



wwPDB EM Validation Summary Report ⓘ

Sep 28, 2026 – 03:32 PM JST

PDB ID : 21WV / pdb_000021wv
EMDB ID : EMD-68060
Title : In situ structure of the C2S2M2L4-type PSII-LHCII supercomplex from *Oryza sativa*
Authors : Li, J.; Elias, E.; Zhang, K.; Croce, R.; Zhu, J.
Deposited on : 2026-01-01
Resolution : 2.89 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:

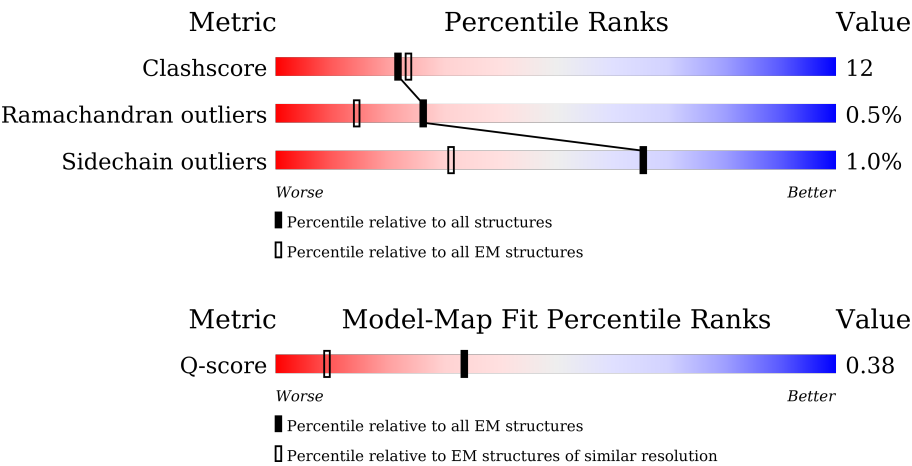
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.2
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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) : 2.51

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.89 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.



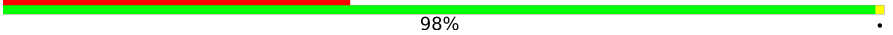
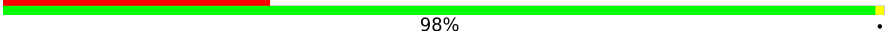
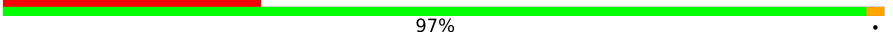
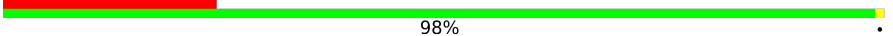
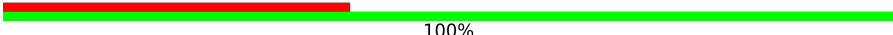
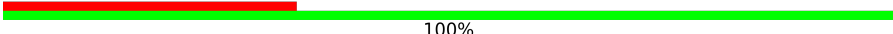
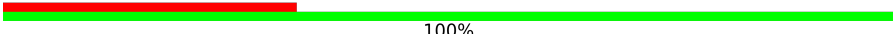
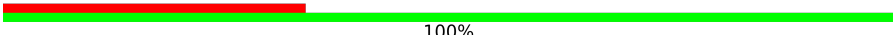
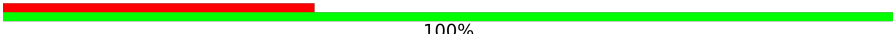
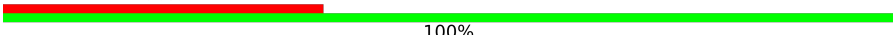
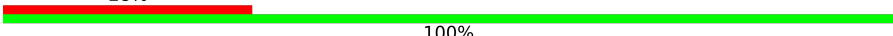
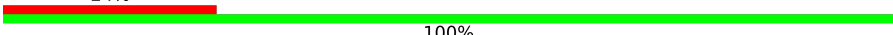
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12148 (2.39 - 3.39)

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	00	219	
1	01	219	
1	02	219	
1	05	219	

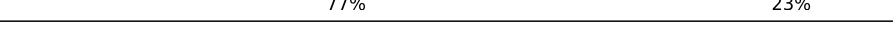
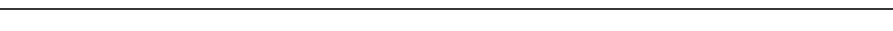
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Mol	Chain	Length	Quality of chain
1	06	219	 78%16%5%
1	09	219	 74%23%
1	11	219	 39%98%
1	14	219	 30%98%
1	17	219	 29%97%
1	1G	219	 80%19%
1	1N	219	 76%22%
1	1g	219	 79%21%
1	1n	219	 79%20%
1	20	219	 24%98%
2	03	220	 79%20%
2	07	220	 81%18%
3	04	205	 79%18%
3	08	205	 78%21%
4	12	222	 39%100%
4	15	222	 33%100%
4	18	222	 33%100%
4	21	222	 34%100%
5	13	218	 35%100%
5	16	218	 36%100%
5	19	218	 28%100%
5	22	218	 24%100%
6	1A	334	 70%30%
6	1a	334	 64%35%
7	1B	503	 73%27%

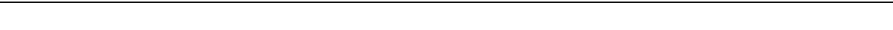
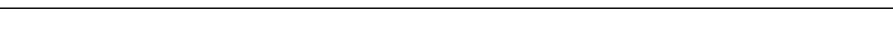
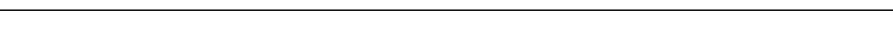
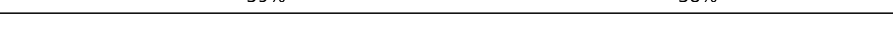
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Mol	Chain	Length	Quality of chain
7	1b	503	
8	1C	450	
8	1c	450	
9	1D	341	
9	1d	341	
10	1E	75	
10	1e	75	
11	1F	35	
11	1f	35	
12	1H	60	
12	1h	60	
13	1I	34	
13	1i	34	
14	1J	35	
14	1j	35	
15	1K	37	
15	1k	37	
16	1L	36	
16	1l	36	
17	1M	33	
17	1m	33	
18	1O	248	
18	1o	248	
19	1P	186	
19	1p	186	

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Mol	Chain	Length	Quality of chain
20	1R	234	
20	1r	234	
21	1S	218	
21	1s	218	
22	1T	32	
22	1t	32	
23	1U	27	
23	1u	27	
24	1V	105	
24	1v	105	
25	1W	54	
25	1w	54	
26	1X	39	
26	1x	39	
27	1Y	36	
27	1y	36	
28	1Z	62	
28	1z	62	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	00	301	X	-	-	-
29	CLA	00	302	X	-	-	-
29	CLA	00	309	X	-	-	-
29	CLA	00	318	X	-	-	-
29	CLA	01	307	X	-	-	-
29	CLA	01	308	X	-	-	-
29	CLA	01	310	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	03	301	X	-	-	-
29	CLA	06	602	X	-	-	-
29	CLA	09	301	X	-	-	-
29	CLA	09	302	X	-	-	-
29	CLA	1A	404	X	-	-	-
29	CLA	1B	601	X	-	-	-
29	CLA	1B	602	X	-	-	-
29	CLA	1B	603	X	-	-	-
29	CLA	1B	604	X	-	-	-
29	CLA	1B	605	X	-	-	-
29	CLA	1B	606	X	-	-	-
29	CLA	1B	607	X	-	-	-
29	CLA	1B	608	X	-	-	-
29	CLA	1B	609	X	-	-	-
29	CLA	1B	610	X	-	-	-
29	CLA	1B	611	X	-	-	-
29	CLA	1B	612	X	-	-	-
29	CLA	1B	613	X	-	-	-
29	CLA	1B	616	X	-	-	-
29	CLA	1C	501	X	-	-	-
29	CLA	1C	502	X	-	-	-
29	CLA	1C	503	X	-	-	-
29	CLA	1C	504	X	-	-	-
29	CLA	1C	505	X	-	-	-
29	CLA	1C	507	X	-	-	-
29	CLA	1C	508	X	-	-	-
29	CLA	1C	509	X	-	-	-
29	CLA	1C	510	X	-	-	-
29	CLA	1C	512	X	-	-	-
29	CLA	1D	401	X	-	-	-
29	CLA	1D	404	X	-	-	-
29	CLA	1G	602	X	-	-	-
29	CLA	1G	612	X	-	-	-
29	CLA	1N	303	X	-	-	-
29	CLA	1R	302	X	-	-	-
29	CLA	1S	313	X	-	-	-
29	CLA	1a	408	X	-	-	-
29	CLA	1b	602	X	-	-	-
29	CLA	1b	603	X	-	-	-
29	CLA	1b	604	X	-	-	-
29	CLA	1b	606	X	-	-	-
29	CLA	1b	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	1b	609	X	-	-	-
29	CLA	1b	610	X	-	-	-
29	CLA	1b	611	X	-	-	-
29	CLA	1b	612	X	-	-	-
29	CLA	1b	613	X	-	-	-
29	CLA	1b	614	X	-	-	-
29	CLA	1b	615	X	-	-	-
29	CLA	1b	616	X	-	-	-
29	CLA	1c	503	X	-	-	-
29	CLA	1c	504	X	-	-	-
29	CLA	1c	505	X	-	-	-
29	CLA	1c	506	X	-	-	-
29	CLA	1c	508	X	-	-	-
29	CLA	1c	509	X	-	-	-
29	CLA	1c	510	X	-	-	-
29	CLA	1c	512	X	-	-	-
29	CLA	1c	514	X	-	-	-
29	CLA	1c	515	X	-	-	-
29	CLA	1d	403	X	-	-	-
29	CLA	1d	406	X	-	-	-
29	CLA	1d	407	X	-	-	-
29	CLA	1g	602	X	-	-	-
29	CLA	1g	610	X	-	-	-
29	CLA	1g	612	X	-	-	-
29	CLA	1g	613	X	-	-	-
29	CLA	1n	602	X	-	-	-
29	CLA	1n	603	X	-	-	-
29	CLA	1n	610	X	-	-	-
29	CLA	1n	611	X	-	-	-
29	CLA	1n	613	X	-	-	-
29	CLA	1r	309	X	-	-	-
29	CLA	1s	312	X	-	-	-
29	CLA	1s	315	X	-	-	-
30	CHL	00	306	X	-	-	-
30	CHL	00	307	X	-	-	-
30	CHL	00	308	X	-	-	-
30	CHL	01	304	X	-	-	-
30	CHL	01	306	X	-	-	-
30	CHL	05	305	X	-	-	-
30	CHL	09	308	X	-	-	-
30	CHL	1G	601	X	-	-	-
30	CHL	1G	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CHL	1N	302	X	-	-	-
30	CHL	1N	308	X	-	-	-
30	CHL	1N	310	X	-	-	-
30	CHL	1g	601	X	-	-	-
30	CHL	1g	609	X	-	-	-
30	CHL	1n	601	X	-	-	-
30	CHL	1n	607	X	-	-	-
30	CHL	1n	609	X	-	-	-
40	PL9	1E	102	-	-	X	-
40	PL9	1a	412	-	-	X	-

2 Entry composition [i](#)

There are 47 unique types of molecules in this entry. The entry contains 107869 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 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	00	219	Total	C	N	O	S	0	0
			1659	1079	269	306	5		
1	01	219	Total	C	N	O	S	0	0
			1637	1061	268	303	5		
1	02	214	Total	C	N	O	S	0	0
			1576	1027	251	294	4		
1	05	210	Total	C	N	O	S	0	0
			1555	1003	258	289	5		
1	06	207	Total	C	N	O	S	0	0
			1450	927	242	276	5		
1	09	219	Total	C	N	O	S	0	0
			1659	1079	269	306	5		
1	11	218	Total	C	N	O		0	0
			1099	662	218	219			
1	14	218	Total	C	N	O		0	0
			1093	656	218	219			
1	17	218	Total	C	N	O		0	0
			1093	656	218	219			
1	1G	219	Total	C	N	O	S	0	0
			1658	1078	269	306	5		
1	1N	219	Total	C	N	O	S	0	0
			1652	1073	269	305	5		
1	1g	219	Total	C	N	O	S	0	0
			1655	1076	268	306	5		
1	1n	219	Total	C	N	O	S	0	0
			1653	1073	269	306	5		
1	20	218	Total	C	N	O		0	0
			1093	656	218	219			

- Molecule 2 is a protein called Chlorophyll a/b-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	03	220	Total	C	N	O	S	0	0
			1685	1098	278	304	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	07	220	Total	C	N	O	S	0	0
			1648	1070	273	300	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	04	200	Total	C	N	O	S	0	0
			1532	1003	249	276	4		
3	08	205	Total	C	N	O	S	0	0
			1570	1029	255	282	4		

- Molecule 4 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	12	222	Total	C	N	O	0	0
			1112	669	222	221		
4	15	222	Total	C	N	O	0	0
			1112	669	222	221		
4	18	222	Total	C	N	O	0	0
			1112	669	222	221		
4	21	222	Total	C	N	O	0	0
			1112	669	222	221		

- Molecule 5 is a protein called Chlorophyll a-b binding protein 1, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	13	218	Total	C	N	O	0	0
			1094	658	218	218		
5	16	218	Total	C	N	O	0	0
			1094	658	218	218		
5	19	218	Total	C	N	O	0	0
			1094	658	218	218		
5	22	218	Total	C	N	O	0	0
			1094	658	218	218		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1A	334	Total	C	N	O	S	0	0
			2612	1706	430	463	13		
6	1a	333	Total	C	N	O	S	0	0
			2606	1703	429	461	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1B	503	Total	C	N	O	S	0	0
			3945	2577	663	693	12		
7	1b	503	Total	C	N	O	S	0	0
			3945	2577	663	693	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1C	450	Total	C	N	O	S	0	0
			3486	2296	582	599	9		
8	1c	450	Total	C	N	O	S	0	0
			3498	2304	583	601	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1D	340	Total	C	N	O	S	0	0
			2708	1790	442	464	12		
9	1d	341	Total	C	N	O	S	0	0
			2716	1794	444	466	12		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	1E	75	Total	C	N	O	0	0
			614	400	100	114		
10	1e	75	Total	C	N	O	0	0
			614	400	100	114		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1F	35	Total	C	N	O	S	0	0
			286	192	49	44	1		
11	1f	30	Total	C	N	O	S	0	0
			241	162	41	37	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1H	60	Total	C	N	O	S	0	0
			454	299	73	79	3		
12	1h	60	Total	C	N	O	S	0	0
			454	299	73	79	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1I	34	Total	C	N	O	S	0	0
			277	190	43	43	1		
13	1i	34	Total	C	N	O	S	0	0
			277	190	43	43	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
14	1J	35	Total	C	N	O	0	0
			255	172	39	44		
14	1j	35	Total	C	N	O	0	0
			255	172	39	44		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1K	37	Total	C	N	O	S	0	0
			305	214	44	46	1		
15	1k	37	Total	C	N	O	S	0	0
			305	214	44	46	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
16	1L	36	Total	C	N	O	0	0
			304	201	48	55		
16	1l	35	Total	C	N	O	0	0
			295	196	46	53		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
17	1M	32	Total	C	N	O	0	0
			247	171	35	41		

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Mol	Chain	Residues	Atoms				AltConf	Trace
17	1m	33	Total	C	N	O	0	0
			251	173	37	41		

- Molecule 18 is a protein called 33 kDa subunit of oxygen evolving system of photosystem II.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	1O	247	Total	C	N	O	S	0	0
			1861	1177	306	373	5		
18	1o	237	Total	C	N	O	S	0	0
			1795	1136	294	360	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1O	248	SER	-	insertion	UNP Q943W1
1o	248	SER	-	insertion	UNP Q943W1

- Molecule 19 is a protein called 23 kDa subunit of oxygen evolving system of photosystem II.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	1P	186	Total	C	N	O	S	0	0
			1422	901	236	284	1		
19	1p	186	Total	C	N	O	S	0	0
			1422	901	236	284	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	1R	234	Total	C	N	O	S	0	0
			1837	1193	299	342	3		
20	1r	234	Total	C	N	O	S	0	0
			1837	1193	299	342	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	1S	218	Total	C	N	O	S	0	0
			1661	1079	269	308	5		
21	1s	217	Total	C	N	O	S	0	0
			1658	1075	270	308	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	1T	32	Total	C	N	O	S	0	0
			261	182	37	41	1		
22	1t	31	Total	C	N	O	S	0	0
			252	176	35	40	1		

- Molecule 23 is a protein called Os02g0581100 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1U	27	Total	C	N	O	S	0	0
			208	130	39	36	3		
23	1u	27	Total	C	N	O	S	0	0
			208	130	39	36	3		

- Molecule 24 is a protein called Photosystem II 10 kDa polypeptide, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1V	98	Total	C	N	O		0	0
			715	464	117	134			
24	1v	99	Total	C	N	O		0	0
			683	437	113	133			

- Molecule 25 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	1W	54	Total	C	N	O	S	0	0
			413	263	61	88	1		
25	1w	44	Total	C	N	O	S	0	0
			333	219	51	62	1		

- Molecule 26 is a protein called Os07g0673550 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1X	39	Total	C	N	O		0	0
			276	181	46	49			
26	1x	38	Total	C	N	O		0	0
			272	179	45	48			

- Molecule 27 is a protein called Os08g0119800 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1Y	34	Total	C	N	O	S	0	0
			270	176	50	43	1		

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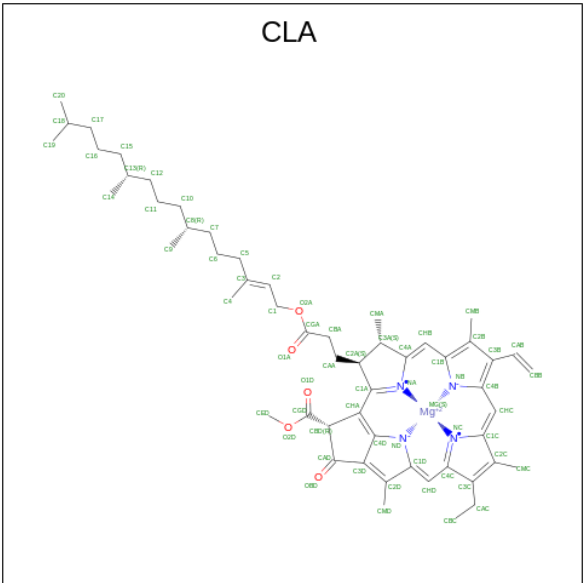
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Mol	Chain	Residues	Atoms					AltConf	Trace
27	1y	34	Total	C	N	O	S	0	0
			268	175	50	42	1		

- Molecule 28 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1Z	62	Total	C	N	O	S	0	0
			466	313	70	82	1		
28	1z	62	Total	C	N	O	S	0	0
			466	313	70	82	1		

- Molecule 29 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
29	00	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
29	00	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	00	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	00	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	00	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	00	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	00	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	00	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	01	1	Total 54	C 44	Mg 1	N 4	O 5	0
29	01	1	Total 56	C 46	Mg 1	N 4	O 5	0
29	01	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	01	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	01	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	01	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	01	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	01	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	02	1	Total 44	C 34	Mg 1	N 4	O 5	0
29	02	1	Total 40	C 32	Mg 1	N 4	O 3	0
29	02	1	Total 42	C 34	Mg 1	N 4	O 3	0
29	02	1	Total 44	C 34	Mg 1	N 4	O 5	0
29	02	1	Total 44	C 34	Mg 1	N 4	O 5	0
29	02	1	Total 44	C 34	Mg 1	N 4	O 5	0
29	02	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	02	1	Total 44	C 34	Mg 1	N 4	O 5	0
29	03	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	03	1	Total 39	C 31	Mg 1	N 4	O 3	0
29	03	1	Total 41	C 33	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
29	03	1	Total 40	C 32	Mg 1	N 4	O 3	0
29	03	1	Total 44	C 34	Mg 1	N 4	O 5	0
29	03	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	03	1	Total 44	C 34	Mg 1	N 4	O 5	0
29	04	1	Total 44	C 34	Mg 1	N 4	O 5	0
29	04	1	Total 44	C 34	Mg 1	N 4	O 5	0
29	04	1	Total 40	C 32	Mg 1	N 4	O 3	0
29	04	1	Total 44	C 34	Mg 1	N 4	O 5	0
29	04	1	Total 44	C 34	Mg 1	N 4	O 5	0
29	04	1	Total 44	C 34	Mg 1	N 4	O 5	0
29	04	1	Total 40	C 32	Mg 1	N 4	O 3	0
29	04	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	05	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	05	1	Total 44	C 34	Mg 1	N 4	O 5	0
29	05	1	Total 44	C 34	Mg 1	N 4	O 5	0
29	05	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	05	1	Total 40	C 32	Mg 1	N 4	O 3	0
29	05	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	05	1	Total 40	C 32	Mg 1	N 4	O 3	0
29	05	1	Total 40	C 32	Mg 1	N 4	O 3	0
29	06	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	06	1	Total 40	C 32	Mg 1	N 4	O 3	0
29	06	1	Total 40	C 32	Mg 1	N 4	O 3	0
29	06	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	06	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	06	1	Total 40	C 32	Mg 1	N 4	O 3	0
29	07	1	Total 40	C 32	Mg 1	N 4	O 3	0
29	07	1	Total 40	C 32	Mg 1	N 4	O 3	0
29	07	1	Total 40	C 32	Mg 1	N 4	O 3	0
29	07	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	07	1	Total 48	C 38	Mg 1	N 4	O 5	0
29	07	1	Total 39	C 31	Mg 1	N 4	O 3	0
29	07	1	Total 44	C 34	Mg 1	N 4	O 5	0
29	08	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	08	1	Total 40	C 32	Mg 1	N 4	O 3	0
29	08	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	08	1	Total 40	C 32	Mg 1	N 4	O 3	0
29	08	1	Total 38	C 32	Mg 1	N 4	O 1	0
29	08	1	Total 40	C 32	Mg 1	N 4	O 3	0
29	08	1	Total 42	C 34	Mg 1	N 4	O 3	0
29	09	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	09	1	Total 56	C 46	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	09	1	Total 40	C 32	Mg 1	N 4	O 3	0
29	09	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	09	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	09	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	09	1	Total 44	C 34	Mg 1	N 4	O 5	0
29	09	1	Total 54	C 44	Mg 1	N 4	O 5	0
29	1A	1	Total 61	C 51	Mg 1	N 4	O 5	0
29	1A	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	1B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	1B	1	Total 61	C 51	Mg 1	N 4	O 5	0
29	1B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	1B	1	Total 56	C 46	Mg 1	N 4	O 5	0
29	1B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	1B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	1B	1	Total 62	C 52	Mg 1	N 4	O 5	0
29	1B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	1B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	1B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	1B	1	Total 56	C 46	Mg 1	N 4	O 5	0
29	1B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	1B	1	Total 58	C 48	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	1B	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	1B	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	1B	1	Total 59	C 49	Mg 1	N 4	O 5	0
29	1C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	1C	1	Total 61	C 51	Mg 1	N 4	O 5	0
29	1C	1	Total 56	C 46	Mg 1	N 4	O 5	0
29	1C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	1C	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	1C	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	1C	1	Total 58	C 48	Mg 1	N 4	O 5	0
29	1C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	1C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	1C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	1C	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	1C	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	1C	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	1D	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	1D	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	1D	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	1D	1	Total 42	C 34	Mg 1	N 4	O 3	0
29	1G	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	1G	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	1G	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	1G	1	Total 44	C 34	Mg 1	N 4	O 5	0
29	1G	1	Total 44	C 34	Mg 1	N 4	O 5	0
29	1G	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	1G	1	Total 44	C 34	Mg 1	N 4	O 5	0
29	1G	1	Total 42	C 34	Mg 1	N 4	O 3	0
29	1N	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	1N	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	1N	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	1N	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	1N	1	Total 40	C 32	Mg 1	N 4	O 3	0
29	1N	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	1N	1	Total 52	C 42	Mg 1	N 4	O 5	0
29	1N	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	1R	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	1R	1	Total 44	C 35	Mg 1	N 4	O 4	0
29	1R	1	Total 40	C 32	Mg 1	N 4	O 3	0
29	1R	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	1R	1	Total 44	C 34	Mg 1	N 4	O 5	0
29	1R	1	Total 49	C 39	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	1R	1	Total 44	C 34	Mg 1	N 4	O 5	0
29	1R	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	1R	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	1S	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	1S	1	Total 40	C 32	Mg 1	N 4	O 3	0
29	1S	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	1S	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	1S	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	1S	1	Total 54	C 44	Mg 1	N 4	O 5	0
29	1S	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	1S	1	Total 44	C 34	Mg 1	N 4	O 5	0
29	1S	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	1a	1	Total 52	C 42	Mg 1	N 4	O 5	0
29	1a	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	1a	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	1b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	1b	1	Total 56	C 46	Mg 1	N 4	O 5	0
29	1b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	1b	1	Total 42	C 34	Mg 1	N 4	O 3	0
29	1b	1	Total 58	C 48	Mg 1	N 4	O 5	0
29	1b	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	1b	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
29	1b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	1b	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
29	1b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	1b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	1b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
29	1b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	1b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	1b	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
29	1b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	1c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	1c	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	1c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	1c	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	1c	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
29	1c	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	1c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	1c	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
29	1c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	1c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	1c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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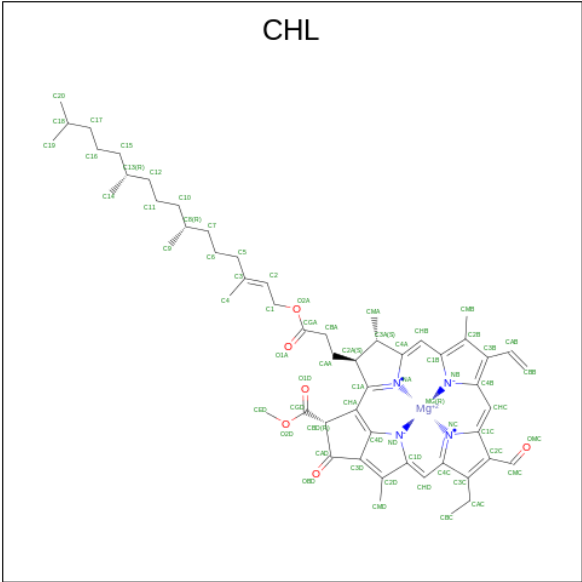
Mol	Chain	Residues	Atoms					AltConf
29	1c	1	Total 61	C 51	Mg 1	N 4	O 5	0
29	1c	1	Total 59	C 49	Mg 1	N 4	O 5	0
29	1d	1	Total 59	C 49	Mg 1	N 4	O 5	0
29	1d	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	1d	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	1g	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	1g	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	1g	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	1g	1	Total 56	C 46	Mg 1	N 4	O 5	0
29	1g	1	Total 42	C 34	Mg 1	N 4	O 3	0
29	1g	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	1g	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	1g	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	1n	1	Total 56	C 46	Mg 1	N 4	O 5	0
29	1n	1	Total 57	C 47	Mg 1	N 4	O 5	0
29	1n	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	1n	1	Total 58	C 48	Mg 1	N 4	O 5	0
29	1n	1	Total 57	C 47	Mg 1	N 4	O 5	0
29	1n	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	1n	1	Total 57	C 47	Mg 1	N 4	O 5	0
29	1n	1	Total 41	C 33	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
29	1r	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	1r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	1r	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	1r	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
29	1r	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
29	1r	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
29	1r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	1r	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
29	1r	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	1s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	1s	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	1s	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	1s	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
29	1s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	1s	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	1s	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
29	1s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	1s	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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



Mol	Chain	Residues	Atoms						AltConf
30	00	1	Total	C	Mg	N	O		0
			45	34	1	4	6		
30	00	1	Total	C	Mg	N	O		0
			47	36	1	4	6		
30	00	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
30	00	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
30	00	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
30	01	1	Total	C	Mg	N	O		0
			46	35	1	4	6		
30	01	1	Total	C	Mg	N	O		0
			46	35	1	4	6		
30	01	1	Total	C	Mg	N	O		0
			63	52	1	4	6		
30	01	1	Total	C	Mg	N	O		0
			46	35	1	4	6		
30	01	1	Total	C	Mg	N	O		0
			62	51	1	4	6		
30	02	1	Total	C	Mg	N	O		0
			46	35	1	4	6		
30	02	1	Total	C	Mg	N	O		0
			46	35	1	4	6		
30	02	1	Total	C	Mg	N	O		0
			45	34	1	4	6		
30	02	1	Total	C	Mg	N	O		0
			45	34	1	4	6		

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Mol	Chain	Residues	Atoms					AltConf
30	02	1	Total 45	C 34	Mg 1	N 4	O 6	0
30	02	1	Total 46	C 35	Mg 1	N 4	O 6	0
30	03	1	Total 40	C 32	Mg 1	N 4	O 3	0
30	03	1	Total 45	C 34	Mg 1	N 4	O 6	0
30	03	1	Total 43	C 34	Mg 1	N 4	O 4	0
30	03	1	Total 46	C 35	Mg 1	N 4	O 6	0
30	03	1	Total 42	C 33	Mg 1	N 4	O 4	0
30	04	1	Total 46	C 35	Mg 1	N 4	O 6	0
30	04	1	Total 41	C 32	Mg 1	N 4	O 4	0
30	04	1	Total 46	C 35	Mg 1	N 4	O 6	0
30	04	1	Total 43	C 34	Mg 1	N 4	O 4	0
30	04	1	Total 42	C 33	Mg 1	N 4	O 4	0
30	05	1	Total 45	C 34	Mg 1	N 4	O 6	0
30	05	1	Total 63	C 52	Mg 1	N 4	O 6	0
30	05	1	Total 41	C 32	Mg 1	N 4	O 4	0
30	05	1	Total 42	C 33	Mg 1	N 4	O 4	0
30	05	1	Total 41	C 32	Mg 1	N 4	O 4	0
30	05	1	Total 42	C 33	Mg 1	N 4	O 4	0
30	06	1	Total 46	C 35	Mg 1	N 4	O 6	0
30	06	1	Total 40	C 31	Mg 1	N 4	O 4	0
30	06	1	Total 41	C 32	Mg 1	N 4	O 4	0

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Mol	Chain	Residues	Atoms					AltConf
30	06	1	Total 45	C 34	Mg 1	N 4	O 6	0
30	06	1	Total 46	C 35	Mg 1	N 4	O 6	0
30	07	1	Total 41	C 32	Mg 1	N 4	O 4	0
30	07	1	Total 41	C 32	Mg 1	N 4	O 4	0
30	07	1	Total 39	C 32	Mg 1	N 4	O 2	0
30	07	1	Total 41	C 32	Mg 1	N 4	O 4	0
30	07	1	Total 41	C 32	Mg 1	N 4	O 4	0
30	08	1	Total 41	C 32	Mg 1	N 4	O 4	0
30	08	1	Total 41	C 32	Mg 1	N 4	O 4	0
30	08	1	Total 45	C 34	Mg 1	N 4	O 6	0
30	08	1	Total 41	C 32	Mg 1	N 4	O 4	0
30	08	1	Total 39	C 32	Mg 1	N 4	O 2	0
30	09	1	Total 41	C 32	Mg 1	N 4	O 4	0
30	09	1	Total 43	C 34	Mg 1	N 4	O 4	0
30	09	1	Total 43	C 34	Mg 1	N 4	O 4	0
30	09	1	Total 43	C 34	Mg 1	N 4	O 4	0
30	09	1	Total 61	C 50	Mg 1	N 4	O 6	0
30	1G	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	1G	1	Total 41	C 32	Mg 1	N 4	O 4	0
30	1G	1	Total 46	C 35	Mg 1	N 4	O 6	0
30	1G	1	Total 64	C 53	Mg 1	N 4	O 6	0

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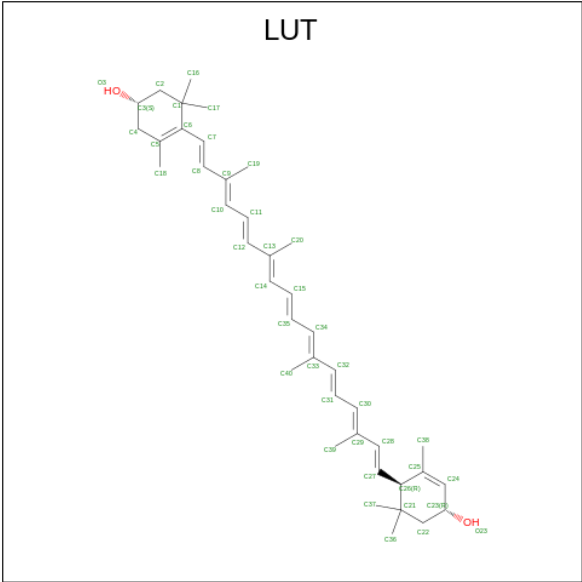
Mol	Chain	Residues	Atoms					AltConf
30	1G	1	Total 43	C 34	Mg 1	N 4	O 4	0
30	1G	1	Total 42	C 33	Mg 1	N 4	O 4	0
30	1N	1	Total 65	C 54	Mg 1	N 4	O 6	0
30	1N	1	Total 42	C 33	Mg 1	N 4	O 4	0
30	1N	1	Total 46	C 35	Mg 1	N 4	O 6	0
30	1N	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	1N	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	1N	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	1R	1	Total 42	C 33	Mg 1	N 4	O 4	0
30	1R	1	Total 42	C 33	Mg 1	N 4	O 4	0
30	1R	1	Total 41	C 32	Mg 1	N 4	O 4	0
30	1R	1	Total 45	C 34	Mg 1	N 4	O 6	0
30	1S	1	Total 46	C 35	Mg 1	N 4	O 6	0
30	1S	1	Total 41	C 32	Mg 1	N 4	O 4	0
30	1S	1	Total 42	C 33	Mg 1	N 4	O 4	0
30	1S	1	Total 42	C 33	Mg 1	N 4	O 4	0
30	1g	1	Total 58	C 47	Mg 1	N 4	O 6	0
30	1g	1	Total 46	C 35	Mg 1	N 4	O 6	0
30	1g	1	Total 50	C 39	Mg 1	N 4	O 6	0
30	1g	1	Total 47	C 36	Mg 1	N 4	O 6	0
30	1g	1	Total 43	C 34	Mg 1	N 4	O 4	0

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Mol	Chain	Residues	Atoms					AltConf
30	1g	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
30	1n	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
30	1n	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	1n	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
30	1n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	1n	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	1n	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
30	1r	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	1r	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	1r	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	1r	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
30	1s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	1s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	1s	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
30	1s	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

- Molecule 31 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂) (labeled as "Ligand of Interest" by depositor).



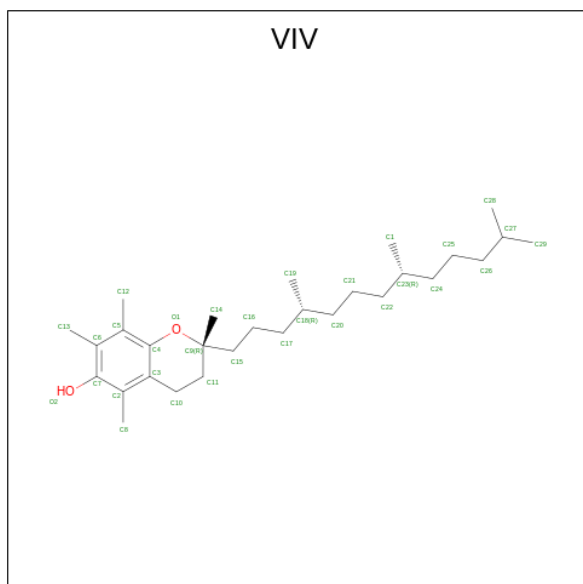
Mol	Chain	Residues	Atoms			AltConf
31	00	1	Total	C	O	0
			42	40	2	
31	00	1	Total	C	O	0
			42	40	2	
31	01	1	Total	C	O	0
			42	40	2	
31	01	1	Total	C	O	0
			42	40	2	
31	03	1	Total	C	O	0
			42	40	2	
31	05	1	Total	C	O	0
			42	40	2	
31	07	1	Total	C	O	0
			42	40	2	
31	09	1	Total	C	O	0
			42	40	2	
31	09	1	Total	C	O	0
			42	40	2	
31	1G	1	Total	C	O	0
			42	40	2	
31	1G	1	Total	C	O	0
			42	40	2	
31	1N	1	Total	C	O	0
			41	39	2	
31	1R	1	Total	C	O	0
			42	40	2	
31	1S	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
31	1S	1	Total	C	O	0
			42	40	2	
31	1g	1	Total	C	O	0
			42	40	2	
31	1g	1	Total	C	O	0
			42	40	2	
31	1n	1	Total	C	O	0
			42	40	2	
31	1r	1	Total	C	O	0
			42	40	2	
31	1s	1	Total	C	O	0
			42	40	2	
31	1s	1	Total	C	O	0
			42	40	2	

- Molecule 32 is (2R)-2,5,7,8-TETRAMETHYL-2-[(4R,8R)-4,8,12-TRIMETHYLTRIDECYL]CHROMAN-6-OL (CCD ID: VIV) (formula: C₂₉H₅₀O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
32	00	1	Total	C	O	0
			21	19	2	
32	09	1	Total	C	O	0
			31	29	2	

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms				AltConf
33	1C	1	Total 40	C 31	O 8	P 1	0
33	1C	1	Total 32	C 23	O 8	P 1	0
33	1C	1	Total 37	C 26	O 10	P 1	0
33	1D	1	Total 31	C 20	O 10	P 1	0
33	1D	1	Total 43	C 32	O 10	P 1	0
33	1D	1	Total 32	C 21	O 10	P 1	0
33	1D	1	Total 41	C 32	O 8	P 1	0
33	1E	1	Total 30	C 19	O 10	P 1	0
33	1F	1	Total 42	C 33	O 8	P 1	0
33	1G	1	Total 41	C 30	O 10	P 1	0
33	1I	1	Total 32	C 23	O 8	P 1	0
33	1I	1	Total 39	C 28	O 10	P 1	0
33	1J	1	Total 45	C 36	O 8	P 1	0
33	1K	1	Total 43	C 34	O 8	P 1	0
33	1L	1	Total 49	C 38	O 10	P 1	0
33	1N	1	Total 40	C 29	O 10	P 1	0
33	1N	1	Total 43	C 32	O 10	P 1	0
33	1N	1	Total 48	C 37	O 10	P 1	0
33	1P	1	Total 45	C 36	O 8	P 1	0
33	1R	1	Total 38	C 27	O 10	P 1	0
33	1R	1	Total 37	C 26	O 10	P 1	0

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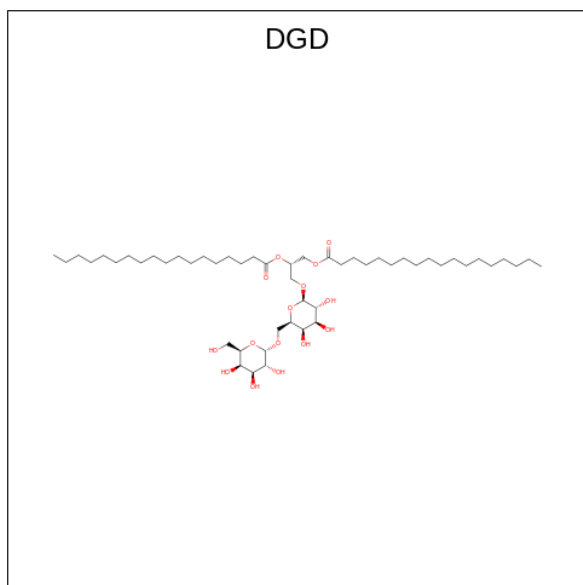
Mol	Chain	Residues	Atoms				AltConf
33	1S	1	Total	C	O	P	0
			34	23	10	1	
33	1S	1	Total	C	O		0
			29	24	5		
33	1S	1	Total	C	O	P	0
			31	20	10	1	
33	1V	1	Total	C	O	P	0
			49	38	10	1	
33	1W	1	Total	C	O	P	0
			35	24	10	1	
33	1W	1	Total	C	O	P	0
			44	33	10	1	
33	1a	1	Total	C	O	P	0
			32	21	10	1	
33	1a	1	Total	C	O	P	0
			41	30	10	1	
33	1b	1	Total	C	O	P	0
			27	18	8	1	
33	1b	1	Total	C	O	P	0
			36	25	10	1	
33	1b	1	Total	C	O	P	0
			45	34	10	1	
33	1b	1	Total	C	O	P	0
			32	21	10	1	
33	1b	1	Total	C	O	P	0
			49	38	10	1	
33	1c	1	Total	C	O	P	0
			42	31	10	1	
33	1c	1	Total	C	O	P	0
			28	19	8	1	
33	1d	1	Total	C	O	P	0
			39	28	10	1	
33	1d	1	Total	C	O	P	0
			38	27	10	1	
33	1e	1	Total	C	O	P	0
			42	31	10	1	
33	1g	1	Total	C	O	P	0
			36	25	10	1	
33	1j	1	Total	C	O	P	0
			41	30	10	1	
33	1n	1	Total	C	O	P	0
			43	32	10	1	

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Mol	Chain	Residues	Atoms				AltConf
33	1n	1	Total	C	O	P	0
			38	32	5	1	
33	1r	1	Total	C	O	P	0
			29	20	8	1	
33	1s	1	Total	C	O	P	0
			29	20	8	1	
33	1s	1	Total	C	O		0
			29	24	5		
33	1s	1	Total	C	O		0
			27	22	5		
33	1t	1	Total	C	O	P	0
			39	31	7	1	
33	1v	1	Total	C	O	P	0
			41	30	10	1	
33	1w	1	Total	C	O	P	0
			35	26	8	1	
33	1w	1	Total	C	O	P	0
			42	31	10	1	
33	1w	1	Total	C	O	P	0
			37	27	9	1	

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



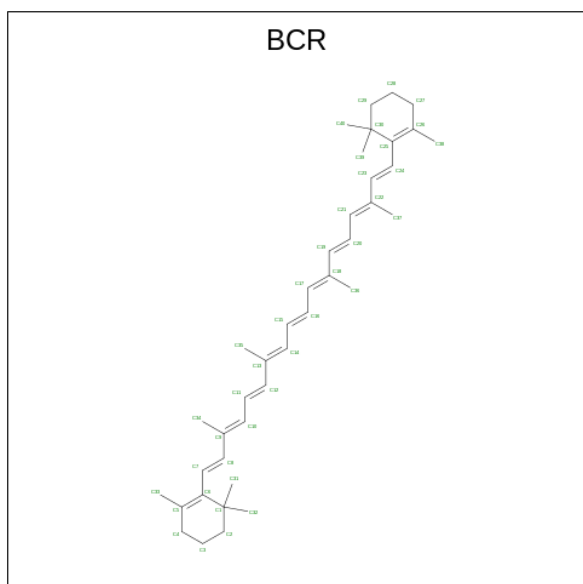
Mol	Chain	Residues	Atoms			AltConf
34	00	1	Total	C	O	0
			61	46	15	

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Mol	Chain	Residues	Atoms			AltConf
34	1A	1	Total	C	O	0
			55	40	15	
34	1B	1	Total	C	O	0
			62	47	15	
34	1B	1	Total	C	O	0
			48	33	15	
34	1B	1	Total	C	O	0
			62	47	15	
34	1C	1	Total	C	O	0
			55	40	15	
34	1C	1	Total	C	O	0
			58	43	15	
34	1C	1	Total	C	O	0
			60	45	15	
34	1S	1	Total	C	O	0
			46	31	15	
34	1b	1	Total	C	O	0
			62	47	15	
34	1c	1	Total	C	O	0
			47	32	15	
34	1c	1	Total	C	O	0
			52	37	15	
34	1c	1	Total	C	O	0
			57	42	15	

- Molecule 35 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
35	04	1	Total C 40 40	0
35	1A	1	Total C 40 40	0
35	1B	1	Total C 40 40	0
35	1B	1	Total C 40 40	0
35	1B	1	Total C 40 40	0
35	1B	1	Total C 40 40	0
35	1D	1	Total C 40 40	0
35	1H	1	Total C 40 40	0
35	1I	1	Total C 40 40	0
35	1J	1	Total C 40 40	0
35	1Z	1	Total C 40 40	0
35	1Z	1	Total C 40 40	0
35	1a	1	Total C 40 40	0
35	1b	1	Total C 40 40	0
35	1b	1	Total C 40 40	0
35	1b	1	Total C 40 40	0
35	1b	1	Total C 40 40	0
35	1c	1	Total C 40 40	0
35	1d	1	Total C 40 40	0
35	1h	1	Total C 40 40	0
35	1i	1	Total C 40 40	0
35	1j	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
35	1k	1	Total C 40 40	0

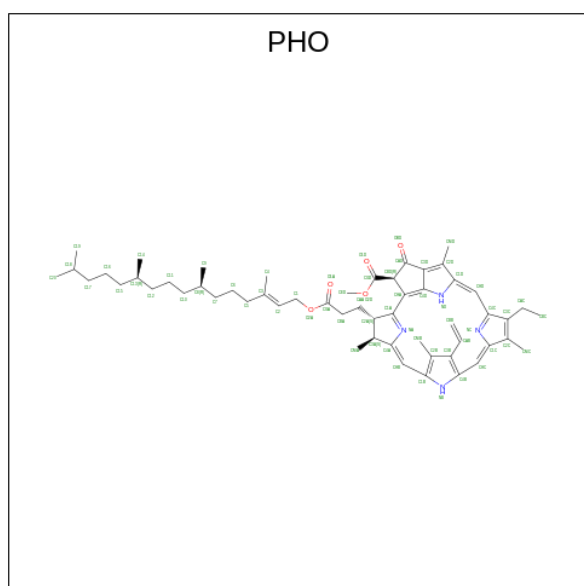
- Molecule 36 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
36	1A	1	Total Fe 1 1	0
36	1a	1	Total Fe 1 1	0

- Molecule 37 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

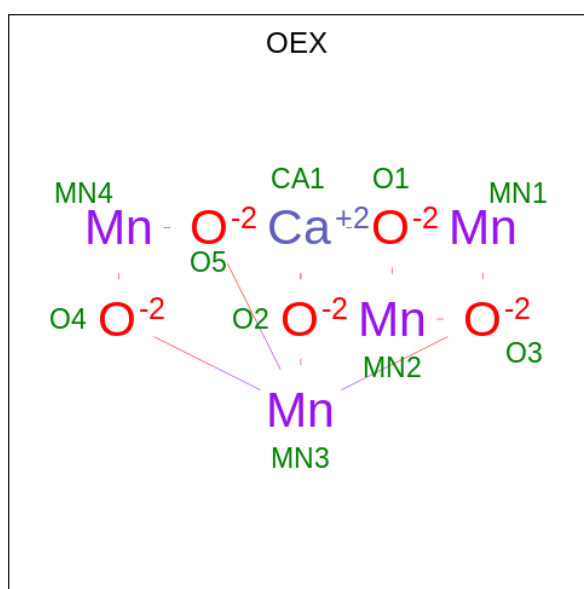
Mol	Chain	Residues	Atoms	AltConf
37	1A	2	Total Cl 2 2	0
37	1a	1	Total Cl 1 1	0
37	1c	1	Total Cl 1 1	0

- Molecule 38 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅) (labeled as "Ligand of Interest" by depositor).



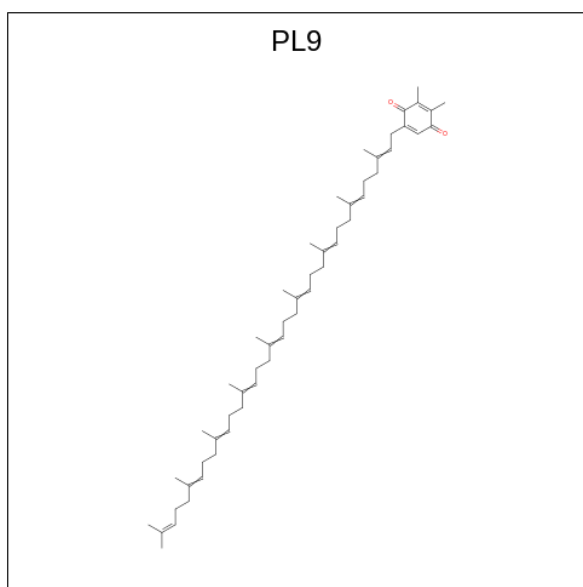
Mol	Chain	Residues	Atoms				AltConf
38	1A	1	Total	C	N	O	0
			64	55	4	5	
38	1A	1	Total	C	N	O	0
			64	55	4	5	
38	1a	1	Total	C	N	O	0
			40	33	4	3	
38	1d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 39 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



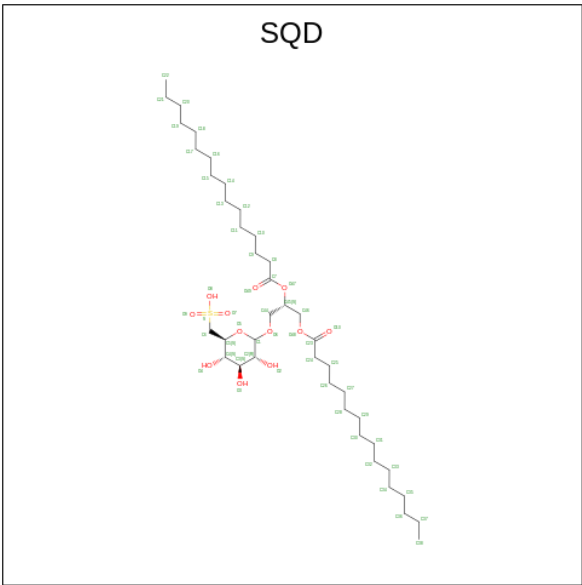
Mol	Chain	Residues	Atoms				AltConf
39	1A	1	Total	Ca	Mn	O	0
			10	1	4	5	
39	1a	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 40 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: $\text{C}_{53}\text{H}_{80}\text{O}_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
40	1A	1	Total	C	O	0
			55	53	2	
40	1D	1	Total	C	O	0
			55	53	2	
40	1E	1	Total	C	O	0
			55	53	2	
40	1R	1	Total	C	O	0
			55	53	2	
40	1a	1	Total	C	O	0
			55	53	2	
40	1d	1	Total	C	O	0
			55	53	2	
40	1e	1	Total	C	O	0
			21	19	2	
40	1r	1	Total	C	O	0
			55	53	2	

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



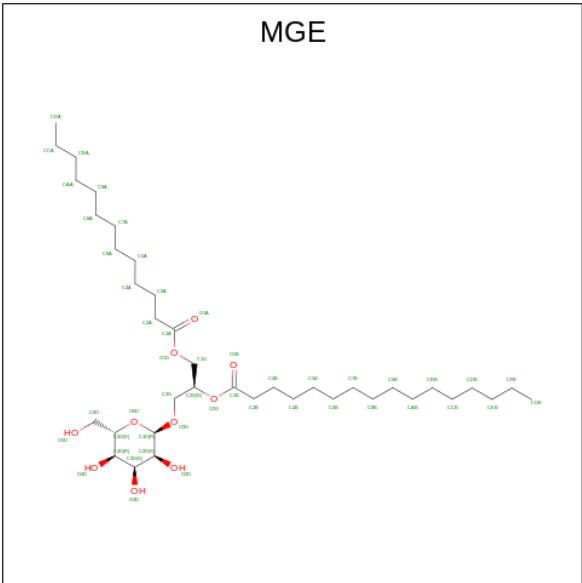
Mol	Chain	Residues	Atoms				AltConf
41	1A	1	Total	C	O	S	0
			48	35	12	1	
41	1A	1	Total	C	O	S	0
			42	29	12	1	
41	1A	1	Total	C	O	S	0
			45	32	12	1	
41	1B	1	Total	C	O	S	0
			45	32	12	1	
41	1B	1	Total	C	O	S	0
			50	37	12	1	
41	1B	1	Total	C	O	S	0
			54	41	12	1	
41	1B	1	Total	C	O	S	0
			40	27	12	1	
41	1C	1	Total	C	O	S	0
			51	38	12	1	
41	1D	1	Total	C	O	S	0
			46	33	12	1	
41	1D	1	Total	C	O	S	0
			43	30	12	1	
41	1L	1	Total	C	O	S	0
			53	40	12	1	
41	1S	1	Total	C	O	S	0
			46	33	12	1	
41	1a	1	Total	C	O	S	0
			50	37	12	1	
41	1a	1	Total	C	O	S	0
			46	33	12	1	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
41	1b	1	Total 54	41	12	1	0
41	1b	1	Total 48	35	12	1	0
41	1c	1	Total 54	41	12	1	0
41	1d	1	Total 48	35	12	1	0
41	1d	1	Total 39	26	12	1	0
41	1l	1	Total 42	29	12	1	0
41	1m	1	Total 42	29	12	1	0
41	1s	1	Total 44	31	12	1	0
41	1w	1	Total 40	27	12	1	0

- Molecule 42 is (1S)-2-(ALPHA-L-ALLOPYRANOSYLOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PALMITATE (CCD ID: MGE) (formula: C₃₈H₇₂O₁₀) (labeled as "Ligand of Interest" by depositor).



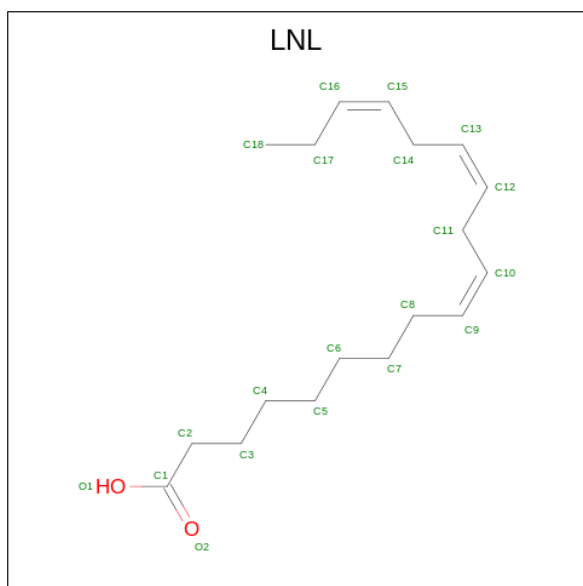
Mol	Chain	Residues	Atoms			AltConf
42	1B	1	Total 44	C 34	O 10	0

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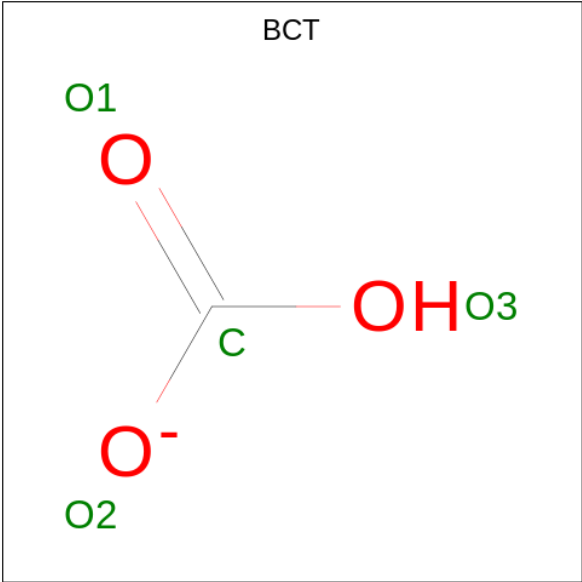
Mol	Chain	Residues	Atoms			AltConf
42	1B	1	Total	C	O	0
			43	33	10	
42	1C	1	Total	C	O	0
			45	35	10	
42	1k	1	Total	C	O	0
			36	26	10	
42	1s	1	Total	C	O	0
			41	31	10	

- Molecule 43 is ALPHA-LINOLENIC ACID (CCD ID: LNL) (formula: $C_{18}H_{30}O_2$) (labeled as "Ligand of Interest" by depositor).



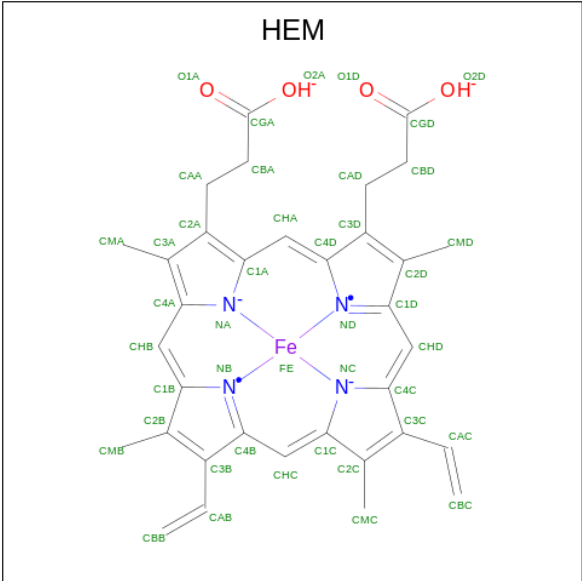
Mol	Chain	Residues	Atoms			AltConf
43	1C	1	Total	C	O	0
			18	16	2	
43	1C	1	Total	C	O	0
			17	15	2	
43	1c	1	Total	C	O	0
			17	15	2	

- Molecule 44 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
44	1D	1	Total	C	O	0
			4	1	3	
44	1d	1	Total	C	O	0
			4	1	3	

- Molecule 45 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄) (labeled as "Ligand of Interest" by depositor).



