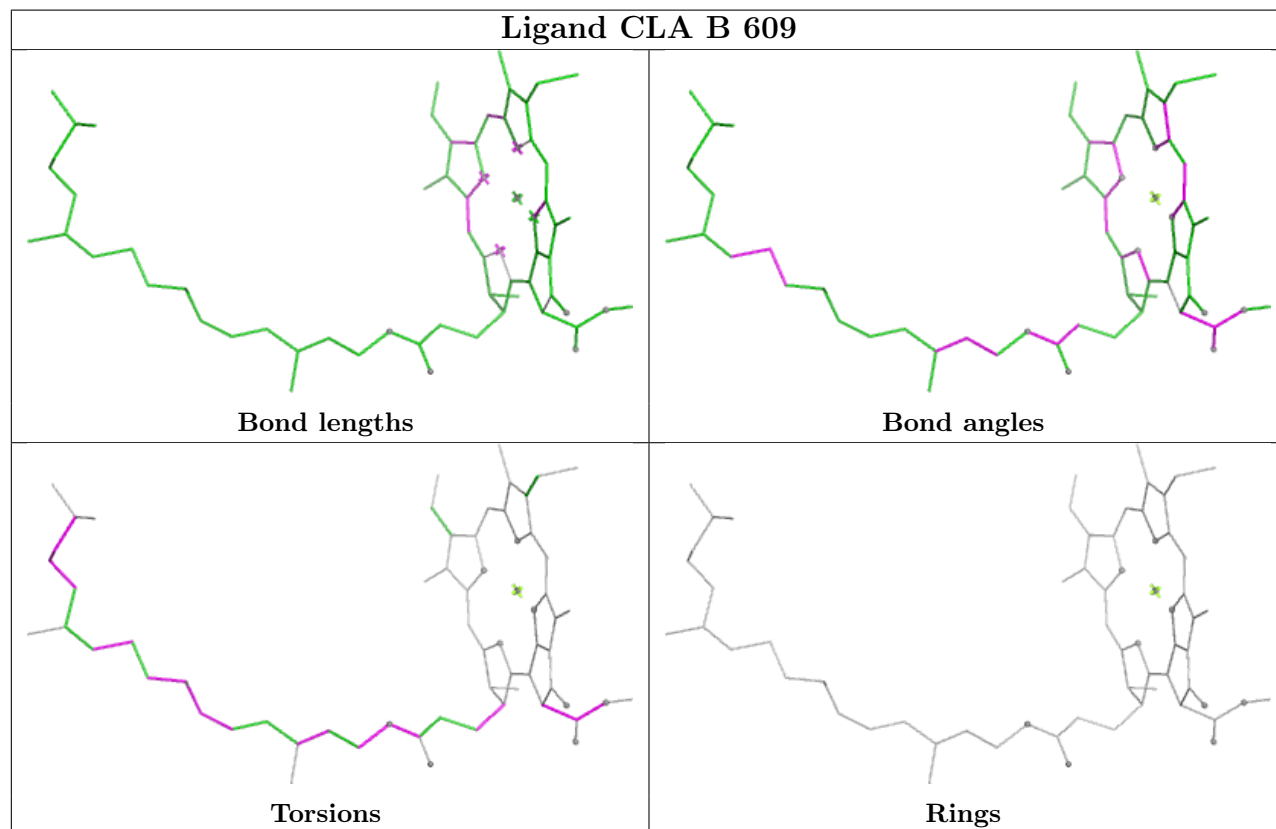
Bond angles

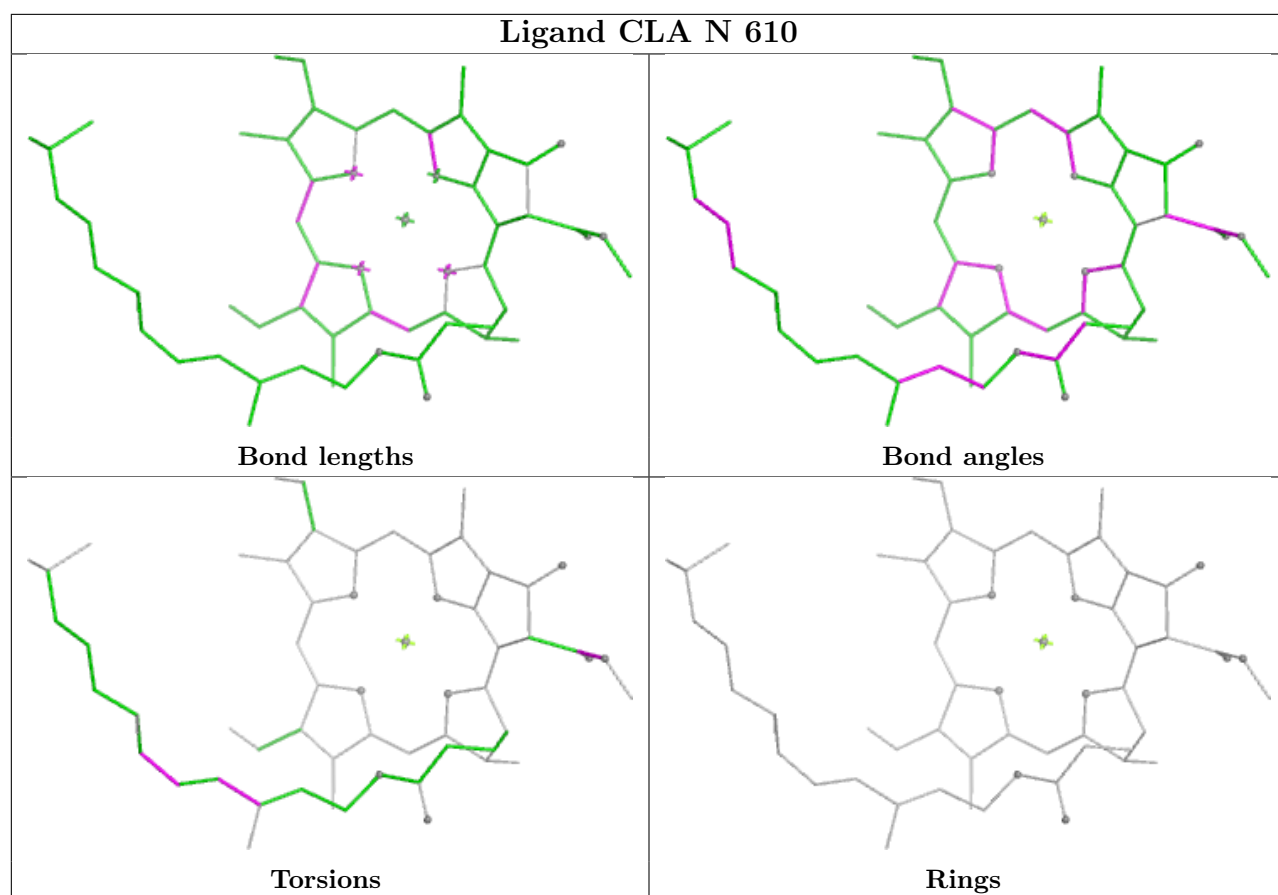


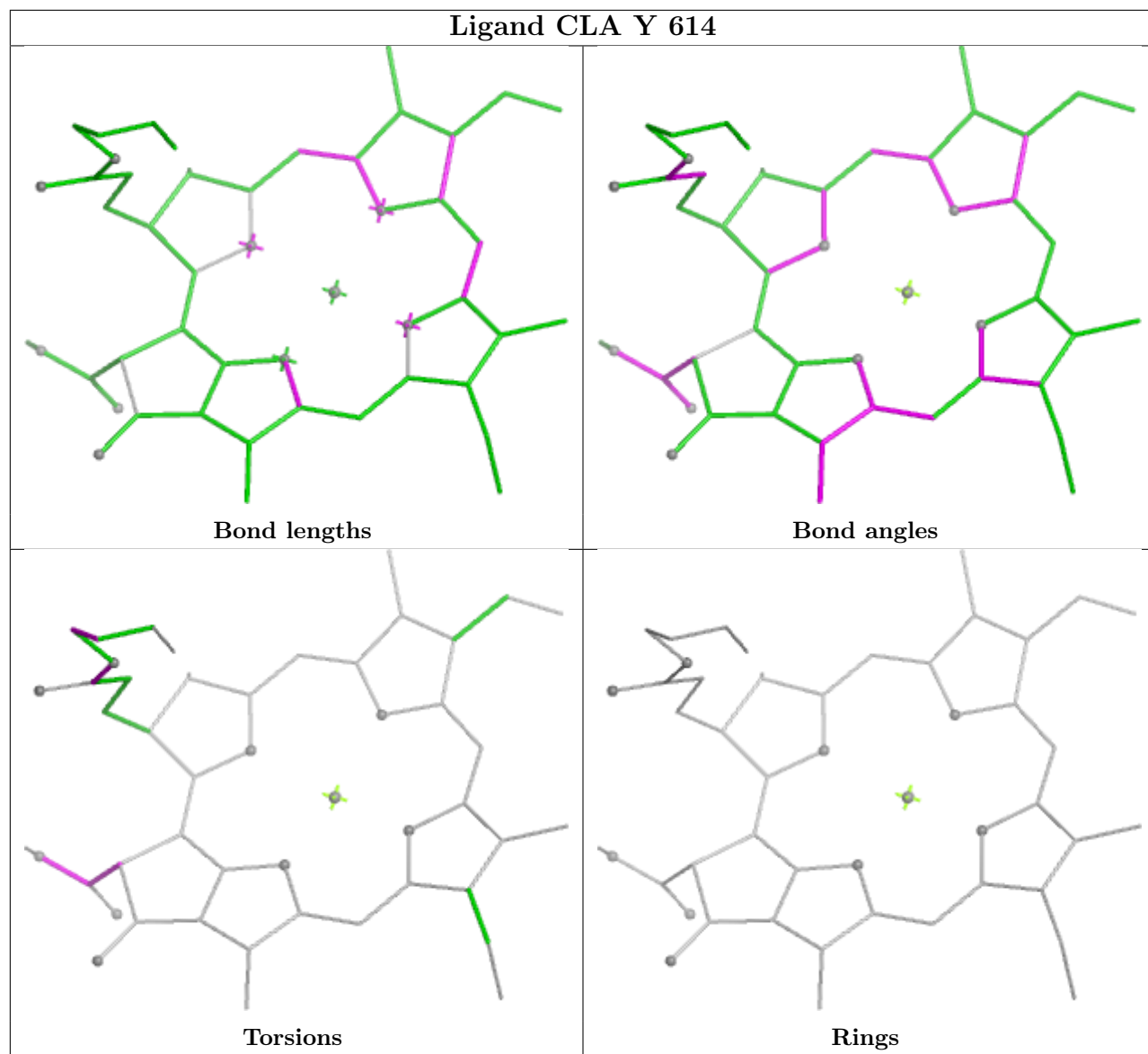
Torsions



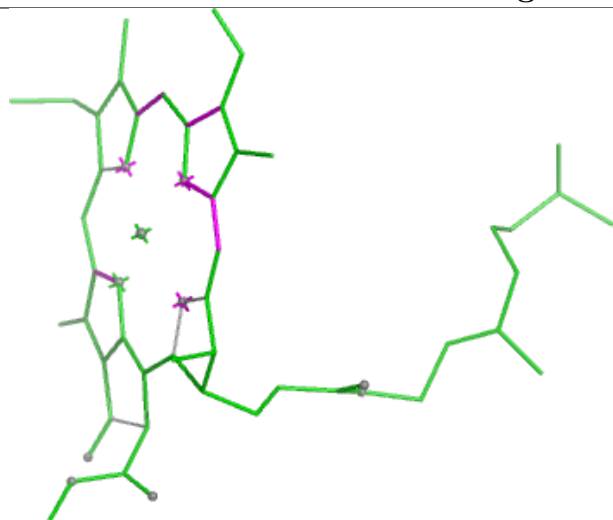
Rings

Ligand CLA B 605**Ligand CLA B 609**

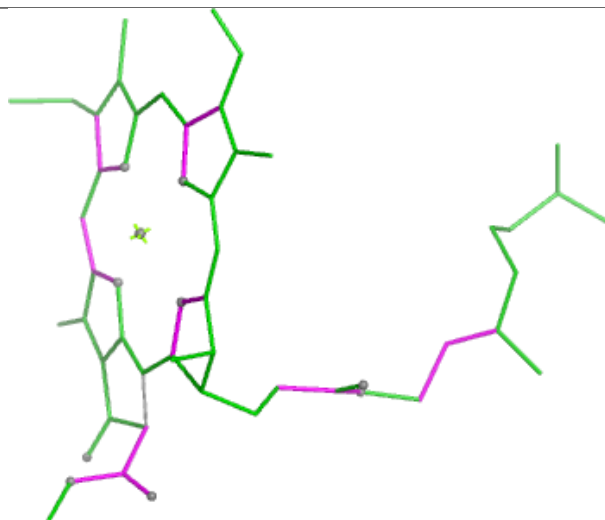




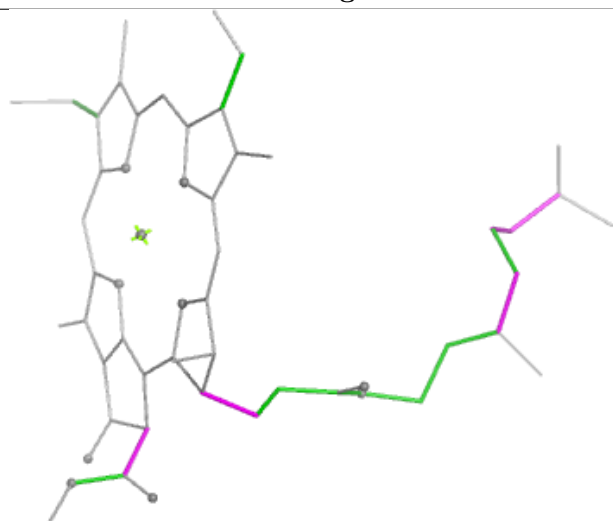
Ligand CLA b 601



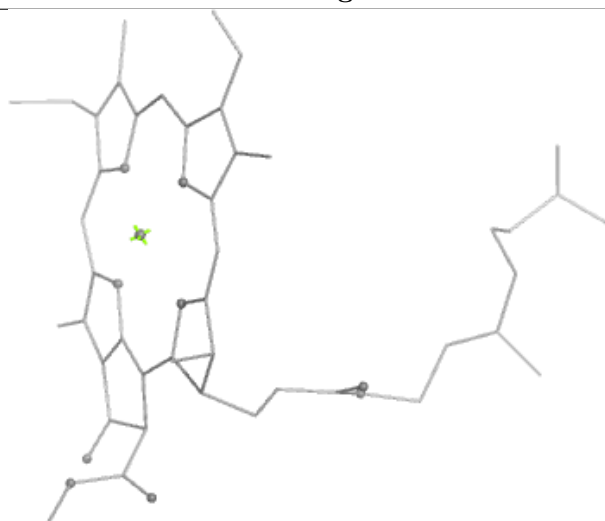
Bond lengths



Bond angles

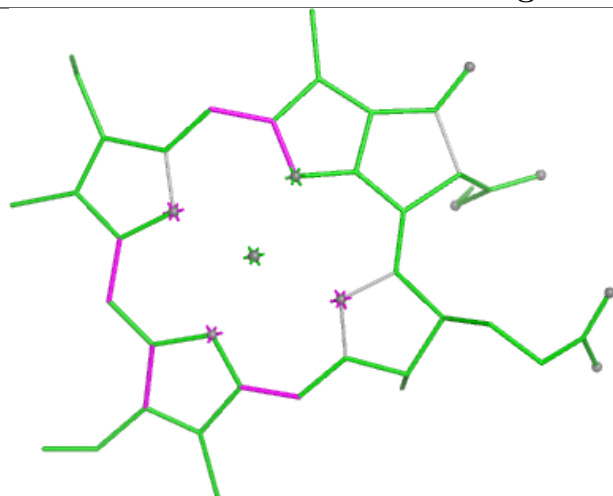


Torsions

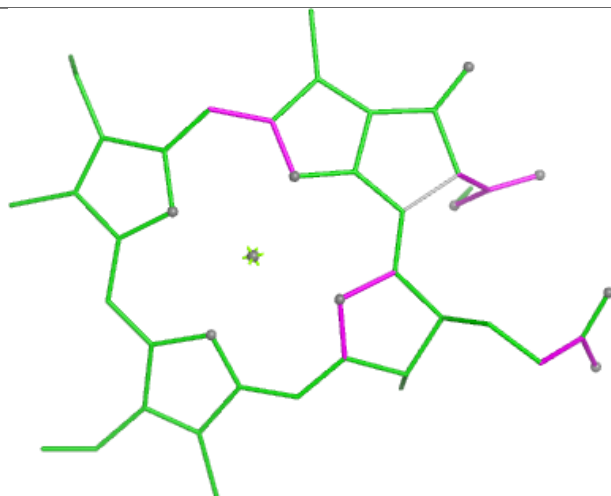


Rings

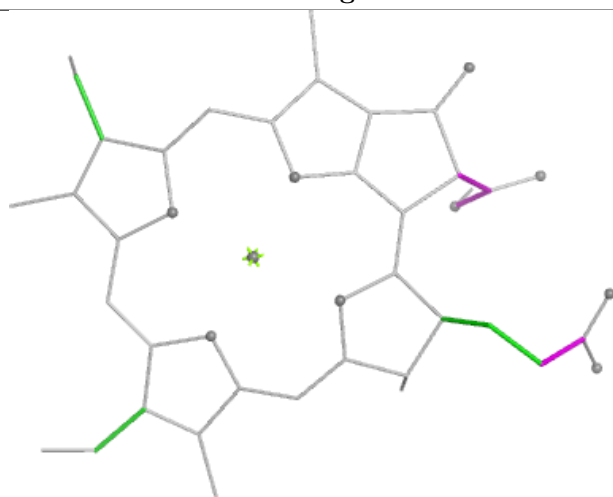
Ligand CLA S 612



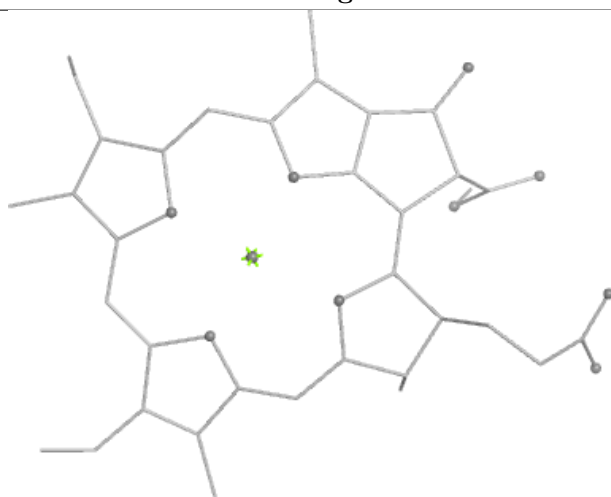
Bond lengths



Bond angles

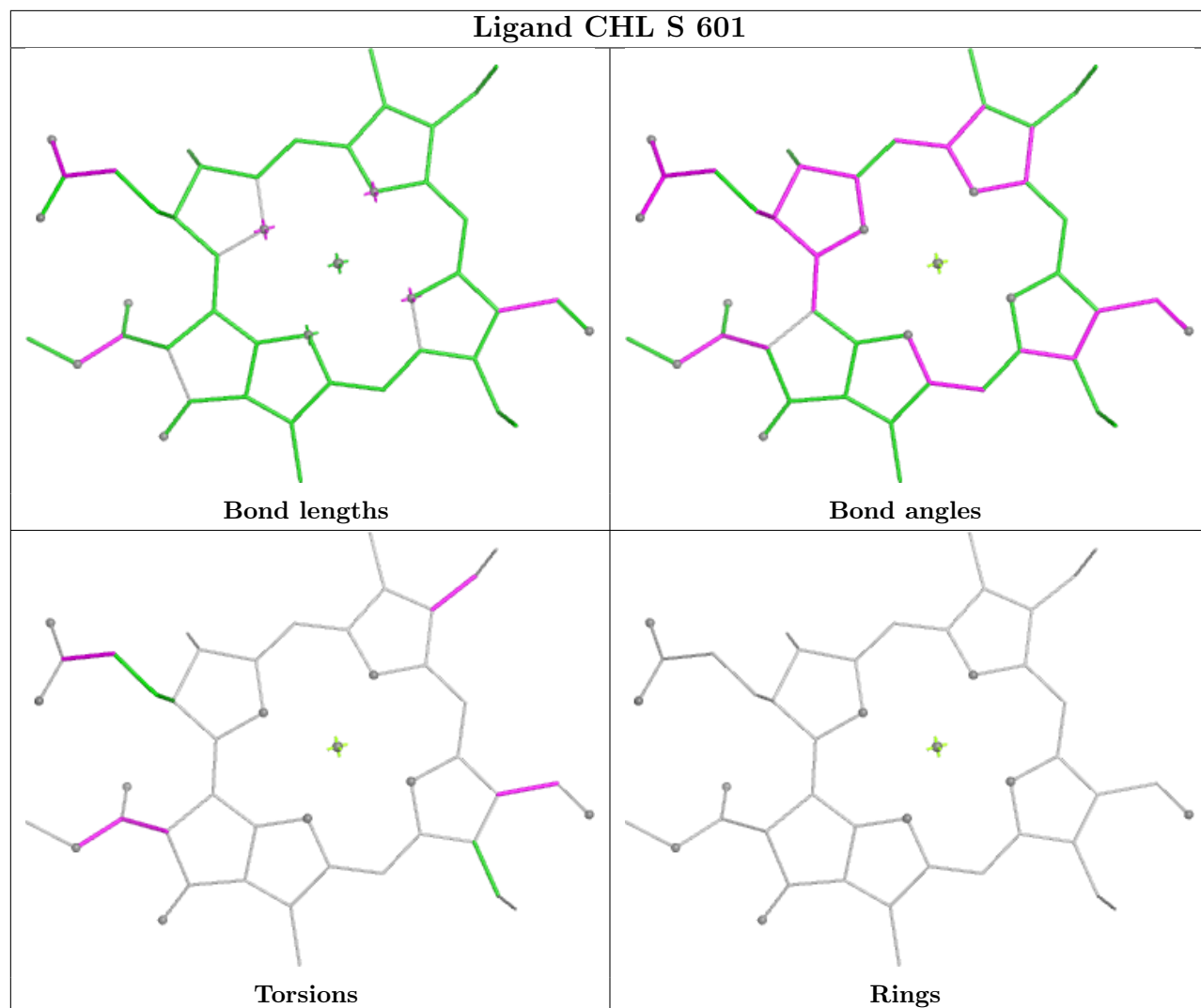


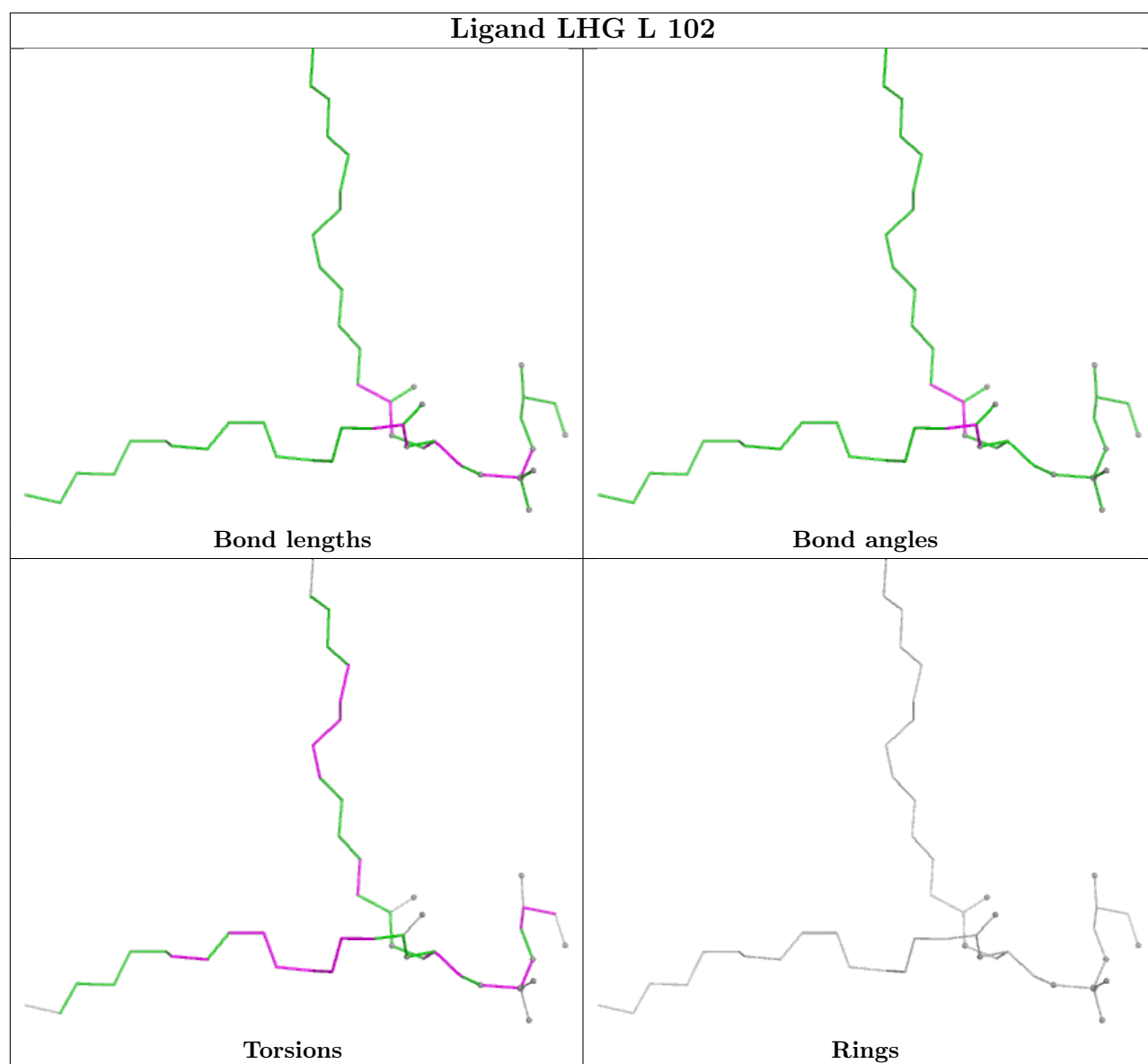
Torsions

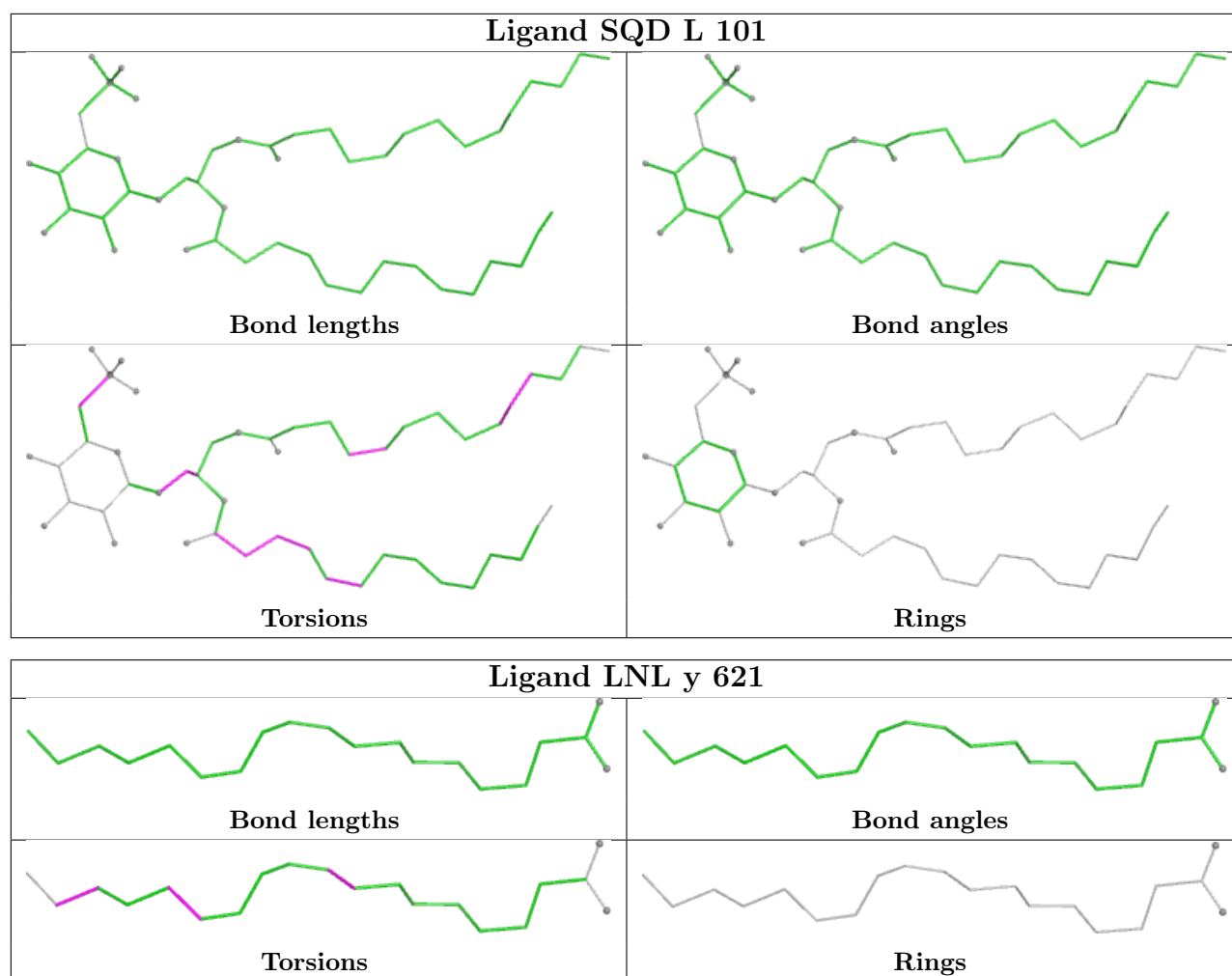


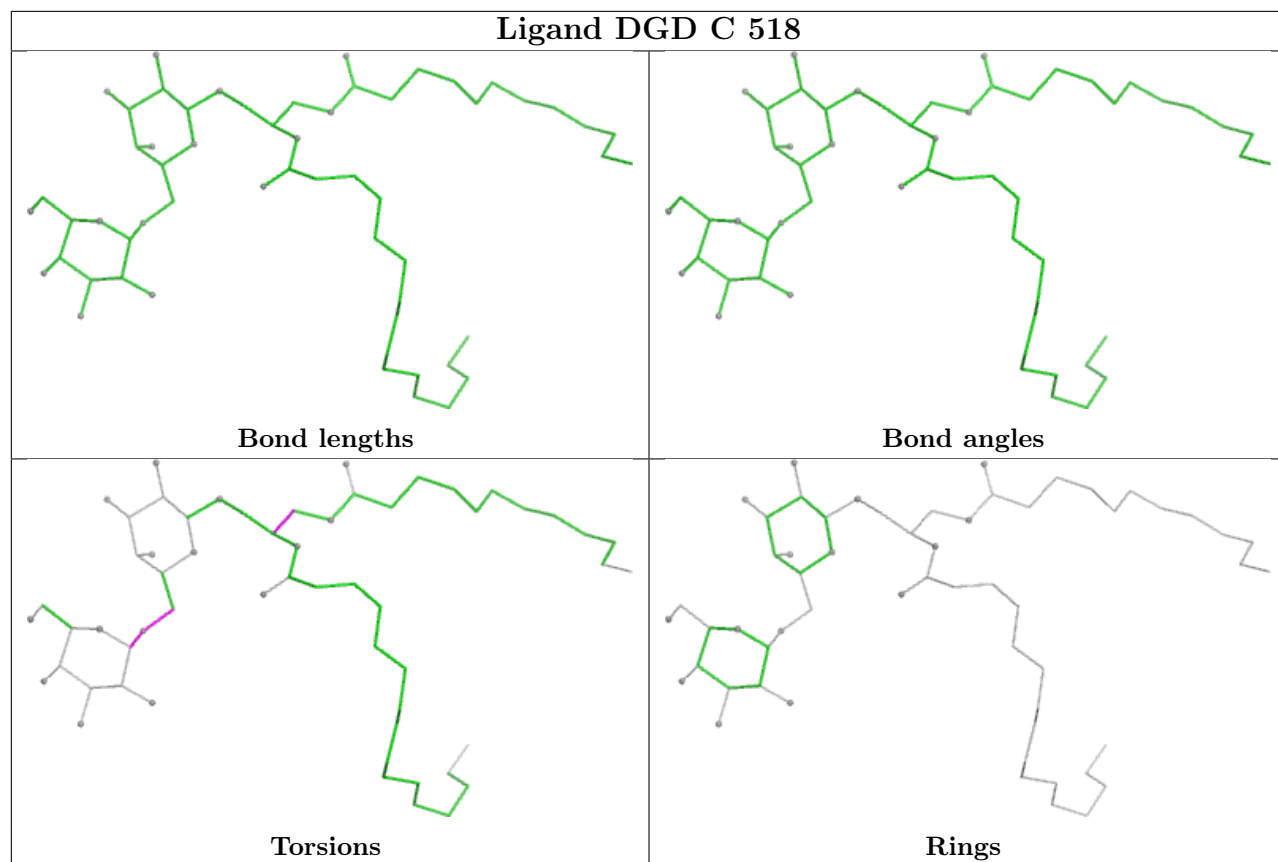
Rings

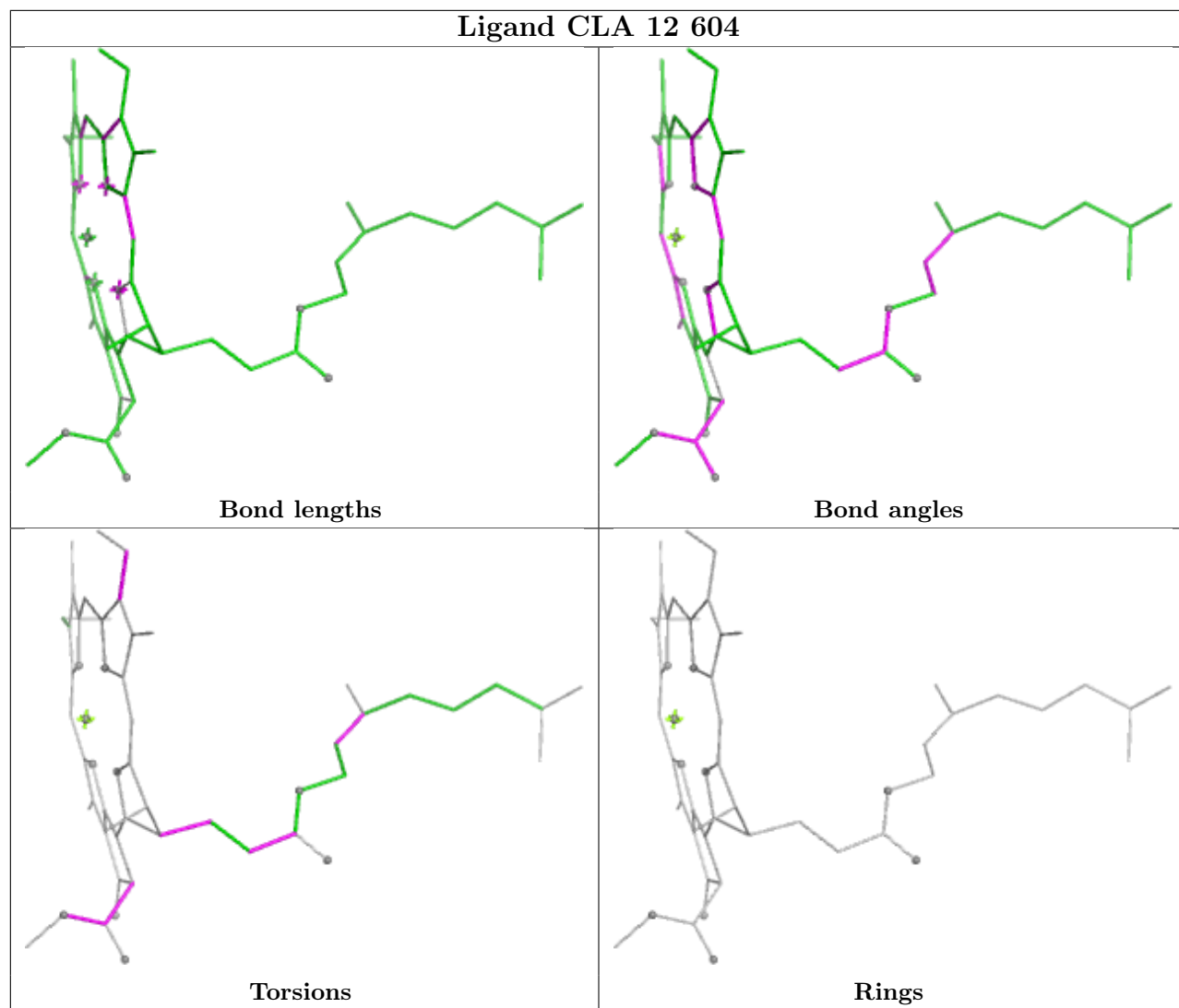
Ligand CHL S 601

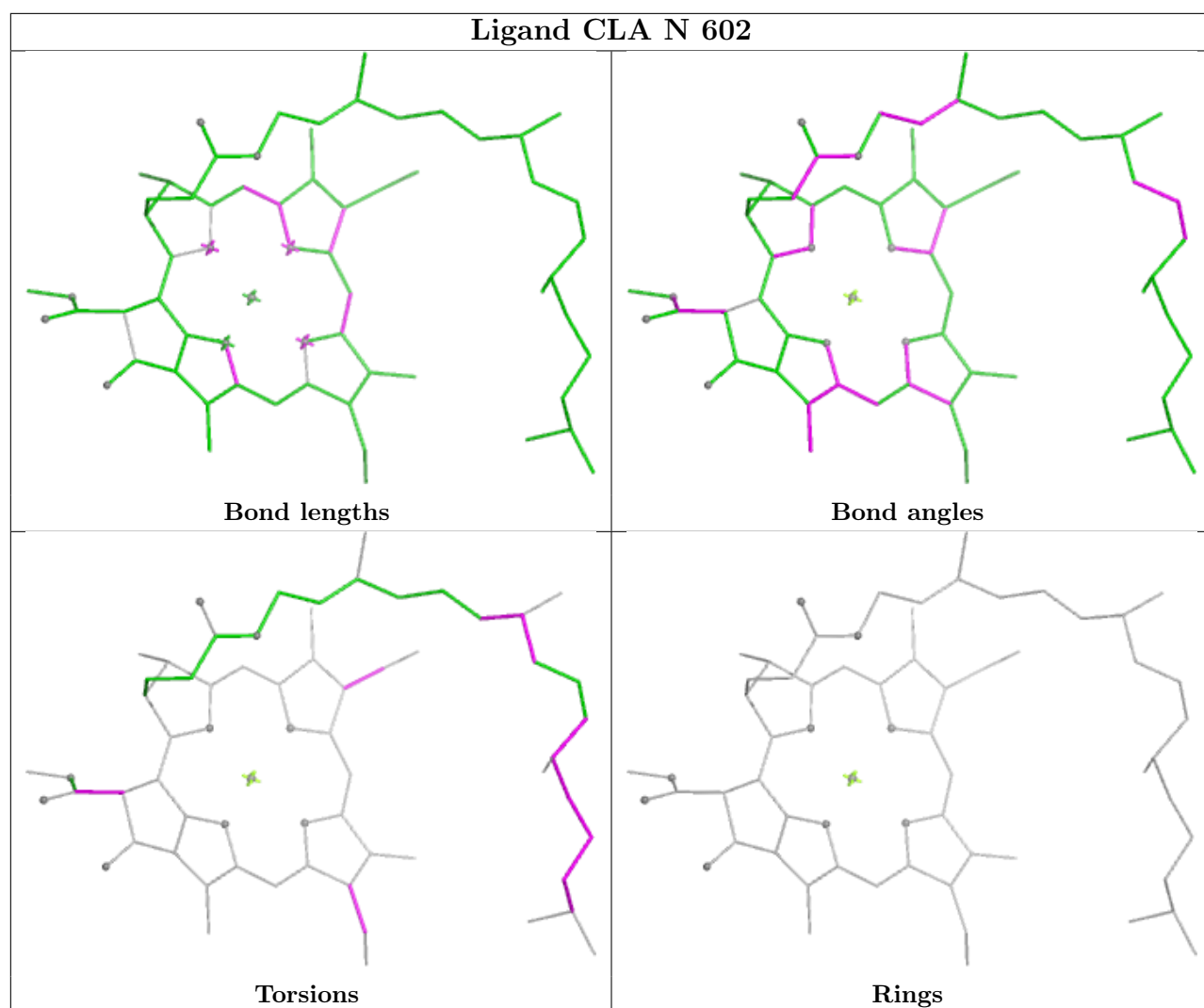




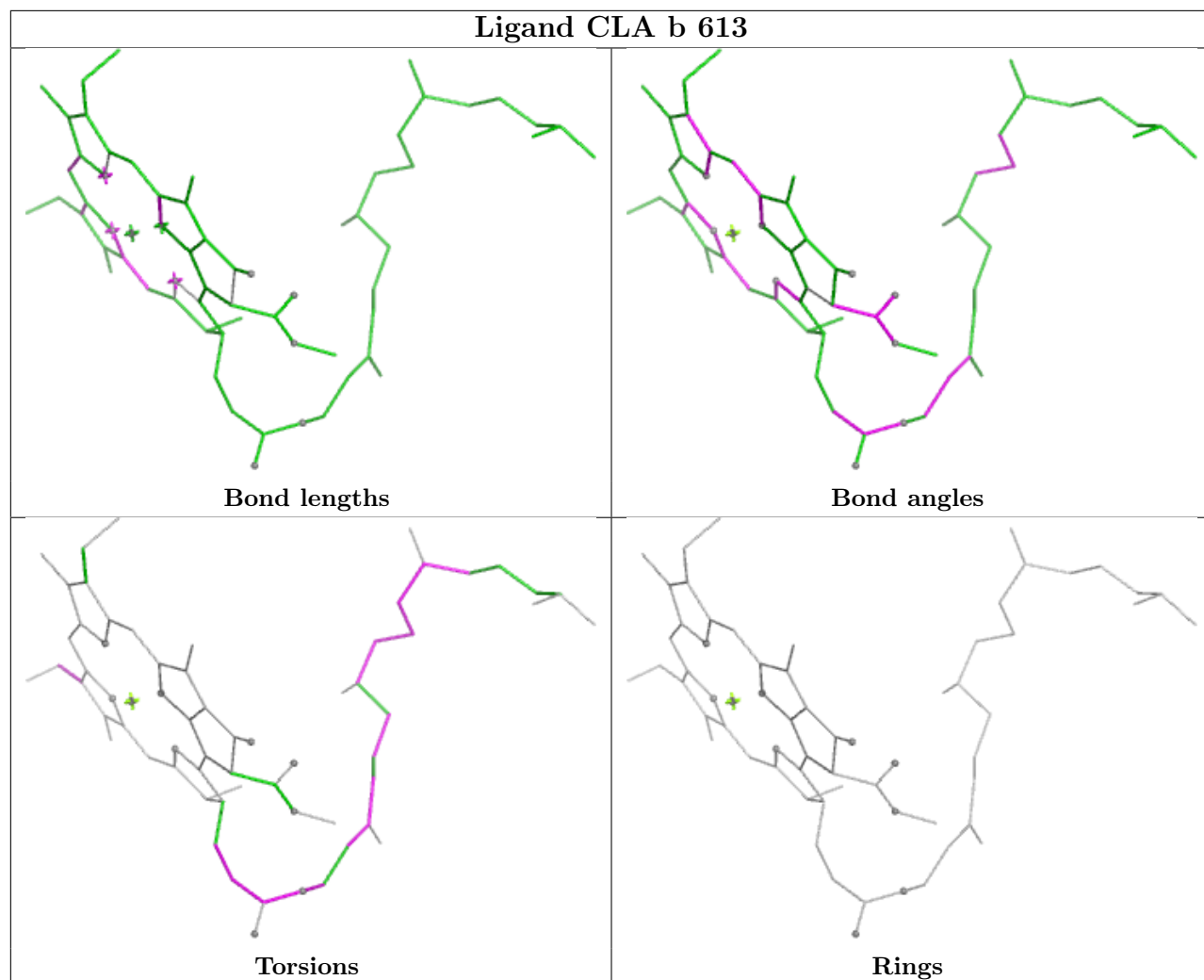




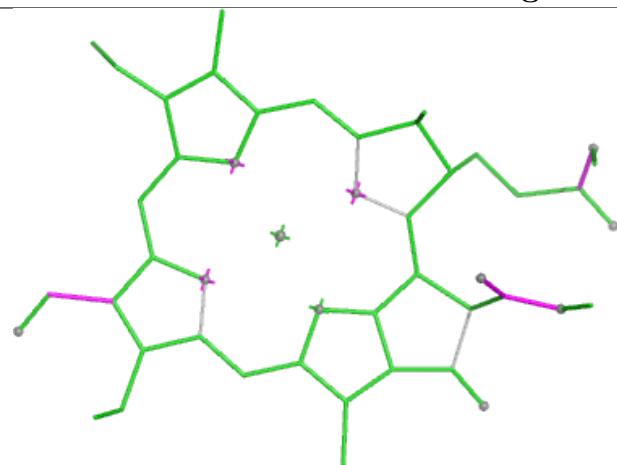




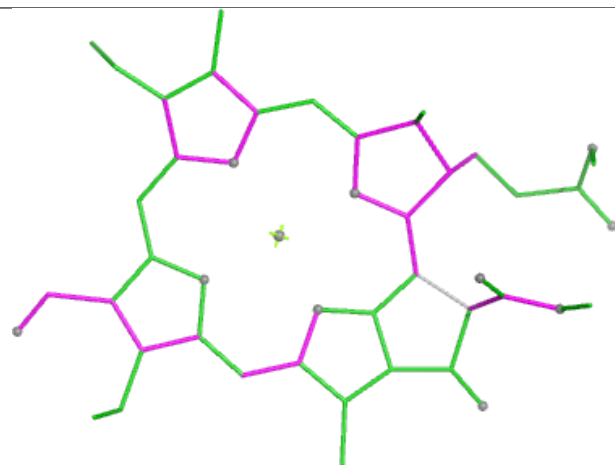
Ligand CLA b 613



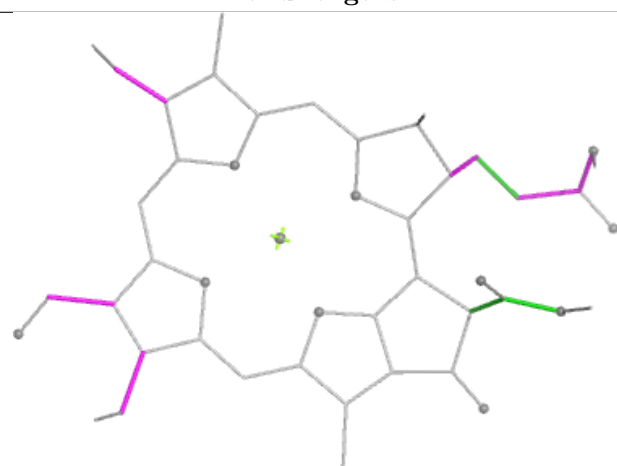
Ligand CHL 1 606



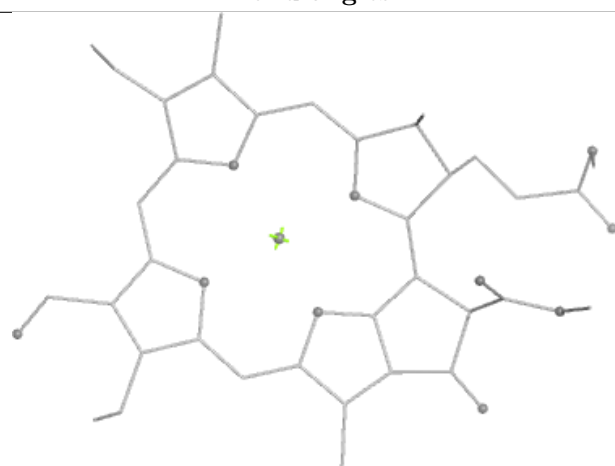
Bond lengths



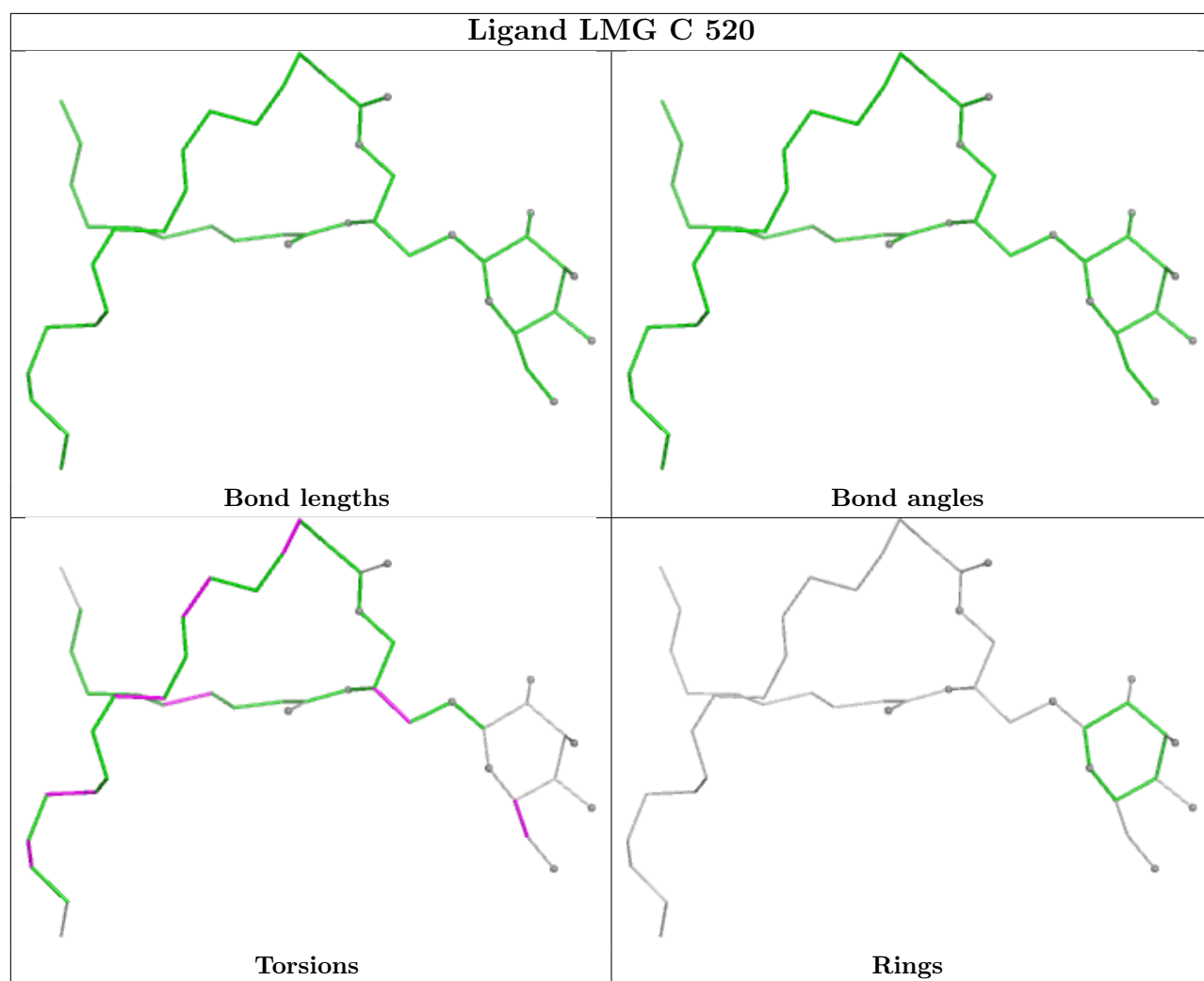
Bond angles

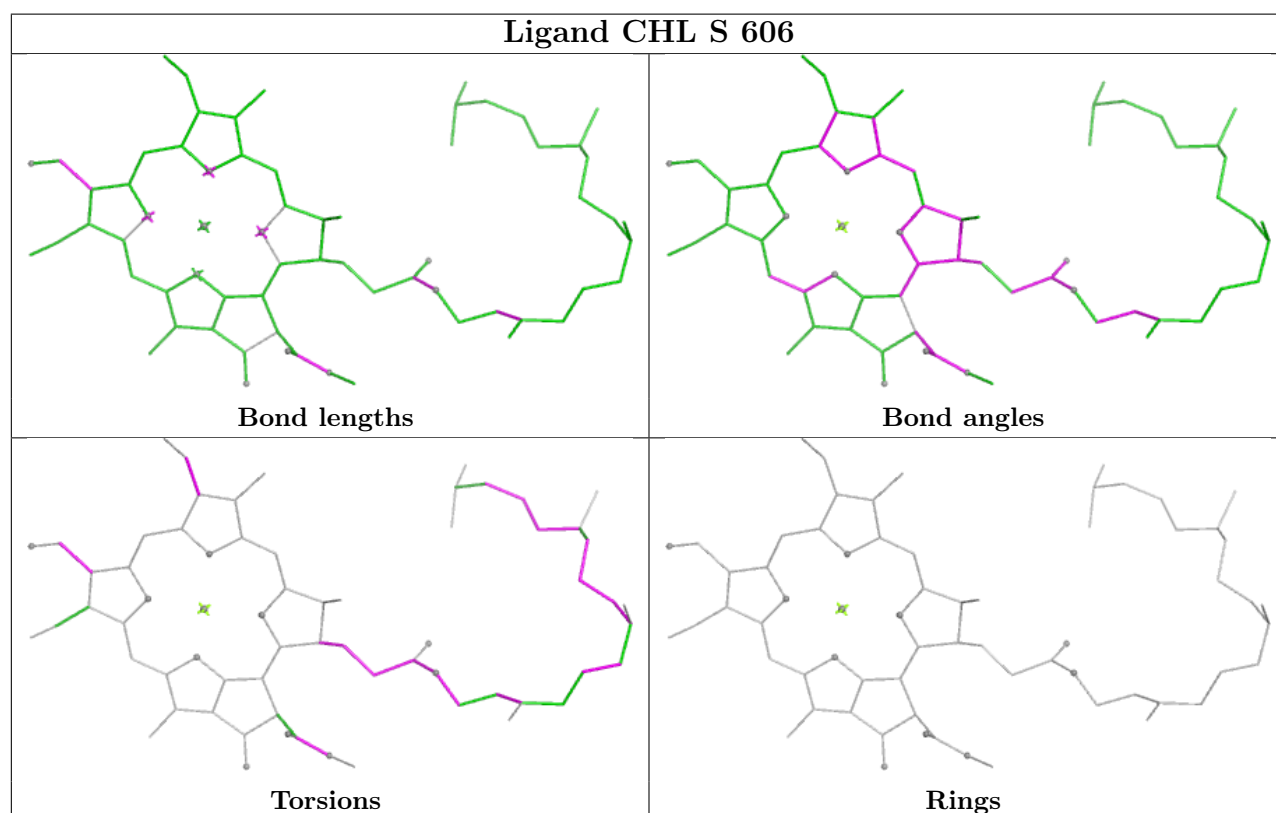
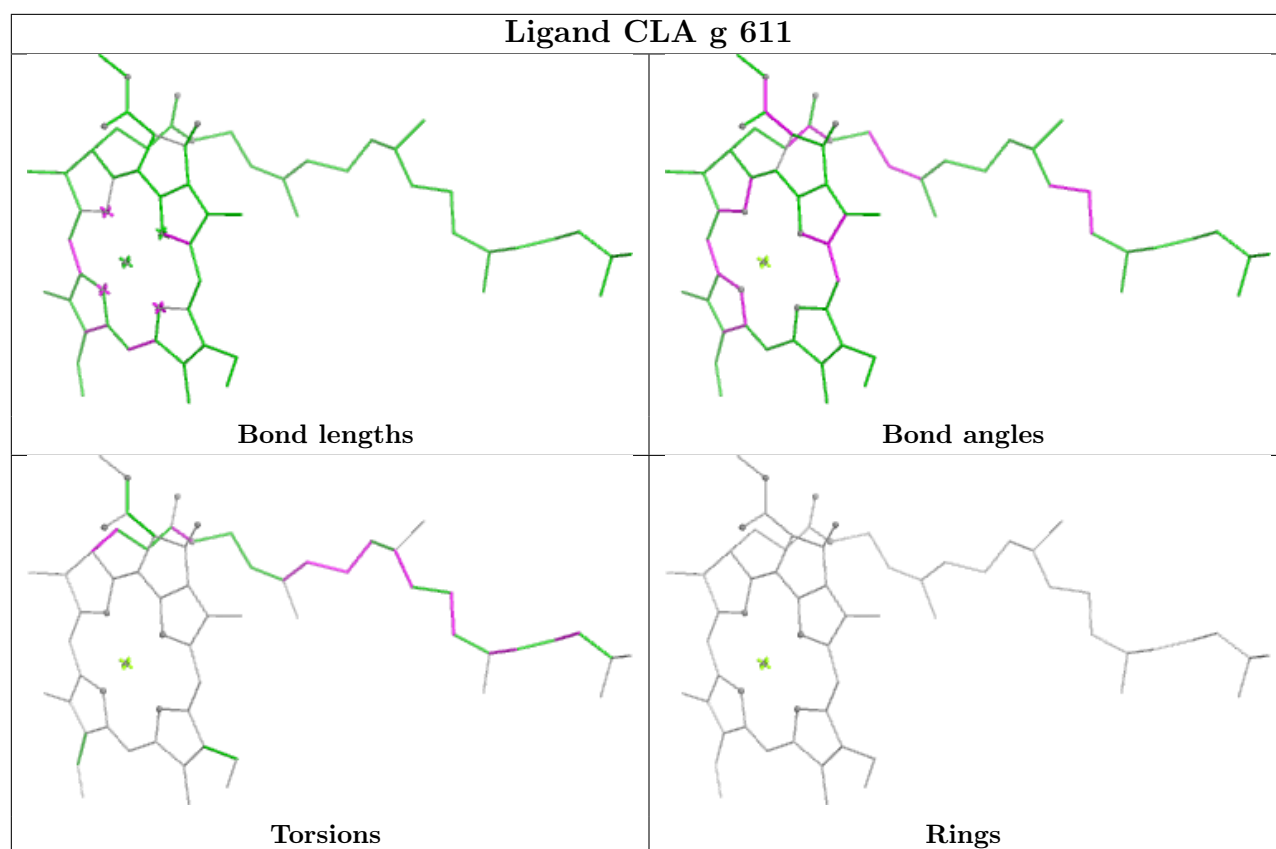


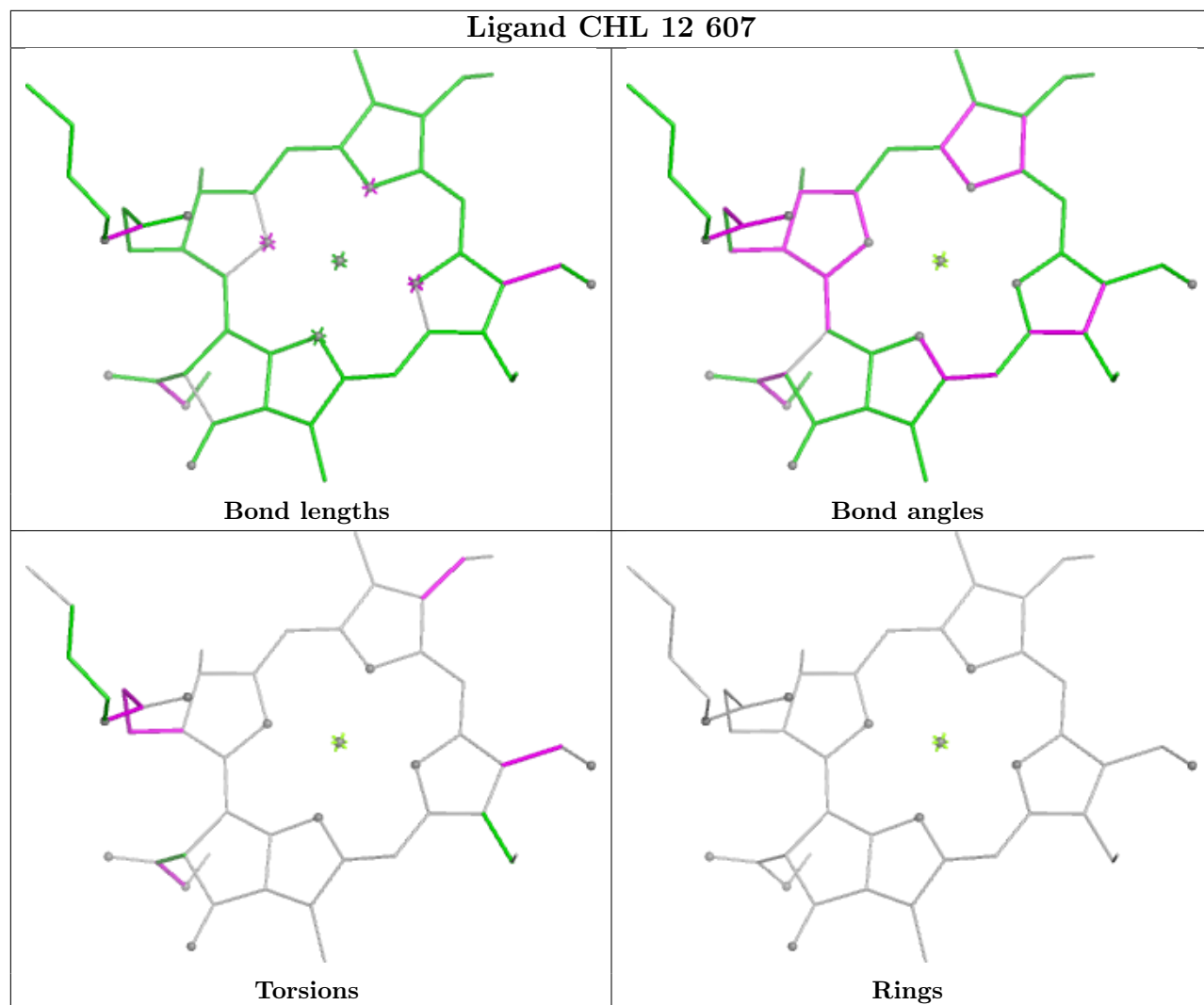
Torsions

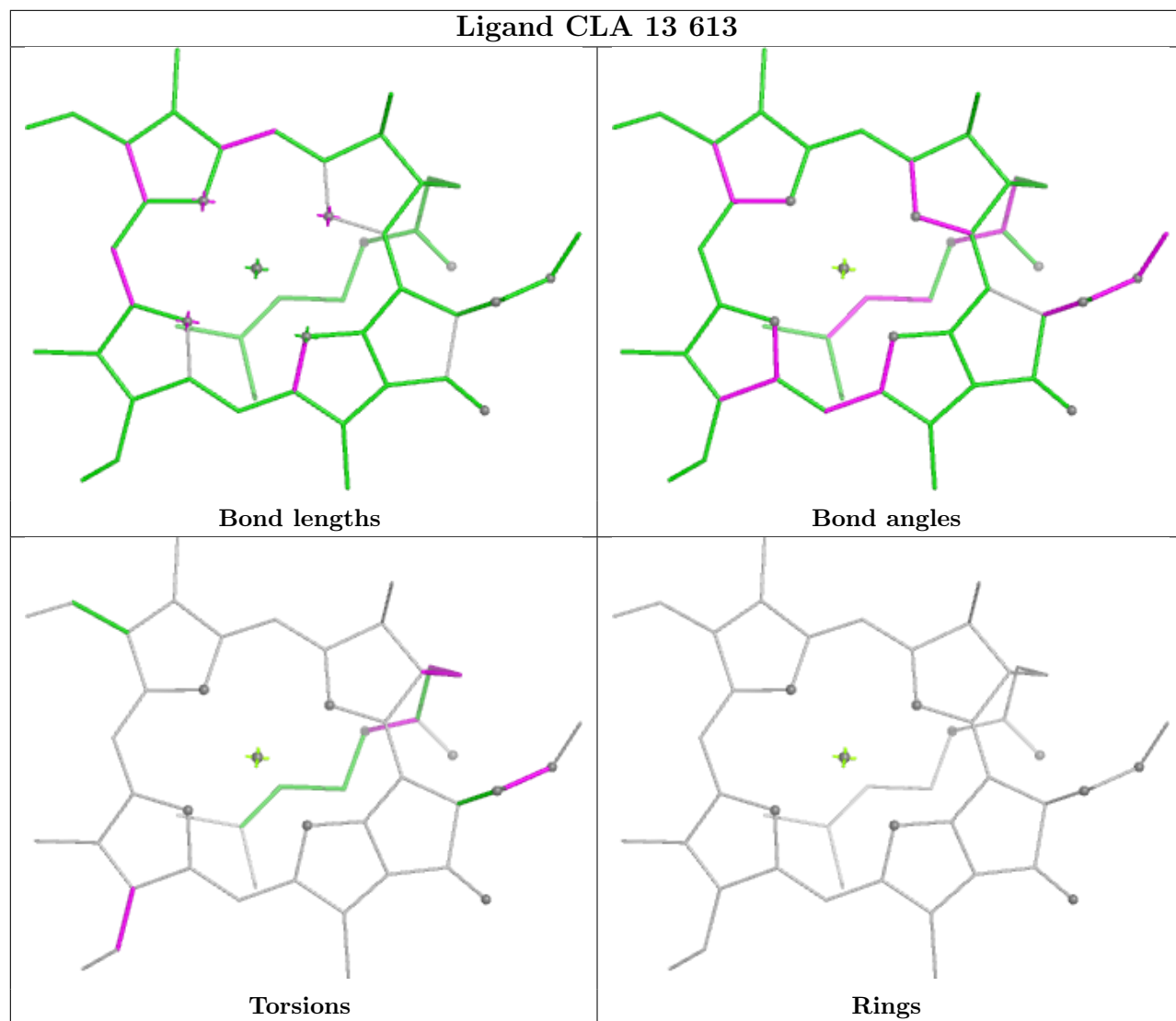


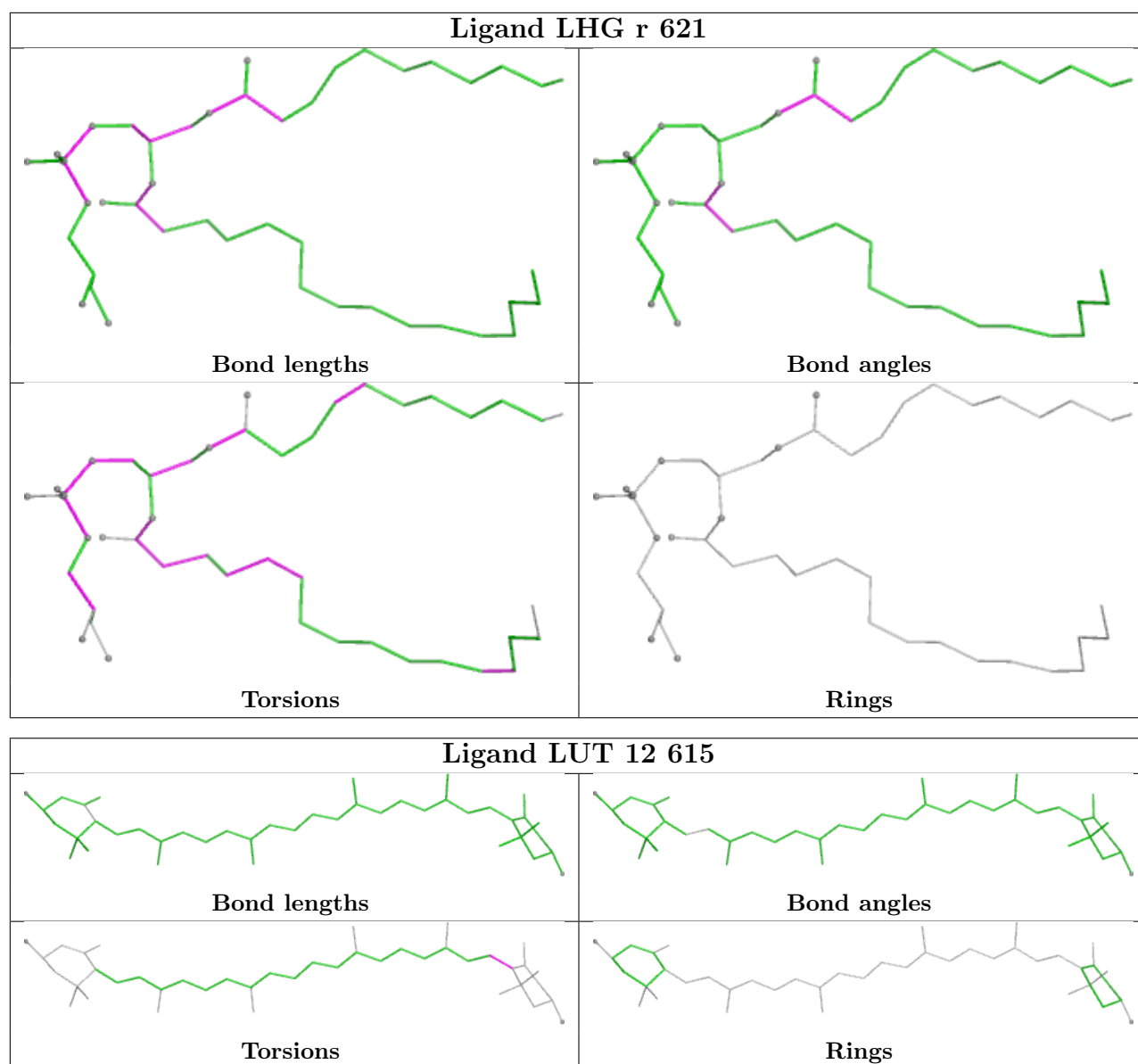
Rings

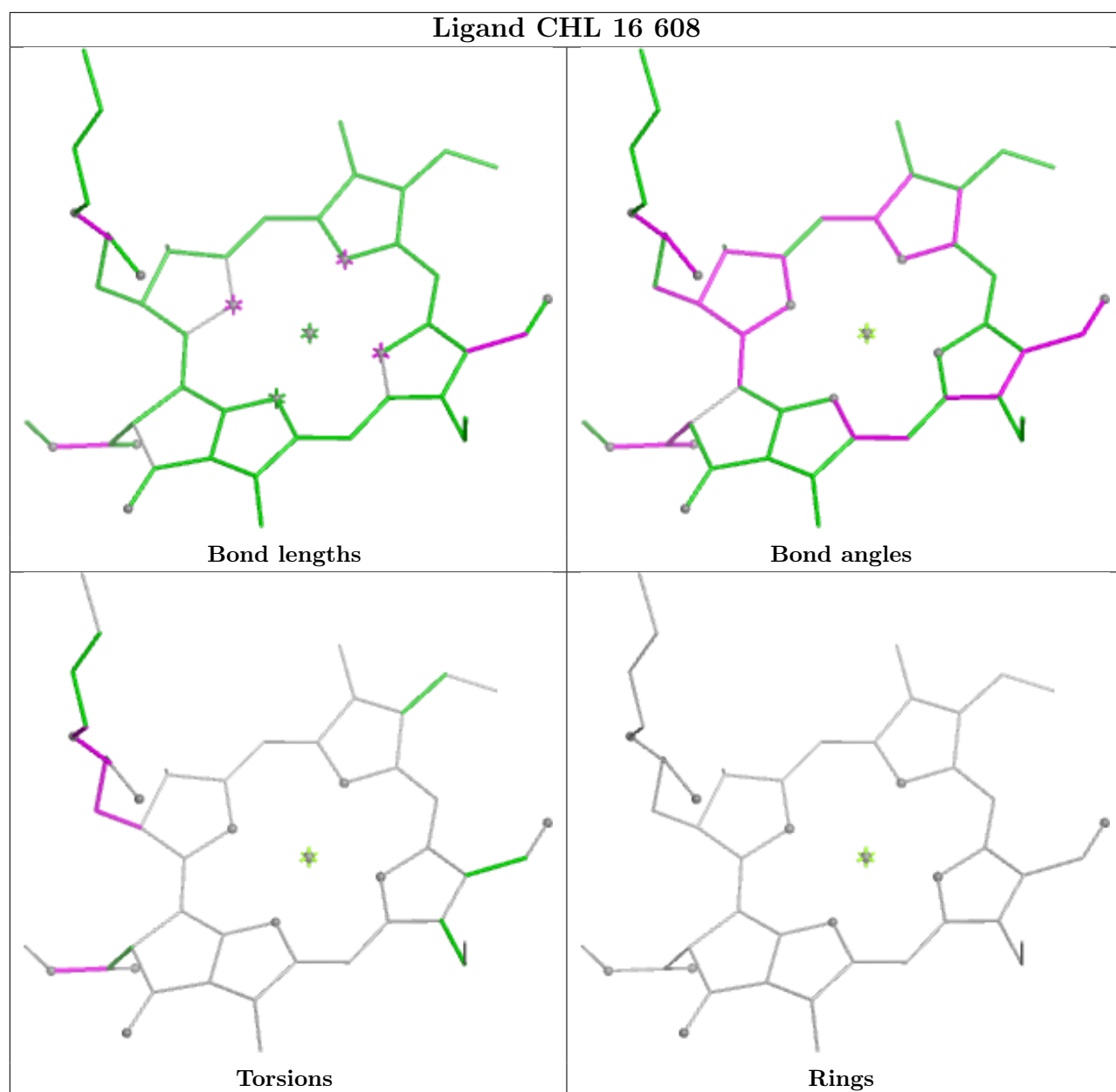


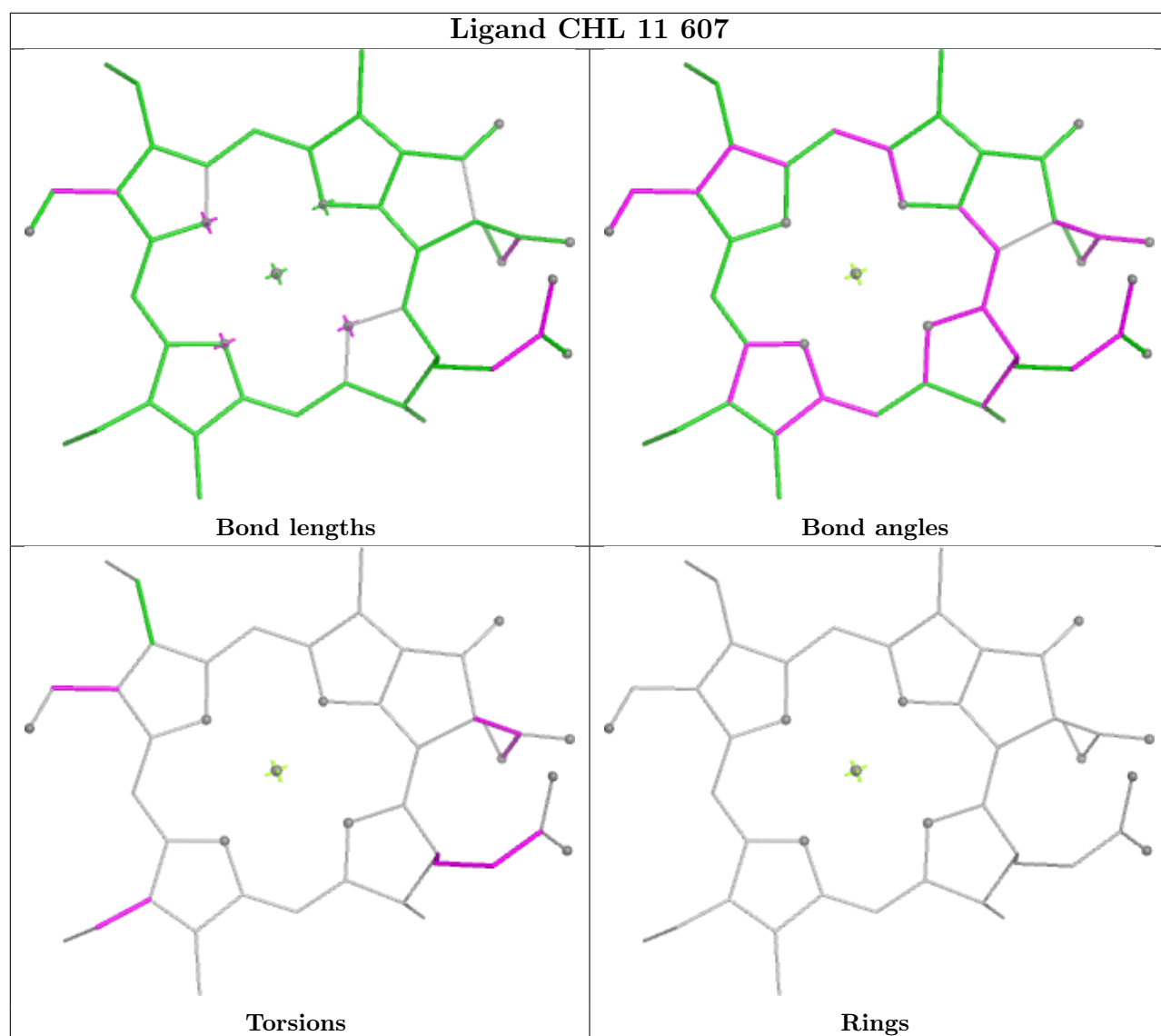


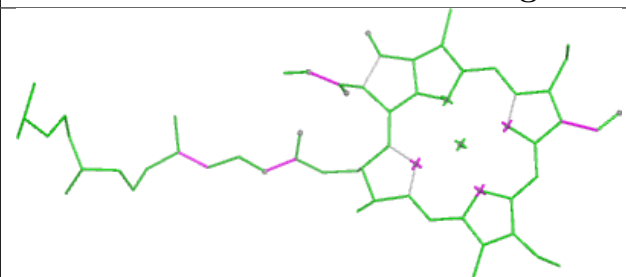
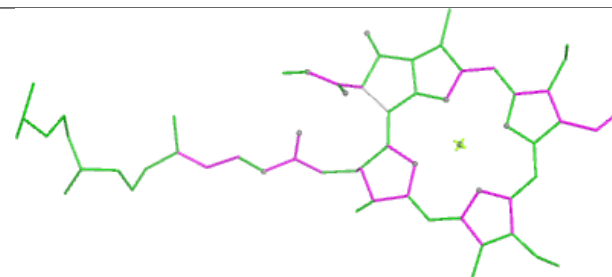
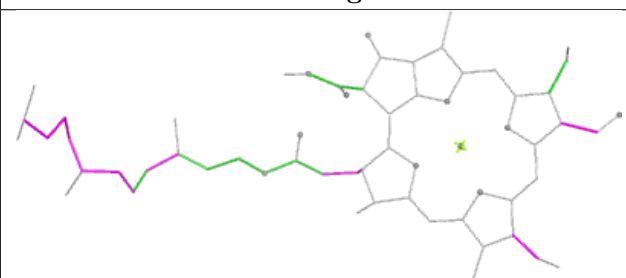
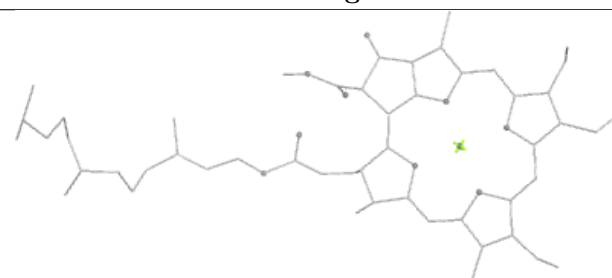


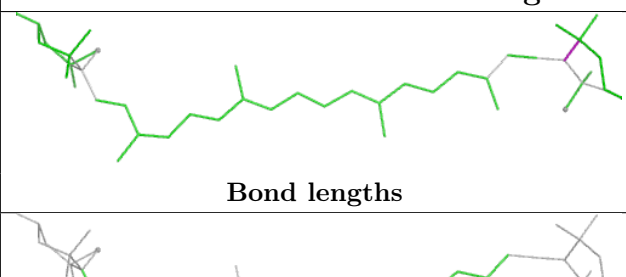
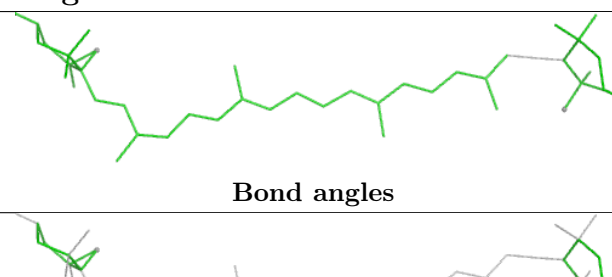
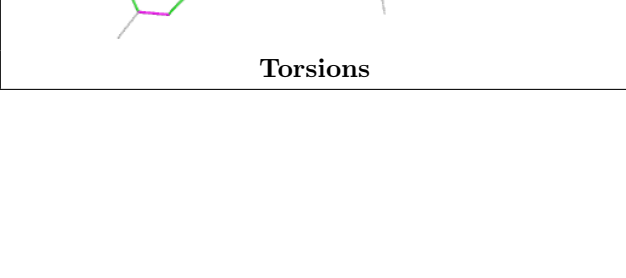
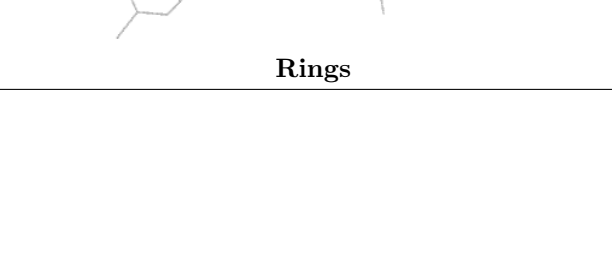


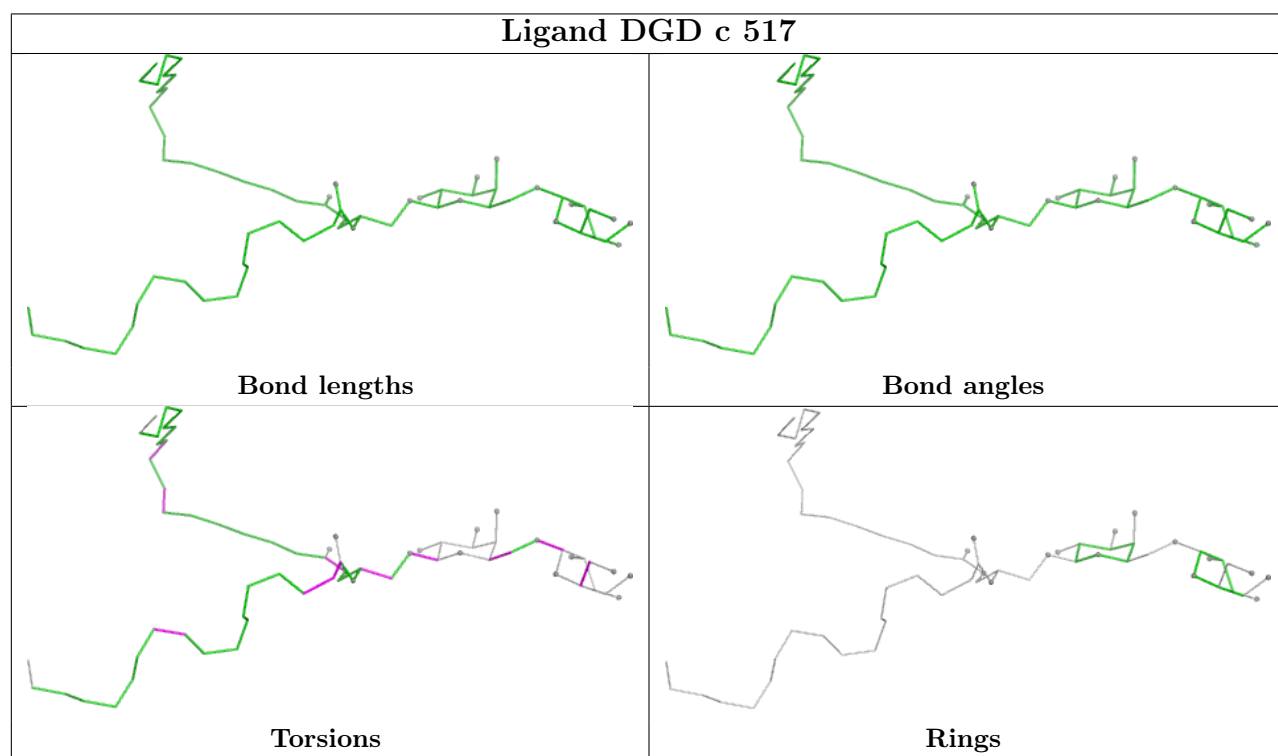
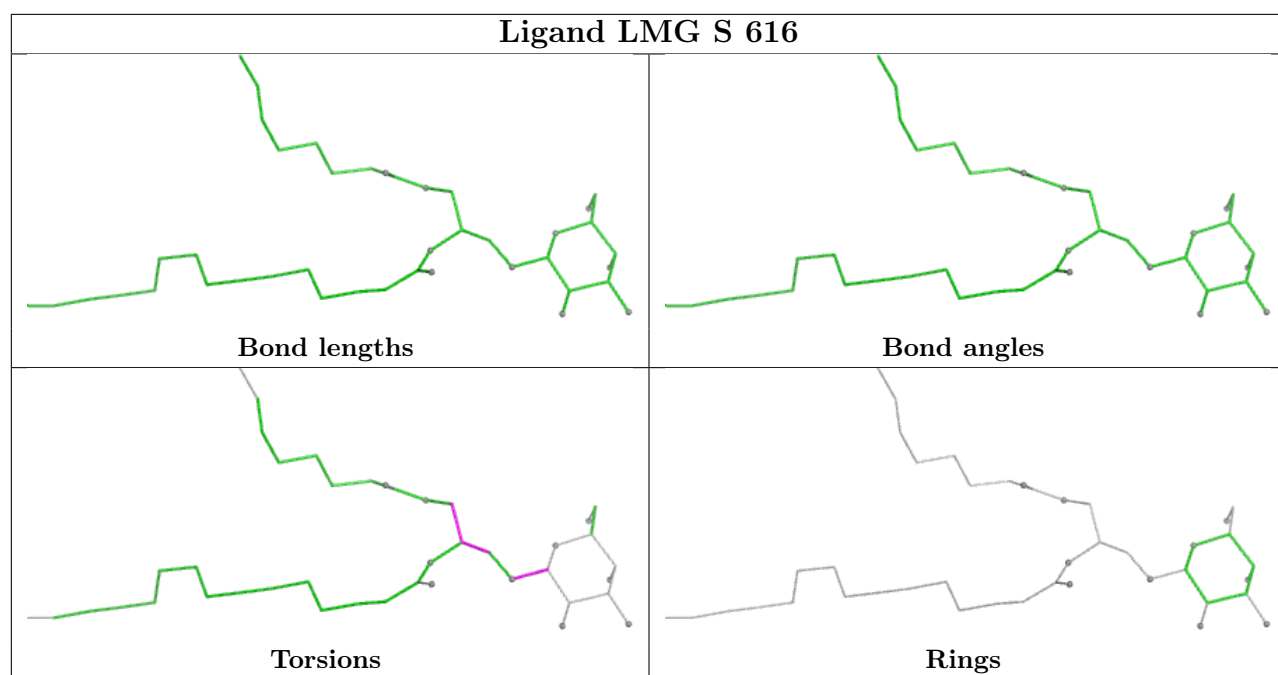


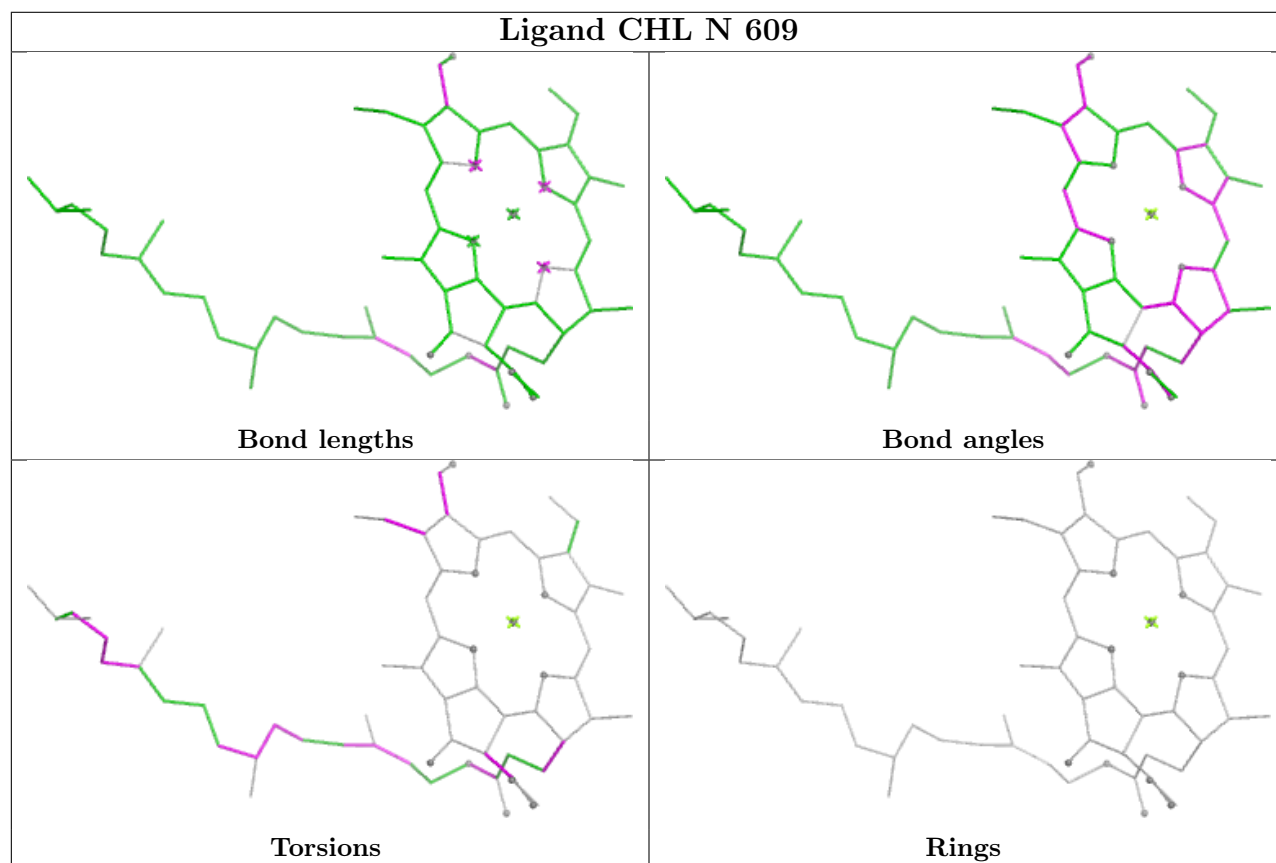
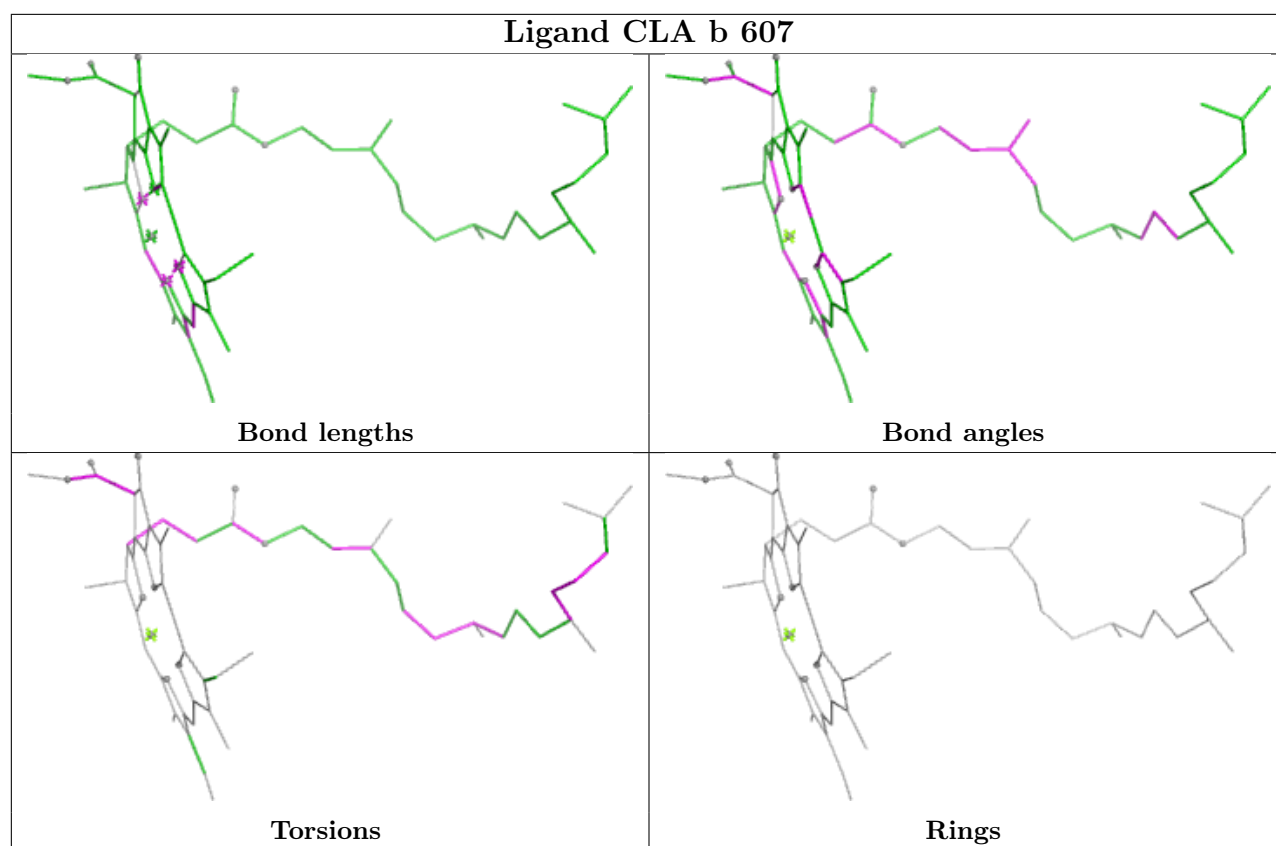


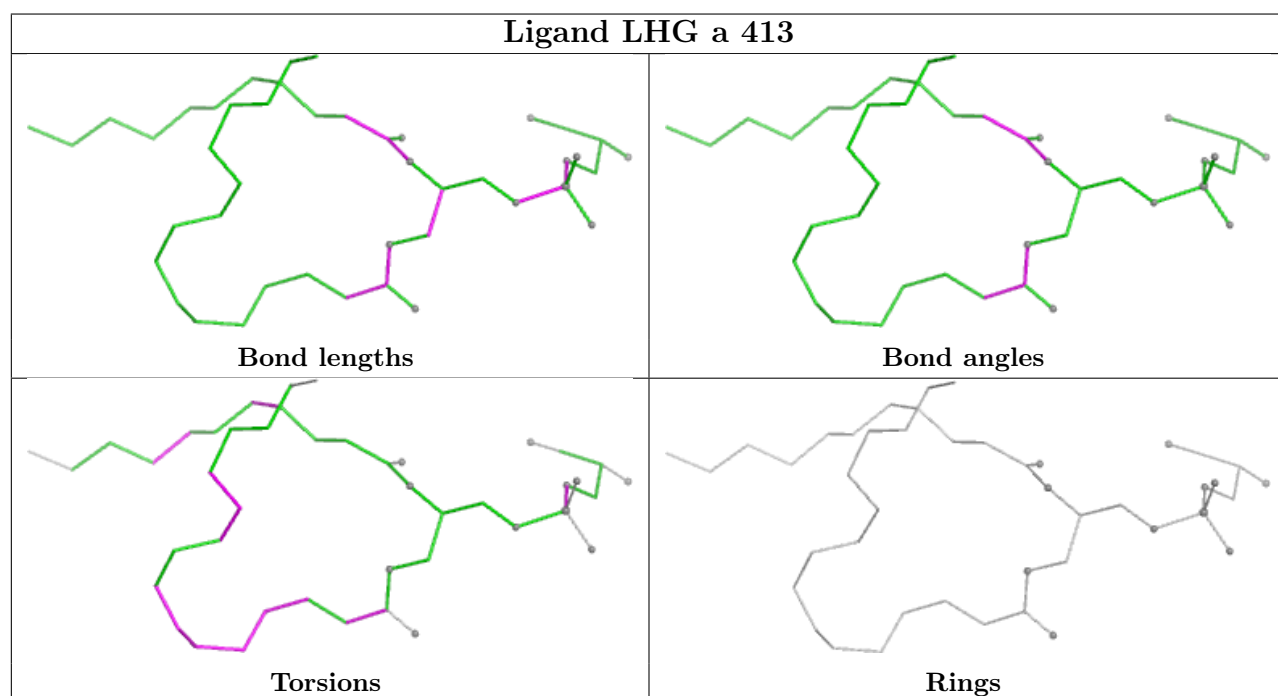
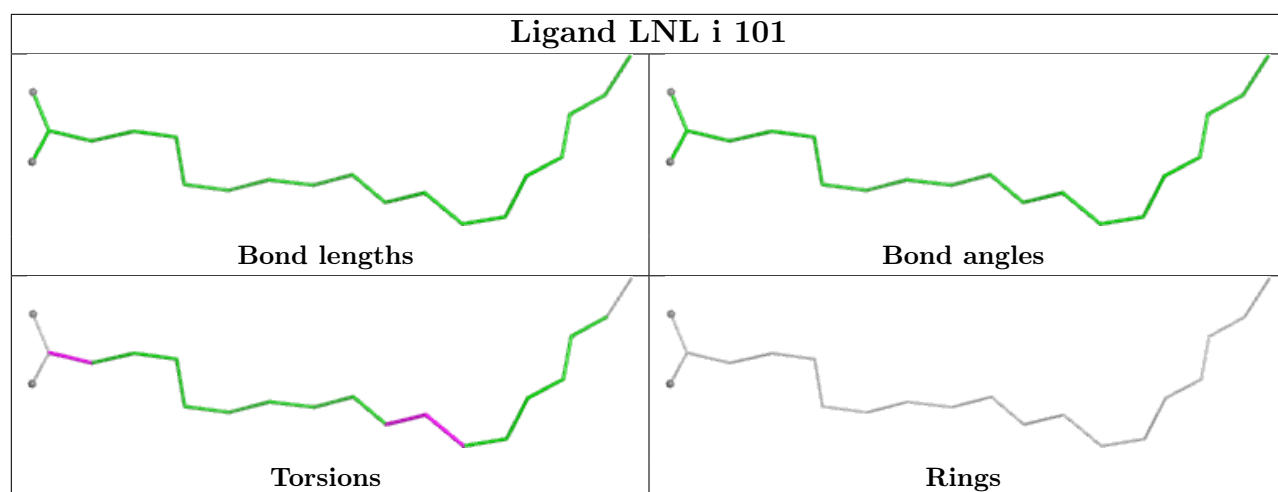


