



wwPDB EM Validation Summary Report ⓘ

Sep 20, 2026 – 02:39 pm BST

PDB ID : 8BD3 / pdb_00008bd3
EMDB ID : EMD-15973
Title : Cryo-EM structure of the Photosystem II - LHCII supercomplex from Chlorella
ohadi
Authors : Fadeeva, M.; Klaiman, D.; Caspy, I.; Nelson, N.
Deposited on : 2022-10-18
Resolution : 2.73 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

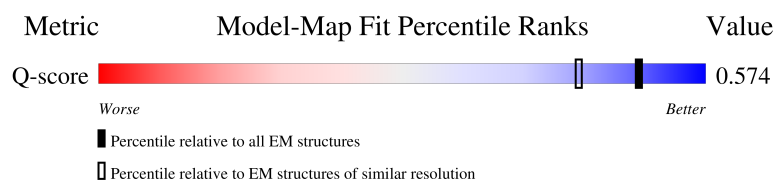
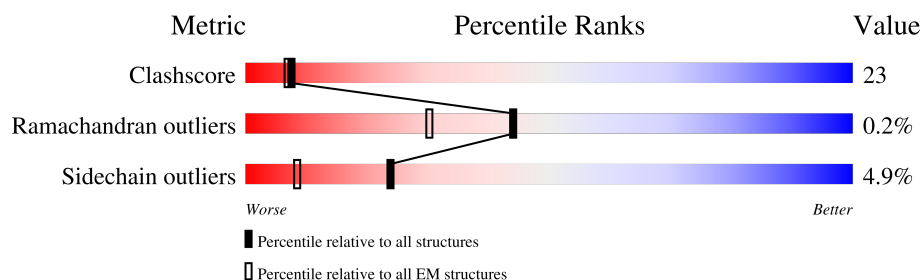
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.73 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.



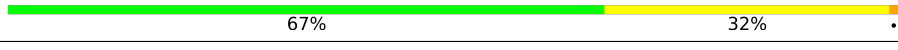
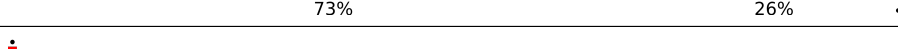
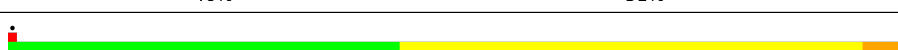
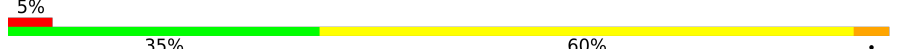
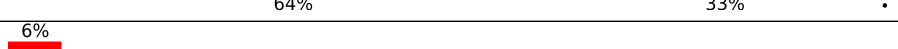
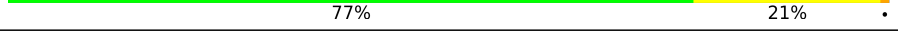
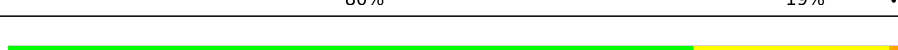
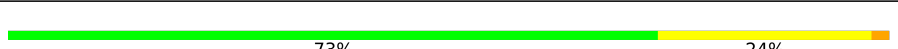
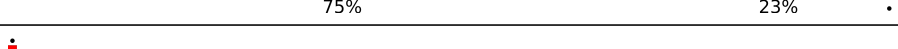
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10432 (2.23 - 3.23)

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	214	
1	7	214	
2	2	222	
2	4	222	

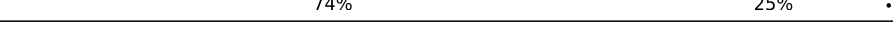
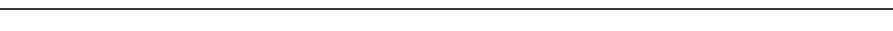
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	9	222	
2	G	222	
2	g	222	
2	q	222	
3	3	221	
3	5	221	
3	8	221	
3	N	221	
3	n	221	
3	p	221	
4	0	217	
4	6	217	
5	A	336	
5	a	336	
6	B	504	
6	b	504	
7	C	448	
7	c	448	
8	D	342	
8	d	342	
9	E	81	
9	e	81	
10	F	37	
10	f	37	
11	H	67	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
11	h	67	 79%21%
12	I	34	 79%21%
12	i	34	 79%21%
13	J	38	 92%5%
13	j	38	 84%13%
14	K	37	 59%38%
14	k	37	 70%27%
15	L	37	 68%32%
15	l	37	 70%27%
16	M	57	 11%77%21%
16	m	57	 11%82%18%
17	O	240	 74%23%
17	o	240	 81%18%
18	R	236	 74%25%
18	r	236	 75%24%
19	S	257	 74%25%
19	s	257	 74%26%
20	T	30	 70%30%
20	t	30	 57%40%
21	V	32	 84%16%
21	v	32	 88%12%
22	W	60	 60%38%
22	w	60	 68%32%
23	X	37	 70%30%
23	x	37	 81%19%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
24	Y	221	 78% 21% .
24	y	221	 72% 25% .
25	Z	62	 89% 11%
25	z	62	 74% 26%
26	U	144	 86% 14%
26	u	144	 83% 16% .
27	Q1	34	 76% 24%
27	q1	34	 62% 38%
28	P1	108	 88% 12%
28	p1	108	 82% 16% .
29	F1	188	 79% 18% .
29	f1	188	 80% 20% .

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	5	610	-	-	X	-
31	CLA	p	613	-	-	X	-
31	CLA	q	312	-	-	X	-
32	LUT	5	616	-	-	X	-
35	RRX	G	614	-	-	X	-
37	XAT	G	620	-	-	X	-
43	BCR	c	614	-	X	-	-
45	DGD	C	620	-	-	X	-
45	DGD	c	619	-	-	X	-

2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 117990 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, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	214	Total	C	N	O	S	0	0
			1630	1056	265	304	5		
1	7	214	Total	C	N	O	S	0	0
			1630	1056	265	304	5		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	195	LEU	PHE	conflict	UNP A0A2P6TPU9
1	225	GLU	ASP	conflict	UNP A0A2P6TPU9
1	250	ASN	THR	conflict	UNP A0A2P6TPU9
7	195	LEU	PHE	conflict	UNP A0A2P6TPU9
7	225	GLU	ASP	conflict	UNP A0A2P6TPU9
7	250	ASN	THR	conflict	UNP A0A2P6TPU9

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	222	Total	C	N	O	S	0	0
			1686	1089	271	321	5		
2	4	222	Total	C	N	O	S	0	0
			1685	1088	271	321	5		
2	G	222	Total	C	N	O	S	0	0
			1686	1089	271	321	5		
2	9	222	Total	C	N	O	S	0	0
			1686	1089	271	321	5		
2	q	222	Total	C	N	O	S	0	0
			1685	1088	271	321	5		
2	g	222	Total	C	N	O	S	0	0
			1686	1089	271	321	5		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	74	THR	SER	conflict	UNP A0A2P6TDA6
4	74	THR	SER	conflict	UNP A0A2P6TDA6
G	74	THR	SER	conflict	UNP A0A2P6TDA6
9	74	THR	SER	conflict	UNP A0A2P6TDA6
q	74	THR	SER	conflict	UNP A0A2P6TDA6
g	74	THR	SER	conflict	UNP A0A2P6TDA6

- Molecule 3 is a protein called Chlorophyll a-b binding of LHCII.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	221	Total	C	N	O	S	0	0
			1686	1090	279	312	5		
3	5	221	Total	C	N	O	S	0	0
			1686	1090	279	312	5		
3	N	221	Total	C	N	O	S	0	0
			1686	1090	279	312	5		
3	8	221	Total	C	N	O	S	0	0
			1686	1090	279	312	5		
3	p	221	Total	C	N	O	S	0	0
			1686	1090	279	312	5		
3	n	221	Total	C	N	O	S	0	0
			1686	1090	279	312	5		

- Molecule 4 is a protein called Chlorophyll a-b binding of LHCII.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	217	Total	C	N	O	S	0	0
			1657	1070	271	311	5		
4	0	217	Total	C	N	O	S	0	0
			1657	1070	271	311	5		

- Molecule 5 is a protein called Photosystem II protein D1.

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

- Molecule 6 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	504	Total	C	N	O	S	0	0
			3954	2583	667	692	12		
6	b	504	Total	C	N	O	S	0	0
			3954	2583	667	692	12		

- Molecule 7 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	448	Total	C	N	O	S	0	0
			3482	2280	584	603	15		
7	c	448	Total	C	N	O	S	0	0
			3482	2280	584	603	15		

- Molecule 8 is a protein called Photosystem II D2 protein.

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

- Molecule 9 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	E	81	Total	C	N	O	0	0
			652	423	106	123		
9	e	81	Total	C	N	O	0	0
			652	423	106	123		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	37	Total	C	N	O	S	0	0
			302	206	49	46	1		
10	f	37	Total	C	N	O	S	0	0
			302	206	49	46	1		

- Molecule 11 is a protein called Photosystem II reaction center protein H.

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	57	Total	C	N	O	S	0	0
			370	242	60	67	1		
16	m	57	Total	C	N	O	S	0	0
			370	242	60	67	1		

- Molecule 17 is a protein called Chloroplast oxygen-evolving enhancer protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	240	Total	C	N	O	S	0	0
			1789	1134	287	362	6		
17	o	240	Total	C	N	O	S	0	0
			1789	1134	287	362	6		

- Molecule 18 is a protein called Chlorophyll a b binding CP29.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	236	Total	C	N	O	S	0	0
			1818	1148	311	352	7		
18	r	236	Total	C	N	O	S	0	0
			1818	1148	311	352	7		

- Molecule 19 is a protein called Chlorophyll a b-binding CP26.

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

- Molecule 20 is a protein called Photosystem II reaction center protein T.

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

- Molecule 21 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	V	32	Total	C	N	O	0	0
			233	155	38	40		
21	v	32	Total	C	N	O	0	0
			233	155	38	40		

- Molecule 22 is a protein called Photosystem II reaction center W protein.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
23	X	37	Total	C	N	O	0	0
			247	156	43	48		
23	x	37	Total	C	N	O	0	0
			247	156	43	48		

- Molecule 24 is a protein called Multifunctional fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	221	Total	C	N	O	S	0	0
			1688	1099	270	314	5		
24	y	221	Total	C	N	O	S	0	0
			1688	1099	270	314	5		

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

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

- Molecule 26 is a protein called Chloroplast oxygen-evolving enhancer protein 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	U	144	Total	C	N	O	0	0
			1122	701	207	214		
26	u	144	Total	C	N	O	0	0
			1122	701	207	214		

- Molecule 27 is a protein called Chloroplast PsbY.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Q1	34	Total	C	N	O	S	0	0
			260	171	44	44	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
27	q1	34	Total	C	N	O	S	0	0
			260	171	44	44	1		

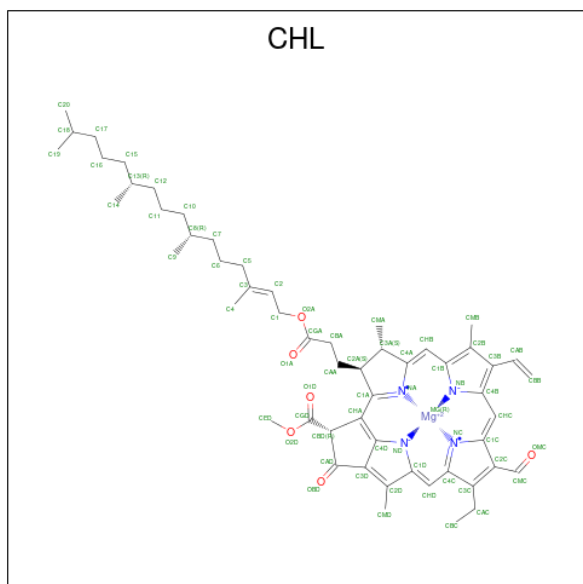
- Molecule 28 is a protein called Chloroplast photosystem II 10 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	P1	108	Total	C	N	O	S	0	0
			820	524	137	157	2		
28	p1	108	Total	C	N	O	S	0	0
			820	524	137	157	2		

- Molecule 29 is a protein called Photosystem II oxygen evolving enhancer 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	F1	188	Total	C	N	O	S	0	0
			1443	918	245	279	1		
29	f1	188	Total	C	N	O	S	0	0
			1443	918	245	279	1		

- Molecule 30 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
30	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	1	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	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	1	1	Total 50	C 39	Mg 1	N 4	O 6	0
30	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	1	1	Total 61	C 50	Mg 1	N 4	O 6	0
30	2	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
30	2	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	2	1	Total 50	C 39	Mg 1	N 4	O 6	0
30	2	1	Total 57	C 46	Mg 1	N 4	O 6	0
30	3	1	Total 57	C 46	Mg 1	N 4	O 6	0
30	3	1	Total 50	C 39	Mg 1	N 4	O 6	0
30	3	1	Total 46	C 35	Mg 1	N 4	O 6	0
30	3	1	Total 47	C 36	Mg 1	N 4	O 6	0
30	3	1	Total 50	C 39	Mg 1	N 4	O 6	0
30	3	1	Total 61	C 50	Mg 1	N 4	O 6	0
30	4	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	4	1	Total 46	C 35	Mg 1	N 4	O 6	0
30	4	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	4	1	Total 57	C 46	Mg 1	N 4	O 6	0
30	4	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	4	1	Total	C	Mg	N	O	0
			57	46	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
			51	40	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
			50	39	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
			56	45	1	4	6	
30	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	6	1	Total	C	Mg	N	O	0
			51	40	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	
30	6	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
			50	39	1	4	6	
30	G	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	G	1	Total	C	Mg	N	O	0
			63	52	1	4	6	
30	G	1	Total	C	Mg	N	O	0
			66	55	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
			56	45	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
30	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	N	1	Total 58	C 47	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	R	1	Total 56	C 45	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 55	C 44	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 44	C 35	Mg 1	N 4	O 4	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 63	C 52	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 46	C 35	Mg 1	N 4	O 6	0
30	Y	1	Total 59	C 48	Mg 1	N 4	O 6	0
30	Y	1	Total 50	C 39	Mg 1	N 4	O 6	0
30	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	O	1	Total 56	C 45	Mg 1	N 4	O 6	0
30	O	1	Total 52	C 41	Mg 1	N 4	O 6	0
30	O	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	O	1	Total 66	C 55	Mg 1	N 4	O 6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
30	0	1	Total 50	C 39	Mg 1	N 4	O 6	0
30	0	1	Total 61	C 50	Mg 1	N 4	O 6	0
30	7	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	7	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	7	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	7	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	7	1	Total 50	C 39	Mg 1	N 4	O 6	0
30	7	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	7	1	Total 63	C 52	Mg 1	N 4	O 6	0
30	8	1	Total 56	C 45	Mg 1	N 4	O 6	0
30	8	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	8	1	Total 58	C 47	Mg 1	N 4	O 6	0
30	8	1	Total 50	C 39	Mg 1	N 4	O 6	0
30	8	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	9	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	9	1	Total 46	C 35	Mg 1	N 4	O 6	0
30	9	1	Total 52	C 41	Mg 1	N 4	O 6	0
30	9	1	Total 53	C 42	Mg 1	N 4	O 6	0
30	9	1	Total 50	C 39	Mg 1	N 4	O 6	0
30	9	1	Total 61	C 50	Mg 1	N 4	O 6	0
30	p	1	Total 51	C 40	Mg 1	N 4	O 6	0

Continued on next page...

Continued from previous page...

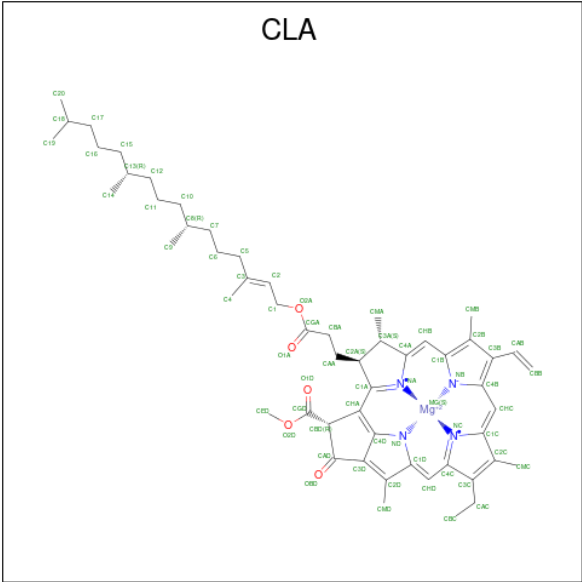
Mol	Chain	Residues	Atoms					AltConf
30	p	1	Total 46	C 35	Mg 1	N 4	O 6	0
30	p	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	p	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	p	1	Total 50	C 39	Mg 1	N 4	O 6	0
30	p	1	Total 56	C 45	Mg 1	N 4	O 6	0
30	q	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	q	1	Total 46	C 35	Mg 1	N 4	O 6	0
30	q	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	q	1	Total 57	C 46	Mg 1	N 4	O 6	0
30	q	1	Total 50	C 39	Mg 1	N 4	O 6	0
30	q	1	Total 56	C 45	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
30	g	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	g	1	Total 63	C 52	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 56	C 45	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 58	C 47	Mg 1	N 4	O 6	0
30	n	1	Total 63	C 52	Mg 1	N 4	O 6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
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	r	1	Total	C	Mg	N	O	0
			56	45	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
			55	44	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
			44	35	1	4	4	
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
			46	35	1	4	6	
30	y	1	Total	C	Mg	N	O	0
			59	48	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
			50	39	1	4	6	
30	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 31 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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
			55	45	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			65	55	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
			54	44	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			60	50	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 65	C 55	Mg 1	N 4	O 5	0
31	2	1	Total 54	C 44	Mg 1	N 4	O 5	0
31	3	1	Total 54	C 44	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 55	C 45	Mg 1	N 4	O 5	0
31	3	1	Total 54	C 44	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 50	C 40	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 54	C 44	Mg 1	N 4	O 5	0
31	3	1	Total 57	C 47	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 55	C 45	Mg 1	N 4	O 5	0
31	4	1	Total 51	C 41	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 43	C 33	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 61	C 51	Mg 1	N 4	O 5	0
31	4	1	Total 54	C 44	Mg 1	N 4	O 5	0
31	5	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	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
31	B	1	Total 49	C 39	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
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	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 56	C 46	Mg 1	N 4	O 5	0
31	C	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	C	1	Total 57	C 47	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 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 55	C 45	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 60	C 50	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 55	C 45	Mg 1	N 4	O 5	0
31	N	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	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	N	1	Total 49	C 39	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 65	C 55	Mg 1	N 4	O 5	0
31	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	N	1	Total 54	C 44	Mg 1	N 4	O 5	0
31	N	1	Total 54	C 44	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 60	C 50	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 48	C 38	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 58	C 48	Mg 1	N 4	O 5	0
31	R	1	Total 57	C 47	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 49	C 39	Mg 1	N 4	O 5	0
31	R	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	R	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 42	C 34	Mg 1	N 4	O 3	0
31	S	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	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	S	1	Total 60	C 50	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 56	C 46	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 48	C 38	Mg 1	N 4	O 5	0
31	S	1	Total 46	C 36	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 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 54	C 44	Mg 1	N 4	O 5	0
31	0	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	0	1	Total 56	C 46	Mg 1	N 4	O 5	0
31	0	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	0	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	0	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	0	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	0	1	Total 56	C 46	Mg 1	N 4	O 5	0
31	0	1	Total 54	C 44	Mg 1	N 4	O 5	0
31	0	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	7	1	Total 54	C 44	Mg 1	N 4	O 5	0
31	7	1	Total 51	C 41	Mg 1	N 4	O 5	0
31	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	8	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	8	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	8	1	Total 54	C 44	Mg 1	N 4	O 5	0
31	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	9	1	Total 54	C 44	Mg 1	N 4	O 5	0
31	9	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	9	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	p	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	p	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	p	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	p	1	Total 56	C 46	Mg 1	N 4	O 5	0
31	p	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	p	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	p	1	Total 54	C 44	Mg 1	N 4	O 5	0
31	p	1	Total 51	C 41	Mg 1	N 4	O 5	0
31	p	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	q	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	q	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	q	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	q	1	Total 53	C 43	Mg 1	N 4	O 5	0
31	q	1	Total 43	C 33	Mg 1	N 4	O 5	0
31	q	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	q	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	q	1	Total 50	C 40	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 60	C 50	Mg 1	N 4	O 5	0
31	b	1	Total 49	C 39	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 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 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 56	C 46	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 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 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 49	C 39	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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
31	g	1	Total 55	C 45	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 60	C 50	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 55	C 45	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 65	C 55	Mg 1	N 4	O 5	0
31	n	1	Total 49	C 39	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 65	C 55	Mg 1	N 4	O 5	0
31	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	n	1	Total 54	C 44	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 60	C 50	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 48	C 38	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 58	C 48	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

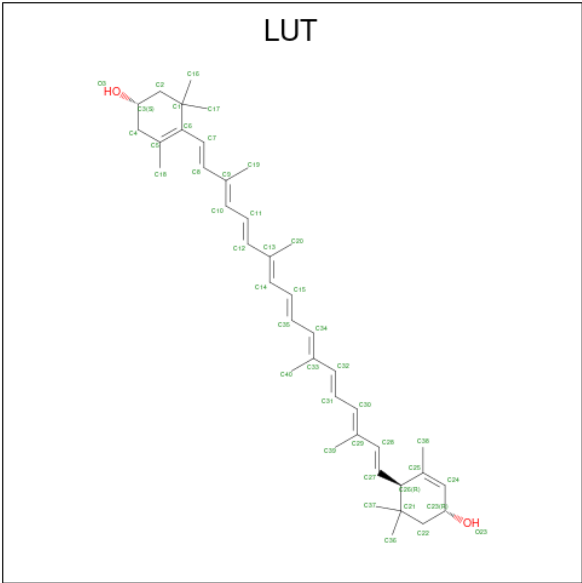
Mol	Chain	Residues	Atoms					AltConf
31	r	1	Total 57	C 47	Mg 1	N 4	O 5	0
31	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	r	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	s	1	Total 42	C 34	Mg 1	N 4	O 3	0
31	s	1	Total 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 60	C 50	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 56	C 46	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 48	C 38	Mg 1	N 4	O 5	0
31	s	1	Total 46	C 36	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 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	C	Mg	N	O	0
			65	55	1	4	5	
31	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	y	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
31	y	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

- Molecule 32 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



Mol	Chain	Residues	Atoms				AltConf
32	1	1	Total	C	O		0
			42	40	2		
32	1	1	Total	C	O		0
			42	40	2		
32	2	1	Total	C	O		0
			42	40	2		
32	3	1	Total	C	O		0
			42	40	2		
32	3	1	Total	C	O		0
			42	40	2		
32	4	1	Total	C	O		0
			42	40	2		
32	5	1	Total	C	O		0
			42	40	2		

Continued on next page...

Continued from previous page...

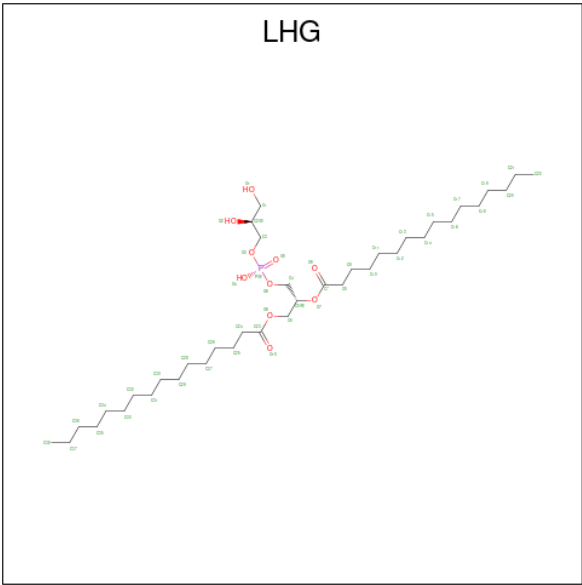
Mol	Chain	Residues	Atoms			AltConf
32	5	1	Total 42	C 40	O 2	0
32	6	1	Total 42	C 40	O 2	0
32	6	1	Total 42	C 40	O 2	0
32	G	1	Total 42	C 40	O 2	0
32	N	1	Total 42	C 40	O 2	0
32	N	1	Total 42	C 40	O 2	0
32	R	1	Total 42	C 40	O 2	0
32	S	1	Total 42	C 40	O 2	0
32	S	1	Total 42	C 40	O 2	0
32	Y	1	Total 42	C 40	O 2	0
32	Y	1	Total 42	C 40	O 2	0
32	0	1	Total 42	C 40	O 2	0
32	0	1	Total 42	C 40	O 2	0
32	7	1	Total 42	C 40	O 2	0
32	7	1	Total 42	C 40	O 2	0
32	8	1	Total 42	C 40	O 2	0
32	8	1	Total 42	C 40	O 2	0
32	9	1	Total 42	C 40	O 2	0
32	p	1	Total 42	C 40	O 2	0
32	p	1	Total 42	C 40	O 2	0
32	q	1	Total 42	C 40	O 2	0

Continued on next page...

Continued from previous page...

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

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
33	1	1	Total	C	O	P	0
			35	24	10	1	
33	2	1	Total	C	O	P	0
			49	38	10	1	
33	3	1	Total	C	O	P	0
			33	22	10	1	

Continued on next page...

Continued from previous page...

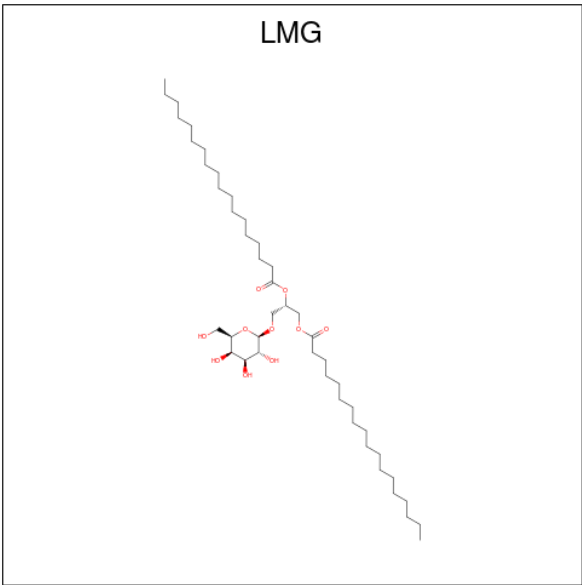
Mol	Chain	Residues	Atoms				AltConf
33	4	1	Total 47	C 36	O 10	P 1	0
33	5	1	Total 35	C 24	O 10	P 1	0
33	6	1	Total 37	C 26	O 10	P 1	0
33	A	1	Total 44	C 33	O 10	P 1	0
33	A	1	Total 39	C 28	O 10	P 1	0
33	B	1	Total 49	C 38	O 10	P 1	0
33	C	1	Total 40	C 29	O 10	P 1	0
33	D	1	Total 44	C 33	O 10	P 1	0
33	D	1	Total 49	C 38	O 10	P 1	0
33	G	1	Total 44	C 33	O 10	P 1	0
33	K	1	Total 36	C 25	O 10	P 1	0
33	L	1	Total 49	C 38	O 10	P 1	0
33	M	1	Total 41	C 30	O 10	P 1	0
33	N	1	Total 49	C 38	O 10	P 1	0
33	R	1	Total 38	C 27	O 10	P 1	0
33	S	1	Total 41	C 30	O 10	P 1	0
33	S	1	Total 44	C 33	O 10	P 1	0
33	Y	1	Total 42	C 31	O 10	P 1	0
33	0	1	Total 36	C 25	O 10	P 1	0
33	7	1	Total 35	C 24	O 10	P 1	0
33	8	1	Total 49	C 38	O 10	P 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
33	9	1	Total 33	C 22	O 10	P 1	0
33	p	1	Total 35	C 24	O 10	P 1	0
33	q	1	Total 46	C 35	O 10	P 1	0
33	a	1	Total 39	C 28	O 10	P 1	0
33	b	1	Total 44	C 33	O 10	P 1	0
33	b	1	Total 49	C 38	O 10	P 1	0
33	c	1	Total 47	C 36	O 10	P 1	0
33	d	1	Total 49	C 38	O 10	P 1	0
33	e	1	Total 44	C 33	O 10	P 1	0
33	g	1	Total 44	C 33	O 10	P 1	0
33	j	1	Total 49	C 38	O 10	P 1	0
33	l	1	Total 49	C 38	O 10	P 1	0
33	n	1	Total 49	C 38	O 10	P 1	0
33	r	1	Total 38	C 27	O 10	P 1	0
33	s	1	Total 41	C 30	O 10	P 1	0
33	s	1	Total 44	C 33	O 10	P 1	0
33	t	1	Total 41	C 30	O 10	P 1	0
33	y	1	Total 46	C 35	O 10	P 1	0
33	z	1	Total 36	C 25	O 10	P 1	0
33	F1	1	Total 35	C 24	O 10	P 1	0

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			AltConf
34	1	1	Total	C	O	0
			38	28	10	
34	2	1	Total	C	O	0
			38	28	10	
34	2	1	Total	C	O	0
			51	41	10	
34	2	1	Total	C	O	0
			40	30	10	
34	3	1	Total	C	O	0
			38	28	10	
34	4	1	Total	C	O	0
			51	41	10	
34	4	1	Total	C	O	0
			40	30	10	
34	5	1	Total	C	O	0
			38	28	10	
34	6	1	Total	C	O	0
			42	32	10	
34	6	1	Total	C	O	0
			39	29	10	
34	6	1	Total	C	O	0
			38	28	10	
34	A	1	Total	C	O	0
			41	31	10	
34	A	1	Total	C	O	0
			38	28	10	
34	A	1	Total	C	O	0
			38	28	10	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
34	B	1	Total	C	O	0
			51	41	10	
34	B	1	Total	C	O	0
			38	28	10	
34	B	1	Total	C	O	0
			38	28	10	
34	C	1	Total	C	O	0
			51	41	10	
34	C	1	Total	C	O	0
			38	28	10	
34	C	1	Total	C	O	0
			32	22	10	
34	C	1	Total	C	O	0
			44	34	10	
34	D	1	Total	C	O	0
			46	36	10	
34	D	1	Total	C	O	0
			46	36	10	
34	D	1	Total	C	O	0
			51	41	10	
34	D	1	Total	C	O	0
			48	38	10	
34	G	1	Total	C	O	0
			38	28	10	
34	G	1	Total	C	O	0
			51	41	10	
34	G	1	Total	C	O	0
			40	30	10	
34	I	1	Total	C	O	0
			38	28	10	
34	J	1	Total	C	O	0
			51	41	10	
34	J	1	Total	C	O	0
			38	28	10	
34	N	1	Total	C	O	0
			38	28	10	
34	R	1	Total	C	O	0
			38	28	10	
34	S	1	Total	C	O	0
			41	31	10	
34	W	1	Total	C	O	0
			55	45	10	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
34	W	1	Total	C	O	0
			38	28	10	
34	W	1	Total	C	O	0
			38	28	10	
34	X	1	Total	C	O	0
			38	28	10	
34	X	1	Total	C	O	0
			38	28	10	
34	Y	1	Total	C	O	0
			38	28	10	
34	0	1	Total	C	O	0
			42	32	10	
34	0	1	Total	C	O	0
			38	28	10	
34	7	1	Total	C	O	0
			39	29	10	
34	7	1	Total	C	O	0
			38	28	10	
34	7	1	Total	C	O	0
			38	28	10	
34	9	1	Total	C	O	0
			51	41	10	
34	9	1	Total	C	O	0
			40	30	10	
34	9	1	Total	C	O	0
			38	28	10	
34	p	1	Total	C	O	0
			38	28	10	
34	q	1	Total	C	O	0
			51	41	10	
34	q	1	Total	C	O	0
			40	30	10	
34	a	1	Total	C	O	0
			38	28	10	
34	a	1	Total	C	O	0
			38	28	10	
34	a	1	Total	C	O	0
			38	28	10	
34	b	1	Total	C	O	0
			45	35	10	
34	b	1	Total	C	O	0
			51	41	10	

Continued on next page...

Continued from previous page...

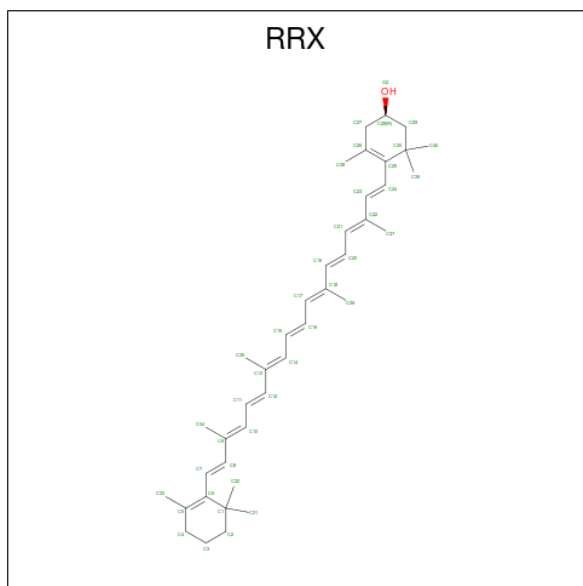
Mol	Chain	Residues	Atoms			AltConf
34	b	1	Total	C	O	0
			38	28	10	
34	b	1	Total	C	O	0
			38	28	10	
34	b	1	Total	C	O	0
			46	36	10	
34	b	1	Total	C	O	0
			38	28	10	
34	c	1	Total	C	O	0
			38	28	10	
34	c	1	Total	C	O	0
			38	28	10	
34	c	1	Total	C	O	0
			44	34	10	
34	d	1	Total	C	O	0
			41	31	10	
34	d	1	Total	C	O	0
			51	41	10	
34	d	1	Total	C	O	0
			48	38	10	
34	f	1	Total	C	O	0
			38	28	10	
34	g	1	Total	C	O	0
			38	28	10	
34	g	1	Total	C	O	0
			49	39	10	
34	j	1	Total	C	O	0
			43	33	10	
34	k	1	Total	C	O	0
			48	38	10	
34	k	1	Total	C	O	0
			38	28	10	
34	m	1	Total	C	O	0
			45	35	10	
34	n	1	Total	C	O	0
			38	28	10	
34	n	1	Total	C	O	0
			40	30	10	
34	r	1	Total	C	O	0
			38	28	10	
34	s	1	Total	C	O	0
			41	31	10	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
34	w	1	Total	C	O	0
			48	38	10	
34	w	1	Total	C	O	0
			55	45	10	
34	w	1	Total	C	O	0
			38	28	10	
34	w	1	Total	C	O	0
			38	28	10	
34	w	1	Total	C	O	0
			38	28	10	
34	x	1	Total	C	O	0
			38	28	10	
34	y	1	Total	C	O	0
			38	28	10	
34	Q1	1	Total	C	O	0
			38	28	10	
34	q1	1	Total	C	O	0
			38	28	10	

- Molecule 35 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: C₄₀H₅₆O).



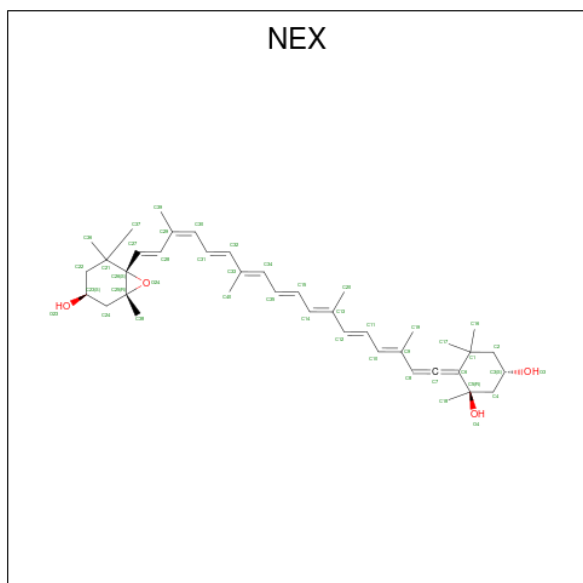
Mol	Chain	Residues	Atoms			AltConf
35	2	1	Total	C	O	0
			41	40	1	
35	4	1	Total	C	O	0
			41	40	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
35	G	1	Total	C	O	0
			41	40	1	
35	9	1	Total	C	O	0
			41	40	1	
35	q	1	Total	C	O	0
			41	40	1	
35	g	1	Total	C	O	0
			41	40	1	

- Molecule 36 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-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).



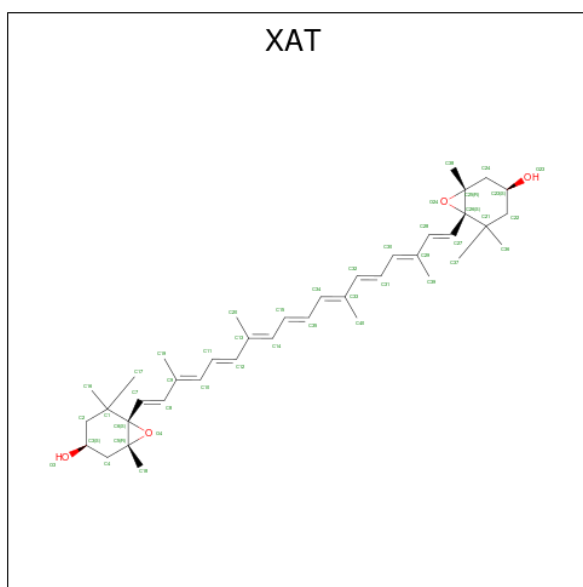
Mol	Chain	Residues	Atoms			AltConf
36	2	1	Total	C	O	0
			44	40	4	
36	3	1	Total	C	O	0
			44	40	4	
36	4	1	Total	C	O	0
			44	40	4	
36	5	1	Total	C	O	0
			44	40	4	
36	6	1	Total	C	O	0
			44	40	4	
36	G	1	Total	C	O	0
			44	40	4	

Continued on next page...

Continued from previous page...

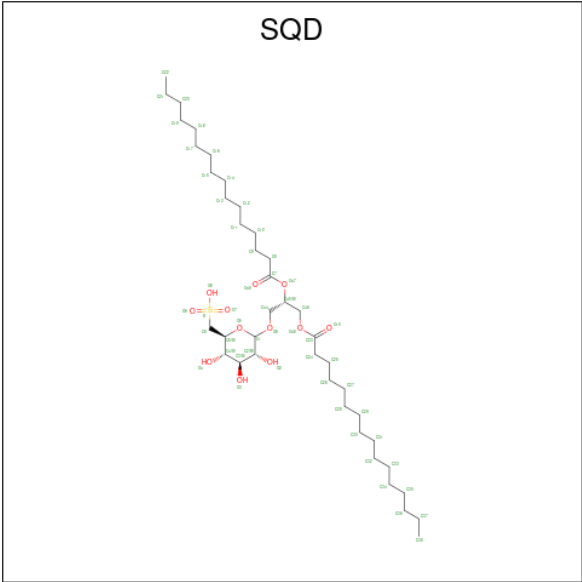
Mol	Chain	Residues	Atoms			AltConf
36	N	1	Total	C	O	0
			44	40	4	
36	R	1	Total	C	O	0
			44	40	4	
36	R	1	Total	C	O	0
			44	40	4	
36	S	1	Total	C	O	0
			44	40	4	
36	Y	1	Total	C	O	0
			44	40	4	
36	0	1	Total	C	O	0
			44	40	4	
36	8	1	Total	C	O	0
			44	40	4	
36	9	1	Total	C	O	0
			44	40	4	
36	p	1	Total	C	O	0
			44	40	4	
36	q	1	Total	C	O	0
			44	40	4	
36	g	1	Total	C	O	0
			44	40	4	
36	n	1	Total	C	O	0
			44	40	4	
36	r	1	Total	C	O	0
			44	40	4	
36	r	1	Total	C	O	0
			44	40	4	
36	s	1	Total	C	O	0
			44	40	4	
36	y	1	Total	C	O	0
			44	40	4	

- Molecule 37 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).



Mol	Chain	Residues	Atoms			AltConf
37	2	1	Total	C	O	0
			44	40	4	
37	4	1	Total	C	O	0
			44	40	4	
37	G	1	Total	C	O	0
			44	40	4	
37	R	1	Total	C	O	0
			44	40	4	
37	9	1	Total	C	O	0
			44	40	4	
37	q	1	Total	C	O	0
			44	40	4	
37	g	1	Total	C	O	0
			44	40	4	
37	r	1	Total	C	O	0
			44	40	4	

- Molecule 38 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



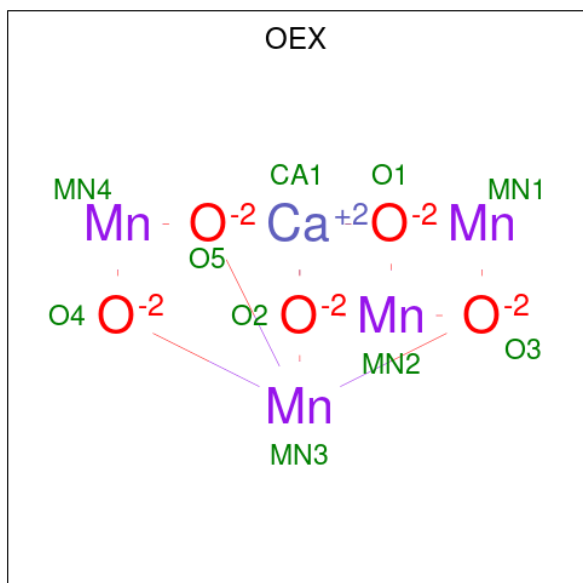
Mol	Chain	Residues	Atoms				AltConf
38	6	1	Total	C	O	S	0
			42	29	12	1	
38	A	1	Total	C	O	S	0
			51	38	12	1	
38	A	1	Total	C	O	S	0
			45	32	12	1	
38	B	1	Total	C	O	S	0
			54	41	12	1	
38	B	1	Total	C	O	S	0
			52	39	12	1	
38	G	1	Total	C	O	S	0
			42	29	12	1	
38	G	1	Total	C	O	S	0
			38	25	12	1	
38	M	1	Total	C	O	S	0
			50	37	12	1	
38	R	1	Total	C	O	S	0
			51	38	12	1	
38	S	1	Total	C	O	S	0
			51	38	12	1	
38	X	1	Total	C	O	S	0
			38	25	12	1	
38	Y	1	Total	C	O	S	0
			42	29	12	1	
38	0	1	Total	C	O	S	0
			42	29	12	1	
38	a	1	Total	C	O	S	0
			48	35	12	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
38	a	1	Total	C	O	S	0
			45	32	12	1	
38	b	1	Total	C	O	S	0
			54	41	12	1	
38	b	1	Total	C	O	S	0
			52	39	12	1	
38	g	1	Total	C	O	S	0
			38	25	12	1	
38	g	1	Total	C	O	S	0
			42	29	12	1	
38	m	1	Total	C	O	S	0
			50	37	12	1	
38	r	1	Total	C	O	S	0
			51	38	12	1	
38	s	1	Total	C	O	S	0
			51	38	12	1	
38	x	1	Total	C	O	S	0
			42	29	12	1	
38	y	1	Total	C	O	S	0
			42	29	12	1	

- Molecule 39 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



Mol	Chain	Residues	Atoms				AltConf
39	A	1	Total	Ca	Mn	O	0
			10	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
39	a	1	Total	Ca	Mn	O	0
			10	1	4	5	

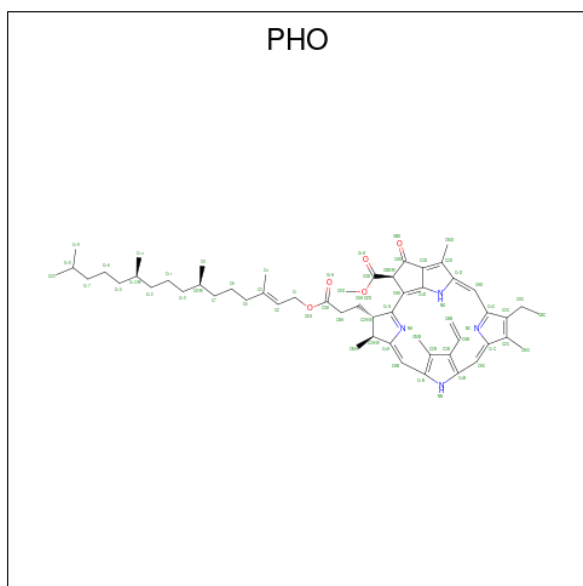
- Molecule 40 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
40	A	1	Total	Fe	0
			1	1	
40	a	1	Total	Fe	0
			1	1	

- Molecule 41 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
41	A	2	Total	Cl	0
			2	2	
41	a	2	Total	Cl	0
			2	2	

- Molecule 42 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



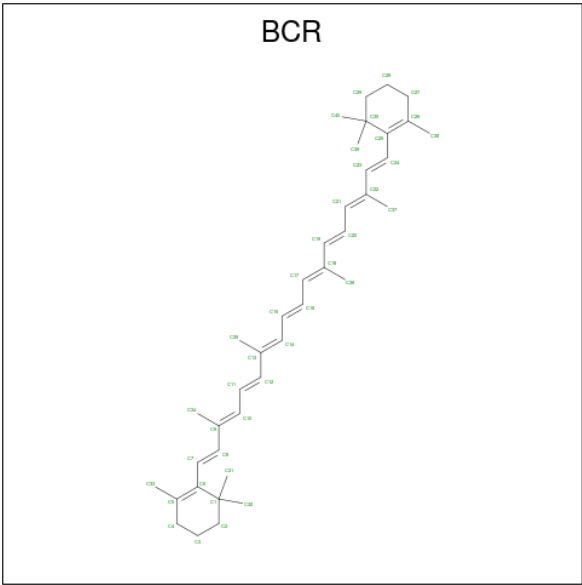
Mol	Chain	Residues	Atoms				AltConf
42	A	1	Total	C	N	O	0
			64	55	4	5	
42	D	1	Total	C	N	O	0
			64	55	4	5	

Continued on next page...

Continued from previous page...

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

- Molecule 43 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



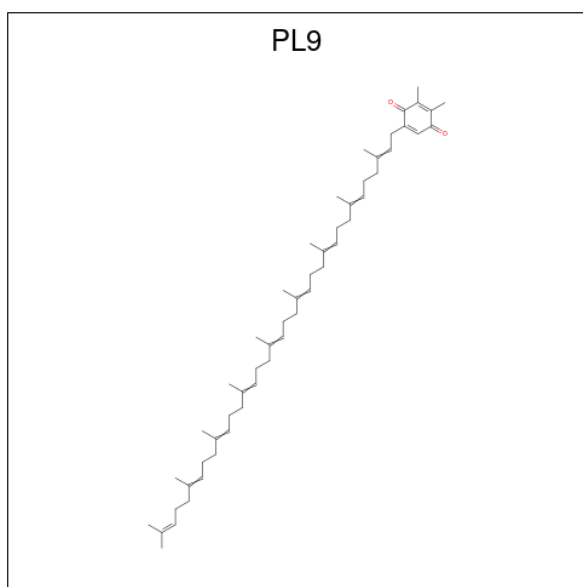
Mol	Chain	Residues	Atoms		AltConf
43	A	1	Total	C	0
			40	40	
43	B	1	Total	C	0
			40	40	
43	B	1	Total	C	0
			40	40	
43	B	1	Total	C	0
			40	40	
43	C	1	Total	C	0
			40	40	
43	C	1	Total	C	0
			40	40	
43	D	1	Total	C	0
			40	40	
43	H	1	Total	C	0
			40	40	
43	T	1	Total	C	0
			40	40	

Continued on next page...

Continued from previous page...

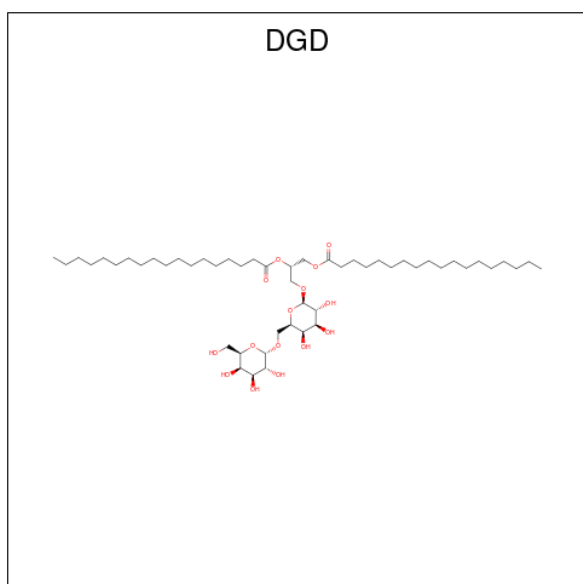
Mol	Chain	Residues	Atoms	AltConf
43	V	1	Total C 40 40	0
43	Z	1	Total C 40 40	0
43	a	1	Total C 40 40	0
43	b	1	Total C 40 40	0
43	b	1	Total C 40 40	0
43	b	1	Total C 40 40	0
43	c	1	Total C 40 40	0
43	c	1	Total C 40 40	0
43	d	1	Total C 40 40	0
43	h	1	Total C 40 40	0
43	t	1	Total C 40 40	0
43	v	1	Total C 40 40	0
43	z	1	Total C 40 40	0

- Molecule 44 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).



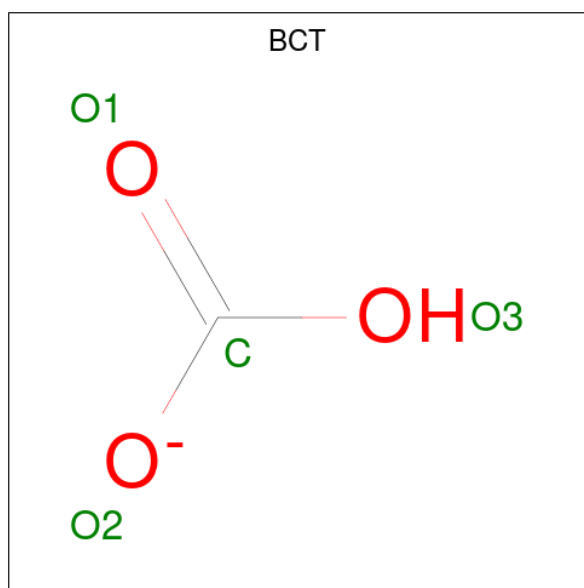
Mol	Chain	Residues	Atoms			AltConf
44	A	1	Total	C	O	0
			55	53	2	
44	D	1	Total	C	O	0
			55	53	2	
44	a	1	Total	C	O	0
			55	53	2	
44	d	1	Total	C	O	0
			55	53	2	

- Molecule 45 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



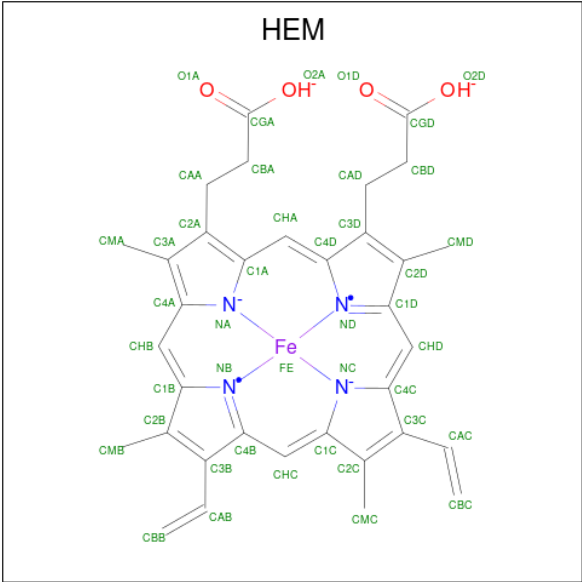
Mol	Chain	Residues	Atoms			AltConf
45	C	1	Total	C	O	0
			50	35	15	
45	C	1	Total	C	O	0
			66	51	15	
45	C	1	Total	C	O	0
			66	51	15	
45	C	1	Total	C	O	0
			66	51	15	
45	c	1	Total	C	O	0
			66	51	15	
45	c	1	Total	C	O	0
			62	47	15	
45	c	1	Total	C	O	0
			66	51	15	
45	c	1	Total	C	O	0
			66	51	15	

- Molecule 46 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



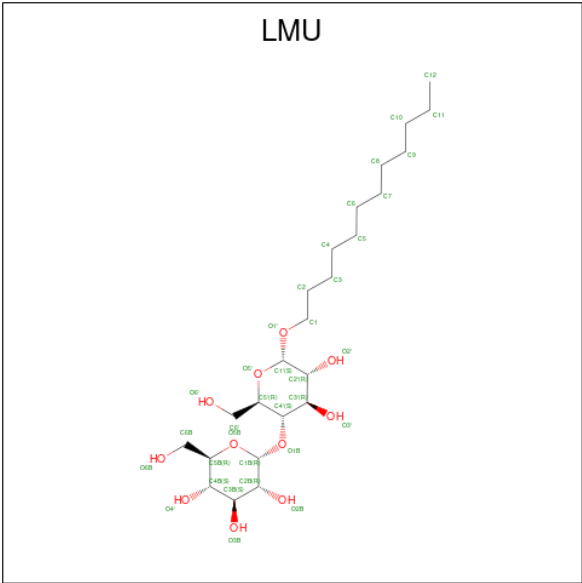
Mol	Chain	Residues	Atoms			AltConf
46	D	1	Total	C	O	0
			4	1	3	
46	d	1	Total	C	O	0
			4	1	3	

- Molecule 47 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



Mol	Chain	Residues	Atoms					AltConf
47	E	1	Total 43	C 34	Fe 1	N 4	O 4	0
47	e	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 48 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			AltConf
48	K	1	Total	C	O	0
			35	24	11	
48	R	1	Total	C	O	0
			35	24	11	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
48	c	1	Total	C	O	0
			28	17	11	
48	r	1	Total	C	O	0
			35	24	11	

- Molecule 49 is water.

Mol	Chain	Residues	Atoms			AltConf
49	1	3	Total	O		0
			3	3		
49	2	3	Total	O		0
			3	3		
49	3	1	Total	O		0
			1	1		
49	4	1	Total	O		0
			1	1		
49	5	1	Total	O		0
			1	1		
49	6	4	Total	O		0
			4	4		
49	A	21	Total	O		0
			21	21		
49	B	6	Total	O		0
			6	6		
49	C	15	Total	O		0
			15	15		
49	D	12	Total	O		0
			12	12		
49	E	1	Total	O		0
			1	1		
49	G	5	Total	O		0
			5	5		
49	I	1	Total	O		0
			1	1		
49	J	1	Total	O		0
			1	1		
49	N	5	Total	O		0
			5	5		
49	O	6	Total	O		0
			6	6		
49	R	4	Total	O		0
			4	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
49	S	3	Total O 3 3	0
49	T	4	Total O 4 4	0
49	Y	8	Total O 8 8	0
49	0	7	Total O 7 7	0
49	7	6	Total O 6 6	0
49	8	4	Total O 4 4	0
49	9	2	Total O 2 2	0
49	q	1	Total O 1 1	0
49	a	14	Total O 14 14	0
49	b	6	Total O 6 6	0
49	c	15	Total O 15 15	0
49	d	15	Total O 15 15	0
49	e	2	Total O 2 2	0
49	f	1	Total O 1 1	0
49	g	4	Total O 4 4	0
49	j	1	Total O 1 1	0
49	m	2	Total O 2 2	0
49	n	7	Total O 7 7	0
49	o	6	Total O 6 6	0
49	r	4	Total O 4 4	0
49	s	3	Total O 3 3	0

Continued on next page...

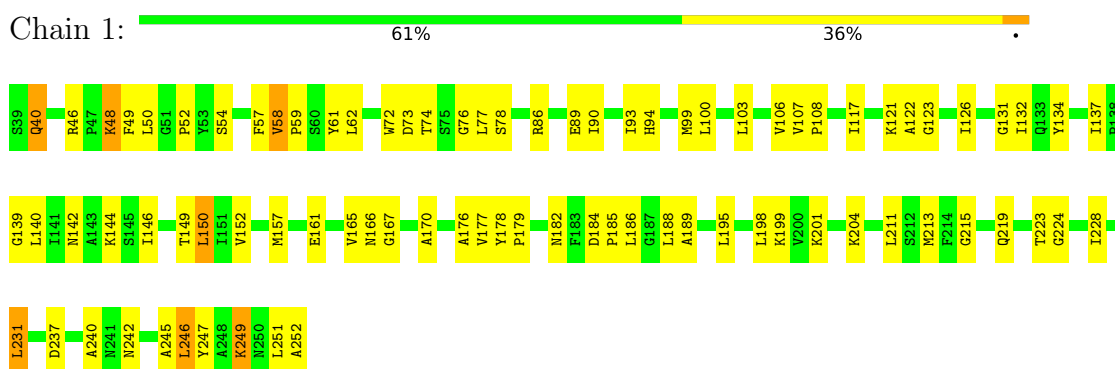
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
49	t	2	Total 2	O 2	0
49	w	2	Total 2	O 2	0
49	y	8	Total 8	O 8	0
49	F1	4	Total 4	O 4	0
49	f1	3	Total 3	O 3	0

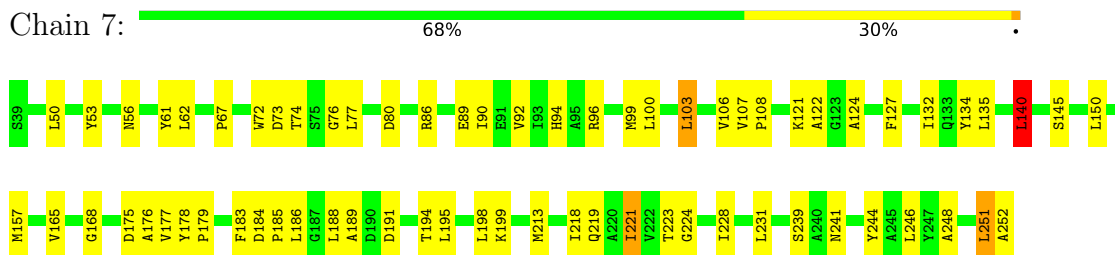
3 Residue-property plots

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.

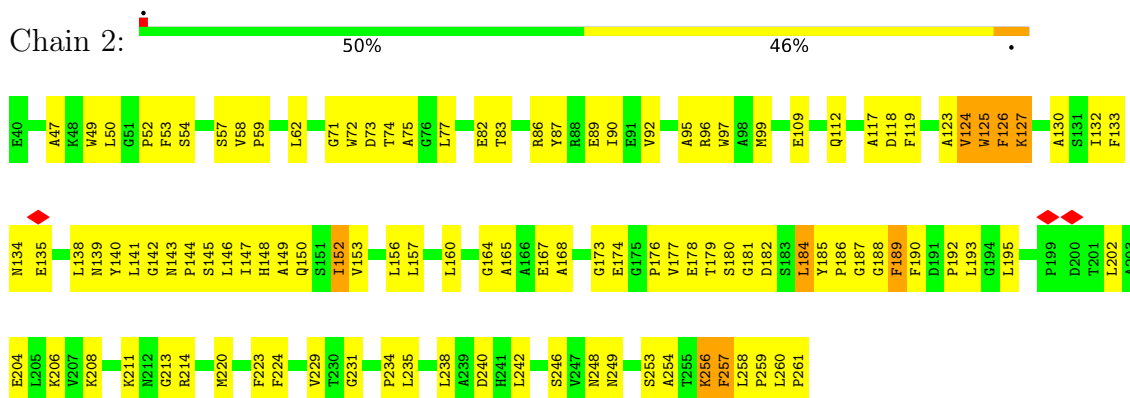
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



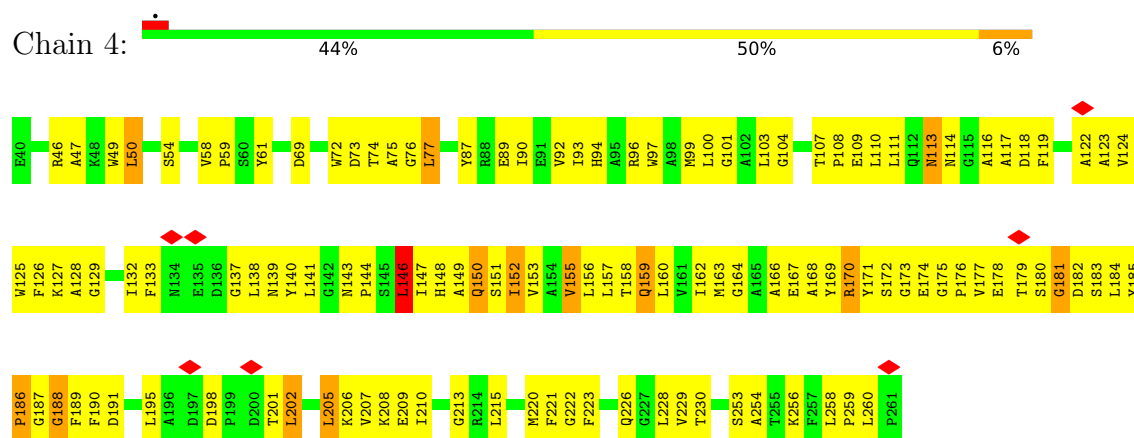
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



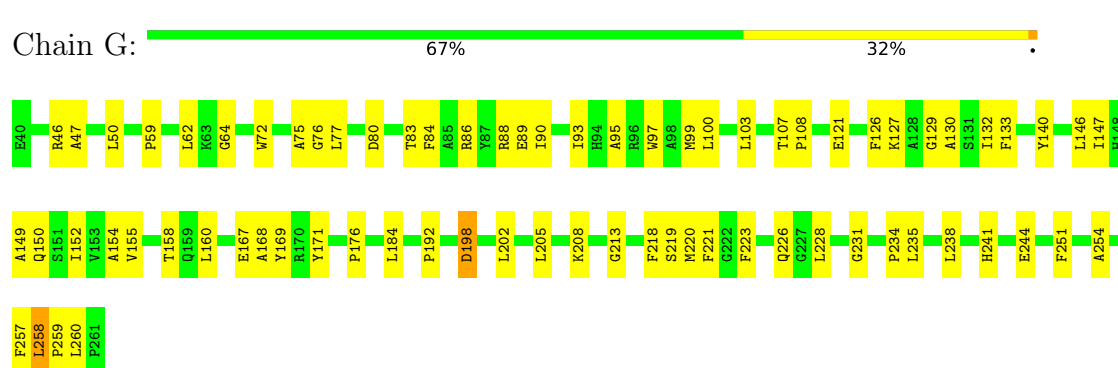
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic



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



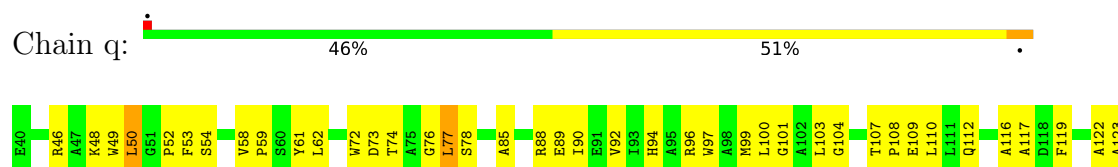
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

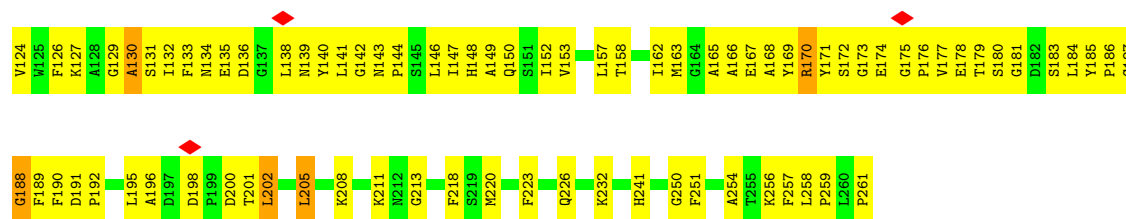


- Molecule 2: Chlorophyll a-b binding protein, chloroplastic



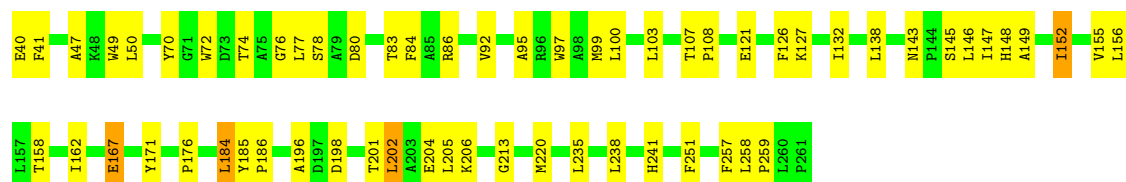
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic





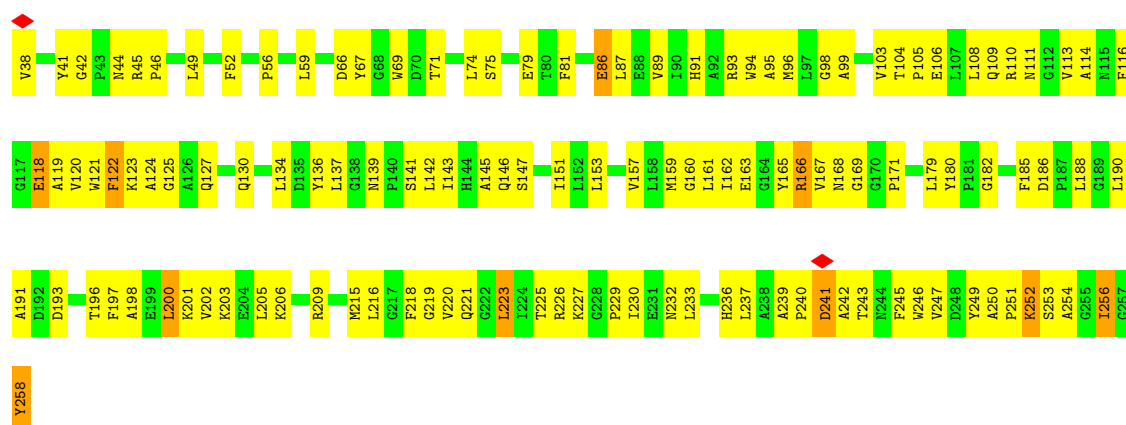
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain g: 73% 26%



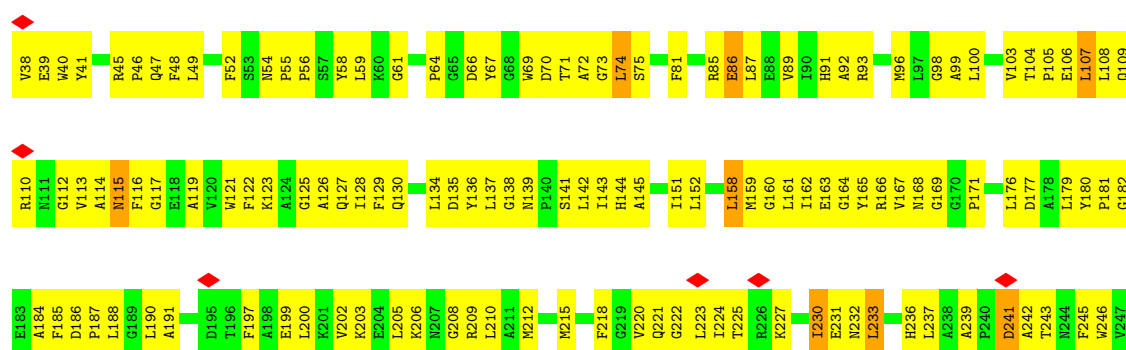
- Molecule 3: Chlorophyll a-b binding of LHCII

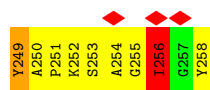
Chain 3: 44% 52% 5%



- Molecule 3: Chlorophyll a-b binding of LHCII

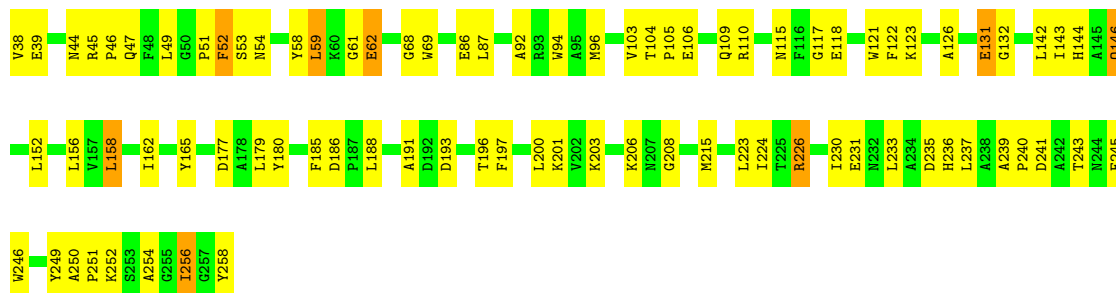
Chain 5: 35% 60%





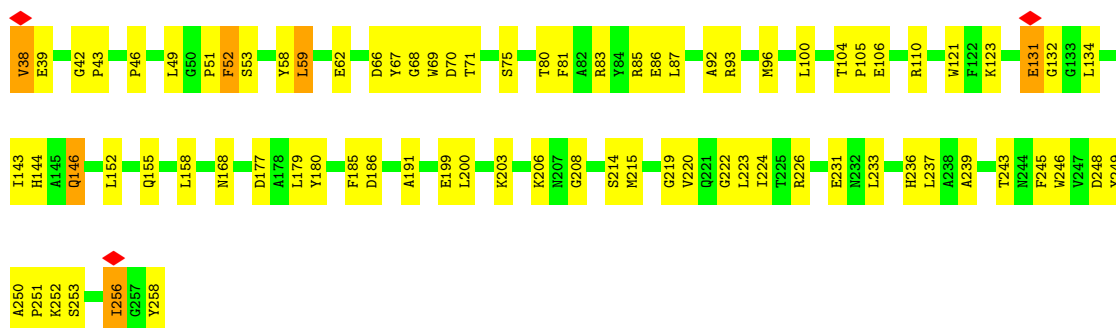
• Molecule 3: Chlorophyll a-b binding of LHCII

Chain N: 62% 34%



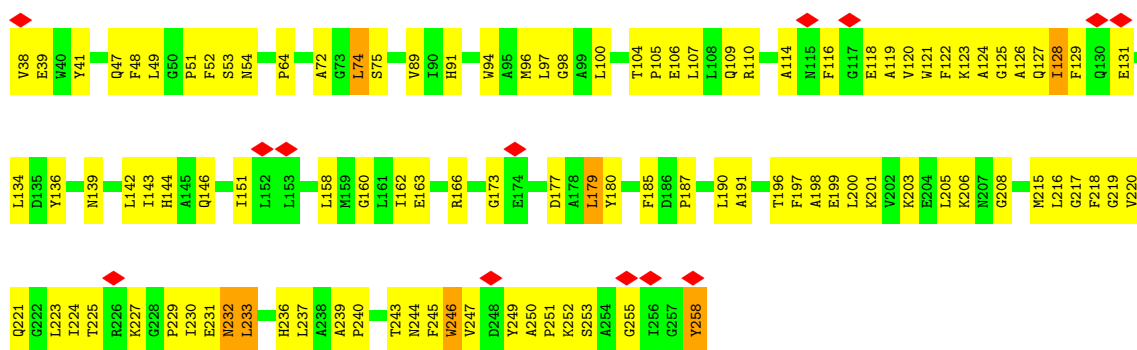
• Molecule 3: Chlorophyll a-b binding of LHCII

Chain 8: 63% 34%



• Molecule 3: Chlorophyll a-b binding of LHCII

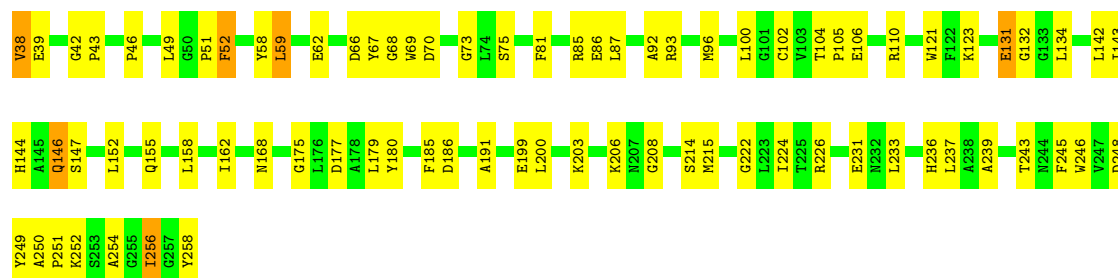
Chain p: 6% 52% 44%



• Molecule 3: Chlorophyll a-b binding of LHCII

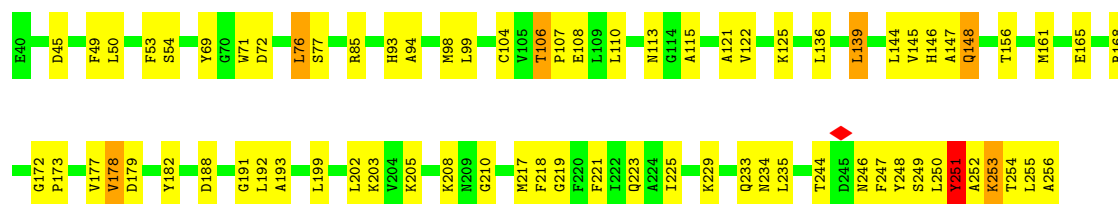
Chain n: 64% 33%





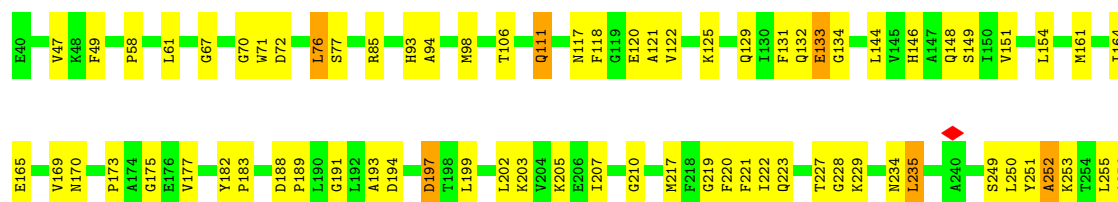
• Molecule 4: Chlorophyll a-b binding of LHCII

Chain 6: 66% 31%



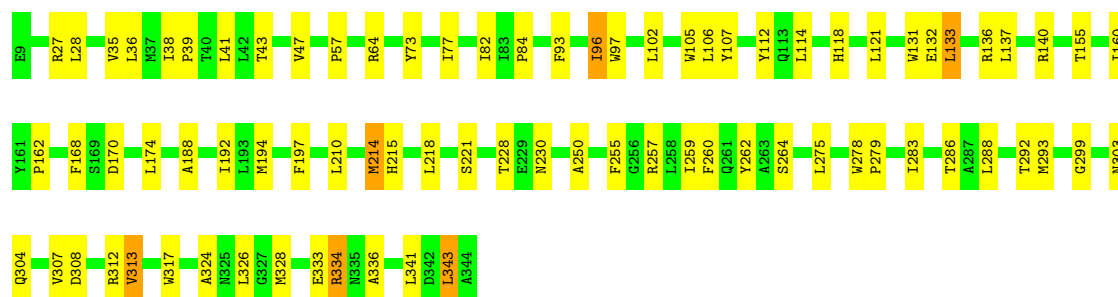
• Molecule 4: Chlorophyll a-b binding of LHCII

Chain 0: 66% 31%



• Molecule 5: Photosystem II protein D1

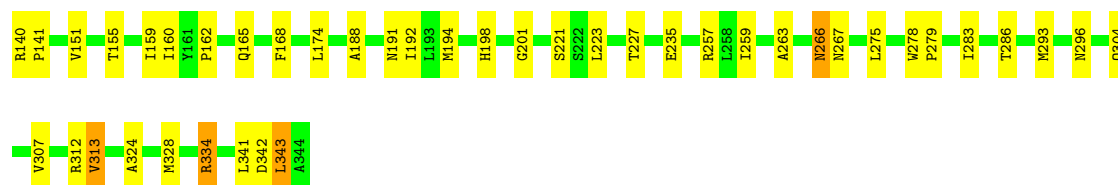
Chain A: 76% 22%



• Molecule 5: Photosystem II protein D1

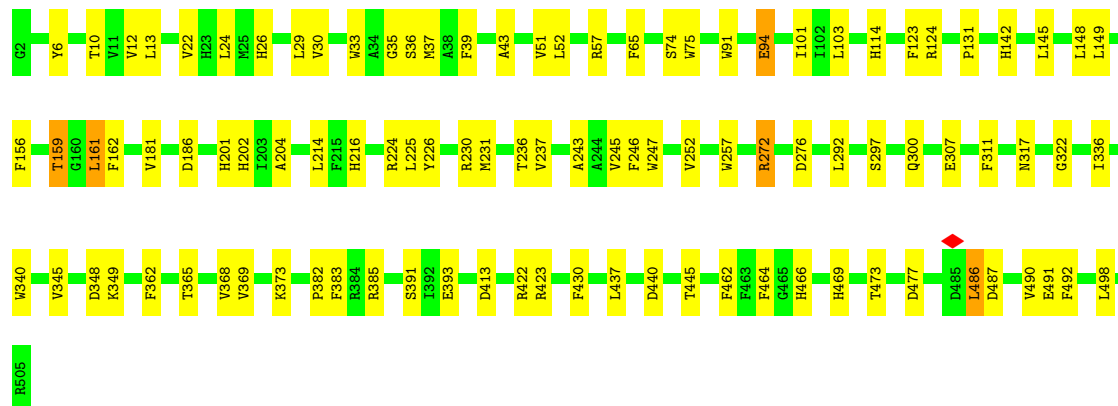
Chain a: 77% 21%





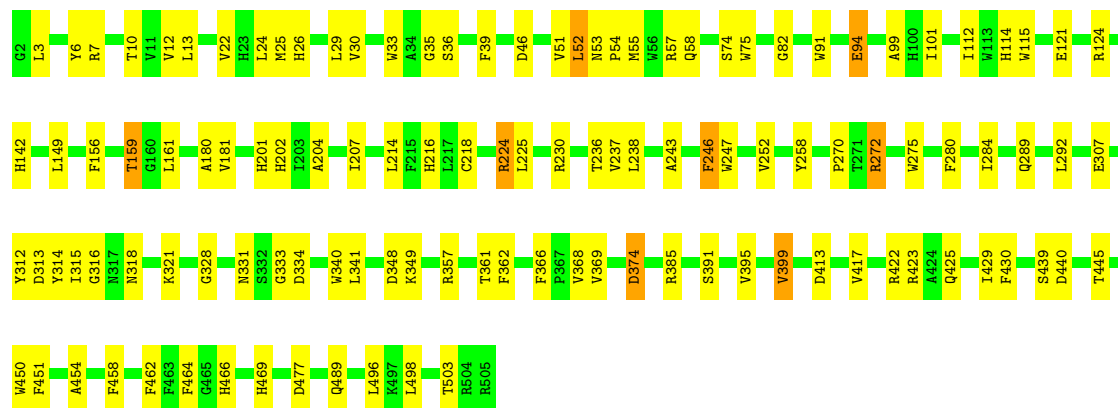
• Molecule 6: Photosystem II CP47 reaction center protein

Chain B: 80% 19% .



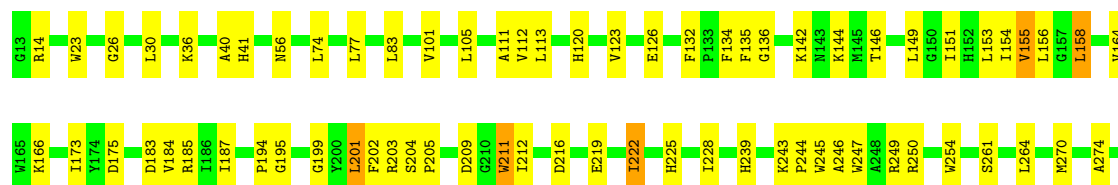
• Molecule 6: Photosystem II CP47 reaction center protein

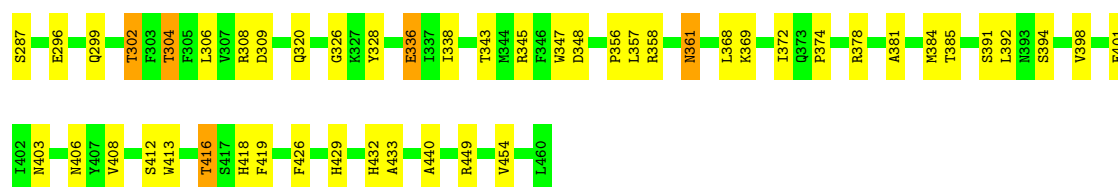
Chain b: 77% 22% .



• Molecule 7: Photosystem II CP43 reaction center protein

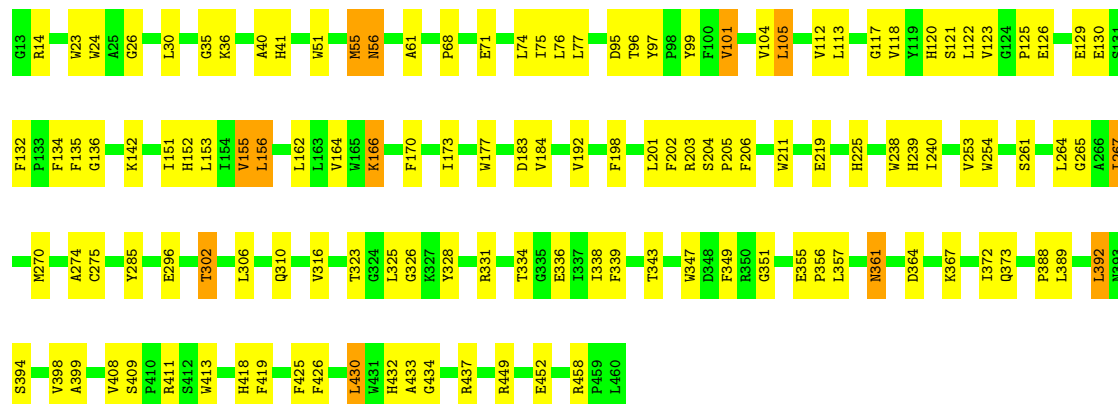
Chain C: 73% 24% .





• Molecule 7: Photosystem II CP43 reaction center protein

Chain c: 71% 26% .



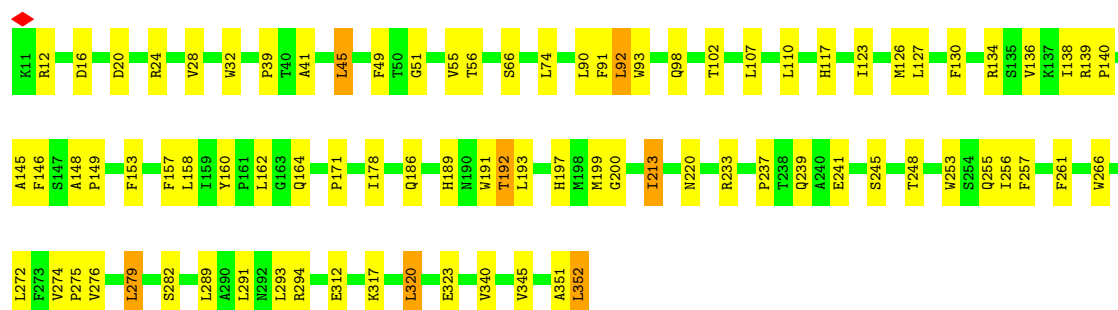
• Molecule 8: Photosystem II D2 protein

Chain D: 75% 24% .



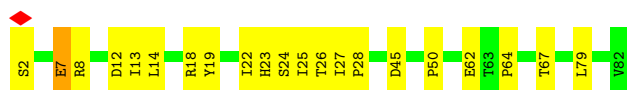
• Molecule 8: Photosystem II D2 protein

Chain d: 75% 23% .



- Molecule 9: Cytochrome b559 subunit alpha

Chain E:  74% 25%



- Molecule 9: Cytochrome b559 subunit alpha

Chain e:  67% 33%



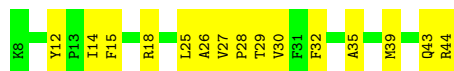
- Molecule 10: Cytochrome b559 subunit beta

Chain F:  54% 46%



- Molecule 10: Cytochrome b559 subunit beta

Chain f:  59% 41%



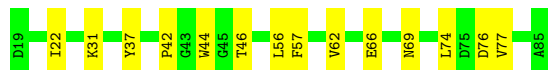
- Molecule 11: Photosystem II reaction center protein H

Chain H:  84% 15%



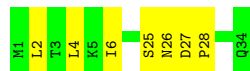
- Molecule 11: Photosystem II reaction center protein H

Chain h:  79% 21%



- Molecule 12: Photosystem II reaction center protein I

Chain I:  79% 21%



- Molecule 12: Photosystem II reaction center protein I

Chain i:  79% 21%



- Molecule 13: Photosystem II reaction center protein J

Chain J:  92% 5%



- Molecule 13: Photosystem II reaction center protein J

Chain j:  84% 13%



- Molecule 14: Photosystem II reaction center protein K

Chain K:  59% 38%



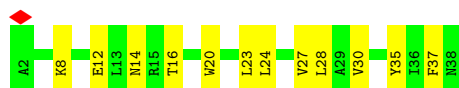
- Molecule 14: Photosystem II reaction center protein K

Chain k:  70% 27%



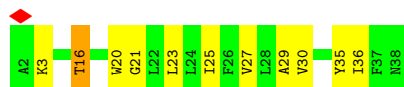
- Molecule 15: Photosystem II reaction center protein L

Chain L:  68% 32%

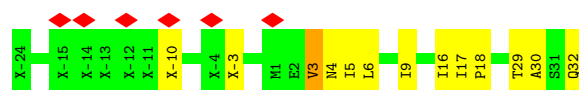
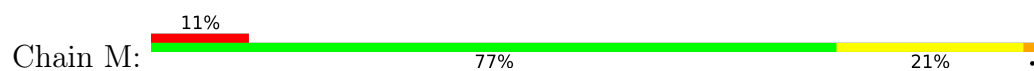


- Molecule 15: Photosystem II reaction center protein L

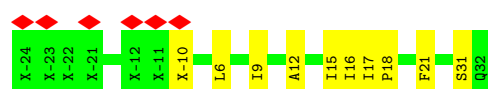
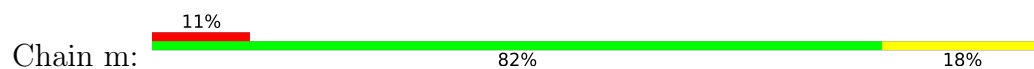
Chain l:  70% 27%



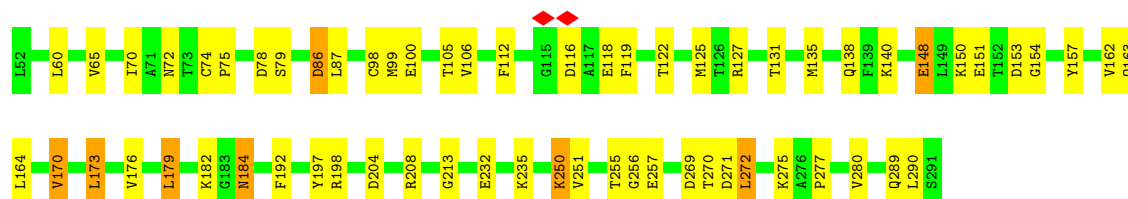
- Molecule 16: Photosystem II reaction center protein M



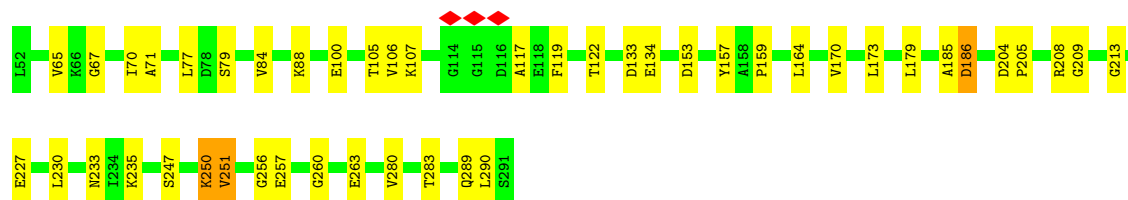
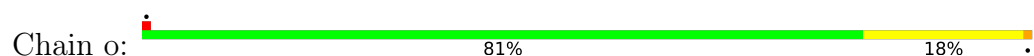
- Molecule 16: Photosystem II reaction center protein M



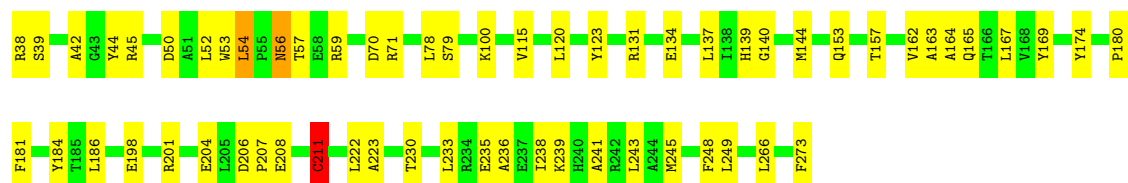
- Molecule 17: Chloroplast oxygen-evolving enhancer protein 1



- Molecule 17: Chloroplast oxygen-evolving enhancer protein 1

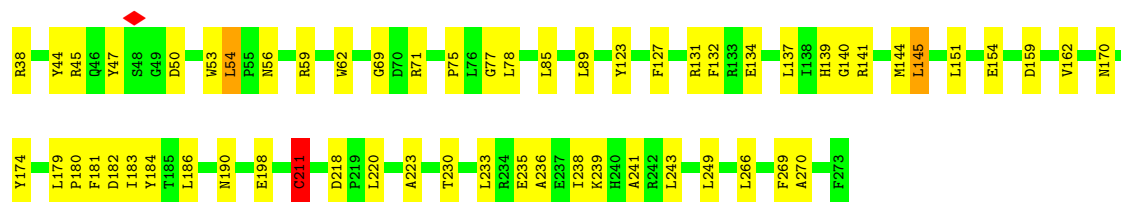


- Molecule 18: Chlorophyll a b binding CP29

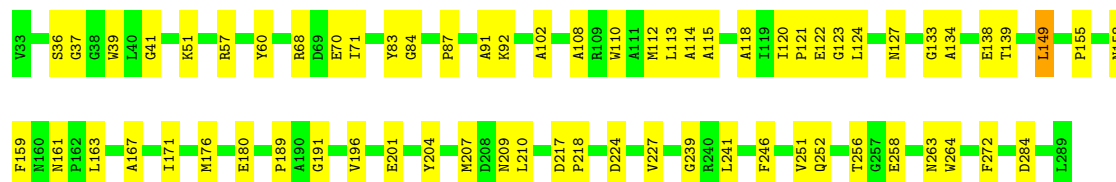


- Molecule 18: Chlorophyll a b binding CP29

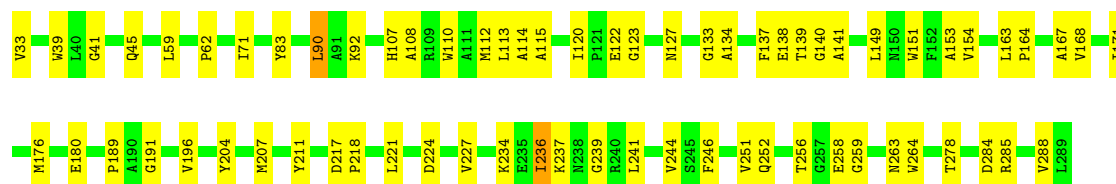




• Molecule 19: Chlorophyll a b-binding CP26



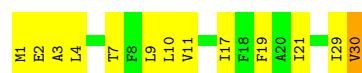
• Molecule 19: Chlorophyll a b-binding CP26



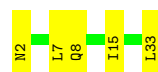
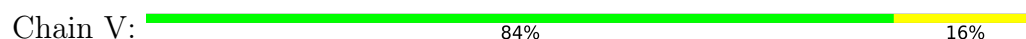
• Molecule 20: Photosystem II reaction center protein T



• Molecule 20: Photosystem II reaction center protein T

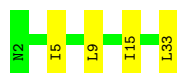


• Molecule 21: Photosystem II reaction center protein Ycf12



• Molecule 21: Photosystem II reaction center protein Ycf12

Chain v:  88% 12%



- Molecule 22: Photosystem II reaction center W protein

Chain W:  60% 38%



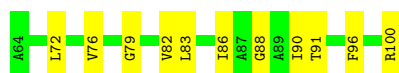
- Molecule 22: Photosystem II reaction center W protein

Chain w:  68% 32%



- Molecule 23: Photosystem II reaction center protein X

Chain X:  70% 30%



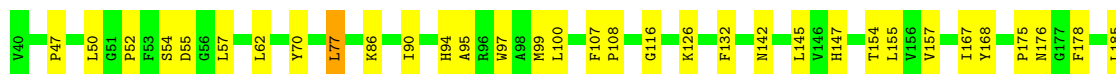
- Molecule 23: Photosystem II reaction center protein X

Chain x:  81% 19%



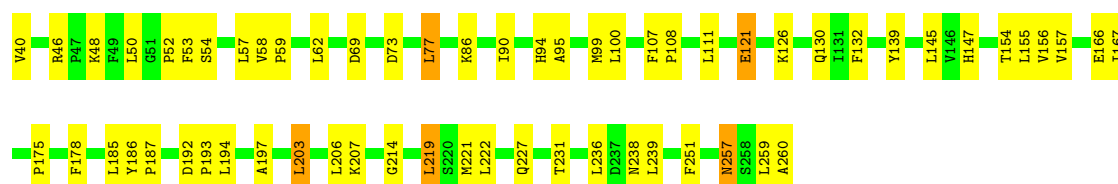
- Molecule 24: Multifunctional fusion protein

Chain Y:  78% 21%



- Molecule 24: Multifunctional fusion protein

Chain y:  72% 25%



- Molecule 25: Photosystem II reaction center protein Z

Chain Z: 89% 11%



- Molecule 25: Photosystem II reaction center protein Z

Chain z: 74% 26%



- Molecule 26: Chloroplast oxygen-evolving enhancer protein 3

Chain U: 86% 14%



- Molecule 26: Chloroplast oxygen-evolving enhancer protein 3

Chain u: 83% 16%



- Molecule 27: Chloroplast PsbY

Chain Q1: 76% 24%



- Molecule 27: Chloroplast PsbY

Chain q1: 62% 38%



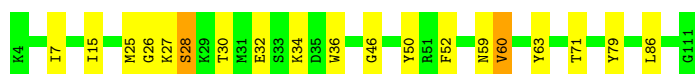
- Molecule 28: Chloroplast photosystem II 10 kDa protein

Chain P1:  88% 12%



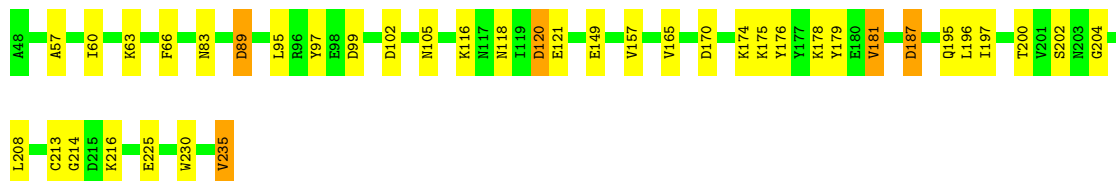
- Molecule 28: Chloroplast photosystem II 10 kDa protein

Chain p1:  82% 16%



- Molecule 29: Photosystem II oxygen evolving enhancer 2

Chain F1:  79% 18%



- Molecule 29: Photosystem II oxygen evolving enhancer 2

Chain f1:  80% 20%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	94893	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.066	Depositor
Minimum map value	-0.028	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	460.8, 460.8, 460.8	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9216, 0.9216, 0.9216	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.72	1/1675 (0.1%)	0.89	0/2283
1	7	0.68	0/1675	0.88	0/2283
2	2	0.70	0/1734	0.91	1/2359 (0.0%)
2	4	0.76	0/1732	0.98	1/2355 (0.0%)
2	9	0.64	0/1734	0.85	0/2359
2	G	0.50	0/1734	0.66	0/2359
2	g	0.53	0/1734	0.69	0/2359
2	q	0.76	0/1732	0.98	1/2355 (0.0%)
3	3	0.67	0/1734	0.90	1/2362 (0.0%)
3	5	0.90	0/1734	1.14	1/2362 (0.0%)
3	8	0.73	0/1734	0.91	0/2362
3	N	0.72	0/1734	0.92	0/2362
3	n	0.72	0/1734	0.91	0/2362
3	p	0.57	0/1734	0.75	0/2362
4	0	0.42	0/1701	0.60	0/2315
4	6	0.49	0/1701	0.65	0/2315
5	A	0.33	0/2714	0.40	0/3701
5	a	0.38	0/2714	0.47	0/3701
6	B	0.32	0/4085	0.37	0/5564
6	b	0.38	0/4085	0.48	0/5564
7	C	0.35	0/3602	0.42	1/4910 (0.0%)
7	c	0.41	0/3602	0.50	0/4910
8	D	0.42	0/2825	0.53	0/3849
8	d	0.43	0/2825	0.52	0/3849
9	E	0.55	0/670	0.69	0/913
9	e	0.71	0/670	0.87	0/913
10	F	0.71	0/312	0.89	0/426
10	f	0.79	0/312	1.02	0/426
11	H	0.24	0/518	0.30	0/708
11	h	0.24	0/518	0.32	0/708
12	I	0.64	0/282	0.76	0/382

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
12	i	0.60	0/282	0.75	0/382
13	J	0.18	0/276	0.24	0/377
13	j	0.28	0/276	0.30	0/377
14	K	0.27	0/305	0.40	0/420
14	k	0.24	0/305	0.42	0/420
15	L	0.41	0/311	0.53	0/422
15	l	0.42	0/311	0.54	0/422
16	M	0.27	0/248	0.45	0/338
16	m	0.24	0/248	0.39	0/338
17	O	0.36	0/1823	0.48	0/2466
17	o	0.35	0/1823	0.46	0/2466
18	R	0.51	0/1850	0.64	0/2515
18	r	0.60	0/1850	0.75	0/2515
19	S	0.44	0/1985	0.61	0/2711
19	s	0.45	0/1985	0.62	0/2711
20	T	0.25	0/253	0.32	0/343
20	t	0.45	0/253	0.57	0/343
21	V	0.13	0/234	0.28	0/319
21	v	0.13	0/234	0.25	0/319
22	W	0.74	0/477	0.90	0/650
22	w	0.74	0/477	0.91	0/650
23	X	0.55	0/248	0.76	0/339
23	x	0.61	0/248	0.79	0/339
24	Y	0.34	0/1735	0.43	1/2359 (0.0%)
24	y	0.32	0/1735	0.39	0/2359
25	Z	0.19	0/491	0.31	0/672
25	z	0.18	0/491	0.28	0/672
26	U	0.24	0/1132	0.35	0/1521
26	u	0.21	0/1132	0.31	0/1521
27	Q1	0.55	0/265	0.69	0/362
27	q1	0.55	0/265	0.75	0/362
28	P1	0.36	0/835	0.47	0/1127
28	p1	0.34	0/835	0.45	0/1127
29	F1	0.49	0/1473	0.60	0/1991
29	f1	0.57	0/1473	0.68	0/1991
All	All	0.51	1/85454 (0.0%)	0.65	7/116284 (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
18	R	0	1
18	r	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	58	VAL	N-CA	5.14	1.49	1.45

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	126	PHE	CA-CB-CG	6.76	120.56	113.80
3	5	112	GLY	CA-C-O	-5.73	118.32	122.45
3	3	122	PHE	CA-CB-CG	5.68	119.48	113.80
2	q	130	ALA	N-CA-C	-5.51	106.46	114.12
24	Y	55	ASP	N-CA-C	-5.25	108.64	114.62

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	R	211	CSU	Mainchain
18	r	211	CSU	Mainchain

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	1630	0	1583	90	0
1	7	1630	0	1583	85	0
2	2	1686	0	1616	136	0
2	4	1685	0	1612	187	0
2	9	1686	0	1616	116	0
2	G	1686	0	1616	79	0
2	g	1686	0	1616	49	0
2	q	1685	0	1612	161	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	3	1686	0	1635	163	0
3	5	1686	0	1635	219	0
3	8	1686	0	1635	86	0
3	N	1686	0	1635	84	0
3	n	1686	0	1635	78	0
3	p	1686	0	1635	146	0
4	0	1657	0	1612	76	0
4	6	1657	0	1612	91	0
5	A	2632	0	2532	62	0
5	a	2632	0	2532	67	0
6	B	3954	0	3823	83	0
6	b	3954	0	3823	98	0
7	C	3482	0	3375	97	0
7	c	3482	0	3375	112	0
8	D	2730	0	2630	73	0
8	d	2730	0	2630	69	0
9	E	652	0	636	20	0
9	e	652	0	636	25	0
10	F	302	0	311	15	0
10	f	302	0	311	16	0
11	H	507	0	520	8	0
11	h	507	0	520	12	0
12	I	274	0	280	6	0
12	i	274	0	280	6	0
13	J	270	0	282	3	0
13	j	270	0	282	7	0
14	K	295	0	311	11	0
14	k	295	0	311	10	0
15	L	303	0	311	10	0
15	l	303	0	311	13	0
16	M	370	0	302	10	0
16	m	370	0	301	7	0
17	O	1789	0	1759	46	0
17	o	1789	0	1759	29	0
18	R	1818	0	1737	59	0
18	r	1818	0	1736	57	0
19	S	1934	0	1879	62	0
19	s	1934	0	1879	67	0
20	T	246	0	262	8	0
20	t	246	0	262	11	0
21	V	233	0	263	4	0
21	v	233	0	263	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	W	468	0	450	26	0
22	w	468	0	450	24	0
23	X	247	0	260	7	0
23	x	247	0	260	5	0
24	Y	1688	0	1637	43	0
24	y	1688	0	1637	56	0
25	Z	478	0	513	5	0
25	z	478	0	513	11	0
26	U	1122	0	1151	16	0
26	u	1122	0	1151	13	0
27	Q1	260	0	269	9	0
27	q1	260	0	269	16	0
28	P1	820	0	834	9	0
28	p1	820	0	834	14	0
29	F1	1443	0	1408	25	0
29	f1	1443	0	1408	34	0
30	0	336	0	282	43	0
30	1	441	0	437	52	0
30	2	270	0	219	43	0
30	3	311	0	236	69	0
30	4	327	0	268	67	0
30	5	305	0	221	58	0
30	6	330	0	275	48	0
30	7	443	0	441	53	0
30	8	296	0	270	34	0
30	9	328	0	269	50	0
30	G	344	0	302	50	0
30	N	346	0	306	52	0
30	R	167	0	138	15	0
30	S	182	0	121	16	0
30	Y	350	0	318	49	0
30	g	278	0	233	34	0
30	n	409	0	366	59	0
30	p	305	0	221	44	0
30	q	326	0	265	60	0
30	r	167	0	138	17	0
30	s	182	0	123	20	0
30	y	353	0	327	42	0
31	0	512	0	481	46	0
31	1	494	0	513	61	0
31	2	468	0	451	57	0
31	3	559	0	506	82	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	4	435	0	386	66	0
31	5	481	0	410	88	0
31	6	535	0	523	67	0
31	7	545	0	552	69	0
31	8	512	0	489	79	0
31	9	437	0	392	62	0
31	A	239	0	242	22	0
31	B	1024	0	1116	92	0
31	C	818	0	870	61	0
31	D	130	0	144	16	0
31	G	457	0	444	55	0
31	N	566	0	539	95	0
31	R	598	0	536	42	0
31	S	627	0	608	65	0
31	Y	484	0	491	56	0
31	a	190	0	203	20	0
31	b	1024	0	1117	98	0
31	c	826	0	888	72	0
31	d	179	0	183	12	0
31	g	457	0	441	44	0
31	n	512	0	489	86	0
31	p	478	0	408	89	0
31	q	432	0	383	63	0
31	r	598	0	534	46	0
31	s	627	0	606	71	0
31	y	538	0	539	68	0
32	0	84	0	112	12	0
32	1	84	0	112	12	0
32	2	42	0	56	8	0
32	3	84	0	112	24	0
32	4	42	0	56	11	0
32	5	84	0	112	38	0
32	6	84	0	112	19	0
32	7	84	0	112	16	0
32	8	84	0	112	18	0
32	9	42	0	56	15	0
32	G	42	0	56	8	0
32	N	84	0	112	22	0
32	R	42	0	56	3	0
32	S	84	0	112	17	0
32	Y	84	0	112	12	0
32	g	42	0	56	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	n	84	0	112	18	0
32	p	84	0	112	24	0
32	q	42	0	56	12	0
32	r	42	0	56	4	0
32	s	84	0	112	24	0
32	y	84	0	112	16	0
33	0	36	0	42	3	0
33	1	35	0	40	5	0
33	2	49	0	74	4	0
33	3	33	0	36	7	0
33	4	47	0	67	5	0
33	5	35	0	40	9	0
33	6	37	0	44	2	0
33	7	35	0	40	3	0
33	8	49	0	74	4	0
33	9	33	0	36	9	0
33	A	83	0	109	8	0
33	B	49	0	74	6	0
33	C	40	0	53	7	0
33	D	93	0	135	12	0
33	F1	35	0	40	1	0
33	G	44	0	61	15	0
33	K	36	0	42	6	0
33	L	49	0	74	4	0
33	M	41	0	55	1	0
33	N	49	0	74	3	0
33	R	38	0	46	1	0
33	S	85	0	113	11	0
33	Y	42	0	57	4	0
33	a	39	0	48	4	0
33	b	93	0	135	21	0
33	c	47	0	67	8	0
33	d	49	0	74	13	0
33	e	44	0	61	7	0
33	g	44	0	61	12	0
33	j	49	0	74	5	0
33	l	49	0	74	11	0
33	n	49	0	74	3	0
33	p	35	0	40	3	0
33	q	46	0	65	12	0
33	r	38	0	46	3	0
33	s	85	0	113	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	t	41	0	55	1	0
33	y	46	0	65	11	0
33	z	36	0	42	3	0
34	0	80	0	100	13	0
34	1	38	0	46	2	0
34	2	129	0	168	14	0
34	3	38	0	46	13	0
34	4	91	0	122	21	0
34	5	38	0	46	11	0
34	6	119	0	148	21	0
34	7	115	0	140	12	0
34	9	129	0	168	32	0
34	A	117	0	144	9	0
34	B	127	0	164	16	0
34	C	165	0	210	17	0
34	D	191	0	262	16	0
34	G	129	0	168	25	0
34	I	38	0	46	5	0
34	J	89	0	118	5	0
34	N	38	0	46	2	0
34	Q1	38	0	46	14	0
34	R	38	0	46	0	0
34	S	41	0	52	2	0
34	W	131	0	178	15	0
34	X	76	0	92	6	0
34	Y	38	0	46	5	0
34	a	114	0	138	12	0
34	b	256	0	332	21	0
34	c	120	0	150	17	0
34	d	140	0	190	11	0
34	f	38	0	46	1	0
34	g	87	0	114	10	0
34	j	43	0	56	4	0
34	k	86	0	112	5	0
34	m	45	0	60	5	0
34	n	78	0	96	20	0
34	p	38	0	46	5	0
34	q	91	0	122	10	0
34	q1	38	0	46	11	0
34	r	38	0	46	5	0
34	s	41	0	52	4	0
34	w	217	0	290	35	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	x	38	0	46	5	0
34	y	38	0	44	4	0
35	2	41	0	56	12	0
35	4	41	0	56	17	0
35	9	41	0	56	13	0
35	G	41	0	56	28	0
35	g	41	0	56	3	0
35	q	41	0	56	20	0
36	0	44	0	54	10	0
36	2	44	0	54	6	0
36	3	44	0	54	10	0
36	4	44	0	54	8	0
36	5	44	0	54	16	0
36	6	44	0	54	11	0
36	8	44	0	54	4	0
36	9	44	0	54	9	0
36	G	44	0	54	1	0
36	N	44	0	55	7	0
36	R	88	0	108	15	0
36	S	44	0	54	4	0
36	Y	44	0	54	2	0
36	g	44	0	54	2	0
36	n	44	0	54	2	0
36	p	44	0	54	2	0
36	q	44	0	54	4	0
36	r	88	0	108	9	0
36	s	44	0	54	4	0
36	y	44	0	54	5	0
37	2	44	0	56	11	0
37	4	44	0	56	9	0
37	9	44	0	56	3	0
37	G	44	0	56	22	0
37	R	44	0	56	7	0
37	g	44	0	56	20	0
37	q	44	0	56	16	0
37	r	44	0	56	4	0
38	0	42	0	47	2	0
38	6	42	0	47	4	0
38	A	96	0	121	4	0
38	B	106	0	147	14	0
38	G	80	0	86	13	0
38	M	50	0	63	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	R	51	0	68	6	0
38	S	51	0	68	4	0
38	X	38	0	39	1	0
38	Y	42	0	47	5	0
38	a	93	0	112	8	0
38	b	106	0	147	11	0
38	g	80	0	86	21	0
38	m	50	0	63	2	0
38	r	51	0	68	4	0
38	s	51	0	68	6	0
38	x	42	0	47	3	0
38	y	42	0	47	3	0
39	A	10	0	0	1	0
39	a	10	0	0	0	0
40	A	1	0	0	0	0
40	a	1	0	0	0	0
41	A	2	0	0	1	0
41	a	2	0	0	1	0
42	A	64	0	74	7	0
42	D	64	0	74	9	0
42	a	64	0	74	3	0
42	d	64	0	74	5	0
43	A	40	0	56	3	0
43	B	120	0	168	20	0
43	C	80	0	112	6	0
43	D	40	0	56	13	0
43	H	40	0	56	4	0
43	T	40	0	56	6	0
43	V	40	0	56	1	0
43	Z	40	0	56	3	0
43	a	40	0	56	4	0
43	b	120	0	168	16	0
43	c	80	0	112	15	0
43	d	40	0	56	5	0
43	h	40	0	56	4	0
43	t	40	0	56	13	0
43	v	40	0	56	3	0
43	z	40	0	56	4	0
44	A	55	0	80	5	0
44	D	55	0	80	7	0
44	a	55	0	80	9	0
44	d	55	0	80	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	C	248	0	346	34	0
45	c	260	0	373	51	0
46	D	4	0	0	0	0
46	d	4	0	1	0	0
47	E	43	0	30	10	0
47	e	43	0	30	11	0
48	K	35	0	46	1	0
48	R	35	0	46	8	0
48	c	28	0	29	3	0
48	r	35	0	46	11	0
49	0	7	0	0	0	0
49	1	3	0	0	0	0
49	2	3	0	0	0	0
49	3	1	0	0	0	0
49	4	1	0	0	0	0
49	5	1	0	0	0	0
49	6	4	0	0	0	0
49	7	6	0	0	0	0
49	8	4	0	0	0	0
49	9	2	0	0	0	0
49	A	21	0	0	1	0
49	B	6	0	0	0	0
49	C	15	0	0	1	0
49	D	12	0	0	0	0
49	E	1	0	0	0	0
49	F1	4	0	0	0	0
49	G	5	0	0	0	0
49	I	1	0	0	1	0
49	J	1	0	0	0	0
49	N	5	0	0	0	0
49	O	6	0	0	0	0
49	R	4	0	0	0	0
49	S	3	0	0	0	0
49	T	4	0	0	0	0
49	Y	8	0	0	0	0
49	a	14	0	0	0	0
49	b	6	0	0	0	0
49	c	15	0	0	0	0
49	d	15	0	0	0	0
49	e	2	0	0	0	0
49	f	1	0	0	0	0
49	f1	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	g	4	0	0	0	0
49	j	1	0	0	0	0
49	m	2	0	0	0	0
49	n	7	0	0	0	0
49	o	6	0	0	0	0
49	q	1	0	0	0	0
49	r	4	0	0	0	0
49	s	3	0	0	0	0
49	t	2	0	0	0	0
49	w	2	0	0	0	0
49	y	8	0	0	0	0
All	All	117990	0	117879	5329	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

The worst 5 of 5329 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)
2:4:223:PHE:HE1	35:4:615:RRX:C32	1.41	1.31
2:4:223:PHE:HE1	35:4:615:RRX:H50	1.09	1.17
2:4:223:PHE:CE1	35:4:615:RRX:C32	2.31	1.13
2:G:223:PHE:HE1	35:G:614:RRX:C32	1.61	1.13
38:g:301:SQD:C13	37:g:321:XAT:H362	1.78	1.11

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	212/214 (99%)	202 (95%)	10 (5%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	7	212/214 (99%)	205 (97%)	6 (3%)	1 (0%)	24	40
2	2	220/222 (99%)	203 (92%)	15 (7%)	2 (1%)	14	26
2	4	220/222 (99%)	200 (91%)	15 (7%)	5 (2%)	5	8
2	9	220/222 (99%)	212 (96%)	8 (4%)	0	100	100
2	G	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
2	g	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
2	q	220/222 (99%)	196 (89%)	22 (10%)	2 (1%)	14	26
3	3	219/221 (99%)	198 (90%)	21 (10%)	0	100	100
3	5	219/221 (99%)	202 (92%)	15 (7%)	2 (1%)	14	26
3	8	219/221 (99%)	212 (97%)	7 (3%)	0	100	100
3	N	219/221 (99%)	211 (96%)	7 (3%)	1 (0%)	24	40
3	n	219/221 (99%)	212 (97%)	7 (3%)	0	100	100
3	p	219/221 (99%)	200 (91%)	16 (7%)	3 (1%)	9	15
4	0	215/217 (99%)	202 (94%)	12 (6%)	1 (0%)	24	40
4	6	215/217 (99%)	205 (95%)	9 (4%)	1 (0%)	24	40
5	A	334/336 (99%)	329 (98%)	5 (2%)	0	100	100
5	a	334/336 (99%)	329 (98%)	5 (2%)	0	100	100
6	B	502/504 (100%)	493 (98%)	9 (2%)	0	100	100
6	b	502/504 (100%)	491 (98%)	11 (2%)	0	100	100
7	C	446/448 (100%)	437 (98%)	9 (2%)	0	100	100
7	c	446/448 (100%)	438 (98%)	8 (2%)	0	100	100
8	D	340/342 (99%)	330 (97%)	10 (3%)	0	100	100
8	d	340/342 (99%)	329 (97%)	10 (3%)	1 (0%)	36	54
9	E	79/81 (98%)	79 (100%)	0	0	100	100
9	e	79/81 (98%)	77 (98%)	2 (2%)	0	100	100
10	F	35/37 (95%)	35 (100%)	0	0	100	100
10	f	35/37 (95%)	35 (100%)	0	0	100	100
11	H	65/67 (97%)	65 (100%)	0	0	100	100
11	h	65/67 (97%)	65 (100%)	0	0	100	100
12	I	32/34 (94%)	32 (100%)	0	0	100	100
12	i	32/34 (94%)	32 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	J	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
13	j	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
14	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
14	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
15	L	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
15	l	35/37 (95%)	35 (100%)	0	0	100	100
16	M	31/57 (54%)	30 (97%)	0	1 (3%)	3	5
16	m	31/57 (54%)	31 (100%)	0	0	100	100
17	O	238/240 (99%)	227 (95%)	11 (5%)	0	100	100
17	o	238/240 (99%)	227 (95%)	11 (5%)	0	100	100
18	R	233/236 (99%)	227 (97%)	6 (3%)	0	100	100
18	r	233/236 (99%)	230 (99%)	3 (1%)	0	100	100
19	S	255/257 (99%)	249 (98%)	6 (2%)	0	100	100
19	s	255/257 (99%)	249 (98%)	6 (2%)	0	100	100
20	T	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
20	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
21	V	30/32 (94%)	30 (100%)	0	0	100	100
21	v	30/32 (94%)	30 (100%)	0	0	100	100
22	W	58/60 (97%)	54 (93%)	4 (7%)	0	100	100
22	w	58/60 (97%)	57 (98%)	1 (2%)	0	100	100
23	X	35/37 (95%)	35 (100%)	0	0	100	100
23	x	35/37 (95%)	35 (100%)	0	0	100	100
24	Y	219/221 (99%)	215 (98%)	4 (2%)	0	100	100
24	y	219/221 (99%)	215 (98%)	4 (2%)	0	100	100
25	Z	60/62 (97%)	60 (100%)	0	0	100	100
25	z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
26	U	142/144 (99%)	139 (98%)	2 (1%)	1 (1%)	18	32
26	u	142/144 (99%)	141 (99%)	1 (1%)	0	100	100
27	Q1	32/34 (94%)	32 (100%)	0	0	100	100
27	q1	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
28	P1	106/108 (98%)	104 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	p1	106/108 (98%)	104 (98%)	2 (2%)	0	100	100
29	F1	186/188 (99%)	183 (98%)	3 (2%)	0	100	100
29	f1	186/188 (99%)	180 (97%)	6 (3%)	0	100	100
All	All	10672/10854 (98%)	10317 (97%)	334 (3%)	21 (0%)	44	62

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	4	181	GLY
2	4	188	GLY
2	4	191	ASP
3	N	52	PHE
4	0	252	ALA

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	165/165 (100%)	156 (94%)	9 (6%)	19	35
1	7	165/165 (100%)	158 (96%)	7 (4%)	26	47
2	2	171/171 (100%)	164 (96%)	7 (4%)	27	48
2	4	171/171 (100%)	161 (94%)	10 (6%)	18	33
2	9	171/171 (100%)	165 (96%)	6 (4%)	32	54
2	G	171/171 (100%)	164 (96%)	7 (4%)	27	48
2	g	171/171 (100%)	161 (94%)	10 (6%)	18	33
2	q	171/171 (100%)	164 (96%)	7 (4%)	27	48
3	3	168/168 (100%)	156 (93%)	12 (7%)	13	24
3	5	168/168 (100%)	156 (93%)	12 (7%)	13	24
3	8	168/168 (100%)	159 (95%)	9 (5%)	20	36
3	N	168/168 (100%)	158 (94%)	10 (6%)	17	31
3	n	168/168 (100%)	159 (95%)	9 (5%)	20	36

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	p	168/168 (100%)	161 (96%)	7 (4%)	26	47
4	0	169/169 (100%)	159 (94%)	10 (6%)	18	32
4	6	169/169 (100%)	161 (95%)	8 (5%)	23	43
5	A	274/274 (100%)	261 (95%)	13 (5%)	23	43
5	a	274/274 (100%)	265 (97%)	9 (3%)	33	55
6	B	402/402 (100%)	375 (93%)	27 (7%)	15	27
6	b	402/402 (100%)	377 (94%)	25 (6%)	16	30
7	C	350/350 (100%)	324 (93%)	26 (7%)	13	23
7	c	350/350 (100%)	332 (95%)	18 (5%)	21	39
8	D	277/277 (100%)	268 (97%)	9 (3%)	34	56
8	d	277/277 (100%)	260 (94%)	17 (6%)	17	30
9	E	72/72 (100%)	69 (96%)	3 (4%)	26	47
9	e	72/72 (100%)	69 (96%)	3 (4%)	26	47
10	F	31/31 (100%)	31 (100%)	0	100	100
10	f	31/31 (100%)	31 (100%)	0	100	100
11	H	57/57 (100%)	56 (98%)	1 (2%)	51	69
11	h	57/57 (100%)	55 (96%)	2 (4%)	32	54
12	I	31/31 (100%)	30 (97%)	1 (3%)	34	56
12	i	31/31 (100%)	30 (97%)	1 (3%)	34	56
13	J	27/27 (100%)	24 (89%)	3 (11%)	6	11
13	j	27/27 (100%)	25 (93%)	2 (7%)	13	23
14	K	33/33 (100%)	29 (88%)	4 (12%)	5	8
14	k	33/33 (100%)	28 (85%)	5 (15%)	3	3
15	L	34/34 (100%)	32 (94%)	2 (6%)	18	32
15	l	34/34 (100%)	32 (94%)	2 (6%)	18	32
16	M	28/28 (100%)	27 (96%)	1 (4%)	31	53
16	m	28/28 (100%)	27 (96%)	1 (4%)	31	53
17	O	189/189 (100%)	176 (93%)	13 (7%)	14	26
17	o	189/189 (100%)	181 (96%)	8 (4%)	26	47
18	R	184/184 (100%)	178 (97%)	6 (3%)	33	55
18	r	184/184 (100%)	177 (96%)	7 (4%)	29	51

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	S	192/192 (100%)	185 (96%)	7 (4%)	31	53
19	s	192/192 (100%)	186 (97%)	6 (3%)	35	57
20	T	26/26 (100%)	26 (100%)	0	100	100
20	t	26/26 (100%)	23 (88%)	3 (12%)	5	10
21	V	26/26 (100%)	24 (92%)	2 (8%)	12	21
21	v	26/26 (100%)	25 (96%)	1 (4%)	29	51
22	W	50/50 (100%)	49 (98%)	1 (2%)	48	67
22	w	50/50 (100%)	50 (100%)	0	100	100
23	X	25/25 (100%)	23 (92%)	2 (8%)	11	20
23	x	25/25 (100%)	25 (100%)	0	100	100
24	Y	170/170 (100%)	161 (95%)	9 (5%)	20	37
24	y	170/170 (100%)	160 (94%)	10 (6%)	18	32
25	Z	52/52 (100%)	50 (96%)	2 (4%)	29	51
25	z	52/52 (100%)	49 (94%)	3 (6%)	18	33
26	U	108/108 (100%)	106 (98%)	2 (2%)	50	68
26	u	108/108 (100%)	100 (93%)	8 (7%)	13	23
27	Q1	28/28 (100%)	28 (100%)	0	100	100
27	q1	28/28 (100%)	28 (100%)	0	100	100
28	P1	88/88 (100%)	88 (100%)	0	100	100
28	p1	88/88 (100%)	84 (96%)	4 (4%)	24	44
29	F1	147/147 (100%)	139 (95%)	8 (5%)	20	36
29	f1	147/147 (100%)	146 (99%)	1 (1%)	76	85
All	All	8504/8504 (100%)	8086 (95%)	418 (5%)	24	41

5 of 418 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	8	146	GLN
6	b	445	THR
26	u	98	LYS
2	9	184	LEU
5	a	275	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
19	s	45	GLN
26	u	171	GLN
29	f1	59	ASN
18	R	130	GLN
18	R	46	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
18	CSU	R	211	18	6,9,10	3.27	3 (50%)	3,12,14	2.40	2 (66%)
18	CSU	r	211	18	6,9,10	3.28	3 (50%)	3,12,14	2.38	2 (66%)

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
18	CSU	R	211	18	-	4/4/8/10	-
18	CSU	r	211	18	-	4/4/8/10	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	r	211	CSU	OD1-S	6.06	1.63	1.45
18	R	211	CSU	OD3-S	6.04	1.63	1.45
18	R	211	CSU	O-C	4.03	1.36	1.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	r	211	CSU	O-C	4.01	1.35	1.19
18	R	211	CSU	OD1-S	-2.73	1.37	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	r	211	CSU	OD2-S-OD3	3.53	125.57	112.78
18	R	211	CSU	OD2-S-OD1	3.15	124.19	112.78
18	R	211	CSU	OD2-S-OD3	-2.70	102.99	112.78
18	r	211	CSU	OD2-S-OD1	-2.10	105.16	112.78

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	R	211	CSU	N-CA-CB-SG
18	R	211	CSU	OD2-S-SG-CB
18	r	211	CSU	OD2-S-SG-CB
18	R	211	CSU	OD1-S-SG-CB
18	R	211	CSU	OD3-S-SG-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	R	211	CSU	1	0
18	r	211	CSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 672 ligands modelled in this entry, 6 are monoatomic - leaving 666 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
43	BCR	b	619	-	41,41,41	4.78	26 (63%)	56,56,56	2.31	20 (35%)
33	LHG	9	320	31	32,32,48	0.46	0	35,38,54	1.25	3 (8%)
35	RRX	G	614	-	42,42,42	5.01	25 (59%)	57,58,58	2.49	22 (38%)
31	CLA	2	611	2	59,63,73	1.46	6 (10%)	71,101,113	2.02	18 (25%)
30	CHL	9	311	2	65,69,74	0.83	2 (3%)	74,108,114	1.33	13 (17%)
31	CLA	3	313	3	54,58,73	1.53	6 (11%)	65,95,113	2.15	20 (30%)
46	BCT	D	402	40	2,3,3	1.35	0	2,3,3	2.67	2 (100%)
31	CLA	C	607	49	69,73,73	1.37	7 (10%)	83,113,113	1.99	21 (25%)
38	SQD	a	412	-	44,45,54	0.90	1 (2%)	53,56,65	1.01	4 (7%)
32	LUT	Y	316	-	42,43,43	6.02	27 (64%)	51,60,60	2.08	18 (35%)
34	LMG	D	410	-	46,46,55	0.93	3 (6%)	54,54,63	1.07	4 (7%)
38	SQD	g	318	-	41,42,54	0.88	0	50,53,65	0.96	2 (4%)
30	CHL	4	606	31	55,59,74	0.88	2 (3%)	62,96,114	1.41	12 (19%)
31	CLA	B	610	49	69,73,73	1.35	6 (8%)	83,113,113	1.96	20 (24%)
31	CLA	y	610	24	69,73,73	1.35	7 (10%)	83,113,113	1.92	17 (20%)
31	CLA	3	306	49	59,63,73	1.47	7 (11%)	71,101,113	2.08	18 (25%)
32	LUT	5	617	-	42,43,43	6.08	27 (64%)	51,60,60	1.87	12 (23%)
30	CHL	3	308	-	51,55,74	0.95	2 (3%)	57,91,114	1.41	10 (17%)
31	CLA	r	311	18	62,66,73	1.44	6 (9%)	74,104,113	2.05	18 (24%)
31	CLA	s	315	19	52,56,73	1.56	6 (11%)	62,92,113	2.05	15 (24%)
30	CHL	Y	302	24	70,74,74	0.80	2 (2%)	80,114,114	1.30	14 (17%)
34	LMG	b	629	-	38,38,55	0.63	1 (2%)	46,46,63	1.12	2 (4%)
30	CHL	G	608	2	67,71,74	0.86	3 (4%)	76,110,114	1.41	14 (18%)
34	LMG	X	203	-	38,38,55	0.61	1 (2%)	46,46,63	1.12	2 (4%)
38	SQD	A	413	-	44,45,54	0.84	0	53,56,65	0.96	2 (3%)
31	CLA	9	313	33	51,55,73	1.59	7 (13%)	61,91,113	2.07	16 (26%)
31	CLA	c	613	7	69,73,73	1.36	7 (10%)	83,113,113	1.99	19 (22%)
34	LMG	3	321	-	38,38,55	0.63	1 (2%)	46,46,63	0.96	2 (4%)
43	BCR	d	406	-	41,41,41	4.70	26 (63%)	56,56,56	3.60	25 (44%)
34	LMG	C	619	-	51,51,55	1.07	6 (11%)	59,59,63	1.18	4 (6%)
31	CLA	s	314	19	69,73,73	1.38	7 (10%)	83,113,113	1.94	19 (22%)
31	CLA	C	604	49	60,64,73	1.47	6 (10%)	72,102,113	2.06	16 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LUT	p	616	-	42,43,43	6.09	27 (64%)	51,60,60	2.78	18 (35%)
31	CLA	N	312	3	49,53,73	1.59	7 (14%)	59,89,113	2.06	17 (28%)
31	CLA	c	609	7	69,73,73	1.38	6 (8%)	83,113,113	1.92	19 (22%)
38	SQD	g	301	-	37,38,54	0.91	0	46,49,65	1.01	2 (4%)
38	SQD	r	322	-	50,51,54	0.80	0	59,62,65	0.93	2 (3%)
31	CLA	G	603	2	59,63,73	1.45	6 (10%)	71,101,113	2.08	18 (25%)
31	CLA	p	603	3	59,63,73	1.47	7 (11%)	71,101,113	2.14	19 (26%)
38	SQD	M	102	-	49,50,54	0.81	0	58,61,65	0.95	2 (3%)
31	CLA	3	314	3	59,63,73	1.46	7 (11%)	71,101,113	2.06	20 (28%)
31	CLA	r	304	18	64,68,73	1.40	6 (9%)	77,107,113	1.99	21 (27%)
38	SQD	G	617	-	41,42,54	0.86	0	50,53,65	0.98	2 (4%)
31	CLA	2	603	2	59,63,73	1.46	6 (10%)	71,101,113	2.05	19 (26%)
43	BCR	D	405	-	41,41,41	4.84	27 (65%)	56,56,56	2.69	22 (39%)
30	CHL	7	310	1	70,74,74	0.80	2 (2%)	80,114,114	1.29	14 (17%)
30	CHL	2	608	2	61,65,74	0.89	3 (4%)	69,103,114	1.42	14 (20%)
31	CLA	B	611	6	69,73,73	1.37	7 (10%)	83,113,113	1.93	18 (21%)
34	LMG	9	301	-	51,51,55	1.10	6 (11%)	59,59,63	1.68	8 (13%)
34	LMG	D	411	-	51,51,55	1.07	6 (11%)	59,59,63	1.08	3 (5%)
31	CLA	N	311	33	53,57,73	1.54	6 (11%)	62,93,113	2.18	17 (27%)
31	CLA	7	305	49	69,73,73	1.35	6 (8%)	83,113,113	1.97	17 (20%)
31	CLA	Y	310	24	69,73,73	1.35	7 (10%)	83,113,113	1.91	18 (21%)
37	XAT	r	318	-	39,47,47	0.65	0	54,74,74	1.94	12 (22%)
31	CLA	n	305	49	69,73,73	1.34	5 (7%)	83,113,113	1.95	18 (21%)
35	RRX	g	315	-	42,42,42	5.02	25 (59%)	57,58,58	2.63	23 (40%)
31	CLA	B	604	6	69,73,73	1.40	7 (10%)	83,113,113	2.05	16 (19%)
31	CLA	S	316	19	50,54,73	1.58	6 (12%)	60,90,113	2.07	16 (26%)
31	CLA	c	610	7	69,73,73	1.36	6 (8%)	83,113,113	2.02	18 (21%)
31	CLA	p	615	3	50,54,73	1.58	7 (14%)	60,90,113	2.06	15 (25%)
33	LHG	D	408	-	48,48,48	0.39	0	51,54,54	1.08	4 (7%)
30	CHL	7	302	1	70,74,74	0.81	2 (2%)	80,114,114	1.32	14 (17%)
32	LUT	S	318	-	42,43,43	6.09	28 (66%)	51,60,60	2.11	14 (27%)
31	CLA	5	613	3	58,62,73	1.48	7 (12%)	69,99,113	2.07	18 (26%)
30	CHL	R	309	18	60,64,74	0.85	2 (3%)	68,102,114	1.33	12 (17%)
30	CHL	0	607	49	70,74,74	0.77	1 (1%)	80,114,114	1.31	14 (17%)
31	CLA	r	312	18	61,65,73	1.46	6 (9%)	73,103,113	2.06	19 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CHL	5	608	-	54,58,74	0.89	2 (3%)	59,94,114	1.44	12 (20%)
34	LMG	c	620	-	38,38,55	0.62	1 (2%)	46,46,63	1.18	5 (10%)
31	CLA	R	314	18	53,57,73	1.55	6 (11%)	62,93,113	2.12	18 (29%)
34	LMG	d	410	-	51,51,55	1.07	6 (11%)	59,59,63	1.08	3 (5%)
31	CLA	6	311	4	69,73,73	1.35	7 (10%)	83,113,113	1.93	19 (22%)
34	LMG	W	203	-	38,38,55	0.64	1 (2%)	46,46,63	1.12	2 (4%)
44	PL9	A	416	-	55,55,55	1.16	7 (12%)	68,69,69	1.60	13 (19%)
30	CHL	6	307	49	55,59,74	0.86	2 (3%)	62,96,114	1.39	11 (17%)
30	CHL	n	309	49	54,58,74	0.91	2 (3%)	59,94,114	1.45	12 (20%)
31	CLA	s	310	19	64,68,73	1.41	7 (10%)	77,107,113	2.02	17 (22%)
33	LHG	8	618	31	48,48,48	0.38	0	51,54,54	1.03	2 (3%)
34	LMG	w	203	-	38,38,55	0.61	1 (2%)	46,46,63	1.46	8 (17%)
31	CLA	S	304	19	46,50,73	1.70	6 (13%)	55,85,113	2.05	18 (32%)
31	CLA	n	314	3	69,73,73	1.35	7 (10%)	83,113,113	1.91	19 (22%)
31	CLA	Y	305	49	59,63,73	1.47	6 (10%)	71,101,113	2.08	18 (25%)
31	CLA	1	603	1	59,63,73	1.48	7 (11%)	71,101,113	2.03	17 (23%)
34	LMG	Y	319	-	38,38,55	0.64	1 (2%)	46,46,63	1.12	3 (6%)
34	LMG	9	302	-	40,40,55	0.68	2 (5%)	48,48,63	1.09	3 (6%)
30	CHL	3	309	-	54,58,74	1.06	3 (5%)	59,94,114	1.43	10 (16%)
31	CLA	4	603	2	59,63,73	1.46	6 (10%)	71,101,113	2.03	19 (26%)
43	BCR	B	617	-	41,41,41	4.69	26 (63%)	56,56,56	2.52	22 (39%)
30	CHL	0	605	4	56,60,74	1.19	5 (8%)	63,97,114	1.61	11 (17%)
31	CLA	C	603	7	69,73,73	1.38	7 (10%)	83,113,113	1.99	15 (18%)
36	NEX	p	618	31	38,46,46	3.38	10 (26%)	50,70,70	1.59	11 (22%)
30	CHL	s	302	19	50,54,74	0.99	2 (4%)	56,90,114	1.32	9 (16%)
31	CLA	r	306	49	52,56,73	1.57	7 (13%)	62,92,113	2.14	15 (24%)
30	CHL	1	606	49	70,74,74	0.81	1 (1%)	80,114,114	1.25	13 (16%)
30	CHL	7	321	49	67,71,74	0.82	2 (2%)	76,110,114	1.34	12 (15%)
34	LMG	Q1	101	-	38,38,55	0.64	1 (2%)	46,46,63	1.20	4 (8%)
38	SQD	6	301	-	41,42,54	0.87	0	50,53,65	1.00	2 (4%)
31	CLA	S	303	19	69,73,73	1.35	7 (10%)	83,113,113	1.97	20 (24%)
31	CLA	Y	314	24	58,62,73	1.48	6 (10%)	69,99,113	2.10	19 (27%)
31	CLA	q	313	33	46,51,73	1.54	5 (10%)	59,86,113	2.20	16 (27%)
31	CLA	5	614	3	55,59,73	1.51	7 (12%)	66,96,113	2.19	19 (28%)
31	CLA	q	306	49	59,63,73	1.49	6 (10%)	71,101,113	2.03	20 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	LMG	g	320	-	38,38,55	0.62	1 (2%)	46,46,63	1.12	4 (8%)
37	XAT	2	619	-	39,47,47	0.64	0	54,74,74	1.91	13 (24%)
31	CLA	c	612	7	59,63,73	1.48	7 (11%)	71,101,113	2.13	18 (25%)
33	LHG	K	102	-	35,35,48	0.45	0	38,41,54	1.21	2 (5%)
31	CLA	1	612	1	69,73,73	1.37	6 (8%)	83,113,113	1.88	18 (21%)
30	CHL	Y	309	24	70,74,74	0.80	2 (2%)	80,114,114	1.32	12 (15%)
34	LMG	N	320	-	38,38,55	0.63	1 (2%)	46,46,63	1.01	2 (4%)
31	CLA	b	614	6	69,73,73	1.35	6 (8%)	83,113,113	1.92	19 (22%)
34	LMG	B	621	-	51,51,55	1.08	6 (11%)	59,59,63	1.29	4 (6%)
43	BCR	z	101	-	41,41,41	4.77	26 (63%)	56,56,56	2.35	21 (37%)
30	CHL	R	310	49	59,63,74	0.97	3 (5%)	66,100,114	1.38	12 (18%)
30	CHL	6	308	49	70,74,74	0.77	1 (1%)	80,114,114	1.24	13 (16%)
32	LUT	S	317	-	42,43,43	6.08	27 (64%)	51,60,60	1.94	13 (25%)
31	CLA	R	307	49	52,56,73	1.59	7 (13%)	62,92,113	2.08	16 (25%)
32	LUT	y	616	-	42,43,43	6.00	28 (66%)	51,60,60	2.00	20 (39%)
34	LMG	6	323	-	38,38,55	0.63	1 (2%)	46,46,63	1.16	4 (8%)
36	NEX	Y	317	-	38,46,46	3.37	11 (28%)	50,70,70	1.73	11 (22%)
30	CHL	3	310	3	65,69,74	0.85	3 (4%)	74,108,114	1.36	12 (16%)
31	CLA	G	613	2	53,57,73	1.56	6 (11%)	62,93,113	2.11	18 (29%)
34	LMG	b	622	-	51,51,55	1.09	6 (11%)	59,59,63	1.33	7 (11%)
31	CLA	N	304	3	59,63,73	1.46	6 (10%)	71,101,113	2.08	19 (26%)
34	LMG	0	622	-	38,38,55	0.65	1 (2%)	46,46,63	1.13	3 (6%)
33	LHG	d	408	-	48,48,48	0.39	0	51,54,54	1.08	3 (5%)
43	BCR	c	614	-	41,41,41	4.75	26 (63%)	56,56,56	2.96	25 (44%)
37	XAT	q	321	-	39,47,47	0.65	0	54,74,74	1.91	13 (24%)
33	LHG	N	319	31	48,48,48	0.38	0	51,54,54	1.02	2 (3%)
31	CLA	2	604	49,36	58,62,73	1.49	7 (12%)	69,99,113	2.14	19 (27%)
43	BCR	Z	101	-	41,41,41	4.77	26 (63%)	56,56,56	2.36	18 (32%)
34	LMG	C	621	-	38,38,55	0.62	1 (2%)	46,46,63	1.11	3 (6%)
34	LMG	x	202	-	38,38,55	0.61	1 (2%)	46,46,63	1.14	4 (8%)
31	CLA	p	611	33	64,68,73	1.41	7 (10%)	77,107,113	1.97	17 (22%)
43	BCR	C	615	-	41,41,41	4.70	25 (60%)	56,56,56	4.03	31 (55%)
32	LUT	4	616	-	42,43,43	6.06	28 (66%)	51,60,60	2.18	13 (25%)
42	PHO	A	408	-	58,69,69	1.94	10 (17%)	56,99,99	1.49	7 (12%)
30	CHL	9	308	-	56,60,74	0.88	1 (1%)	63,97,114	1.43	13 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	b	615	6	69,73,73	1.35	7 (10%)	83,113,113	1.97	18 (21%)
31	CLA	5	602	3	64,68,73	1.41	6 (9%)	77,107,113	2.00	19 (24%)
43	BCR	C	614	-	41,41,41	4.70	25 (60%)	56,56,56	2.59	23 (41%)
31	CLA	q	316	2	54,58,73	1.54	7 (12%)	65,95,113	2.16	18 (27%)
39	OEX	a	402	7,5	0,14,14	-	-	-	-	-
45	DGD	c	619	-	67,67,67	1.16	7 (10%)	81,81,81	1.02	3 (3%)
31	CLA	b	613	6	69,73,73	1.35	7 (10%)	83,113,113	1.99	20 (24%)
30	CHL	N	307	49	62,66,74	0.88	2 (3%)	70,104,114	1.38	12 (17%)
31	CLA	b	611	49	69,73,73	1.36	7 (10%)	83,113,113	1.92	18 (21%)
34	LMG	p	620	-	38,38,55	0.62	1 (2%)	46,46,63	1.10	4 (8%)
30	CHL	Y	307	49	63,67,74	0.87	3 (4%)	71,105,114	1.36	13 (18%)
42	PHO	d	402	-	58,69,69	0.79	3 (5%)	56,99,99	0.98	3 (5%)
31	CLA	B	602	6	69,73,73	1.37	7 (10%)	83,113,113	2.02	19 (22%)
31	CLA	8	614	3	58,62,73	1.48	7 (12%)	69,99,113	2.04	18 (26%)
36	NEX	R	319	-	38,46,46	3.39	11 (28%)	50,70,70	1.61	9 (18%)
34	LMG	a	401	-	38,38,55	0.62	1 (2%)	46,46,63	1.04	3 (6%)
31	CLA	N	315	3	58,62,73	1.47	6 (10%)	69,99,113	2.10	19 (27%)
30	CHL	R	308	18	60,64,74	0.88	2 (3%)	68,102,114	1.40	13 (19%)
31	CLA	c	608	7	69,73,73	1.38	6 (8%)	83,113,113	1.82	19 (22%)
34	LMG	n	322	-	40,40,55	0.71	3 (7%)	48,48,63	1.39	5 (10%)
31	CLA	8	611	3	49,53,73	1.59	7 (14%)	59,89,113	2.07	14 (23%)
31	CLA	g	314	2	53,57,73	1.54	6 (11%)	62,93,113	2.18	19 (30%)
33	LHG	t	102	-	40,40,48	0.43	0	43,46,54	1.18	4 (9%)
32	LUT	N	317	-	42,43,43	6.07	28 (66%)	51,60,60	2.10	14 (27%)
32	LUT	6	318	-	42,43,43	6.06	28 (66%)	51,60,60	1.94	12 (23%)
33	LHG	y	619	31	45,45,48	0.43	0	48,51,54	1.05	3 (6%)
31	CLA	0	615	-	59,63,73	1.46	6 (10%)	71,101,113	2.06	18 (25%)
37	XAT	G	620	-	39,47,47	0.65	0	54,74,74	1.91	13 (24%)
30	CHL	s	309	49	53,57,74	0.98	2 (3%)	59,93,114	1.40	11 (18%)
30	CHL	p	606	-	55,59,74	0.86	2 (3%)	62,96,114	1.41	13 (20%)
36	NEX	y	618	-	38,46,46	3.41	11 (28%)	50,70,70	1.59	11 (22%)
34	LMG	w	204	-	38,38,55	0.65	1 (2%)	46,46,63	1.11	4 (8%)
31	CLA	6	315	4	58,62,73	1.46	6 (10%)	69,99,113	2.13	18 (26%)
30	CHL	G	607	49	55,59,74	0.93	2 (3%)	62,96,114	1.44	14 (22%)
30	CHL	g	302	2	70,74,74	0.80	2 (2%)	80,114,114	1.28	14 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	LMG	n	321	-	38,38,55	0.66	1 (2%)	46,46,63	1.20	3 (6%)
36	NEX	g	317	31	38,46,46	3.36	11 (28%)	50,70,70	1.67	10 (20%)
30	CHL	q	307	2	50,54,74	0.93	2 (4%)	56,90,114	1.46	12 (21%)
31	CLA	A	405	5	69,73,73	1.36	6 (8%)	83,113,113	1.99	20 (24%)
31	CLA	5	610	3	64,68,73	1.40	6 (9%)	77,107,113	2.03	19 (24%)
30	CHL	7	309	49	54,58,74	0.91	1 (1%)	59,94,114	1.49	12 (20%)
33	LHG	S	320	31	40,40,48	0.43	0	43,46,54	1.17	4 (9%)
31	CLA	5	603	3	56,60,73	1.49	5 (8%)	67,97,113	2.17	19 (28%)
35	RRX	q	317	-	42,42,42	4.96	25 (59%)	57,58,58	2.57	19 (33%)
30	CHL	p	609	3	60,64,74	0.88	3 (5%)	68,102,114	1.39	13 (19%)
33	LHG	C	623	-	39,39,48	0.42	0	42,45,54	1.21	4 (9%)
30	CHL	n	310	3	70,74,74	0.82	3 (4%)	80,114,114	1.38	12 (15%)
31	CLA	G	610	33	64,68,73	1.42	7 (10%)	77,107,113	1.94	17 (22%)
30	CHL	7	307	49	70,74,74	0.81	1 (1%)	80,114,114	1.34	14 (17%)
34	LMG	2	618	-	38,38,55	0.62	1 (2%)	46,46,63	1.11	3 (6%)
31	CLA	b	609	6	69,73,73	1.38	6 (8%)	83,113,113	1.91	16 (19%)
30	CHL	Y	308	49	54,58,74	0.93	2 (3%)	59,94,114	1.45	13 (22%)
34	LMG	2	621	-	40,40,55	0.67	2 (5%)	48,48,63	1.16	4 (8%)
33	LHG	6	320	31	36,36,48	0.44	0	39,42,54	1.19	3 (7%)
30	CHL	8	606	49	62,66,74	0.85	1 (1%)	70,104,114	1.36	12 (17%)
31	CLA	C	611	7	69,73,73	1.38	7 (10%)	83,113,113	2.00	19 (22%)
31	CLA	B	601	49	53,57,73	1.56	7 (13%)	62,93,113	2.15	18 (29%)
32	LUT	Y	315	-	42,43,43	6.00	28 (66%)	51,60,60	1.95	18 (35%)
33	LHG	G	618	31	43,43,48	0.40	0	46,49,54	1.10	3 (6%)
31	CLA	2	610	33	64,68,73	1.40	6 (9%)	77,107,113	2.01	17 (22%)
34	LMG	J	102	-	38,38,55	0.60	1 (2%)	46,46,63	1.10	2 (4%)
34	LMG	a	413	-	38,38,55	0.64	1 (2%)	46,46,63	1.49	6 (13%)
32	LUT	3	318	-	42,43,43	6.07	28 (66%)	51,60,60	2.00	13 (25%)
30	CHL	p	605	3	50,54,74	0.92	2 (4%)	56,90,114	1.46	12 (21%)
32	LUT	7	318	-	42,43,43	6.07	28 (66%)	51,60,60	1.88	12 (23%)
31	CLA	q	305	2	59,63,73	1.45	6 (10%)	71,101,113	2.08	18 (25%)
33	LHG	3	320	31	32,32,48	0.45	0	35,38,54	1.29	4 (11%)
31	CLA	g	310	2	69,73,73	1.37	7 (10%)	83,113,113	1.91	21 (25%)
31	CLA	c	605	7	69,73,73	1.38	6 (8%)	83,113,113	1.87	16 (19%)
30	CHL	N	309	3	70,74,74	0.81	3 (4%)	80,114,114	1.34	13 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CHL	9	310	49	54,58,74	0.89	2 (3%)	59,94,114	1.41	12 (20%)
38	SQD	X	201	-	37,38,54	0.91	0	46,49,65	1.02	2 (4%)
31	CLA	2	609	2	64,68,73	1.41	7 (10%)	77,107,113	2.02	21 (27%)
38	SQD	b	627	-	51,52,54	0.87	0	60,63,65	1.02	2 (3%)
31	CLA	6	313	4	64,68,73	1.41	7 (10%)	77,107,113	1.98	18 (23%)
33	LHG	A	417	-	38,38,48	0.45	0	41,44,54	1.09	3 (7%)
30	CHL	3	307	3	50,54,74	0.93	2 (4%)	56,90,114	1.46	12 (21%)
34	LMG	6	321	-	42,42,55	0.77	2 (4%)	50,50,63	1.24	5 (10%)
30	CHL	6	306	4	50,54,74	0.90	1 (2%)	56,90,114	1.47	12 (21%)
30	CHL	s	307	19	48,52,74	0.95	1 (2%)	53,87,114	1.47	10 (18%)
31	CLA	3	316	3	61,65,73	1.47	7 (11%)	73,103,113	2.08	21 (28%)
30	CHL	S	309	49	53,57,74	0.97	2 (3%)	59,93,114	1.44	13 (22%)
31	CLA	2	602	2	69,73,73	1.35	6 (8%)	83,113,113	1.94	17 (20%)
33	LHG	1	617	31	34,34,48	0.44	0	37,40,54	1.17	3 (8%)
31	CLA	s	313	19	60,64,73	1.46	6 (10%)	72,102,113	2.11	18 (25%)
33	LHG	S	322	-	43,43,48	0.41	0	46,49,54	1.08	3 (6%)
31	CLA	C	606	7	61,65,73	1.45	6 (9%)	73,103,113	2.05	18 (24%)
34	LMG	c	624	-	44,44,55	0.86	3 (6%)	52,52,63	1.05	3 (5%)
30	CHL	4	607	-	61,65,74	0.88	2 (3%)	69,103,114	1.38	12 (17%)
30	CHL	8	601	3	60,64,74	0.86	2 (3%)	68,102,114	1.42	14 (20%)
31	CLA	c	602	7	69,73,73	1.38	6 (8%)	83,113,113	1.94	16 (19%)
43	BCR	B	618	-	41,41,41	4.77	25 (60%)	56,56,56	2.19	20 (35%)
31	CLA	8	603	3	59,63,73	1.46	6 (10%)	71,101,113	2.09	18 (25%)
31	CLA	b	610	6	69,73,73	1.36	7 (10%)	83,113,113	1.98	18 (21%)
31	CLA	6	316	4	59,63,73	1.47	5 (8%)	71,101,113	2.07	18 (25%)
33	LHG	7	319	31	34,34,48	0.44	0	37,40,54	1.11	2 (5%)
31	CLA	G	602	2	69,73,73	1.36	7 (10%)	83,113,113	1.90	20 (24%)
34	LMG	k	101	-	48,48,55	0.99	5 (10%)	56,56,63	1.14	4 (7%)
38	SQD	s	301	-	50,51,54	0.79	0	59,62,65	0.94	3 (5%)
33	LHG	2	617	31	48,48,48	0.39	0	51,54,54	1.09	3 (5%)
32	LUT	R	317	-	42,43,43	6.05	27 (64%)	51,60,60	2.98	15 (29%)
31	CLA	3	315	3	58,62,73	1.48	7 (12%)	69,99,113	2.10	19 (27%)
33	LHG	r	320	31	37,37,48	0.45	0	40,43,54	1.14	3 (7%)
31	CLA	0	613	4	60,64,73	1.46	7 (11%)	72,102,113	2.03	19 (26%)
31	CLA	5	604	-	54,58,73	1.53	7 (12%)	65,95,113	2.14	18 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	C	605	7	69,73,73	1.46	8 (11%)	83,113,113	1.92	16 (19%)
31	CLA	Y	304	24	59,63,73	1.46	7 (11%)	71,101,113	2.06	20 (28%)
30	CHL	p	601	3	55,59,74	0.89	2 (3%)	62,96,114	1.39	14 (22%)
31	CLA	R	304	18	64,68,73	1.42	6 (9%)	77,107,113	1.95	17 (22%)
32	LUT	3	317	-	42,43,43	6.08	28 (66%)	51,60,60	1.88	12 (23%)
34	LMG	r	321	-	38,38,55	0.69	2 (5%)	46,46,63	1.27	4 (8%)
31	CLA	p	610	3	60,64,73	1.46	7 (11%)	72,102,113	2.03	20 (27%)
30	CHL	y	606	49	63,67,74	0.84	2 (3%)	71,105,114	1.34	14 (19%)
31	CLA	0	611	33	64,68,73	1.41	7 (10%)	77,107,113	1.93	16 (20%)
34	LMG	q	302	-	40,40,55	0.69	2 (5%)	48,48,63	1.13	2 (4%)
31	CLA	6	304	4	60,64,73	1.46	7 (11%)	72,102,113	2.08	21 (29%)
36	NEX	s	319	-	38,46,46	3.46	10 (26%)	50,70,70	1.56	10 (20%)
37	XAT	4	619	-	39,47,47	0.64	0	54,74,74	1.91	13 (24%)
31	CLA	R	313	33	53,57,73	1.56	7 (13%)	62,93,113	2.12	17 (27%)
31	CLA	p	612	3	50,54,73	1.59	7 (14%)	60,90,113	2.08	17 (28%)
31	CLA	9	314	2	54,58,73	1.55	6 (11%)	65,95,113	2.12	17 (26%)
31	CLA	y	614	24	58,62,73	1.47	6 (10%)	69,99,113	2.08	20 (28%)
33	LHG	q	320	31	45,45,48	0.43	0	48,51,54	1.09	2 (4%)
30	CHL	3	302	49	61,65,74	1.02	4 (6%)	69,103,114	1.53	15 (21%)
33	LHG	B	624	-	48,48,48	0.37	0	51,54,54	0.98	2 (3%)
33	LHG	5	619	31	34,34,48	0.46	0	37,40,54	1.14	3 (8%)
31	CLA	8	610	33	53,57,73	1.54	7 (13%)	62,93,113	2.15	17 (27%)
30	CHL	4	601	2	70,74,74	0.81	2 (2%)	80,114,114	1.27	14 (17%)
32	LUT	G	615	-	42,43,43	6.12	28 (66%)	51,60,60	6.98	17 (33%)
30	CHL	N	301	-	54,58,74	0.92	2 (3%)	59,94,114	1.40	12 (20%)
33	LHG	L	101	-	48,48,48	0.39	0	51,54,54	1.02	3 (5%)
34	LMG	B	622	-	38,38,55	0.64	1 (2%)	46,46,63	1.22	4 (8%)
34	LMG	s	321	-	41,41,55	0.85	2 (4%)	49,49,63	1.28	5 (10%)
32	LUT	r	317	-	42,43,43	6.02	28 (66%)	51,60,60	2.07	20 (39%)
31	CLA	b	606	6	69,73,73	1.37	6 (8%)	83,113,113	1.95	16 (19%)
37	XAT	R	318	-	39,47,47	0.64	0	54,74,74	1.94	14 (25%)
31	CLA	R	312	18	61,65,73	1.45	6 (9%)	73,103,113	2.05	18 (24%)
30	CHL	S	308	49	47,51,74	1.08	3 (6%)	52,86,114	1.56	12 (23%)
31	CLA	b	607	6	69,73,73	1.37	6 (8%)	83,113,113	1.98	17 (20%)
31	CLA	g	305	49,36	59,63,73	1.46	7 (11%)	71,101,113	2.08	17 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	LMG	f	101	-	38,38,55	0.58	1 (2%)	46,46,63	1.13	2 (4%)
31	CLA	b	616	6	69,73,73	1.35	7 (10%)	83,113,113	1.97	16 (19%)
47	HEM	E	101	9,10	50,50,50	1.58	8 (16%)	66,82,82	1.70	13 (19%)
31	CLA	4	613	2	65,69,73	1.39	6 (9%)	78,108,113	1.96	20 (25%)
31	CLA	7	303	1	64,68,73	1.40	6 (9%)	77,107,113	1.97	19 (24%)
31	CLA	8	612	3	69,73,73	1.35	7 (10%)	83,113,113	1.91	19 (22%)
31	CLA	9	305	2	59,63,73	1.46	7 (11%)	71,101,113	2.10	20 (28%)
34	LMG	7	322	-	38,38,55	0.65	1 (2%)	46,46,63	1.06	4 (8%)
44	PL9	D	406	-	55,55,55	0.66	1 (1%)	68,69,69	0.62	1 (1%)
45	DGD	C	616	-	51,51,67	0.82	2 (3%)	65,65,81	1.00	2 (3%)
33	LHG	b	625	-	43,43,48	0.41	0	46,49,54	1.07	3 (6%)
33	LHG	0	619	31	35,35,48	0.44	0	38,41,54	1.20	4 (10%)
31	CLA	b	608	49	69,73,73	1.37	7 (10%)	83,113,113	1.99	16 (19%)
31	CLA	r	316	18	69,73,73	1.37	6 (8%)	83,113,113	1.95	16 (19%)
36	NEX	S	319	-	38,46,46	3.44	10 (26%)	50,70,70	1.55	11 (22%)
30	CHL	G	605	2	52,56,74	0.92	2 (3%)	58,92,114	1.47	14 (24%)
34	LMG	C	622	-	32,32,55	0.48	0	40,40,63	1.08	2 (5%)
31	CLA	R	316	18	69,73,73	1.36	7 (10%)	83,113,113	2.00	19 (22%)
46	BCT	d	403	40	2,3,3	1.15	0	2,3,3	4.30	2 (100%)
32	LUT	q	318	-	42,43,43	6.07	28 (66%)	51,60,60	2.12	14 (27%)
31	CLA	y	611	33	69,73,73	1.36	7 (10%)	83,113,113	1.84	16 (19%)
31	CLA	4	604	30	55,59,73	1.51	6 (10%)	66,96,113	2.20	18 (27%)
31	CLA	d	405	8	69,73,73	1.35	7 (10%)	83,113,113	2.04	20 (24%)
36	NEX	0	618	-	38,46,46	3.37	10 (26%)	50,70,70	1.59	11 (22%)
36	NEX	r	301	-	38,46,46	3.37	9 (23%)	50,70,70	1.69	12 (24%)
30	CHL	g	309	2	67,71,74	0.84	3 (4%)	76,110,114	1.41	14 (18%)
31	CLA	b	603	6	69,73,73	1.36	7 (10%)	83,113,113	2.03	17 (20%)
31	CLA	S	314	19	69,73,73	1.37	7 (10%)	83,113,113	1.91	18 (21%)
30	CHL	9	309	-	57,61,74	0.92	2 (3%)	64,98,114	1.49	13 (20%)
45	DGD	C	618	-	67,67,67	1.16	7 (10%)	81,81,81	0.93	3 (3%)
31	CLA	C	601	7	69,73,73	1.37	7 (10%)	83,113,113	1.93	18 (21%)
32	LUT	5	616	-	42,43,43	6.10	27 (64%)	51,60,60	1.89	11 (21%)
34	LMG	G	621	-	51,51,55	1.07	6 (11%)	59,59,63	1.07	3 (5%)
33	LHG	c	622	-	46,46,48	0.40	0	49,52,54	1.01	2 (4%)
30	CHL	9	307	2	50,54,74	0.96	2 (4%)	56,90,114	1.42	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	c	607	49	69,73,73	1.39	6 (8%)	83,113,113	1.91	19 (22%)
33	LHG	e	101	-	43,43,48	0.40	0	46,49,54	1.18	4 (8%)
30	CHL	p	608	-	54,58,74	0.88	2 (3%)	59,94,114	1.39	11 (18%)
34	LMG	A	414	-	38,38,55	0.64	1 (2%)	46,46,63	1.14	4 (8%)
31	CLA	Y	312	24	69,73,73	1.38	6 (8%)	83,113,113	1.93	19 (22%)
31	CLA	C	612	7	59,63,73	1.48	7 (11%)	71,101,113	2.14	16 (22%)
31	CLA	s	303	19	69,73,73	1.36	7 (10%)	83,113,113	1.96	21 (25%)
38	SQD	A	411	-	50,51,54	0.80	0	59,62,65	0.97	3 (5%)
34	LMG	b	626	-	46,46,55	0.92	3 (6%)	54,54,63	1.10	4 (7%)
31	CLA	6	312	33	64,68,73	1.42	8 (12%)	77,107,113	1.99	17 (22%)
43	BCR	b	620	-	41,41,41	4.75	25 (60%)	56,56,56	2.33	20 (35%)
34	LMG	w	205	-	38,38,55	0.62	1 (2%)	46,46,63	1.13	2 (4%)
33	LHG	4	618	31	46,46,48	0.39	0	49,52,54	1.06	4 (8%)
30	CHL	2	601	2	70,74,74	0.80	2 (2%)	80,114,114	1.28	14 (17%)
31	CLA	4	612	2	50,54,73	1.58	6 (12%)	60,90,113	2.18	15 (25%)
33	LHG	Y	318	31	41,41,48	0.45	0	44,47,54	1.07	3 (6%)
34	LMG	W	202	-	38,38,55	0.64	1 (2%)	46,46,63	1.25	5 (10%)
34	LMG	4	620	-	51,51,55	1.06	5 (9%)	59,59,63	1.07	3 (5%)
38	SQD	Y	320	-	41,42,54	0.87	0	50,53,65	0.99	2 (4%)
31	CLA	d	401	49	53,57,73	1.55	6 (11%)	62,93,113	2.19	18 (29%)
31	CLA	G	609	2	69,73,73	1.37	6 (8%)	83,113,113	1.90	19 (22%)
34	LMG	7	301	-	39,39,55	0.62	1 (2%)	47,47,63	1.00	2 (4%)
30	CHL	7	308	49	70,74,74	0.77	2 (2%)	80,114,114	1.25	13 (16%)
31	CLA	B	607	49	69,73,73	1.43	6 (8%)	83,113,113	2.10	20 (24%)
30	CHL	y	601	24	70,74,74	0.79	2 (2%)	80,114,114	1.29	13 (16%)
31	CLA	B	612	6	69,73,73	1.35	7 (10%)	83,113,113	1.93	18 (21%)
30	CHL	q	310	-	54,58,74	1.02	3 (5%)	59,94,114	1.56	13 (22%)
34	LMG	S	321	-	41,41,55	0.83	2 (4%)	49,49,63	1.23	3 (6%)
34	LMG	G	622	-	40,40,55	0.69	2 (5%)	48,48,63	1.09	4 (8%)
31	CLA	G	604	49	59,63,73	1.46	6 (10%)	71,101,113	2.05	17 (23%)
31	CLA	7	315	1	58,62,73	1.46	5 (8%)	69,99,113	2.05	19 (27%)
31	CLA	q	315	2	69,73,73	1.38	6 (8%)	83,113,113	1.93	19 (22%)
31	CLA	3	311	-	58,62,73	1.49	7 (12%)	69,99,113	2.12	19 (27%)
31	CLA	y	615	24	58,62,73	1.47	7 (12%)	69,99,113	2.18	20 (28%)
31	CLA	S	310	19	64,68,73	1.41	7 (10%)	77,107,113	2.00	18 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CHL	5	605	3	50,54,74	0.92	2 (4%)	56,90,114	1.42	13 (23%)
32	LUT	n	318	-	42,43,43	6.07	28 (66%)	51,60,60	1.94	13 (25%)
31	CLA	4	610	2	64,68,73	1.44	6 (9%)	77,107,113	2.01	22 (28%)
43	BCR	t	101	-	41,41,41	4.71	25 (60%)	56,56,56	3.99	27 (48%)
33	LHG	a	415	-	38,38,48	0.45	0	41,44,54	1.24	3 (7%)
33	LHG	g	319	31	43,43,48	0.40	0	46,49,54	1.13	4 (8%)
33	LHG	b	628	-	48,48,48	0.40	0	51,54,54	1.11	3 (5%)
36	NEX	r	319	-	38,46,46	3.39	11 (28%)	50,70,70	1.61	10 (20%)
32	LUT	1	616	-	42,43,43	6.03	27 (64%)	51,60,60	1.89	16 (31%)
31	CLA	N	313	3	69,73,73	1.35	6 (8%)	83,113,113	1.91	18 (21%)
31	CLA	R	305	18	64,68,73	1.42	6 (9%)	77,107,113	2.04	14 (18%)
33	LHG	l	101	-	48,48,48	0.39	0	51,54,54	1.03	3 (5%)
30	CHL	s	308	49	47,51,74	0.93	2 (4%)	52,86,114	1.46	11 (21%)
36	NEX	5	618	-	38,46,46	3.36	10 (26%)	50,70,70	1.56	9 (18%)
32	LUT	0	617	-	42,43,43	6.02	28 (66%)	51,60,60	1.96	14 (27%)
31	CLA	B	606	6	69,73,73	1.38	6 (8%)	83,113,113	1.94	19 (22%)
31	CLA	r	303	18	53,57,73	1.60	6 (11%)	62,93,113	2.32	19 (30%)
34	LMG	W	201	-	55,55,55	1.18	6 (10%)	63,63,63	1.20	4 (6%)
30	CHL	8	608	3	70,74,74	0.79	3 (4%)	80,114,114	1.35	12 (15%)
38	SQD	a	411	-	47,48,54	0.82	0	56,59,65	0.97	2 (3%)
31	CLA	7	316	1	55,59,73	1.52	7 (12%)	66,96,113	2.14	19 (28%)
34	LMG	q1	101	-	38,38,55	0.64	1 (2%)	46,46,63	1.10	2 (4%)
43	BCR	T	101	-	41,41,41	4.76	27 (65%)	56,56,56	2.30	19 (33%)
36	NEX	4	617	-	38,46,46	3.38	11 (28%)	50,70,70	1.53	9 (18%)
31	CLA	p	614	3	55,59,73	1.52	7 (12%)	66,96,113	2.18	19 (28%)
31	CLA	c	611	7	69,73,73	1.37	7 (10%)	83,113,113	1.99	19 (22%)
33	LHG	M	101	-	40,40,48	0.42	0	43,46,54	1.10	3 (6%)
31	CLA	4	611	33	46,51,73	1.54	5 (10%)	59,86,113	2.12	15 (25%)
32	LUT	y	617	-	42,43,43	6.02	28 (66%)	51,60,60	2.00	17 (33%)
31	CLA	q	304	2	69,73,73	1.36	7 (10%)	83,113,113	1.95	19 (22%)
30	CHL	0	606	49	55,59,74	0.94	2 (3%)	62,96,114	1.38	9 (14%)
31	CLA	R	303	18	53,57,73	1.56	7 (13%)	62,93,113	2.30	17 (27%)
31	CLA	A	407	49	53,57,73	1.56	6 (11%)	62,93,113	2.17	19 (30%)
31	CLA	N	314	3	53,57,73	1.54	6 (11%)	62,93,113	2.15	17 (27%)
30	CHL	n	307	49	62,66,74	0.85	1 (1%)	70,104,114	1.36	12 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	LMG	1	618	-	38,38,55	0.62	1 (2%)	46,46,63	1.04	2 (4%)
31	CLA	0	614	4	58,62,73	1.46	6 (10%)	69,99,113	2.10	20 (28%)
31	CLA	3	312	33	69,73,73	1.36	7 (10%)	83,113,113	1.90	17 (20%)
30	CHL	2	605	2	50,54,74	0.92	2 (4%)	56,90,114	1.46	13 (23%)
38	SQD	x	201	-	41,42,54	0.88	1 (2%)	50,53,65	0.98	4 (8%)
36	NEX	N	318	-	38,46,46	3.36	11 (28%)	50,70,70	1.79	14 (28%)
31	CLA	R	306	49	52,56,73	1.58	7 (13%)	62,92,113	2.32	18 (29%)
36	NEX	9	319	31	38,46,46	3.44	10 (26%)	50,70,70	1.63	9 (18%)
30	CHL	y	608	49	54,58,74	0.92	2 (3%)	59,94,114	1.49	13 (22%)
30	CHL	1	601	1	70,74,74	1.05	5 (7%)	80,114,114	1.39	11 (13%)
30	CHL	1	619	-	65,69,74	1.10	4 (6%)	74,108,114	1.54	16 (21%)
30	CHL	q	303	2	70,74,74	0.79	2 (2%)	80,114,114	1.25	13 (16%)
32	LUT	7	317	-	42,43,43	6.01	27 (64%)	51,60,60	2.12	15 (29%)
31	CLA	g	303	2	69,73,73	1.33	6 (8%)	83,113,113	1.94	17 (20%)
35	RRX	2	614	-	42,42,42	5.00	25 (59%)	57,58,58	2.53	22 (38%)
30	CHL	q	311	2	60,64,74	0.84	2 (3%)	68,102,114	1.31	12 (17%)
31	CLA	a	406	5	69,73,73	1.37	6 (8%)	83,113,113	1.96	16 (19%)
31	CLA	s	316	19	50,54,73	1.58	7 (14%)	60,90,113	2.08	17 (28%)
30	CHL	9	303	2	70,74,74	0.78	2 (2%)	80,114,114	1.28	13 (16%)
31	CLA	y	603	24	59,63,73	1.47	7 (11%)	71,101,113	2.06	19 (26%)
32	LUT	8	615	-	42,43,43	6.09	28 (66%)	51,60,60	1.83	17 (33%)
31	CLA	3	301	1	58,62,73	1.51	6 (10%)	69,99,113	2.17	19 (27%)
31	CLA	6	314	4	69,73,73	1.35	5 (7%)	83,113,113	1.95	19 (22%)
30	CHL	1	607	-	70,74,74	0.78	2 (2%)	80,114,114	1.24	13 (16%)
31	CLA	S	313	19	60,64,73	1.49	6 (10%)	72,102,113	2.11	20 (27%)
31	CLA	c	606	7	69,73,73	1.39	6 (8%)	83,113,113	1.91	15 (18%)
42	PHO	D	401	-	58,69,69	1.94	9 (15%)	56,99,99	1.51	9 (16%)
32	LUT	6	317	-	42,43,43	6.05	28 (66%)	51,60,60	1.94	16 (31%)
30	CHL	r	310	49	59,63,74	0.93	2 (3%)	66,100,114	1.40	13 (19%)
45	DGD	C	620	-	67,67,67	1.18	7 (10%)	81,81,81	1.02	4 (4%)
30	CHL	2	607	49	54,58,74	0.91	2 (3%)	59,94,114	1.49	12 (20%)
30	CHL	6	309	49	54,58,74	0.92	3 (5%)	59,94,114	1.50	13 (22%)
43	BCR	h	101	-	41,41,41	4.72	25 (60%)	56,56,56	2.41	20 (35%)
30	CHL	1	605	1	70,74,74	0.82	2 (2%)	80,114,114	1.28	10 (12%)
31	CLA	2	612	2	69,73,73	1.34	8 (11%)	83,113,113	1.92	19 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LUT	s	318	-	42,43,43	6.04	28 (66%)	51,60,60	1.92	15 (29%)
30	CHL	4	605	2	50,54,74	0.92	2 (4%)	56,90,114	1.43	12 (21%)
30	CHL	0	609	4	65,69,74	0.86	3 (4%)	74,108,114	1.38	14 (18%)
31	CLA	S	305	49	69,73,73	1.35	5 (7%)	83,113,113	1.94	18 (21%)
34	LMG	j	101	-	43,43,55	0.82	2 (4%)	51,51,63	1.03	3 (5%)
31	CLA	3	304	3	64,68,73	1.41	6 (9%)	77,107,113	2.02	19 (24%)
34	LMG	5	620	-	38,38,55	0.63	1 (2%)	46,46,63	1.09	2 (4%)
31	CLA	p	604	36	54,58,73	1.53	8 (14%)	65,95,113	2.14	18 (27%)
32	LUT	g	316	-	42,43,43	6.09	28 (66%)	51,60,60	2.29	15 (29%)
34	LMG	D	409	-	46,46,55	0.94	4 (8%)	54,54,63	1.14	4 (7%)
31	CLA	B	614	6	69,73,73	1.37	7 (10%)	83,113,113	1.91	18 (21%)
31	CLA	7	304	1	59,63,73	1.46	7 (11%)	71,101,113	2.08	20 (28%)
30	CHL	Y	306	24	50,54,74	1.01	3 (6%)	56,90,114	1.45	13 (23%)
36	NEX	3	319	-	38,46,46	3.45	9 (23%)	50,70,70	1.67	12 (24%)
32	LUT	N	316	-	42,43,43	6.09	28 (66%)	51,60,60	2.01	12 (23%)
34	LMG	R	321	-	38,38,55	0.63	1 (2%)	46,46,63	1.11	2 (4%)
31	CLA	7	313	1	69,73,73	1.36	6 (8%)	83,113,113	1.90	20 (24%)
43	BCR	H	101	-	41,41,41	4.74	26 (63%)	56,56,56	2.38	20 (35%)
31	CLA	B	615	6	69,73,73	1.36	7 (10%)	83,113,113	2.00	16 (19%)
30	CHL	5	607	-	55,59,74	0.96	3 (5%)	62,96,114	1.40	11 (17%)
37	XAT	g	321	-	39,47,47	0.64	0	54,74,74	1.91	13 (24%)
31	CLA	0	604	49	59,63,73	1.46	6 (10%)	71,101,113	2.09	16 (22%)
34	LMG	c	621	-	38,38,55	0.63	1 (2%)	46,46,63	1.11	4 (8%)
30	CHL	3	303	3	54,58,74	0.91	2 (3%)	59,94,114	1.46	13 (22%)
31	CLA	1	610	1	69,73,73	1.35	7 (10%)	83,113,113	1.95	19 (22%)
30	CHL	4	609	2	61,65,74	0.86	2 (3%)	69,103,114	1.43	15 (21%)
33	LHG	s	322	-	43,43,48	0.40	0	46,49,54	1.14	3 (6%)
31	CLA	p	613	-	58,62,73	1.47	7 (12%)	69,99,113	2.07	15 (21%)
31	CLA	d	404	8	69,73,73	1.37	6 (8%)	83,113,113	1.90	16 (19%)
34	LMG	J	101	-	51,51,55	1.08	6 (11%)	59,59,63	1.08	3 (5%)
30	CHL	5	606	49	55,59,74	0.90	2 (3%)	62,96,114	1.44	12 (19%)
34	LMG	4	621	-	40,40,55	0.68	2 (5%)	48,48,63	1.04	2 (4%)
31	CLA	g	311	33	64,68,73	1.44	7 (10%)	77,107,113	1.97	18 (23%)
31	CLA	C	609	7	69,73,73	1.37	7 (10%)	83,113,113	1.91	15 (18%)
43	BCR	c	615	-	41,41,41	4.78	25 (60%)	56,56,56	2.74	24 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CHL	g	308	49	55,59,74	0.90	2 (3%)	62,96,114	1.46	14 (22%)
31	CLA	a	409	5	64,68,73	1.41	7 (10%)	77,107,113	2.09	18 (23%)
30	CHL	6	310	4	65,69,74	0.83	2 (3%)	74,108,114	1.34	15 (20%)
30	CHL	1	608	49	54,58,74	0.92	2 (3%)	59,94,114	1.45	10 (16%)
31	CLA	7	312	33	69,73,73	1.35	6 (8%)	83,113,113	1.95	18 (21%)
37	XAT	9	322	-	39,47,47	0.64	0	54,74,74	1.91	13 (24%)
32	LUT	8	616	-	42,43,43	6.07	28 (66%)	51,60,60	1.93	14 (27%)
45	DGD	C	617	-	67,67,67	1.17	7 (10%)	81,81,81	0.92	3 (3%)
48	LMU	r	302	-	36,36,36	0.38	0	47,47,47	0.78	0
31	CLA	s	304	19	46,50,73	1.64	5 (10%)	55,85,113	2.17	17 (30%)
33	LHG	R	320	31	37,37,48	0.46	0	40,43,54	1.21	3 (7%)
32	LUT	s	317	-	42,43,43	6.07	28 (66%)	51,60,60	1.89	16 (31%)
30	CHL	p	607	-	55,59,74	0.94	2 (3%)	62,96,114	1.42	11 (17%)
31	CLA	R	311	18	62,66,73	1.45	6 (9%)	74,104,113	2.00	18 (24%)
38	SQD	B	623	-	51,52,54	0.81	0	60,63,65	0.95	3 (5%)
30	CHL	0	601	4	60,64,74	0.87	2 (3%)	68,102,114	1.40	14 (20%)
34	LMG	A	412	-	41,41,55	0.75	2 (4%)	49,49,63	1.06	2 (4%)
30	CHL	7	306	1	70,74,74	0.83	3 (4%)	80,114,114	1.30	14 (17%)
31	CLA	8	613	3	53,57,73	1.54	6 (11%)	62,93,113	2.16	18 (29%)
34	LMG	d	409	-	41,41,55	0.72	2 (4%)	49,49,63	1.08	3 (6%)
30	CHL	6	302	4	60,64,74	0.86	2 (3%)	68,102,114	1.38	14 (20%)
38	SQD	R	322	-	50,51,54	0.81	0	59,62,65	0.92	2 (3%)
43	BCR	a	410	-	41,41,41	4.73	25 (60%)	56,56,56	2.54	21 (37%)
33	LHG	n	320	31	48,48,48	0.38	0	51,54,54	1.03	2 (3%)
31	CLA	r	315	18	59,63,73	1.47	7 (11%)	71,101,113	2.16	20 (28%)
31	CLA	G	611	2	47,51,73	1.67	6 (12%)	56,86,113	2.09	15 (26%)
31	CLA	1	611	33	69,73,73	1.35	7 (10%)	83,113,113	1.90	19 (22%)
30	CHL	n	308	49	67,71,74	0.81	2 (2%)	76,110,114	1.34	12 (15%)
30	CHL	N	308	49	54,58,74	0.93	3 (5%)	59,94,114	1.43	11 (18%)
31	CLA	2	613	2	58,62,73	1.48	6 (10%)	69,99,113	2.12	19 (27%)
34	LMG	I	101	-	38,38,55	0.62	1 (2%)	46,46,63	1.10	2 (4%)
31	CLA	N	310	3	69,73,73	1.36	7 (10%)	83,113,113	1.96	20 (24%)
31	CLA	c	604	49	60,64,73	1.44	6 (10%)	72,102,113	2.08	19 (26%)
31	CLA	N	321	24	58,62,73	1.48	7 (12%)	69,99,113	2.09	18 (26%)
31	CLA	A	406	49	69,73,73	1.36	7 (10%)	83,113,113	1.99	18 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	8	604	49,36	69,73,73	1.35	6 (8%)	83,113,113	1.96	18 (21%)
34	LMG	D	412	-	48,48,55	0.99	5 (10%)	56,56,63	1.11	2 (3%)
30	CHL	8	607	49	54,58,74	0.91	2 (3%)	59,94,114	1.45	12 (20%)
31	CLA	n	311	3	69,73,73	1.35	7 (10%)	83,113,113	1.94	19 (22%)
31	CLA	r	305	18	64,68,73	1.40	6 (9%)	77,107,113	2.01	18 (23%)
31	CLA	s	312	33	69,73,73	1.35	6 (8%)	83,113,113	1.94	15 (18%)
30	CHL	G	623	49	70,74,74	0.79	1 (1%)	80,114,114	1.31	14 (17%)
36	NEX	2	616	31	38,46,46	3.38	10 (26%)	50,70,70	1.60	10 (20%)
31	CLA	R	315	18	59,63,73	1.48	6 (10%)	71,101,113	2.08	18 (25%)
43	BCR	b	618	-	41,41,41	4.69	25 (60%)	56,56,56	2.52	23 (41%)
47	HEM	e	102	9,10	50,50,50	1.57	8 (16%)	66,82,82	1.68	11 (16%)
31	CLA	A	409	5	64,68,73	1.42	7 (10%)	77,107,113	2.09	18 (23%)
31	CLA	c	601	7	69,73,73	1.36	7 (10%)	83,113,113	1.91	18 (21%)
30	CHL	y	609	24	70,74,74	0.80	2 (2%)	80,114,114	1.29	11 (13%)
31	CLA	n	315	3	53,57,73	1.54	6 (11%)	62,93,113	2.17	18 (29%)
31	CLA	b	612	6	69,73,73	1.35	6 (8%)	83,113,113	1.94	19 (22%)
30	CHL	r	309	18	60,64,74	0.84	2 (3%)	68,102,114	1.34	10 (14%)
34	LMG	a	416	-	38,38,55	0.61	1 (2%)	46,46,63	1.06	3 (6%)
30	CHL	5	609	3	60,64,74	0.89	3 (5%)	68,102,114	1.44	14 (20%)
32	LUT	n	317	-	42,43,43	6.09	28 (66%)	51,60,60	1.83	17 (33%)
31	CLA	Y	311	33	69,73,73	1.37	6 (8%)	83,113,113	1.88	16 (19%)
31	CLA	C	613	7	69,73,73	1.36	7 (10%)	83,113,113	2.06	21 (25%)
31	CLA	s	306	-	54,58,73	1.53	6 (11%)	65,95,113	2.23	19 (29%)
33	LHG	D	407	-	43,43,48	0.41	0	46,49,54	1.10	3 (6%)
30	CHL	4	608	-	54,58,74	0.88	2 (3%)	59,94,114	1.46	12 (20%)
31	CLA	S	306	-	54,58,73	1.53	6 (11%)	65,95,113	2.20	18 (27%)
31	CLA	N	305	49	69,73,73	1.35	5 (7%)	83,113,113	1.96	18 (21%)
30	CHL	n	302	3	60,64,74	0.86	2 (3%)	68,102,114	1.42	14 (20%)
31	CLA	S	315	19	52,56,73	1.57	6 (11%)	62,92,113	2.05	16 (25%)
31	CLA	r	314	18	53,57,73	1.56	6 (11%)	62,93,113	2.12	18 (29%)
48	LMU	R	302	-	36,36,36	0.44	0	47,47,47	0.95	2 (4%)
34	LMG	b	623	-	38,38,55	0.62	1 (2%)	46,46,63	1.09	2 (4%)
38	SQD	0	621	-	41,42,54	0.86	0	50,53,65	0.96	3 (6%)
30	CHL	2	606	-	55,59,74	0.87	2 (3%)	62,96,114	1.43	13 (20%)
31	CLA	y	602	24	64,68,73	1.41	7 (10%)	77,107,113	2.01	19 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	LMG	g	322	-	49,49,55	1.03	5 (10%)	57,57,63	1.22	2 (3%)
38	SQD	S	301	-	50,51,54	0.80	0	59,62,65	0.94	2 (3%)
31	CLA	n	316	3	58,62,73	1.48	7 (12%)	69,99,113	2.07	19 (27%)
36	NEX	R	301	-	38,46,46	3.42	11 (28%)	50,70,70	1.56	9 (18%)
31	CLA	5	611	33	62,66,73	1.43	7 (11%)	74,104,113	2.03	18 (24%)
31	CLA	C	610	7	69,73,73	1.38	7 (10%)	83,113,113	1.97	17 (20%)
31	CLA	y	612	24	69,73,73	1.37	6 (8%)	83,113,113	1.94	18 (21%)
31	CLA	B	608	6	69,73,73	1.38	6 (8%)	83,113,113	1.89	16 (19%)
31	CLA	N	303	3	69,73,73	1.35	7 (10%)	83,113,113	1.93	21 (25%)
34	LMG	7	320	-	38,38,55	0.61	1 (2%)	46,46,63	1.17	3 (6%)
36	NEX	8	617	31	38,46,46	3.38	11 (28%)	50,70,70	1.65	12 (24%)
31	CLA	Y	313	24	69,73,73	1.38	7 (10%)	83,113,113	1.92	17 (20%)
30	CHL	n	306	3	70,74,74	0.79	2 (2%)	80,114,114	1.30	14 (17%)
35	RRX	9	317	-	42,42,42	5.01	25 (59%)	57,58,58	2.49	22 (38%)
31	CLA	a	407	49	69,73,73	1.37	7 (10%)	83,113,113	1.96	17 (20%)
32	LUT	p	617	-	42,43,43	6.06	29 (69%)	51,60,60	2.82	20 (39%)
31	CLA	p	602	3	64,68,73	1.41	7 (10%)	77,107,113	1.96	18 (23%)
31	CLA	6	305	49	59,63,73	1.46	6 (10%)	71,101,113	2.10	18 (25%)
30	CHL	S	302	19	50,54,74	1.01	2 (4%)	56,90,114	1.35	10 (17%)
31	CLA	S	312	33	69,73,73	1.35	6 (8%)	83,113,113	1.95	16 (19%)
34	LMG	m	102	-	45,45,55	0.91	3 (6%)	53,53,63	1.25	5 (9%)
30	CHL	5	601	3	55,59,74	0.88	2 (3%)	62,96,114	1.47	13 (20%)
31	CLA	y	613	24	69,73,73	1.44	6 (8%)	83,113,113	1.97	20 (24%)
30	CHL	S	307	19	48,52,74	0.95	2 (4%)	53,87,114	1.46	10 (18%)
34	LMG	G	619	-	38,38,55	0.63	1 (2%)	46,46,63	1.10	3 (6%)
35	RRX	4	615	-	42,42,42	5.02	25 (59%)	57,58,58	2.49	22 (38%)
31	CLA	B	616	6	69,73,73	1.38	6 (8%)	83,113,113	1.95	14 (16%)
32	LUT	1	615	-	42,43,43	6.01	27 (64%)	51,60,60	2.01	18 (35%)
31	CLA	5	612	3	54,58,73	1.54	7 (12%)	65,95,113	2.16	20 (30%)
31	CLA	6	303	4	69,73,73	1.35	7 (10%)	83,113,113	1.95	19 (22%)
31	CLA	9	316	2	50,54,73	1.59	7 (14%)	60,90,113	2.05	16 (26%)
31	CLA	4	602	2	69,73,73	1.35	7 (10%)	83,113,113	1.97	20 (24%)
31	CLA	5	615	3	50,54,73	1.59	6 (12%)	60,90,113	2.20	16 (26%)
34	LMG	6	322	-	39,39,55	0.61	1 (2%)	47,47,63	1.18	3 (6%)
30	CHL	G	606	49	54,58,74	0.91	2 (3%)	59,94,114	1.41	13 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	3	305	3	59,63,73	1.47	7 (11%)	71,101,113	2.03	18 (25%)
31	CLA	C	608	7	69,73,73	1.38	6 (8%)	83,113,113	1.85	18 (21%)
30	CHL	q	308	-	55,59,74	0.98	4 (7%)	62,96,114	1.51	10 (16%)
31	CLA	g	304	2	59,63,73	1.46	6 (10%)	71,101,113	2.09	18 (25%)
31	CLA	1	614	1	58,62,73	1.46	5 (8%)	69,99,113	2.07	19 (27%)
30	CHL	y	607	49	70,74,74	0.79	2 (2%)	80,114,114	1.29	14 (17%)
31	CLA	8	602	3	69,73,73	1.35	6 (8%)	83,113,113	1.92	20 (24%)
34	LMG	d	411	-	48,48,55	0.99	5 (10%)	56,56,63	1.15	3 (5%)
31	CLA	9	304	2	69,73,73	1.35	6 (8%)	83,113,113	2.00	20 (24%)
30	CHL	1	609	1	70,74,74	0.82	3 (4%)	80,114,114	1.33	14 (17%)
31	CLA	1	613	1	69,73,73	1.36	7 (10%)	83,113,113	1.89	17 (20%)
32	LUT	9	318	-	42,43,43	6.10	27 (64%)	51,60,60	2.23	17 (33%)
48	LMU	c	623	-	29,29,36	0.44	0	40,40,47	1.11	2 (5%)
30	CHL	0	608	49	54,58,74	0.91	1 (1%)	59,94,114	1.53	12 (20%)
31	CLA	r	307	49	52,56,73	1.59	6 (11%)	62,92,113	2.06	17 (27%)
31	CLA	c	603	7	69,73,73	1.38	7 (10%)	83,113,113	2.00	19 (22%)
34	LMG	A	418	-	38,38,55	0.61	1 (2%)	46,46,63	1.09	3 (6%)
31	CLA	0	612	4	50,54,73	1.61	7 (14%)	60,90,113	2.03	17 (28%)
33	LHG	A	415	-	43,43,48	0.40	0	46,49,54	1.15	5 (10%)
34	LMG	k	102	-	38,38,55	0.61	1 (2%)	46,46,63	1.10	3 (6%)
48	LMU	K	101	-	36,36,36	0.42	0	47,47,47	1.10	4 (8%)
34	LMG	X	202	-	38,38,55	0.62	1 (2%)	46,46,63	1.06	2 (4%)
34	LMG	0	620	-	42,42,55	0.81	2 (4%)	50,50,63	1.16	4 (8%)
33	LHG	s	320	31	40,40,48	0.43	0	43,46,54	1.11	3 (6%)
36	NEX	q	319	-	38,46,46	3.39	11 (28%)	50,70,70	1.55	10 (20%)
31	CLA	s	311	19	69,73,73	1.36	6 (8%)	83,113,113	1.94	22 (26%)
30	CHL	y	605	24	50,54,74	1.01	2 (4%)	56,90,114	1.44	10 (17%)
31	CLA	g	312	2	47,51,73	1.63	7 (14%)	56,86,113	2.13	15 (26%)
31	CLA	n	304	3	59,63,73	1.46	6 (10%)	71,101,113	2.09	18 (25%)
34	LMG	q	301	-	51,51,55	1.07	5 (9%)	59,59,63	1.16	5 (8%)
30	CHL	q	309	-	61,65,74	1.06	3 (4%)	69,103,114	1.39	11 (15%)
34	LMG	C	624	-	44,44,55	0.88	3 (6%)	52,52,63	1.05	2 (3%)
31	CLA	9	312	2	58,62,73	1.48	6 (10%)	69,99,113	2.19	21 (30%)
44	PL9	d	407	-	55,55,55	0.72	1 (1%)	68,69,69	0.59	1 (1%)
30	CHL	G	601	2	70,74,74	0.80	2 (2%)	80,114,114	1.27	14 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	s	305	49	69,73,73	1.35	7 (10%)	83,113,113	1.97	18 (21%)
31	CLA	q	314	2	50,54,73	1.59	6 (12%)	60,90,113	2.09	15 (25%)
31	CLA	C	602	7	69,73,73	1.37	6 (8%)	83,113,113	1.95	18 (21%)
31	CLA	n	313	3	49,53,73	1.59	6 (12%)	59,89,113	2.08	14 (23%)
31	CLA	0	603	4	60,64,73	1.47	7 (11%)	72,102,113	2.00	18 (25%)
36	NEX	n	319	-	38,46,46	3.30	9 (23%)	50,70,70	1.78	14 (28%)
43	BCR	B	619	-	41,41,41	4.74	25 (60%)	56,56,56	2.46	21 (37%)
31	CLA	1	602	1	64,68,73	1.42	7 (10%)	77,107,113	1.97	19 (24%)
38	SQD	y	621	-	41,42,54	0.87	0	50,53,65	1.00	2 (4%)
31	CLA	g	313	2	69,73,73	1.35	7 (10%)	83,113,113	1.90	19 (22%)
30	CHL	g	306	2	52,56,74	0.94	2 (3%)	58,92,114	1.46	12 (20%)
31	CLA	D	403	8	69,73,73	1.39	6 (8%)	83,113,113	1.90	16 (19%)
31	CLA	9	306	49,36	69,73,73	1.35	6 (8%)	83,113,113	1.99	18 (21%)
31	CLA	7	314	1	69,73,73	1.37	7 (10%)	83,113,113	1.89	19 (22%)
30	CHL	N	306	3	70,74,74	0.81	2 (2%)	80,114,114	1.33	14 (17%)
31	CLA	0	610	4	69,73,73	1.41	6 (8%)	83,113,113	1.95	21 (25%)
31	CLA	n	303	3	69,73,73	1.35	7 (10%)	83,113,113	1.93	21 (25%)
32	LUT	0	616	-	42,43,43	6.02	27 (64%)	51,60,60	1.99	17 (33%)
34	LMG	B	625	-	38,38,55	0.62	1 (2%)	46,46,63	1.09	4 (8%)
38	SQD	B	620	-	53,54,54	0.77	0	62,65,65	0.91	2 (3%)
39	OEX	A	401	7,5	0,14,14	-	-	-		
45	DGD	c	616	-	67,67,67	1.16	7 (10%)	81,81,81	1.07	2 (2%)
33	LHG	z	102	-	35,35,48	0.43	0	38,41,54	1.20	3 (7%)
31	CLA	n	312	33	53,57,73	1.54	7 (13%)	62,93,113	2.15	16 (25%)
30	CHL	r	308	18	60,64,74	0.89	3 (5%)	68,102,114	1.39	14 (20%)
31	CLA	B	609	6	69,73,73	1.36	6 (8%)	83,113,113	1.96	19 (22%)
34	LMG	2	620	-	51,51,55	1.06	5 (9%)	59,59,63	1.06	3 (5%)
44	PL9	a	414	-	55,55,55	1.21	5 (9%)	68,69,69	1.51	15 (22%)
31	CLA	9	315	2	59,63,73	1.46	6 (10%)	71,101,113	2.02	18 (25%)
36	NEX	G	616	-	38,46,46	3.40	9 (23%)	50,70,70	1.68	10 (20%)
31	CLA	D	404	8	69,73,73	1.36	7 (10%)	83,113,113	2.04	19 (22%)
30	CHL	8	605	3	70,74,74	0.79	2 (2%)	80,114,114	1.31	15 (18%)
31	CLA	B	613	6	69,73,73	1.35	7 (10%)	83,113,113	1.86	18 (21%)
38	SQD	b	621	-	53,54,54	0.79	0	62,65,65	0.91	3 (4%)
30	CHL	n	301	49	54,58,74	0.93	2 (3%)	59,94,114	1.43	13 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	b	617	6	69,73,73	1.39	6 (8%)	83,113,113	1.93	17 (20%)
33	LHG	j	102	-	48,48,48	0.39	0	51,54,54	1.08	3 (5%)
31	CLA	S	311	19	69,73,73	1.37	6 (8%)	83,113,113	1.93	22 (26%)
30	CHL	N	302	3	60,64,74	0.86	2 (3%)	68,102,114	1.44	14 (20%)
34	LMG	9	321	-	38,38,55	0.65	1 (2%)	46,46,63	1.14	4 (8%)
33	LHG	p	619	31	34,34,48	0.44	0	37,40,54	1.18	3 (8%)
34	LMG	b	624	-	38,38,55	0.66	1 (2%)	46,46,63	1.33	7 (15%)
45	DGD	c	618	-	67,67,67	1.16	7 (10%)	81,81,81	1.02	2 (2%)
31	CLA	l	604	49	69,73,73	1.37	6 (8%)	83,113,113	1.98	18 (21%)
43	BCR	v	101	-	41,41,41	4.75	25 (60%)	56,56,56	2.24	18 (32%)
30	CHL	g	307	49	54,58,74	0.93	1 (1%)	59,94,114	1.45	11 (18%)
31	CLA	b	602	49	53,57,73	1.54	6 (11%)	62,93,113	2.16	15 (24%)
42	PHO	a	408	-	58,69,69	0.78	2 (3%)	56,99,99	0.97	3 (5%)
31	CLA	B	603	6	69,73,73	1.39	6 (8%)	83,113,113	1.87	16 (19%)
34	LMG	w	202	-	55,55,55	1.14	6 (10%)	63,63,63	1.13	3 (4%)
38	SQD	m	101	-	49,50,54	0.82	0	58,61,65	0.96	2 (3%)
31	CLA	y	604	49	59,63,73	1.47	6 (10%)	71,101,113	2.11	19 (26%)
31	CLA	Y	303	24	64,68,73	1.40	7 (10%)	77,107,113	2.05	20 (25%)
36	NEX	6	319	-	38,46,46	3.37	11 (28%)	50,70,70	1.59	11 (22%)
30	CHL	Y	301	49	67,71,74	0.83	3 (4%)	76,110,114	1.32	12 (15%)
33	LHG	F1	301	-	34,34,48	0.44	0	37,40,54	1.09	2 (5%)
34	LMG	w	201	-	48,48,55	1.00	5 (10%)	56,56,63	1.08	3 (5%)
31	CLA	G	612	2	69,73,73	1.37	7 (10%)	83,113,113	1.93	17 (20%)
31	CLA	4	614	2	58,62,73	1.48	8 (13%)	69,99,113	2.13	20 (28%)
43	BCR	A	410	-	41,41,41	4.72	25 (60%)	56,56,56	2.56	20 (35%)
43	BCR	V	101	-	41,41,41	4.71	25 (60%)	56,56,56	2.39	22 (39%)
32	LUT	2	615	-	42,43,43	5.91	28 (66%)	51,60,60	3.00	18 (35%)
31	CLA	7	311	1	69,73,73	1.35	7 (10%)	83,113,113	1.91	18 (21%)
31	CLA	b	605	6	69,73,73	1.40	7 (10%)	83,113,113	1.96	17 (20%)
31	CLA	8	609	3	69,73,73	1.35	6 (8%)	83,113,113	1.95	19 (22%)
38	SQD	G	624	-	37,38,54	0.94	1 (2%)	46,49,65	1.04	2 (4%)
31	CLA	0	602	4	69,73,73	1.35	6 (8%)	83,113,113	1.93	19 (22%)
31	CLA	r	313	33	53,57,73	1.56	8 (15%)	62,93,113	2.14	17 (27%)
31	CLA	b	604	6	69,73,73	1.39	6 (8%)	83,113,113	1.88	17 (20%)
31	CLA	B	605	6	69,73,73	1.37	6 (8%)	83,113,113	1.95	16 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	LMG	b	601	-	45,45,55	0.90	3 (6%)	53,53,63	1.07	3 (5%)
34	LMG	y	620	-	38,38,55	0.60	1 (2%)	46,46,63	1.13	3 (6%)
31	CLA	q	312	2	56,61,73	1.40	6 (10%)	71,98,113	2.21	19 (26%)
45	DGD	c	617	-	63,63,67	1.14	7 (11%)	77,77,81	1.29	9 (11%)

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
43	BCR	b	619	-	-	15/29/63/63	0/2/2/2
33	LHG	9	320	31	-	24/37/37/53	-
35	RRX	G	614	-	-	15/29/65/65	0/2/2/2
31	CLA	2	611	2	-	10/27/103/115	-
30	CHL	9	311	2	-	14/35/111/117	-
31	CLA	3	313	3	-	11/21/97/115	-
31	CLA	C	607	49	-	15/39/115/115	-
38	SQD	a	412	-	-	18/40/60/69	0/1/1/1
32	LUT	Y	316	-	-	3/29/67/67	0/2/2/2
34	LMG	D	410	-	-	12/41/61/70	0/1/1/1
38	SQD	g	318	-	-	3/37/57/69	0/1/1/1
30	CHL	4	606	31	-	6/23/99/117	-
31	CLA	B	610	49	-	14/39/115/115	-
31	CLA	y	610	24	-	11/39/115/115	-
31	CLA	3	306	49	-	17/27/103/115	-
32	LUT	5	617	-	-	7/29/67/67	0/2/2/2
30	CHL	3	308	-	-	3/19/95/117	-
31	CLA	r	311	18	-	17/31/107/115	-
31	CLA	s	315	19	-	8/19/95/115	-
30	CHL	Y	302	24	-	11/41/117/117	-
34	LMG	b	629	-	-	12/33/53/70	0/1/1/1
30	CHL	G	608	2	-	4/38/114/117	-
34	LMG	X	203	-	-	10/33/53/70	0/1/1/1
38	SQD	A	413	-	-	15/40/60/69	0/1/1/1
31	CLA	9	313	33	-	10/18/94/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	c	613	7	-	10/39/115/115	-
34	LMG	3	321	-	-	10/33/53/70	0/1/1/1
43	BCR	d	406	-	-	11/29/63/63	0/2/2/2
34	LMG	C	619	-	-	10/46/66/70	0/1/1/1
31	CLA	s	314	19	-	17/39/115/115	-
31	CLA	C	604	49	-	10/29/105/115	-
32	LUT	p	616	-	-	9/29/67/67	0/2/2/2
31	CLA	N	312	3	-	6/15/91/115	-
31	CLA	c	609	7	-	12/39/115/115	-
38	SQD	g	301	-	-	6/33/53/69	0/1/1/1
38	SQD	r	322	-	-	15/46/66/69	0/1/1/1
31	CLA	G	603	2	-	11/27/103/115	-
31	CLA	p	603	3	-	13/27/103/115	-
38	SQD	M	102	-	-	16/45/65/69	0/1/1/1
31	CLA	3	314	3	-	6/27/103/115	-
31	CLA	r	304	18	-	11/33/109/115	-
38	SQD	G	617	-	-	11/37/57/69	0/1/1/1
31	CLA	2	603	2	-	13/27/103/115	-
43	BCR	D	405	-	-	13/29/63/63	0/2/2/2
30	CHL	7	310	1	-	9/41/117/117	-
30	CHL	2	608	2	-	7/31/107/117	-
31	CLA	B	611	6	-	13/39/115/115	-
34	LMG	9	301	-	-	11/46/66/70	0/1/1/1
34	LMG	D	411	-	-	15/46/66/70	0/1/1/1
31	CLA	N	311	33	-	9/20/96/115	-
31	CLA	7	305	49	-	14/39/115/115	-
31	CLA	Y	310	24	-	11/39/115/115	-
37	XAT	r	318	-	-	1/31/93/93	0/4/4/4
31	CLA	n	305	49	-	19/39/115/115	-
35	RRX	g	315	-	-	7/29/65/65	0/2/2/2
31	CLA	B	604	6	-	16/39/115/115	-
31	CLA	S	316	19	-	7/17/93/115	-
31	CLA	c	610	7	-	14/39/115/115	-
31	CLA	p	615	3	-	7/17/93/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LHG	D	408	-	-	30/53/53/53	-
30	CHL	7	302	1	-	12/41/117/117	-
32	LUT	S	318	-	-	9/29/67/67	0/2/2/2
31	CLA	5	613	3	-	11/26/102/115	-
30	CHL	R	309	18	-	6/29/105/117	-
30	CHL	0	607	49	-	19/41/117/117	-
31	CLA	r	312	18	-	12/30/106/115	-
30	CHL	5	608	-	-	8/22/98/117	-
34	LMG	c	620	-	-	14/33/53/70	0/1/1/1
31	CLA	R	314	18	-	6/20/96/115	-
34	LMG	d	410	-	-	15/46/66/70	0/1/1/1
31	CLA	6	311	4	-	16/39/115/115	-
34	LMG	W	203	-	-	13/33/53/70	0/1/1/1
44	PL9	A	416	-	-	13/53/73/73	0/1/1/1
30	CHL	6	307	49	-	5/23/99/117	-
30	CHL	n	309	49	-	5/22/98/117	-
31	CLA	s	310	19	-	15/33/109/115	-
33	LHG	8	618	31	-	35/53/53/53	-
34	LMG	w	203	-	-	6/33/53/70	0/1/1/1
31	CLA	S	304	19	-	5/12/88/115	-
31	CLA	n	314	3	-	15/39/115/115	-
31	CLA	Y	305	49	-	13/27/103/115	-
31	CLA	1	603	1	-	10/27/103/115	-
34	LMG	Y	319	-	-	8/33/53/70	0/1/1/1
34	LMG	9	302	-	-	13/35/55/70	0/1/1/1
30	CHL	3	309	-	-	10/22/98/117	-
31	CLA	4	603	2	-	10/27/103/115	-
43	BCR	B	617	-	-	14/29/63/63	0/2/2/2
30	CHL	0	605	4	-	10/25/101/117	-
31	CLA	C	603	7	-	18/39/115/115	-
36	NEX	p	618	31	-	9/27/83/83	0/3/3/3
30	CHL	s	302	19	-	2/17/93/117	-
31	CLA	r	306	49	-	8/19/95/115	-
30	CHL	1	606	49	-	16/41/117/117	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	7	321	49	-	13/38/114/117	-
34	LMG	Q1	101	-	-	10/33/53/70	0/1/1/1
38	SQD	6	301	-	-	18/37/57/69	0/1/1/1
31	CLA	S	303	19	-	17/39/115/115	-
31	CLA	Y	314	24	-	11/26/102/115	-
31	CLA	q	313	33	-	7/13/89/115	-
31	CLA	5	614	3	-	8/23/99/115	-
31	CLA	q	306	49	-	12/27/103/115	-
34	LMG	g	320	-	-	11/33/53/70	0/1/1/1
37	XAT	2	619	-	-	9/31/93/93	0/4/4/4
31	CLA	c	612	7	-	12/27/103/115	-
33	LHG	K	102	-	-	24/40/40/53	-
31	CLA	1	612	1	-	19/39/115/115	-
30	CHL	Y	309	24	-	10/41/117/117	-
34	LMG	N	320	-	-	9/33/53/70	0/1/1/1
31	CLA	b	614	6	-	13/39/115/115	-
34	LMG	B	621	-	-	15/46/66/70	0/1/1/1
43	BCR	z	101	-	-	4/29/63/63	0/2/2/2
30	CHL	R	310	49	-	4/28/104/117	-
30	CHL	6	308	49	-	13/41/117/117	-
32	LUT	S	317	-	-	6/29/67/67	0/2/2/2
31	CLA	R	307	49	-	11/19/95/115	-
32	LUT	y	616	-	-	2/29/67/67	0/2/2/2
34	LMG	6	323	-	-	14/33/53/70	0/1/1/1
36	NEX	Y	317	-	-	2/27/83/83	0/3/3/3
30	CHL	3	310	3	-	8/35/111/117	-
31	CLA	G	613	2	-	10/20/96/115	-
34	LMG	b	622	-	-	16/46/66/70	0/1/1/1
31	CLA	N	304	3	-	12/27/103/115	-
34	LMG	0	622	-	-	15/33/53/70	0/1/1/1
33	LHG	d	408	-	-	29/53/53/53	-
43	BCR	c	614	-	-	16/29/63/63	0/2/2/2
37	XAT	q	321	-	-	9/31/93/93	0/4/4/4
33	LHG	N	319	31	-	32/53/53/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	2	604	49,36	-	11/26/102/115	-
43	BCR	Z	101	-	-	4/29/63/63	0/2/2/2
34	LMG	C	621	-	-	9/33/53/70	0/1/1/1
34	LMG	x	202	-	-	19/33/53/70	0/1/1/1
31	CLA	p	611	33	-	19/33/109/115	-
43	BCR	C	615	-	-	8/29/63/63	0/2/2/2
32	LUT	4	616	-	-	6/29/67/67	0/2/2/2
42	PHO	A	408	-	-	13/37/103/103	0/5/6/6
30	CHL	9	308	-	-	6/25/101/117	-
31	CLA	b	615	6	-	16/39/115/115	-
31	CLA	5	602	3	-	14/33/109/115	-
43	BCR	C	614	-	-	12/29/63/63	0/2/2/2
31	CLA	q	316	2	-	10/21/97/115	-
45	DGD	c	619	-	-	16/55/95/95	0/2/2/2
31	CLA	b	613	6	-	18/39/115/115	-
30	CHL	N	307	49	-	6/32/108/117	-
31	CLA	b	611	49	-	12/39/115/115	-
34	LMG	p	620	-	-	7/33/53/70	0/1/1/1
30	CHL	Y	307	49	-	10/33/109/117	-
42	PHO	d	402	-	-	6/37/103/103	0/5/6/6
31	CLA	B	602	6	-	16/39/115/115	-
31	CLA	8	614	3	-	10/26/102/115	-
36	NEX	R	319	-	-	7/27/83/83	0/3/3/3
34	LMG	a	401	-	-	6/33/53/70	0/1/1/1
31	CLA	N	315	3	-	8/26/102/115	-
30	CHL	R	308	18	-	5/29/105/117	-
31	CLA	c	608	7	-	11/39/115/115	-
34	LMG	n	322	-	-	12/35/55/70	0/1/1/1
31	CLA	8	611	3	-	4/15/91/115	-
31	CLA	g	314	2	-	7/20/96/115	-
33	LHG	t	102	-	-	30/45/45/53	-
32	LUT	N	317	-	-	6/29/67/67	0/2/2/2
32	LUT	6	318	-	-	6/29/67/67	0/2/2/2
33	LHG	y	619	31	-	30/50/50/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	0	615	-	-	14/27/103/115	-
37	XAT	G	620	-	-	9/31/93/93	0/4/4/4
30	CHL	s	309	49	-	2/21/97/117	-
30	CHL	p	606	-	-	2/23/99/117	-
36	NEX	y	618	-	-	2/27/83/83	0/3/3/3
34	LMG	w	204	-	-	12/33/53/70	0/1/1/1
31	CLA	6	315	4	-	16/26/102/115	-
30	CHL	G	607	49	-	5/23/99/117	-
30	CHL	g	302	2	-	14/41/117/117	-
34	LMG	n	321	-	-	12/33/53/70	0/1/1/1
36	NEX	g	317	31	-	12/27/83/83	0/3/3/3
30	CHL	q	307	2	-	4/17/93/117	-
31	CLA	A	405	5	-	10/39/115/115	-
31	CLA	5	610	3	-	11/33/109/115	-
30	CHL	7	309	49	-	7/22/98/117	-
33	LHG	S	320	31	-	30/45/45/53	-
31	CLA	5	603	3	-	10/24/100/115	-
35	RRX	q	317	-	-	9/29/65/65	0/2/2/2
30	CHL	p	609	3	-	4/29/105/117	-
33	LHG	C	623	-	-	28/44/44/53	-
30	CHL	n	310	3	-	6/41/117/117	-
31	CLA	G	610	33	-	17/33/109/115	-
30	CHL	7	307	49	-	9/41/117/117	-
34	LMG	2	618	-	-	13/33/53/70	0/1/1/1
31	CLA	b	609	6	-	14/39/115/115	-
30	CHL	Y	308	49	-	7/22/98/117	-
34	LMG	2	621	-	-	9/35/55/70	0/1/1/1
33	LHG	6	320	31	-	24/41/41/53	-
30	CHL	8	606	49	-	3/32/108/117	-
31	CLA	C	611	7	-	15/39/115/115	-
31	CLA	B	601	49	-	10/20/96/115	-
32	LUT	Y	315	-	-	0/29/67/67	0/2/2/2
33	LHG	G	618	31	-	29/48/48/53	-
31	CLA	2	610	33	-	15/33/109/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMG	J	102	-	-	7/33/53/70	0/1/1/1
34	LMG	a	413	-	-	9/33/53/70	0/1/1/1
32	LUT	3	318	-	-	8/29/67/67	0/2/2/2
30	CHL	p	605	3	-	3/17/93/117	-
32	LUT	7	318	-	-	6/29/67/67	0/2/2/2
31	CLA	q	305	2	-	14/27/103/115	-
33	LHG	3	320	31	-	25/37/37/53	-
31	CLA	g	310	2	-	14/39/115/115	-
31	CLA	c	605	7	-	18/39/115/115	-
30	CHL	N	309	3	-	7/41/117/117	-
30	CHL	9	310	49	-	7/22/98/117	-
38	SQD	X	201	-	-	9/33/53/69	0/1/1/1
31	CLA	2	609	2	-	18/33/109/115	-
38	SQD	b	627	-	-	14/47/67/69	0/1/1/1
31	CLA	6	313	4	-	12/33/109/115	-
33	LHG	A	417	-	-	24/43/43/53	-
30	CHL	3	307	3	-	7/17/93/117	-
34	LMG	6	321	-	-	13/37/57/70	0/1/1/1
30	CHL	6	306	4	-	8/17/93/117	-
30	CHL	s	307	19	-	0/15/91/117	-
31	CLA	3	316	3	-	13/30/106/115	-
30	CHL	S	309	49	-	1/21/97/117	-
31	CLA	2	602	2	-	25/39/115/115	-
33	LHG	1	617	31	-	29/39/39/53	-
31	CLA	s	313	19	-	9/29/105/115	-
33	LHG	S	322	-	-	31/48/48/53	-
31	CLA	C	606	7	-	15/30/106/115	-
34	LMG	c	624	-	-	11/39/59/70	0/1/1/1
30	CHL	4	607	-	-	15/31/107/117	-
30	CHL	8	601	3	-	8/29/105/117	-
31	CLA	c	602	7	-	12/39/115/115	-
43	BCR	B	618	-	-	10/29/63/63	0/2/2/2
31	CLA	8	603	3	-	13/27/103/115	-
31	CLA	b	610	6	-	20/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	6	316	4	-	14/27/103/115	-
33	LHG	7	319	31	-	28/39/39/53	-
31	CLA	G	602	2	-	16/39/115/115	-
34	LMG	k	101	-	-	9/43/63/70	0/1/1/1
38	SQD	s	301	-	-	16/46/66/69	0/1/1/1
33	LHG	2	617	31	-	32/53/53/53	-
32	LUT	R	317	-	-	8/29/67/67	0/2/2/2
31	CLA	3	315	3	-	12/26/102/115	-
33	LHG	r	320	31	-	23/42/42/53	-
31	CLA	0	613	4	-	10/29/105/115	-
31	CLA	5	604	-	-	6/21/97/115	-
31	CLA	C	605	7	-	18/39/115/115	-
31	CLA	Y	304	24	-	13/27/103/115	-
30	CHL	p	601	3	-	8/23/99/117	-
31	CLA	R	304	18	-	14/33/109/115	-
32	LUT	3	317	-	-	2/29/67/67	0/2/2/2
34	LMG	r	321	-	-	15/33/53/70	0/1/1/1
31	CLA	p	610	3	-	15/29/105/115	-
30	CHL	y	606	49	-	9/33/109/117	-
31	CLA	0	611	33	-	12/33/109/115	-
34	LMG	q	302	-	-	9/35/55/70	0/1/1/1
31	CLA	6	304	4	-	18/29/105/115	-
36	NEX	s	319	-	-	3/27/83/83	0/3/3/3
37	XAT	4	619	-	-	9/31/93/93	0/4/4/4
31	CLA	R	313	33	-	8/20/96/115	-
31	CLA	p	612	3	-	8/17/93/115	-
31	CLA	9	314	2	-	5/21/97/115	-
31	CLA	y	614	24	-	10/26/102/115	-
33	LHG	q	320	31	-	31/50/50/53	-
30	CHL	3	302	49	-	13/31/107/117	-
33	LHG	B	624	-	-	35/53/53/53	-
33	LHG	5	619	31	-	27/39/39/53	-
31	CLA	8	610	33	-	7/20/96/115	-
30	CHL	4	601	2	-	12/41/117/117	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LUT	G	615	-	-	10/29/67/67	0/2/2/2
30	CHL	N	301	-	-	6/22/98/117	-
33	LHG	L	101	-	-	31/53/53/53	-
34	LMG	B	622	-	-	8/33/53/70	0/1/1/1
34	LMG	s	321	-	-	11/36/56/70	0/1/1/1
32	LUT	r	317	-	-	5/29/67/67	0/2/2/2
31	CLA	b	606	6	-	16/39/115/115	-
37	XAT	R	318	-	-	6/31/93/93	0/4/4/4
31	CLA	R	312	18	-	12/30/106/115	-
30	CHL	S	308	49	-	1/14/90/117	-
31	CLA	b	607	6	-	16/39/115/115	-
31	CLA	g	305	49,36	-	13/27/103/115	-
34	LMG	f	101	-	-	11/33/53/70	0/1/1/1
31	CLA	b	616	6	-	17/39/115/115	-
47	HEM	E	101	9,10	-	5/14/54/54	-
31	CLA	4	613	2	-	15/35/111/115	-
31	CLA	7	303	1	-	11/33/109/115	-
31	CLA	8	612	3	-	15/39/115/115	-
31	CLA	9	305	2	-	12/27/103/115	-
34	LMG	7	322	-	-	13/33/53/70	0/1/1/1
44	PL9	D	406	-	-	9/53/73/73	0/1/1/1
45	DGD	C	616	-	-	9/39/79/95	0/2/2/2
33	LHG	b	625	-	-	30/48/48/53	-
33	LHG	0	619	31	-	29/40/40/53	-
31	CLA	b	608	49	-	24/39/115/115	-
31	CLA	r	316	18	-	20/39/115/115	-
36	NEX	S	319	-	-	2/27/83/83	0/3/3/3
30	CHL	G	605	2	-	5/20/96/117	-
34	LMG	C	622	-	-	6/27/47/70	0/1/1/1
31	CLA	R	316	18	-	22/39/115/115	-
32	LUT	q	318	-	-	6/29/67/67	0/2/2/2
31	CLA	y	611	33	-	17/39/115/115	-
31	CLA	4	604	30	-	12/23/99/115	-
31	CLA	d	405	8	-	13/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	NEX	0	618	-	-	9/27/83/83	0/3/3/3
36	NEX	r	301	-	-	2/27/83/83	0/3/3/3
30	CHL	g	309	2	-	7/38/114/117	-
31	CLA	b	603	6	-	19/39/115/115	-
31	CLA	S	314	19	-	16/39/115/115	-
30	CHL	9	309	-	-	11/26/102/117	-
45	DGD	C	618	-	-	16/55/95/95	0/2/2/2
31	CLA	C	601	7	-	20/39/115/115	-
32	LUT	5	616	-	-	7/29/67/67	0/2/2/2
34	LMG	G	621	-	-	13/46/66/70	0/1/1/1
33	LHG	c	622	-	-	32/51/51/53	-
30	CHL	9	307	2	-	7/17/93/117	-
31	CLA	c	607	49	-	12/39/115/115	-
33	LHG	e	101	-	-	31/48/48/53	-
30	CHL	p	608	-	-	10/22/98/117	-
34	LMG	A	414	-	-	10/33/53/70	0/1/1/1
31	CLA	Y	312	24	-	17/39/115/115	-
31	CLA	C	612	7	-	14/27/103/115	-
31	CLA	s	303	19	-	14/39/115/115	-
38	SQD	A	411	-	-	13/46/66/69	0/1/1/1
34	LMG	b	626	-	-	14/41/61/70	0/1/1/1
31	CLA	6	312	33	-	19/33/109/115	-
43	BCR	b	620	-	-	9/29/63/63	0/2/2/2
34	LMG	w	205	-	-	13/33/53/70	0/1/1/1
33	LHG	4	618	31	-	28/51/51/53	-
30	CHL	2	601	2	-	10/41/117/117	-
31	CLA	4	612	2	-	6/17/93/115	-
33	LHG	Y	318	31	-	30/46/46/53	-
34	LMG	W	202	-	-	11/33/53/70	0/1/1/1
34	LMG	4	620	-	-	15/46/66/70	0/1/1/1
38	SQD	Y	320	-	-	8/37/57/69	0/1/1/1
31	CLA	d	401	49	-	8/20/96/115	-
31	CLA	G	609	2	-	7/39/115/115	-
34	LMG	7	301	-	-	11/34/54/70	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	7	308	49	-	10/41/117/117	-
31	CLA	B	607	49	-	20/39/115/115	-
30	CHL	y	601	24	-	13/41/117/117	-
31	CLA	B	612	6	-	11/39/115/115	-
30	CHL	q	310	-	-	4/22/98/117	-
34	LMG	S	321	-	-	9/36/56/70	0/1/1/1
34	LMG	G	622	-	-	7/35/55/70	0/1/1/1
31	CLA	G	604	49	-	14/27/103/115	-
31	CLA	7	315	1	-	16/26/102/115	-
31	CLA	q	315	2	-	15/39/115/115	-
31	CLA	3	311	-	-	6/26/102/115	-
31	CLA	y	615	24	-	12/26/102/115	-
31	CLA	S	310	19	-	16/33/109/115	-
30	CHL	5	605	3	-	3/17/93/117	-
32	LUT	n	318	-	-	6/29/67/67	0/2/2/2
31	CLA	4	610	2	-	20/33/109/115	-
43	BCR	t	101	-	-	6/29/63/63	0/2/2/2
33	LHG	a	415	-	-	23/43/43/53	-
33	LHG	g	319	31	-	26/48/48/53	-
33	LHG	b	628	-	-	31/53/53/53	-
36	NEX	r	319	-	-	4/27/83/83	0/3/3/3
32	LUT	1	616	-	-	3/29/67/67	0/2/2/2
31	CLA	N	313	3	-	13/39/115/115	-
31	CLA	R	305	18	-	8/33/109/115	-
33	LHG	l	101	-	-	29/53/53/53	-
30	CHL	s	308	49	-	3/14/90/117	-
36	NEX	5	618	-	-	9/27/83/83	0/3/3/3
32	LUT	0	617	-	-	0/29/67/67	0/2/2/2
31	CLA	B	606	6	-	16/39/115/115	-
31	CLA	r	303	18	-	9/20/96/115	-
34	LMG	W	201	-	-	19/50/70/70	0/1/1/1
30	CHL	8	608	3	-	8/41/117/117	-
38	SQD	a	411	-	-	16/43/63/69	0/1/1/1
31	CLA	7	316	1	-	7/23/99/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMG	q1	101	-	-	7/33/53/70	0/1/1/1
43	BCR	T	101	-	-	14/29/63/63	0/2/2/2
36	NEX	4	617	-	-	6/27/83/83	0/3/3/3
31	CLA	p	614	3	-	11/23/99/115	-
31	CLA	c	611	7	-	15/39/115/115	-
33	LHG	M	101	-	-	25/45/45/53	-
31	CLA	4	611	33	-	5/13/89/115	-
32	LUT	y	617	-	-	2/29/67/67	0/2/2/2
31	CLA	q	304	2	-	12/39/115/115	-
30	CHL	0	606	49	-	3/23/99/117	-
31	CLA	R	303	18	-	11/20/96/115	-
31	CLA	A	407	49	-	6/20/96/115	-
31	CLA	N	314	3	-	9/20/96/115	-
30	CHL	n	307	49	-	3/32/108/117	-
34	LMG	1	618	-	-	8/33/53/70	0/1/1/1
31	CLA	0	614	4	-	12/26/102/115	-
31	CLA	3	312	33	-	15/39/115/115	-
30	CHL	2	605	2	-	4/17/93/117	-
38	SQD	x	201	-	-	14/37/57/69	0/1/1/1
36	NEX	N	318	-	-	15/27/83/83	0/3/3/3
31	CLA	R	306	49	-	7/19/95/115	-
36	NEX	9	319	31	-	6/27/83/83	0/3/3/3
30	CHL	y	608	49	-	3/22/98/117	-
30	CHL	1	601	1	-	12/41/117/117	-
30	CHL	1	619	-	-	11/35/111/117	-
30	CHL	q	303	2	-	9/41/117/117	-
32	LUT	7	317	-	-	6/29/67/67	0/2/2/2
31	CLA	g	303	2	-	11/39/115/115	-
35	RRX	2	614	-	-	15/29/65/65	0/2/2/2
30	CHL	q	311	2	-	3/29/105/117	-
31	CLA	a	406	5	-	15/39/115/115	-
31	CLA	s	316	19	-	6/17/93/115	-
30	CHL	9	303	2	-	11/41/117/117	-
31	CLA	y	603	24	-	12/27/103/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LUT	8	615	-	-	6/29/67/67	0/2/2/2
31	CLA	3	301	1	-	13/26/102/115	-
31	CLA	6	314	4	-	13/39/115/115	-
30	CHL	1	607	-	-	14/41/117/117	-
31	CLA	S	313	19	-	9/29/105/115	-
31	CLA	c	606	7	-	20/39/115/115	-
42	PHO	D	401	-	-	12/37/103/103	0/5/6/6
32	LUT	6	317	-	-	6/29/67/67	0/2/2/2
30	CHL	r	310	49	-	3/28/104/117	-
45	DGD	C	620	-	-	17/55/95/95	0/2/2/2
30	CHL	2	607	49	-	6/22/98/117	-
30	CHL	6	309	49	-	2/22/98/117	-
43	BCR	h	101	-	-	9/29/63/63	0/2/2/2
30	CHL	1	605	1	-	13/41/117/117	-
31	CLA	2	612	2	-	17/39/115/115	-
32	LUT	s	318	-	-	5/29/67/67	0/2/2/2
30	CHL	4	605	2	-	4/17/93/117	-
30	CHL	0	609	4	-	4/35/111/117	-
31	CLA	S	305	49	-	11/39/115/115	-
34	LMG	j	101	-	-	12/38/58/70	0/1/1/1
31	CLA	3	304	3	-	14/33/109/115	-
34	LMG	5	620	-	-	14/33/53/70	0/1/1/1
31	CLA	p	604	36	-	8/21/97/115	-
32	LUT	g	316	-	-	10/29/67/67	0/2/2/2
34	LMG	D	409	-	-	12/41/61/70	0/1/1/1
31	CLA	B	614	6	-	19/39/115/115	-
31	CLA	7	304	1	-	12/27/103/115	-
30	CHL	Y	306	24	-	0/17/93/117	-
36	NEX	3	319	-	-	9/27/83/83	0/3/3/3
32	LUT	N	316	-	-	6/29/67/67	0/2/2/2
34	LMG	R	321	-	-	9/33/53/70	0/1/1/1
31	CLA	7	313	1	-	15/39/115/115	-
43	BCR	H	101	-	-	5/29/63/63	0/2/2/2
31	CLA	B	615	6	-	11/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	5	607	-	-	8/23/99/117	-
37	XAT	g	321	-	-	9/31/93/93	0/4/4/4
31	CLA	0	604	49	-	15/27/103/115	-
34	LMG	c	621	-	-	8/33/53/70	0/1/1/1
30	CHL	3	303	3	-	6/22/98/117	-
31	CLA	1	610	1	-	19/39/115/115	-
30	CHL	4	609	2	-	10/31/107/117	-
33	LHG	s	322	-	-	29/48/48/53	-
31	CLA	p	613	-	-	9/26/102/115	-
31	CLA	d	404	8	-	13/39/115/115	-
34	LMG	J	101	-	-	13/46/66/70	0/1/1/1
30	CHL	5	606	49	-	2/23/99/117	-
34	LMG	4	621	-	-	11/35/55/70	0/1/1/1
31	CLA	g	311	33	-	15/33/109/115	-
31	CLA	C	609	7	-	12/39/115/115	-
43	BCR	c	615	-	-	11/29/63/63	0/2/2/2
30	CHL	g	308	49	-	4/23/99/117	-
31	CLA	a	409	5	-	16/33/109/115	-
30	CHL	6	310	4	-	12/35/111/117	-
30	CHL	1	608	49	-	5/22/98/117	-
31	CLA	7	312	33	-	19/39/115/115	-
37	XAT	9	322	-	-	9/31/93/93	0/4/4/4
32	LUT	8	616	-	-	6/29/67/67	0/2/2/2
45	DGD	C	617	-	-	16/55/95/95	0/2/2/2
48	LMU	r	302	-	-	9/21/61/61	0/2/2/2
31	CLA	s	304	19	-	6/12/88/115	-
33	LHG	R	320	31	-	26/42/42/53	-
32	LUT	s	317	-	-	6/29/67/67	0/2/2/2
30	CHL	p	607	-	-	7/23/99/117	-
31	CLA	R	311	18	-	18/31/107/115	-
38	SQD	B	623	-	-	20/47/67/69	0/1/1/1
30	CHL	0	601	4	-	8/29/105/117	-
34	LMG	A	412	-	-	11/36/56/70	0/1/1/1
30	CHL	7	306	1	-	17/41/117/117	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	8	613	3	-	8/20/96/115	-
34	LMG	d	409	-	-	10/36/56/70	0/1/1/1
30	CHL	6	302	4	-	5/29/105/117	-
38	SQD	R	322	-	-	16/46/66/69	0/1/1/1
43	BCR	a	410	-	-	11/29/63/63	0/2/2/2
33	LHG	n	320	31	-	34/53/53/53	-
31	CLA	r	315	18	-	13/27/103/115	-
31	CLA	G	611	2	-	2/13/89/115	-
31	CLA	1	611	33	-	11/39/115/115	-
30	CHL	n	308	49	-	13/38/114/117	-
30	CHL	N	308	49	-	8/22/98/117	-
31	CLA	2	613	2	-	13/26/102/115	-
34	LMG	I	101	-	-	15/33/53/70	0/1/1/1
31	CLA	N	310	3	-	11/39/115/115	-
31	CLA	c	604	49	-	11/29/105/115	-
31	CLA	N	321	24	-	9/26/102/115	-
31	CLA	A	406	49	-	12/39/115/115	-
31	CLA	8	604	49,36	-	21/39/115/115	-
34	LMG	D	412	-	-	7/43/63/70	0/1/1/1
30	CHL	8	607	49	-	5/22/98/117	-
31	CLA	n	311	3	-	10/39/115/115	-
31	CLA	r	305	18	-	14/33/109/115	-
31	CLA	s	312	33	-	25/39/115/115	-
30	CHL	G	623	49	-	12/41/117/117	-
36	NEX	2	616	31	-	14/27/83/83	0/3/3/3
31	CLA	R	315	18	-	8/27/103/115	-
43	BCR	b	618	-	-	14/29/63/63	0/2/2/2
47	HEM	e	102	9,10	-	7/14/54/54	-
31	CLA	A	409	5	-	16/33/109/115	-
31	CLA	c	601	7	-	24/39/115/115	-
30	CHL	y	609	24	-	6/41/117/117	-
31	CLA	n	315	3	-	8/20/96/115	-
31	CLA	b	612	6	-	13/39/115/115	-
30	CHL	r	309	18	-	5/29/105/117	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMG	a	416	-	-	11/33/53/70	0/1/1/1
30	CHL	5	609	3	-	5/29/105/117	-
32	LUT	n	317	-	-	6/29/67/67	0/2/2/2
31	CLA	Y	311	33	-	16/39/115/115	-
31	CLA	C	613	7	-	13/39/115/115	-
31	CLA	s	306	-	-	5/21/97/115	-
33	LHG	D	407	-	-	31/48/48/53	-
30	CHL	4	608	-	-	5/22/98/117	-
31	CLA	S	306	-	-	4/21/97/115	-
31	CLA	N	305	49	-	18/39/115/115	-
30	CHL	n	302	3	-	8/29/105/117	-
31	CLA	S	315	19	-	5/19/95/115	-
31	CLA	r	314	18	-	8/20/96/115	-
48	LMU	R	302	-	-	12/21/61/61	0/2/2/2
34	LMG	b	623	-	-	7/33/53/70	0/1/1/1
38	SQD	0	621	-	-	9/37/57/69	0/1/1/1
30	CHL	2	606	-	-	6/23/99/117	-
31	CLA	y	602	24	-	10/33/109/115	-
34	LMG	g	322	-	-	15/44/64/70	0/1/1/1
38	SQD	S	301	-	-	14/46/66/69	0/1/1/1
31	CLA	n	316	3	-	10/26/102/115	-
36	NEX	R	301	-	-	3/27/83/83	0/3/3/3
31	CLA	5	611	33	-	15/31/107/115	-
31	CLA	C	610	7	-	14/39/115/115	-
31	CLA	y	612	24	-	18/39/115/115	-
31	CLA	B	608	6	-	12/39/115/115	-
31	CLA	N	303	3	-	19/39/115/115	-
34	LMG	7	320	-	-	7/33/53/70	0/1/1/1
36	NEX	8	617	31	-	11/27/83/83	0/3/3/3
31	CLA	Y	313	24	-	12/39/115/115	-
30	CHL	n	306	3	-	15/41/117/117	-
35	RRX	9	317	-	-	15/29/65/65	0/2/2/2
31	CLA	a	407	49	-	13/39/115/115	-
32	LUT	p	617	-	-	9/29/67/67	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	p	602	3	-	12/33/109/115	-
31	CLA	6	305	49	-	16/27/103/115	-
30	CHL	S	302	19	-	0/17/93/117	-
31	CLA	S	312	33	-	19/39/115/115	-
34	LMG	m	102	-	-	10/40/60/70	0/1/1/1
30	CHL	5	601	3	-	9/23/99/117	-
31	CLA	y	613	24	-	17/39/115/115	-
30	CHL	S	307	19	-	0/15/91/117	-
34	LMG	G	619	-	-	11/33/53/70	0/1/1/1
35	RRX	4	615	-	-	15/29/65/65	0/2/2/2
31	CLA	B	616	6	-	15/39/115/115	-
32	LUT	1	615	-	-	1/29/67/67	0/2/2/2
31	CLA	5	612	3	-	8/21/97/115	-
31	CLA	6	303	4	-	15/39/115/115	-
31	CLA	9	316	2	-	9/17/93/115	-
31	CLA	4	602	2	-	15/39/115/115	-
31	CLA	5	615	3	-	11/17/93/115	-
34	LMG	6	322	-	-	11/34/54/70	0/1/1/1
30	CHL	G	606	49	-	6/22/98/117	-
31	CLA	3	305	3	-	13/27/103/115	-
31	CLA	C	608	7	-	13/39/115/115	-
30	CHL	q	308	-	-	6/23/99/117	-
31	CLA	g	304	2	-	12/27/103/115	-
31	CLA	1	614	1	-	16/26/102/115	-
30	CHL	y	607	49	-	11/41/117/117	-
31	CLA	8	602	3	-	13/39/115/115	-
34	LMG	d	411	-	-	8/43/63/70	0/1/1/1
31	CLA	9	304	2	-	19/39/115/115	-
30	CHL	1	609	1	-	6/41/117/117	-
31	CLA	1	613	1	-	15/39/115/115	-
32	LUT	9	318	-	-	5/29/67/67	0/2/2/2
48	LMU	c	623	-	-	5/14/54/61	0/2/2/2
30	CHL	0	608	49	-	5/22/98/117	-
31	CLA	r	307	49	-	11/19/95/115	-
31	CLA	c	603	7	-	22/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMG	A	418	-	-	11/33/53/70	0/1/1/1
31	CLA	0	612	4	-	8/17/93/115	-
33	LHG	A	415	-	-	31/48/48/53	-
34	LMG	k	102	-	-	10/33/53/70	0/1/1/1
48	LMU	K	101	-	-	7/21/61/61	0/2/2/2
34	LMG	X	202	-	-	5/33/53/70	0/1/1/1
34	LMG	0	620	-	-	13/37/57/70	0/1/1/1
33	LHG	s	320	31	-	25/45/45/53	-
36	NEX	q	319	-	-	11/27/83/83	0/3/3/3
31	CLA	s	311	19	-	13/39/115/115	-
30	CHL	y	605	24	-	2/17/93/117	-
31	CLA	g	312	2	-	3/13/89/115	-
31	CLA	n	304	3	-	13/27/103/115	-
34	LMG	q	301	-	-	14/46/66/70	0/1/1/1
30	CHL	q	309	-	-	19/31/107/117	-
34	LMG	C	624	-	-	13/39/59/70	0/1/1/1
31	CLA	9	312	2	-	13/26/102/115	-
44	PL9	d	407	-	-	7/53/73/73	0/1/1/1
30	CHL	G	601	2	-	10/41/117/117	-
31	CLA	s	305	49	-	16/39/115/115	-
31	CLA	q	314	2	-	9/17/93/115	-
31	CLA	C	602	7	-	11/39/115/115	-
31	CLA	n	313	3	-	4/15/91/115	-
31	CLA	0	603	4	-	16/29/105/115	-
36	NEX	n	319	-	-	10/27/83/83	0/3/3/3
43	BCR	B	619	-	-	9/29/63/63	0/2/2/2
31	CLA	1	602	1	-	14/33/109/115	-
38	SQD	y	621	-	-	9/37/57/69	0/1/1/1
31	CLA	g	313	2	-	13/39/115/115	-
30	CHL	g	306	2	-	5/20/96/117	-
31	CLA	D	403	8	-	14/39/115/115	-
31	CLA	9	306	49,36	-	17/39/115/115	-
31	CLA	7	314	1	-	17/39/115/115	-
30	CHL	N	306	3	-	12/41/117/117	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	0	610	4	-	15/39/115/115	-
31	CLA	n	303	3	-	13/39/115/115	-
32	LUT	0	616	-	-	2/29/67/67	0/2/2/2
34	LMG	B	625	-	-	13/33/53/70	0/1/1/1
38	SQD	B	620	-	-	18/49/69/69	0/1/1/1
45	DGD	c	616	-	-	22/55/95/95	0/2/2/2
33	LHG	z	102	-	-	22/40/40/53	-
31	CLA	n	312	33	-	7/20/96/115	-
30	CHL	r	308	18	-	8/29/105/117	-
31	CLA	B	609	6	-	20/39/115/115	-
34	LMG	2	620	-	-	18/46/66/70	0/1/1/1
44	PL9	a	414	-	-	16/53/73/73	0/1/1/1
31	CLA	9	315	2	-	8/27/103/115	-
36	NEX	G	616	-	-	2/27/83/83	0/3/3/3
31	CLA	D	404	8	-	19/39/115/115	-
30	CHL	8	605	3	-	15/41/117/117	-
31	CLA	B	613	6	-	9/39/115/115	-
38	SQD	b	621	-	-	13/49/69/69	0/1/1/1
30	CHL	n	301	49	-	6/22/98/117	-
31	CLA	b	617	6	-	15/39/115/115	-
33	LHG	j	102	-	-	36/53/53/53	-
31	CLA	S	311	19	-	13/39/115/115	-
30	CHL	N	302	3	-	4/29/105/117	-
34	LMG	9	321	-	-	10/33/53/70	0/1/1/1
33	LHG	p	619	31	-	26/39/39/53	-
34	LMG	b	624	-	-	14/33/53/70	0/1/1/1
45	DGD	c	618	-	-	19/55/95/95	0/2/2/2
31	CLA	1	604	49	-	14/39/115/115	-
43	BCR	v	101	-	-	15/29/63/63	0/2/2/2
30	CHL	g	307	49	-	3/22/98/117	-
31	CLA	b	602	49	-	14/20/96/115	-
42	PHO	a	408	-	-	10/37/103/103	0/5/6/6
31	CLA	B	603	6	-	19/39/115/115	-
34	LMG	w	202	-	-	12/50/70/70	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	SQD	m	101	-	-	13/45/65/69	0/1/1/1
31	CLA	y	604	49	-	15/27/103/115	-
31	CLA	Y	303	24	-	10/33/109/115	-
36	NEX	6	319	-	-	9/27/83/83	0/3/3/3
30	CHL	Y	301	49	-	10/38/114/117	-
33	LHG	F1	301	-	-	26/39/39/53	-
34	LMG	w	201	-	-	13/43/63/70	0/1/1/1
31	CLA	G	612	2	-	19/39/115/115	-
31	CLA	4	614	2	-	8/26/102/115	-
43	BCR	A	410	-	-	6/29/63/63	0/2/2/2
43	BCR	V	101	-	-	15/29/63/63	0/2/2/2
32	LUT	2	615	-	-	5/29/67/67	0/2/2/2
31	CLA	7	311	1	-	17/39/115/115	-
31	CLA	b	605	6	-	25/39/115/115	-
31	CLA	8	609	3	-	10/39/115/115	-
38	SQD	G	624	-	-	12/33/53/69	0/1/1/1
31	CLA	0	602	4	-	18/39/115/115	-
31	CLA	r	313	33	-	8/20/96/115	-
31	CLA	b	604	6	-	16/39/115/115	-
31	CLA	B	605	6	-	19/39/115/115	-
34	LMG	b	601	-	-	10/40/60/70	0/1/1/1
34	LMG	y	620	-	-	10/33/53/70	0/1/1/1
31	CLA	q	312	2	-	11/25/101/115	-
45	DGD	c	617	-	-	23/51/91/95	0/2/2/2

The worst 5 of 4254 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	N	316	LUT	C24-C25	23.29	1.62	1.33
32	5	616	LUT	C24-C25	23.25	1.62	1.33
32	G	615	LUT	C24-C25	23.25	1.62	1.33
32	3	317	LUT	C24-C25	23.24	1.62	1.33
32	9	318	LUT	C24-C25	23.23	1.62	1.33

The worst 5 of 8510 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	G	615	LUT	C40-C33-C34	-33.47	76.04	122.92
32	G	615	LUT	C32-C33-C34	25.38	157.89	118.94
32	G	615	LUT	C40-C33-C32	-22.99	81.85	118.08
43	C	615	BCR	C15-C14-C13	-12.84	108.99	127.31
43	t	101	BCR	C11-C10-C9	-11.88	110.35	127.31

There are no chirality outliers.

5 of 7923 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	1	601	CHL	CHA-CBD-CGD-O1D
30	1	601	CHL	CHA-CBD-CGD-O2D
30	1	606	CHL	CAD-CBD-CGD-O1D
30	1	606	CHL	CAD-CBD-CGD-O2D
30	1	607	CHL	C1A-C2A-CAA-CBA

There are no ring outliers.

654 monomers are involved in 3749 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	b	619	BCR	4	0
33	9	320	LHG	9	0
35	G	614	RRX	28	0
31	2	611	CLA	9	0
30	9	311	CHL	6	0
31	3	313	CLA	4	0
31	C	607	CLA	5	0
38	a	412	SQD	4	0
32	Y	316	LUT	3	0
34	D	410	LMG	5	0
38	g	318	SQD	9	0
30	4	606	CHL	17	0
31	B	610	CLA	11	0
31	y	610	CLA	14	0
31	3	306	CLA	12	0
32	5	617	LUT	15	0
30	3	308	CHL	11	0
31	r	311	CLA	5	0
31	s	315	CLA	3	0
30	Y	302	CHL	10	0
34	b	629	LMG	5	0
30	G	608	CHL	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	X	203	LMG	1	0
38	A	413	SQD	3	0
31	9	313	CLA	4	0
31	c	613	CLA	8	0
34	3	321	LMG	13	0
43	d	406	BCR	5	0
31	s	314	CLA	4	0
31	C	604	CLA	6	0
32	p	616	LUT	15	0
31	N	312	CLA	5	0
31	c	609	CLA	2	0
38	g	301	SQD	12	0
38	r	322	SQD	4	0
31	G	603	CLA	10	0
31	p	603	CLA	5	0
38	M	102	SQD	3	0
31	3	314	CLA	13	0
31	r	304	CLA	3	0
38	G	617	SQD	9	0
31	2	603	CLA	10	0
43	D	405	BCR	13	0
30	7	310	CHL	6	0
30	2	608	CHL	10	0
31	B	611	CLA	11	0
34	9	301	LMG	14	0
34	D	411	LMG	1	0
31	N	311	CLA	4	0
31	7	305	CLA	13	0
31	Y	310	CLA	13	0
37	r	318	XAT	4	0
31	n	305	CLA	14	0
35	g	315	RRX	3	0
31	B	604	CLA	8	0
31	S	316	CLA	4	0
31	c	610	CLA	6	0
31	p	615	CLA	9	0
33	D	408	LHG	8	0
30	7	302	CHL	4	0
32	S	318	LUT	8	0
31	5	613	CLA	10	0
30	R	309	CHL	9	0
30	0	607	CHL	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	r	312	CLA	5	0
30	5	608	CHL	11	0
34	c	620	LMG	9	0
34	d	410	LMG	5	0
31	6	311	CLA	15	0
34	W	203	LMG	1	0
44	A	416	PL9	5	0
30	6	307	CHL	12	0
30	n	309	CHL	3	0
31	s	310	CLA	3	0
33	8	618	LHG	4	0
34	w	203	LMG	1	0
31	S	304	CLA	4	0
31	n	314	CLA	14	0
31	Y	305	CLA	5	0
31	1	603	CLA	9	0
34	Y	319	LMG	5	0
34	9	302	LMG	11	0
30	3	309	CHL	13	0
31	4	603	CLA	10	0
43	B	617	BCR	7	0
30	0	605	CHL	7	0
31	C	603	CLA	3	0
36	p	618	NEX	2	0
30	s	302	CHL	1	0
31	r	306	CLA	5	0
30	1	606	CHL	13	0
30	7	321	CHL	17	0
34	Q1	101	LMG	14	0
38	6	301	SQD	4	0
31	S	303	CLA	9	0
31	Y	314	CLA	3	0
31	q	313	CLA	8	0
31	5	614	CLA	6	0
31	q	306	CLA	8	0
34	g	320	LMG	4	0
37	2	619	XAT	11	0
31	c	612	CLA	8	0
33	K	102	LHG	6	0
31	1	612	CLA	12	0
30	Y	309	CHL	11	0
34	N	320	LMG	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	b	614	CLA	13	0
34	B	621	LMG	8	0
43	z	101	BCR	4	0
30	R	310	CHL	2	0
30	6	308	CHL	11	0
32	S	317	LUT	9	0
31	R	307	CLA	2	0
32	y	616	LUT	11	0
34	6	323	LMG	2	0
36	Y	317	NEX	2	0
30	3	310	CHL	7	0
31	G	613	CLA	1	0
34	b	622	LMG	8	0
31	N	304	CLA	10	0
34	0	622	LMG	5	0
33	d	408	LHG	13	0
43	c	614	BCR	6	0
37	q	321	XAT	16	0
33	N	319	LHG	3	0
31	2	604	CLA	6	0
43	Z	101	BCR	3	0
34	C	621	LMG	9	0
34	x	202	LMG	5	0
31	p	611	CLA	8	0
43	C	615	BCR	3	0
32	4	616	LUT	11	0
42	A	408	PHO	7	0
30	9	308	CHL	9	0
31	b	615	CLA	6	0
31	5	602	CLA	9	0
43	C	614	BCR	3	0
45	c	619	DGD	26	0
31	b	613	CLA	9	0
30	N	307	CHL	13	0
31	b	611	CLA	10	0
34	p	620	LMG	5	0
30	Y	307	CHL	8	0
42	d	402	PHO	5	0
31	B	602	CLA	4	0
31	8	614	CLA	12	0
36	R	319	NEX	8	0
34	a	401	LMG	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	N	315	CLA	9	0
30	R	308	CHL	5	0
31	c	608	CLA	9	0
34	n	322	LMG	14	0
31	8	611	CLA	4	0
31	g	314	CLA	4	0
33	t	102	LHG	1	0
32	N	317	LUT	8	0
32	6	318	LUT	10	0
33	y	619	LHG	11	0
31	0	615	CLA	5	0
37	G	620	XAT	22	0
30	s	309	CHL	3	0
30	p	606	CHL	8	0
36	y	618	NEX	5	0
34	w	204	LMG	1	0
31	6	315	CLA	10	0
30	G	607	CHL	3	0
30	g	302	CHL	7	0
34	n	321	LMG	6	0
36	g	317	NEX	2	0
30	q	307	CHL	9	0
31	A	405	CLA	7	0
31	5	610	CLA	27	0
30	7	309	CHL	3	0
33	S	320	LHG	6	0
31	5	603	CLA	12	0
35	q	317	RRX	20	0
30	p	609	CHL	7	0
33	C	623	LHG	7	0
30	n	310	CHL	9	0
31	G	610	CLA	8	0
30	7	307	CHL	10	0
34	2	618	LMG	7	0
31	b	609	CLA	7	0
30	Y	308	CHL	5	0
34	2	621	LMG	5	0
33	6	320	LHG	2	0
30	8	606	CHL	9	0
31	C	611	CLA	5	0
31	B	601	CLA	2	0
32	Y	315	LUT	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	G	618	LHG	15	0
31	2	610	CLA	7	0
34	J	102	LMG	1	0
34	a	413	LMG	4	0
32	3	318	LUT	13	0
30	p	605	CHL	7	0
32	7	318	LUT	5	0
31	q	305	CLA	7	0
33	3	320	LHG	7	0
31	g	310	CLA	5	0
31	c	605	CLA	6	0
30	N	309	CHL	14	0
30	9	310	CHL	11	0
38	X	201	SQD	1	0
31	2	609	CLA	16	0
38	b	627	SQD	9	0
31	6	313	CLA	3	0
33	A	417	LHG	4	0
30	3	307	CHL	16	0
34	6	321	LMG	10	0
30	6	306	CHL	6	0
30	s	307	CHL	9	0
31	3	316	CLA	10	0
30	S	309	CHL	3	0
31	2	602	CLA	8	0
33	1	617	LHG	5	0
31	s	313	CLA	9	0
33	S	322	LHG	5	0
31	C	606	CLA	8	0
34	c	624	LMG	7	0
30	4	607	CHL	18	0
30	8	601	CHL	10	0
31	c	602	CLA	6	0
43	B	618	BCR	5	0
31	8	603	CLA	12	0
31	b	610	CLA	10	0
31	6	316	CLA	4	0
33	7	319	LHG	3	0
31	G	602	CLA	5	0
34	k	101	LMG	3	0
38	s	301	SQD	6	0
33	2	617	LHG	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	R	317	LUT	3	0
31	3	315	CLA	7	0
33	r	320	LHG	3	0
31	0	613	CLA	2	0
31	5	604	CLA	4	0
31	C	605	CLA	6	0
31	Y	304	CLA	15	0
30	p	601	CHL	2	0
31	R	304	CLA	7	0
32	3	317	LUT	11	0
34	r	321	LMG	5	0
31	p	610	CLA	19	0
30	y	606	CHL	10	0
31	0	611	CLA	5	0
34	q	302	LMG	6	0
31	6	304	CLA	7	0
36	s	319	NEX	4	0
37	4	619	XAT	9	0
31	R	313	CLA	2	0
31	p	612	CLA	8	0
31	9	314	CLA	9	0
31	y	614	CLA	5	0
33	q	320	LHG	12	0
30	3	302	CHL	15	0
33	B	624	LHG	6	0
33	5	619	LHG	9	0
31	8	610	CLA	3	0
30	4	601	CHL	6	0
32	G	615	LUT	8	0
30	N	301	CHL	10	0
33	L	101	LHG	4	0
34	B	622	LMG	3	0
34	s	321	LMG	4	0
32	r	317	LUT	4	0
31	b	606	CLA	5	0
37	R	318	XAT	7	0
31	R	312	CLA	5	0
30	S	308	CHL	5	0
31	b	607	CLA	3	0
31	g	305	CLA	7	0
34	f	101	LMG	1	0
31	b	616	CLA	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	E	101	HEM	10	0
31	4	613	CLA	5	0
31	7	303	CLA	3	0
31	8	612	CLA	13	0
31	9	305	CLA	9	0
34	7	322	LMG	4	0
44	D	406	PL9	7	0
33	b	625	LHG	8	0
33	0	619	LHG	3	0
31	b	608	CLA	7	0
31	r	316	CLA	4	0
36	S	319	NEX	4	0
30	G	605	CHL	7	0
34	C	622	LMG	2	0
31	R	316	CLA	6	0
32	q	318	LUT	12	0
31	y	611	CLA	7	0
31	4	604	CLA	16	0
31	d	405	CLA	6	0
36	0	618	NEX	10	0
36	r	301	NEX	6	0
30	g	309	CHL	5	0
31	b	603	CLA	7	0
31	S	314	CLA	4	0
30	9	309	CHL	13	0
45	C	618	DGD	6	0
31	C	601	CLA	4	0
32	5	616	LUT	23	0
34	G	621	LMG	10	0
33	c	622	LHG	8	0
30	9	307	CHL	6	0
31	c	607	CLA	5	0
33	e	101	LHG	7	0
30	p	608	CHL	10	0
34	A	414	LMG	2	0
31	Y	312	CLA	8	0
31	C	612	CLA	5	0
31	s	303	CLA	12	0
38	A	411	SQD	1	0
34	b	626	LMG	2	0
31	6	312	CLA	4	0
43	b	620	BCR	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	w	205	LMG	6	0
33	4	618	LHG	5	0
30	2	601	CHL	5	0
31	4	612	CLA	5	0
33	Y	318	LHG	4	0
34	W	202	LMG	1	0
34	4	620	LMG	13	0
38	Y	320	SQD	5	0
31	G	609	CLA	10	0
34	7	301	LMG	6	0
30	7	308	CHL	11	0
31	B	607	CLA	5	0
30	y	601	CHL	8	0
31	B	612	CLA	9	0
30	q	310	CHL	14	0
34	S	321	LMG	2	0
34	G	622	LMG	12	0
31	G	604	CLA	7	0
31	7	315	CLA	3	0
31	q	315	CLA	7	0
31	3	311	CLA	8	0
31	y	615	CLA	11	0
31	S	310	CLA	2	0
30	5	605	CHL	11	0
32	n	318	LUT	8	0
31	4	610	CLA	18	0
43	t	101	BCR	13	0
33	a	415	LHG	4	0
33	g	319	LHG	12	0
33	b	628	LHG	13	0
36	r	319	NEX	3	0
32	1	616	LUT	3	0
31	N	313	CLA	15	0
31	R	305	CLA	7	0
33	l	101	LHG	11	0
30	s	308	CHL	8	0
36	5	618	NEX	16	0
32	0	617	LUT	6	0
31	B	606	CLA	6	0
31	r	303	CLA	3	0
34	W	201	LMG	13	0
30	8	608	CHL	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	a	411	SQD	4	0
31	7	316	CLA	11	0
34	q1	101	LMG	11	0
43	T	101	BCR	6	0
36	4	617	NEX	8	0
31	p	614	CLA	11	0
31	c	611	CLA	5	0
33	M	101	LHG	1	0
31	4	611	CLA	4	0
32	y	617	LUT	5	0
31	q	304	CLA	7	0
30	0	606	CHL	5	0
31	R	303	CLA	1	0
31	N	314	CLA	17	0
30	n	307	CHL	8	0
34	1	618	LMG	2	0
31	0	614	CLA	7	0
31	3	312	CLA	4	0
30	2	605	CHL	9	0
38	x	201	SQD	3	0
36	N	318	NEX	7	0
31	R	306	CLA	9	0
36	9	319	NEX	9	0
30	y	608	CHL	4	0
30	1	601	CHL	7	0
30	1	619	CHL	8	0
30	q	303	CHL	8	0
32	7	317	LUT	11	0
31	g	303	CLA	4	0
35	2	614	RRX	12	0
30	q	311	CHL	6	0
31	a	406	CLA	3	0
31	s	316	CLA	5	0
30	9	303	CHL	8	0
31	y	603	CLA	9	0
32	8	615	LUT	9	0
31	3	301	CLA	10	0
31	6	314	CLA	9	0
30	1	607	CHL	12	0
31	S	313	CLA	9	0
31	c	606	CLA	14	0
42	D	401	PHO	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	6	317	LUT	9	0
30	r	310	CHL	3	0
45	C	620	DGD	21	0
30	2	607	CHL	10	0
30	6	309	CHL	8	0
43	h	101	BCR	4	0
30	1	605	CHL	6	0
32	s	318	LUT	12	0
30	4	605	CHL	12	0
30	0	609	CHL	7	0
31	S	305	CLA	10	0
34	j	101	LMG	4	0
31	3	304	CLA	5	0
34	5	620	LMG	11	0
31	p	604	CLA	4	0
32	g	316	LUT	8	0
34	D	409	LMG	8	0
31	B	614	CLA	6	0
31	7	304	CLA	10	0
30	Y	306	CHL	2	0
36	3	319	NEX	10	0
32	N	316	LUT	14	0
31	7	313	CLA	3	0
43	H	101	BCR	4	0
31	B	615	CLA	6	0
30	5	607	CHL	11	0
37	g	321	XAT	20	0
31	0	604	CLA	2	0
34	c	621	LMG	1	0
30	3	303	CHL	8	0
31	1	610	CLA	15	0
30	4	609	CHL	9	0
33	s	322	LHG	6	0
31	p	613	CLA	25	0
31	d	404	CLA	6	0
34	J	101	LMG	4	0
30	5	606	CHL	12	0
34	4	621	LMG	12	0
31	g	311	CLA	5	0
31	C	609	CLA	2	0
43	c	615	BCR	9	0
30	g	308	CHL	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	a	409	CLA	14	0
30	6	310	CHL	7	0
30	1	608	CHL	3	0
31	7	312	CLA	7	0
37	9	322	XAT	3	0
32	8	616	LUT	9	0
45	C	617	DGD	9	0
48	r	302	LMU	11	0
31	s	304	CLA	4	0
33	R	320	LHG	1	0
32	s	317	LUT	12	0
30	p	607	CHL	13	0
31	R	311	CLA	5	0
38	B	623	SQD	7	0
30	0	601	CHL	4	0
34	A	412	LMG	4	0
30	7	306	CHL	5	0
31	8	613	CLA	15	0
34	d	409	LMG	4	0
30	6	302	CHL	6	0
38	R	322	SQD	6	0
43	a	410	BCR	4	0
33	n	320	LHG	3	0
31	r	315	CLA	7	0
31	G	611	CLA	3	0
31	1	611	CLA	14	0
30	n	308	CHL	15	0
30	N	308	CHL	4	0
31	2	613	CLA	7	0
34	I	101	LMG	5	0
31	N	310	CLA	16	0
31	c	604	CLA	2	0
31	N	321	CLA	14	0
31	A	406	CLA	8	0
31	8	604	CLA	9	0
34	D	412	LMG	2	0
30	8	607	CHL	3	0
31	n	311	CLA	14	0
31	r	305	CLA	8	0
31	s	312	CLA	6	0
30	G	623	CHL	14	0
36	2	616	NEX	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	R	315	CLA	2	0
43	b	618	BCR	11	0
47	e	102	HEM	11	0
31	A	409	CLA	7	0
31	c	601	CLA	4	0
30	y	609	CHL	11	0
31	n	315	CLA	16	0
31	b	612	CLA	14	0
30	r	309	CHL	9	0
34	a	416	LMG	3	0
30	5	609	CHL	9	0
32	n	317	LUT	10	0
31	Y	311	CLA	8	0
31	C	613	CLA	7	0
31	s	306	CLA	11	0
33	D	407	LHG	4	0
30	4	608	CHL	9	0
31	S	306	CLA	14	0
31	N	305	CLA	13	0
30	n	302	CHL	8	0
31	S	315	CLA	5	0
31	r	314	CLA	1	0
48	R	302	LMU	8	0
38	0	621	SQD	2	0
30	2	606	CHL	11	0
31	y	602	CLA	1	0
34	g	322	LMG	6	0
38	S	301	SQD	4	0
31	n	316	CLA	11	0
36	R	301	NEX	7	0
31	5	611	CLA	8	0
31	C	610	CLA	5	0
31	y	612	CLA	9	0
31	B	608	CLA	5	0
31	N	303	CLA	2	0
34	7	320	LMG	2	0
36	8	617	NEX	4	0
31	Y	313	CLA	2	0
30	n	306	CHL	10	0
35	9	317	RRX	13	0
31	a	407	CLA	3	0
32	p	617	LUT	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	p	602	CLA	9	0
31	6	305	CLA	12	0
30	S	302	CHL	3	0
31	S	312	CLA	6	0
34	m	102	LMG	5	0
30	5	601	CHL	7	0
31	y	613	CLA	8	0
30	S	307	CHL	6	0
34	G	619	LMG	3	0
35	4	615	RRX	17	0
31	B	616	CLA	9	0
32	1	615	LUT	9	0
31	5	612	CLA	6	0
31	6	303	CLA	4	0
31	9	316	CLA	1	0
31	4	602	CLA	10	0
31	5	615	CLA	10	0
34	6	322	LMG	11	0
30	G	606	CHL	10	0
31	3	305	CLA	14	0
31	C	608	CLA	9	0
30	q	308	CHL	7	0
31	g	304	CLA	4	0
31	1	614	CLA	4	0
30	y	607	CHL	12	0
31	8	602	CLA	8	0
34	d	411	LMG	2	0
31	9	304	CLA	9	0
30	1	609	CHL	6	0
31	1	613	CLA	2	0
32	9	318	LUT	15	0
48	c	623	LMU	3	0
30	0	608	CHL	7	0
31	r	307	CLA	5	0
31	c	603	CLA	5	0
34	A	418	LMG	3	0
31	0	612	CLA	3	0
33	A	415	LHG	4	0
34	k	102	LMG	2	0
48	K	101	LMU	1	0
34	X	202	LMG	5	0
34	0	620	LMG	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	s	320	LHG	5	0
36	q	319	NEX	4	0
31	s	311	CLA	8	0
30	y	605	CHL	2	0
31	g	312	CLA	6	0
31	n	304	CLA	11	0
34	q	301	LMG	4	0
30	q	309	CHL	19	0
34	C	624	LMG	6	0
31	9	312	CLA	15	0
44	d	407	PL9	9	0
30	G	601	CHL	11	0
31	s	305	CLA	9	0
31	q	314	CLA	8	0
31	C	602	CLA	4	0
31	n	313	CLA	4	0
31	0	603	CLA	5	0
36	n	319	NEX	2	0
43	B	619	BCR	8	0
31	1	602	CLA	5	0
38	y	621	SQD	3	0
31	g	313	CLA	12	0
30	g	306	CHL	7	0
31	D	403	CLA	8	0
31	9	306	CLA	10	0
31	7	314	CLA	4	0
30	N	306	CHL	10	0
31	0	610	CLA	15	0
31	n	303	CLA	8	0
32	0	616	LUT	6	0
34	B	625	LMG	5	0
38	B	620	SQD	7	0
39	A	401	OEX	1	0
45	c	616	DGD	13	0
33	z	102	LHG	3	0
31	n	312	CLA	3	0
30	r	308	CHL	6	0
31	B	609	CLA	7	0
34	2	620	LMG	2	0
44	a	414	PL9	9	0
31	9	315	CLA	8	0
36	G	616	NEX	1	0

Continued on next page...

Continued from previous page...

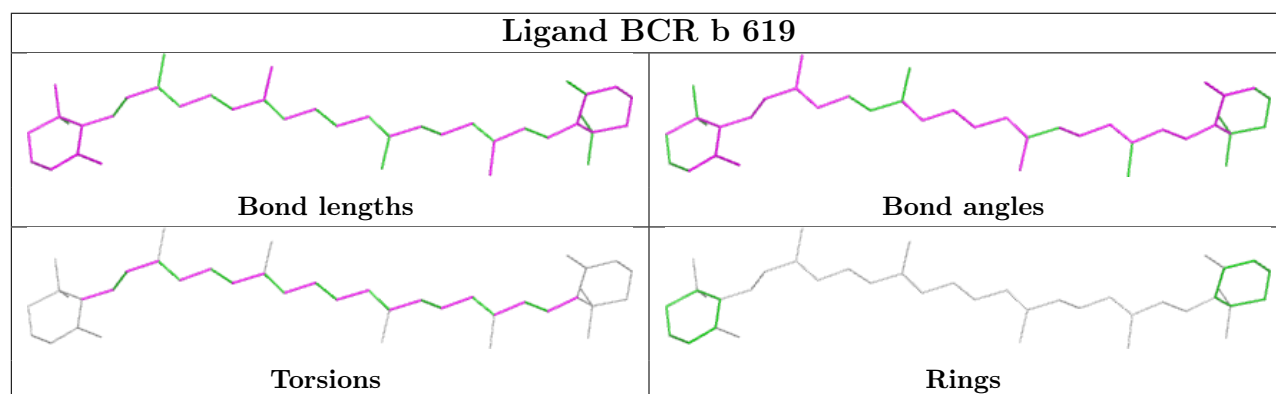
Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	D	404	CLA	8	0
30	8	605	CHL	5	0
31	B	613	CLA	10	0
38	b	621	SQD	2	0
30	n	301	CHL	8	0
31	b	617	CLA	7	0
33	j	102	LHG	5	0
31	S	311	CLA	6	0
30	N	302	CHL	3	0
34	9	321	LMG	7	0
33	p	619	LHG	3	0
34	b	624	LMG	2	0
45	c	618	DGD	5	0
31	l	604	CLA	8	0
43	v	101	BCR	3	0
30	g	307	CHL	9	0
31	b	602	CLA	3	0
42	a	408	PHO	3	0
31	B	603	CLA	3	0
34	w	202	LMG	20	0
38	m	101	SQD	2	0
31	y	604	CLA	8	0
31	Y	303	CLA	5	0
36	6	319	NEX	11	0
30	Y	301	CHL	18	0
33	F1	301	LHG	1	0
34	w	201	LMG	7	0
31	G	612	CLA	12	0
31	4	614	CLA	3	0
43	A	410	BCR	3	0
43	V	101	BCR	1	0
32	2	615	LUT	8	0
31	7	311	CLA	17	0
31	b	605	CLA	6	0
31	8	609	CLA	11	0
38	G	624	SQD	4	0
31	0	602	CLA	4	0
31	r	313	CLA	4	0
31	b	604	CLA	3	0
31	B	605	CLA	7	0
34	b	601	LMG	4	0
34	y	620	LMG	4	0

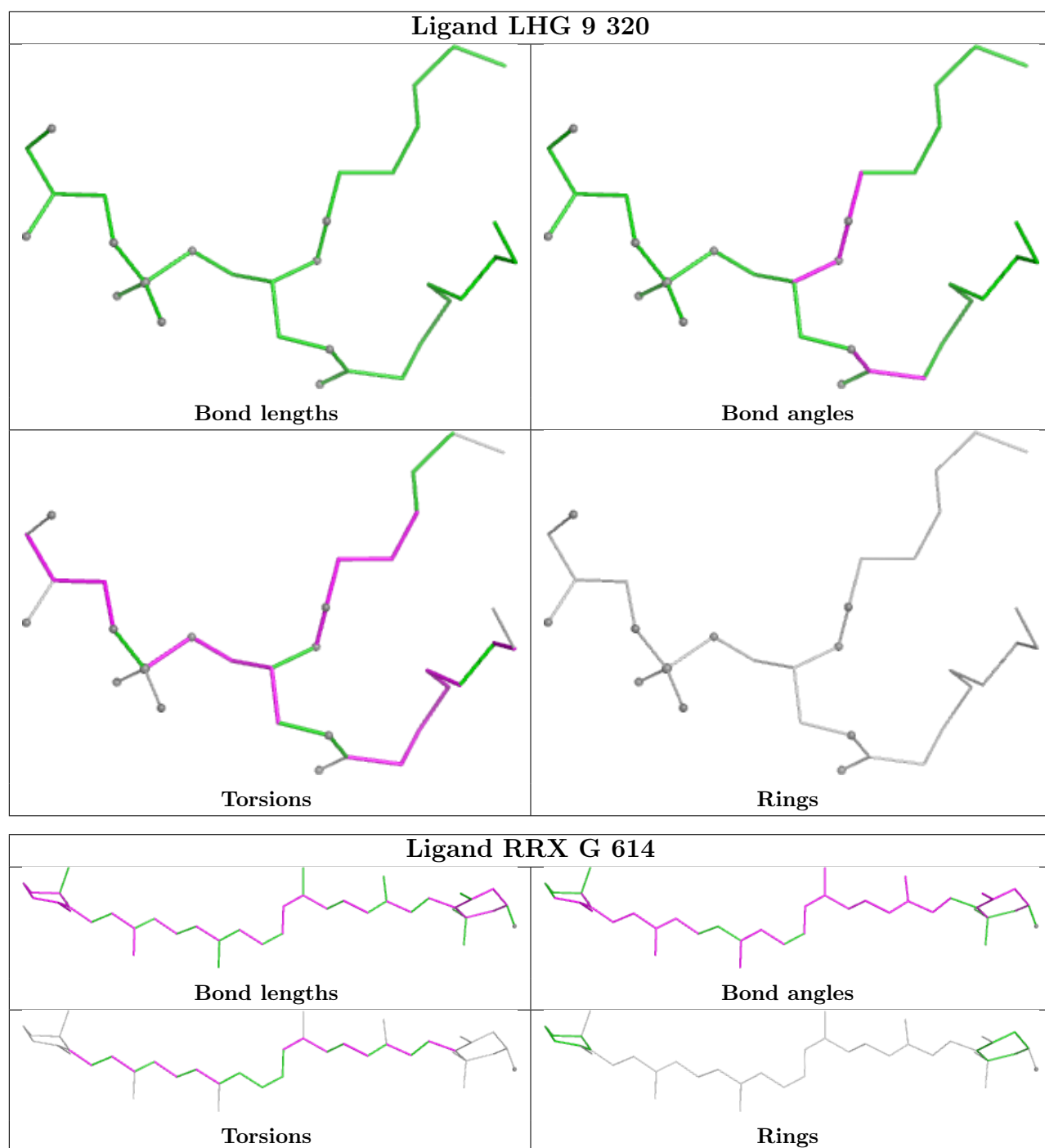
Continued on next page...

Continued from previous page...