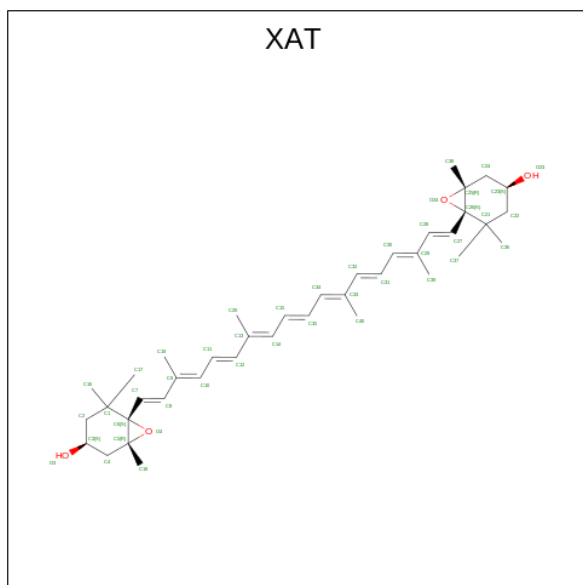
Mol	Chain	Residues	Atoms					AltConf
45	1E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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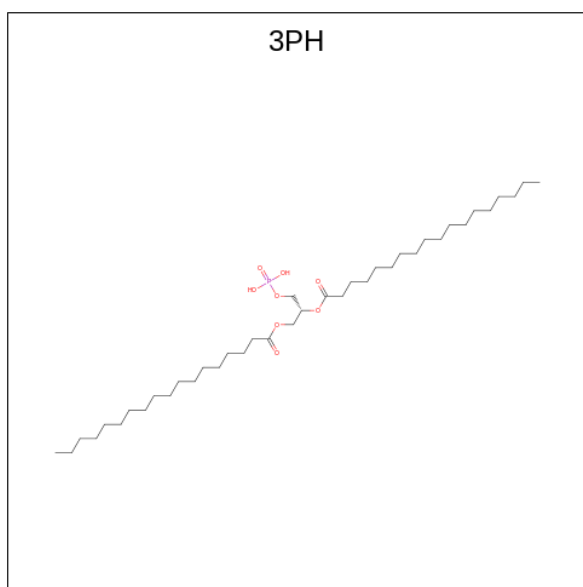
Mol	Chain	Residues	Atoms					AltConf
45	1f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 46 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'-TETRAHYDRO-BETA, BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
46	1G	1	Total	C	O	0
			44	40	4	
46	1G	1	Total	C	O	0
			44	40	4	
46	1R	1	Total	C	O	0
			44	40	4	
46	1g	1	Total	C	O	0
			44	40	4	
46	1g	1	Total	C	O	0
			44	40	4	
46	1r	1	Total	C	O	0
			44	40	4	

- Molecule 47 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$) (labeled as "Ligand of Interest" by depositor).

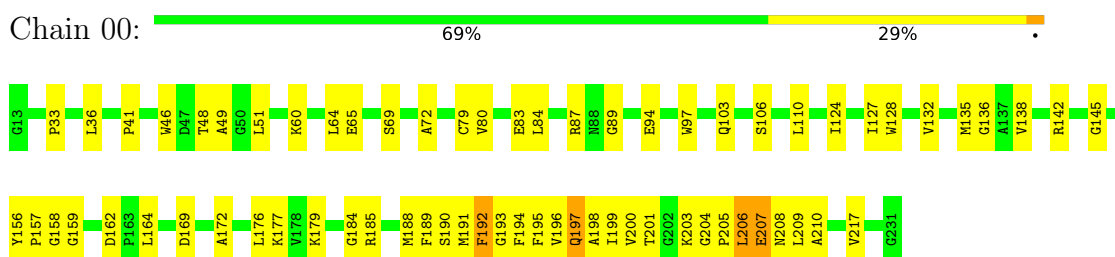


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
47	1X	1	39	30	8	1	0

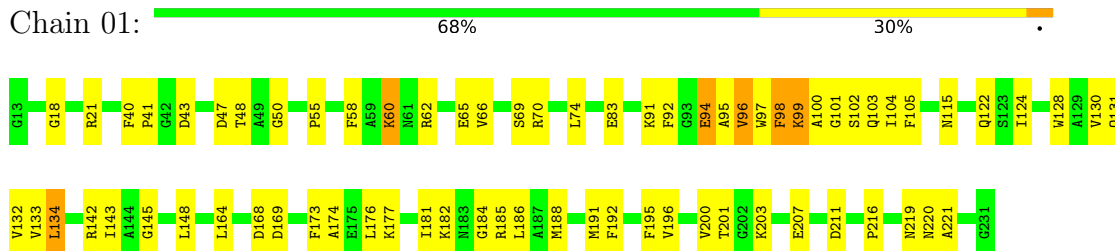
3 Residue-property plots

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.

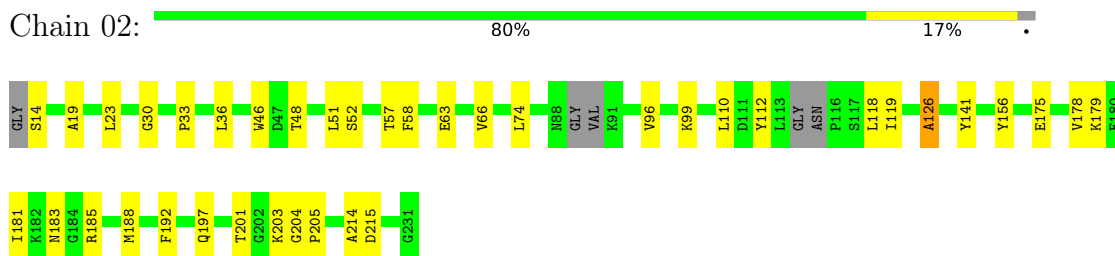
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic



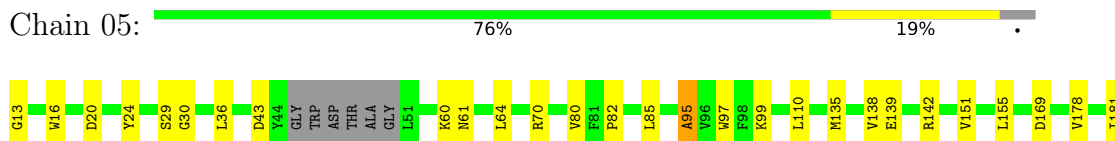
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic



- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic



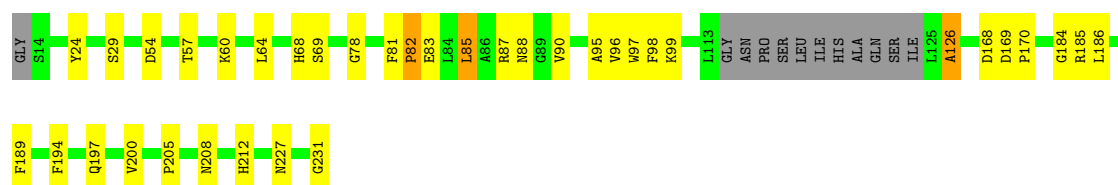
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic





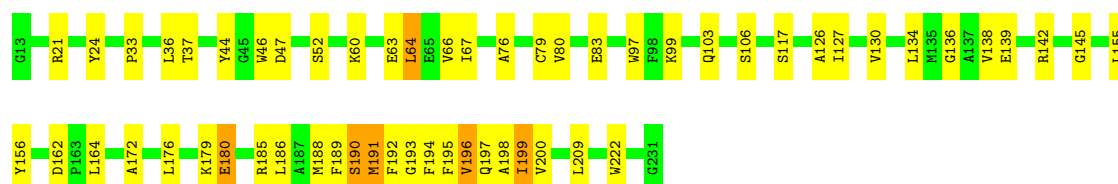
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic

Chain 06: 78% 16% 5%



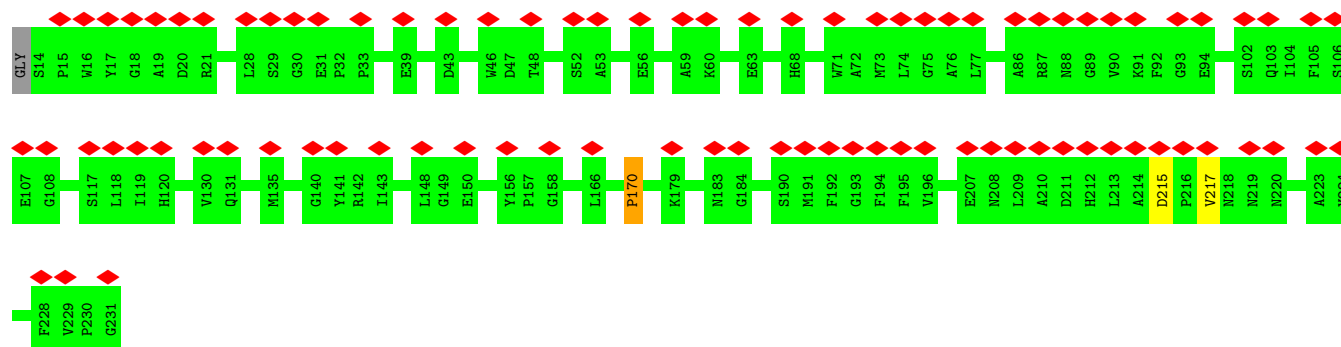
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic

Chain 09: 74% 23%



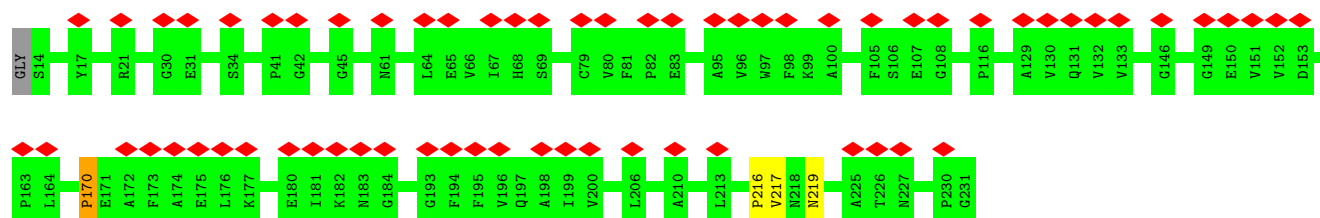
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic

Chain 11: 39% 98%

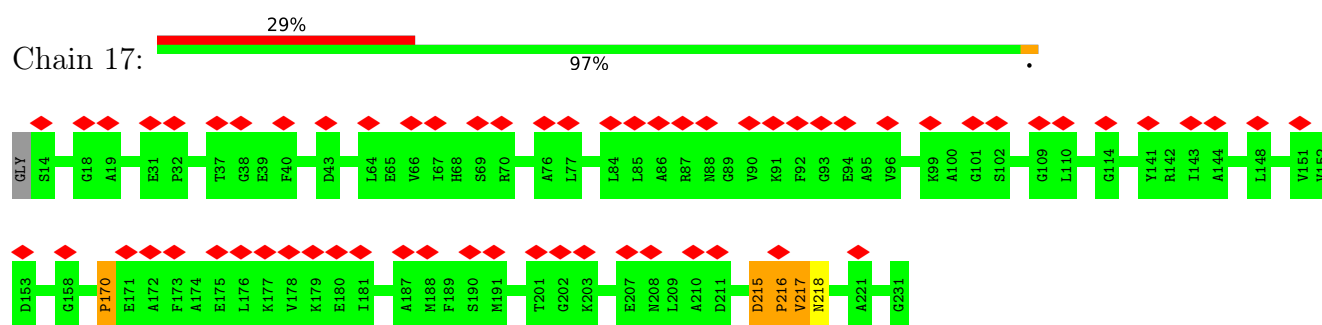


- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic

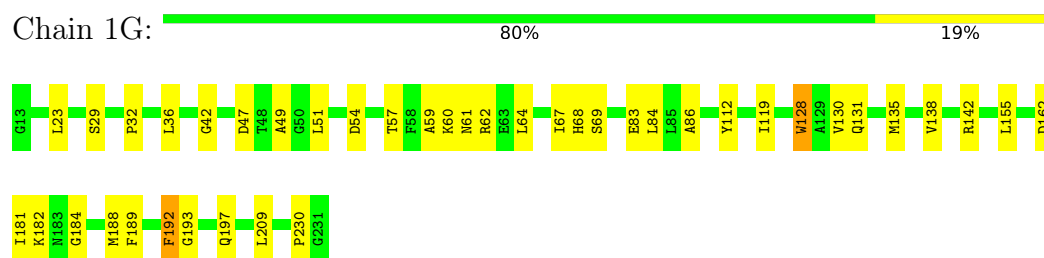
Chain 14: 30% 98%



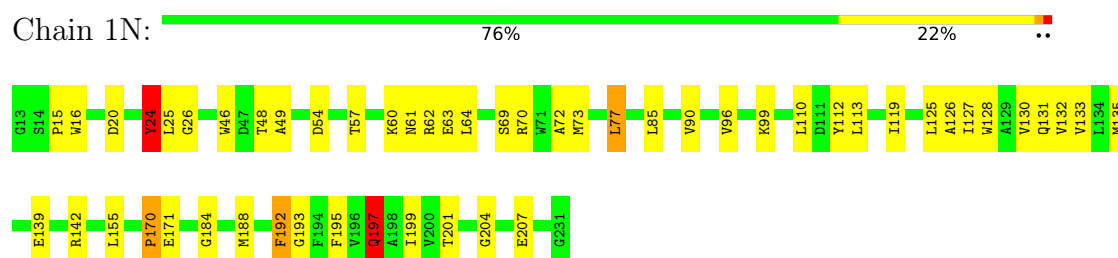
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic



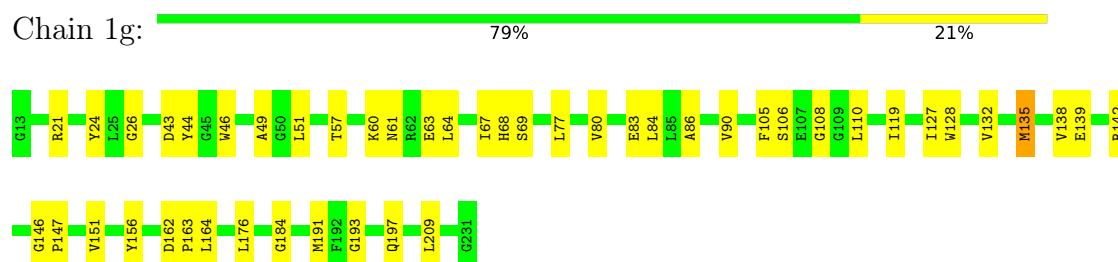
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic



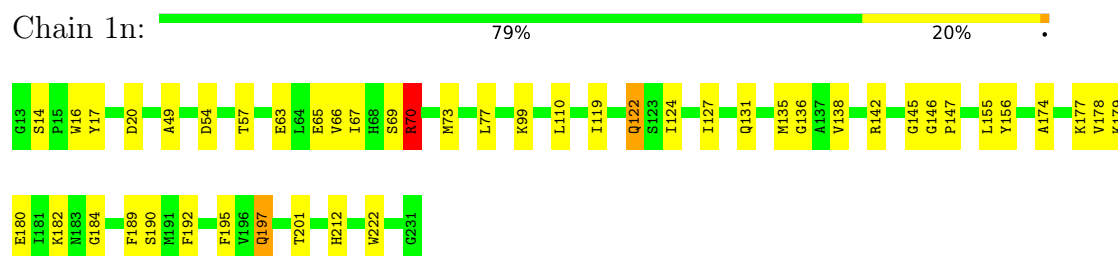
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic



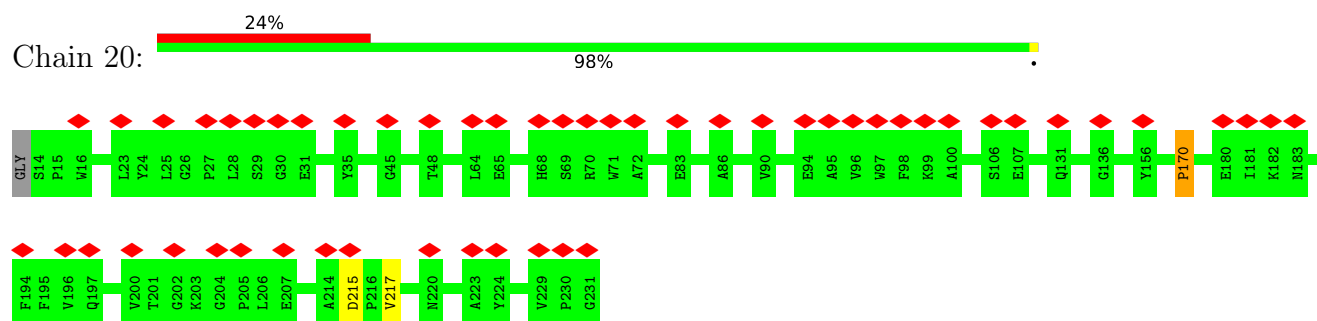
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic



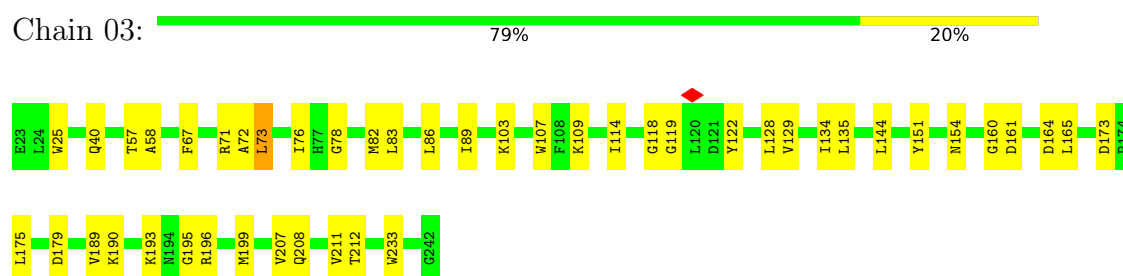
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic



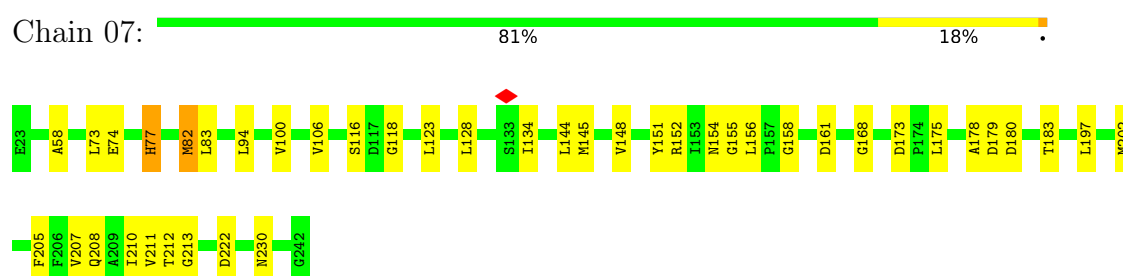
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic



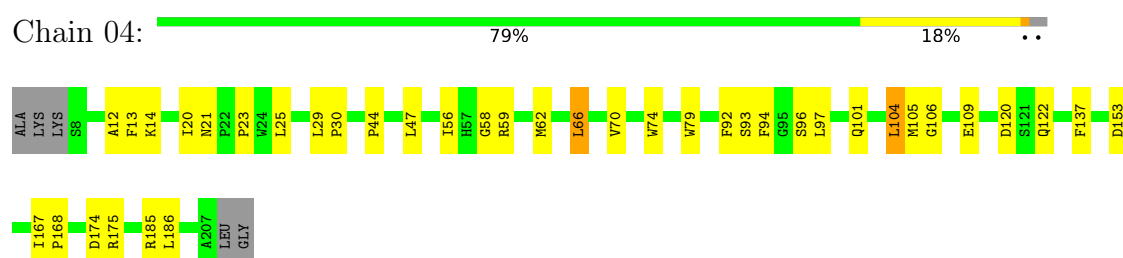
- Molecule 2: Chlorophyll a/b-binding protein



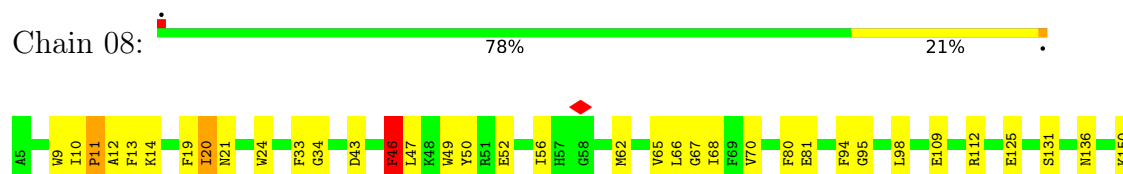
- Molecule 2: Chlorophyll a/b-binding protein



- Molecule 3: Chlorophyll a-b binding protein, chloroplastic



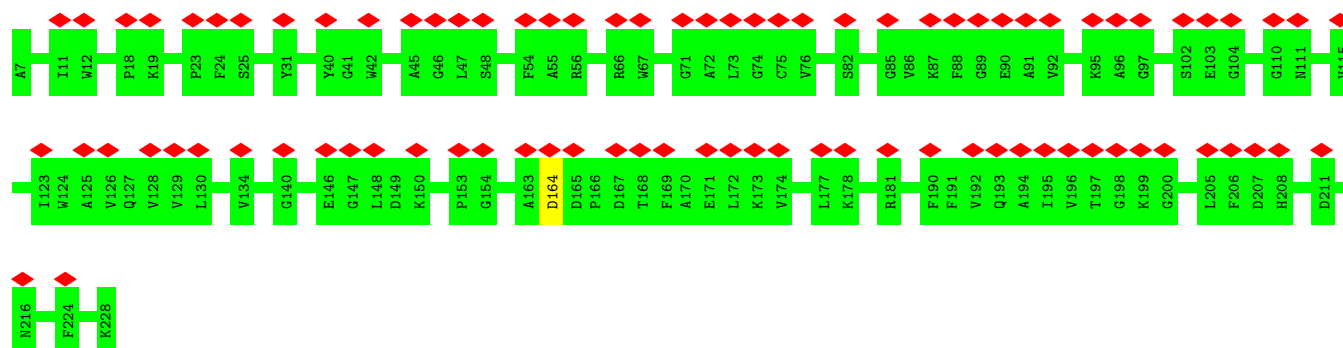
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic





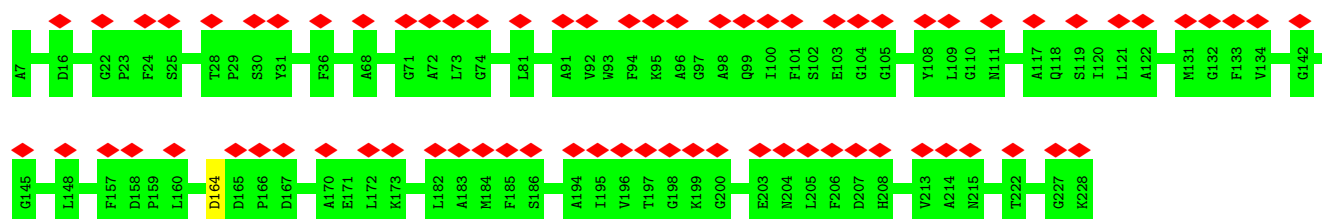
- Molecule 4: Chlorophyll a-b binding protein, chloroplastic

Chain 12: 39% 100%



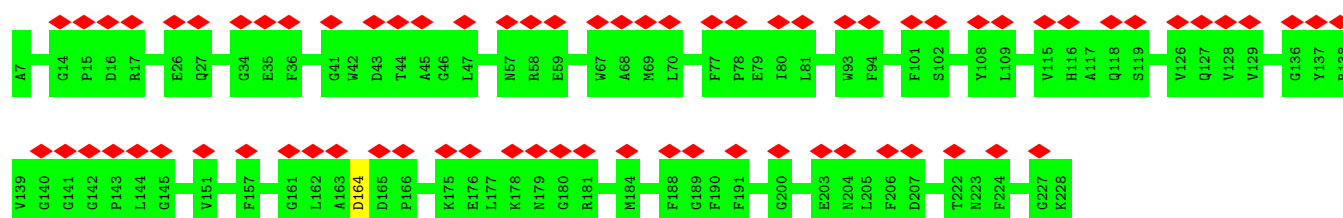
- Molecule 4: Chlorophyll a-b binding protein, chloroplastic

Chain 15: 33% 100%



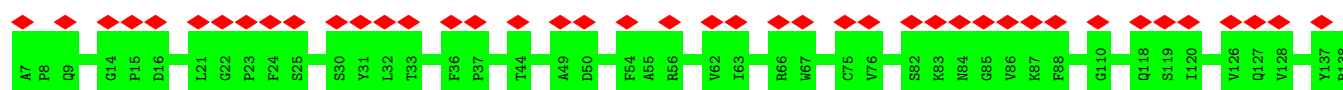
- Molecule 4: Chlorophyll a-b binding protein, chloroplastic

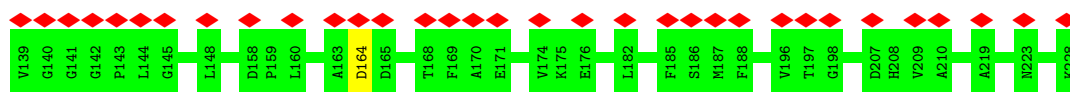
Chain 18: 33% 100%



- Molecule 4: Chlorophyll a-b binding protein, chloroplastic

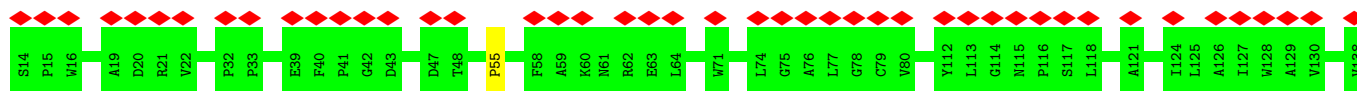
Chain 21: 34% 100%





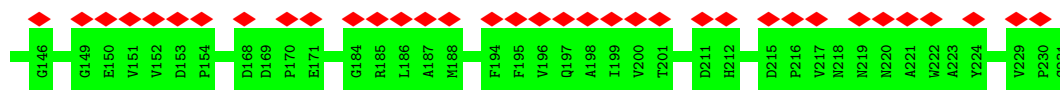
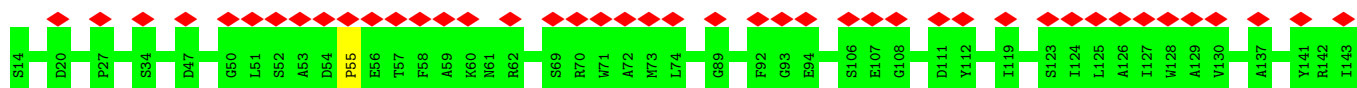
- Molecule 5: Chlorophyll a-b binding protein 1, chloroplastic

Chain 13: 35% 100%



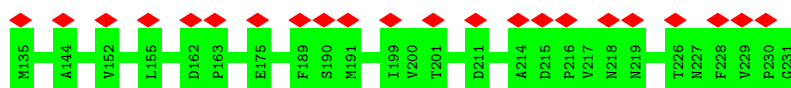
- Molecule 5: Chlorophyll a-b binding protein 1, chloroplastic

Chain 16: 36% 100%



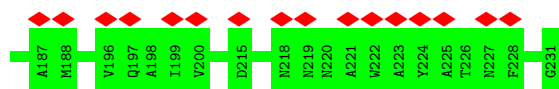
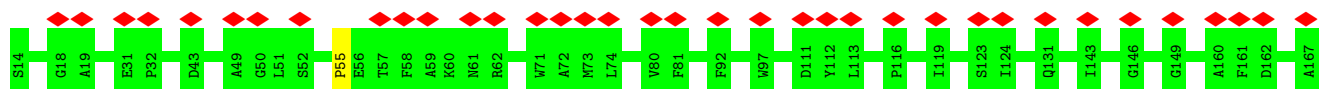
- Molecule 5: Chlorophyll a-b binding protein 1, chloroplastic

Chain 19: 28% 100%



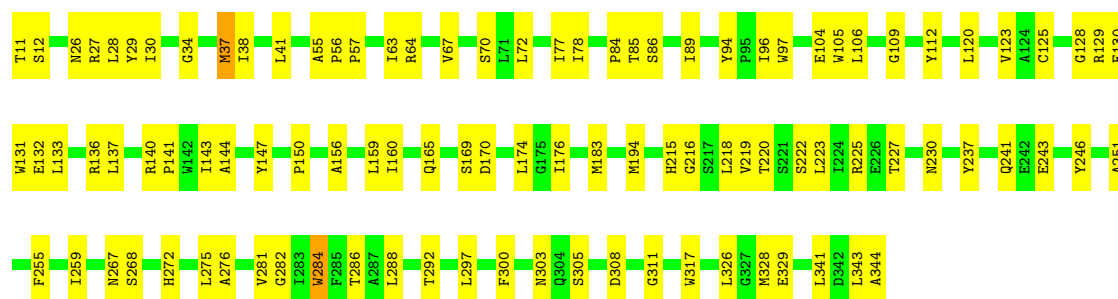
- Molecule 5: Chlorophyll a-b binding protein 1, chloroplastic

Chain 22: 24% 100%



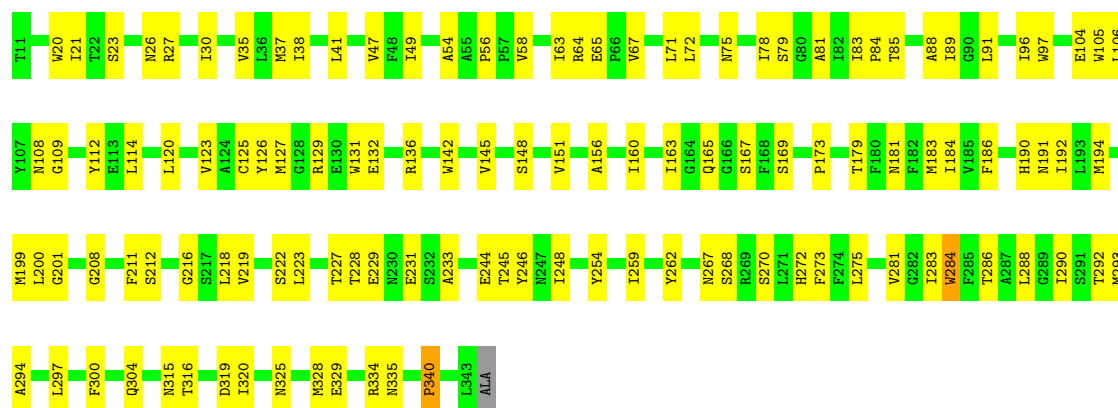
- Molecule 6: Photosystem II protein D1

Chain 1A:  70% 30%



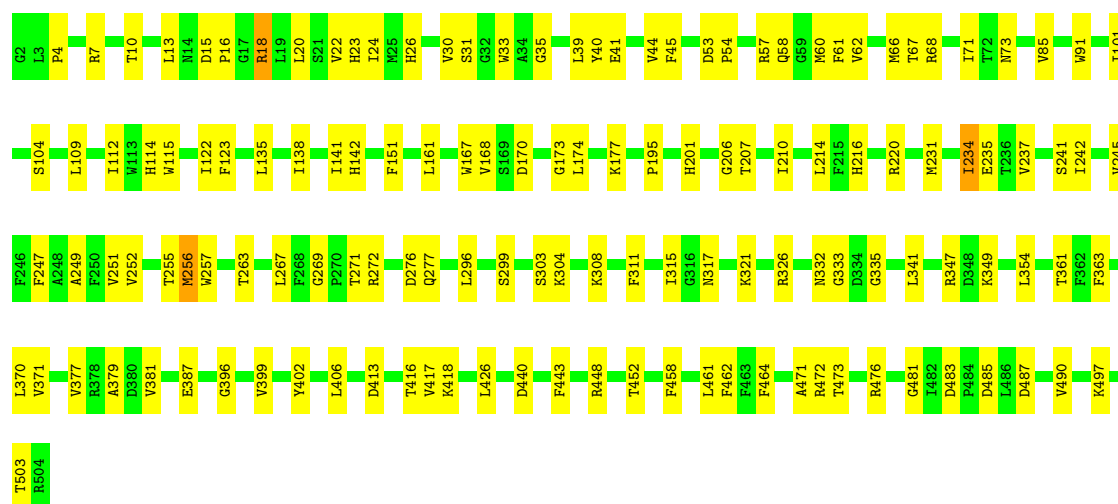
• Molecule 6: Photosystem II protein D1

Chain 1a:  64% 35%



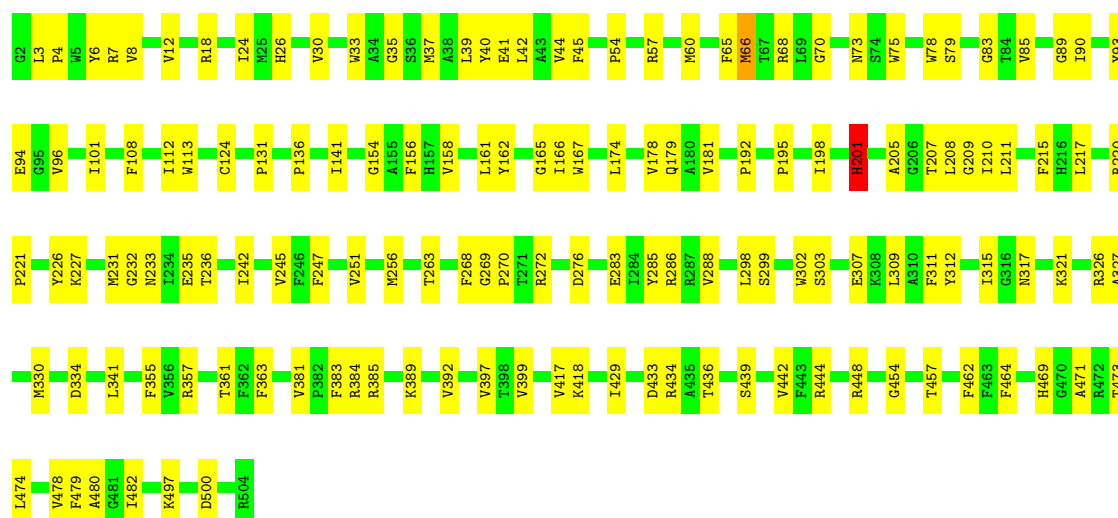
• Molecule 7: Photosystem II CP47 reaction center protein

Chain 1B:  73% 27%



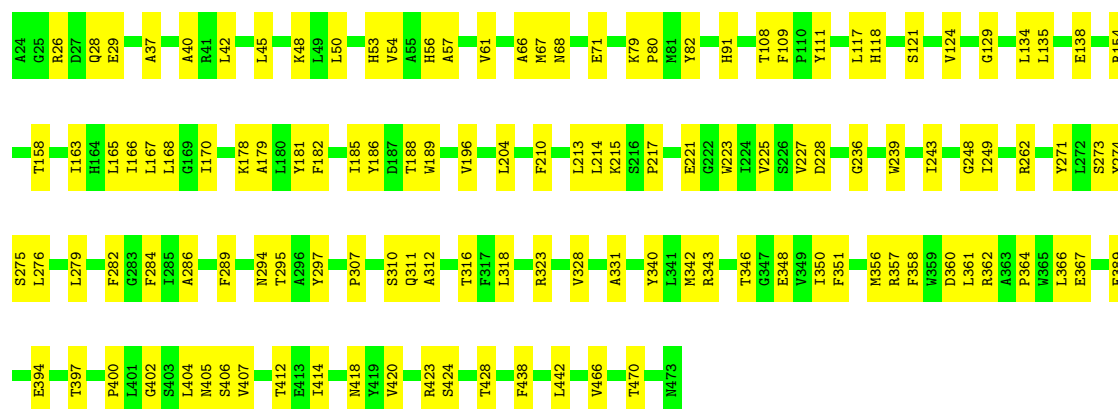
• Molecule 7: Photosystem II CP47 reaction center protein

Chain 1b:  71% 28%



• Molecule 8: Photosystem II CP43 reaction center protein

Chain 1C: 72% 28%



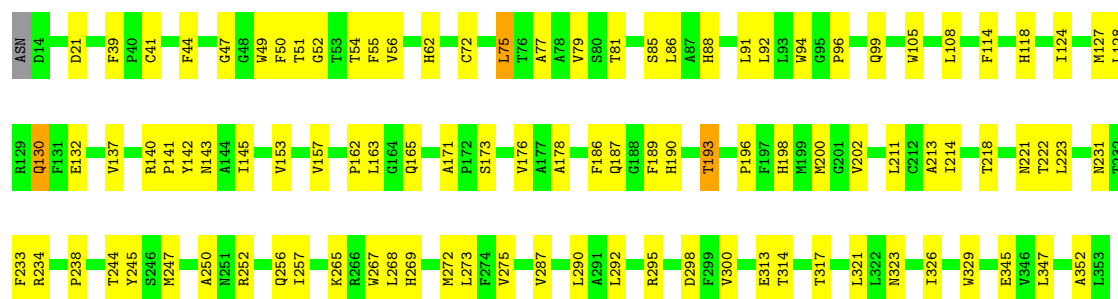
• Molecule 8: Photosystem II CP43 reaction center protein

Chain 1c: 74% 26%



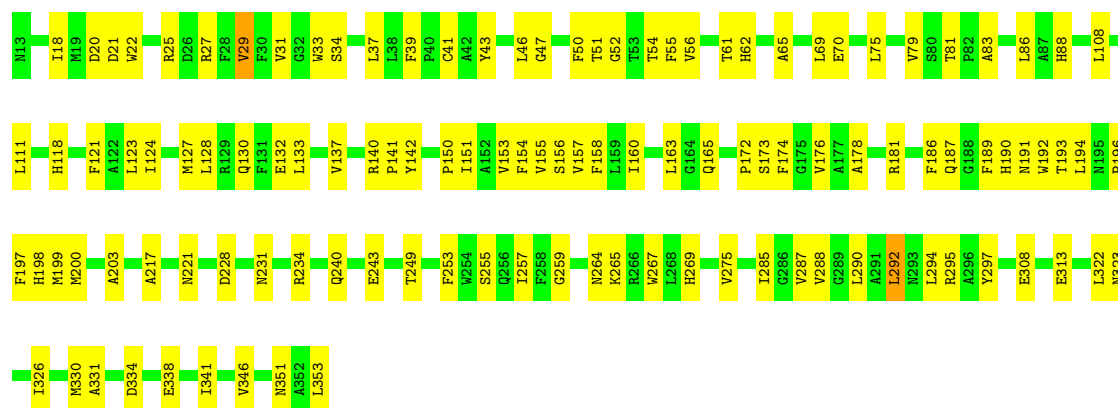
• Molecule 9: Photosystem II D2 protein

Chain 1D:  70% 28%



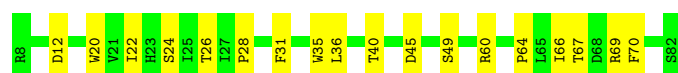
• Molecule 9: Photosystem II D2 protein

Chain 1d:  66% 34%



• Molecule 10: Cytochrome b559 subunit alpha

Chain 1E:  76% 24%



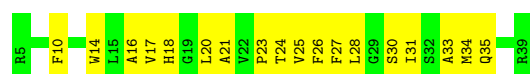
• Molecule 10: Cytochrome b559 subunit alpha

Chain 1e:  67% 33%



• Molecule 11: Cytochrome b559 subunit beta

Chain 1F:  49% 51%



• Molecule 11: Cytochrome b559 subunit beta

Chain 1f:  49% 37% 14%



- Molecule 12: Photosystem II reaction center protein H

Chain 1H:  83% 17%

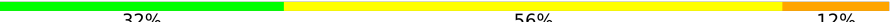


- Molecule 12: Photosystem II reaction center protein H

Chain 1h:  77% 22% .



- Molecule 13: Photosystem II reaction center protein I

Chain 1I:  32% 56% 12%



- Molecule 13: Photosystem II reaction center protein I

Chain 1i:  56% 44%



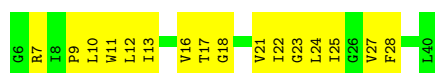
- Molecule 14: Photosystem II reaction center protein J

Chain 1J:  77% 23%



- Molecule 14: Photosystem II reaction center protein J

Chain 1j:  54% 46%



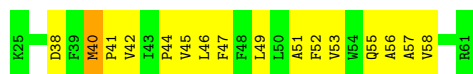
- Molecule 15: Photosystem II reaction center protein K

Chain 1K:  73% 27%



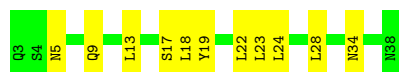
- Molecule 15: Photosystem II reaction center protein K

Chain 1k:  57% 41% .



- Molecule 16: Photosystem II reaction center protein L

Chain 1L:  69% 31%



- Molecule 16: Photosystem II reaction center protein L

Chain 1l:  61% 36% .



- Molecule 17: Photosystem II reaction center protein M

Chain 1M:  67% 27% . .



- Molecule 17: Photosystem II reaction center protein M

Chain 1m:  64% 36%

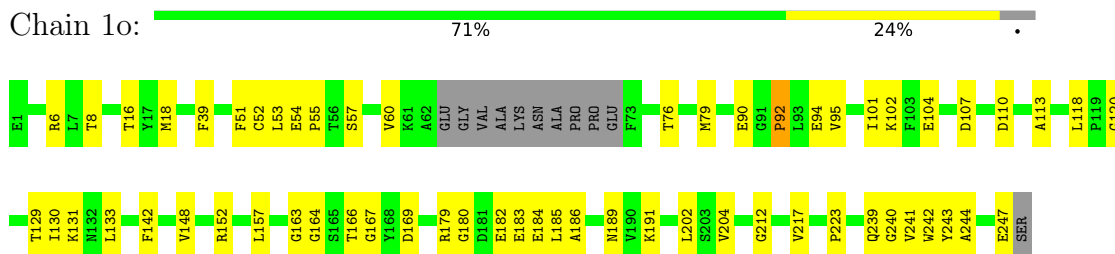


- Molecule 18: 33 kDa subunit of oxygen evolving system of photosystem II

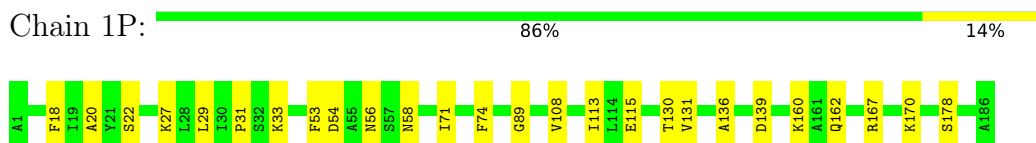
Chain 1O:  73% 26%



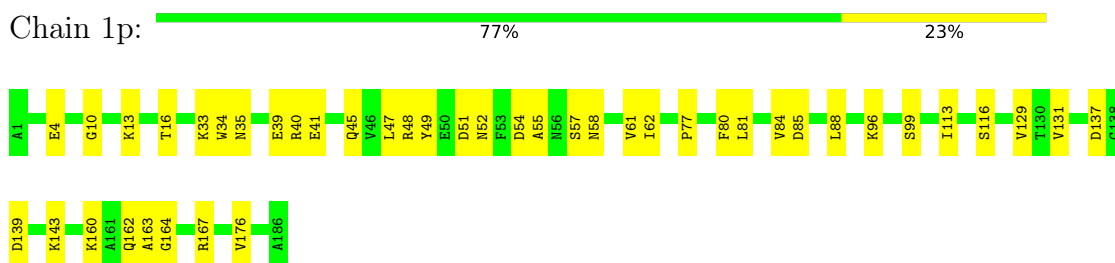
- Molecule 18: 33 kDa subunit of oxygen evolving system of photosystem II



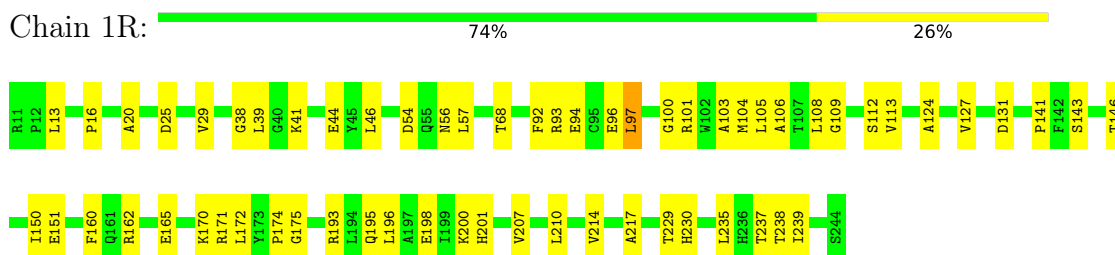
- Molecule 19: 23 kDa subunit of oxygen evolving system of photosystem II



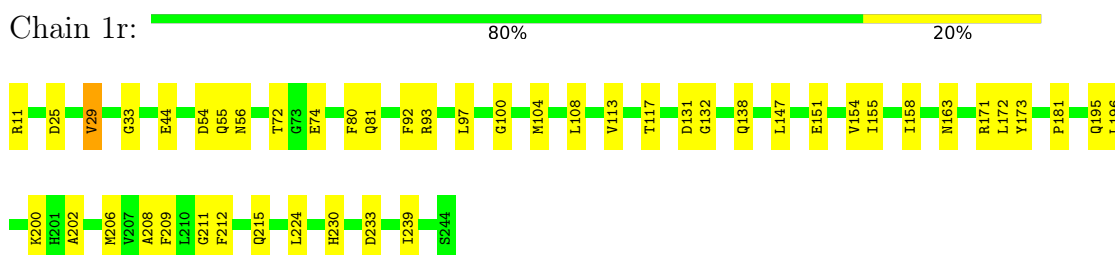
- Molecule 19: 23 kDa subunit of oxygen evolving system of photosystem II



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

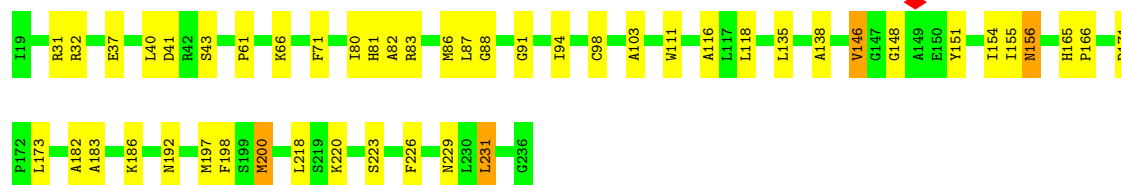


- Molecule 20: Chlorophyll a-b binding protein, chloroplastic



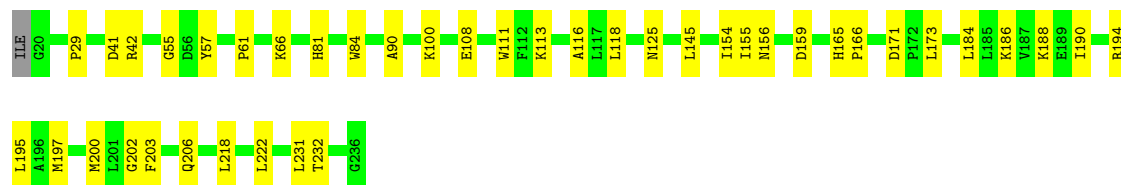
- Molecule 21: Chlorophyll a-b binding protein, chloroplastic

Chain 1S:  78% 20% .



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

Chain 1s:  81% 19%



- Molecule 22: Photosystem II reaction center protein T

Chain 1T:  66% 34%



- Molecule 22: Photosystem II reaction center protein T

Chain 1t:  75% 22% .



- Molecule 23: Os02g0581100 protein

Chain 1U:  89% 11%



- Molecule 23: Os02g0581100 protein

Chain 1u:  78% 19% .



- Molecule 24: Photosystem II 10 kDa polypeptide, chloroplastic

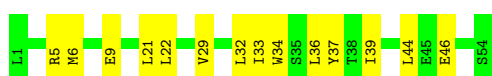
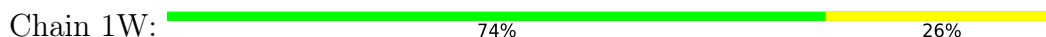
Chain 1V:  70% 23% . 7%



- Molecule 24: Photosystem II 10 kDa polypeptide, chloroplastic



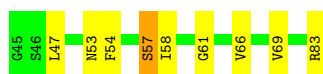
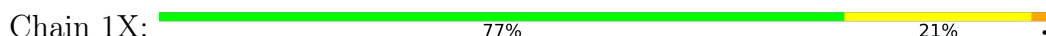
- Molecule 25: Photosystem II reaction center W protein, chloroplastic



- Molecule 25: Photosystem II reaction center W protein, chloroplastic



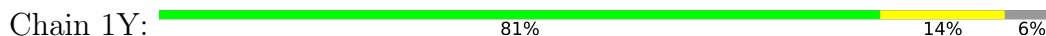
- Molecule 26: Os07g0673550 protein



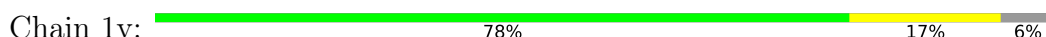
- Molecule 26: Os07g0673550 protein

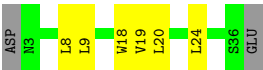


- Molecule 27: Os08g0119800 protein



- Molecule 27: Os08g0119800 protein

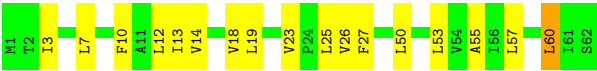




● Molecule 28: Photosystem II reaction center protein Z



● Molecule 28: Photosystem II reaction center protein Z



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	172752	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.375	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.753	Depositor
Minimum map value	0.000	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0004	Depositor
Map size (Å)	656.0, 656.0, 656.0	wwPDB
Map dimensions	800, 800, 800	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	00	0.30	0/1710	0.63	3/2332 (0.1%)
1	01	0.32	1/1685 (0.1%)	0.71	4/2297 (0.2%)
1	02	0.27	0/1623	0.63	0/2219
1	05	0.25	0/1597	0.67	0/2176
1	06	0.35	1/1485 (0.1%)	0.71	5/2030 (0.2%)
1	09	0.28	0/1710	0.55	2/2332 (0.1%)
1	11	0.34	1/1114 (0.1%)	0.69	3/1552 (0.2%)
1	14	0.34	1/1107 (0.1%)	0.69	3/1543 (0.2%)
1	17	0.35	1/1107 (0.1%)	0.71	3/1543 (0.2%)
1	1G	0.31	0/1707	0.62	1/2325 (0.0%)
1	1N	0.35	0/1702	0.72	5/2321 (0.2%)
1	1g	0.25	0/1706	0.58	1/2328 (0.0%)
1	1n	0.25	0/1703	0.55	2/2323 (0.1%)
1	20	0.34	1/1107 (0.1%)	0.69	3/1543 (0.2%)
2	03	0.23	0/1736	0.63	0/2366
2	07	0.28	0/1696	0.69	1/2312 (0.0%)
3	04	0.31	0/1585	0.78	5/2162 (0.2%)
3	08	0.31	0/1626	0.69	1/2217 (0.0%)
4	12	0.18	0/1127	0.45	0/1571
4	15	0.18	0/1127	0.45	0/1571
4	18	0.18	0/1127	0.45	0/1571
4	21	0.18	0/1127	0.45	0/1571
5	13	0.17	0/1109	0.42	1/1547 (0.1%)
5	16	0.17	0/1109	0.42	1/1547 (0.1%)
5	19	0.17	0/1109	0.42	1/1547 (0.1%)
5	22	0.17	0/1109	0.42	1/1547 (0.1%)
6	1A	0.30	0/2693	0.61	2/3672 (0.1%)
6	1a	0.31	0/2687	0.58	2/3665 (0.1%)
7	1B	0.27	0/4077	0.52	1/5551 (0.0%)
7	1b	0.26	0/4077	0.52	3/5551 (0.1%)
8	1C	0.24	0/3603	0.48	0/4910

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	1c	0.25	0/3615	0.50	0/4922
9	1D	0.30	1/2801 (0.0%)	0.59	2/3818 (0.1%)
9	1d	0.29	0/2809	0.58	2/3829 (0.1%)
10	1E	0.26	0/632	0.53	0/860
10	1e	0.23	0/632	0.52	0/860
11	1F	0.43	0/295	0.62	0/400
11	1f	0.22	0/248	0.46	0/335
12	1H	0.25	0/464	0.56	0/630
12	1h	0.26	0/464	0.62	0/630
13	1I	0.51	0/285	0.62	0/385
13	1i	0.26	0/285	0.60	0/385
14	1J	0.24	0/261	0.63	0/353
14	1j	0.30	0/261	0.71	1/353 (0.3%)
15	1K	0.27	0/317	0.57	0/433
15	1k	0.25	0/317	0.51	0/433
16	1L	0.26	0/312	0.51	0/424
16	1l	0.29	0/303	0.61	0/412
17	1M	0.34	0/251	0.89	0/344
17	1m	0.32	0/255	0.64	0/350
18	1O	0.25	0/1898	0.59	1/2567 (0.0%)
18	1o	0.24	0/1829	0.52	0/2470
19	1P	0.19	0/1452	0.48	0/1961
19	1p	0.19	0/1452	0.43	0/1961
20	1R	0.24	0/1890	0.55	0/2574
20	1r	0.22	0/1890	0.54	0/2574
21	1S	0.23	0/1706	0.55	0/2322
21	1s	0.25	0/1702	0.59	0/2313
22	1T	0.19	0/269	0.40	0/365
22	1t	0.17	0/260	0.37	0/354
23	1U	0.12	0/211	0.31	0/281
23	1u	0.21	0/211	0.63	1/281 (0.4%)
24	1V	0.22	0/731	0.50	0/991
24	1v	0.28	0/697	0.68	2/952 (0.2%)
25	1W	0.27	0/419	0.62	0/567
25	1w	0.23	0/339	0.57	0/462
26	1X	0.23	0/279	0.47	0/380
26	1x	0.23	0/275	0.48	0/375
27	1Y	0.29	0/275	0.57	0/376
27	1y	0.24	0/273	0.56	0/373
28	1Z	0.33	0/476	0.70	0/652
28	1z	0.23	0/476	0.51	0/652
All	All	0.27	7/87604 (0.0%)	0.58	63/119701 (0.1%)

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
1	02	0	1
1	05	0	1
1	06	0	1
1	1G	0	1
1	1N	0	4
1	1n	0	2
3	04	0	1
6	1a	0	1
7	1b	0	1
18	1o	0	1
All	All	0	14

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	06	170	PRO	CG-CD	-9.04	1.20	1.50
1	14	170	PRO	CG-CD	-7.22	1.26	1.50
1	17	170	PRO	CG-CD	-7.21	1.26	1.50
1	20	170	PRO	CG-CD	-7.20	1.26	1.50
1	11	170	PRO	CG-CD	-7.19	1.26	1.50

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	20	170	PRO	N-CD-CG	-14.12	82.01	103.20
1	17	170	PRO	N-CD-CG	-14.11	82.04	103.20
1	11	170	PRO	N-CD-CG	-14.10	82.05	103.20
1	14	170	PRO	N-CD-CG	-14.08	82.08	103.20
1	06	170	PRO	N-CD-CG	-10.77	87.04	103.20

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	02	156	TYR	Peptide
3	04	104	LEU	Peptide
1	05	95	ALA	Peptide
1	06	189	PHE	Peptide