Ligand CHL N 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

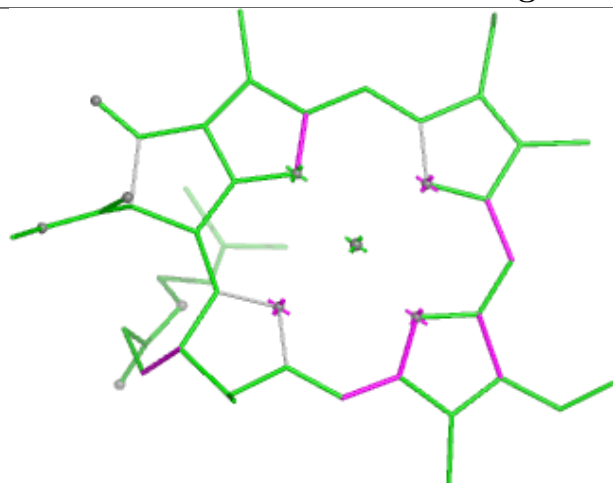
Ligand NEX g 618	
	
Bond lengths	Bond angles
	
Torsions	Rings



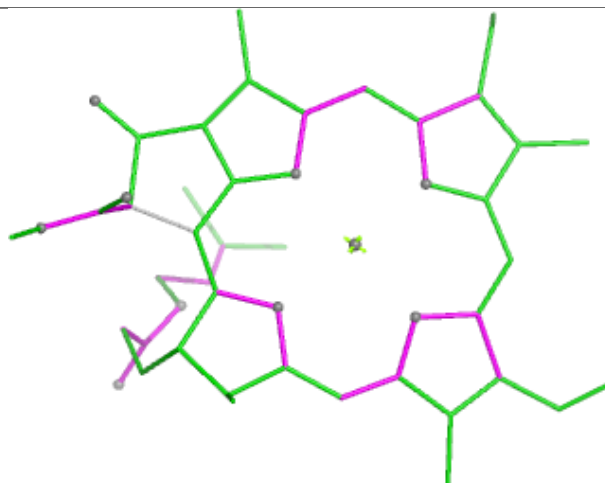




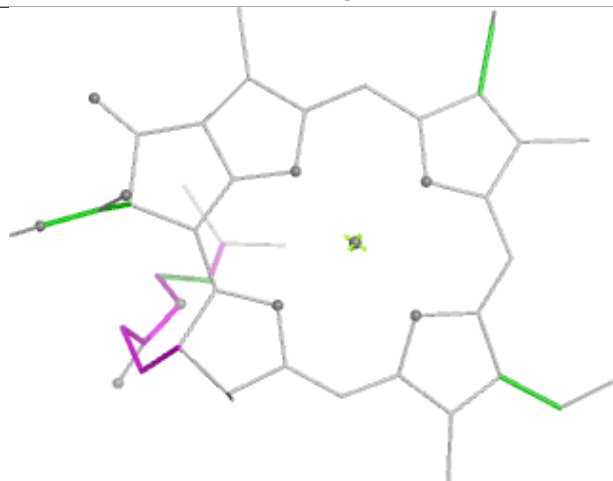
Ligand CLA 1 611



Bond lengths



Bond angles

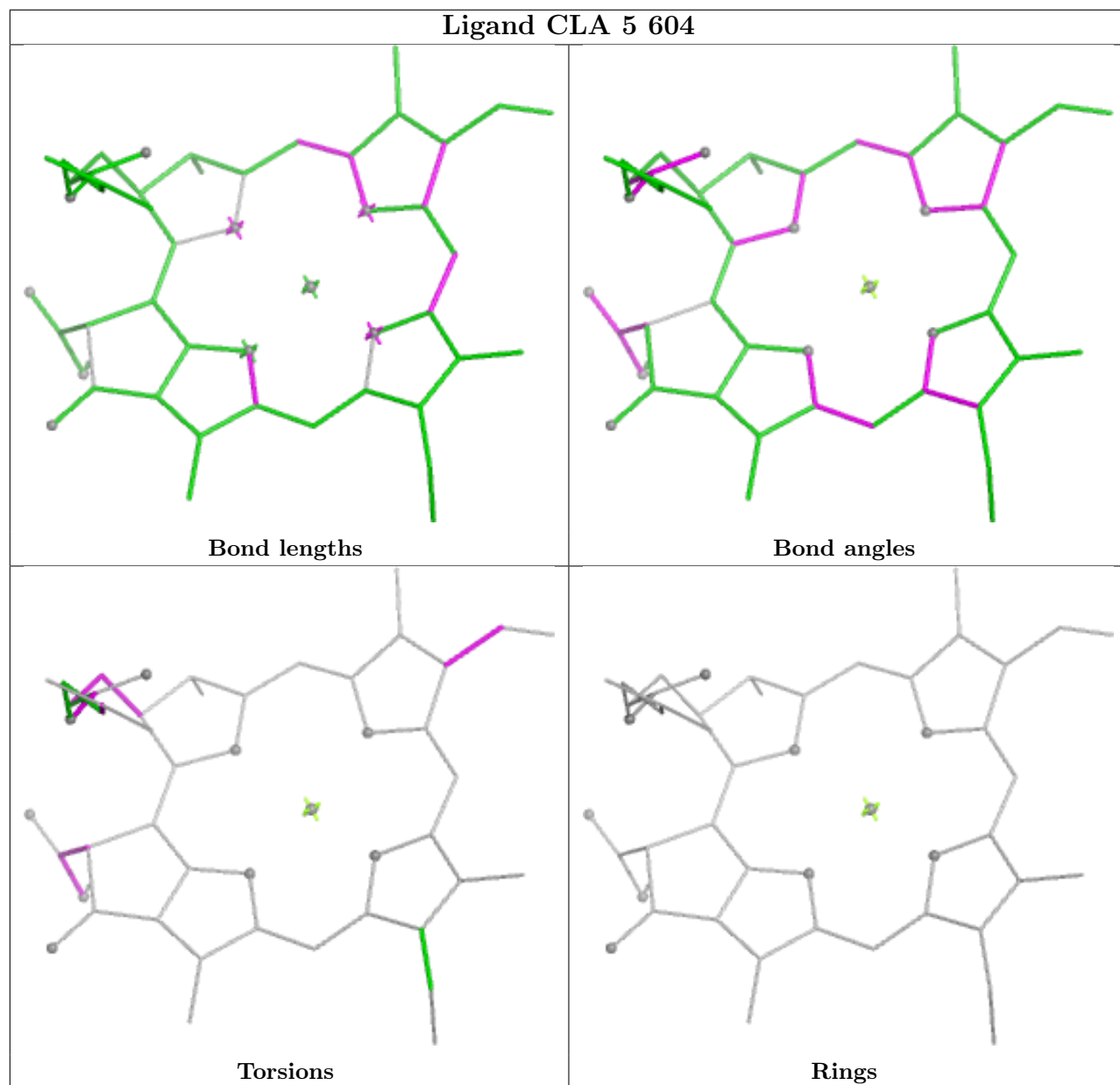


Torsions

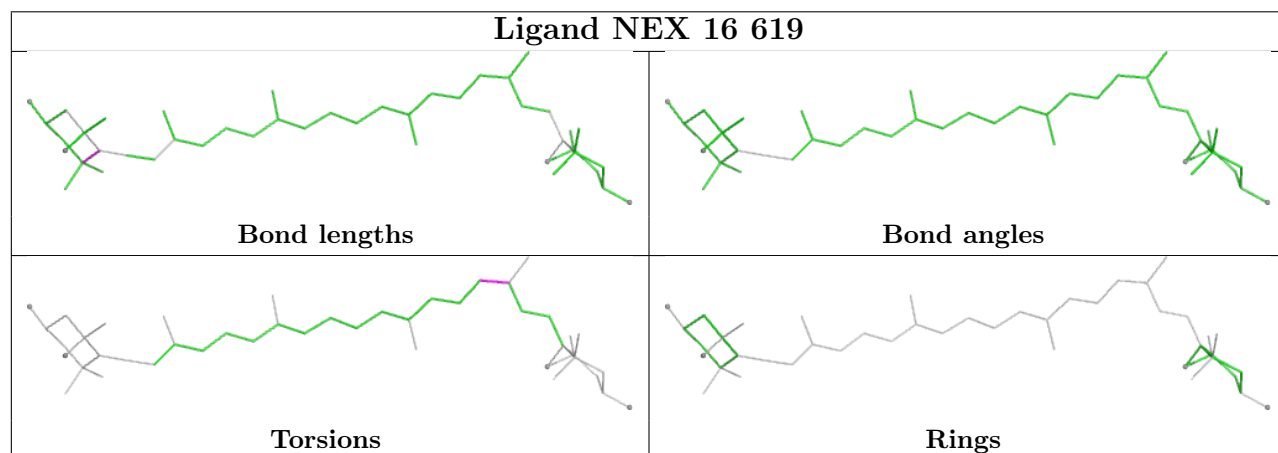


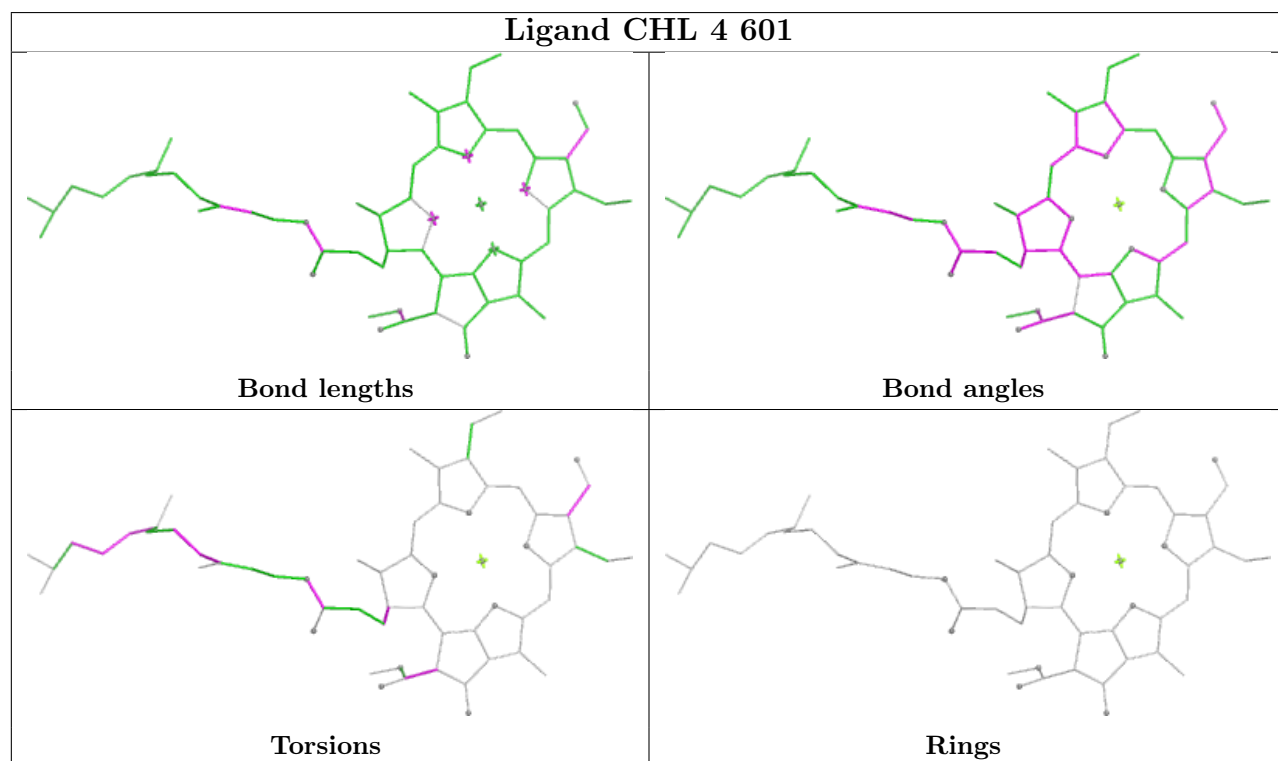
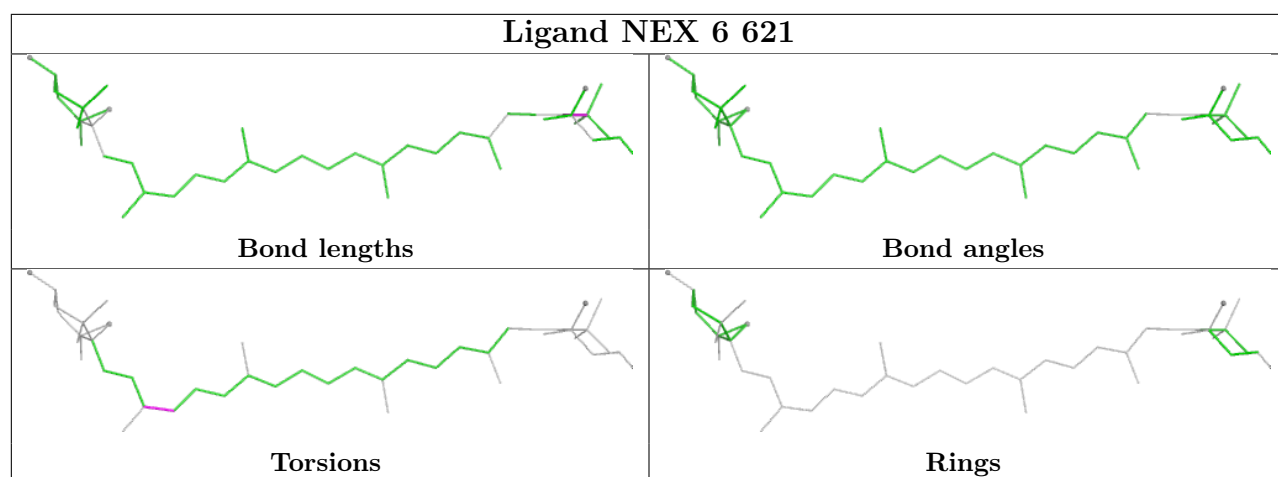
Rings

Ligand CLA 5 604

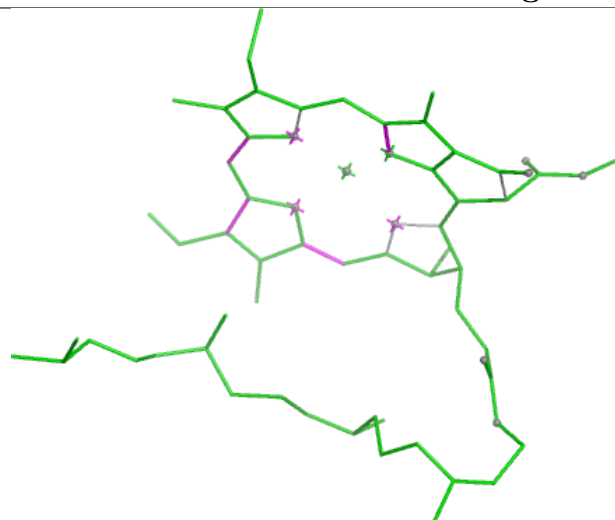


Ligand NEX 16 619

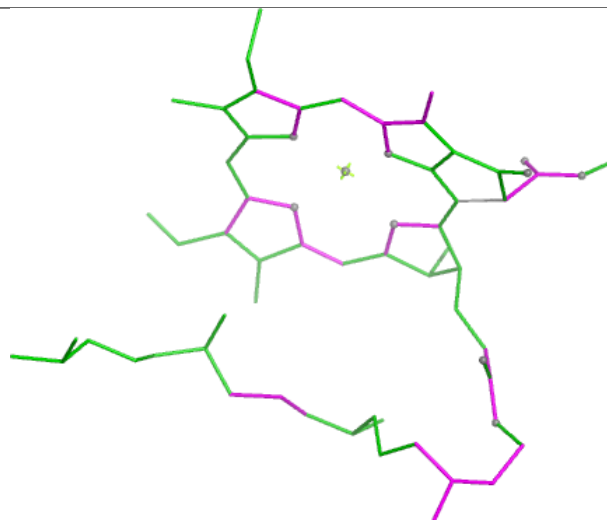




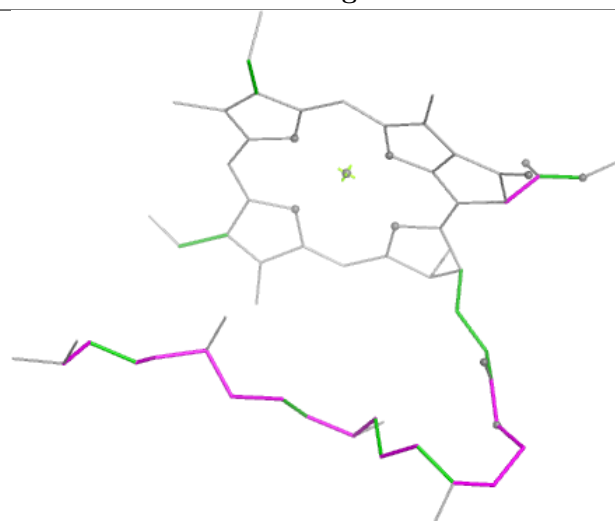
Ligand CLA s 614



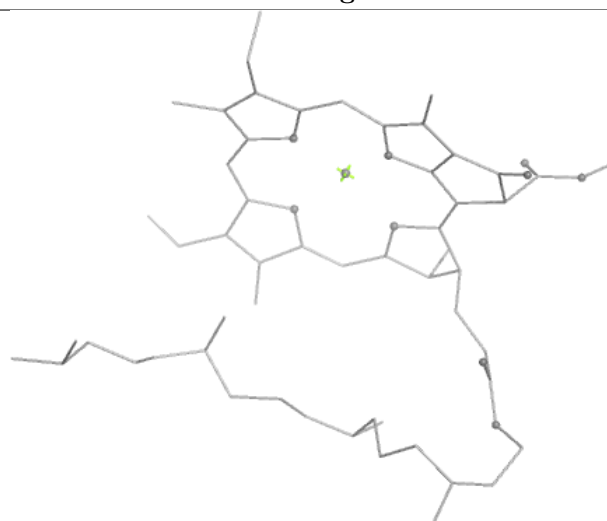
Bond lengths



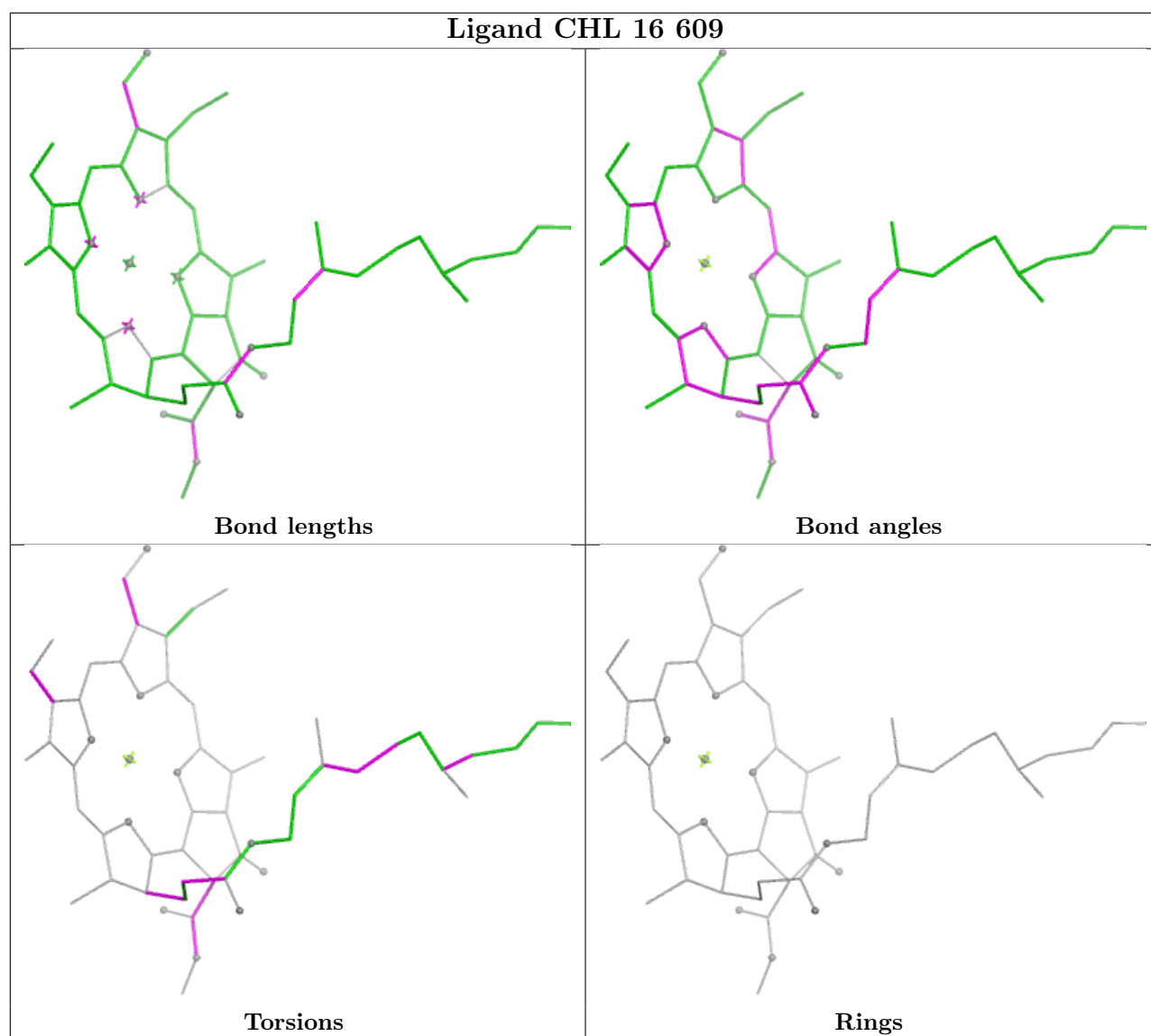
Bond angles



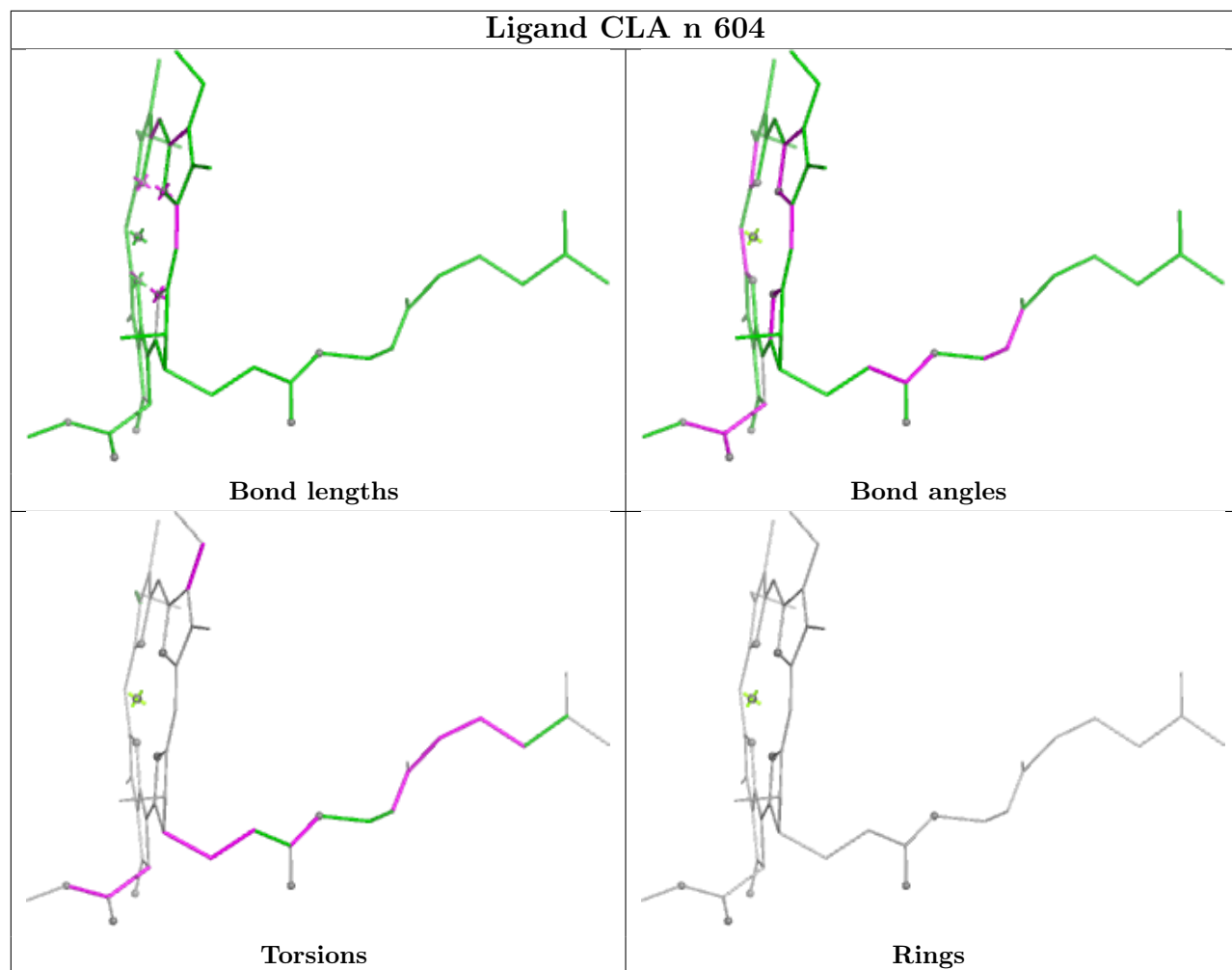
Torsions

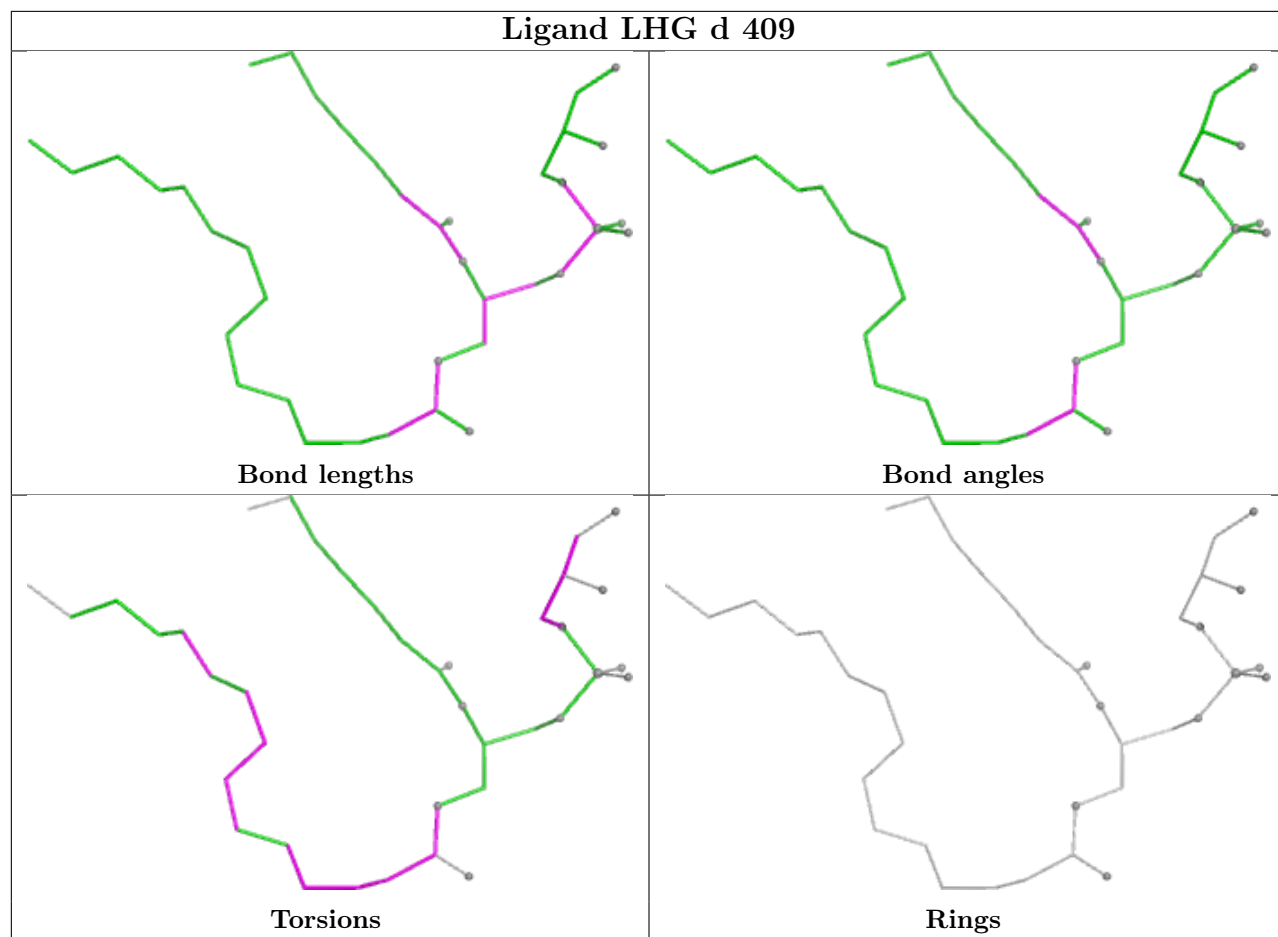


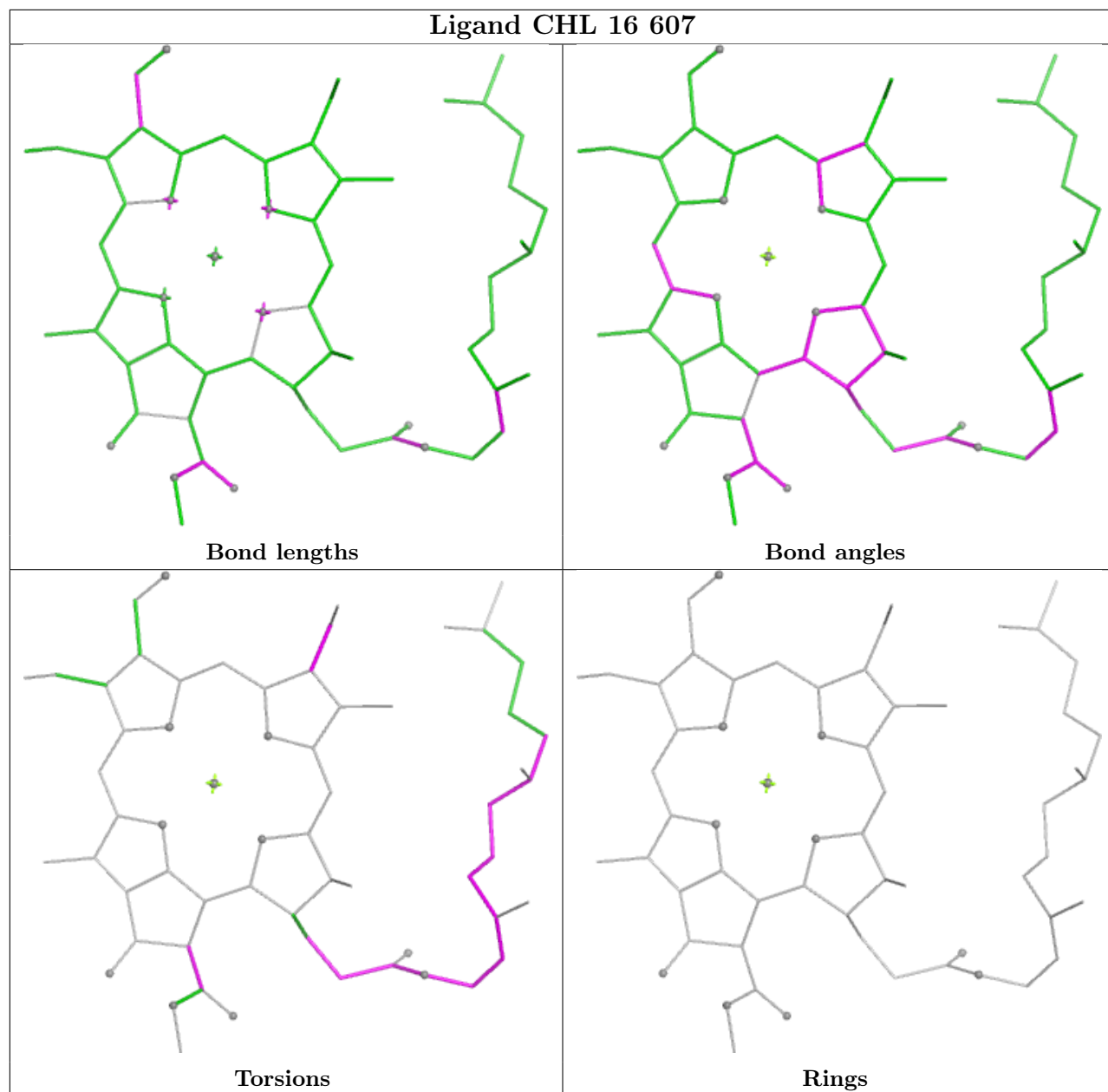
Rings

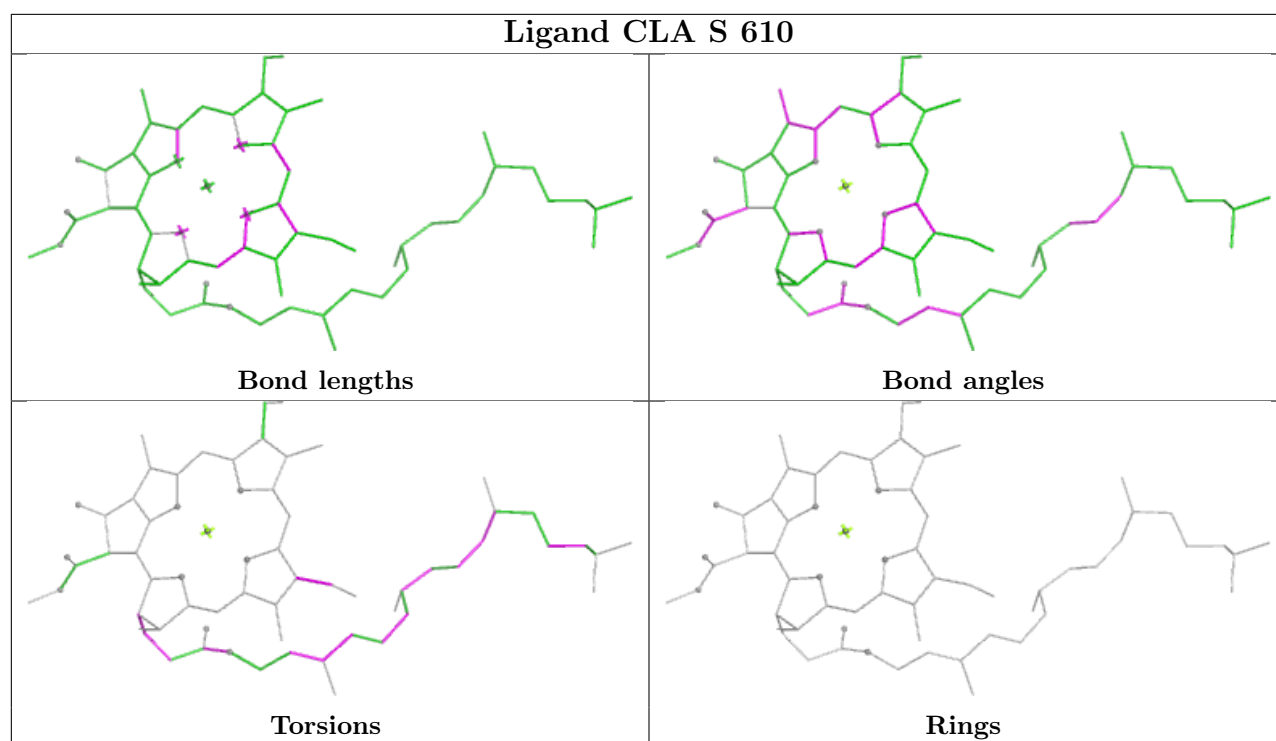


Ligand CLA n 604

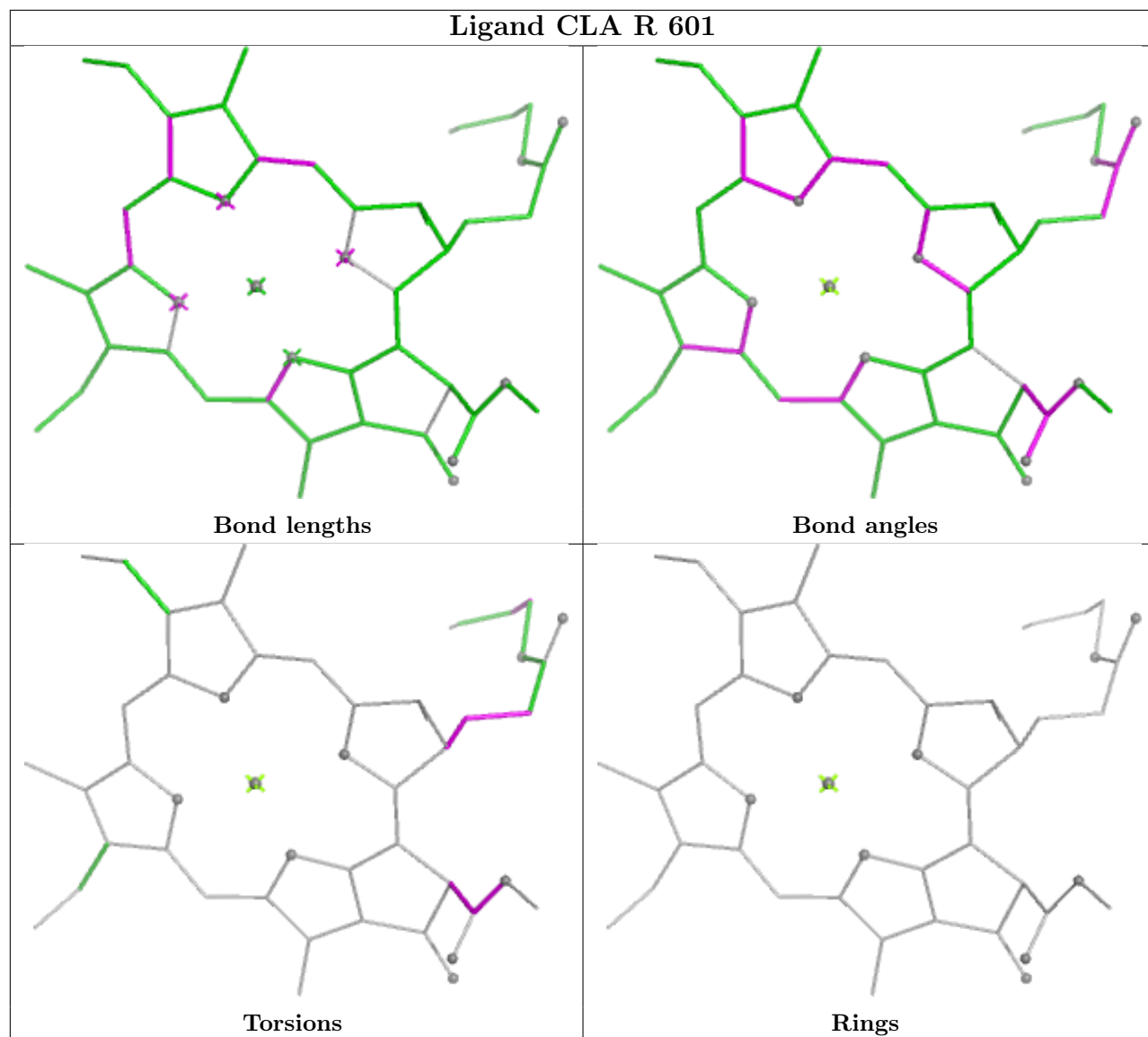


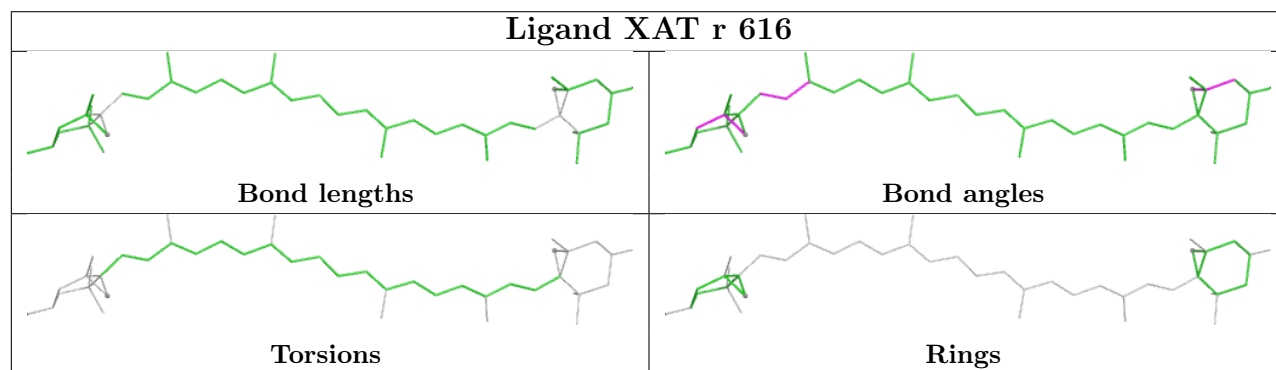
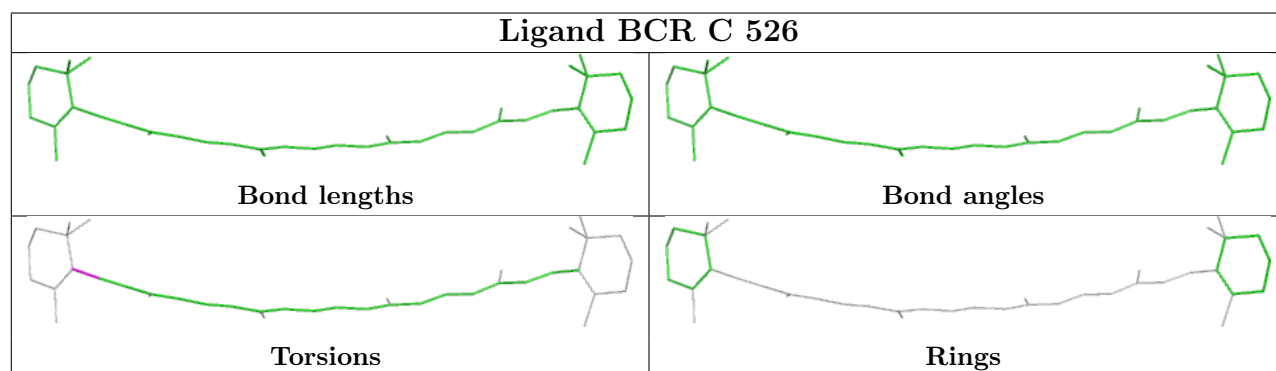
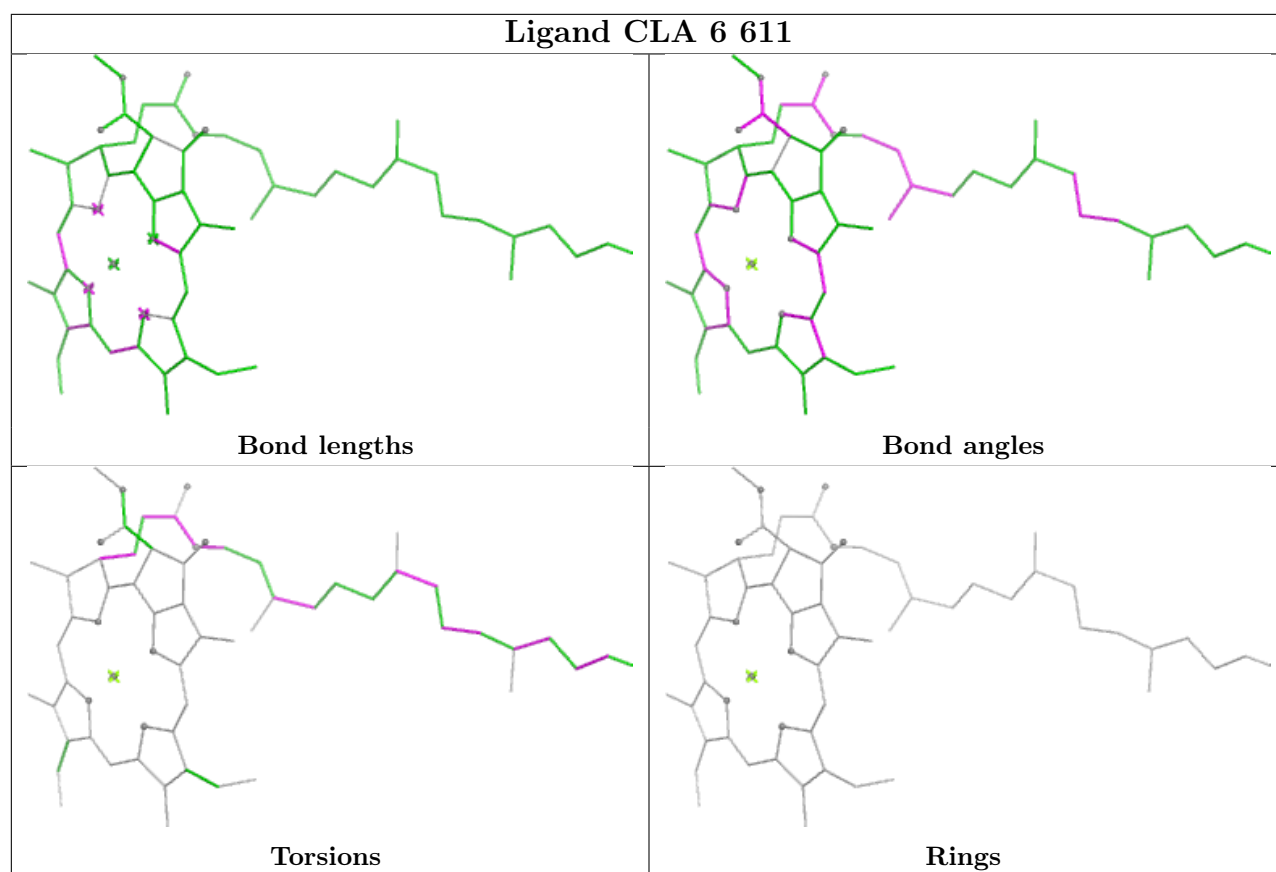


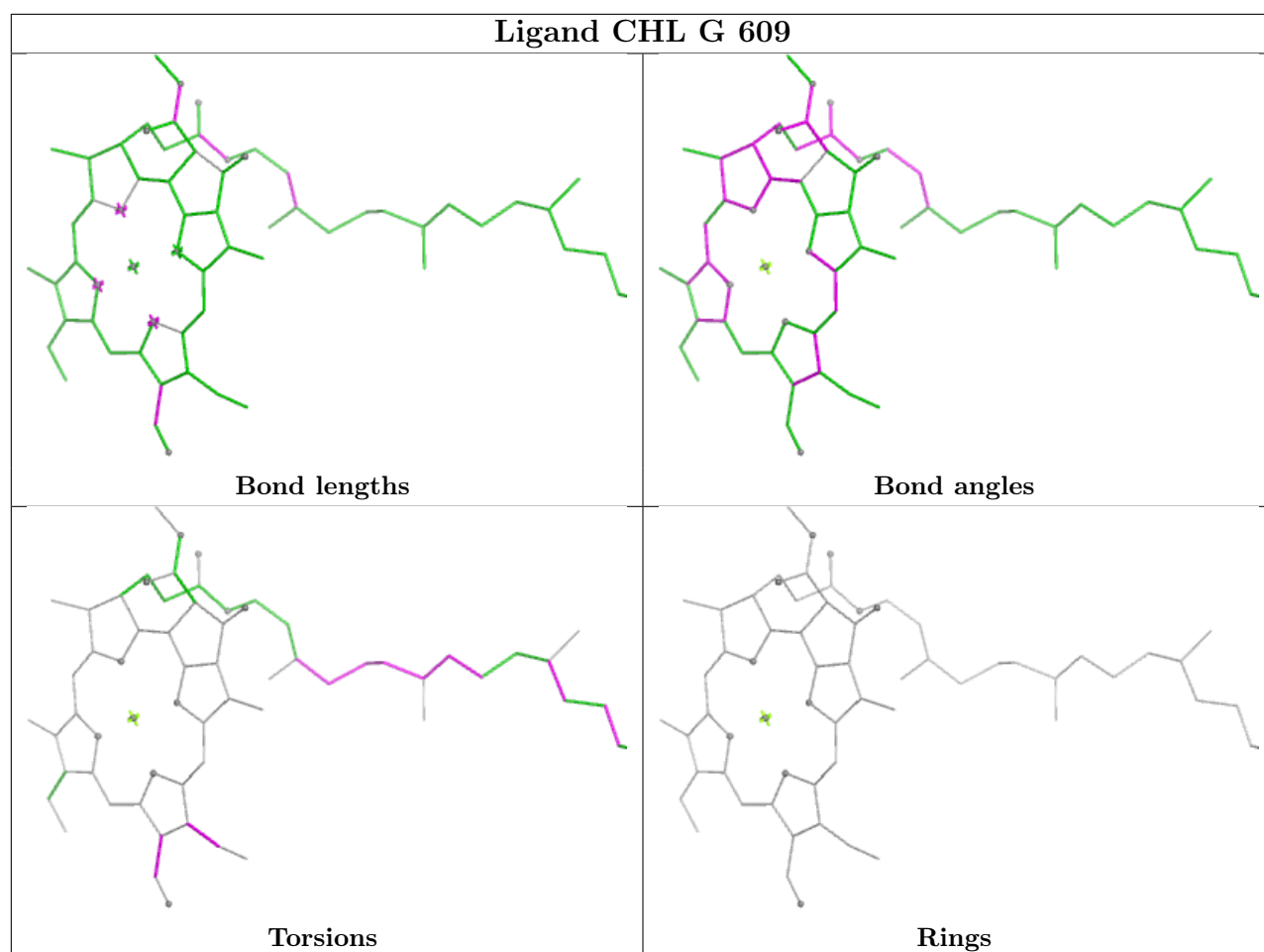




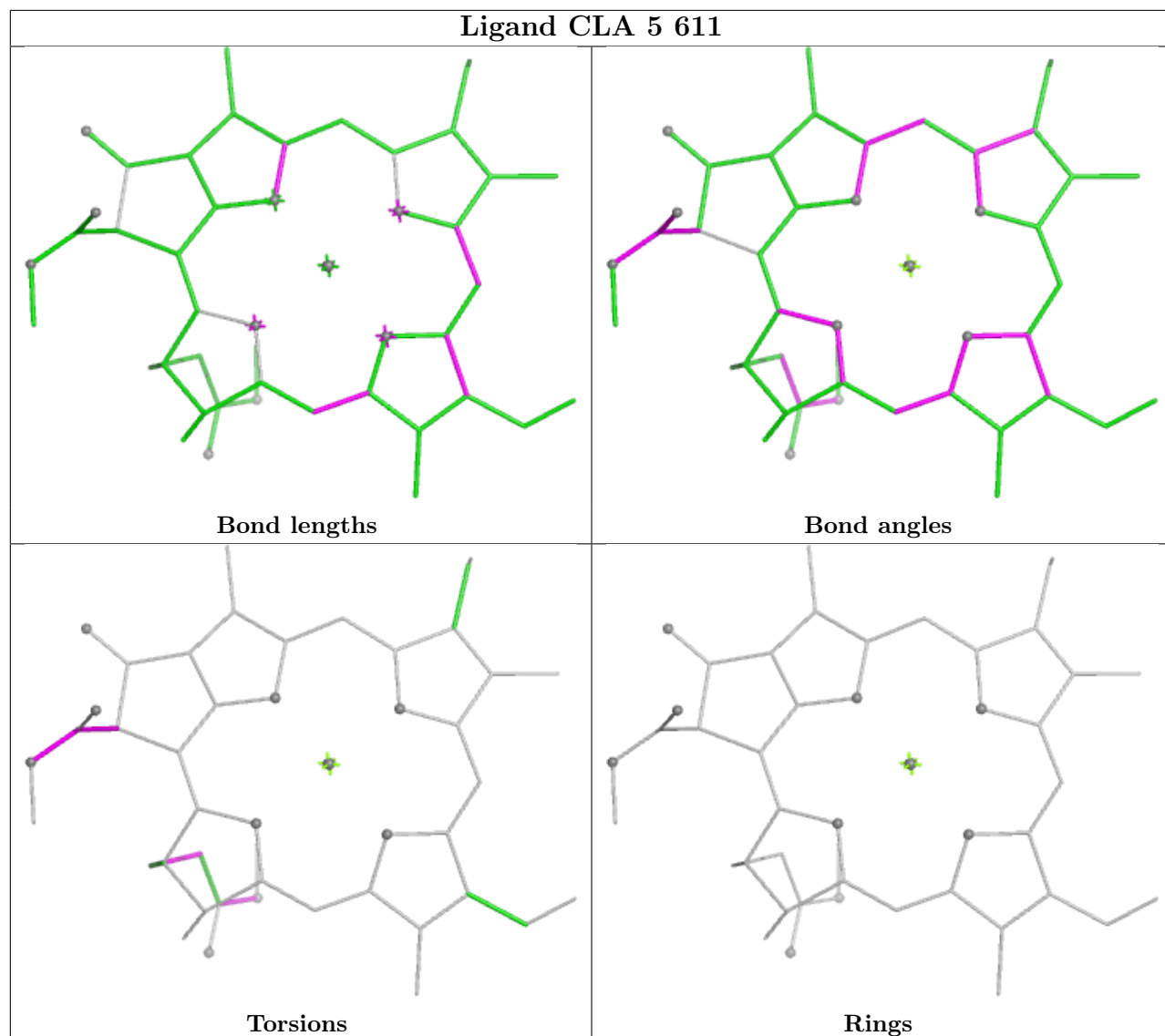
Ligand CLA R 601



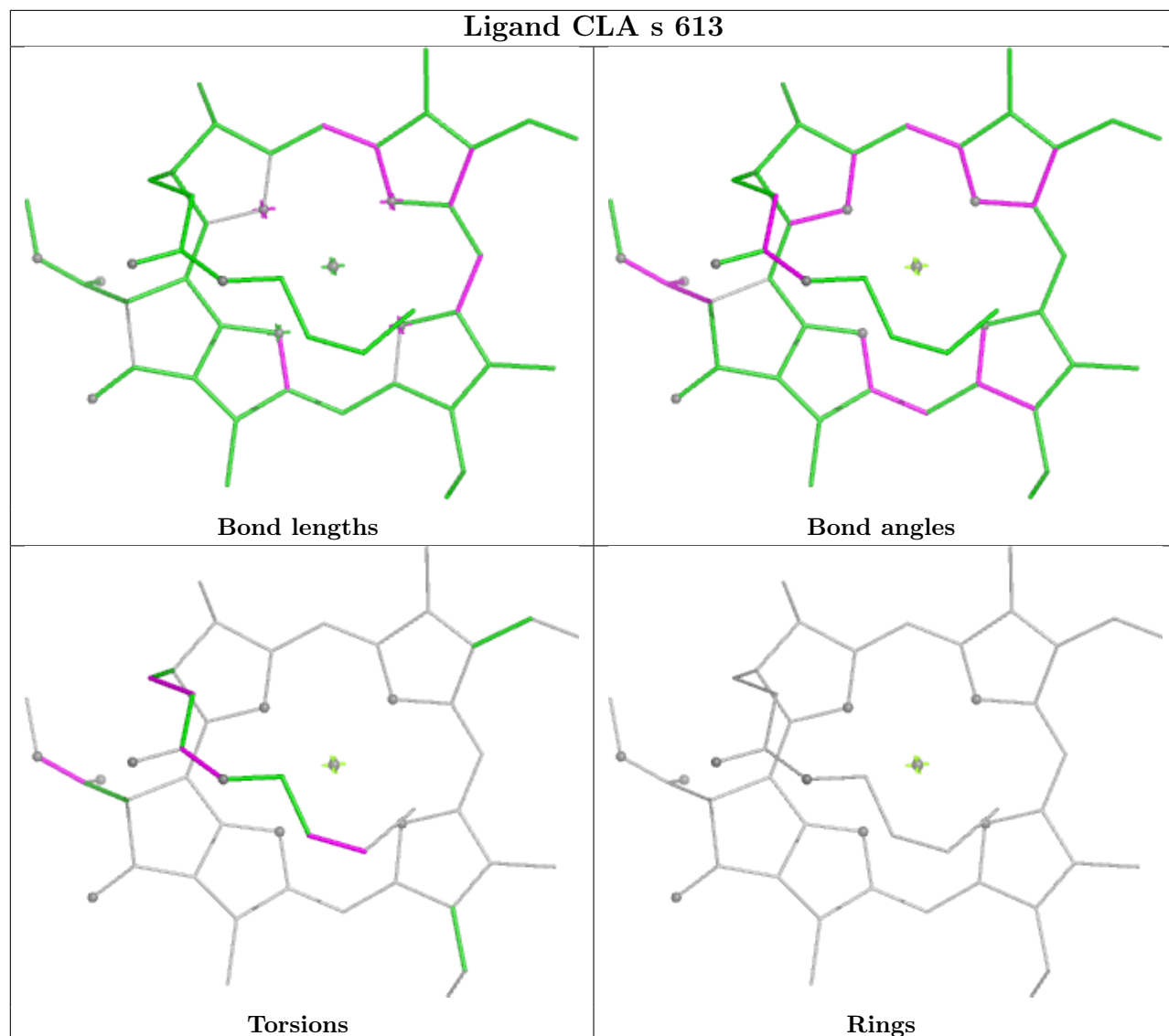


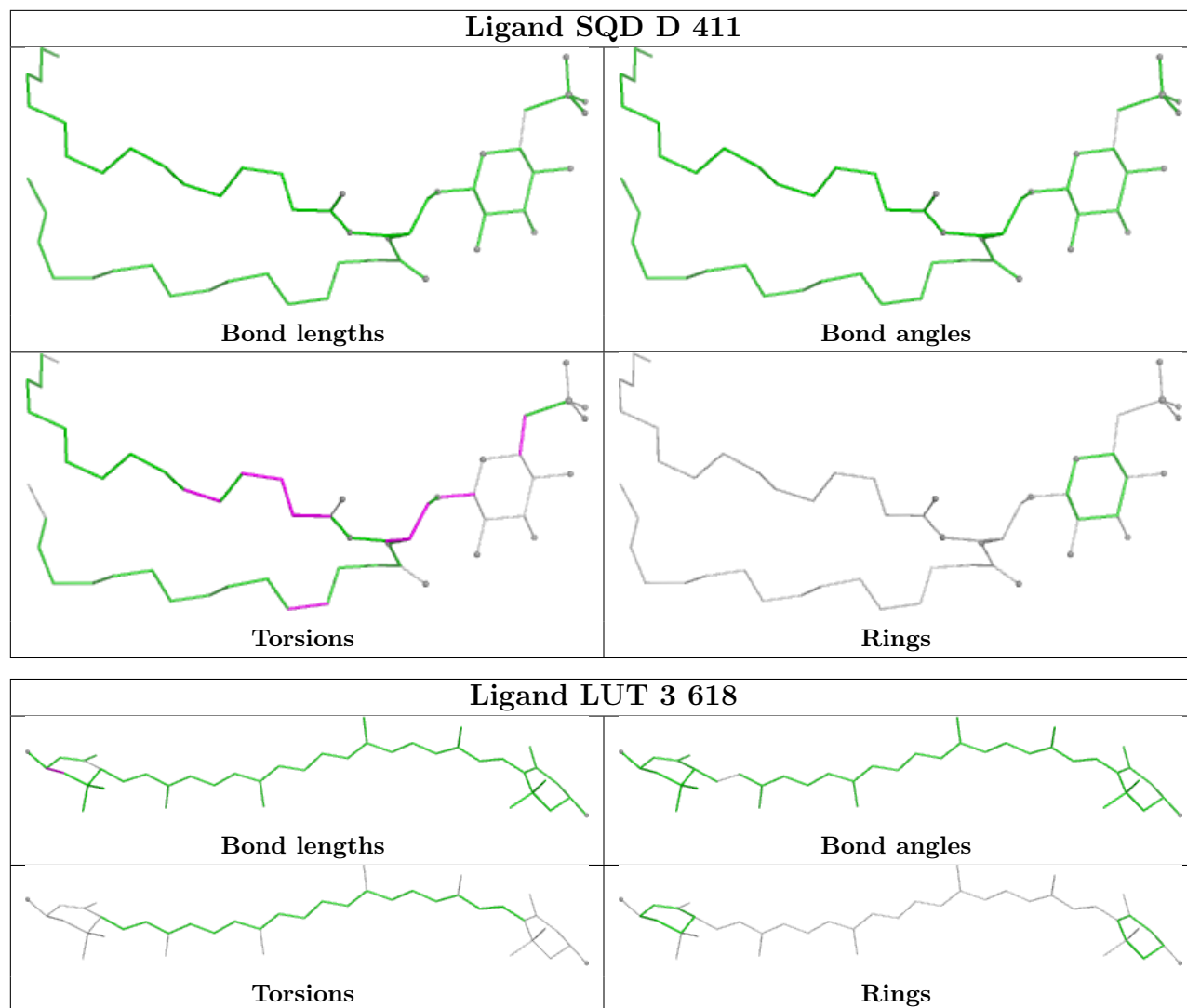


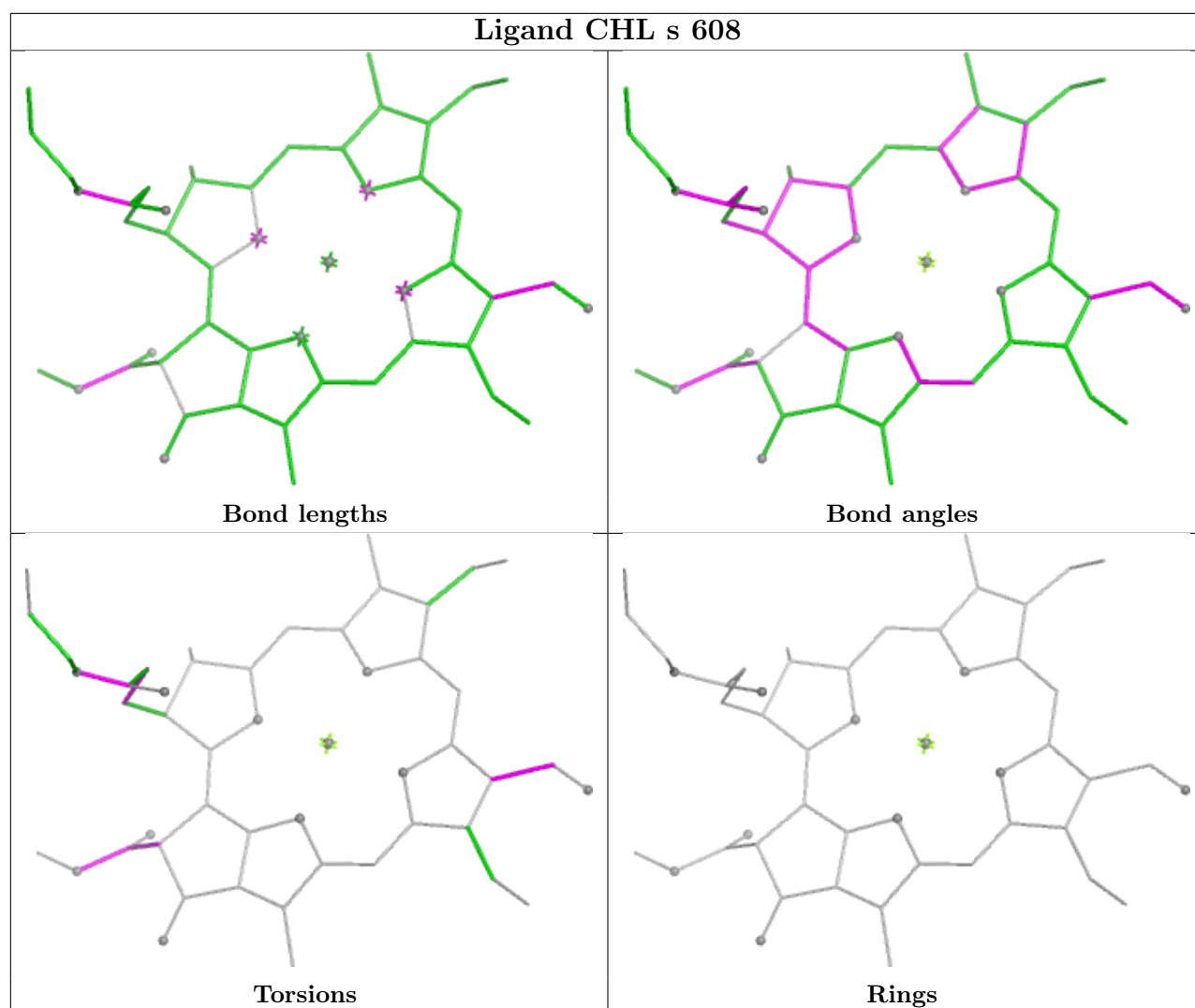
Ligand CLA 5 611



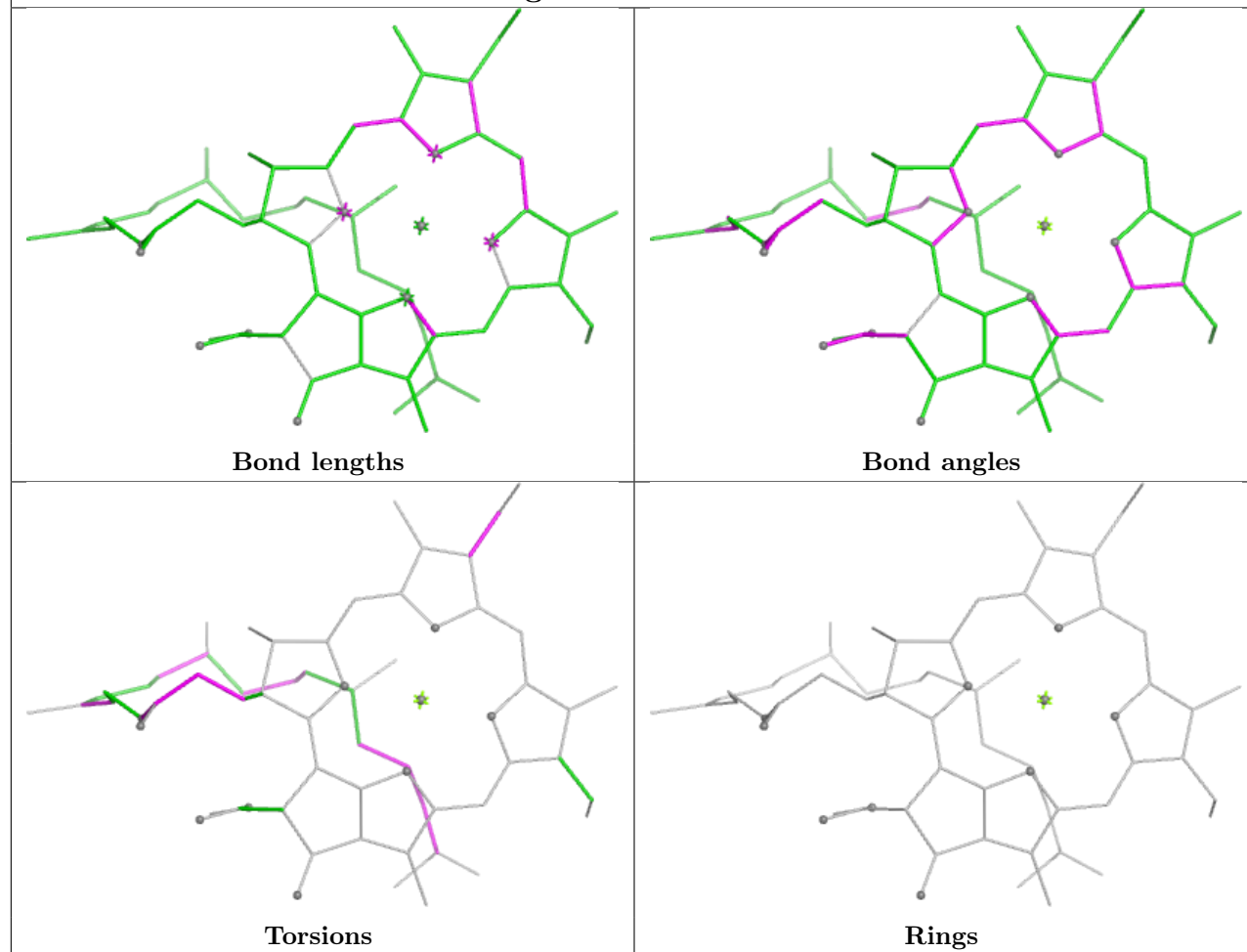
Ligand CLA s 613



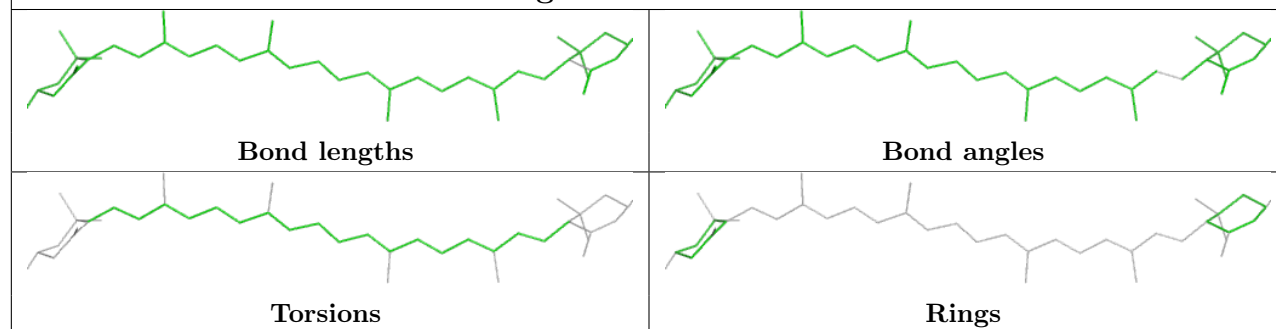




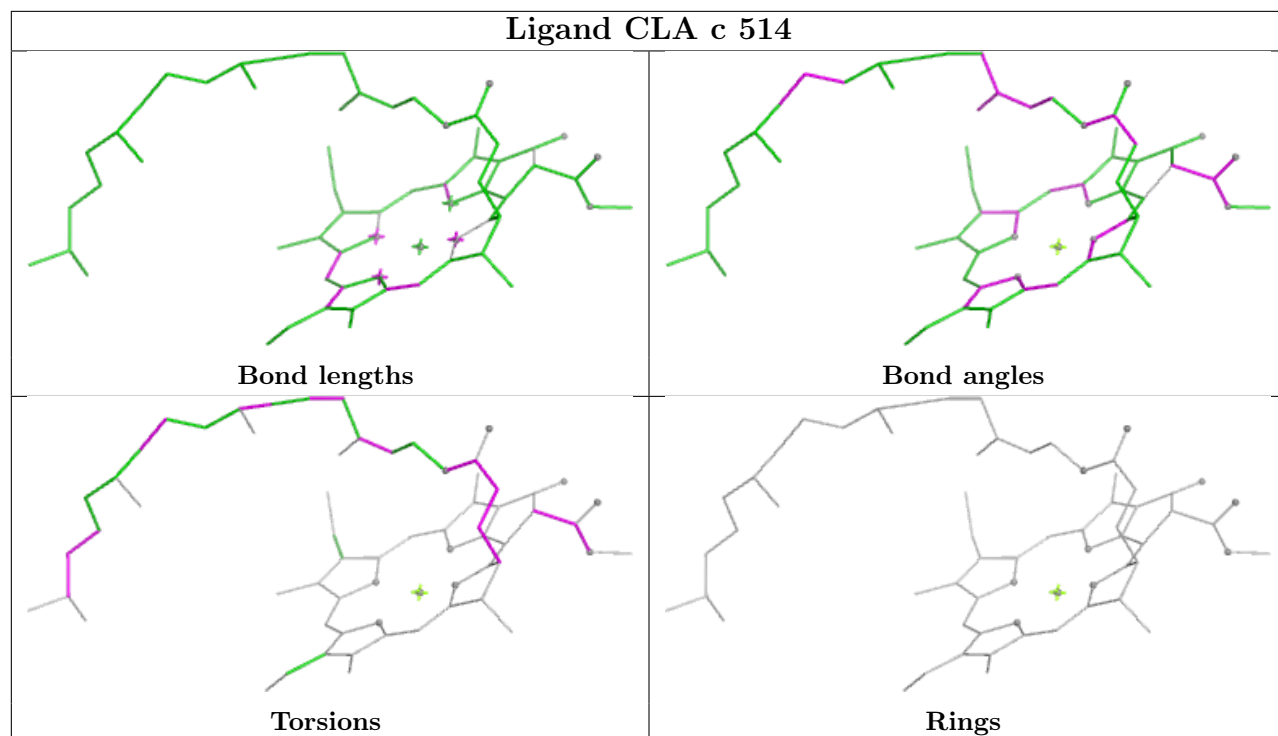
Ligand CLA c 511



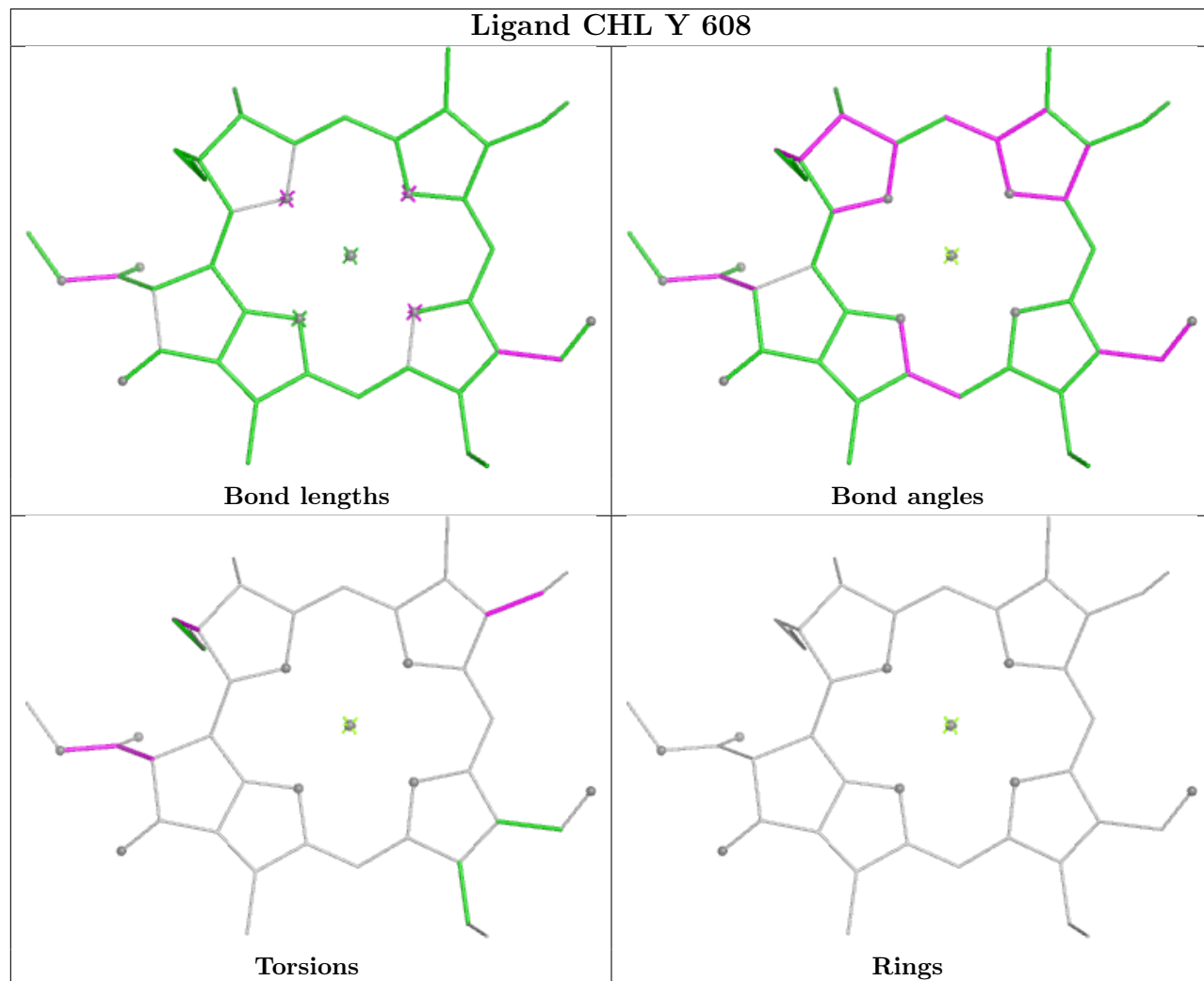
Ligand LUT 2 614

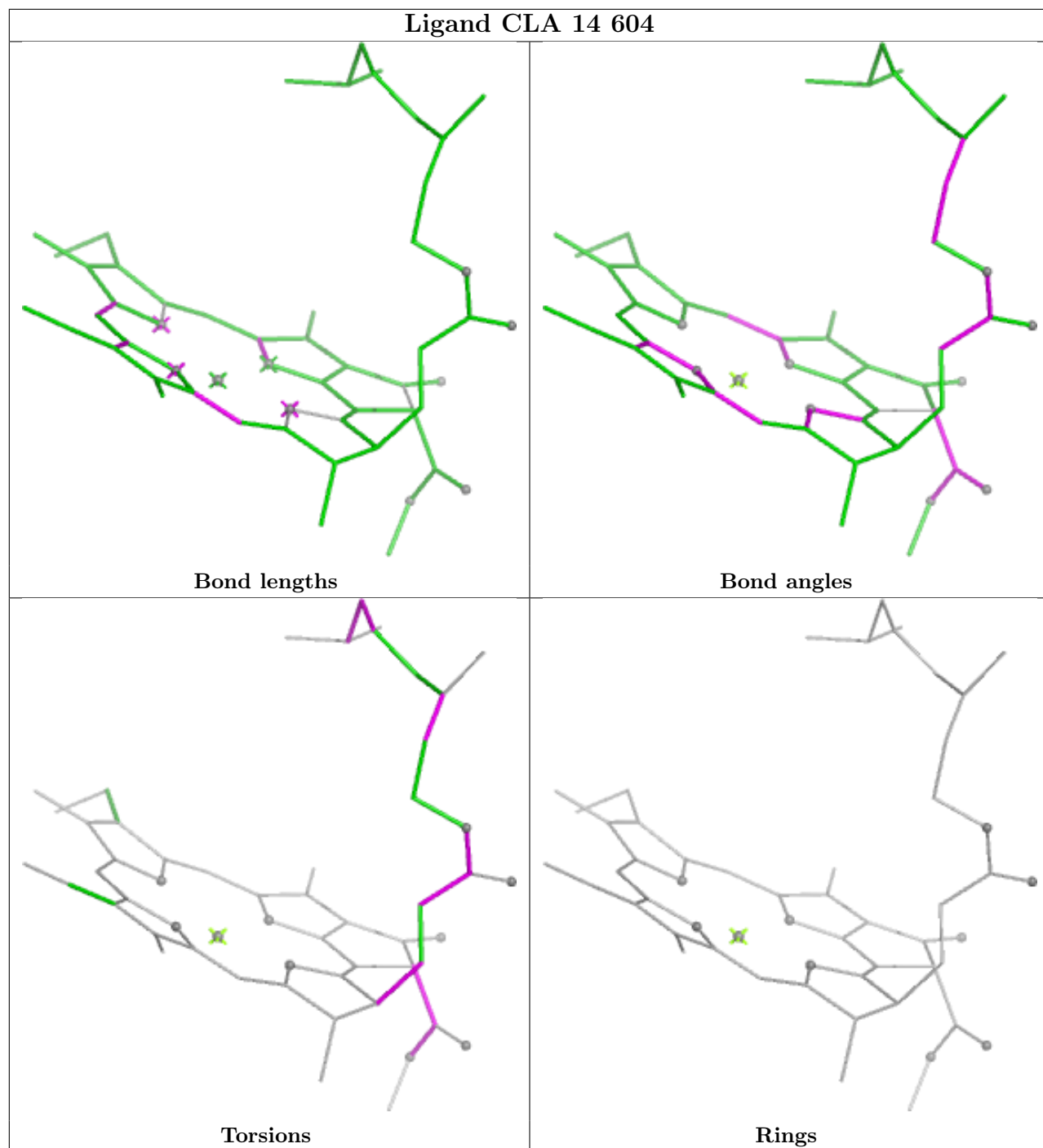


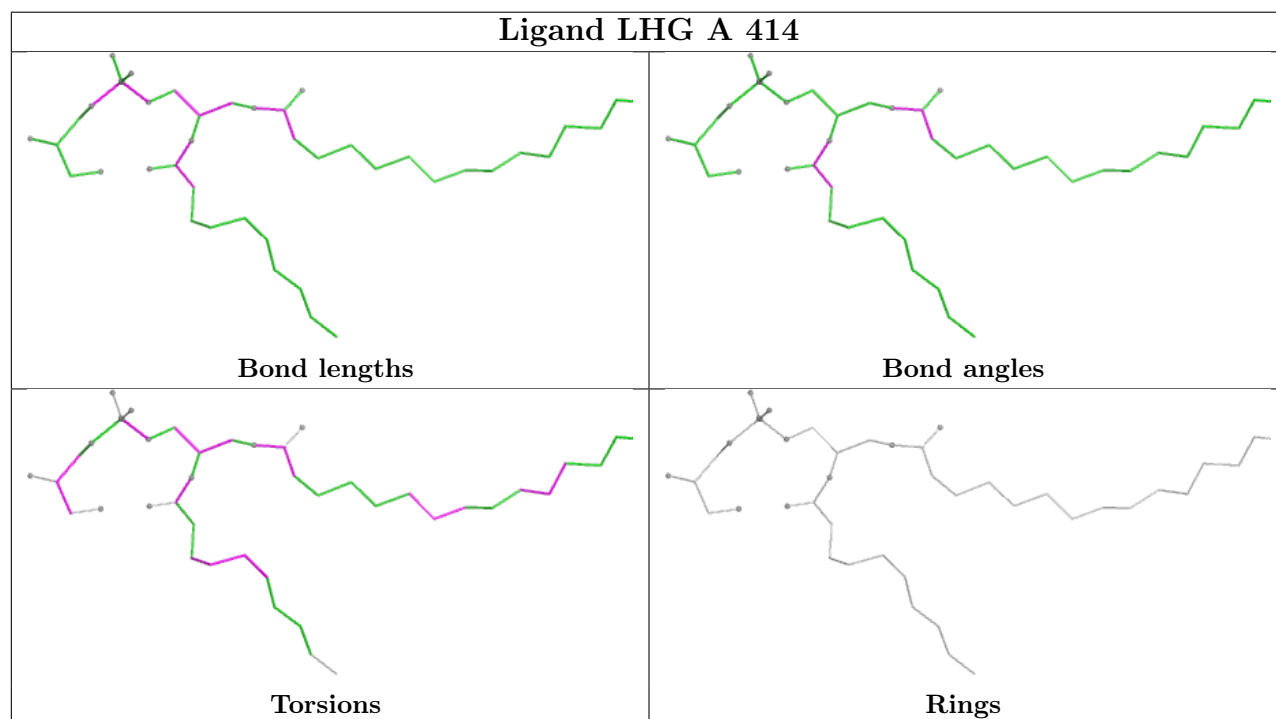
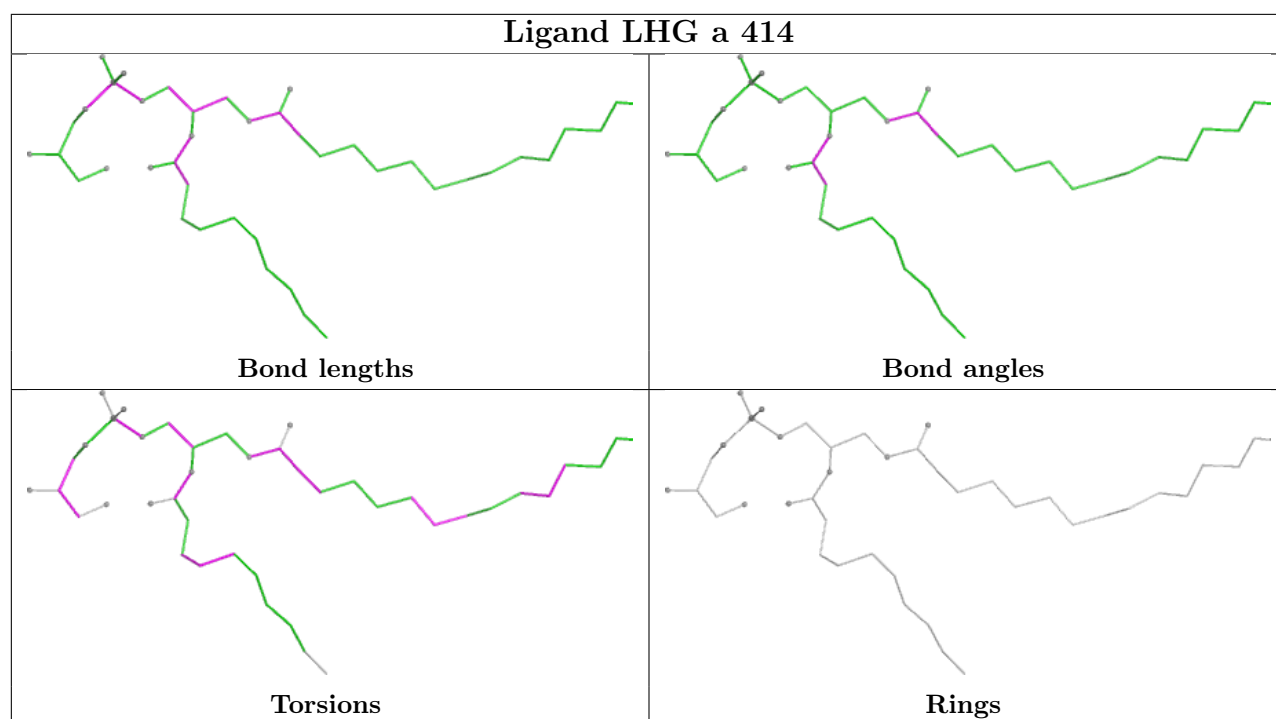
Ligand CLA c 514

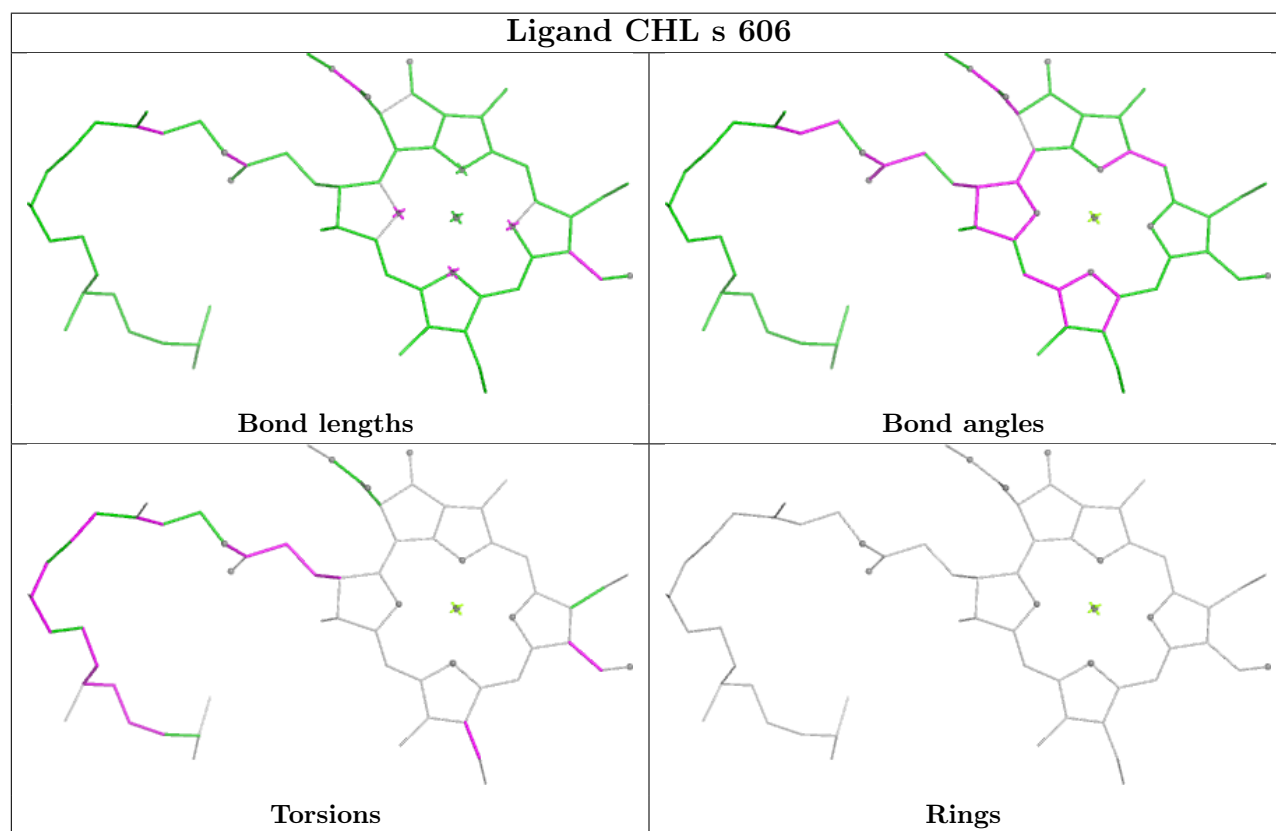
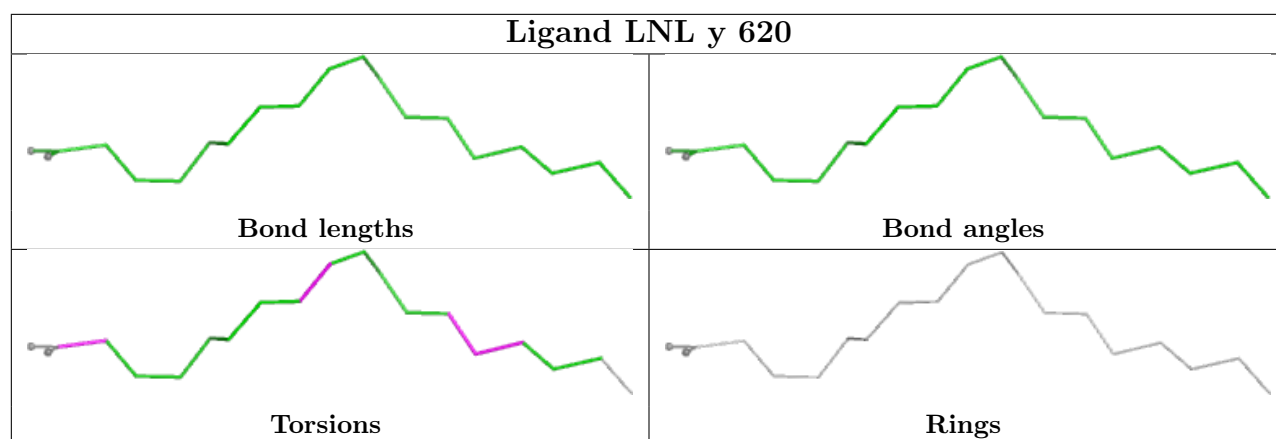