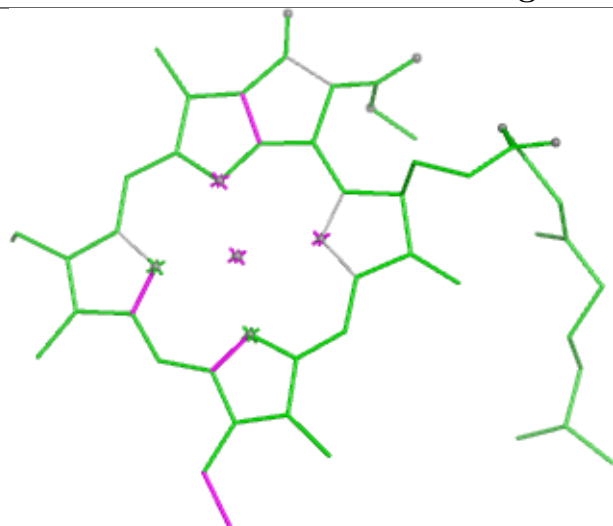
Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	q	312	CLA	22	0
45	c	617	DGD	9	0

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

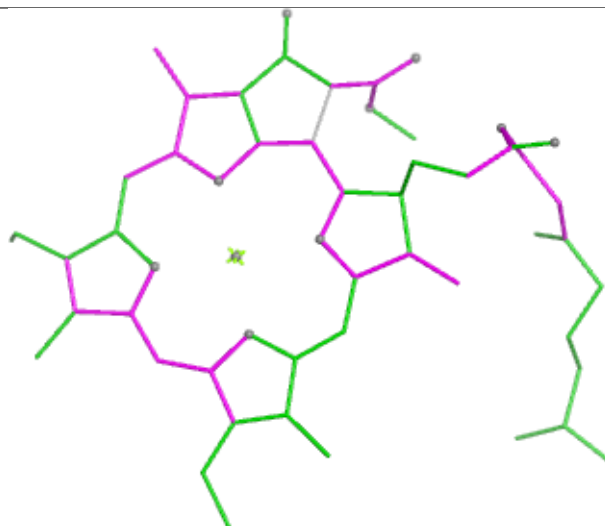




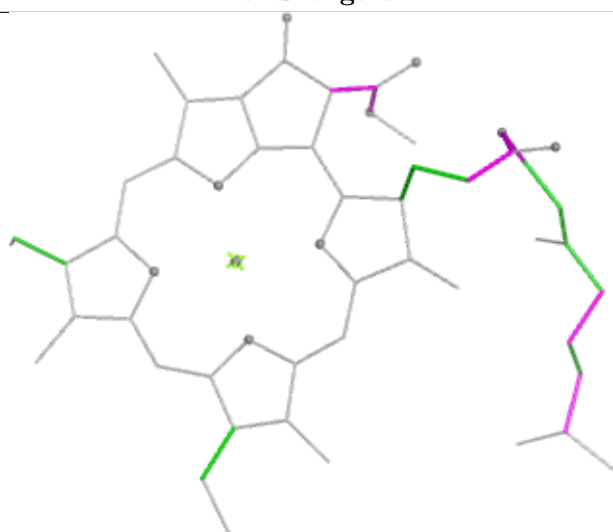
Ligand CLA 2 611



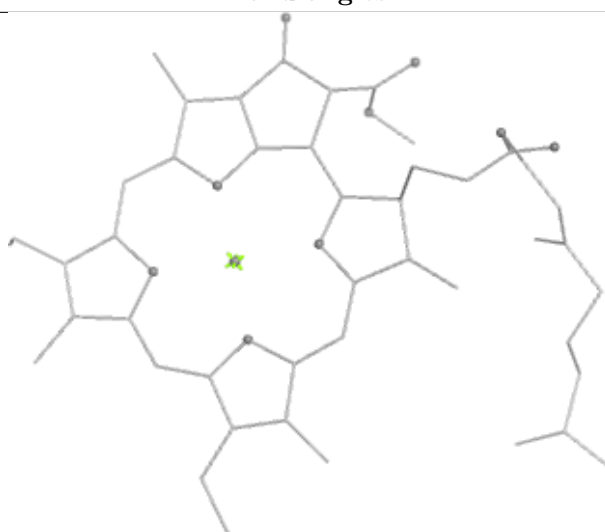
Bond lengths



Bond angles

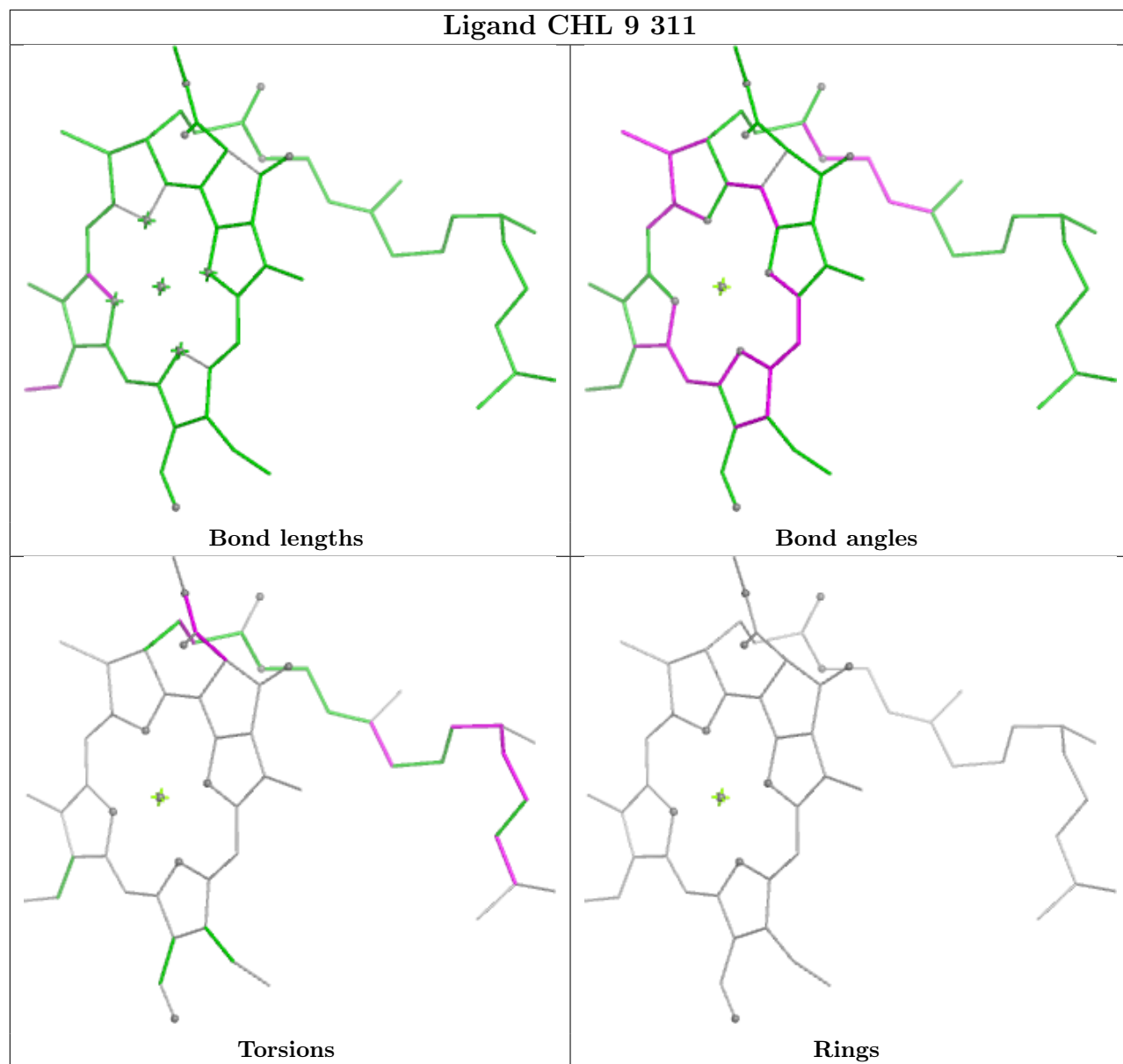


Torsions

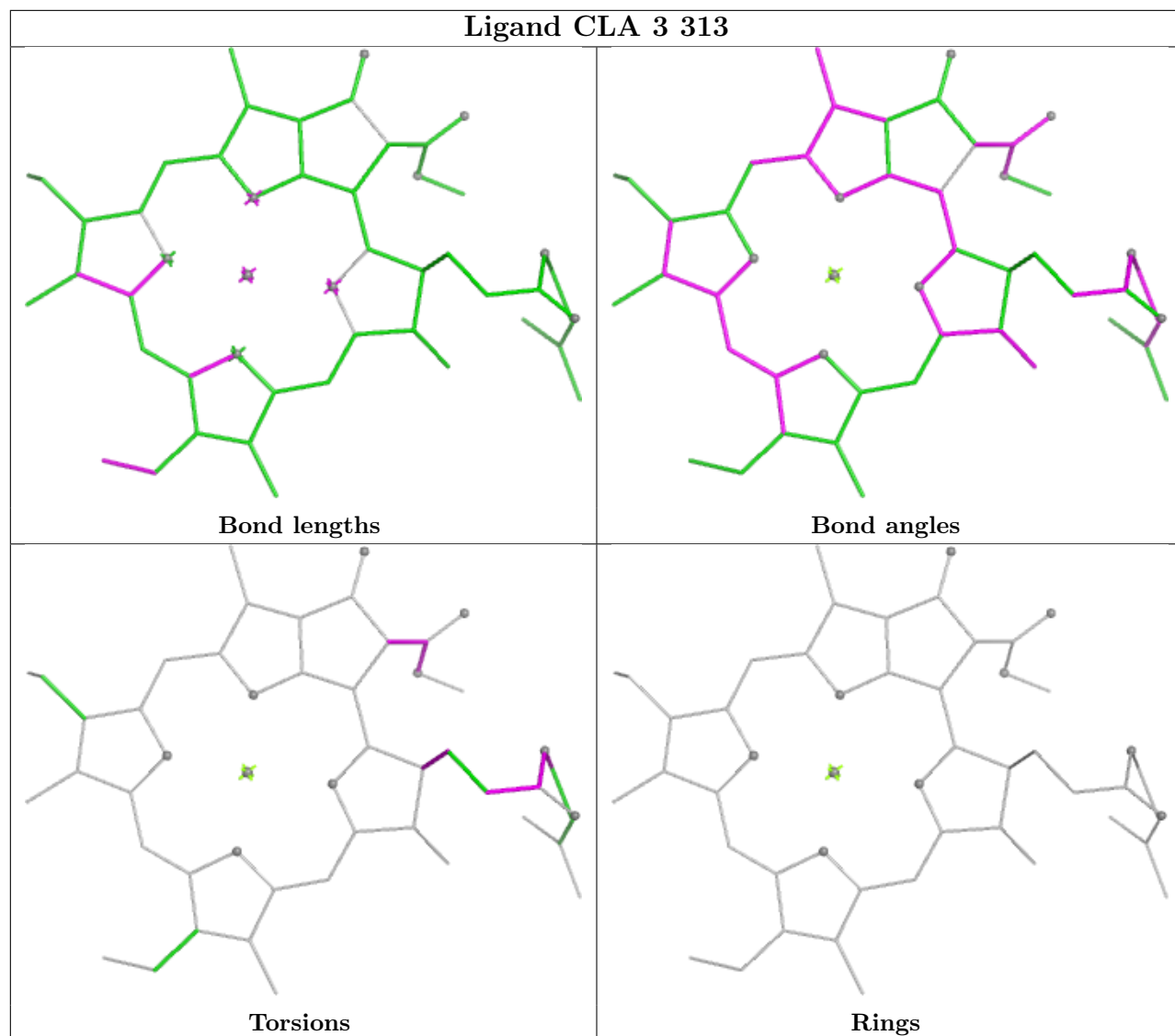


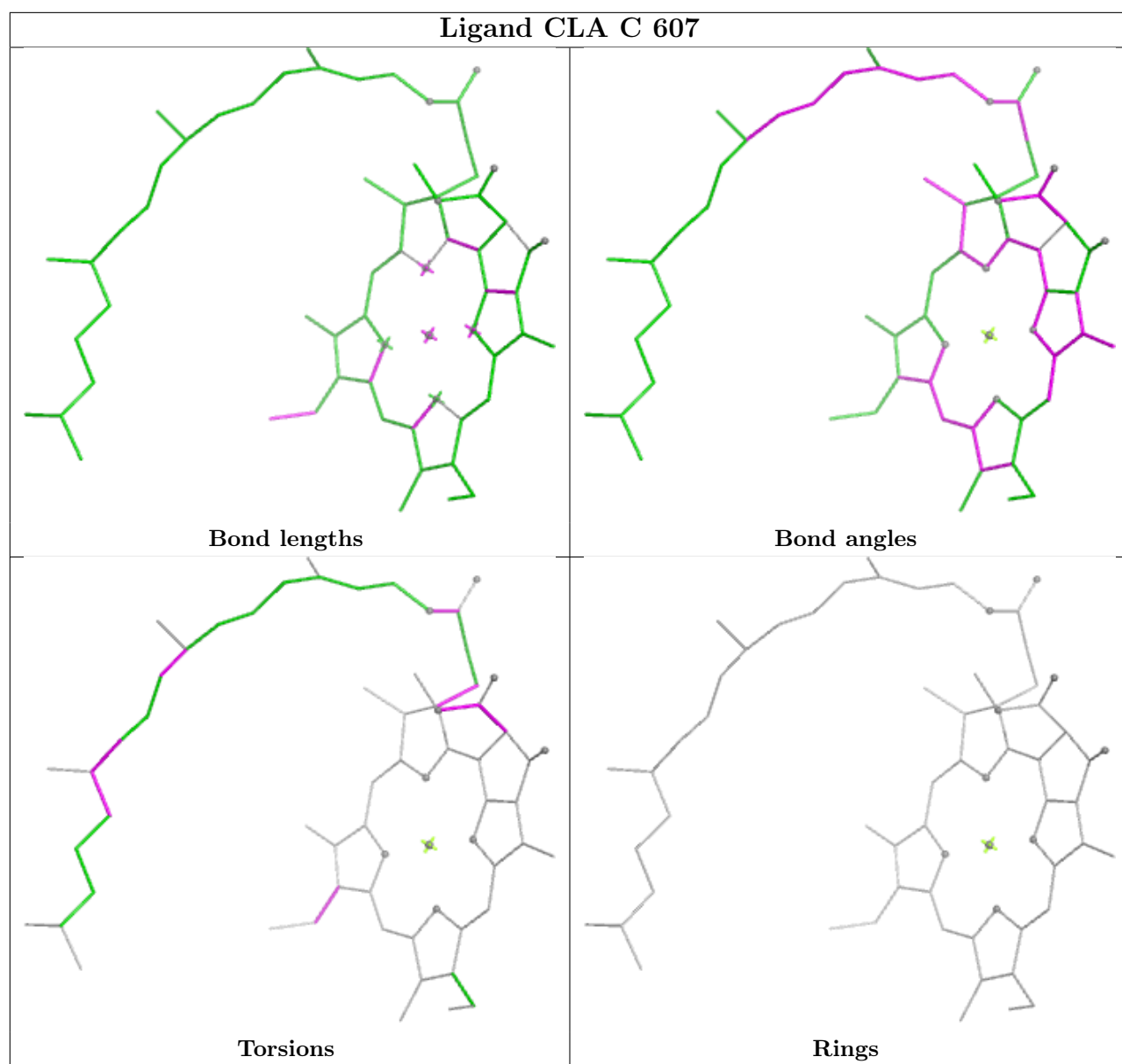
Rings

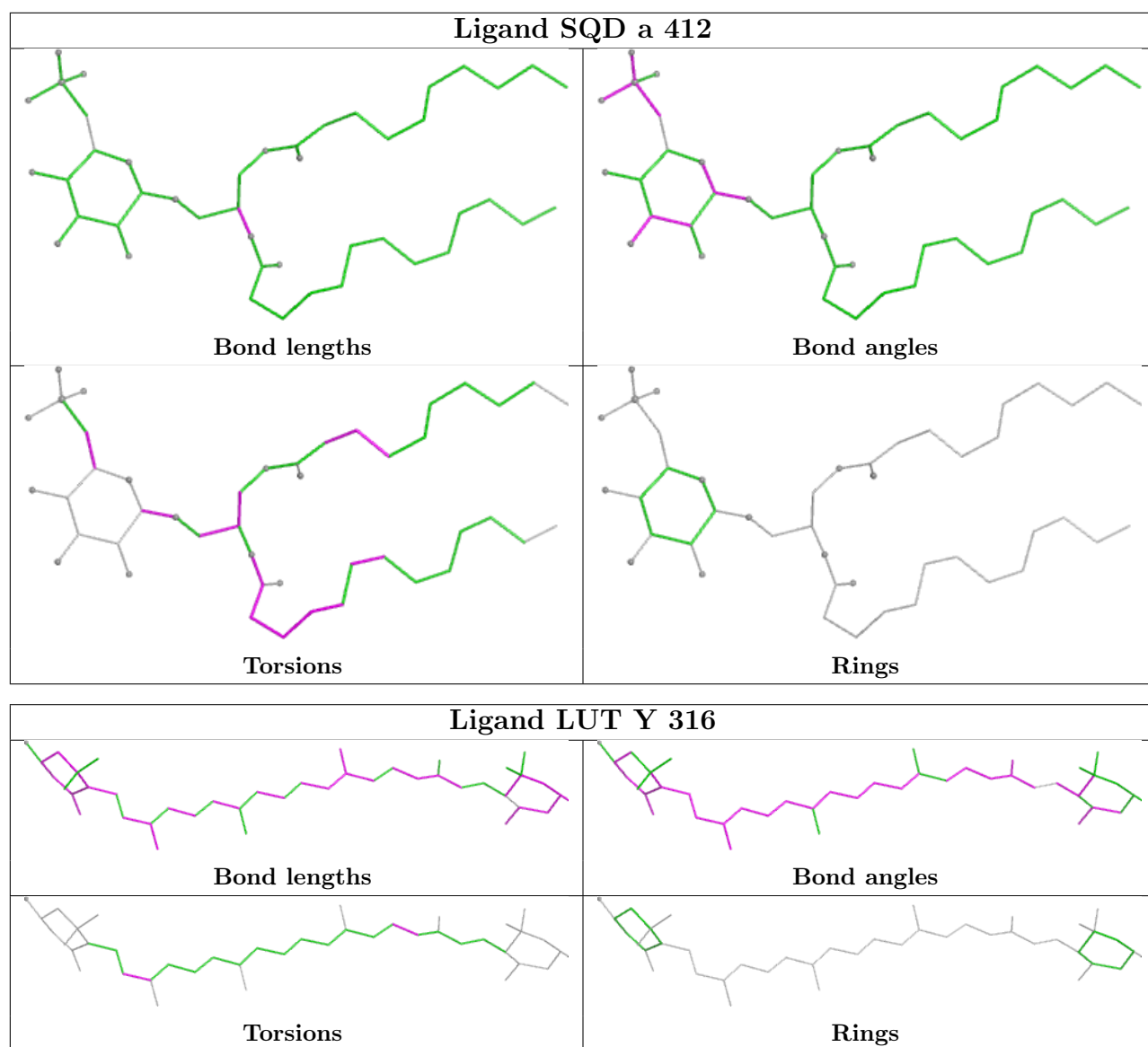
Ligand CHL 9 311

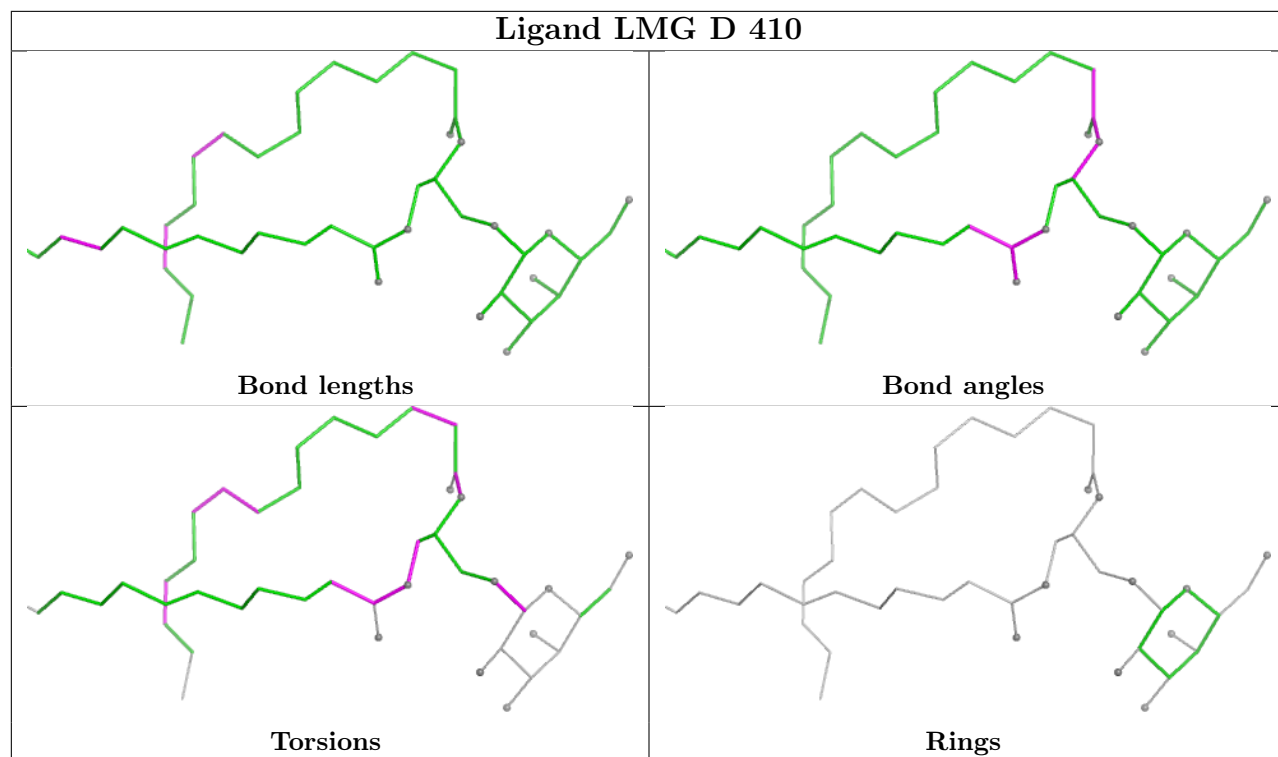


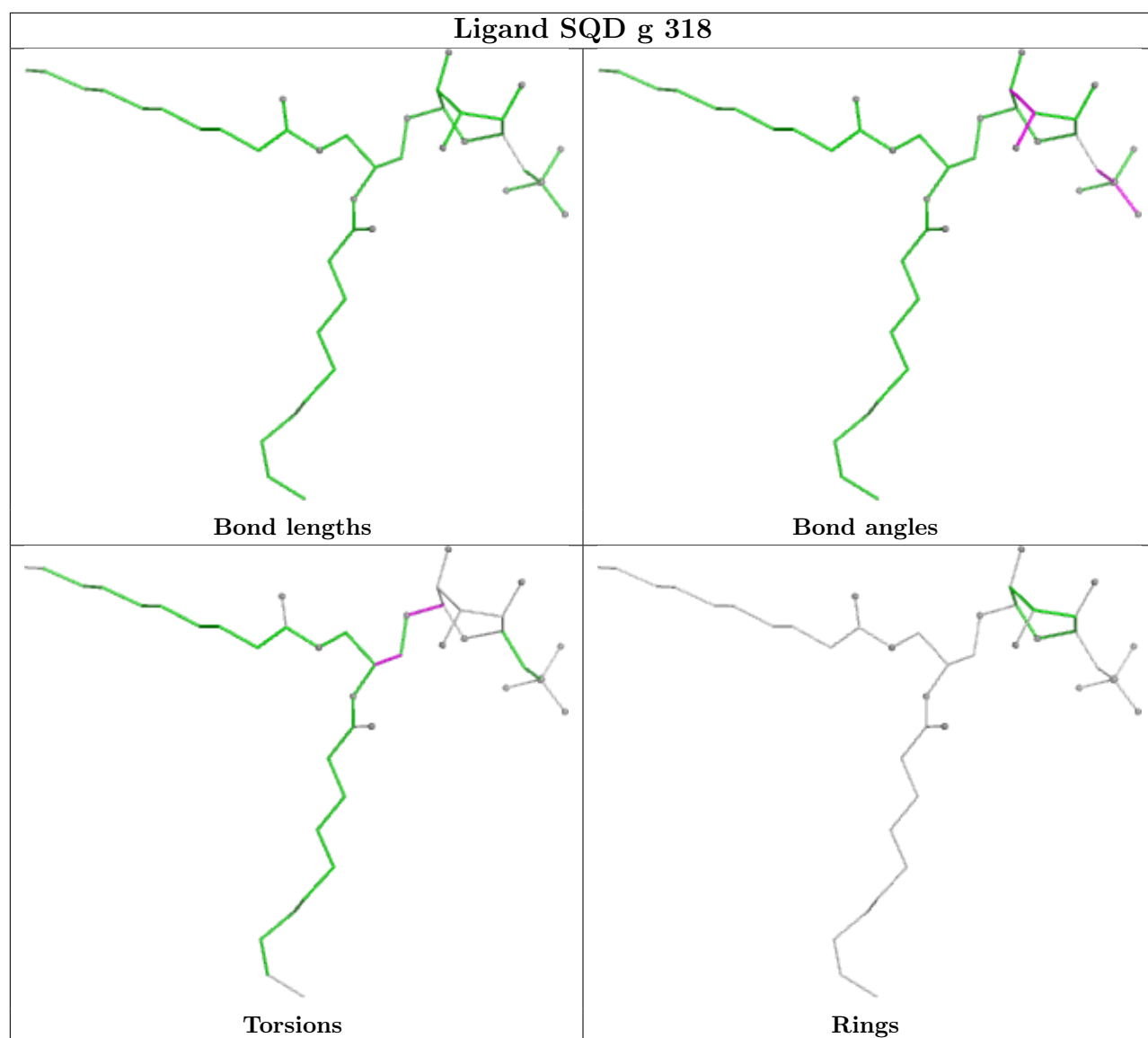
Ligand CLA 3 313



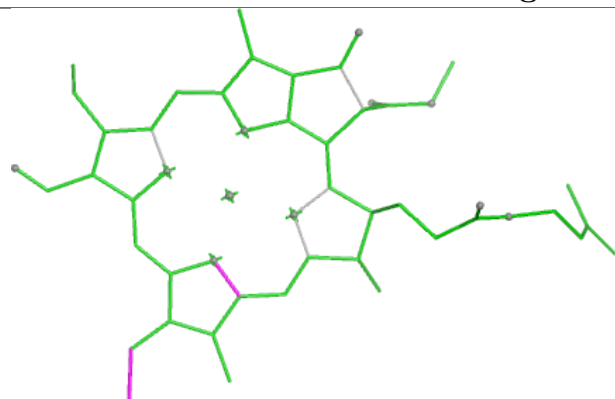




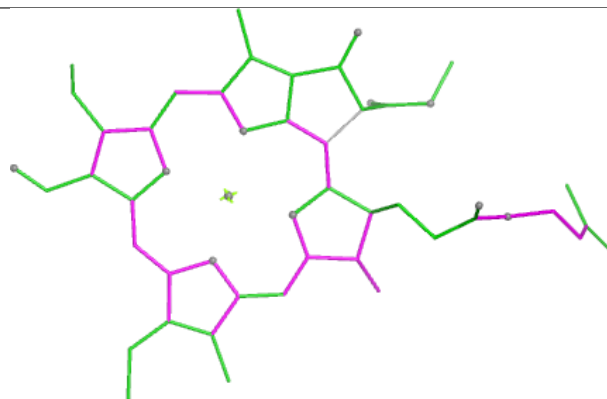




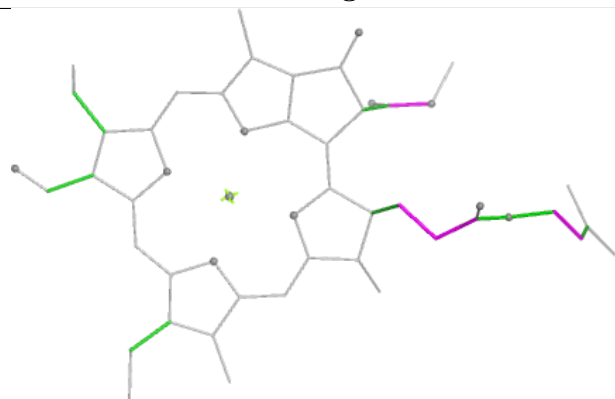
Ligand CHL 4 606



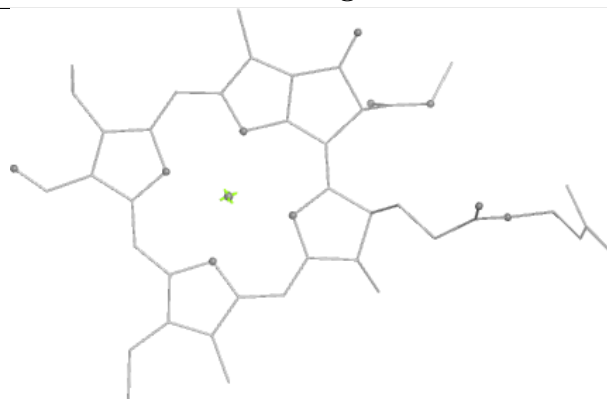
Bond lengths



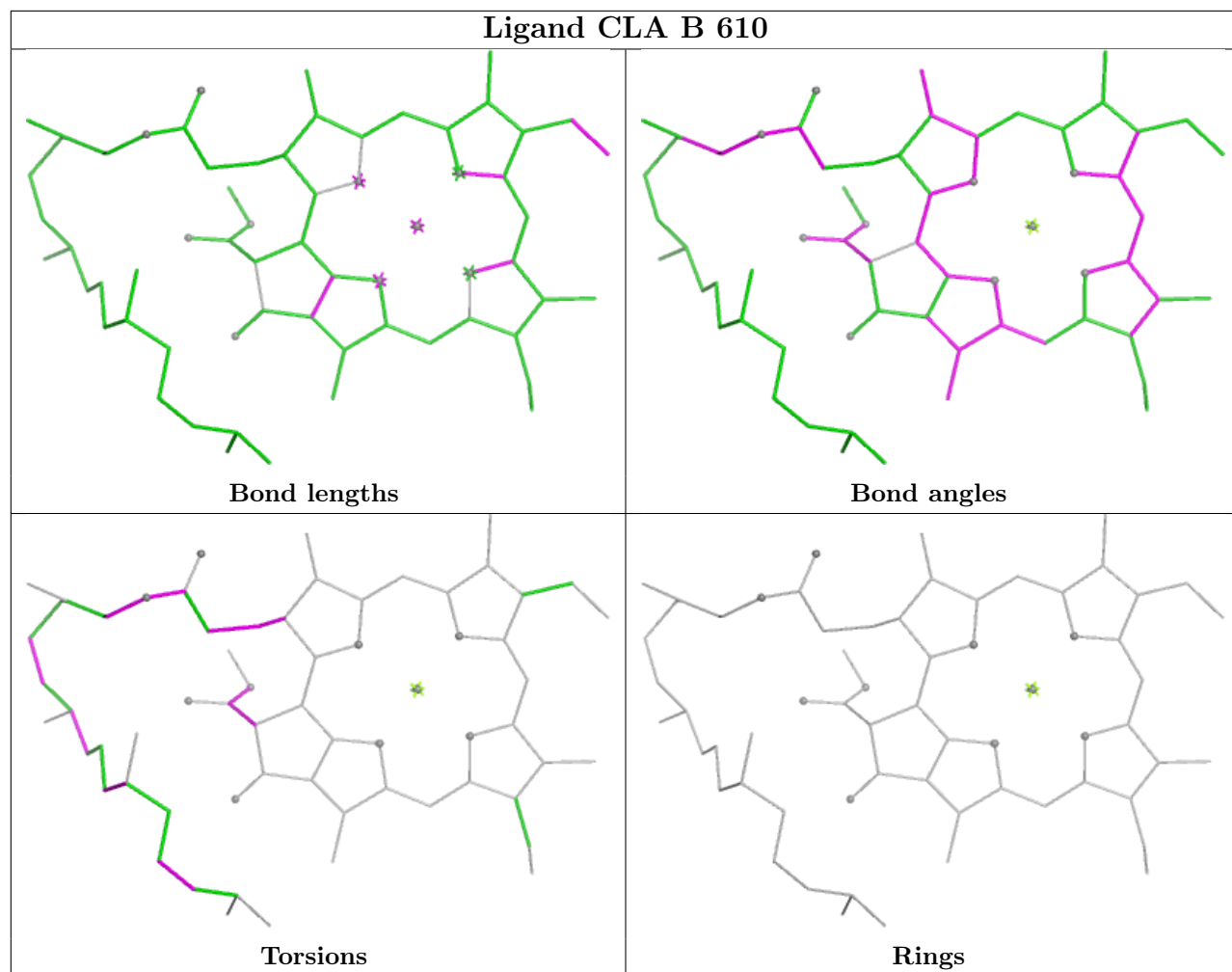
Bond angles

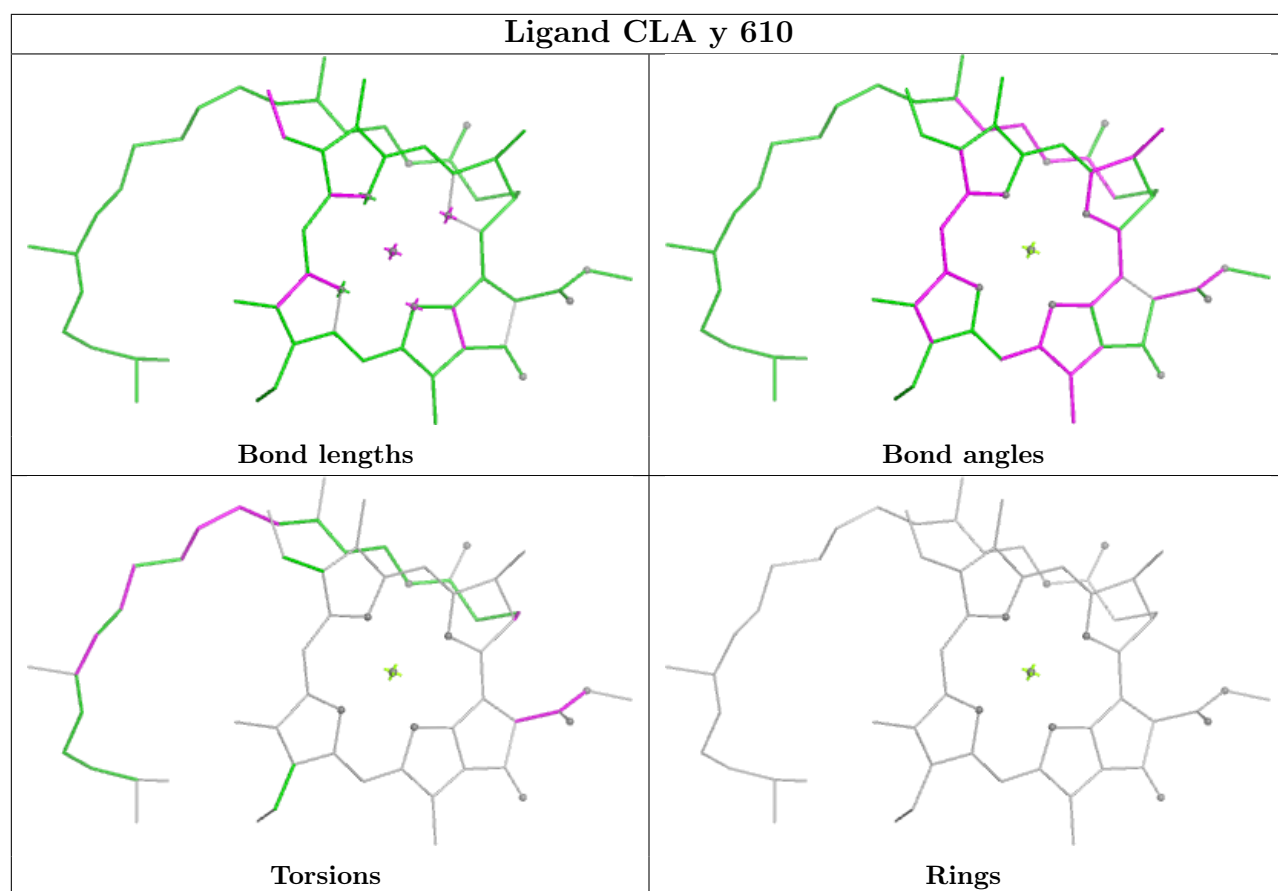


Torsions

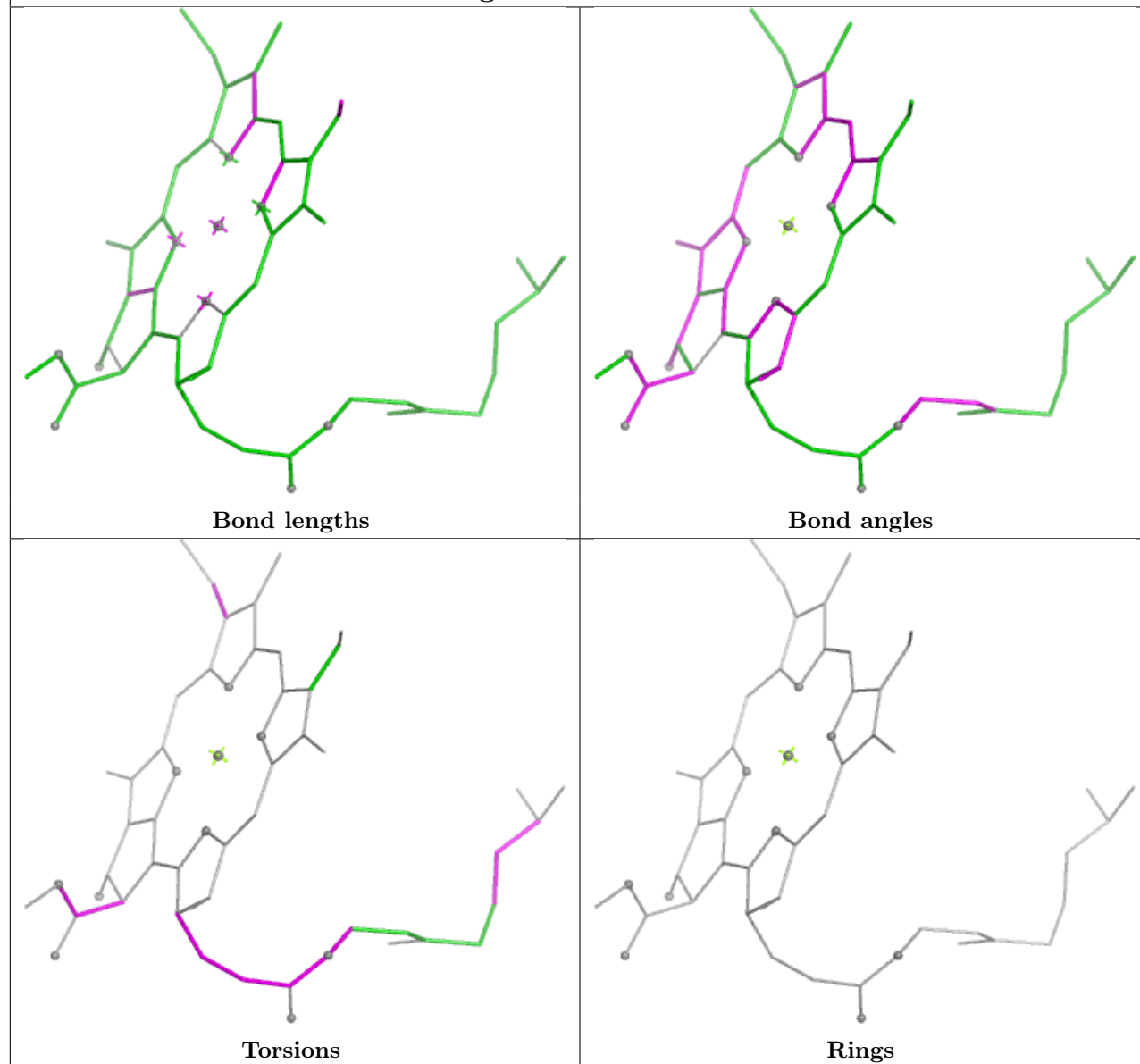


Rings





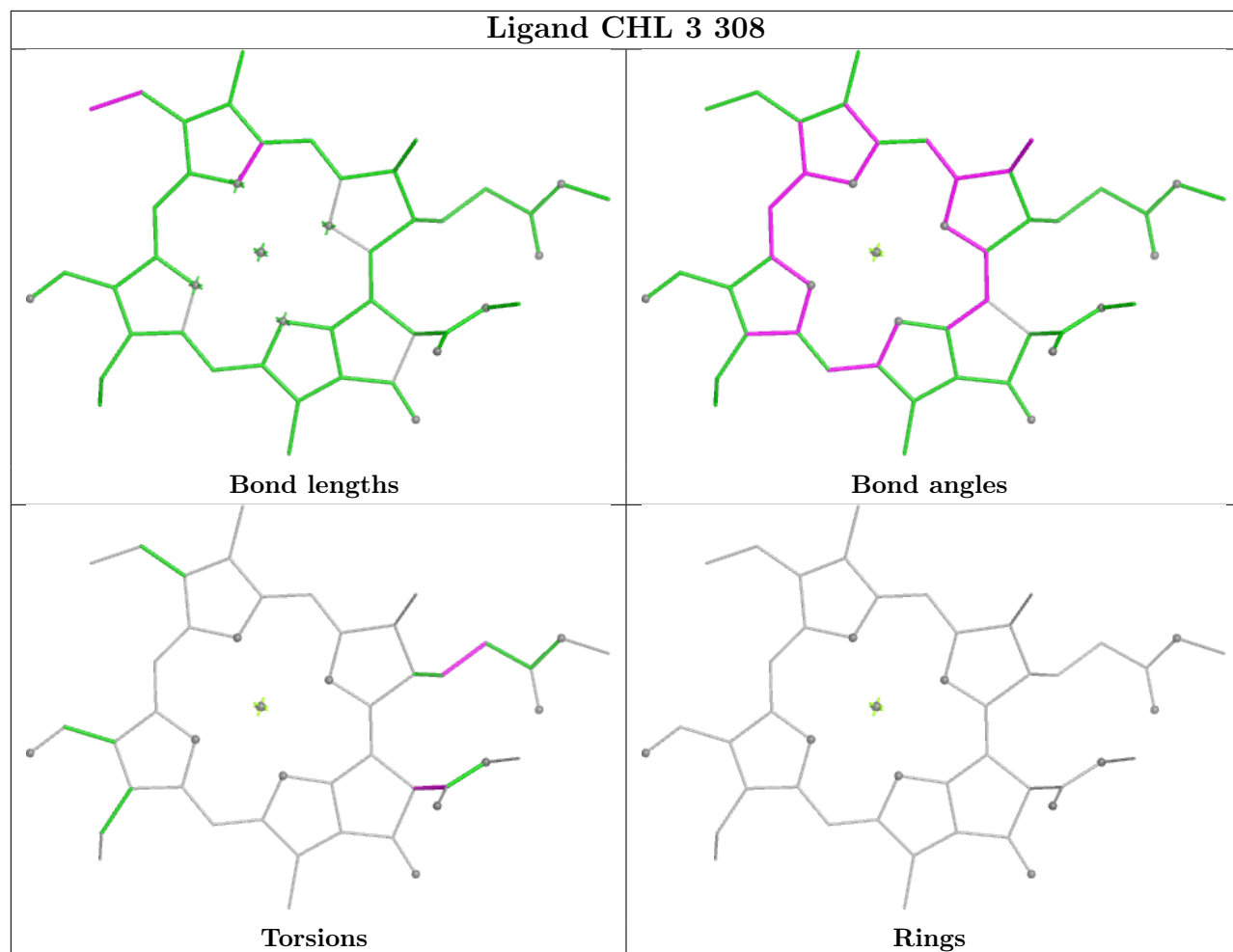
Ligand CLA 3 306



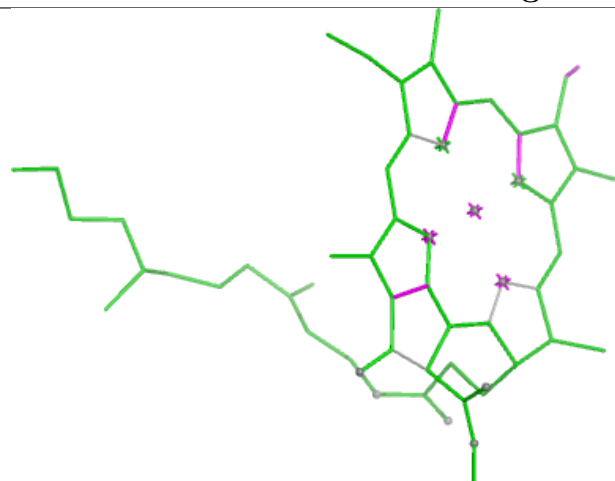
Ligand LUT 5 617



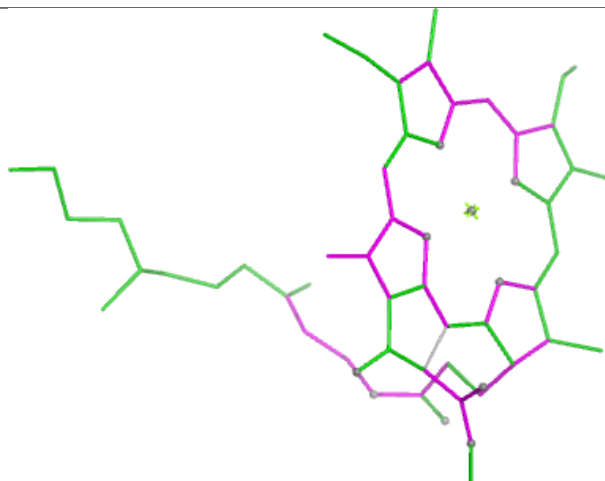
Ligand CHL 3 308



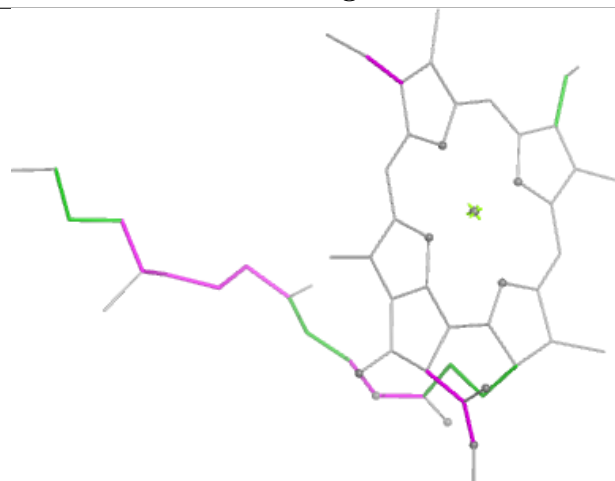
Ligand CLA r 311



Bond lengths



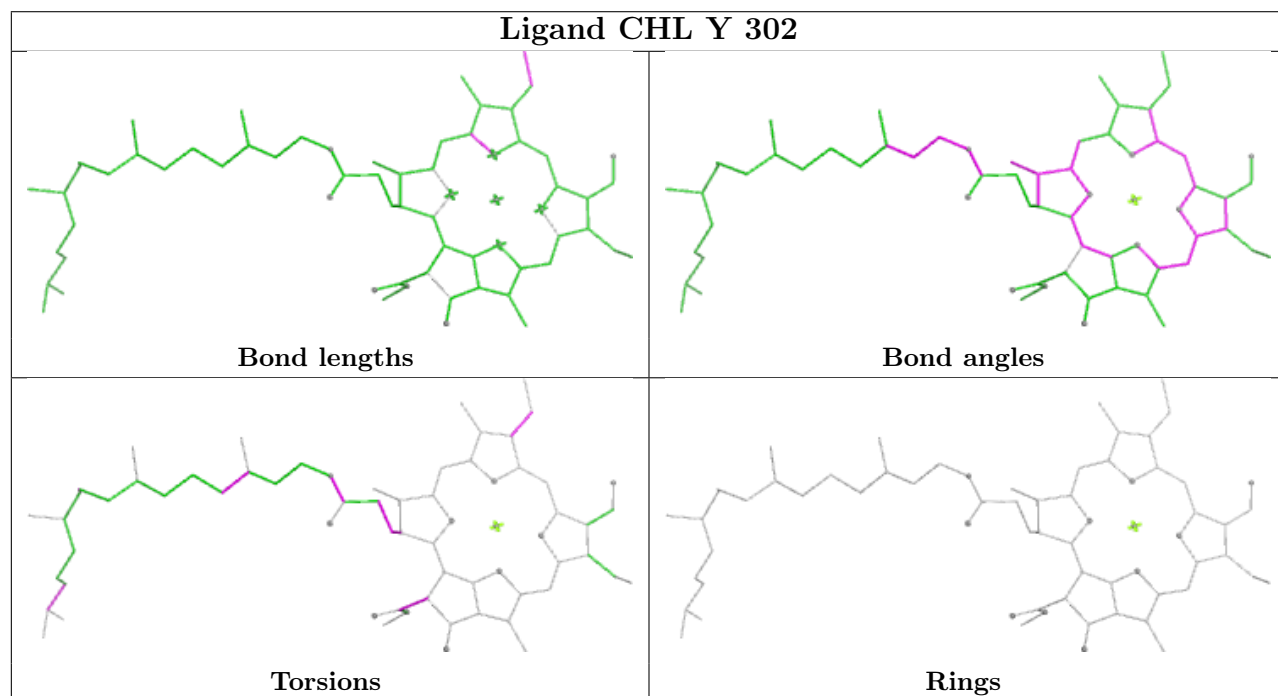
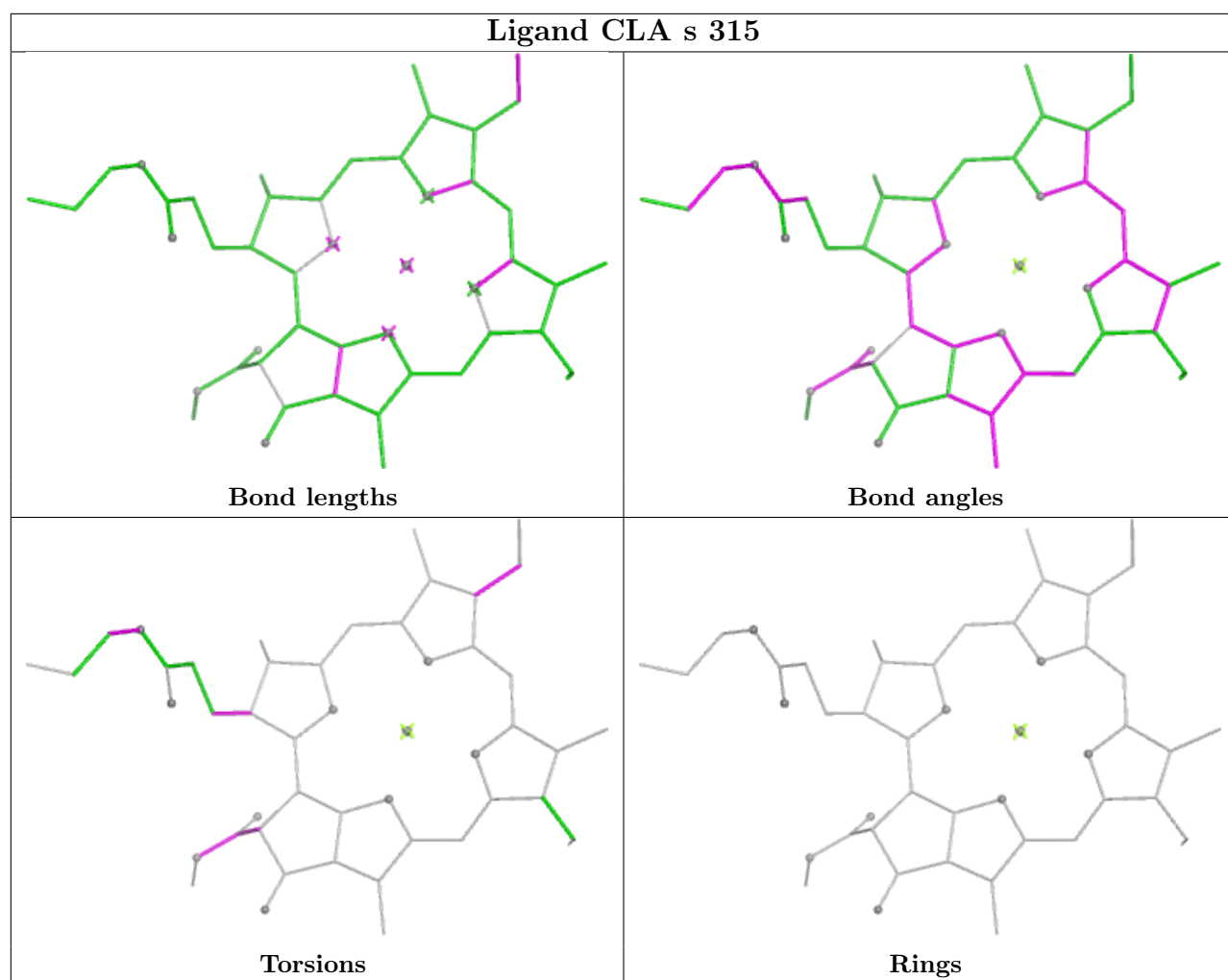
Bond angles

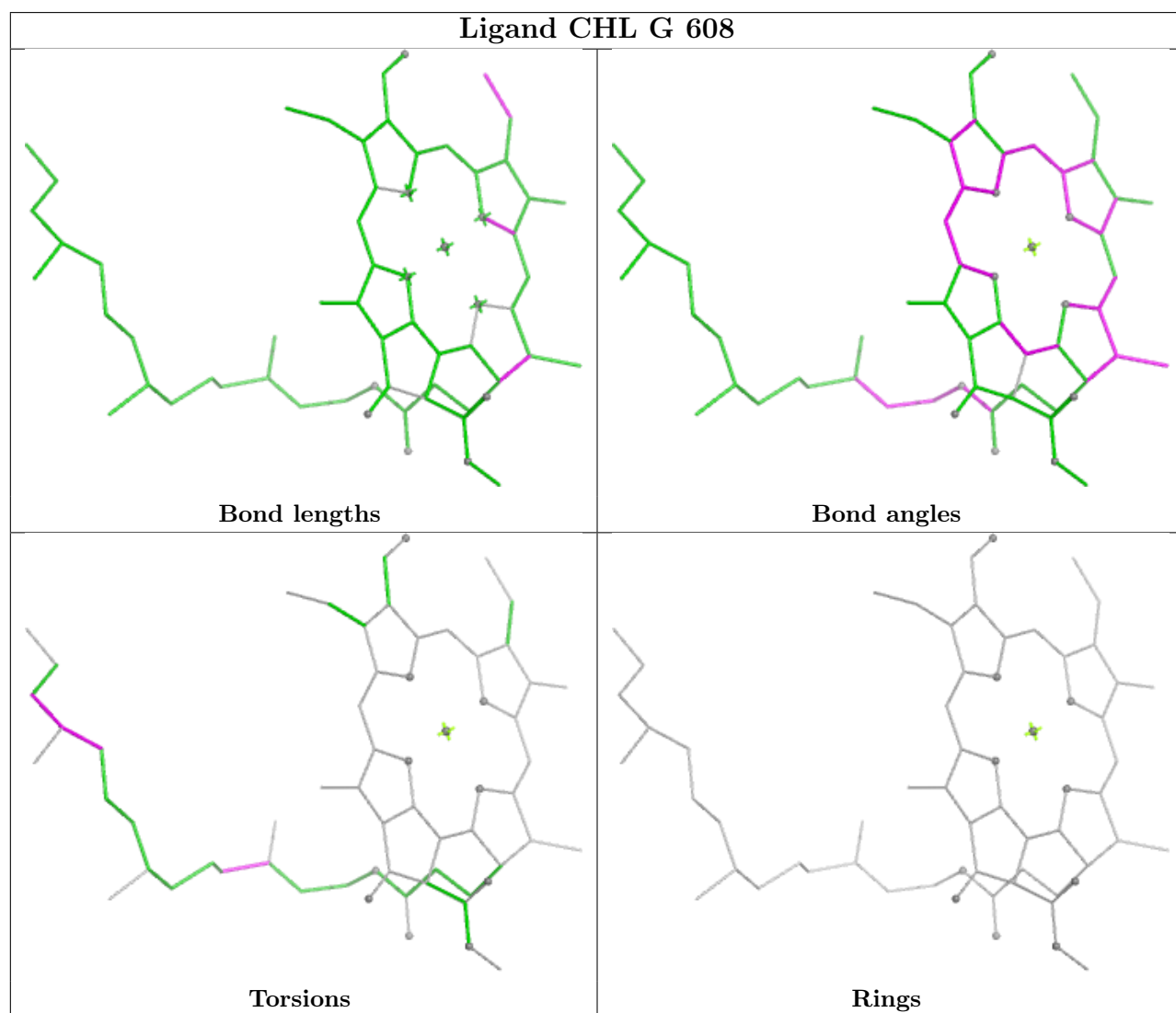
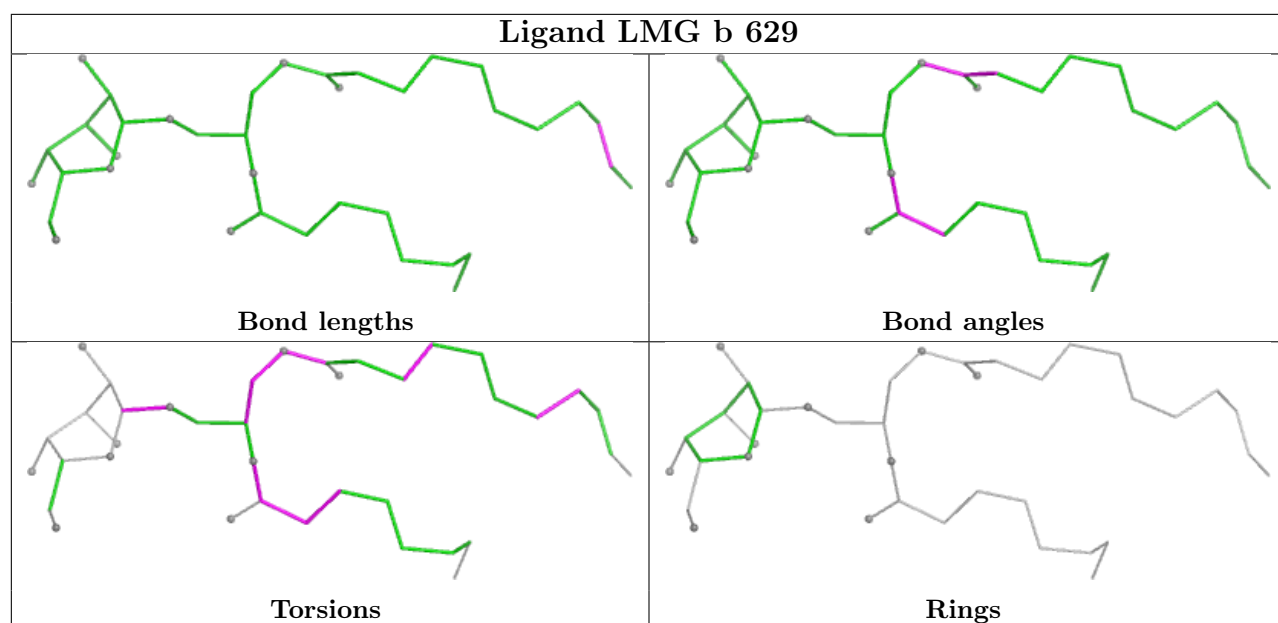


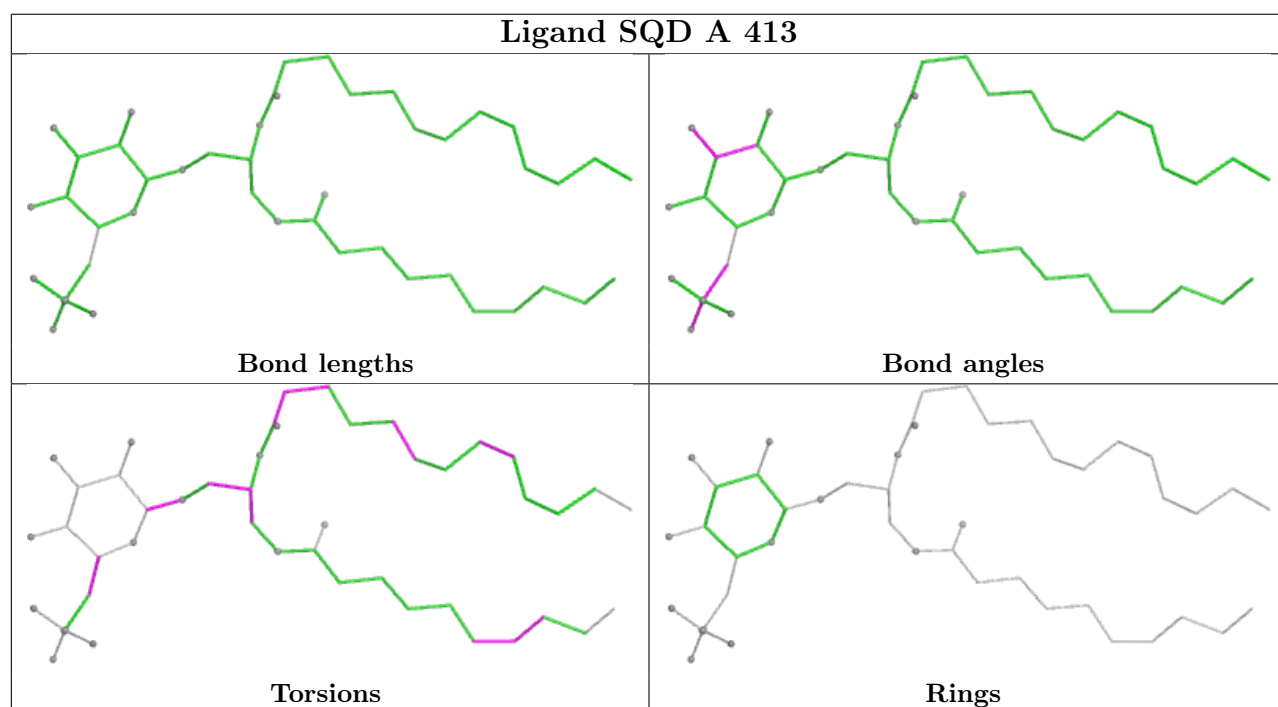
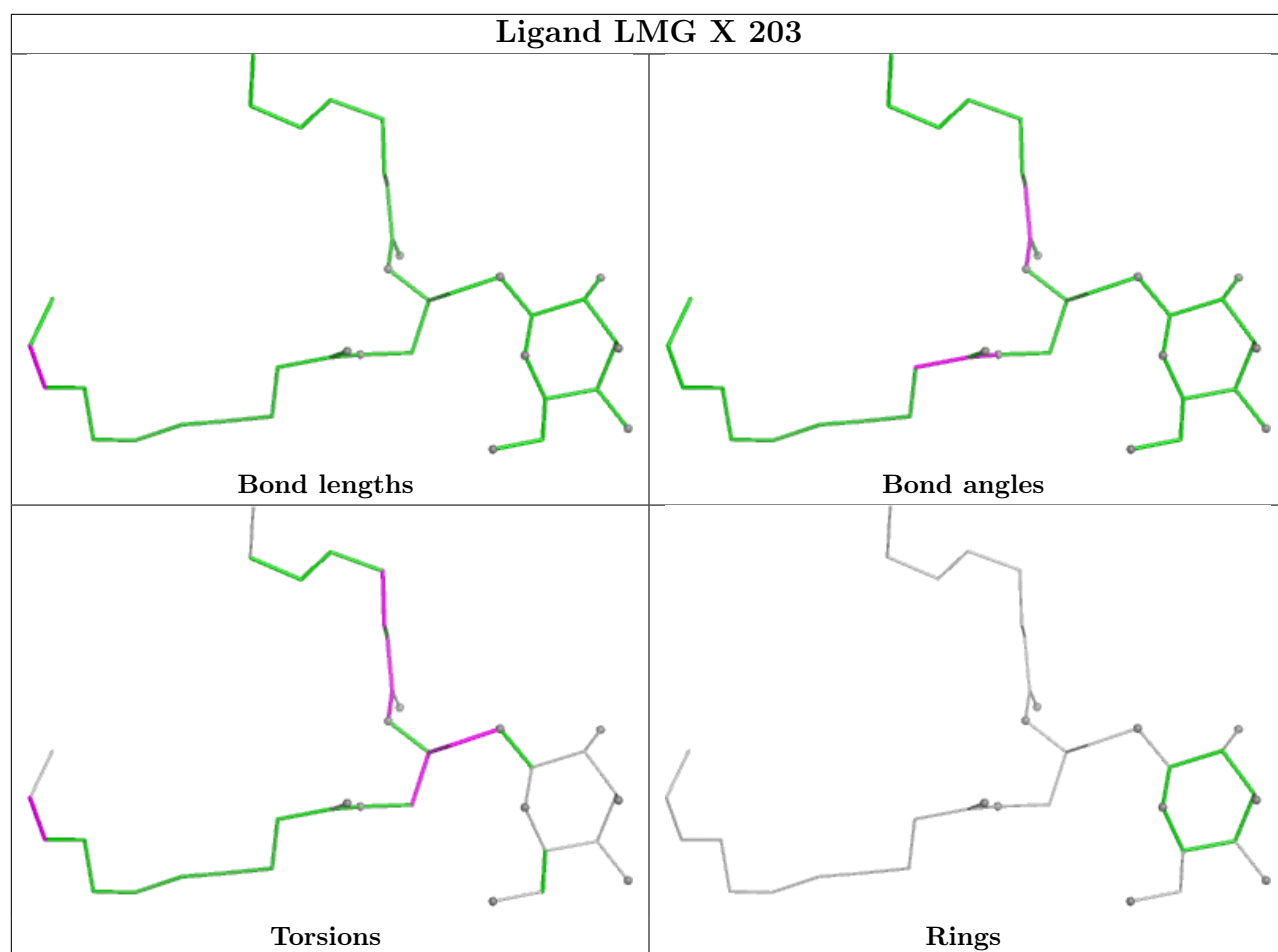
Torsions



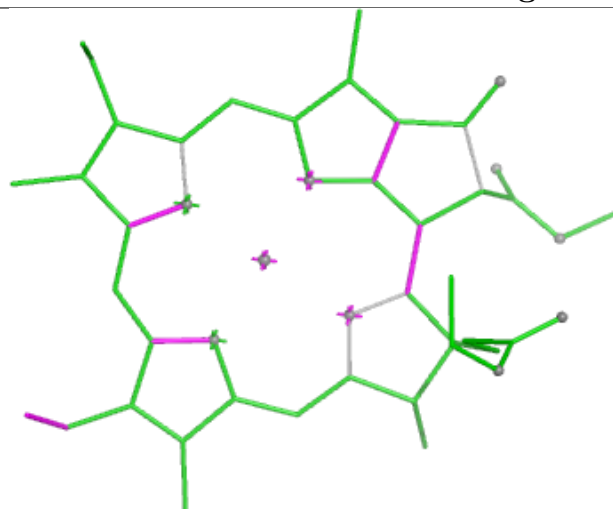
Rings



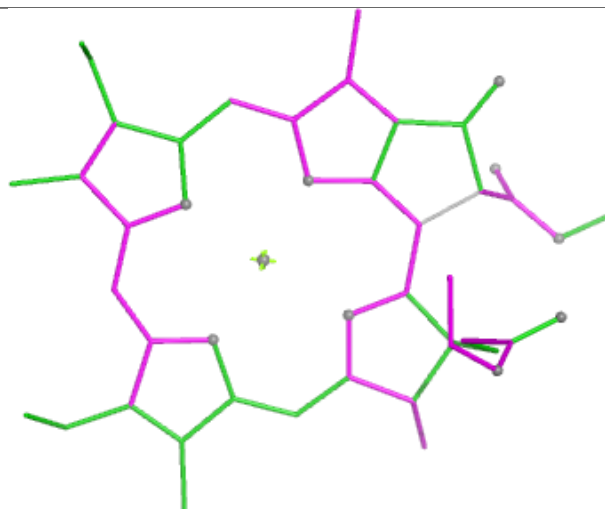




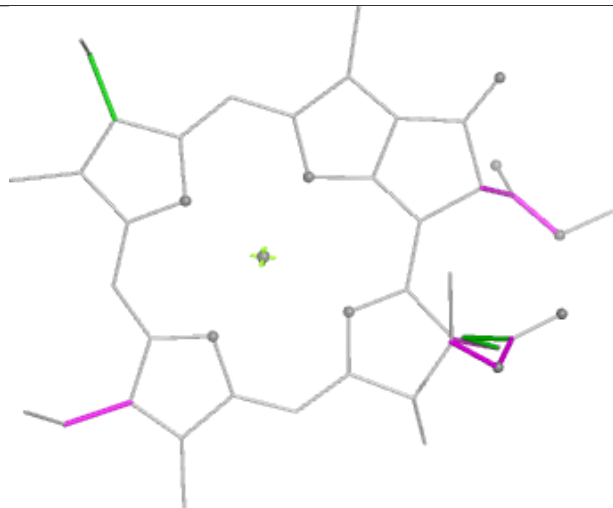
Ligand CLA 9 313



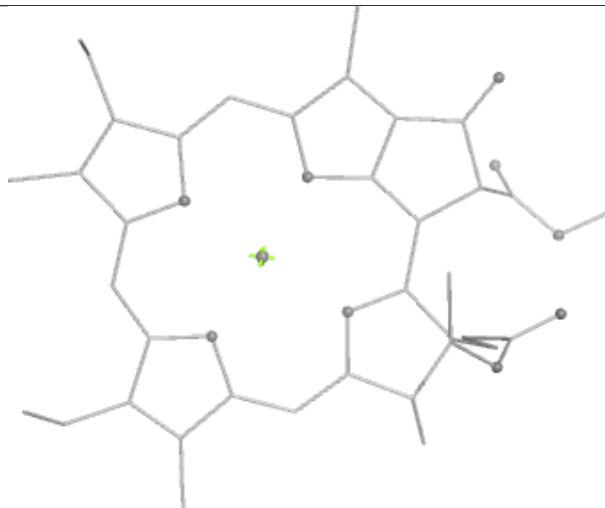
Bond lengths



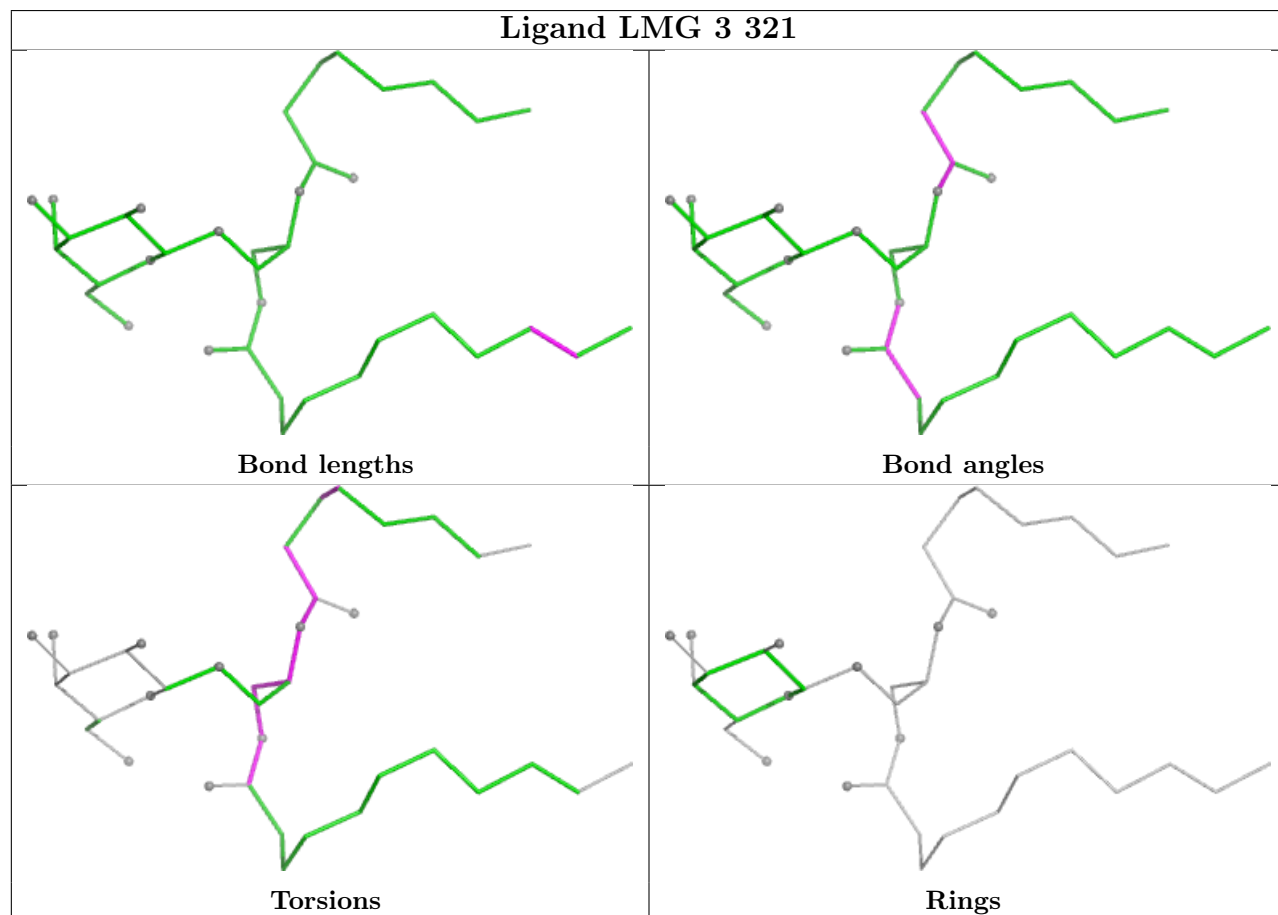
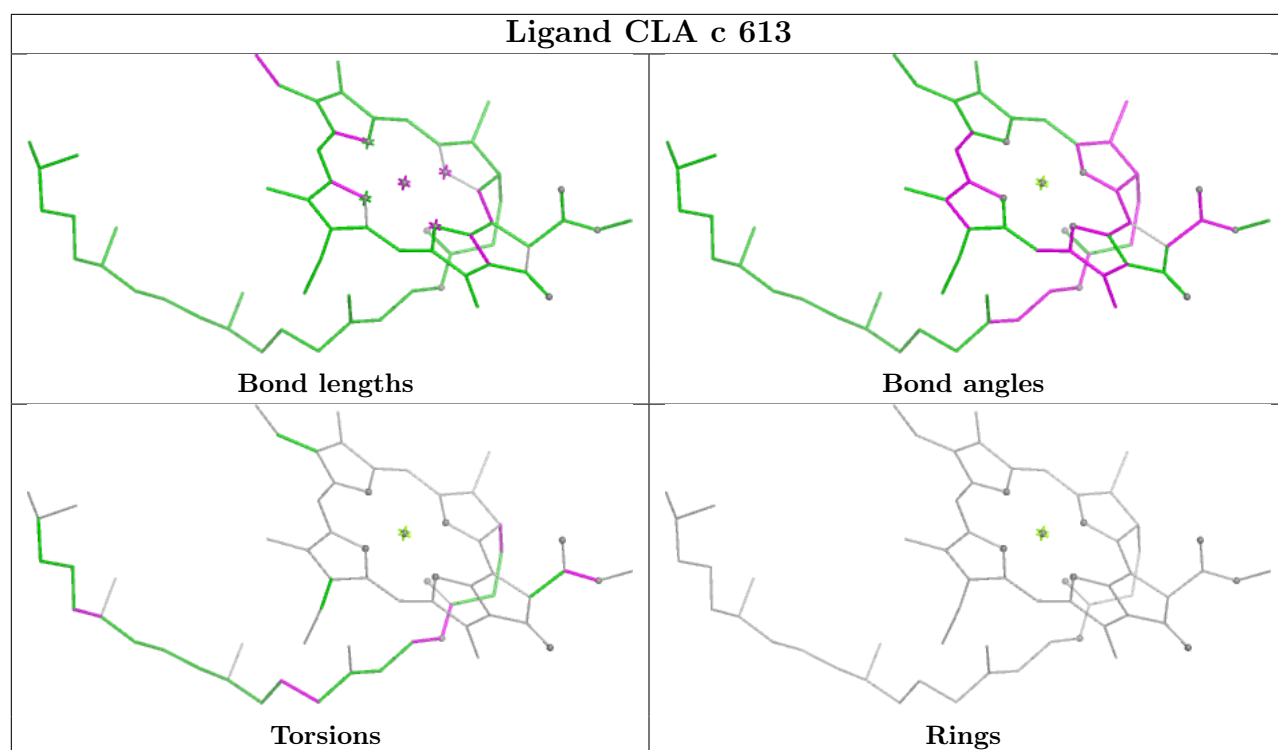
Bond angles

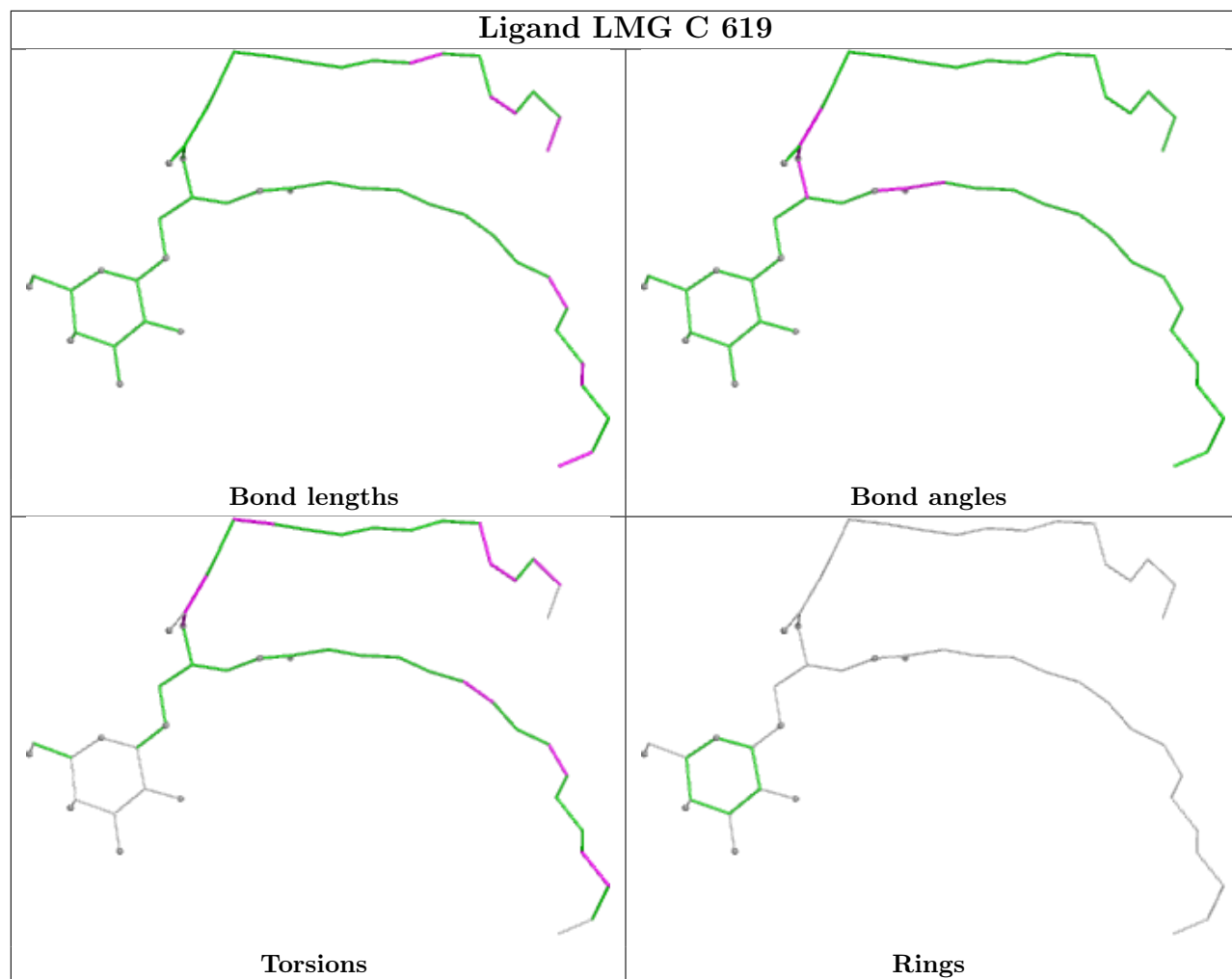
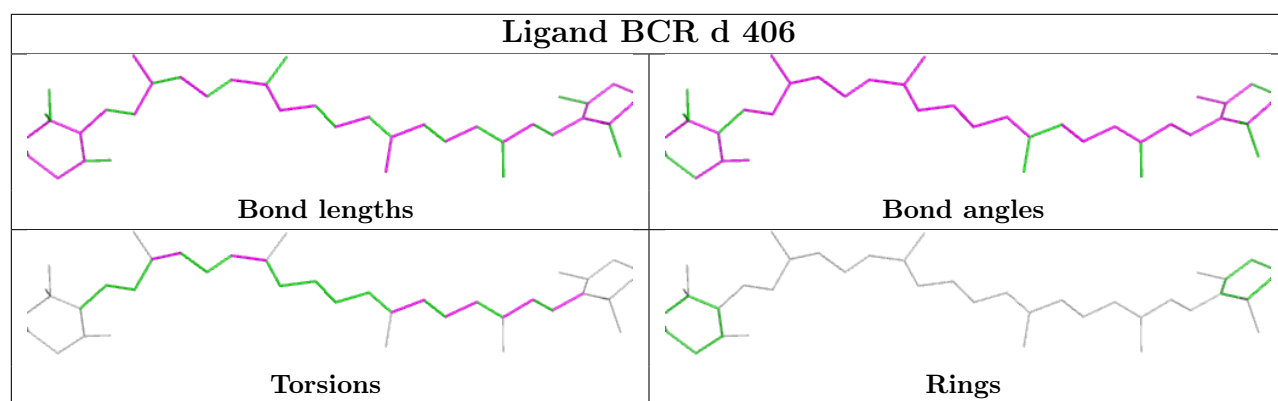


Torsions

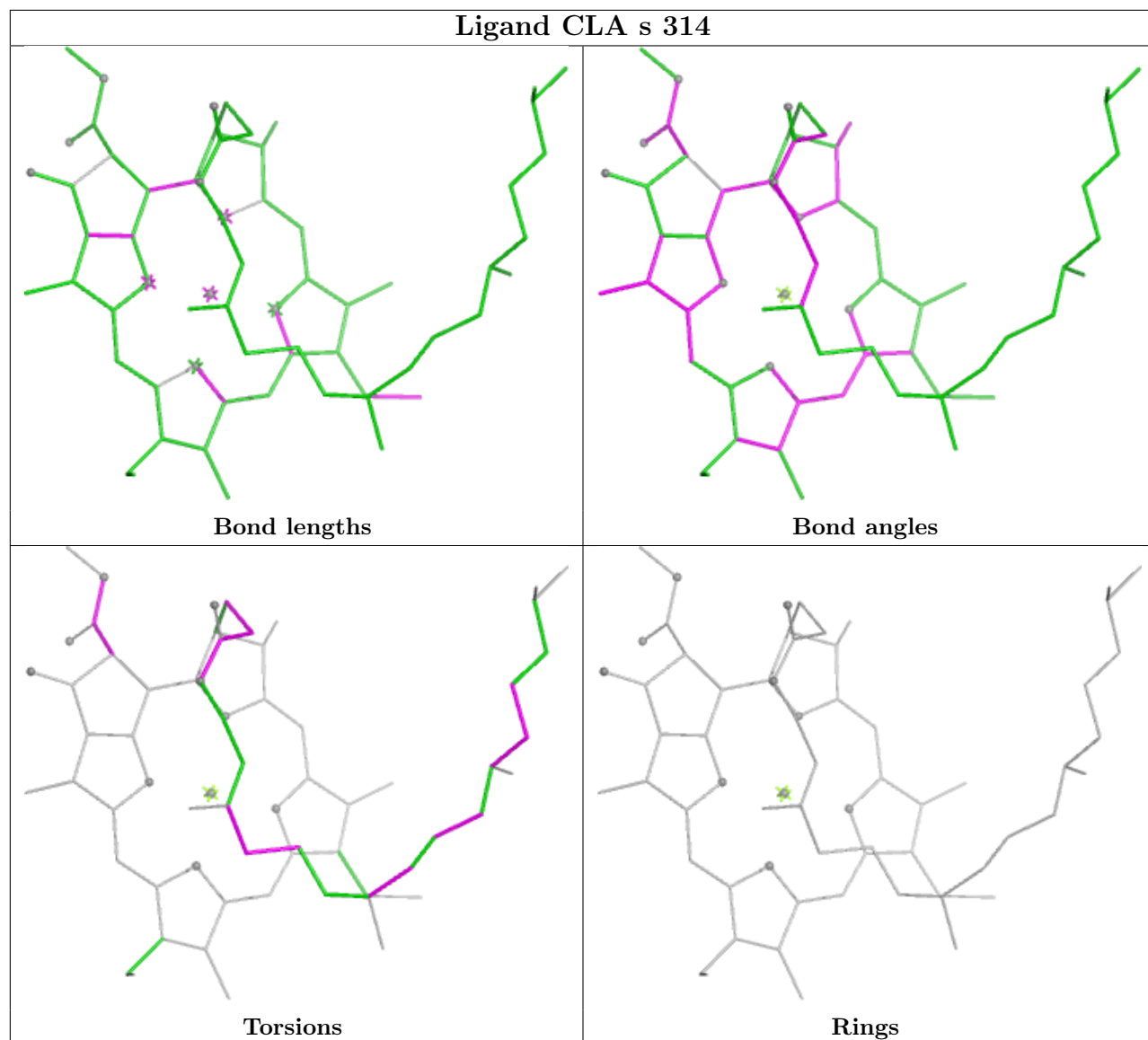


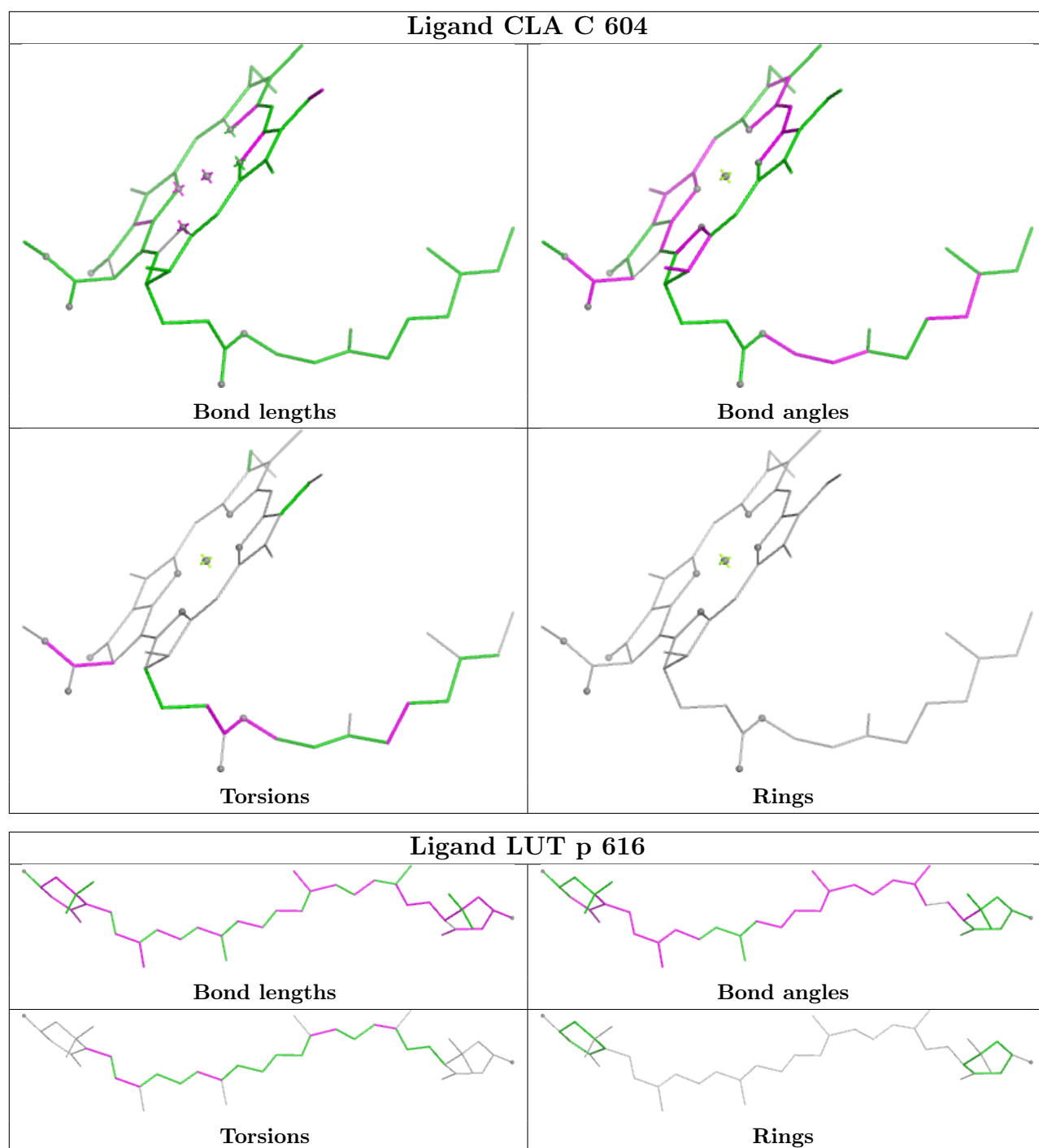
Rings

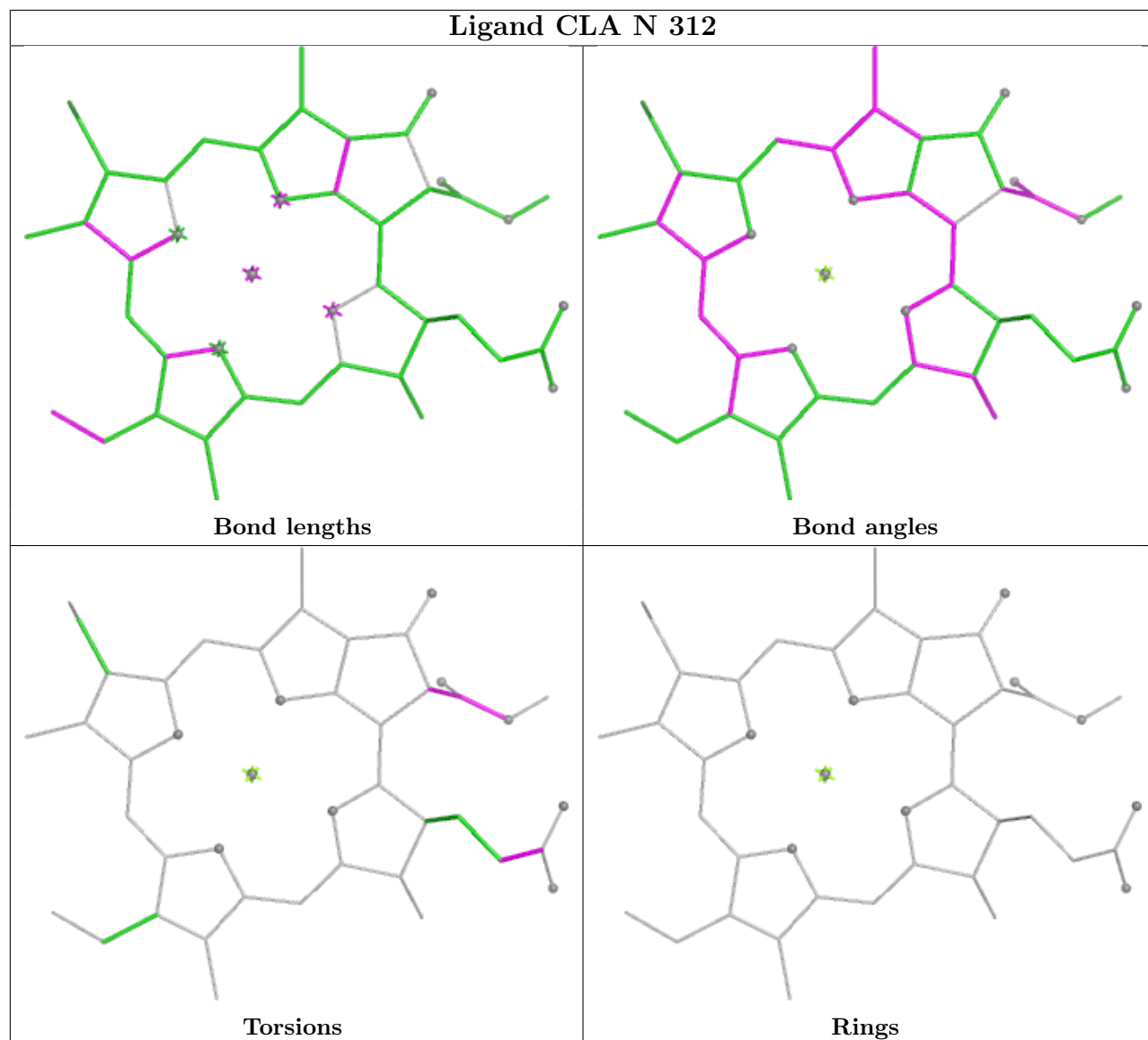


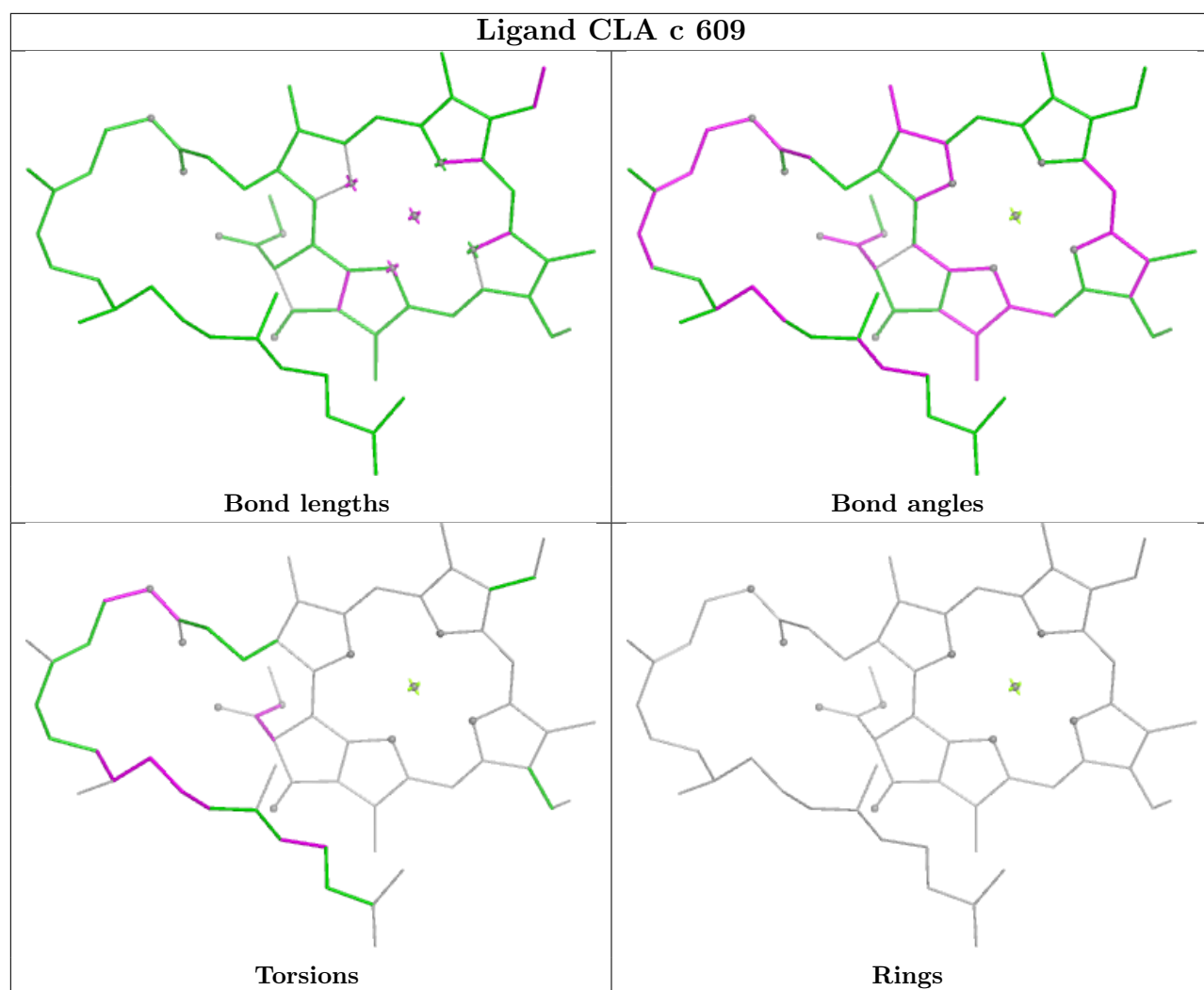


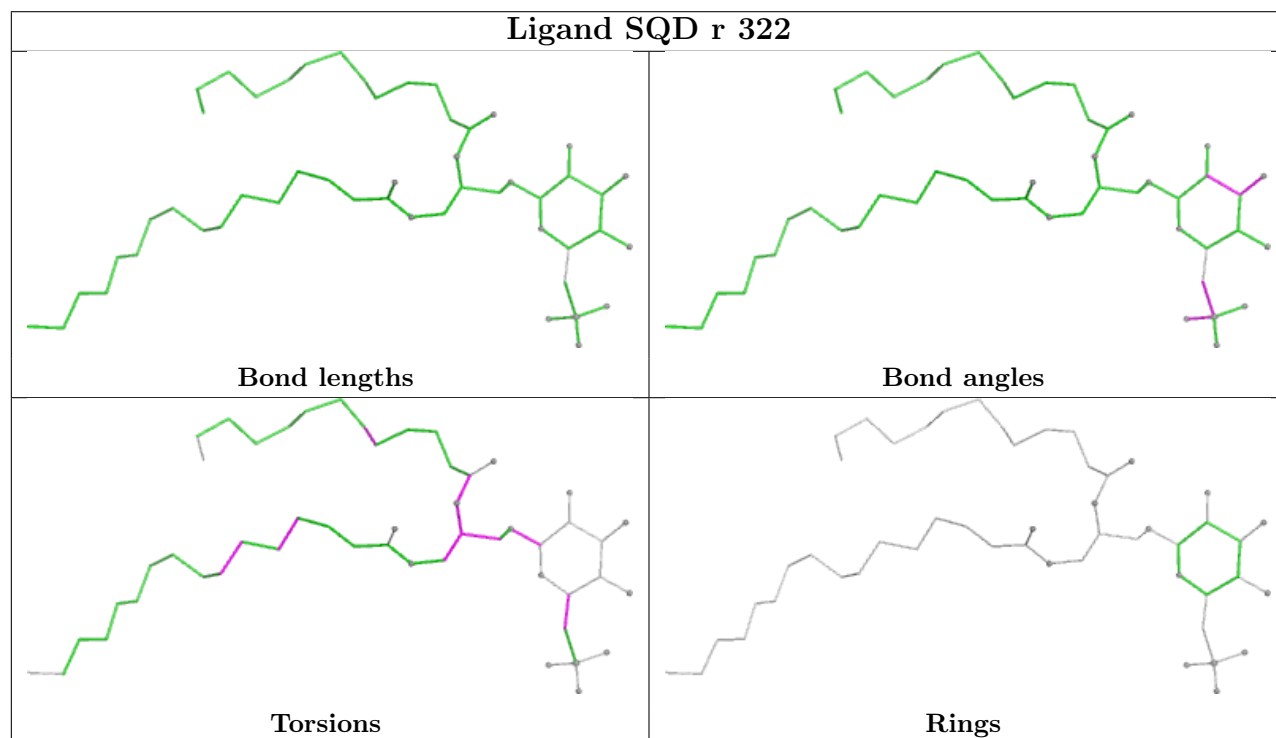
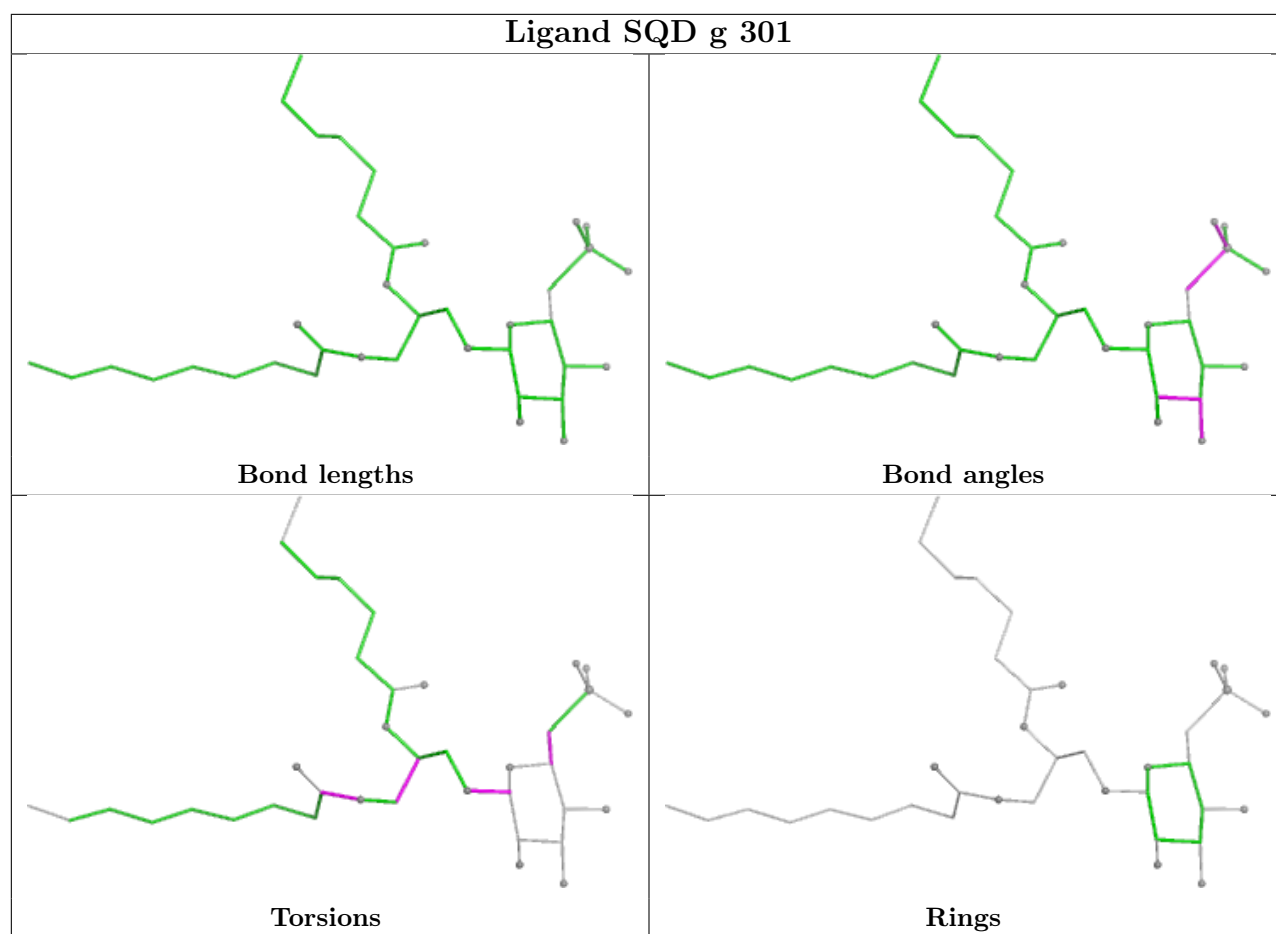
Ligand CLA s 314

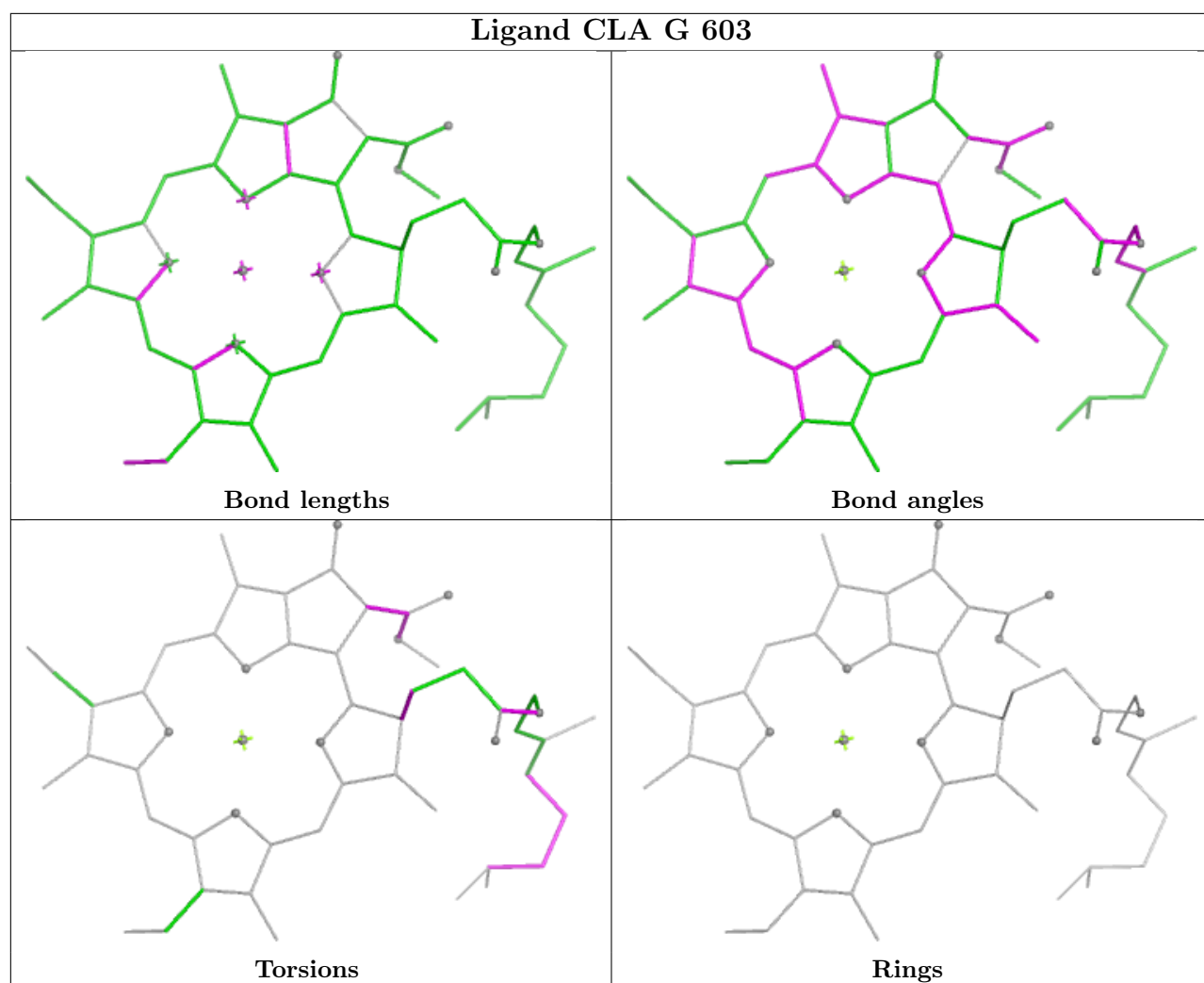


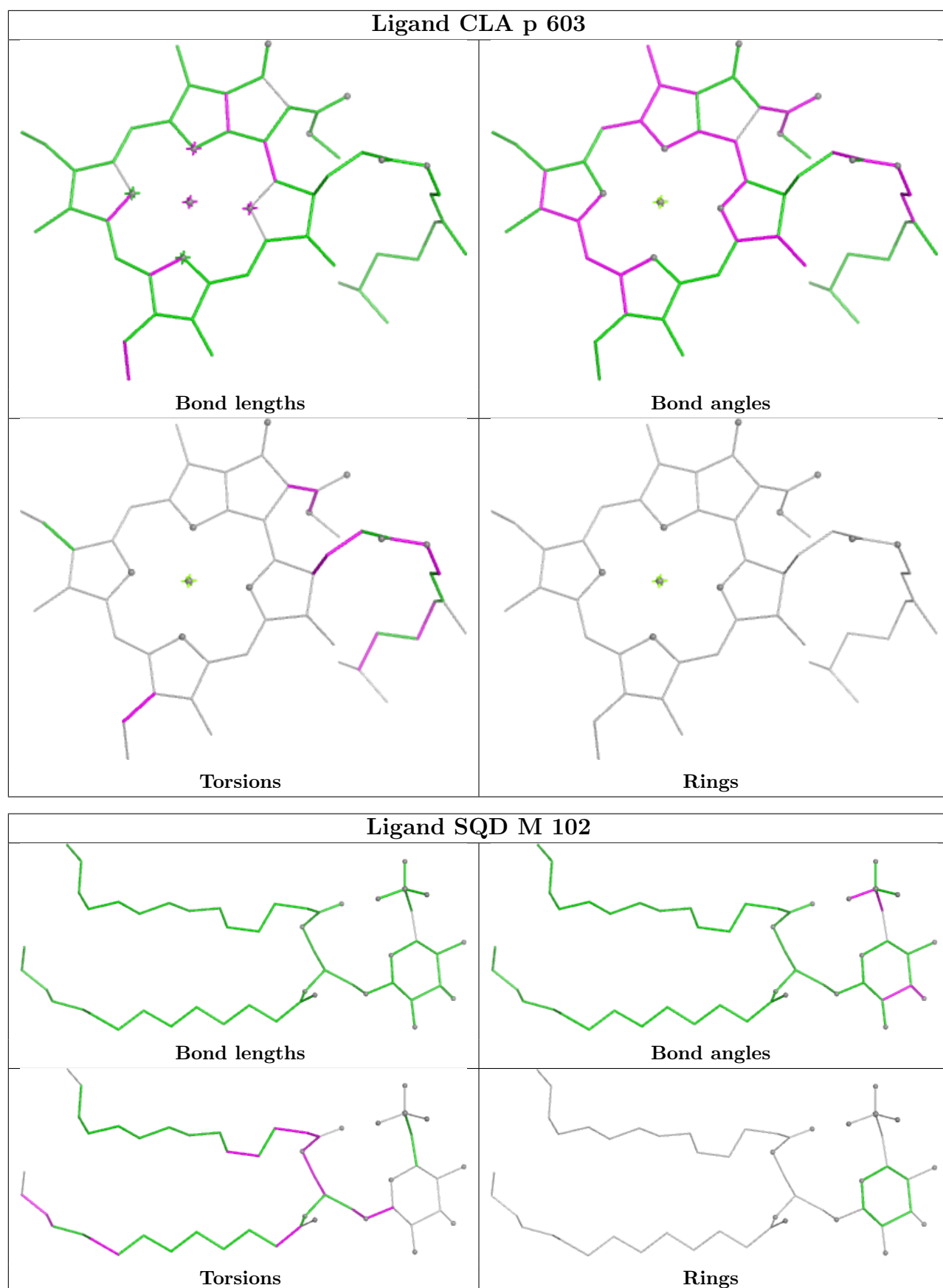




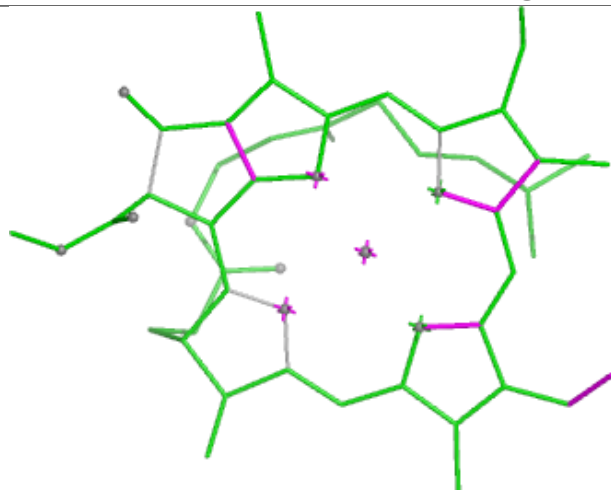




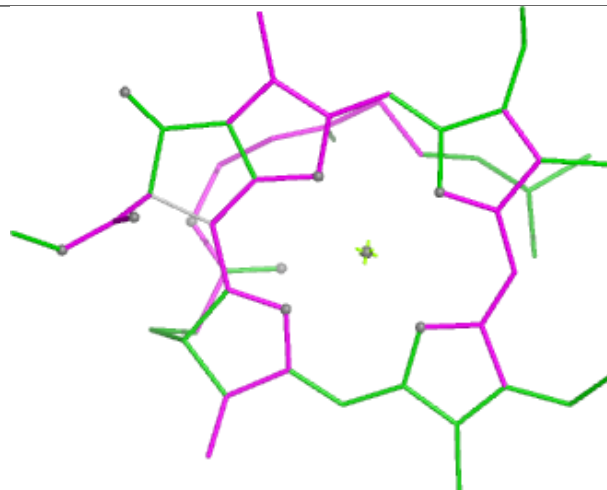




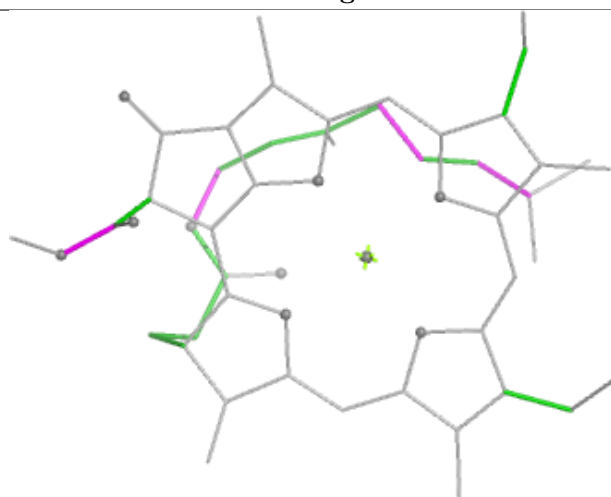
Ligand CLA 3 314



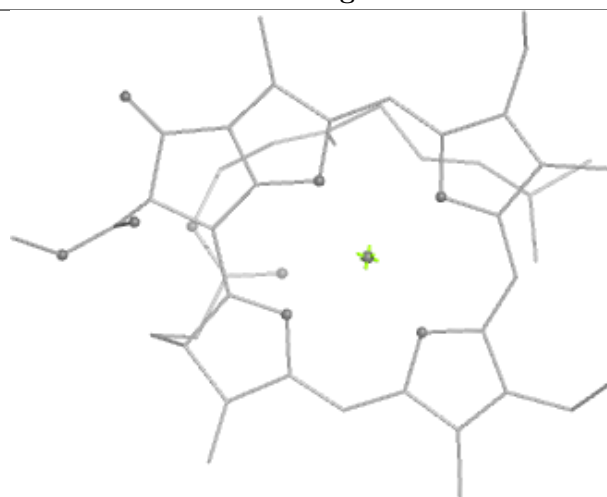
Bond lengths



Bond angles

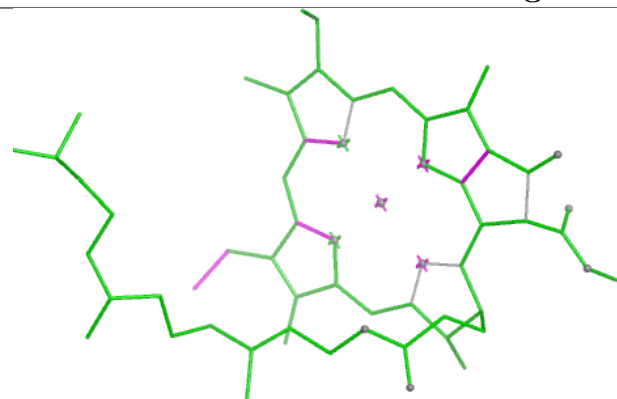


Torsions

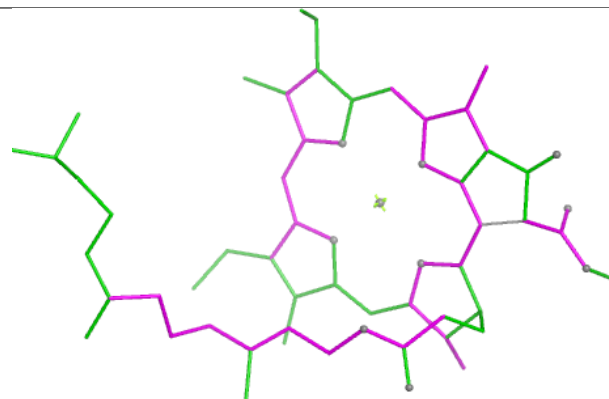


Rings

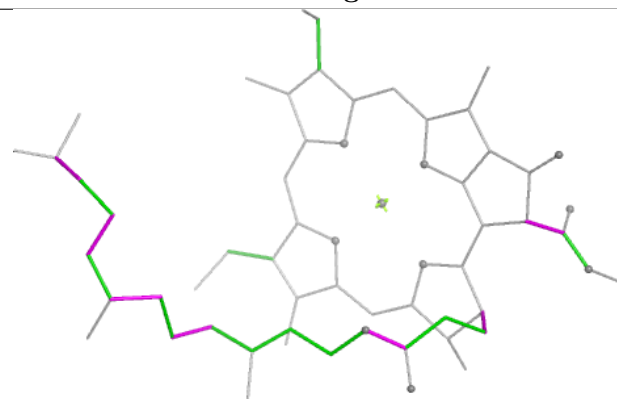
Ligand CLA r 304



Bond lengths



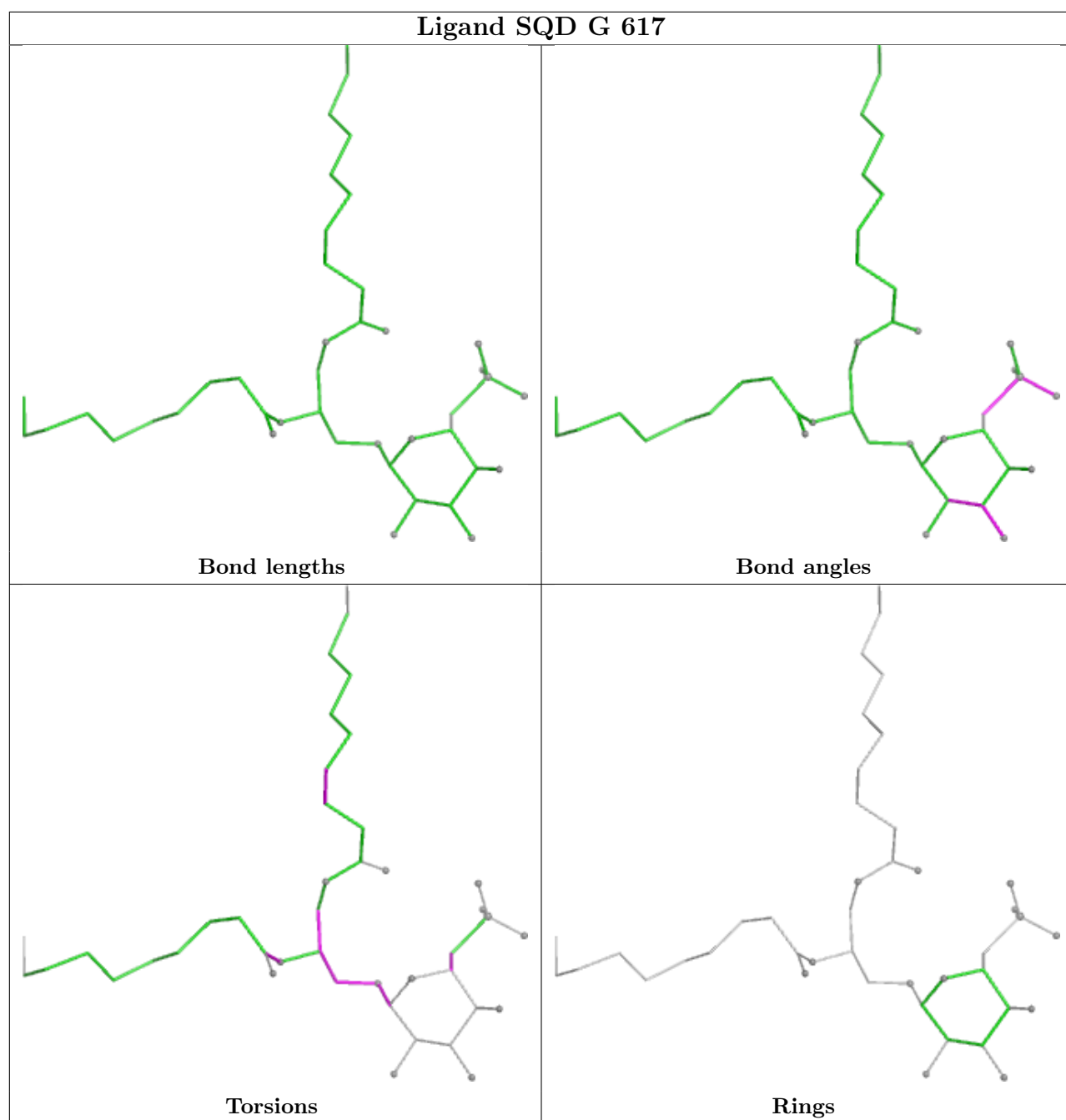
Bond angles



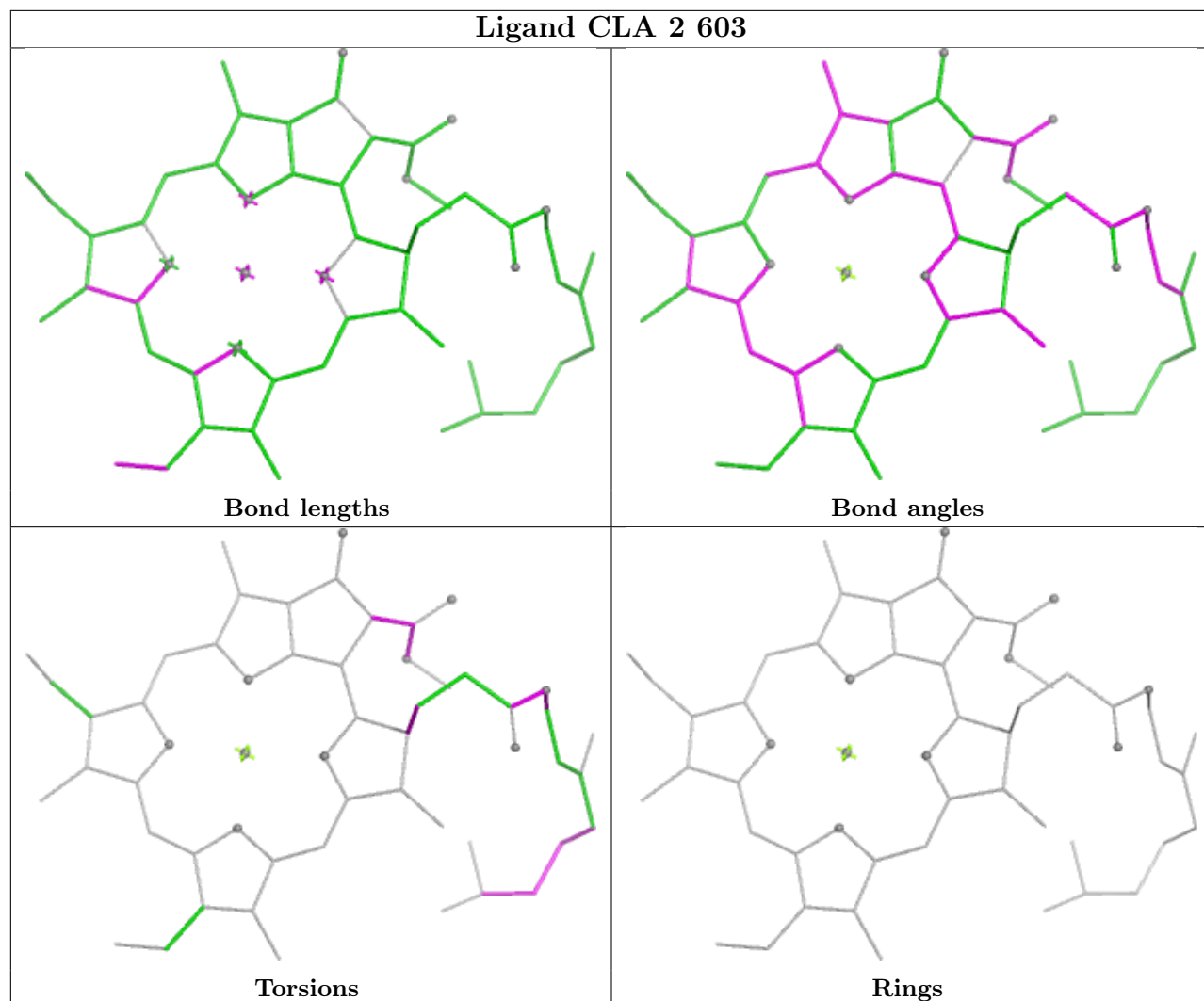
Torsions



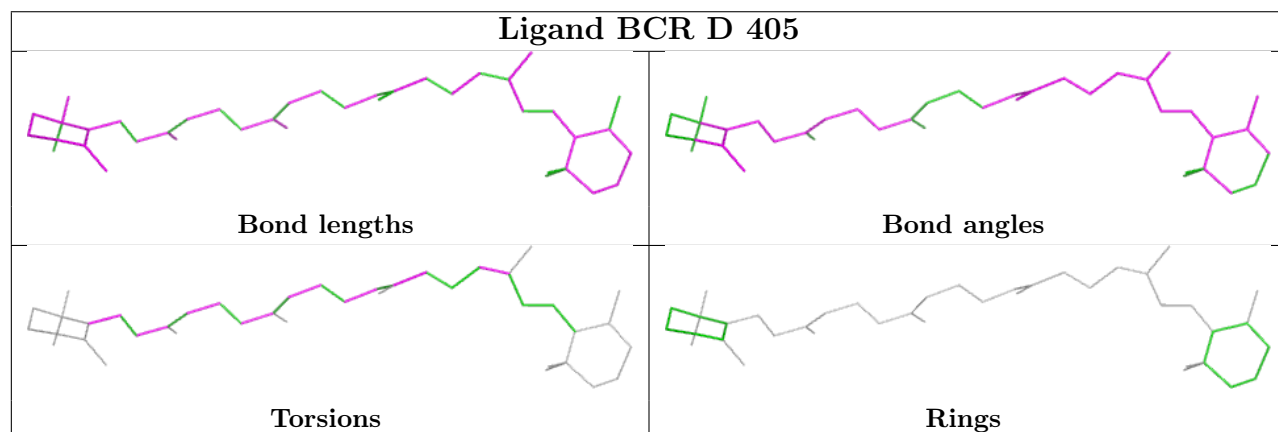
Rings

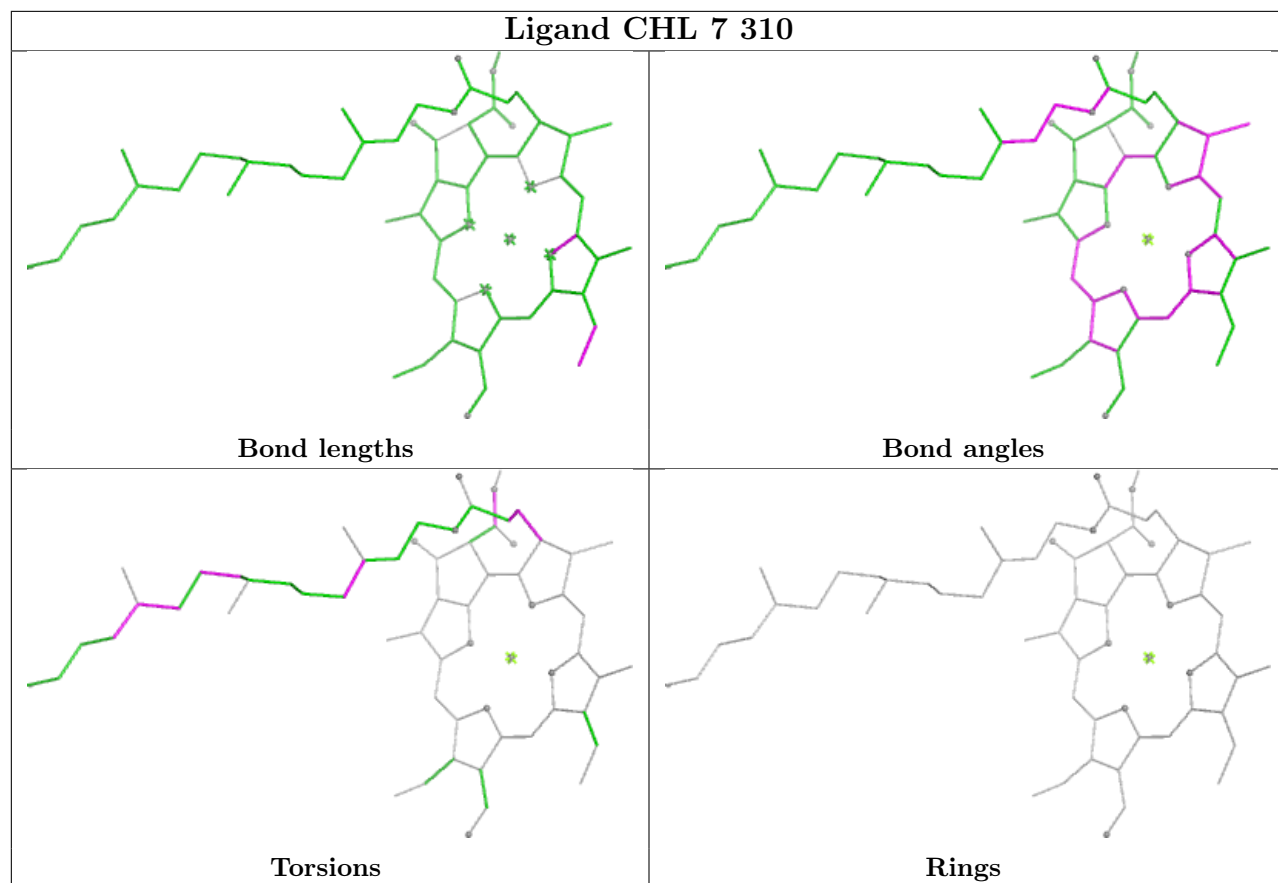


Ligand CLA 2 603

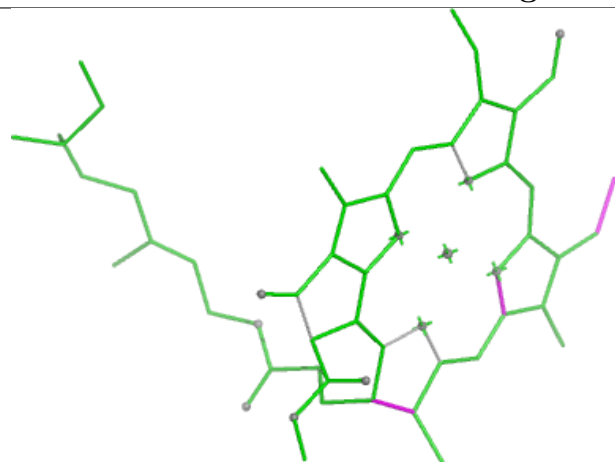


Ligand BCR D 405

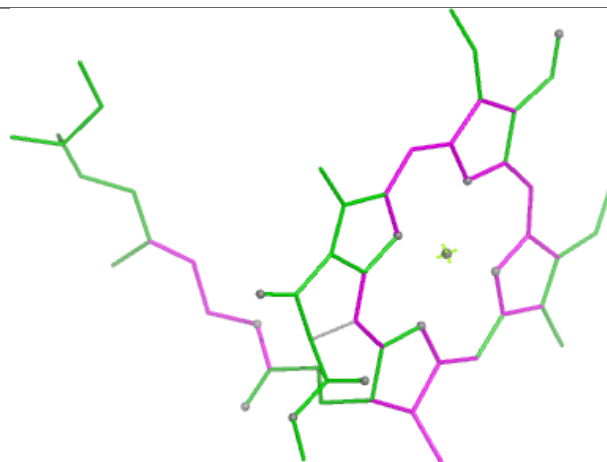




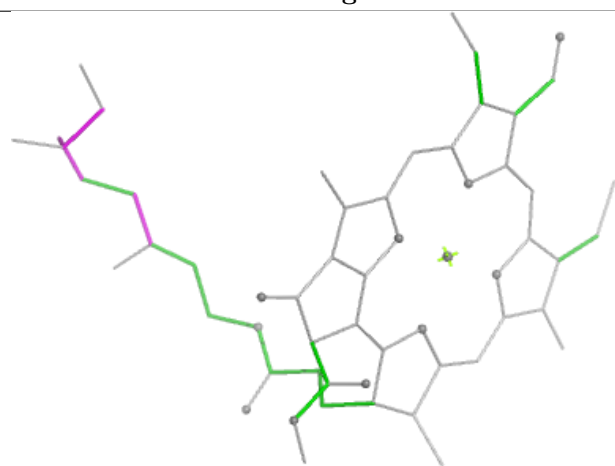
Ligand CHL 2 608



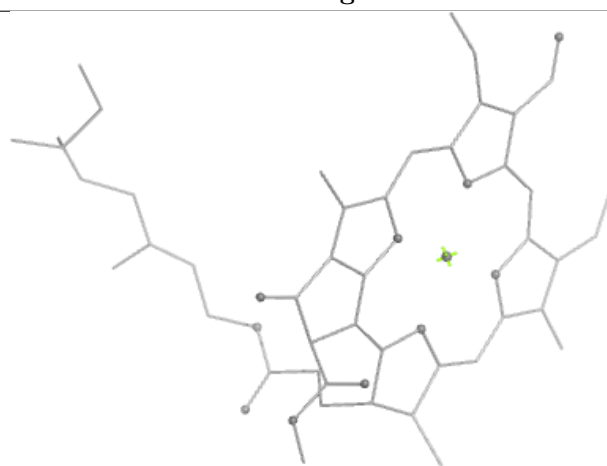
Bond lengths



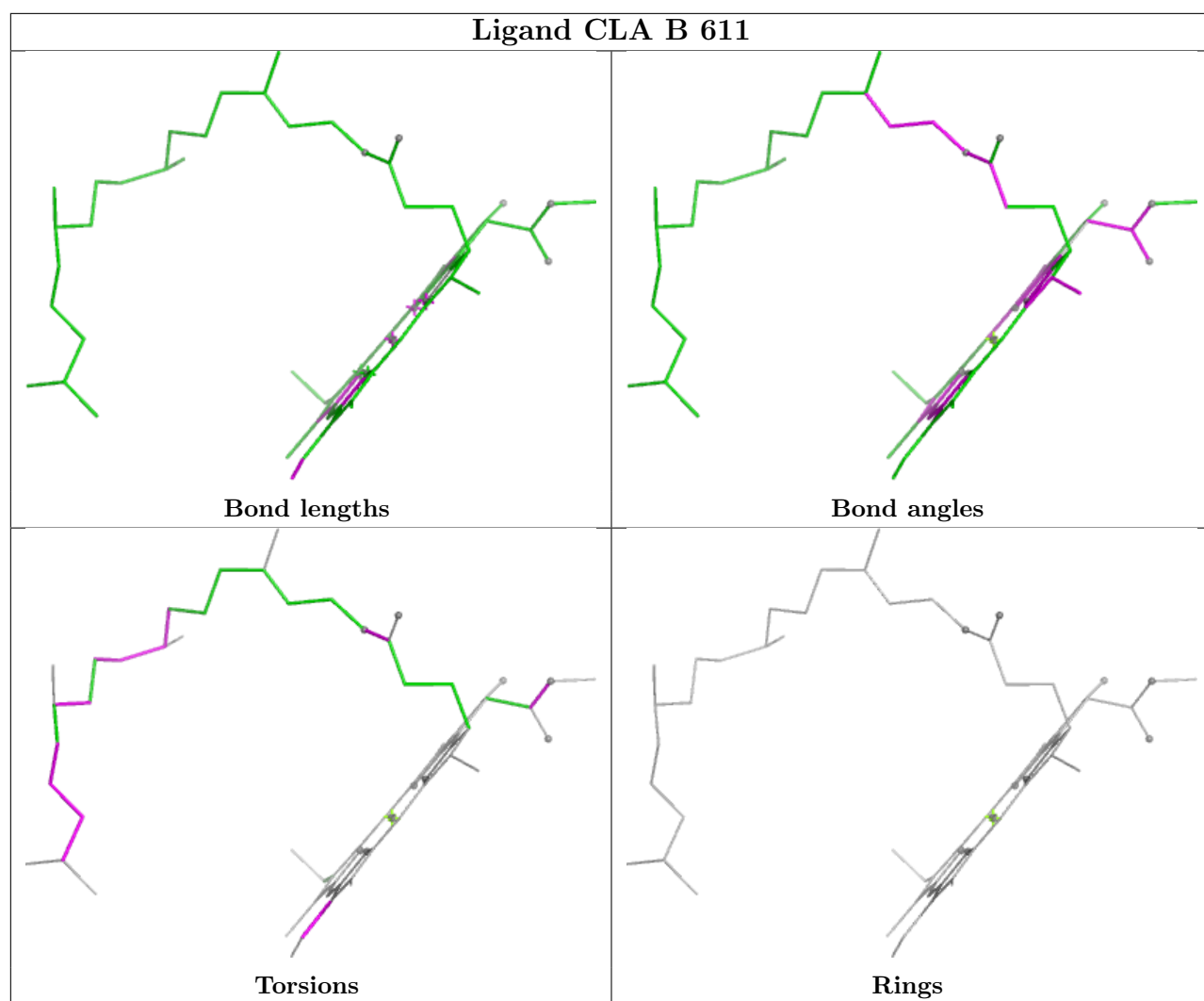
Bond angles



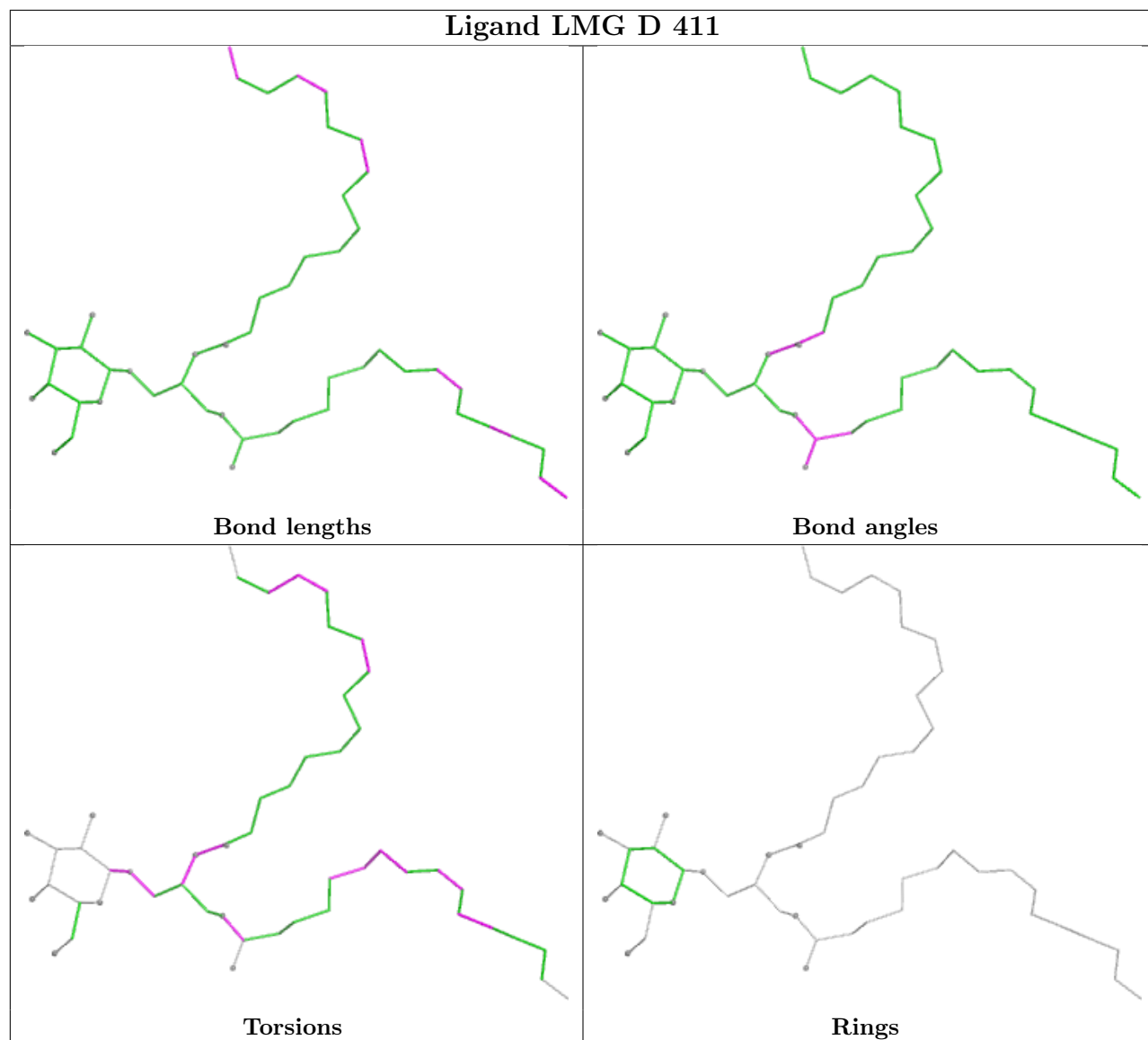
Torsions



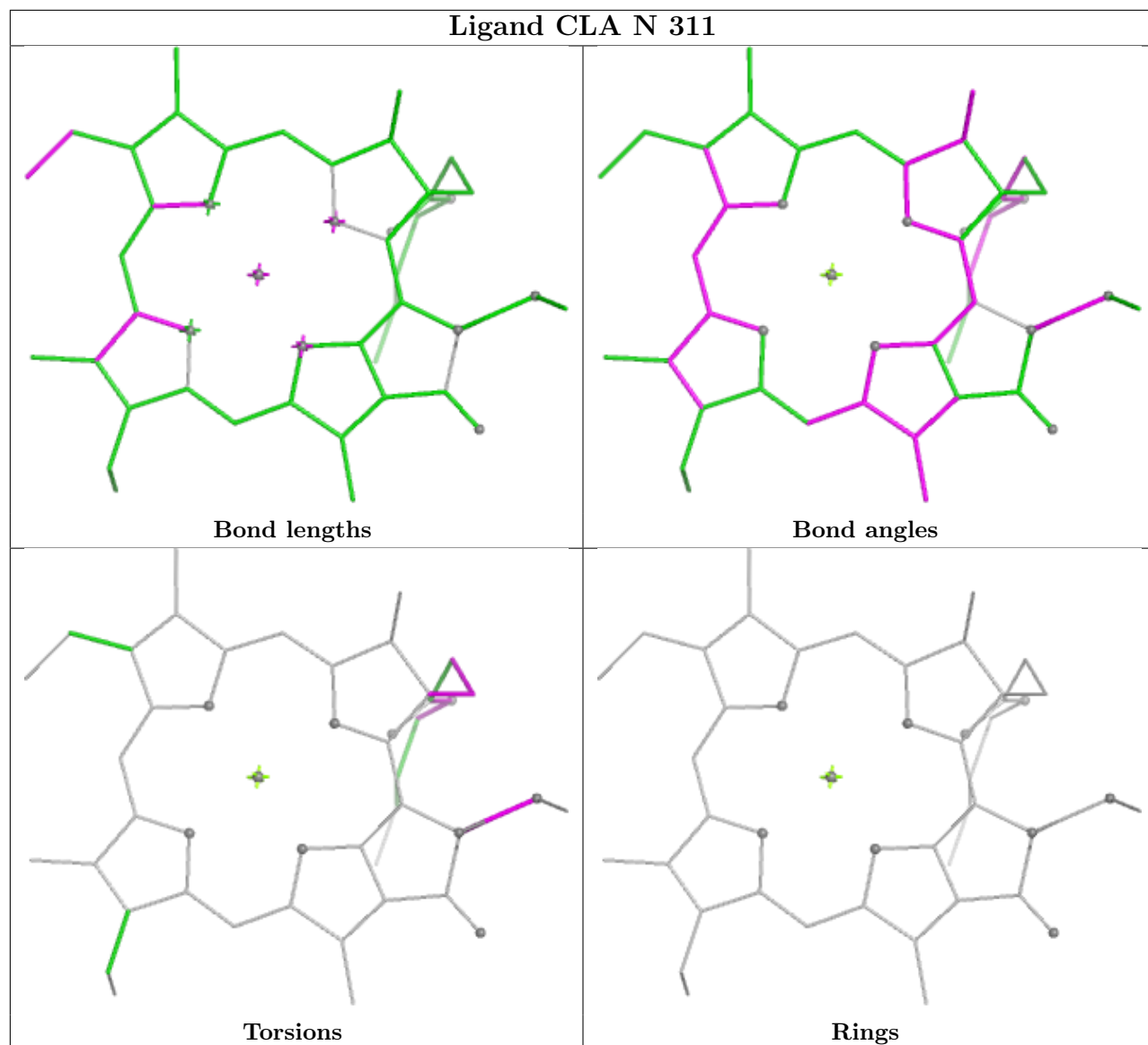
Rings

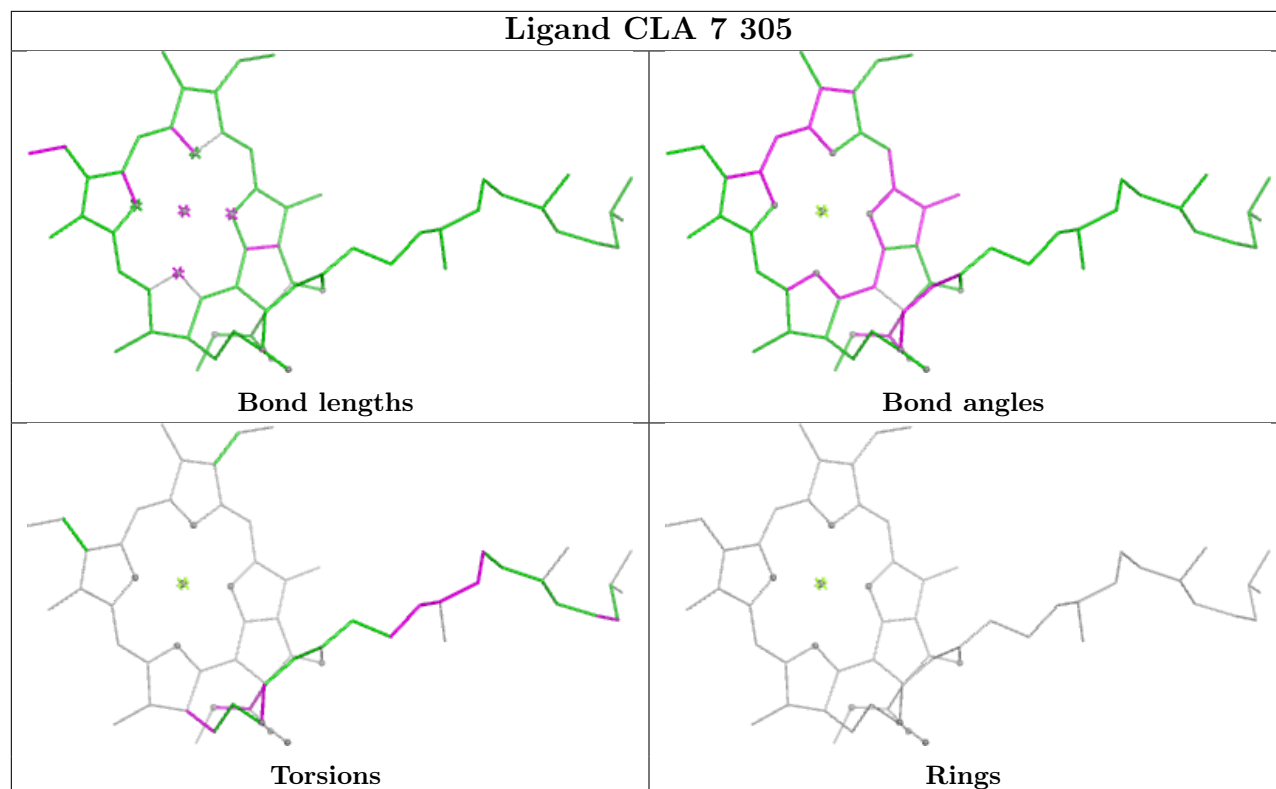
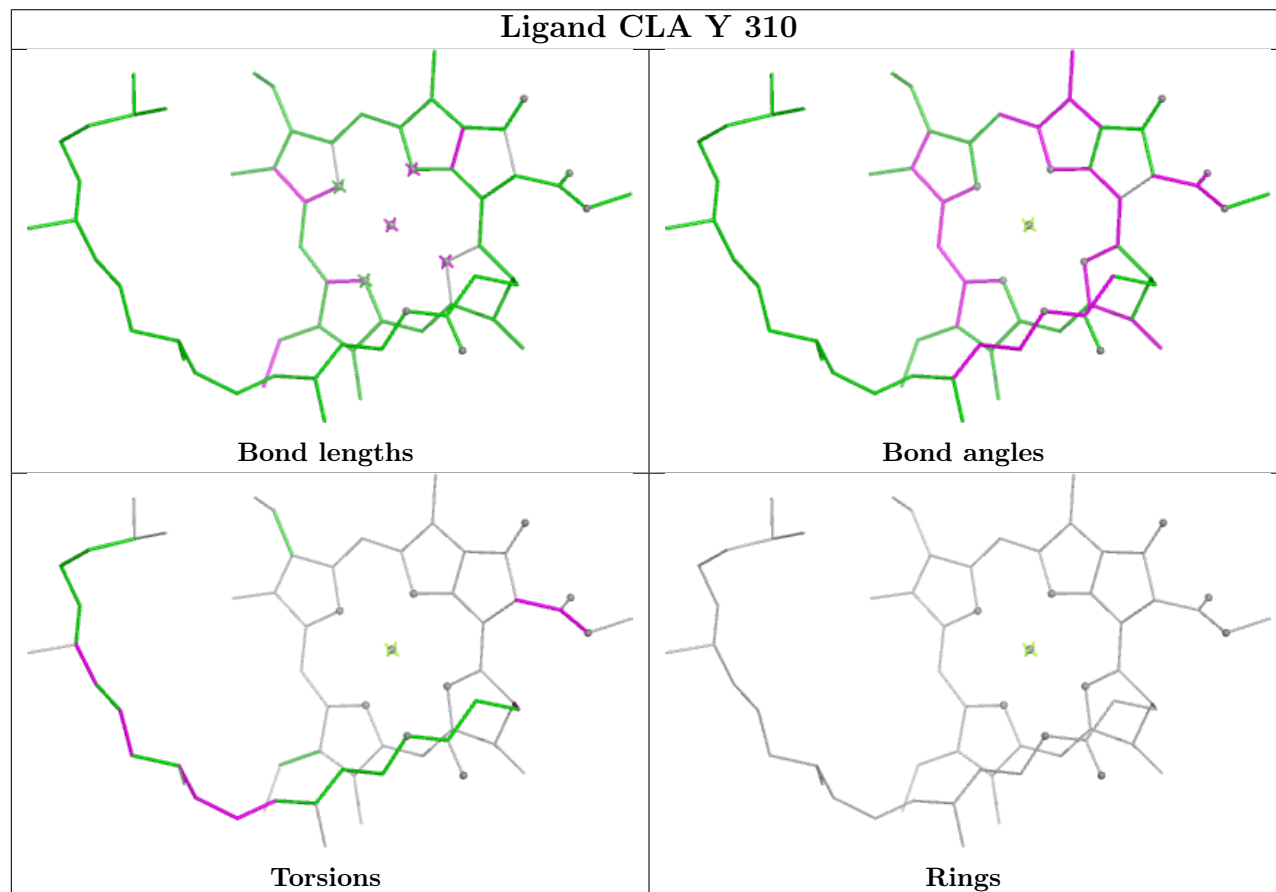


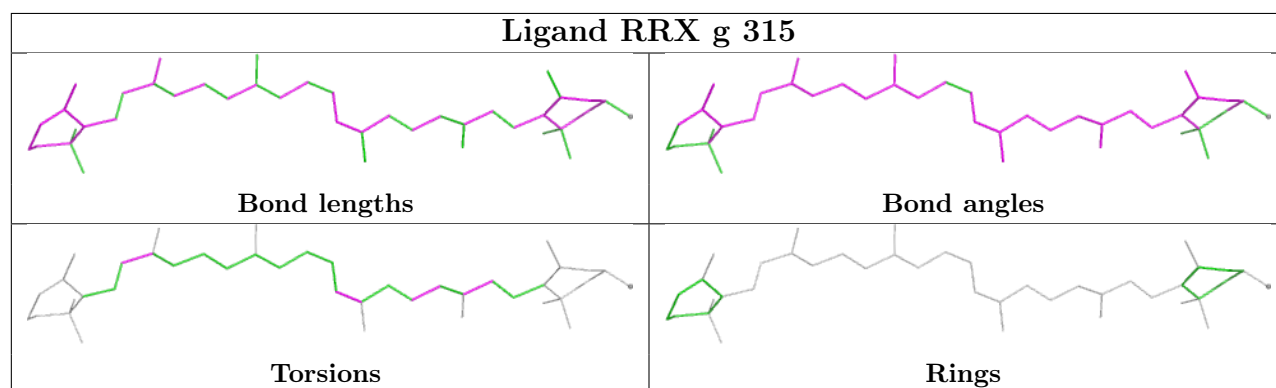
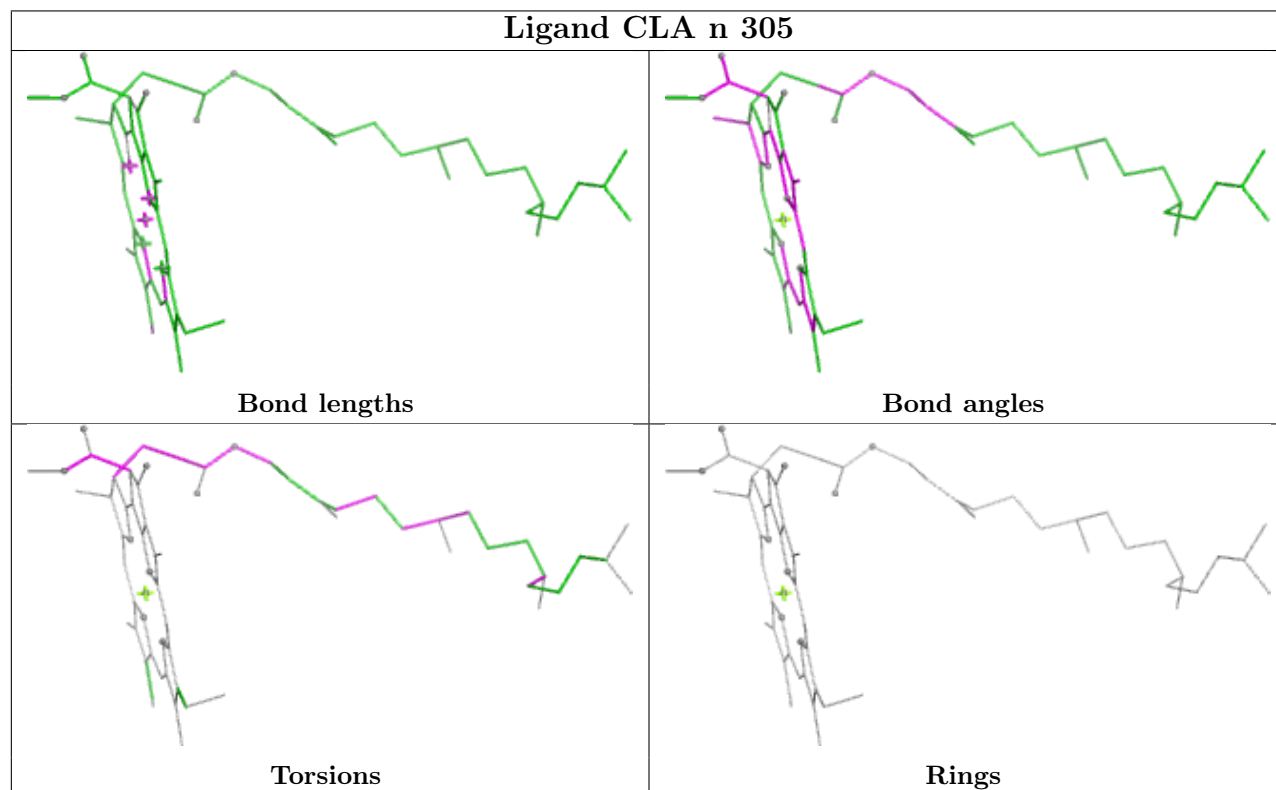
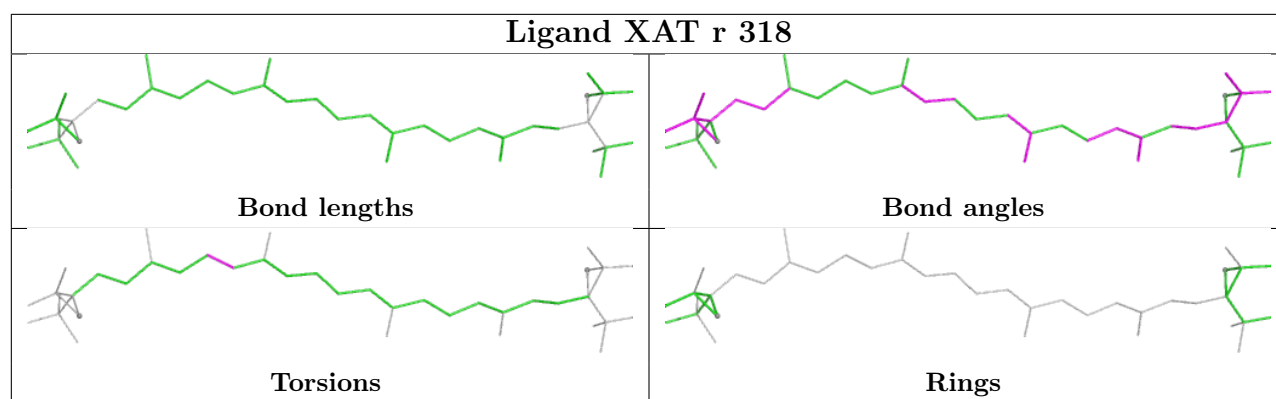


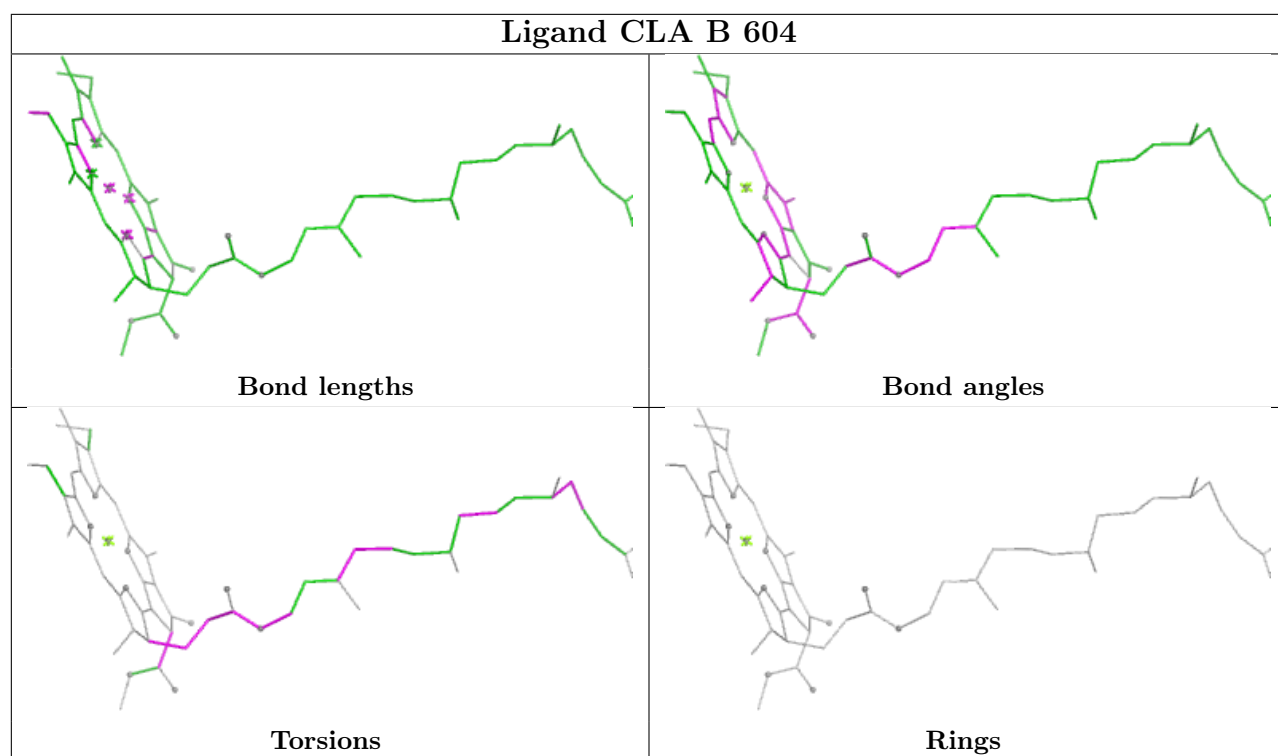


Ligand CLA N 311

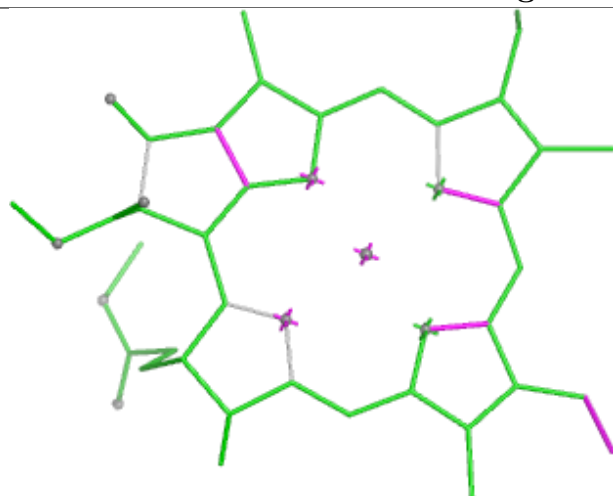


Ligand CLA 7 305**Ligand CLA Y 310**

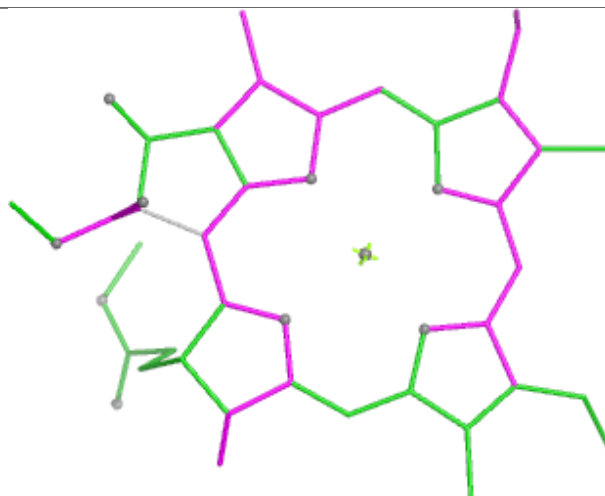




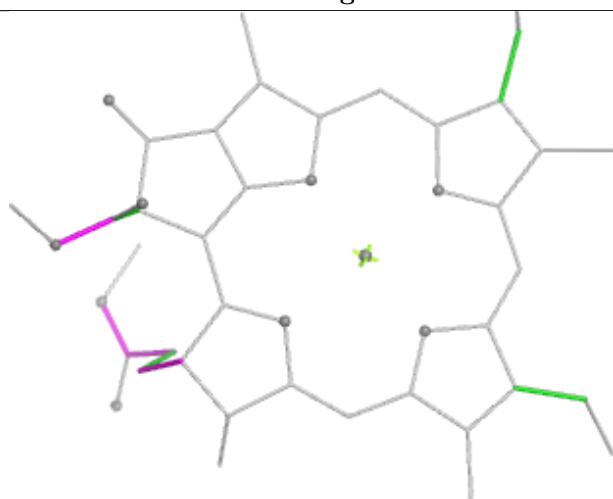
Ligand CLA S 316



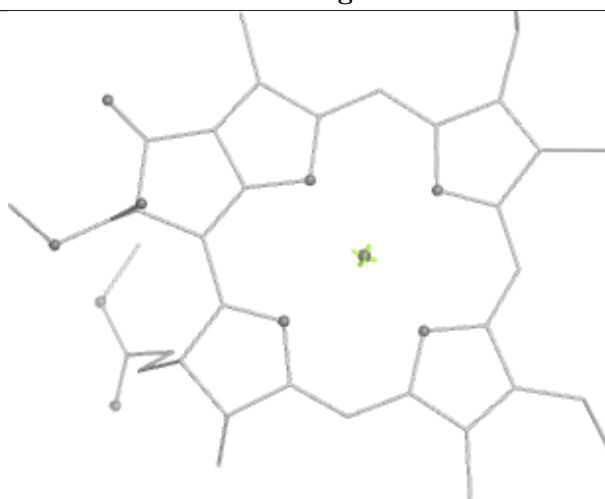
Bond lengths



Bond angles

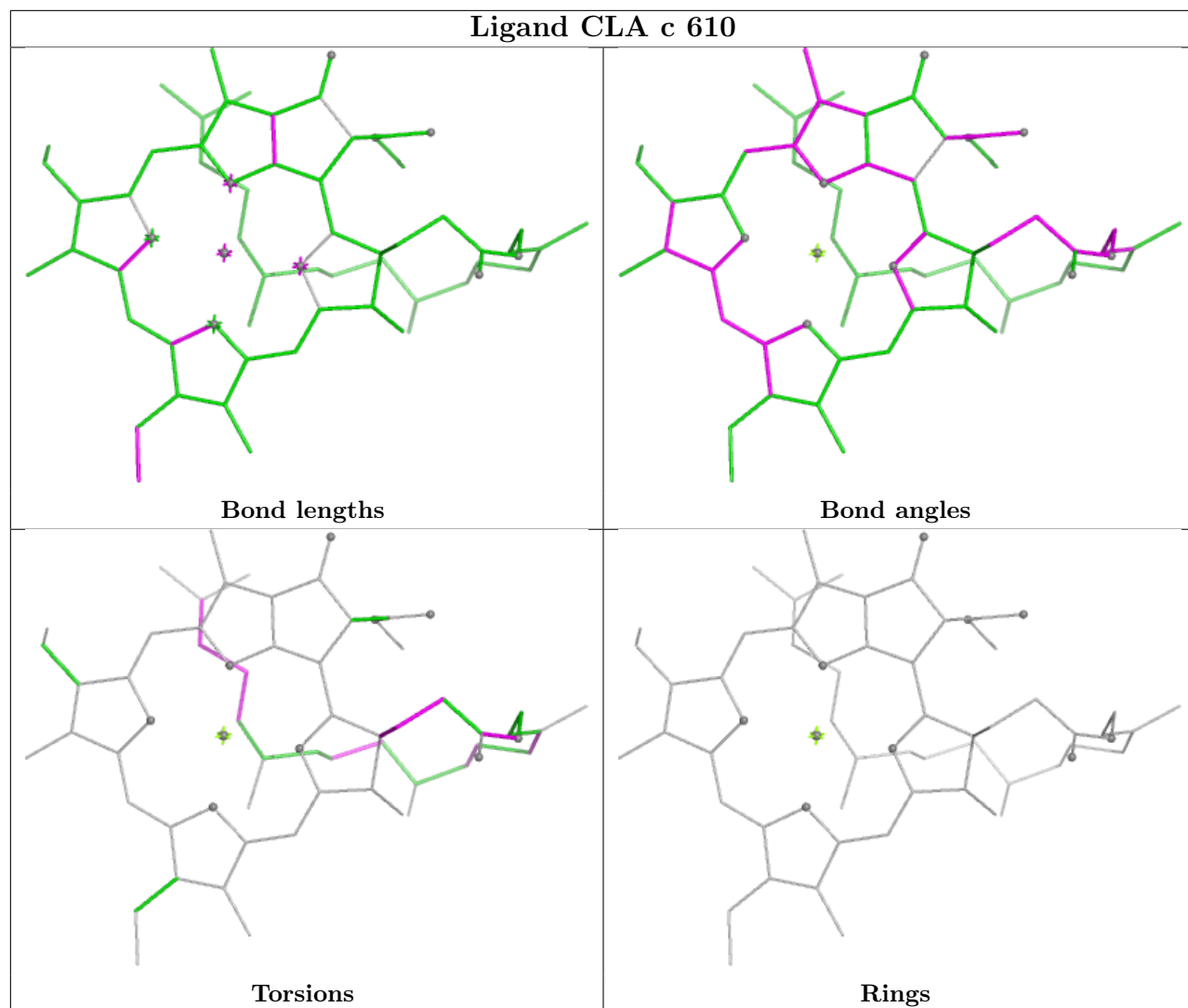


Torsions

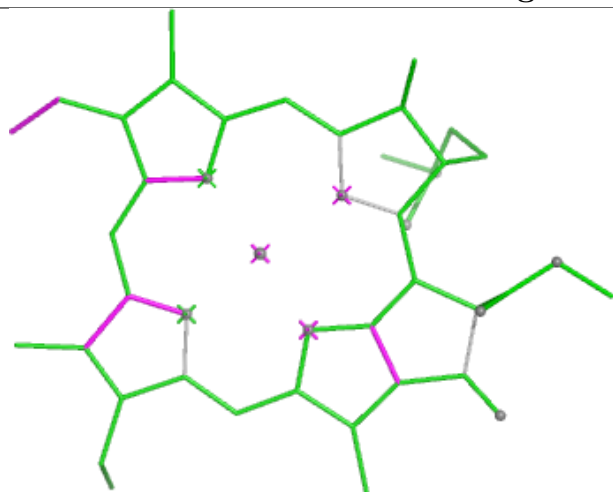


Rings

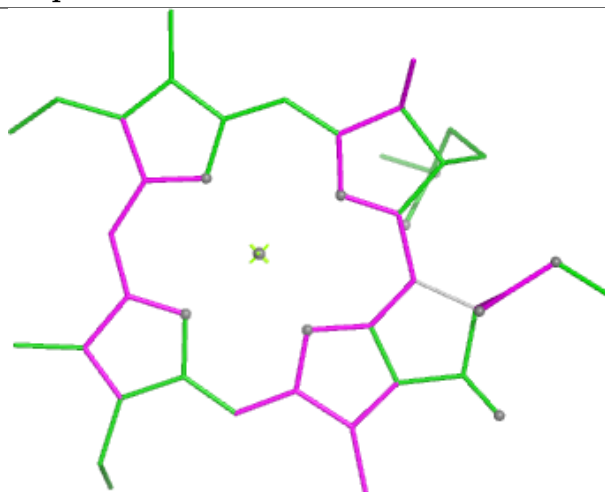
Ligand CLA c 610



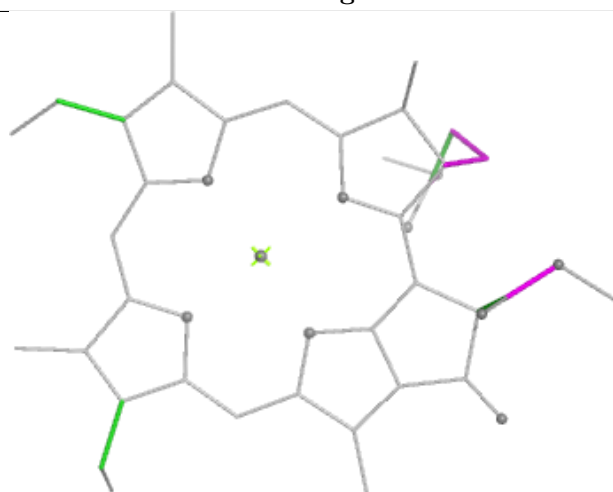
Ligand CLA p 615



Bond lengths



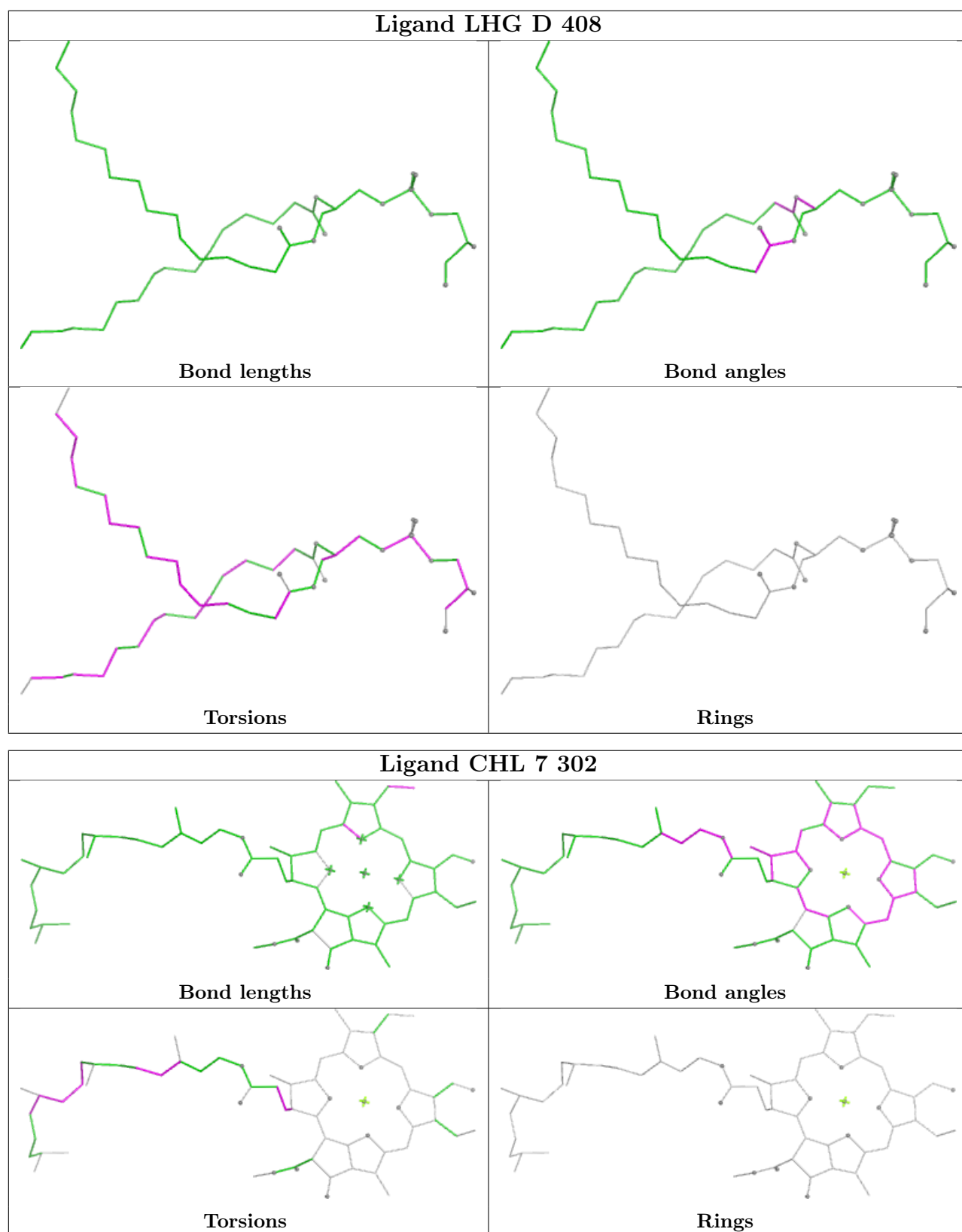
Bond angles

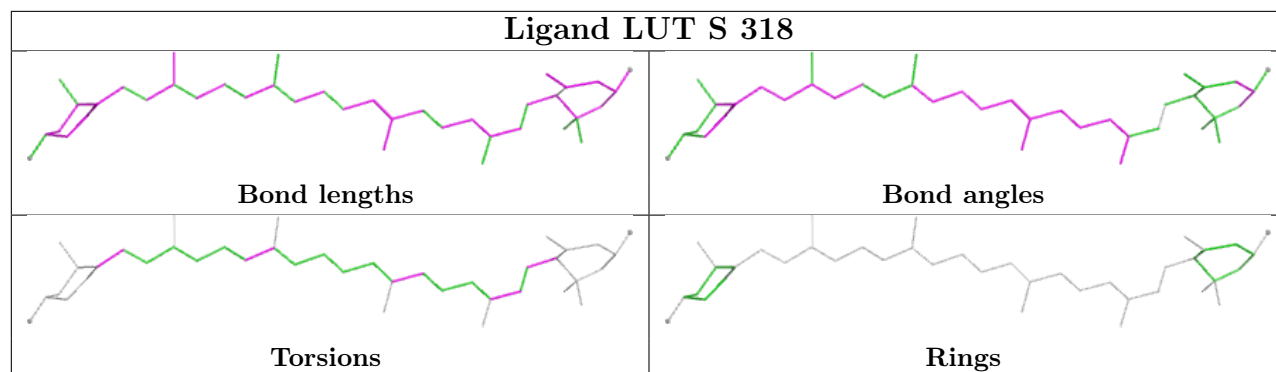
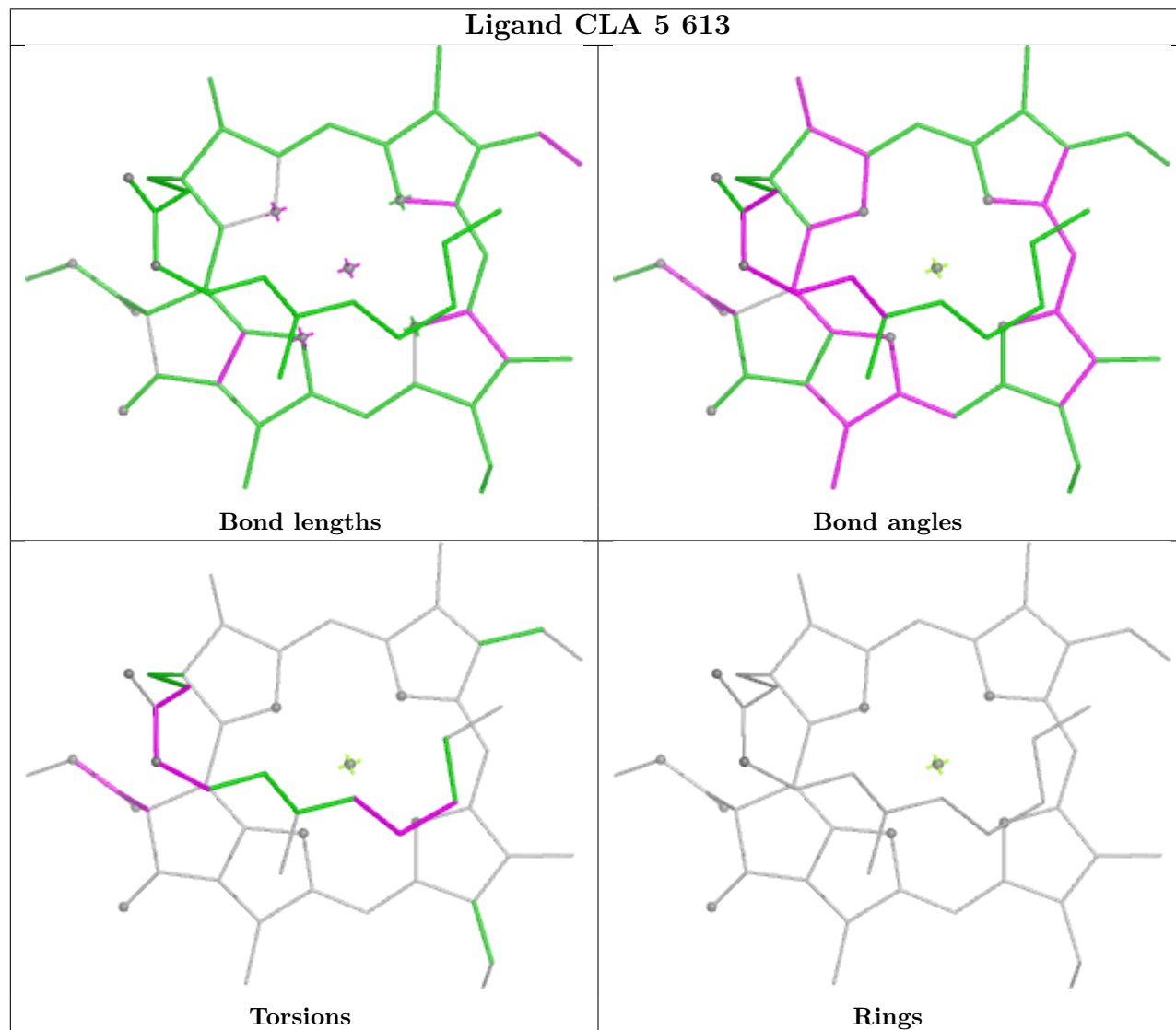


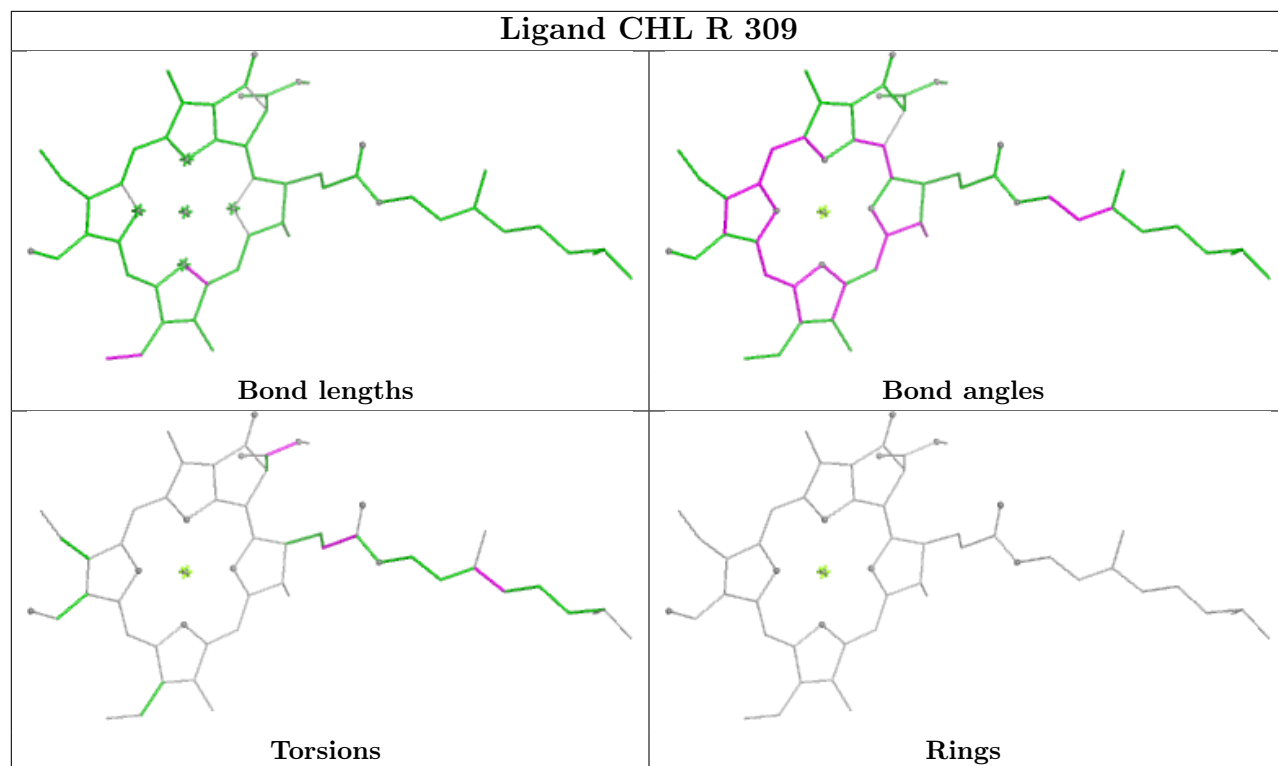
Torsions

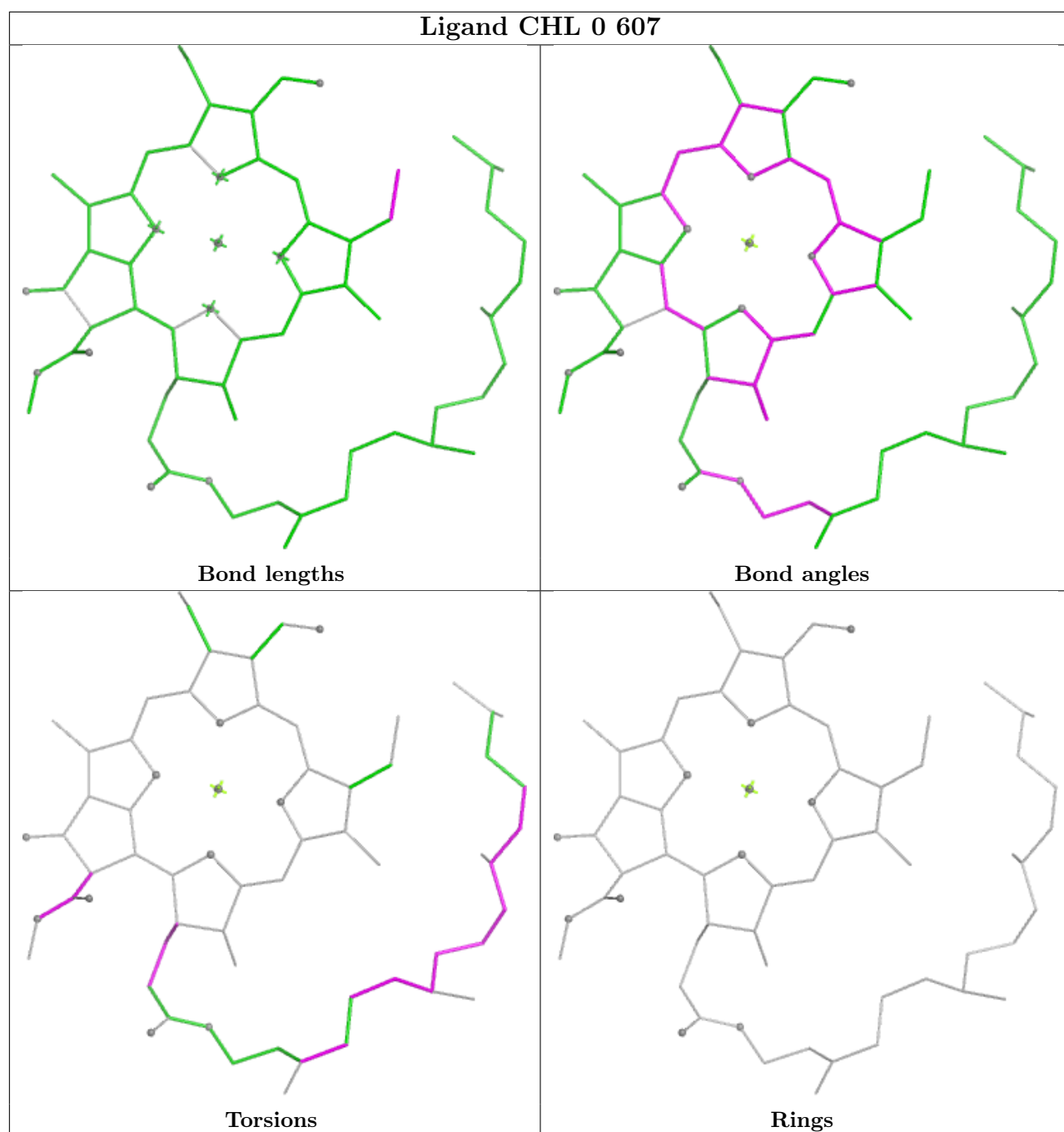


Rings

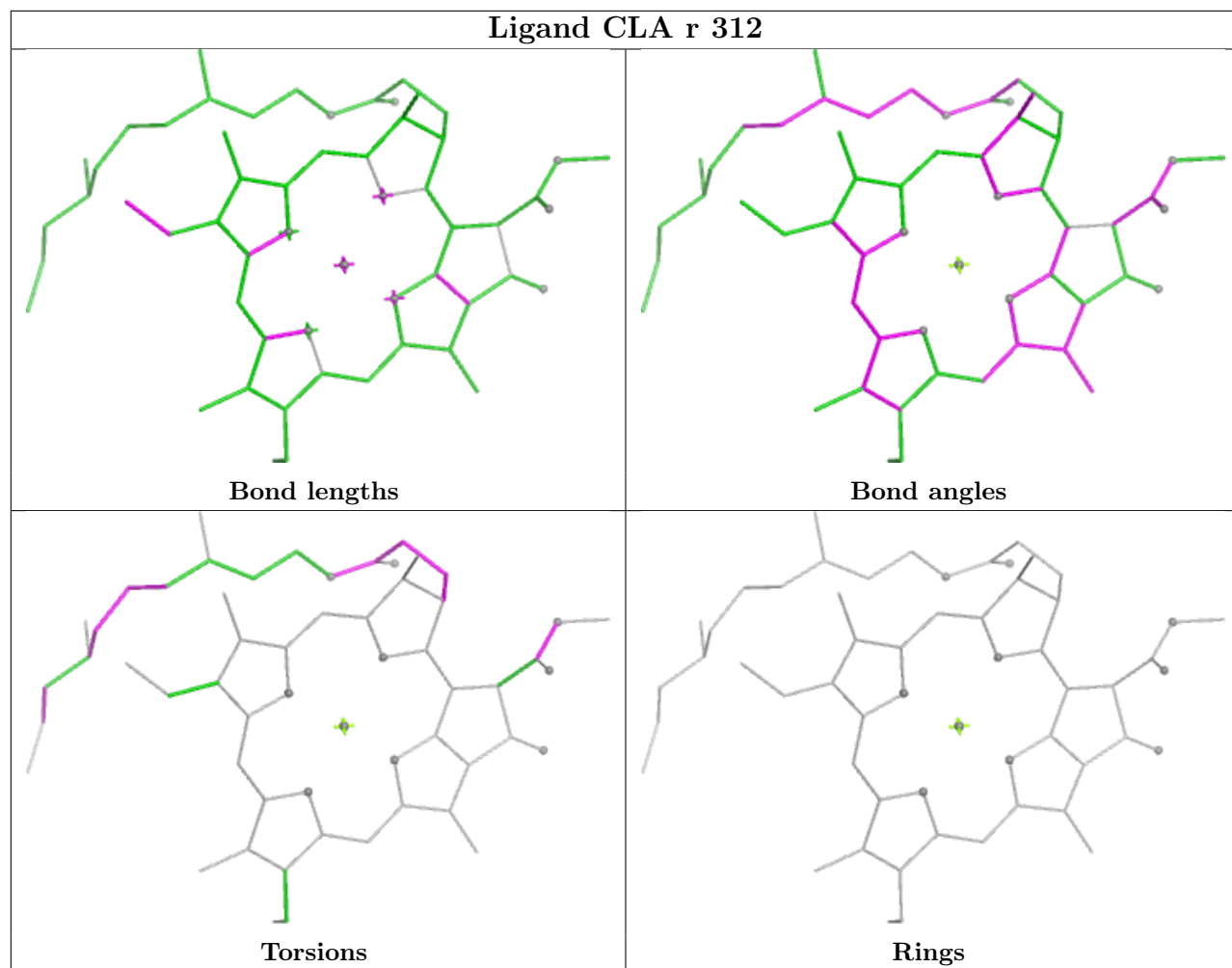


Ligand LUT S 318**Ligand CLA 5 613**

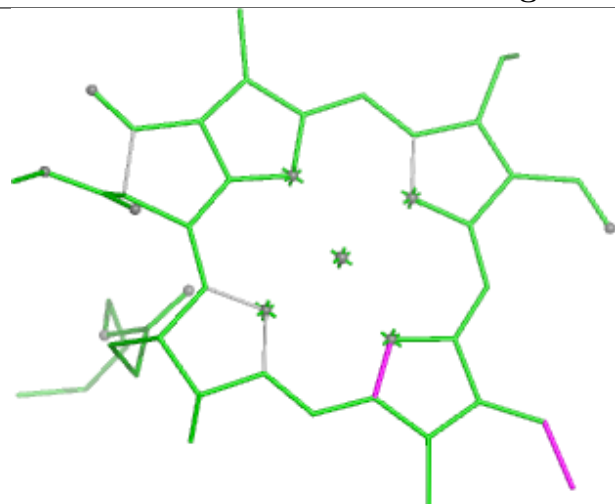




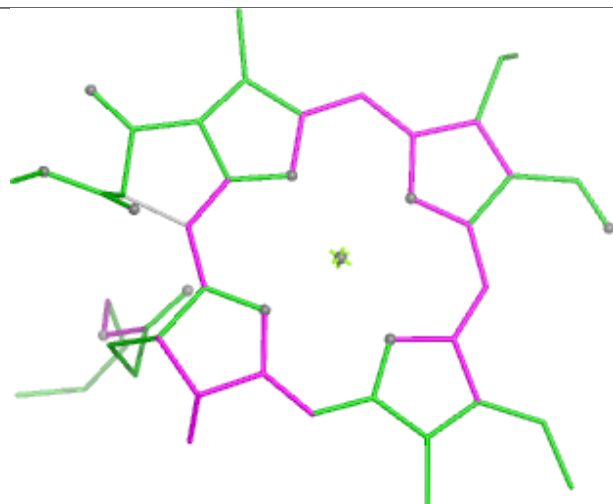
Ligand CLA r 312



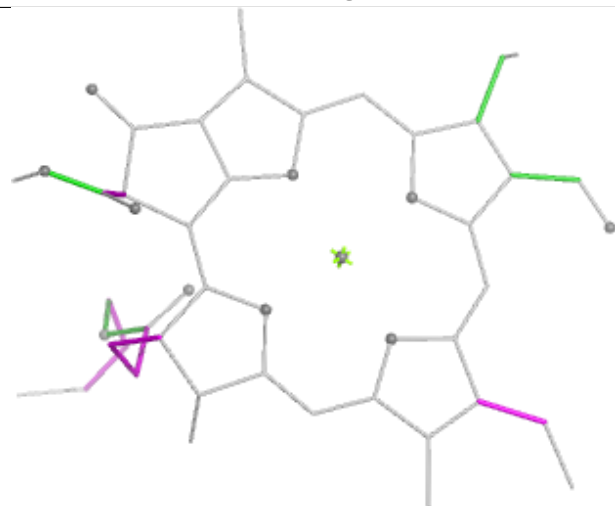
Ligand CHL 5 608



Bond lengths



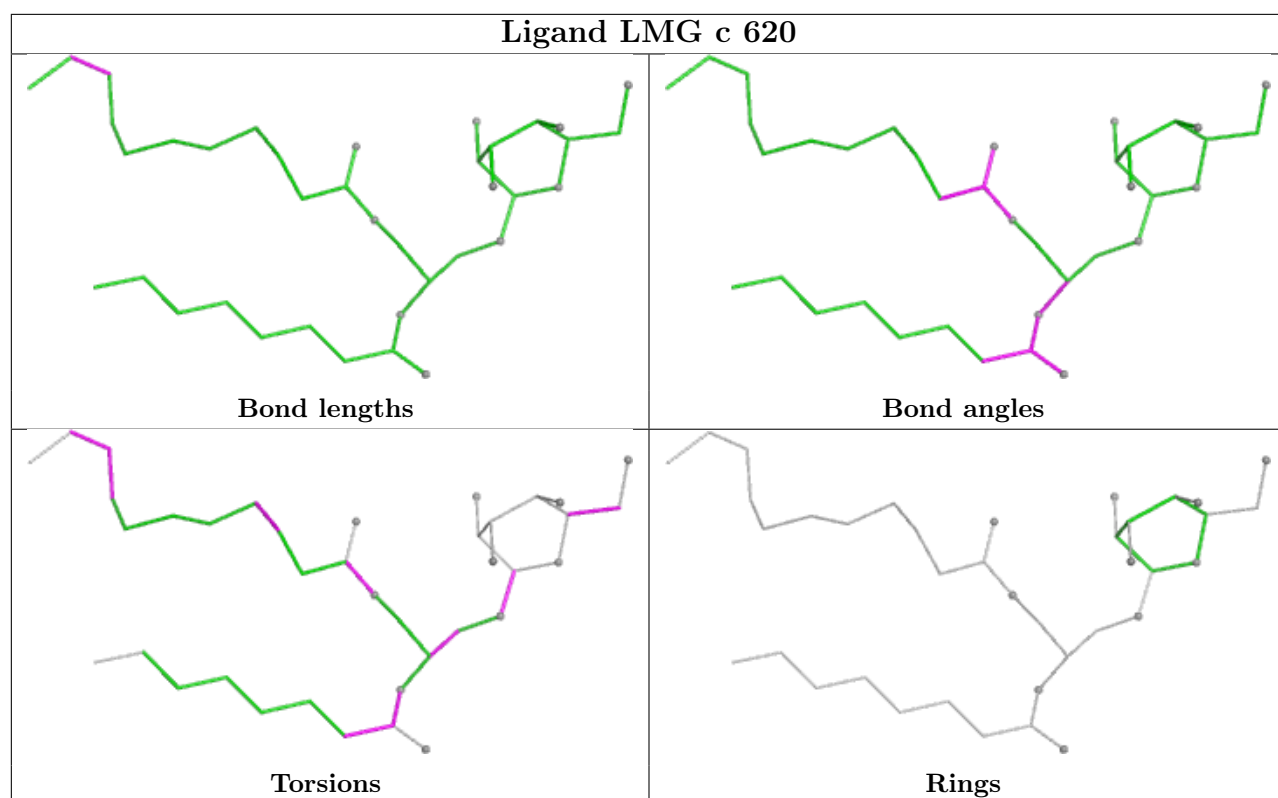
Bond angles



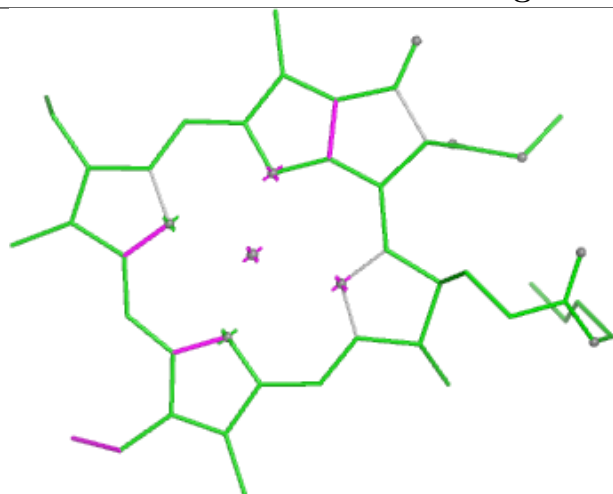
Torsions



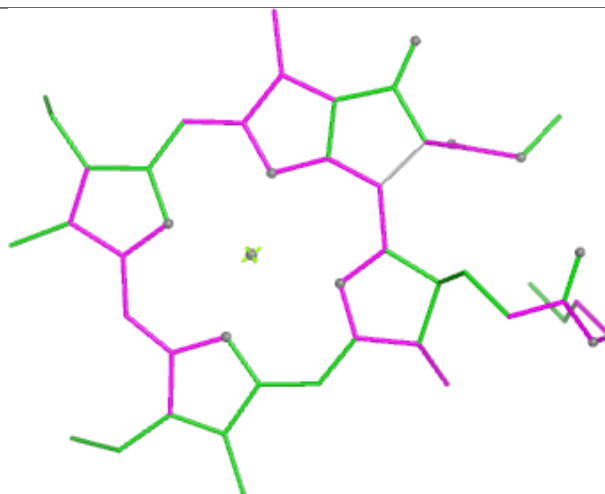
Rings



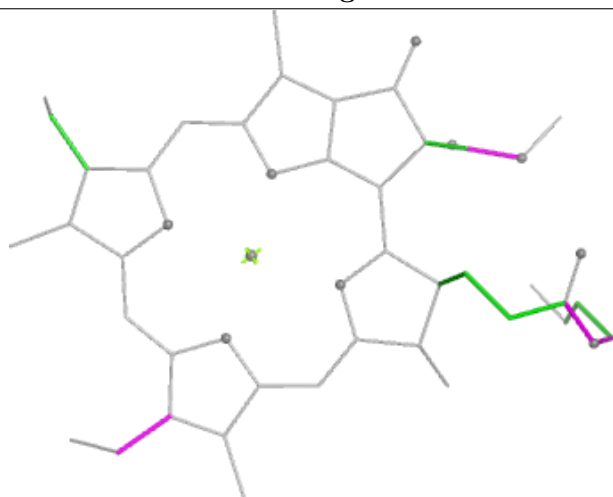
Ligand CLA R 314



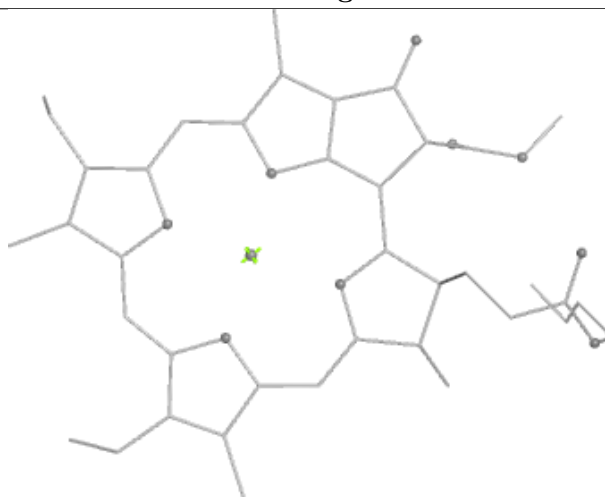
Bond lengths



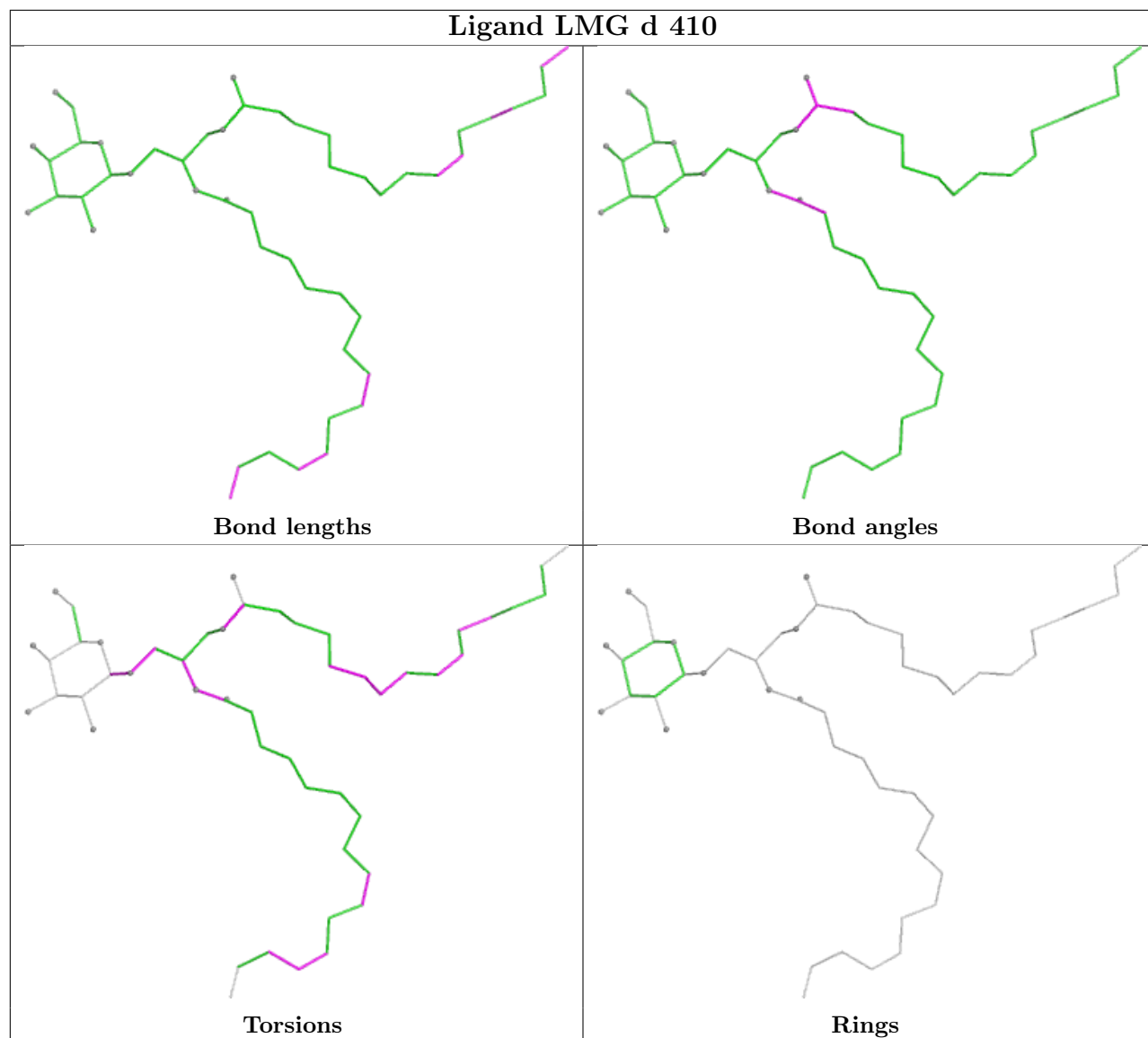
Bond angles

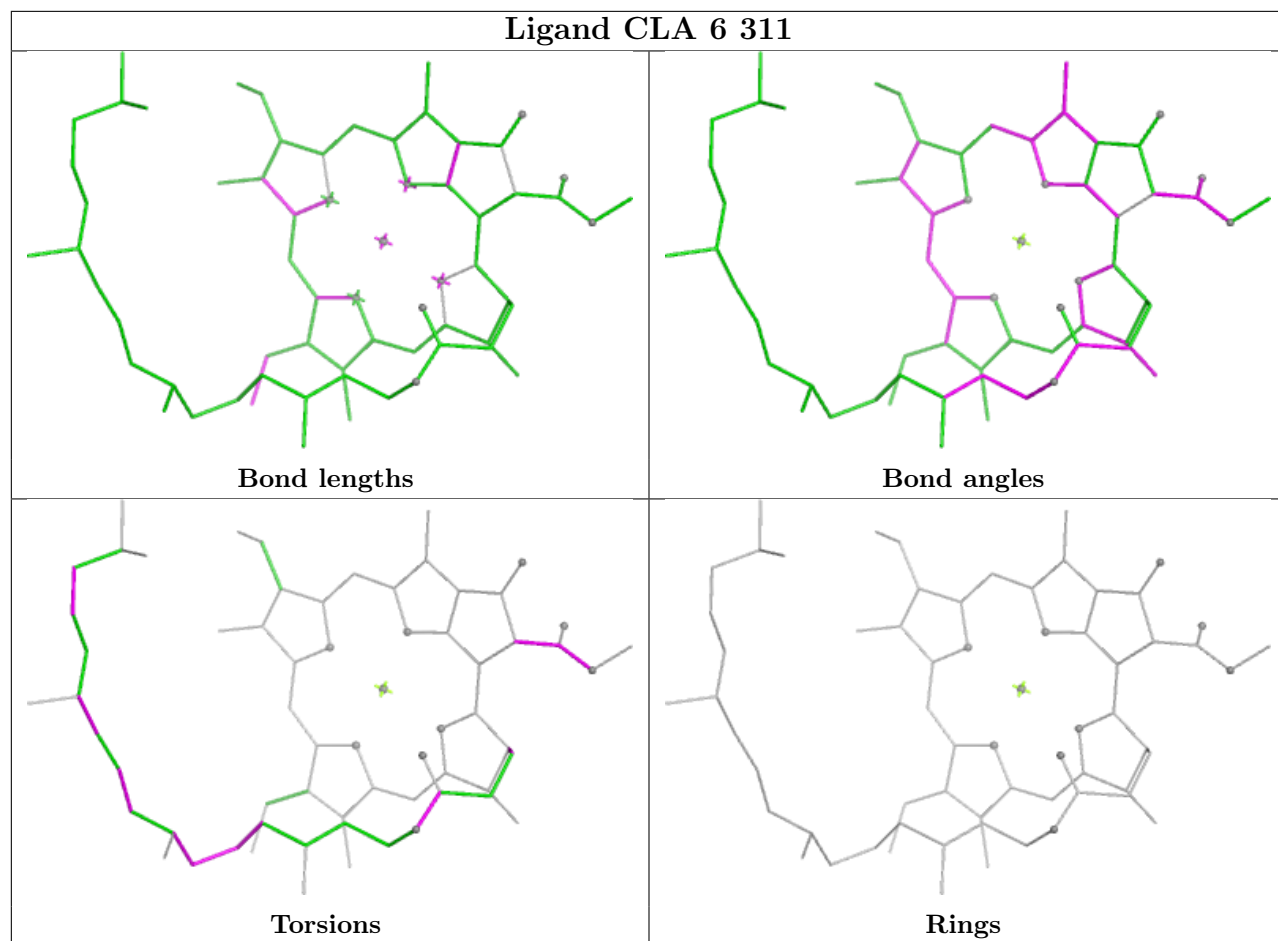
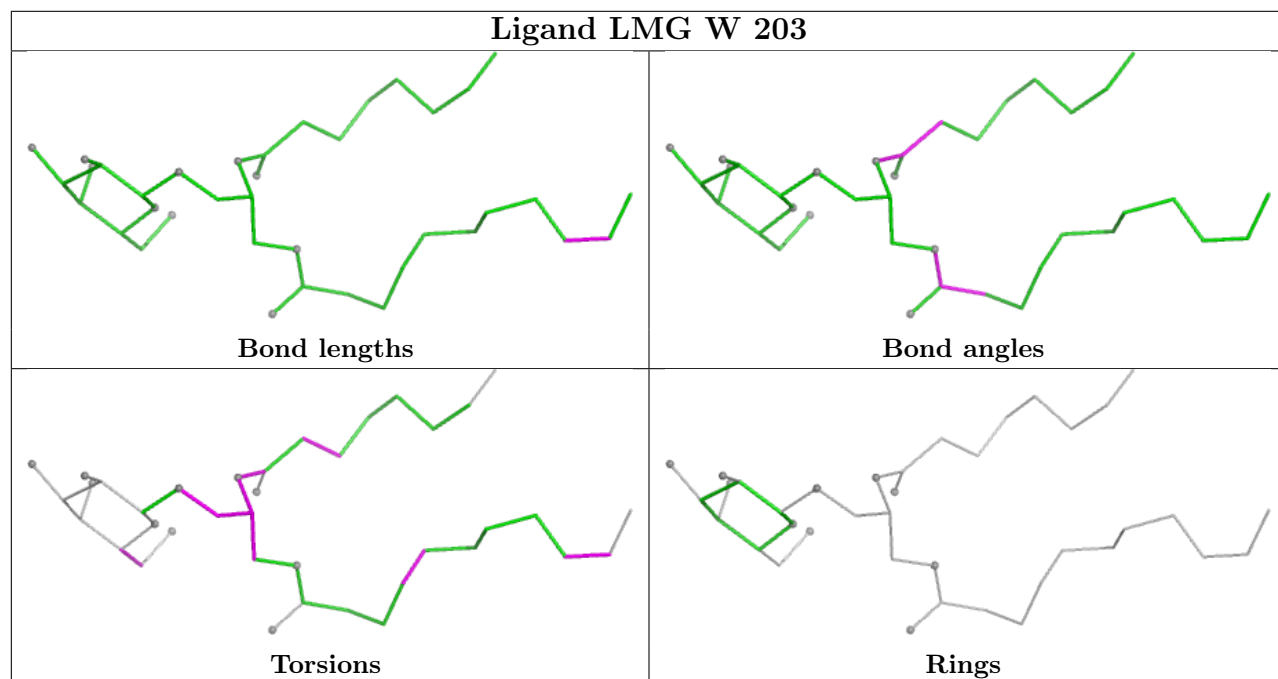


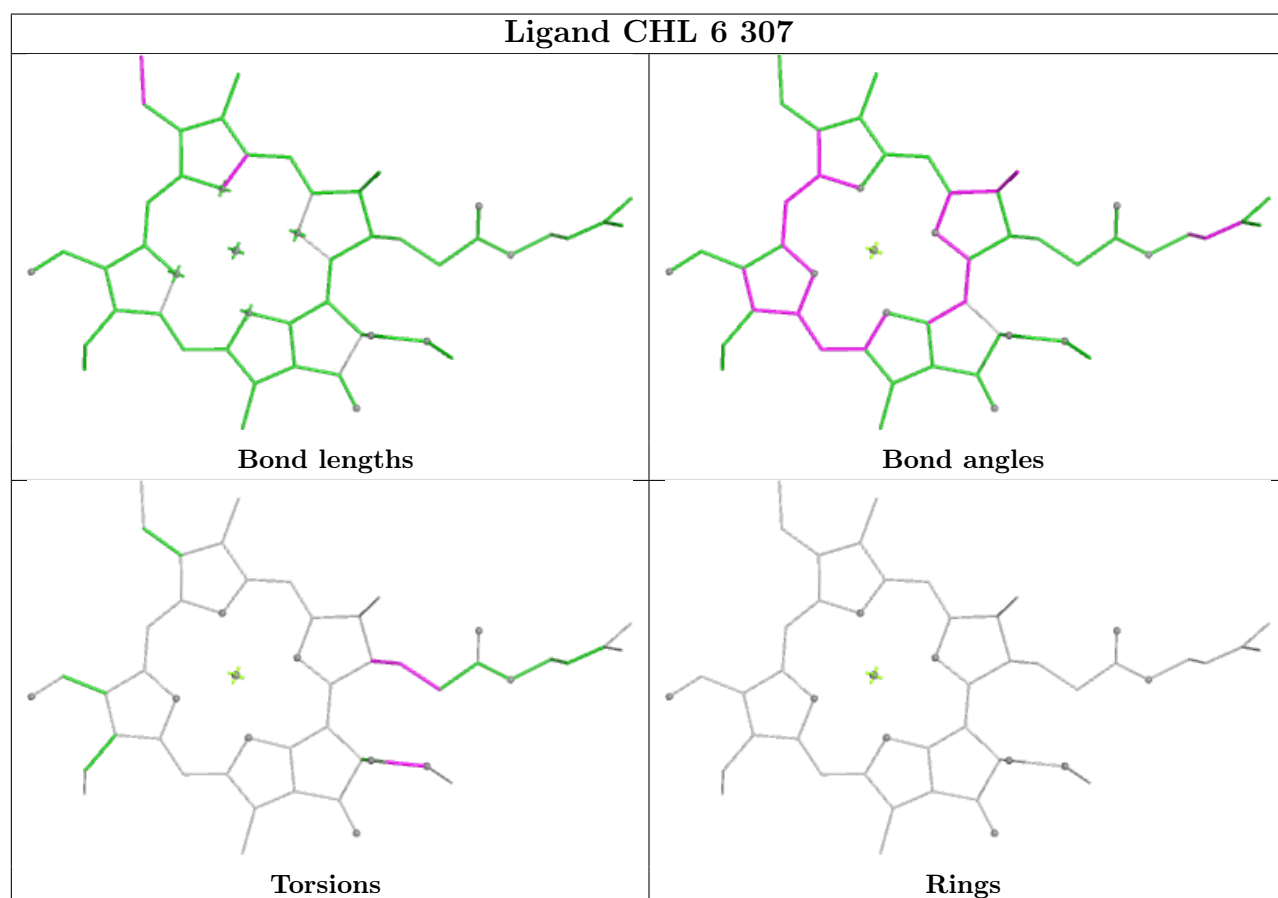
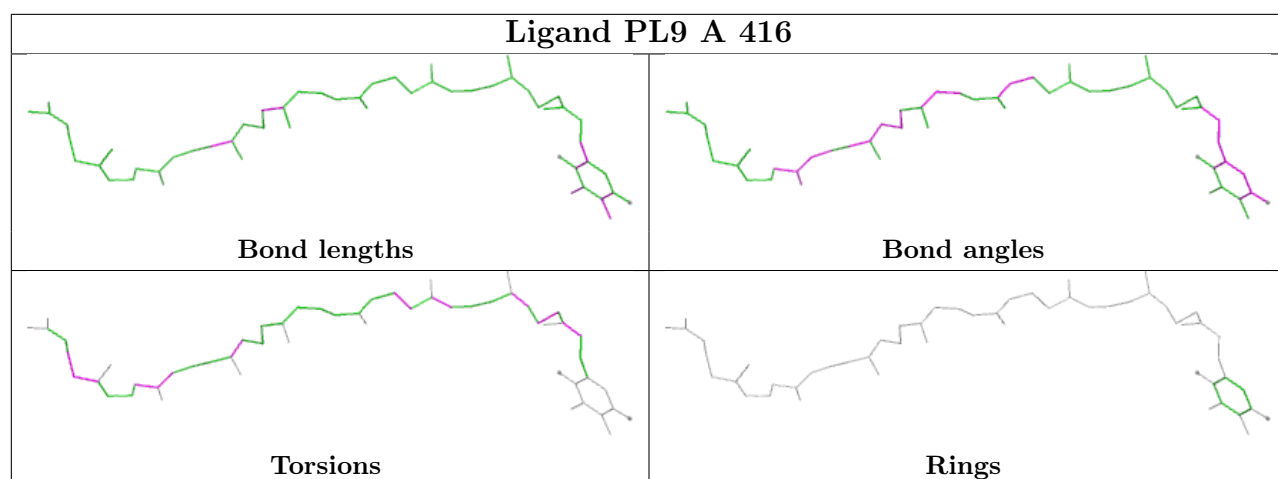
Torsions



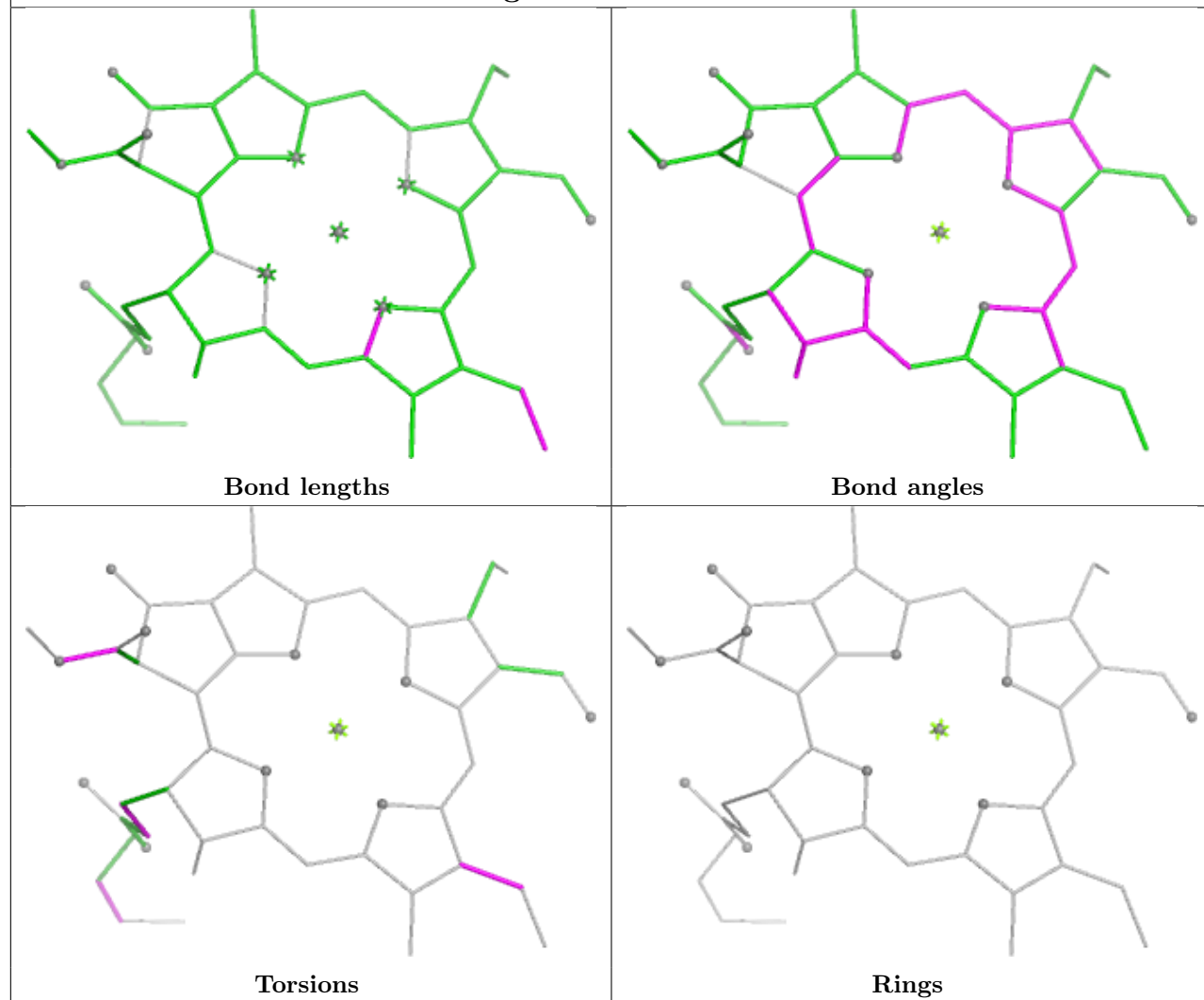
Rings

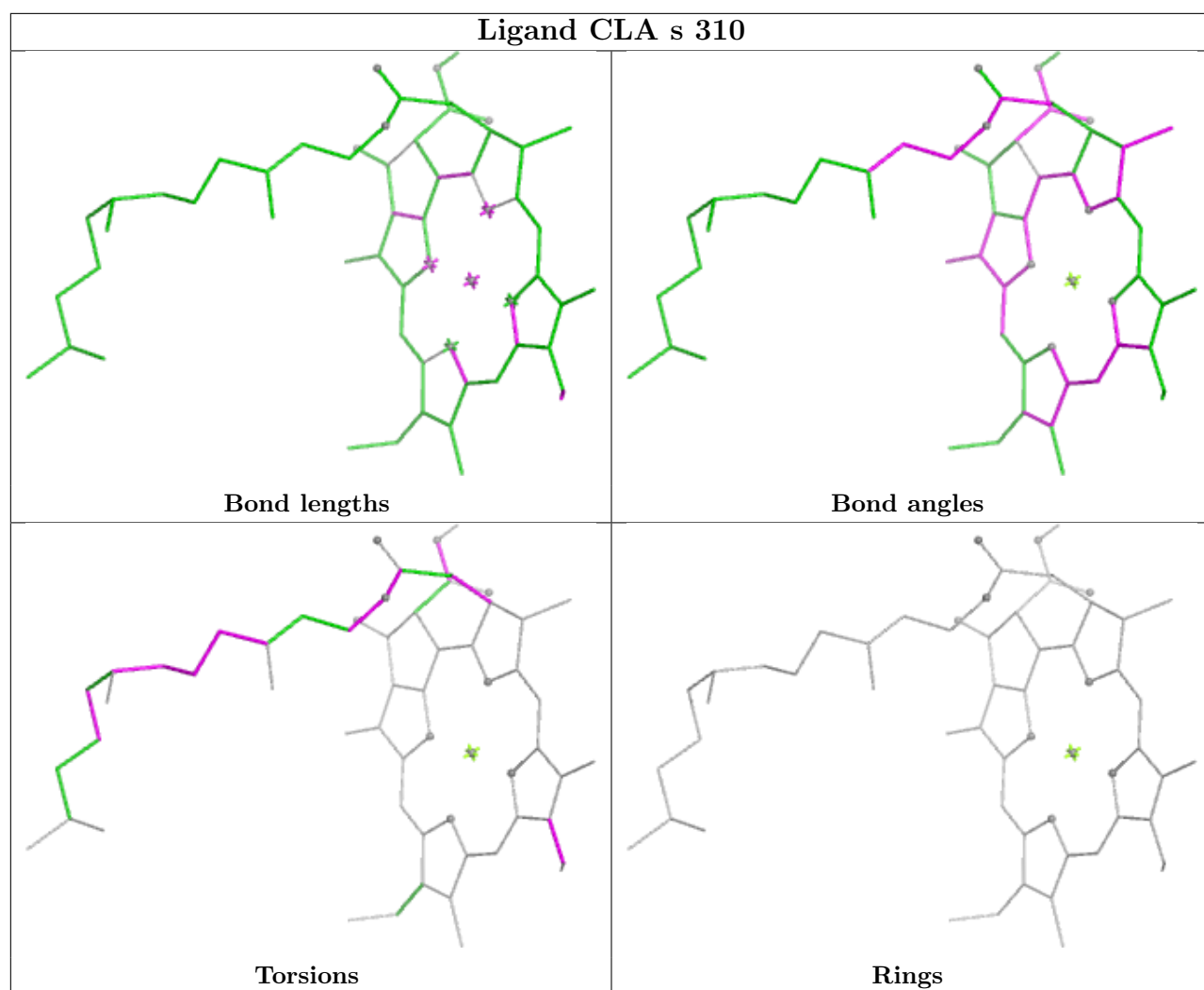


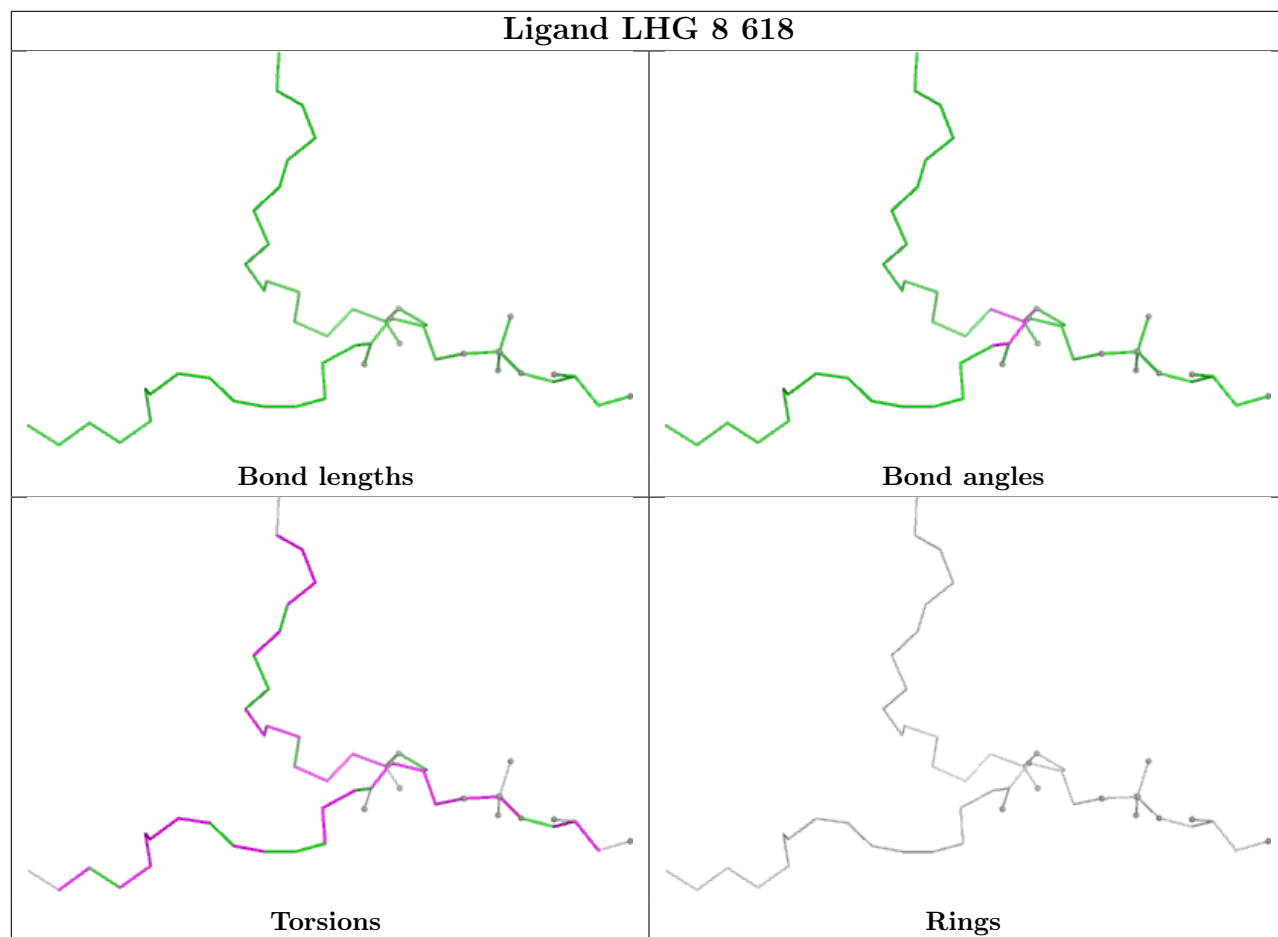
Ligand CLA 6 311**Ligand LMG W 203**

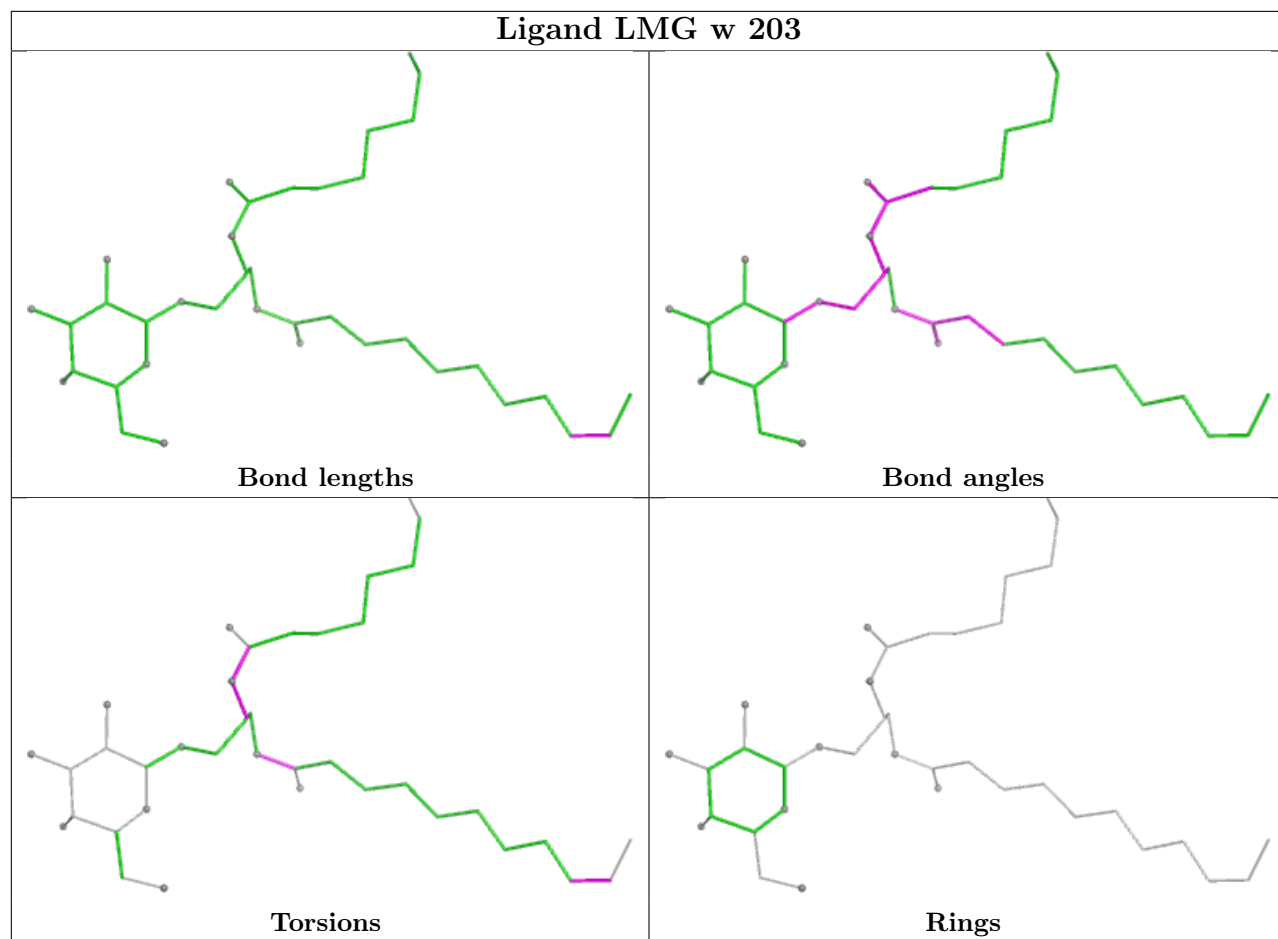


Ligand CHL n 309

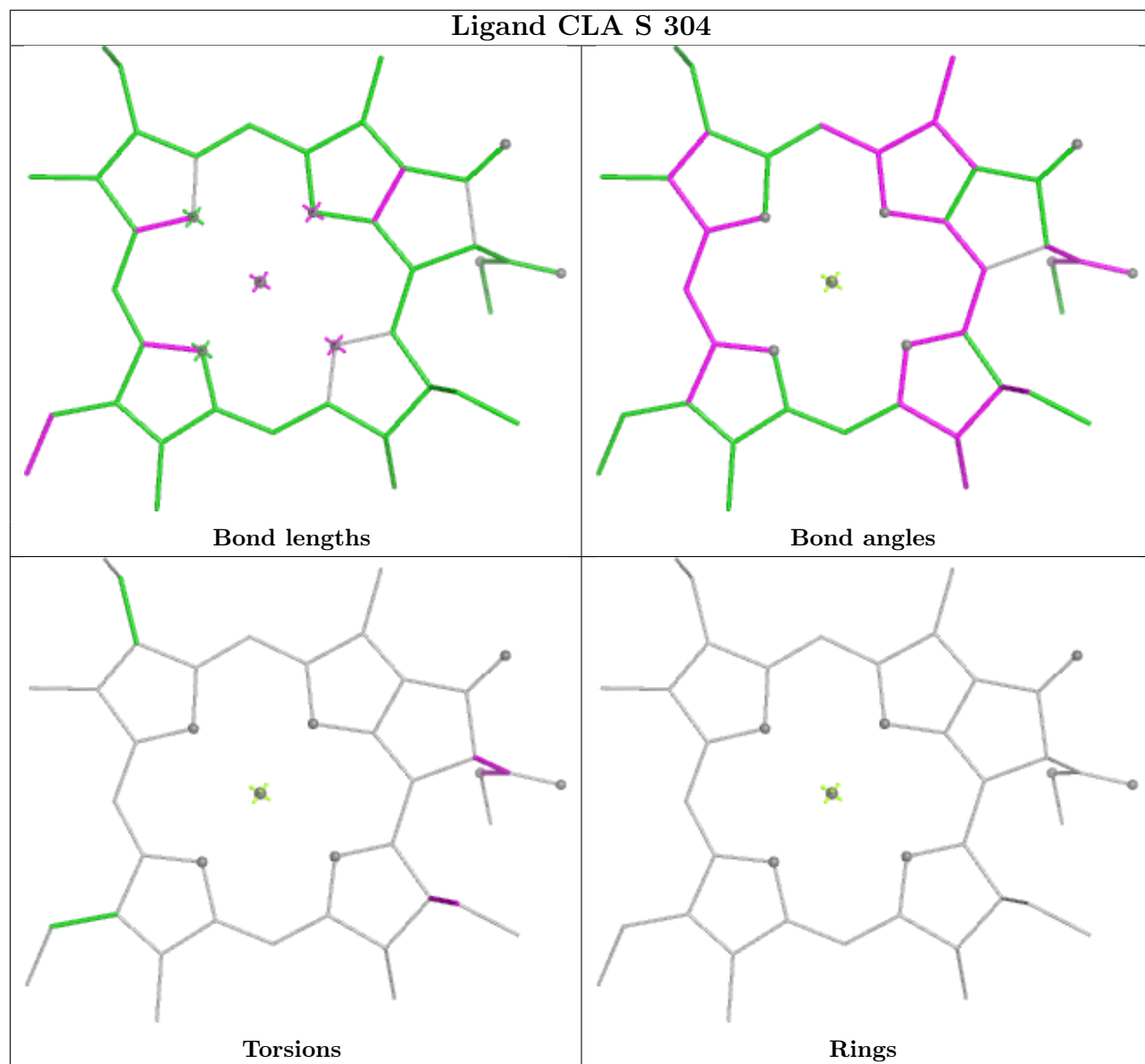




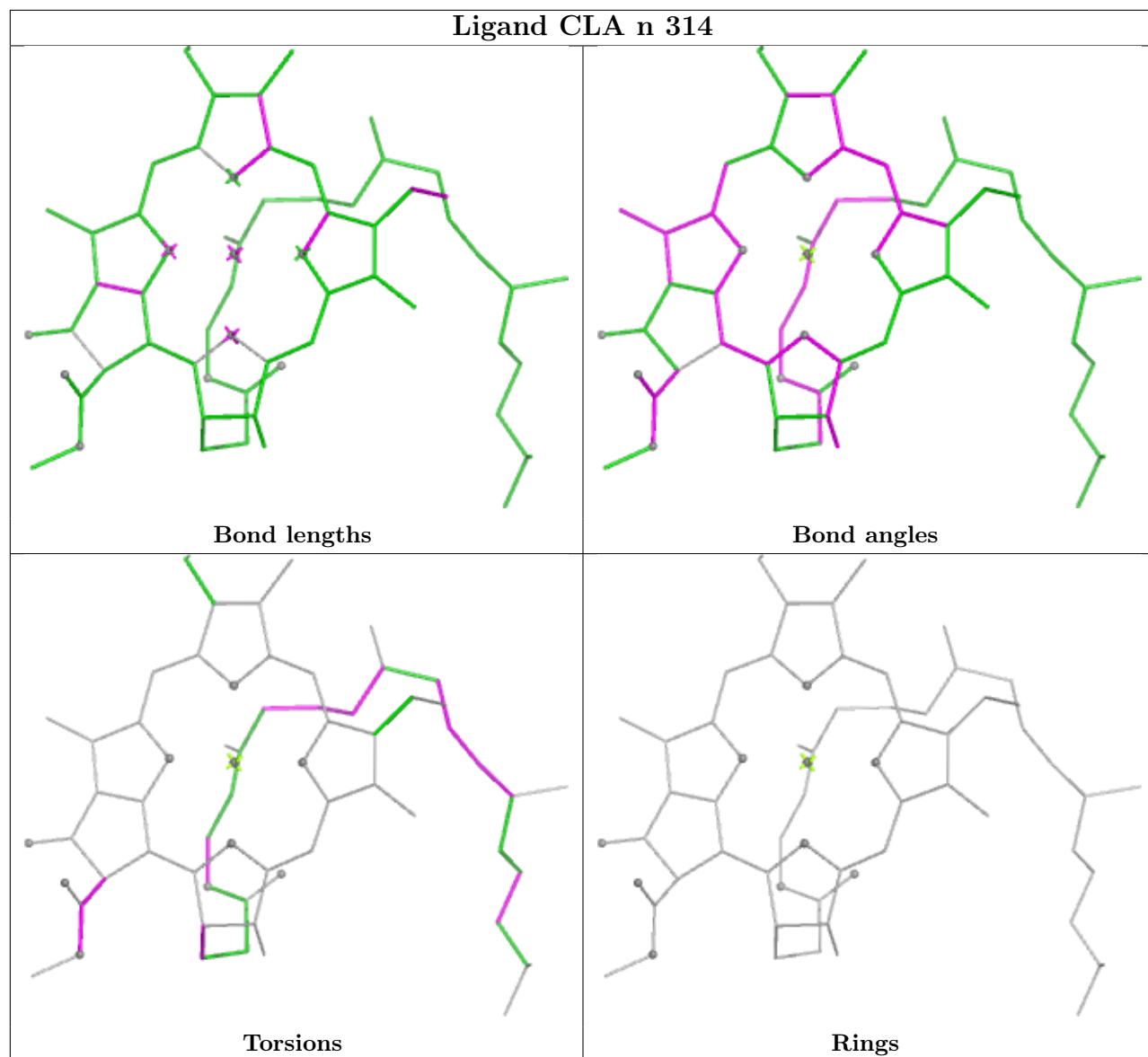




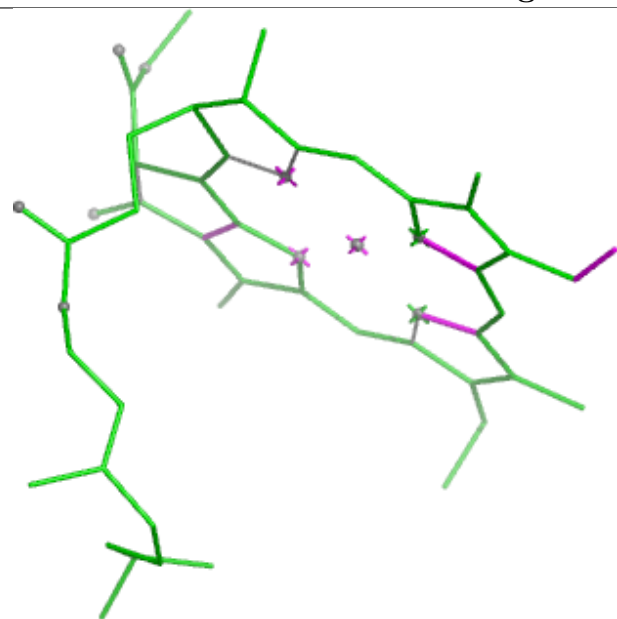
Ligand CLA S 304



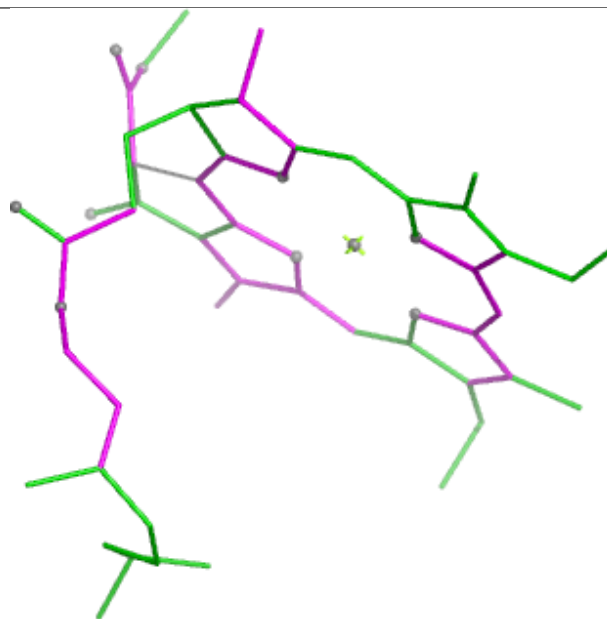
Ligand CLA n 314



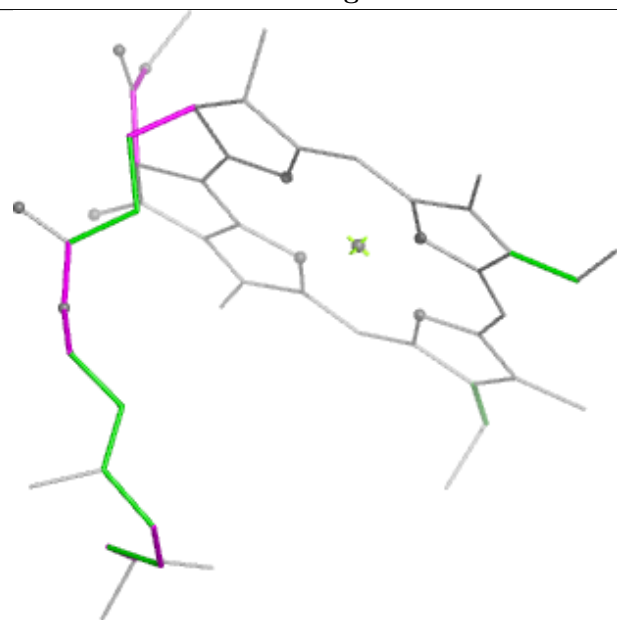
Ligand CLA Y 305



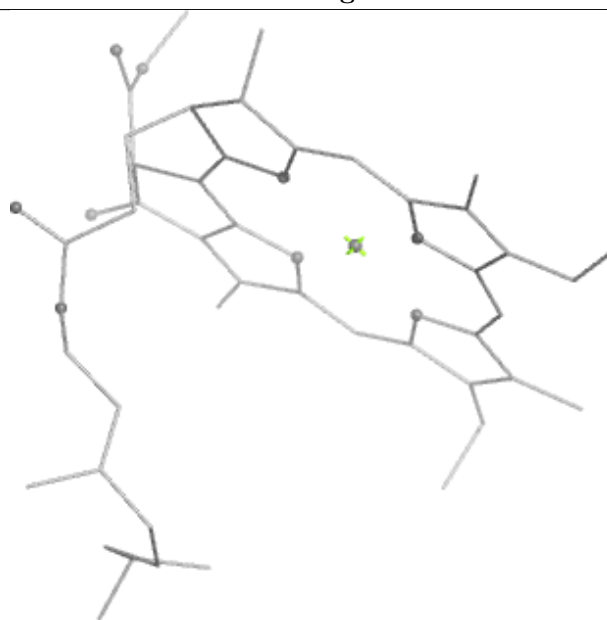
Bond lengths



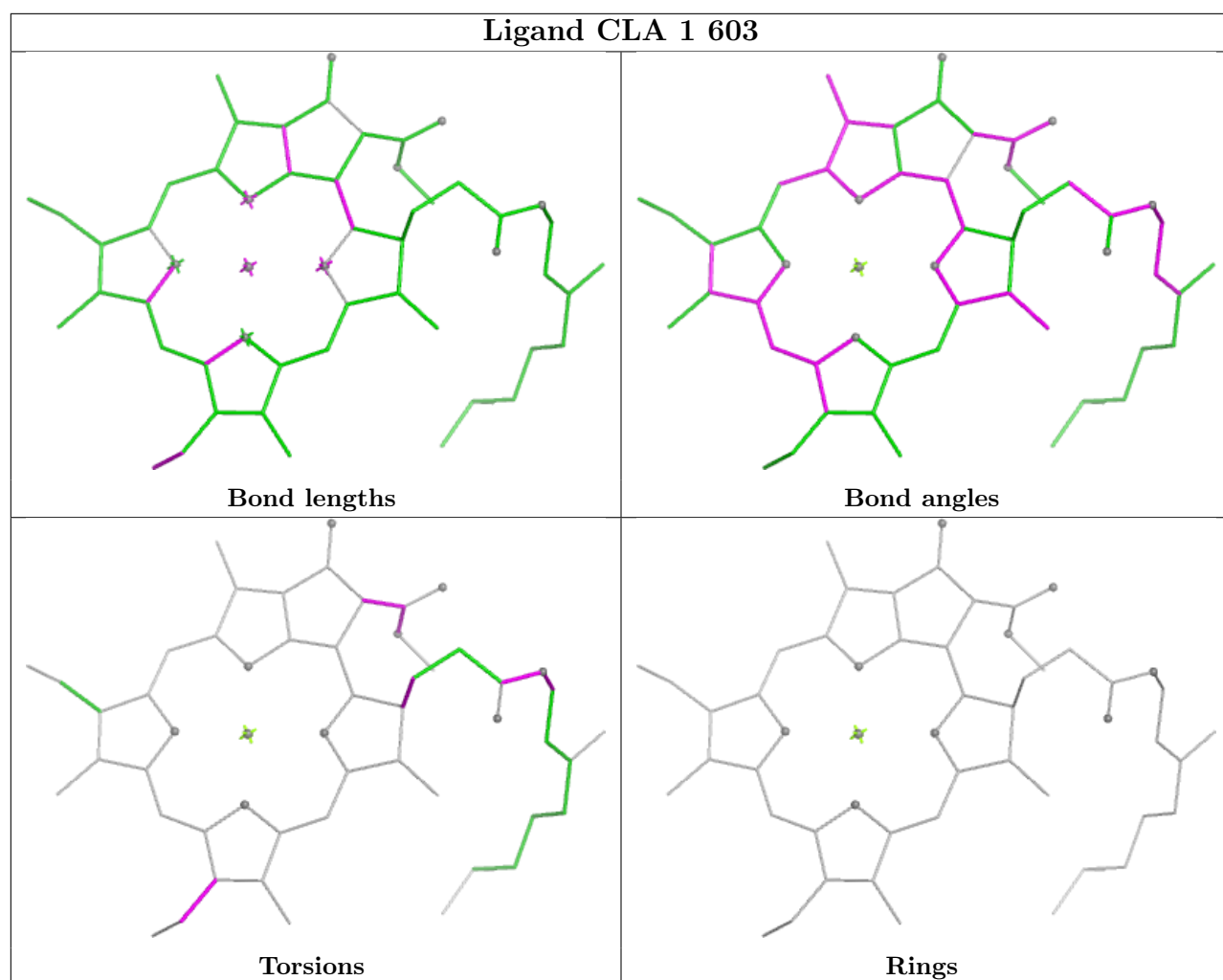
Bond angles

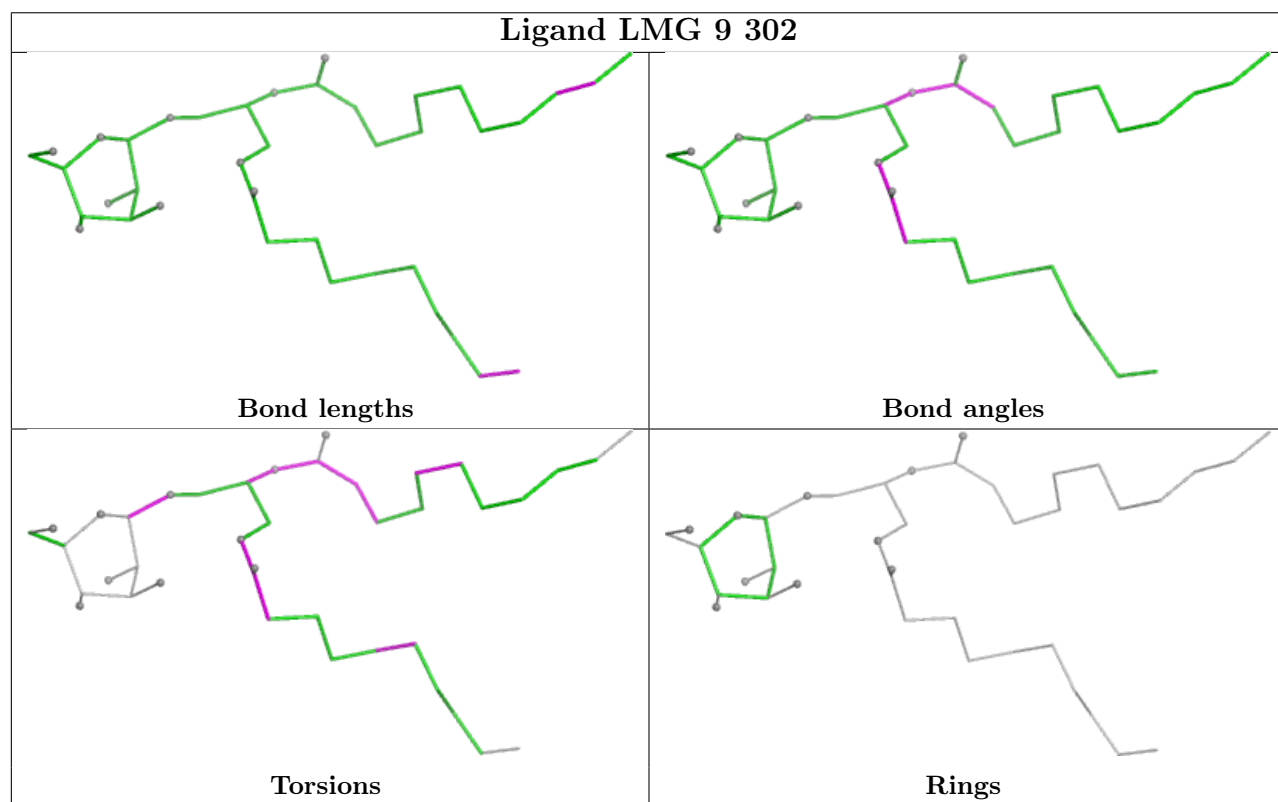
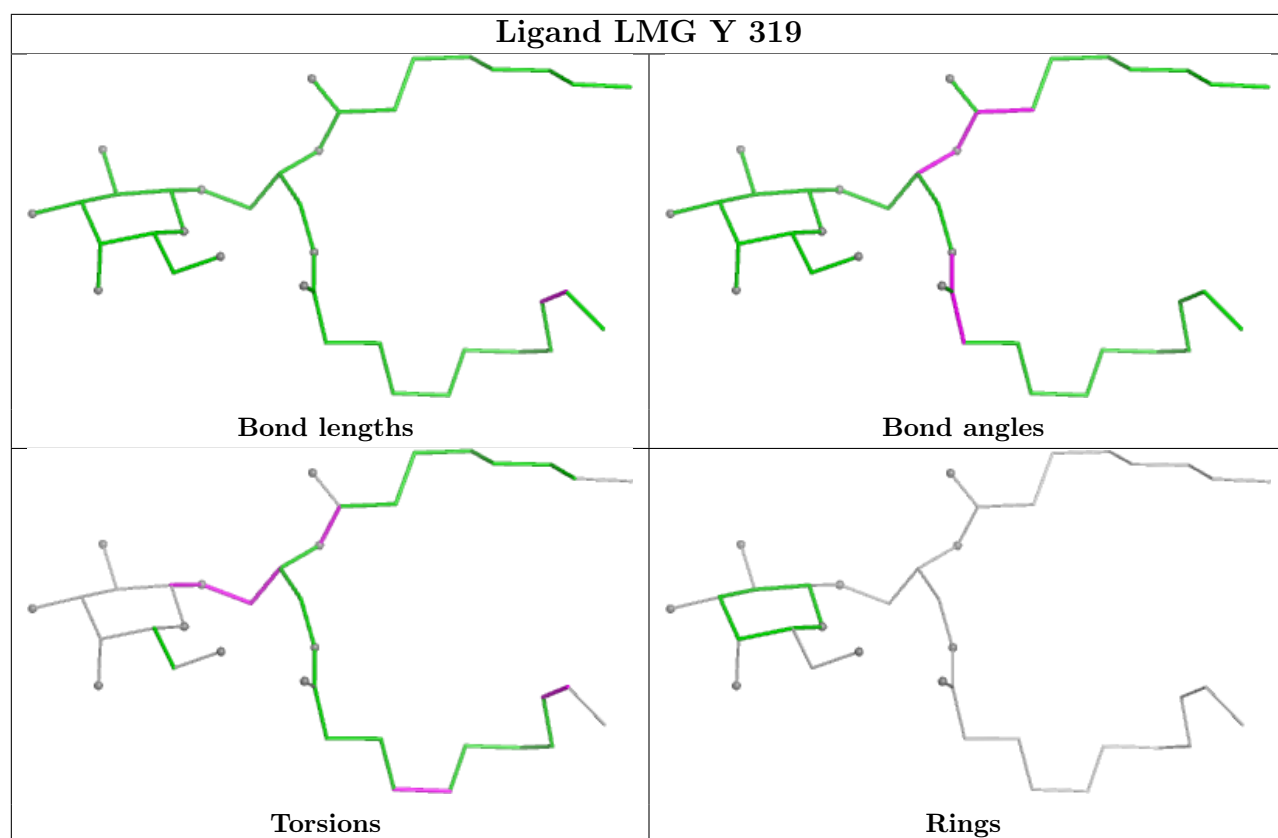


Torsions

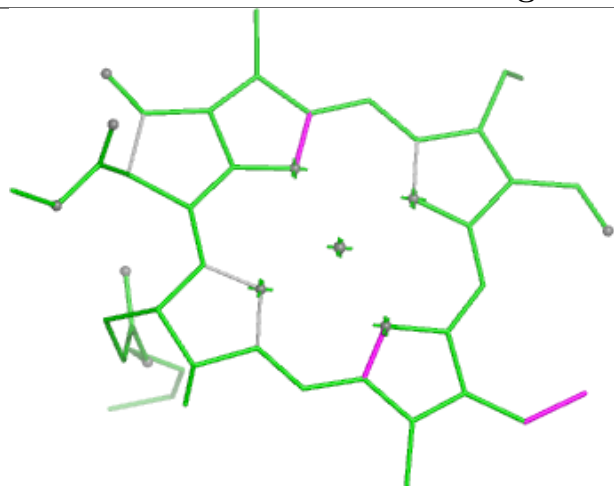


Rings

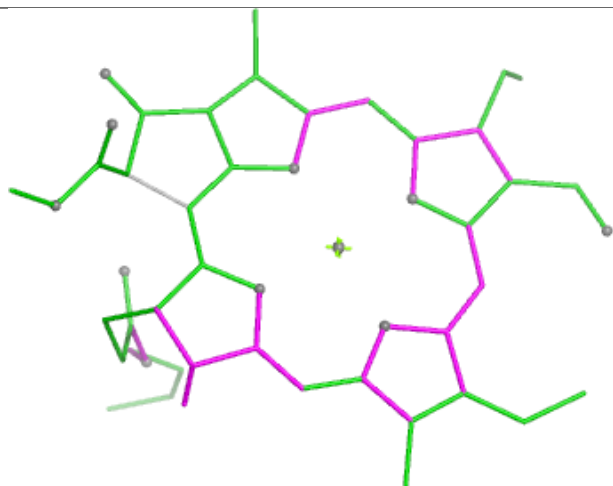




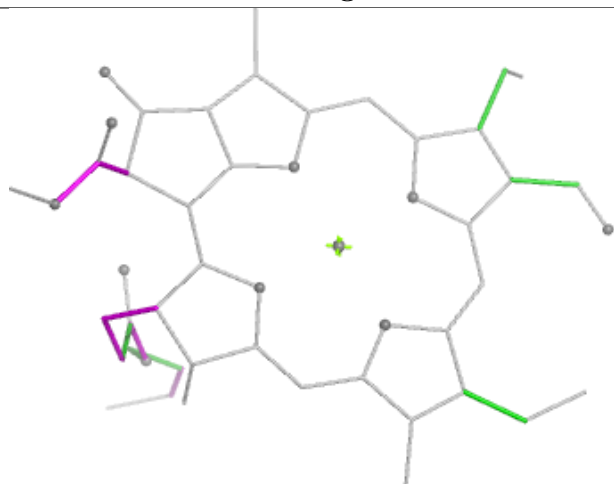
Ligand CHL 3 309



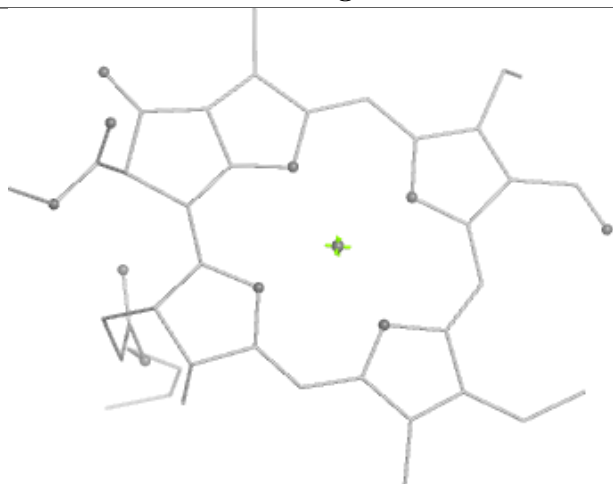
Bond lengths



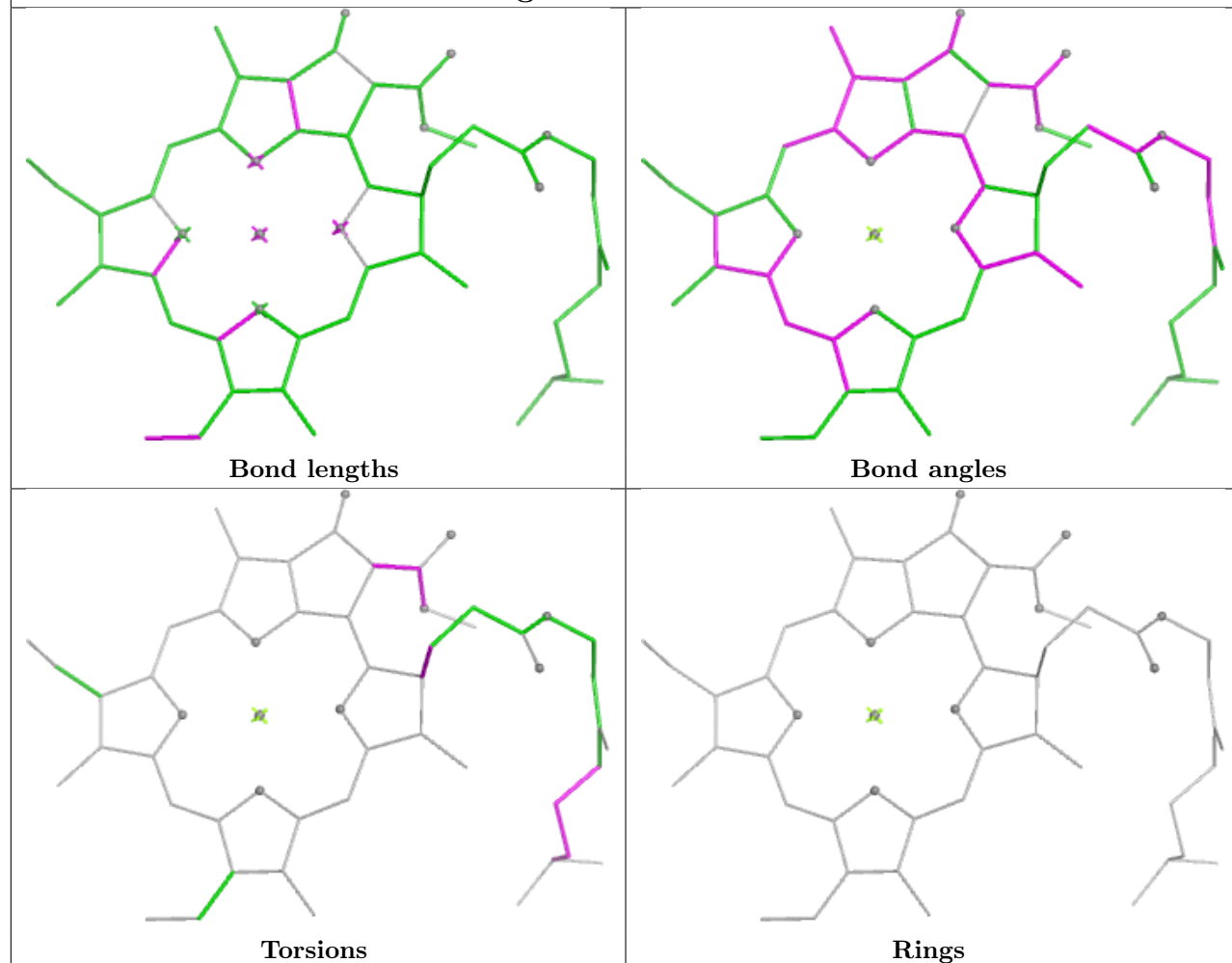
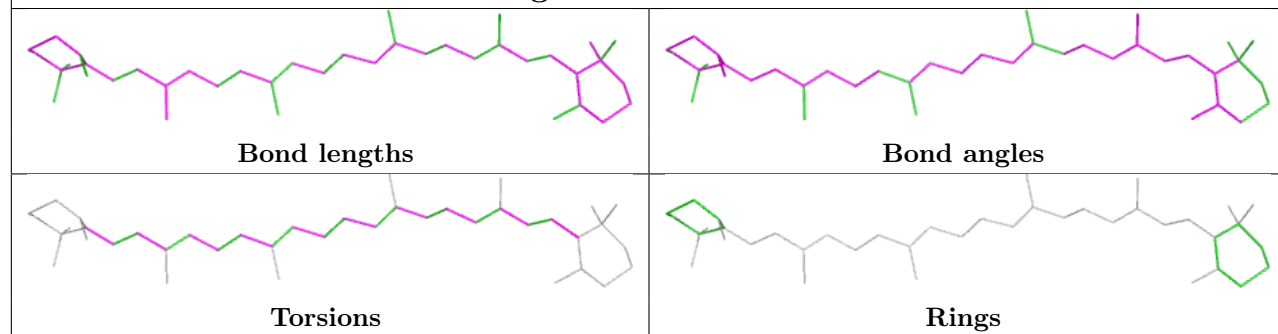
Bond angles



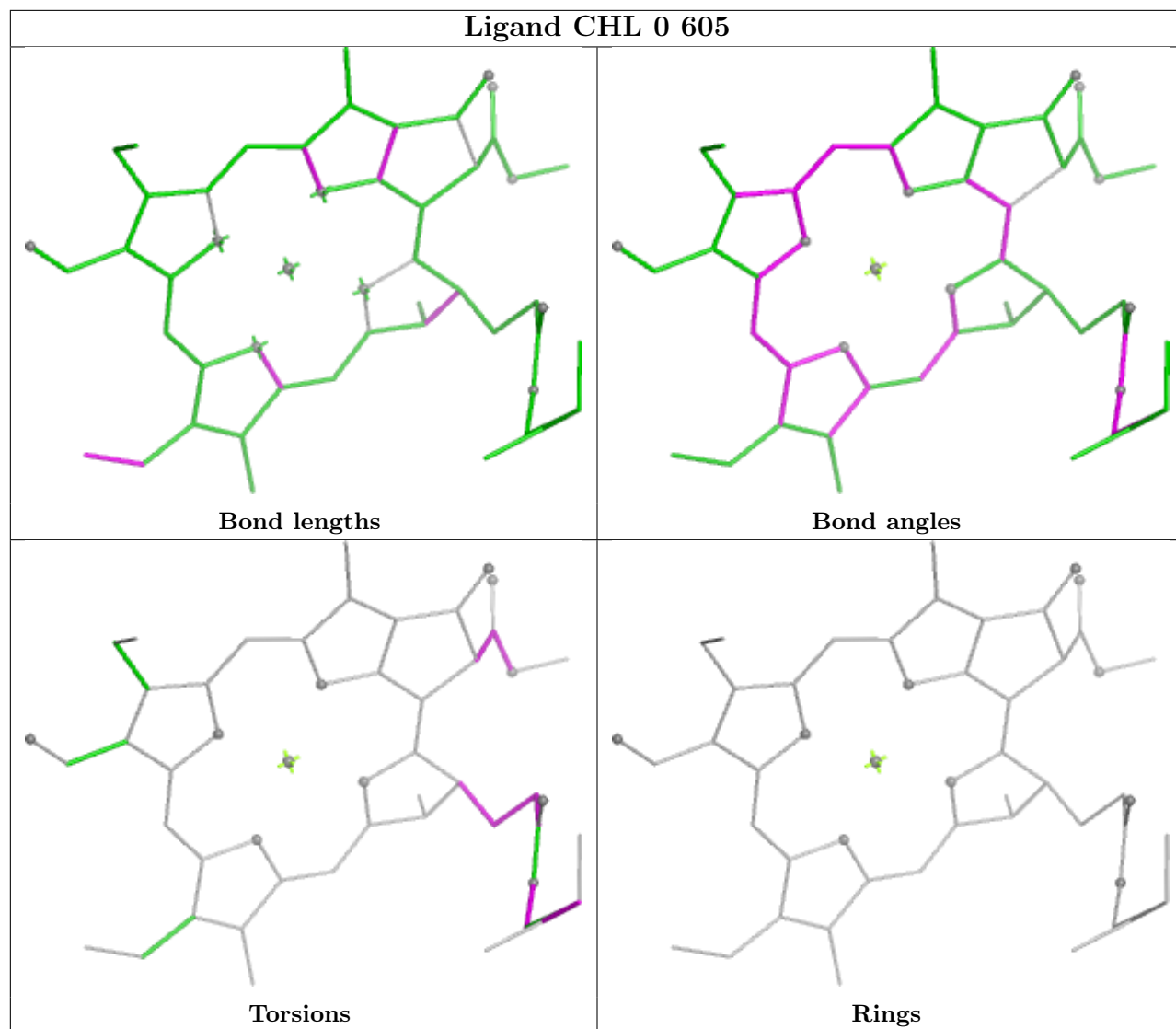
Torsions

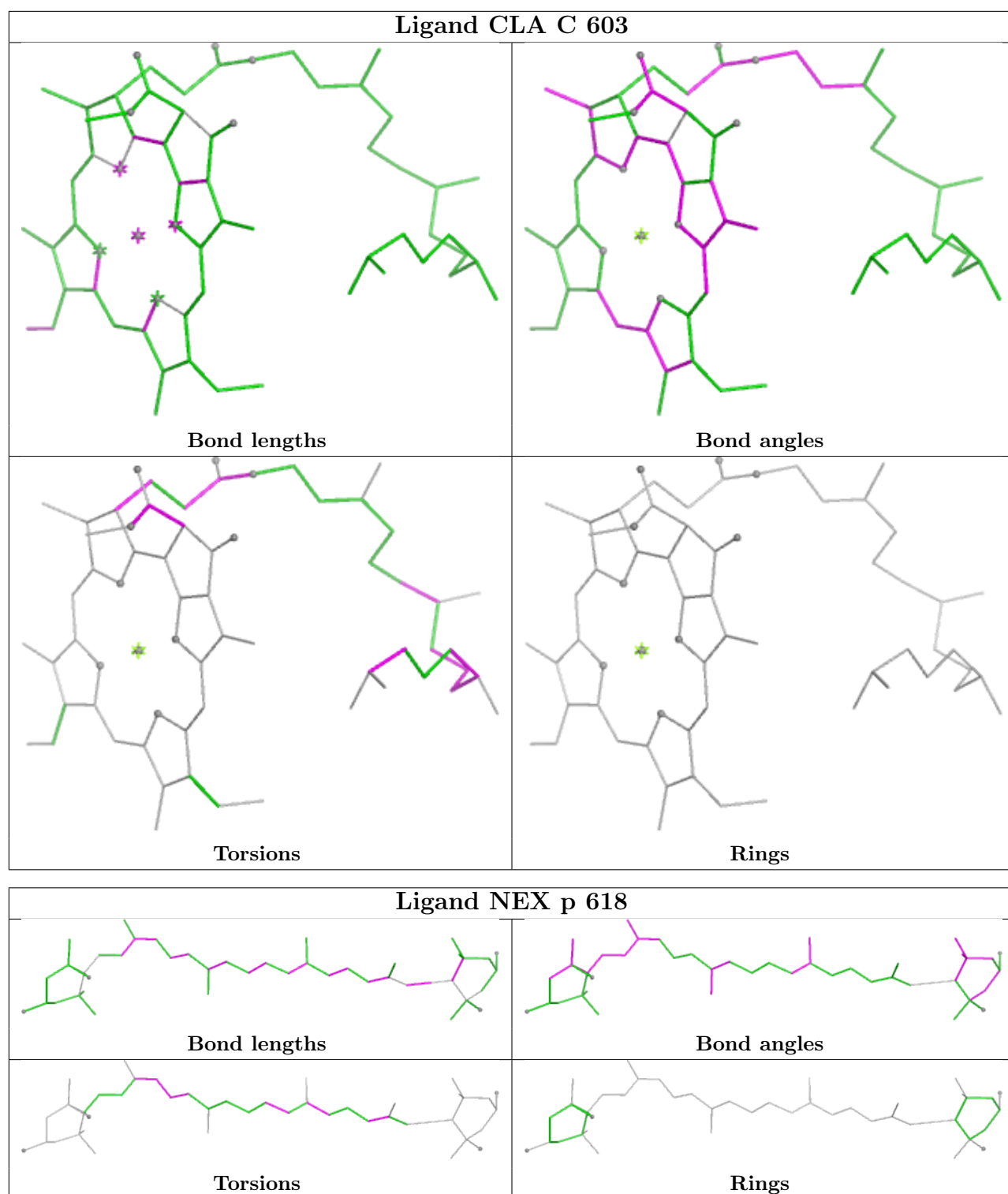


Rings

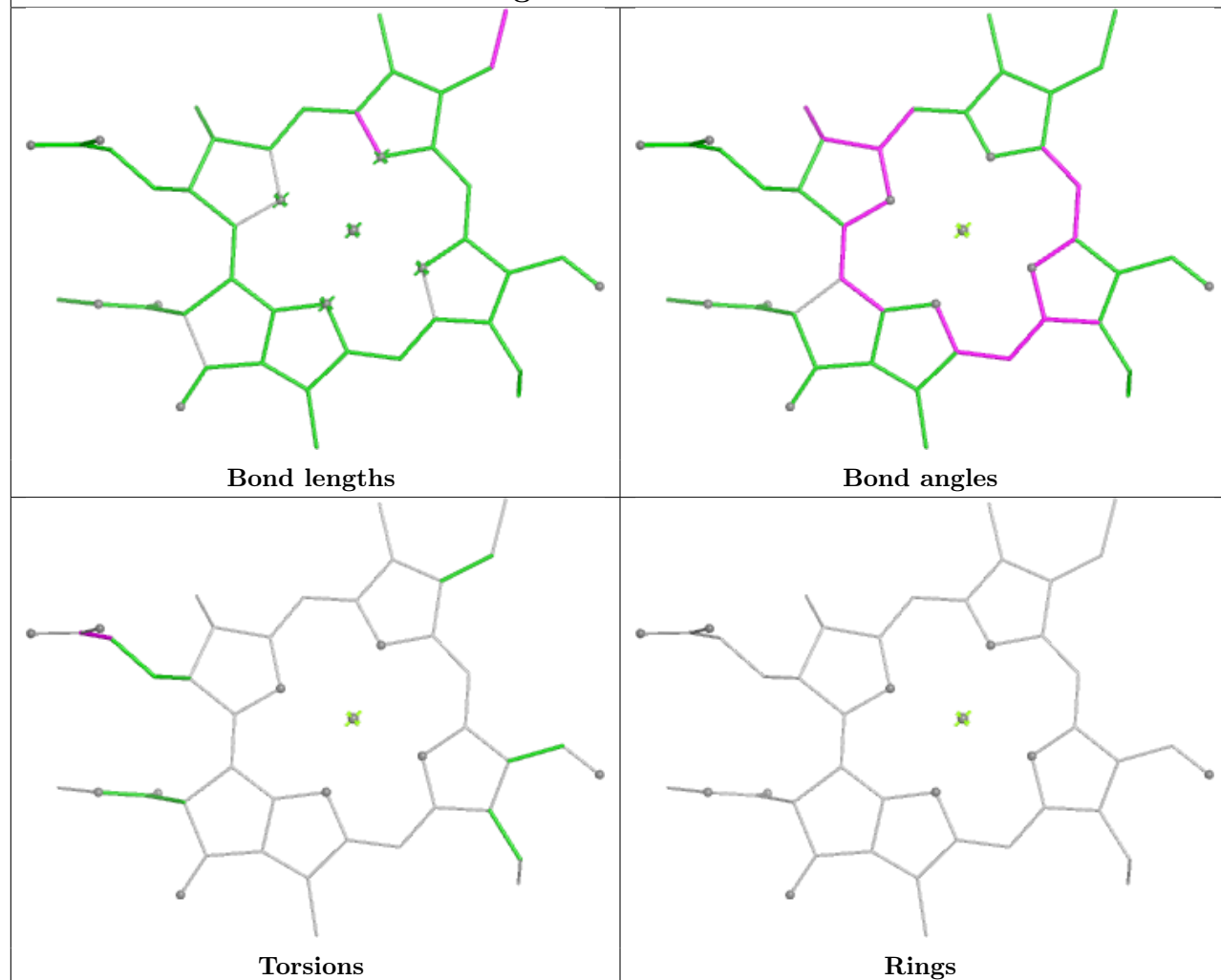
Ligand CLA 4 603**Ligand BCR B 617**

Ligand CHL 0 605

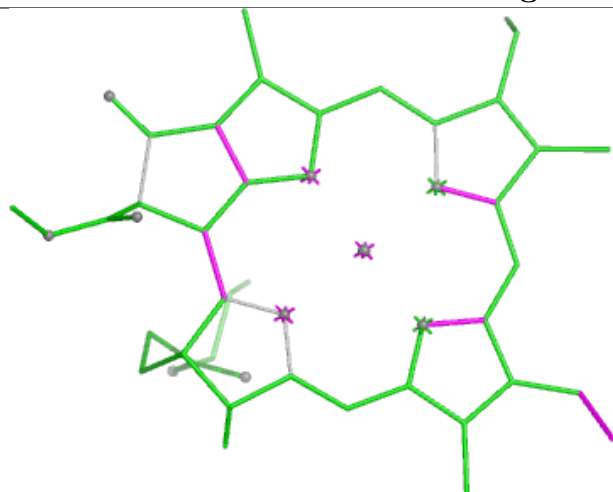




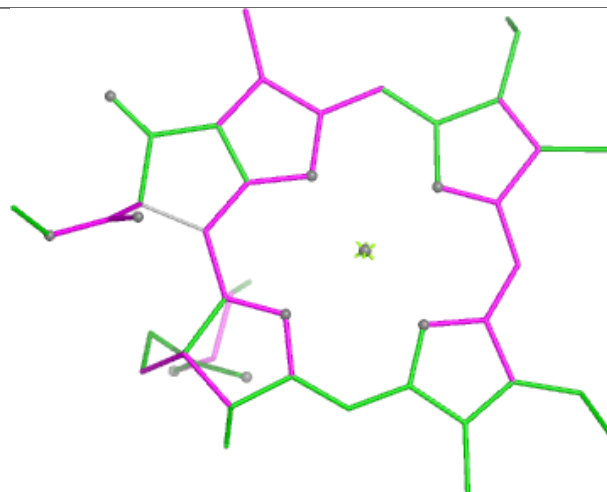
Ligand CHL s 302



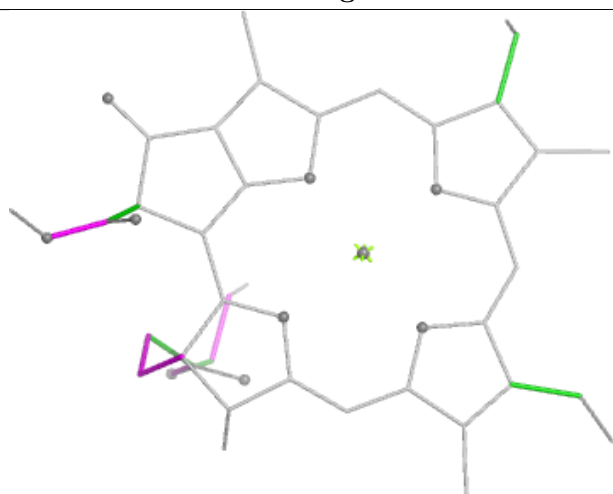
Ligand CLA r 306



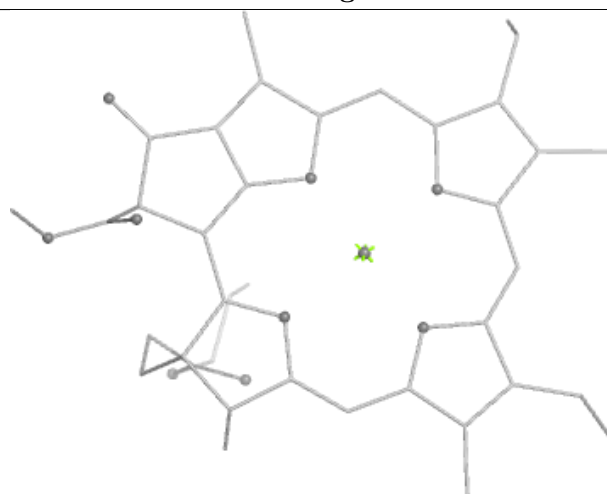
Bond lengths



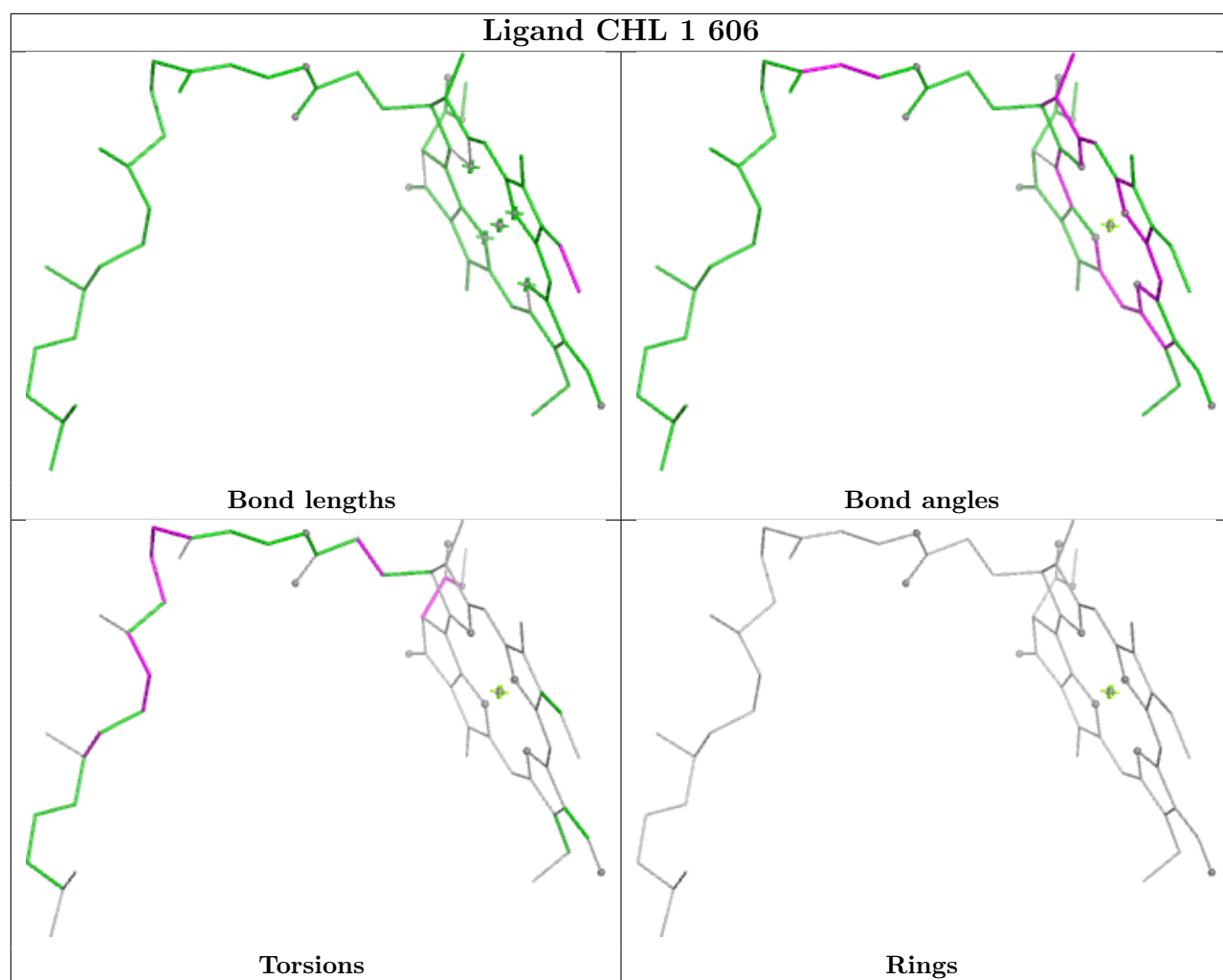
Bond angles

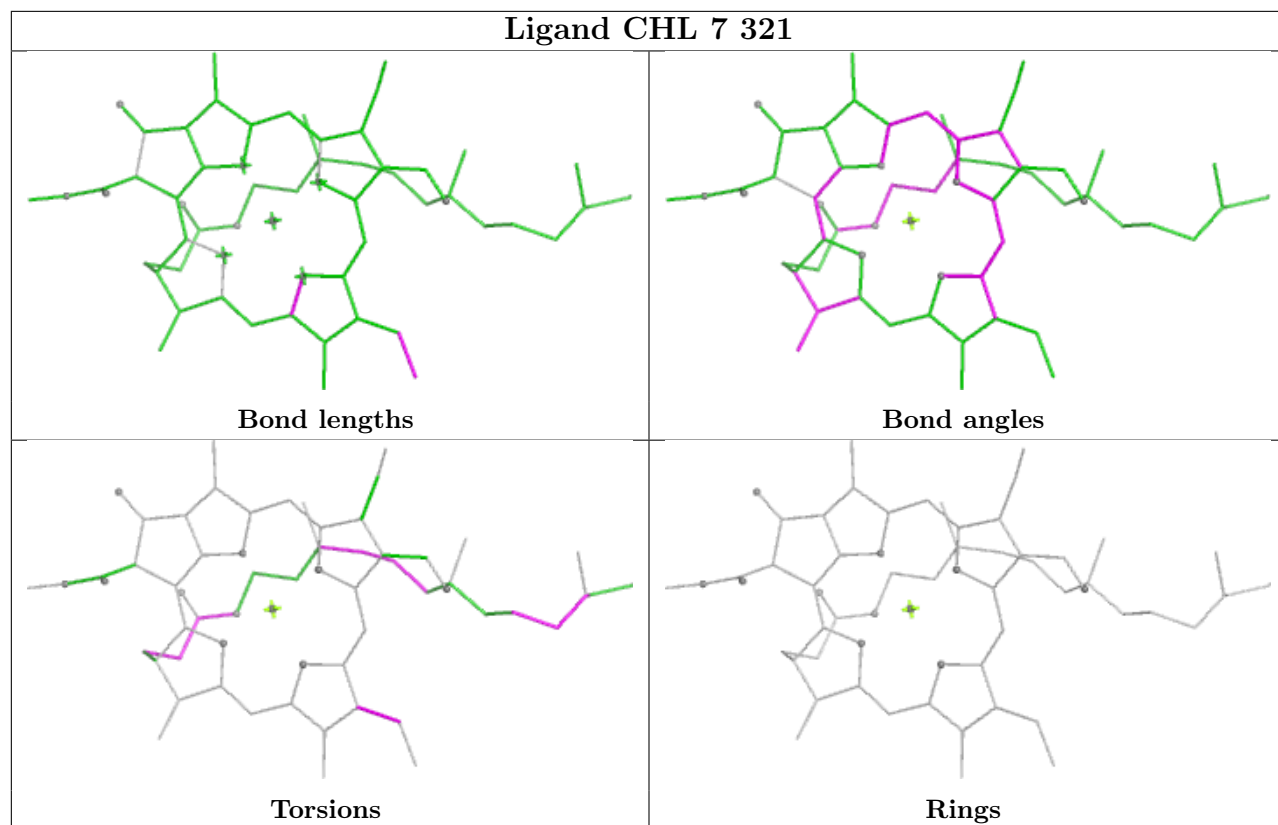


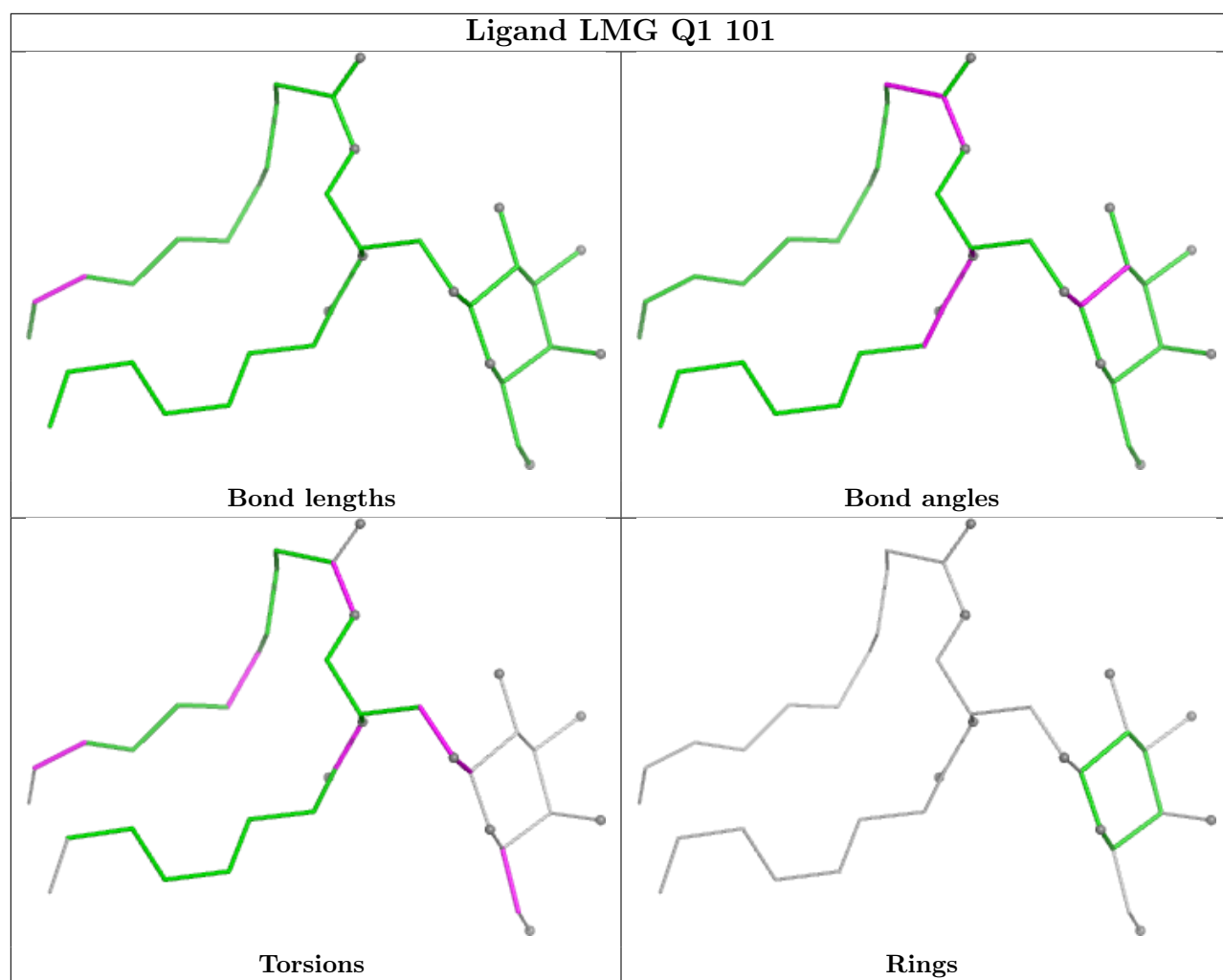
Torsions

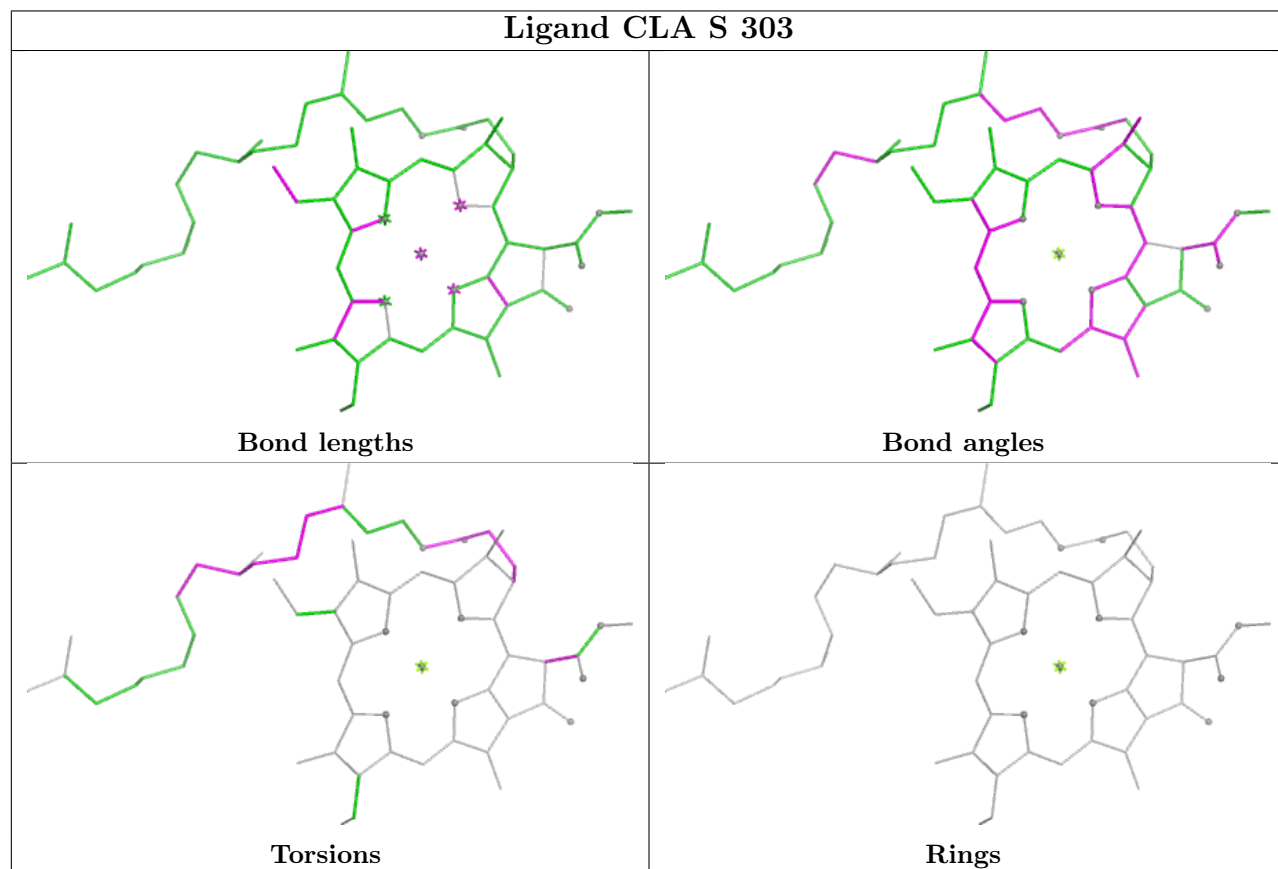
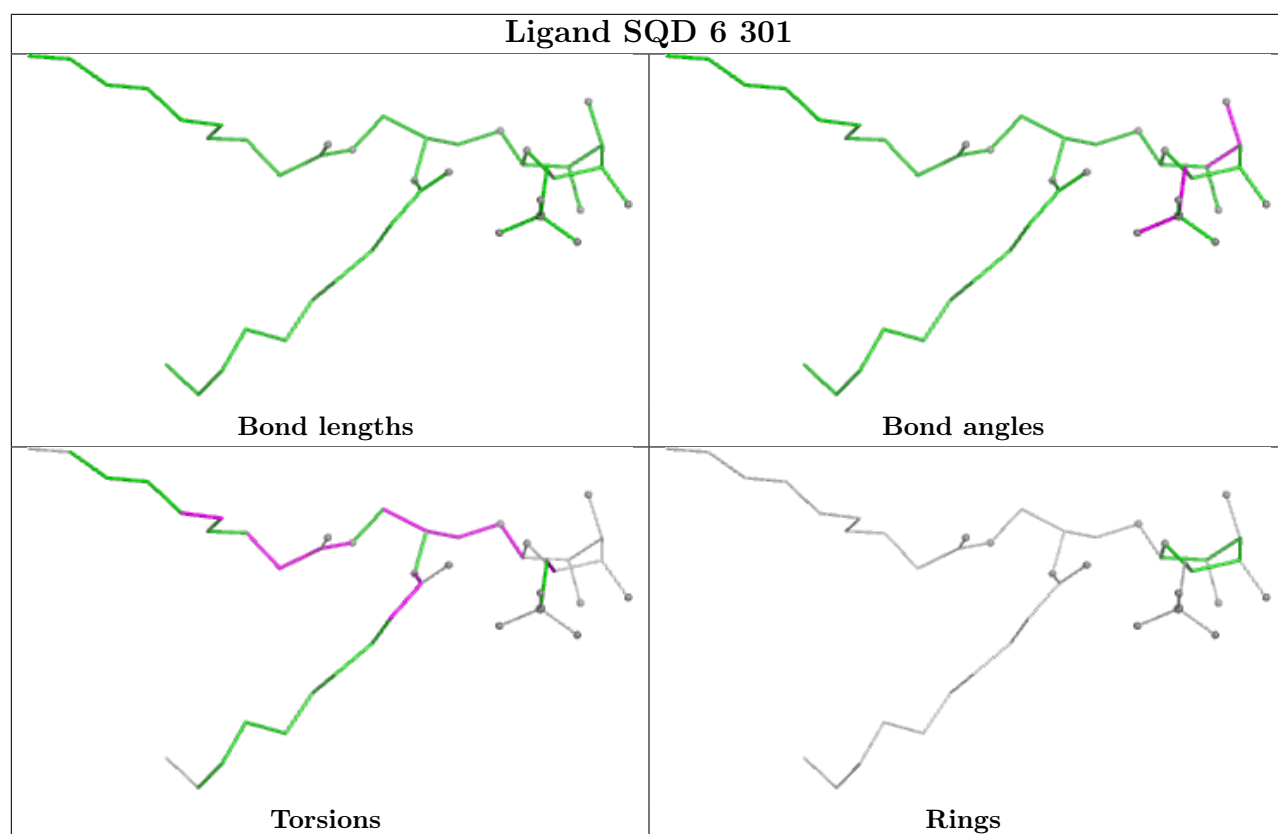