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Mol	Chain	Res	Type	Group
1	1G	192	PHE	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	00	1659	0	1598	75	0
1	01	1637	0	1572	64	0
1	02	1576	0	1470	21	0
1	05	1555	0	1473	32	0
1	06	1450	0	1320	28	0
1	09	1659	0	1598	62	0
1	11	1099	0	619	2	0
1	14	1093	0	612	2	0
1	17	1093	0	612	3	0
1	1G	1658	0	1595	36	0
1	1N	1652	0	1589	46	0
1	1g	1655	0	1586	35	0
1	1n	1653	0	1591	41	0
1	20	1093	0	612	1	0
2	03	1685	0	1612	34	0
2	07	1648	0	1561	31	0
3	04	1532	0	1450	26	0
3	08	1570	0	1469	31	0
4	12	1112	0	618	0	0
4	15	1112	0	618	0	0
4	18	1112	0	618	0	0
4	21	1112	0	618	0	0
5	13	1094	0	618	0	0
5	16	1094	0	618	0	0
5	19	1094	0	618	0	0
5	22	1094	0	618	0	0
6	1A	2612	0	2522	88	0
6	1a	2606	0	2517	115	0
7	1B	3945	0	3810	110	0
7	1b	3945	0	3810	116	0
8	1C	3486	0	3396	100	0
8	1c	3498	0	3421	96	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	1D	2708	0	2598	87	0
9	1d	2716	0	2604	109	0
10	1E	614	0	592	19	0
10	1e	614	0	592	28	0
11	1F	286	0	293	21	0
11	1f	241	0	246	13	0
12	1H	454	0	473	11	0
12	1h	454	0	473	13	0
13	1I	277	0	289	27	0
13	1i	277	0	289	14	0
14	1J	255	0	265	8	0
14	1j	255	0	265	12	0
15	1K	305	0	311	11	0
15	1k	305	0	311	14	0
16	1L	304	0	292	12	0
16	1l	295	0	284	13	0
17	1M	247	0	272	10	0
17	1m	251	0	274	11	0
18	1O	1861	0	1847	43	0
18	1o	1795	0	1783	39	0
19	1P	1422	0	1384	15	0
19	1p	1422	0	1384	30	0
20	1R	1837	0	1786	46	0
20	1r	1837	0	1785	40	0
21	1S	1661	0	1613	44	0
21	1s	1658	0	1620	40	0
22	1T	261	0	280	10	0
22	1t	252	0	267	7	0
23	1U	208	0	221	3	0
23	1u	208	0	221	6	0
24	1V	715	0	721	18	0
24	1v	683	0	648	27	0
25	1W	413	0	401	14	0
25	1w	333	0	332	9	0
26	1X	276	0	303	8	0
26	1x	272	0	300	10	0
27	1Y	270	0	289	5	0
27	1y	268	0	290	4	0
28	1Z	466	0	494	15	0
28	1z	466	0	494	13	0
29	00	437	0	397	24	0
29	01	424	0	375	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	02	348	0	240	7	0
29	03	313	0	233	11	0
29	04	341	0	231	5	0
29	05	331	0	224	7	0
29	06	257	0	183	8	0
29	07	292	0	198	4	0
29	08	282	0	191	8	0
29	09	372	0	291	29	0
29	1A	106	0	94	3	0
29	1B	958	0	977	61	0
29	1C	751	0	736	38	0
29	1D	222	0	214	16	0
29	1G	380	0	304	13	0
29	1N	366	0	289	10	0
29	1R	422	0	319	20	0
29	1S	389	0	280	14	0
29	1a	162	0	141	6	0
29	1b	940	0	935	45	0
29	1c	751	0	731	45	0
29	1d	174	0	166	11	0
29	1g	414	0	354	17	0
29	1n	412	0	356	22	0
29	1r	425	0	329	16	0
29	1s	415	0	316	16	0
30	00	290	0	269	26	0
30	01	263	0	213	19	0
30	02	273	0	177	5	0
30	03	216	0	139	4	0
30	04	218	0	143	7	0
30	05	274	0	191	10	0
30	06	218	0	137	1	0
30	07	203	0	120	3	0
30	08	207	0	125	1	0
30	09	231	0	168	11	0
30	1G	302	0	244	13	0
30	1N	330	0	295	27	0
30	1R	170	0	104	4	0
30	1S	171	0	109	9	0
30	1g	305	0	236	12	0
30	1n	328	0	279	27	0
30	1r	185	0	124	4	0
30	1s	176	0	115	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	00	84	0	112	13	0
31	01	84	0	112	10	0
31	03	42	0	56	7	0
31	05	42	0	56	4	0
31	07	42	0	56	6	0
31	09	84	0	112	16	0
31	1G	84	0	112	12	0
31	1N	41	0	53	3	0
31	1R	42	0	56	5	0
31	1S	84	0	112	17	0
31	1g	84	0	112	9	0
31	1n	42	0	56	4	0
31	1r	42	0	56	6	0
31	1s	84	0	112	18	0
32	00	21	0	26	3	0
32	09	31	0	49	1	0
33	00	175	0	246	13	0
33	01	36	0	42	4	0
33	03	45	0	63	2	0
33	07	49	0	74	0	0
33	09	86	0	118	9	0
33	1B	38	0	46	2	0
33	1C	243	0	285	13	0
33	1D	147	0	181	5	0
33	1E	30	0	30	0	0
33	1F	42	0	58	2	0
33	1G	41	0	55	4	0
33	1I	71	0	88	5	0
33	1J	45	0	67	5	0
33	1K	43	0	60	1	0
33	1L	49	0	74	2	0
33	1N	131	0	178	14	0
33	1P	45	0	67	7	0
33	1R	75	0	93	4	0
33	1S	94	0	109	9	0
33	1V	49	0	74	2	0
33	1W	79	0	101	4	0
33	1a	73	0	86	13	0
33	1b	189	0	238	19	0
33	1c	70	0	86	7	0
33	1d	77	0	97	4	0
33	1e	42	0	57	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	1g	36	0	42	0	0
33	1j	41	0	52	2	0
33	1n	81	0	114	5	0
33	1r	29	0	29	1	0
33	1s	85	0	103	7	0
33	1t	39	0	56	3	0
33	1v	41	0	52	3	0
33	1w	114	0	147	9	0
34	00	61	0	83	7	0
34	1A	55	0	68	6	0
34	1B	172	0	221	11	0
34	1C	173	0	220	16	0
34	1S	46	0	50	3	0
34	1b	62	0	82	4	0
34	1c	156	0	186	8	0
35	04	40	0	56	6	0
35	1A	40	0	56	4	0
35	1B	160	0	224	22	0
35	1D	40	0	56	4	0
35	1H	40	0	56	2	0
35	1I	40	0	56	6	0
35	1J	40	0	56	4	0
35	1Z	80	0	112	9	0
35	1a	40	0	56	5	0
35	1b	160	0	224	23	0
35	1c	40	0	56	6	0
35	1d	40	0	56	1	0
35	1h	40	0	56	3	0
35	1i	40	0	56	7	0
35	1j	40	0	56	5	0
35	1k	40	0	56	4	0
36	1A	1	0	0	0	0
36	1a	1	0	0	0	0
37	1A	2	0	0	0	0
37	1a	1	0	0	1	0
37	1c	1	0	0	0	0
38	1A	128	0	148	7	0
38	1a	40	0	31	1	0
38	1d	64	0	74	6	0
39	1A	10	0	0	0	0
39	1a	10	0	0	0	0
40	1A	55	0	80	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	1D	55	0	80	6	0
40	1E	55	0	80	28	0
40	1R	55	0	80	7	0
40	1a	55	0	80	21	0
40	1d	55	0	80	7	0
40	1e	21	0	23	9	0
40	1r	55	0	80	4	0
41	1A	135	0	162	10	0
41	1B	189	0	243	17	0
41	1C	51	0	69	5	0
41	1D	89	0	106	7	0
41	1L	53	0	73	5	0
41	1S	46	0	56	5	0
41	1a	96	0	123	7	0
41	1b	102	0	138	13	0
41	1c	54	0	78	8	0
41	1d	87	0	105	6	0
41	1l	42	0	48	3	0
41	1m	42	0	48	6	0
41	1s	44	0	52	4	0
41	1w	40	0	44	3	0
42	1B	87	0	120	5	0
42	1C	45	0	63	4	0
42	1k	36	0	42	5	0
42	1s	41	0	52	2	0
43	1C	35	0	45	1	0
43	1c	17	0	22	4	0
44	1D	4	0	0	1	0
44	1d	4	0	0	0	0
45	1E	43	0	30	4	0
45	1f	43	0	30	6	0
46	1G	88	0	112	8	0
46	1R	44	0	56	8	0
46	1g	88	0	112	8	0
46	1r	44	0	56	3	0
47	1X	39	0	51	1	0
All	All	107869	0	99523	2414	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 2414 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)
1:09:190:SER:HA	29:09:317:CLA:HBB1	1.51	0.92
40:1a:412:PL9:H312	38:1d:404:PHO:H2	1.55	0.88
40:1E:102:PL9:H371	33:1P:201:LHG:H202	1.59	0.85
9:1D:130:GLN:NE2	9:1D:143:ASN:OD1	2.09	0.84
30:01:303:CHL:HBB2	30:01:304:CHL:HBB1	1.60	0.82

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	00	217/219 (99%)	193 (89%)	24 (11%)	0	100	100
1	01	217/219 (99%)	186 (86%)	27 (12%)	4 (2%)	6	25
1	02	208/219 (95%)	173 (83%)	31 (15%)	4 (2%)	6	23
1	05	206/219 (94%)	175 (85%)	29 (14%)	2 (1%)	12	39
1	06	203/219 (93%)	167 (82%)	33 (16%)	3 (2%)	8	28
1	09	217/219 (99%)	192 (88%)	24 (11%)	1 (0%)	24	54
1	11	216/219 (99%)	197 (91%)	19 (9%)	0	100	100
1	14	216/219 (99%)	196 (91%)	20 (9%)	0	100	100
1	17	216/219 (99%)	195 (90%)	17 (8%)	4 (2%)	6	23
1	1G	217/219 (99%)	199 (92%)	17 (8%)	1 (0%)	24	54
1	1N	217/219 (99%)	199 (92%)	17 (8%)	1 (0%)	24	54
1	1g	217/219 (99%)	197 (91%)	19 (9%)	1 (0%)	24	54
1	1n	217/219 (99%)	199 (92%)	17 (8%)	1 (0%)	24	54
1	20	216/219 (99%)	197 (91%)	19 (9%)	0	100	100
2	03	218/220 (99%)	186 (85%)	30 (14%)	2 (1%)	14	41
2	07	218/220 (99%)	188 (86%)	28 (13%)	2 (1%)	14	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	04	198/205 (97%)	152 (77%)	44 (22%)	2 (1%)	12	39
3	08	203/205 (99%)	170 (84%)	28 (14%)	5 (2%)	4	17
4	12	220/222 (99%)	202 (92%)	17 (8%)	1 (0%)	24	54
4	15	220/222 (99%)	202 (92%)	17 (8%)	1 (0%)	24	54
4	18	220/222 (99%)	202 (92%)	17 (8%)	1 (0%)	24	54
4	21	220/222 (99%)	202 (92%)	17 (8%)	1 (0%)	24	54
5	13	216/218 (99%)	206 (95%)	10 (5%)	0	100	100
5	16	216/218 (99%)	206 (95%)	10 (5%)	0	100	100
5	19	216/218 (99%)	206 (95%)	10 (5%)	0	100	100
5	22	216/218 (99%)	206 (95%)	10 (5%)	0	100	100
6	1A	332/334 (99%)	314 (95%)	18 (5%)	0	100	100
6	1a	331/334 (99%)	313 (95%)	18 (5%)	0	100	100
7	1B	501/503 (100%)	476 (95%)	24 (5%)	1 (0%)	43	72
7	1b	501/503 (100%)	486 (97%)	15 (3%)	0	100	100
8	1C	448/450 (100%)	428 (96%)	20 (4%)	0	100	100
8	1c	448/450 (100%)	428 (96%)	17 (4%)	3 (1%)	18	48
9	1D	338/341 (99%)	319 (94%)	17 (5%)	2 (1%)	21	51
9	1d	339/341 (99%)	316 (93%)	23 (7%)	0	100	100
10	1E	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
10	1e	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
11	1F	33/35 (94%)	33 (100%)	0	0	100	100
11	1f	28/35 (80%)	27 (96%)	1 (4%)	0	100	100
12	1H	58/60 (97%)	53 (91%)	5 (9%)	0	100	100
12	1h	58/60 (97%)	57 (98%)	1 (2%)	0	100	100
13	1I	32/34 (94%)	23 (72%)	8 (25%)	1 (3%)	3	14
13	1i	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
14	1J	33/35 (94%)	33 (100%)	0	0	100	100
14	1j	33/35 (94%)	33 (100%)	0	0	100	100
15	1K	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
15	1k	35/37 (95%)	34 (97%)	0	1 (3%)	3	15
16	1L	34/36 (94%)	33 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	1l	33/36 (92%)	33 (100%)	0	0	100	100
17	1M	30/33 (91%)	24 (80%)	5 (17%)	1 (3%)	3	13
17	1m	31/33 (94%)	31 (100%)	0	0	100	100
18	1O	245/248 (99%)	211 (86%)	34 (14%)	0	100	100
18	1o	233/248 (94%)	210 (90%)	23 (10%)	0	100	100
19	1P	184/186 (99%)	164 (89%)	19 (10%)	1 (0%)	24	54
19	1p	184/186 (99%)	170 (92%)	14 (8%)	0	100	100
20	1R	232/234 (99%)	209 (90%)	22 (10%)	1 (0%)	30	59
20	1r	232/234 (99%)	216 (93%)	16 (7%)	0	100	100
21	1S	216/218 (99%)	186 (86%)	28 (13%)	2 (1%)	14	41
21	1s	215/218 (99%)	188 (87%)	26 (12%)	1 (0%)	24	54
22	1T	30/32 (94%)	30 (100%)	0	0	100	100
22	1t	29/32 (91%)	29 (100%)	0	0	100	100
23	1U	25/27 (93%)	23 (92%)	2 (8%)	0	100	100
23	1u	25/27 (93%)	22 (88%)	3 (12%)	0	100	100
24	1V	96/105 (91%)	79 (82%)	16 (17%)	1 (1%)	12	39
24	1v	97/105 (92%)	81 (84%)	12 (12%)	4 (4%)	2	9
25	1W	52/54 (96%)	47 (90%)	5 (10%)	0	100	100
25	1w	42/54 (78%)	40 (95%)	2 (5%)	0	100	100
26	1X	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
26	1x	36/39 (92%)	34 (94%)	2 (6%)	0	100	100
27	1Y	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
27	1y	32/36 (89%)	32 (100%)	0	0	100	100
28	1Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
28	1z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
All	All	11864/12104 (98%)	10839 (91%)	969 (8%)	56 (0%)	26	54

5 of 56 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	01	98	PHE
3	08	13	PHE
1	17	215	ASP

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Mol	Chain	Res	Type
1	17	216	PRO
1	17	217	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	00	166/166 (100%)	161 (97%)	5 (3%)	36	70
1	01	162/166 (98%)	157 (97%)	5 (3%)	35	69
1	02	150/166 (90%)	149 (99%)	1 (1%)	76	92
1	05	150/166 (90%)	149 (99%)	1 (1%)	76	92
1	06	129/166 (78%)	128 (99%)	1 (1%)	73	90
1	09	166/166 (100%)	163 (98%)	3 (2%)	51	80
1	11	17/166 (10%)	16 (94%)	1 (6%)	18	48
1	14	16/166 (10%)	15 (94%)	1 (6%)	16	45
1	17	16/166 (10%)	15 (94%)	1 (6%)	16	45
1	1G	166/166 (100%)	164 (99%)	2 (1%)	63	86
1	1N	165/166 (99%)	165 (100%)	0	100	100
1	1g	165/166 (99%)	163 (99%)	2 (1%)	63	86
1	1n	165/166 (99%)	162 (98%)	3 (2%)	51	80
1	20	16/166 (10%)	15 (94%)	1 (6%)	16	45
2	03	166/172 (96%)	164 (99%)	2 (1%)	63	86
2	07	159/172 (92%)	156 (98%)	3 (2%)	50	79
3	04	147/157 (94%)	145 (99%)	2 (1%)	59	85
3	08	149/157 (95%)	146 (98%)	3 (2%)	48	78
4	12	16/171 (9%)	16 (100%)	0	100	100
4	15	16/171 (9%)	16 (100%)	0	100	100
4	18	16/171 (9%)	16 (100%)	0	100	100
4	21	16/171 (9%)	16 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	13	16/165 (10%)	16 (100%)	0	100	100
5	16	16/165 (10%)	16 (100%)	0	100	100
5	19	16/165 (10%)	16 (100%)	0	100	100
5	22	16/165 (10%)	16 (100%)	0	100	100
6	1A	270/270 (100%)	268 (99%)	2 (1%)	76	92
6	1a	270/270 (100%)	269 (100%)	1 (0%)	84	94
7	1B	402/402 (100%)	400 (100%)	2 (0%)	81	93
7	1b	402/402 (100%)	401 (100%)	1 (0%)	87	96
8	1C	346/350 (99%)	344 (99%)	2 (1%)	78	93
8	1c	349/350 (100%)	348 (100%)	1 (0%)	86	96
9	1D	274/275 (100%)	271 (99%)	3 (1%)	65	88
9	1d	275/275 (100%)	274 (100%)	1 (0%)	84	94
10	1E	68/68 (100%)	68 (100%)	0	100	100
10	1e	68/68 (100%)	68 (100%)	0	100	100
11	1F	30/30 (100%)	30 (100%)	0	100	100
11	1f	25/30 (83%)	25 (100%)	0	100	100
12	1H	49/49 (100%)	49 (100%)	0	100	100
12	1h	49/49 (100%)	48 (98%)	1 (2%)	48	78
13	1I	31/31 (100%)	28 (90%)	3 (10%)	8	25
13	1i	31/31 (100%)	31 (100%)	0	100	100
14	1J	26/26 (100%)	26 (100%)	0	100	100
14	1j	26/26 (100%)	26 (100%)	0	100	100
15	1K	32/32 (100%)	32 (100%)	0	100	100
15	1k	32/32 (100%)	32 (100%)	0	100	100
16	1L	34/34 (100%)	34 (100%)	0	100	100
16	1l	33/34 (97%)	33 (100%)	0	100	100
17	1M	27/29 (93%)	27 (100%)	0	100	100
17	1m	27/29 (93%)	27 (100%)	0	100	100
18	1O	202/204 (99%)	200 (99%)	2 (1%)	68	89
18	1o	196/204 (96%)	195 (100%)	1 (0%)	81	93
19	1P	149/149 (100%)	149 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	1p	149/149 (100%)	149 (100%)	0	100	100
20	1R	191/191 (100%)	188 (98%)	3 (2%)	55	83
20	1r	191/191 (100%)	189 (99%)	2 (1%)	68	89
21	1S	169/173 (98%)	165 (98%)	4 (2%)	43	75
21	1s	170/173 (98%)	169 (99%)	1 (1%)	78	93
22	1T	29/29 (100%)	28 (97%)	1 (3%)	32	66
22	1t	28/29 (97%)	28 (100%)	0	100	100
23	1U	23/23 (100%)	23 (100%)	0	100	100
23	1u	23/23 (100%)	23 (100%)	0	100	100
24	1V	70/77 (91%)	70 (100%)	0	100	100
24	1v	62/77 (80%)	60 (97%)	2 (3%)	34	68
25	1W	46/46 (100%)	45 (98%)	1 (2%)	45	77
25	1w	35/46 (76%)	35 (100%)	0	100	100
26	1X	32/32 (100%)	31 (97%)	1 (3%)	35	69
26	1x	32/32 (100%)	32 (100%)	0	100	100
27	1Y	28/30 (93%)	28 (100%)	0	100	100
27	1y	28/30 (93%)	27 (96%)	1 (4%)	31	65
28	1Z	54/54 (100%)	54 (100%)	0	100	100
28	1z	54/54 (100%)	52 (96%)	2 (4%)	30	64
All	All	7535/9534 (79%)	7460 (99%)	75 (1%)	65	89

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	1c	469	MET
27	1y	9	LEU
1	1g	135	MET
18	1o	8	THR
1	09	191	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
7	1b	182	ASN

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Mol	Chain	Res	Type
16	1l	34	ASN
7	1b	274	GLN
9	1d	302	GLN
18	1o	13	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 492 ligands modelled in this entry, 6 are monoatomic - leaving 486 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	$\# Z > 2$
29	CLA	02	610	-	47,52,73	2.58	20 (42%)	56,88,113	3.35	26 (46%)
29	CLA	1N	305	-	45,49,73	2.60	19 (42%)	54,84,113	3.42	30 (55%)
47	3PH	1X	101	-	38,38,47	0.70	1 (2%)	42,43,52	0.65	1 (2%)
46	XAT	1G	619	-	39,47,47	0.87	0	54,74,74	2.66	19 (35%)
29	CLA	1G	611	-	47,52,73	2.55	19 (40%)	56,88,113	3.40	24 (42%)
29	CLA	1c	509	-	69,73,73	2.14	19 (27%)	83,113,113	2.90	31 (37%)
46	XAT	1G	617	-	39,47,47	0.83	0	54,74,74	3.02	27 (50%)
40	PL9	1R	301	-	55,55,55	0.69	1 (1%)	68,69,69	0.76	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	1N	311	1	45,49,73	2.56	19 (42%)	54,84,113	3.42	28 (51%)
34	DGD	1b	627	-	63,63,67	0.85	2 (3%)	77,77,81	0.91	2 (2%)
29	CLA	1c	508	8	59,63,73	2.27	18 (30%)	71,101,113	2.92	27 (38%)
34	DGD	1C	517	-	59,59,67	0.87	2 (3%)	73,73,81	1.03	5 (6%)
29	CLA	1b	609	7	69,73,73	2.04	16 (23%)	83,113,113	2.67	28 (33%)
29	CLA	1B	615	-	45,49,73	2.62	19 (42%)	54,84,113	3.50	28 (51%)
33	LHG	1D	409	-	42,42,48	0.30	0	45,48,54	0.36	0
29	CLA	1N	314	1	56,60,73	2.39	20 (35%)	67,97,113	3.24	30 (44%)
29	CLA	1c	512	8	69,73,73	2.12	19 (27%)	83,113,113	2.88	27 (32%)
29	CLA	03	310	-	49,53,73	2.53	20 (40%)	59,89,113	3.19	27 (45%)
29	CLA	1r	303	-	49,53,73	2.52	19 (38%)	59,89,113	3.34	26 (44%)
29	CLA	1N	315	1	45,49,73	2.62	20 (44%)	54,84,113	3.45	29 (53%)
29	CLA	1r	302	20	45,49,73	2.62	19 (42%)	54,84,113	3.42	29 (53%)
29	CLA	01	311	-	50,54,73	2.51	20 (40%)	60,90,113	3.34	27 (45%)
29	CLA	1C	509	8	69,73,73	2.12	19 (27%)	83,113,113	2.89	30 (36%)
29	CLA	01	308	-	69,73,73	2.10	19 (27%)	83,113,113	2.93	31 (37%)
29	CLA	1d	407	9	59,63,73	2.28	20 (33%)	71,101,113	3.11	30 (42%)
30	CHL	07	306	-	44,49,74	2.35	16 (36%)	48,84,114	3.32	22 (45%)
29	CLA	1s	312	21	59,63,73	2.32	20 (33%)	71,101,113	3.03	31 (43%)
30	CHL	1g	601	1	62,66,74	2.00	14 (22%)	70,104,114	2.91	25 (35%)
29	CLA	1B	607	7	66,70,73	2.15	19 (28%)	79,109,113	3.00	32 (40%)
29	CLA	1b	604	-	69,73,73	2.07	19 (27%)	83,113,113	2.63	26 (31%)
33	LHG	1W	101	-	34,34,48	0.31	0	37,40,54	0.40	0
41	SQD	1d	411	-	38,39,54	0.47	1 (2%)	47,50,65	0.65	2 (4%)
29	CLA	1B	605	-	69,73,73	2.07	19 (27%)	83,113,113	2.77	29 (34%)
29	CLA	1B	611	7	60,64,73	2.27	18 (30%)	72,102,113	3.14	29 (40%)
38	PHO	1A	406	-	58,69,69	0.76	1 (1%)	56,99,99	1.07	4 (7%)
29	CLA	1b	605	7	46,50,73	2.48	18 (39%)	55,85,113	3.43	28 (50%)
29	CLA	1b	613	-	62,66,73	2.16	19 (30%)	74,104,113	2.98	33 (44%)
29	CLA	08	307	-	43,48,73	2.64	20 (46%)	51,83,113	3.45	27 (52%)
33	LHG	1R	317	29	37,37,48	0.29	0	40,43,54	0.45	0
30	CHL	06	605	-	48,53,74	2.28	16 (33%)	53,89,114	3.15	20 (37%)
30	CHL	1G	608	-	47,51,74	2.20	16 (34%)	52,86,114	3.34	21 (40%)
29	CLA	1B	614	7	49,53,73	2.57	19 (38%)	59,89,113	3.60	27 (45%)
29	CLA	08	311	-	43,48,73	2.69	19 (44%)	51,83,113	3.51	28 (54%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LHG	1D	408	-	30,30,48	0.35	0	33,36,54	0.39	0
33	LHG	1N	317	29	42,42,48	0.29	0	45,48,54	0.36	0
30	CHL	05	307	1	46,50,74	2.32	15 (32%)	51,85,114	3.26	24 (47%)
29	CLA	1b	608	-	63,67,73	2.17	19 (30%)	75,105,113	2.92	31 (41%)
30	CHL	02	607	-	50,54,74	2.25	17 (34%)	56,90,114	3.12	22 (39%)
29	CLA	1b	610	7	65,69,73	2.12	18 (27%)	78,108,113	2.99	30 (38%)
29	CLA	1a	406	-	54,58,73	2.41	19 (35%)	65,95,113	3.26	31 (47%)
30	CHL	1n	608	-	50,54,74	2.24	19 (38%)	56,90,114	3.18	23 (41%)
33	LHG	1g	618	29	35,35,48	0.32	0	38,41,54	0.45	0
29	CLA	1d	403	-	63,67,73	2.23	19 (30%)	75,105,113	3.13	30 (40%)
29	CLA	1A	407	6	49,53,73	2.44	19 (38%)	59,89,113	3.34	28 (47%)
30	CHL	00	308	1	70,74,74	1.89	18 (25%)	80,114,114	2.67	24 (30%)
29	CLA	1C	507	8	62,66,73	2.19	19 (30%)	74,104,113	2.95	28 (37%)
29	CLA	1S	312	-	45,49,73	2.62	19 (42%)	54,84,113	3.53	28 (51%)
33	LHG	1I	103	-	38,38,48	0.30	0	41,44,54	0.38	0
29	CLA	1S	316	-	50,54,73	2.49	20 (40%)	60,90,113	3.27	27 (45%)
30	CHL	1n	606	-	51,55,74	2.15	17 (33%)	57,91,114	2.89	21 (36%)
29	CLA	1C	503	8	60,64,73	2.24	20 (33%)	72,102,113	3.12	30 (41%)
29	CLA	1c	514	-	65,69,73	2.12	18 (27%)	78,108,113	3.02	30 (38%)
33	LHG	00	317	-	48,48,48	0.27	0	51,54,54	0.63	1 (1%)
31	LUT	00	313	-	42,43,43	1.65	8 (19%)	51,60,60	1.56	12 (23%)
30	CHL	06	601	-	50,54,74	2.27	15 (30%)	56,90,114	3.16	21 (37%)
29	CLA	00	309	1	64,68,73	2.19	19 (29%)	77,107,113	2.90	30 (38%)
32	VIV	09	315	-	32,32,32	0.48	1 (3%)	41,45,45	0.84	2 (4%)
33	LHG	1F	101	-	41,41,48	0.31	0	44,46,54	0.39	0
41	SQD	1B	620	-	44,45,54	0.43	1 (2%)	53,56,65	0.55	1 (1%)
40	PL9	1A	410	-	55,55,55	0.69	1 (1%)	68,69,69	0.72	1 (1%)
29	CLA	01	309	-	50,54,73	2.48	20 (40%)	60,90,113	3.19	27 (45%)
33	LHG	1C	519	-	28,28,48	0.37	0	31,34,54	0.45	0
33	LHG	1S	303	-	28,28,48	0.31	0	30,30,54	0.70	1 (3%)
29	CLA	06	602	1	59,63,73	2.35	22 (37%)	71,101,113	3.15	31 (43%)
29	CLA	1s	316	21	50,54,73	2.50	19 (38%)	60,90,113	3.30	27 (45%)
43	LNL	1c	501	-	16,16,19	0.61	0	15,16,19	0.63	0
34	DGD	1B	626	-	49,49,67	1.00	2 (4%)	63,63,81	1.26	7 (11%)
35	BCR	1B	618	-	41,41,41	1.71	8 (19%)	56,56,56	1.76	14 (25%)
33	LHG	1W	102	-	43,43,48	0.31	0	46,49,54	0.73	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CHL	06	604	-	44,49,74	2.36	16 (36%)	48,84,114	3.32	22 (45%)
30	CHL	05	306	-	44,49,74	2.36	18 (40%)	48,84,114	3.35	22 (45%)
30	CHL	07	311	2	44,49,74	2.32	17 (38%)	48,84,114	3.23	21 (43%)
33	LHG	1b	626	-	31,31,48	0.32	0	34,37,54	0.39	0
29	CLA	02	602	-	47,52,73	2.54	20 (42%)	56,88,113	3.35	26 (46%)
29	CLA	02	612	1	47,52,73	2.54	19 (40%)	56,88,113	3.54	26 (46%)
35	BCR	1i	101	-	41,41,41	1.71	8 (19%)	56,56,56	1.61	11 (19%)
30	CHL	08	305	-	44,47,74	2.11	14 (31%)	48,80,114	3.29	21 (43%)
29	CLA	01	307	1	60,64,73	2.26	19 (31%)	72,102,113	2.97	31 (43%)
29	CLA	1G	612	1	59,63,73	2.25	20 (33%)	71,101,113	3.04	30 (42%)
29	CLA	03	309	-	47,52,73	2.57	20 (42%)	56,88,113	3.38	26 (46%)
29	CLA	09	301	1	59,63,73	2.30	19 (32%)	71,101,113	3.09	29 (40%)
30	CHL	09	304	1	44,49,74	2.32	16 (36%)	48,84,114	3.34	22 (45%)
33	LHG	1D	410	-	31,31,48	0.33	0	34,37,54	0.47	0
30	CHL	1r	305	-	50,54,74	2.24	17 (34%)	56,90,114	3.11	23 (41%)
29	CLA	1A	404	6	65,69,73	2.13	19 (29%)	78,108,113	3.03	27 (34%)
35	BCR	04	313	-	41,41,41	1.72	8 (19%)	56,56,56	1.67	12 (21%)
41	SQD	1C	521	-	50,51,54	0.40	1 (2%)	59,62,65	0.43	1 (1%)
29	CLA	1b	617	-	49,53,73	2.49	19 (38%)	59,89,113	3.30	26 (44%)
30	CHL	1S	304	21	50,54,74	2.25	16 (32%)	56,90,114	3.21	23 (41%)
46	XAT	1r	316	-	39,47,47	0.89	0	54,74,74	3.46	24 (44%)
29	CLA	00	301	1	65,69,73	2.17	19 (29%)	78,108,113	2.95	30 (38%)
33	LHG	09	316	29	36,36,48	0.32	0	39,42,54	0.37	0
33	LHG	00	321	-	43,43,48	0.30	0	46,49,54	0.37	0
41	SQD	1S	302	-	45,46,54	0.44	1 (2%)	54,57,65	0.40	0
29	CLA	1B	608	-	69,73,73	2.12	18 (26%)	83,113,113	2.89	28 (33%)
42	MGE	1s	320	-	41,41,48	0.25	0	49,49,56	0.79	1 (2%)
29	CLA	1S	311	33	45,49,73	2.59	20 (44%)	54,84,113	3.44	26 (48%)
33	LHG	1w	103	-	41,41,48	0.30	0	44,47,54	0.34	0
29	CLA	08	310	3	41,46,73	2.64	19 (46%)	51,80,113	3.54	27 (52%)
29	CLA	1R	307	-	43,48,73	2.65	19 (44%)	51,83,113	3.52	28 (54%)
33	LHG	1N	318	-	47,47,48	0.28	0	50,53,54	0.43	1 (2%)
30	CHL	00	304	1	48,53,74	2.26	17 (35%)	53,89,114	3.20	21 (39%)
33	LHG	1t	101	-	35,38,48	0.26	0	36,41,54	0.34	0
29	CLA	01	301	-	58,62,73	2.35	20 (34%)	69,99,113	3.13	30 (43%)
38	PHO	1A	405	-	58,69,69	0.80	3 (5%)	56,99,99	1.07	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	02	613	-	50,54,73	2.49	19 (38%)	60,90,113	3.32	28 (46%)
30	CHL	09	305	-	47,51,74	2.19	17 (36%)	52,86,114	3.17	25 (48%)
41	SQD	1D	411	-	45,46,54	0.44	0	54,57,65	1.05	6 (11%)
40	PL9	1r	301	-	55,55,55	0.66	1 (1%)	68,69,69	0.86	4 (5%)
29	CLA	1B	612	7	69,73,73	2.09	19 (27%)	83,113,113	2.84	30 (36%)
45	HEM	1f	101	11	50,50,50	1.57	7 (14%)	66,82,82	1.64	11 (16%)
29	CLA	1S	310	21	45,49,73	2.66	19 (42%)	54,84,113	3.40	29 (53%)
29	CLA	03	308	2	43,48,73	2.60	18 (41%)	52,82,113	3.51	30 (57%)
29	CLA	1B	616	7	63,67,73	2.17	19 (30%)	75,105,113	3.11	33 (44%)
33	LHG	1N	301	-	39,39,48	0.29	0	42,45,54	0.36	0
30	CHL	1n	607	-	70,74,74	1.89	19 (27%)	80,114,114	2.74	24 (30%)
29	CLA	1C	513	8	45,49,73	2.59	19 (42%)	54,84,113	3.53	27 (50%)
30	CHL	08	301	-	44,49,74	2.37	16 (36%)	48,84,114	3.23	23 (47%)
31	LUT	1N	316	-	41,42,43	1.62	8 (19%)	48,57,60	1.63	12 (25%)
41	SQD	1D	412	-	42,43,54	0.43	1 (2%)	51,54,65	0.66	2 (3%)
30	CHL	1s	308	-	50,54,74	2.22	18 (36%)	56,90,114	3.15	22 (39%)
33	LHG	1c	521	-	41,41,48	0.29	0	44,47,54	0.39	0
29	CLA	1c	505	8	69,73,73	2.07	20 (28%)	83,113,113	2.91	31 (37%)
30	CHL	1g	609	1	65,69,74	1.97	18 (27%)	74,108,114	2.76	26 (35%)
30	CHL	1r	307	-	50,54,74	2.23	17 (34%)	56,90,114	3.17	20 (35%)
35	BCR	1Z	102	-	41,41,41	1.68	8 (19%)	56,56,56	1.83	17 (30%)
41	SQD	1l	101	-	41,42,54	0.44	1 (2%)	50,53,65	0.76	2 (4%)
44	BCT	1d	408	36	2,3,3	0.98	0	2,3,3	0.37	0
31	LUT	1s	317	-	42,43,43	1.69	8 (19%)	51,60,60	1.81	14 (27%)
30	CHL	03	303	-	48,53,74	2.26	15 (31%)	53,89,114	3.06	20 (37%)
29	CLA	01	312	-	50,54,73	2.52	20 (40%)	60,90,113	3.27	27 (45%)
30	CHL	04	301	-	50,54,74	2.24	18 (36%)	56,90,114	3.09	25 (44%)
30	CHL	03	302	2	44,48,74	2.26	16 (36%)	46,82,114	3.39	20 (43%)
30	CHL	09	307	-	47,51,74	2.21	16 (34%)	52,86,114	3.28	23 (44%)
33	LHG	1a	401	-	31,31,48	0.34	0	34,37,54	0.48	0
29	CLA	03	301	2	64,68,73	2.22	19 (29%)	77,107,113	3.01	30 (38%)
29	CLA	04	310	-	47,52,73	2.59	20 (42%)	56,88,113	3.41	26 (46%)
29	CLA	02	611	-	47,52,73	2.56	20 (42%)	56,88,113	3.33	26 (46%)
29	CLA	06	610	-	44,49,73	2.58	19 (43%)	52,84,113	3.45	26 (50%)
29	CLA	01	310	1	69,73,73	2.13	20 (28%)	83,113,113	2.90	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	1b	607	7	54,58,73	2.40	19 (35%)	65,95,113	3.24	31 (47%)
29	CLA	1n	602	1	60,64,73	2.27	19 (31%)	72,102,113	3.02	31 (43%)
38	PHO	1d	404	-	58,69,69	0.82	2 (3%)	56,99,99	1.07	5 (8%)
35	BCR	1A	409	-	41,41,41	1.71	8 (19%)	56,56,56	1.71	12 (21%)
31	LUT	1S	318	-	42,43,43	1.63	8 (19%)	51,60,60	1.65	14 (27%)
29	CLA	03	312	-	47,52,73	2.55	20 (42%)	56,88,113	3.34	26 (46%)
31	LUT	01	315	-	42,43,43	1.62	8 (19%)	51,60,60	2.11	18 (35%)
29	CLA	05	310	1	44,49,73	2.56	19 (43%)	52,84,113	3.46	26 (50%)
29	CLA	1N	313	-	44,49,73	2.57	18 (40%)	52,84,113	3.48	27 (51%)
41	SQD	1d	405	-	47,48,54	0.42	1 (2%)	56,59,65	0.65	2 (3%)
35	BCR	1b	619	-	41,41,41	1.68	8 (19%)	56,56,56	1.73	15 (26%)
29	CLA	1R	309	20	47,52,73	2.66	24 (51%)	56,88,113	3.72	28 (50%)
35	BCR	1B	630	-	41,41,41	1.68	10 (24%)	56,56,56	1.83	15 (26%)
30	CHL	04	303	-	50,54,74	2.23	20 (40%)	56,90,114	3.16	22 (39%)
33	LHG	1c	522	-	27,27,48	0.46	0	31,32,54	0.64	1 (3%)
42	MGE	1C	524	-	45,45,48	0.24	0	53,53,56	0.52	0
29	CLA	1R	310	-	52,57,73	2.45	20 (38%)	62,94,113	3.22	29 (46%)
30	CHL	1N	309	-	49,53,74	2.15	16 (32%)	53,88,114	3.29	23 (43%)
30	CHL	00	305	-	51,55,74	2.16	17 (33%)	57,91,114	3.08	23 (40%)
29	CLA	1c	506	-	59,63,73	2.25	20 (33%)	71,101,113	3.00	29 (40%)
29	CLA	1n	612	-	49,53,73	2.50	20 (40%)	59,89,113	3.34	28 (47%)
29	CLA	1G	602	1	69,73,73	2.10	19 (27%)	83,113,113	2.83	30 (36%)
35	BCR	1D	406	-	41,41,41	1.75	8 (19%)	56,56,56	1.78	14 (25%)
42	MGE	1B	624	-	43,43,48	0.33	0	51,51,56	0.53	0
33	LHG	1v	201	-	40,40,48	0.29	0	43,46,54	0.39	0
29	CLA	1g	604	-	54,58,73	2.37	18 (33%)	65,95,113	3.10	30 (46%)
33	LHG	1E	101	-	29,29,48	0.32	0	32,35,54	0.40	0
30	CHL	07	303	2	44,49,74	2.33	17 (38%)	48,84,114	3.34	21 (43%)
46	XAT	1R	316	-	39,47,47	0.96	0	54,74,74	3.50	28 (51%)
30	CHL	1s	304	21	50,54,74	2.24	18 (36%)	56,90,114	3.13	22 (39%)
30	CHL	1n	609	1	65,69,74	1.95	18 (27%)	74,108,114	2.84	25 (33%)
29	CLA	03	307	-	44,49,73	2.55	19 (43%)	52,84,113	3.46	26 (50%)
40	PL9	1a	412	-	55,55,55	0.58	1 (1%)	68,69,69	1.85	20 (29%)
30	CHL	07	304	2	44,49,74	2.36	16 (36%)	48,84,114	3.32	22 (45%)
29	CLA	06	609	-	44,49,73	2.56	19 (43%)	52,84,113	3.47	26 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	1s	311	-	46,50,73	2.52	18 (39%)	55,85,113	3.43	27 (49%)
29	CLA	1C	501	8	69,73,73	2.15	20 (28%)	83,113,113	2.85	29 (34%)
29	CLA	07	301	-	43,48,73	2.62	20 (46%)	51,83,113	3.46	28 (54%)
29	CLA	05	311	-	43,48,73	2.62	19 (44%)	51,83,113	3.59	30 (58%)
31	LUT	09	314	-	42,43,43	1.65	8 (19%)	51,60,60	1.62	12 (23%)
34	DGD	1B	625	-	63,63,67	0.86	2 (3%)	77,77,81	0.88	2 (2%)
29	CLA	1s	314	-	47,52,73	2.55	19 (40%)	56,88,113	3.37	26 (46%)
29	CLA	1c	504	-	64,68,73	2.12	18 (28%)	77,107,113	2.97	30 (38%)
30	CHL	03	305	-	50,54,74	2.23	18 (36%)	56,90,114	3.14	21 (37%)
29	CLA	08	309	3	43,48,73	2.74	19 (44%)	51,83,113	3.49	28 (54%)
33	LHG	1D	413	-	40,40,48	0.30	0	43,45,54	0.36	0
34	DGD	1B	627	-	63,63,67	0.89	3 (4%)	77,77,81	1.08	6 (7%)
29	CLA	1D	404	9	69,73,73	2.01	19 (27%)	83,113,113	2.76	30 (36%)
30	CHL	1G	606	-	50,54,74	2.23	18 (36%)	56,90,114	3.17	23 (41%)
33	LHG	1b	623	-	26,26,48	0.38	0	29,31,54	0.92	2 (6%)
35	BCR	1B	617	-	41,41,41	1.69	9 (21%)	56,56,56	1.78	13 (23%)
29	CLA	1S	305	21	45,49,73	2.58	19 (42%)	54,84,113	3.46	29 (53%)
29	CLA	1s	306	21	50,54,73	2.58	20 (40%)	60,90,113	3.36	28 (46%)
33	LHG	1L	101	-	48,48,48	0.28	0	51,54,54	0.39	0
33	LHG	1C	523	-	38,38,48	0.31	0	41,44,54	0.38	0
30	CHL	05	304	-	48,53,74	2.21	15 (31%)	53,89,114	2.77	19 (35%)
30	CHL	01	304	-	67,71,74	1.93	17 (25%)	76,110,114	2.82	25 (32%)
30	CHL	02	601	-	50,54,74	2.24	16 (32%)	56,90,114	3.13	21 (37%)
30	CHL	07	305	-	42,47,74	2.30	16 (38%)	48,81,114	3.34	21 (43%)
41	SQD	1B	629	-	39,40,54	0.44	1 (2%)	48,51,65	0.39	0
29	CLA	1a	405	6	56,60,73	2.29	19 (33%)	67,97,113	3.14	31 (46%)
30	CHL	1N	310	1	70,74,74	1.90	19 (27%)	80,114,114	2.68	24 (30%)
30	CHL	1g	607	-	51,55,74	2.21	19 (37%)	57,91,114	3.05	22 (38%)
29	CLA	1g	603	-	50,54,73	2.45	18 (36%)	60,90,113	3.28	29 (48%)
29	CLA	1r	311	-	49,53,73	2.53	19 (38%)	59,89,113	3.33	26 (44%)
29	CLA	1b	603	7	60,64,73	2.19	16 (26%)	72,102,113	3.06	30 (41%)
29	CLA	04	306	3	47,52,73	2.57	20 (42%)	56,88,113	3.29	26 (46%)
30	CHL	1S	308	-	46,50,74	2.31	18 (39%)	51,85,114	3.33	24 (47%)
29	CLA	1C	511	-	50,54,73	2.42	19 (38%)	60,90,113	3.38	28 (46%)
30	CHL	1R	313	20	48,53,74	2.27	17 (35%)	53,89,114	3.14	22 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LHG	1b	625	-	44,44,48	0.29	0	47,50,54	0.33	0
30	CHL	05	313	1	44,49,74	2.34	15 (34%)	48,84,114	3.32	21 (43%)
29	CLA	06	608	-	43,48,73	2.66	20 (46%)	51,83,113	3.48	27 (52%)
30	CHL	02	604	-	48,53,74	2.28	15 (31%)	53,89,114	3.16	20 (37%)
31	LUT	1s	318	-	42,43,43	1.79	8 (19%)	51,60,60	1.99	17 (33%)
30	CHL	08	303	-	48,53,74	2.23	18 (37%)	53,89,114	3.13	20 (37%)
31	LUT	01	314	-	42,43,43	1.66	8 (19%)	51,60,60	1.98	15 (29%)
29	CLA	00	310	33	55,59,73	2.38	19 (34%)	66,96,113	3.21	30 (45%)
30	CHL	03	311	-	46,50,74	2.34	19 (41%)	51,85,114	3.33	24 (47%)
29	CLA	04	309	3	47,52,73	2.58	20 (42%)	56,88,113	3.37	29 (51%)
30	CHL	08	302	-	44,49,74	2.36	18 (40%)	48,84,114	3.36	22 (45%)
29	CLA	09	302	-	60,64,73	2.25	18 (30%)	72,102,113	3.14	31 (43%)
33	LHG	1s	319	-	26,26,48	0.33	0	28,28,54	0.48	0
30	CHL	08	304	3	44,49,74	2.35	17 (38%)	48,84,114	3.34	22 (45%)
29	CLA	1c	510	8	63,67,73	2.11	17 (26%)	75,105,113	2.94	31 (41%)
30	CHL	01	306	1	66,70,74	1.97	19 (28%)	75,109,114	2.75	24 (32%)
29	CLA	1B	604	7	60,64,73	2.25	18 (30%)	72,102,113	3.05	31 (43%)
35	BCR	1J	101	-	41,41,41	1.72	8 (19%)	56,56,56	1.96	15 (26%)
29	CLA	1G	614	33	46,50,73	2.51	19 (41%)	55,85,113	3.41	29 (52%)
29	CLA	1c	513	8	49,53,73	2.49	20 (40%)	59,89,113	3.40	28 (47%)
29	CLA	06	611	-	43,48,73	2.66	20 (46%)	51,83,113	3.53	26 (50%)
35	BCR	1h	101	-	41,41,41	1.79	10 (24%)	56,56,56	2.06	18 (32%)
30	CHL	1G	601	-	70,74,74	1.87	17 (24%)	80,114,114	2.70	25 (31%)
31	LUT	1G	615	-	42,43,43	1.71	8 (19%)	51,60,60	1.59	11 (21%)
33	LHG	03	314	-	44,44,48	0.29	0	47,50,54	0.37	0
29	CLA	09	312	1	47,52,73	2.55	20 (42%)	56,88,113	3.32	26 (46%)
30	CHL	04	302	-	44,49,74	2.30	17 (38%)	49,83,114	3.38	25 (51%)
29	CLA	1n	610	1	62,66,73	2.28	18 (29%)	74,104,113	3.05	34 (45%)
29	CLA	1n	611	33	61,65,73	2.26	20 (32%)	73,103,113	3.08	31 (42%)
29	CLA	1B	613	-	62,66,73	2.20	19 (30%)	74,104,113	3.20	30 (40%)
29	CLA	1G	610	1	47,52,73	2.55	18 (38%)	56,88,113	3.34	25 (44%)
33	LHG	1n	617	-	36,37,48	0.28	0	38,39,54	1.47	4 (10%)
29	CLA	1S	315	21	47,52,73	2.69	21 (44%)	56,88,113	3.39	24 (42%)
33	LHG	1b	624	-	35,35,48	0.31	0	38,41,54	0.53	0
46	XAT	1g	619	-	39,47,47	0.98	1 (2%)	54,74,74	3.92	31 (57%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	DGD	1c	520	-	58,58,67	0.89	2 (3%)	72,72,81	0.90	3 (4%)
31	LUT	1n	615	-	42,43,43	1.71	8 (19%)	51,60,60	1.71	11 (21%)
34	DGD	00	320	-	62,62,67	0.90	2 (3%)	76,76,81	0.89	2 (2%)
29	CLA	04	311	-	47,52,73	2.57	20 (42%)	56,88,113	3.36	26 (46%)
29	CLA	1r	310	33	46,50,73	2.52	19 (41%)	55,85,113	3.41	26 (47%)
29	CLA	1C	502	8	65,69,73	2.11	18 (27%)	78,108,113	2.92	29 (37%)
29	CLA	1b	612	7	69,73,73	2.01	17 (24%)	83,113,113	2.70	29 (34%)
33	LHG	1V	201	-	48,48,48	0.27	0	51,54,54	0.34	0
34	DGD	1A	414	-	56,56,67	0.90	2 (3%)	70,70,81	0.95	3 (4%)
41	SQD	1c	517	-	53,54,54	0.39	1 (1%)	62,65,65	0.89	4 (6%)
30	CHL	05	305	-	67,71,74	1.93	18 (26%)	76,110,114	2.80	27 (35%)
30	CHL	02	603	-	50,54,74	2.25	16 (32%)	56,90,114	3.17	22 (39%)
30	CHL	01	305	-	50,54,74	2.21	19 (38%)	56,90,114	3.04	20 (35%)
41	SQD	1L	102	-	52,53,54	0.39	1 (1%)	61,64,65	0.63	1 (1%)
41	SQD	1a	411	-	45,46,54	0.41	1 (2%)	54,57,65	0.52	1 (1%)
29	CLA	1g	611	33	46,50,73	2.47	18 (39%)	55,85,113	3.34	27 (49%)
33	LHG	1d	402	-	37,37,48	0.33	0	40,43,54	0.38	0
33	LHG	1e	102	-	41,41,48	0.29	0	44,47,54	0.39	0
29	CLA	1B	603	7	69,73,73	2.07	18 (26%)	83,113,113	2.91	30 (36%)
29	CLA	1b	611	-	69,73,73	2.13	20 (28%)	83,113,113	2.93	29 (34%)
35	BCR	1Z	101	-	41,41,41	1.70	8 (19%)	56,56,56	1.69	12 (21%)
29	CLA	1C	505	8	64,68,73	2.17	19 (29%)	77,107,113	2.97	30 (38%)
29	CLA	1b	615	7	69,73,73	2.13	20 (28%)	83,113,113	2.83	30 (36%)
29	CLA	08	308	3	44,49,73	2.57	18 (40%)	52,84,113	3.38	26 (50%)
31	LUT	1G	616	-	42,43,43	1.67	8 (19%)	51,60,60	1.98	12 (23%)
33	LHG	1C	525	-	39,39,48	0.31	0	42,44,54	0.73	1 (2%)
33	LHG	1C	527	-	36,36,48	0.34	0	39,42,54	0.53	1 (2%)
41	SQD	1m	101	-	41,42,54	0.44	1 (2%)	50,53,65	0.46	0
41	SQD	1a	410	-	49,50,54	0.40	1 (2%)	58,61,65	0.93	3 (5%)
29	CLA	1S	306	-	43,48,73	2.62	20 (46%)	51,83,113	3.47	27 (52%)
30	CHL	1S	309	-	46,50,74	2.34	17 (36%)	51,85,114	3.32	23 (45%)
29	CLA	01	313	-	50,54,73	2.52	20 (40%)	60,90,113	3.32	28 (46%)
30	CHL	06	603	-	42,48,74	2.32	14 (33%)	46,82,114	3.39	23 (50%)
35	BCR	1c	516	-	41,41,41	1.71	8 (19%)	56,56,56	1.68	16 (28%)
29	CLA	00	311	-	49,53,73	2.47	18 (36%)	59,89,113	3.43	27 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CHL	1R	304	-	45,50,74	2.23	16 (35%)	49,85,114	3.33	22 (44%)
39	OEX	1A	408	6,8	0,14,14	-	-	-		
30	CHL	1G	605	1	44,49,74	2.35	16 (36%)	48,84,114	3.33	22 (45%)
29	CLA	04	312	-	43,48,73	2.65	20 (46%)	51,83,113	3.53	27 (52%)
35	BCR	1b	620	-	41,41,41	1.65	8 (19%)	56,56,56	1.81	16 (28%)
29	CLA	1R	311	-	47,52,73	2.55	19 (40%)	56,88,113	3.38	26 (46%)
33	LHG	1j	102	-	40,40,48	0.29	0	43,46,54	0.78	1 (2%)
30	CHL	1S	307	-	44,49,74	2.37	18 (40%)	48,84,114	3.32	21 (43%)
30	CHL	01	303	-	50,54,74	2.24	18 (36%)	56,90,114	3.13	23 (41%)
29	CLA	00	318	1	64,68,73	2.17	19 (29%)	77,107,113	2.94	29 (37%)
29	CLA	06	607	1	43,48,73	2.67	20 (46%)	51,83,113	3.47	28 (54%)
29	CLA	07	310	-	41,47,73	2.63	19 (46%)	49,81,113	3.57	27 (55%)
35	BCR	1b	601	-	41,41,41	1.87	9 (21%)	56,56,56	2.15	19 (33%)
32	VIV	00	315	-	22,22,32	0.48	0	29,33,45	1.13	2 (6%)
33	LHG	00	319	-	48,48,48	0.27	0	51,54,54	0.40	0
29	CLA	1g	610	1	60,64,73	2.26	18 (30%)	72,102,113	3.00	30 (41%)
30	CHL	1n	601	-	66,70,74	1.94	17 (25%)	75,109,114	2.83	28 (37%)
29	CLA	1s	305	21	49,53,73	2.48	19 (38%)	59,89,113	3.30	26 (44%)
29	CLA	1S	313	21	57,62,73	2.27	18 (31%)	68,100,113	3.11	30 (44%)
33	LHG	1C	520	-	30,31,48	0.34	0	33,37,54	0.41	0
29	CLA	1r	304	-	50,54,73	2.46	19 (38%)	60,90,113	3.25	29 (48%)
31	LUT	1S	317	-	42,43,43	1.62	8 (19%)	51,60,60	1.62	13 (25%)
29	CLA	1D	401	-	69,73,73	2.11	18 (26%)	83,113,113	2.98	32 (38%)
30	CHL	1r	306	-	50,54,74	2.23	18 (36%)	56,90,114	3.18	24 (42%)
29	CLA	04	308	-	43,48,73	2.66	20 (46%)	51,83,113	3.52	28 (54%)
30	CHL	1g	606	-	54,58,74	2.14	17 (31%)	59,94,114	2.99	23 (38%)
29	CLA	00	312	1	49,53,73	2.48	18 (36%)	59,89,113	3.35	28 (47%)
33	LHG	1w	104	-	36,36,48	0.46	0	38,41,54	0.37	0
29	CLA	1n	614	1	45,49,73	2.63	20 (44%)	54,84,113	3.41	28 (51%)
39	OEX	1a	402	6,8	0,14,14	-	-	-		
33	LHG	1G	618	29	40,40,48	0.29	0	43,46,54	0.37	0
41	SQD	1b	622	-	47,48,54	0.42	1 (2%)	56,59,65	0.58	2 (3%)
29	CLA	1s	315	21	59,63,73	2.25	19 (32%)	71,101,113	3.05	32 (45%)
40	PL9	1e	101	-	21,21,55	0.86	1 (4%)	27,28,69	1.83	7 (25%)
30	CHL	03	304	-	47,51,74	2.21	18 (38%)	52,86,114	3.28	23 (44%)
29	CLA	05	309	-	43,48,73	2.62	20 (46%)	51,83,113	3.53	25 (49%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	1b	616	-	65,69,73	2.16	18 (27%)	78,108,113	3.02	29 (37%)
29	CLA	02	614	-	47,52,73	2.57	20 (42%)	56,88,113	3.34	26 (46%)
30	CHL	1G	609	1	46,50,74	2.33	17 (36%)	51,85,114	3.33	24 (47%)
29	CLA	1s	313	-	45,49,73	2.61	20 (44%)	54,84,113	3.43	29 (53%)
34	DGD	1c	519	-	53,53,67	0.92	2 (3%)	67,67,81	1.05	5 (7%)
29	CLA	1b	606	7	62,66,73	2.20	18 (29%)	74,104,113	3.20	32 (43%)
29	CLA	00	303	-	54,58,73	2.36	19 (35%)	65,95,113	3.10	31 (47%)
33	LHG	1d	401	-	38,38,48	0.30	0	41,44,54	0.42	0
30	CHL	1R	305	-	44,49,74	2.36	16 (36%)	48,84,114	3.37	21 (43%)
33	LHG	1B	621	-	37,37,48	0.30	0	40,43,54	0.37	0
29	CLA	08	312	-	46,50,73	2.53	18 (39%)	55,85,113	3.41	29 (52%)
29	CLA	1C	512	8	59,63,73	2.31	18 (30%)	71,101,113	3.11	33 (46%)
30	CHL	04	304	-	47,51,74	2.22	15 (31%)	52,86,114	3.27	23 (44%)
29	CLA	1r	312	20	56,60,73	2.37	20 (35%)	67,97,113	3.20	31 (46%)
30	CHL	1s	309	-	46,50,74	2.36	19 (41%)	51,85,114	3.32	25 (49%)
35	BCR	1k	102	-	41,41,41	1.81	8 (19%)	56,56,56	1.83	13 (23%)
29	CLA	1S	314	21	45,49,73	2.64	20 (44%)	54,84,113	3.43	29 (53%)
31	LUT	03	313	-	42,43,43	1.64	8 (19%)	51,60,60	1.70	12 (23%)
42	MGE	1B	623	-	44,44,48	0.25	0	52,52,56	0.65	1 (1%)
33	LHG	1s	303	-	28,28,48	0.31	0	30,30,54	0.84	1 (3%)
29	CLA	1c	515	8	63,67,73	2.23	20 (31%)	75,105,113	3.05	30 (40%)
30	CHL	02	605	-	48,53,74	2.25	19 (39%)	53,89,114	2.95	21 (39%)
29	CLA	1N	303	-	69,73,73	2.10	19 (27%)	83,113,113	2.88	31 (37%)
29	CLA	04	314	-	45,49,73	2.64	20 (44%)	54,84,113	3.45	30 (55%)
41	SQD	1A	412	-	41,42,54	0.46	1 (2%)	50,53,65	0.63	1 (2%)
29	CLA	1N	304	-	49,53,73	2.50	19 (38%)	59,89,113	3.33	27 (45%)
33	LHG	1s	302	-	28,28,48	0.37	0	31,33,54	0.44	0
29	CLA	02	608	1	43,48,73	2.68	19 (44%)	51,83,113	3.45	28 (54%)
31	LUT	00	314	-	42,43,43	1.63	8 (19%)	51,60,60	1.60	10 (19%)
30	CHL	1N	306	1	46,50,74	2.35	18 (39%)	51,85,114	3.34	24 (47%)
41	SQD	1B	622	-	49,50,54	0.41	1 (2%)	58,61,65	0.64	1 (1%)
29	CLA	1B	610	-	69,73,73	2.03	17 (24%)	83,113,113	2.77	31 (37%)
30	CHL	1g	605	1	50,54,74	2.24	16 (32%)	56,90,114	3.19	23 (41%)
41	SQD	1A	411	-	47,48,54	0.39	1 (2%)	56,59,65	0.46	0
29	CLA	1B	609	7	69,73,73	2.05	19 (27%)	83,113,113	2.71	28 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	1d	406	9	64,68,73	2.15	18 (28%)	77,107,113	2.94	32 (41%)
40	PL9	1D	407	-	55,55,55	0.81	1 (1%)	68,69,69	0.59	2 (2%)
29	CLA	1c	503	8	69,73,73	2.13	19 (27%)	83,113,113	2.87	29 (34%)
29	CLA	1g	612	-	64,68,73	2.20	19 (29%)	77,107,113	3.01	30 (38%)
30	CHL	04	305	-	45,50,74	2.24	15 (33%)	49,85,114	3.25	22 (44%)
29	CLA	09	309	1	45,49,73	2.59	19 (42%)	54,84,113	3.37	28 (51%)
33	LHG	1w	102	-	34,34,48	0.34	0	37,39,54	0.40	0
29	CLA	1n	613	1	61,65,73	2.25	18 (29%)	73,103,113	2.84	29 (39%)
33	LHG	1I	101	-	31,31,48	0.43	0	35,36,54	0.56	1 (2%)
41	SQD	1b	621	-	53,54,54	0.39	1 (1%)	62,65,65	0.88	3 (4%)
35	BCR	1j	101	-	41,41,41	1.78	8 (19%)	56,56,56	2.11	15 (26%)
33	LHG	1P	201	-	44,44,48	0.28	0	47,49,54	0.35	0
35	BCR	1I	102	-	41,41,41	1.70	8 (19%)	56,56,56	1.64	12 (21%)
29	CLA	05	301	1	45,49,73	2.64	20 (44%)	54,84,113	3.41	28 (51%)
29	CLA	1r	308	20	56,60,73	2.32	20 (35%)	67,97,113	3.14	30 (44%)
29	CLA	1G	604	-	45,49,73	2.60	19 (42%)	54,84,113	3.39	29 (53%)
29	CLA	1R	302	20	64,68,73	2.19	19 (29%)	77,107,113	2.99	31 (40%)
29	CLA	00	302	-	69,73,73	2.11	20 (28%)	83,113,113	2.94	32 (38%)
33	LHG	1n	616	29	42,42,48	0.29	0	45,48,54	0.43	0
33	LHG	09	318	-	48,48,48	0.29	0	51,54,54	0.38	0
34	DGD	1c	518	-	48,48,67	0.98	2 (4%)	62,62,81	1.20	7 (11%)
31	LUT	1R	315	-	42,43,43	1.69	8 (19%)	51,60,60	1.81	11 (21%)
29	CLA	1n	603	-	61,65,73	2.24	20 (32%)	73,103,113	3.01	31 (42%)
41	SQD	1A	413	-	44,45,54	0.43	1 (2%)	53,56,65	1.12	5 (9%)
30	CHL	09	306	-	47,51,74	2.17	17 (36%)	52,86,114	3.30	20 (38%)
29	CLA	07	312	-	47,52,73	2.57	20 (42%)	56,88,113	3.34	27 (48%)
29	CLA	07	308	-	45,49,73	2.59	20 (44%)	54,84,113	3.47	28 (51%)
29	CLA	1G	613	1	47,52,73	2.55	20 (42%)	56,88,113	3.36	25 (44%)
29	CLA	04	307	-	47,52,73	2.56	20 (42%)	56,88,113	3.33	26 (46%)
31	LUT	09	313	-	42,43,43	1.74	8 (19%)	51,60,60	1.67	11 (21%)
41	SQD	1s	301	-	43,44,54	0.44	1 (2%)	52,55,65	0.48	0
35	BCR	1B	619	-	41,41,41	1.69	9 (21%)	56,56,56	1.98	17 (30%)
35	BCR	1a	409	-	41,41,41	1.72	8 (19%)	56,56,56	1.65	13 (23%)
30	CHL	00	307	-	70,74,74	1.89	18 (25%)	80,114,114	2.78	25 (31%)
34	DGD	1C	518	-	61,61,67	0.85	2 (3%)	75,75,81	0.96	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	PHO	1a	407	-	34,45,69	1.05	2 (5%)	28,70,99	1.48	5 (17%)
29	CLA	1b	614	7	64,68,73	2.28	20 (31%)	77,107,113	3.29	31 (40%)
42	MGE	1k	101	-	36,36,48	0.29	0	44,44,56	0.59	0
29	CLA	1c	511	8	49,53,73	2.55	20 (40%)	59,89,113	3.32	28 (47%)
29	CLA	1D	405	9	46,50,73	2.51	19 (41%)	55,85,113	3.45	27 (49%)
29	CLA	1G	603	-	49,53,73	2.49	19 (38%)	59,89,113	3.29	29 (49%)
29	CLA	1R	312	-	50,54,73	2.47	19 (38%)	60,90,113	3.25	27 (45%)
29	CLA	1r	314	20	50,54,73	2.48	20 (40%)	60,90,113	3.37	28 (46%)
33	LHG	1C	526	-	31,31,48	0.43	0	35,36,54	0.74	2 (5%)
33	LHG	1r	317	29	28,28,48	0.36	0	31,33,54	0.76	2 (6%)
29	CLA	05	312	1	43,48,73	2.74	21 (48%)	51,83,113	3.61	28 (54%)
29	CLA	1C	504	-	69,73,73	2.09	19 (27%)	83,113,113	2.86	29 (34%)
29	CLA	1a	408	6	64,68,73	2.16	19 (29%)	77,107,113	2.93	30 (38%)
29	CLA	02	609	-	46,50,73	2.54	19 (41%)	55,85,113	3.46	29 (52%)
40	PL9	1d	410	-	55,55,55	0.78	1 (1%)	68,69,69	0.53	1 (1%)
33	LHG	1K	101	-	42,42,48	0.30	0	45,47,54	0.36	0
29	CLA	03	306	-	41,47,73	2.63	18 (43%)	49,81,113	3.61	27 (55%)
33	LHG	00	316	29	32,32,48	0.34	0	35,37,54	0.37	0
33	LHG	1C	522	-	33,33,48	0.35	0	36,39,54	0.93	1 (2%)
46	XAT	1g	617	-	39,47,47	0.83	0	54,74,74	3.12	23 (42%)
33	LHG	1J	102	-	44,44,48	0.30	0	47,49,54	0.56	0
30	CHL	1g	608	-	47,51,74	2.21	17 (36%)	52,86,114	3.26	25 (48%)
35	BCR	1H	101	-	41,41,41	1.76	8 (19%)	56,56,56	1.74	14 (25%)
29	CLA	1C	508	8	69,73,73	2.12	19 (27%)	83,113,113	2.94	31 (37%)
41	SQD	1w	101	-	39,40,54	0.43	1 (2%)	48,51,65	0.71	1 (2%)
29	CLA	1B	606	7	69,73,73	2.05	18 (26%)	83,113,113	2.67	29 (34%)
30	CHL	1N	308	-	70,74,74	1.87	18 (25%)	80,114,114	2.74	24 (30%)
33	LHG	01	316	-	35,35,48	0.30	0	38,41,54	0.45	0
41	SQD	1B	628	-	53,54,54	0.39	1 (1%)	62,65,65	0.47	1 (1%)
29	CLA	1C	506	-	53,57,73	2.39	19 (35%)	62,93,113	3.32	28 (45%)
29	CLA	09	311	-	45,49,73	2.60	19 (42%)	54,84,113	3.49	27 (50%)
30	CHL	1r	313	20	51,55,74	2.21	16 (31%)	57,91,114	3.12	22 (38%)
34	DGD	1C	516	-	56,56,67	0.89	2 (3%)	70,70,81	0.95	3 (4%)
30	CHL	1R	303	-	45,50,74	2.24	16 (35%)	49,85,114	3.11	22 (44%)
29	CLA	08	306	-	44,49,73	2.55	18 (40%)	52,84,113	3.49	26 (50%)
33	LHG	1S	319	29	30,30,48	0.34	0	33,36,54	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	LNL	1C	515	-	16,16,19	0.62	0	15,16,19	0.64	0
43	LNL	1C	514	-	17,17,19	0.63	0	17,17,19	0.59	0
29	CLA	1g	602	1	64,68,73	2.16	19 (29%)	77,107,113	2.94	30 (38%)
29	CLA	05	308	1	45,49,73	2.67	19 (42%)	54,84,113	3.46	31 (57%)
29	CLA	1b	602	-	69,73,73	2.16	19 (27%)	83,113,113	2.81	27 (32%)
30	CHL	1s	310	-	45,50,74	2.26	16 (35%)	49,85,114	3.26	21 (42%)
33	LHG	1R	318	-	36,36,48	0.30	0	39,42,54	0.36	0
30	CHL	1G	607	-	68,72,74	1.96	19 (27%)	77,111,114	2.75	26 (33%)
29	CLA	1R	308	33	53,57,73	2.43	20 (37%)	62,93,113	3.13	28 (45%)
29	CLA	07	302	2	43,48,73	2.75	21 (48%)	51,83,113	4.03	29 (56%)
44	BCT	1D	403	36	2,3,3	0.96	0	2,3,3	0.36	0
29	CLA	1c	507	8	56,60,73	2.32	20 (35%)	67,97,113	3.14	31 (46%)
31	LUT	1r	315	-	42,43,43	1.69	8 (19%)	51,60,60	1.72	11 (21%)
30	CHL	05	315	-	46,50,74	2.35	16 (34%)	51,85,114	3.31	24 (47%)
29	CLA	1C	510	8	69,73,73	2.10	20 (28%)	83,113,113	2.88	30 (36%)
45	HEM	1E	103	10	50,50,50	1.63	10 (20%)	66,82,82	1.74	12 (18%)
31	LUT	07	313	-	42,43,43	1.58	7 (16%)	51,60,60	1.91	13 (25%)
29	CLA	07	309	2	52,56,73	2.48	19 (36%)	62,92,113	3.29	27 (43%)
30	CHL	1N	302	1	69,73,74	1.91	15 (21%)	78,112,114	2.76	26 (33%)
40	PL9	1E	102	-	55,55,55	0.58	1 (1%)	68,69,69	1.92	22 (32%)
29	CLA	1B	602	7	65,69,73	2.13	19 (29%)	78,108,113	2.75	27 (34%)
30	CHL	00	306	-	70,74,74	1.86	19 (27%)	80,114,114	2.69	23 (28%)
31	LUT	05	314	-	42,43,43	1.70	9 (21%)	51,60,60	1.97	14 (27%)
29	CLA	1g	613	-	59,63,73	2.23	19 (32%)	71,101,113	3.04	28 (39%)
30	CHL	06	606	-	50,54,74	2.25	16 (32%)	56,90,114	3.12	22 (39%)
30	CHL	1n	605	1	50,54,74	2.25	17 (34%)	56,90,114	3.20	21 (37%)
29	CLA	09	317	1	58,62,73	2.27	20 (34%)	69,99,113	3.14	30 (43%)
29	CLA	05	303	-	47,52,73	2.54	19 (40%)	56,88,113	3.27	27 (48%)
33	LHG	1a	413	-	40,40,48	1.01	2 (5%)	43,46,54	1.09	3 (6%)
33	LHG	1S	301	-	33,33,48	0.32	0	36,39,54	0.37	0
29	CLA	1g	614	1	49,53,73	2.51	20 (40%)	59,89,113	3.34	27 (45%)
31	LUT	1g	616	-	42,43,43	1.78	8 (19%)	51,60,60	2.36	14 (27%)
29	CLA	09	310	33	45,49,73	2.61	20 (44%)	54,84,113	3.46	28 (51%)
29	CLA	05	302	1	47,52,73	2.57	19 (40%)	56,88,113	3.40	28 (50%)
29	CLA	1B	601	7	69,73,73	2.04	19 (27%)	83,113,113	2.88	32 (38%)
29	CLA	1R	306	20	48,52,73	2.46	18 (37%)	56,87,113	3.42	27 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	07	307	-	43,48,73	2.64	19 (44%)	51,83,113	3.53	27 (52%)
35	BCR	1d	409	-	41,41,41	1.80	10 (24%)	56,56,56	1.89	17 (30%)
29	CLA	1N	312	33	43,48,73	2.67	20 (46%)	51,83,113	3.51	27 (52%)
30	CHL	1N	307	-	50,54,74	2.20	17 (34%)	56,90,114	3.02	22 (39%)
35	BCR	1b	618	-	41,41,41	1.67	12 (29%)	56,56,56	1.57	12 (21%)
30	CHL	01	302	-	50,54,74	2.24	17 (34%)	56,90,114	3.16	22 (39%)
29	CLA	1r	309	20	60,64,73	2.30	19 (31%)	72,102,113	3.03	33 (45%)
33	LHG	07	314	-	48,48,48	0.29	0	51,54,54	0.67	1 (1%)
31	LUT	1g	615	-	42,43,43	1.73	8 (19%)	51,60,60	1.73	11 (21%)
29	CLA	1D	402	-	54,58,73	2.38	18 (33%)	65,95,113	3.19	30 (46%)
33	LHG	1b	628	-	48,48,48	0.28	0	51,54,54	0.32	0
30	CHL	02	606	-	48,53,74	2.27	16 (33%)	53,89,114	3.14	21 (39%)
29	CLA	1R	314	20	50,54,73	2.50	20 (40%)	60,90,113	3.37	27 (45%)
30	CHL	09	308	1	65,69,74	1.93	18 (27%)	74,108,114	2.71	25 (33%)
34	DGD	1S	320	-	47,47,67	1.02	2 (4%)	61,61,81	1.17	7 (11%)
29	CLA	09	303	-	43,48,73	2.61	19 (44%)	51,83,113	3.36	25 (49%)
29	CLA	1s	307	-	45,49,73	2.58	20 (44%)	54,84,113	3.40	28 (51%)
29	CLA	1n	604	-	45,49,73	2.59	19 (42%)	54,84,113	3.37	29 (53%)