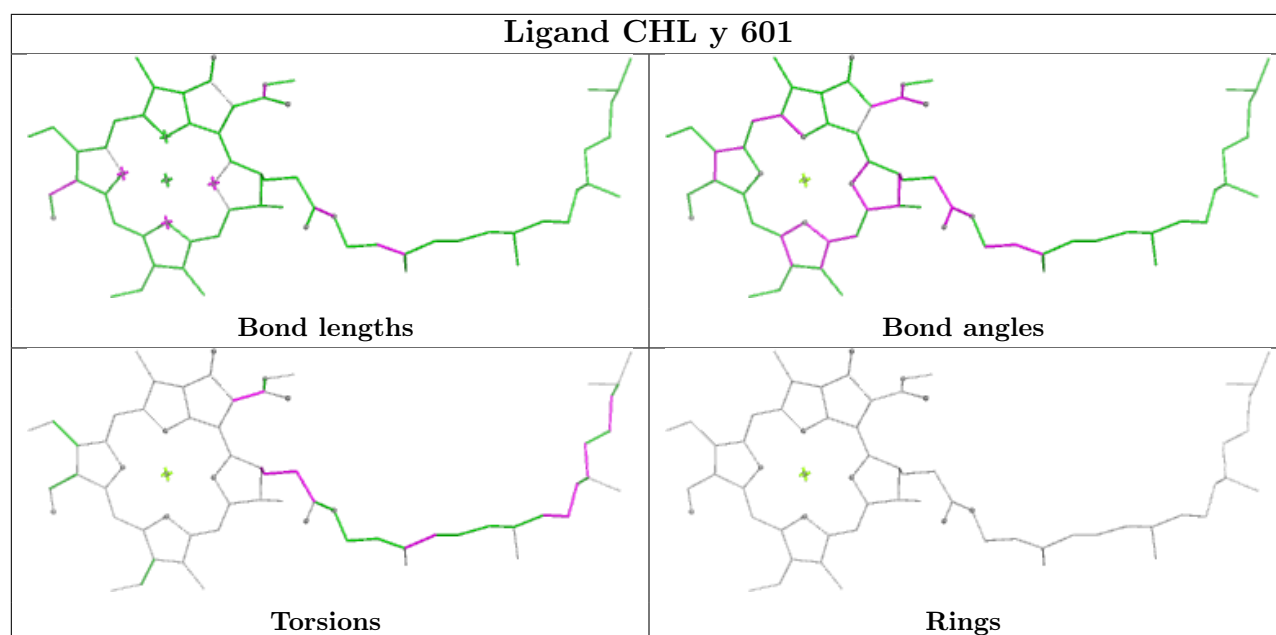
Ligand CHL Y 608

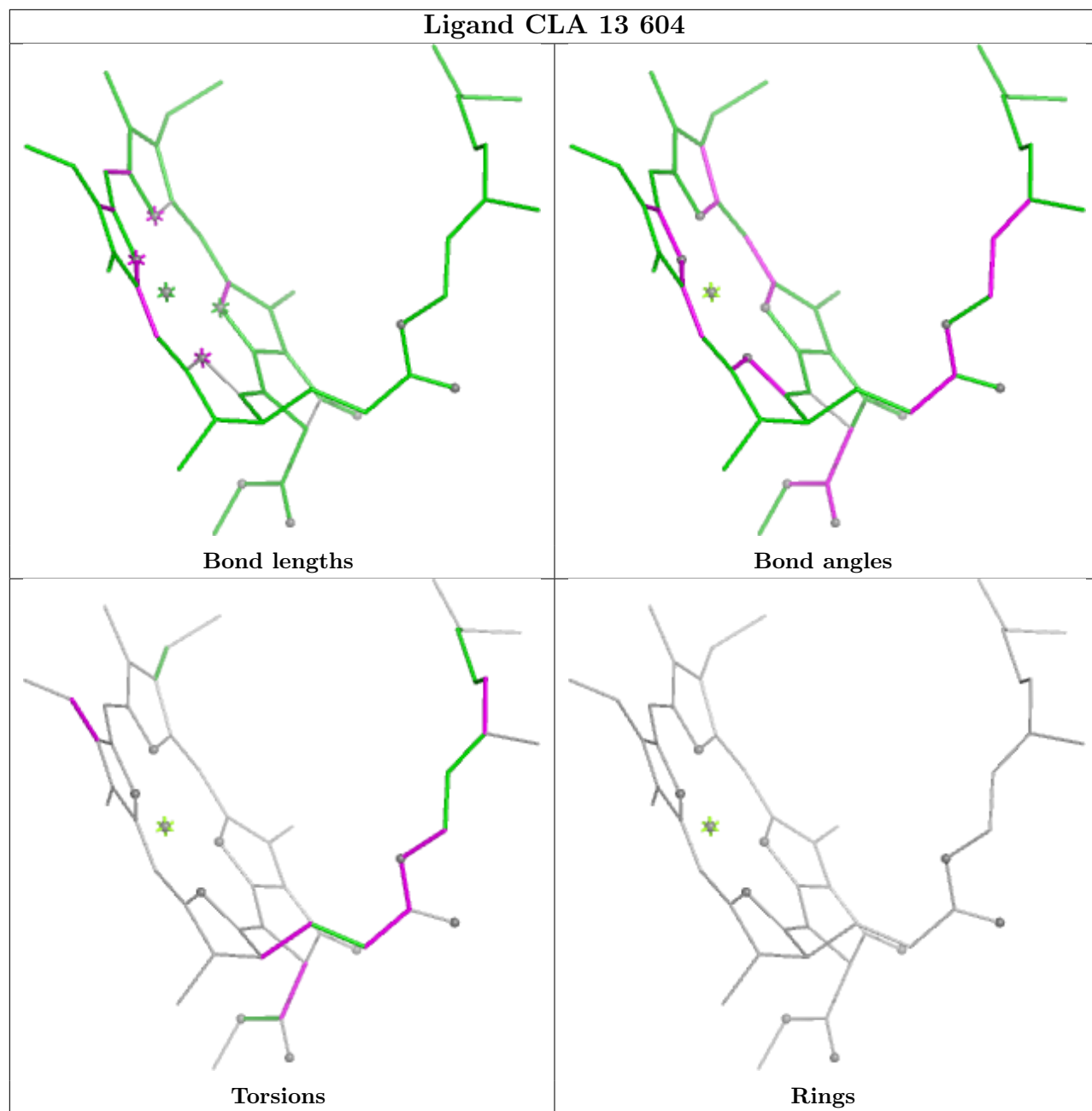


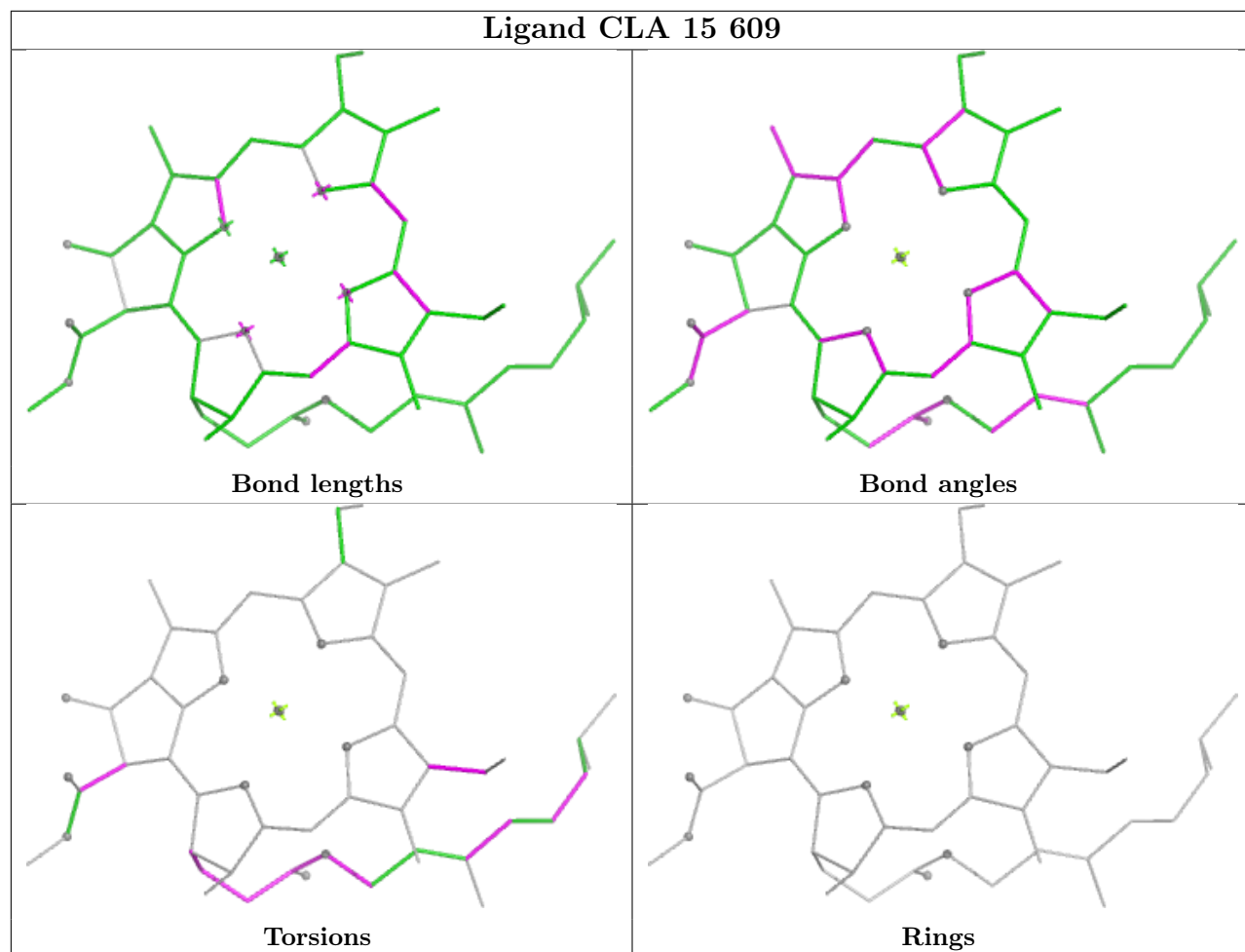


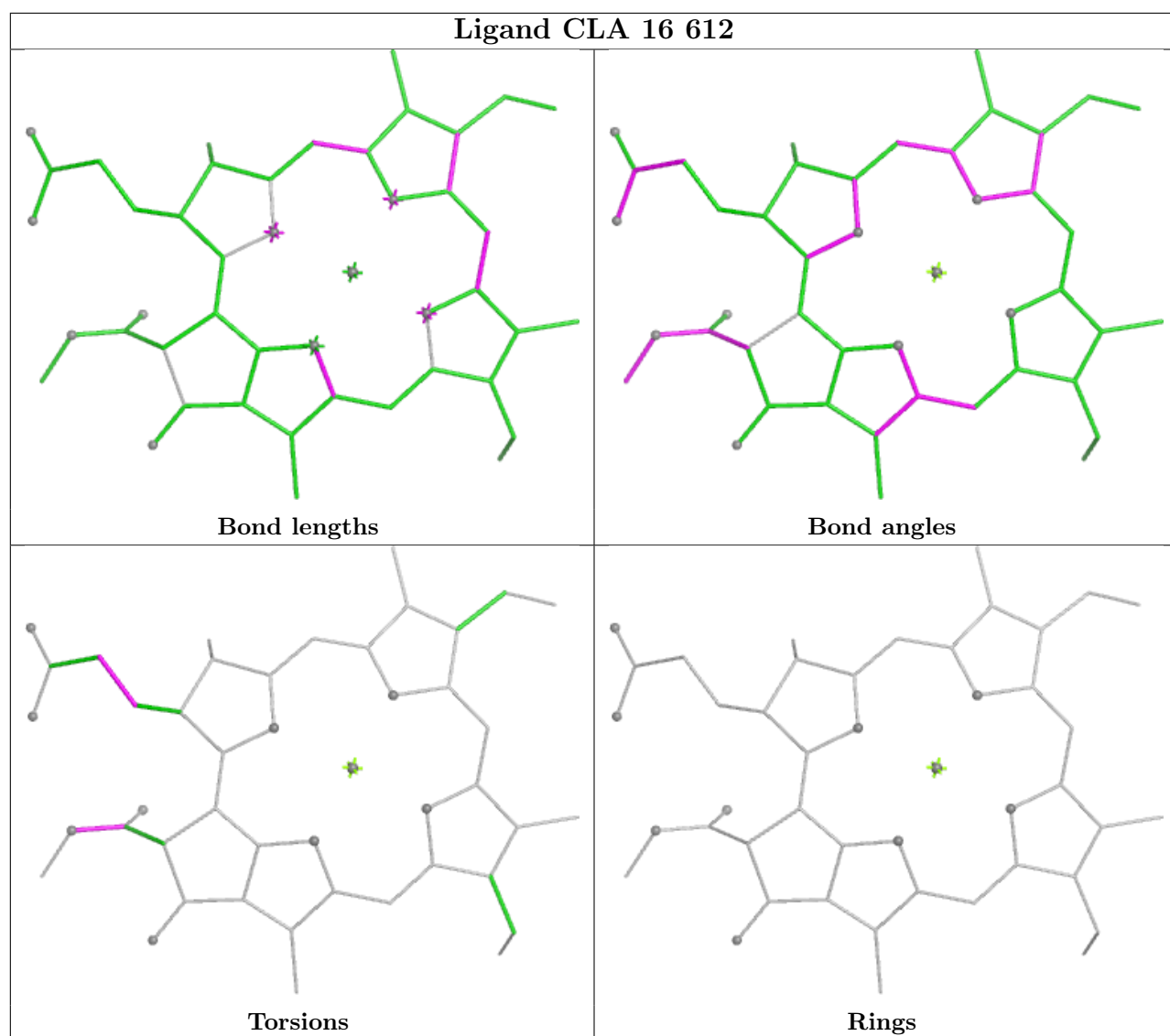




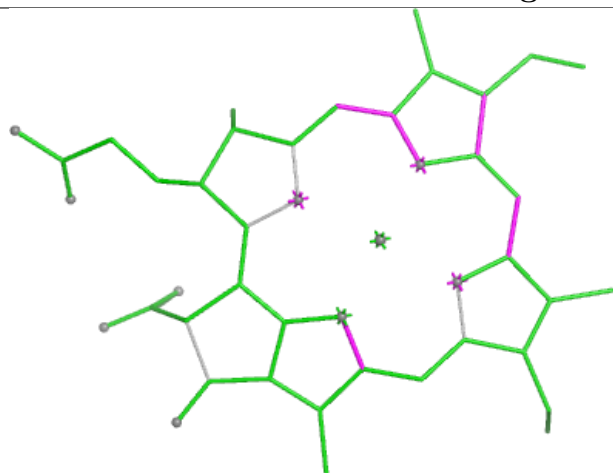




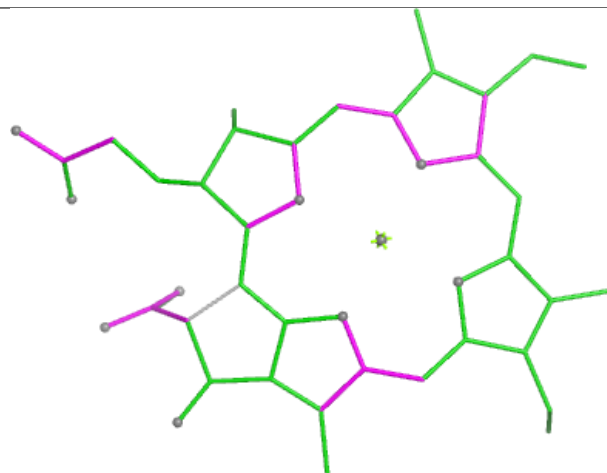




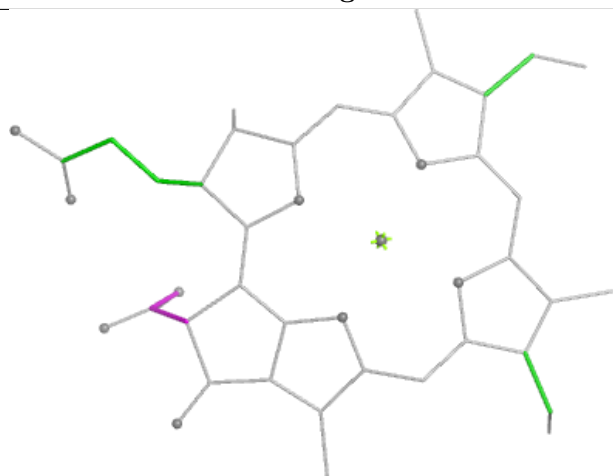
Ligand CLA s 612



Bond lengths



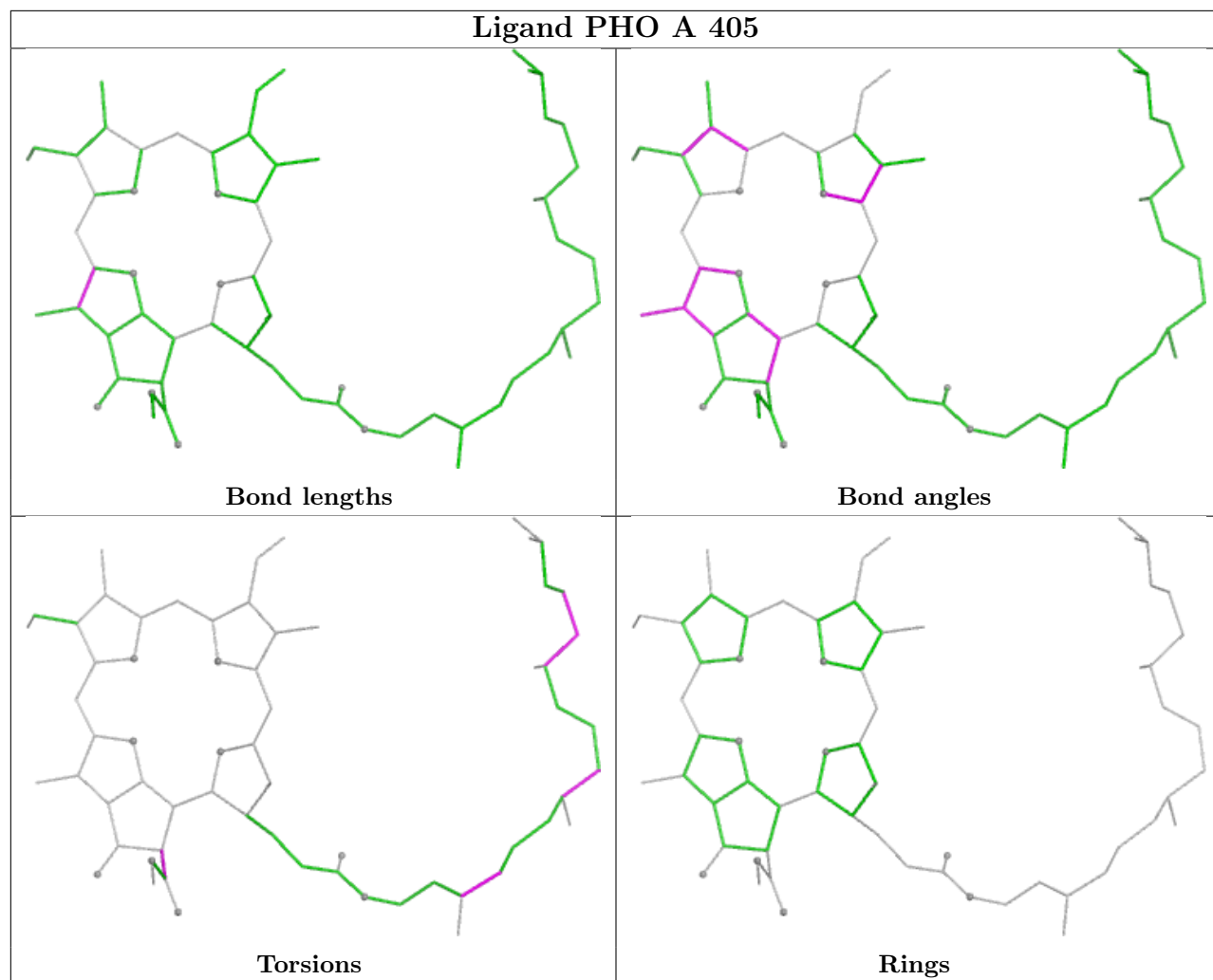
Bond angles



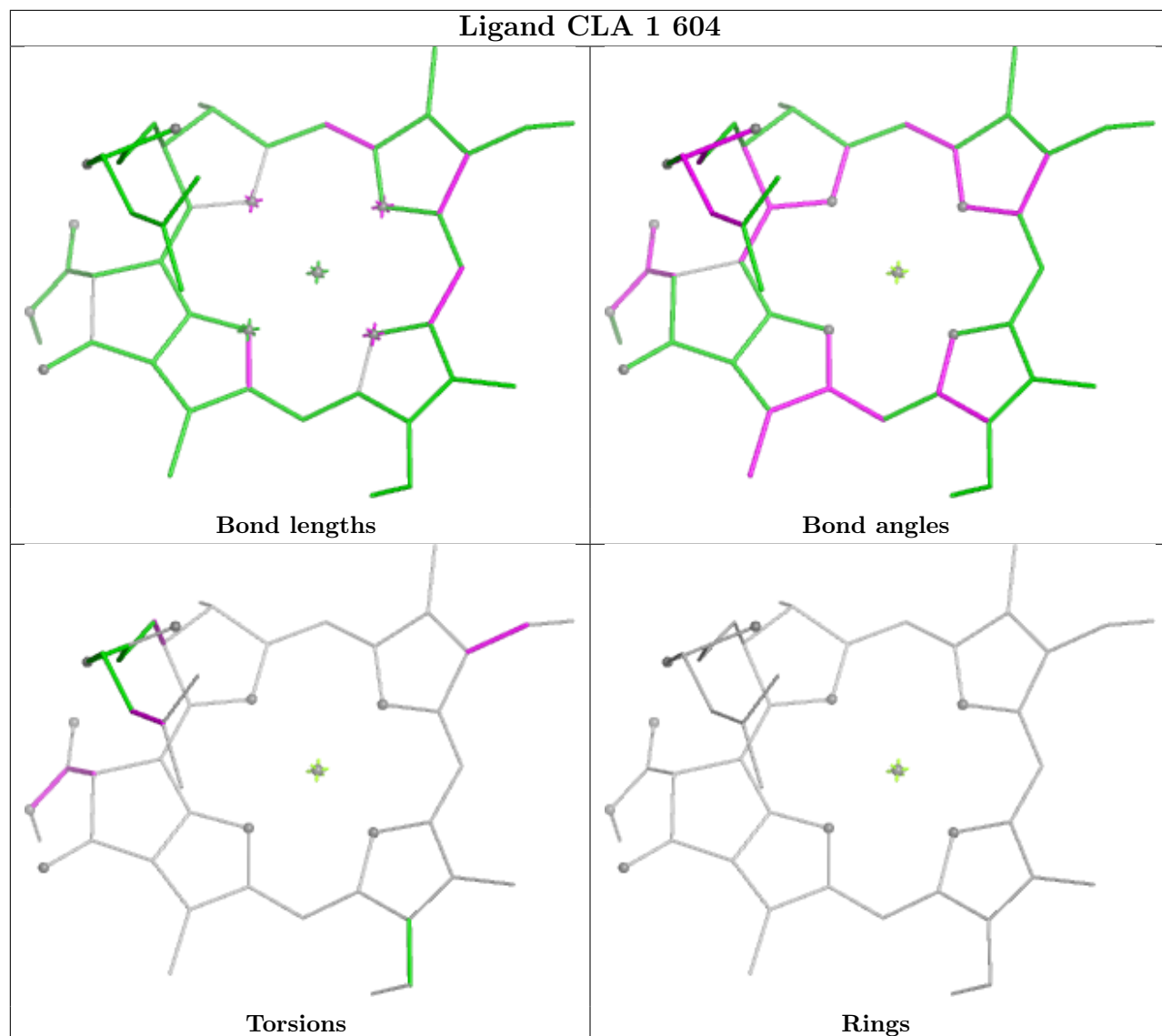
Torsions

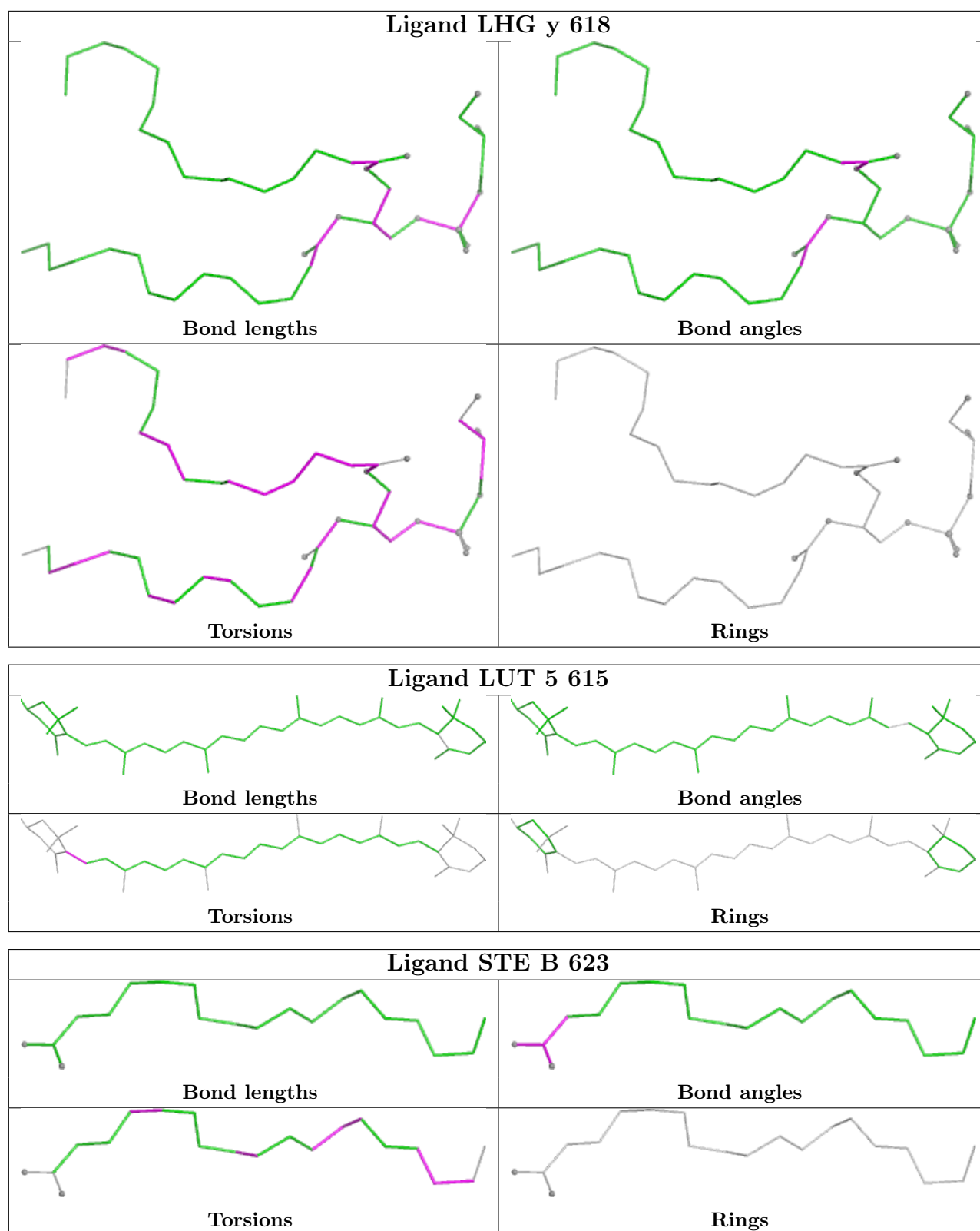


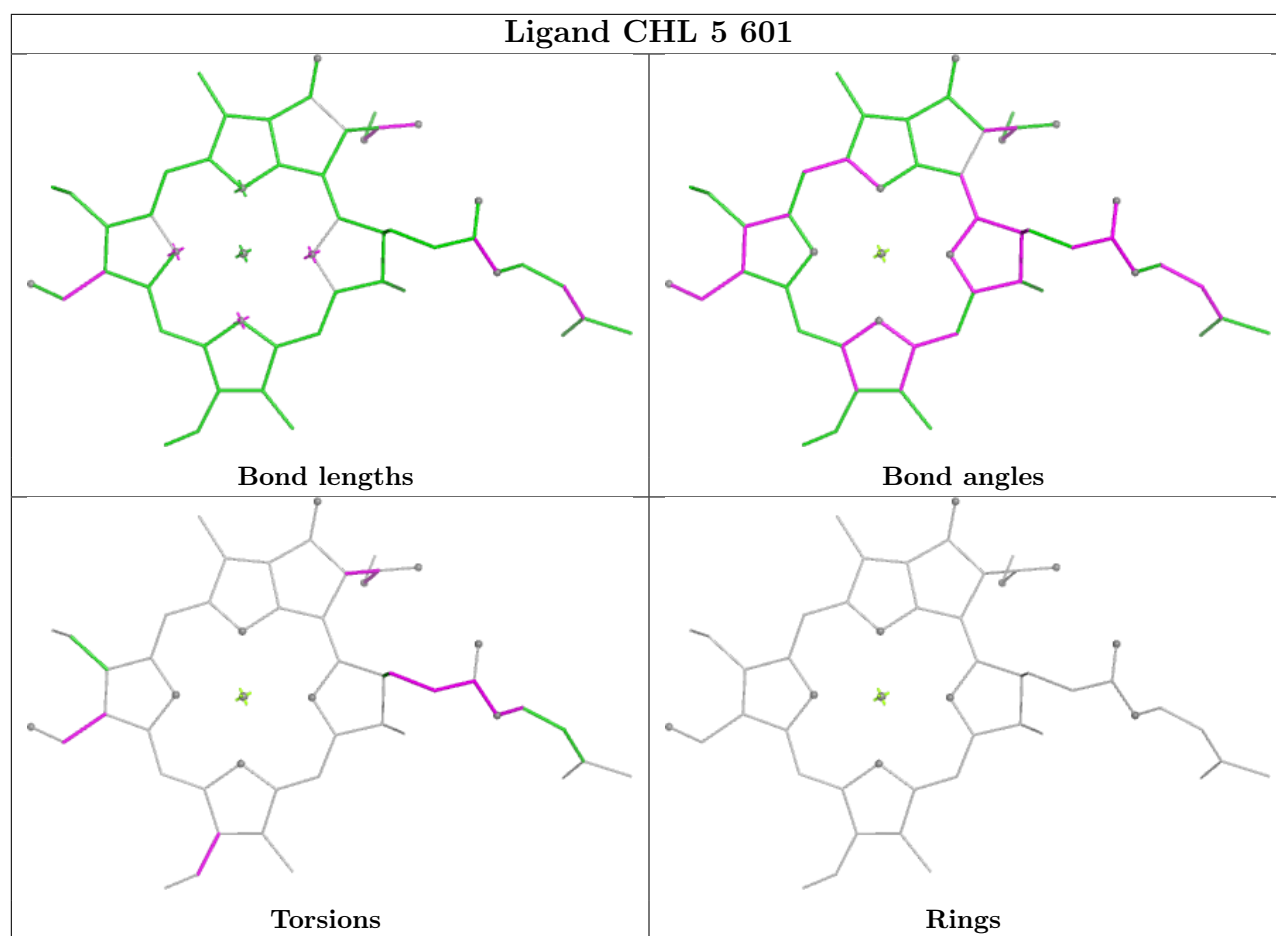
Rings

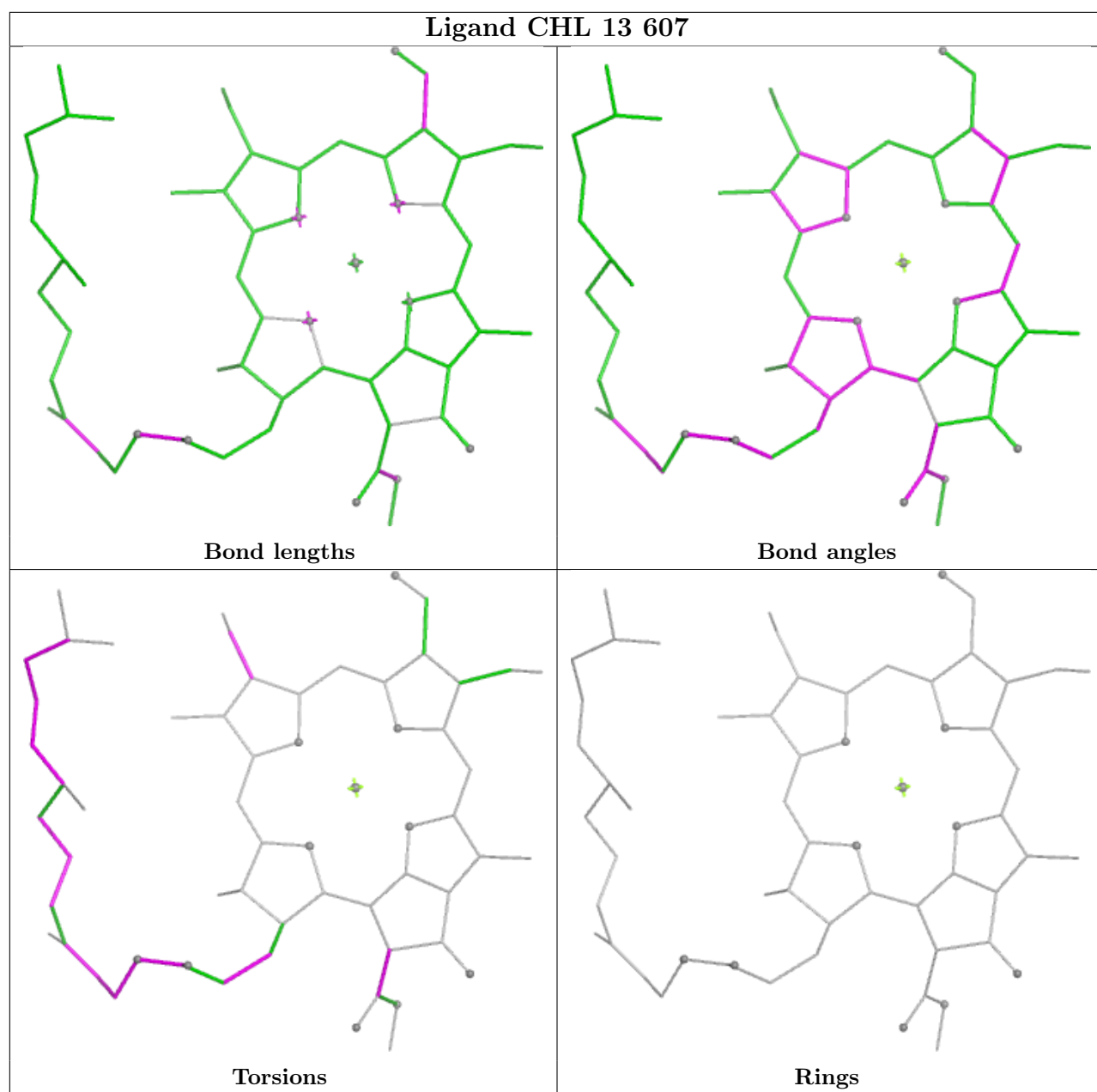


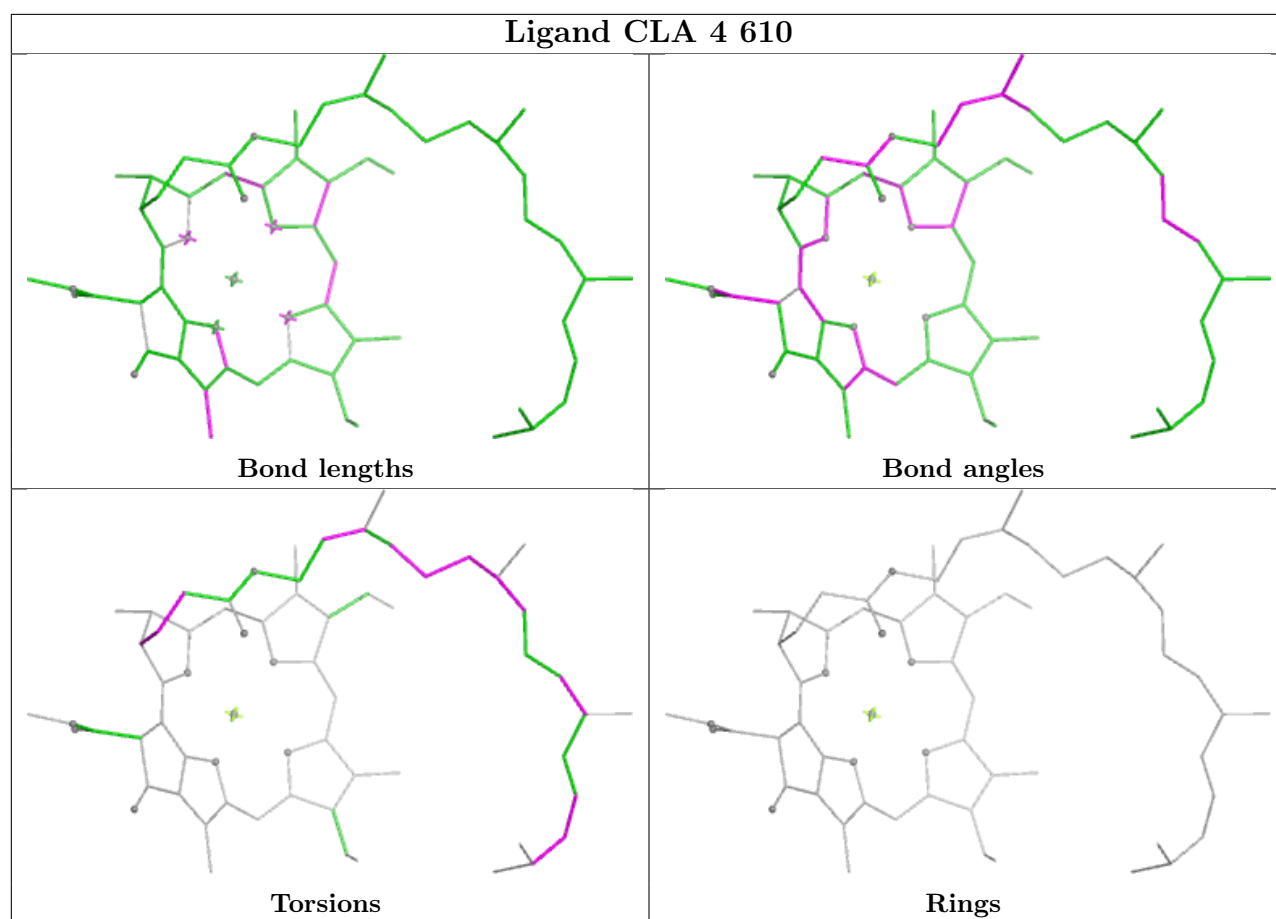
Ligand CLA 1 604



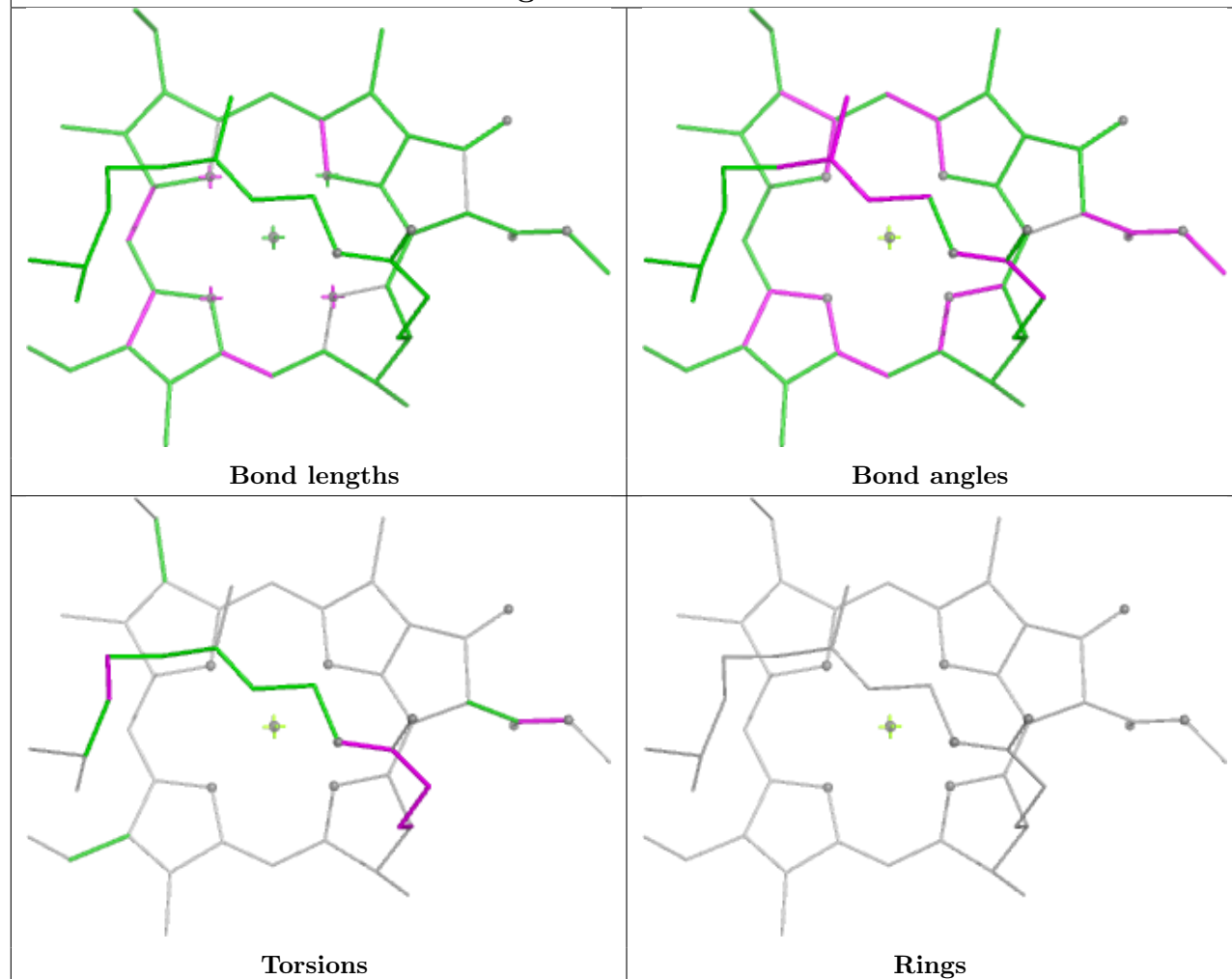




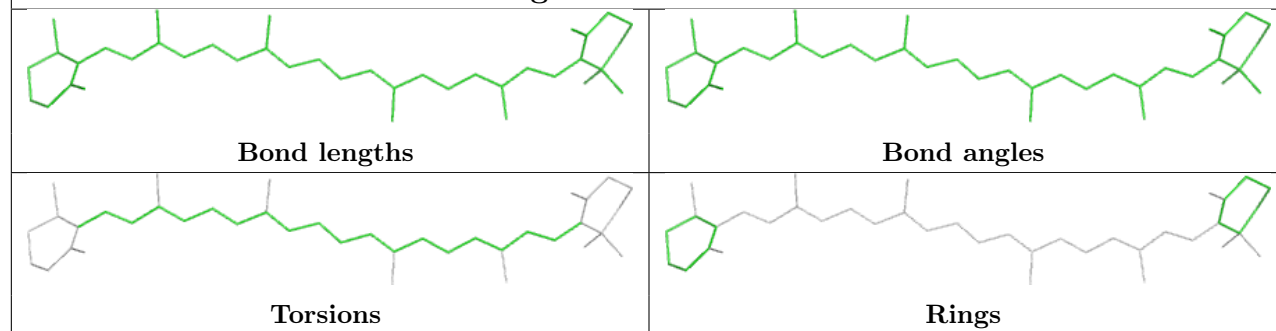


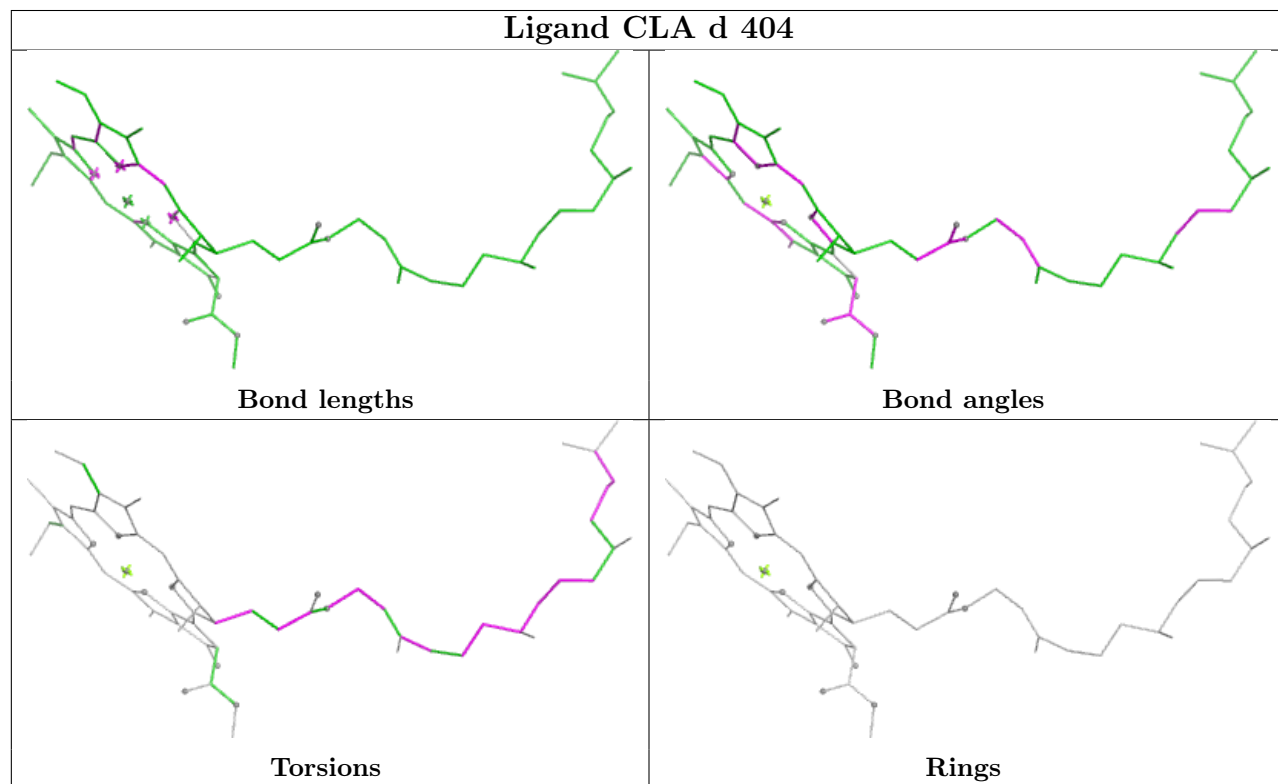
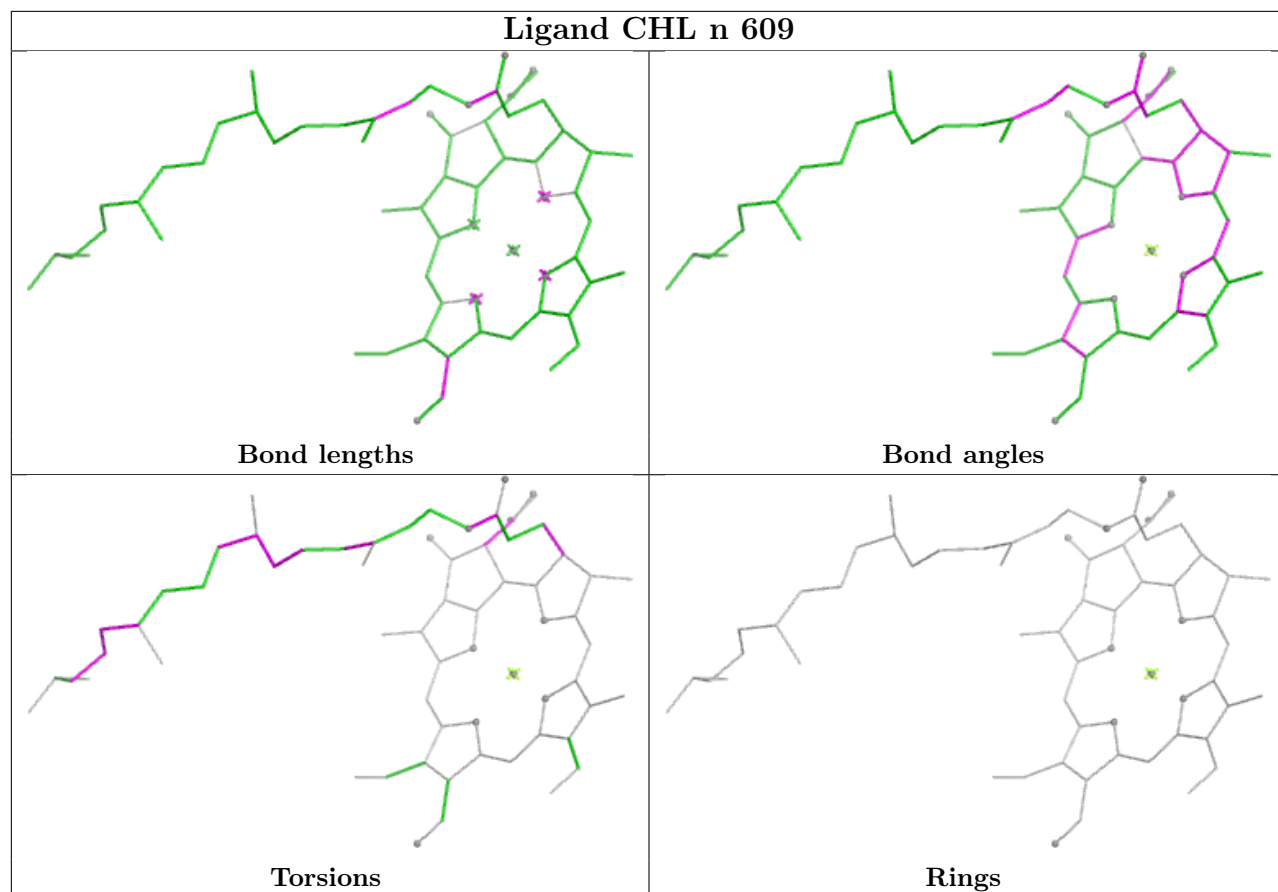


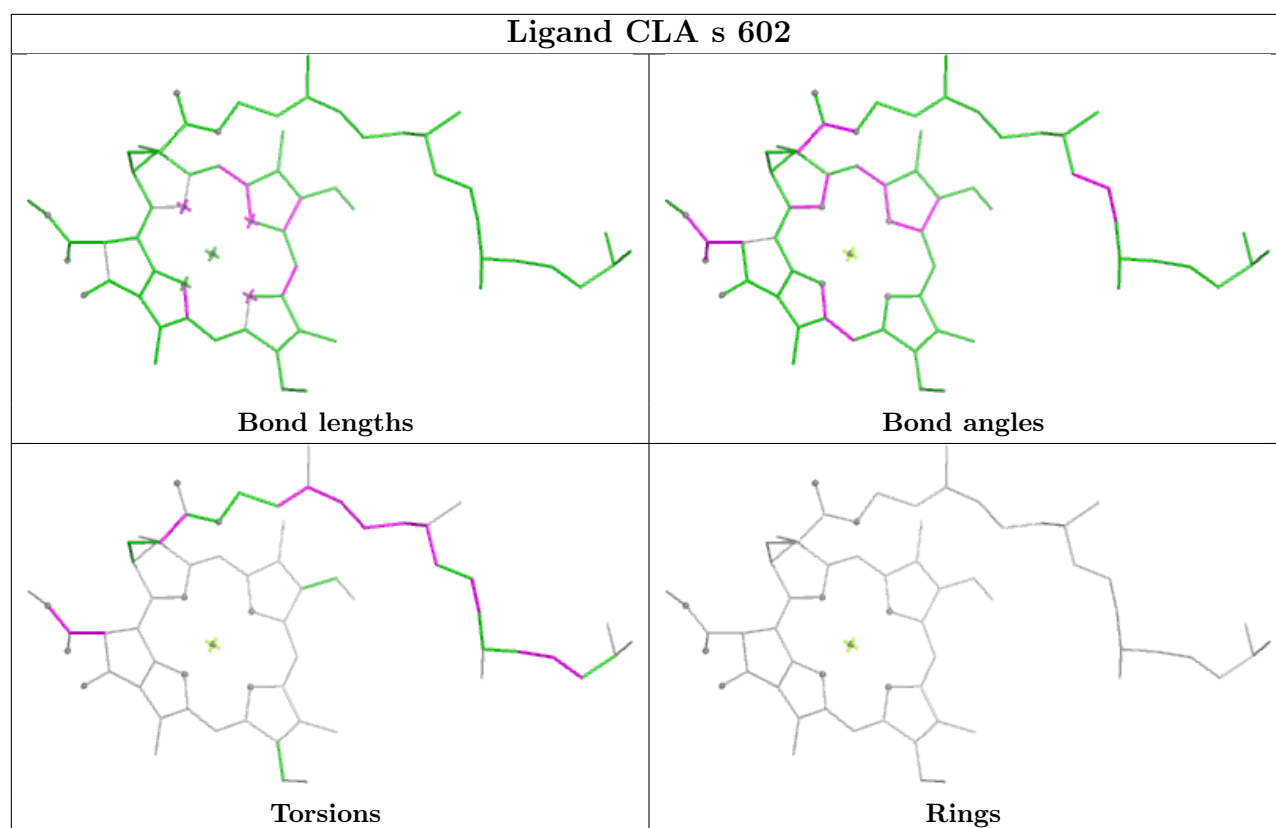
Ligand CLA 4 613



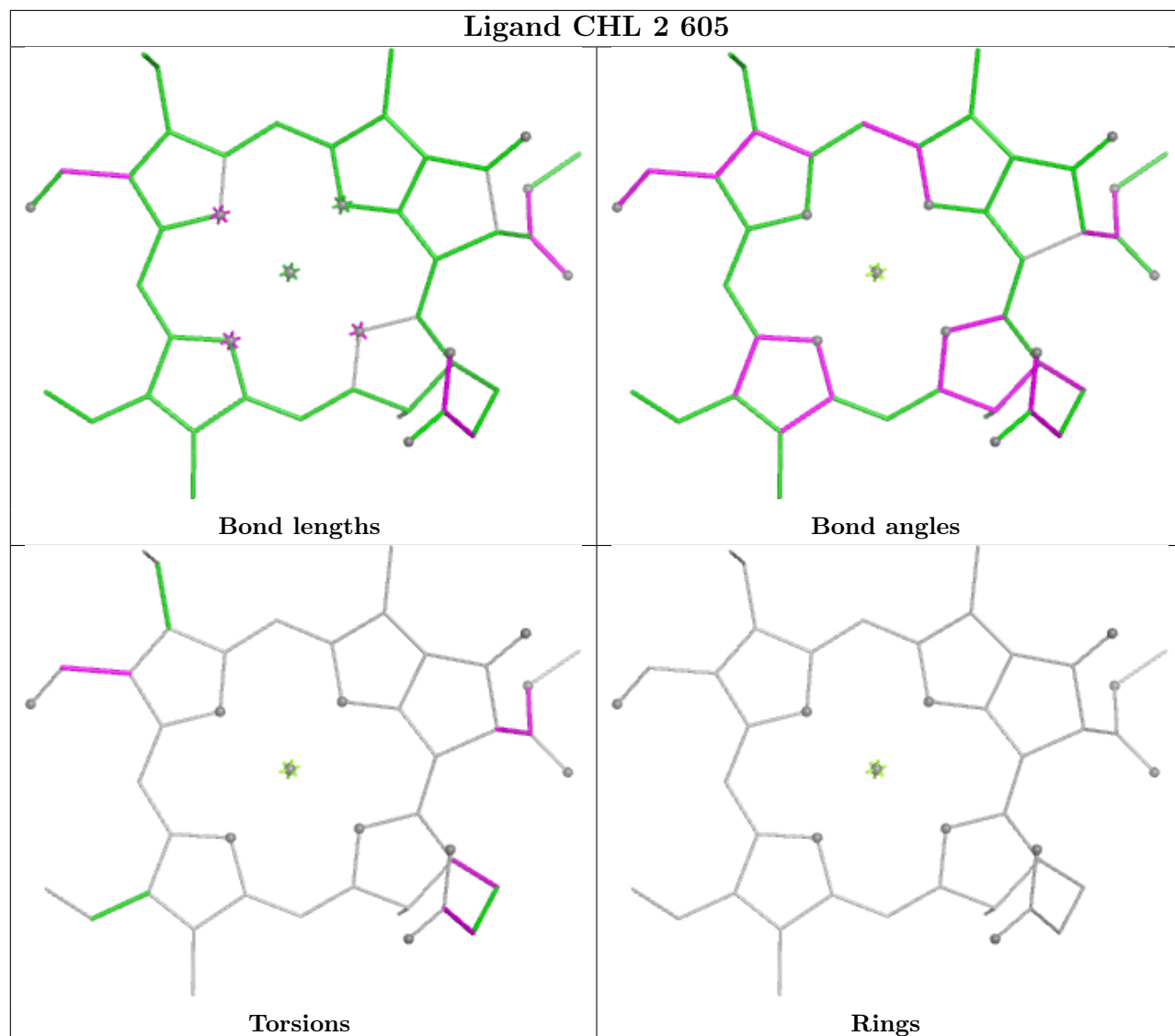
Ligand BCR B 618



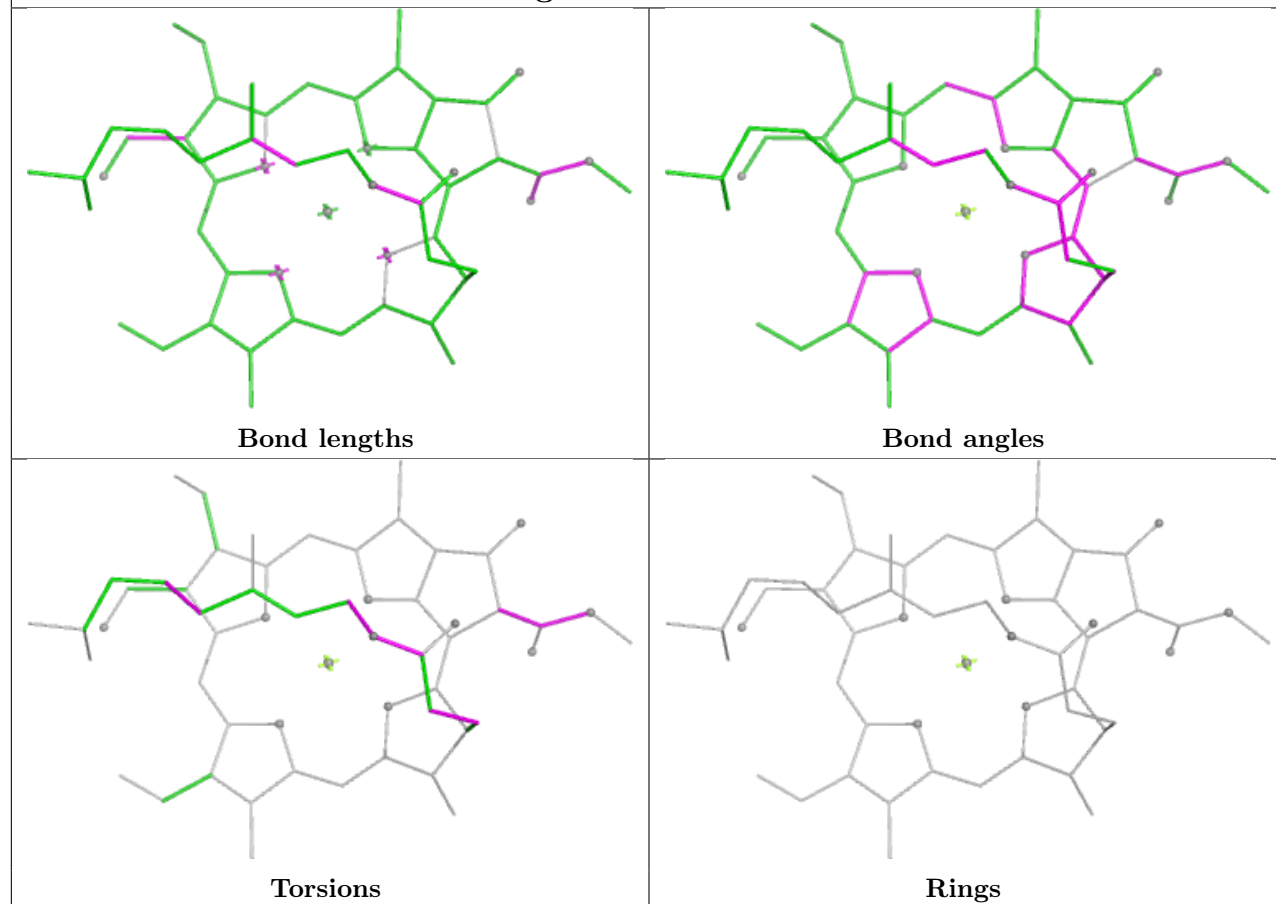




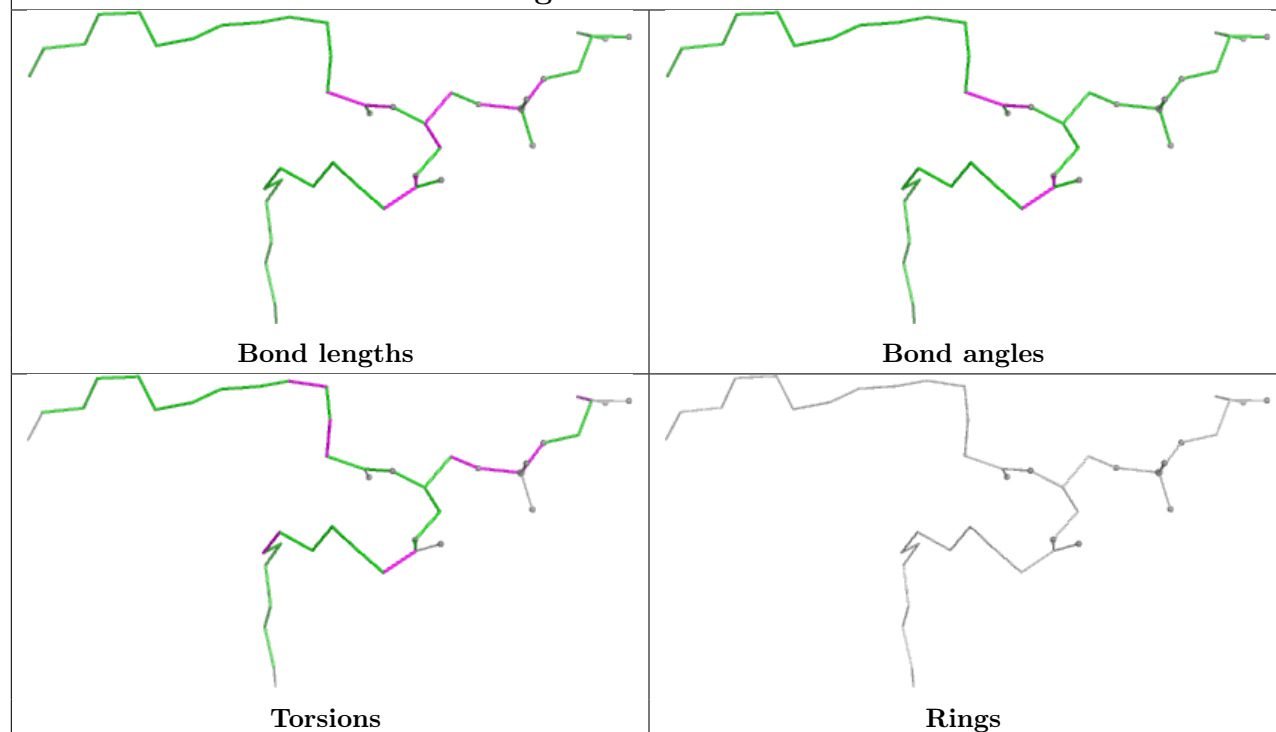
Ligand CHL 2 605

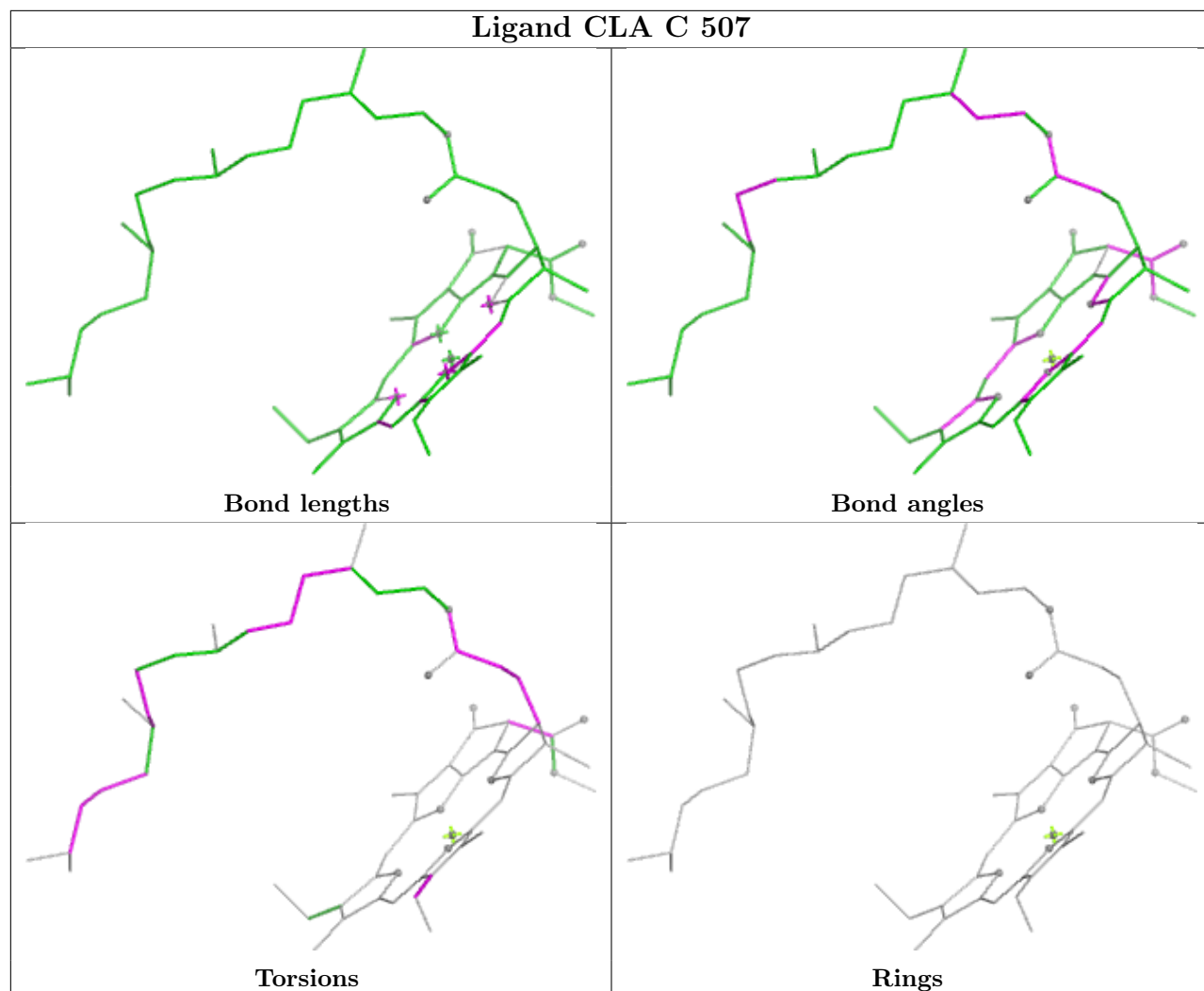
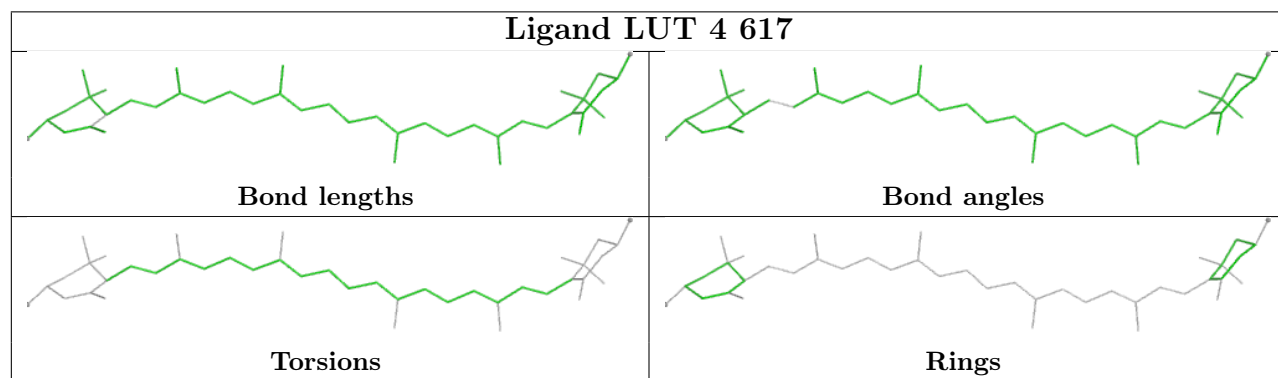


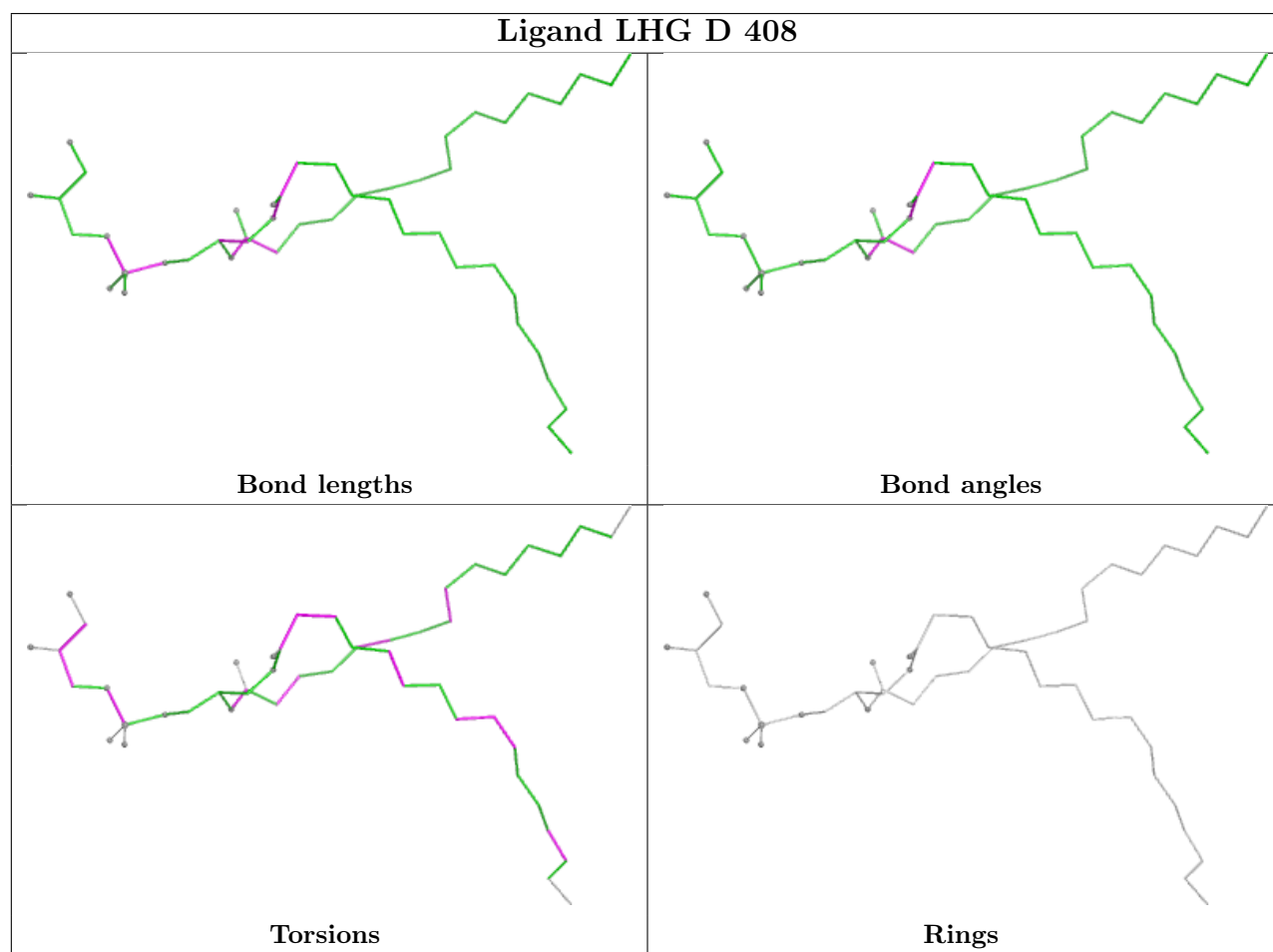
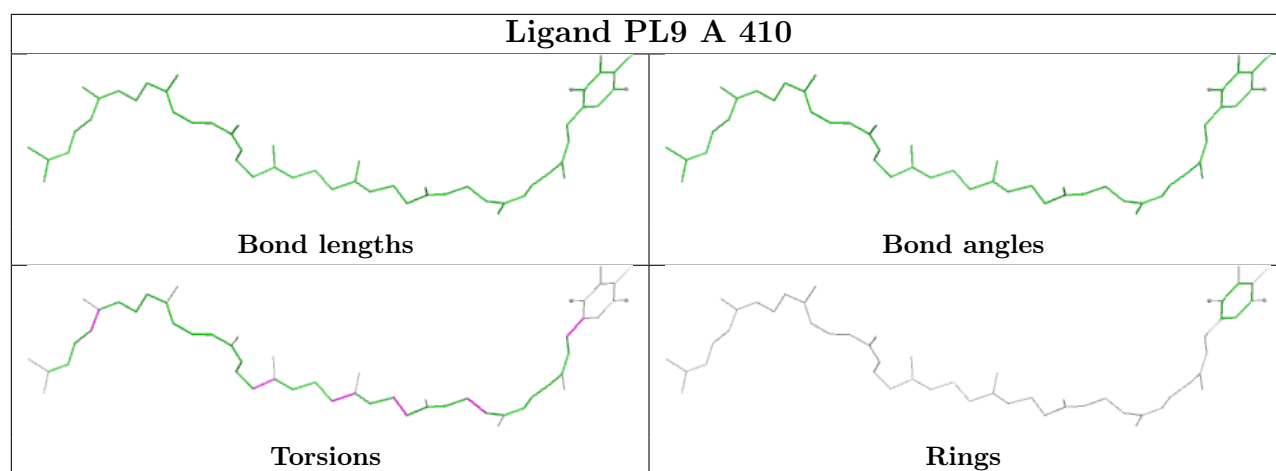
Ligand CHL 5 607

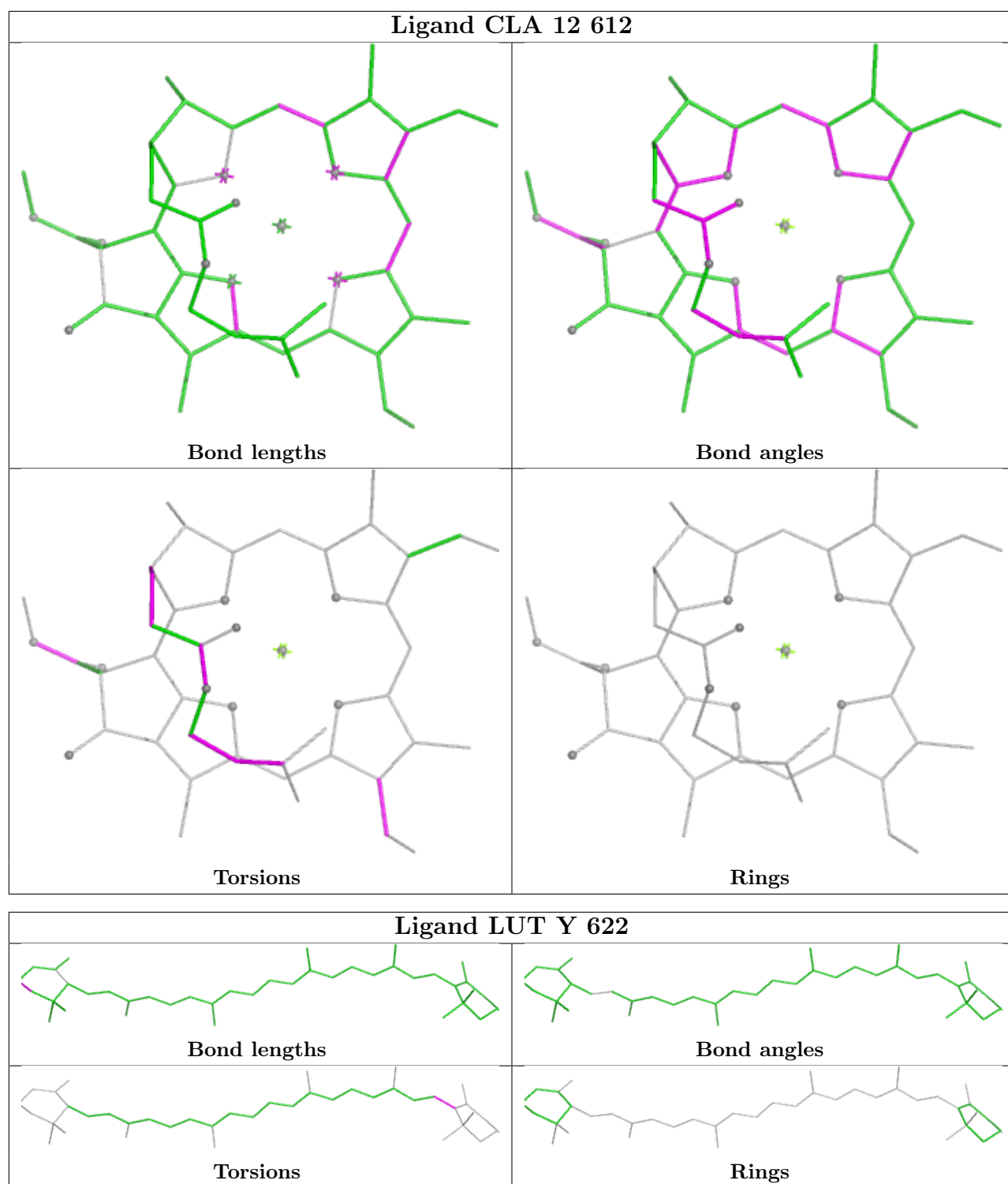


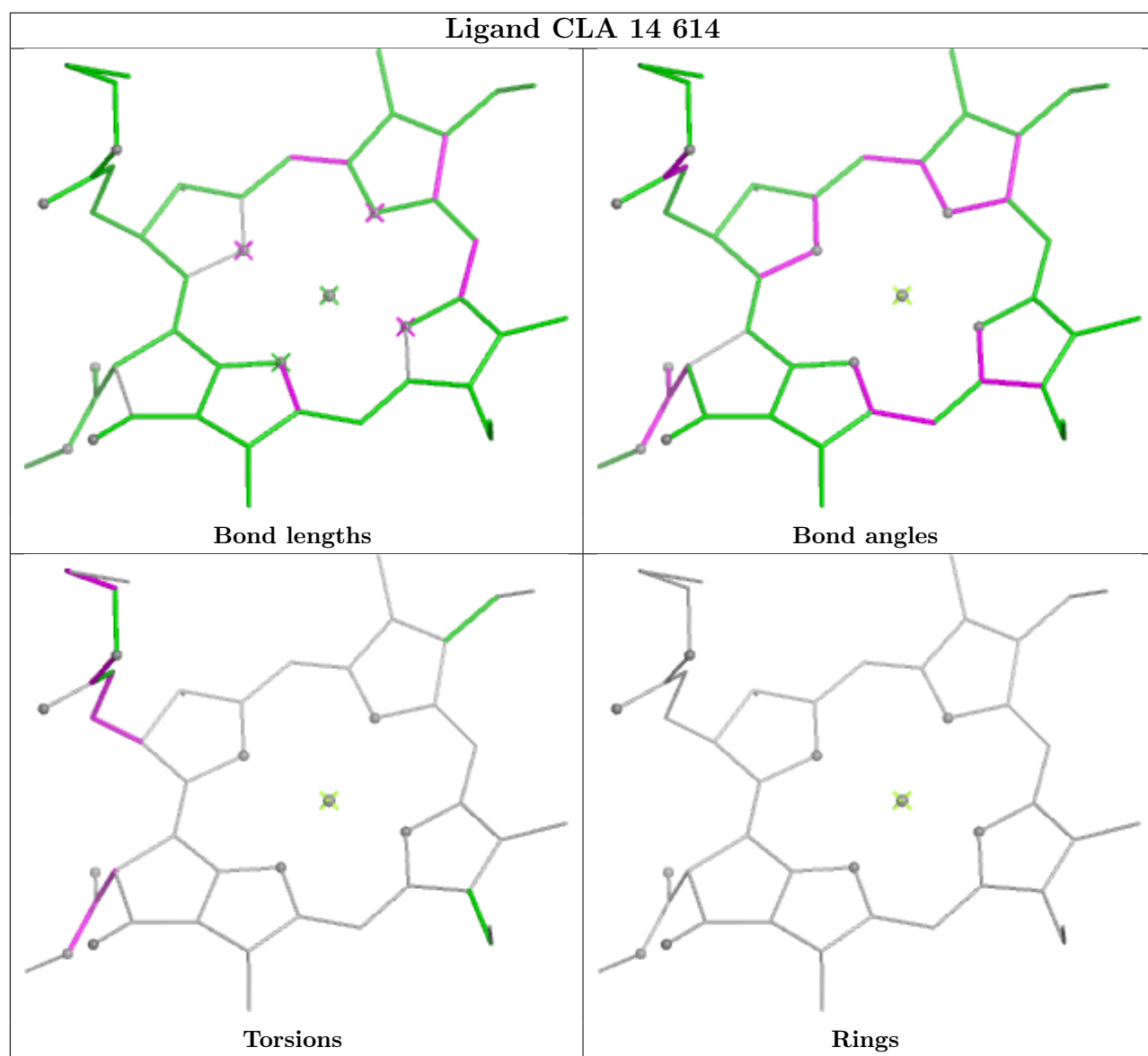
Ligand LHG 3 616

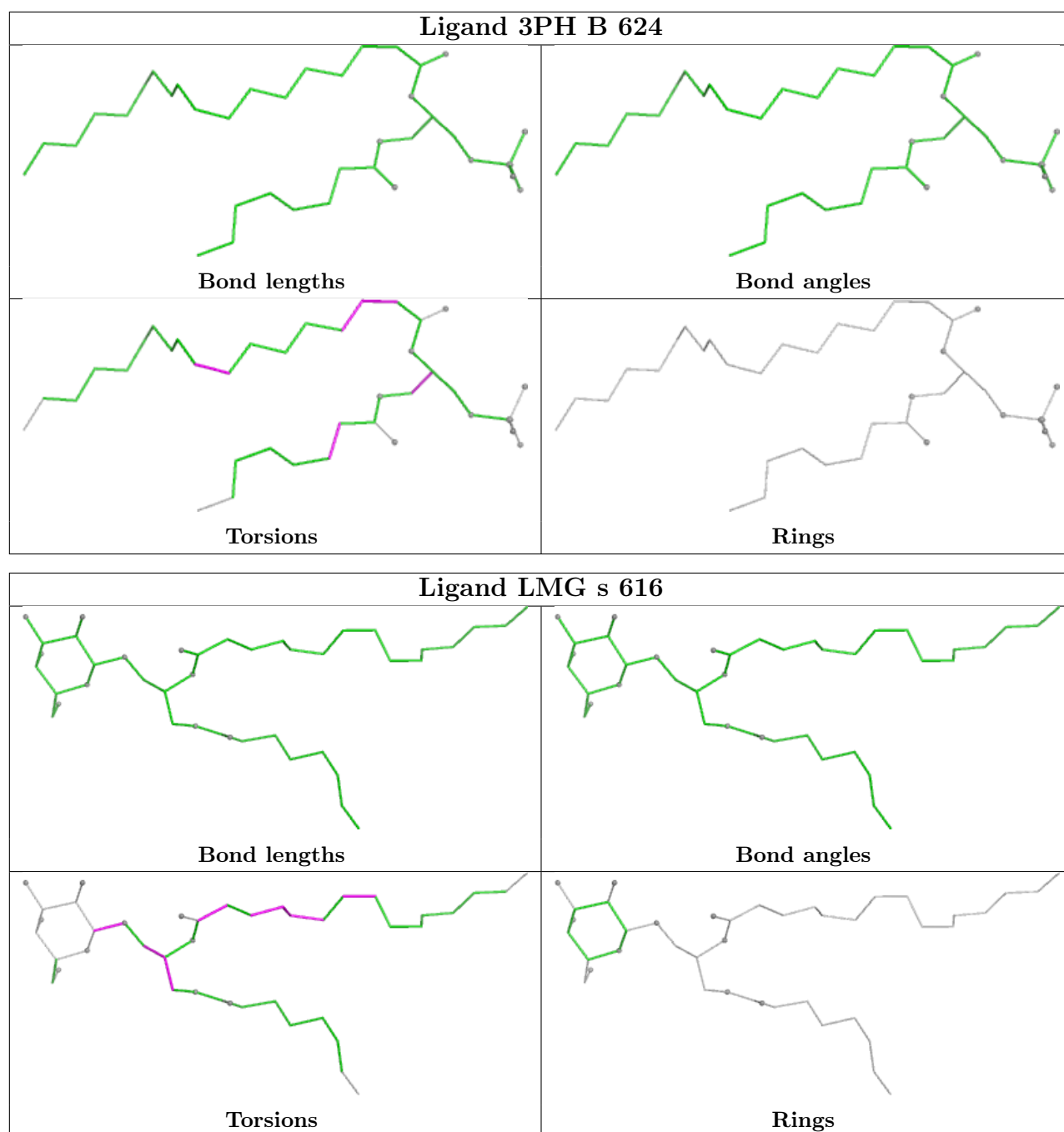


Ligand CLA C 507**Ligand LUT 4 617**

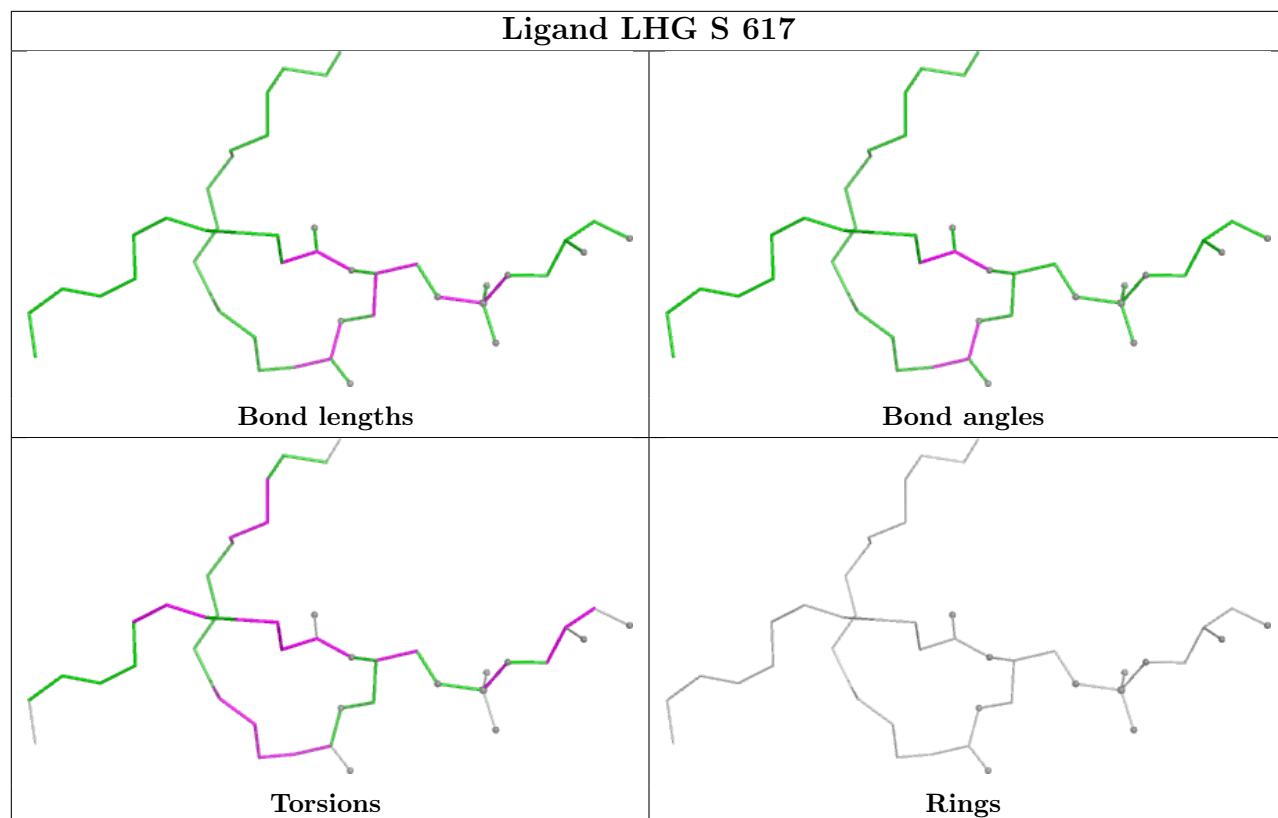




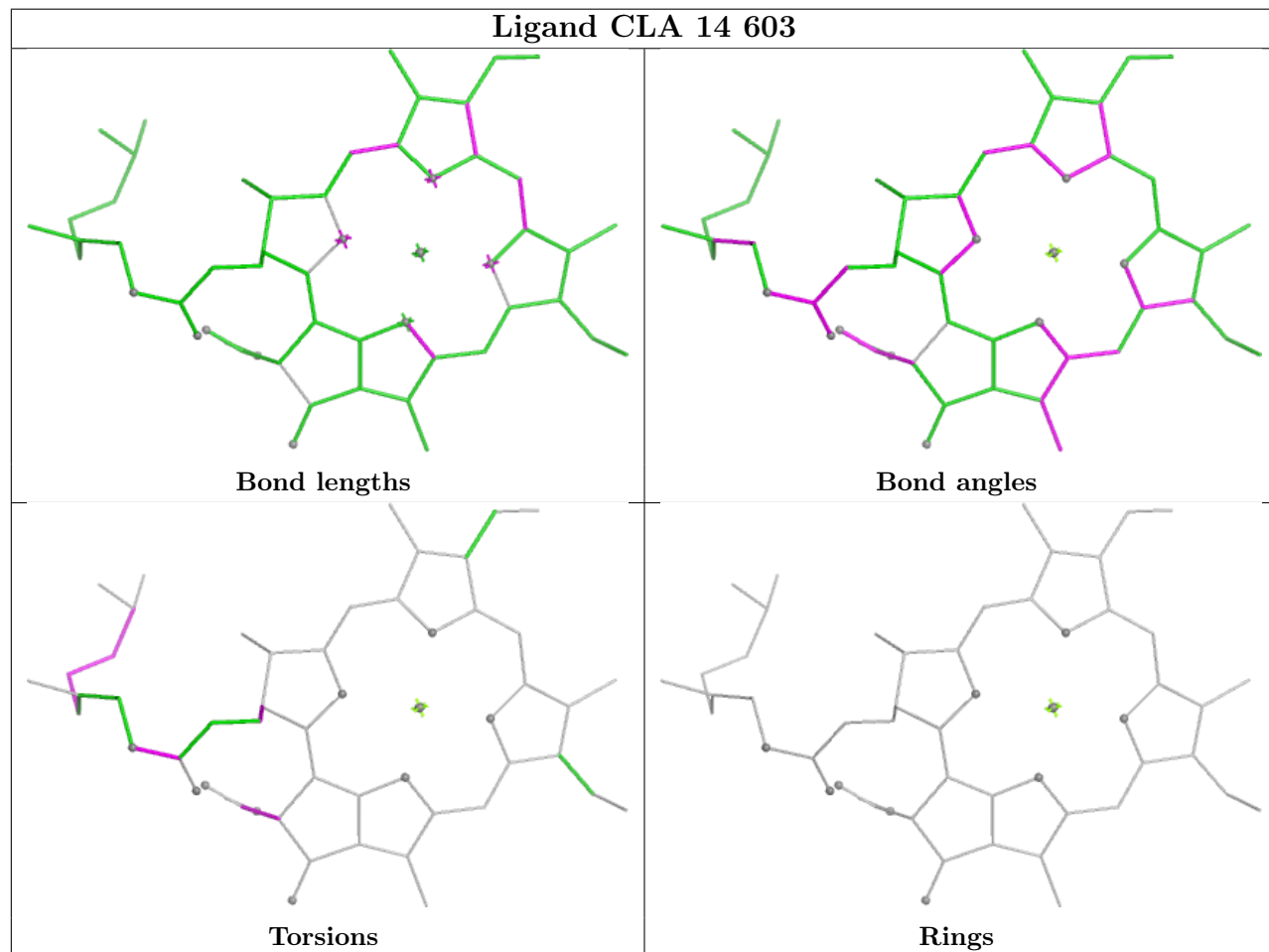


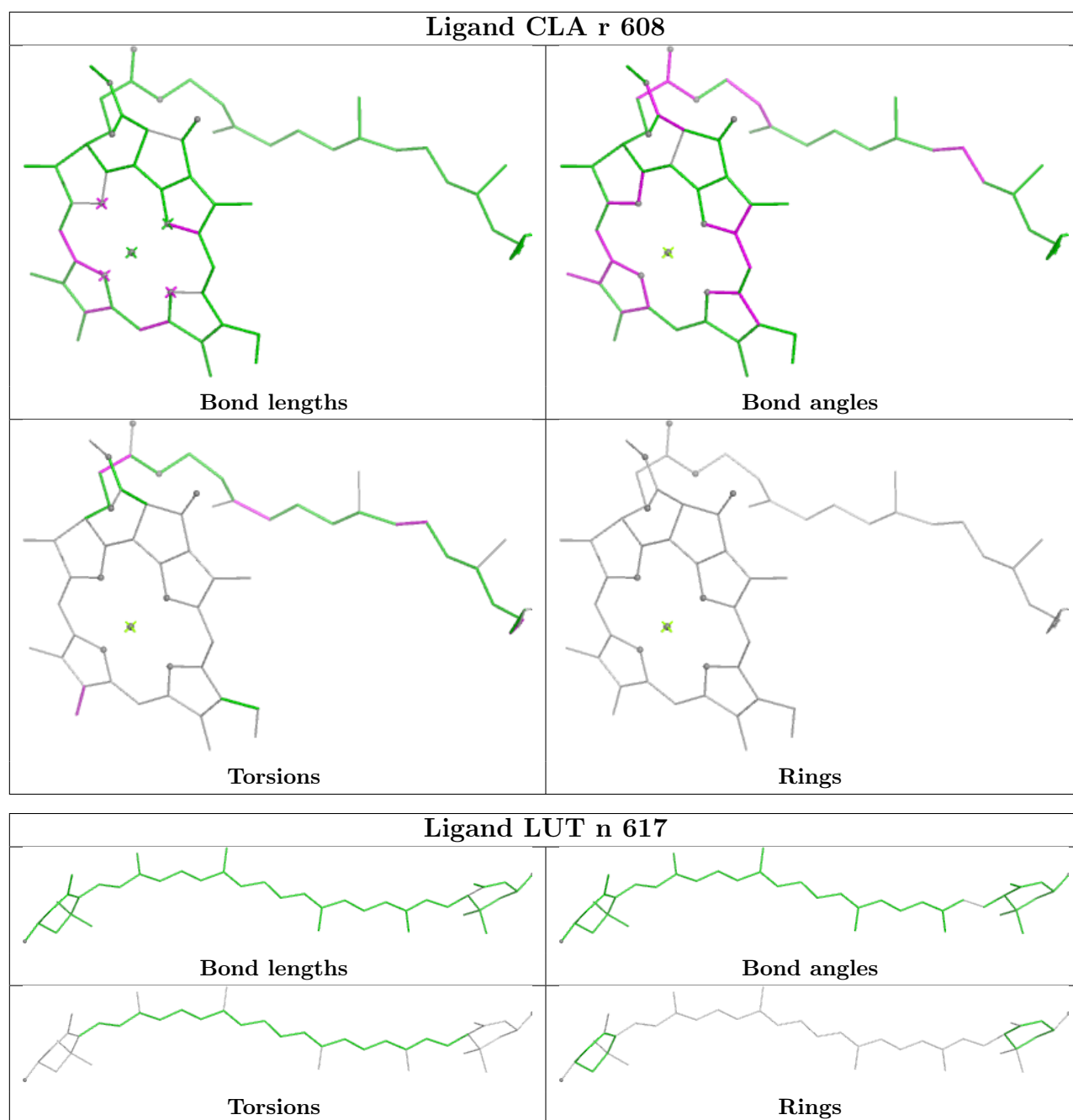


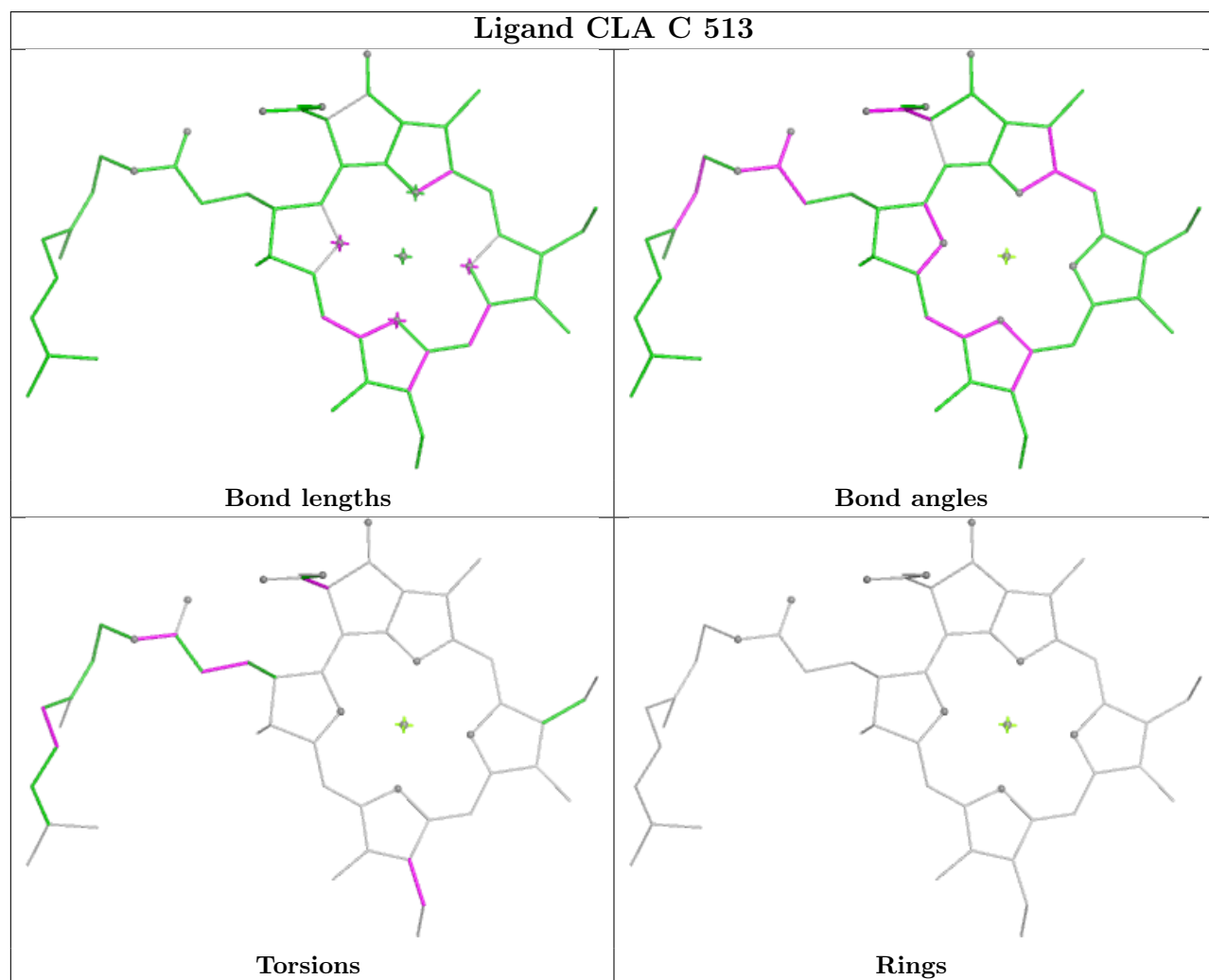
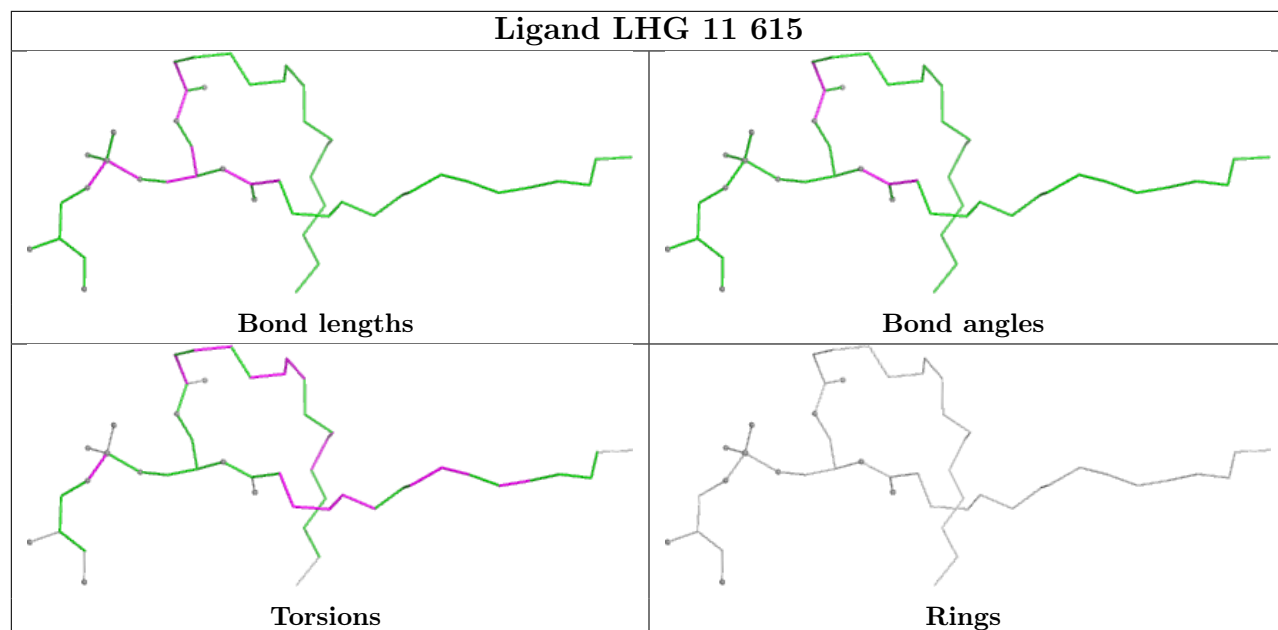
Ligand LHG S 617