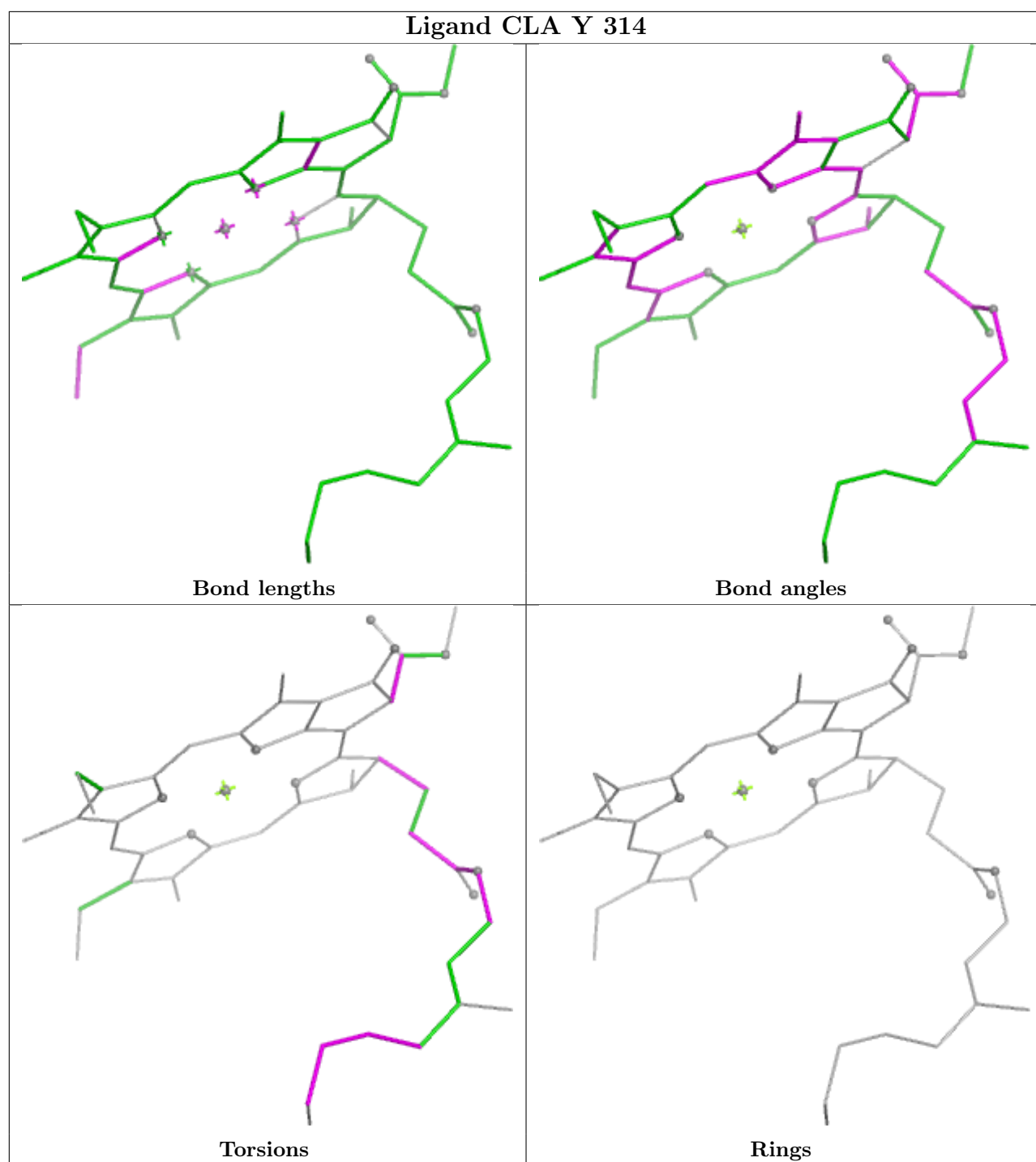
Rings



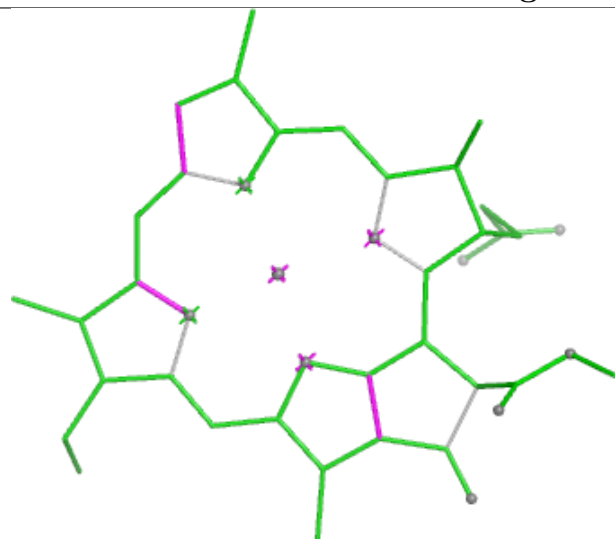




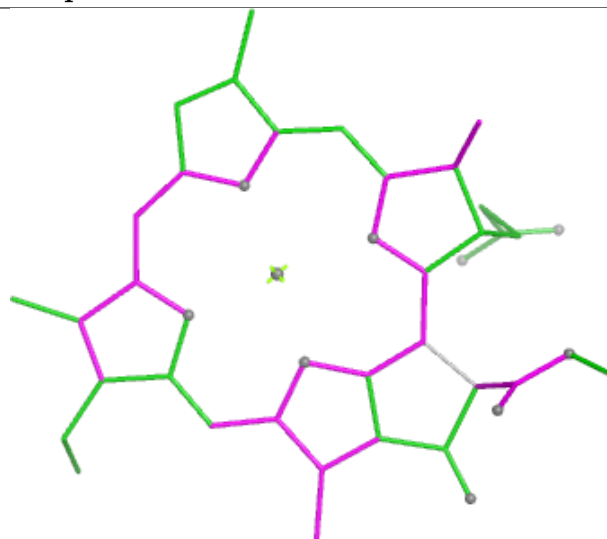




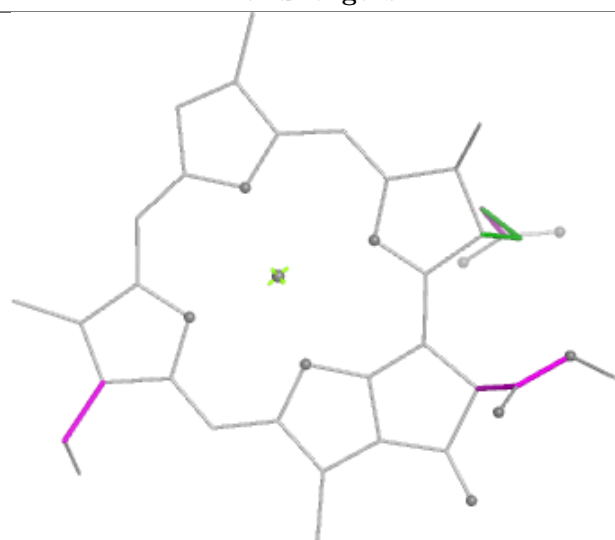
Ligand CLA q 313



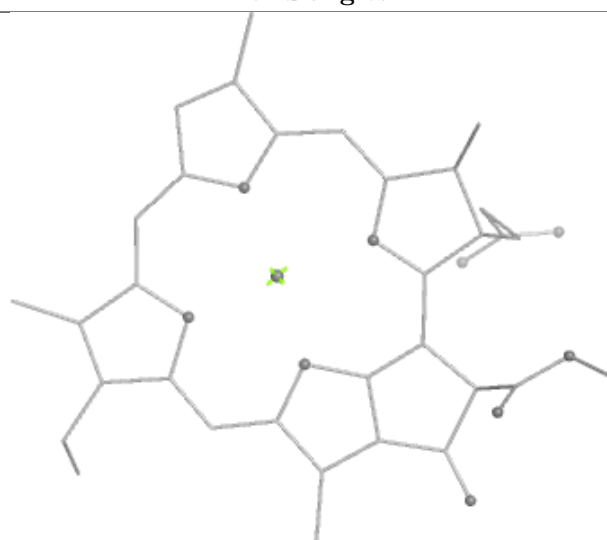
Bond lengths



Bond angles

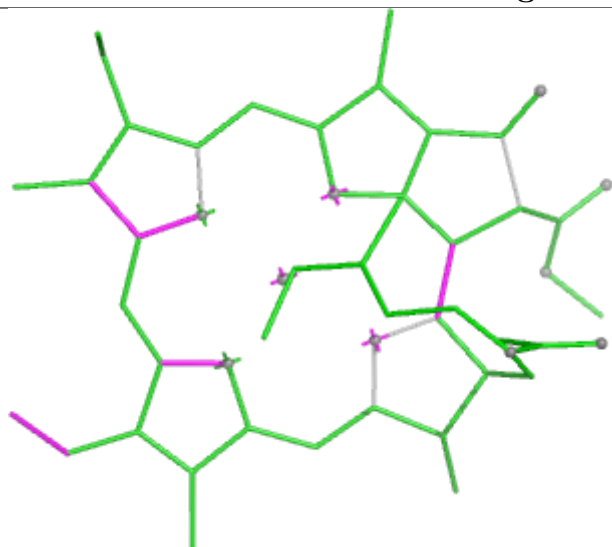


Torsions

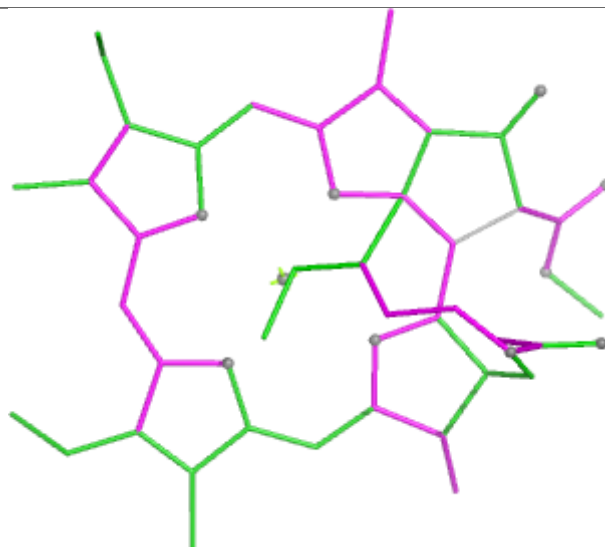


Rings

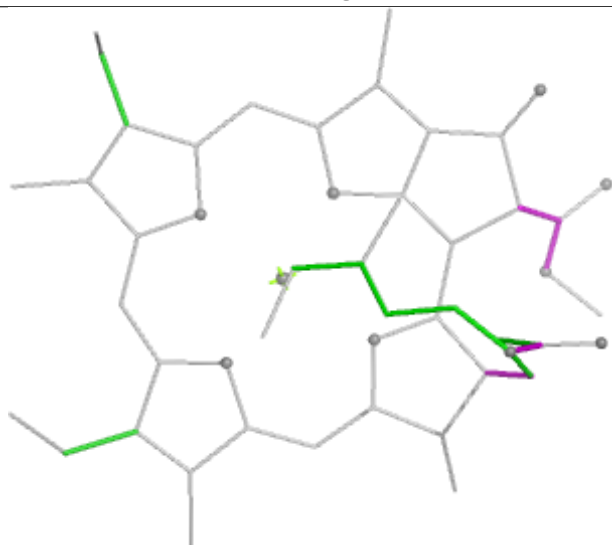
Ligand CLA 5 614



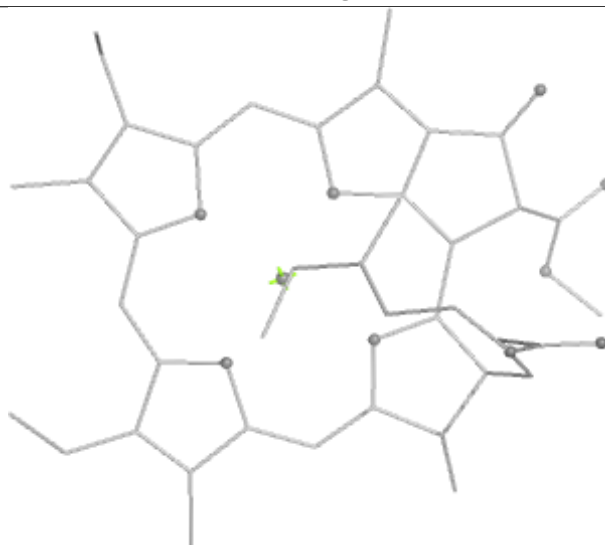
Bond lengths



Bond angles

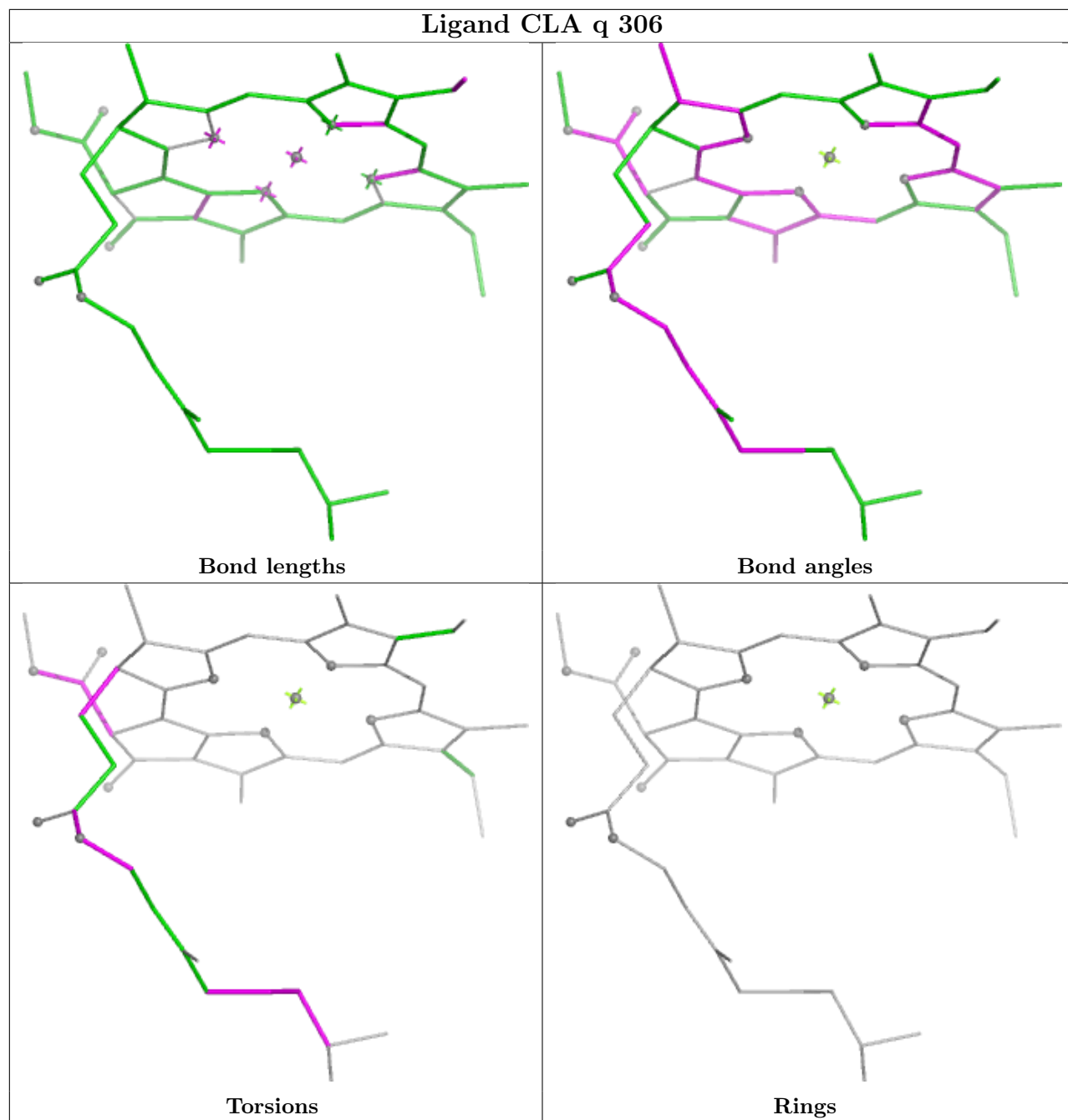


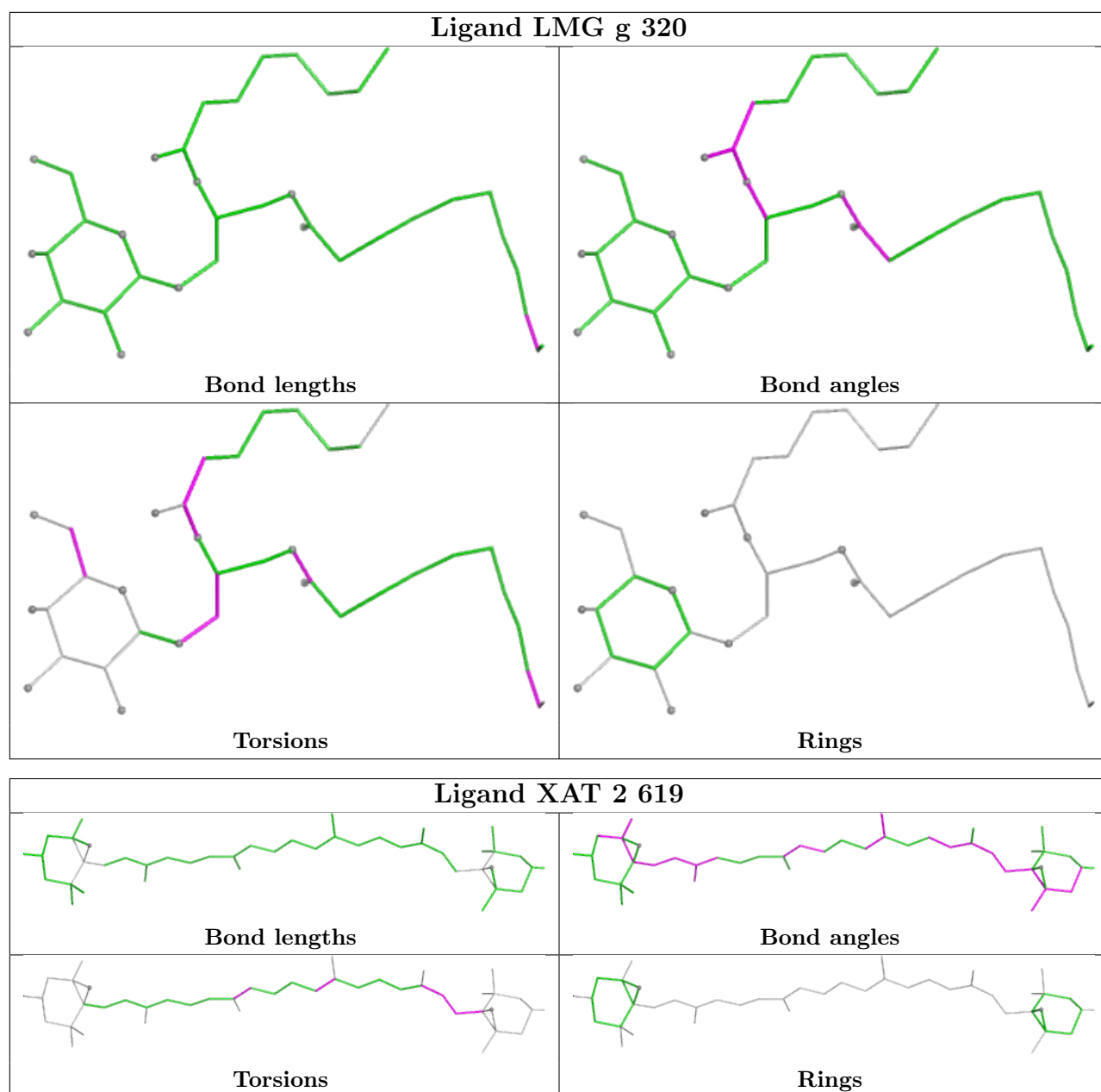
Torsions



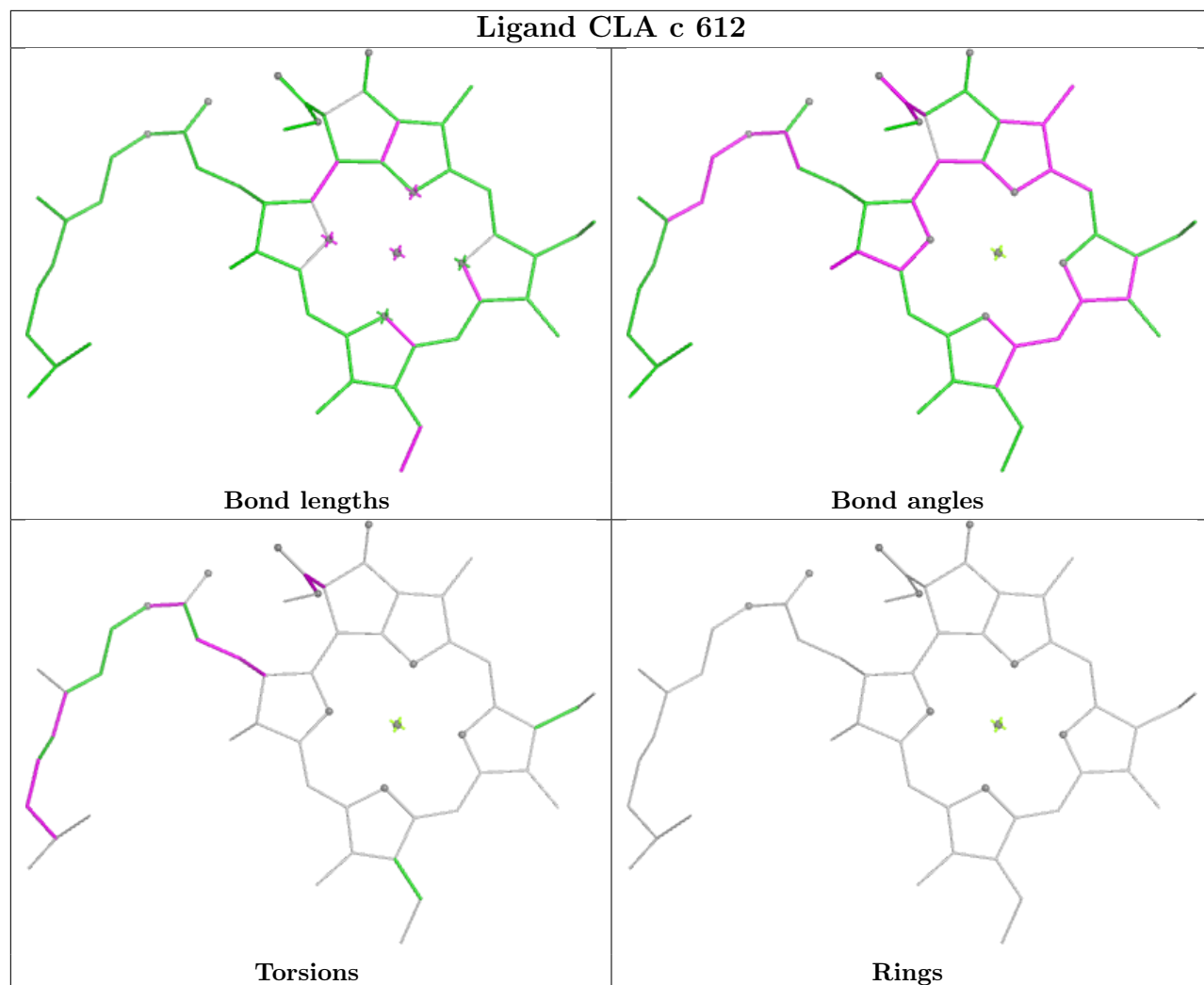
Rings

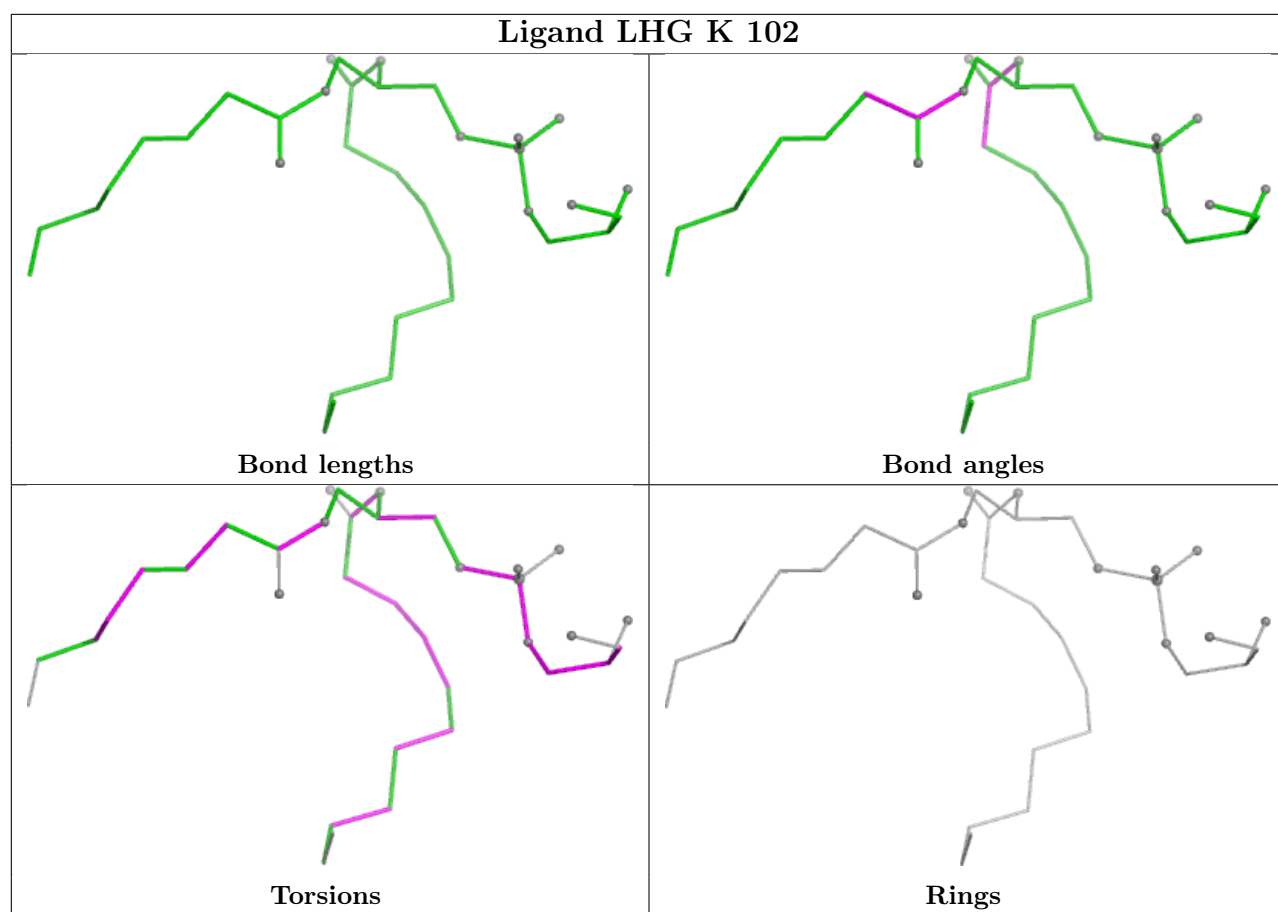
Ligand CLA q 306



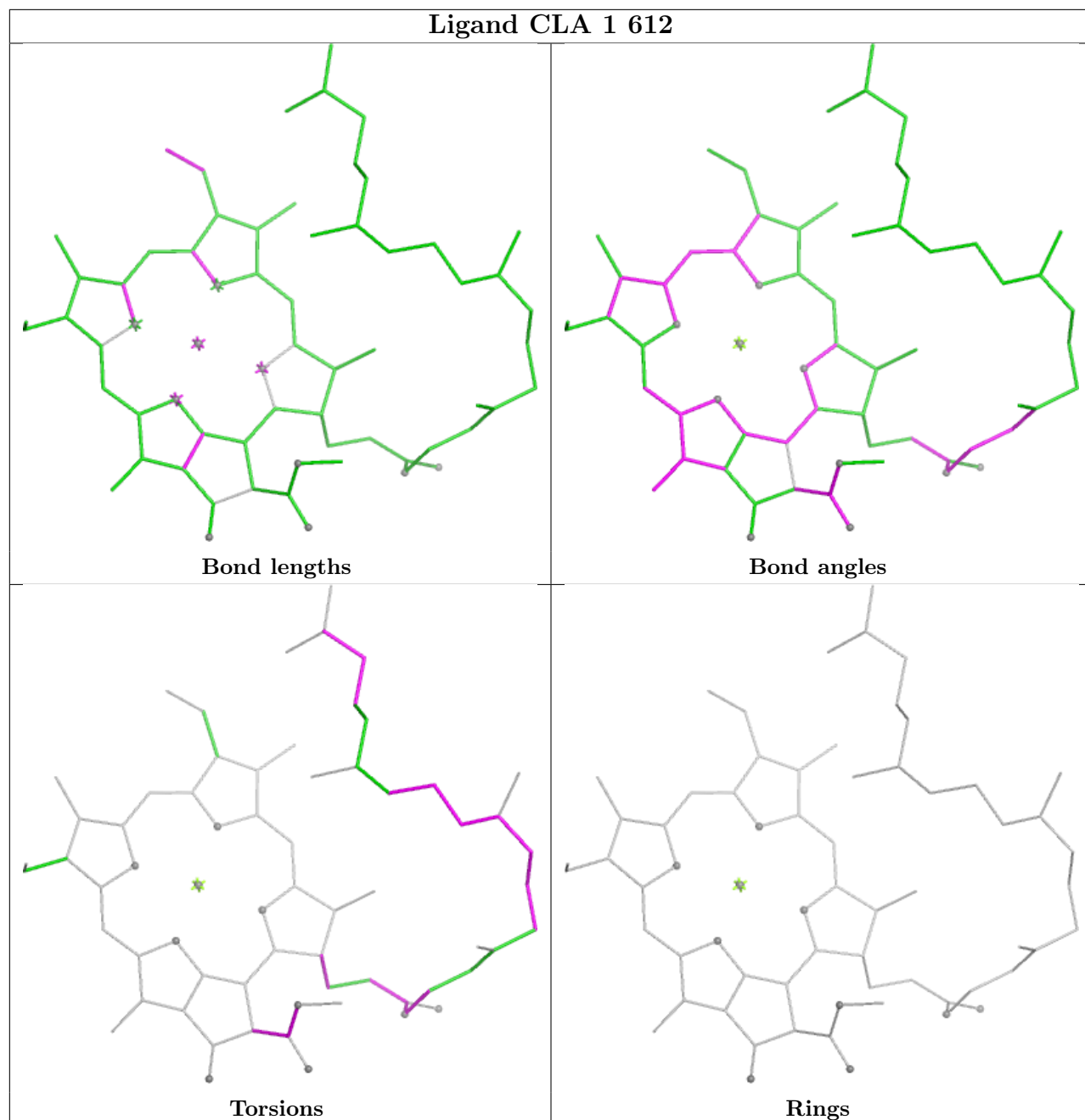


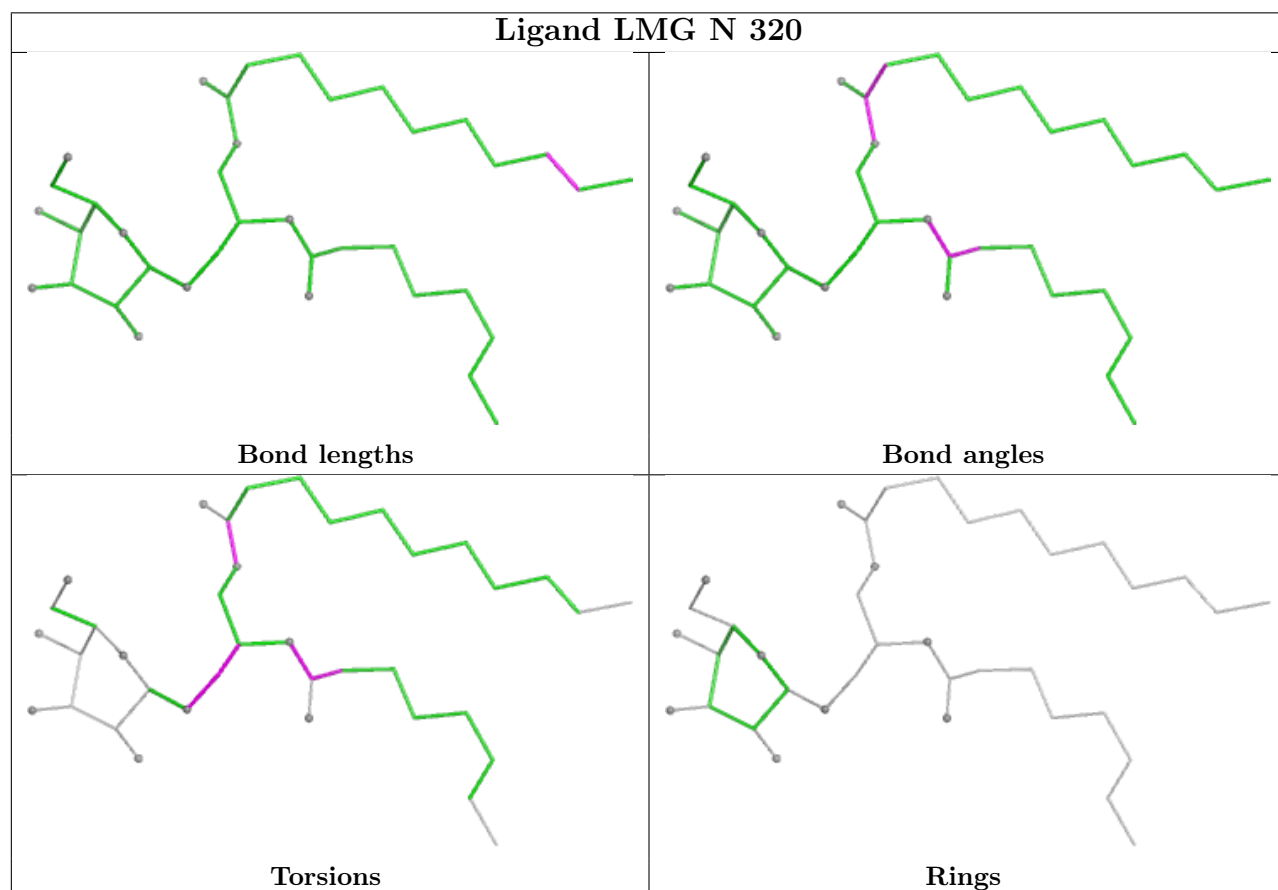
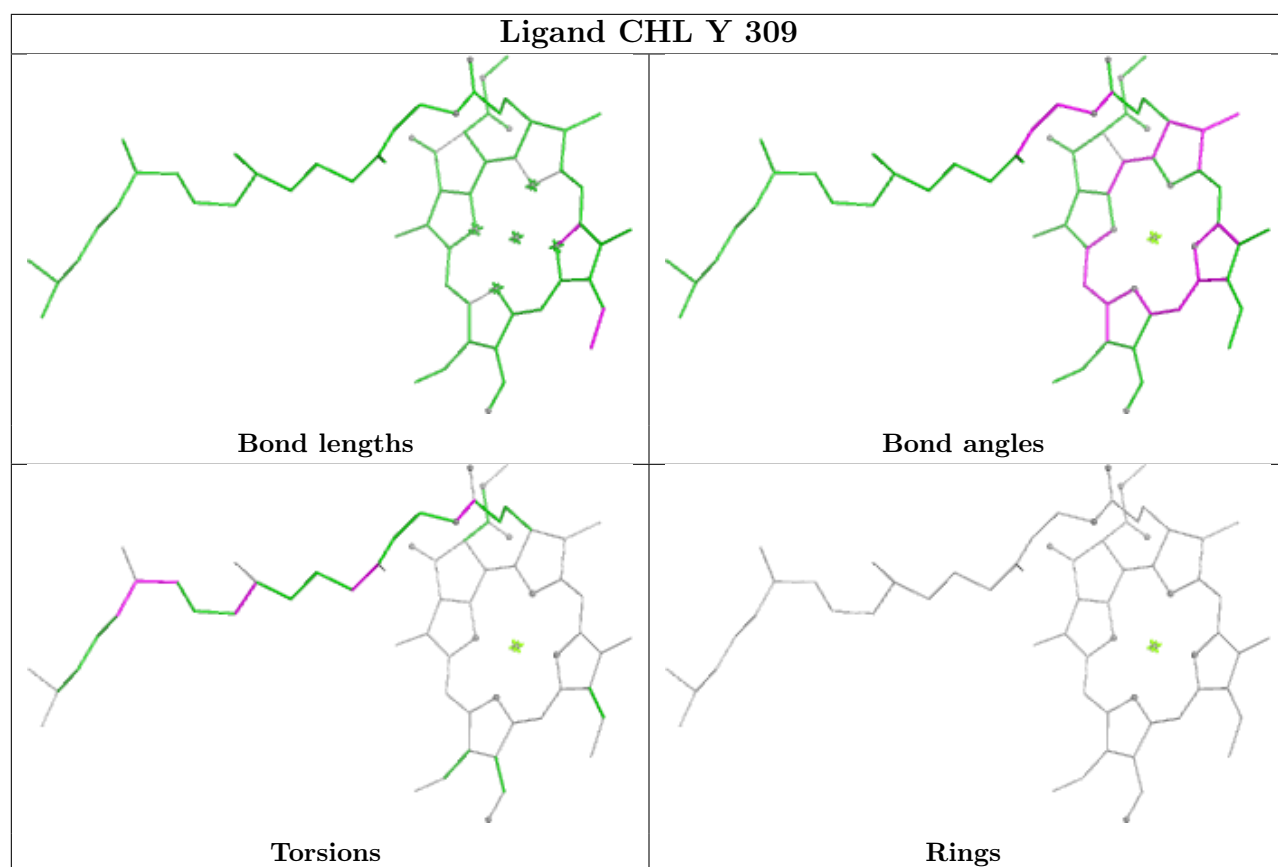
Ligand CLA c 612

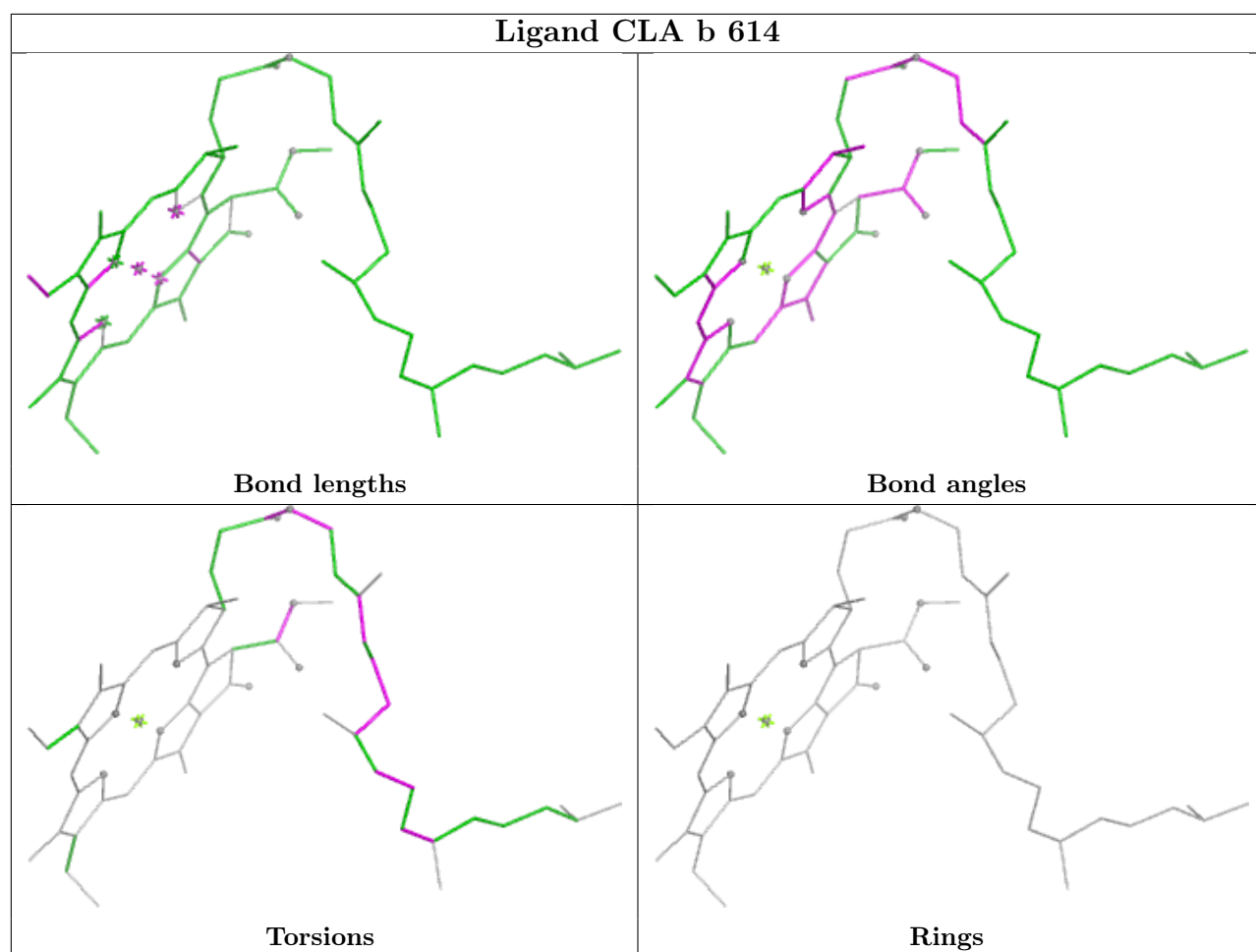


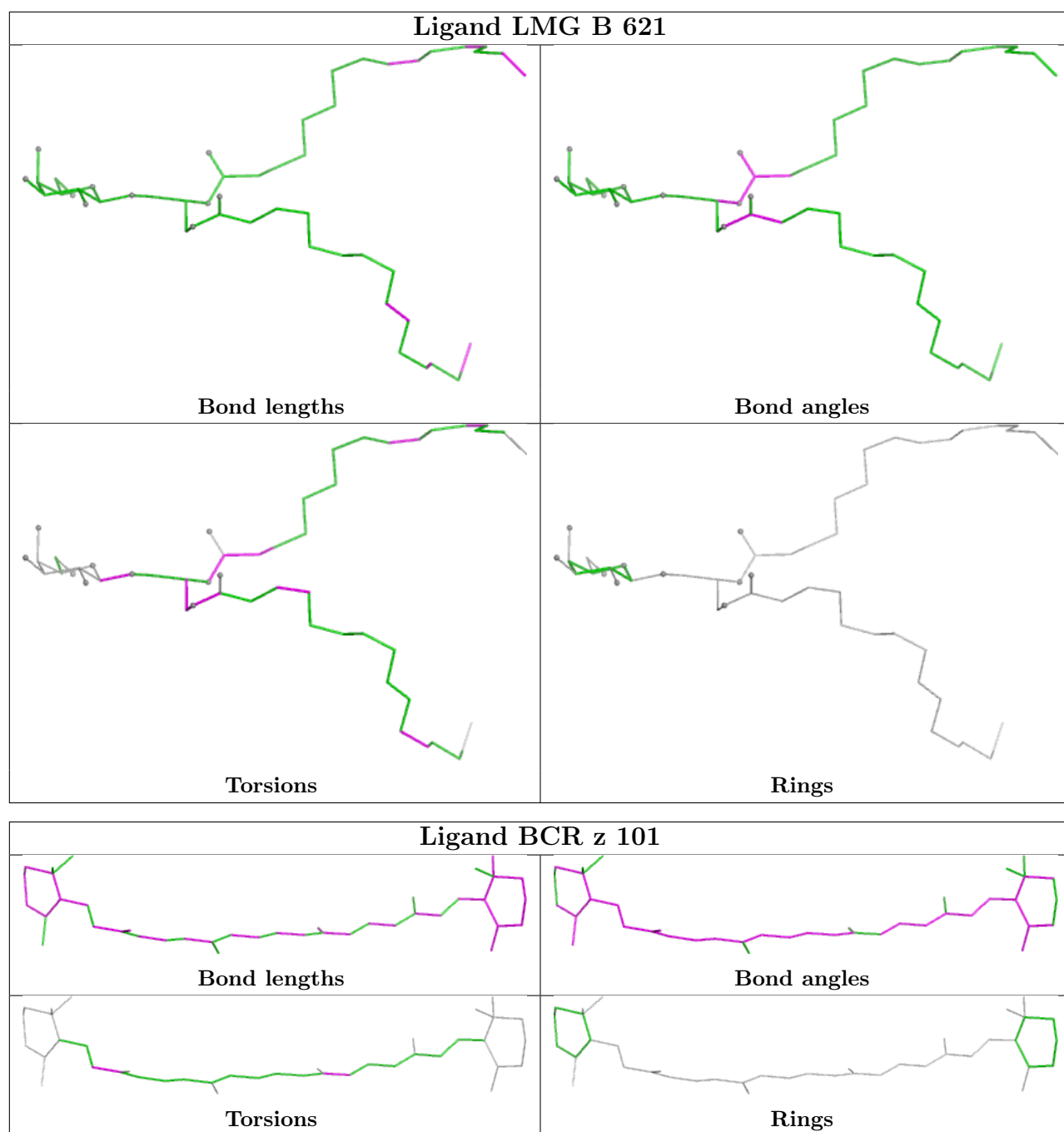


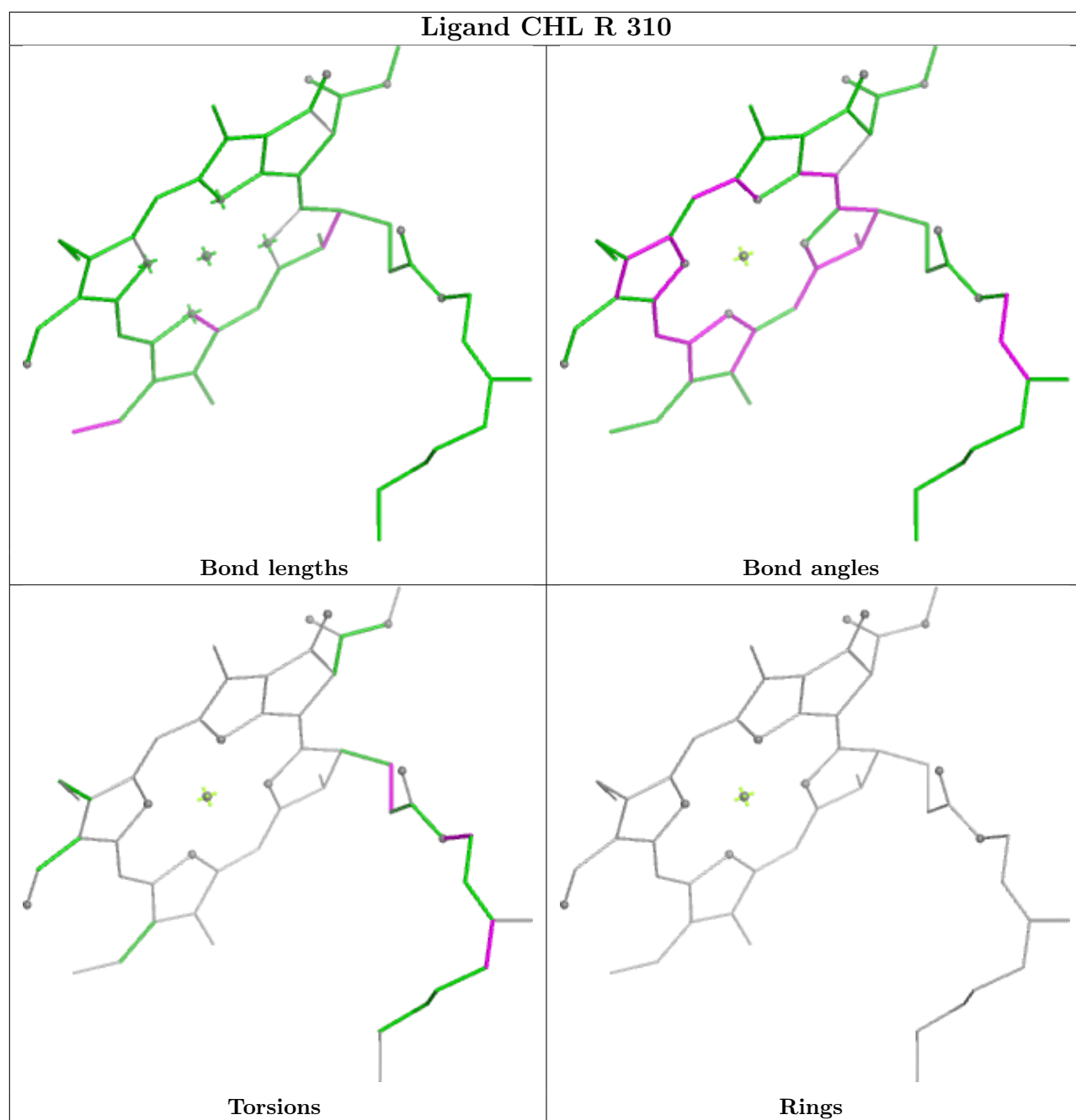
Ligand CLA 1 612

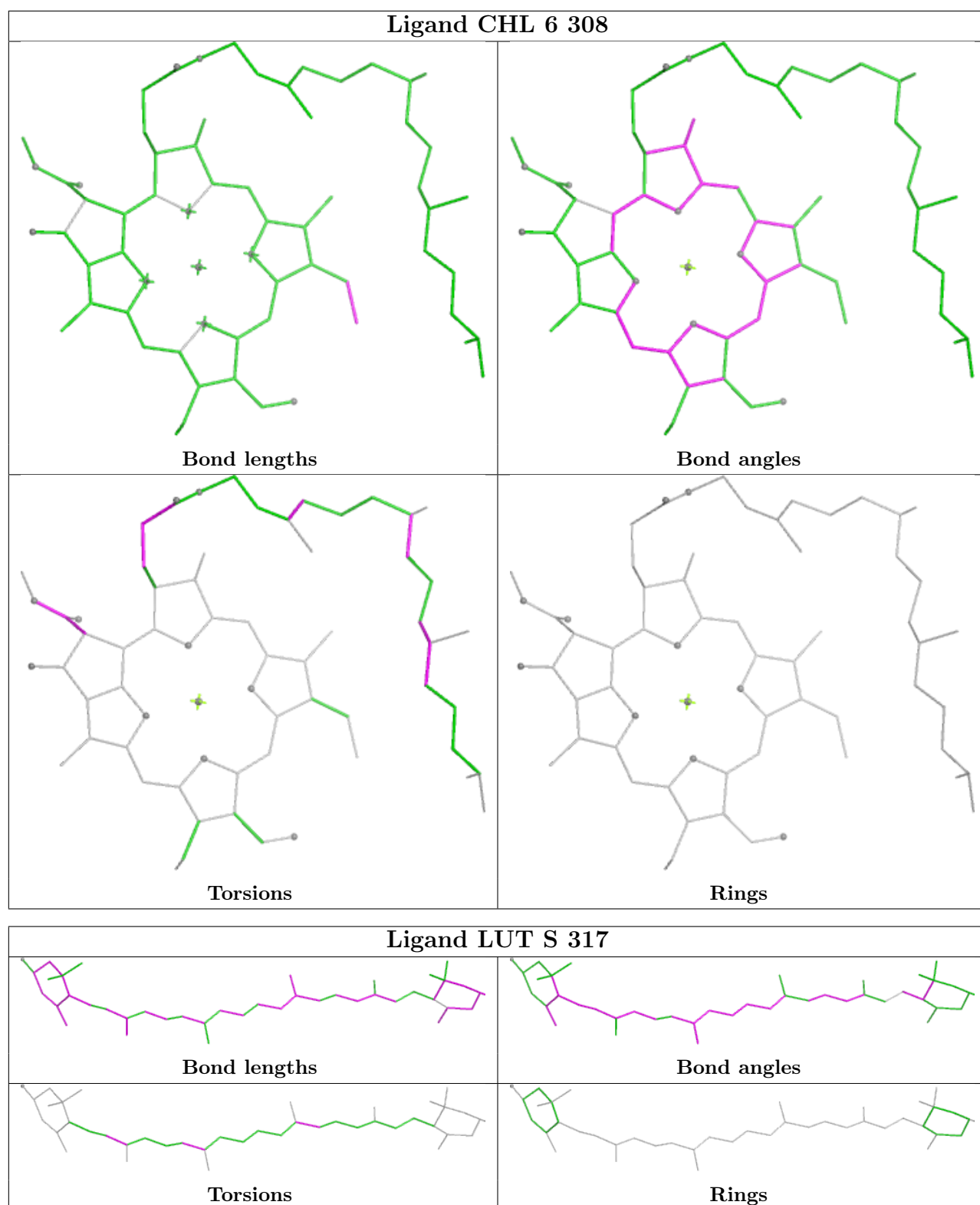




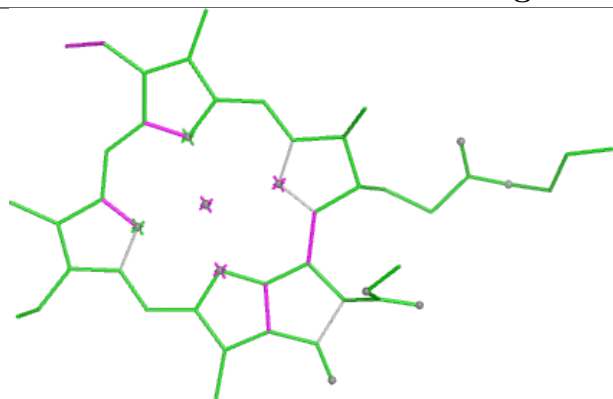




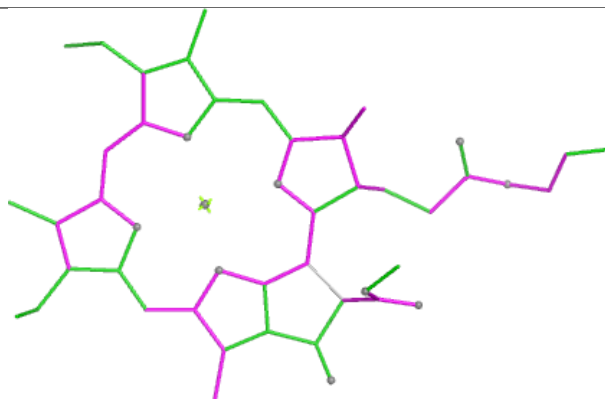




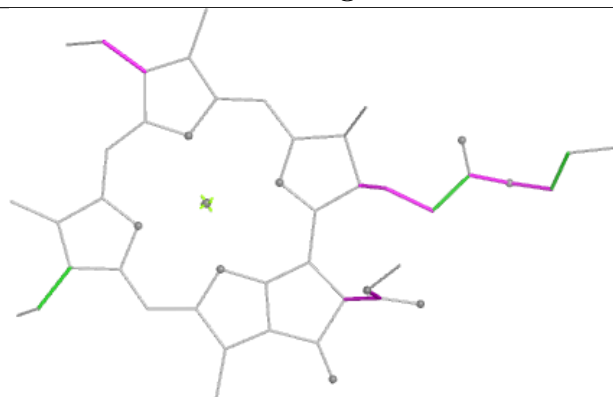
Ligand CLA R 307



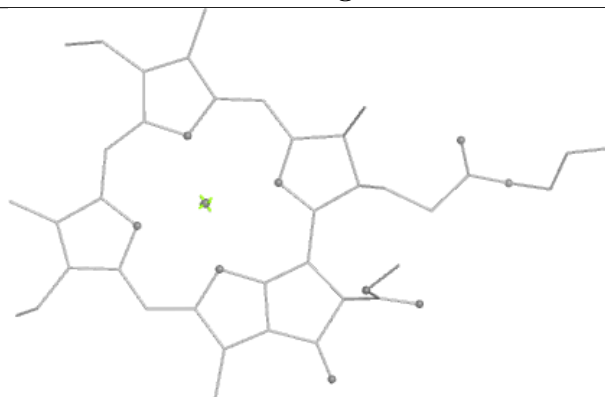
Bond lengths



Bond angles



Torsions



Rings

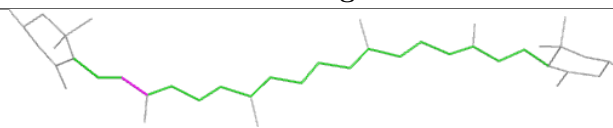
Ligand LUT y 616



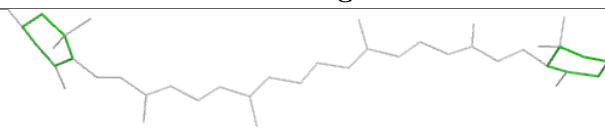
Bond lengths



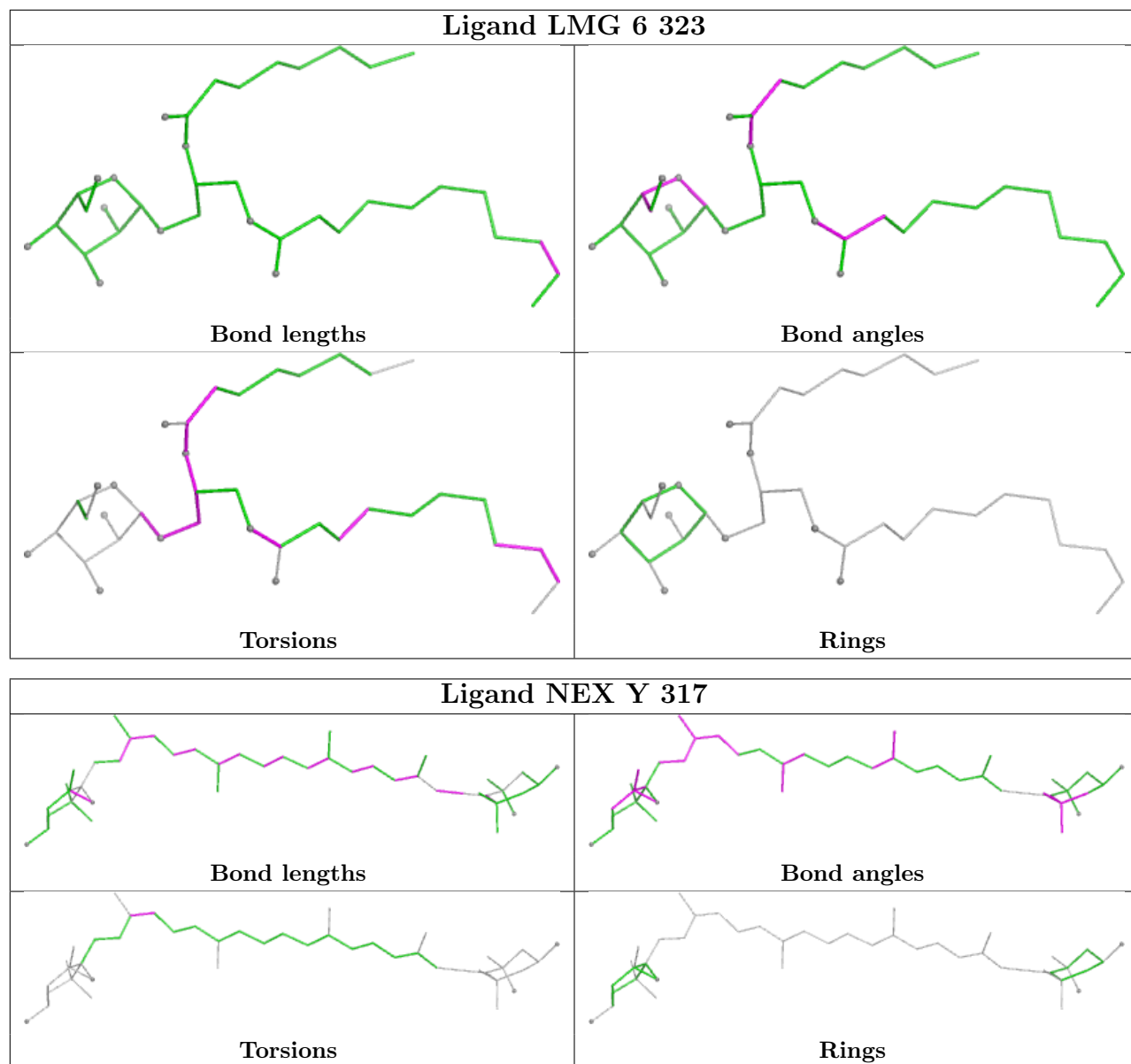
Bond angles



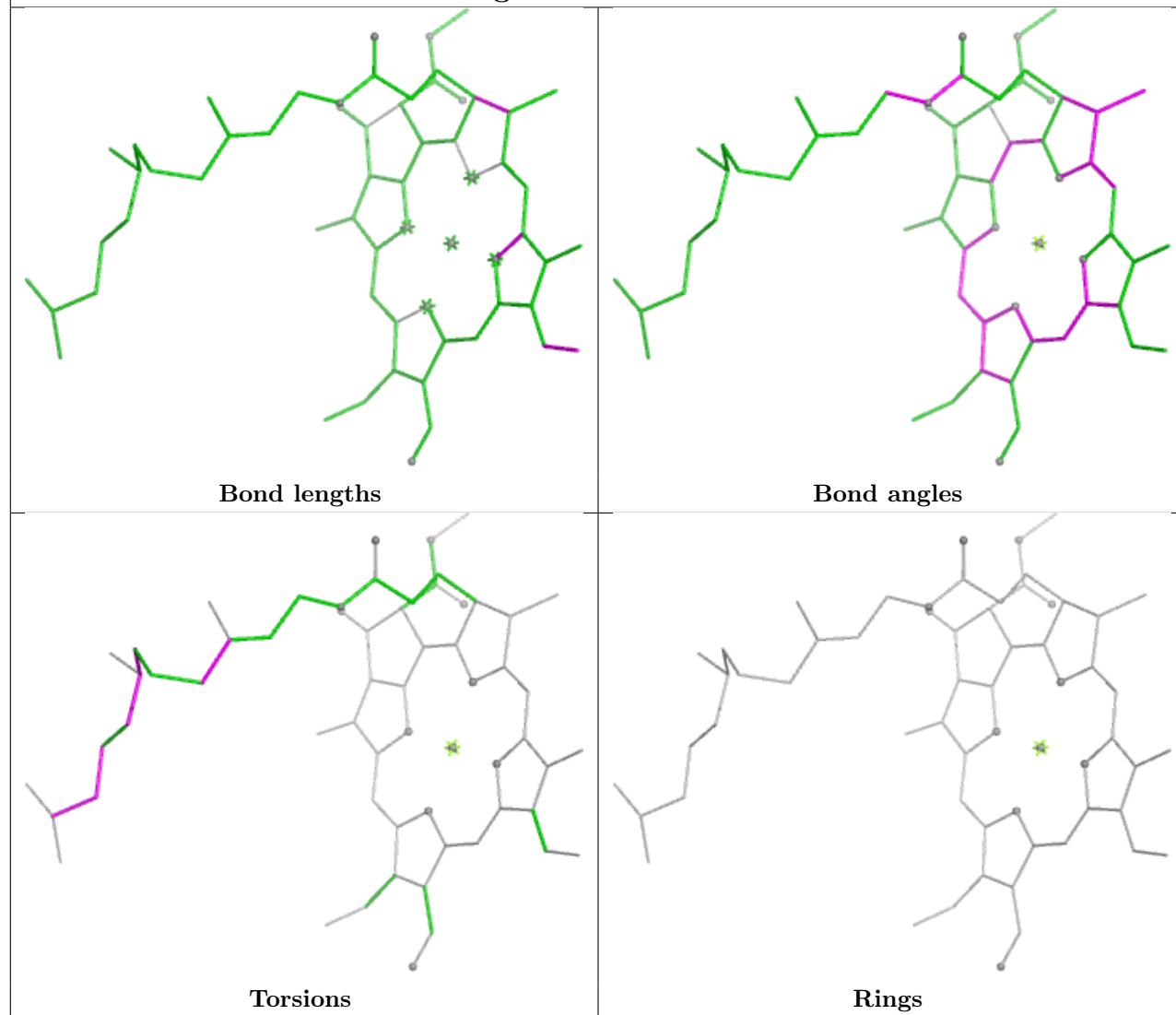
Torsions



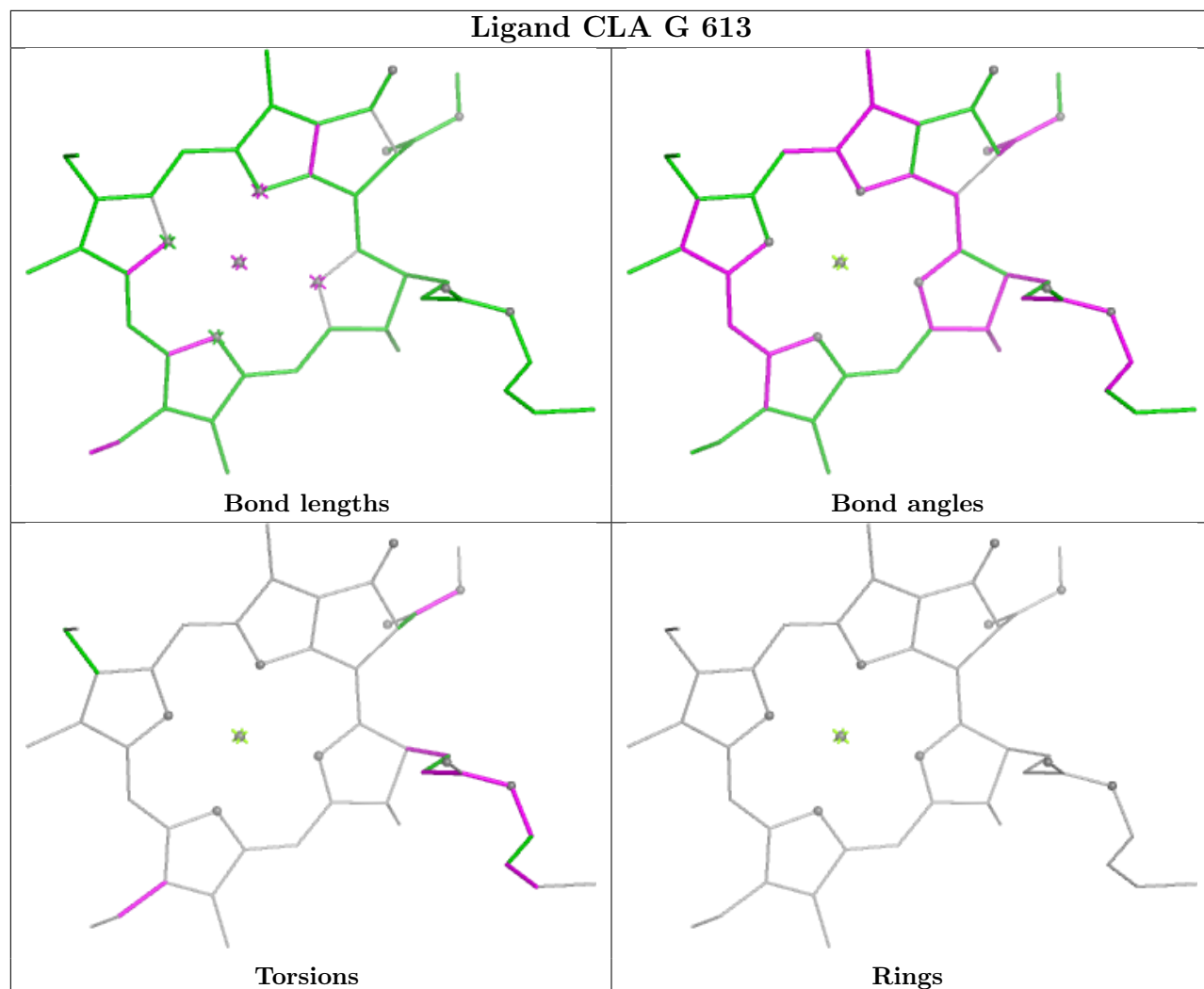
Rings

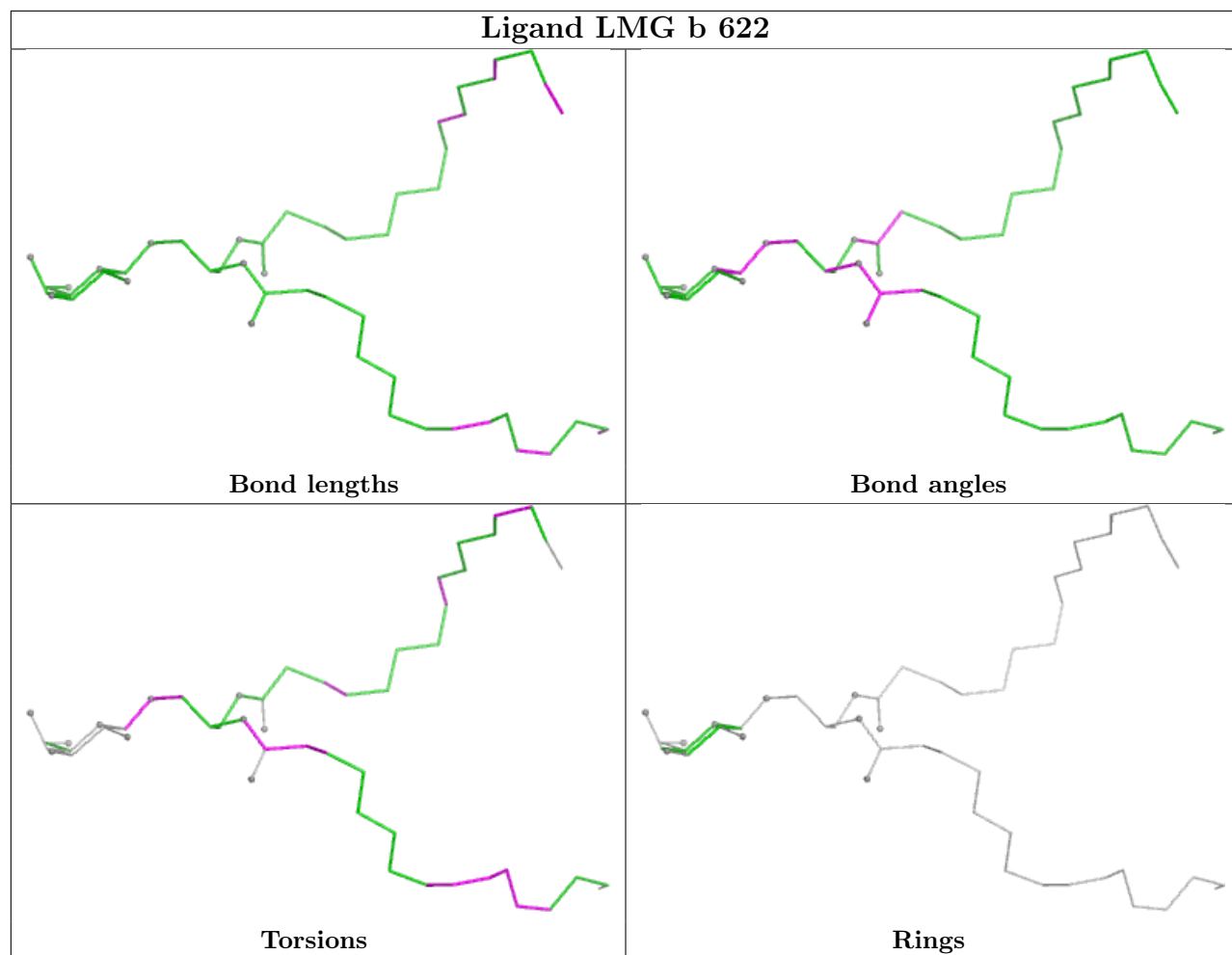


Ligand CHL 3 310

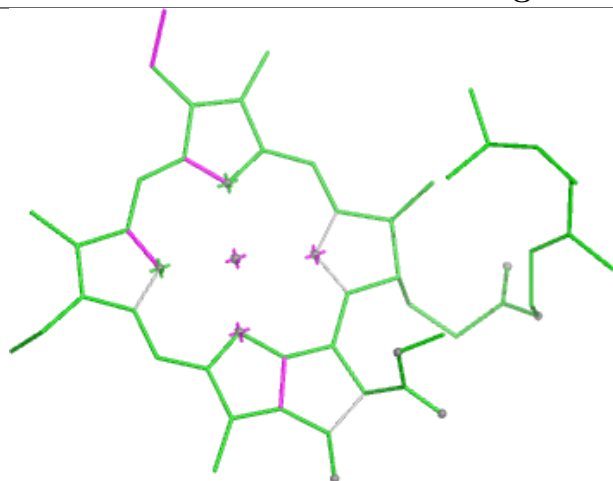


Ligand CLA G 613

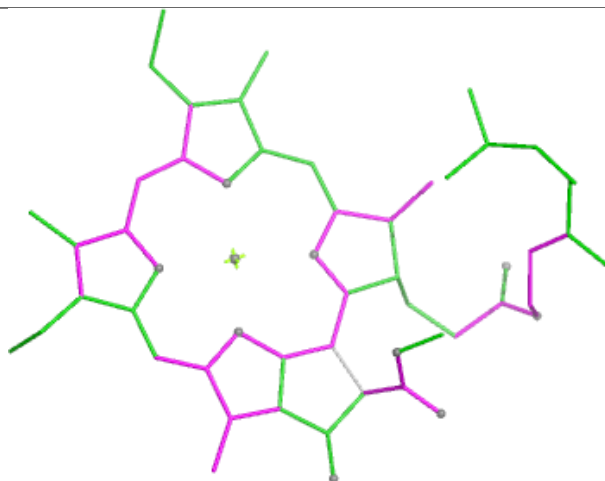




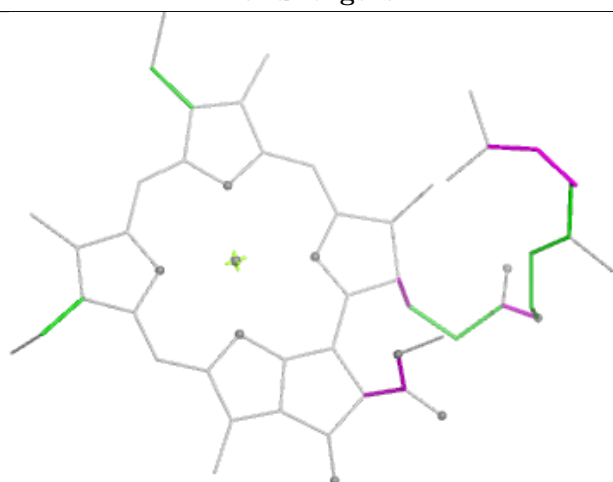
Ligand CLA N 304



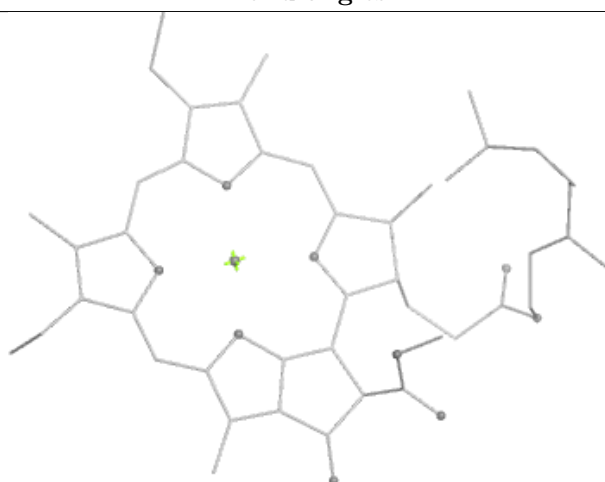
Bond lengths



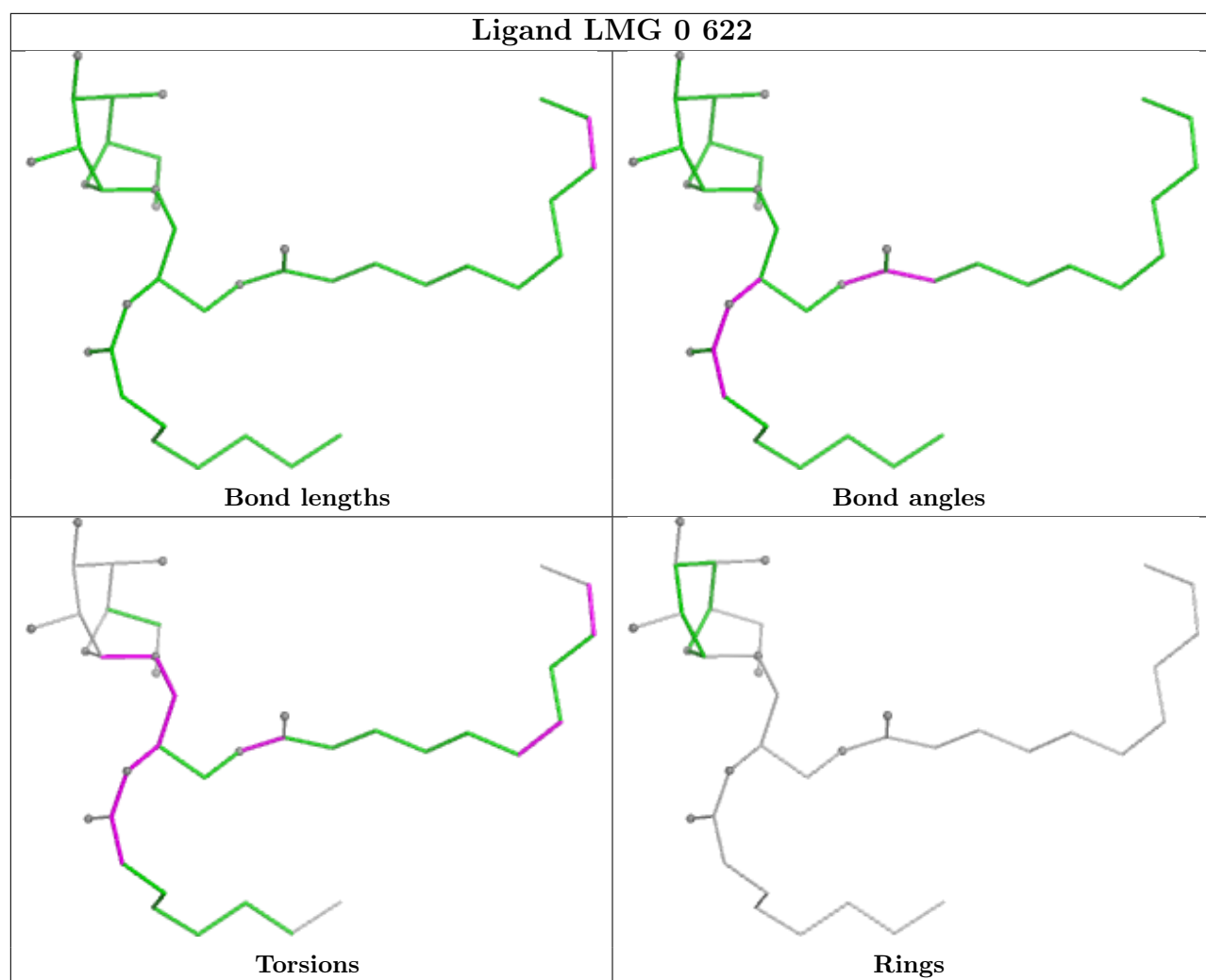
Bond angles

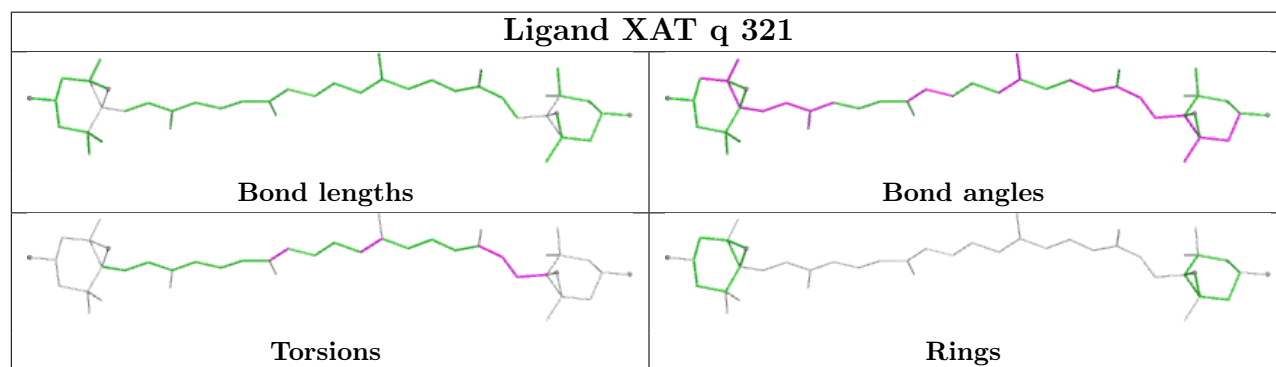
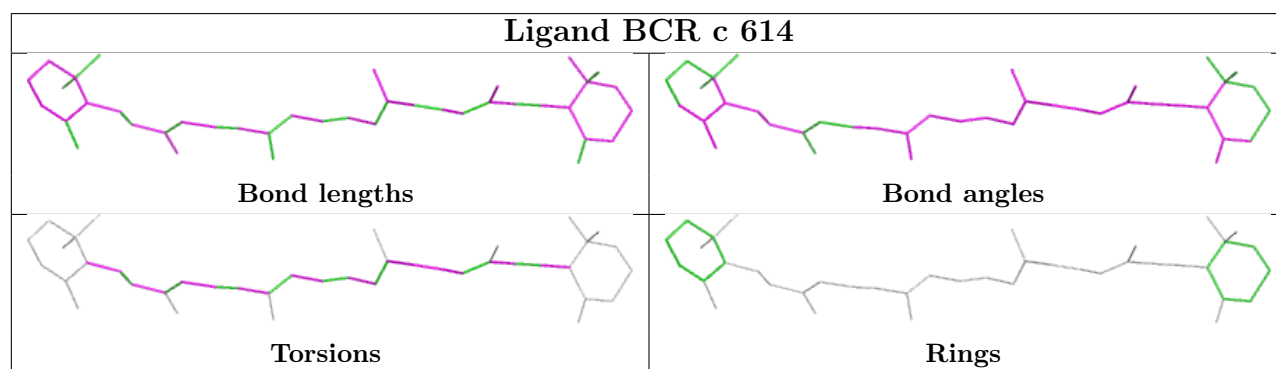
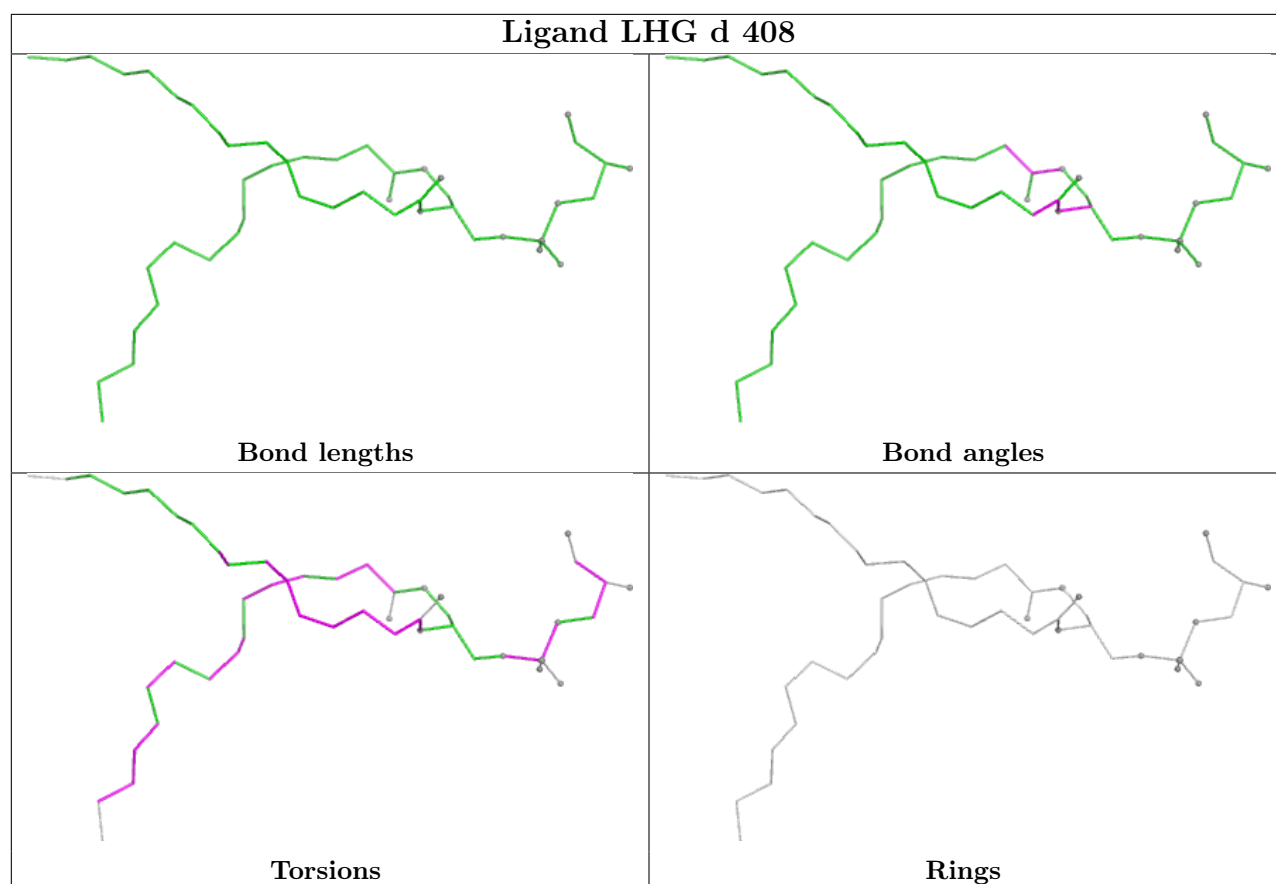


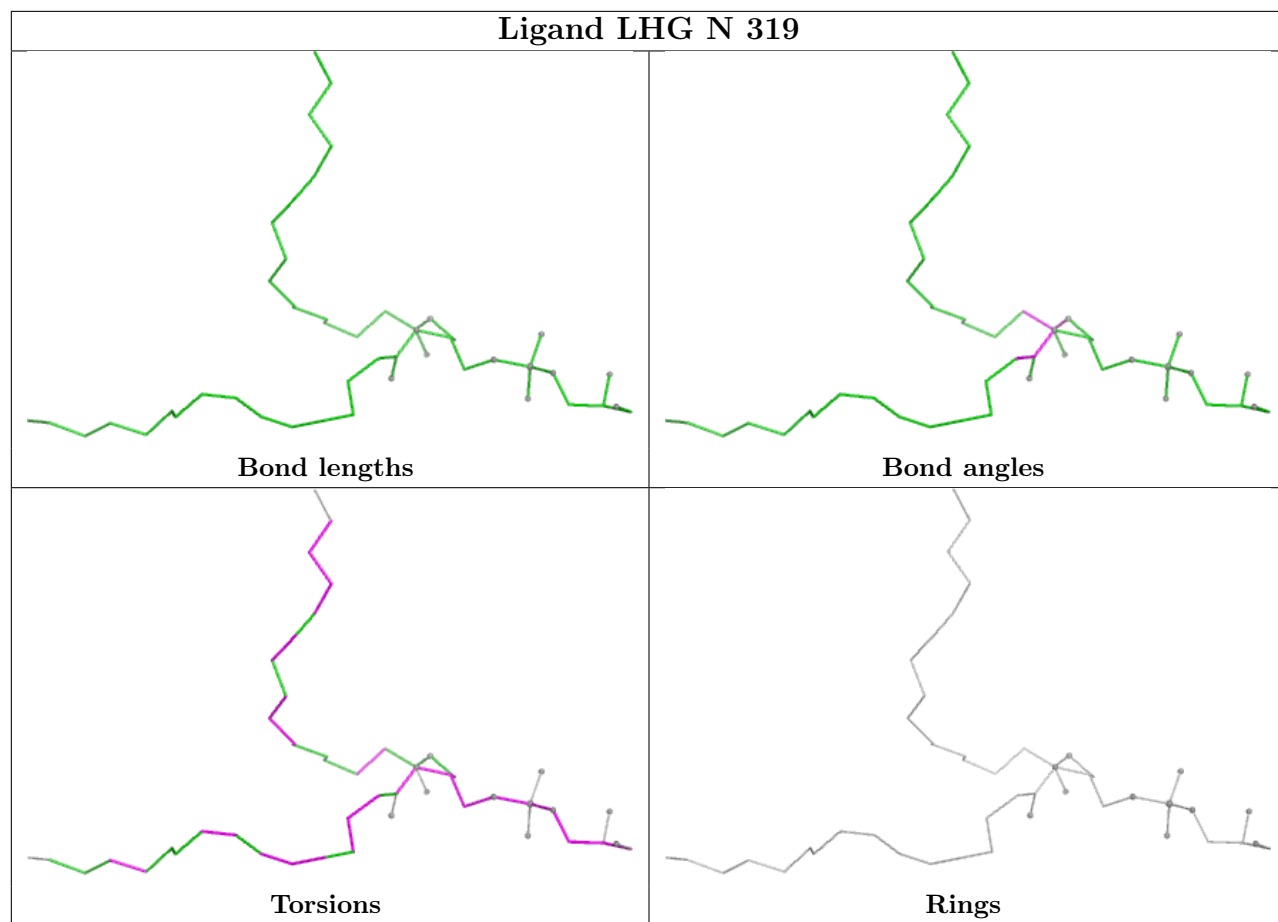
Torsions

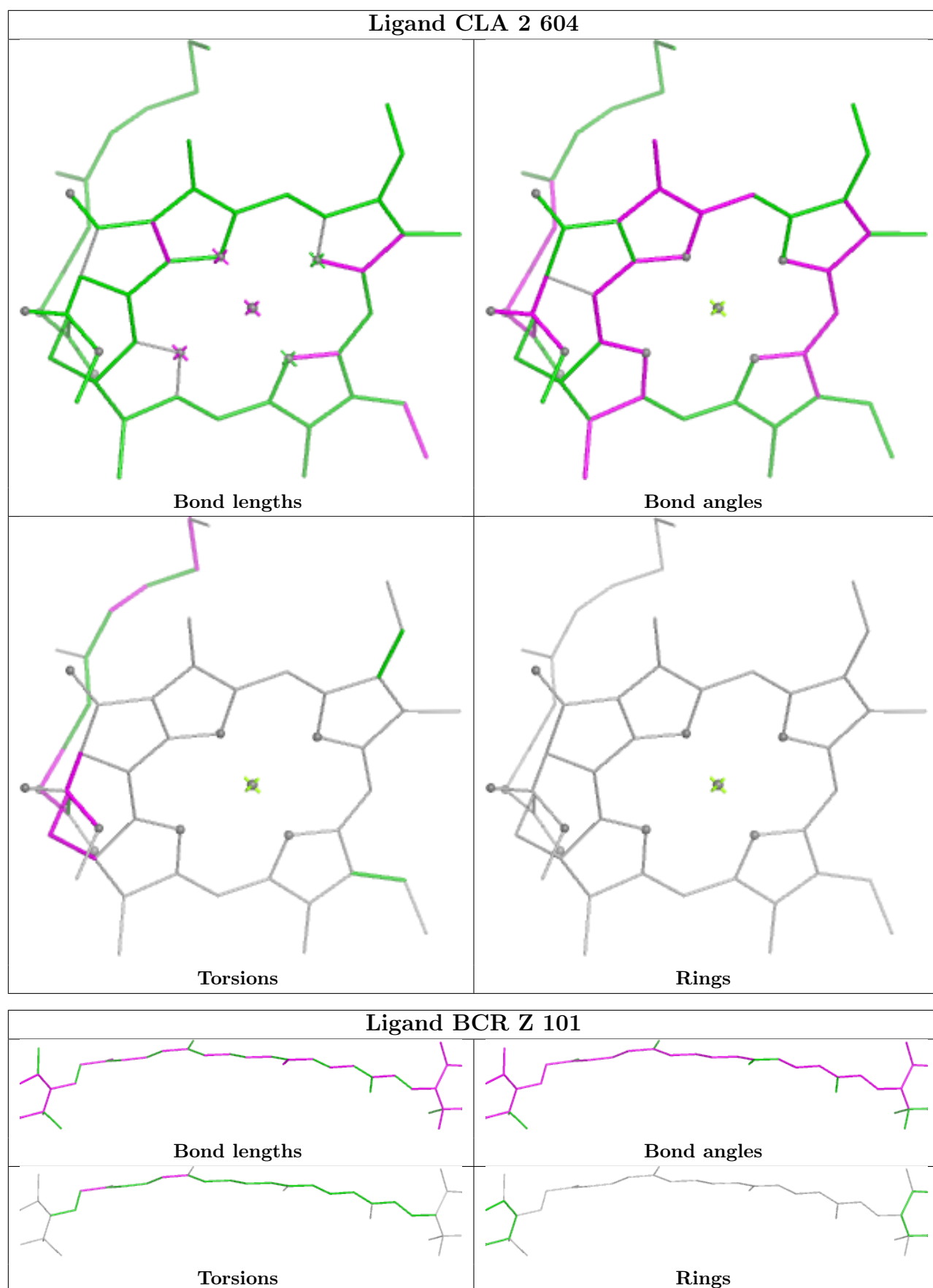


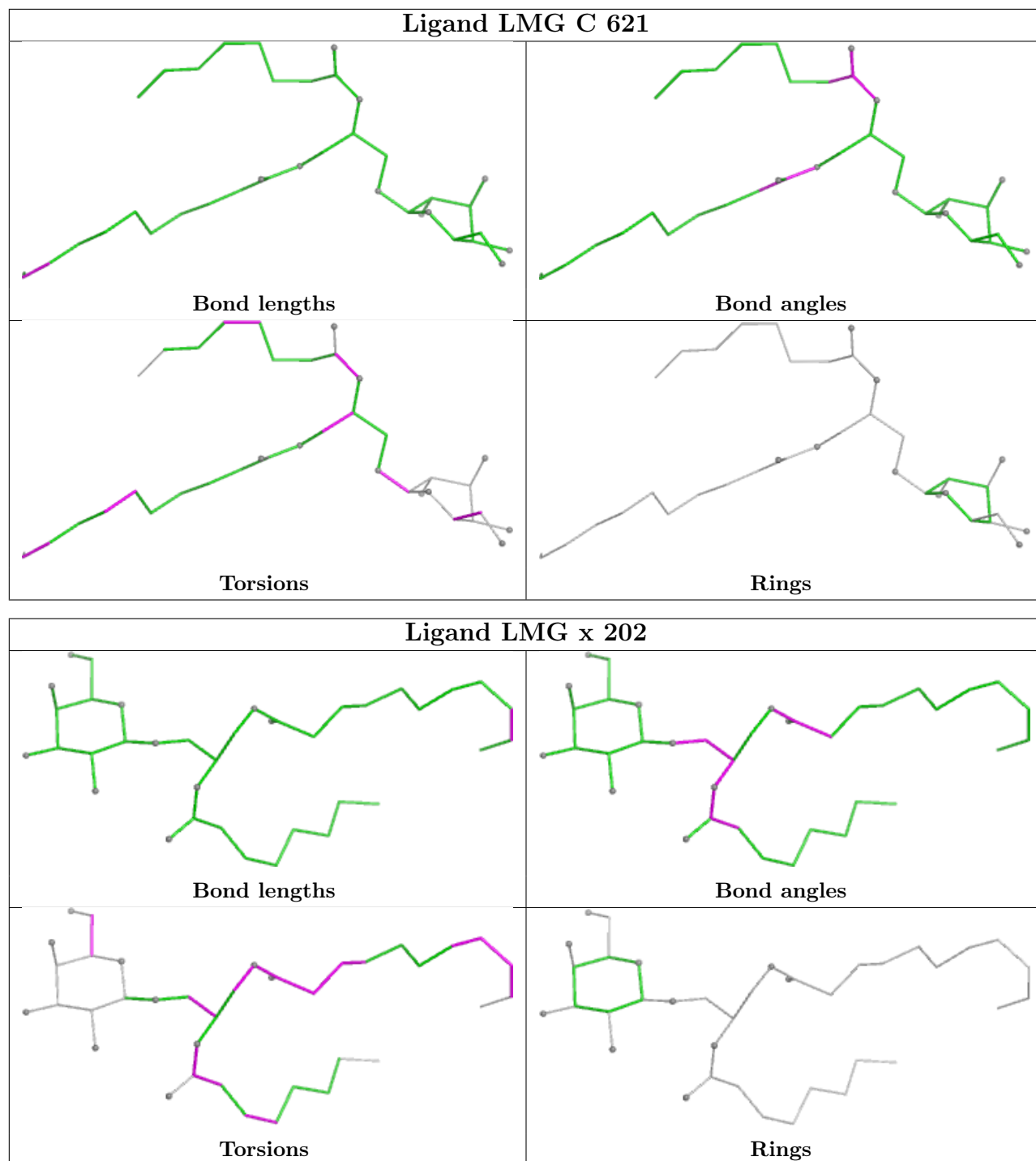
Rings



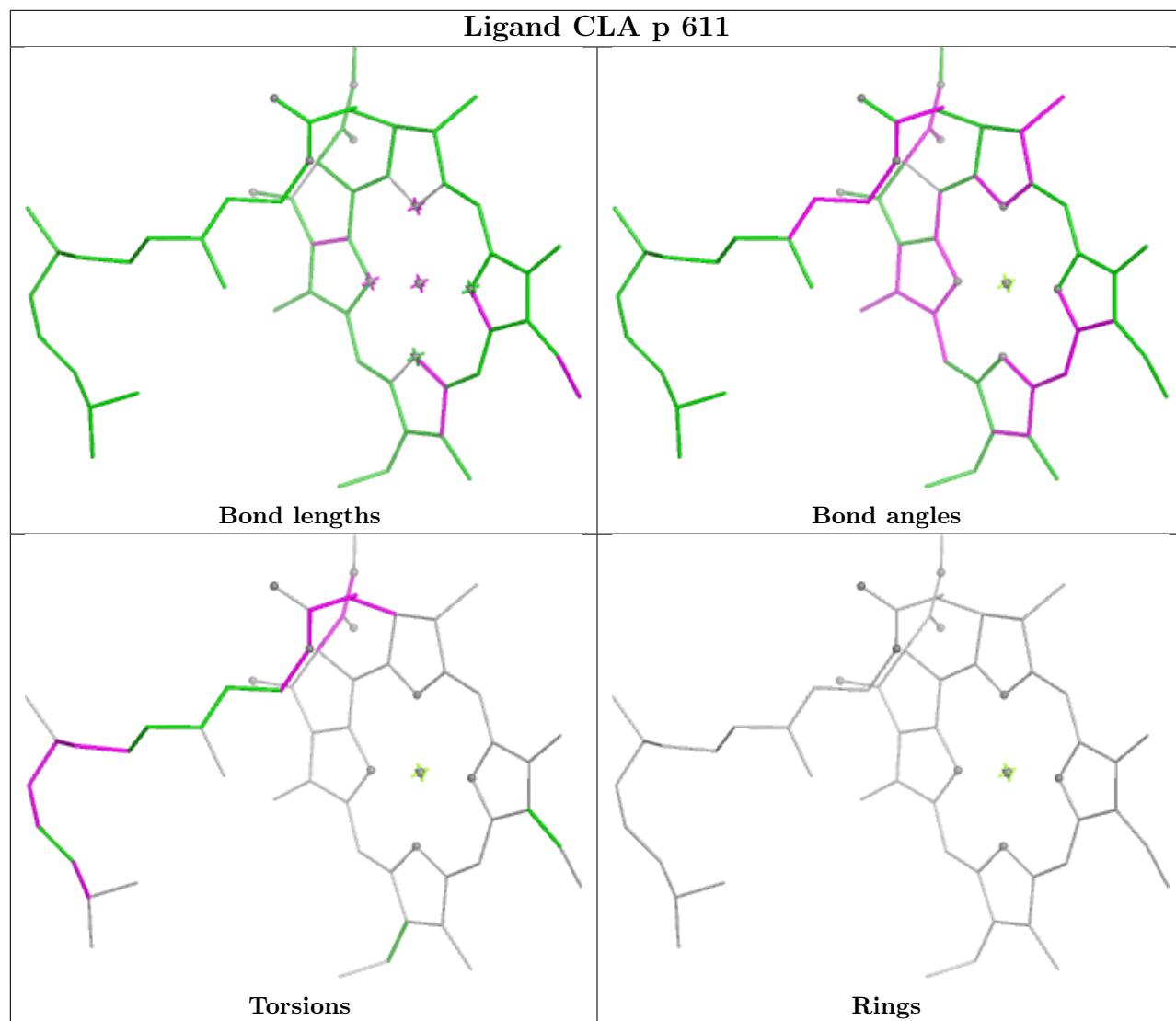




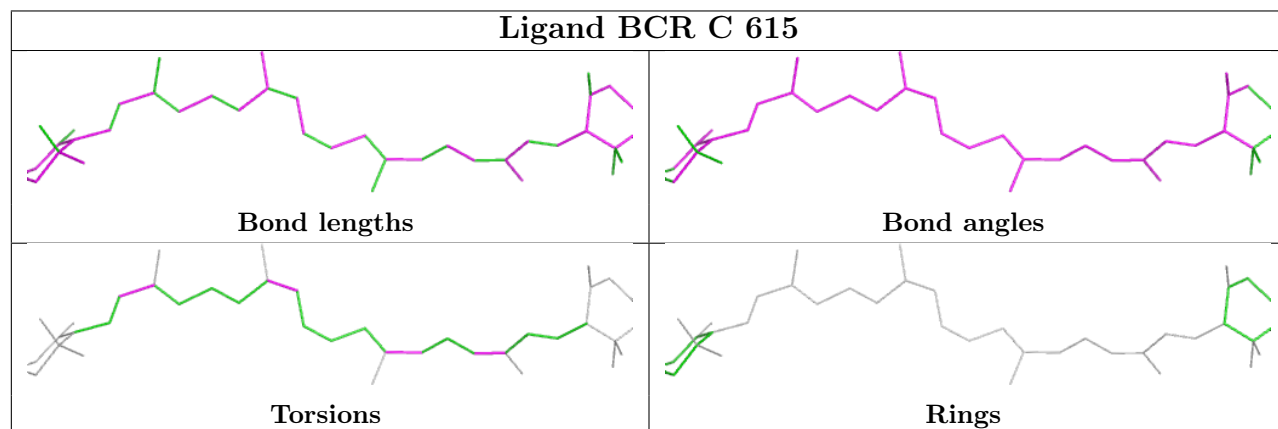


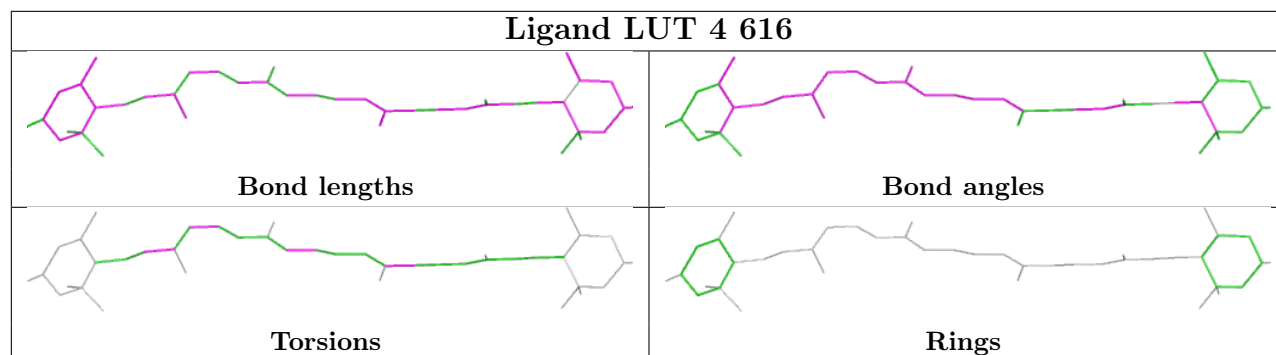
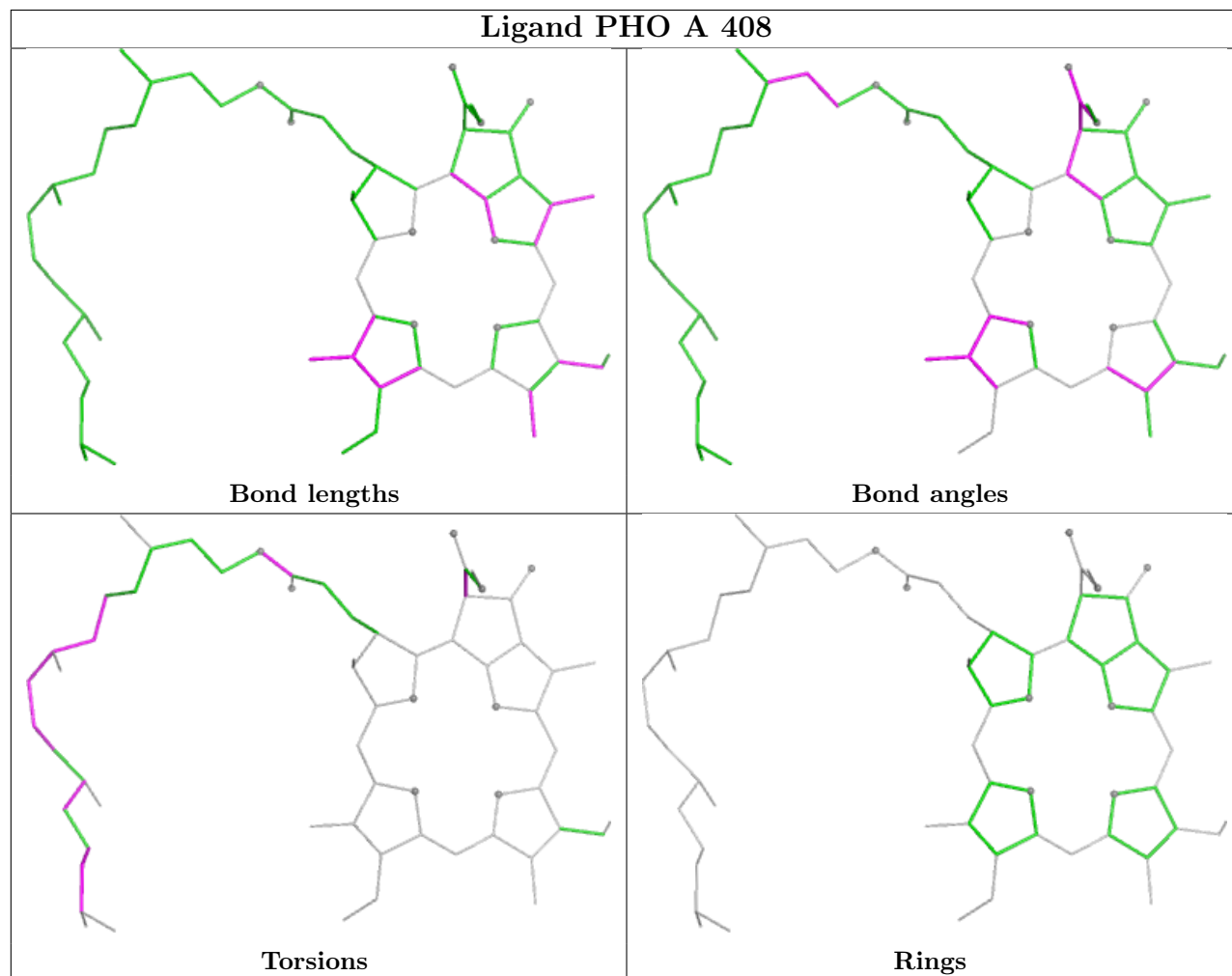


Ligand CLA p 611

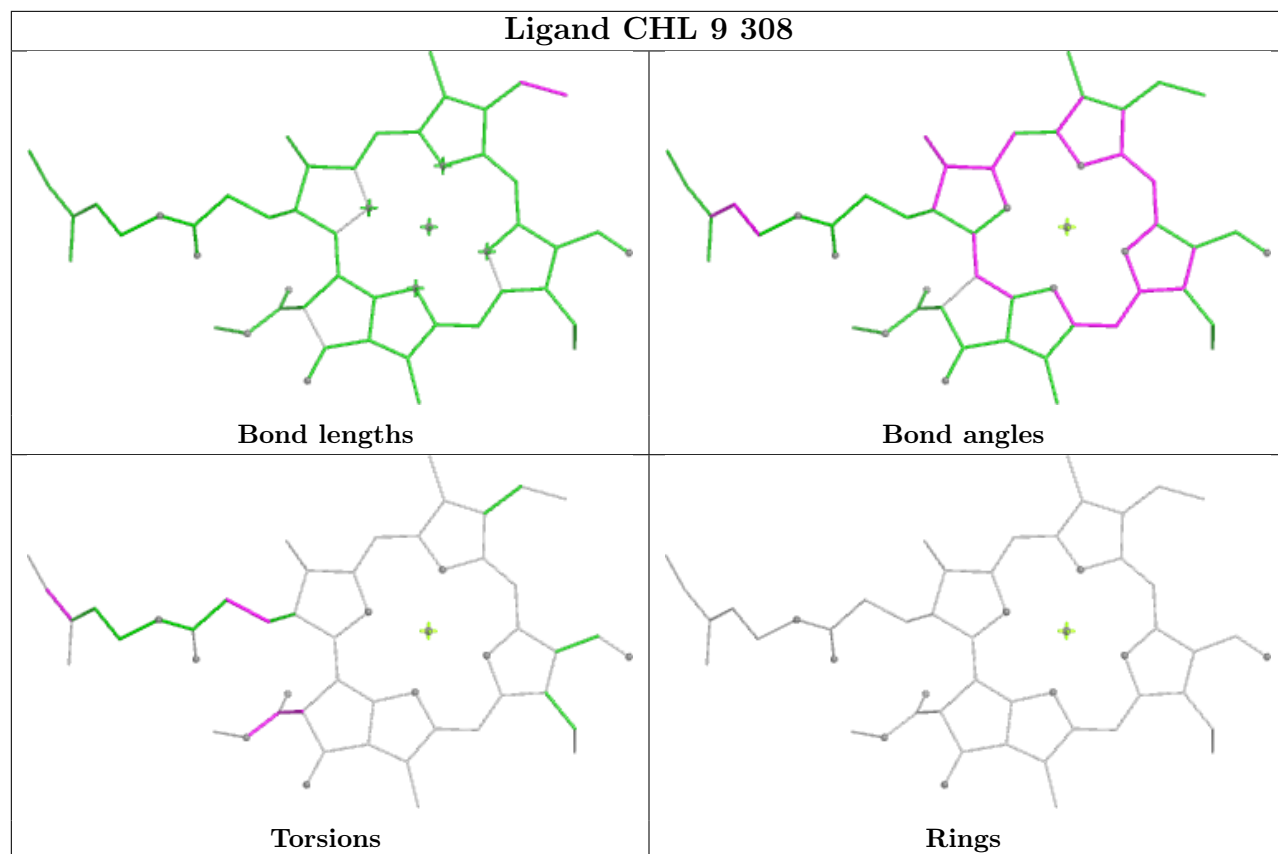


Ligand BCR C 615

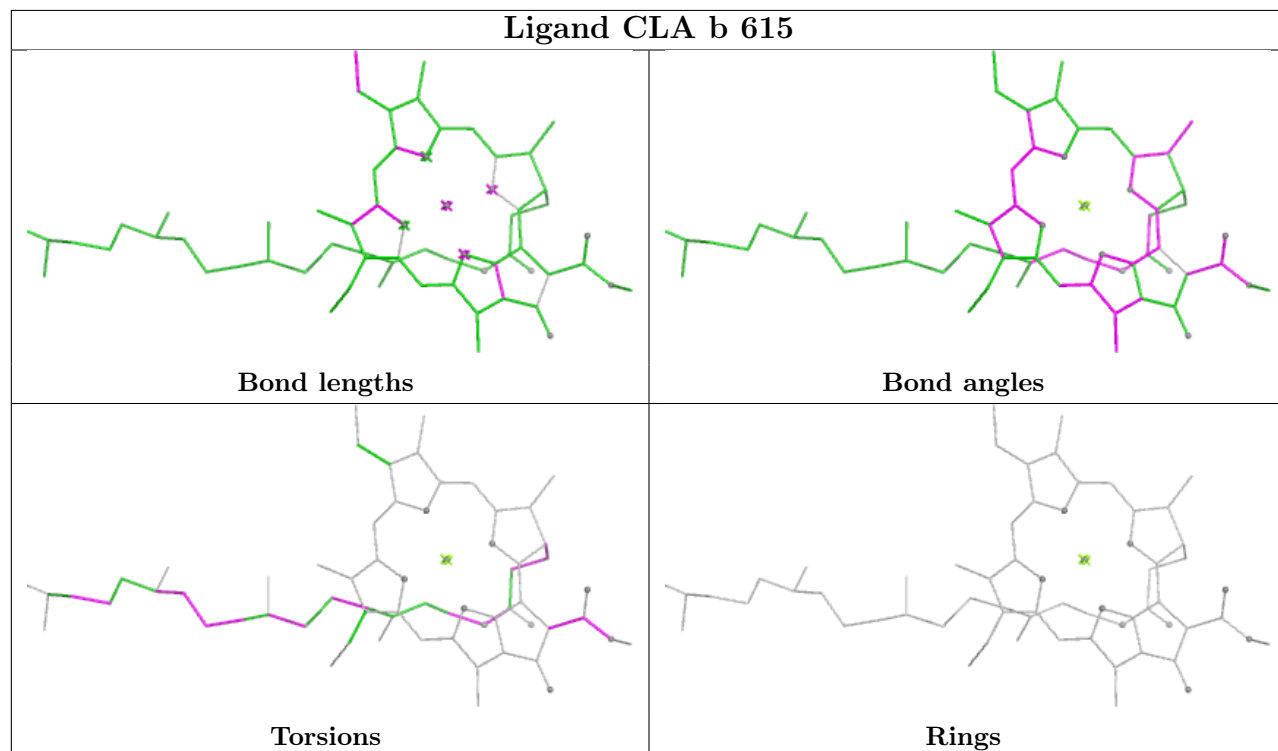


Ligand LUT 4 616**Ligand PHO A 408**

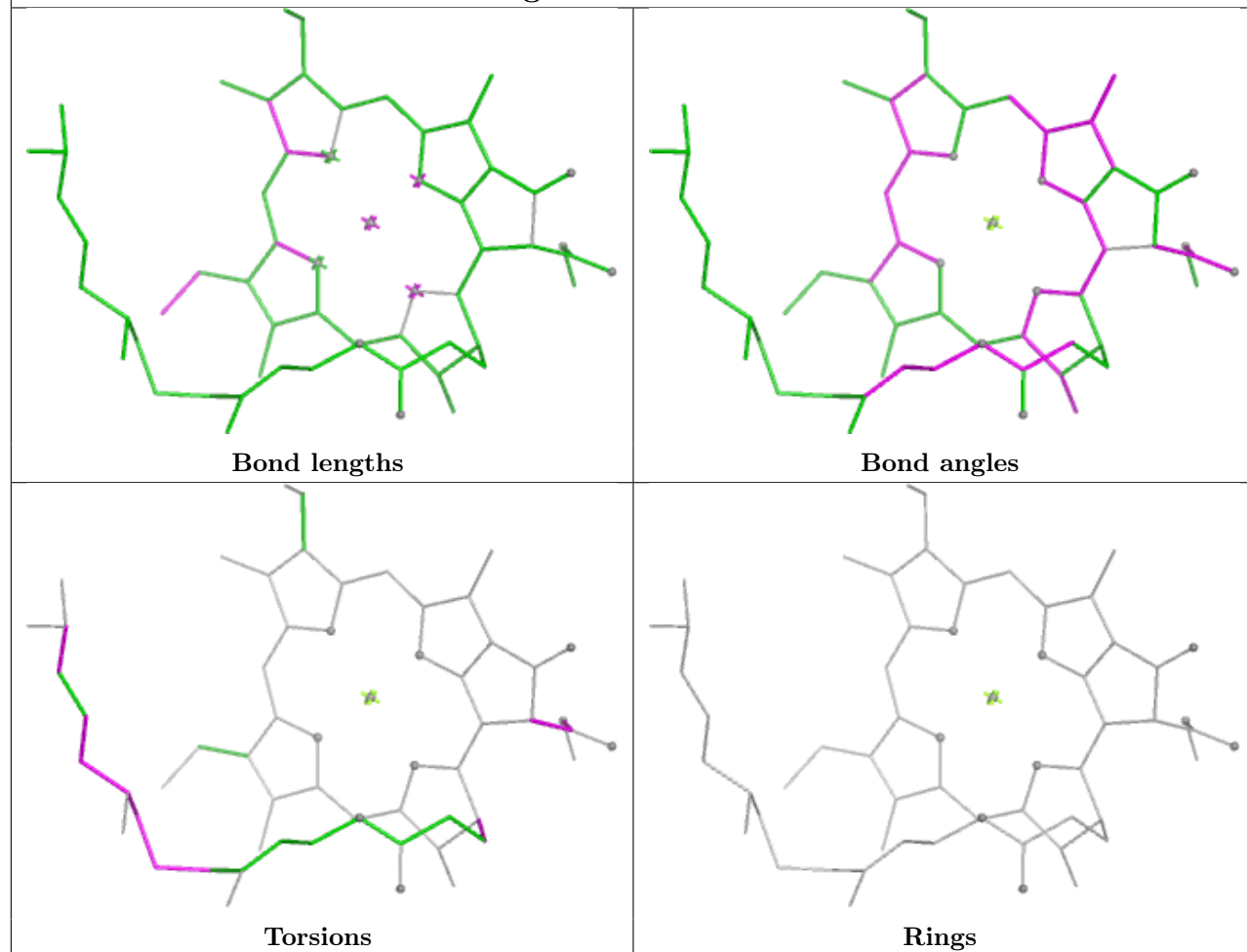
Ligand CHL 9 308



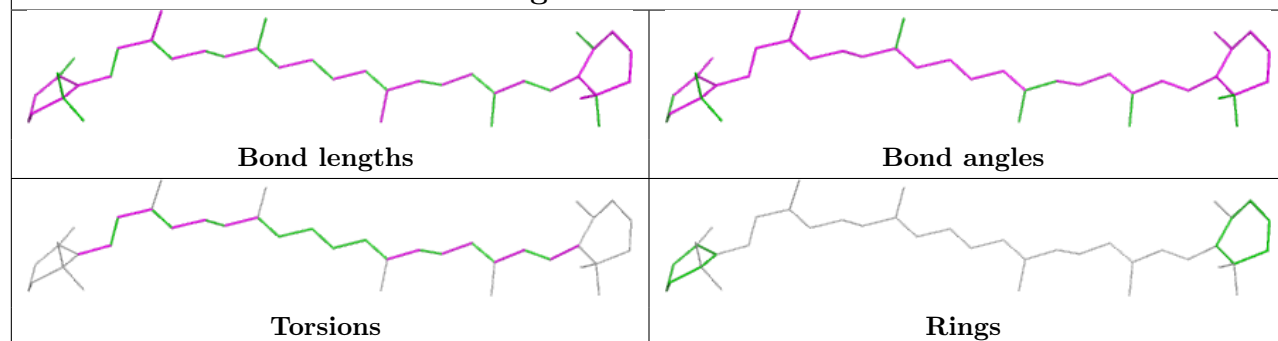
Ligand CLA b 615



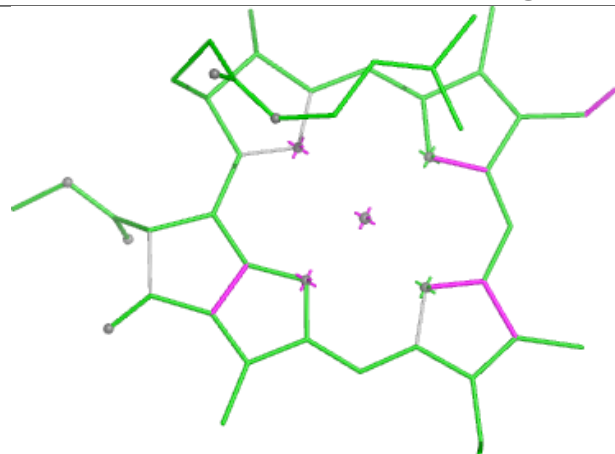
Ligand CLA 5 602



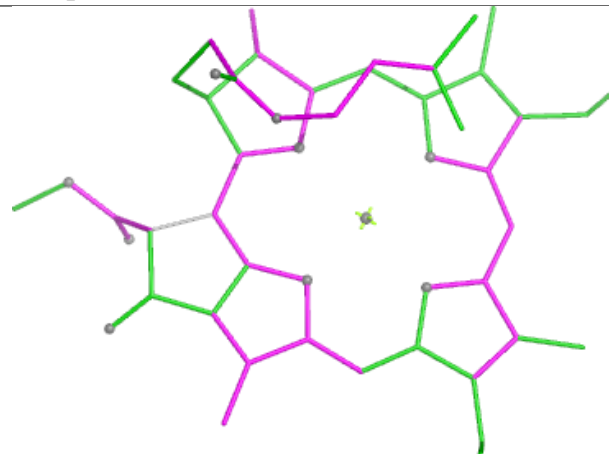
Ligand BCR C 614



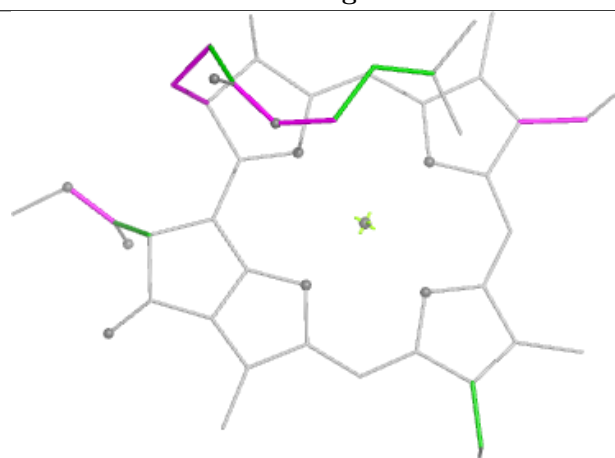
Ligand CLA q 316



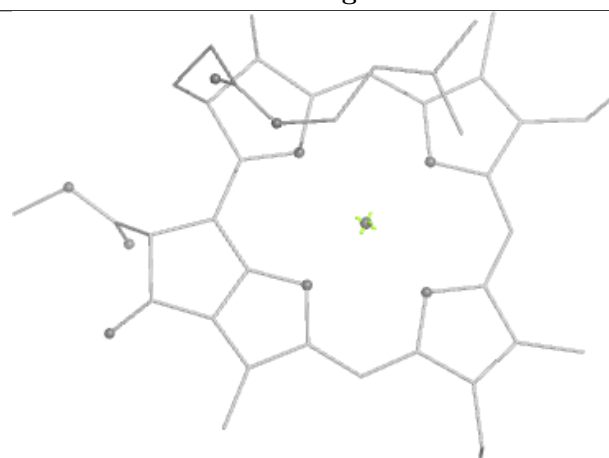
Bond lengths



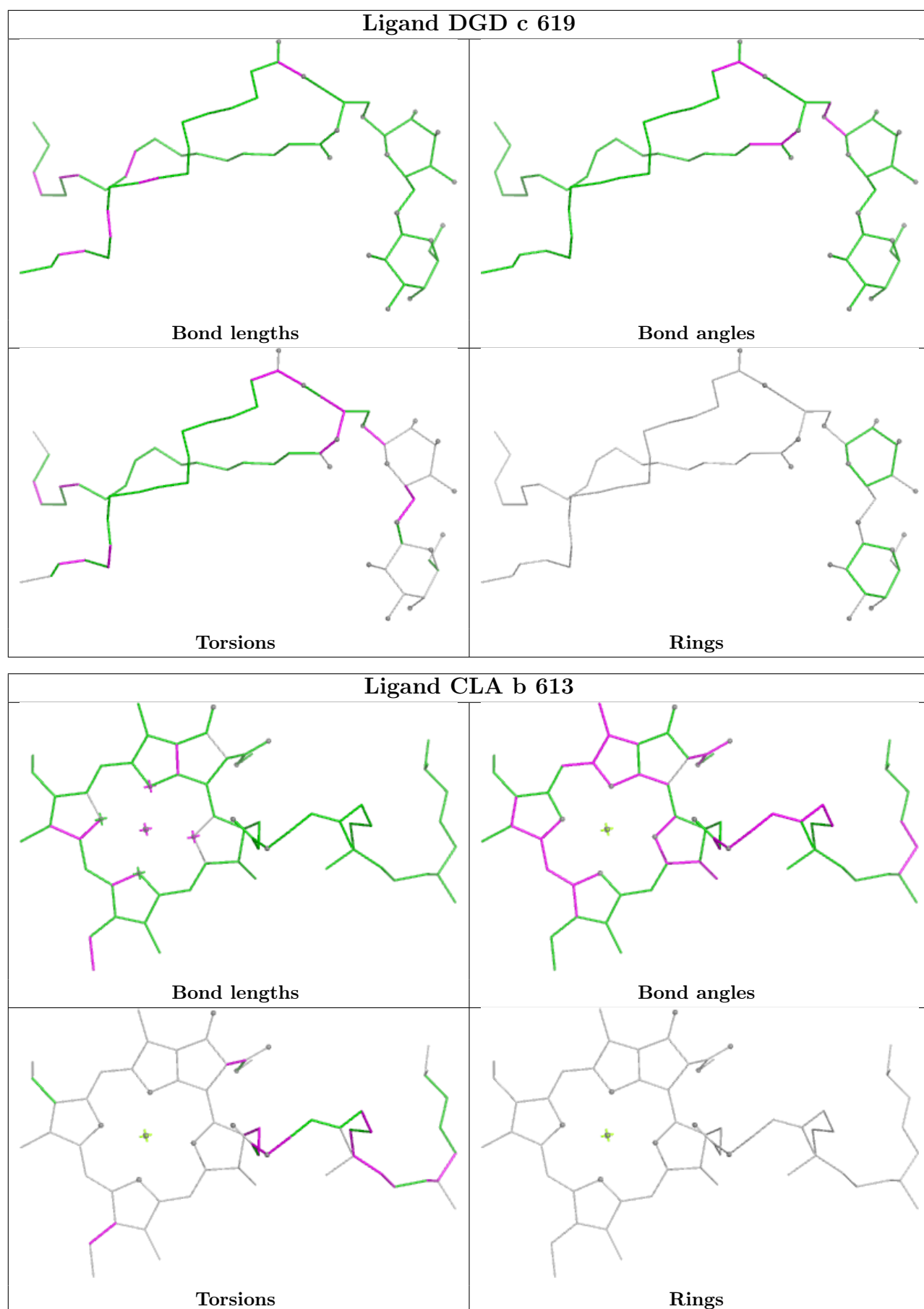
Bond angles

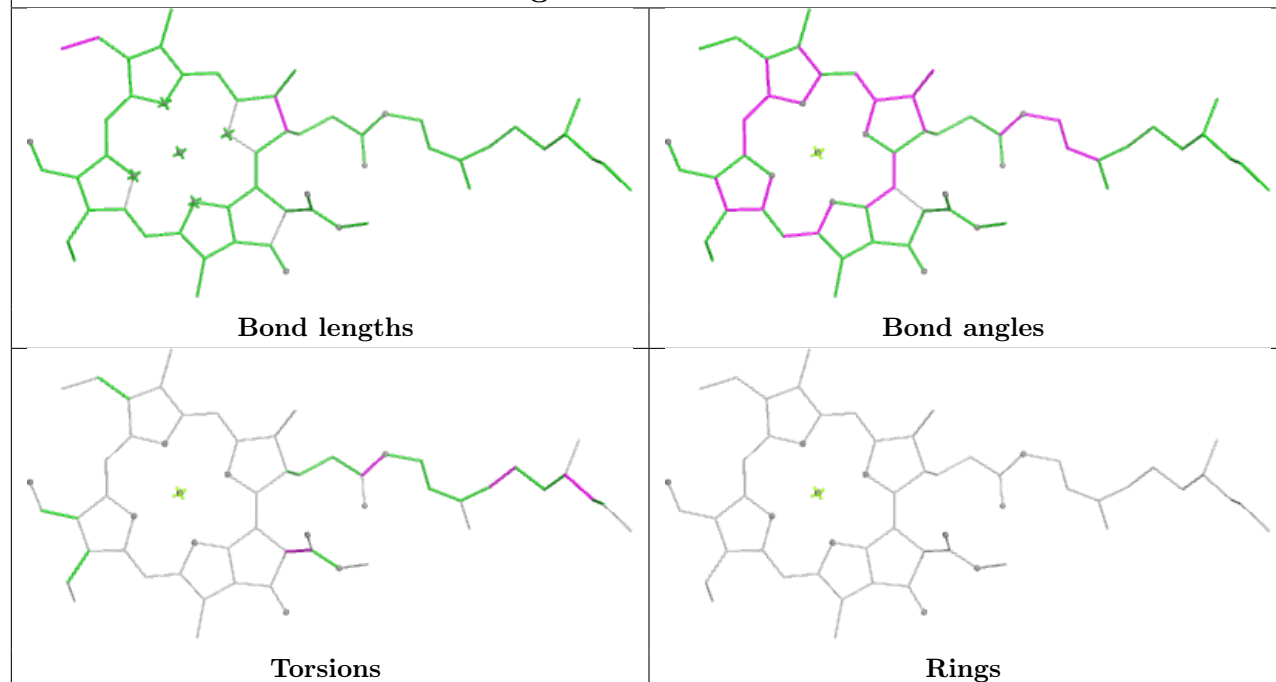
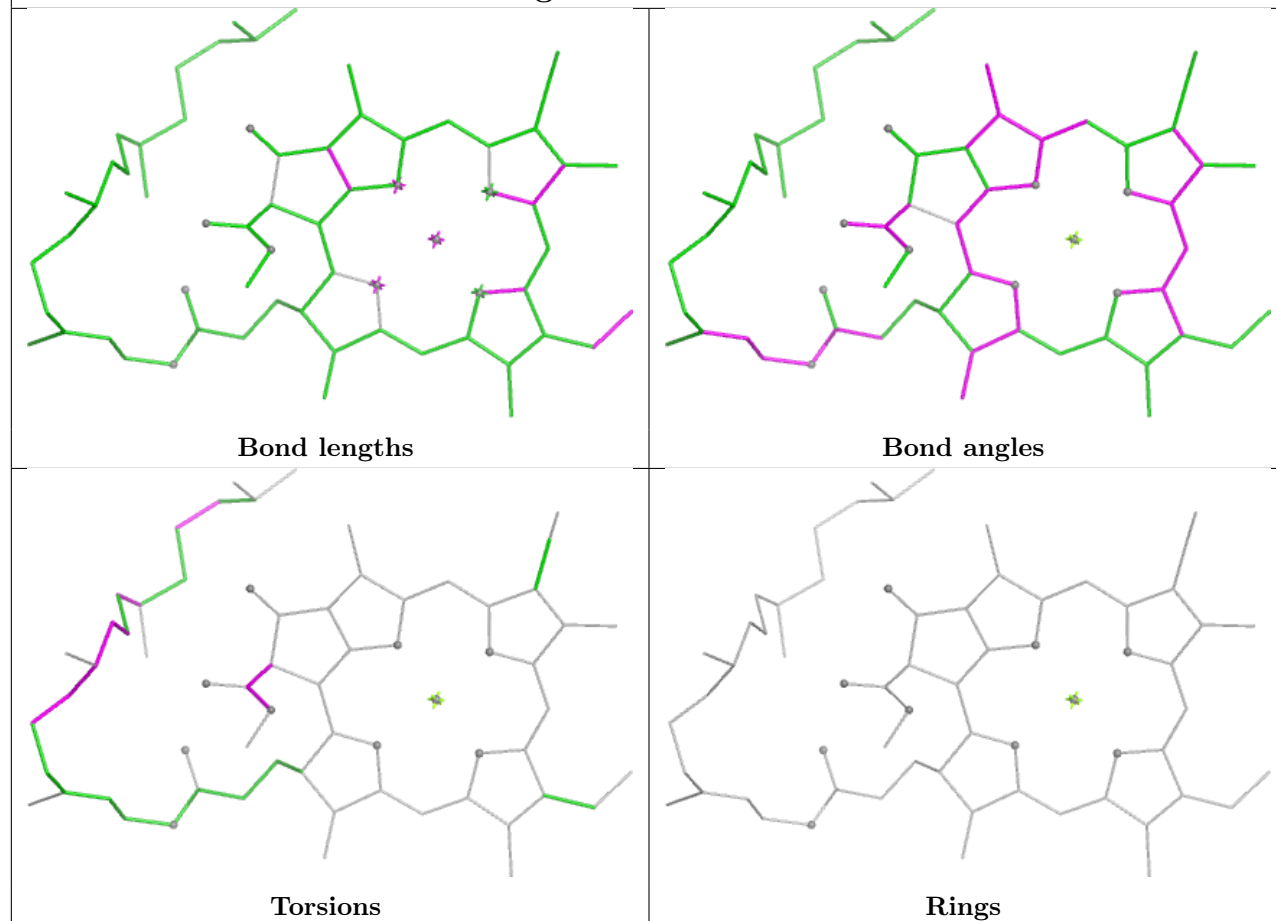


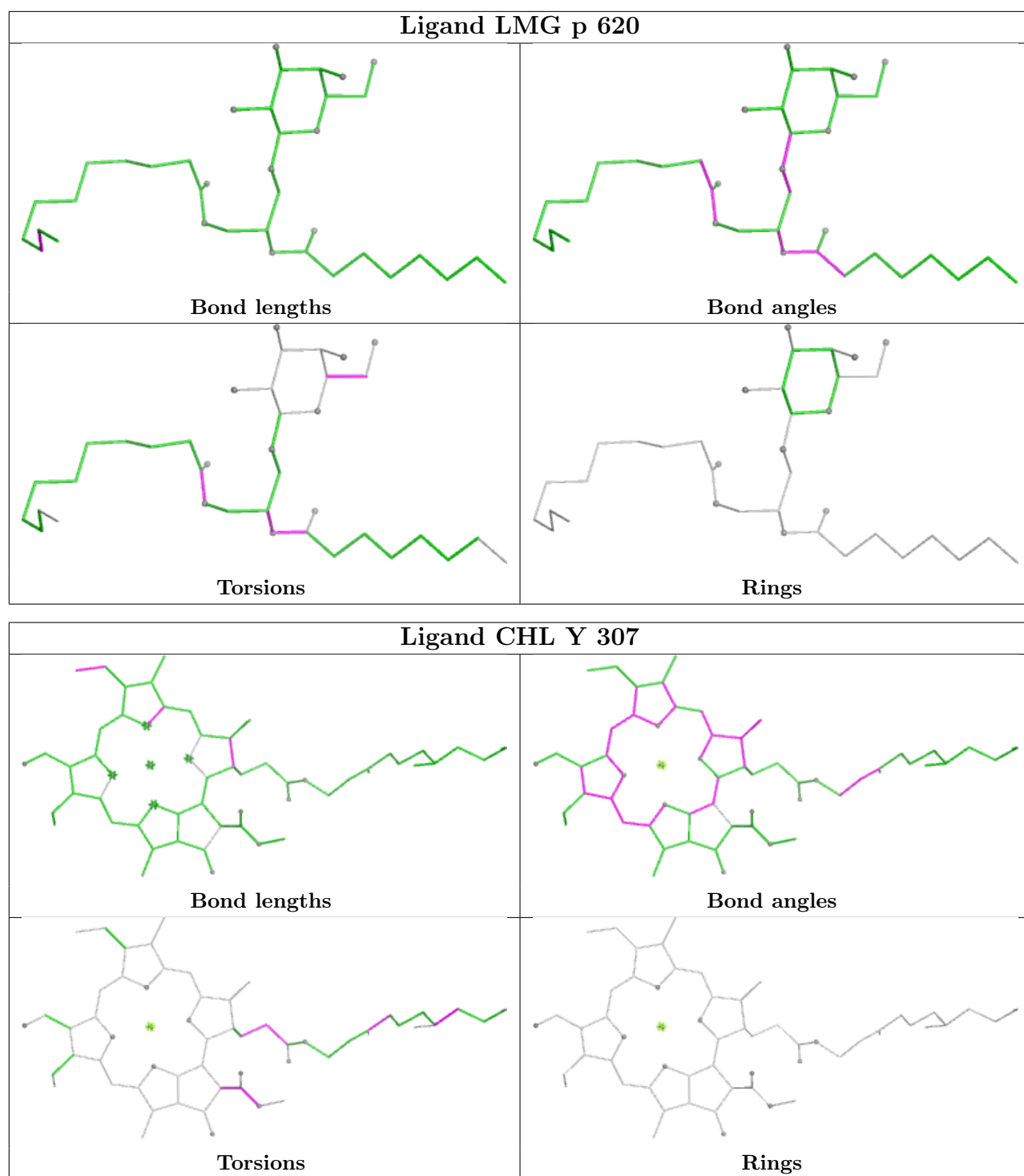
Torsions

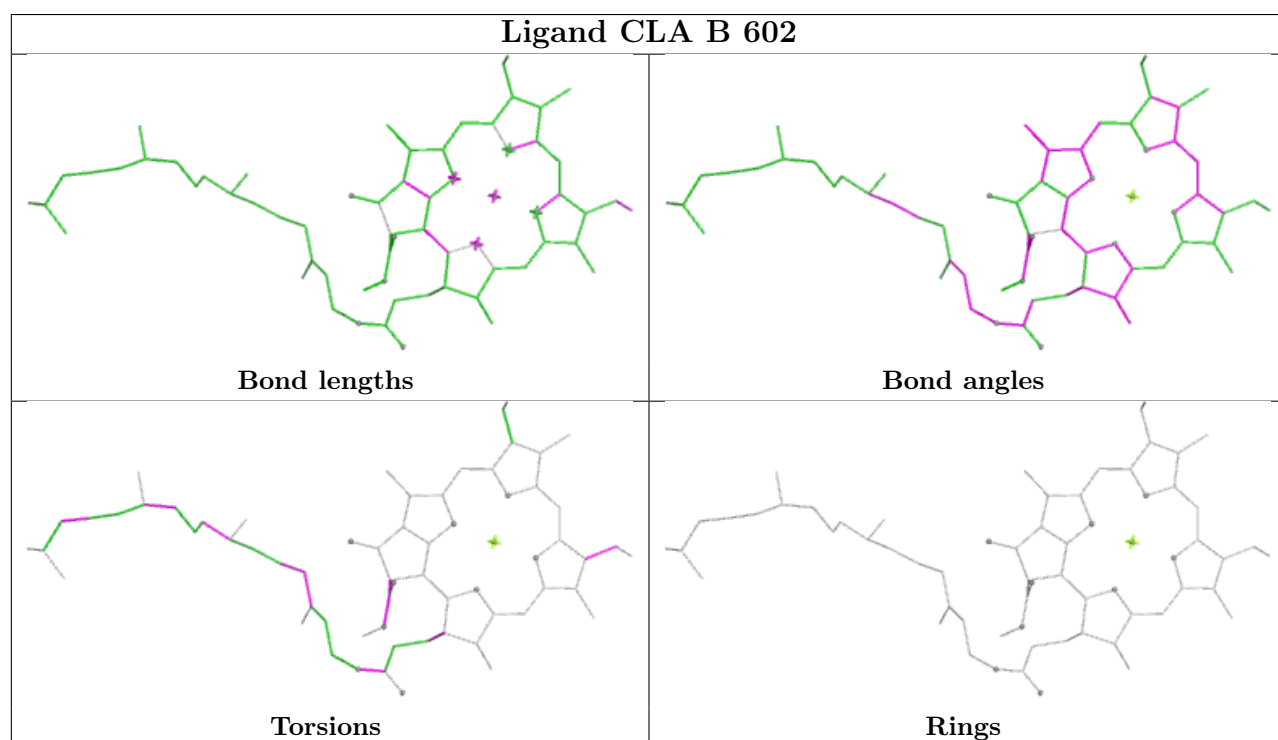
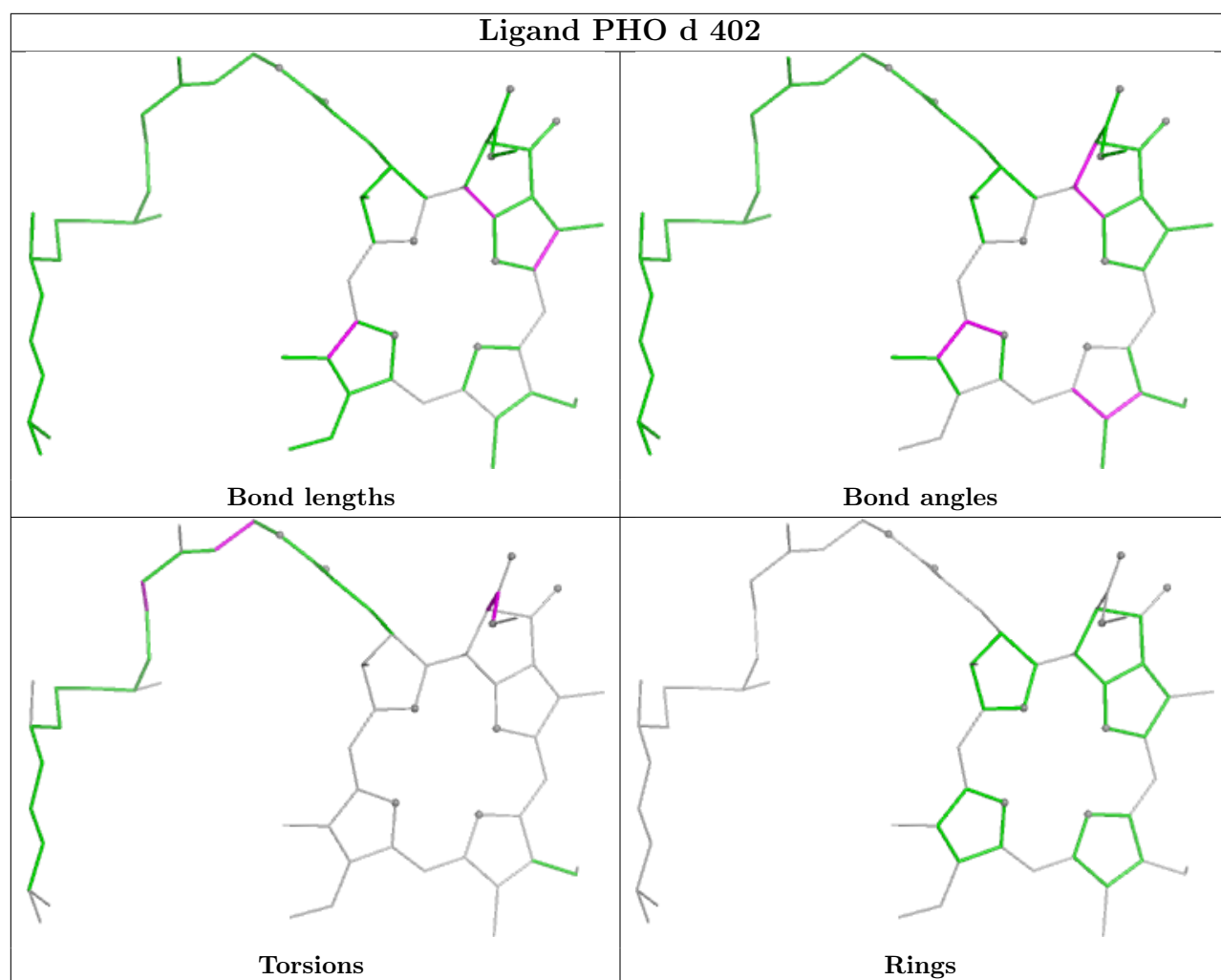


Rings

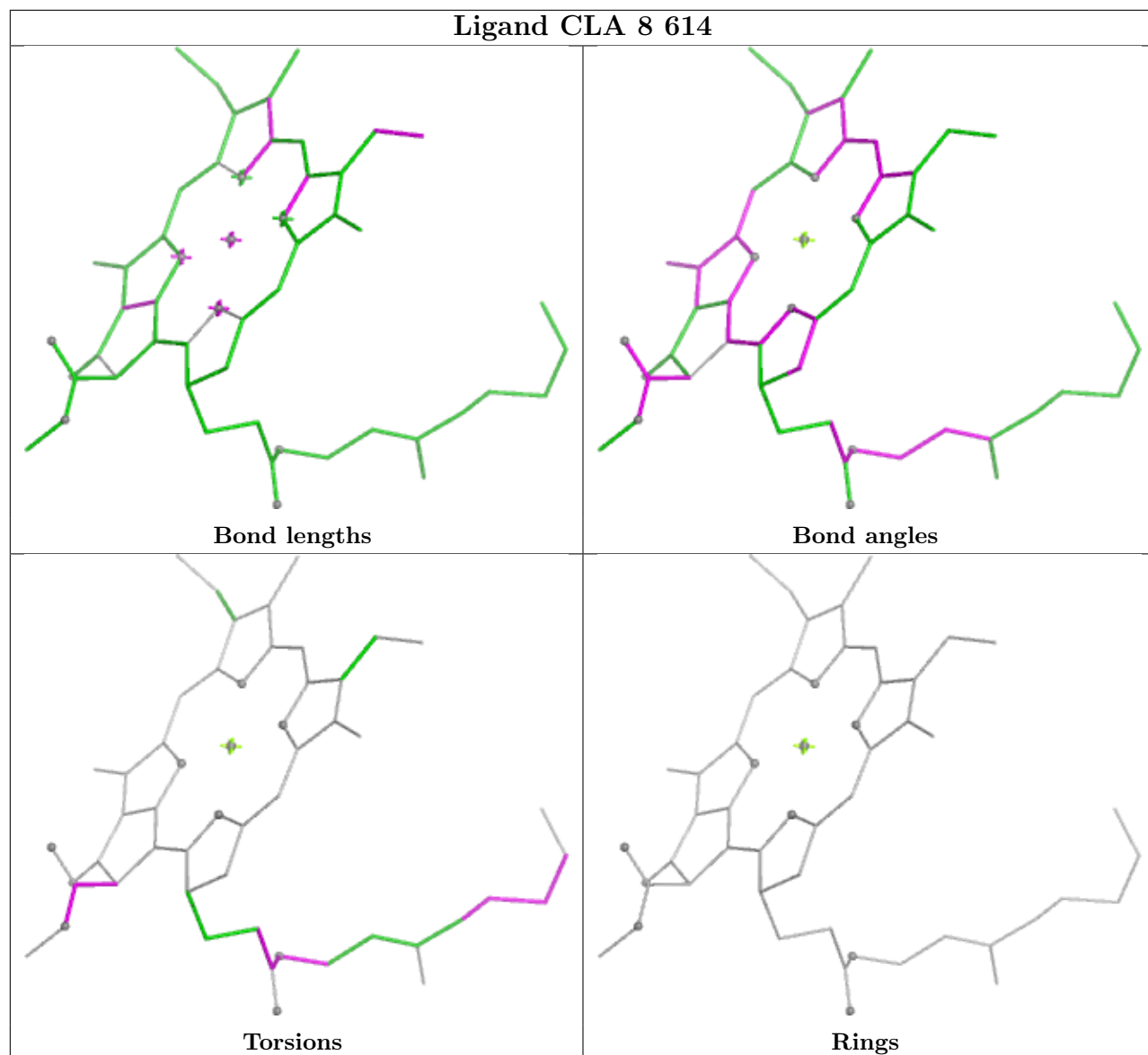


Ligand CHL N 307**Ligand CLA b 611**

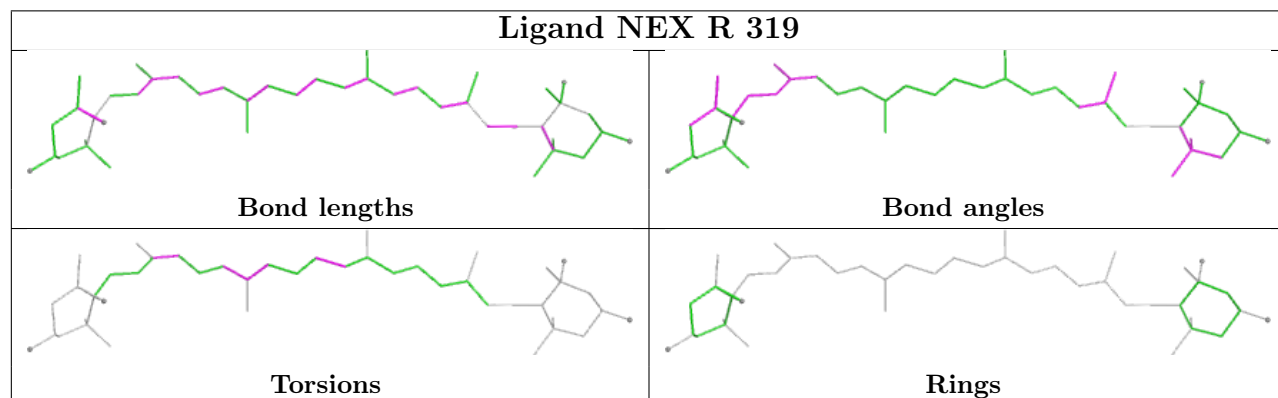


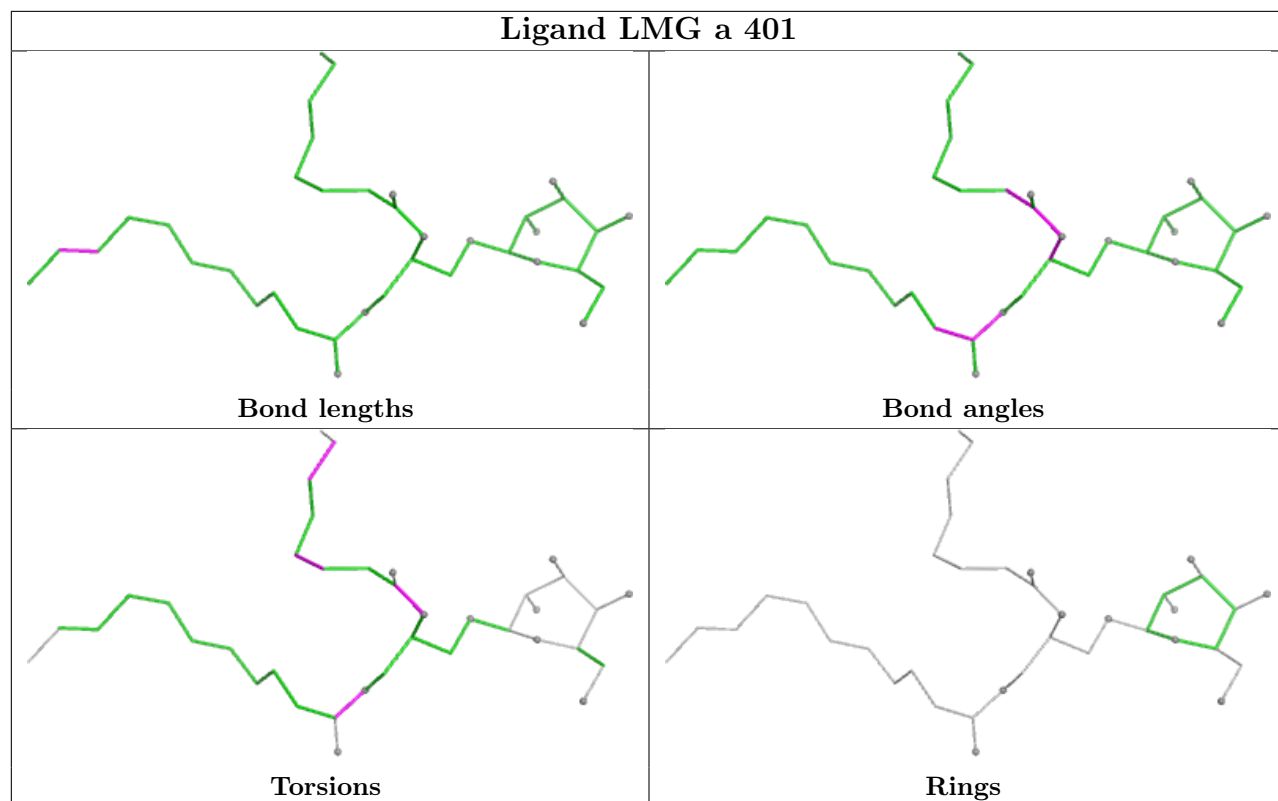


Ligand CLA 8 614

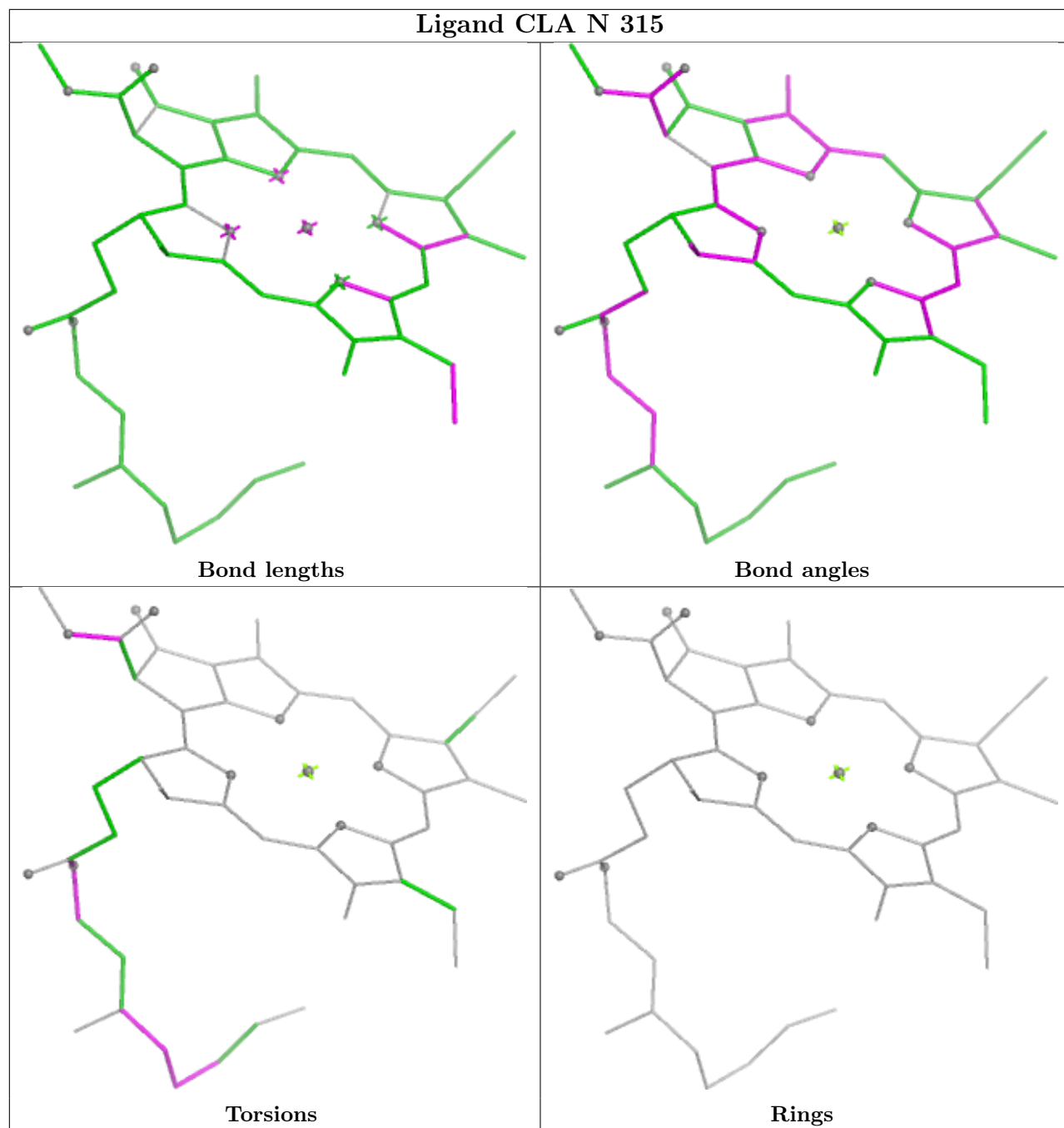


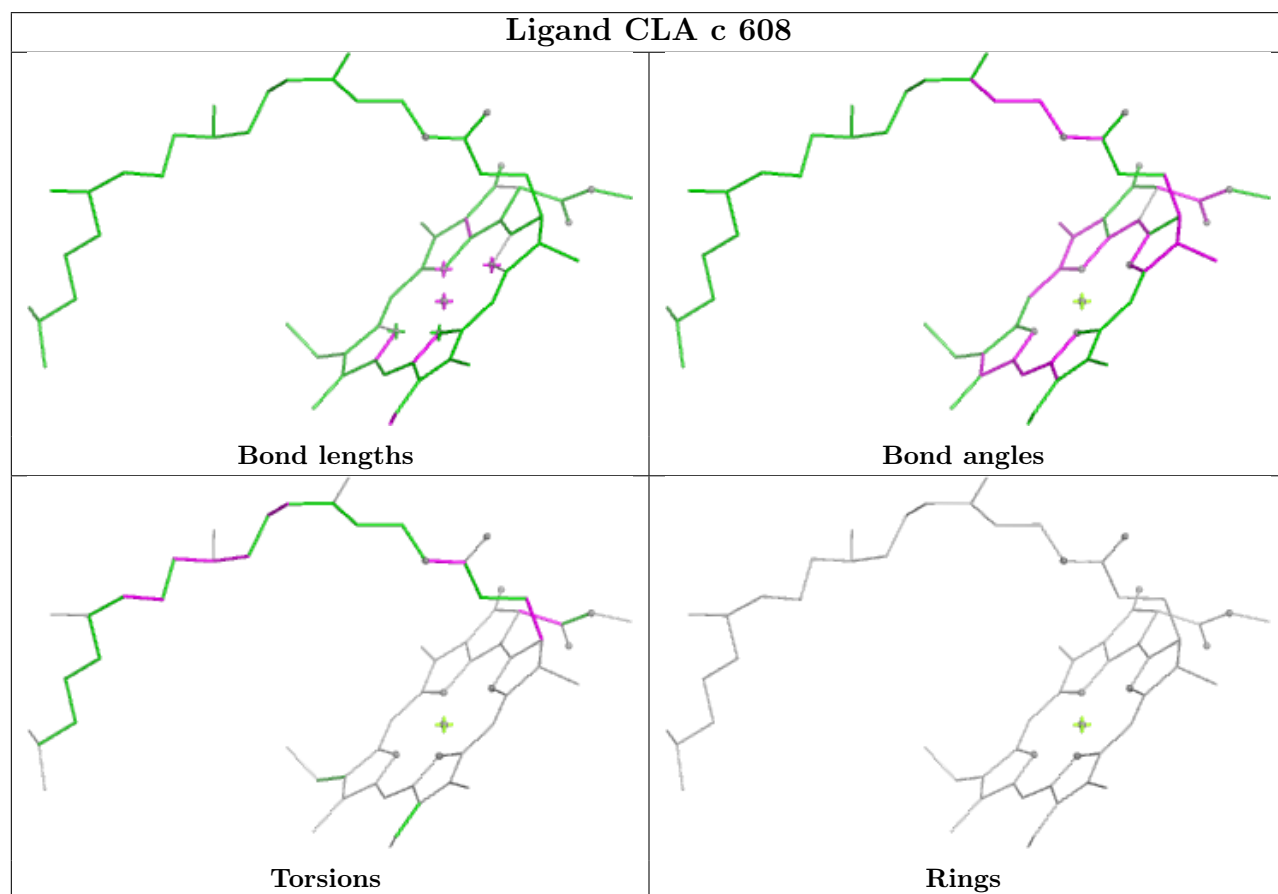
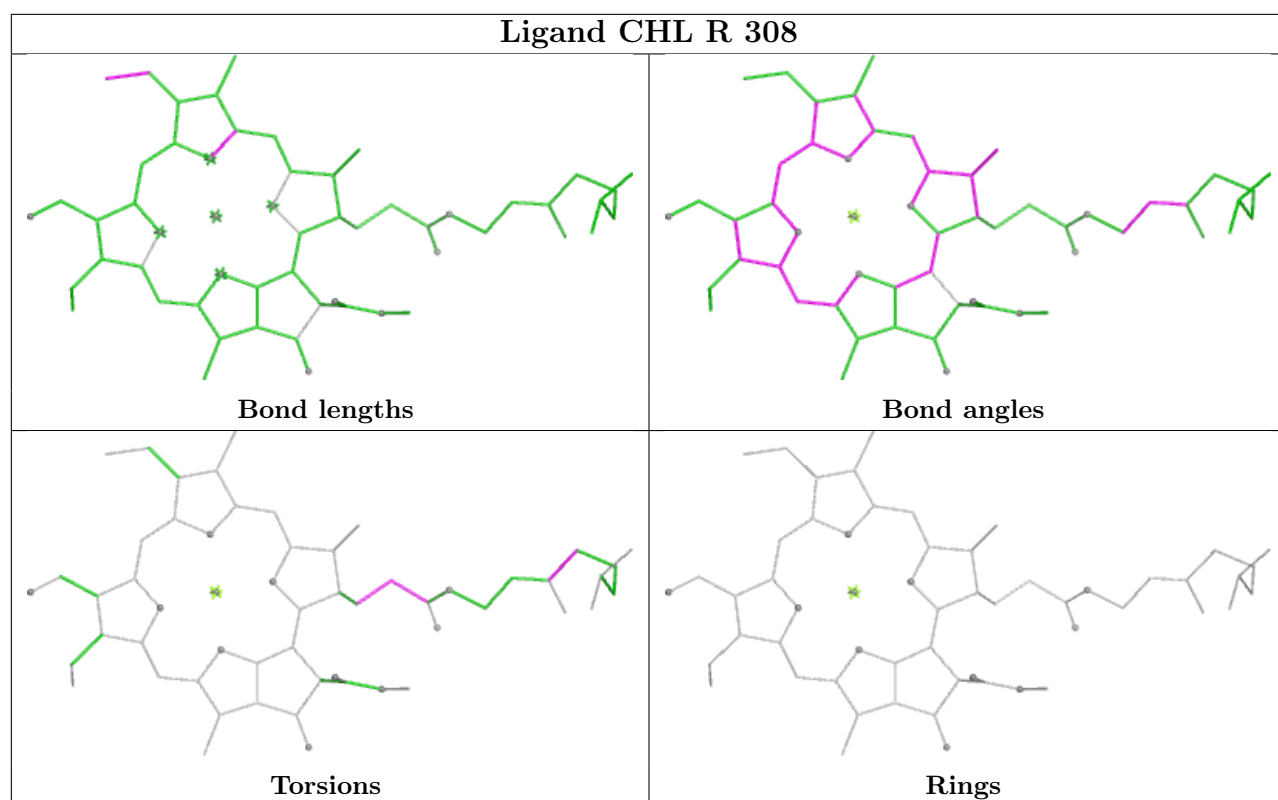
Ligand NEX R 319

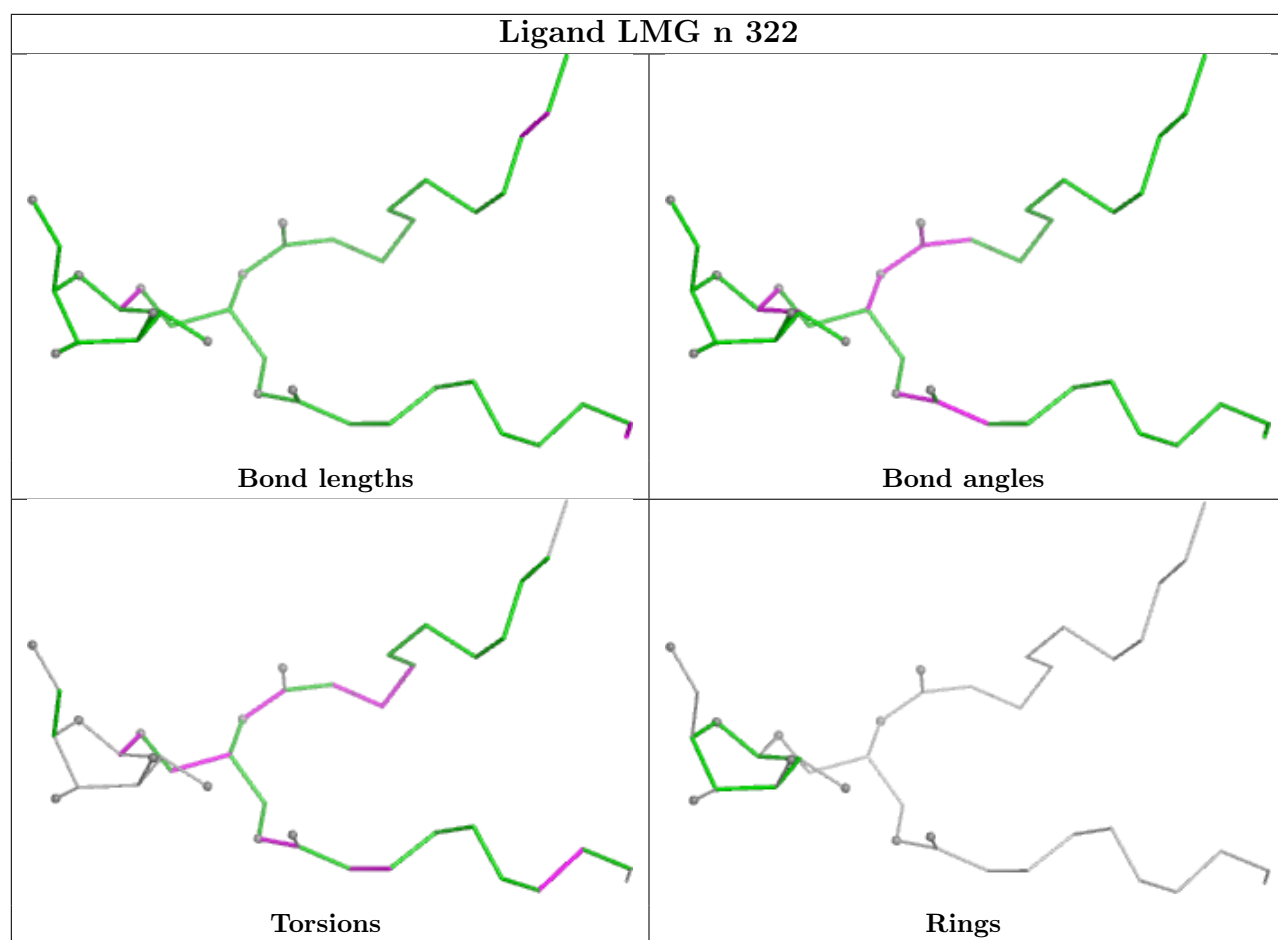




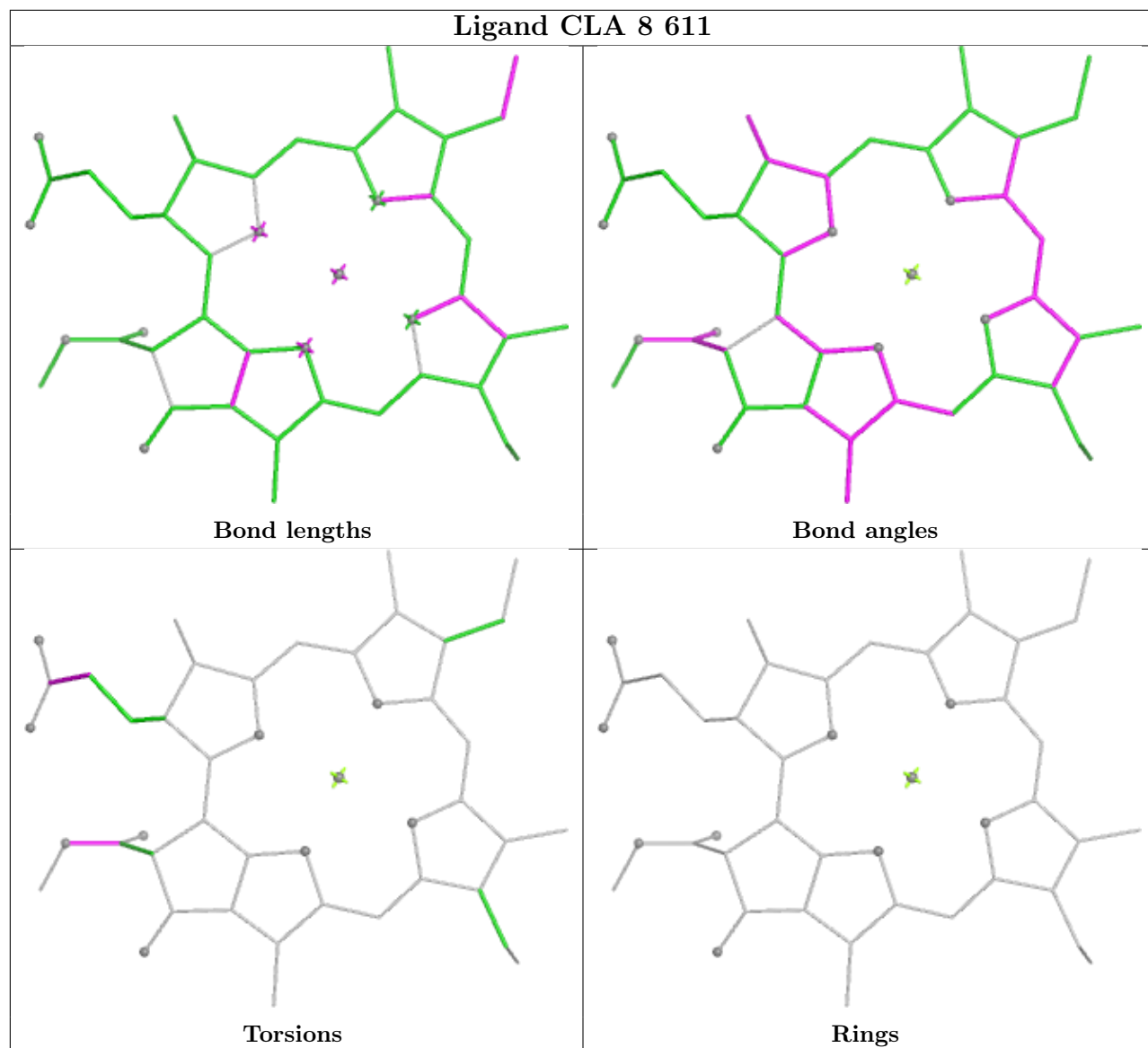
Ligand CLA N 315



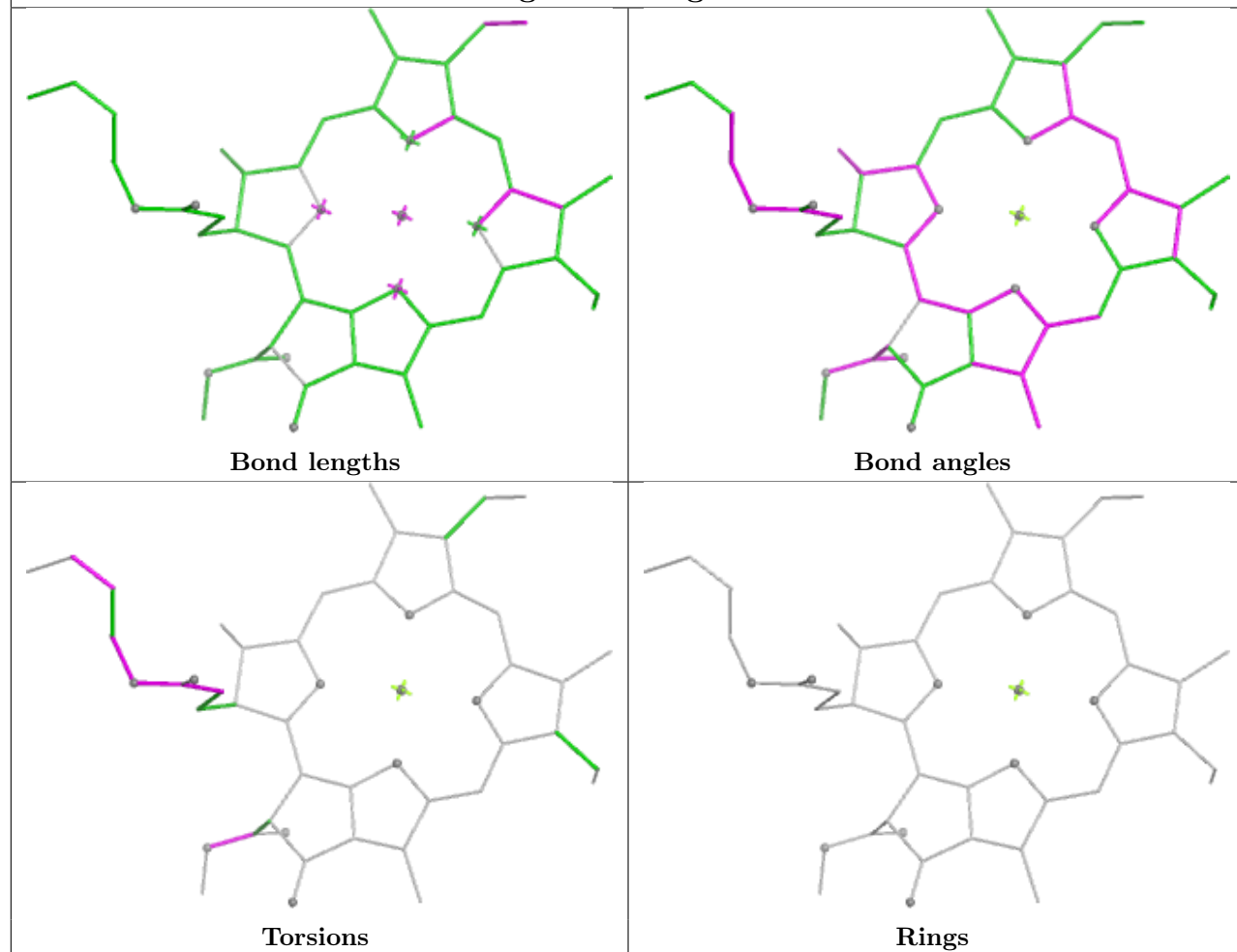




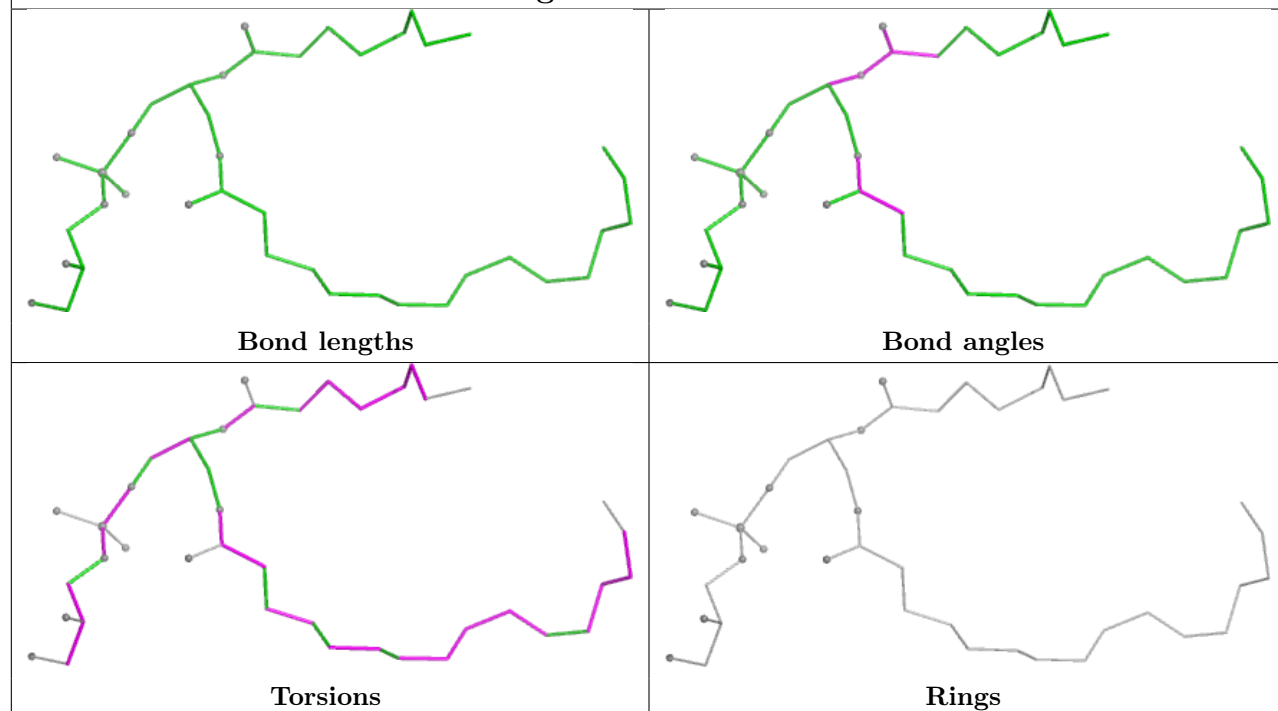
Ligand CLA 8 611

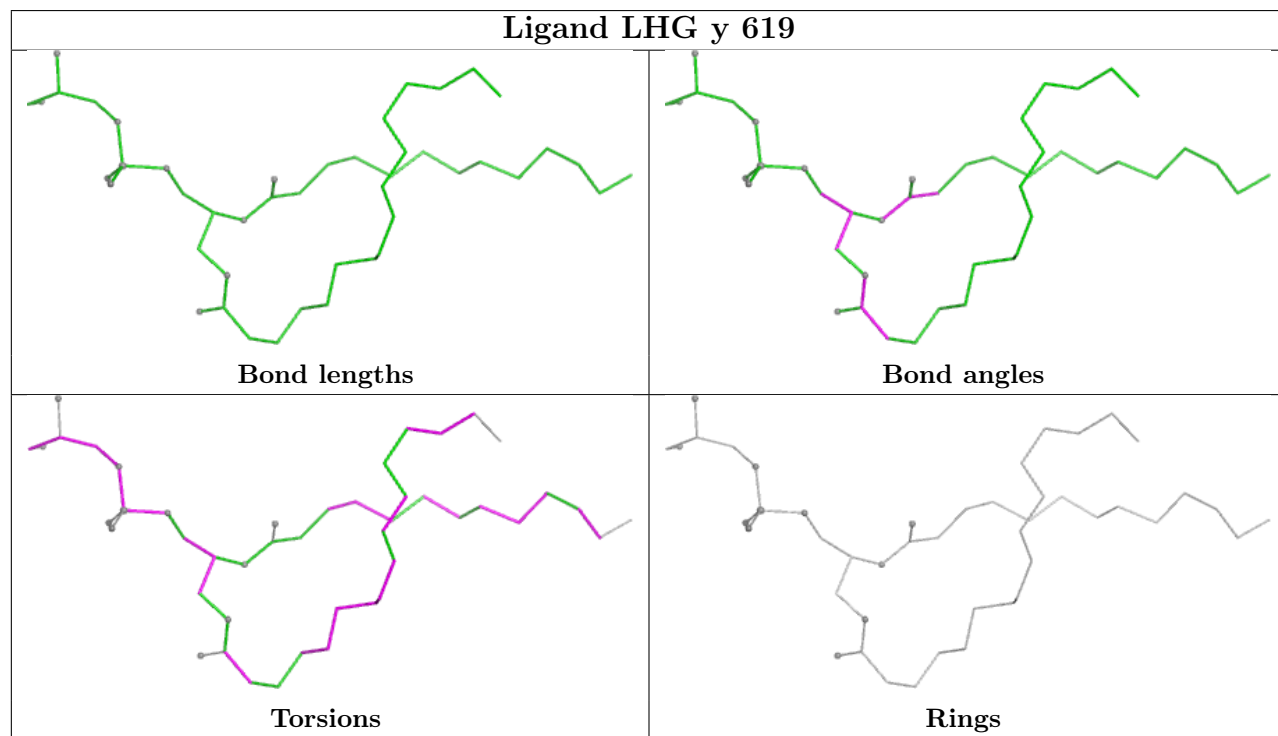
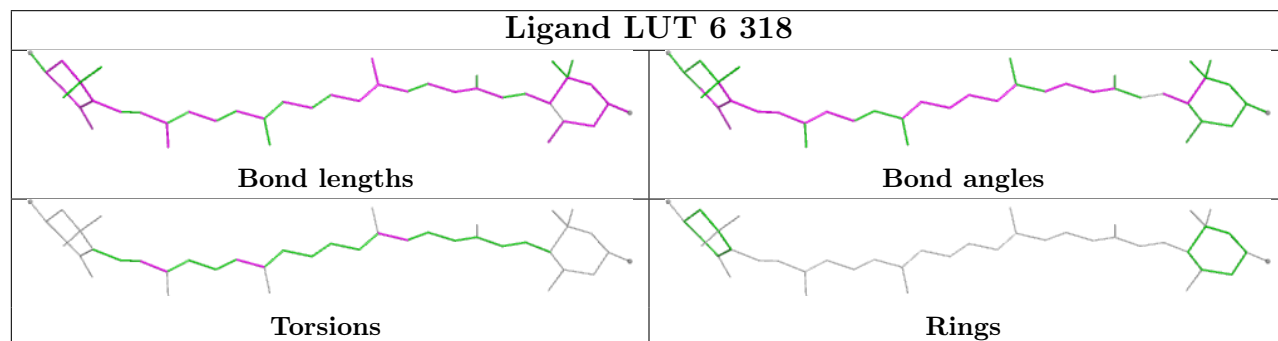
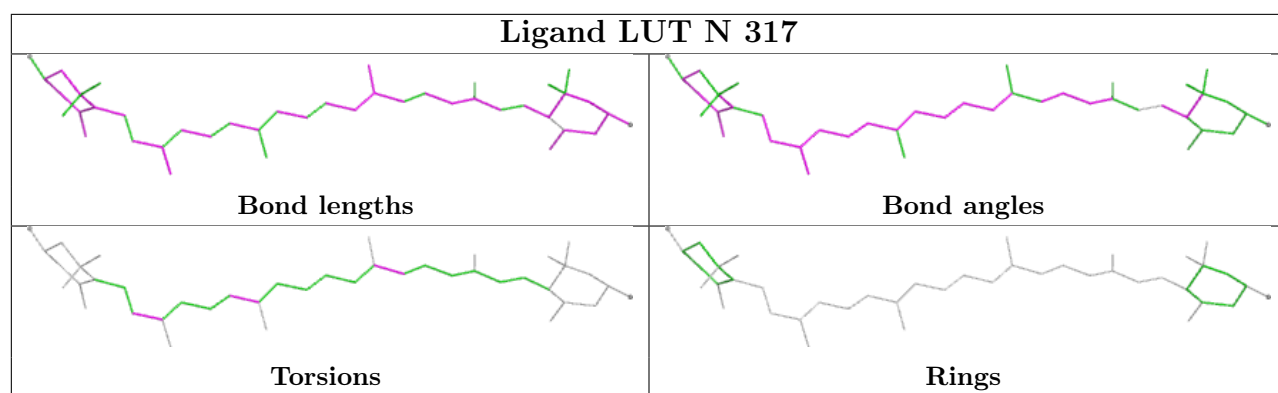


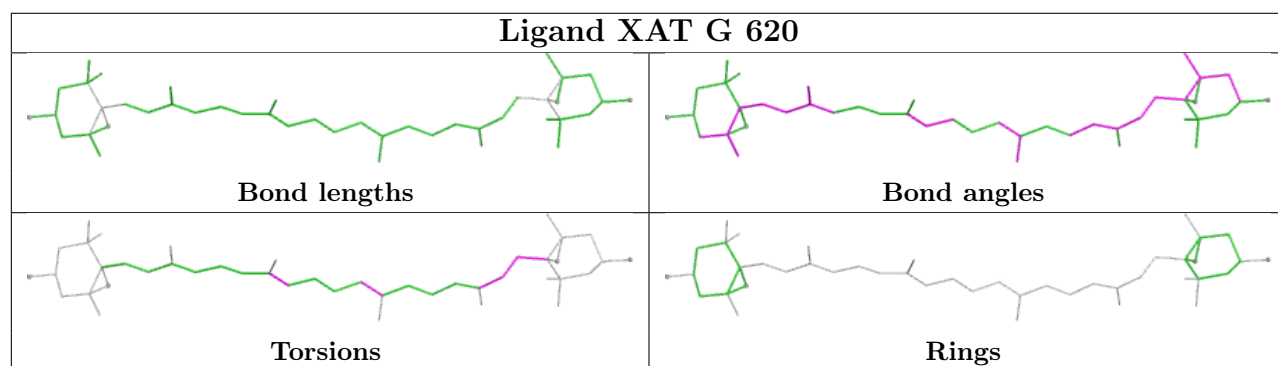
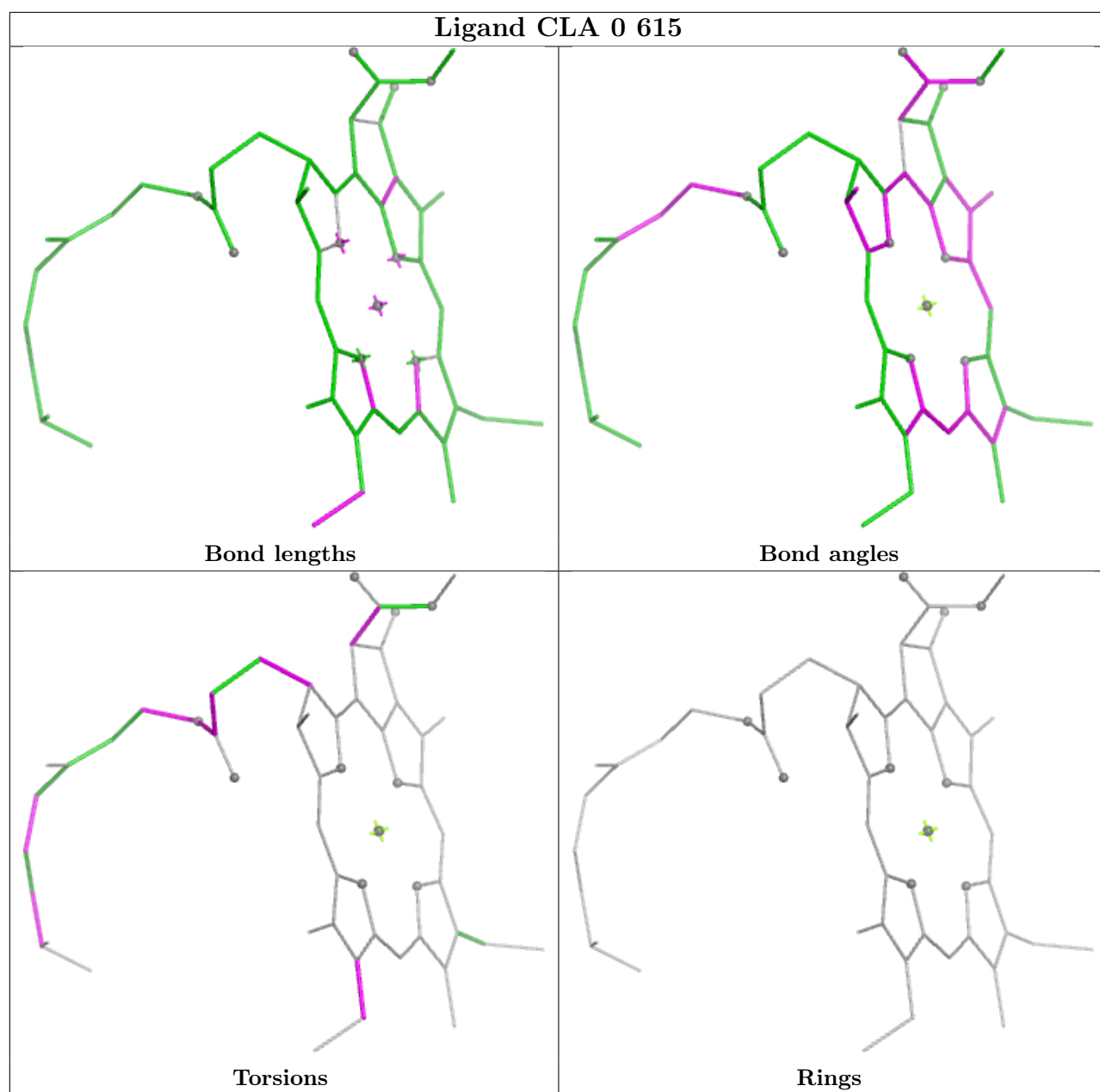
Ligand CLA g 314



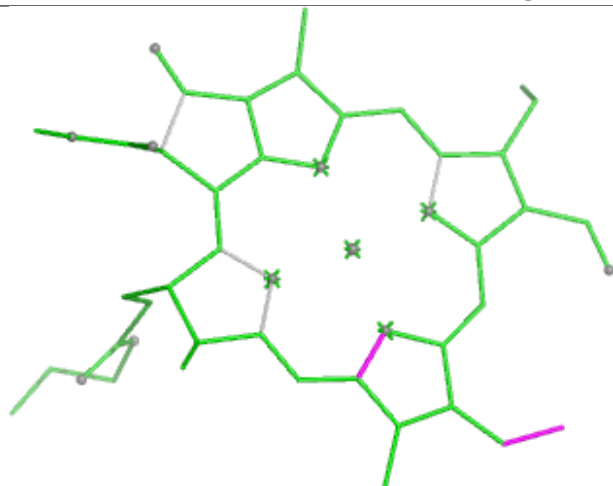
Ligand LHG t 102



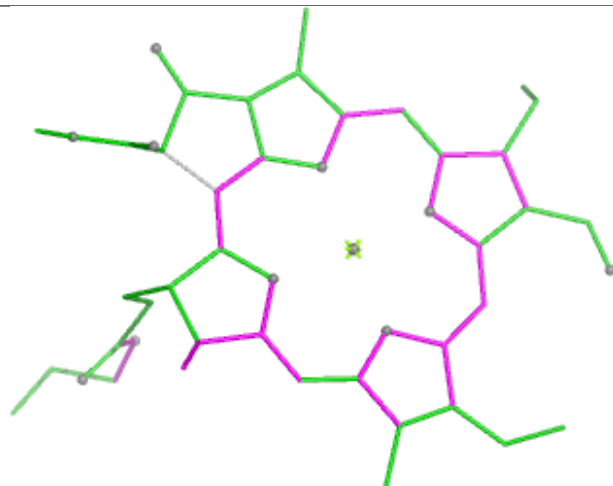




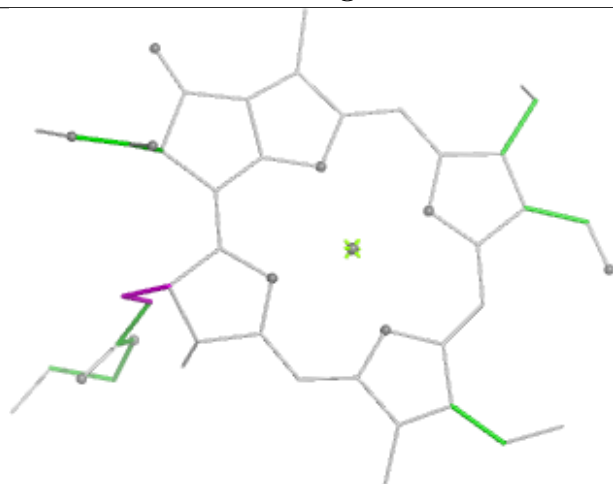
Ligand CHL s 309



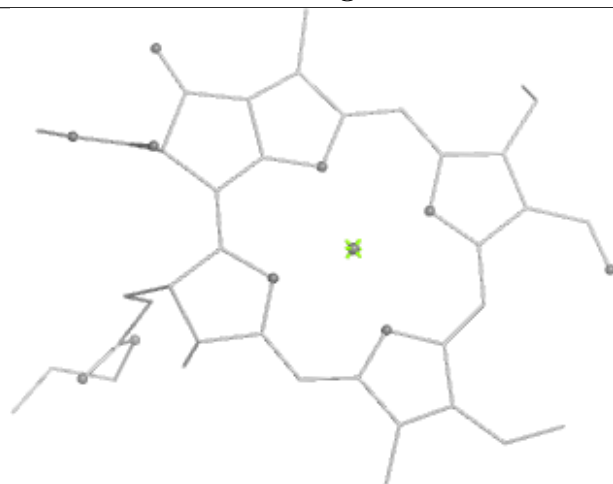
Bond lengths



Bond angles

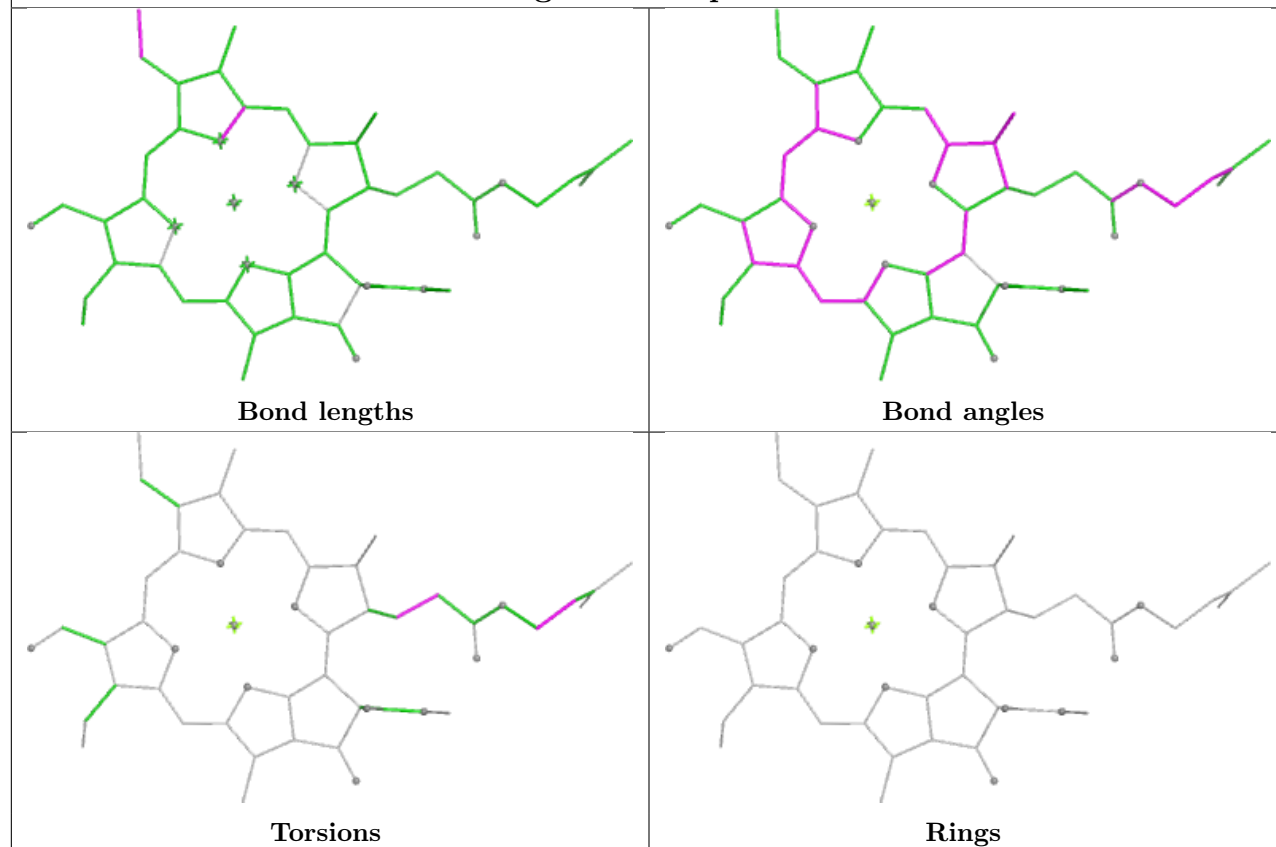


Torsions

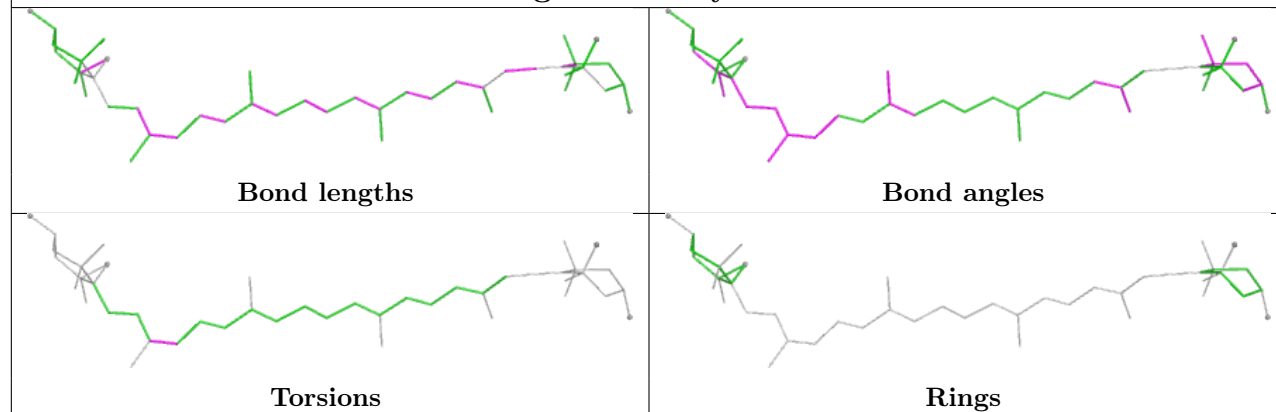


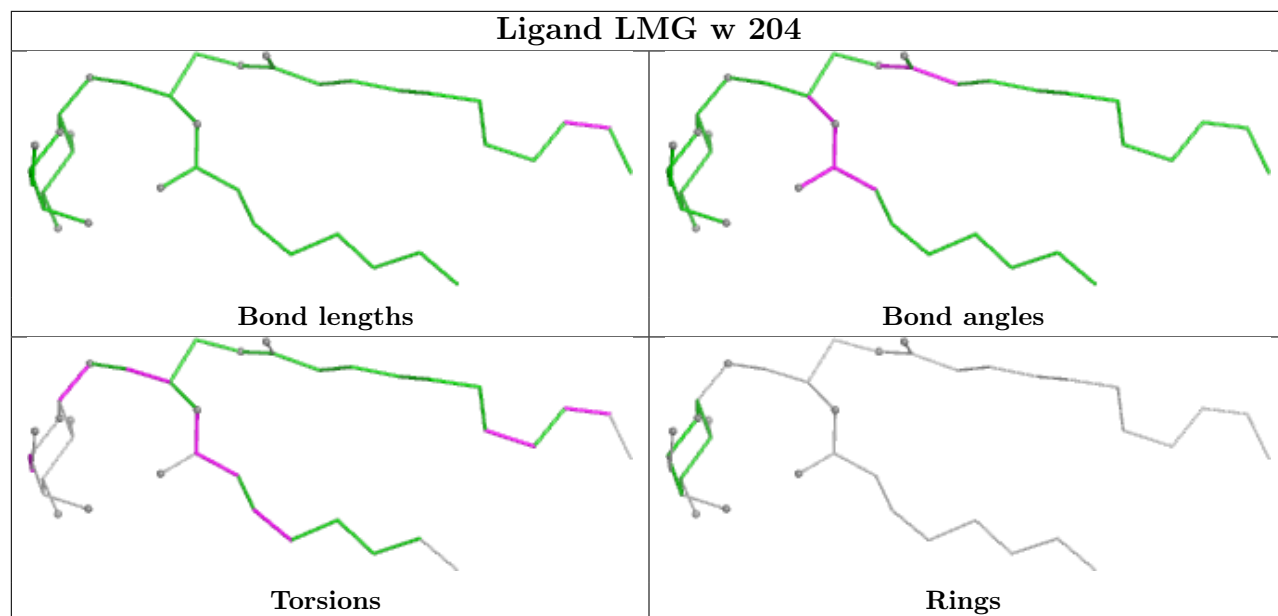
Rings

Ligand CHL p 606

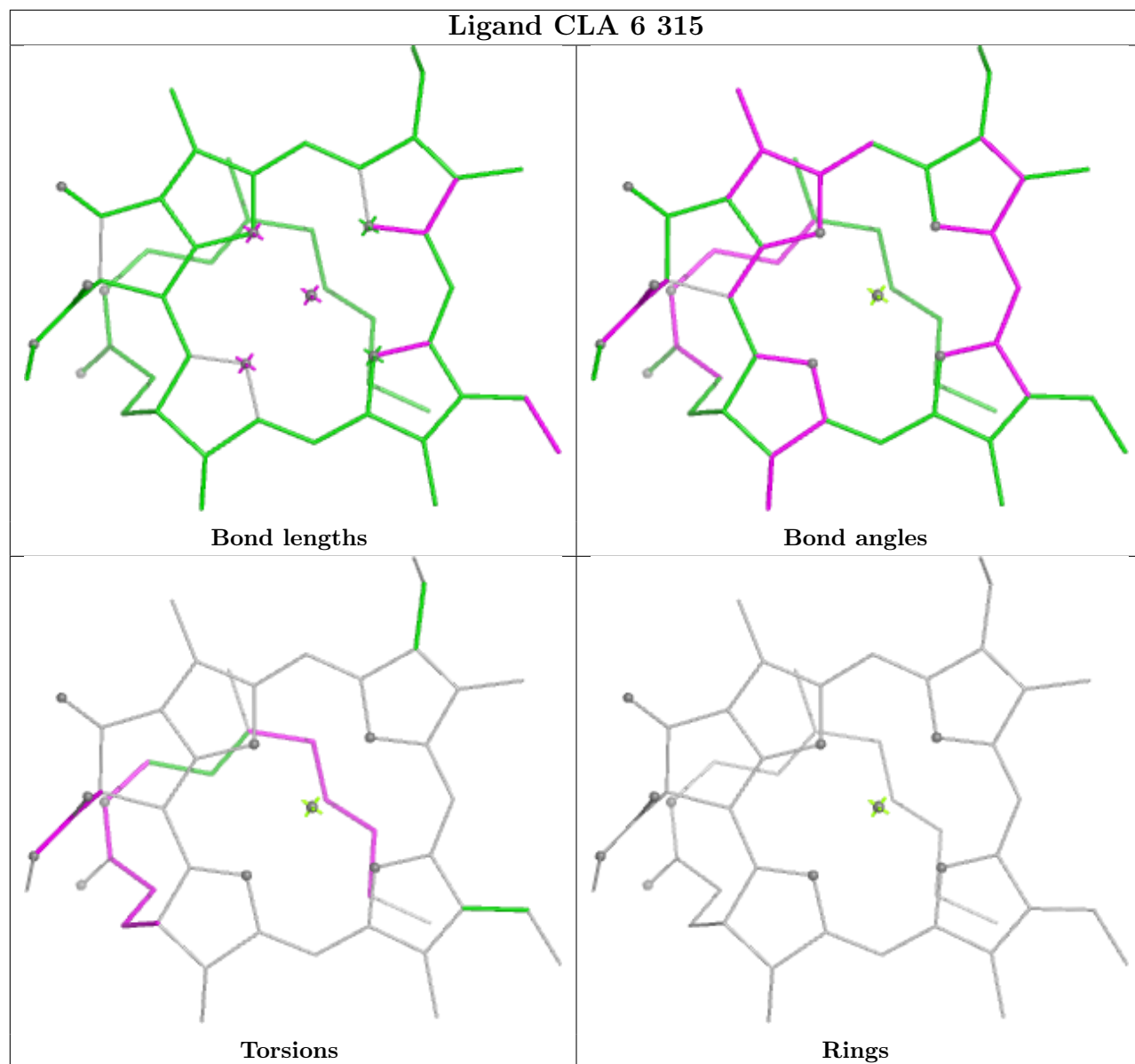


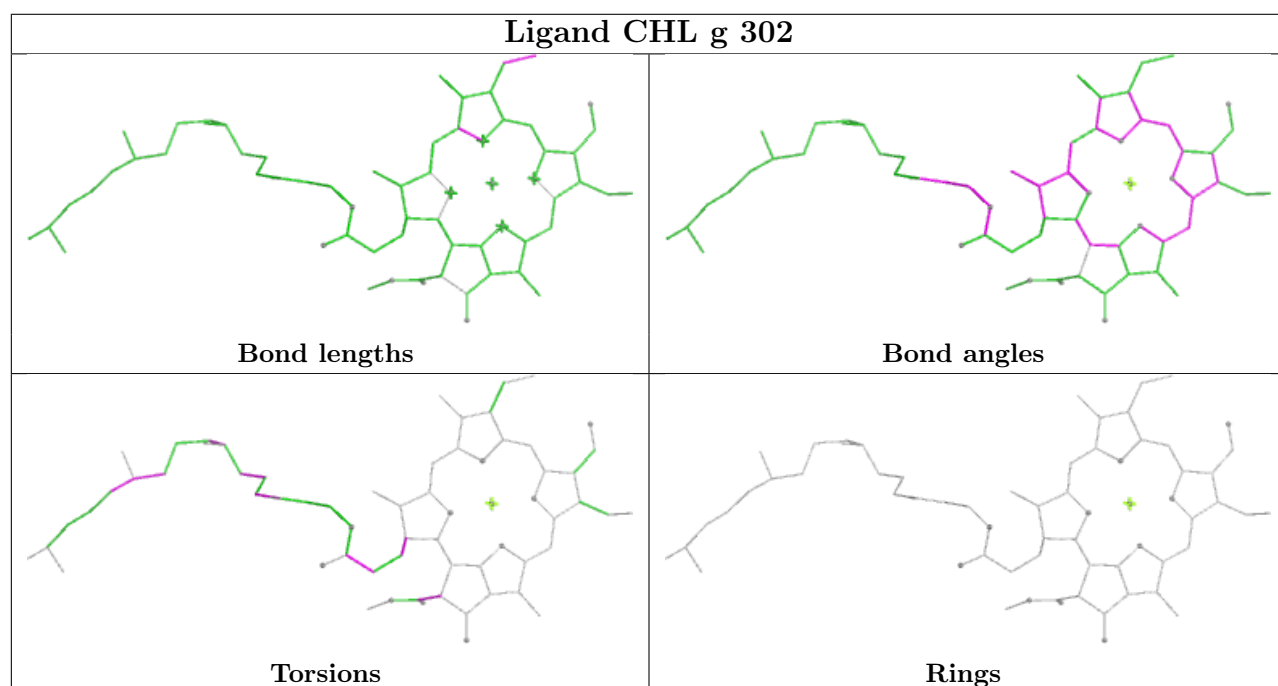
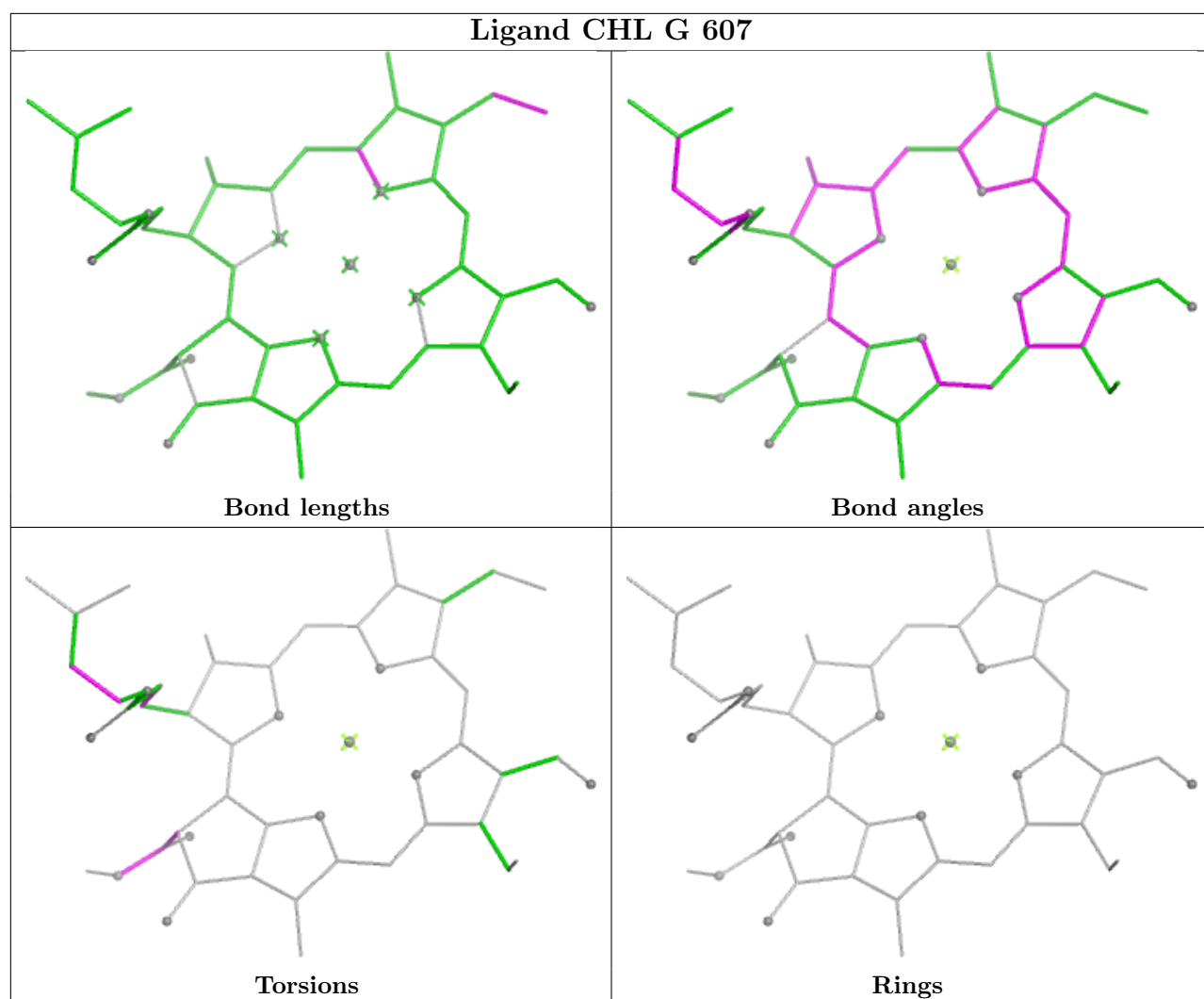
Ligand NEX y 618

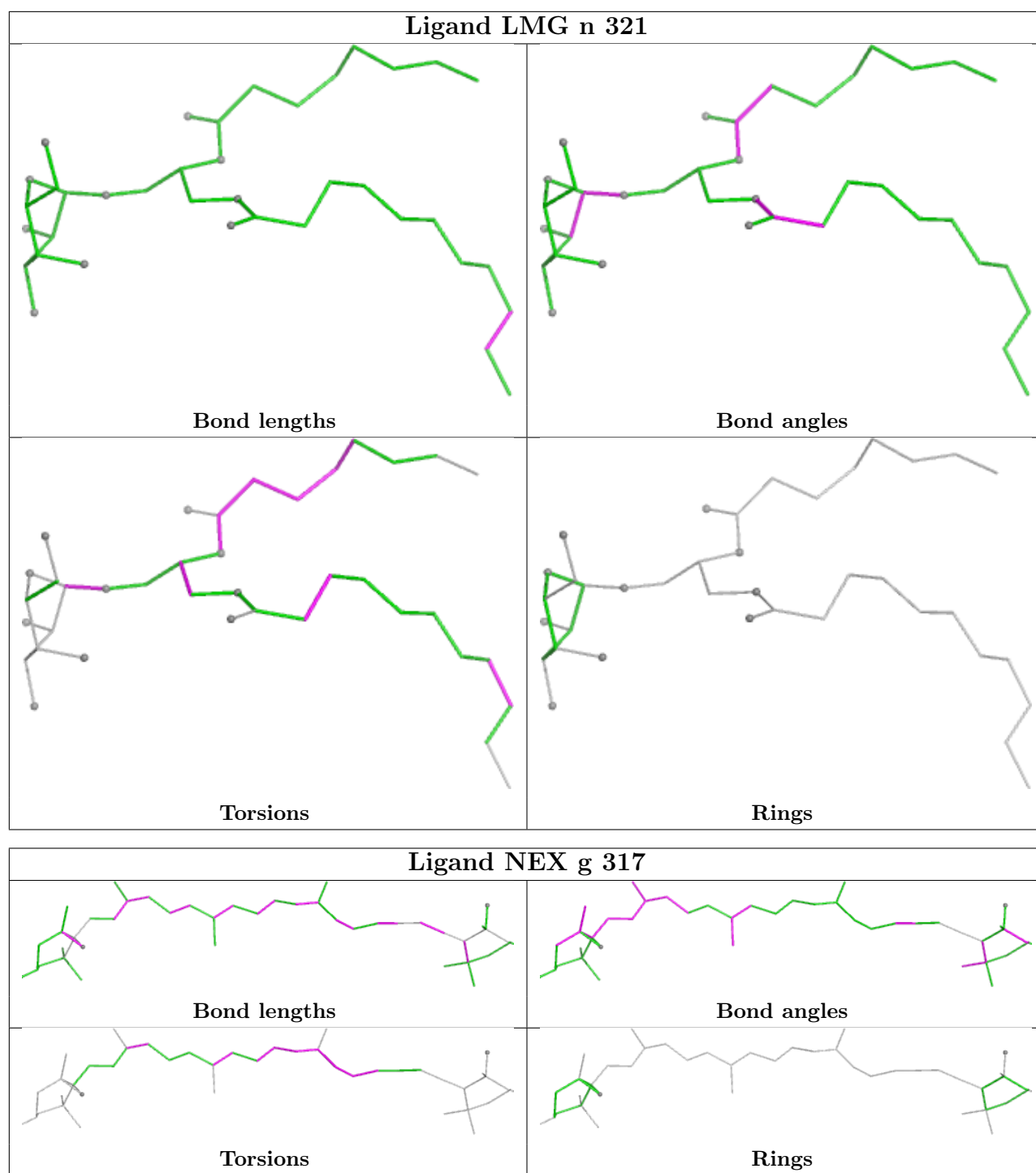




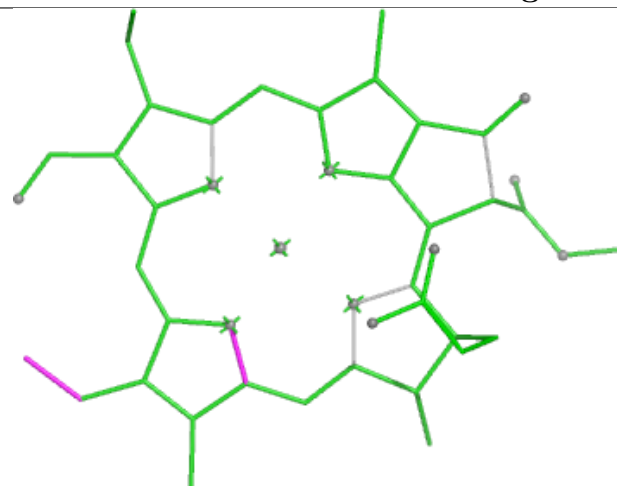
Ligand CLA 6 315



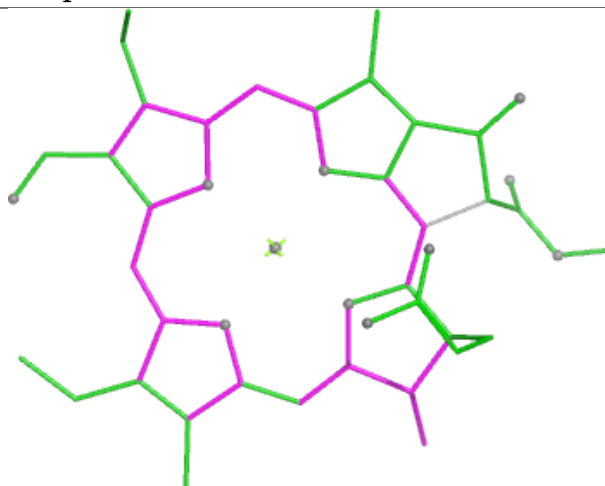




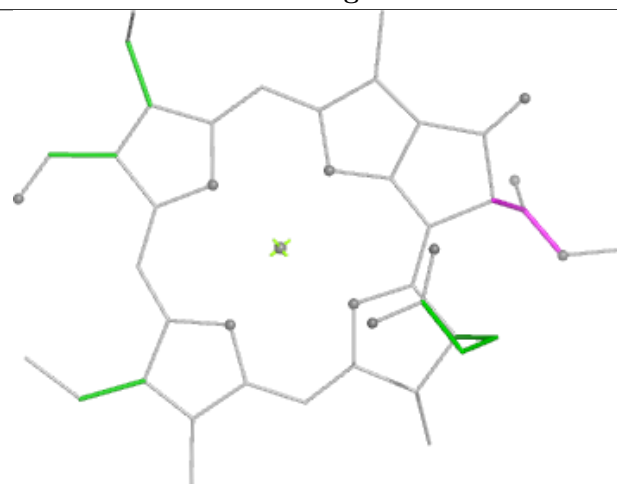
Ligand CHL q 307



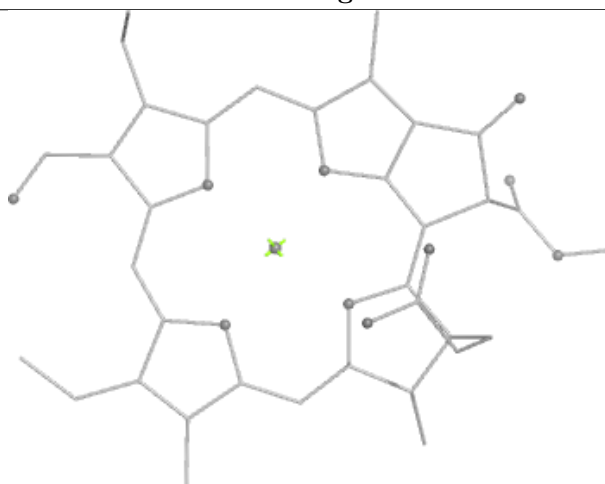
Bond lengths



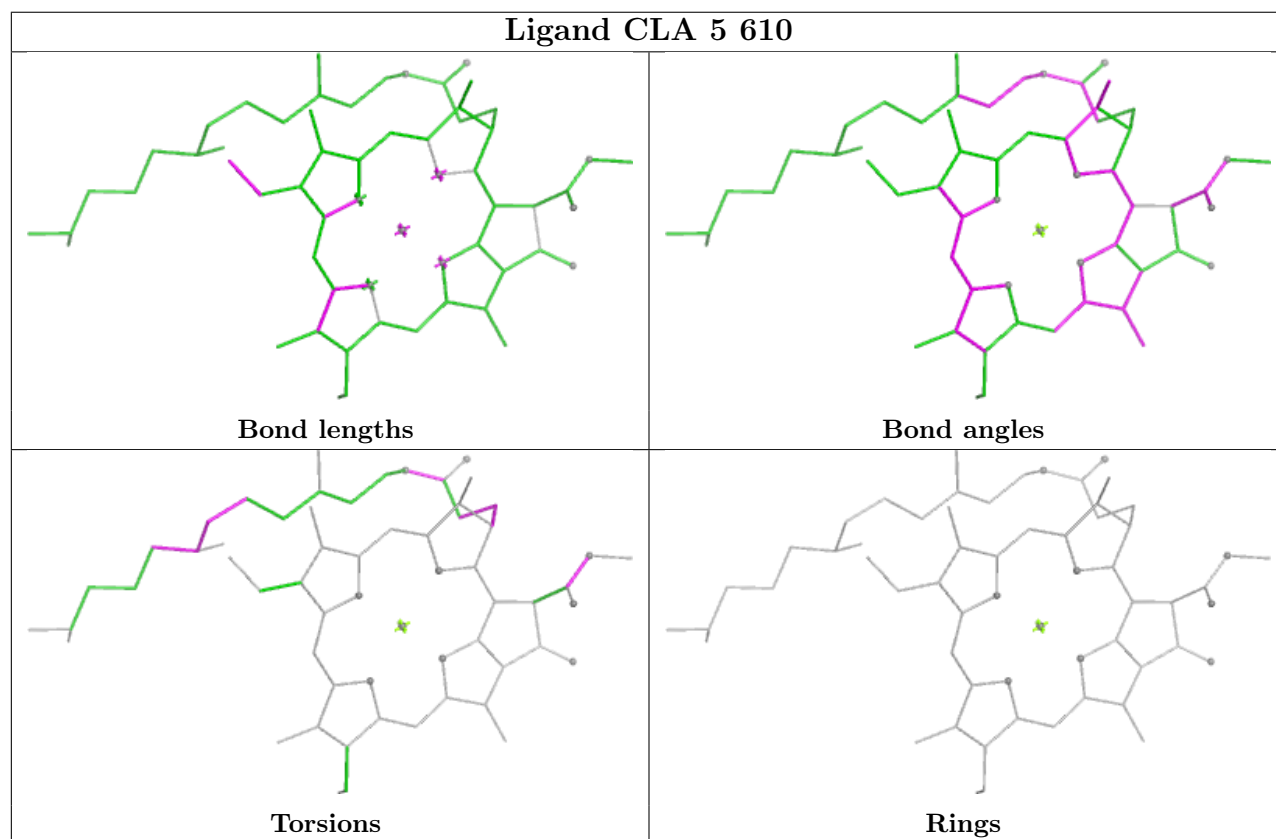
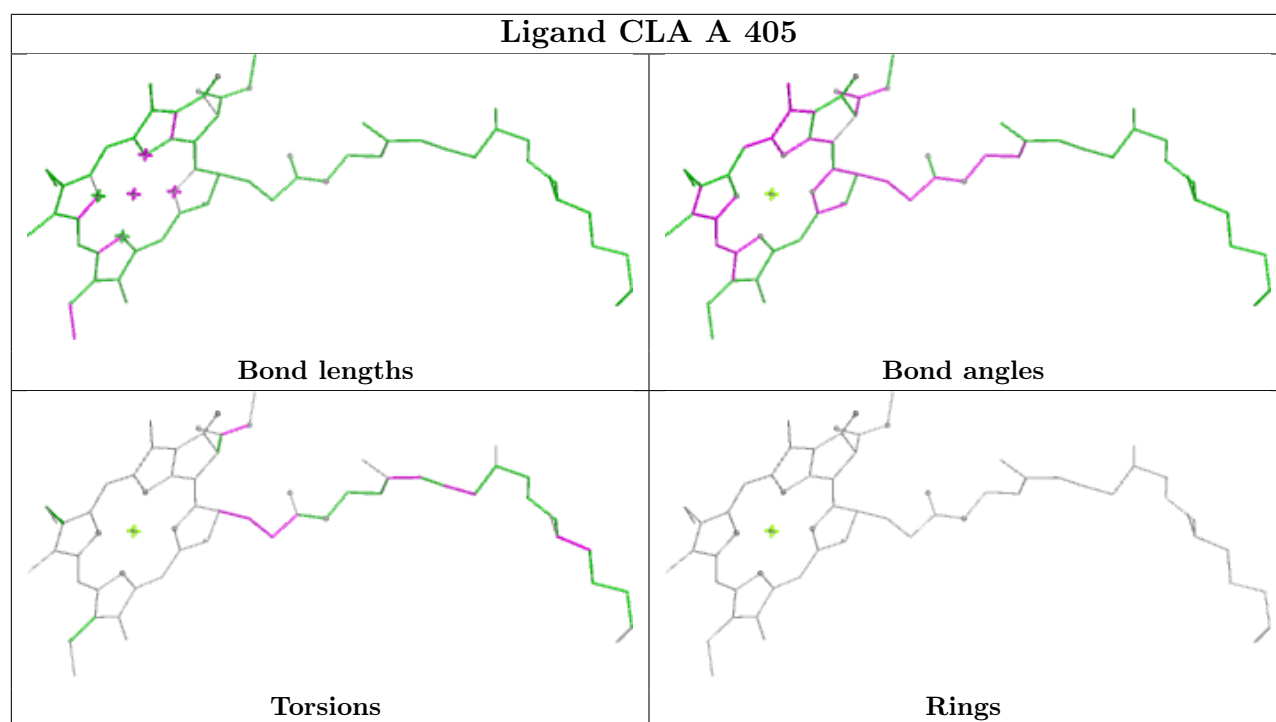
Bond angles



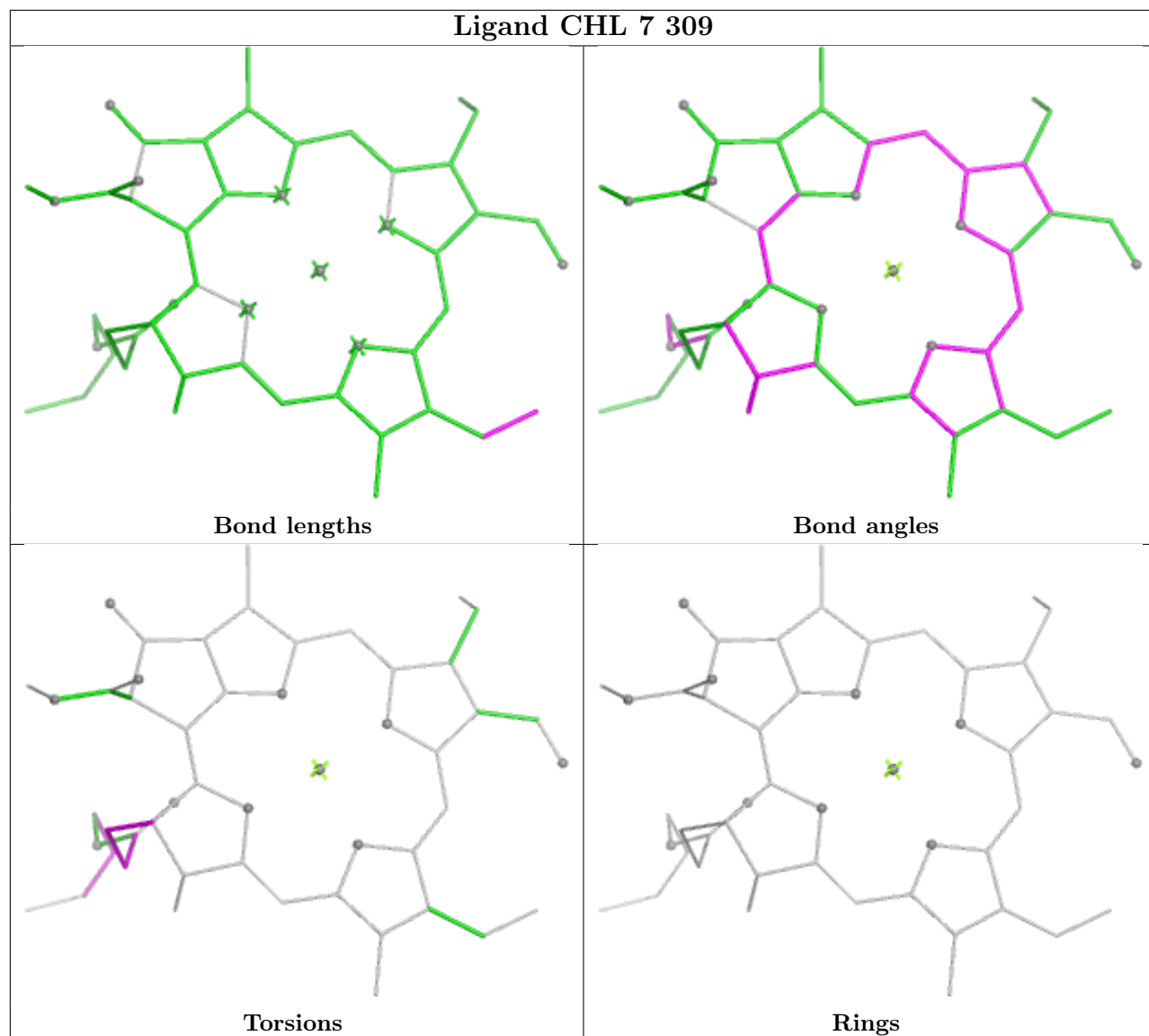
Torsions



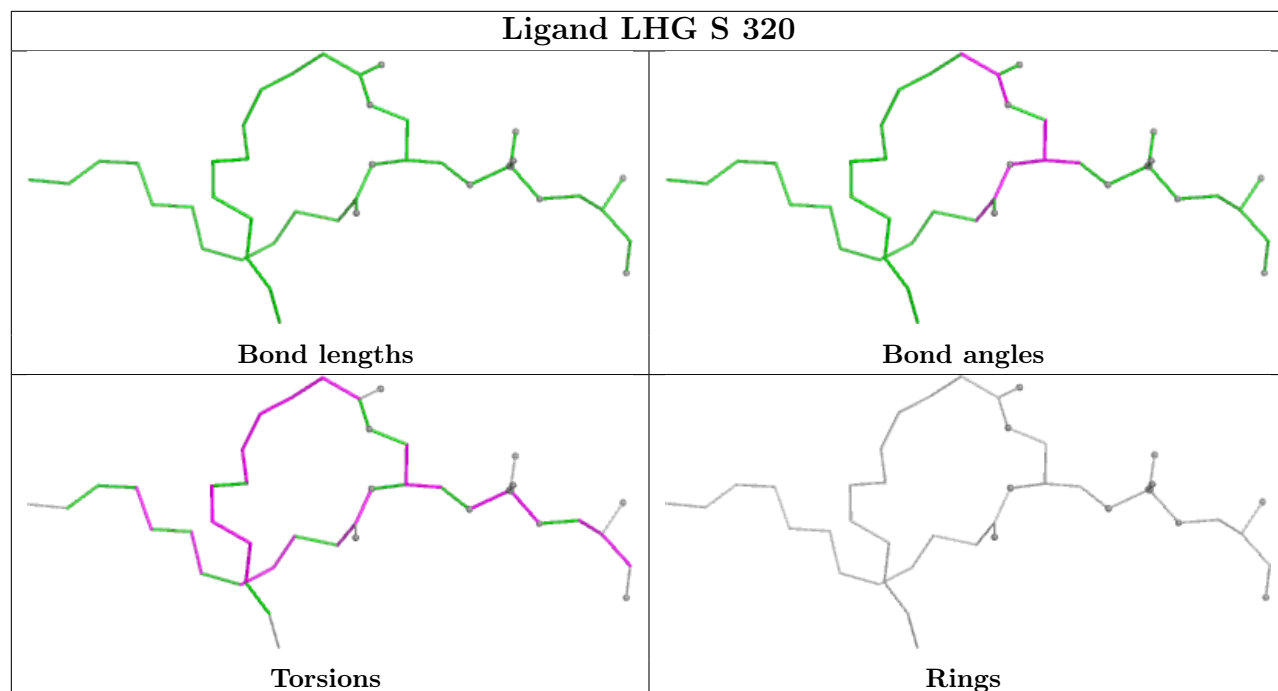
Rings



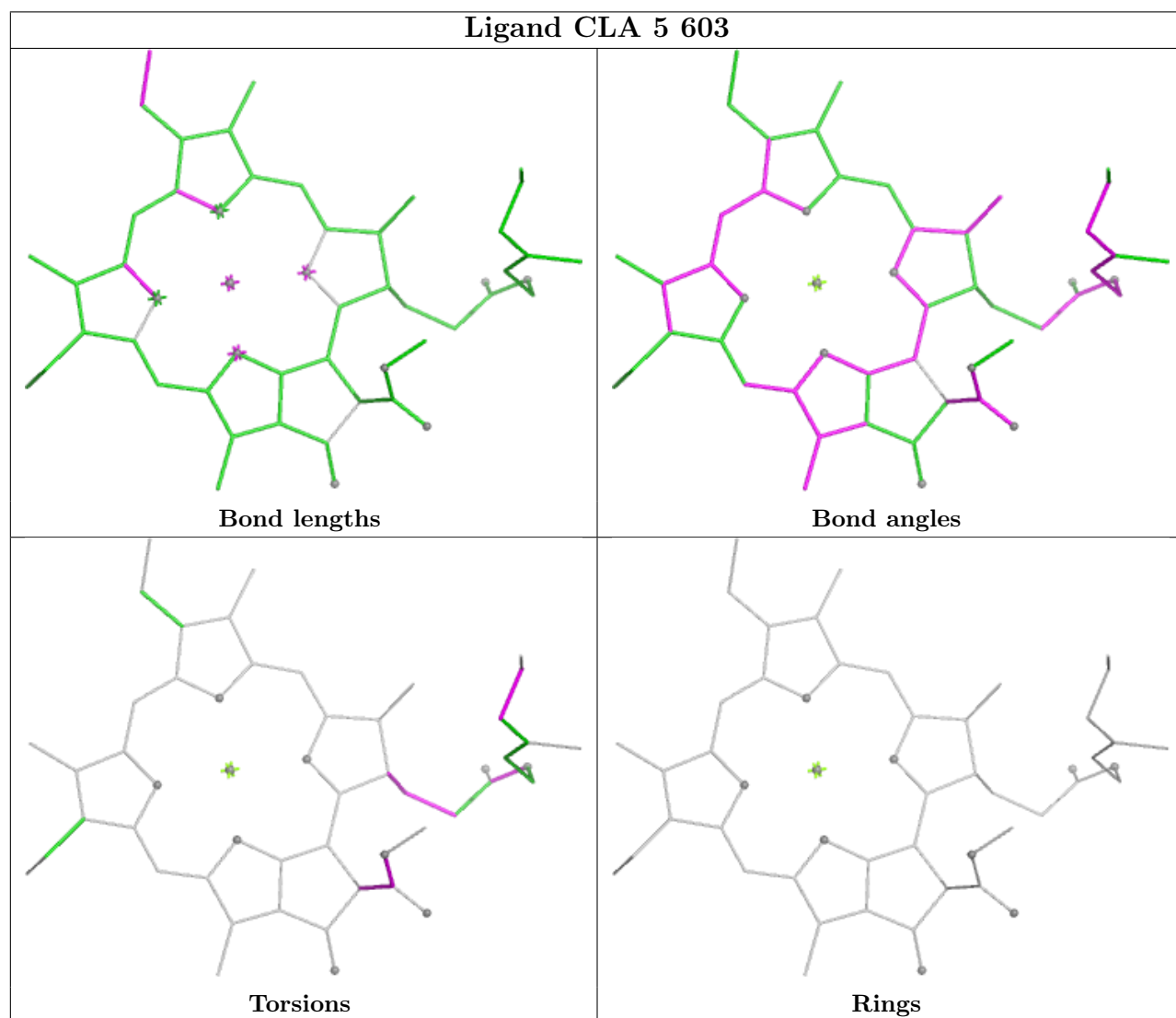
Ligand CHL 7 309

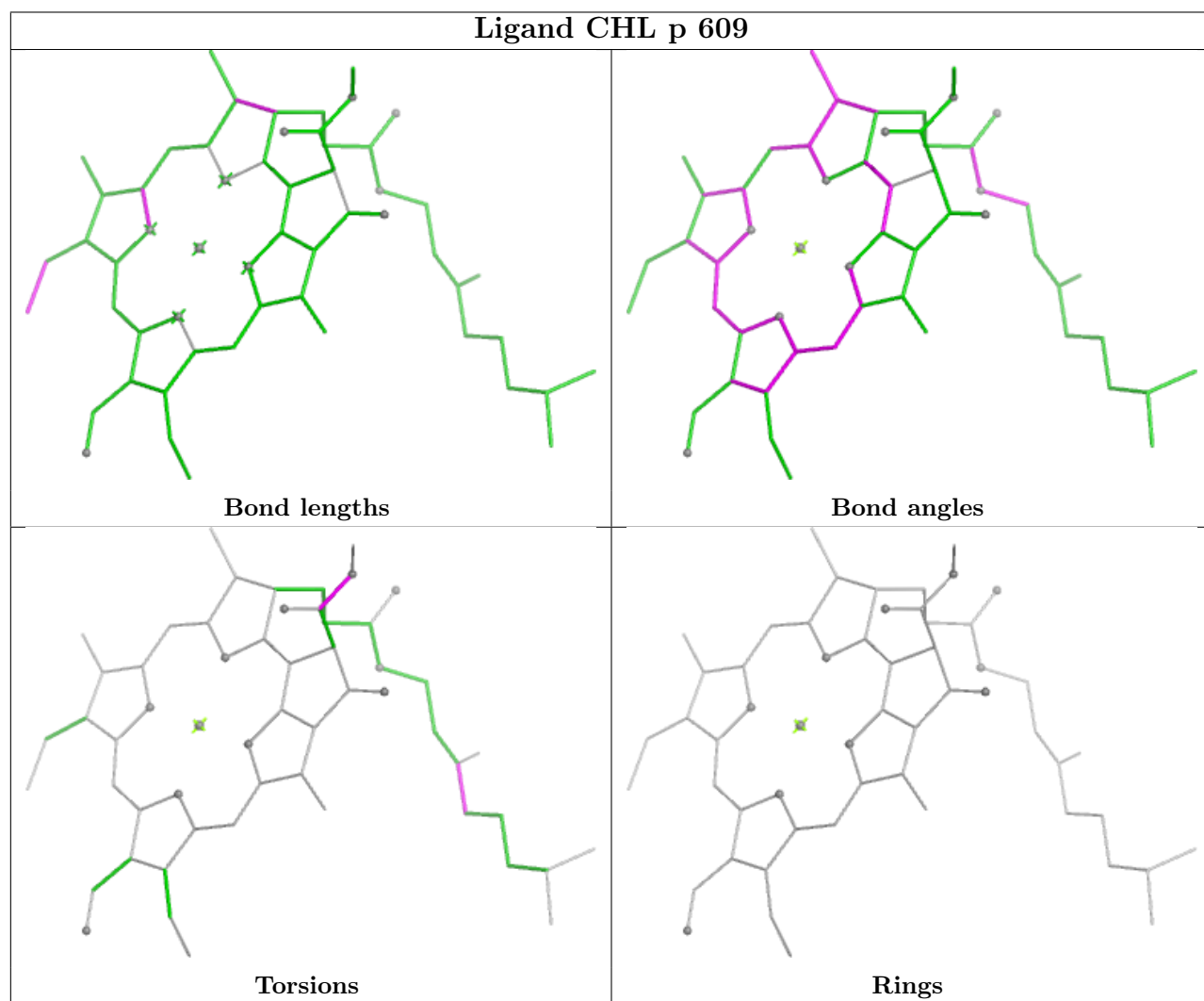
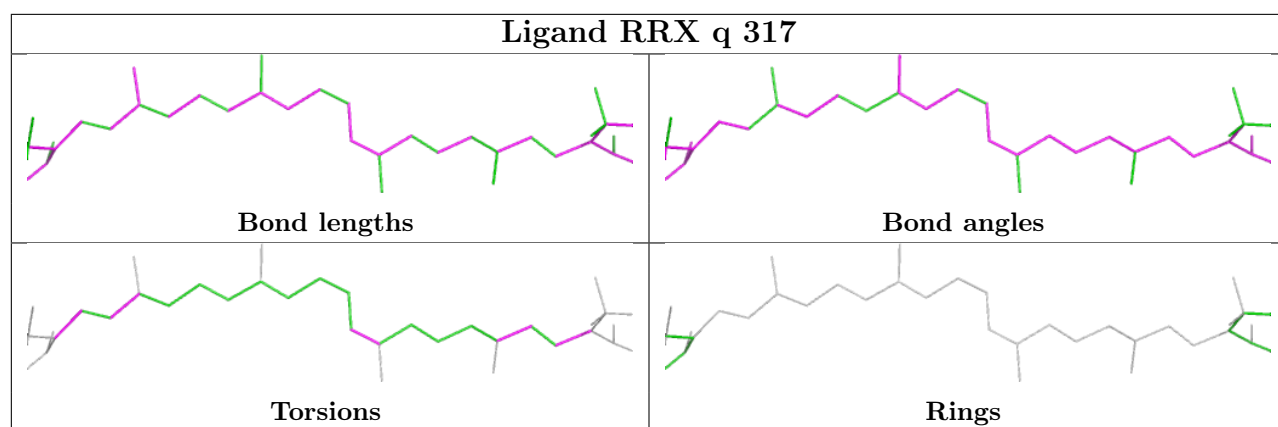


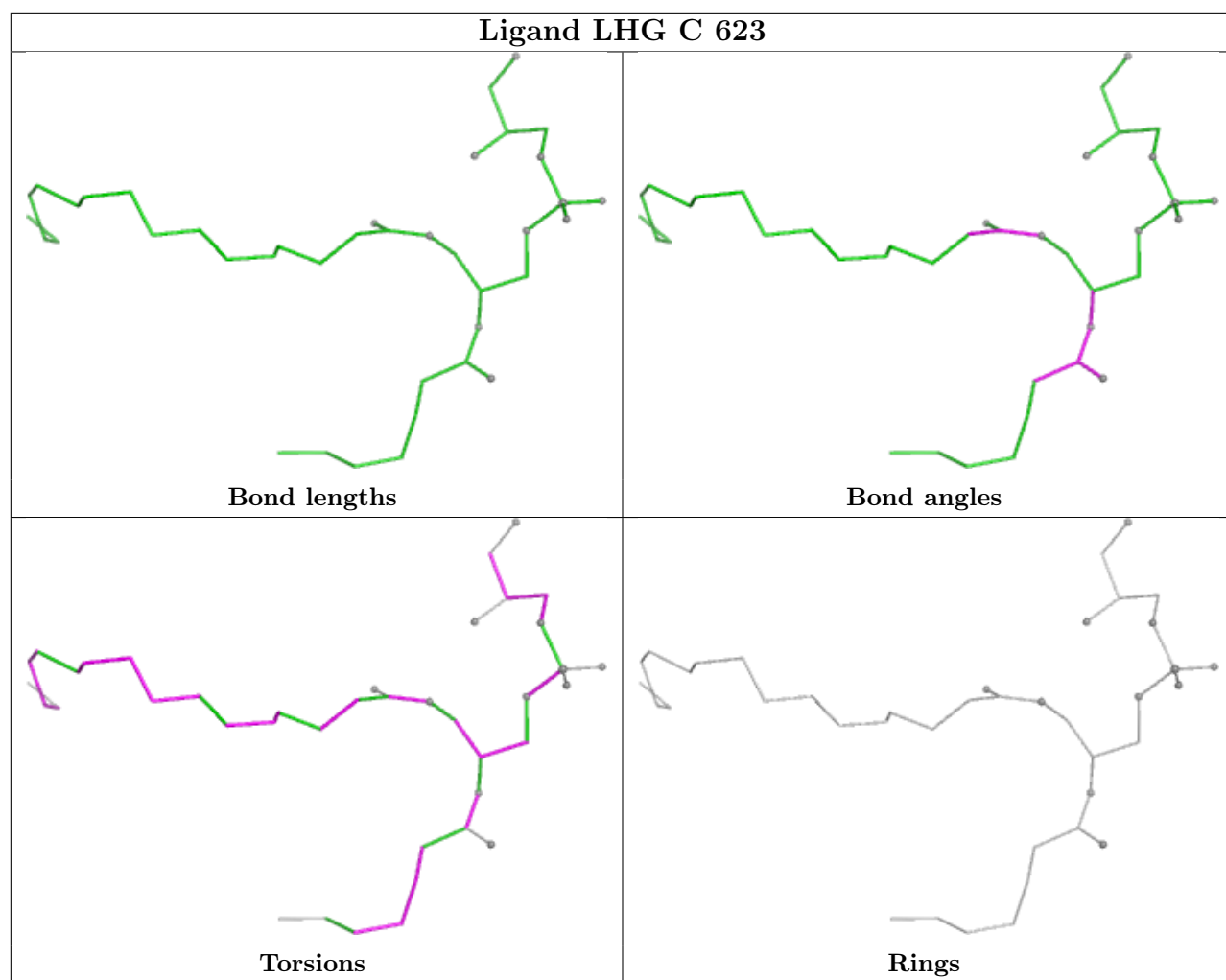
Ligand LHG S 320

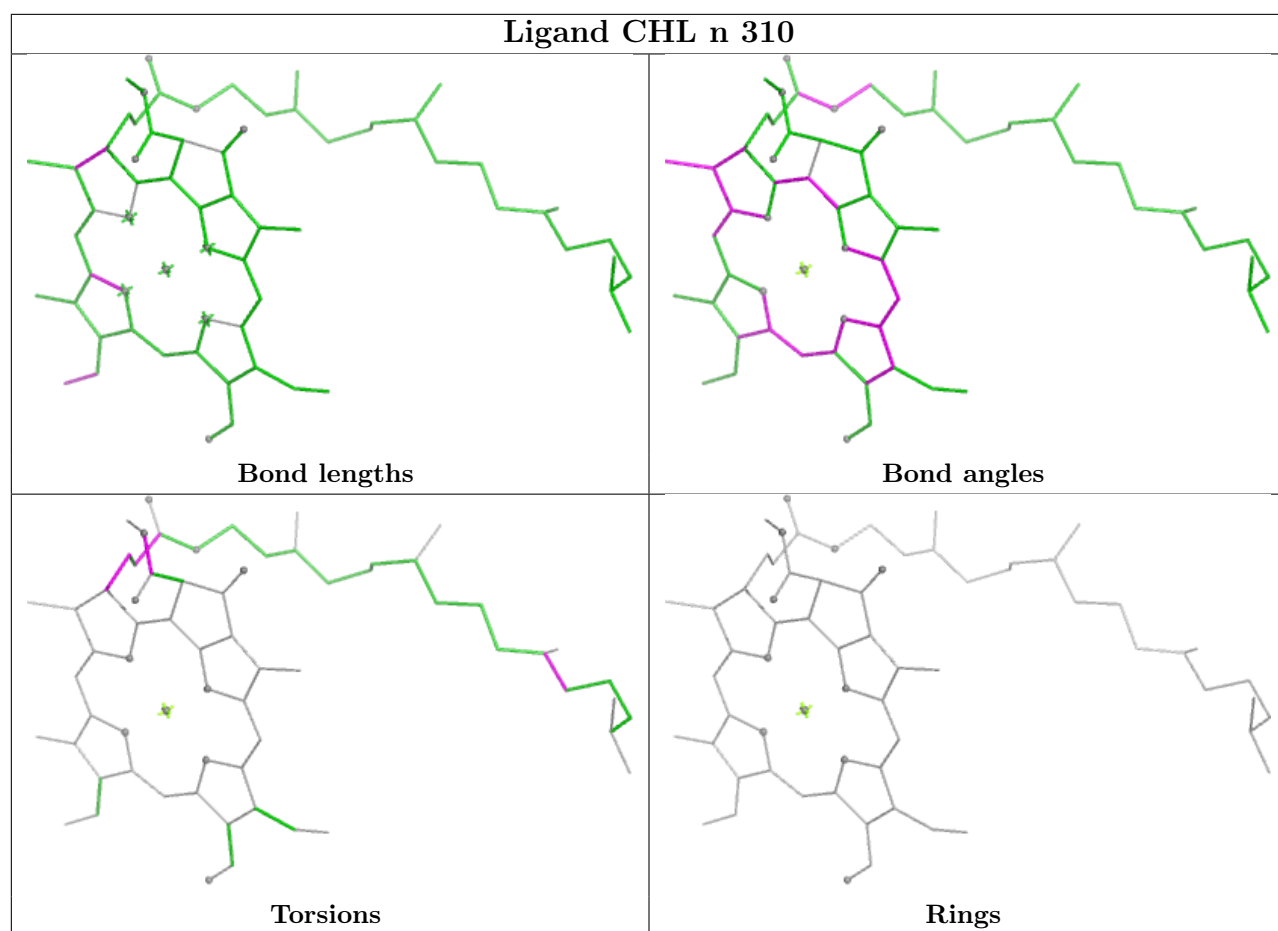


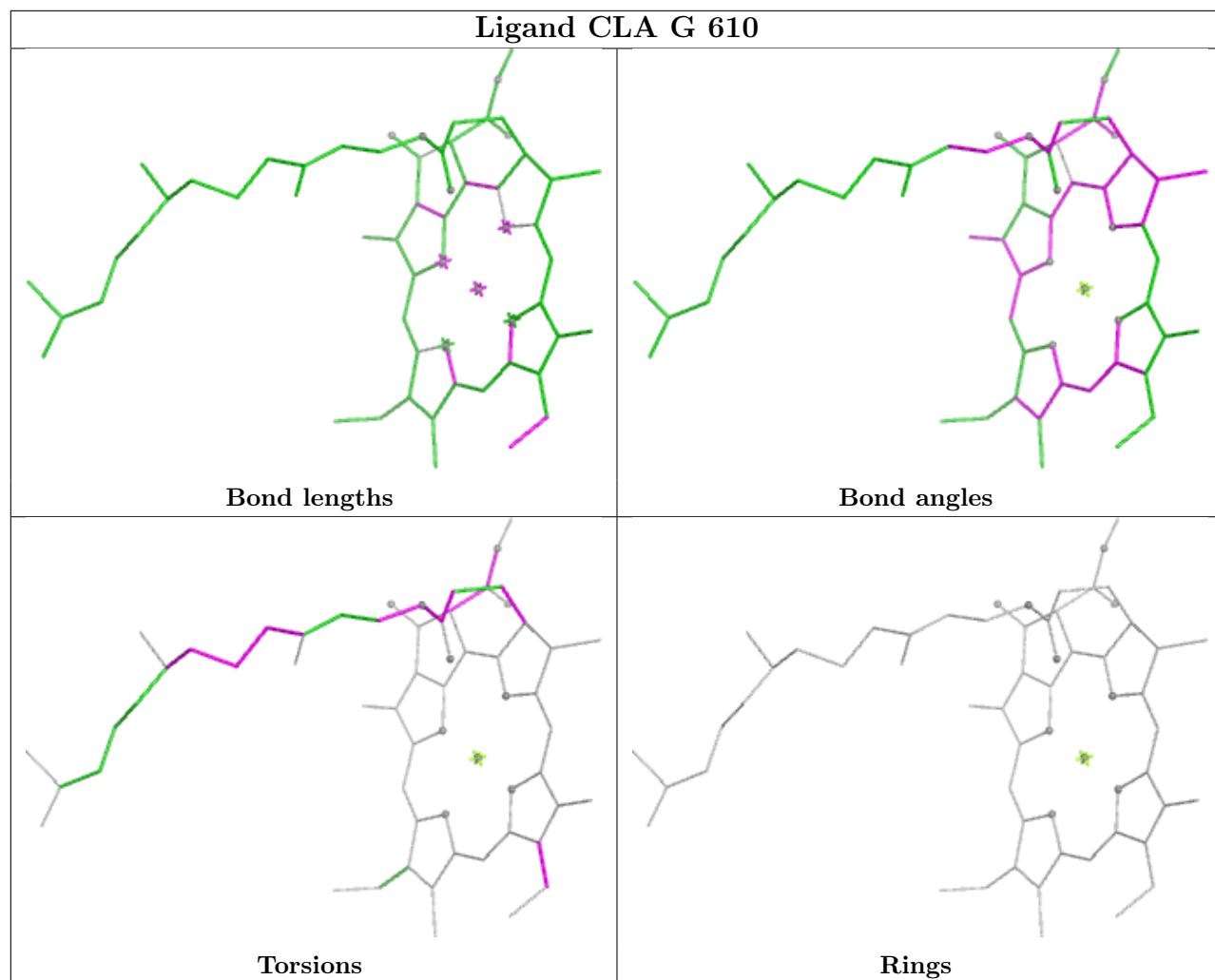
Ligand CLA 5 603

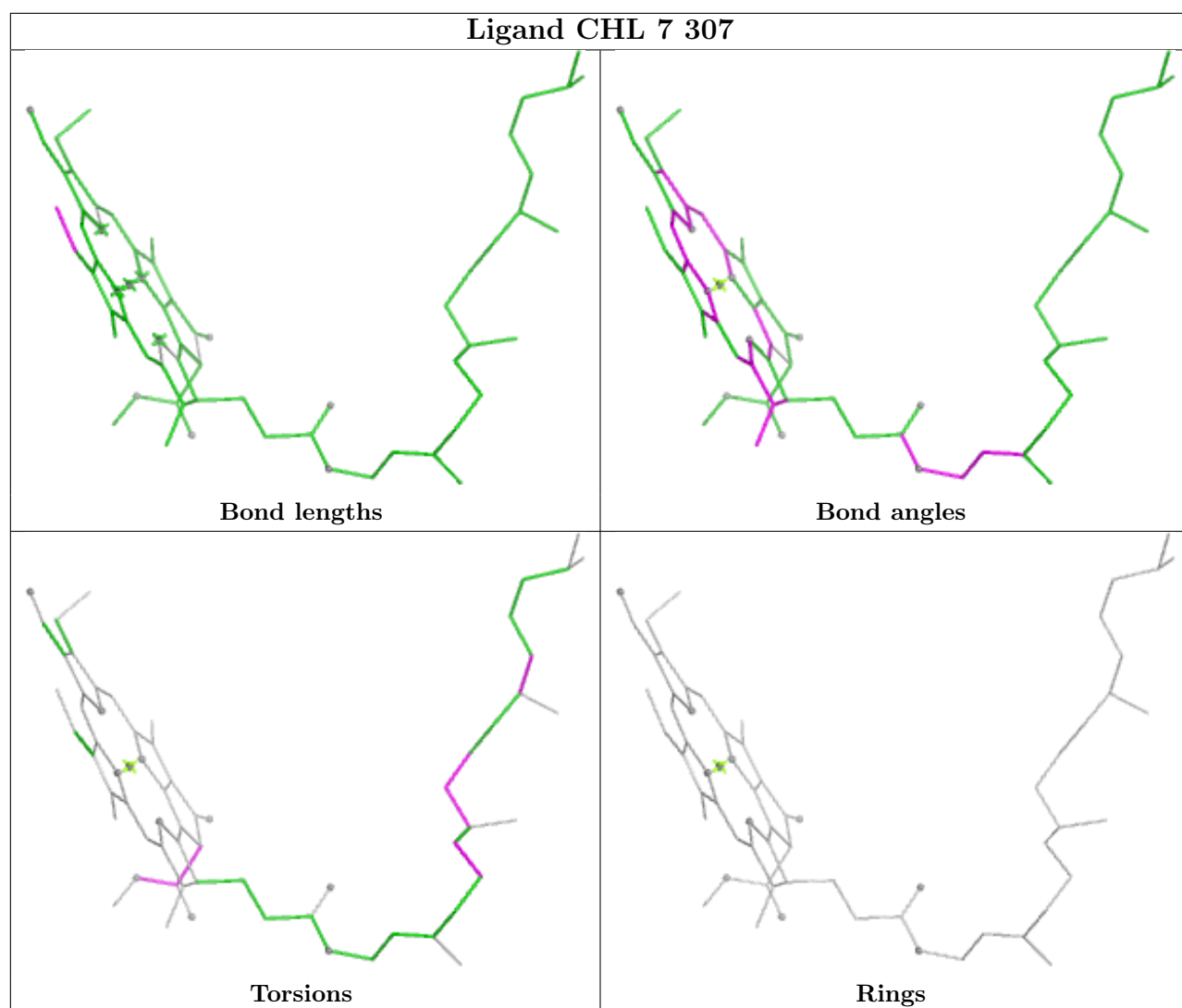


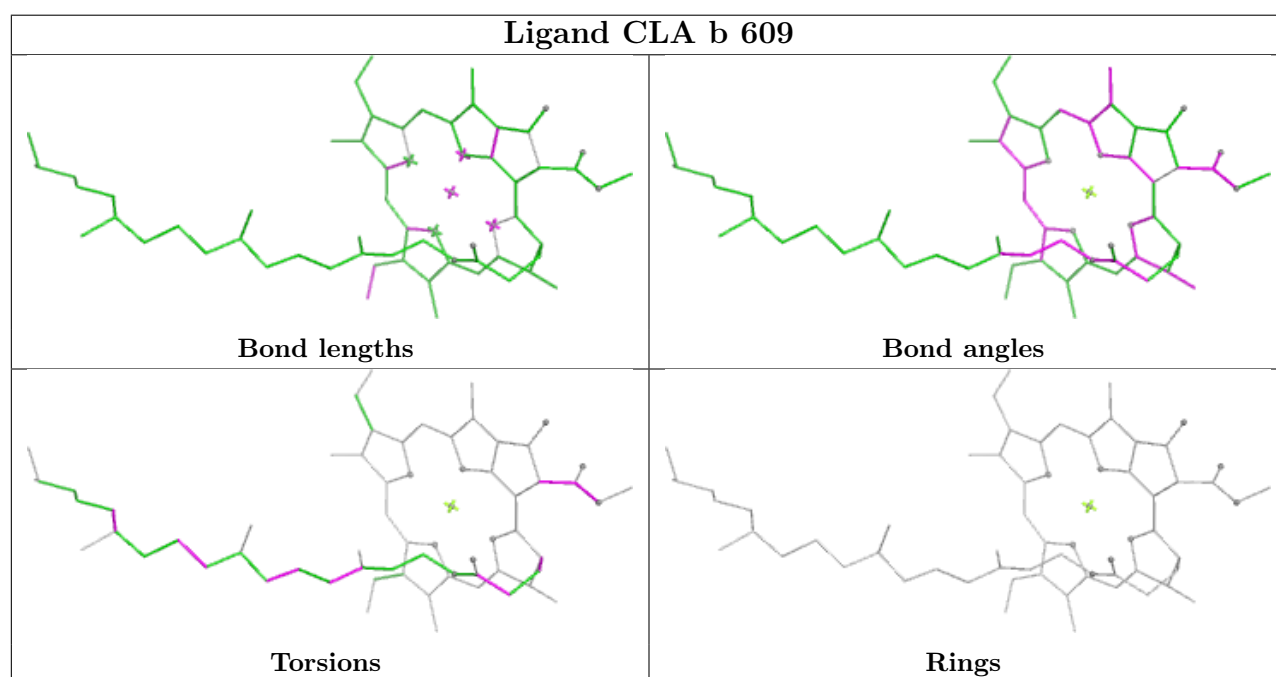
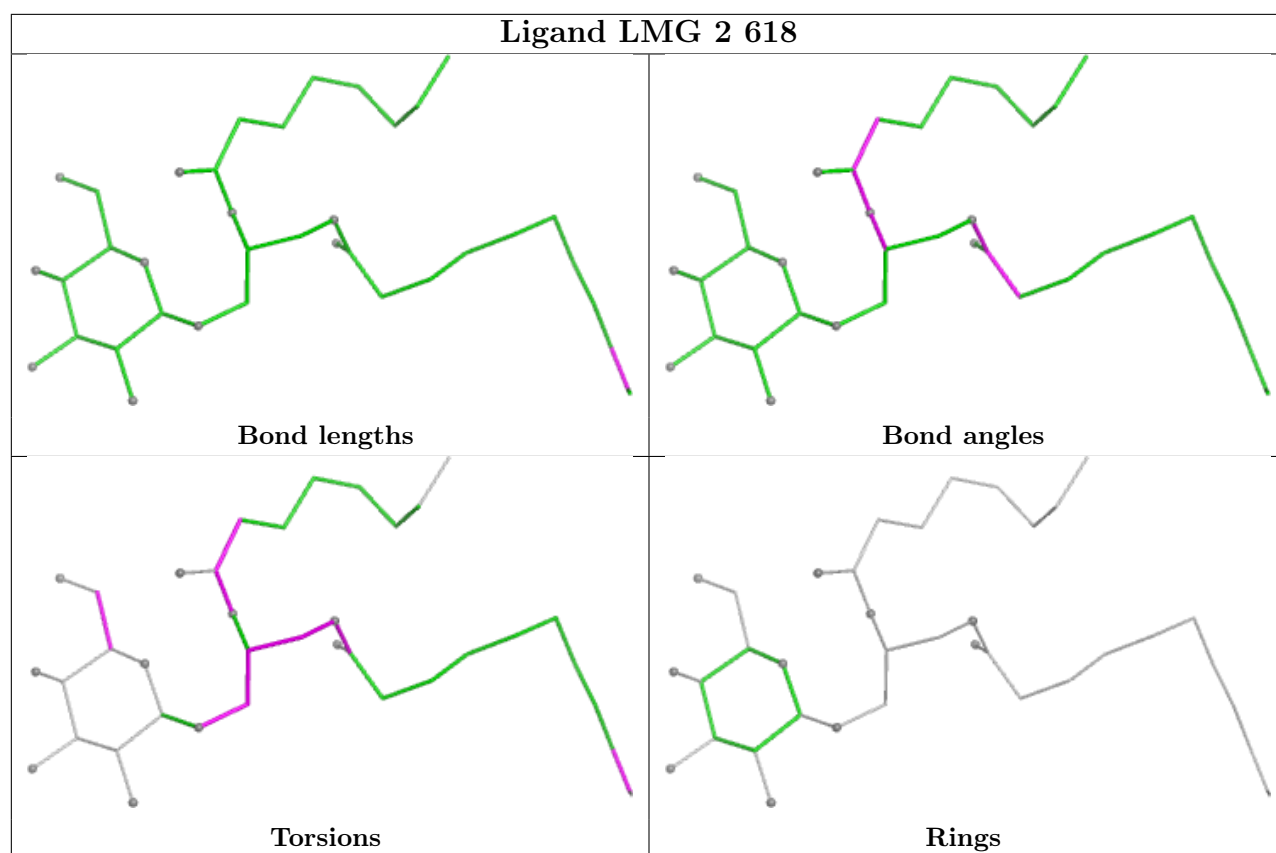




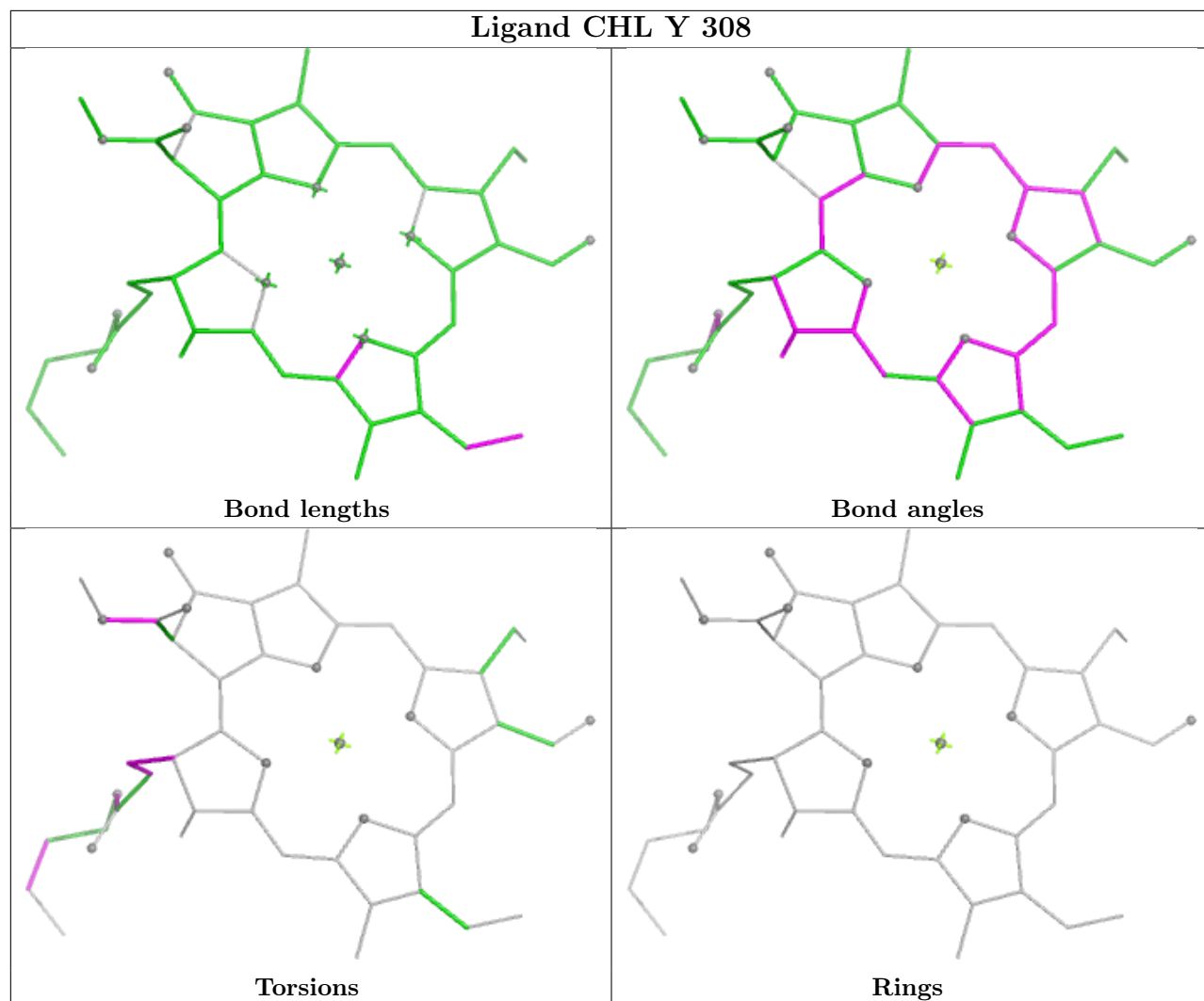


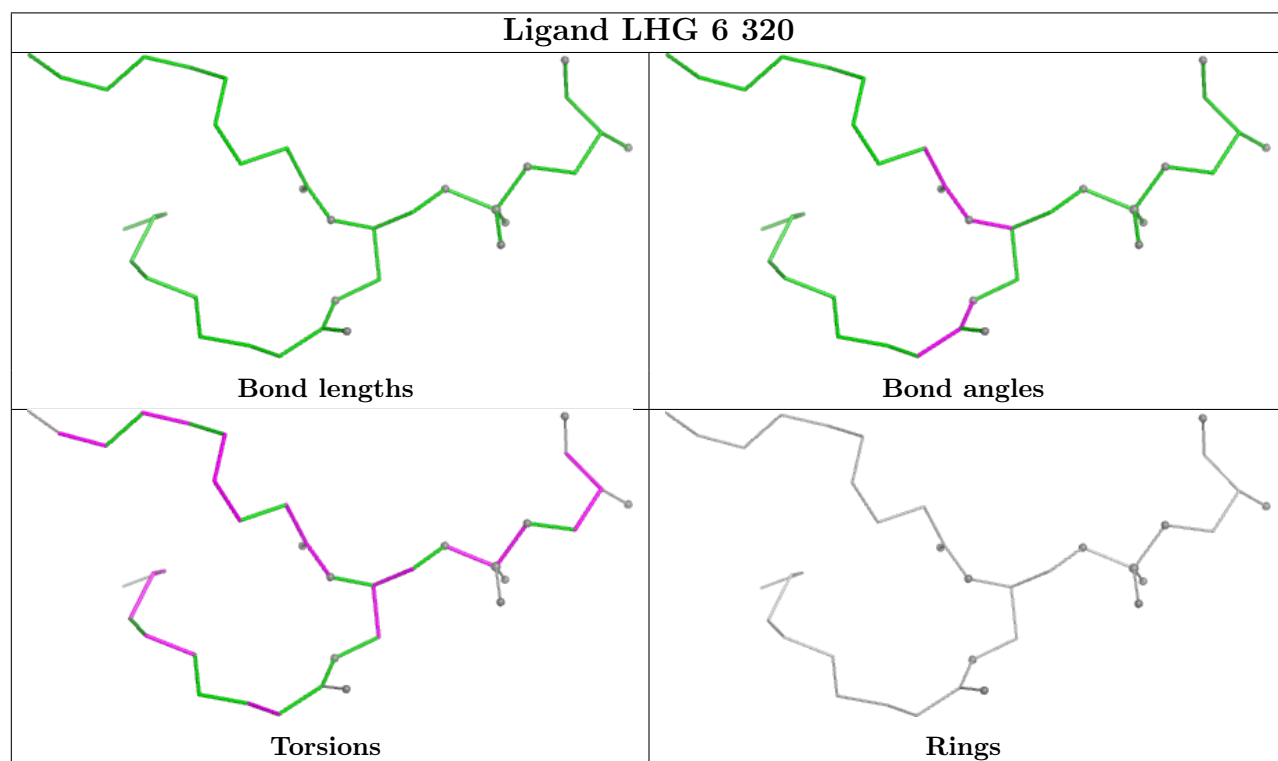
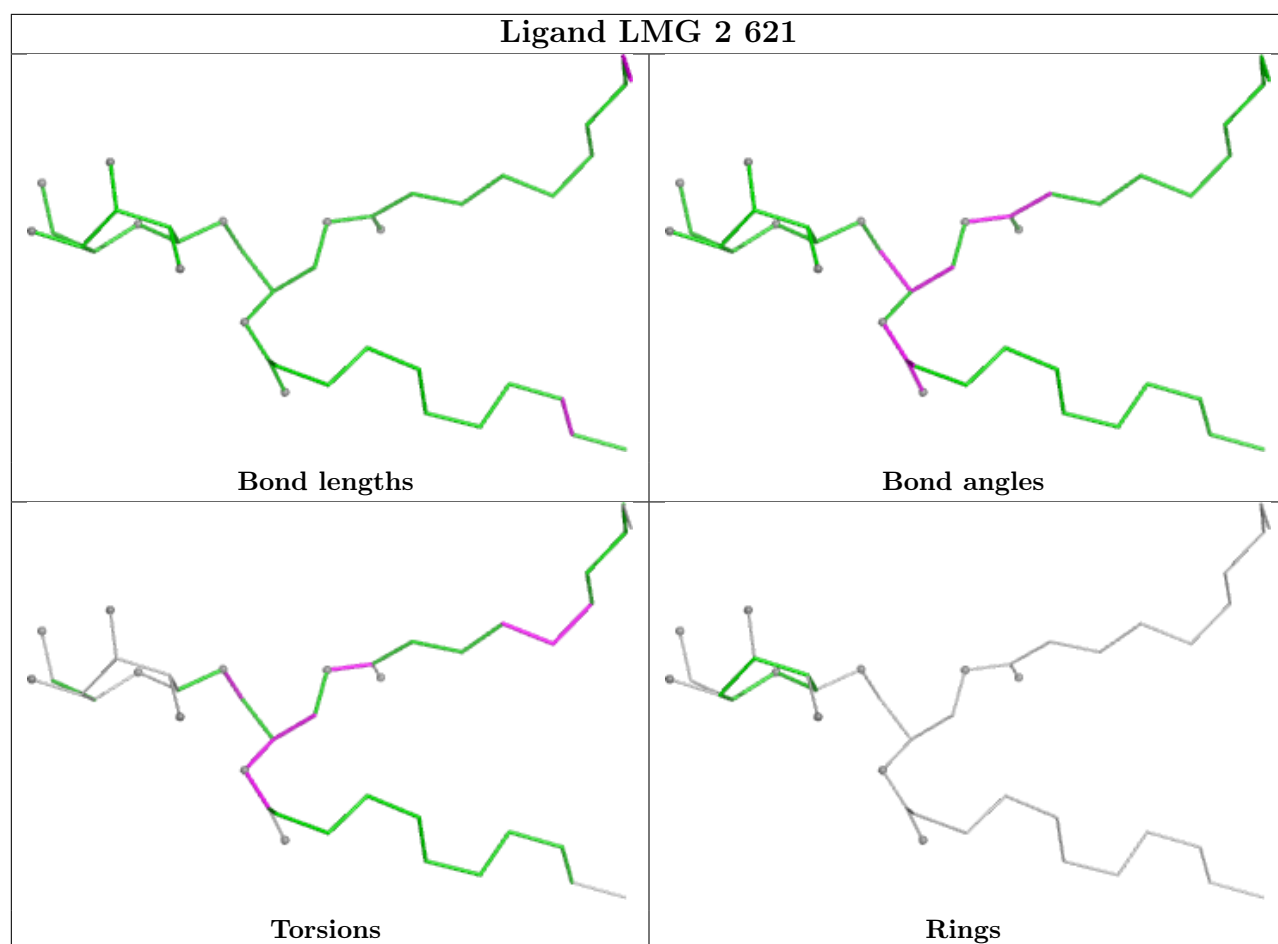


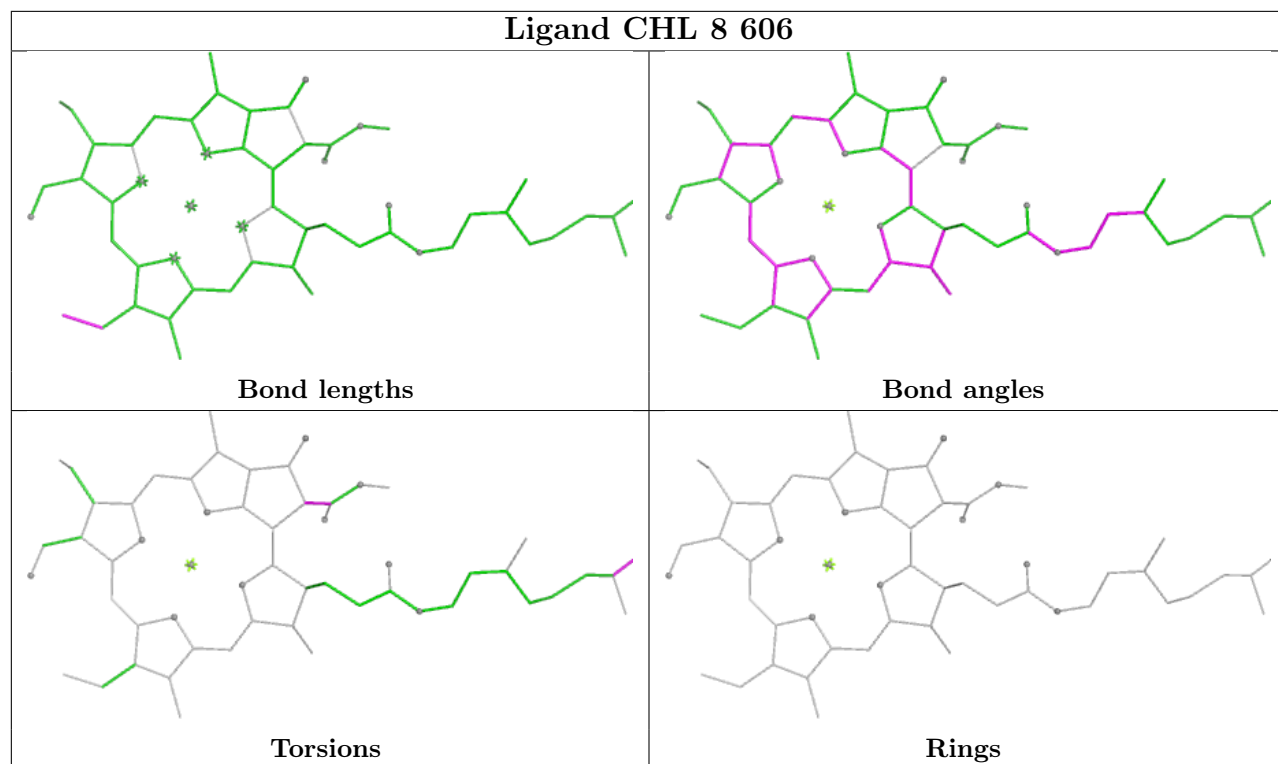
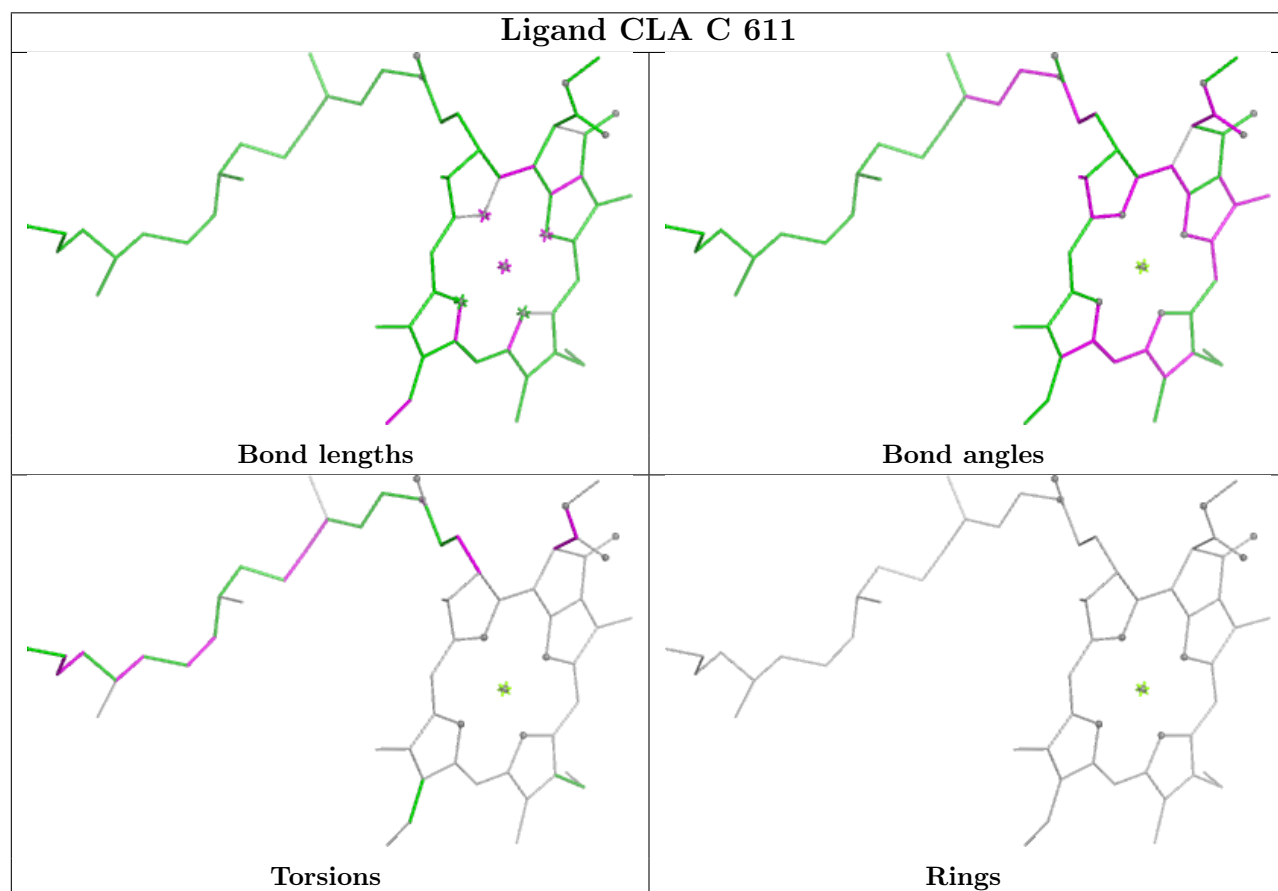


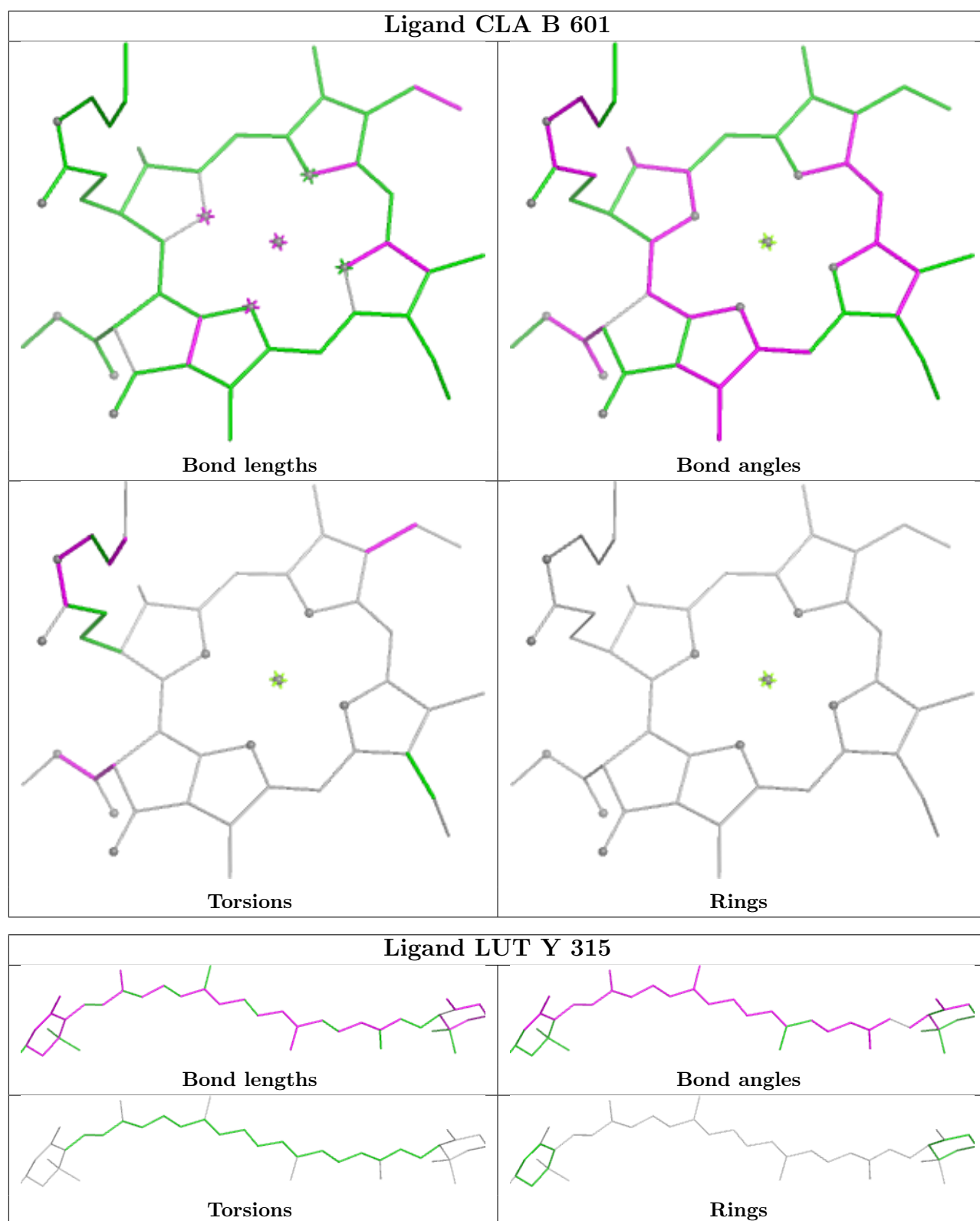


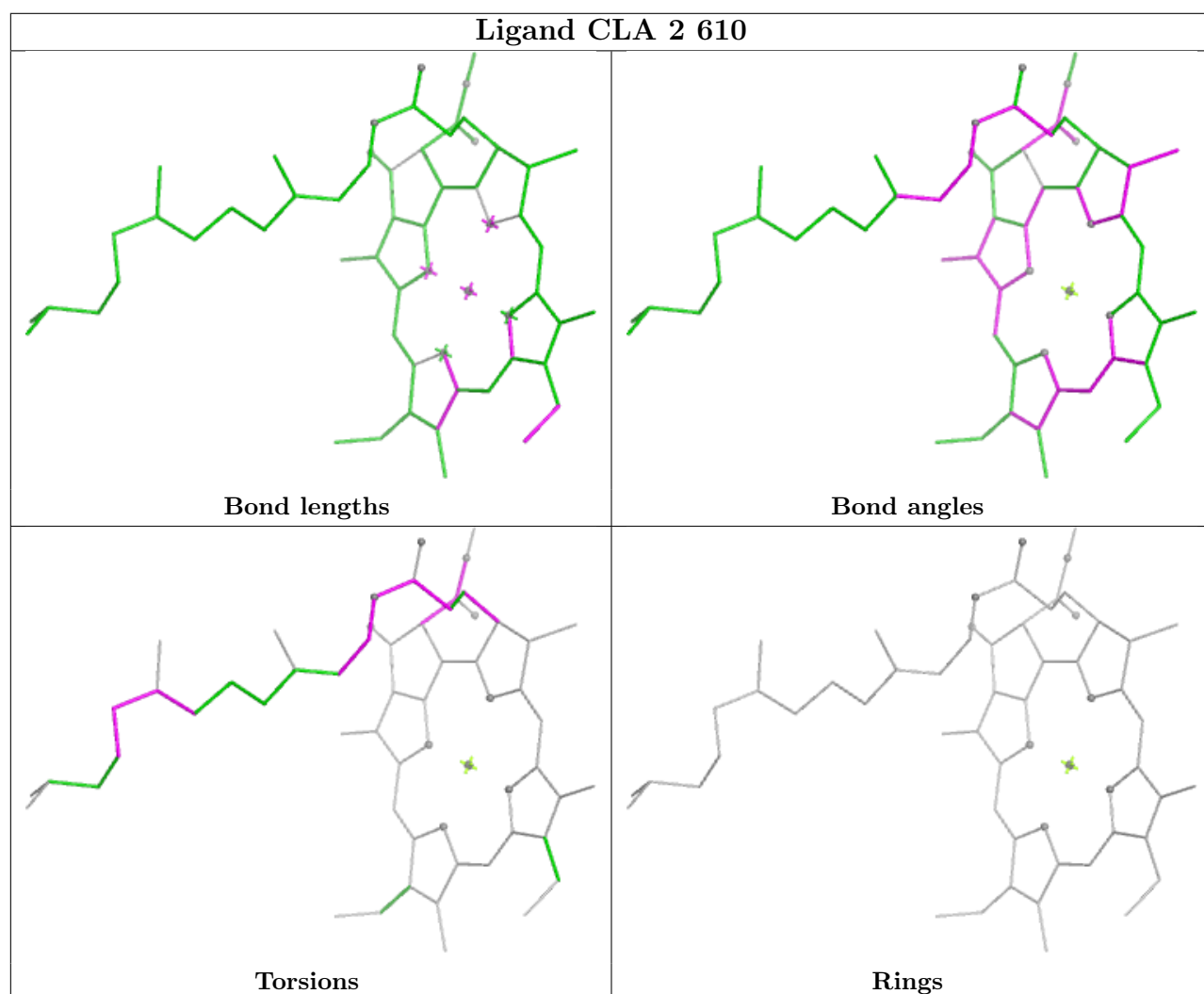
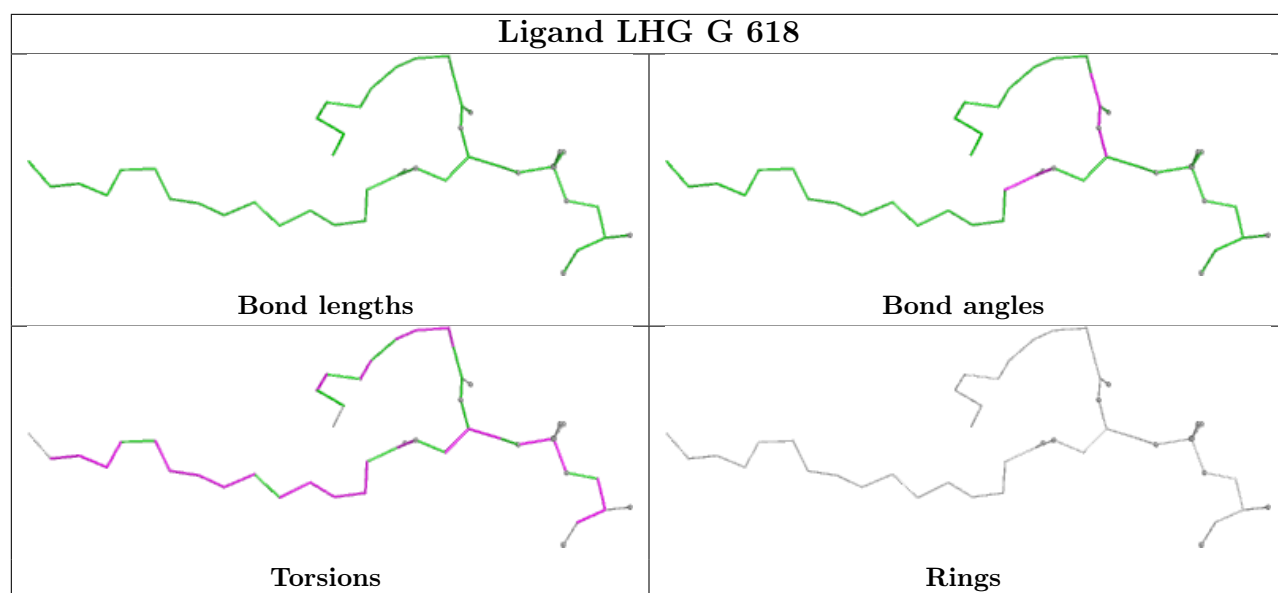
Ligand CHL Y 308