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
29	CLA	02	610	-	-	2/13/89/115	-
29	CLA	1N	305	-	-	2/10/86/115	-
47	3PH	1X	101	-	-	18/40/40/49	-
46	XAT	1G	619	-	-	10/31/93/93	0/4/4/4
29	CLA	1G	611	-	-	6/13/89/115	-
29	CLA	1c	509	-	1/1/15/20	9/39/115/115	-
46	XAT	1G	617	-	-	7/31/93/93	0/4/4/4
40	PL9	1R	301	-	-	18/53/73/73	0/1/1/1
29	CLA	1N	311	1	-	2/10/86/115	-
34	DGD	1b	627	-	-	9/51/91/95	0/2/2/2
29	CLA	1c	508	8	1/1/13/20	14/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	DGD	1C	517	-	-	11/47/87/95	0/2/2/2
29	CLA	1b	609	7	1/1/15/20	4/39/115/115	-
29	CLA	1B	615	-	-	4/10/86/115	-
33	LHG	1D	409	-	-	7/47/47/53	-
29	CLA	1N	314	1	-	8/24/100/115	-
29	CLA	1c	512	8	1/1/15/20	12/39/115/115	-
29	CLA	03	310	-	-	5/15/91/115	-
29	CLA	1r	303	-	-	3/15/91/115	-
29	CLA	1N	315	1	-	3/10/86/115	-
29	CLA	1r	302	20	-	2/10/86/115	-
29	CLA	01	311	-	-	0/17/93/115	-
29	CLA	1C	509	8	1/1/15/20	11/39/115/115	-
29	CLA	01	308	-	1/1/15/20	16/39/115/115	-
29	CLA	1d	407	9	1/1/13/20	9/27/103/115	-
30	CHL	07	306	-	-	4/10/86/117	-
29	CLA	1s	312	21	1/1/13/20	9/27/103/115	-
30	CHL	1g	601	1	1/1/13/21	13/32/108/117	-
29	CLA	1B	607	7	1/1/14/20	10/36/112/115	-
29	CLA	1b	604	-	1/1/15/20	9/39/115/115	-
33	LHG	1W	101	-	-	6/39/39/53	-
41	SQD	1d	411	-	-	0/34/54/69	0/1/1/1
29	CLA	1B	605	-	1/1/15/20	11/39/115/115	-
29	CLA	1B	611	7	1/1/13/20	8/29/105/115	-
38	PHO	1A	406	-	-	10/37/103/103	0/5/6/6
29	CLA	1b	605	7	-	1/12/88/115	-
29	CLA	1b	613	-	1/1/13/20	19/31/107/115	-
29	CLA	08	307	-	-	2/8/84/115	-
33	LHG	1R	317	29	-	10/42/42/53	-
30	CHL	06	605	-	-	7/15/91/117	-
30	CHL	1G	608	-	-	8/14/90/117	-
29	CLA	1B	614	7	-	6/15/91/115	-
29	CLA	08	311	-	-	1/8/84/115	-
33	LHG	1D	408	-	-	1/35/35/53	-
33	LHG	1N	317	29	-	6/47/47/53	-
30	CHL	05	307	1	-	6/12/88/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	1b	608	-	1/1/13/20	10/32/108/115	-
30	CHL	02	607	-	-	11/17/93/117	-
29	CLA	1b	610	7	1/1/14/20	10/35/111/115	-
29	CLA	1a	406	-	-	3/21/97/115	-
30	CHL	1n	608	-	-	6/17/93/117	-
33	LHG	1g	618	29	-	12/40/40/53	-
29	CLA	1d	403	-	1/1/13/20	10/32/108/115	-
30	CHL	00	308	1	1/1/15/21	19/41/117/117	-
29	CLA	1A	407	6	-	3/15/91/115	-
29	CLA	1C	507	8	1/1/13/20	6/31/107/115	-
29	CLA	1S	312	-	-	1/10/86/115	-
33	LHG	1I	103	-	-	4/43/43/53	-
29	CLA	1S	316	-	-	5/17/93/115	-
30	CHL	1n	606	-	-	7/19/95/117	-
29	CLA	1C	503	8	1/1/13/20	6/29/105/115	-
29	CLA	1c	514	-	1/1/14/20	11/35/111/115	-
33	LHG	00	317	-	-	8/53/53/53	-
31	LUT	00	313	-	-	0/29/67/67	0/2/2/2
30	CHL	06	601	-	-	11/17/93/117	-
29	CLA	00	309	1	1/1/14/20	14/33/109/115	-
32	VIV	09	315	-	-	12/19/30/30	0/2/2/2
33	LHG	1F	101	-	-	12/45/45/53	-
41	SQD	1B	620	-	-	7/40/60/69	0/1/1/1
40	PL9	1A	410	-	-	11/53/73/73	0/1/1/1
29	CLA	01	309	-	-	7/17/93/115	-
33	LHG	1C	519	-	-	4/33/33/53	-
33	LHG	1S	303	-	-	3/30/30/53	-
29	CLA	06	602	1	1/1/13/20	6/27/103/115	-
29	CLA	1s	316	21	-	5/17/93/115	-
43	LNL	1c	501	-	-	2/14/14/17	-
34	DGD	1B	626	-	-	19/37/77/95	0/2/2/2
35	BCR	1B	618	-	-	3/29/63/63	0/2/2/2
33	LHG	1W	102	-	-	21/48/48/53	-
30	CHL	06	604	-	-	3/10/86/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	05	306	-	-	2/10/86/117	-
30	CHL	07	311	2	-	8/10/86/117	-
33	LHG	1b	626	-	-	2/36/36/53	-
29	CLA	02	602	-	-	3/13/89/115	-
29	CLA	02	612	1	-	1/13/89/115	-
35	BCR	1i	101	-	-	1/29/63/63	0/2/2/2
30	CHL	08	305	-	-	5/8/80/117	-
29	CLA	01	307	1	1/1/13/20	11/29/105/115	-
29	CLA	1G	612	1	1/1/13/20	14/27/103/115	-
29	CLA	09	301	1	1/1/13/20	12/27/103/115	-
29	CLA	03	309	-	-	5/13/89/115	-
30	CHL	09	304	1	-	6/10/86/117	-
33	LHG	1D	410	-	-	3/36/36/53	-
30	CHL	1r	305	-	-	9/17/93/117	-
29	CLA	1A	404	6	1/1/14/20	8/35/111/115	-
35	BCR	04	313	-	-	6/29/63/63	0/2/2/2
41	SQD	1C	521	-	-	5/46/66/69	0/1/1/1
29	CLA	1b	617	-	-	8/15/91/115	-
30	CHL	1S	304	21	-	7/17/93/117	-
46	XAT	1r	316	-	-	5/31/93/93	0/4/4/4
29	CLA	00	301	1	1/1/14/20	9/35/111/115	-
33	LHG	09	316	29	-	5/41/41/53	-
33	LHG	00	321	-	-	13/48/48/53	-
41	SQD	1S	302	-	-	6/41/61/69	0/1/1/1
29	CLA	1B	608	-	1/1/15/20	17/39/115/115	-
42	MGE	1s	320	-	-	12/36/56/63	0/1/1/1
29	CLA	1S	311	33	-	2/10/86/115	-
33	LHG	1w	103	-	-	7/46/46/53	-
29	CLA	08	310	3	-	0/4/80/115	-
29	CLA	1R	307	-	-	2/8/84/115	-
33	LHG	1N	318	-	-	13/52/52/53	-
30	CHL	00	304	1	-	8/15/91/117	-
33	LHG	1t	101	-	-	7/38/40/53	-
29	CLA	01	301	-	-	14/26/102/115	-
38	PHO	1A	405	-	-	7/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	02	613	-	-	7/17/93/115	-
30	CHL	09	305	-	-	4/14/90/117	-
41	SQD	1D	411	-	-	9/41/61/69	0/1/1/1
40	PL9	1r	301	-	-	13/53/73/73	0/1/1/1
29	CLA	1B	612	7	1/1/15/20	16/39/115/115	-
45	HEM	1f	101	11	-	8/14/54/54	-
29	CLA	1S	310	21	-	0/10/86/115	-
29	CLA	03	308	2	-	2/10/82/115	-
29	CLA	1B	616	7	1/1/13/20	5/32/108/115	-
33	LHG	1N	301	-	-	6/44/44/53	-
30	CHL	1n	607	-	1/1/15/21	23/41/117/117	-
29	CLA	1C	513	8	-	5/10/86/115	-
30	CHL	08	301	-	-	4/10/86/117	-
31	LUT	1N	316	-	-	0/29/64/67	0/2/2/2
41	SQD	1D	412	-	-	4/38/58/69	0/1/1/1
30	CHL	1s	308	-	-	13/17/93/117	-
33	LHG	1c	521	-	-	9/46/46/53	-
29	CLA	1c	505	8	1/1/15/20	15/39/115/115	-
30	CHL	1g	609	1	1/1/14/21	13/35/111/117	-
30	CHL	1r	307	-	-	7/17/93/117	-
35	BCR	1Z	102	-	-	4/29/63/63	0/2/2/2
41	SQD	1l	101	-	-	4/37/57/69	0/1/1/1
31	LUT	1s	317	-	-	4/29/67/67	0/2/2/2
30	CHL	03	303	-	-	9/15/91/117	-
29	CLA	01	312	-	-	5/17/93/115	-
30	CHL	04	301	-	-	10/17/93/117	-
30	CHL	03	302	2	-	4/6/84/117	-
30	CHL	09	307	-	-	2/14/90/117	-
33	LHG	1a	401	-	-	4/36/36/53	-
29	CLA	03	301	2	1/1/14/20	6/33/109/115	-
29	CLA	04	310	-	-	2/13/89/115	-
29	CLA	02	611	-	-	2/13/89/115	-
29	CLA	06	610	-	-	0/10/86/115	-
29	CLA	01	310	1	1/1/15/20	11/39/115/115	-
29	CLA	1b	607	7	-	4/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	1n	602	1	1/1/13/20	5/29/105/115	-
38	PHO	1d	404	-	-	3/37/103/103	0/5/6/6
35	BCR	1A	409	-	-	3/29/63/63	0/2/2/2
31	LUT	1S	318	-	-	1/29/67/67	0/2/2/2
29	CLA	03	312	-	-	2/13/89/115	-
31	LUT	01	315	-	-	1/29/67/67	0/2/2/2
29	CLA	05	310	1	-	2/10/86/115	-
29	CLA	1N	313	-	-	3/10/86/115	-
41	SQD	1d	405	-	-	3/43/63/69	0/1/1/1
35	BCR	1b	619	-	-	4/29/63/63	0/2/2/2
29	CLA	1R	309	20	-	7/13/89/115	-
35	BCR	1B	630	-	-	2/29/63/63	0/2/2/2
30	CHL	04	303	-	-	6/17/93/117	-
33	LHG	1c	522	-	-	6/29/29/53	-
42	MGE	1C	524	-	-	6/40/60/63	0/1/1/1
29	CLA	1R	310	-	-	3/19/95/115	-
30	CHL	1N	309	-	-	6/15/92/117	-
30	CHL	00	305	-	-	8/19/95/117	-
29	CLA	1c	506	-	1/1/13/20	8/27/103/115	-
29	CLA	1n	612	-	-	7/15/91/115	-
29	CLA	1G	602	1	1/1/15/20	18/39/115/115	-
35	BCR	1D	406	-	-	4/29/63/63	0/2/2/2
42	MGE	1B	624	-	-	4/38/58/63	0/1/1/1
33	LHG	1v	201	-	-	8/45/45/53	-
29	CLA	1g	604	-	-	8/21/97/115	-
33	LHG	1E	101	-	-	8/34/34/53	-
30	CHL	07	303	2	-	6/10/86/117	-
46	XAT	1R	316	-	-	4/31/93/93	0/4/4/4
30	CHL	1s	304	21	-	11/17/93/117	-
30	CHL	1n	609	1	1/1/14/21	21/35/111/117	-
29	CLA	03	307	-	-	3/10/86/115	-
40	PL9	1a	412	-	-	16/53/73/73	0/1/1/1
30	CHL	07	304	2	-	4/10/86/117	-
29	CLA	06	609	-	-	0/10/86/115	-
29	CLA	1s	311	-	-	1/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	1C	501	8	1/1/15/20	9/39/115/115	-
29	CLA	07	301	-	-	2/8/84/115	-
29	CLA	05	311	-	-	0/8/84/115	-
31	LUT	09	314	-	-	0/29/67/67	0/2/2/2
34	DGD	1B	625	-	-	10/51/91/95	0/2/2/2
29	CLA	1s	314	-	-	4/13/89/115	-
29	CLA	1c	504	-	1/1/14/20	11/33/109/115	-
30	CHL	03	305	-	-	8/17/93/117	-
29	CLA	08	309	3	-	3/8/84/115	-
33	LHG	1D	413	-	-	2/44/44/53	-
34	DGD	1B	627	-	-	17/51/91/95	0/2/2/2
29	CLA	1D	404	9	1/1/15/20	15/39/115/115	-
30	CHL	1G	606	-	-	8/17/93/117	-
33	LHG	1b	623	-	-	4/30/30/53	-
35	BCR	1B	617	-	-	4/29/63/63	0/2/2/2
29	CLA	1S	305	21	-	5/10/86/115	-
29	CLA	1s	306	21	-	0/17/93/115	-
33	LHG	1L	101	-	-	10/53/53/53	-
33	LHG	1C	523	-	-	8/43/43/53	-
30	CHL	05	304	-	-	9/15/91/117	-
30	CHL	01	304	-	1/1/14/21	22/38/114/117	-
30	CHL	02	601	-	-	11/17/93/117	-
30	CHL	07	305	-	-	4/6/82/117	-
41	SQD	1B	629	-	-	3/35/55/69	0/1/1/1
30	CHL	1N	310	1	1/1/15/21	24/41/117/117	-
29	CLA	1a	405	6	-	6/24/100/115	-
30	CHL	1g	607	-	-	9/19/95/117	-
29	CLA	1g	603	-	-	4/17/93/115	-
29	CLA	1r	311	-	-	4/15/91/115	-
29	CLA	1b	603	7	1/1/13/20	8/29/105/115	-
29	CLA	04	306	3	-	5/13/89/115	-
30	CHL	1S	308	-	-	9/12/88/117	-
29	CLA	1C	511	-	-	7/17/93/115	-
30	CHL	1R	313	20	-	9/15/91/117	-
33	LHG	1b	625	-	-	7/49/49/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	05	313	1	-	6/10/86/117	-
29	CLA	06	608	-	-	1/8/84/115	-
30	CHL	02	604	-	-	6/15/91/117	-
31	LUT	1s	318	-	-	4/29/67/67	0/2/2/2
30	CHL	08	303	-	-	8/15/91/117	-
31	LUT	01	314	-	-	1/29/67/67	0/2/2/2
29	CLA	00	310	33	-	4/23/99/115	-
30	CHL	03	311	-	-	6/12/88/117	-
29	CLA	04	309	3	-	4/13/89/115	-
29	CLA	09	302	-	1/1/13/20	7/29/105/115	-
30	CHL	08	302	-	-	2/10/86/117	-
33	LHG	1s	319	-	-	3/28/28/53	-
30	CHL	08	304	3	-	6/10/86/117	-
29	CLA	1c	510	8	1/1/13/20	6/32/108/115	-
30	CHL	01	306	1	1/1/14/21	17/37/113/117	-
29	CLA	1B	604	7	1/1/13/20	6/29/105/115	-
35	BCR	1J	101	-	-	5/29/63/63	0/2/2/2
29	CLA	1G	614	33	-	0/12/88/115	-
29	CLA	1c	513	8	-	3/15/91/115	-
29	CLA	06	611	-	-	0/8/84/115	-
35	BCR	1h	101	-	-	3/29/63/63	0/2/2/2
30	CHL	1G	601	-	1/1/15/21	19/41/117/117	-
31	LUT	1G	615	-	-	1/29/67/67	0/2/2/2
33	LHG	03	314	-	-	10/49/49/53	-
29	CLA	09	312	1	-	4/13/89/115	-
30	CHL	04	302	-	-	4/12/84/117	-
29	CLA	1n	610	1	1/1/13/20	12/31/107/115	-
29	CLA	1n	611	33	1/1/13/20	5/30/106/115	-
29	CLA	1B	613	-	1/1/13/20	4/31/107/115	-
29	CLA	1G	610	1	-	6/13/89/115	-
33	LHG	1n	617	-	-	8/38/39/53	-
29	CLA	1S	315	21	-	2/13/89/115	-
33	LHG	1b	624	-	-	7/40/40/53	-
46	XAT	1g	619	-	-	8/31/93/93	0/4/4/4
34	DGD	1c	520	-	-	8/46/86/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LUT	1n	615	-	-	2/29/67/67	0/2/2/2
34	DGD	00	320	-	-	16/50/90/95	0/2/2/2
29	CLA	04	311	-	-	4/13/89/115	-
29	CLA	1r	310	33	-	3/12/88/115	-
29	CLA	1C	502	8	1/1/14/20	10/35/111/115	-
29	CLA	1b	612	7	1/1/15/20	11/39/115/115	-
33	LHG	1V	201	-	-	9/53/53/53	-
34	DGD	1A	414	-	-	10/44/84/95	0/2/2/2
41	SQD	1c	517	-	-	3/49/69/69	0/1/1/1
30	CHL	05	305	-	1/1/14/21	18/38/114/117	-
30	CHL	02	603	-	-	11/17/93/117	-
30	CHL	01	305	-	-	7/17/93/117	-
41	SQD	1L	102	-	-	10/48/68/69	0/1/1/1
41	SQD	1a	411	-	-	3/41/61/69	0/1/1/1
29	CLA	1g	611	33	-	2/12/88/115	-
33	LHG	1d	402	-	-	3/42/42/53	-
33	LHG	1e	102	-	-	10/46/46/53	-
29	CLA	1B	603	7	1/1/15/20	10/39/115/115	-
29	CLA	1b	611	-	1/1/15/20	13/39/115/115	-
35	BCR	1Z	101	-	-	2/29/63/63	0/2/2/2
29	CLA	1C	505	8	1/1/14/20	16/33/109/115	-
29	CLA	1b	615	7	1/1/15/20	14/39/115/115	-
29	CLA	08	308	3	-	4/10/86/115	-
31	LUT	1G	616	-	-	1/29/67/67	0/2/2/2
33	LHG	1C	525	-	-	8/43/43/53	-
33	LHG	1C	527	-	-	12/41/41/53	-
41	SQD	1m	101	-	-	5/37/57/69	0/1/1/1
41	SQD	1a	410	-	-	9/45/65/69	0/1/1/1
29	CLA	1S	306	-	-	4/8/84/115	-
30	CHL	1S	309	-	-	7/12/88/117	-
29	CLA	01	313	-	-	3/17/93/115	-
30	CHL	06	603	-	-	6/10/82/117	-
35	BCR	1c	516	-	-	1/29/63/63	0/2/2/2
29	CLA	00	311	-	-	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	1R	304	-	-	4/12/88/117	-
30	CHL	1G	605	1	-	6/10/86/117	-
29	CLA	04	312	-	-	2/8/84/115	-
35	BCR	1b	620	-	-	2/29/63/63	0/2/2/2
29	CLA	1R	311	-	-	2/13/89/115	-
33	LHG	1j	102	-	-	14/45/45/53	-
30	CHL	1S	307	-	-	8/10/86/117	-
30	CHL	01	303	-	-	6/17/93/117	-
29	CLA	00	318	1	1/1/14/20	17/33/109/115	-
29	CLA	06	607	1	-	0/8/84/115	-
29	CLA	07	310	-	-	2/8/80/115	-
35	BCR	1b	601	-	-	7/29/63/63	0/2/2/2
32	VIV	00	315	-	-	4/7/18/30	0/2/2/2
33	LHG	00	319	-	-	11/53/53/53	-
29	CLA	1g	610	1	1/1/13/20	11/29/105/115	-
30	CHL	1n	601	-	1/1/14/21	6/37/113/117	-
29	CLA	1s	305	21	-	8/15/91/115	-
29	CLA	1S	313	21	1/1/13/20	10/25/101/115	-
33	LHG	1C	520	-	-	4/35/35/53	-
29	CLA	1r	304	-	-	4/17/93/115	-
31	LUT	1S	317	-	-	0/29/67/67	0/2/2/2
29	CLA	1D	401	-	1/1/15/20	7/39/115/115	-
30	CHL	1r	306	-	-	9/17/93/117	-
29	CLA	04	308	-	-	2/8/84/115	-
30	CHL	1g	606	-	-	8/22/98/117	-
29	CLA	00	312	1	-	7/15/91/115	-
33	LHG	1w	104	-	-	10/40/40/53	-
29	CLA	1n	614	1	-	3/10/86/115	-
33	LHG	1G	618	29	-	7/45/45/53	-
41	SQD	1b	622	-	-	13/43/63/69	0/1/1/1
29	CLA	1s	315	21	1/1/13/20	11/27/103/115	-
40	PL9	1e	101	-	-	4/13/33/73	0/1/1/1
30	CHL	03	304	-	-	6/14/90/117	-
29	CLA	05	309	-	-	2/8/84/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	1b	616	-	1/1/14/20	10/35/111/115	-
29	CLA	02	614	-	-	7/13/89/115	-
30	CHL	1G	609	1	-	8/12/88/117	-
29	CLA	1s	313	-	-	2/10/86/115	-
34	DGD	1c	519	-	-	14/41/81/95	0/2/2/2
29	CLA	1b	606	7	1/1/13/20	9/31/107/115	-
29	CLA	00	303	-	-	4/21/97/115	-
33	LHG	1d	401	-	-	10/43/43/53	-
30	CHL	1R	305	-	-	5/10/86/117	-
33	LHG	1B	621	-	-	6/42/42/53	-
29	CLA	08	312	-	-	9/12/88/115	-
29	CLA	1C	512	8	1/1/13/20	10/27/103/115	-
30	CHL	04	304	-	-	4/14/90/117	-
29	CLA	1r	312	20	-	7/24/100/115	-
30	CHL	1s	309	-	-	10/12/88/117	-
35	BCR	1k	102	-	-	5/29/63/63	0/2/2/2
29	CLA	1S	314	21	-	3/10/86/115	-
31	LUT	03	313	-	-	0/29/67/67	0/2/2/2
42	MGE	1B	623	-	-	8/39/59/63	0/1/1/1
33	LHG	1s	303	-	-	7/30/30/53	-
29	CLA	1c	515	8	1/1/13/20	7/32/108/115	-
30	CHL	02	605	-	-	7/15/91/117	-
29	CLA	1N	303	-	1/1/15/20	11/39/115/115	-
29	CLA	04	314	-	-	2/10/86/115	-
41	SQD	1A	412	-	-	4/37/57/69	0/1/1/1
29	CLA	1N	304	-	-	7/15/91/115	-
33	LHG	1s	302	-	-	4/32/32/53	-
29	CLA	02	608	1	-	2/8/84/115	-
31	LUT	00	314	-	-	0/29/67/67	0/2/2/2
30	CHL	1N	306	1	-	7/12/88/117	-
41	SQD	1B	622	-	-	6/45/65/69	0/1/1/1
29	CLA	1B	610	-	1/1/15/20	17/39/115/115	-
30	CHL	1g	605	1	-	10/17/93/117	-
41	SQD	1A	411	-	-	2/43/63/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	1B	609	7	1/1/15/20	11/39/115/115	-
29	CLA	1d	406	9	1/1/14/20	7/33/109/115	-
40	PL9	1D	407	-	-	5/53/73/73	0/1/1/1
29	CLA	1c	503	8	1/1/15/20	8/39/115/115	-
29	CLA	1g	612	-	1/1/14/20	5/33/109/115	-
30	CHL	04	305	-	-	4/12/88/117	-
29	CLA	09	309	1	-	5/10/86/115	-
33	LHG	1w	102	-	-	10/38/38/53	-
29	CLA	1n	613	1	1/1/13/20	14/30/106/115	-
33	LHG	1I	101	-	-	3/33/33/53	-
41	SQD	1b	621	-	-	7/49/69/69	0/1/1/1
35	BCR	1j	101	-	-	5/29/63/63	0/2/2/2
33	LHG	1P	201	-	-	6/48/48/53	-
35	BCR	1I	102	-	-	3/29/63/63	0/2/2/2
29	CLA	05	301	1	-	5/10/86/115	-
29	CLA	1r	308	20	-	9/24/100/115	-
29	CLA	1G	604	-	-	6/10/86/115	-
29	CLA	1R	302	20	1/1/14/20	9/33/109/115	-
29	CLA	00	302	-	1/1/15/20	12/39/115/115	-
33	LHG	1n	616	29	-	6/47/47/53	-
33	LHG	09	318	-	-	12/53/53/53	-
34	DGD	1c	518	-	-	9/36/76/95	0/2/2/2
31	LUT	1R	315	-	-	0/29/67/67	0/2/2/2
29	CLA	1n	603	-	1/1/13/20	11/30/106/115	-
41	SQD	1A	413	-	-	9/40/60/69	0/1/1/1
30	CHL	09	306	-	-	7/14/90/117	-
29	CLA	07	312	-	-	2/13/89/115	-
29	CLA	07	308	-	-	4/10/86/115	-
29	CLA	1G	613	1	-	3/13/89/115	-
29	CLA	04	307	-	-	4/13/89/115	-
31	LUT	09	313	-	-	0/29/67/67	0/2/2/2
41	SQD	1s	301	-	-	2/39/59/69	0/1/1/1
35	BCR	1B	619	-	-	4/29/63/63	0/2/2/2
35	BCR	1a	409	-	-	1/29/63/63	0/2/2/2
30	CHL	00	307	-	1/1/15/21	21/41/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	DGD	1C	518	-	-	7/49/89/95	0/2/2/2
38	PHO	1a	407	-	-	2/8/74/103	0/5/6/6
29	CLA	1b	614	7	1/1/14/20	7/33/109/115	-
42	MGE	1k	101	-	-	11/31/51/63	0/1/1/1
29	CLA	1c	511	8	-	7/15/91/115	-
29	CLA	1D	405	9	-	4/12/88/115	-
29	CLA	1G	603	-	-	7/15/91/115	-
29	CLA	1R	312	-	-	8/17/93/115	-
29	CLA	1r	314	20	-	8/17/93/115	-
33	LHG	1C	526	-	-	8/33/33/53	-
33	LHG	1r	317	29	-	4/32/32/53	-
29	CLA	1a	408	6	1/1/14/20	5/33/109/115	-
29	CLA	1C	504	-	1/1/15/20	7/39/115/115	-
29	CLA	05	312	1	-	0/8/84/115	-
29	CLA	02	609	-	-	1/12/88/115	-
40	PL9	1d	410	-	-	3/53/73/73	0/1/1/1
33	LHG	1K	101	-	-	12/46/46/53	-
29	CLA	03	306	-	-	0/8/80/115	-
33	LHG	00	316	29	-	2/36/36/53	-
33	LHG	1C	522	-	-	11/38/38/53	-
46	XAT	1g	617	-	-	10/31/93/93	0/4/4/4
33	LHG	1J	102	-	-	12/48/48/53	-
30	CHL	1g	608	-	-	3/14/90/117	-
35	BCR	1H	101	-	-	5/29/63/63	0/2/2/2
29	CLA	1C	508	8	1/1/15/20	13/39/115/115	-
41	SQD	1w	101	-	-	5/35/55/69	0/1/1/1
29	CLA	1B	606	7	1/1/15/20	8/39/115/115	-
30	CHL	1N	308	-	1/1/15/21	22/41/117/117	-
33	LHG	01	316	-	-	13/40/40/53	-
41	SQD	1B	628	-	-	8/49/69/69	0/1/1/1
29	CLA	1C	506	-	-	7/20/96/115	-
29	CLA	09	311	-	-	0/10/86/115	-
30	CHL	1r	313	20	-	8/19/95/117	-
34	DGD	1C	516	-	-	6/44/84/95	0/2/2/2
30	CHL	1R	303	-	-	6/12/88/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	08	306	-	-	2/10/86/115	-
33	LHG	1S	319	29	-	8/35/35/53	-
43	LNL	1C	515	-	-	3/14/14/17	-
43	LNL	1C	514	-	-	7/15/15/17	-
29	CLA	1g	602	1	1/1/14/20	15/33/109/115	-
29	CLA	05	308	1	-	2/10/86/115	-
29	CLA	1b	602	-	1/1/15/20	6/39/115/115	-
30	CHL	1s	310	-	-	5/12/88/117	-
33	LHG	1R	318	-	-	4/41/41/53	-
30	CHL	1G	607	-	1/1/14/21	18/39/115/117	-
29	CLA	1R	308	33	-	7/20/96/115	-
29	CLA	07	302	2	-	1/8/84/115	-
29	CLA	1c	507	8	-	10/24/100/115	-
31	LUT	1r	315	-	-	0/29/67/67	0/2/2/2
30	CHL	05	315	-	-	7/12/88/117	-
29	CLA	1C	510	8	1/1/15/20	5/39/115/115	-
45	HEM	1E	103	10	-	6/14/54/54	-
31	LUT	07	313	-	-	0/29/67/67	0/2/2/2
29	CLA	07	309	2	-	7/19/95/115	-
30	CHL	1N	302	1	1/1/14/21	20/40/116/117	-
40	PL9	1E	102	-	-	10/53/73/73	0/1/1/1
29	CLA	1B	602	7	1/1/14/20	14/35/111/115	-
30	CHL	00	306	-	1/1/15/21	23/41/117/117	-
31	LUT	05	314	-	-	2/29/67/67	0/2/2/2
29	CLA	1g	613	-	1/1/13/20	13/27/103/115	-
30	CHL	06	606	-	-	10/17/93/117	-
30	CHL	1n	605	1	-	11/17/93/117	-
29	CLA	09	317	1	-	13/26/102/115	-
29	CLA	05	303	-	-	6/13/89/115	-
33	LHG	1a	413	-	-	29/45/45/53	-
33	LHG	1S	301	-	-	9/38/38/53	-
29	CLA	1g	614	1	-	9/15/91/115	-
31	LUT	1g	616	-	-	4/29/67/67	0/2/2/2
29	CLA	09	310	33	-	5/10/86/115	-
29	CLA	05	302	1	-	4/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	1B	601	7	1/1/15/20	15/39/115/115	-
29	CLA	1R	306	20	-	2/13/90/115	-
29	CLA	07	307	-	-	1/8/84/115	-
35	BCR	1d	409	-	-	4/29/63/63	0/2/2/2
29	CLA	1N	312	33	-	0/8/84/115	-
30	CHL	1N	307	-	-	7/17/93/117	-
35	BCR	1b	618	-	-	2/29/63/63	0/2/2/2
30	CHL	01	302	-	-	14/17/93/117	-
29	CLA	1r	309	20	1/1/13/20	5/29/105/115	-
33	LHG	07	314	-	-	13/53/53/53	-
31	LUT	1g	615	-	-	0/29/67/67	0/2/2/2
29	CLA	1D	402	-	-	8/21/97/115	-
33	LHG	1b	628	-	-	3/53/53/53	-
30	CHL	02	606	-	-	8/15/91/117	-
29	CLA	1R	314	20	-	5/17/93/115	-
30	CHL	09	308	1	1/1/14/21	16/35/111/117	-
34	DGD	1S	320	-	-	15/35/75/95	0/2/2/2
29	CLA	09	303	-	-	2/8/84/115	-
29	CLA	1s	307	-	-	4/10/86/115	-
29	CLA	1n	604	-	-	6/10/86/115	-

The worst 5 of 6095 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	1b	602	CLA	C1D-ND	8.88	1.48	1.37
29	1S	315	CLA	C1D-ND	8.87	1.48	1.37
29	1B	613	CLA	C1D-ND	8.86	1.48	1.37
29	1c	511	CLA	C1D-ND	8.86	1.48	1.37
29	1B	614	CLA	C1D-ND	8.77	1.48	1.37

The worst 5 of 9150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	00	307	CHL	C2B-C1B-NB	11.08	117.66	110.23
46	1g	617	XAT	O24-C25-C24	10.94	121.60	113.38
30	1N	309	CHL	C2B-C1B-NB	10.92	117.55	110.23
30	03	304	CHL	C2B-C1B-NB	10.90	117.54	110.23
30	1n	608	CHL	C2B-C1B-NB	10.87	117.52	110.23

5 of 99 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
29	00	301	CLA	C8
29	00	302	CLA	C8
29	00	309	CLA	C8
29	00	318	CLA	C8
29	01	307	CLA	C8

5 of 3335 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	00	301	CLA	C2-C3-C5-C6
29	00	301	CLA	C4-C3-C5-C6
29	00	303	CLA	C2B-C3B-CAB-CBB
29	00	303	CLA	C4B-C3B-CAB-CBB
29	00	309	CLA	C2-C3-C5-C6

There are no ring outliers.

413 monomers are involved in 1160 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	02	610	CLA	1	0
29	1N	305	CLA	1	0
47	1X	101	3PH	1	0
46	1G	619	XAT	1	0
29	1c	509	CLA	9	0
46	1G	617	XAT	7	0
40	1R	301	PL9	7	0
29	1N	311	CLA	1	0
34	1b	627	DGD	4	0
29	1c	508	CLA	10	0
34	1C	517	DGD	5	0
29	1b	609	CLA	7	0
33	1D	409	LHG	2	0
29	1N	314	CLA	2	0
29	1c	512	CLA	9	0
29	03	310	CLA	1	0
29	1r	303	CLA	1	0
29	1N	315	CLA	1	0
29	1r	302	CLA	4	0
29	01	311	CLA	1	0
29	1C	509	CLA	2	0
29	01	308	CLA	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	1d	407	CLA	1	0
29	1s	312	CLA	4	0
30	1g	601	CHL	3	0
29	1B	607	CLA	7	0
29	1b	604	CLA	2	0
33	1W	101	LHG	1	0
41	1d	411	SQD	2	0
29	1B	605	CLA	4	0
29	1B	611	CLA	8	0
38	1A	406	PHO	1	0
29	1b	605	CLA	1	0
29	1b	613	CLA	3	0
29	08	307	CLA	1	0
33	1R	317	LHG	1	0
29	1B	614	CLA	3	0
29	08	311	CLA	3	0
33	1D	408	LHG	1	0
33	1N	317	LHG	3	0
30	05	307	CHL	2	0
29	1b	608	CLA	5	0
29	1b	610	CLA	2	0
29	1a	406	CLA	1	0
30	1n	608	CHL	1	0
29	1d	403	CLA	2	0
30	00	308	CHL	7	0
29	1C	507	CLA	5	0
33	1I	103	LHG	3	0
29	1S	316	CLA	1	0
30	1n	606	CHL	4	0
29	1C	503	CLA	1	0
29	1c	514	CLA	2	0
33	00	317	LHG	4	0
31	00	313	LUT	7	0
29	00	309	CLA	3	0
32	09	315	VIV	1	0
33	1F	101	LHG	2	0
41	1B	620	SQD	8	0
40	1A	410	PL9	6	0
29	01	309	CLA	1	0
33	1S	303	LHG	4	0
29	06	602	CLA	4	0
29	1s	316	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	1c	501	LNL	4	0
34	1B	626	DGD	4	0
35	1B	618	BCR	2	0
33	1W	102	LHG	3	0
30	07	311	CHL	3	0
33	1b	626	LHG	4	0
29	02	602	CLA	1	0
35	1i	101	BCR	7	0
29	01	307	CLA	1	0
29	1G	612	CLA	4	0
29	03	309	CLA	1	0
29	09	301	CLA	7	0
33	1D	410	LHG	2	0
30	1r	305	CHL	2	0
29	1A	404	CLA	3	0
35	04	313	BCR	6	0
41	1C	521	SQD	5	0
29	1b	617	CLA	1	0
30	1S	304	CHL	1	0
46	1r	316	XAT	3	0
29	00	301	CLA	4	0
33	09	316	LHG	3	0
33	00	321	LHG	4	0
41	1S	302	SQD	5	0
29	1B	608	CLA	9	0
42	1s	320	MGE	2	0
29	1S	311	CLA	2	0
33	1w	103	LHG	4	0
29	08	310	CLA	2	0
29	1R	307	CLA	3	0
33	1N	318	LHG	9	0
30	00	304	CHL	1	0
33	1t	101	LHG	3	0
29	01	301	CLA	6	0
38	1A	405	PHO	6	0
29	02	613	CLA	1	0
30	09	305	CHL	3	0
41	1D	411	SQD	3	0
40	1r	301	PL9	4	0
29	1B	612	CLA	5	0
45	1f	101	HEM	6	0
29	1S	310	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	03	308	CLA	2	0
29	1B	616	CLA	4	0
33	1N	301	LHG	2	0
30	1n	607	CHL	7	0
29	1C	513	CLA	2	0
31	1N	316	LUT	3	0
41	1D	412	SQD	4	0
30	1s	308	CHL	1	0
33	1c	521	LHG	5	0
29	1c	505	CLA	3	0
30	1g	609	CHL	5	0
35	1Z	102	BCR	5	0
41	1l	101	SQD	3	0
31	1s	317	LUT	8	0
30	03	303	CHL	1	0
29	01	312	CLA	2	0
30	03	302	CHL	1	0
30	09	307	CHL	1	0
33	1a	401	LHG	2	0
29	03	301	CLA	3	0
29	04	310	CLA	2	0
29	01	310	CLA	3	0
29	1n	602	CLA	6	0
38	1d	404	PHO	6	0
35	1A	409	BCR	4	0
31	1S	318	LUT	9	0
29	03	312	CLA	4	0
31	01	315	LUT	8	0
29	05	310	CLA	1	0
29	1N	313	CLA	1	0
41	1d	405	SQD	4	0
35	1b	619	BCR	6	0
29	1R	309	CLA	2	0
35	1B	630	BCR	7	0
30	04	303	CHL	3	0
33	1c	522	LHG	3	0
42	1C	524	MGE	4	0
29	1R	310	CLA	1	0
30	00	305	CHL	7	0
29	1c	506	CLA	2	0
29	1n	612	CLA	2	0
29	1G	602	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	1D	406	BCR	4	0
42	1B	624	MGE	2	0
33	1v	201	LHG	3	0
29	1g	604	CLA	1	0
46	1R	316	XAT	8	0
30	1s	304	CHL	3	0
30	1n	609	CHL	4	0
40	1a	412	PL9	21	0
30	07	304	CHL	1	0
29	06	609	CLA	1	0
29	1C	501	CLA	2	0
29	05	311	CLA	1	0
31	09	314	LUT	5	0
34	1B	625	DGD	5	0
29	1c	504	CLA	1	0
30	03	305	CHL	1	0
29	08	309	CLA	1	0
34	1B	627	DGD	2	0
29	1D	404	CLA	7	0
30	1G	606	CHL	1	0
33	1b	623	LHG	1	0
35	1B	617	BCR	6	0
29	1S	305	CLA	2	0
29	1s	306	CLA	2	0
33	1L	101	LHG	2	0
33	1C	523	LHG	2	0
30	05	304	CHL	5	0
30	01	304	CHL	3	0
41	1B	629	SQD	4	0
29	1a	405	CLA	4	0
30	1N	310	CHL	6	0
30	1g	607	CHL	3	0
29	1g	603	CLA	1	0
29	1r	311	CLA	1	0
29	1b	603	CLA	4	0
29	04	306	CLA	1	0
30	1S	308	CHL	3	0
29	1C	511	CLA	1	0
30	1R	313	CHL	1	0
33	1b	625	LHG	4	0
30	02	604	CHL	1	0
31	1s	318	LUT	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	01	314	LUT	2	0
29	00	310	CLA	2	0
30	03	311	CHL	1	0
29	04	309	CLA	1	0
29	09	302	CLA	4	0
33	1s	319	LHG	3	0
30	08	304	CHL	1	0
29	1c	510	CLA	5	0
30	01	306	CHL	8	0
29	1B	604	CLA	2	0
35	1J	101	BCR	4	0
29	1G	614	CLA	1	0
29	1c	513	CLA	2	0
29	06	611	CLA	1	0
35	1h	101	BCR	3	0
30	1G	601	CHL	8	0
31	1G	615	LUT	4	0
33	03	314	LHG	2	0
29	09	312	CLA	1	0
30	04	302	CHL	2	0
29	1n	610	CLA	4	0
29	1n	611	CLA	3	0
29	1B	613	CLA	1	0
29	1G	610	CLA	1	0
33	1n	617	LHG	3	0
29	1S	315	CLA	3	0
33	1b	624	LHG	3	0
46	1g	619	XAT	6	0
34	1c	520	DGD	3	0
31	1n	615	LUT	4	0
34	00	320	DGD	7	0
29	1C	502	CLA	2	0
29	1b	612	CLA	8	0
33	1V	201	LHG	2	0
34	1A	414	DGD	6	0
41	1c	517	SQD	8	0
30	05	305	CHL	4	0
30	02	603	CHL	1	0
30	01	305	CHL	5	0
41	1L	102	SQD	5	0
41	1a	411	SQD	1	0
33	1d	402	LHG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	1e	102	LHG	3	0
29	1B	603	CLA	4	0
29	1b	611	CLA	2	0
35	1Z	101	BCR	4	0
29	1C	505	CLA	4	0
29	1b	615	CLA	2	0
31	1G	616	LUT	8	0
33	1C	525	LHG	3	0
33	1C	527	LHG	3	0
41	1m	101	SQD	6	0
41	1a	410	SQD	6	0
29	1S	306	CLA	1	0
30	1S	309	CHL	3	0
30	06	603	CHL	1	0
35	1c	516	BCR	6	0
29	00	311	CLA	1	0
30	1R	304	CHL	3	0
30	1G	605	CHL	1	0
35	1b	620	BCR	5	0
29	1R	311	CLA	1	0
33	1j	102	LHG	2	0
30	1S	307	CHL	3	0
30	01	303	CHL	3	0
29	00	318	CLA	7	0
29	06	607	CLA	2	0
29	07	310	CLA	1	0
35	1b	601	BCR	4	0
32	00	315	VIV	3	0
33	00	319	LHG	4	0
29	1g	610	CLA	3	0
30	1n	601	CHL	7	0
29	1s	305	CLA	2	0
33	1C	520	LHG	4	0
29	1r	304	CLA	1	0
31	1S	317	LUT	8	0
29	1D	401	CLA	7	0
30	1r	306	CHL	2	0
30	1g	606	CHL	1	0
33	1w	104	LHG	6	0
29	1n	614	CLA	2	0
33	1G	618	LHG	4	0
41	1b	622	SQD	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	1s	315	CLA	1	0
40	1e	101	PL9	9	0
30	03	304	CHL	1	0
29	05	309	CLA	1	0
29	1b	616	CLA	3	0
29	02	614	CLA	2	0
30	1G	609	CHL	3	0
29	1s	313	CLA	2	0
34	1c	519	DGD	5	0
29	1b	606	CLA	3	0
33	1d	401	LHG	2	0
33	1B	621	LHG	2	0
29	08	312	CLA	1	0
29	1C	512	CLA	3	0
30	04	304	CHL	2	0
29	1r	312	CLA	3	0
30	1s	309	CHL	2	0
35	1k	102	BCR	4	0
29	1S	314	CLA	1	0
31	03	313	LUT	7	0
42	1B	623	MGE	3	0
33	1s	303	LHG	2	0
29	1c	515	CLA	1	0
30	02	605	CHL	1	0
29	1N	303	CLA	1	0
29	04	314	CLA	1	0
41	1A	412	SQD	3	0
29	1N	304	CLA	4	0
33	1s	302	LHG	2	0
29	02	608	CLA	1	0
31	00	314	LUT	6	0
30	1N	306	CHL	5	0
41	1B	622	SQD	3	0
29	1B	610	CLA	6	0
30	1g	605	CHL	1	0
41	1A	411	SQD	5	0
29	1B	609	CLA	8	0
29	1d	406	CLA	8	0
40	1D	407	PL9	6	0
29	1c	503	CLA	4	0
30	04	305	CHL	1	0
29	09	309	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	1n	613	CLA	4	0
33	1I	101	LHG	2	0
41	1b	621	SQD	9	0
35	1j	101	BCR	5	0
33	1P	201	LHG	7	0
35	1I	102	BCR	6	0
29	05	301	CLA	3	0
29	1r	308	CLA	2	0
29	1R	302	CLA	6	0
29	00	302	CLA	8	0
33	1n	616	LHG	2	0
33	09	318	LHG	6	0
34	1c	518	DGD	1	0
31	1R	315	LUT	5	0
29	1n	603	CLA	4	0
41	1A	413	SQD	2	0
30	09	306	CHL	2	0
29	07	308	CLA	1	0
29	1G	613	CLA	1	0
31	09	313	LUT	11	0
41	1s	301	SQD	4	0
35	1B	619	BCR	7	0
35	1a	409	BCR	5	0
30	00	307	CHL	4	0
34	1C	518	DGD	1	0
38	1a	407	PHO	1	0
29	1b	614	CLA	5	0
42	1k	101	MGE	5	0
29	1c	511	CLA	3	0
29	1D	405	CLA	2	0
29	1R	312	CLA	1	0
29	1r	314	CLA	1	0
33	1r	317	LHG	1	0
29	05	312	CLA	1	0
29	1C	504	CLA	2	0
29	1a	408	CLA	1	0
29	02	609	CLA	1	0
40	1d	410	PL9	7	0
33	1K	101	LHG	1	0
29	03	306	CLA	1	0
33	00	316	LHG	1	0
33	1C	522	LHG	1	0