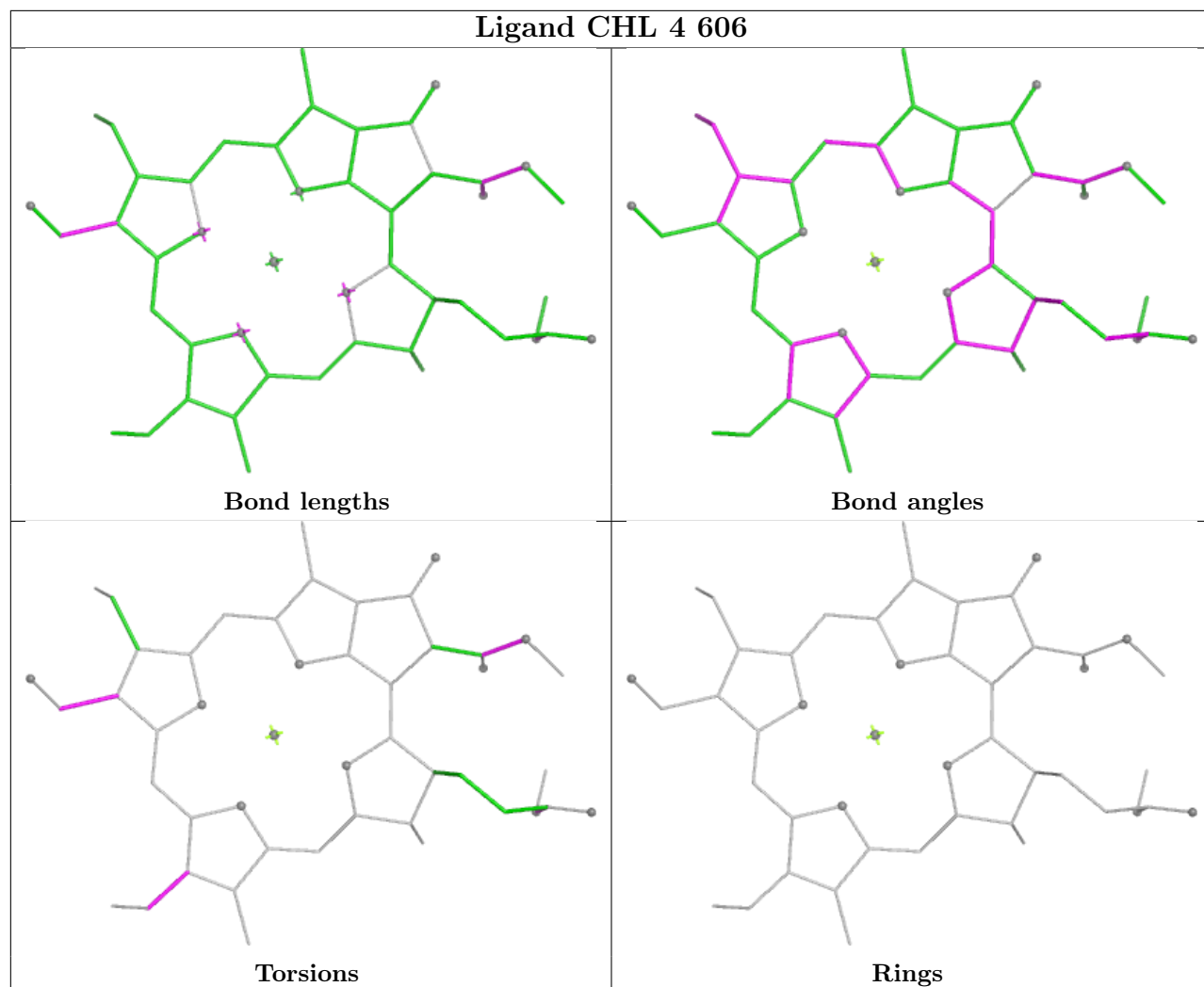
Ligand CLA 14 603

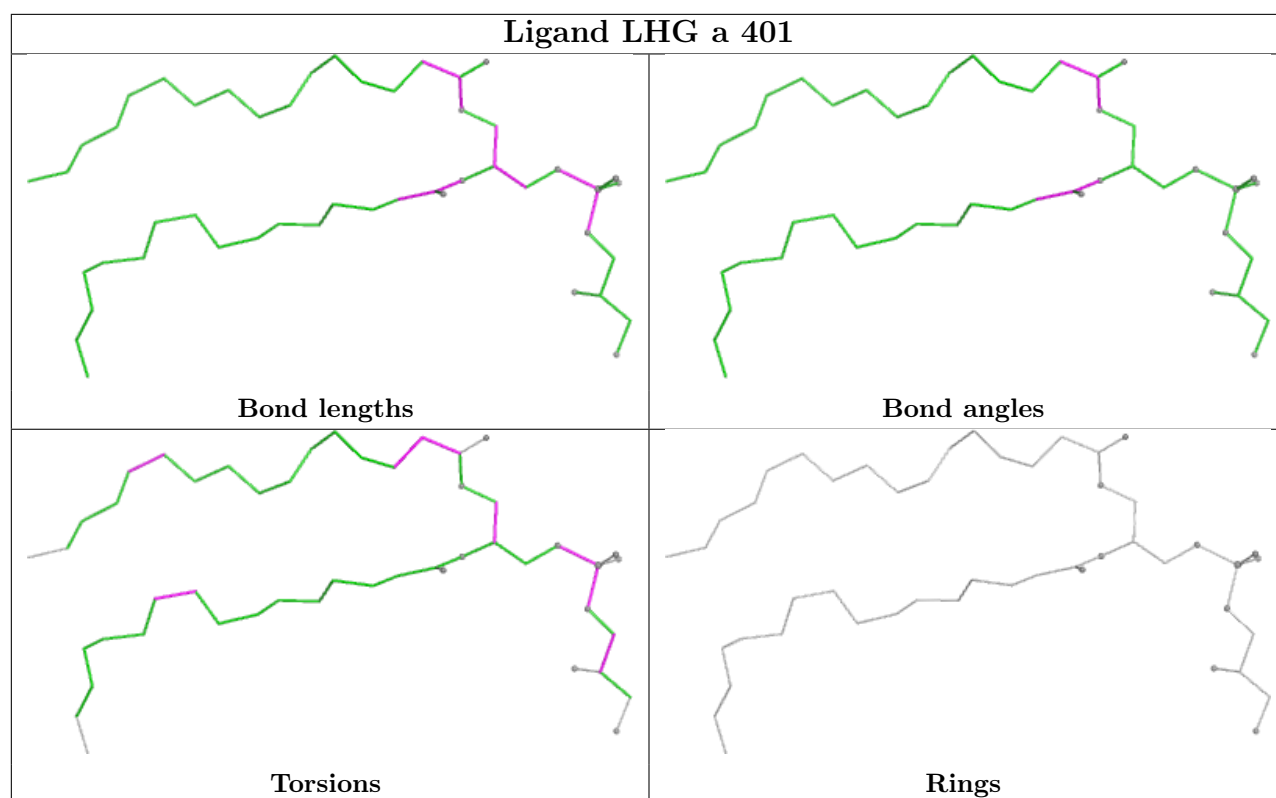




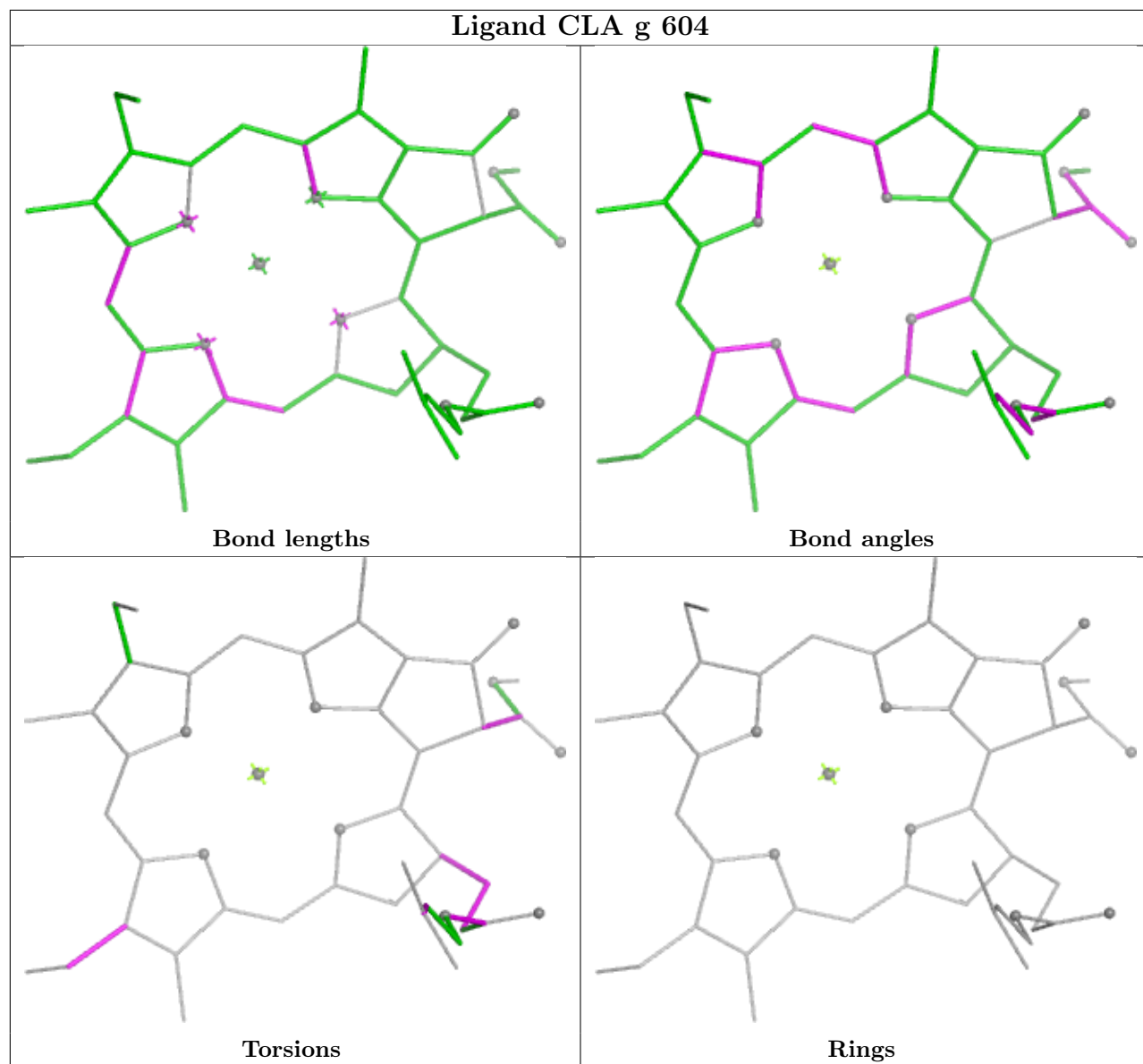


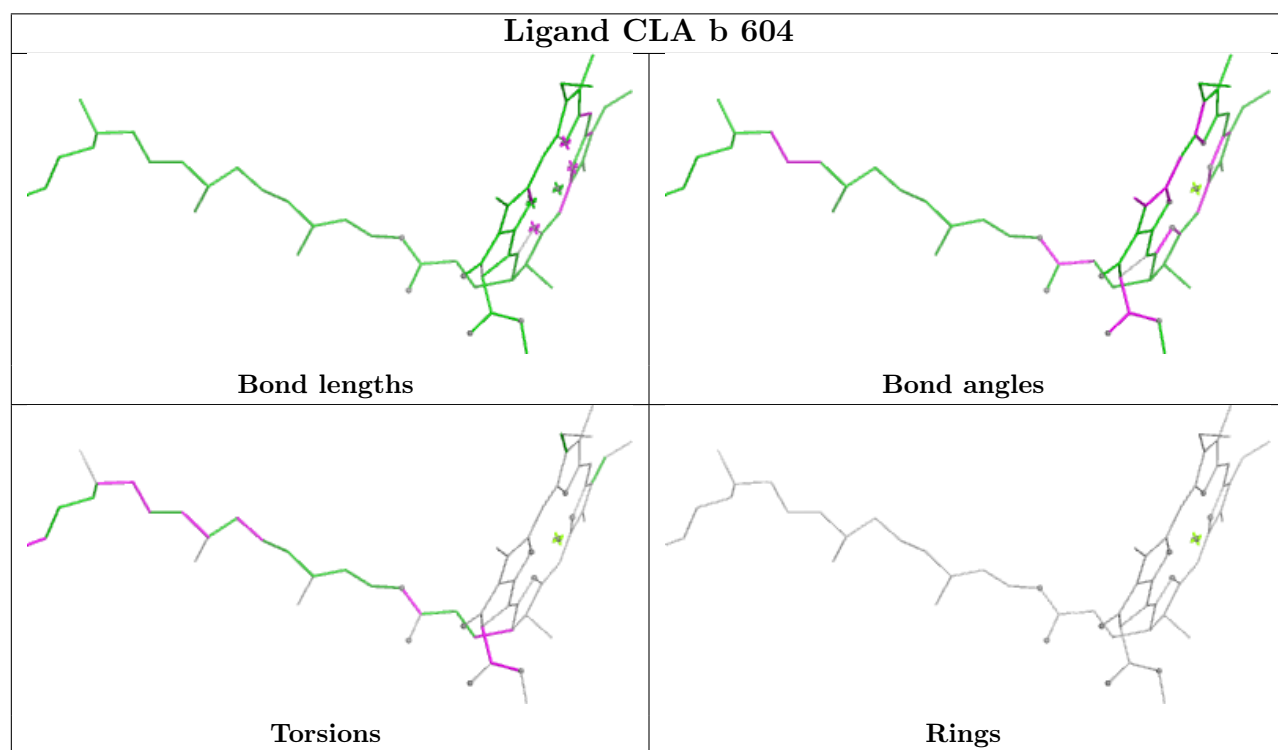
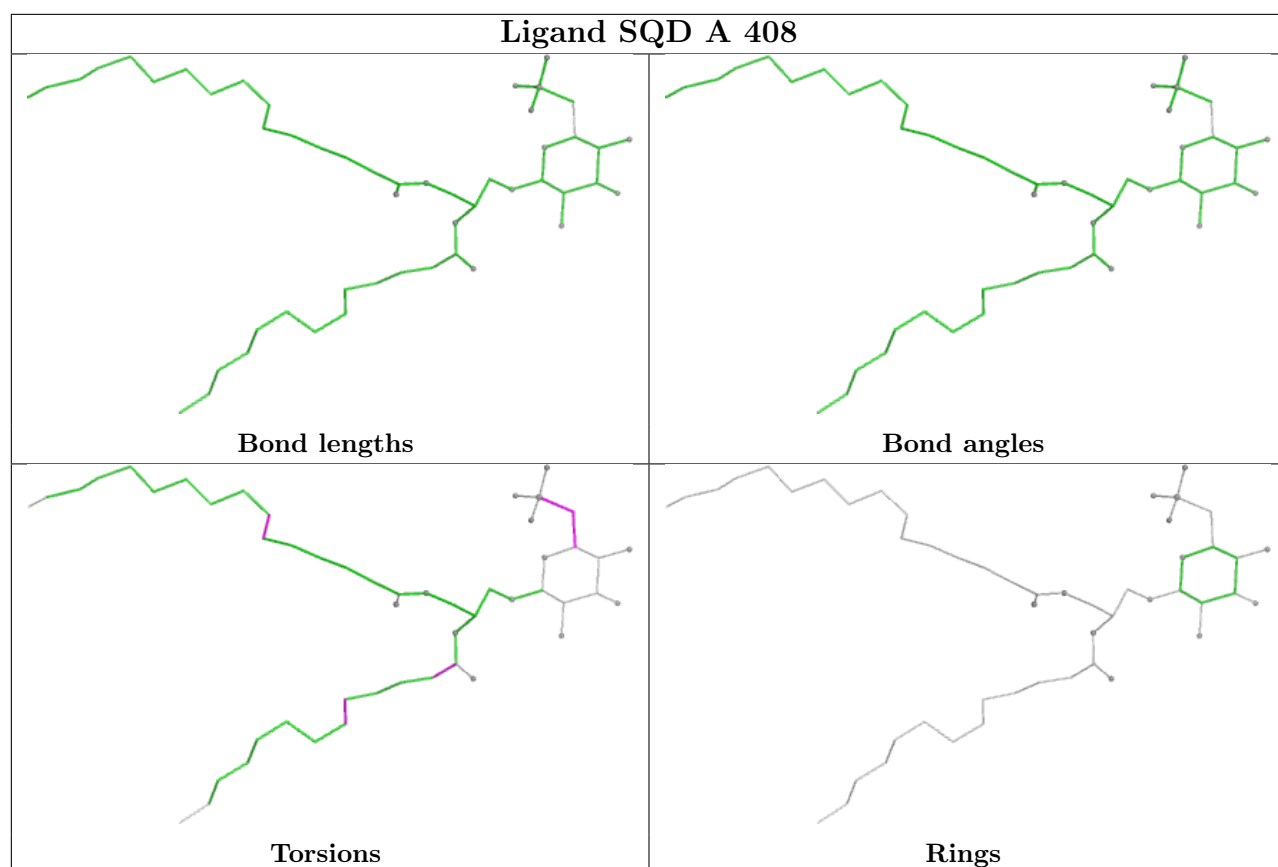
Ligand CHL 4 606

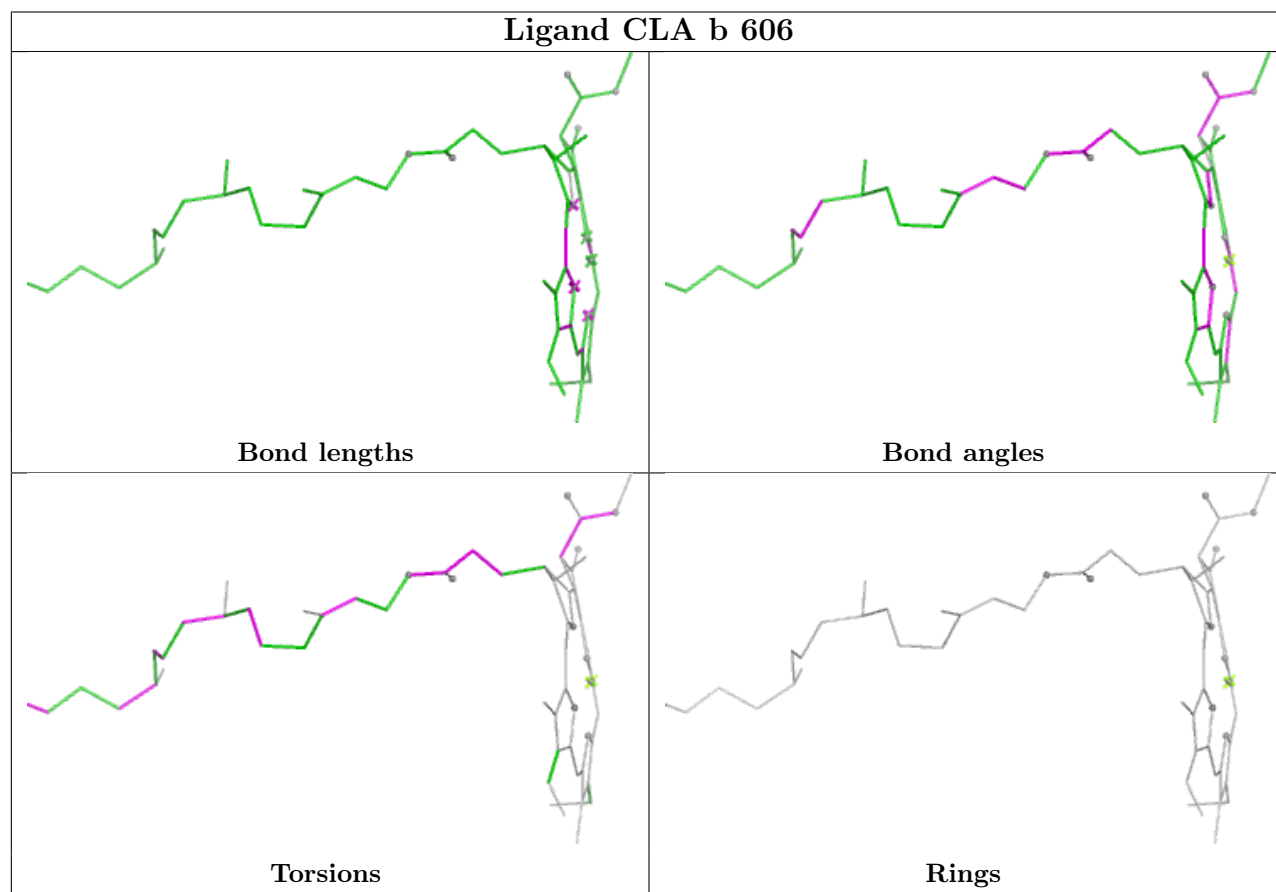
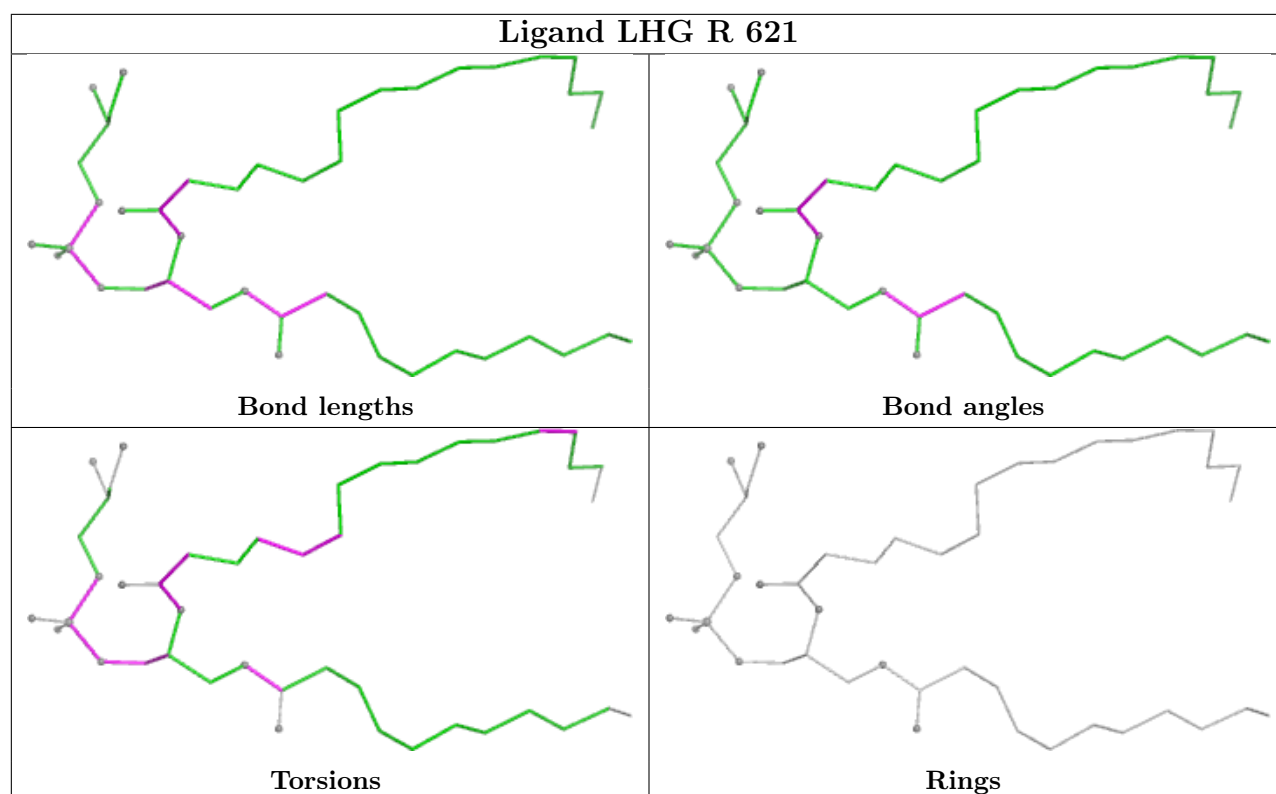


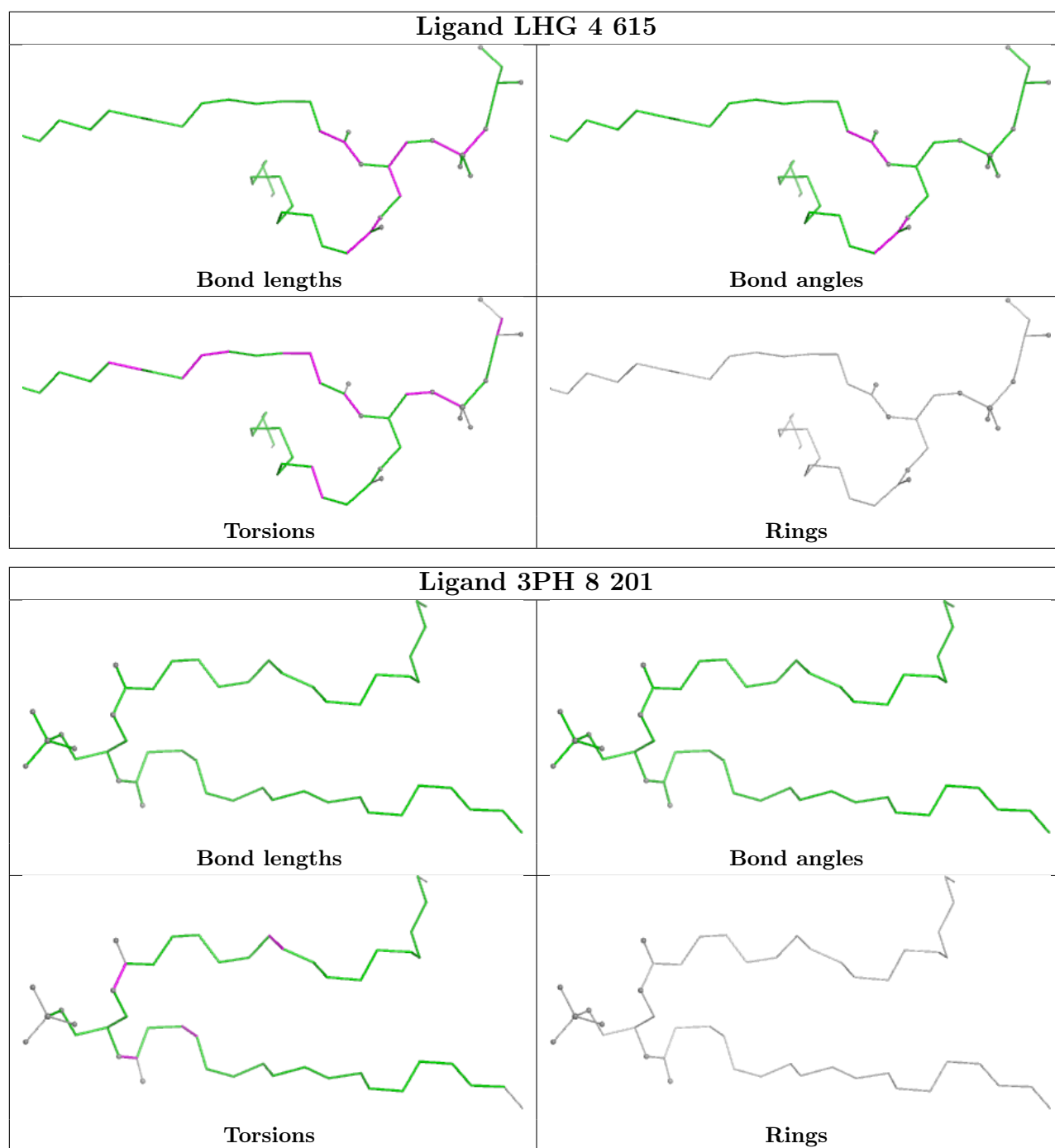


Ligand CLA g 604

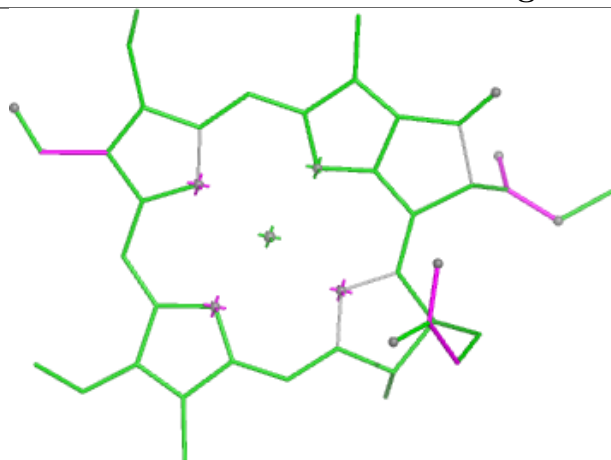




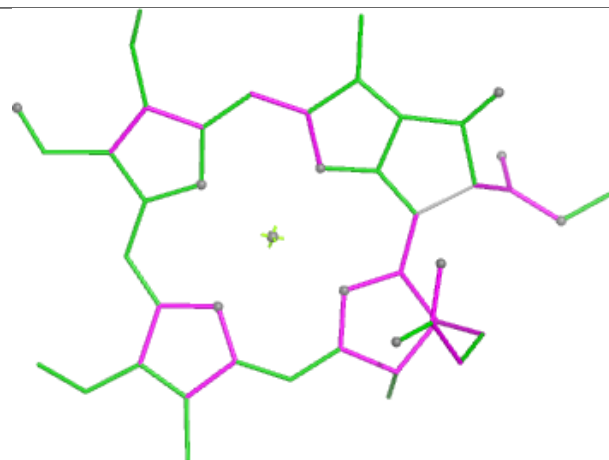




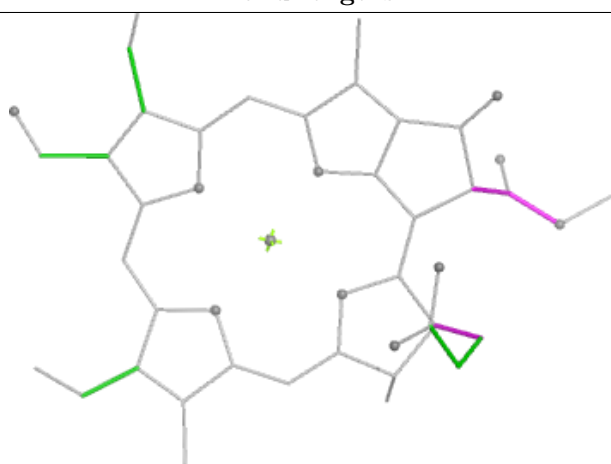
Ligand CHL 4 605



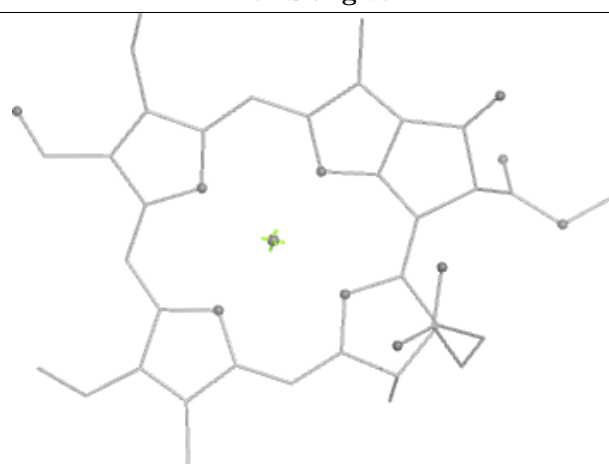
Bond lengths



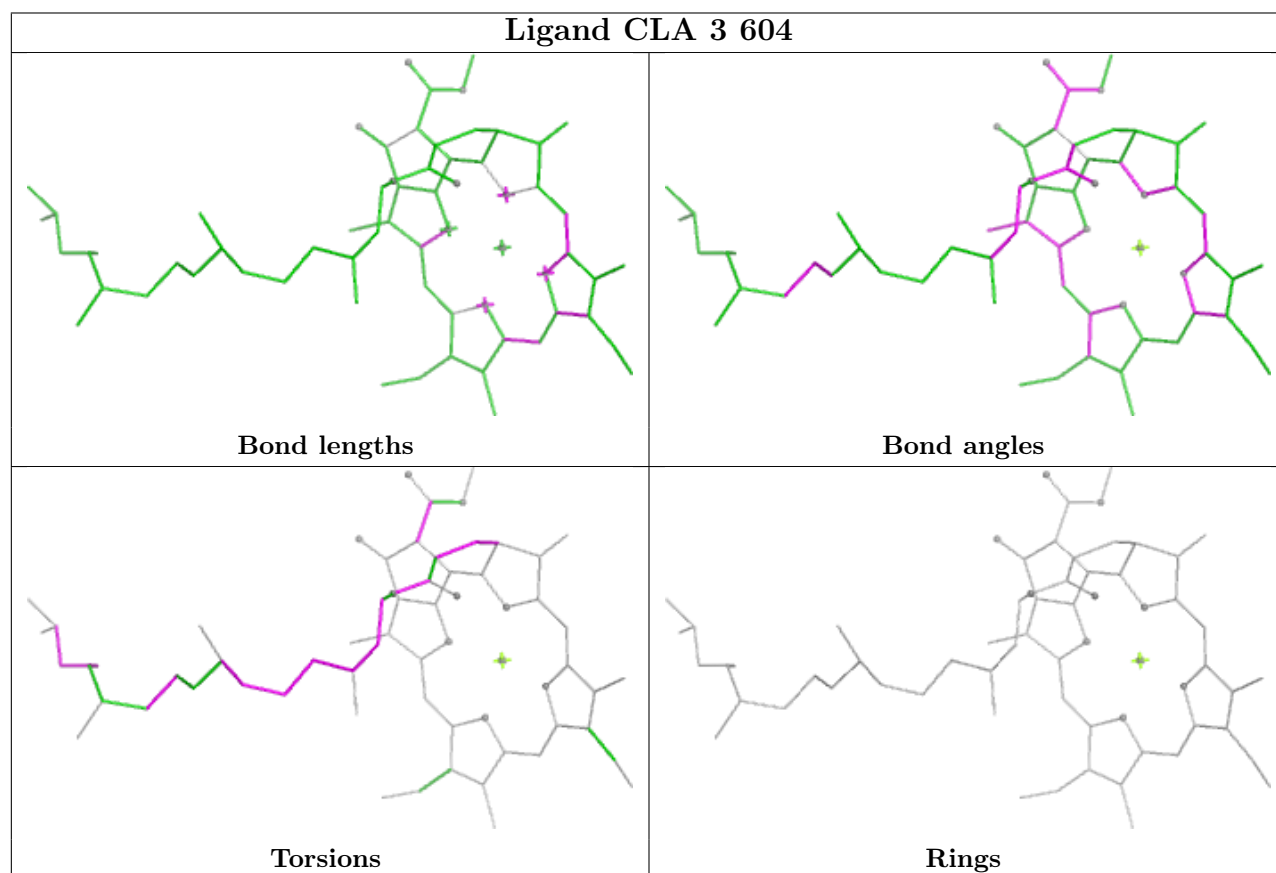
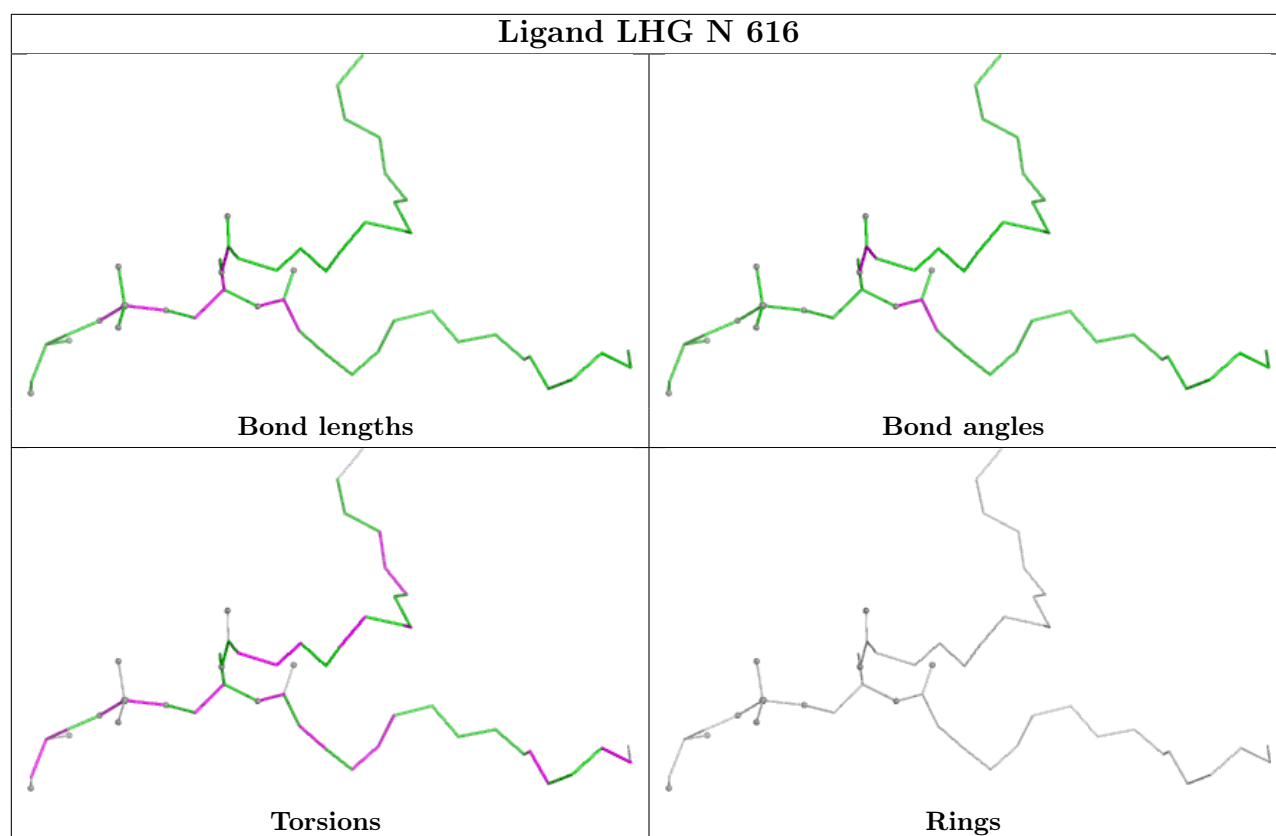
Bond angles

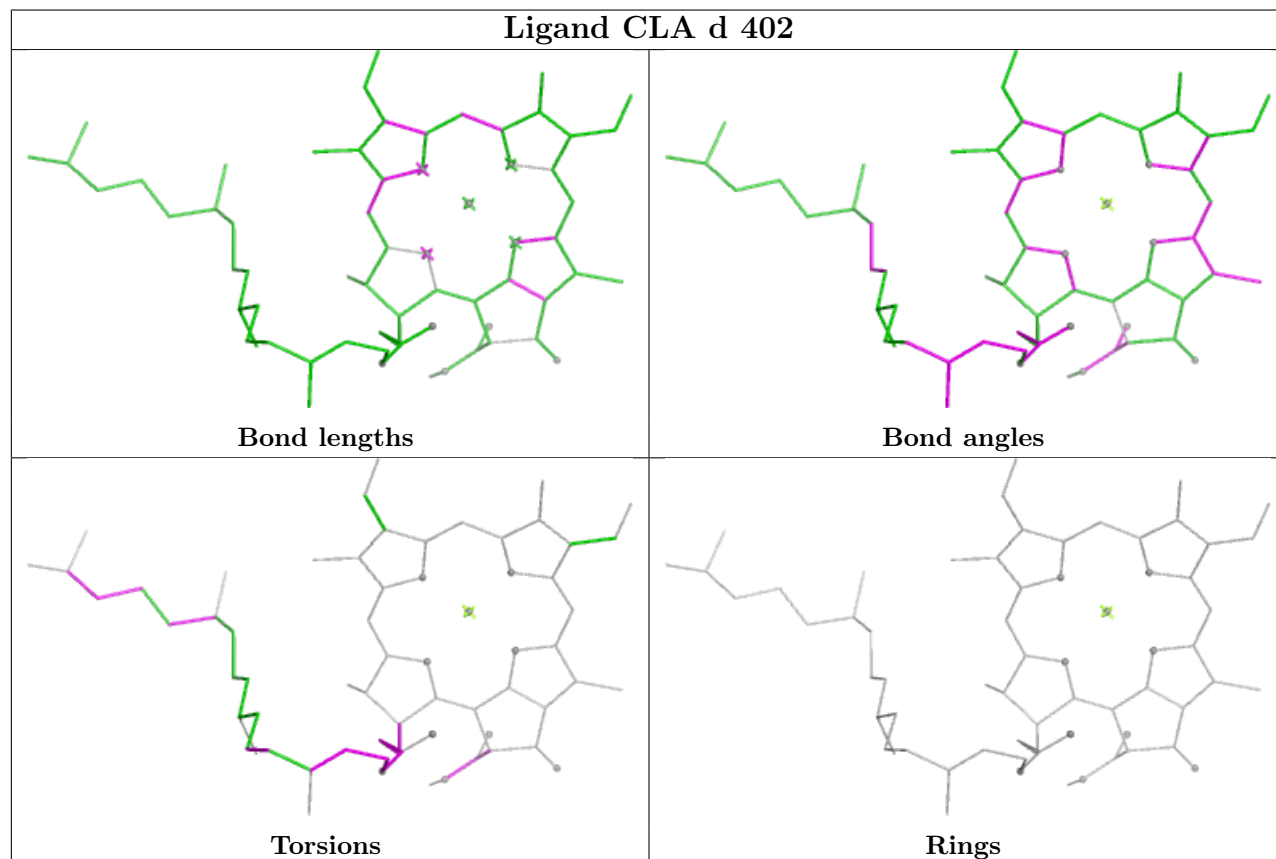
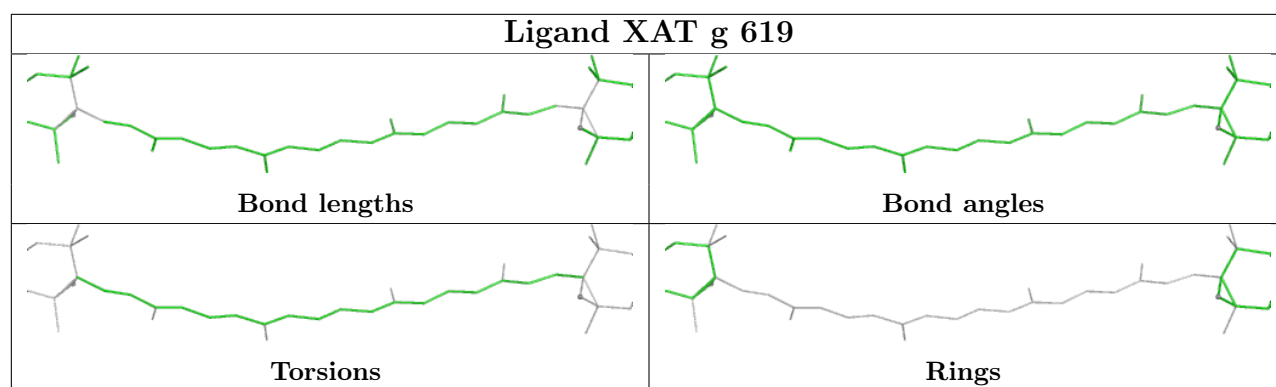


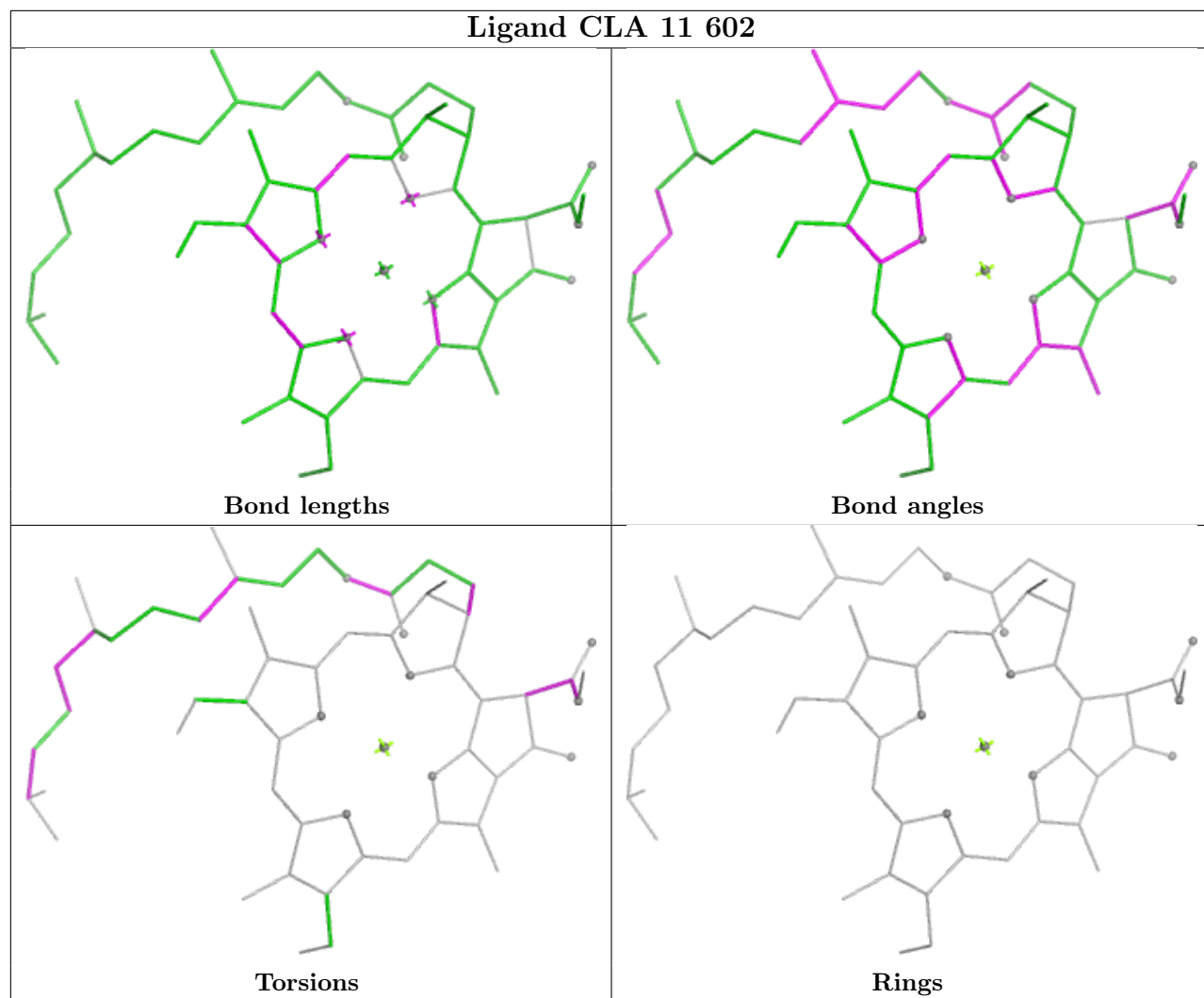
Torsions

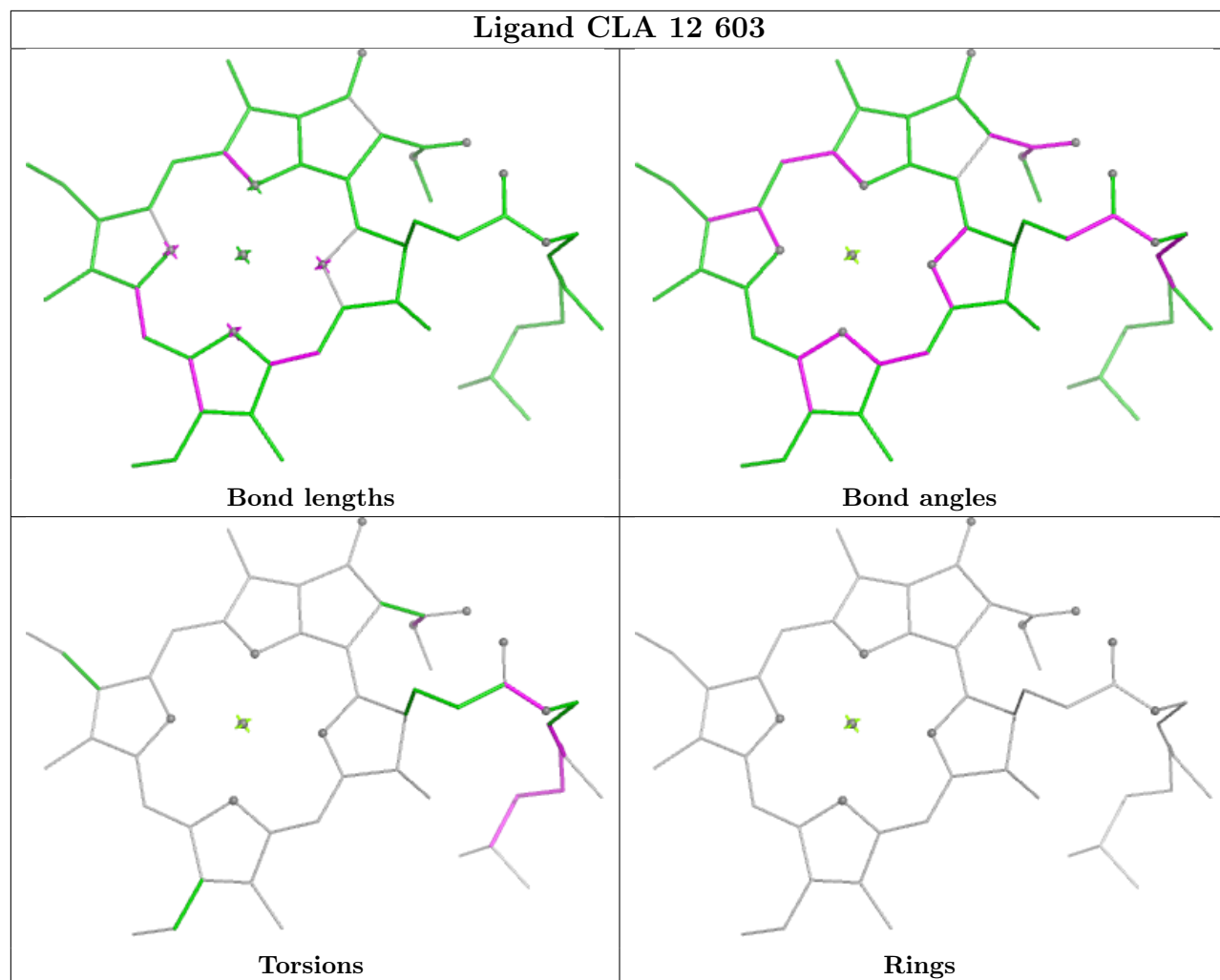


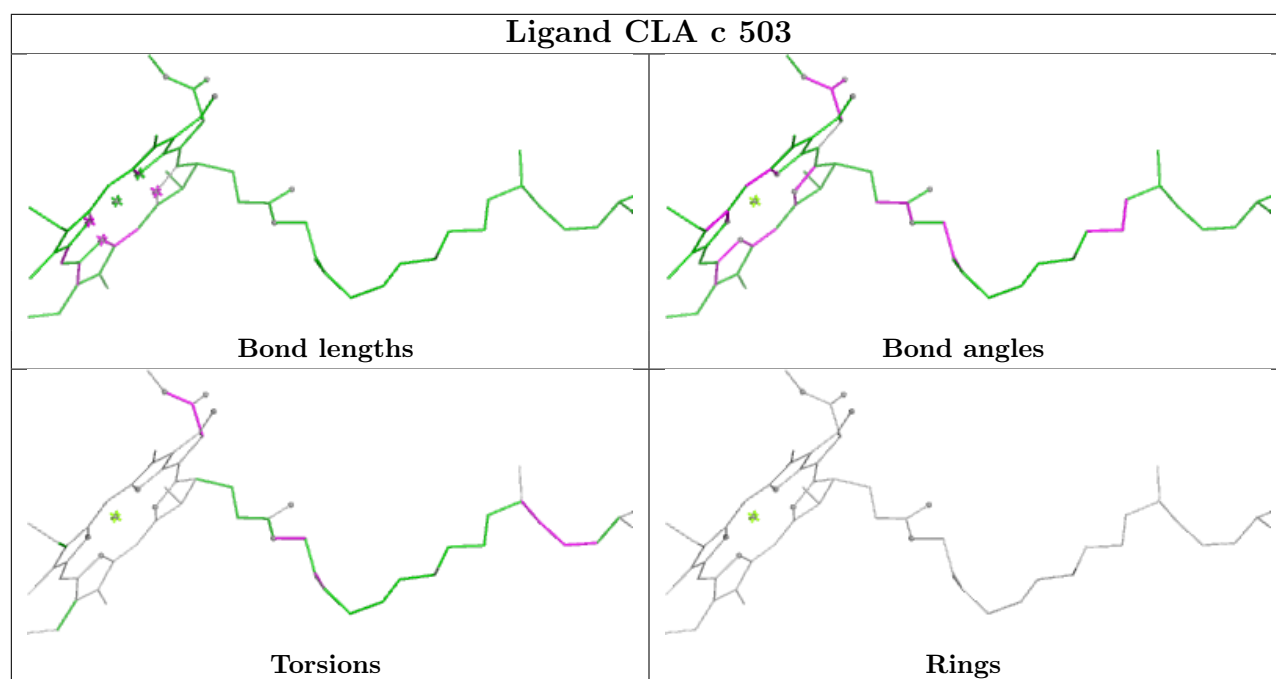
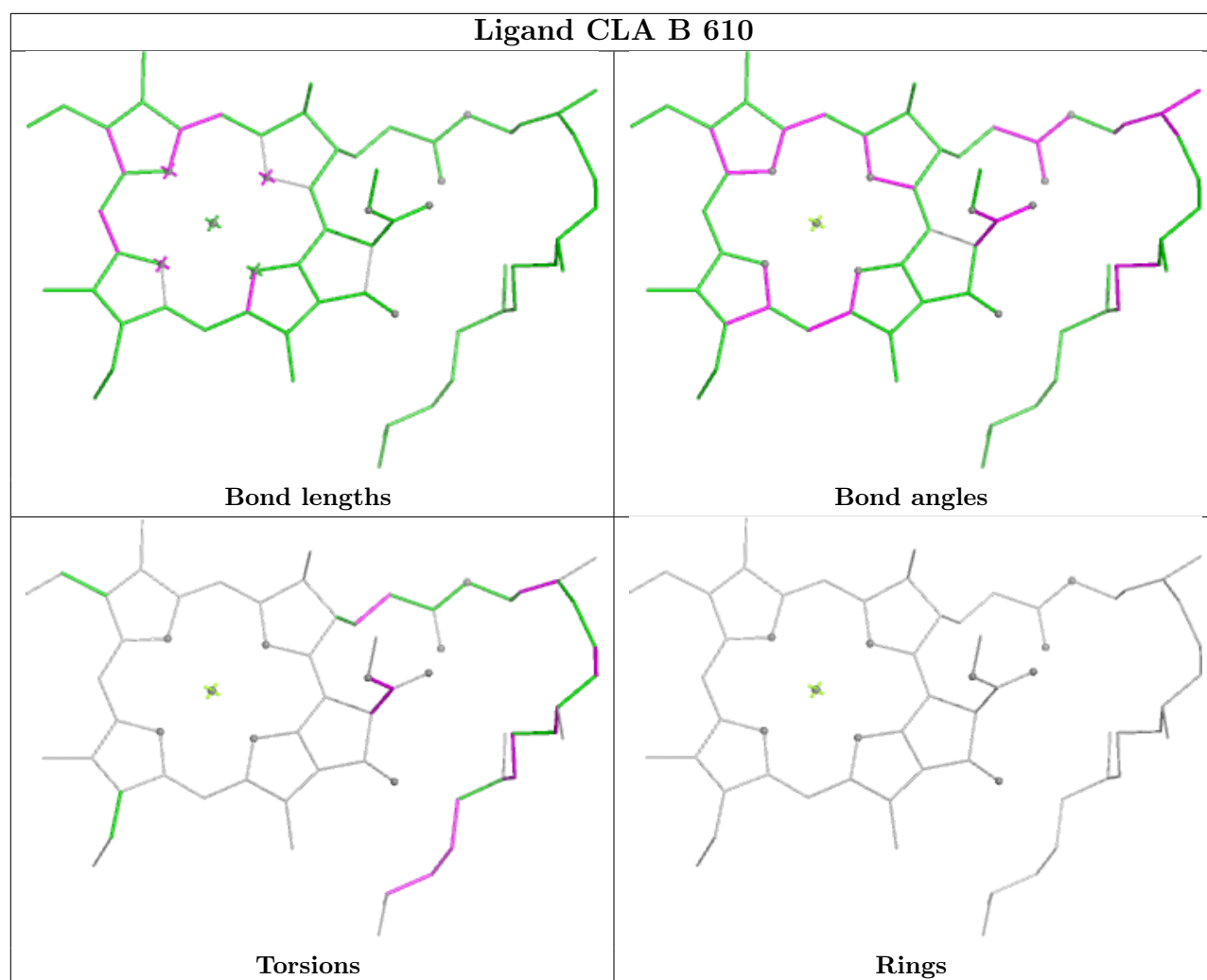
Rings



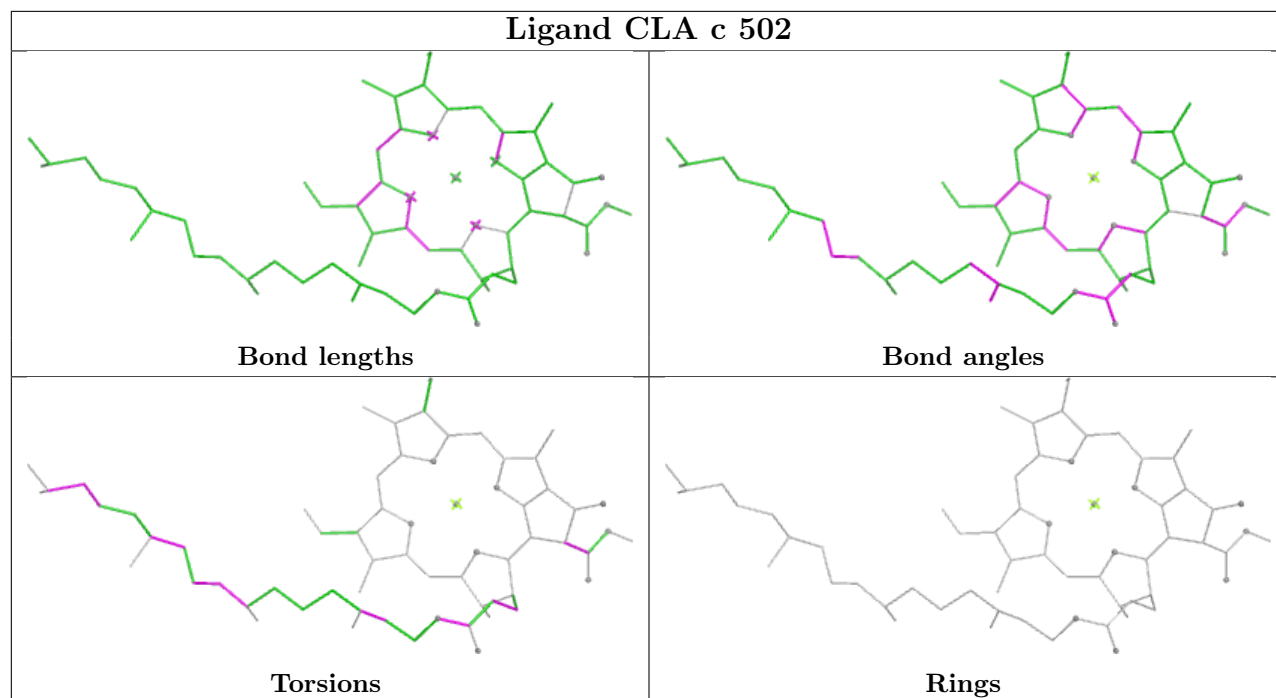




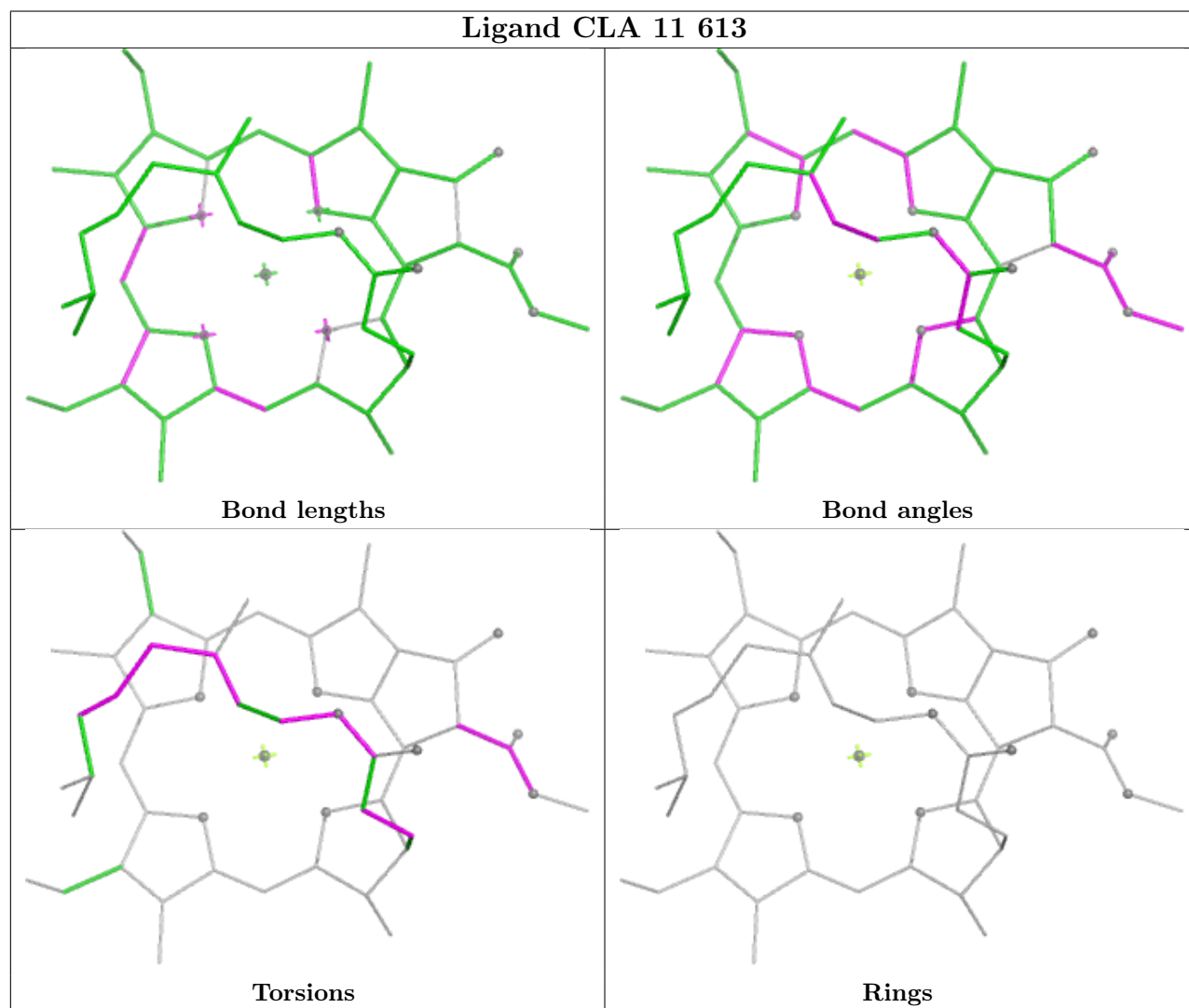


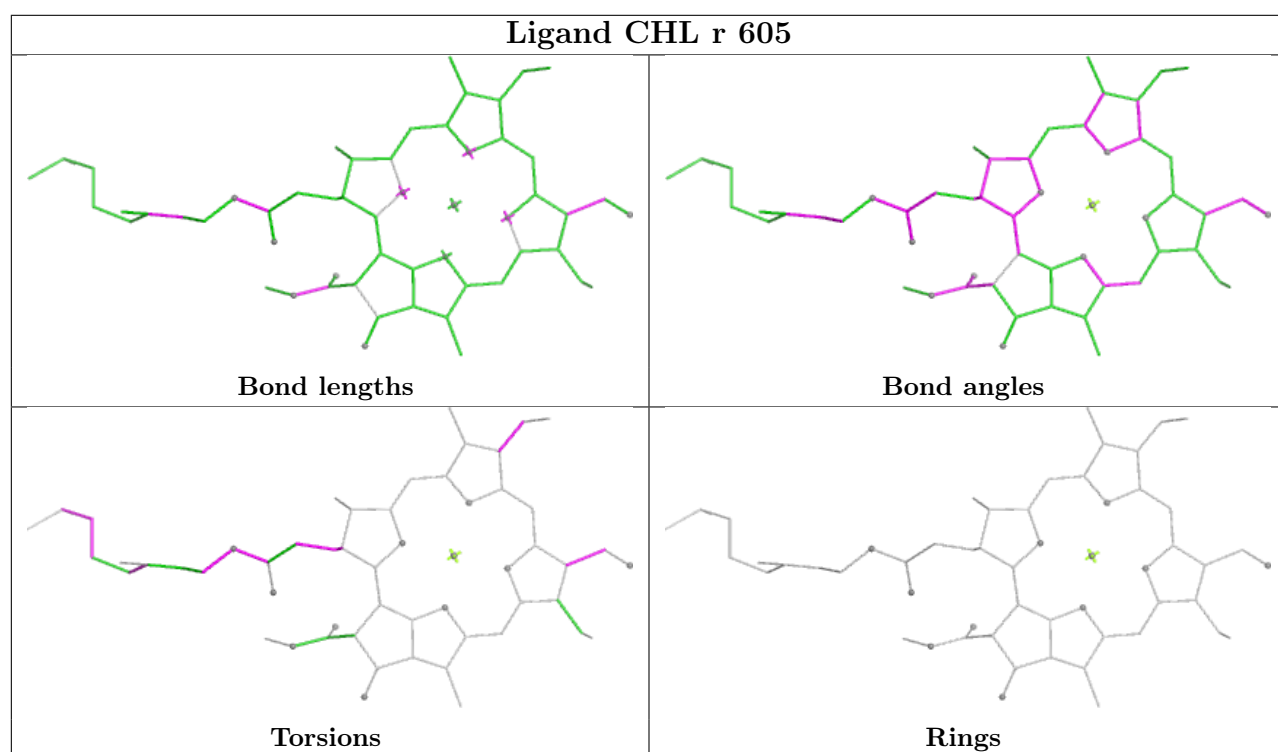
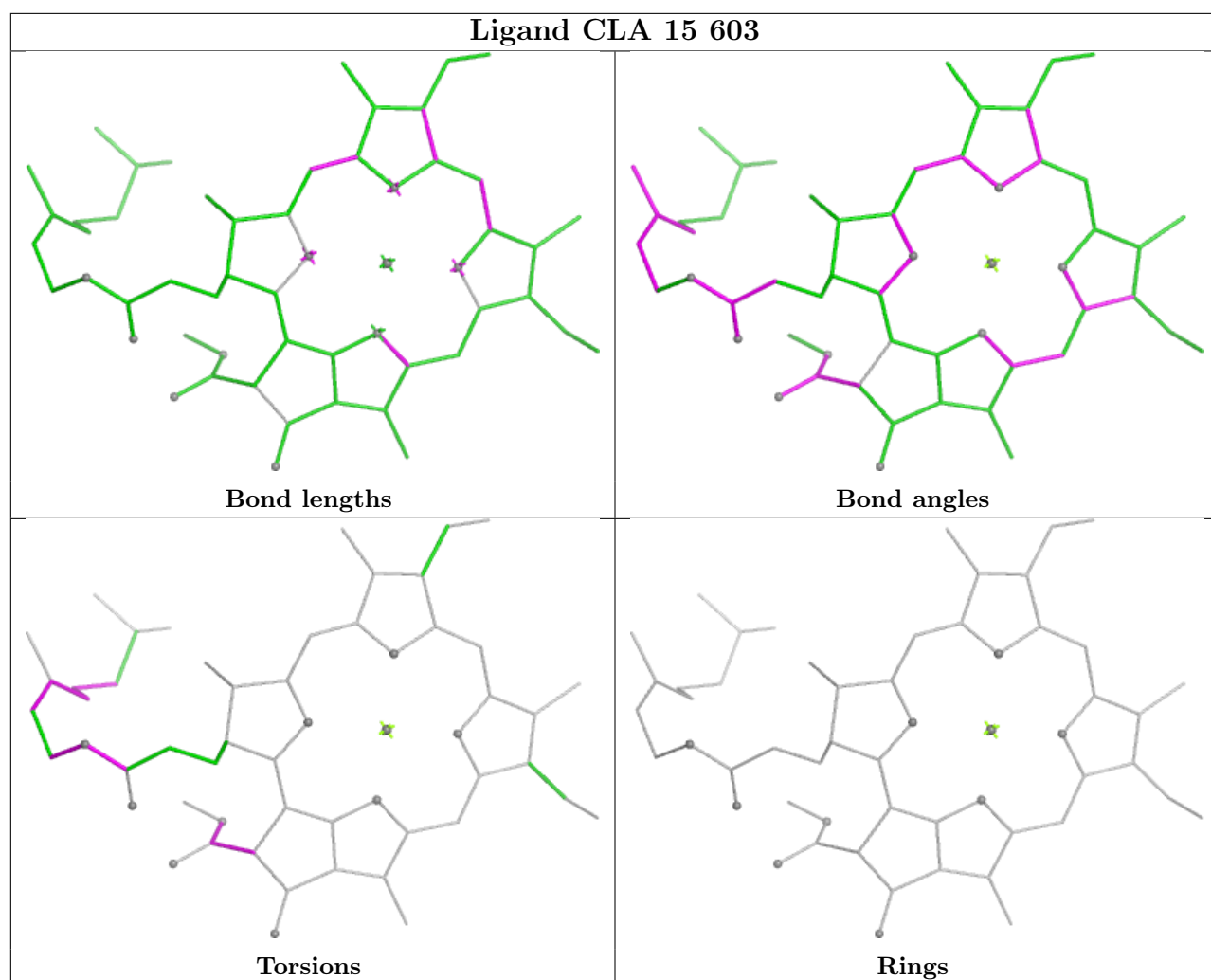


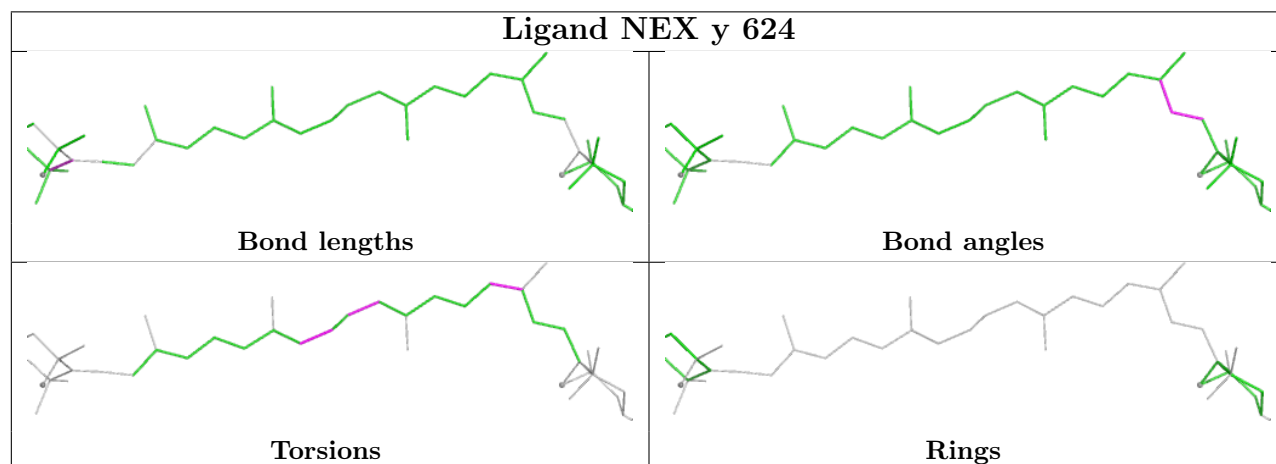
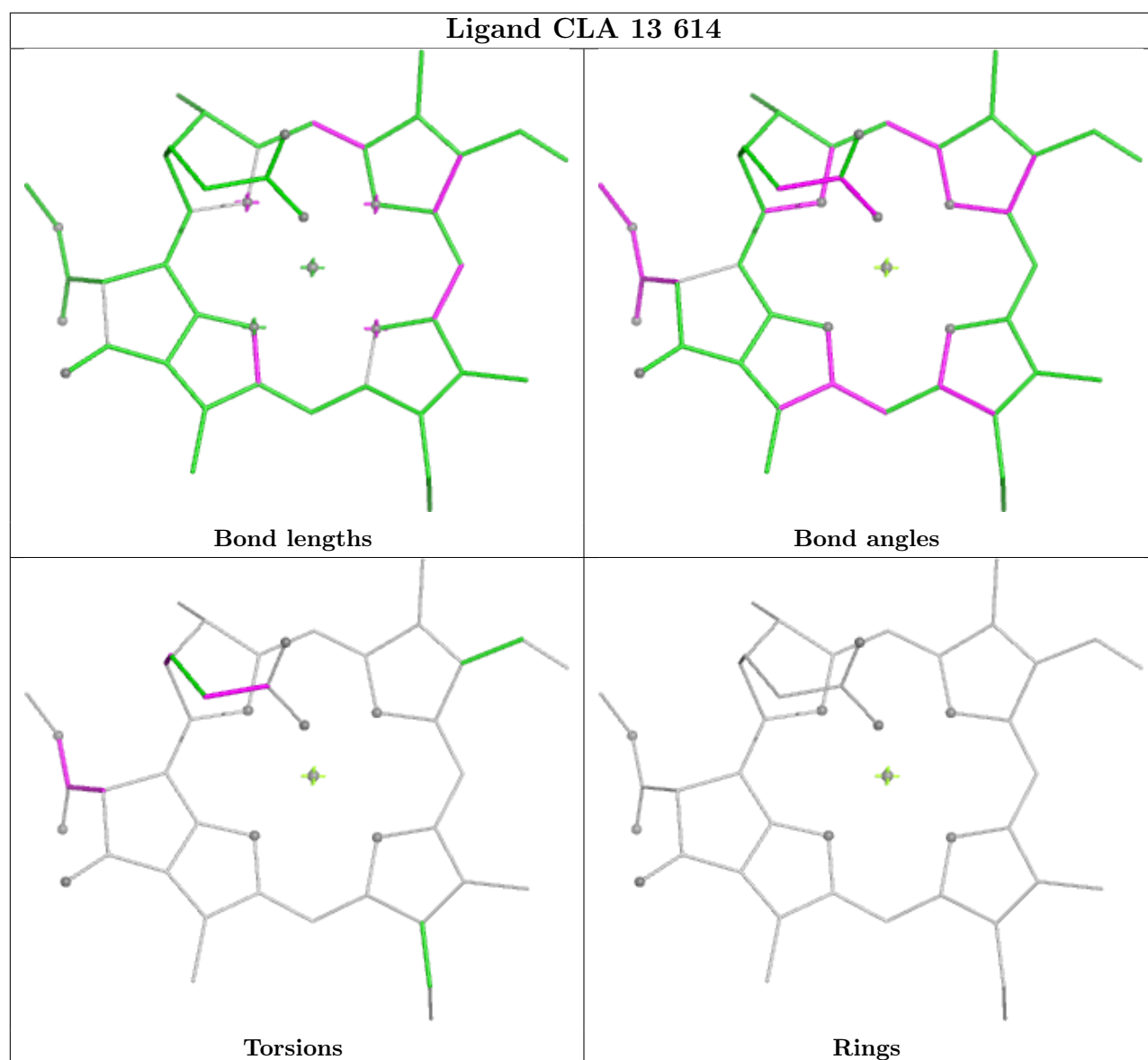
Ligand CLA c 502