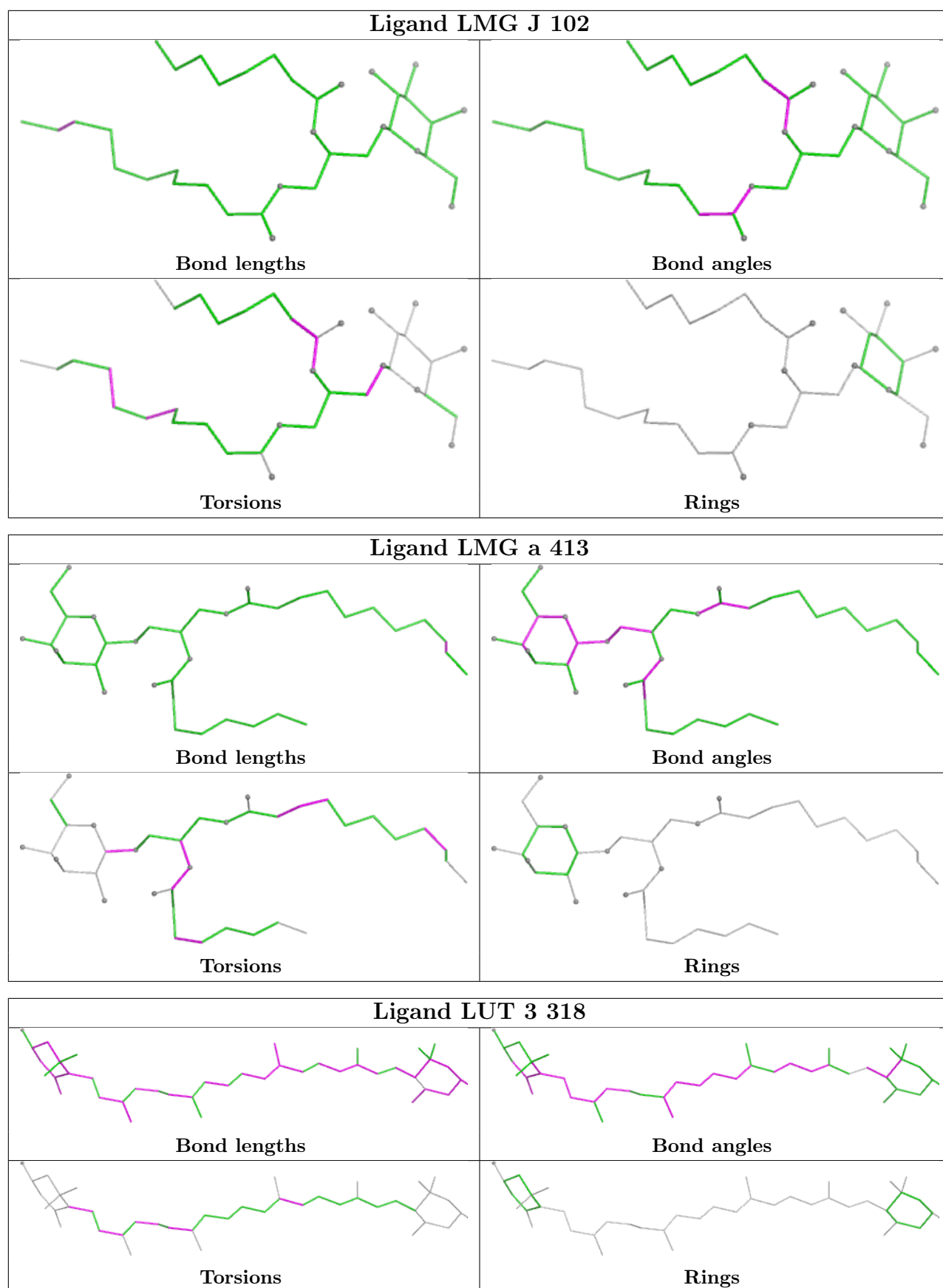




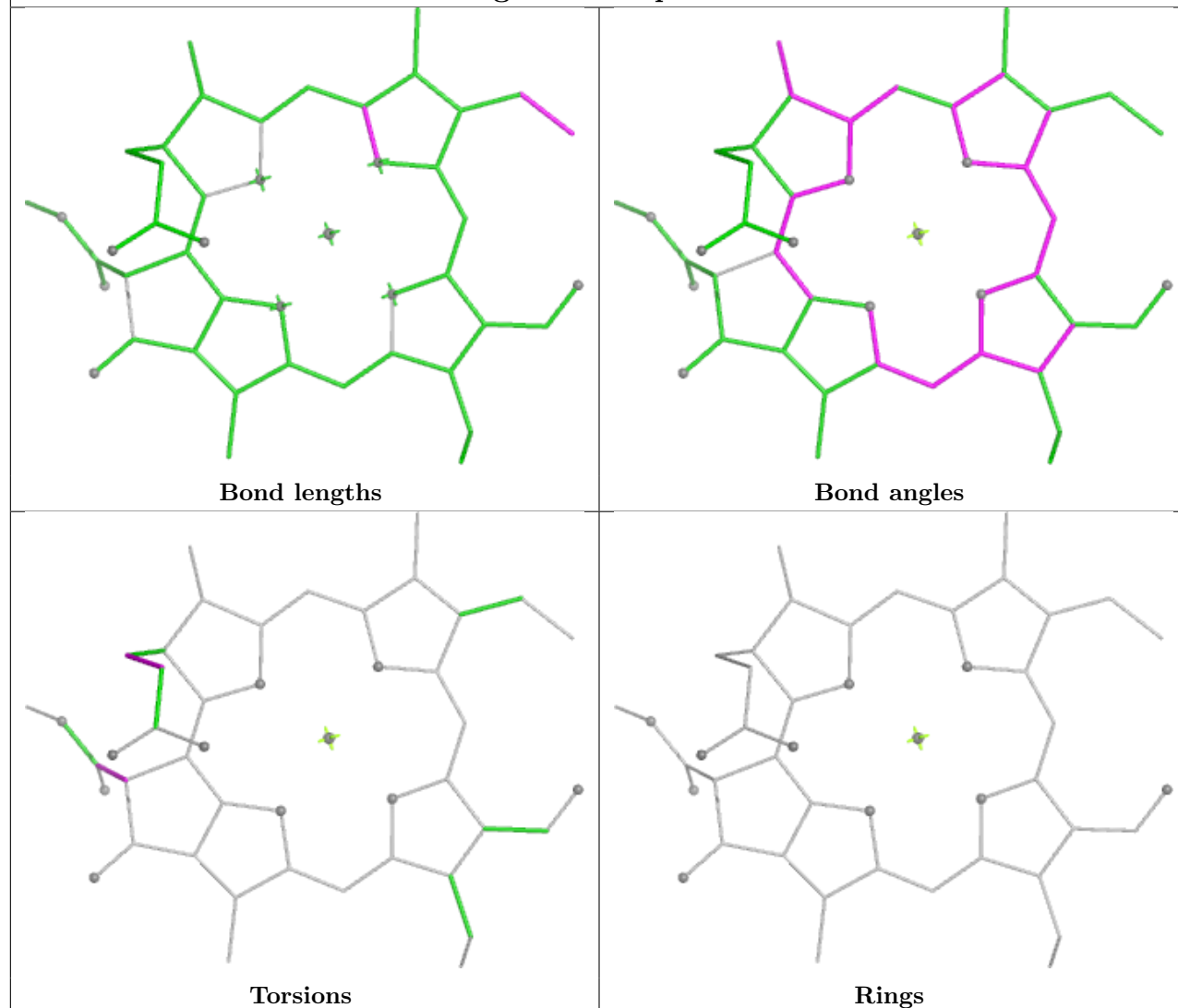
Ligand CHL 8 606**Ligand CLA C 611**



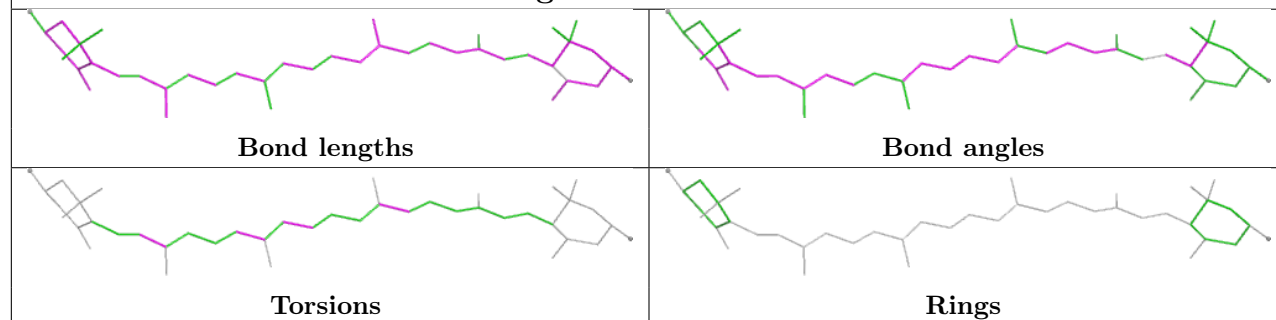


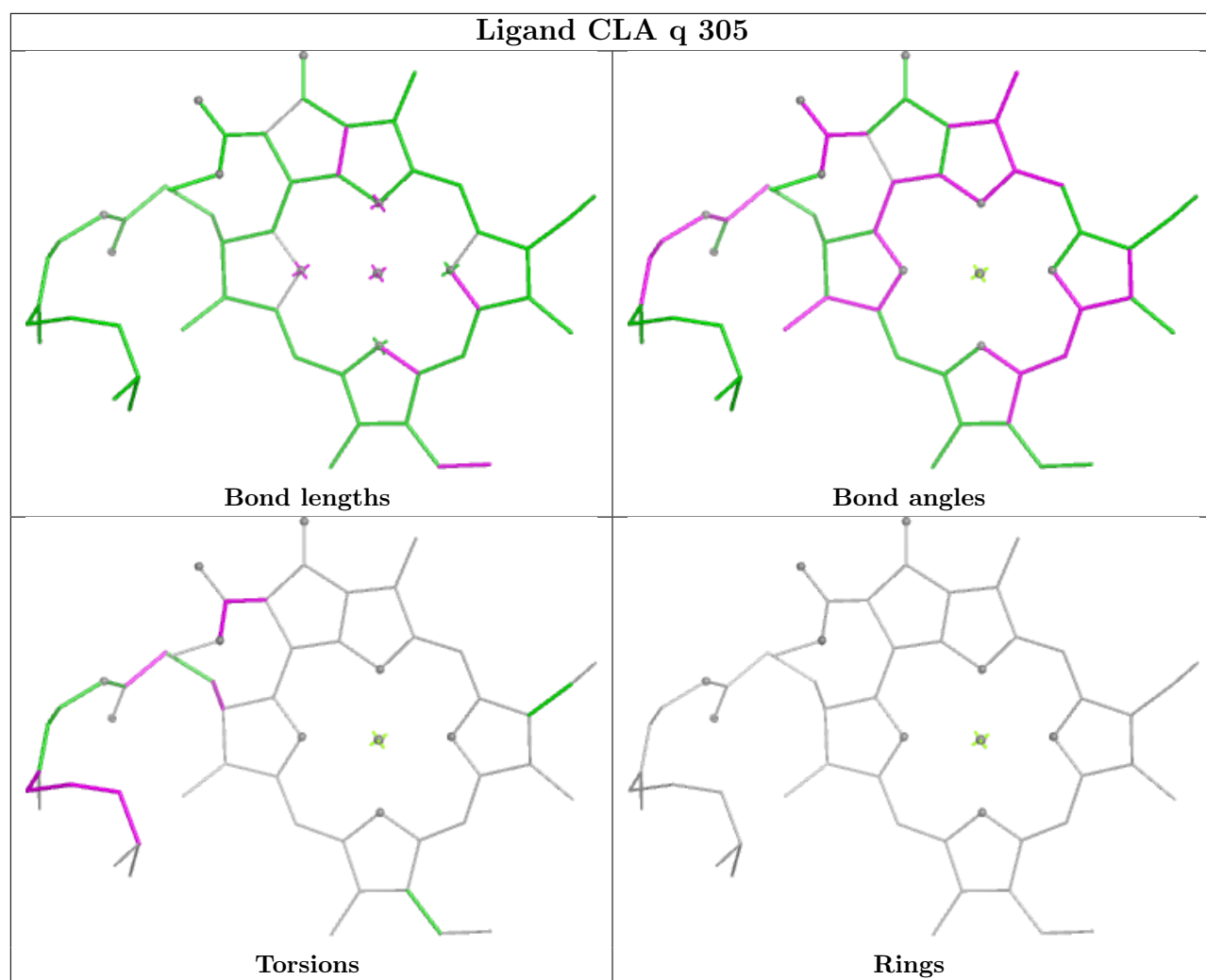


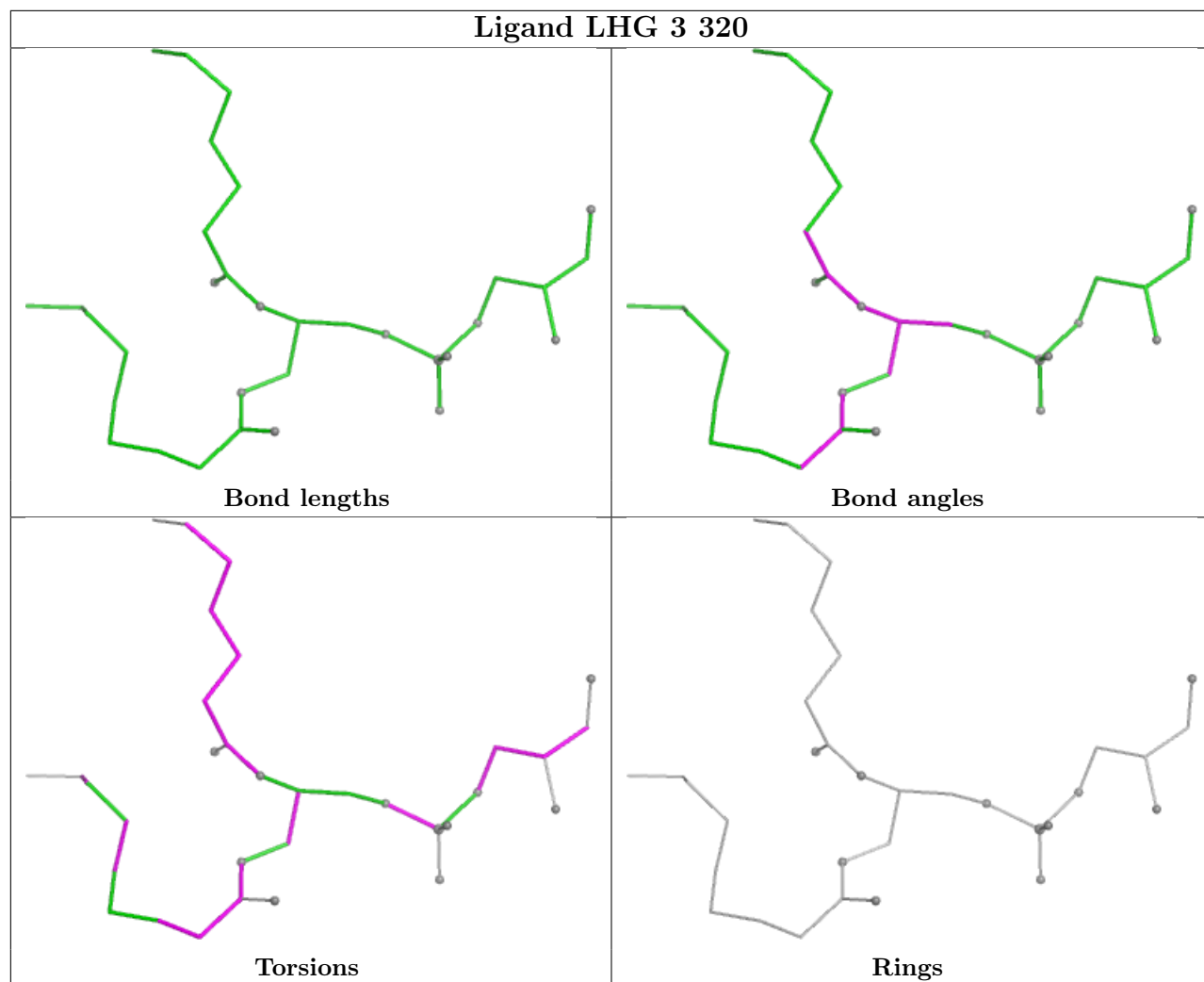
Ligand CHL p 605



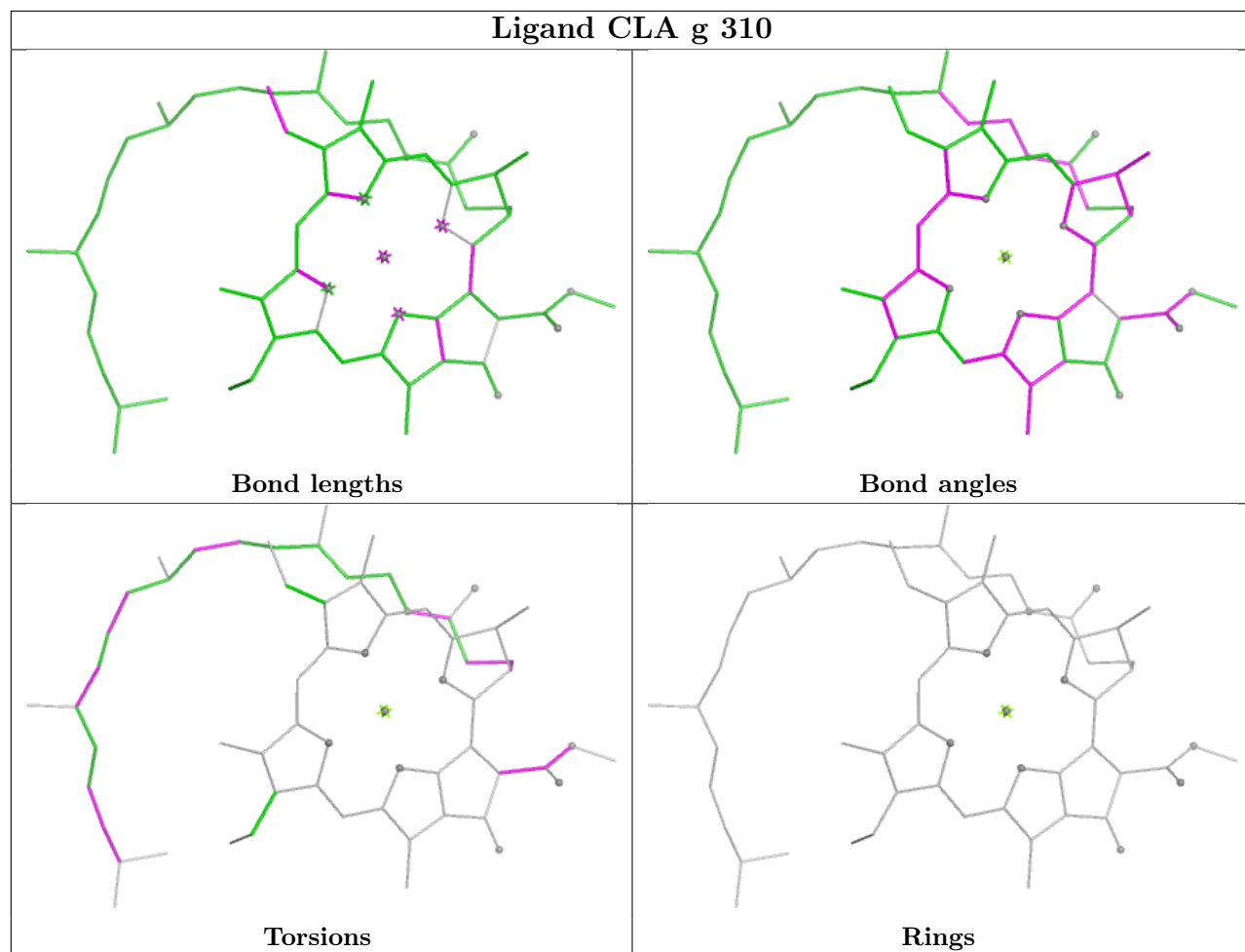
Ligand LUT 7 318



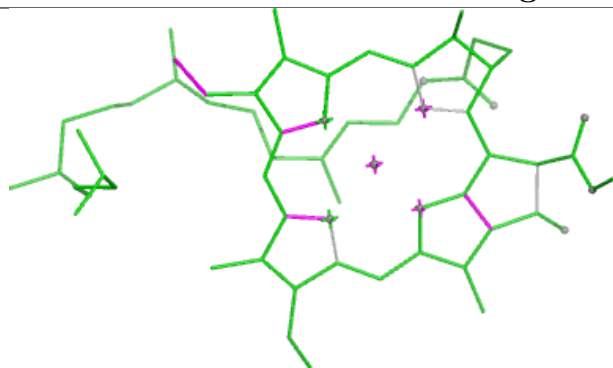




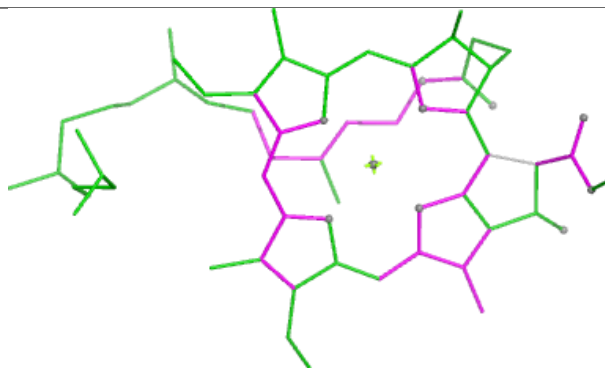
Ligand CLA g 310



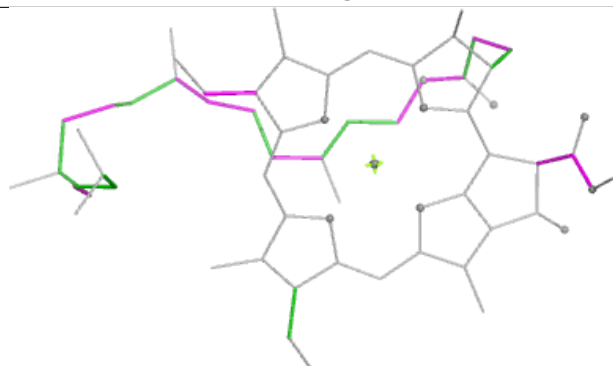
Ligand CLA c 605



Bond lengths



Bond angles

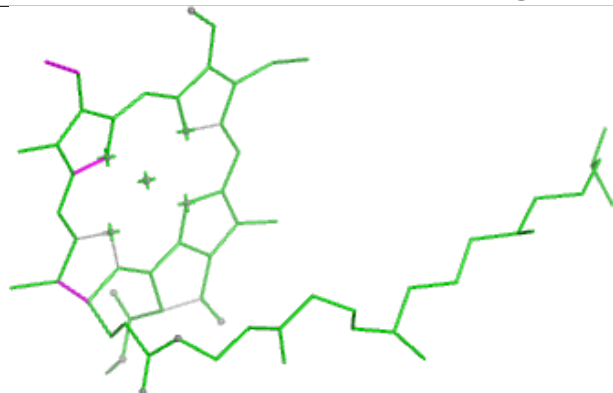


Torsions

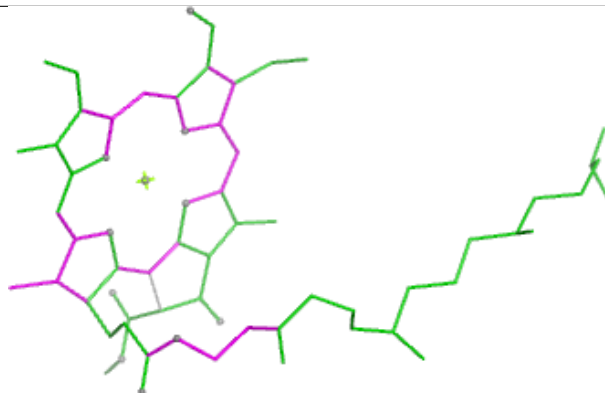


Rings

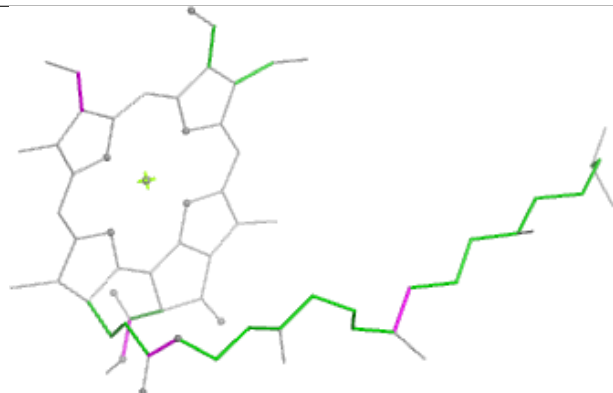
Ligand CHL N 309



Bond lengths



Bond angles

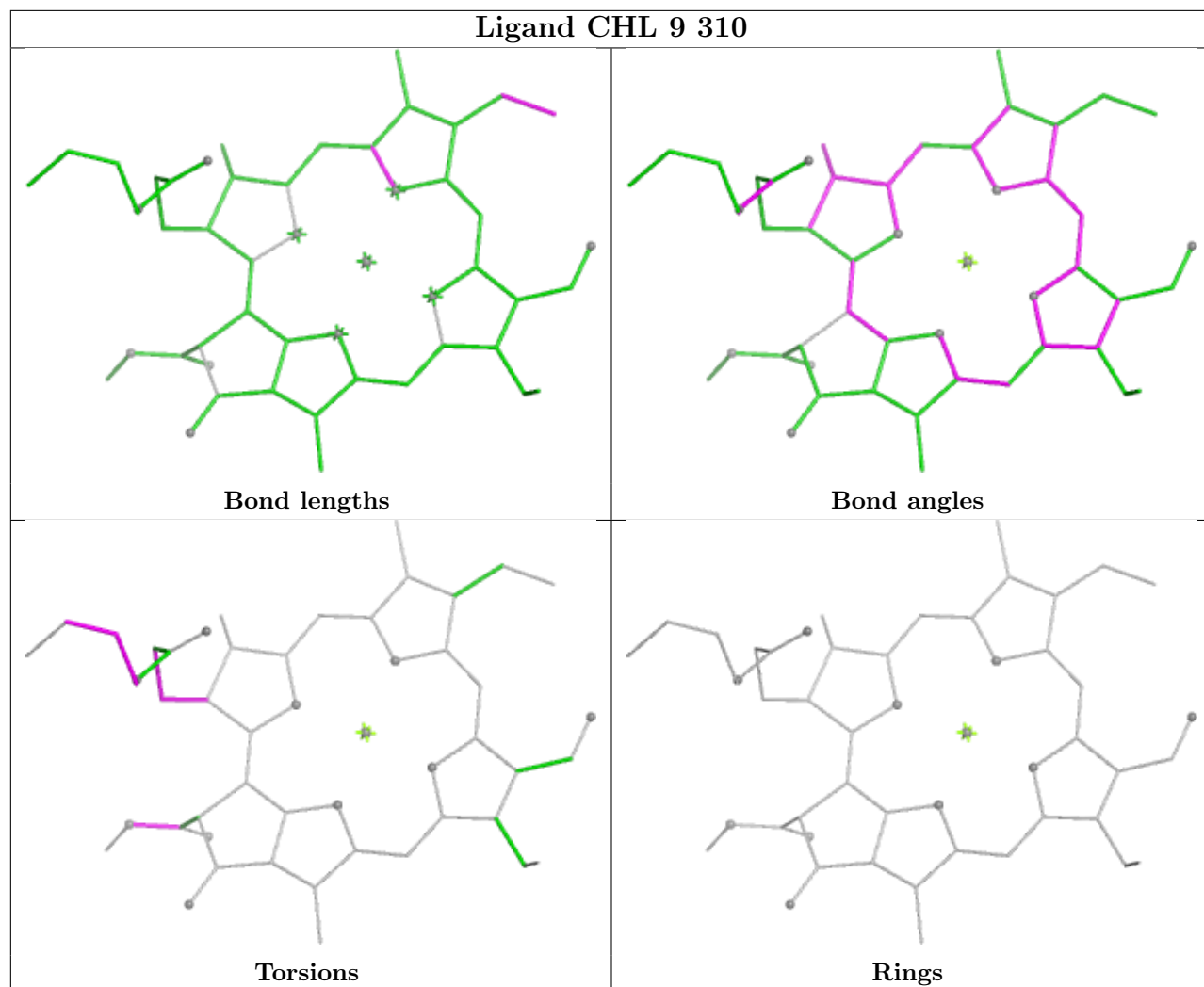


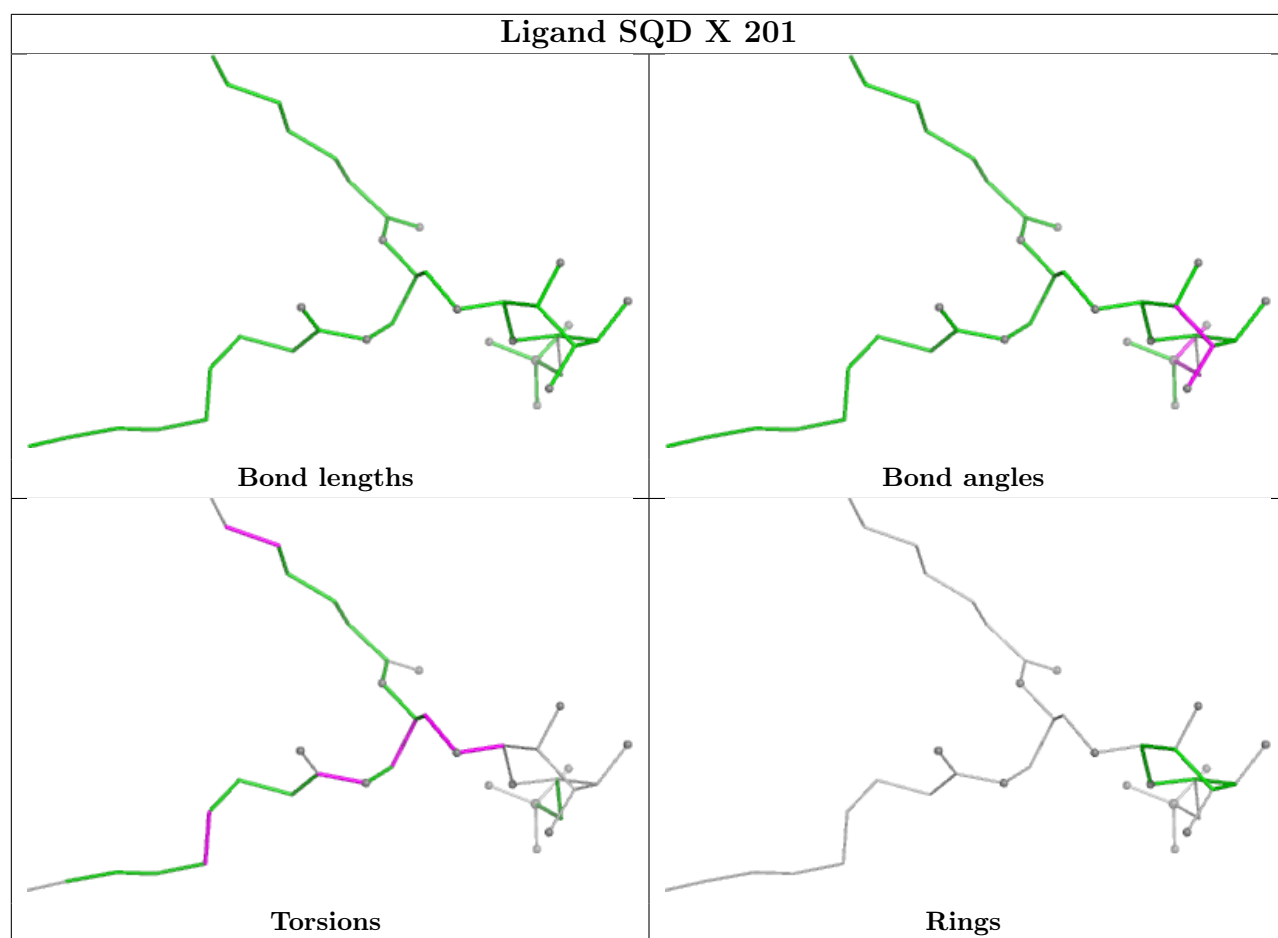
Torsions

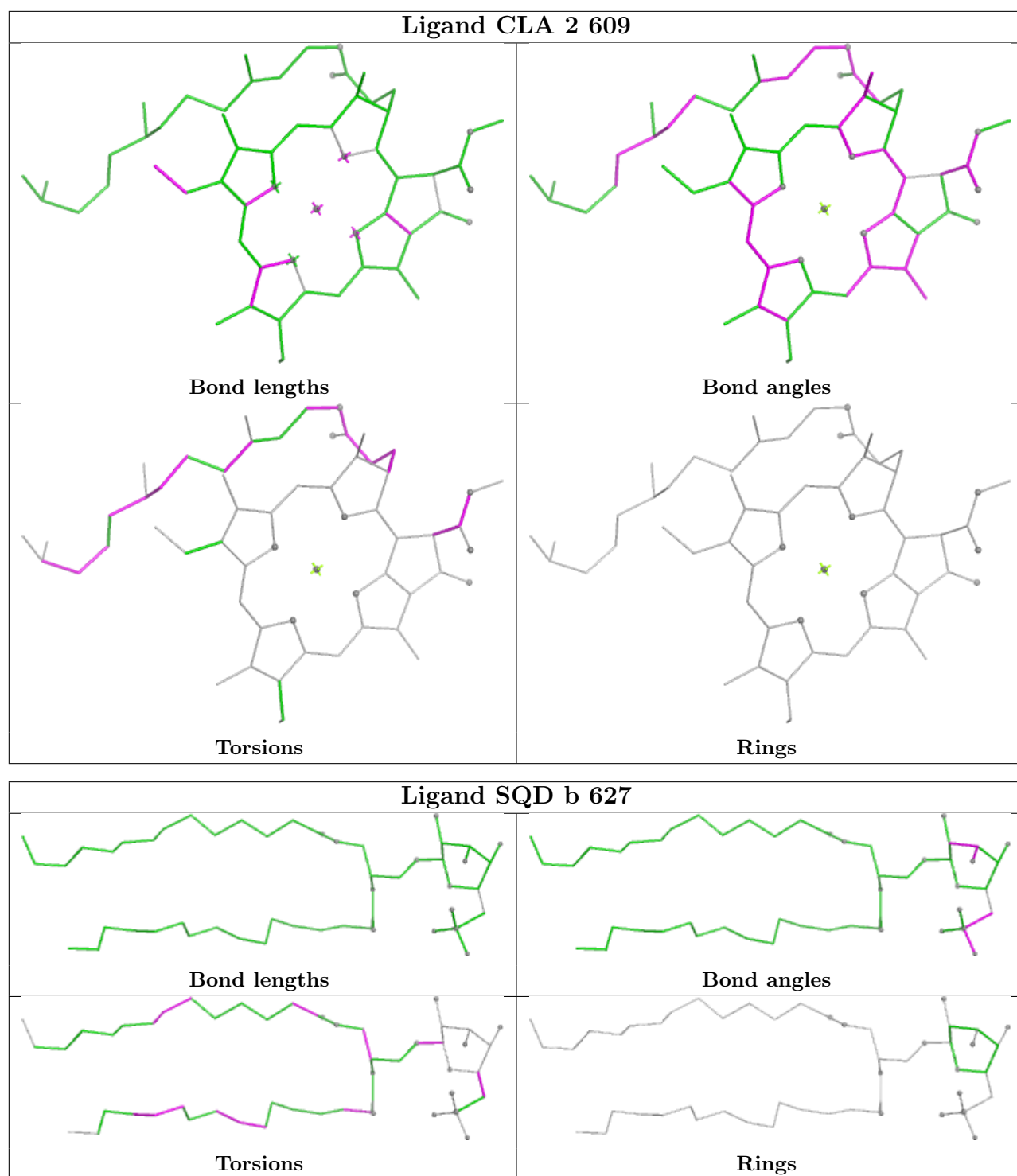


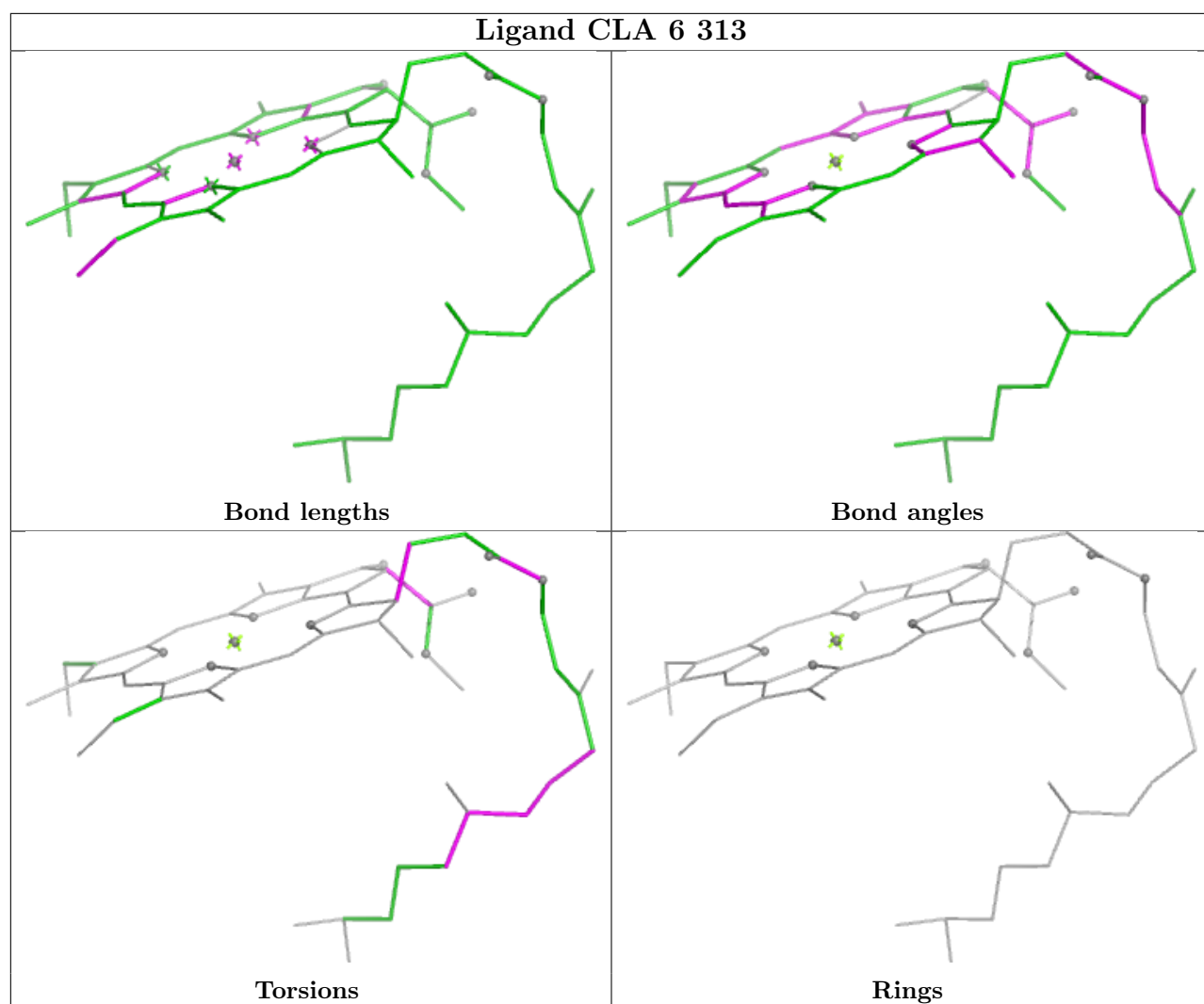
Rings

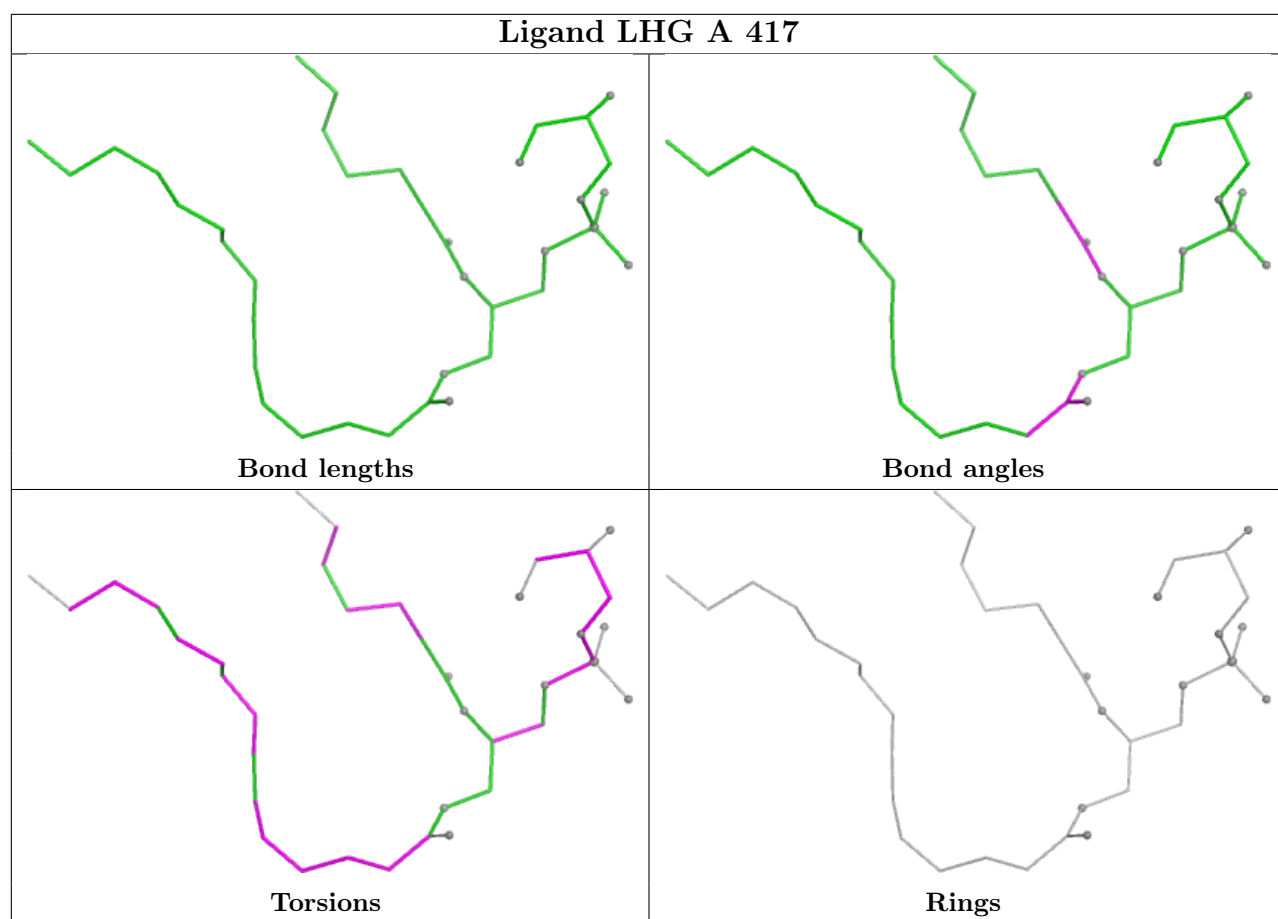
Ligand CHL 9 310



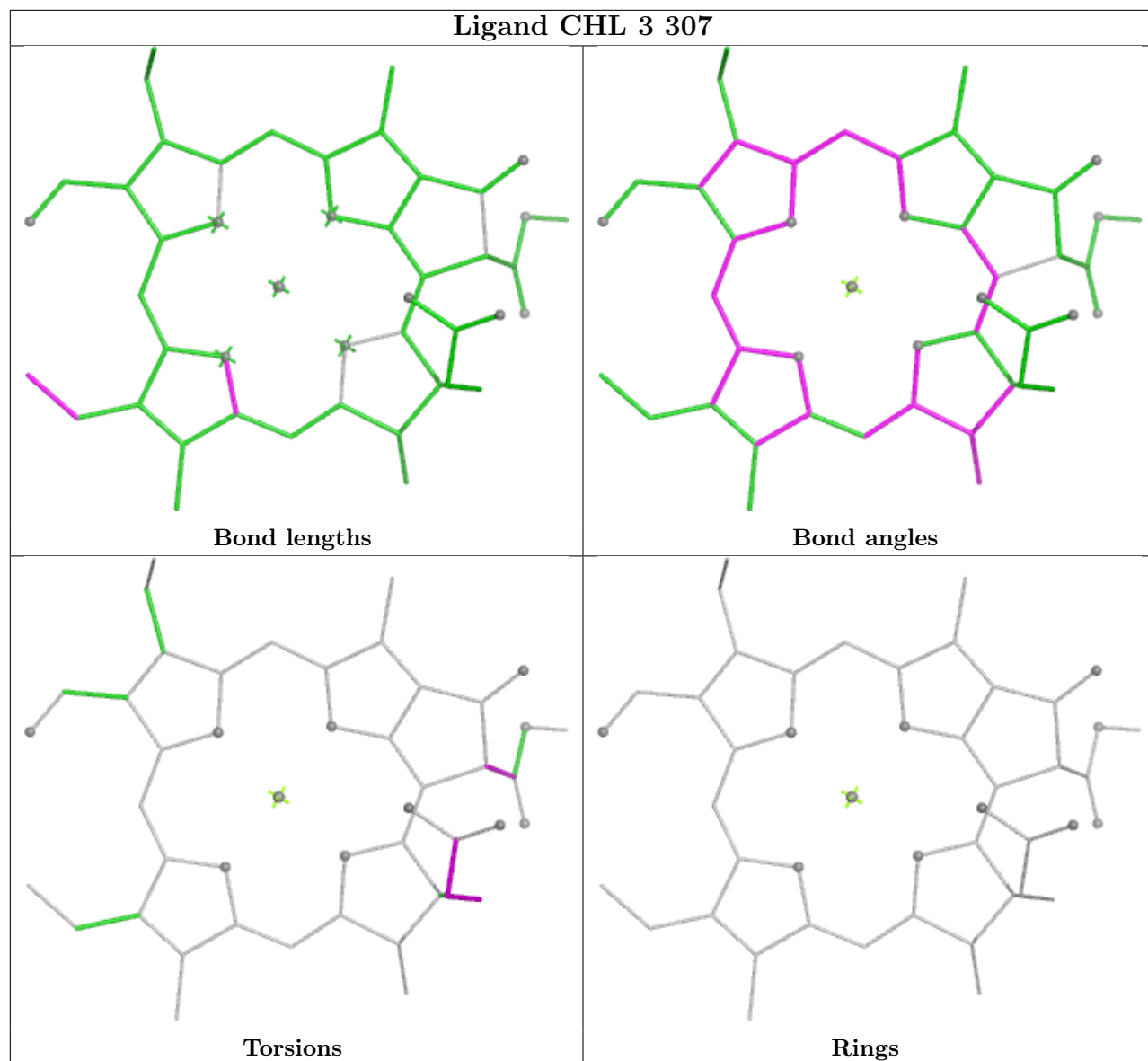


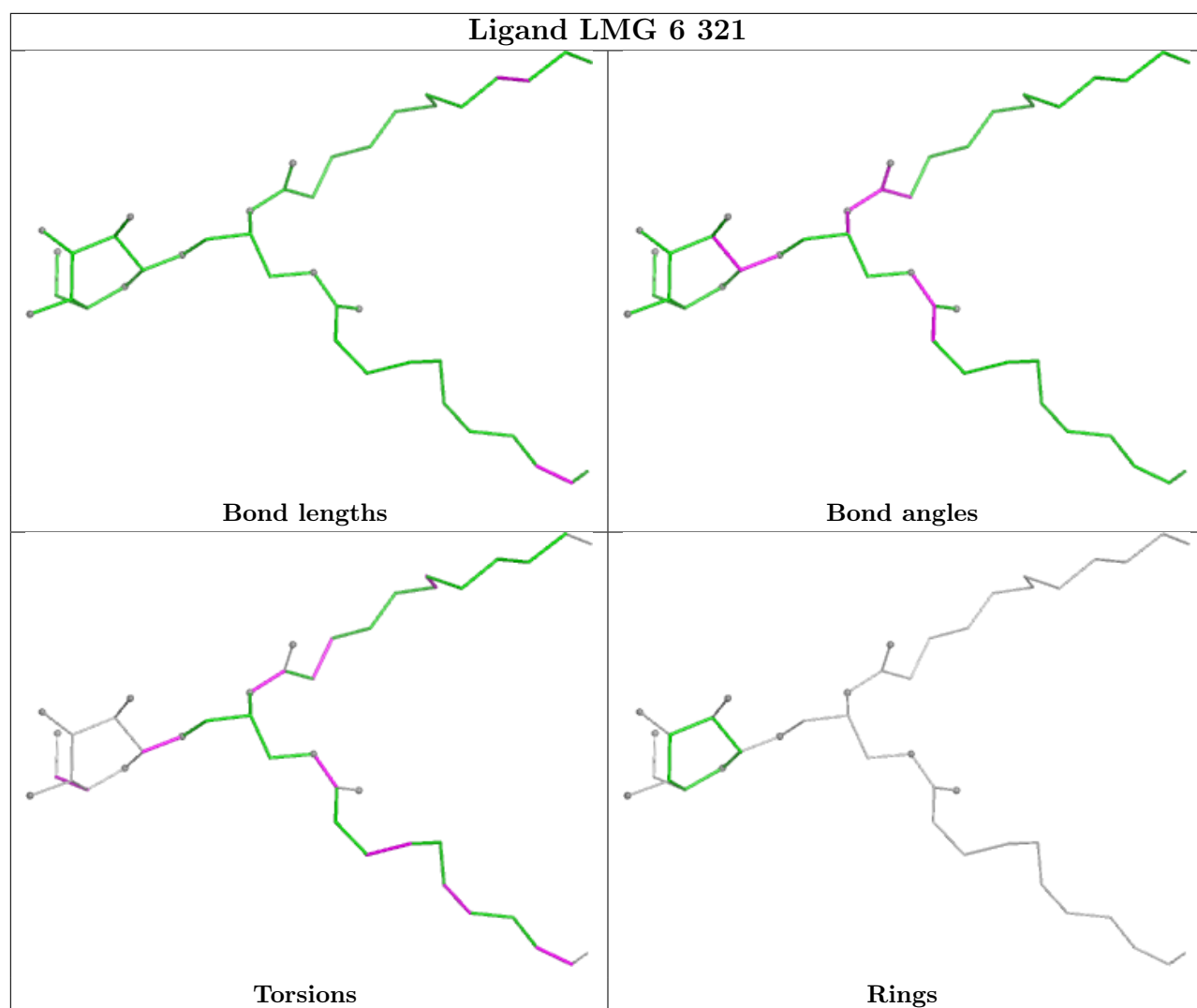




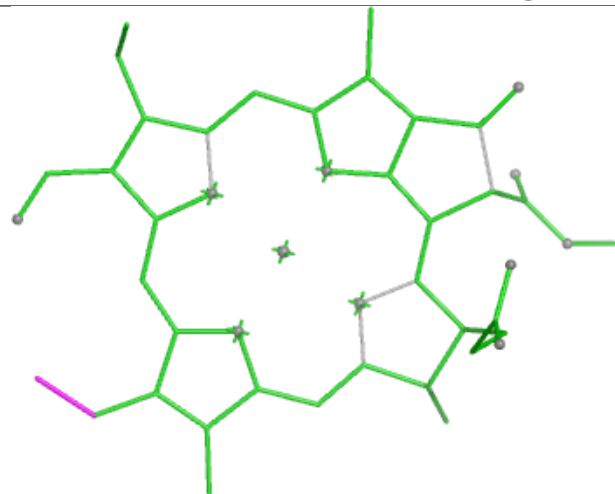


Ligand CHL 3 307

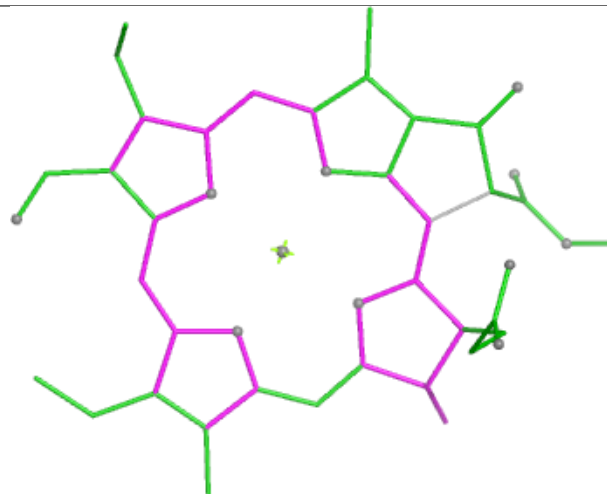




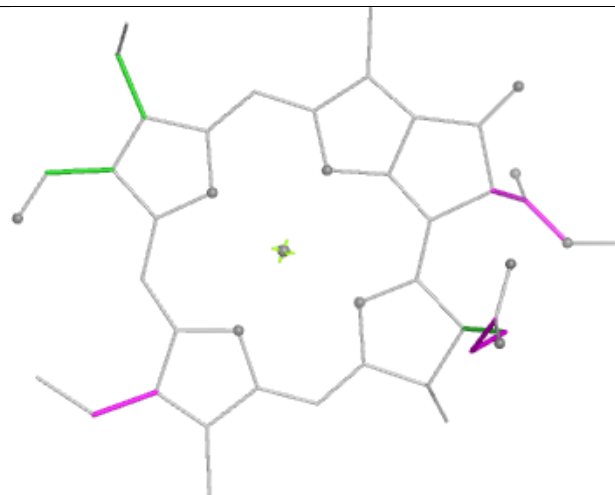
Ligand CHL 6 306



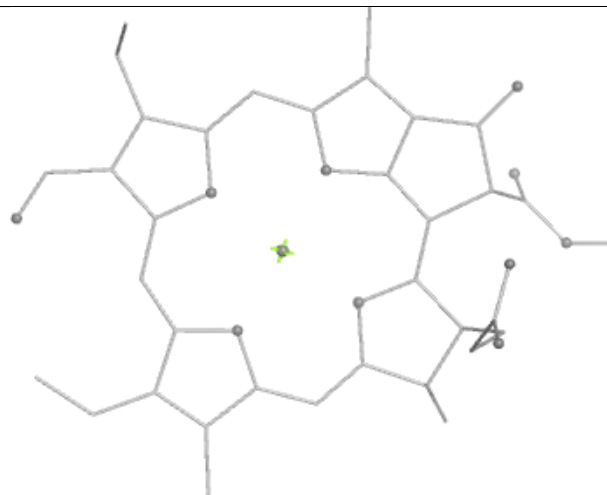
Bond lengths



Bond angles

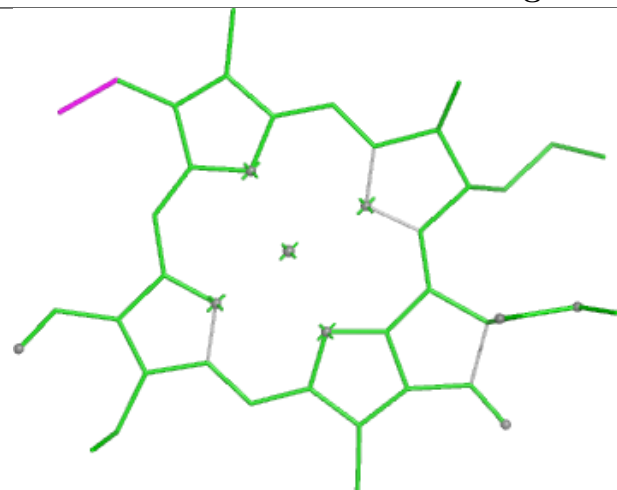


Torsions

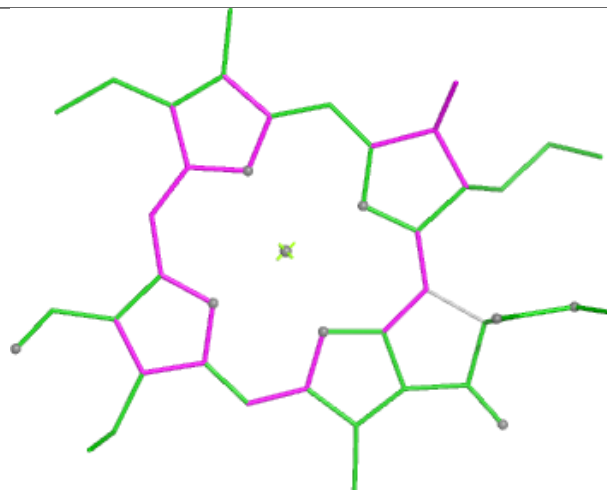


Rings

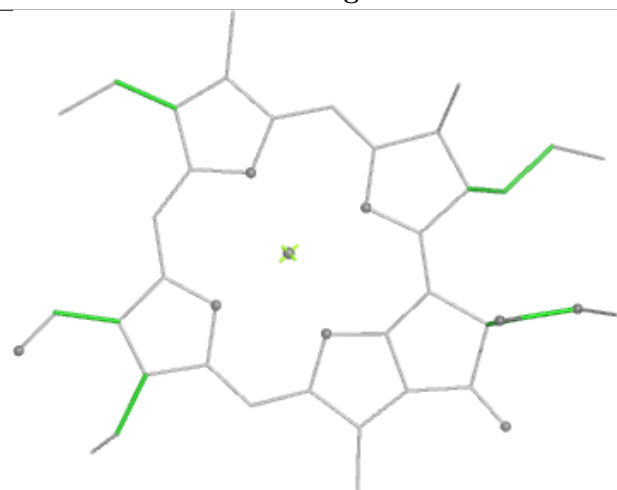
Ligand CHL s 307



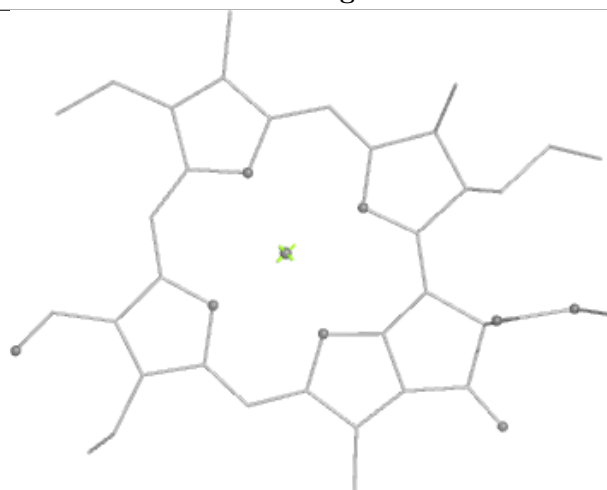
Bond lengths



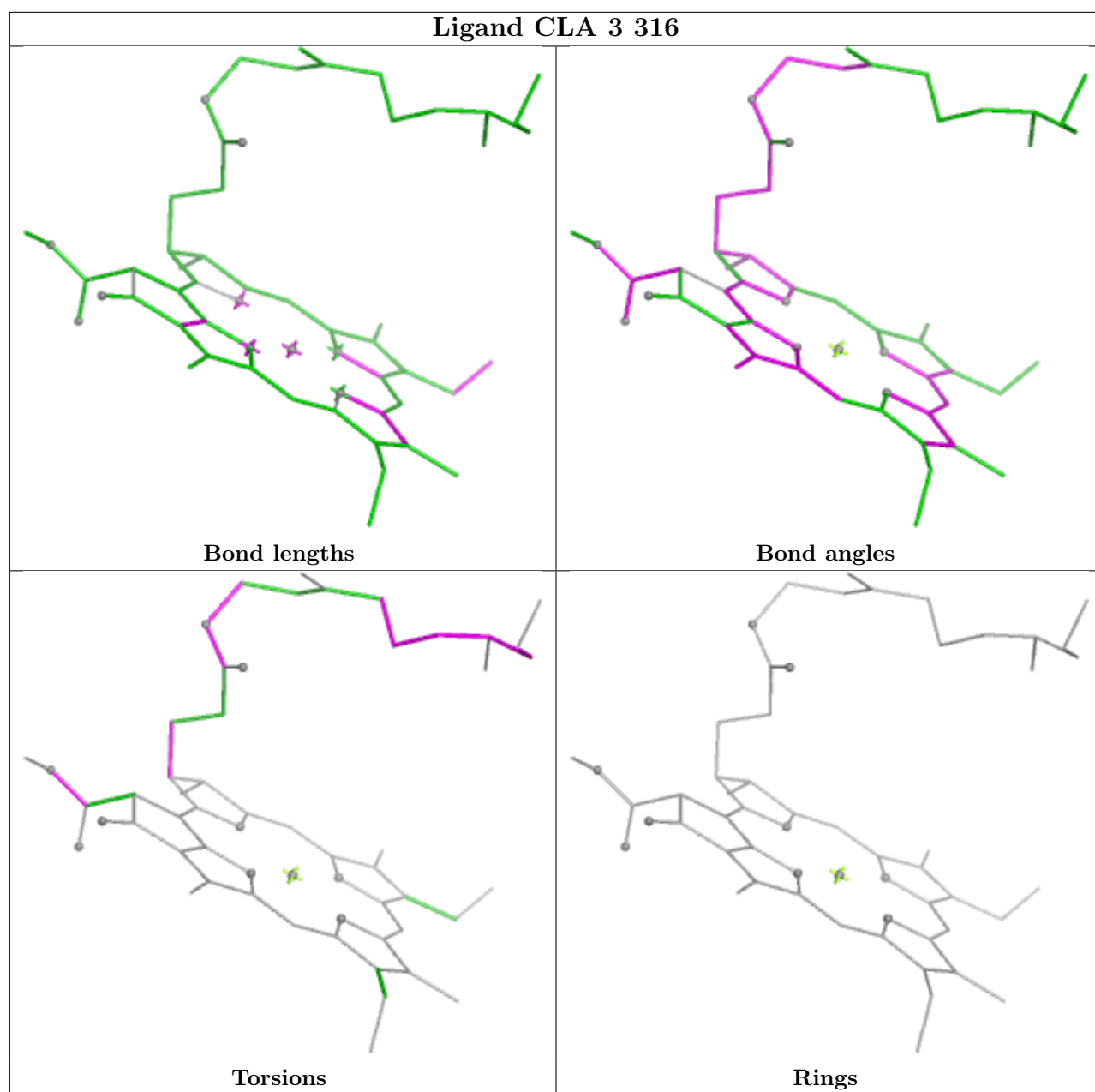
Bond angles



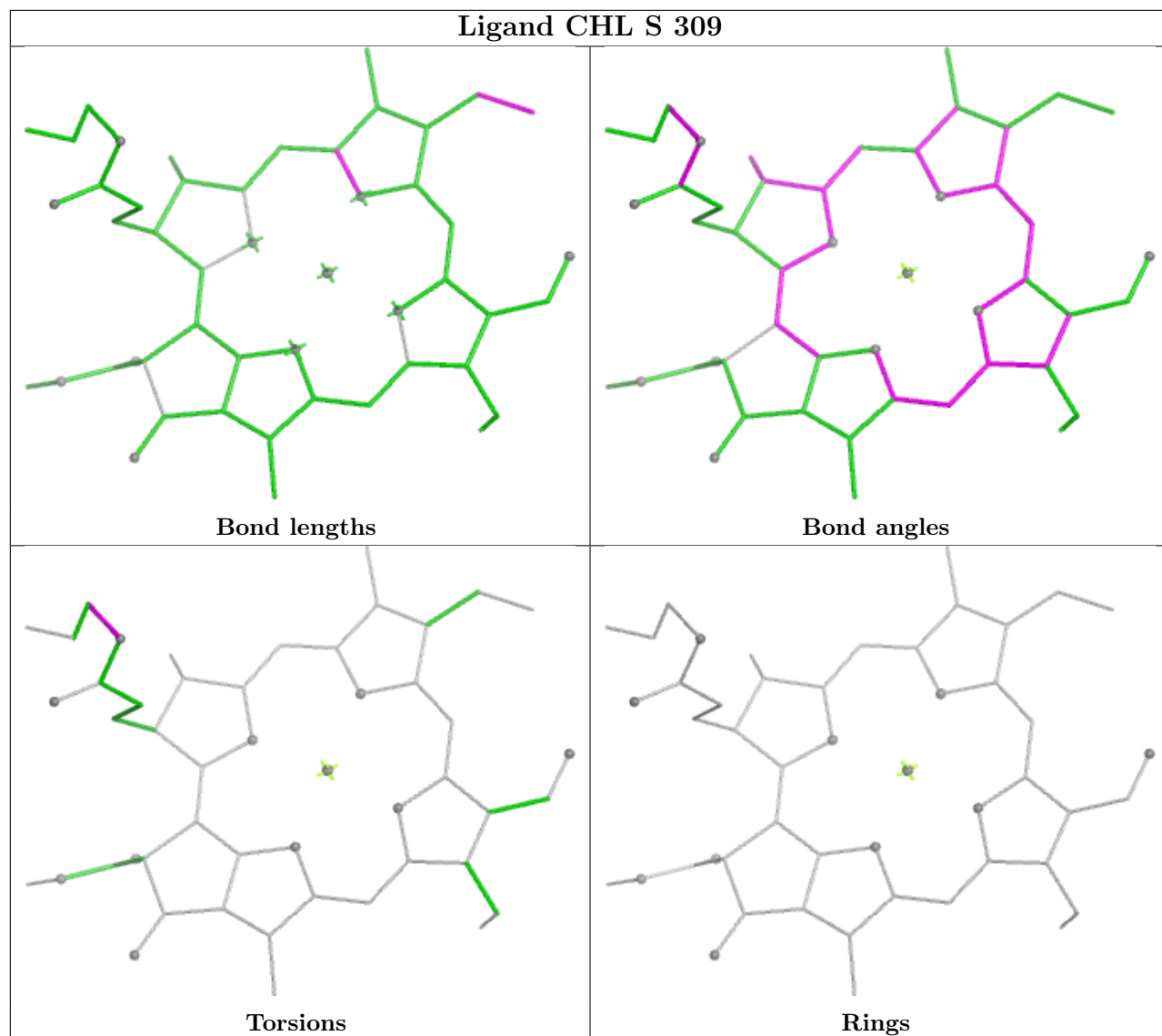
Torsions



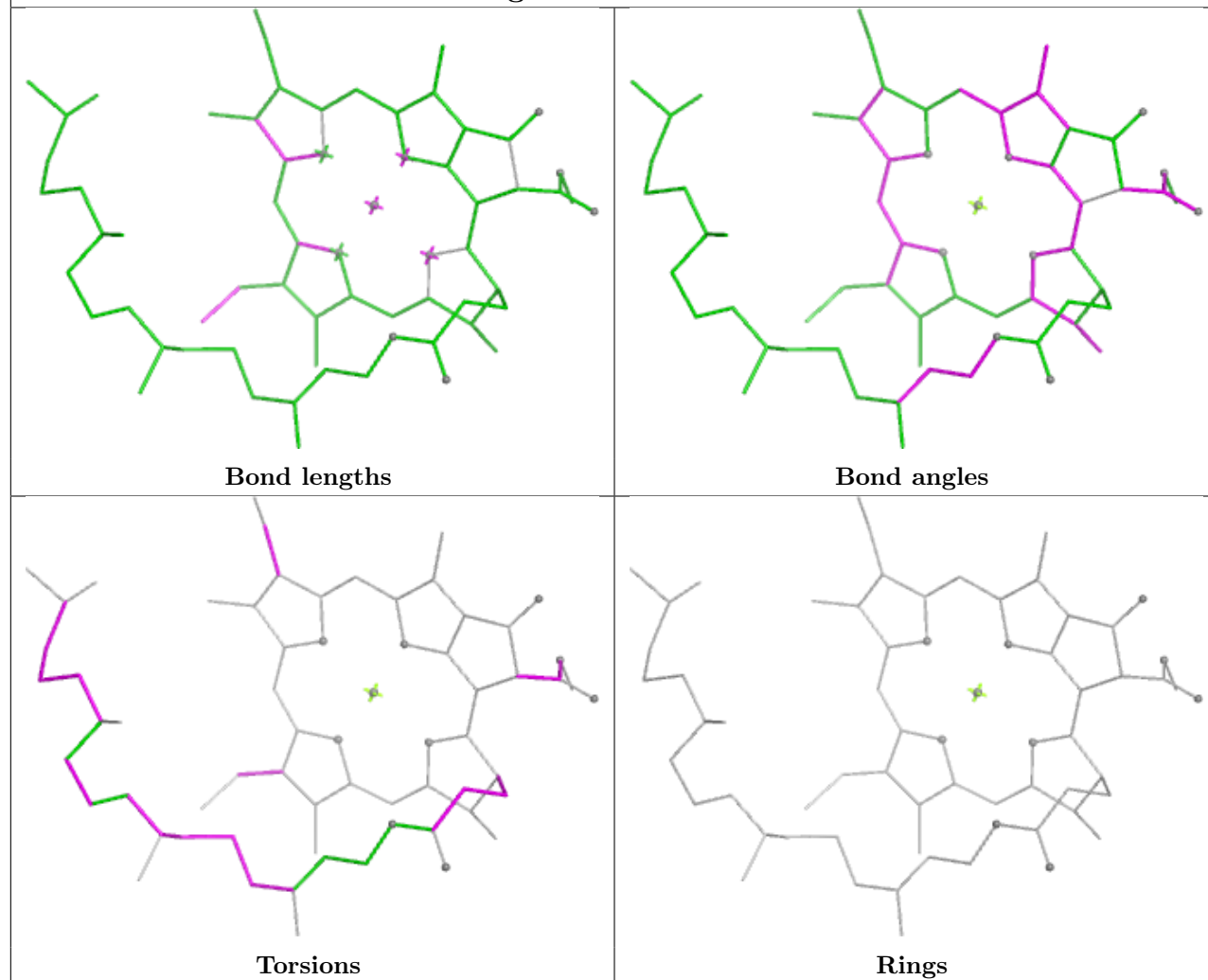
Rings



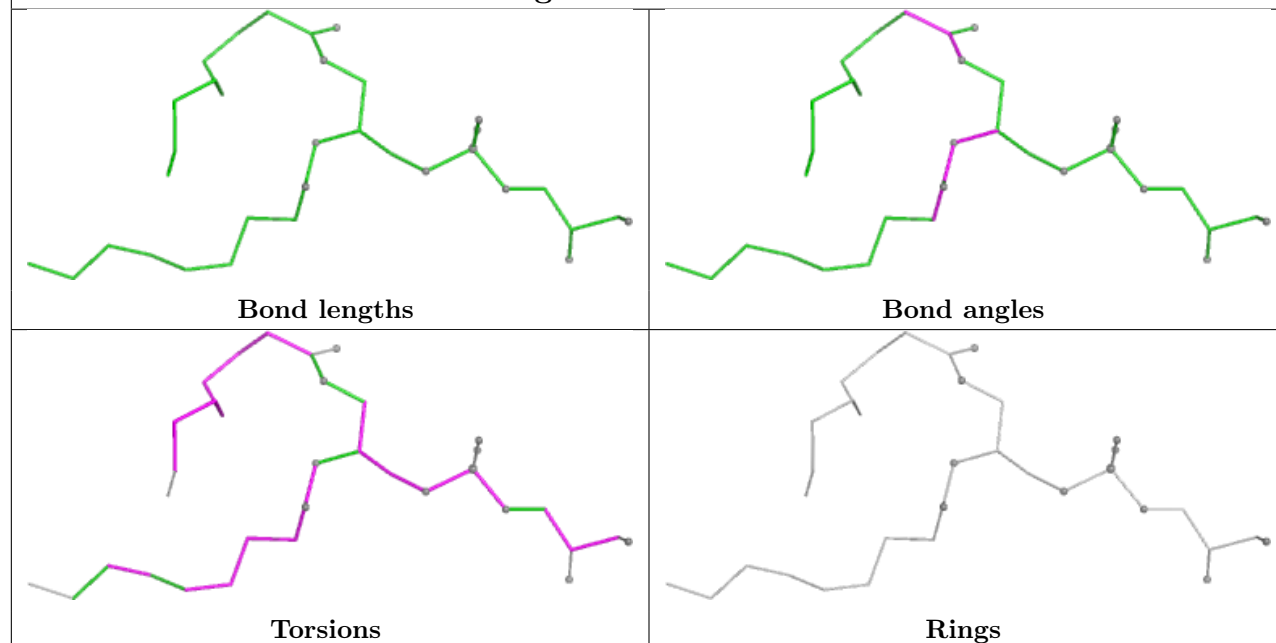
Ligand CHL S 309

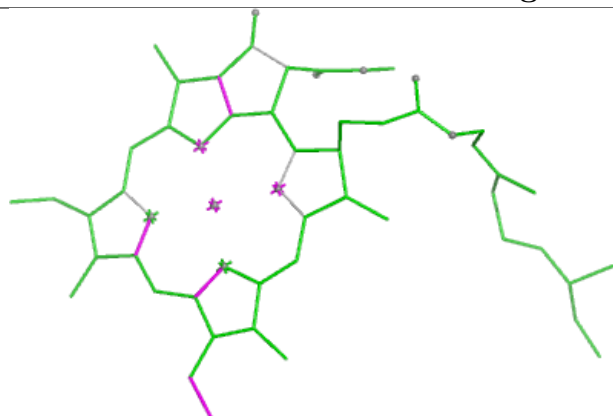
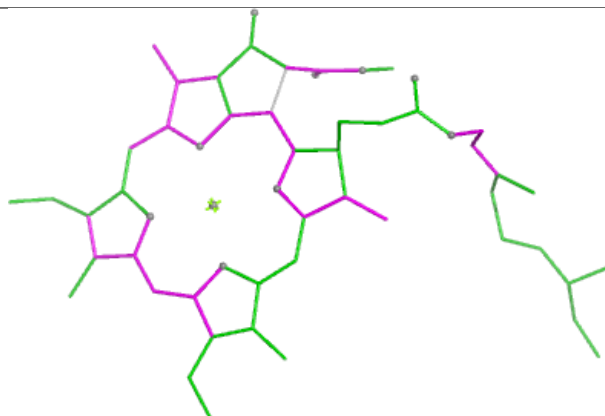
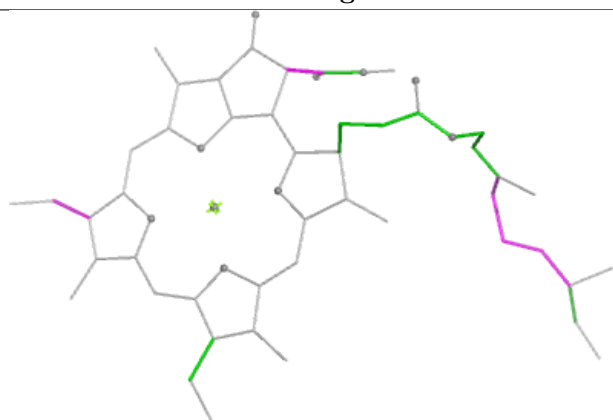
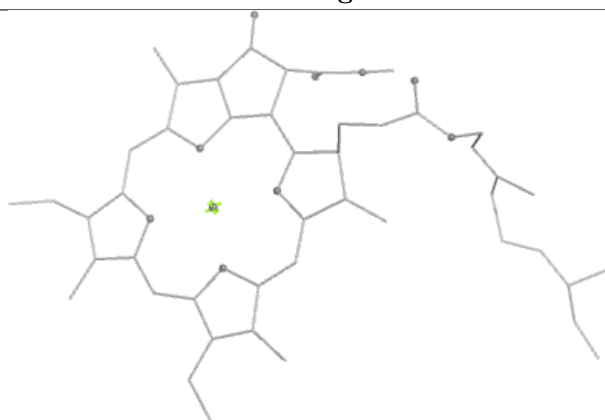
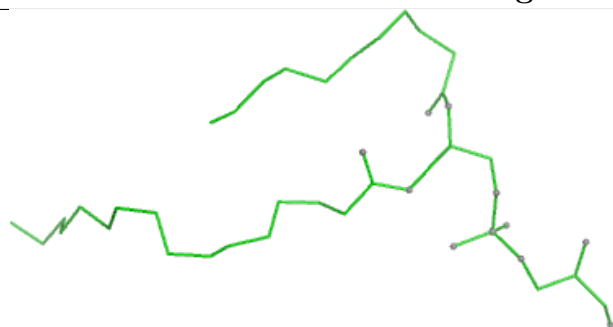
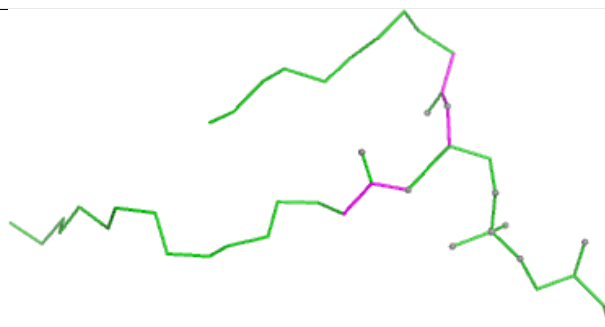
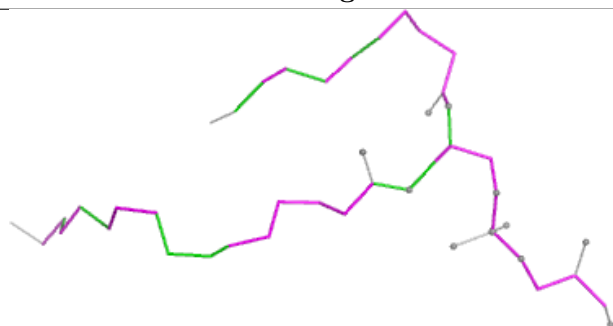
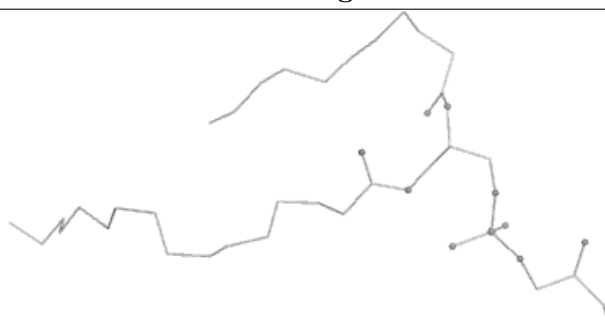


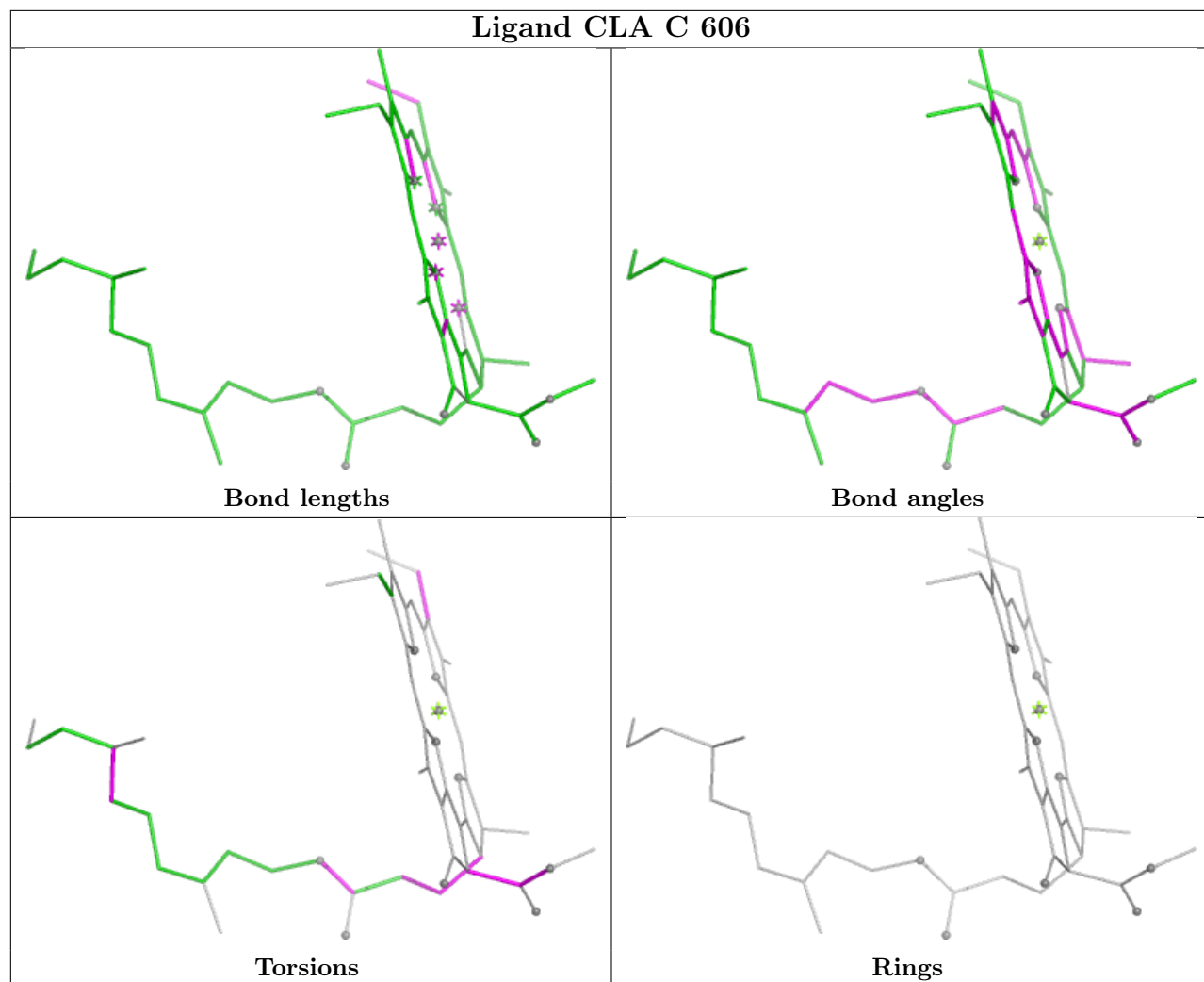
Ligand CLA 2 602

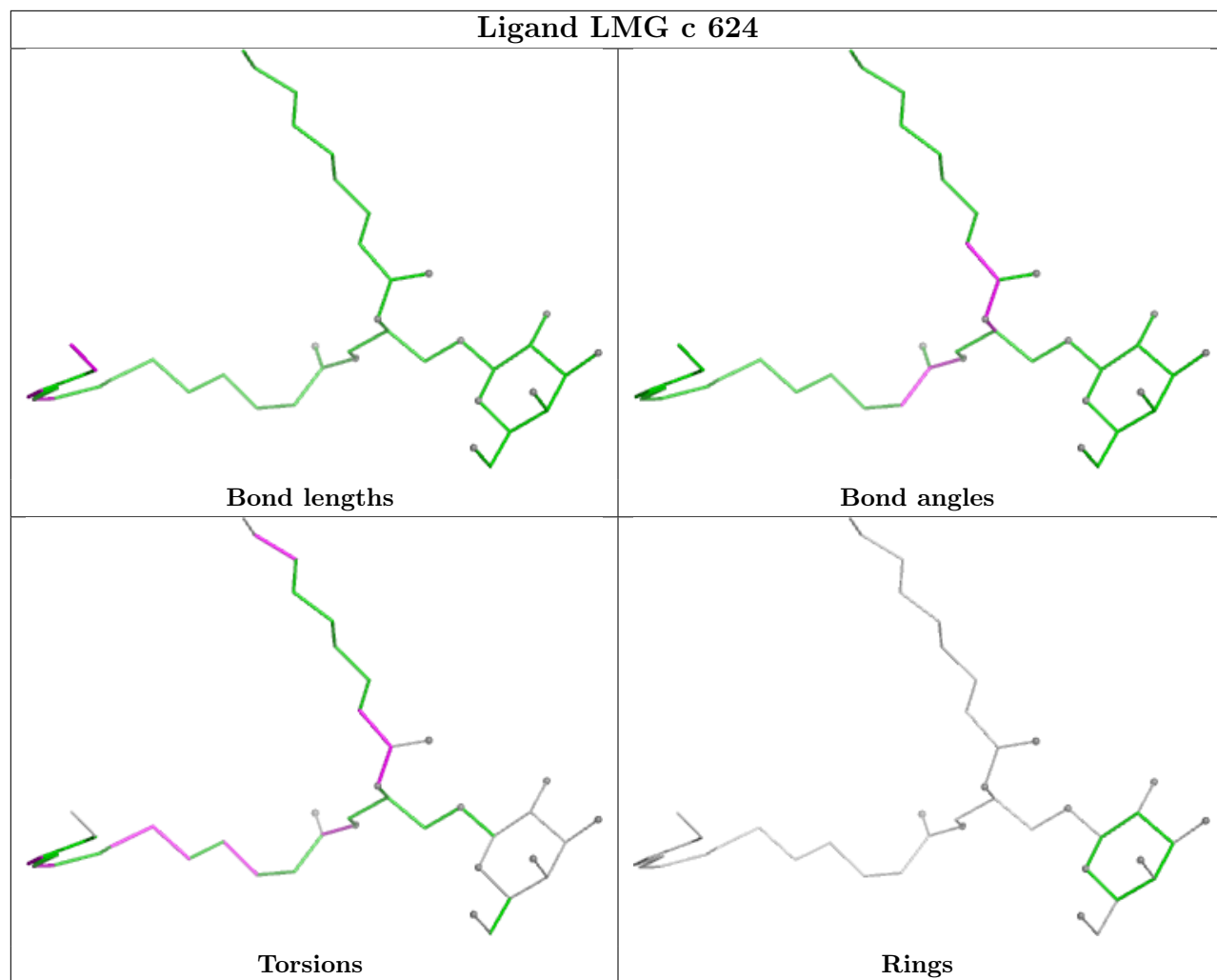


Ligand LHG 1 617

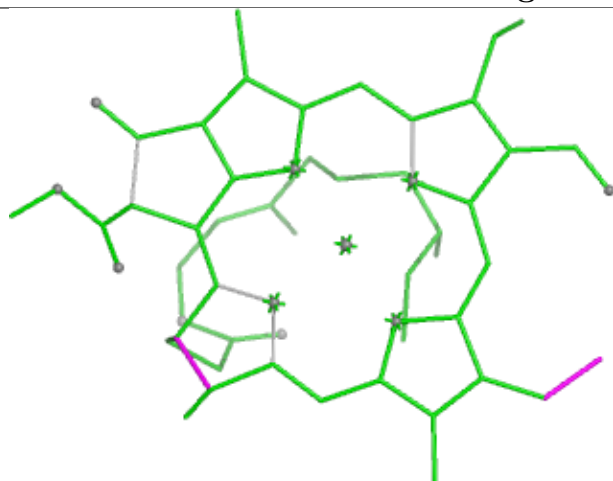


Ligand CLA s 313**Bond lengths****Bond angles****Torsions****Rings****Ligand LHG S 322****Bond lengths****Bond angles****Torsions****Rings**

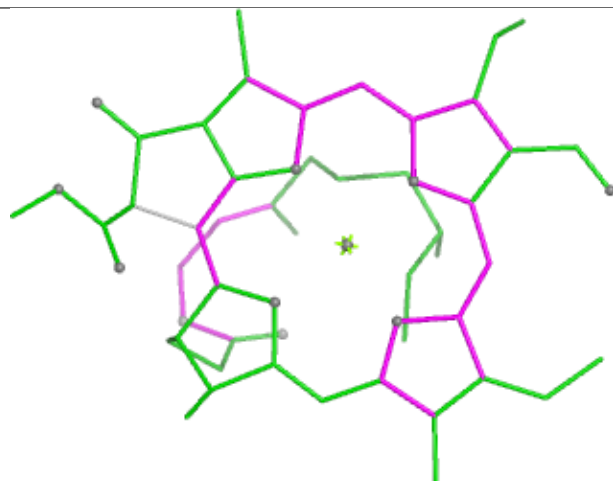




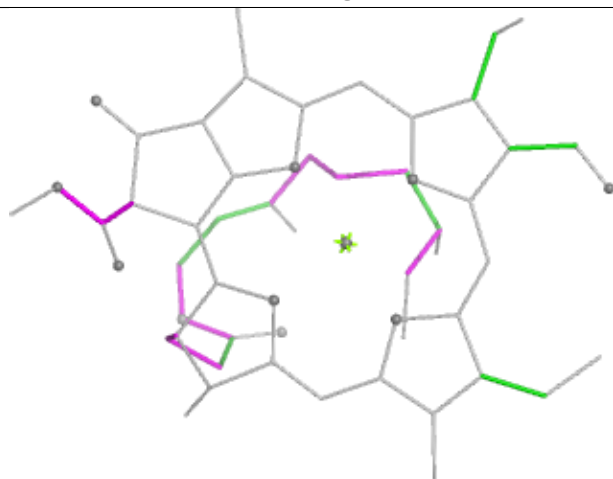
Ligand CHL 4 607



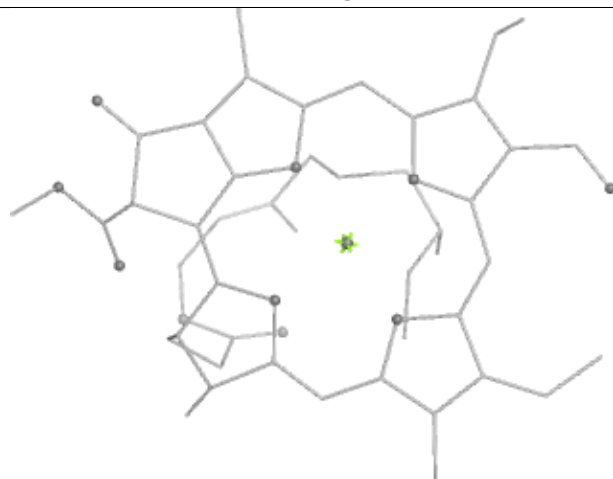
Bond lengths



Bond angles

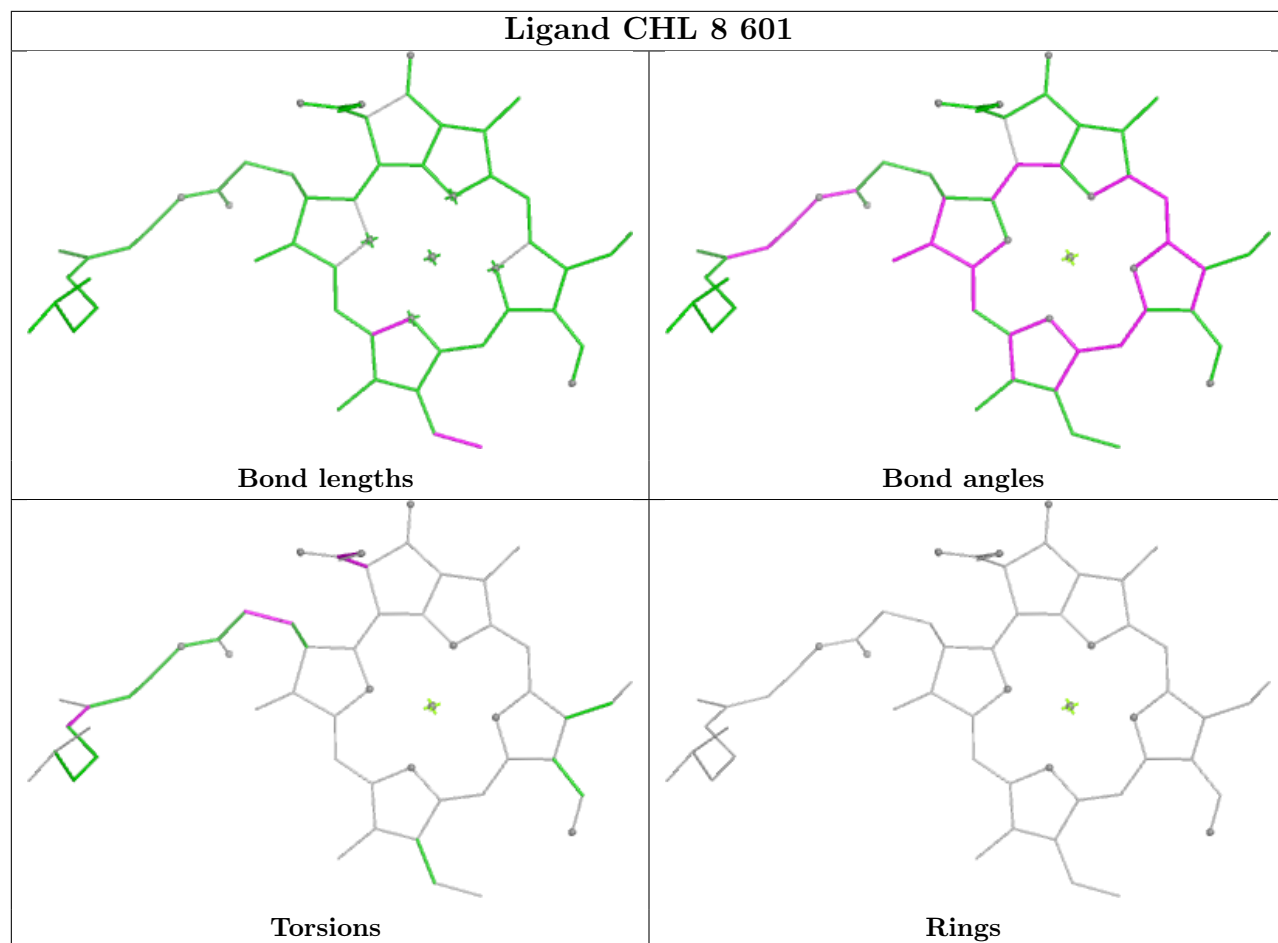


Torsions

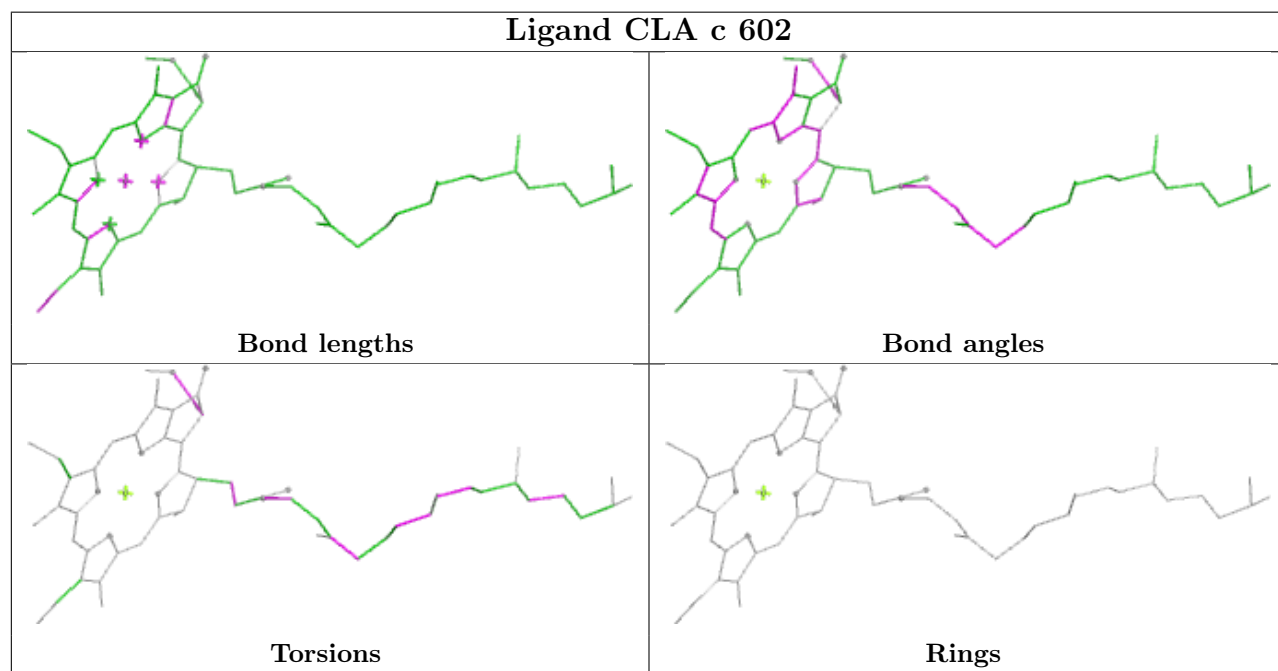


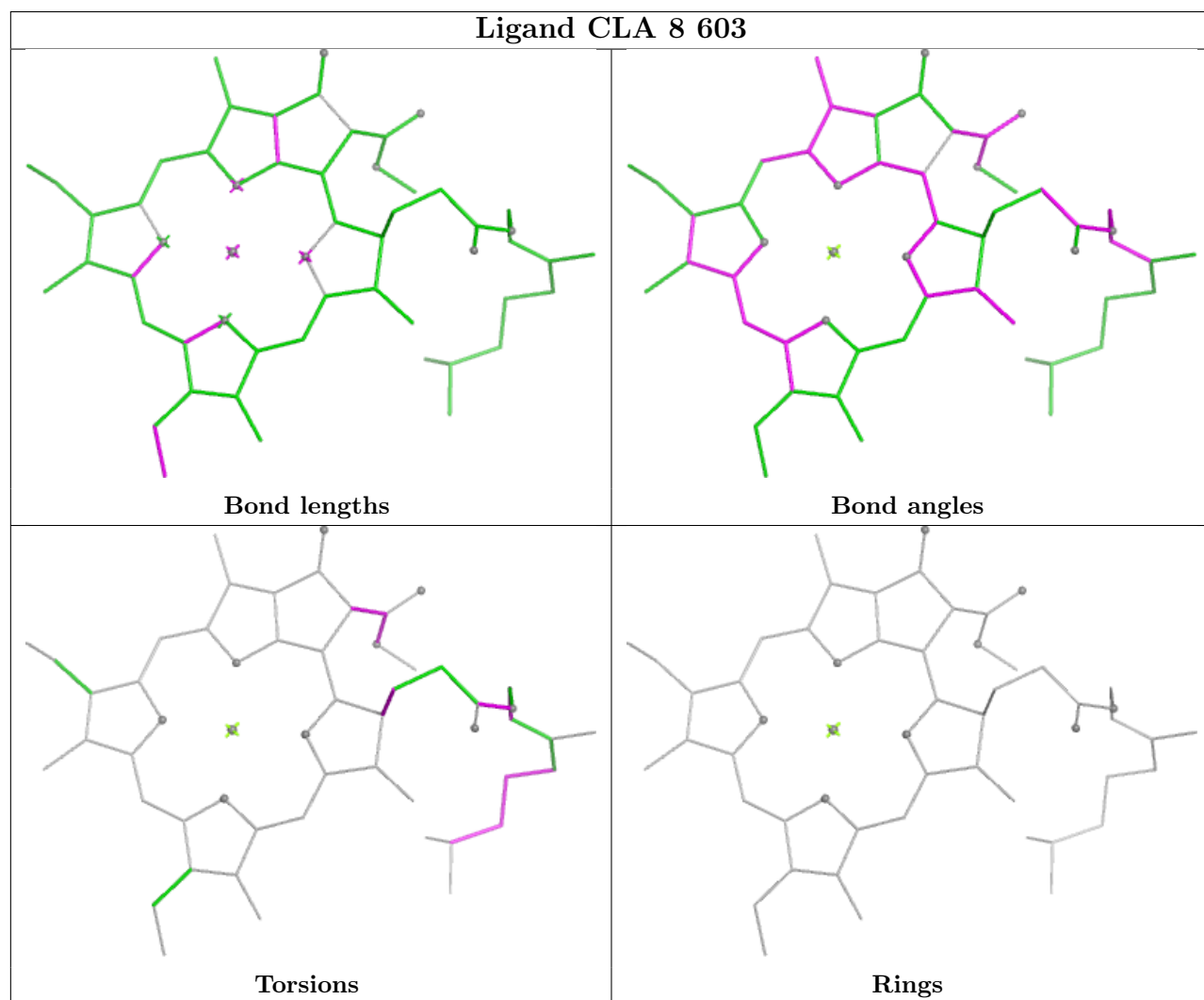
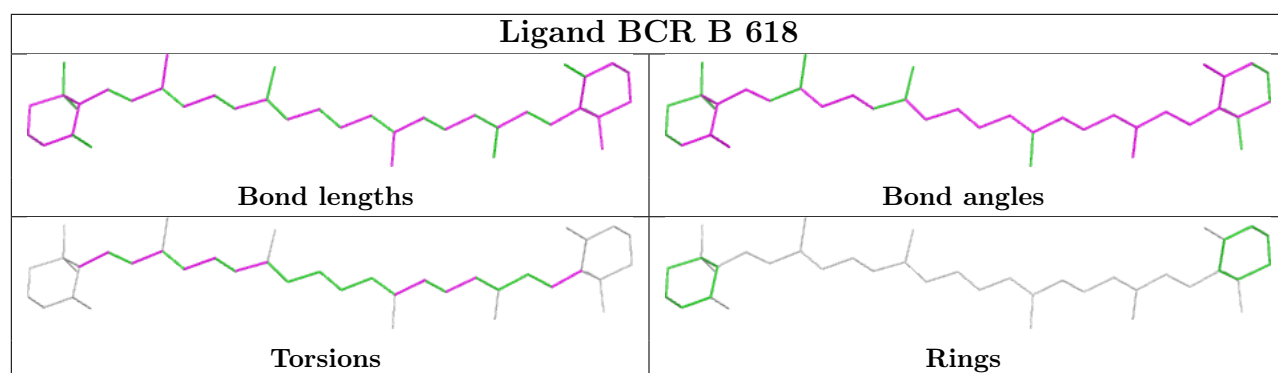
Rings

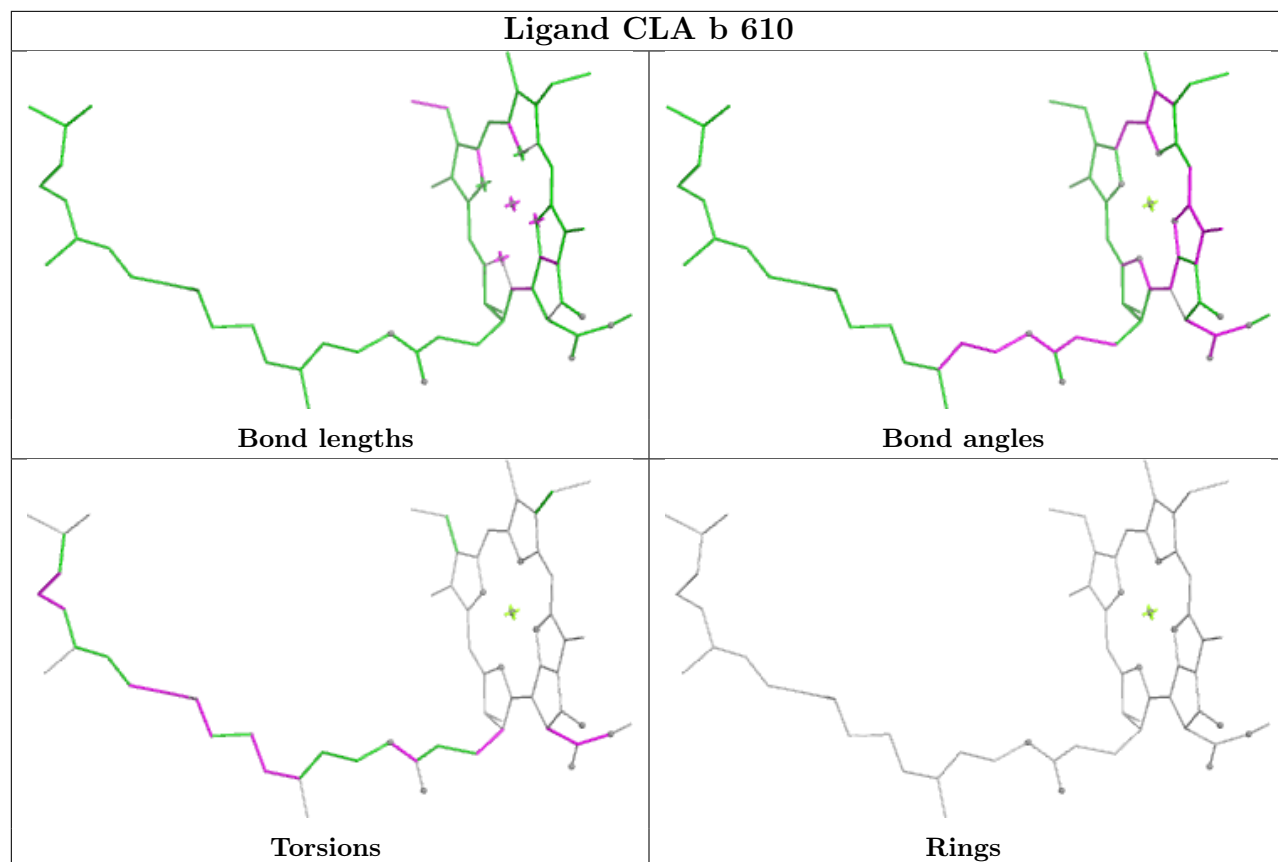
Ligand CHL 8 601



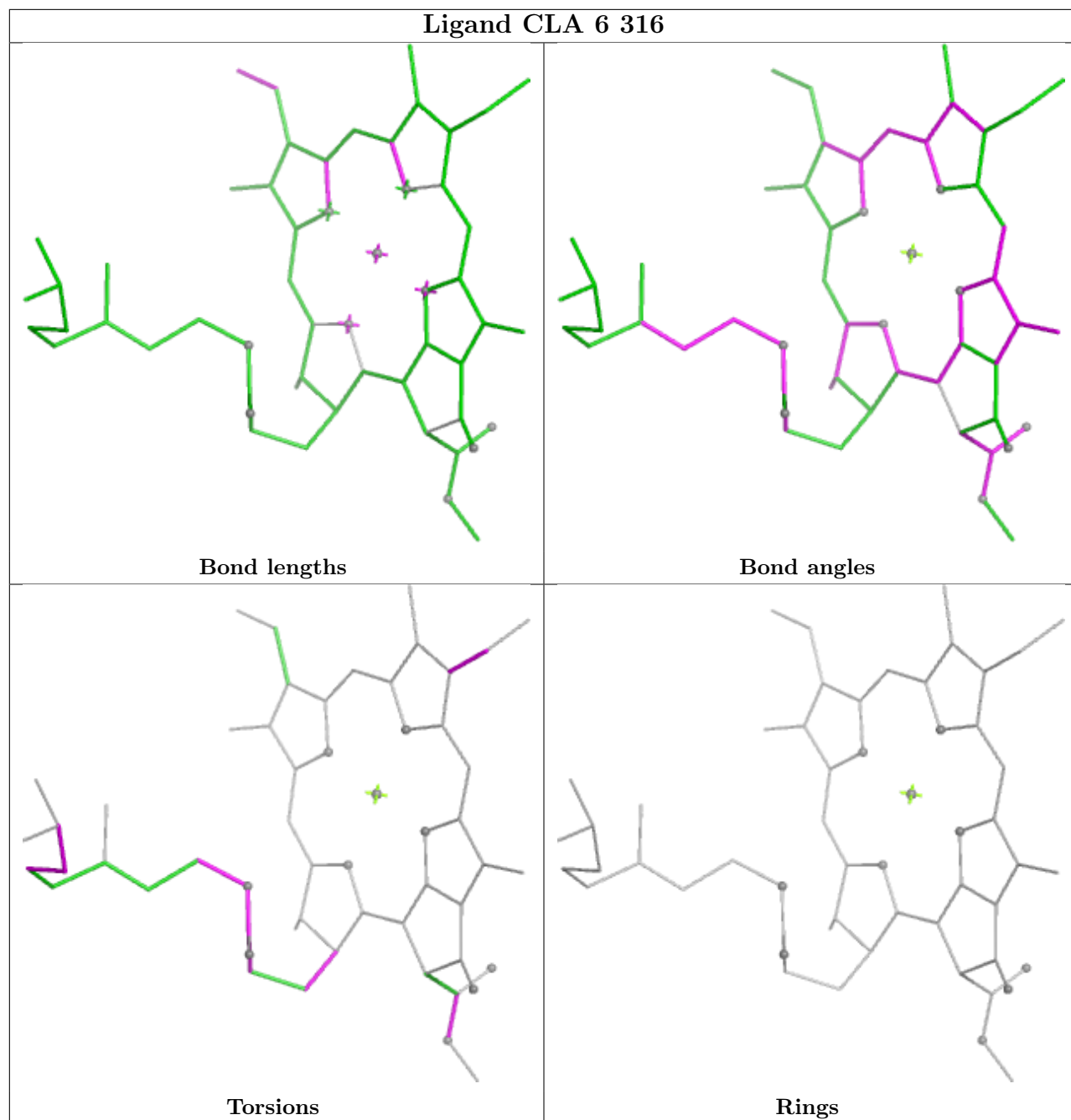
Ligand CLA c 602

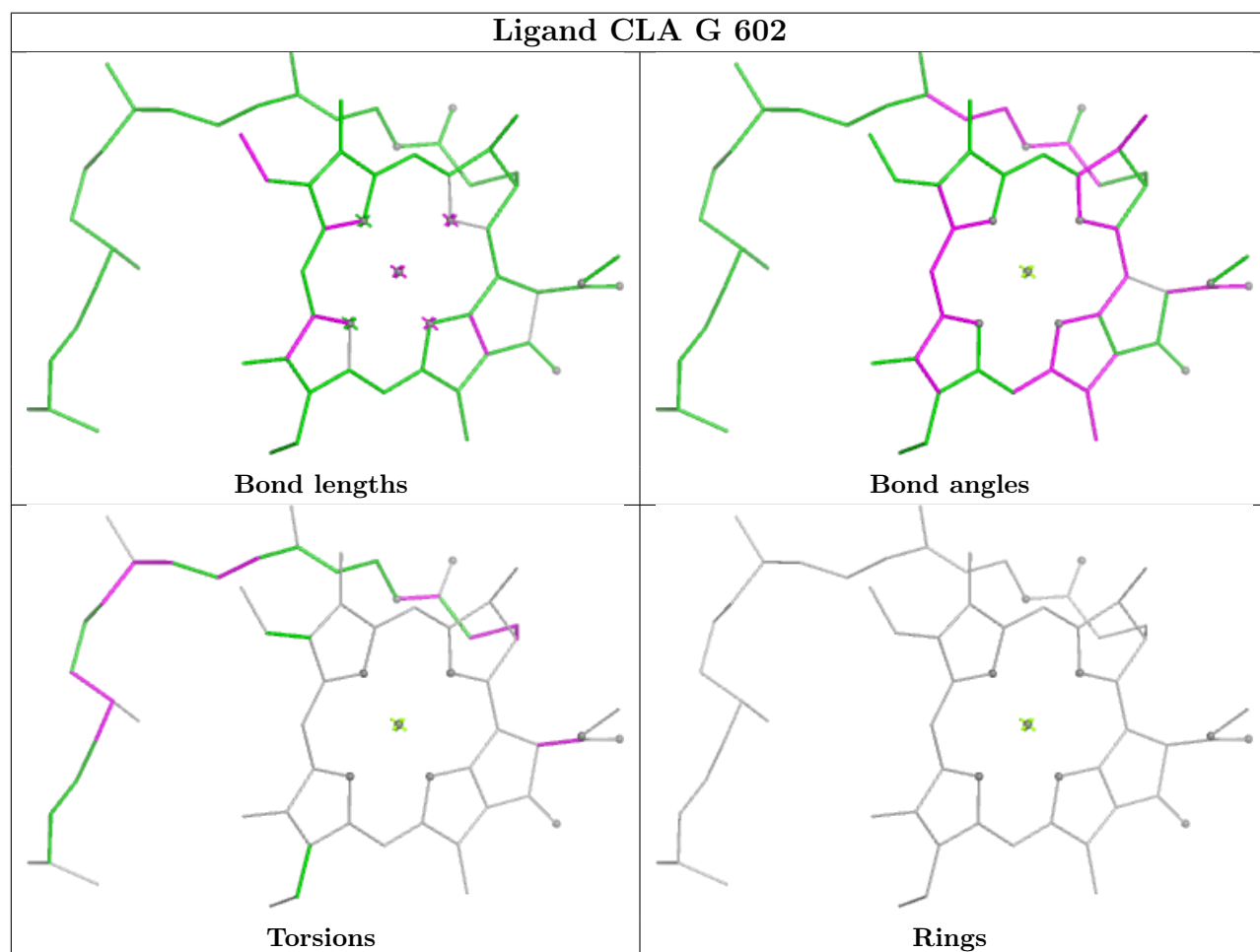
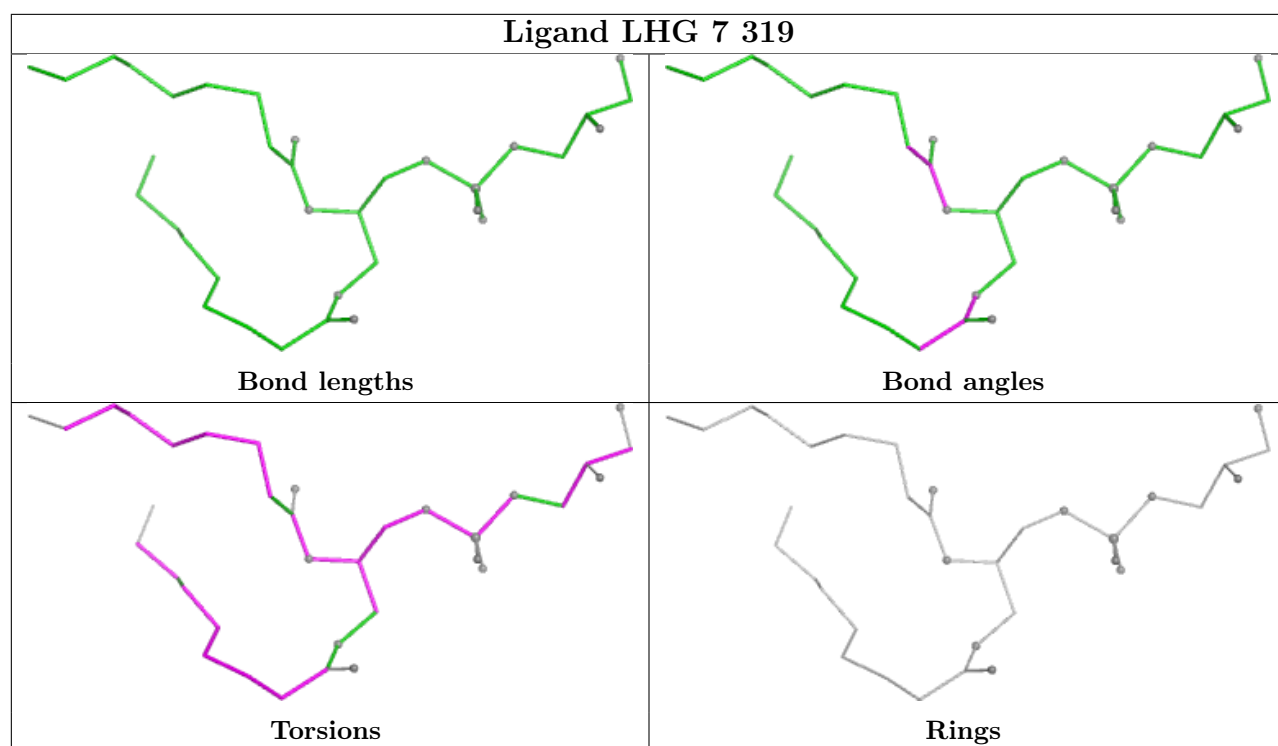


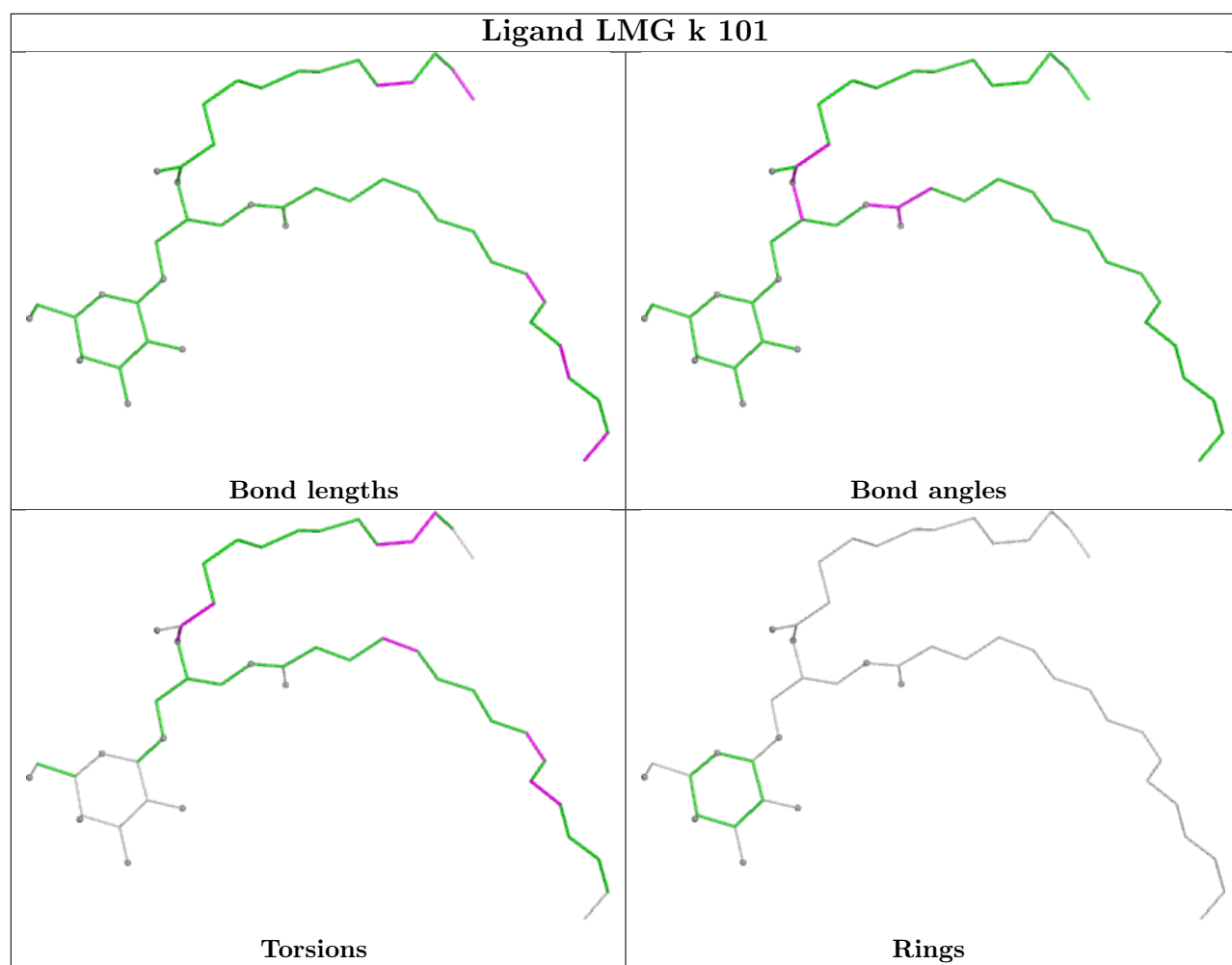


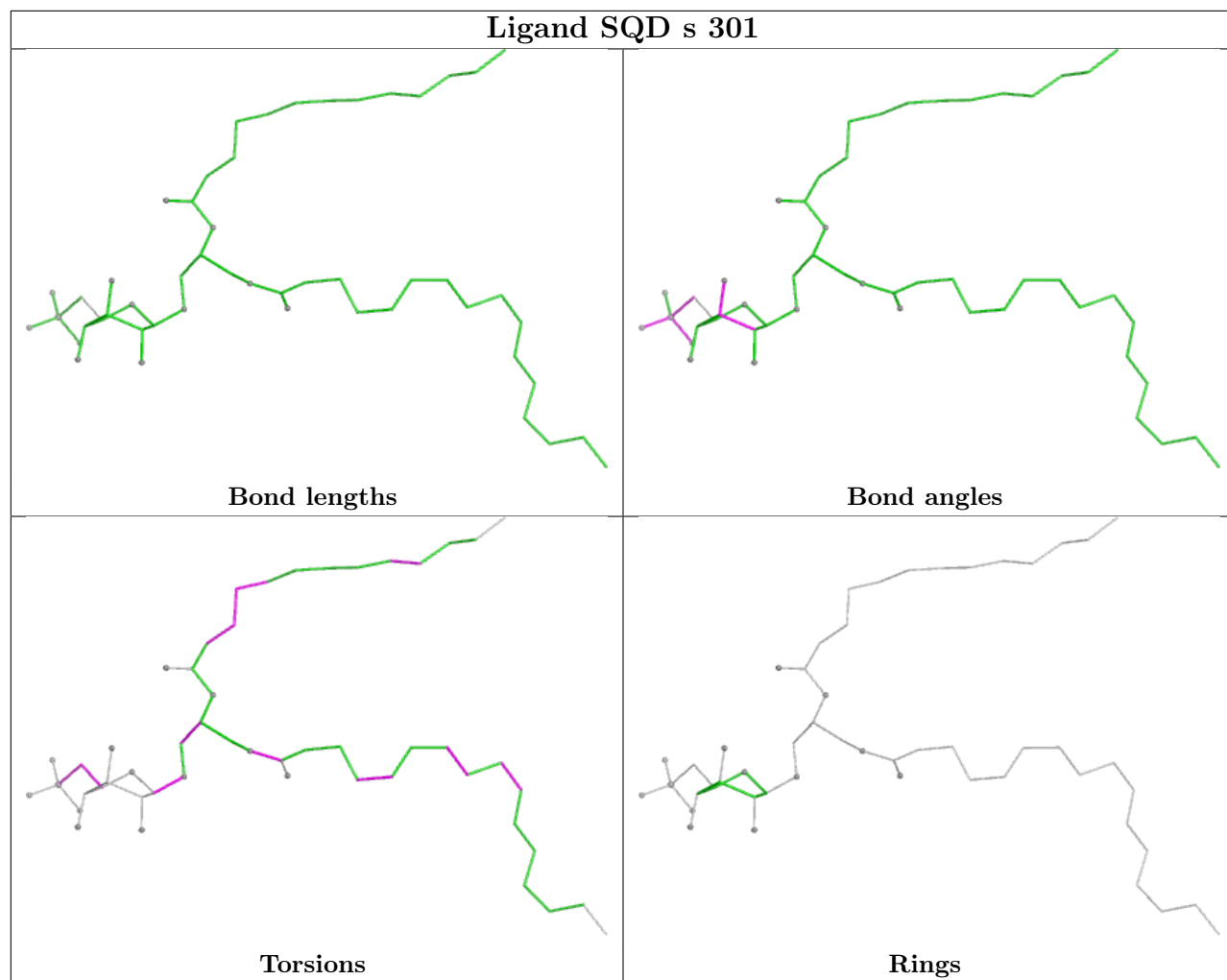


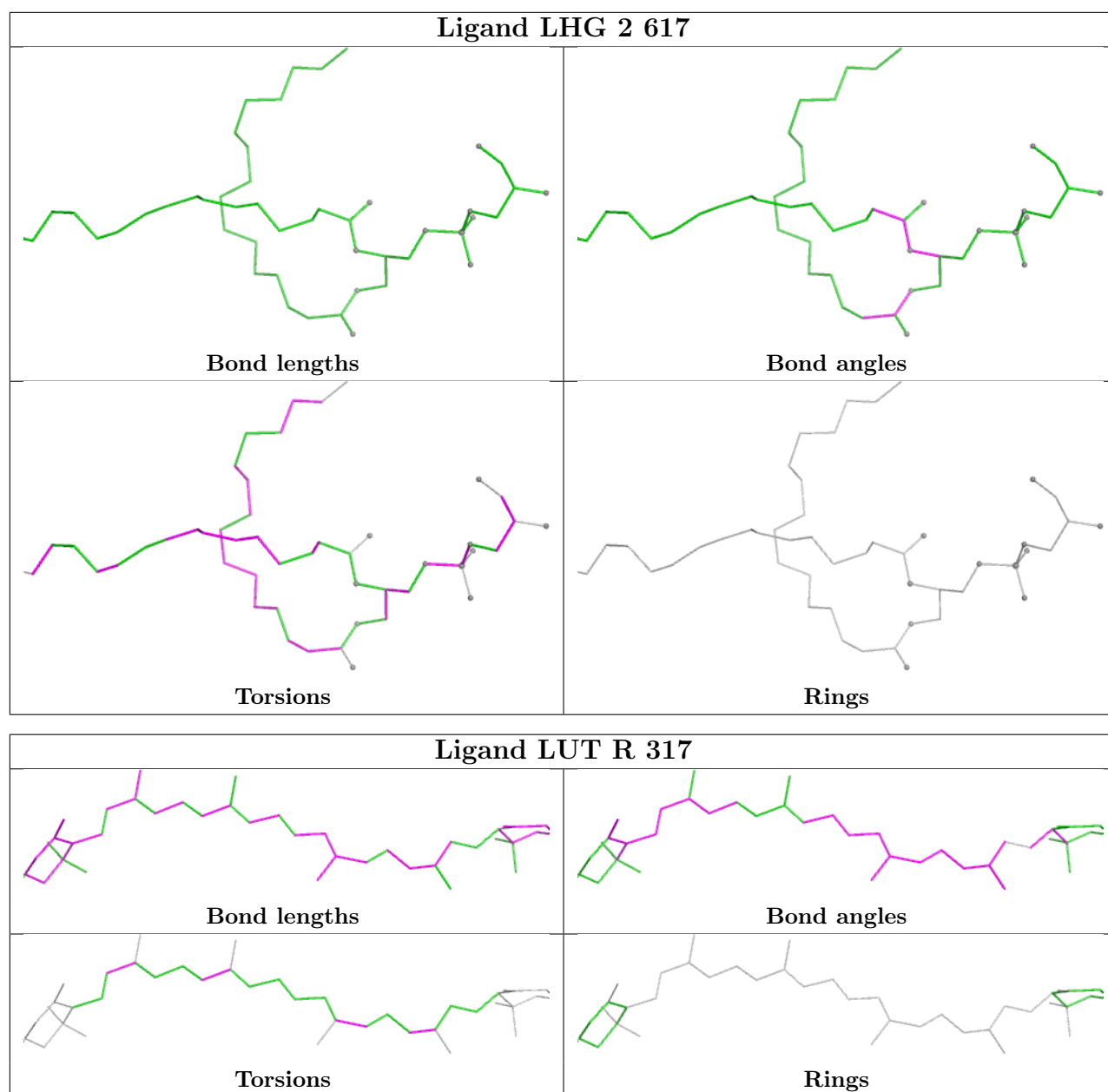
Ligand CLA 6 316

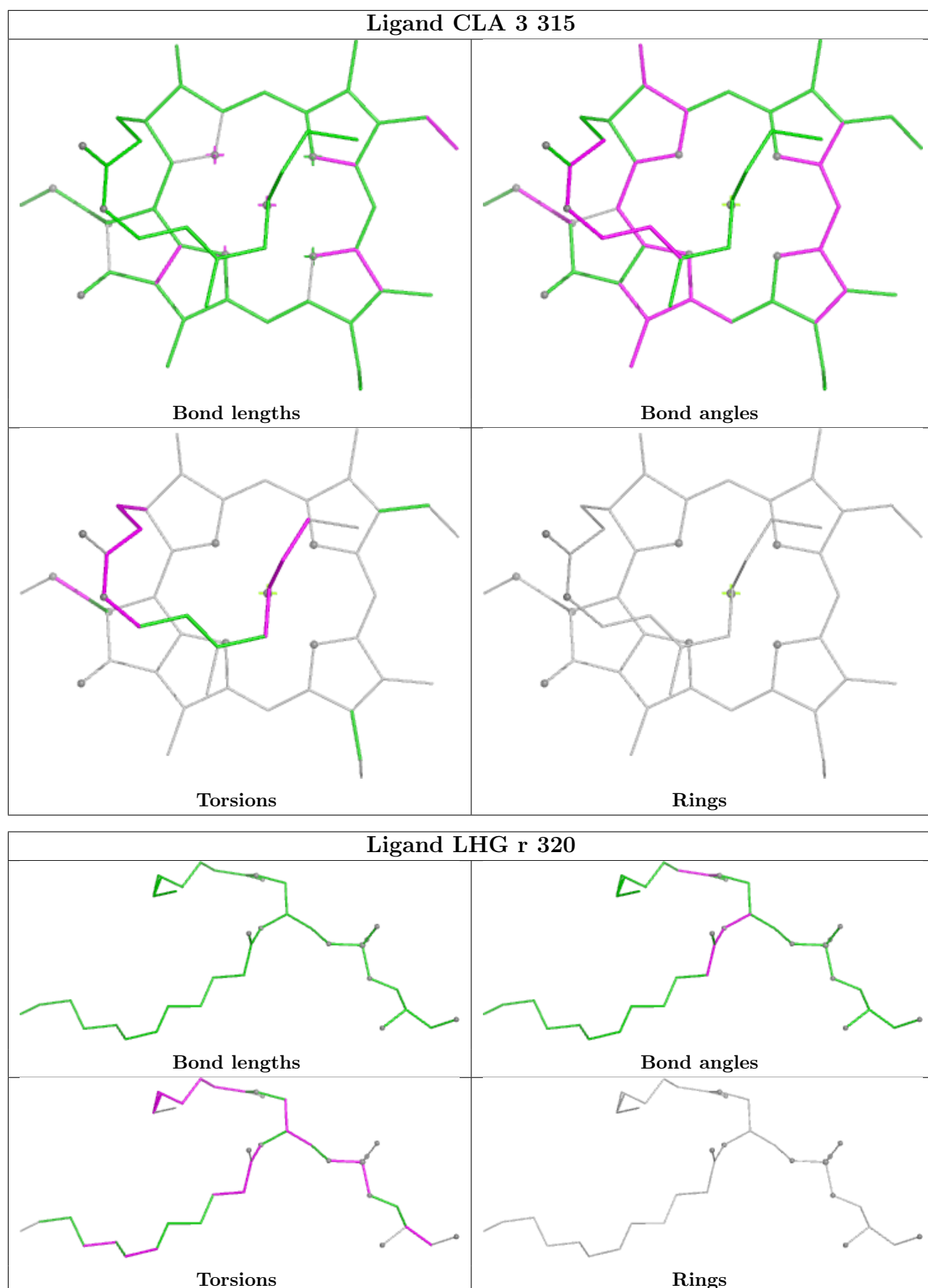




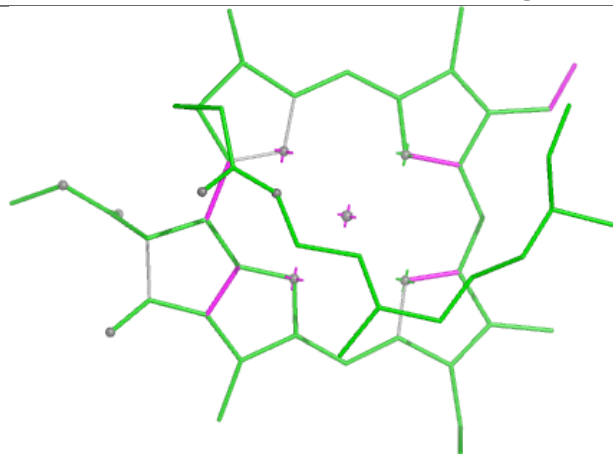




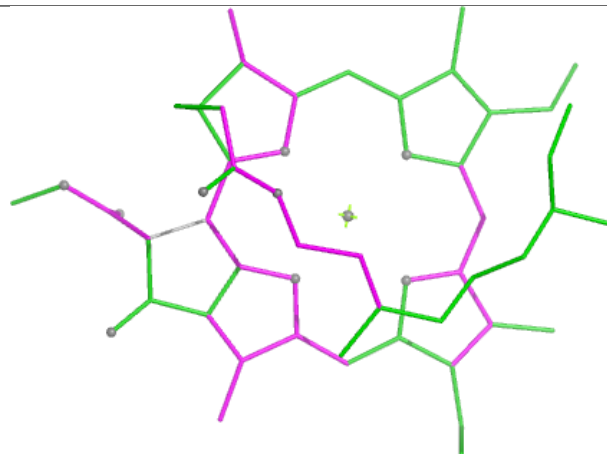




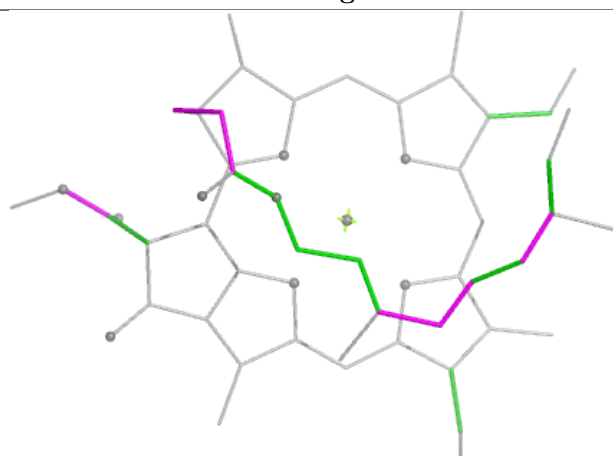
Ligand CLA 0 613



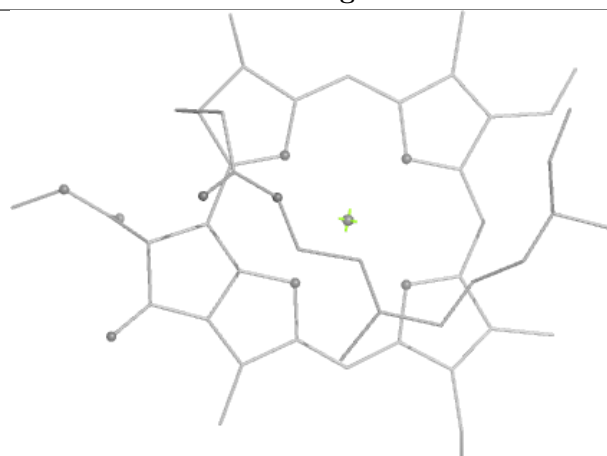
Bond lengths



Bond angles

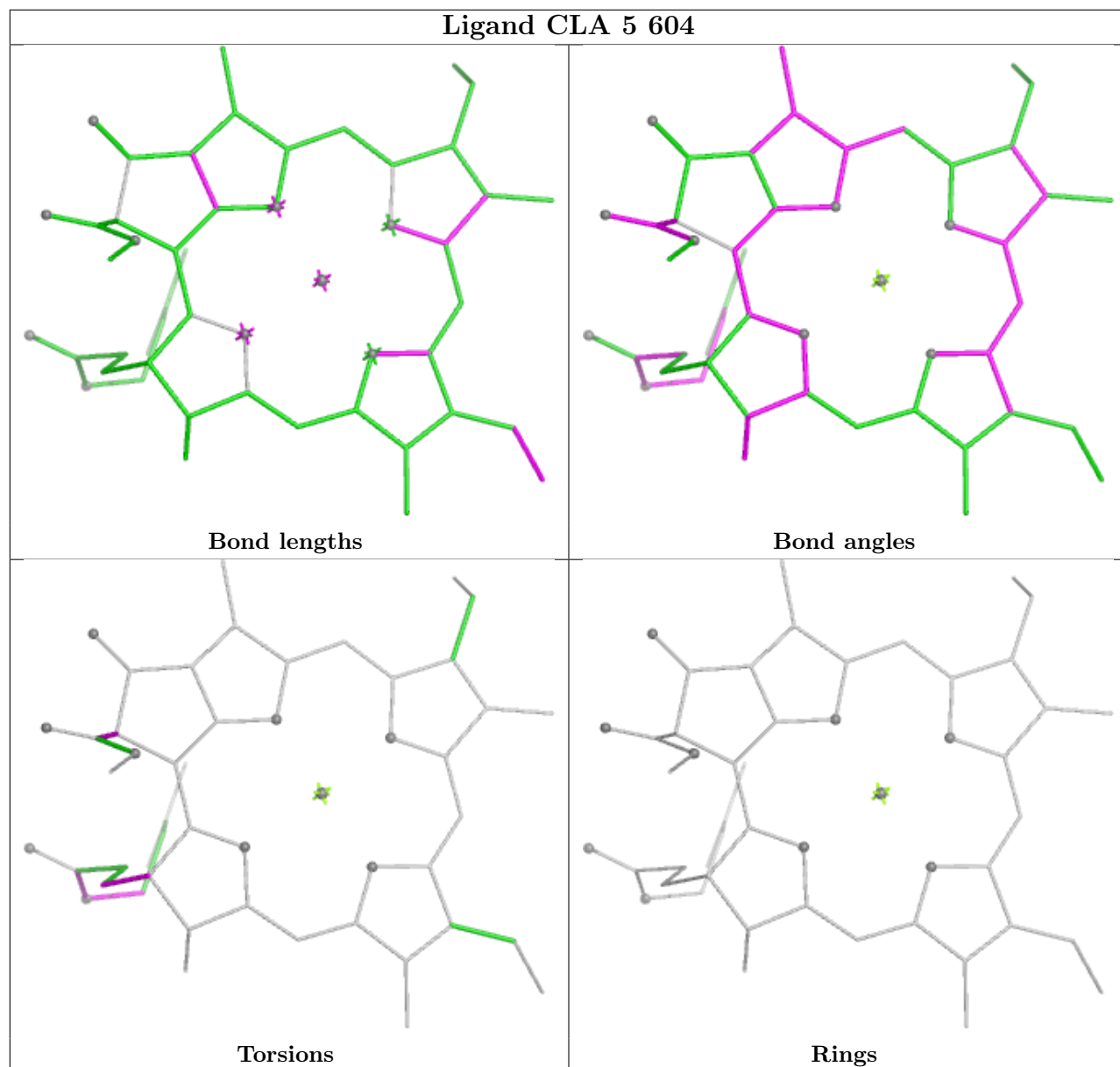


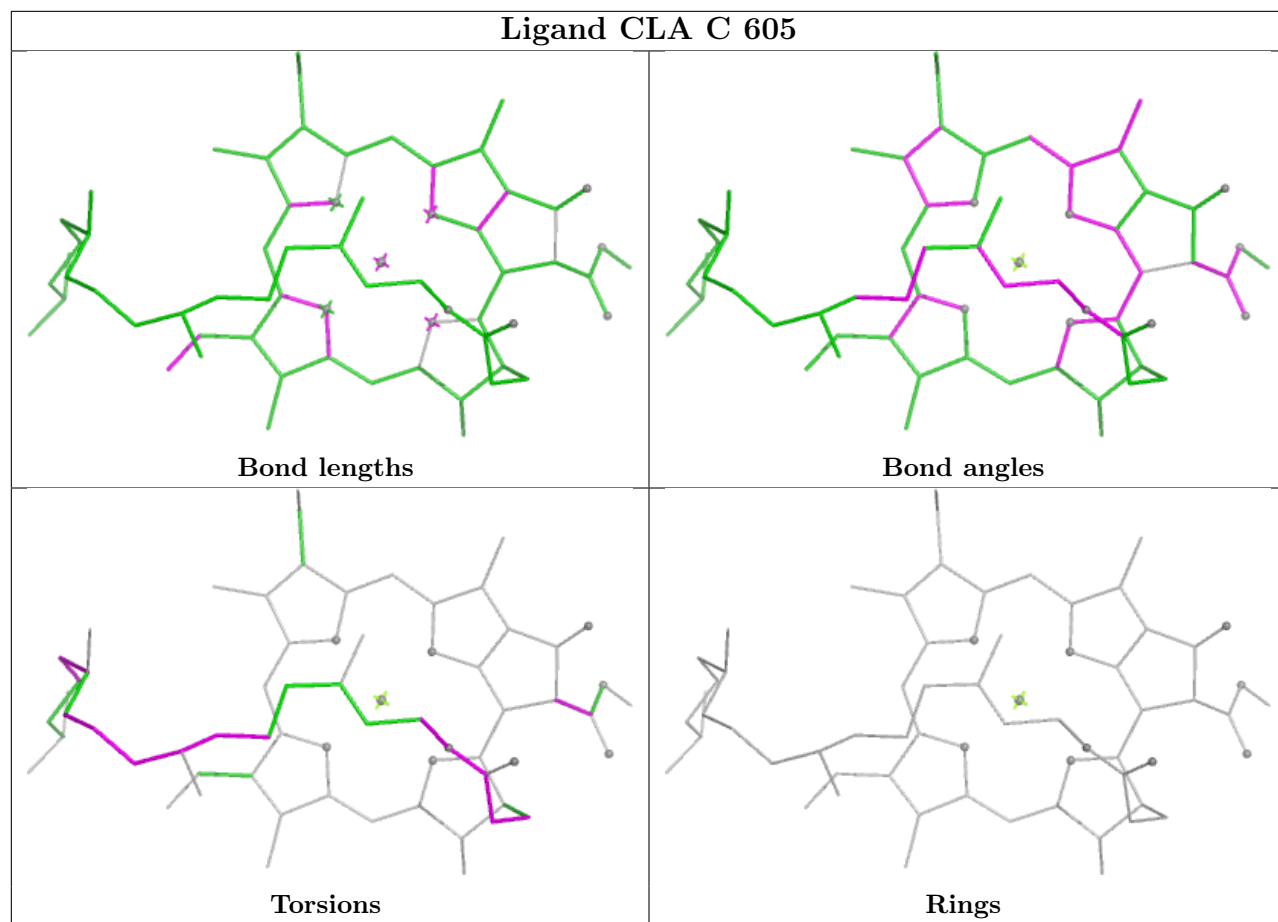
Torsions

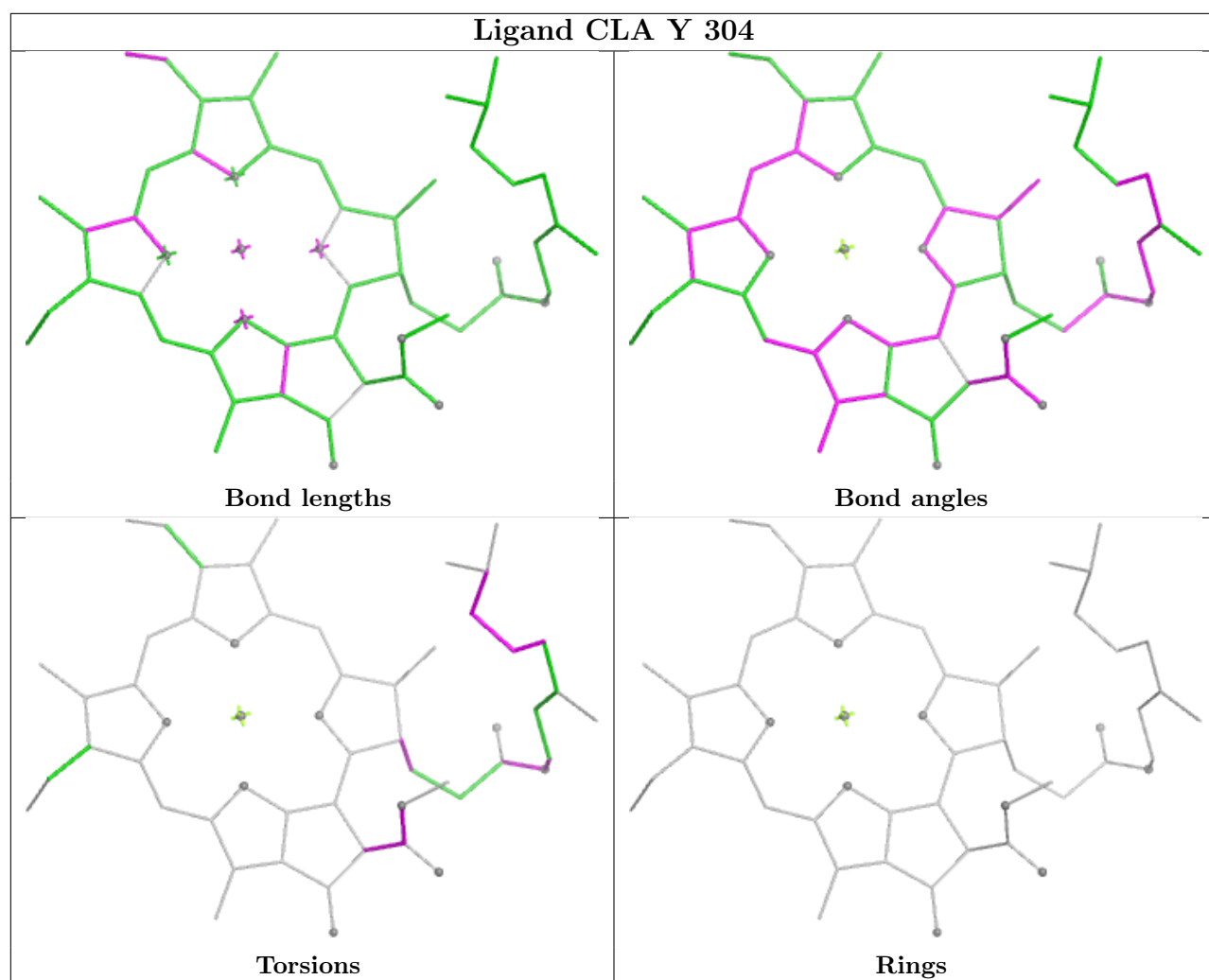


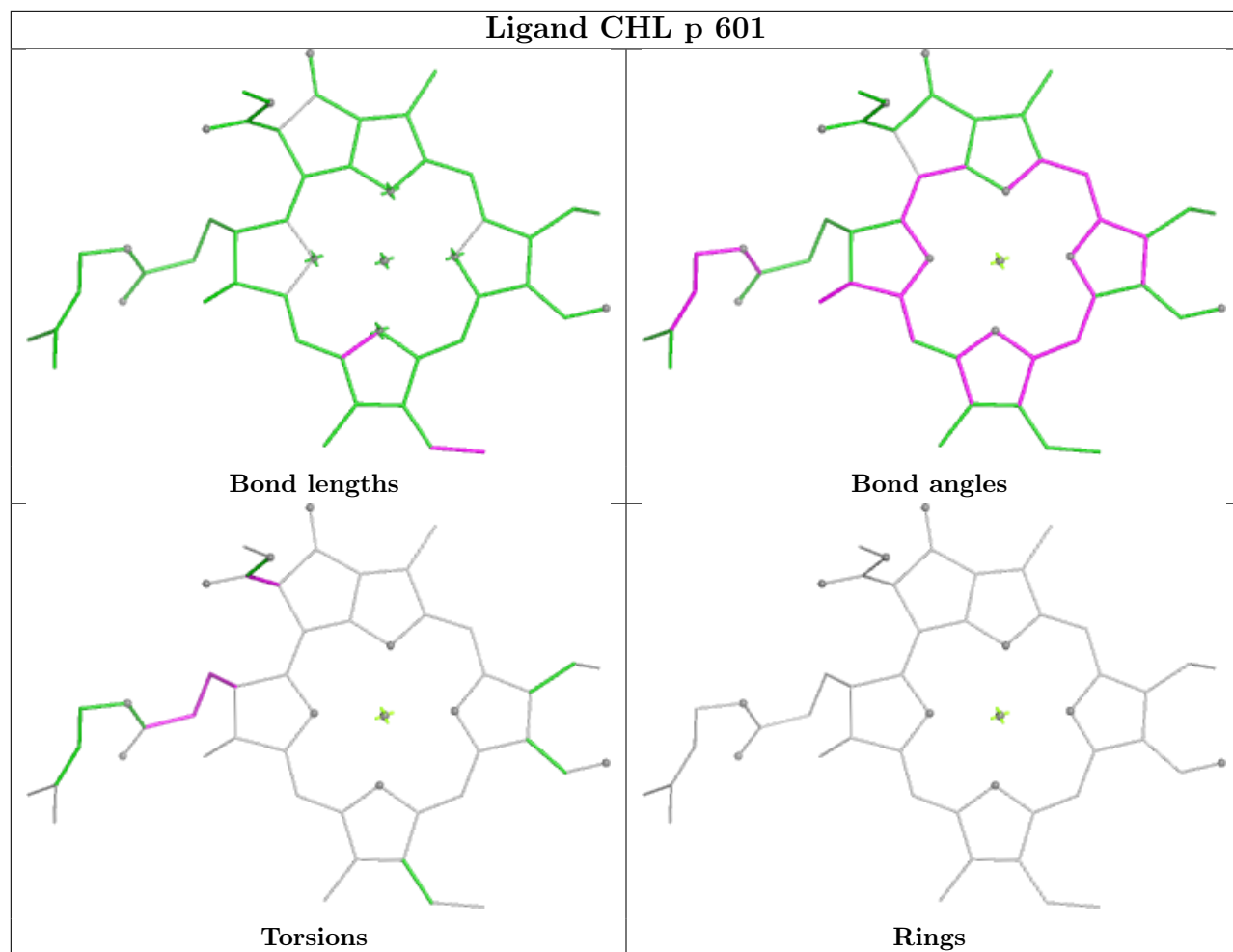
Rings

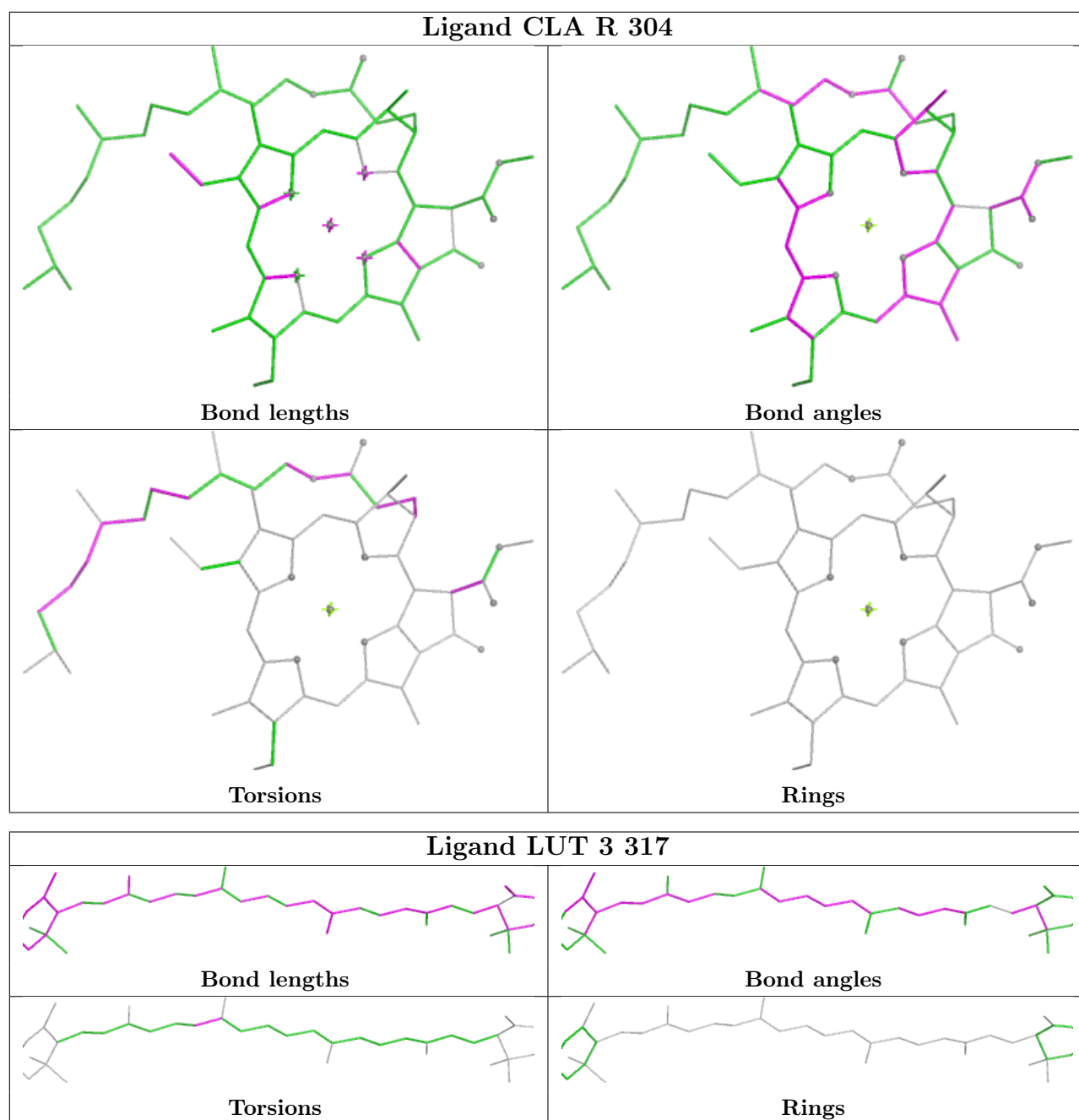
Ligand CLA 5 604

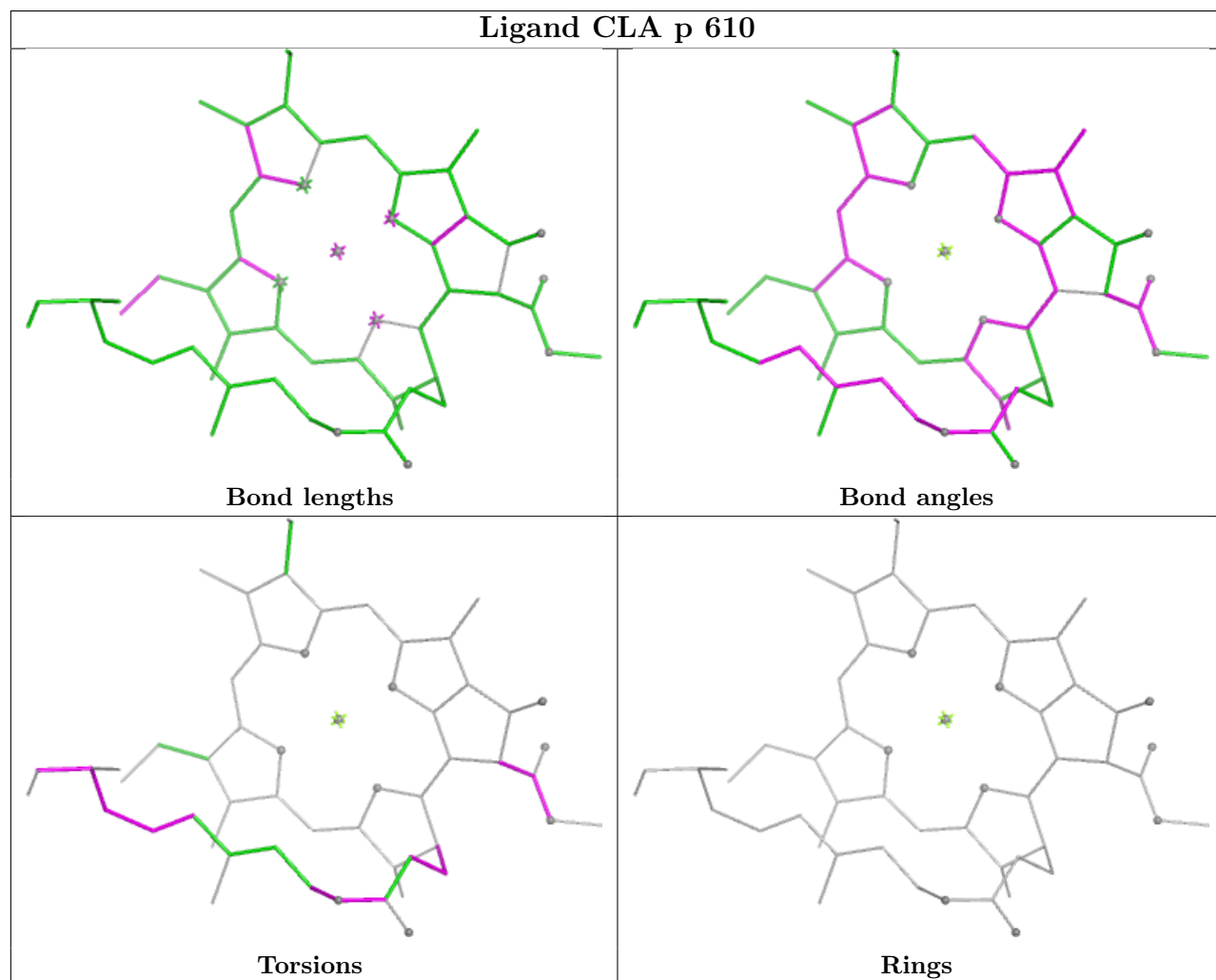
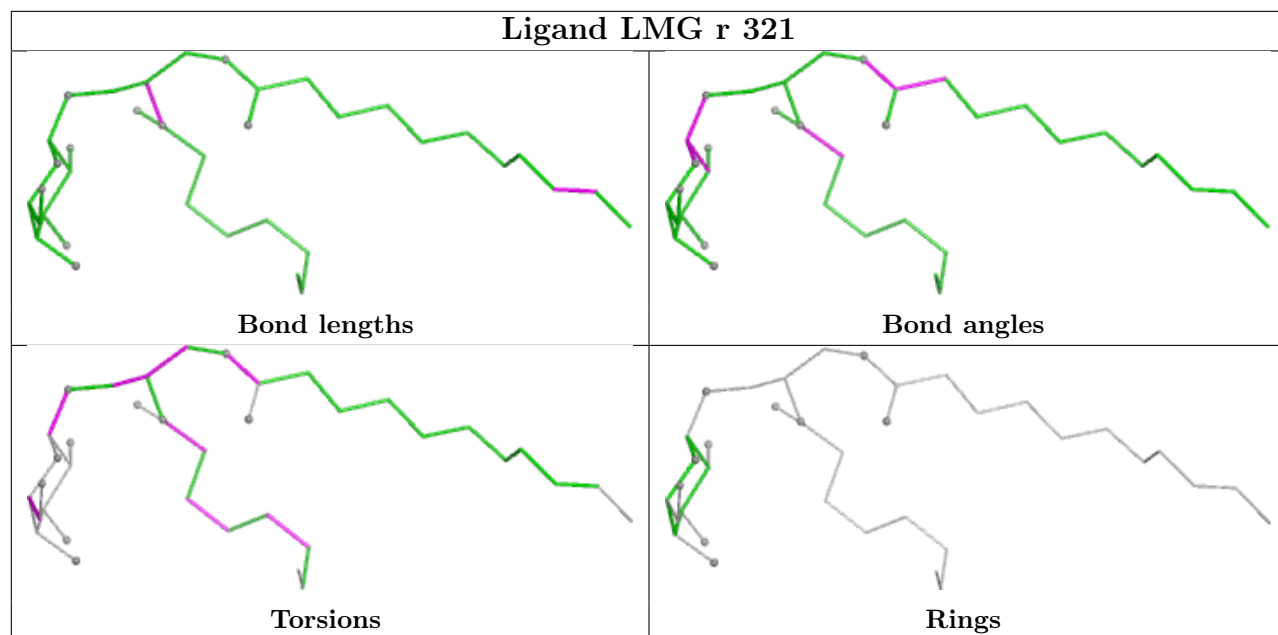


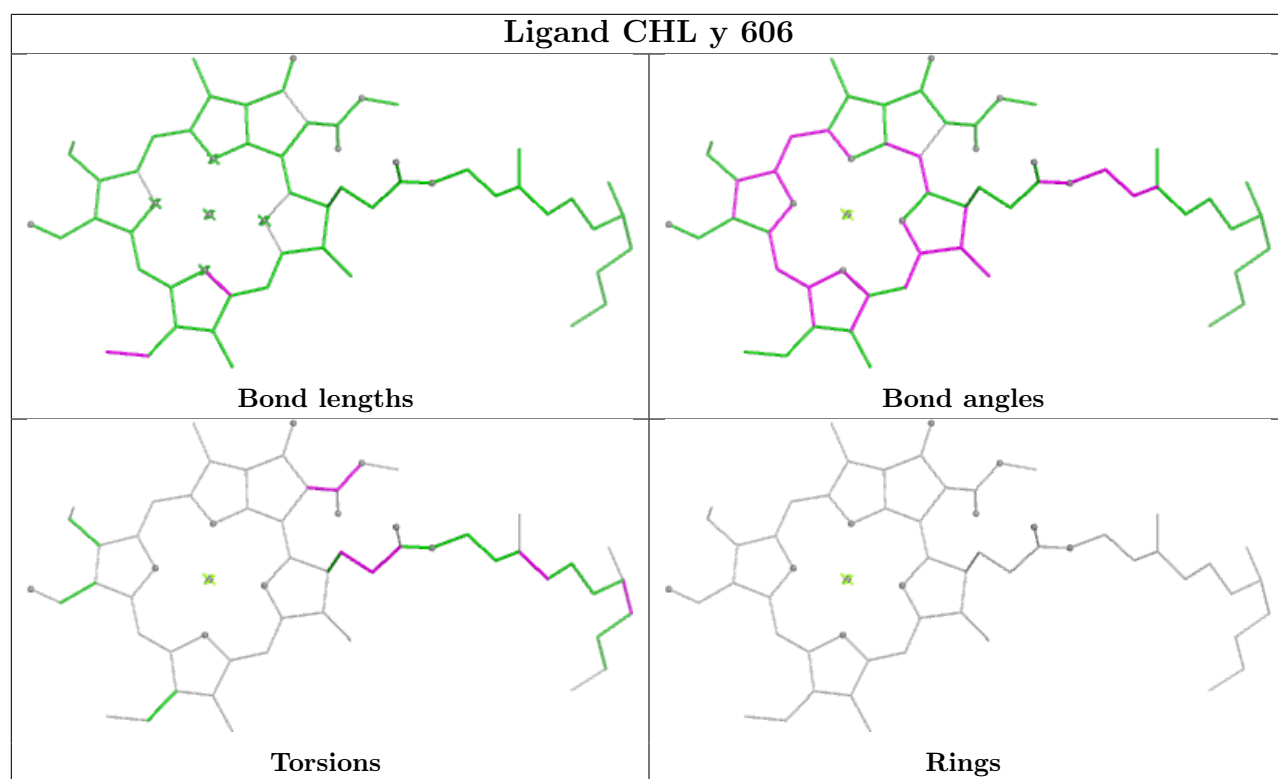


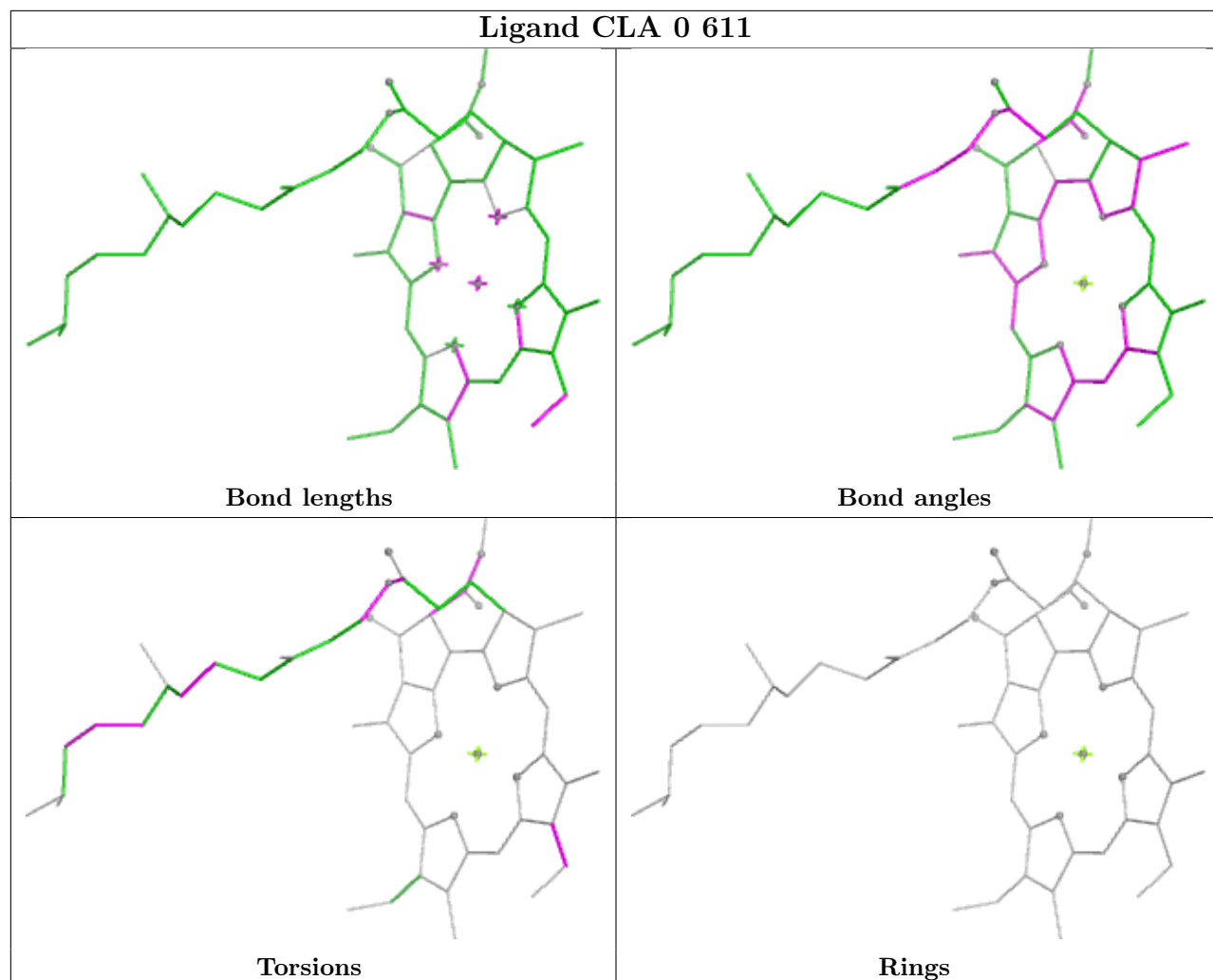


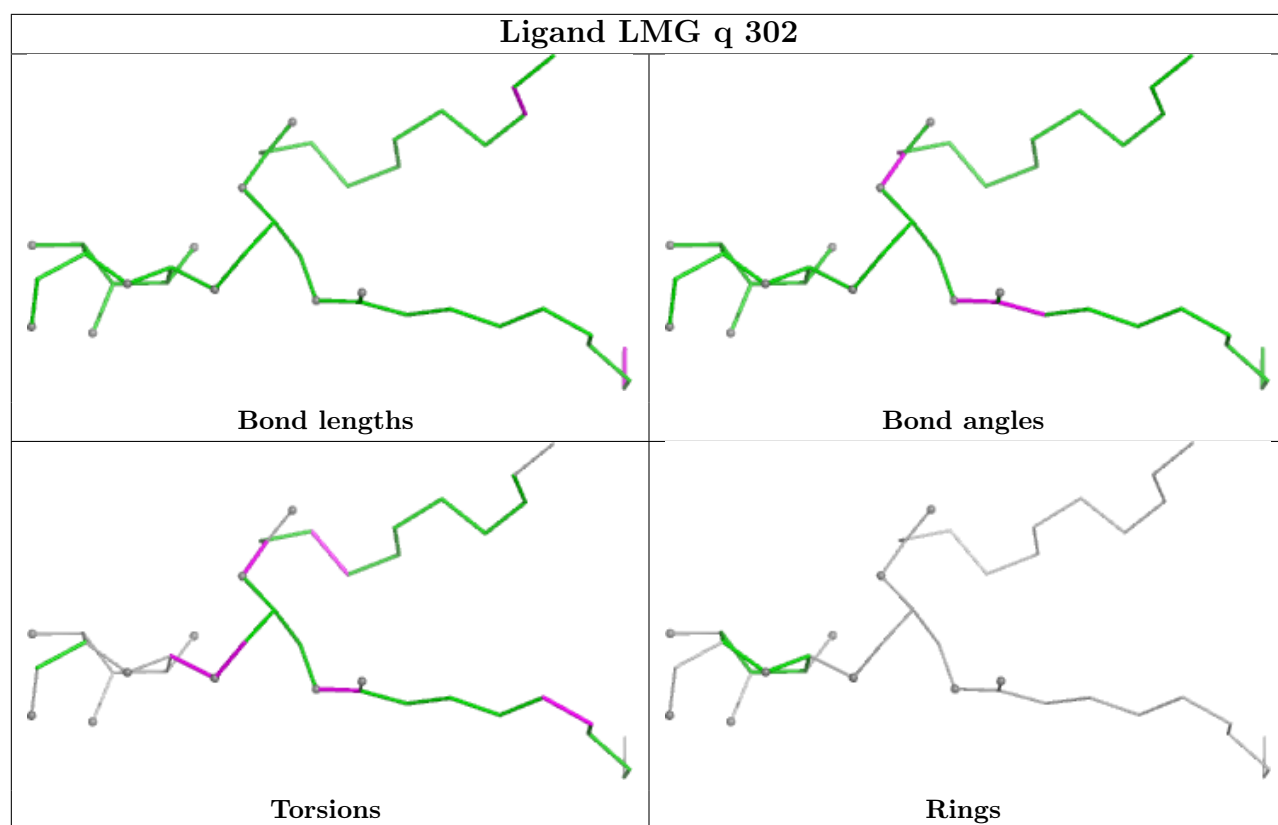


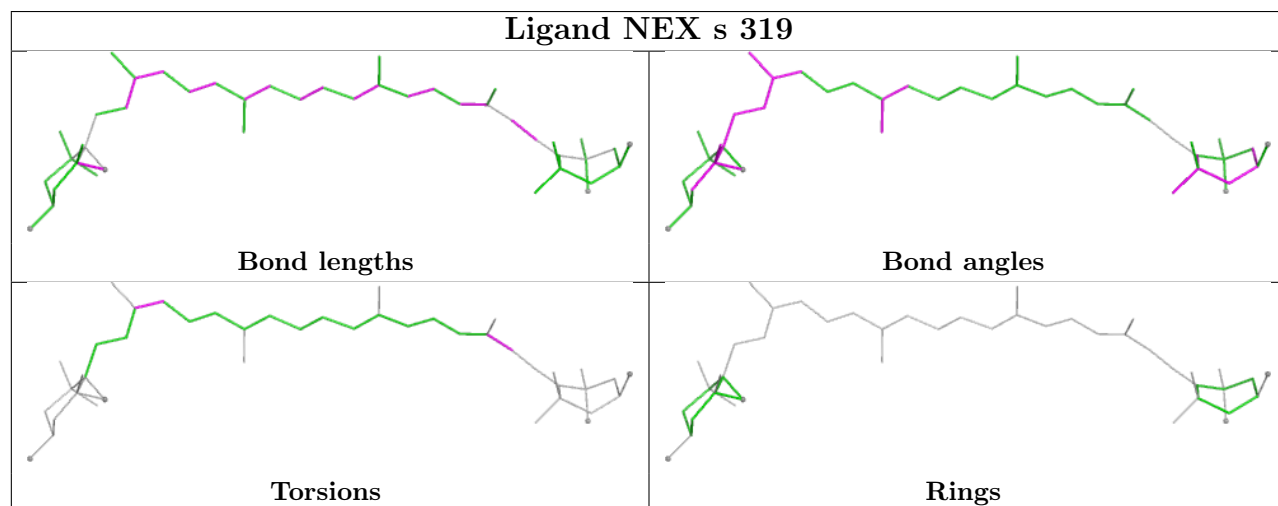
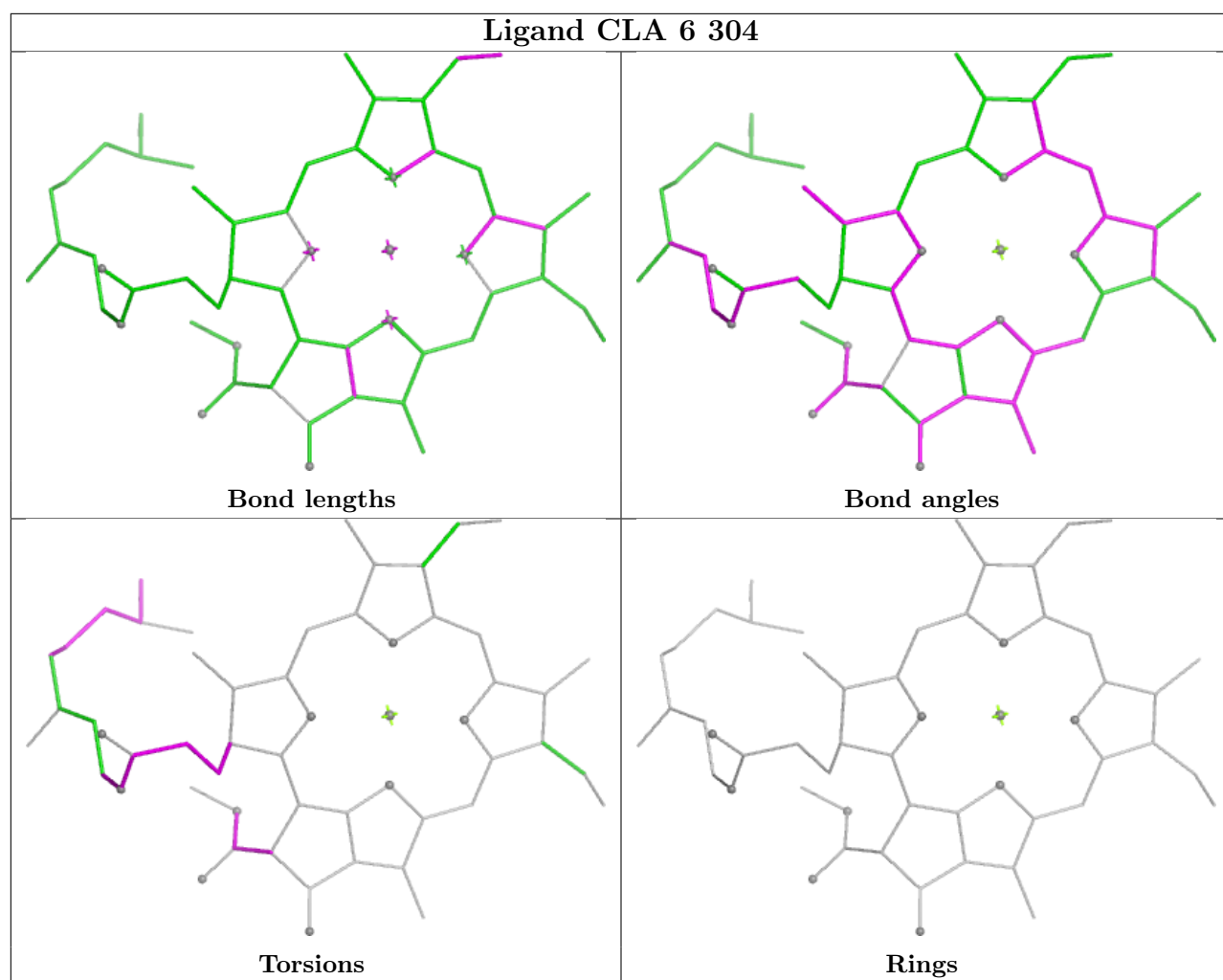


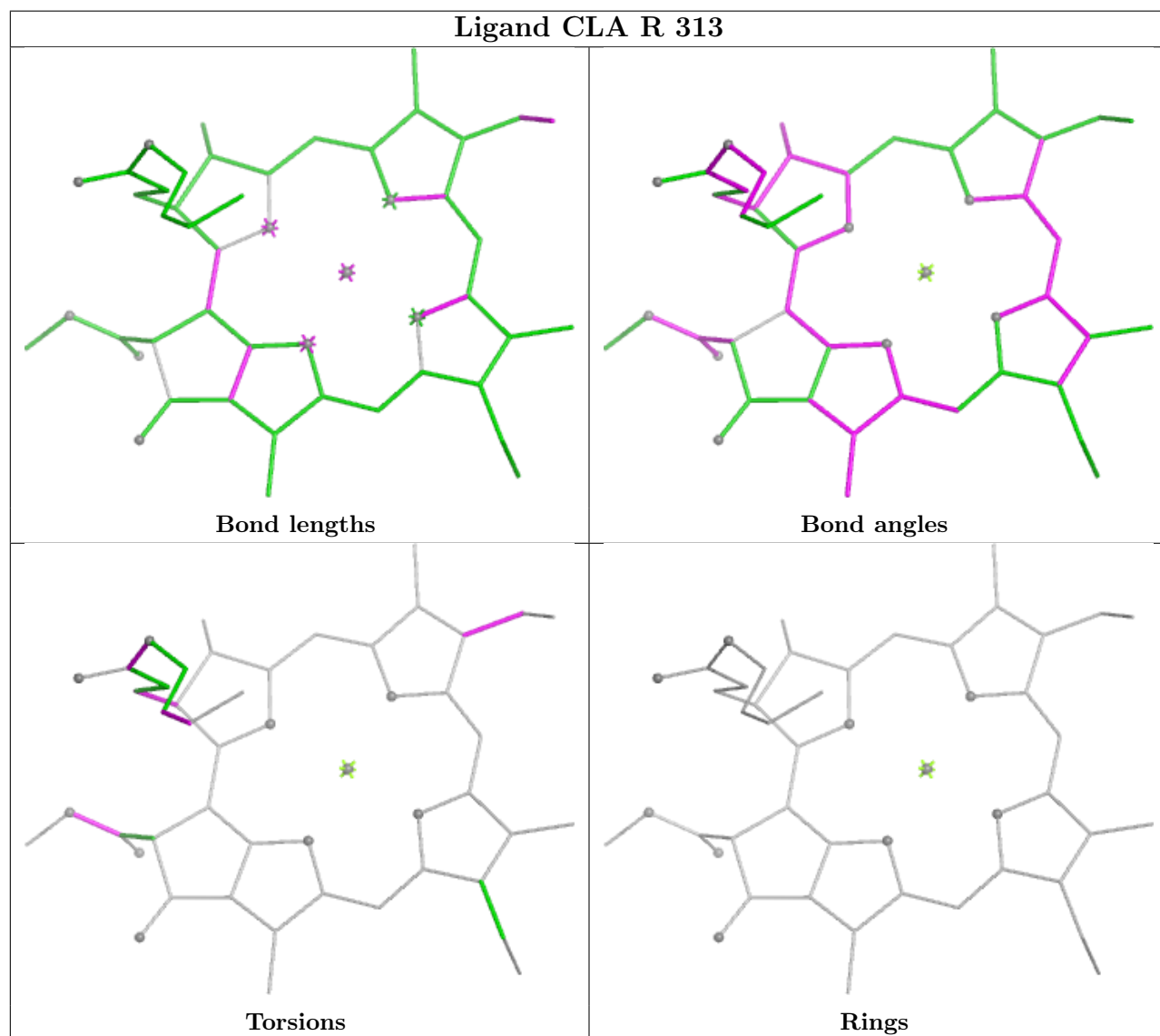
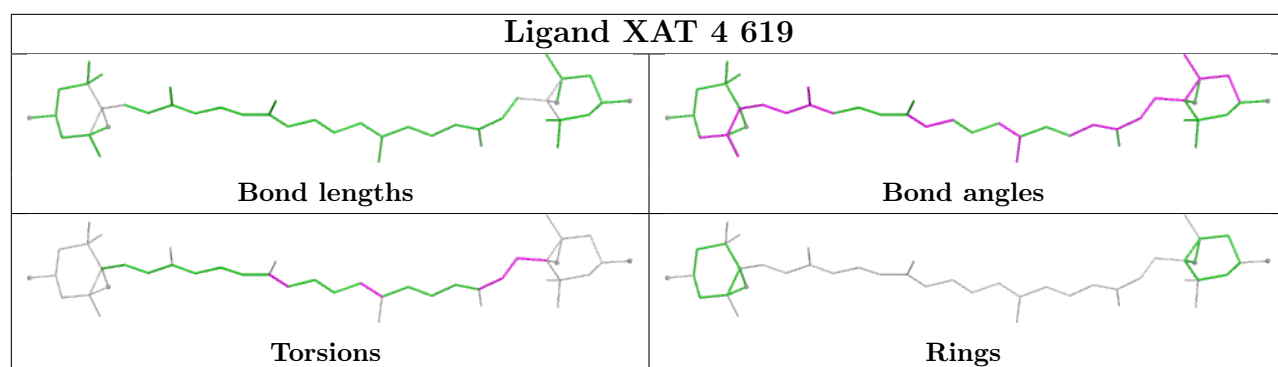




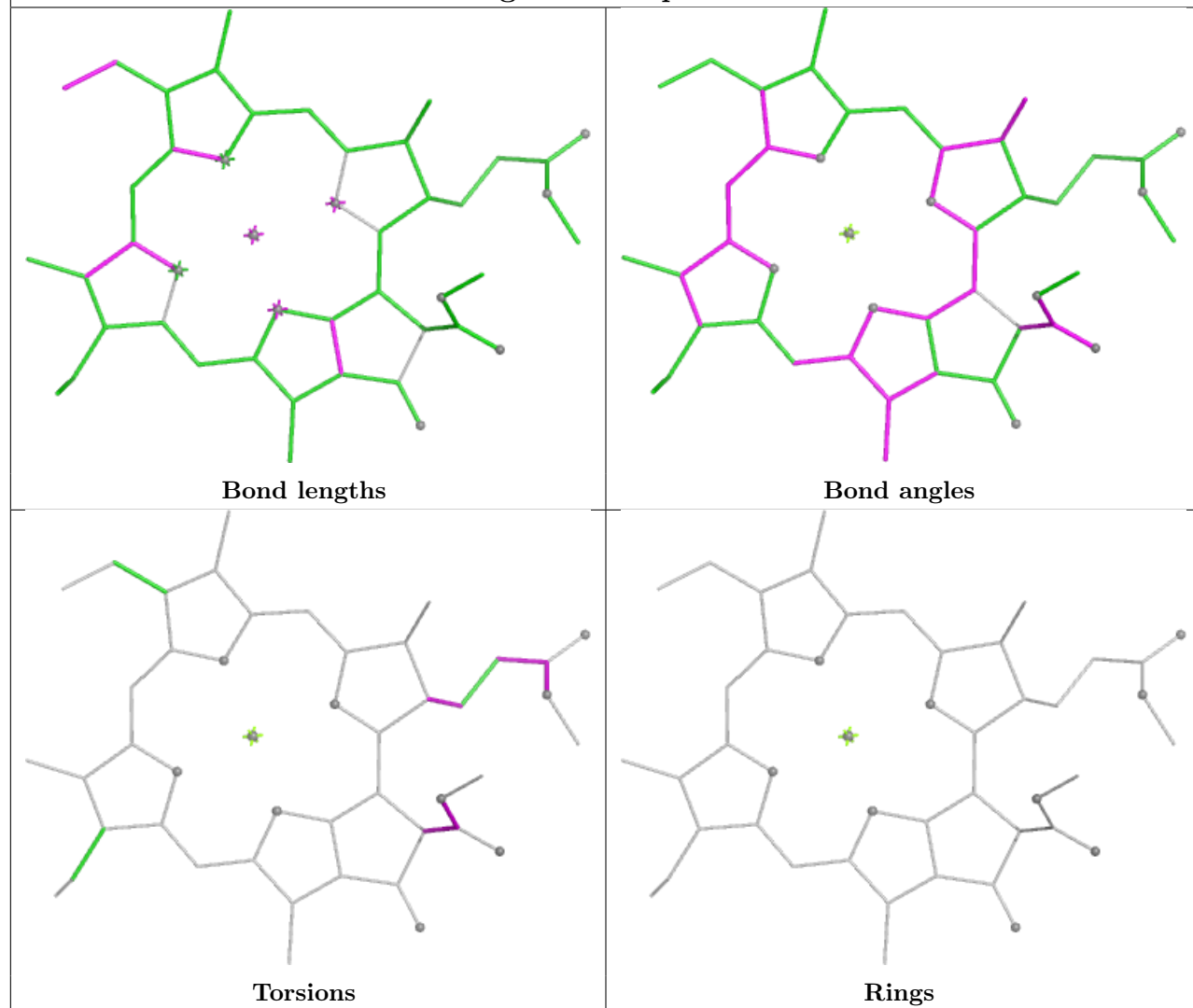
Ligand CLA 0 611



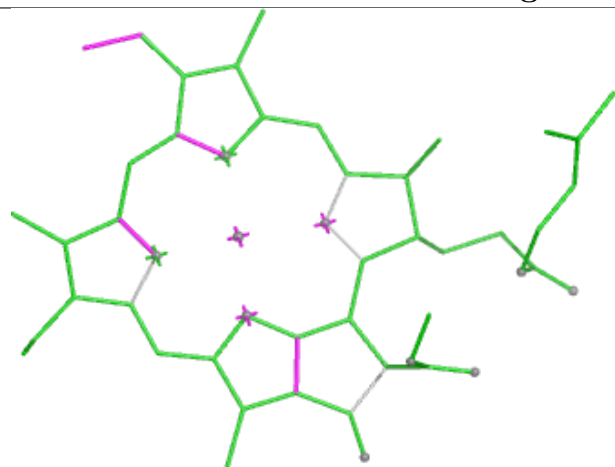




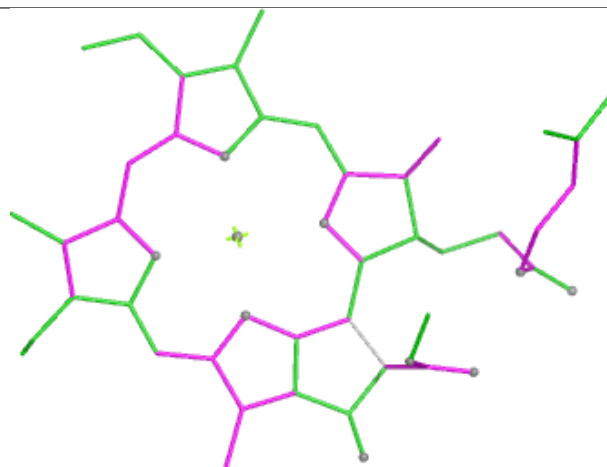
Ligand CLA p 612



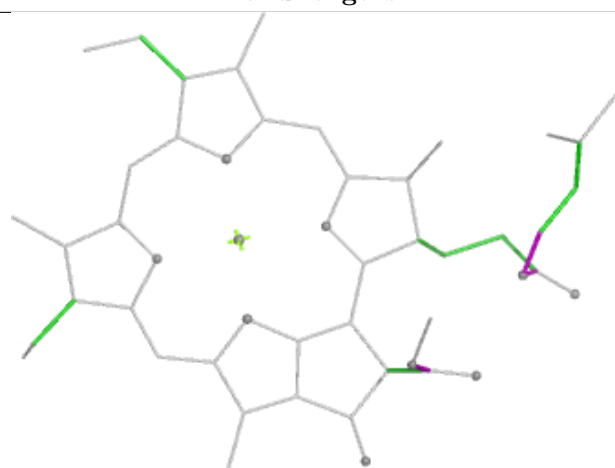
Ligand CLA 9 314



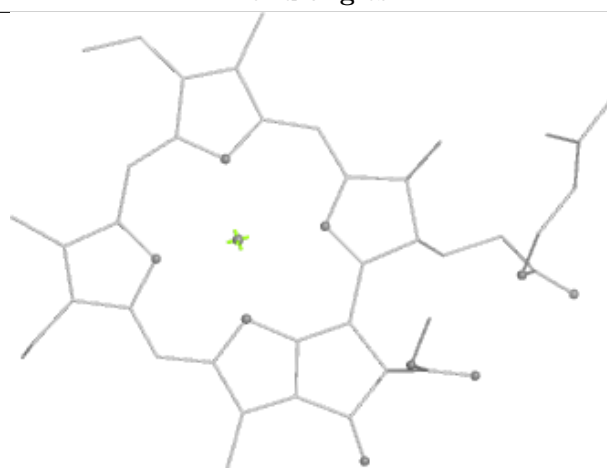
Bond lengths



Bond angles

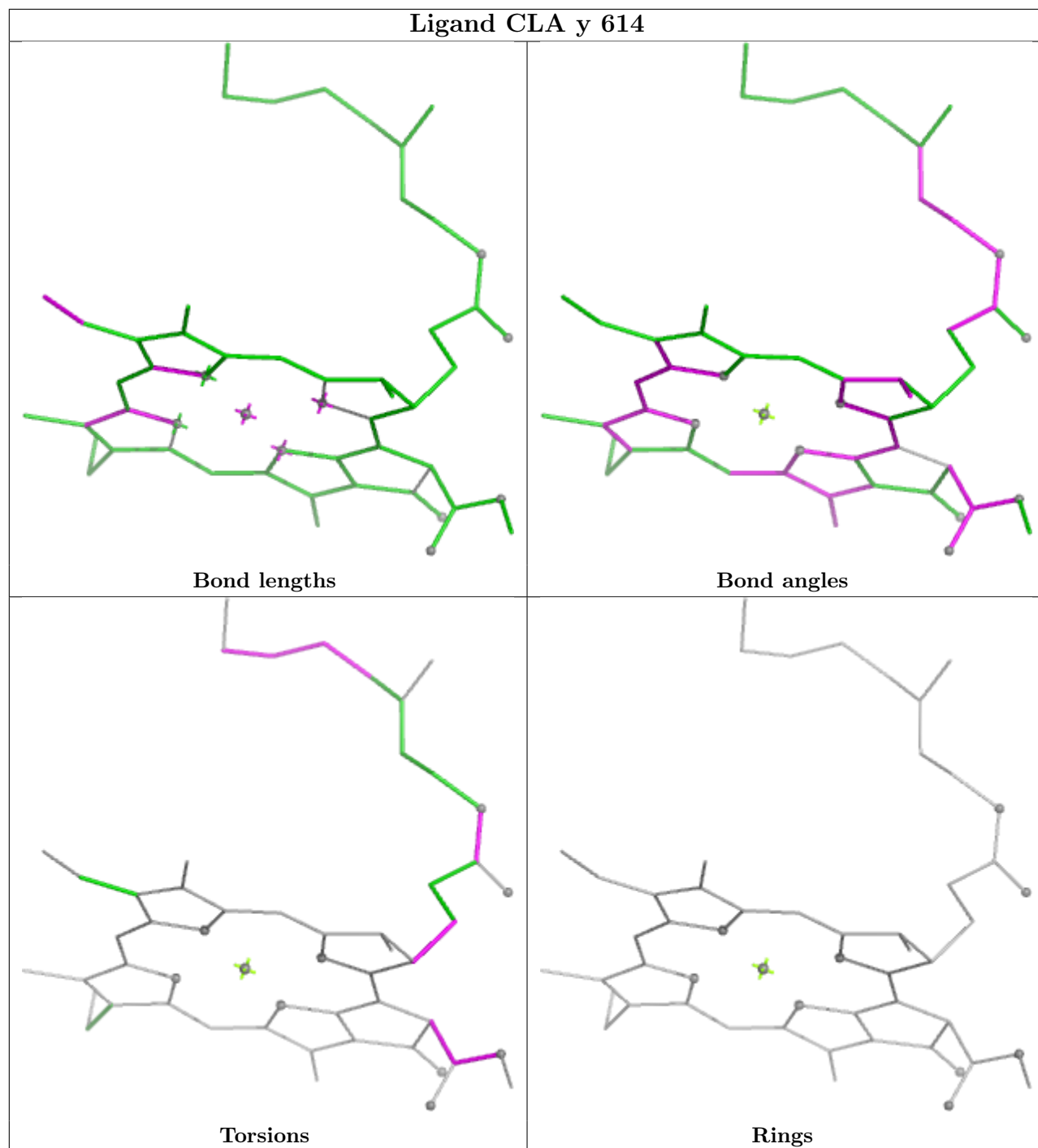


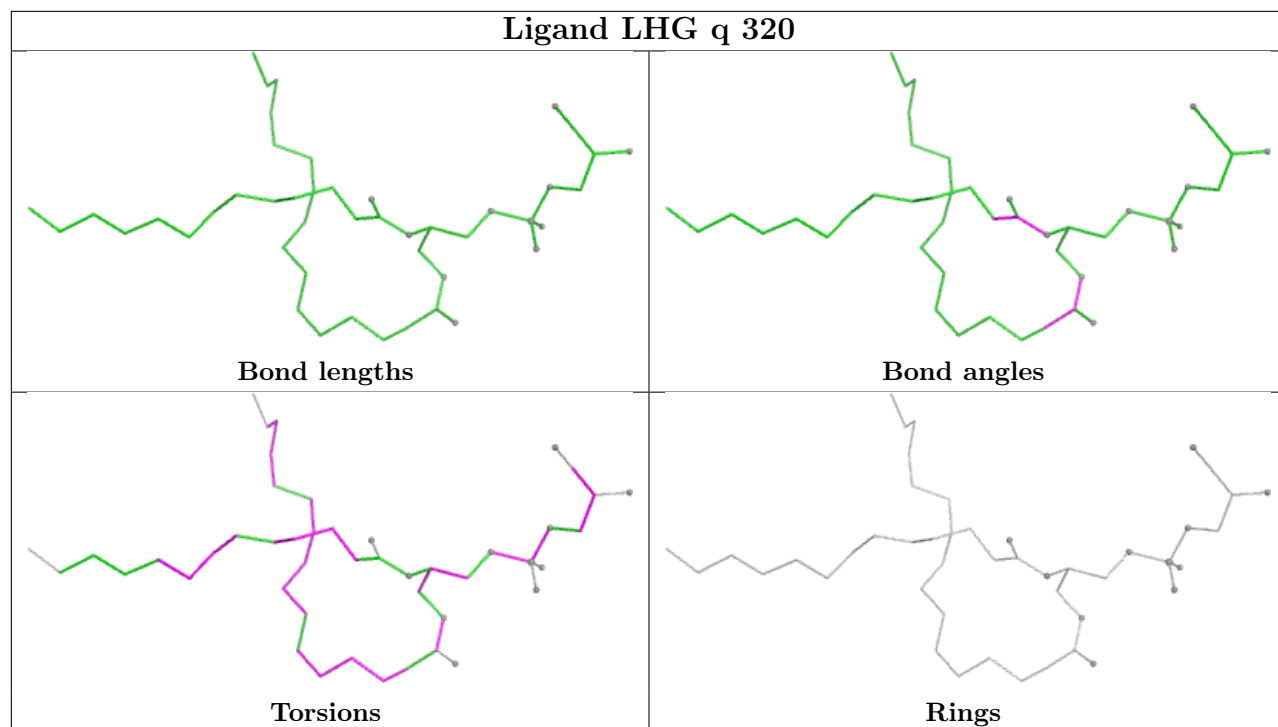
Torsions



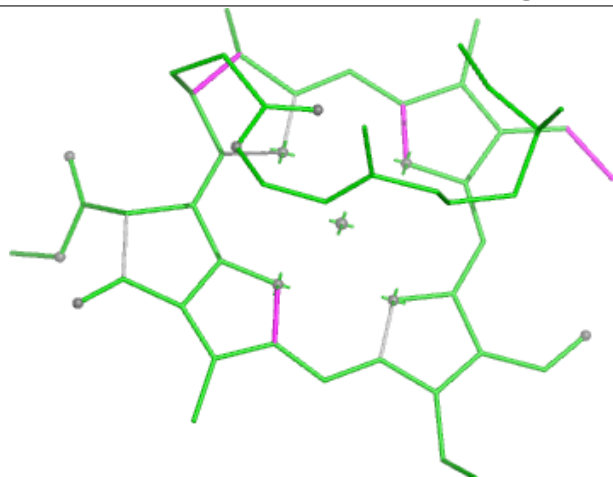
Rings

Ligand CLA y 614

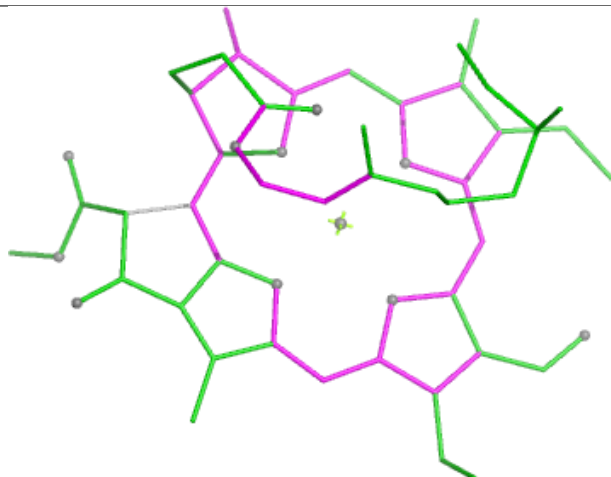




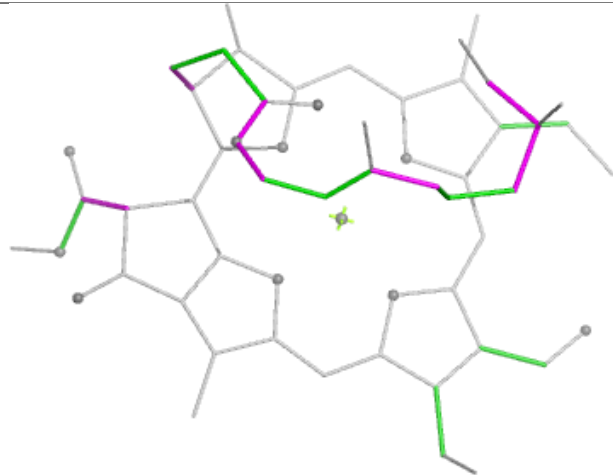
Ligand CHL 3 302



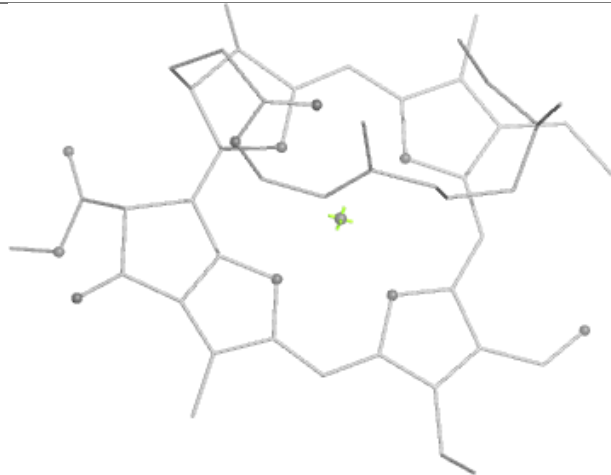
Bond lengths



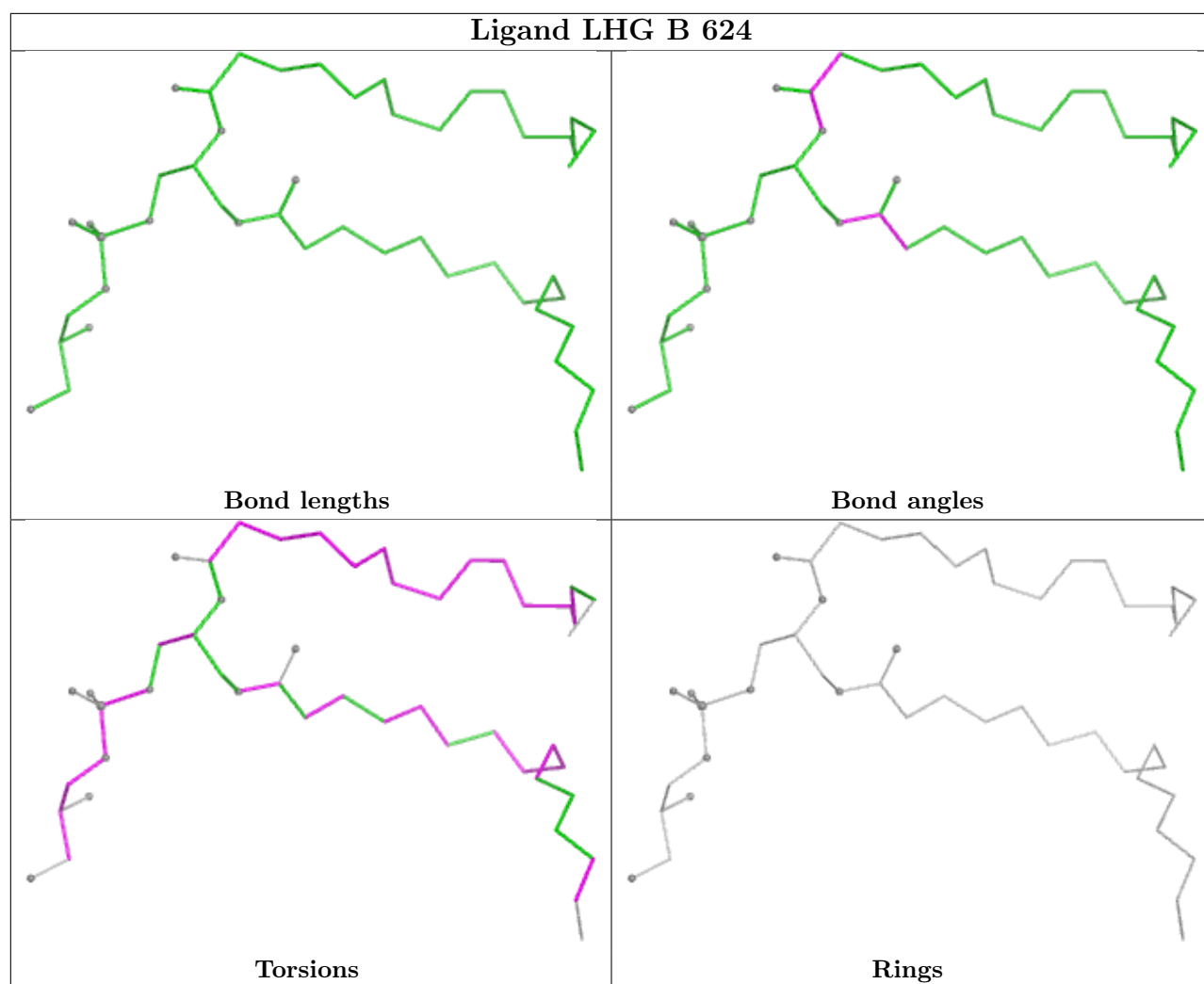
Bond angles

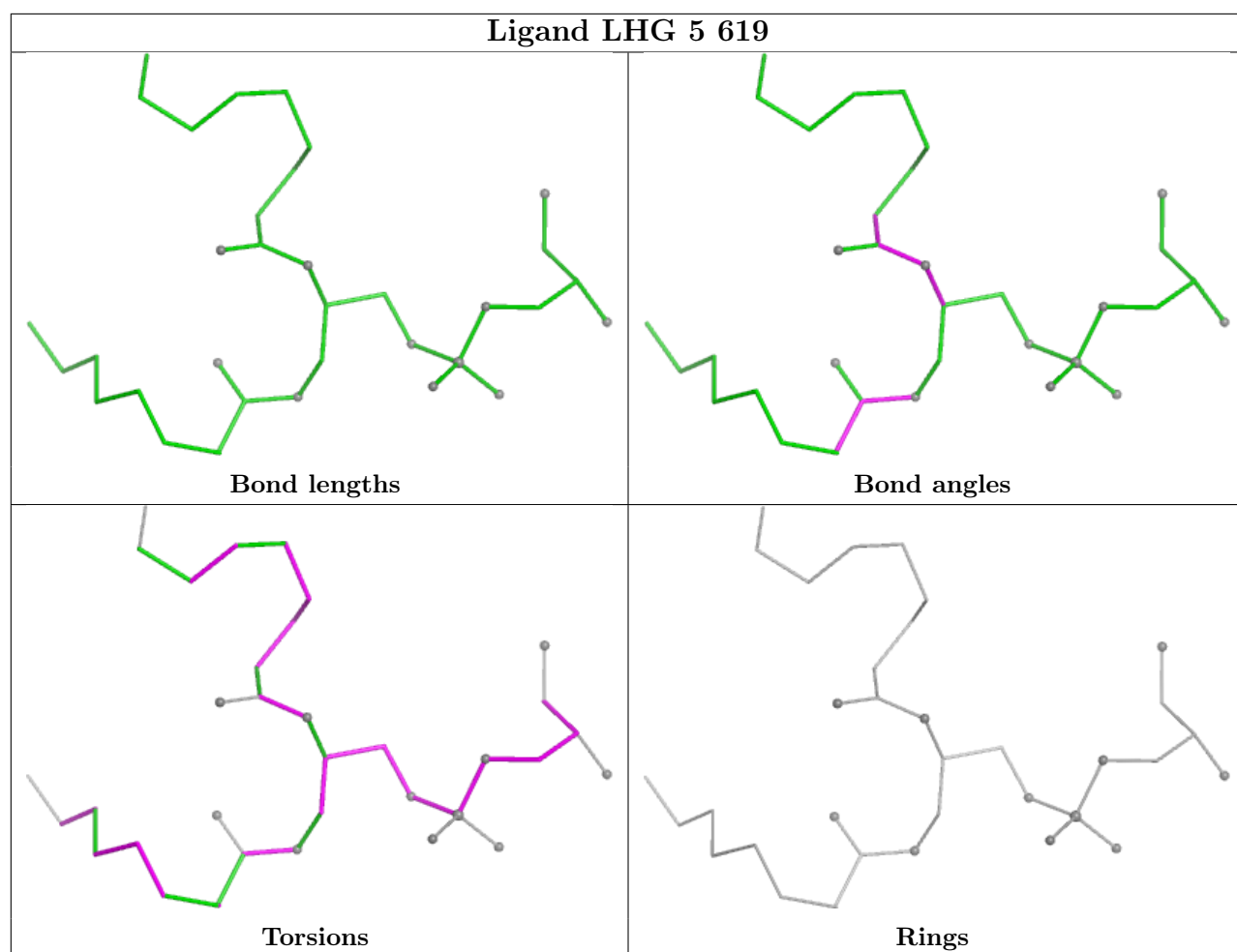


Torsions

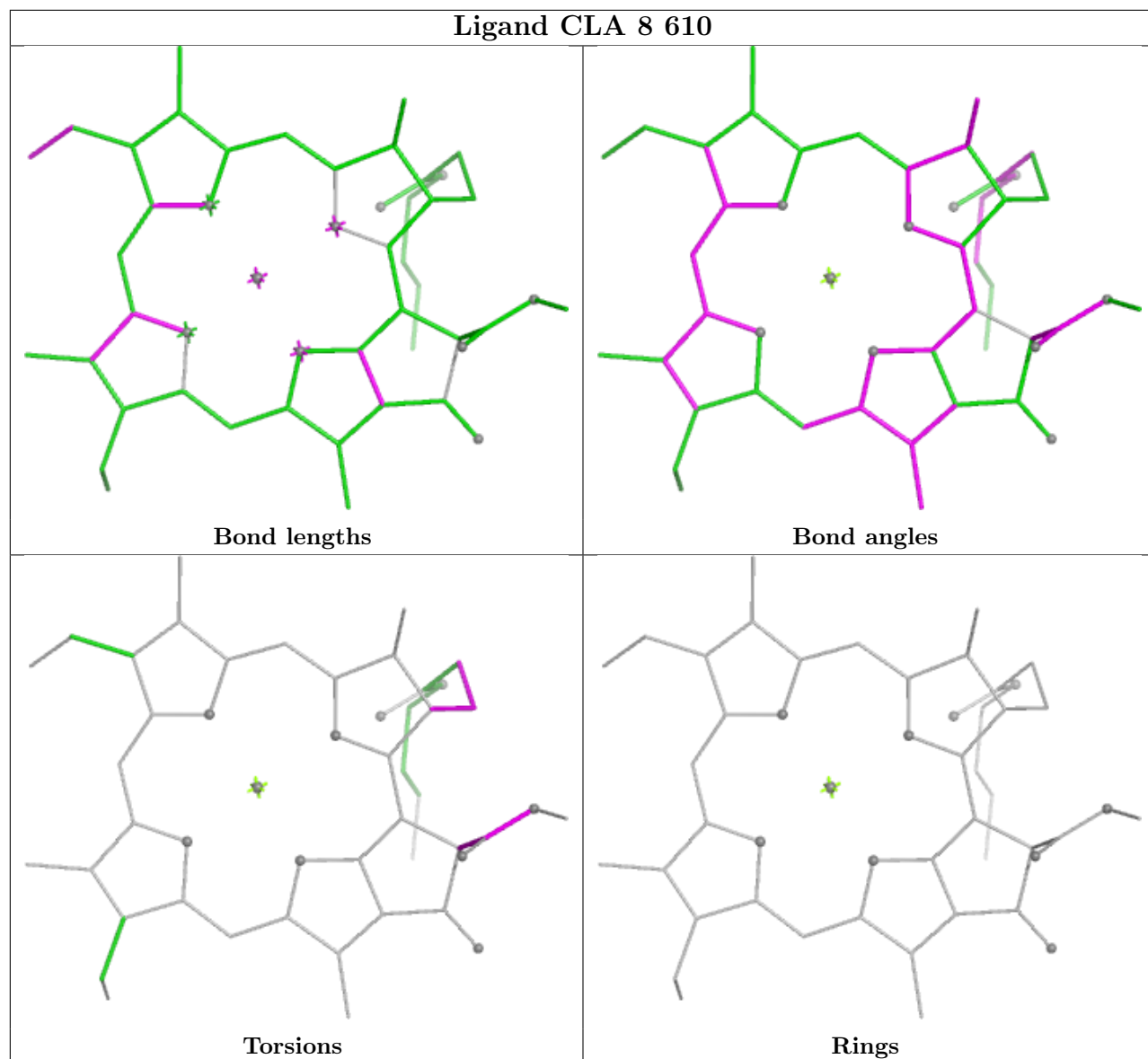


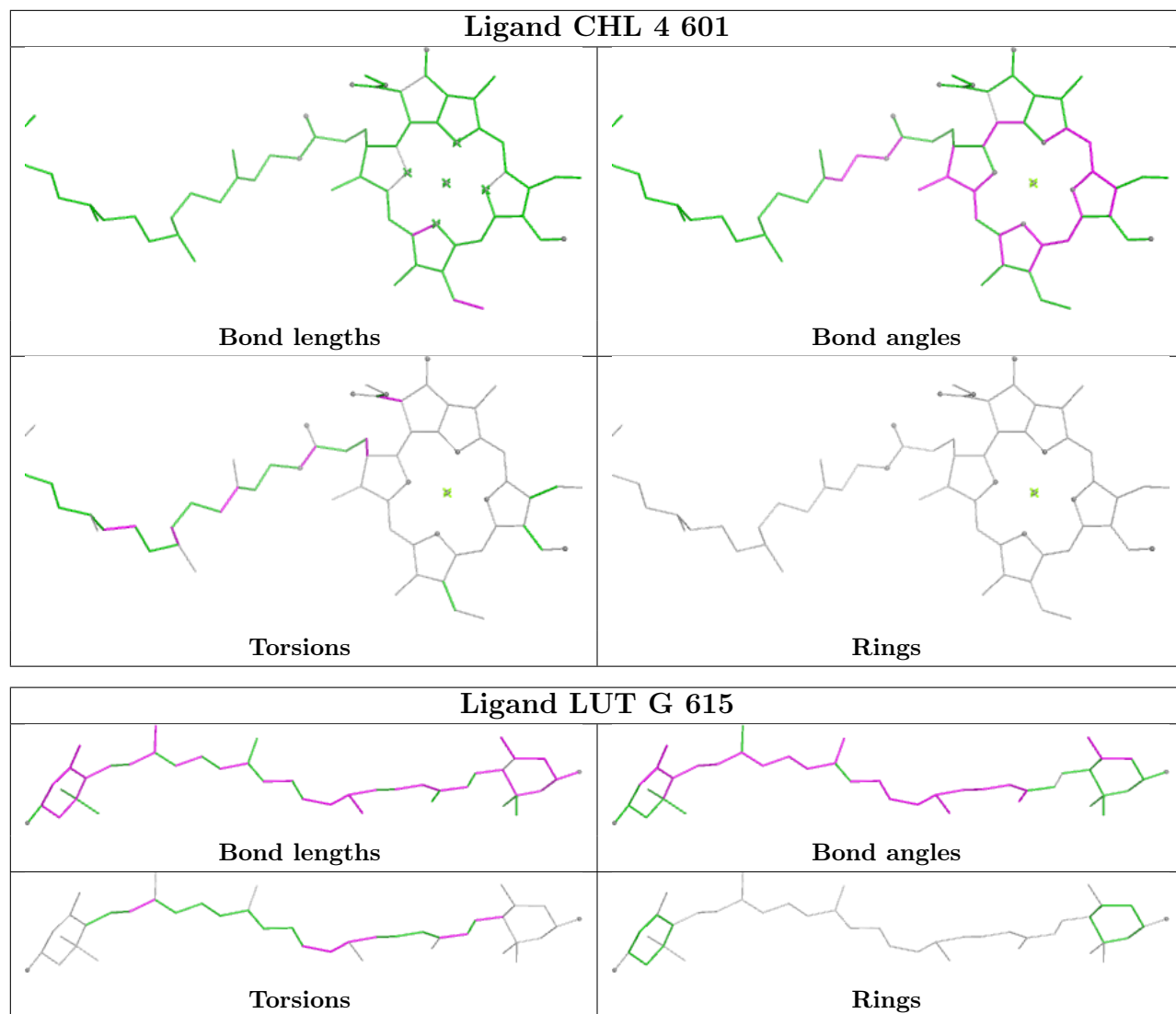
Rings

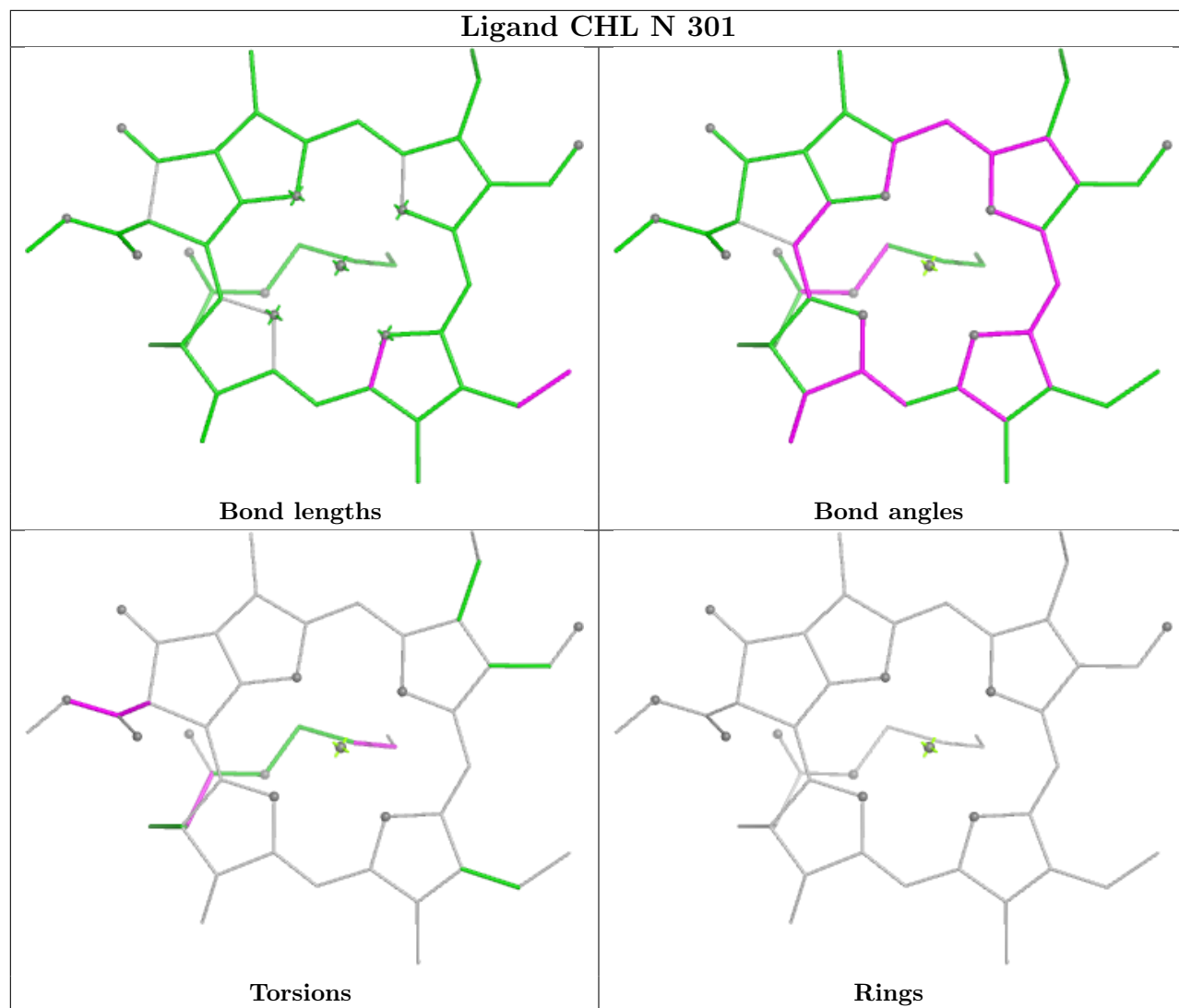


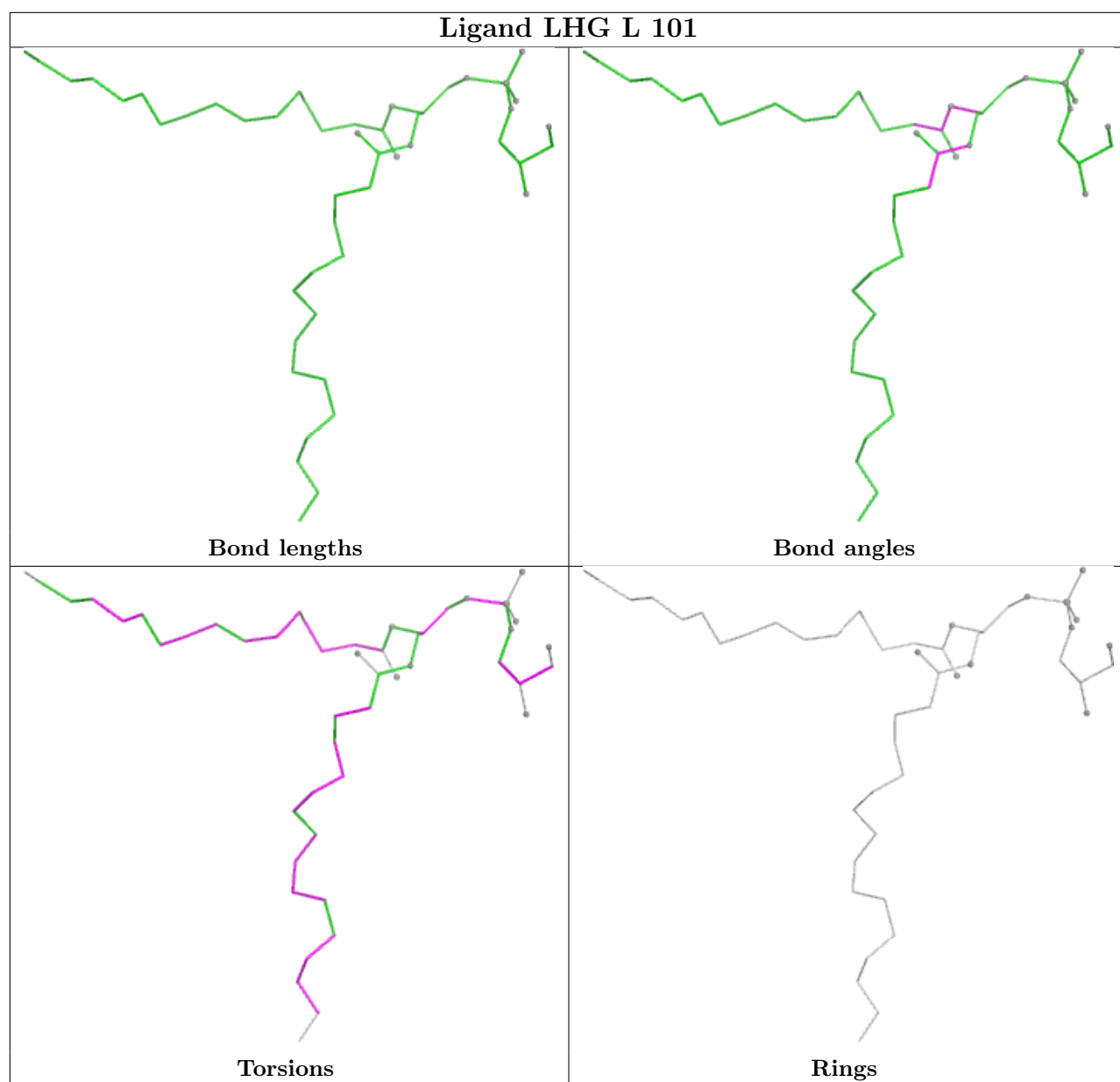


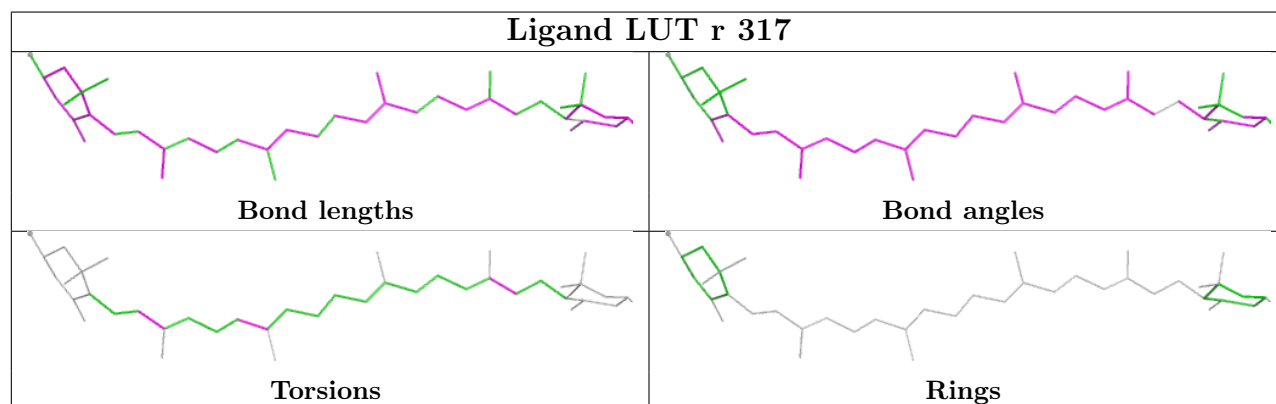
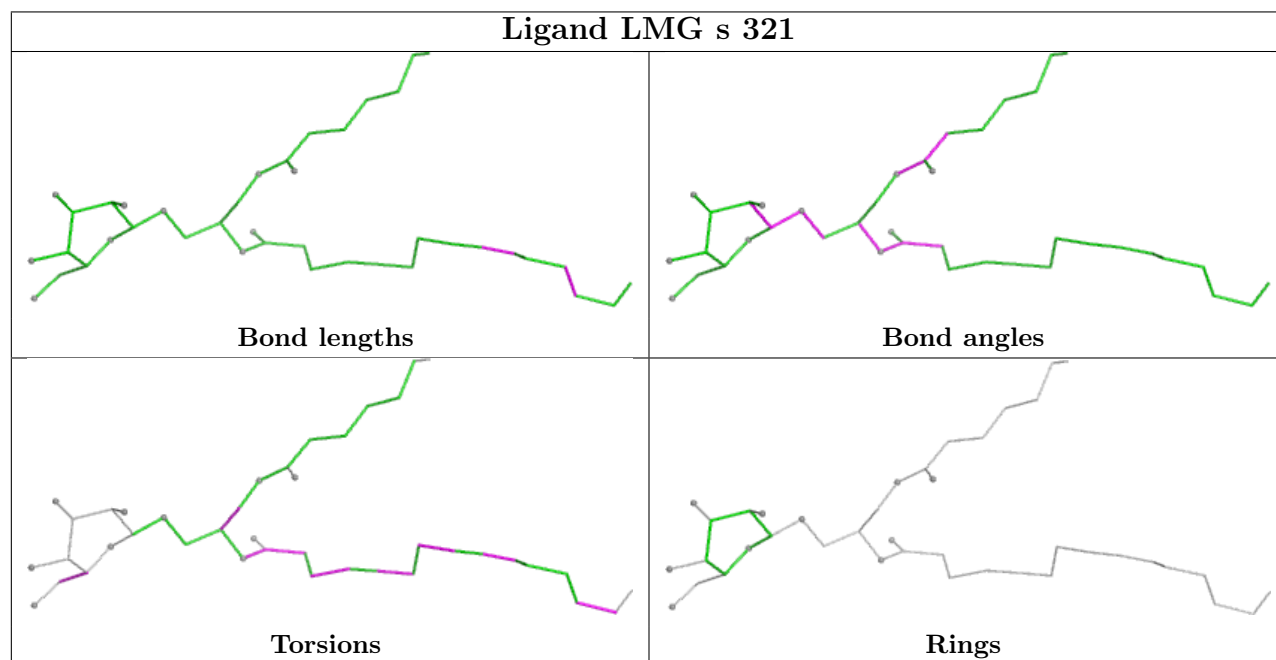
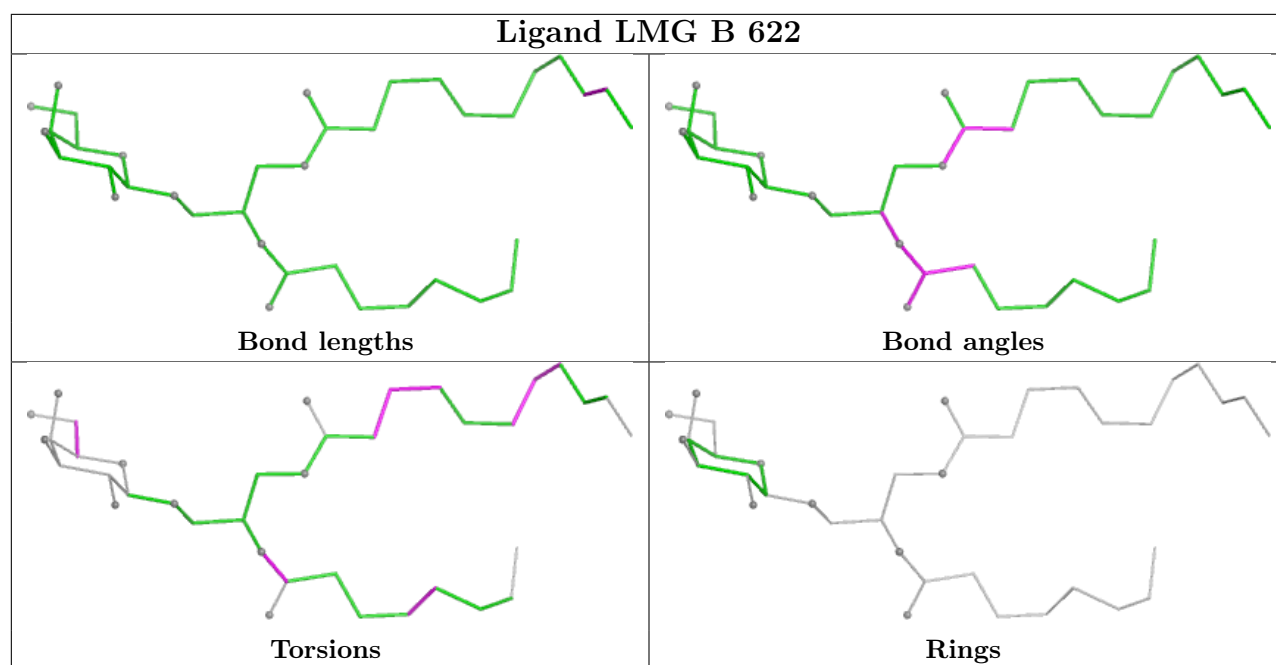
Ligand CLA 8 610

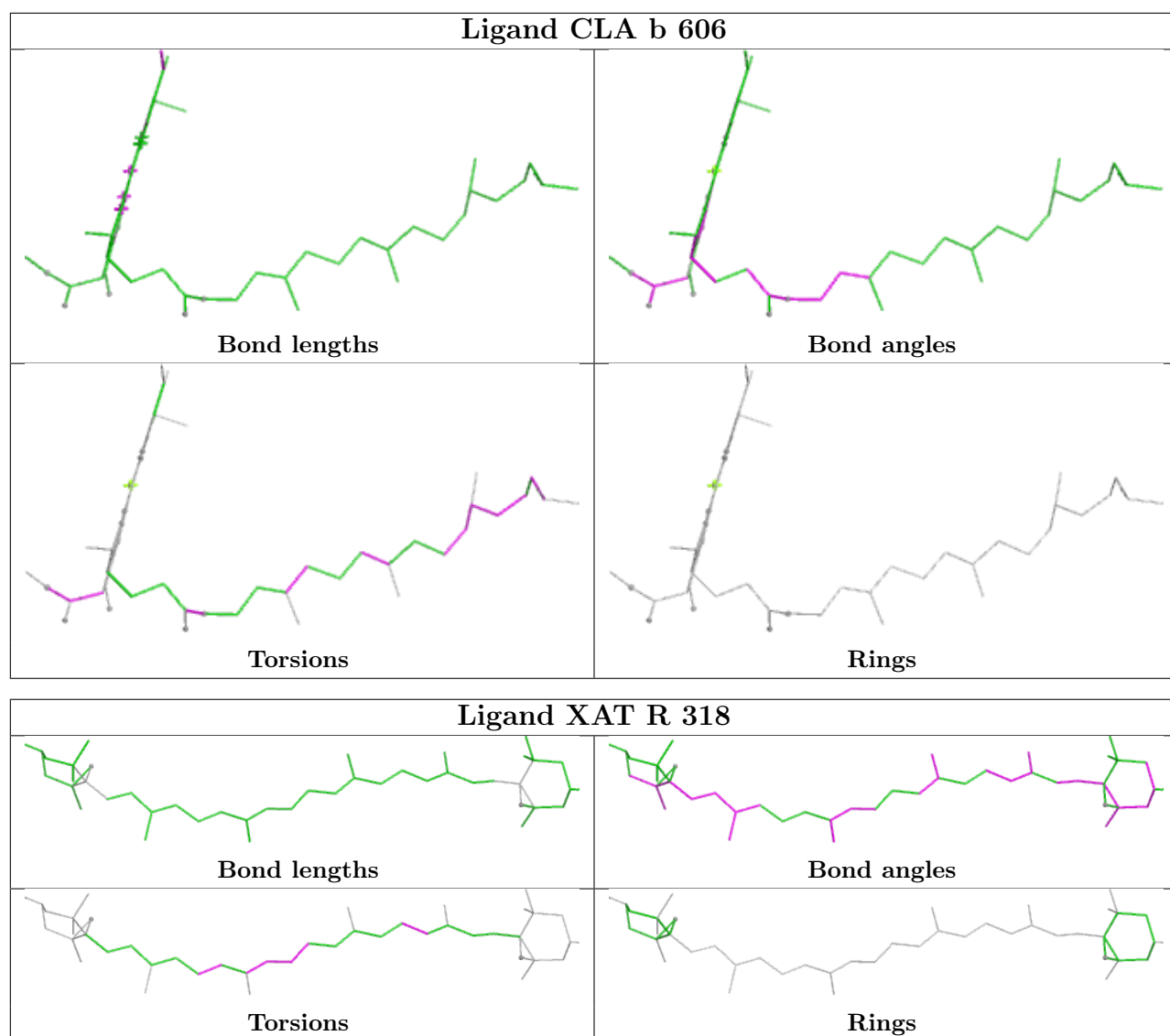


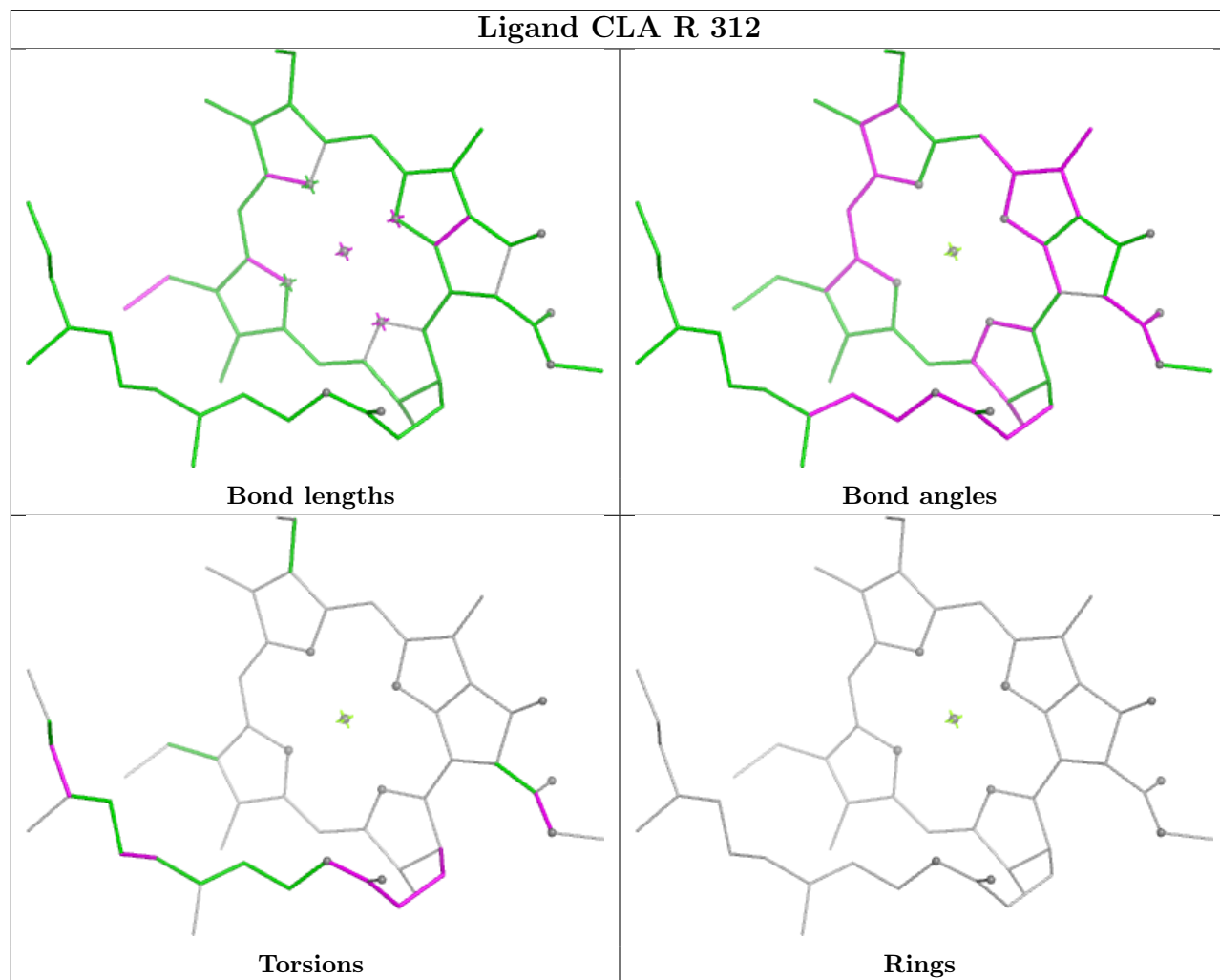




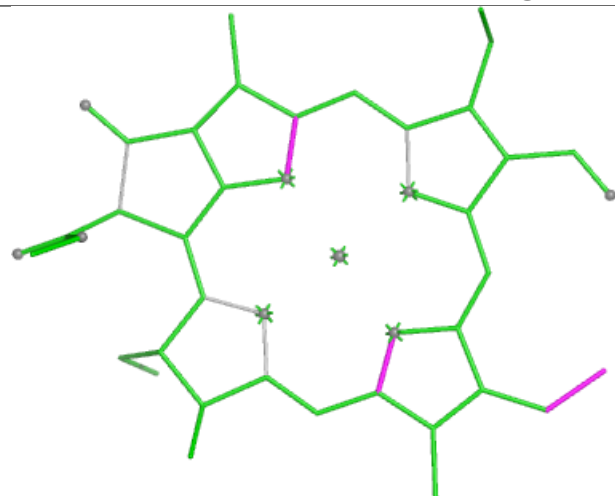




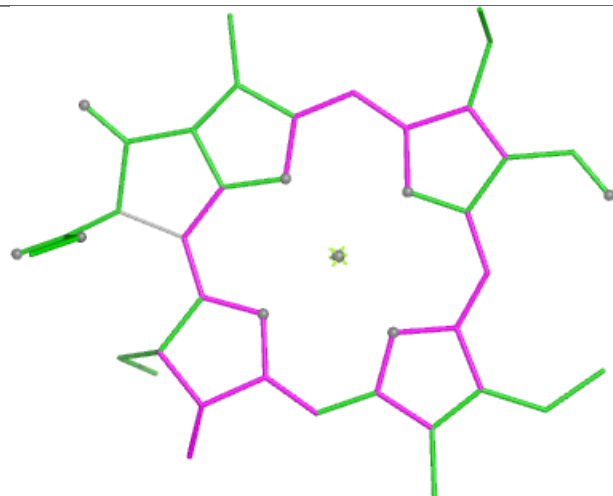




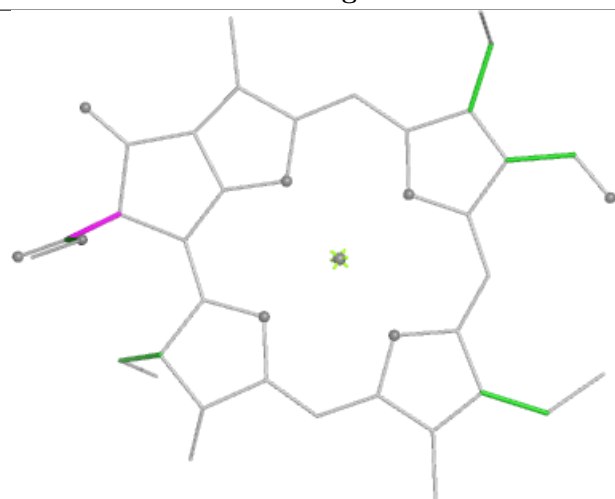
Ligand CHL S 308



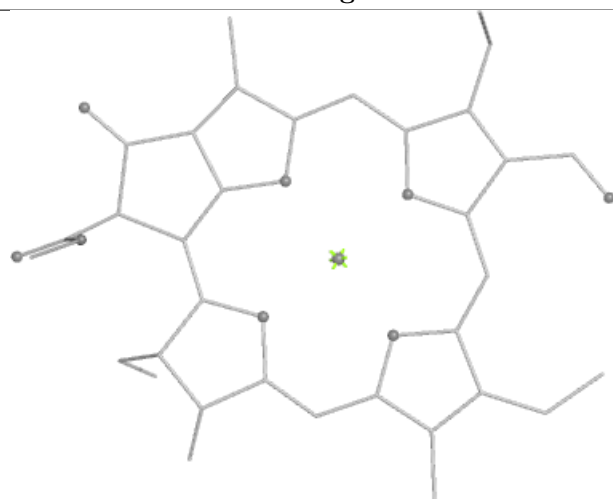
Bond lengths



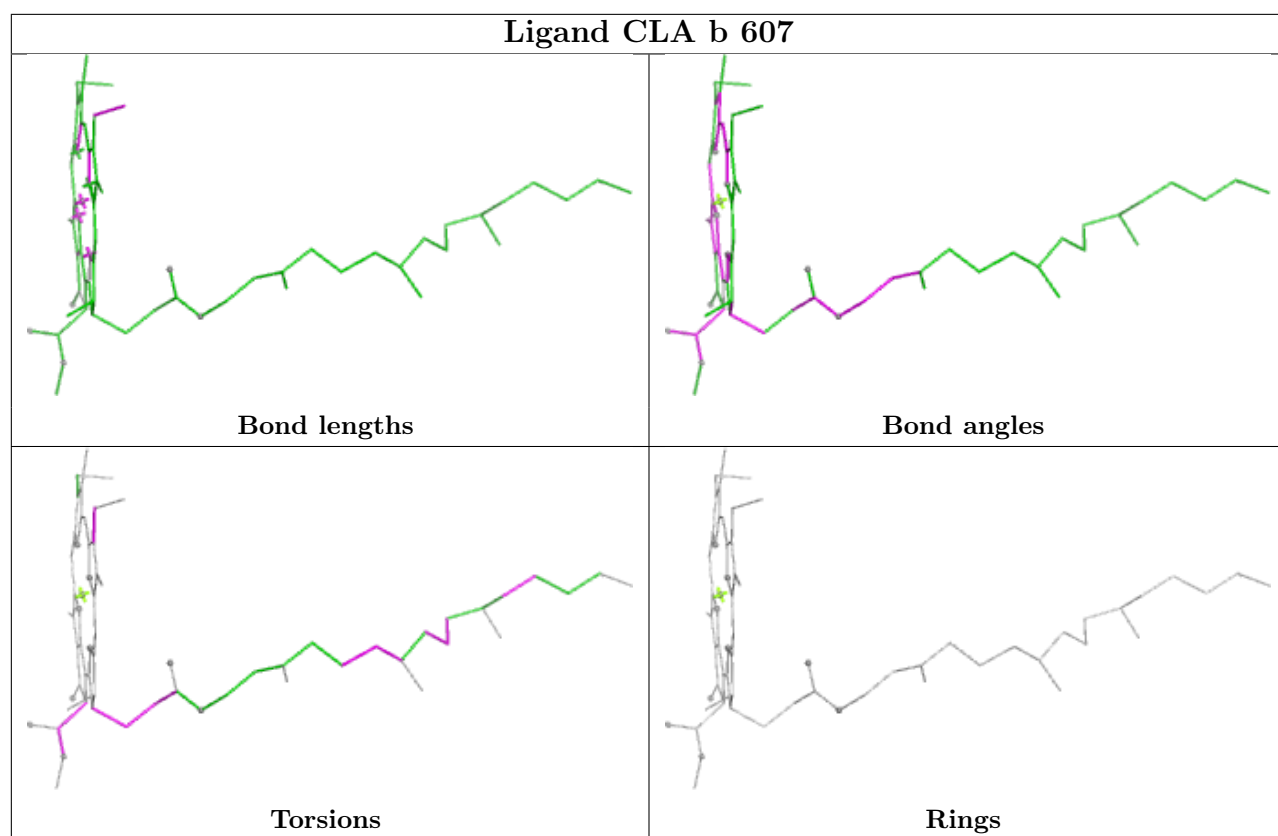
Bond angles

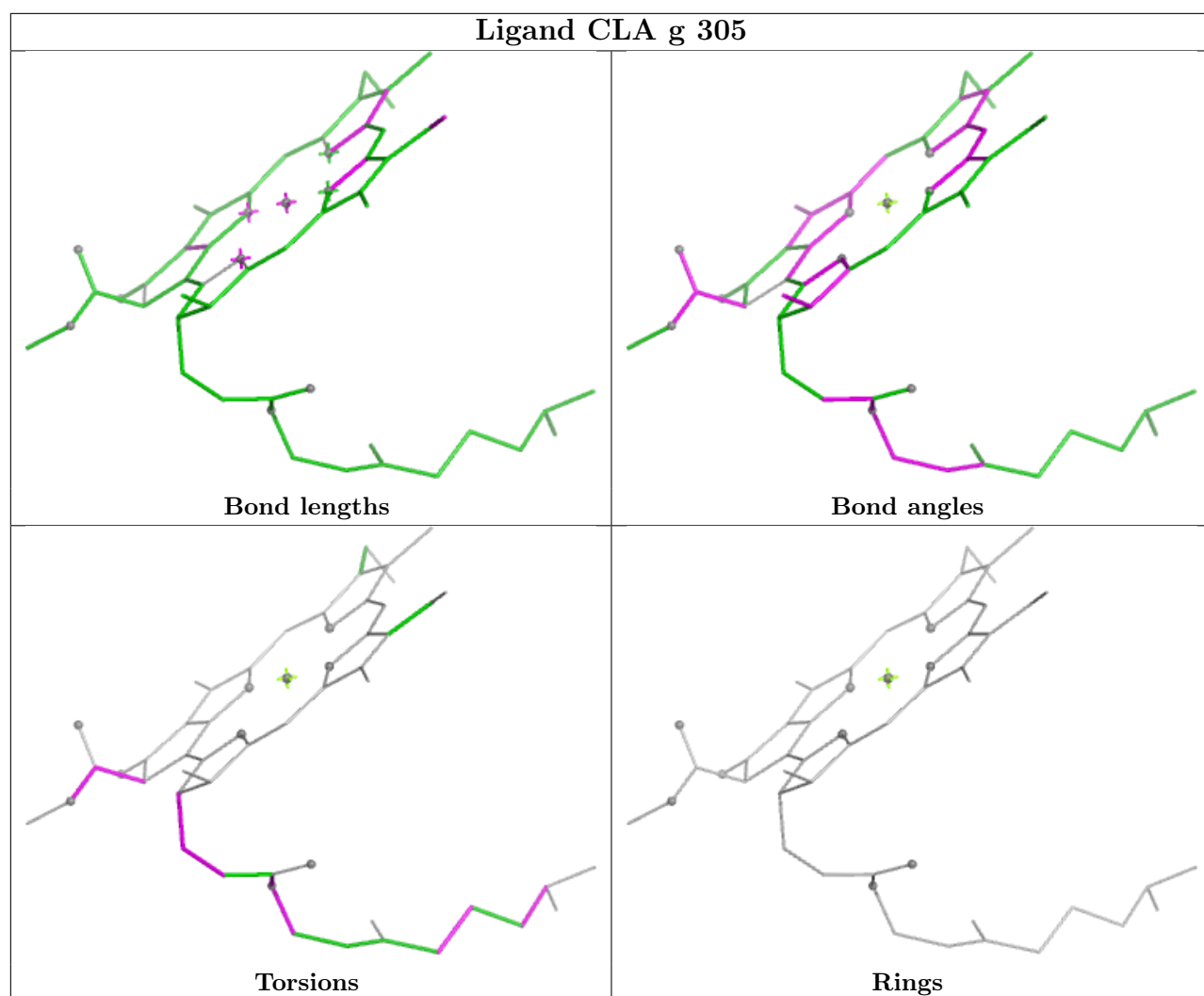


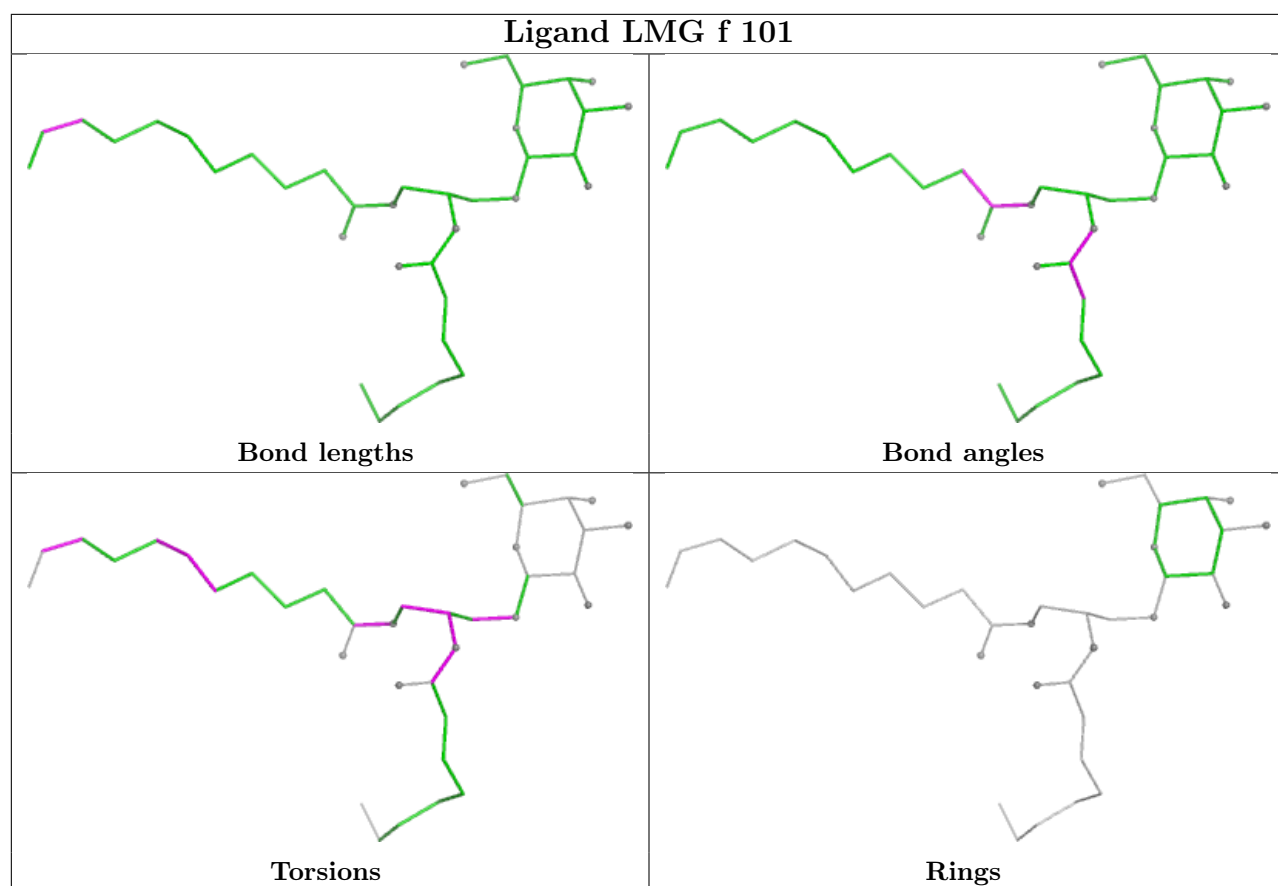
Torsions



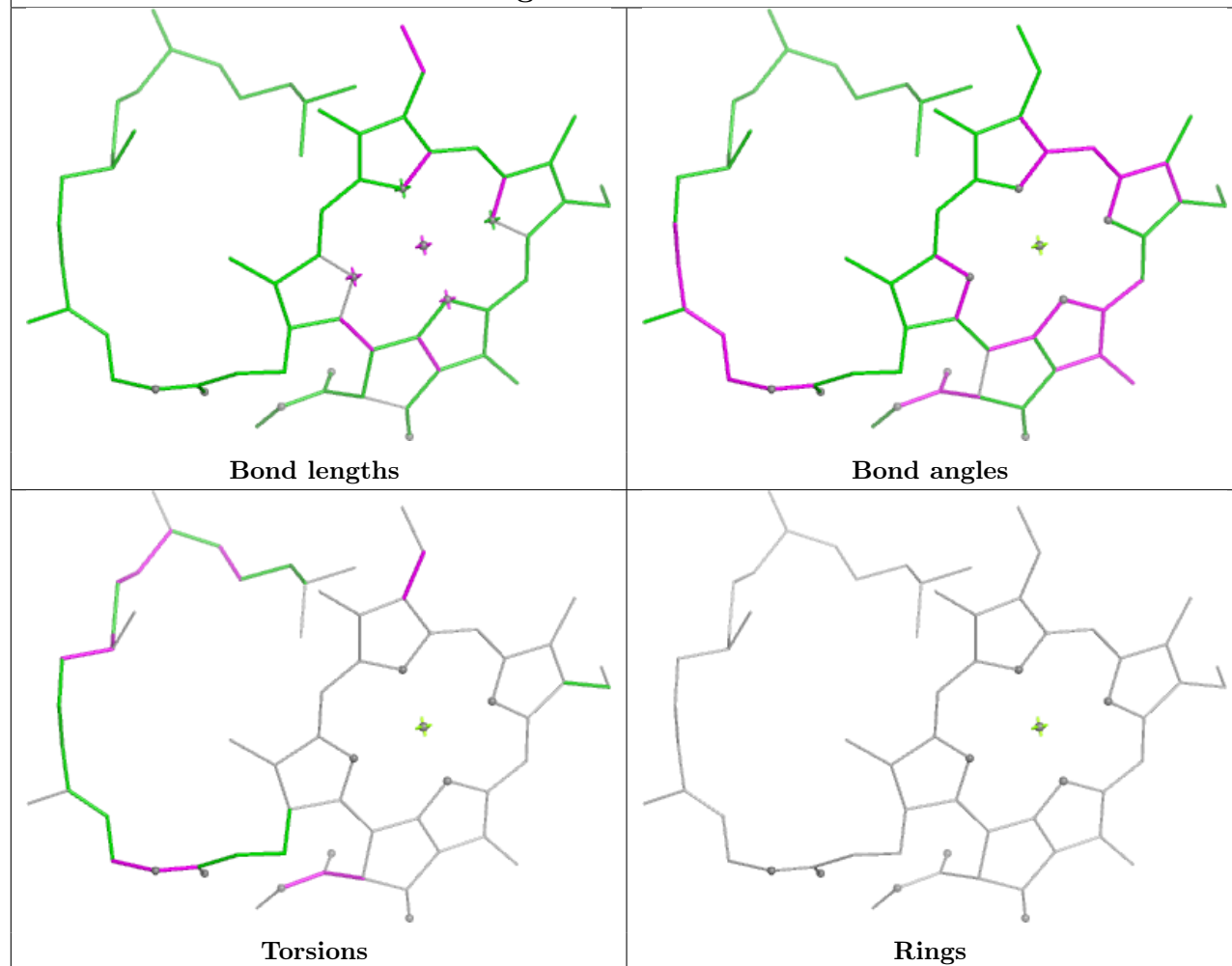
Rings

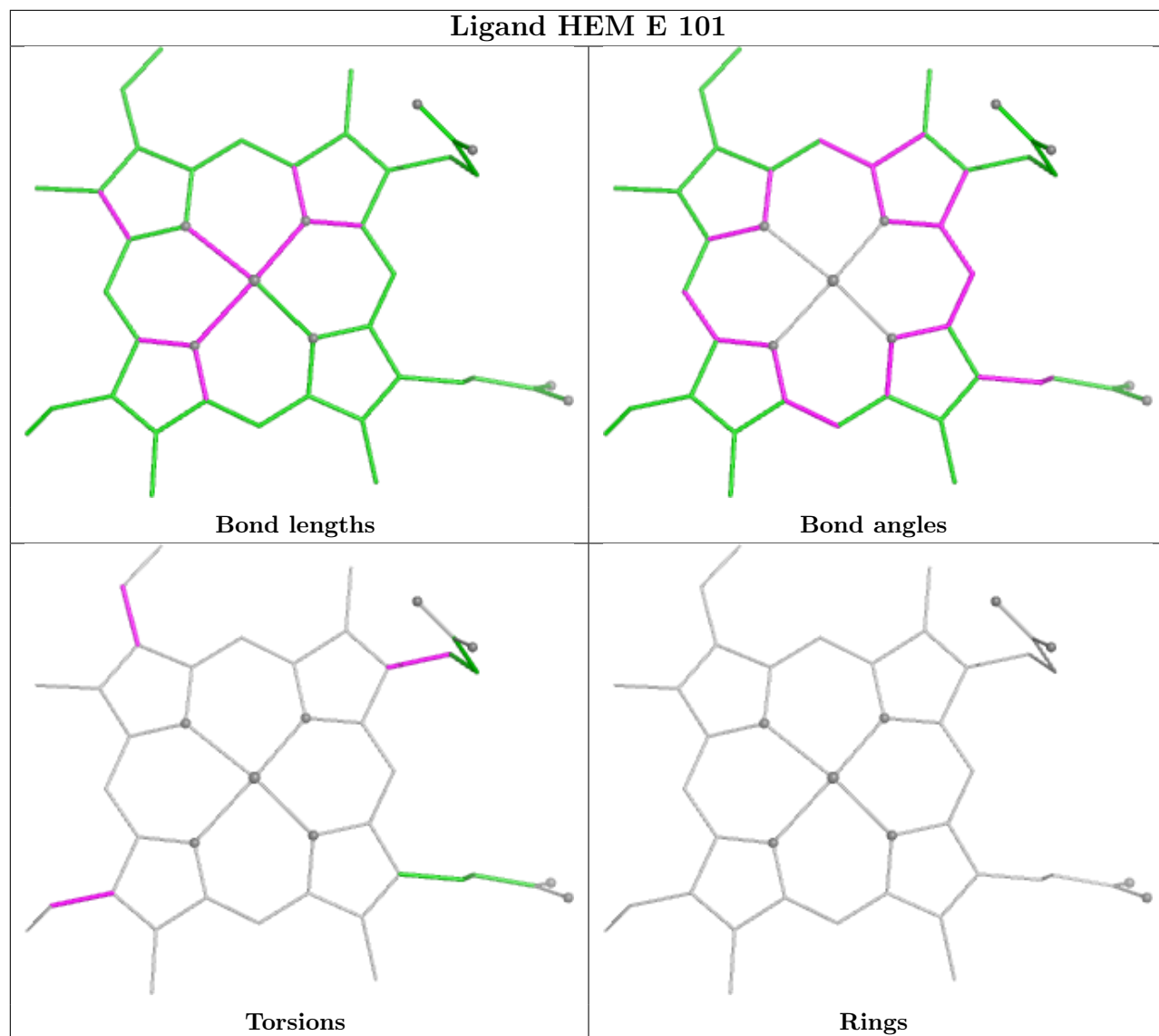




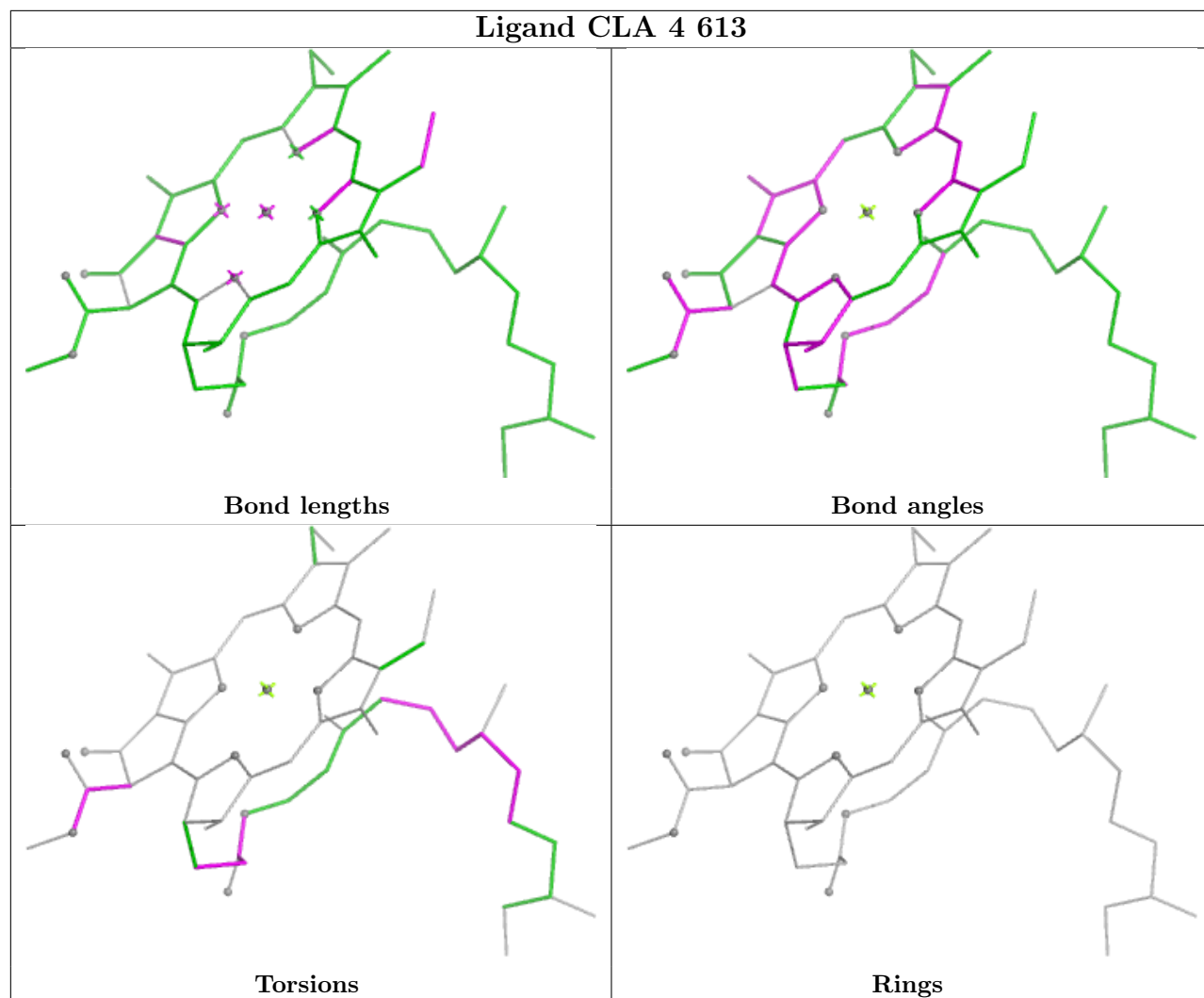


Ligand CLA b 616

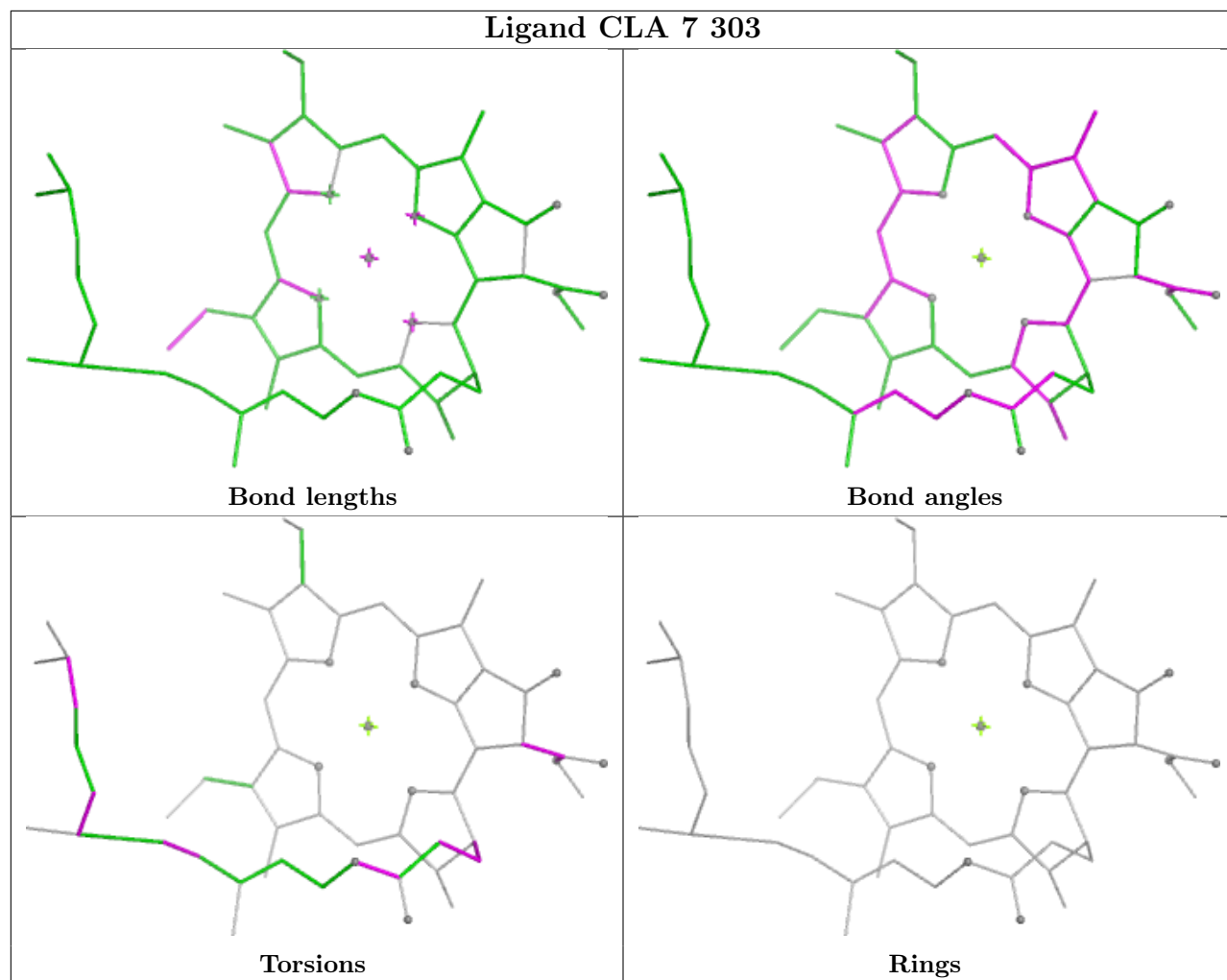


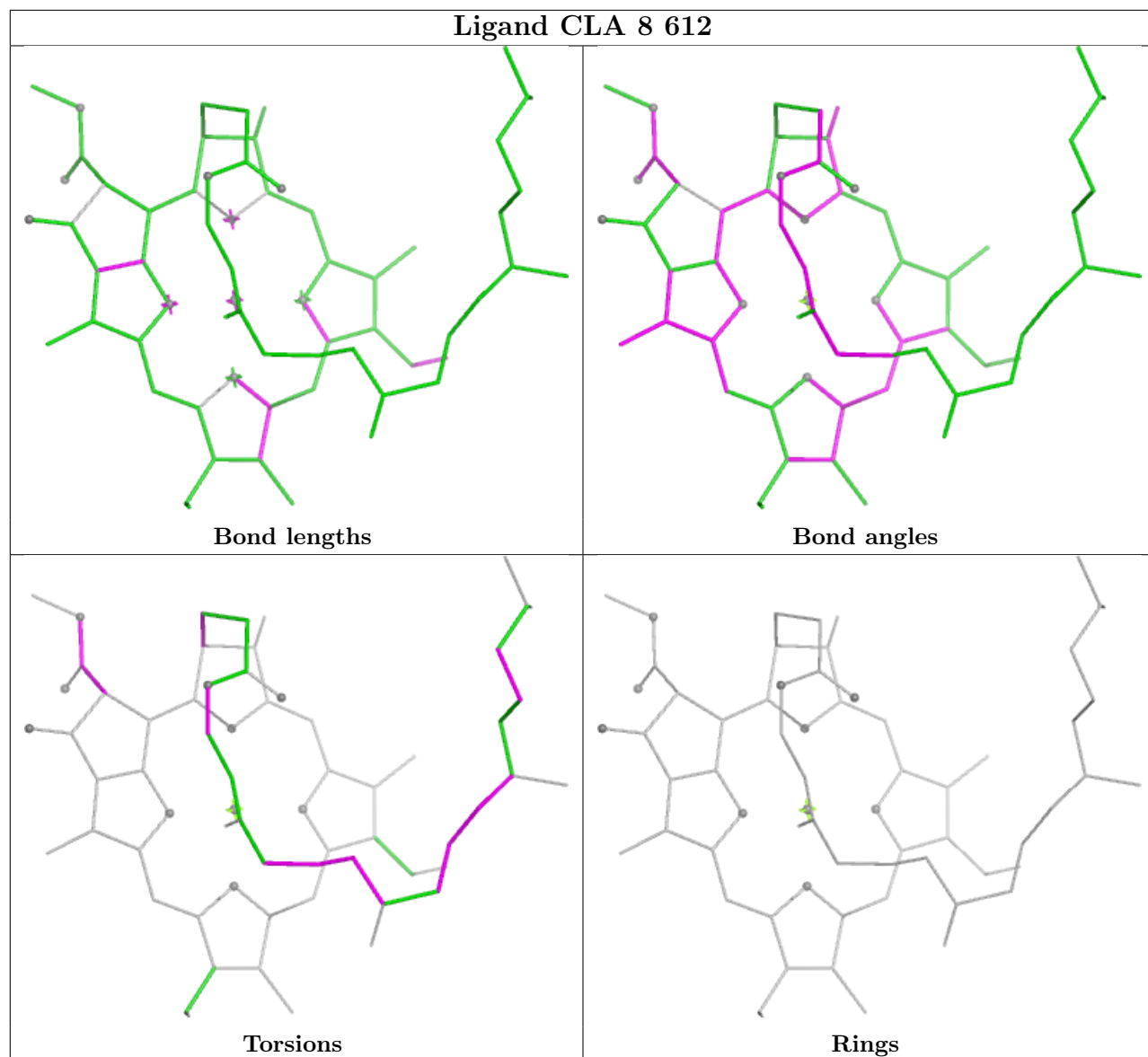


Ligand CLA 4 613

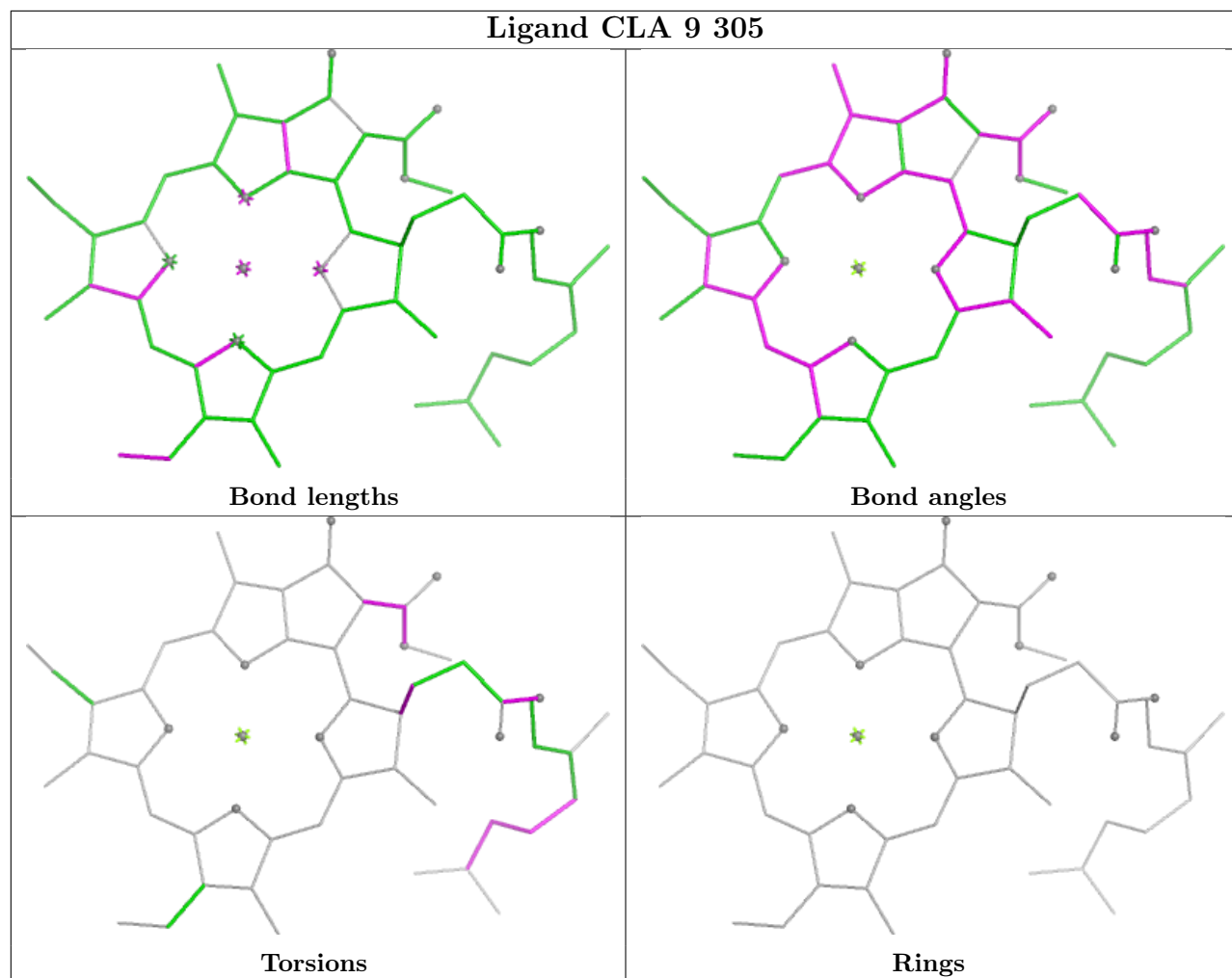


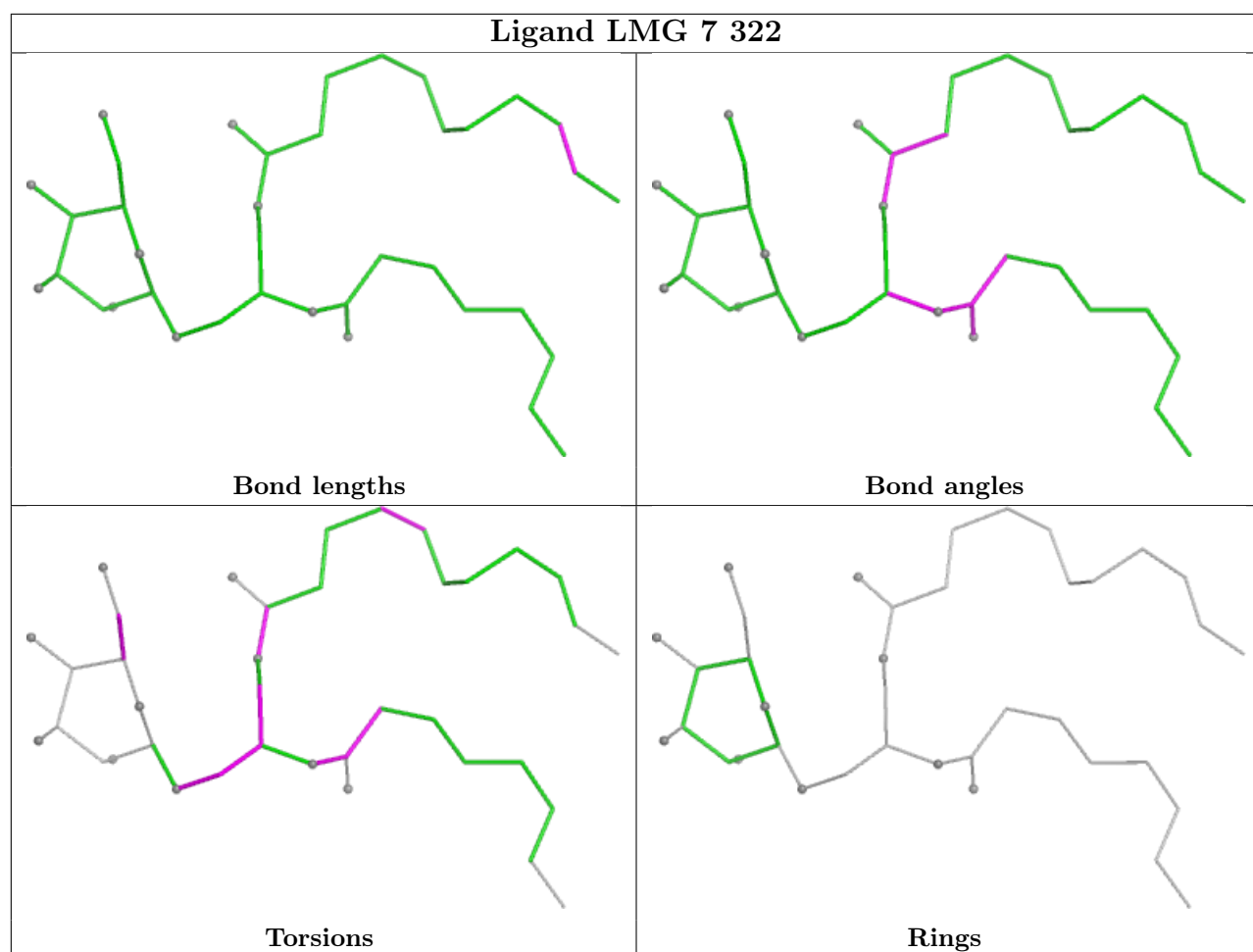
Ligand CLA 7 303

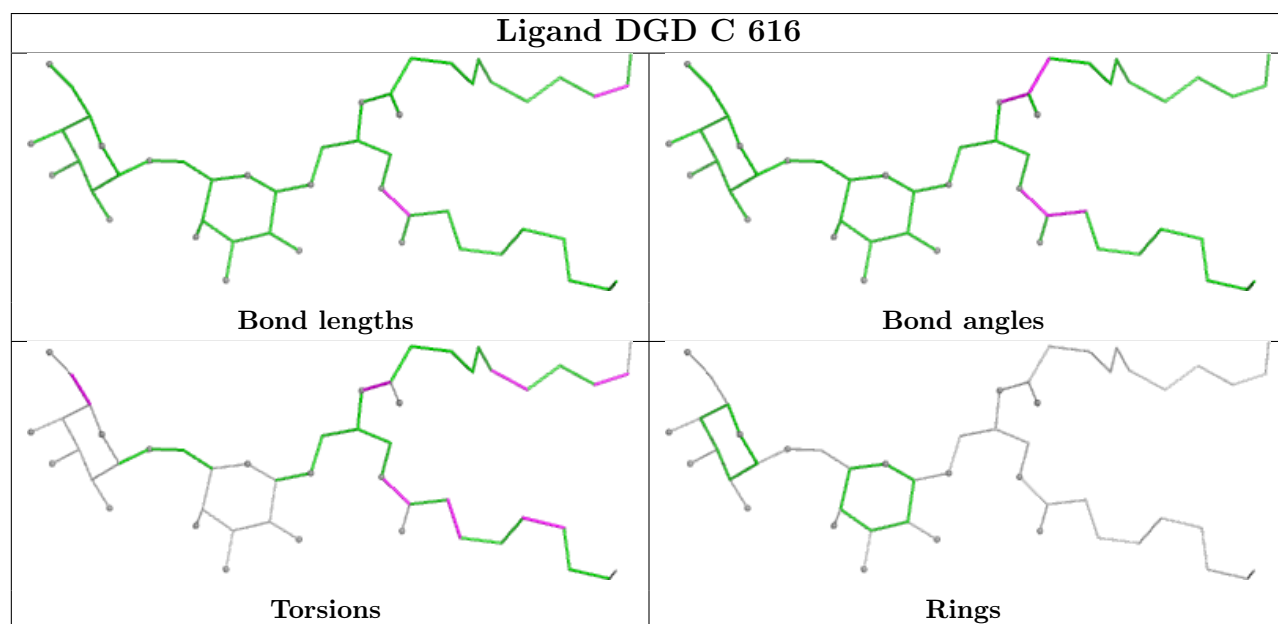
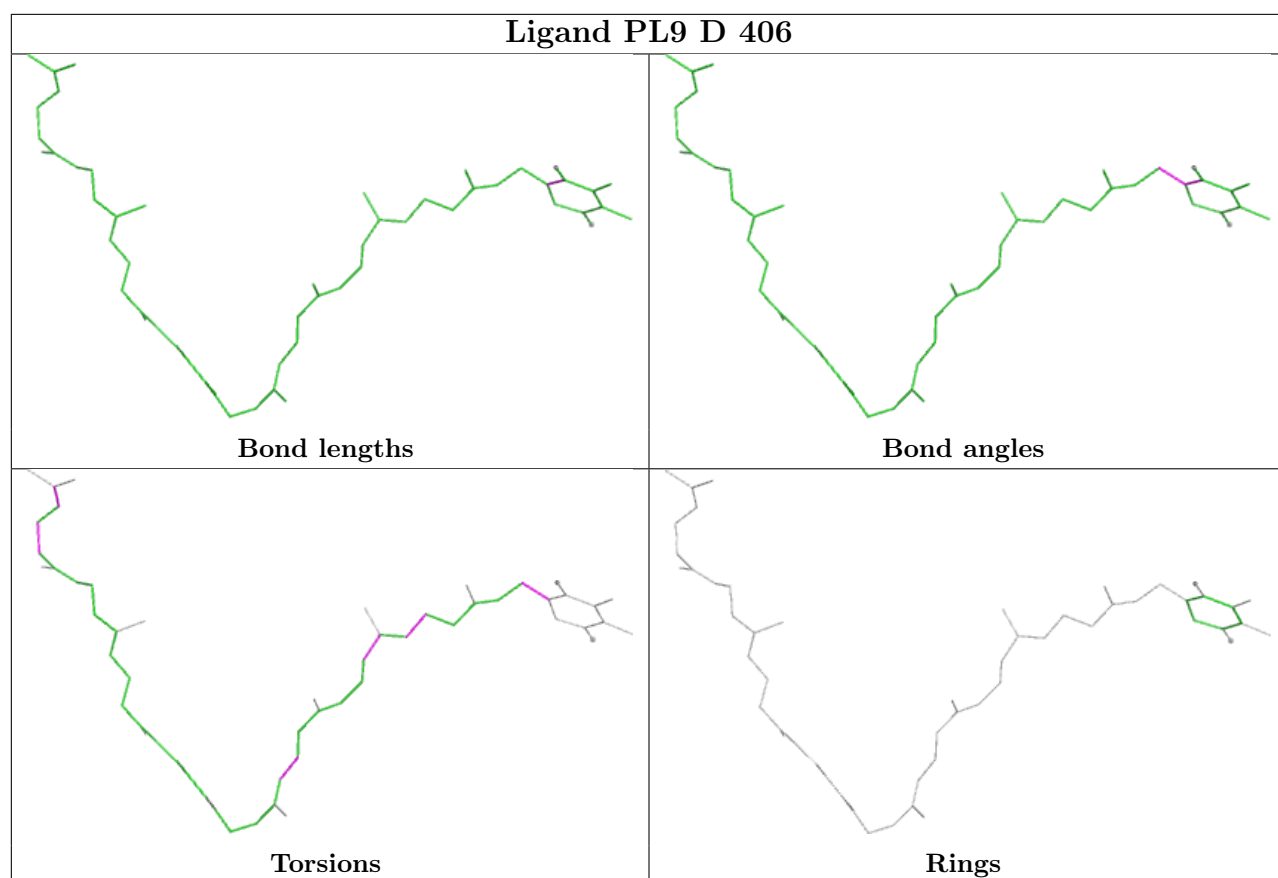


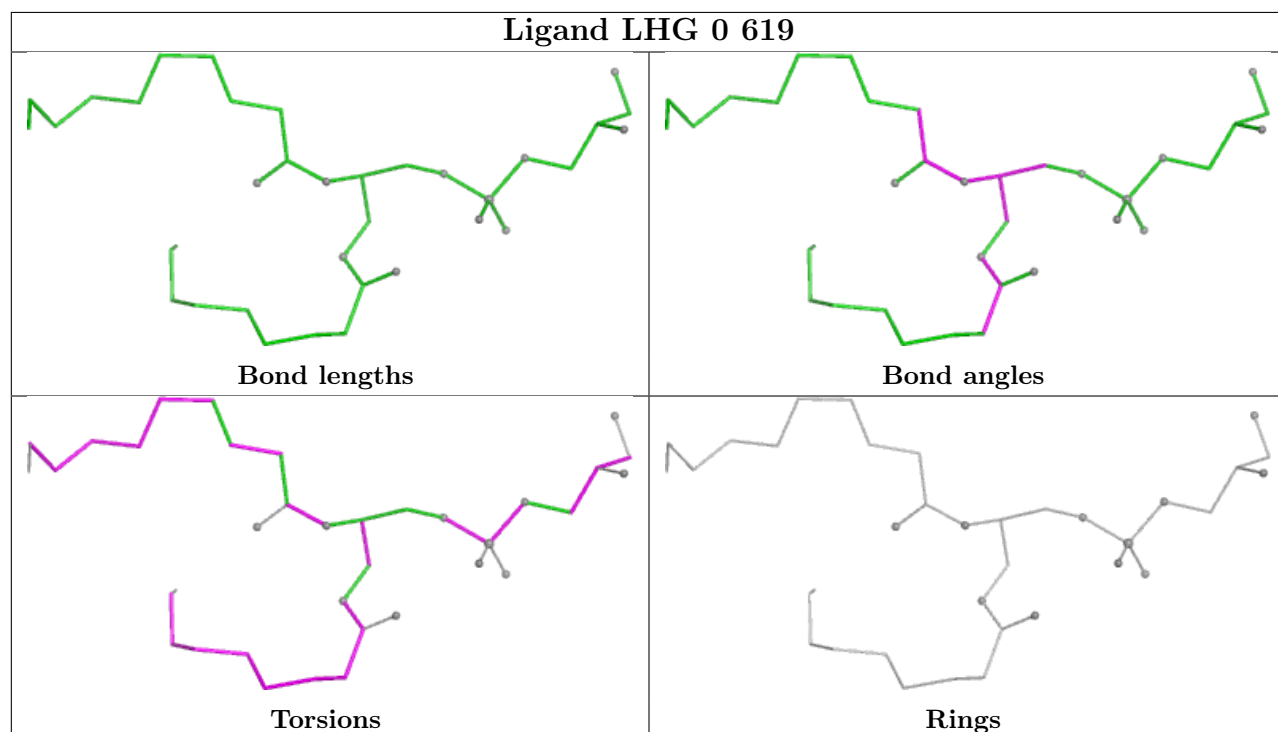
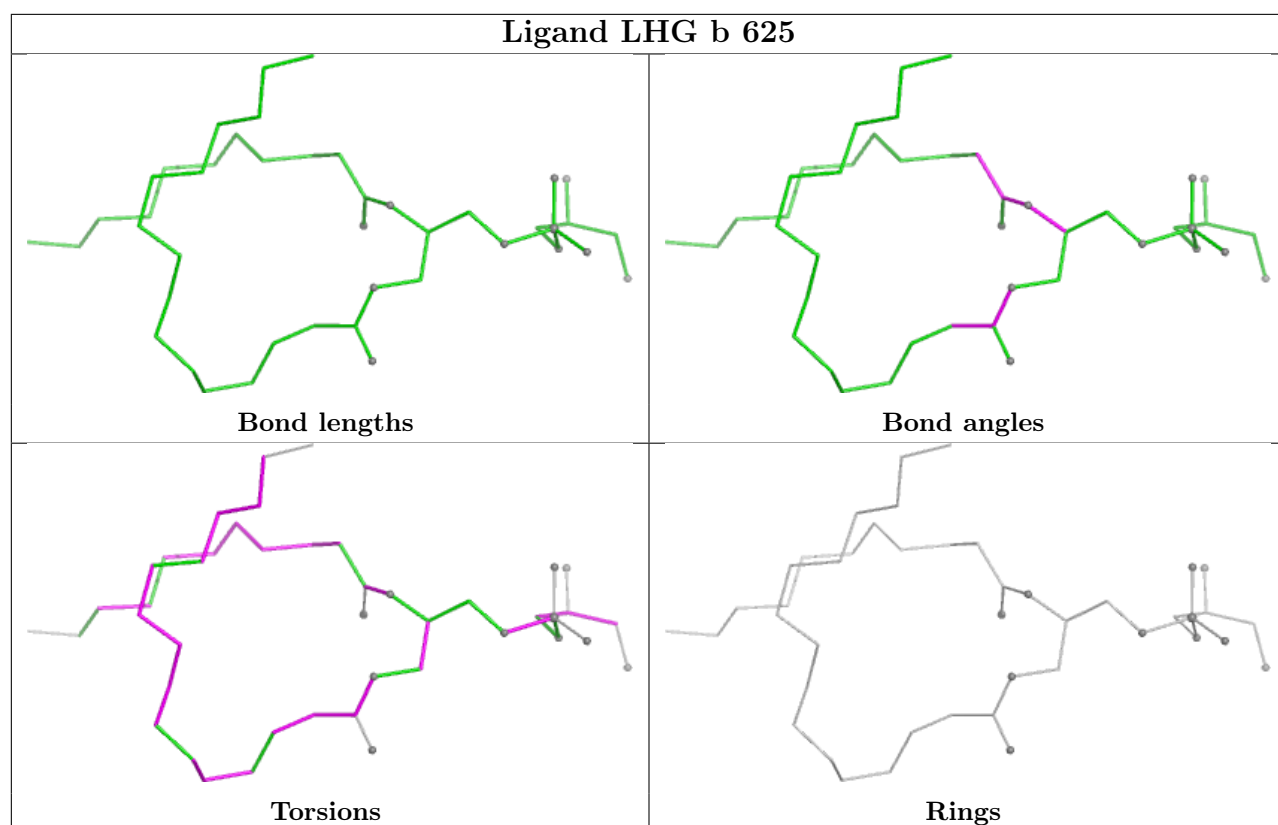


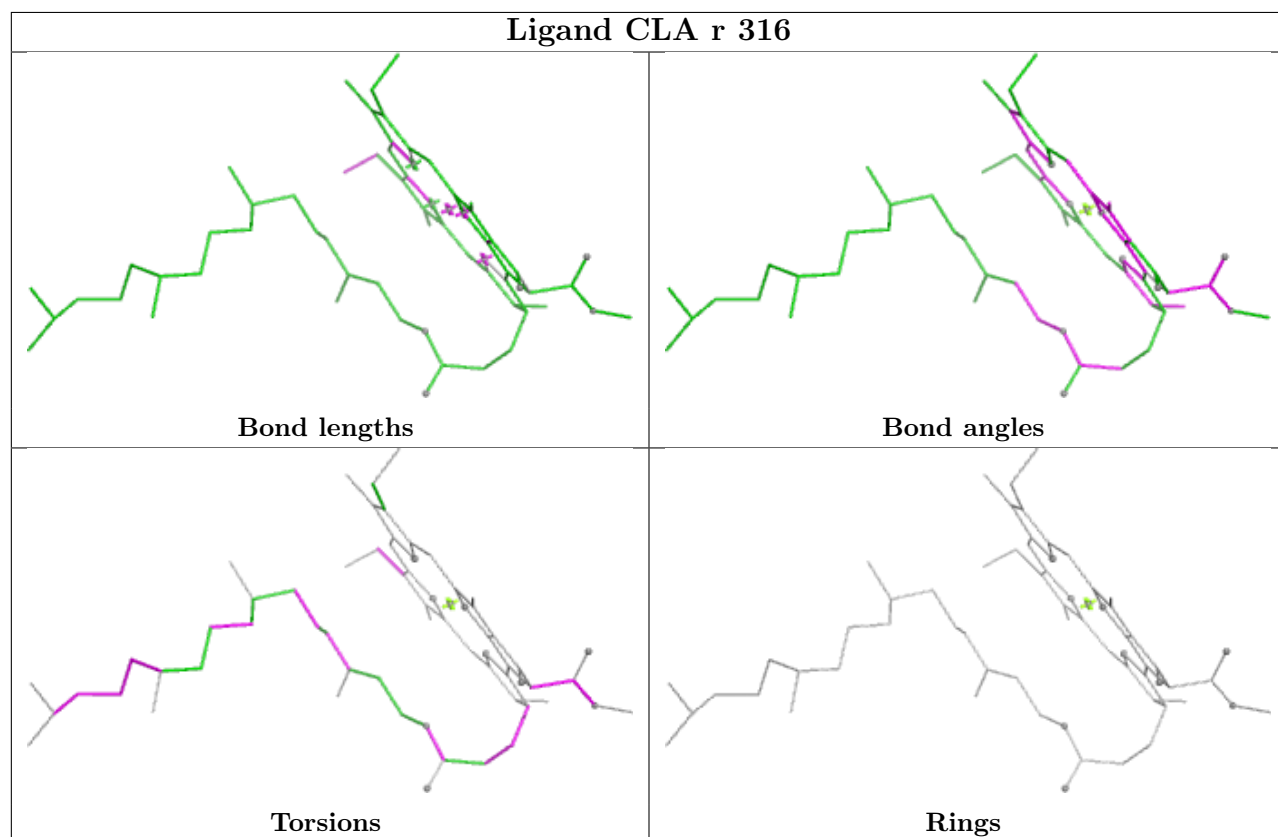
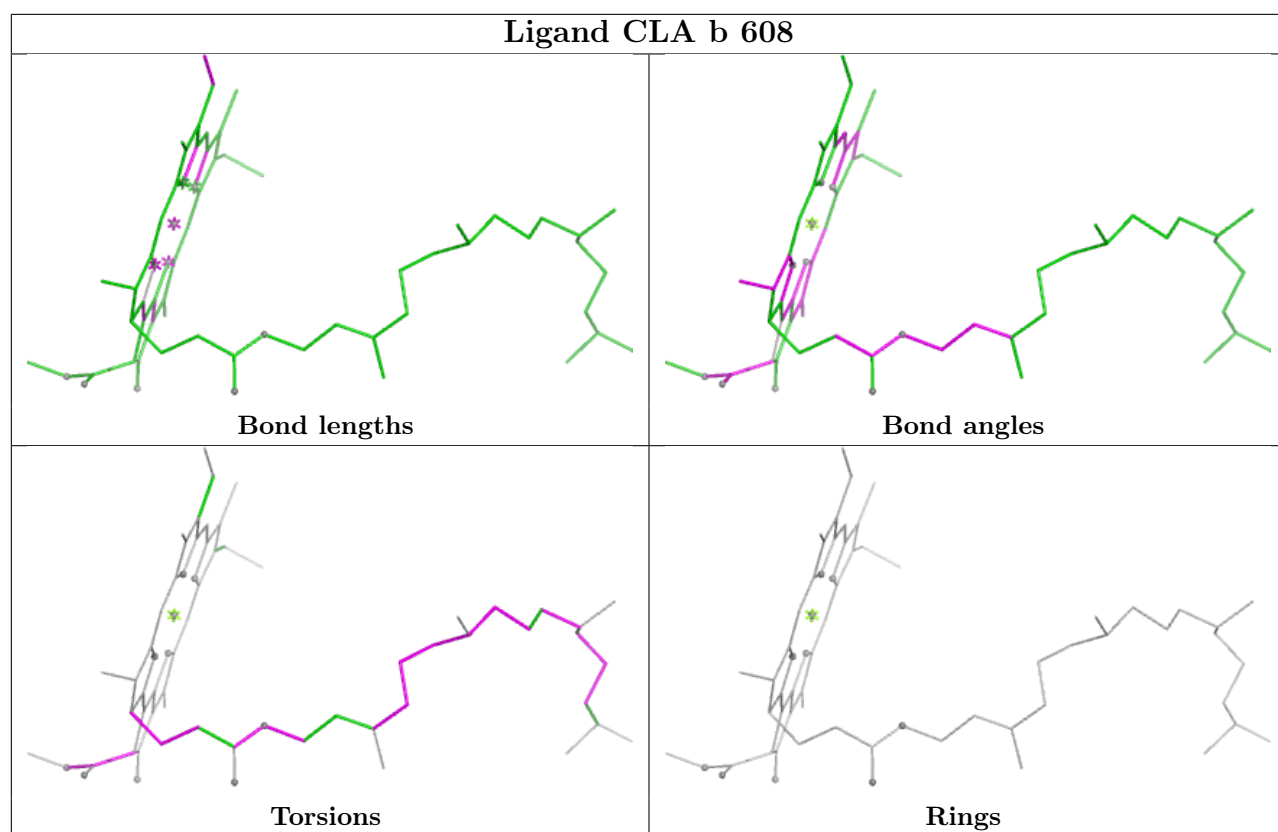
Ligand CLA 9 305



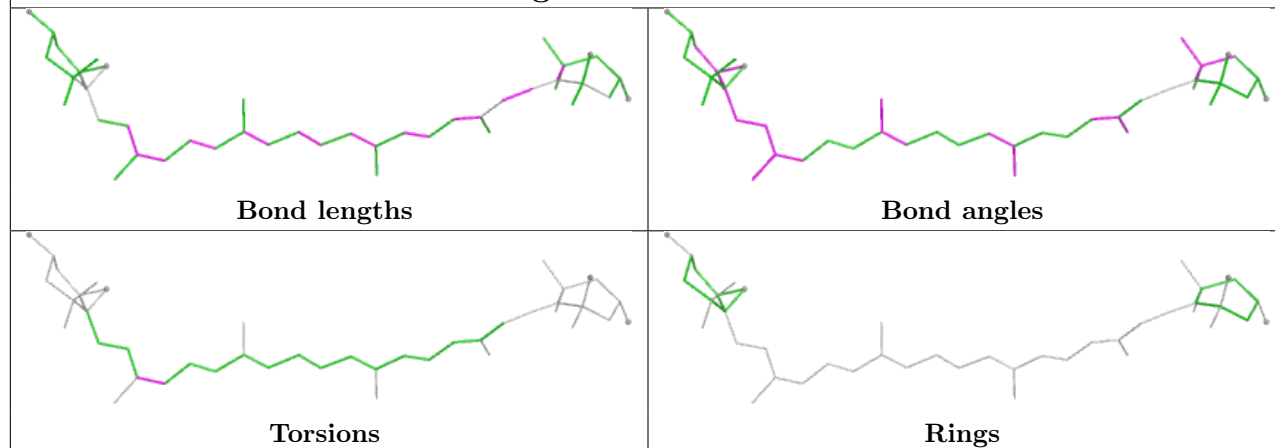




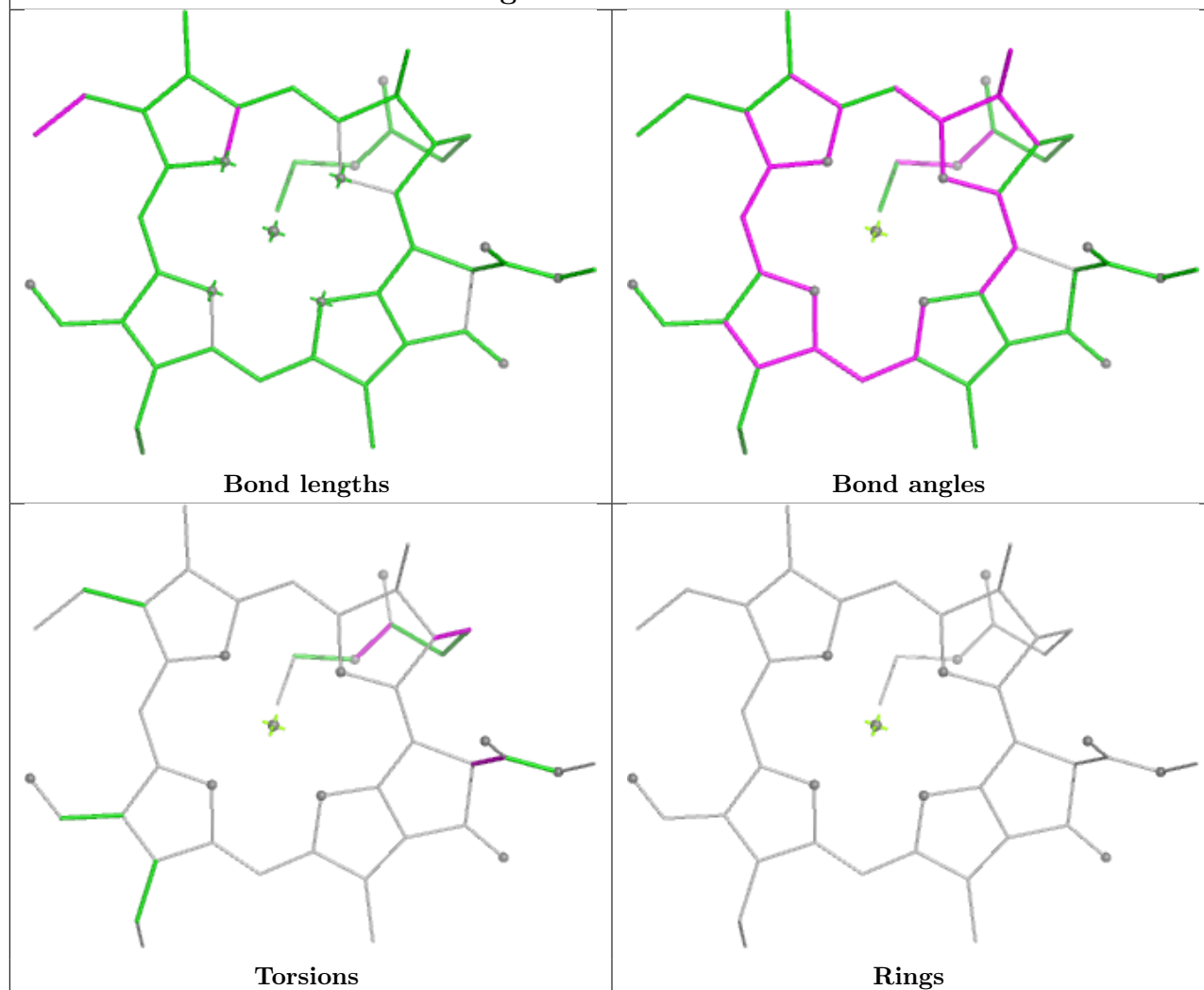


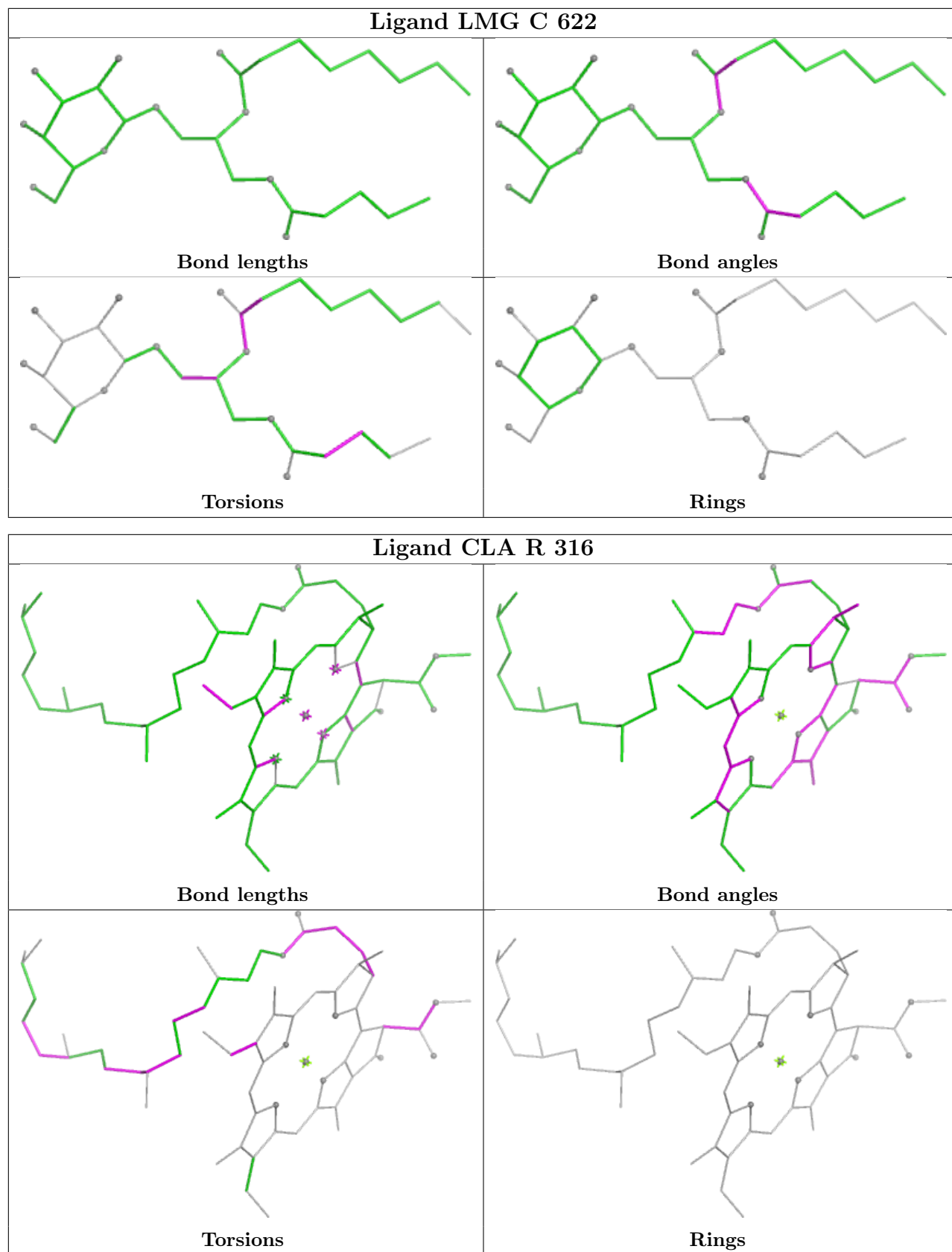


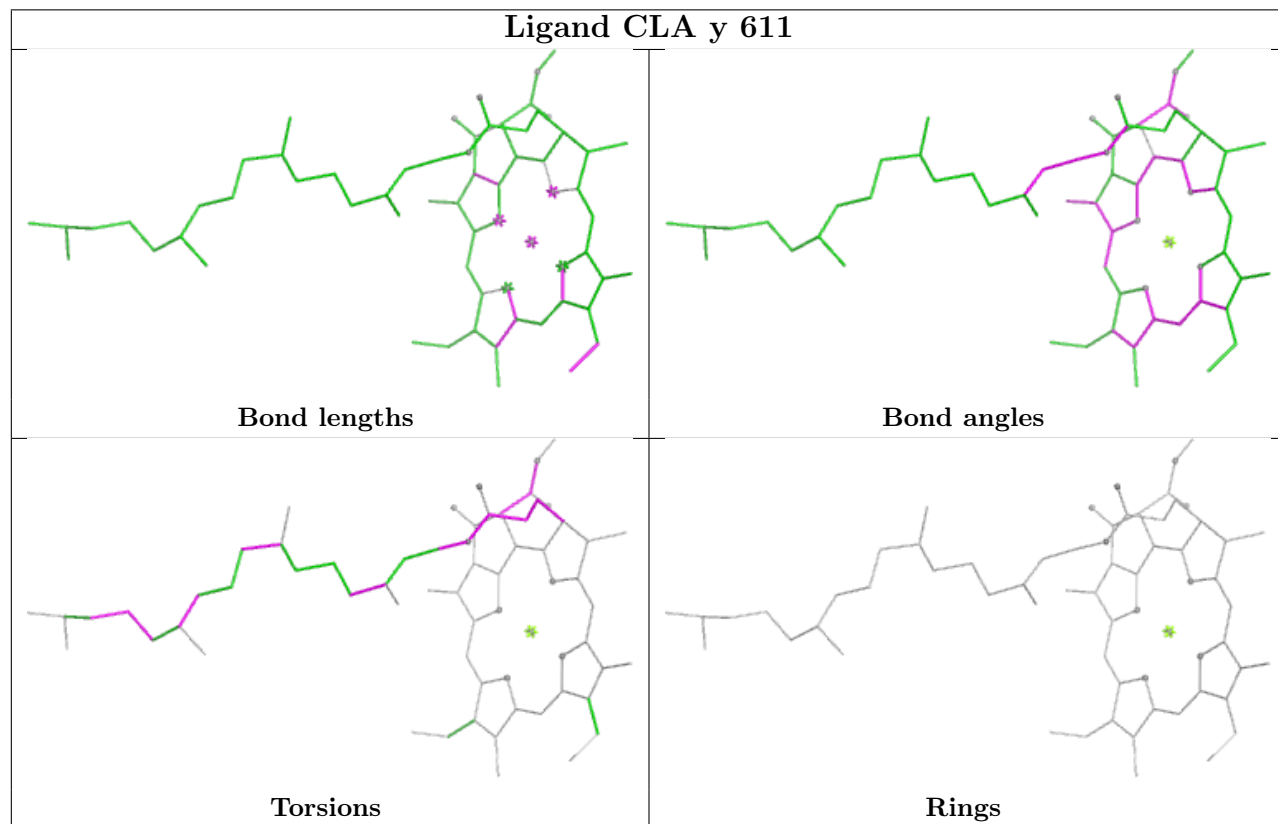
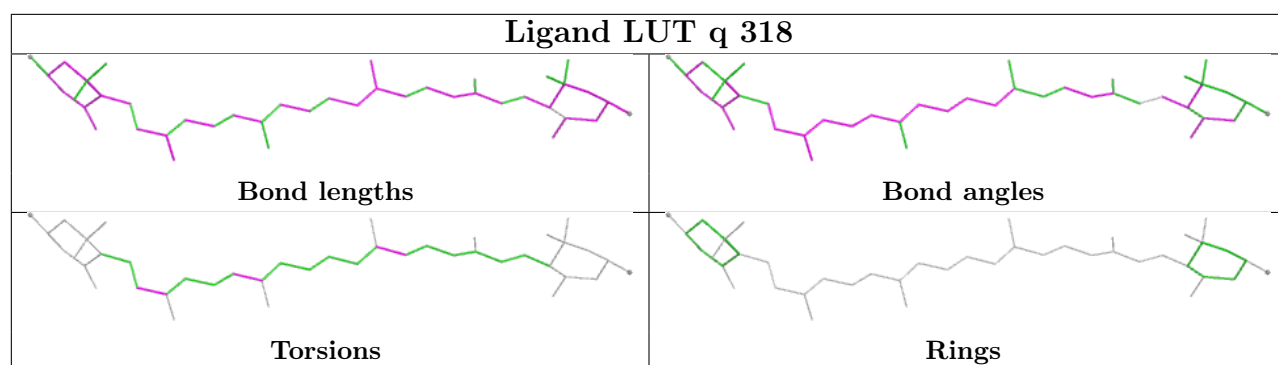
Ligand NEX S 319