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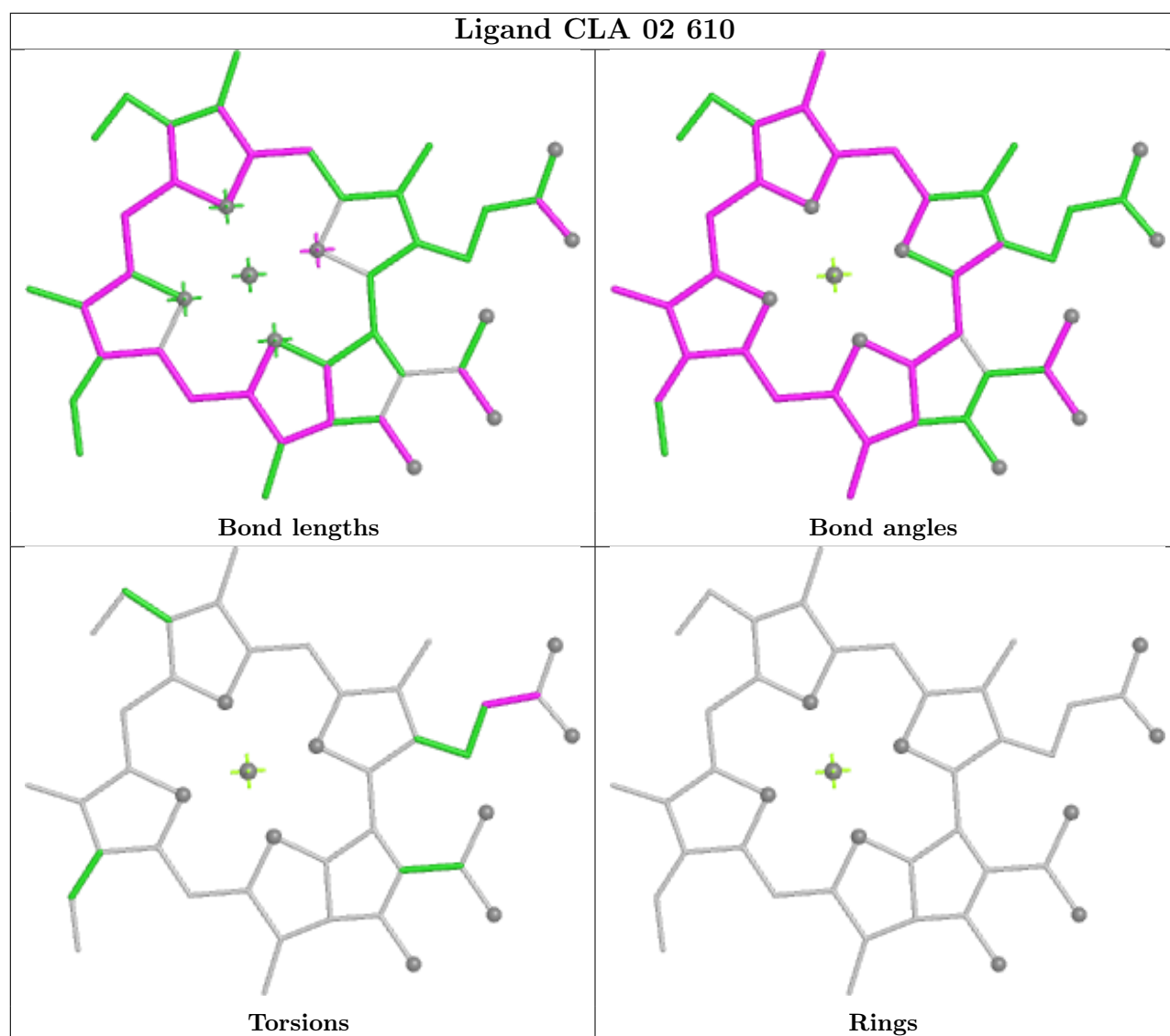
Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	1g	617	XAT	2	0
33	1J	102	LHG	5	0
35	1H	101	BCR	2	0
29	1C	508	CLA	8	0
41	1w	101	SQD	3	0
29	1B	606	CLA	5	0
30	1N	308	CHL	6	0
33	0I	316	LHG	4	0
41	1B	628	SQD	2	0
29	1C	506	CLA	2	0
30	1r	313	CHL	1	0
34	1C	516	DGD	10	0
30	1R	303	CHL	1	0
33	1S	319	LHG	4	0
43	1C	514	LNL	1	0
29	1g	602	CLA	11	0
29	1b	602	CLA	5	0
30	1s	310	CHL	1	0
33	1R	318	LHG	3	0
30	1G	607	CHL	1	0
29	1R	308	CLA	2	0
44	1D	403	BCT	1	0
29	1c	507	CLA	2	0
31	1r	315	LUT	6	0
30	05	315	CHL	1	0
29	1C	510	CLA	5	0
45	1E	103	HEM	4	0
31	07	313	LUT	6	0
30	1N	302	CHL	6	0
40	1E	102	PL9	28	0
29	1B	602	CLA	2	0
30	00	306	CHL	8	0
31	05	314	LUT	4	0
29	1g	613	CLA	1	0
30	1n	605	CHL	4	0
29	09	317	CLA	14	0
33	1a	413	LHG	11	0
33	1S	301	LHG	1	0
31	1g	616	LUT	6	0
29	09	310	CLA	1	0
29	1B	601	CLA	5	0
29	1R	306	CLA	3	0

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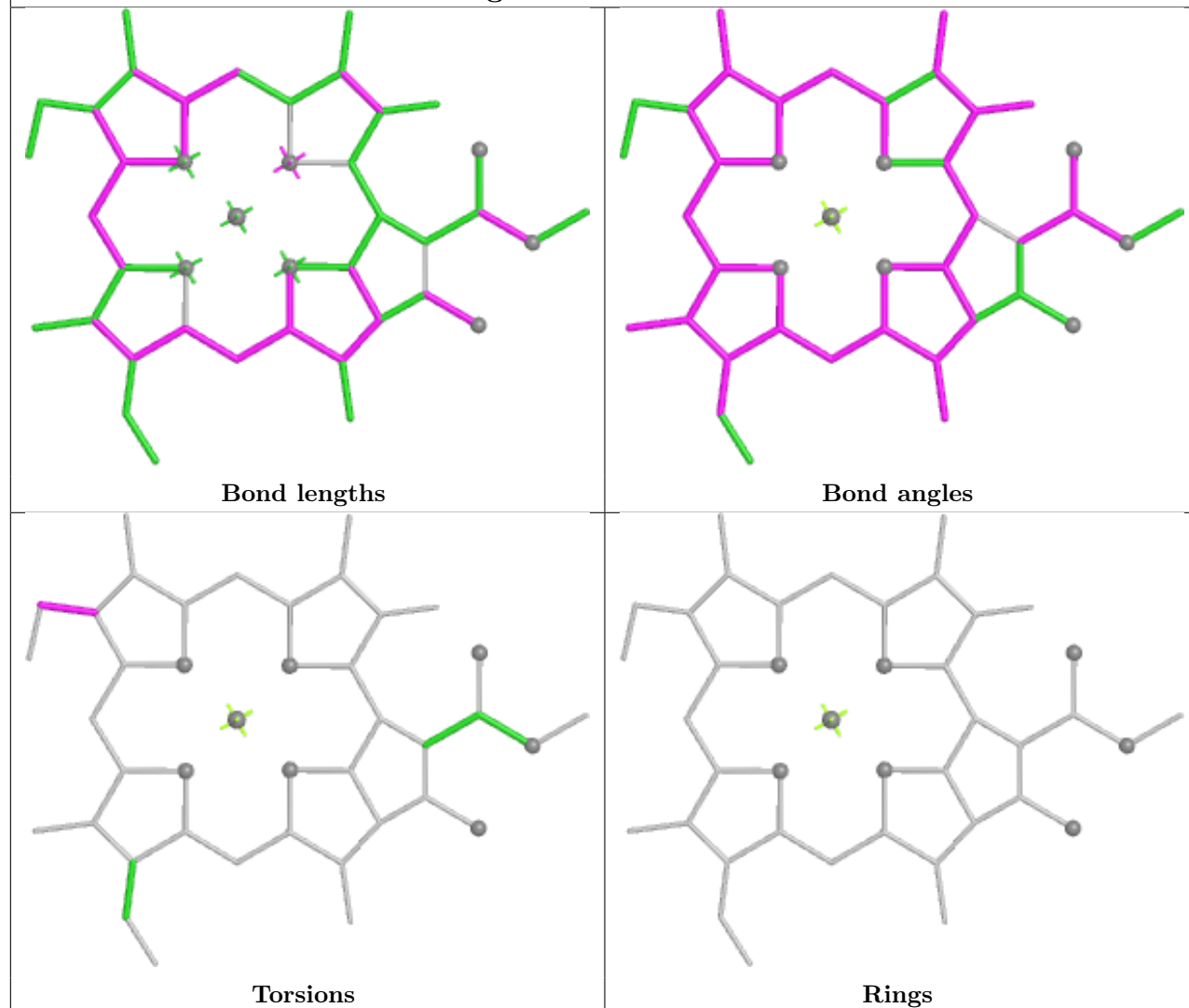
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	07	307	CLA	2	0
35	1d	409	BCR	1	0
30	1N	307	CHL	5	0
35	1b	618	BCR	9	0
30	01	302	CHL	1	0
29	1r	309	CLA	3	0
31	1g	615	LUT	3	0
29	1D	402	CLA	1	0
33	1b	628	LHG	7	0
30	02	606	CHL	3	0
29	1R	314	CLA	2	0
30	09	308	CHL	7	0
34	1S	320	DGD	3	0

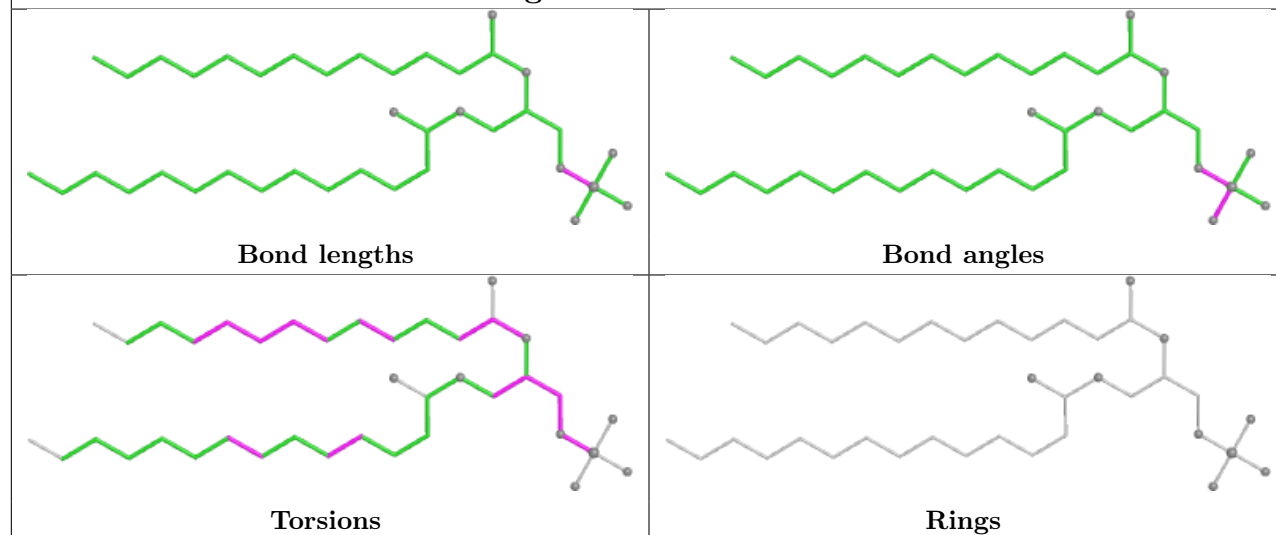
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

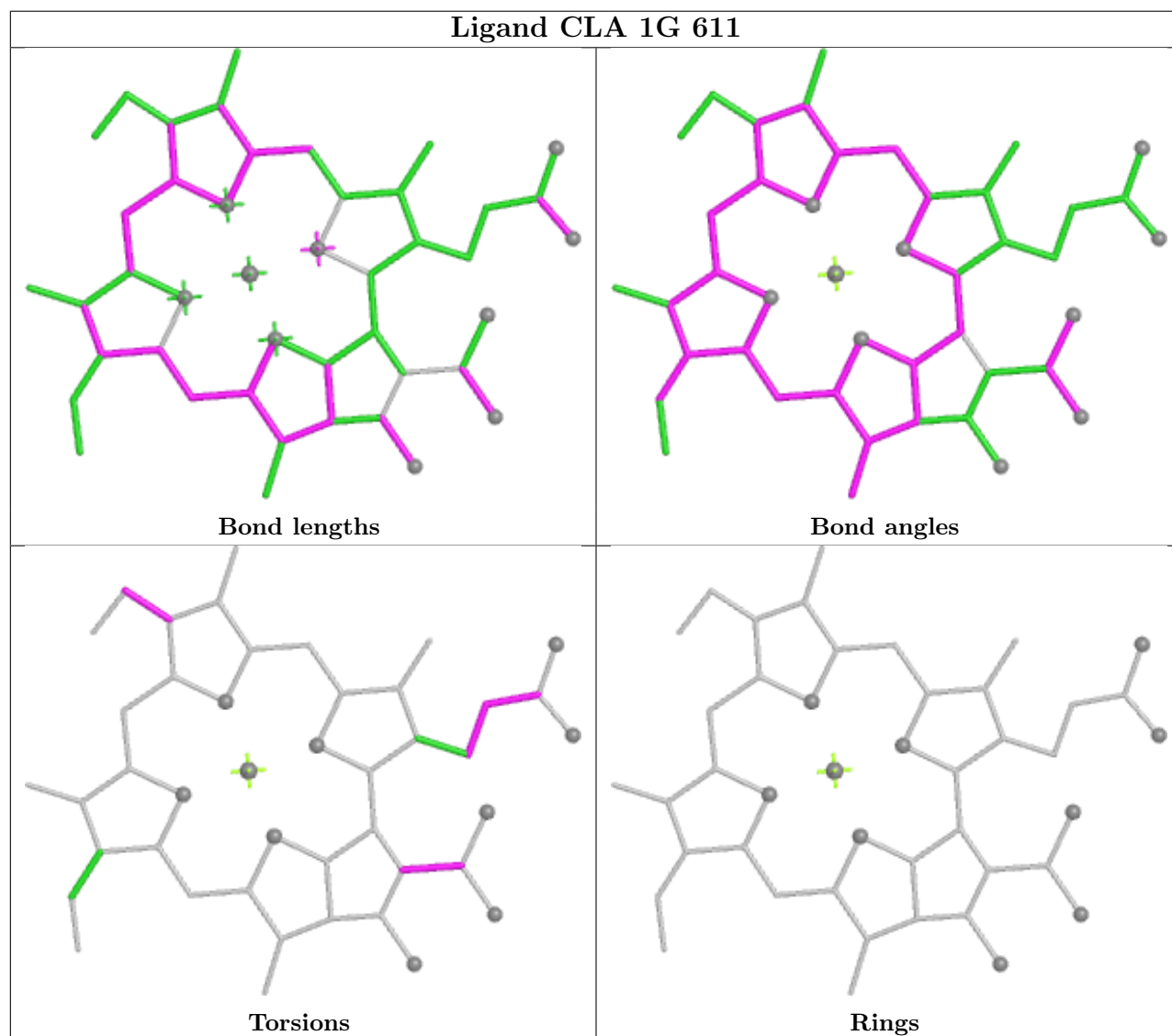
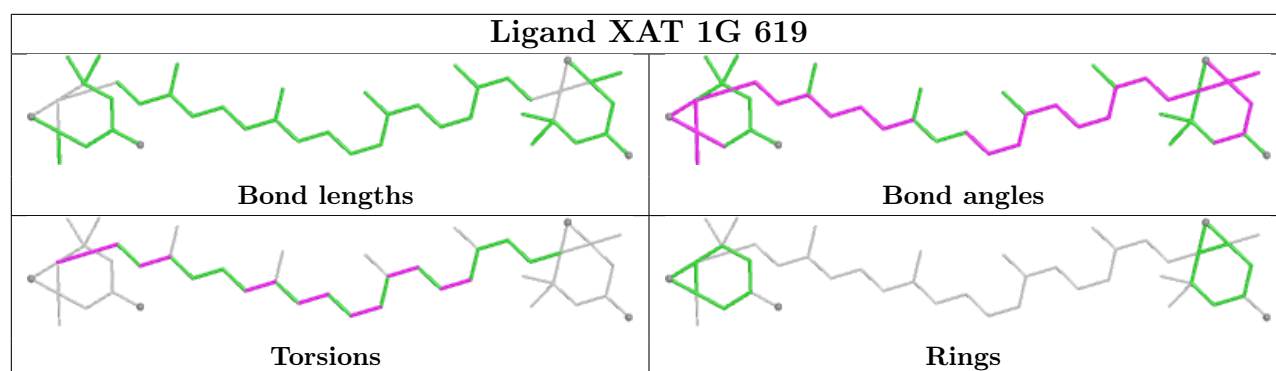


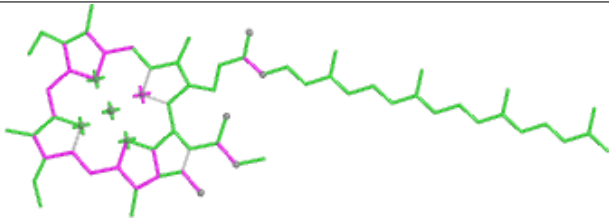
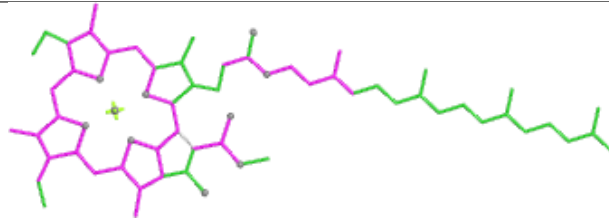
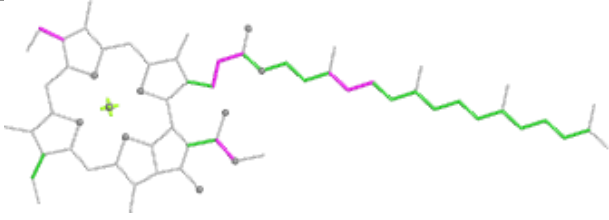
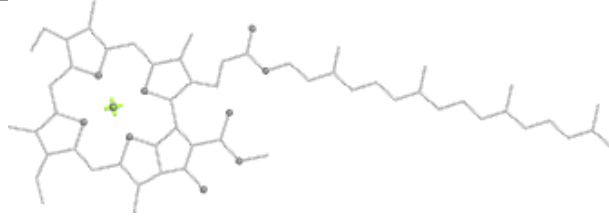
Ligand CLA 1N 305

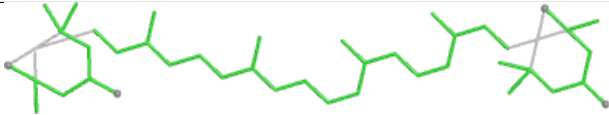
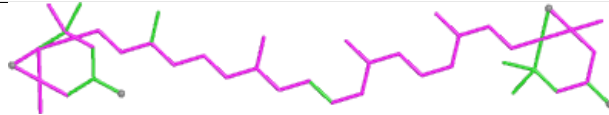
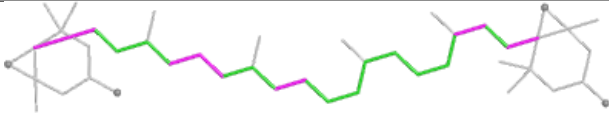
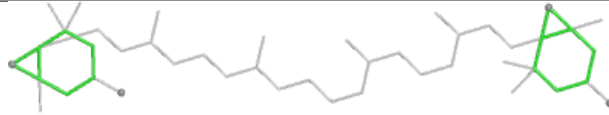


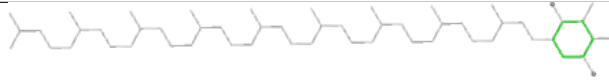
Ligand 3PH 1X 101



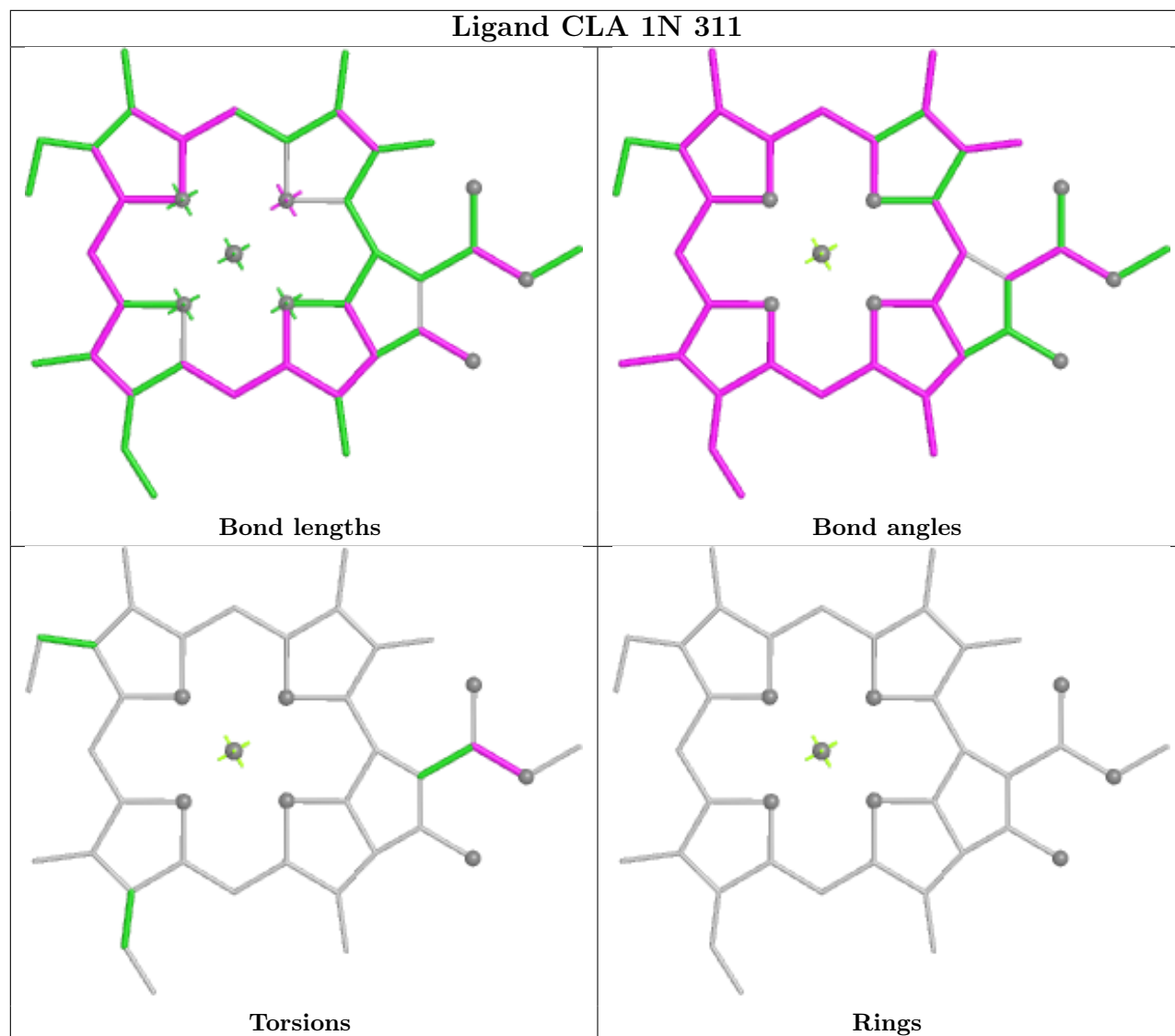


Ligand CLA 1c 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

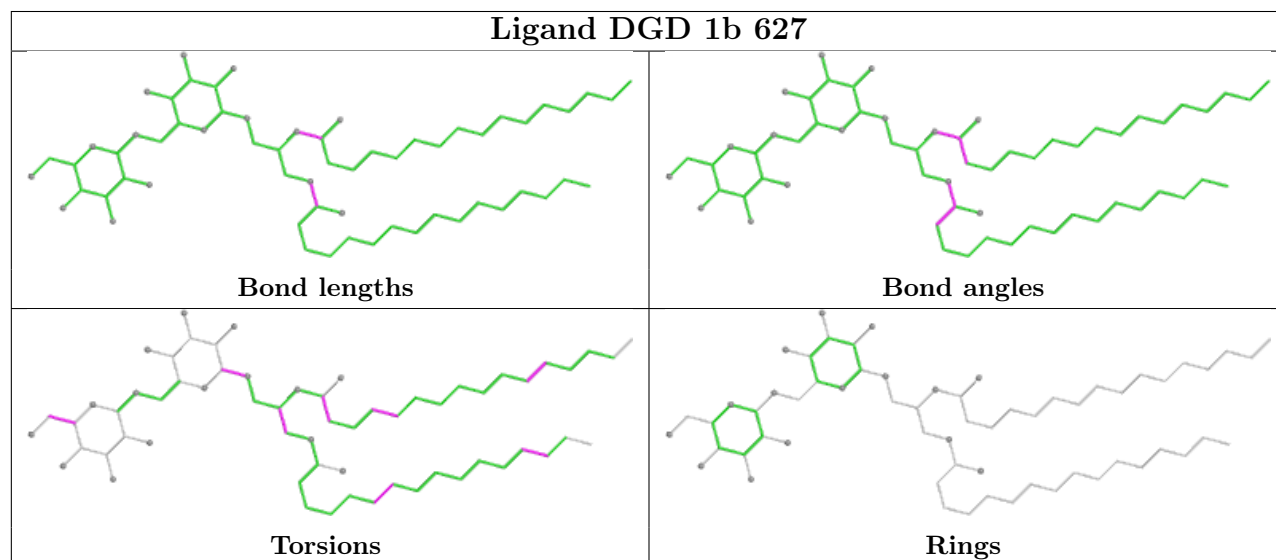
Ligand XAT 1G 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

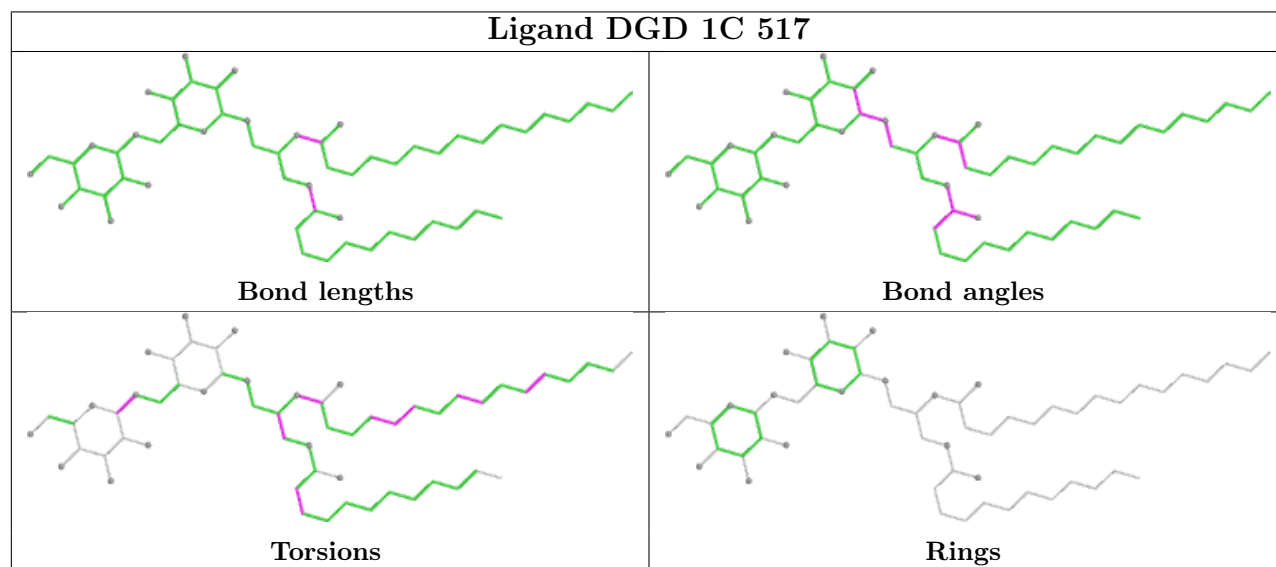
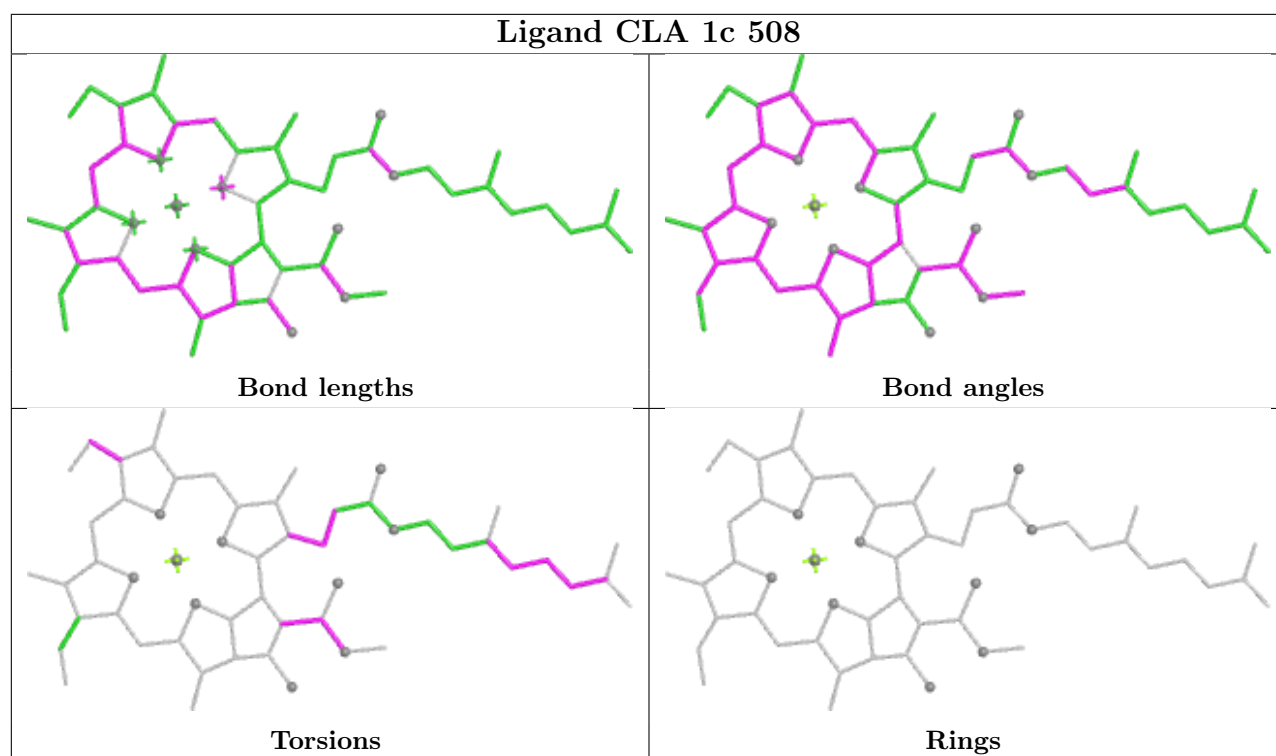
Ligand PL9 1R 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

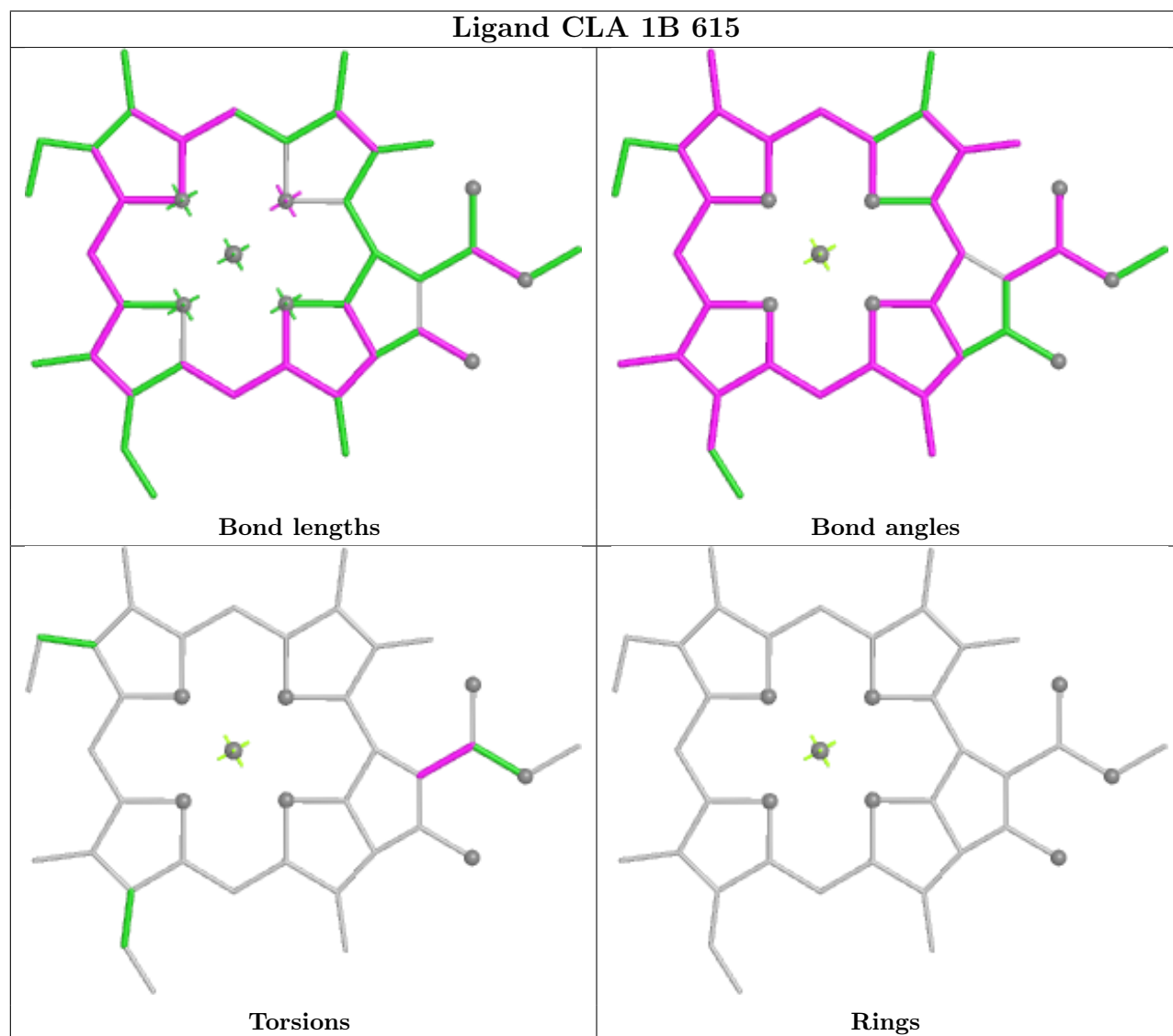
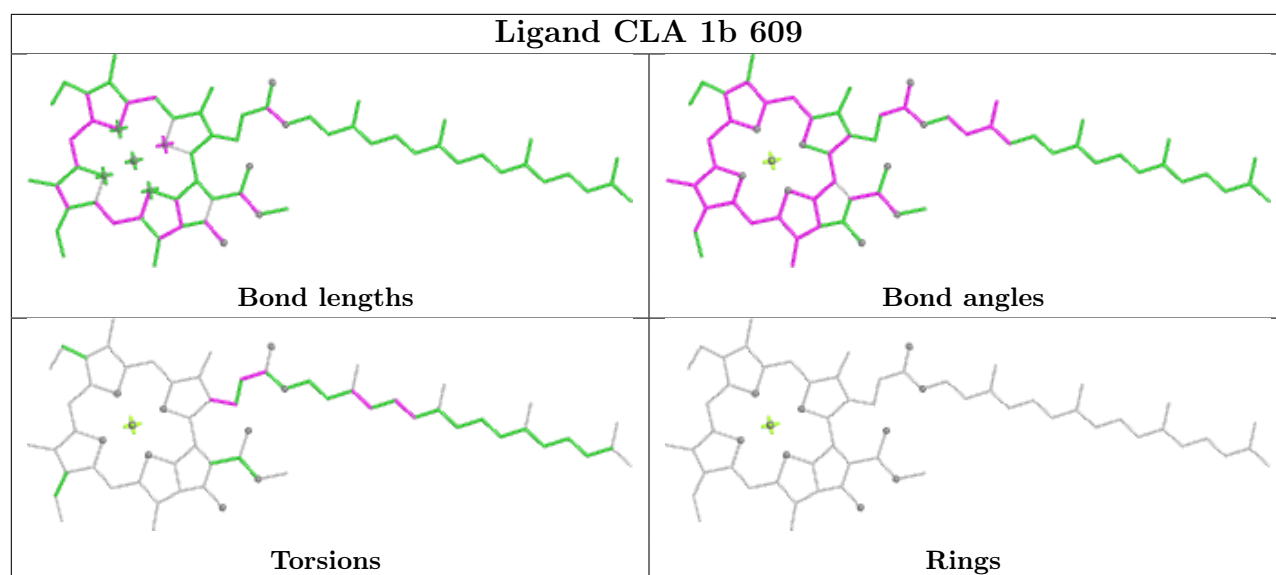
Ligand CLA 1N 311

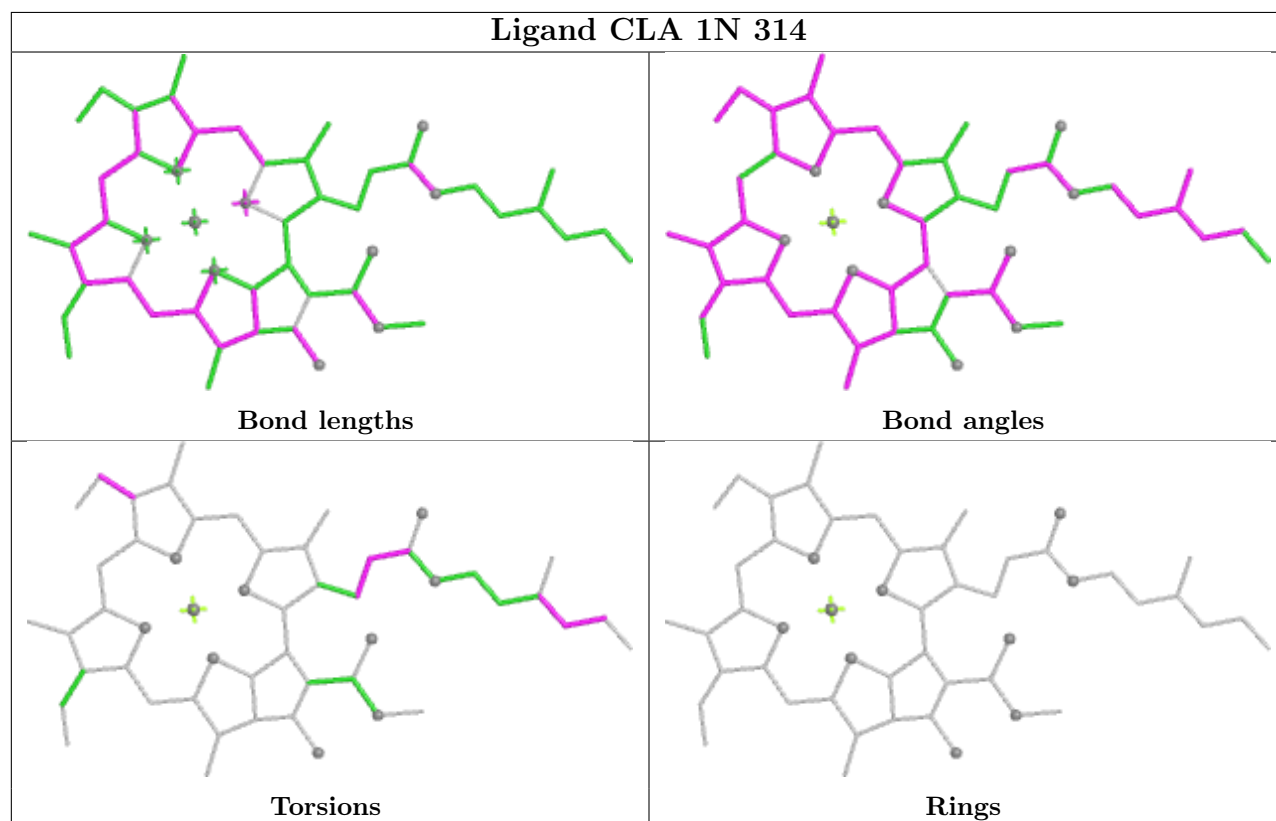
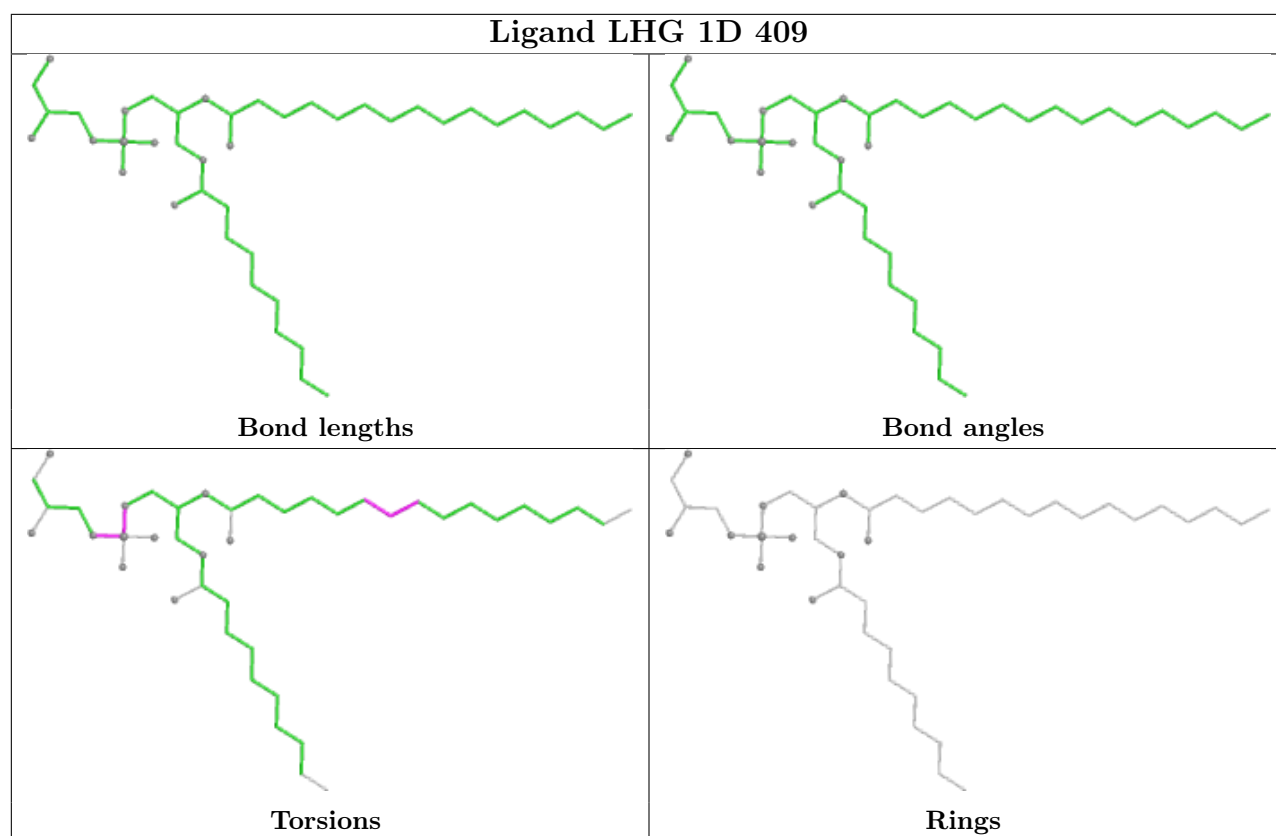


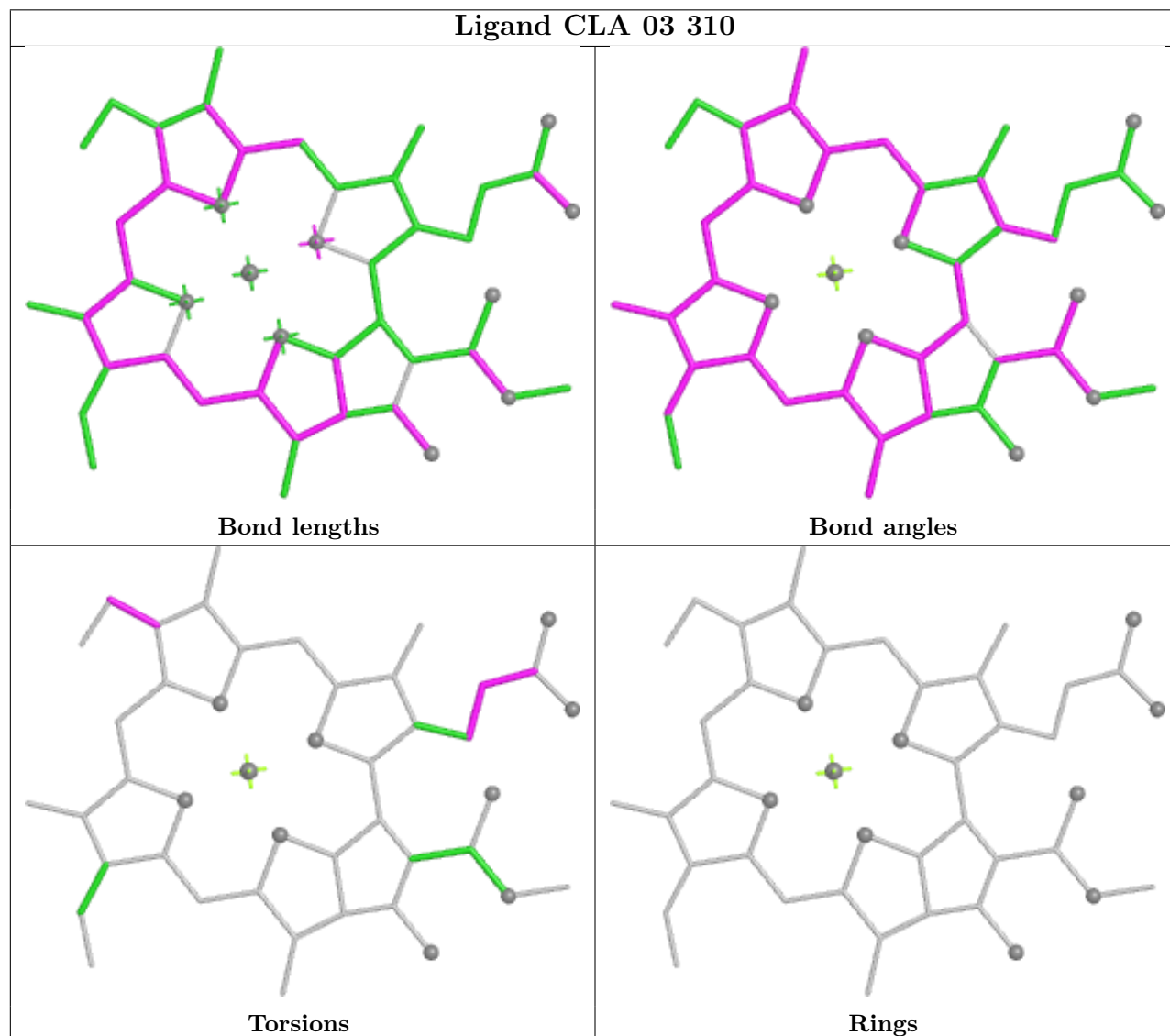
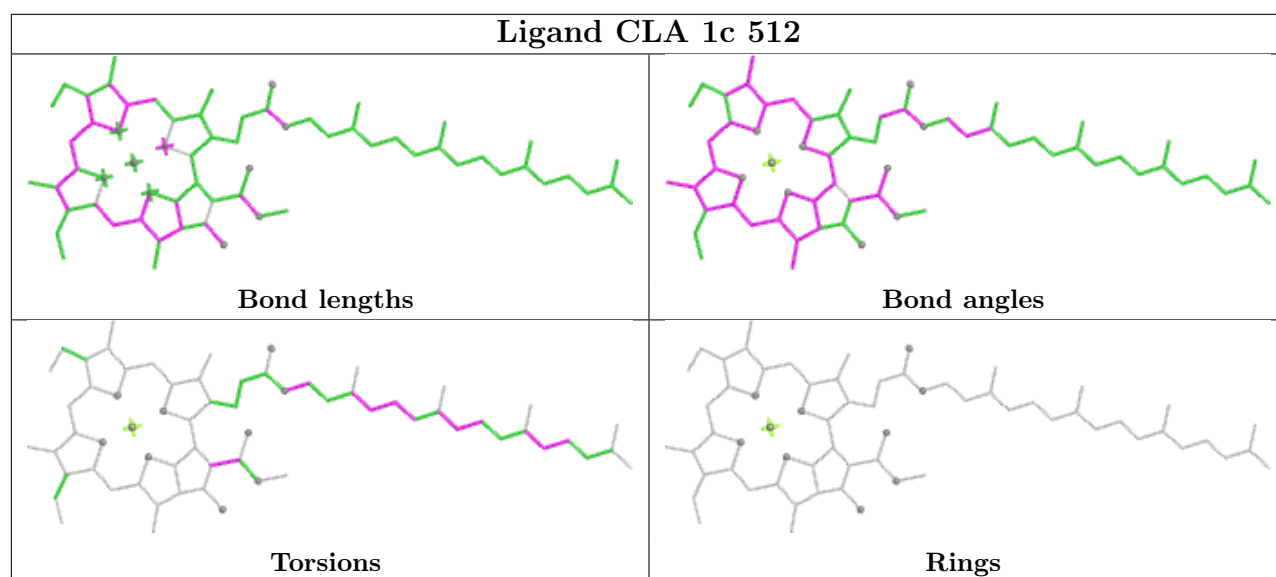
Ligand DGD 1b 627