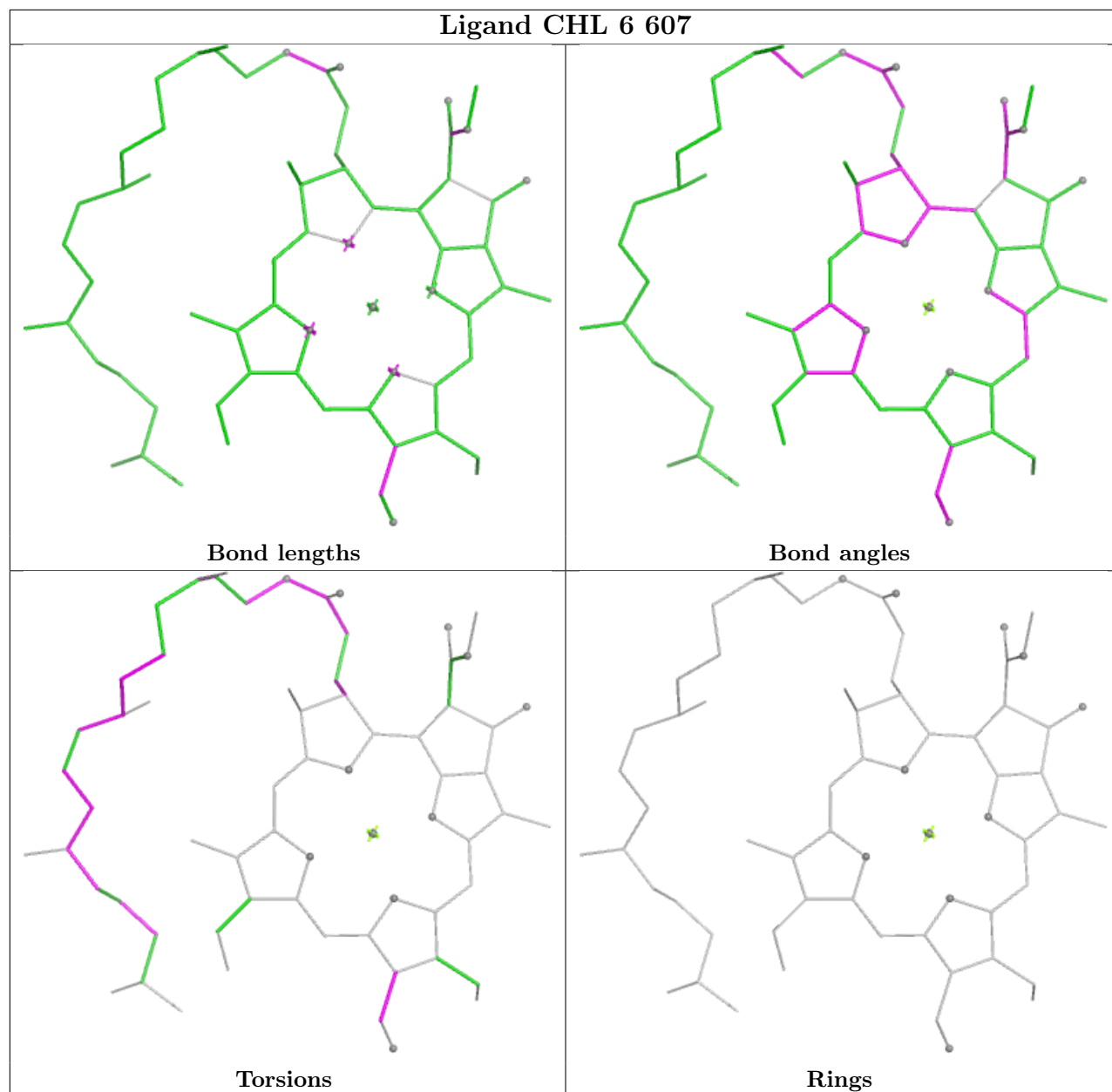
Ligand CLA 11 613



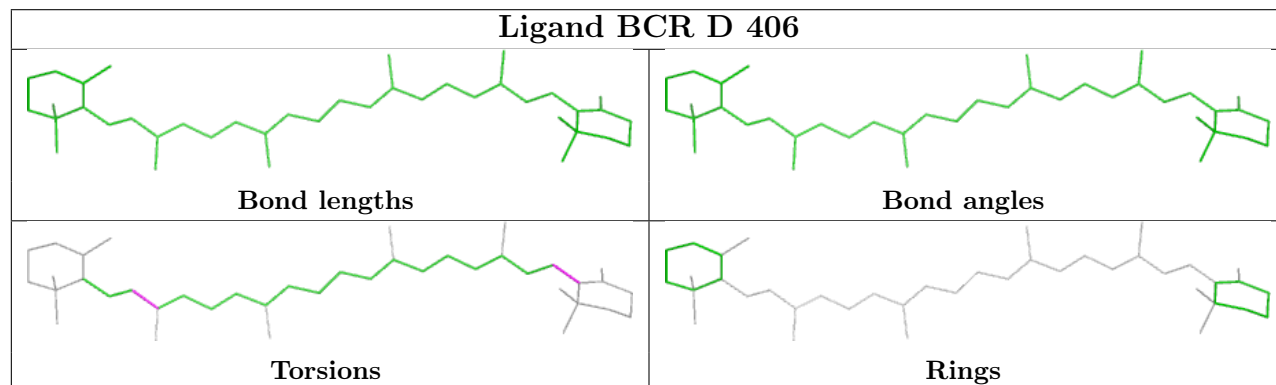


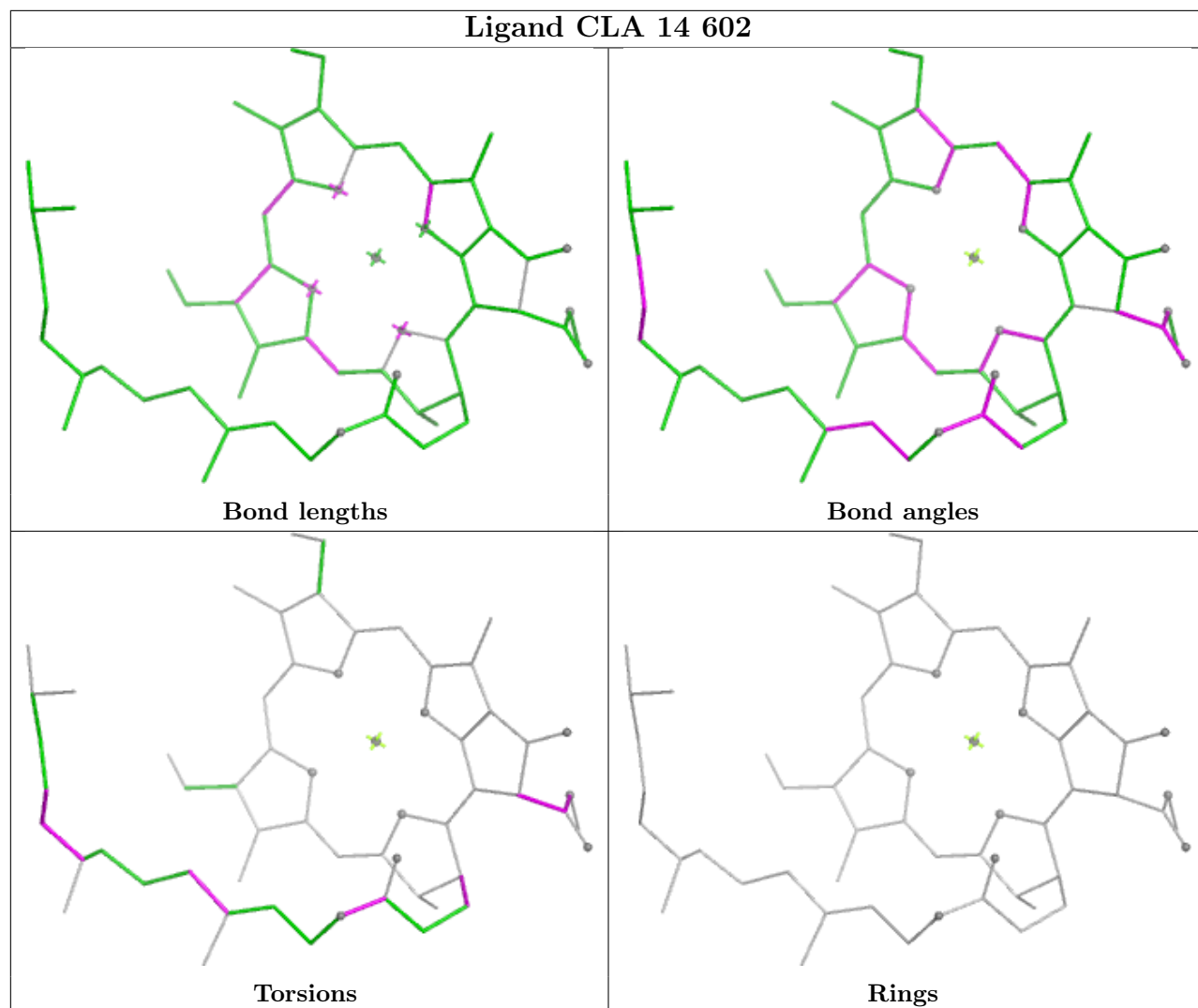


Ligand CHL 6 607

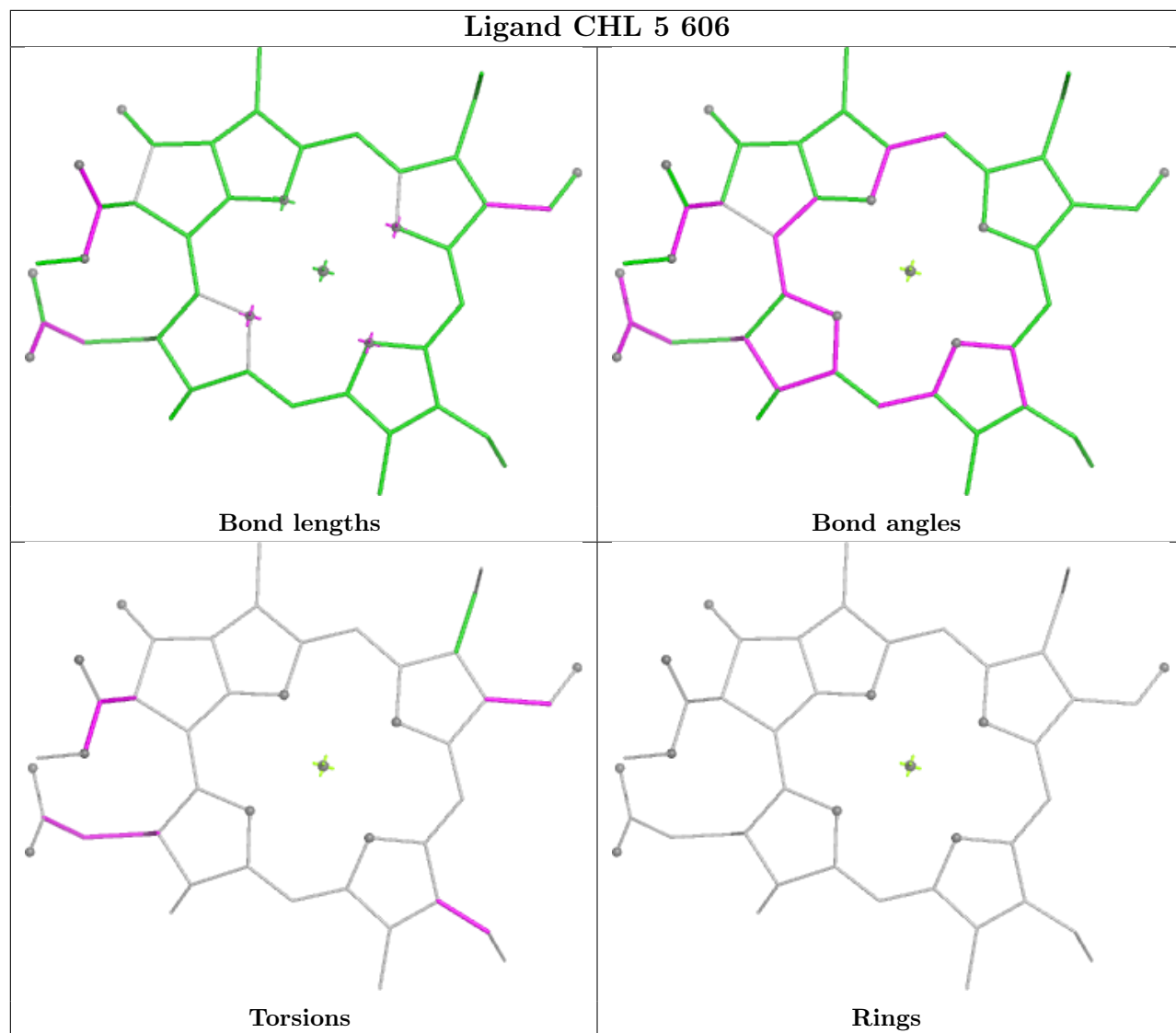


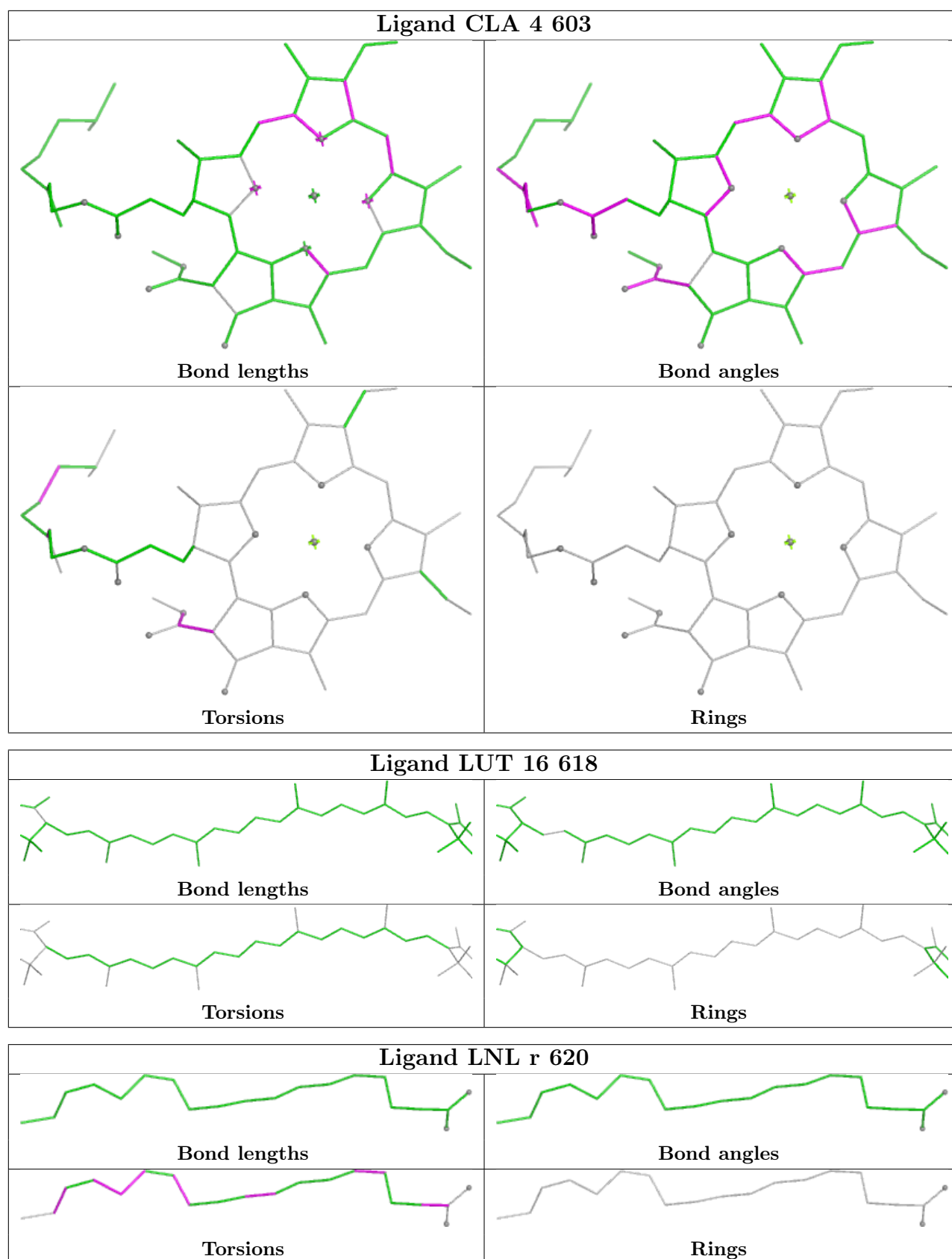
Ligand BCR D 406

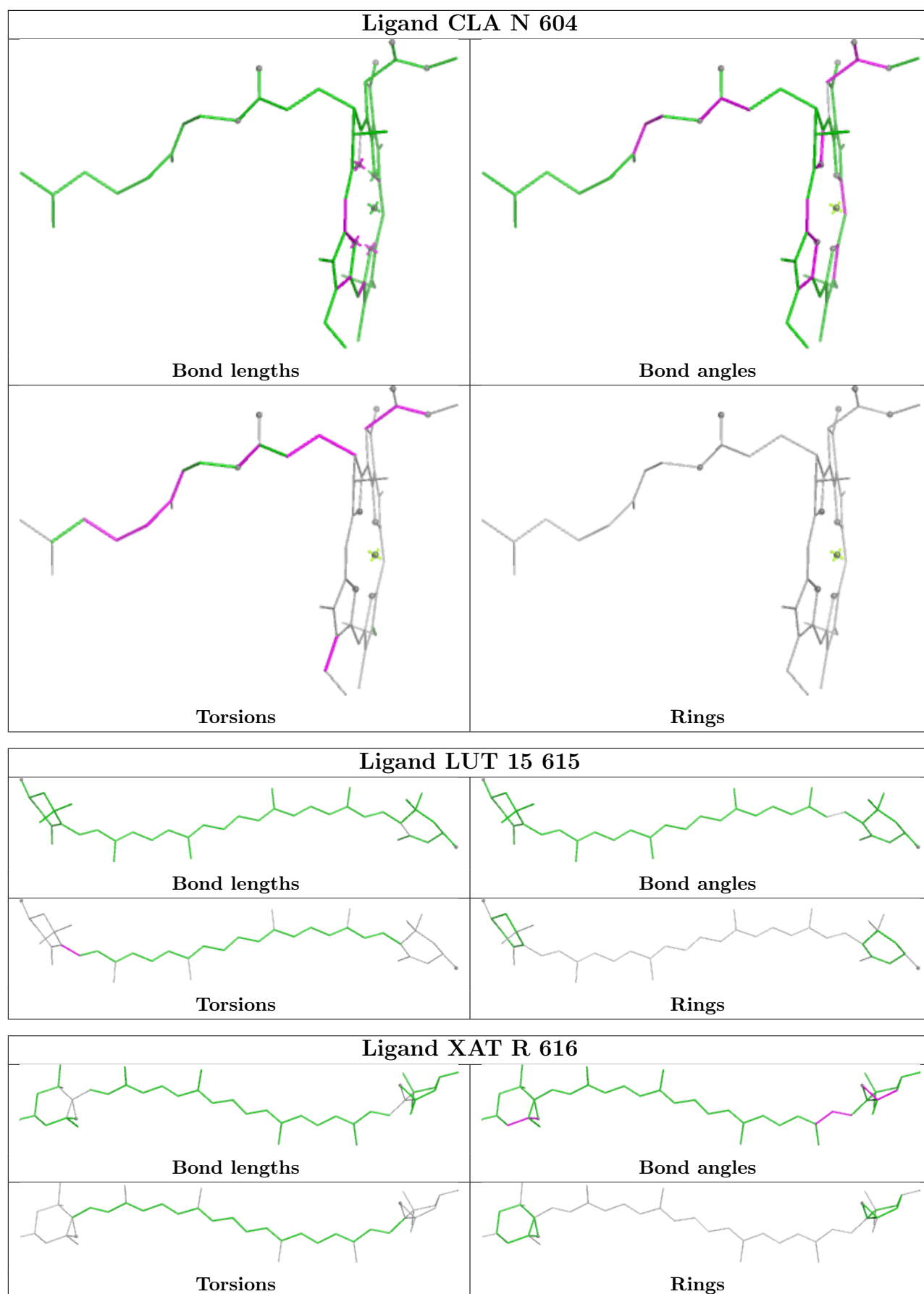


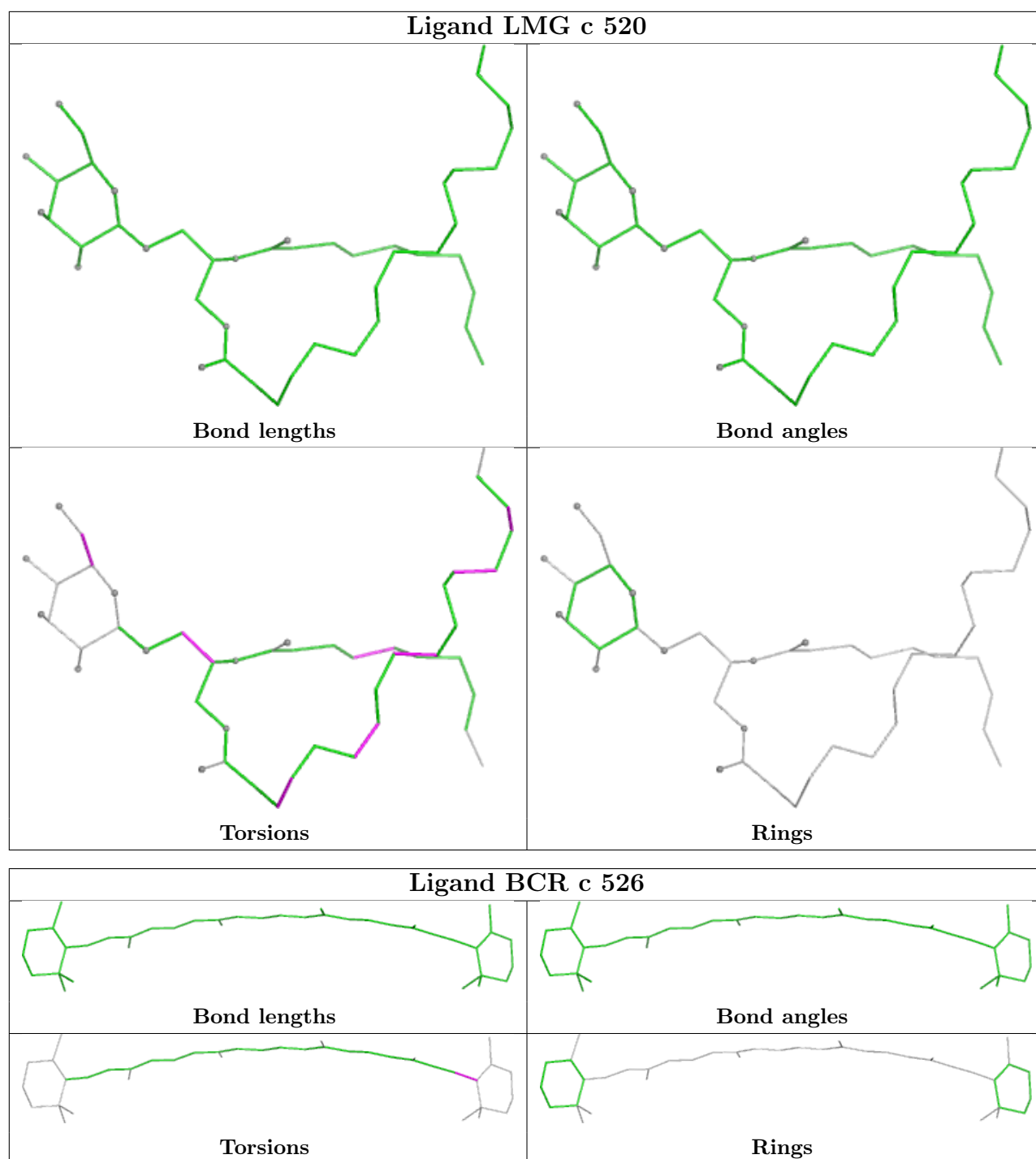


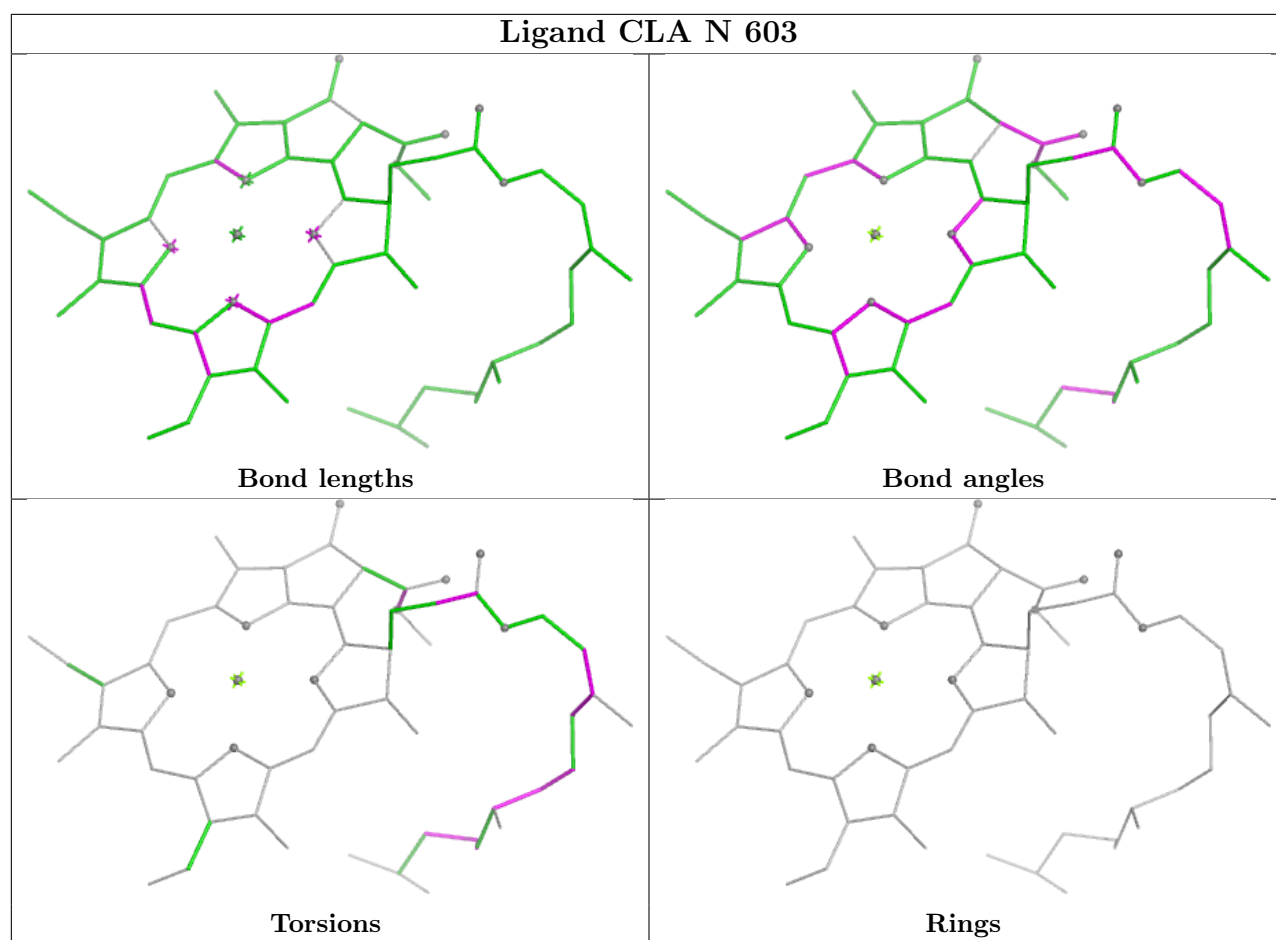
Ligand CHL 5 606

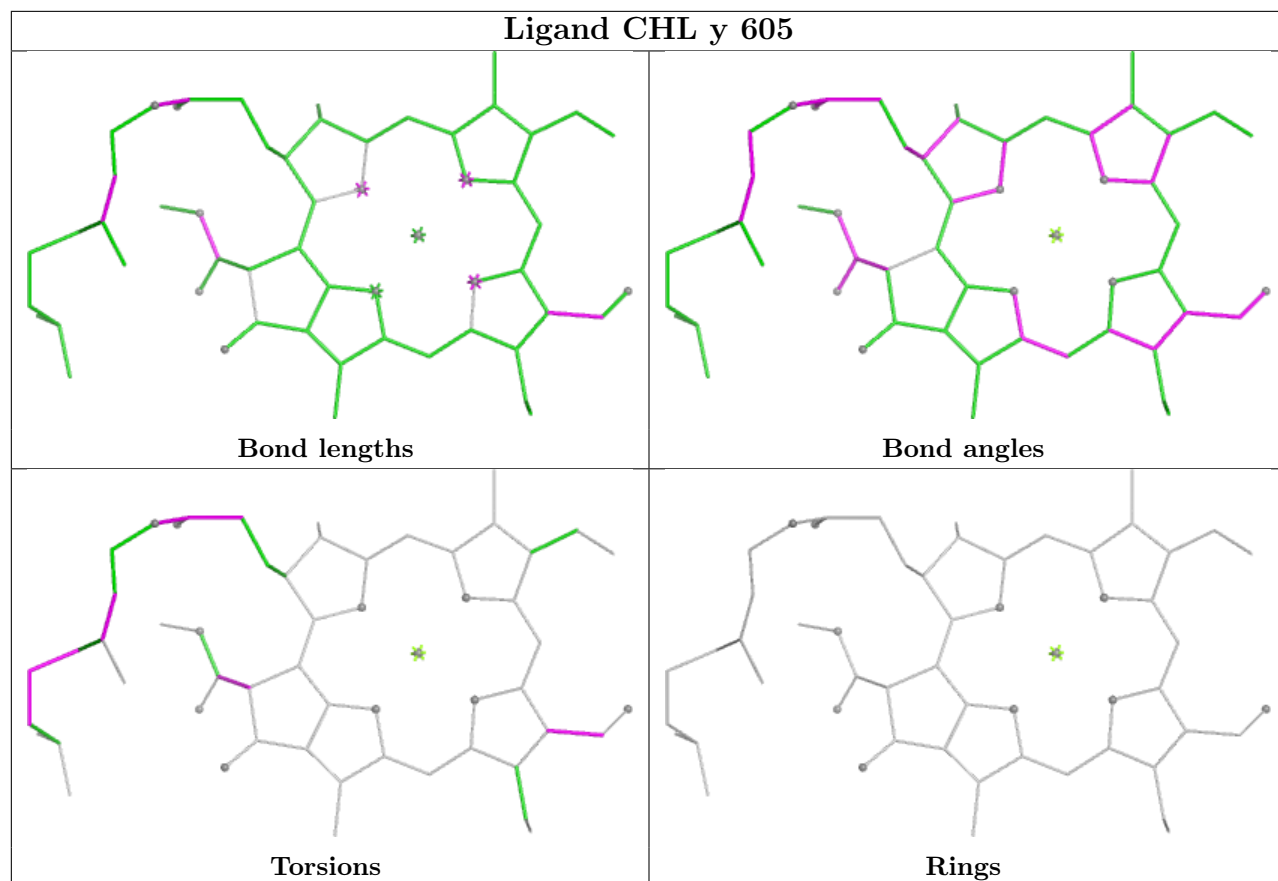


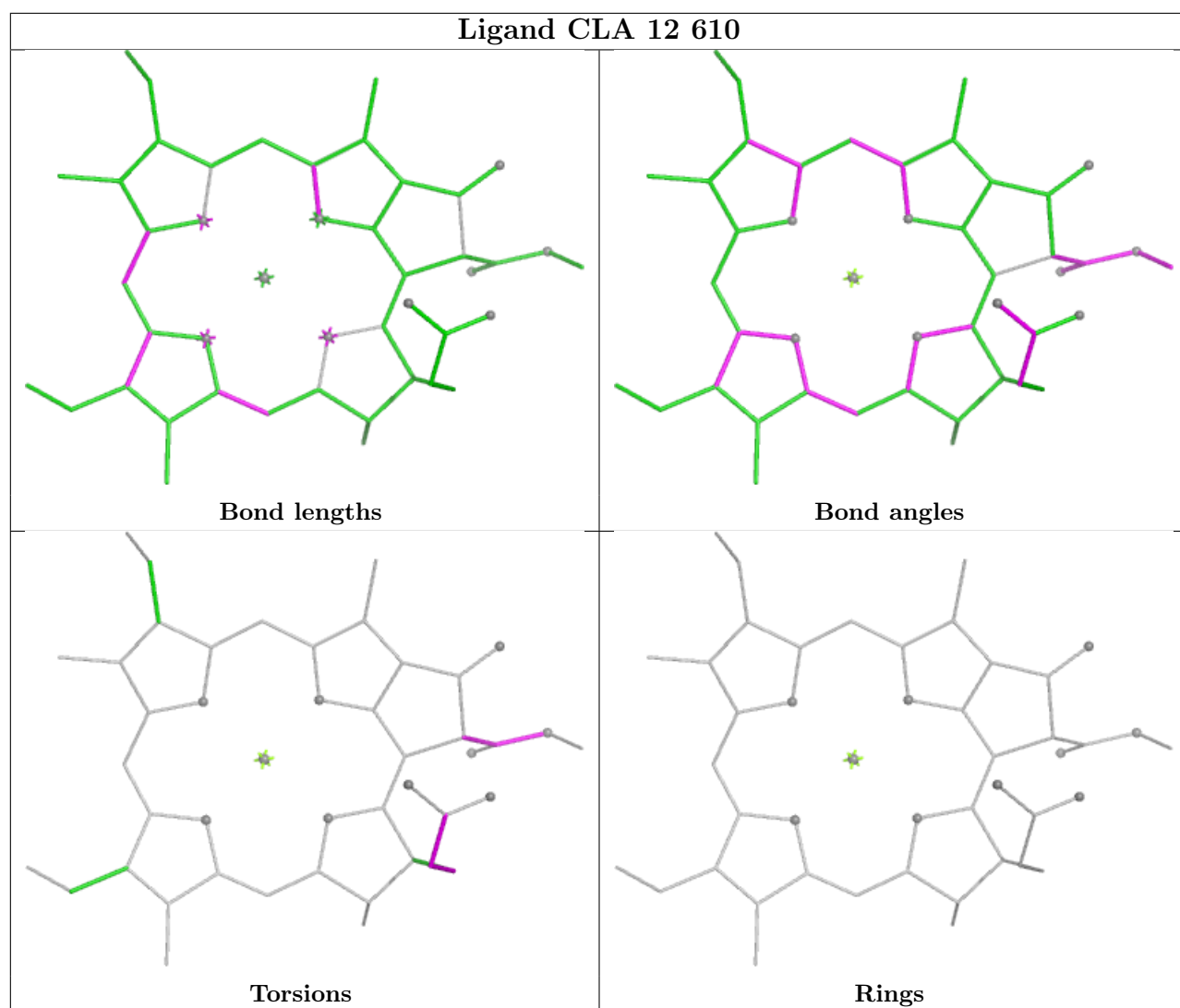




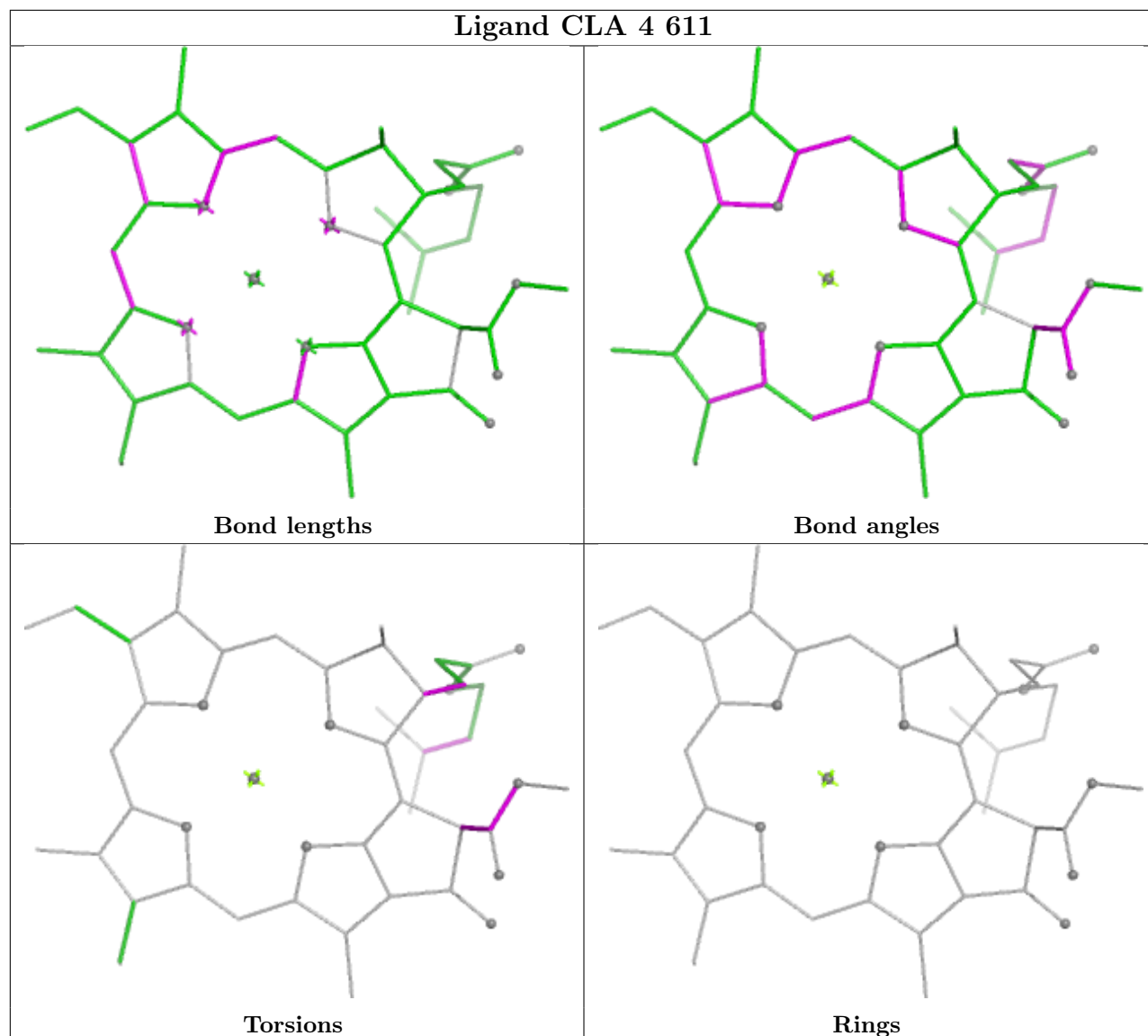




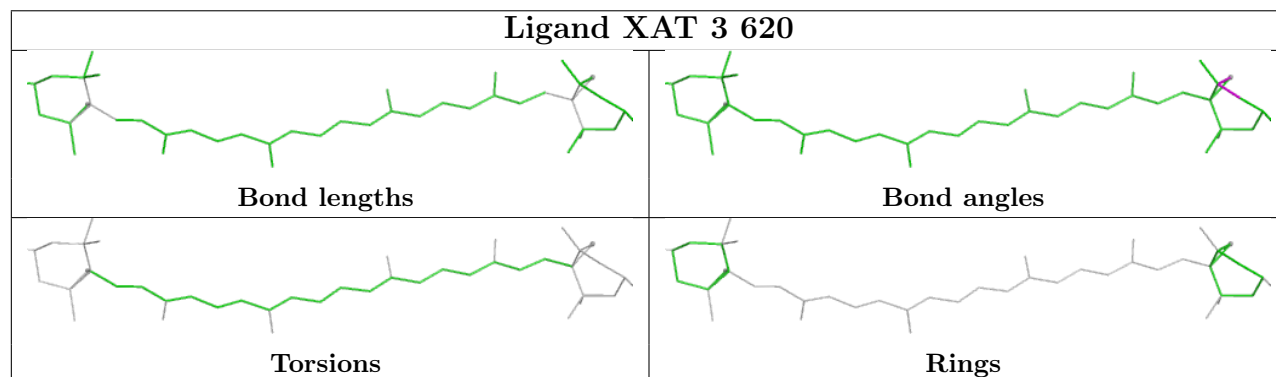


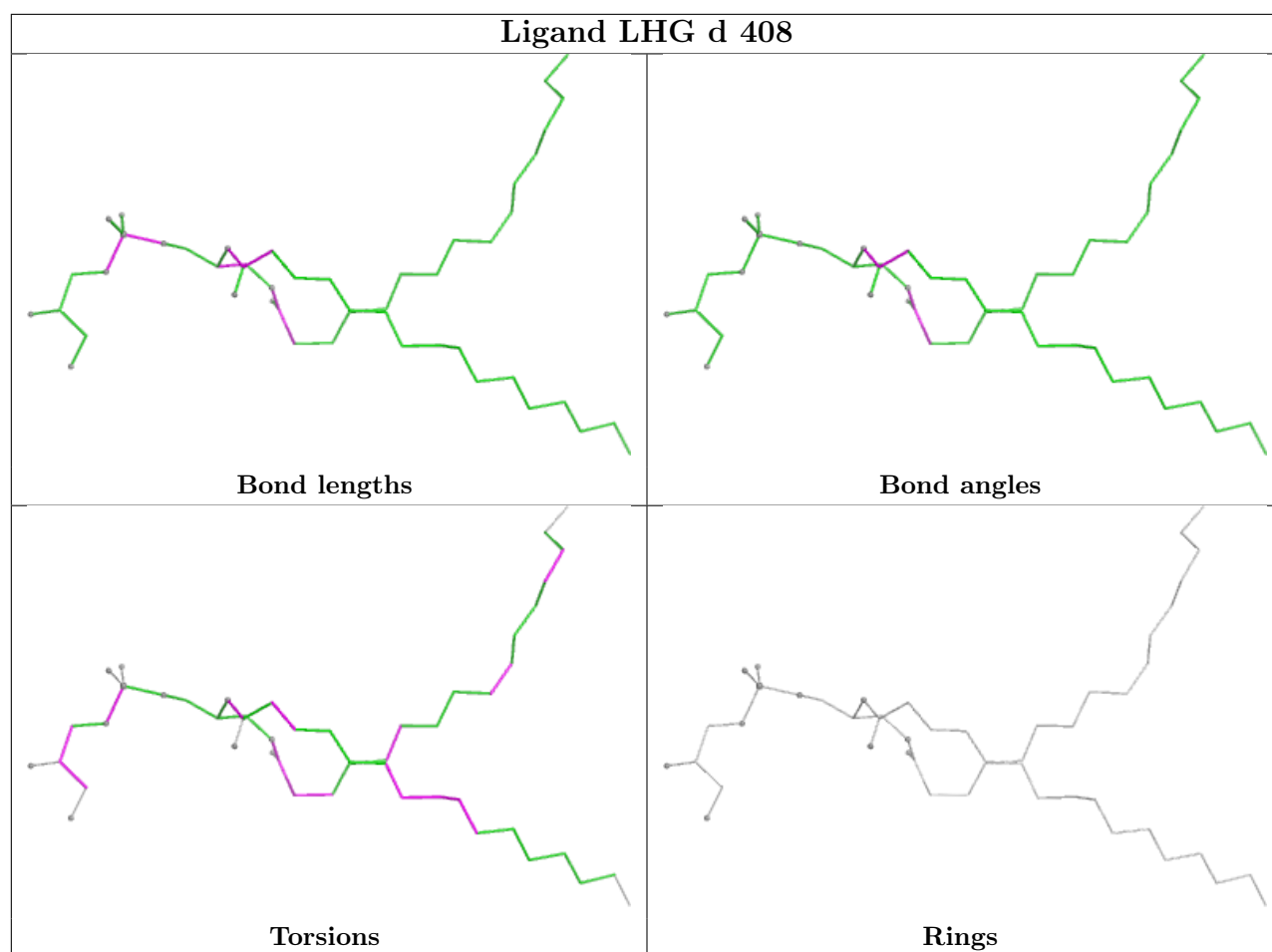


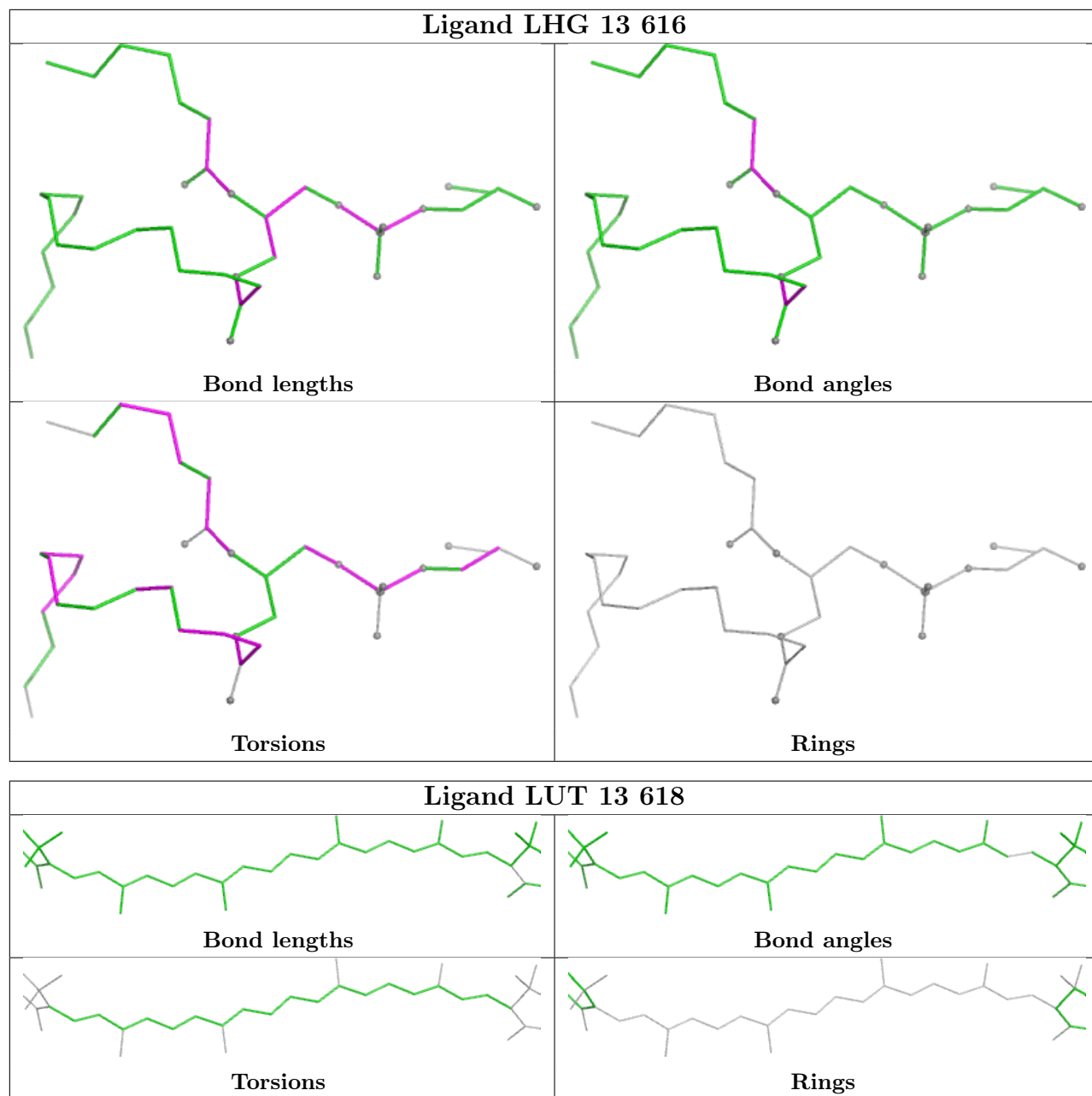
Ligand CLA 4 611



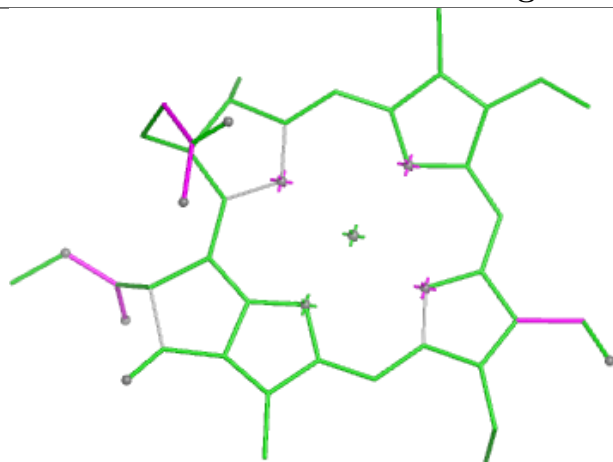
Ligand XAT 3 620



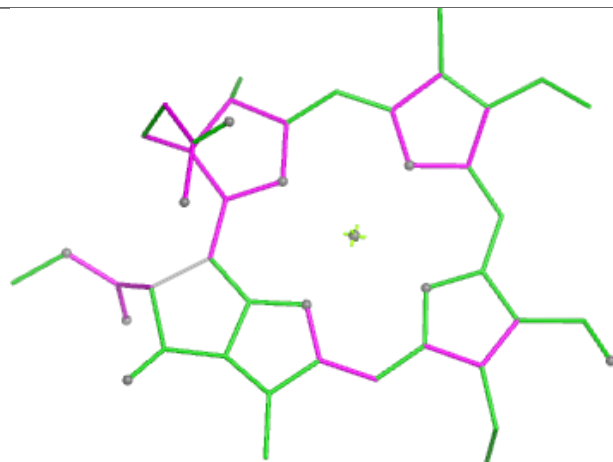




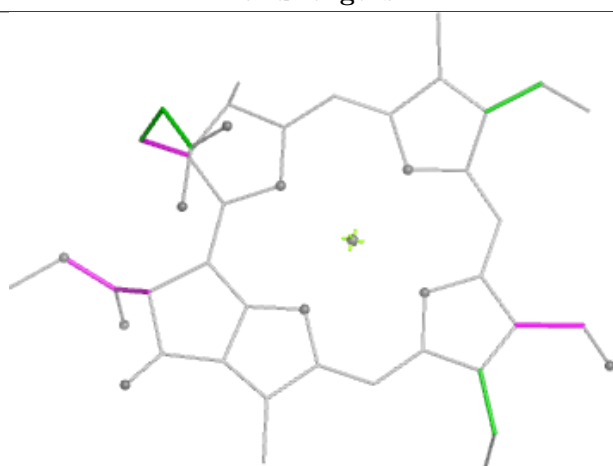
Ligand CHL 1 605



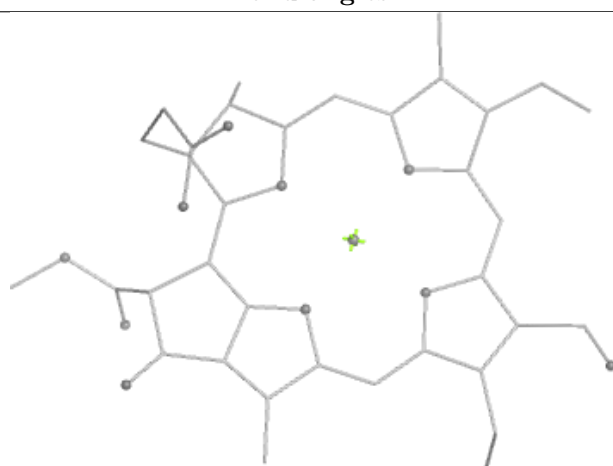
Bond lengths



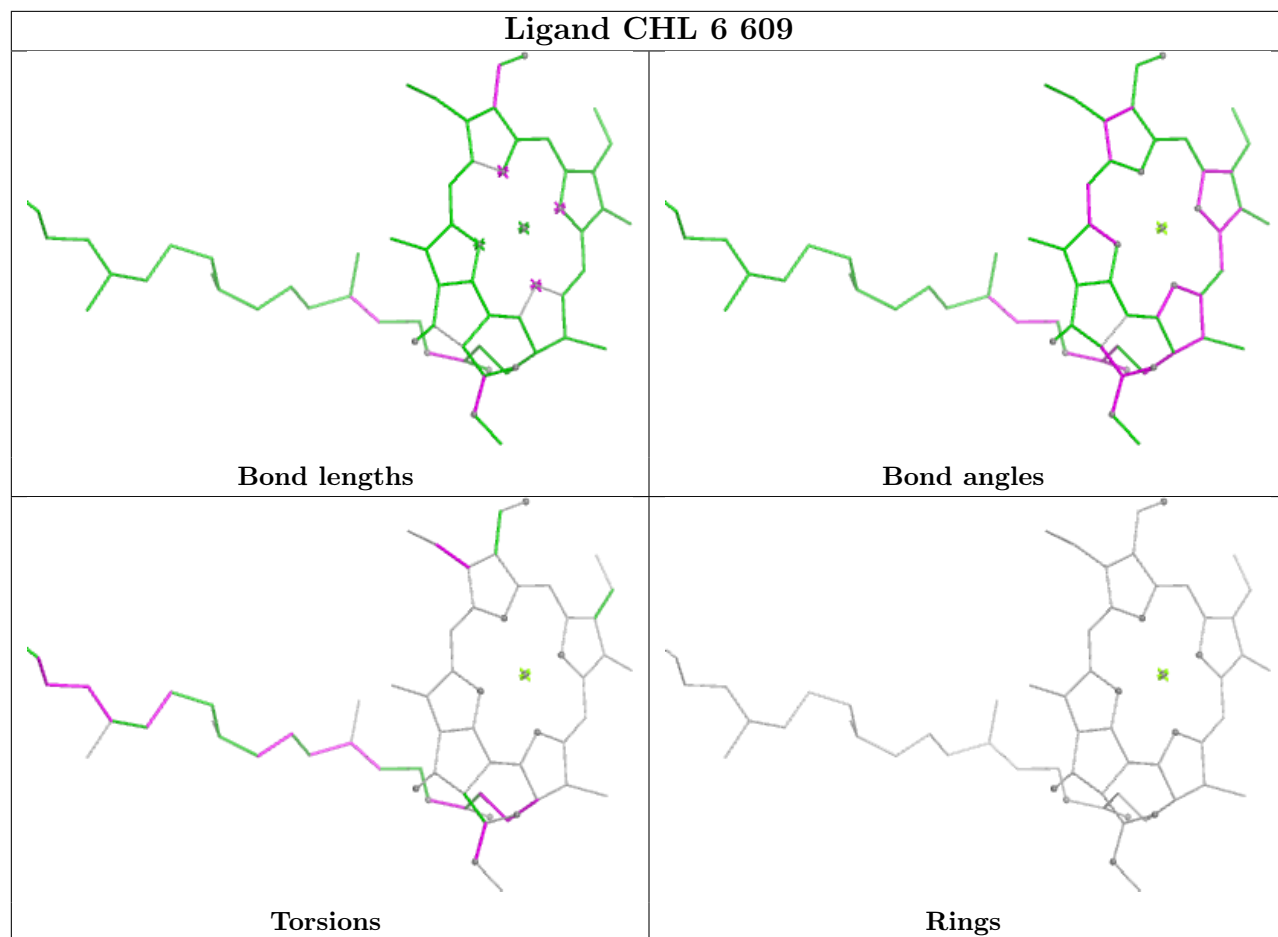
Bond angles



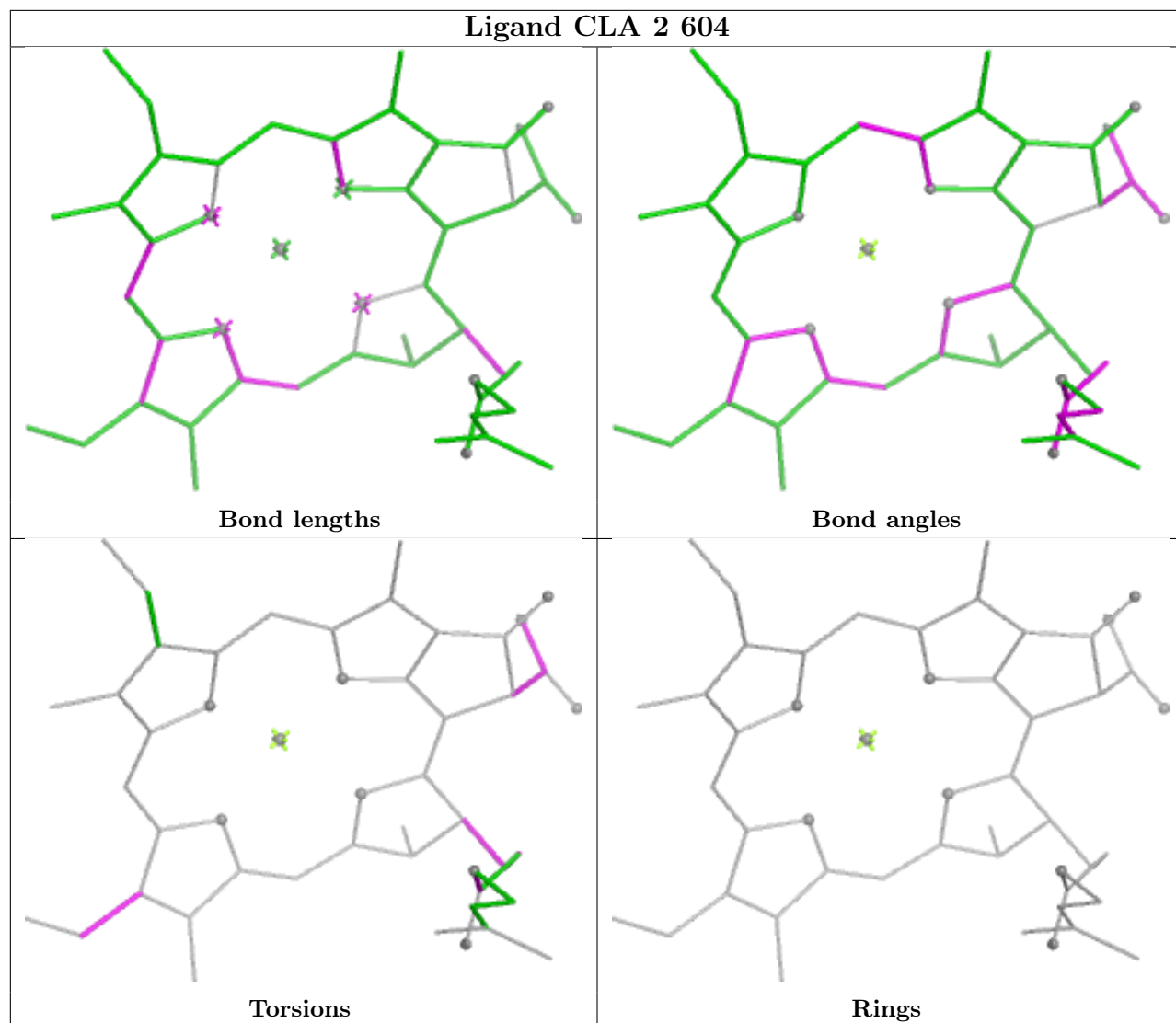
Torsions



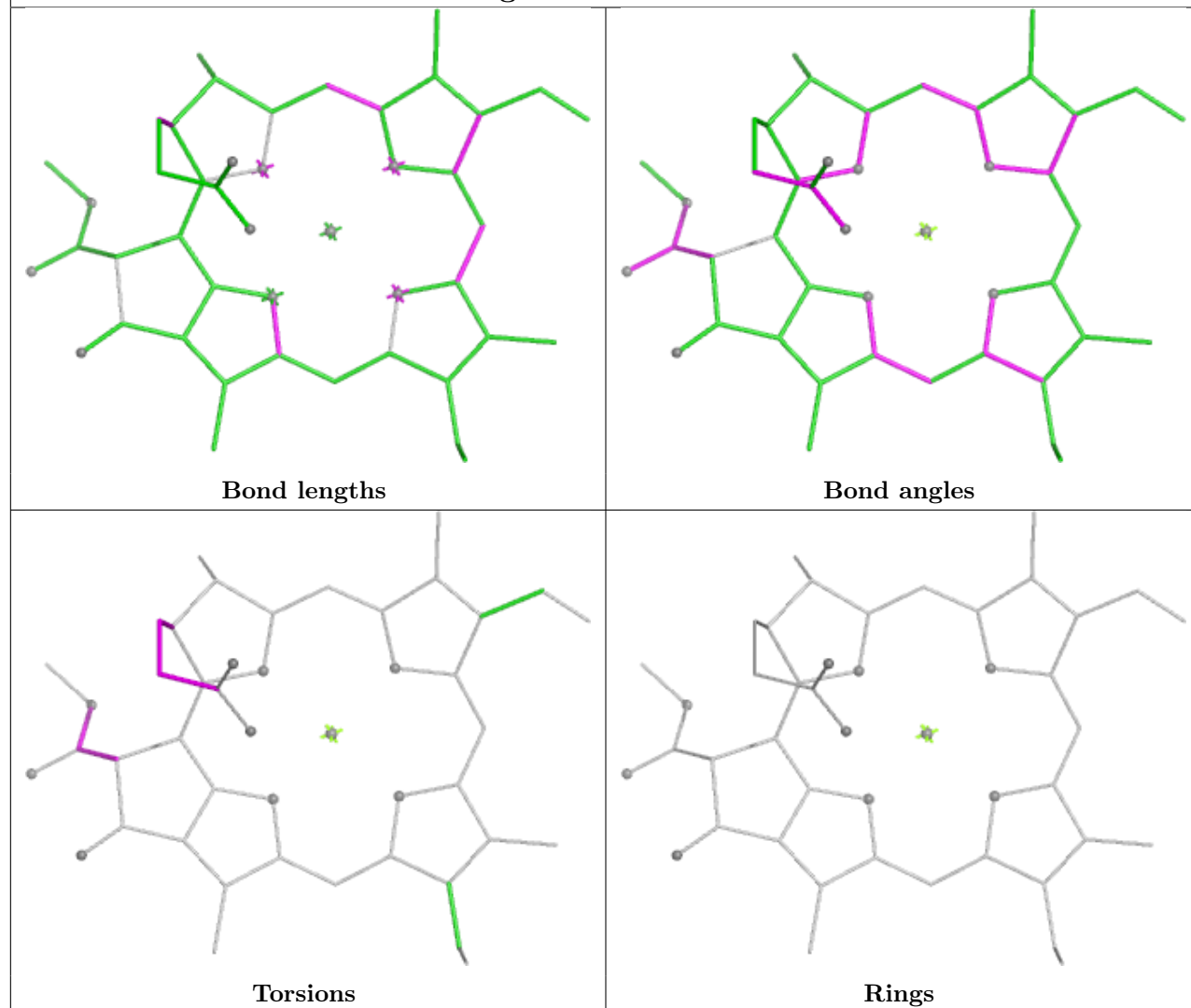
Rings



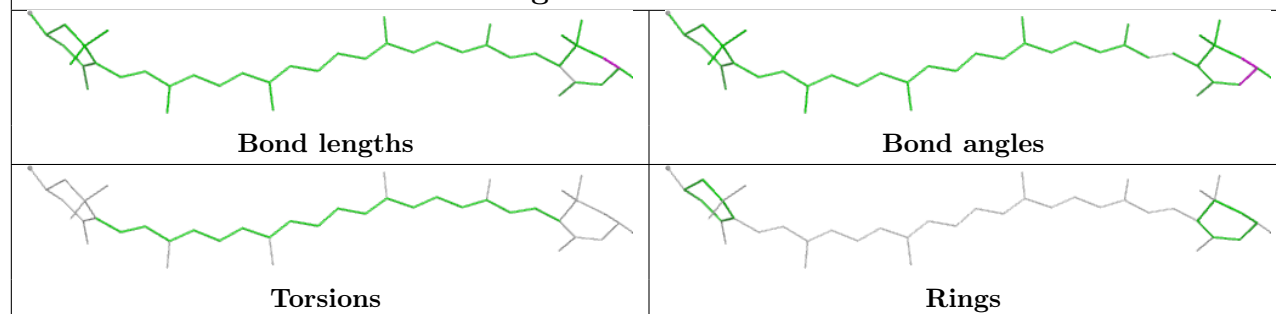
Ligand CLA 2 604

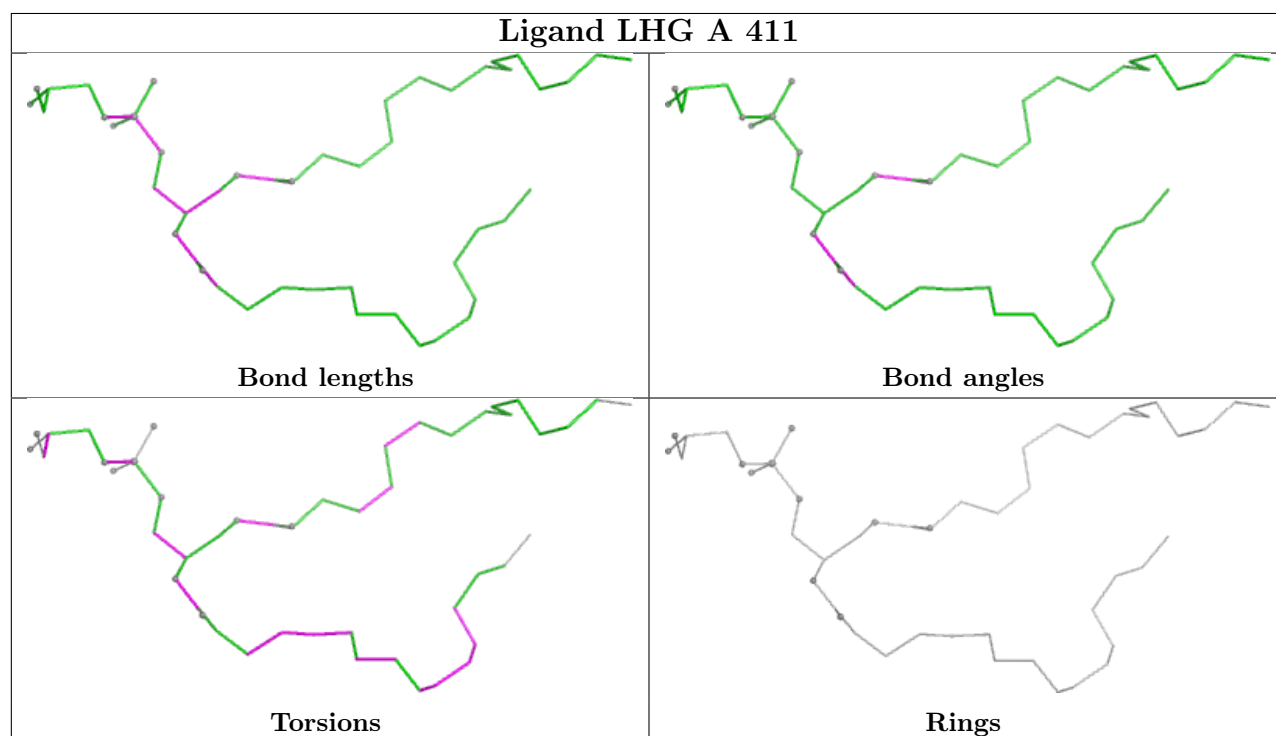
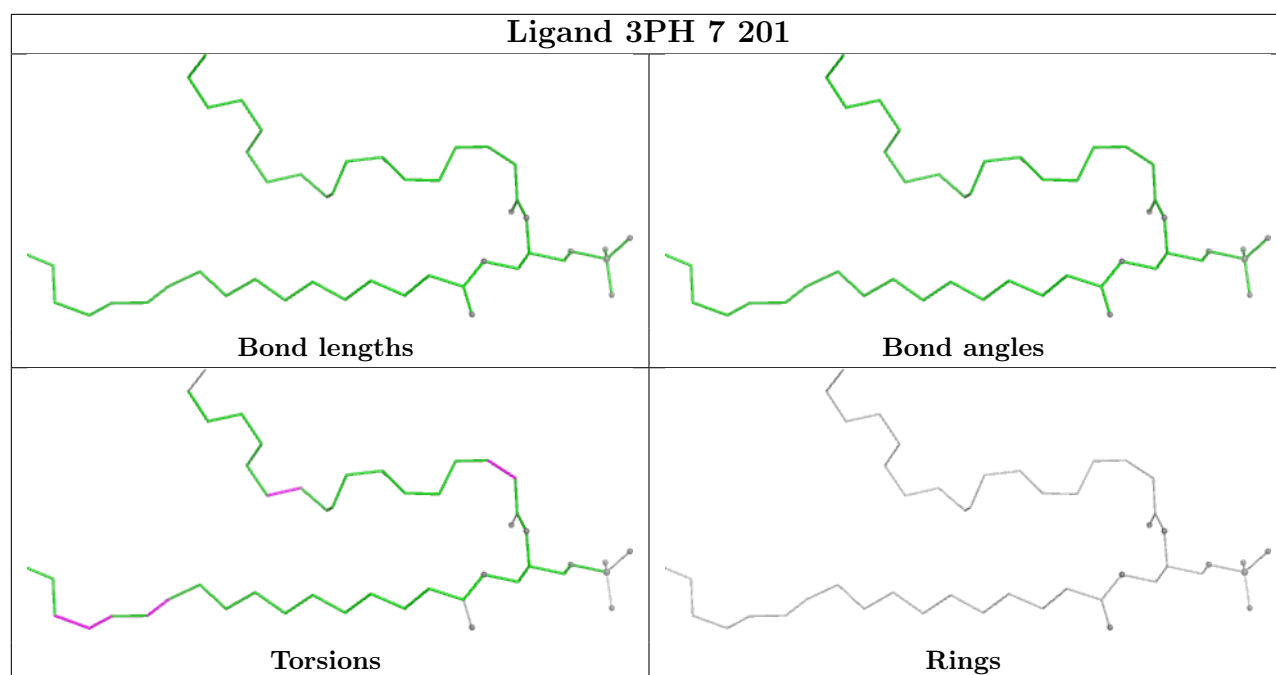


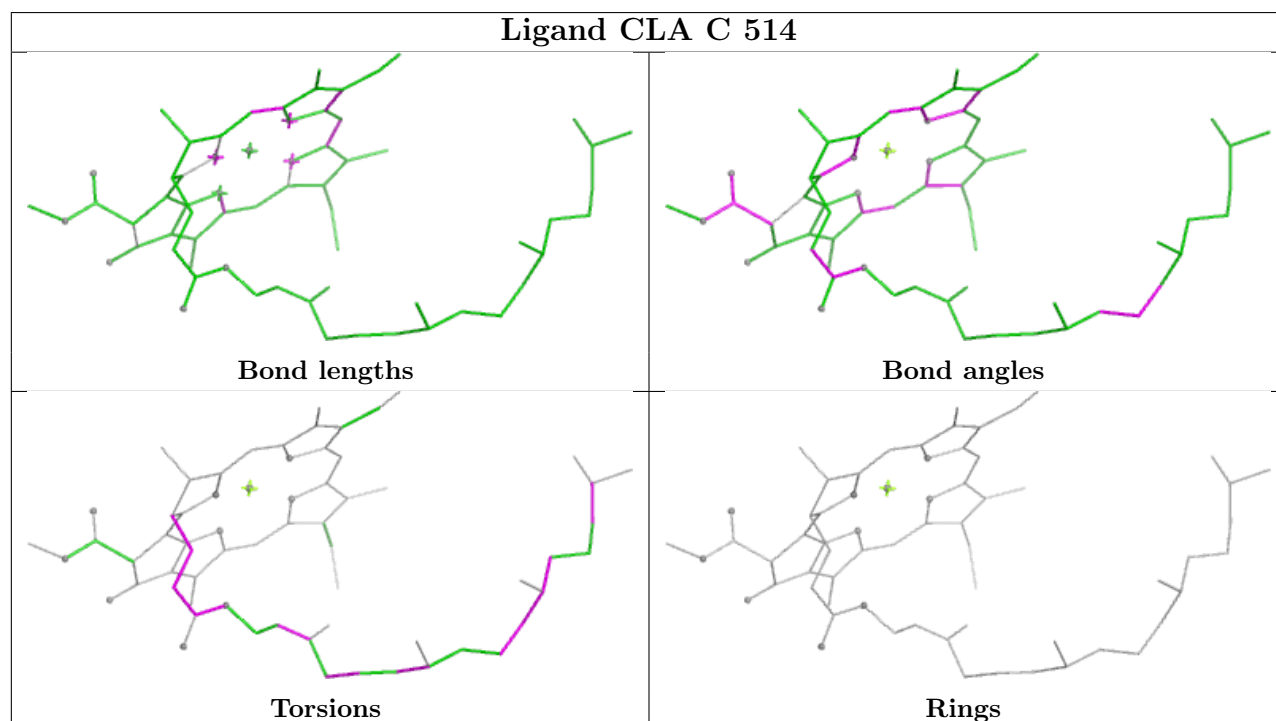
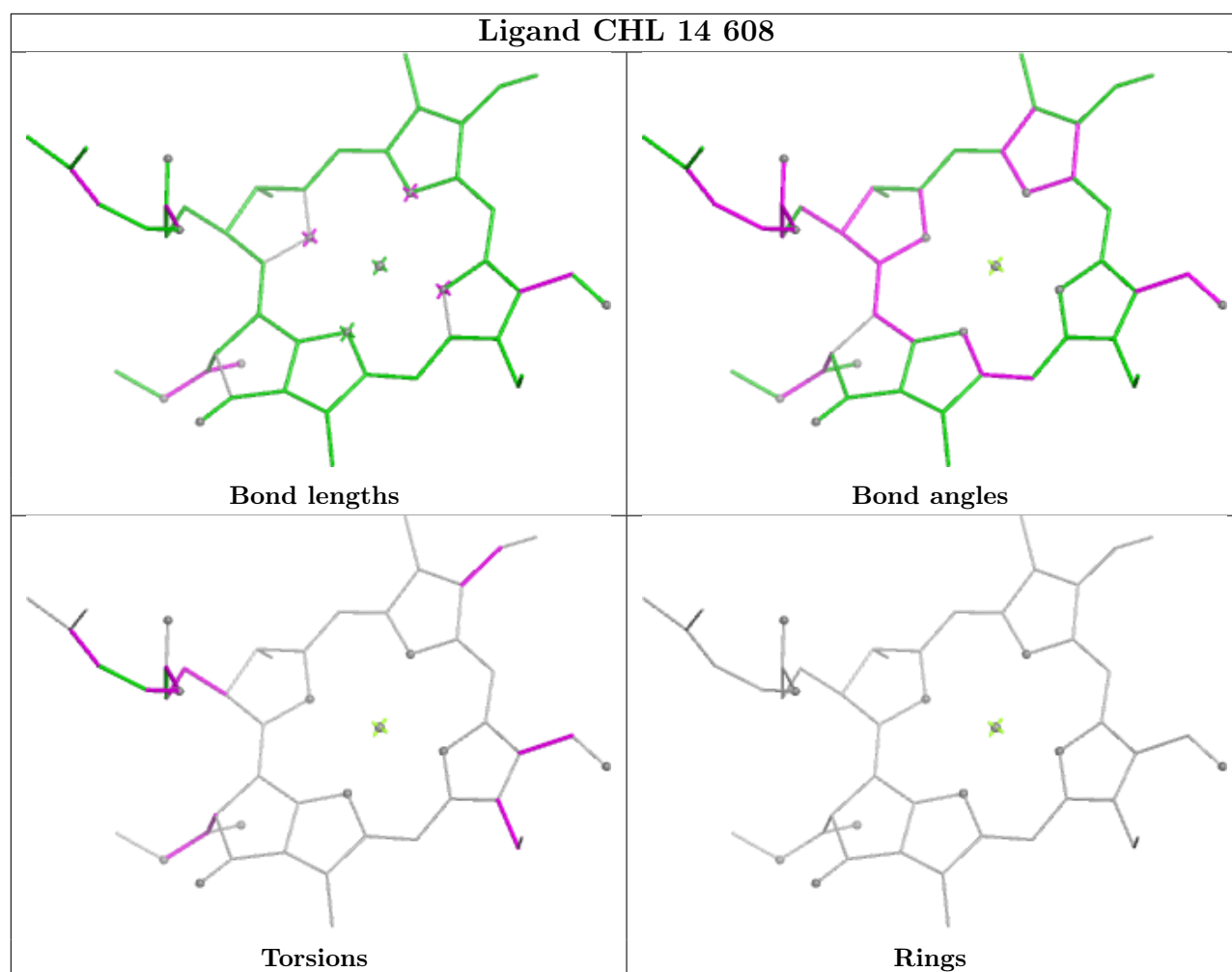
Ligand CLA n 614

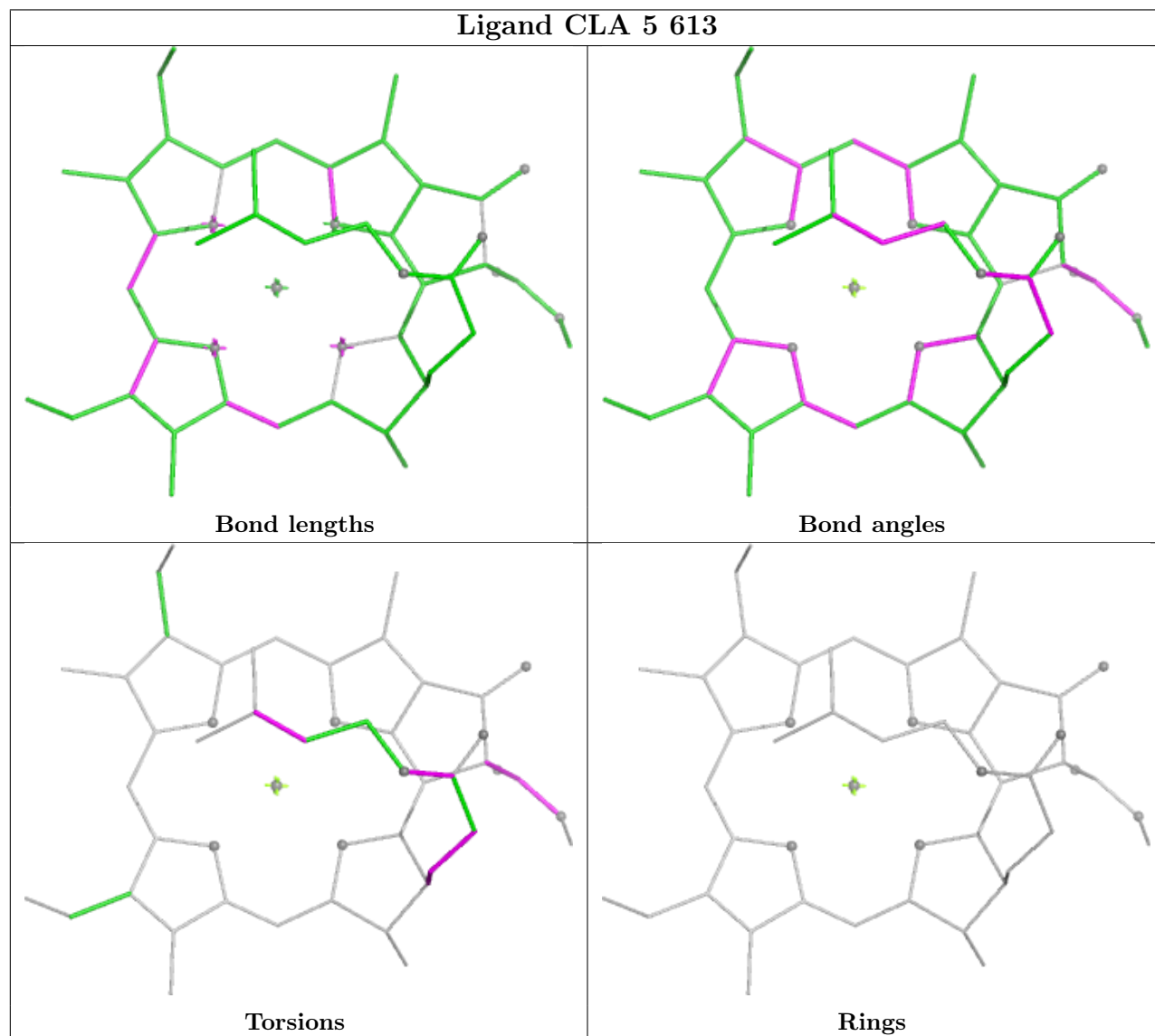
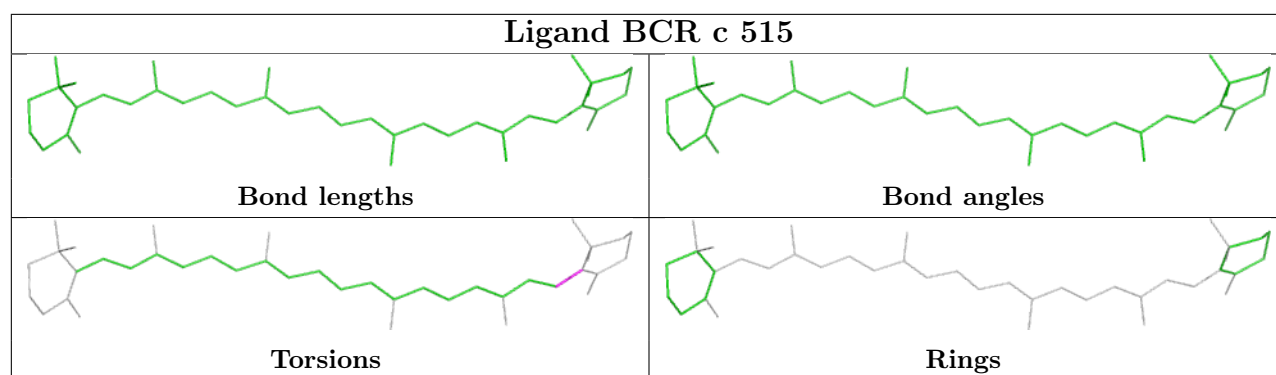


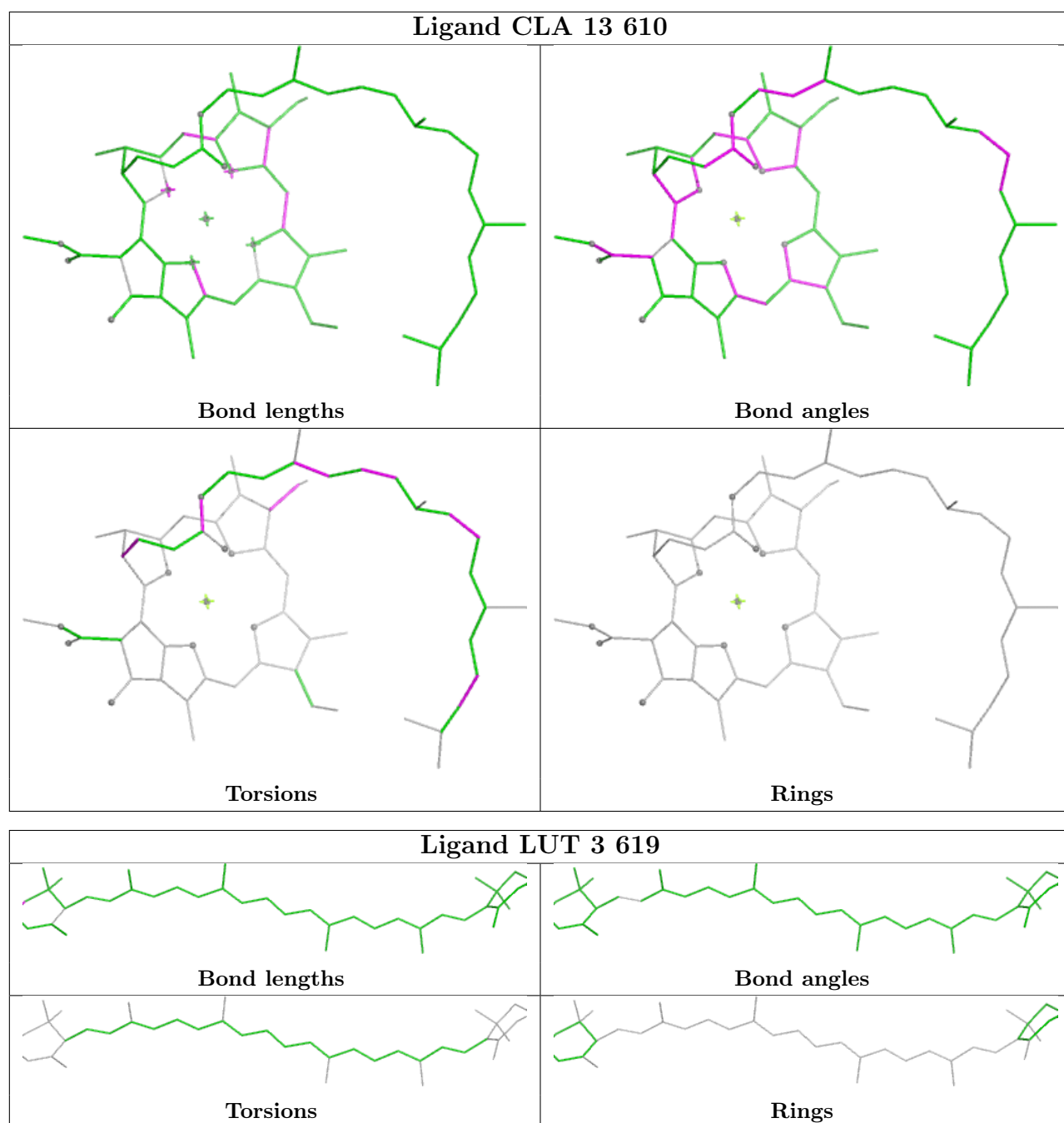
Ligand LUT G 617



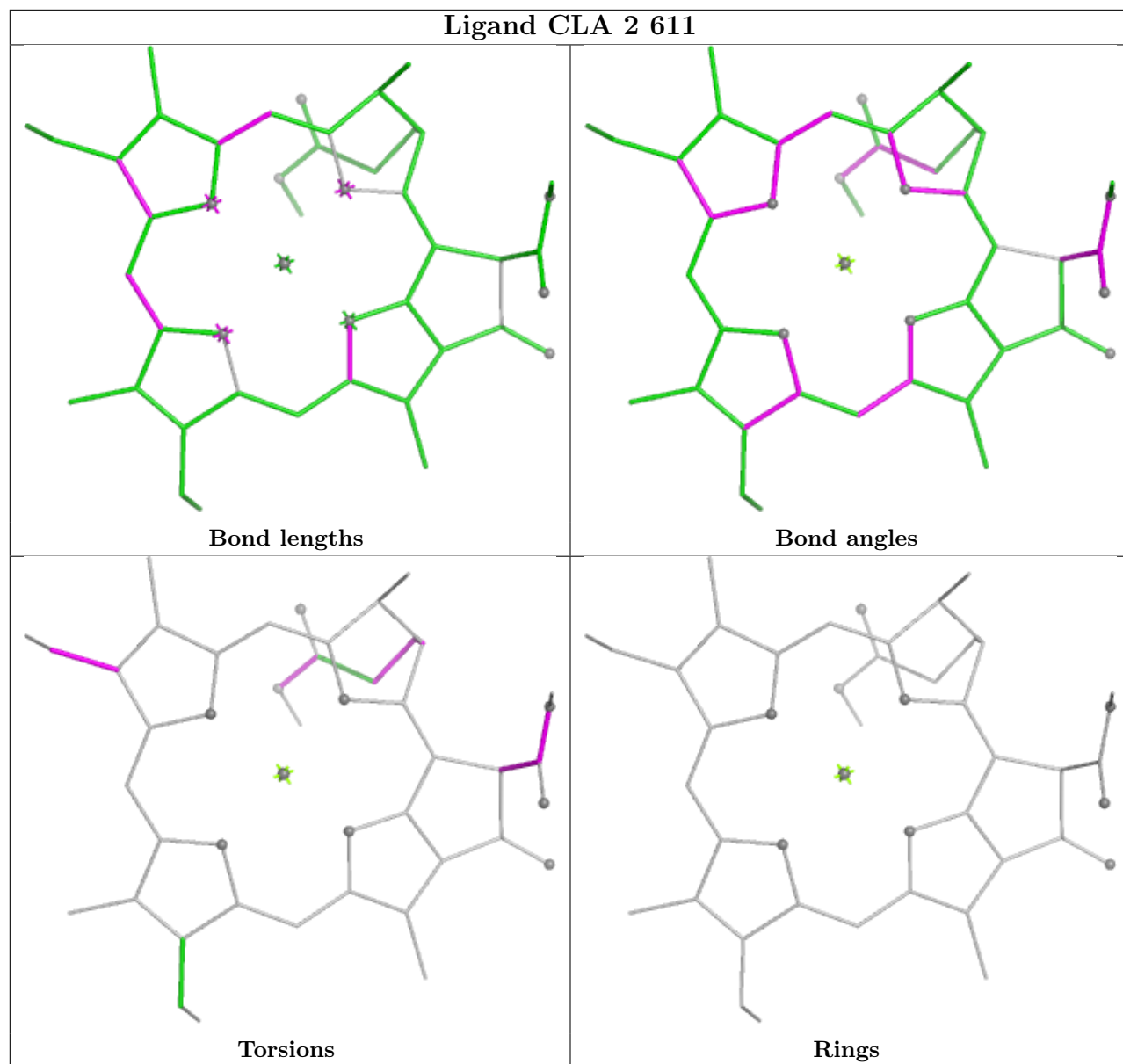


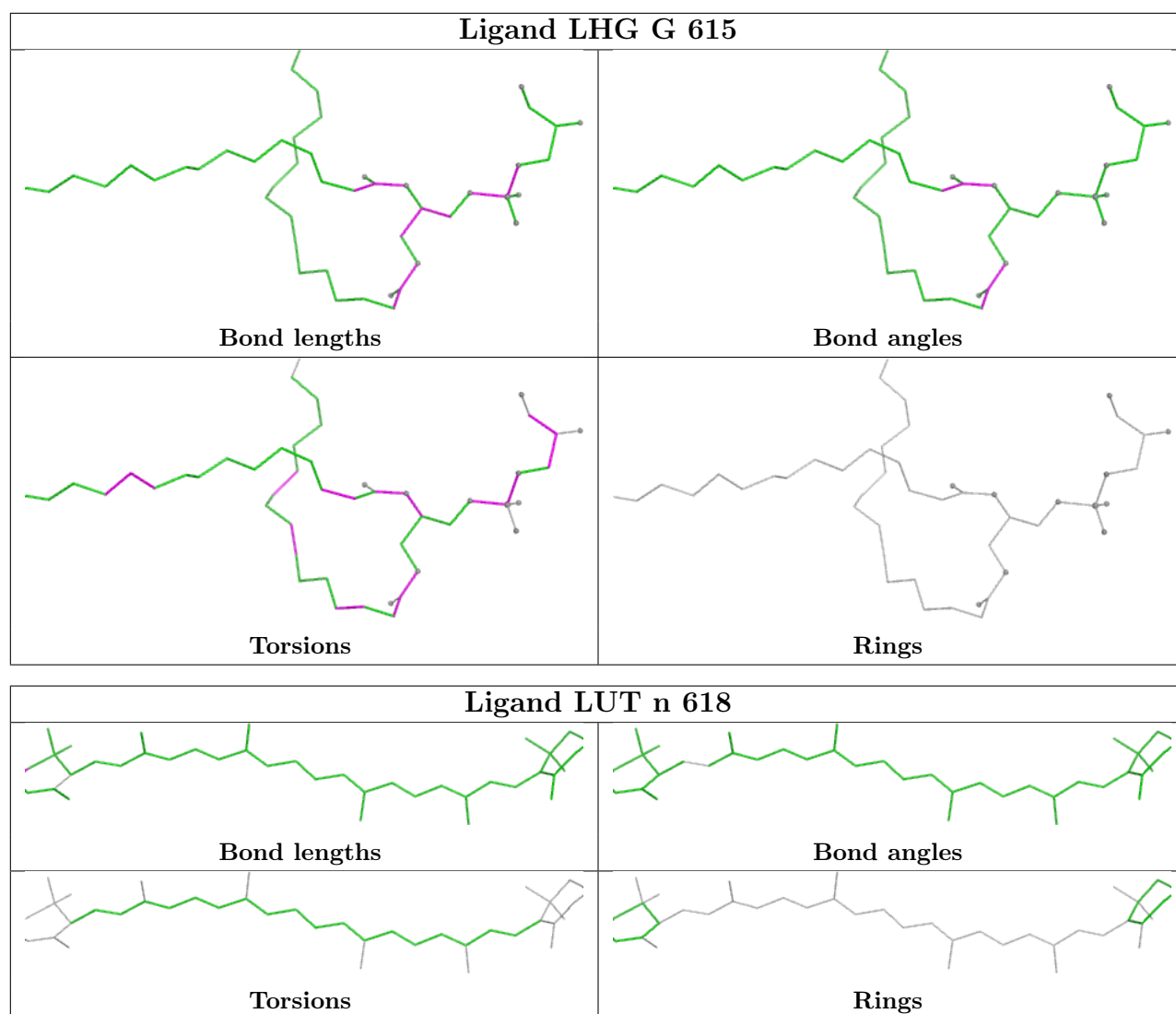




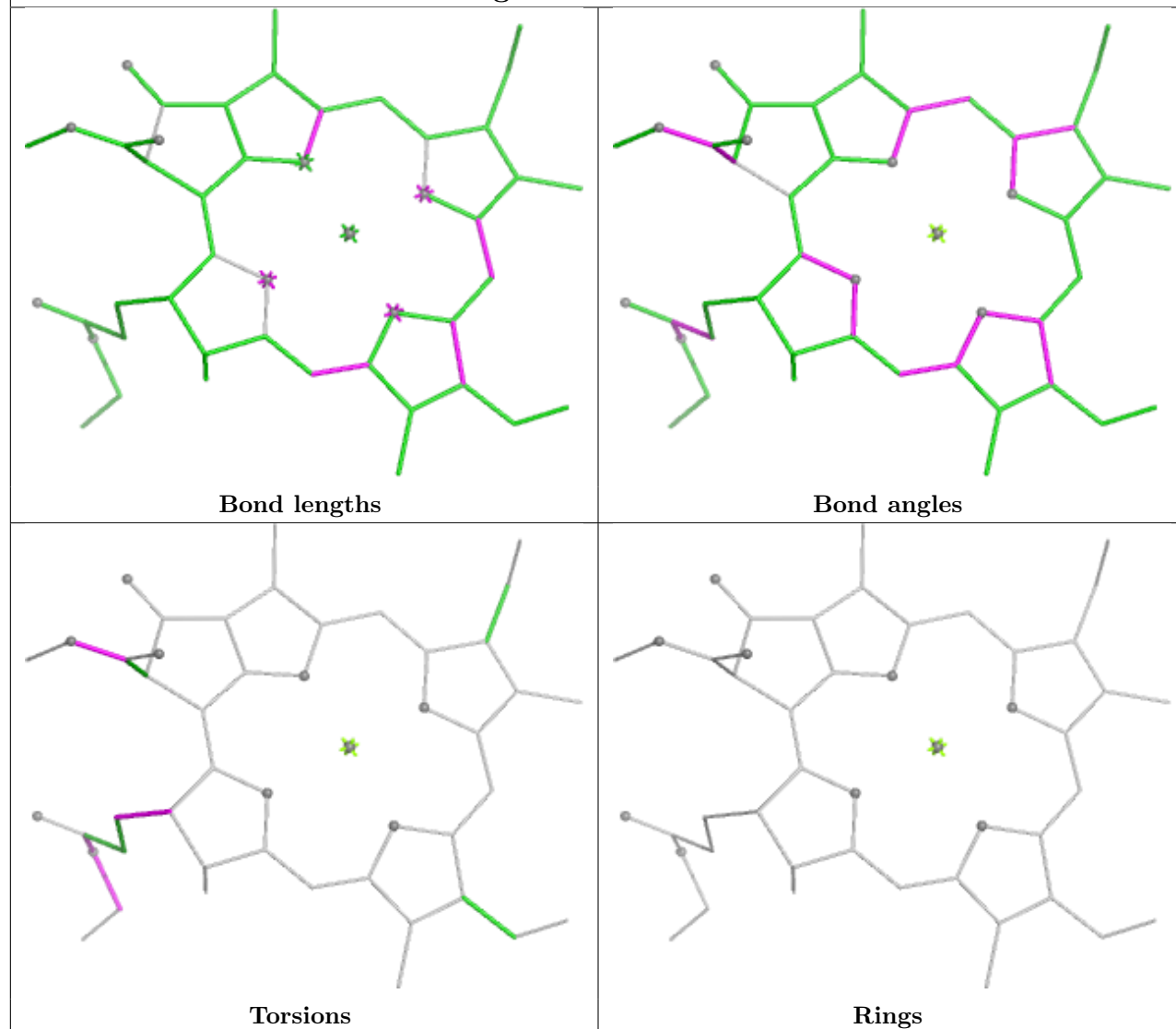


Ligand CLA 2 611

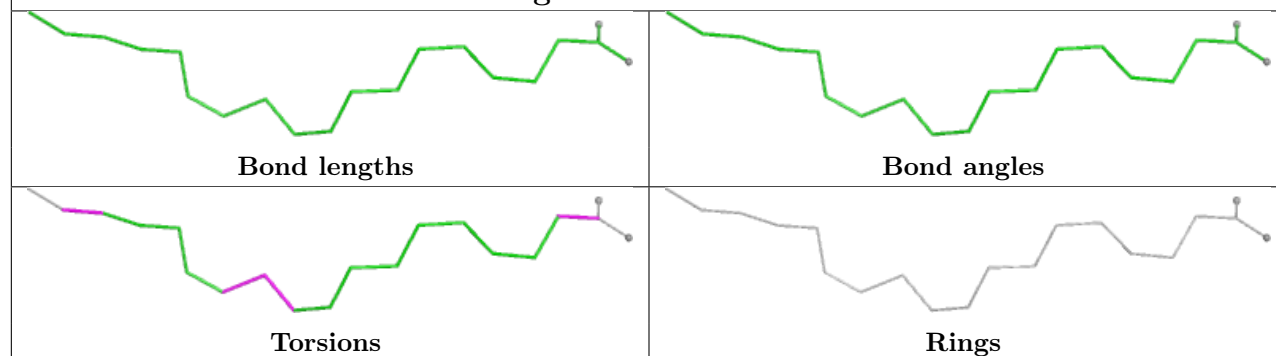


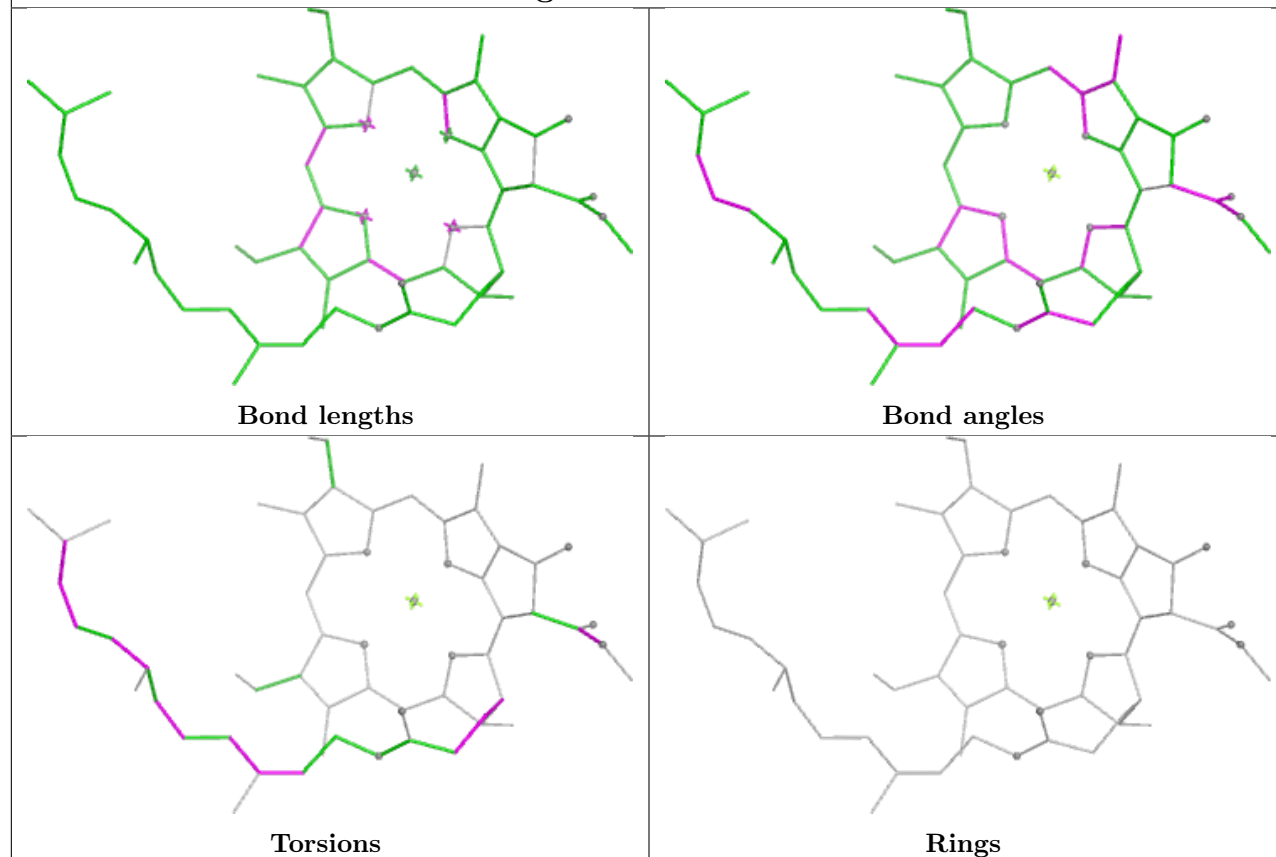
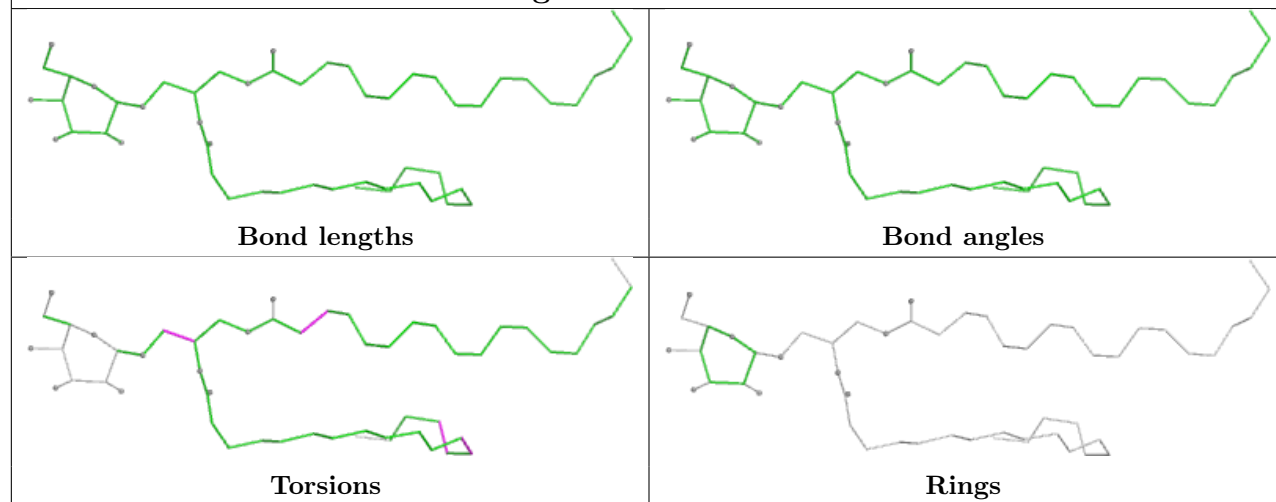


Ligand CLA S 615

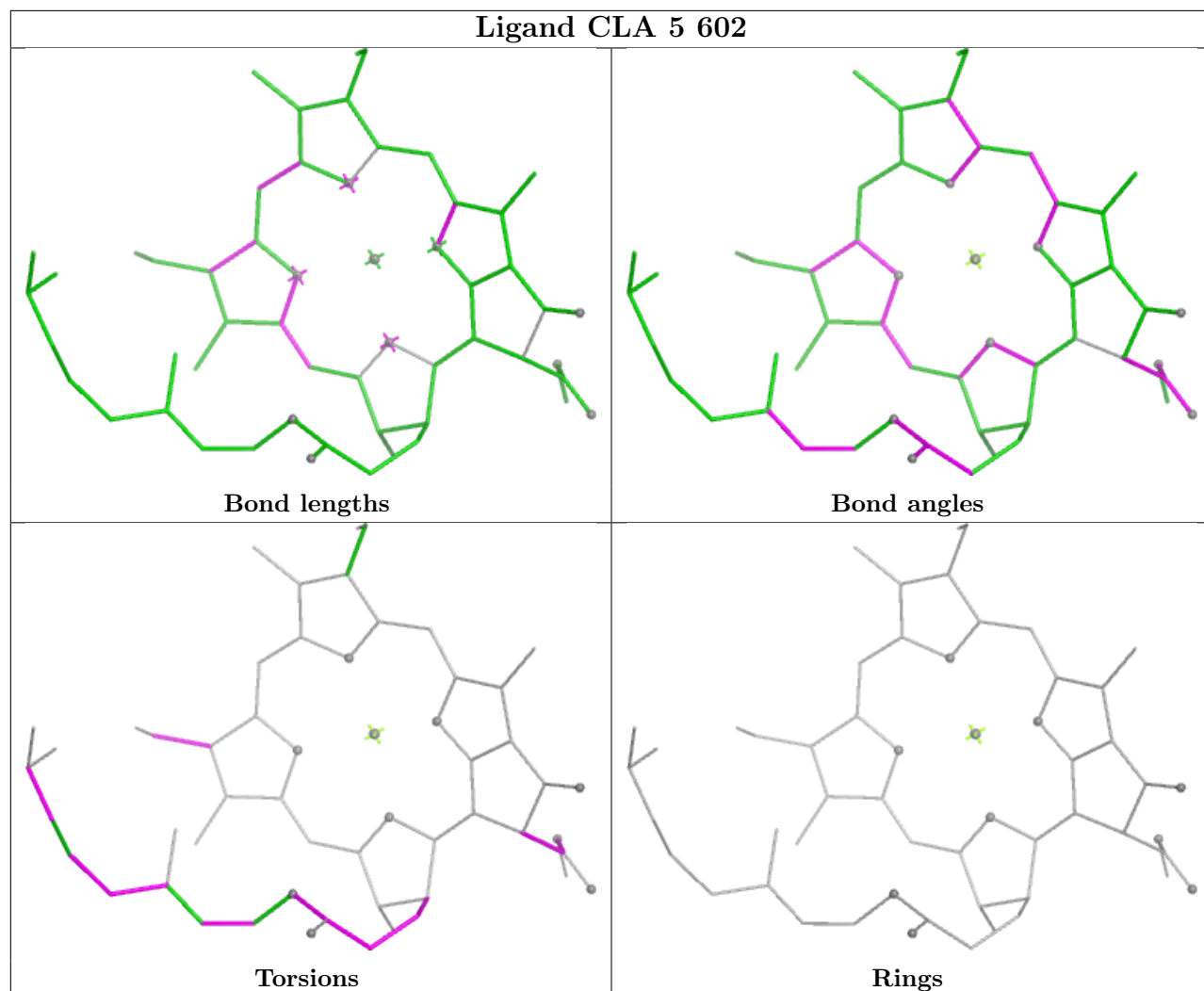


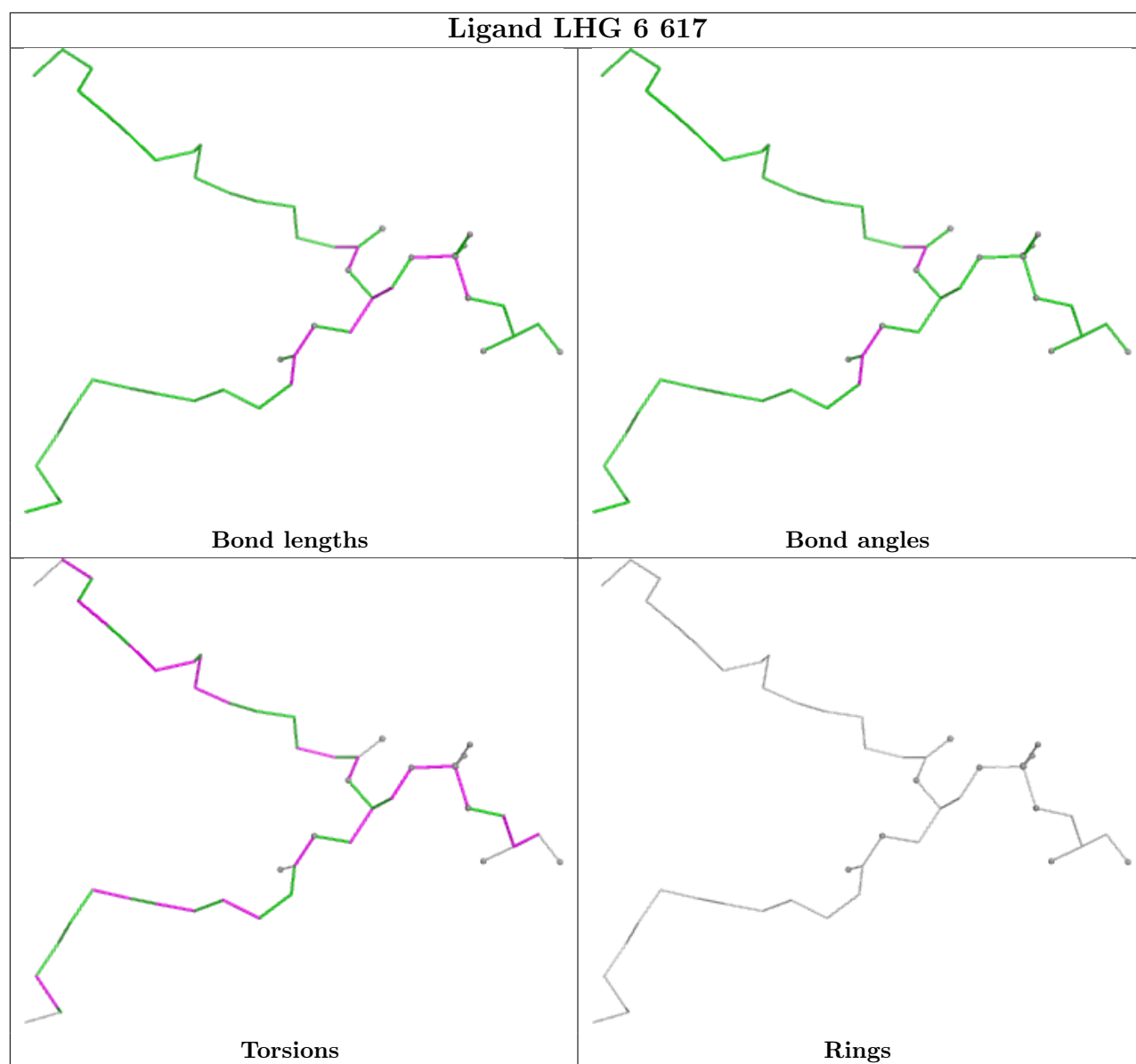
Ligand LNL Y 620

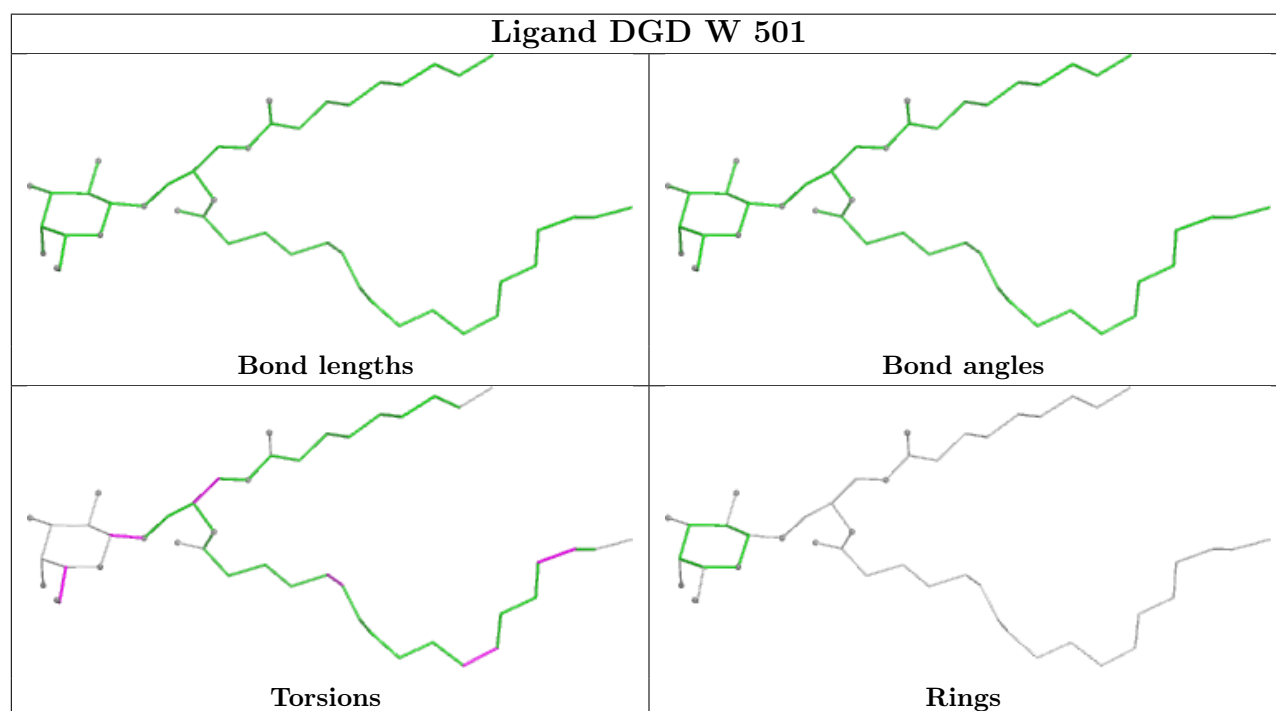
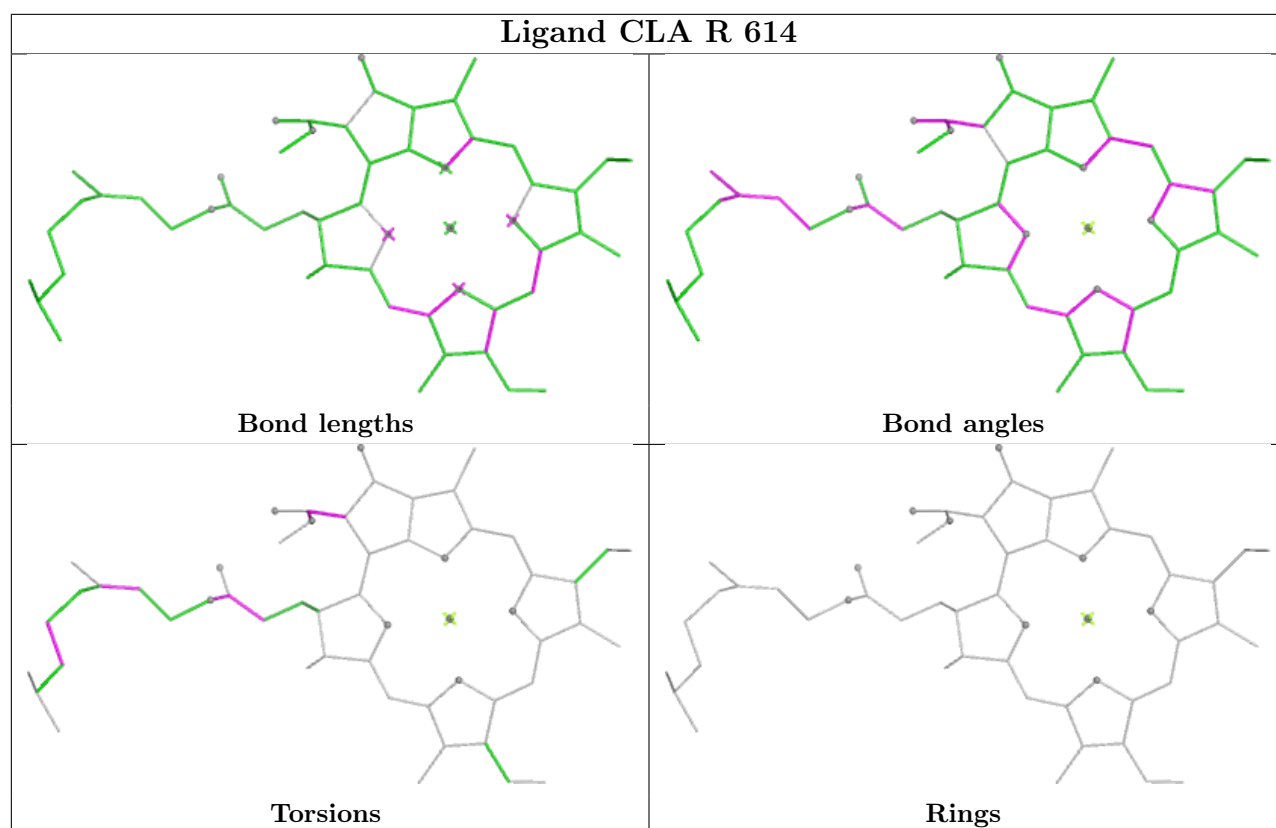