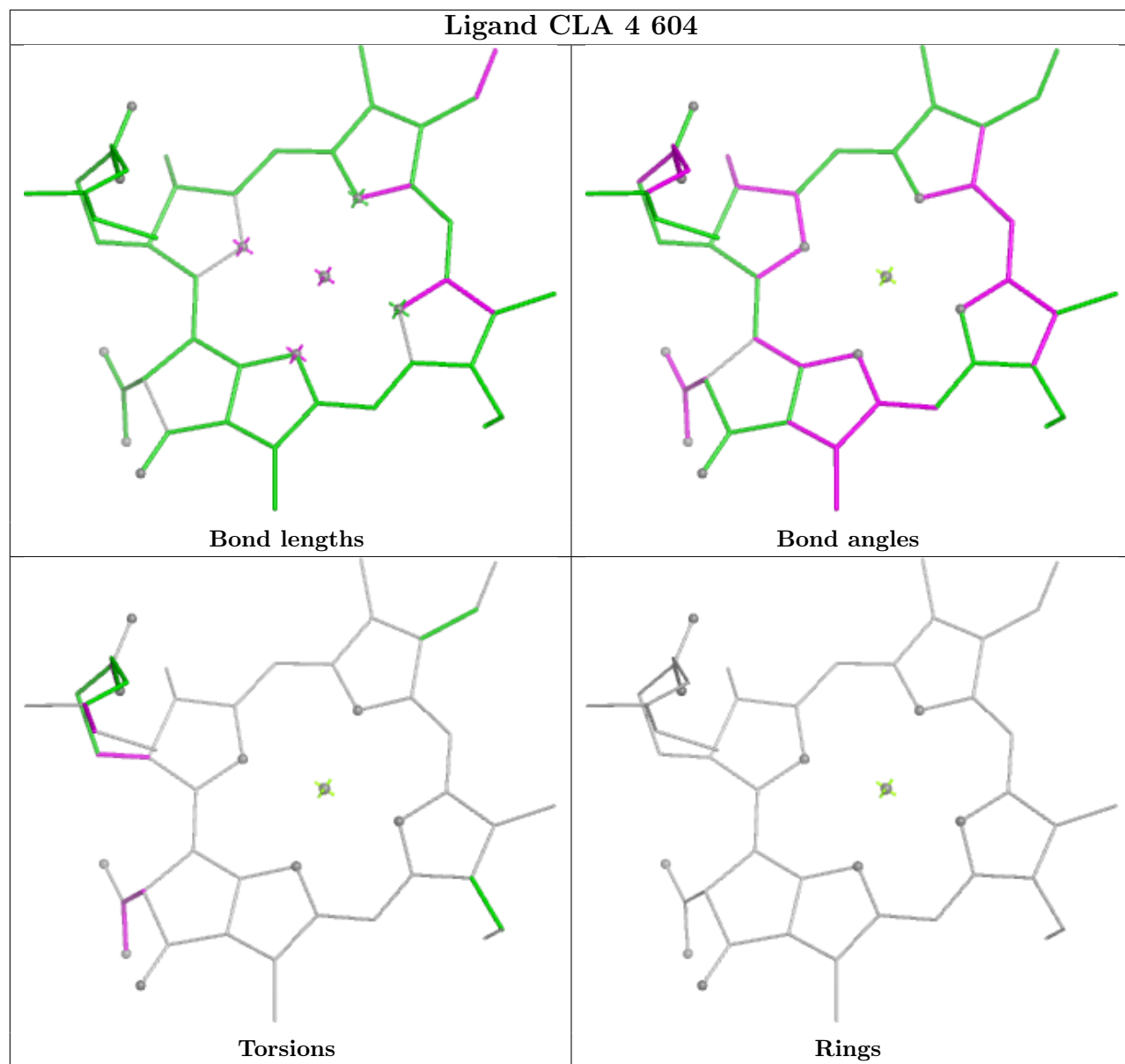


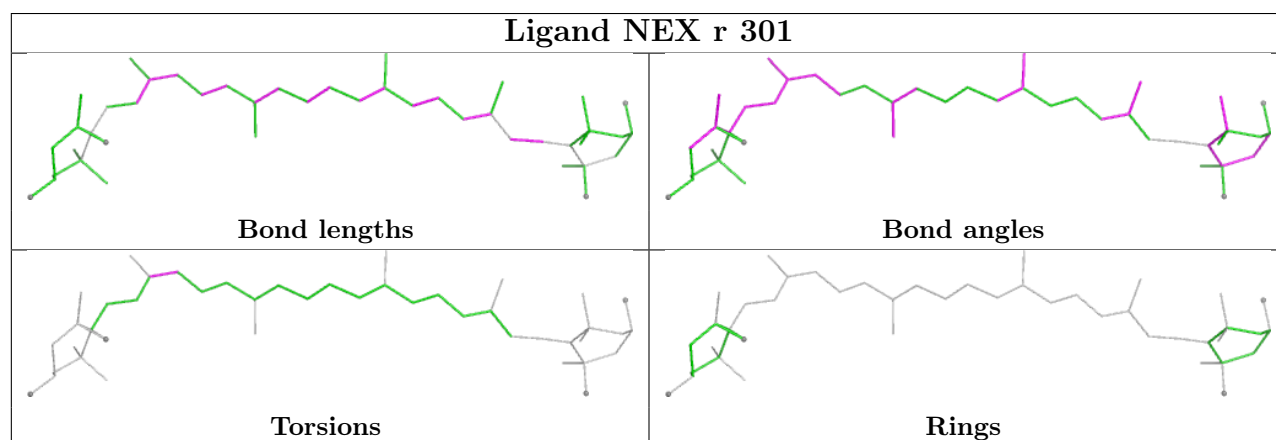
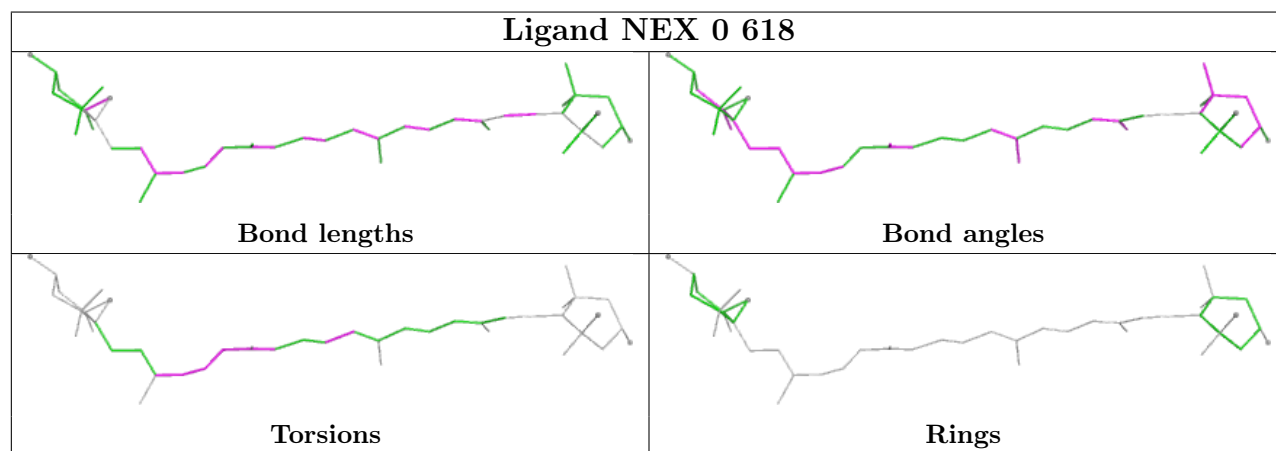
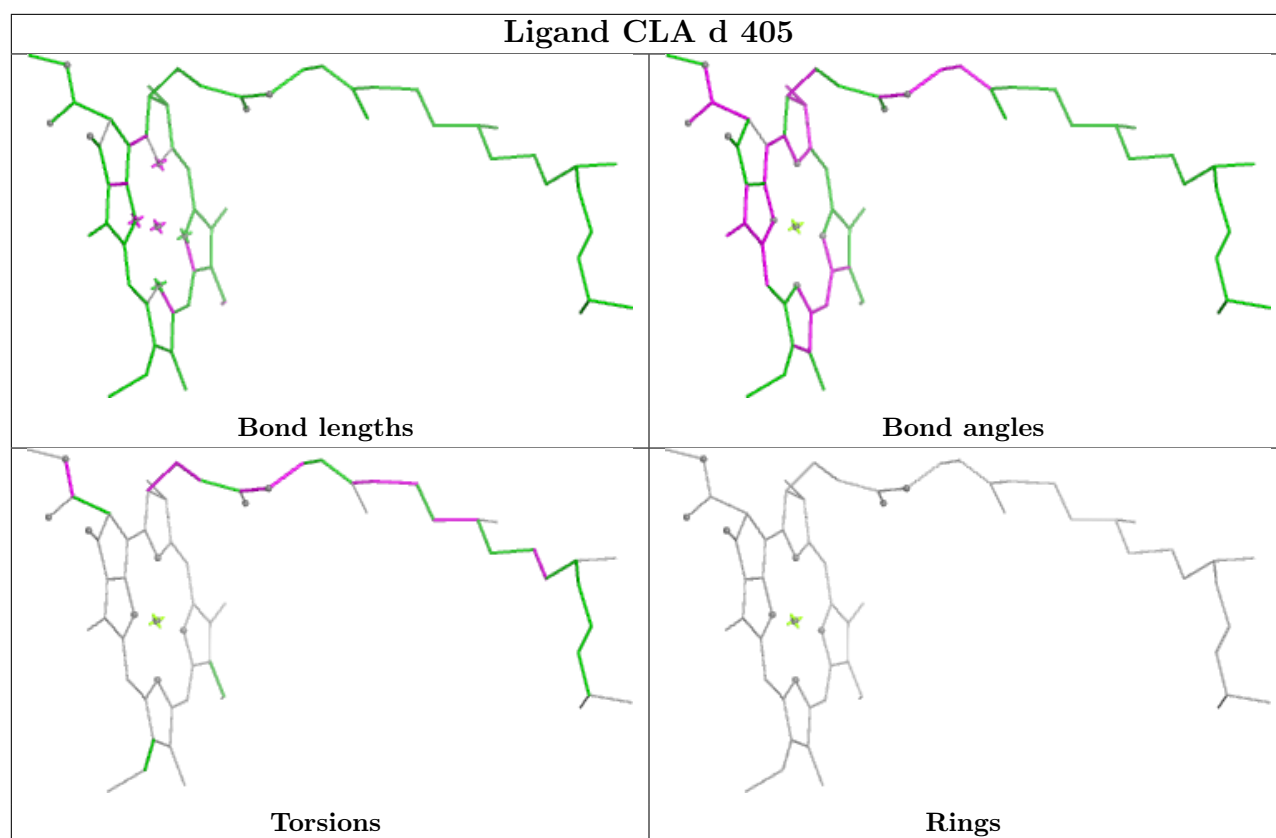
Ligand CHL G 605

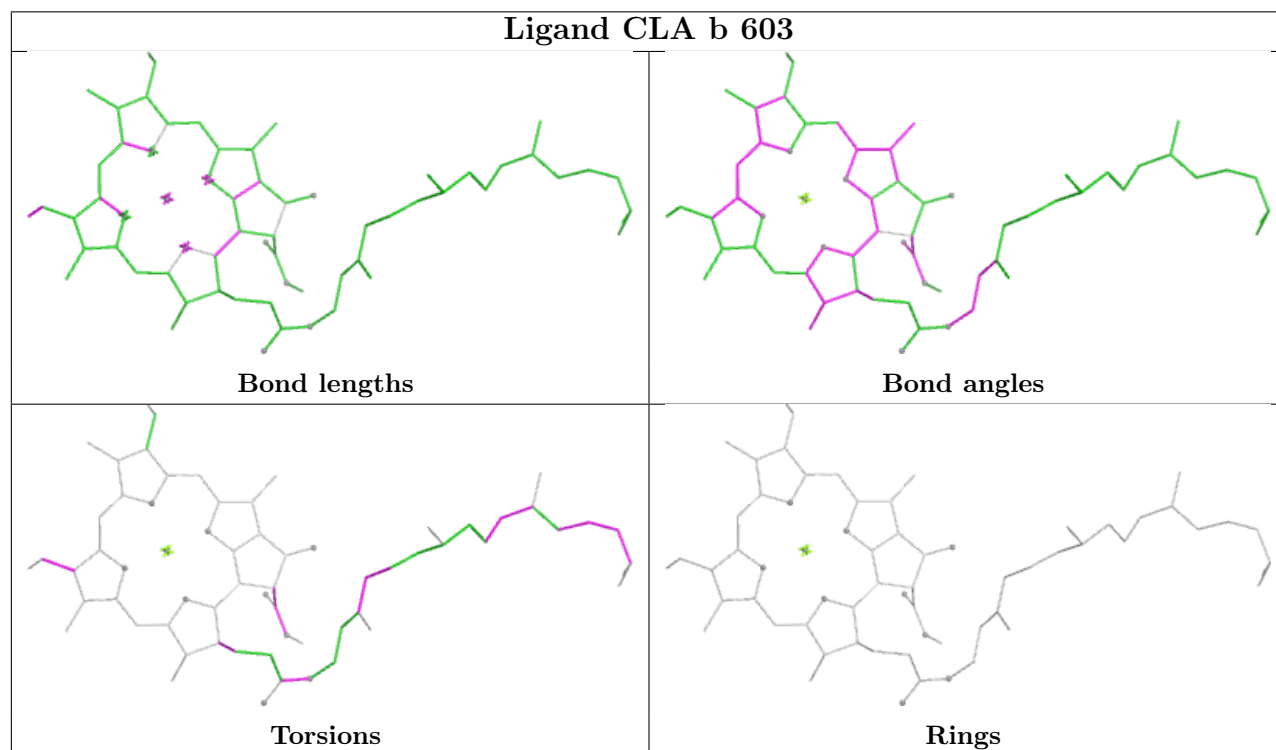
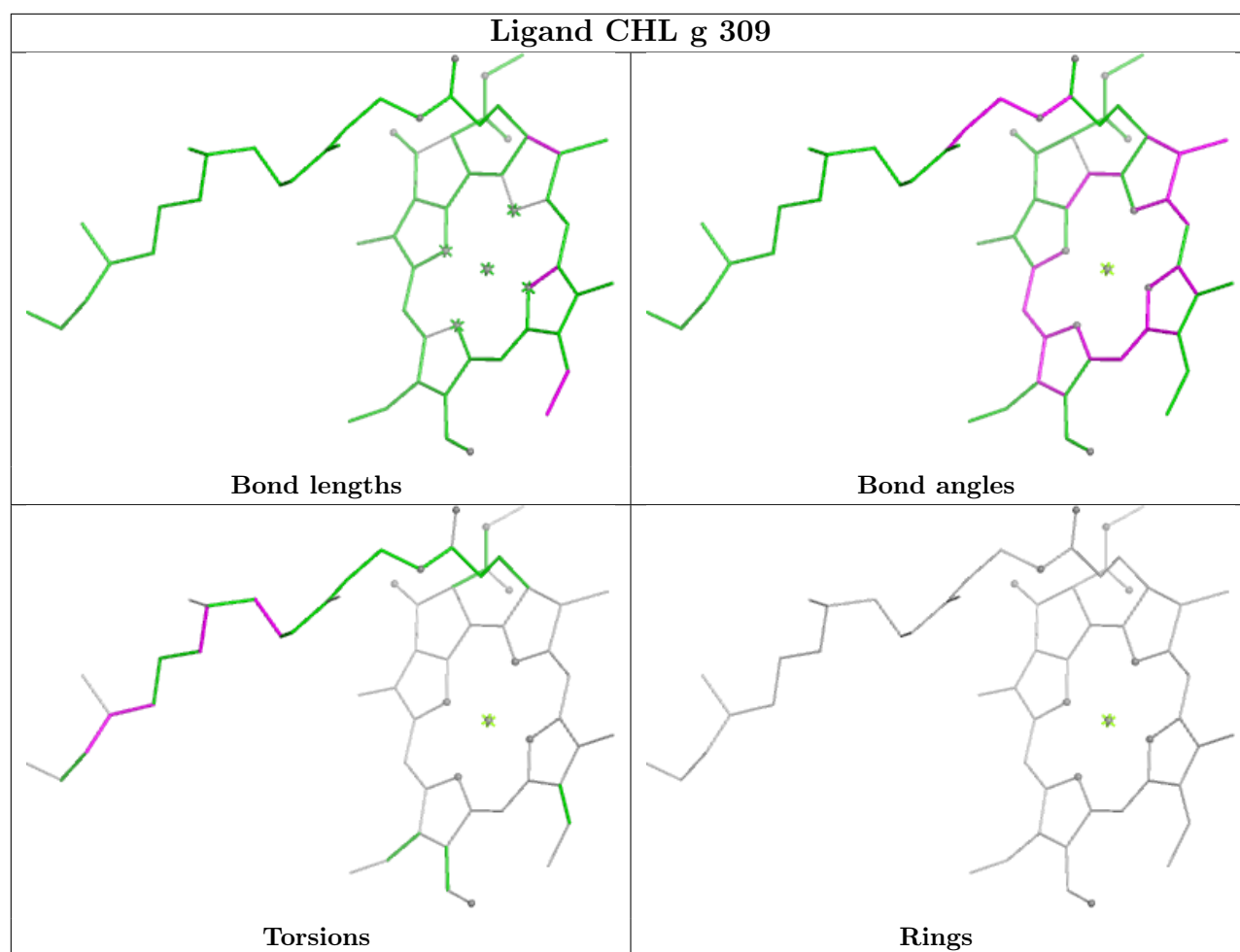




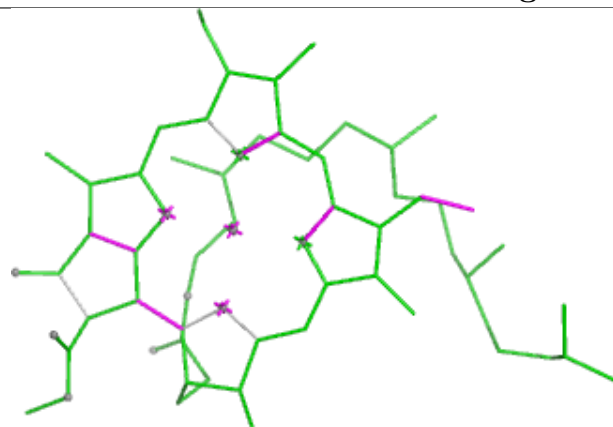




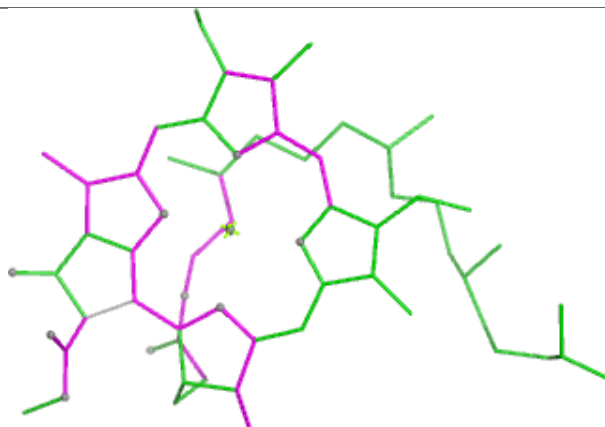




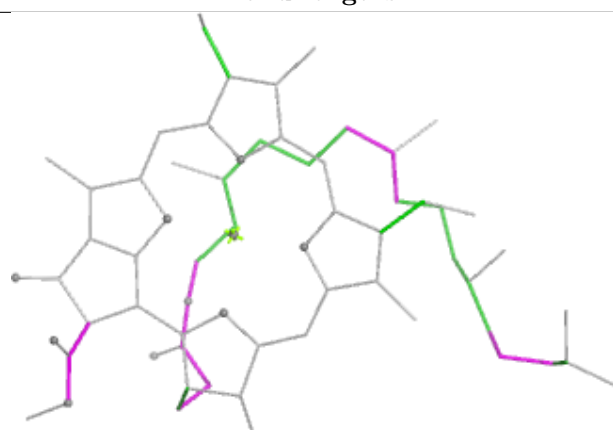
Ligand CLA S 314



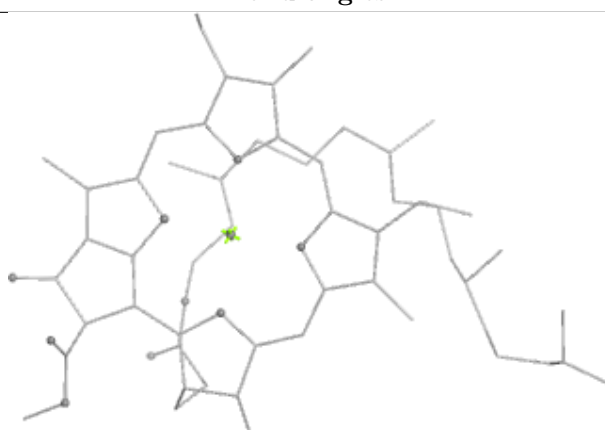
Bond lengths



Bond angles

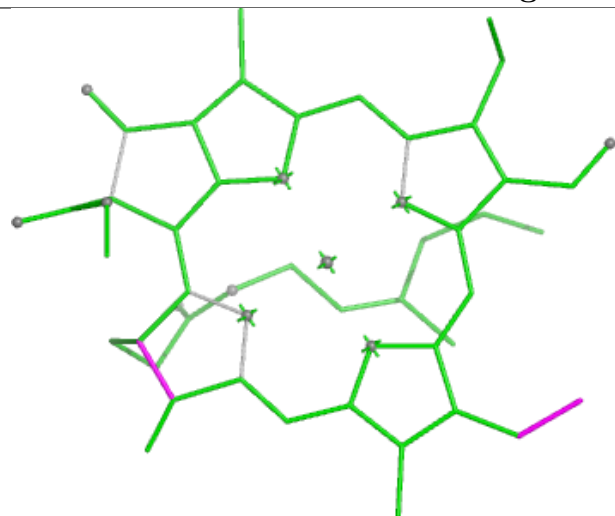


Torsions

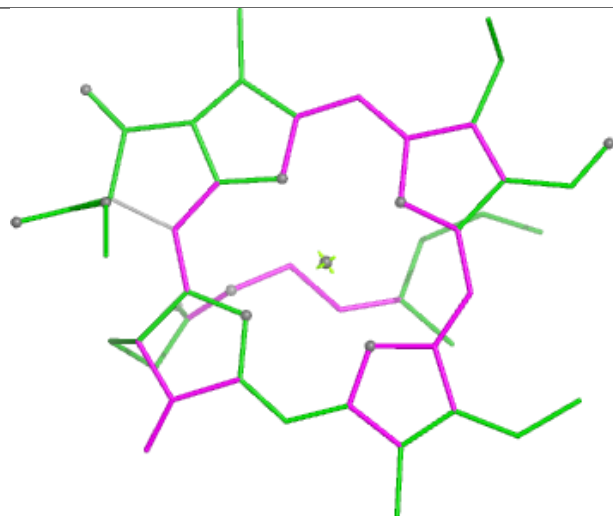


Rings

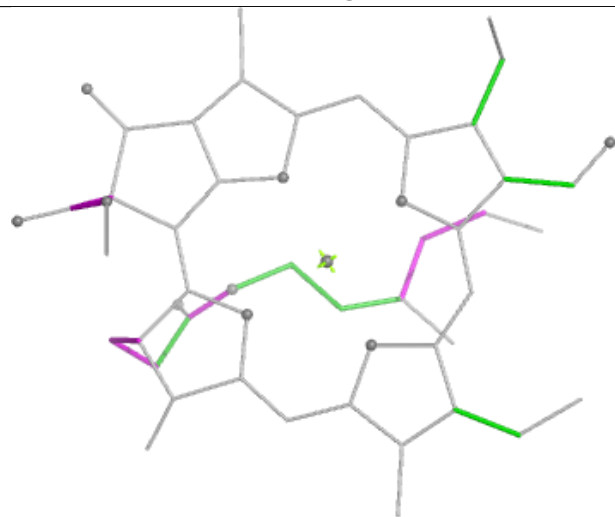
Ligand CHL 9 309



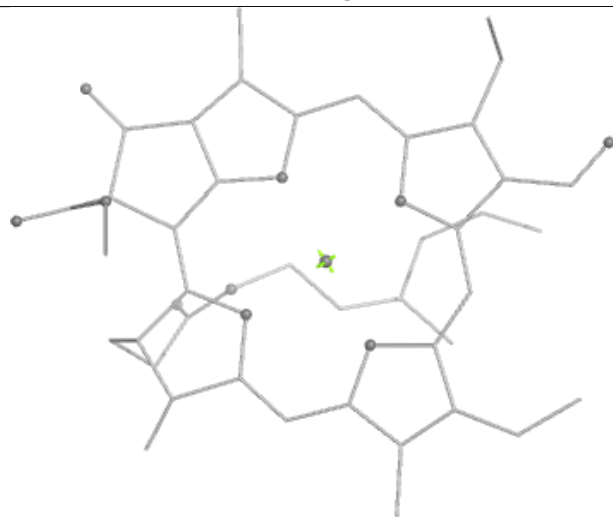
Bond lengths



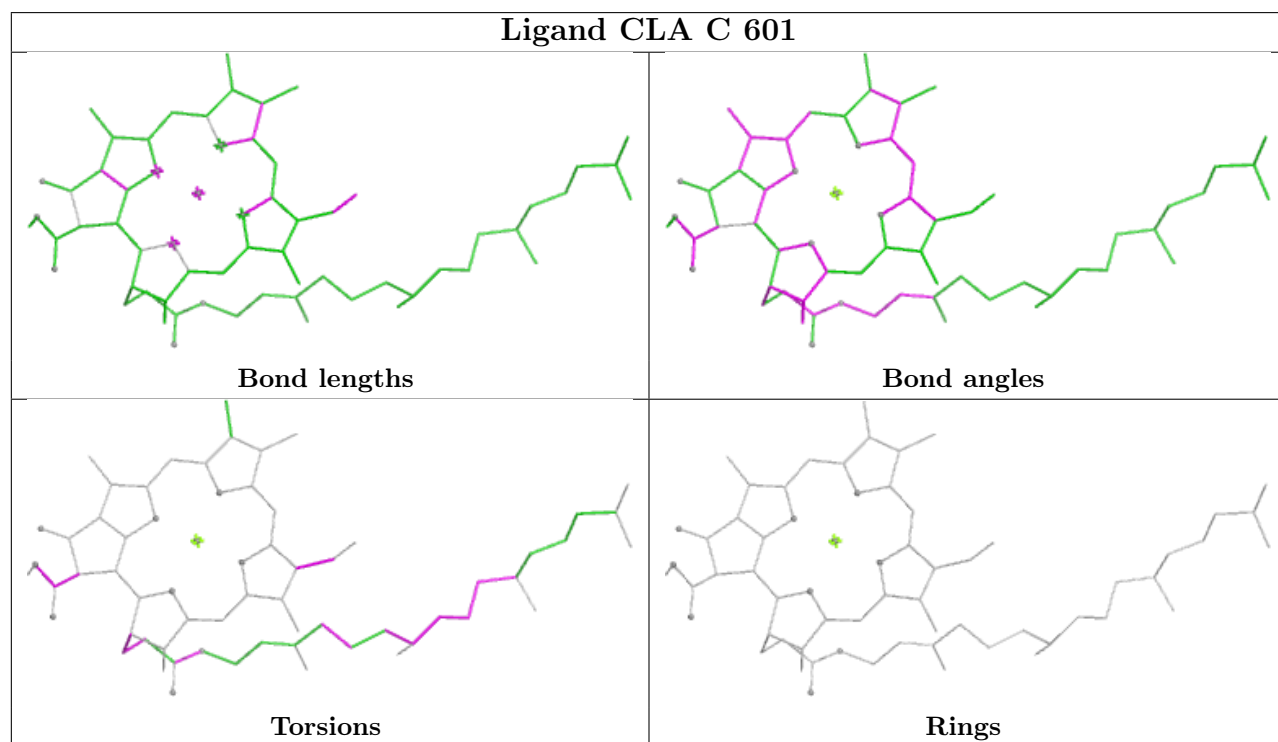
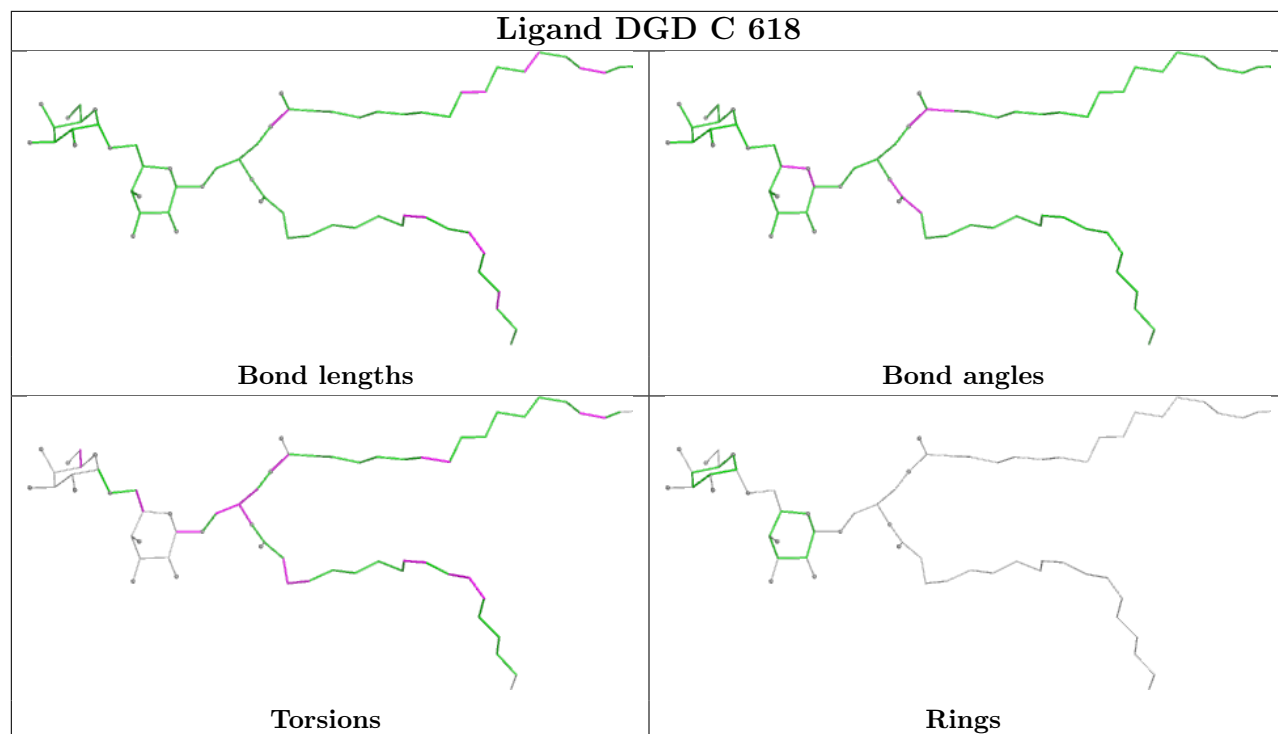
Bond angles

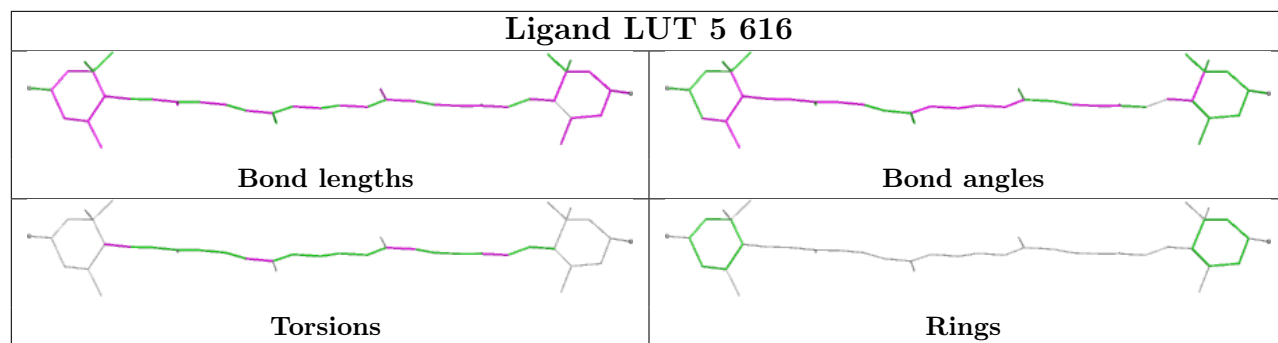


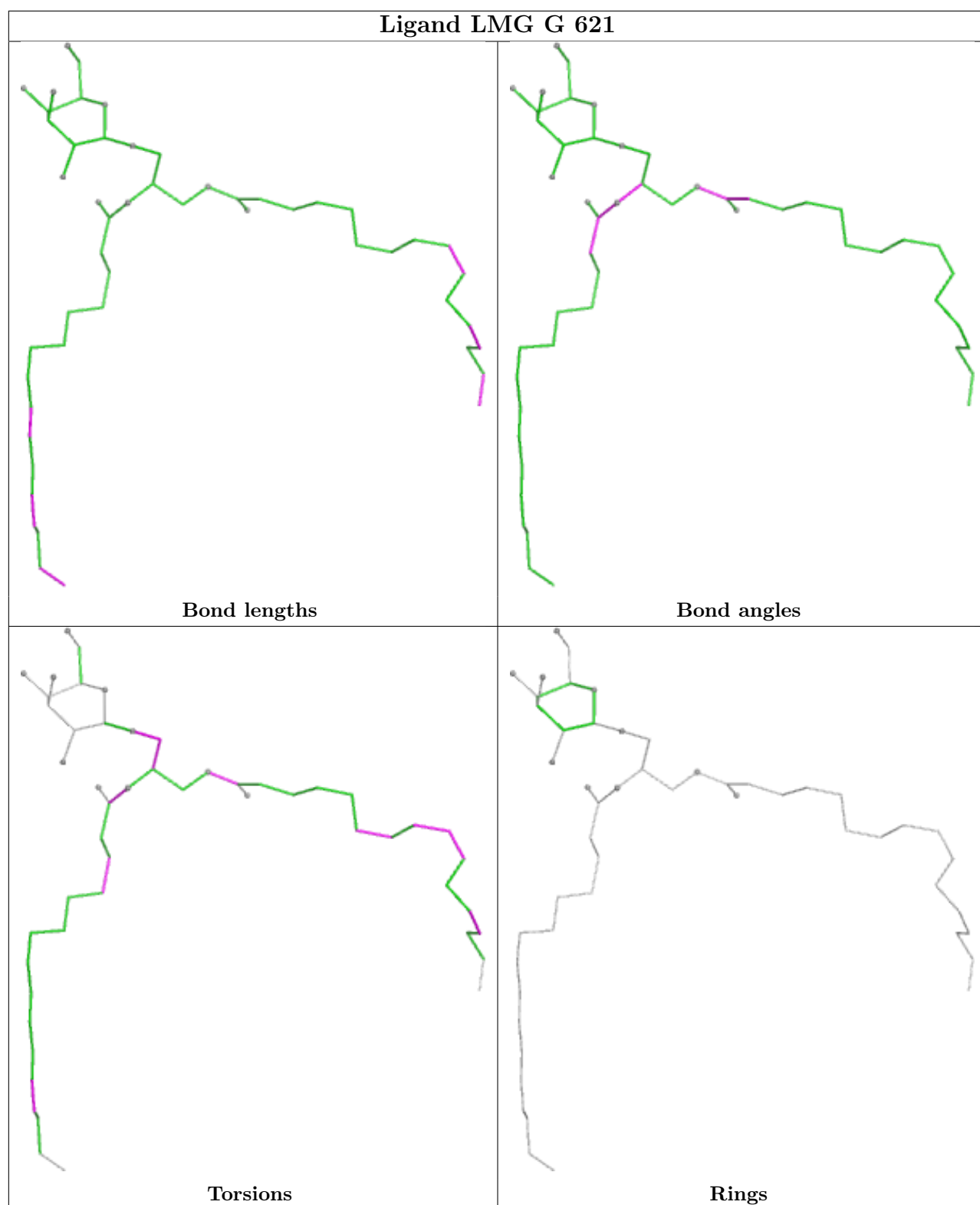
Torsions

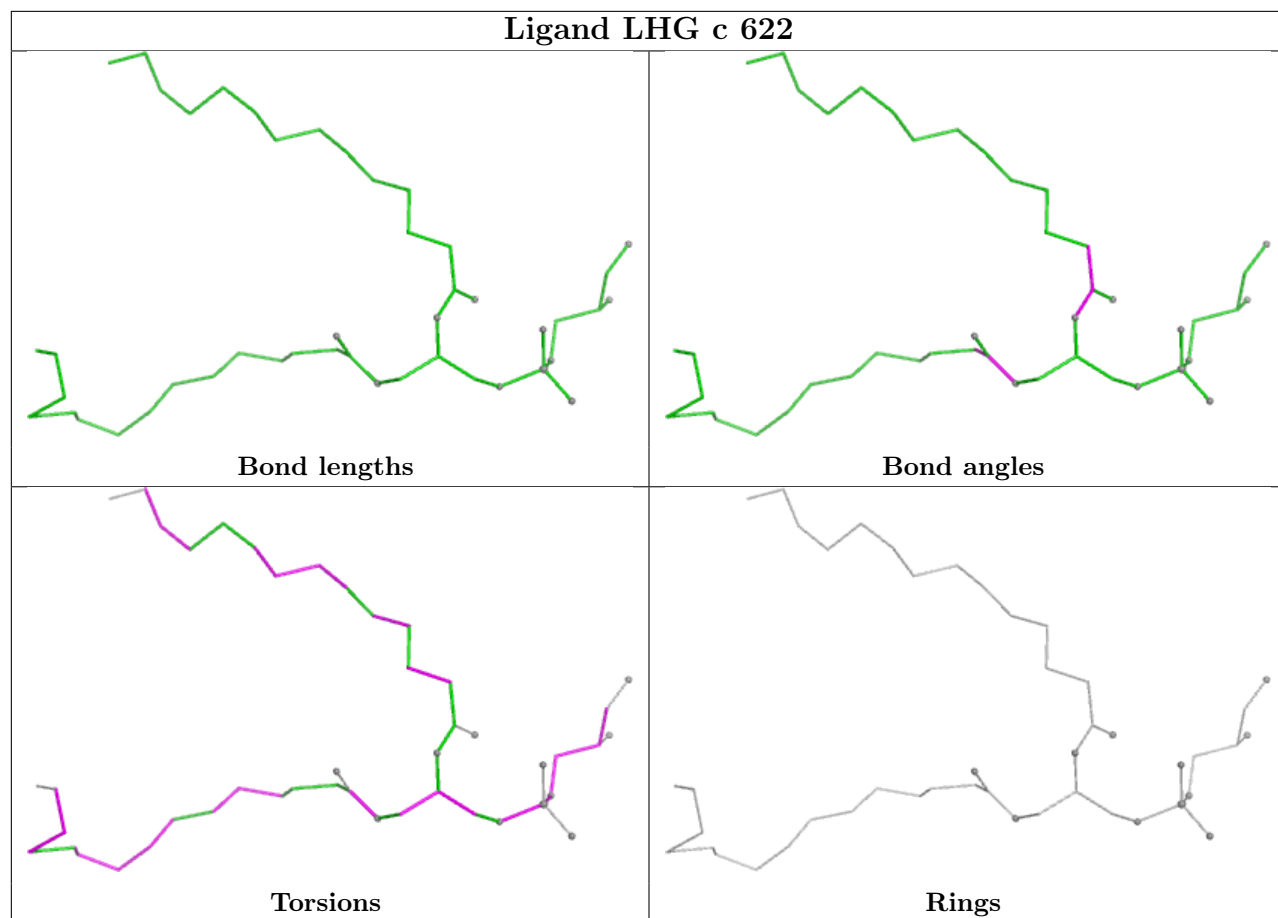


Rings

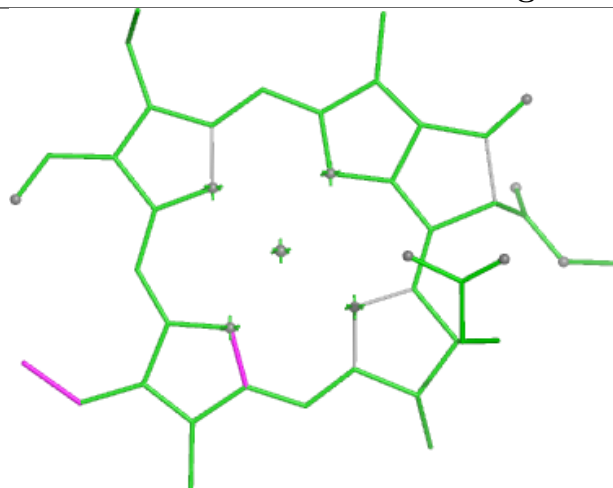




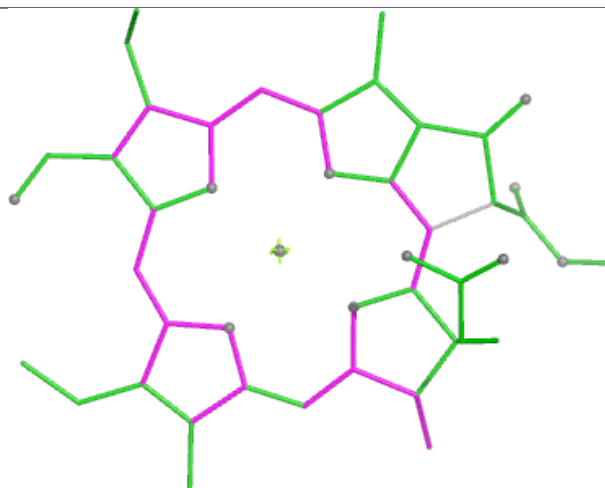




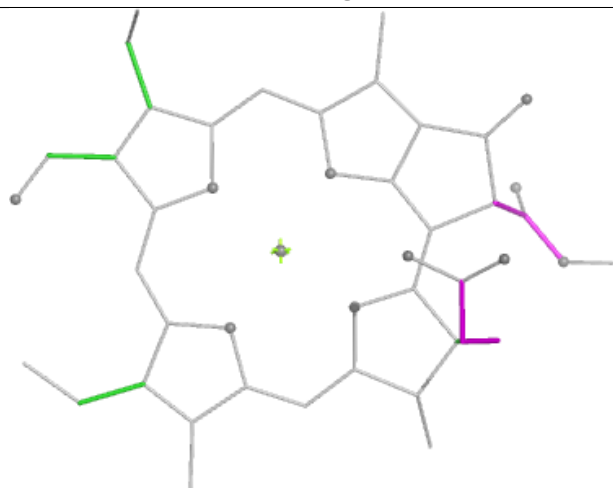
Ligand CHL 9 307



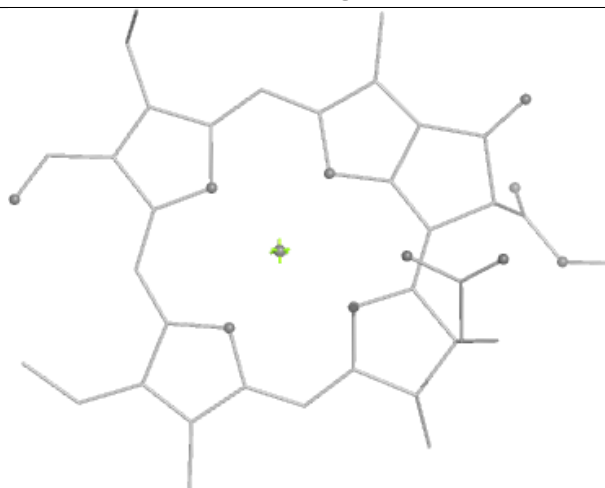
Bond lengths



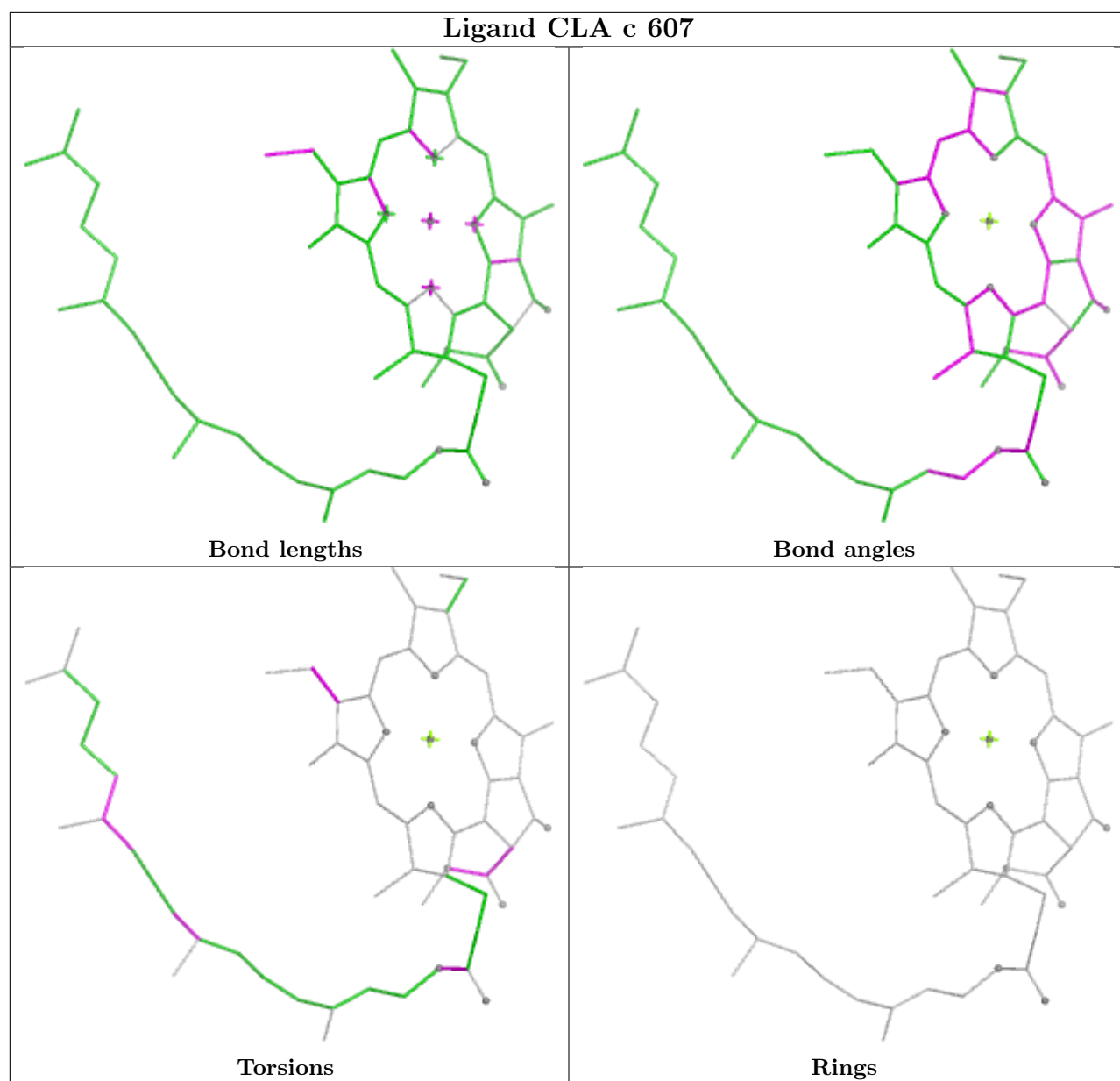
Bond angles

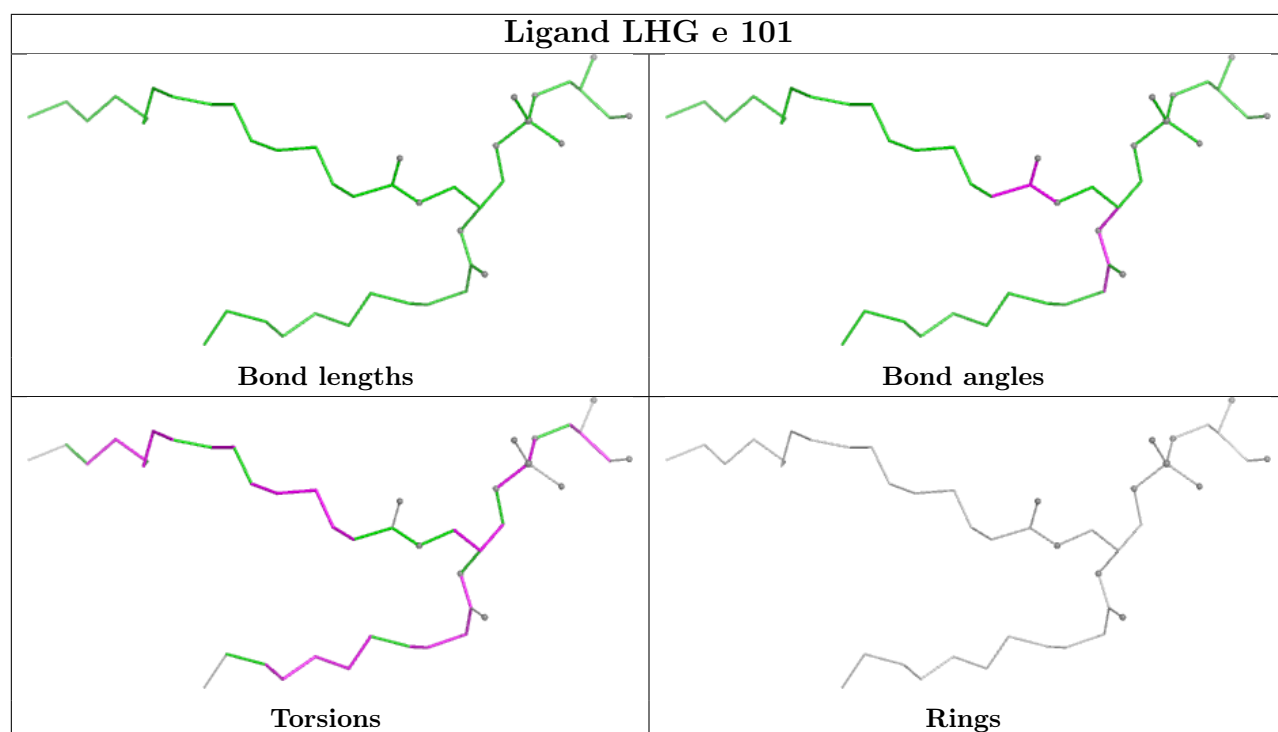


Torsions

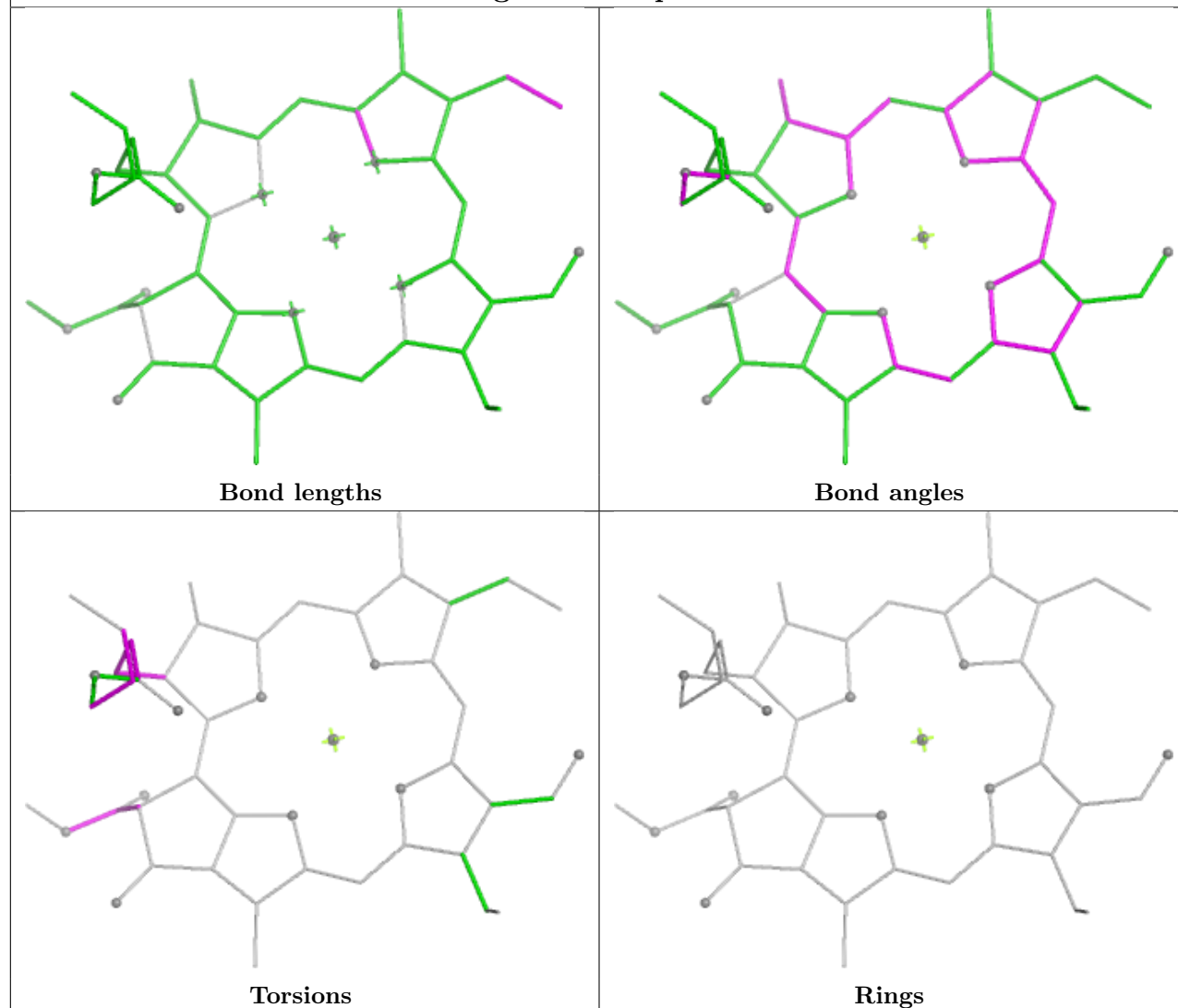


Rings

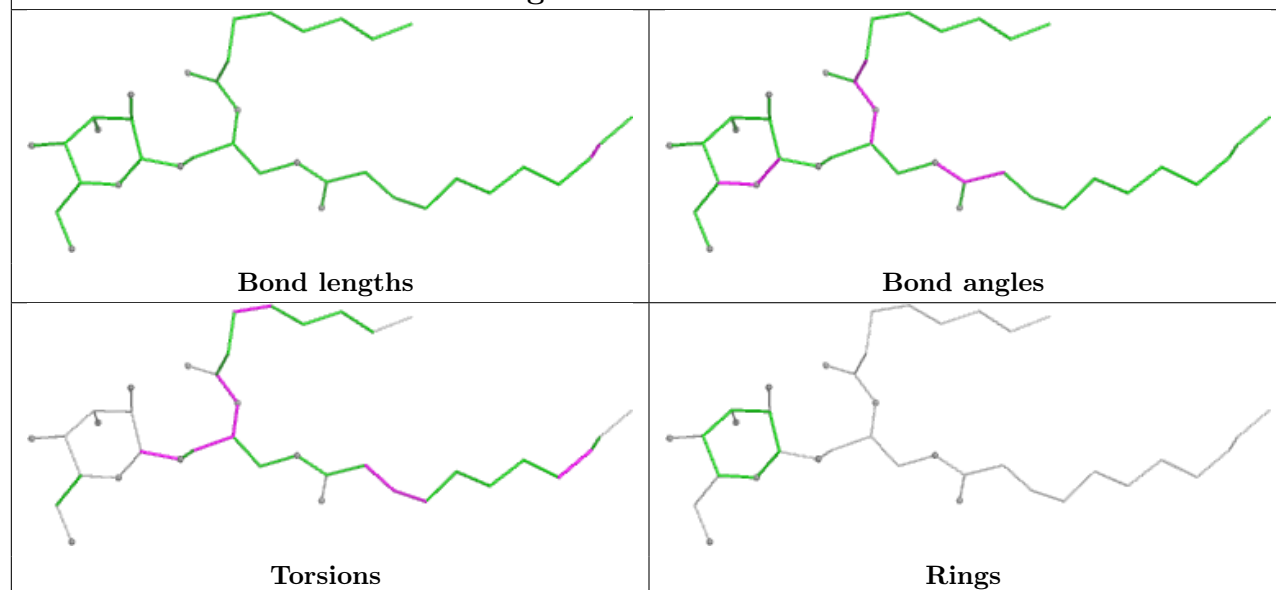




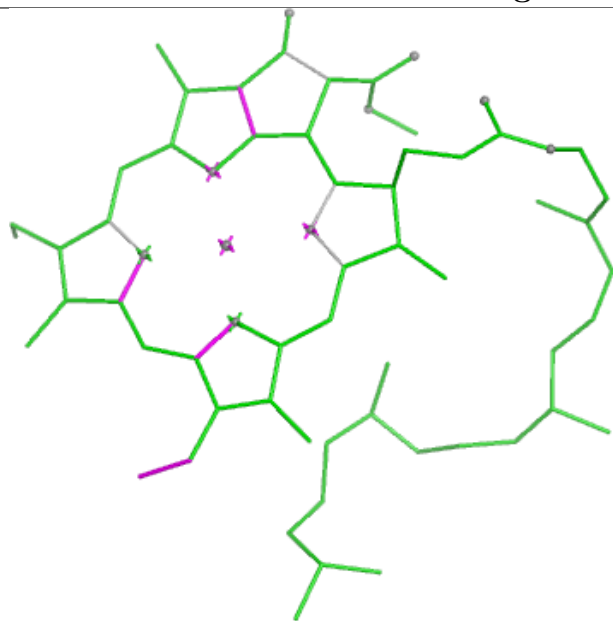
Ligand CHL p 608



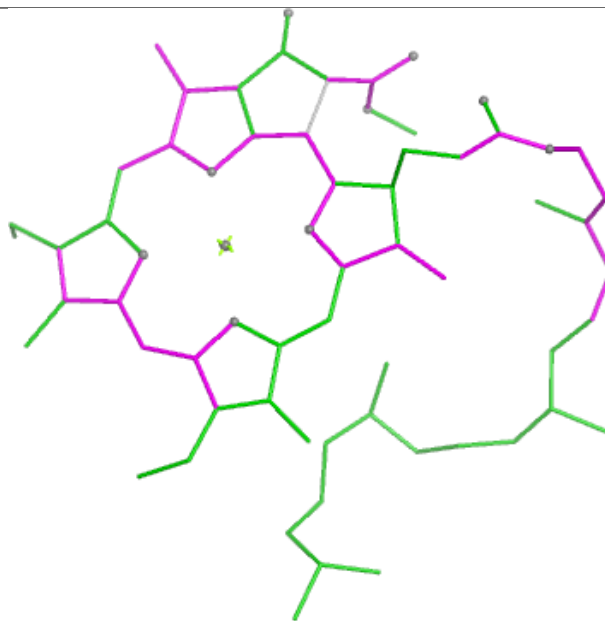
Ligand LMG A 414



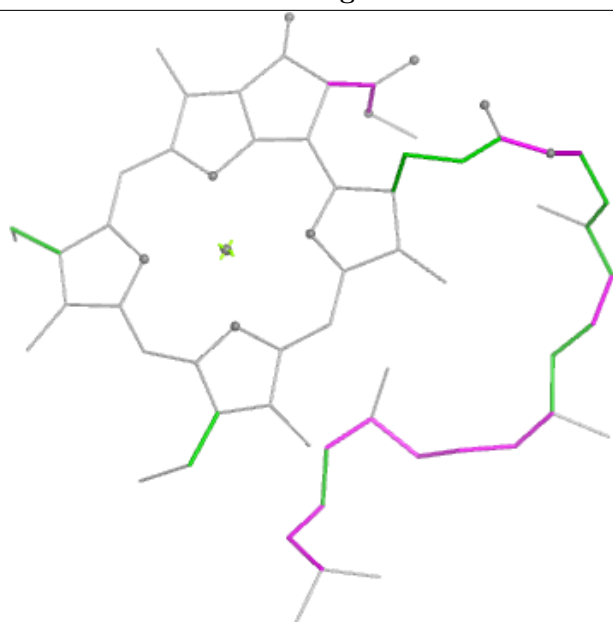
Ligand CLA Y 312



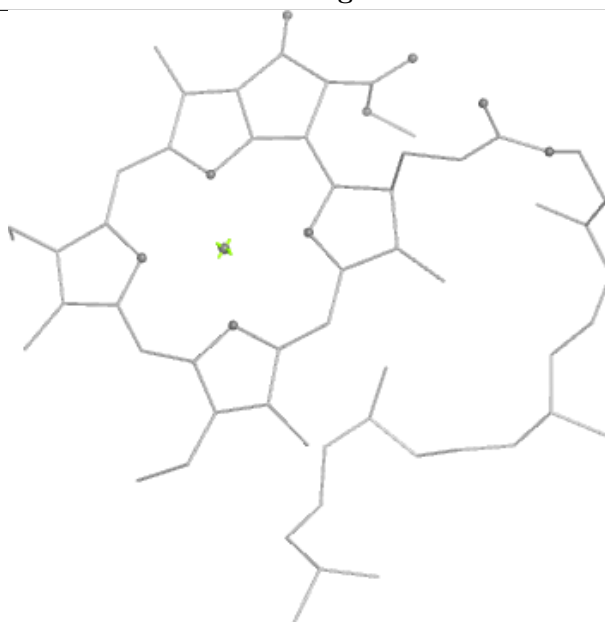
Bond lengths



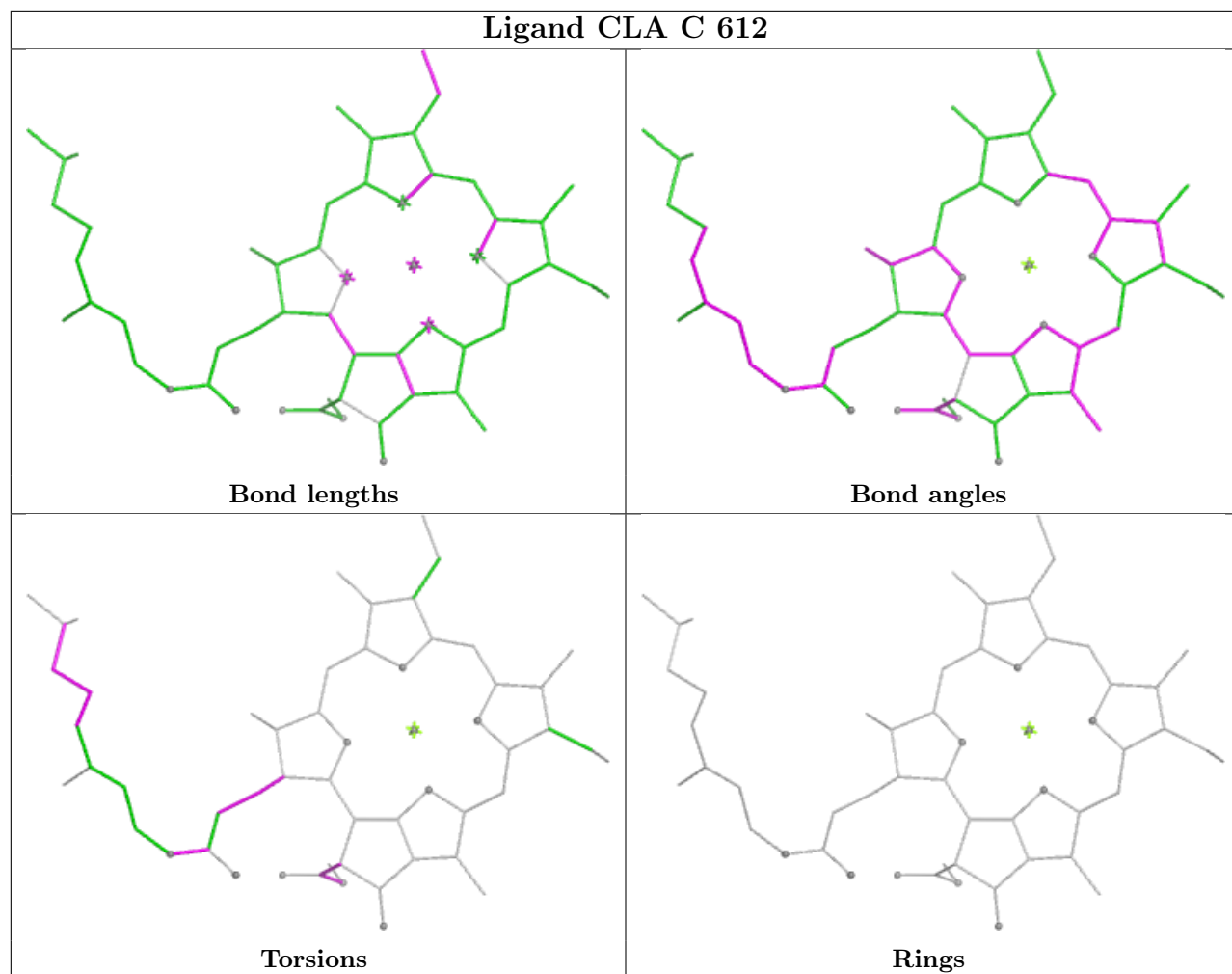
Bond angles

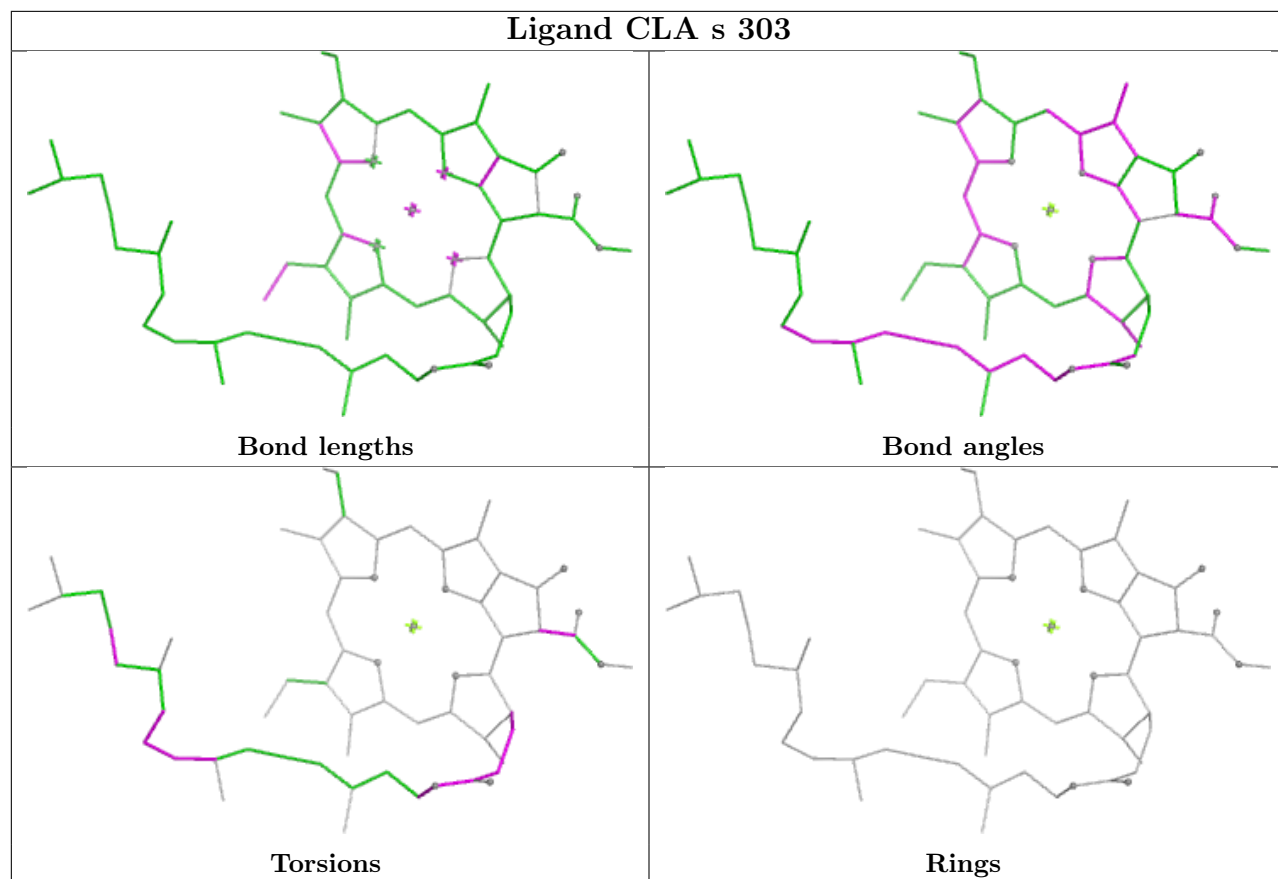


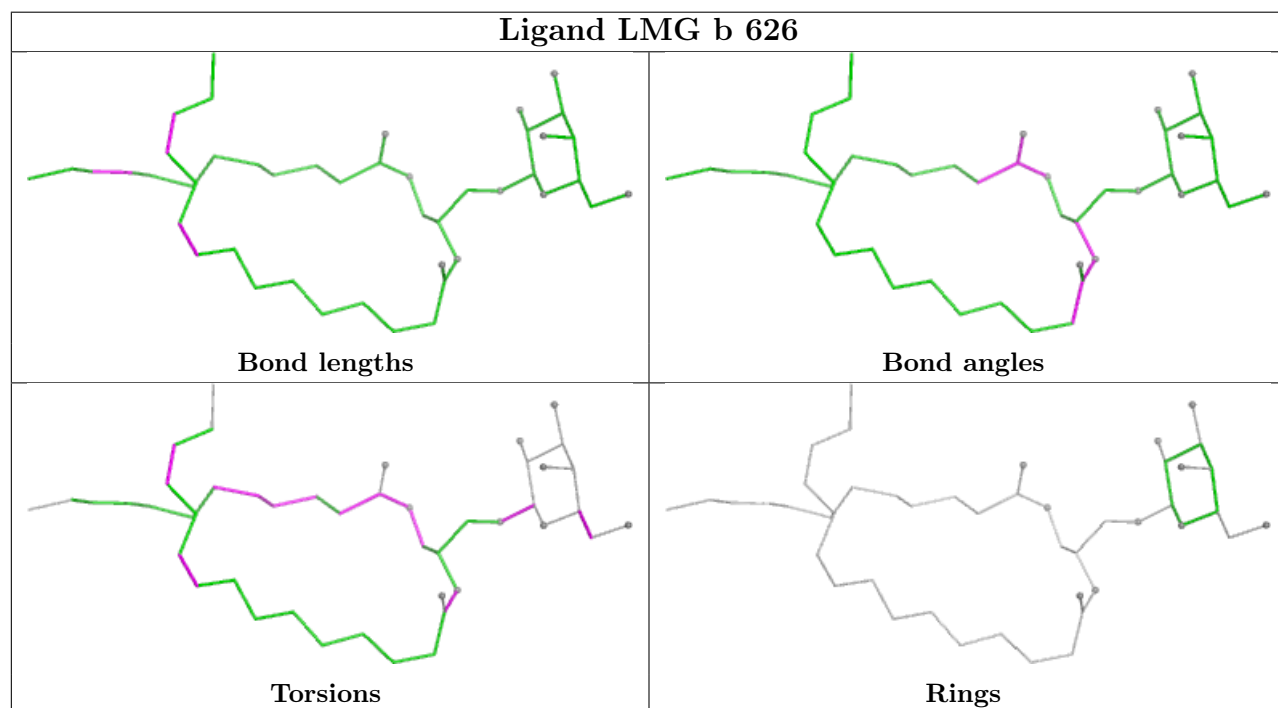
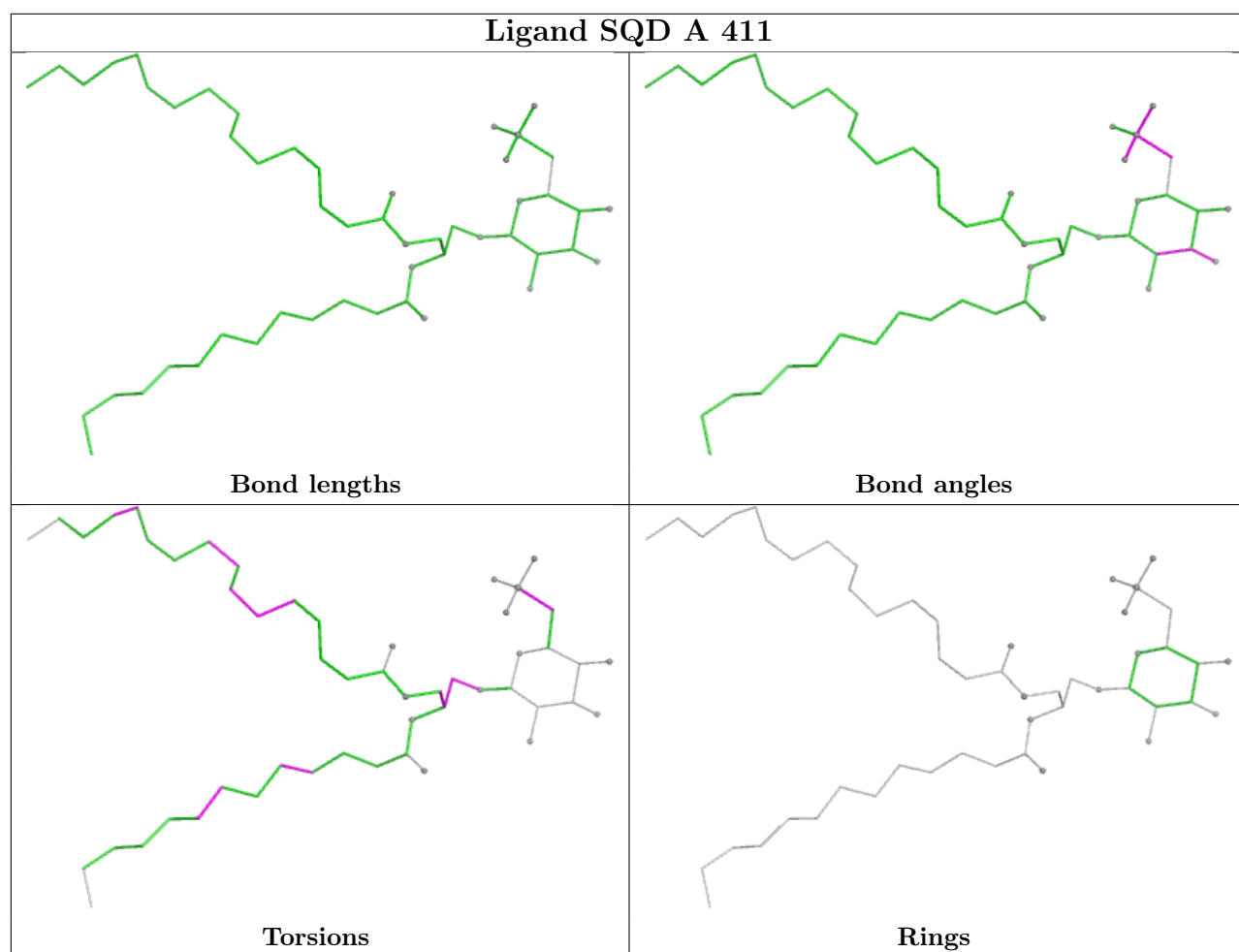
Torsions

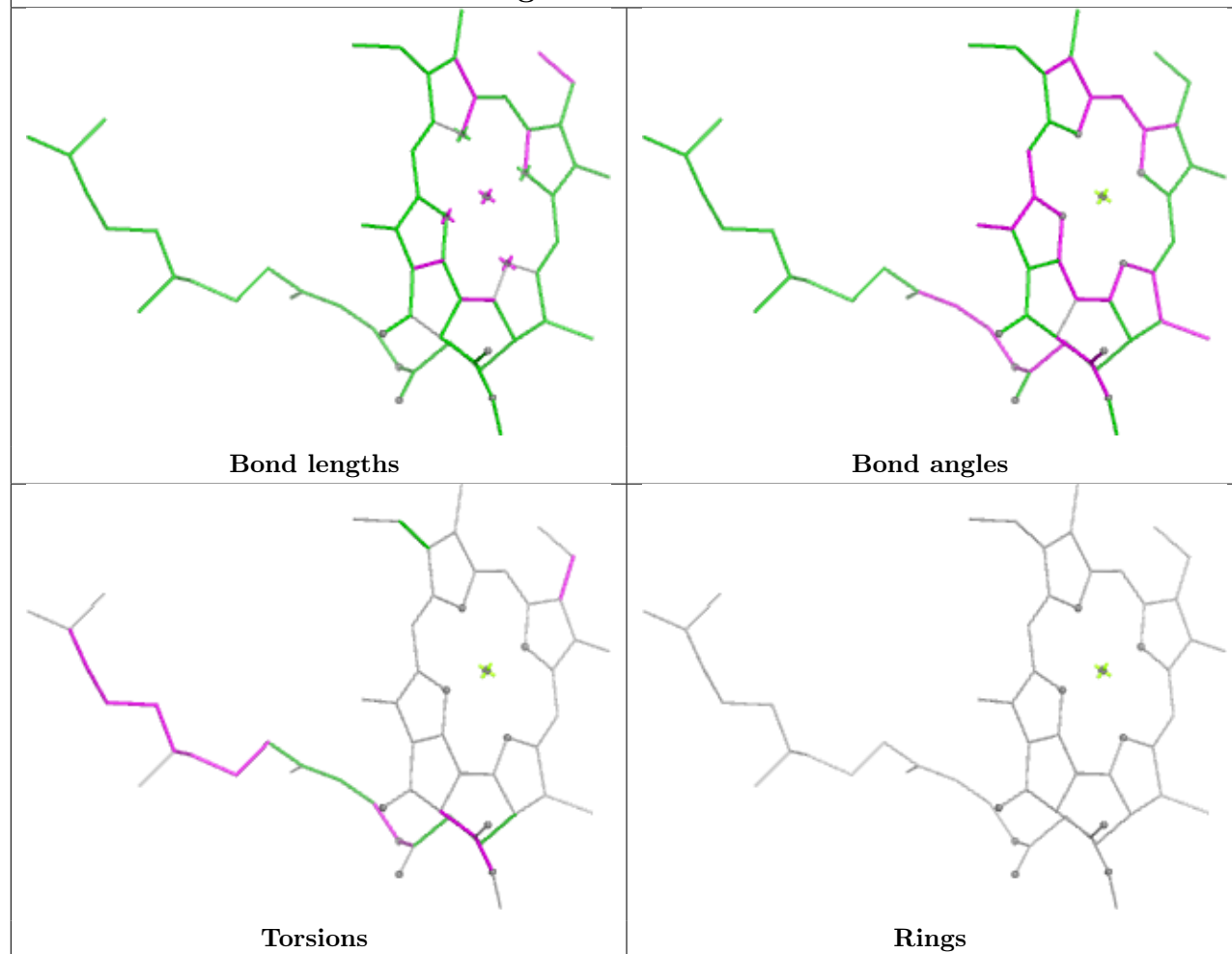
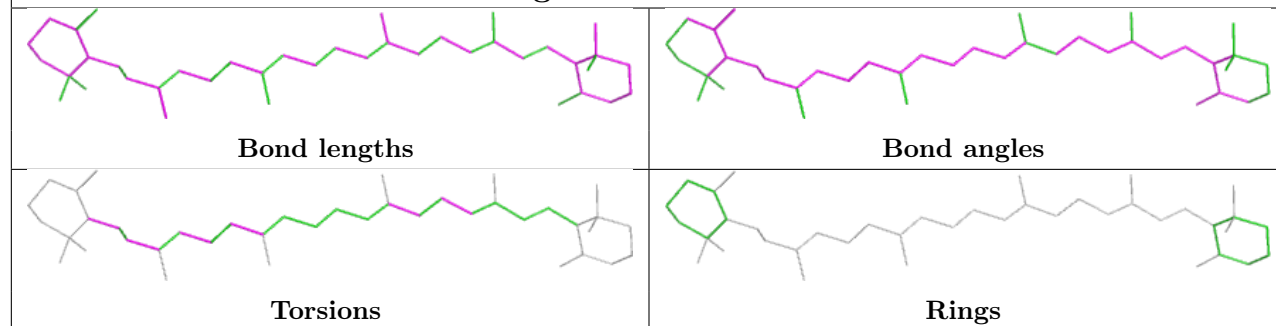


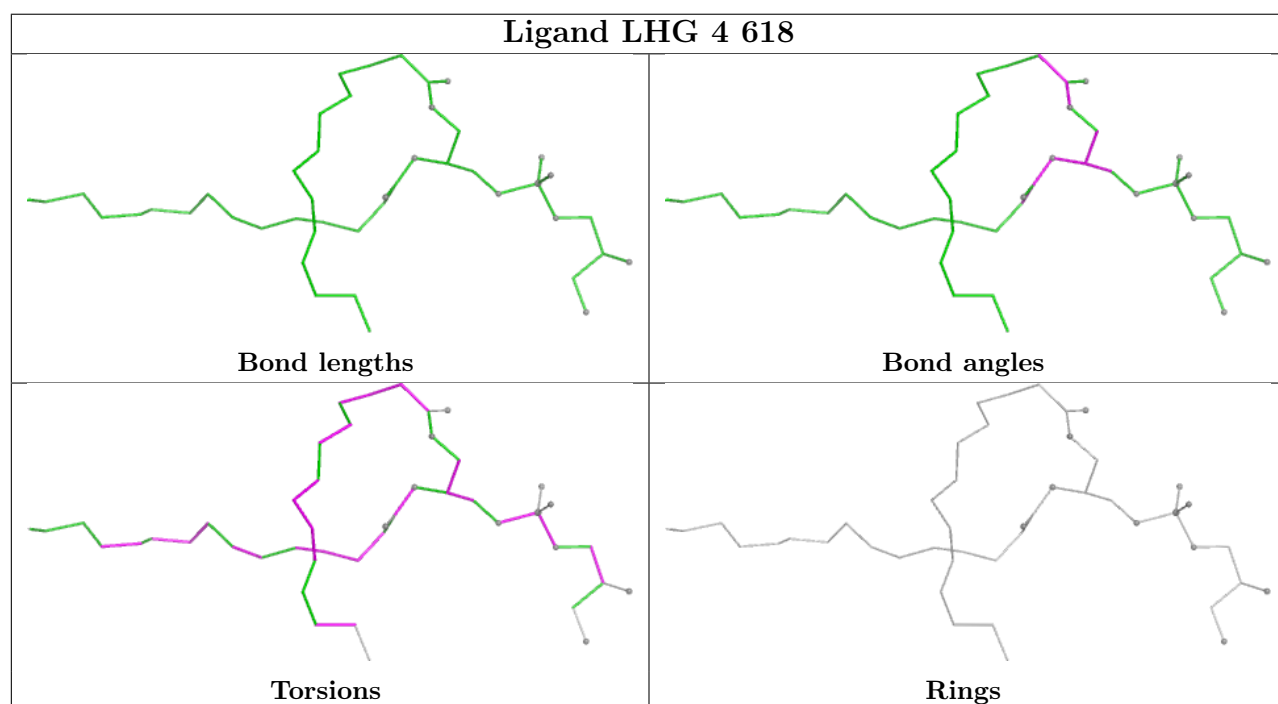
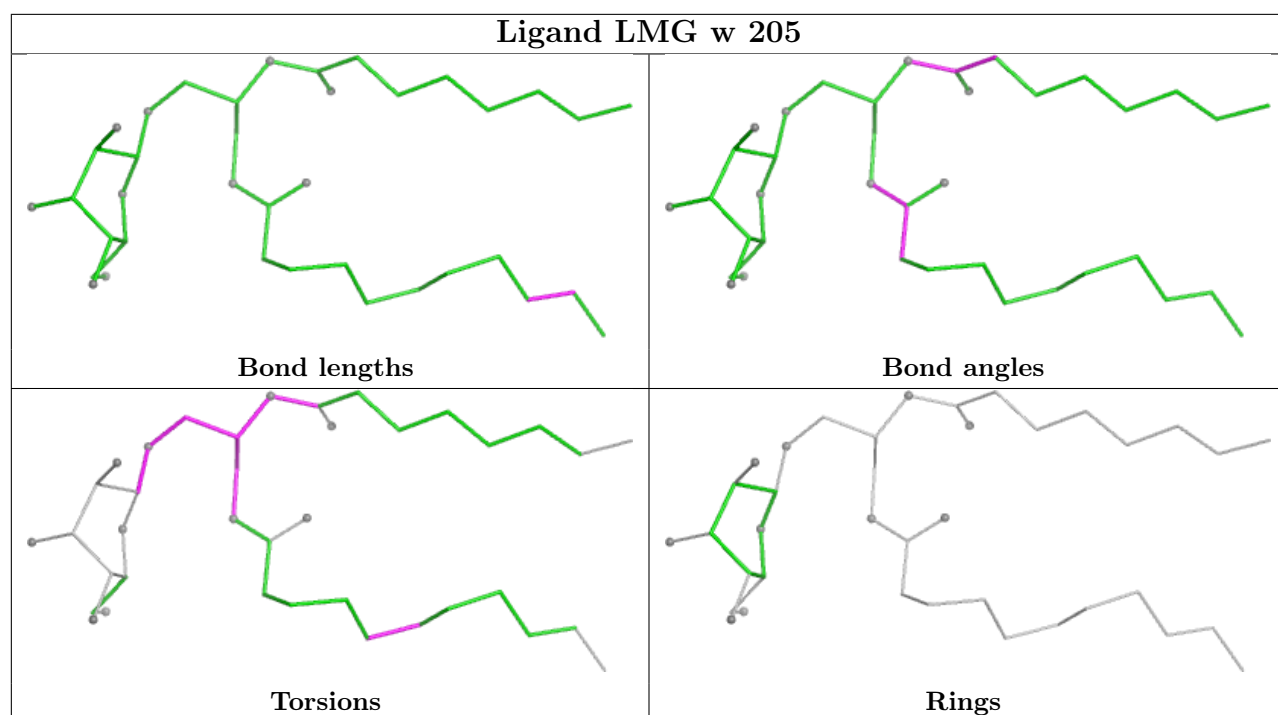
Rings

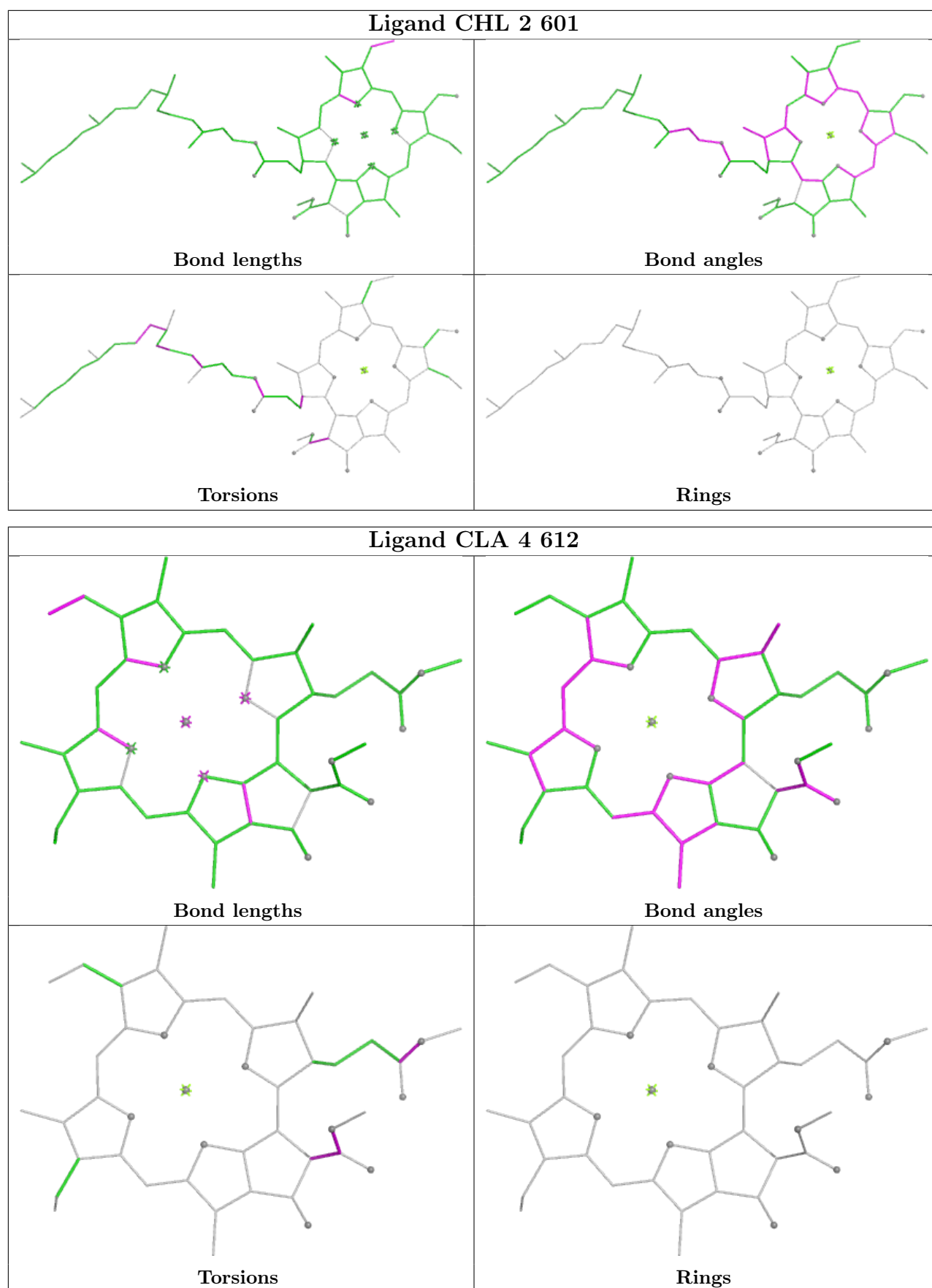


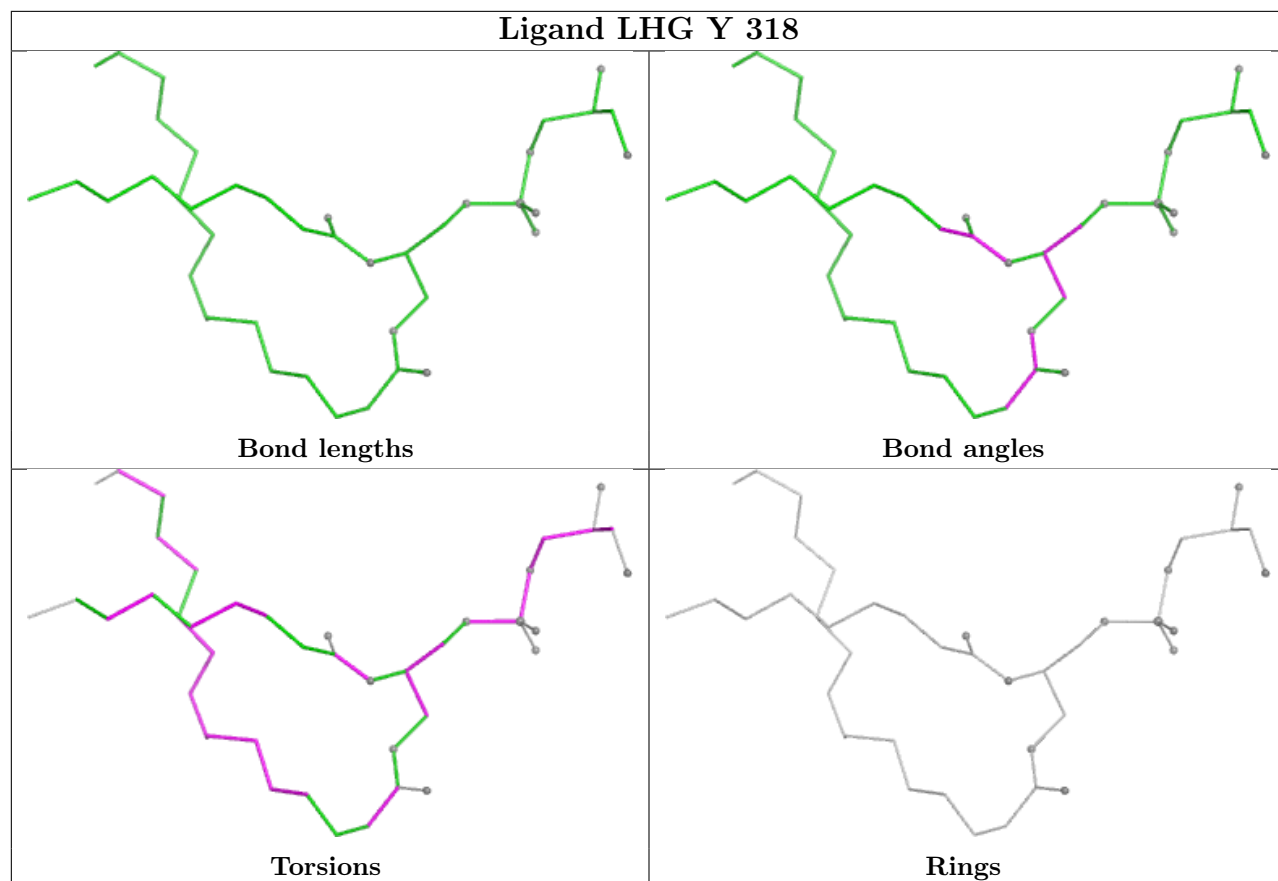


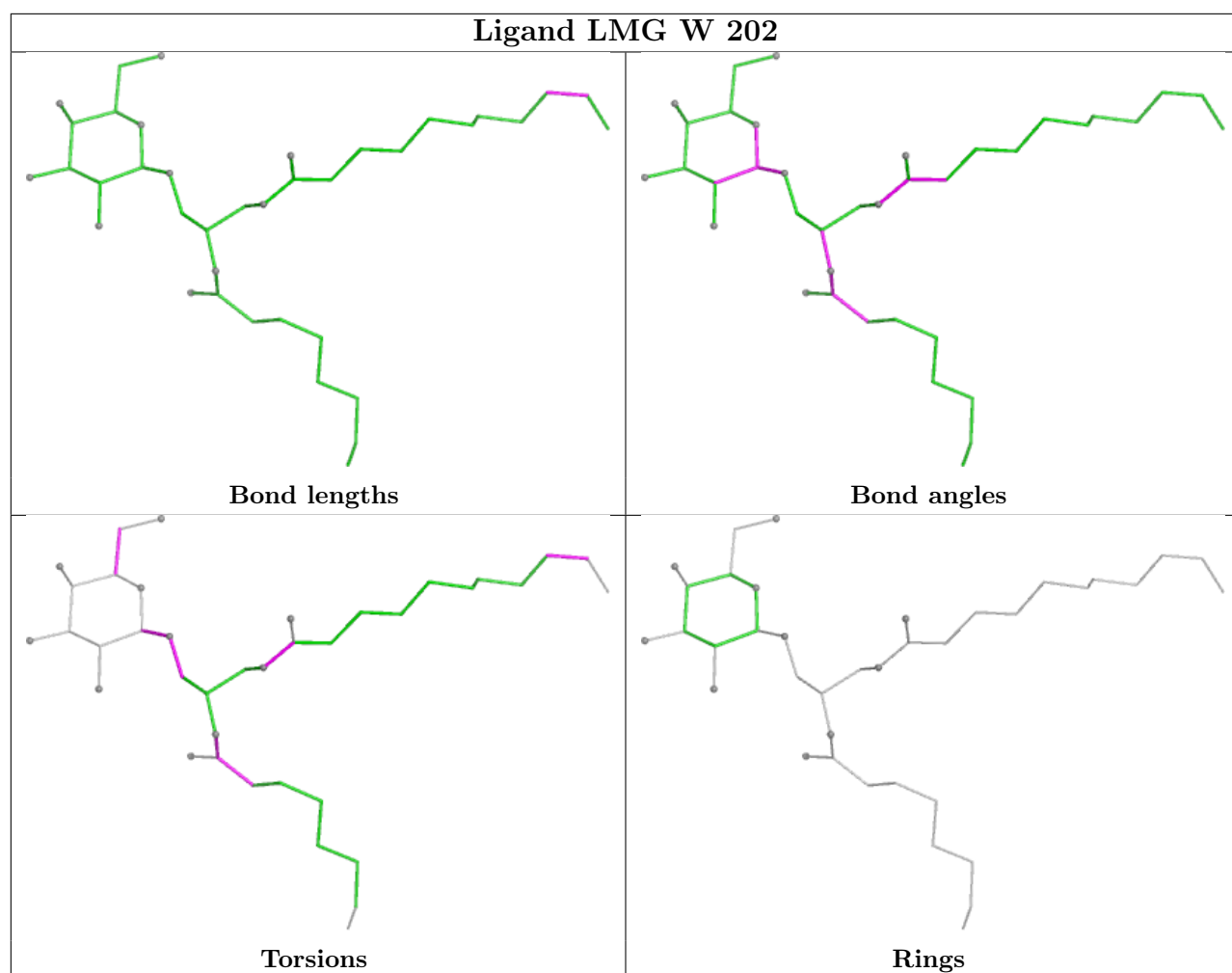


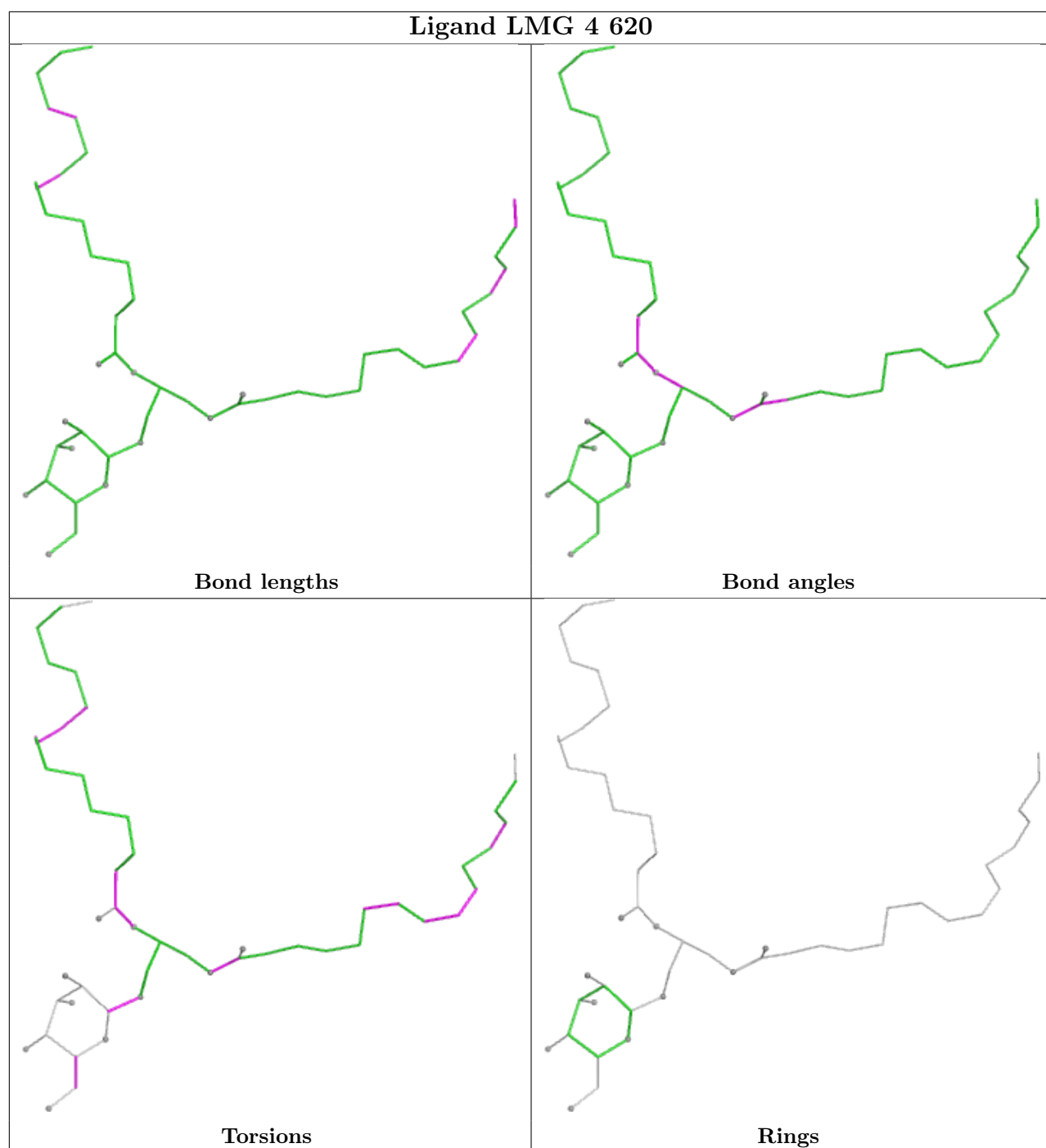
Ligand CLA 6 312**Ligand BCR b 620**

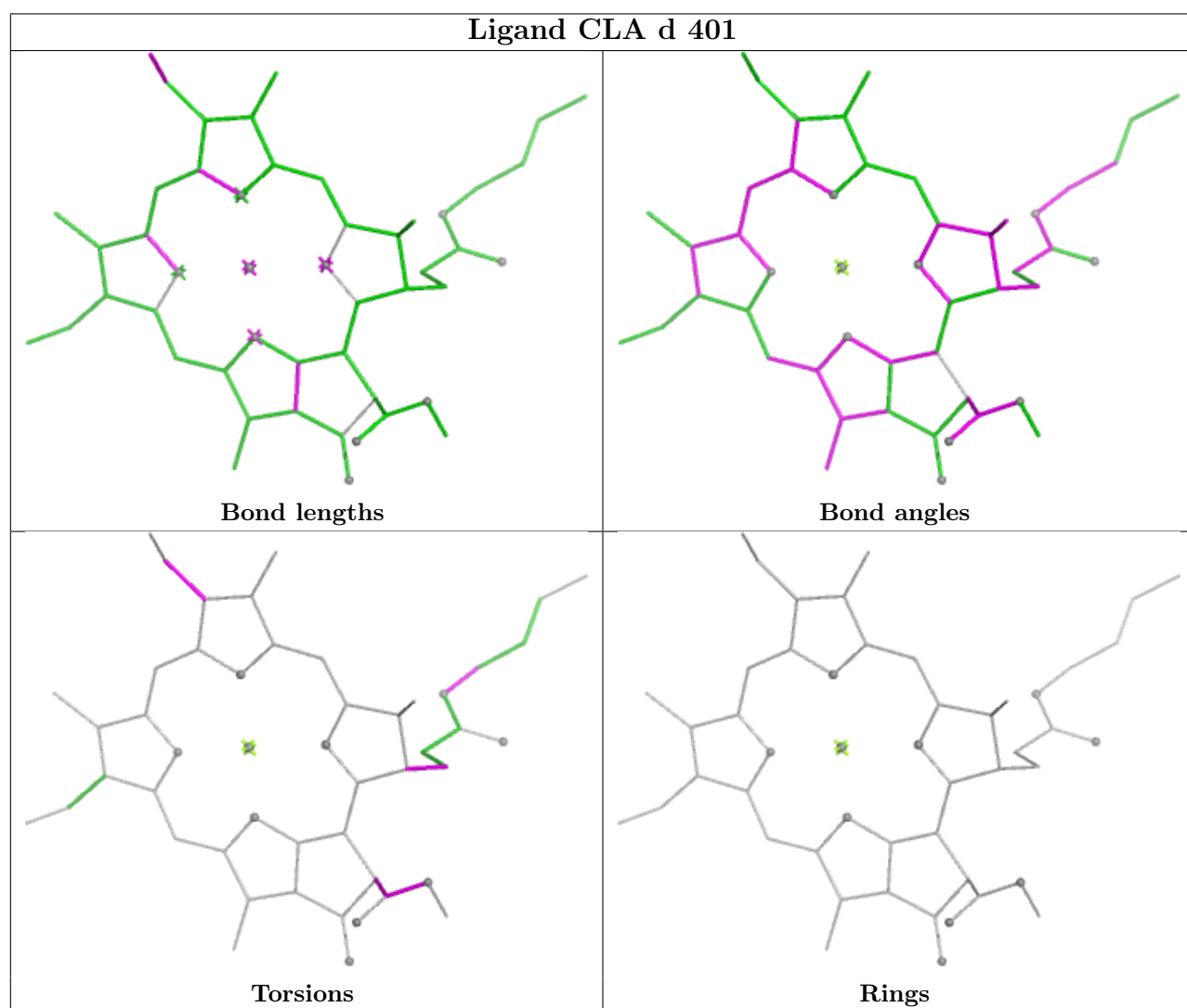
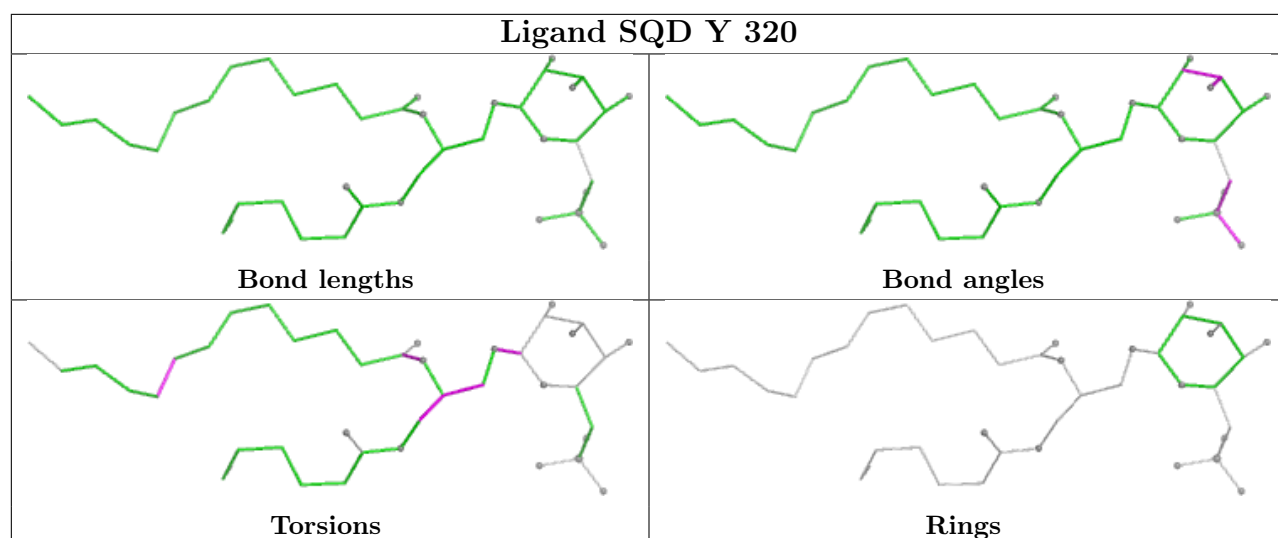




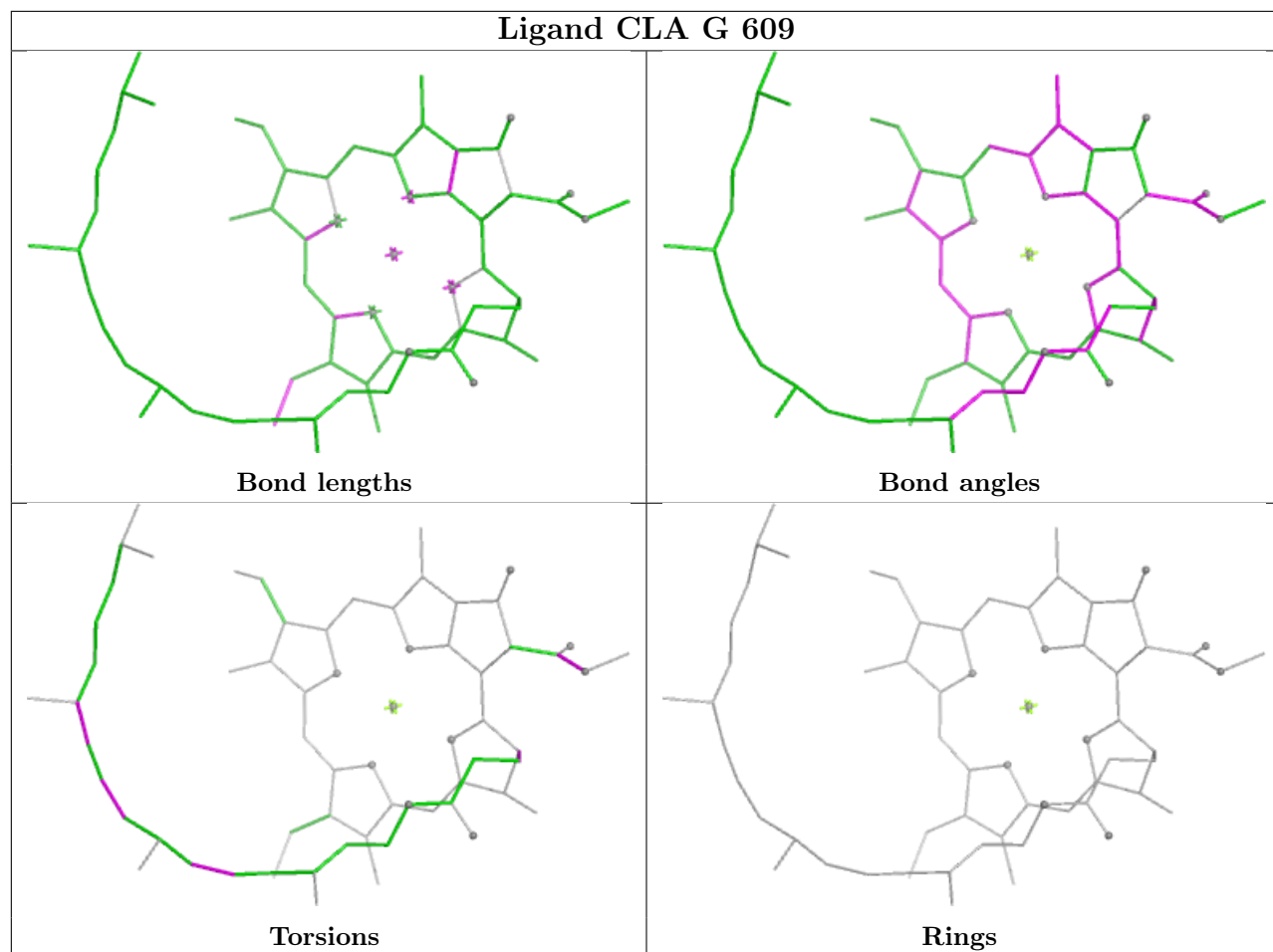




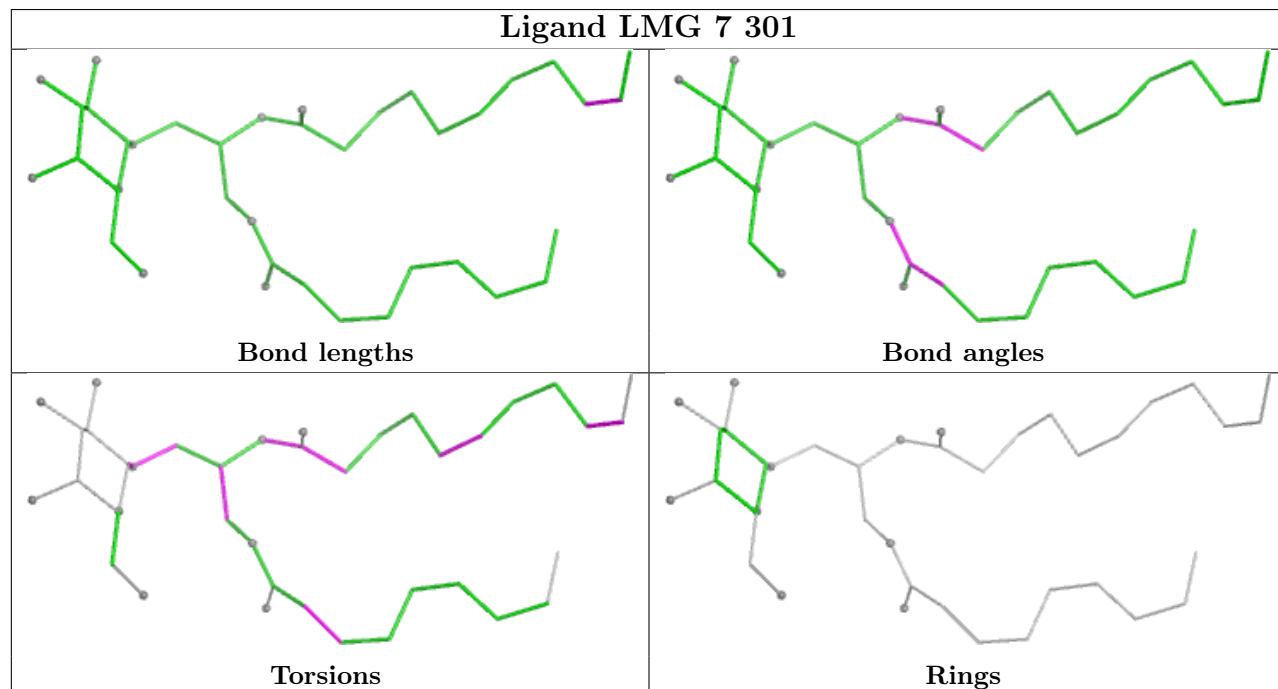


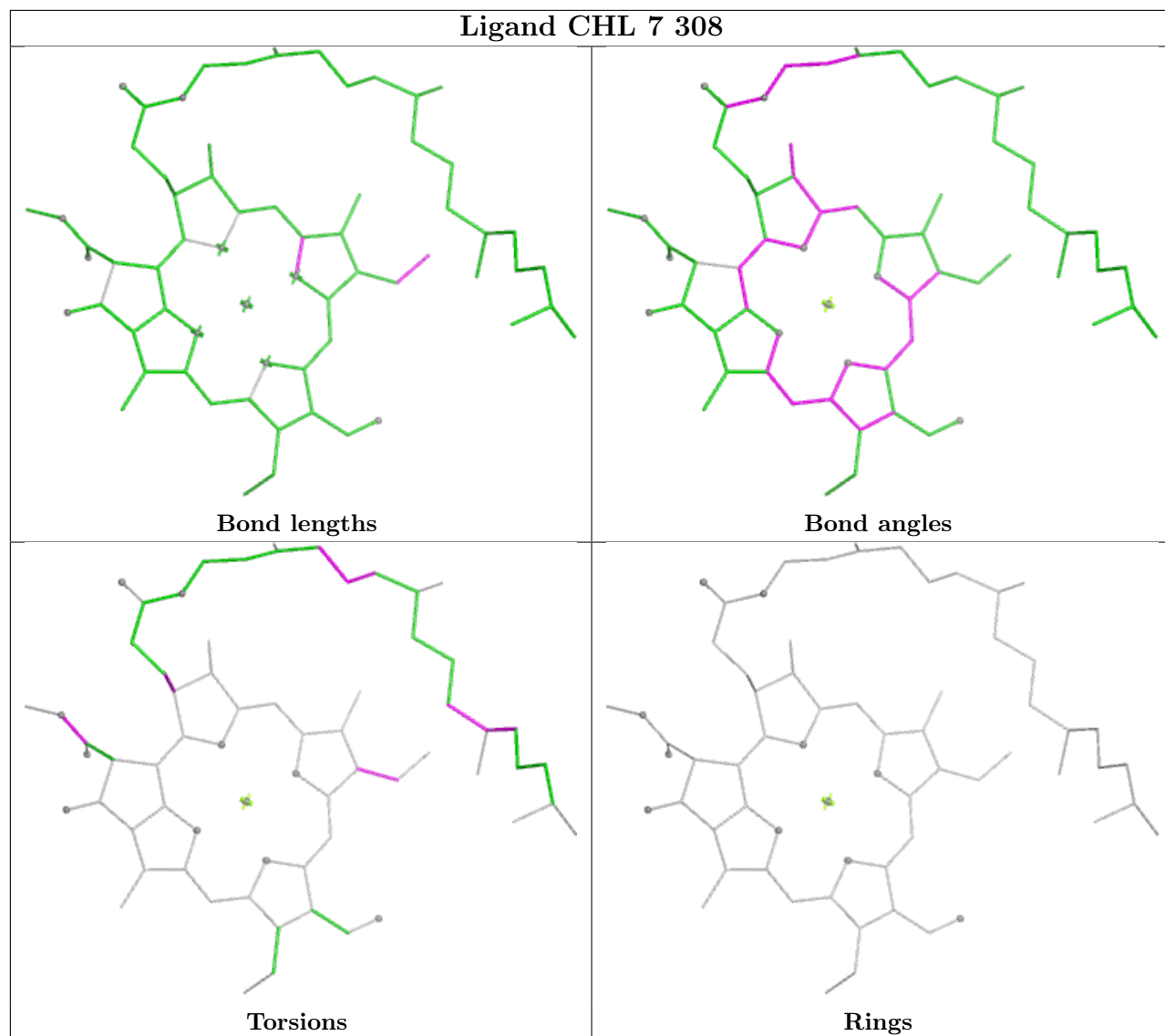


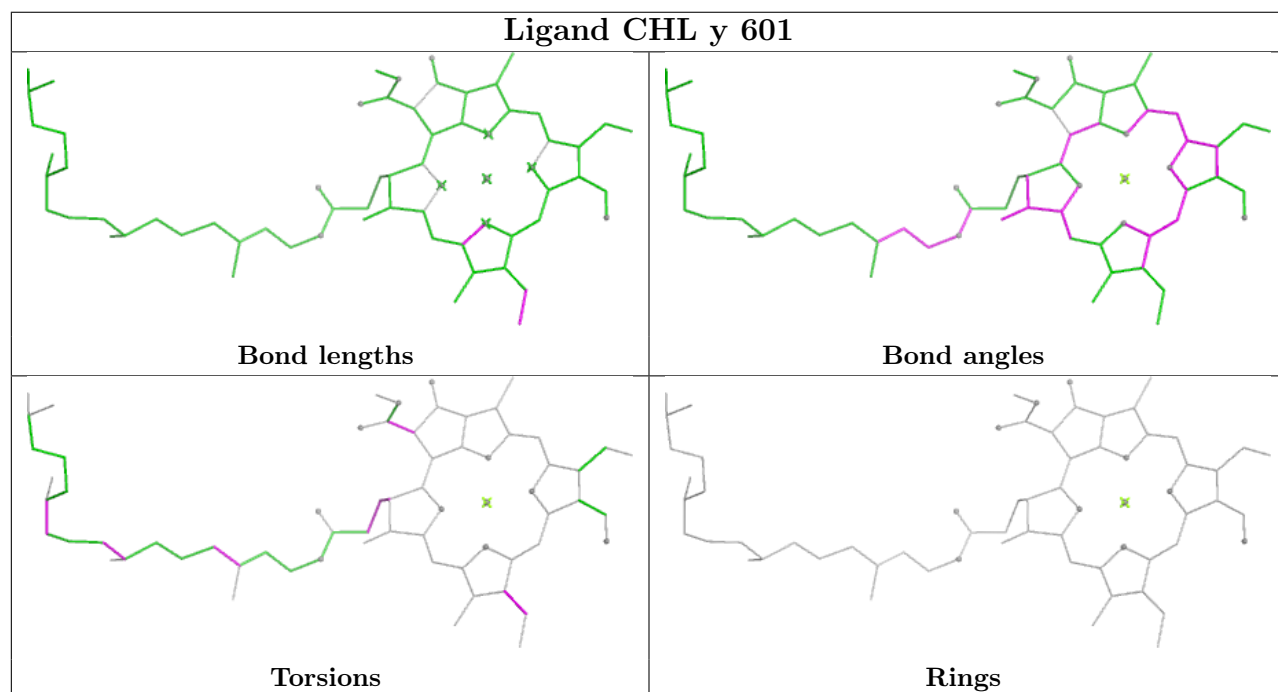
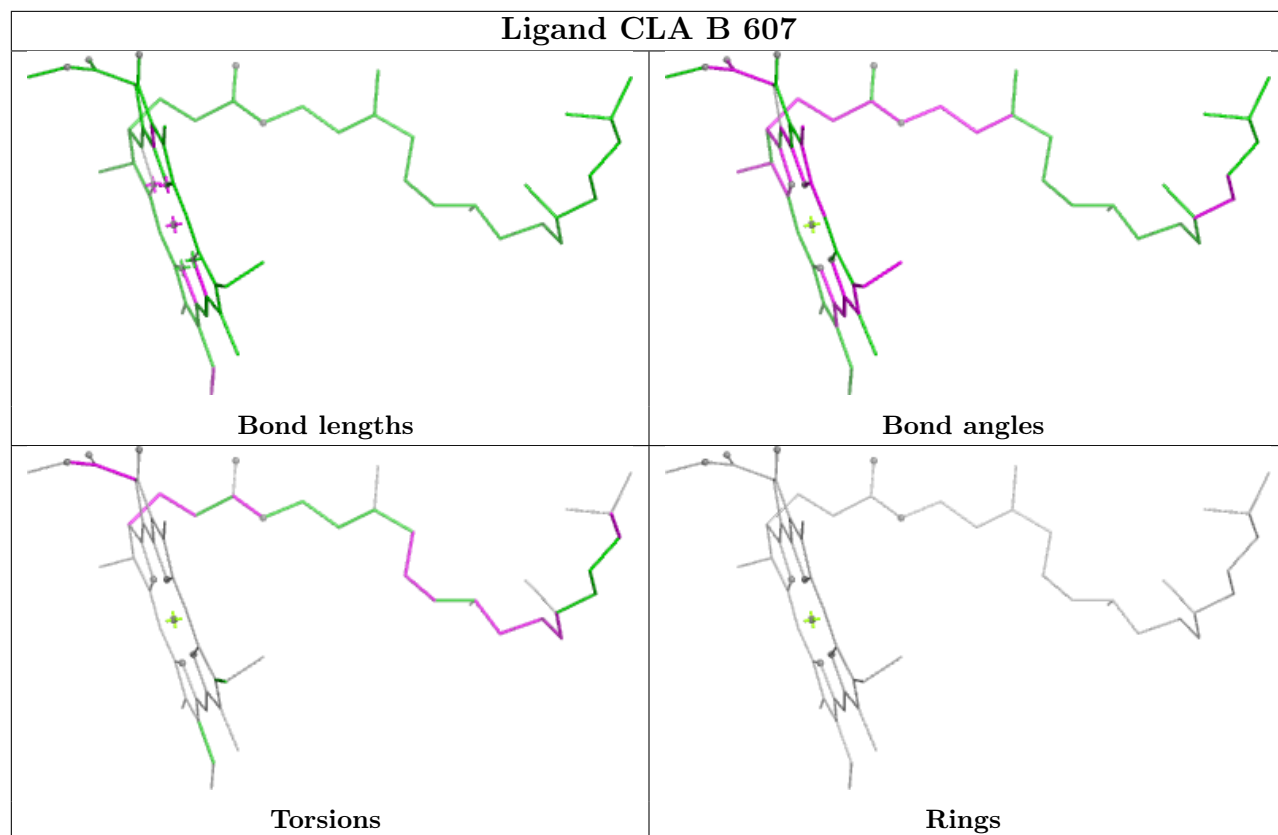
Ligand CLA G 609

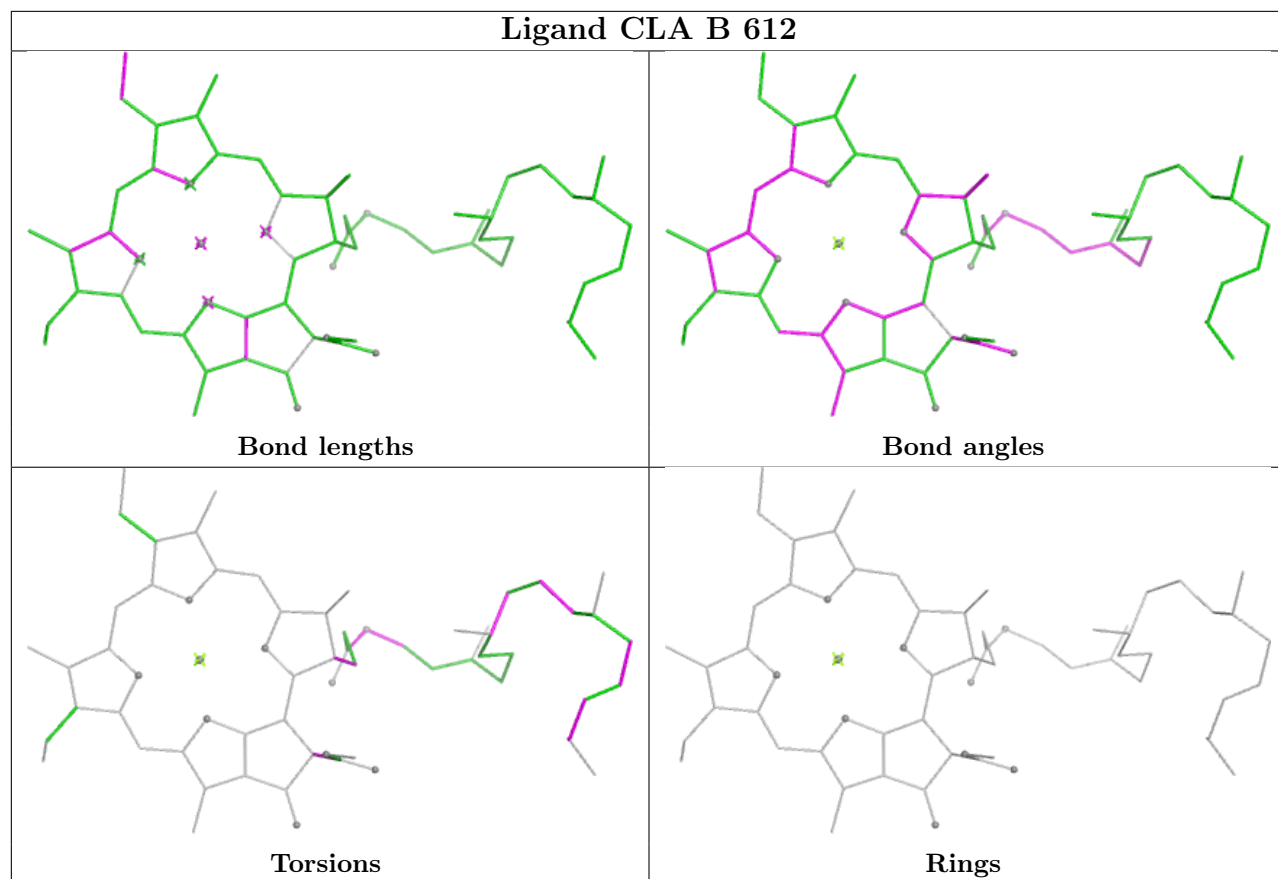


Ligand LMG 7 301

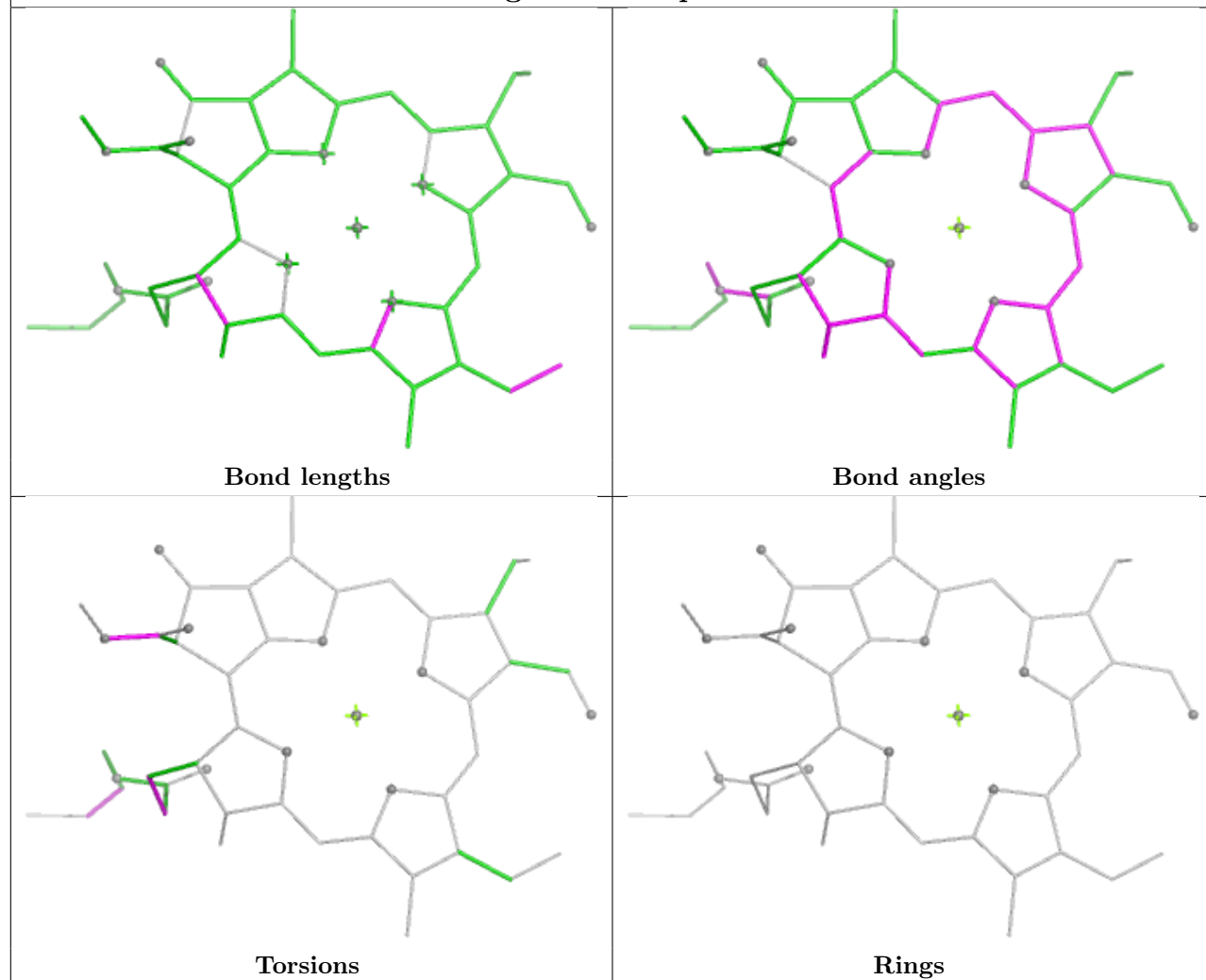




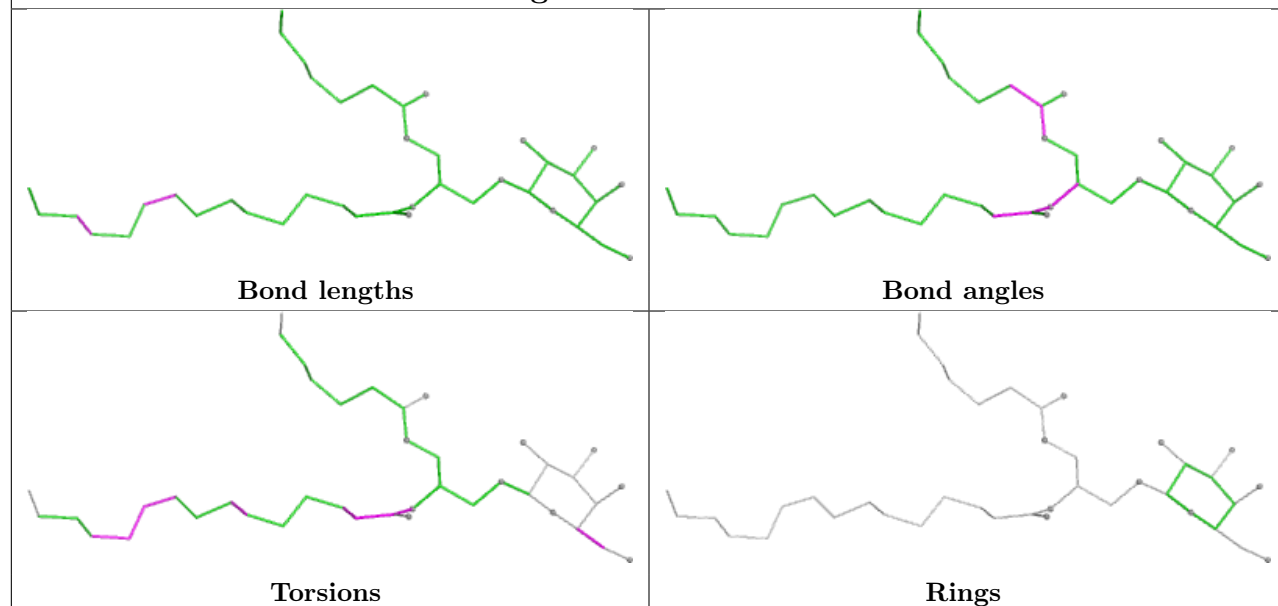


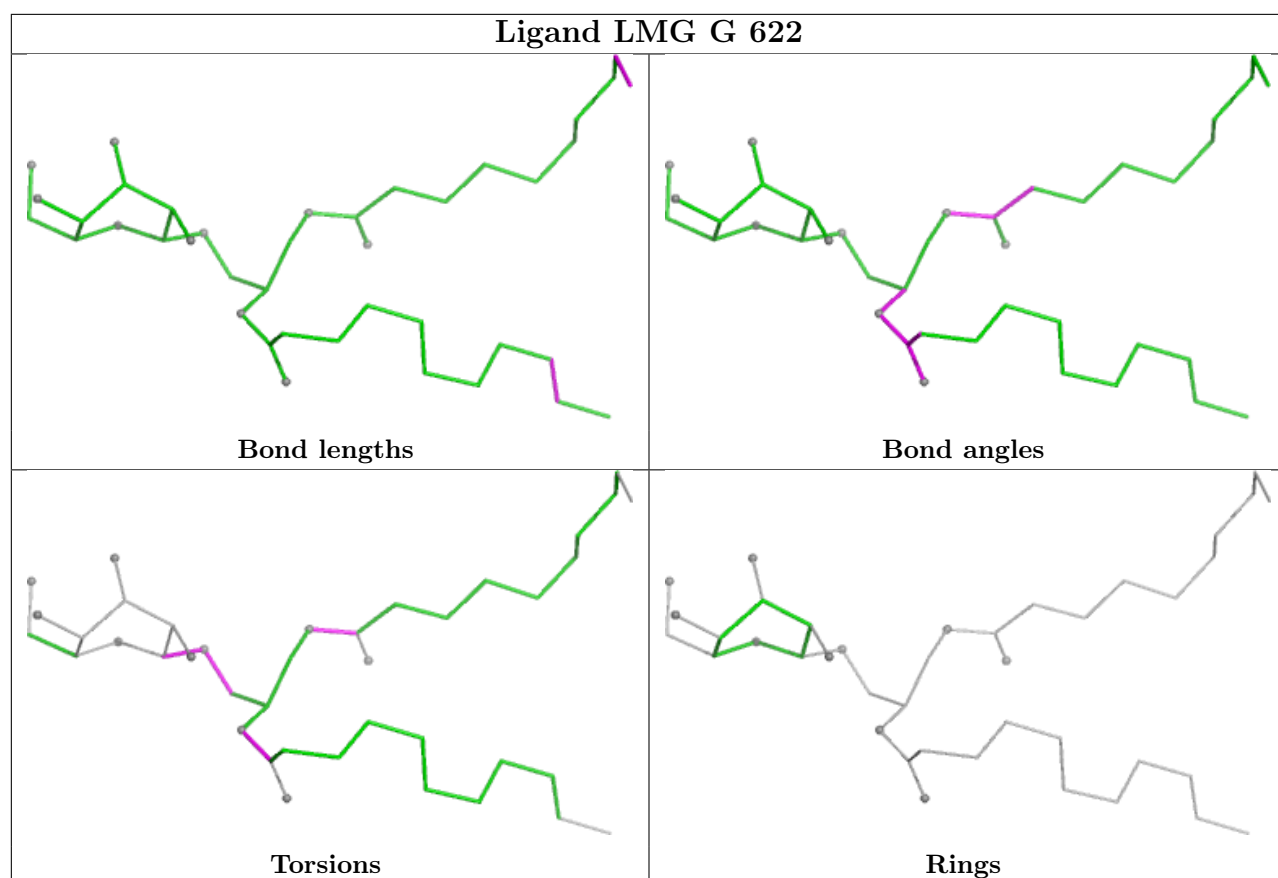


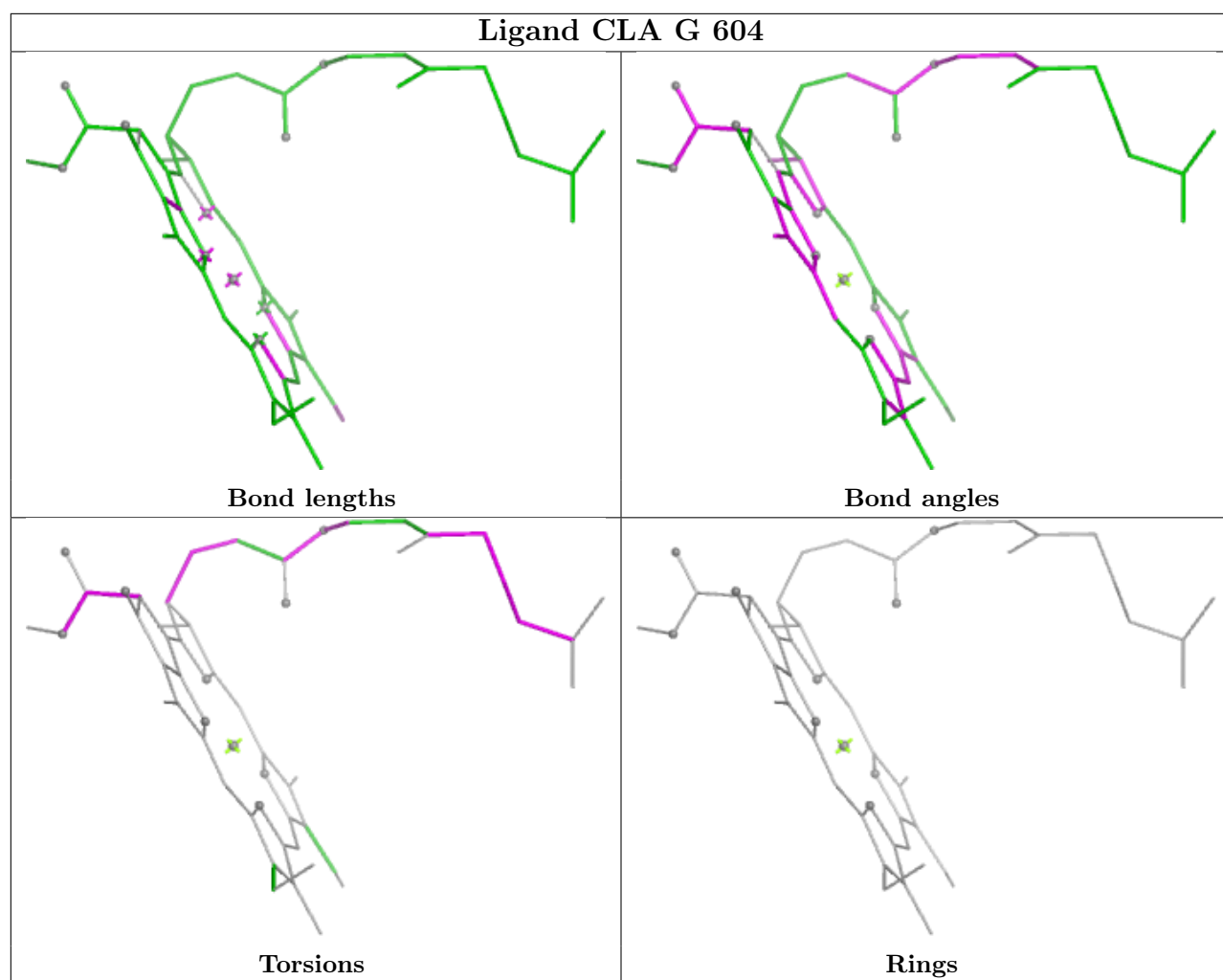
Ligand CHL q 310



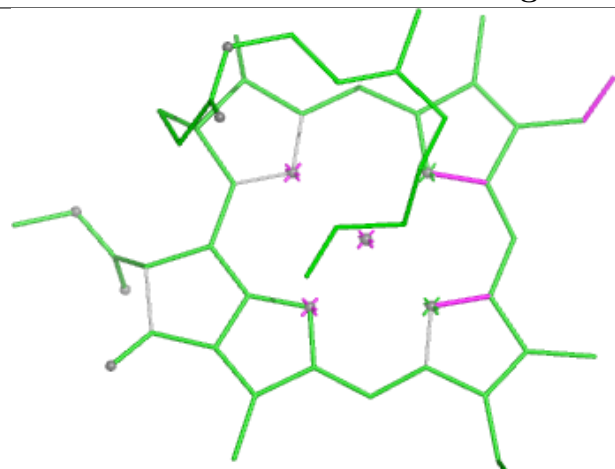
Ligand LMG S 321



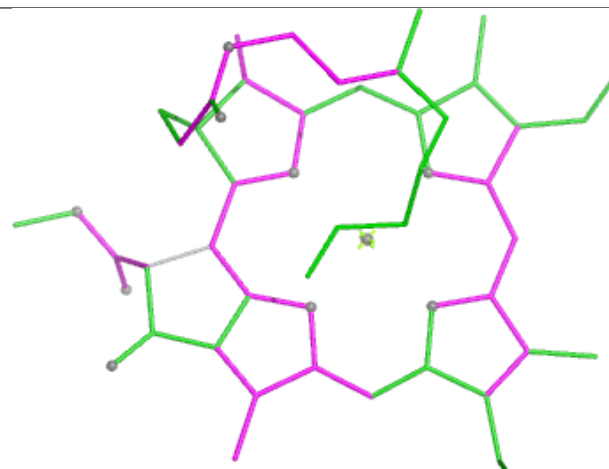




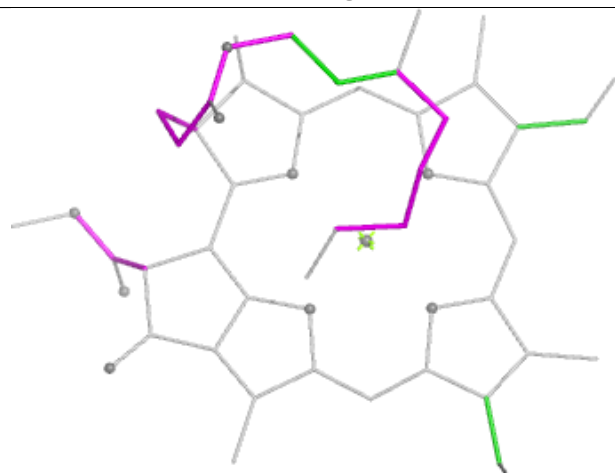
Ligand CLA 7 315



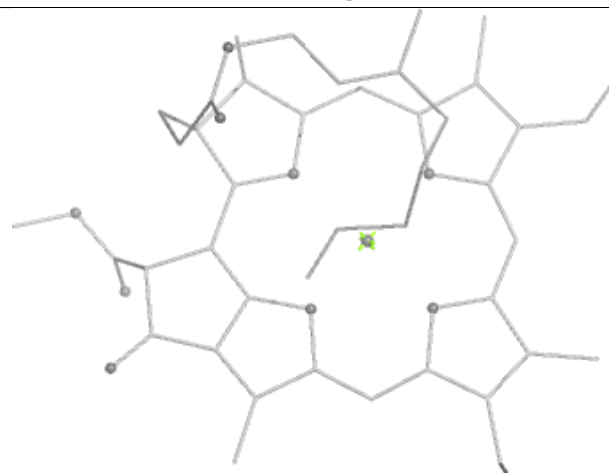
Bond lengths



Bond angles

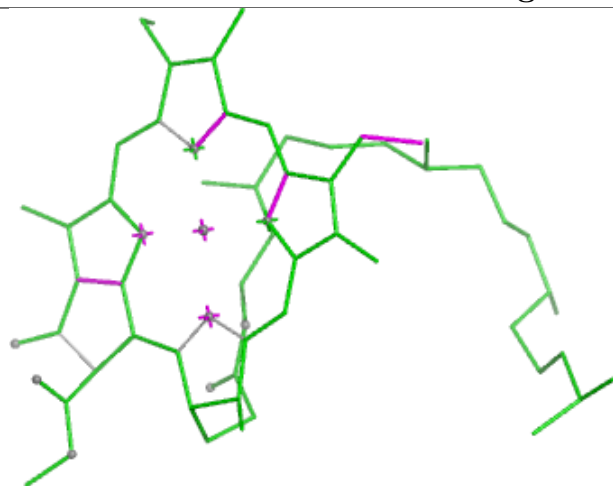


Torsions

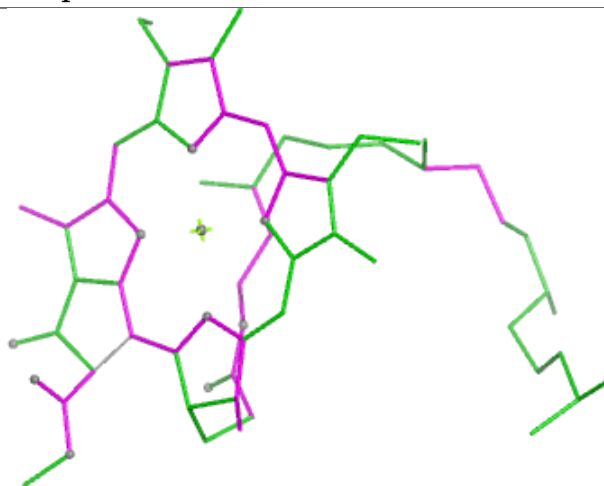


Rings

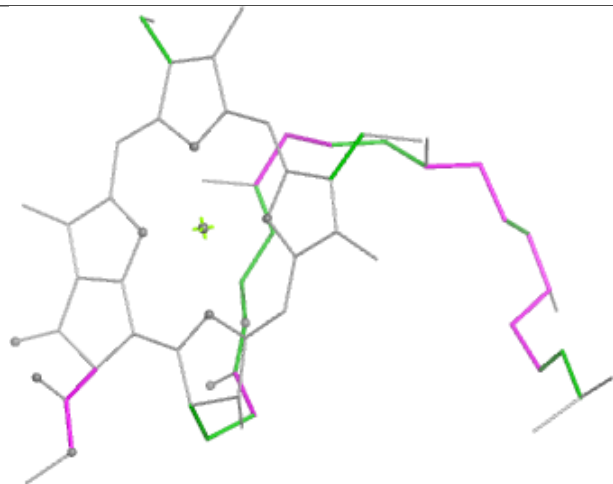
Ligand CLA q 315



Bond lengths



Bond angles

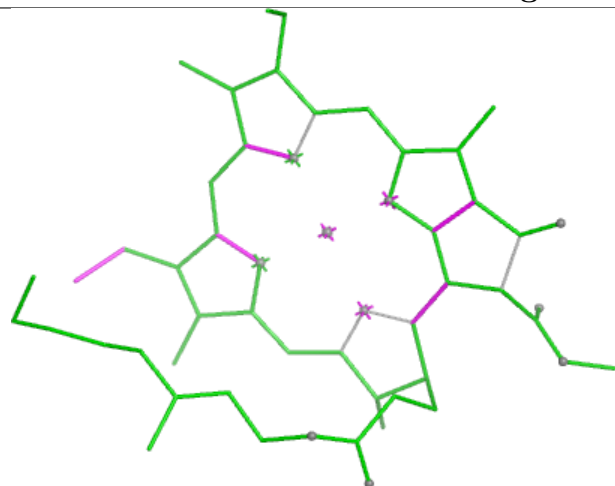


Torsions

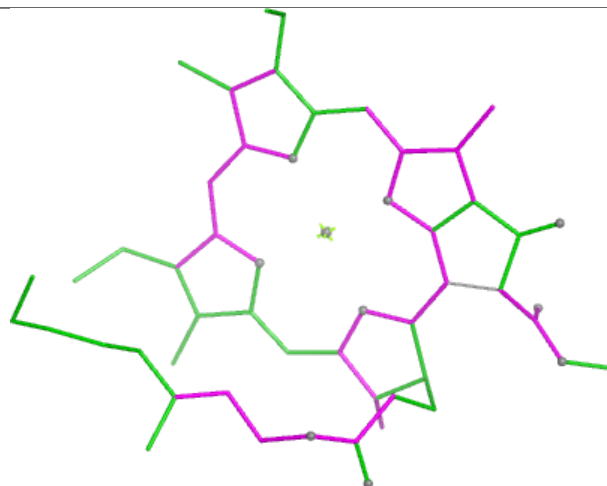


Rings

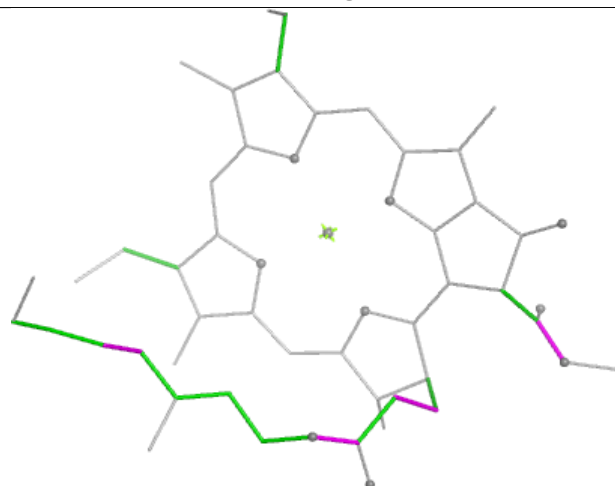
Ligand CLA 3 311



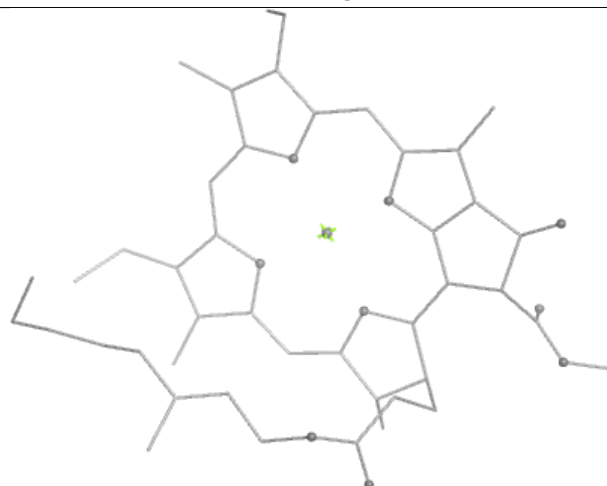
Bond lengths



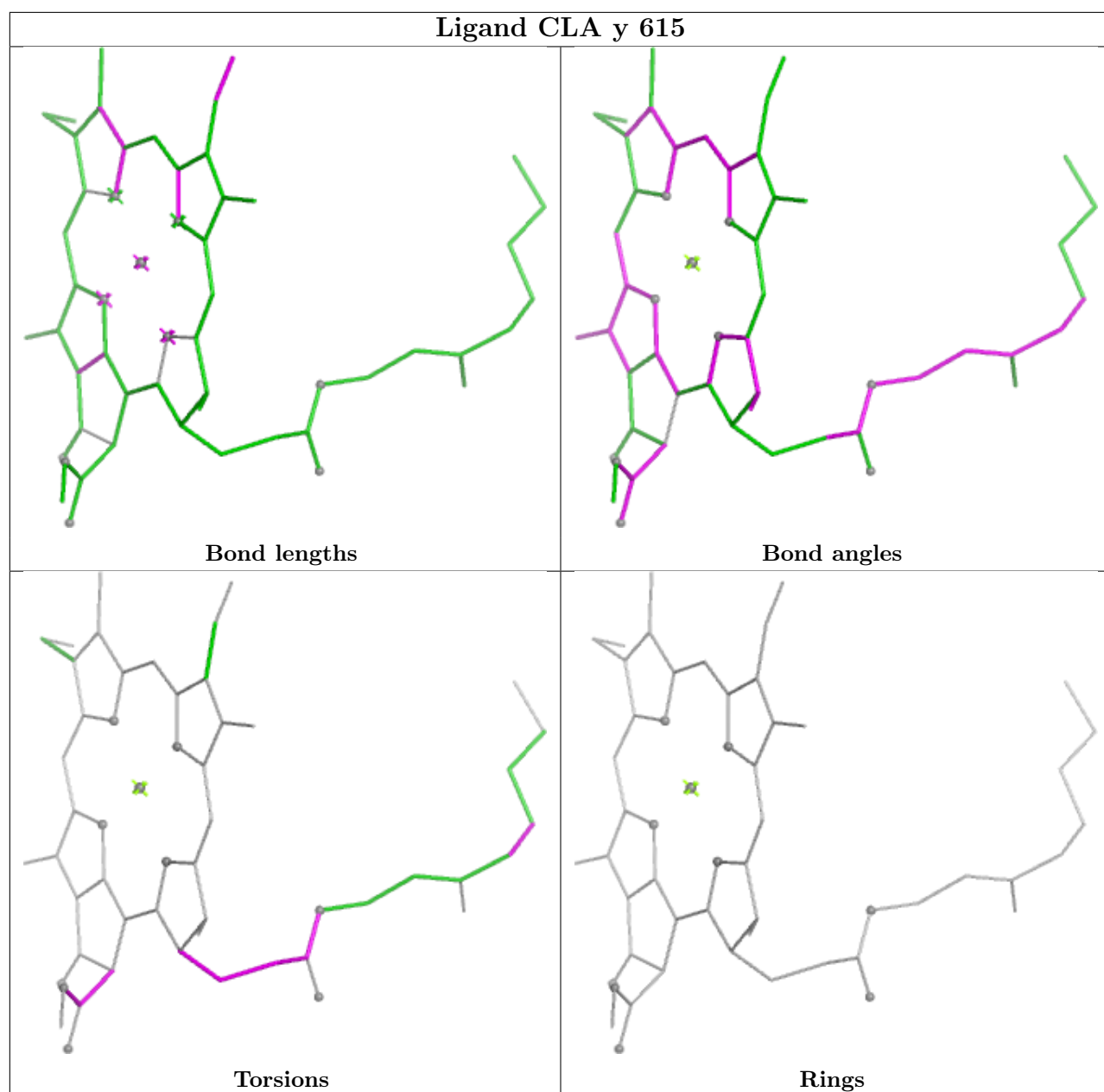
Bond angles

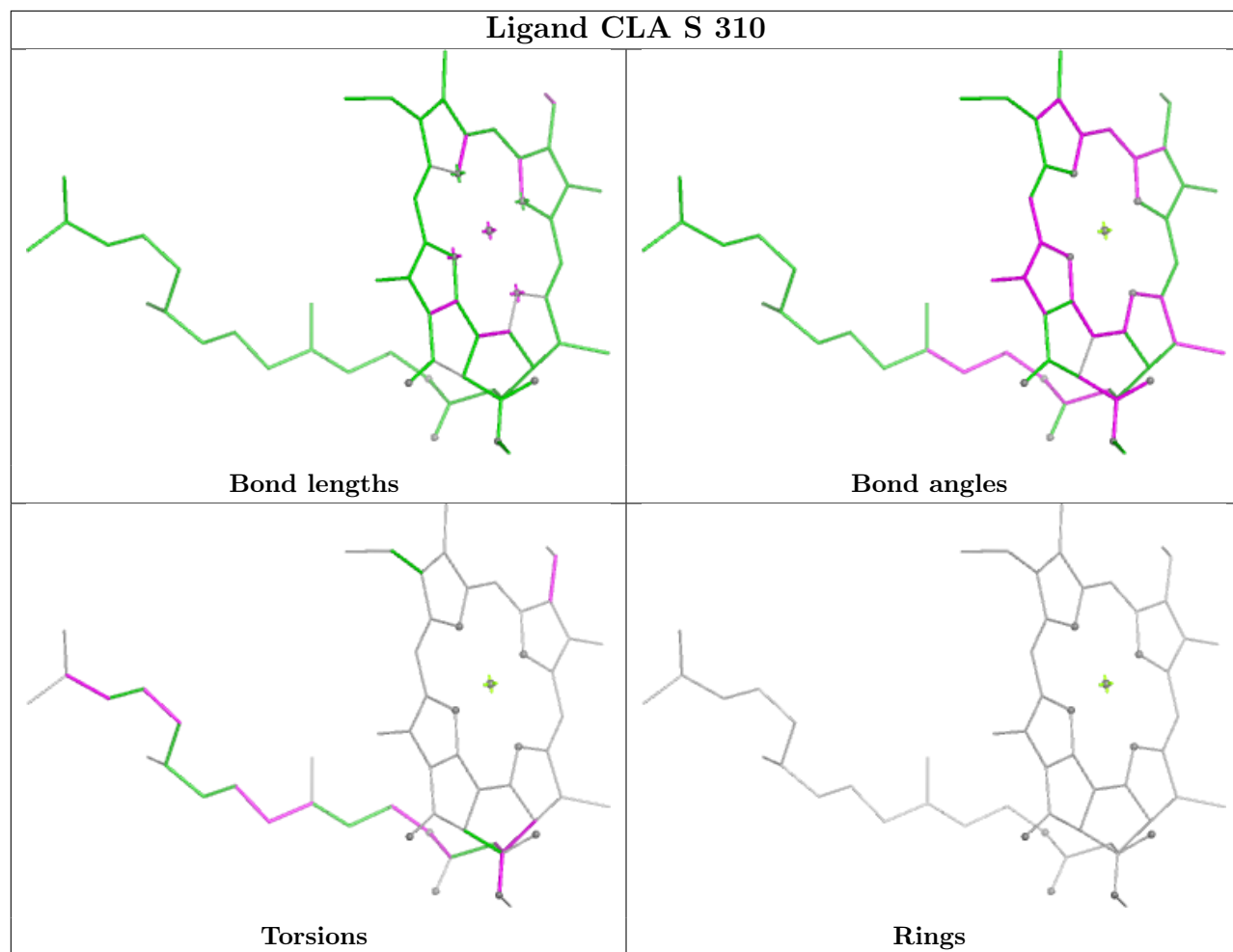


Torsions

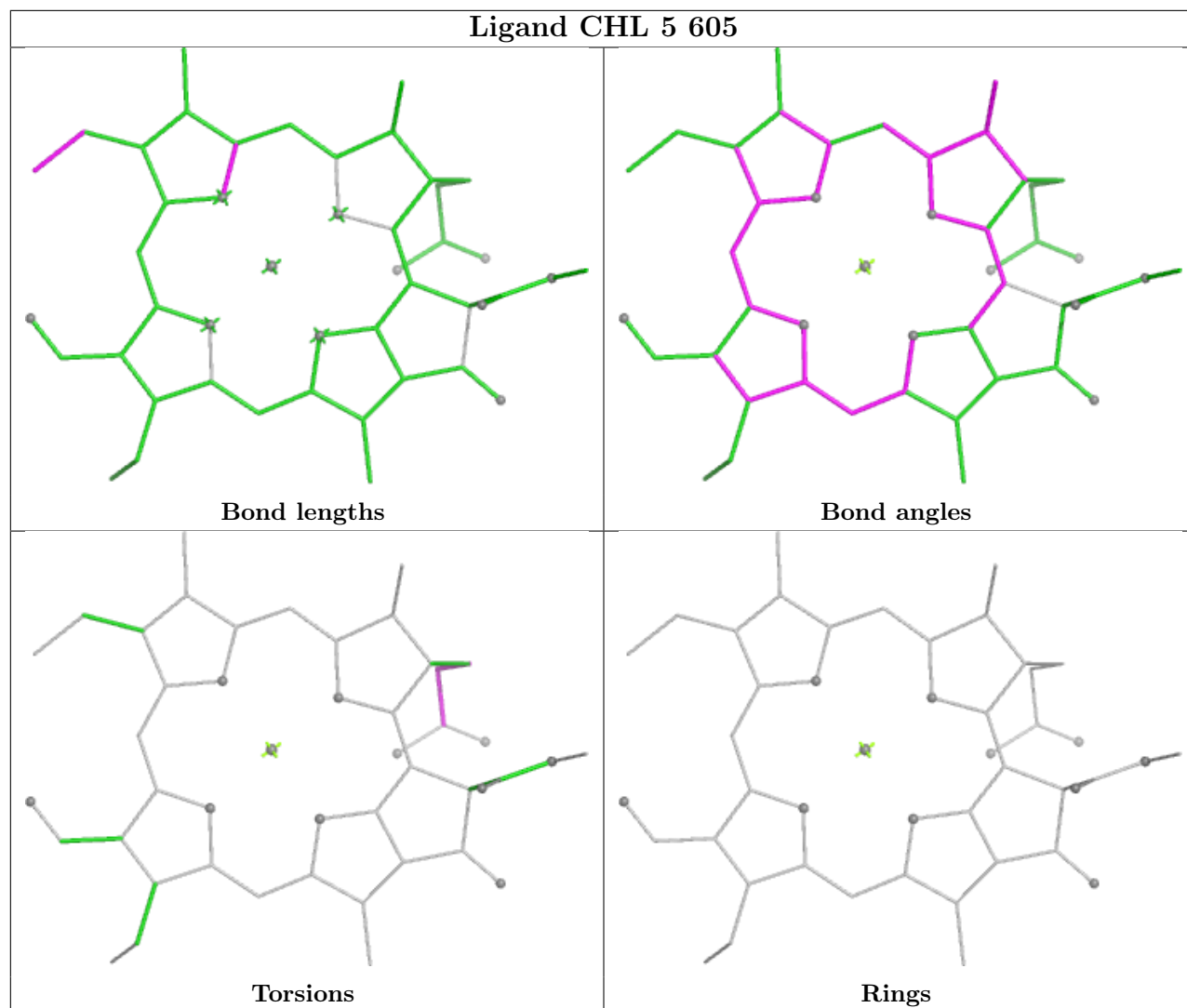


Rings

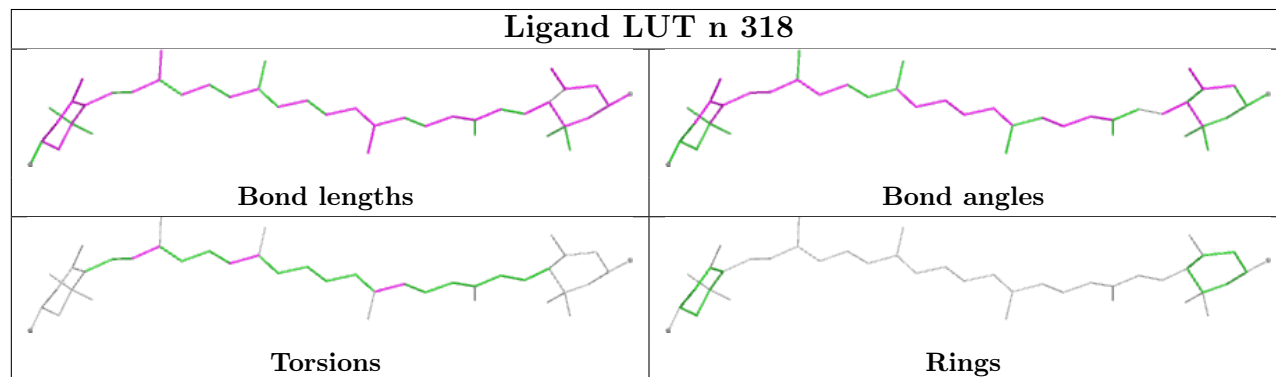


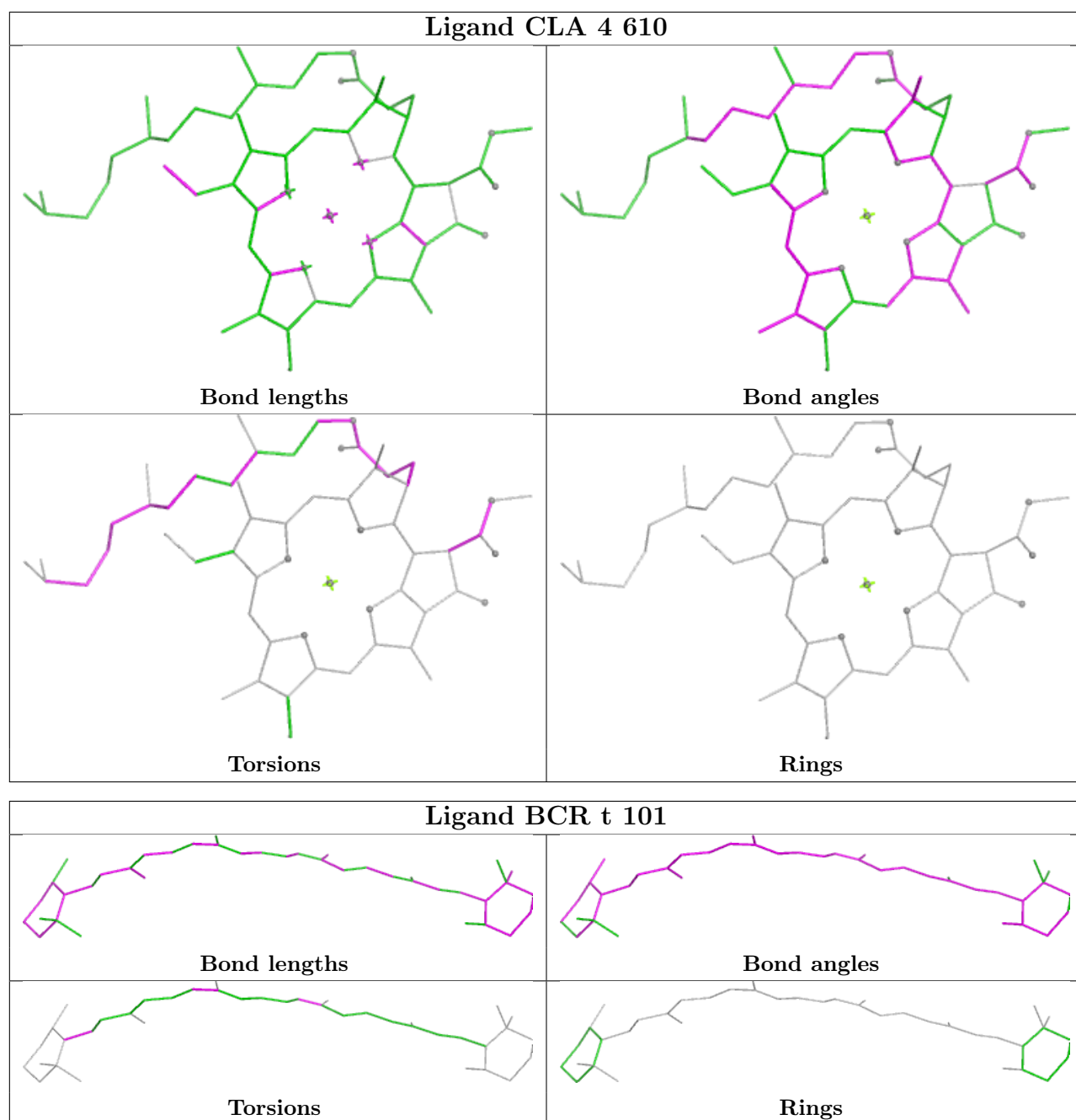


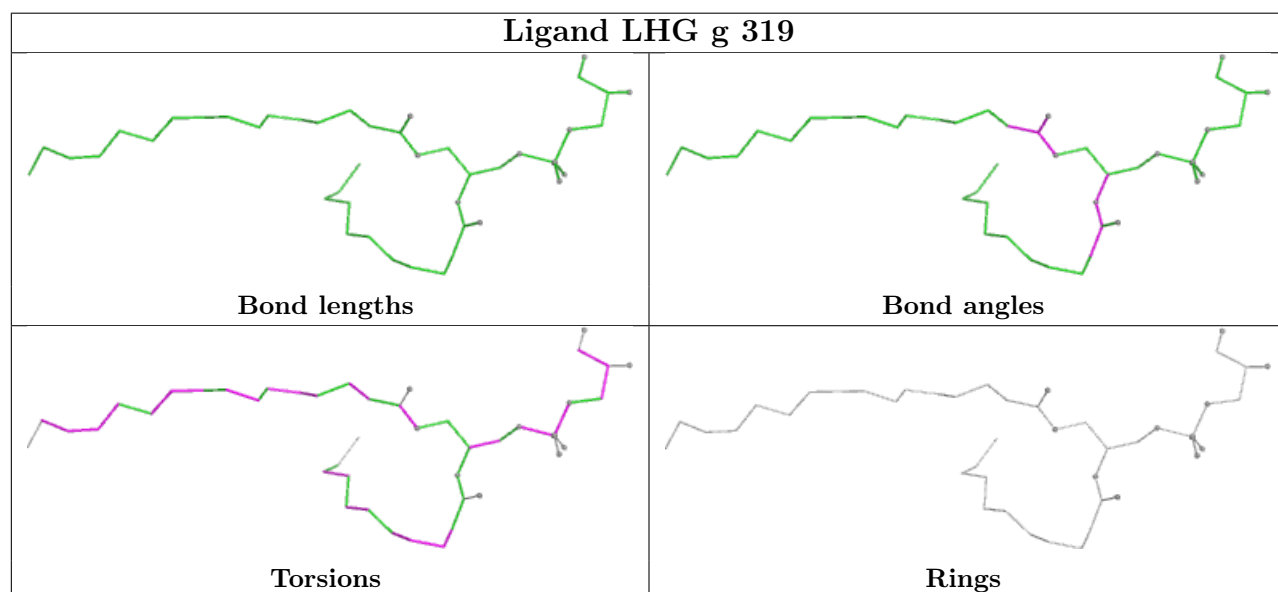
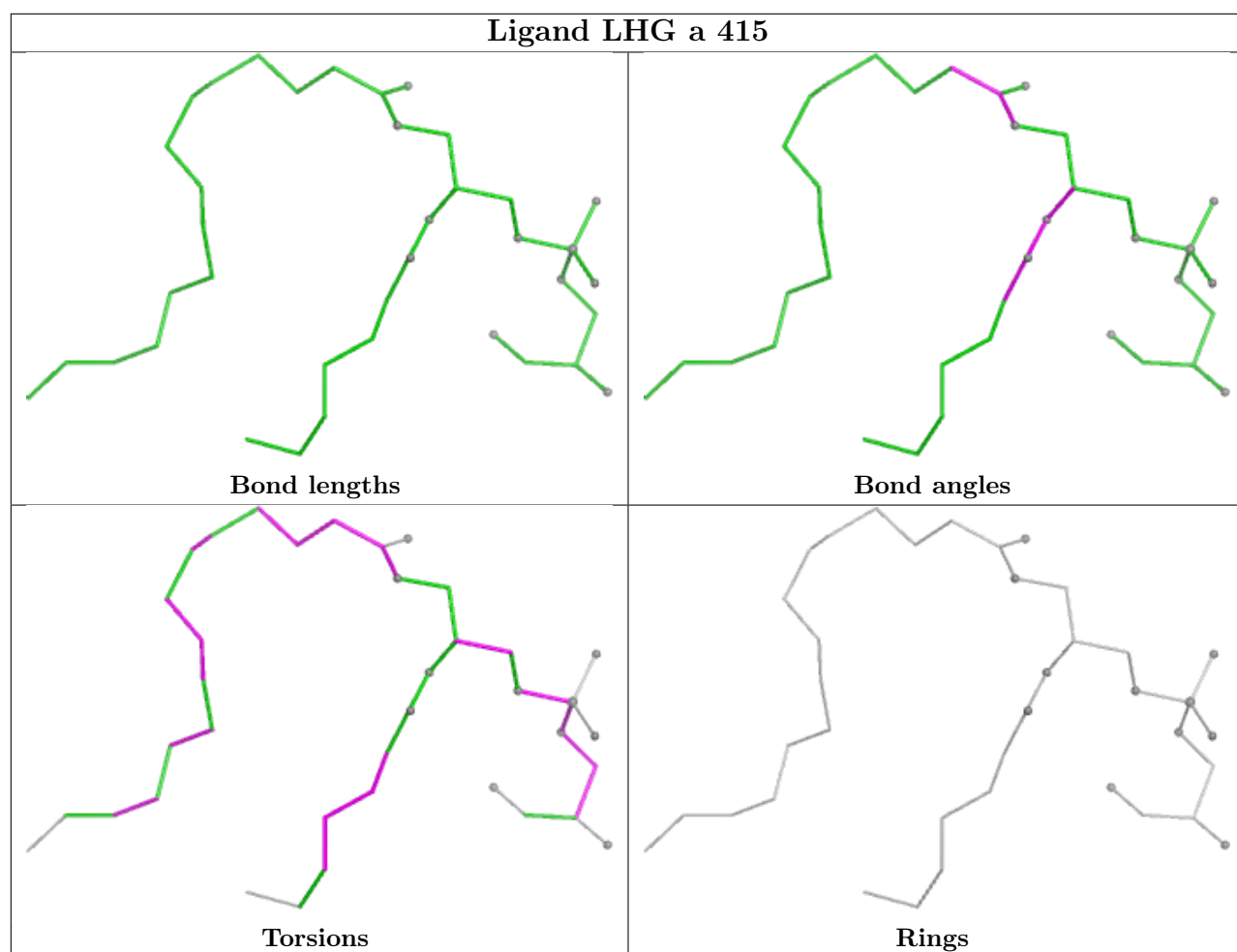
Ligand CHL 5 605

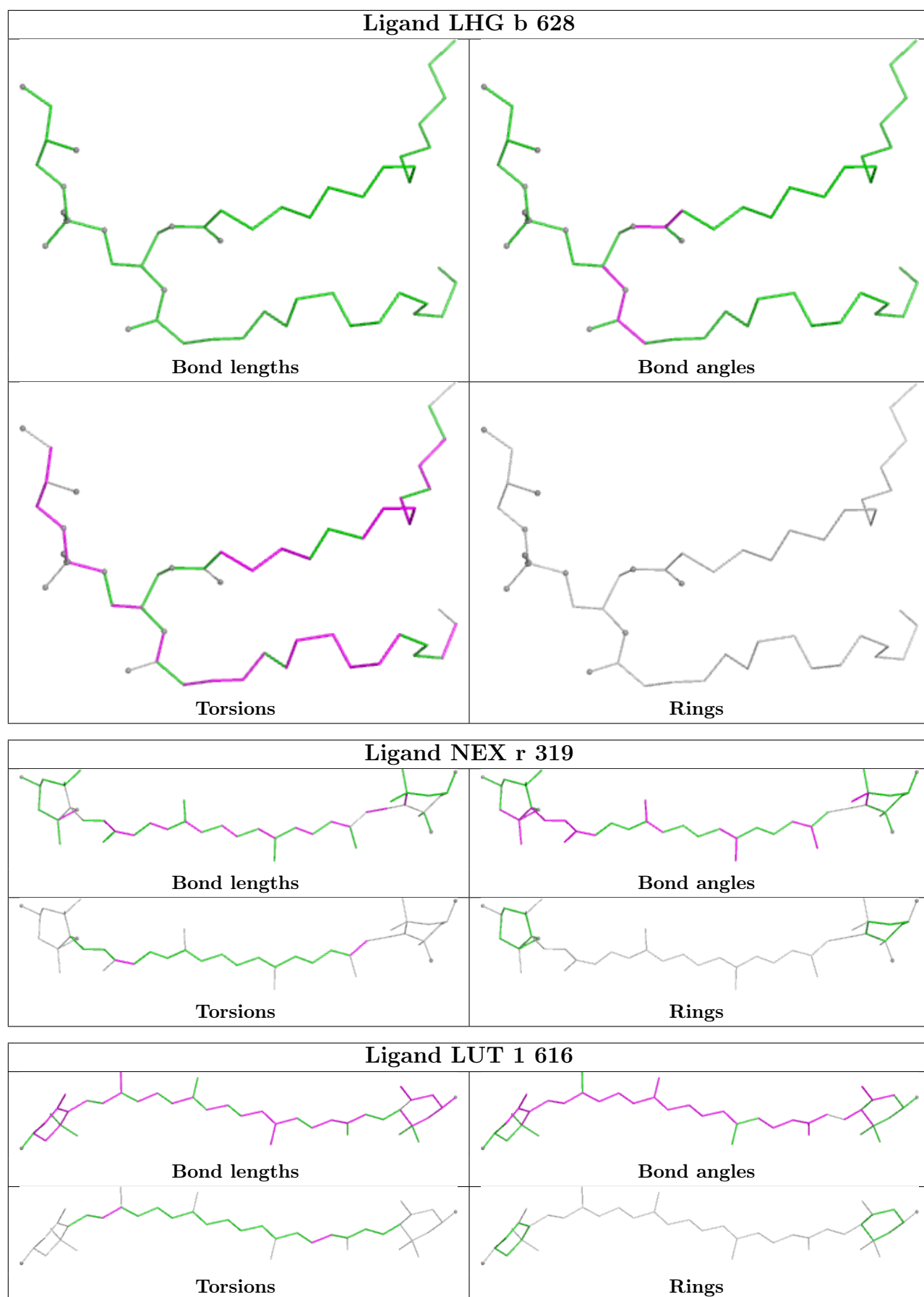


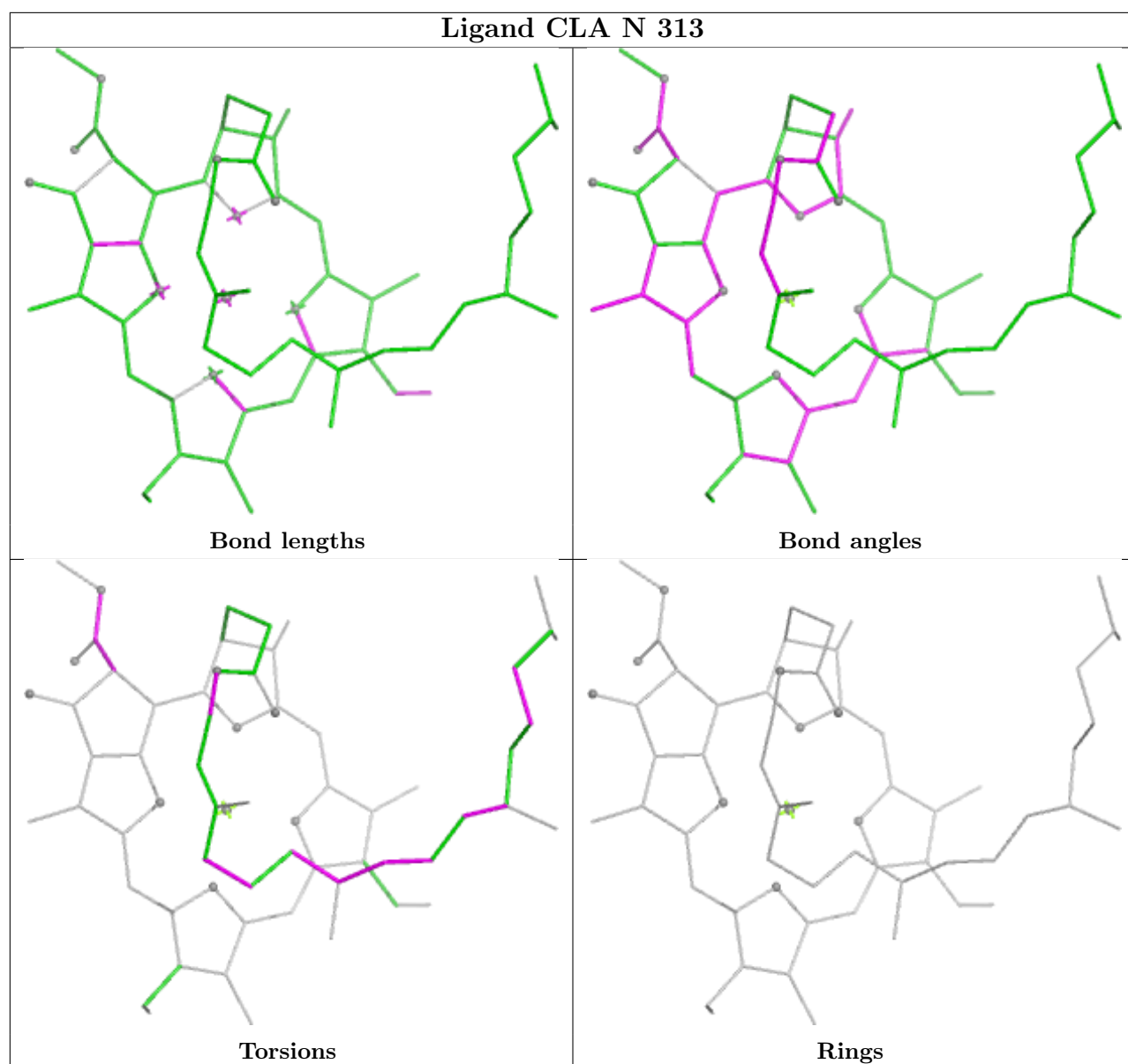
Ligand LUT n 318



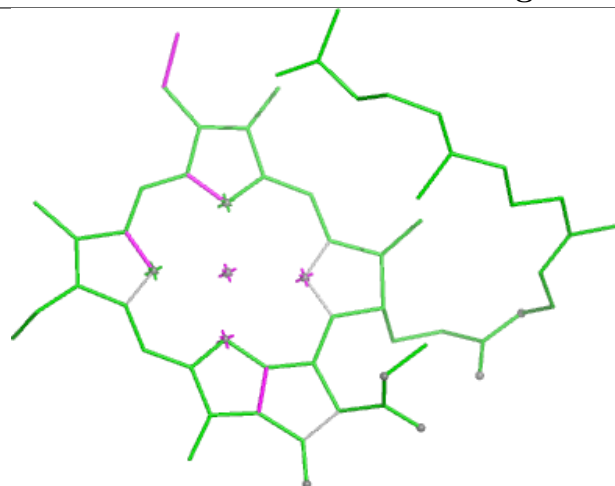




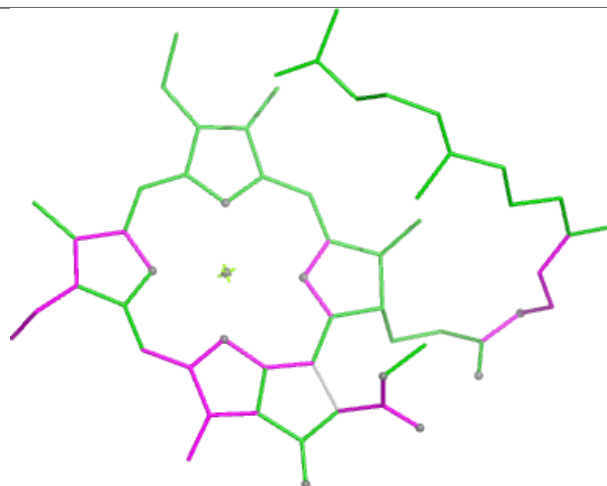




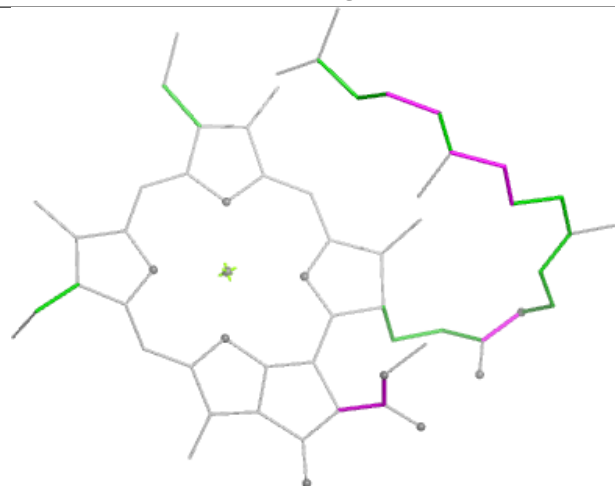
Ligand CLA R 305



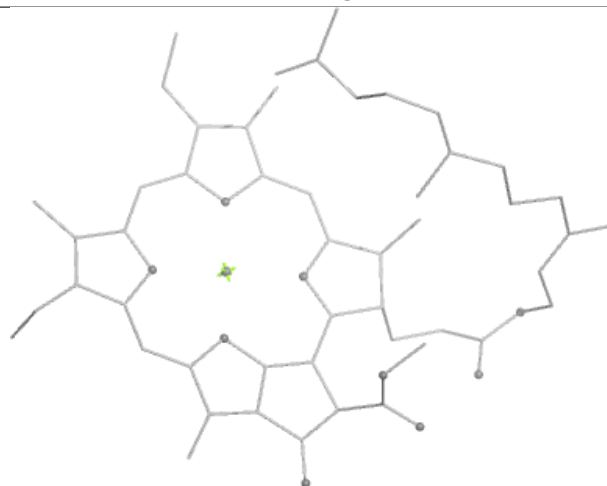
Bond lengths



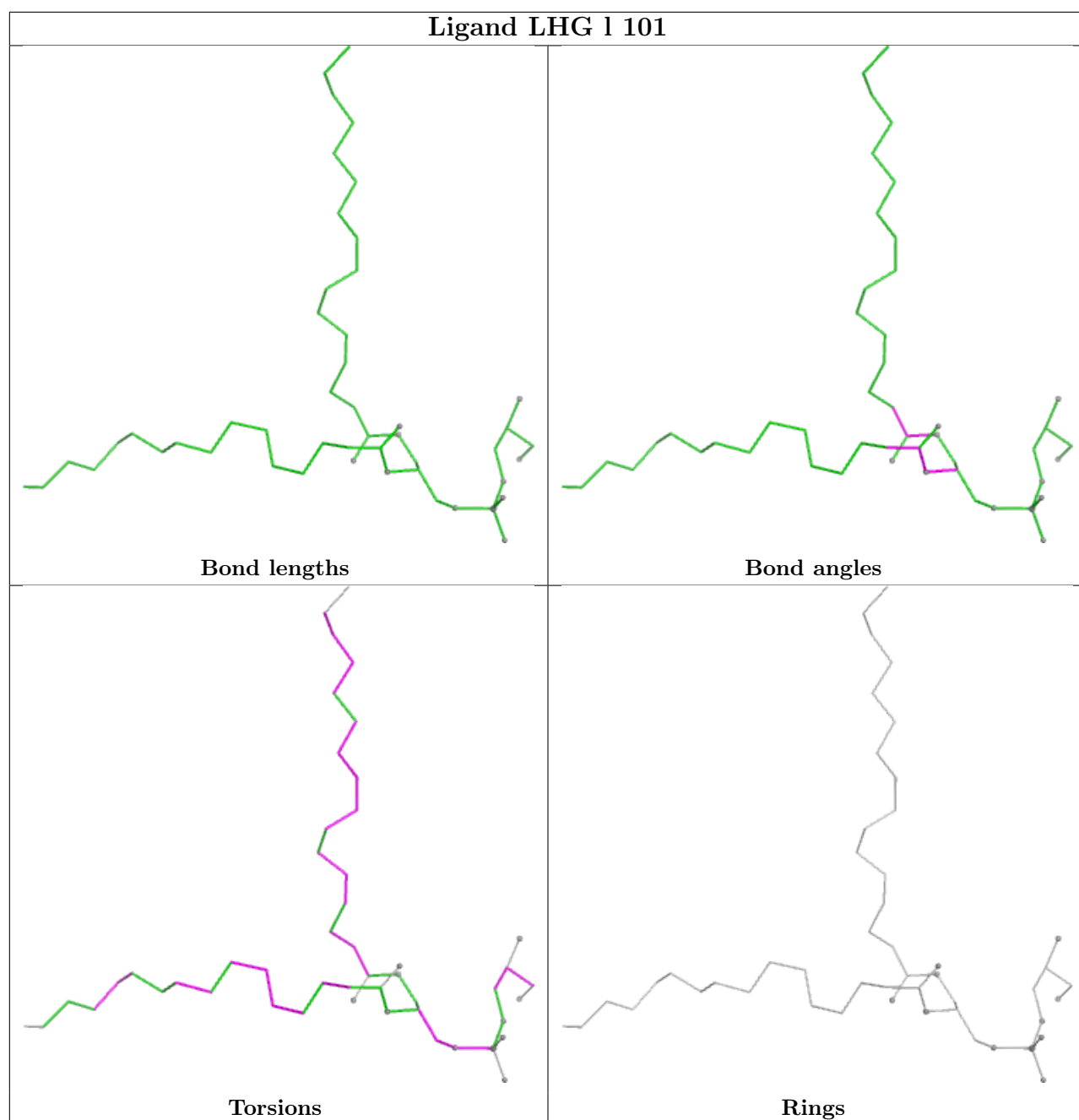
Bond angles



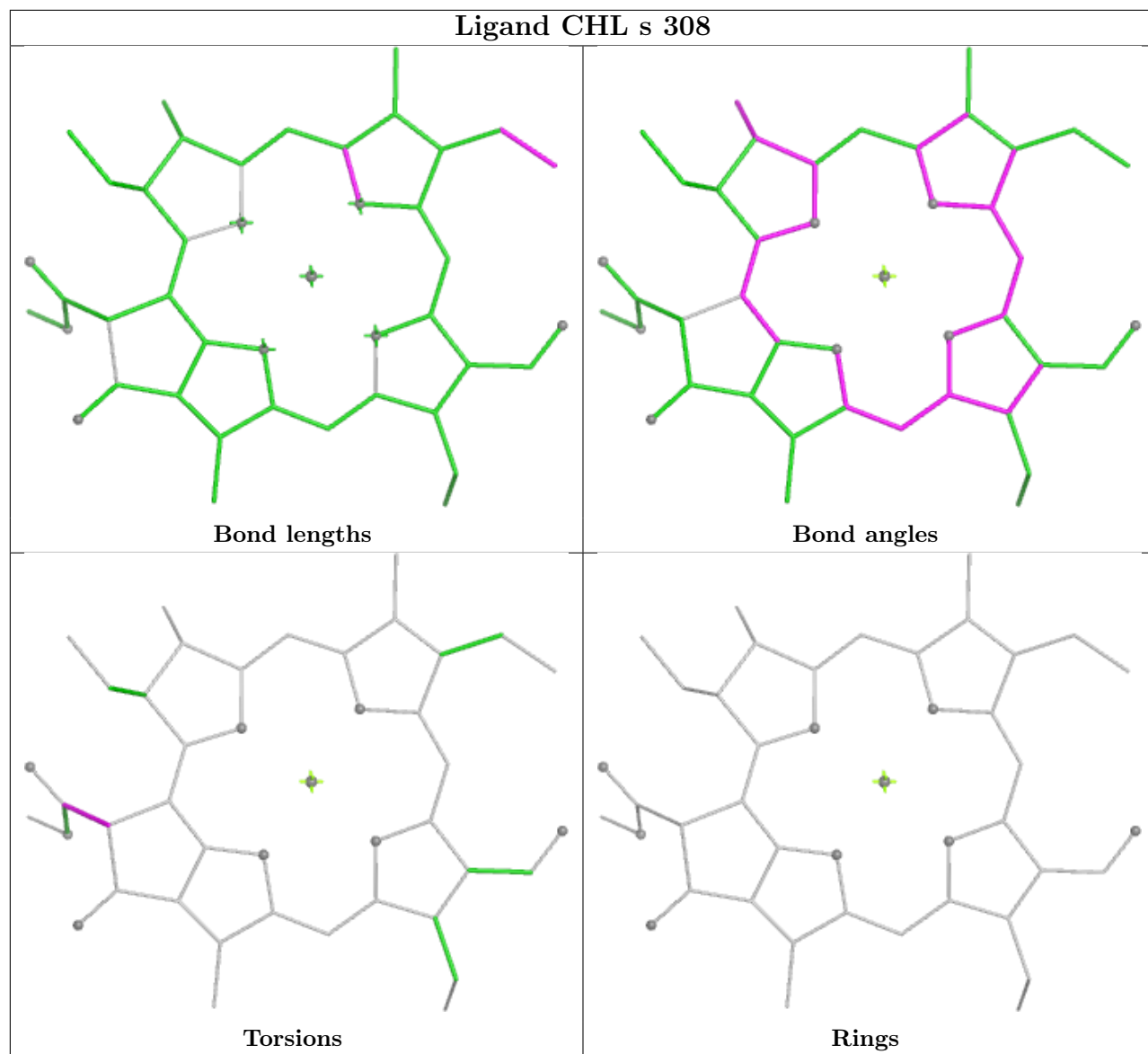
Torsions



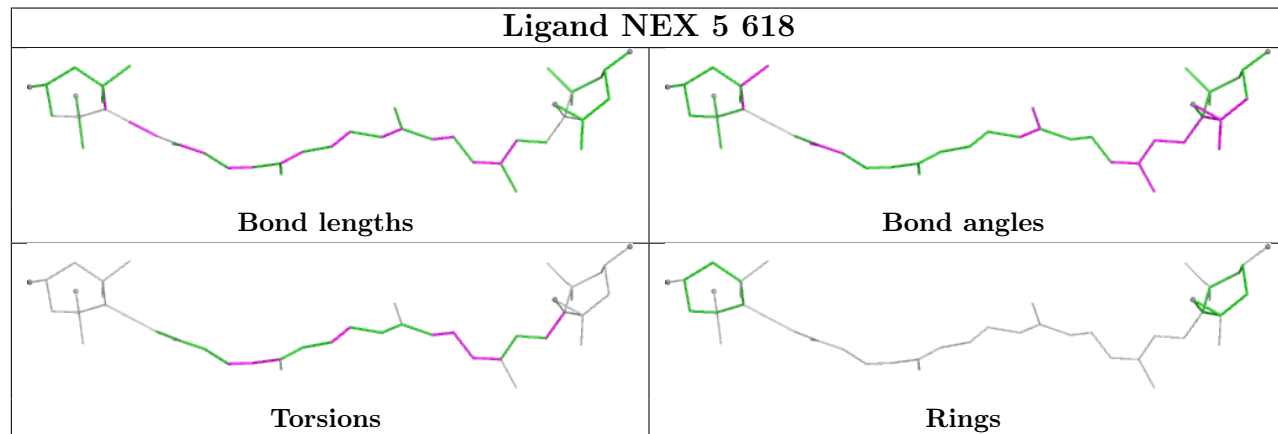
Rings

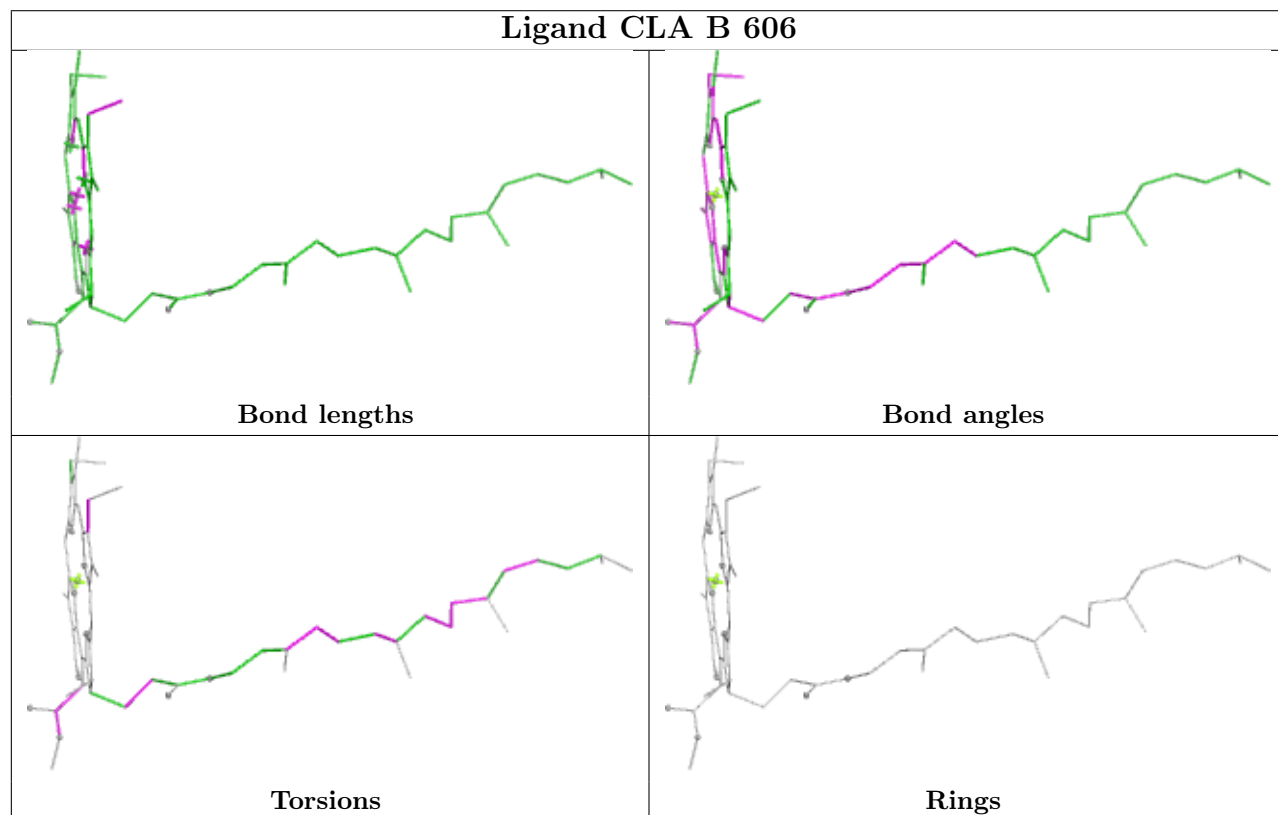
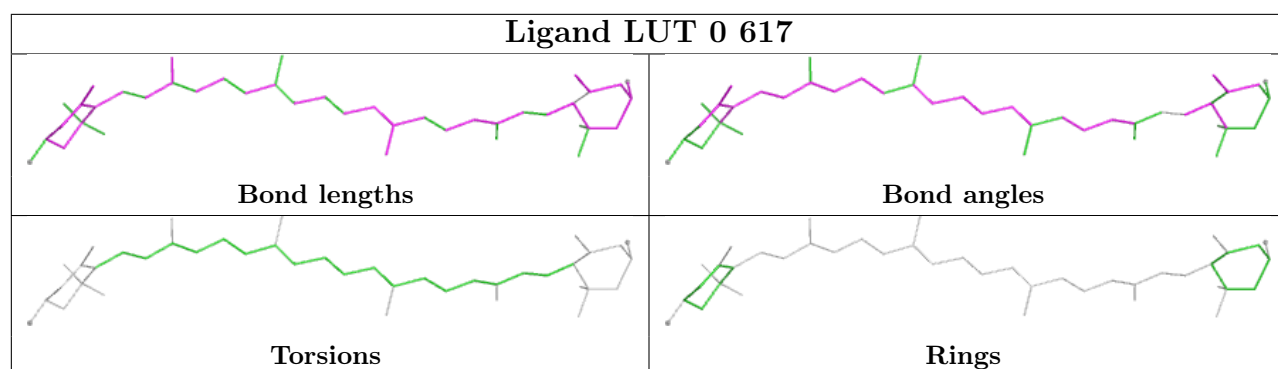


Ligand CHL s 308

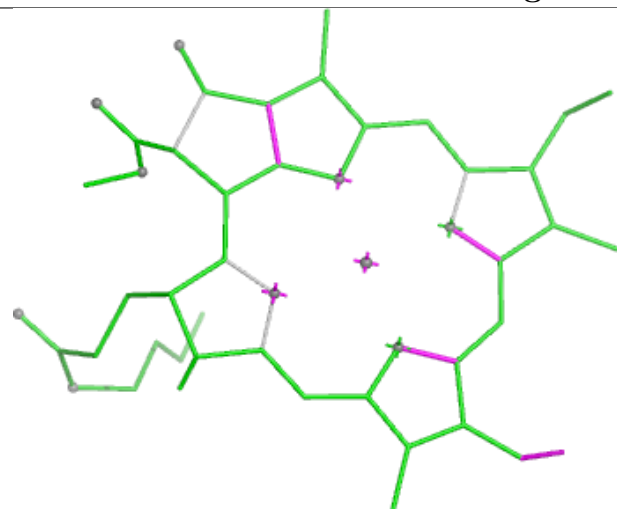


Ligand NEX 5 618

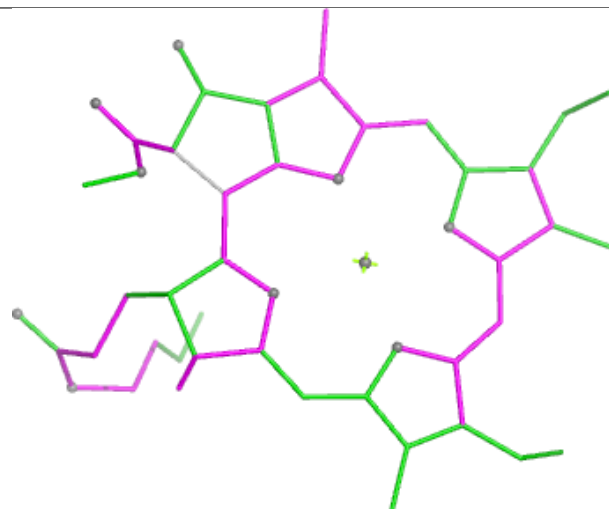




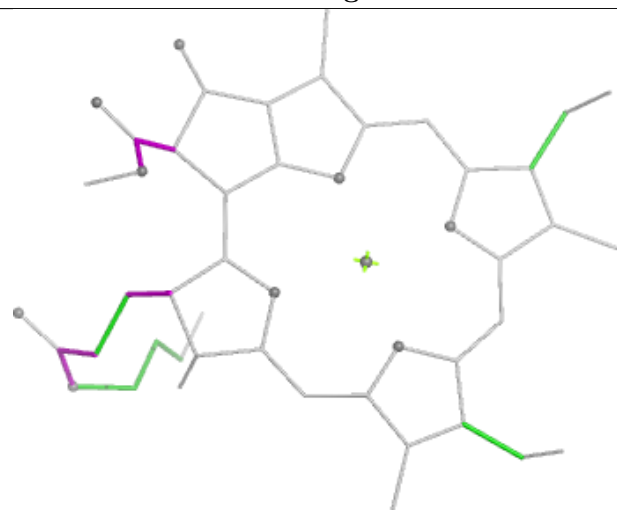
Ligand CLA r 303



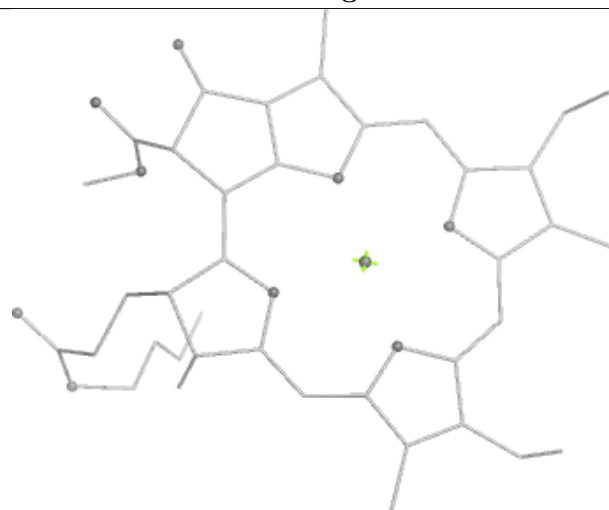
Bond lengths



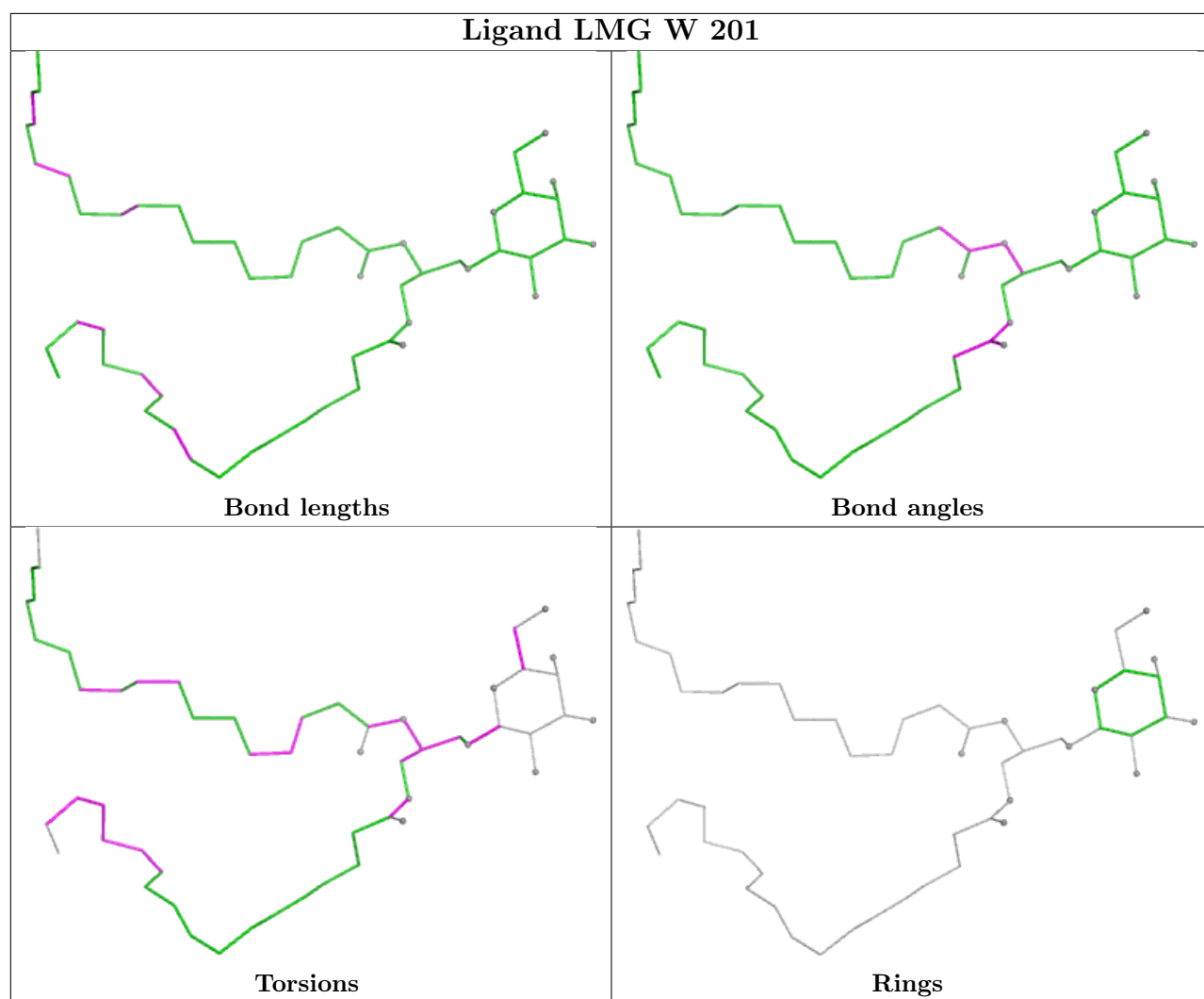
Bond angles

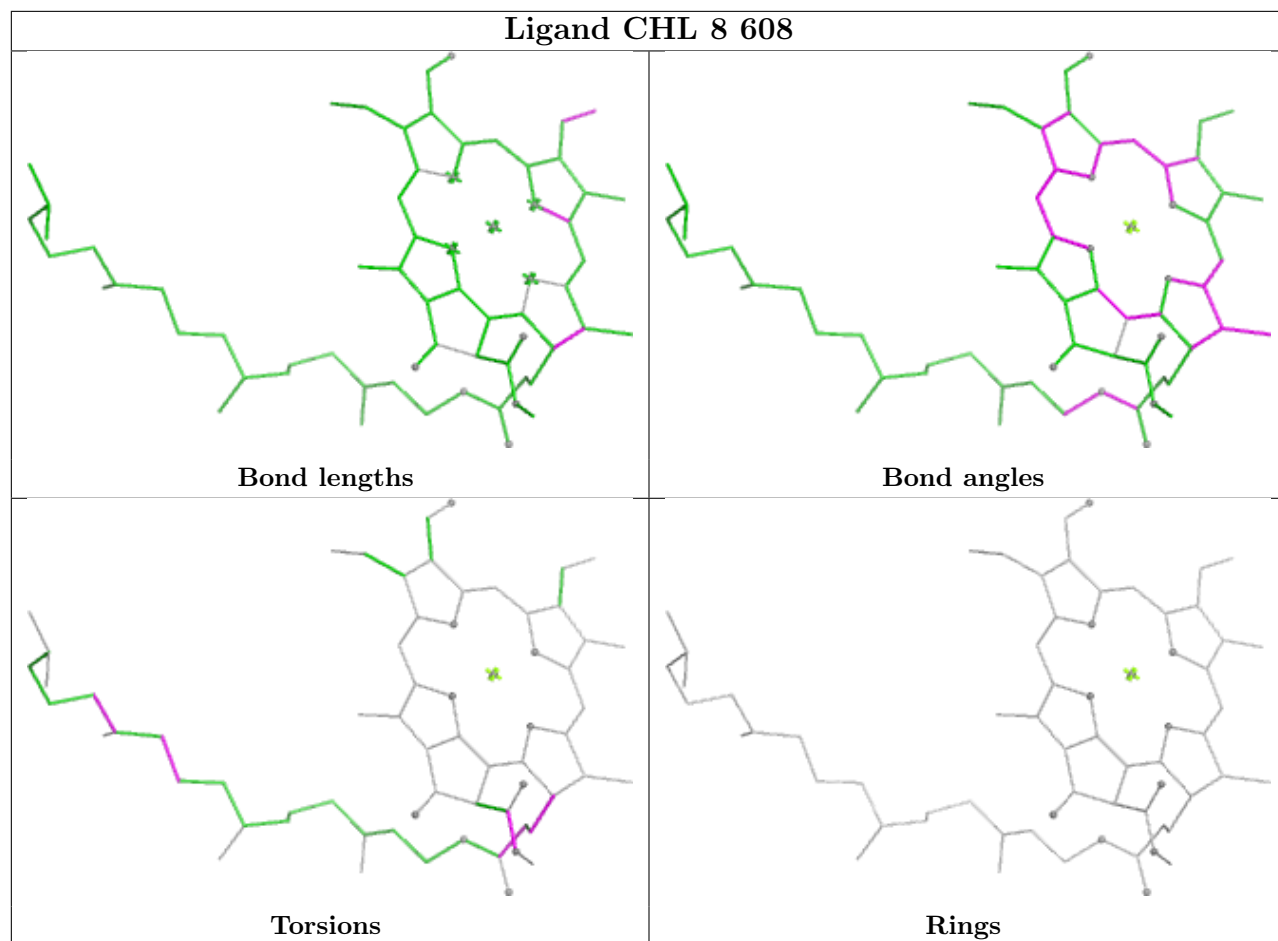


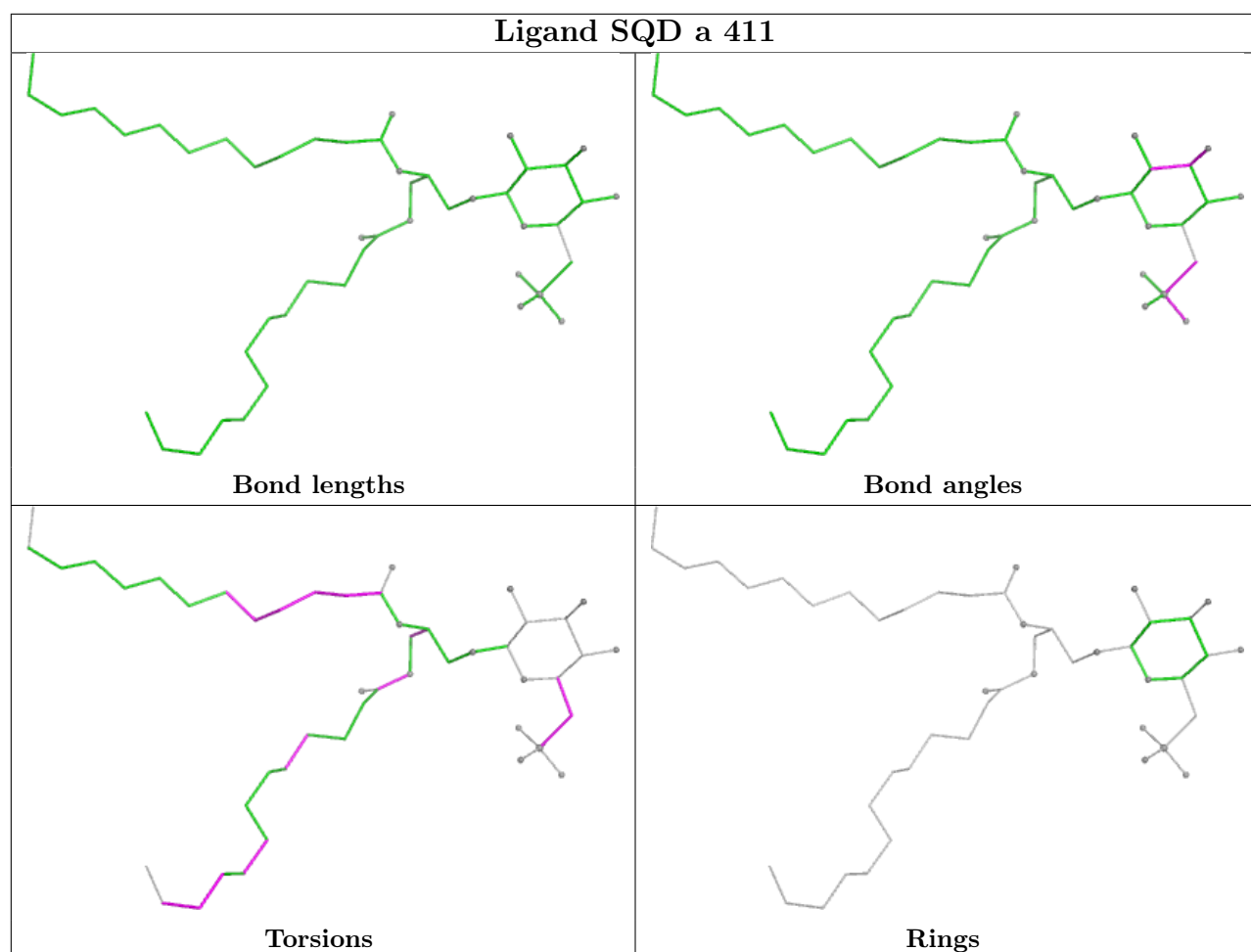
Torsions



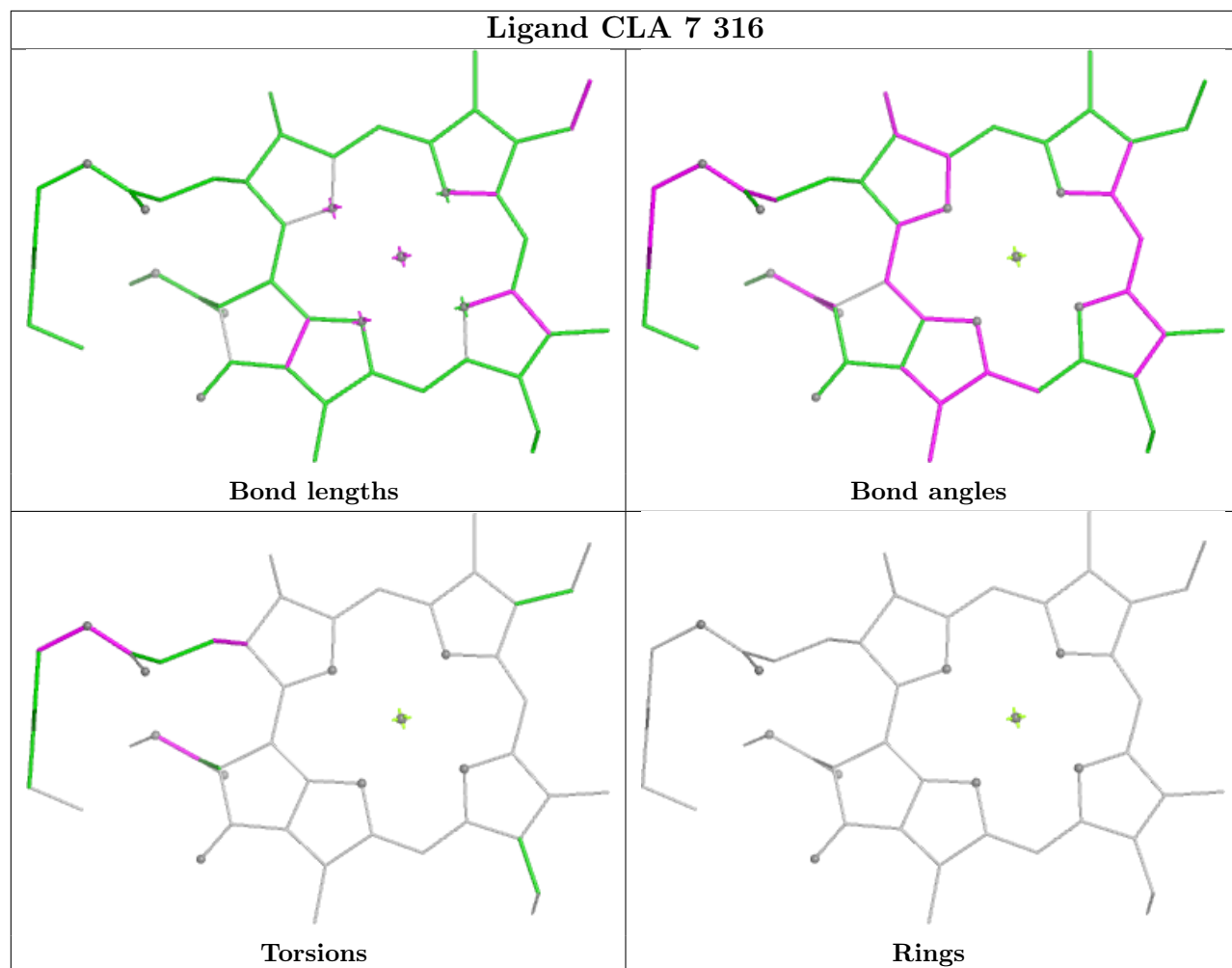
Rings

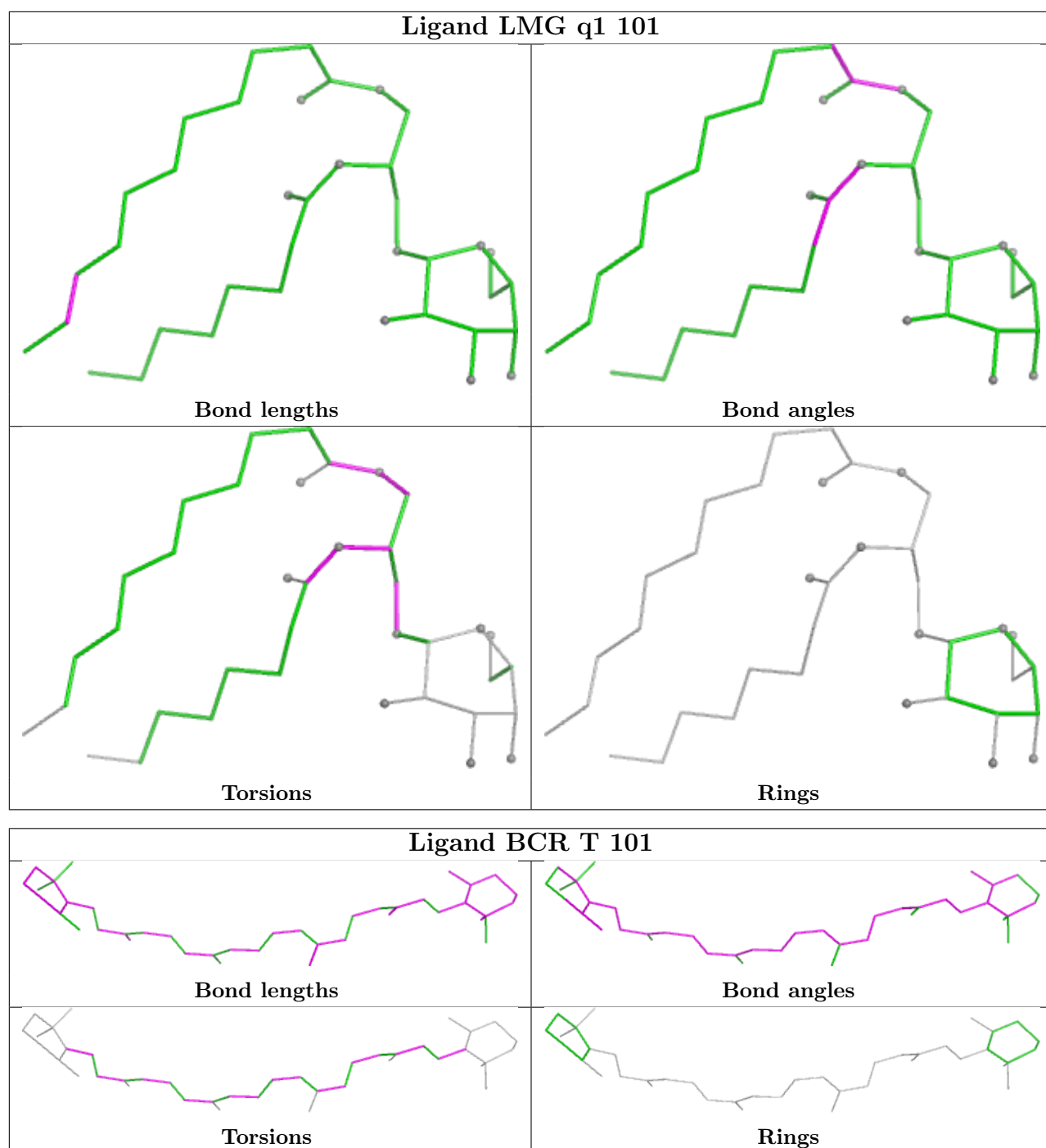


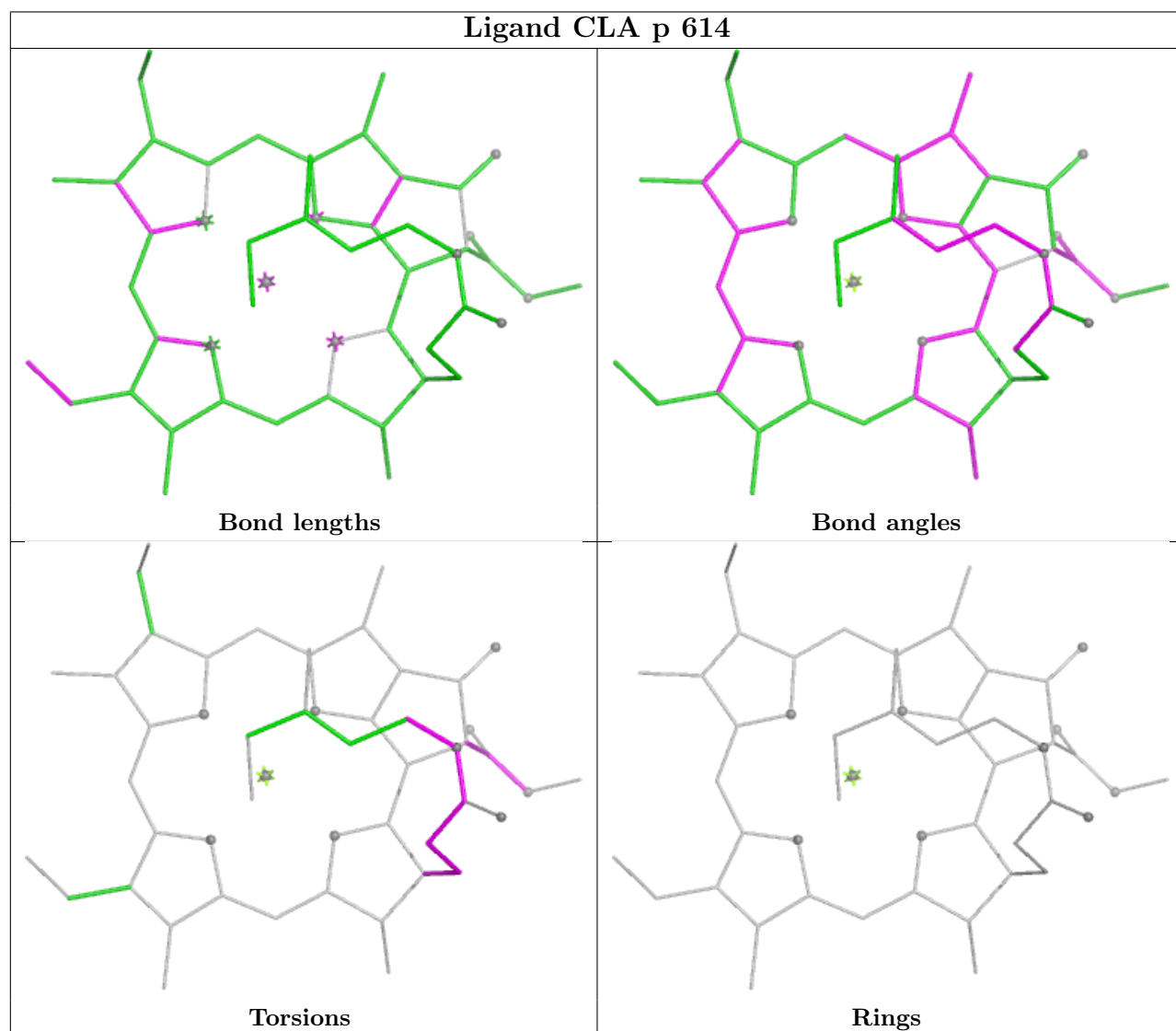
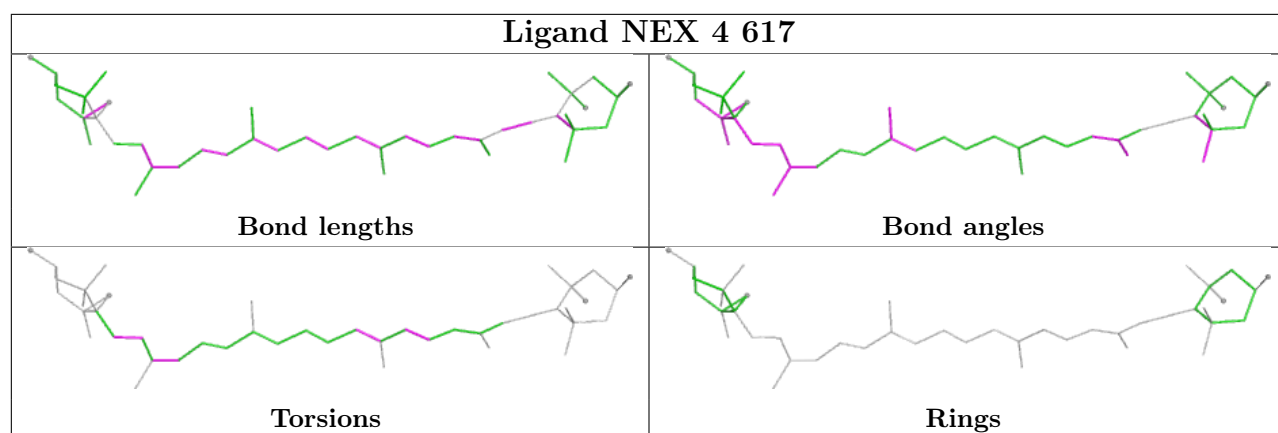


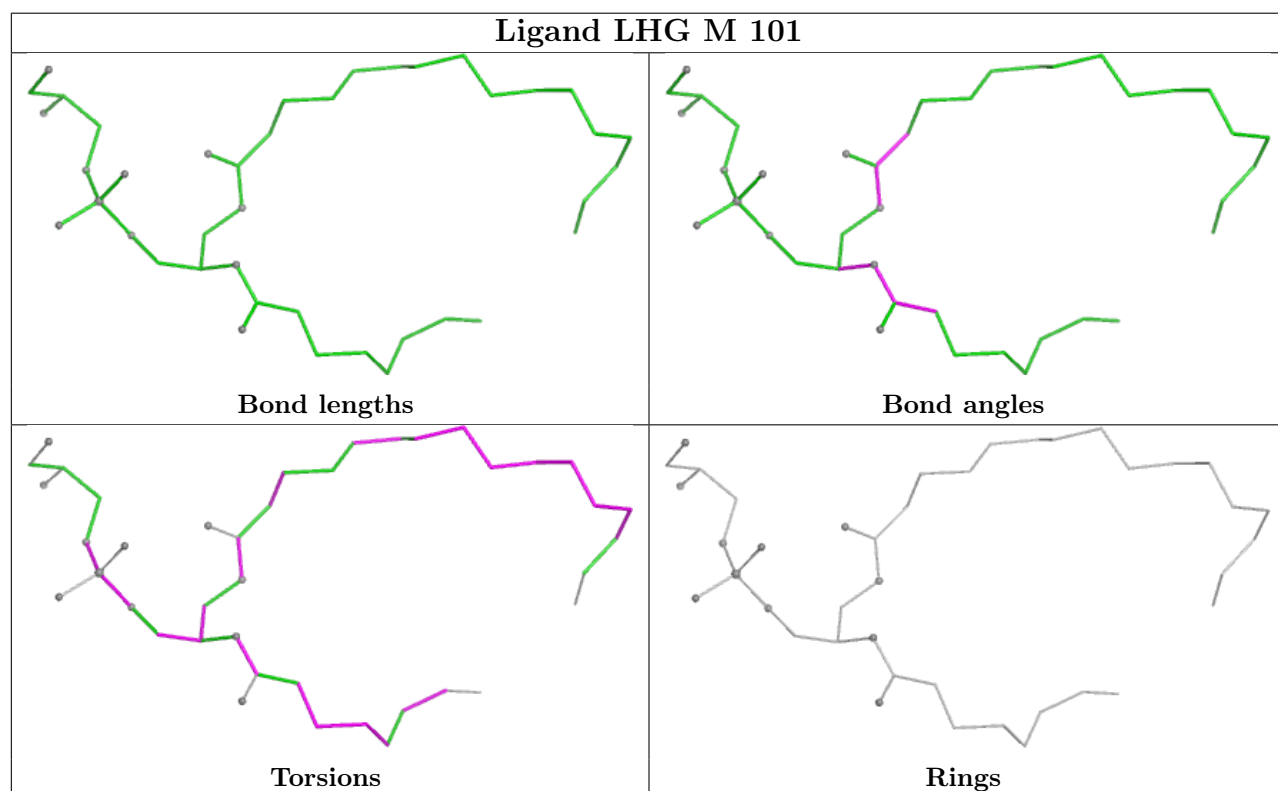
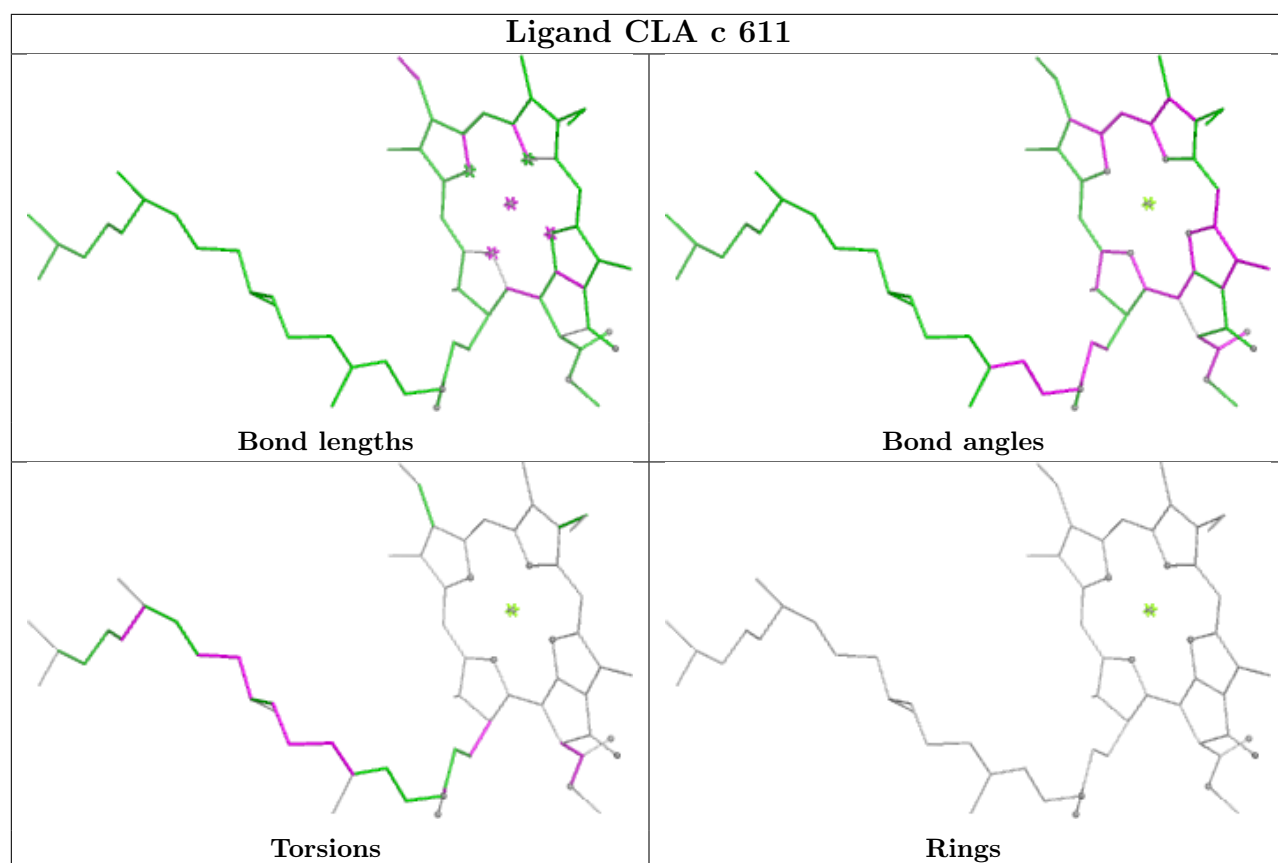


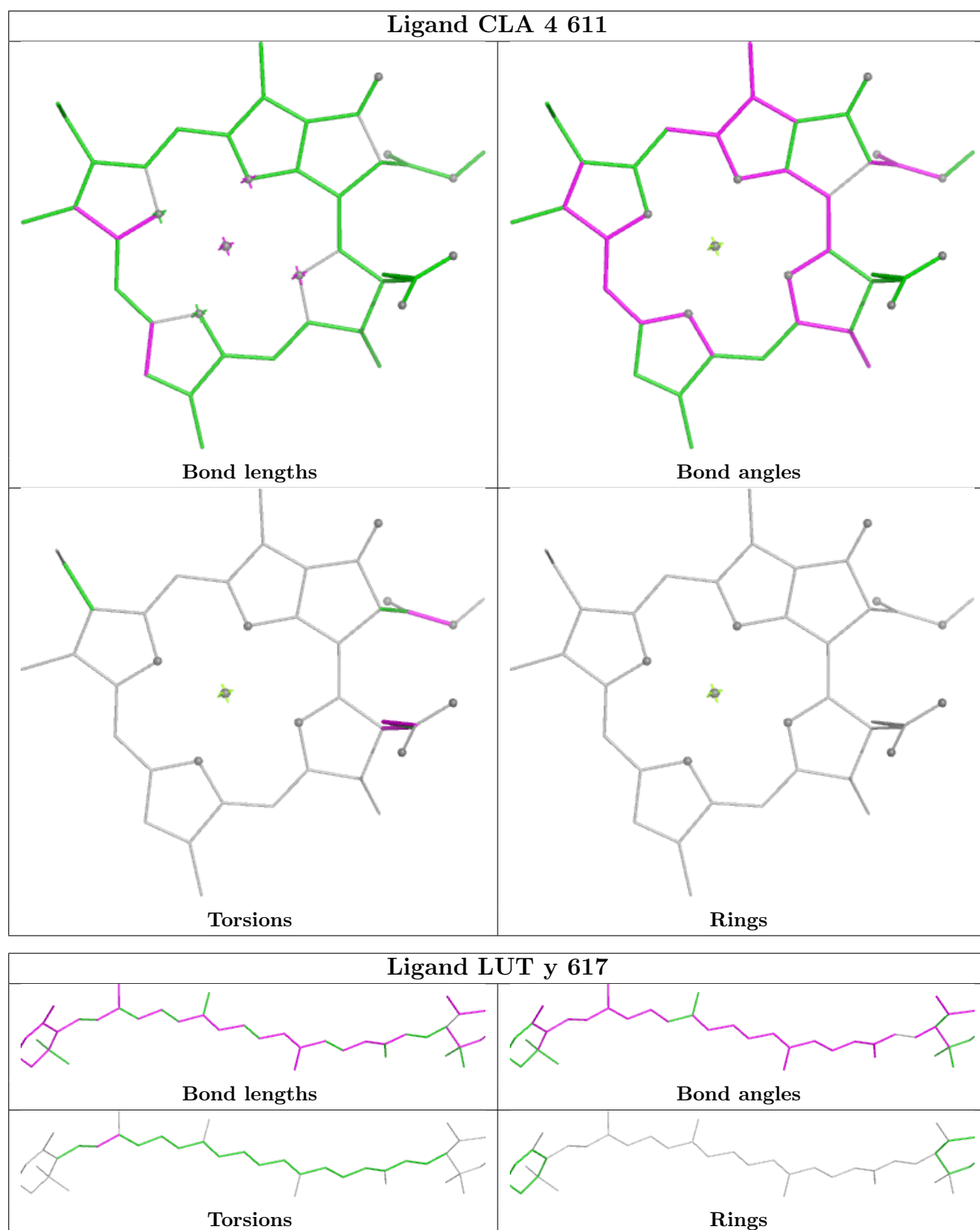
Ligand CLA 7 316



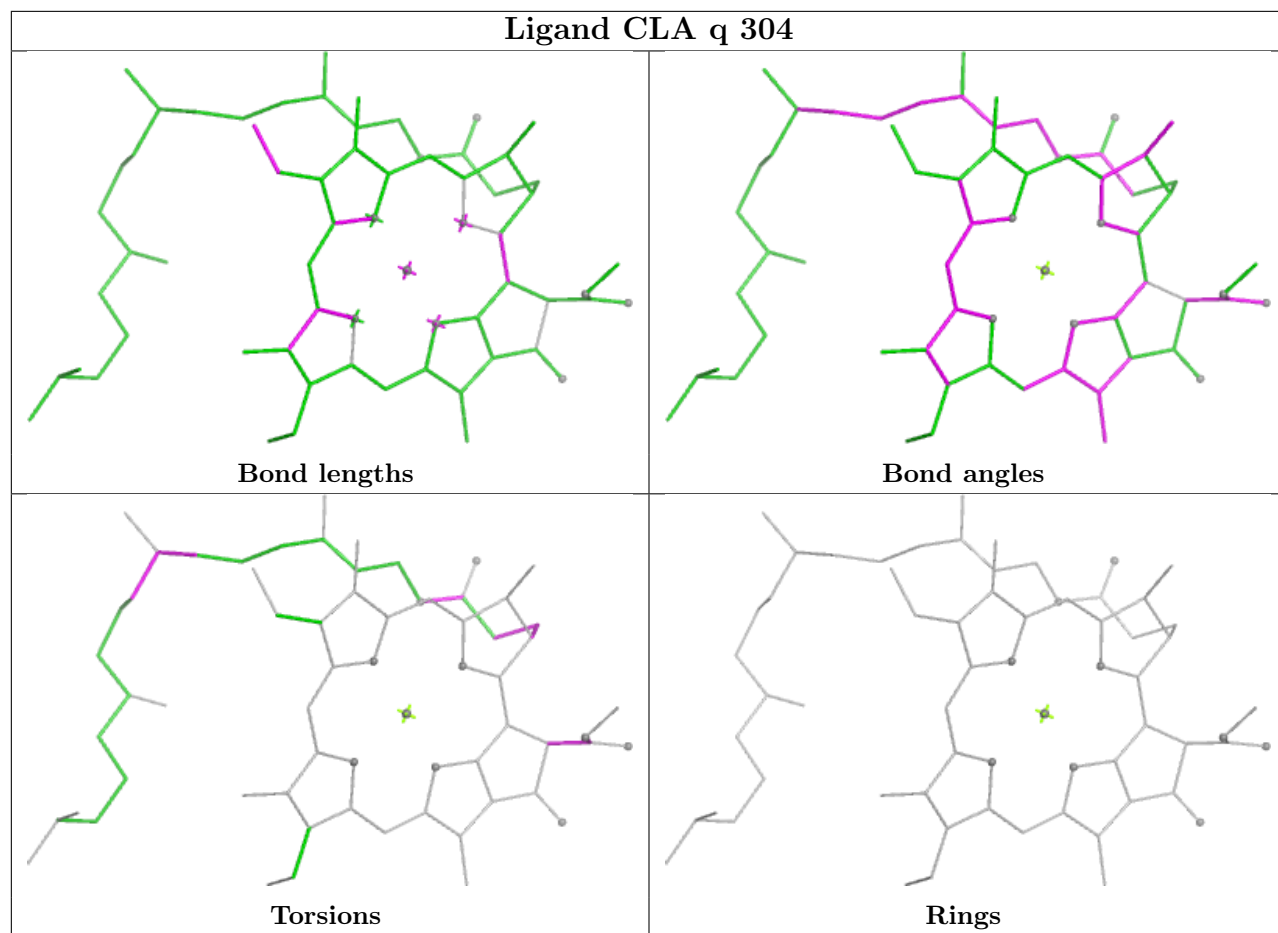




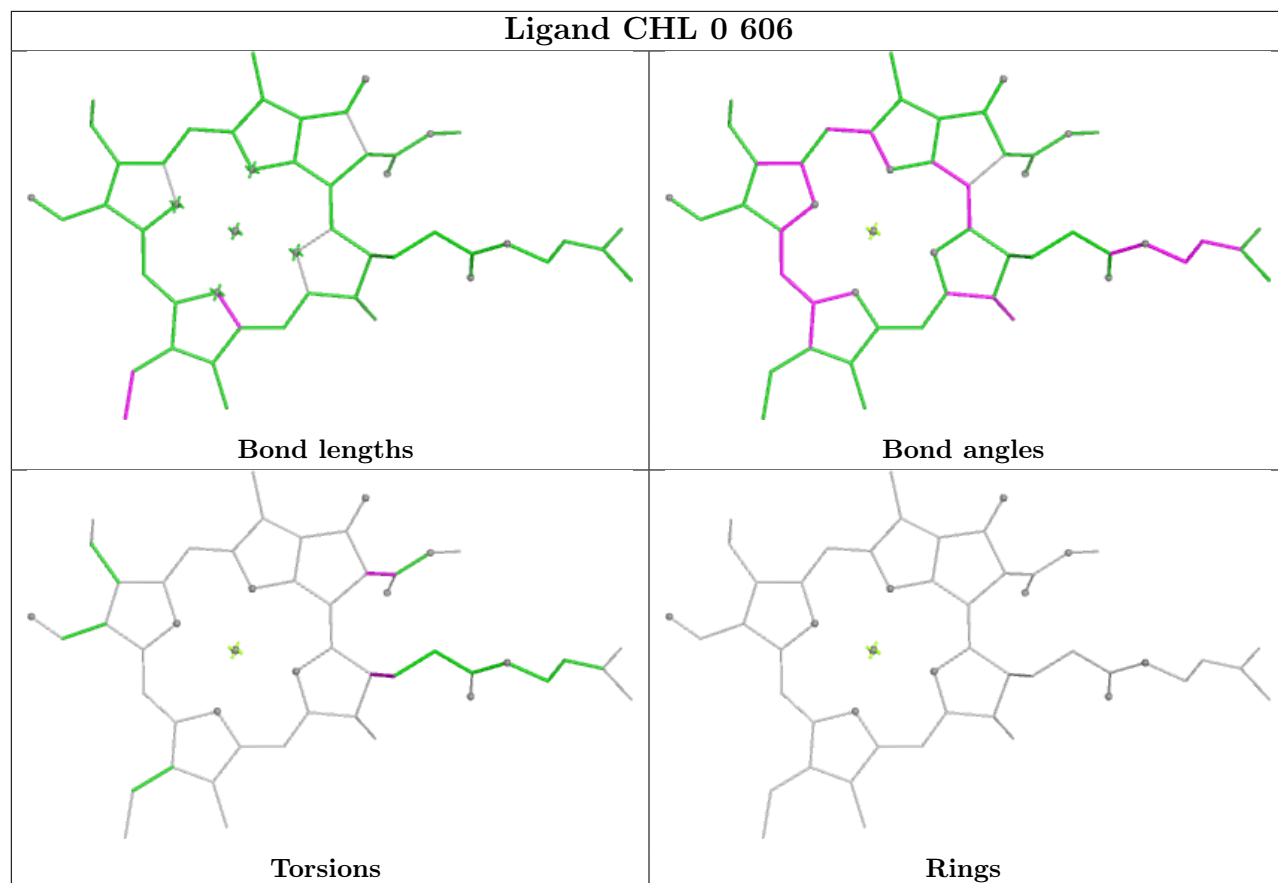




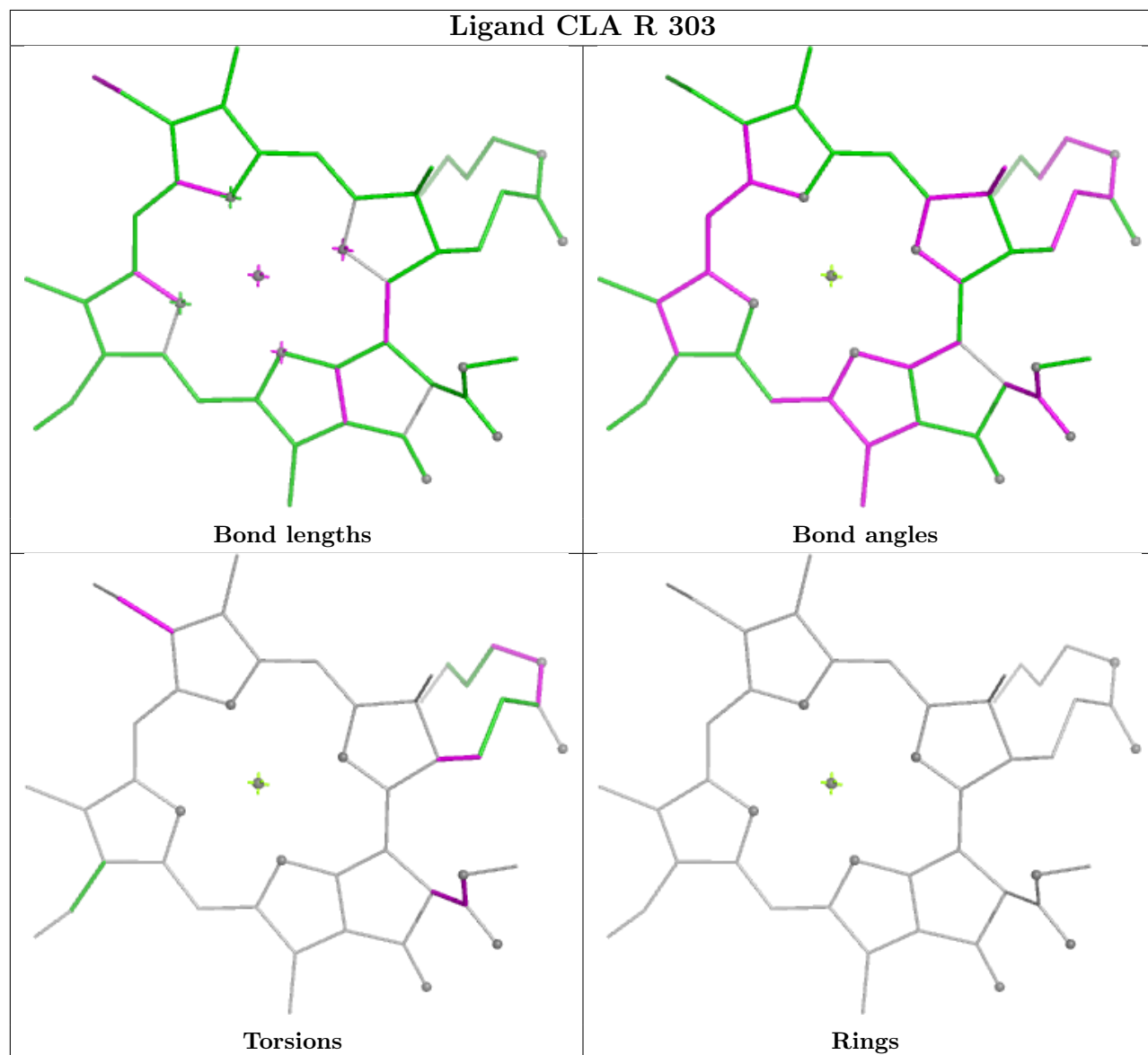
Ligand CLA q 304



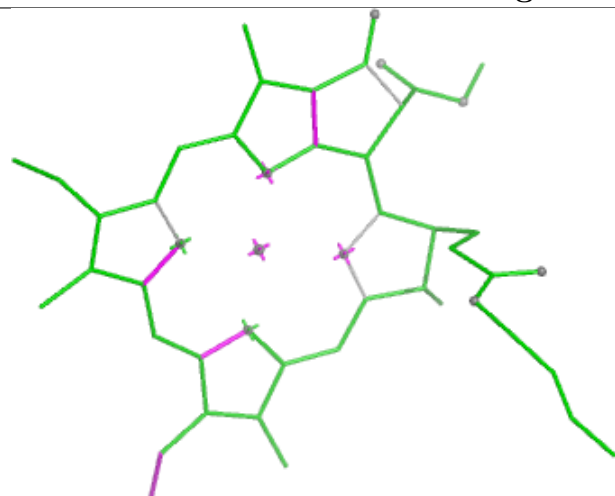
Ligand CHL 0 606



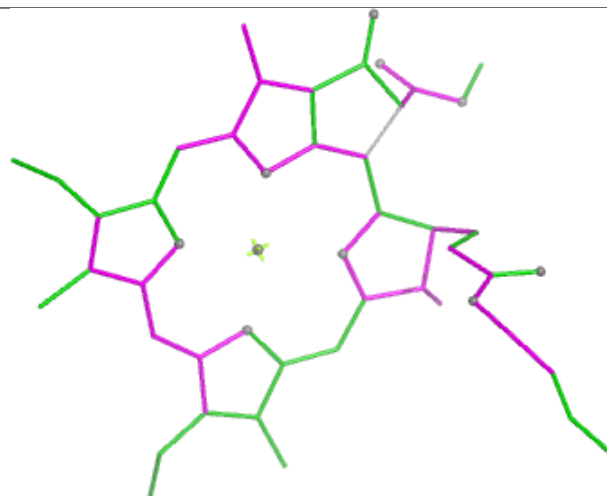
Ligand CLA R 303



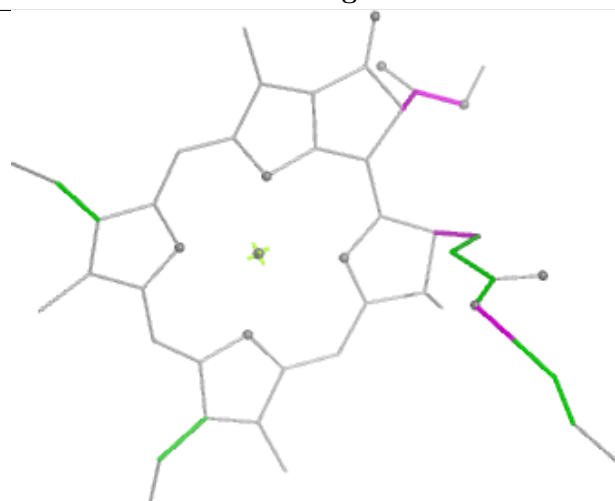
Ligand CLA A 407



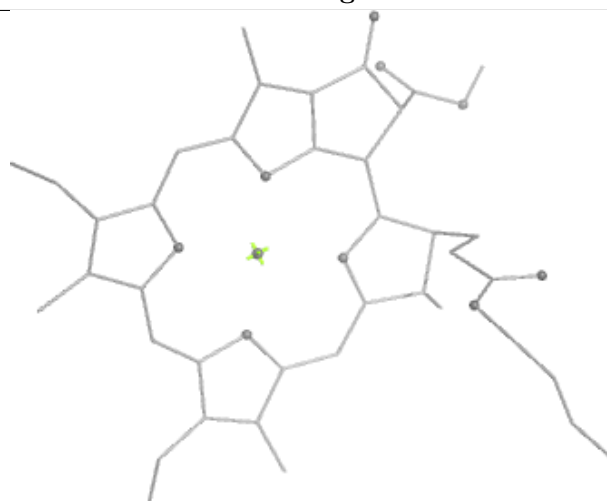
Bond lengths



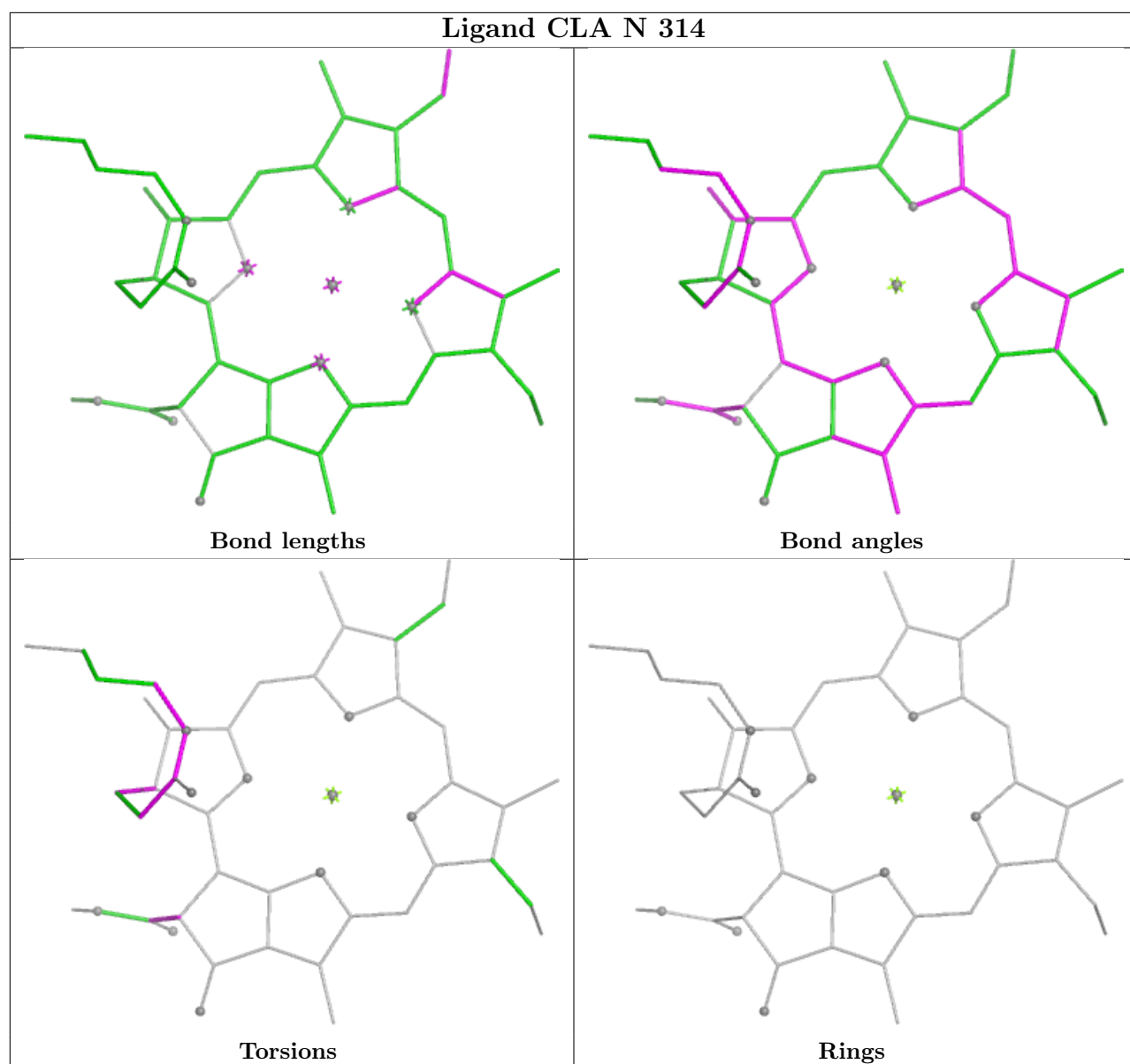
Bond angles

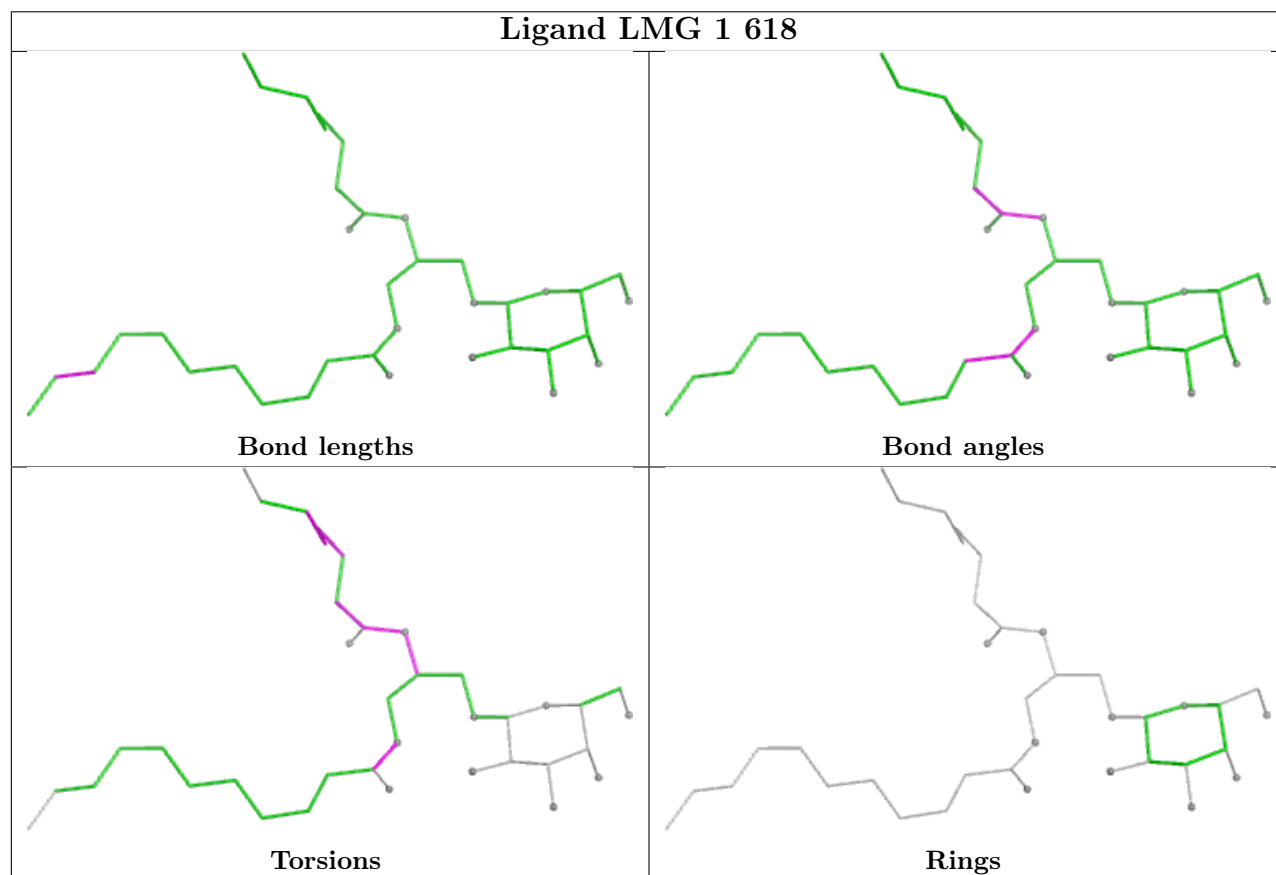
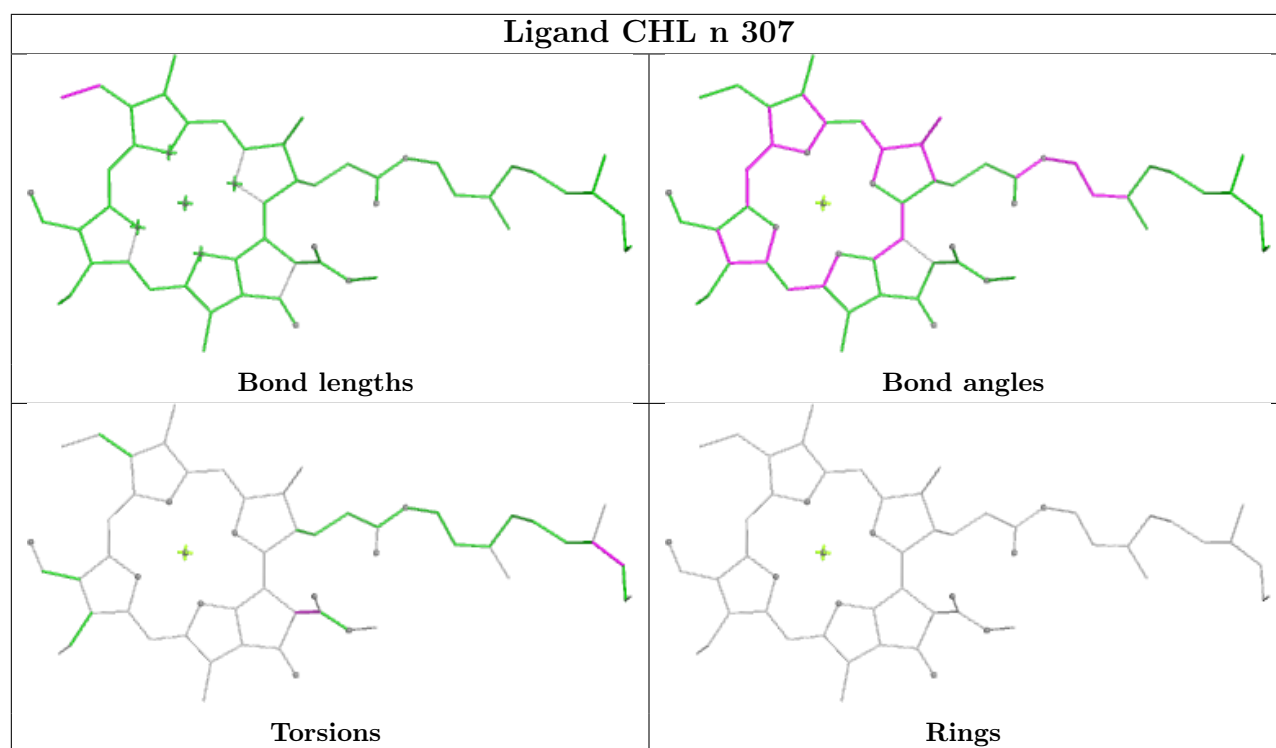


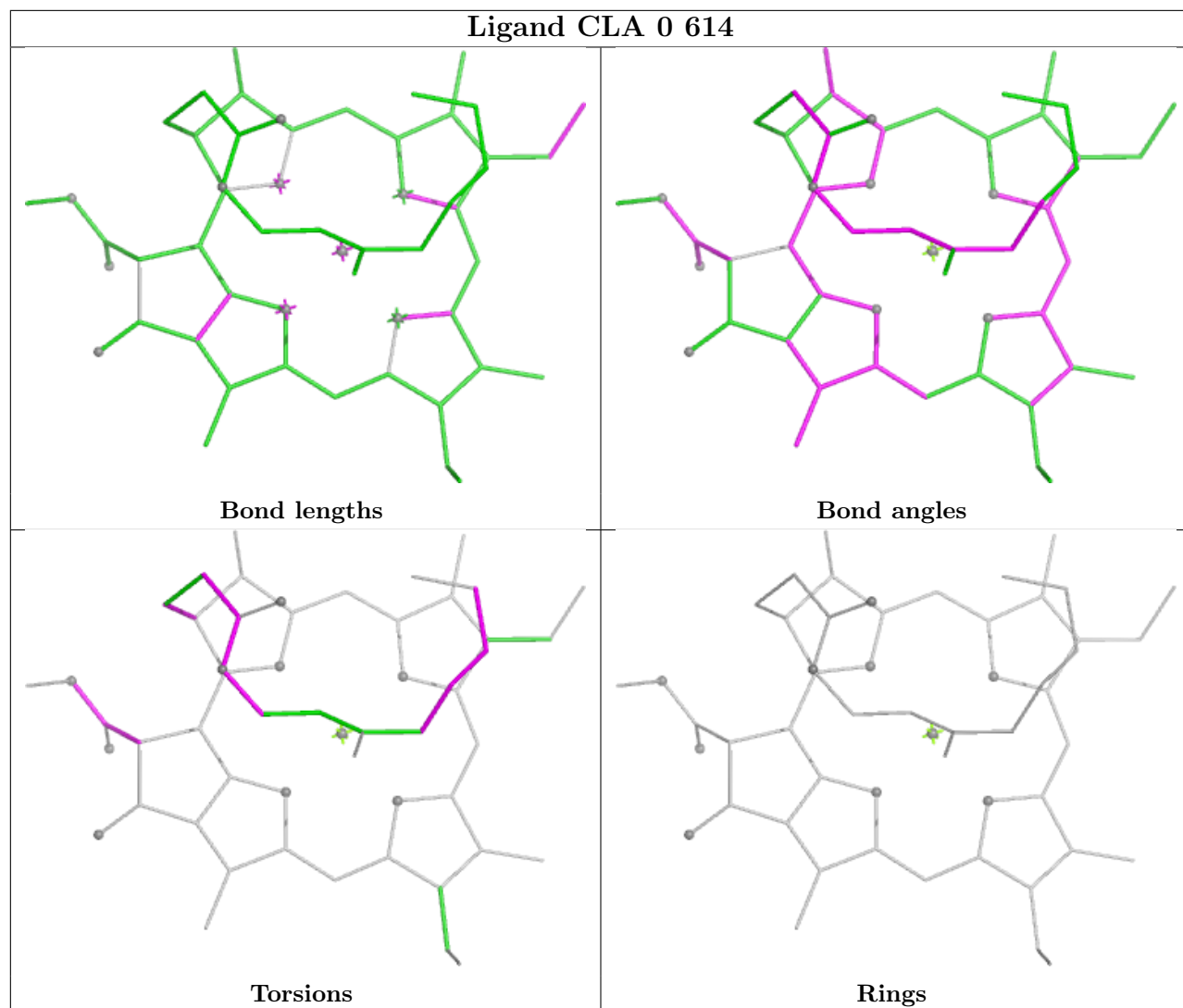
Torsions

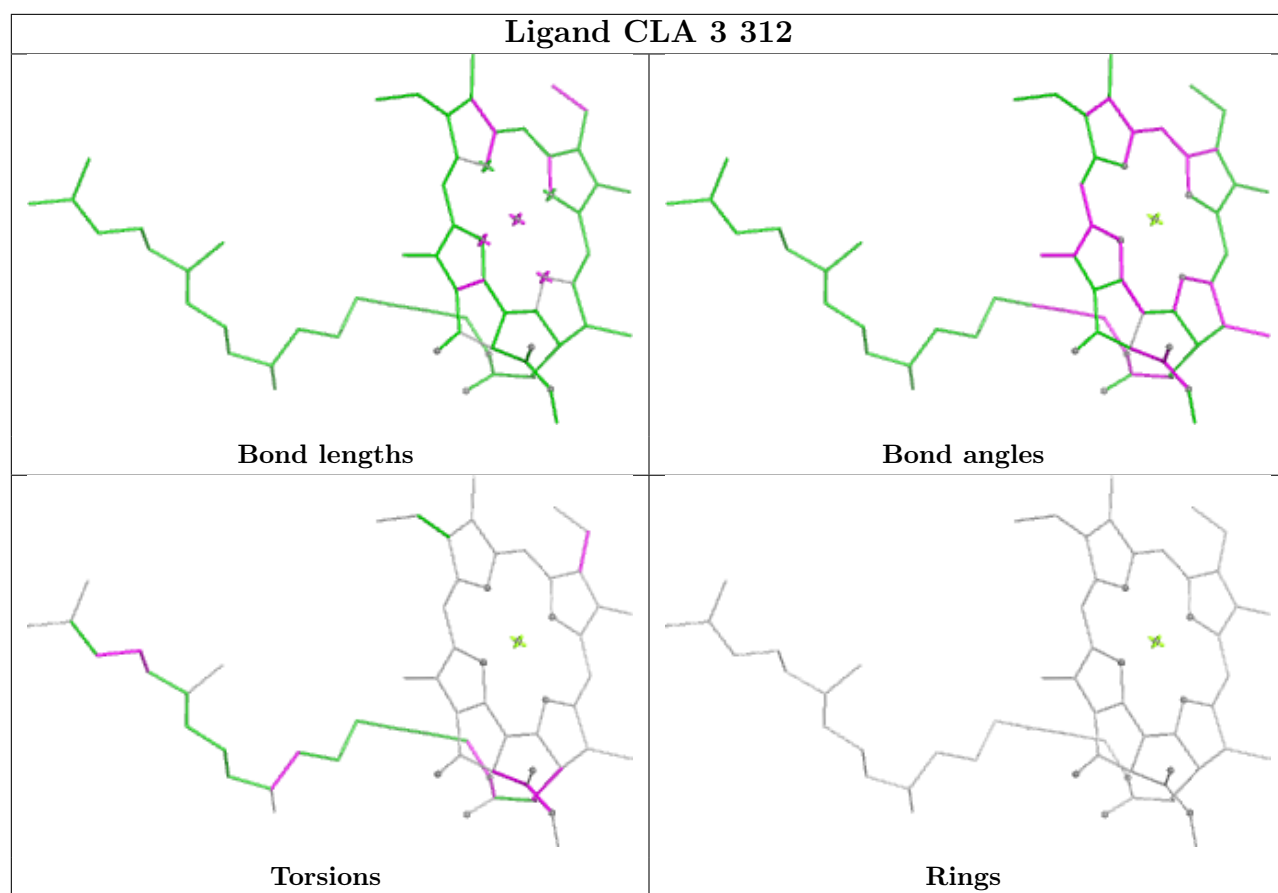


Rings

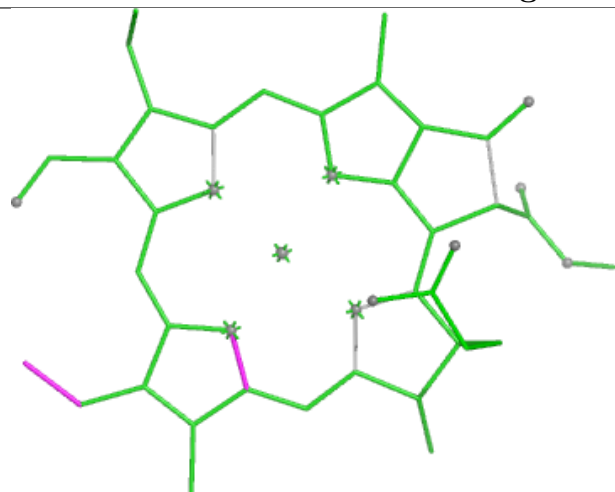




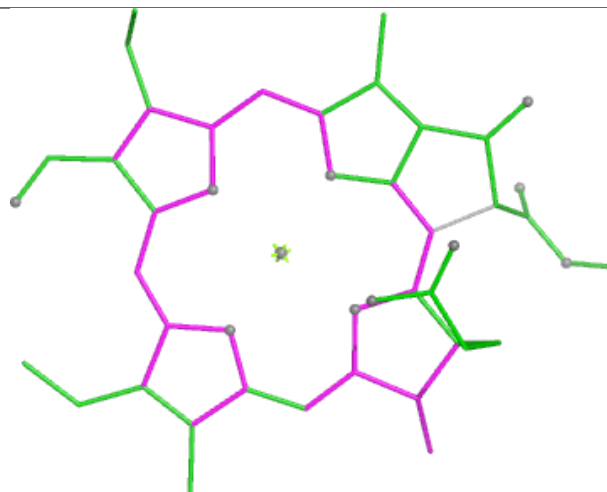




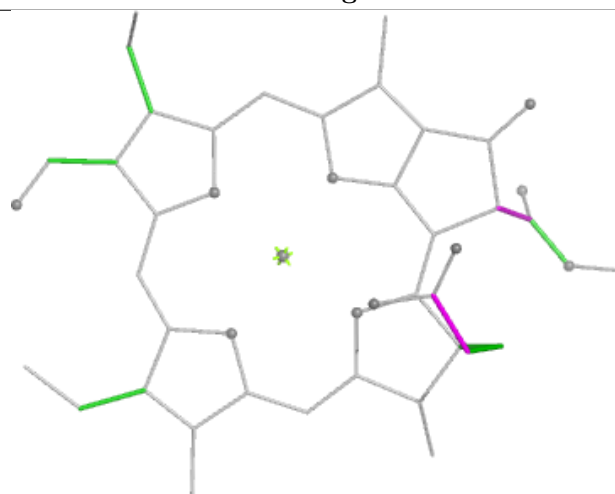
Ligand CHL 2 605



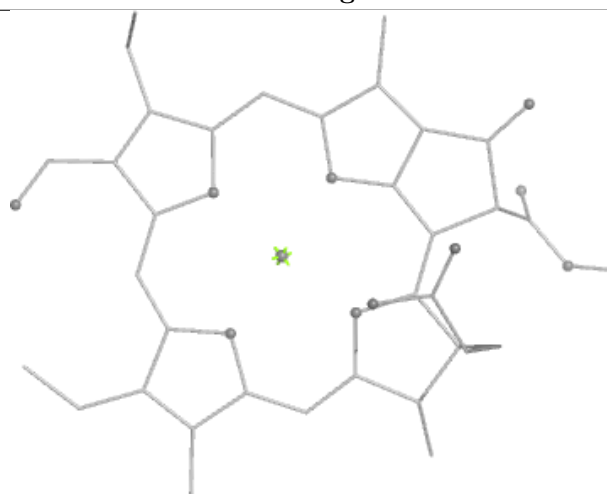
Bond lengths



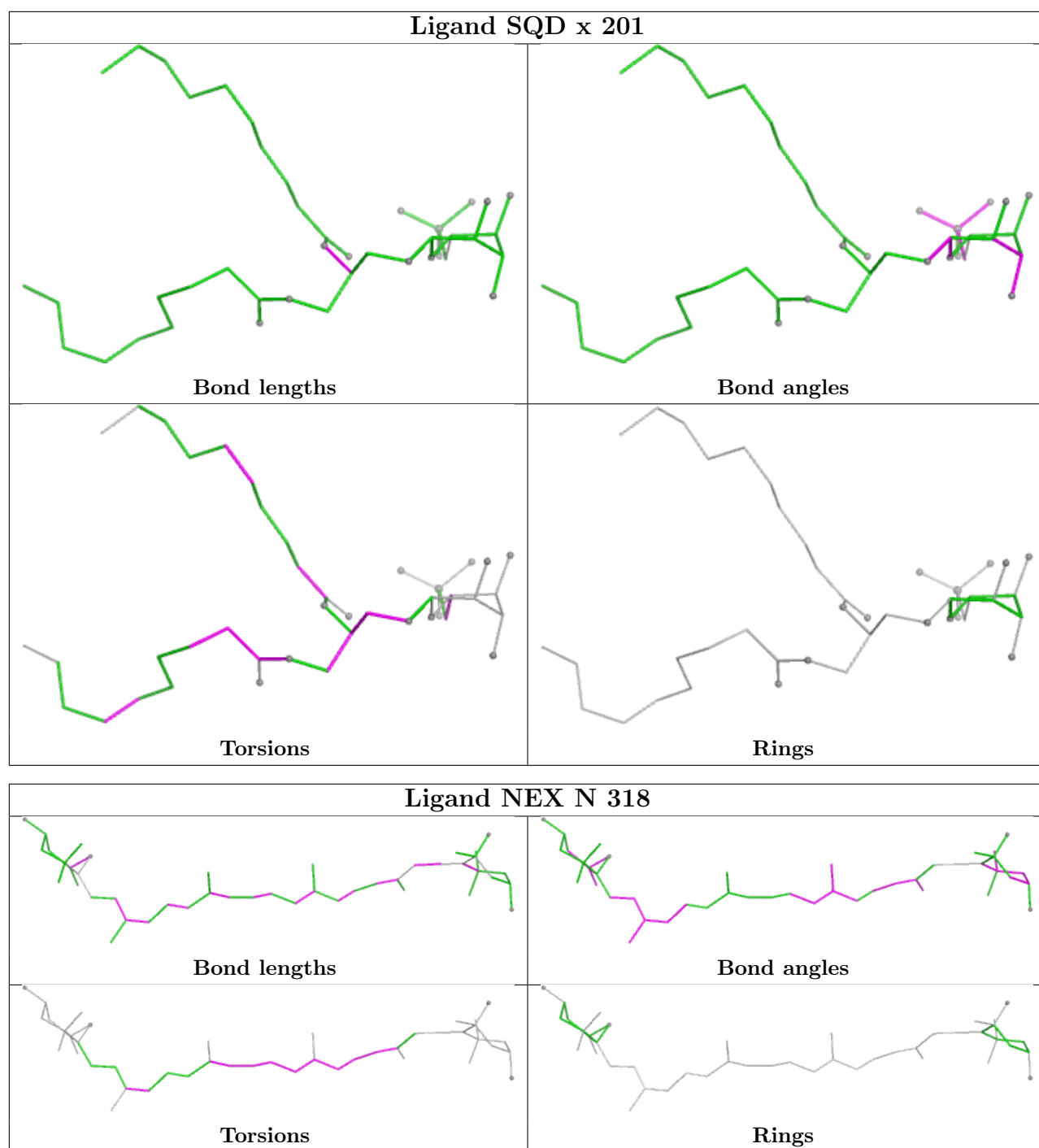
Bond angles



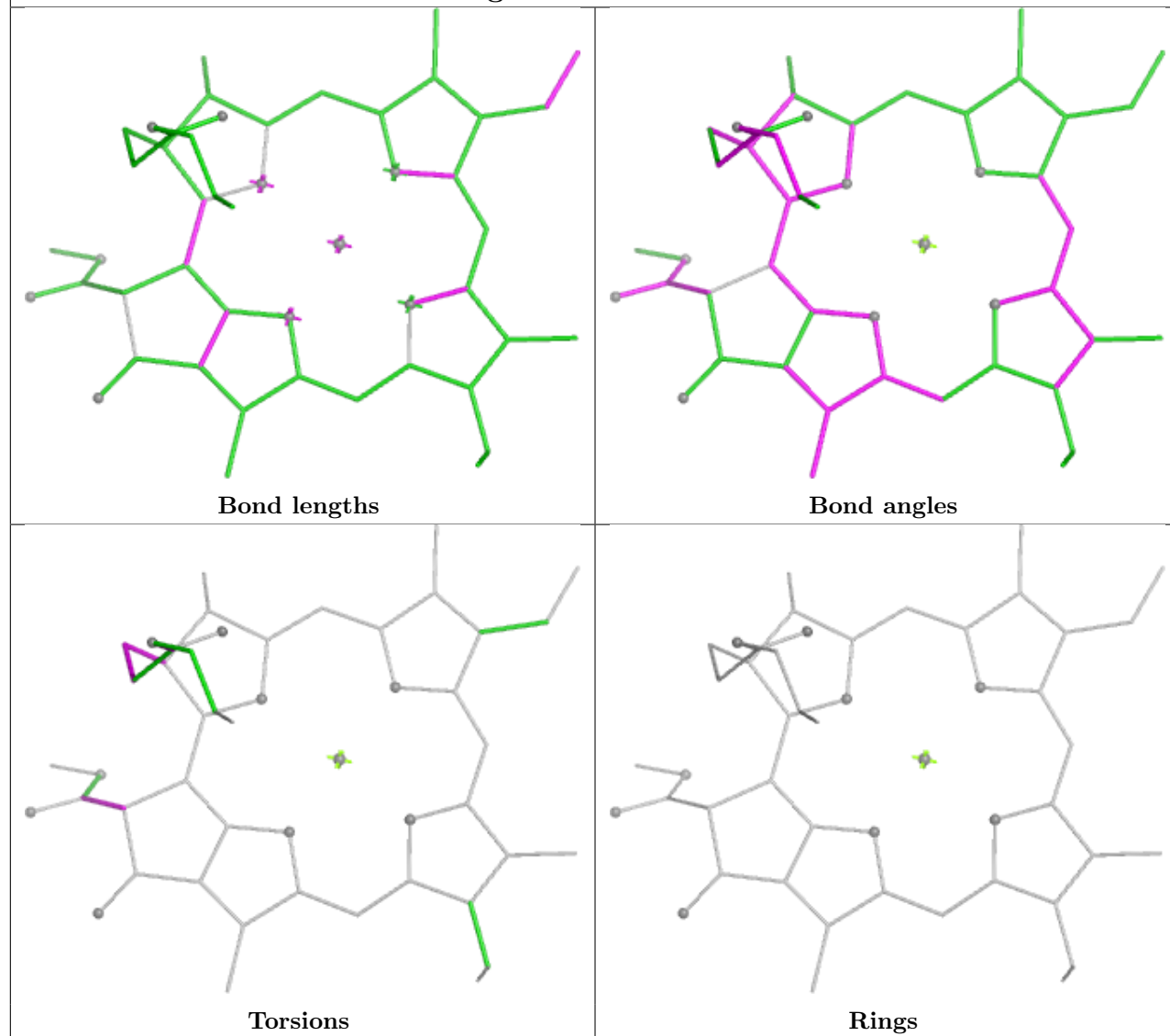
Torsions



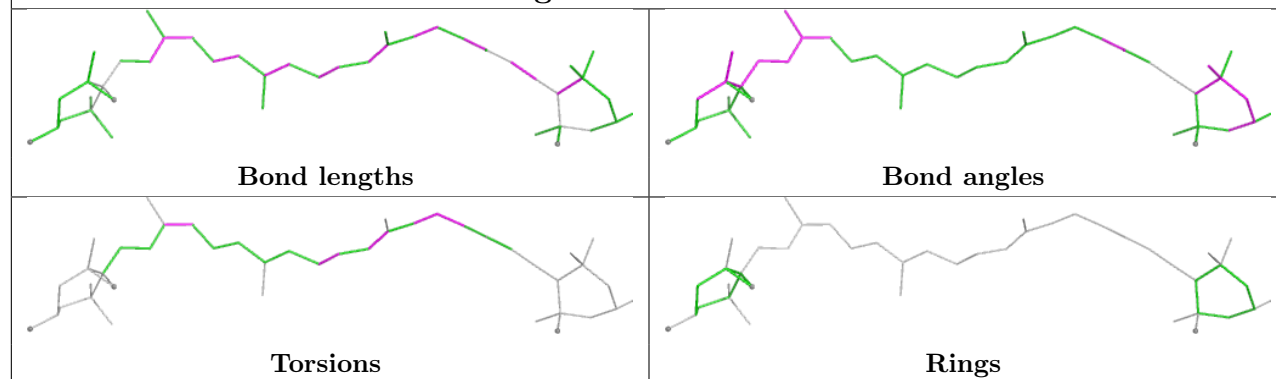
Rings

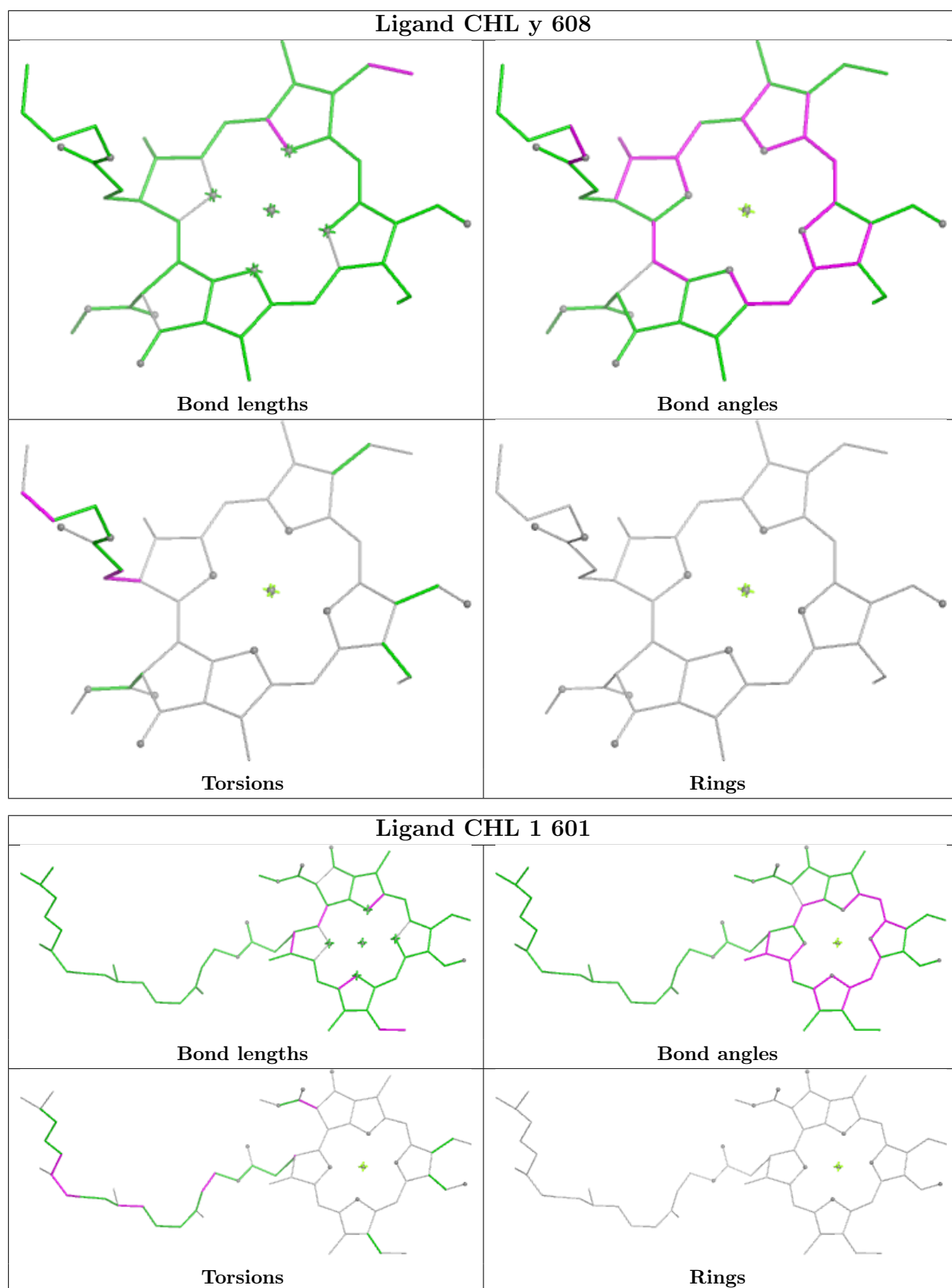


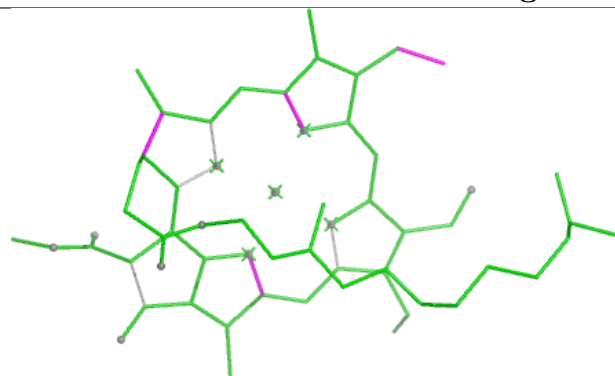
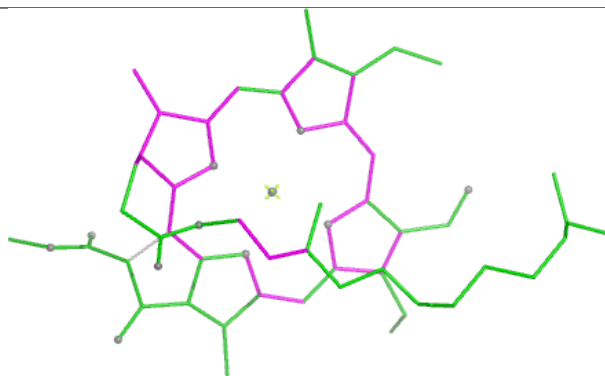
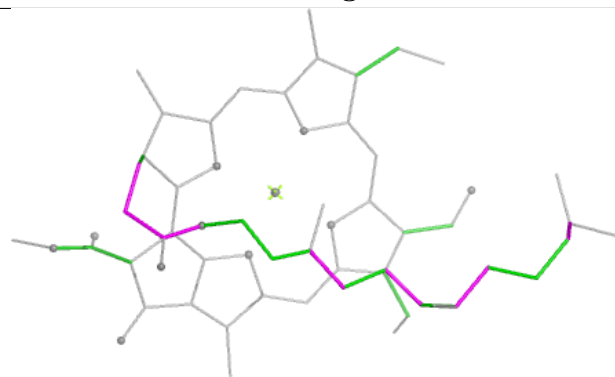
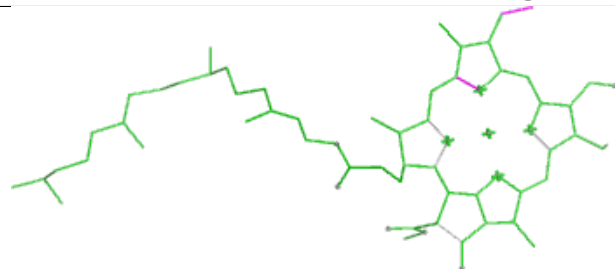
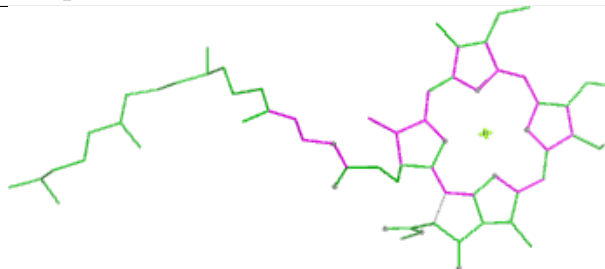
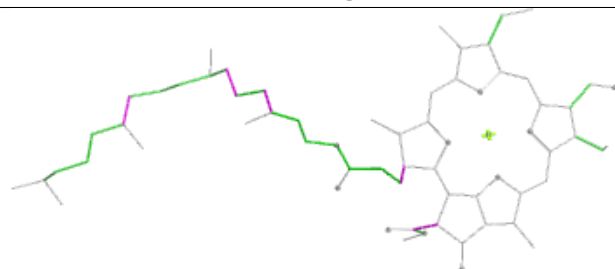
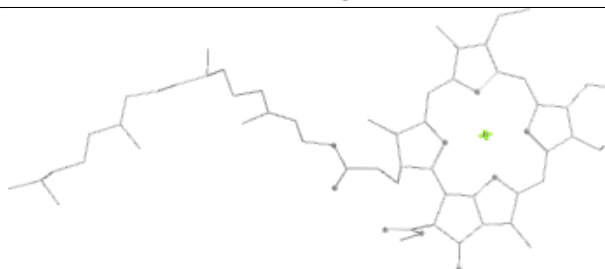
Ligand CLA R 306