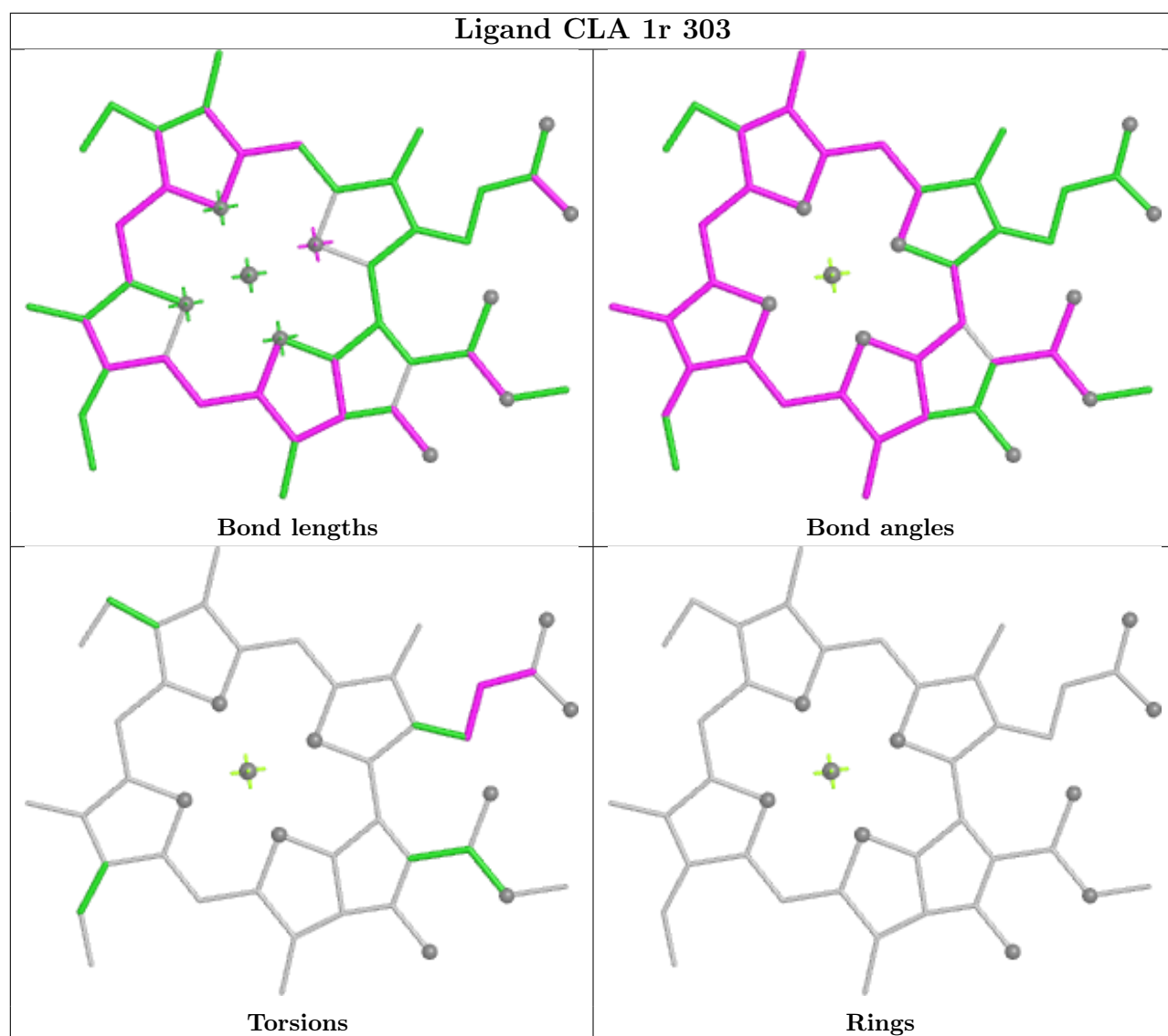




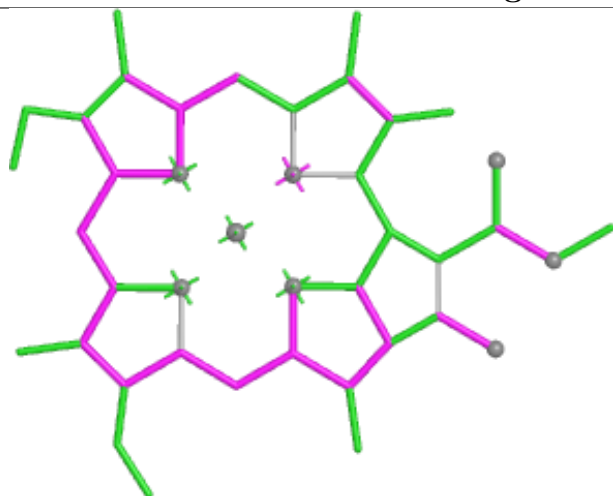








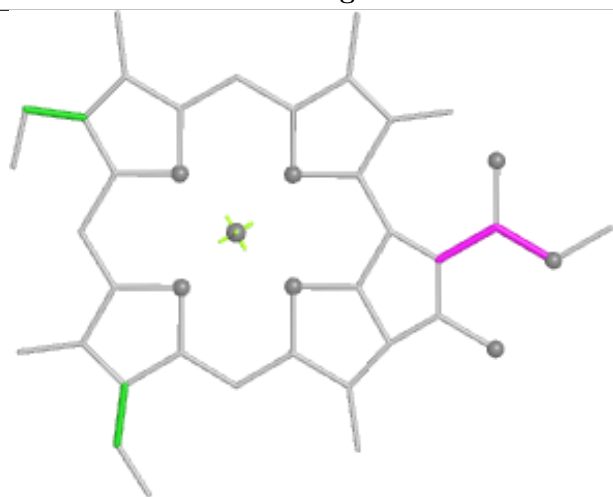
Ligand CLA 1N 315



Bond lengths



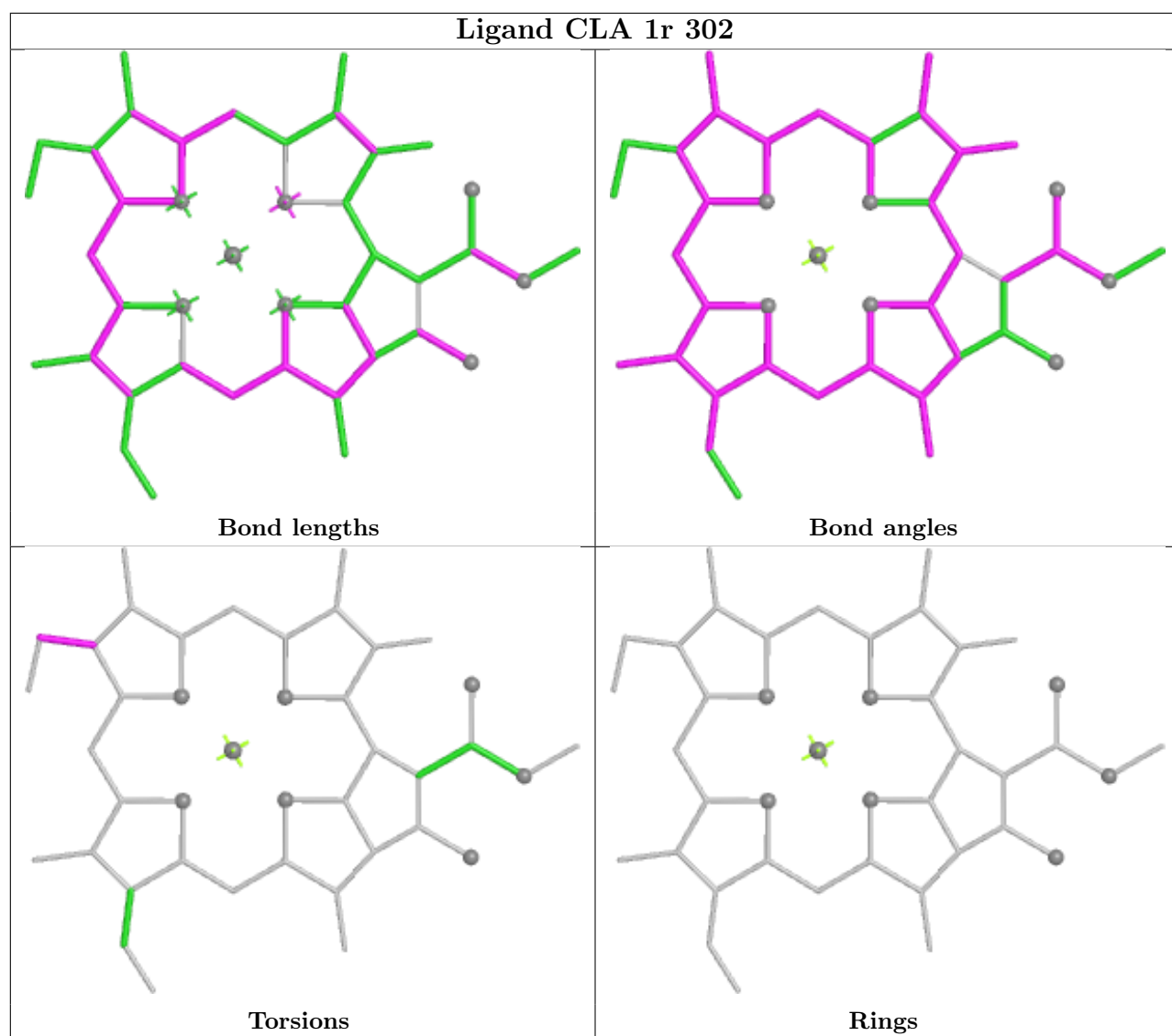
Bond angles

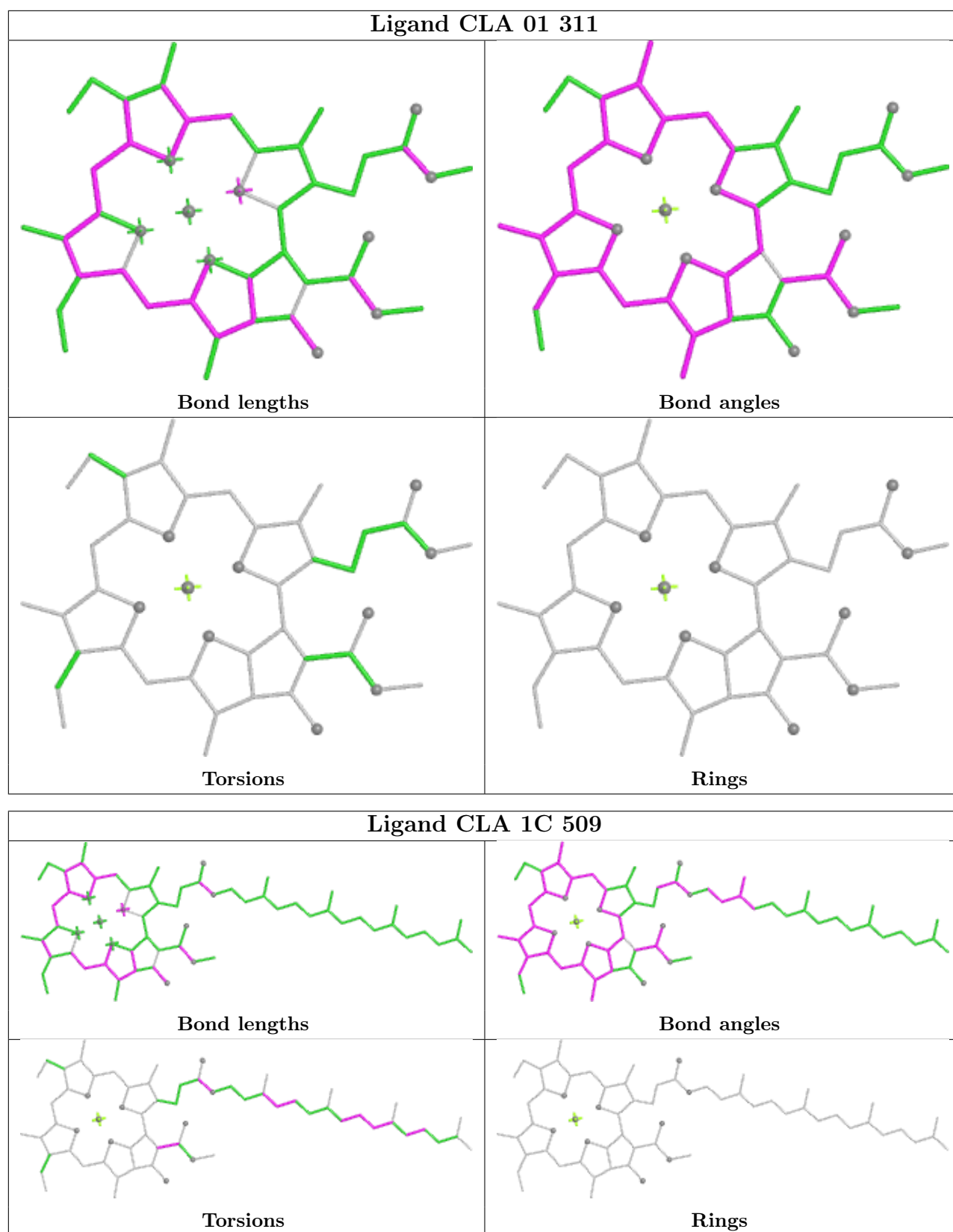


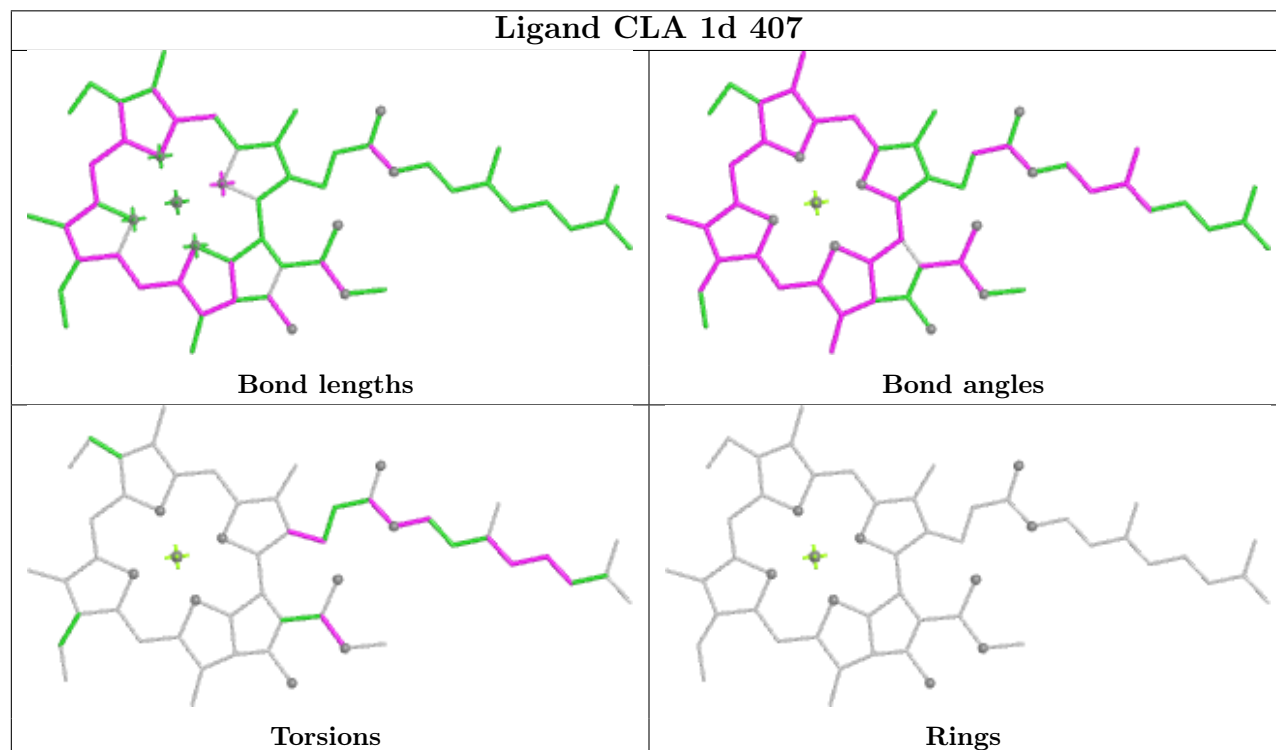
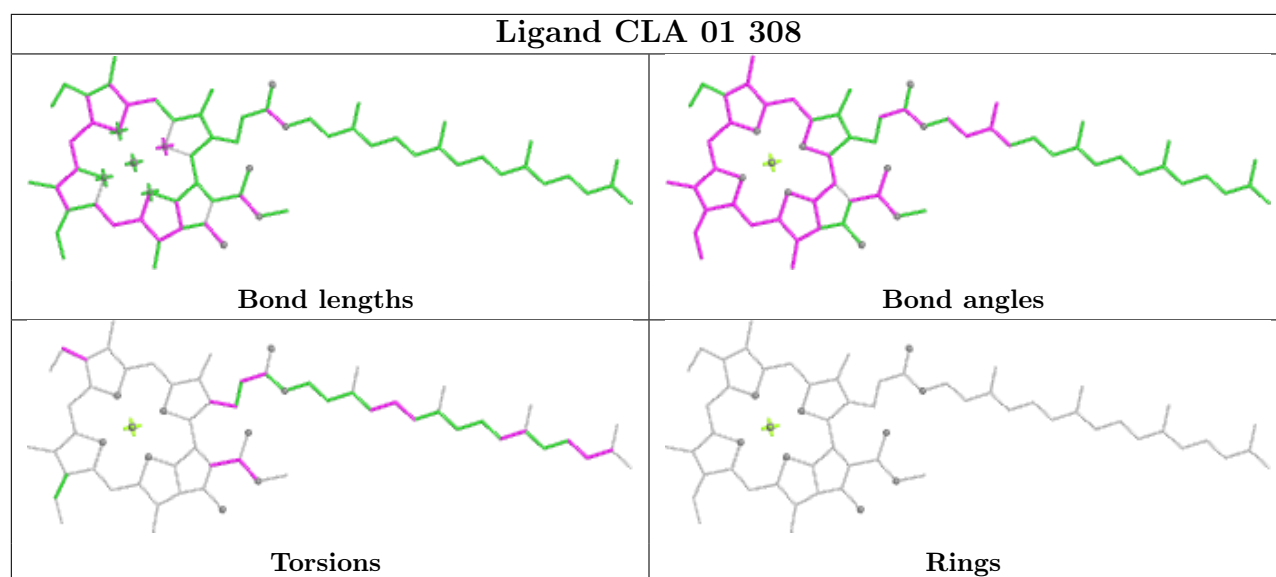
Torsions

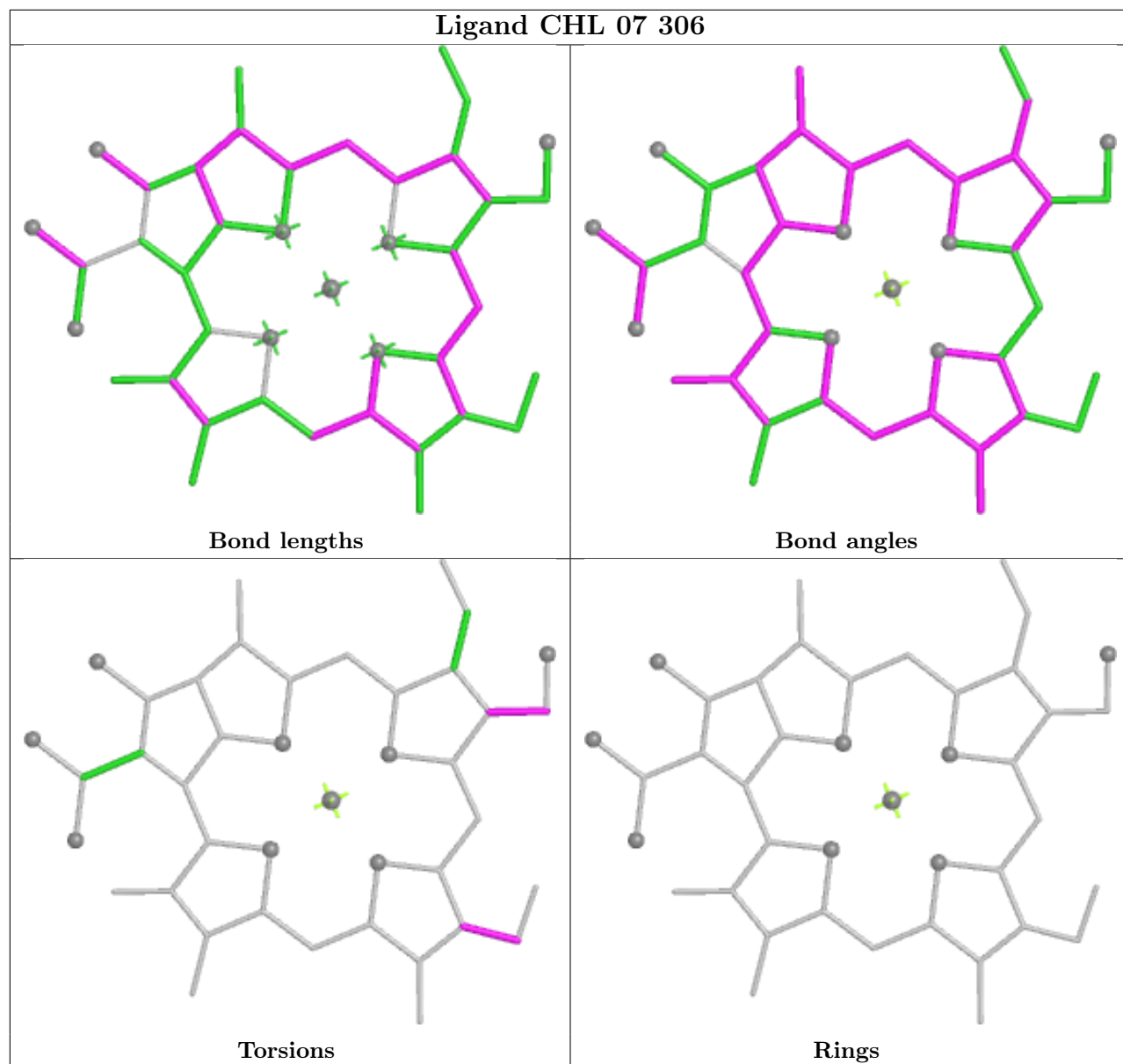


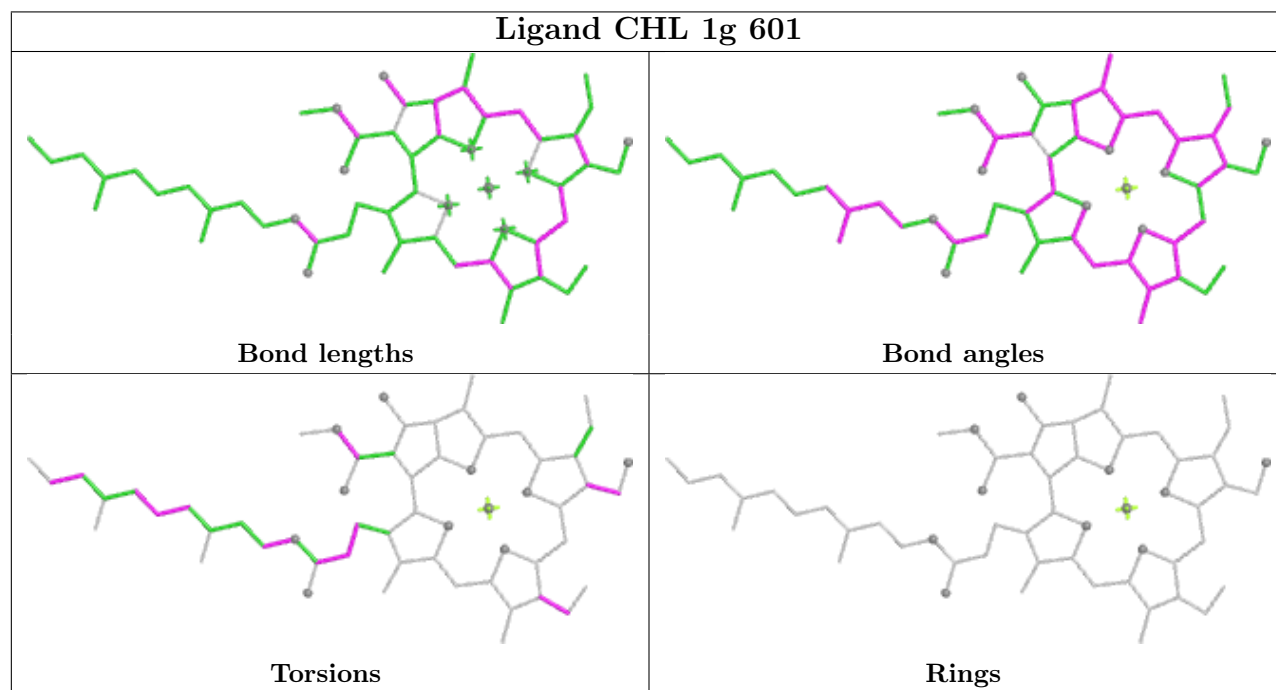
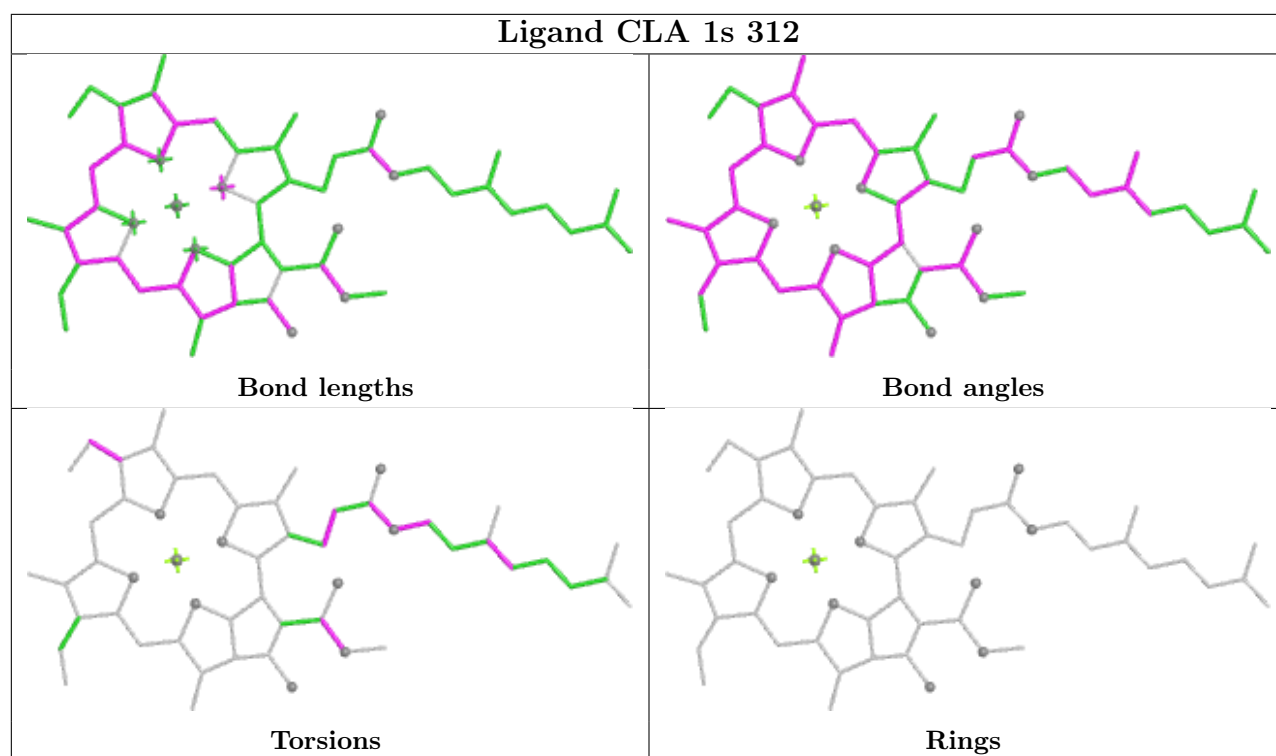
Rings

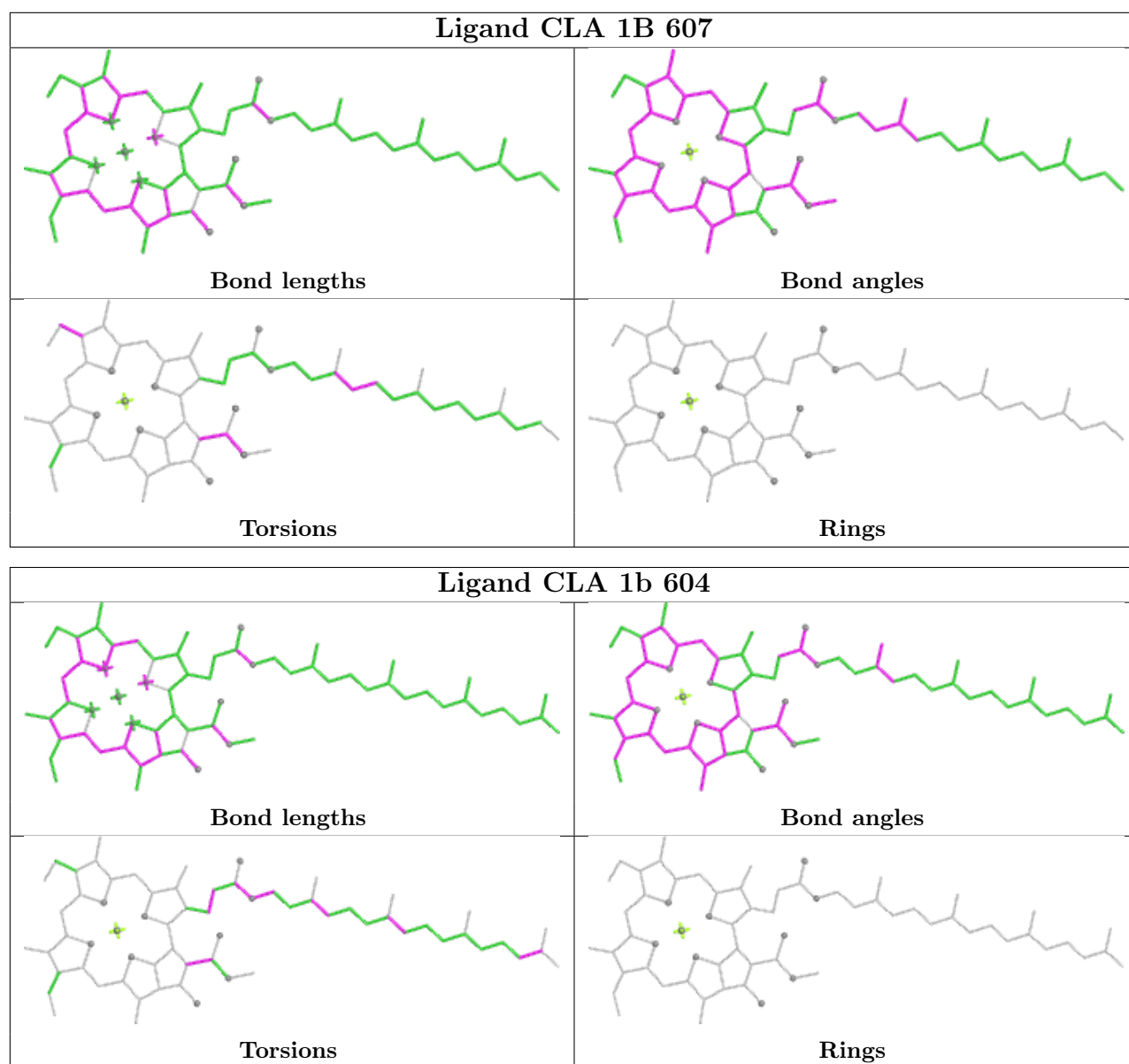


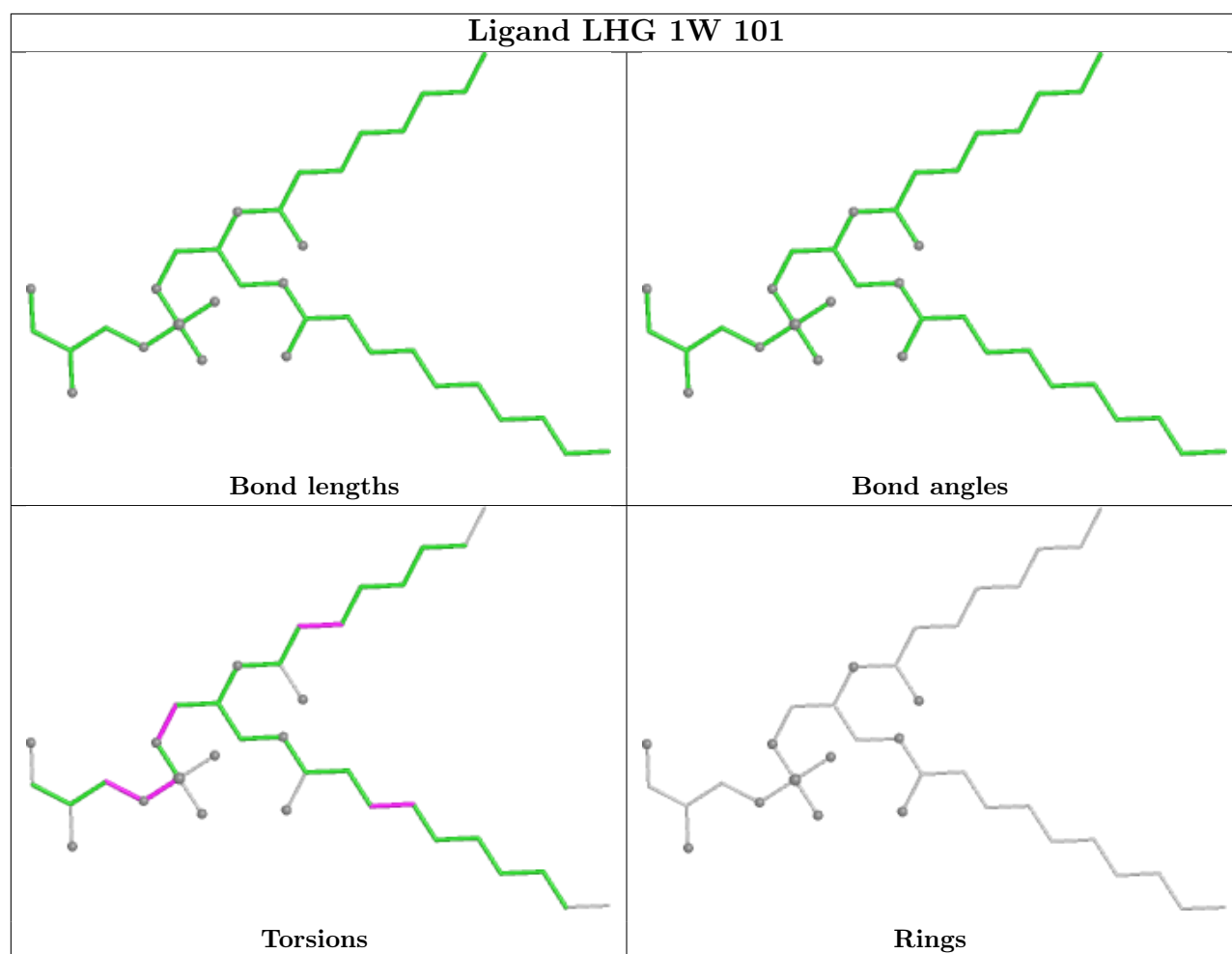


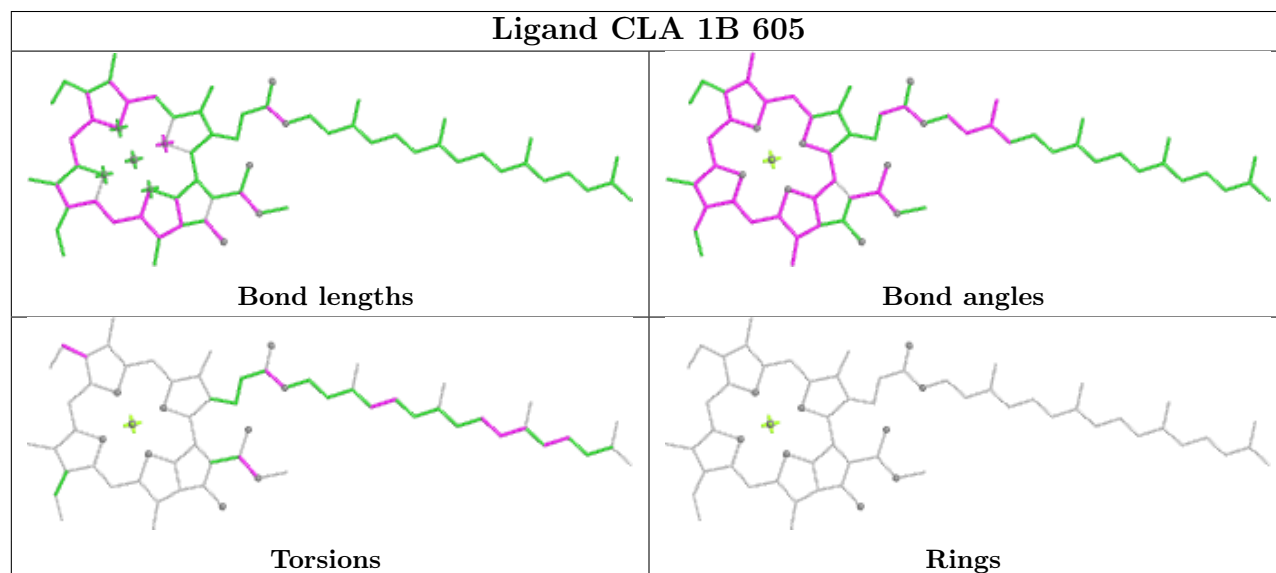
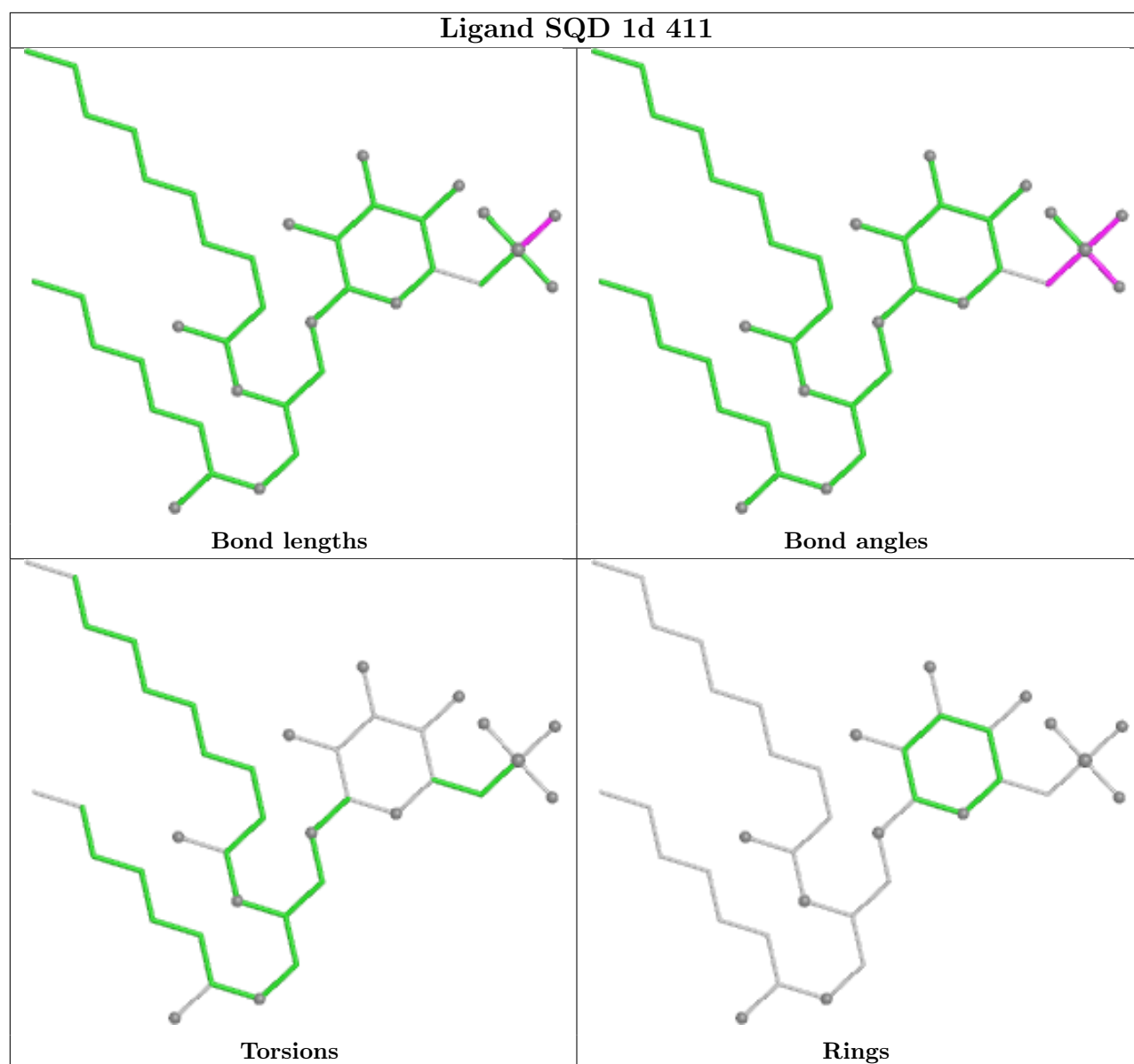