Ligand CLA 6 610**Ligand LMG c 522**

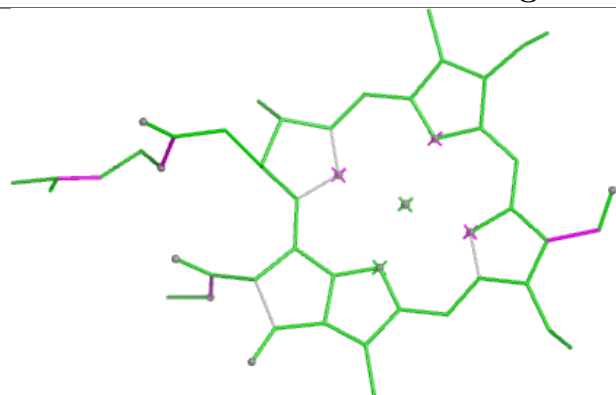
Ligand CLA 5 602



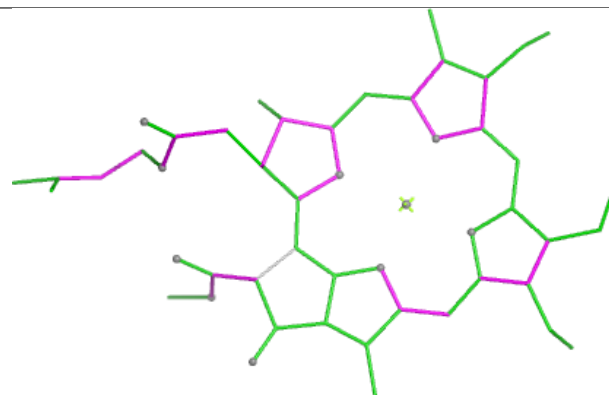




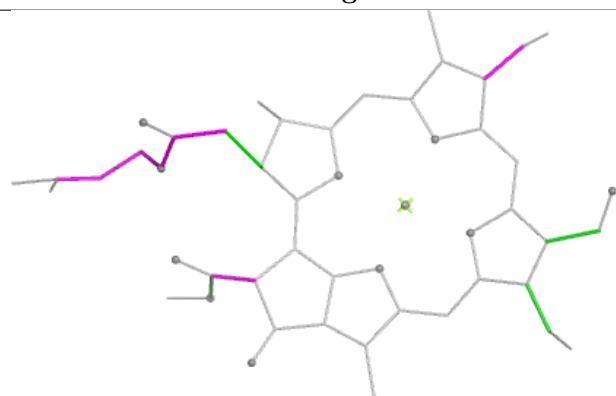
Ligand CHL 4 607



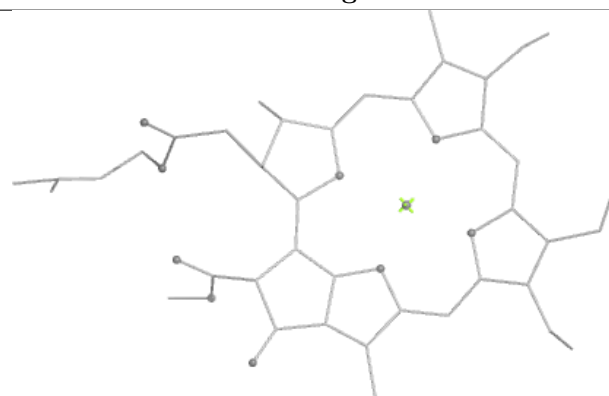
Bond lengths



Bond angles

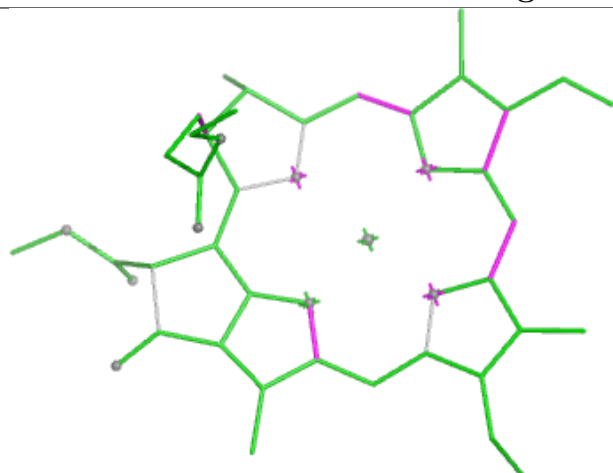


Torsions

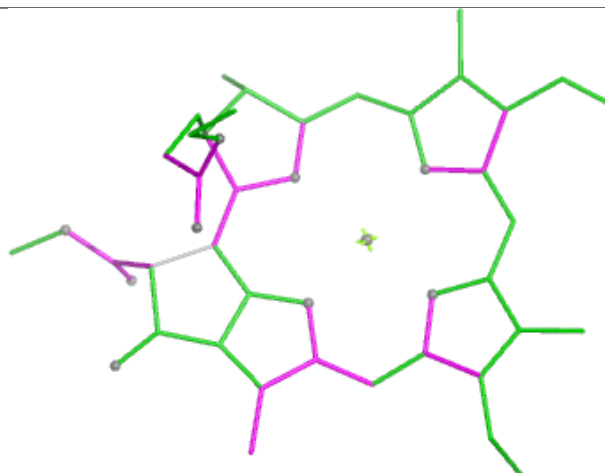


Rings

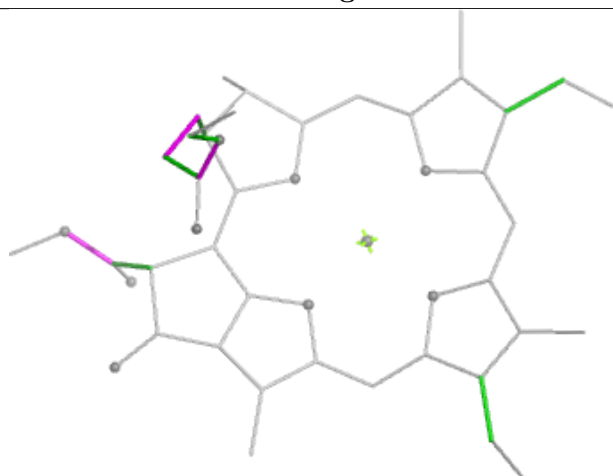
Ligand CLA n 615



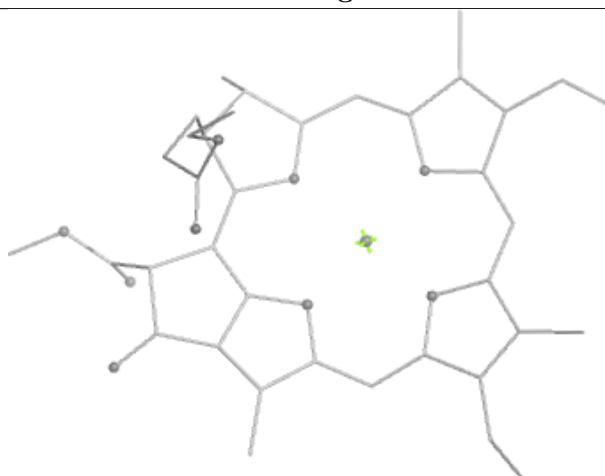
Bond lengths



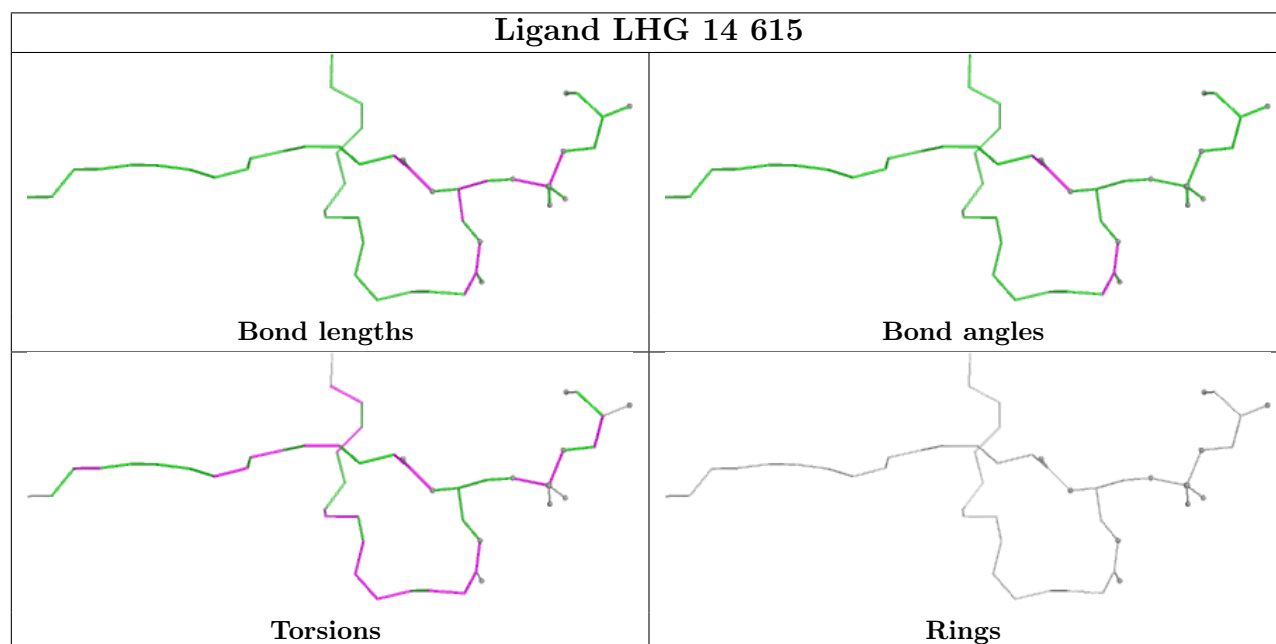
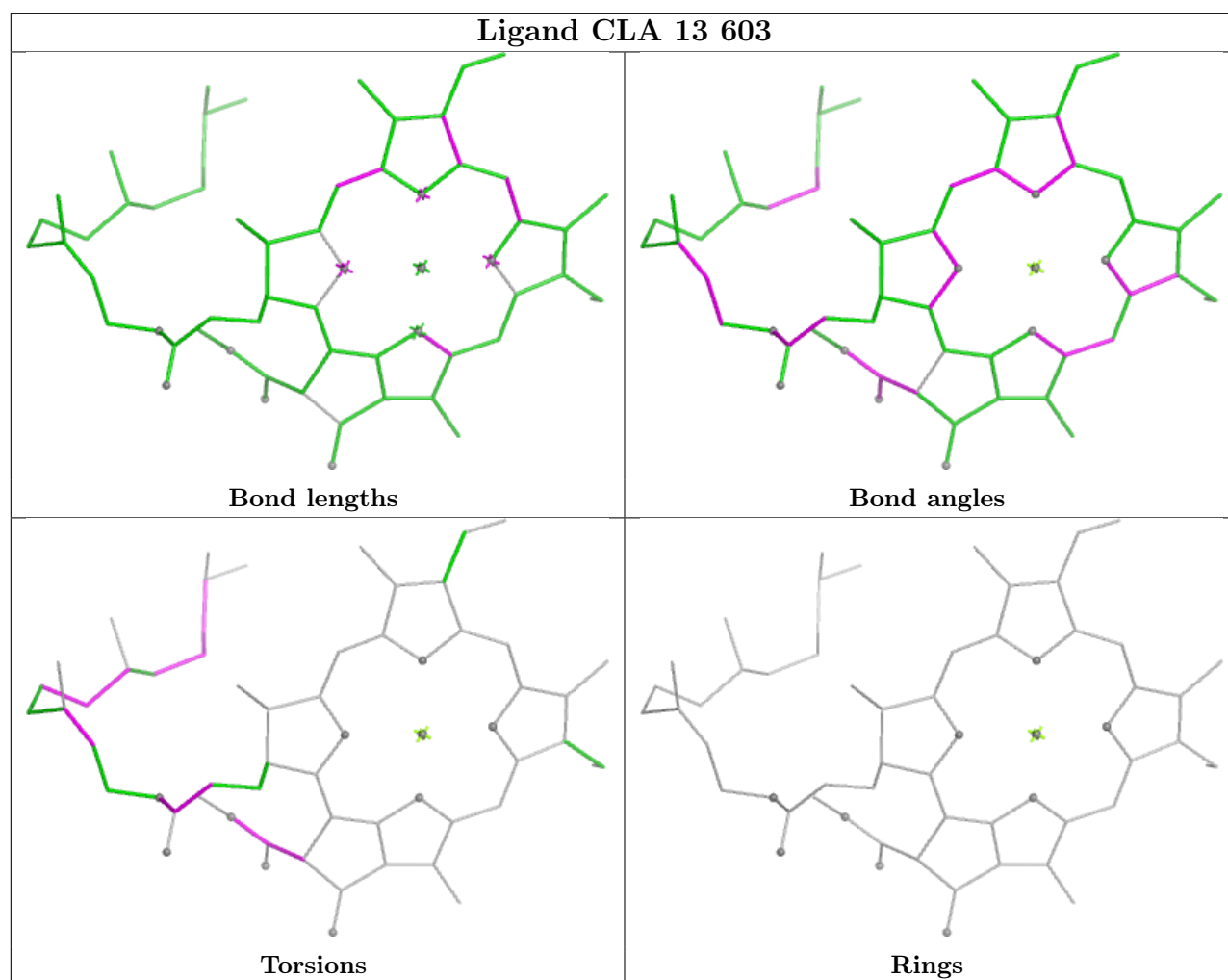
Bond angles

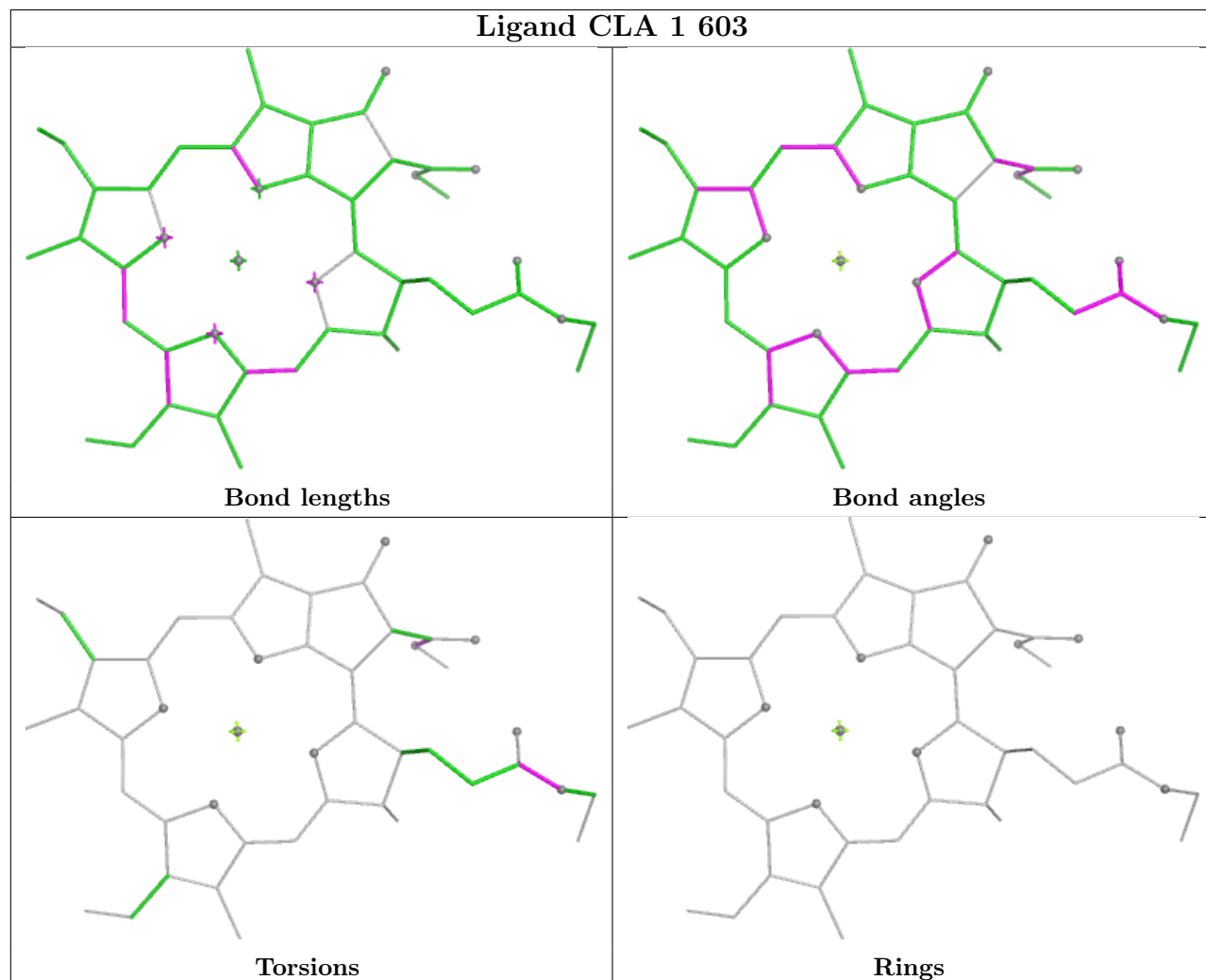
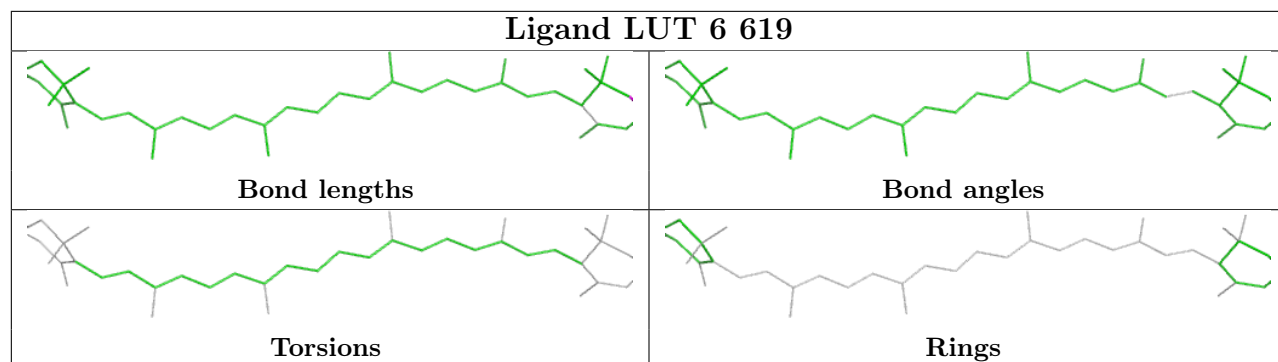


Torsions

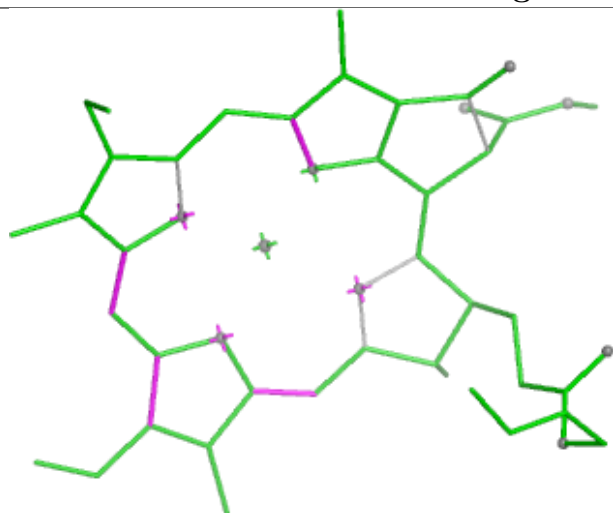


Rings

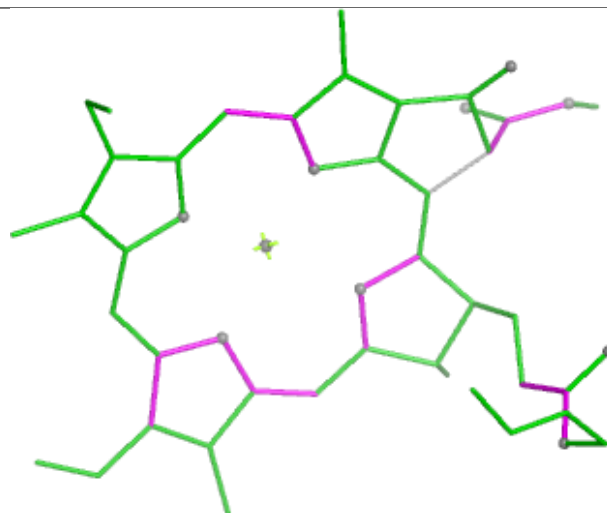




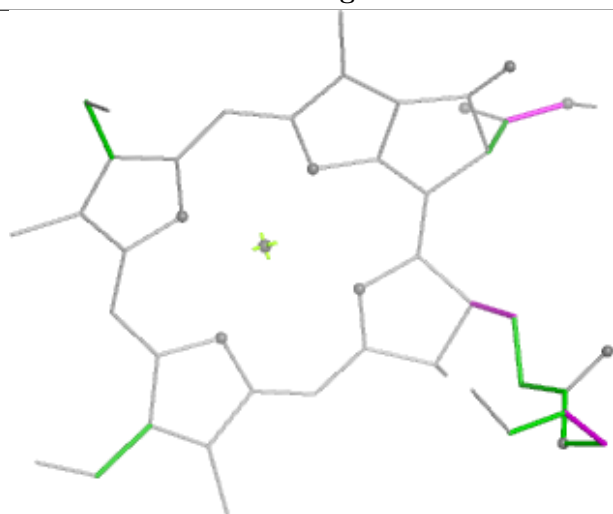
Ligand CLA G 614



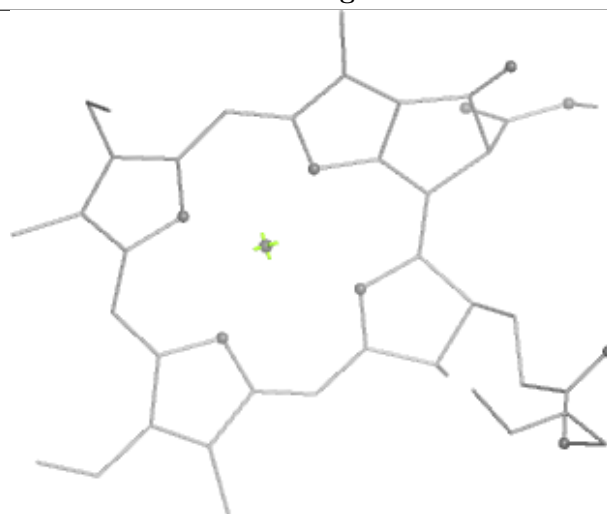
Bond lengths



Bond angles

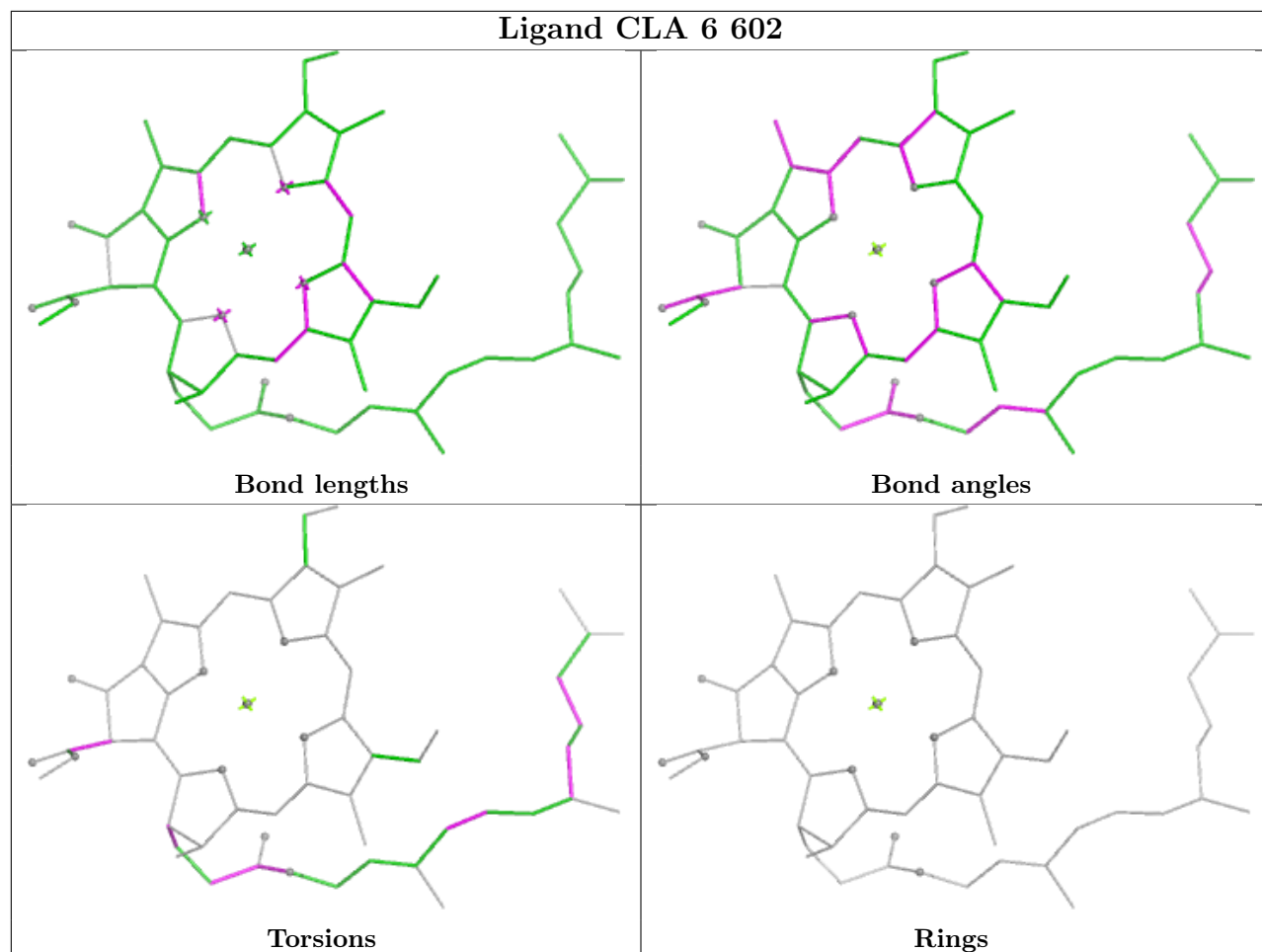


Torsions

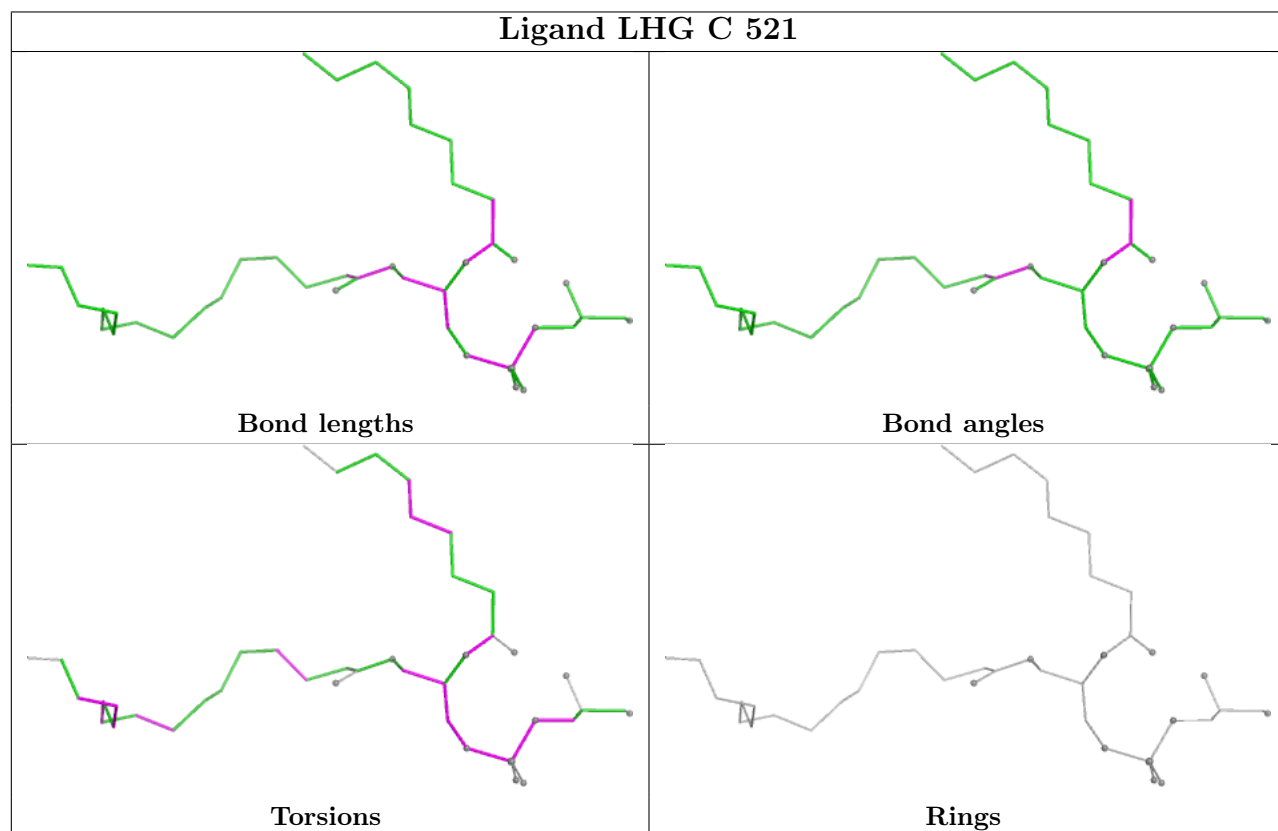


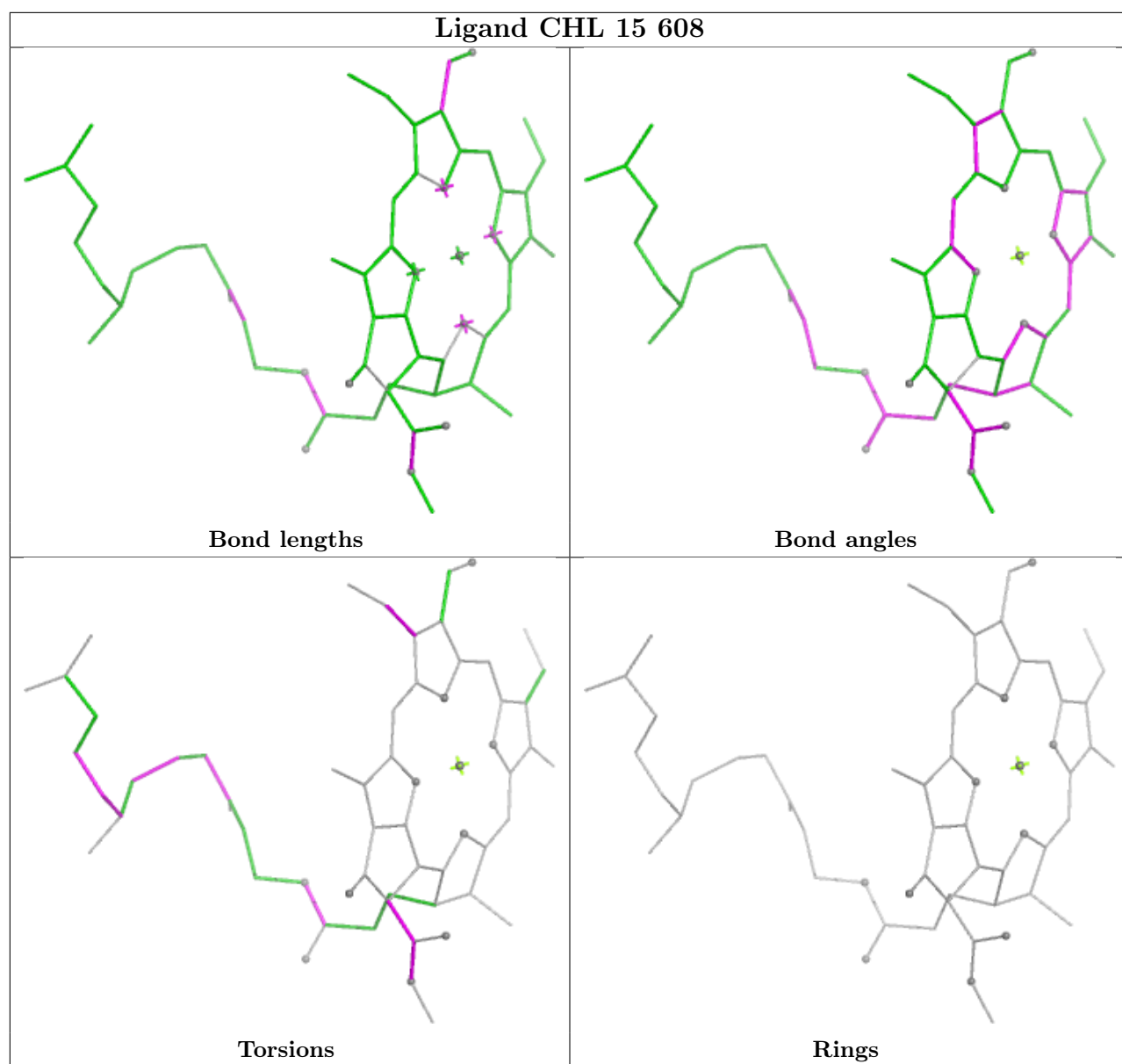
Rings

Ligand CLA 6 602

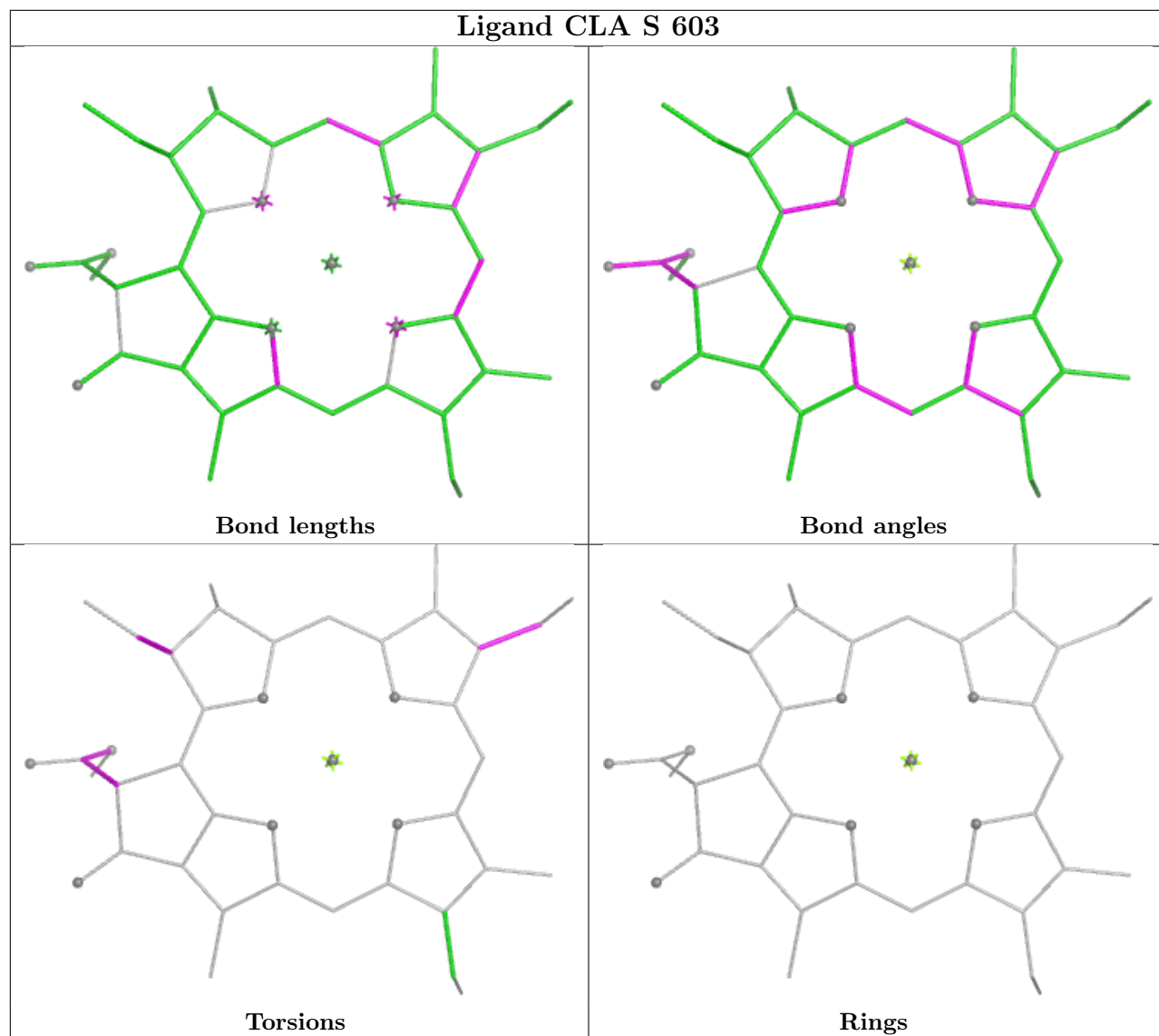


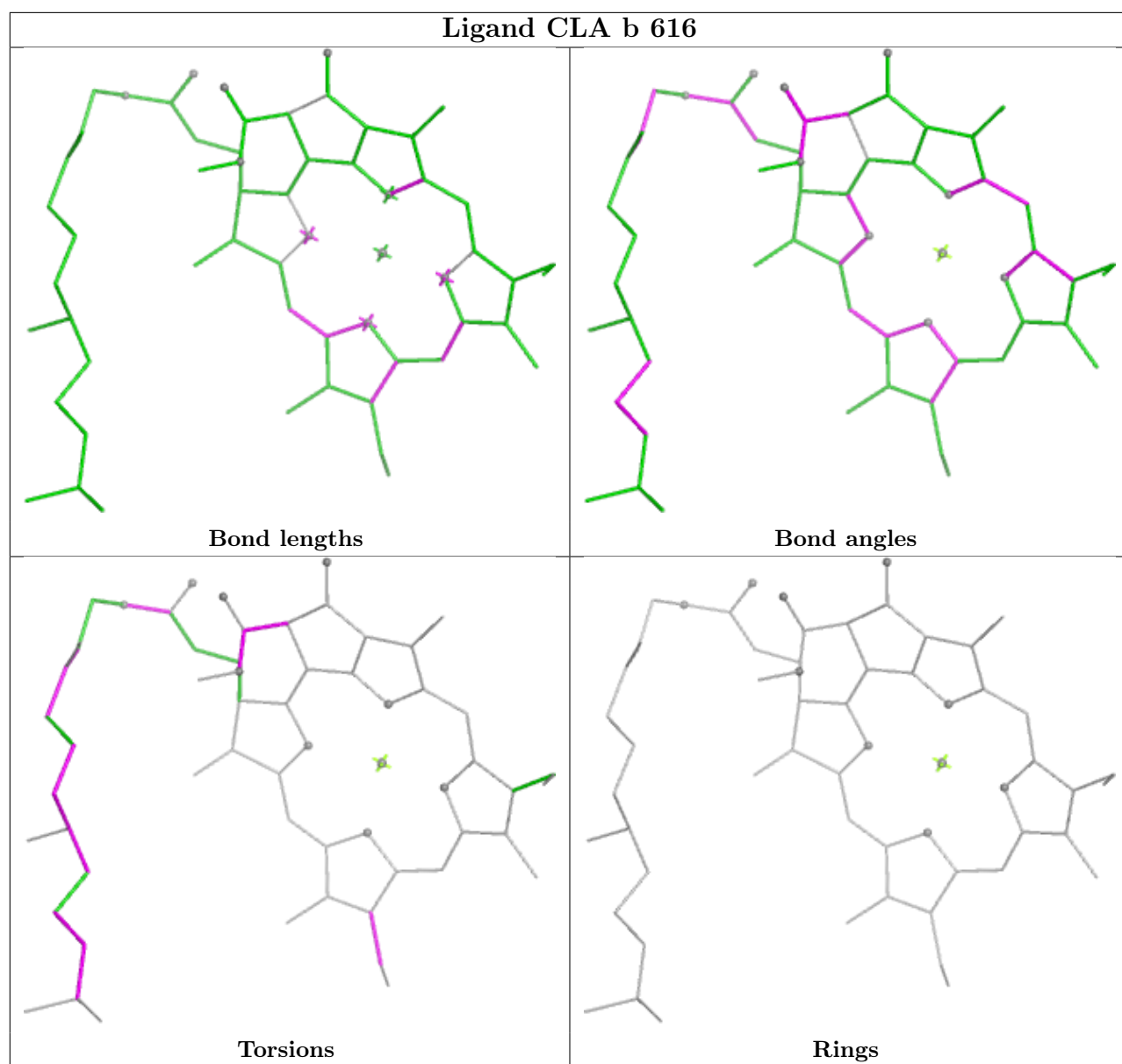
Ligand LHG C 521



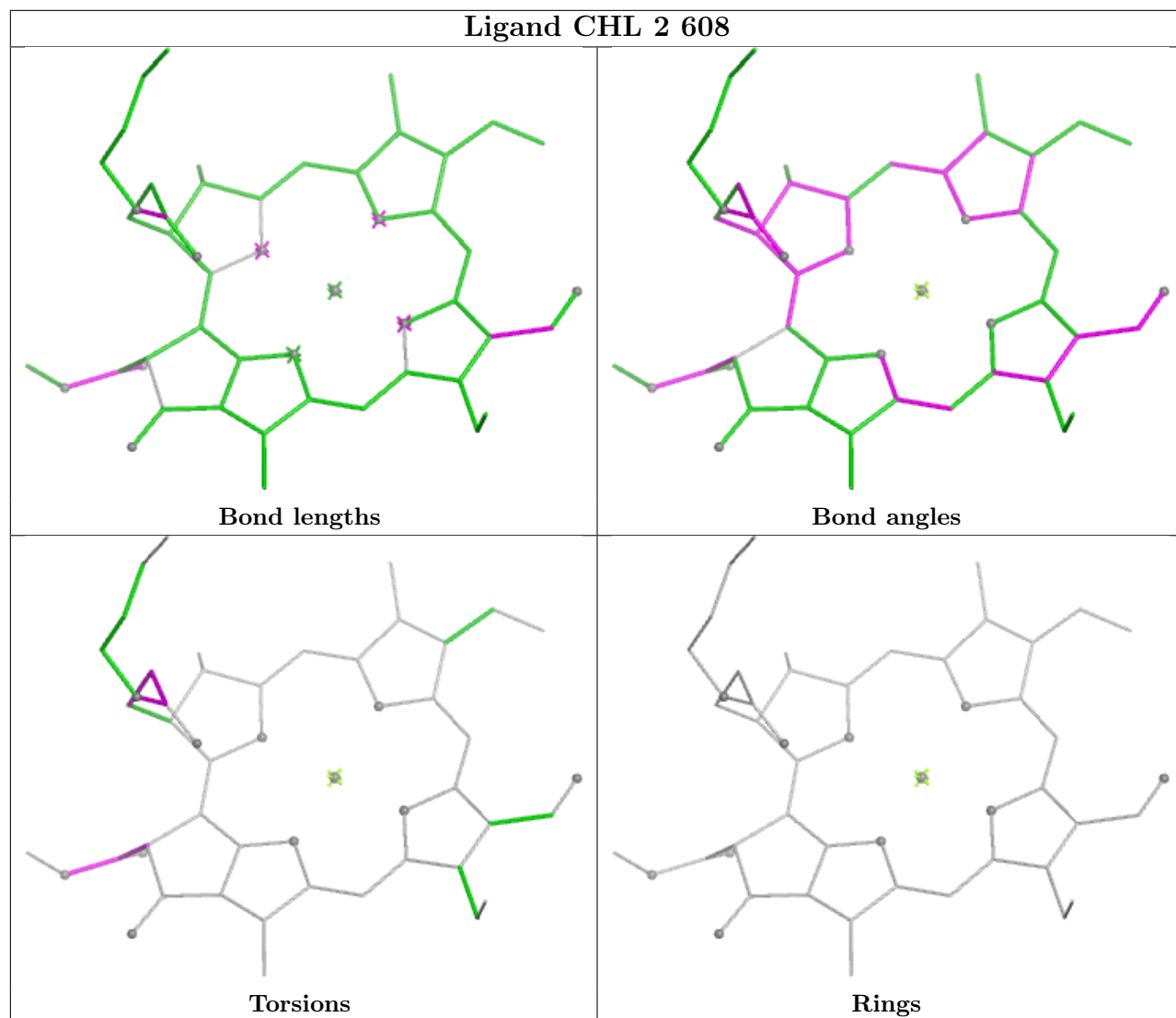


Ligand CLA S 603

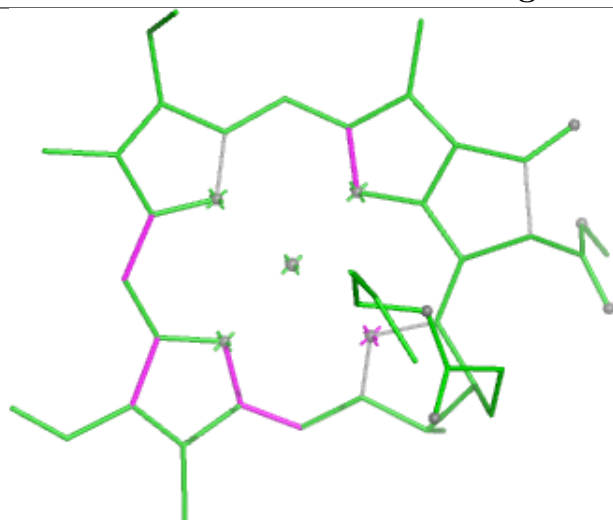




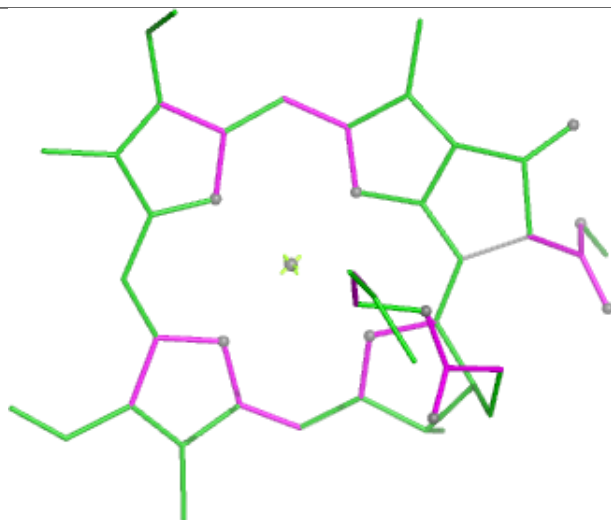
Ligand CHL 2 608



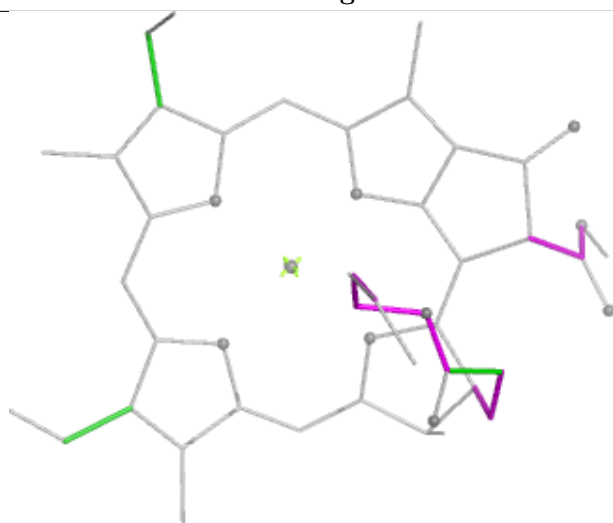
Ligand CLA 6 615



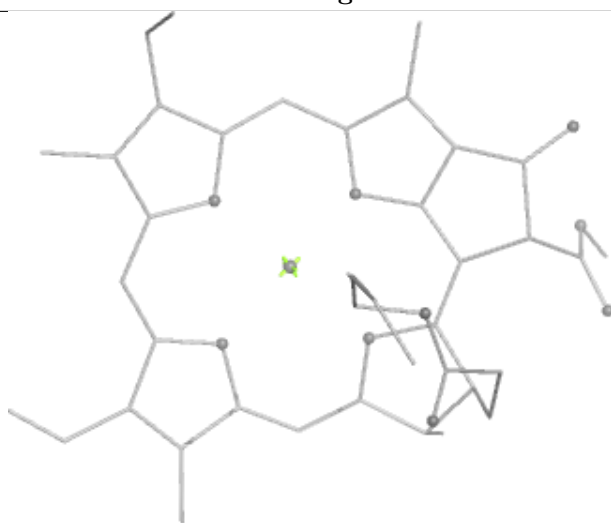
Bond lengths



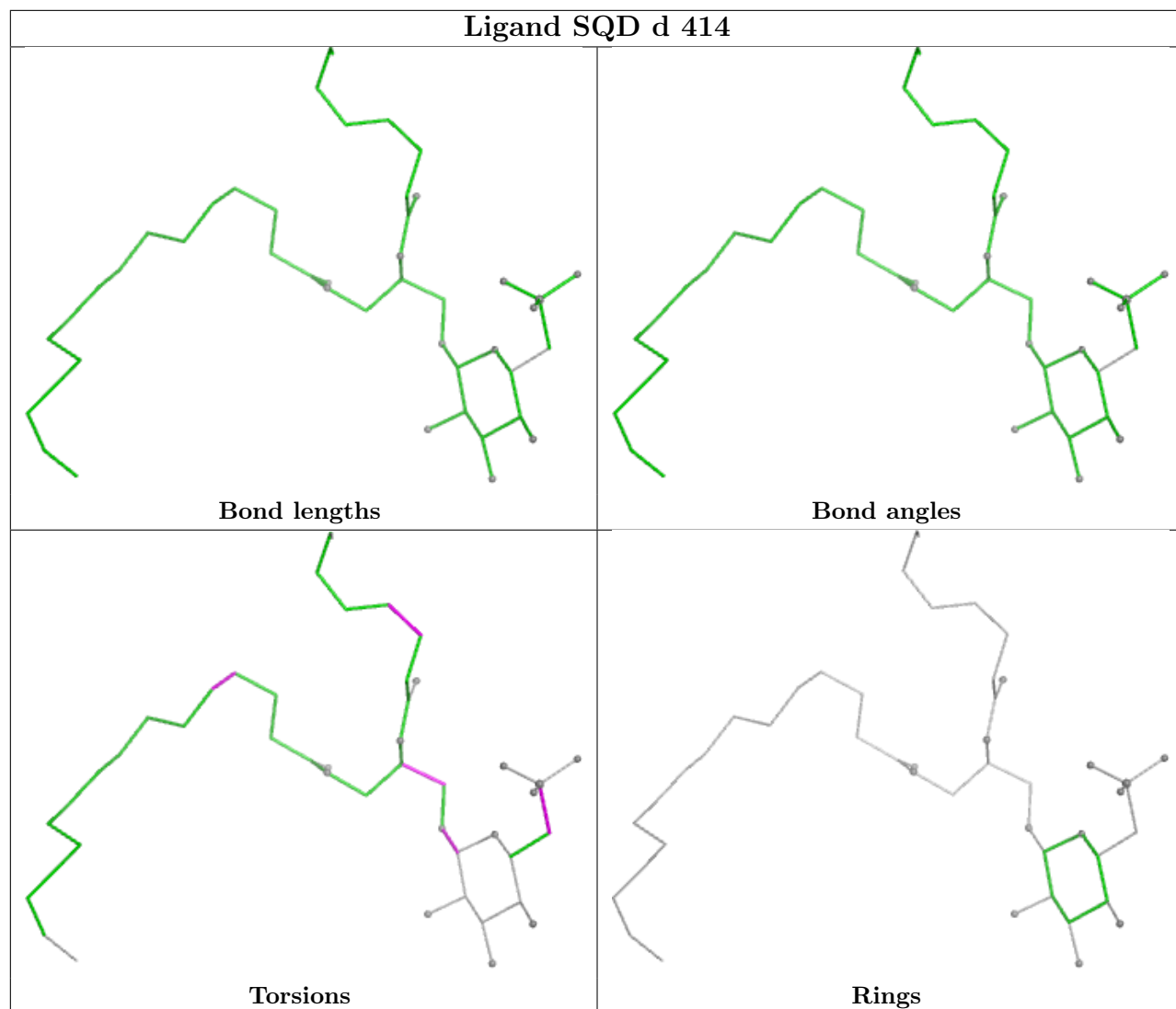
Bond angles



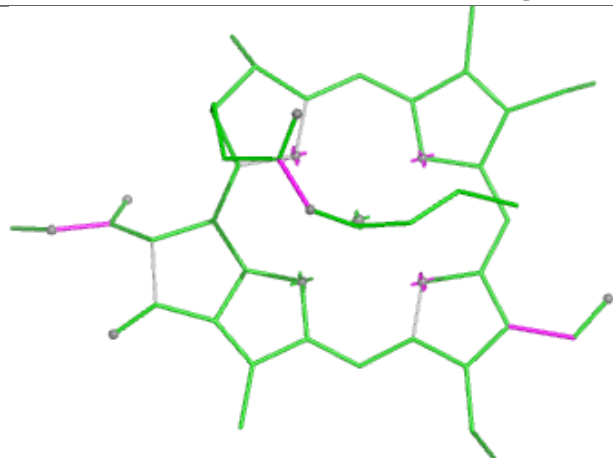
Torsions



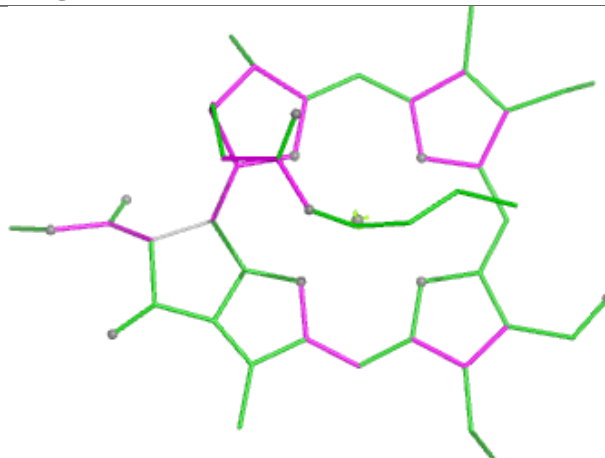
Rings



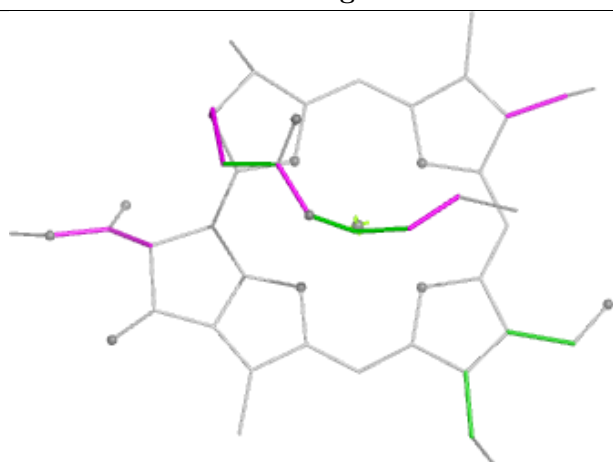
Ligand CHL g 607



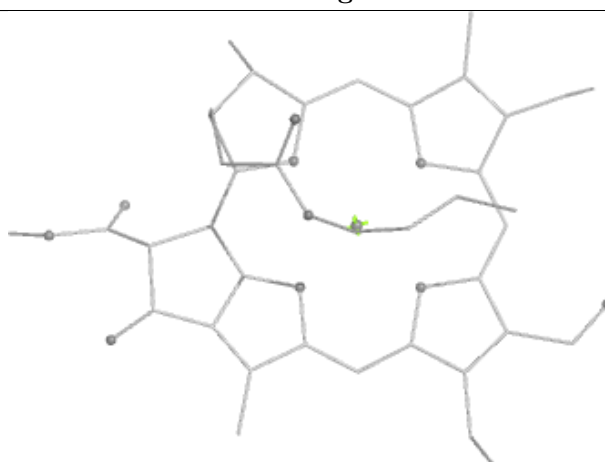
Bond lengths



Bond angles

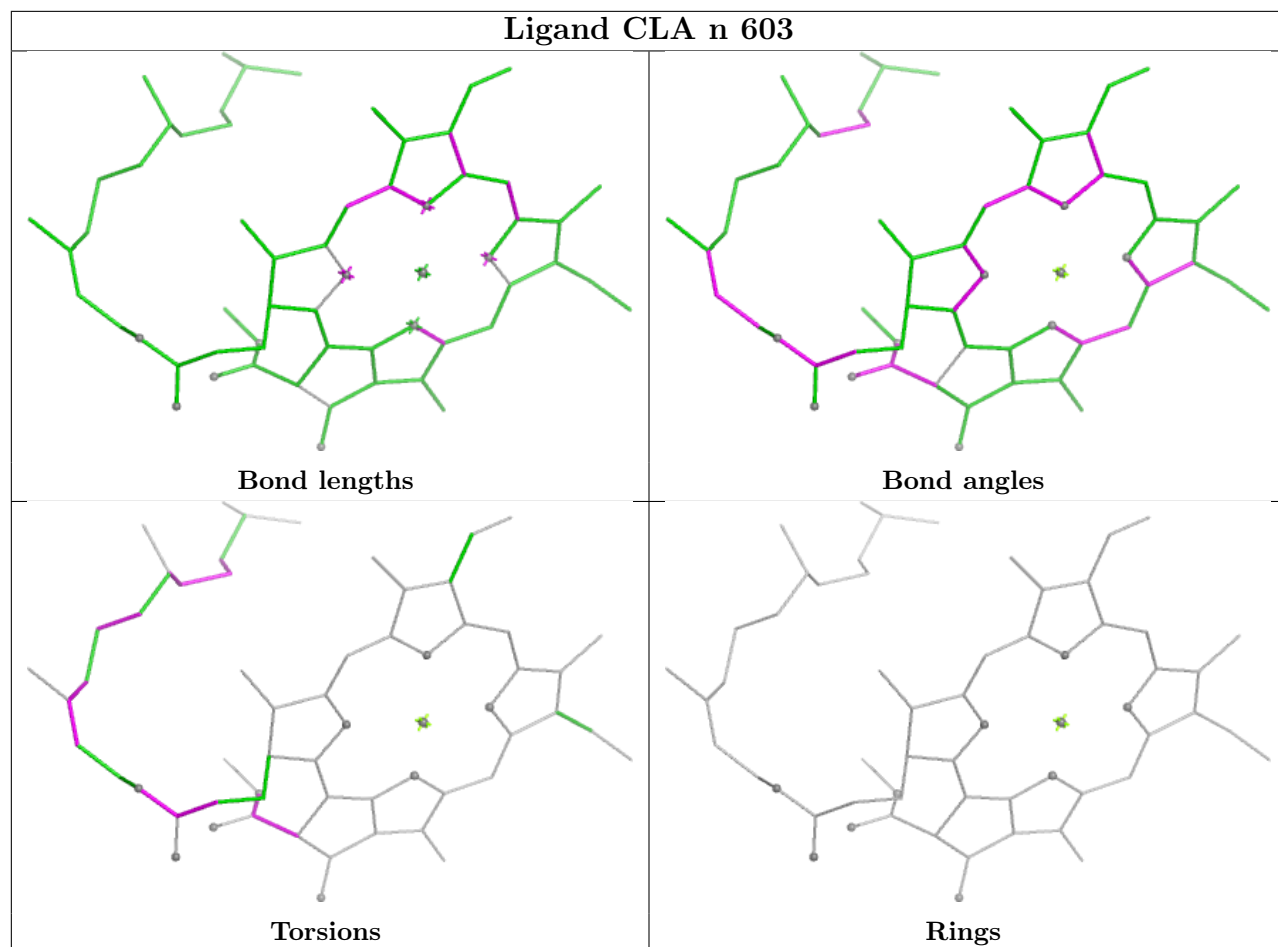


Torsions

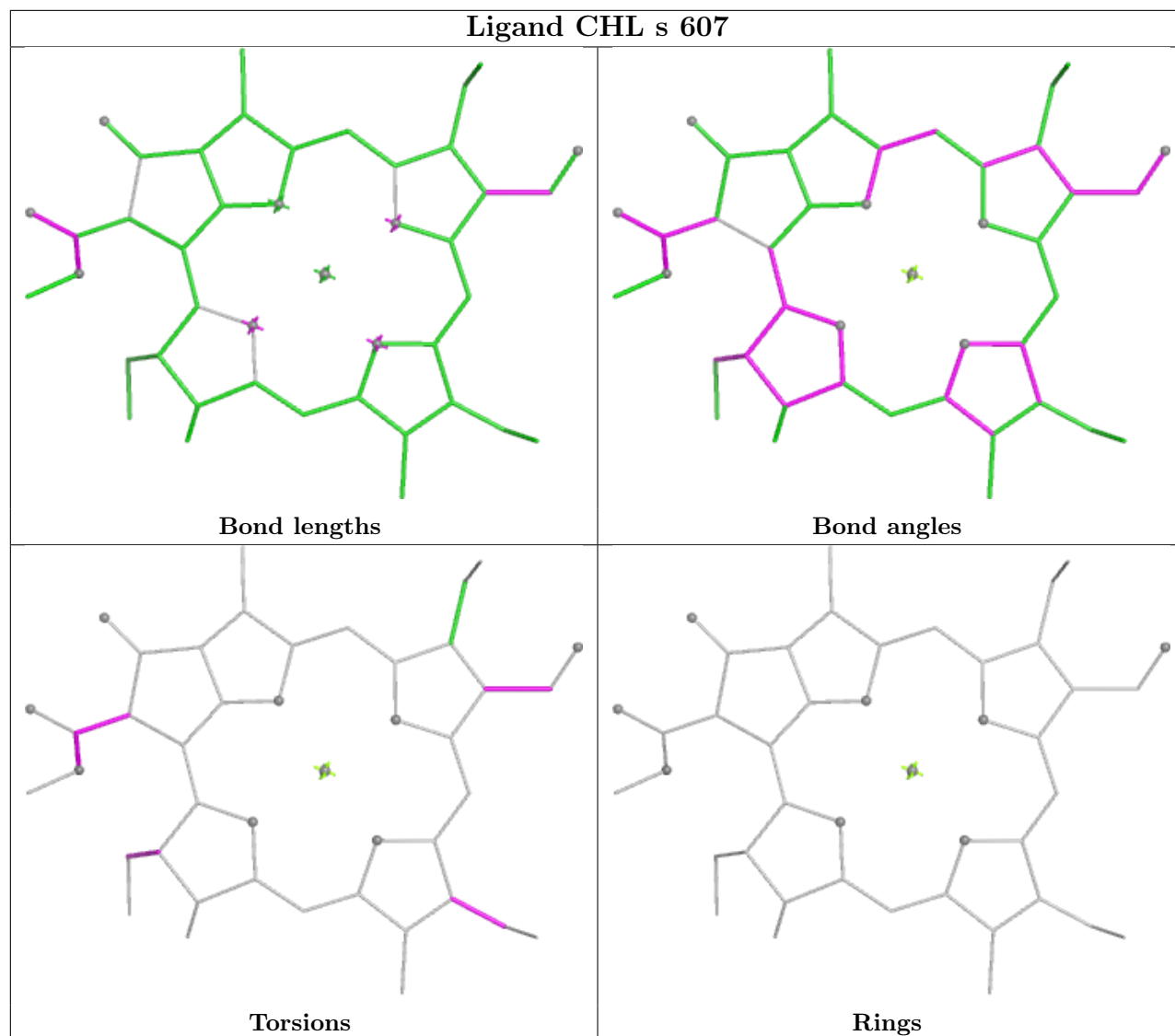


Rings

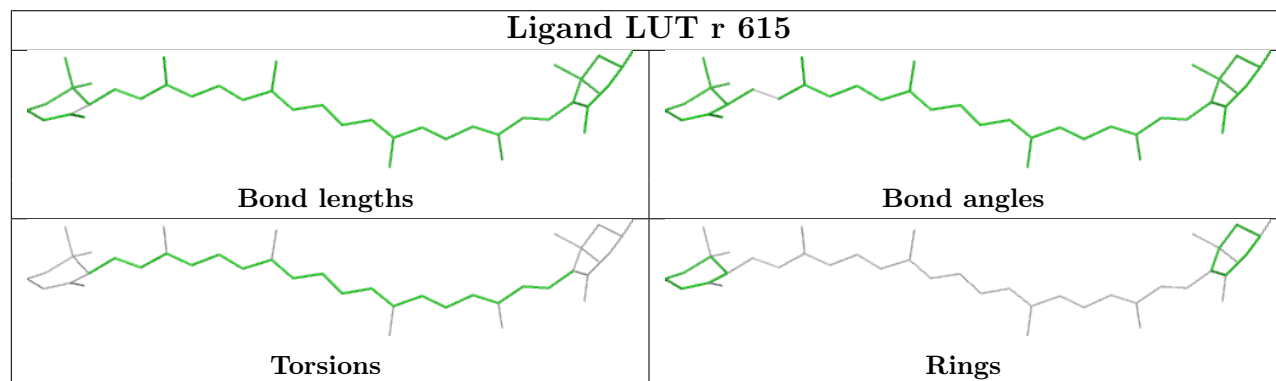
Ligand CLA n 603

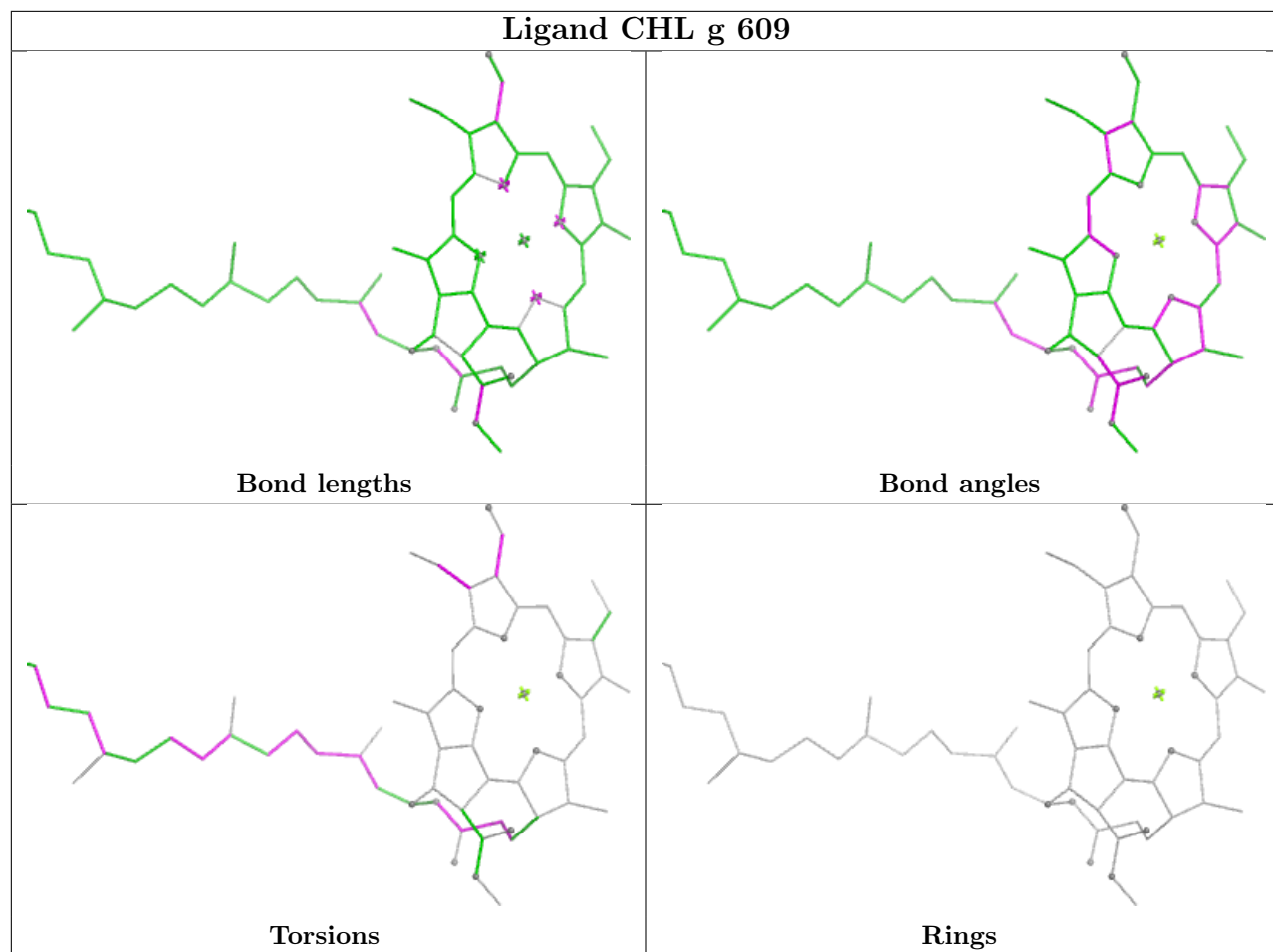


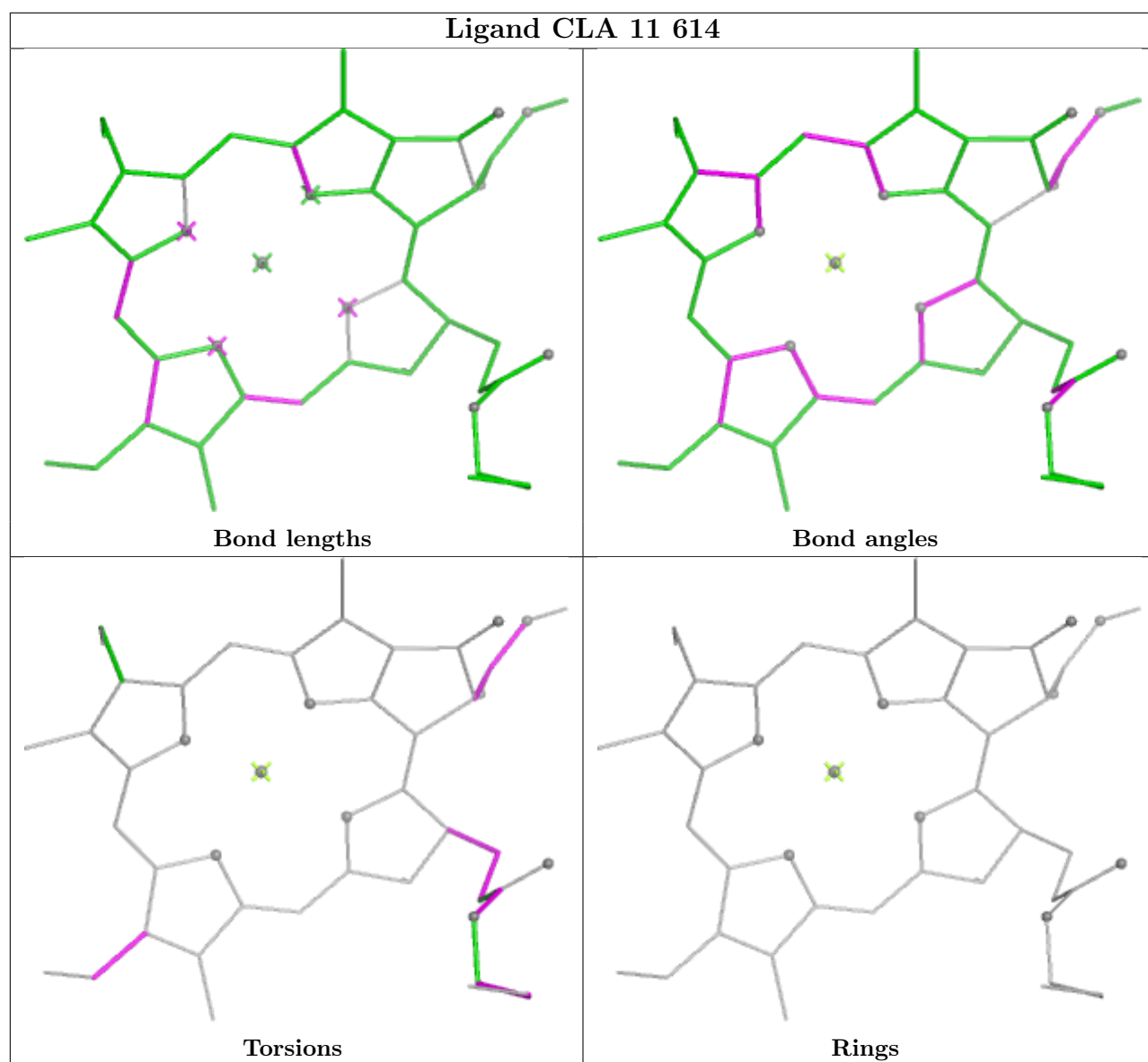
Ligand CHL s 607

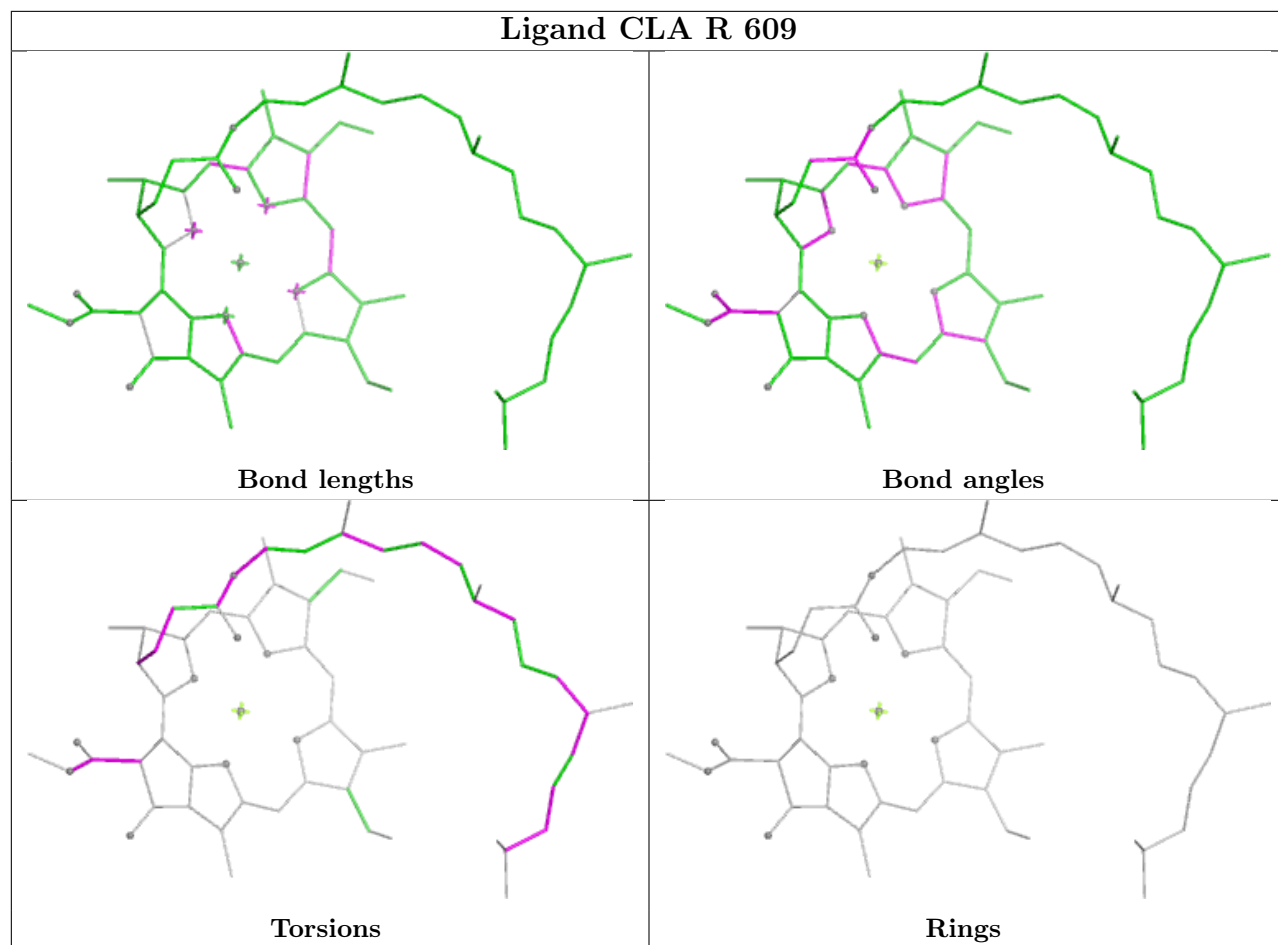


Ligand LUT r 615

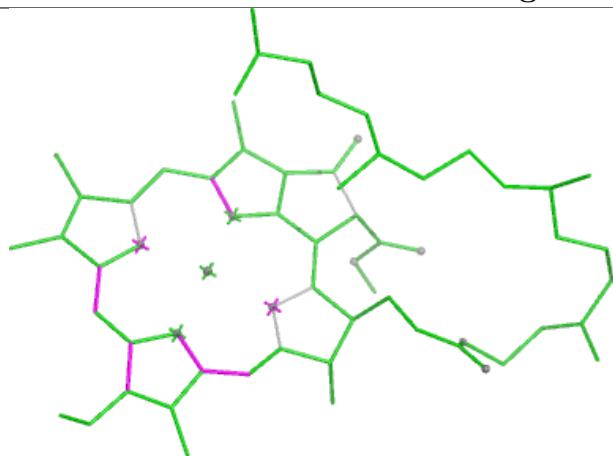




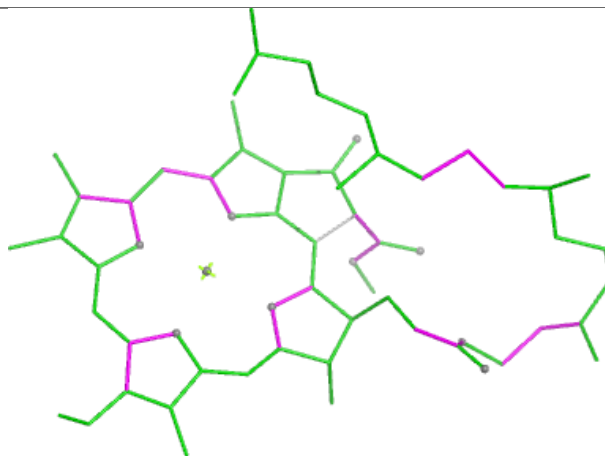




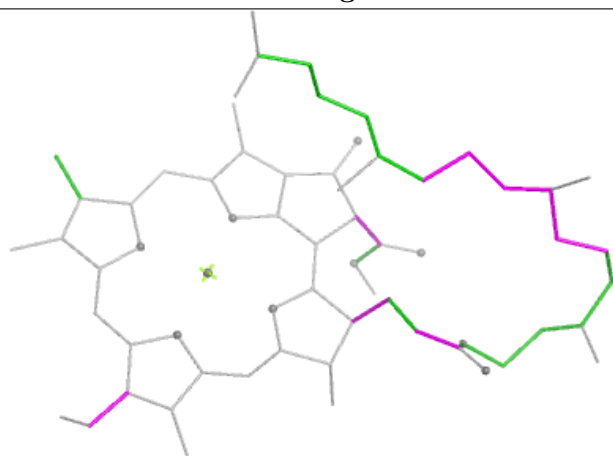
Ligand CLA c 510



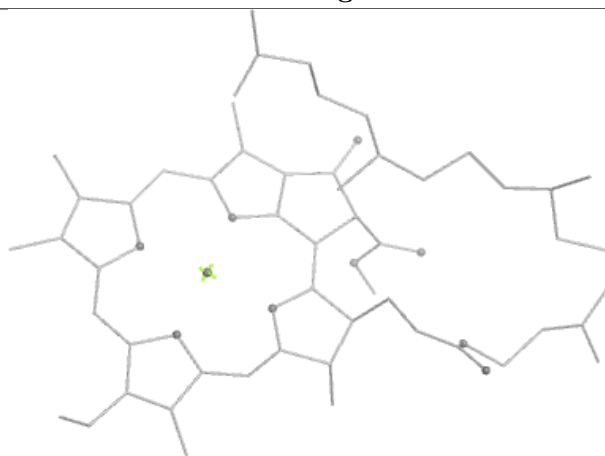
Bond lengths



Bond angles

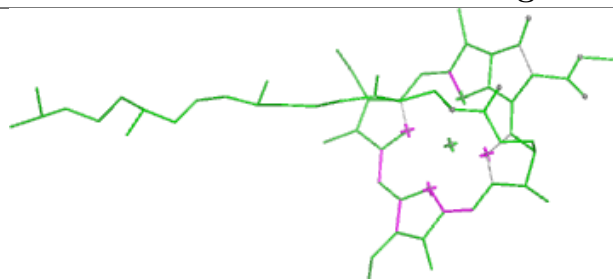


Torsions

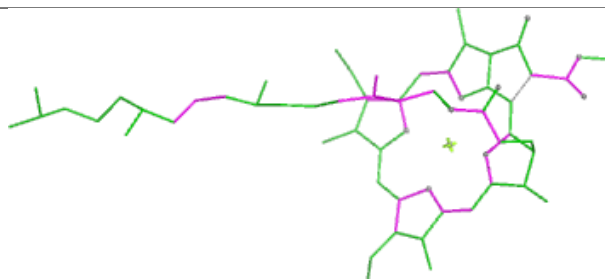


Rings

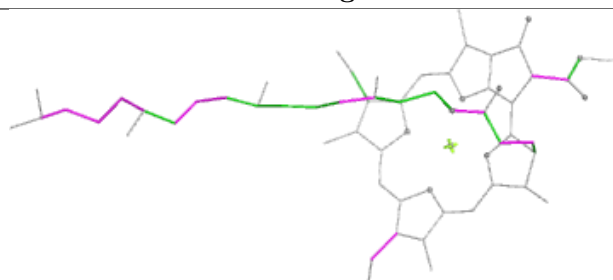
Ligand CLA b 614



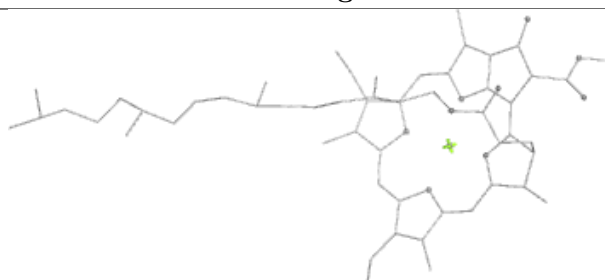
Bond lengths



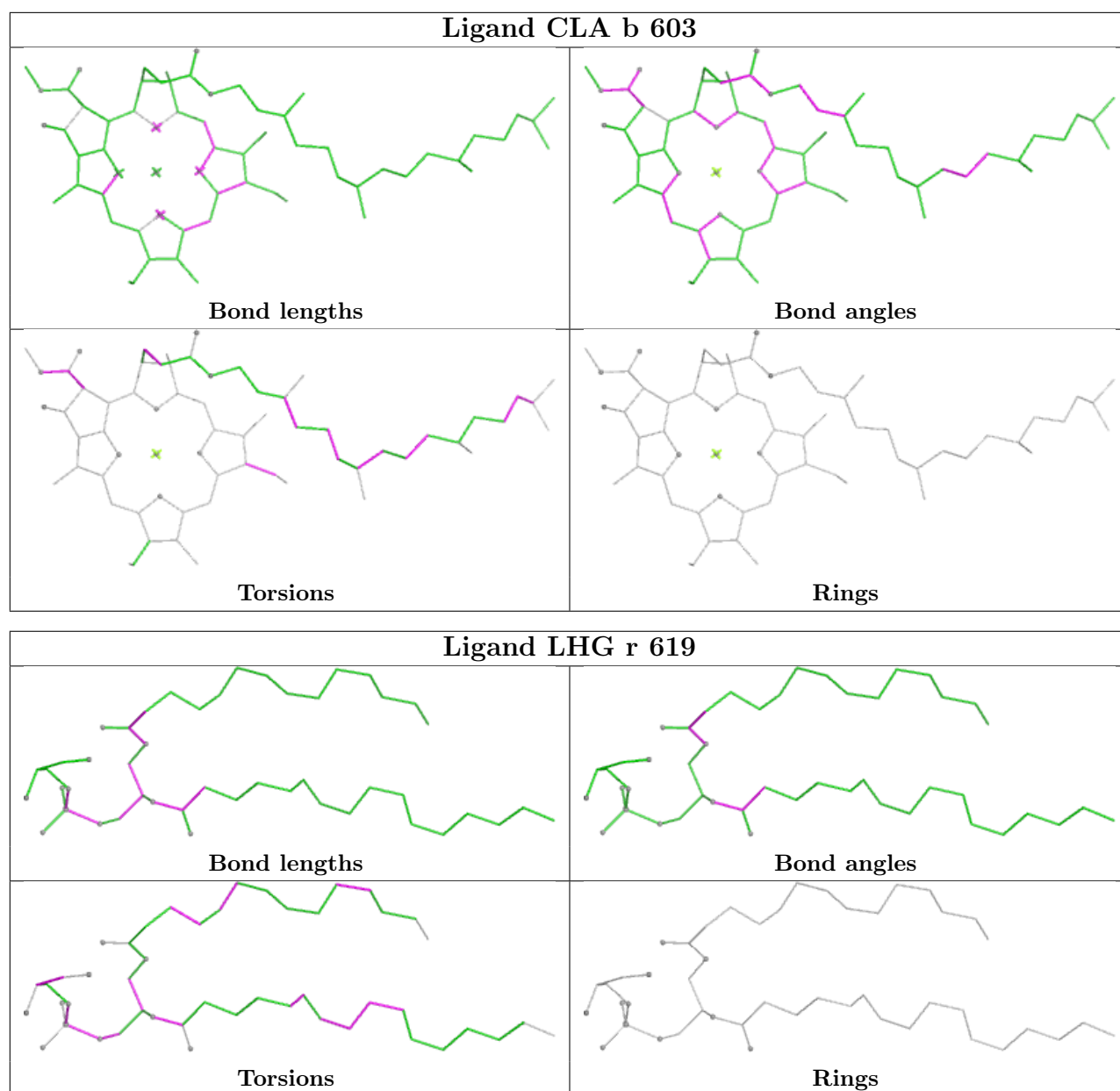
Bond angles

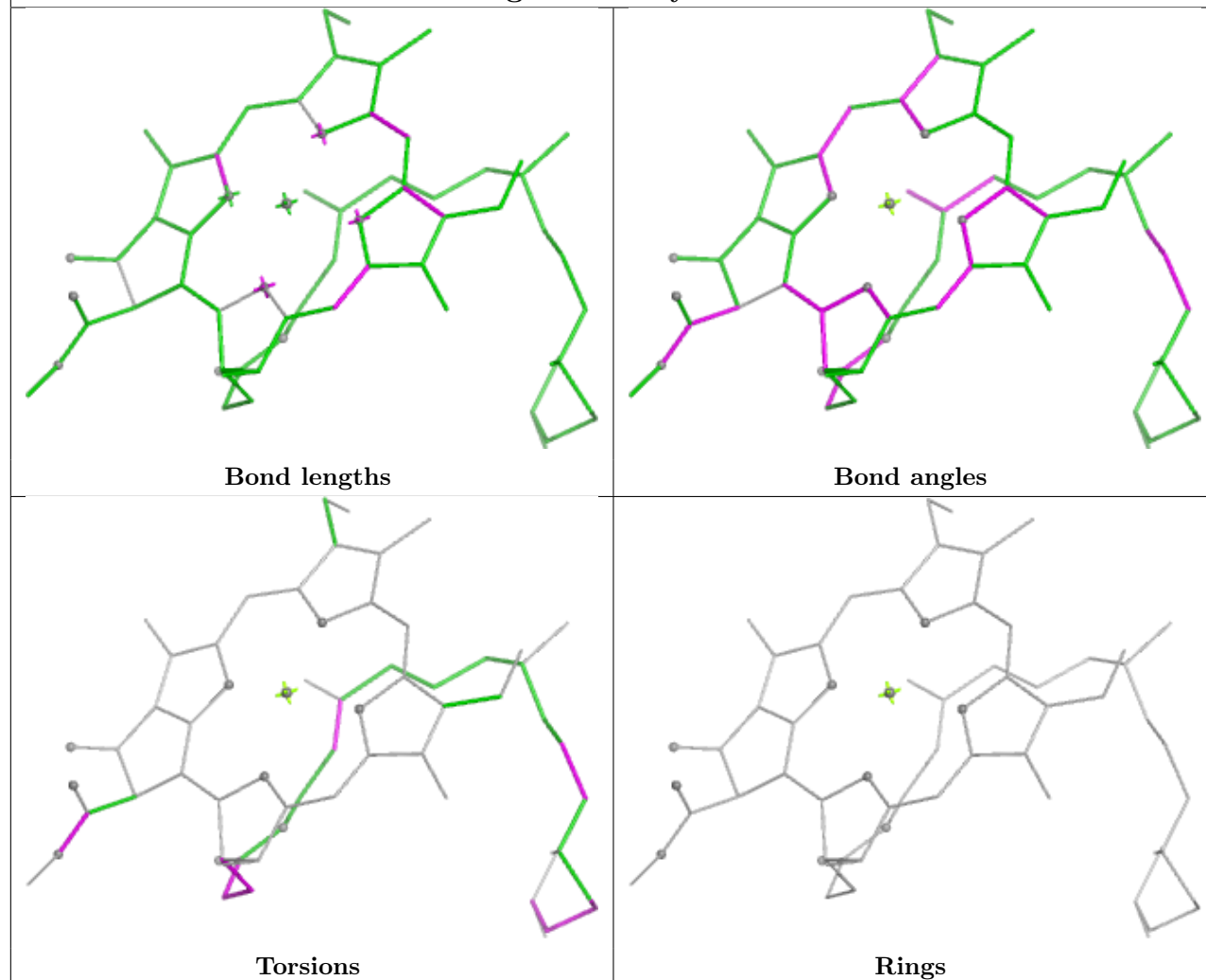
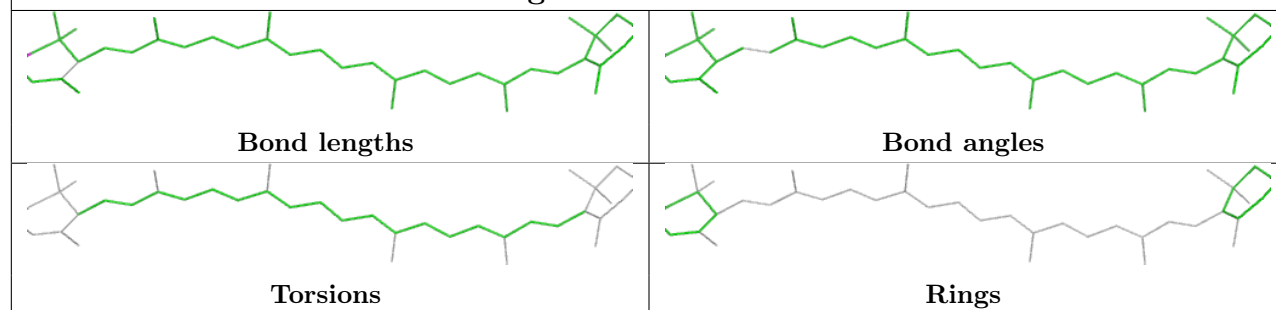


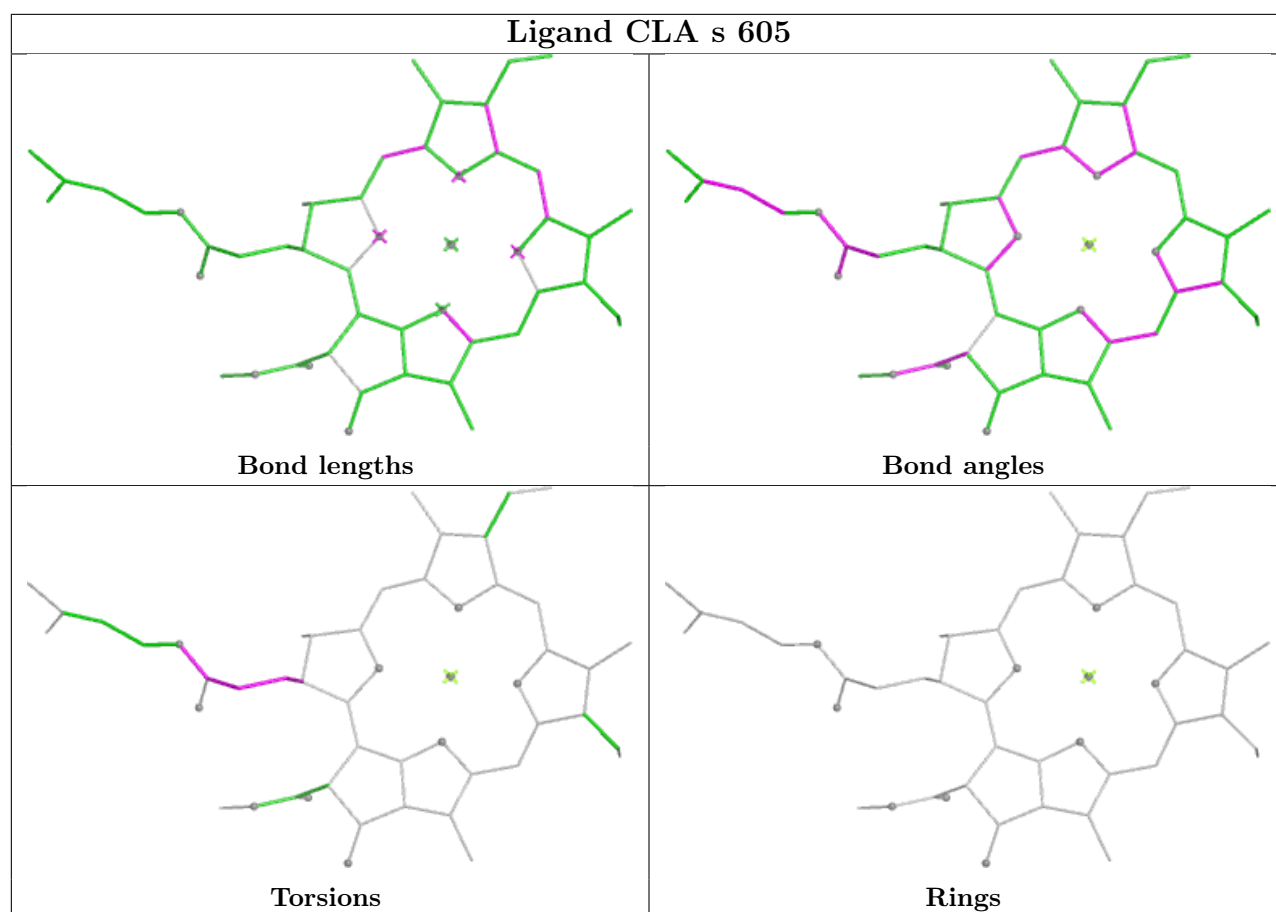
Torsions



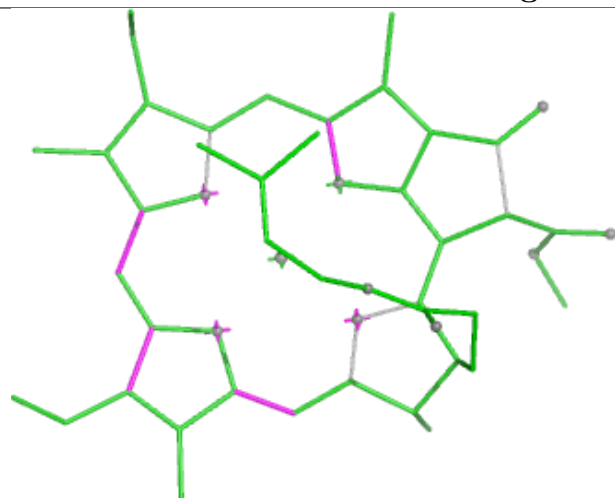
Rings



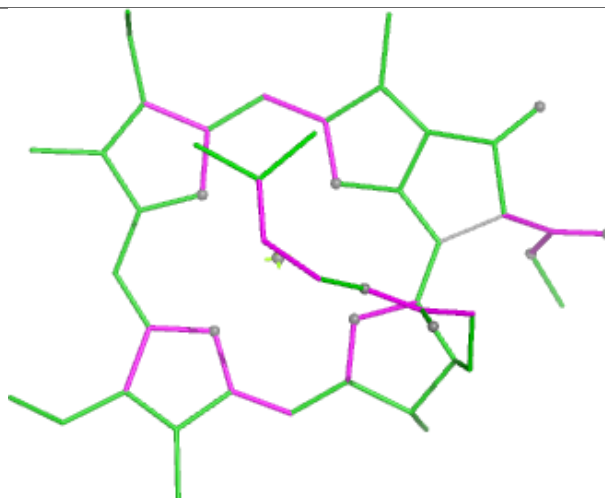
Ligand CLA y 613**Ligand LUT 11 617**



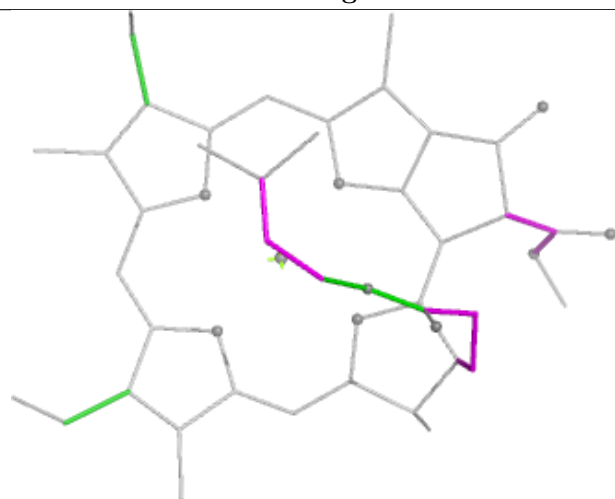
Ligand CLA 3 614



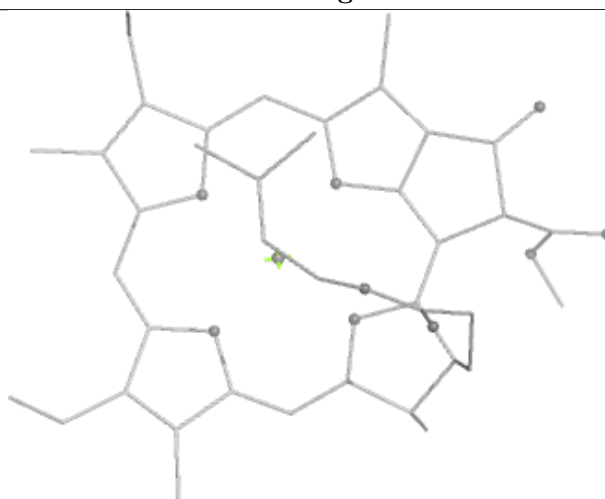
Bond lengths



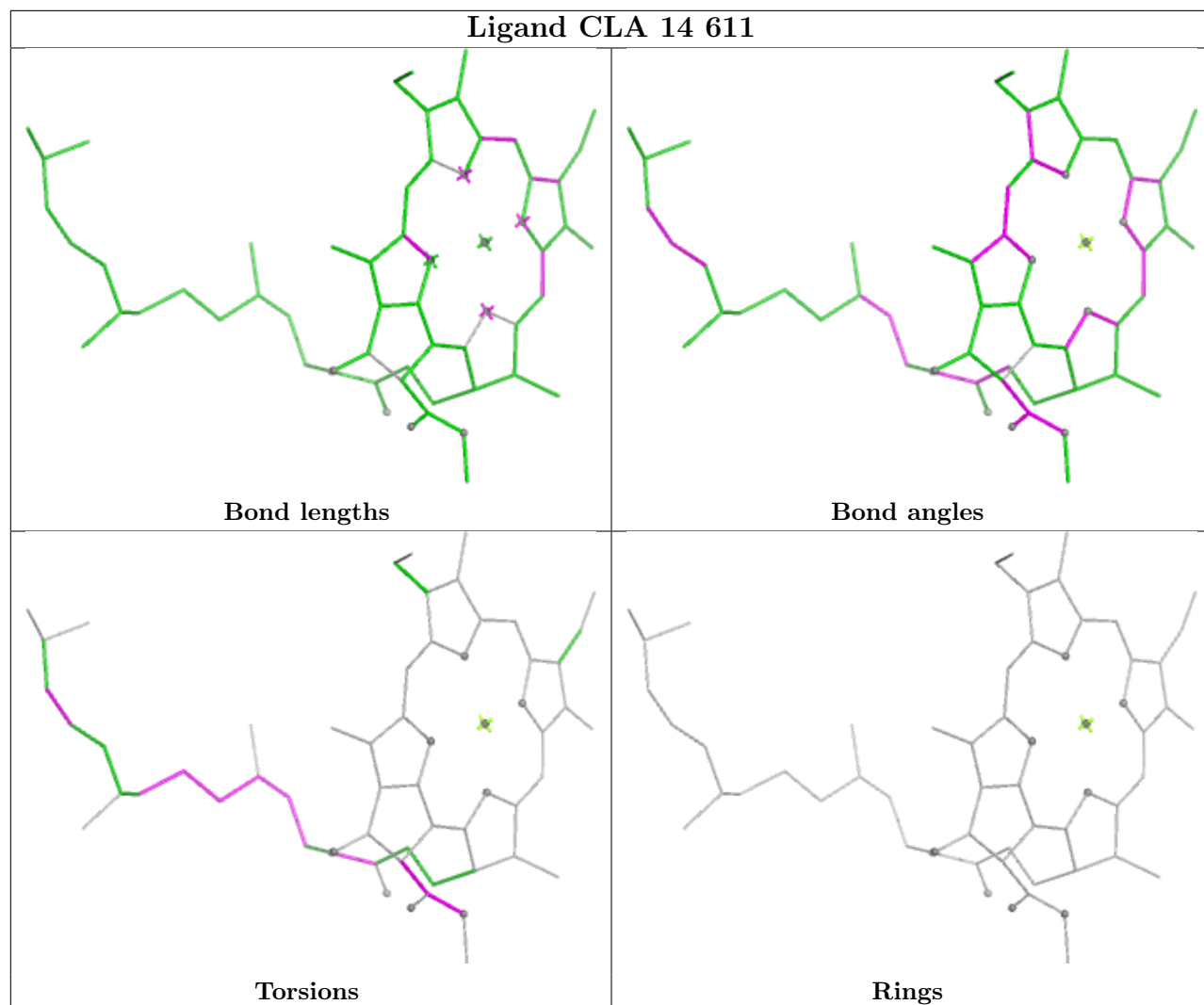
Bond angles

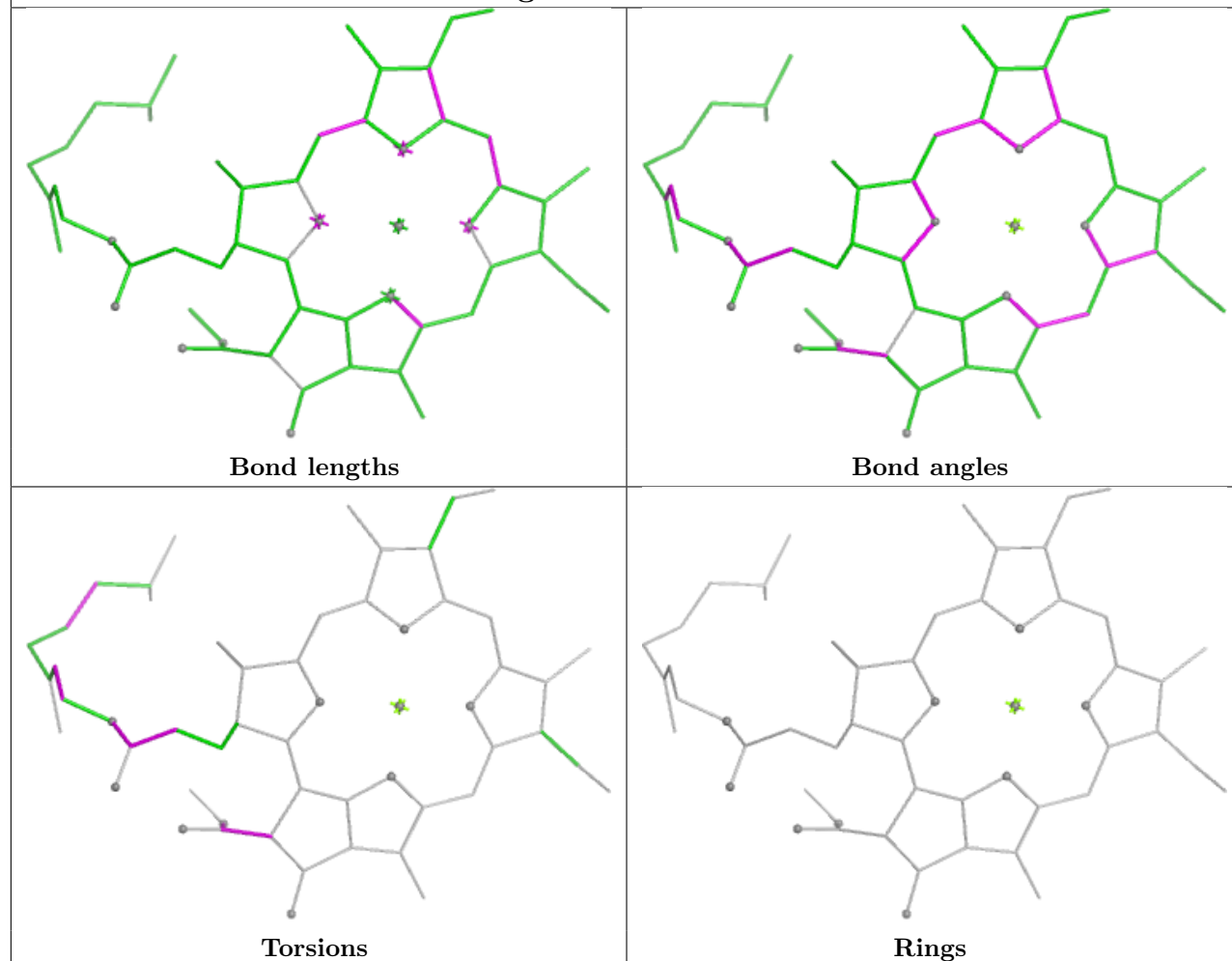
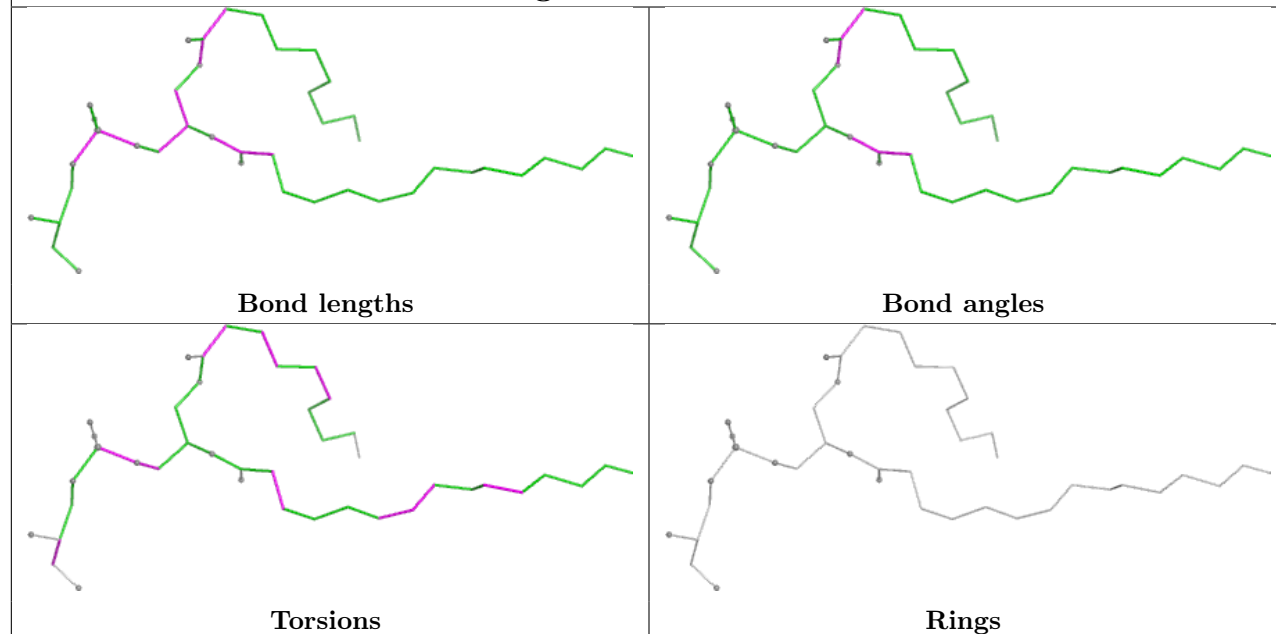