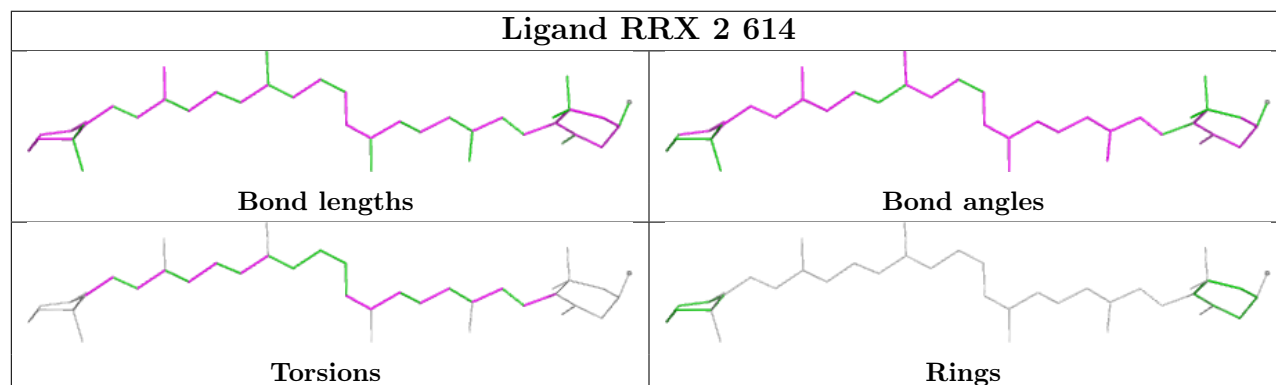
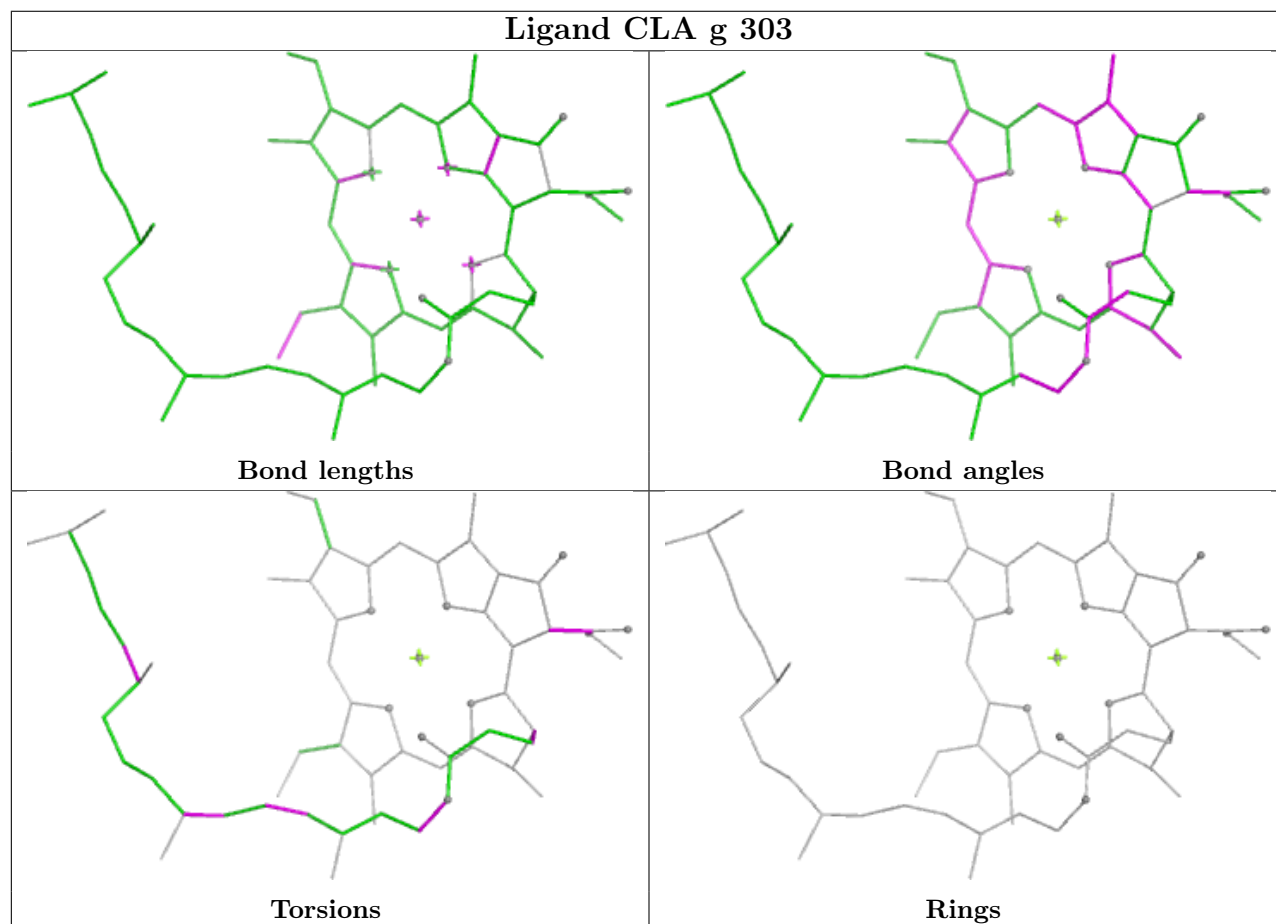
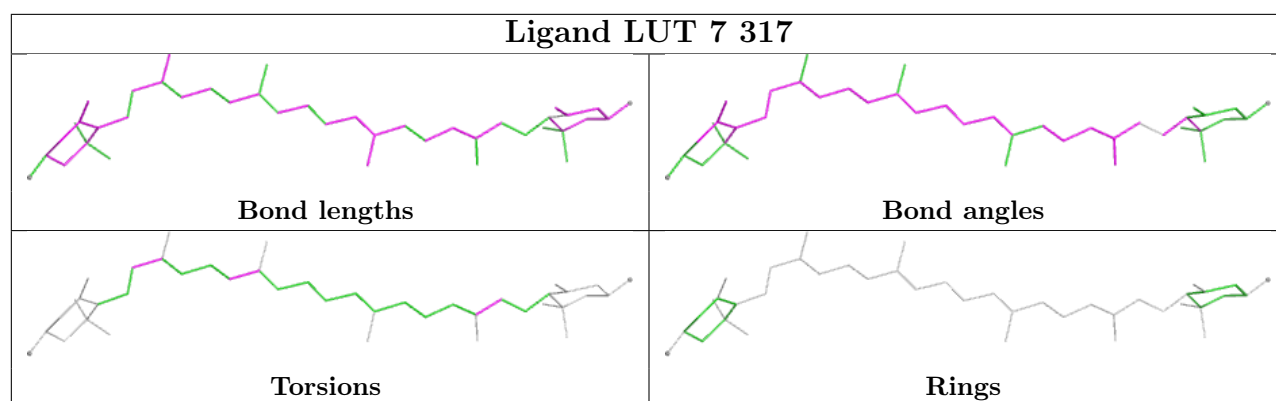


Ligand NEX 9 319

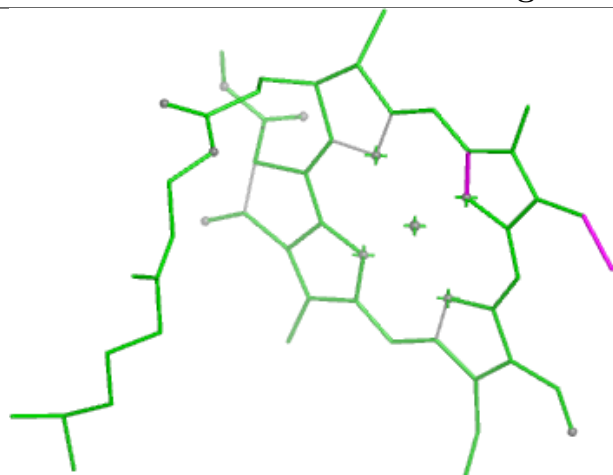




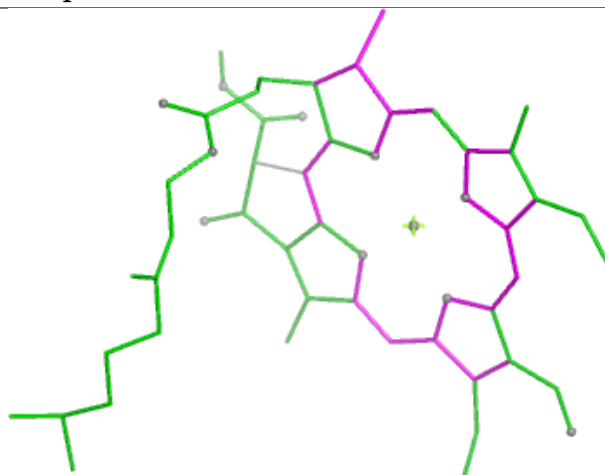
Ligand CHL 1 619**Bond lengths****Bond angles****Torsions****Rings****Ligand CHL q 303****Bond lengths****Bond angles****Torsions****Rings**



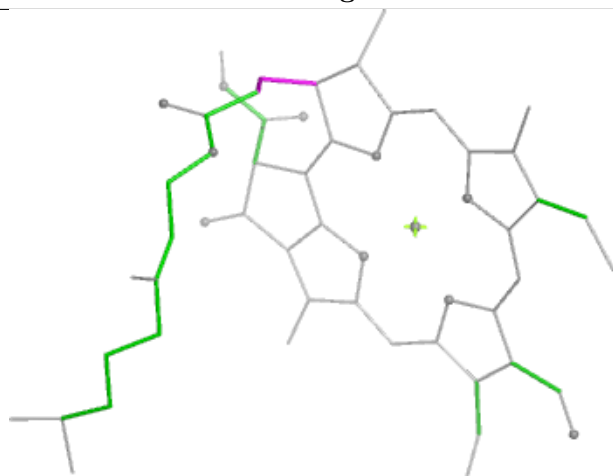
Ligand CHL q 311



Bond lengths



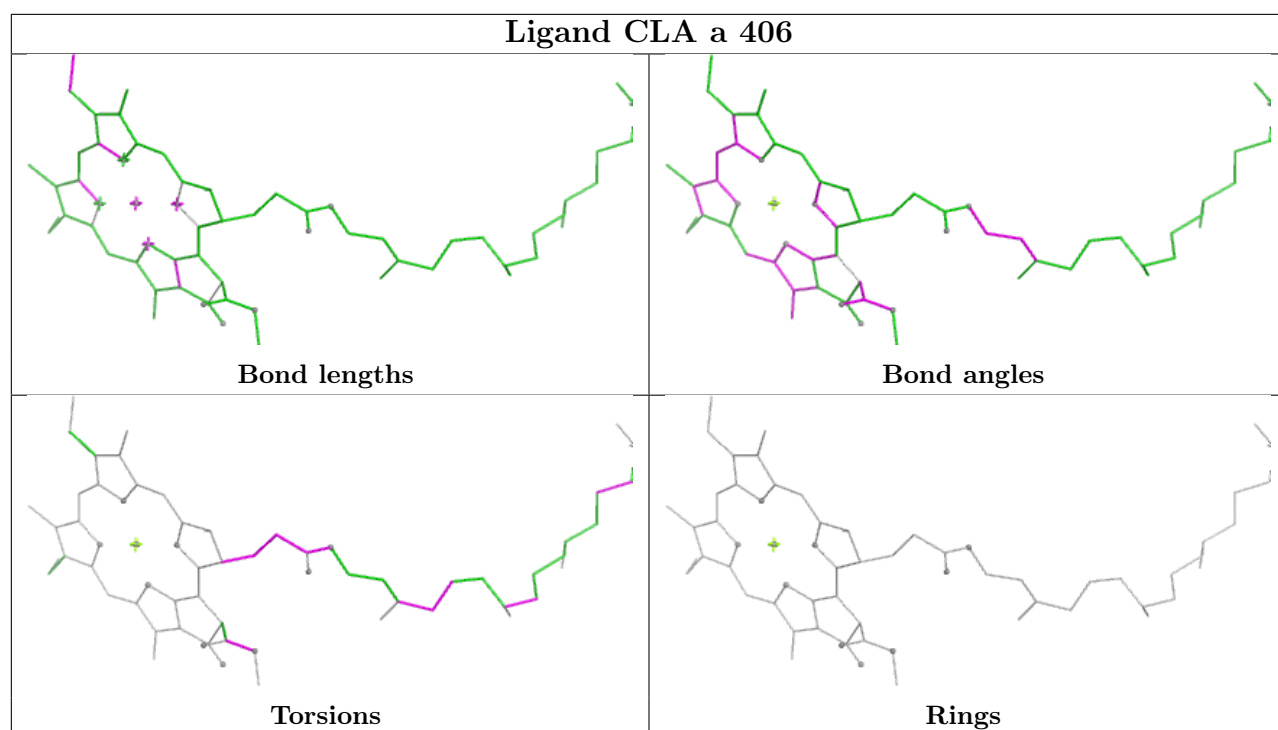
Bond angles



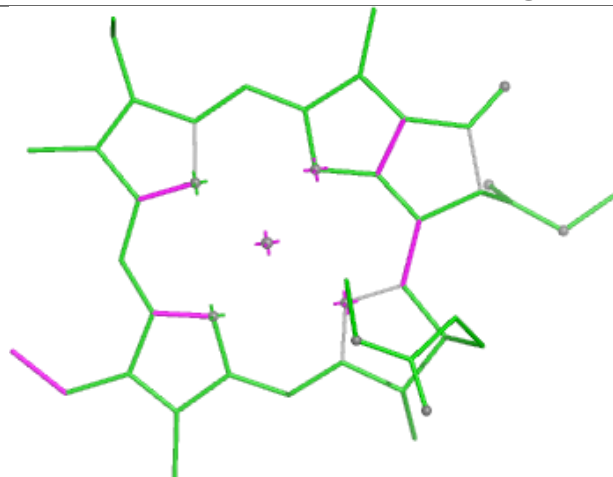
Torsions



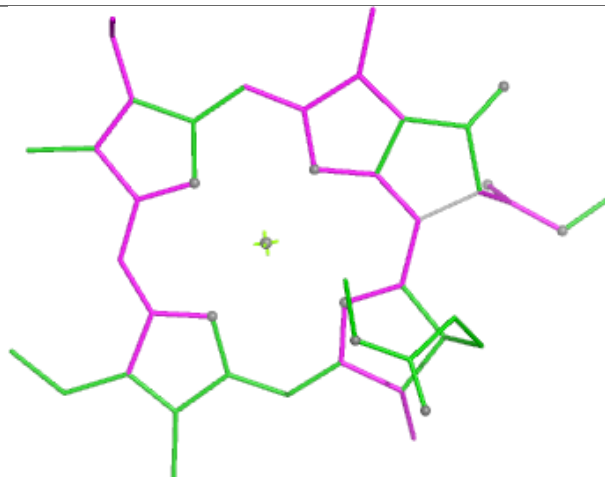
Rings



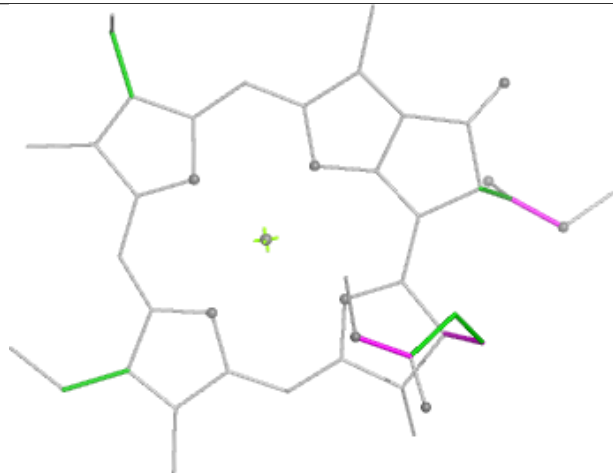
Ligand CLA s 316



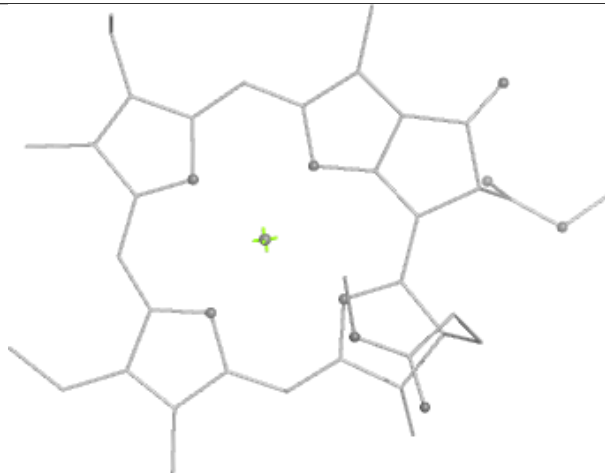
Bond lengths



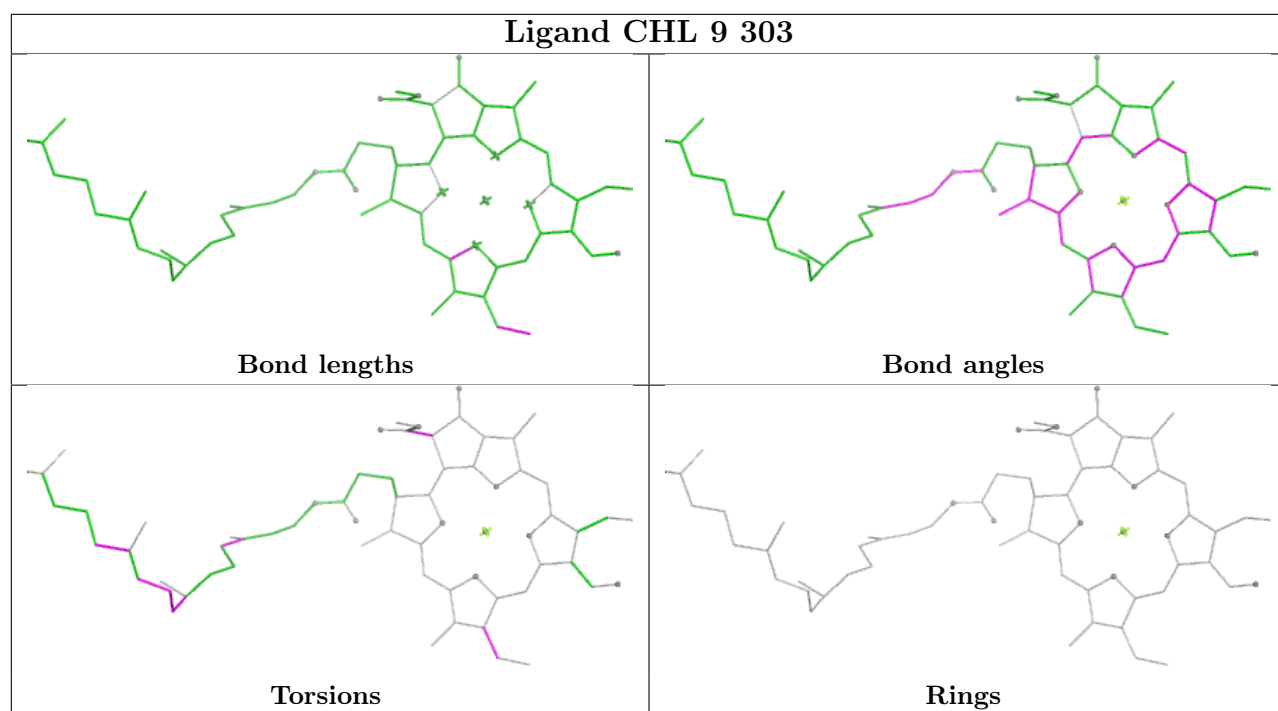
Bond angles



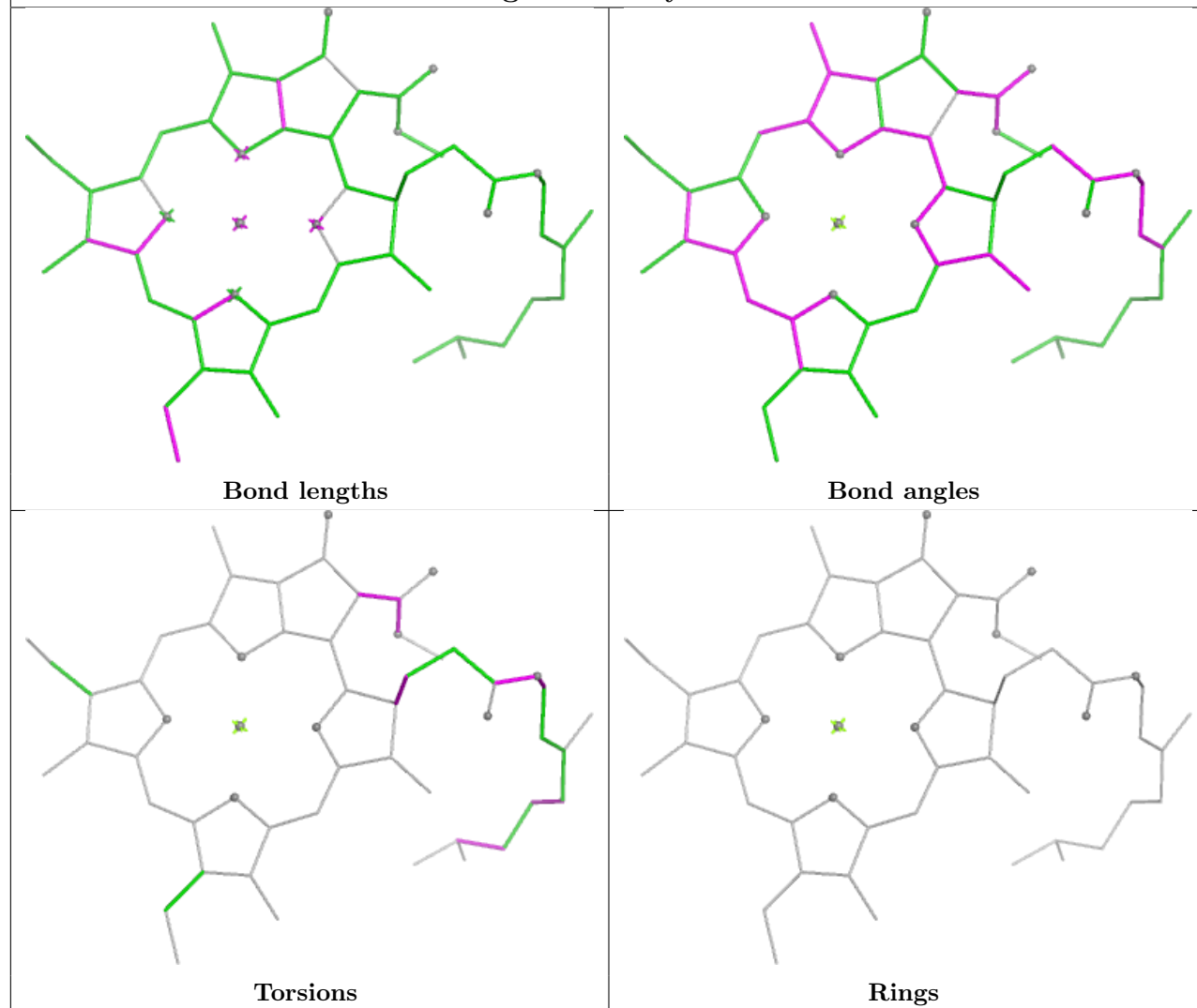
Torsions



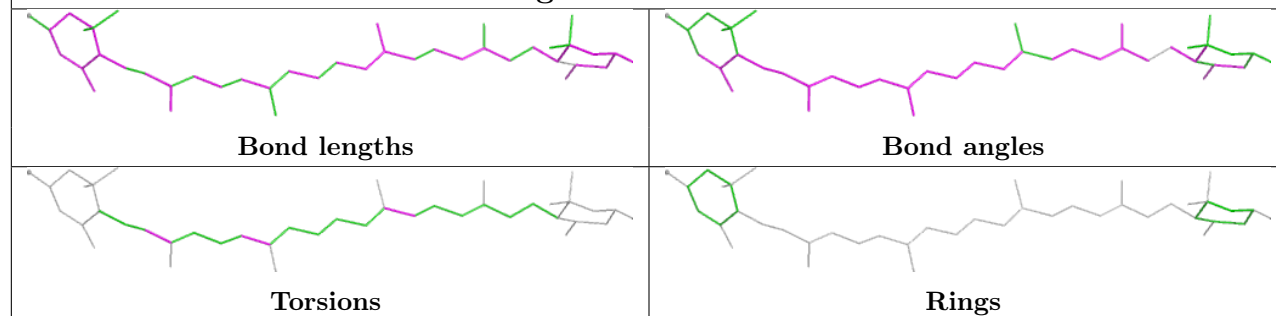
Rings



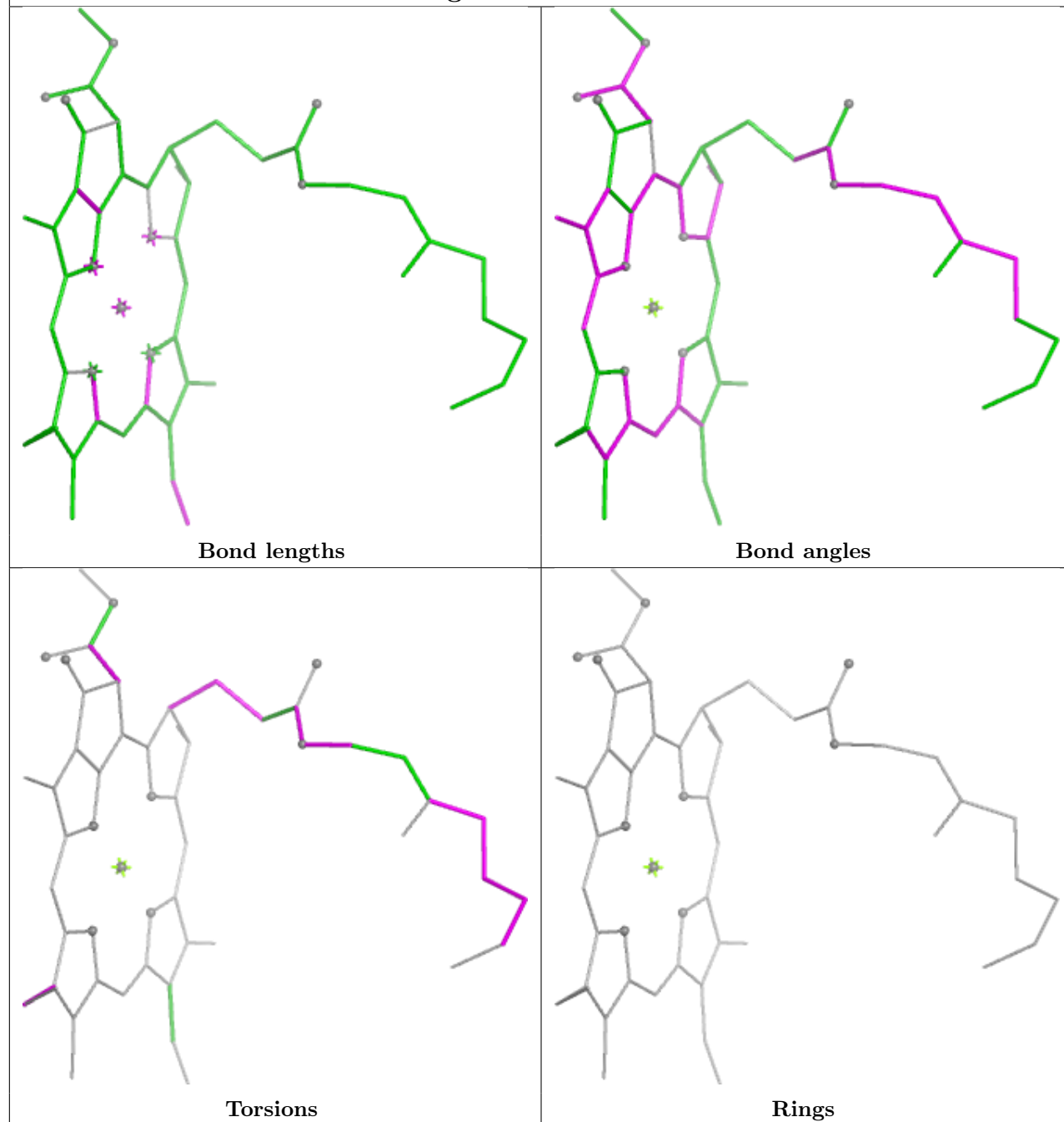
Ligand CLA y 603

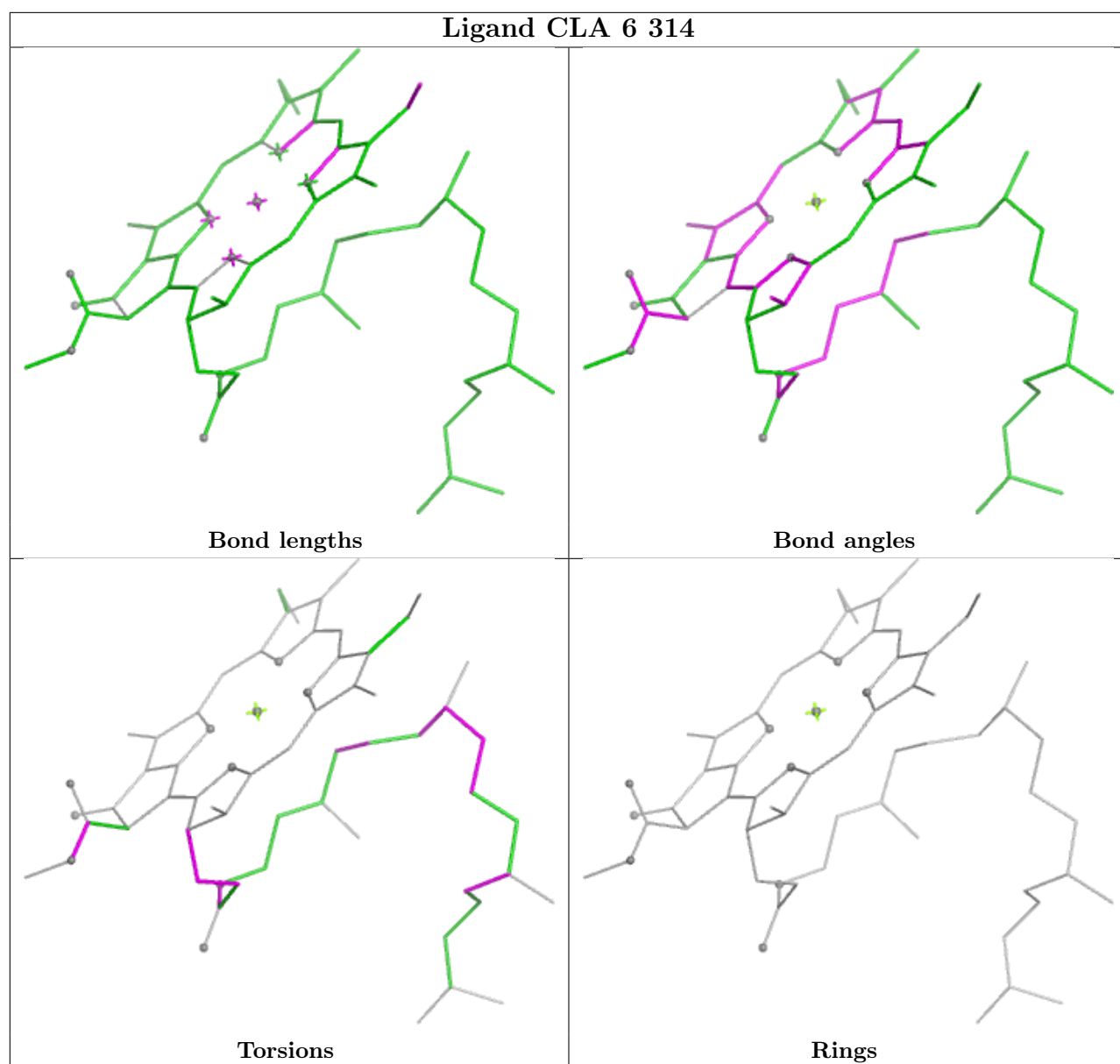


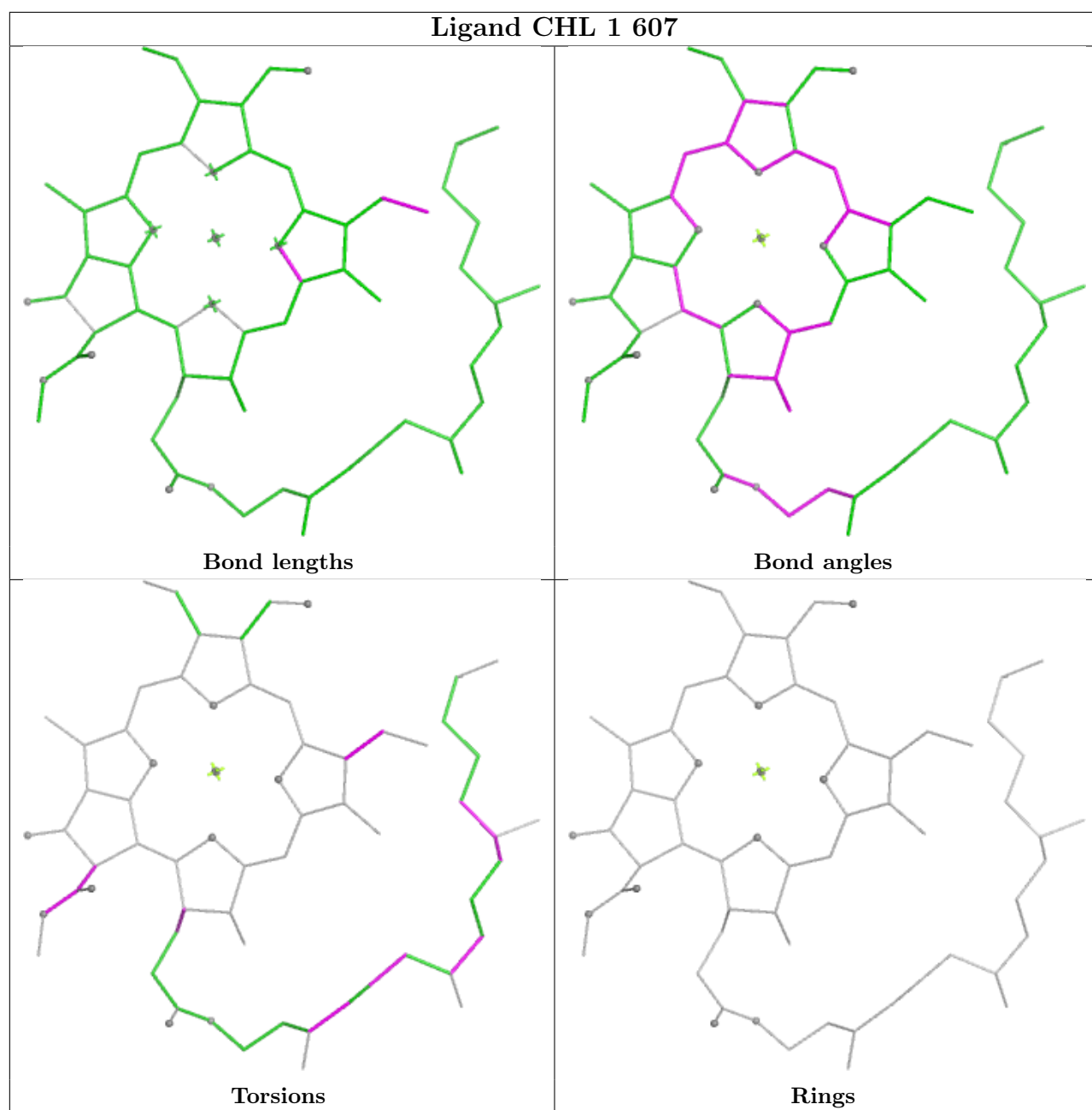
Ligand LUT 8 615



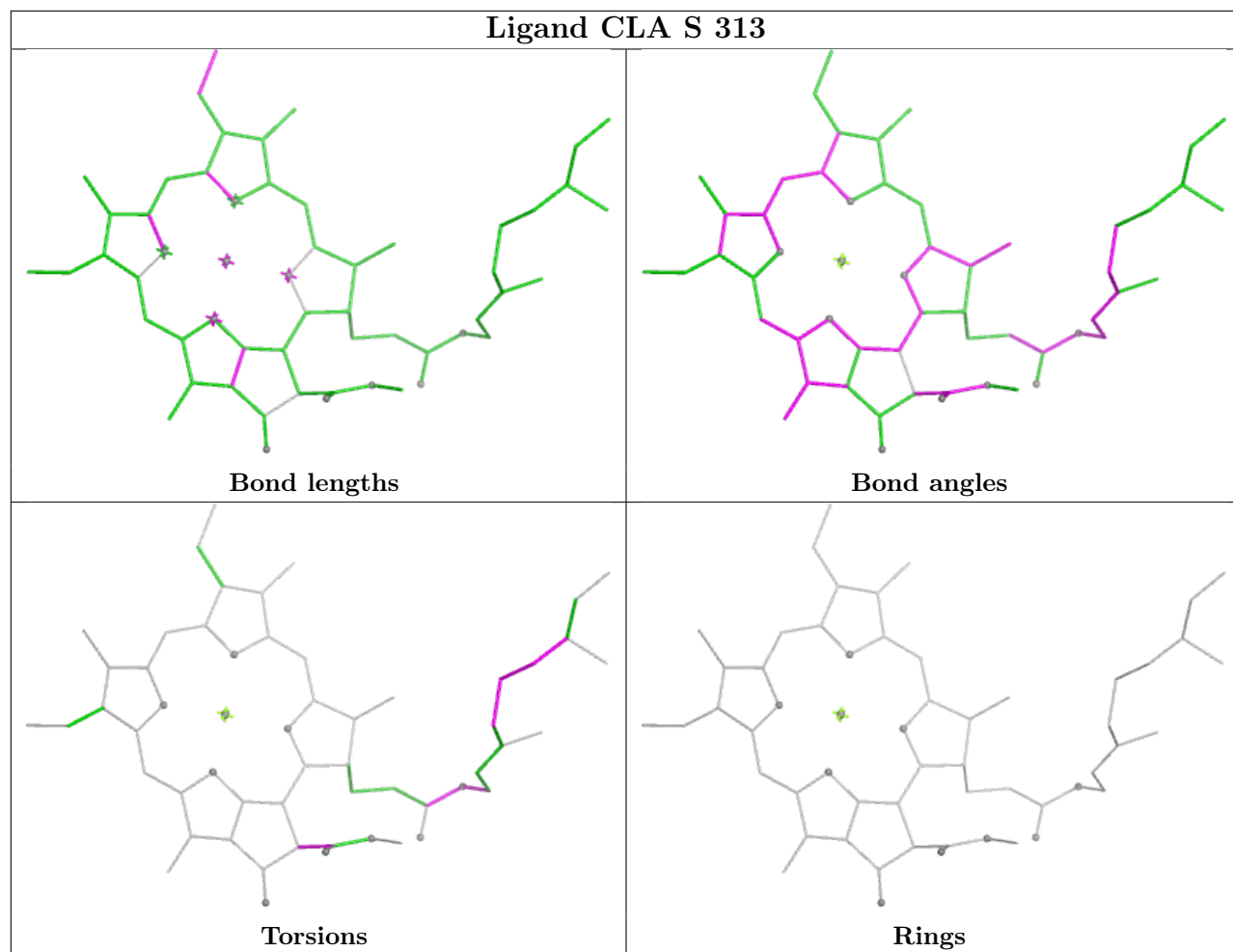
Ligand CLA 3 301

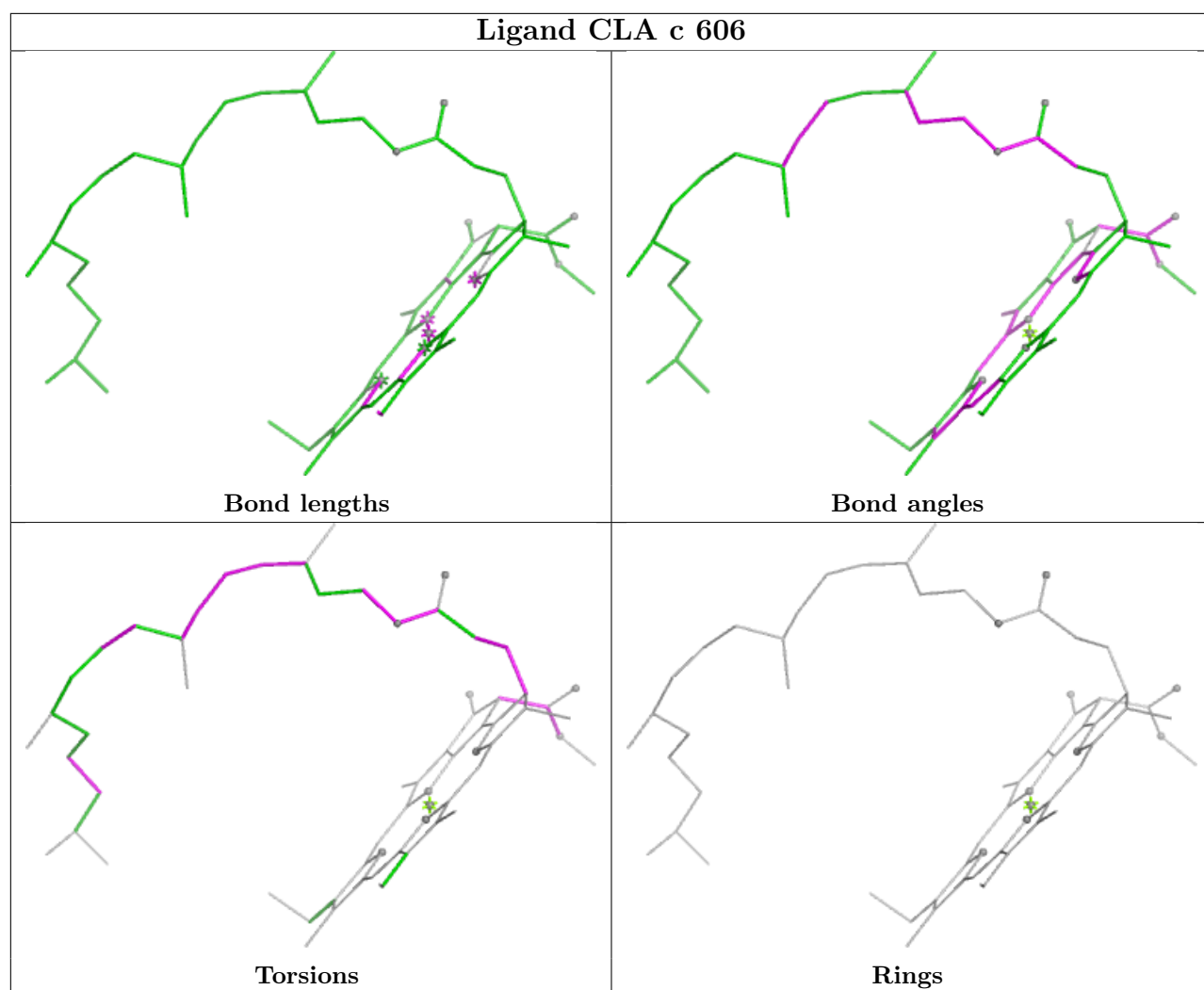


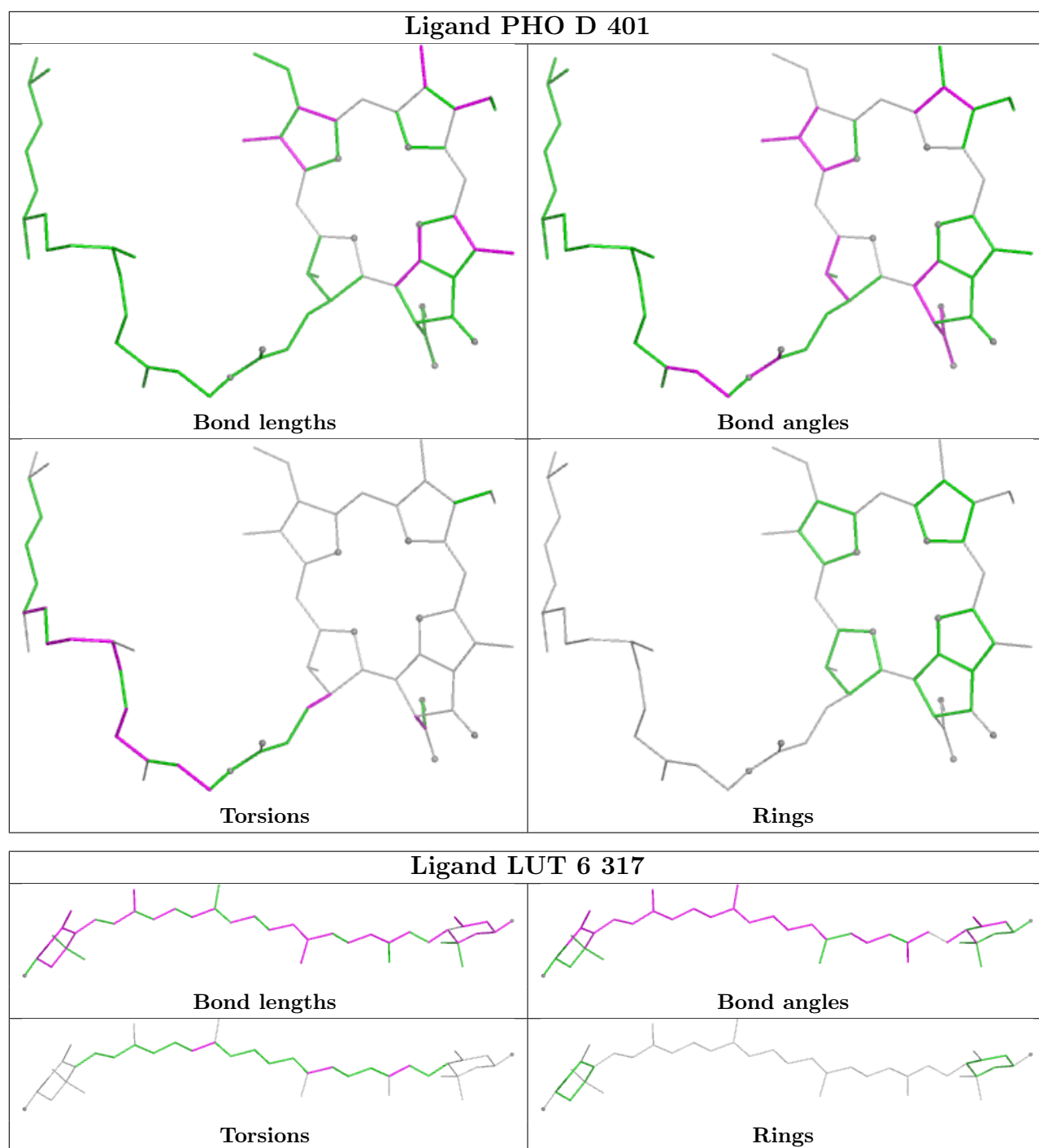




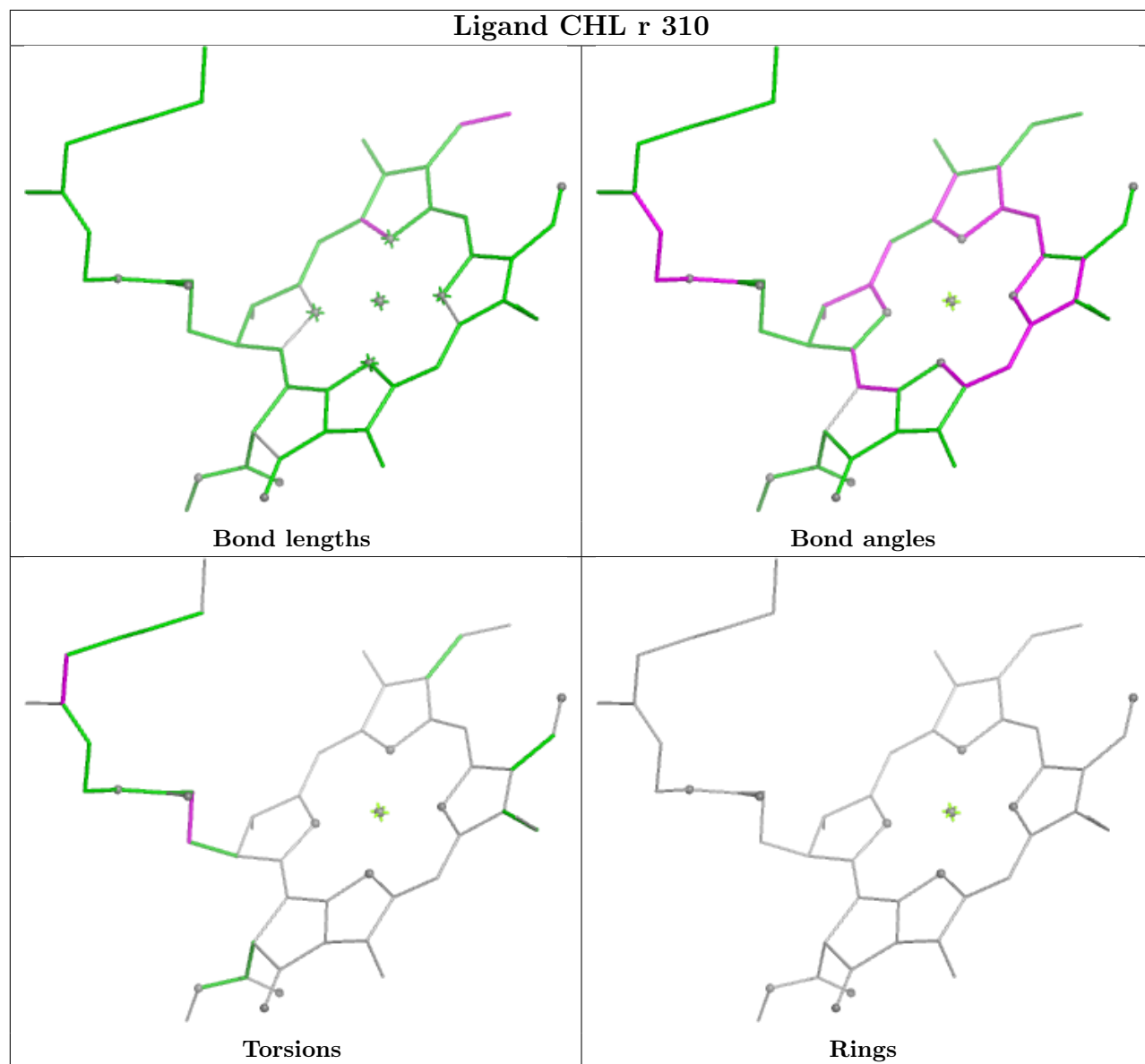
Ligand CLA S 313

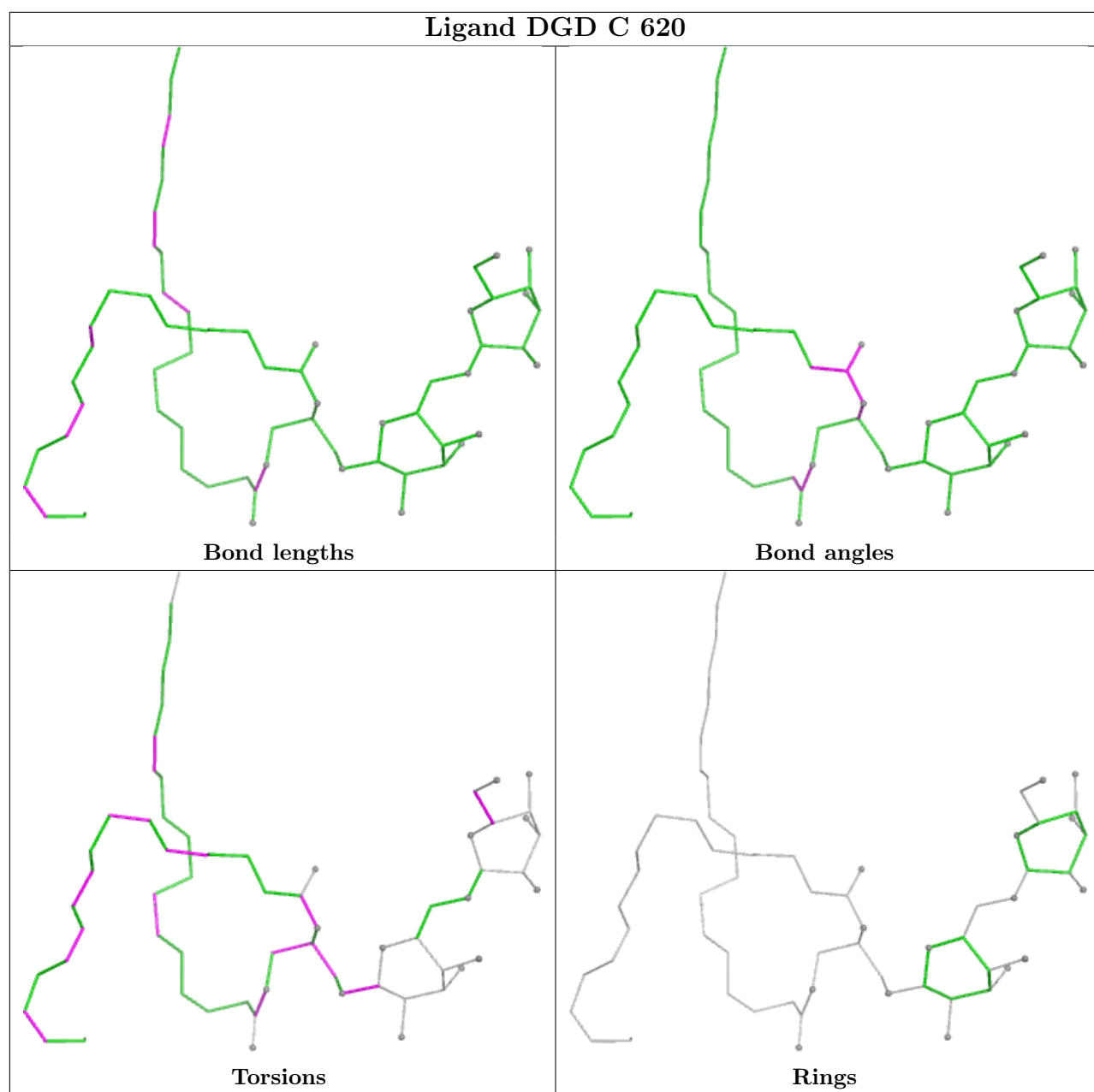




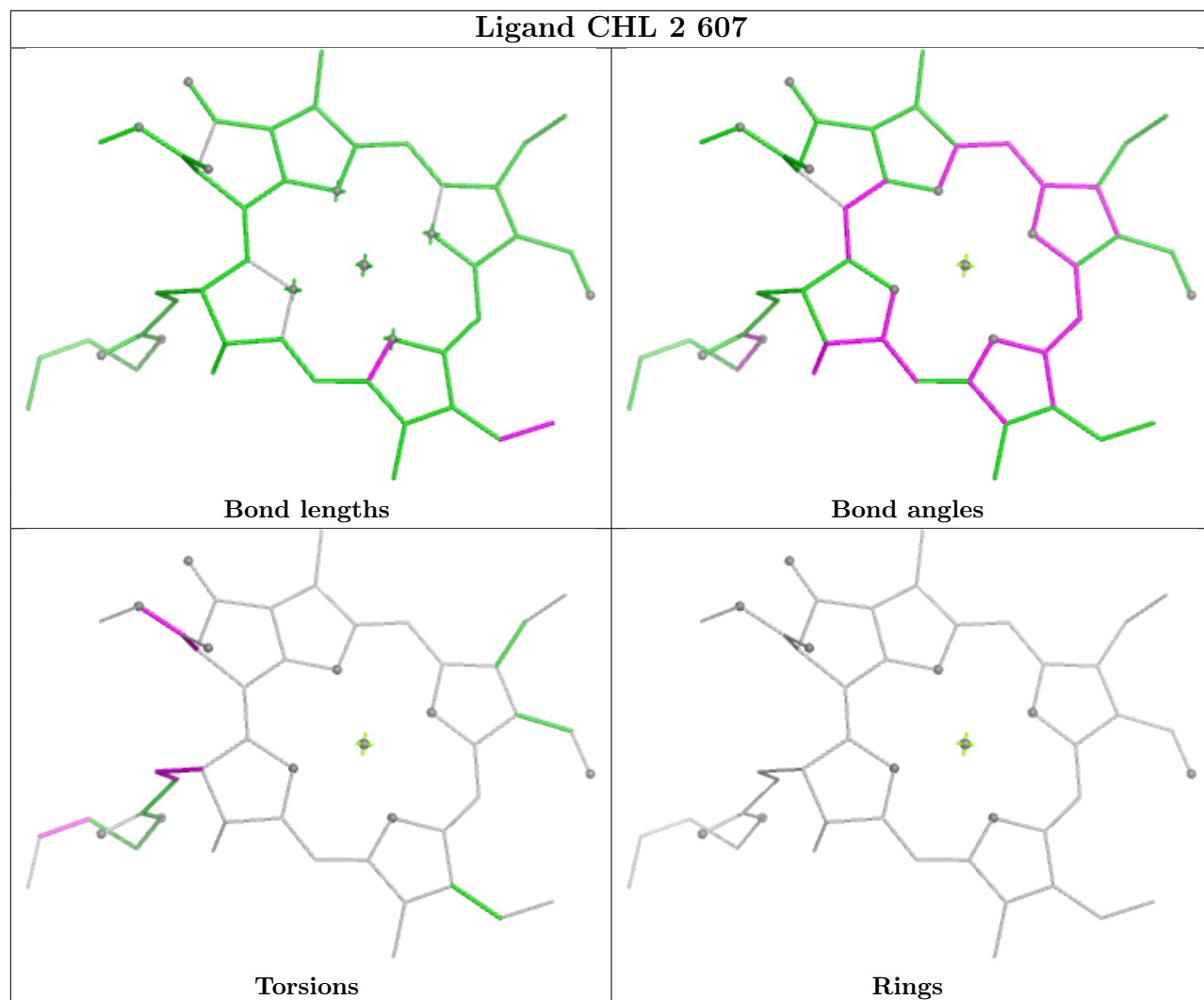


Ligand CHL r 310

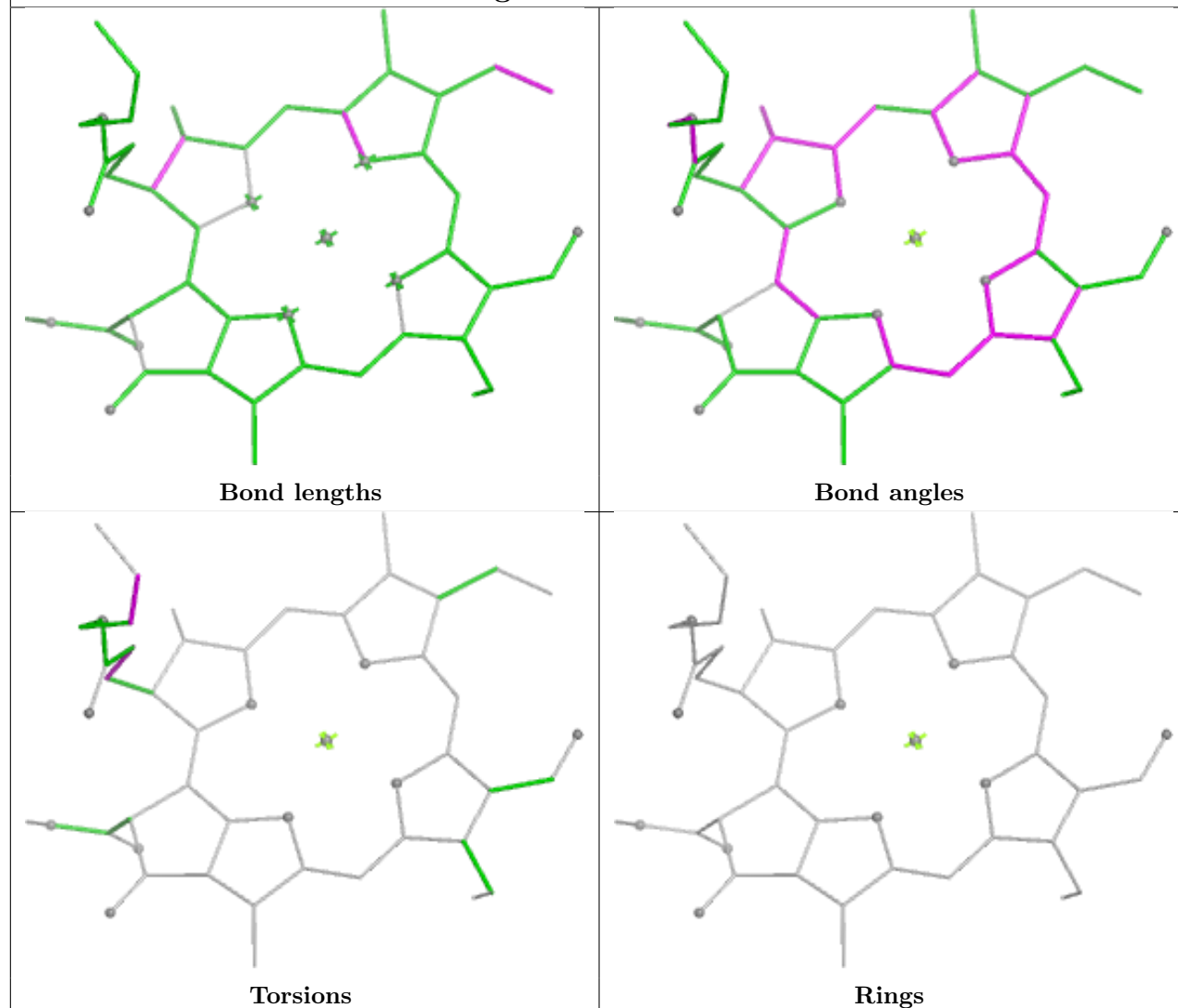




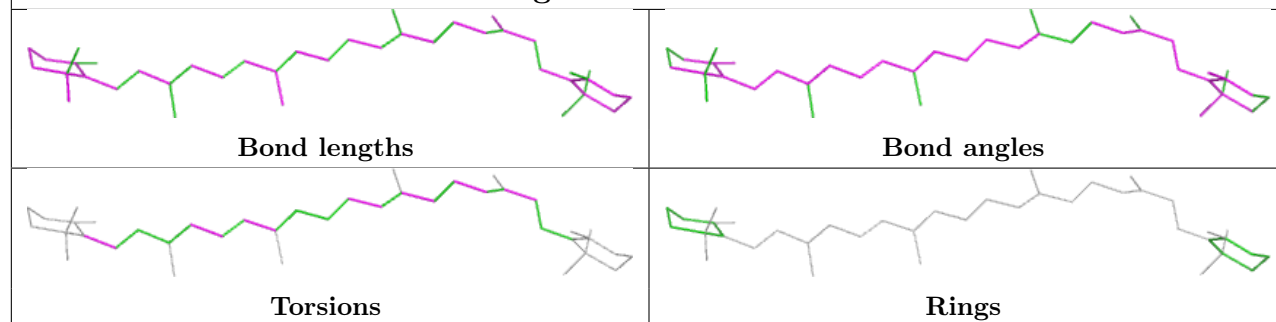
Ligand CHL 2 607



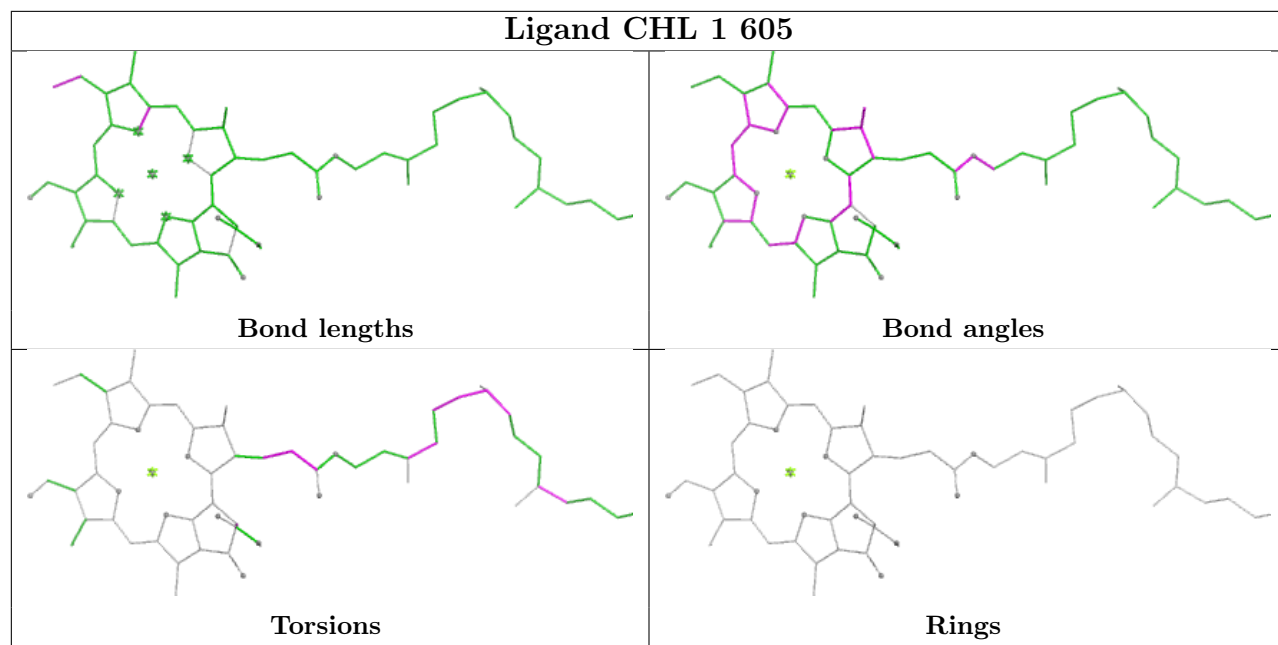
Ligand CHL 6 309



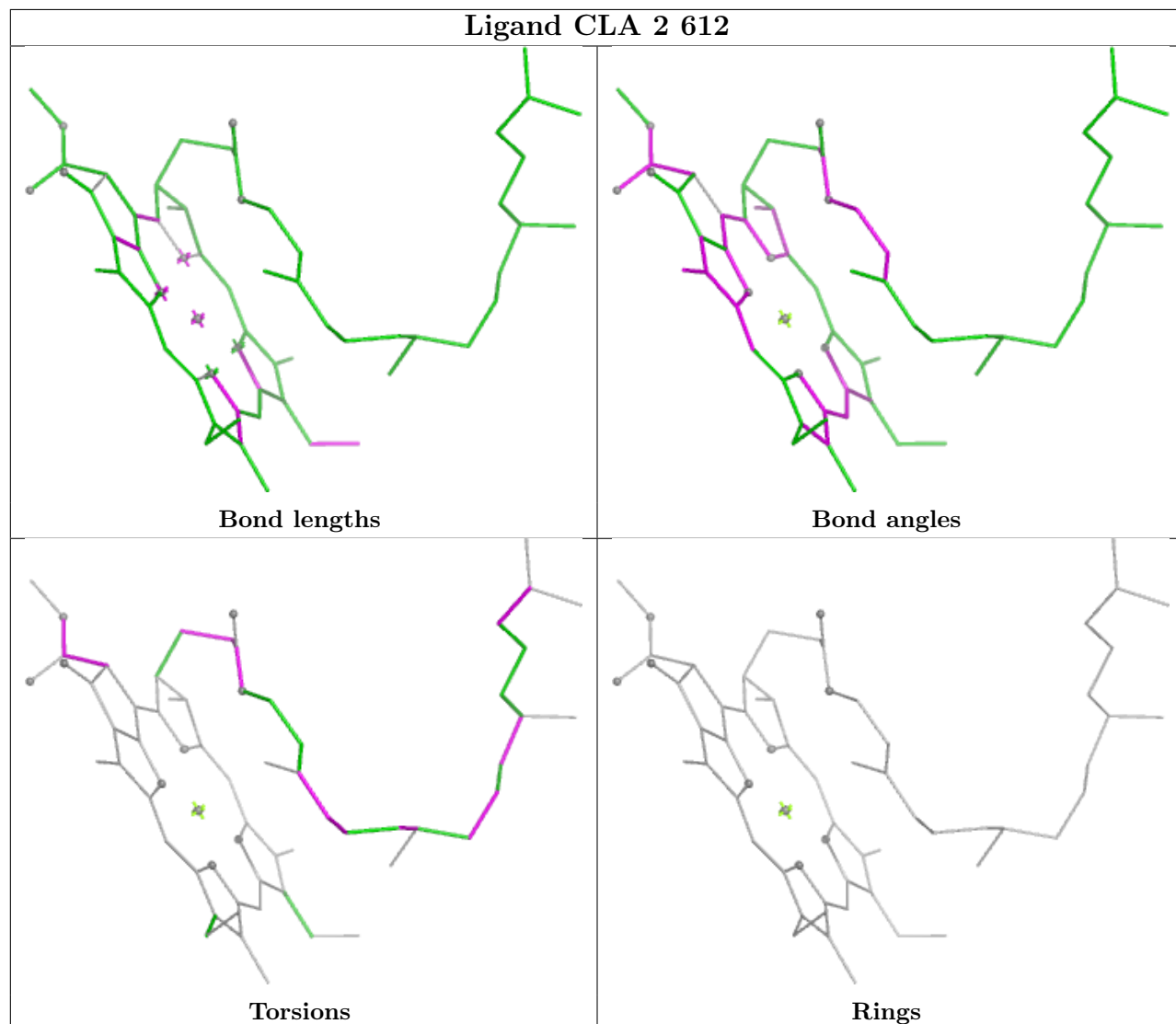
Ligand BCR h 101

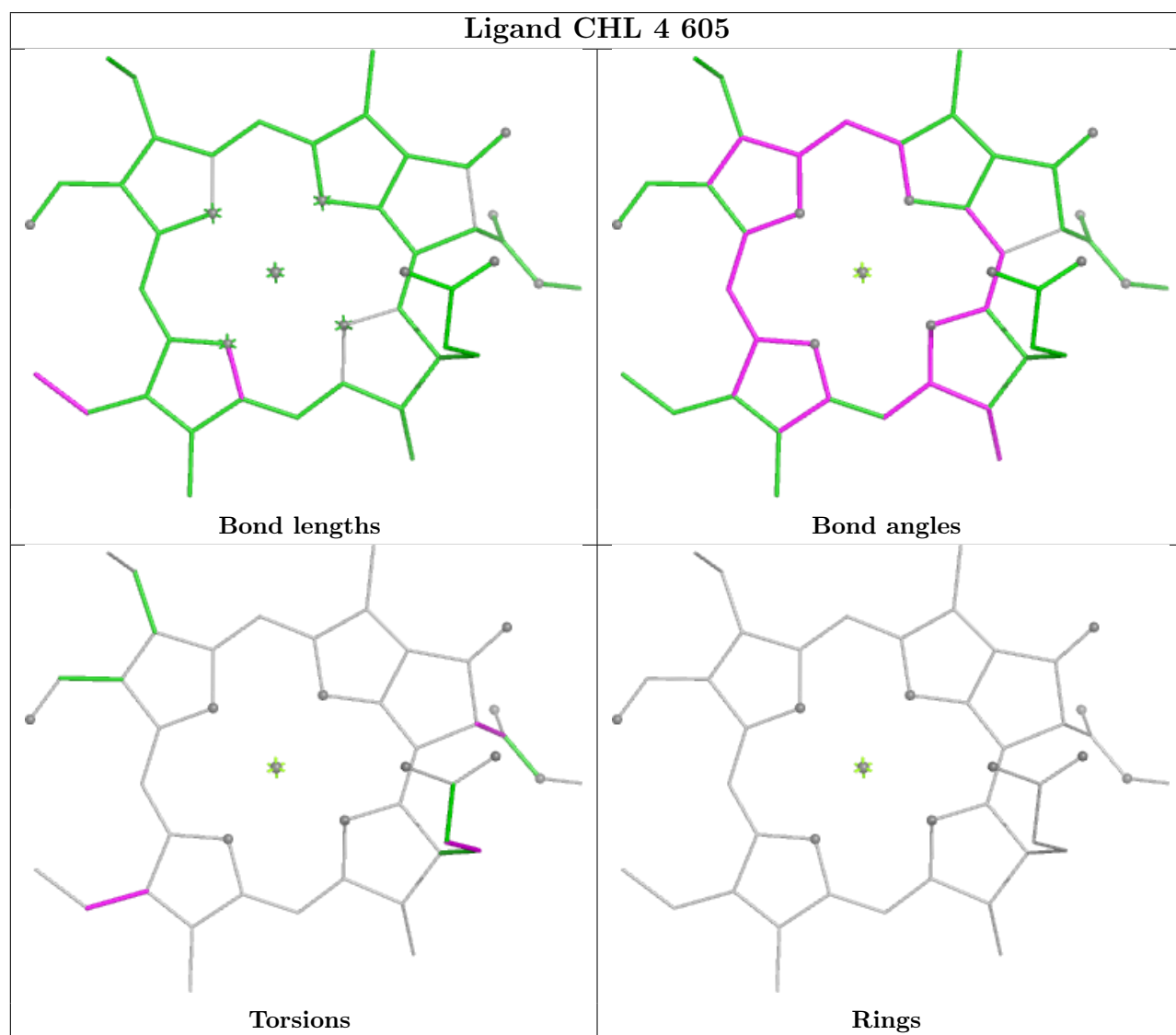
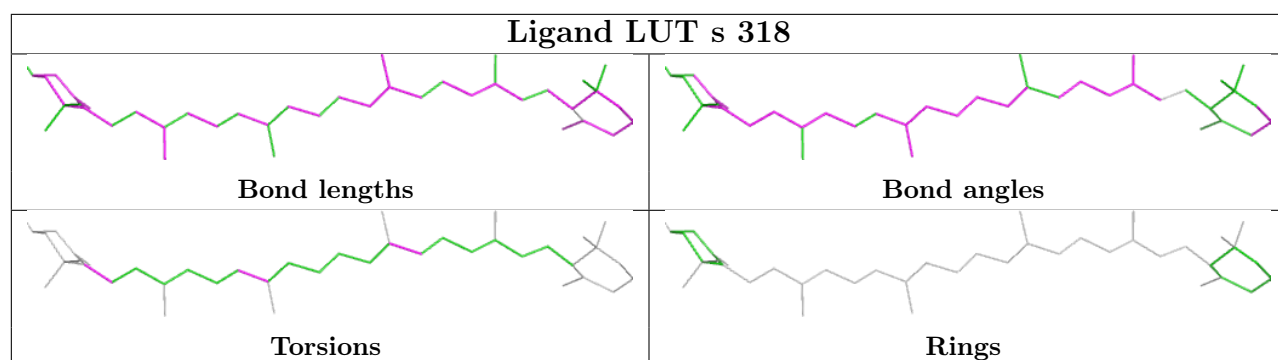


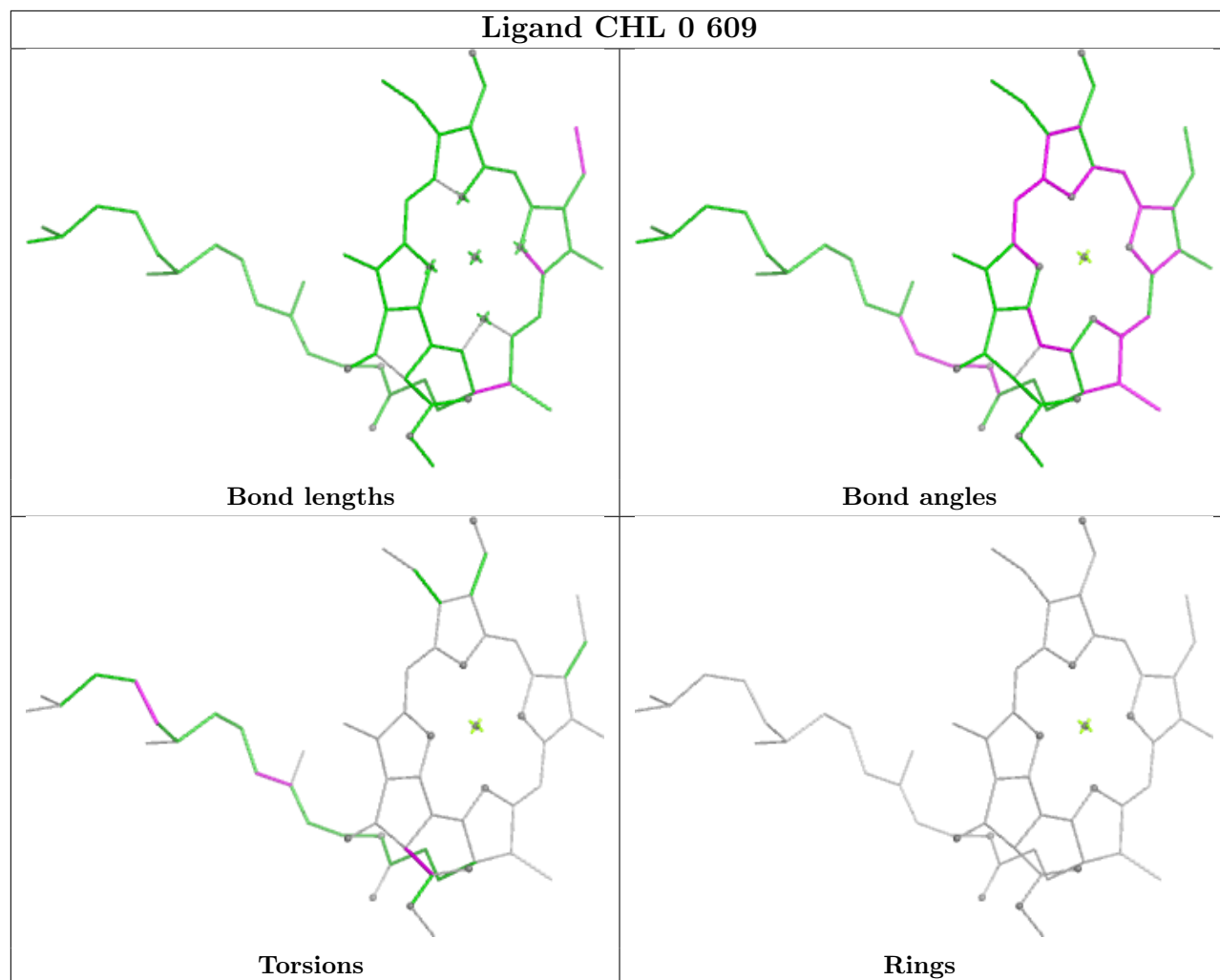
Ligand CHL 1 605

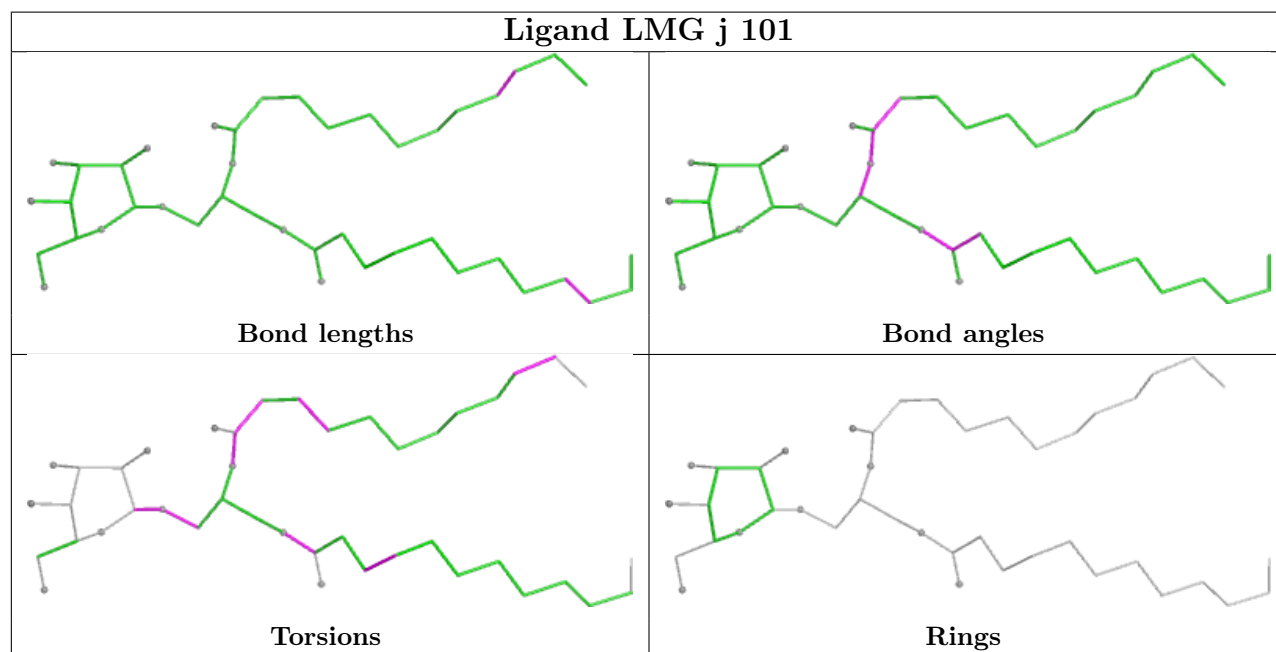
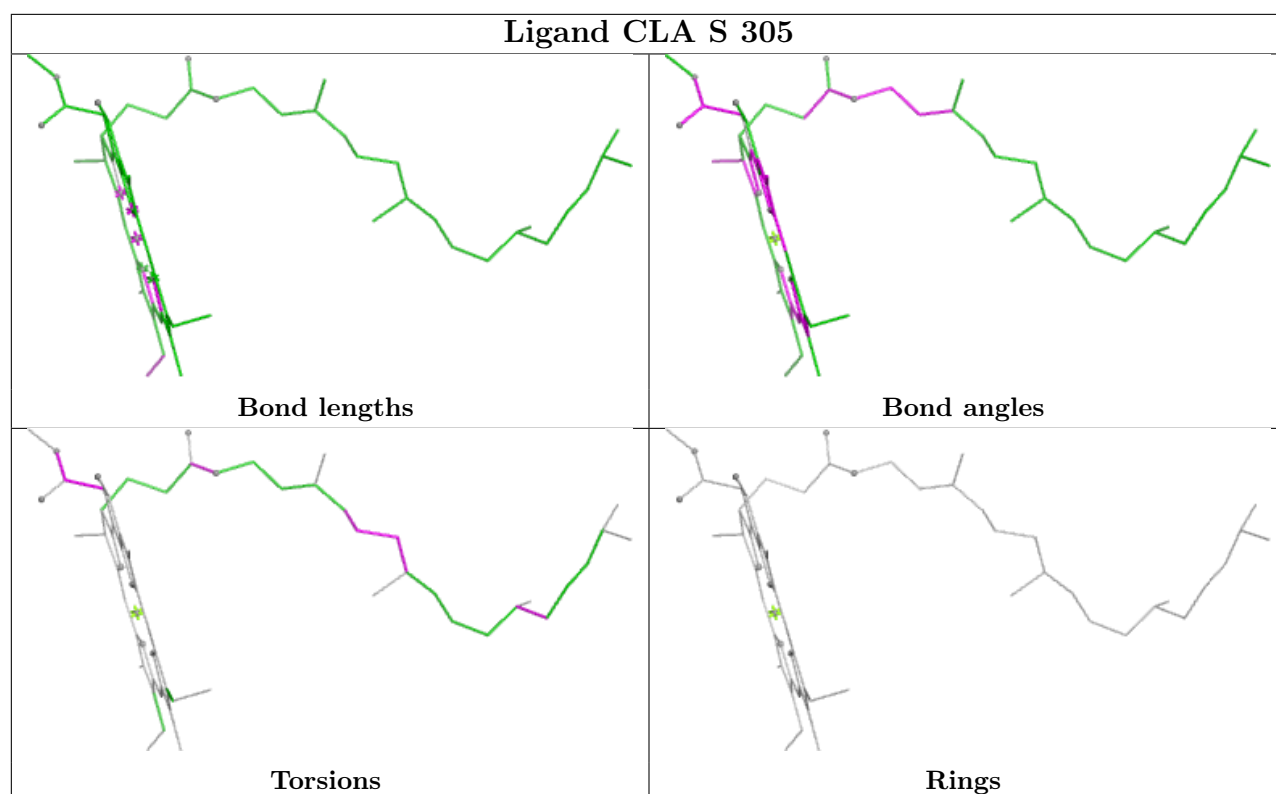


Ligand CLA 2 612

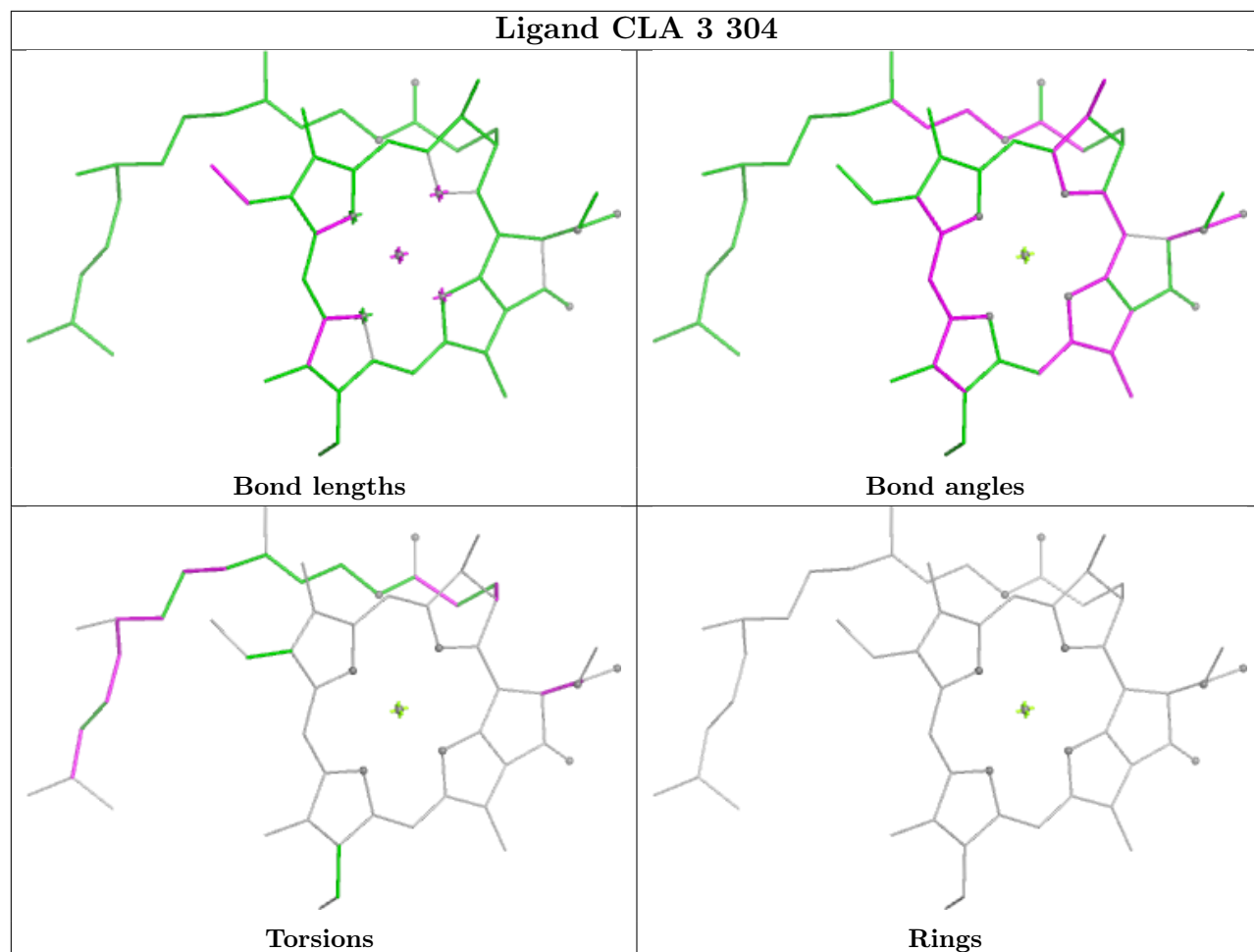


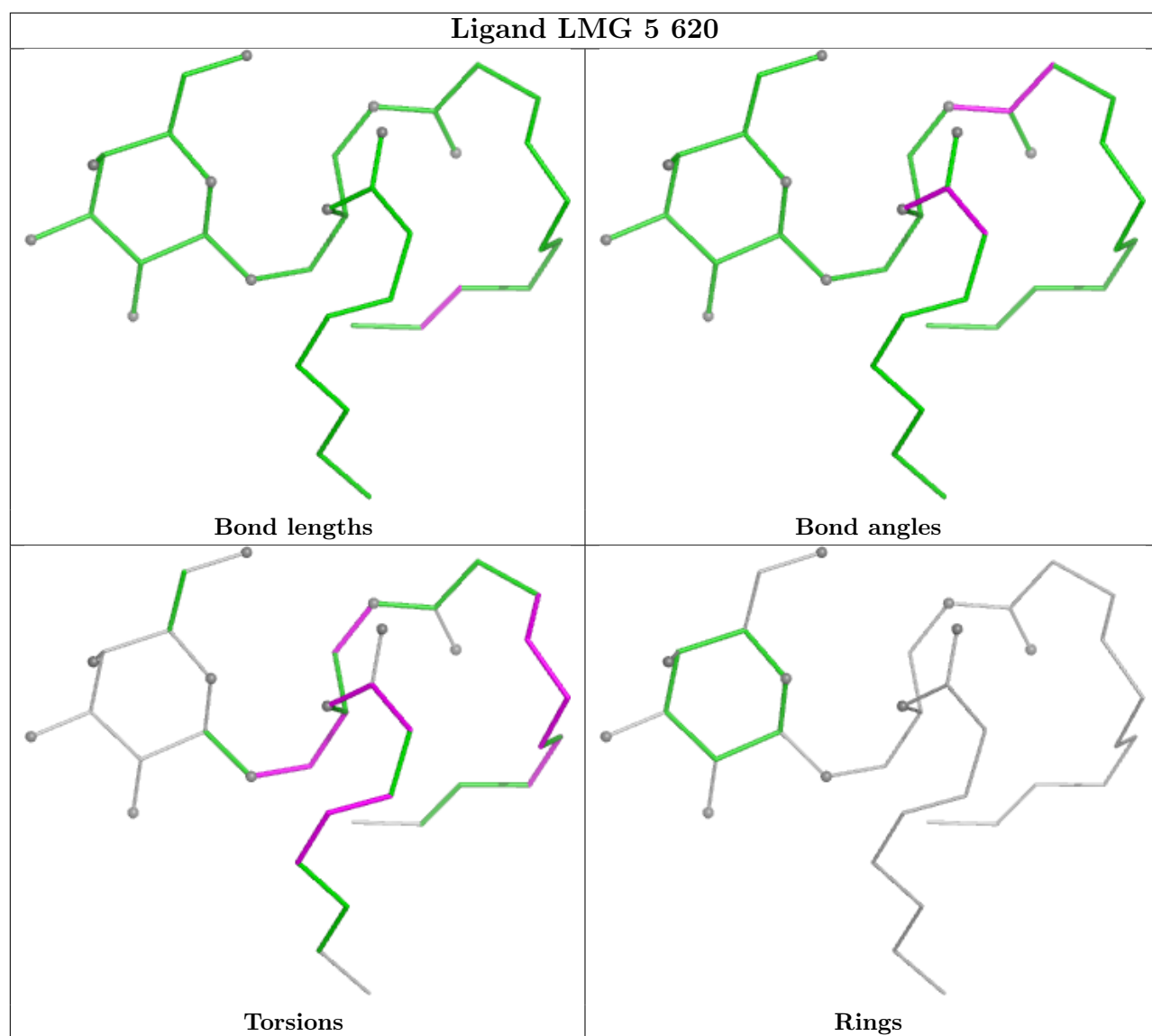


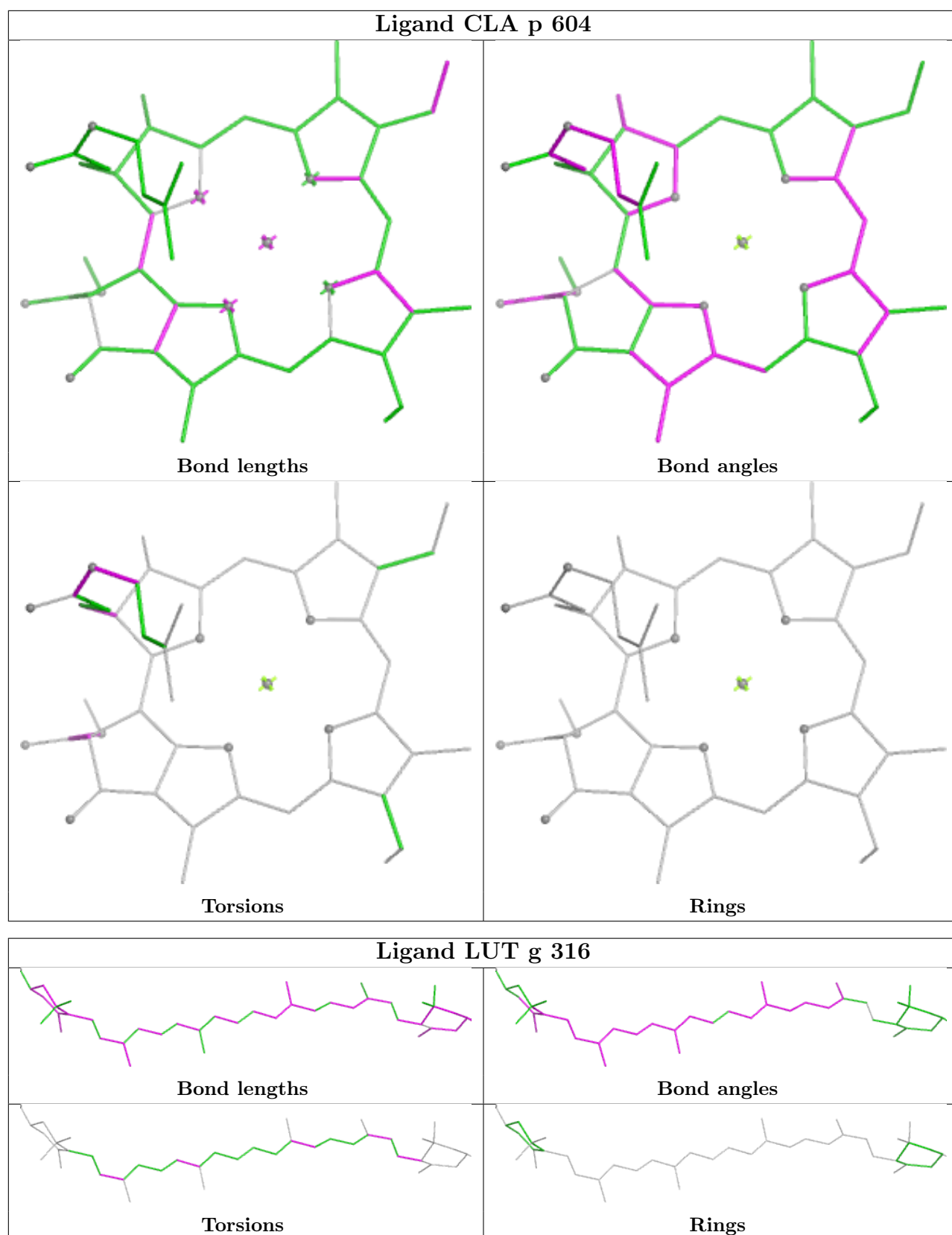


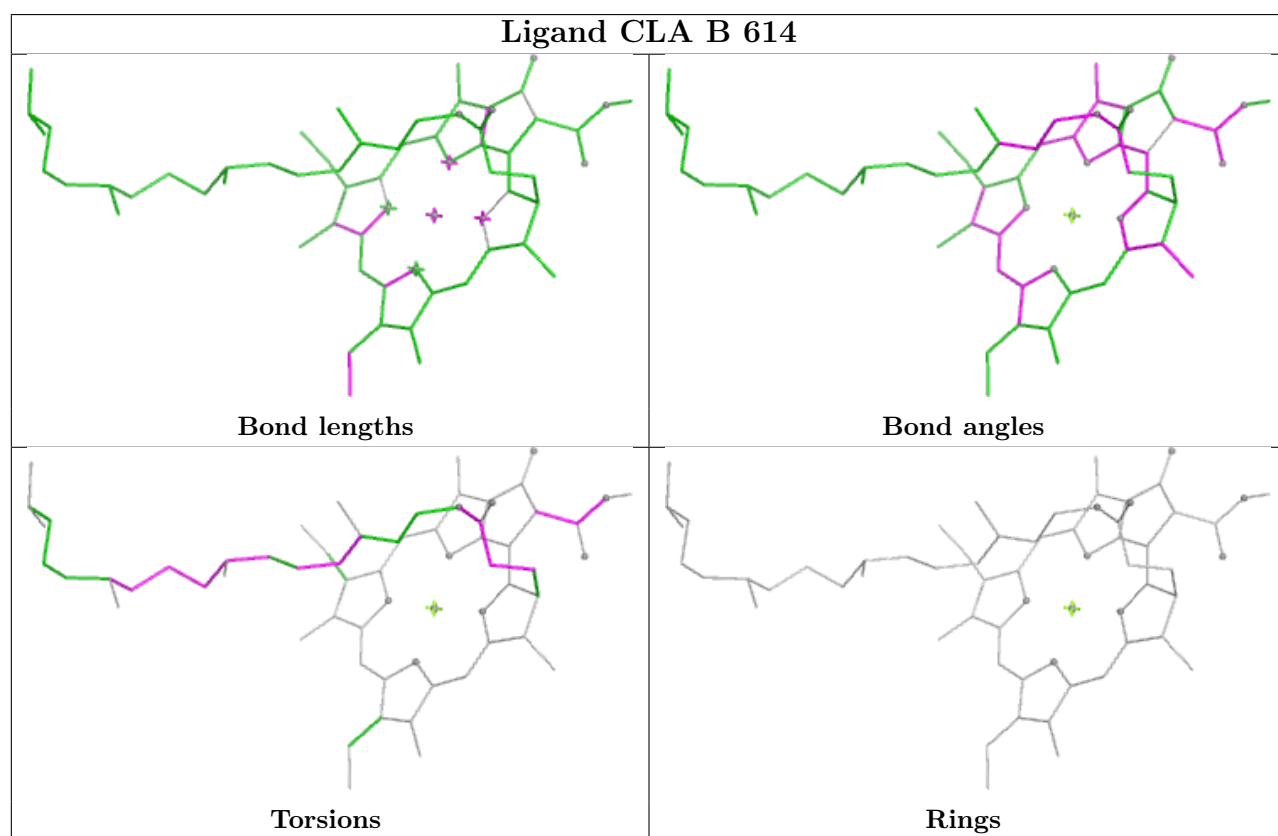
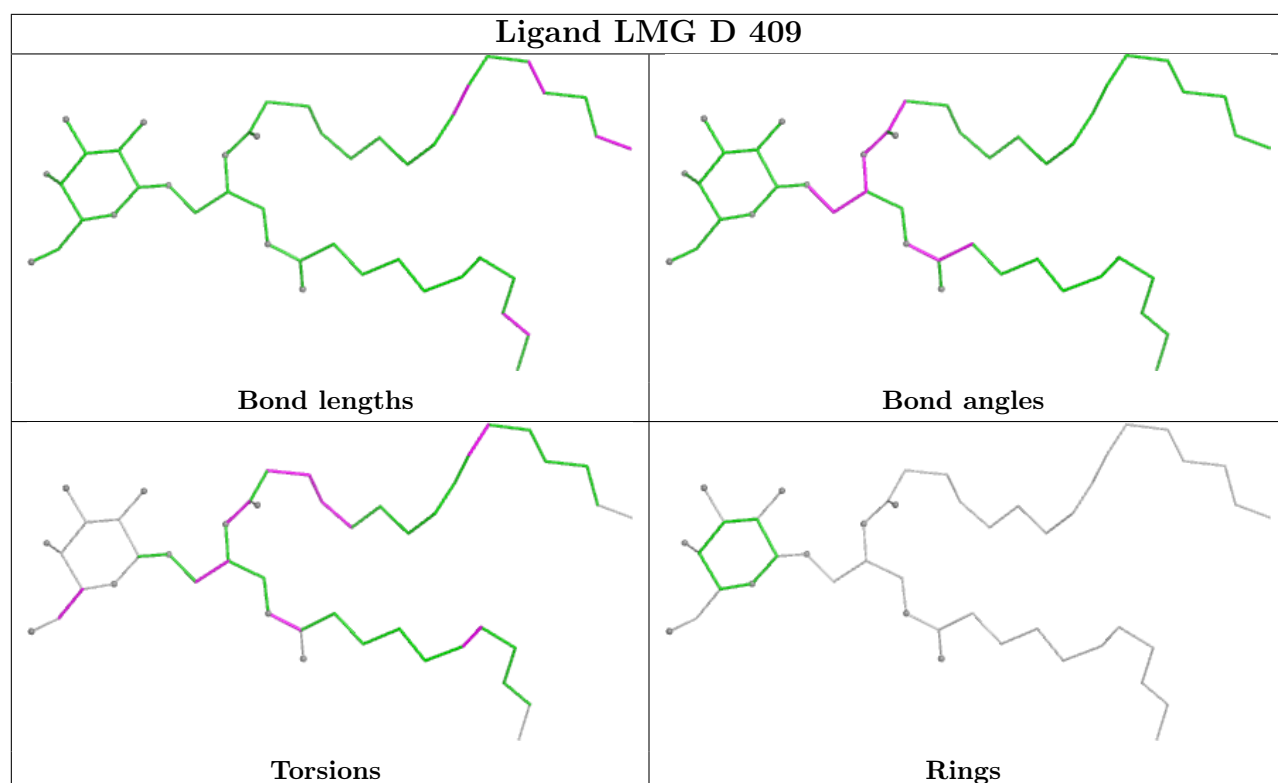


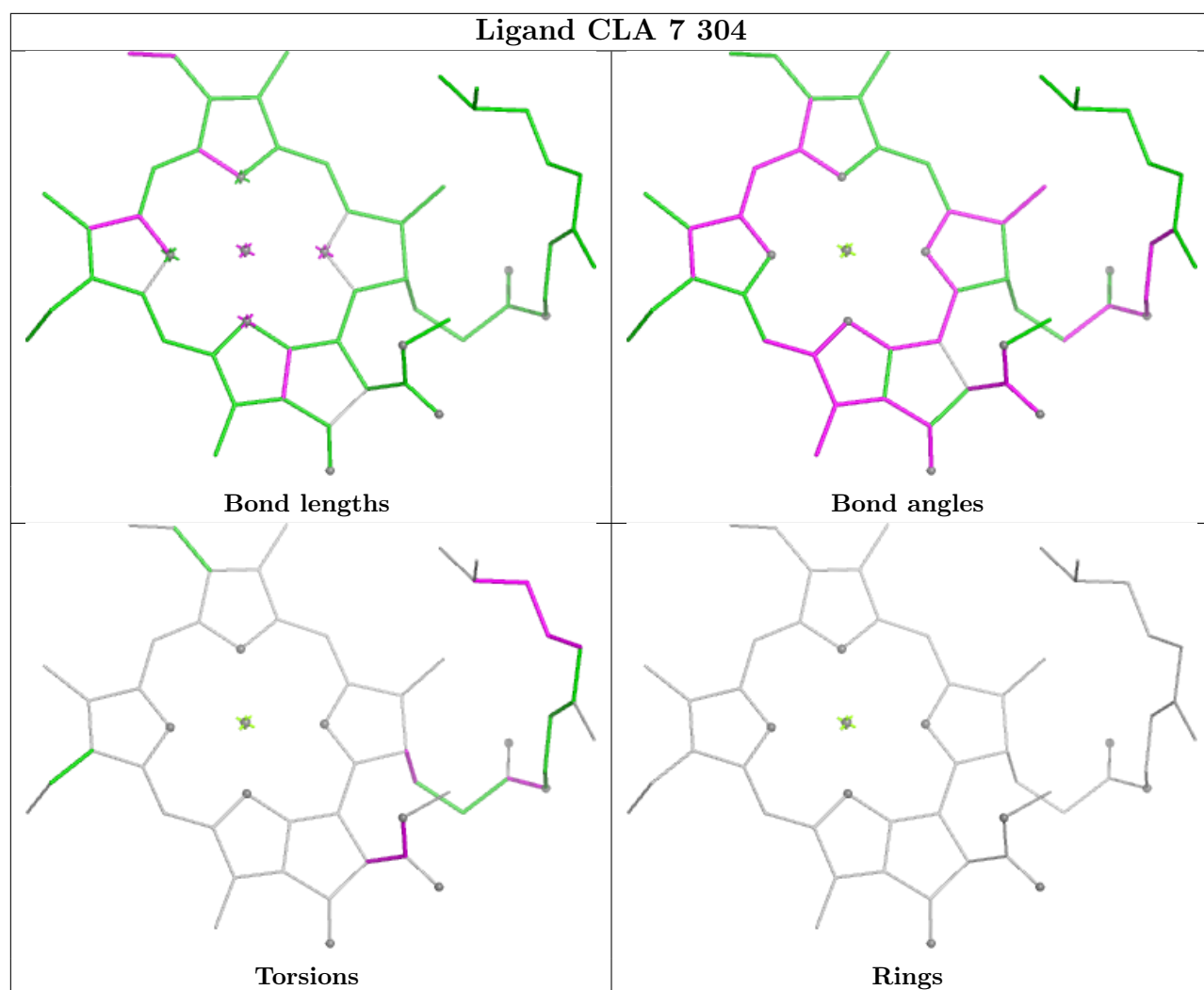
Ligand CLA 3 304



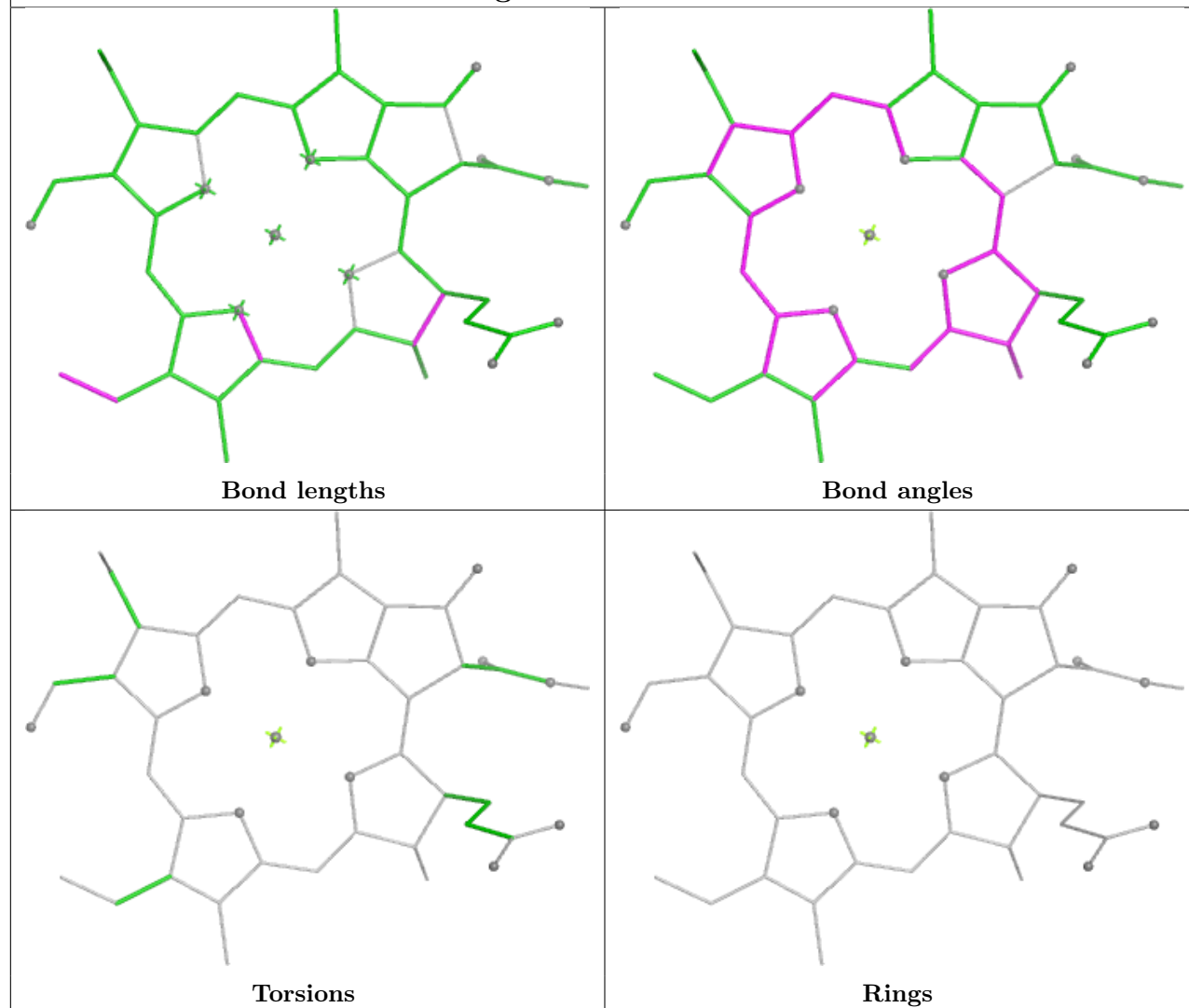




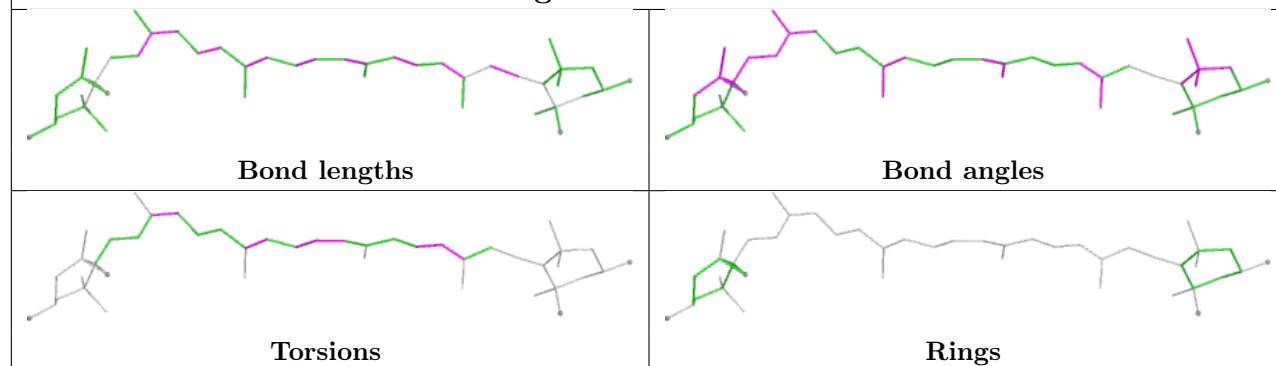


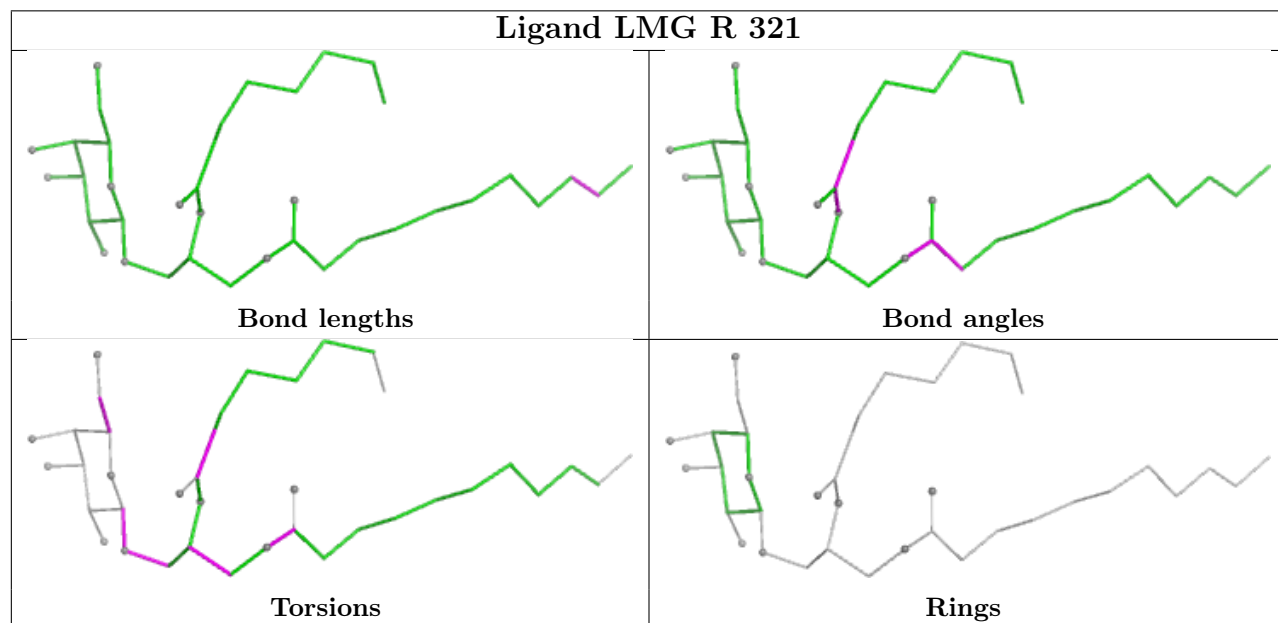
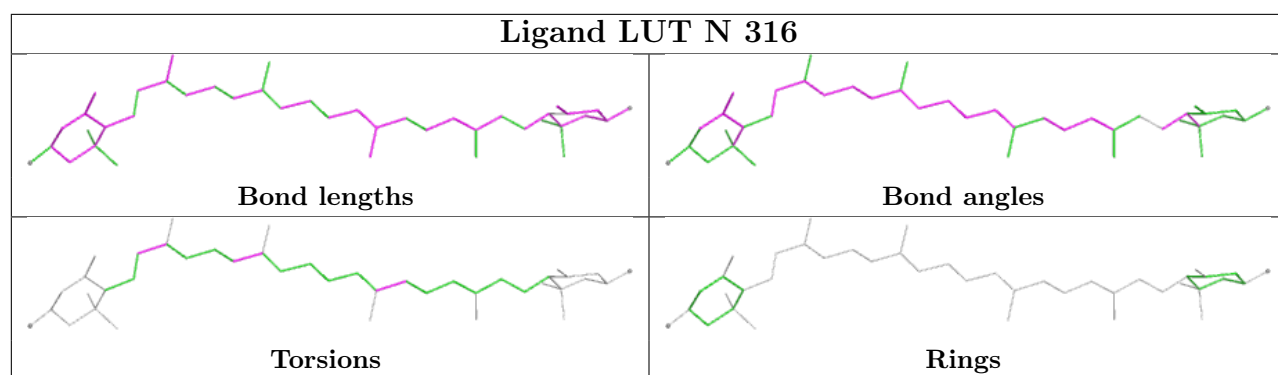


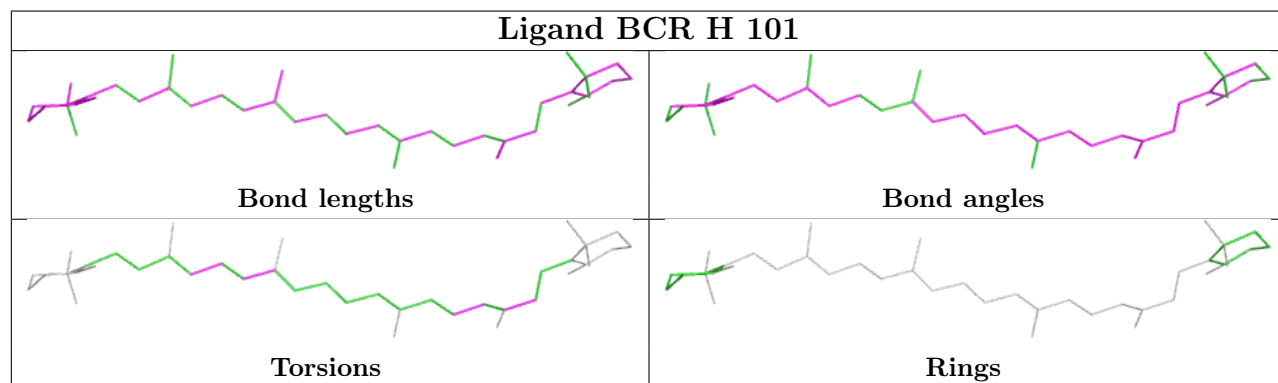
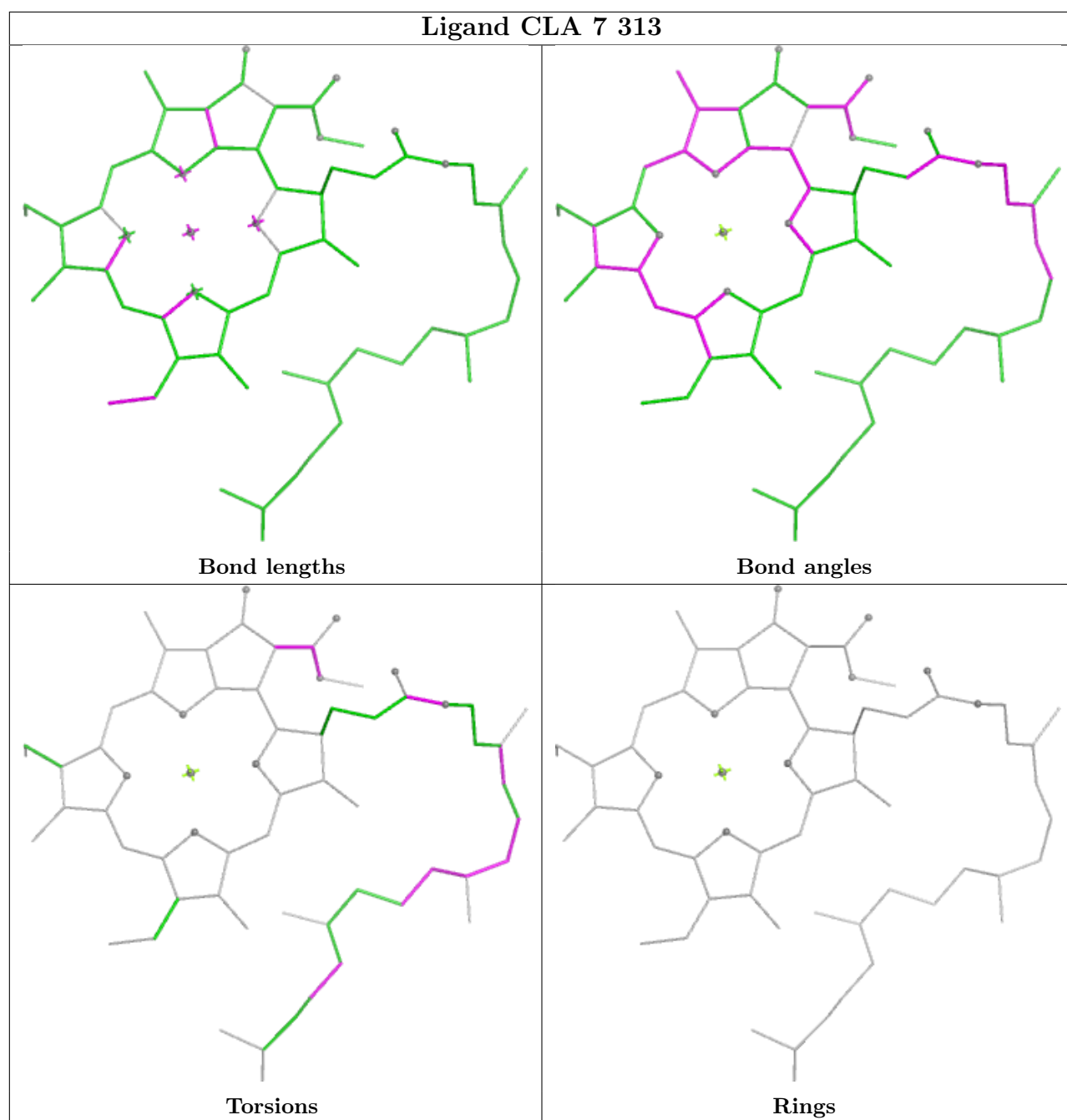
Ligand CHL Y 306



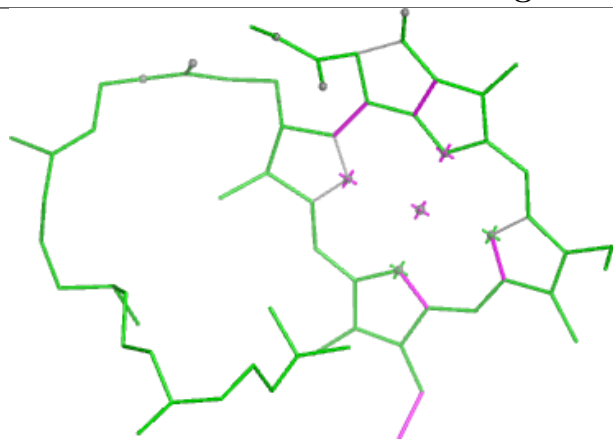
Ligand NEX 3 319



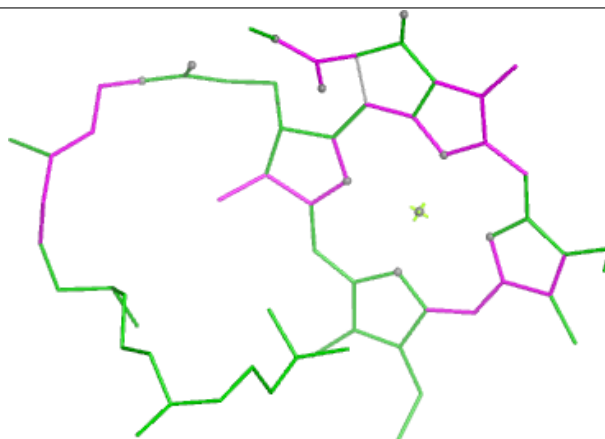




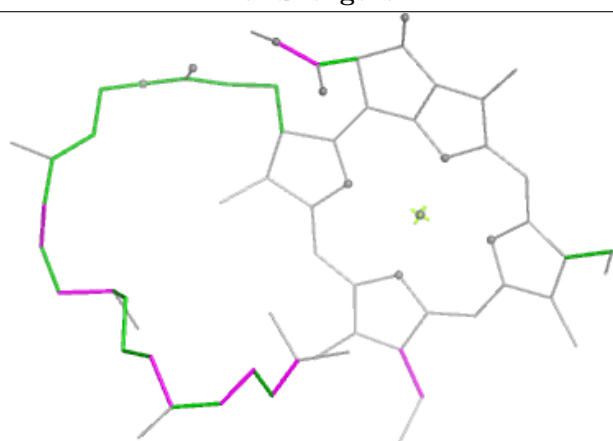
Ligand CLA B 615



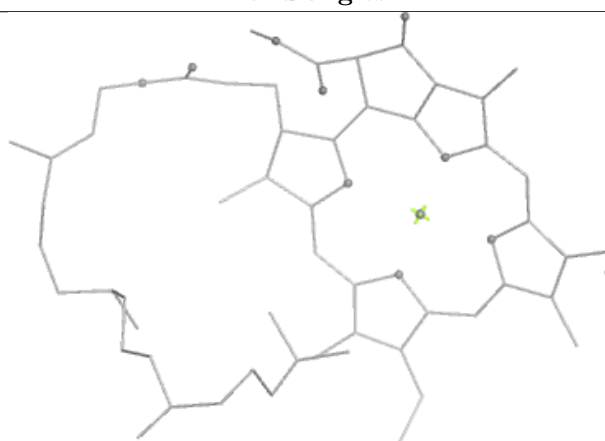
Bond lengths



Bond angles

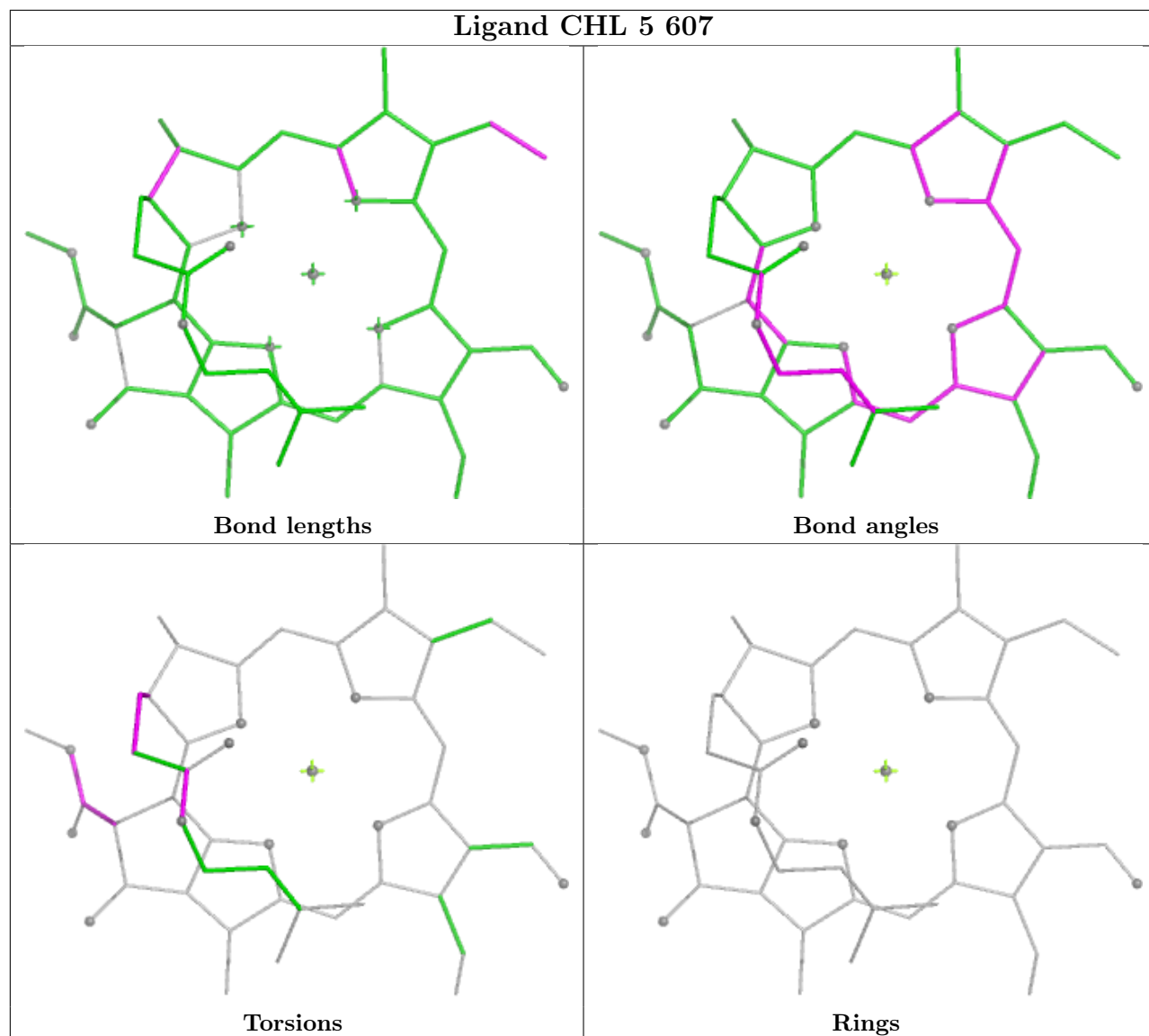


Torsions

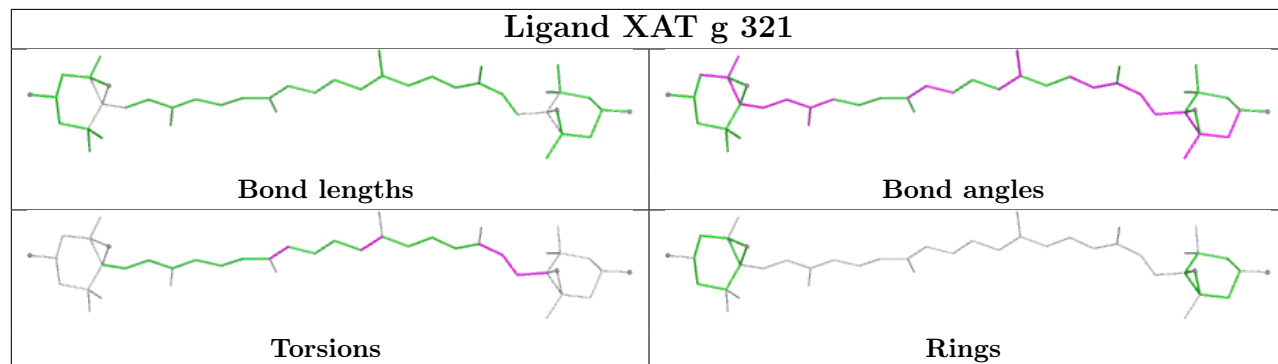


Rings

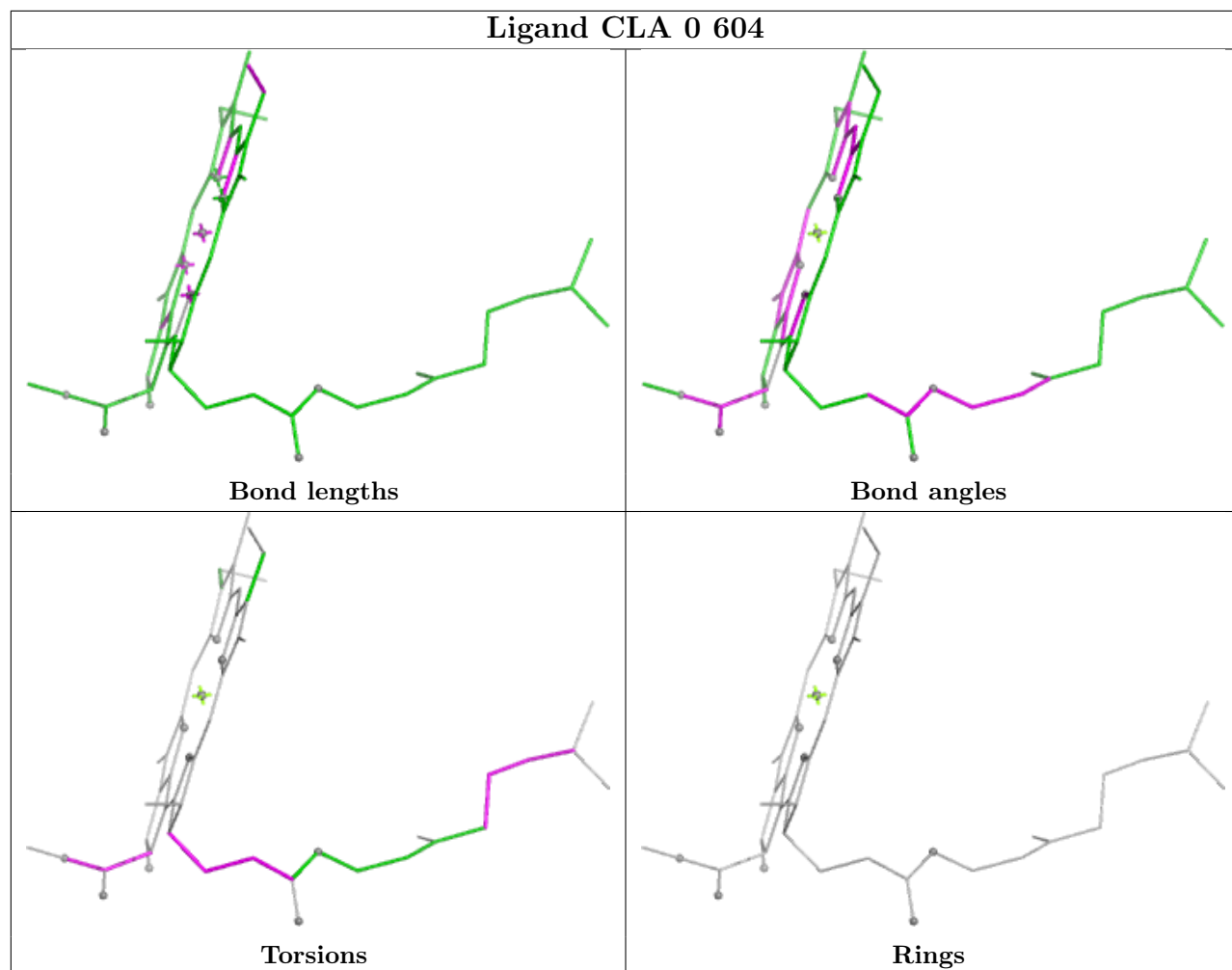
Ligand CHL 5 607



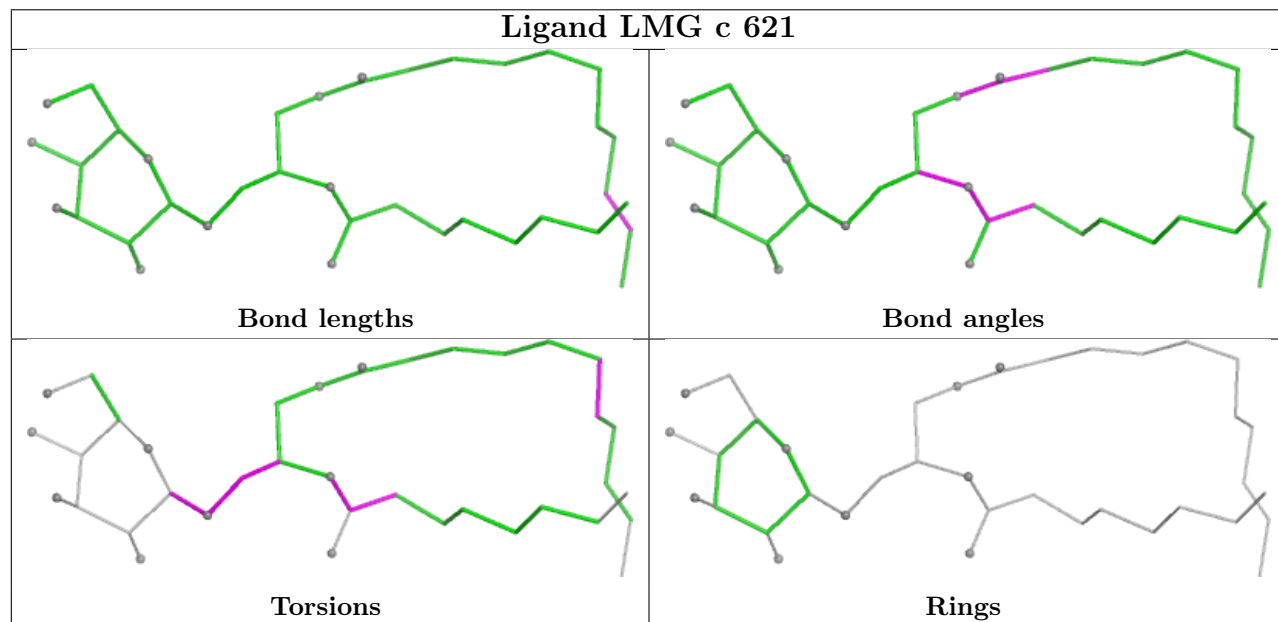
Ligand XAT g 321

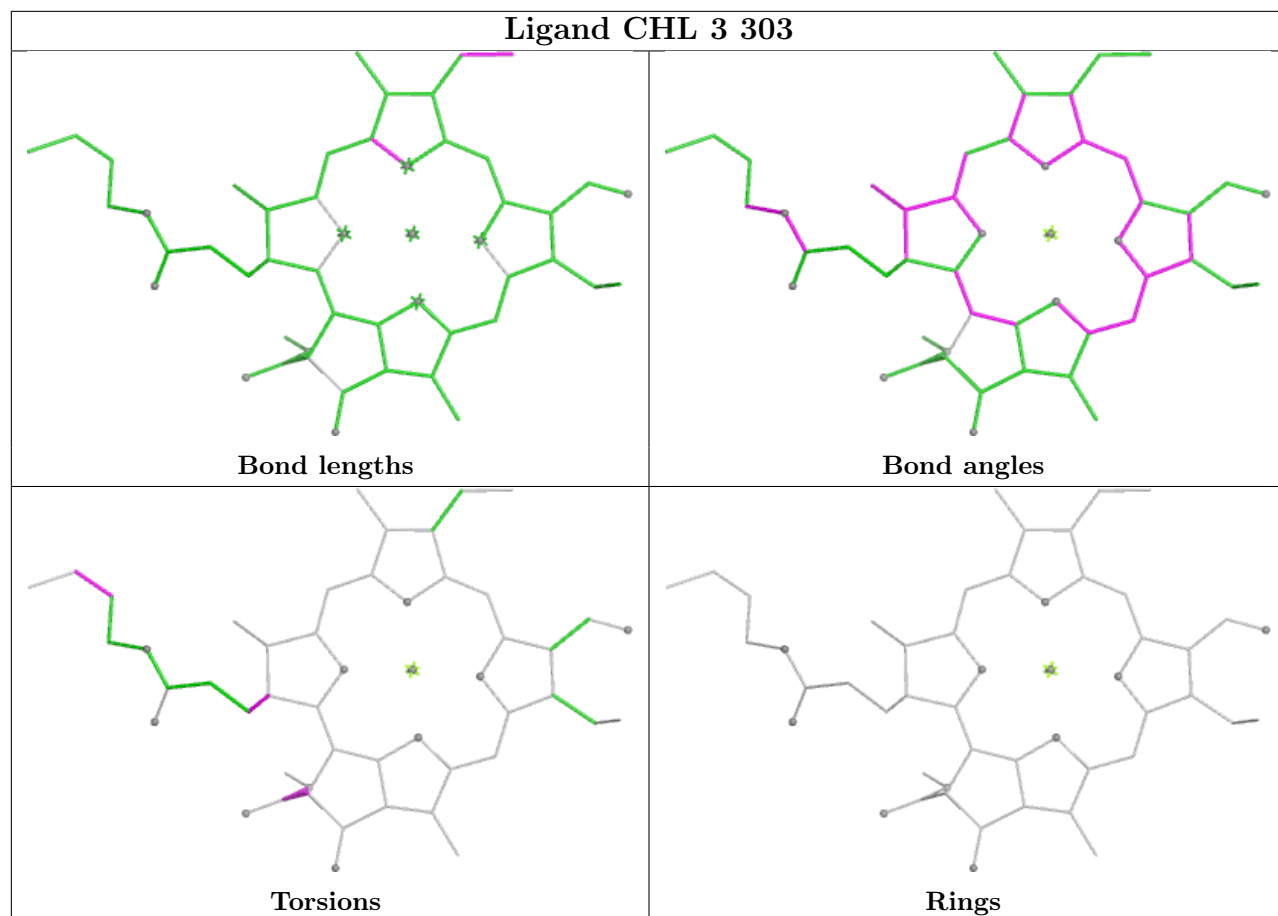
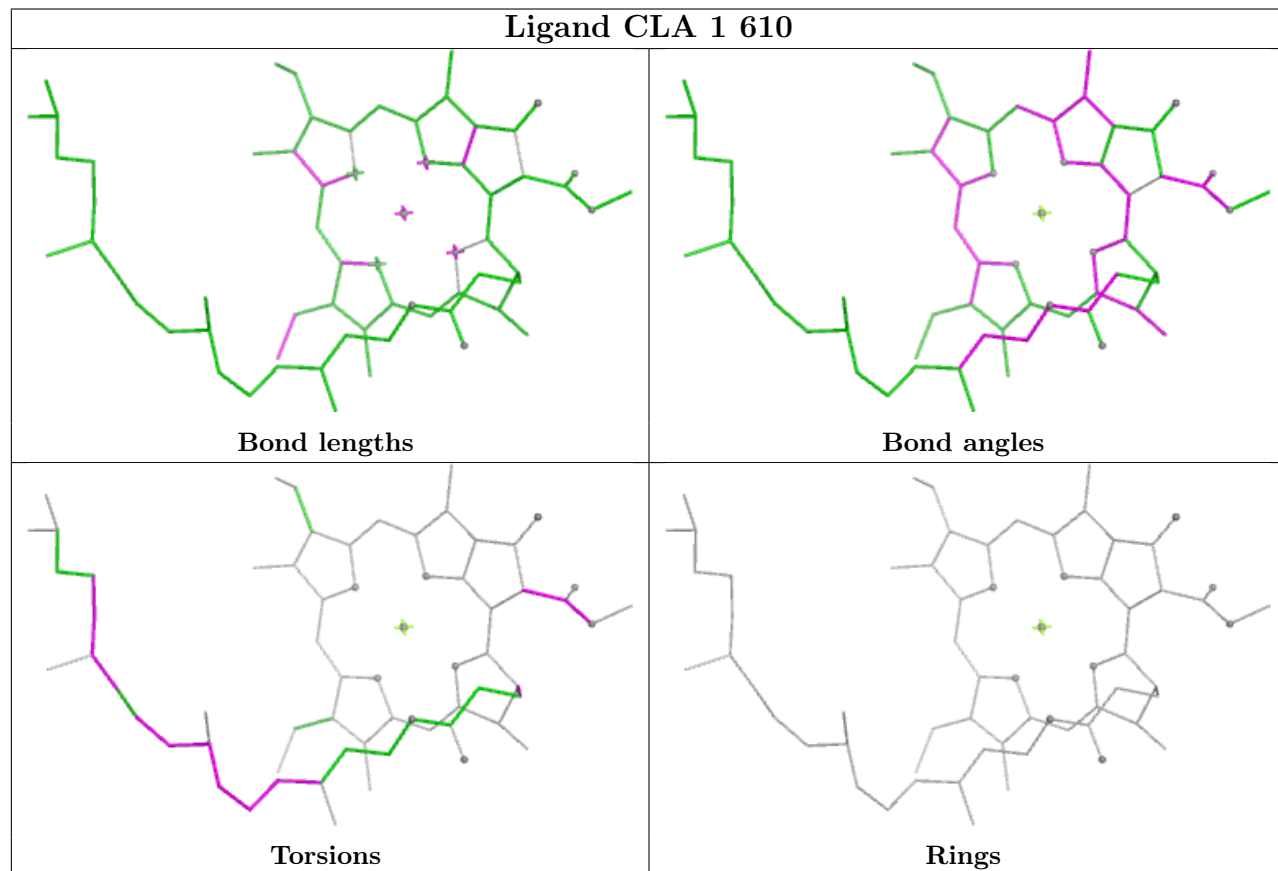


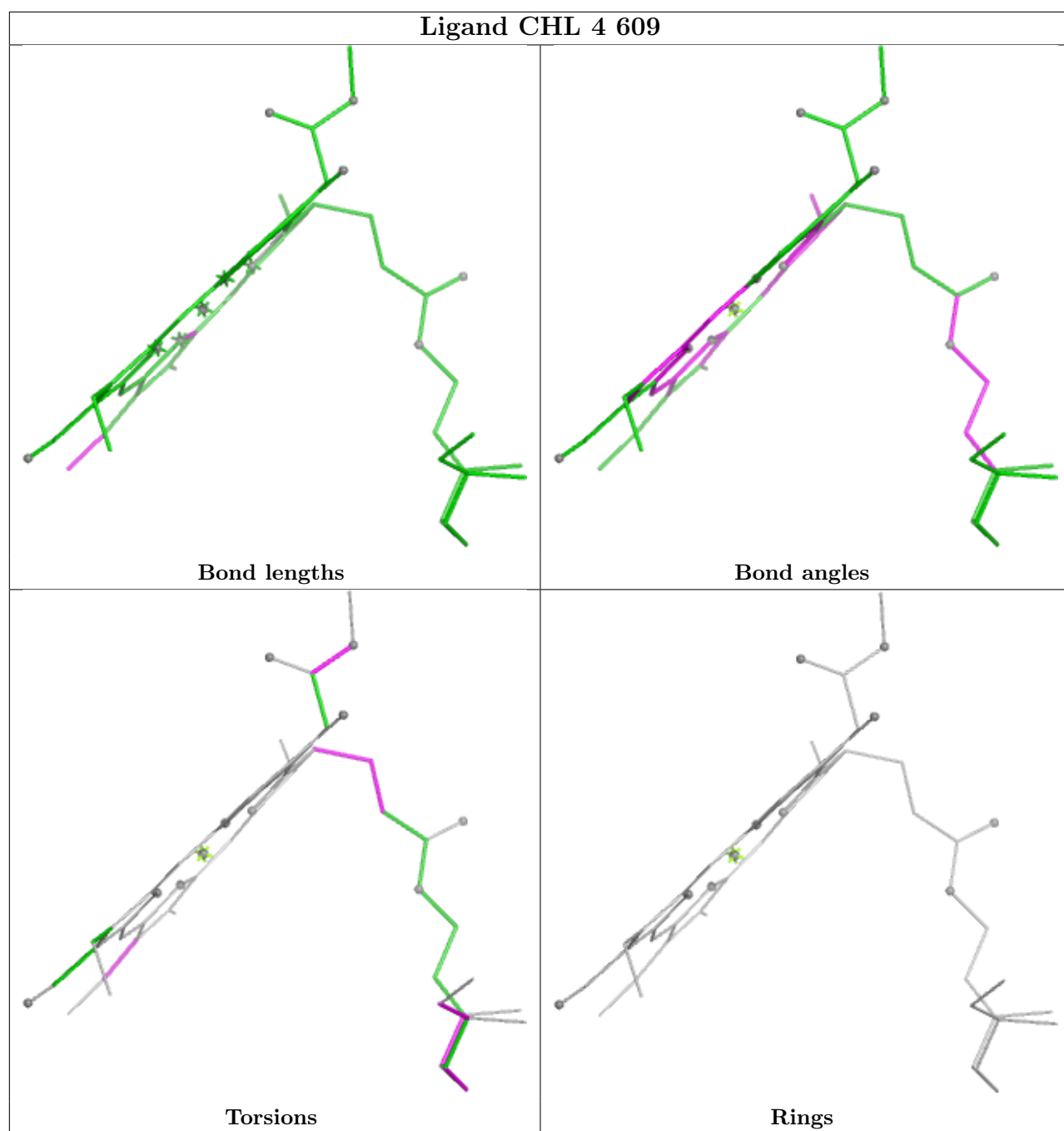
Ligand CLA 0 604

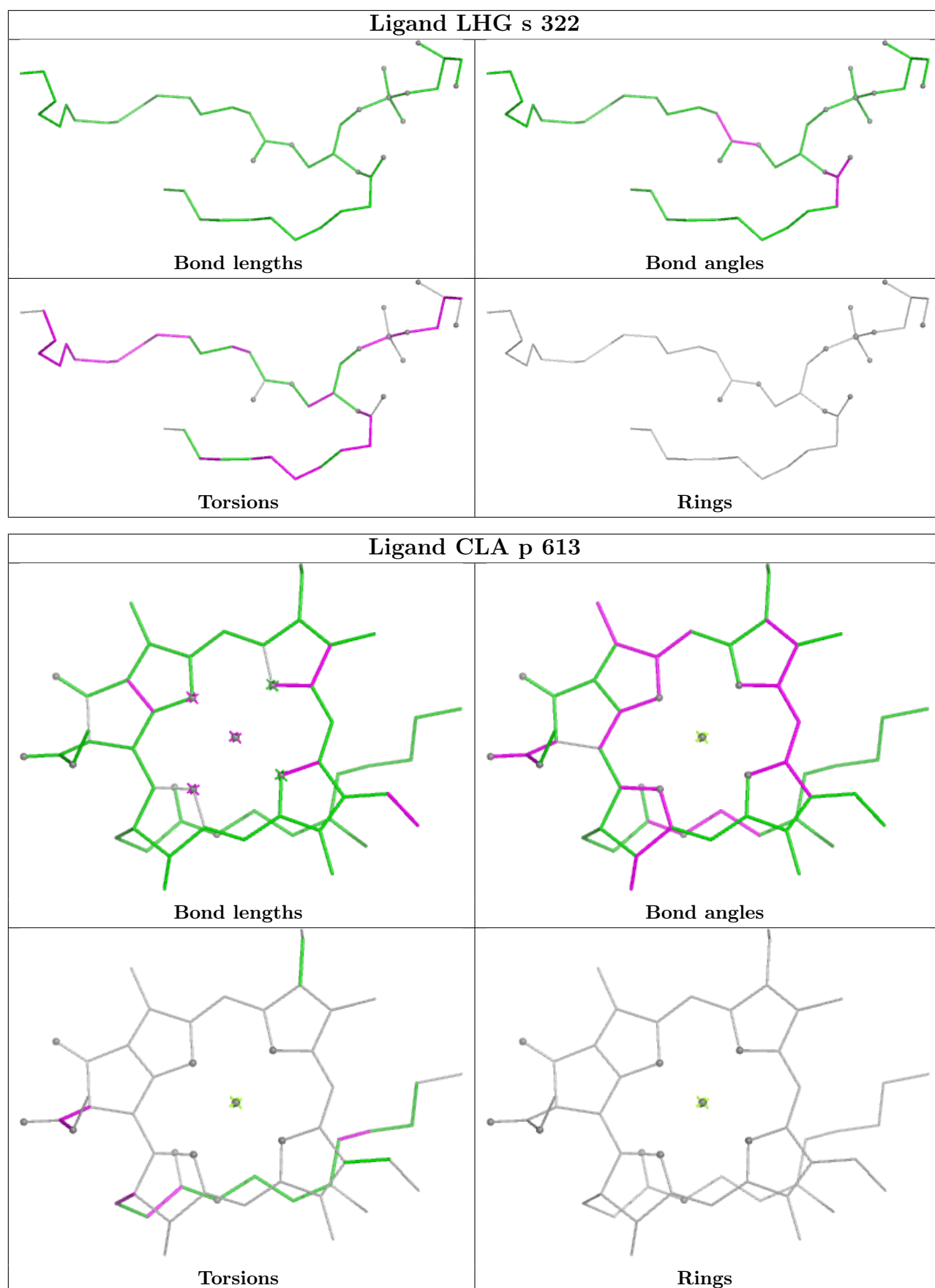


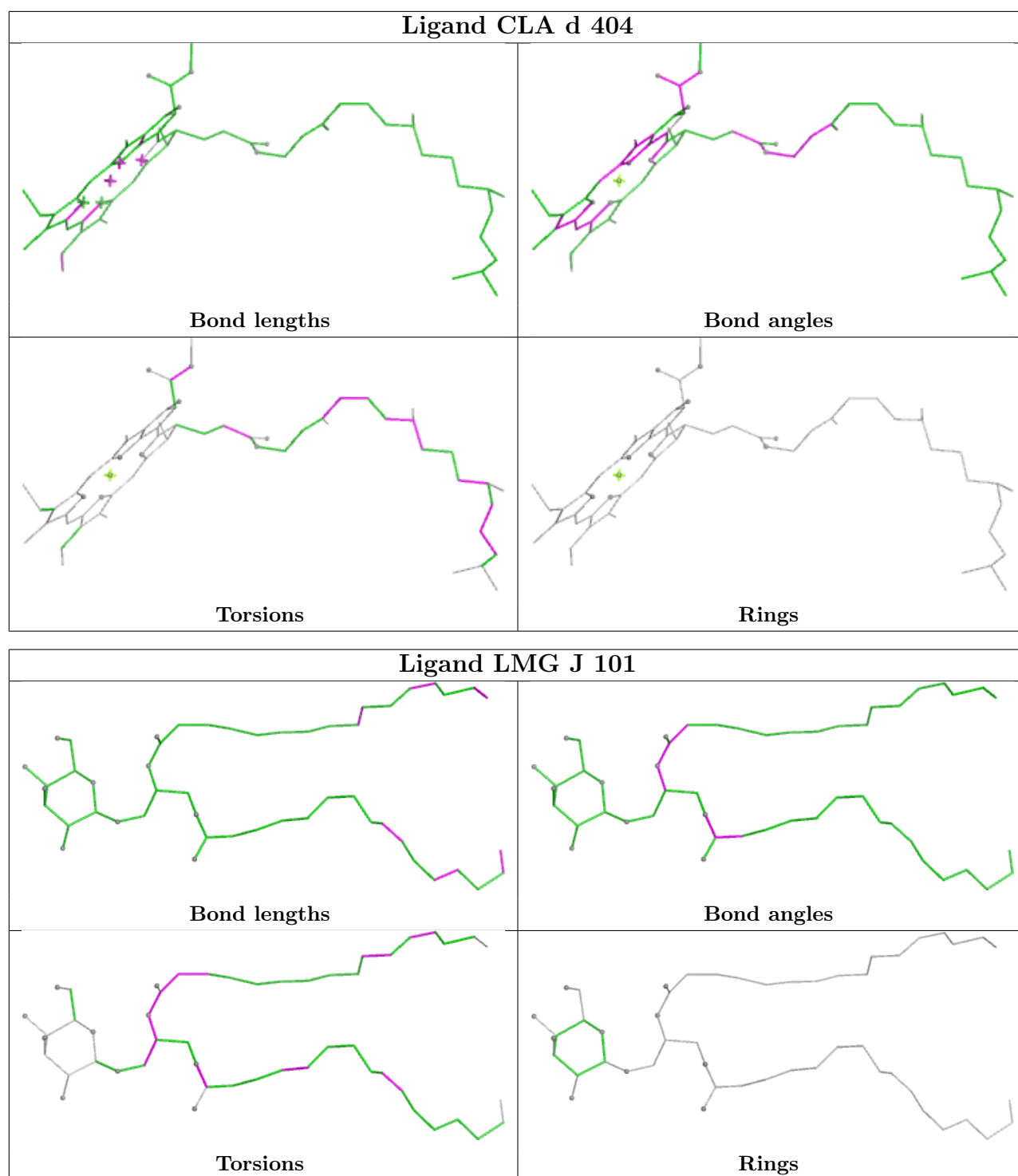
Ligand LMG c 621



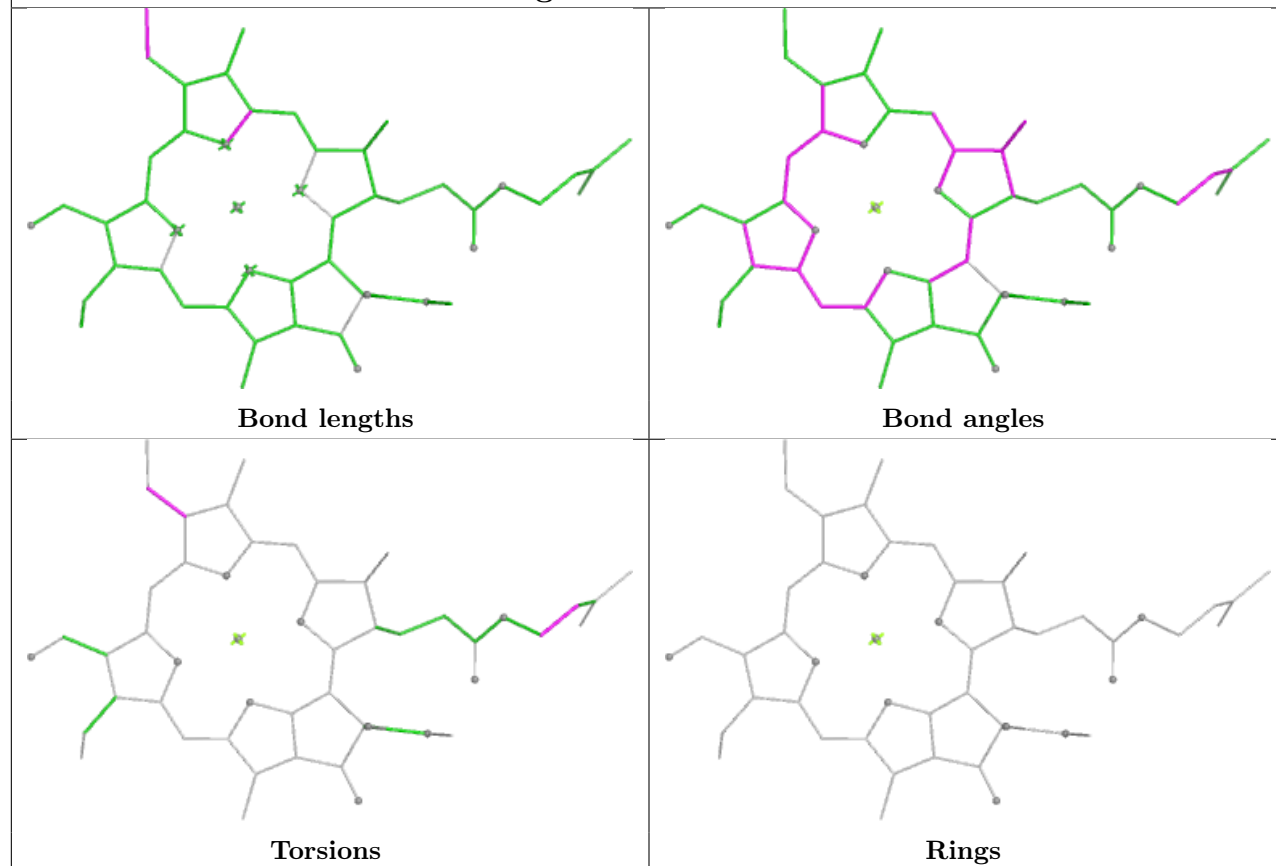
Ligand CHL 3 303**Ligand CLA 1 610**



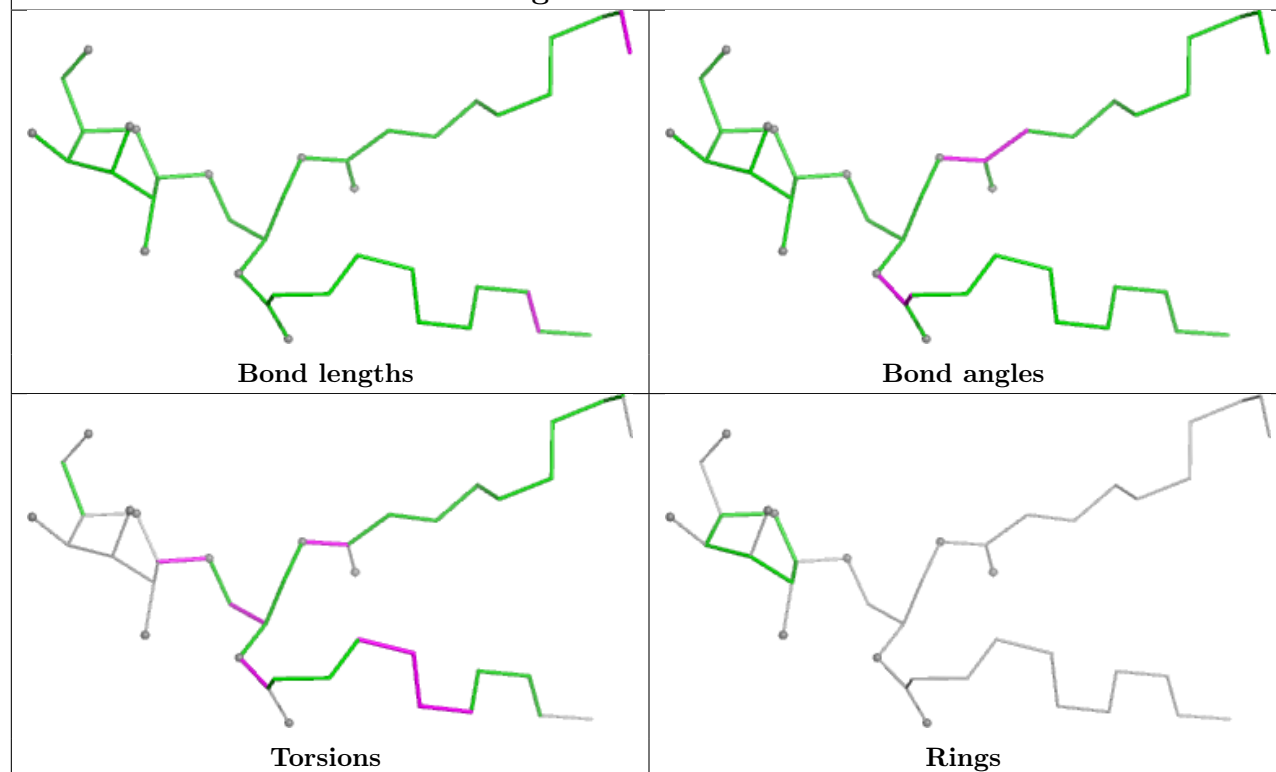




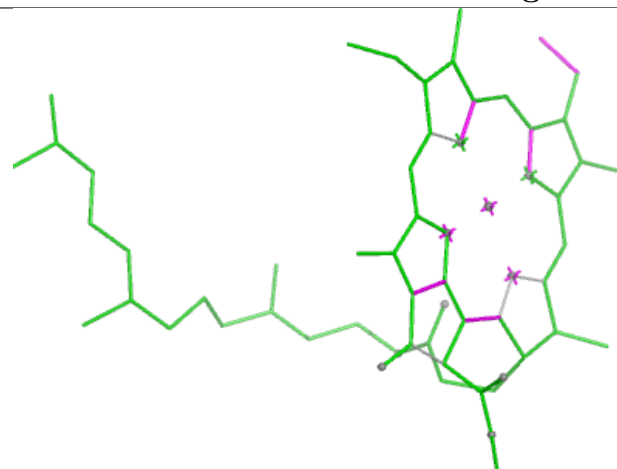
Ligand CHL 5 606



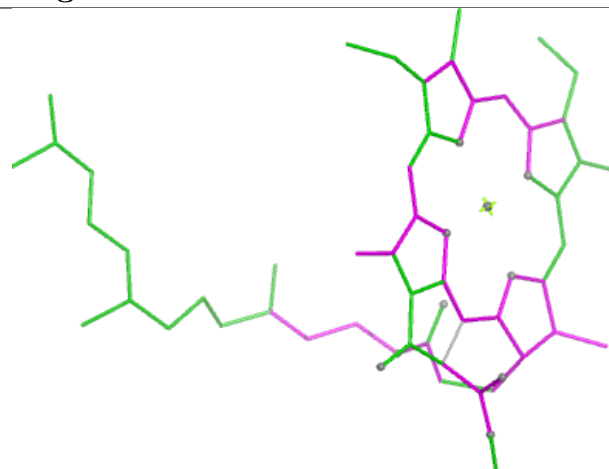
Ligand LMG 4 621



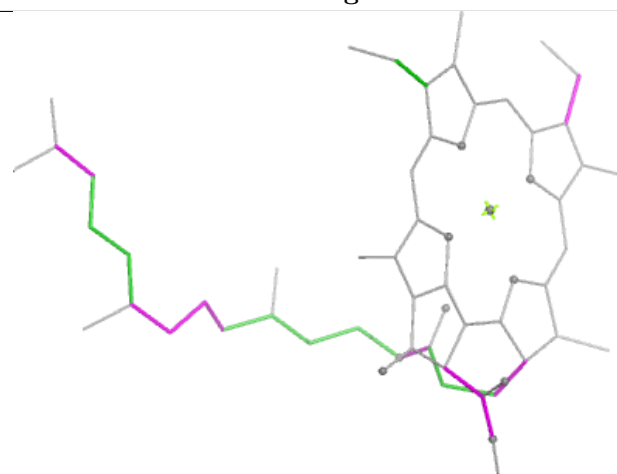
Ligand CLA g 311



Bond lengths



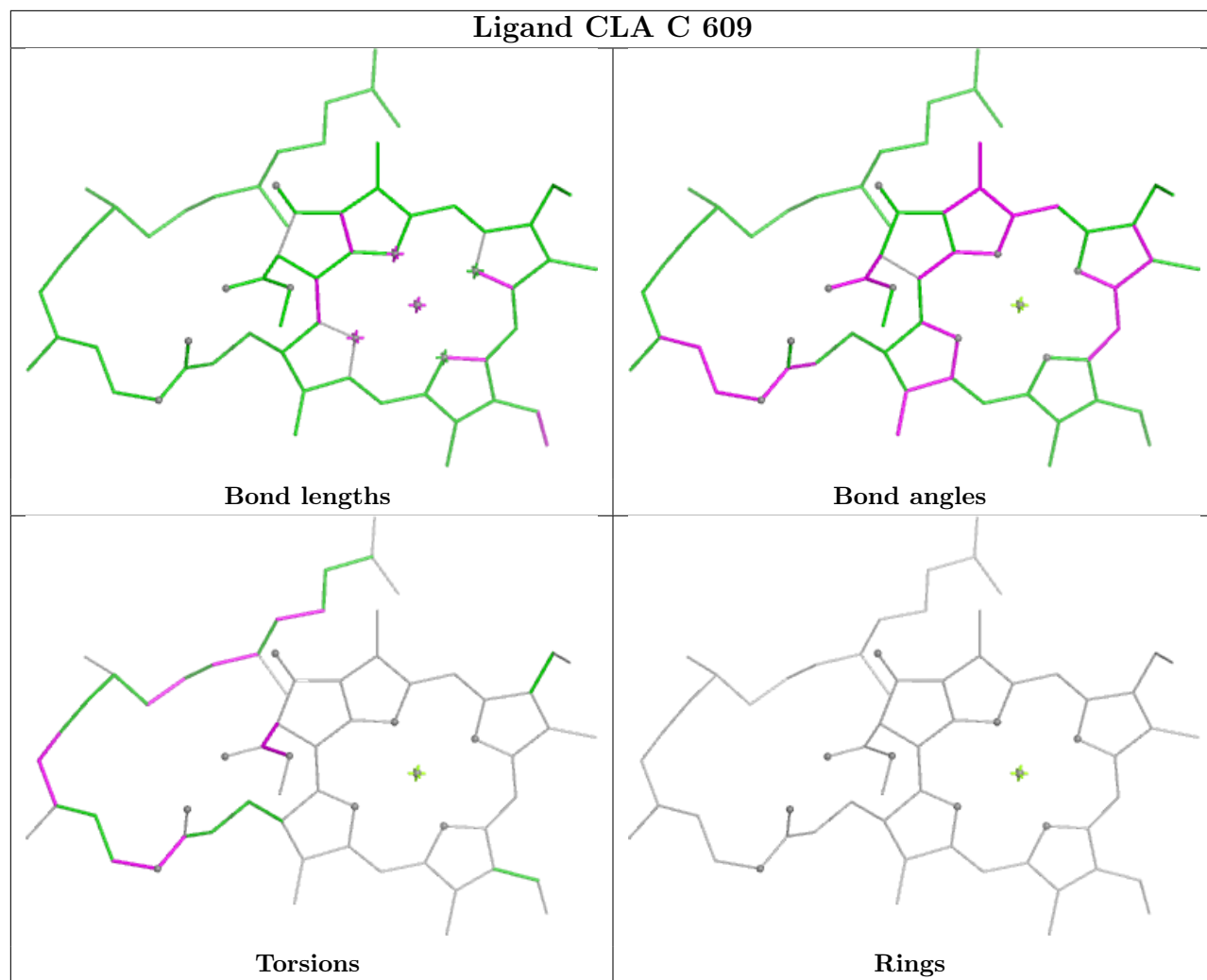
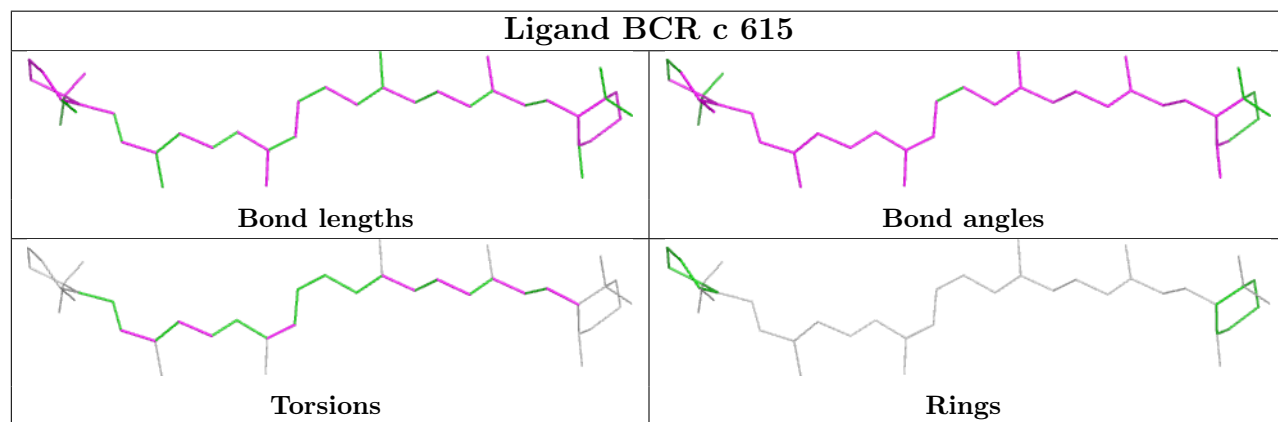
Bond angles

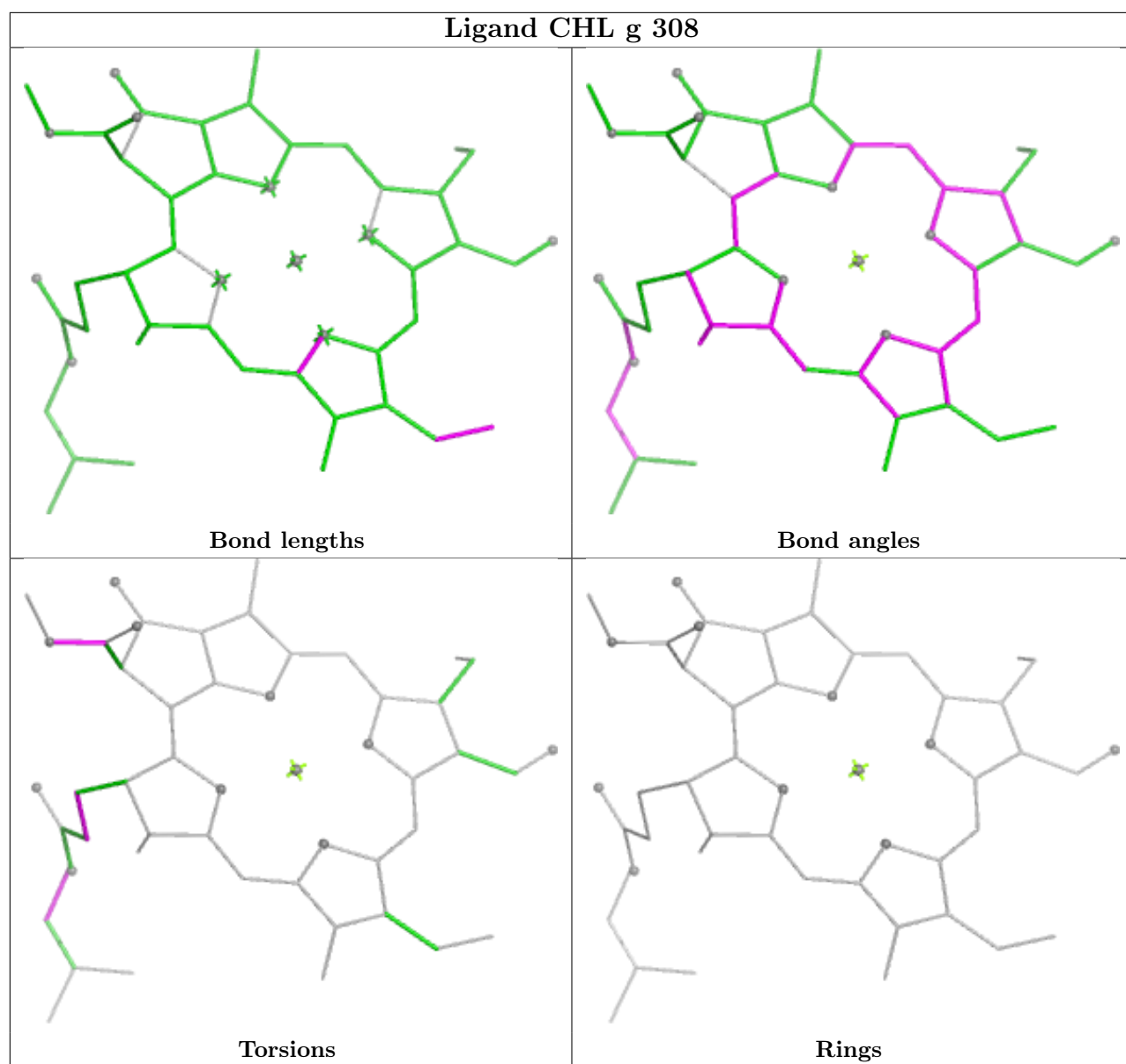


Torsions

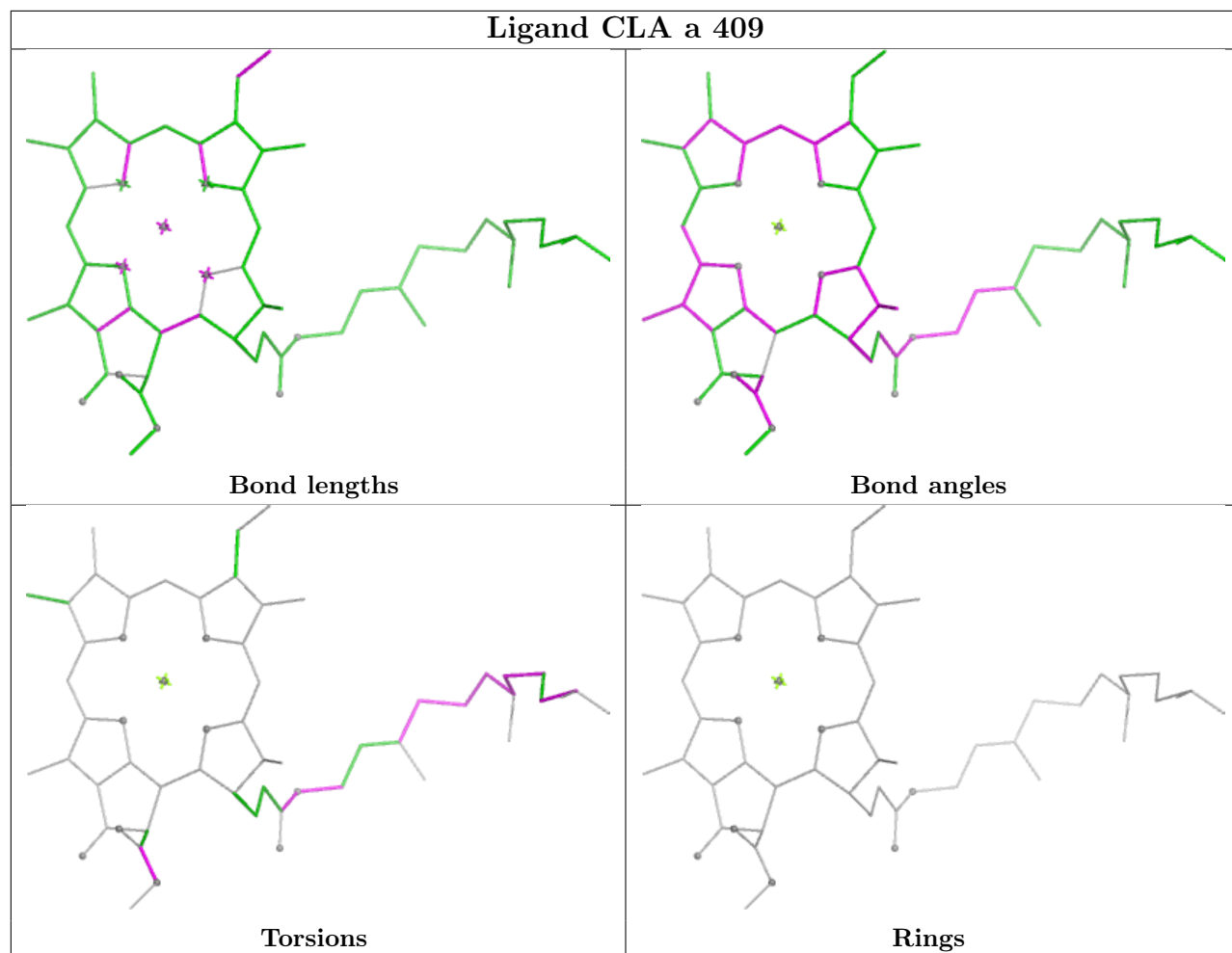


Rings

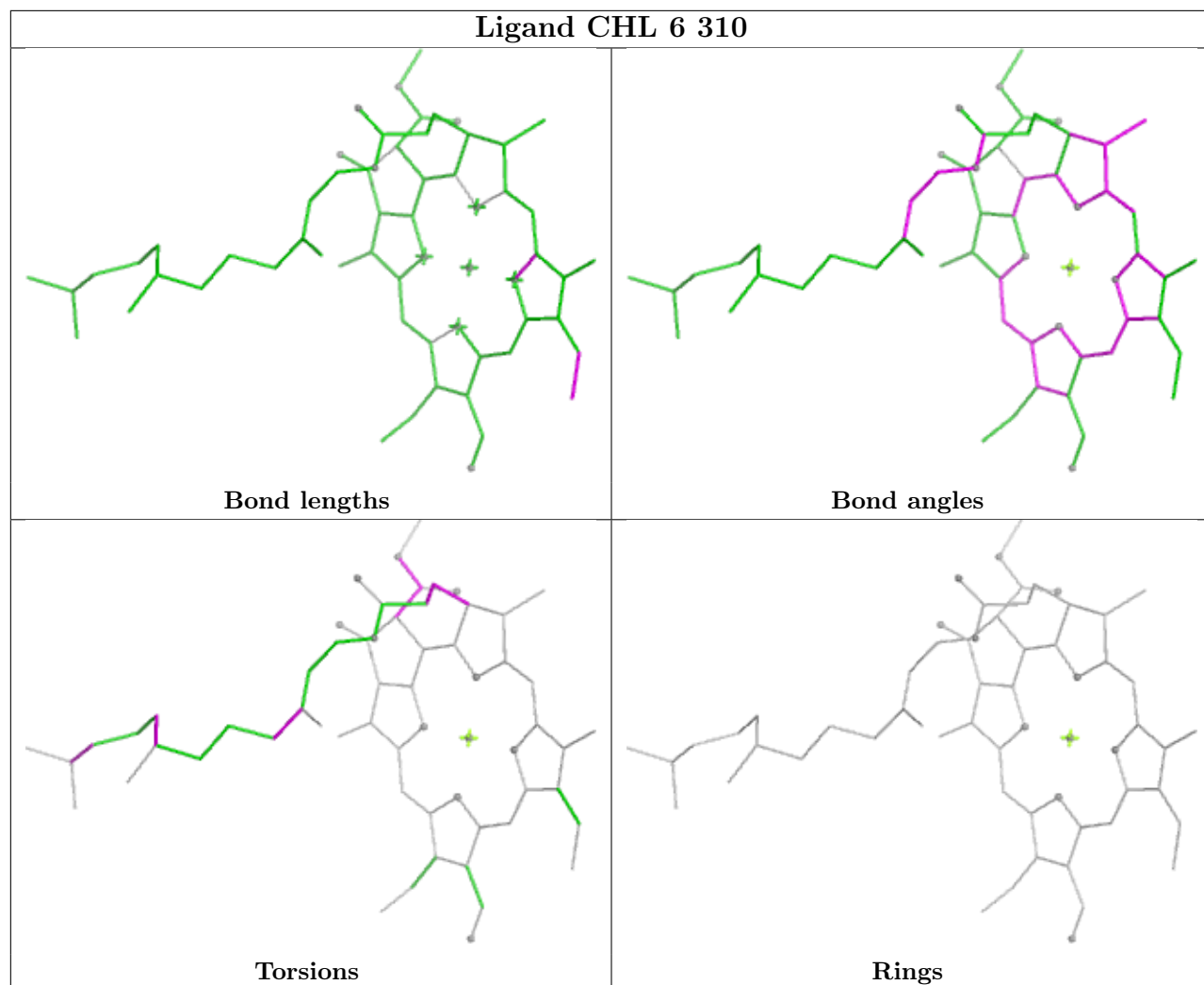
Ligand CLA C 609**Ligand BCR c 615**



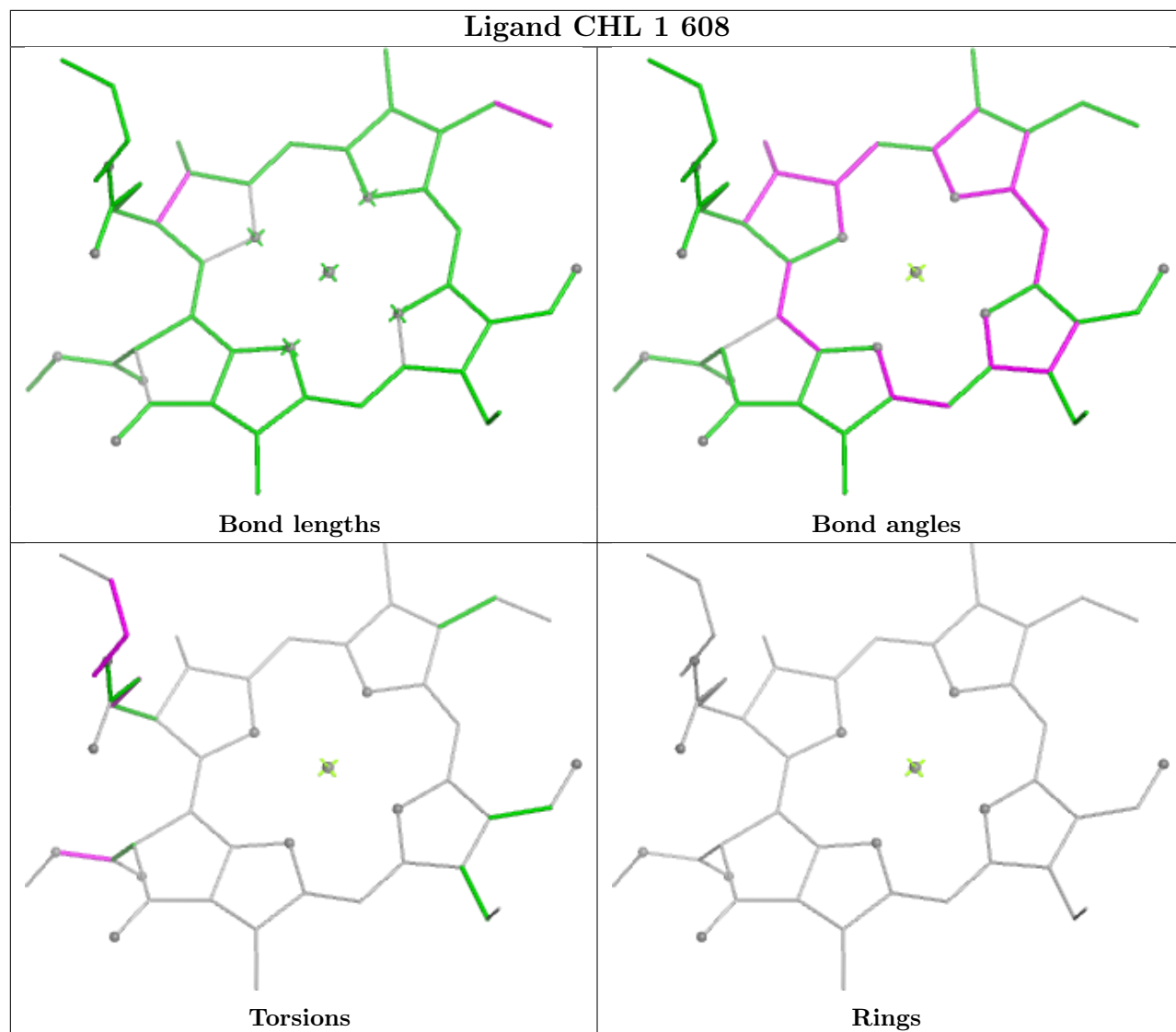
Ligand CLA a 409

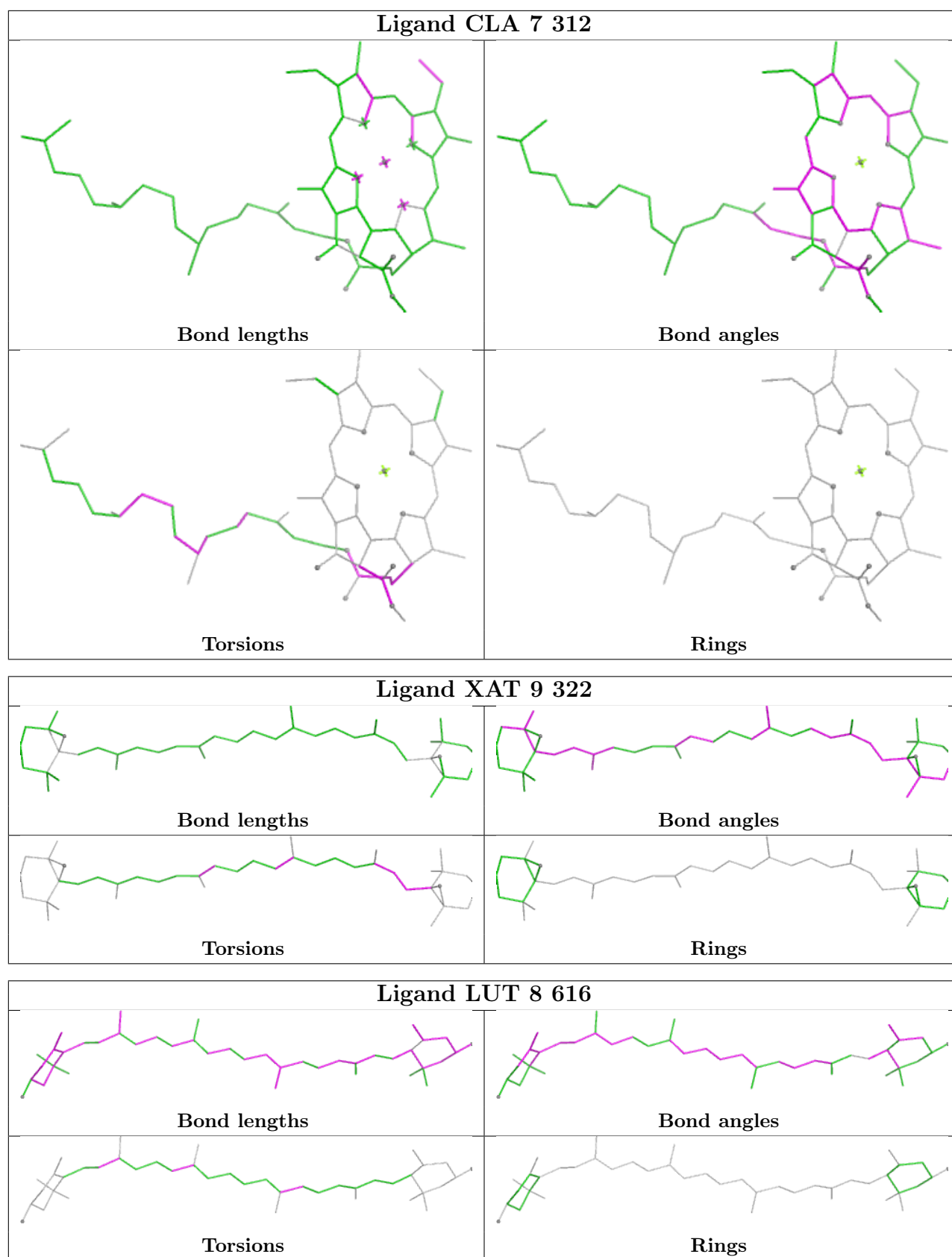


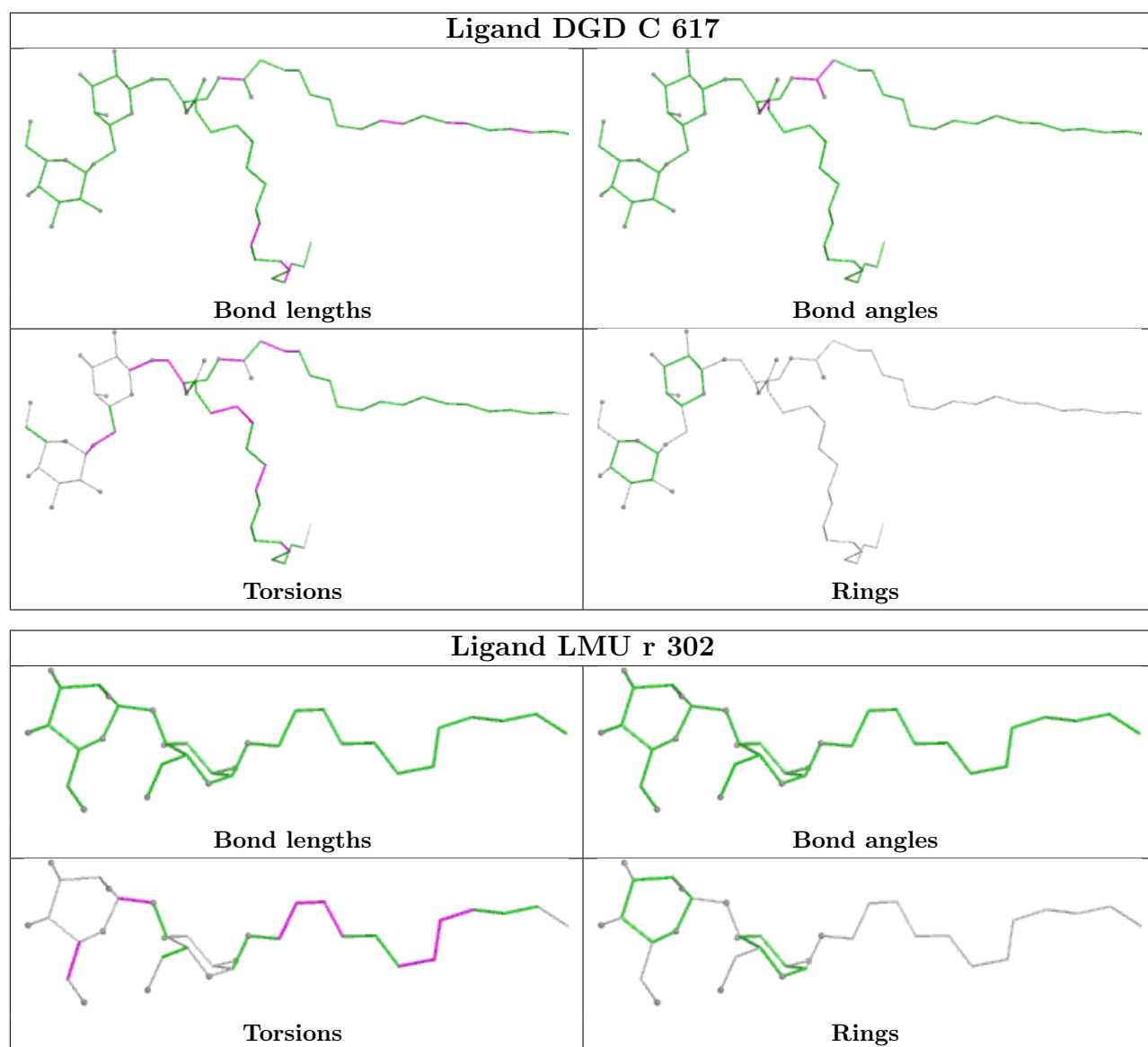
Ligand CHL 6 310



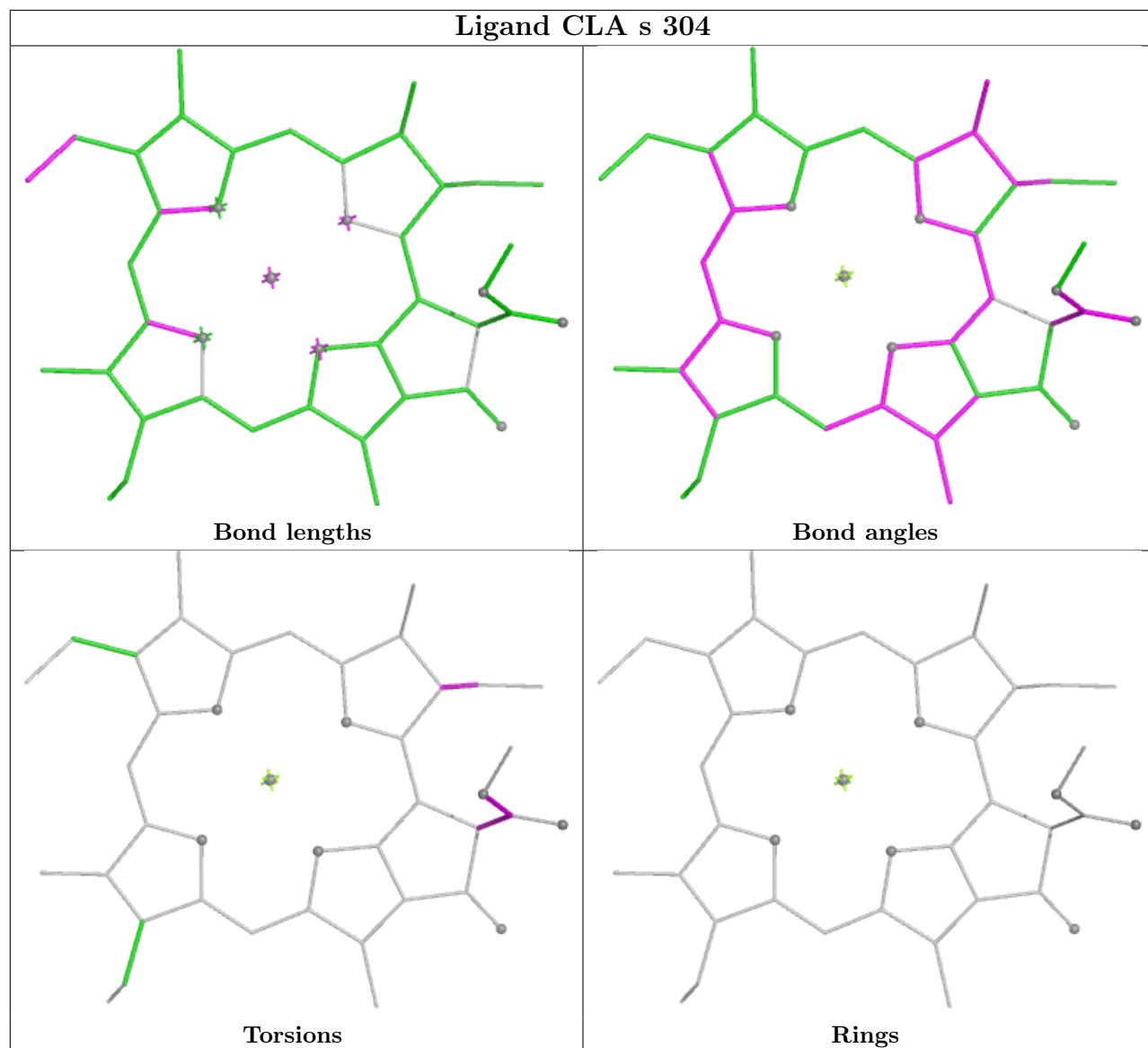
Ligand CHL 1 608

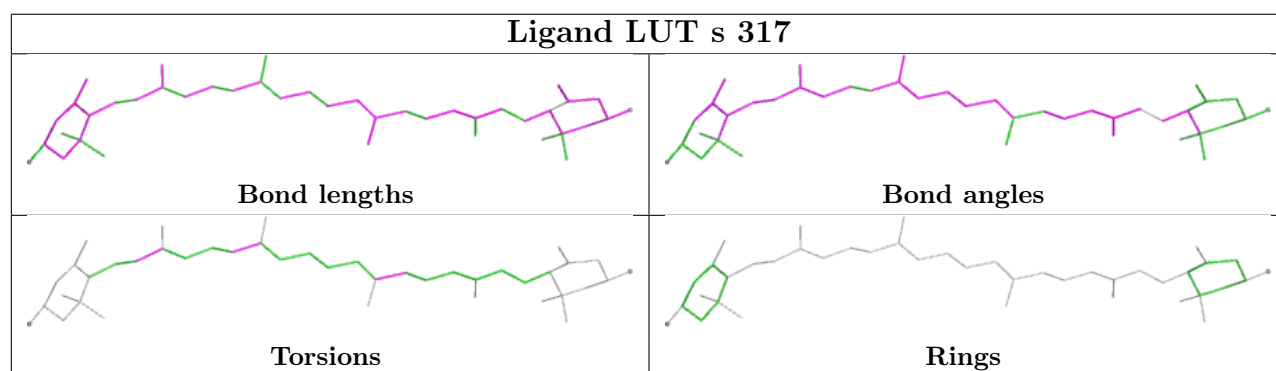
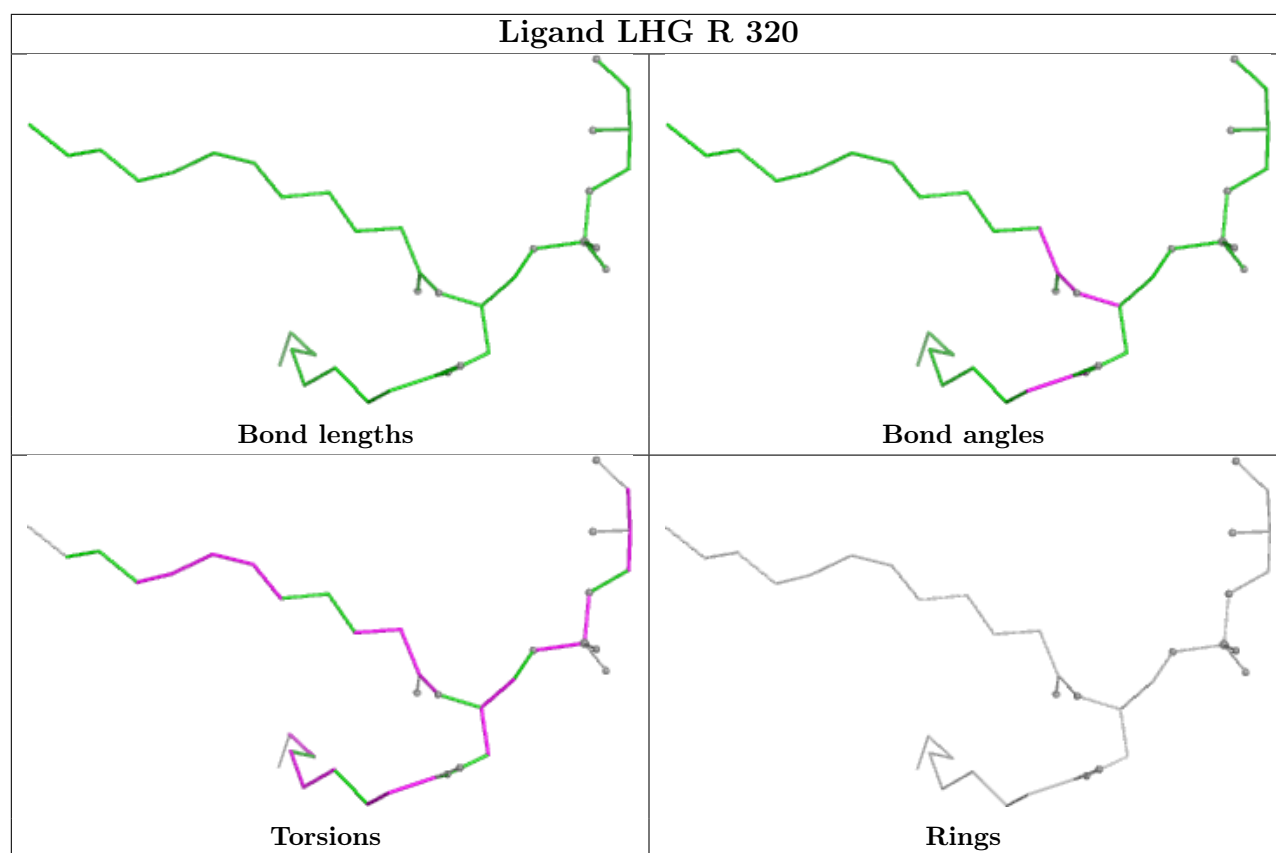




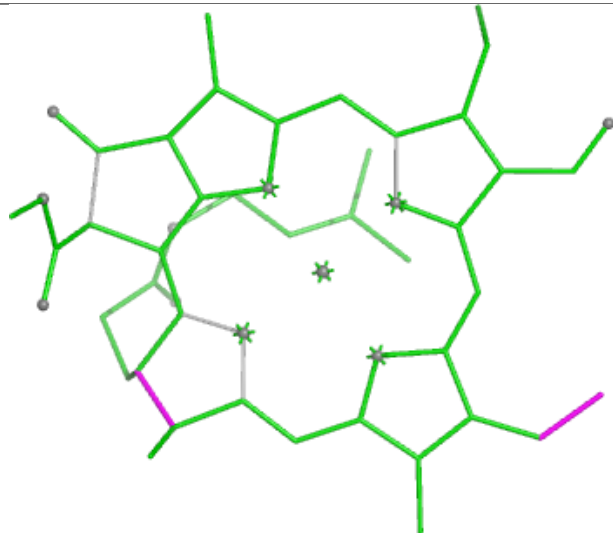


Ligand CLA s 304

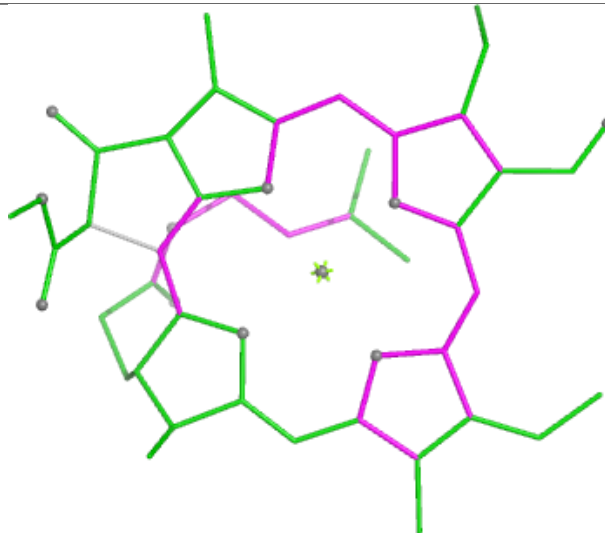




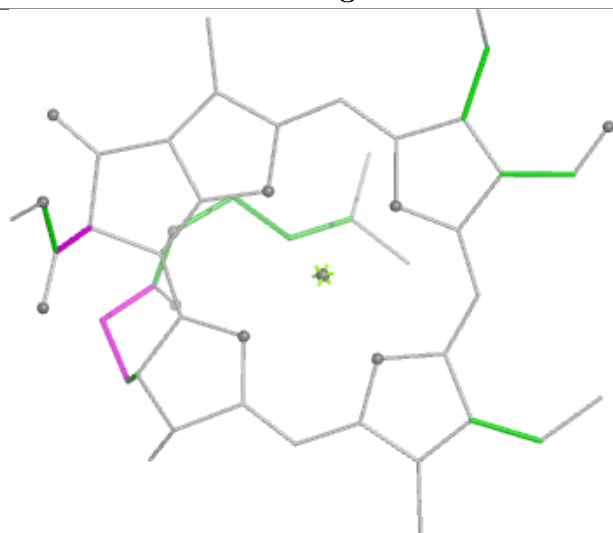
Ligand CHL p 607



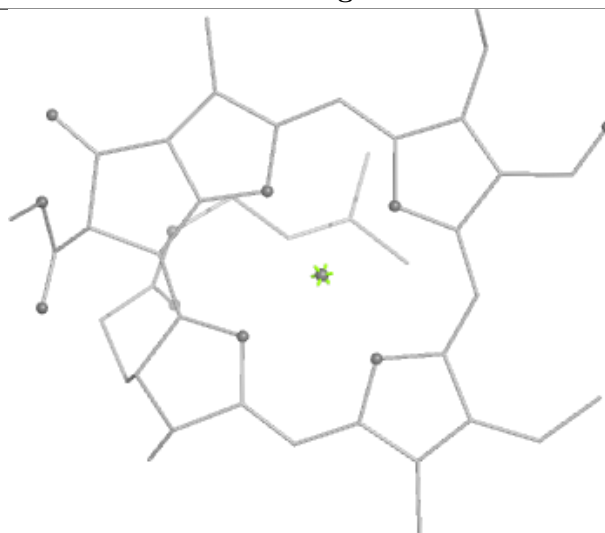
Bond lengths



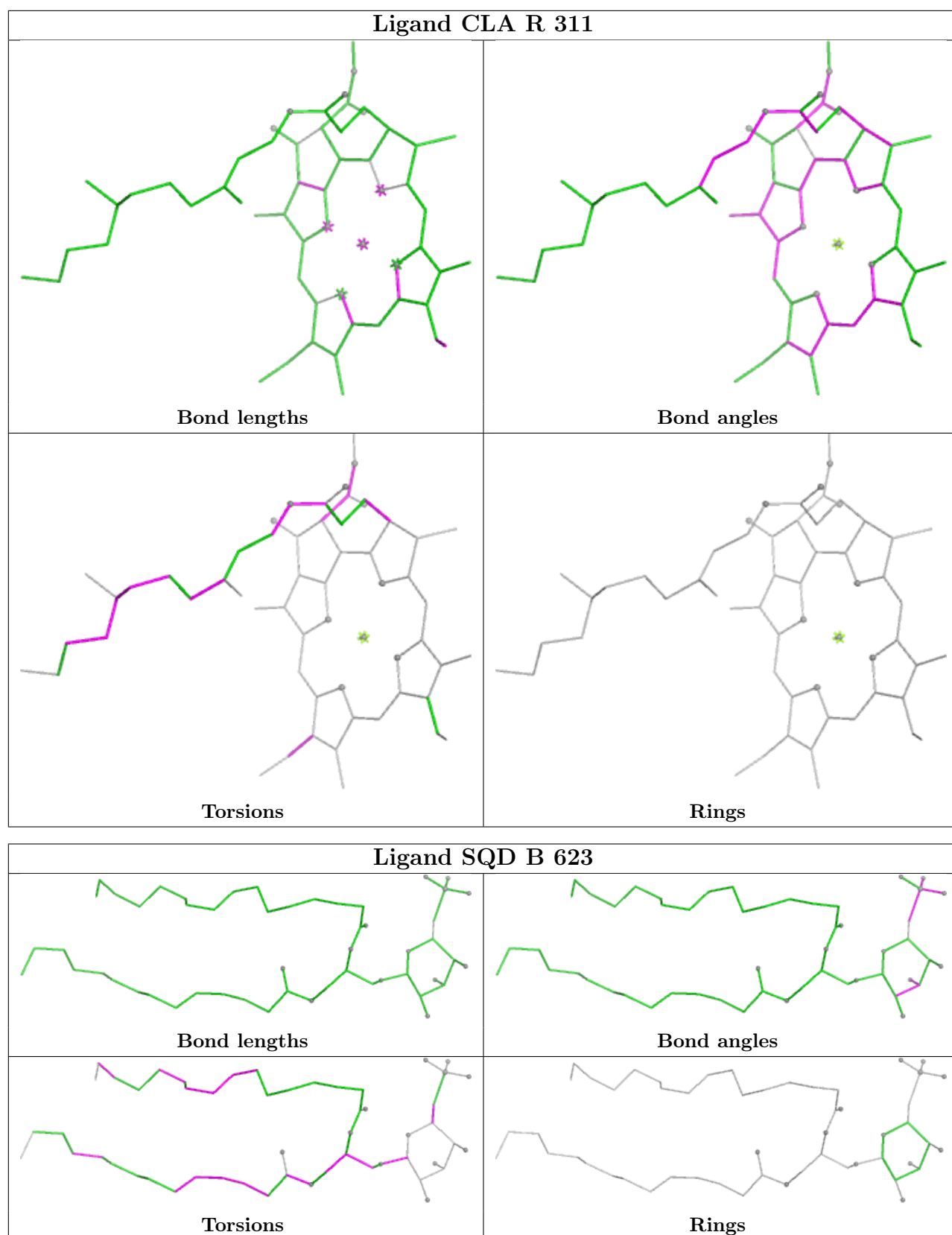
Bond angles

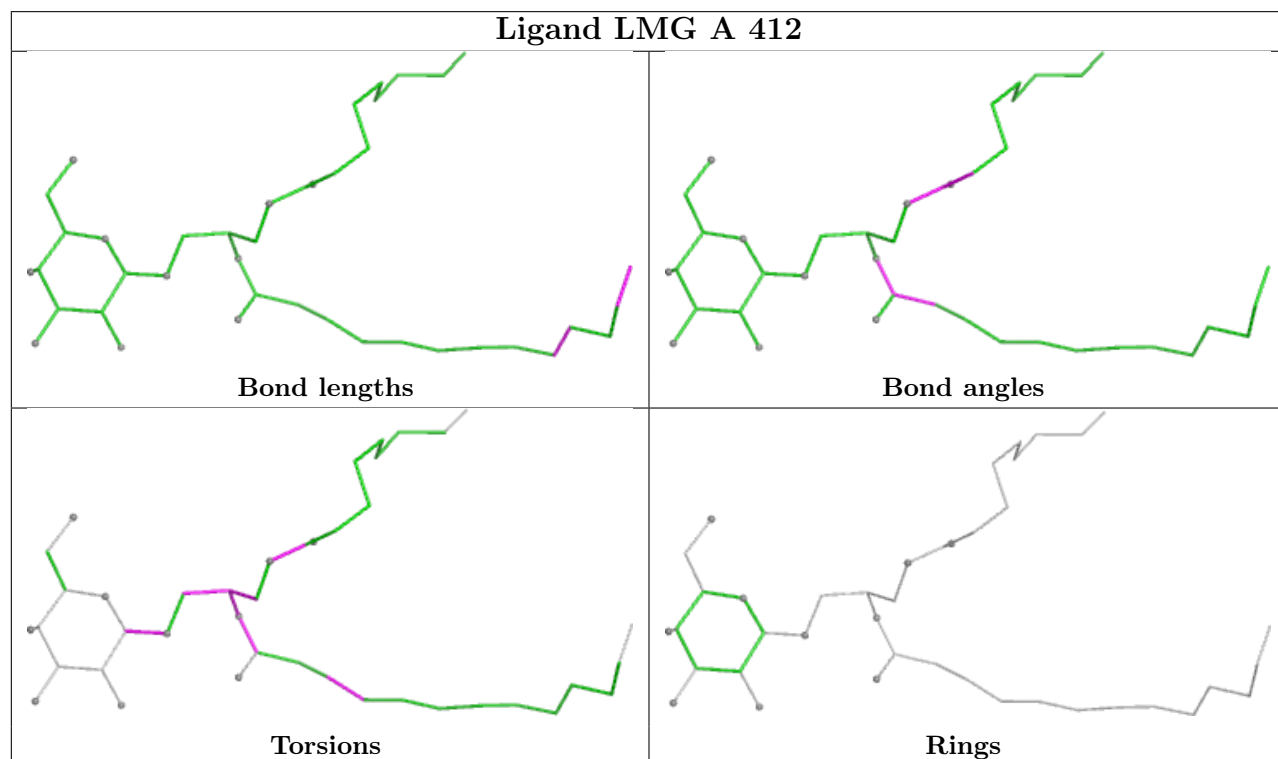
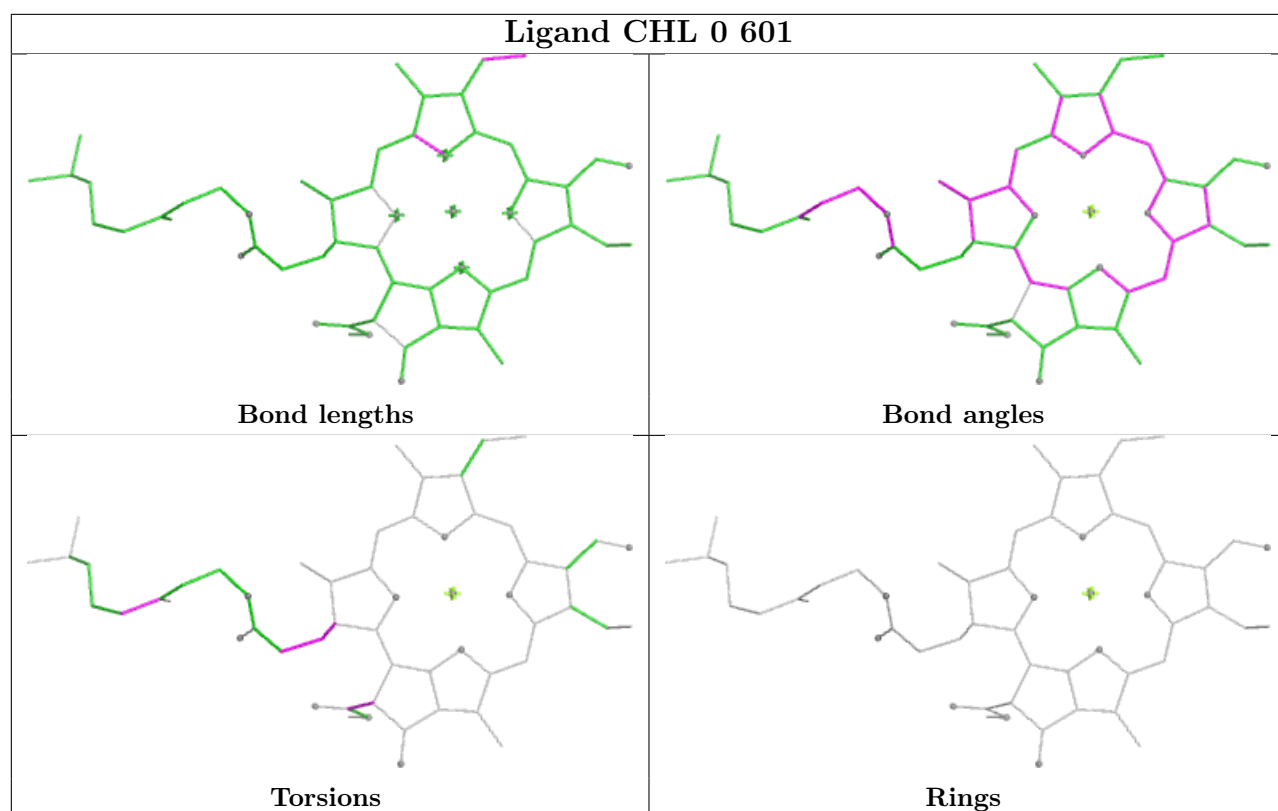


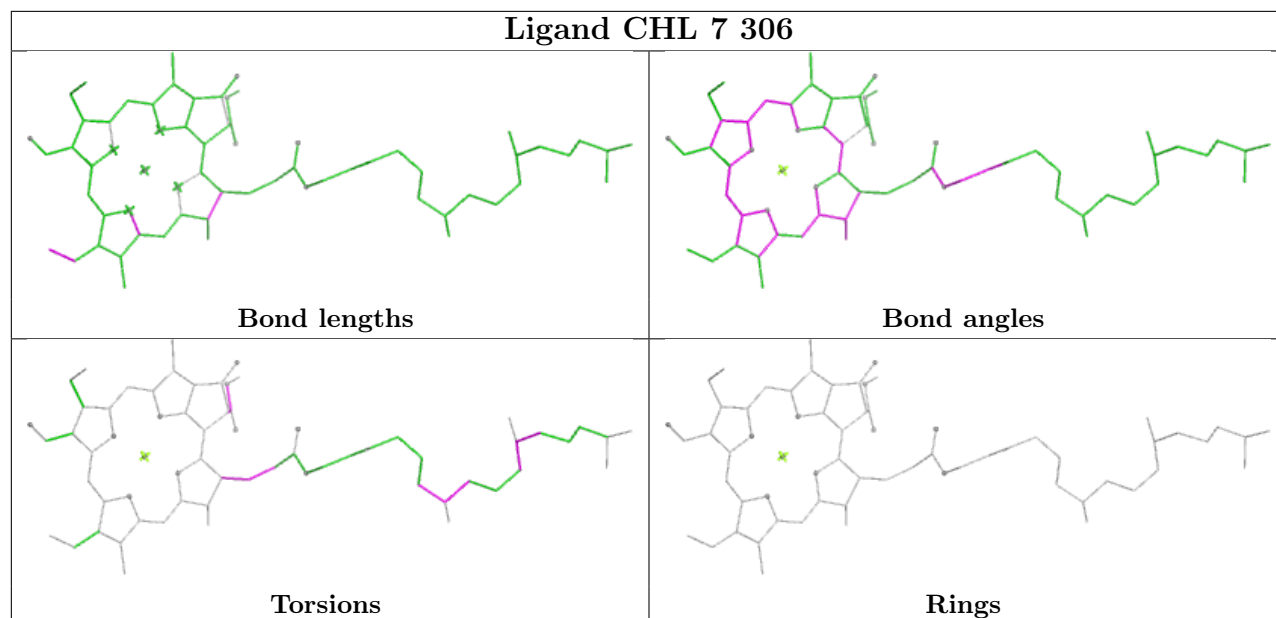
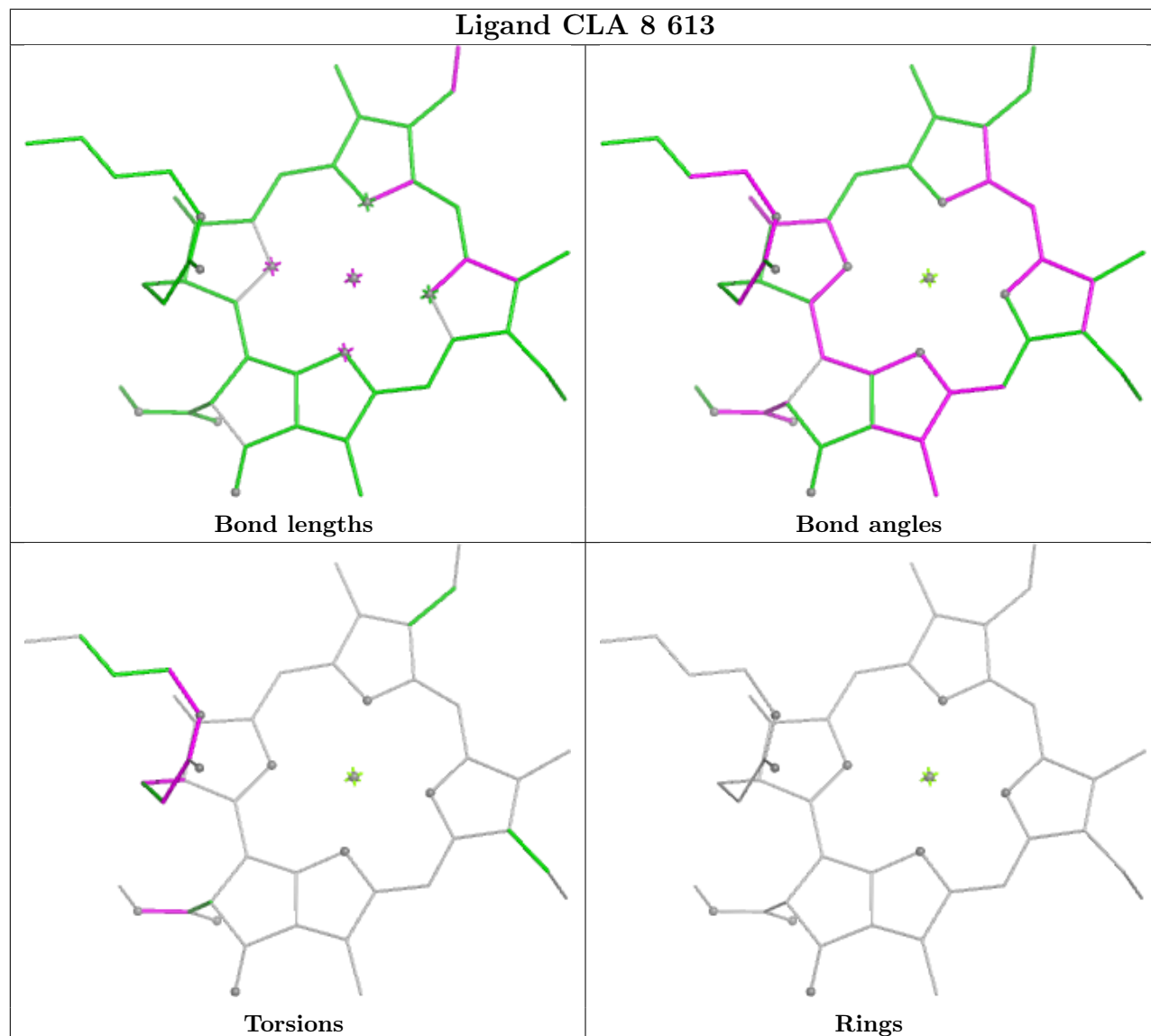
Torsions

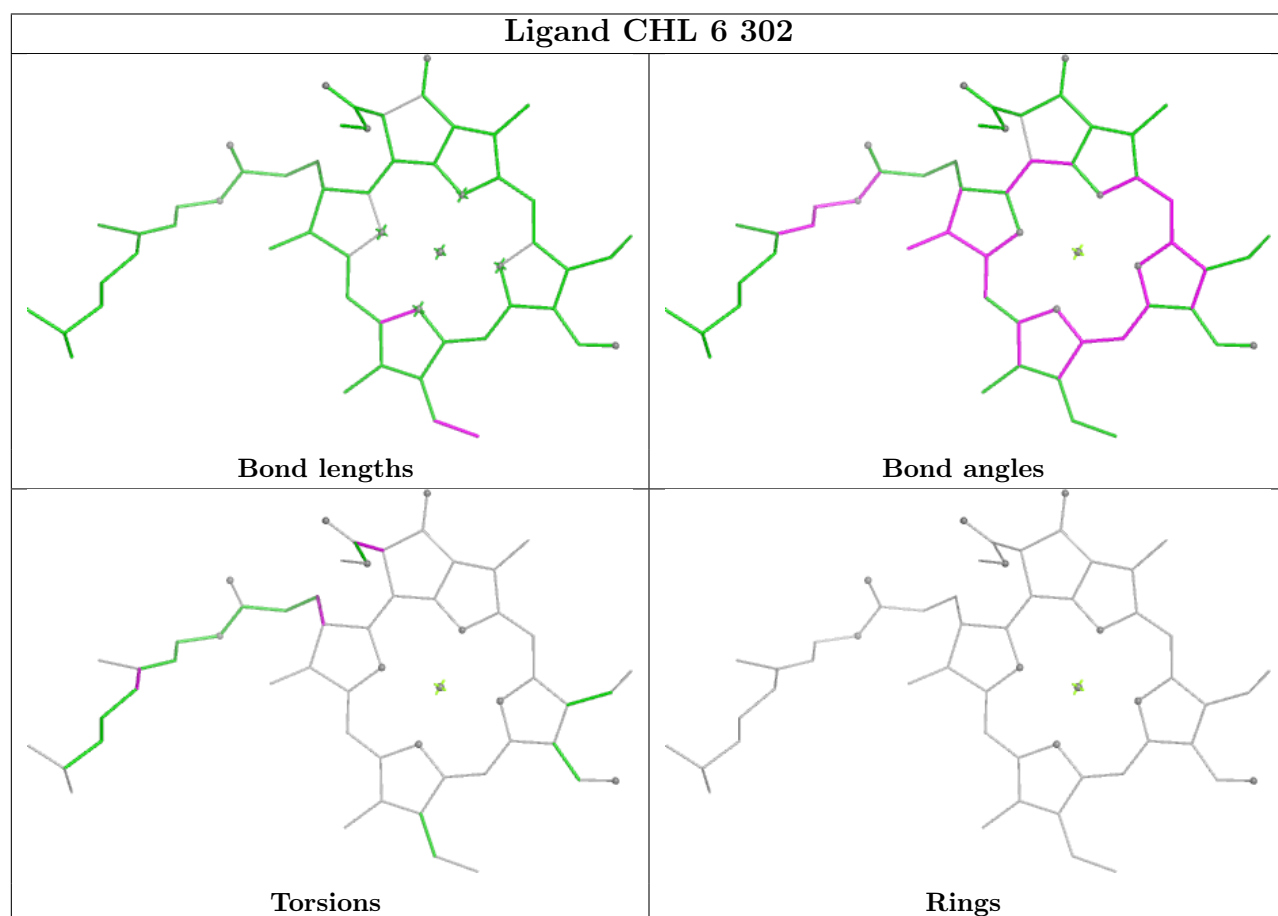
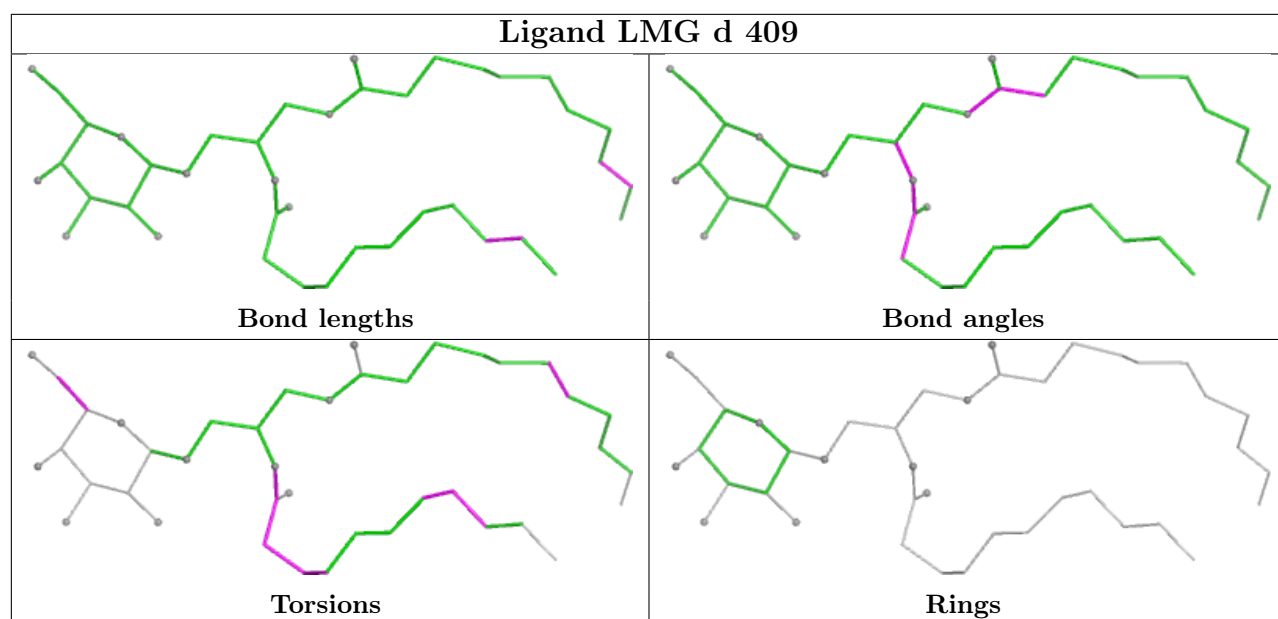


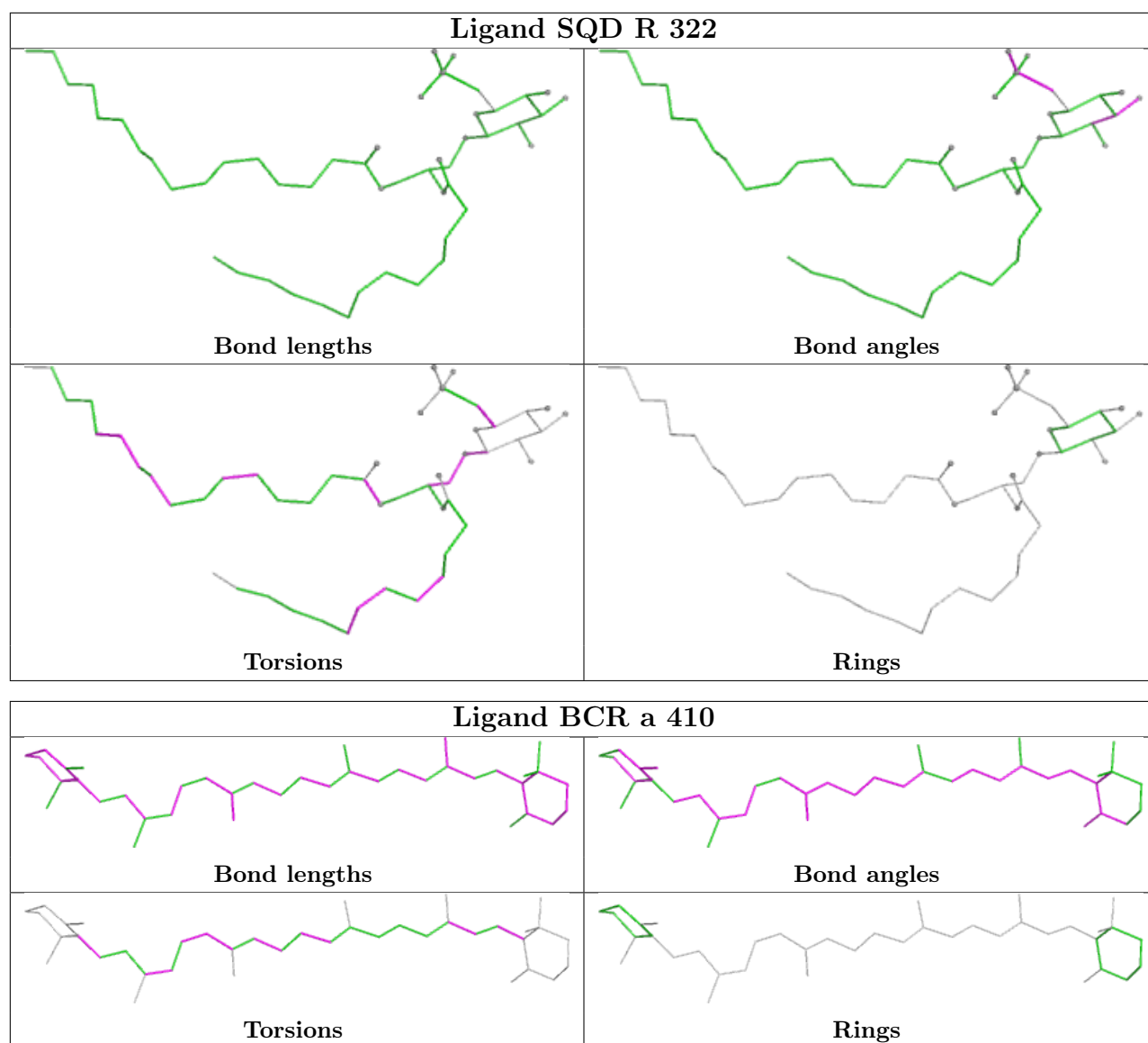
Rings

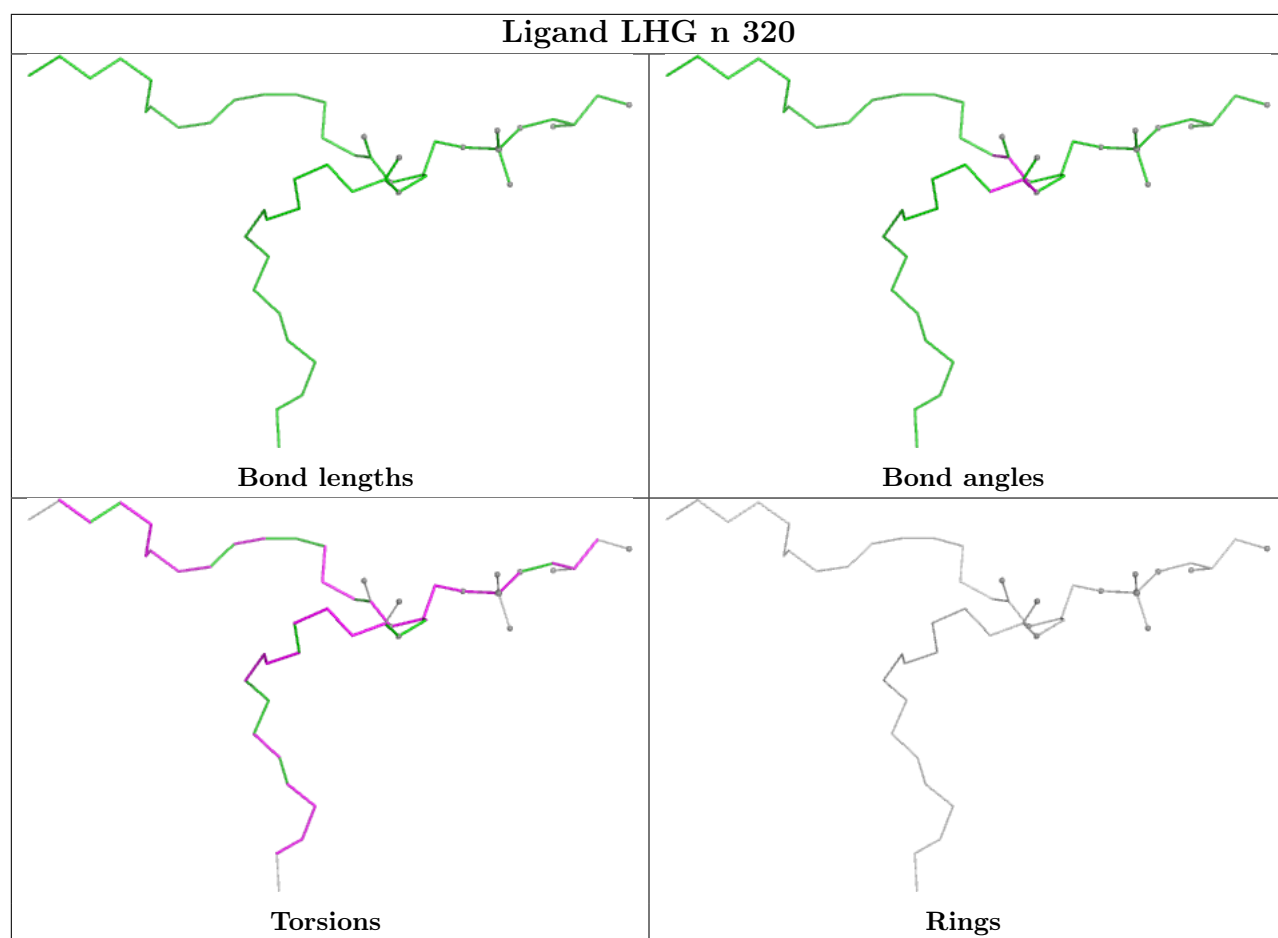




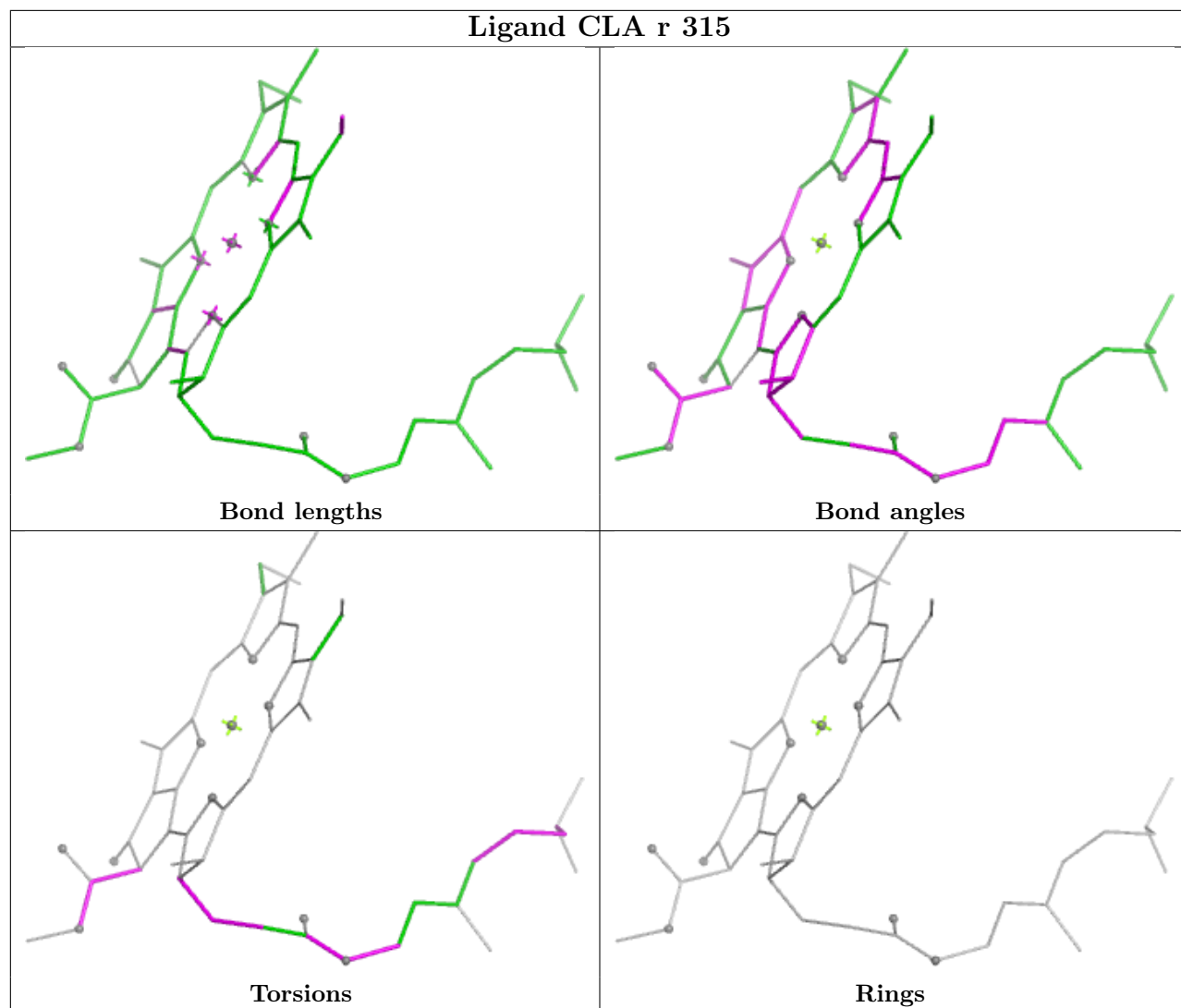
Ligand CHL 7 306**Ligand CLA 8 613**



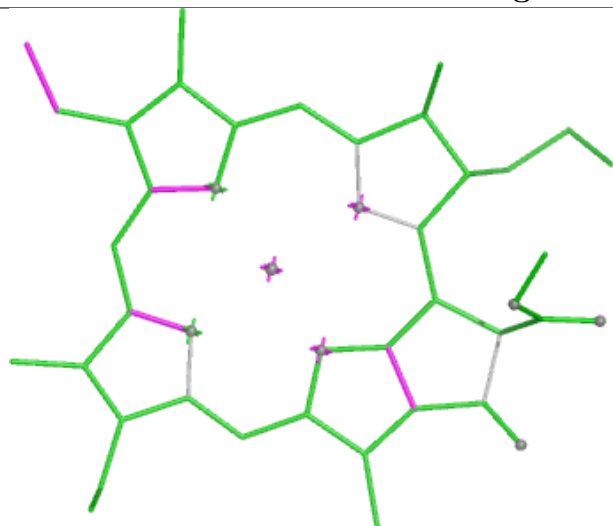




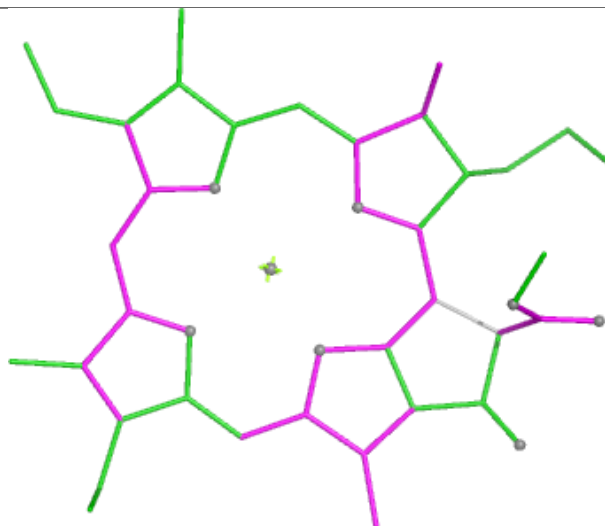
Ligand CLA r 315



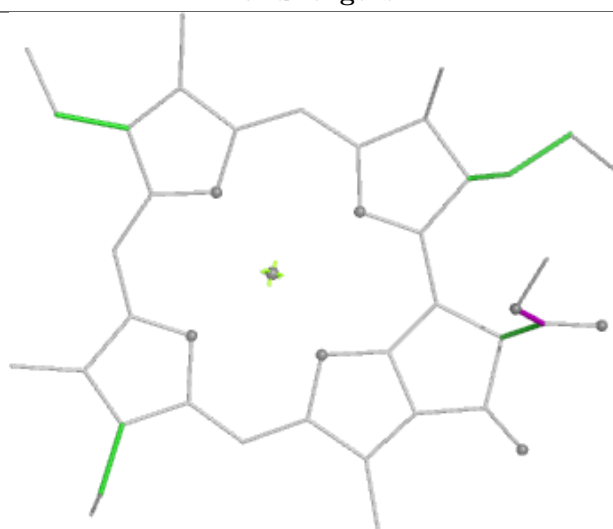
Ligand CLA G 611



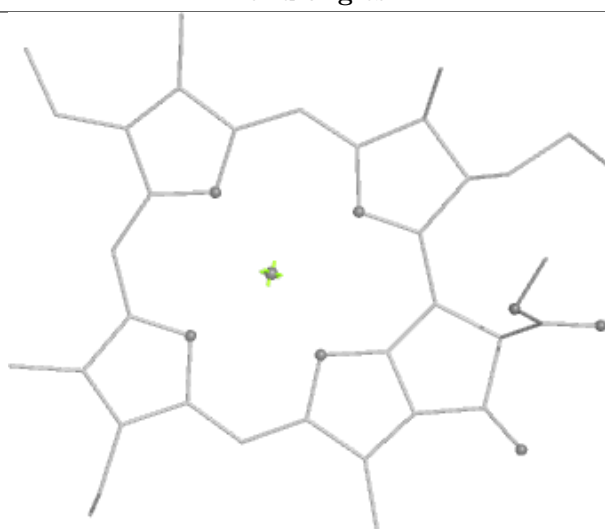
Bond lengths



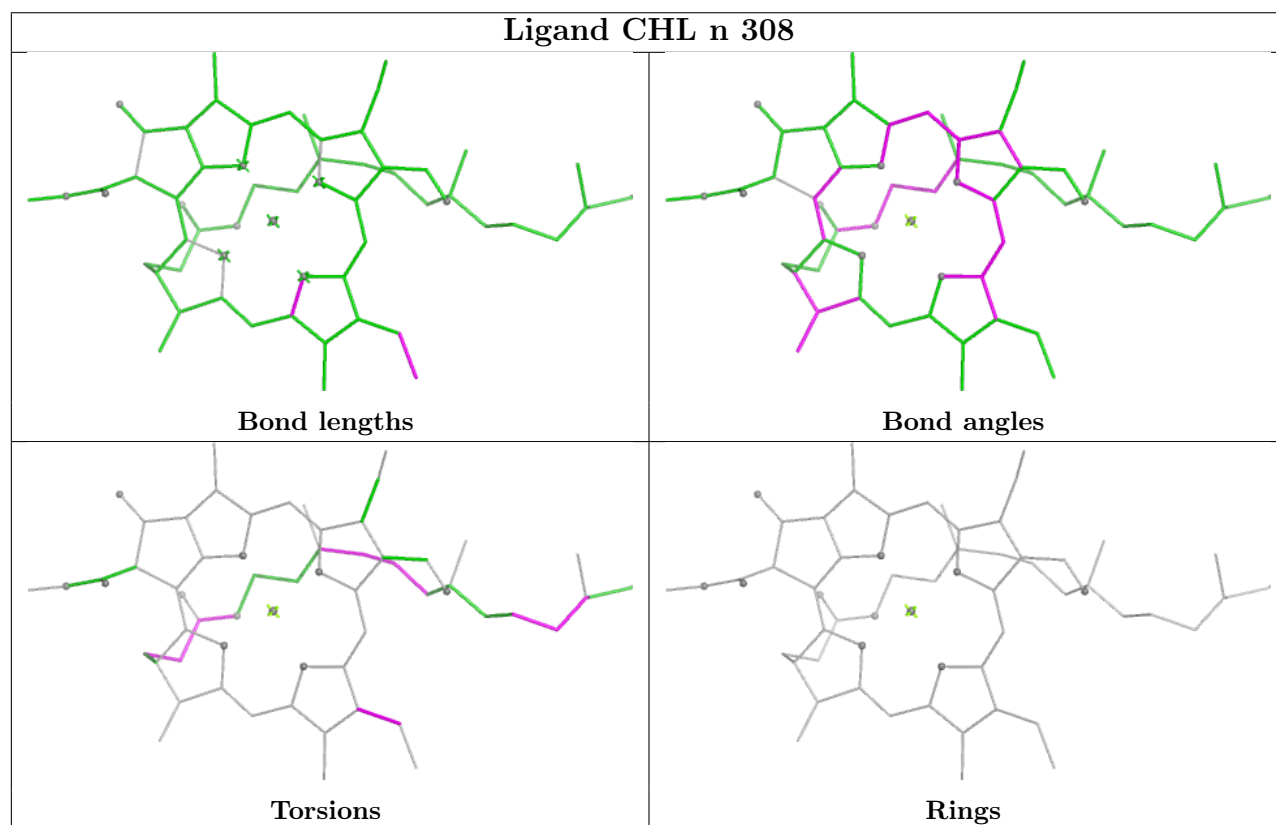
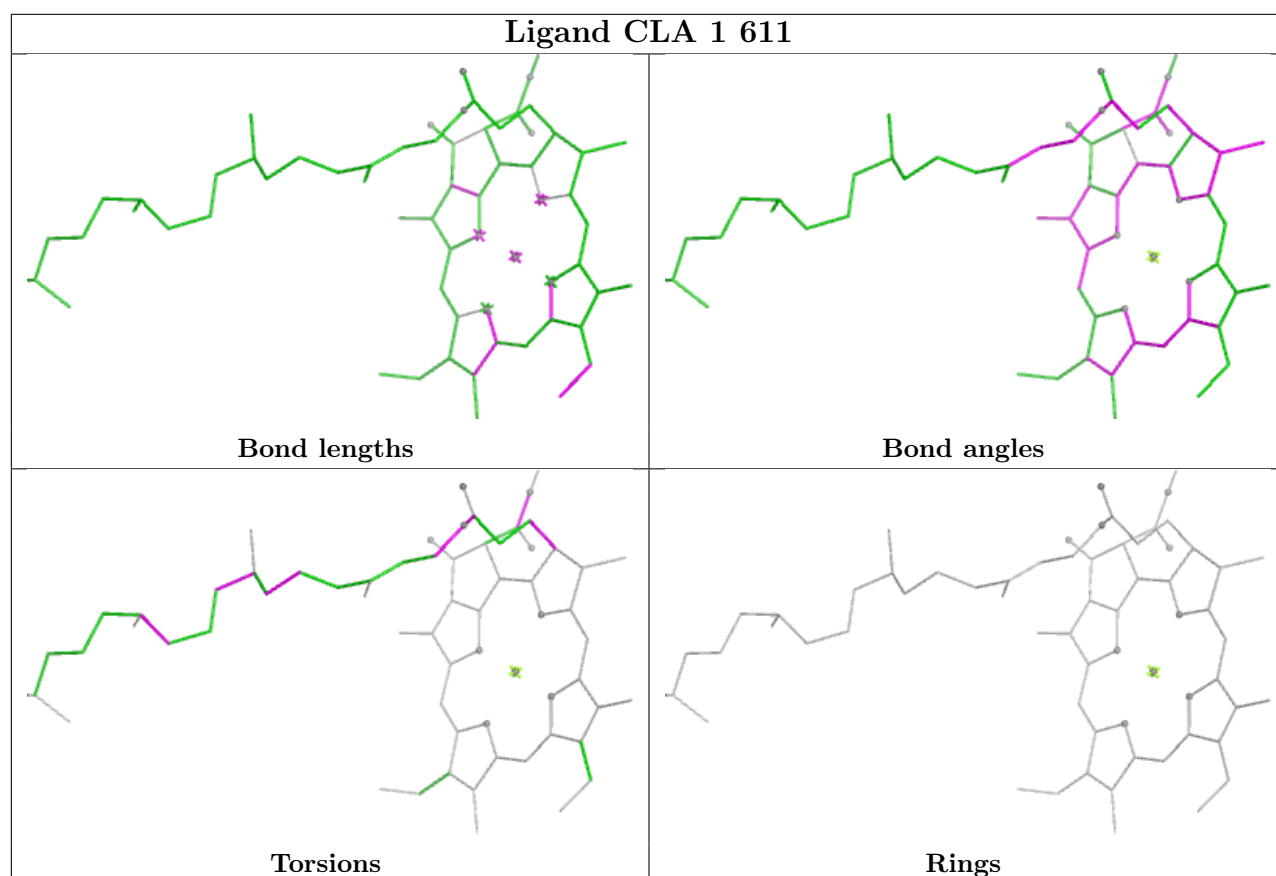
Bond angles

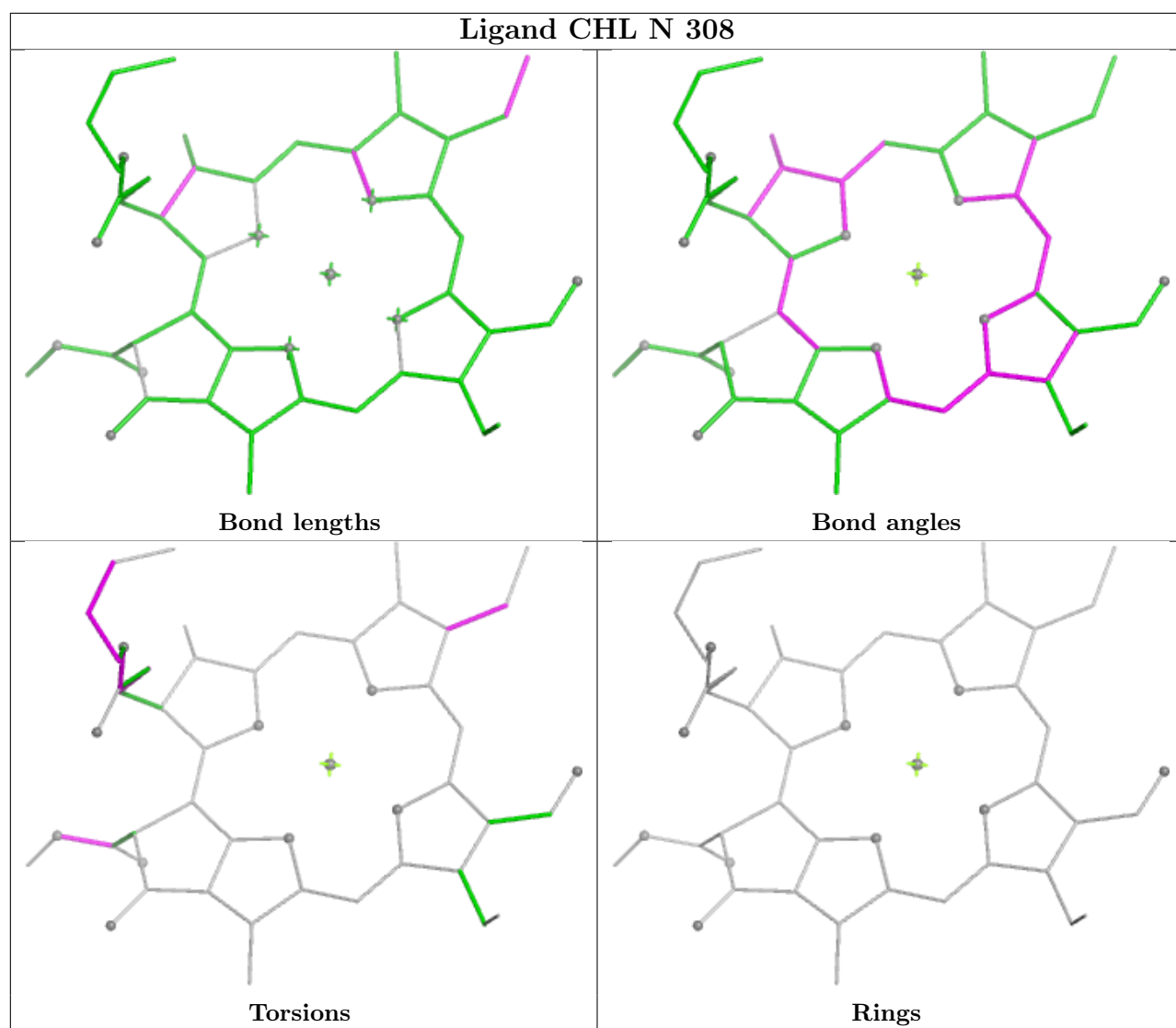


Torsions

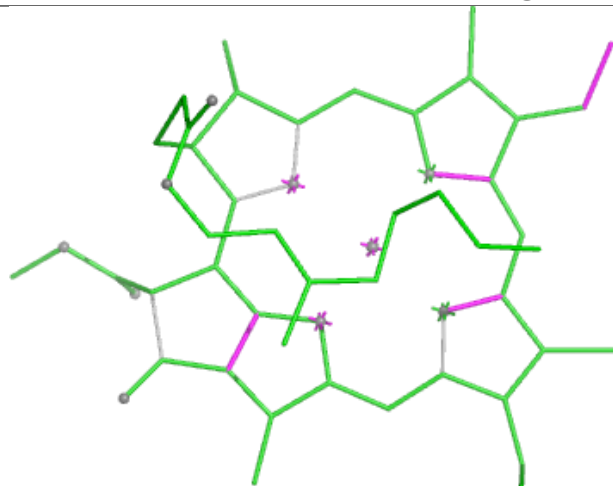


Rings

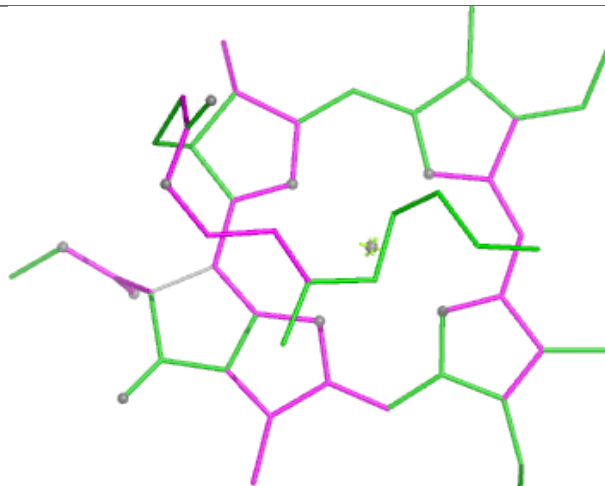




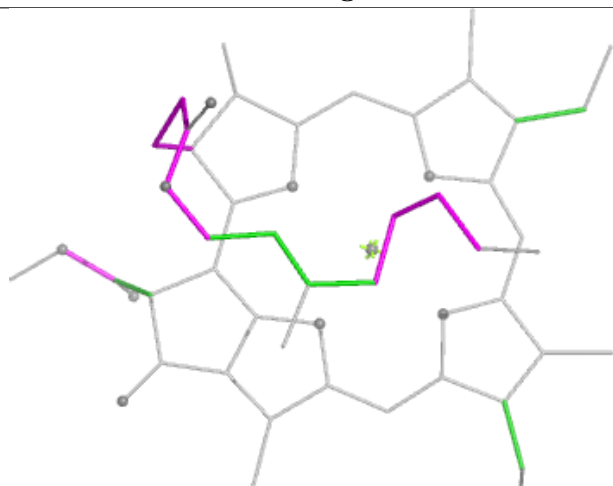
Ligand CLA 2 613



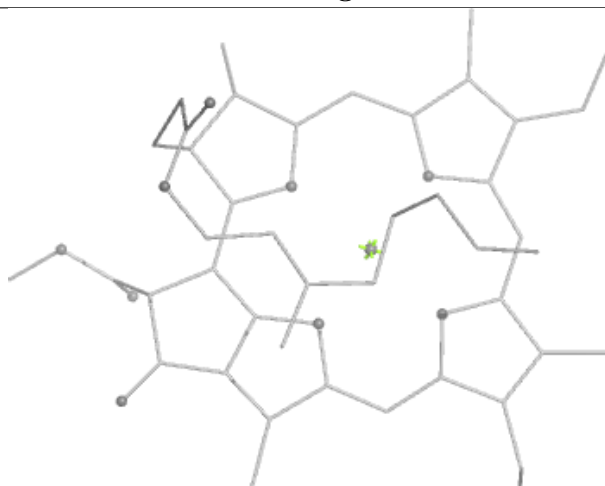
Bond lengths



Bond angles

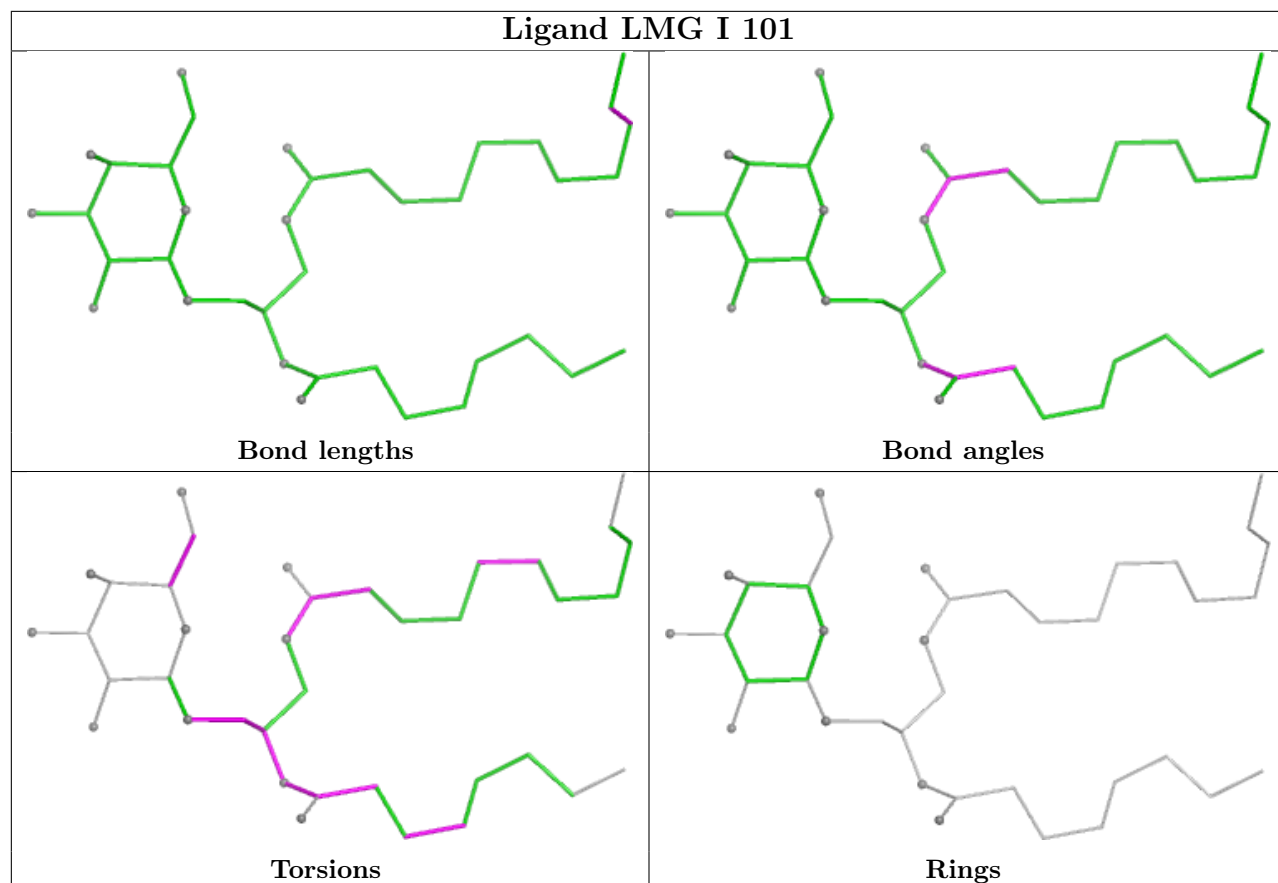


Torsions

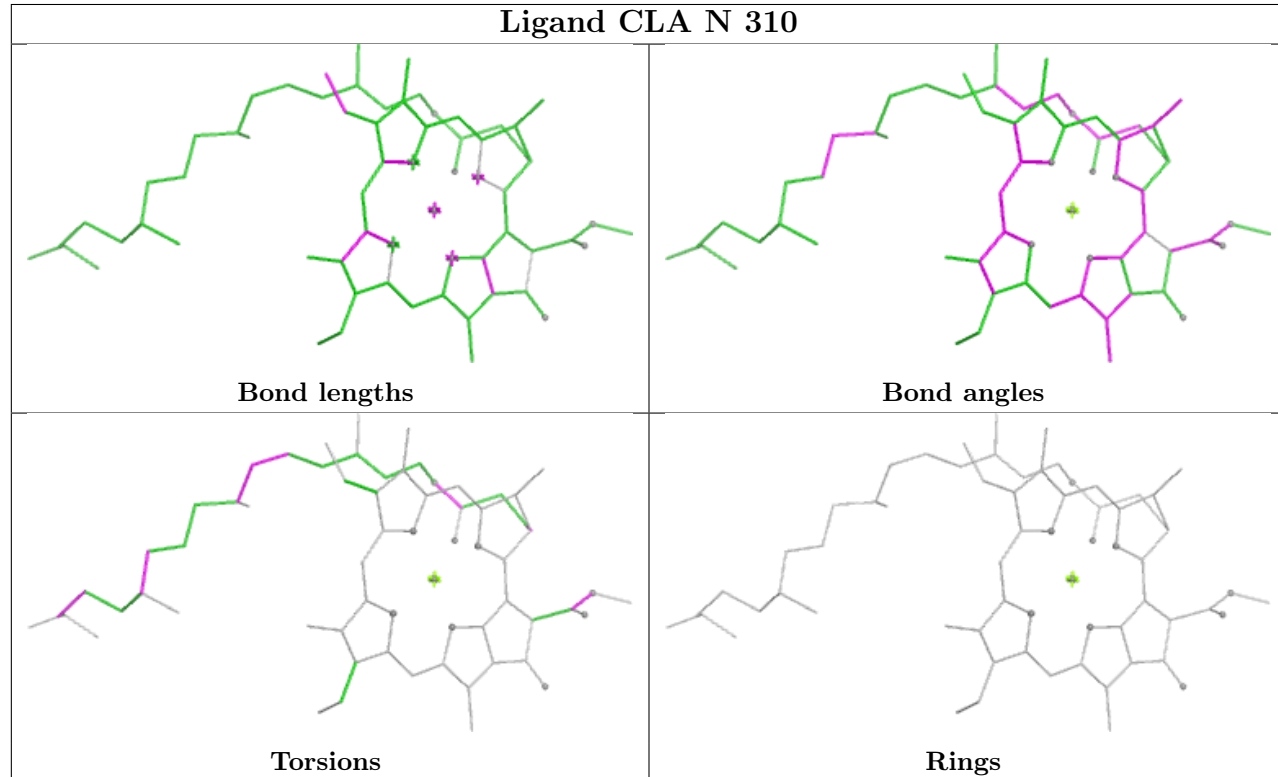


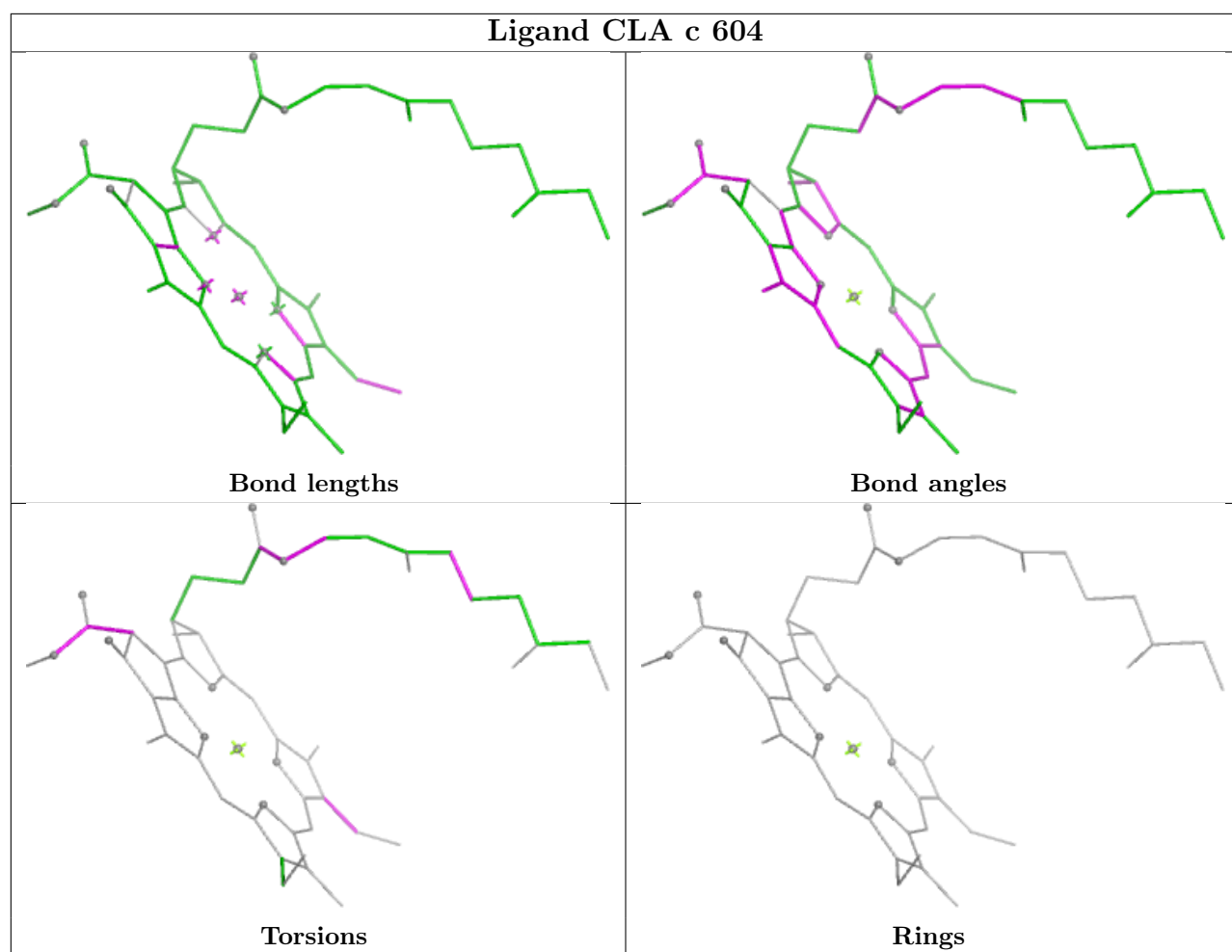
Rings

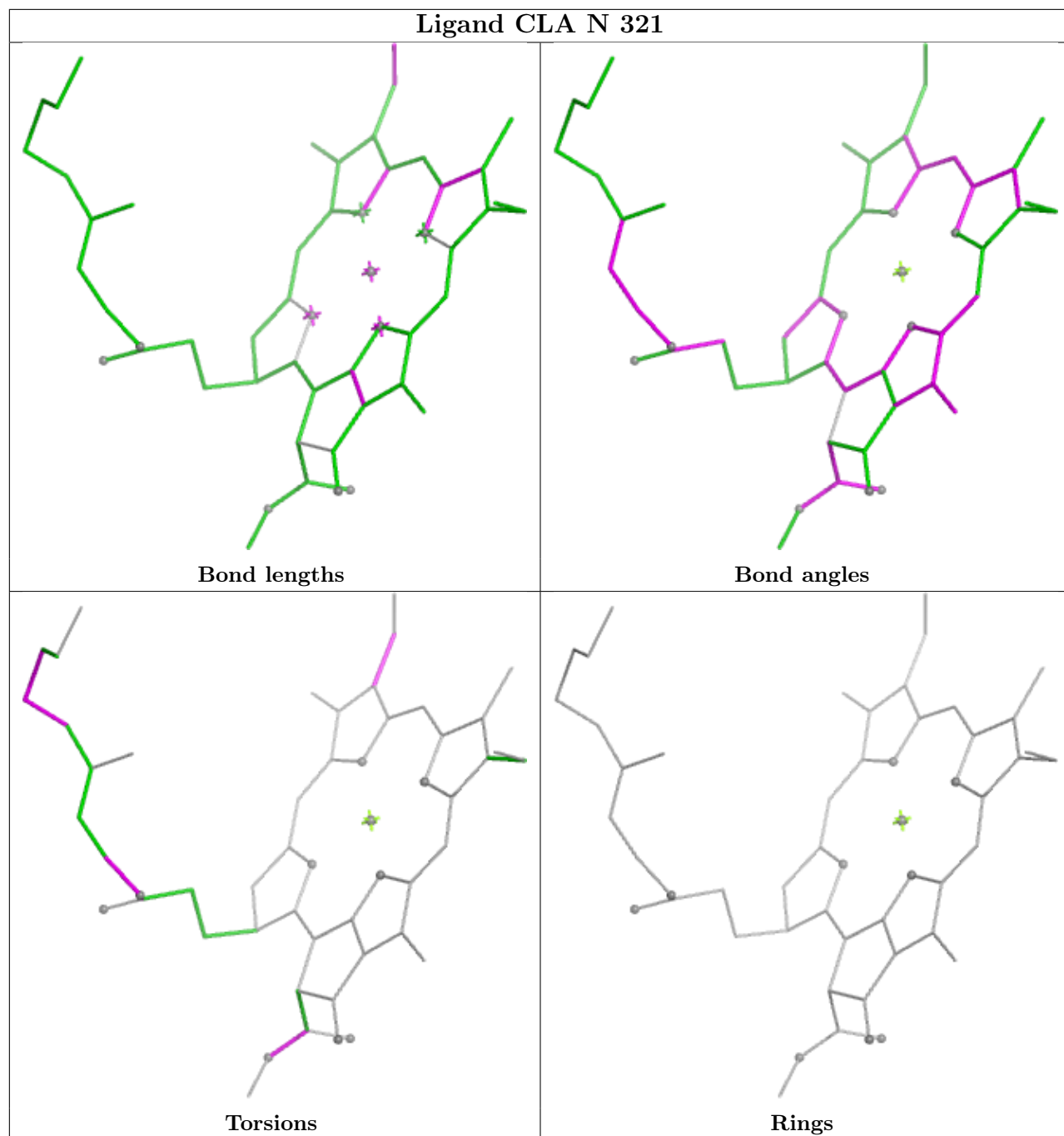
Ligand LMG I 101

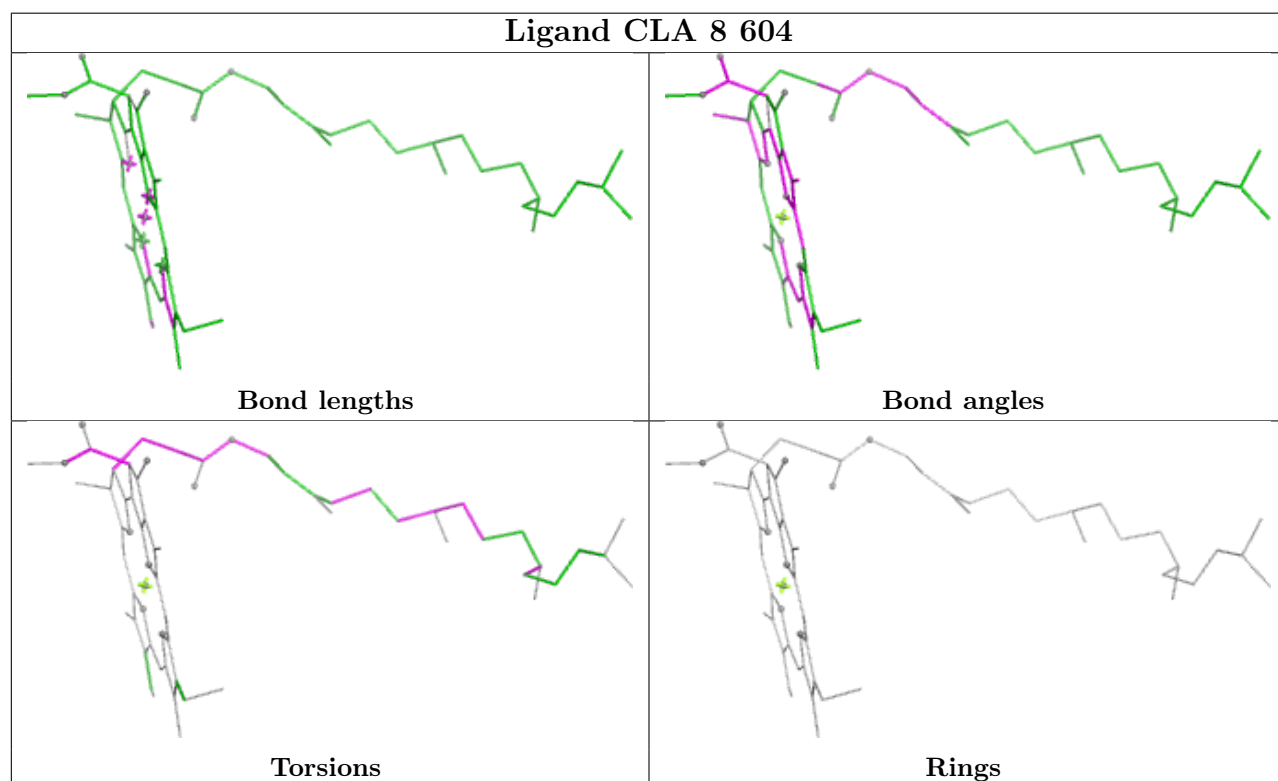
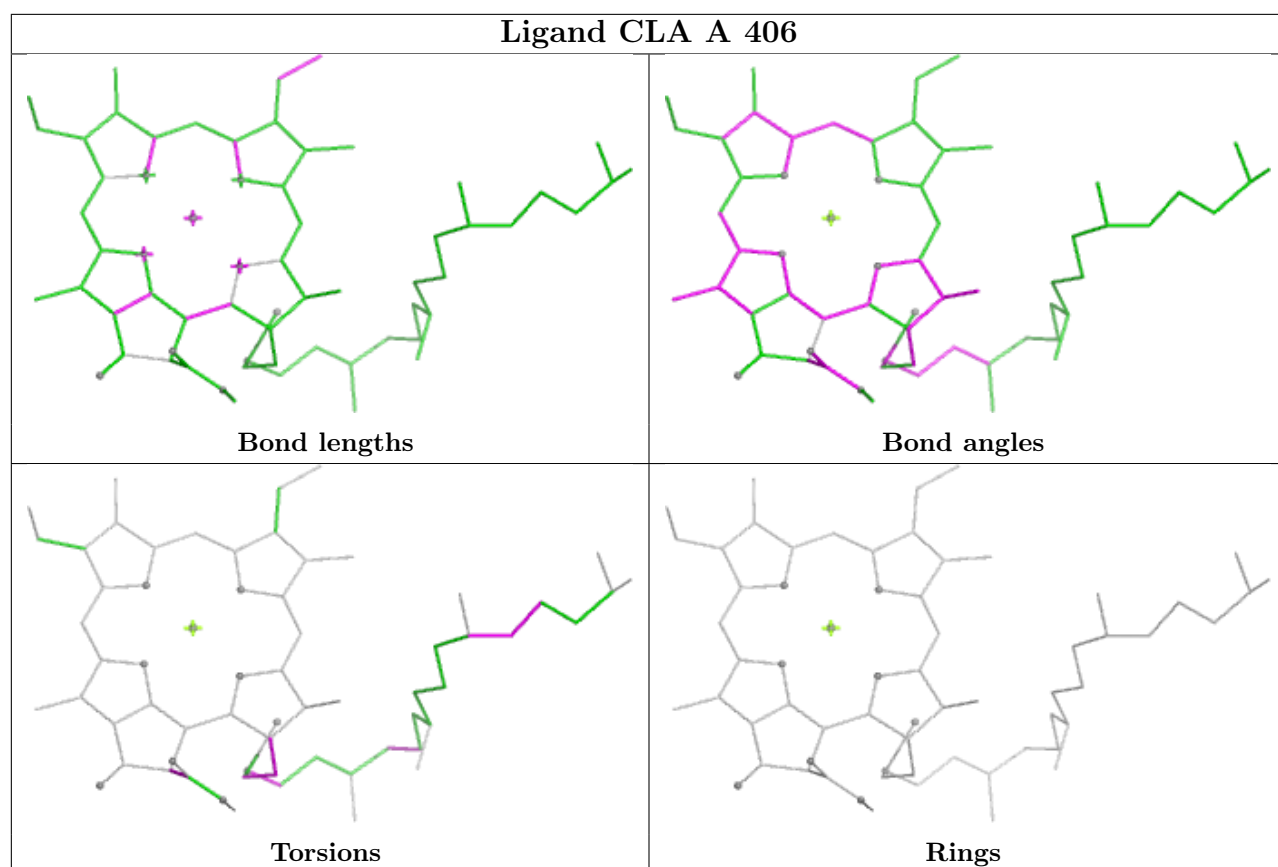


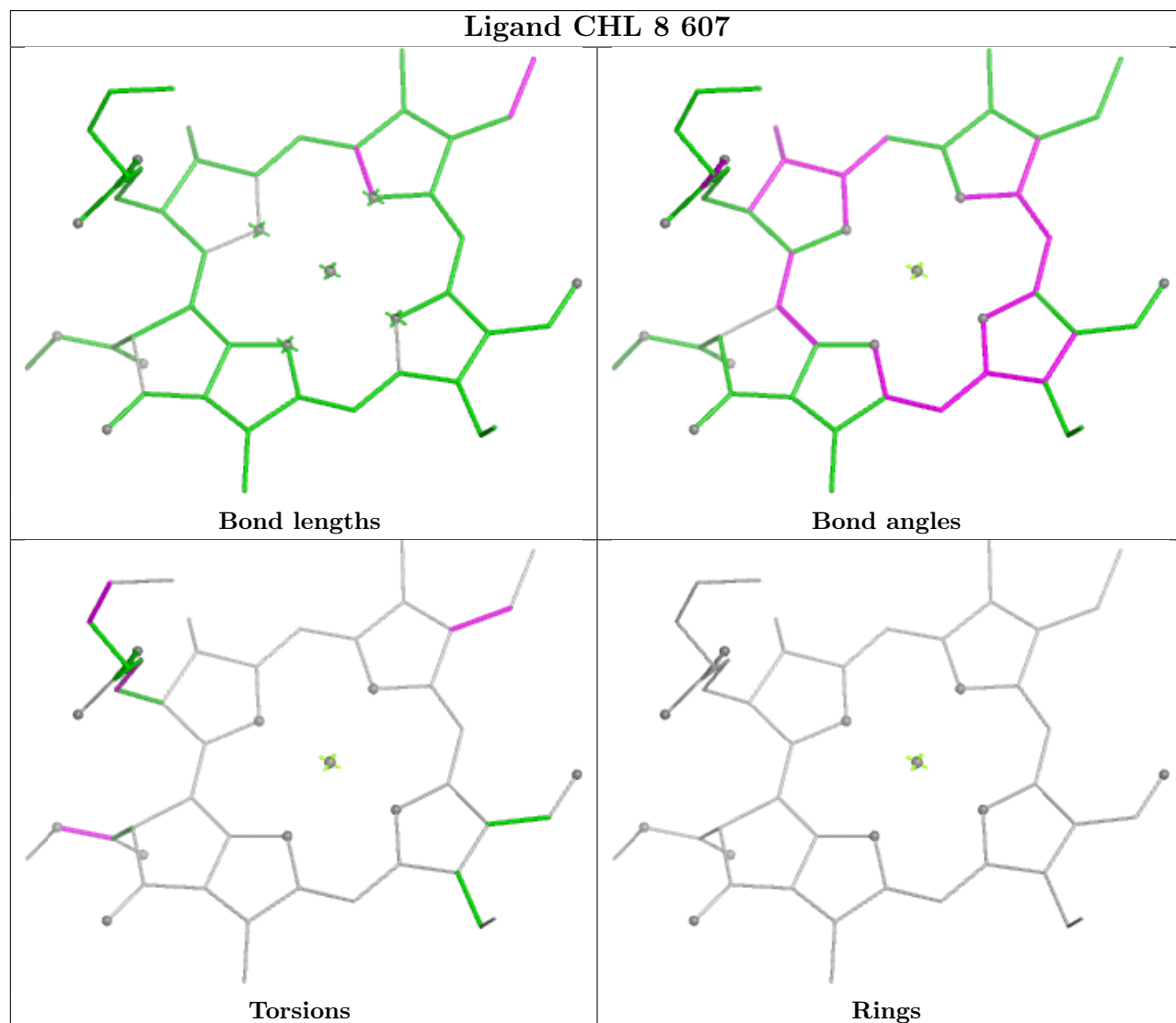
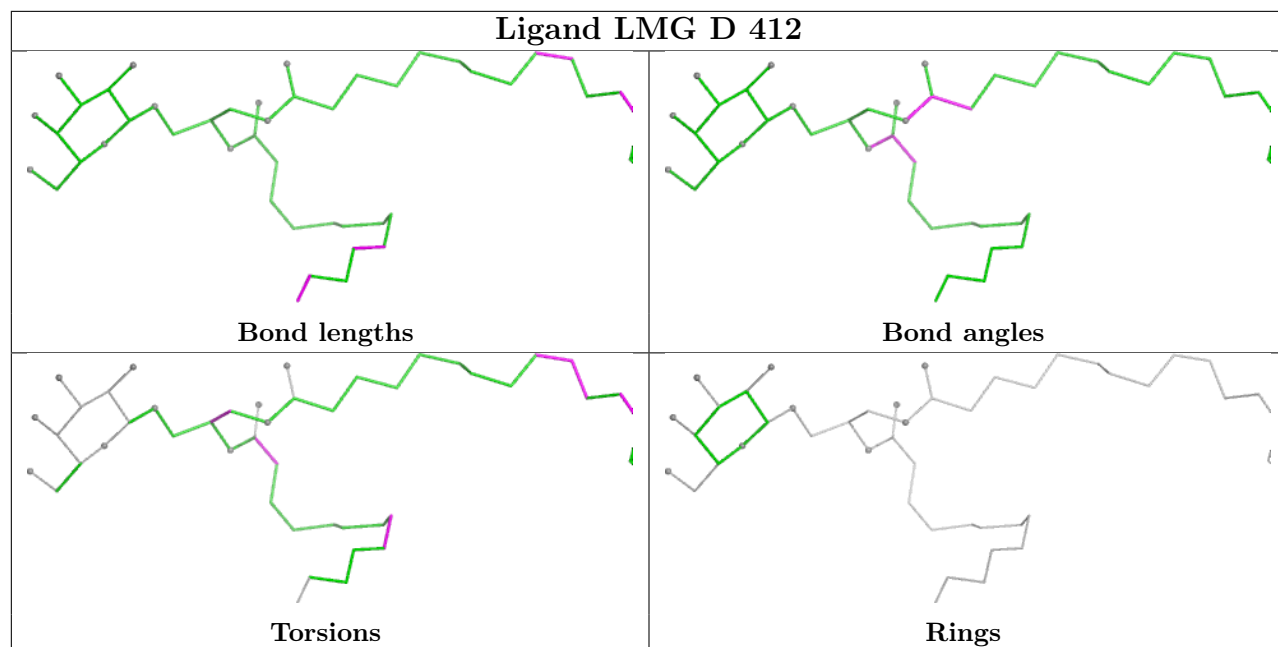
Ligand CLA N 310