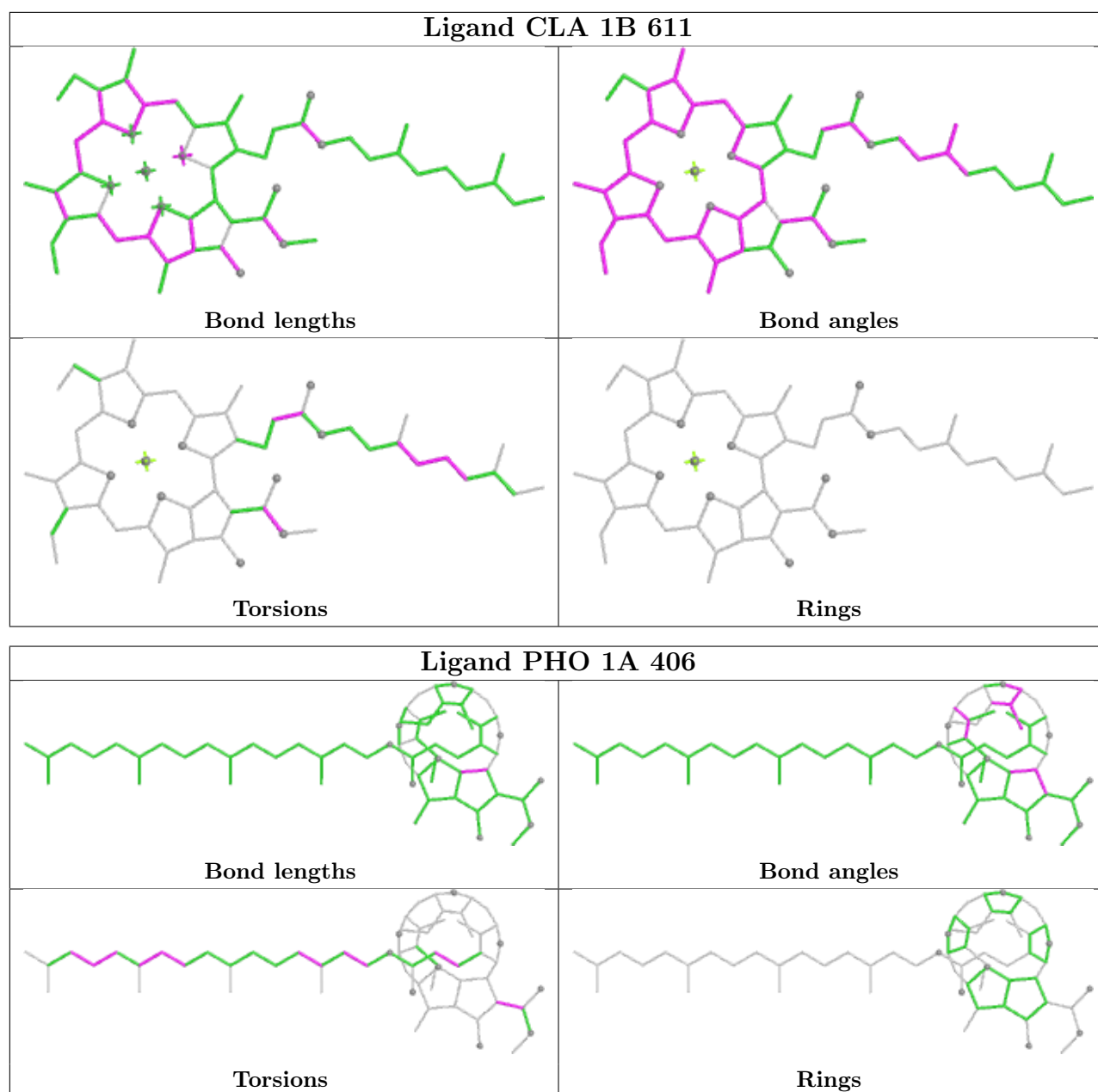


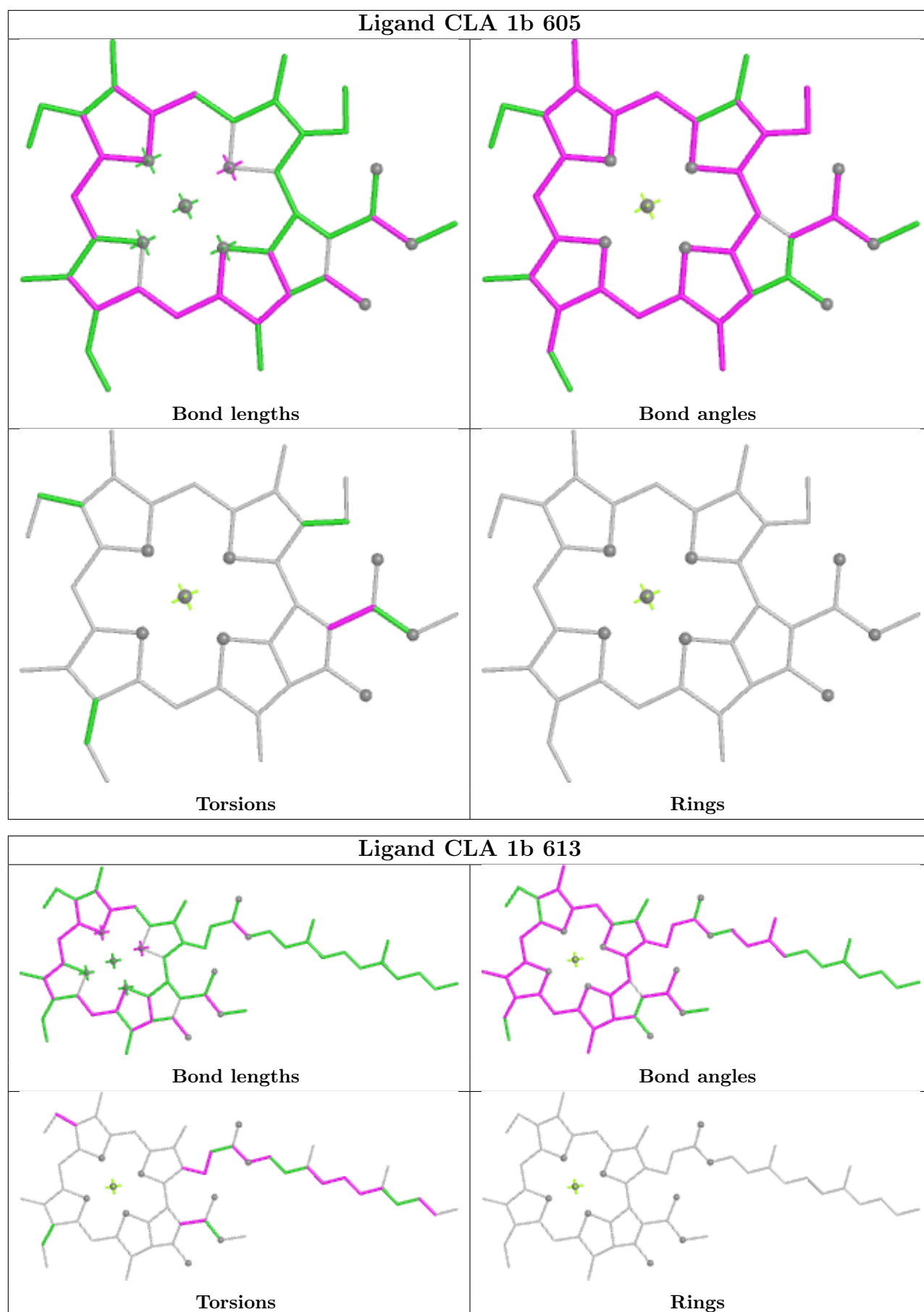


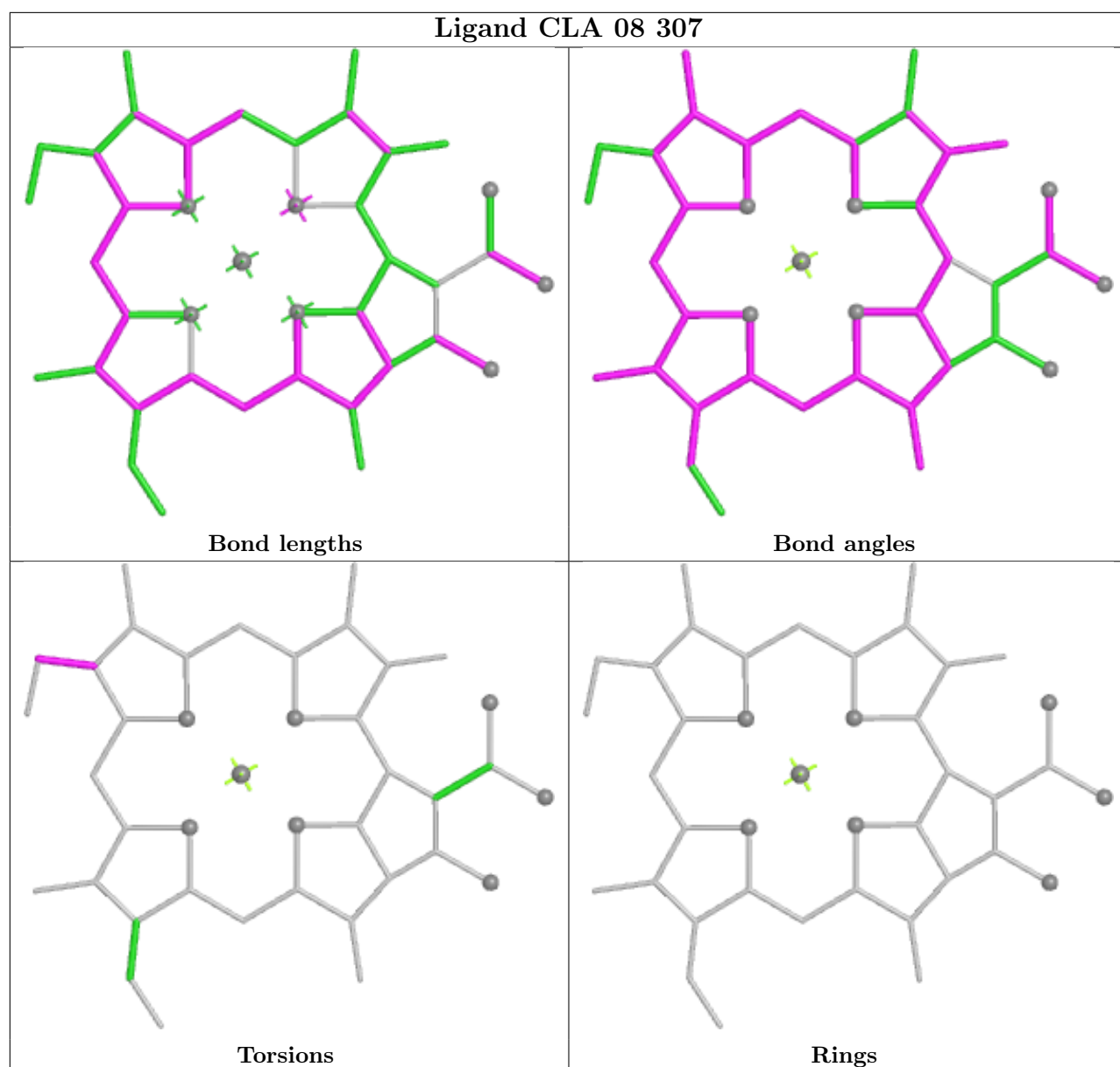


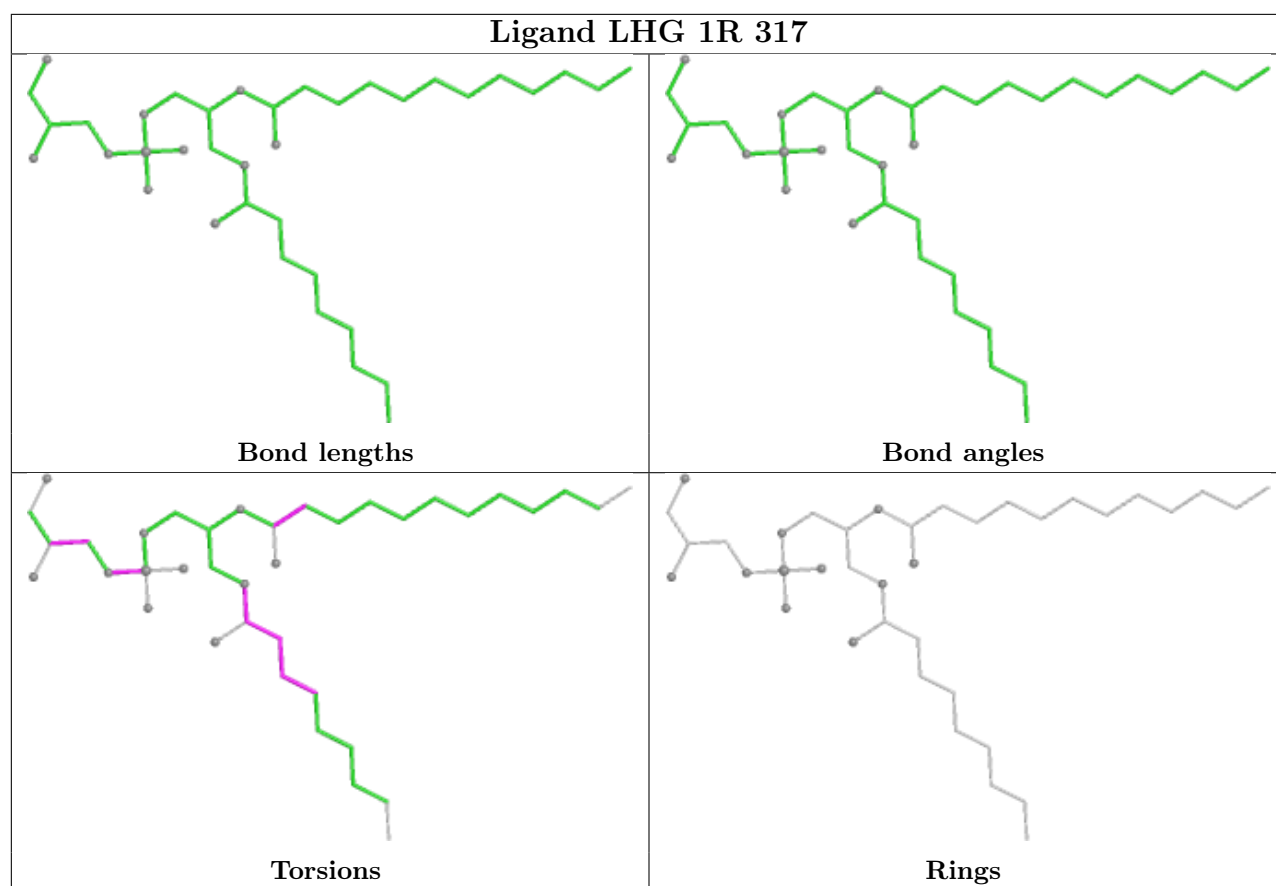


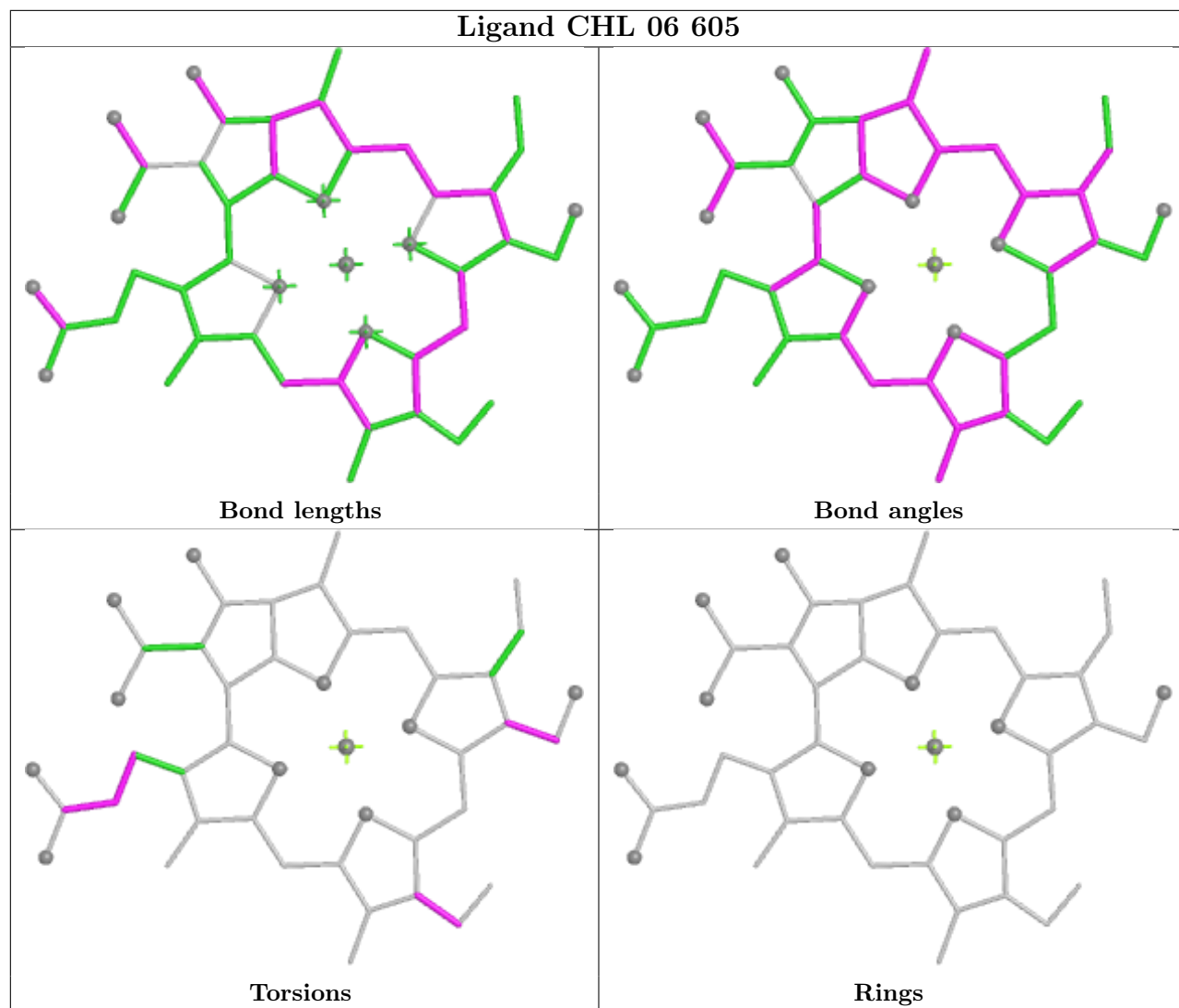


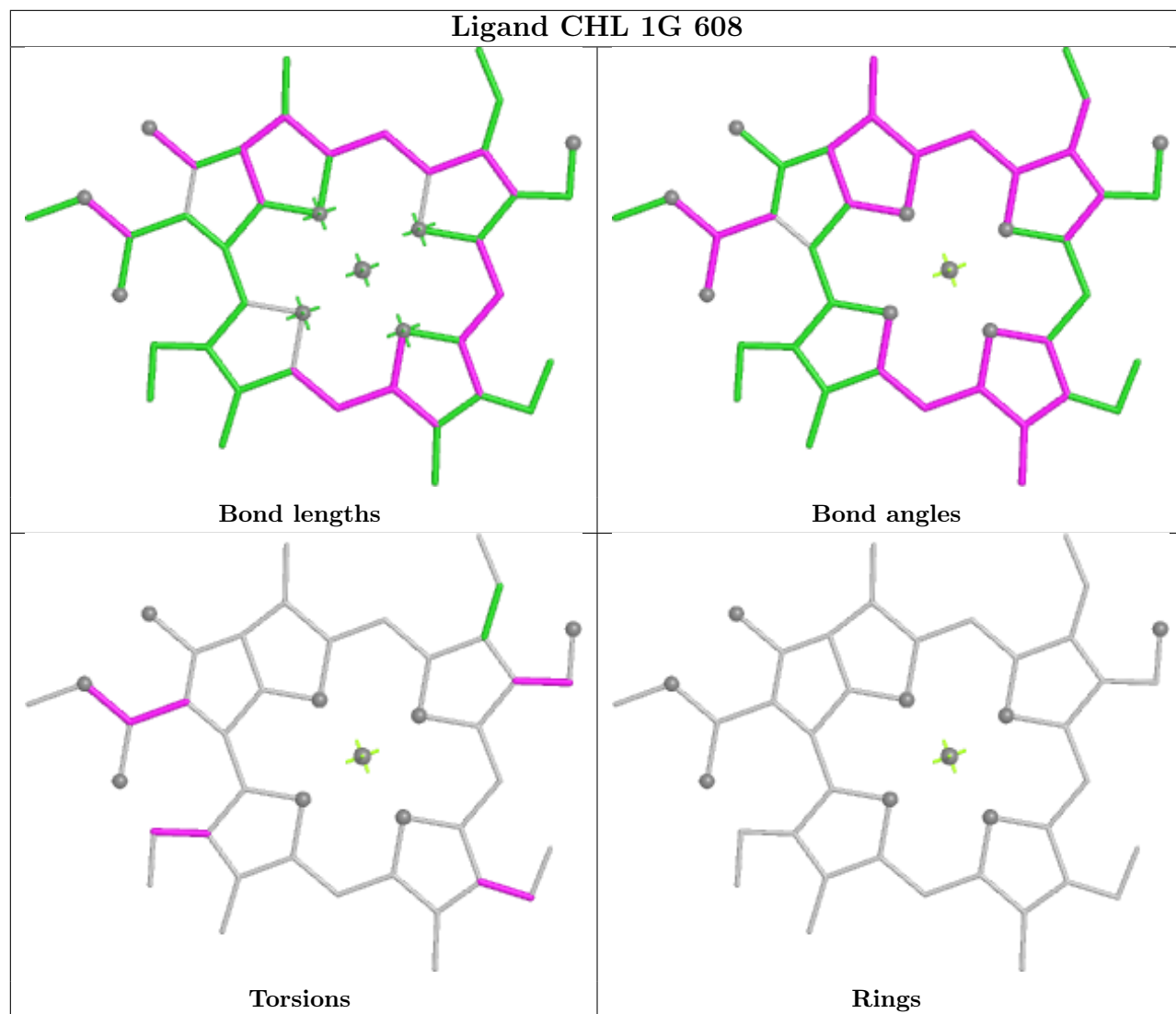


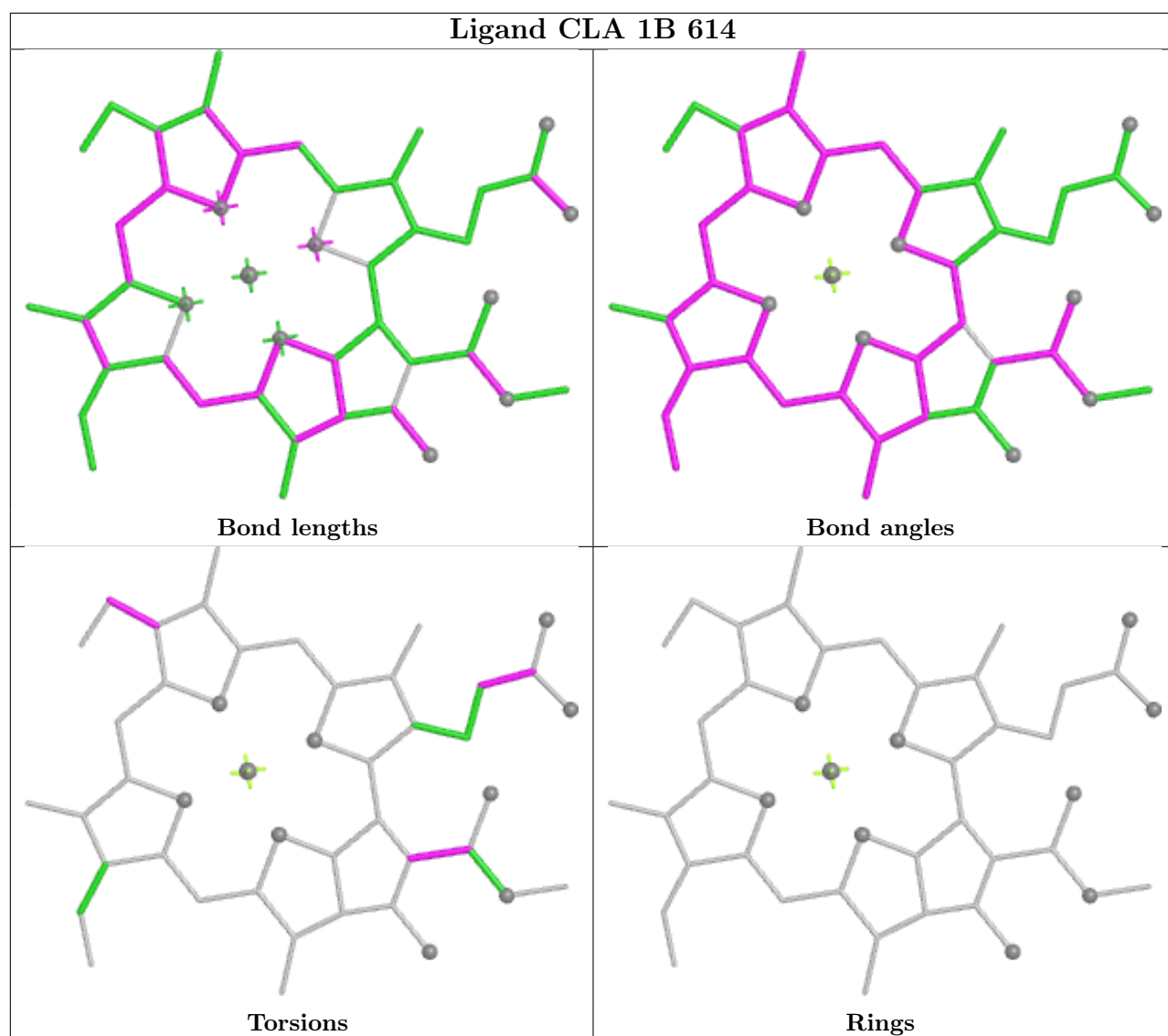


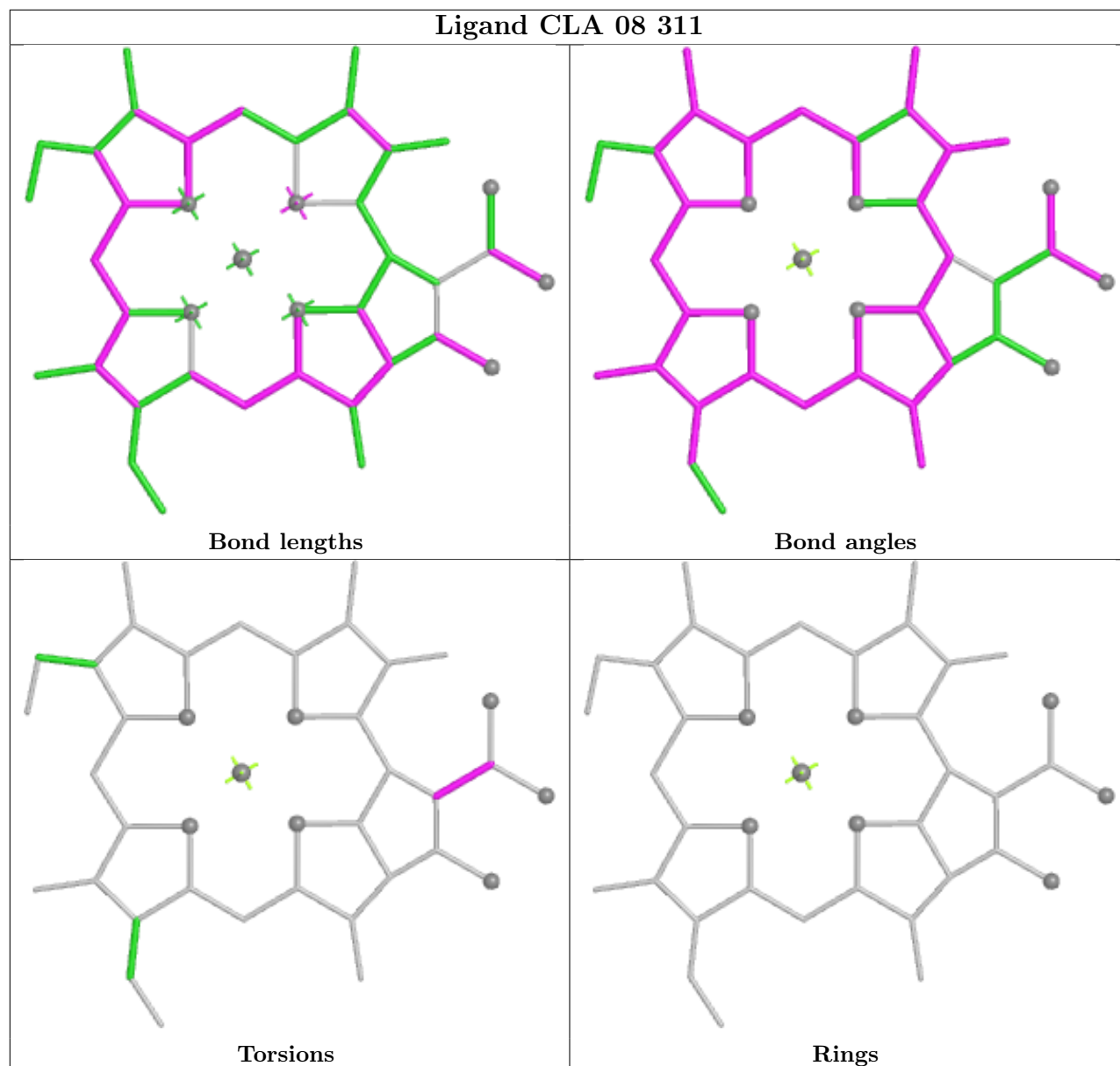


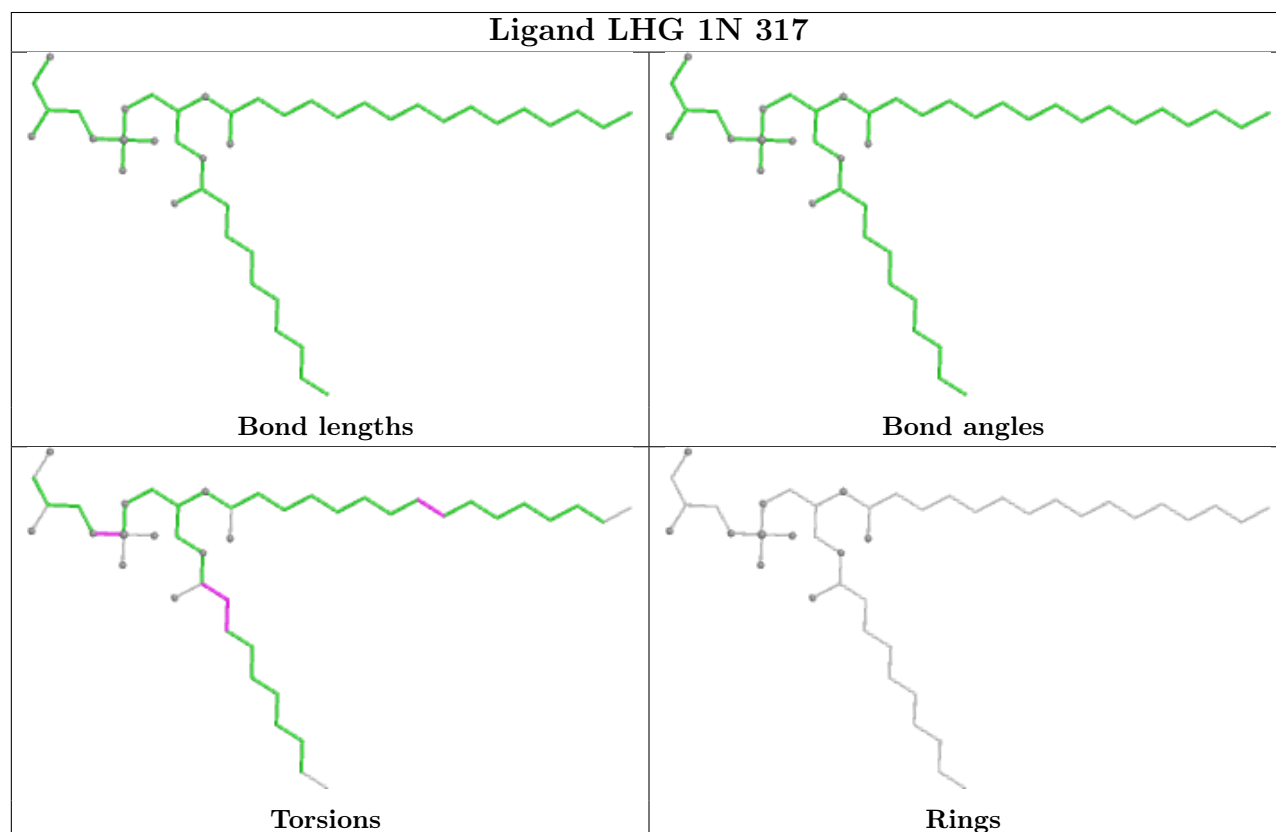
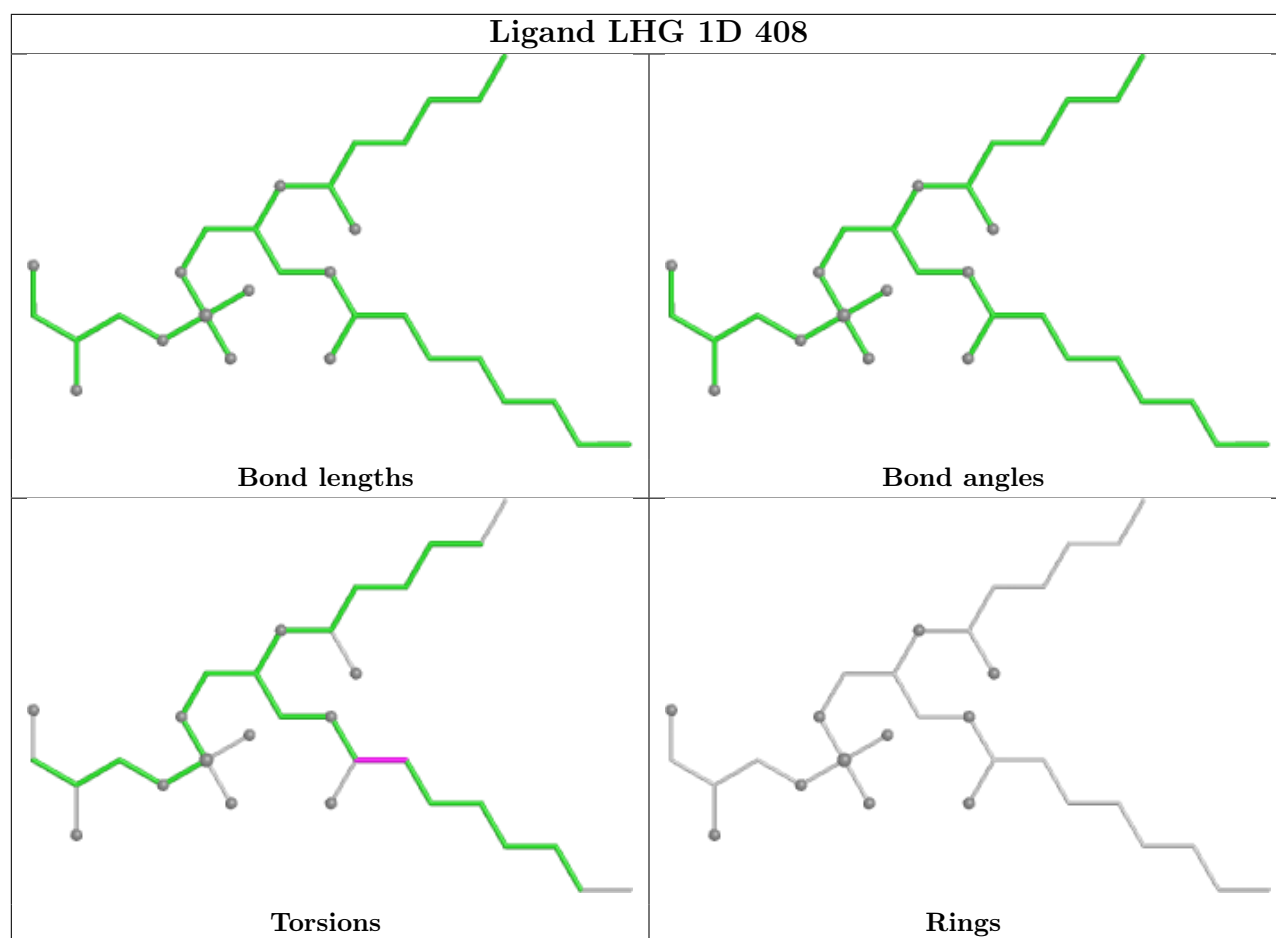


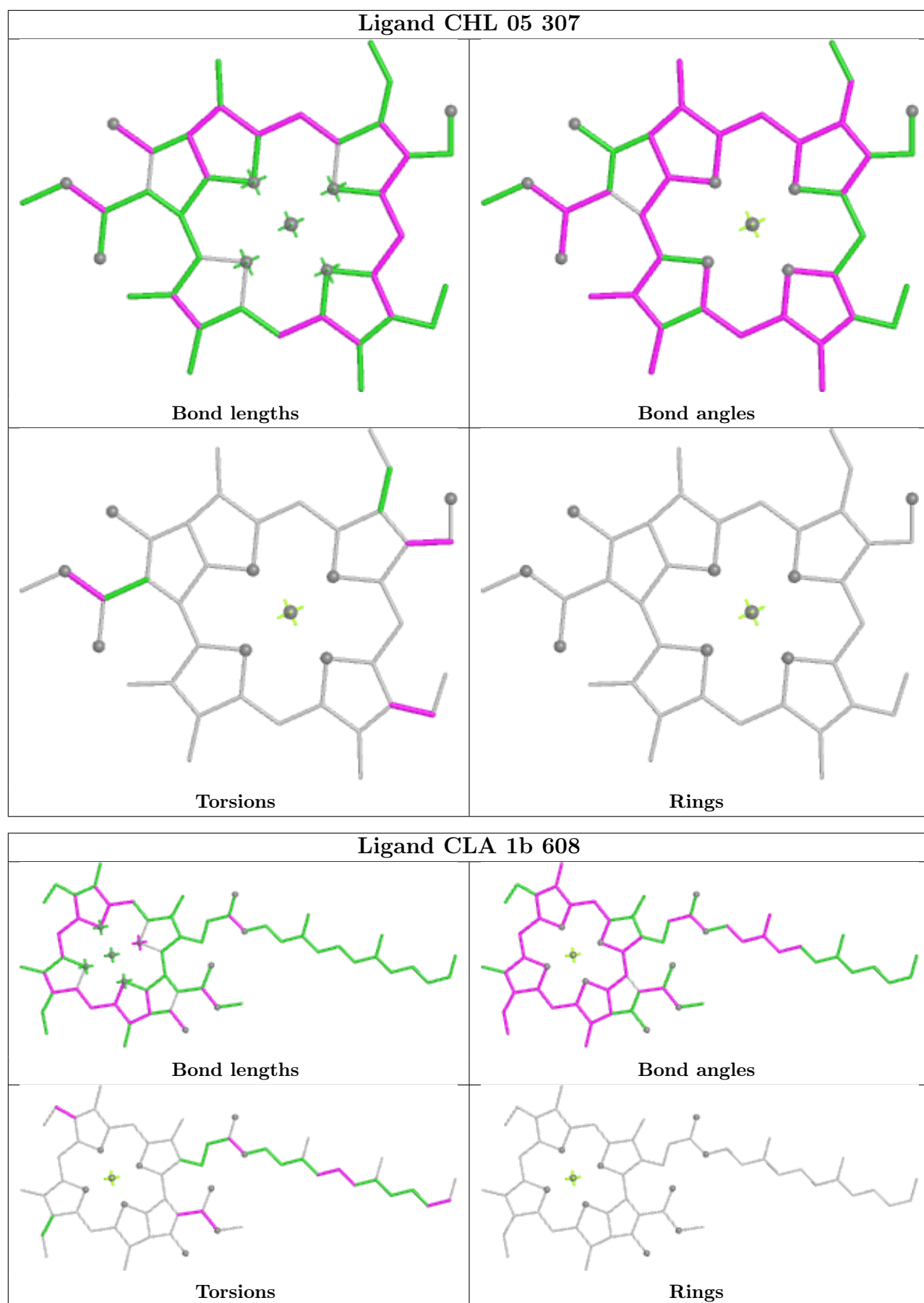


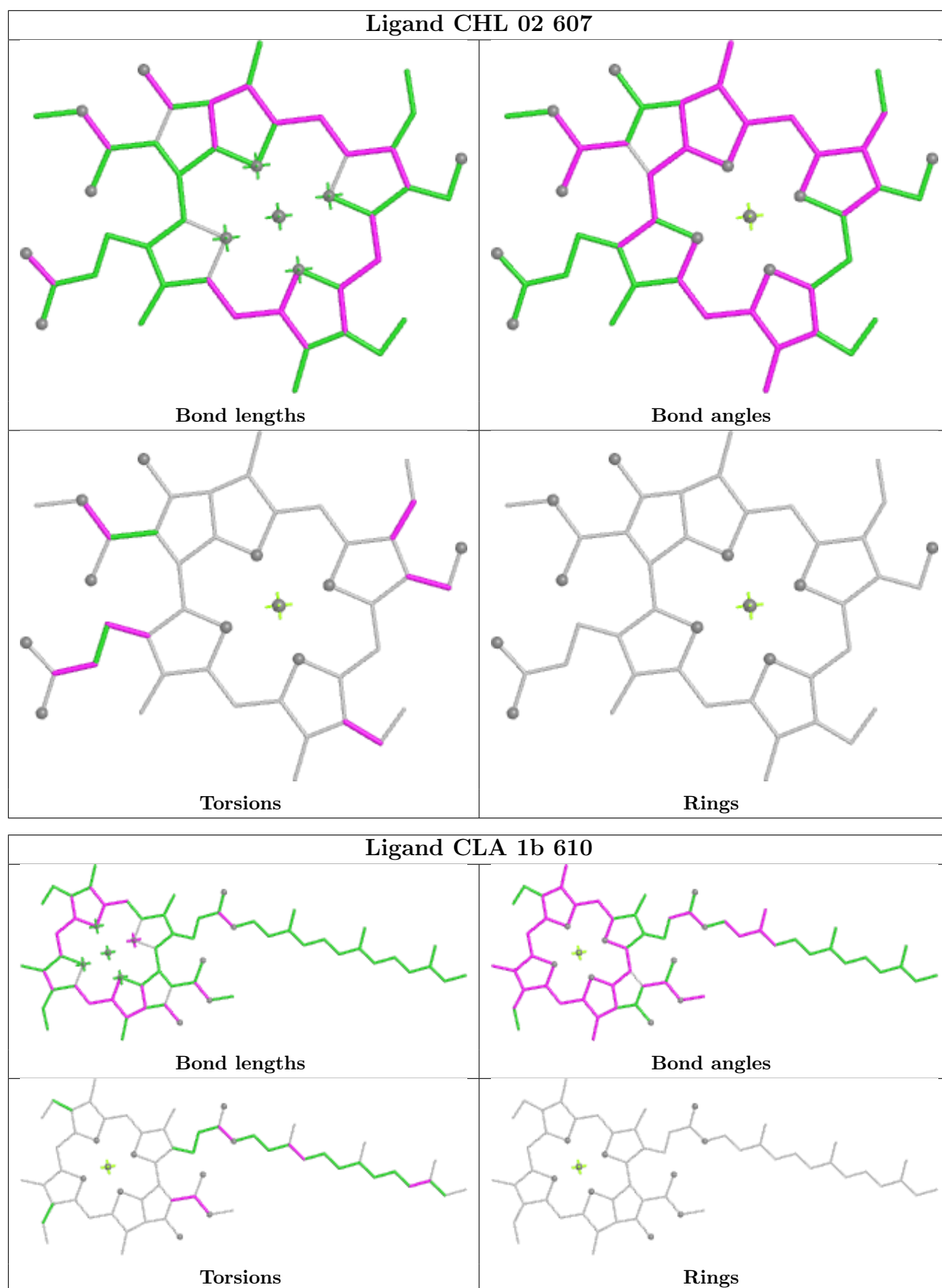


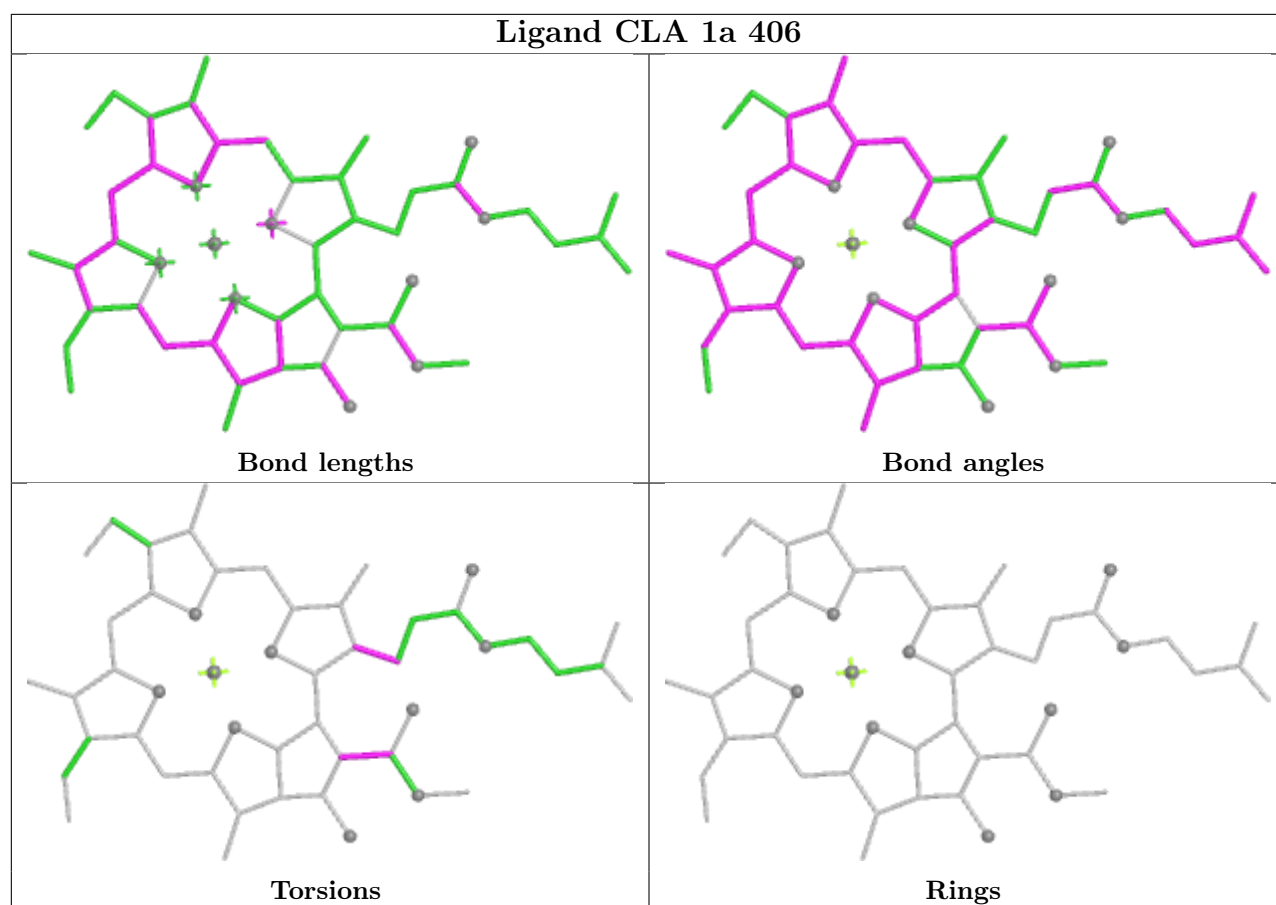


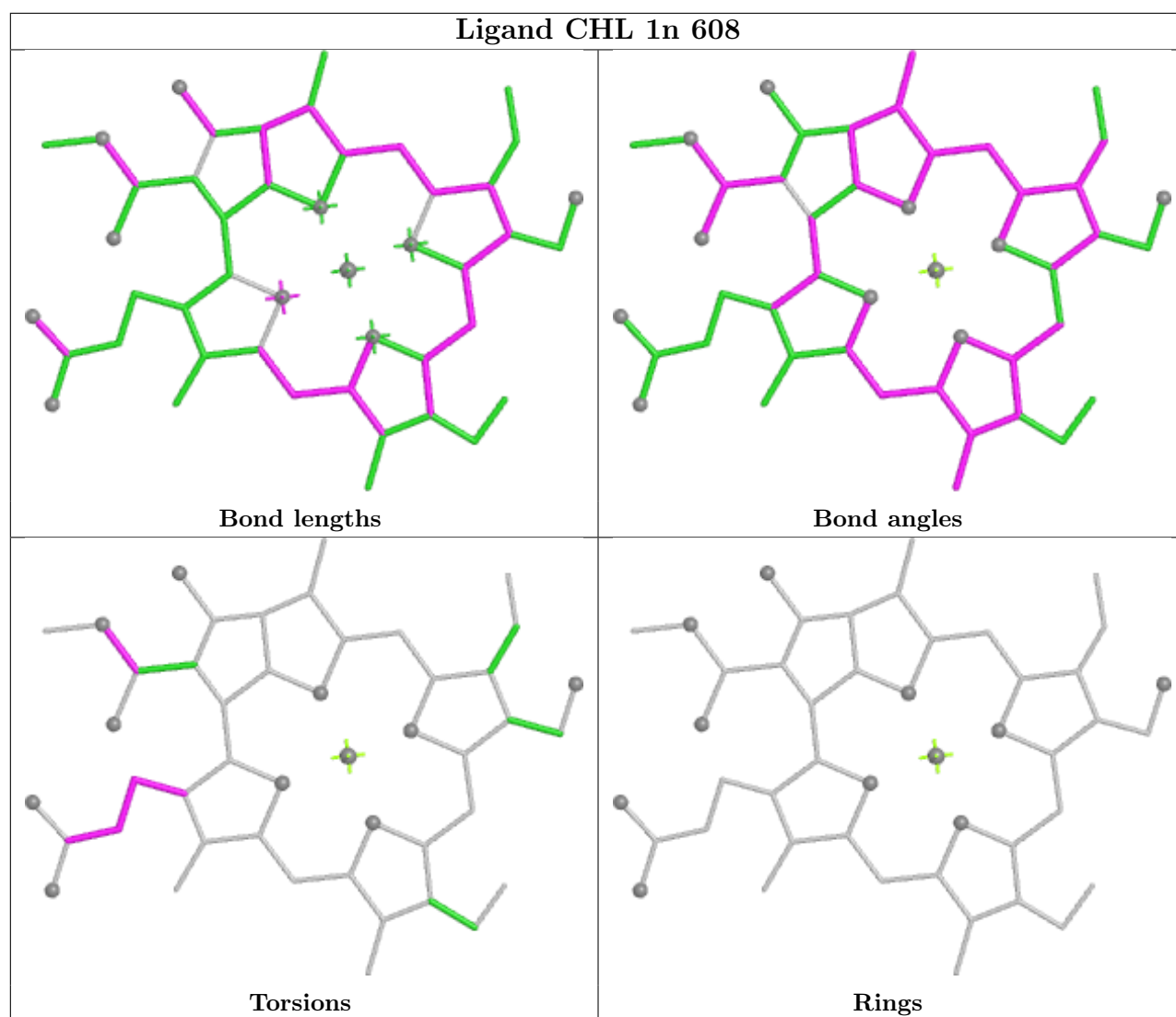


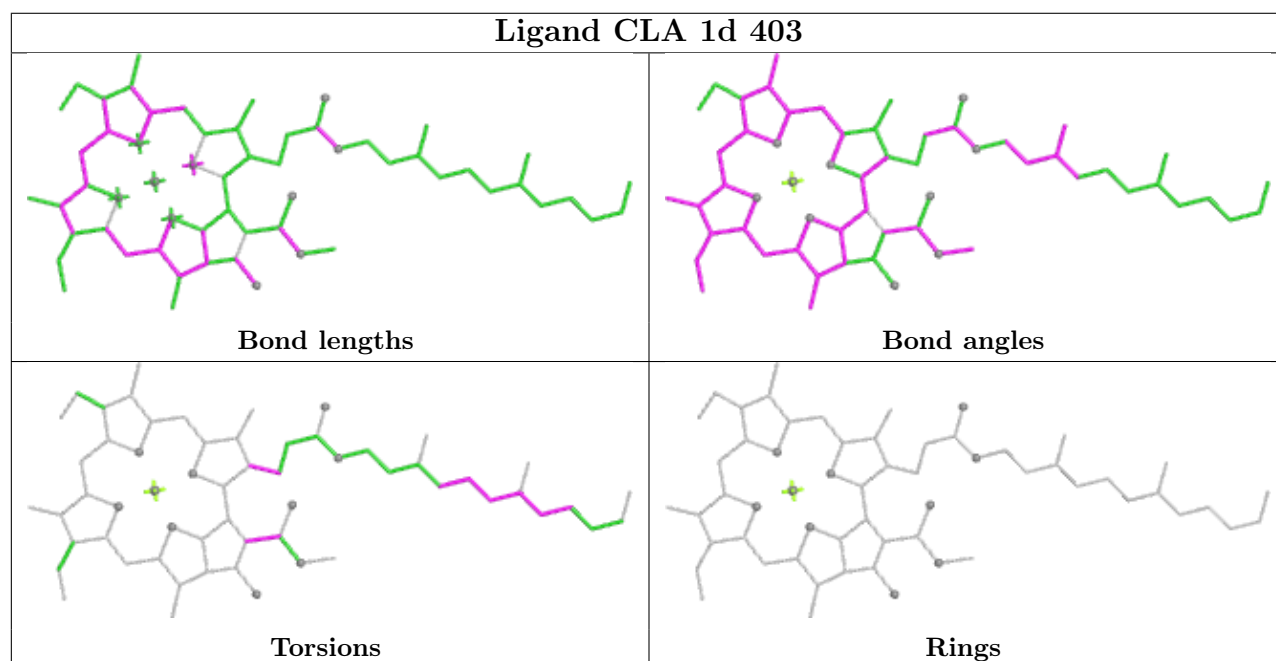
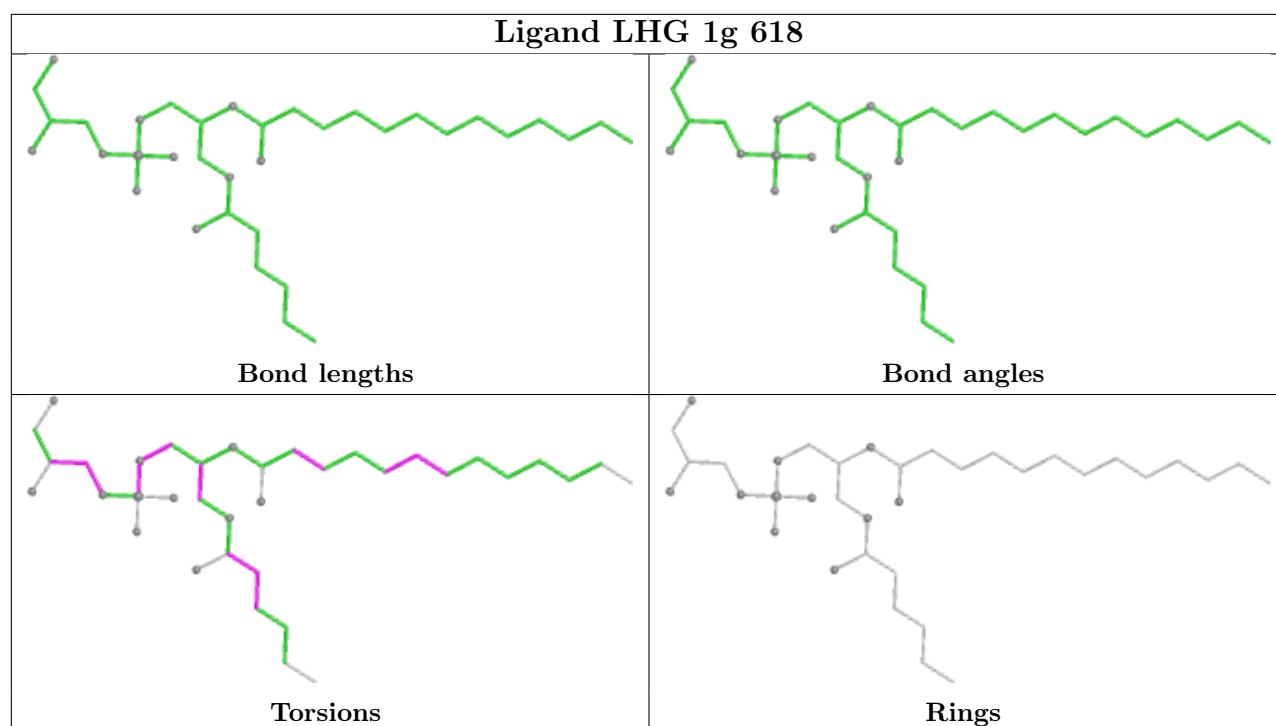




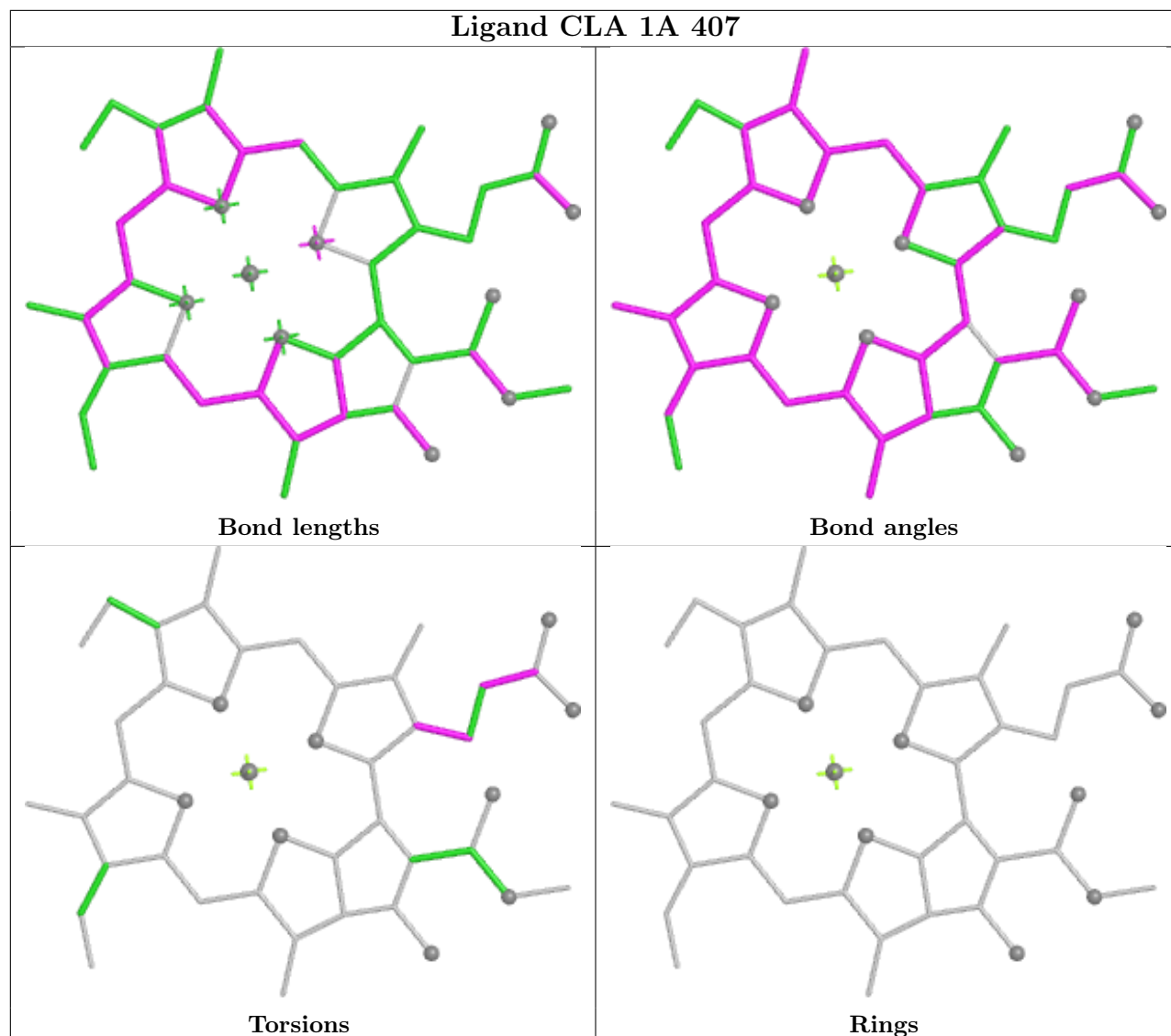




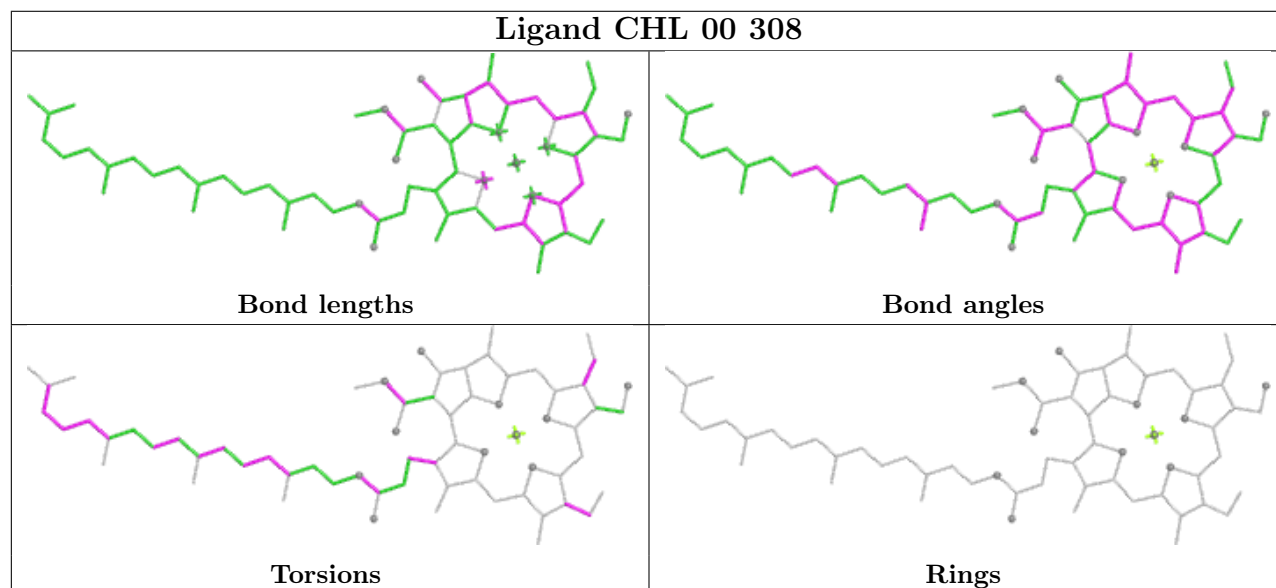


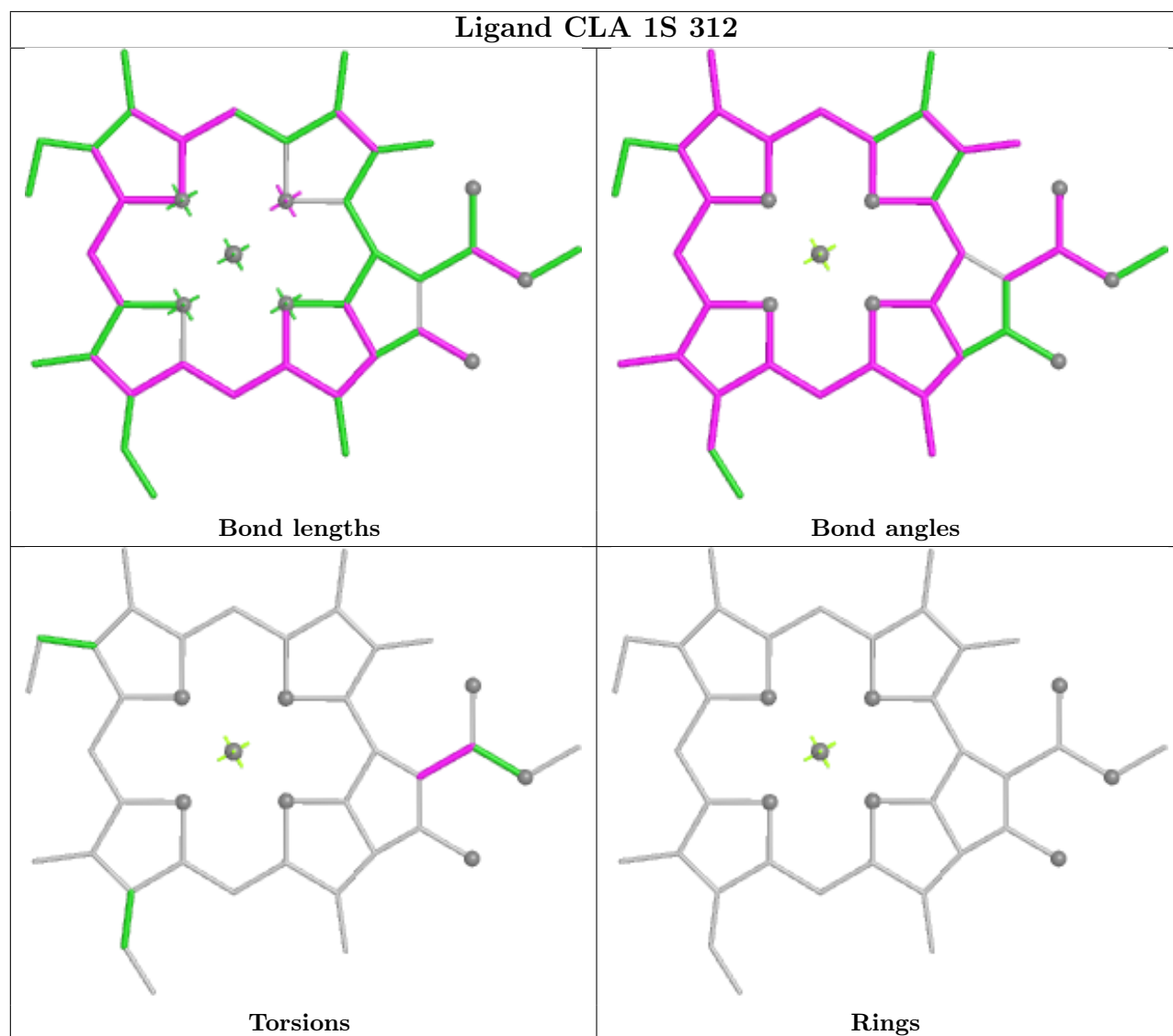
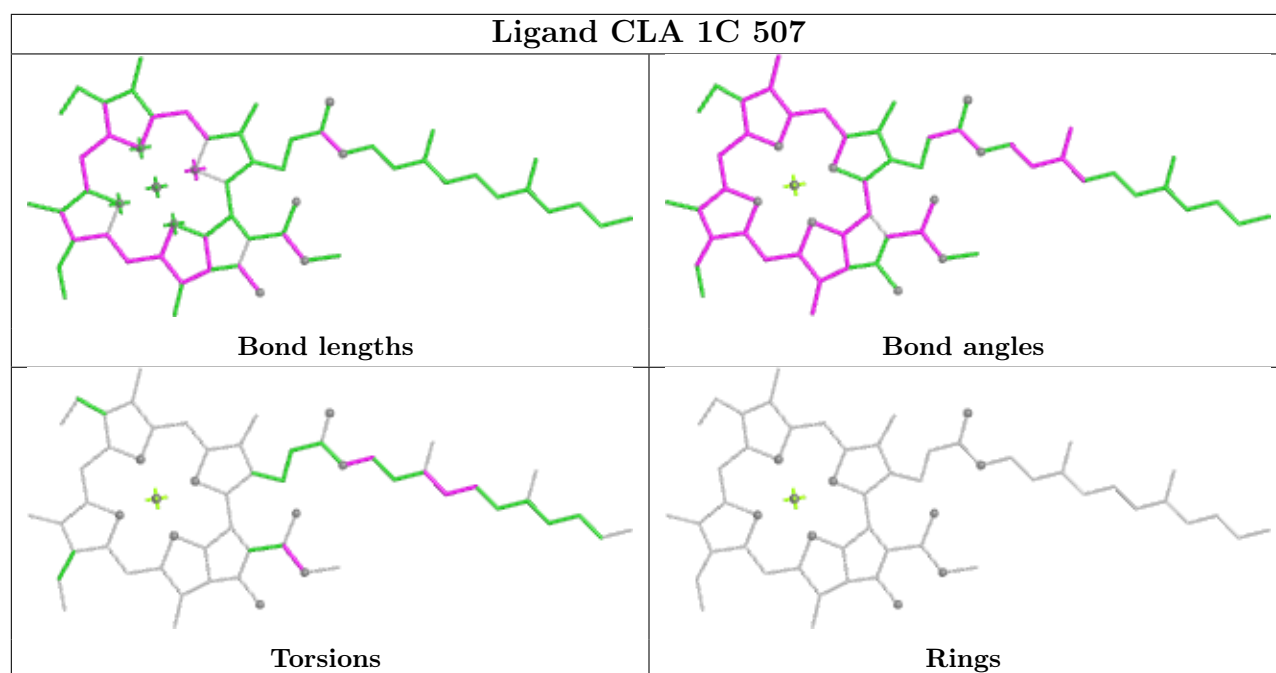


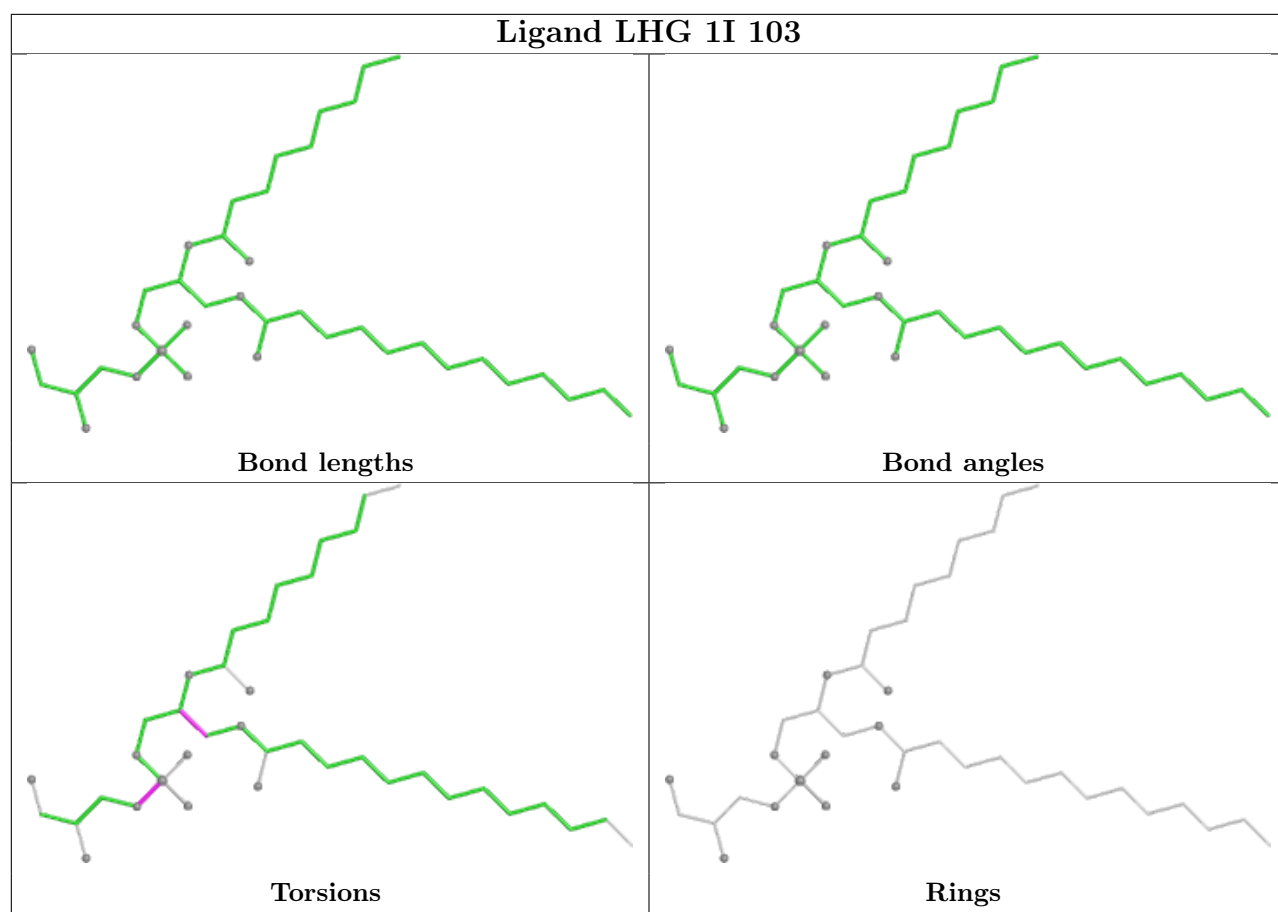
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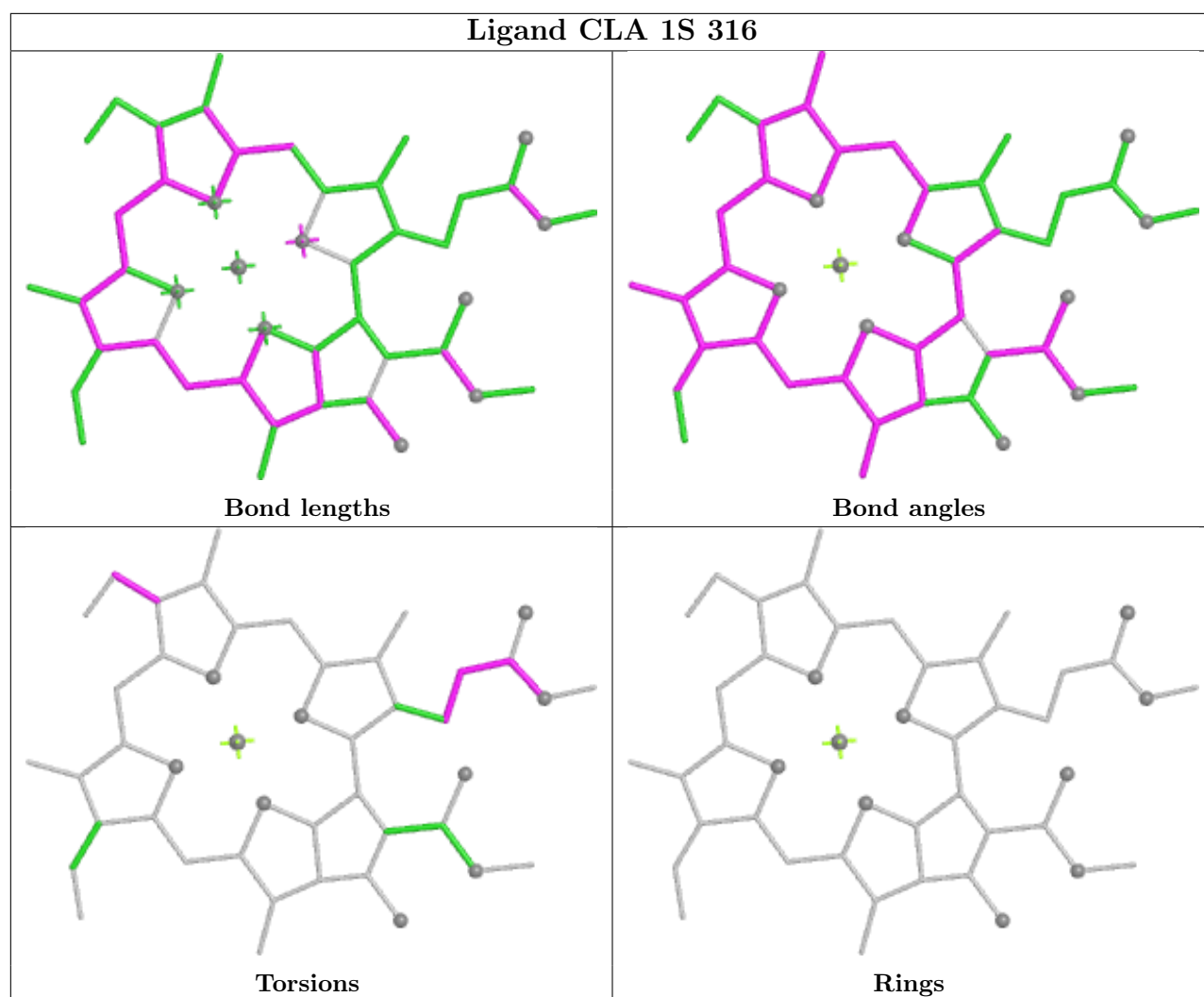