Torsions

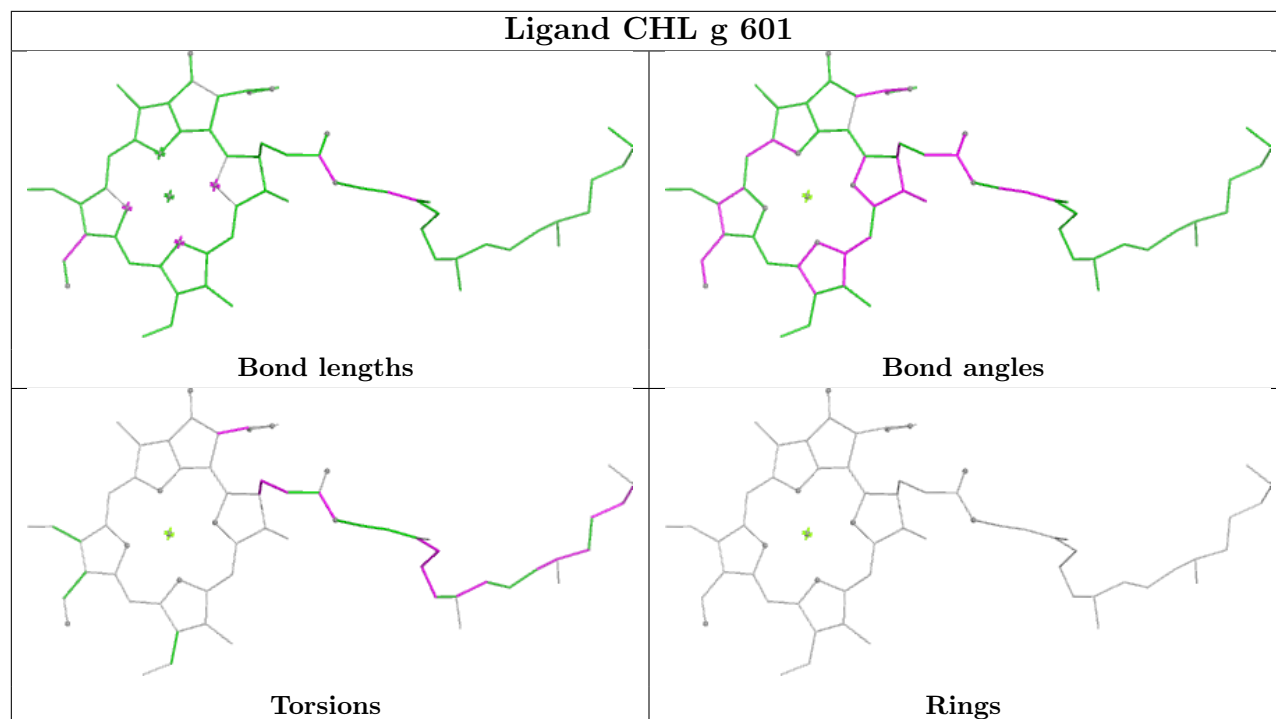


Rings

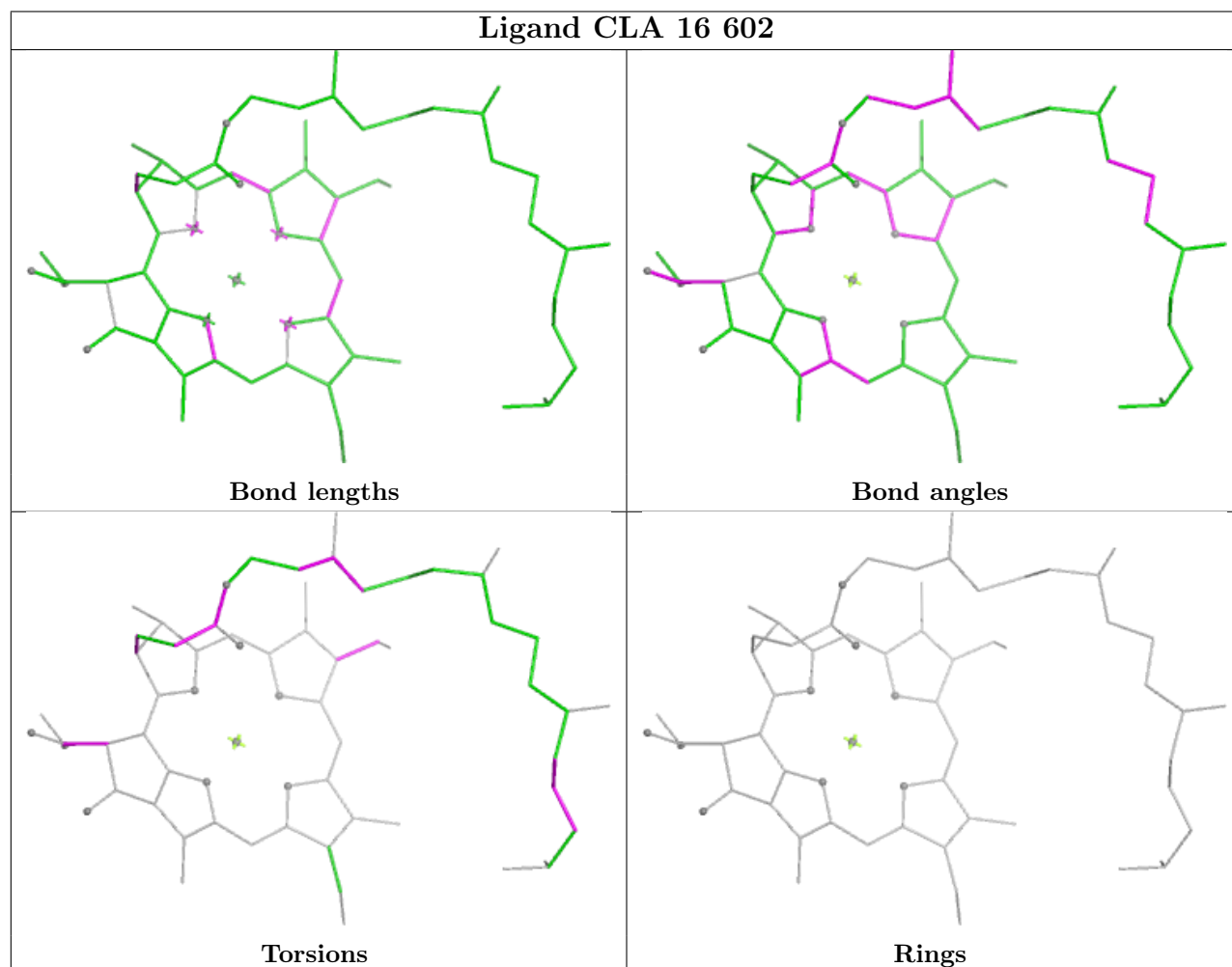


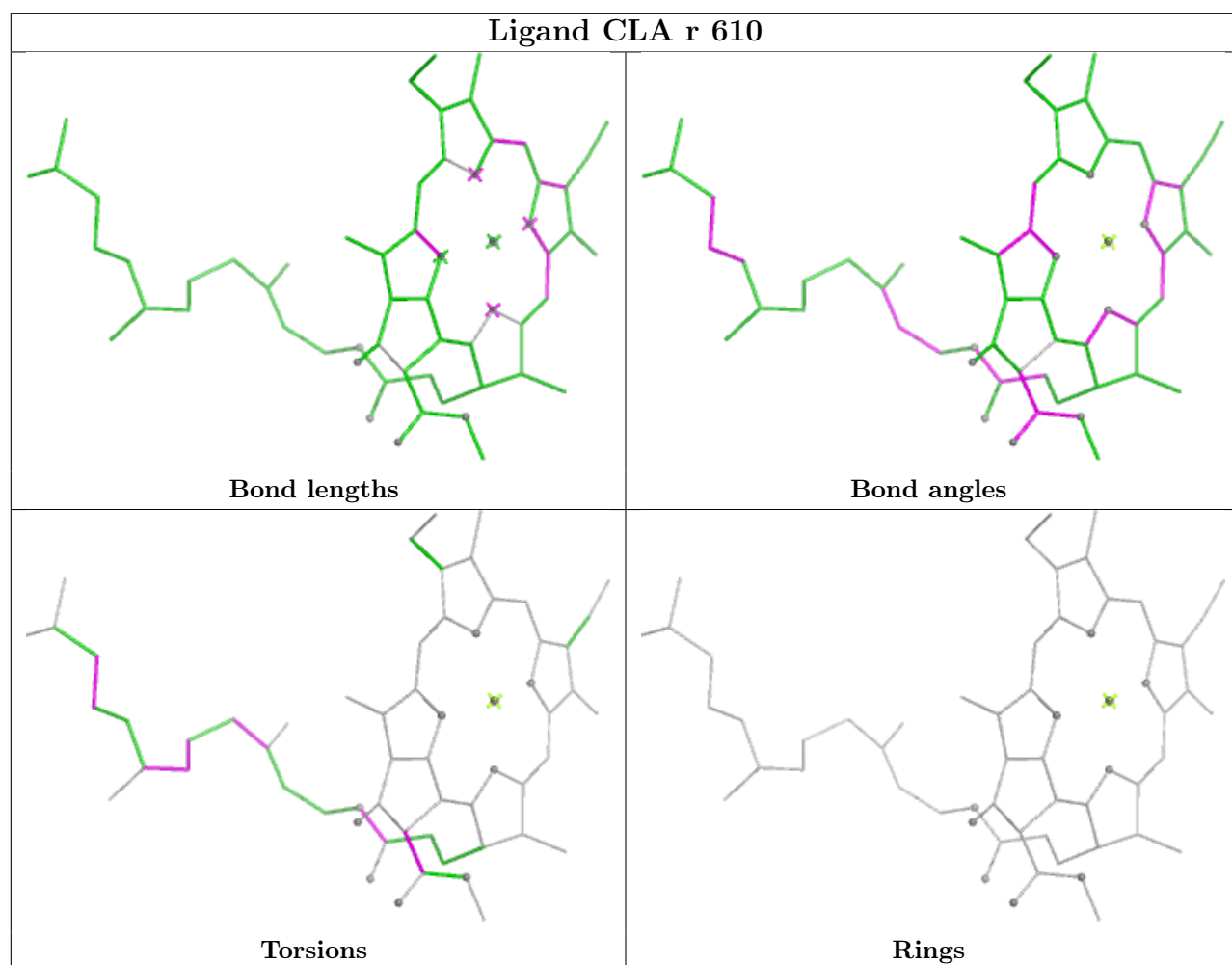
Ligand CLA 3 603**Ligand LHG 1 615**

Ligand CHL g 601

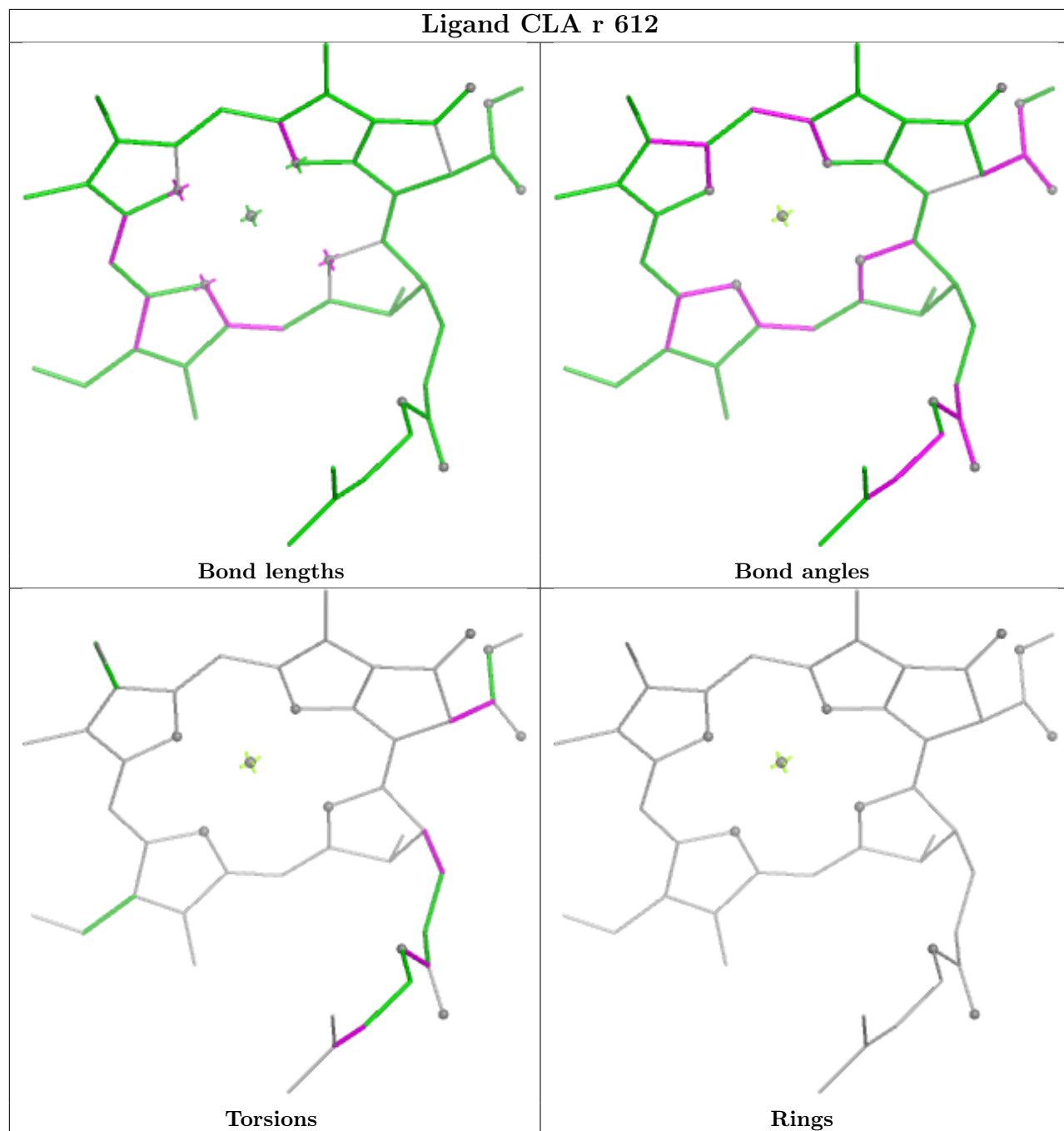


Ligand CLA 16 602

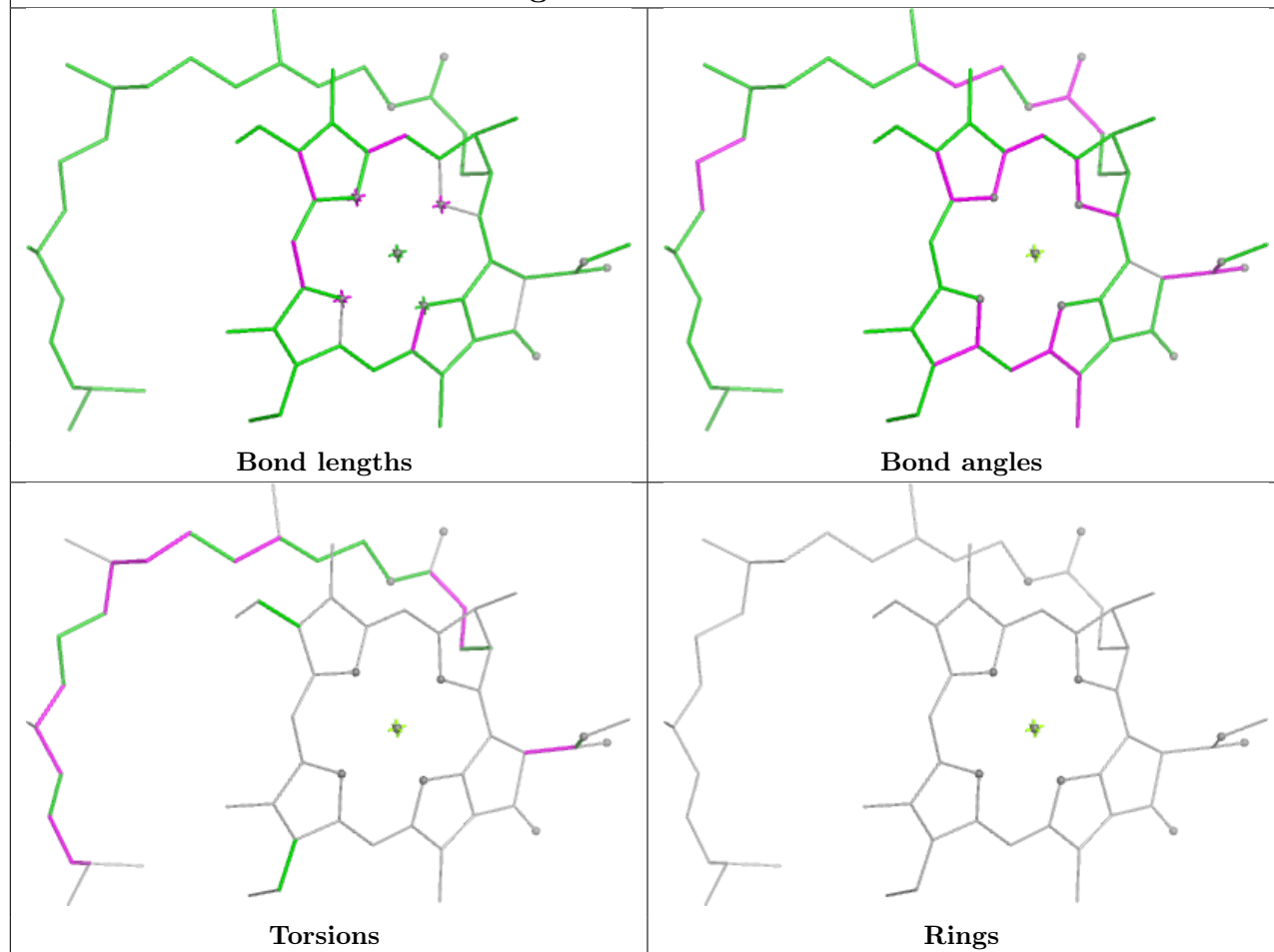




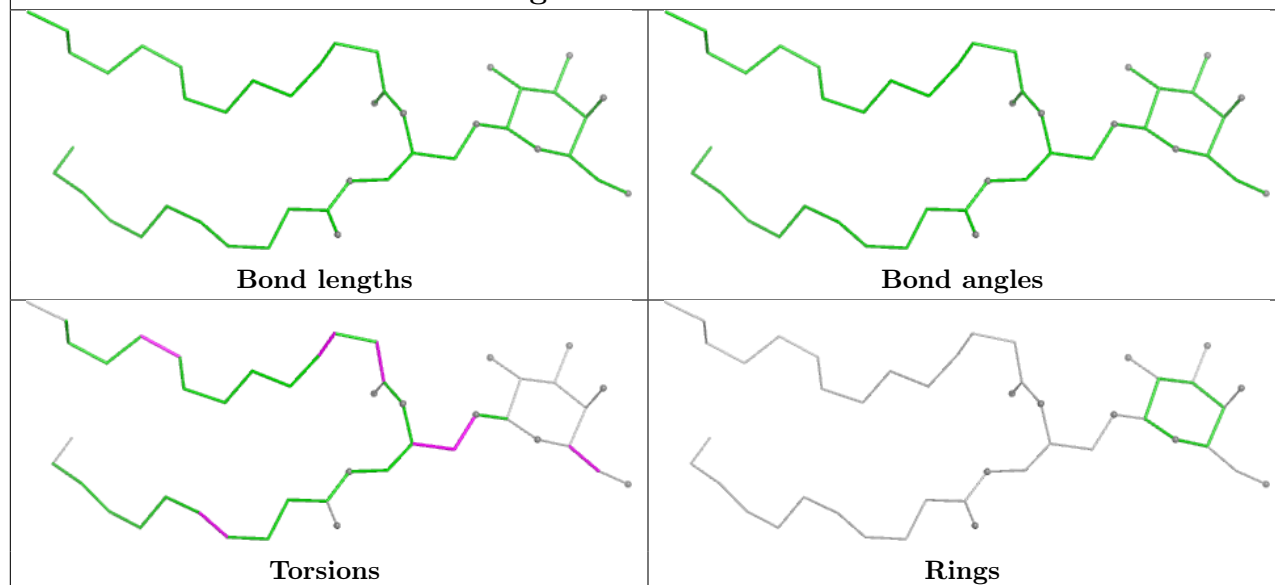
Ligand CLA r 612



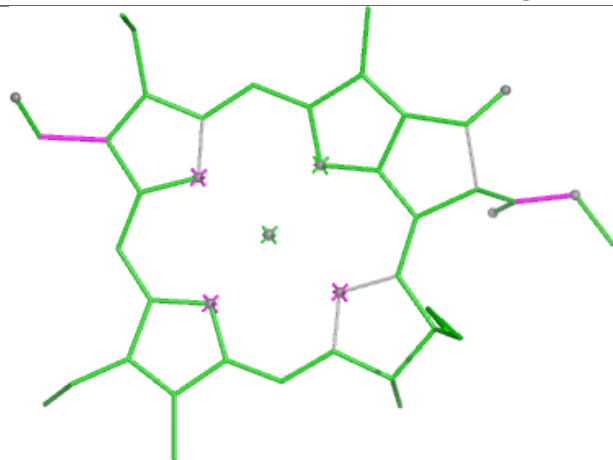
Ligand CLA G 602



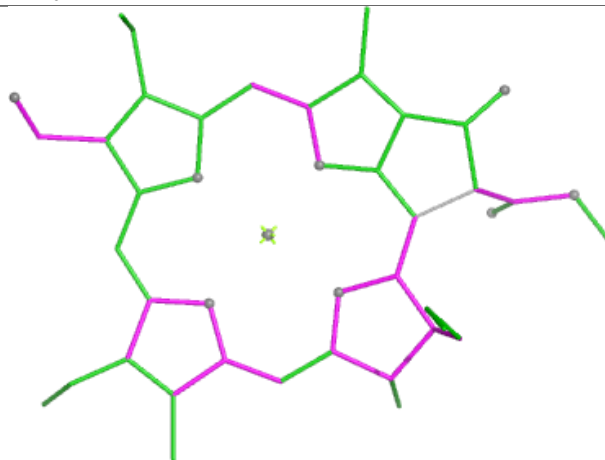
Ligand LMG d 410



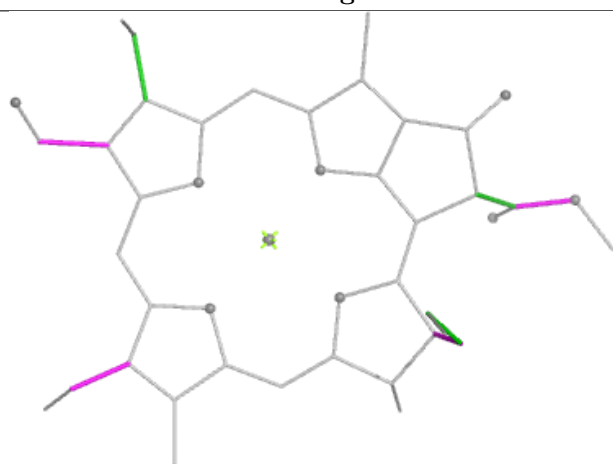
Ligand CHL y 608



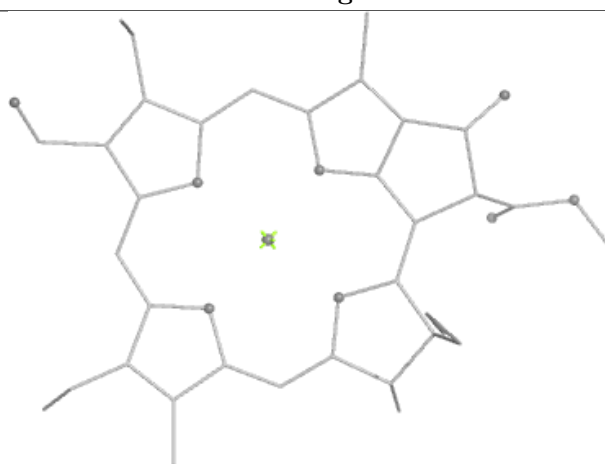
Bond lengths



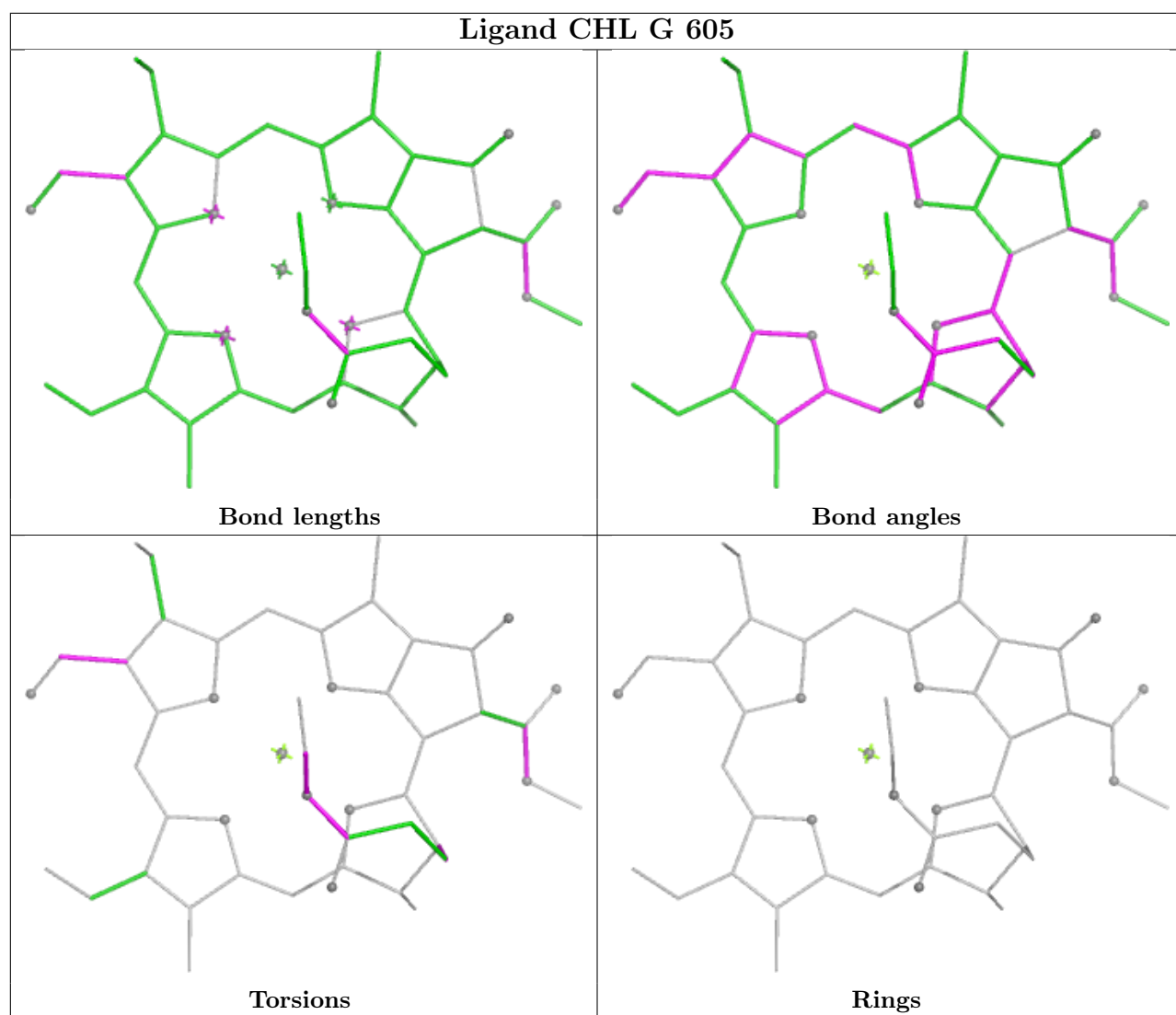
Bond angles



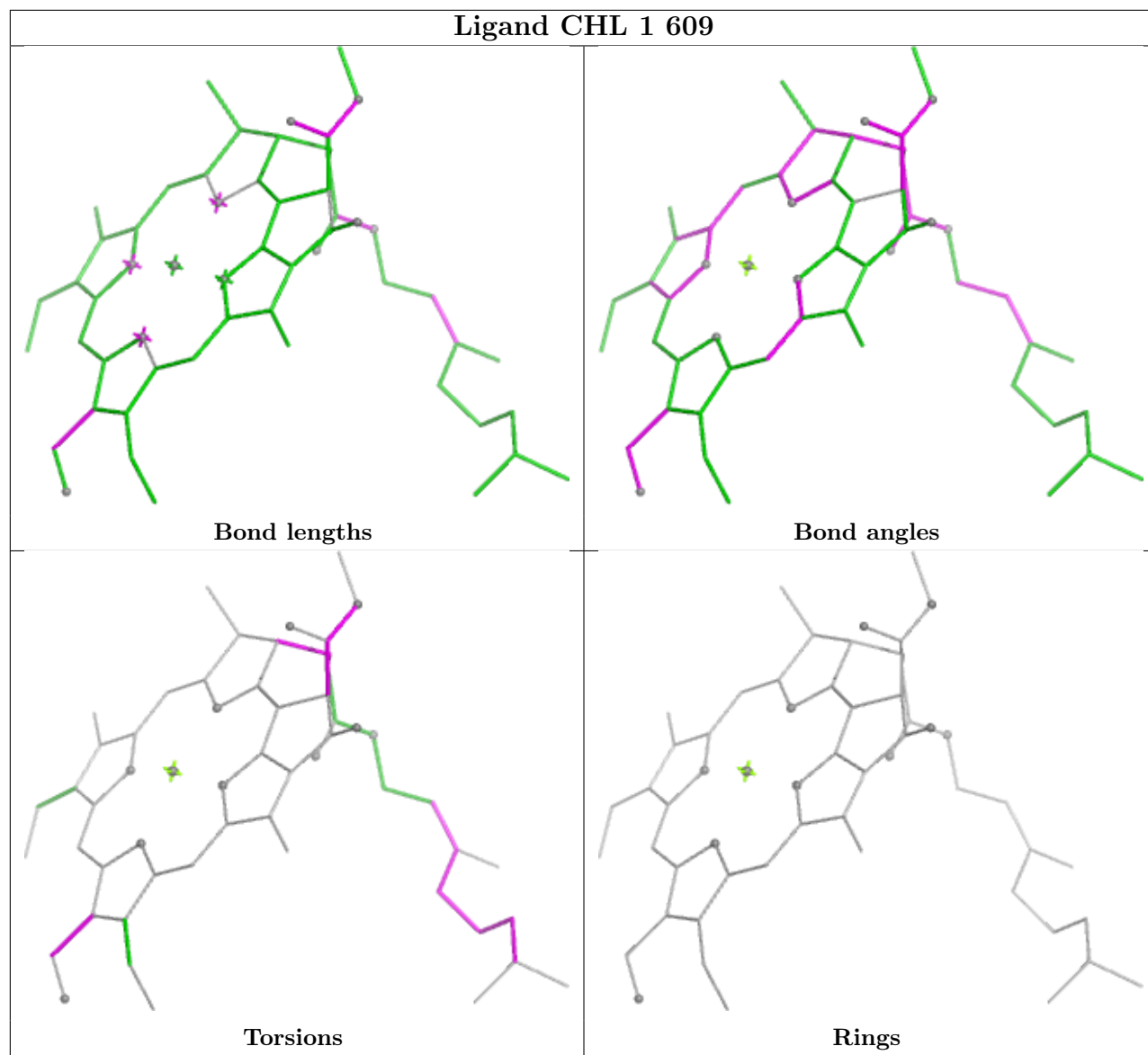
Torsions



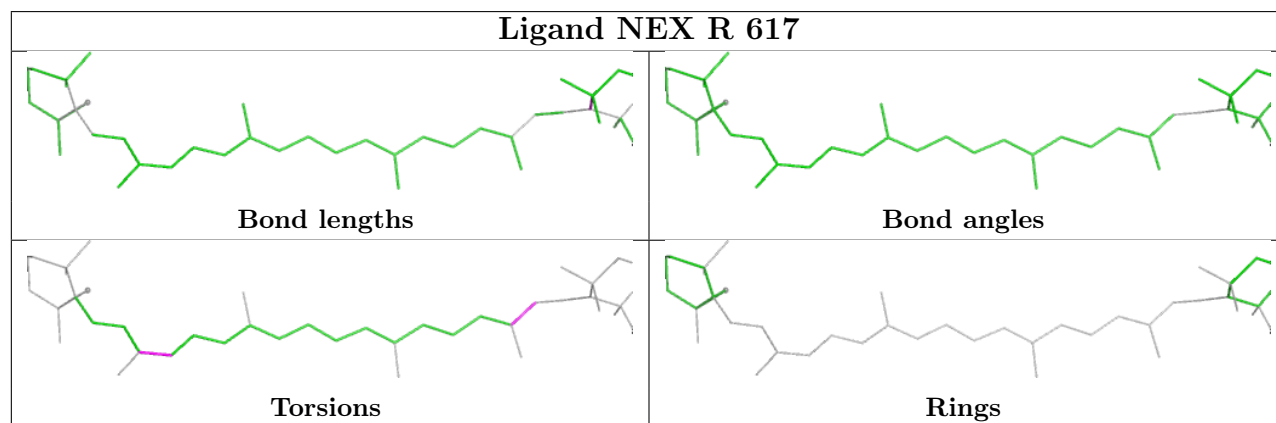
Rings



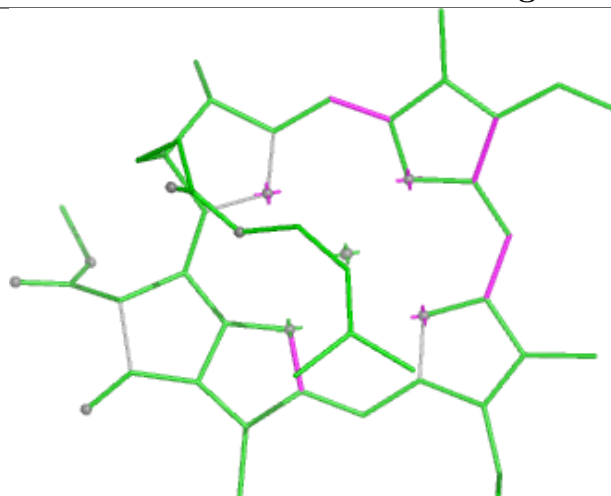
Ligand CHL 1 609



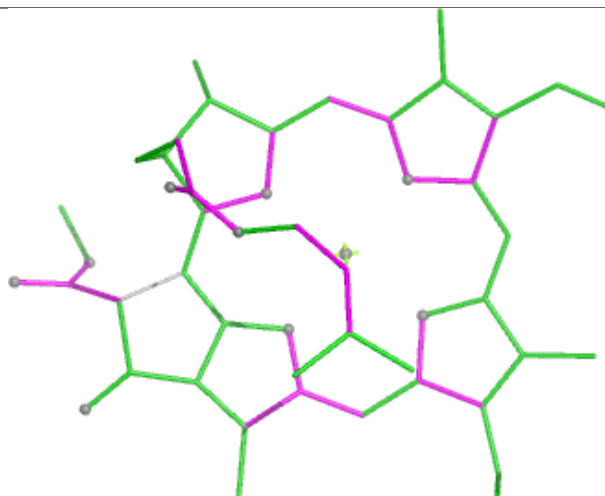
Ligand NEX R 617



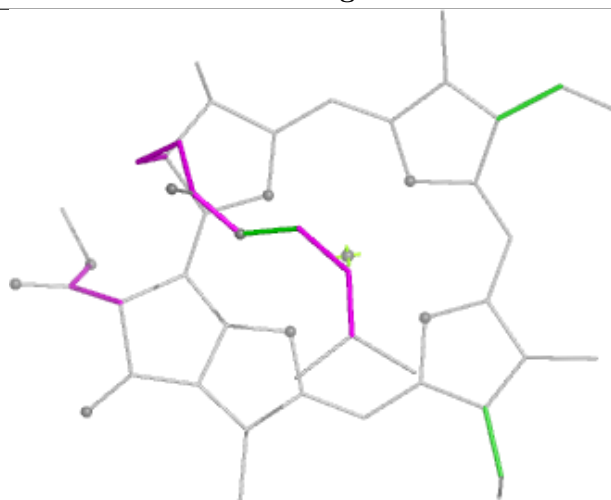
Ligand CLA 6 614



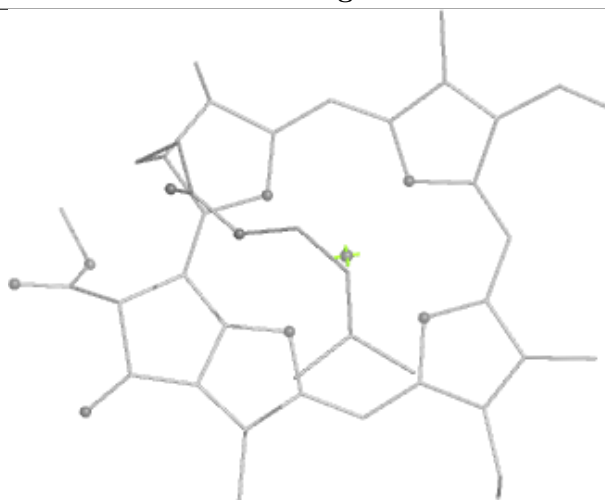
Bond lengths



Bond angles

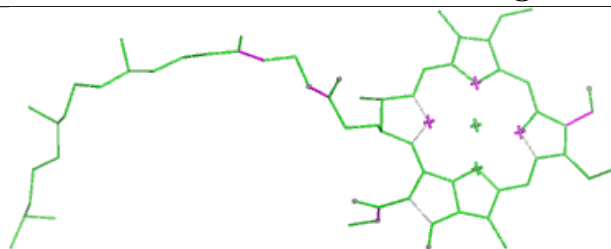


Torsions

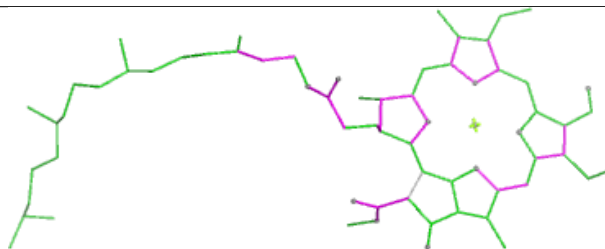


Rings

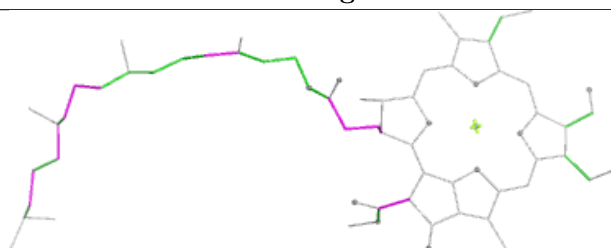
Ligand CHL Y 601



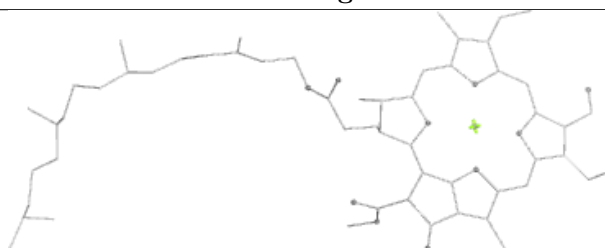
Bond lengths



Bond angles

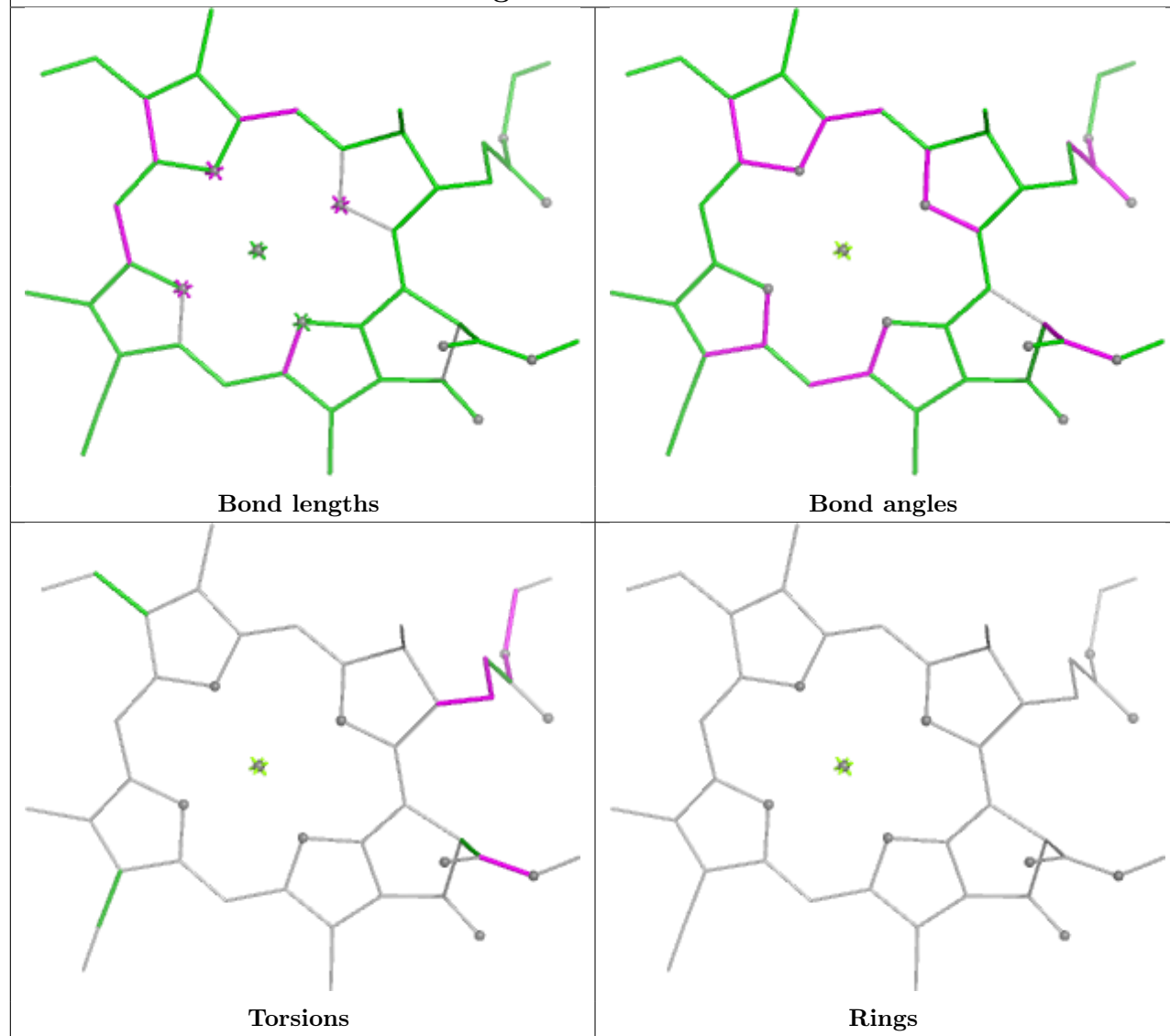


Torsions

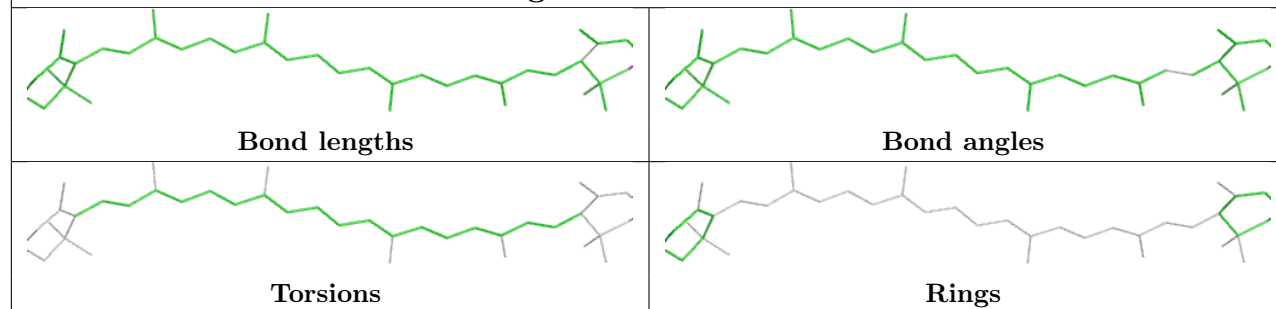


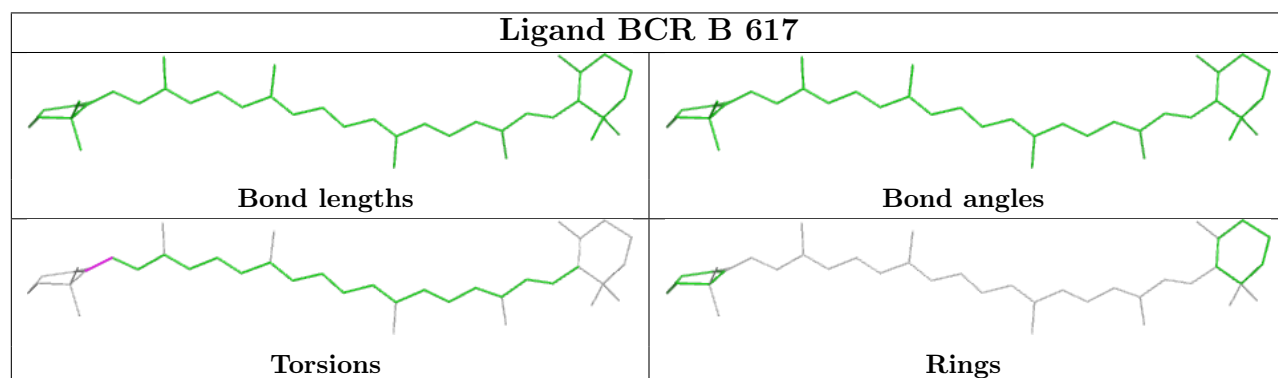
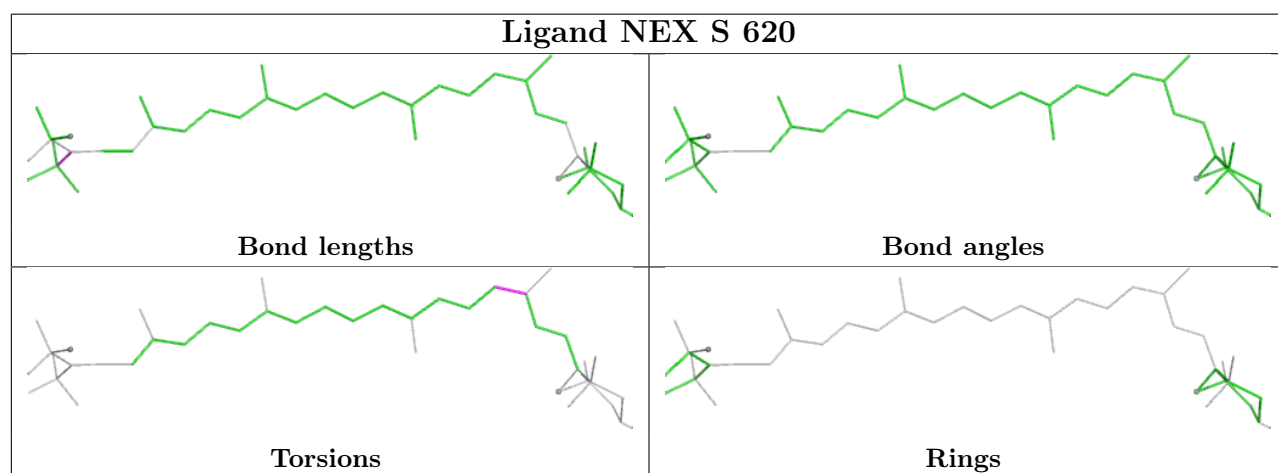
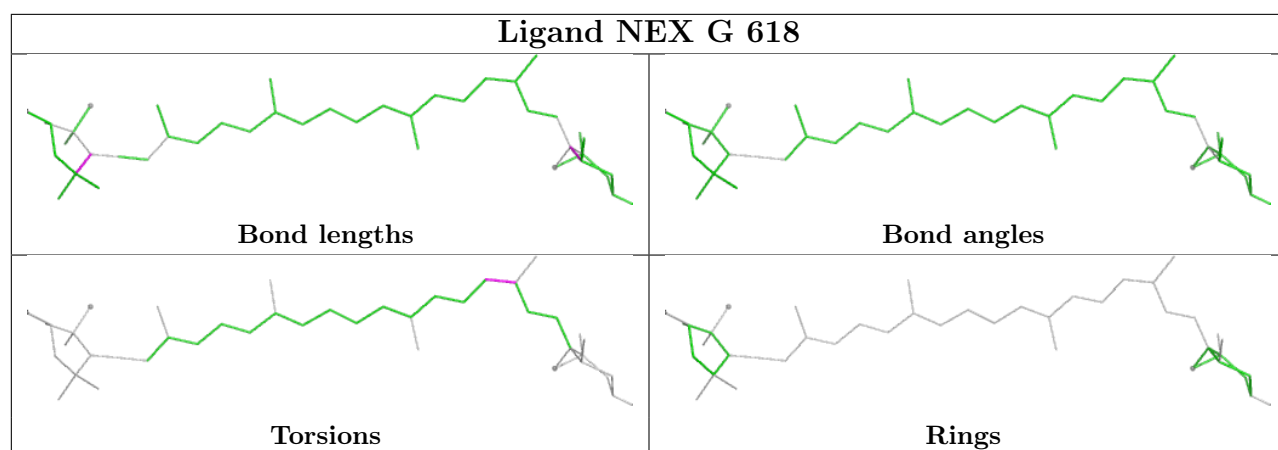
Rings

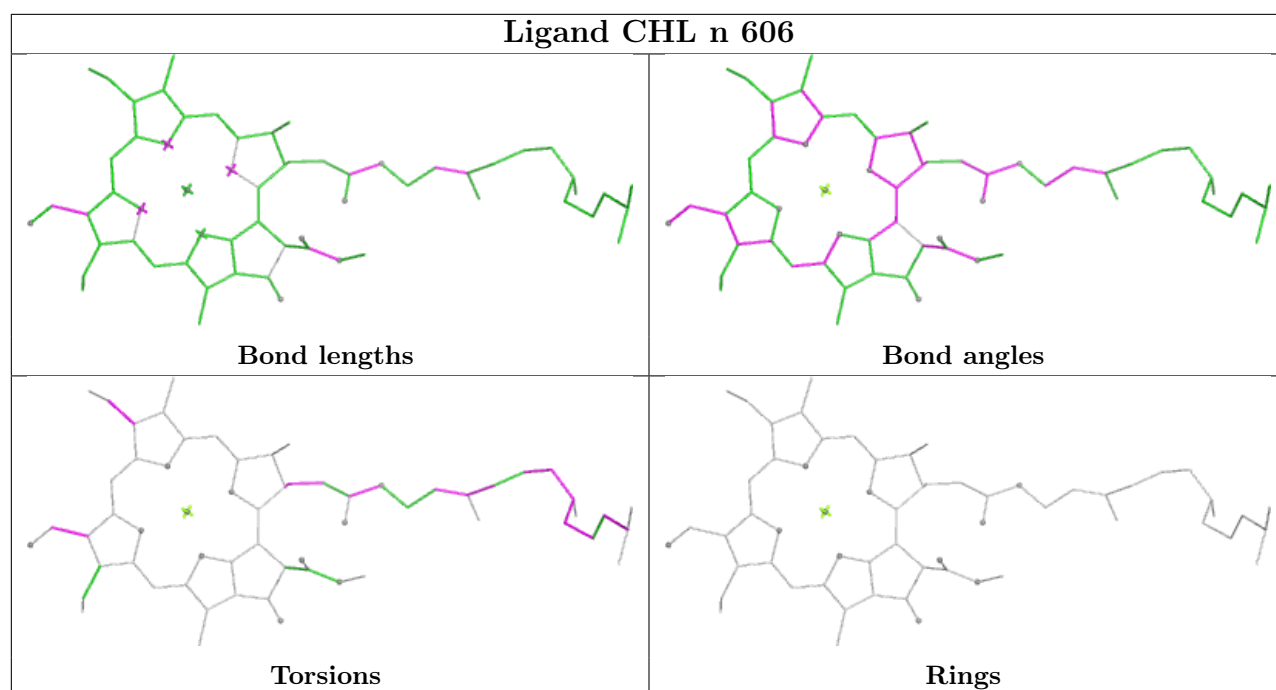
Ligand CLA s 615

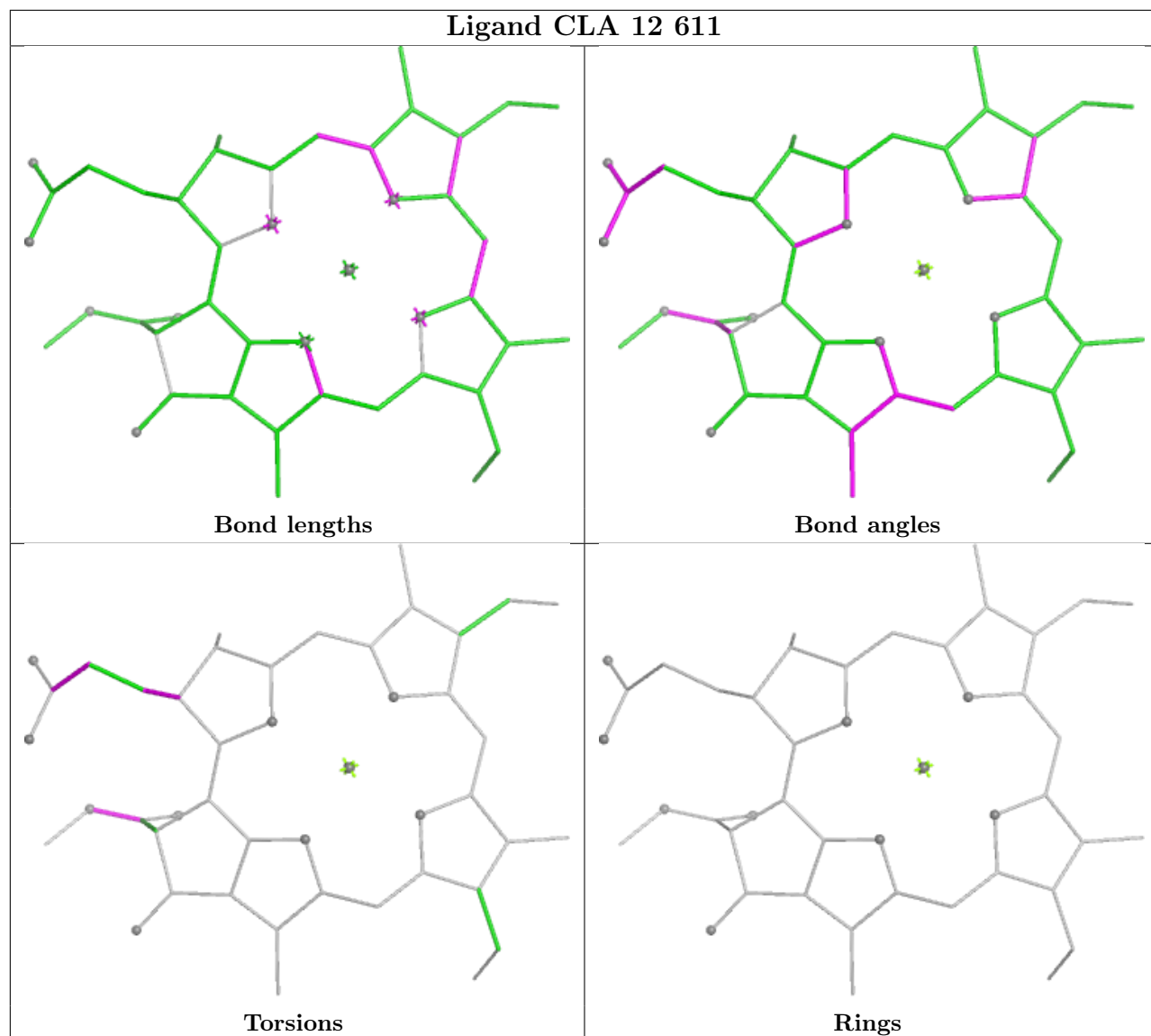


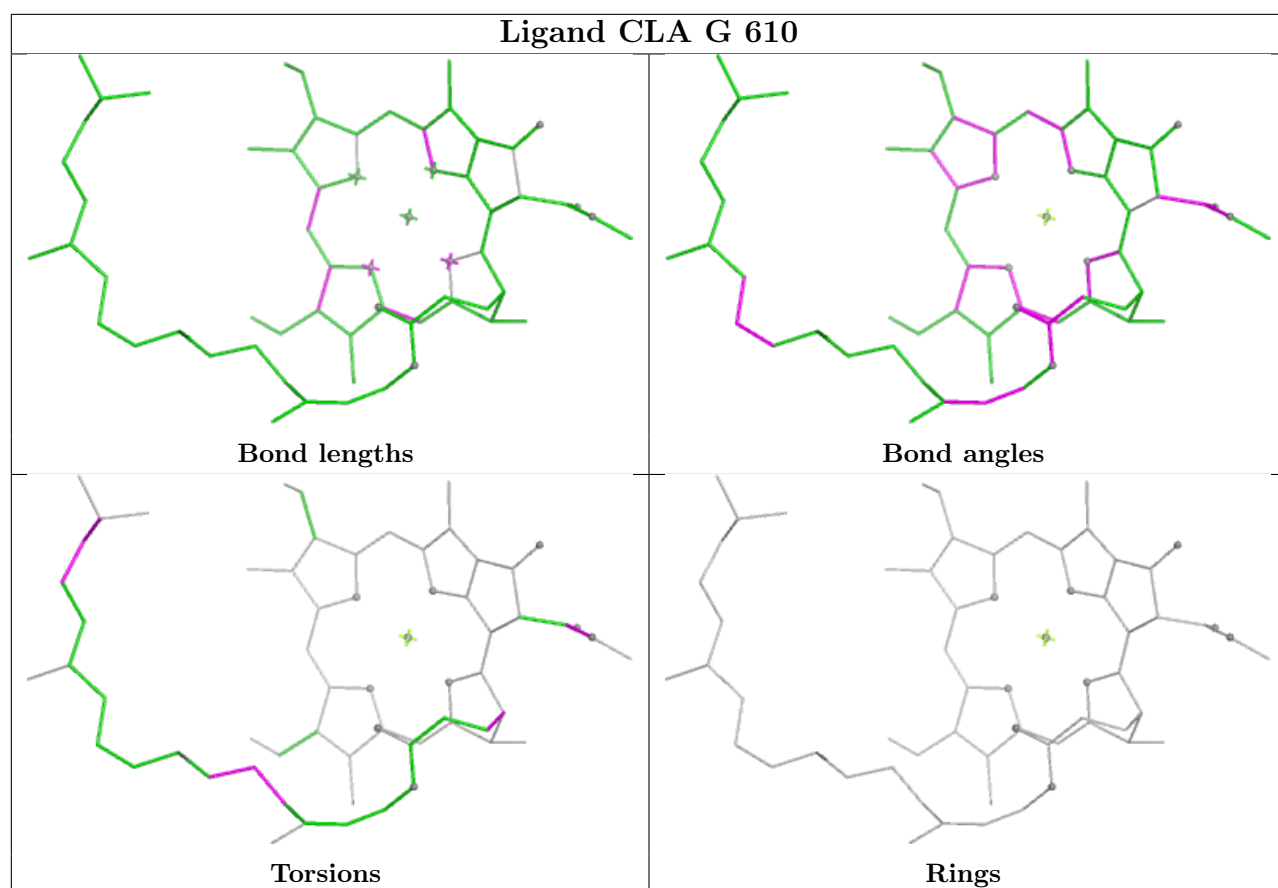
Ligand LUT 14 617



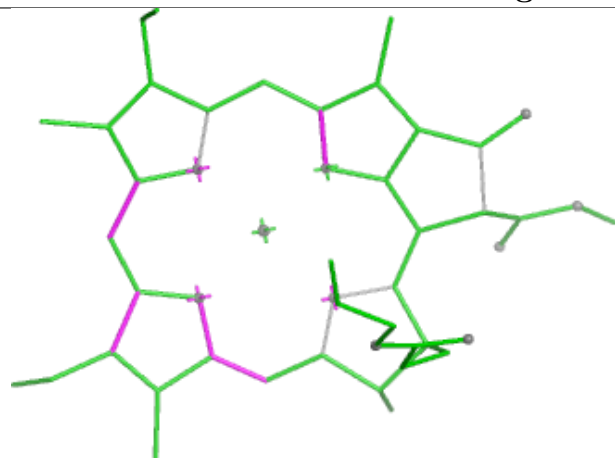




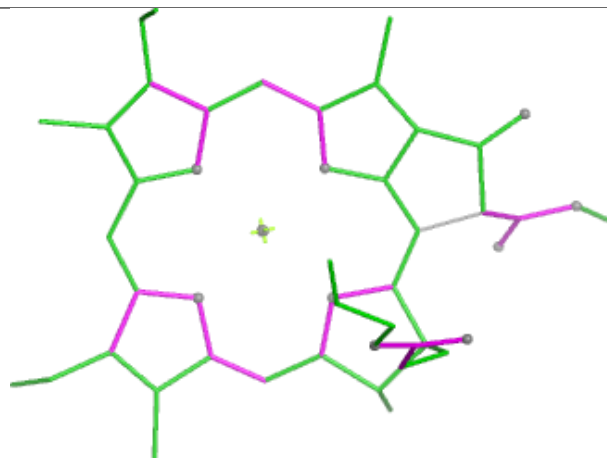




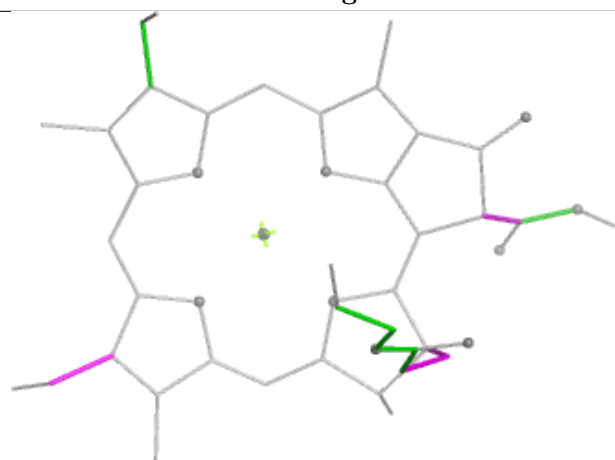
Ligand CLA R 604



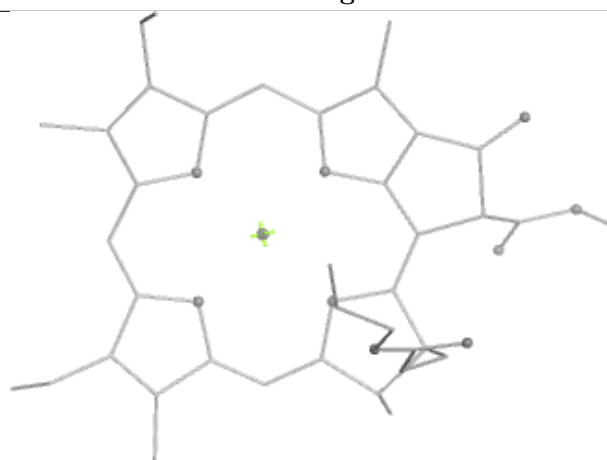
Bond lengths



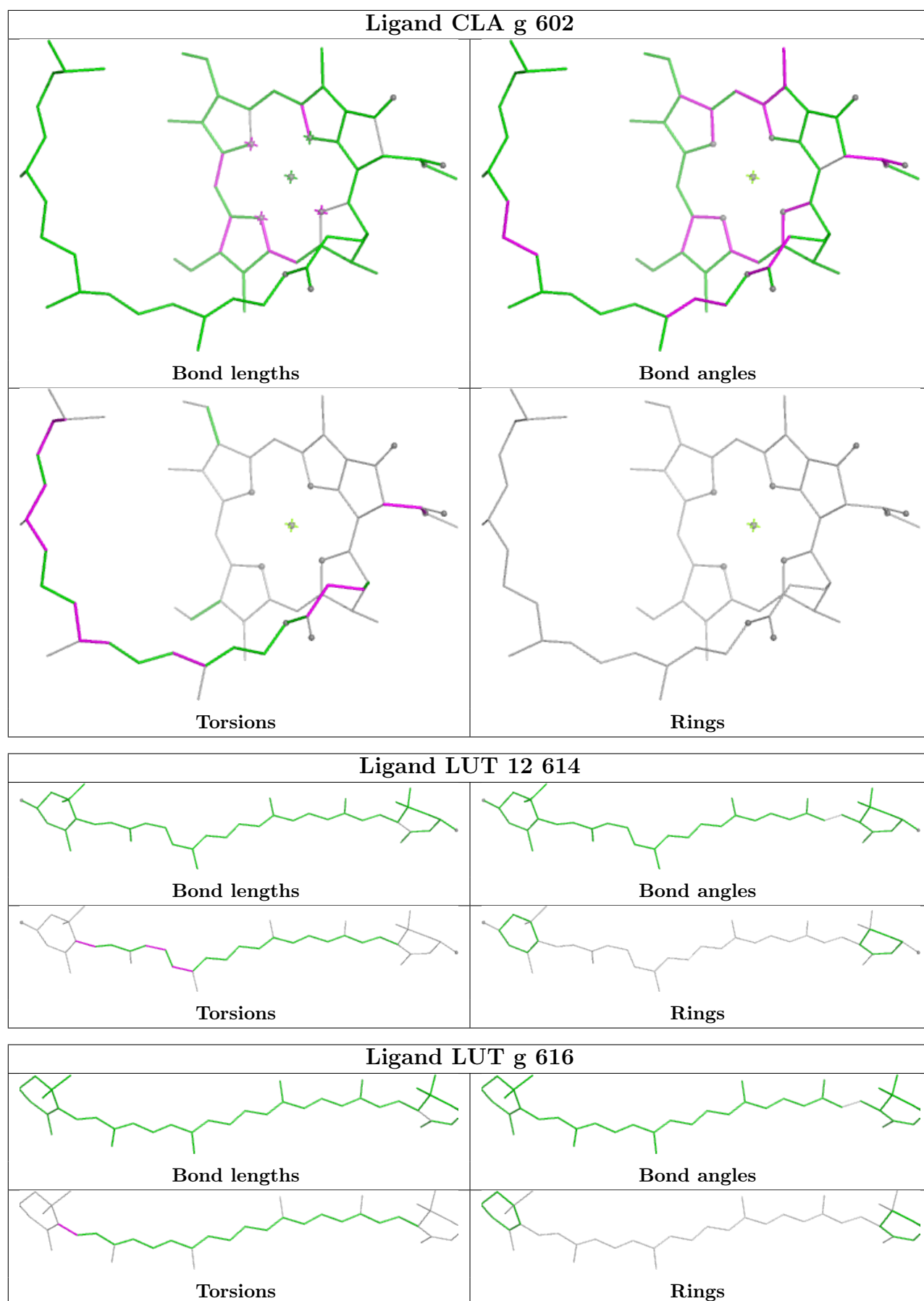
Bond angles

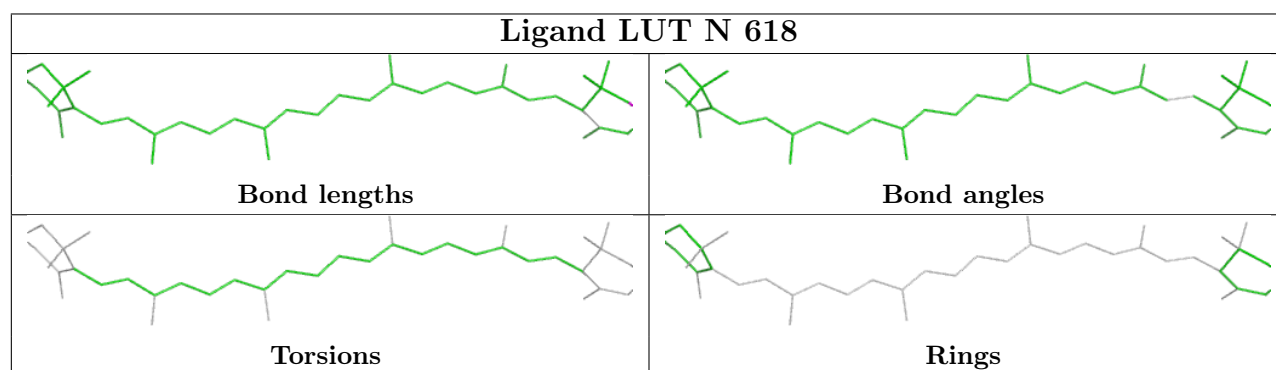
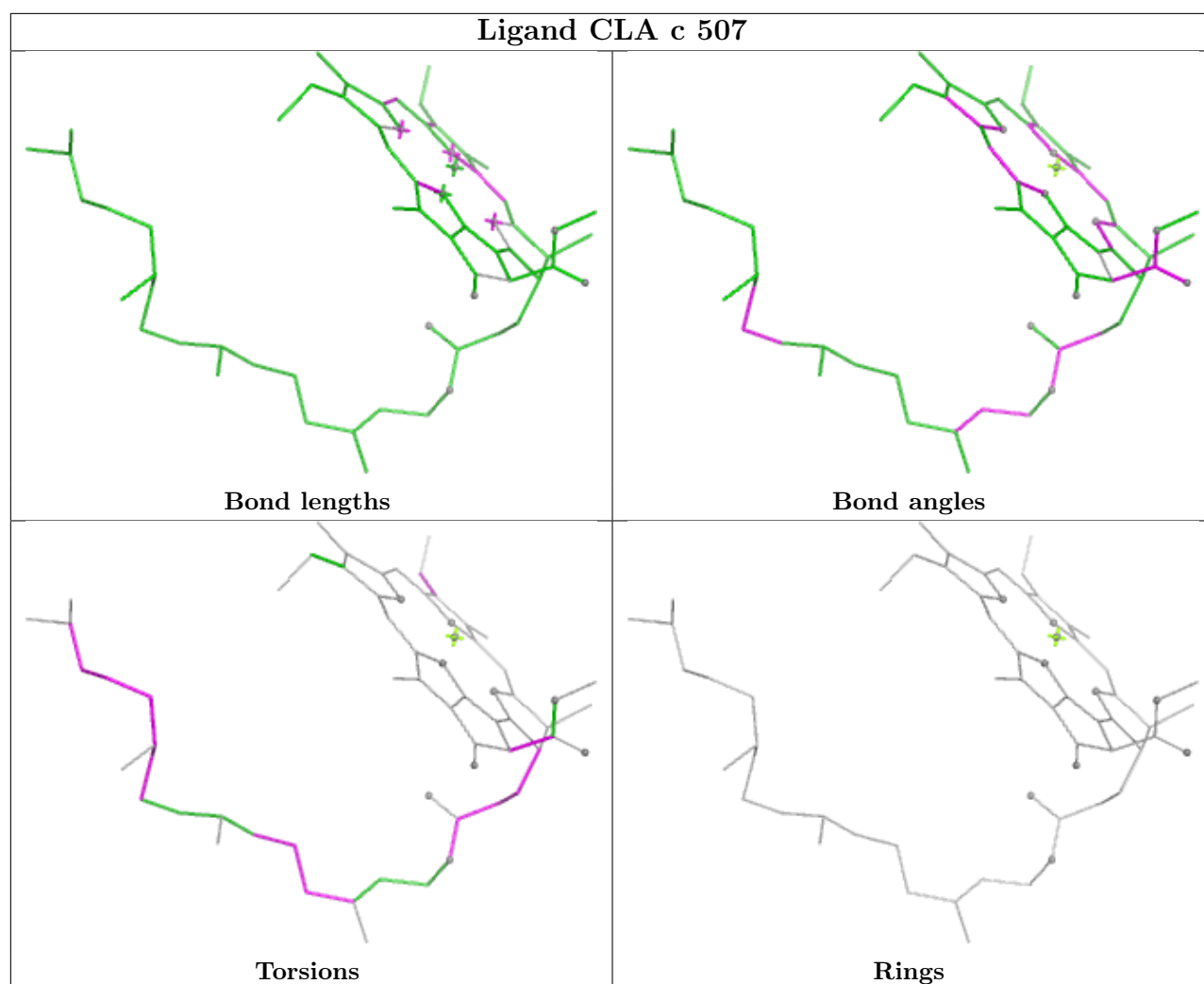


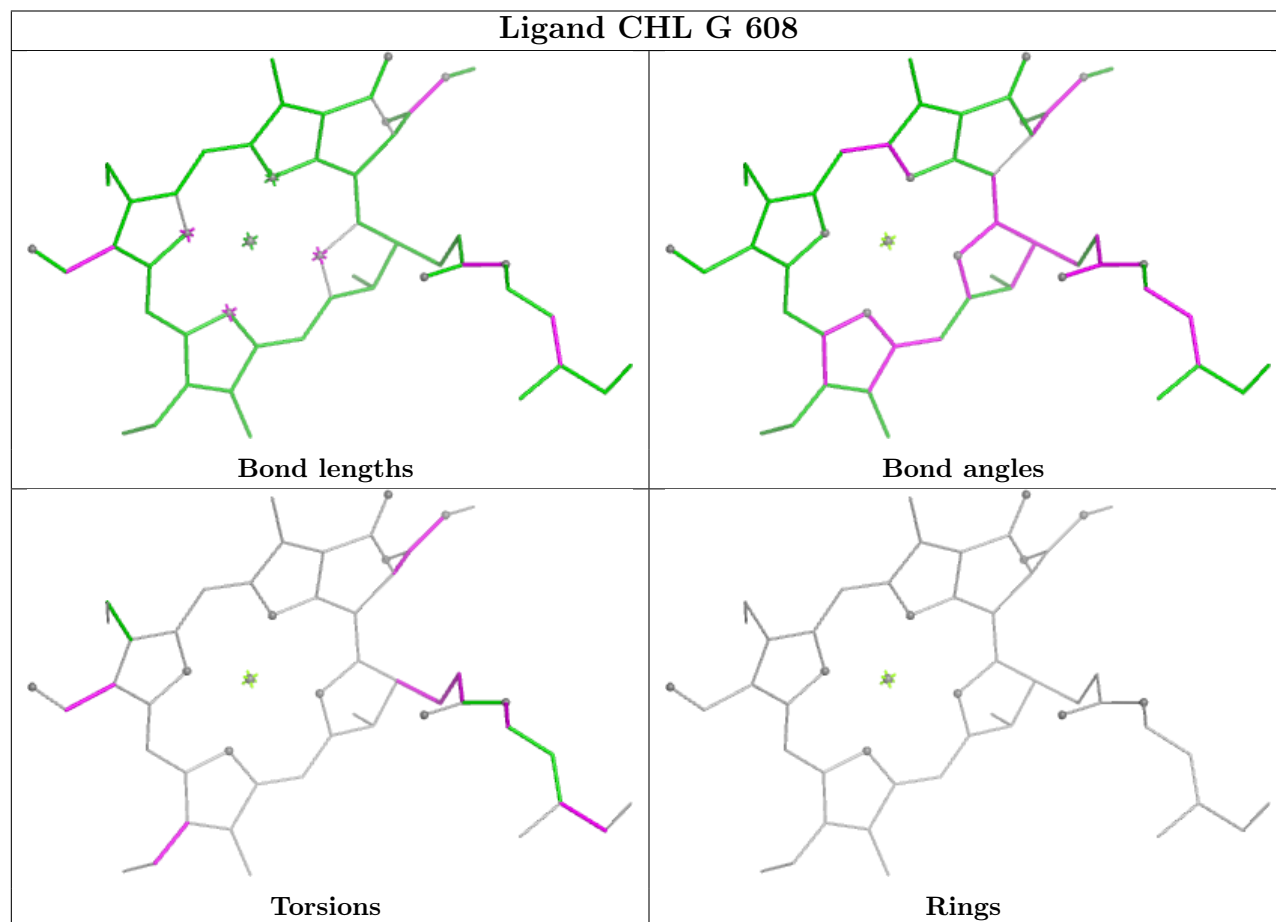
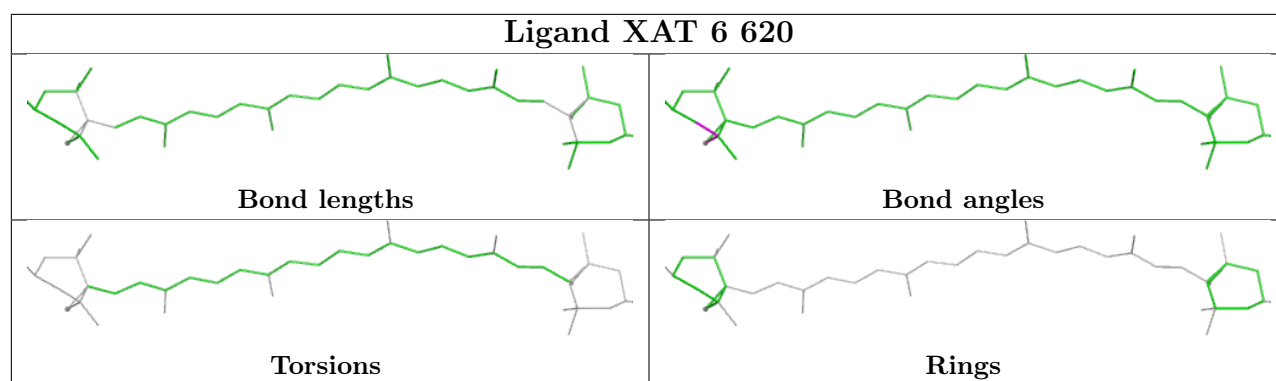
Torsions

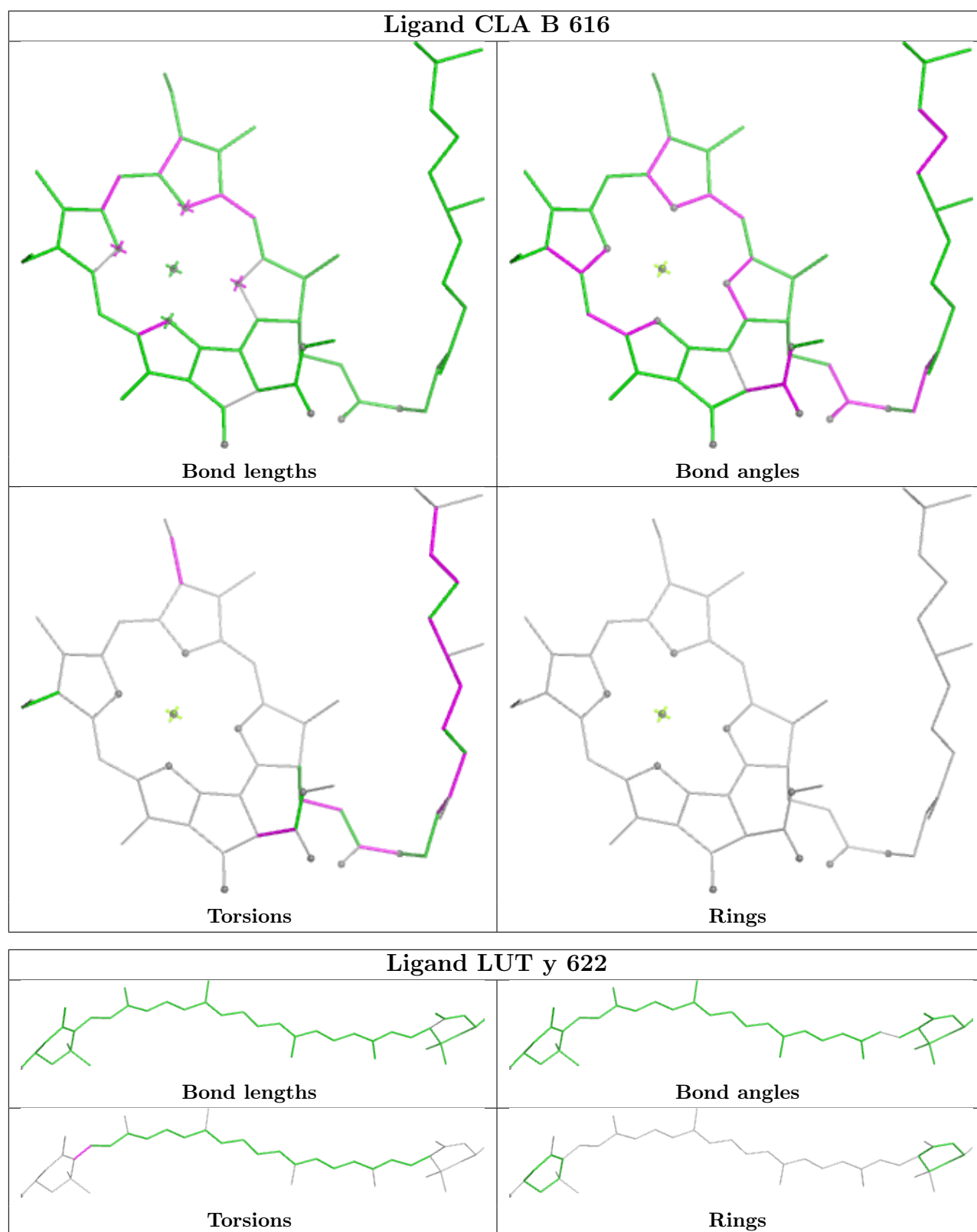


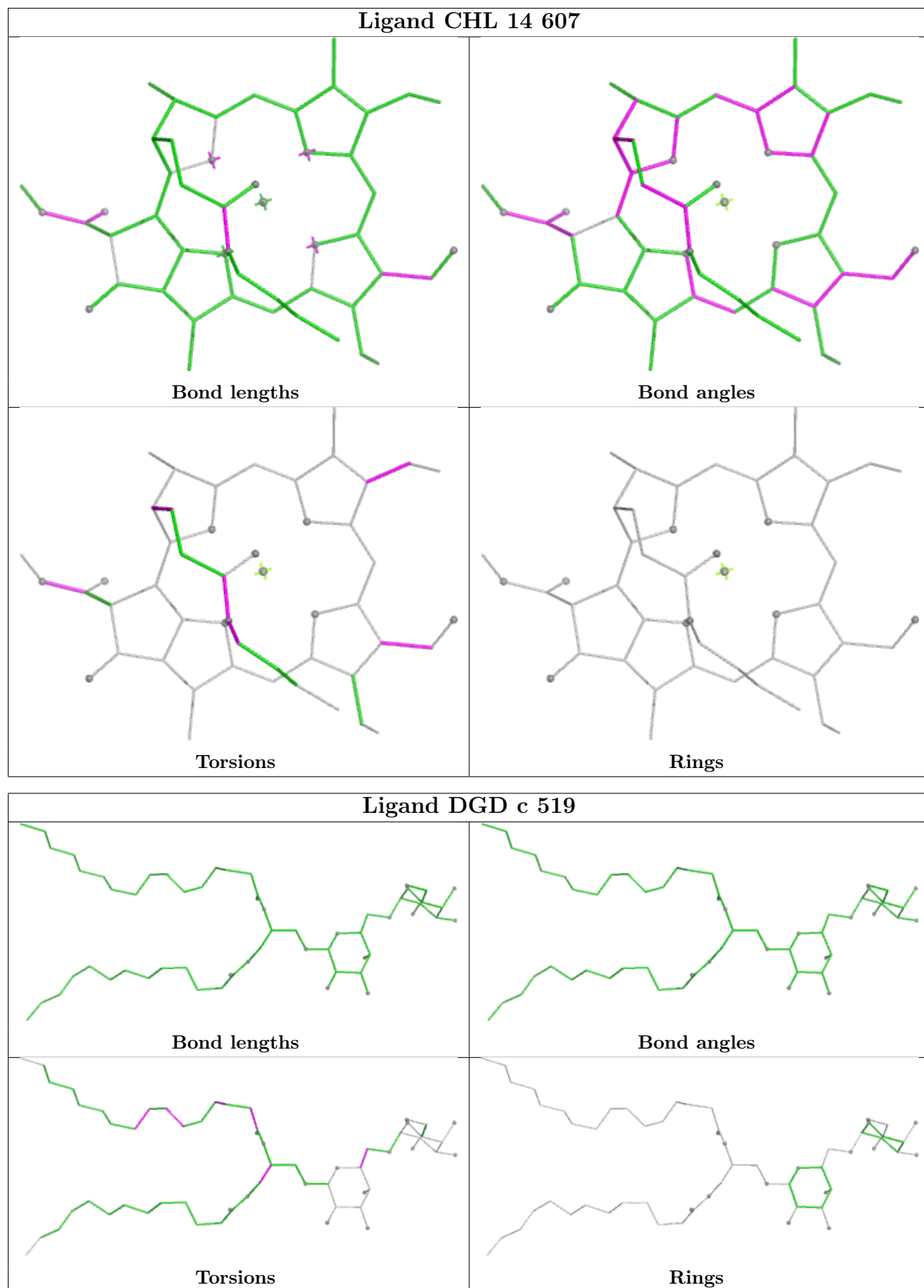
Rings



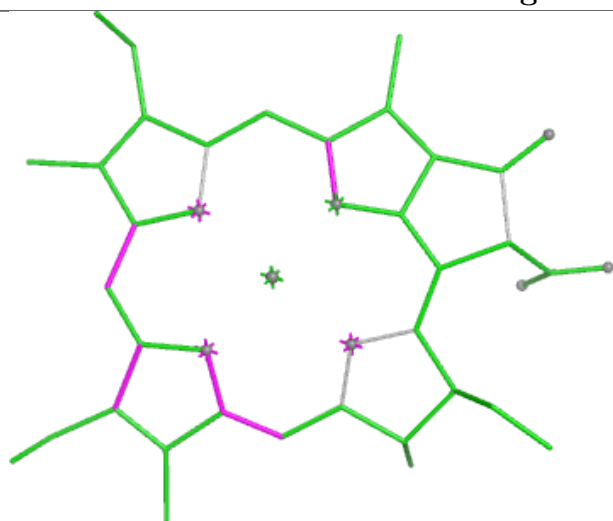




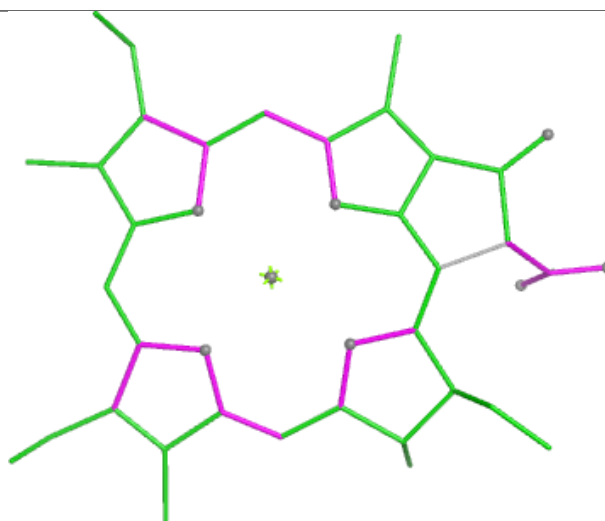




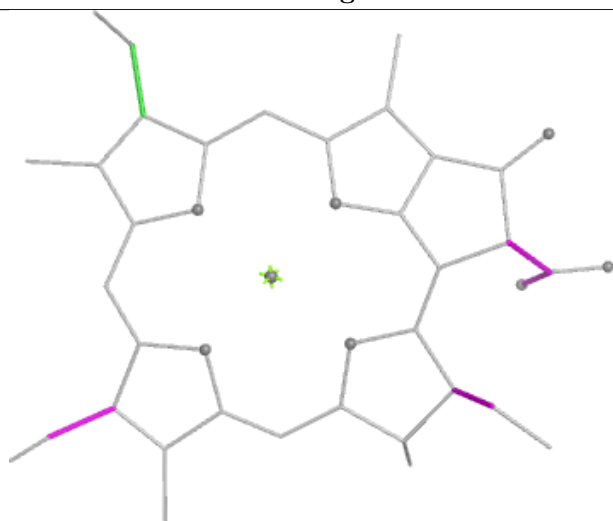
Ligand CLA s 603



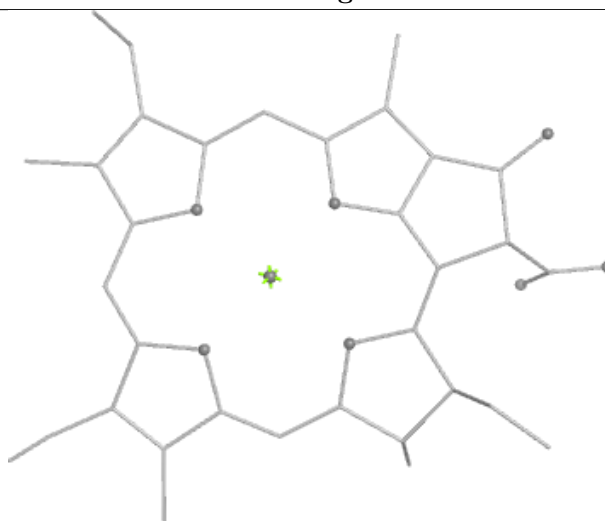
Bond lengths



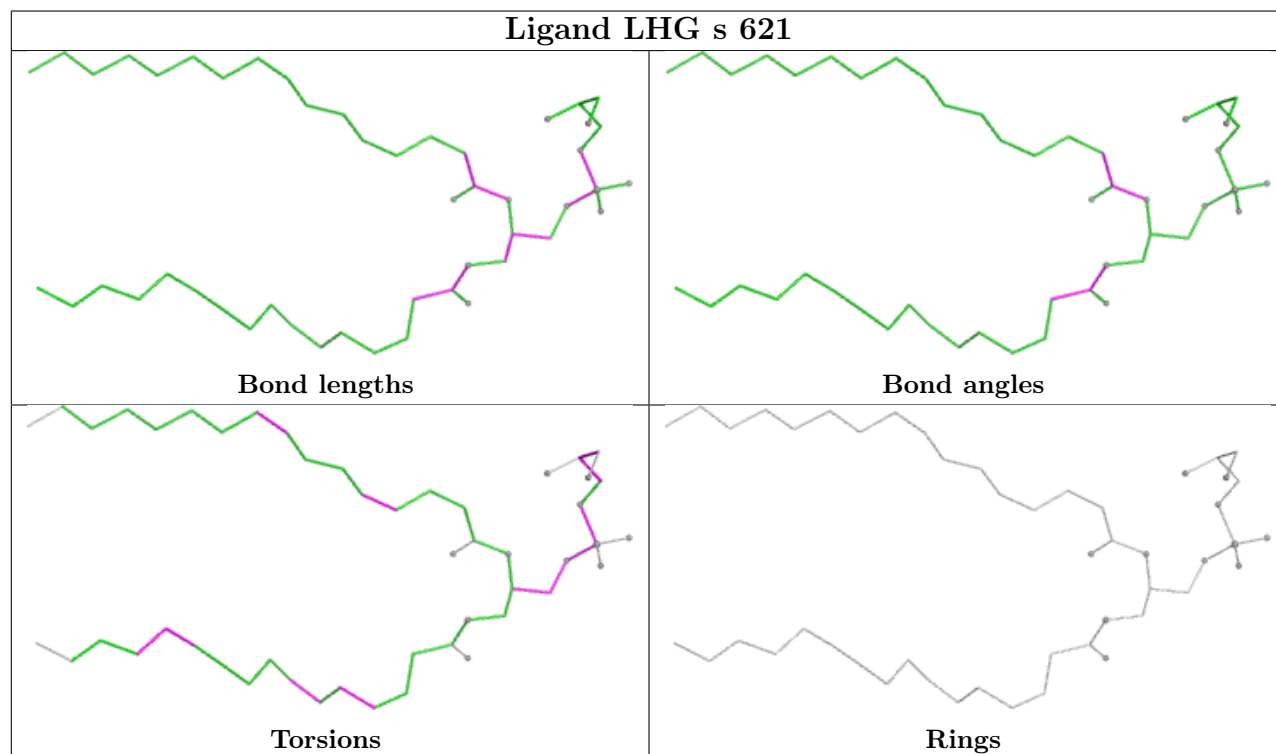
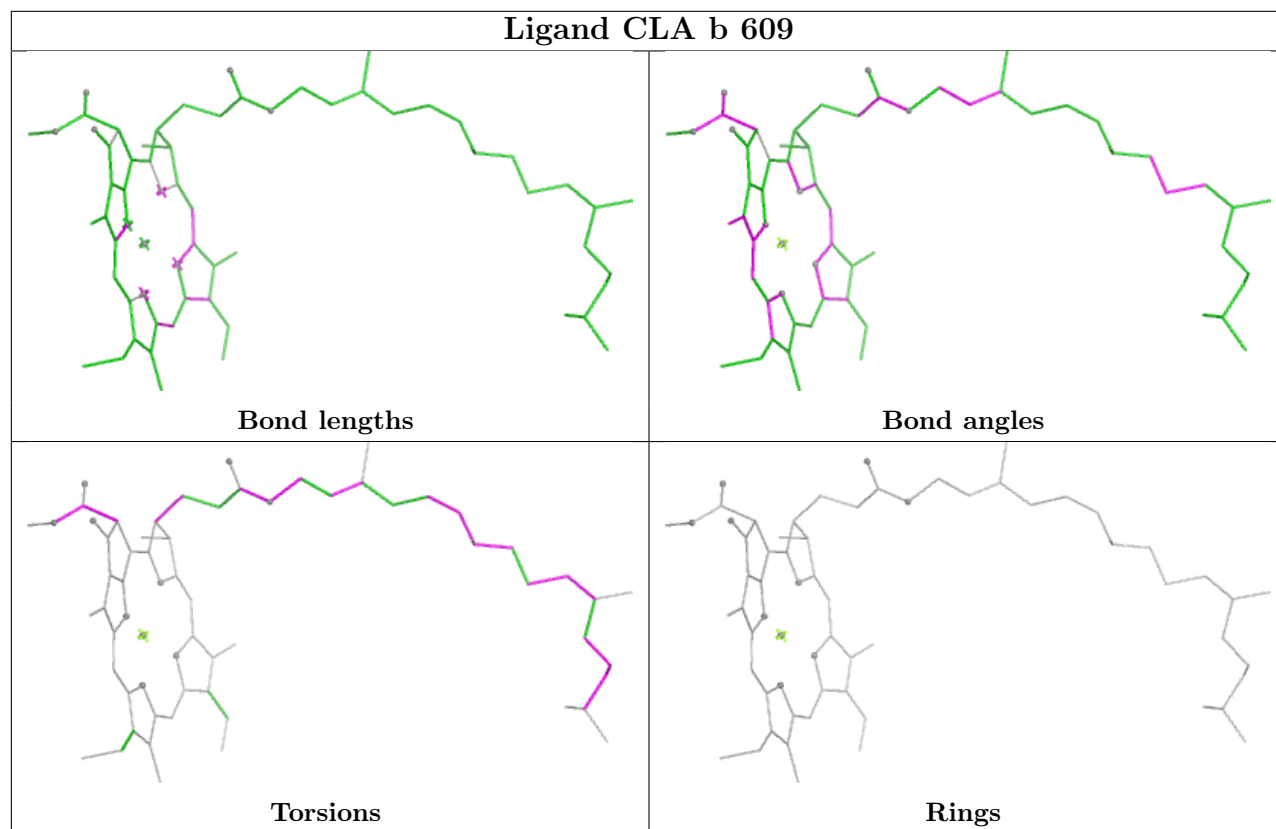
Bond angles