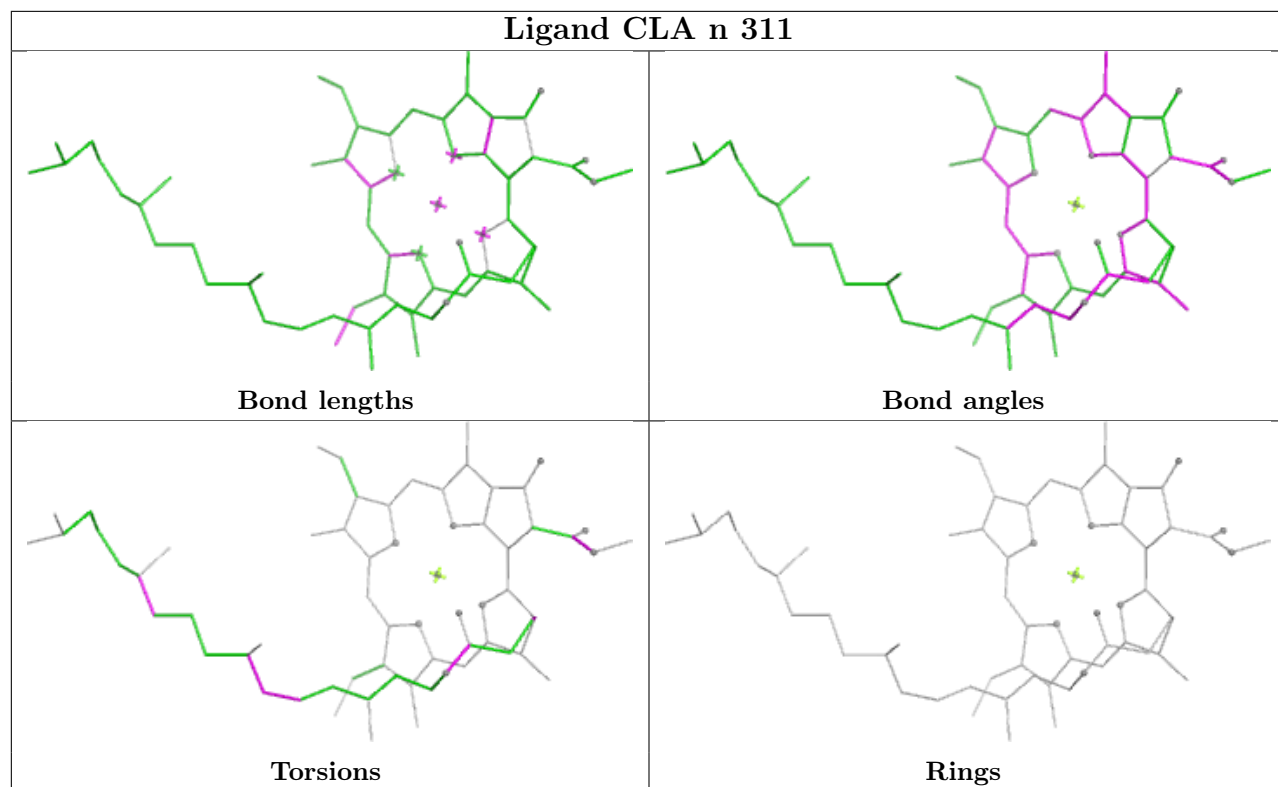




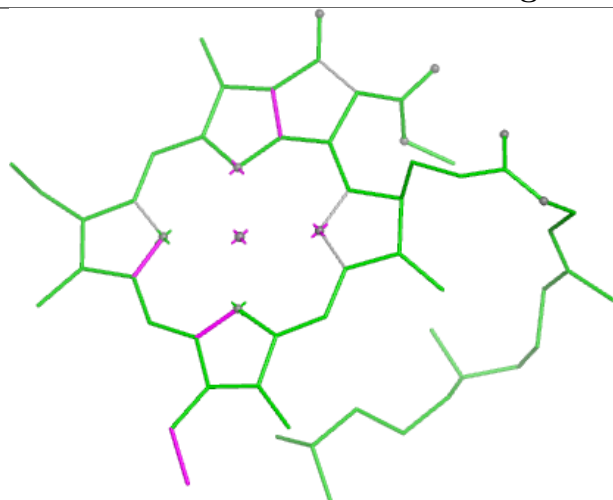




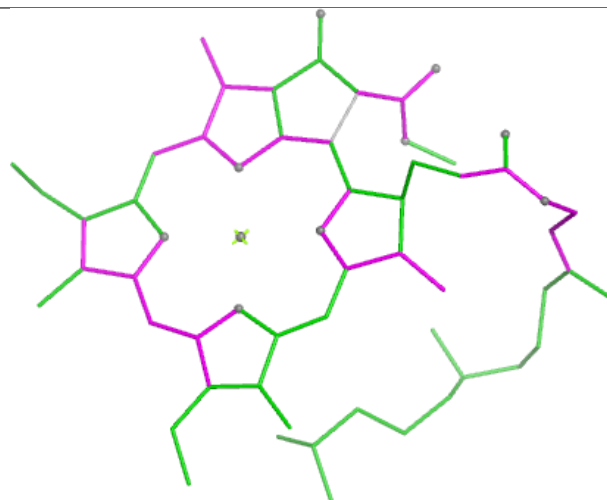




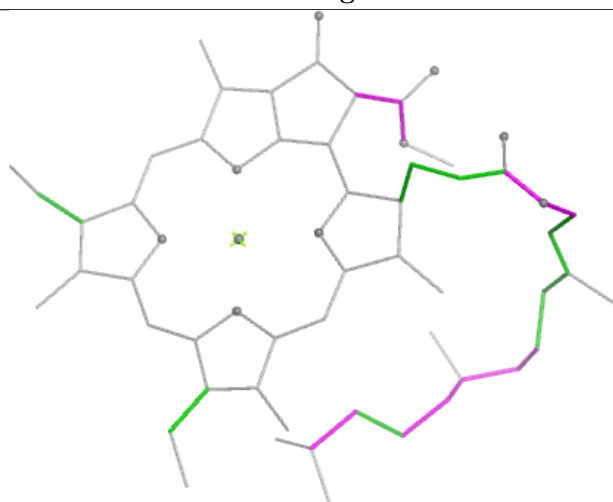
Ligand CLA r 305



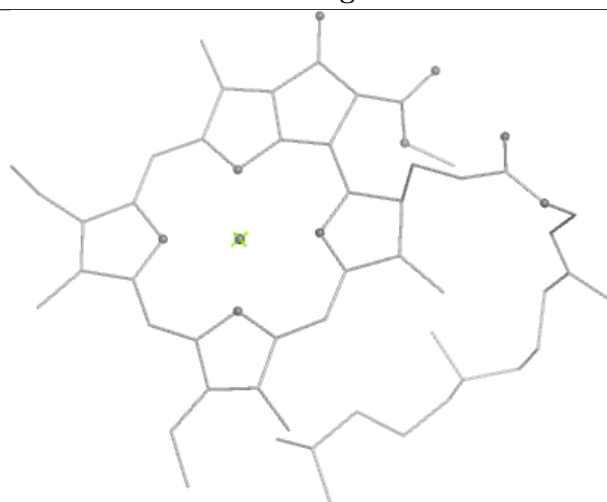
Bond lengths



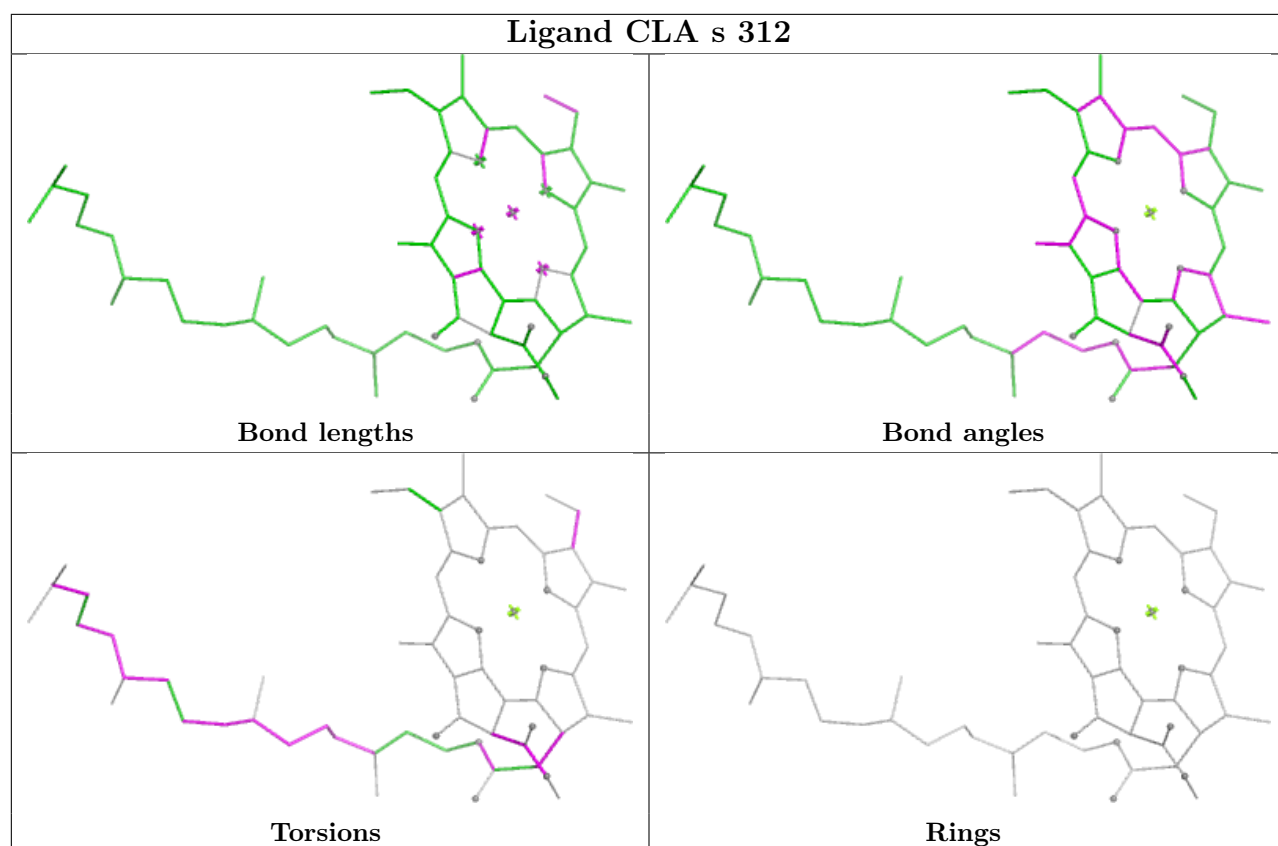
Bond angles

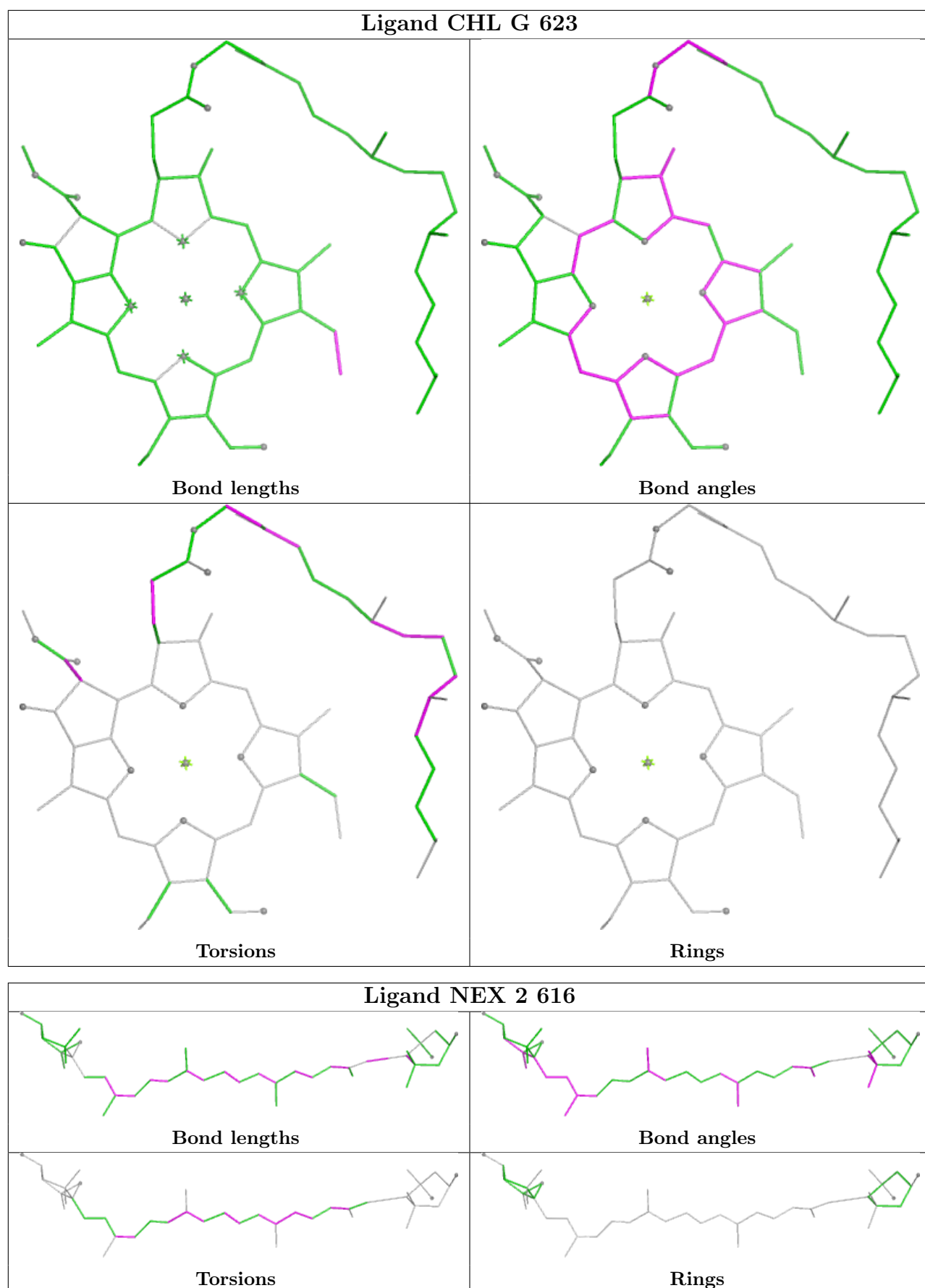


Torsions

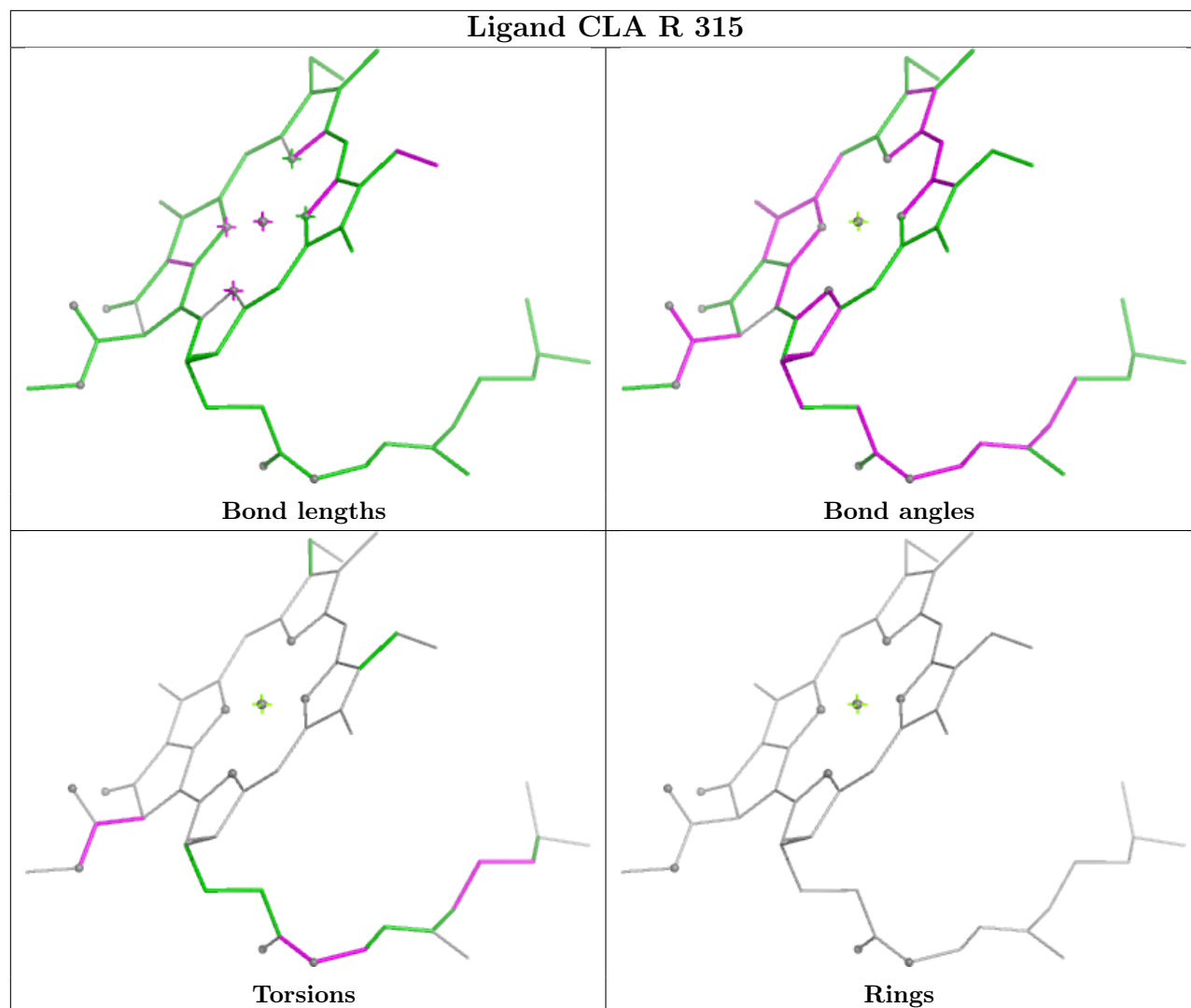


Rings

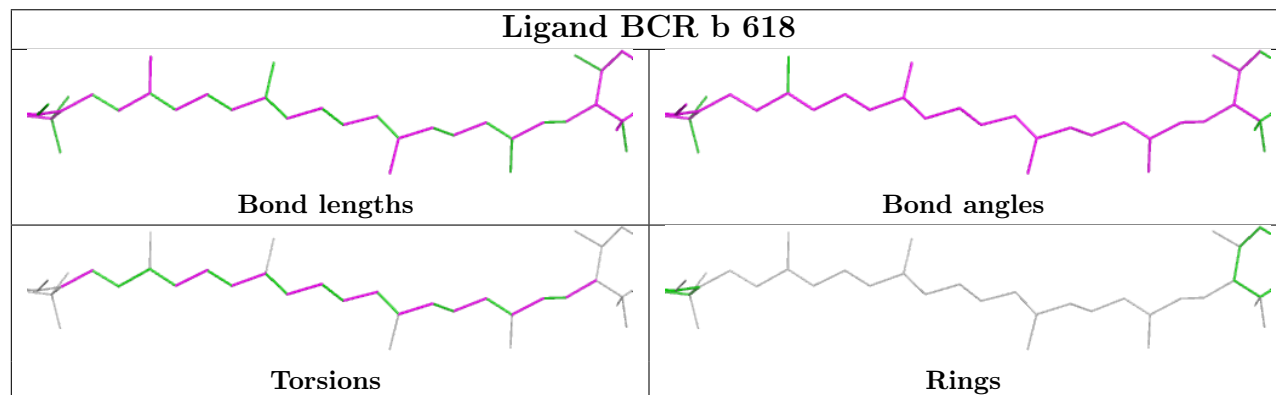


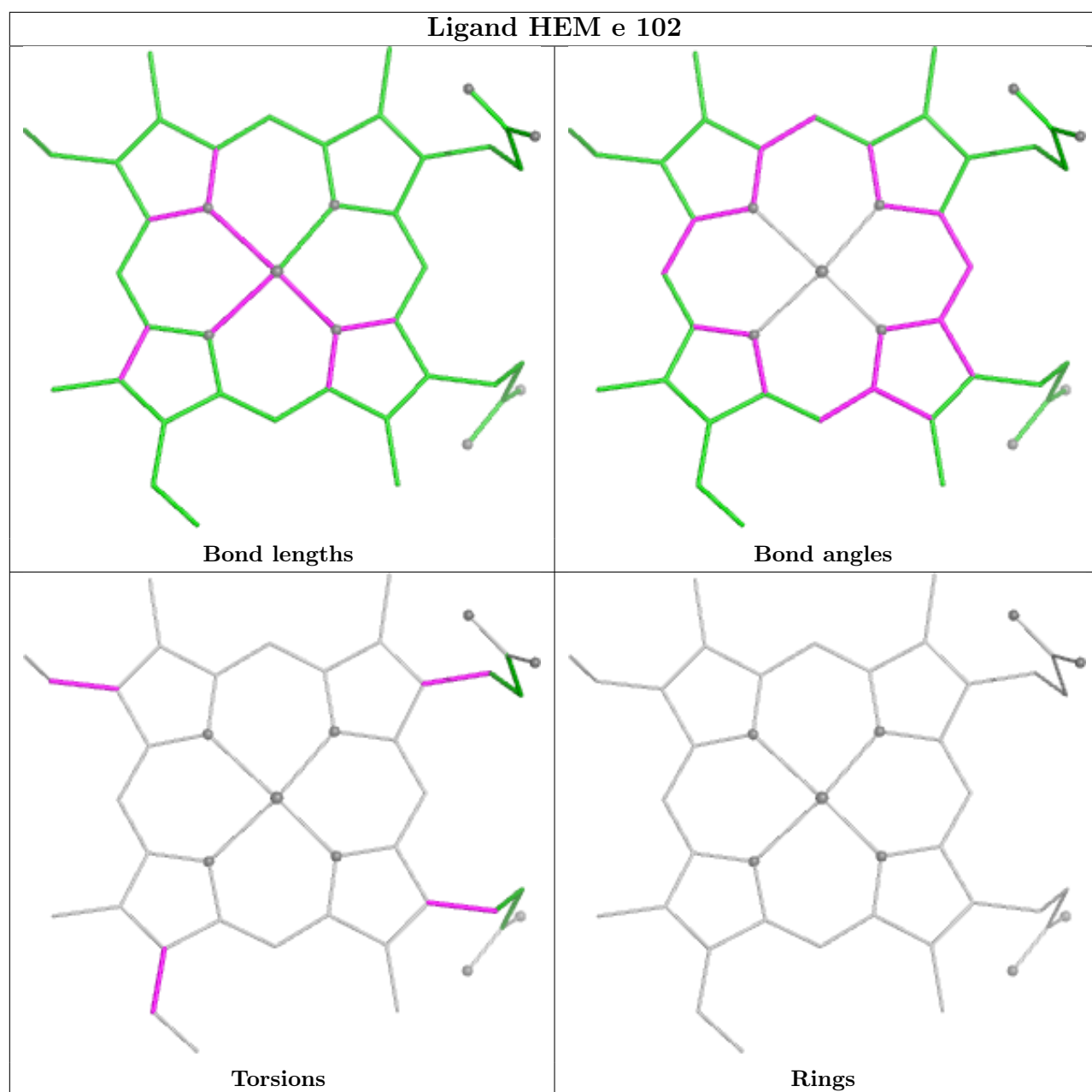


Ligand CLA R 315

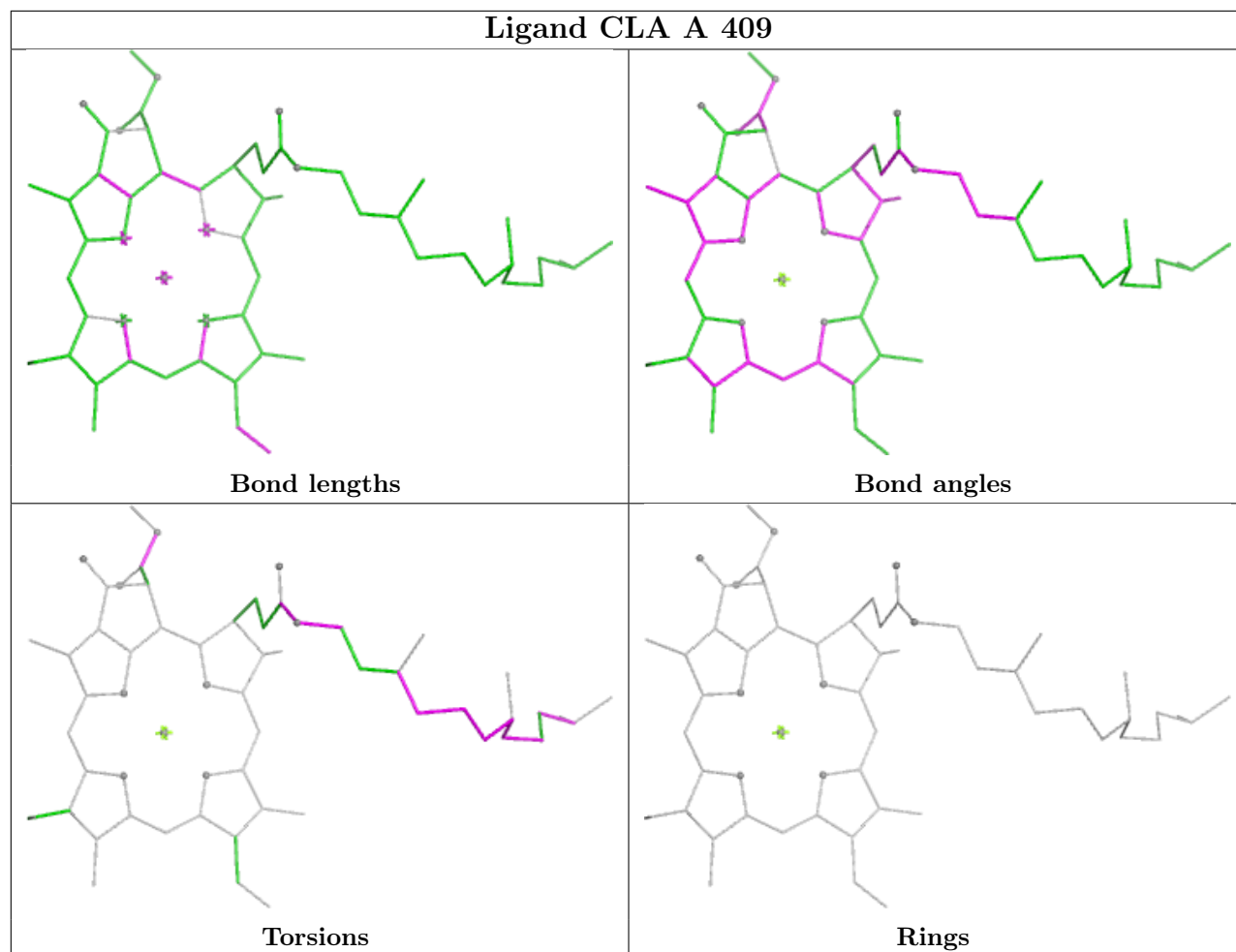


Ligand BCR b 618

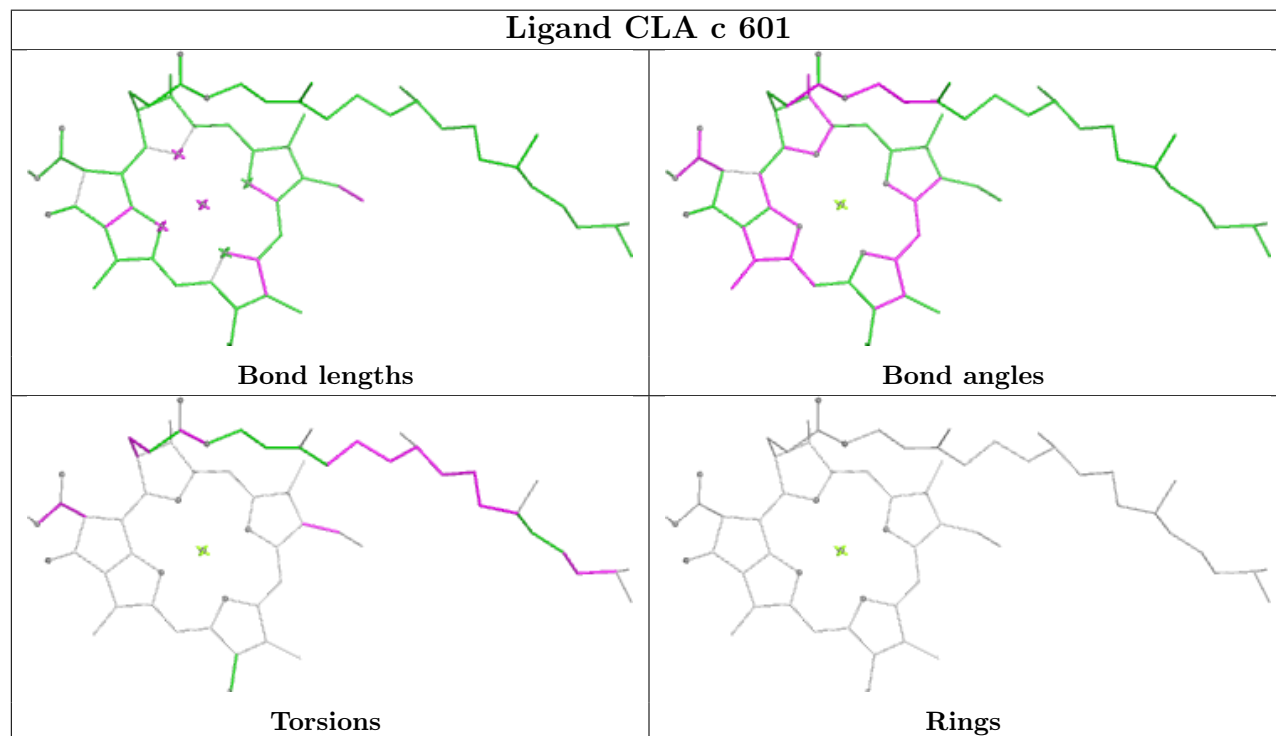


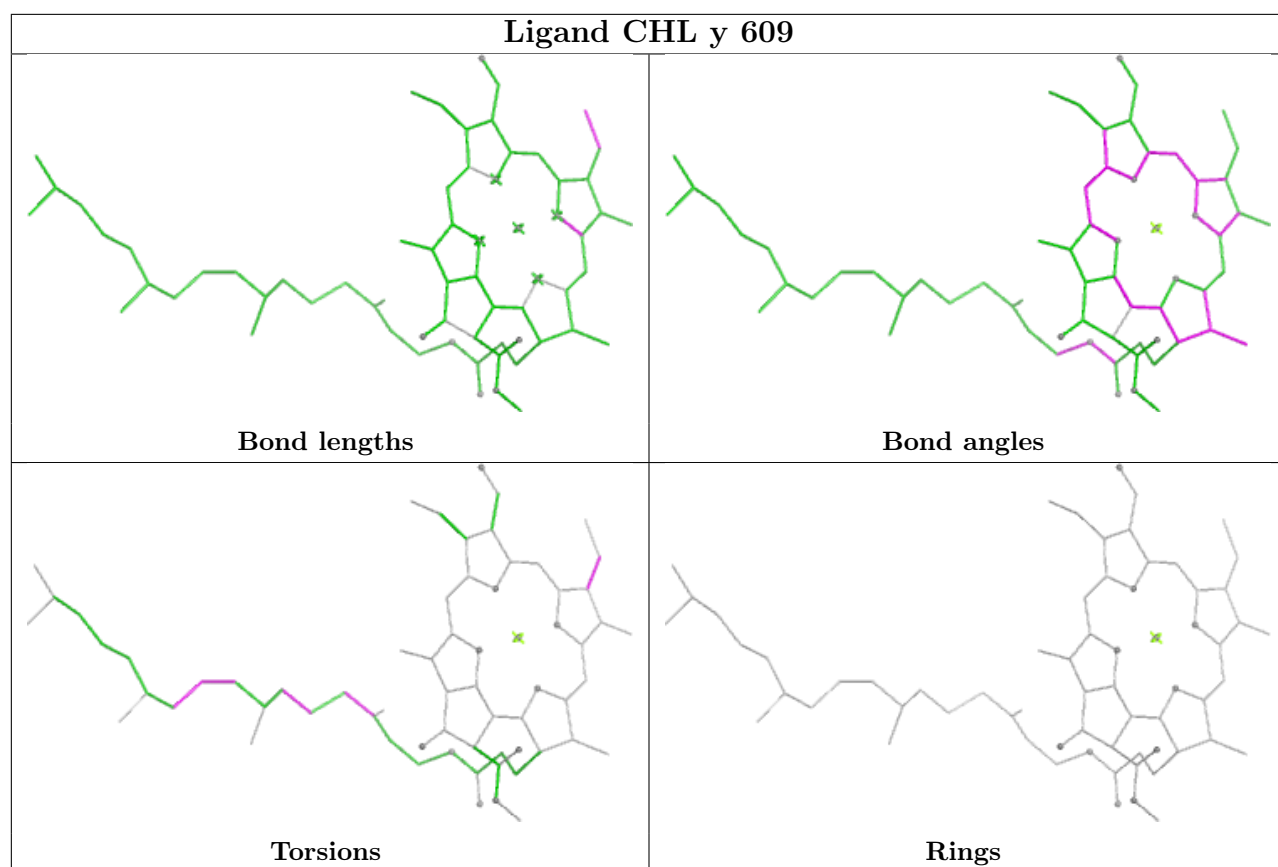


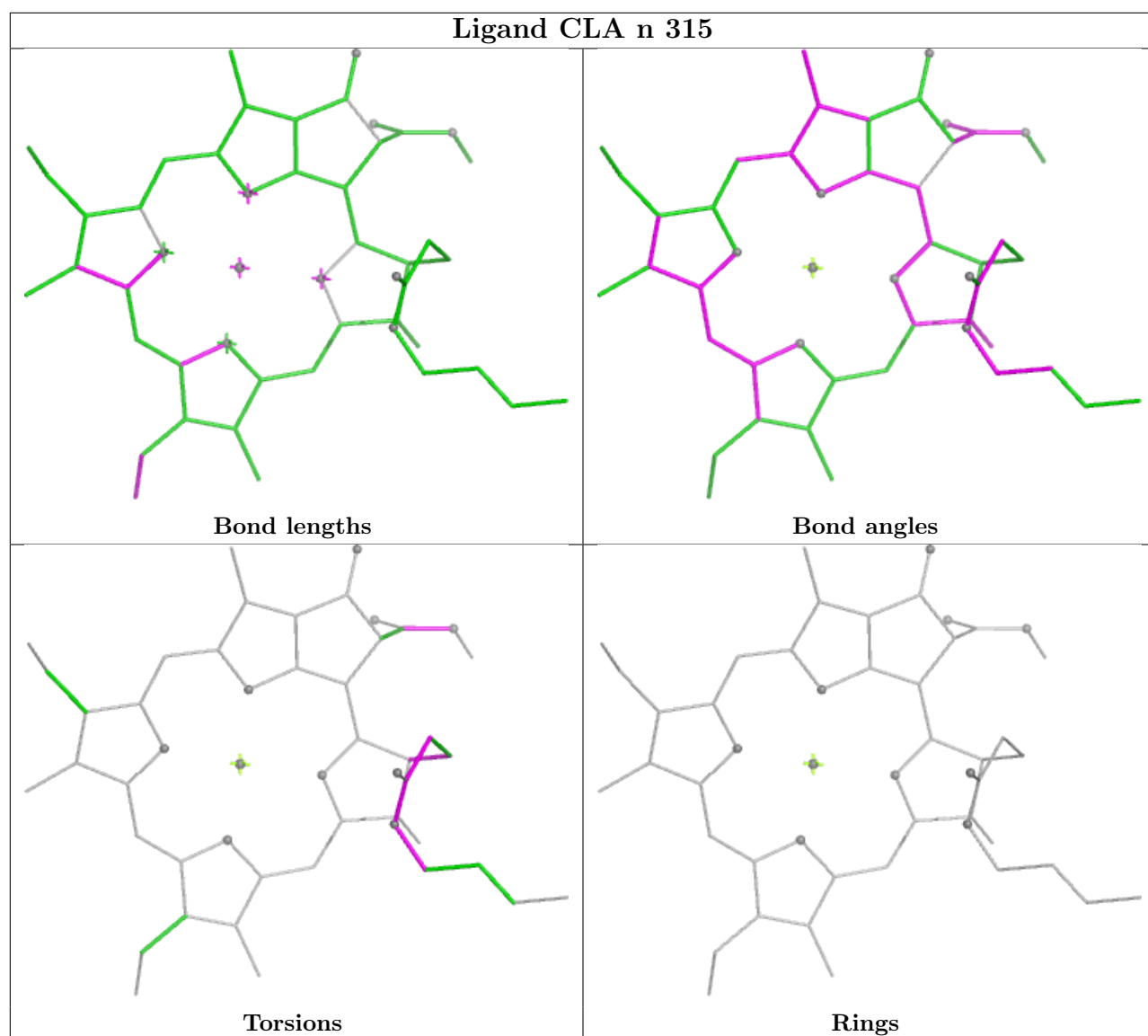
Ligand CLA A 409

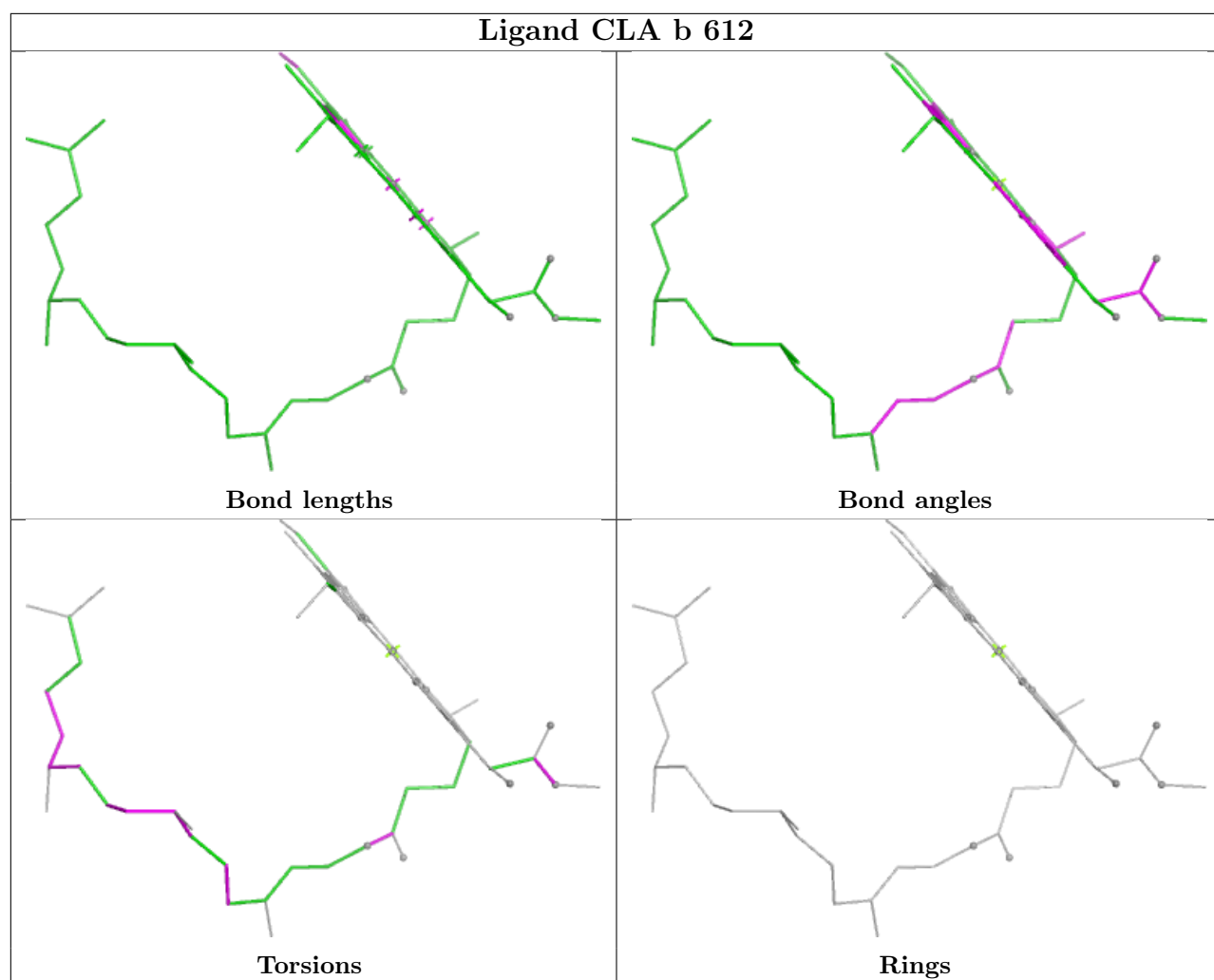


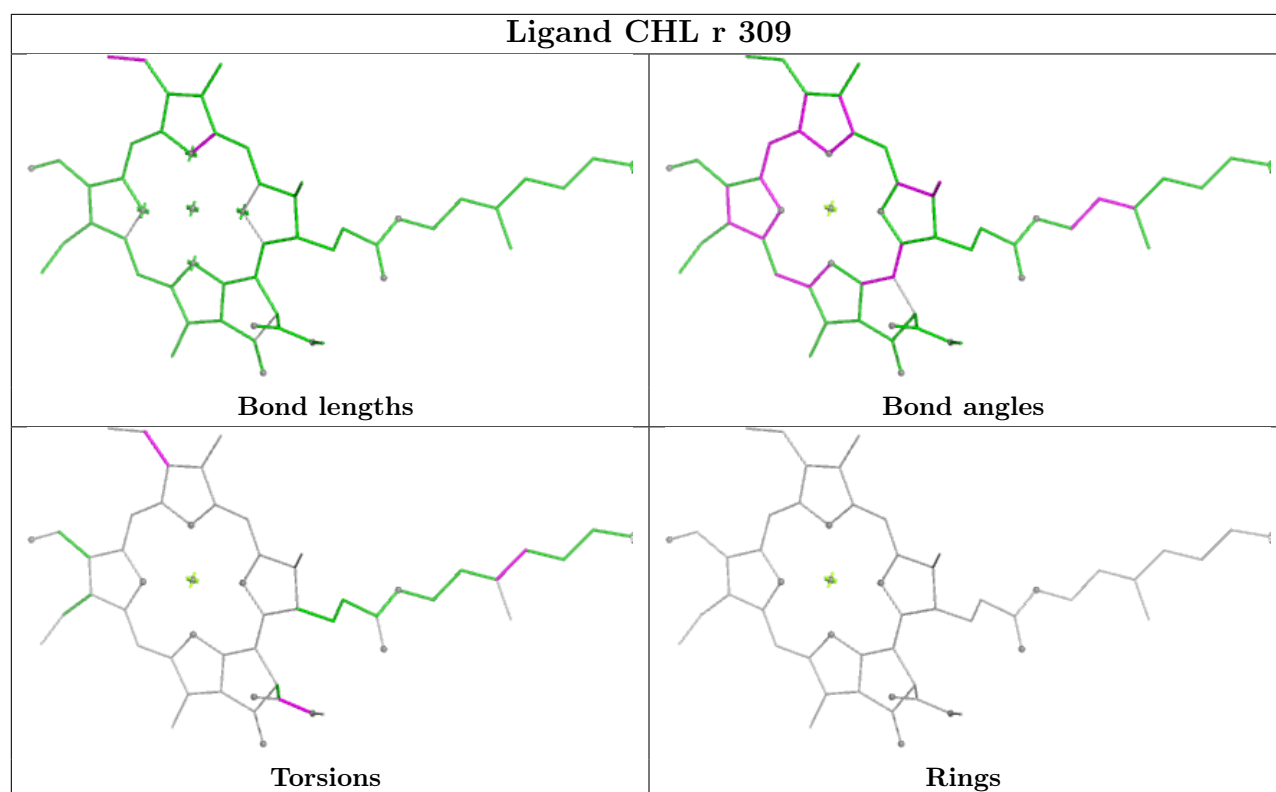
Ligand CLA c 601

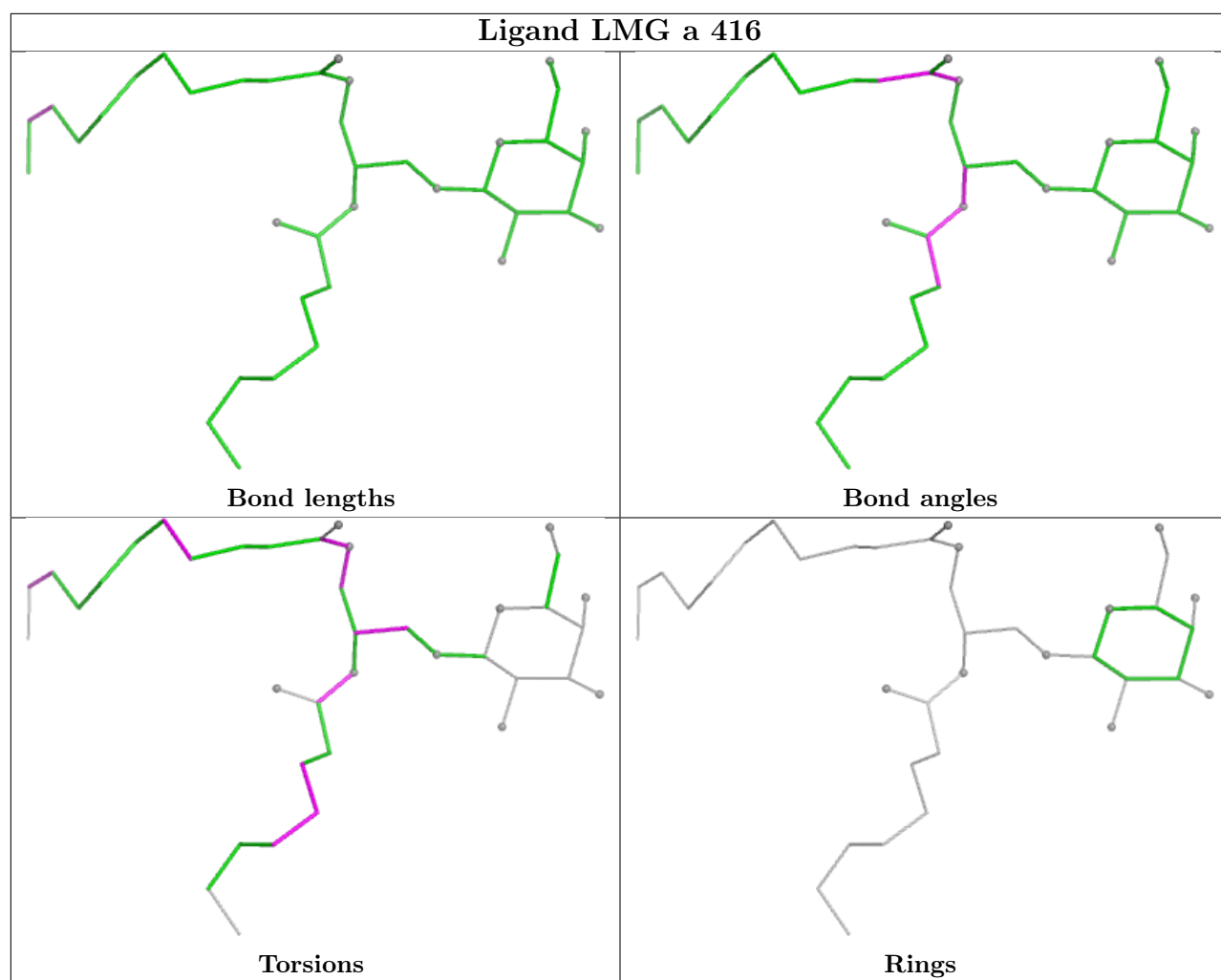




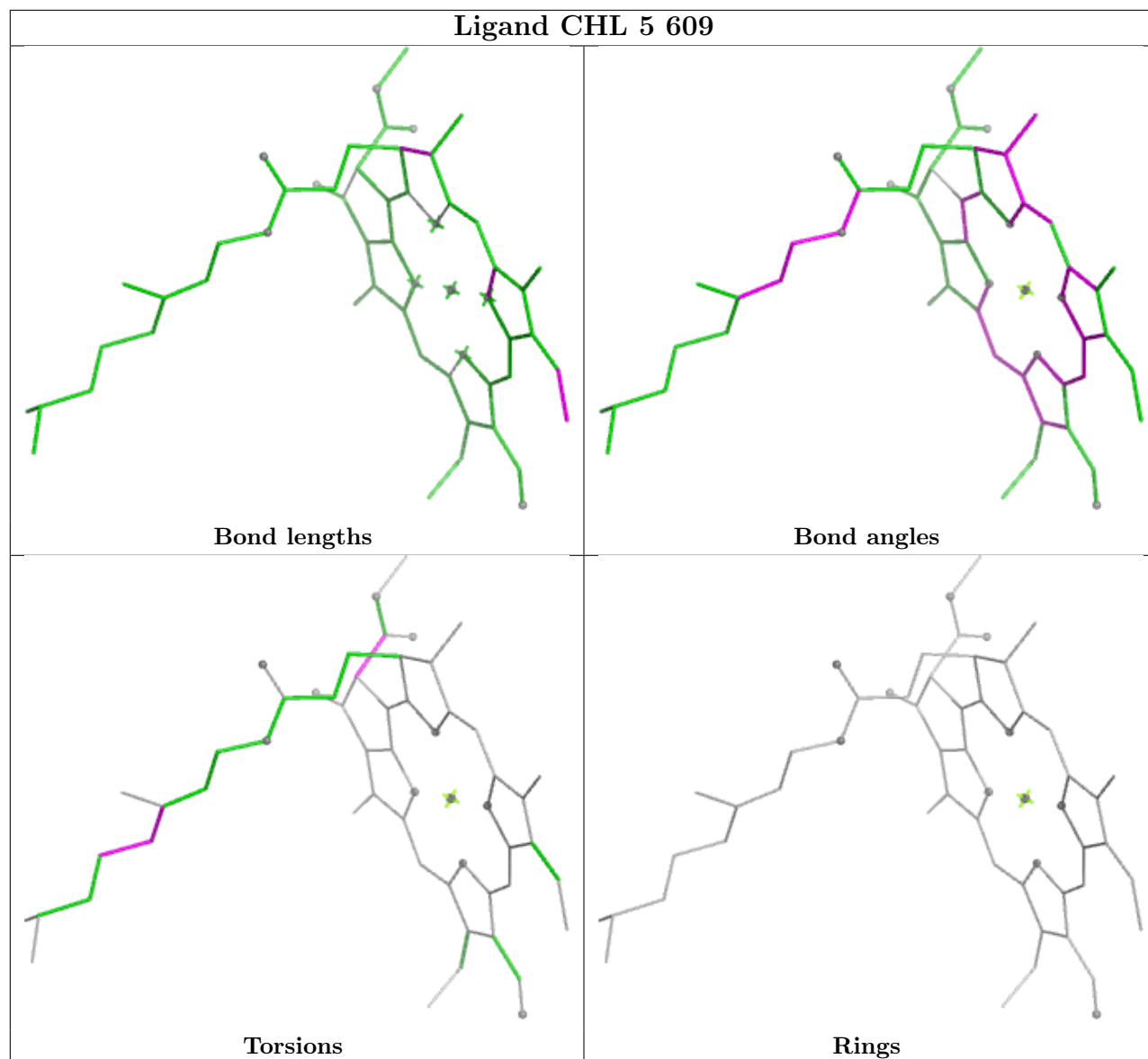




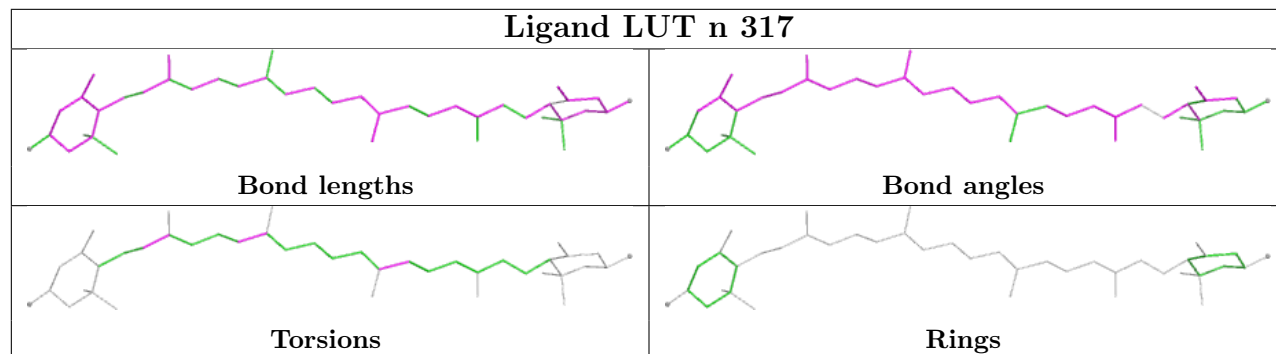


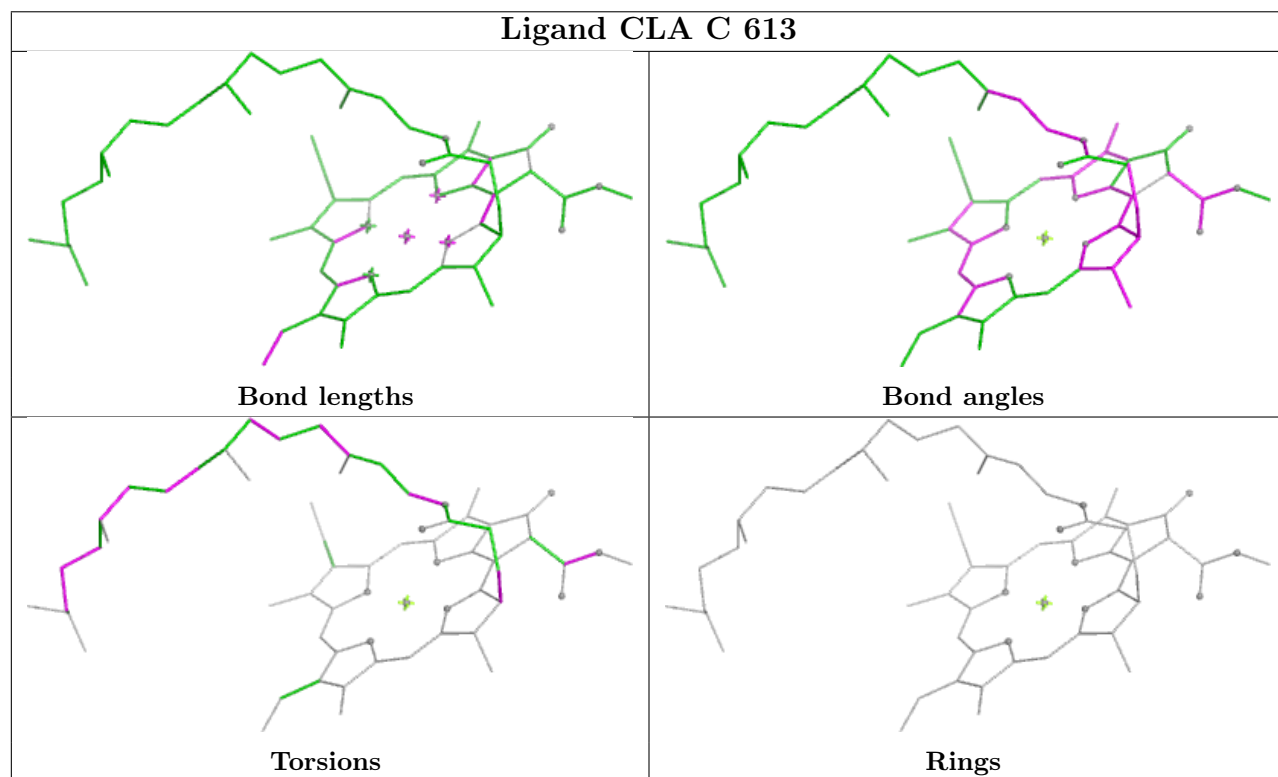
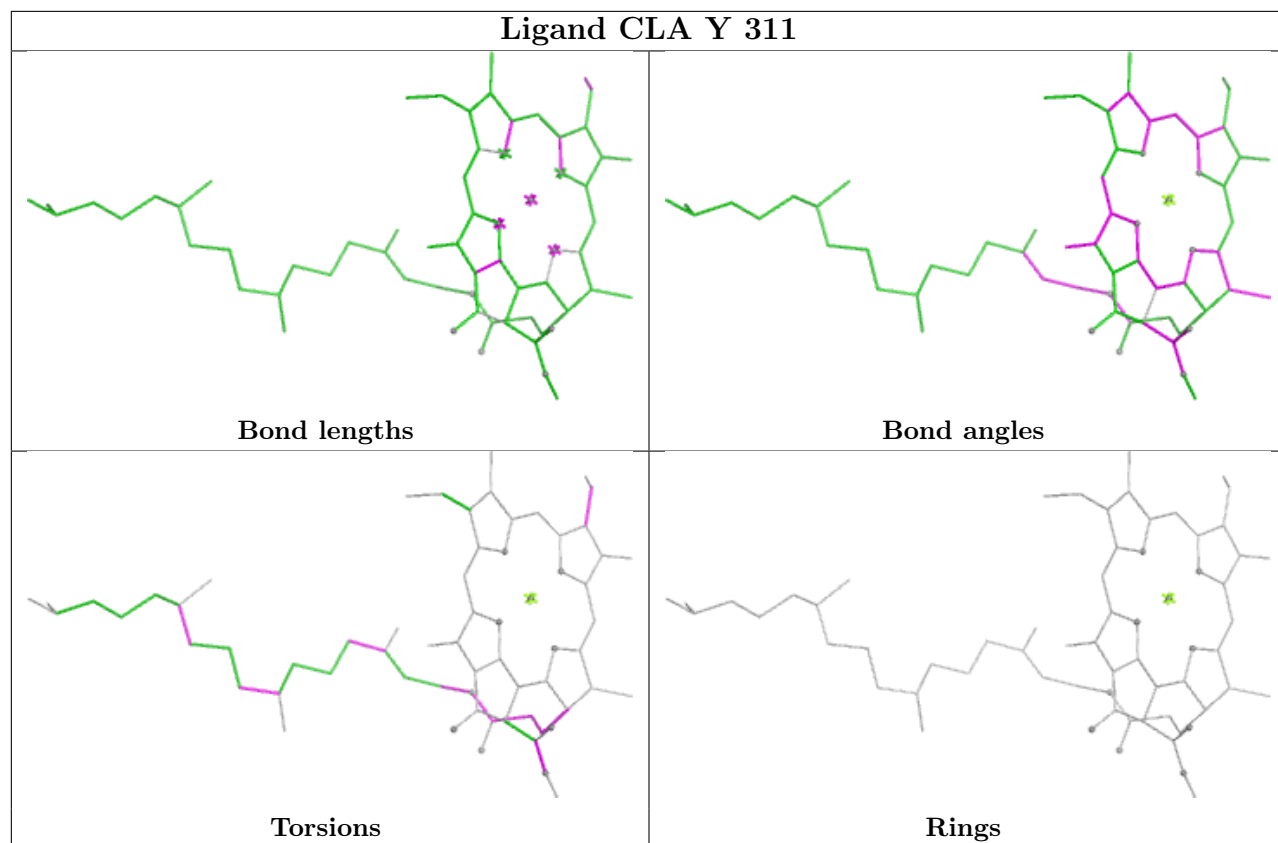


Ligand CHL 5 609

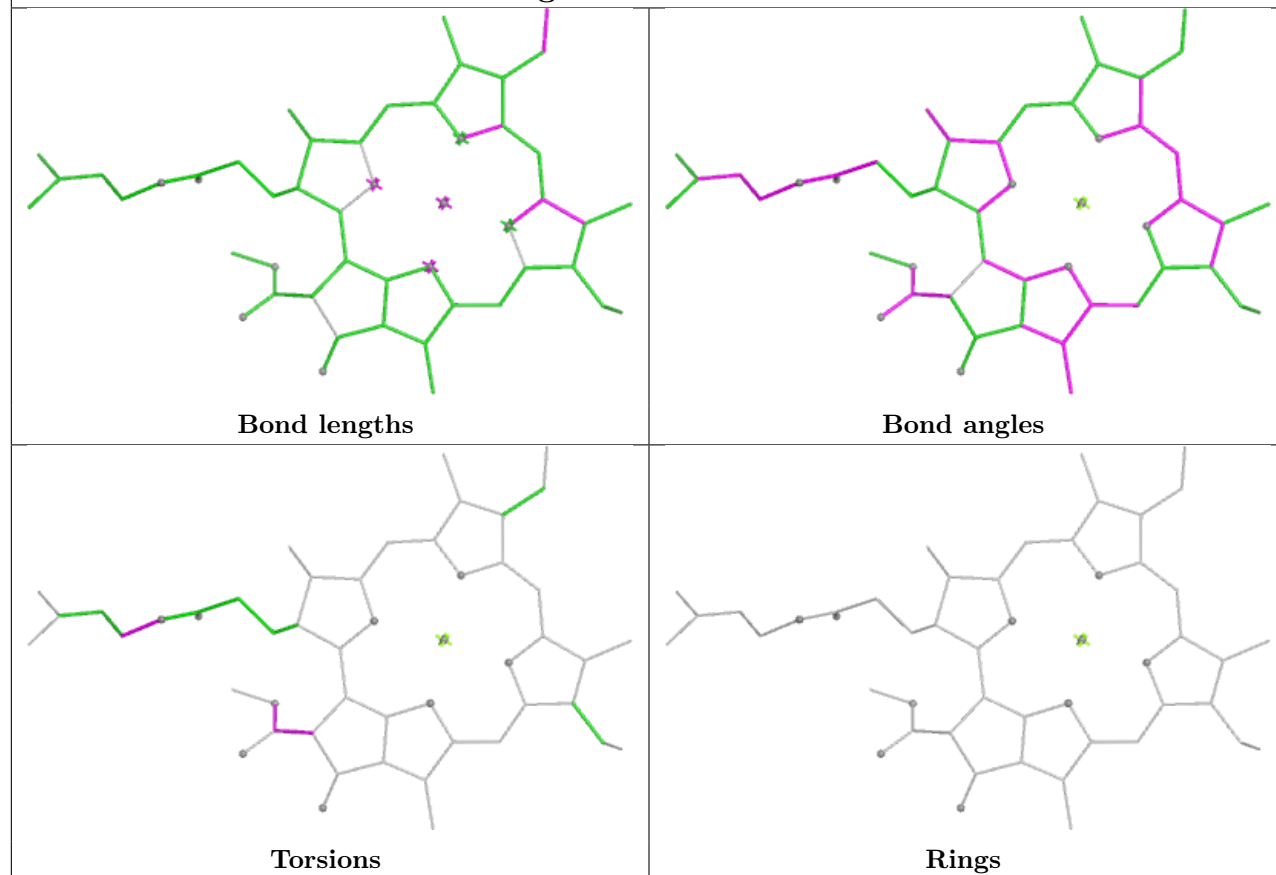


Ligand LUT n 317

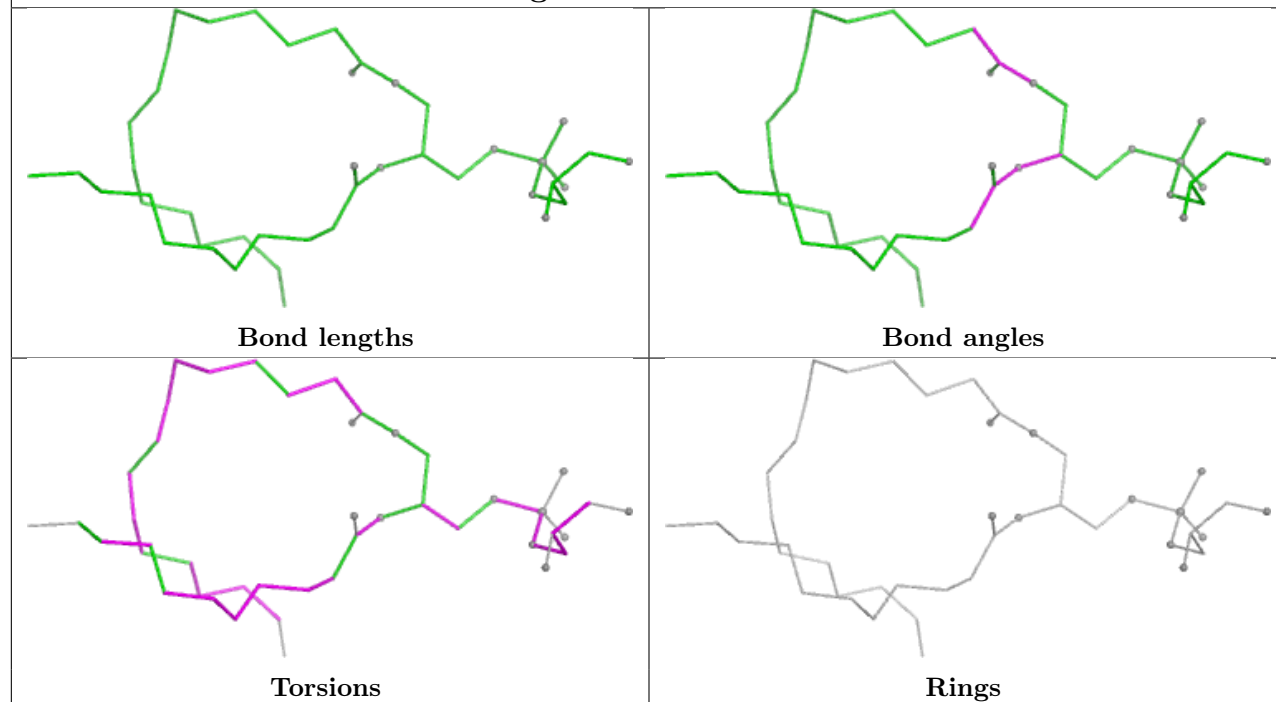


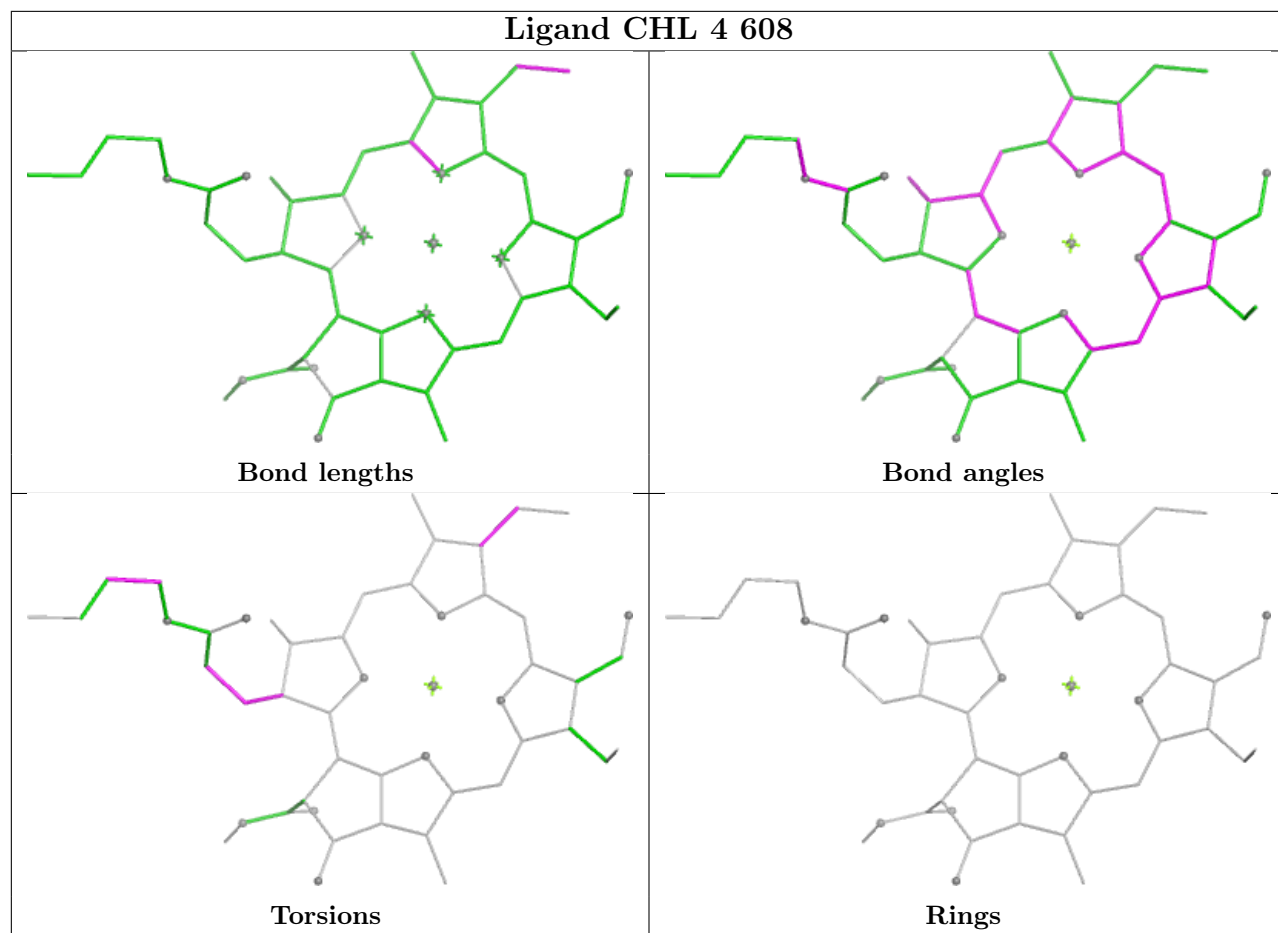


Ligand CLA s 306

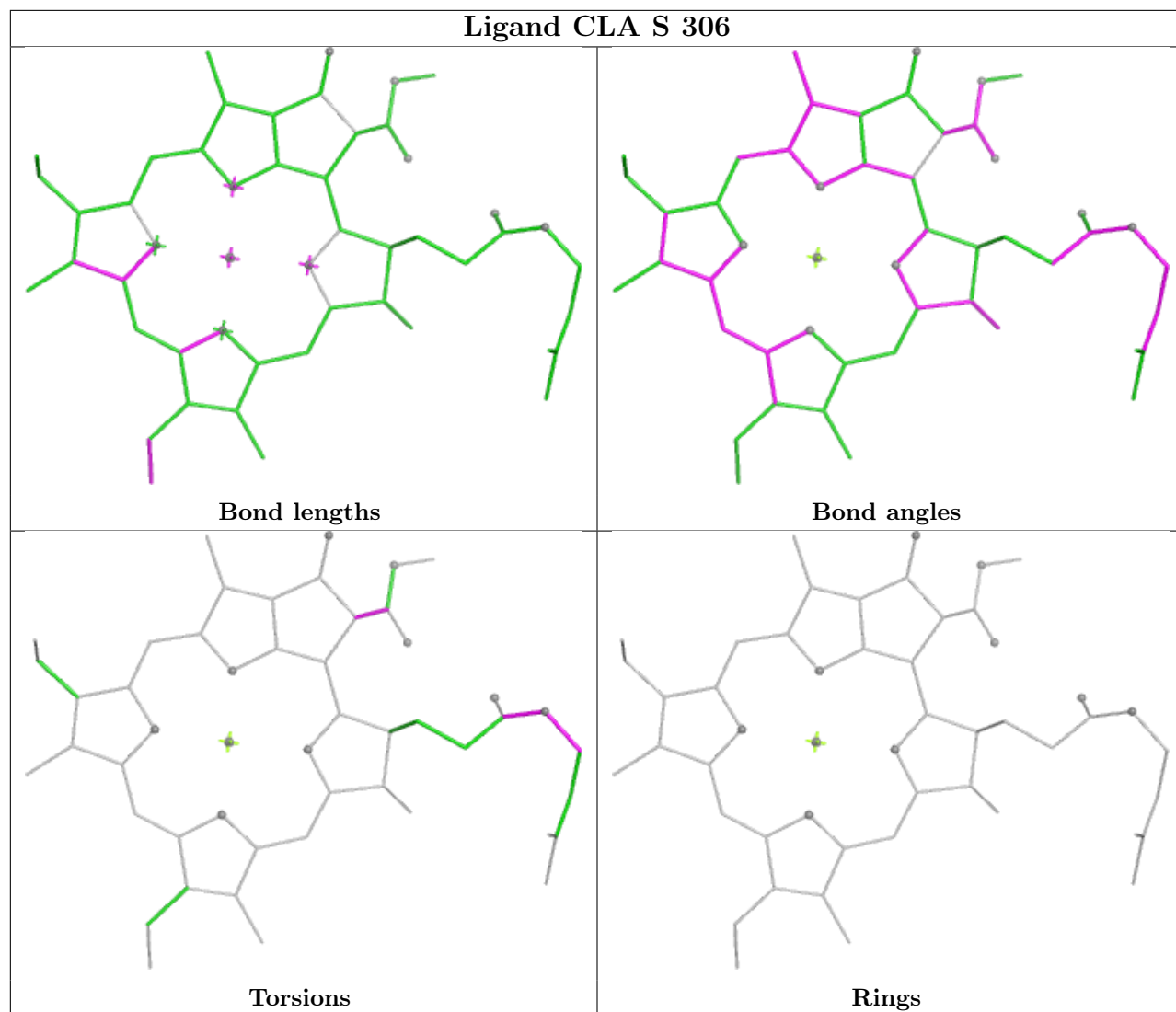


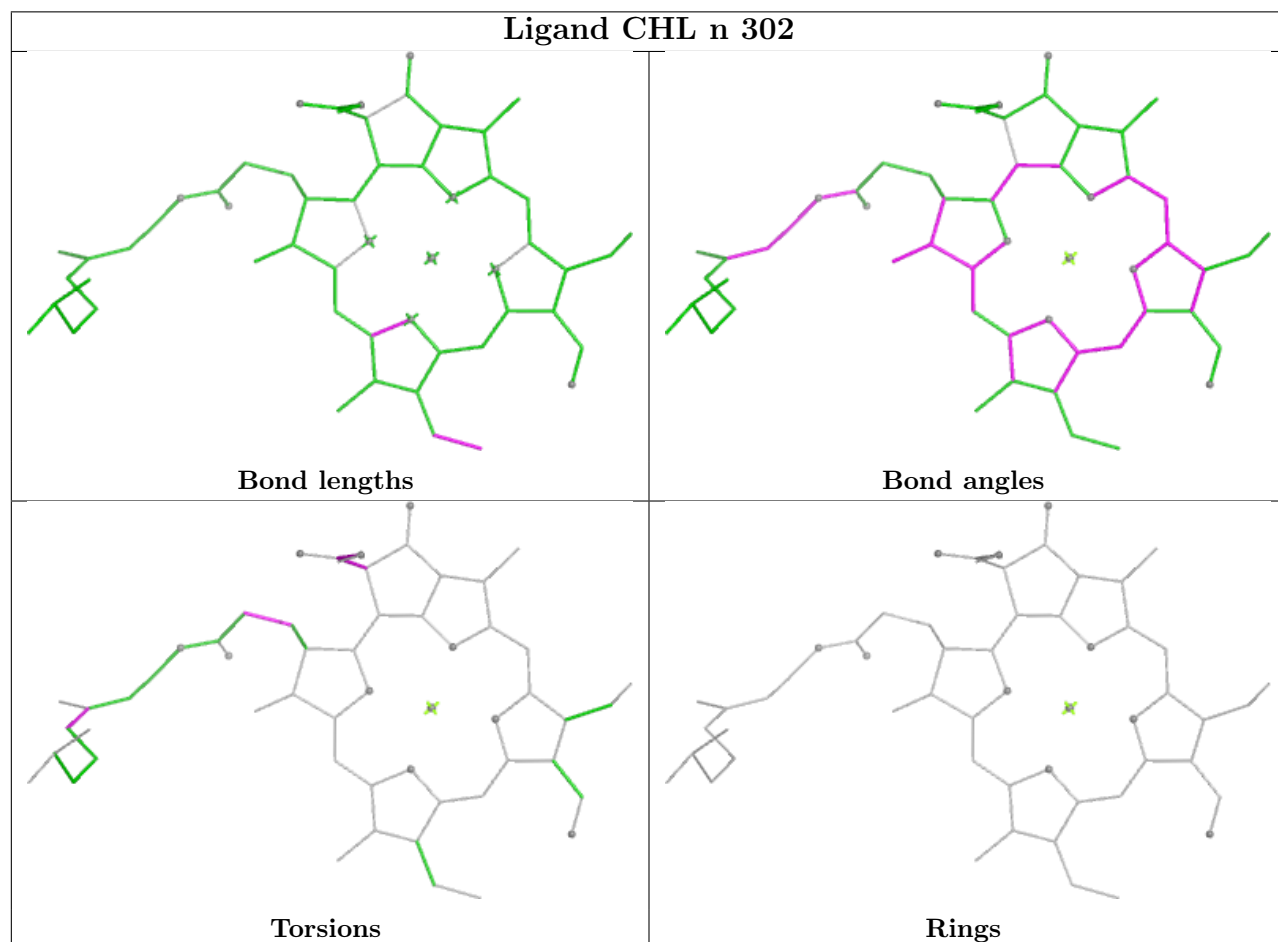
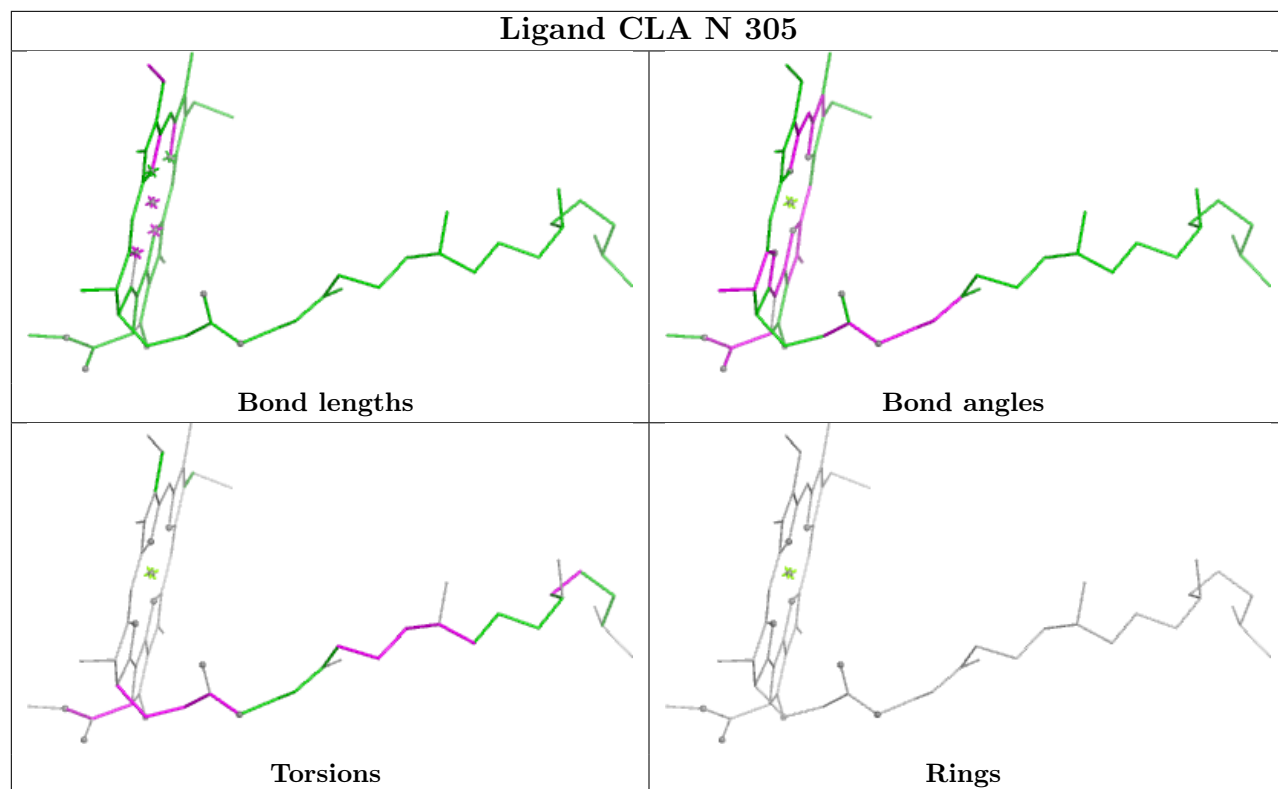
Ligand LHG D 407





Ligand CLA S 306

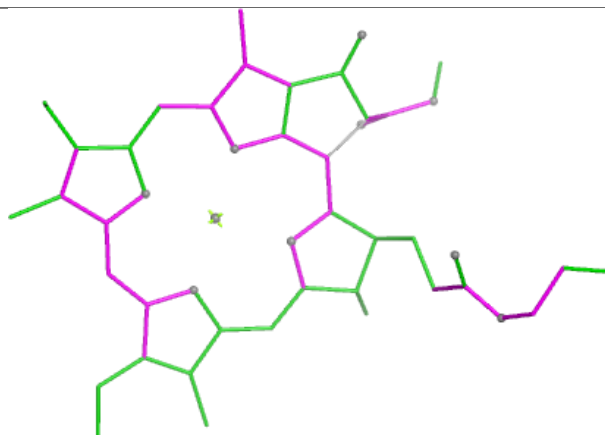




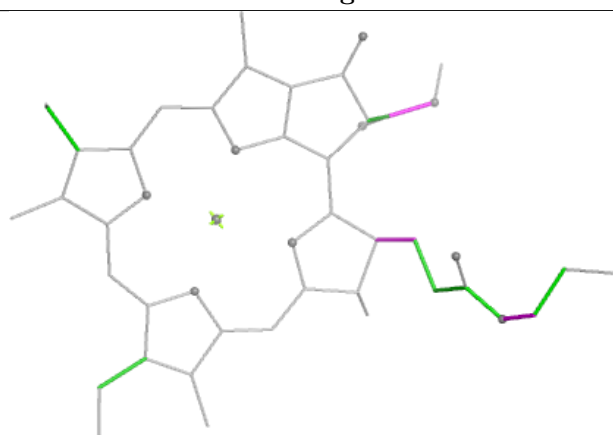
Ligand CLA S 315



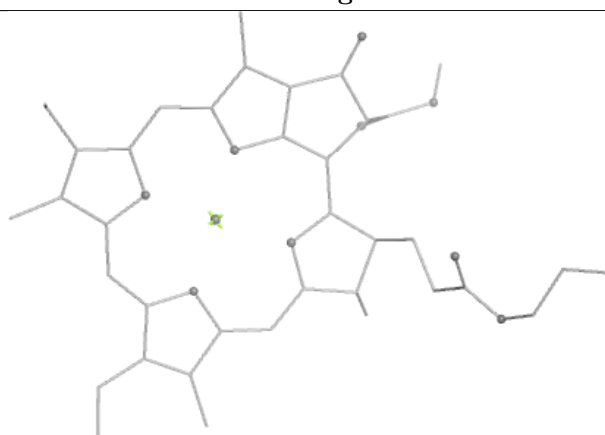
Bond lengths



Bond angles

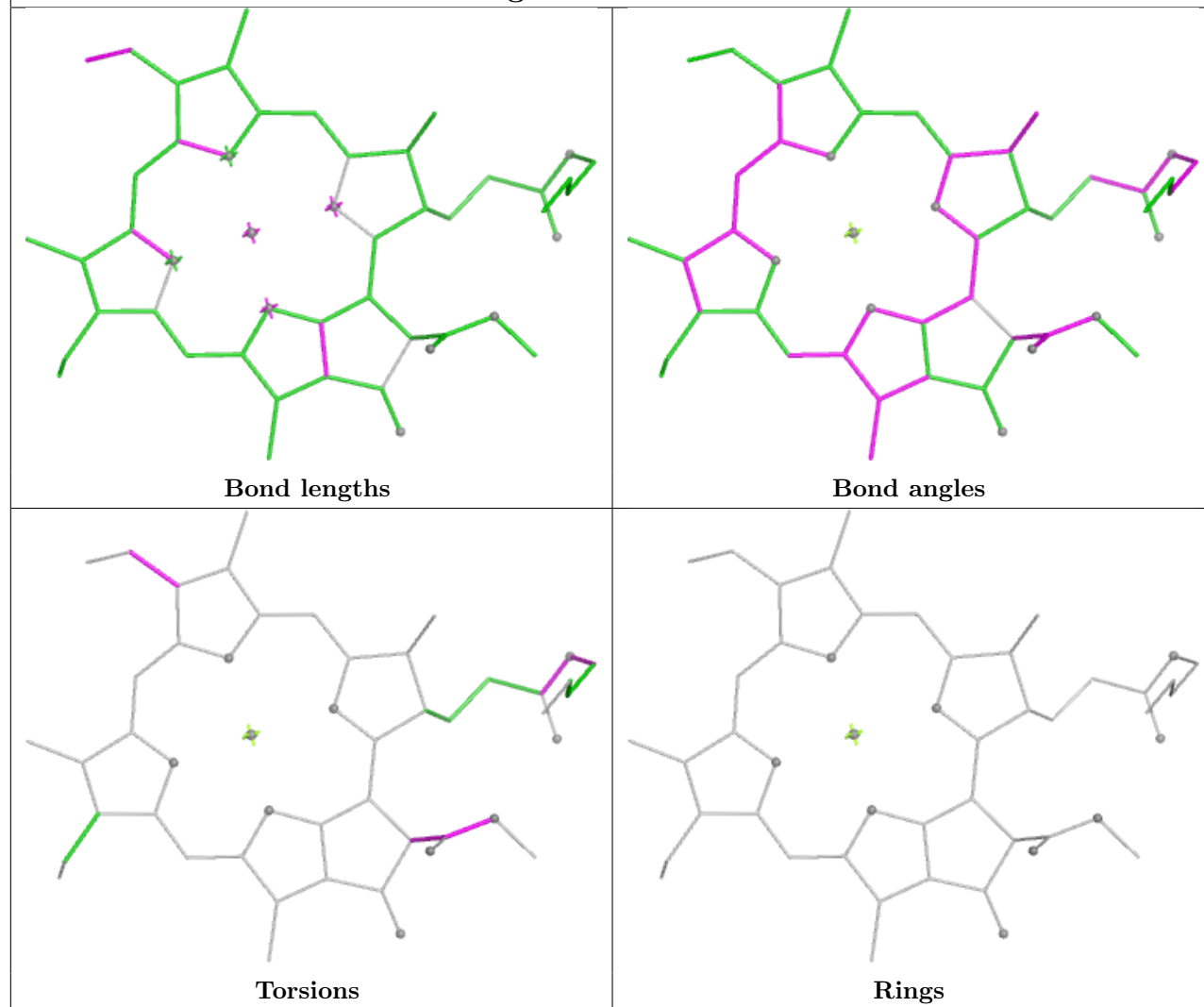


Torsions

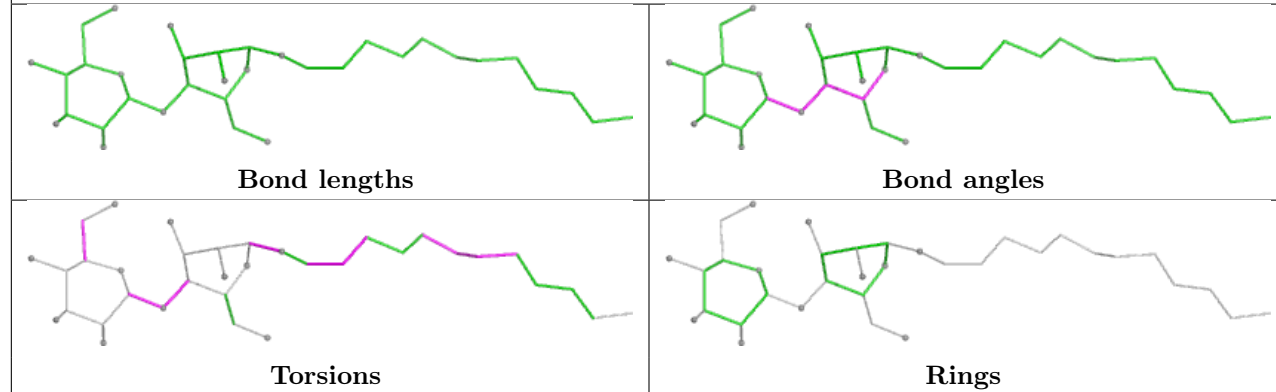


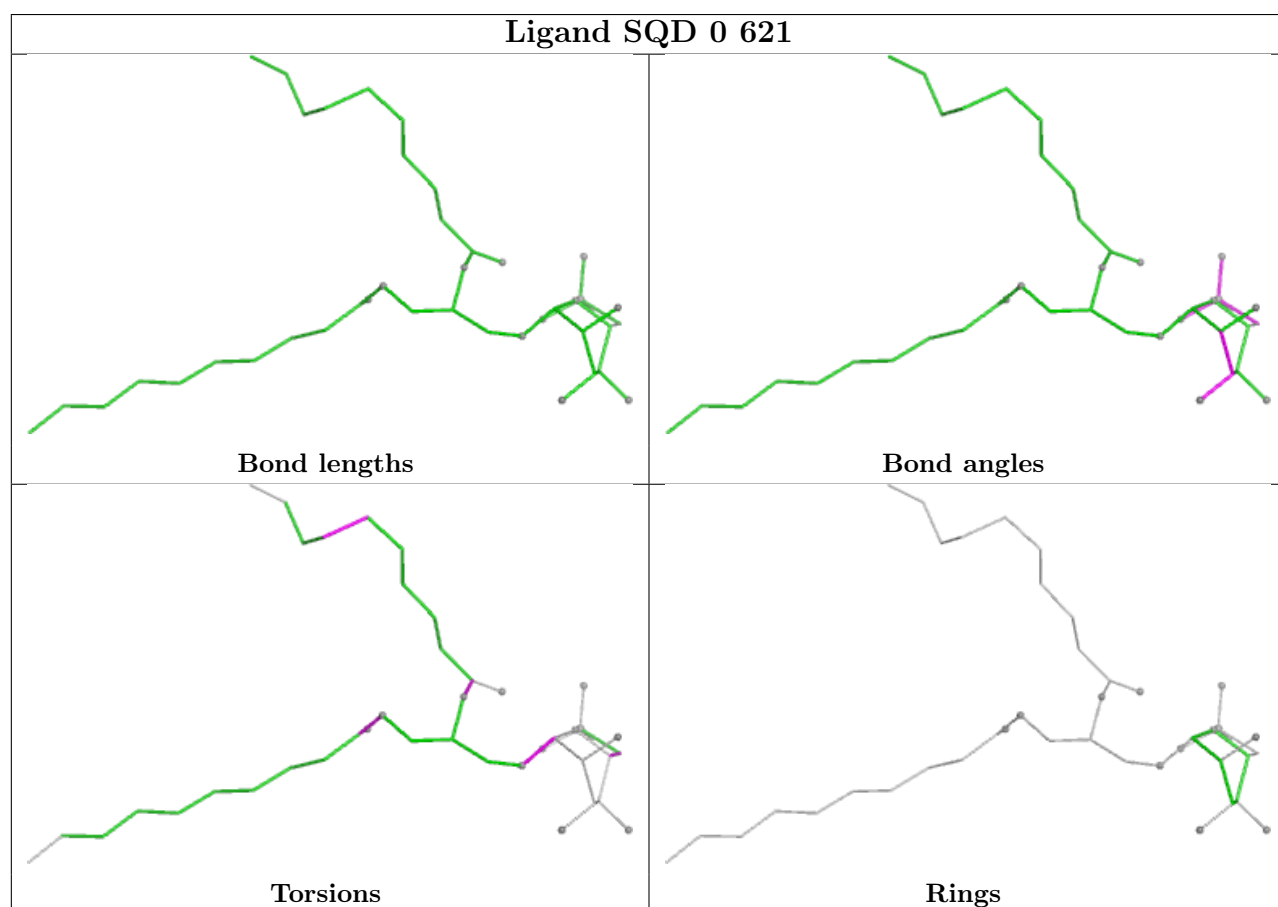
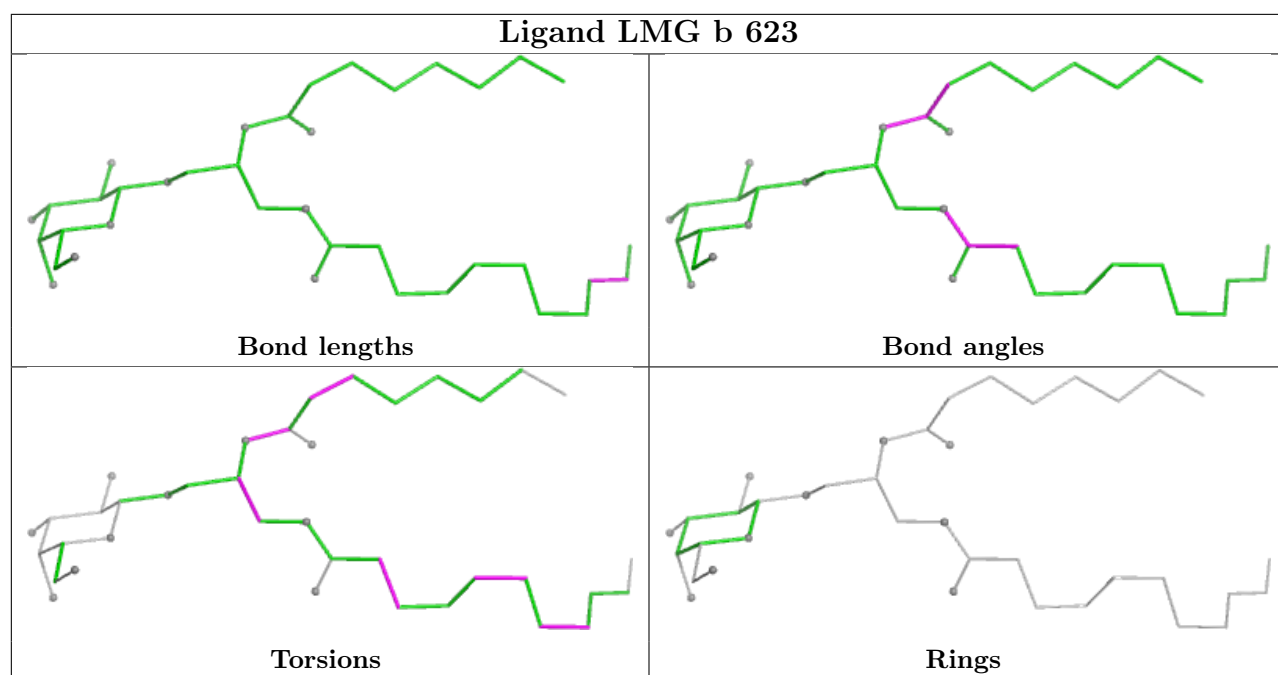
Rings

Ligand CLA r 314

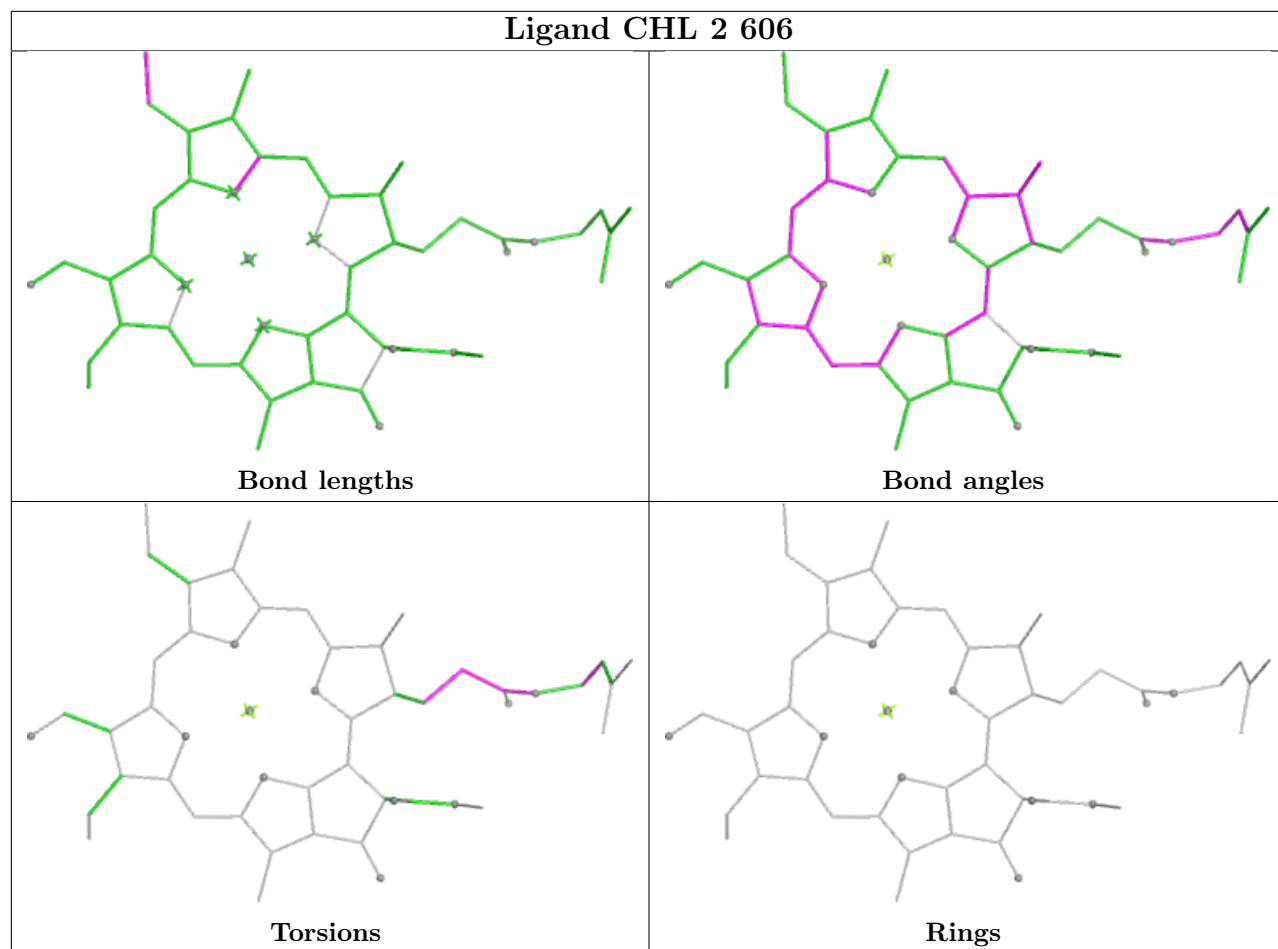


Ligand LMU R 302

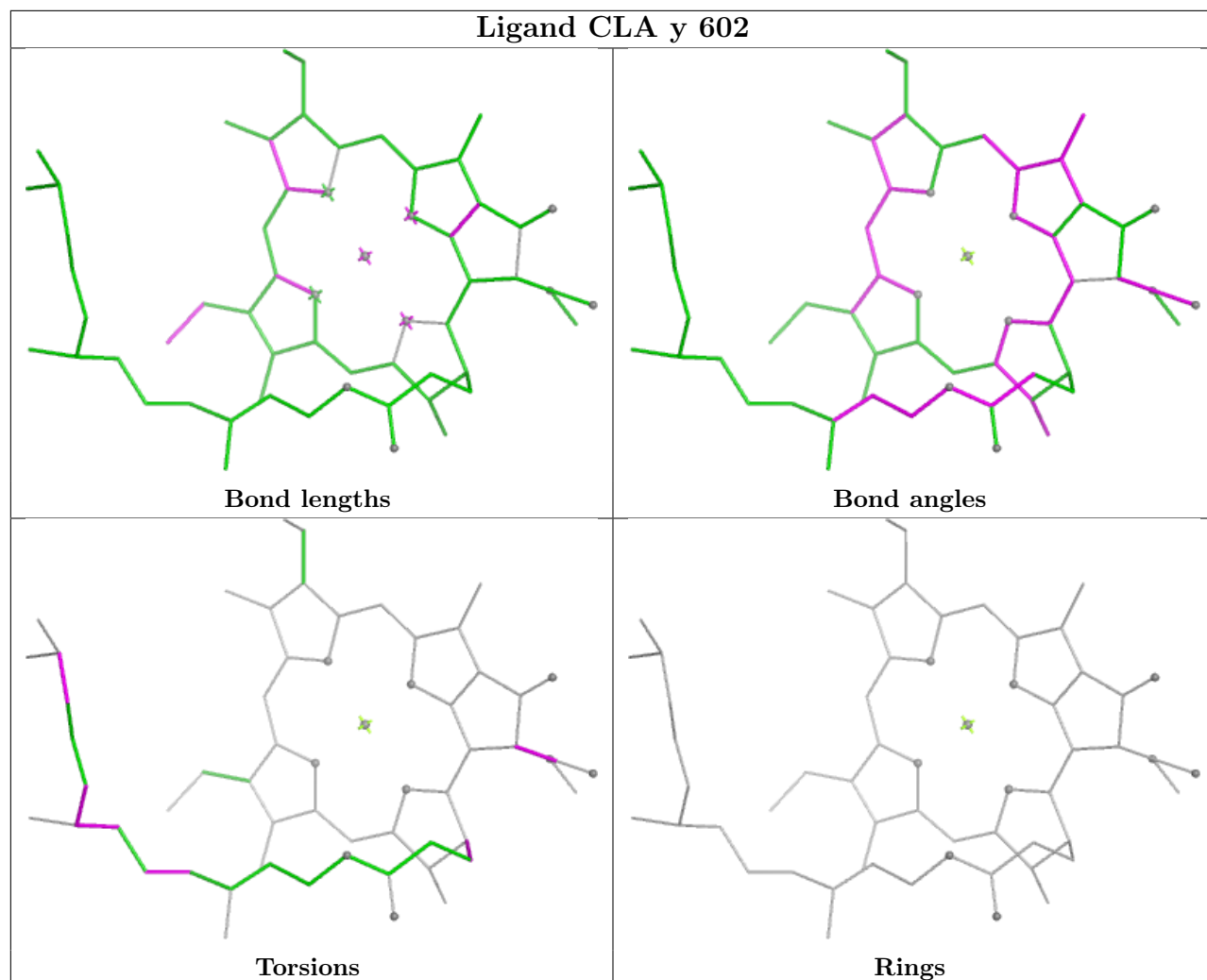


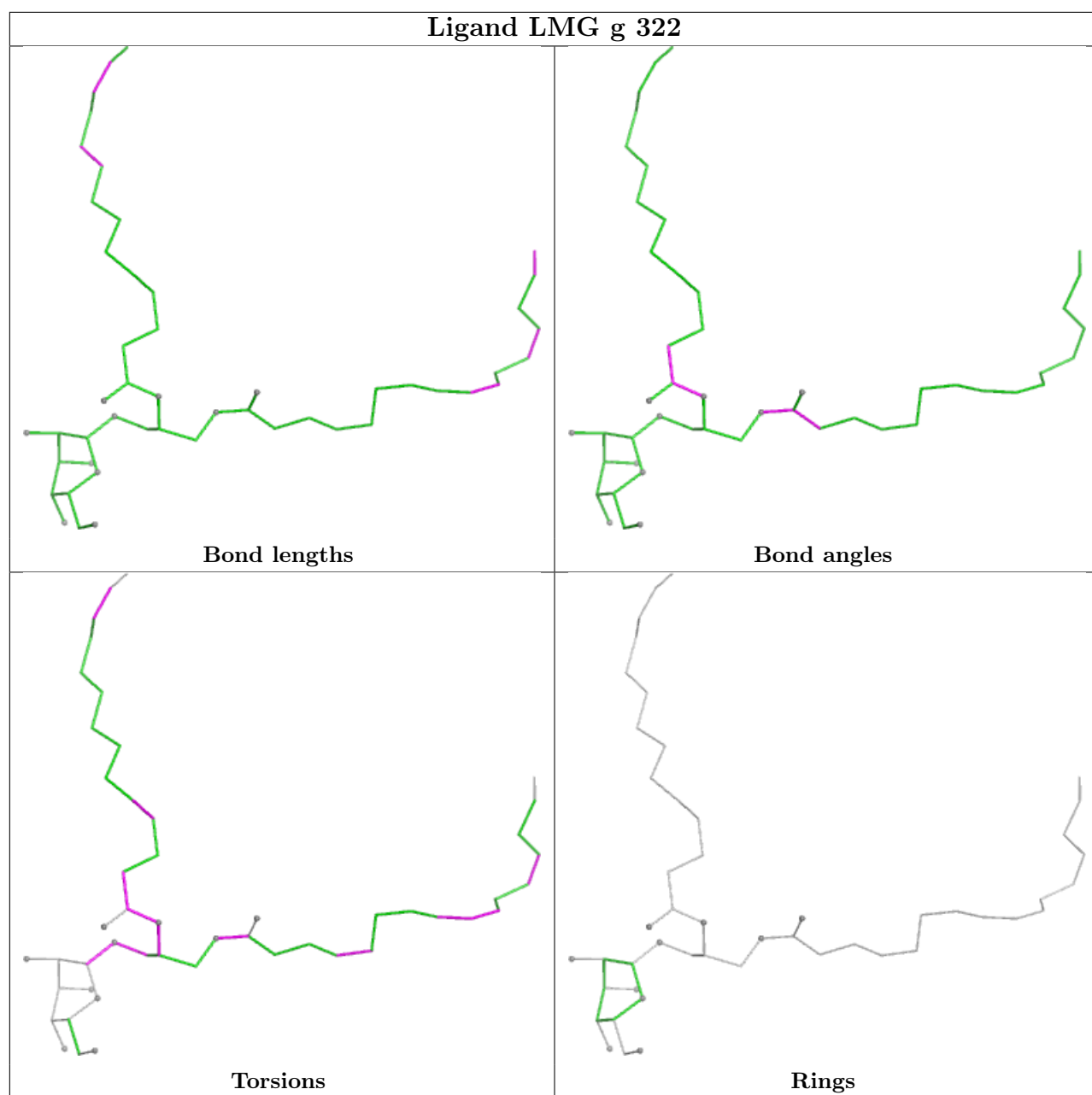


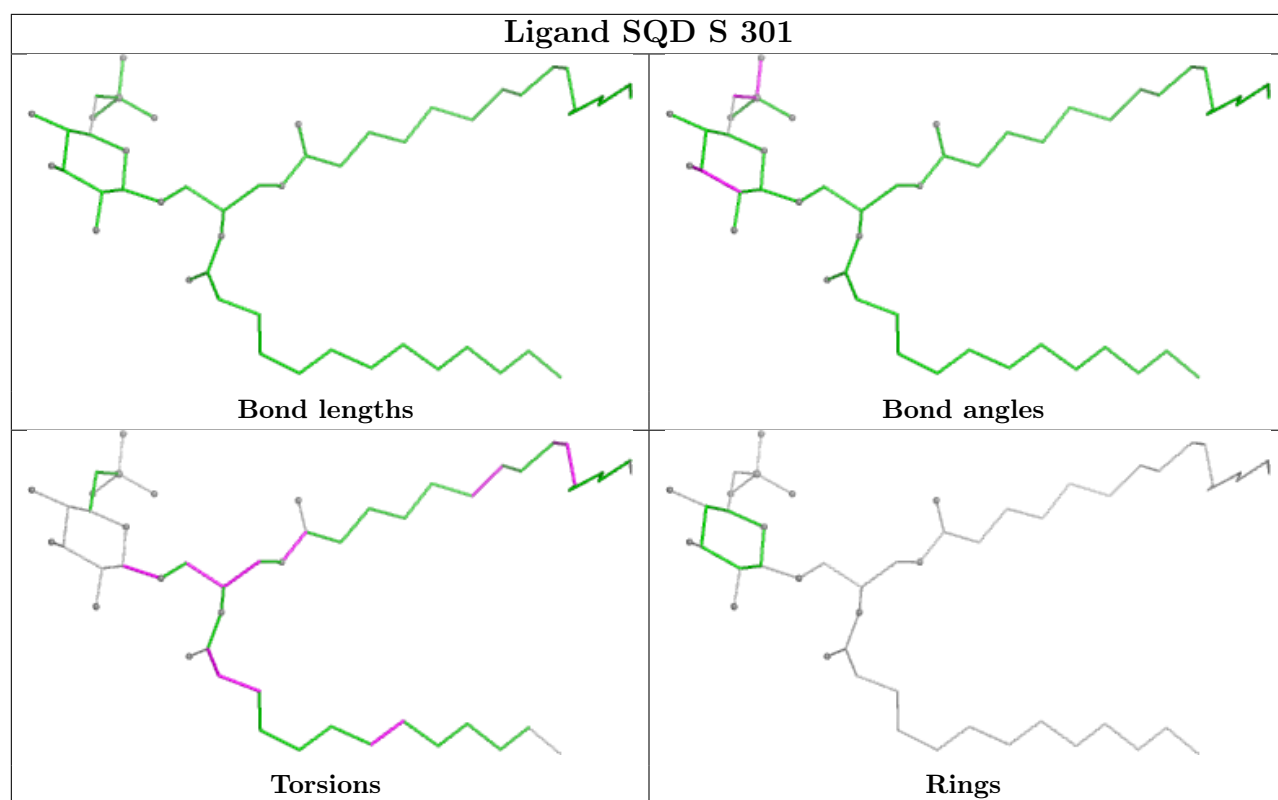
Ligand CHL 2 606

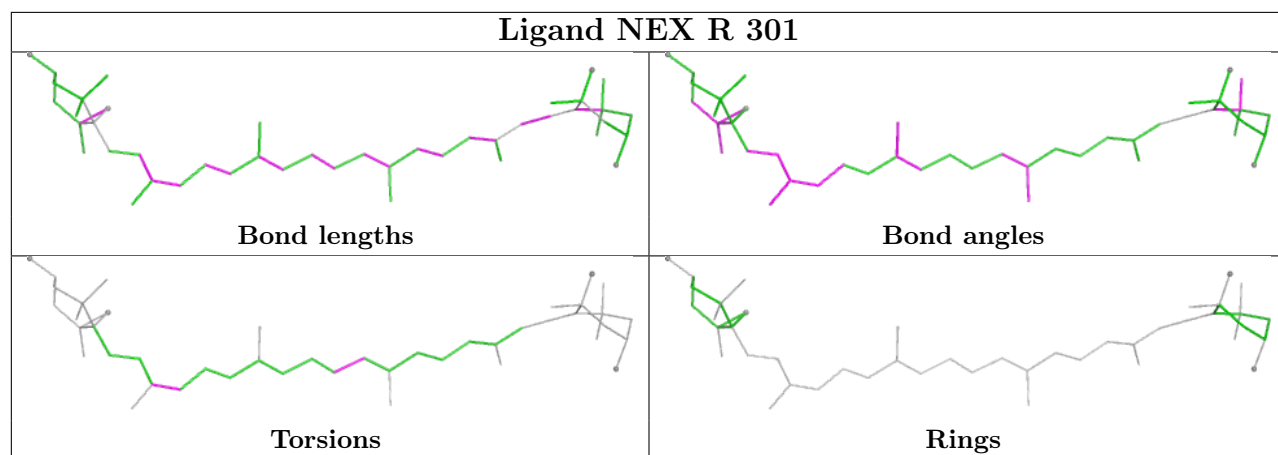
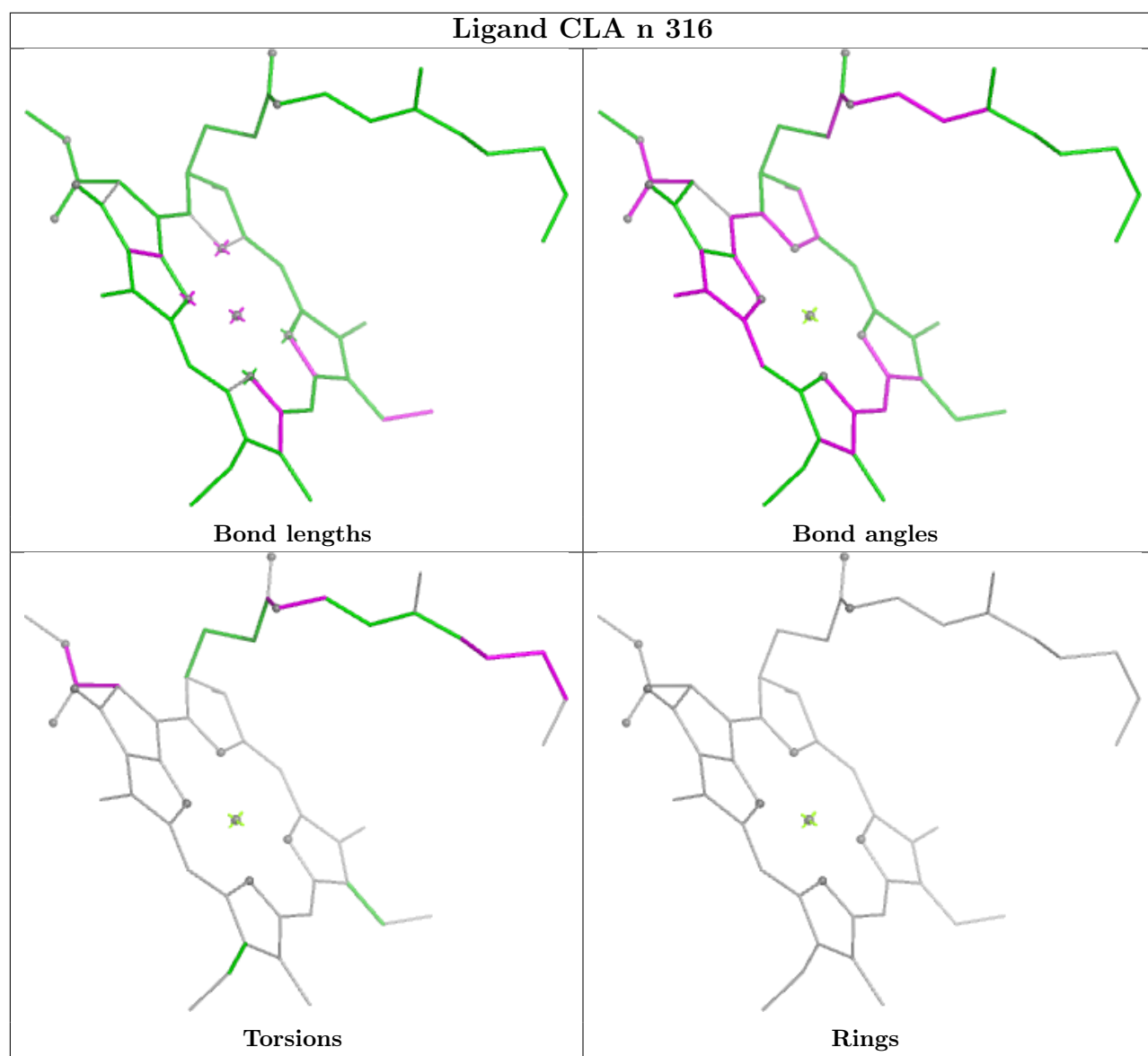


Ligand CLA y 602

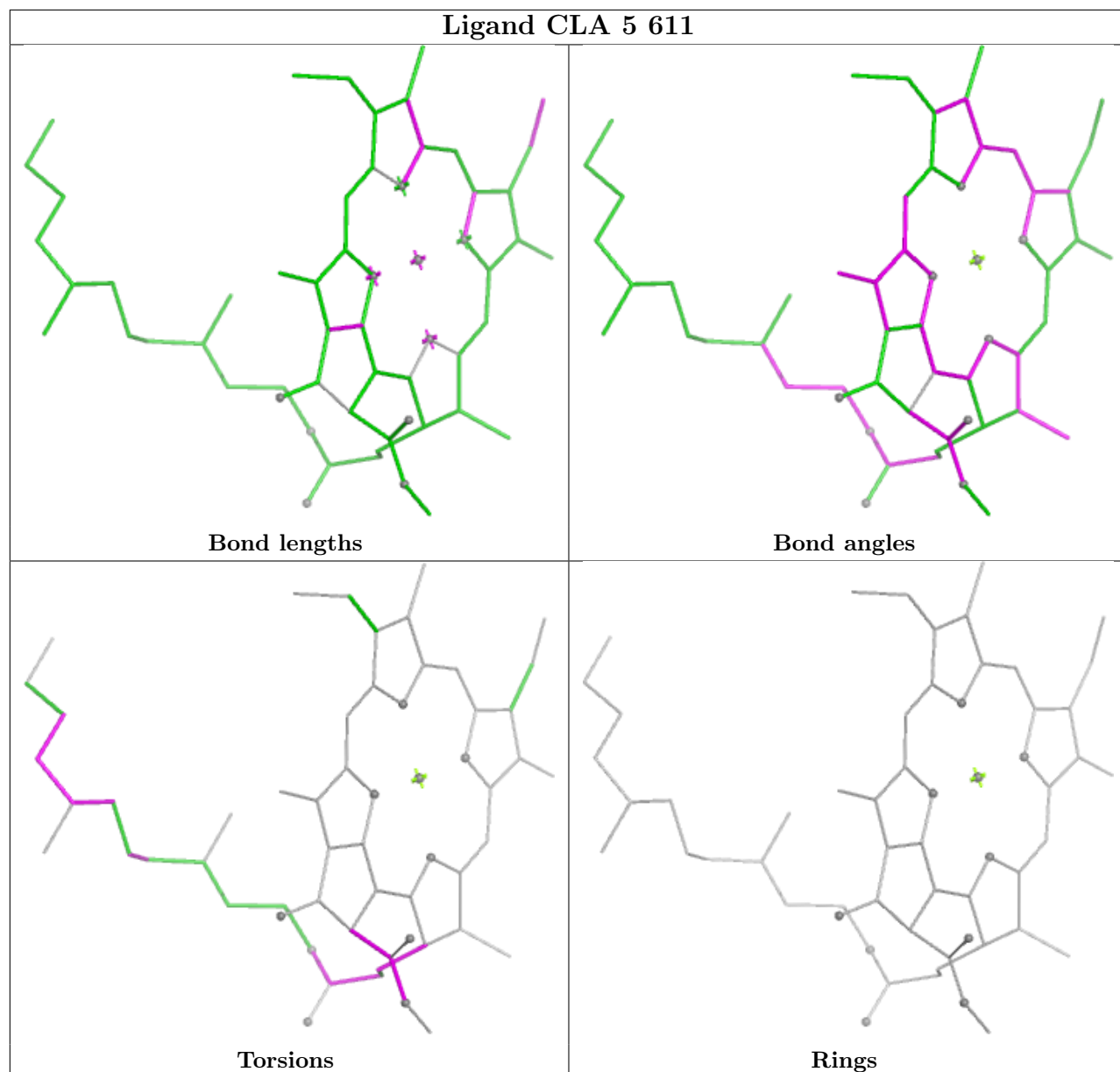




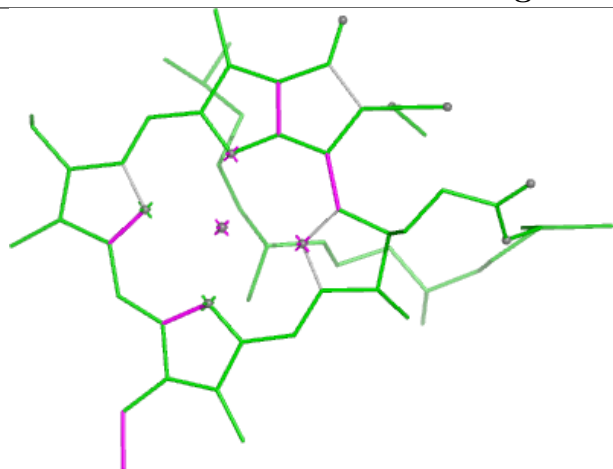




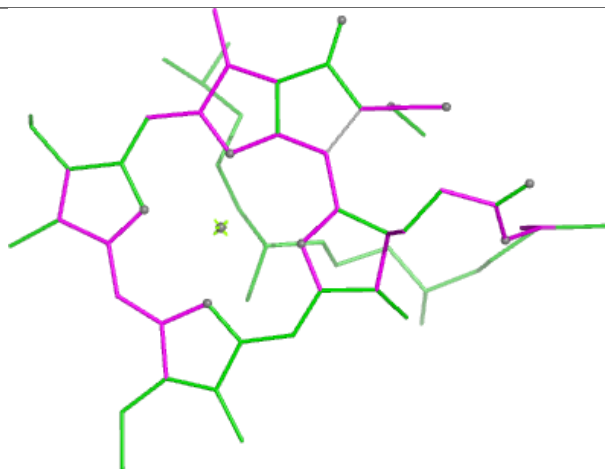
Ligand CLA 5 611



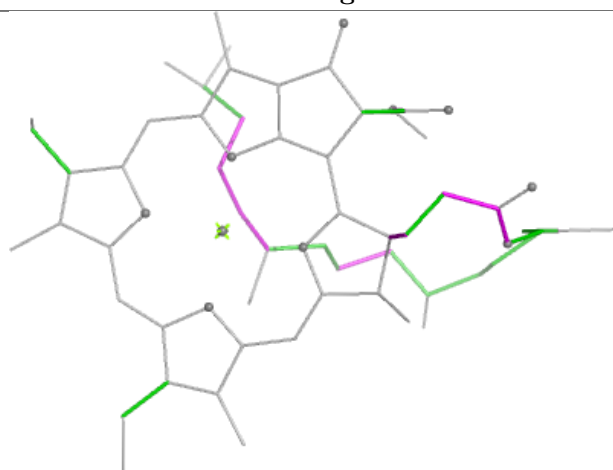
Ligand CLA C 610



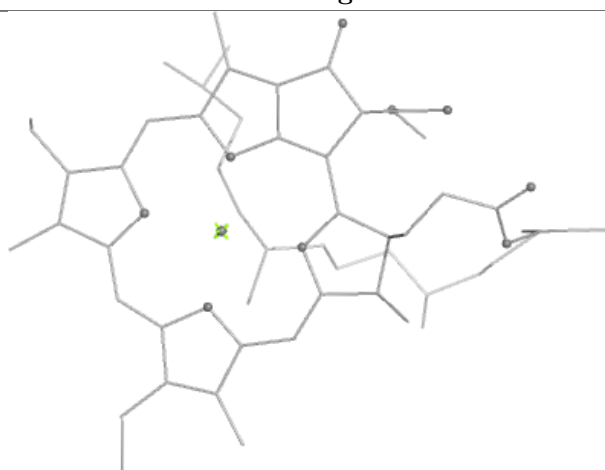
Bond lengths



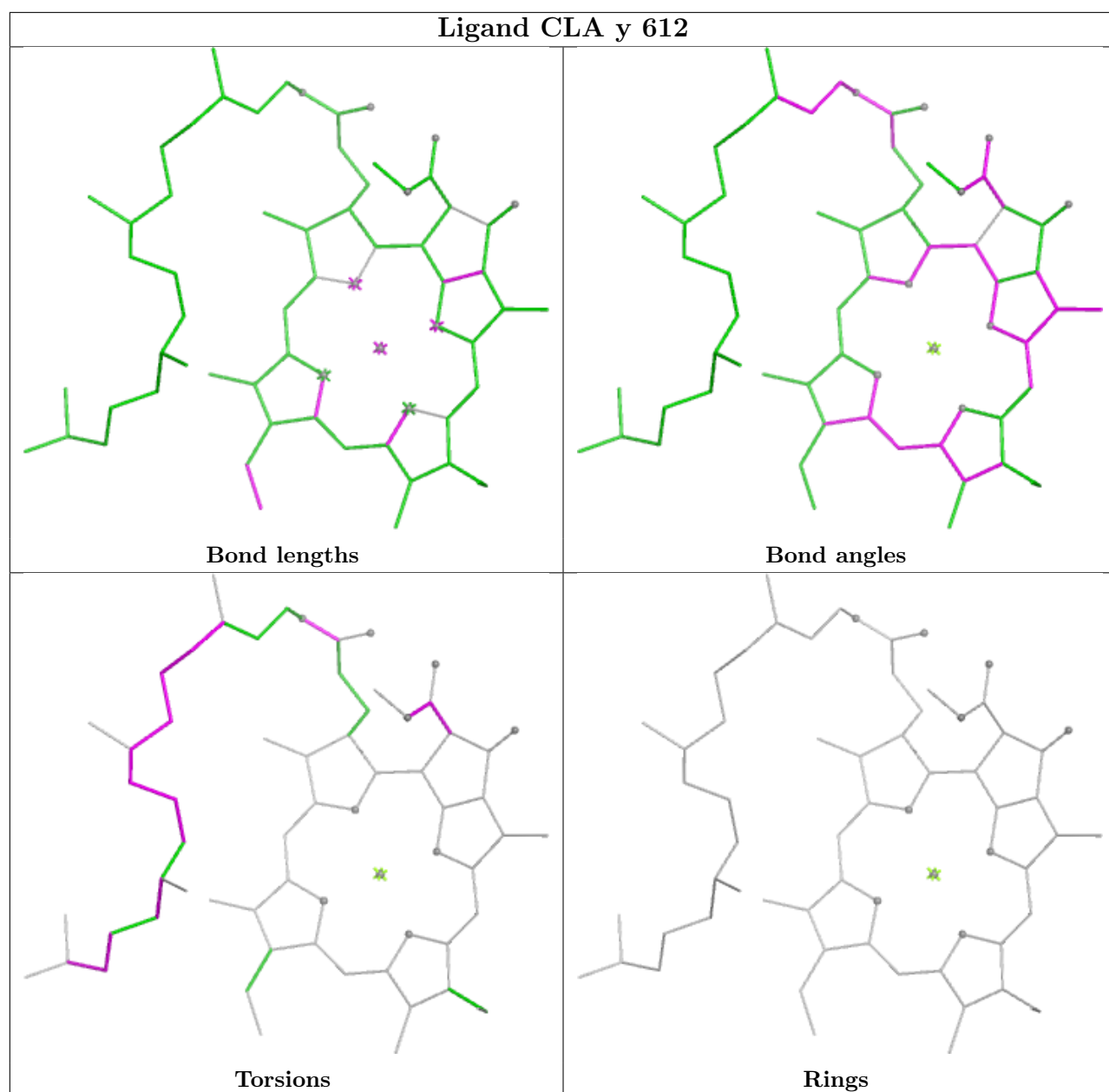
Bond angles



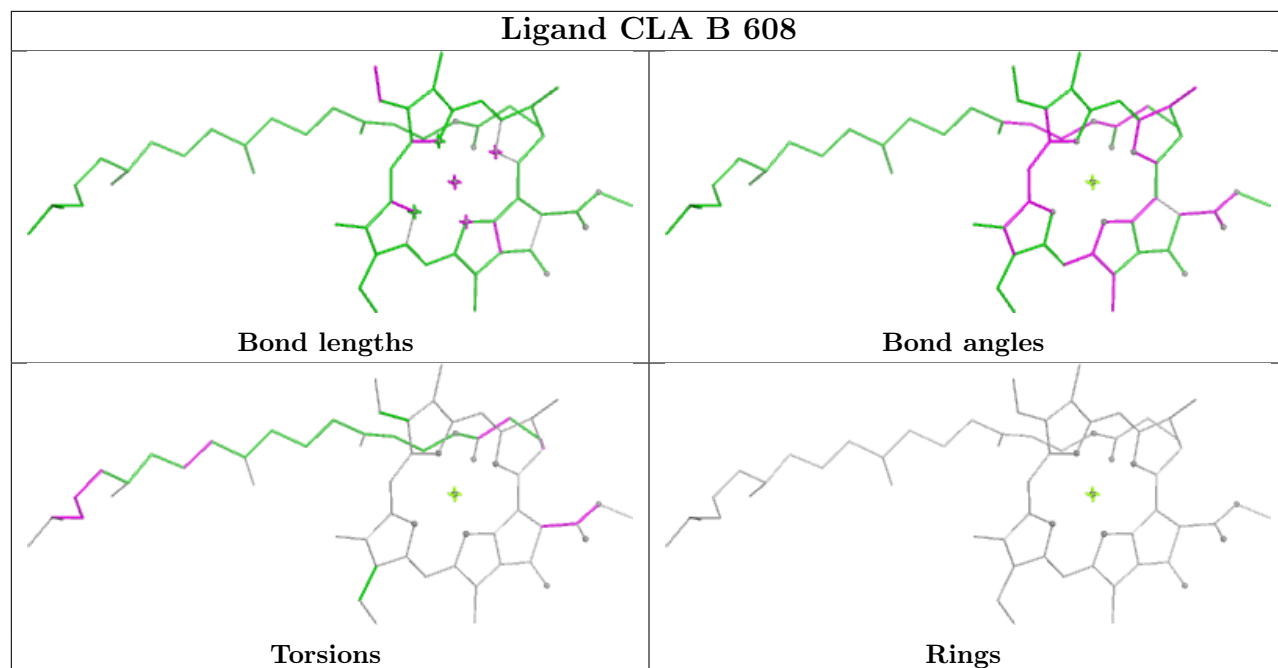
Torsions



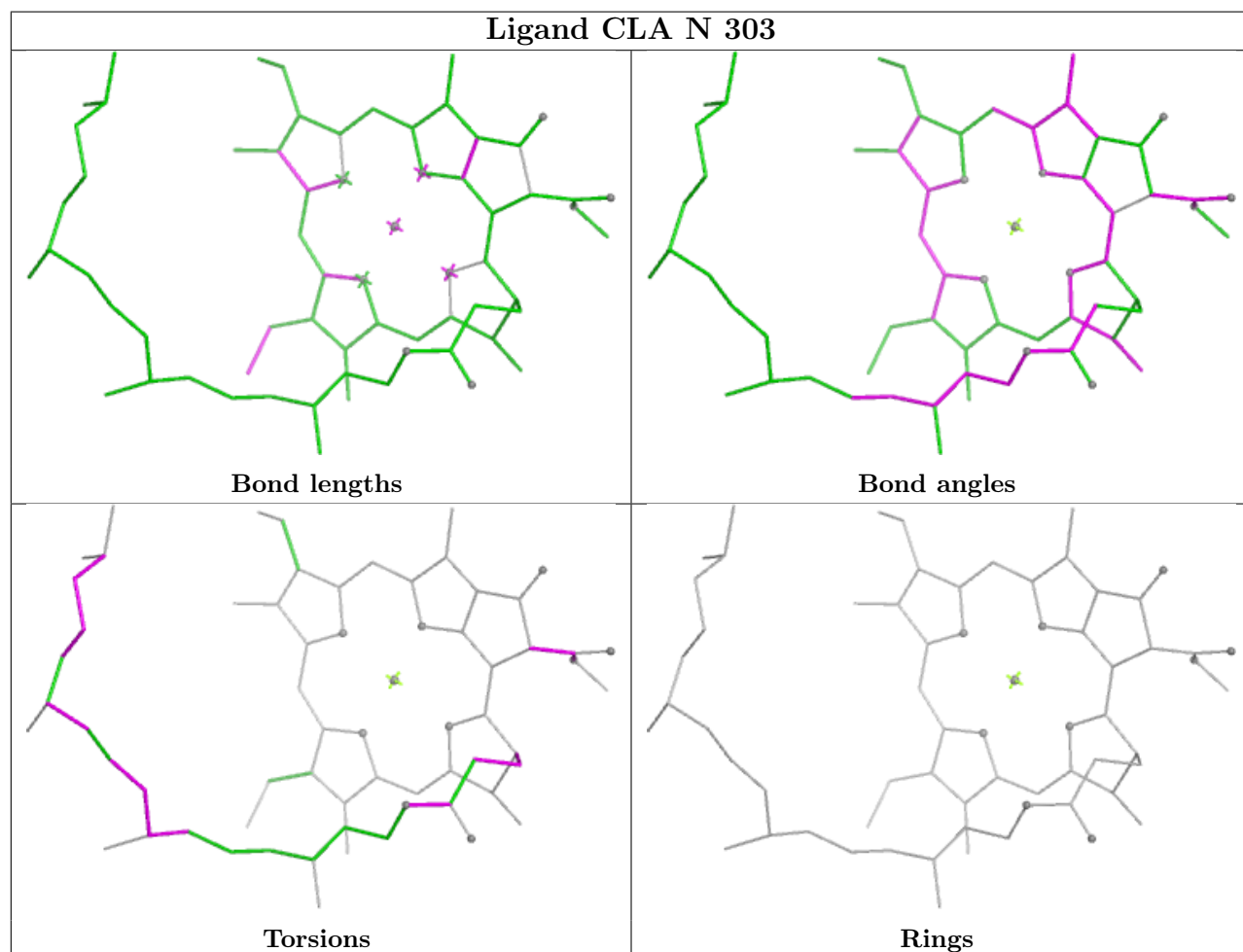
Rings

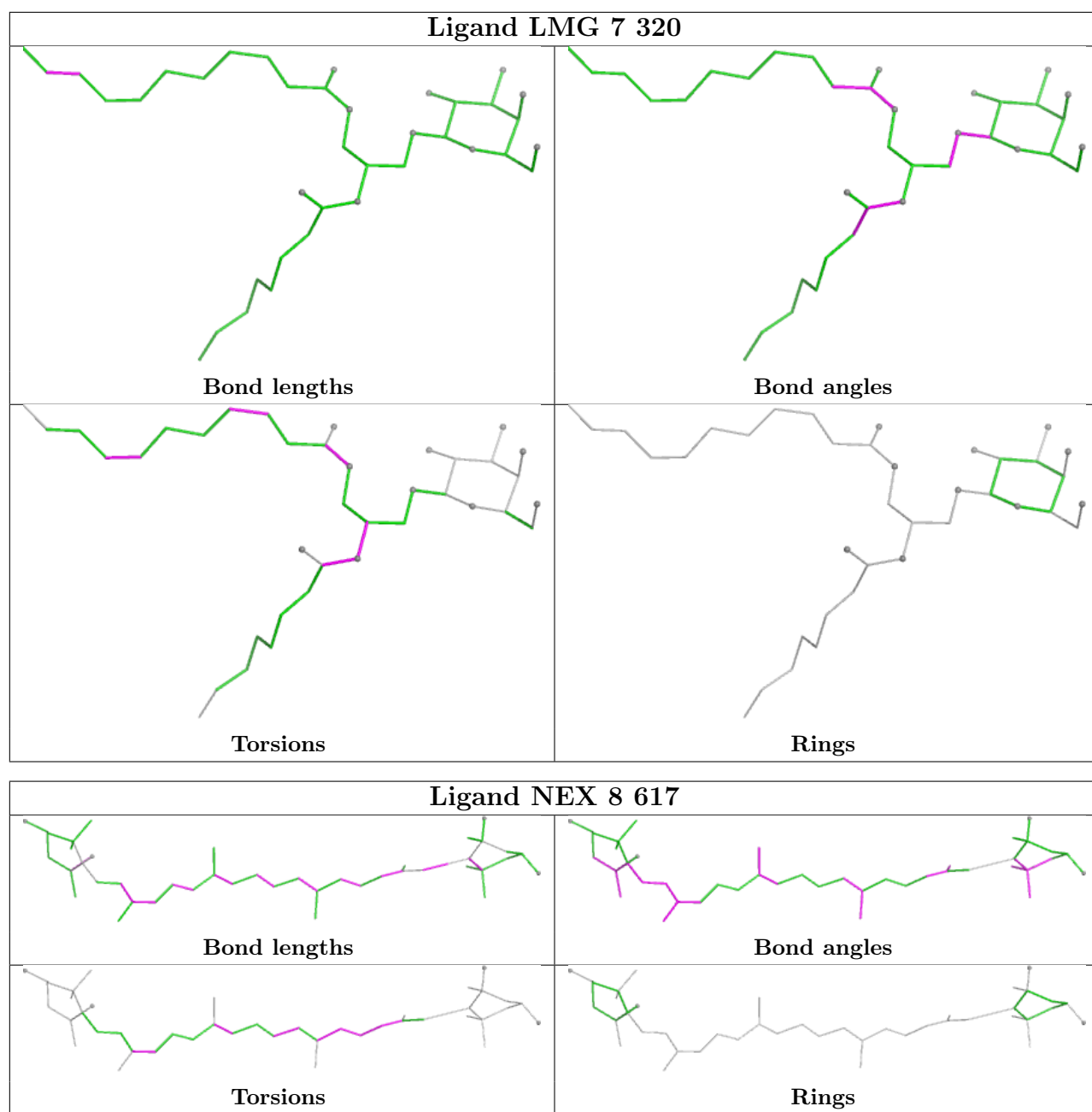


Ligand CLA B 608

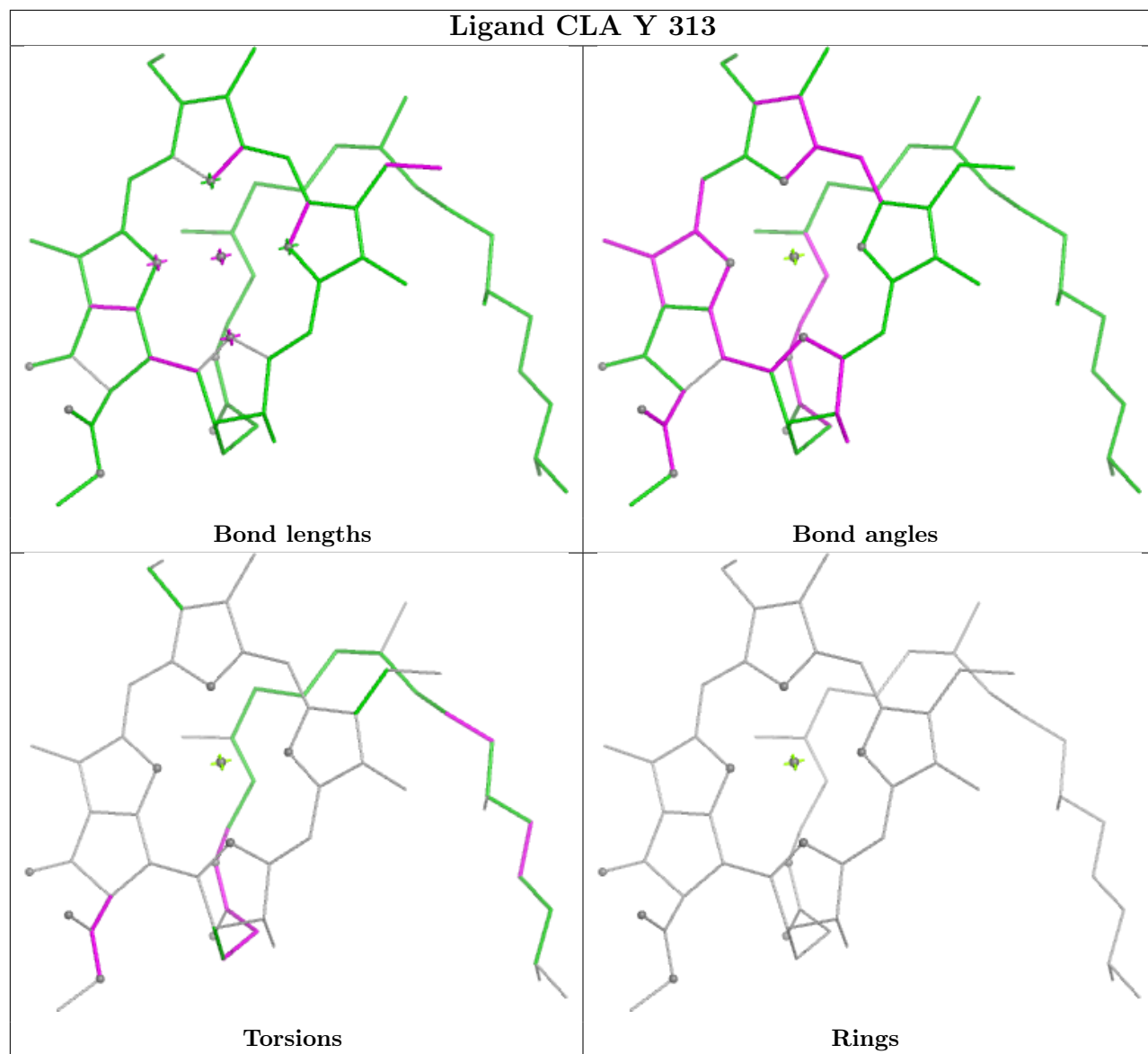


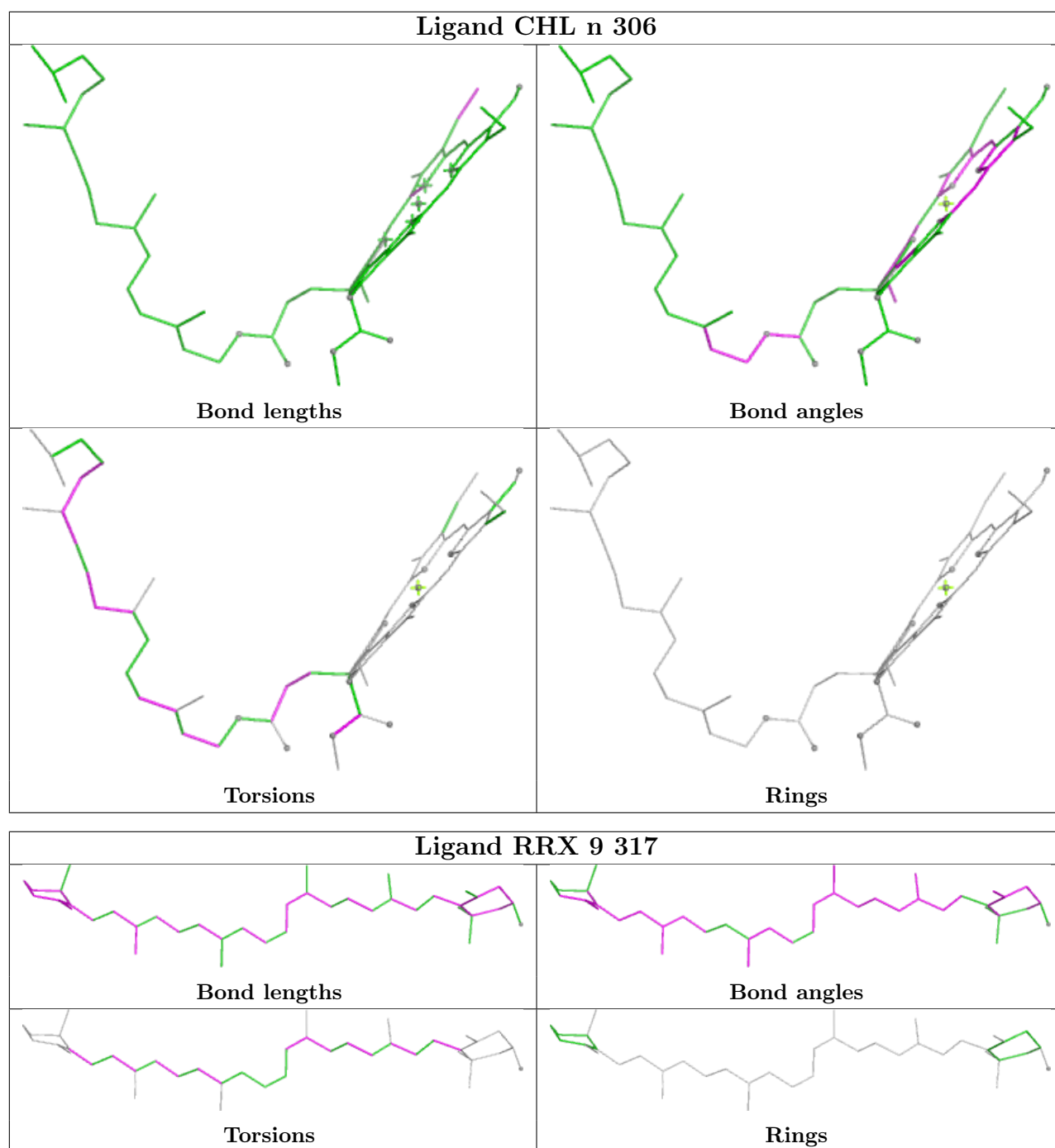
Ligand CLA N 303

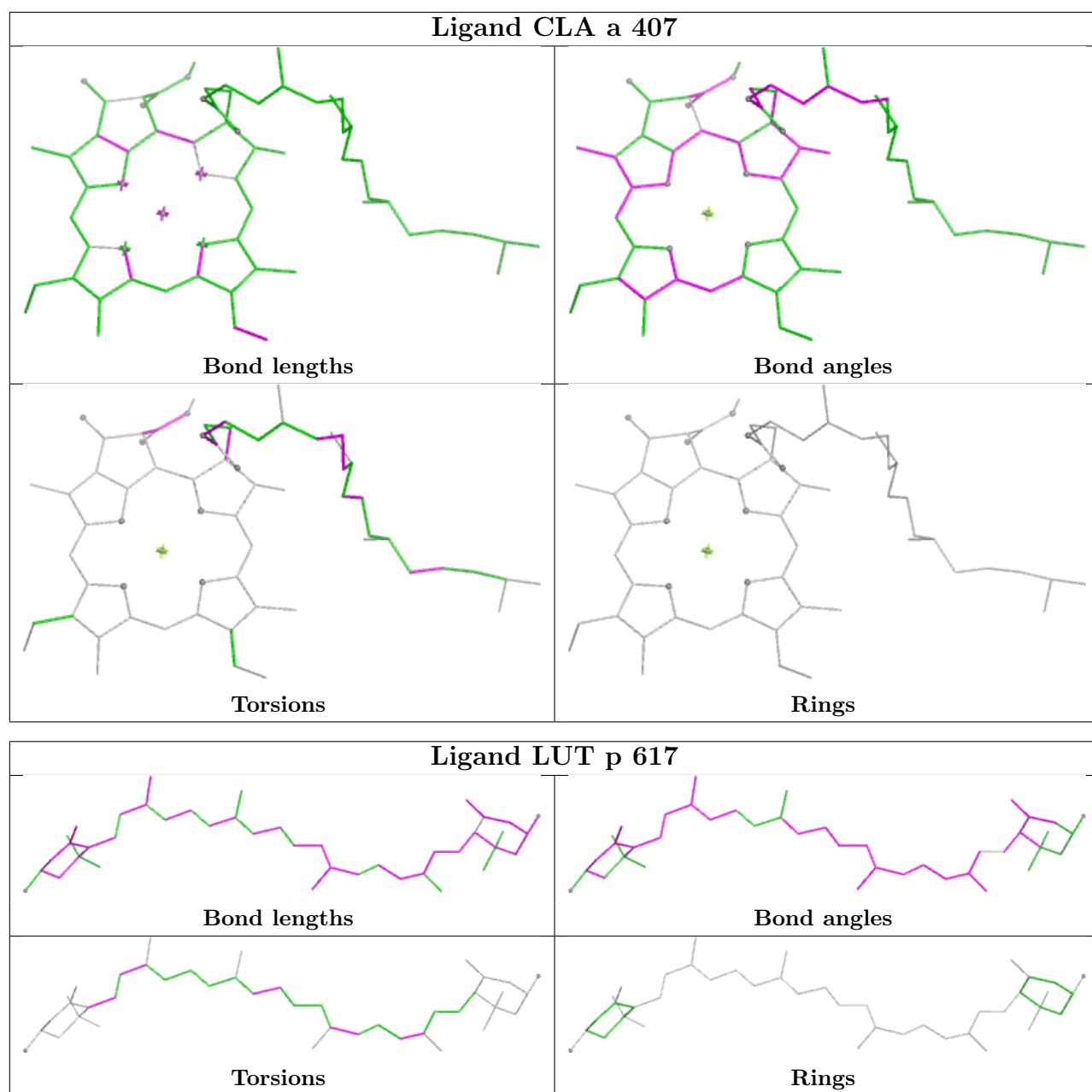




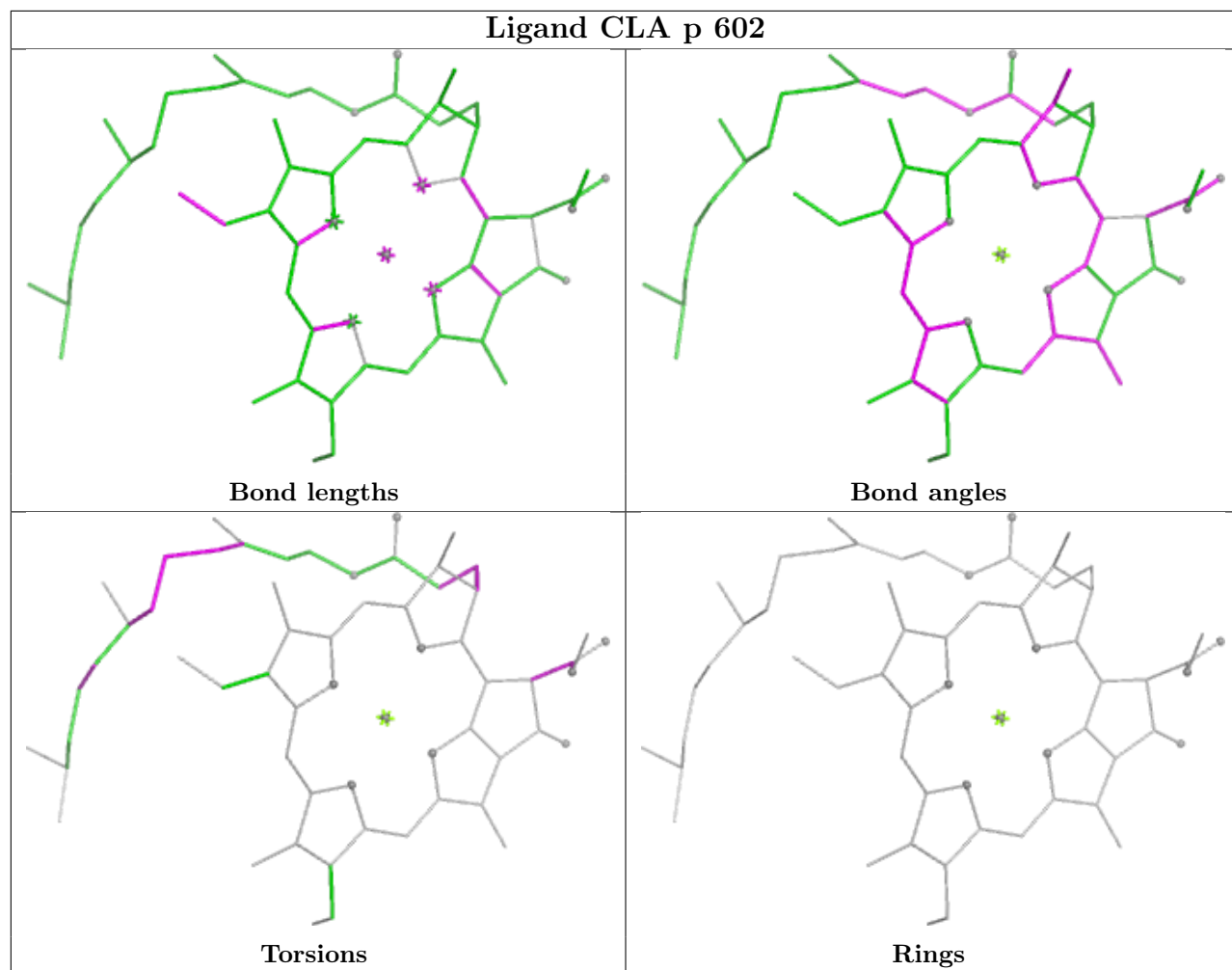
Ligand CLA Y 313

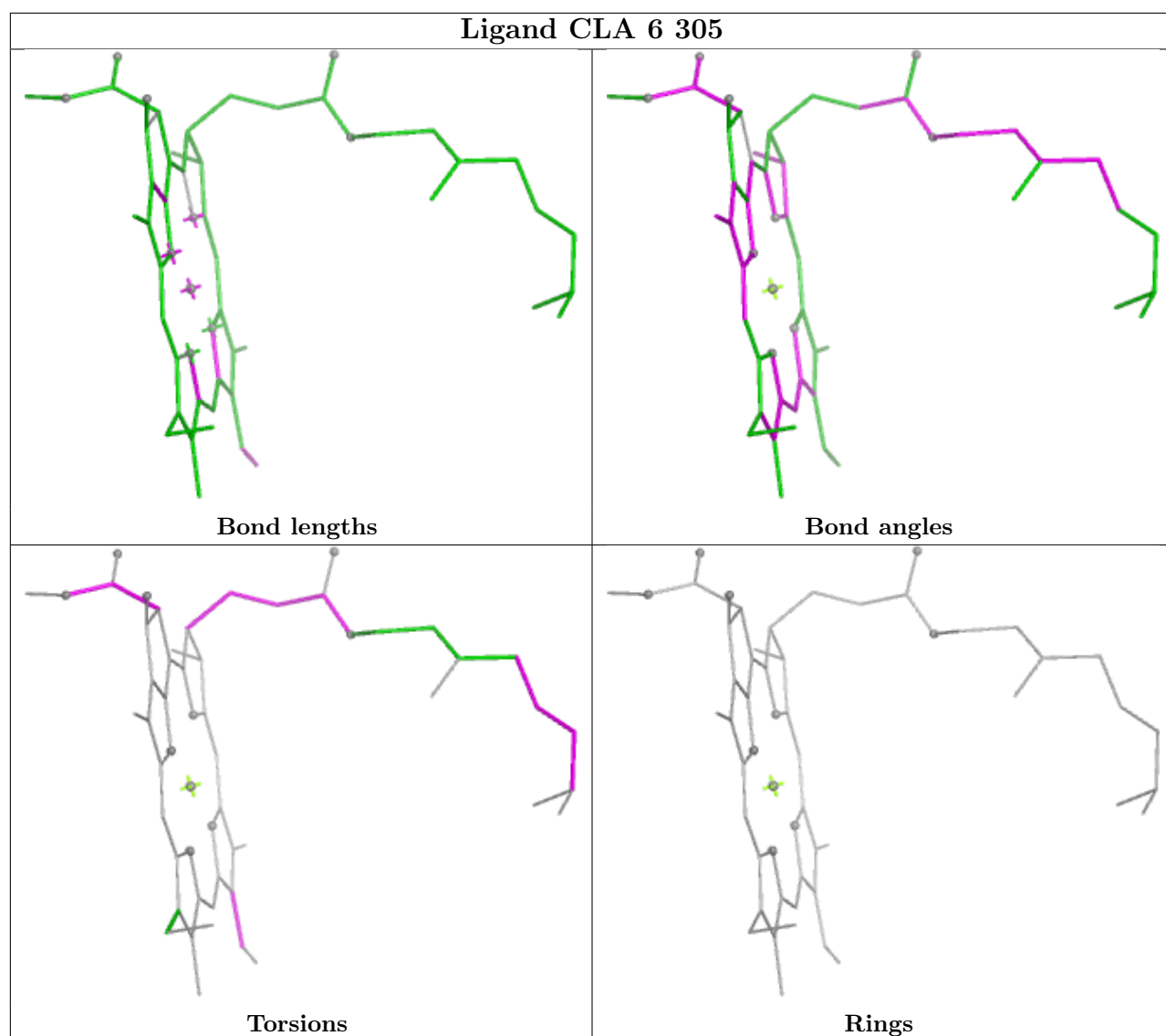




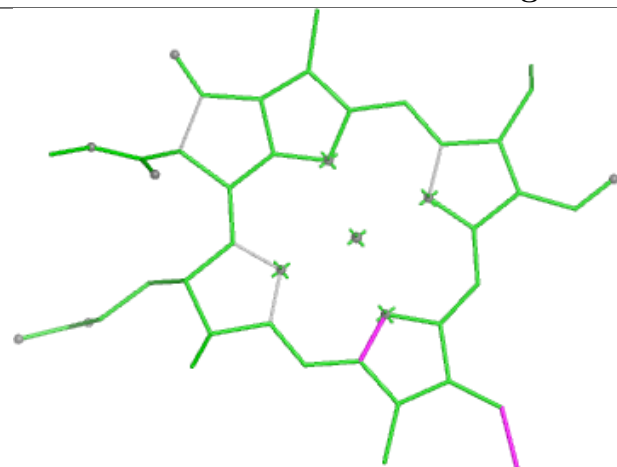


Ligand CLA p 602

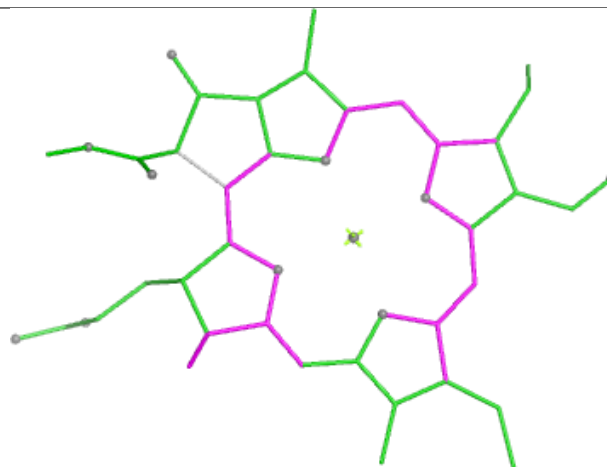




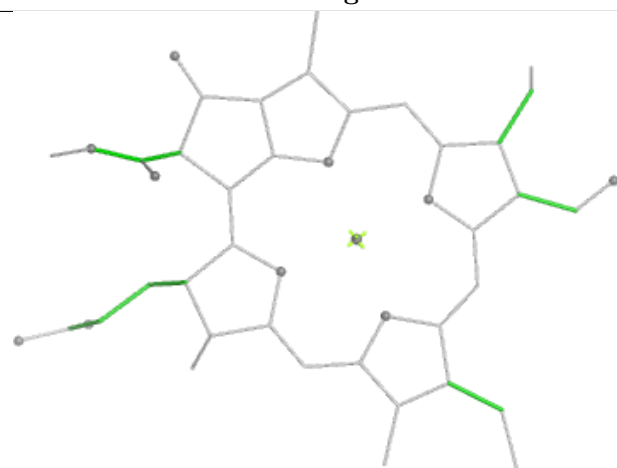
Ligand CHL S 302



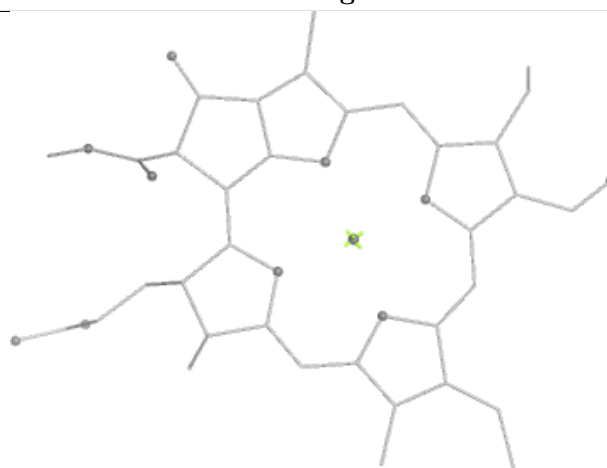
Bond lengths



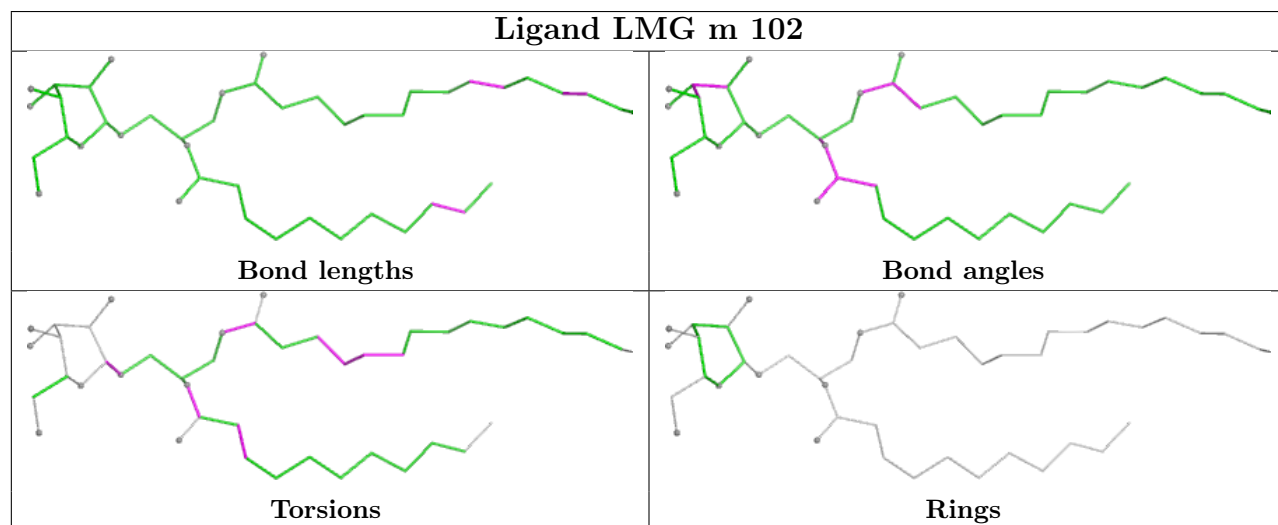
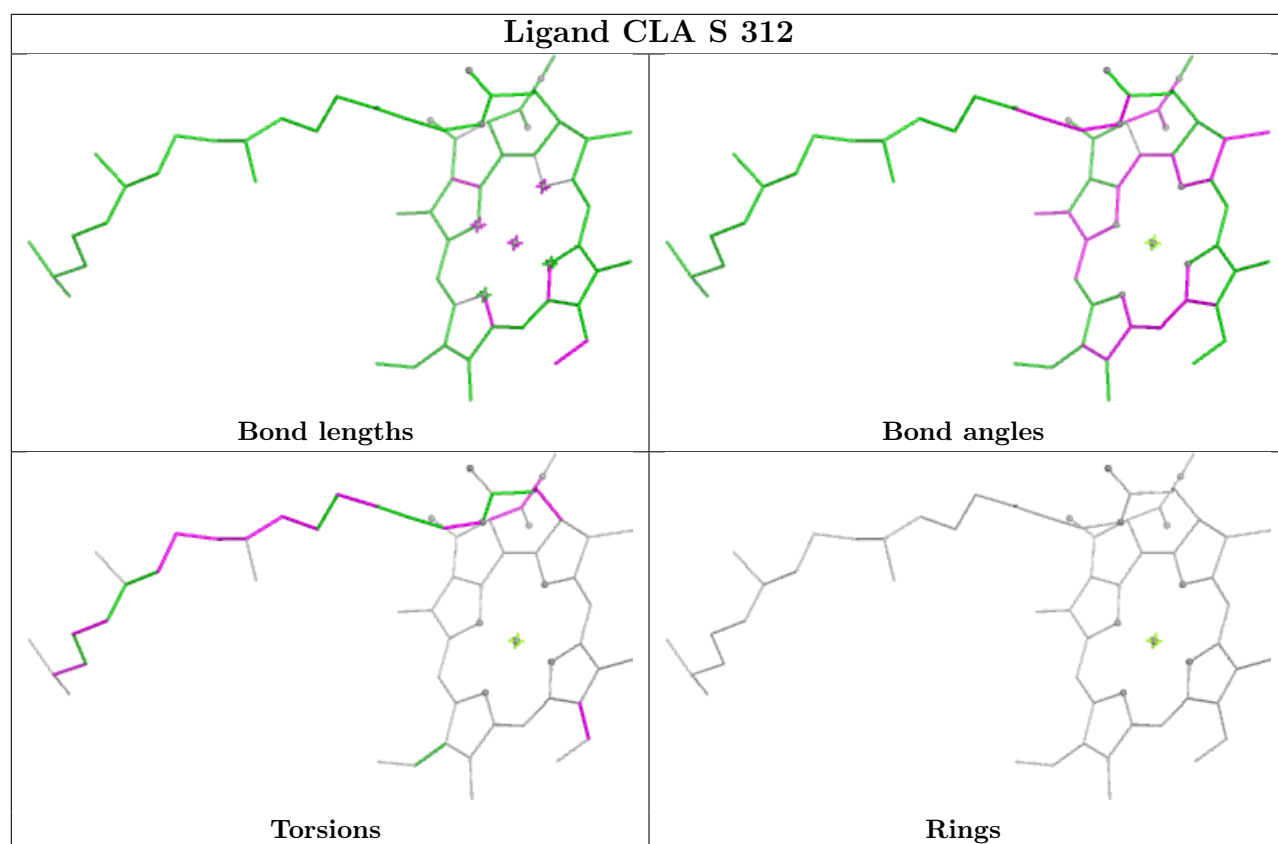
Bond angles



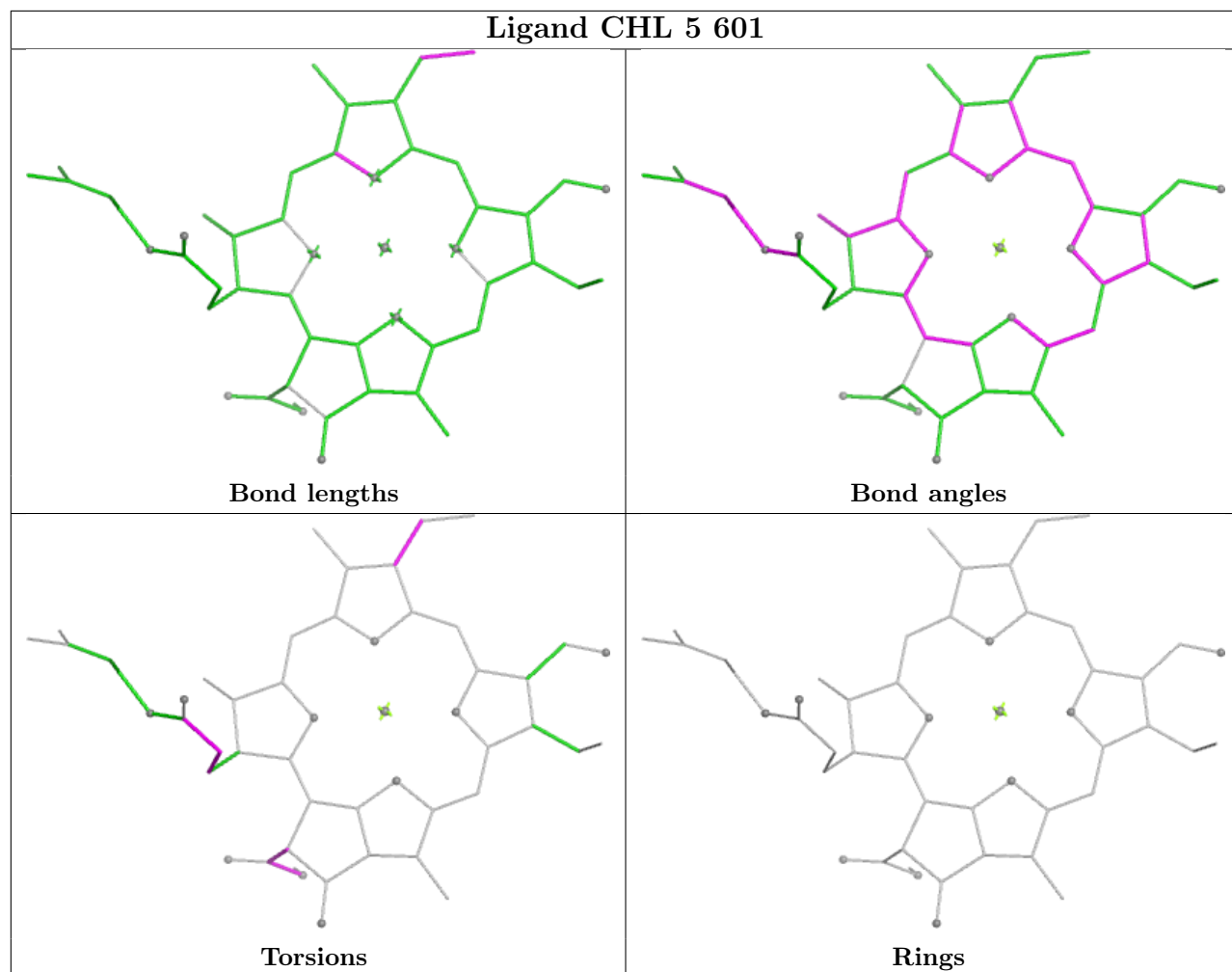
Torsions

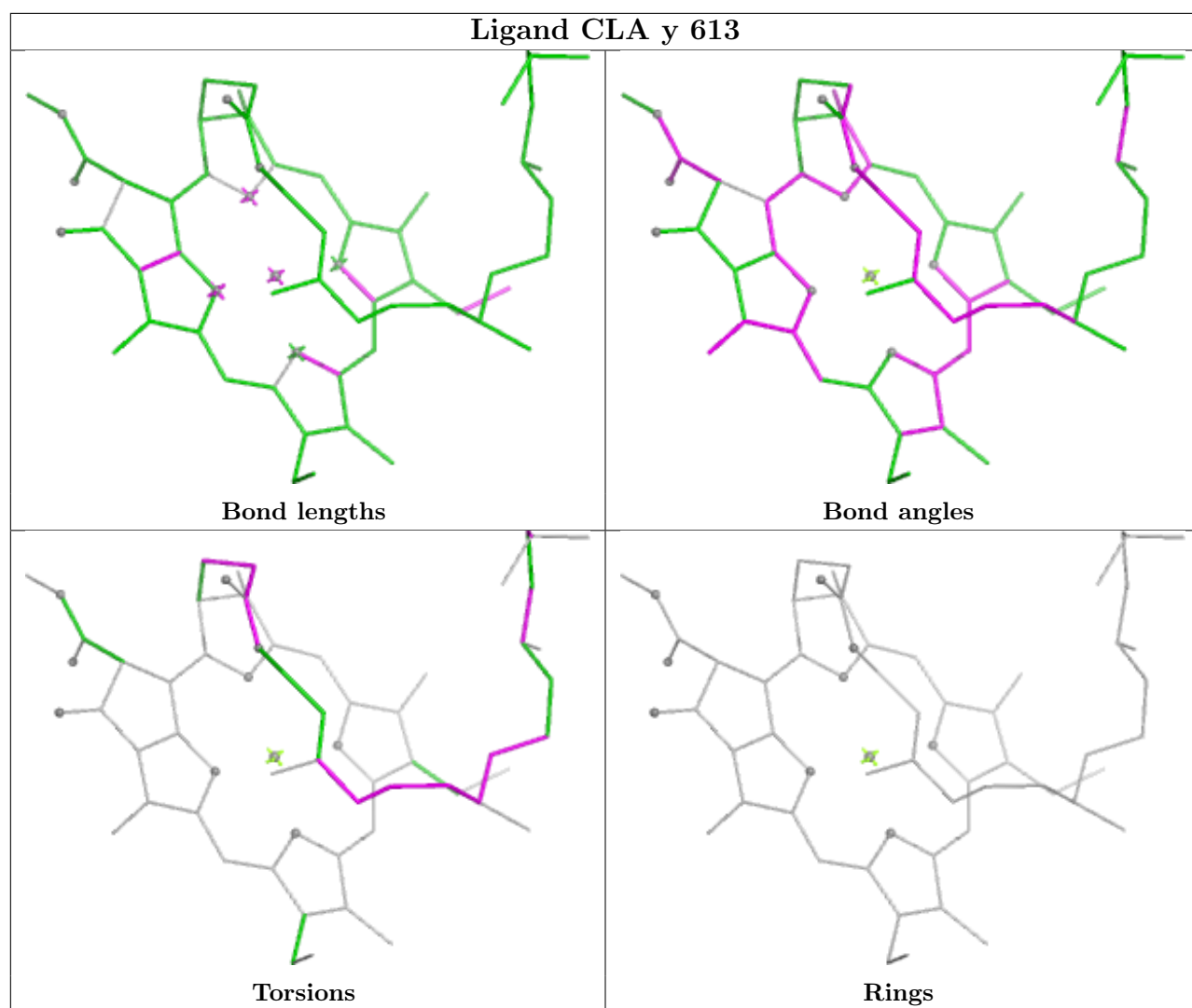


Rings

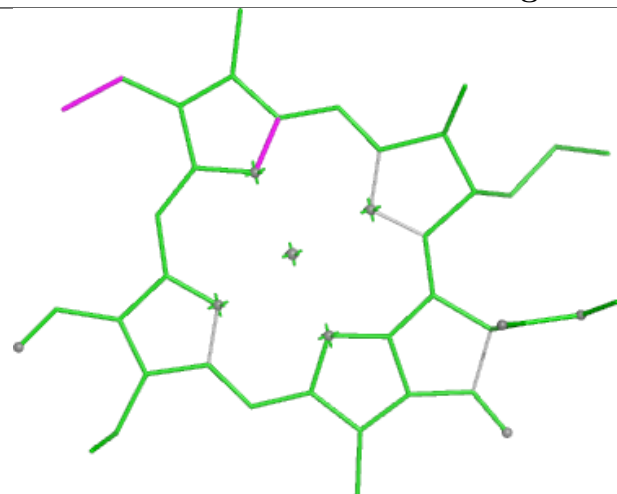


Ligand CHL 5 601

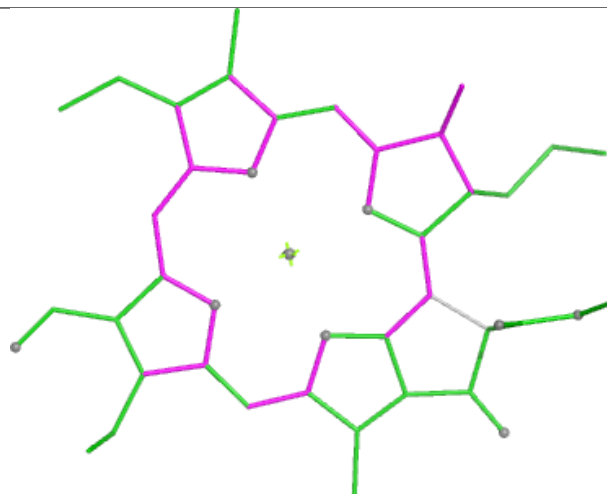




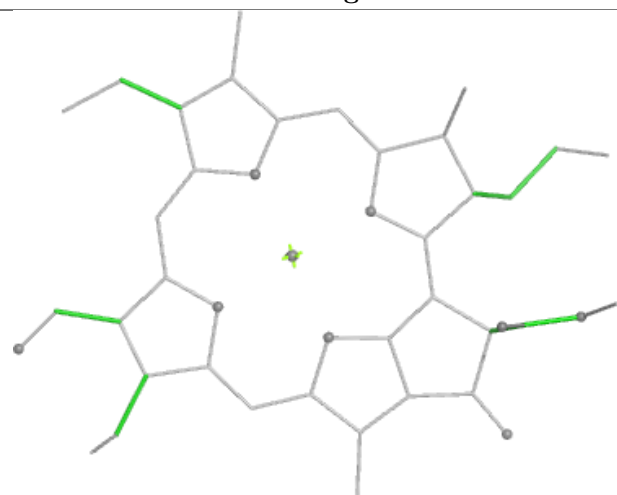
Ligand CHL S 307



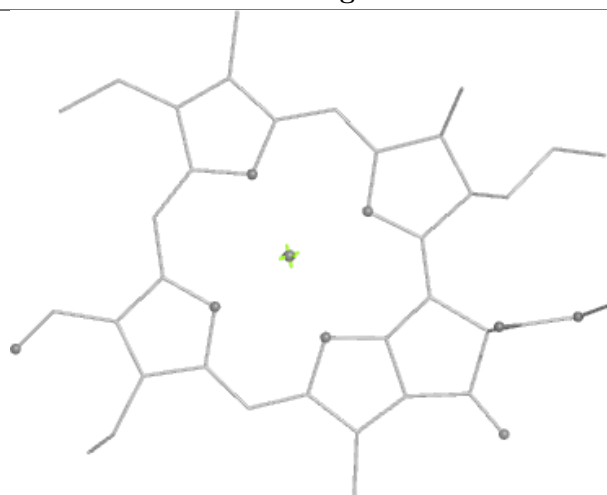
Bond lengths



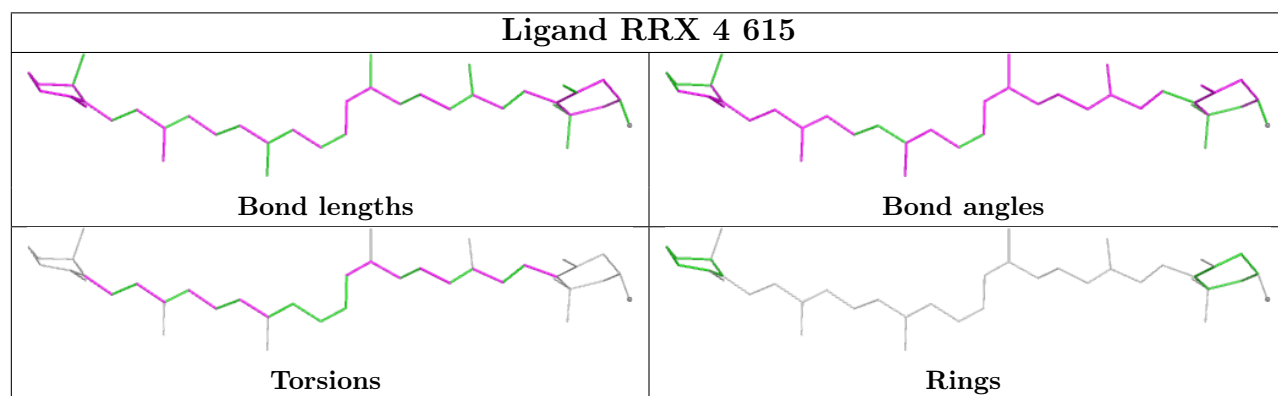
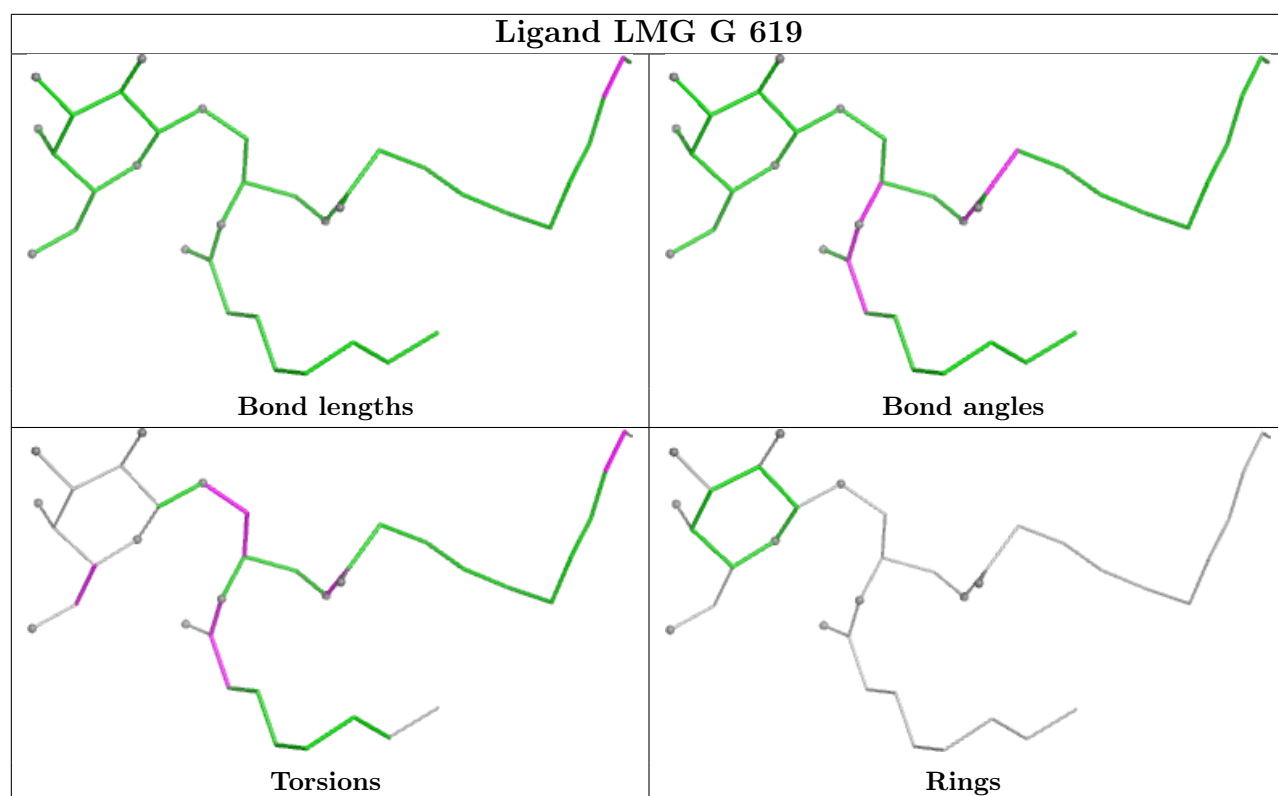
Bond angles



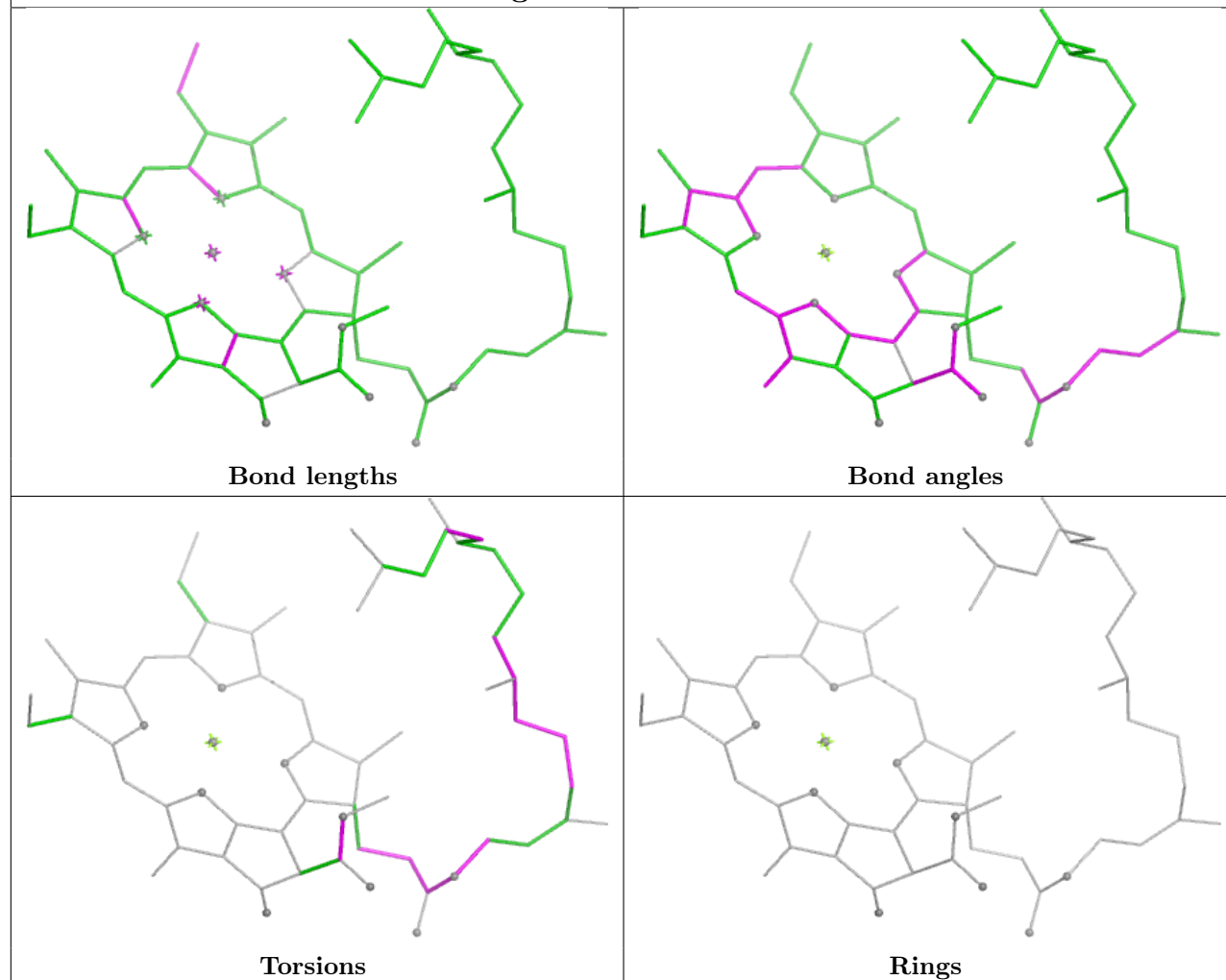
Torsions



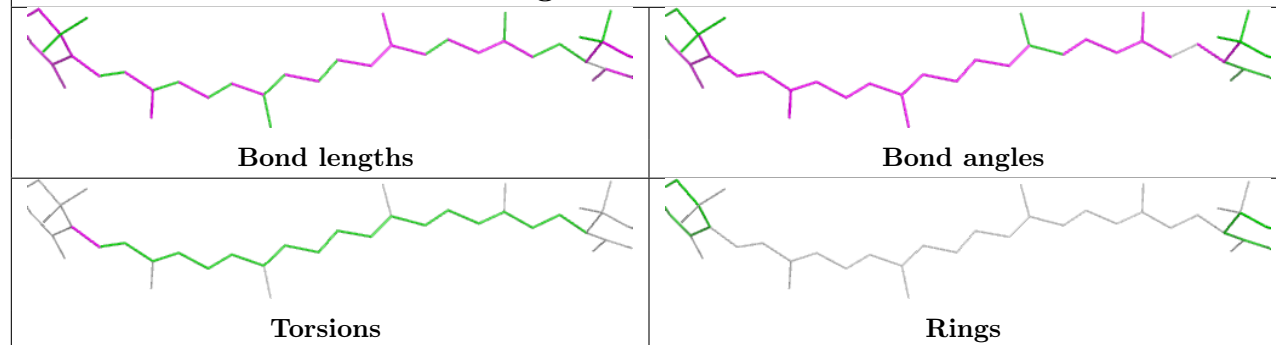
Rings



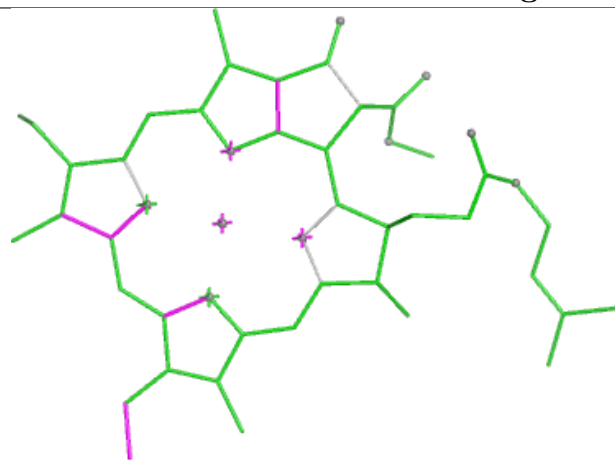
Ligand CLA B 616



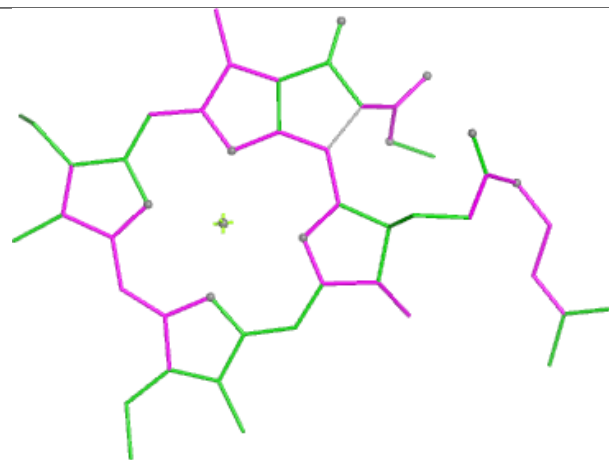
Ligand LUT 1 615



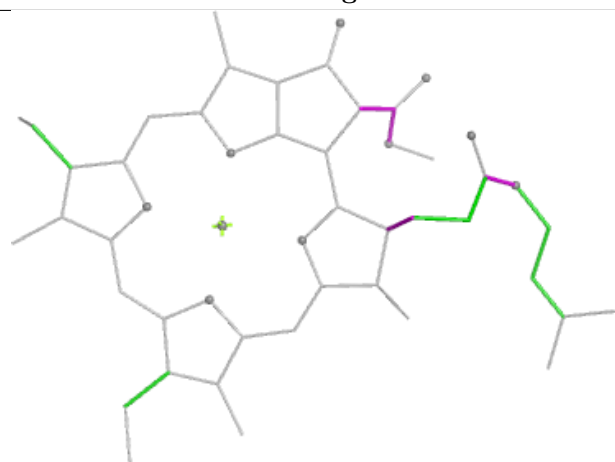
Ligand CLA 5 612



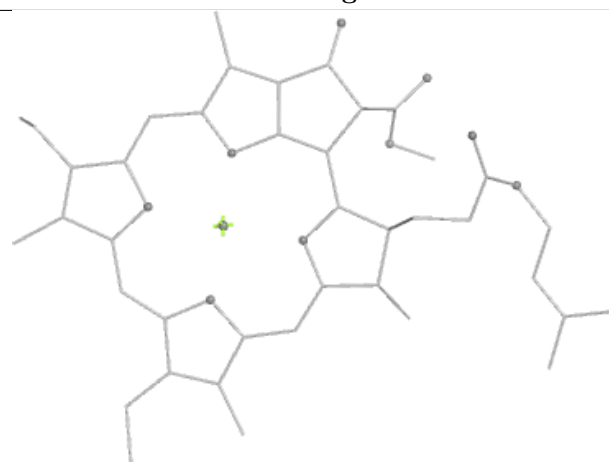
Bond lengths



Bond angles

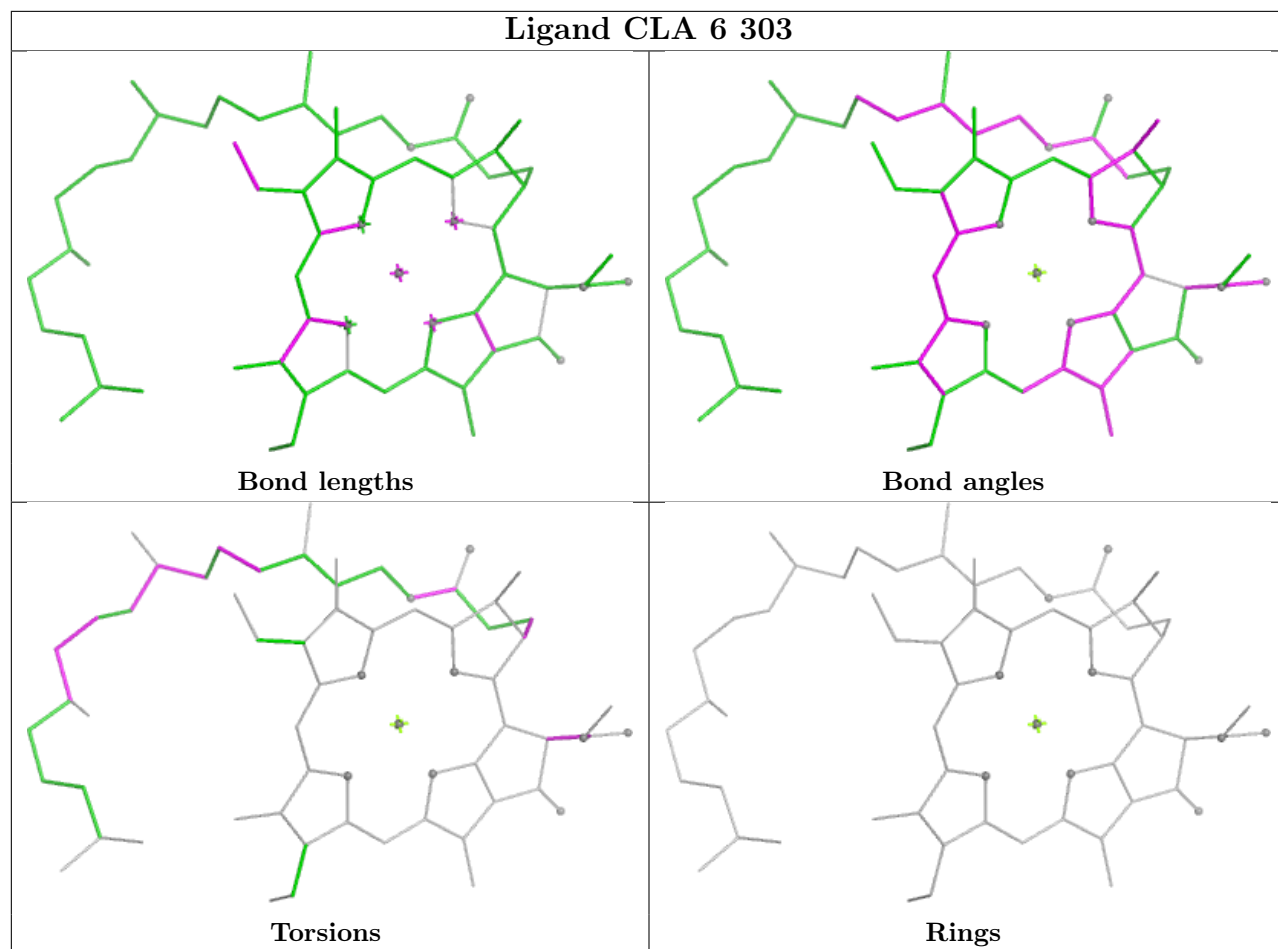


Torsions

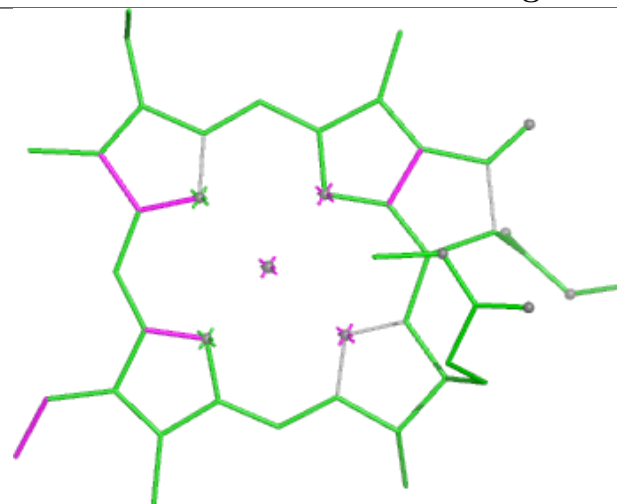


Rings

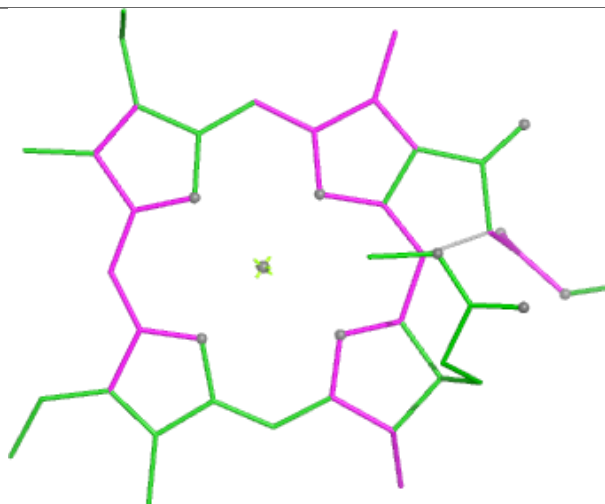
Ligand CLA 6 303



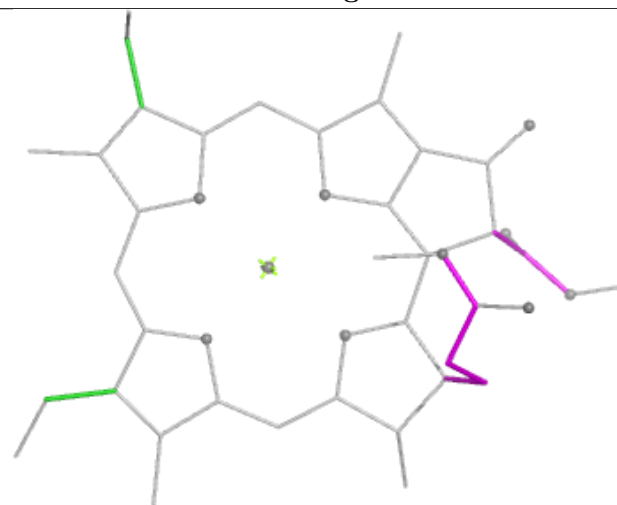
Ligand CLA 9 316



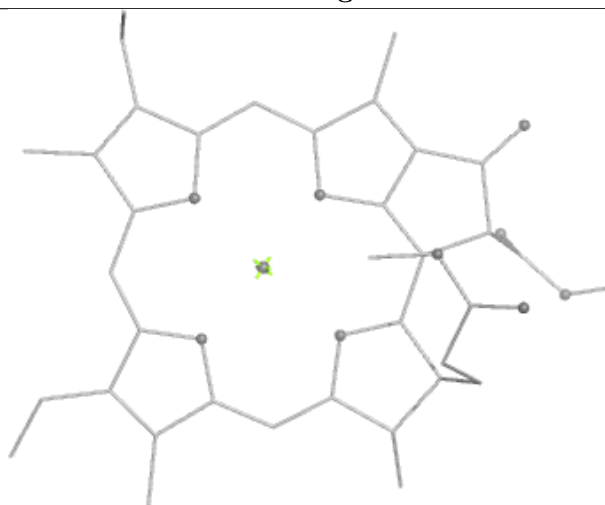
Bond lengths



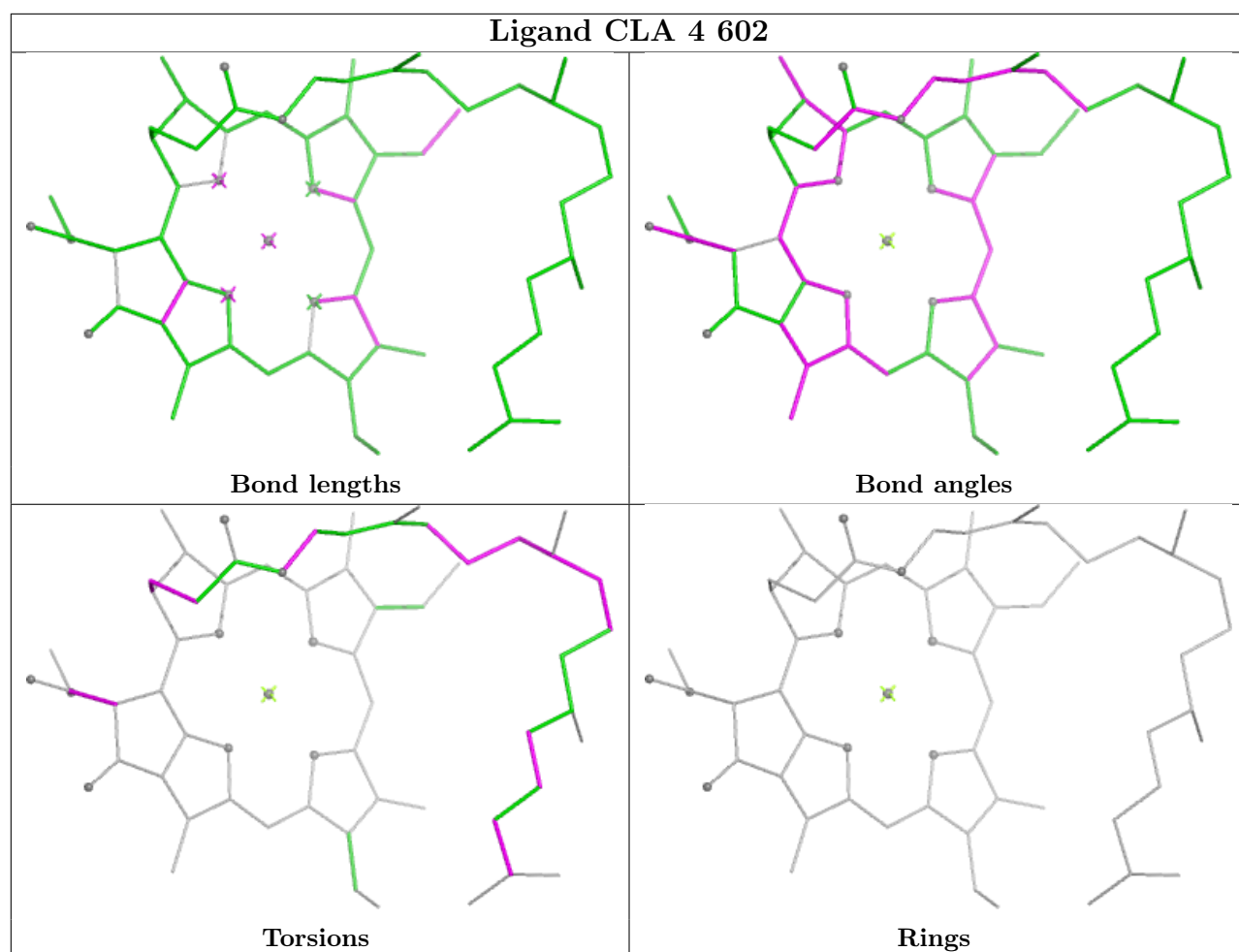
Bond angles



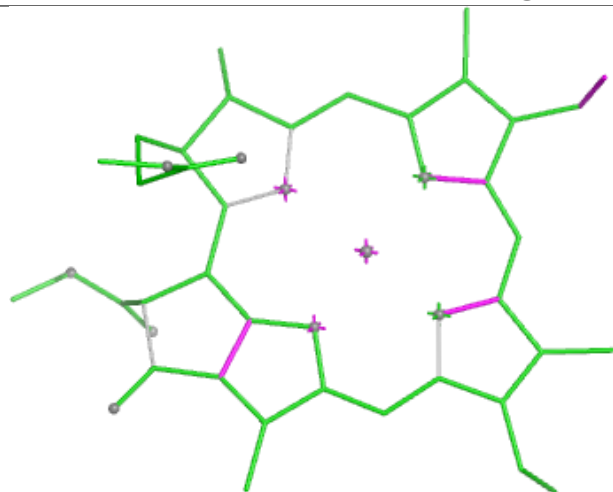
Torsions



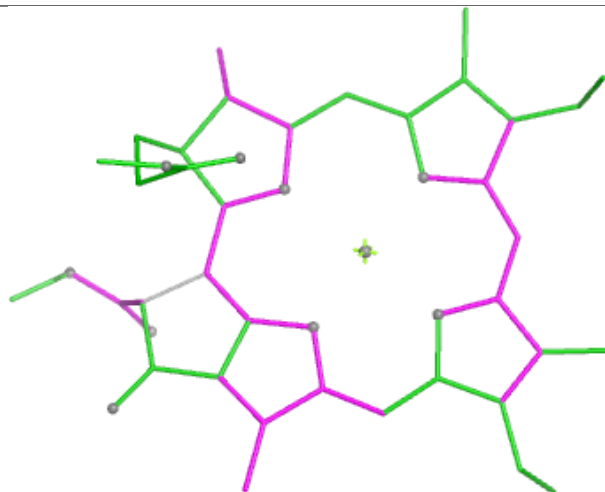
Rings



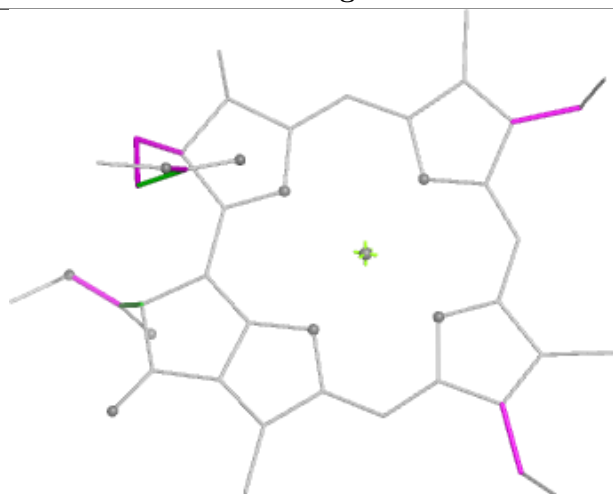
Ligand CLA 5 615



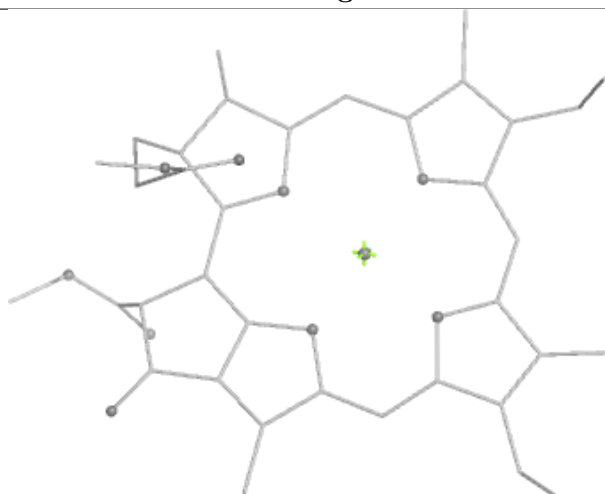
Bond lengths



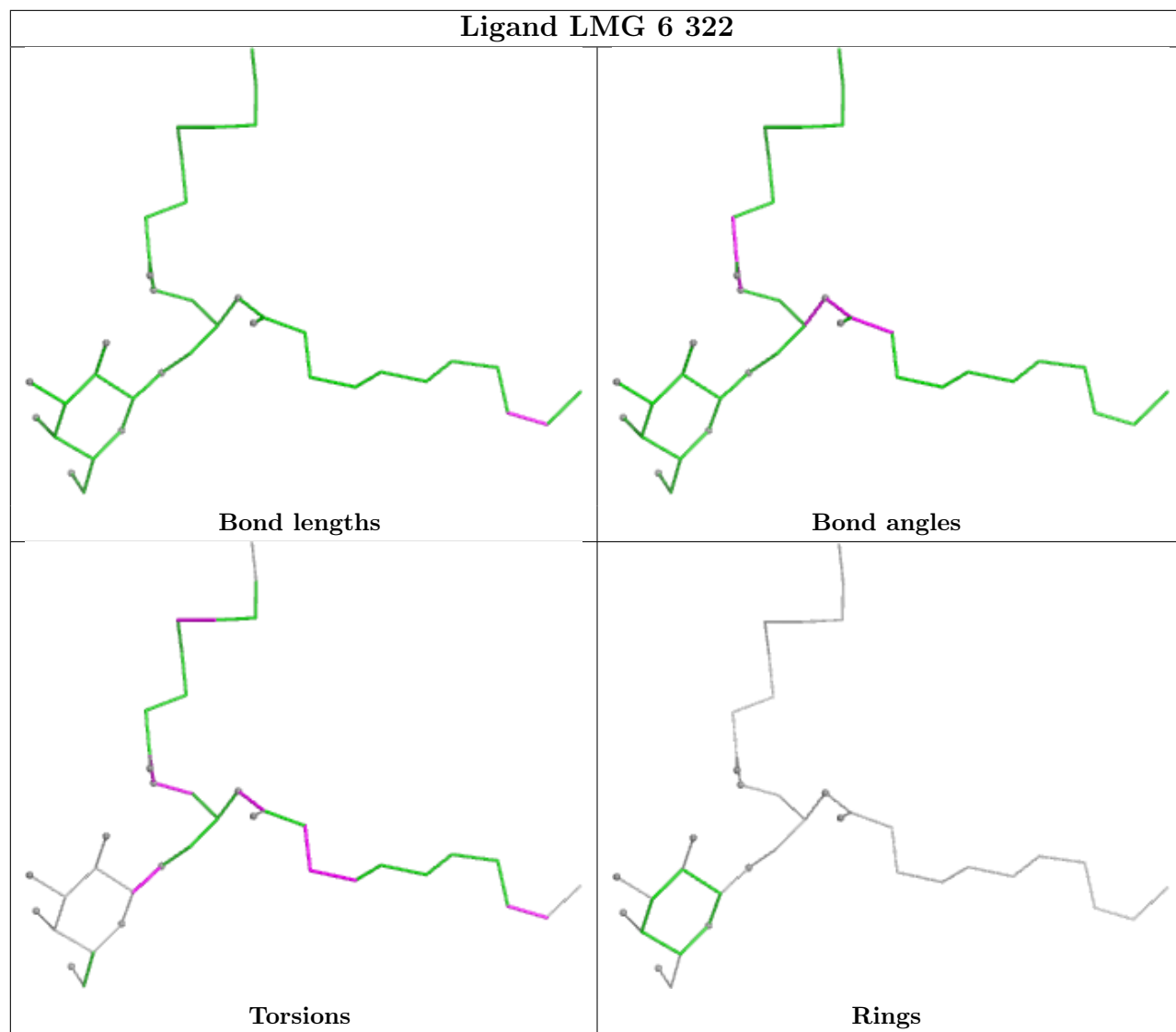
Bond angles

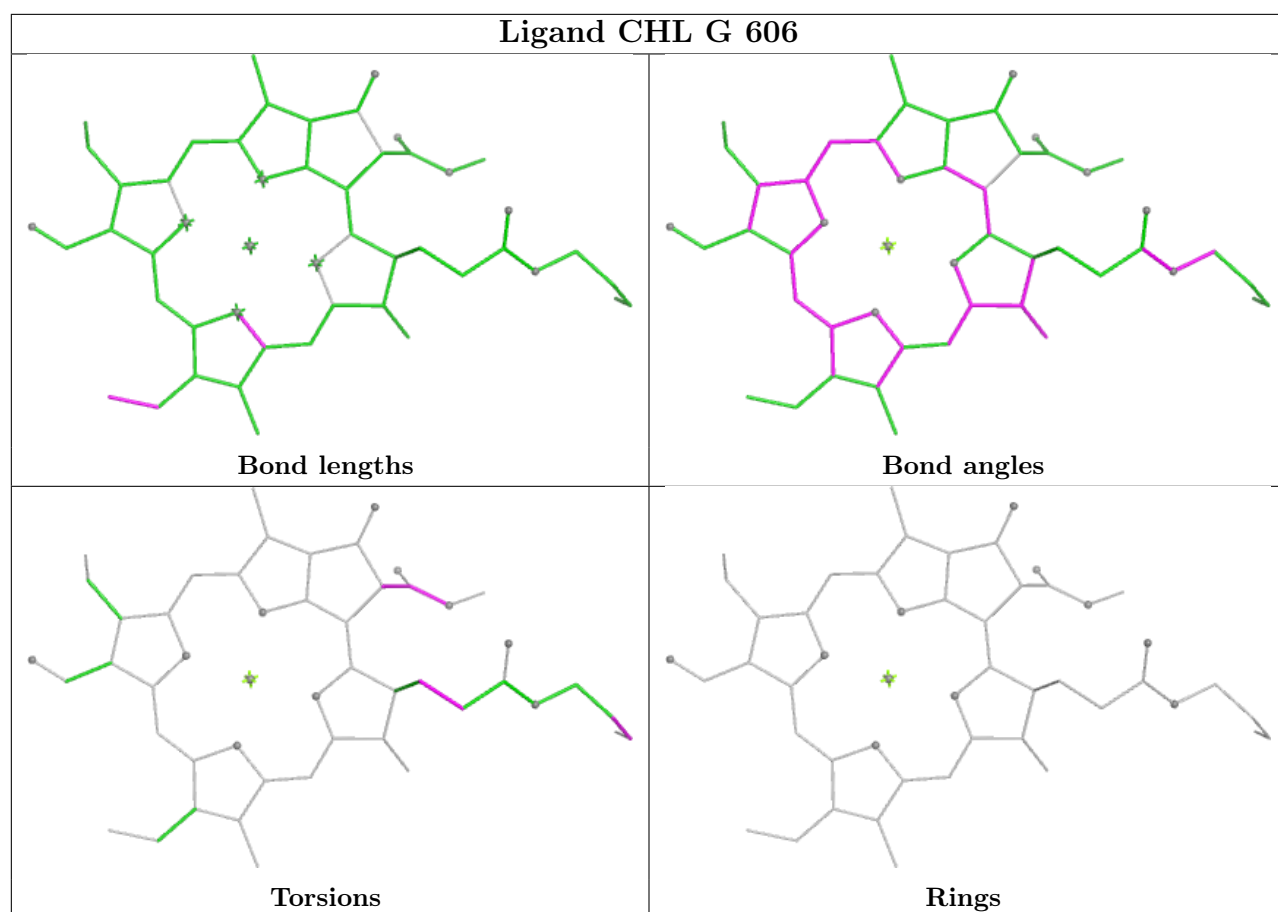


Torsions

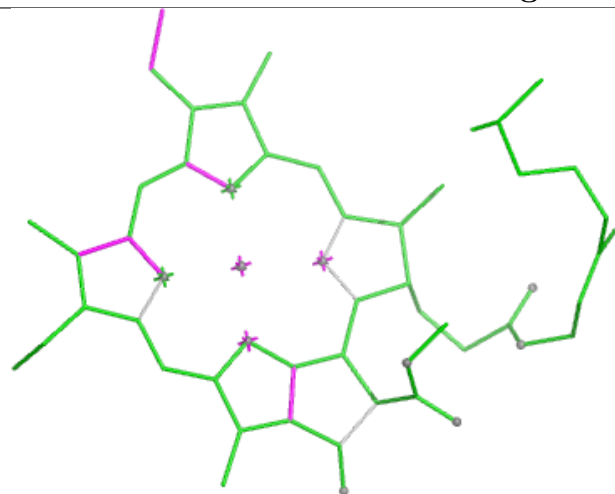


Rings

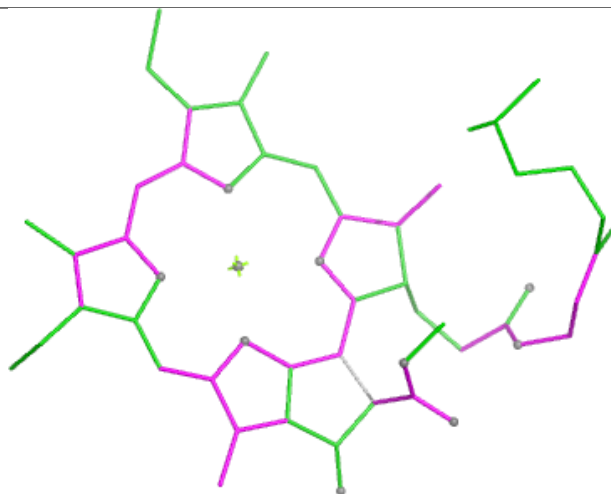




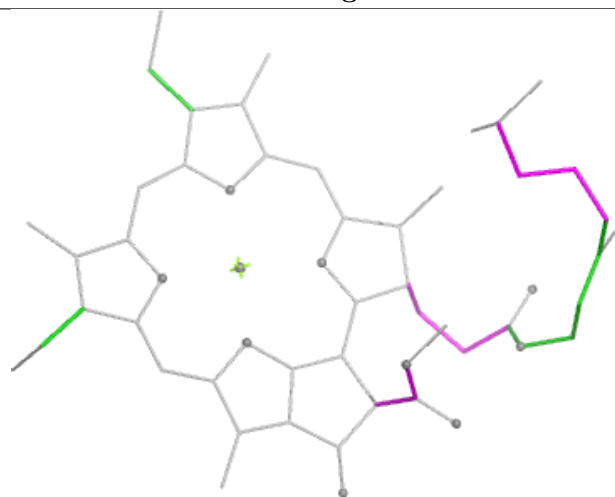
Ligand CLA 3 305



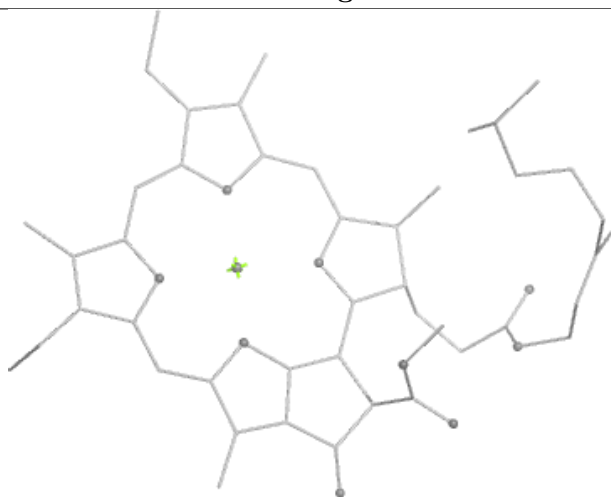
Bond lengths



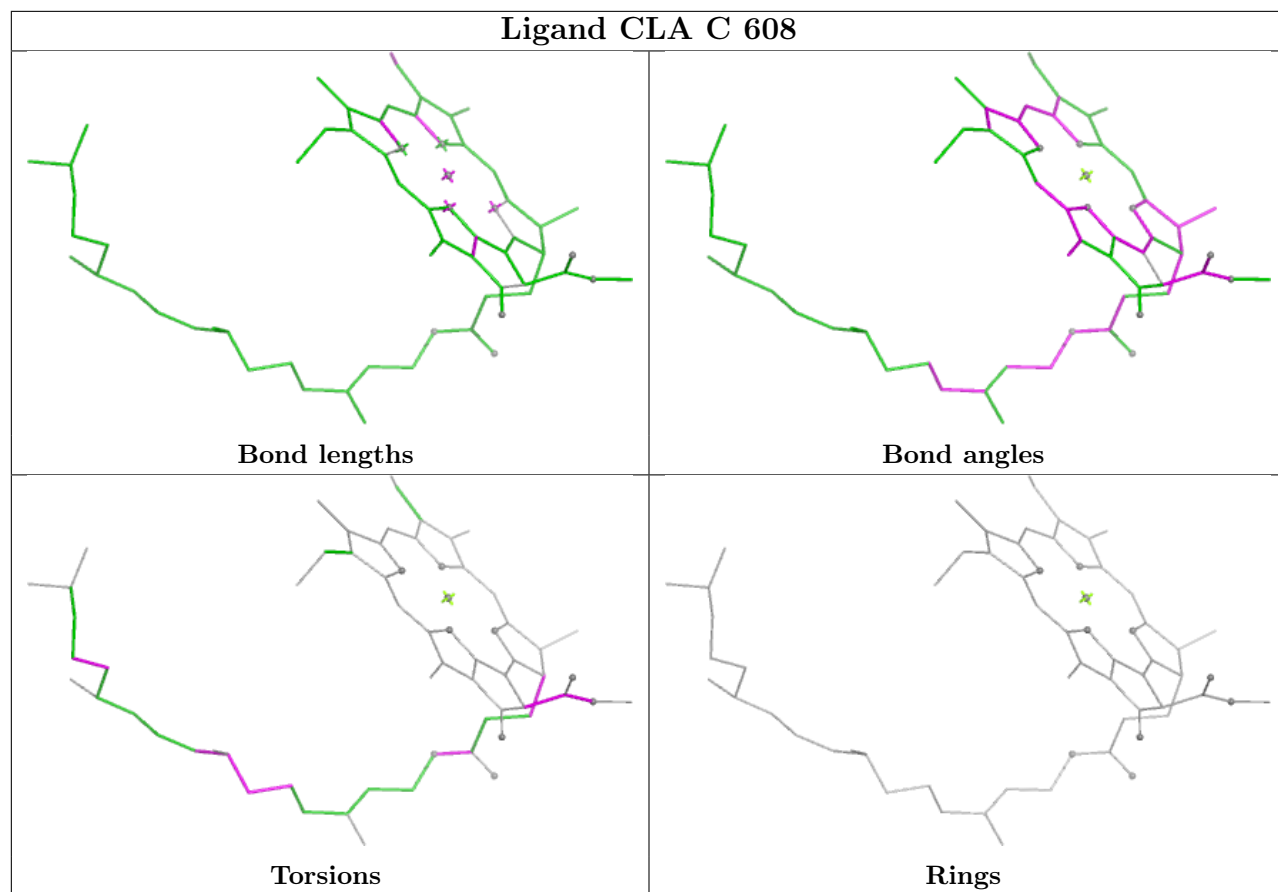
Bond angles

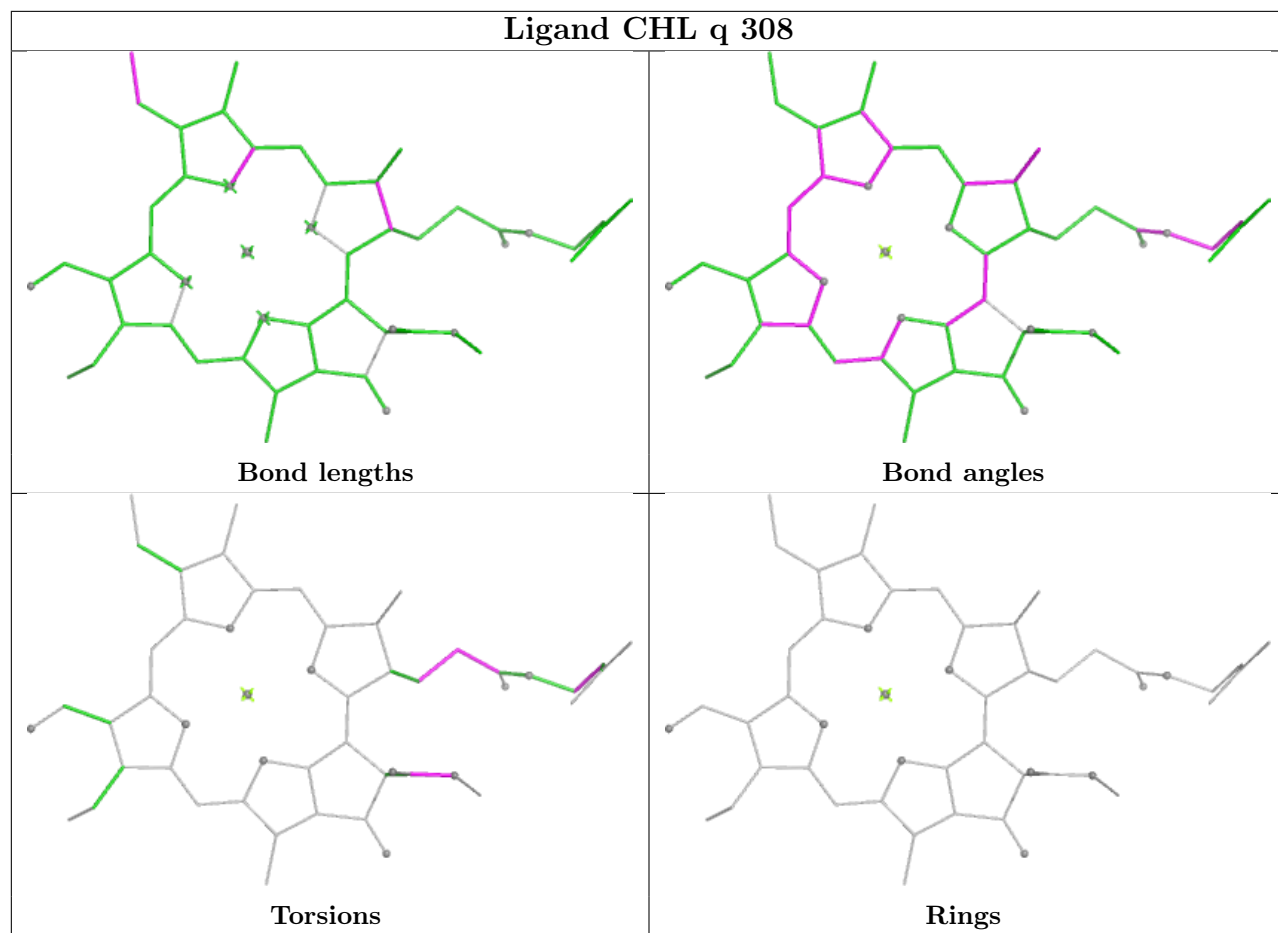


Torsions

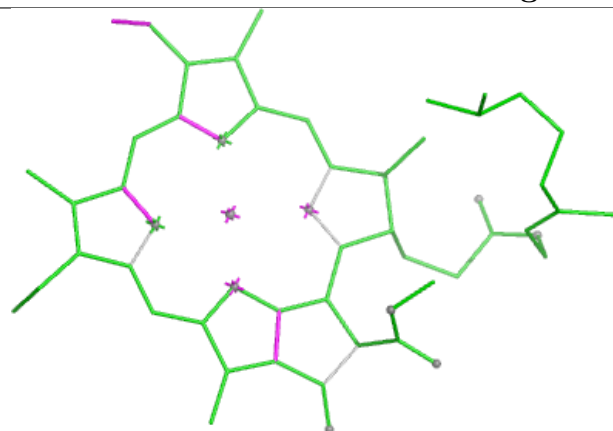


Rings

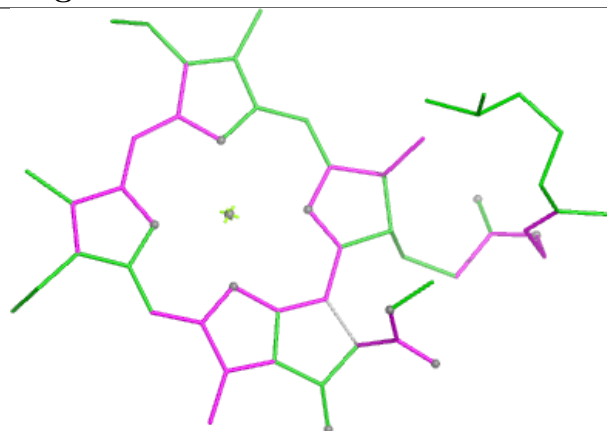




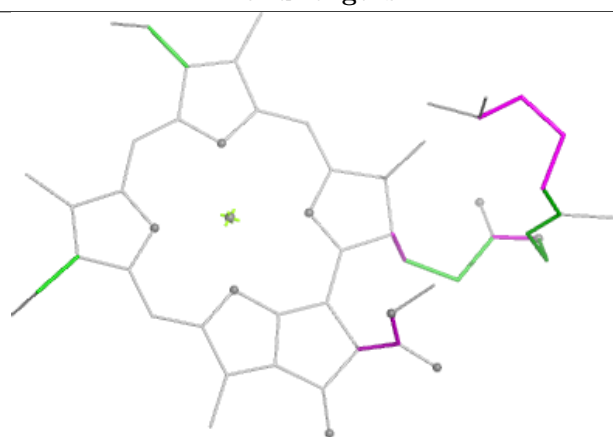
Ligand CLA g 304



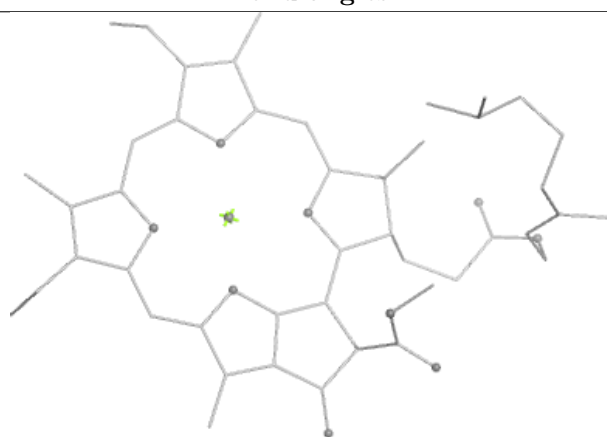
Bond lengths



Bond angles

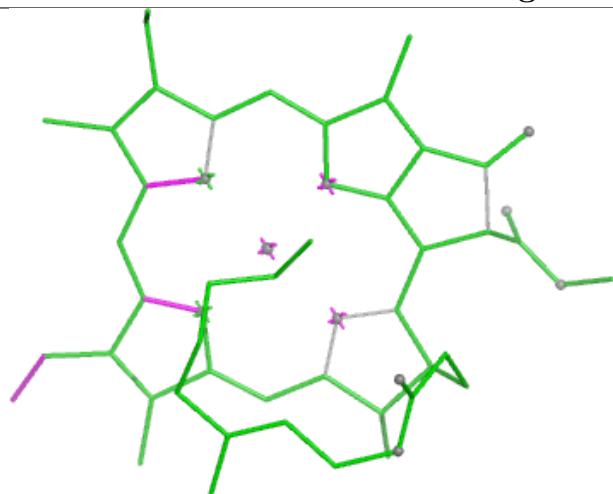


Torsions

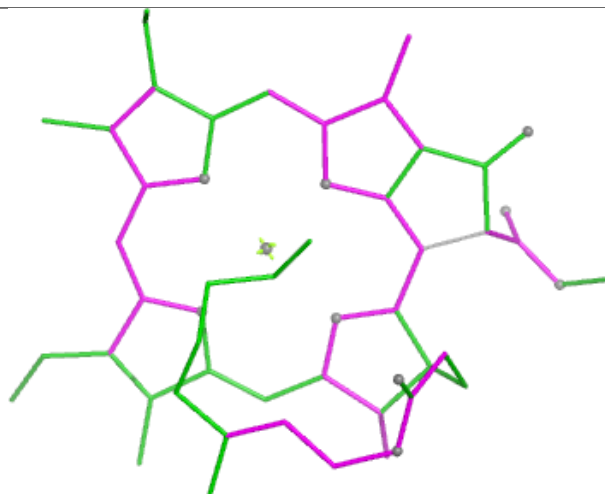


Rings

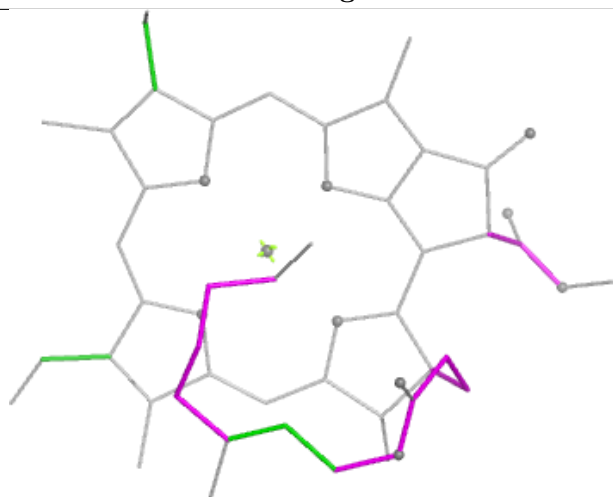
Ligand CLA 1 614



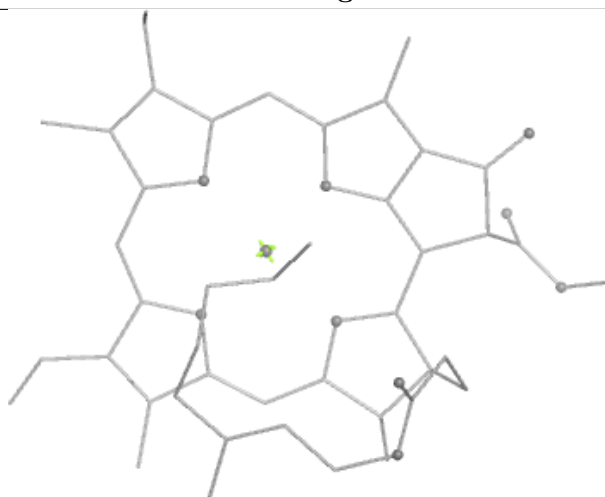
Bond lengths



Bond angles

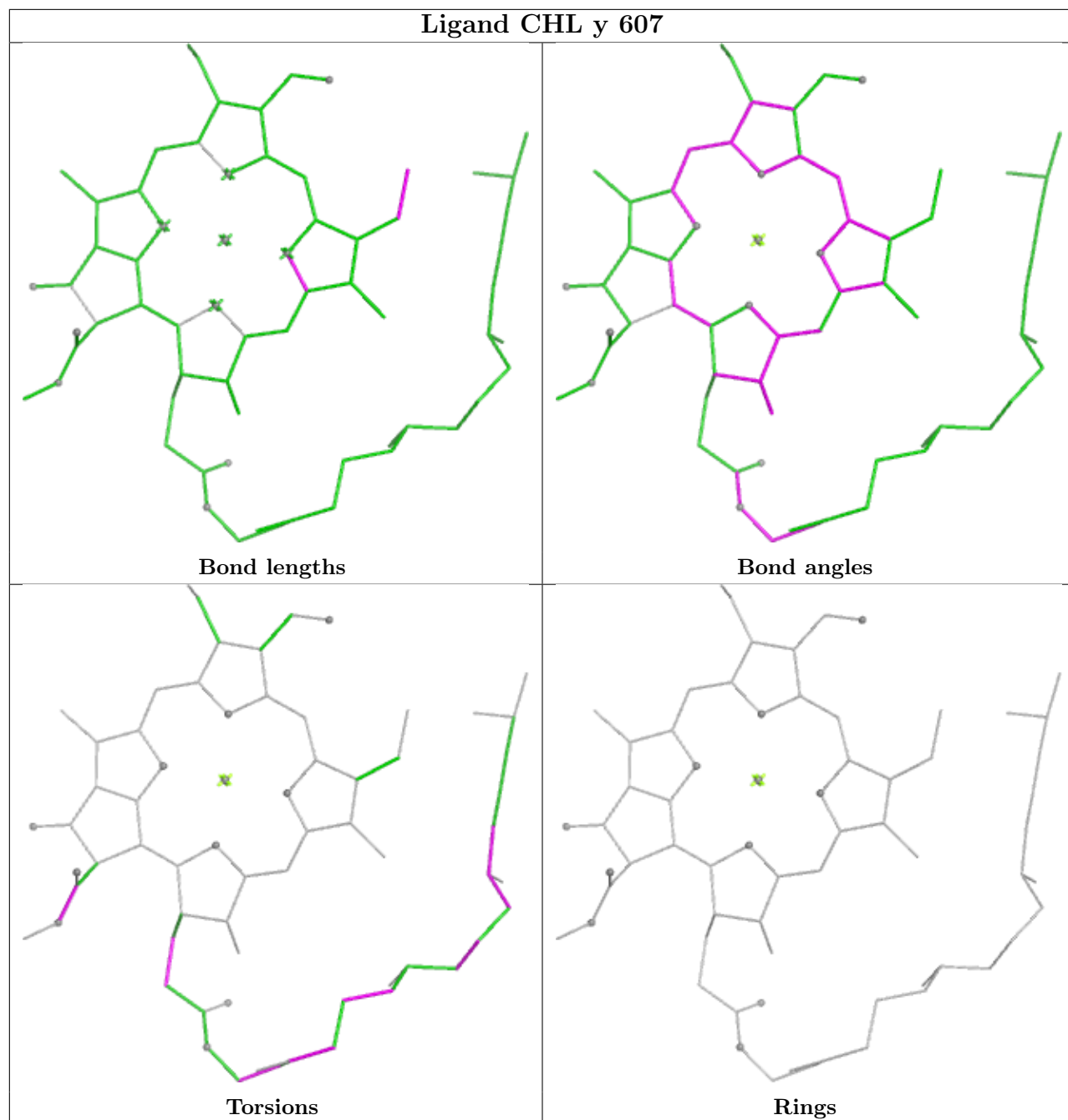


Torsions

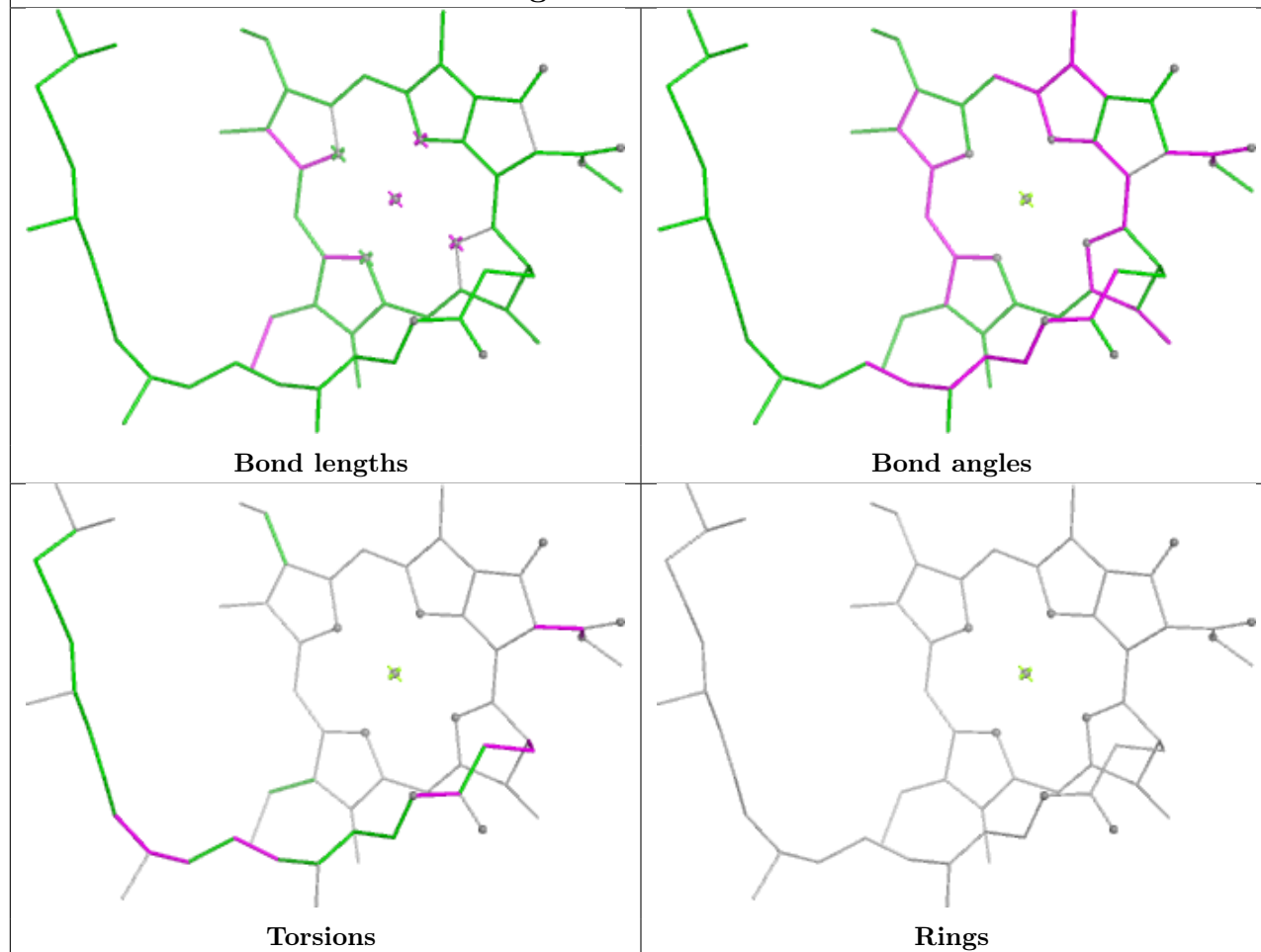


Rings

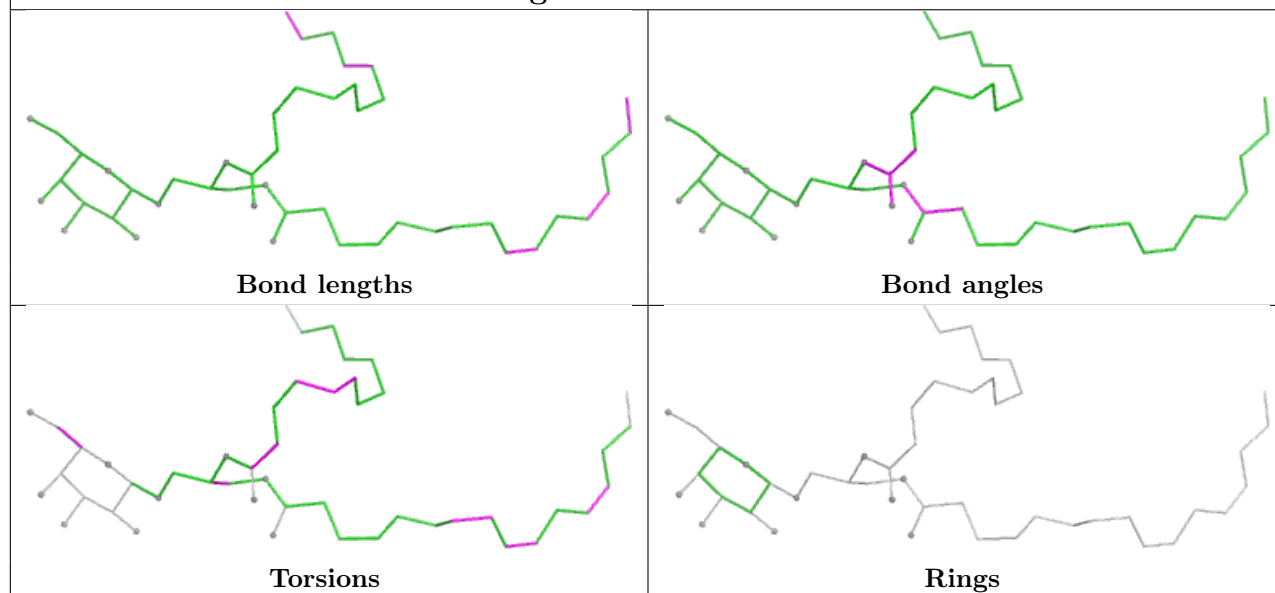
Ligand CHL y 607



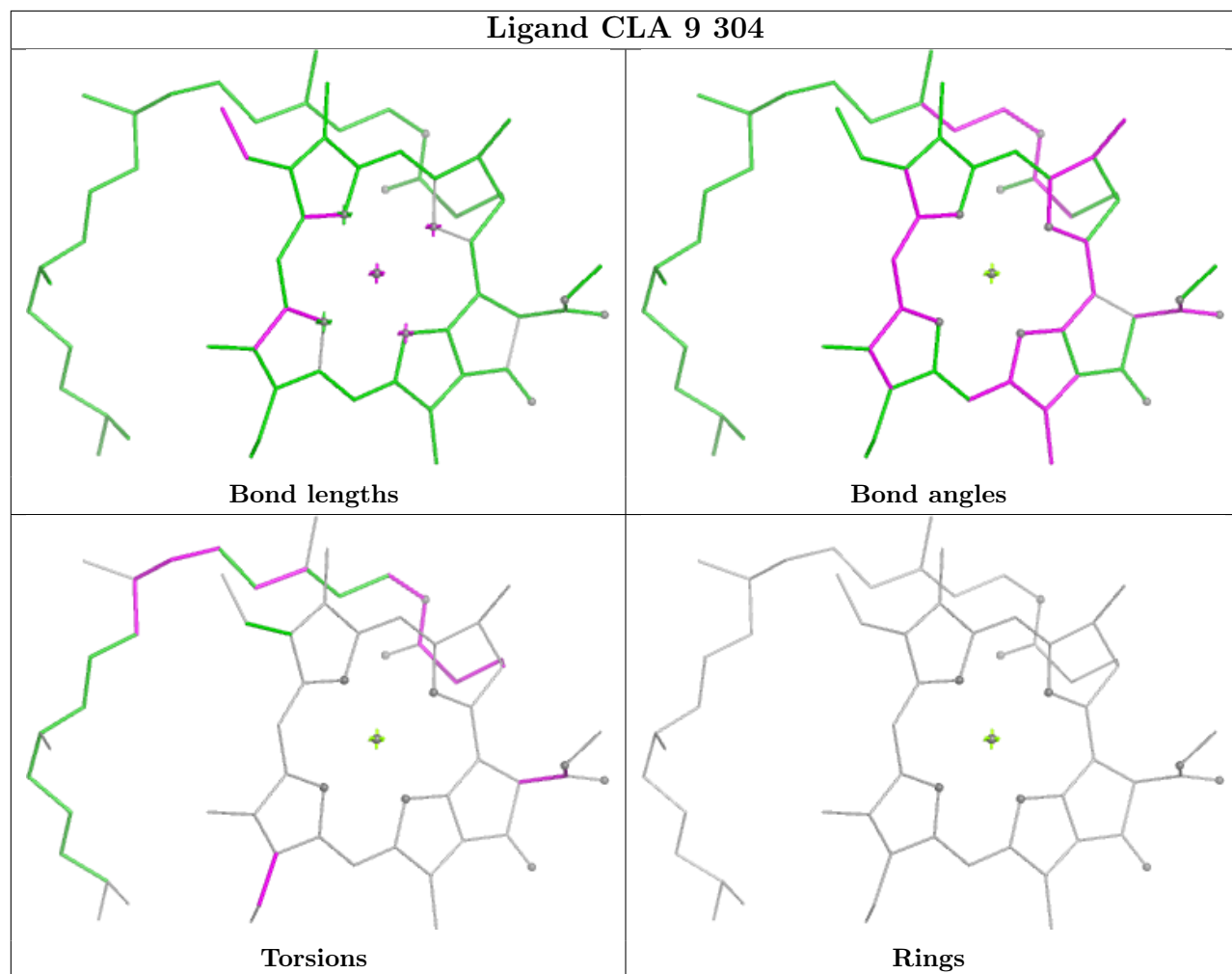
Ligand CLA 8 602

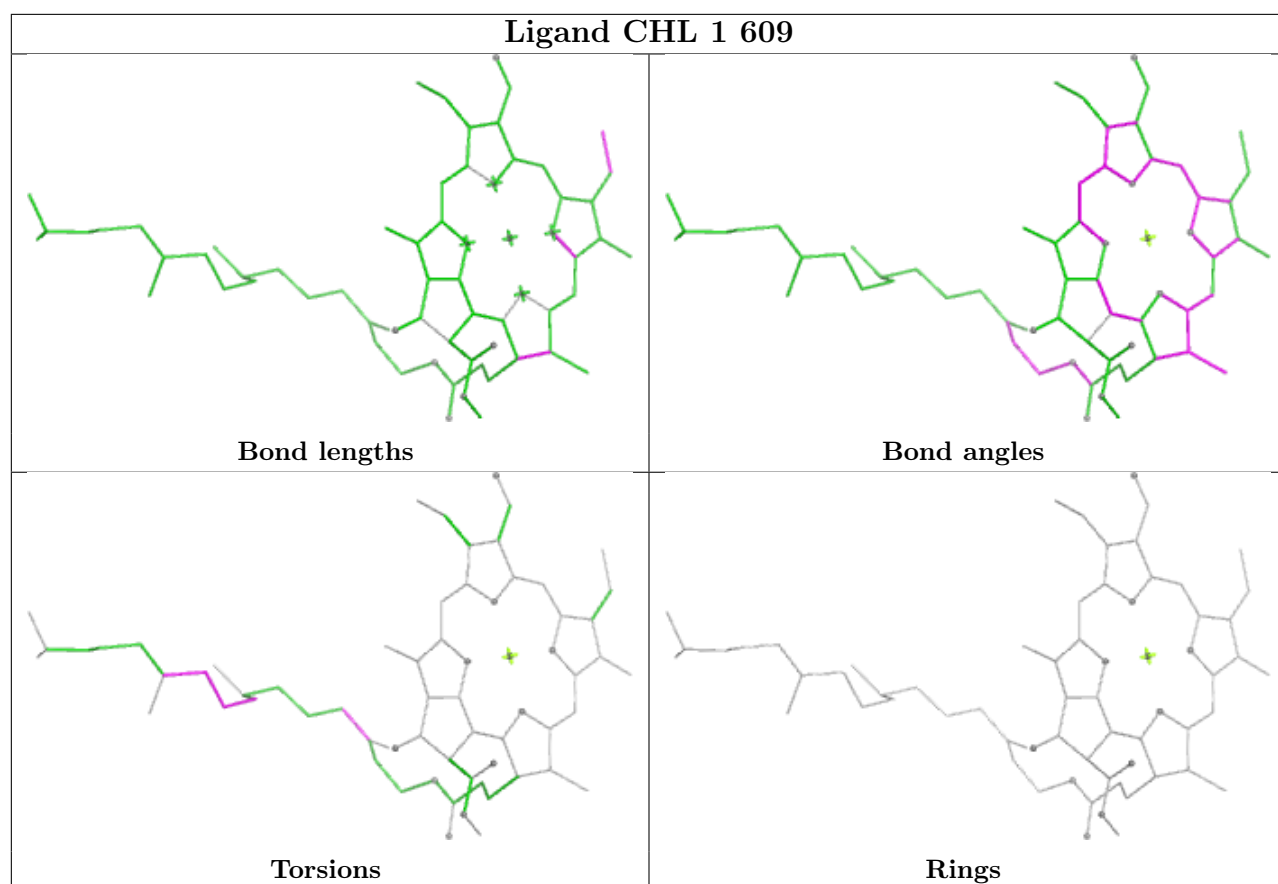


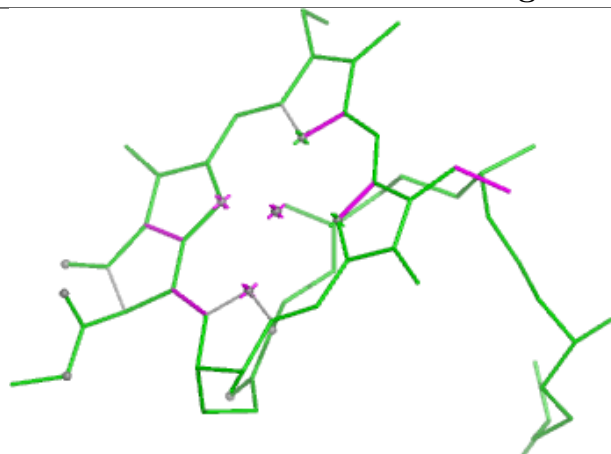
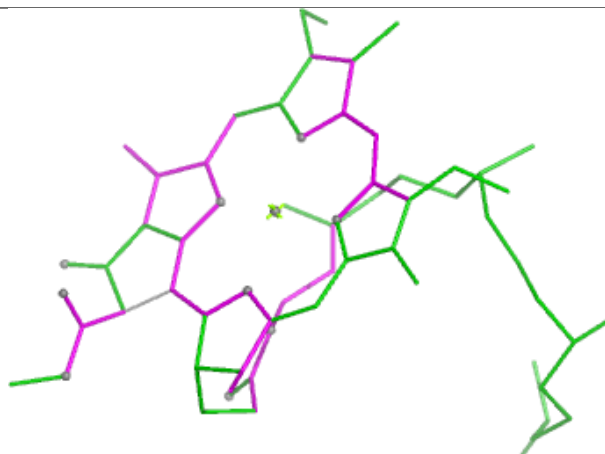
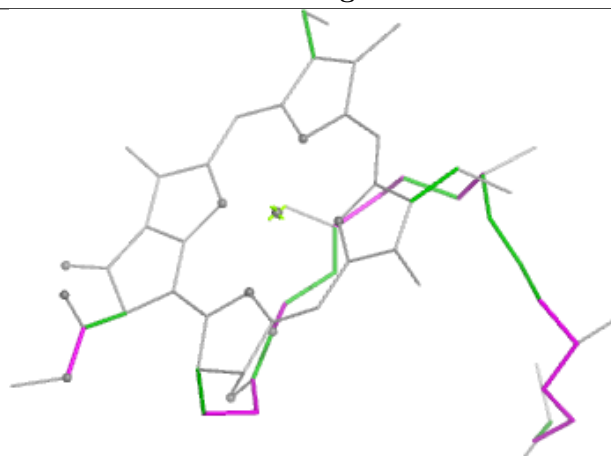
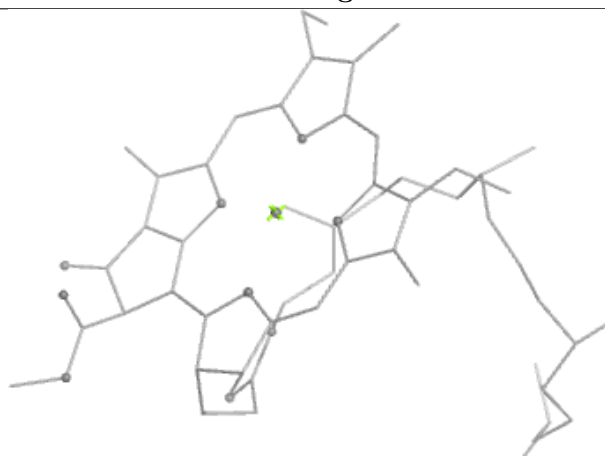
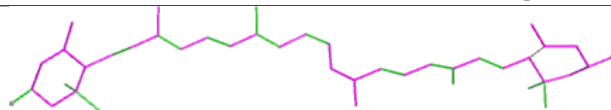
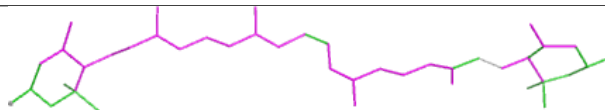
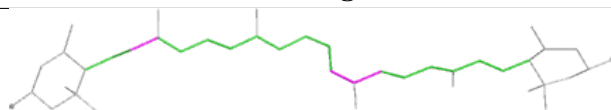
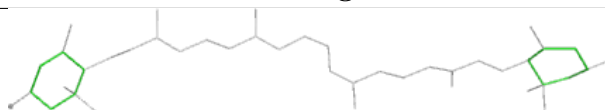
Ligand LMG d 411

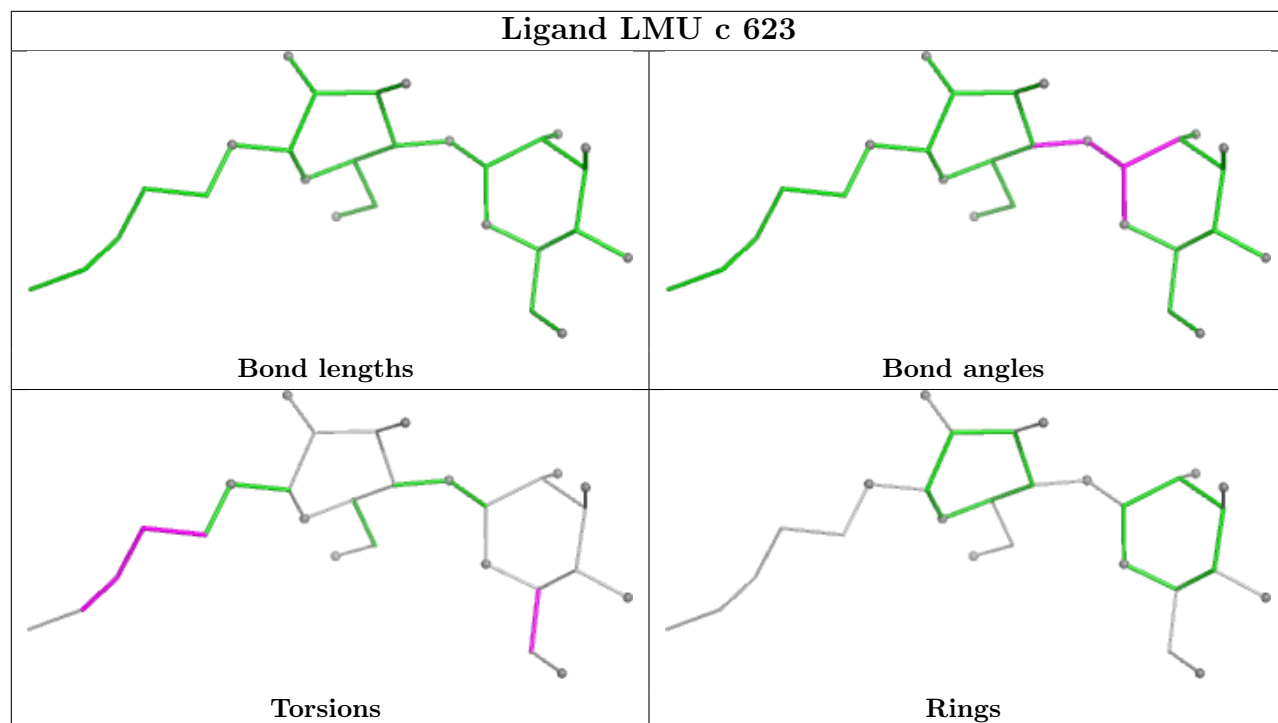


Ligand CLA 9 304

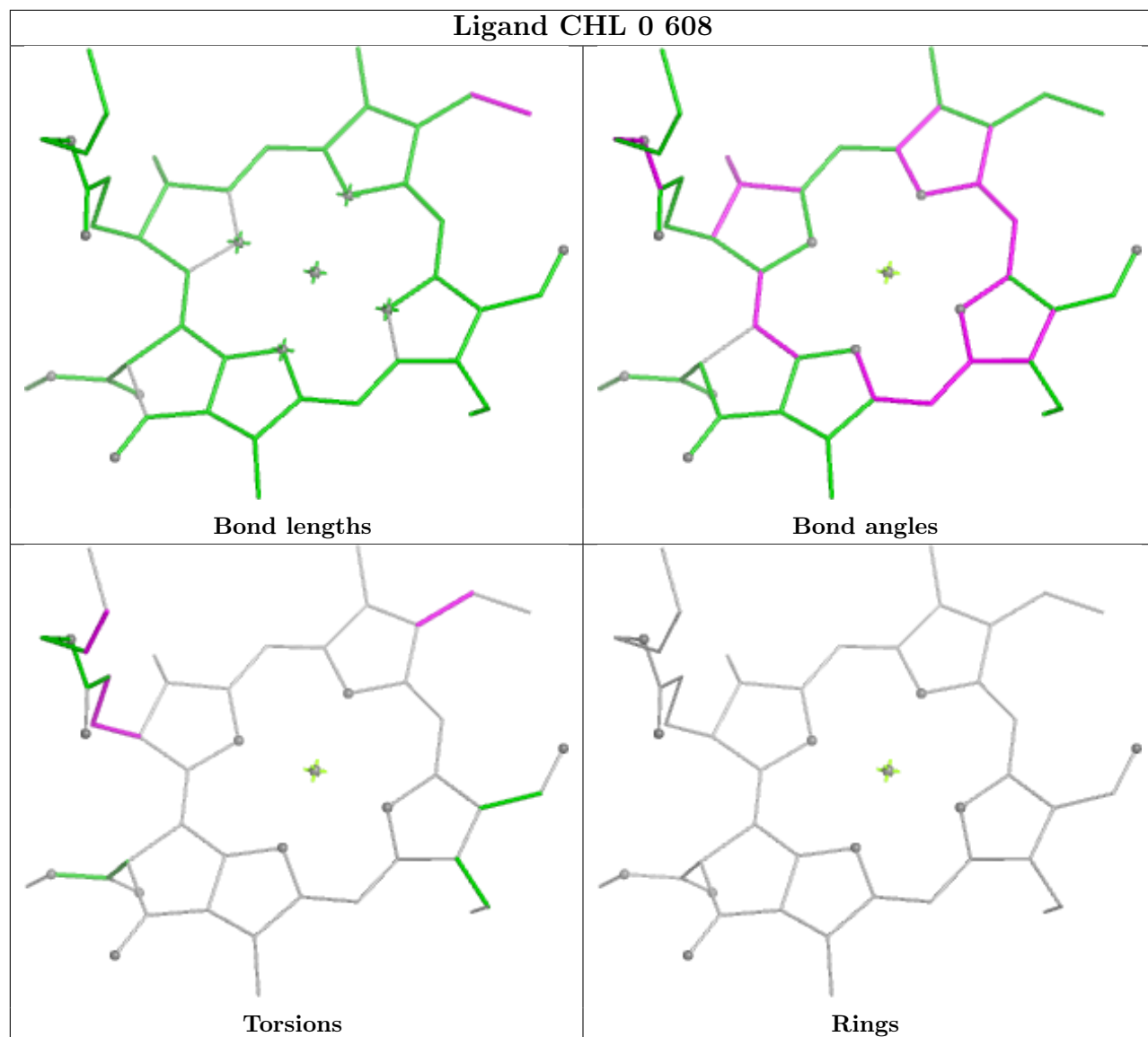




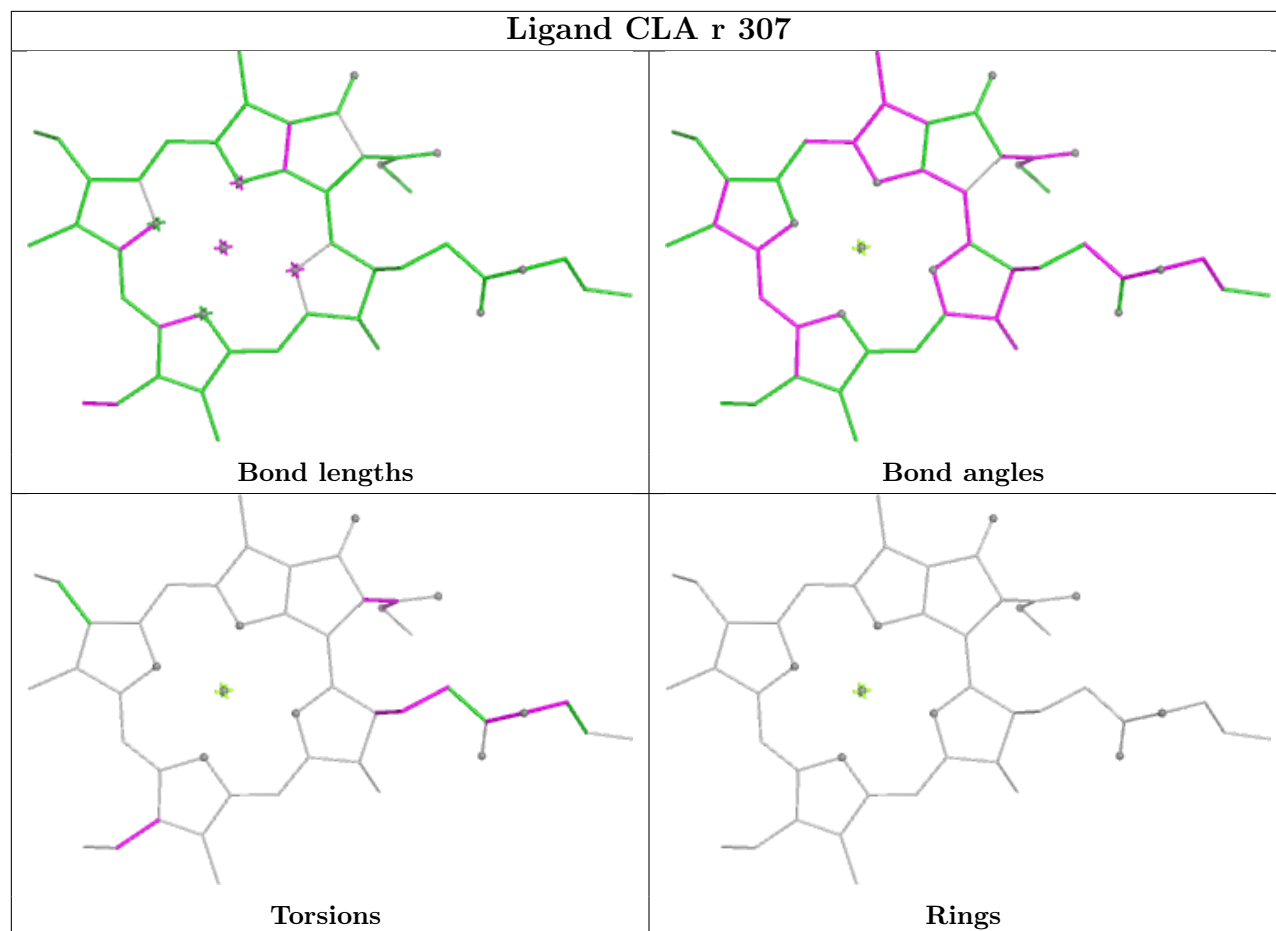
Ligand CLA 1 613**Bond lengths****Bond angles****Torsions****Rings****Ligand LUT 9 318****Bond lengths****Bond angles****Torsions****Rings**

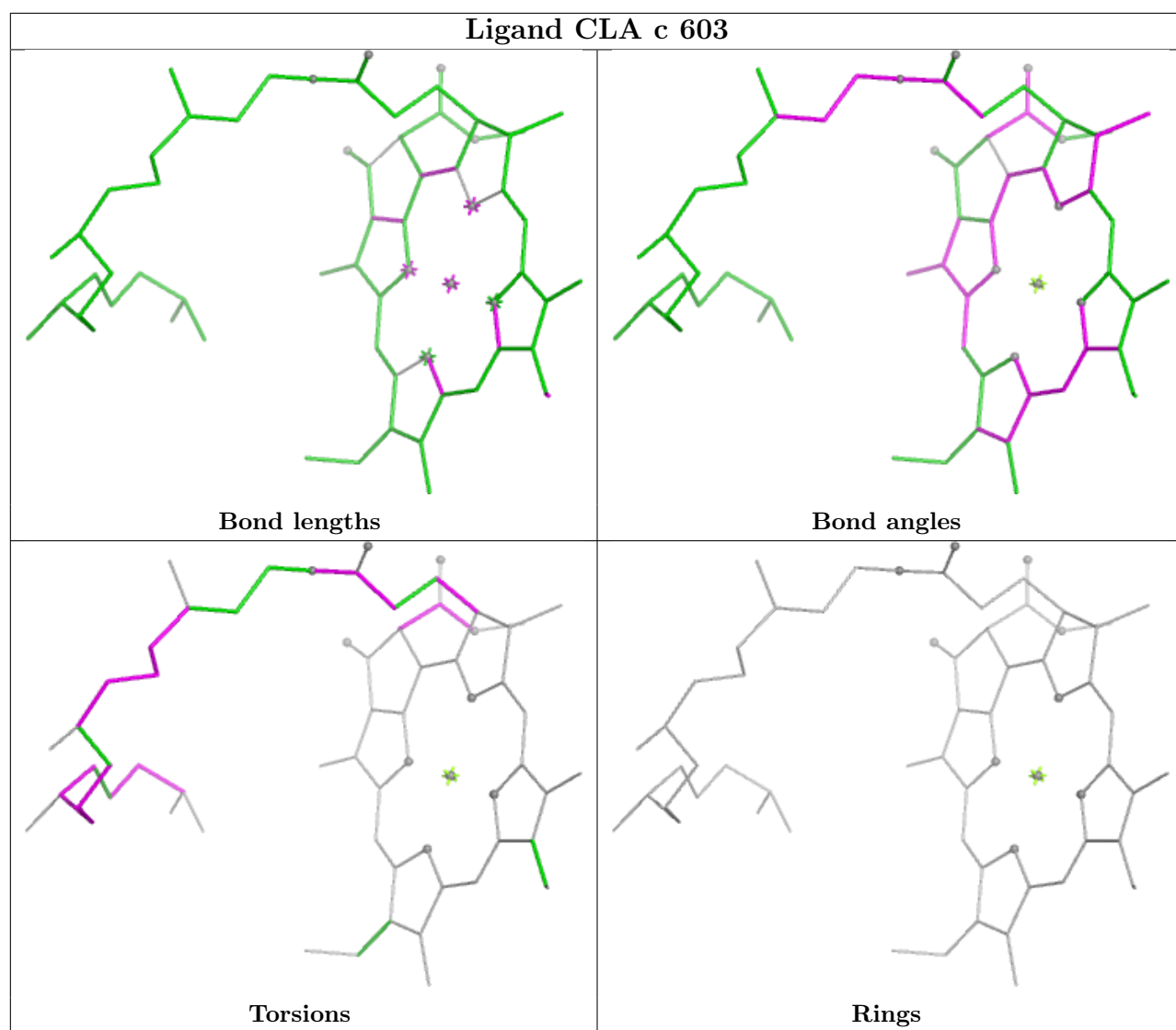


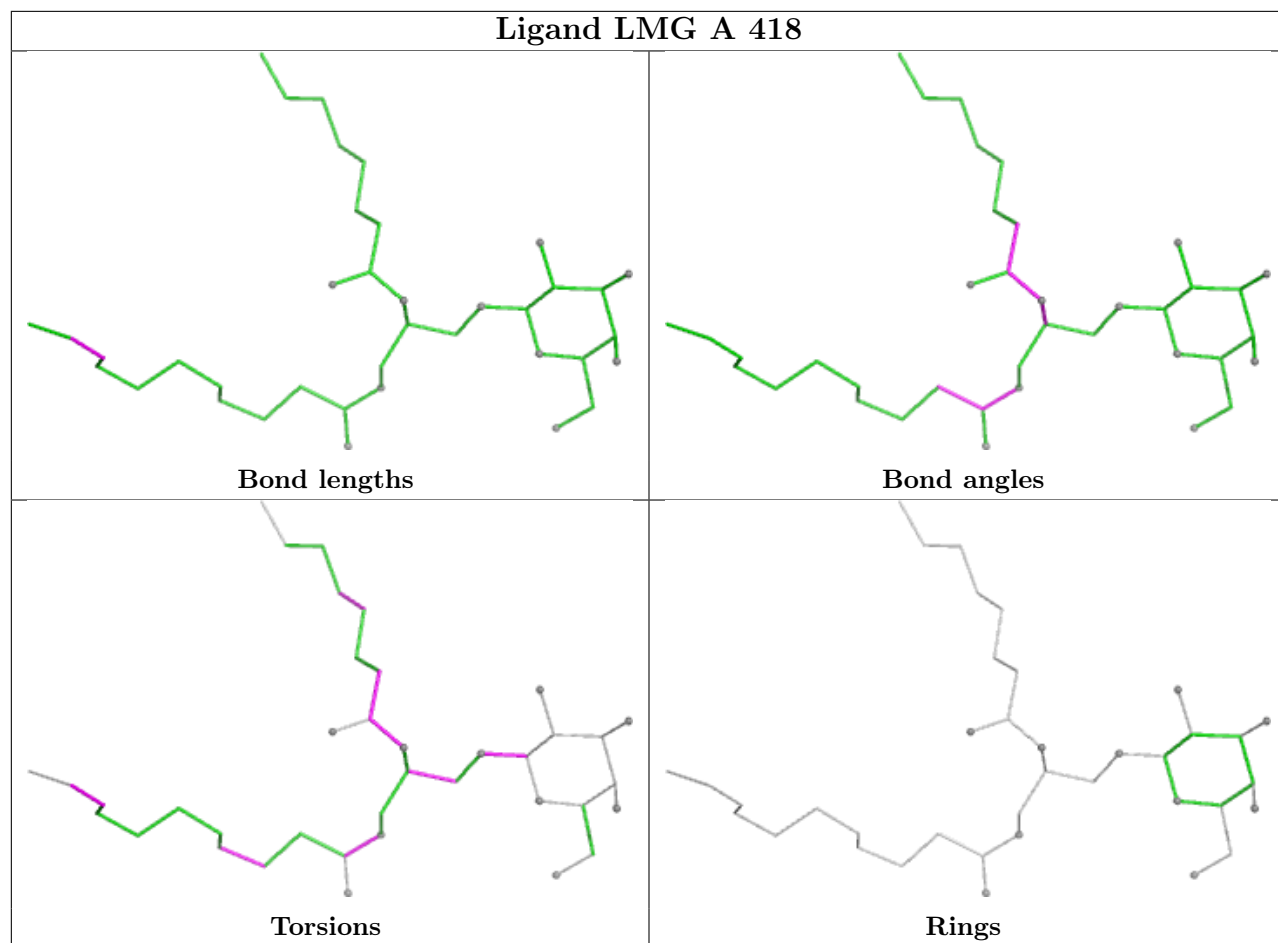
Ligand CHL 0 608



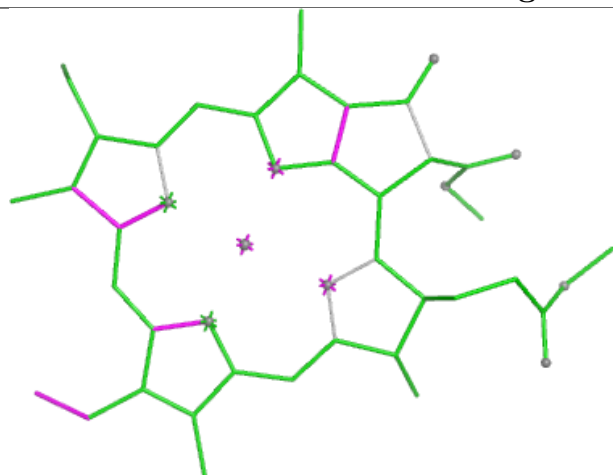
Ligand CLA r 307



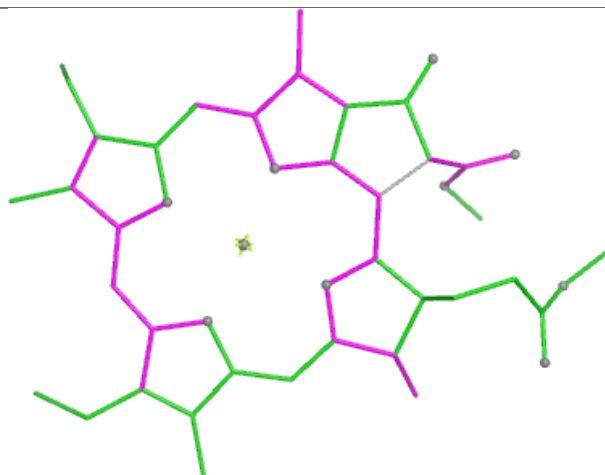




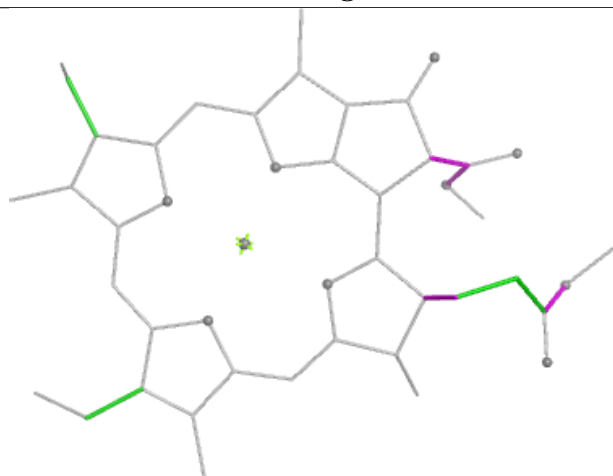
Ligand CLA 0 612



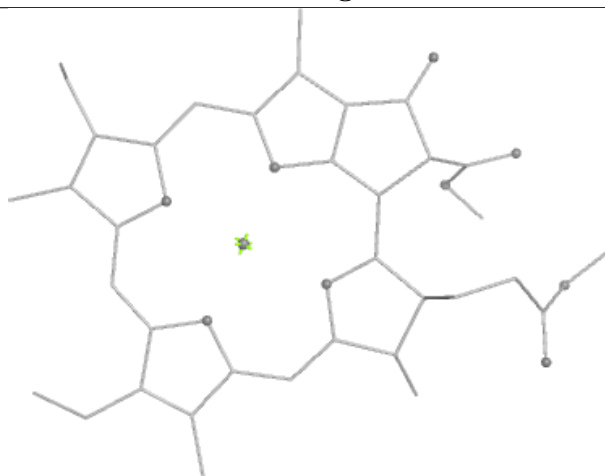
Bond lengths



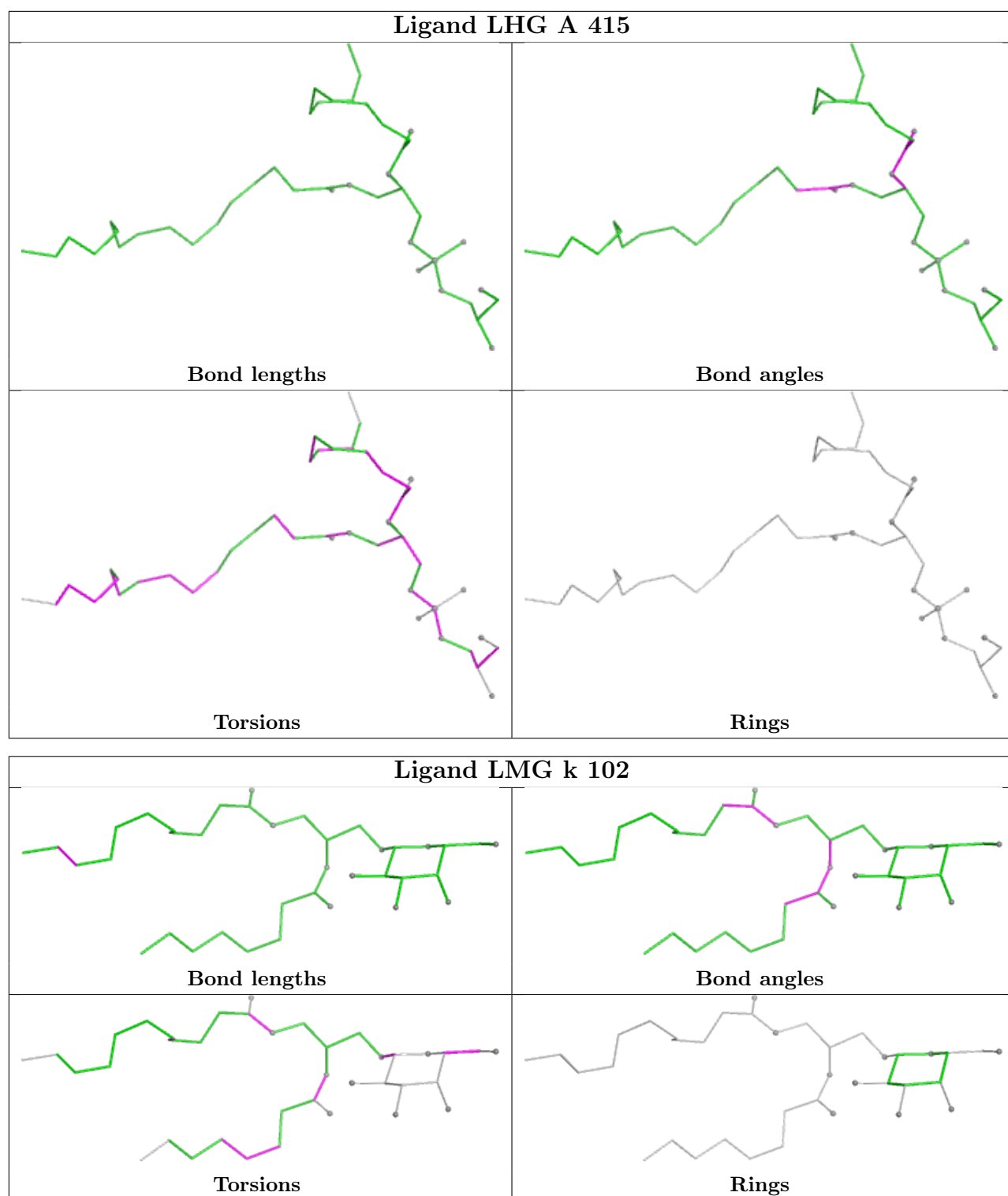
Bond angles

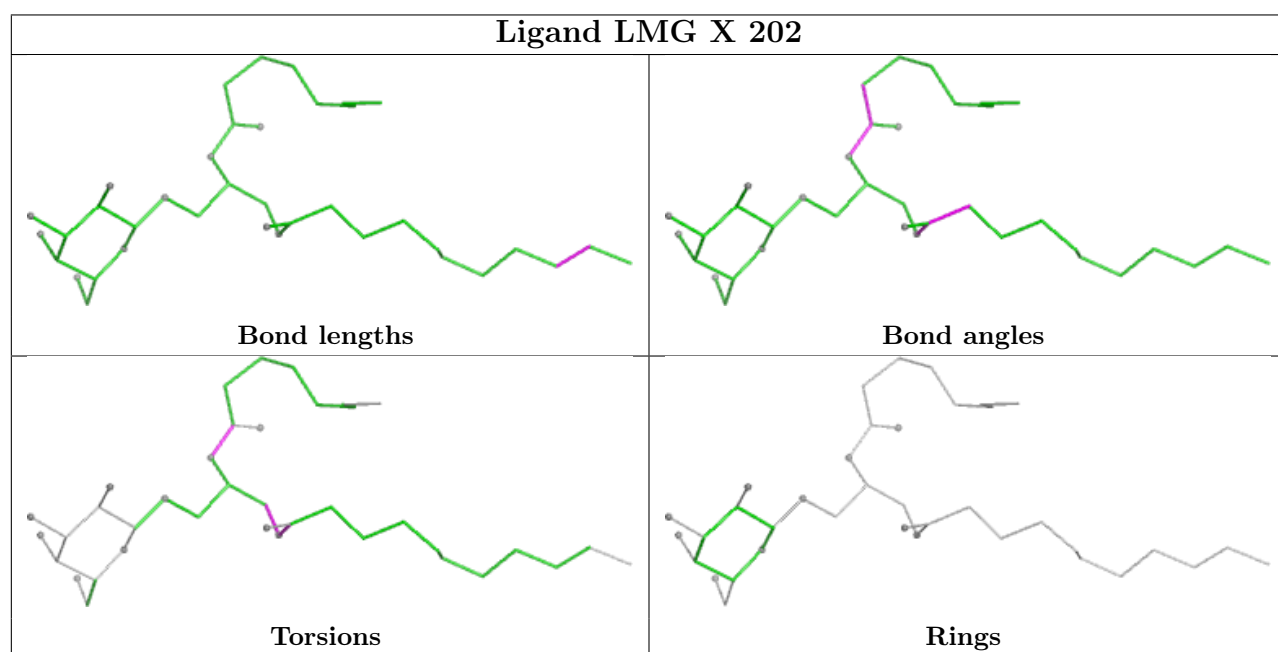
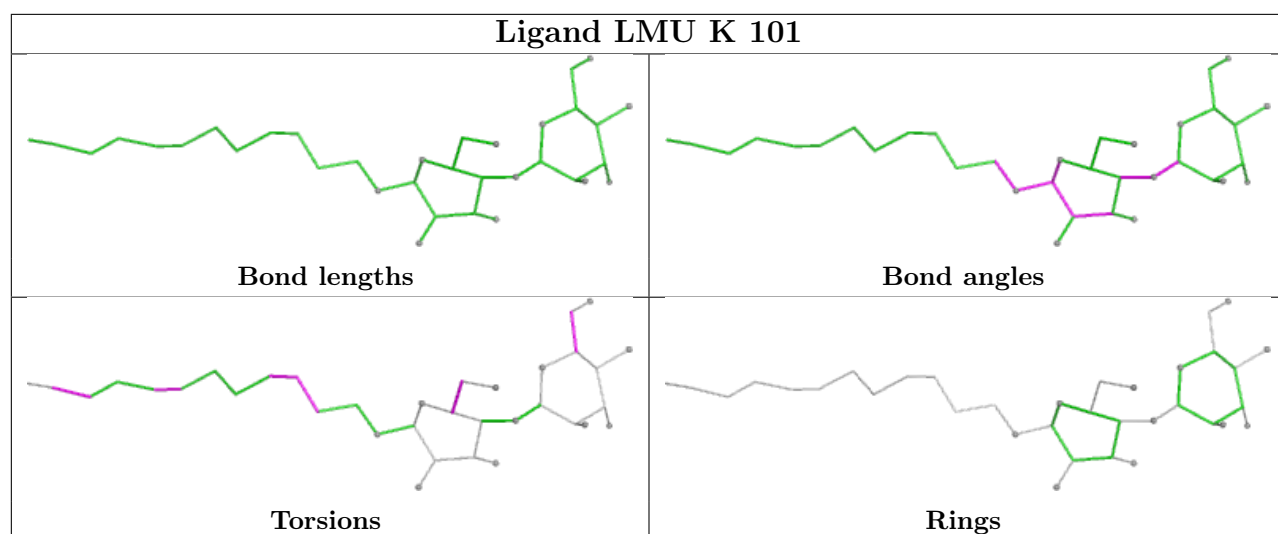


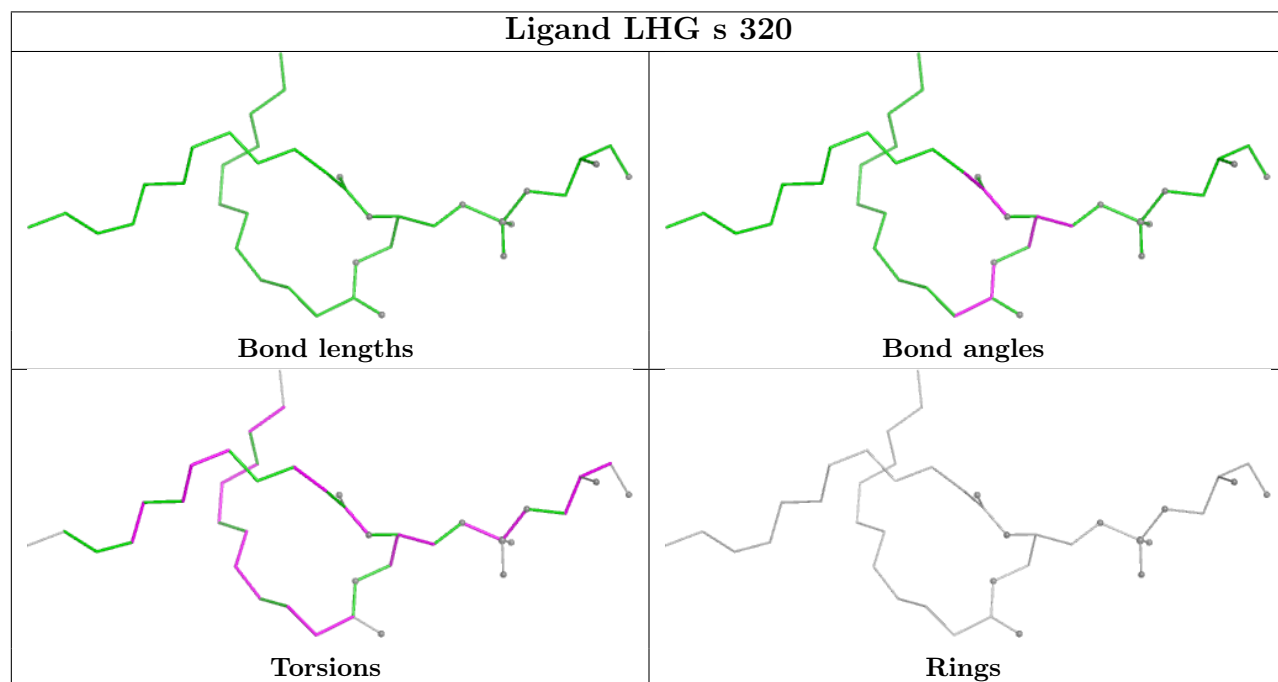
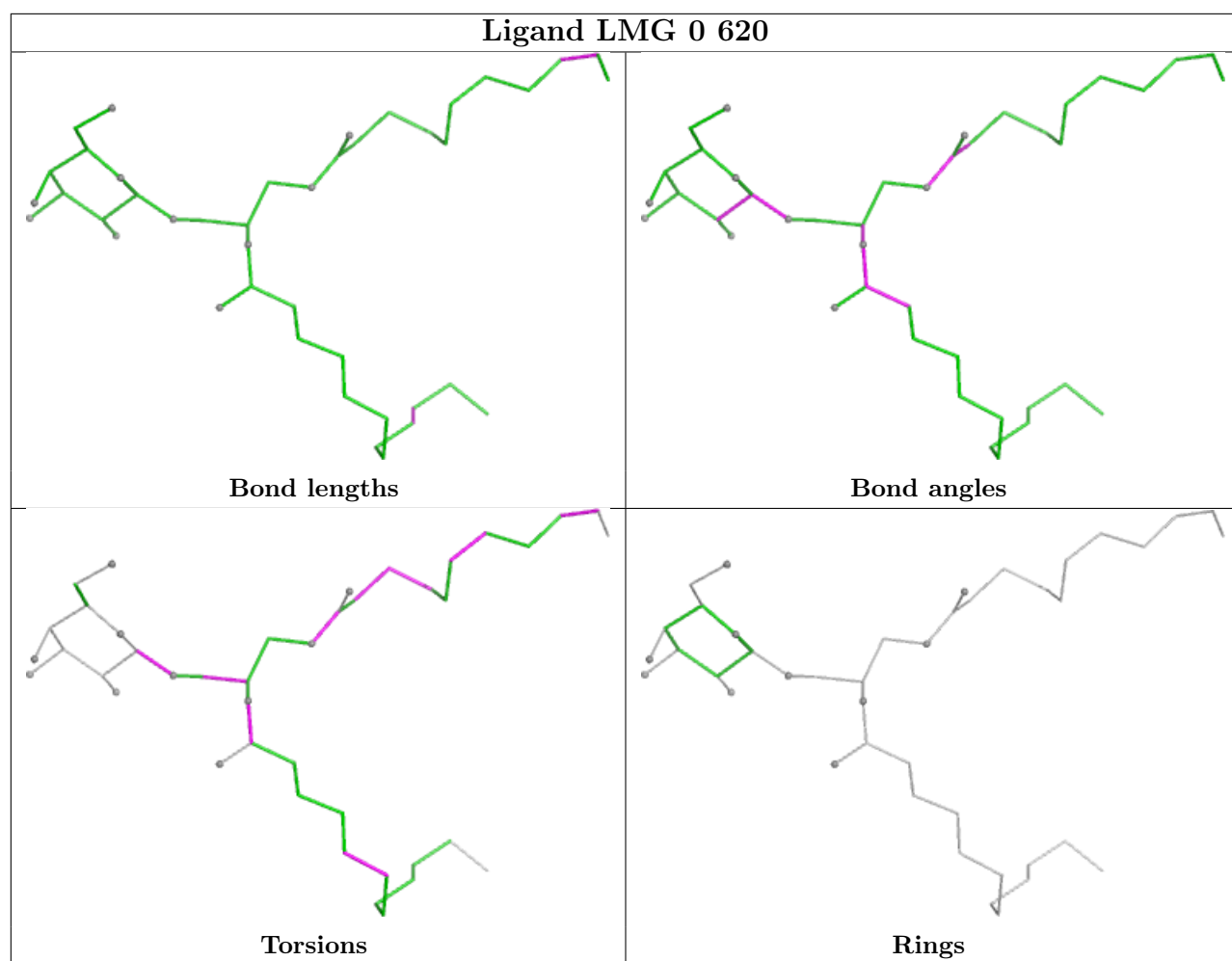
Torsions

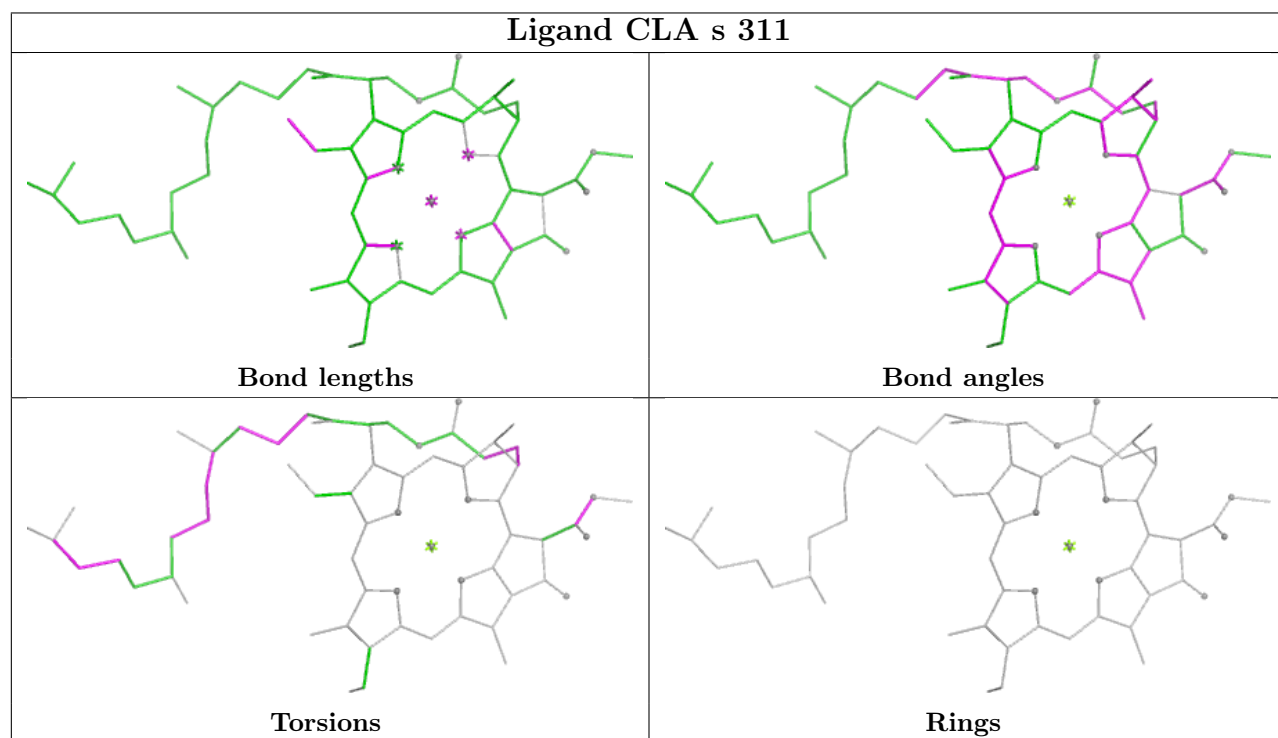
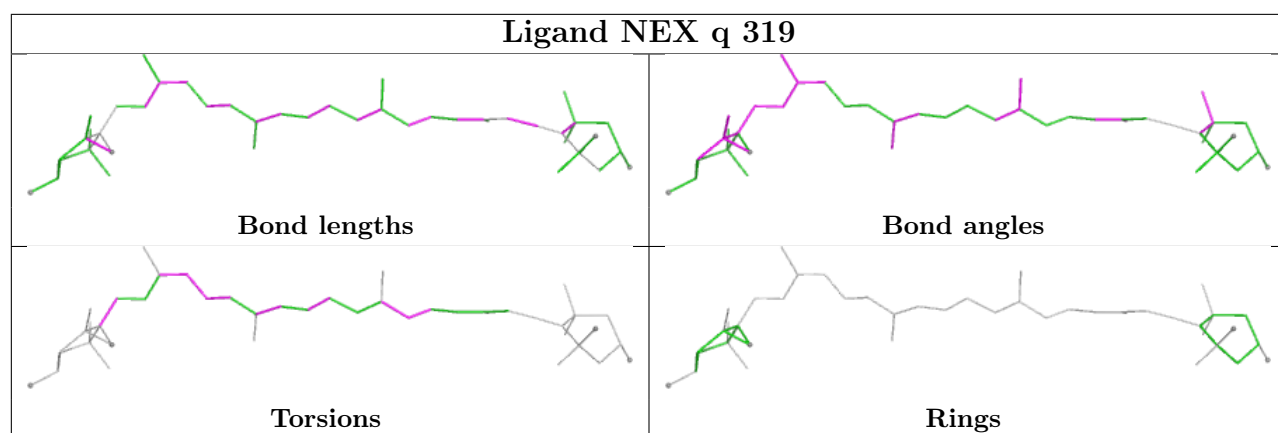