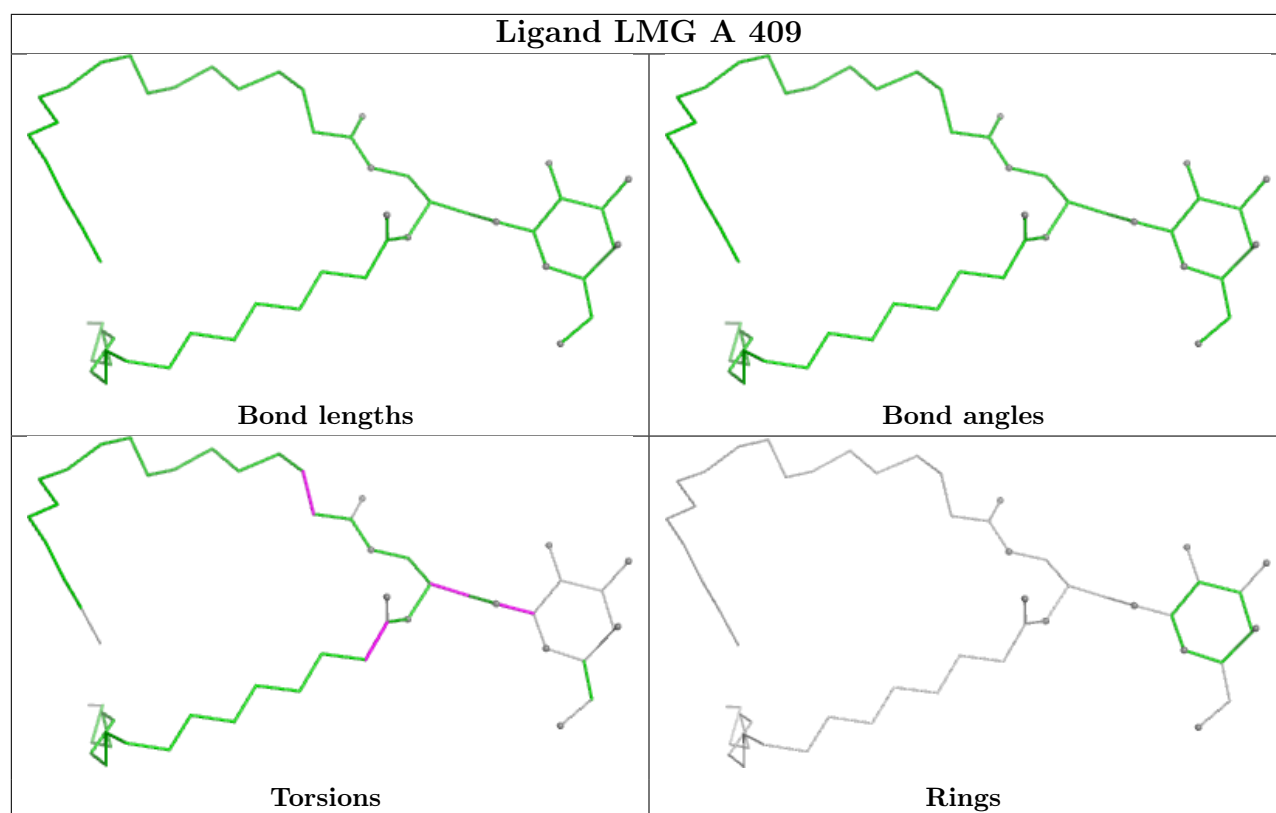


Torsions

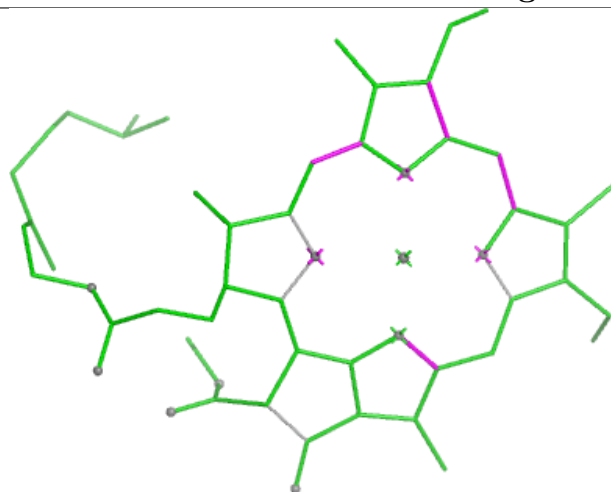


Rings

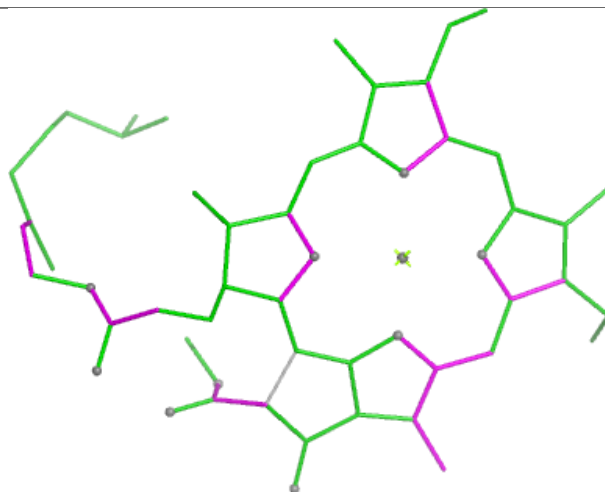




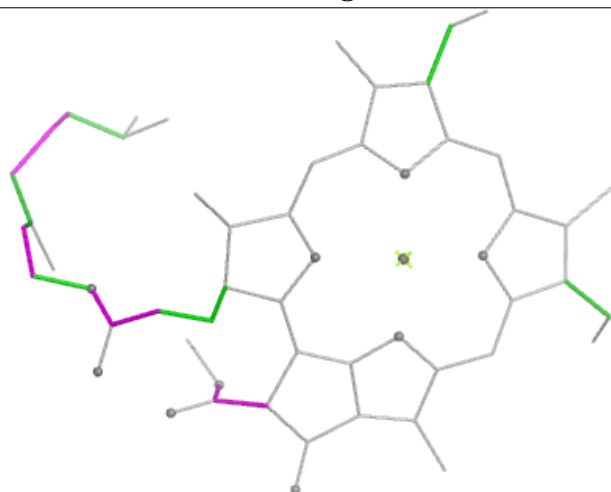
Ligand CLA 2 603



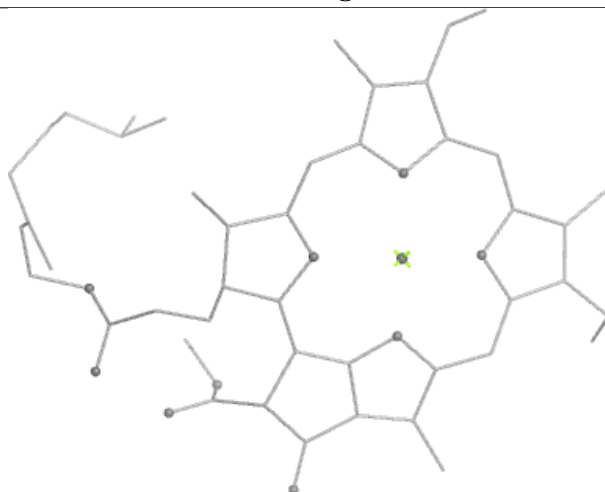
Bond lengths



Bond angles

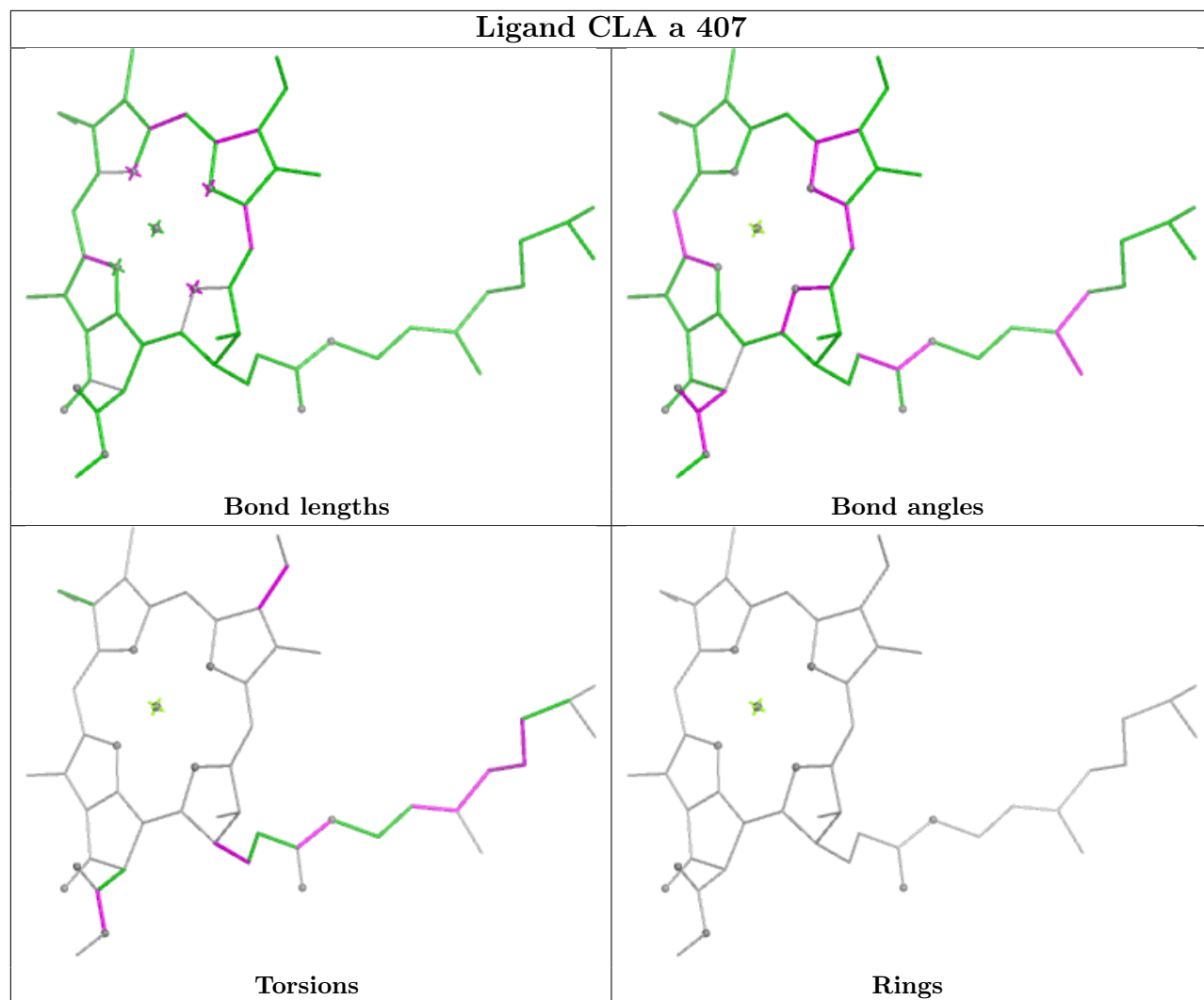


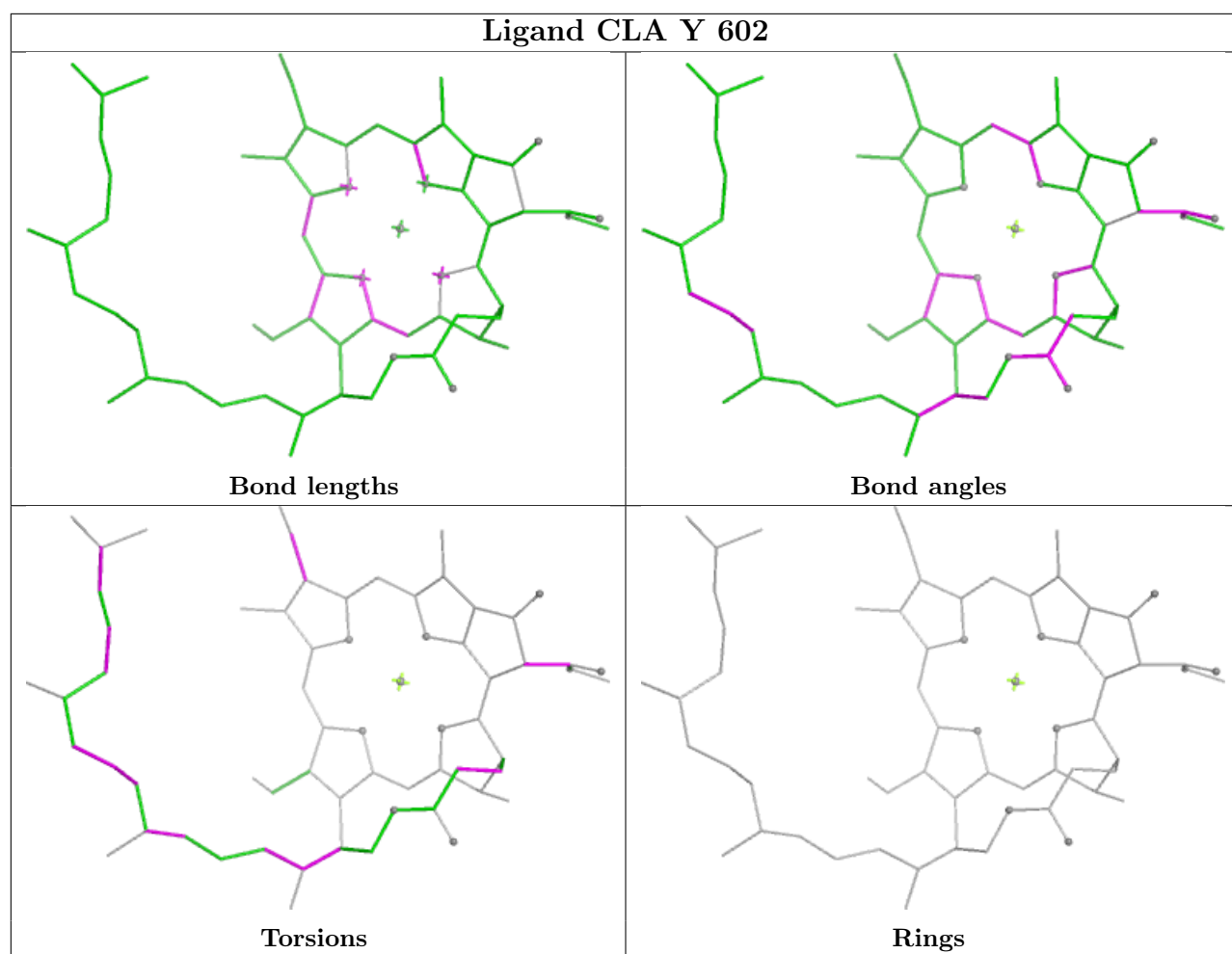
Torsions

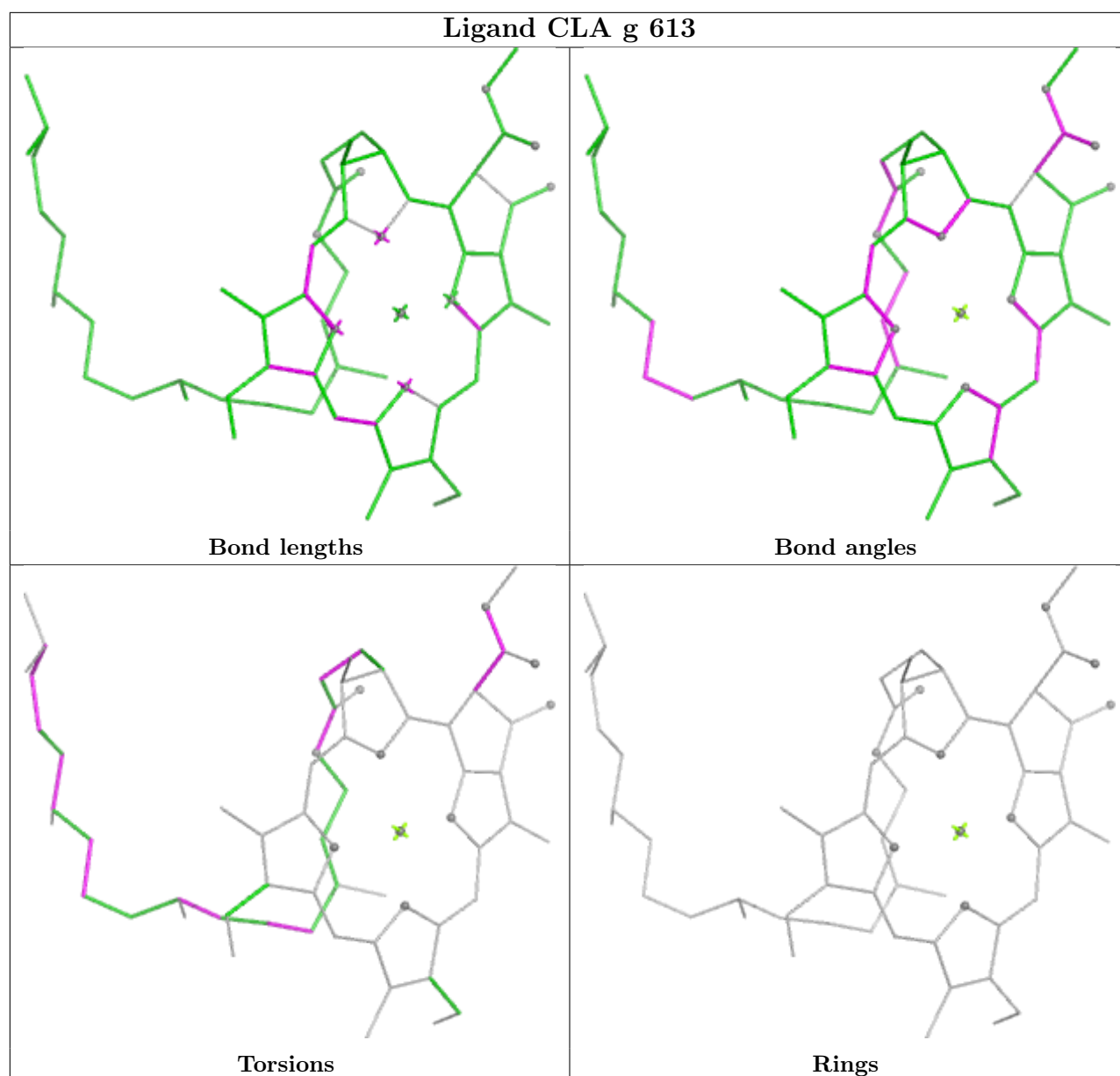


Rings

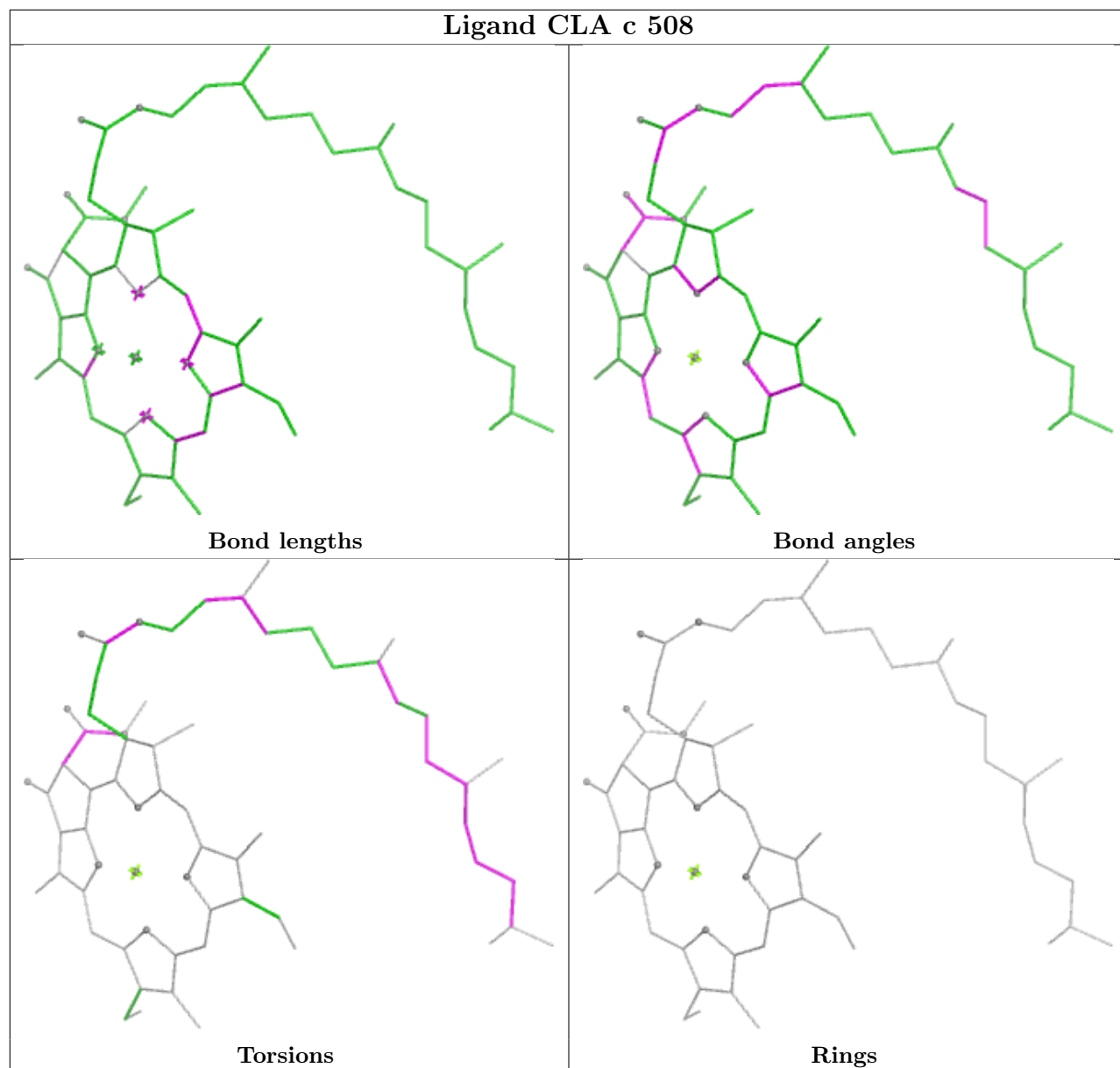
Ligand CLA a 407

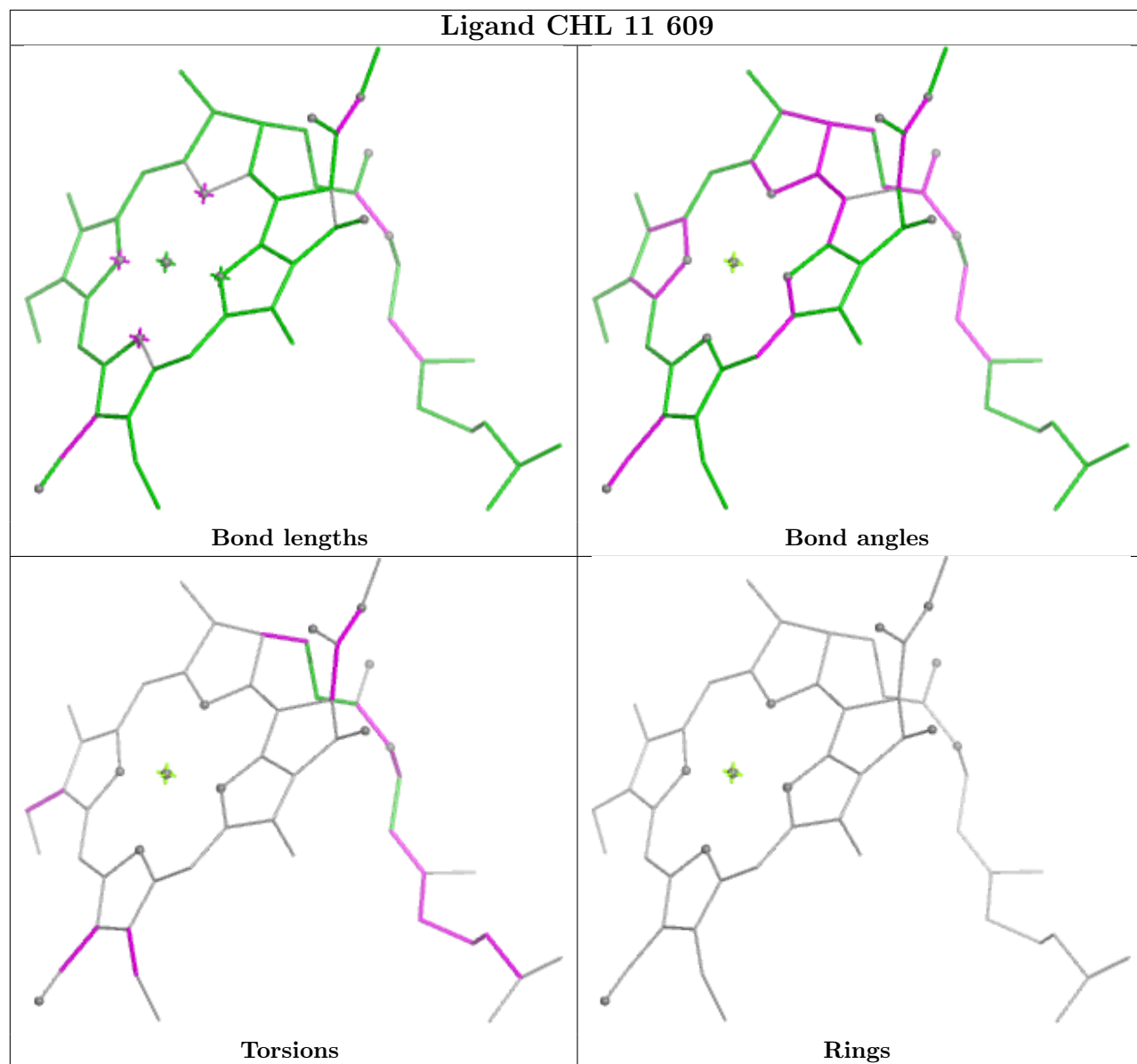




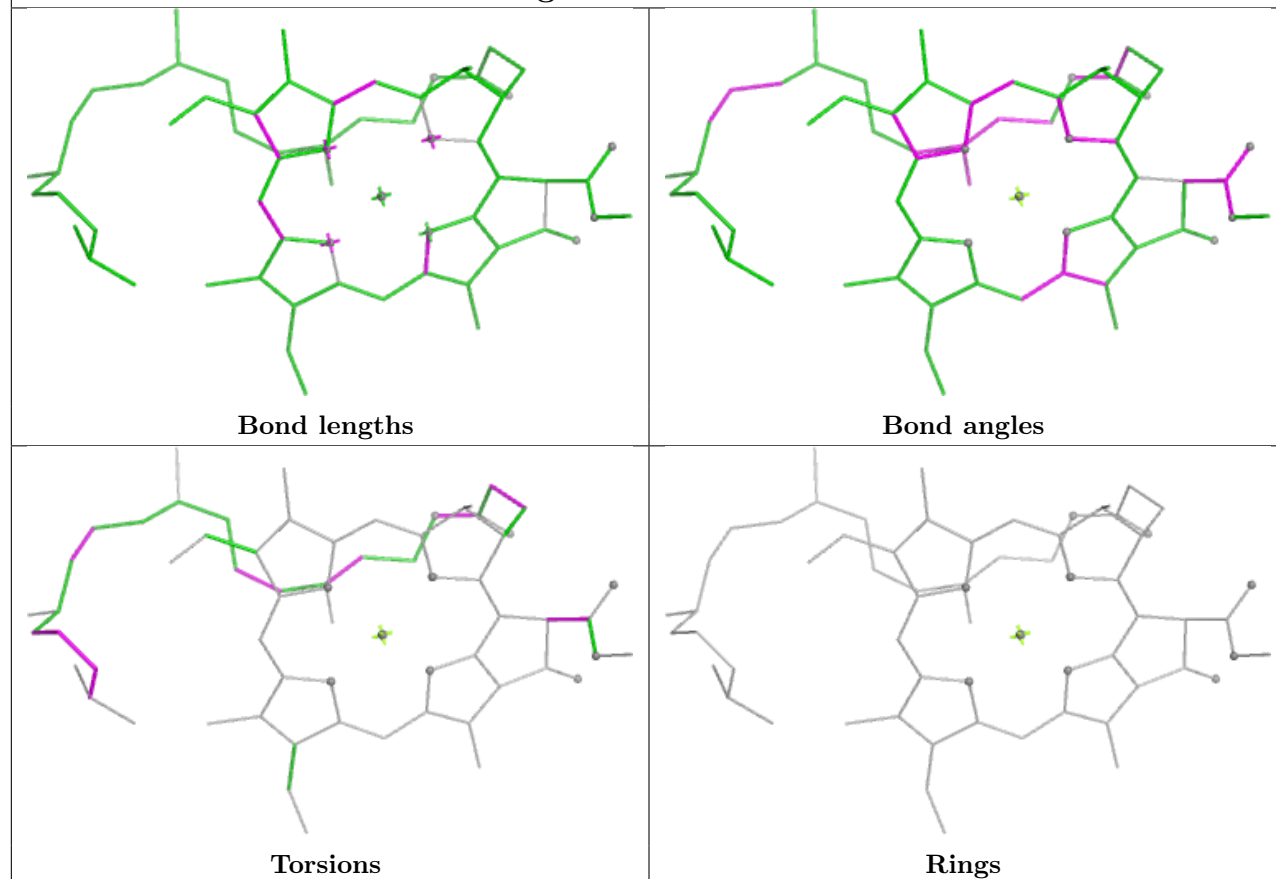


Ligand CLA c 508

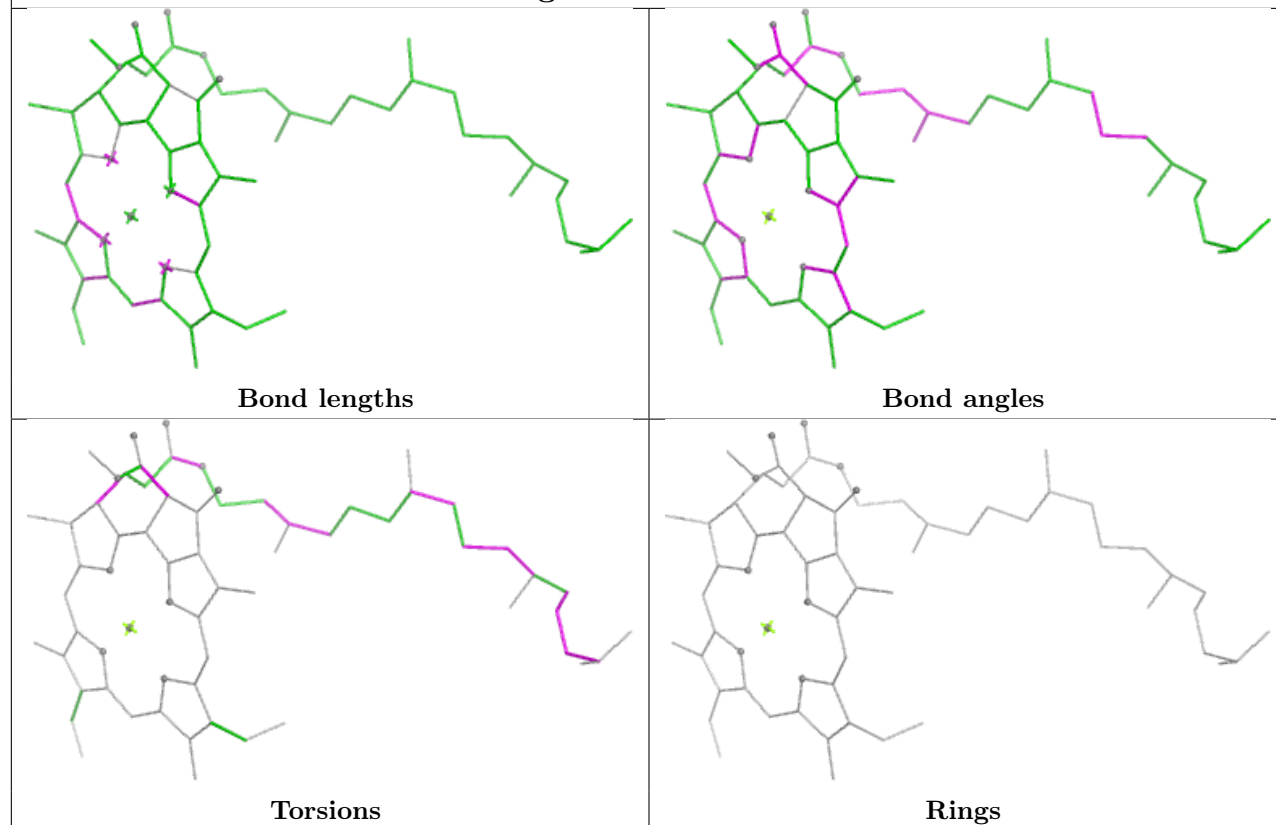


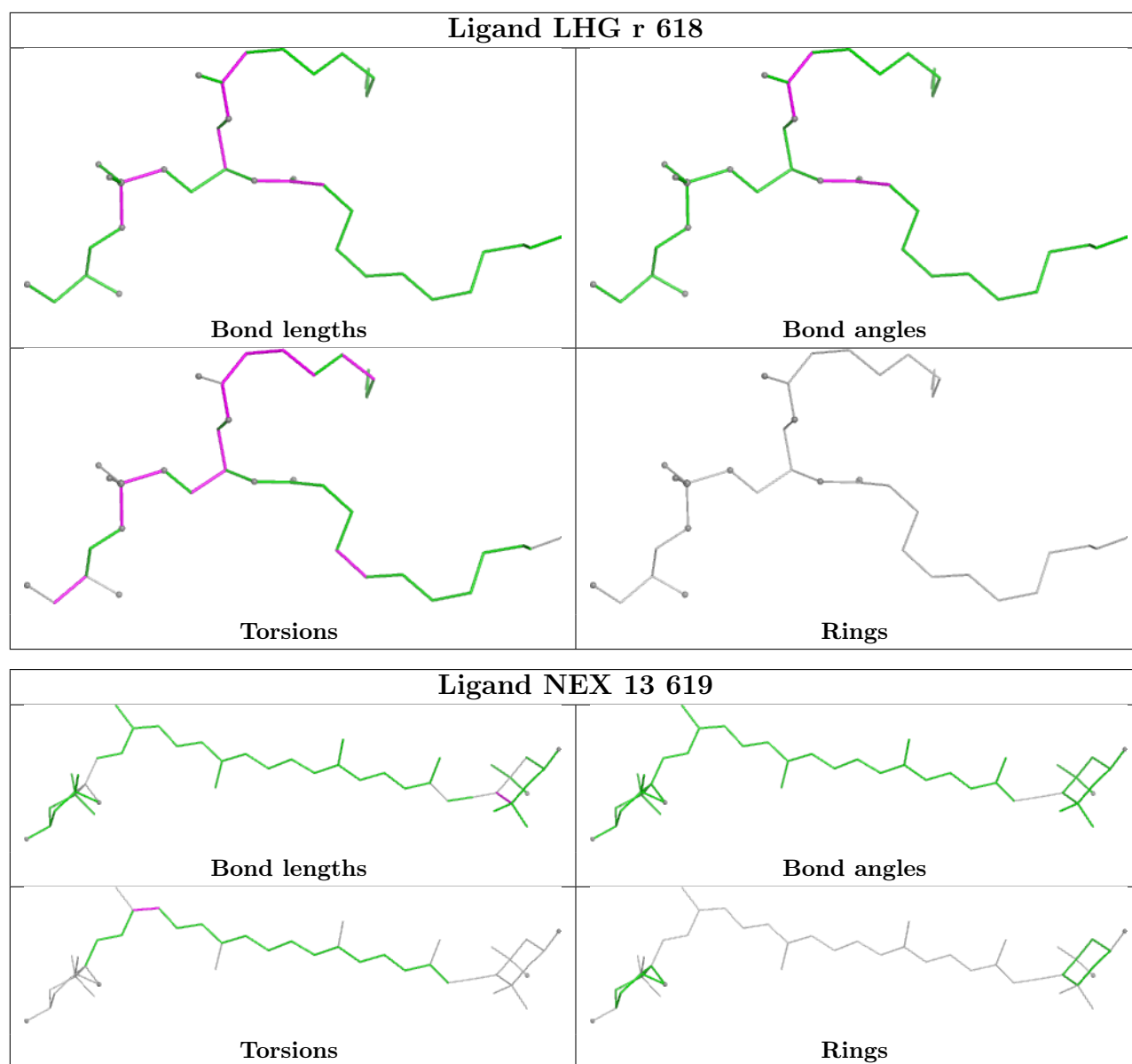


Ligand CLA c 506

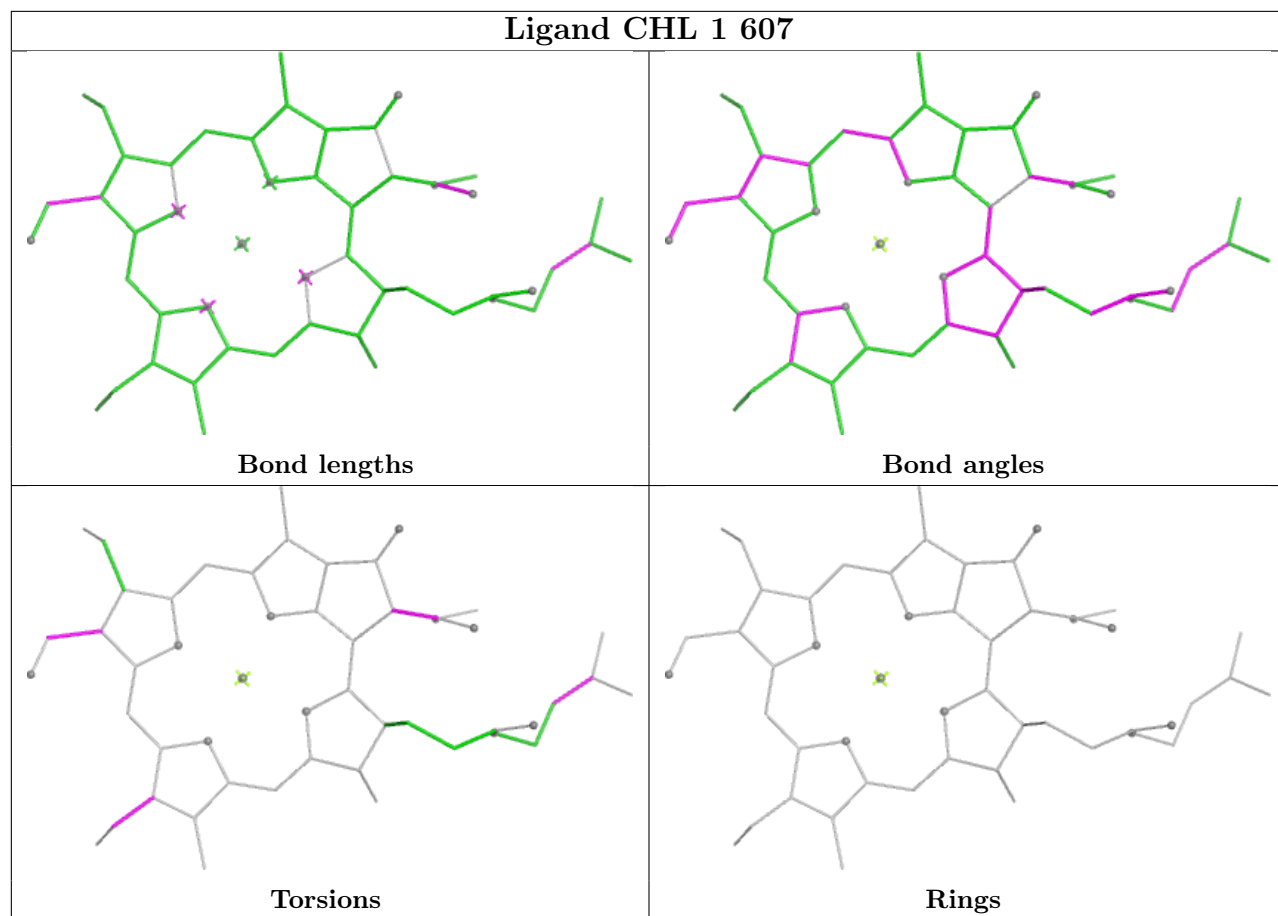


Ligand CLA s 611

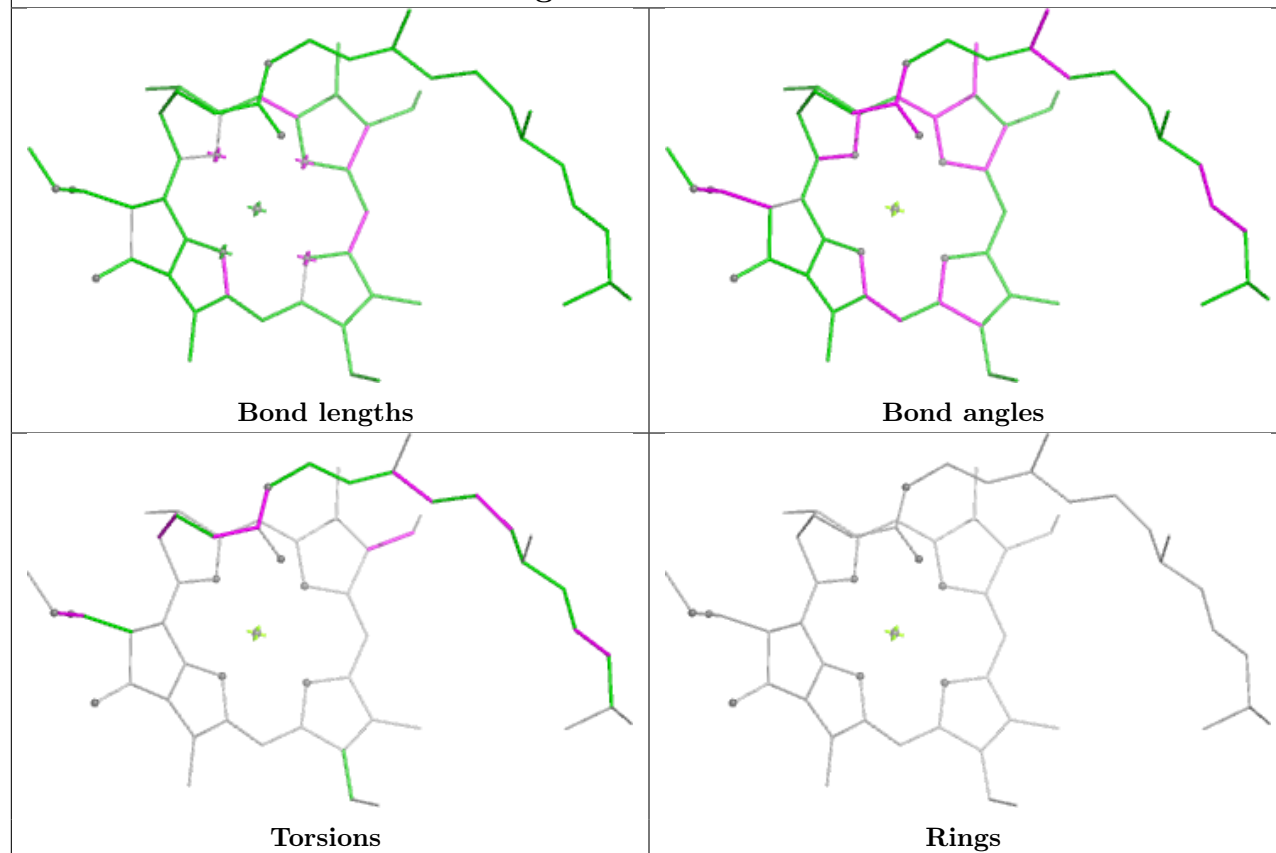




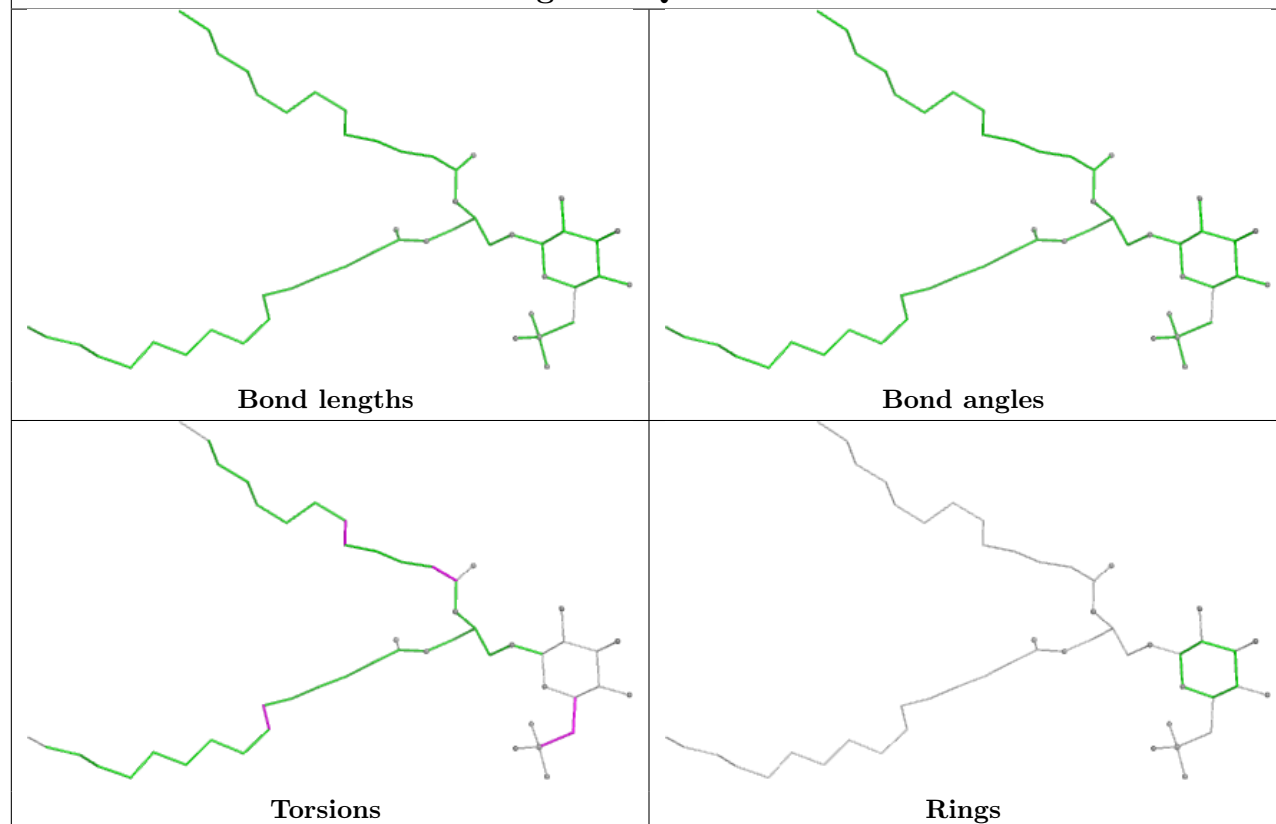
Ligand CHL 1 607

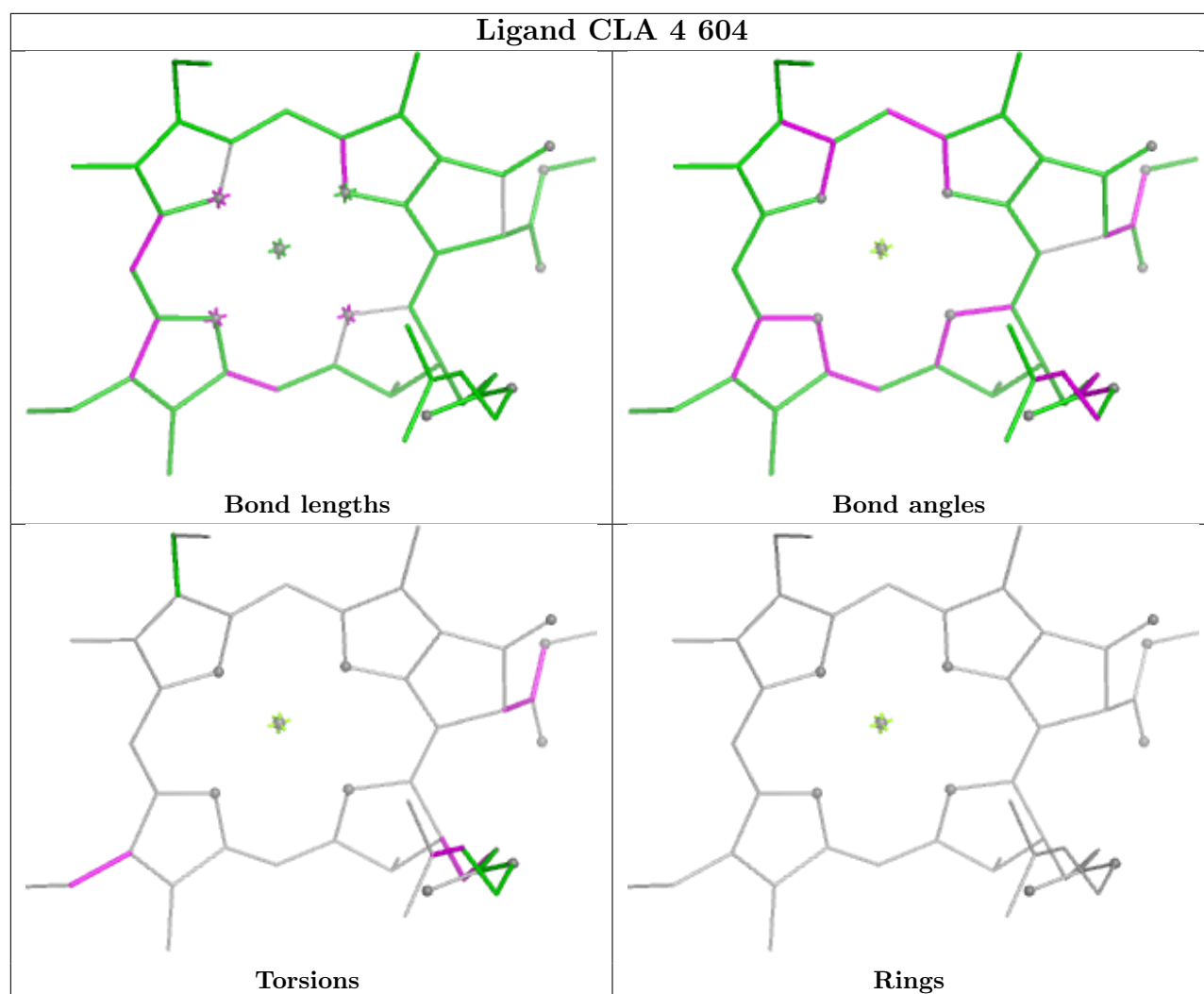


Ligand CLA n 610



Ligand SQD a 409





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.

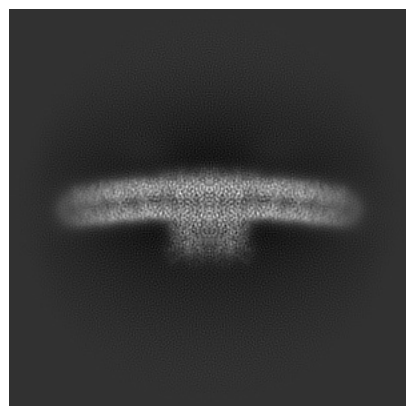
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52056. These allow visual inspection of the internal detail of the map and identification of artifacts.

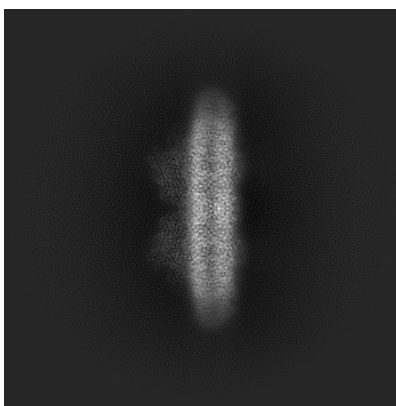
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

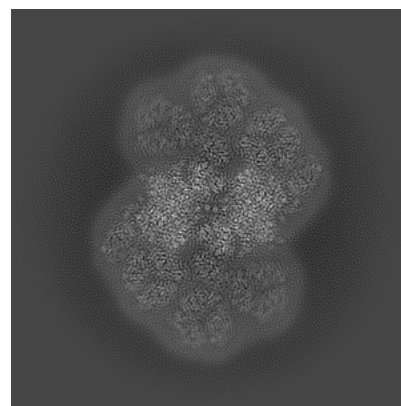
6.1.1 Primary map



X

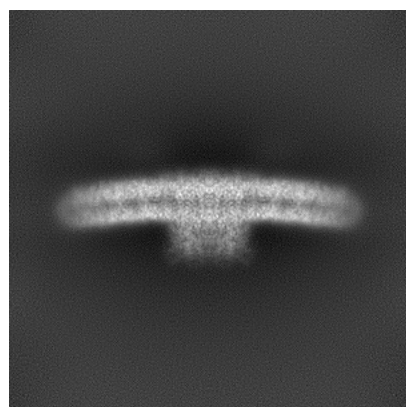


Y

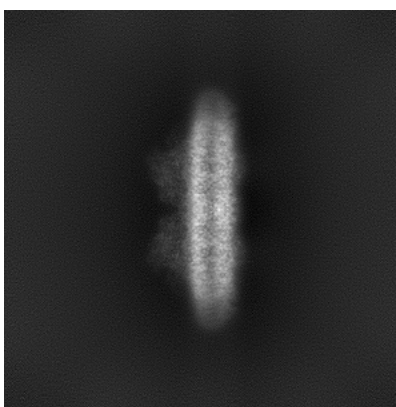


Z

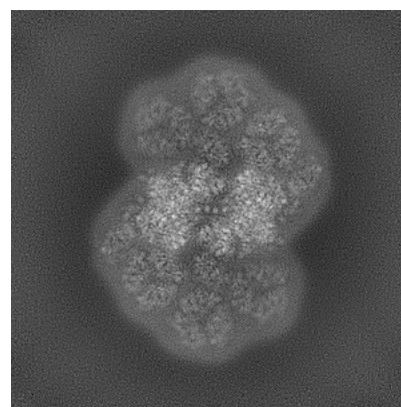
6.1.2 Raw map



X



Y

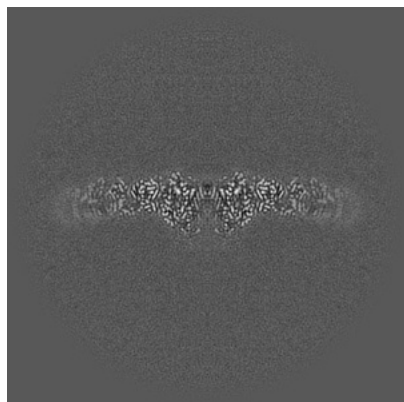


Z

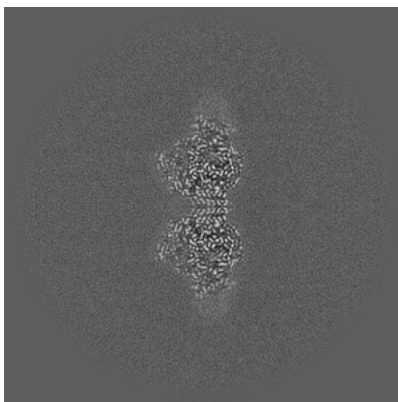
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

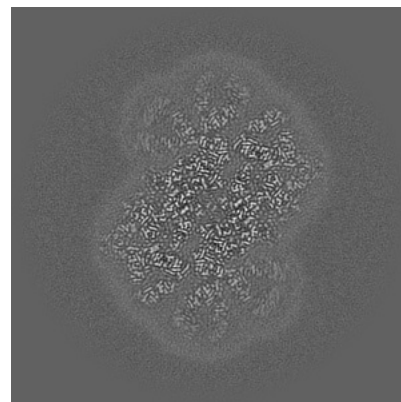
6.2.1 Primary map



X Index: 240

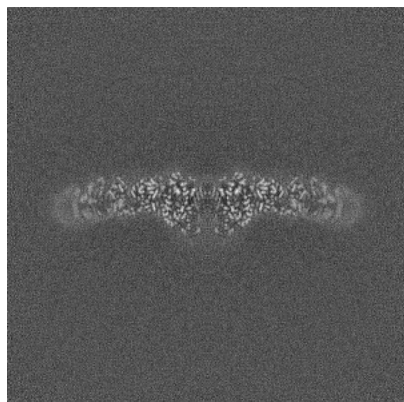


Y Index: 240

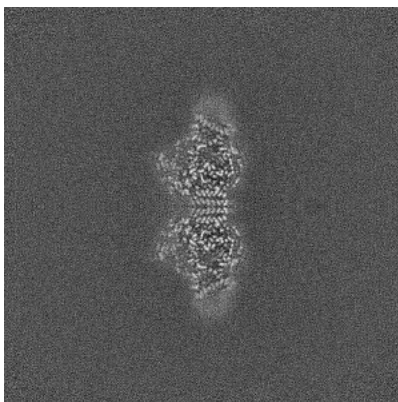


Z Index: 240

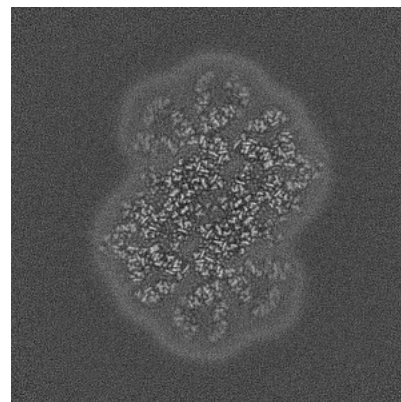
6.2.2 Raw map



X Index: 240



Y Index: 240

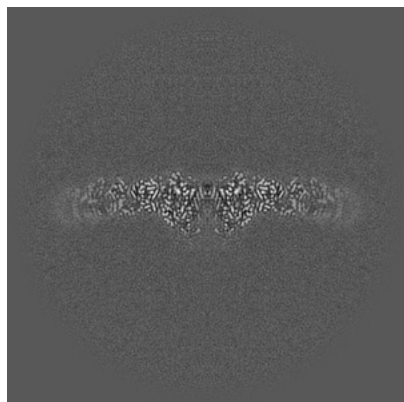


Z Index: 240

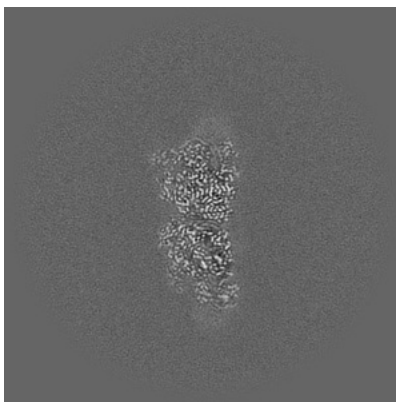
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

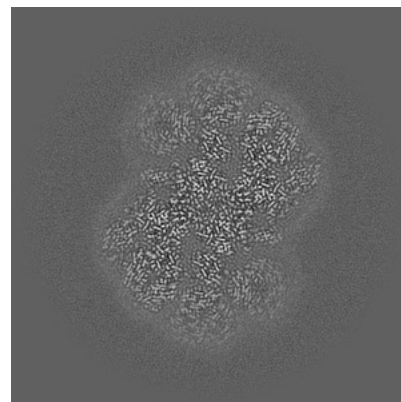
6.3.1 Primary map



X Index: 240

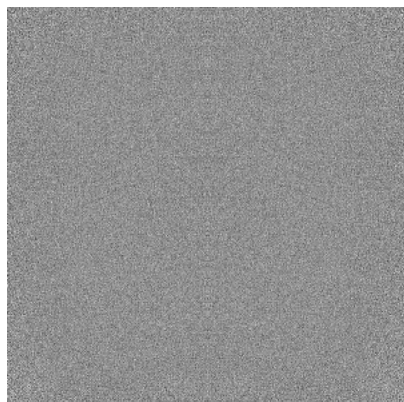


Y Index: 214

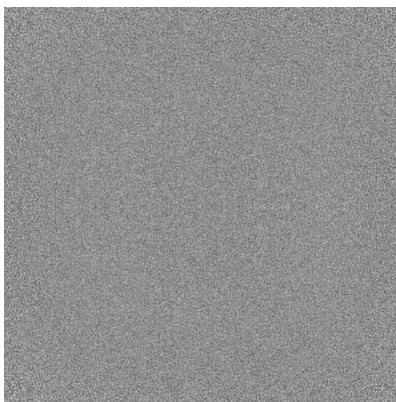


Z Index: 259

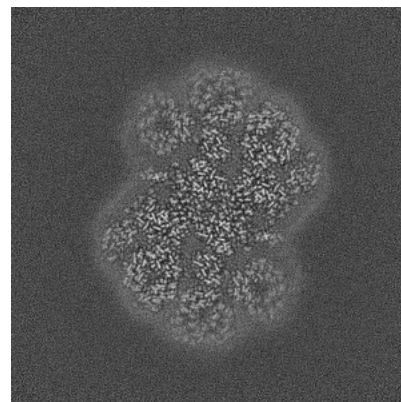
6.3.2 Raw map



X Index: 0



Y Index: 0

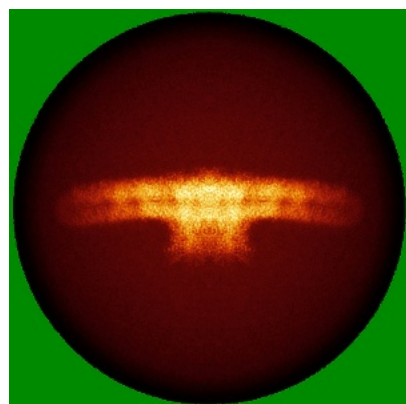


Z Index: 259

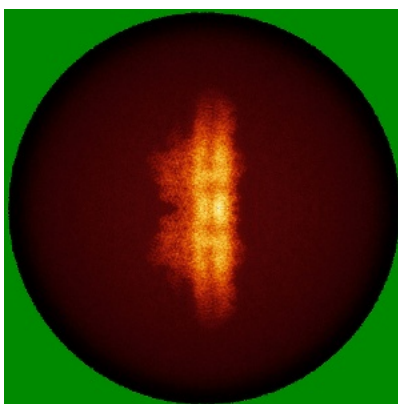
The images above show the largest variance slices of the map in three orthogonal directions.

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

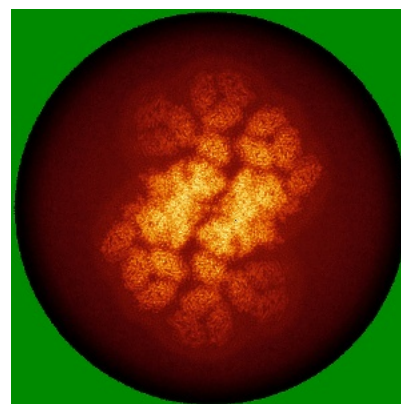
6.4.1 Primary map



X

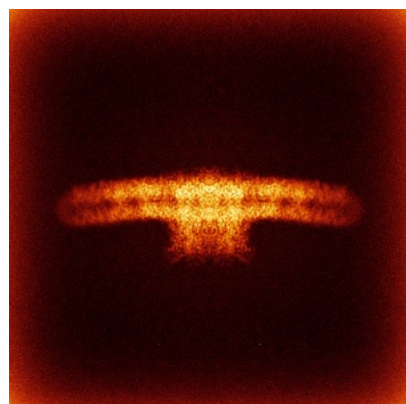


Y

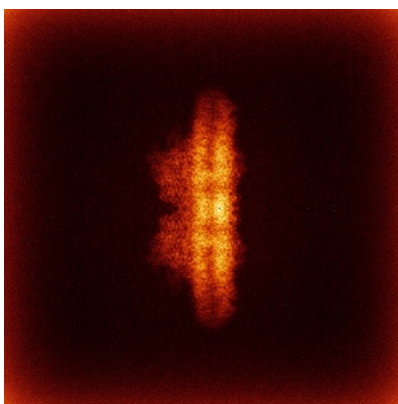


Z

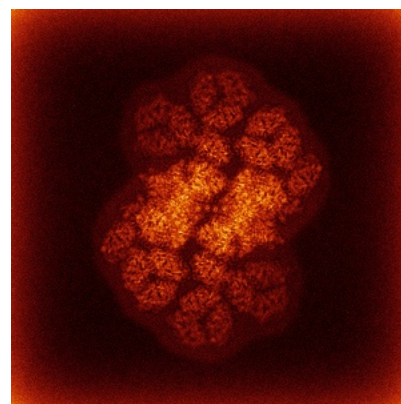
6.4.2 Raw map



X



Y

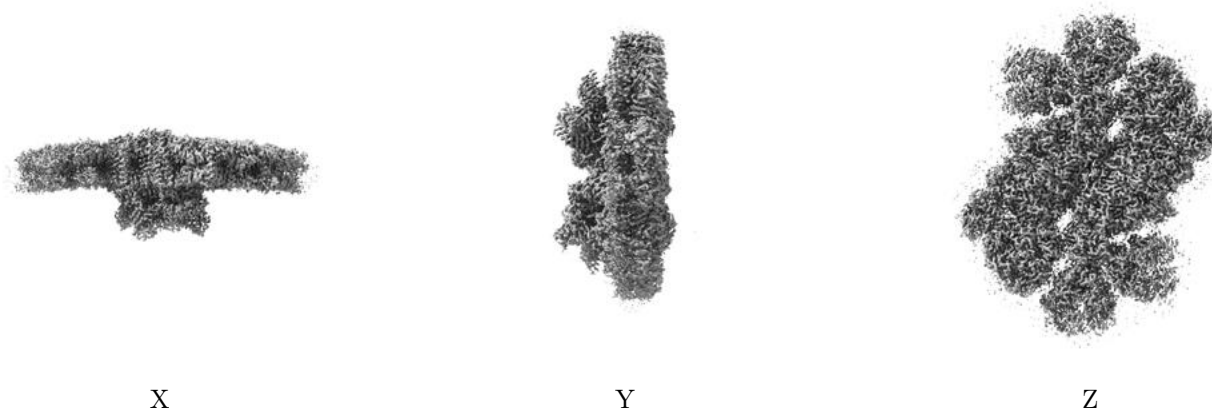


Z

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.

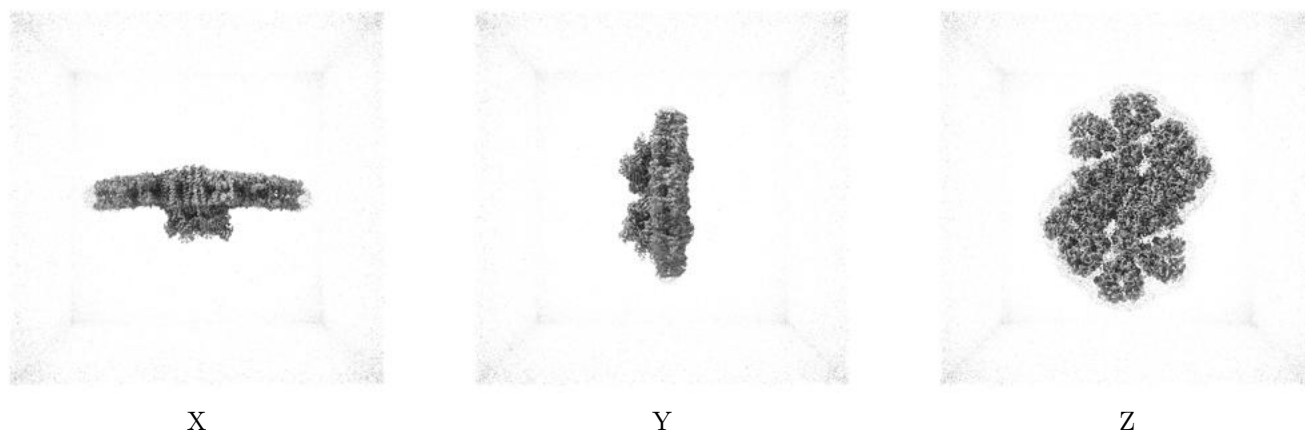
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

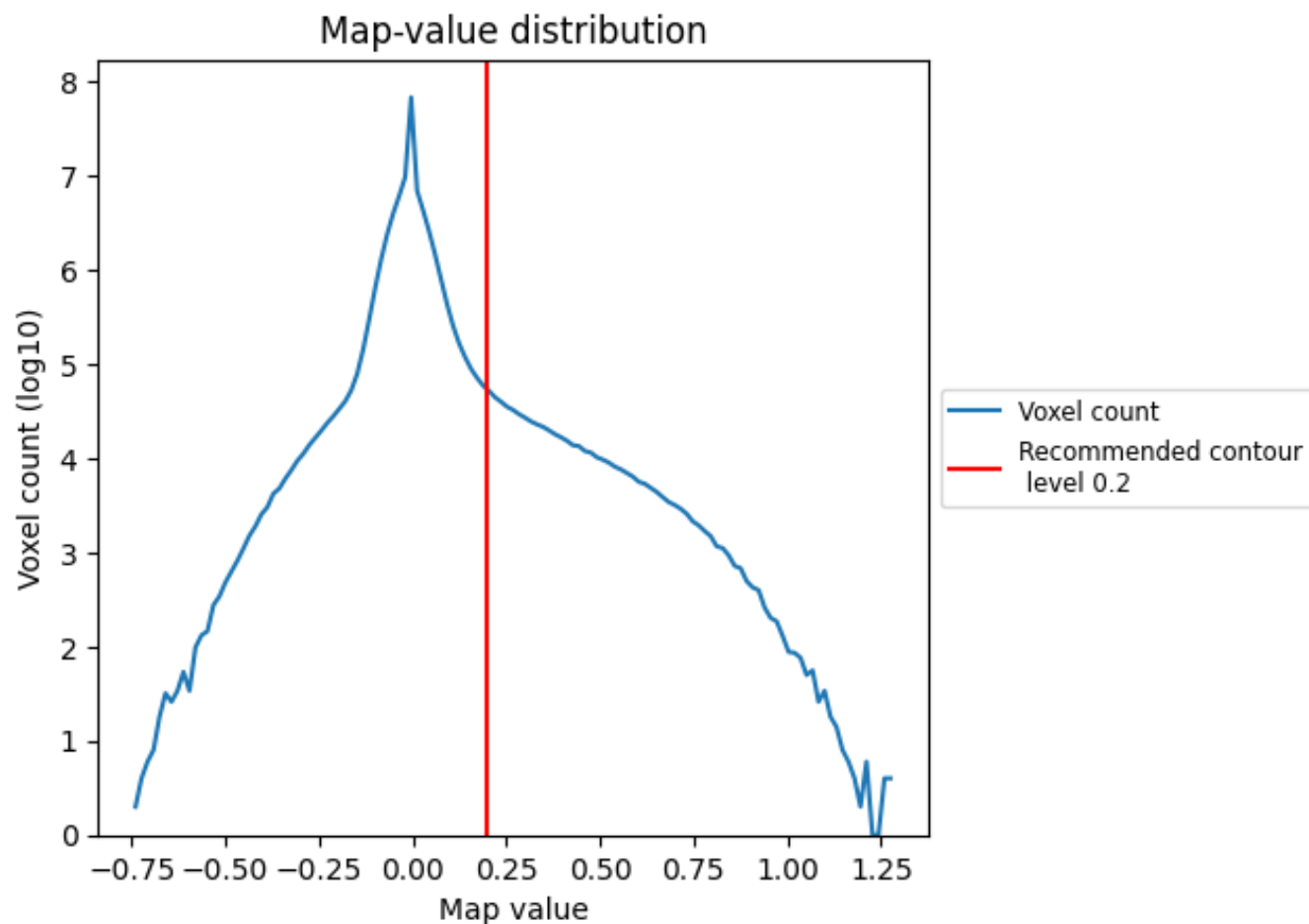
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

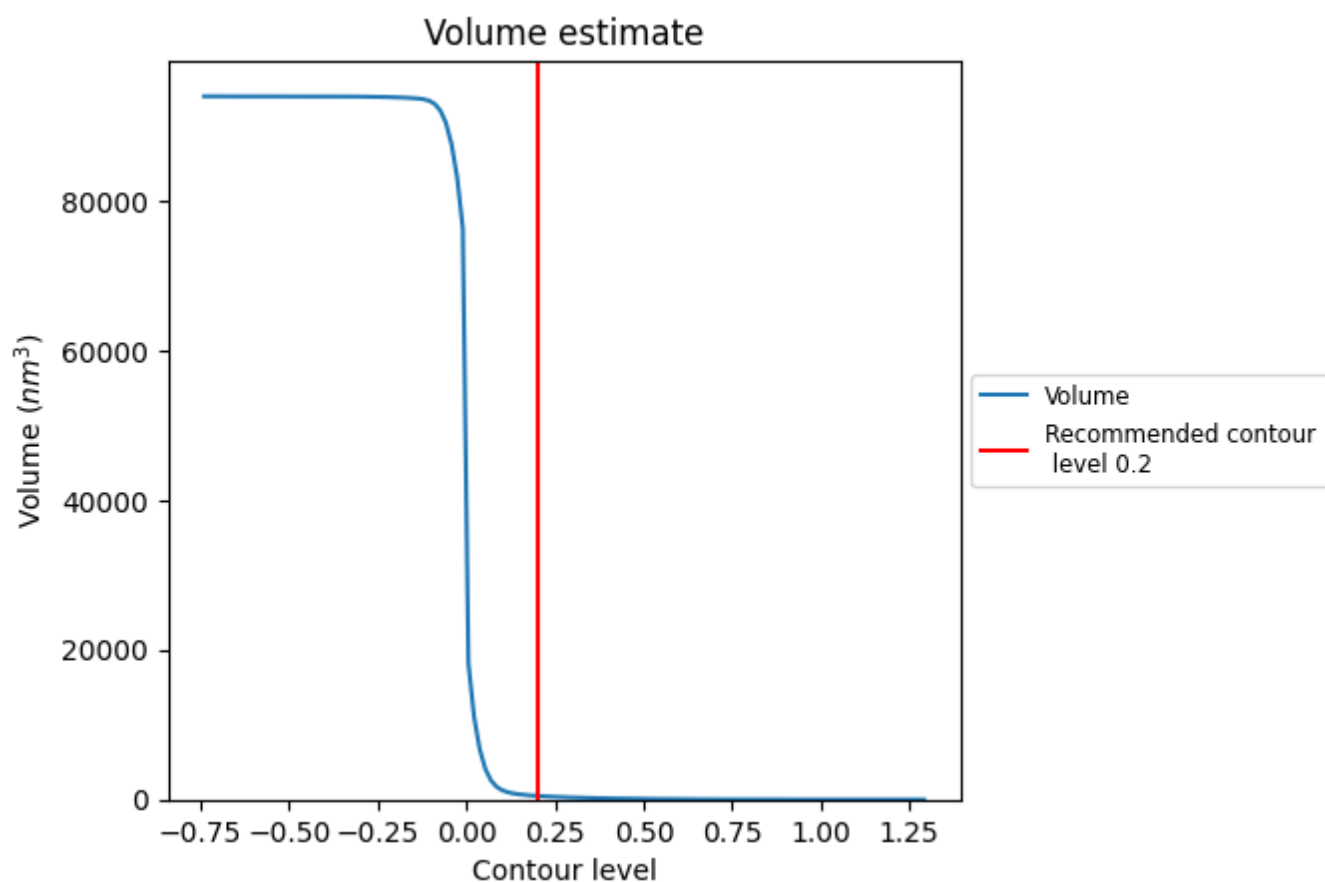
This section contains the results of statistical analysis of the map.

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.

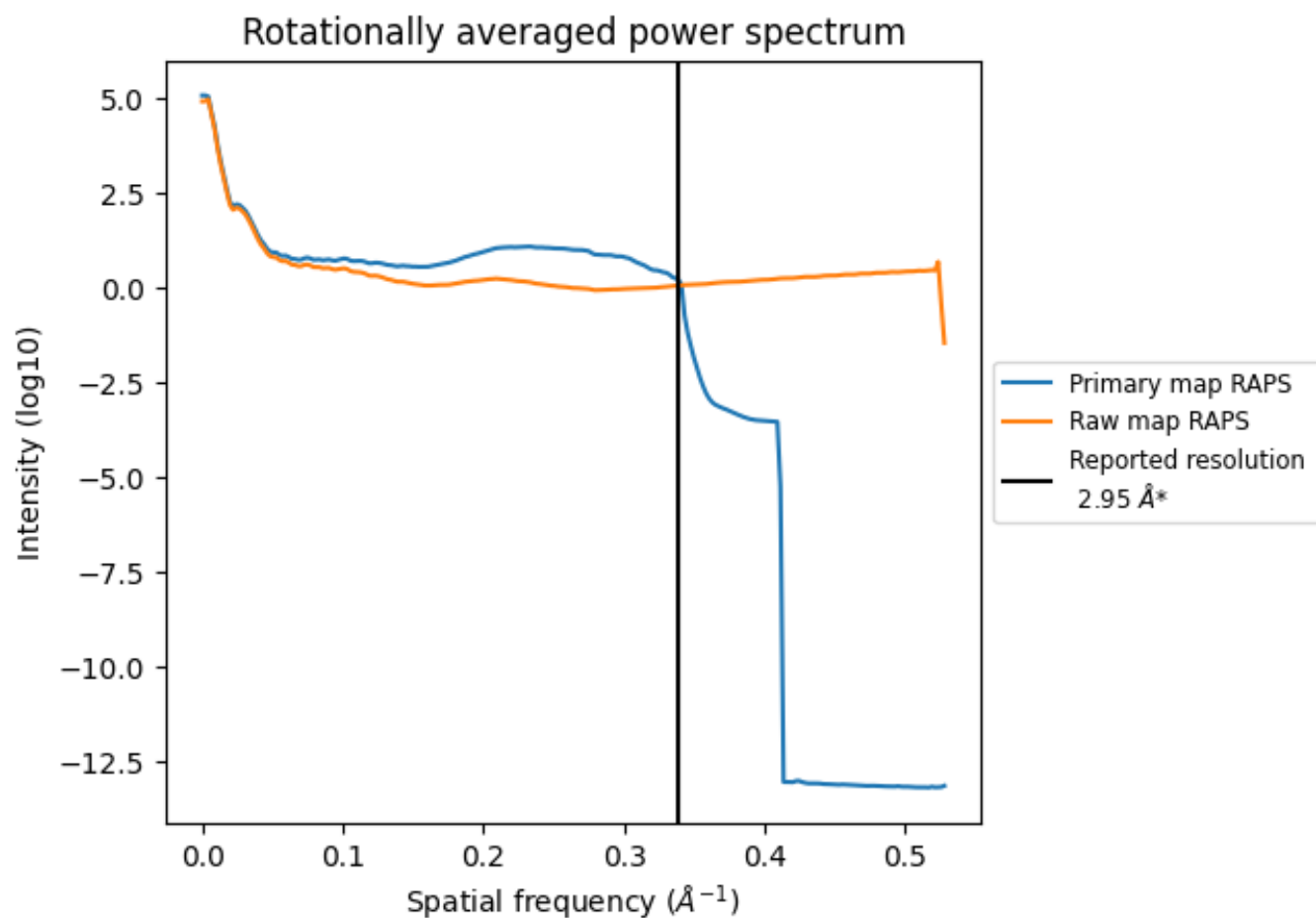
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 486 nm³; this corresponds to an approximate mass of 439 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

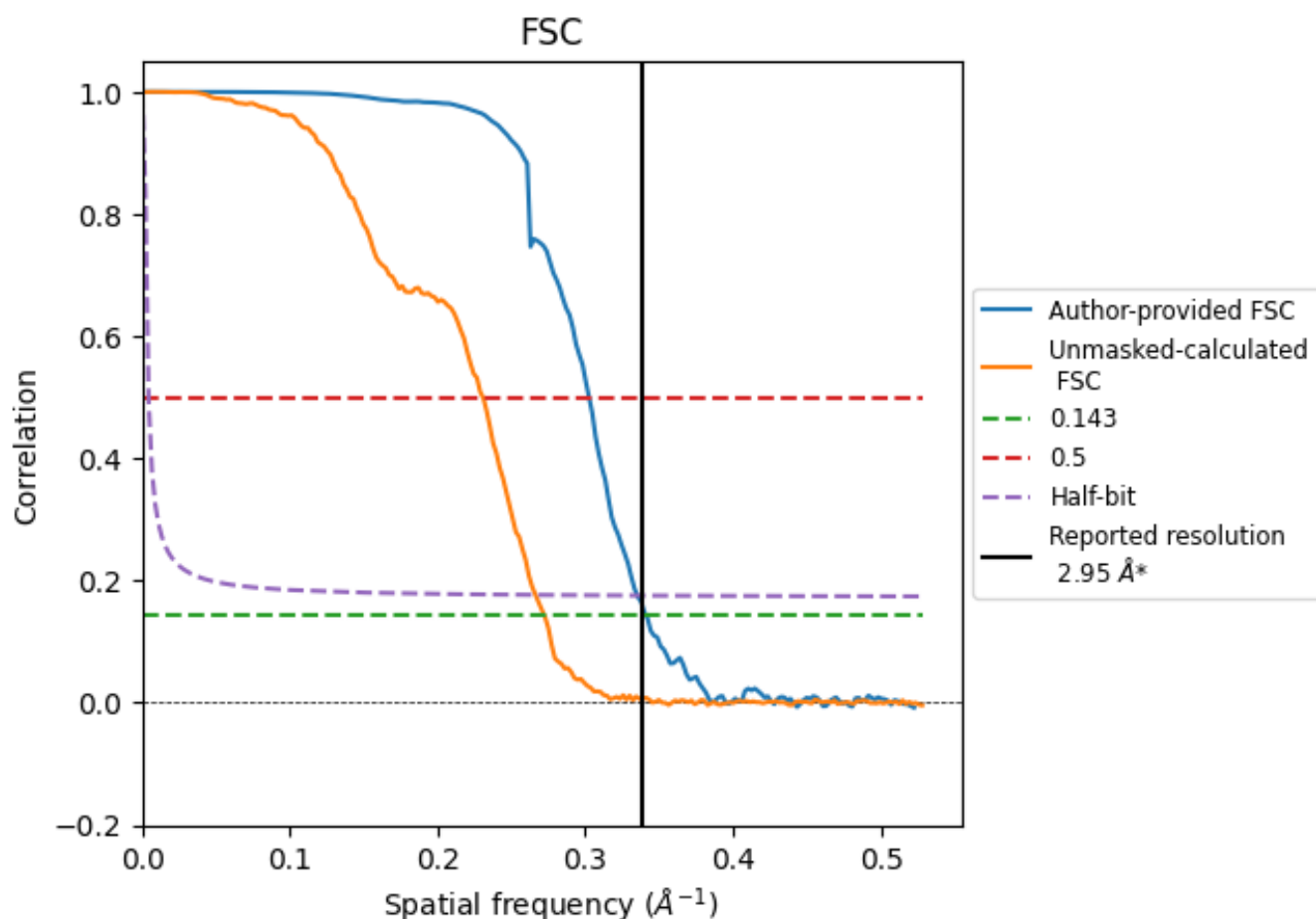


*Reported resolution corresponds to spatial frequency of 0.339 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.339 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

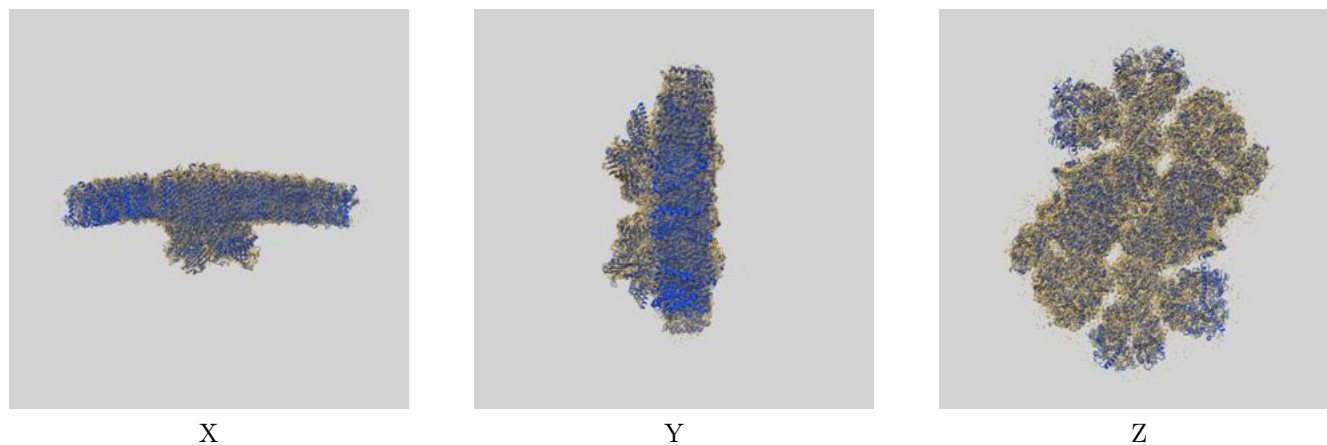
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.95	-	-
Author-provided FSC curve	2.93	3.31	2.98
Unmasked-calculated*	3.67	4.33	3.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.67 differs from the reported value 2.95 by more than 10 %

9 Map-model fit [i](#)

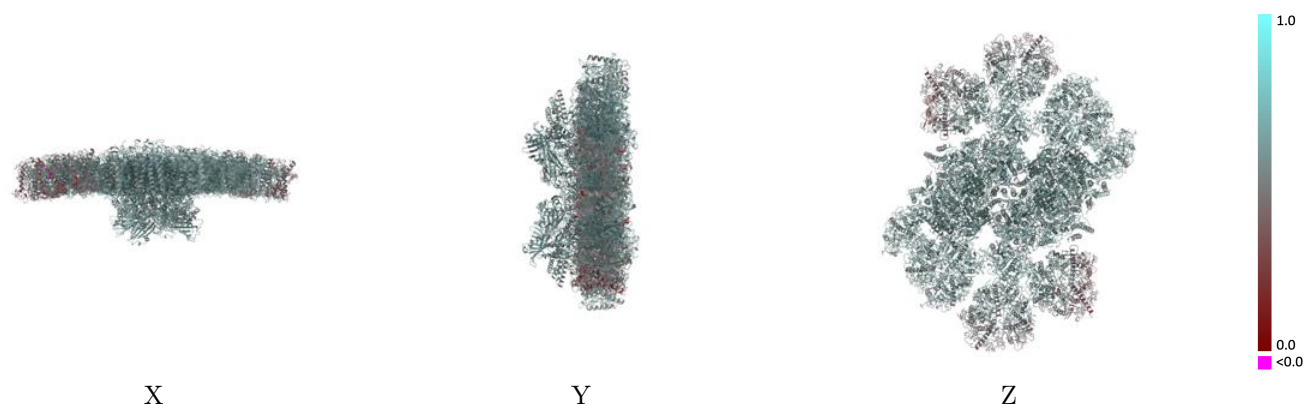
This section contains information regarding the fit between EMDB map EMD-52056 and PDB model 9HD7. Per-residue inclusion information can be found in [section 3](#) on [page 51](#).

9.1 Map-model overlay [i](#)



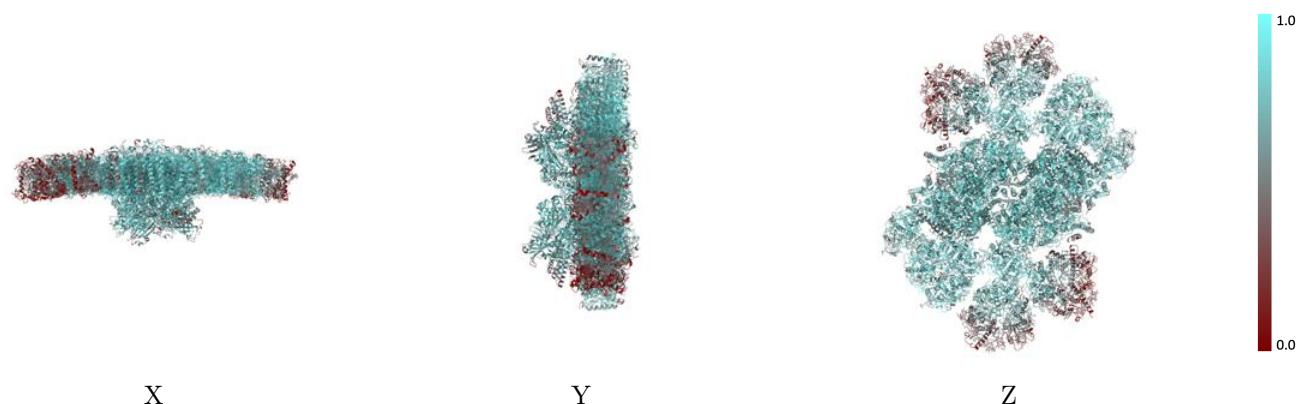
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



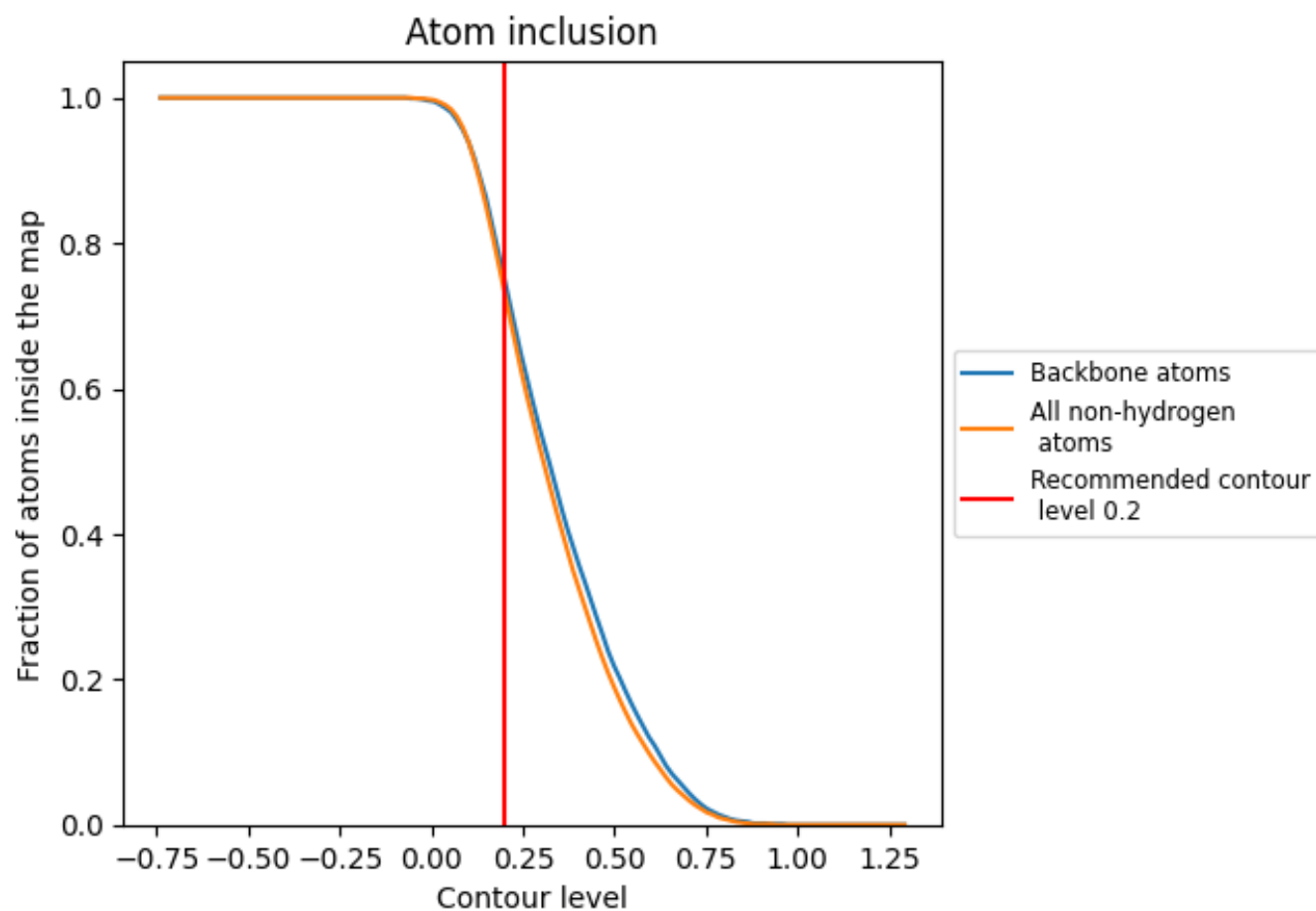
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 73% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7310	 0.5760
1	 0.4700	 0.5130
11	 0.4260	 0.4850
12	 0.2500	 0.4300
13	 0.6560	 0.5560
14	 0.4220	 0.4860
15	 0.2480	 0.4320
16	 0.6510	 0.5550
2	 0.3760	 0.4700
3	 0.7550	 0.5810
4	 0.4620	 0.5080
5	 0.3760	 0.4760
6	 0.7570	 0.5790
7	 0.6010	 0.5670
8	 0.6000	 0.5670
A	 0.8840	 0.6170
B	 0.8780	 0.6130
C	 0.8840	 0.6110
D	 0.8990	 0.6200
E	 0.8340	 0.6050
F	 0.8600	 0.6090
G	 0.7700	 0.5830
H	 0.8650	 0.6040
I	 0.8970	 0.6150
J	 0.7330	 0.5830
K	 0.7920	 0.5790
L	 0.8230	 0.5940
M	 0.7750	 0.5830
N	 0.7950	 0.5870
O	 0.7220	 0.5880
P	 0.6690	 0.5880
Q	 0.5370	 0.5550
R	 0.8390	 0.6050
S	 0.7130	 0.5740
T	 0.7730	 0.5840



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
U	 0.4520	 0.5170
V	 0.5520	 0.5230
W	 0.8050	 0.6020
X	 0.8100	 0.6010
Y	 0.8720	 0.6150
Z	 0.7120	 0.5670
a	 0.8900	 0.6180
b	 0.8820	 0.6160
c	 0.8820	 0.6110
d	 0.8970	 0.6190
e	 0.8380	 0.6050
f	 0.8510	 0.6090
g	 0.7660	 0.5830
h	 0.8700	 0.6070
i	 0.9000	 0.6140
j	 0.7420	 0.5820
k	 0.8320	 0.5760
l	 0.8230	 0.5950
m	 0.7800	 0.5820
n	 0.7960	 0.5850
o	 0.7230	 0.5880
p	 0.6770	 0.5890
q	 0.5380	 0.5530
r	 0.8360	 0.6070
s	 0.7150	 0.5760
t	 0.8090	 0.5910
u	 0.4570	 0.5240
v	 0.5660	 0.5370
w	 0.8060	 0.6010
x	 0.7990	 0.6060
y	 0.8730	 0.6140
z	 0.7040	 0.5670