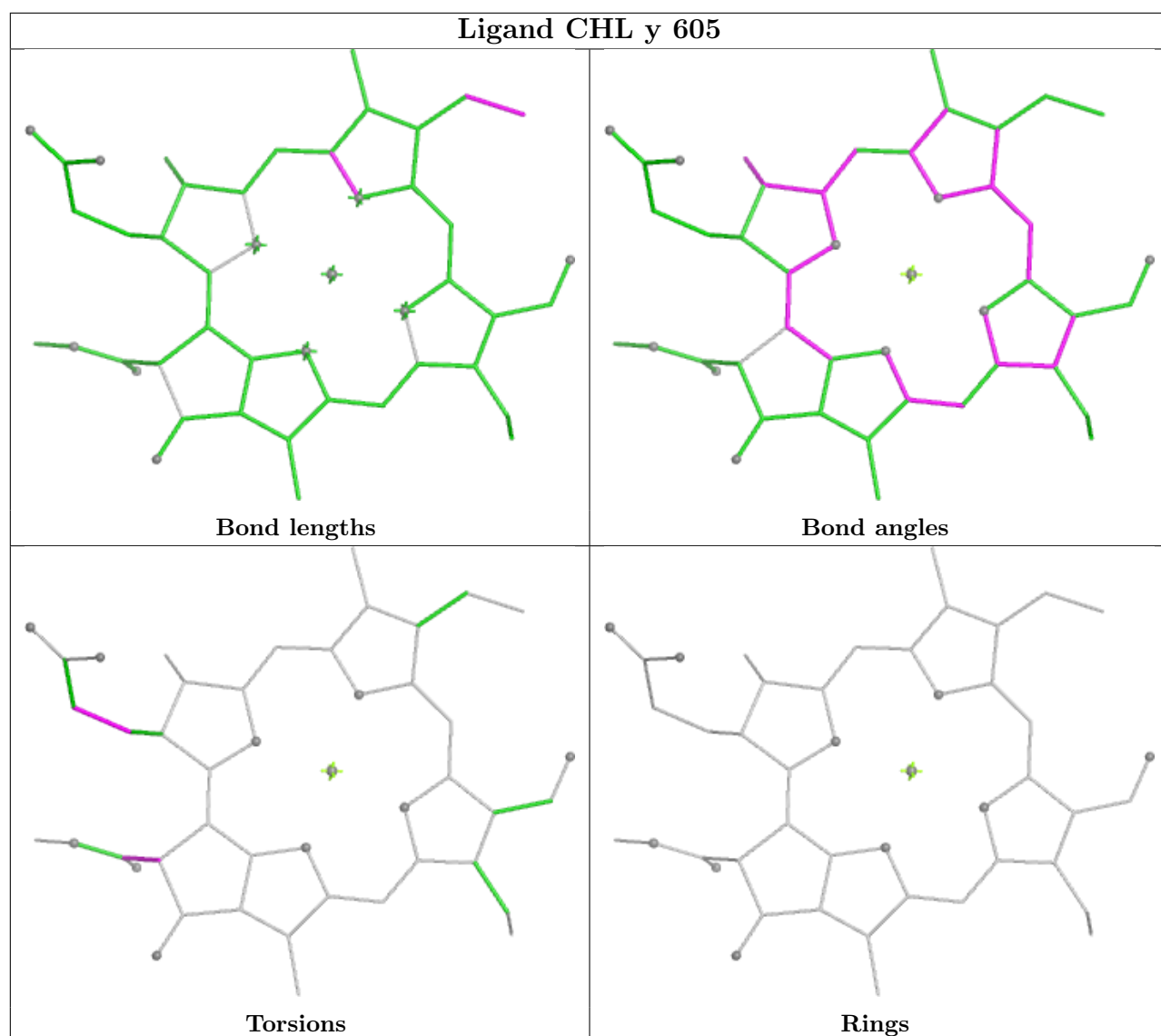
Rings



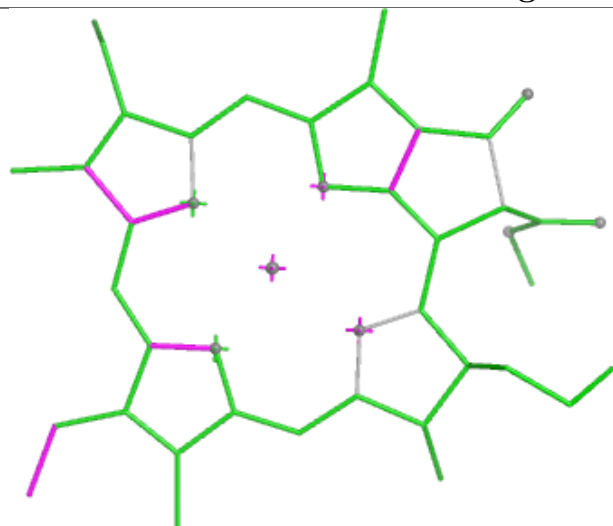




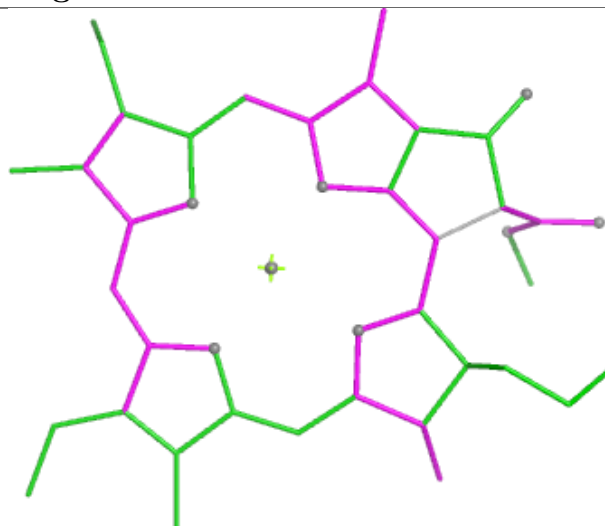




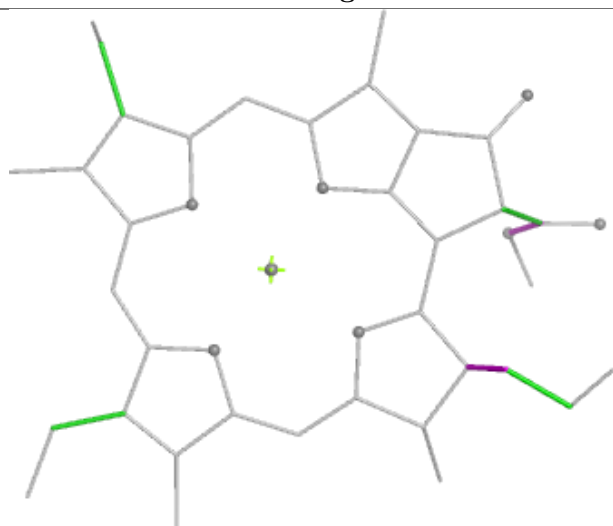
Ligand CLA g 312



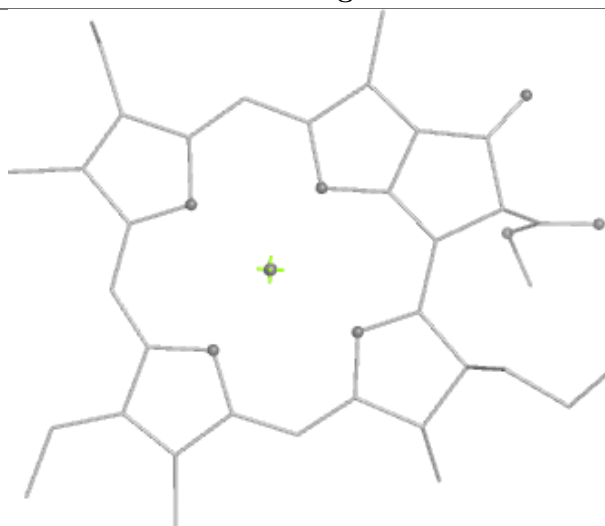
Bond lengths



Bond angles

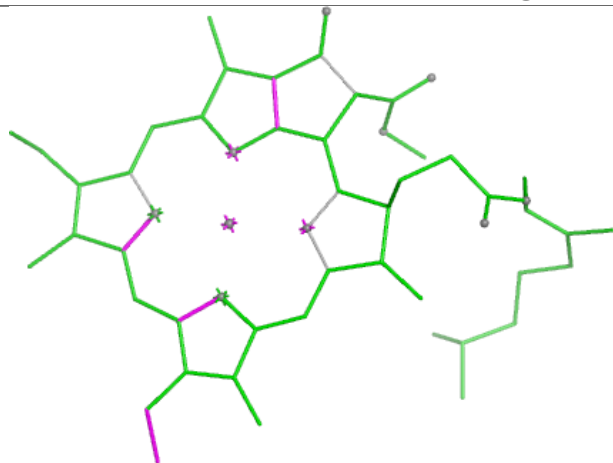


Torsions

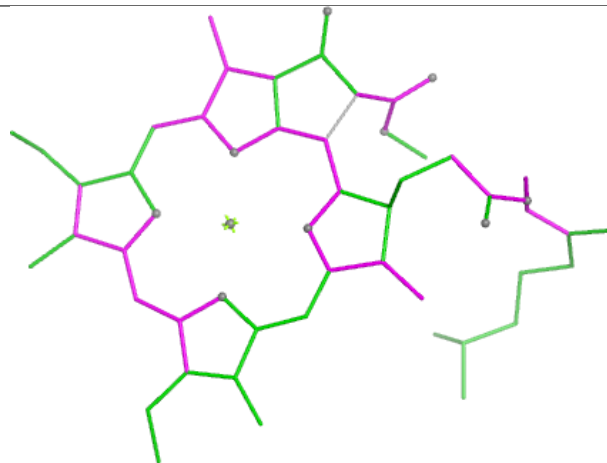


Rings

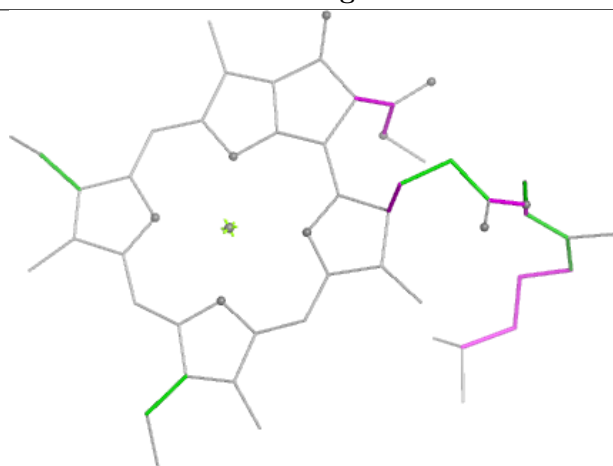
Ligand CLA n 304



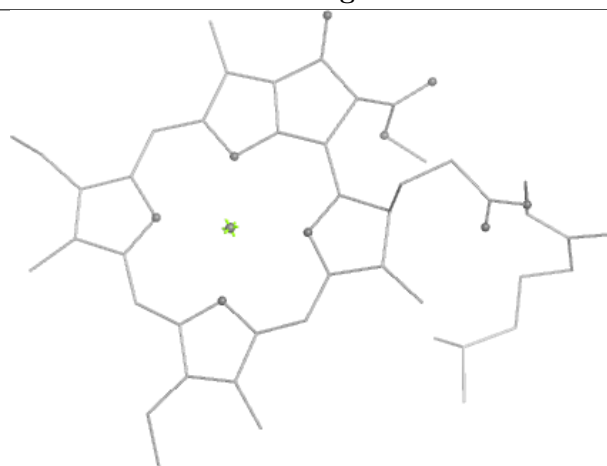
Bond lengths



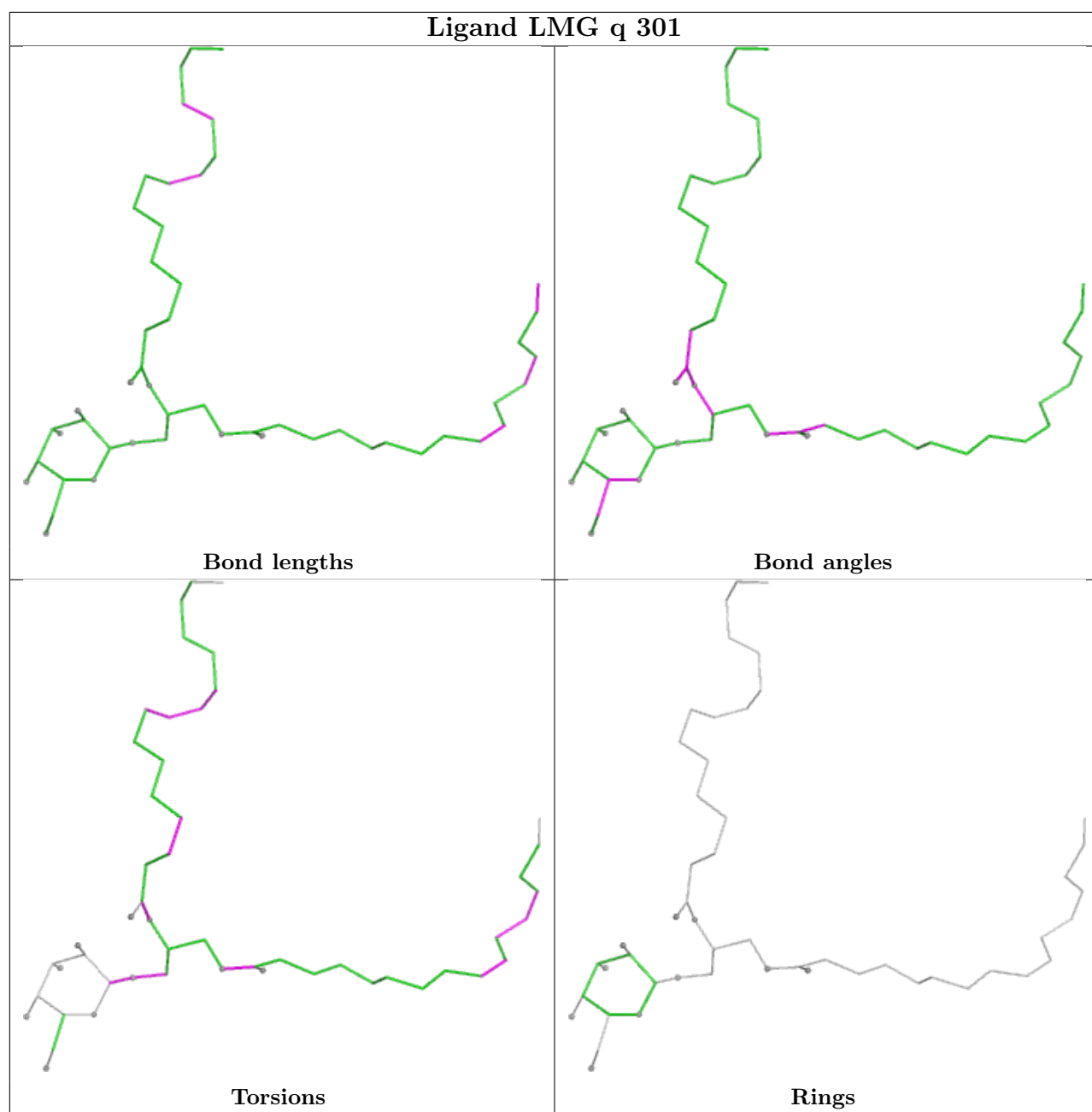
Bond angles



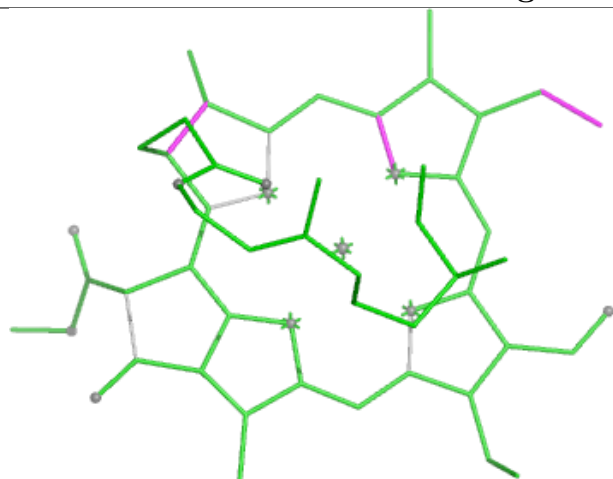
Torsions



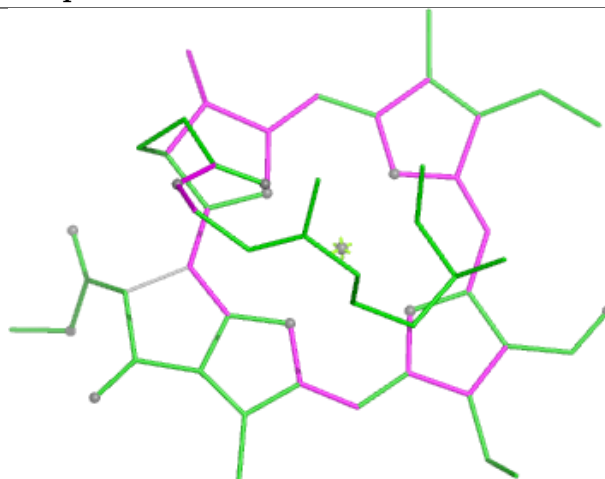
Rings



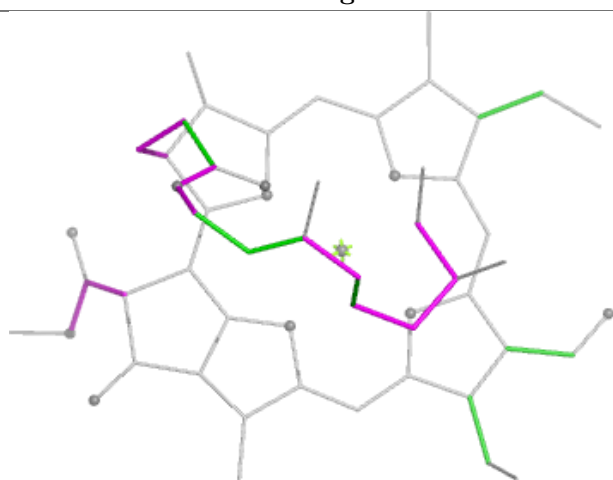
Ligand CHL q 309



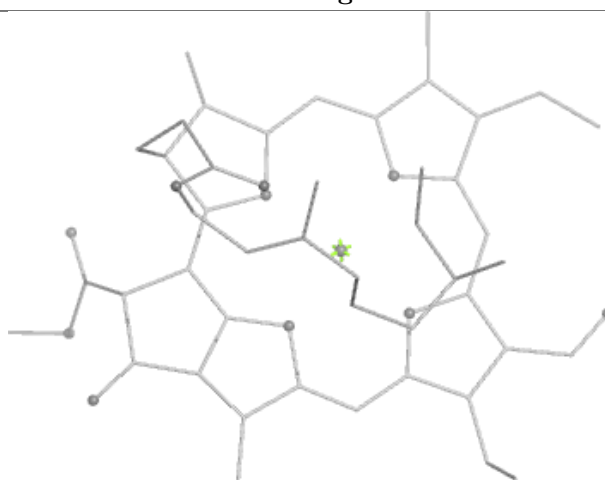
Bond lengths



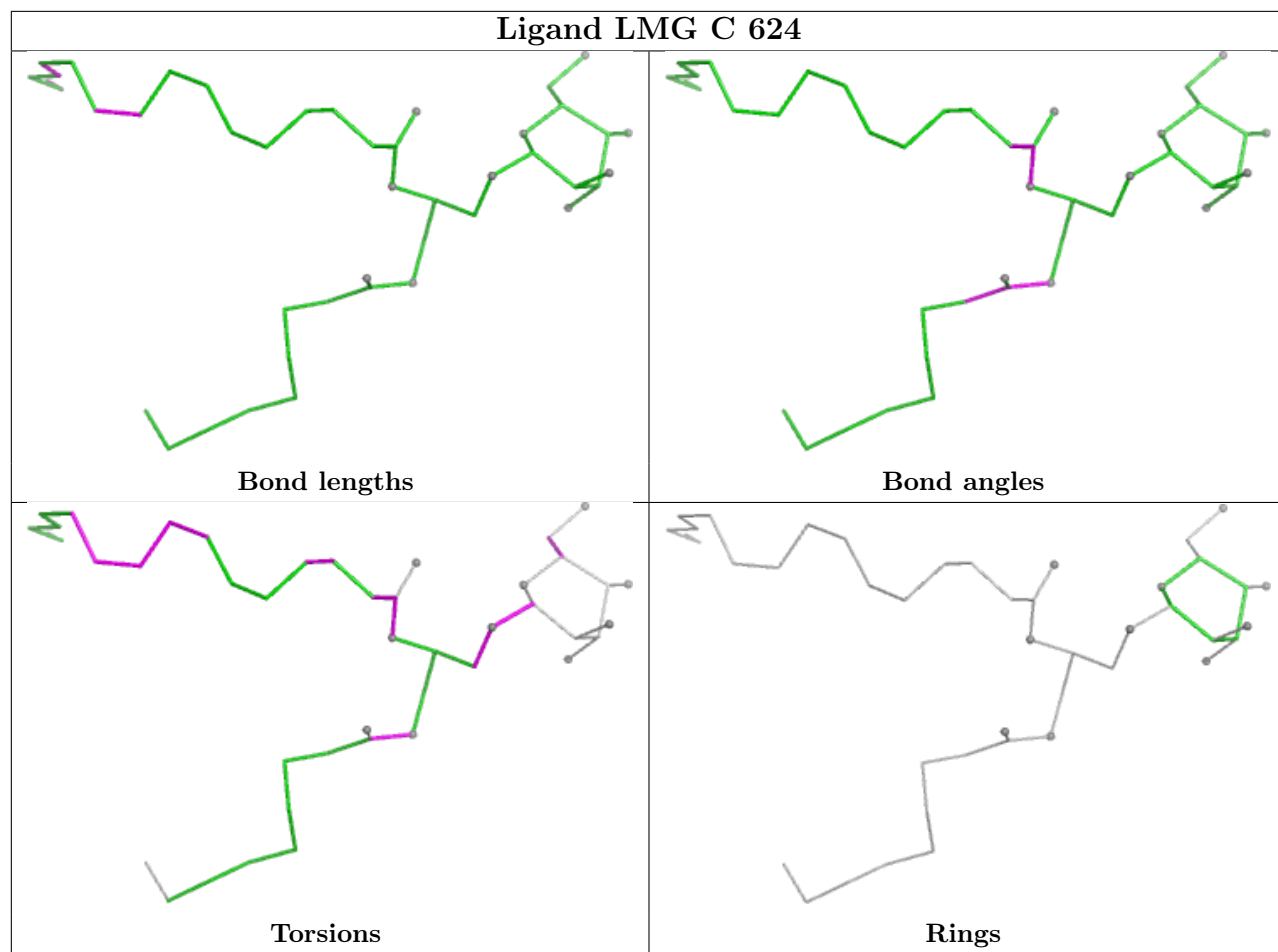
Bond angles



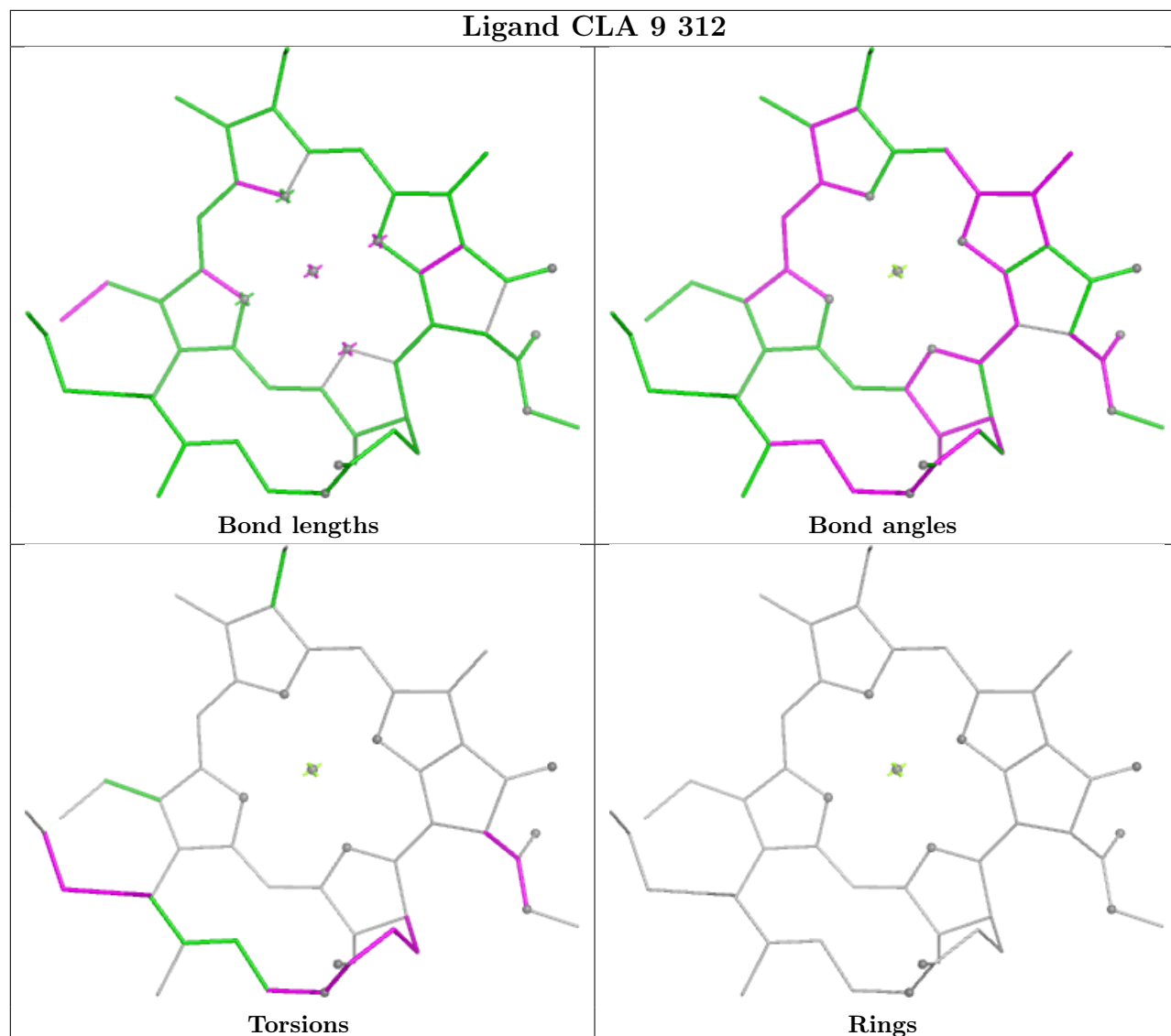
Torsions

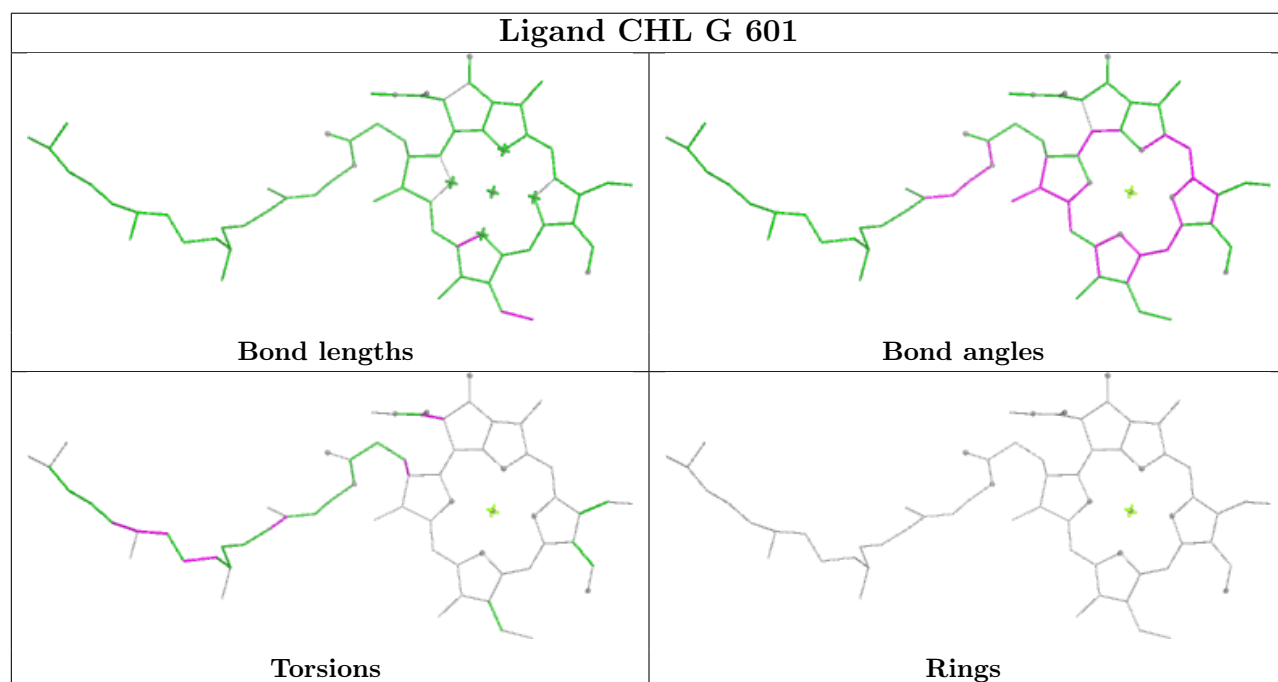
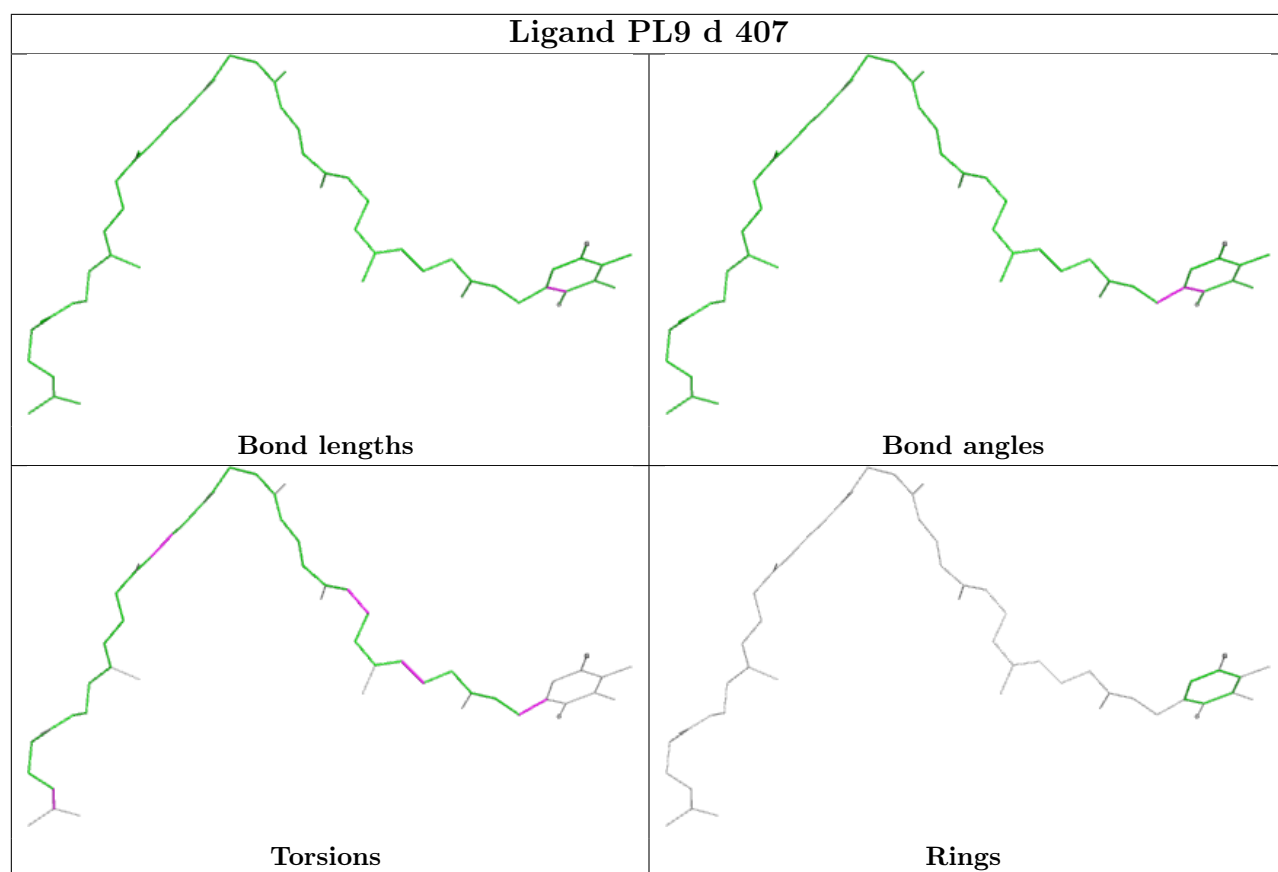


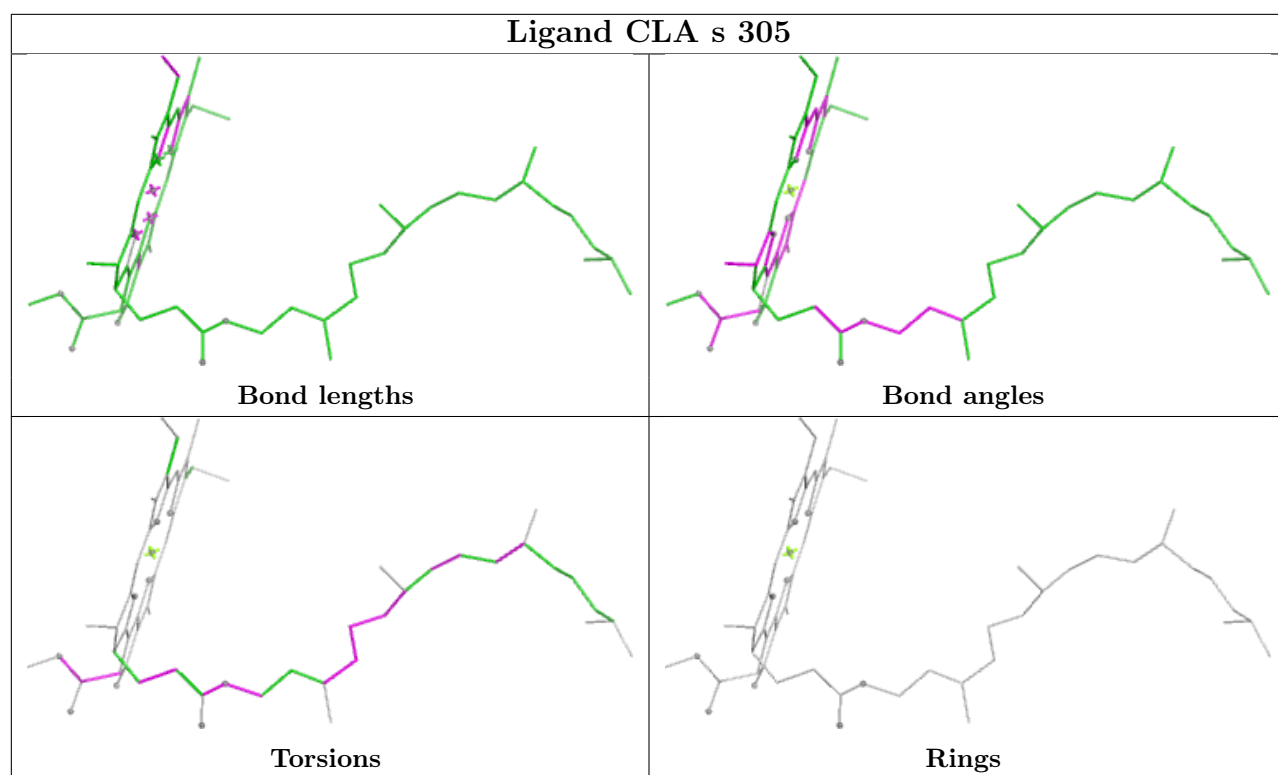
Rings



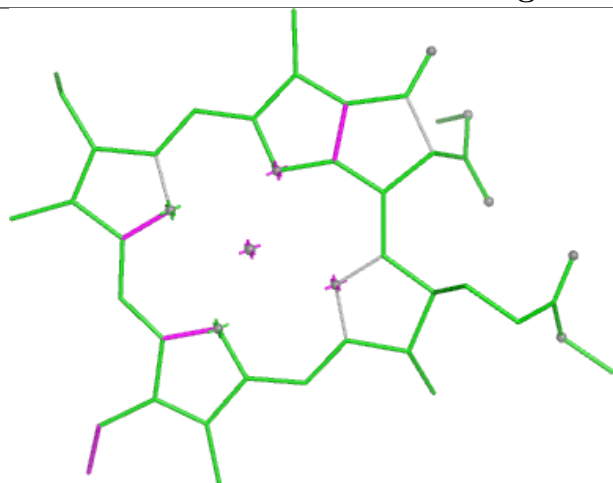
Ligand CLA 9 312



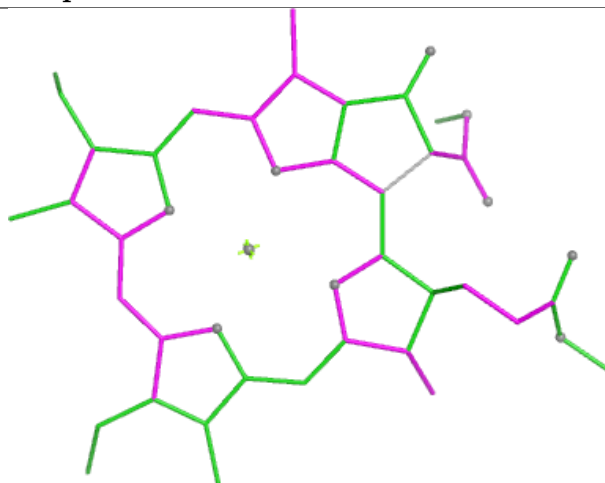




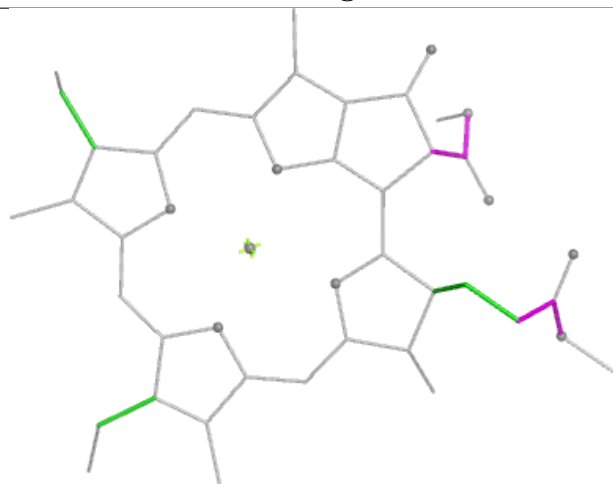
Ligand CLA q 314



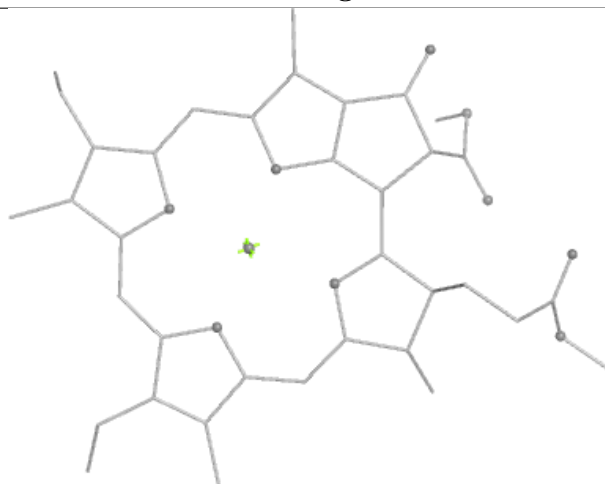
Bond lengths



Bond angles



Torsions

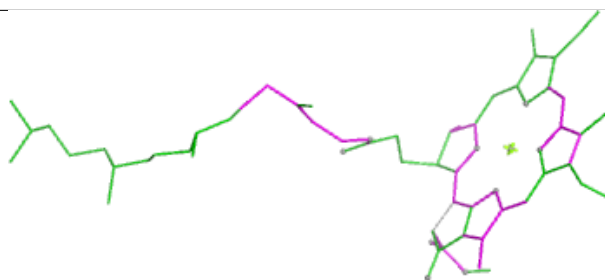


Rings

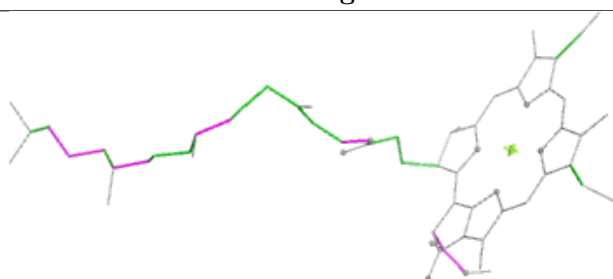
Ligand CLA C 602



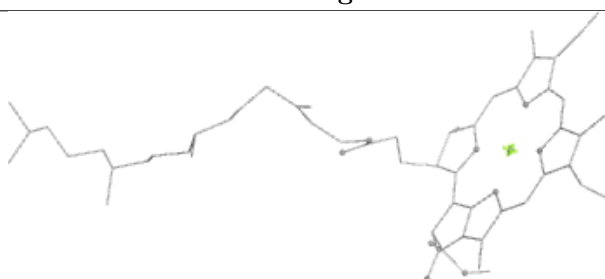
Bond lengths



Bond angles

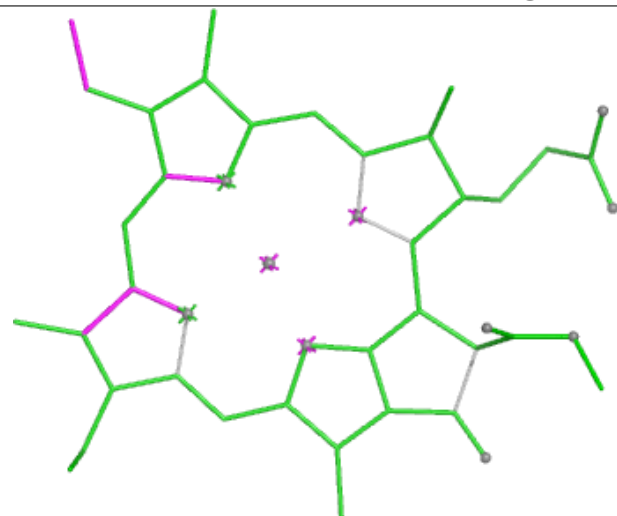


Torsions

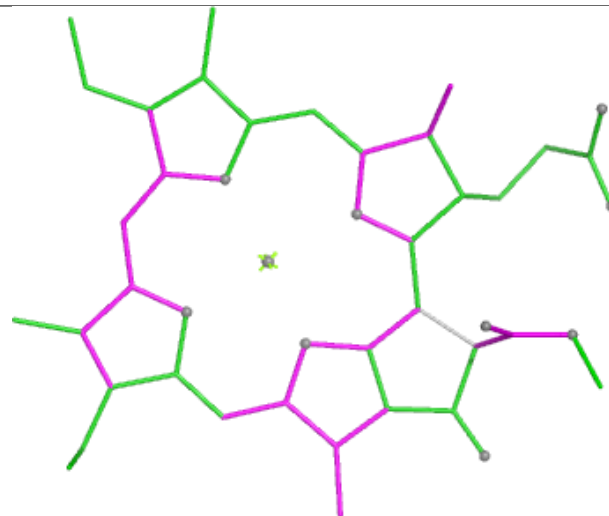


Rings

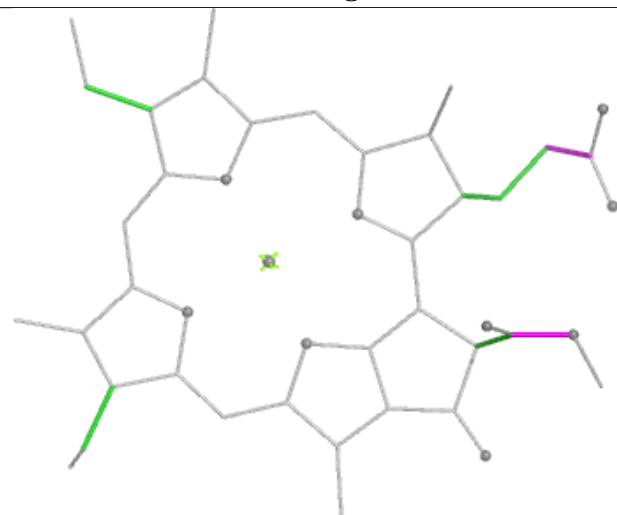
Ligand CLA n 313



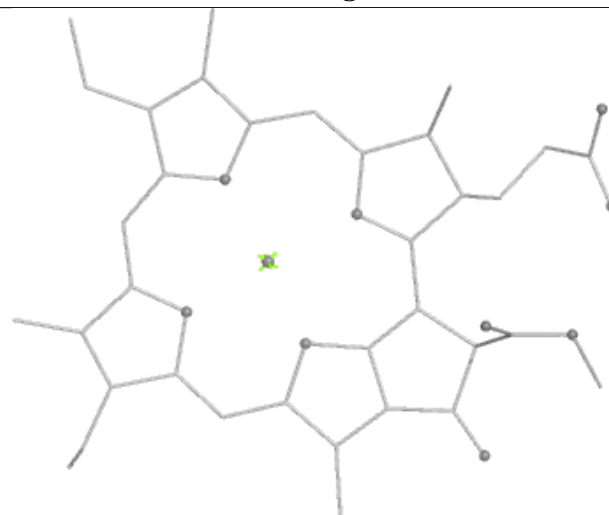
Bond lengths



Bond angles

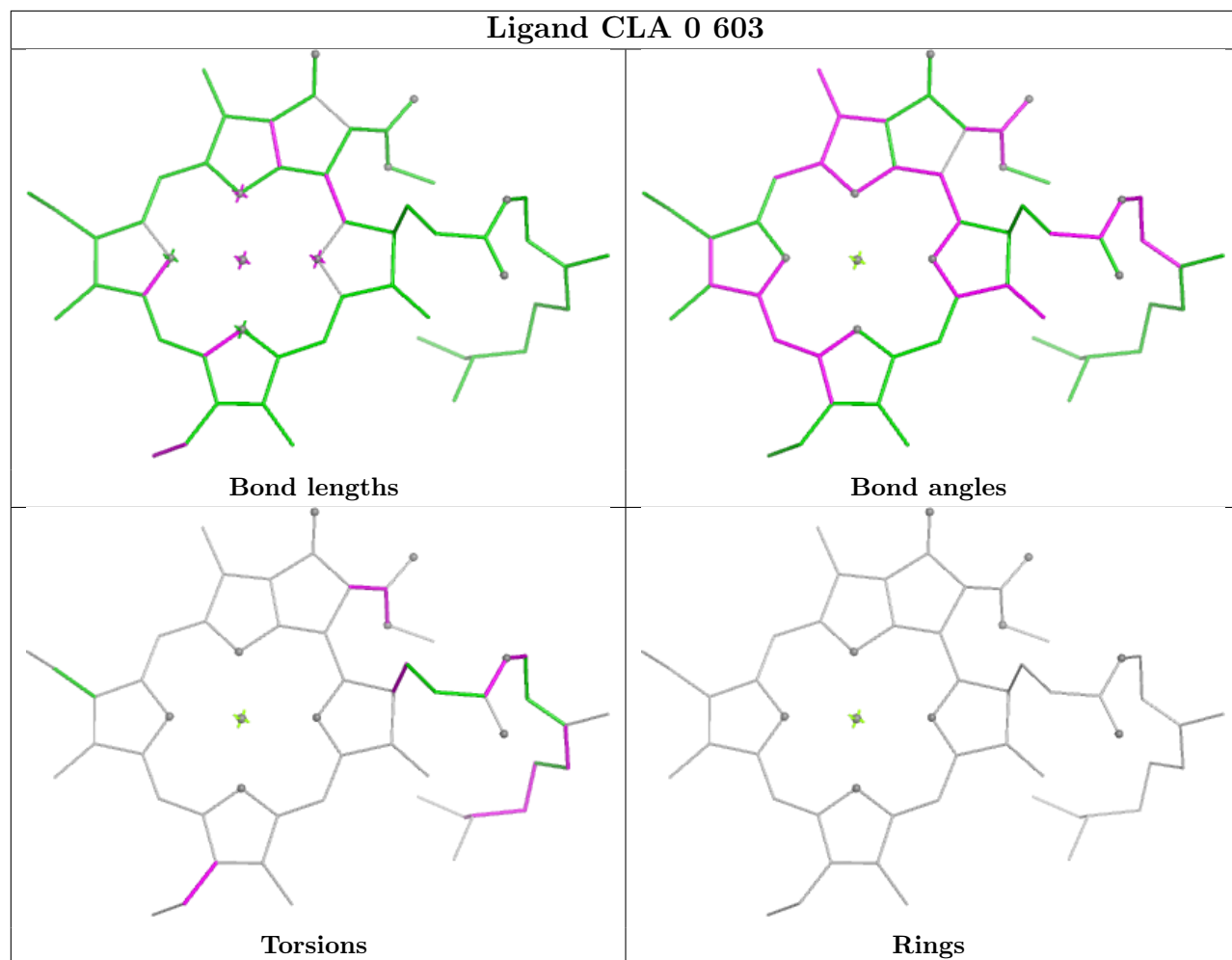


Torsions

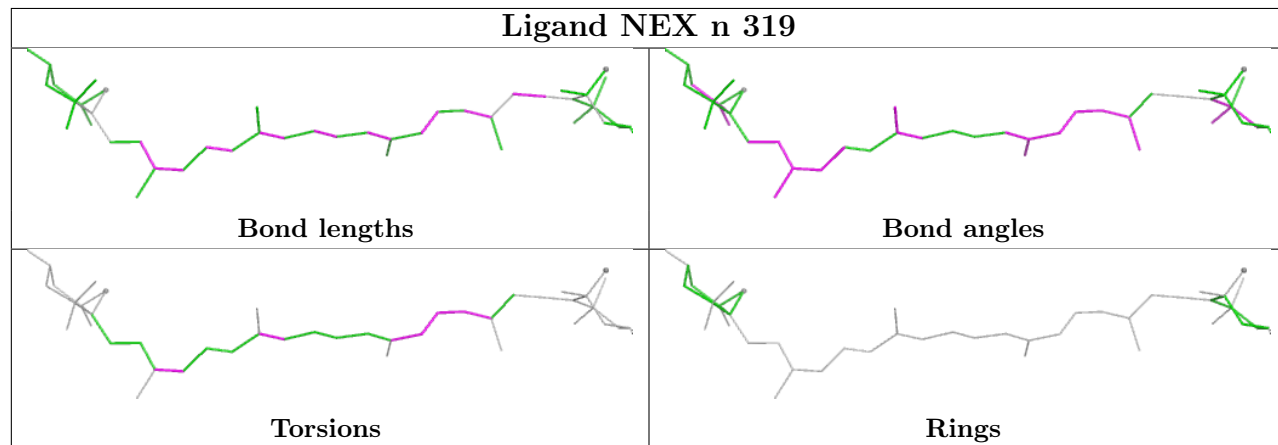


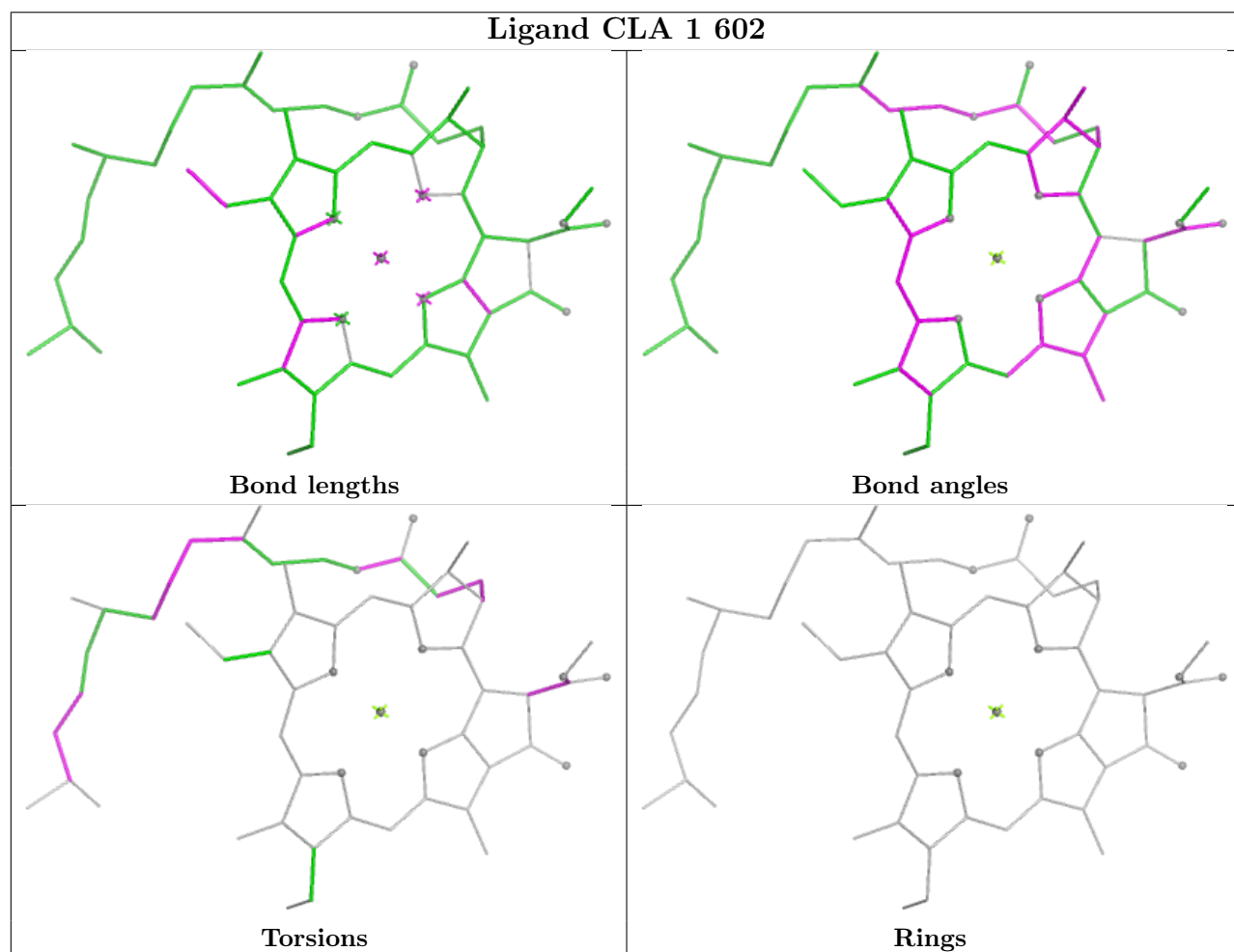
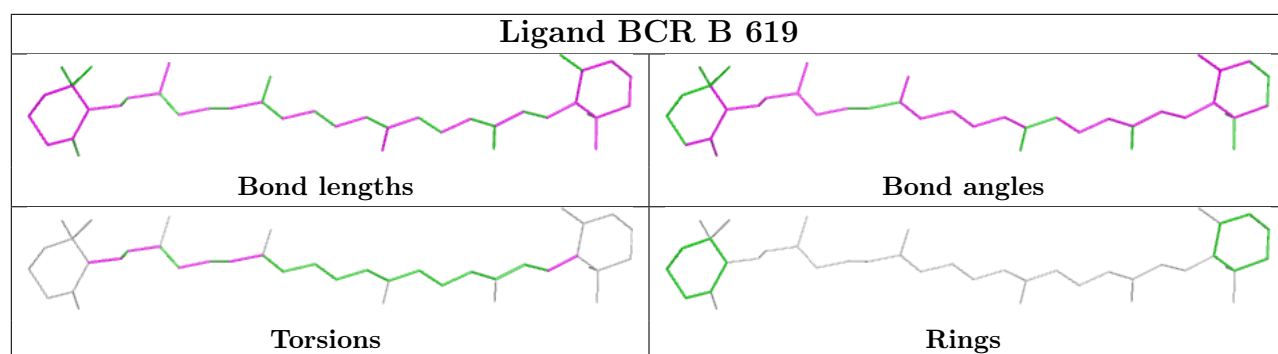
Rings

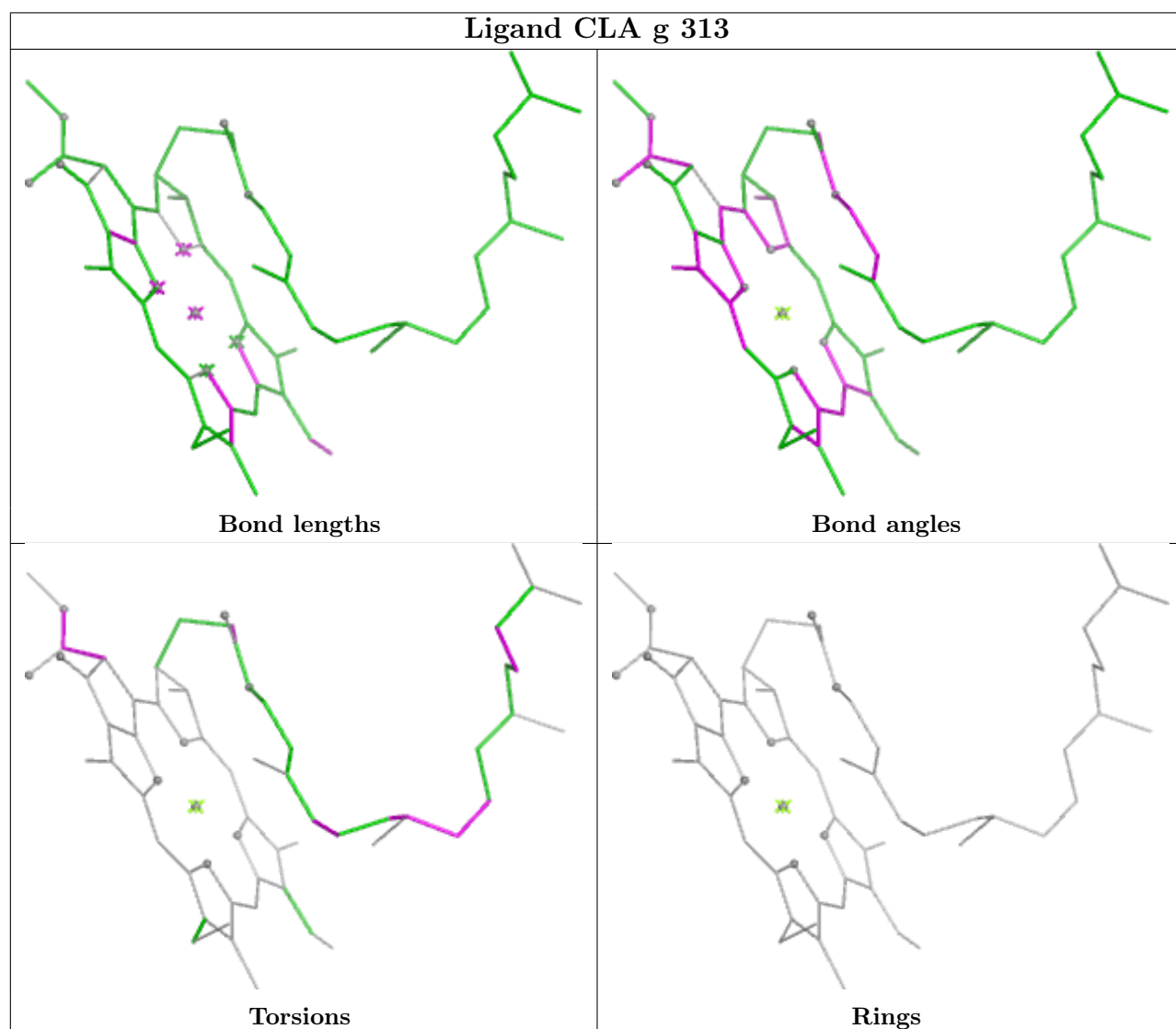
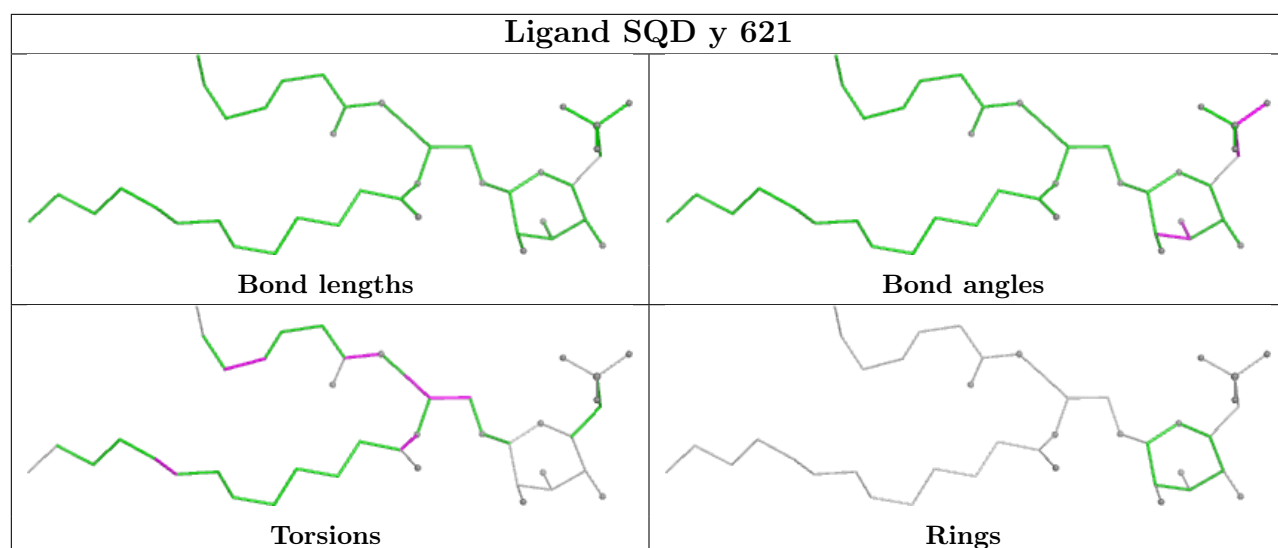
Ligand CLA 0 603



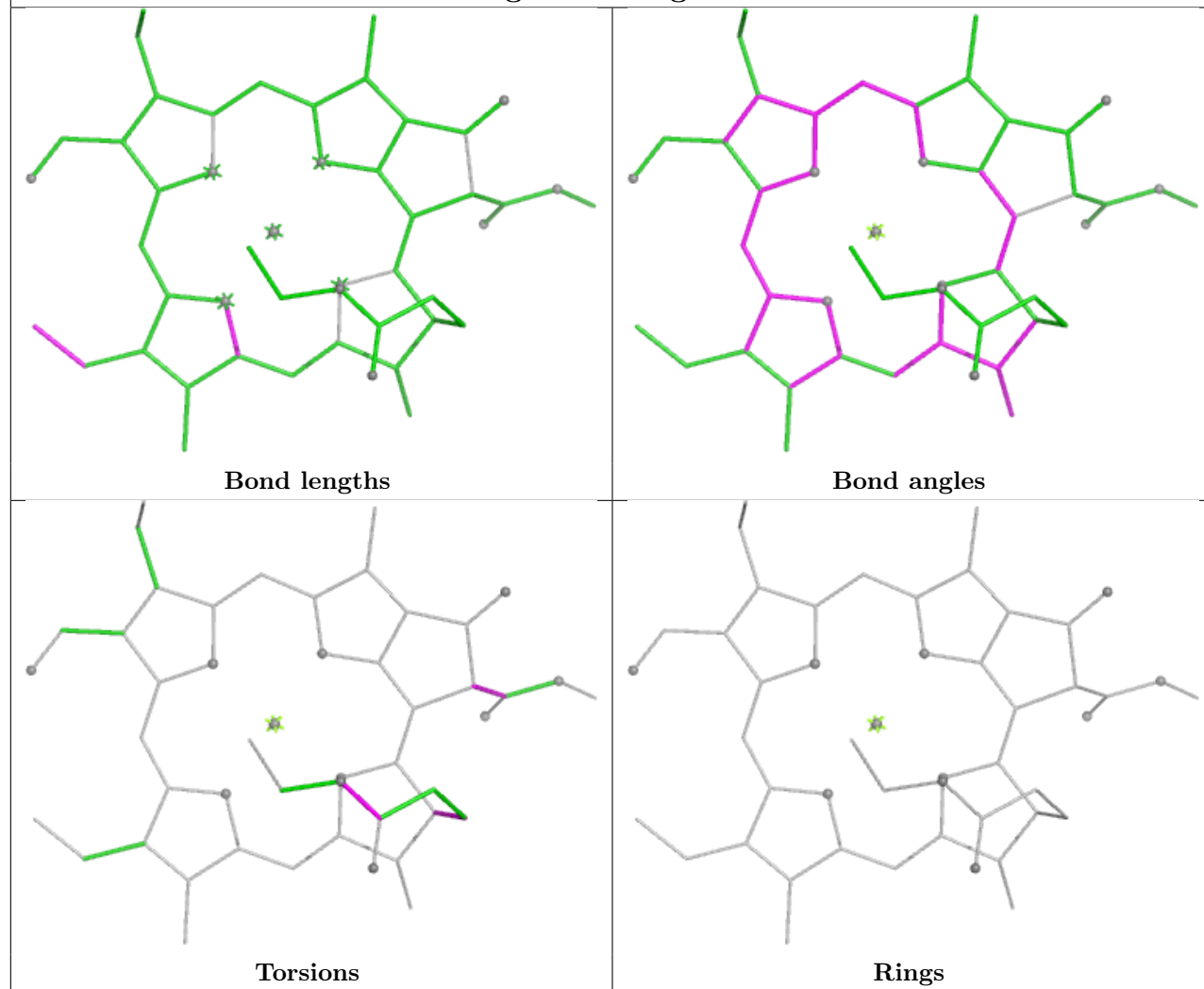
Ligand NEX n 319

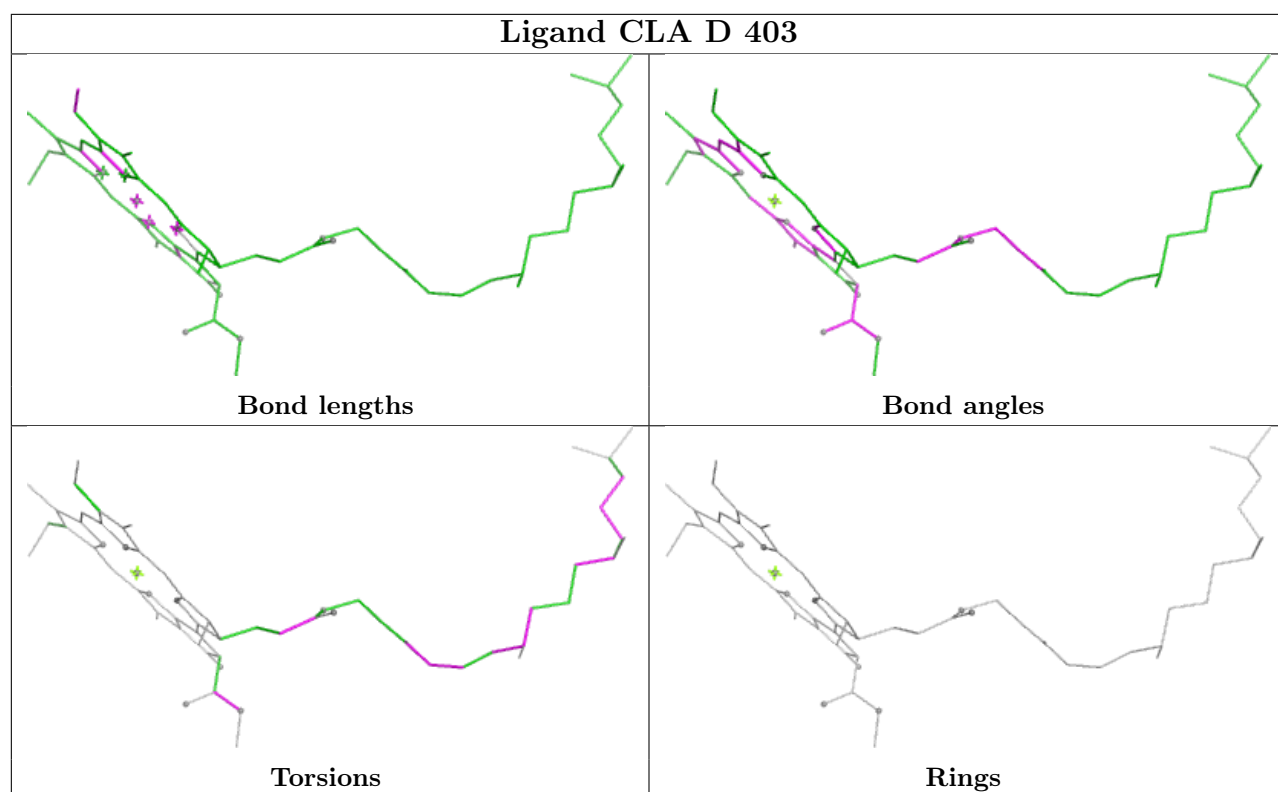




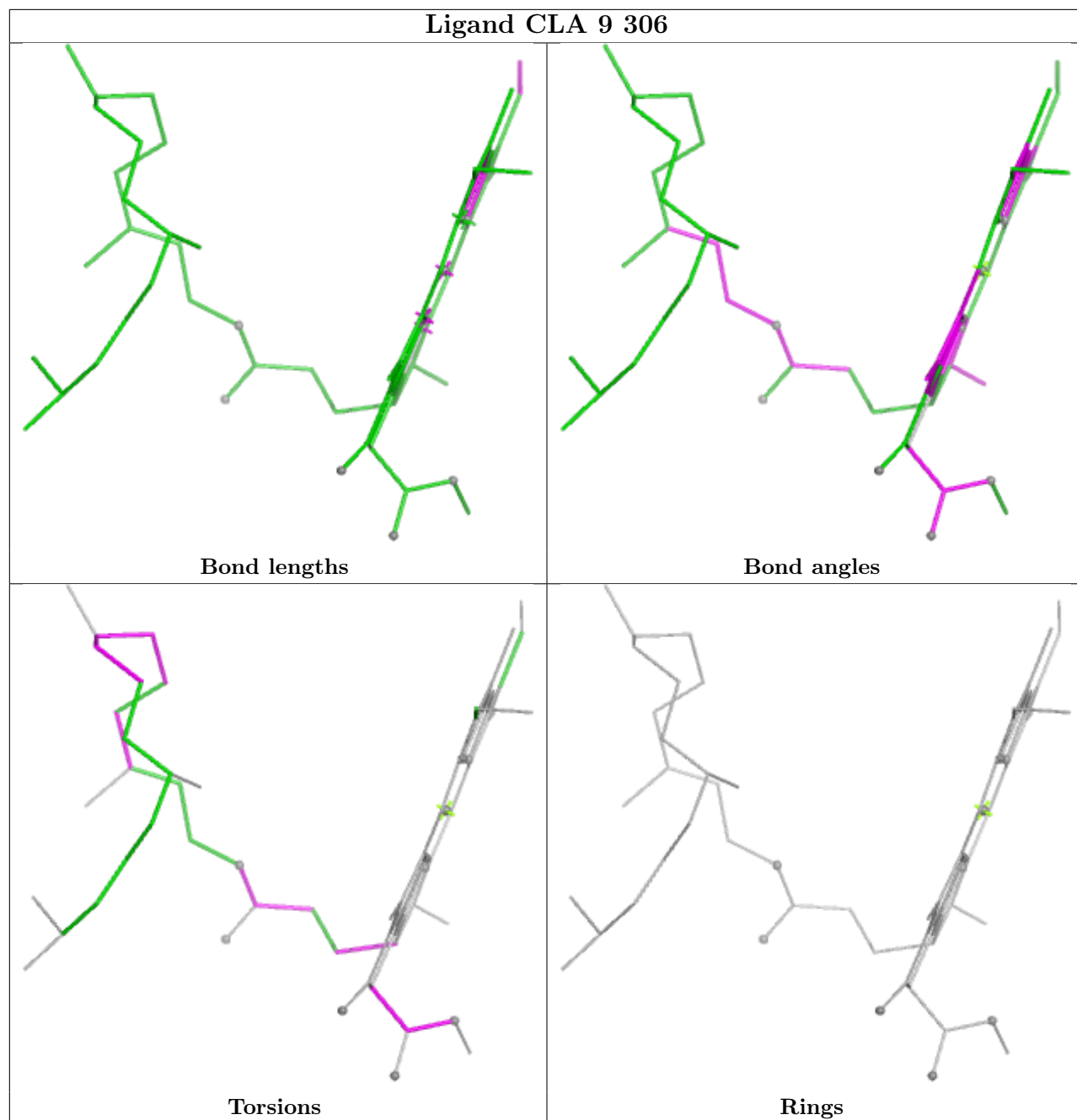


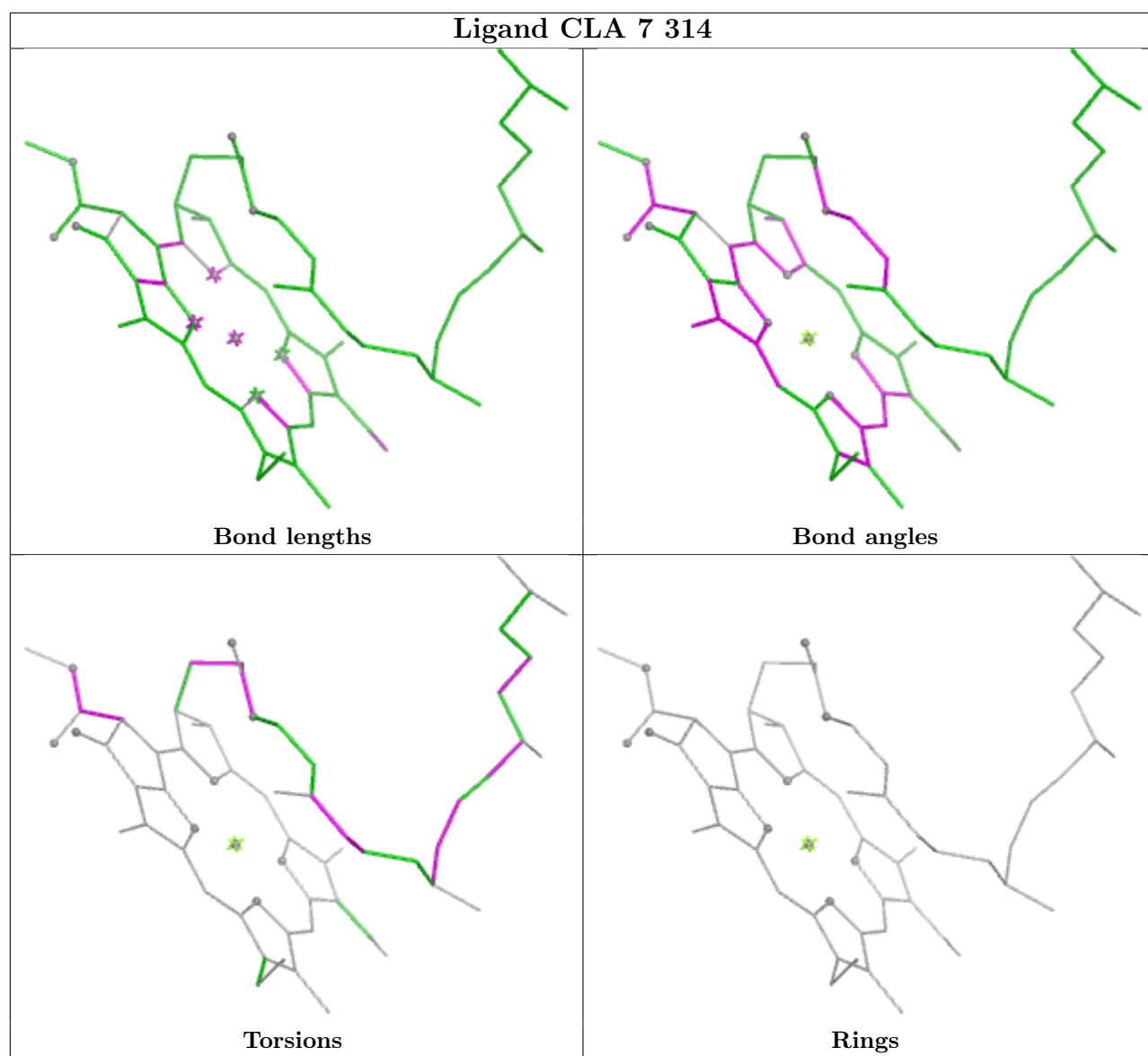
Ligand CHL g 306

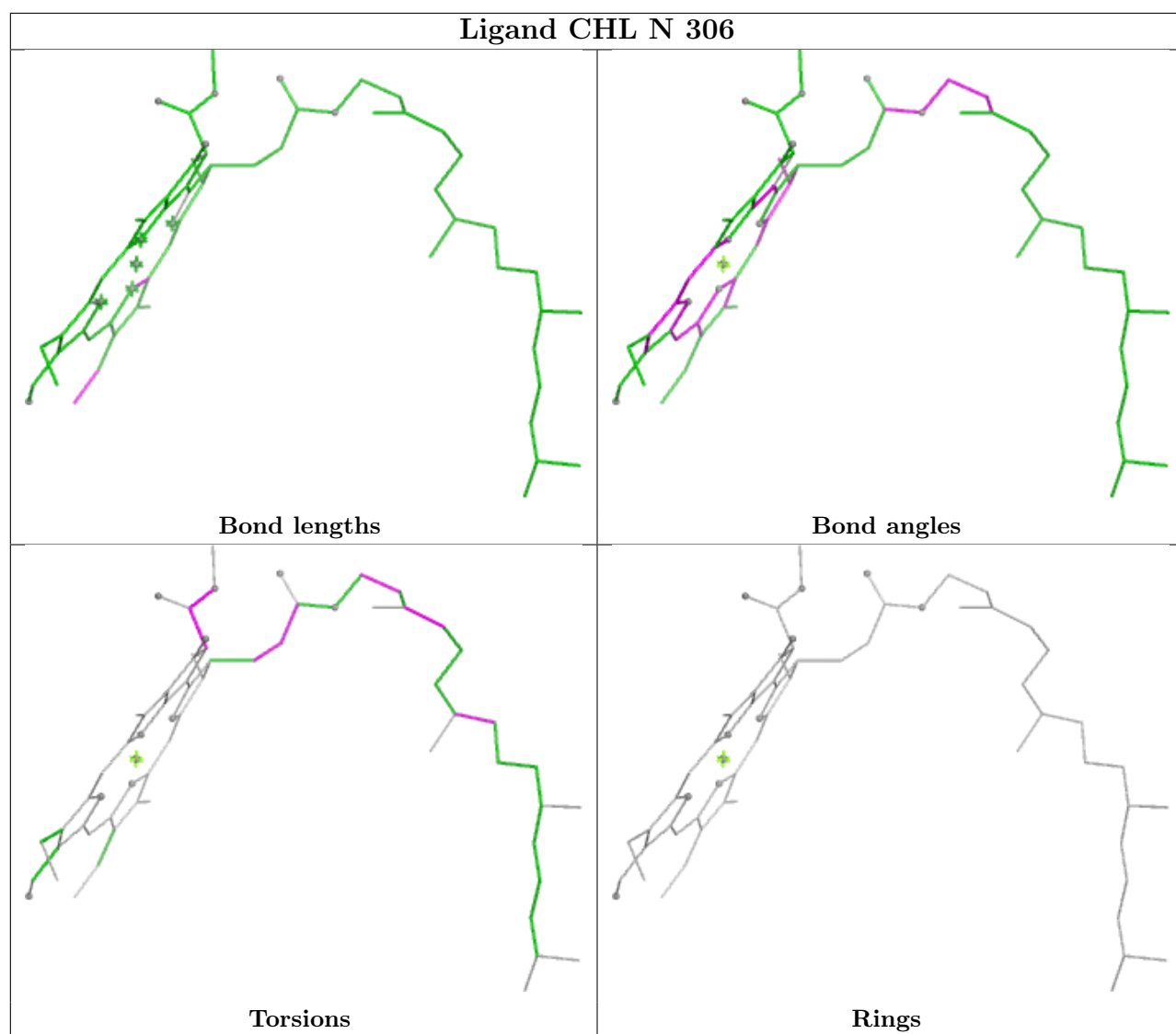




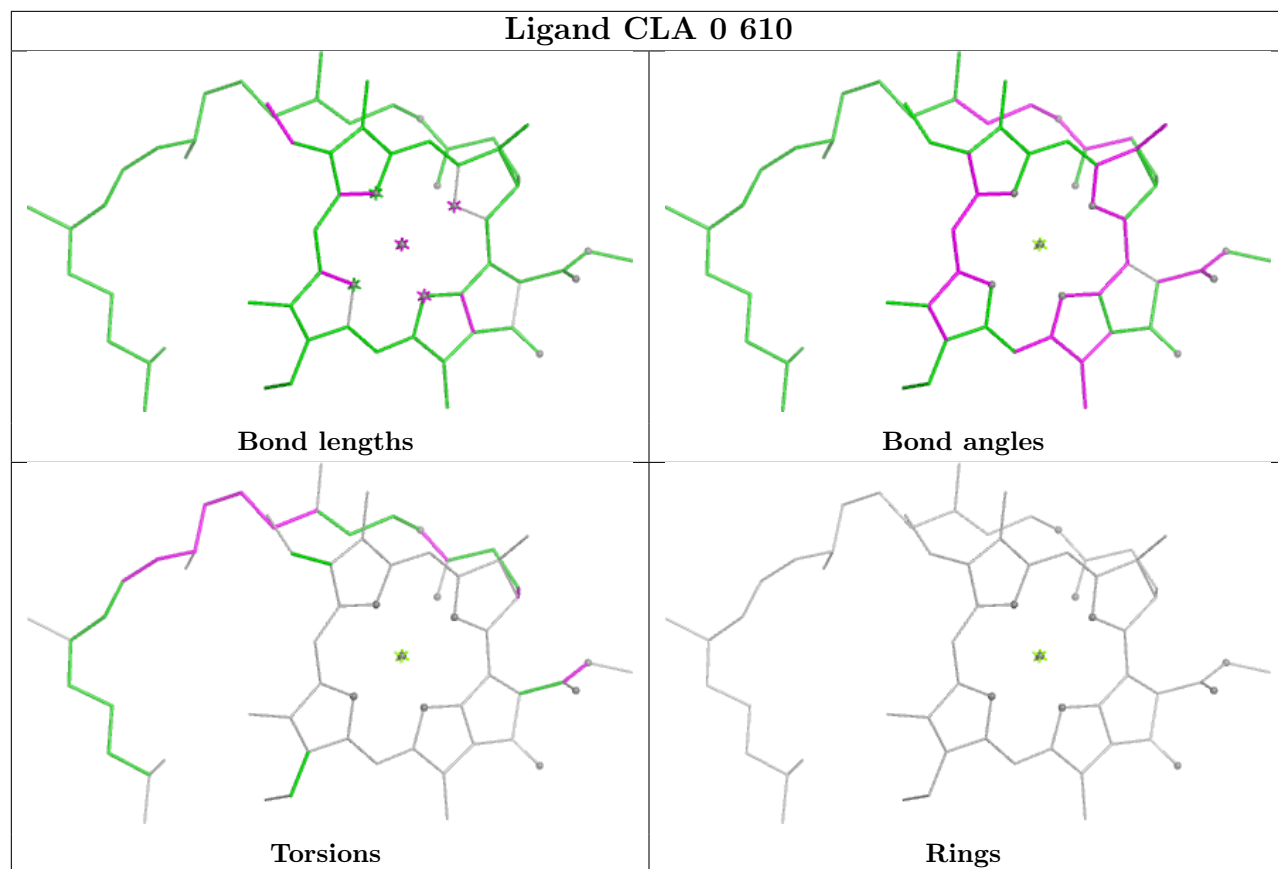
Ligand CLA 9 306

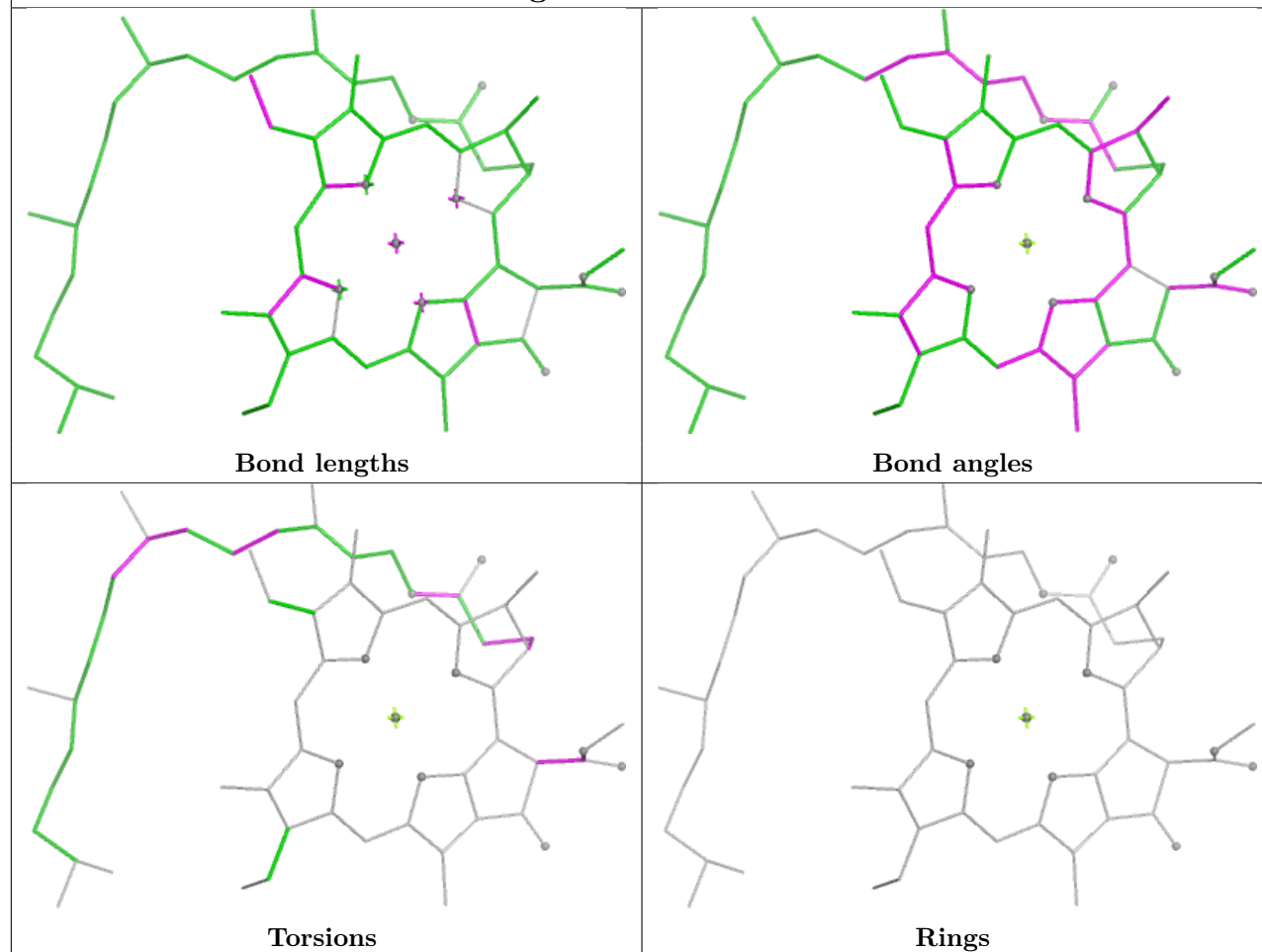
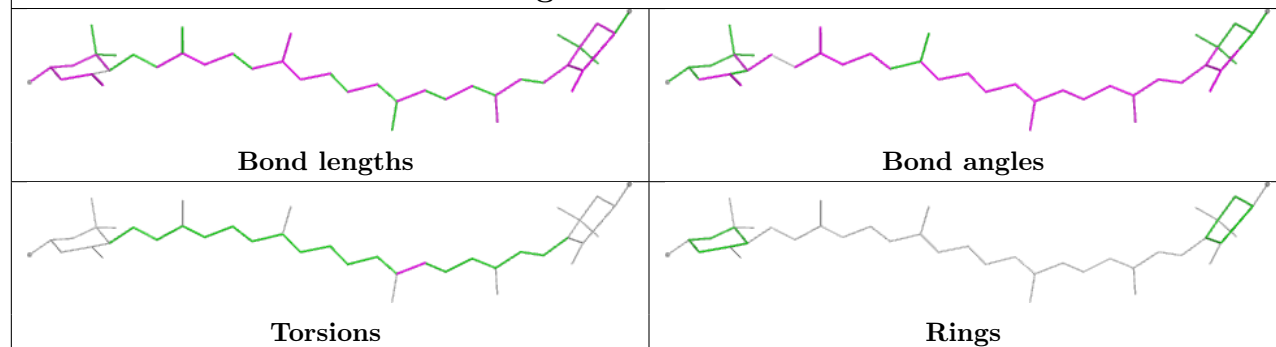


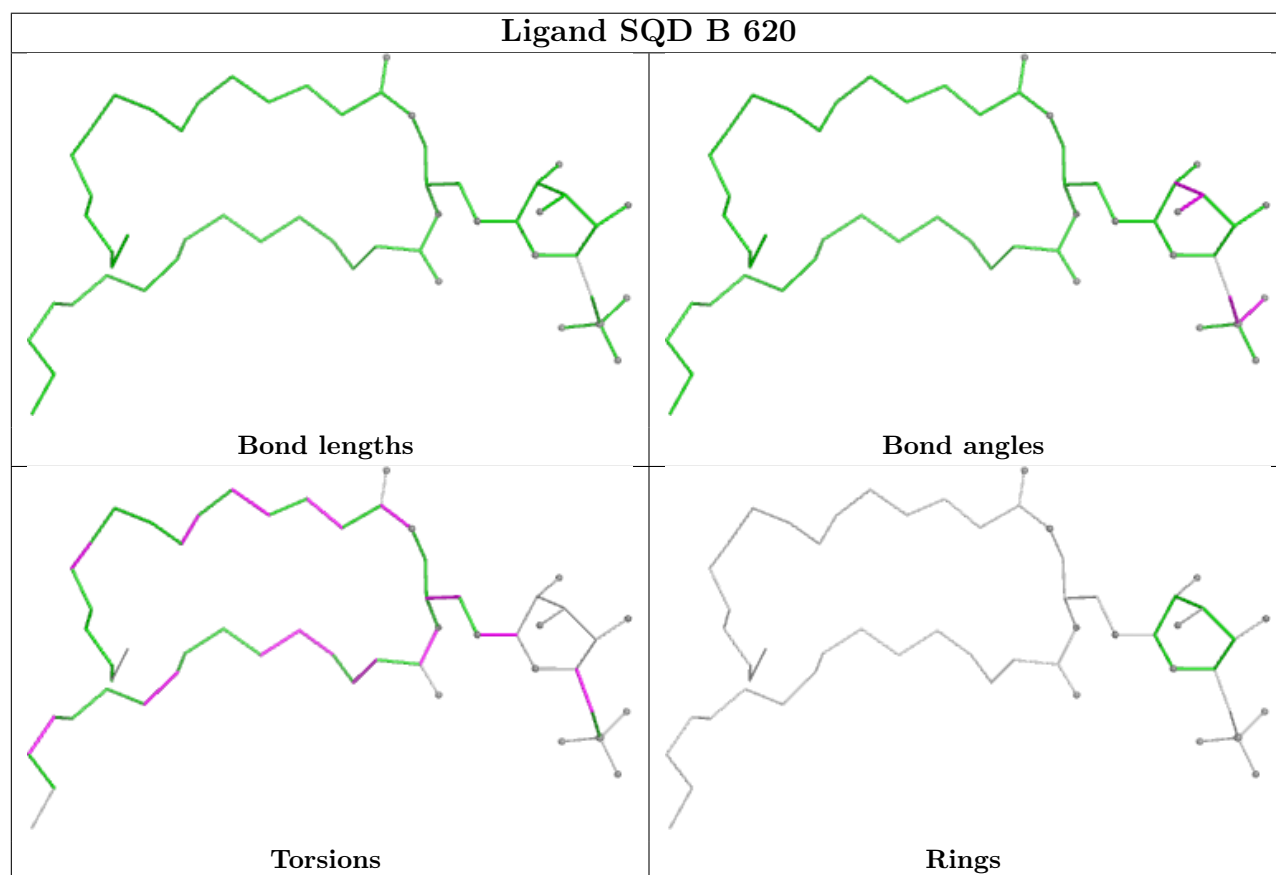
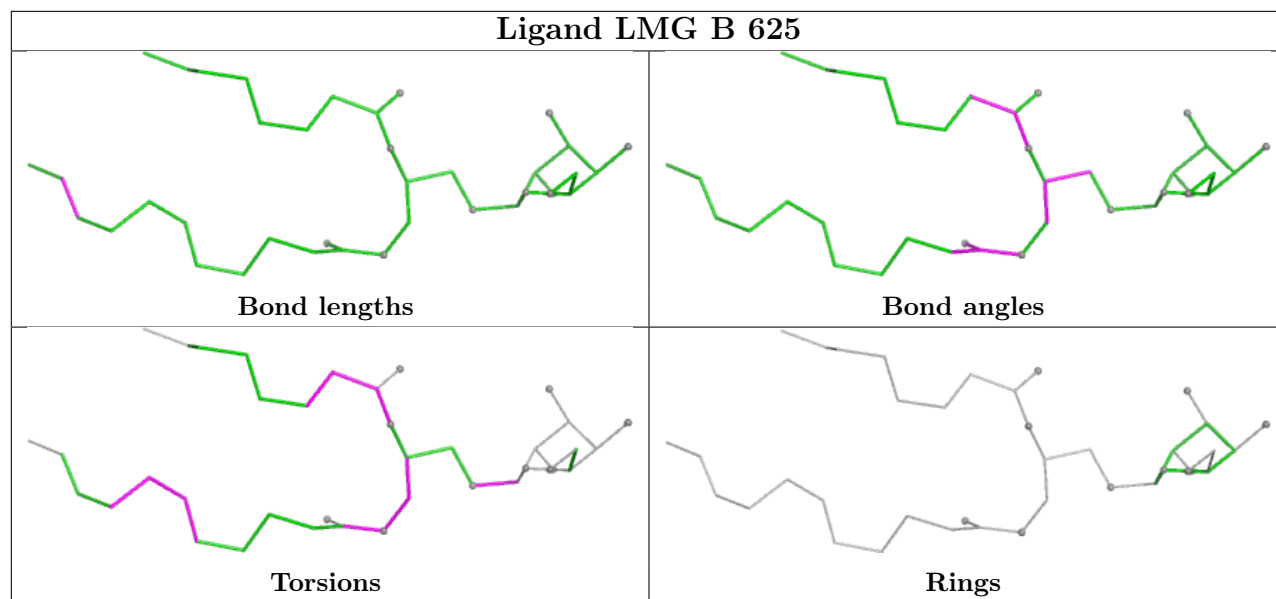


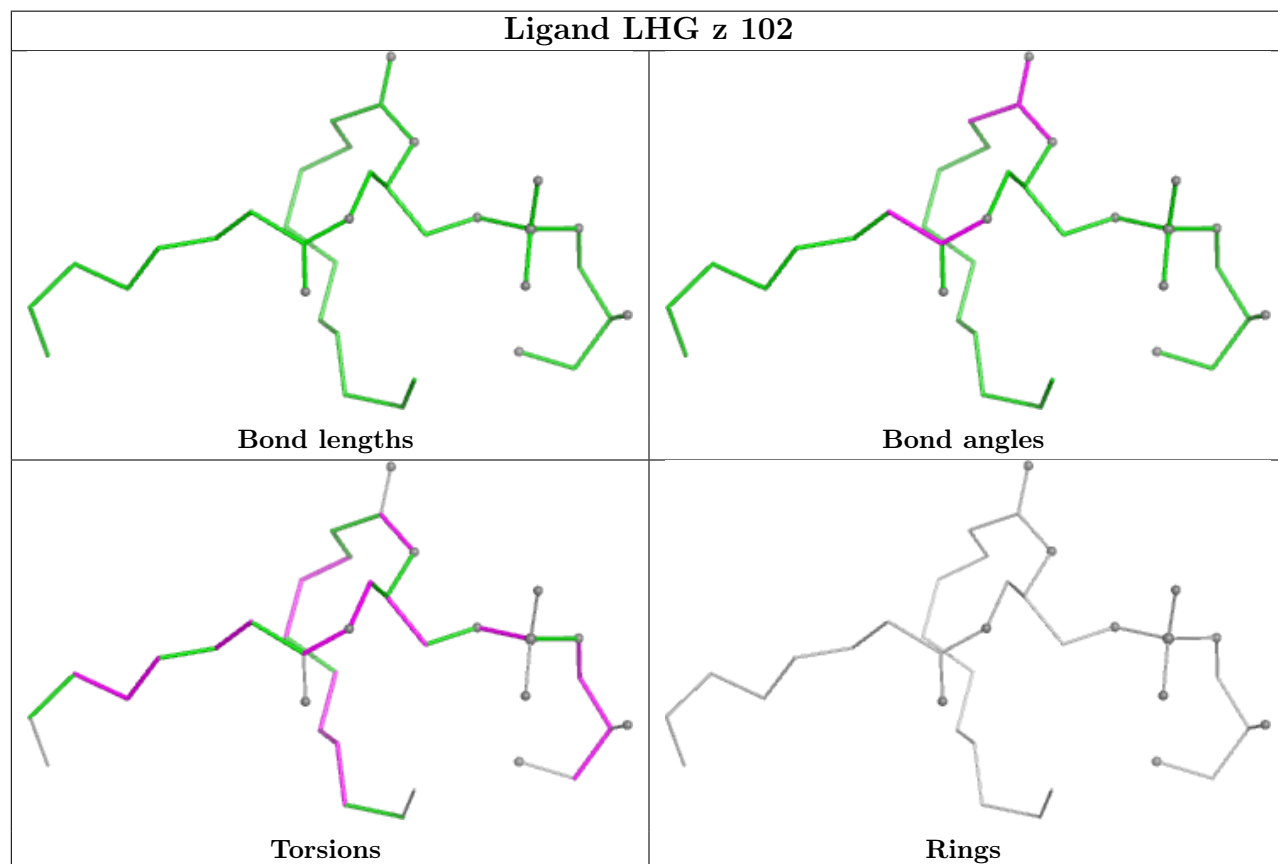
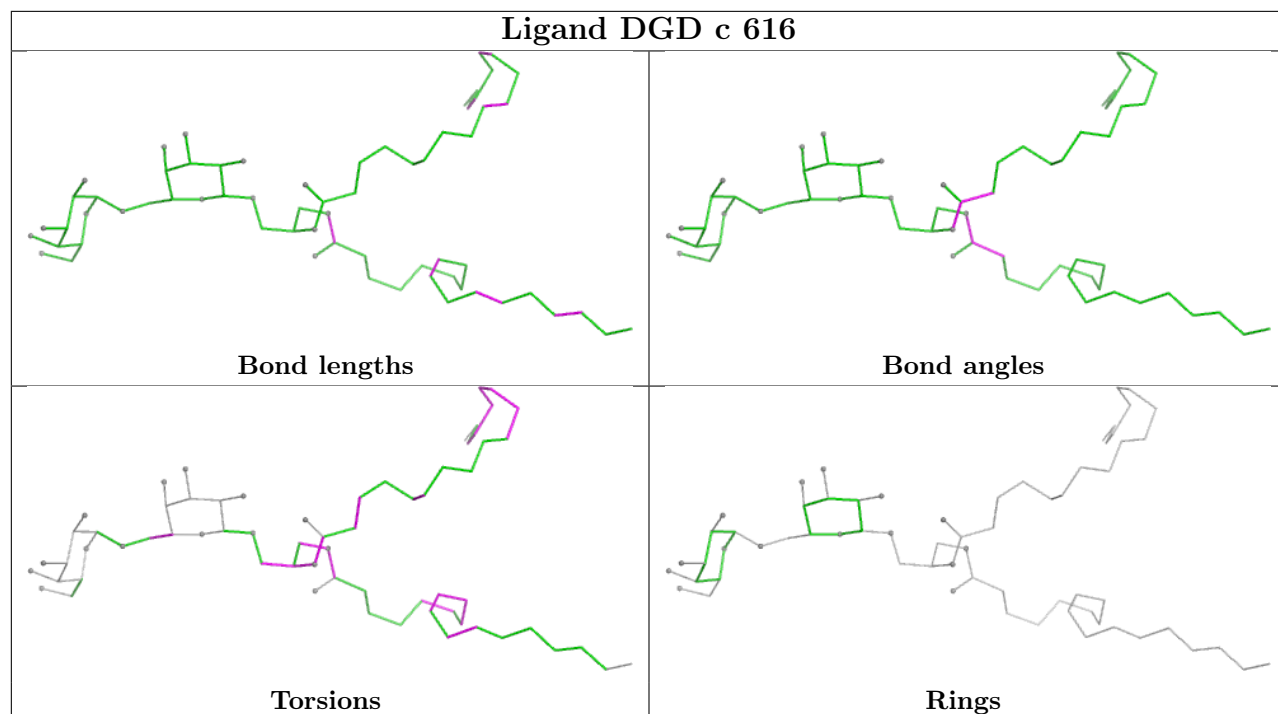


Ligand CLA 0 610

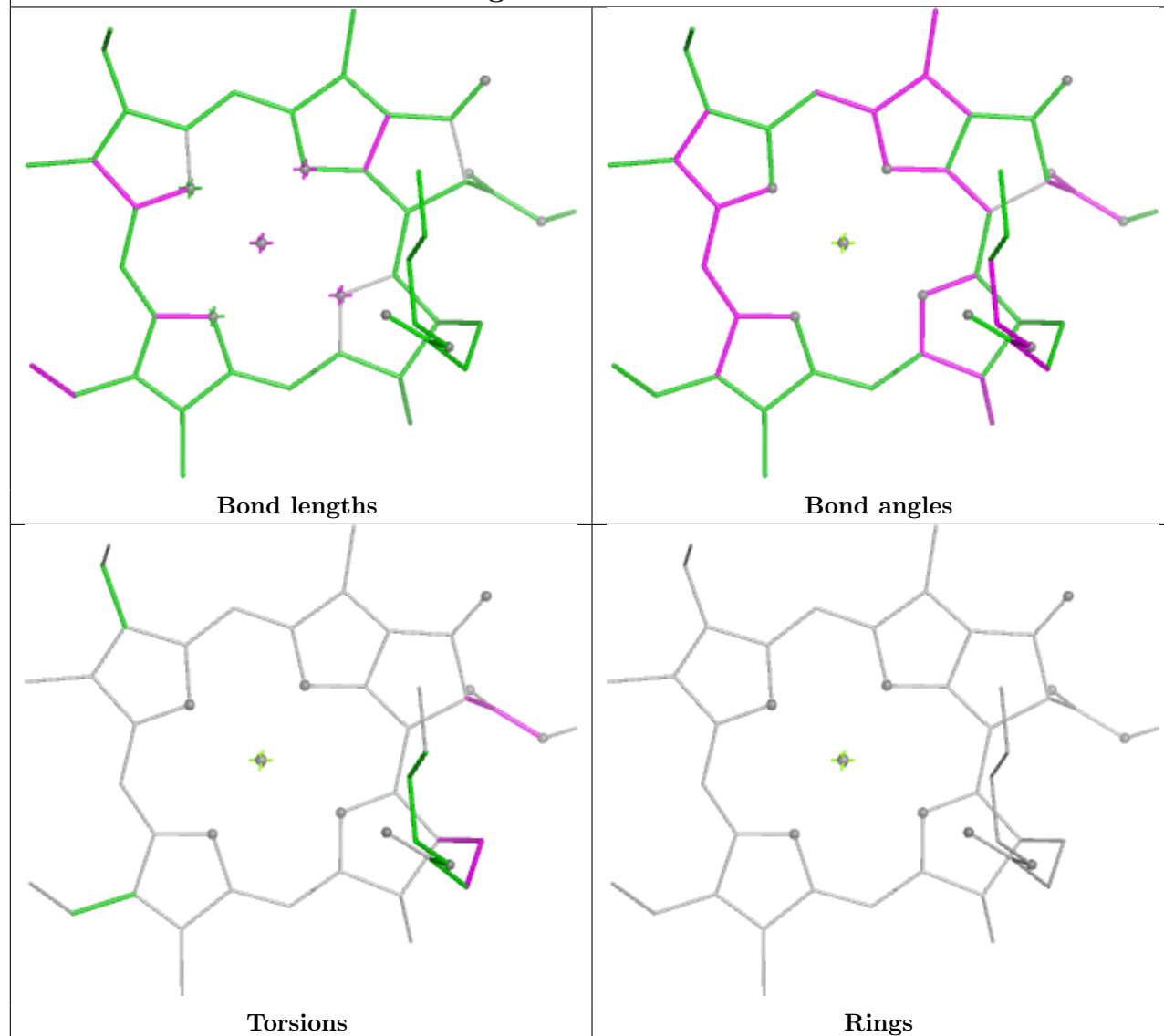


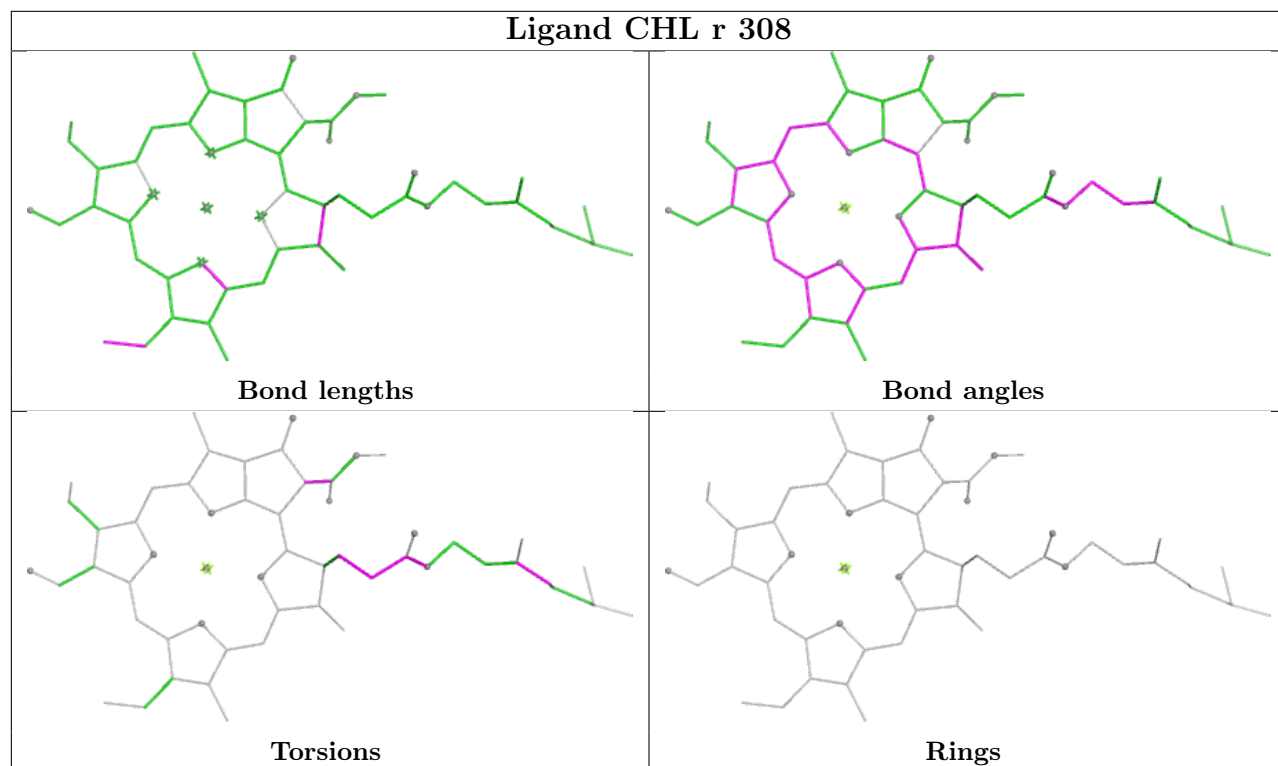
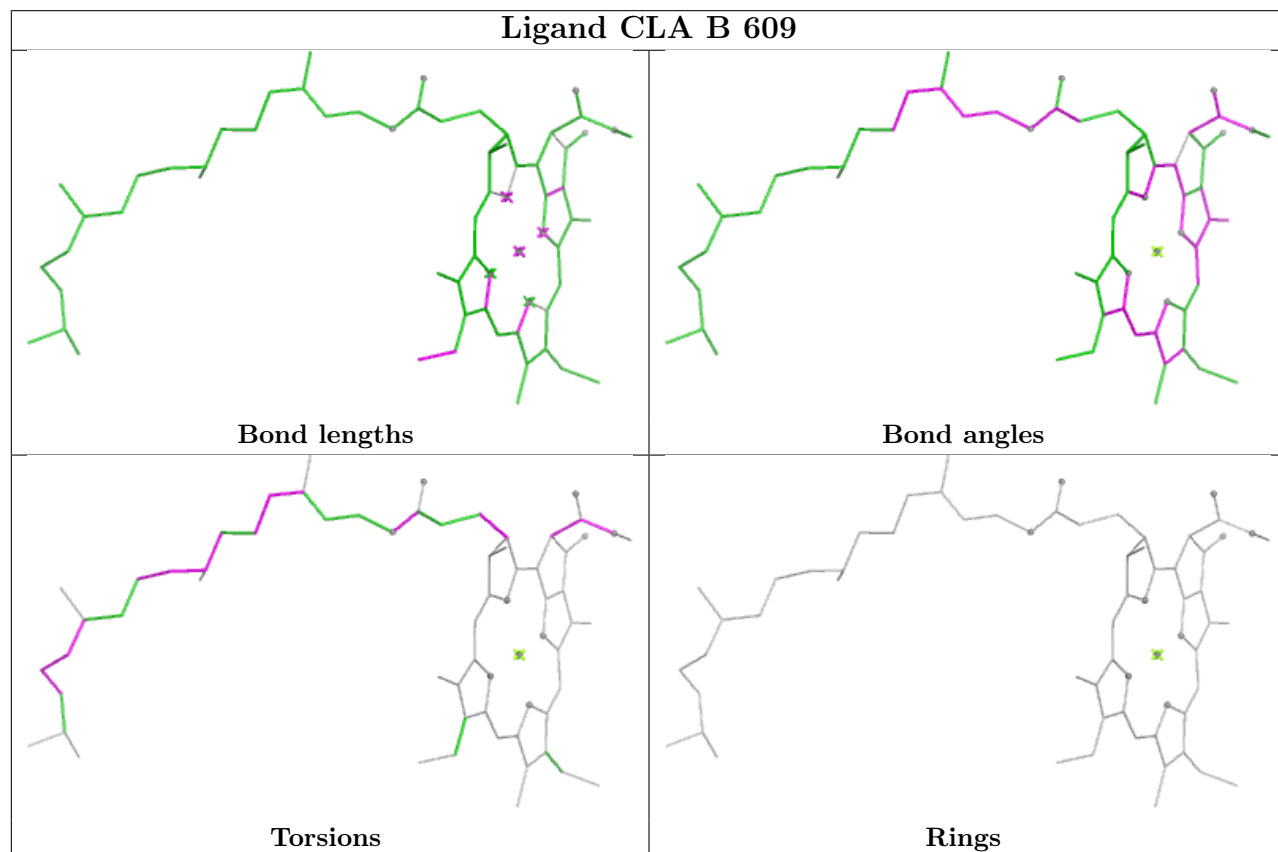
Ligand CLA n 303**Ligand LUT 0 616**

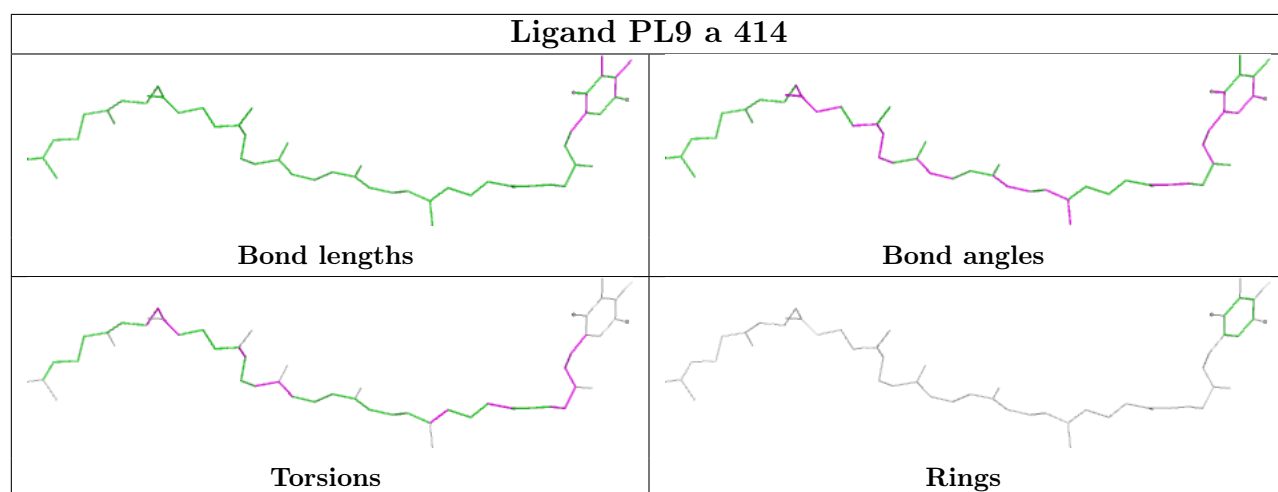
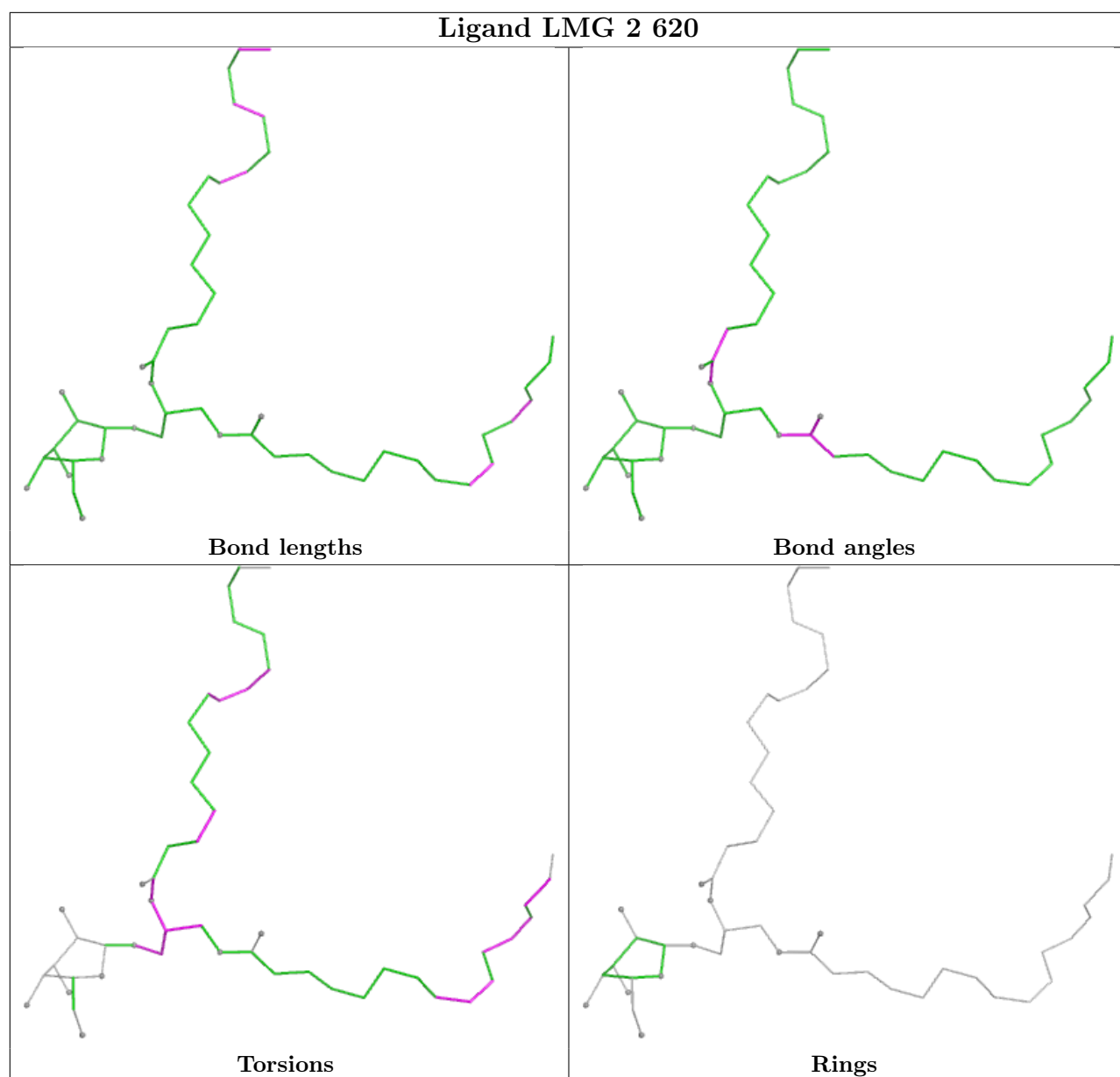




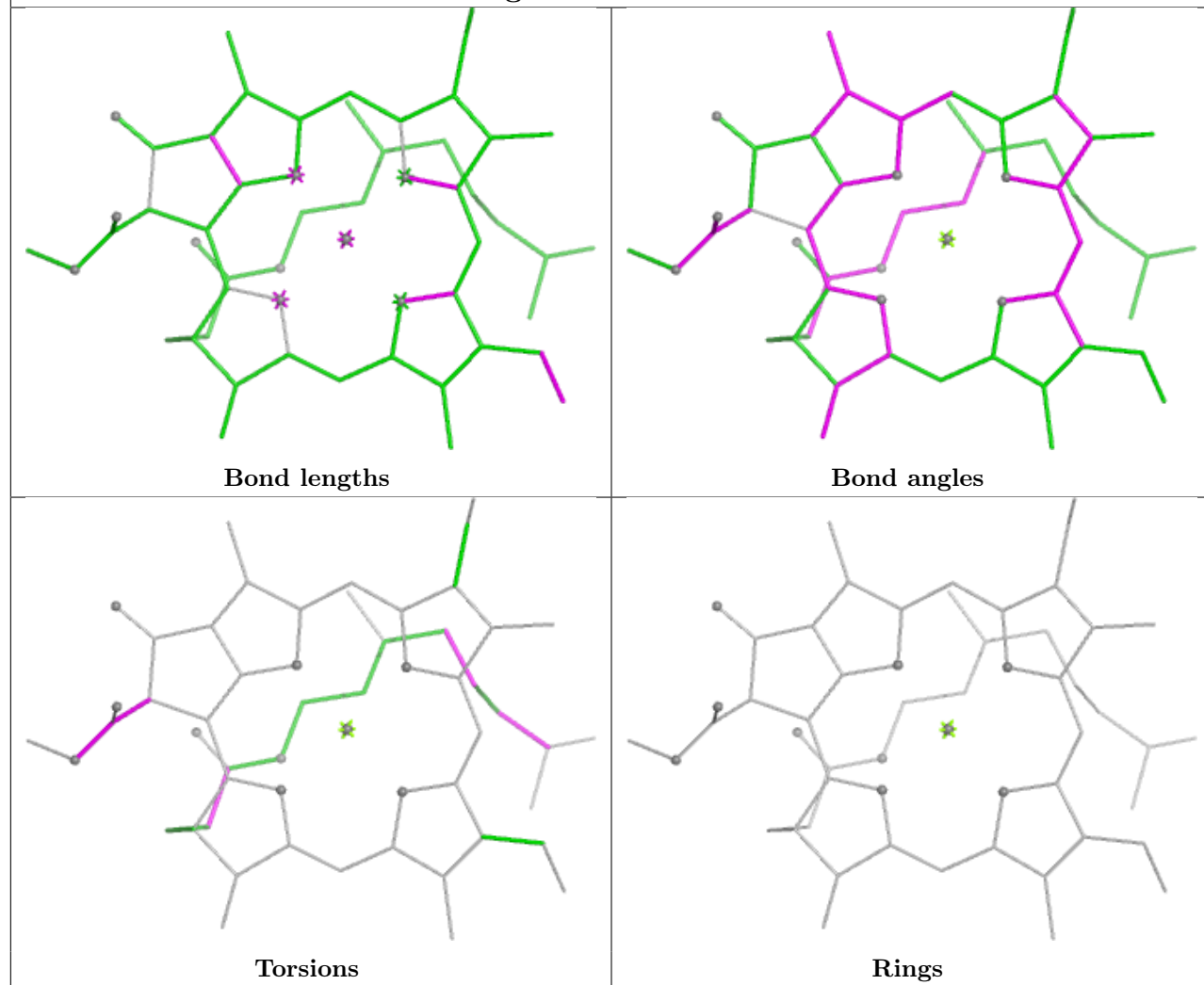
Ligand CLA n 312



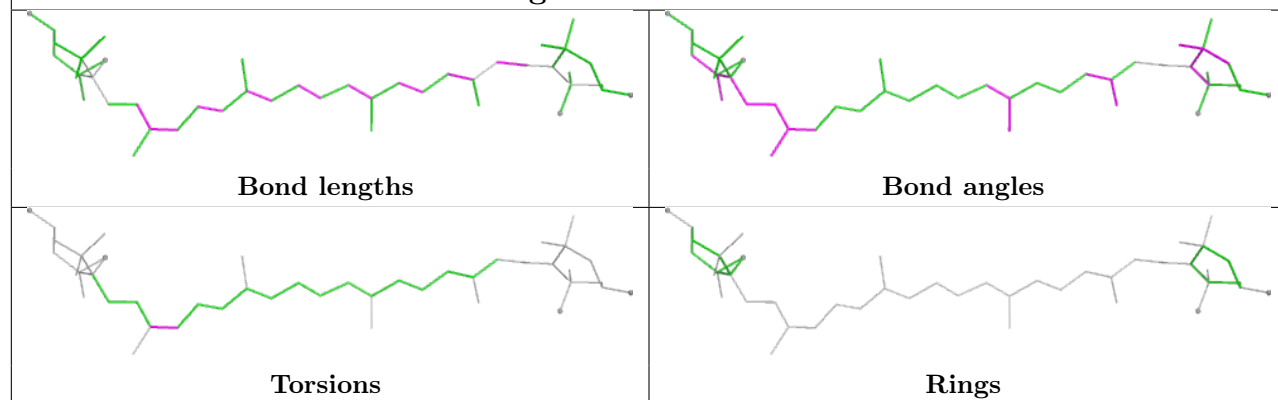
Ligand CHL r 308**Ligand CLA B 609**

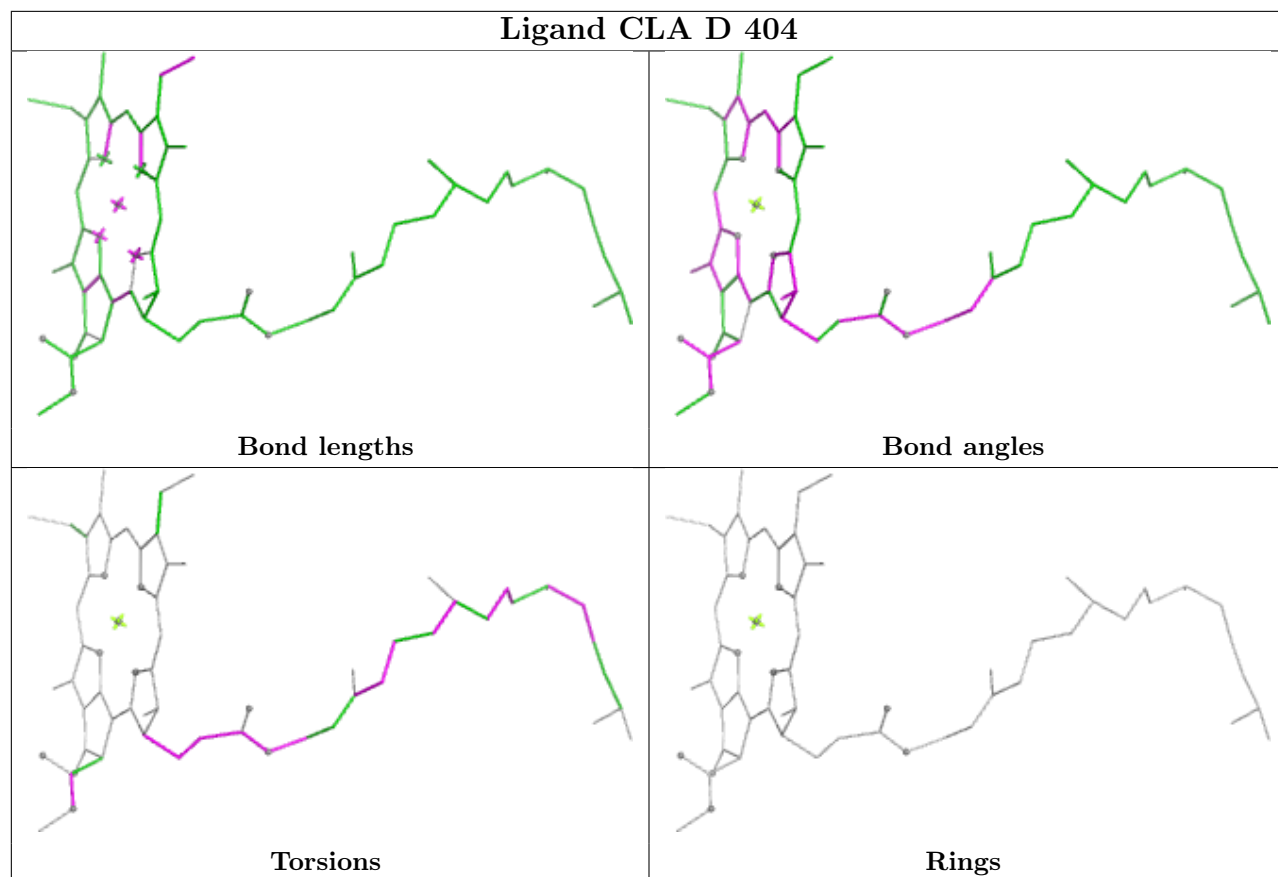


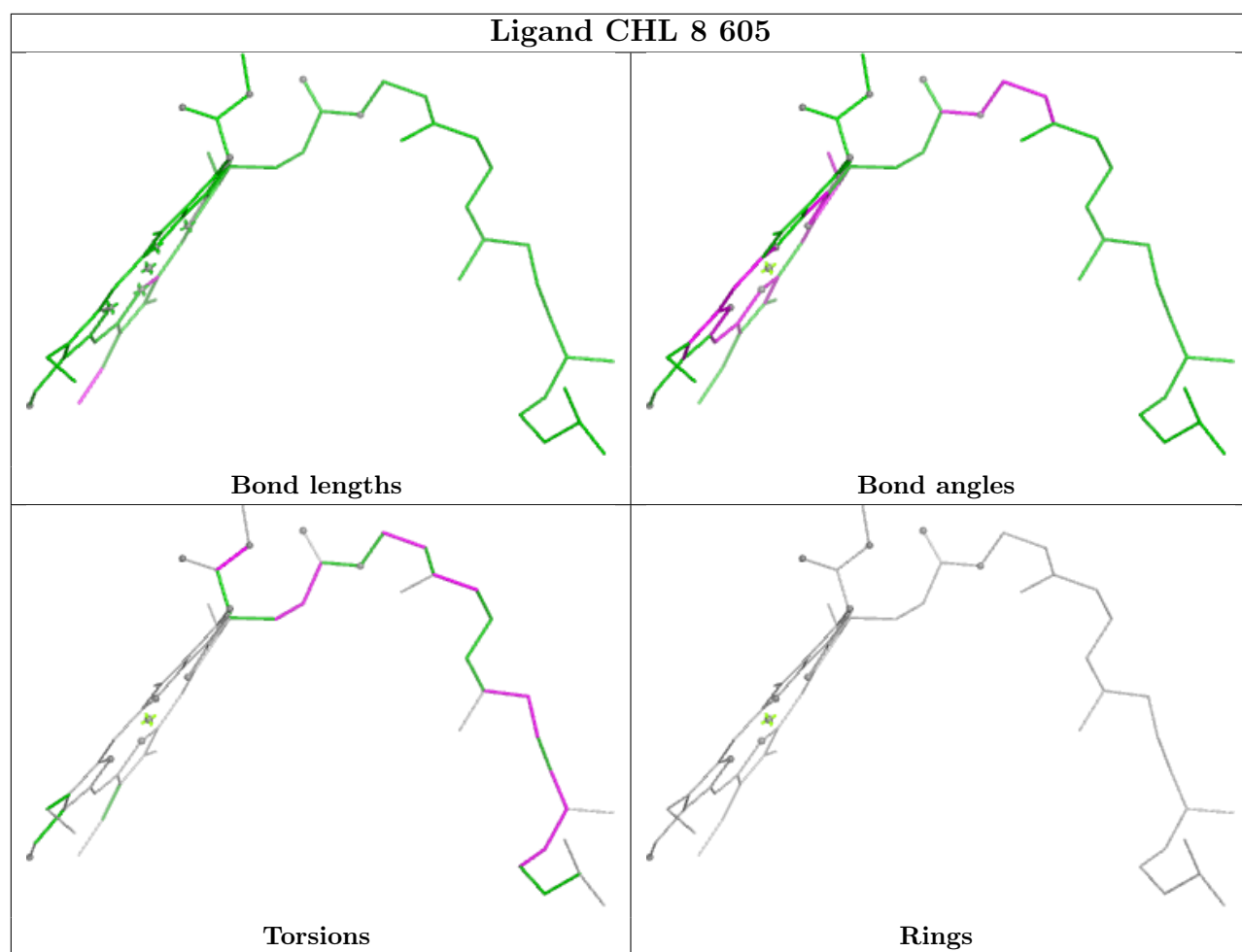
Ligand CLA 9 315

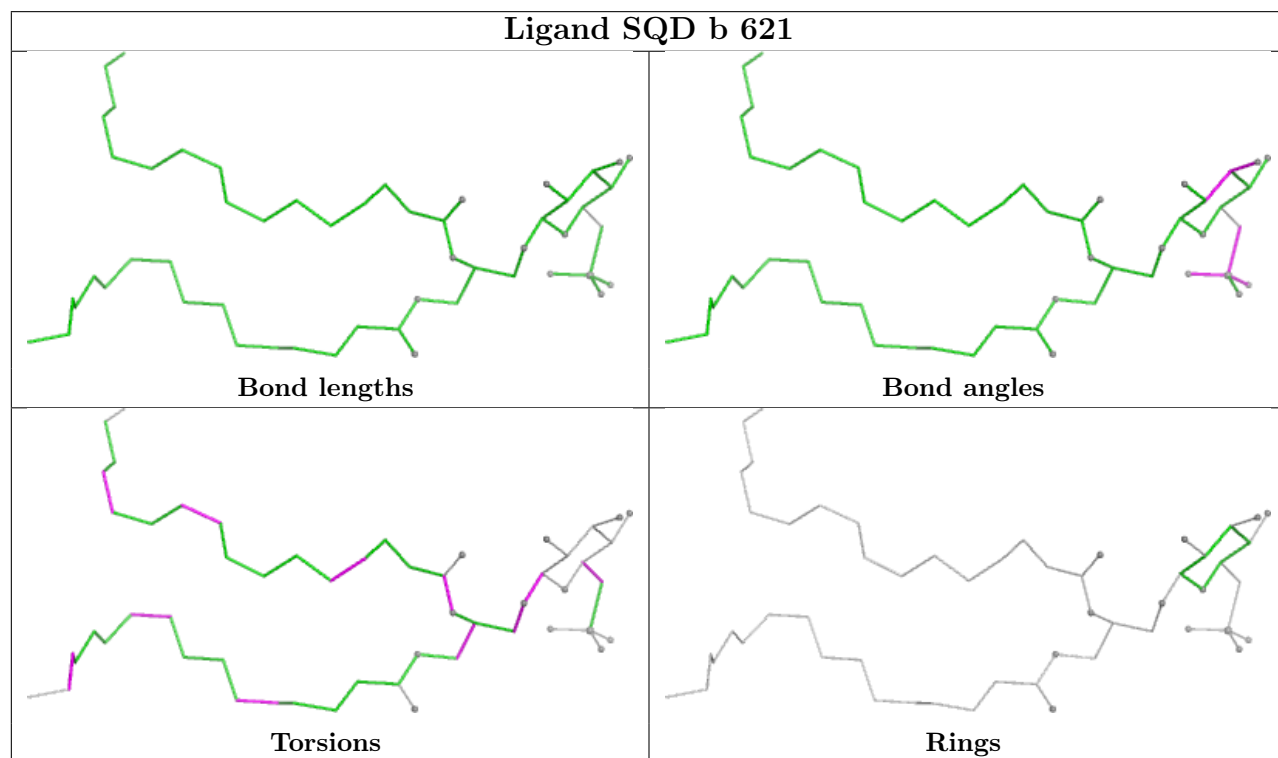
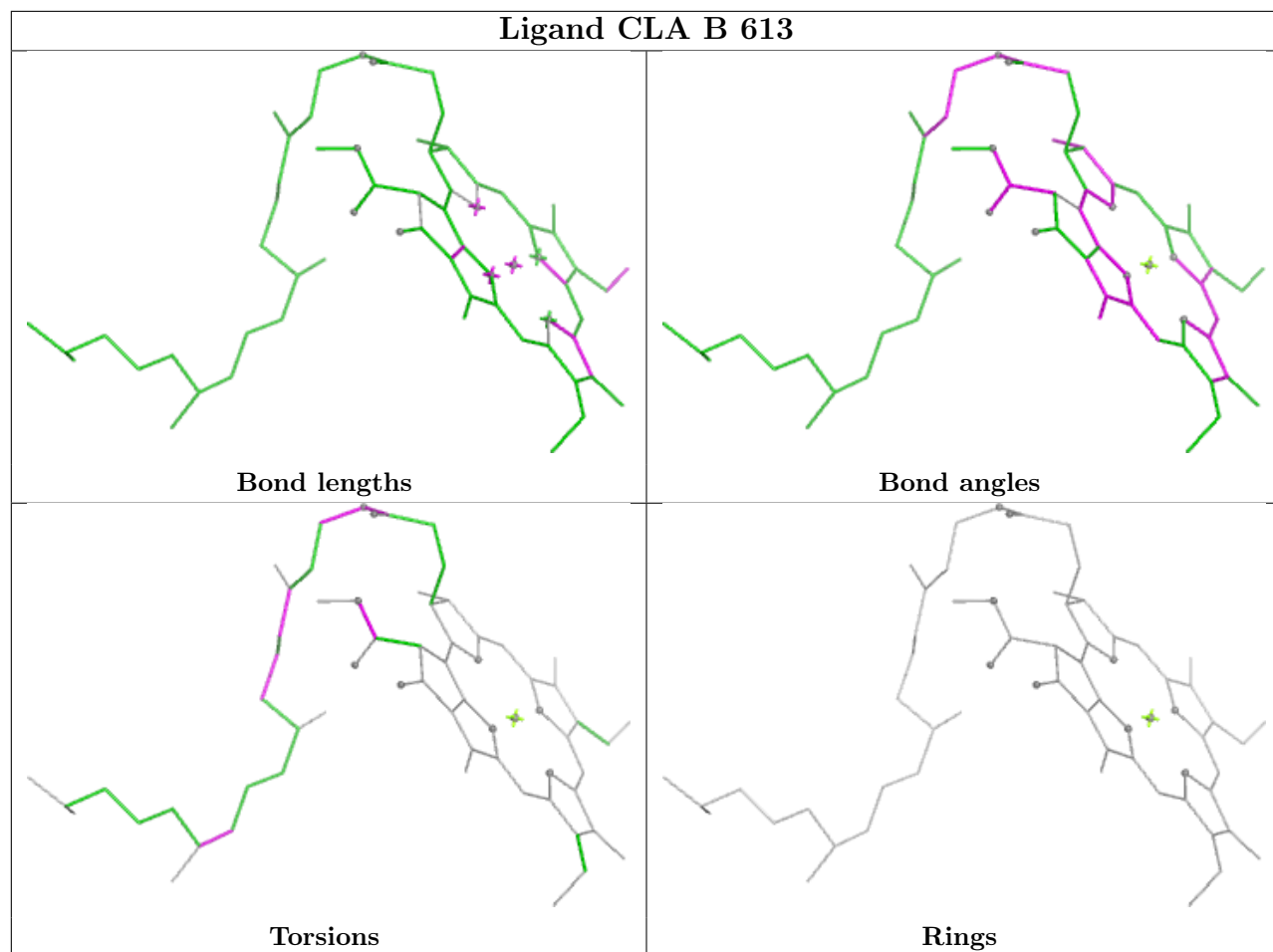


Ligand NEX G 616

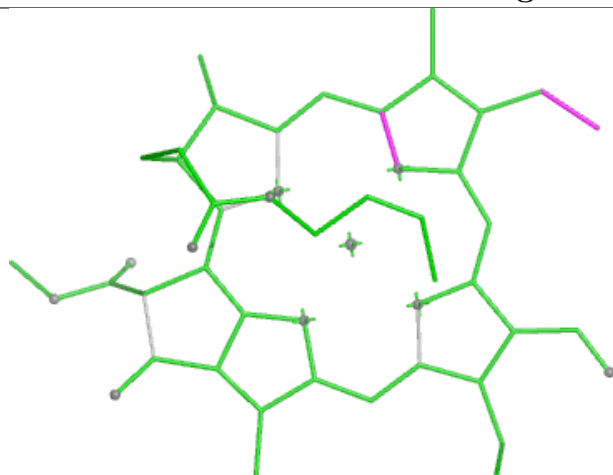




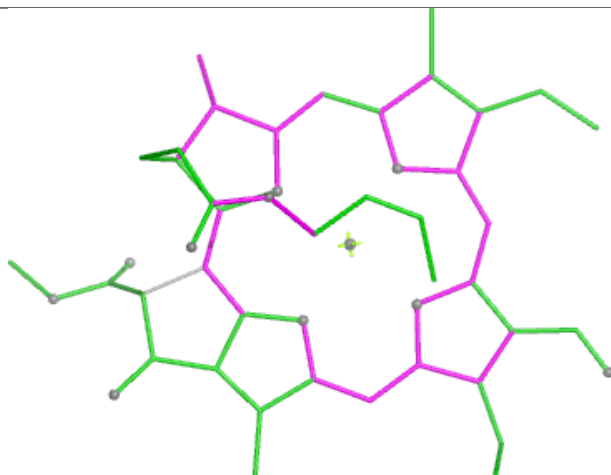




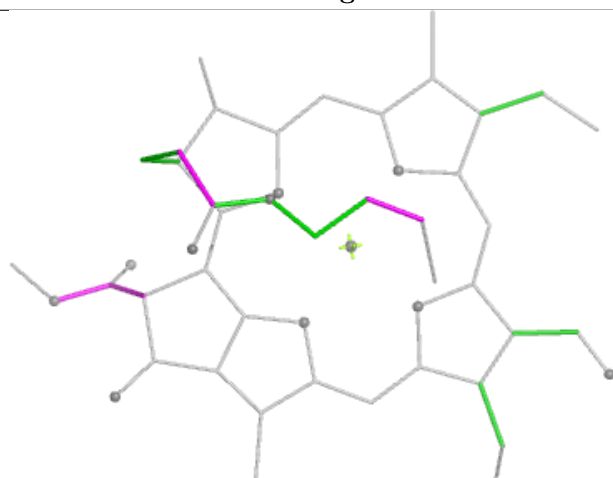
Ligand CHL n 301



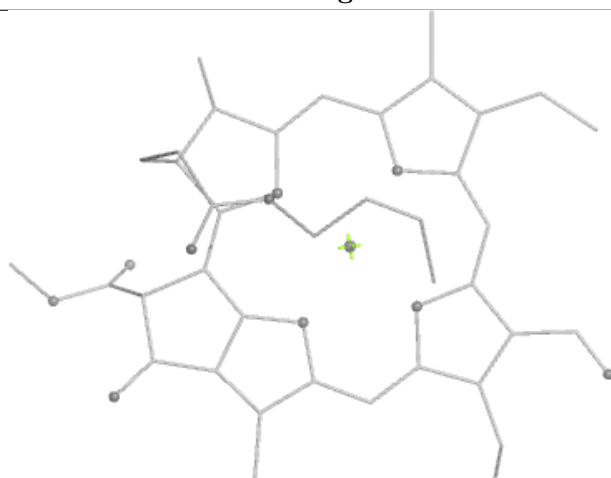
Bond lengths



Bond angles

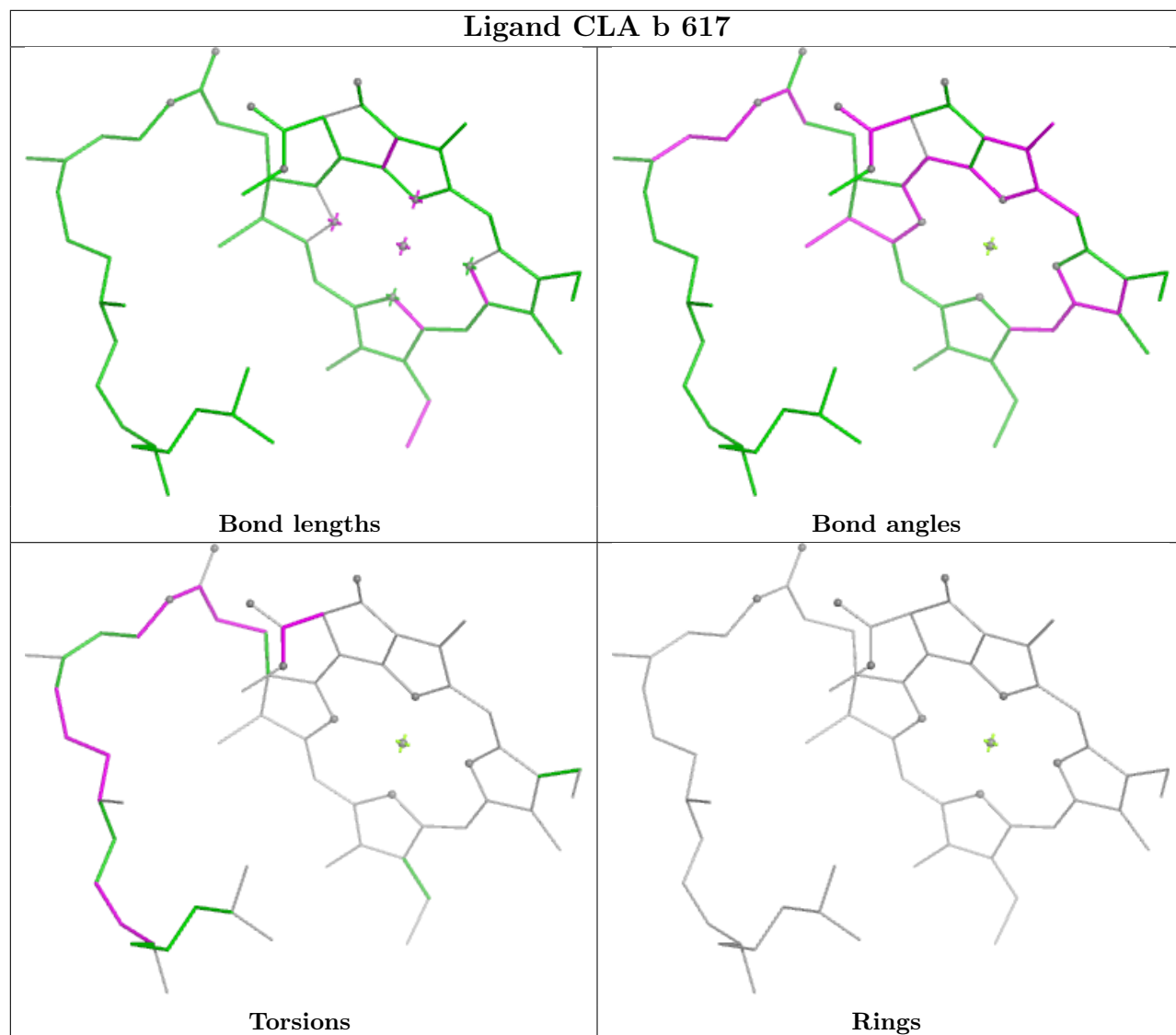


Torsions

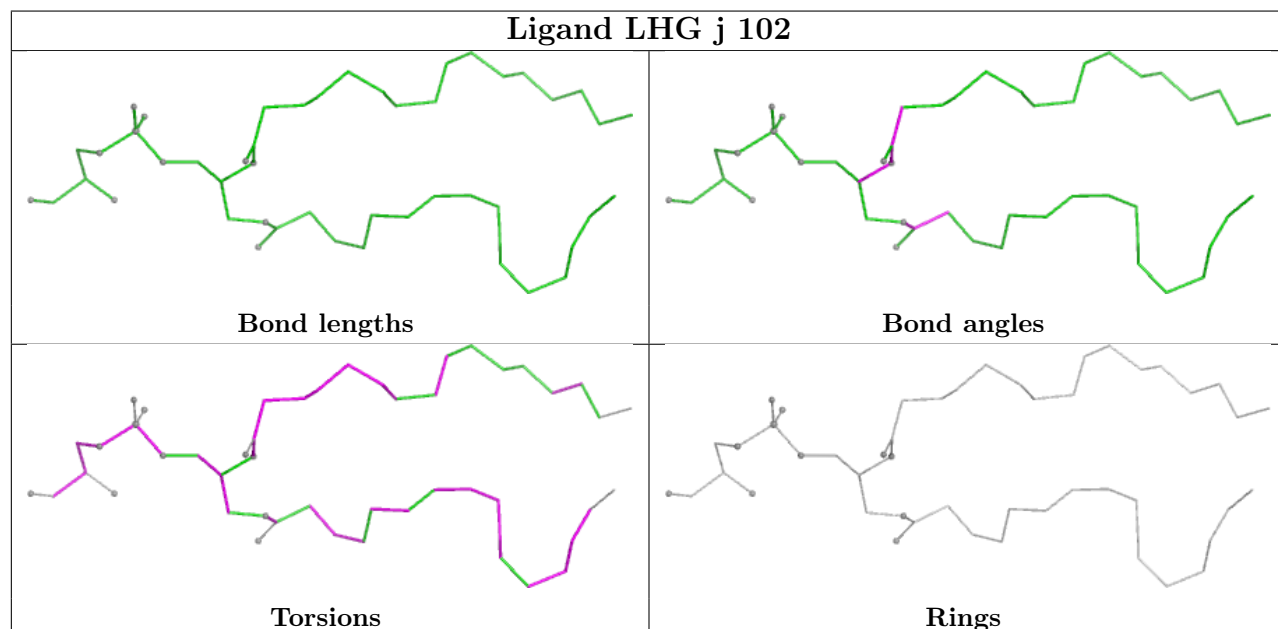


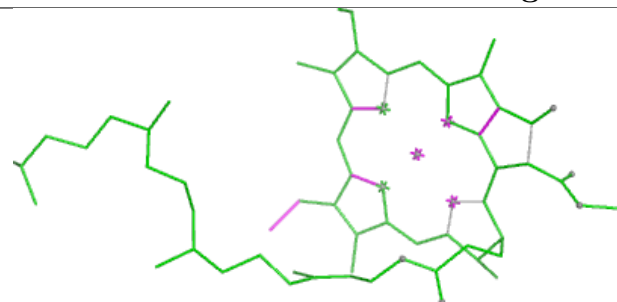
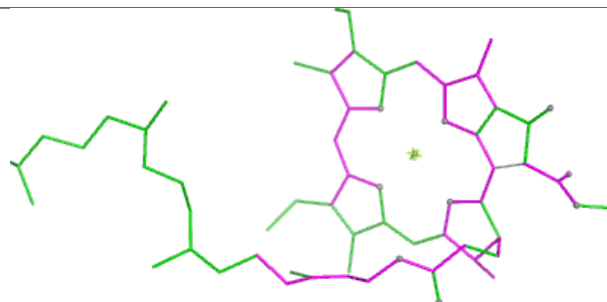
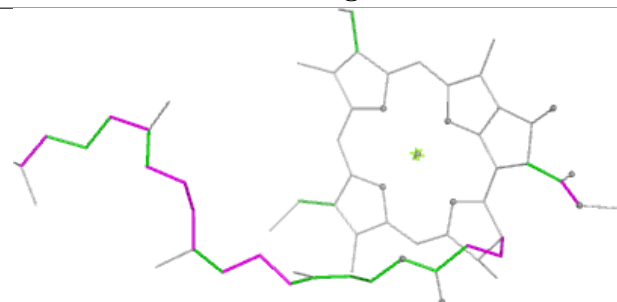
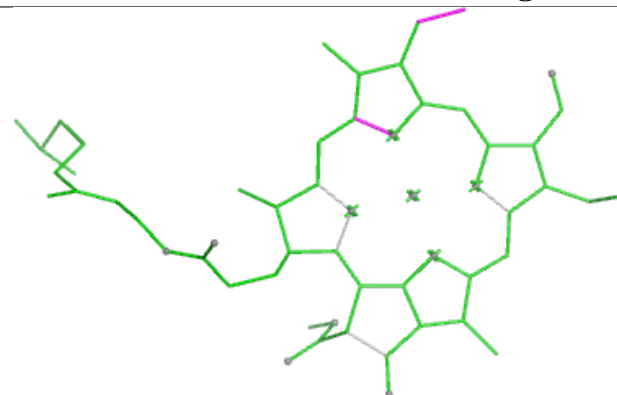
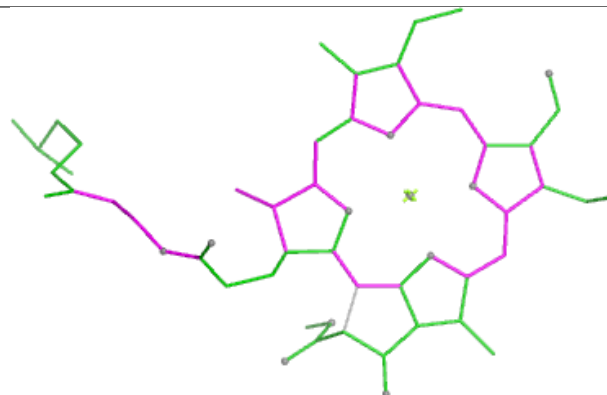
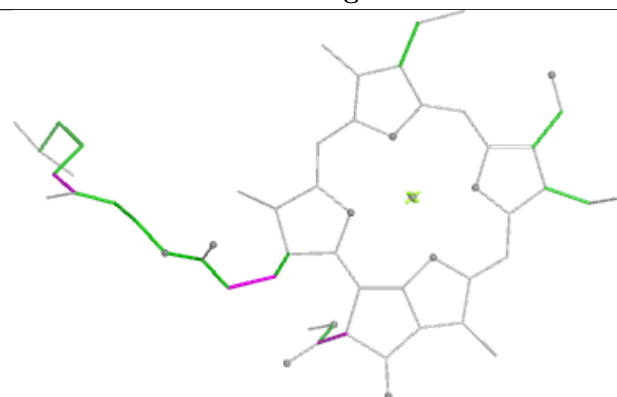
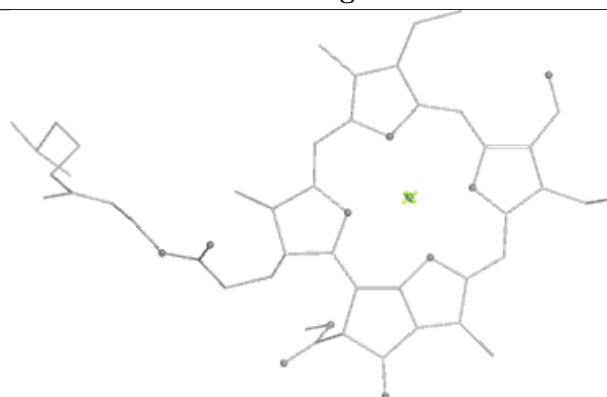
Rings

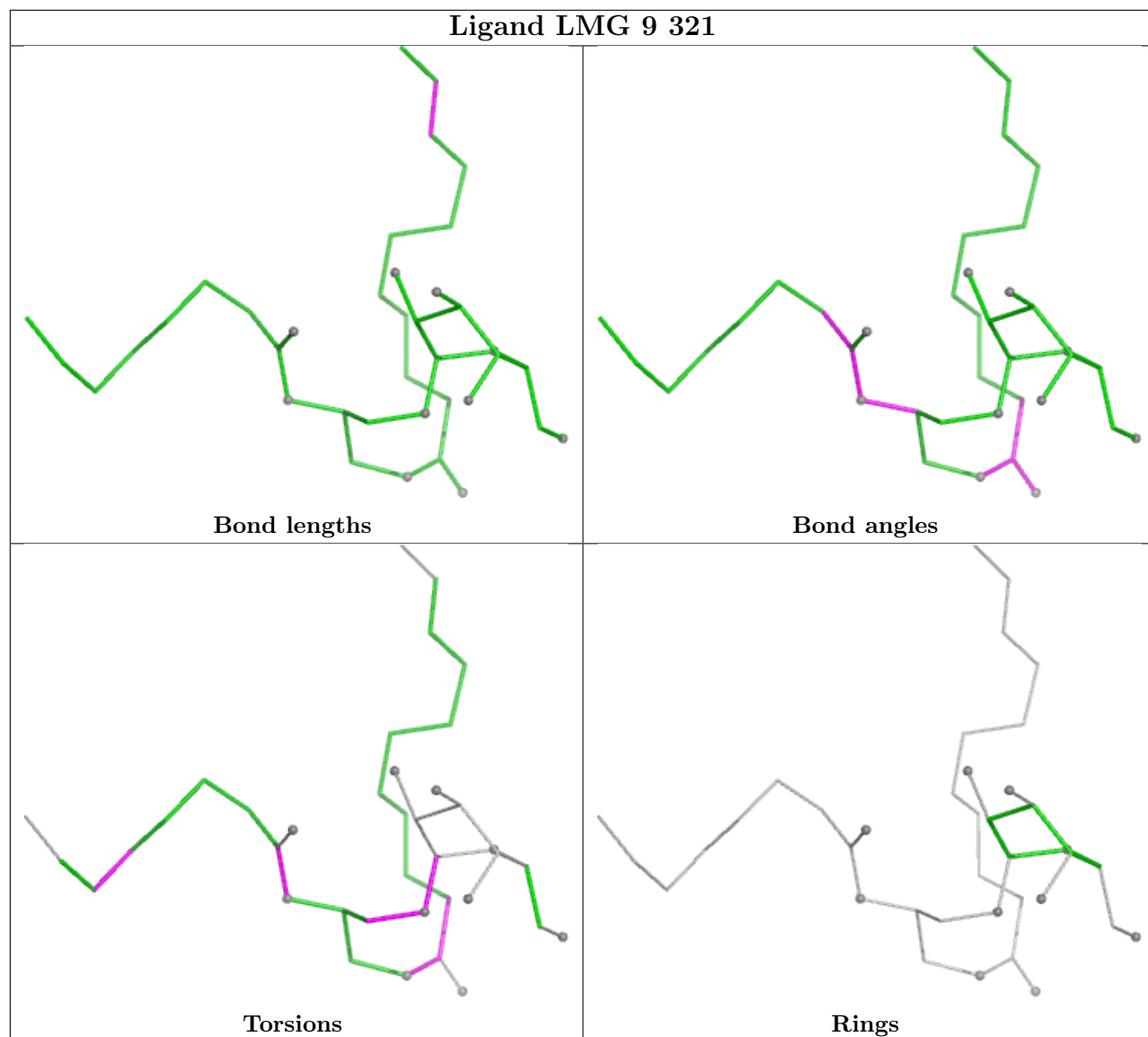
Ligand CLA b 617

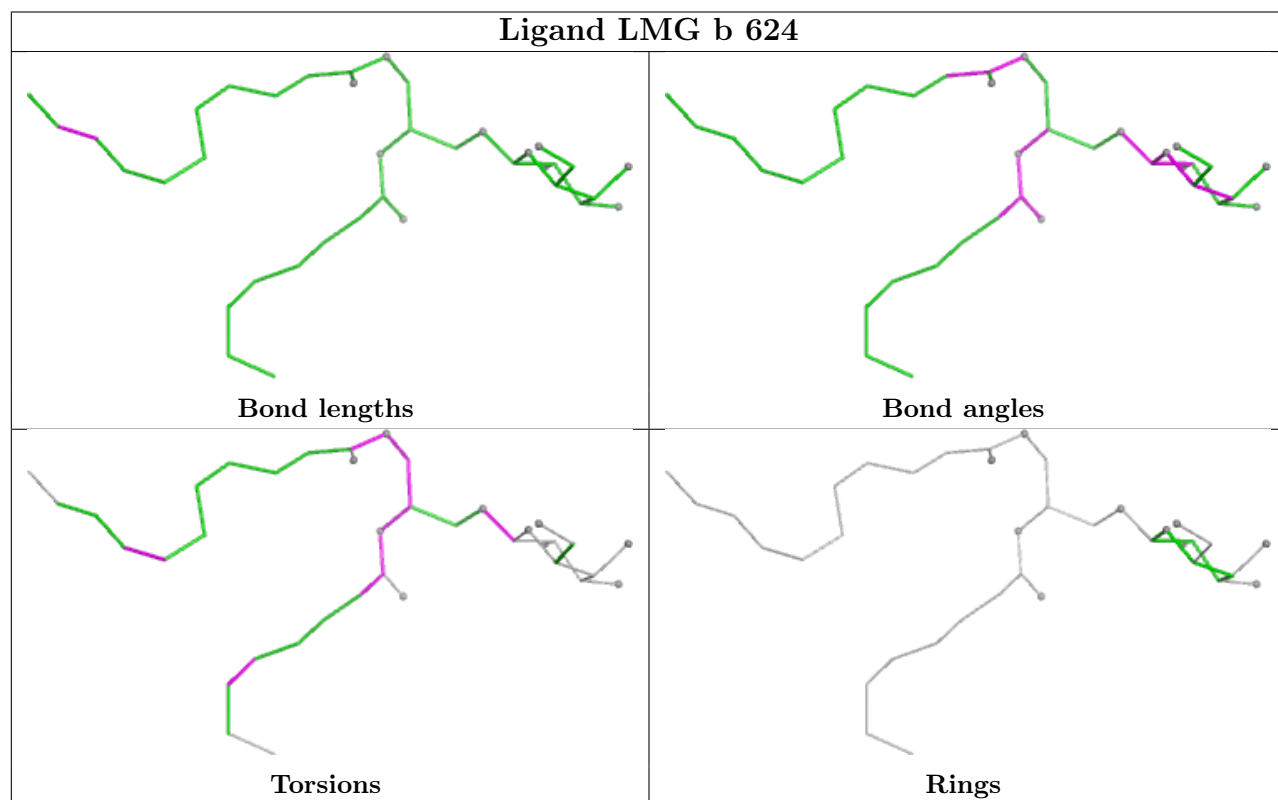
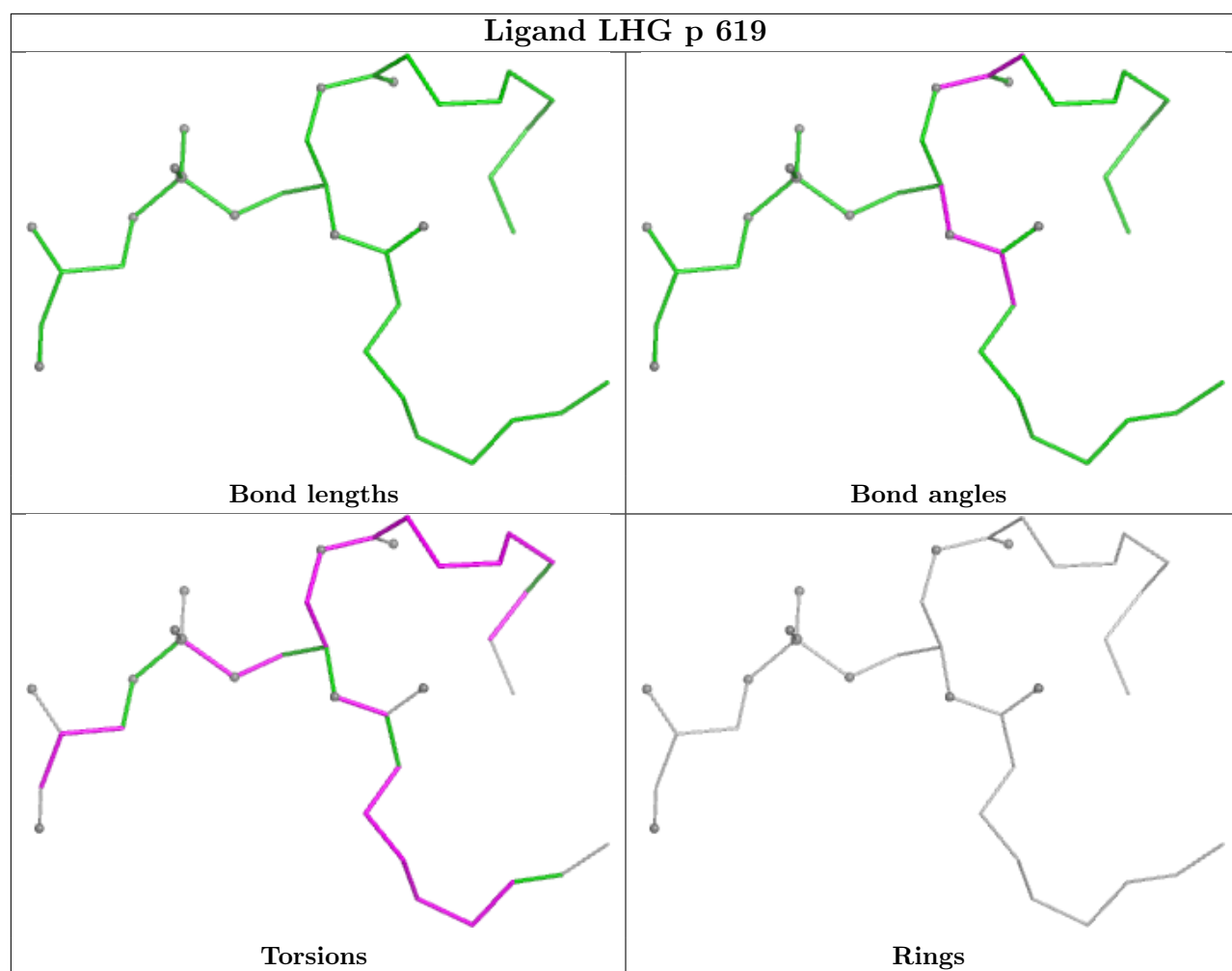


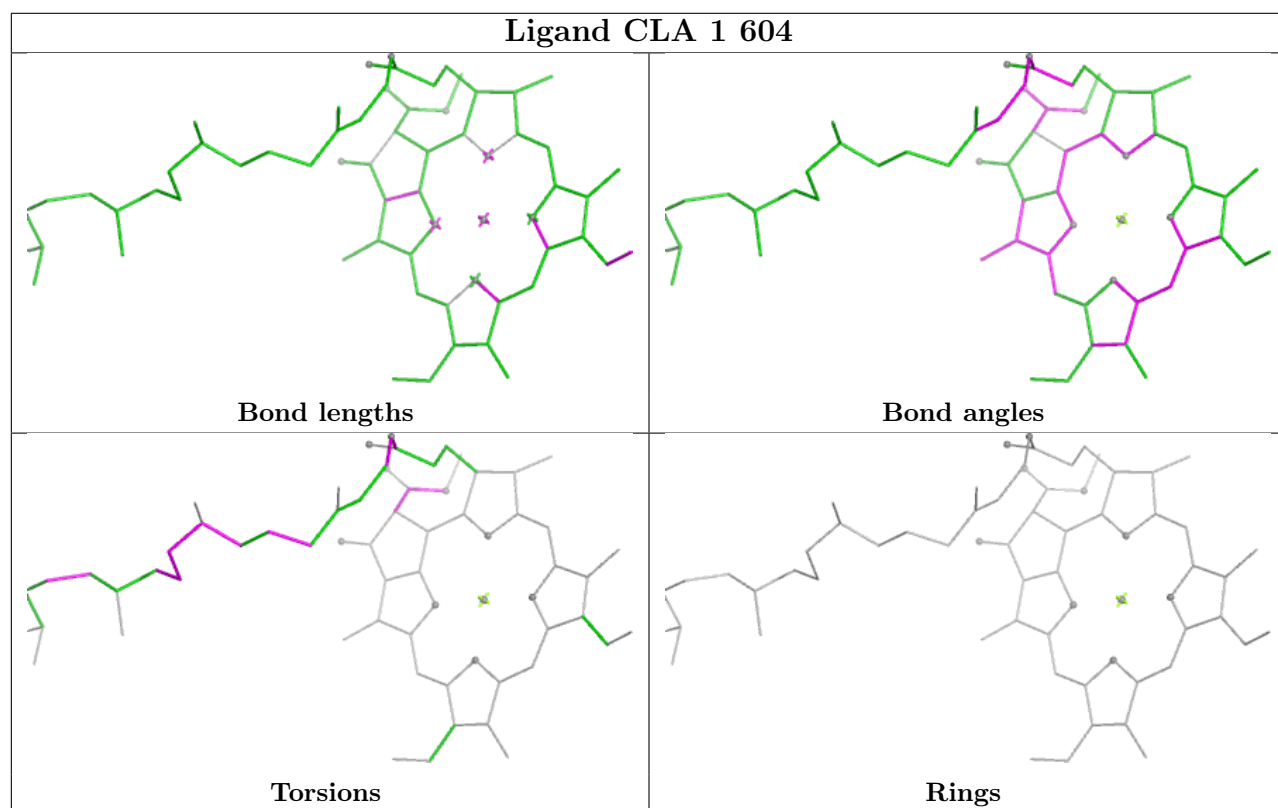
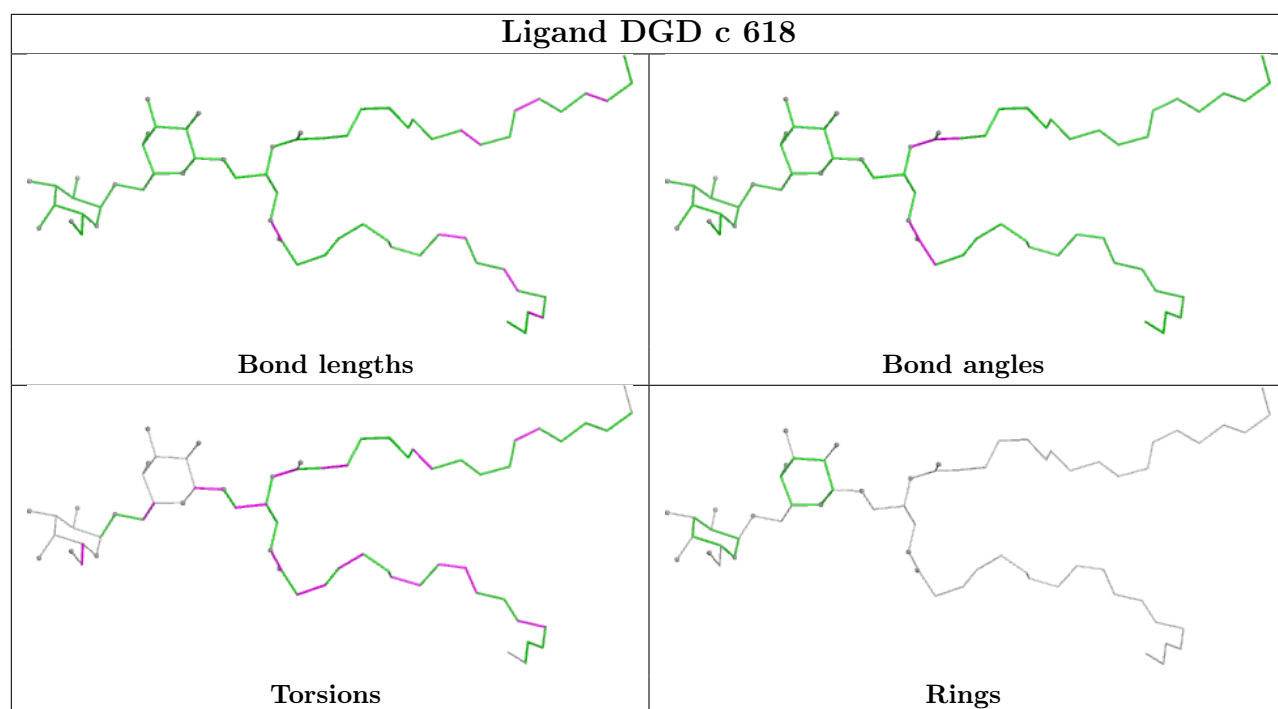
Ligand LHG j 102

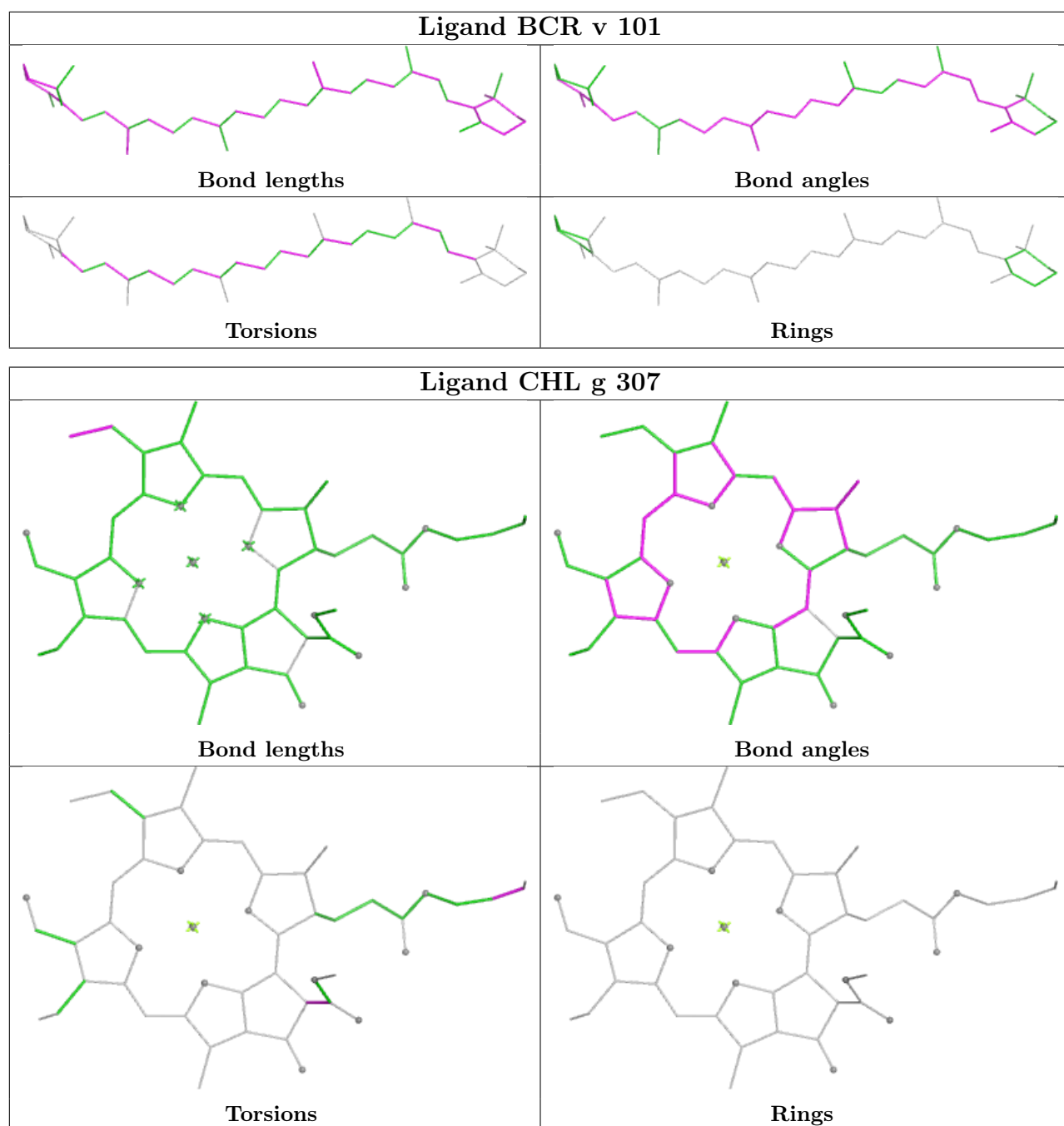


Ligand CLA S 311**Bond lengths****Bond angles****Torsions****Rings****Ligand CHL N 302****Bond lengths****Bond angles****Torsions****Rings**

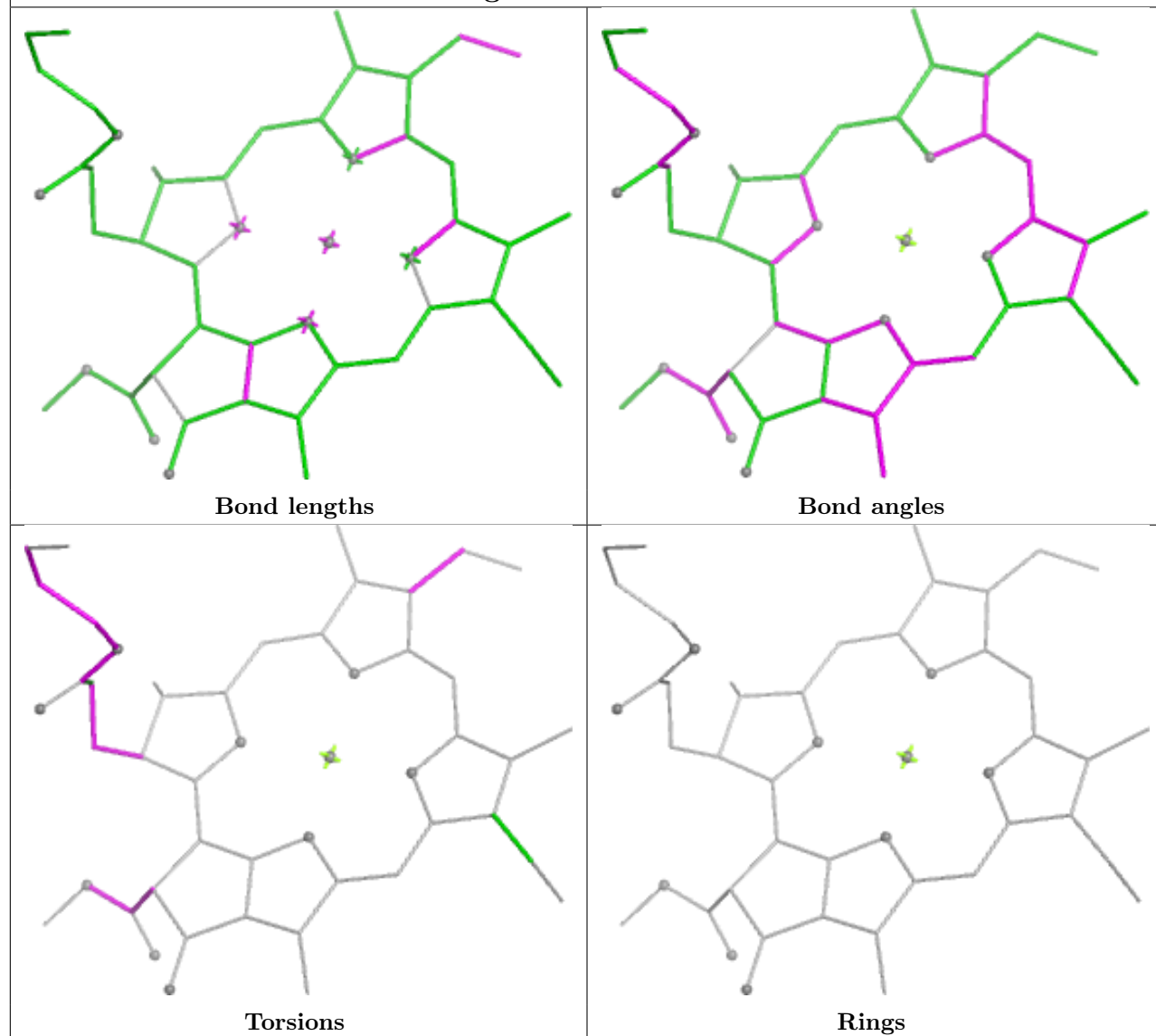




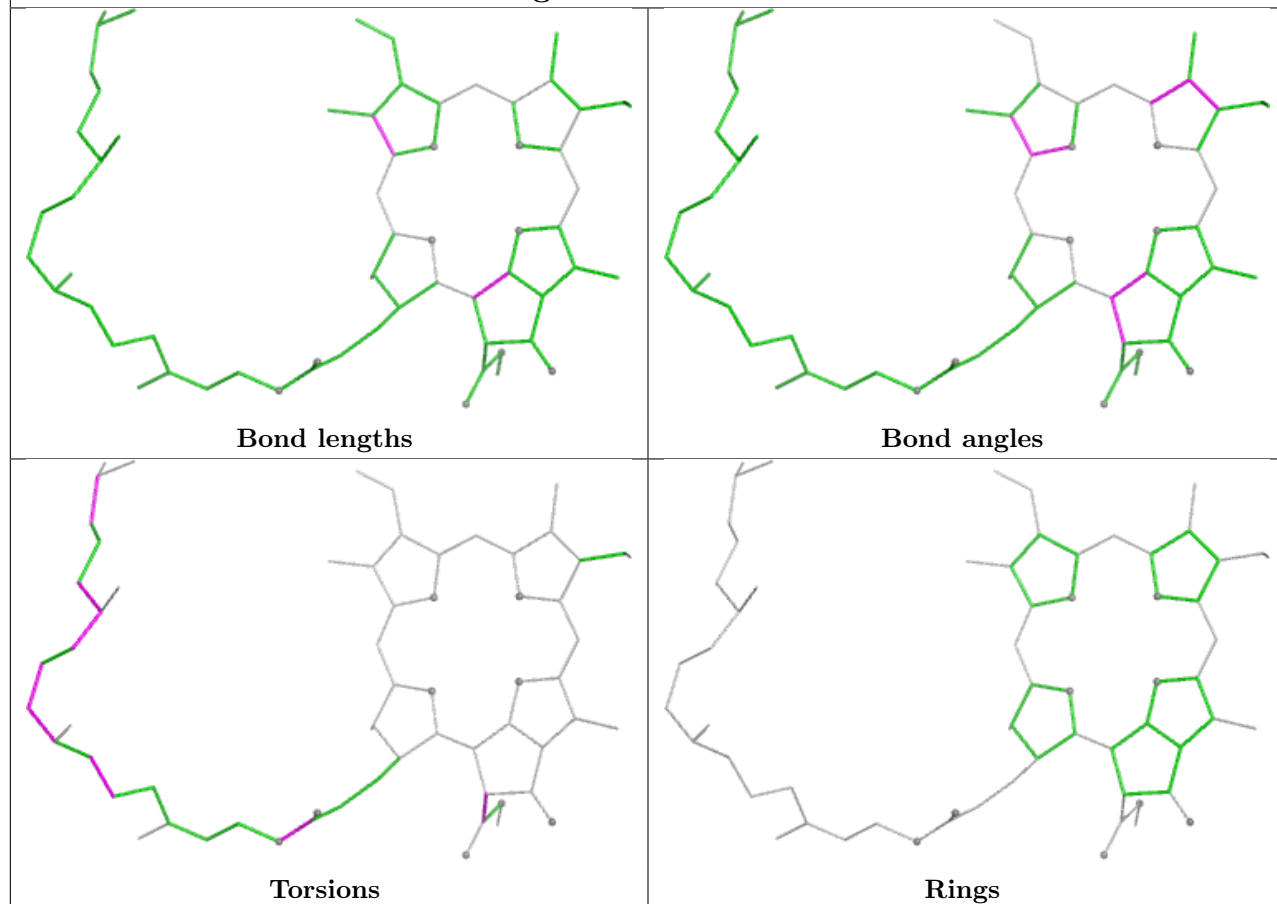




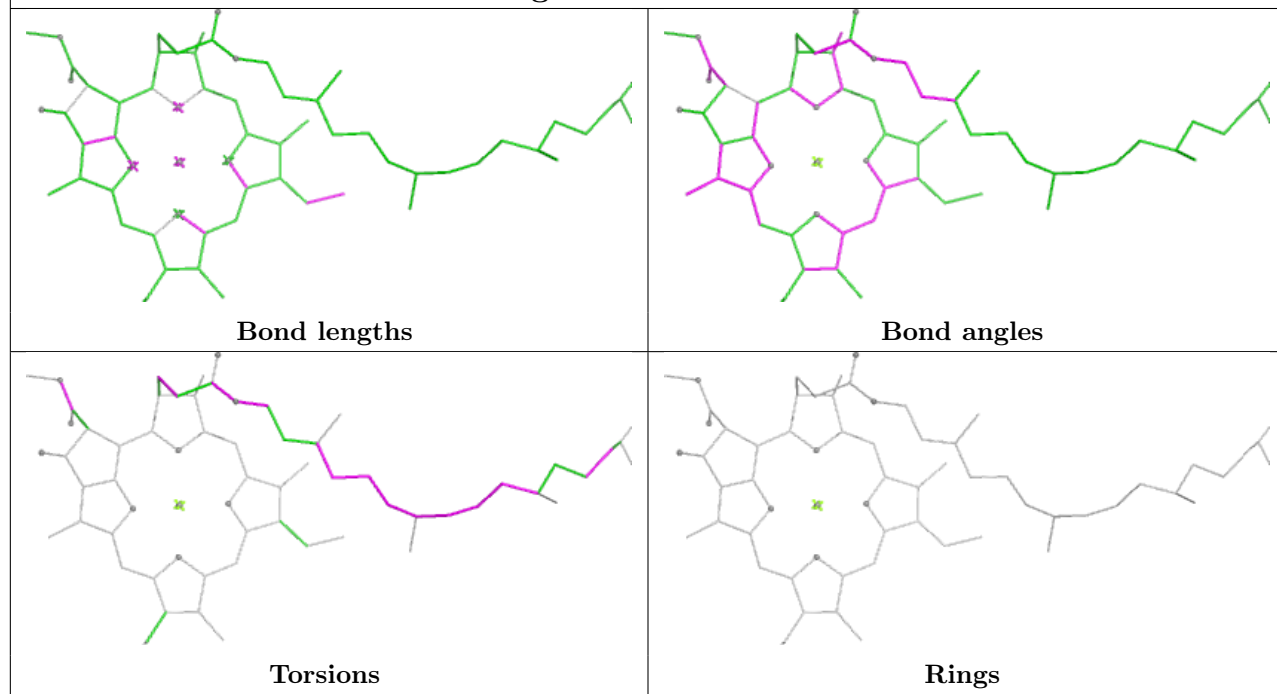
Ligand CLA b 602

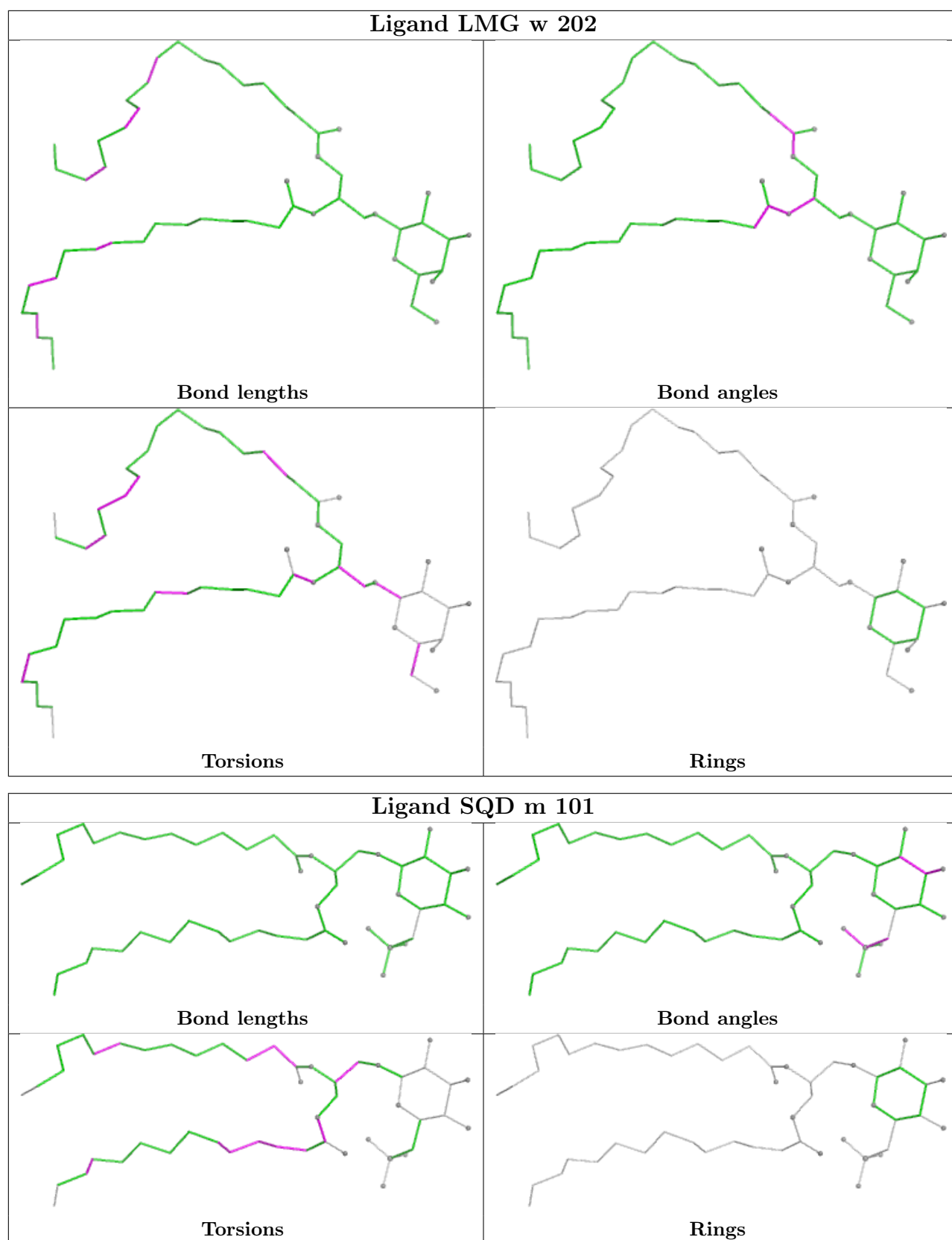


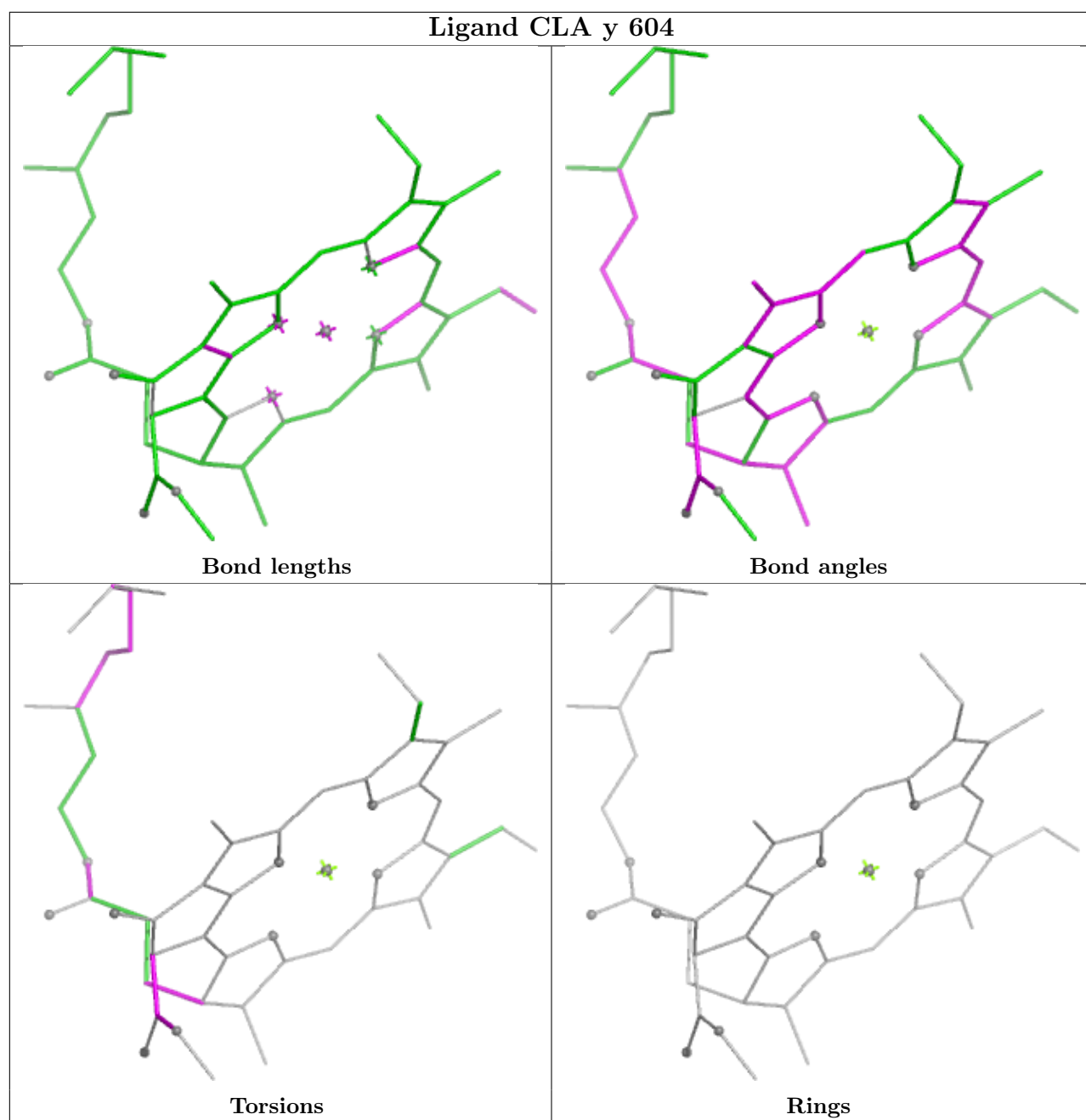
Ligand PHO a 408



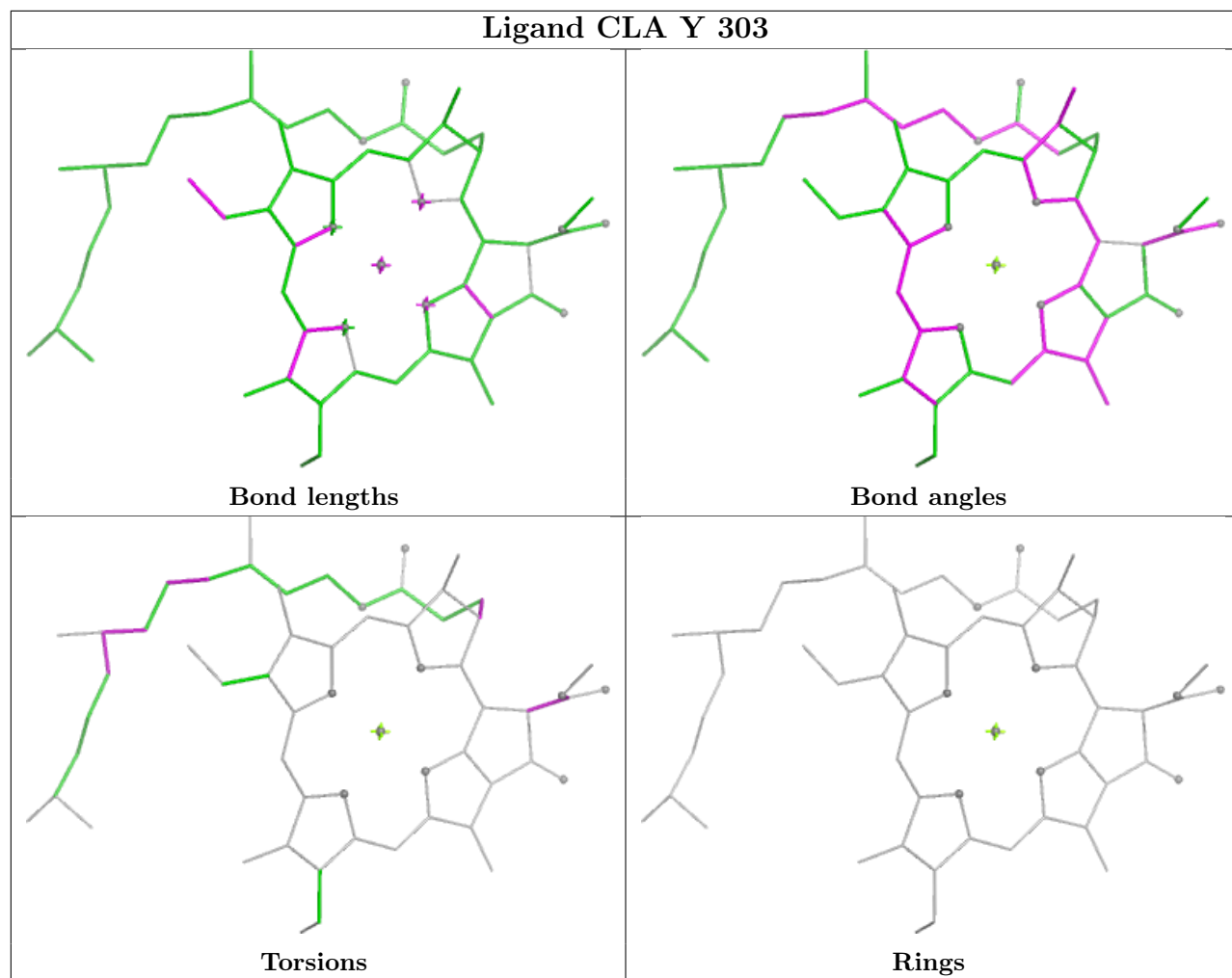
Ligand CLA B 603



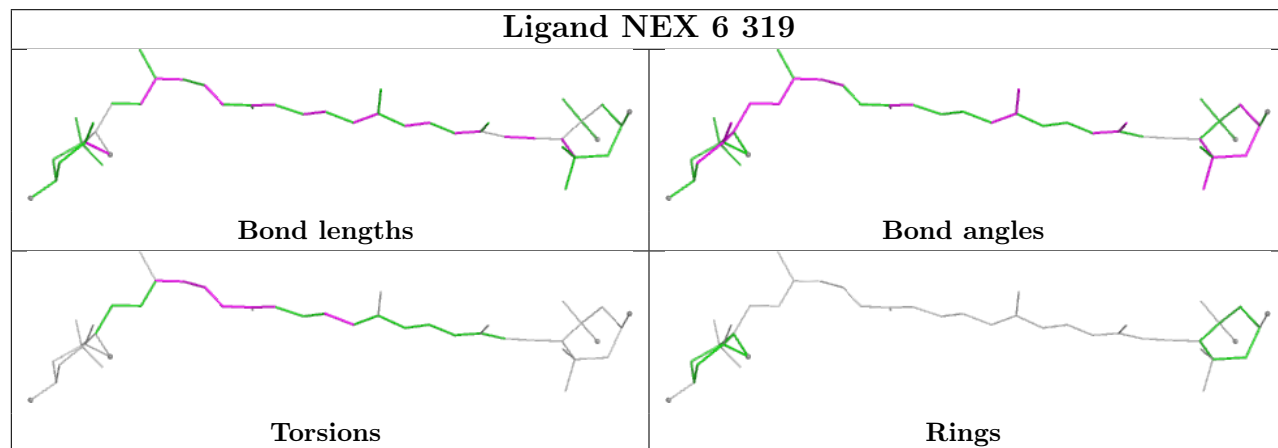


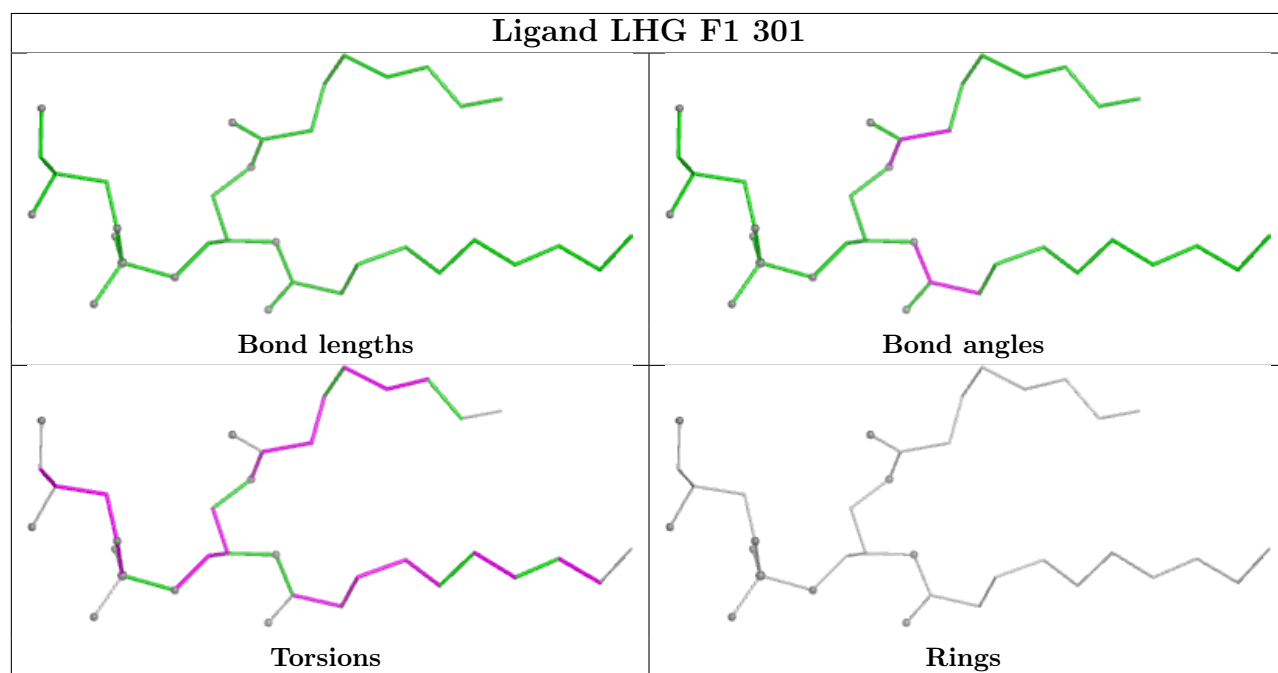
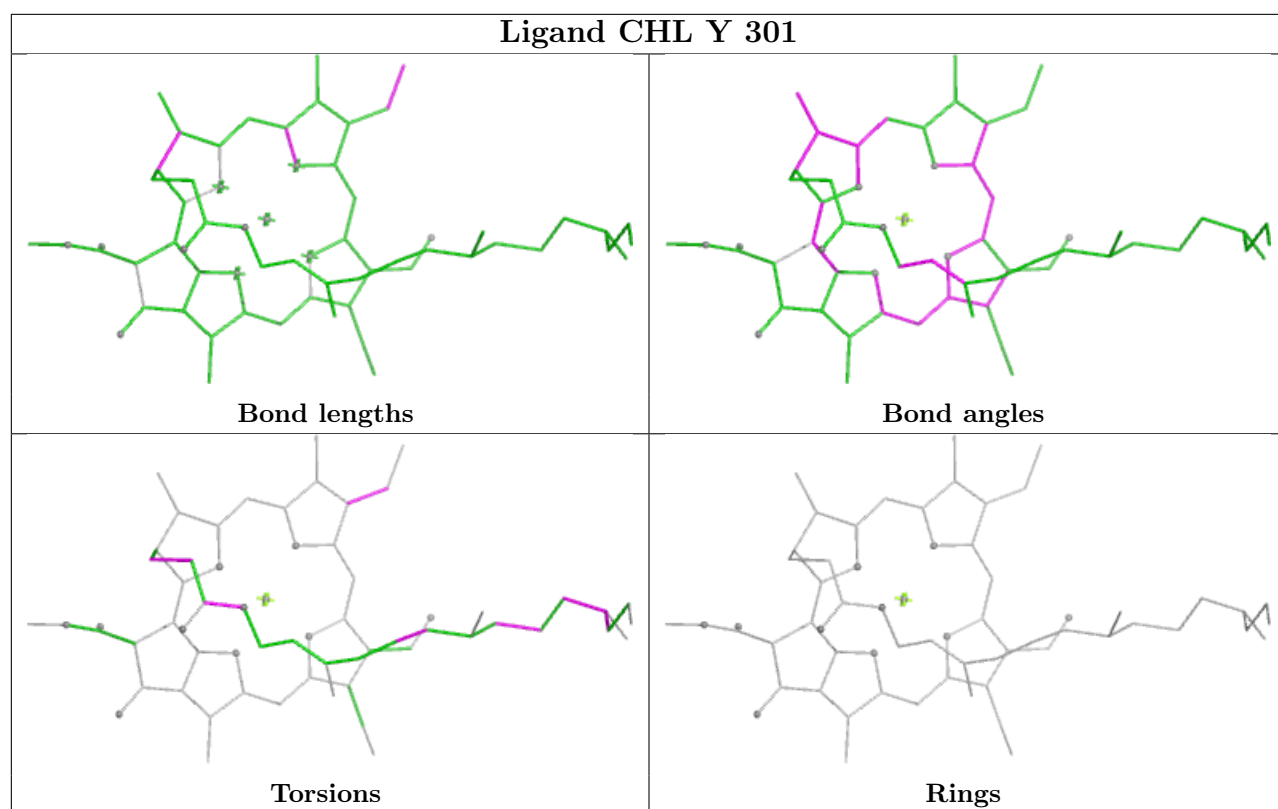


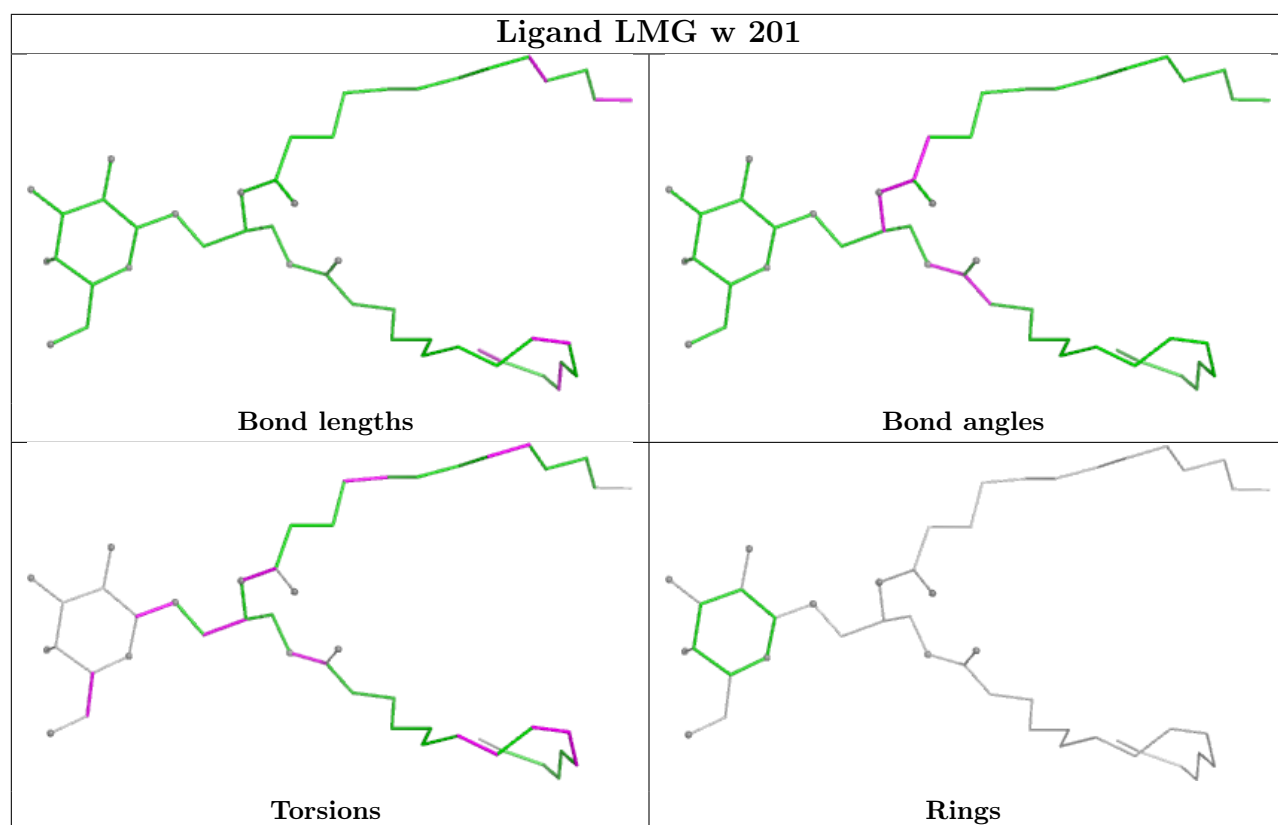
Ligand CLA Y 303

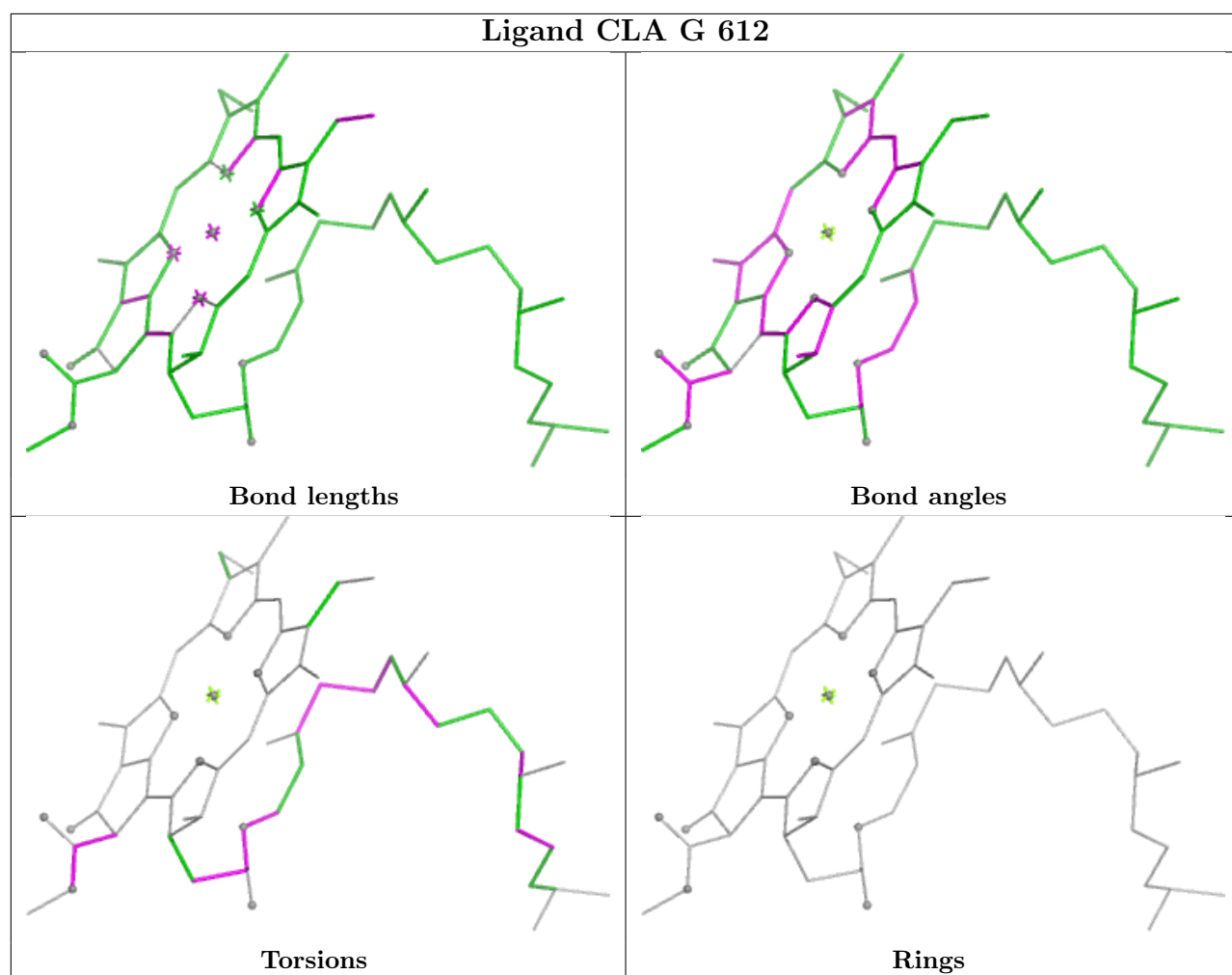


Ligand NEX 6 319

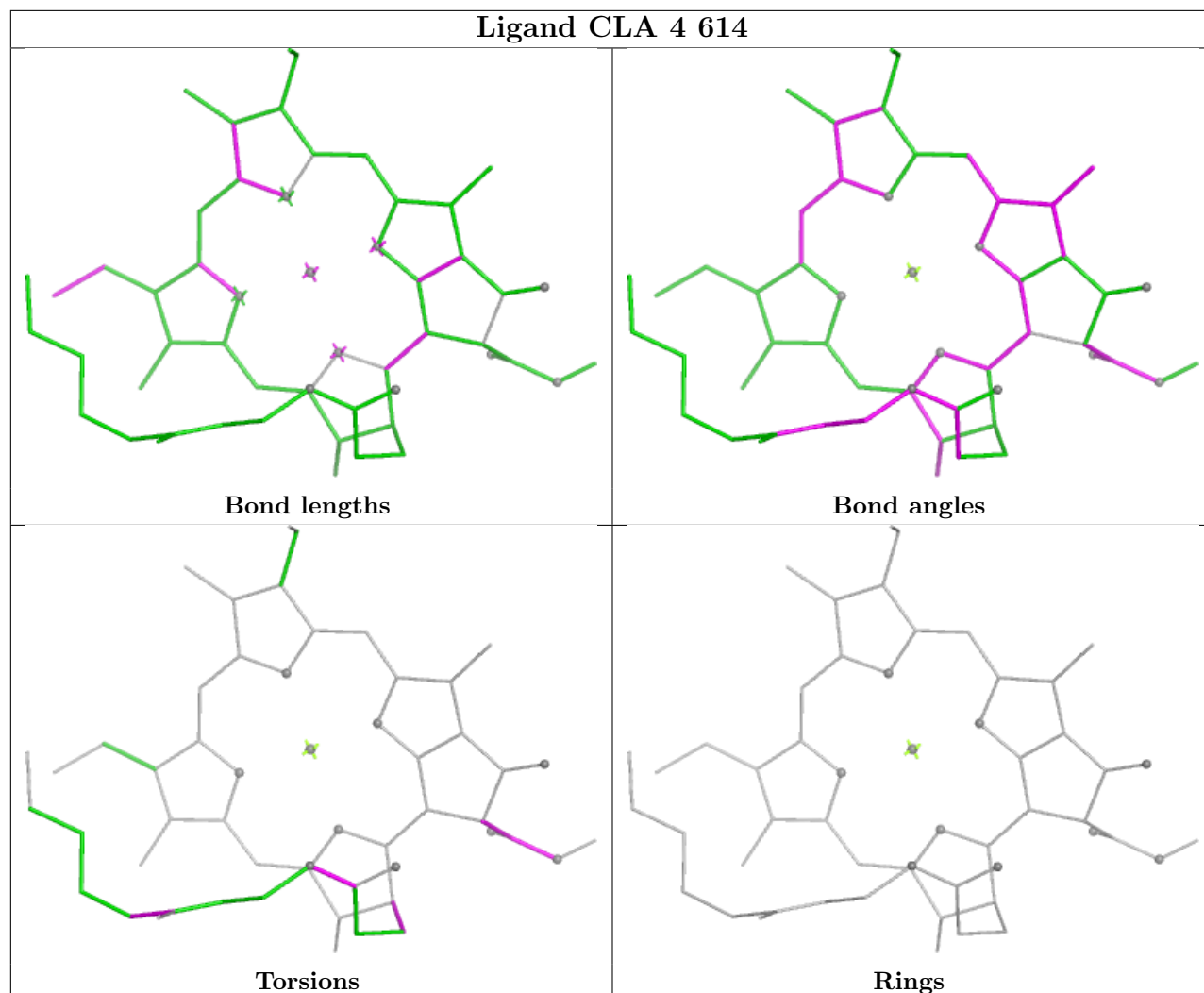




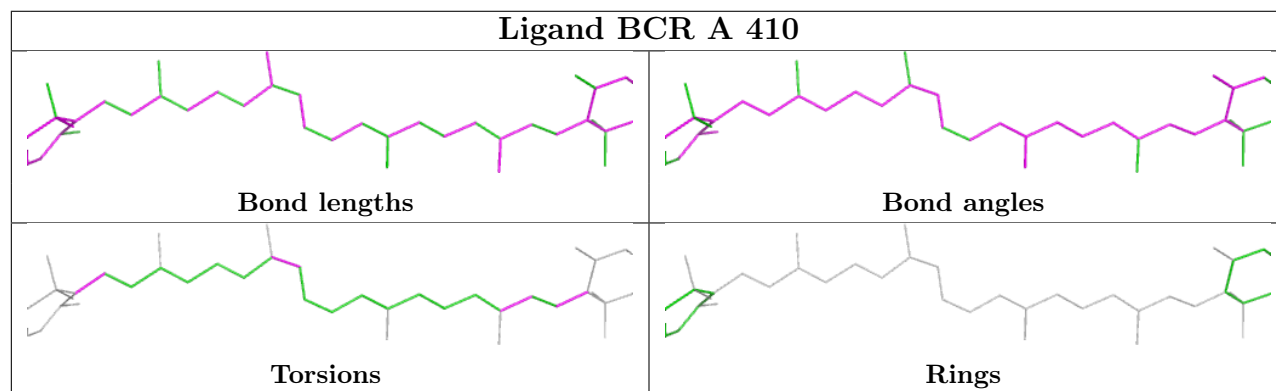


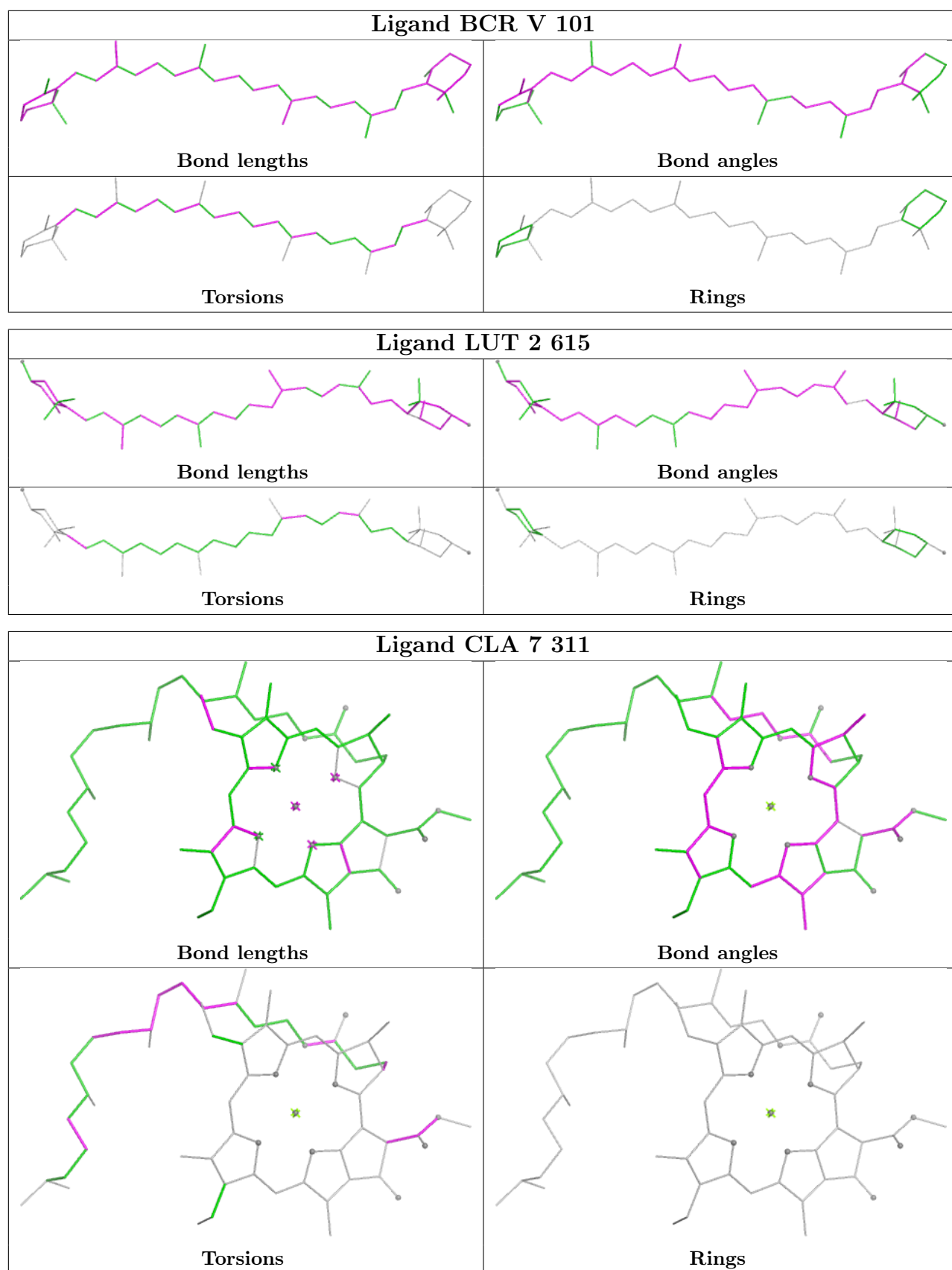


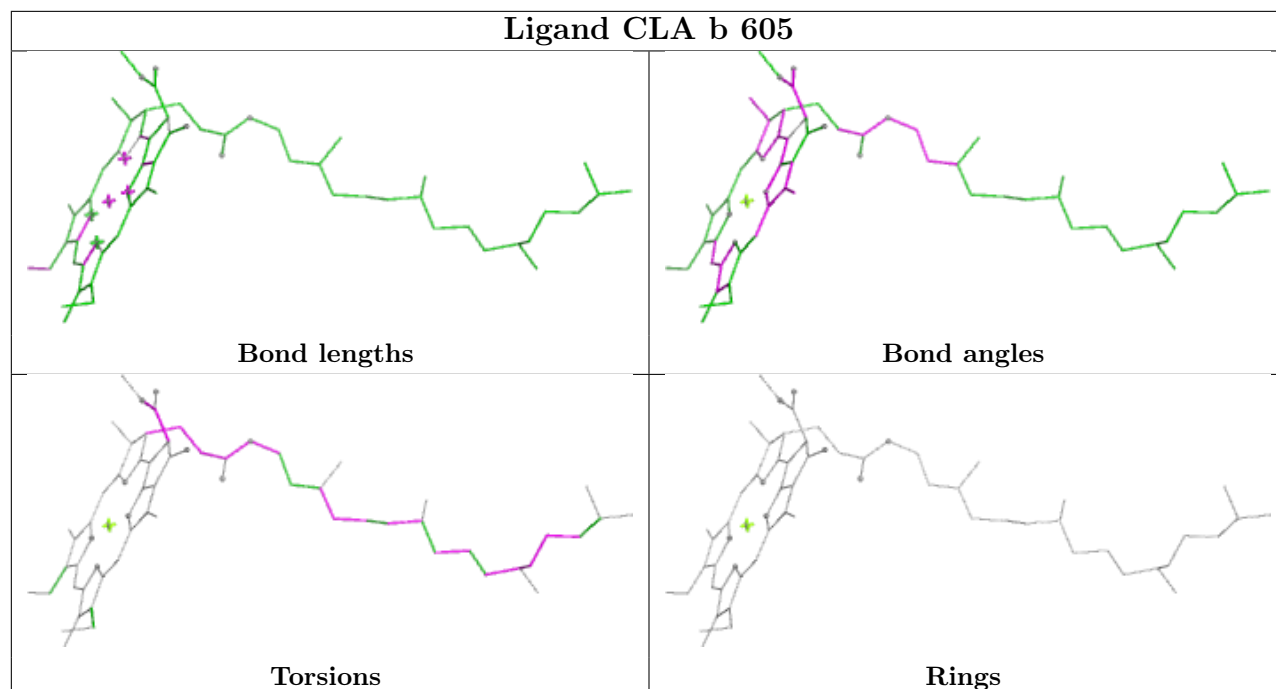
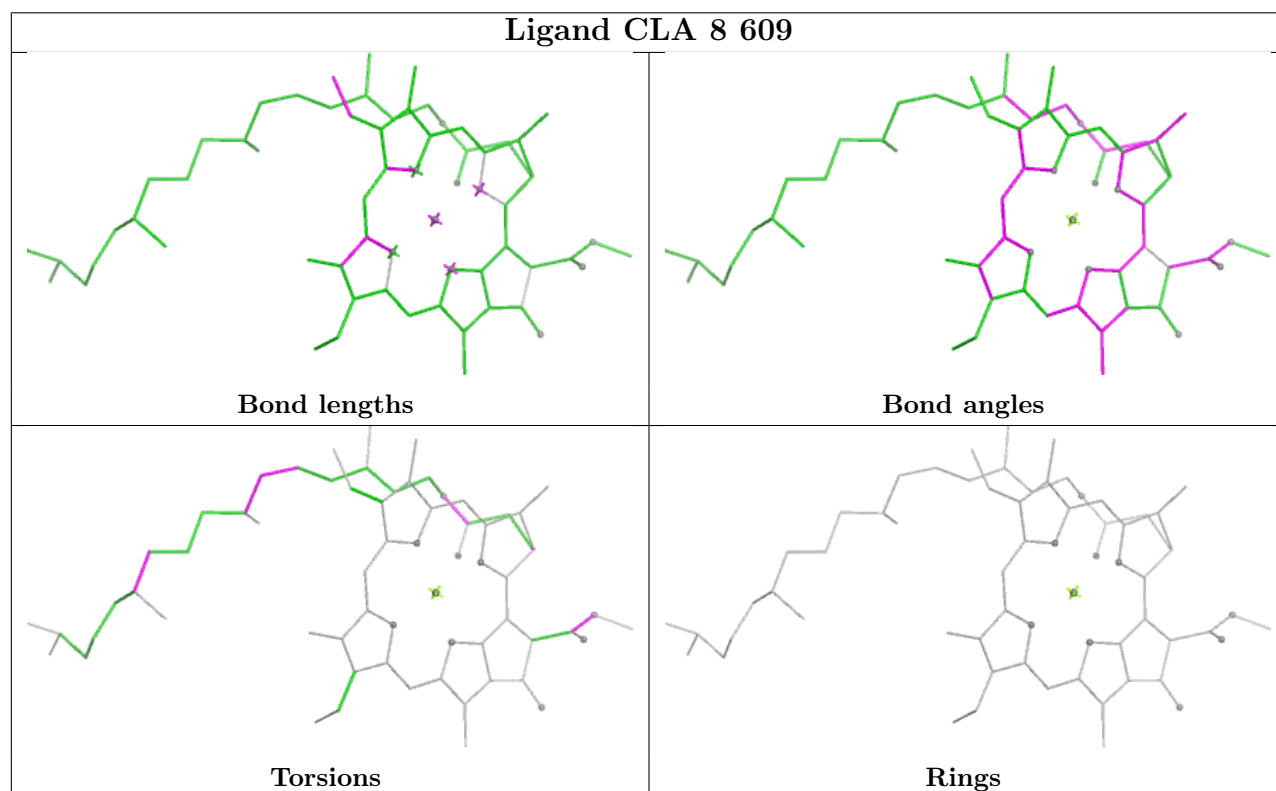
Ligand CLA 4 614

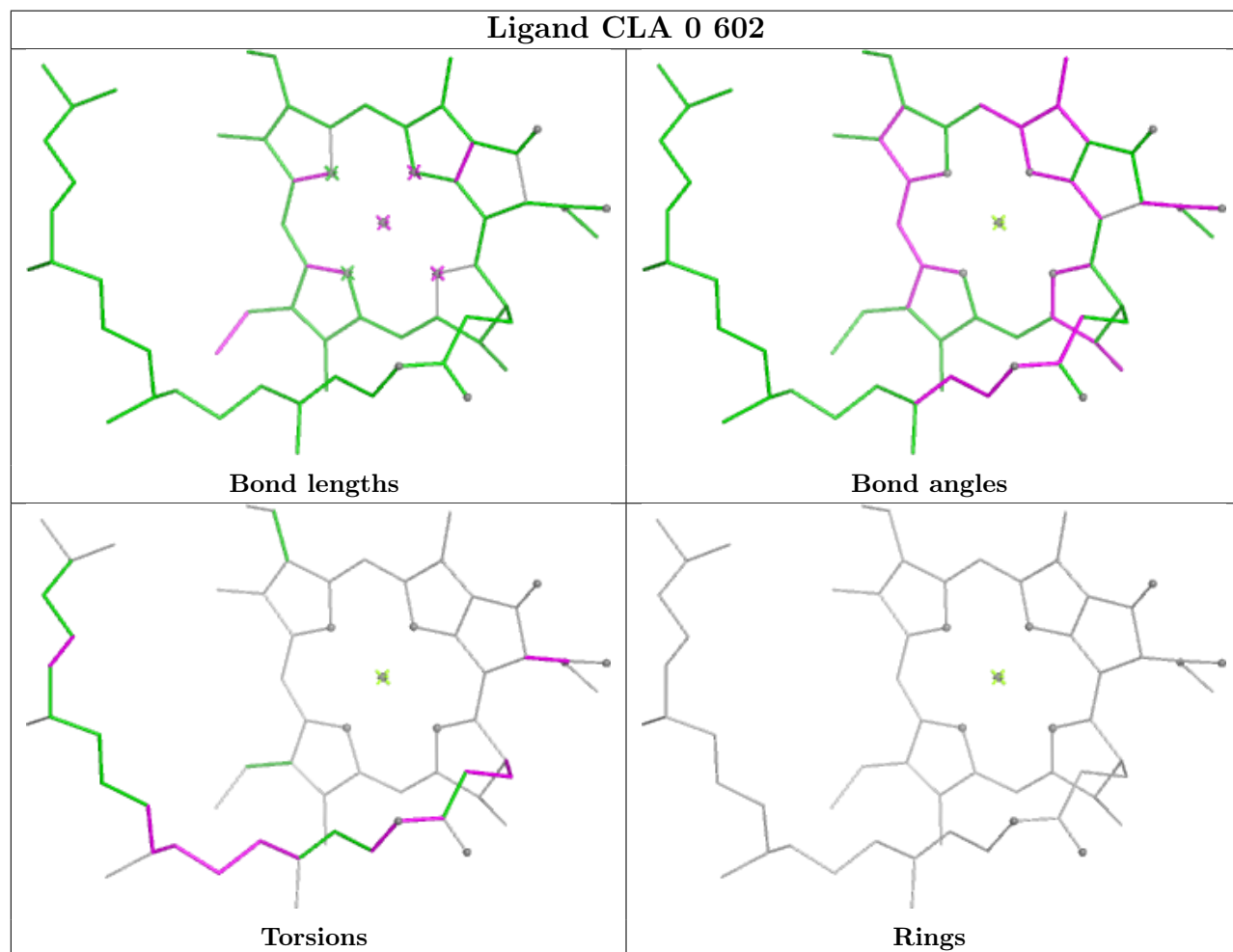
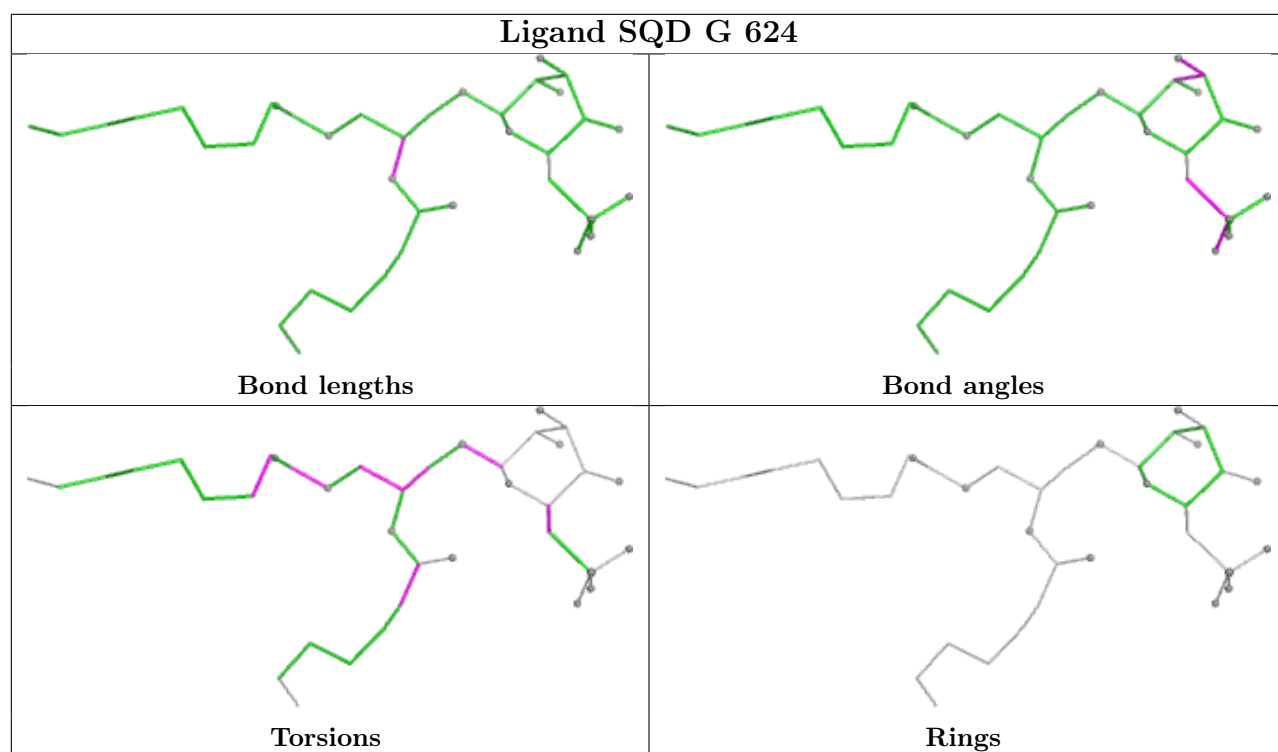


Ligand BCR A 410

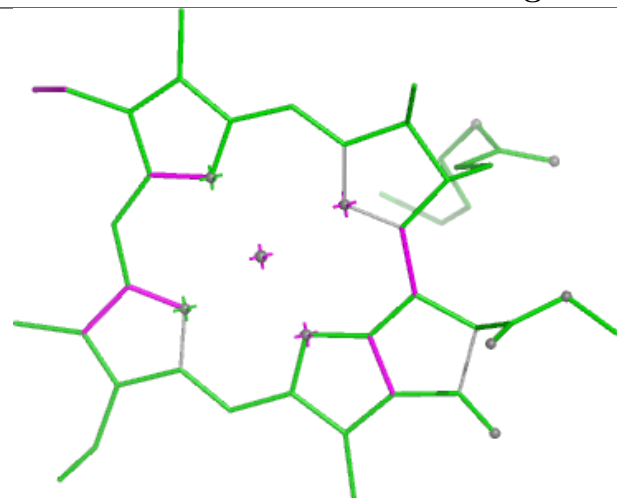




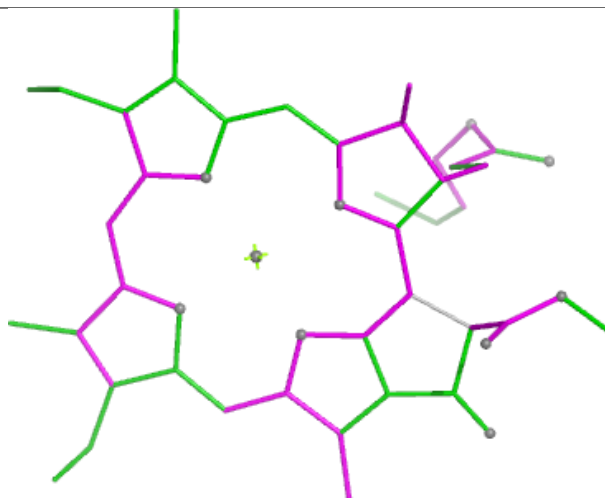
Ligand CLA b 605**Ligand CLA 8 609**



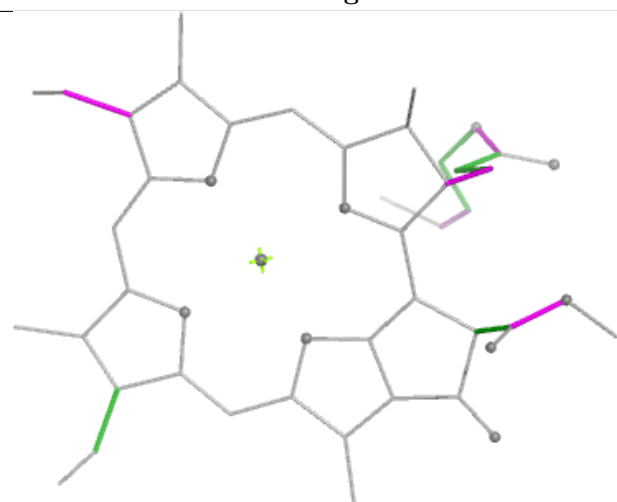
Ligand CLA r 313



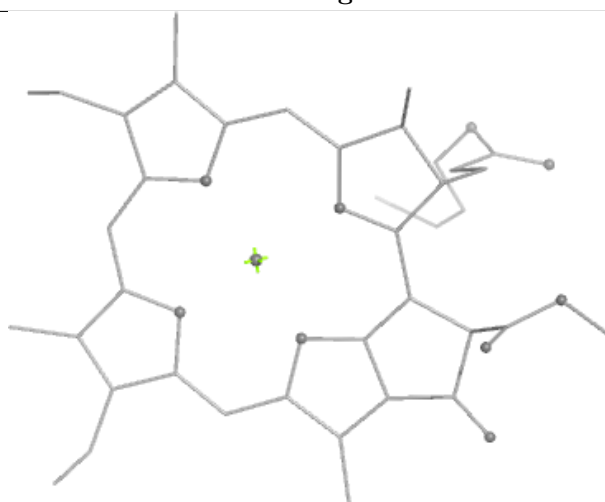
Bond lengths



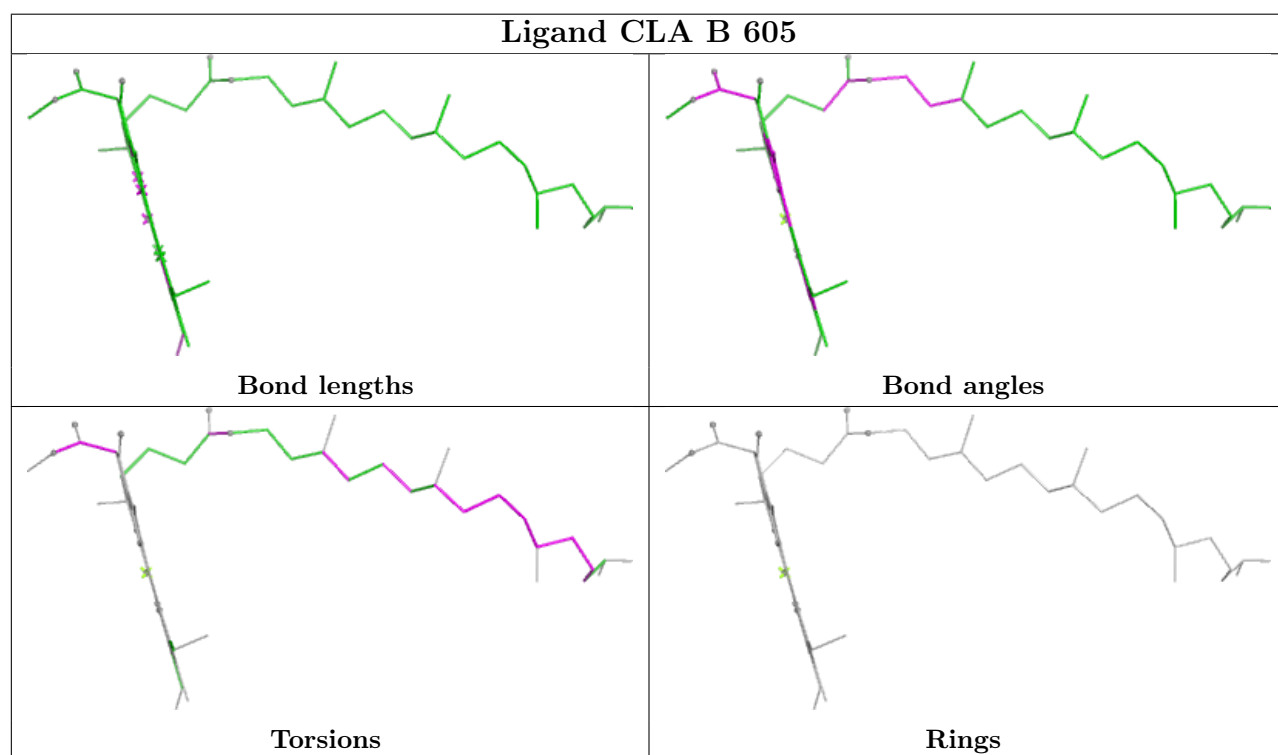
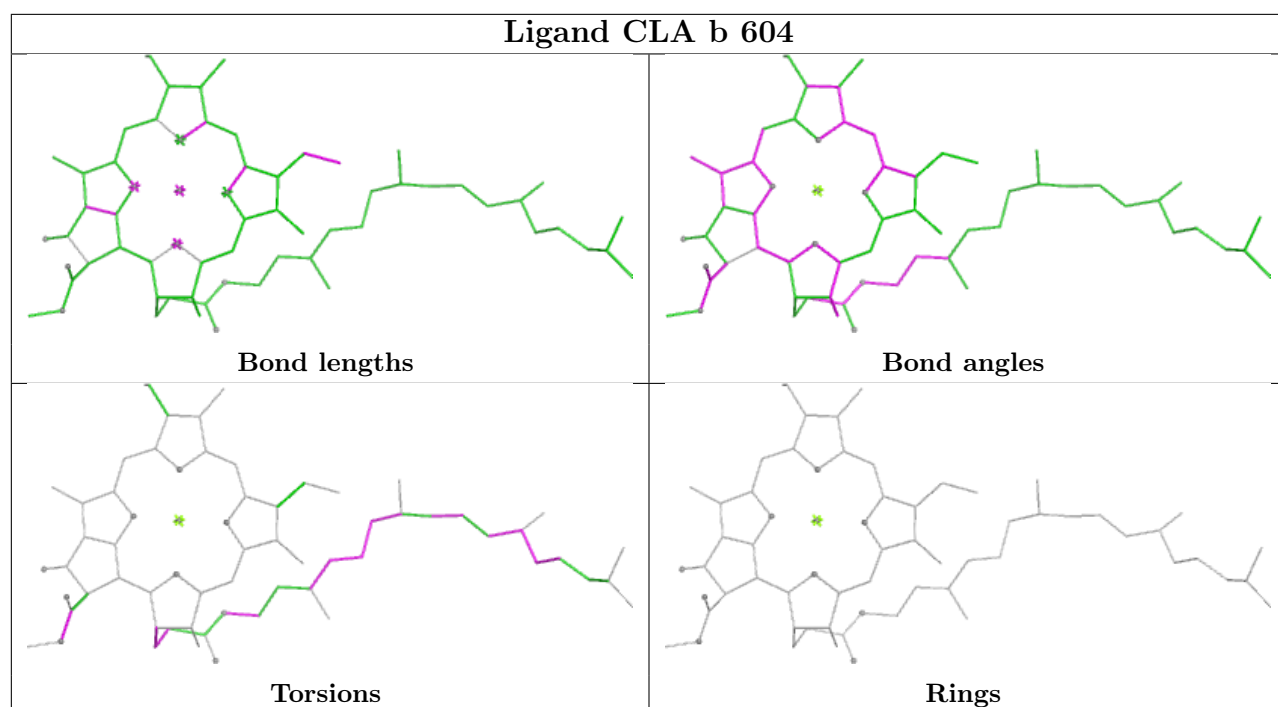
Bond angles

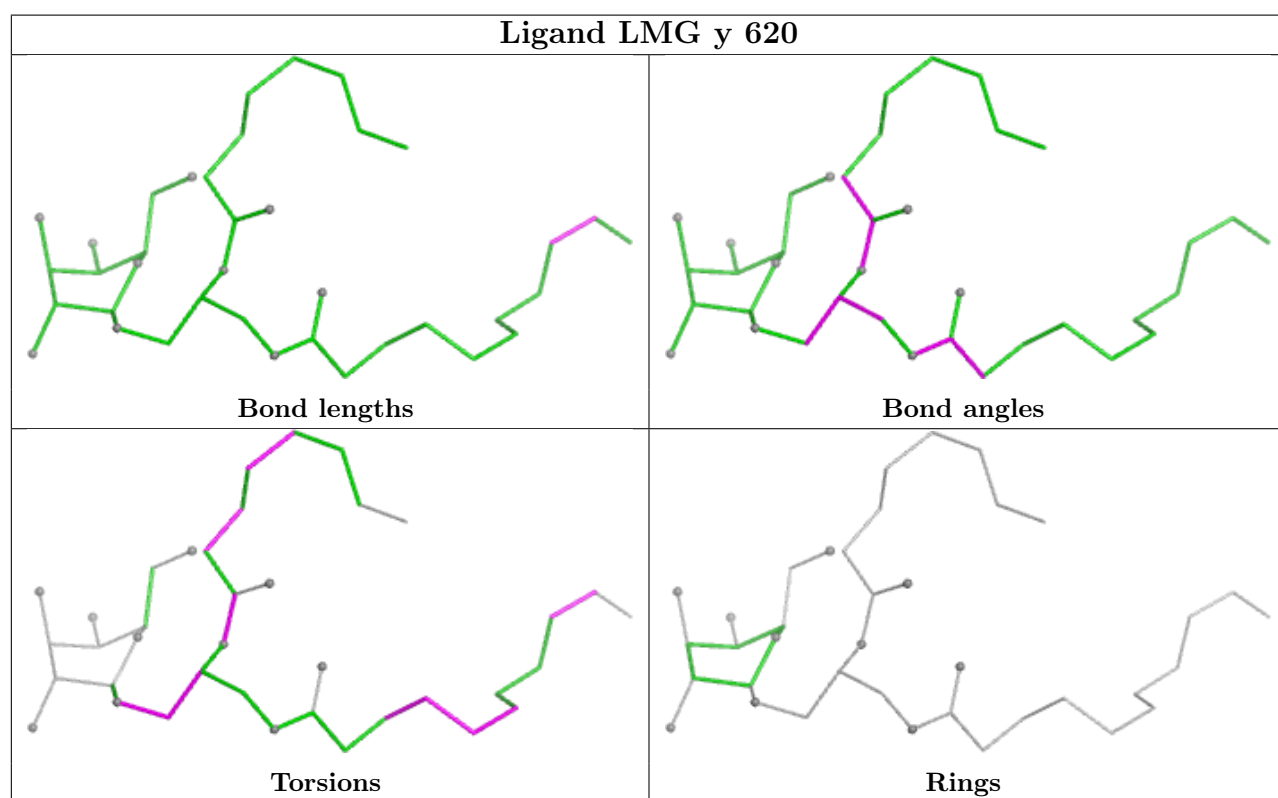
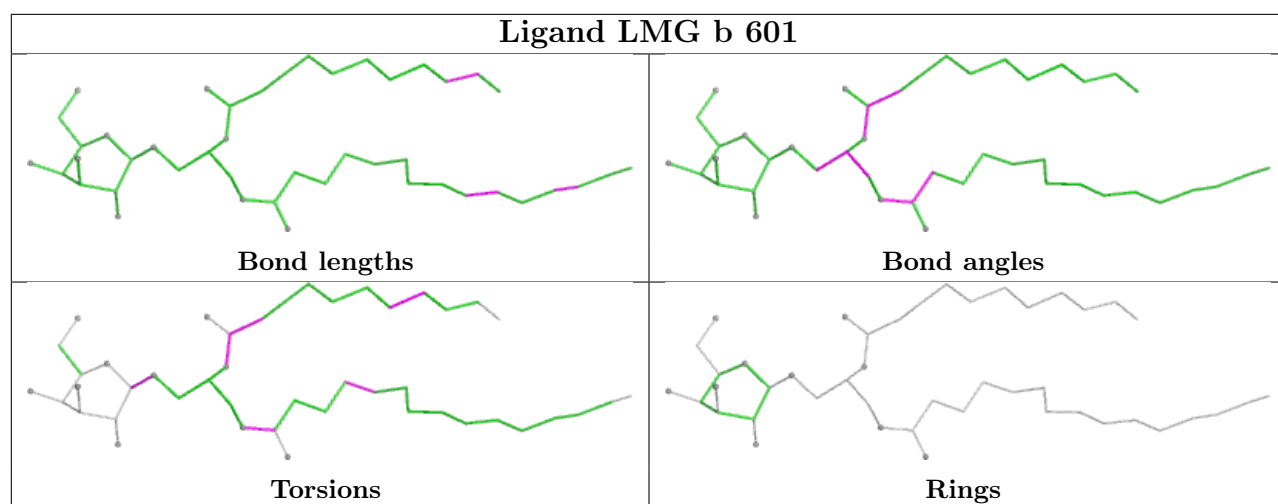


Torsions

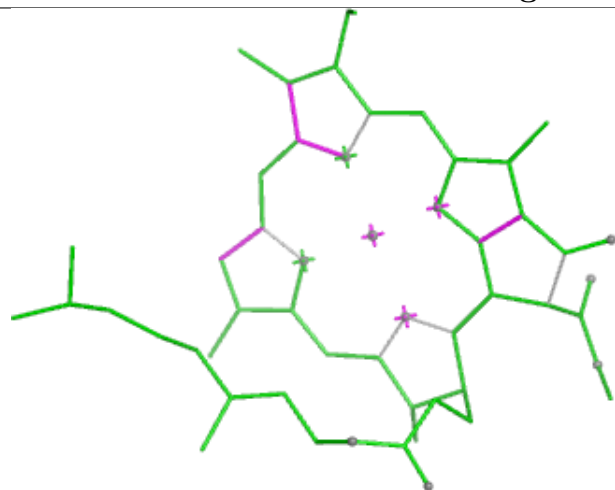


Rings

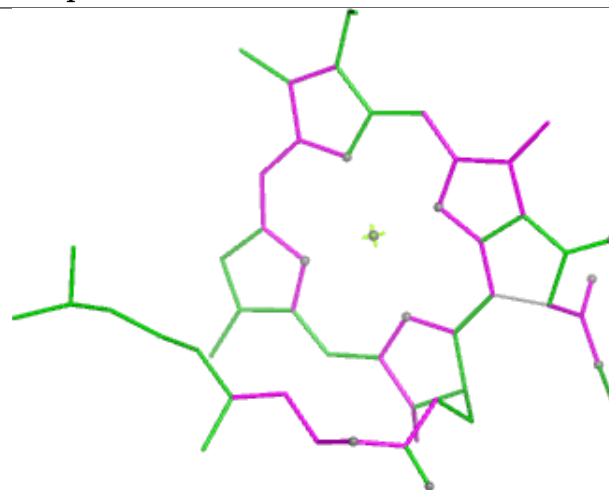




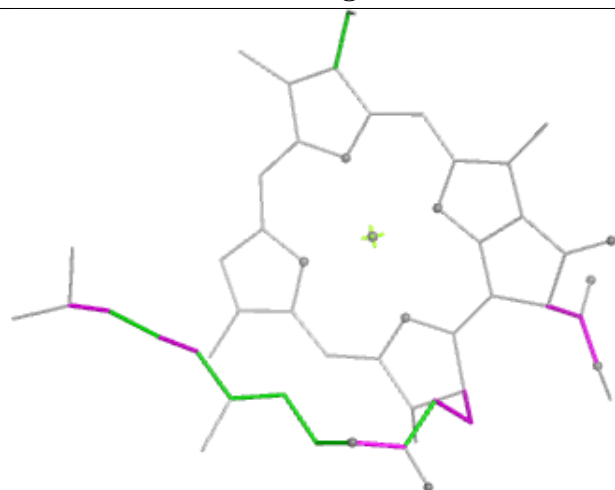
Ligand CLA q 312



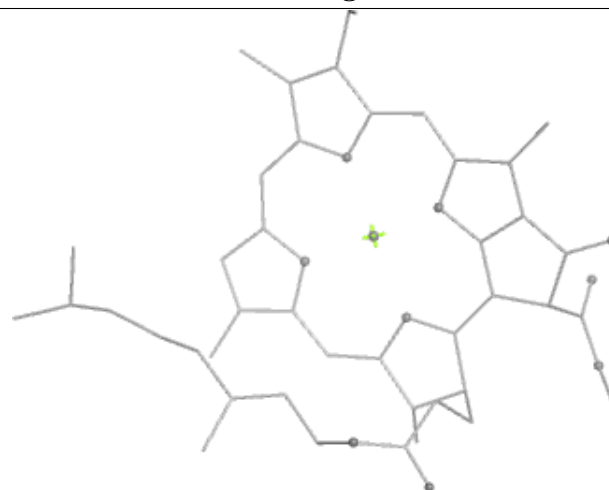
Bond lengths



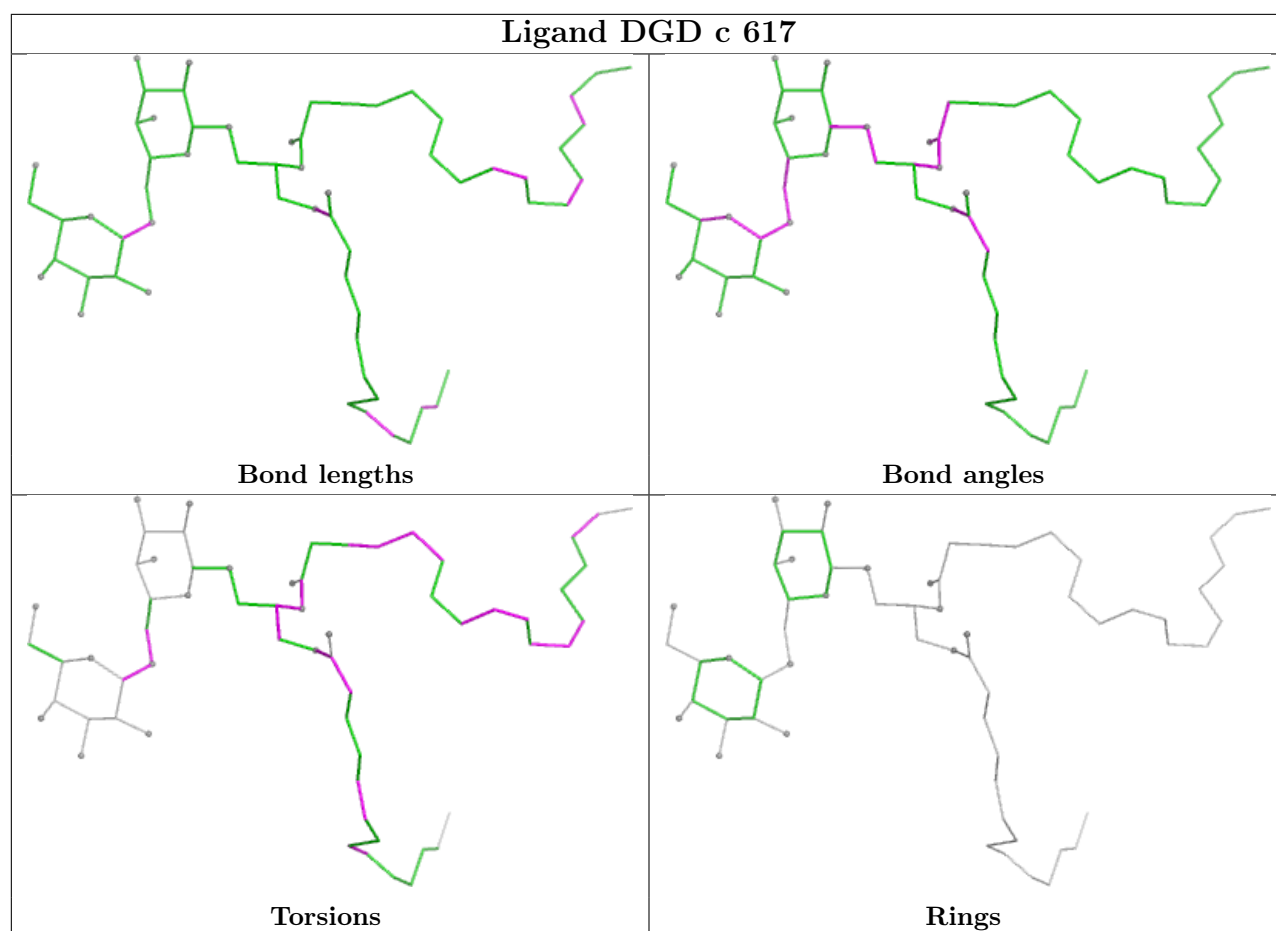
Bond angles



Torsions



Rings



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.

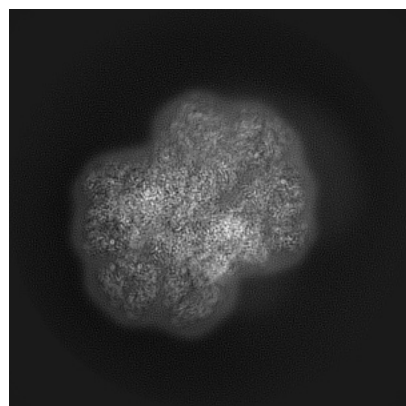
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15973. These allow visual inspection of the internal detail of the map and identification of artifacts.

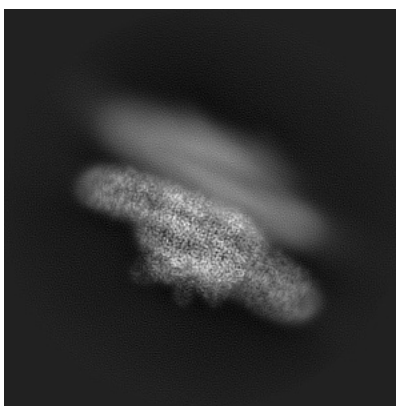
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

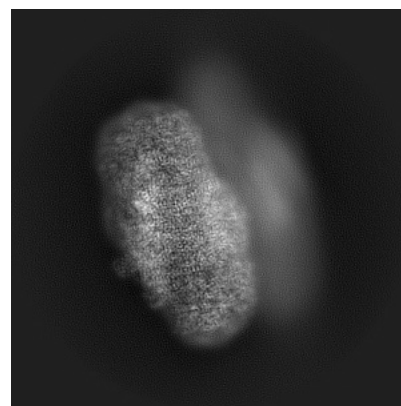
6.1.1 Primary map



X

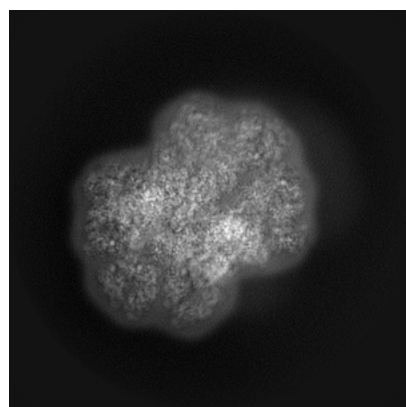


Y

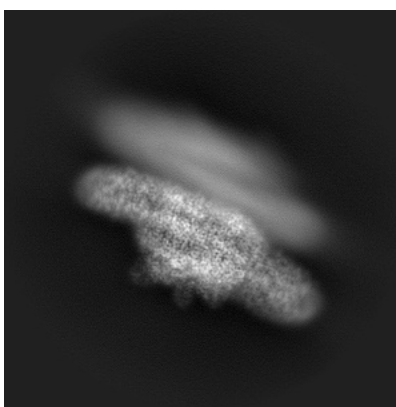


Z

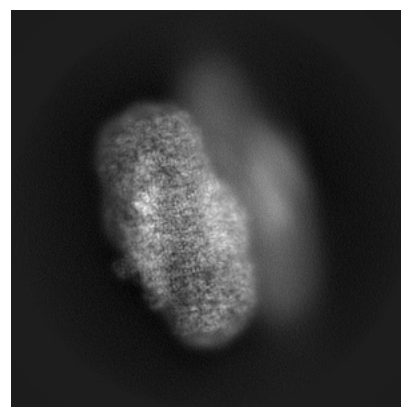
6.1.2 Raw map



X



Y

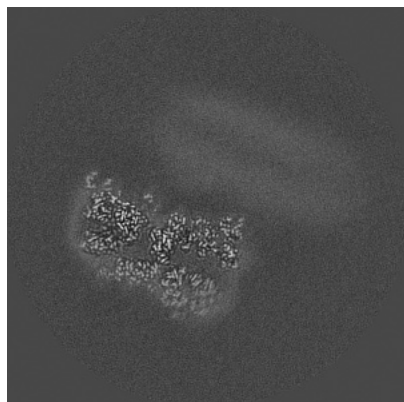


Z

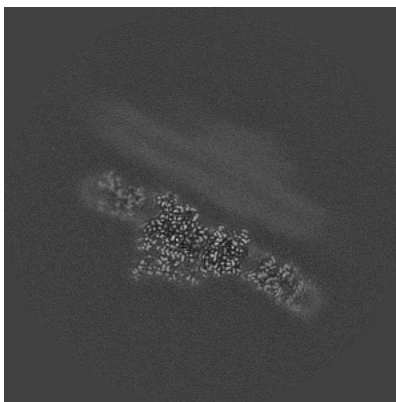
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

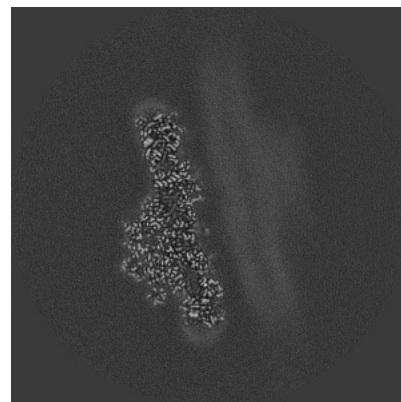
6.2.1 Primary map



X Index: 250

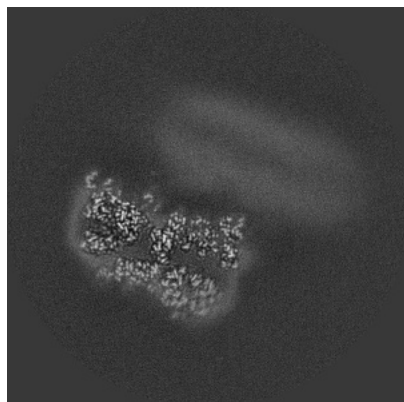


Y Index: 250

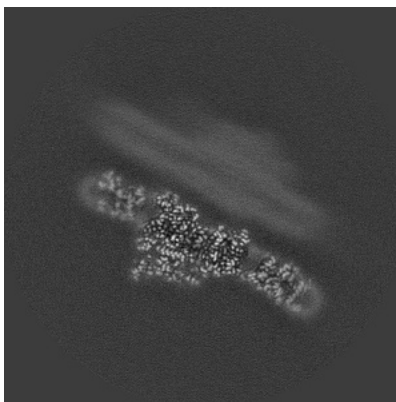


Z Index: 250

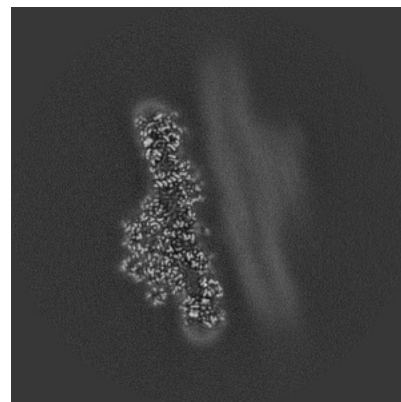
6.2.2 Raw map



X Index: 250



Y Index: 250

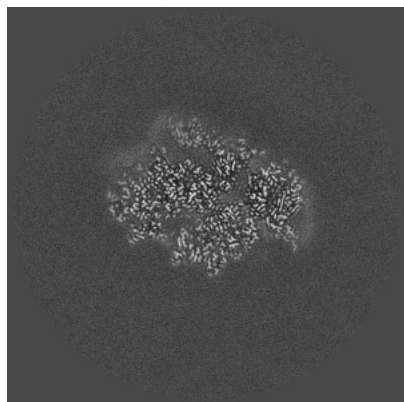


Z Index: 250

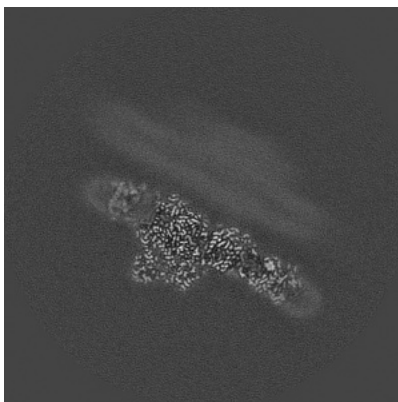
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

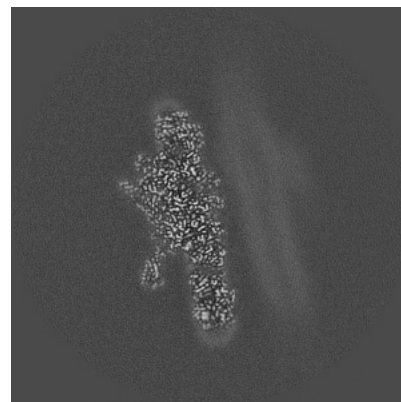
6.3.1 Primary map



X Index: 183

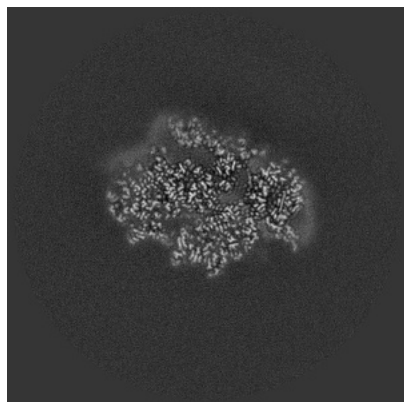


Y Index: 257

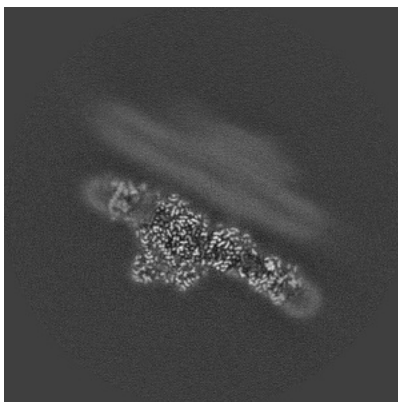


Z Index: 213

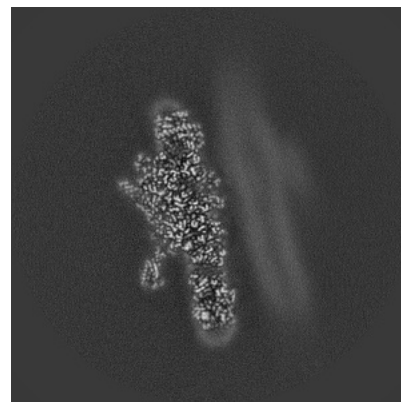
6.3.2 Raw map



X Index: 183



Y Index: 257

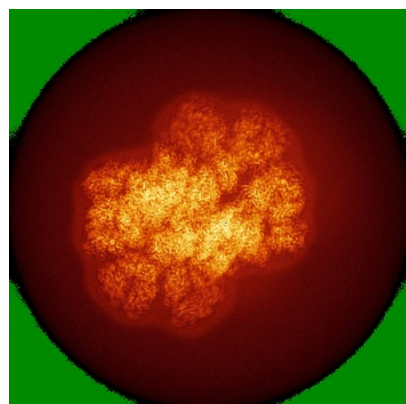


Z Index: 213

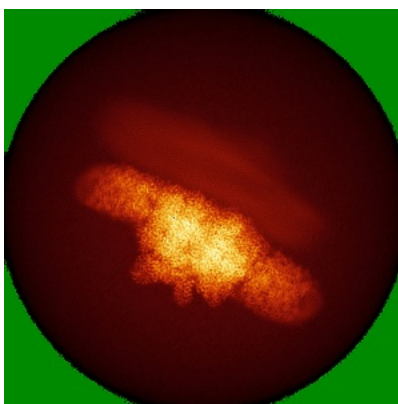
The images above show the largest variance slices of the map in three orthogonal directions.

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

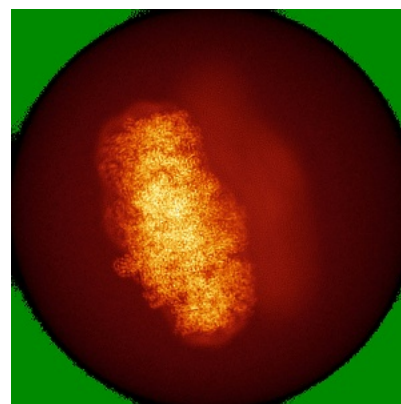
6.4.1 Primary map



X

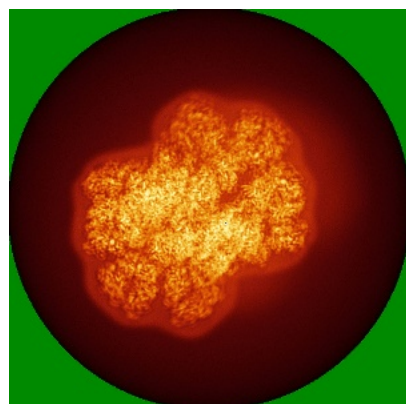


Y

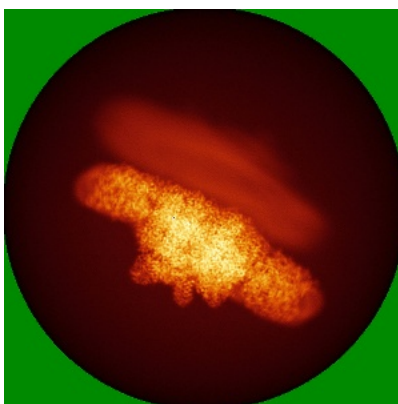


Z

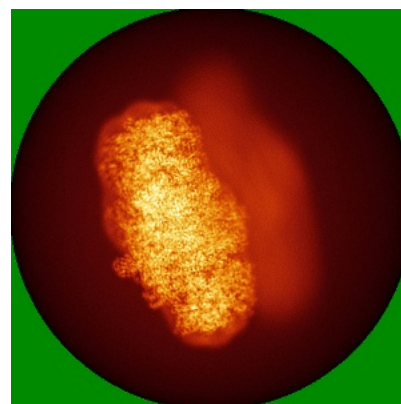
6.4.2 Raw map



X



Y

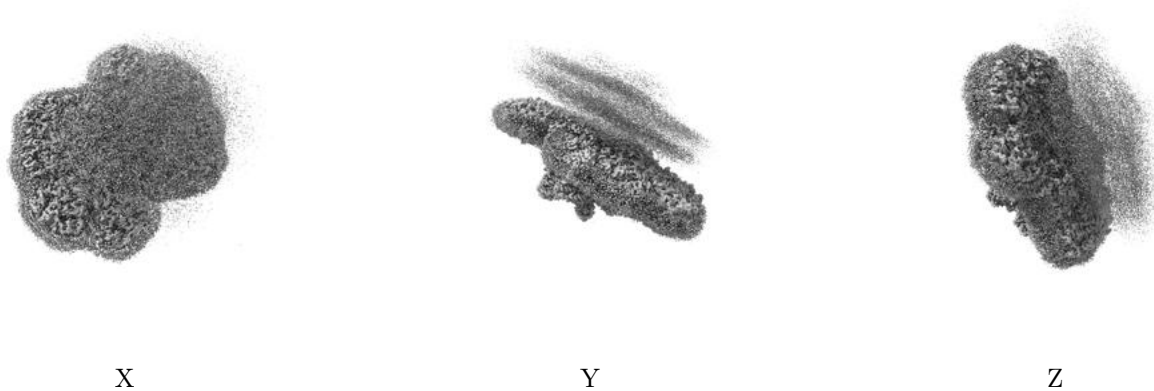


Z

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.

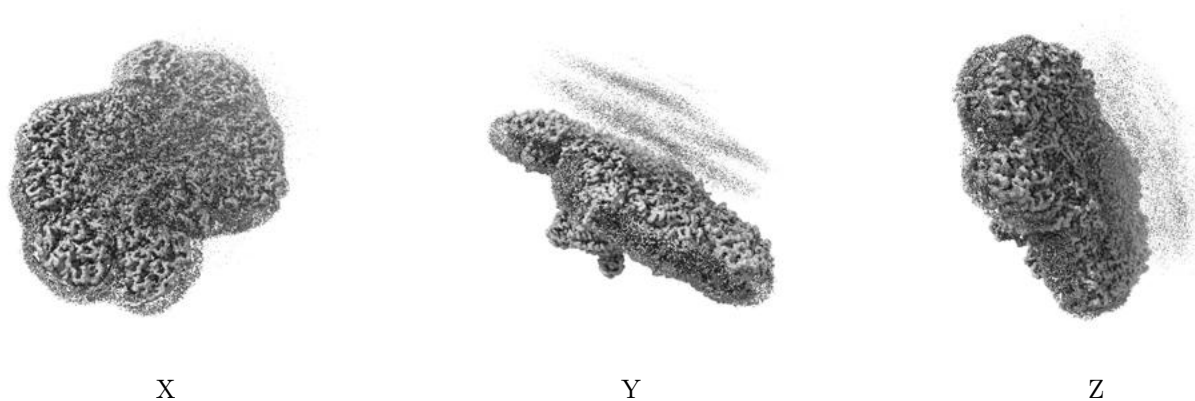
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.008. 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.

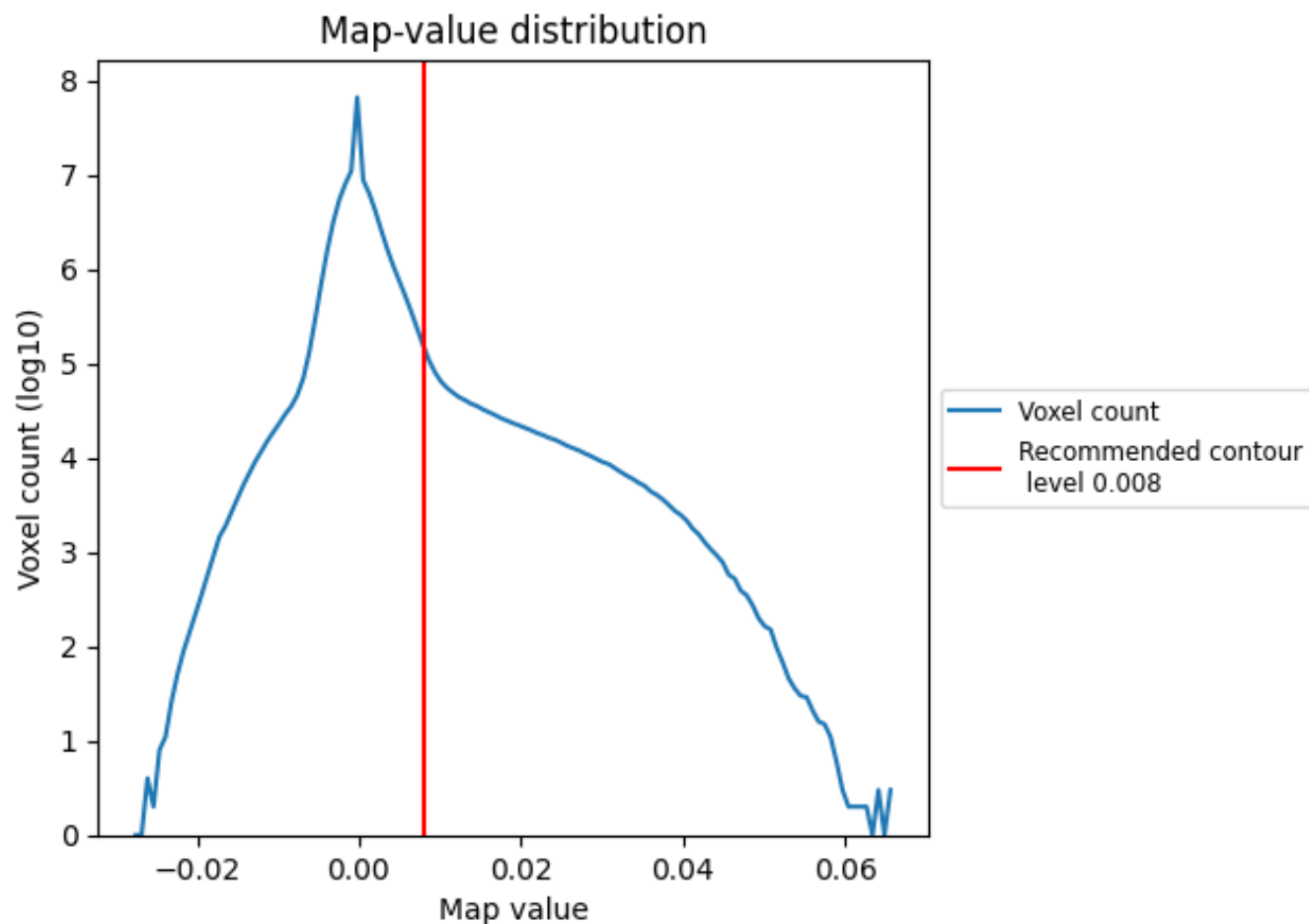
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

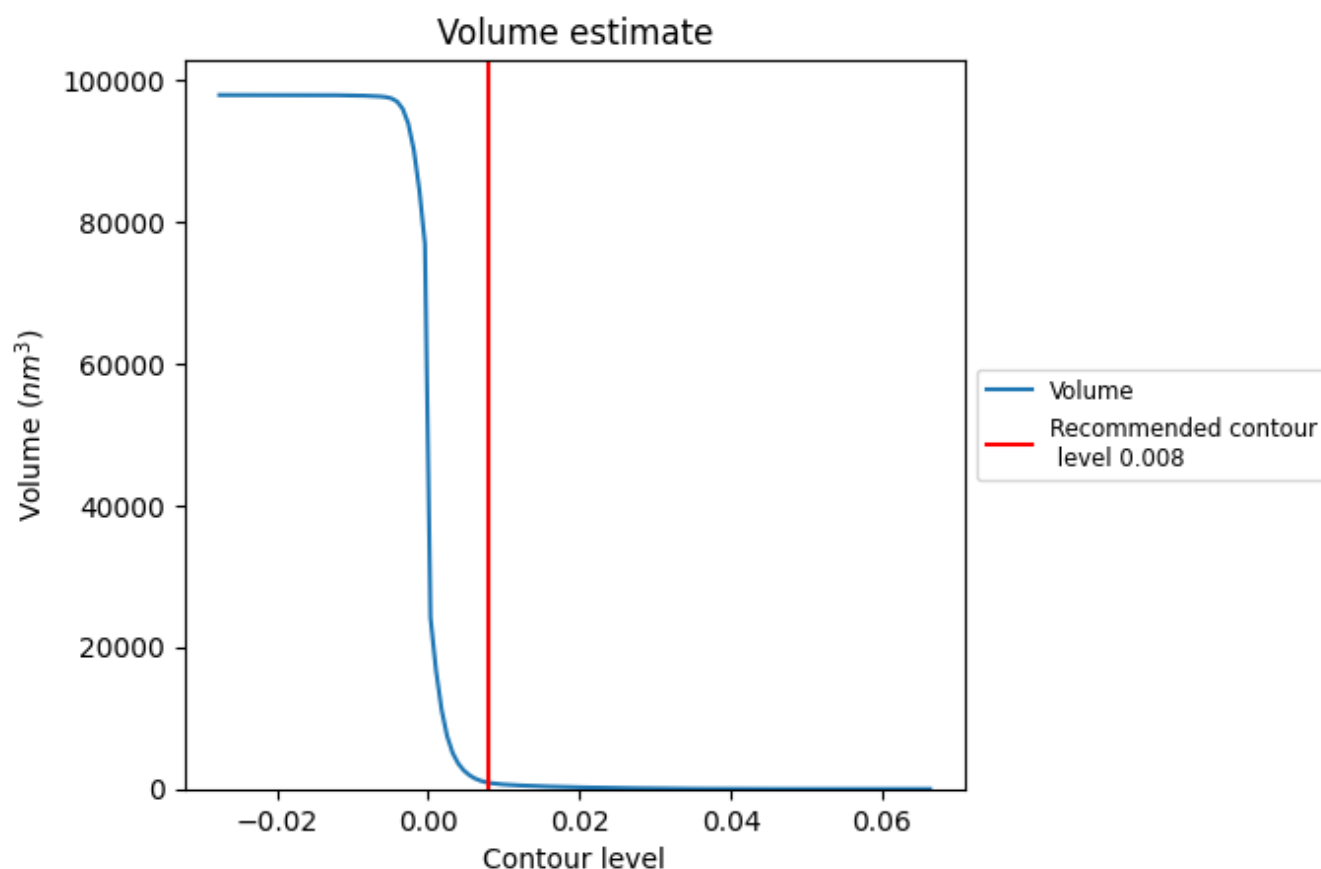
This section contains the results of statistical analysis of the map.

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.

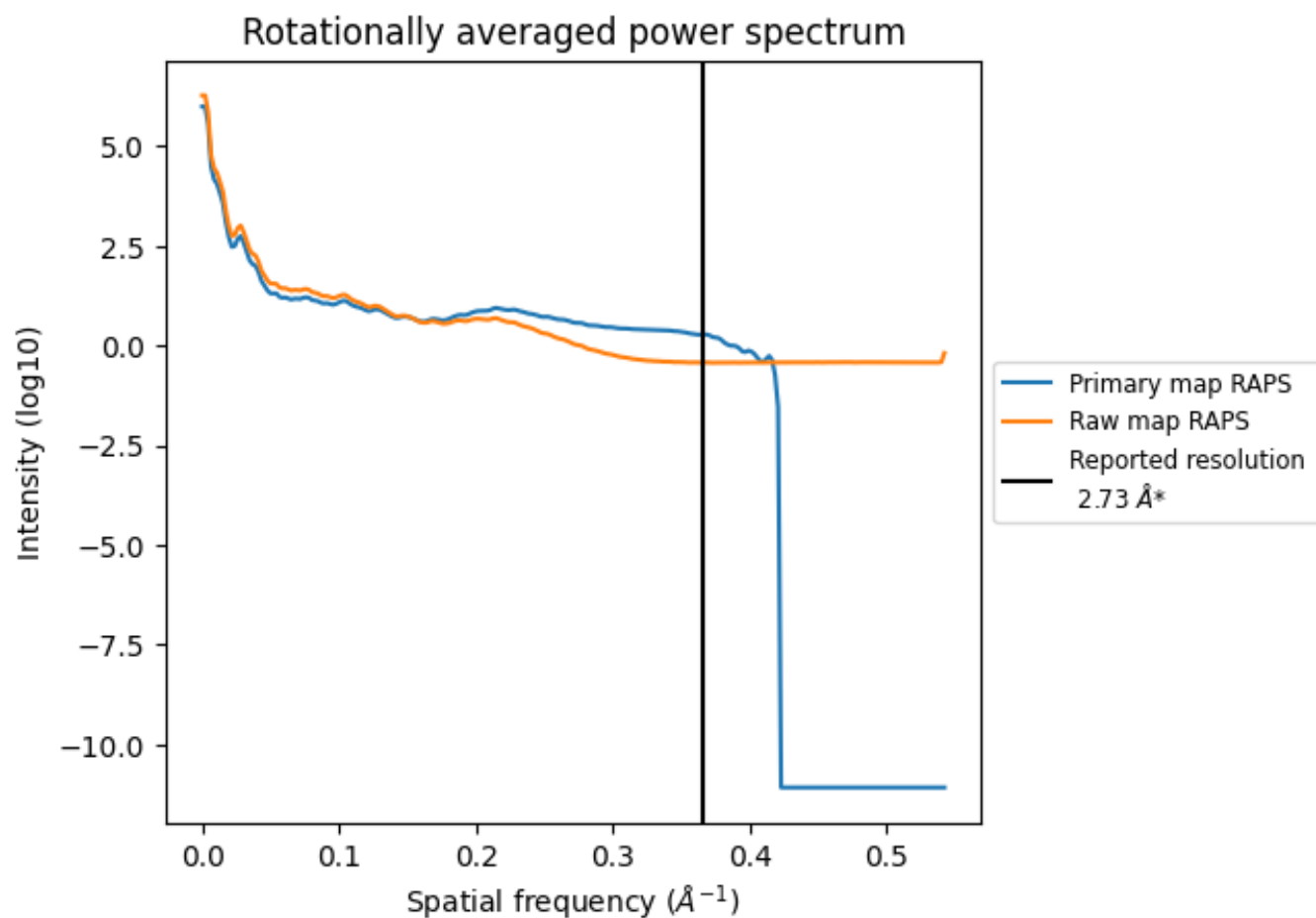
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 885 nm³; this corresponds to an approximate mass of 799 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 ⓘ

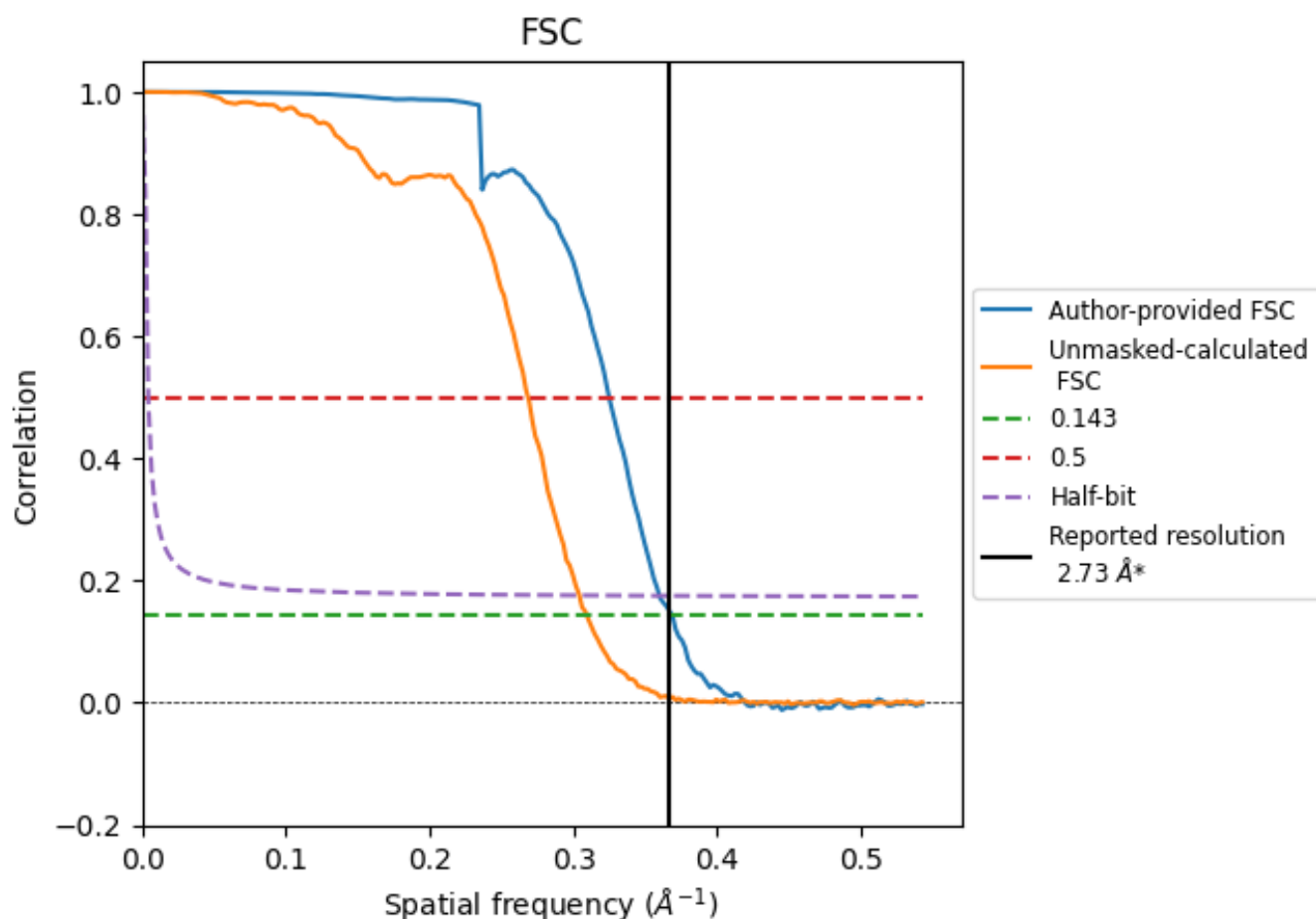


*Reported resolution corresponds to spatial frequency of 0.366 Å⁻¹

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 0.366 Å⁻¹

8.2 Resolution estimates [i](#)

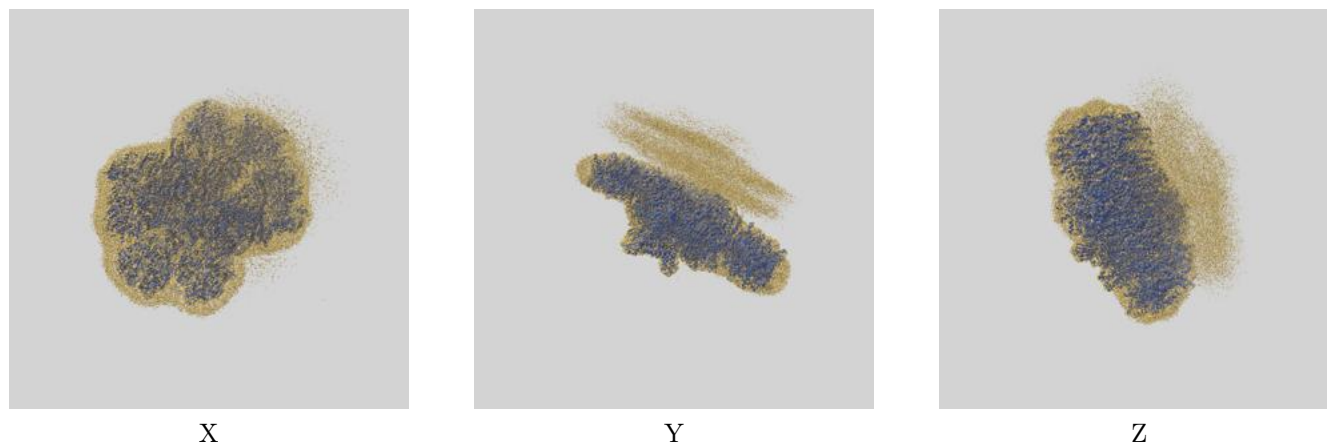
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.73	-	-
Author-provided FSC curve	2.71	3.08	2.78
Unmasked-calculated*	3.23	3.73	3.29

*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 3.23 differs from the reported value 2.73 by more than 10 %

9 Map-model fit [i](#)

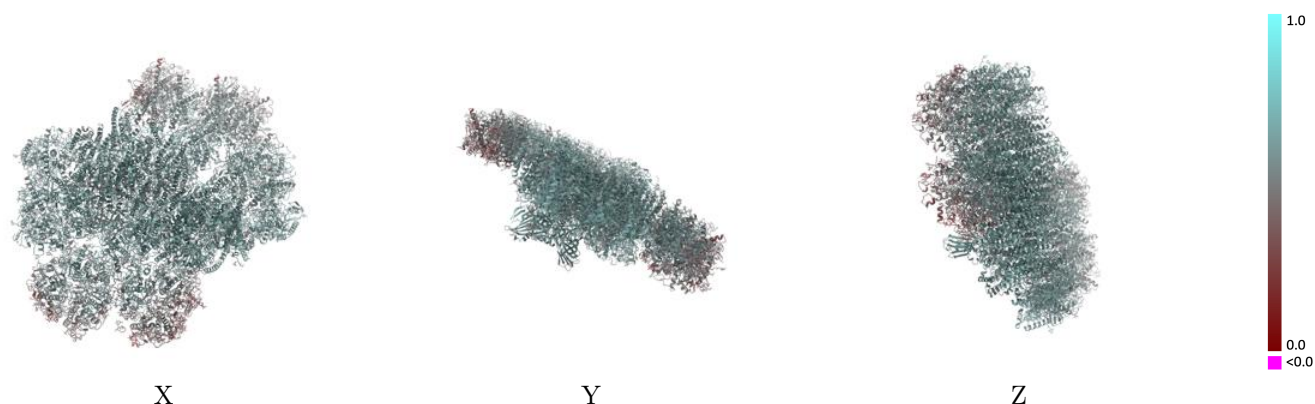
This section contains information regarding the fit between EMDB map EMD-15973 and PDB model 8BD3. Per-residue inclusion information can be found in section [3](#) on page [56](#).

9.1 Map-model overlay [i](#)



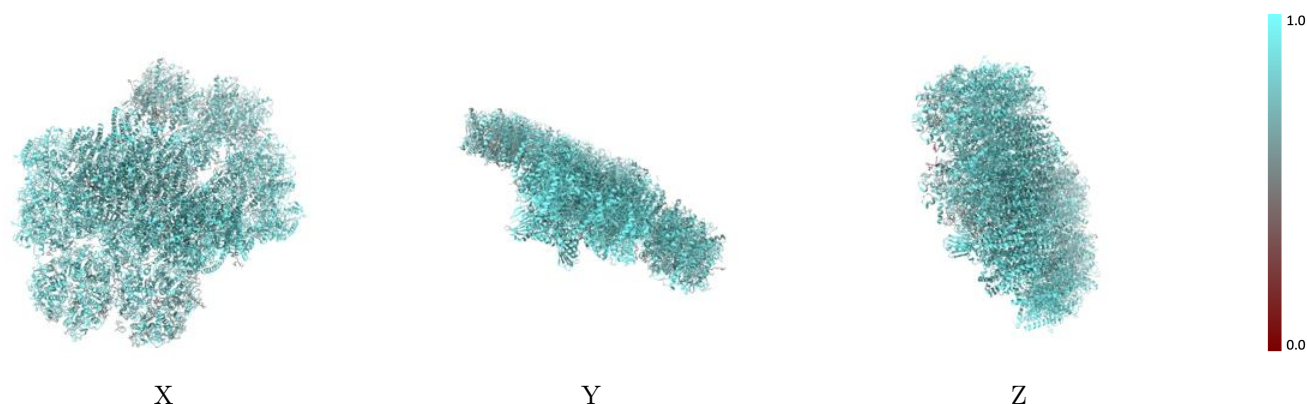
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



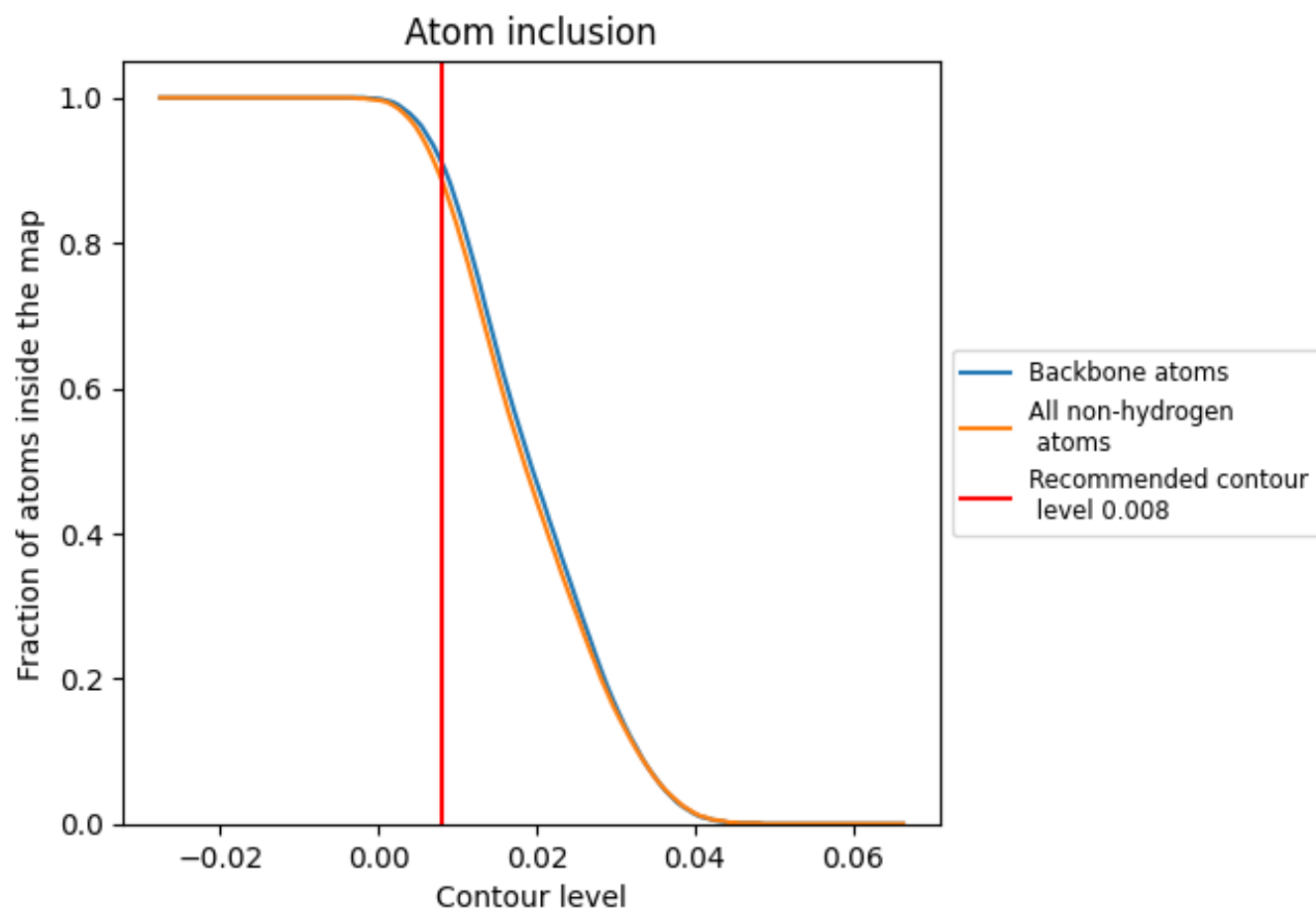
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.008).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 89% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8870	 0.5740
0	 0.8560	 0.5540
1	 0.8750	 0.5670
2	 0.8000	 0.5010
3	 0.8160	 0.4830
4	 0.7510	 0.4600
5	 0.7340	 0.4100
6	 0.8510	 0.5480
7	 0.8590	 0.5610
8	 0.7870	 0.4560
9	 0.7940	 0.4860
A	 0.9550	 0.6360
B	 0.9450	 0.6280
C	 0.9450	 0.6240
D	 0.9590	 0.6370
E	 0.9350	 0.6170
F	 0.9590	 0.6310
F1	 0.9210	 0.5910
G	 0.8990	 0.5780
H	 0.9560	 0.6210
I	 0.9350	 0.6110
J	 0.8950	 0.6030
K	 0.8510	 0.5810
L	 0.9280	 0.6150
M	 0.7890	 0.5400
N	 0.9150	 0.5880
O	 0.8970	 0.5770
P1	 0.8790	 0.5930
Q1	 0.7590	 0.5390
R	 0.9020	 0.6000
S	 0.8980	 0.5830
T	 0.9070	 0.6020
U	 0.8870	 0.5770
V	 0.8380	 0.5670
W	 0.8310	 0.5780



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
X	 0.8580	 0.5780
Y	 0.9280	 0.6150
Z	 0.9200	 0.5810
a	 0.9540	 0.6320
b	 0.9410	 0.6240
c	 0.9370	 0.6190
d	 0.9640	 0.6400
e	 0.9260	 0.6050
f	 0.9310	 0.6210
fl	 0.9180	 0.5860
g	 0.8950	 0.5790
h	 0.9580	 0.6240
i	 0.9740	 0.6400
j	 0.8940	 0.5880
k	 0.9420	 0.6090
l	 0.9340	 0.6190
m	 0.8210	 0.5590
n	 0.9170	 0.5890
o	 0.8930	 0.5850
p	 0.7040	 0.4150
p1	 0.8800	 0.5840
q	 0.7420	 0.4650
q1	 0.7490	 0.5230
r	 0.9090	 0.6030
s	 0.9000	 0.5820
t	 0.8760	 0.5990
u	 0.8940	 0.5850
v	 0.8520	 0.5680
w	 0.8480	 0.5680
x	 0.8280	 0.5630
y	 0.9350	 0.6170
z	 0.8880	 0.5610