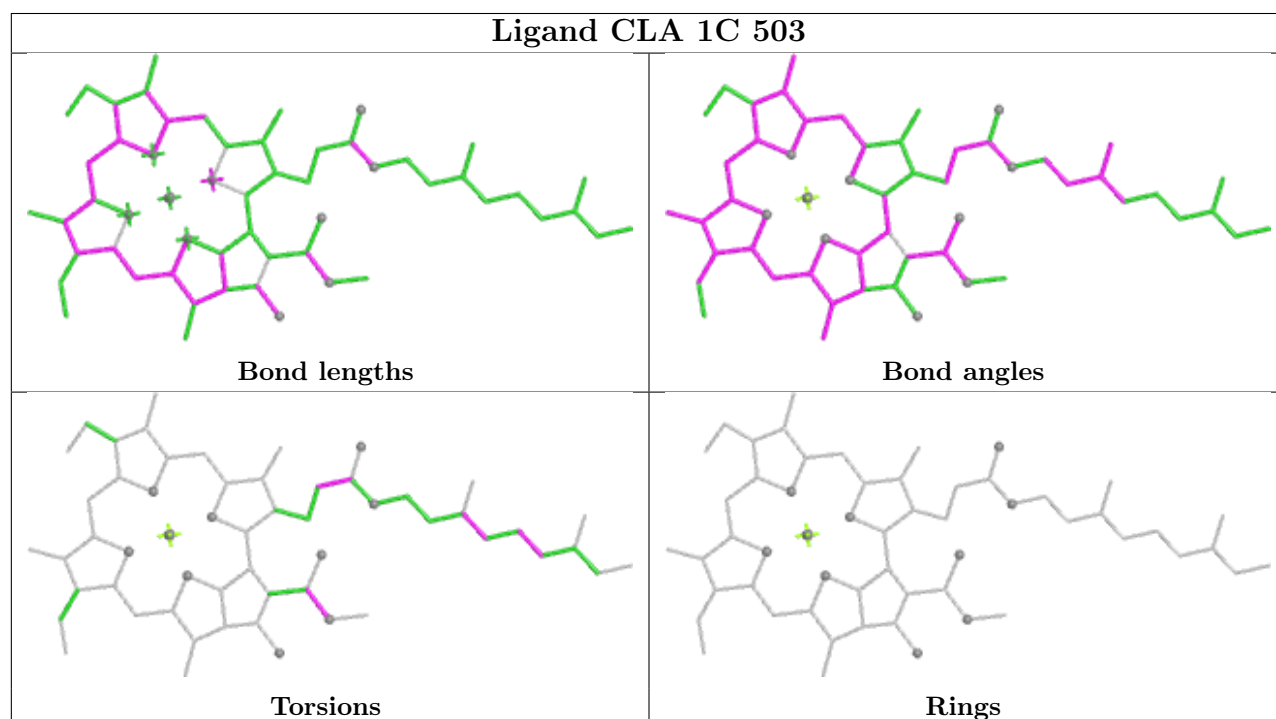
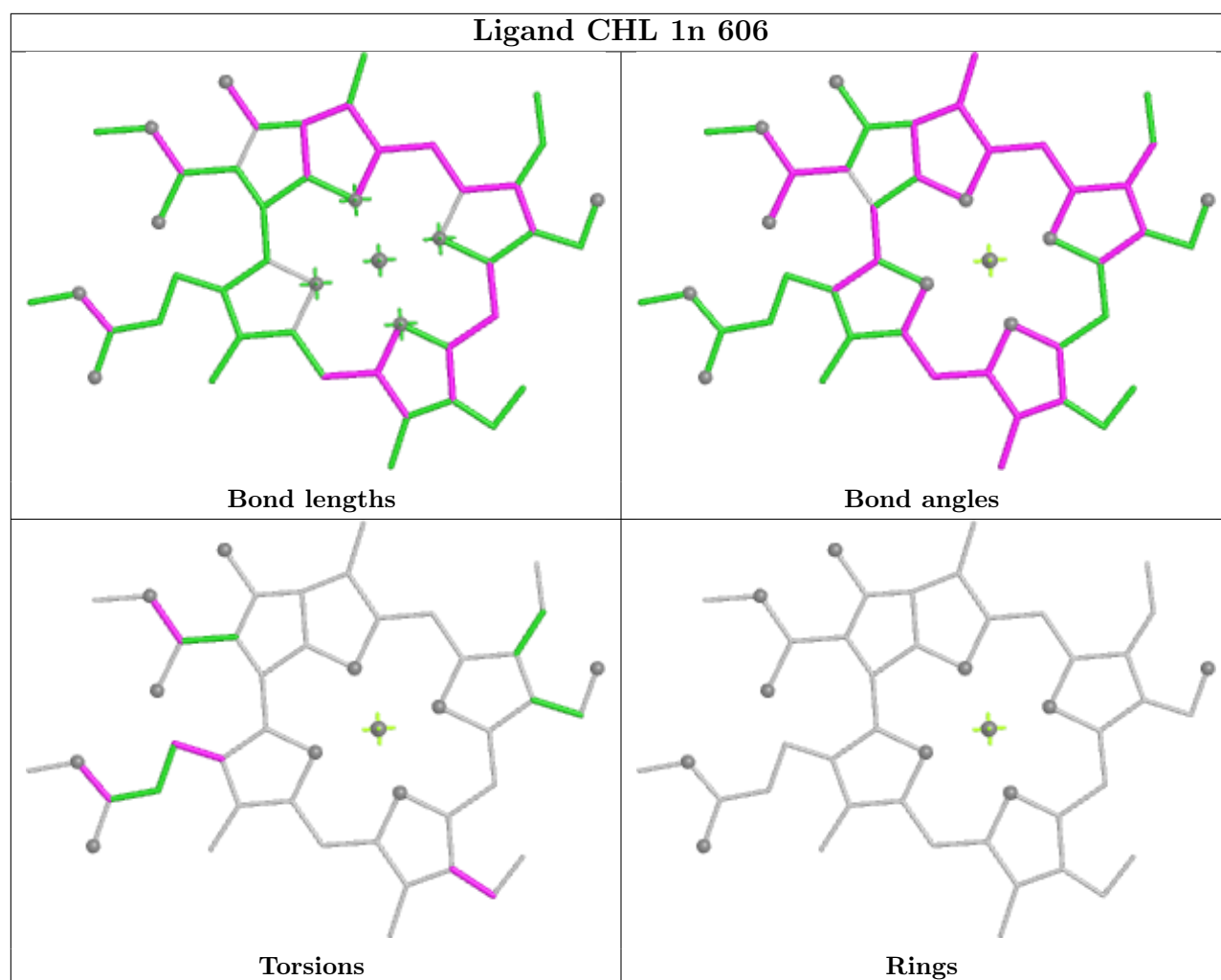
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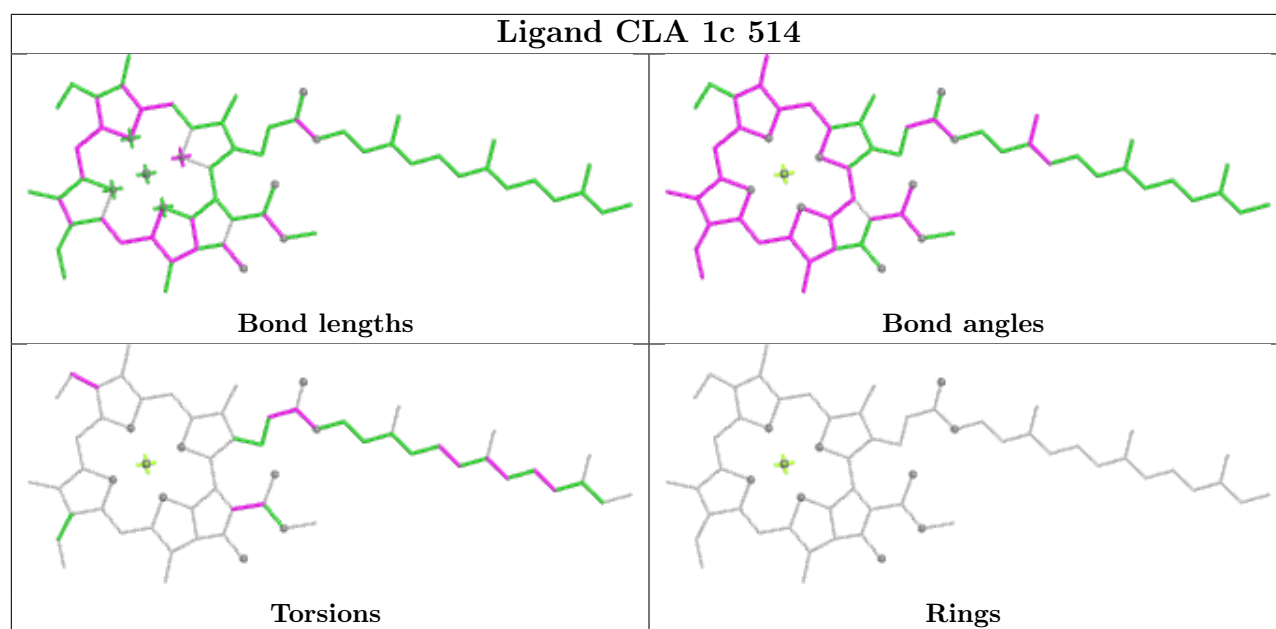


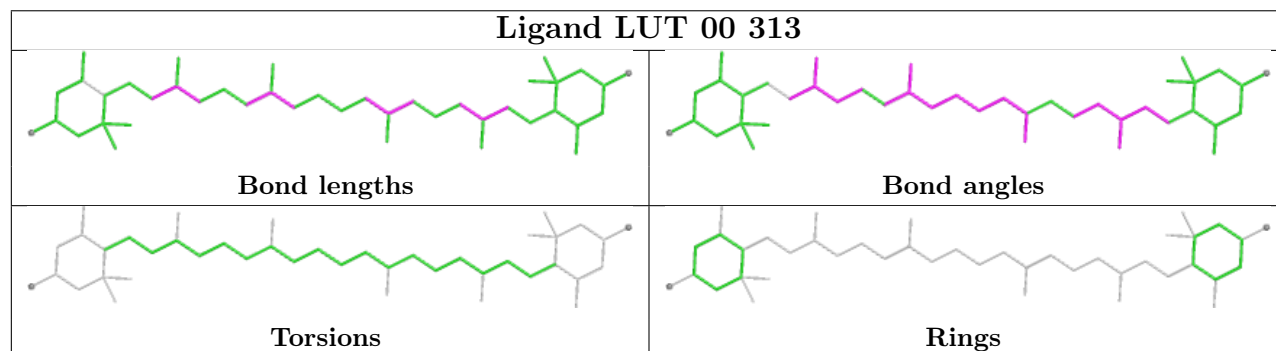
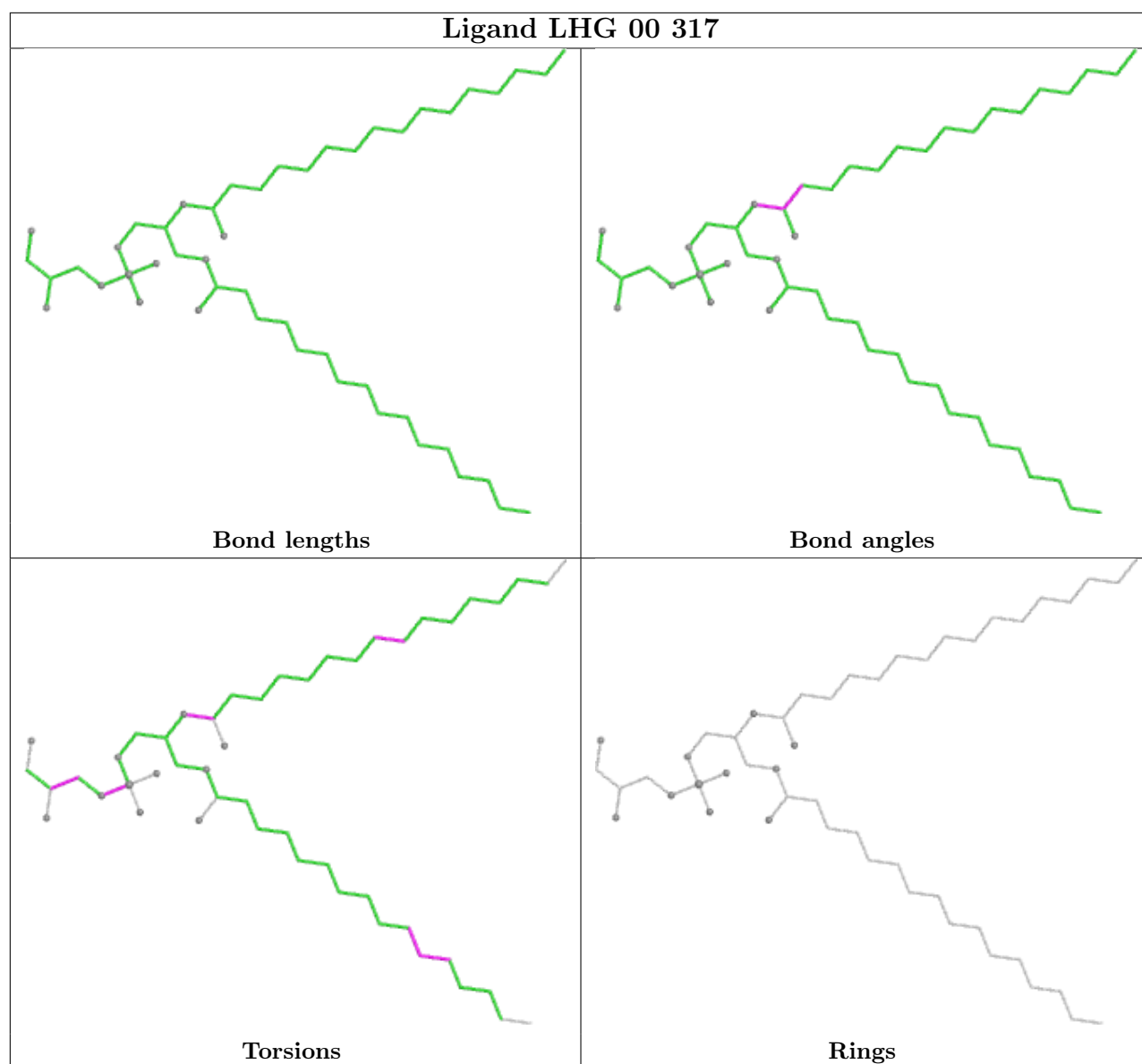


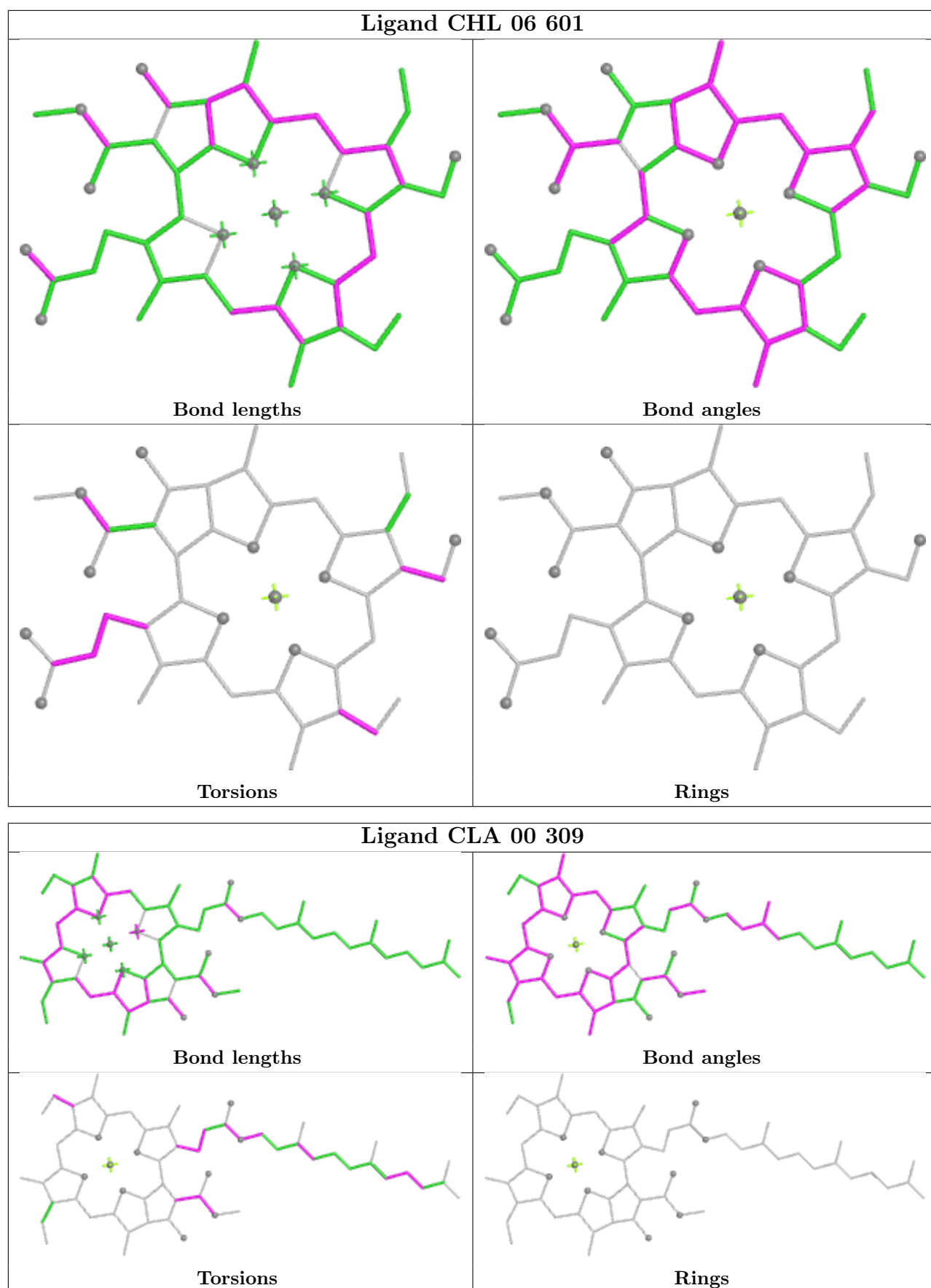


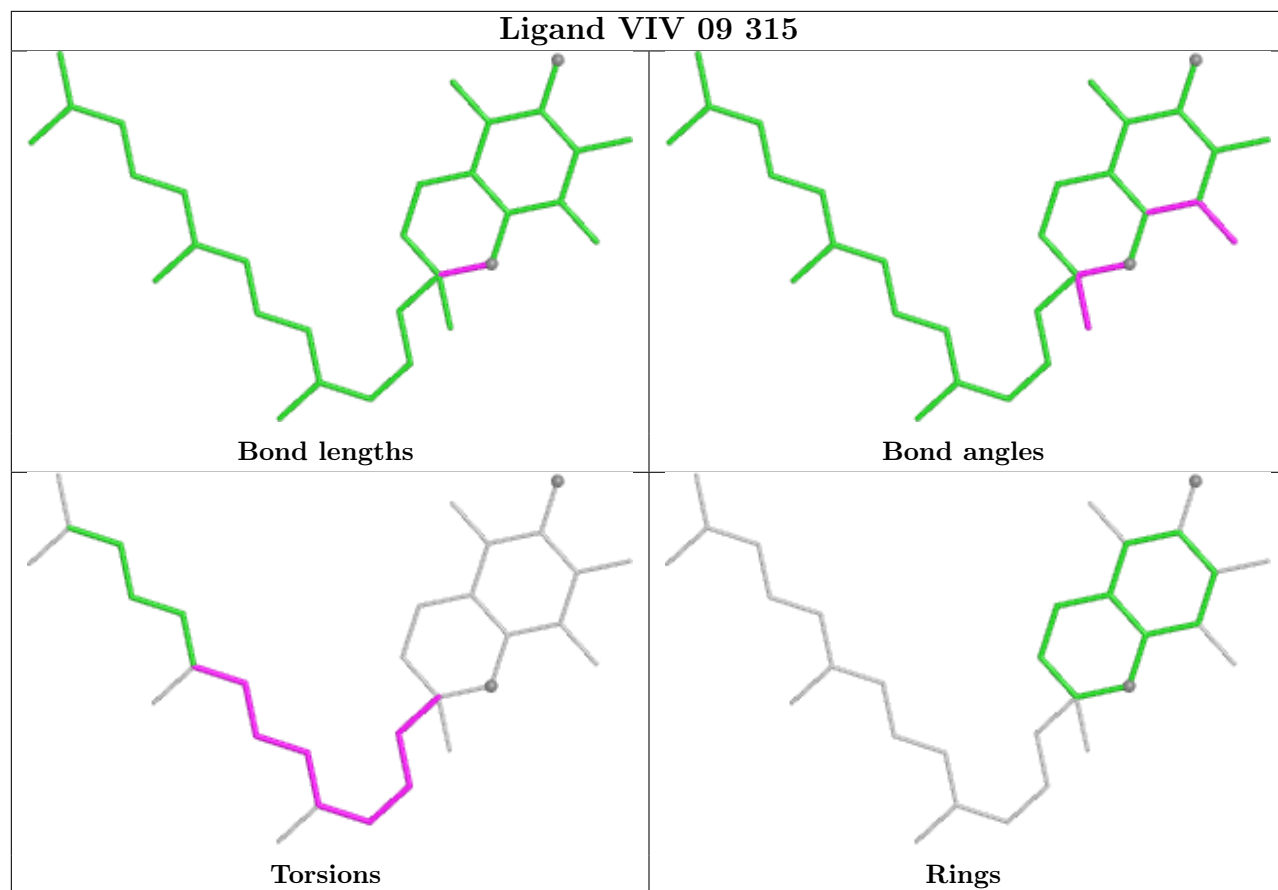


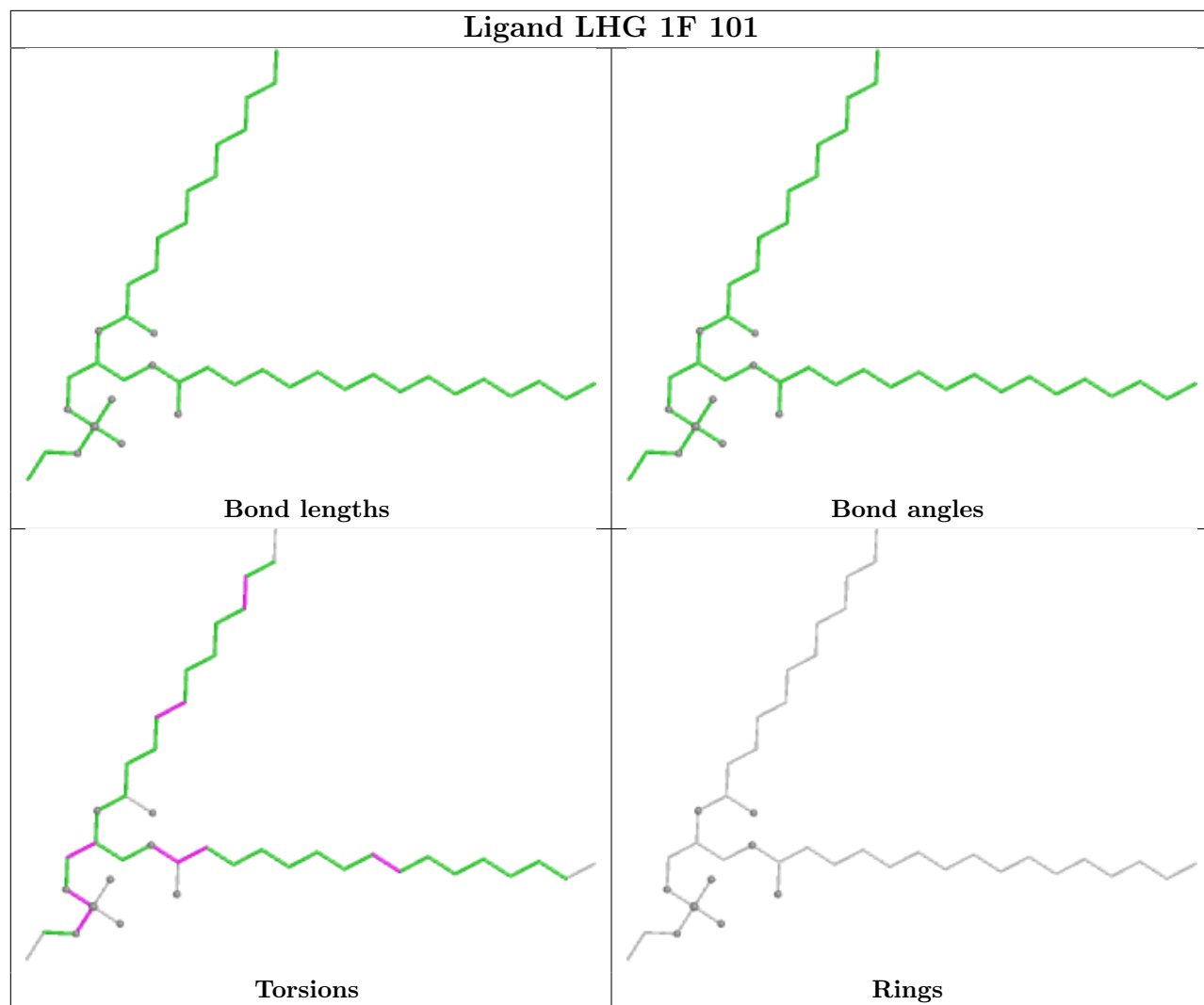


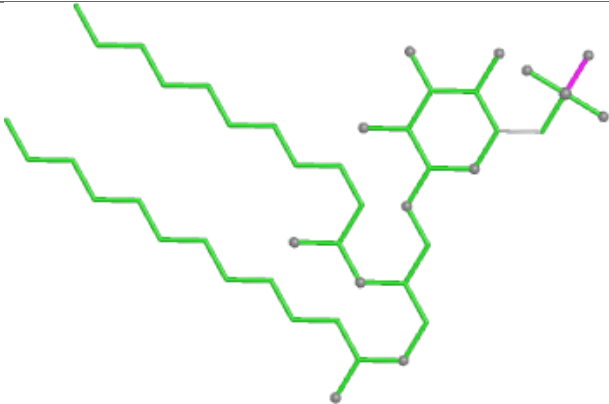
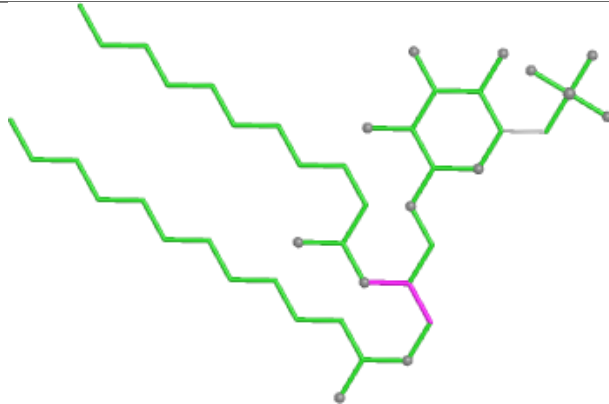
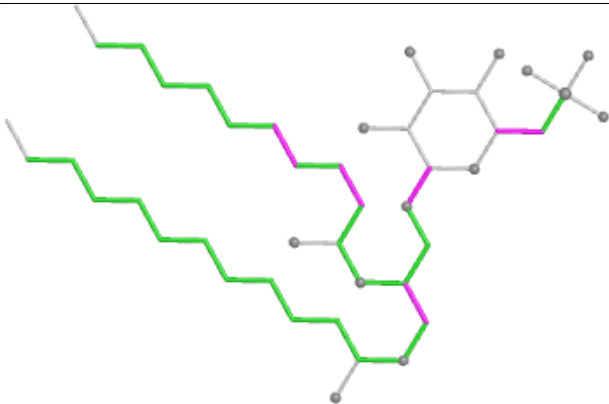
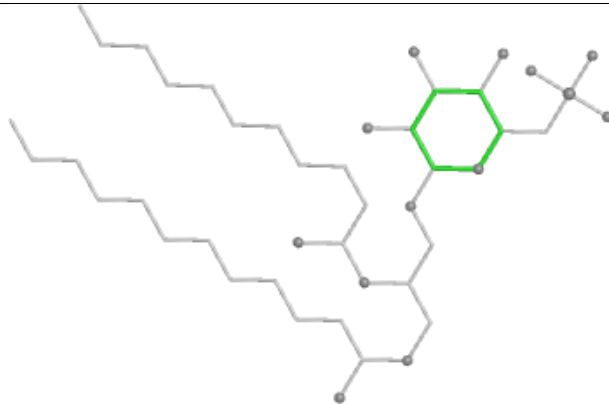


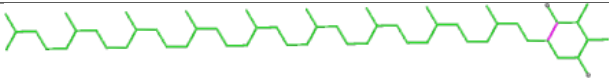
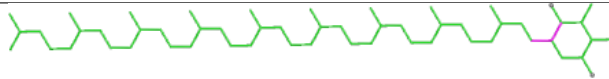
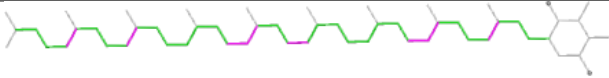
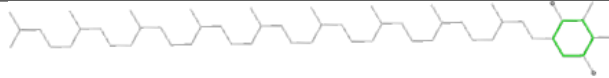


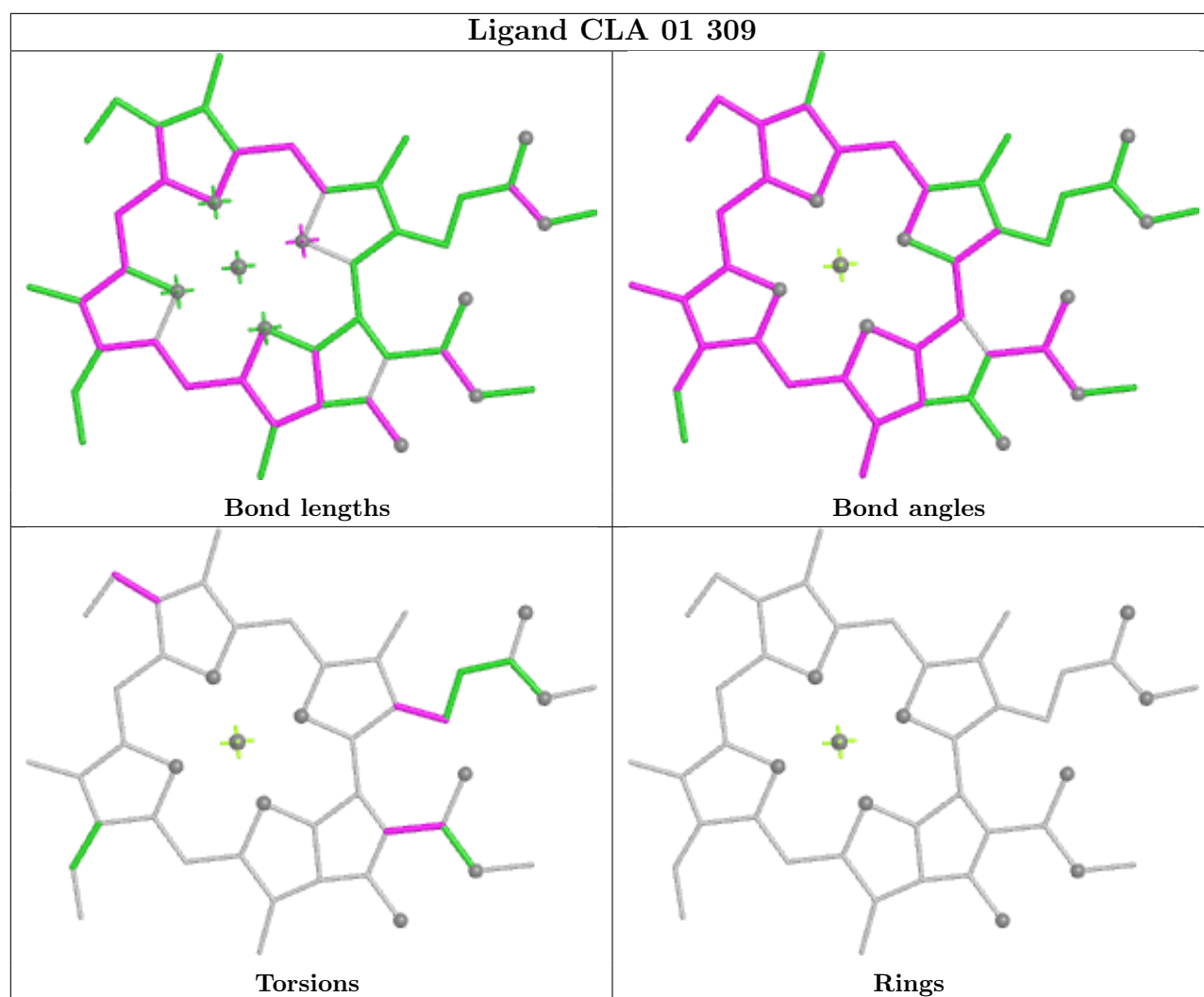


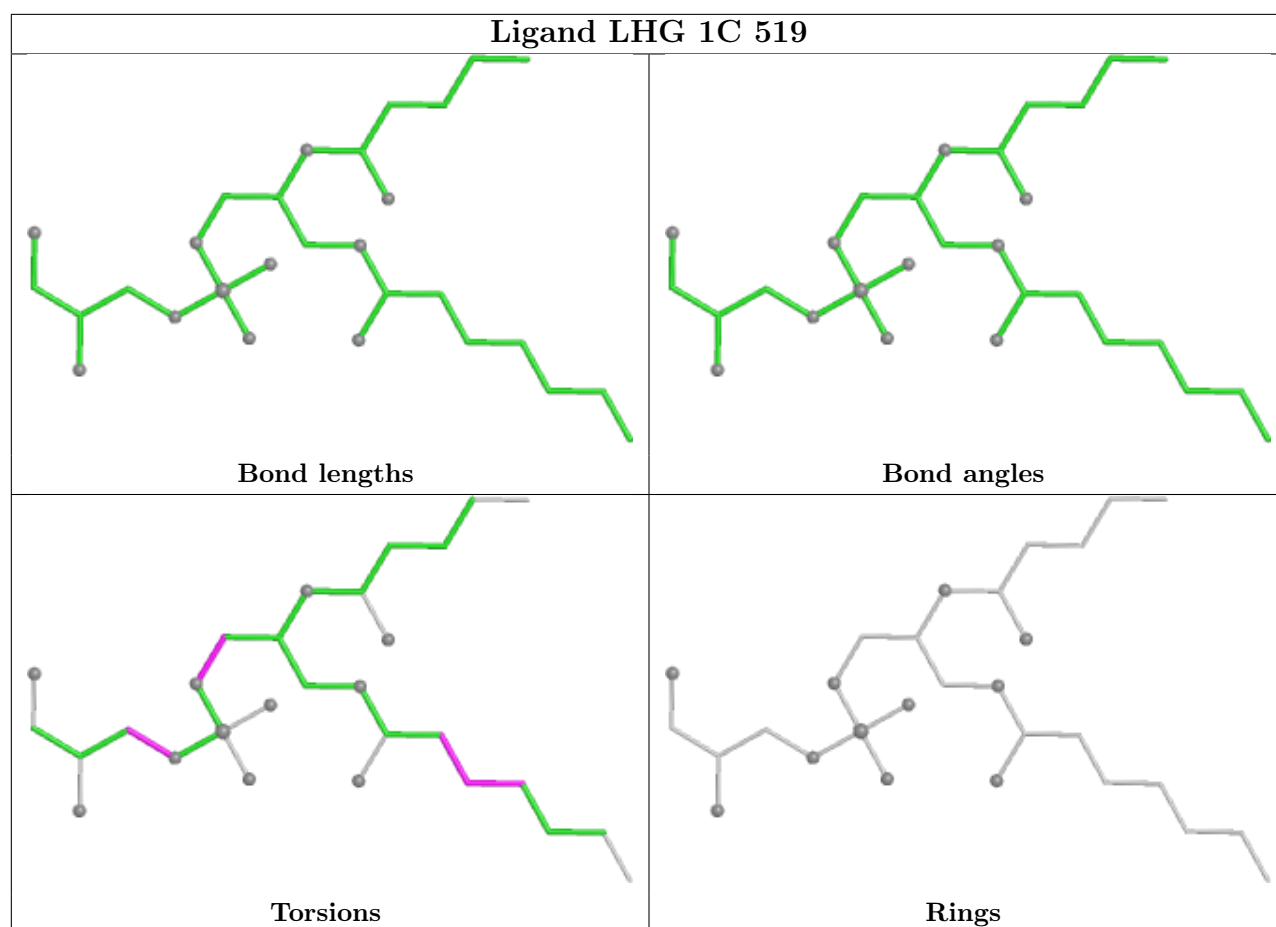


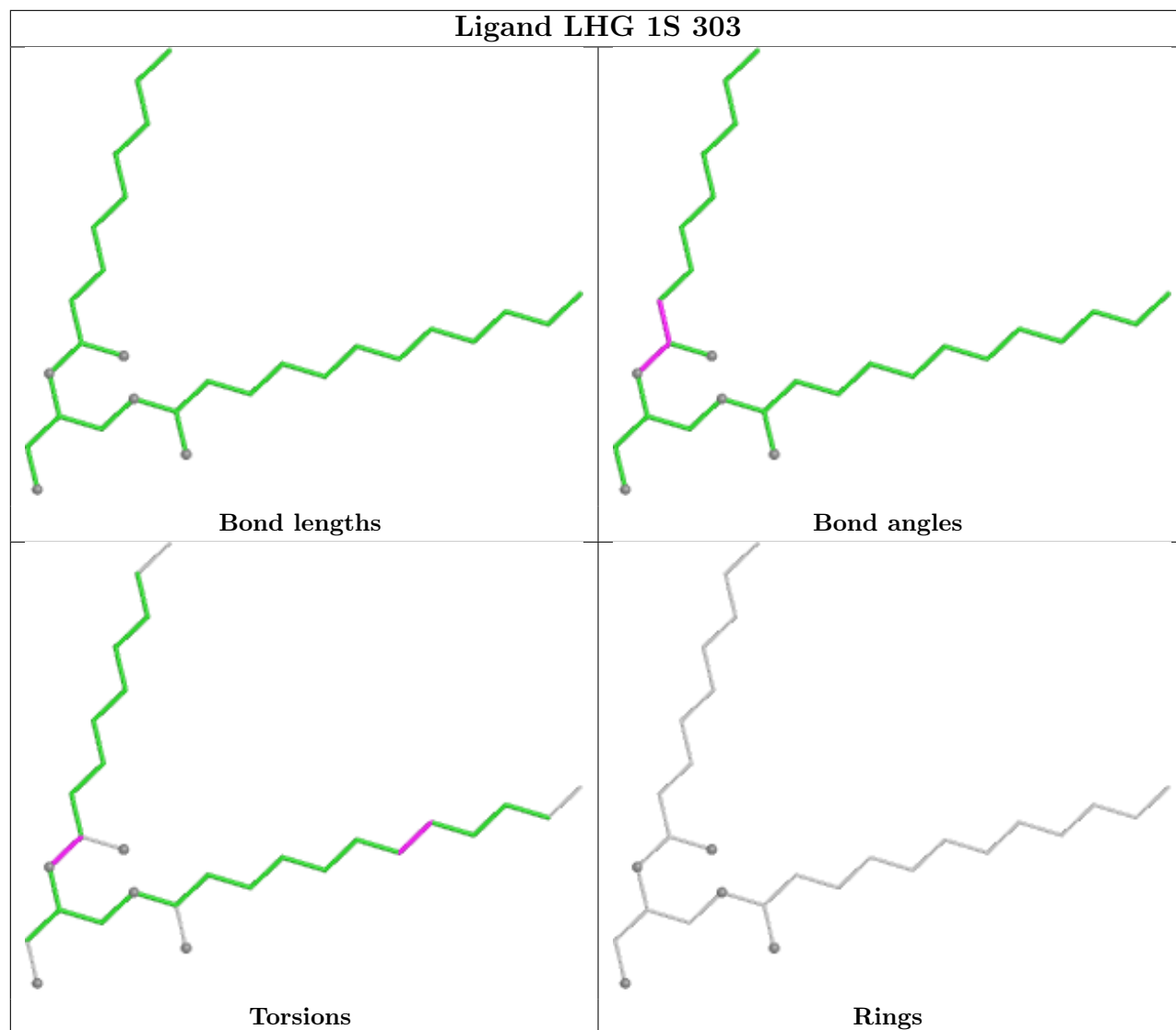


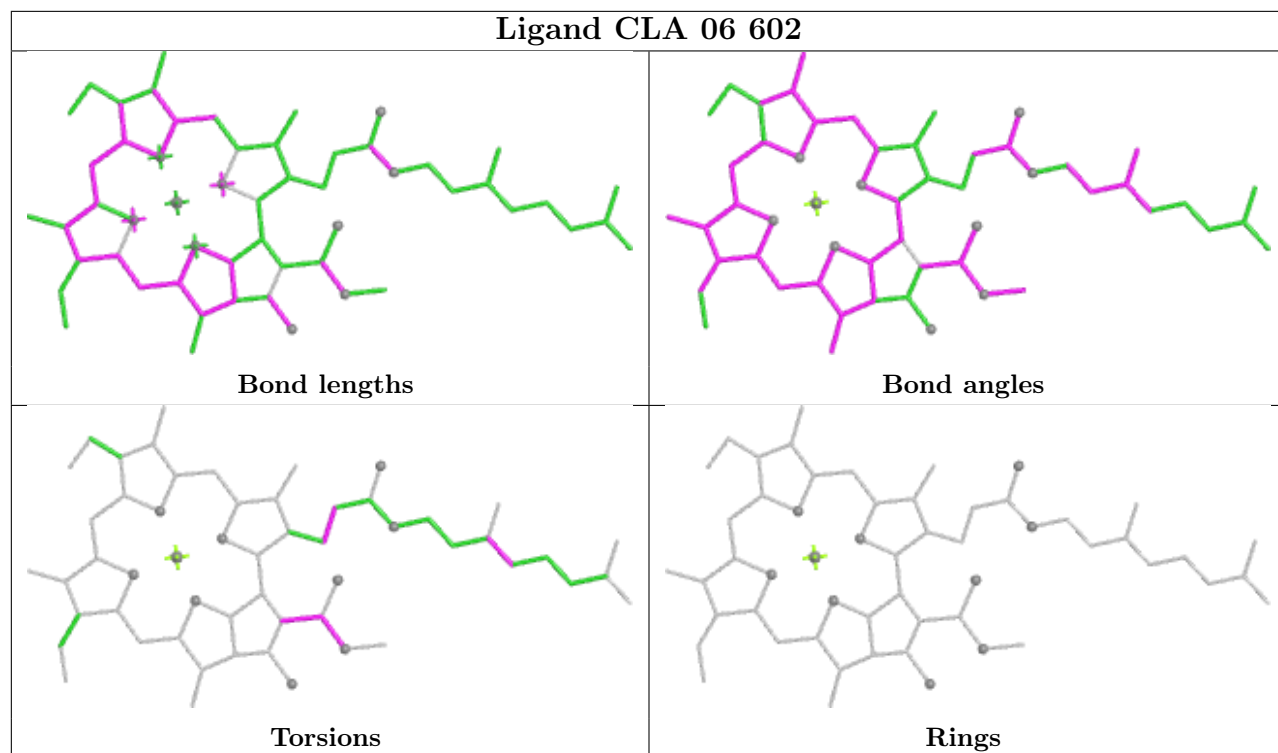
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Bond lengths	Bond angles
	
Torsions	Rings

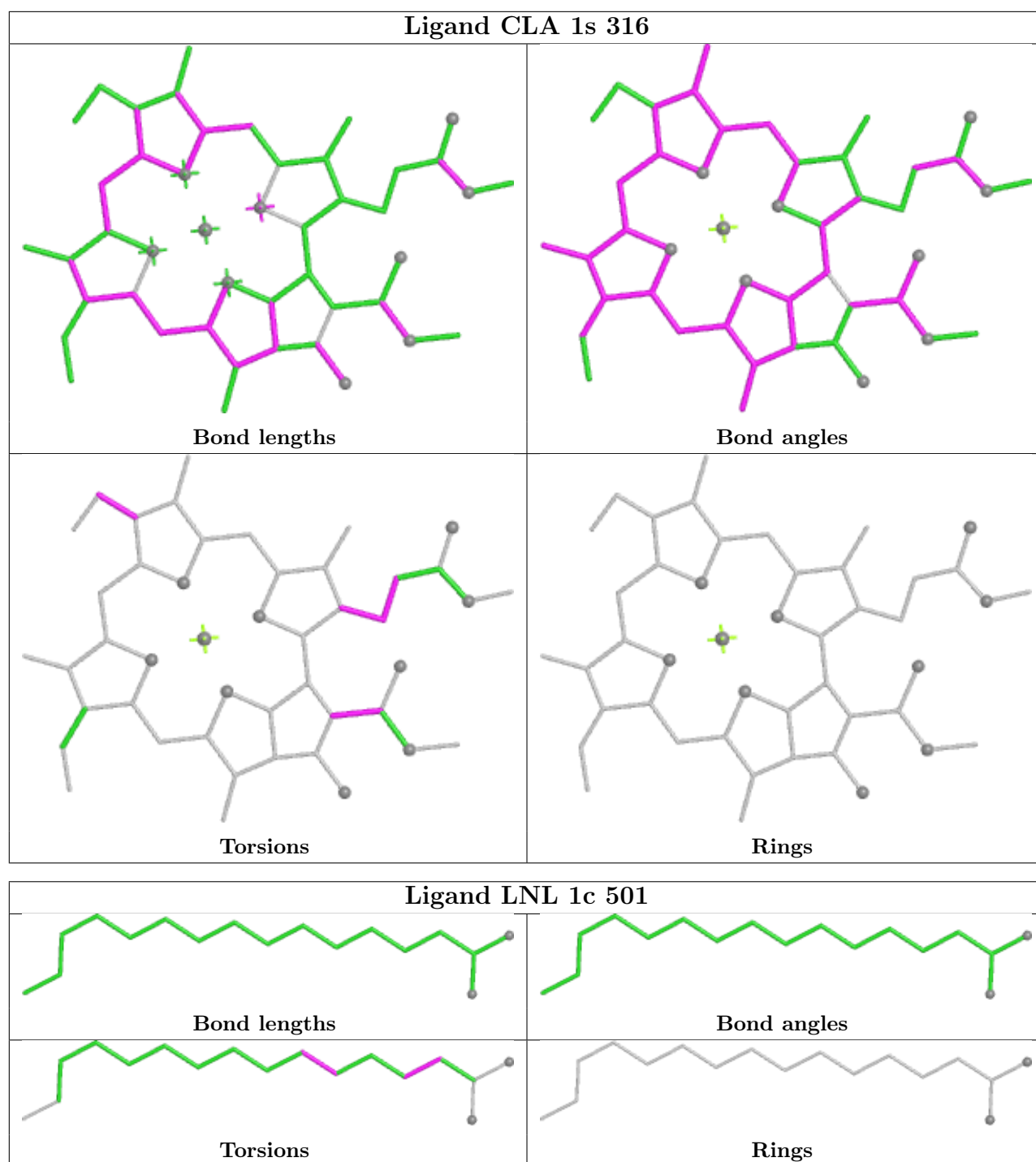
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Bond lengths	Bond angles
	
Torsions	Rings

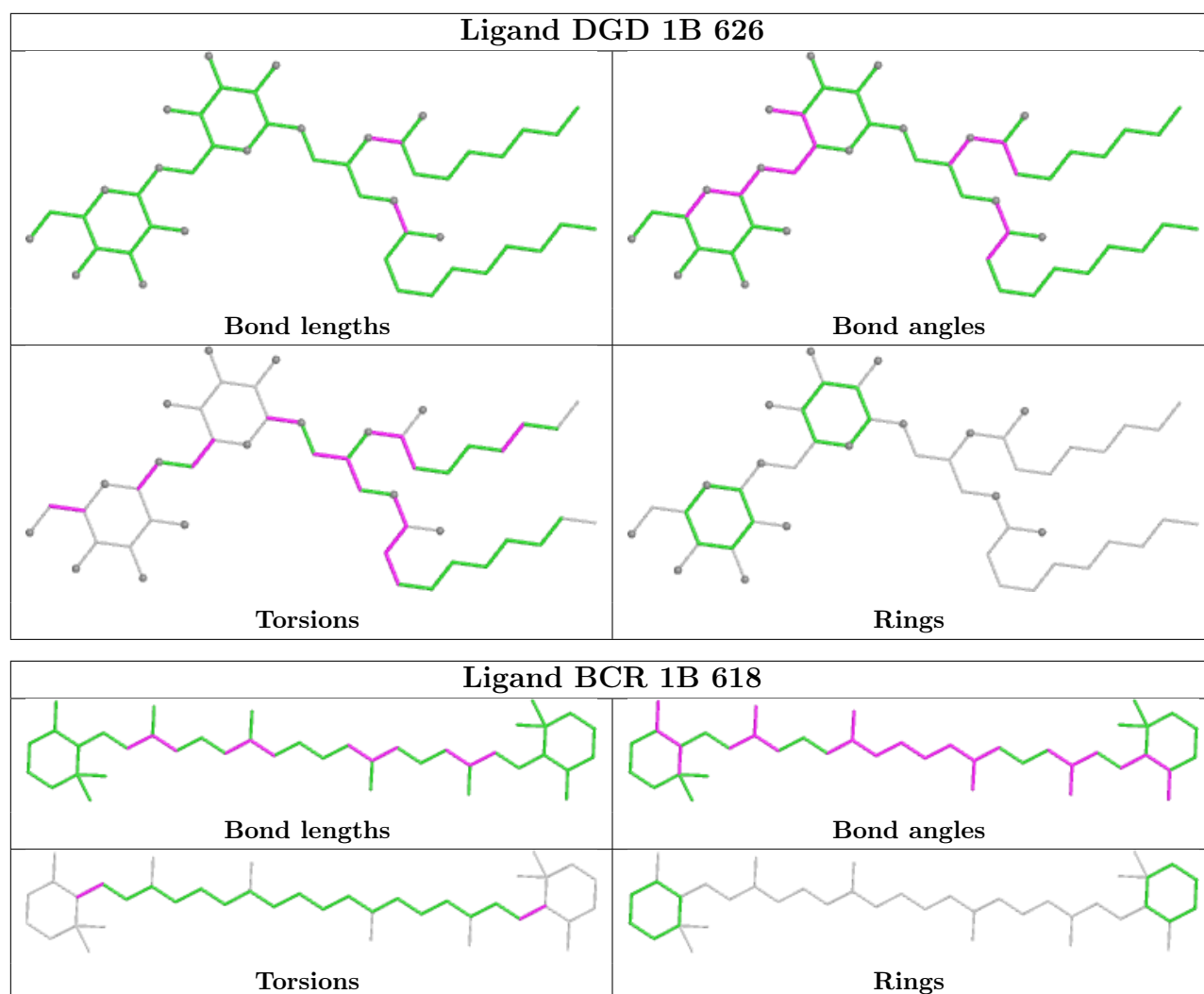


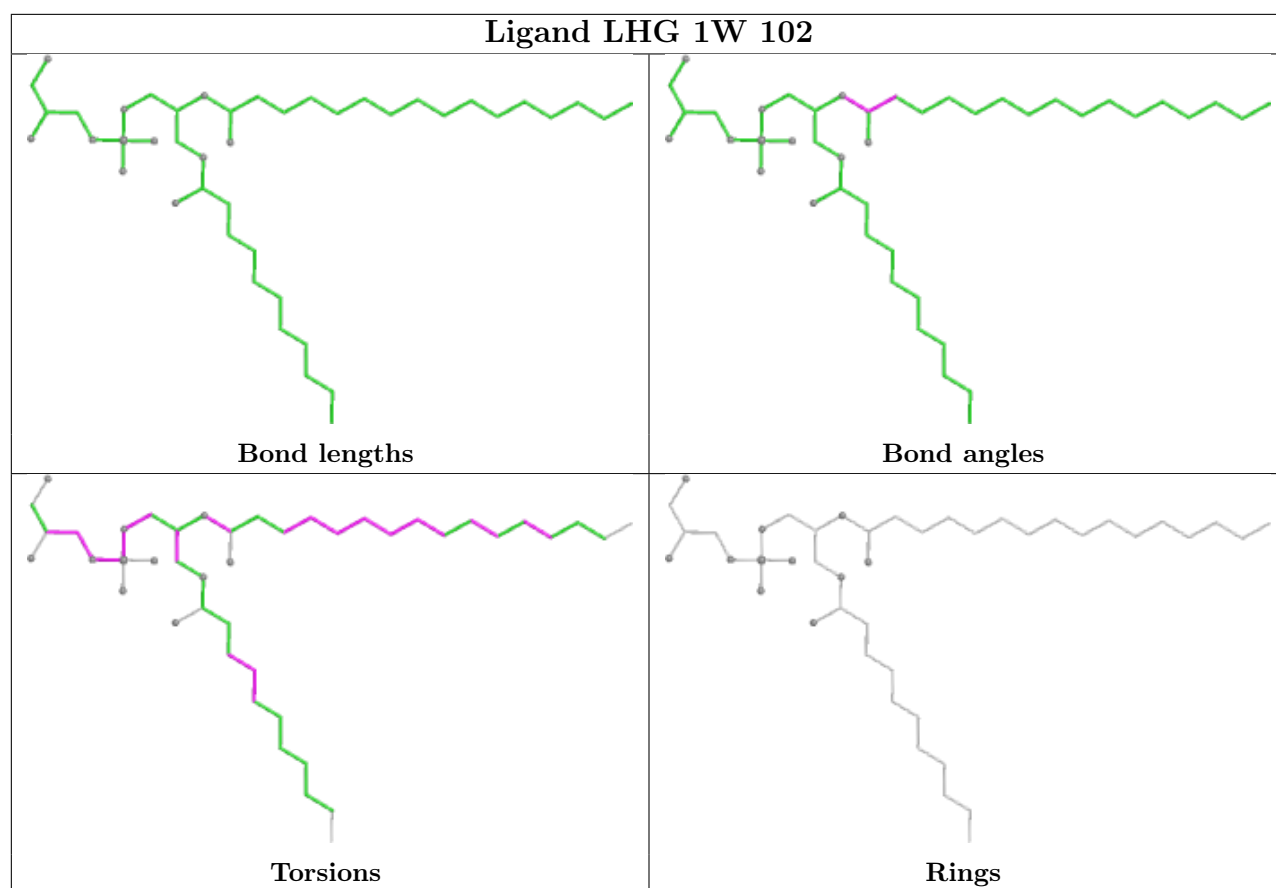


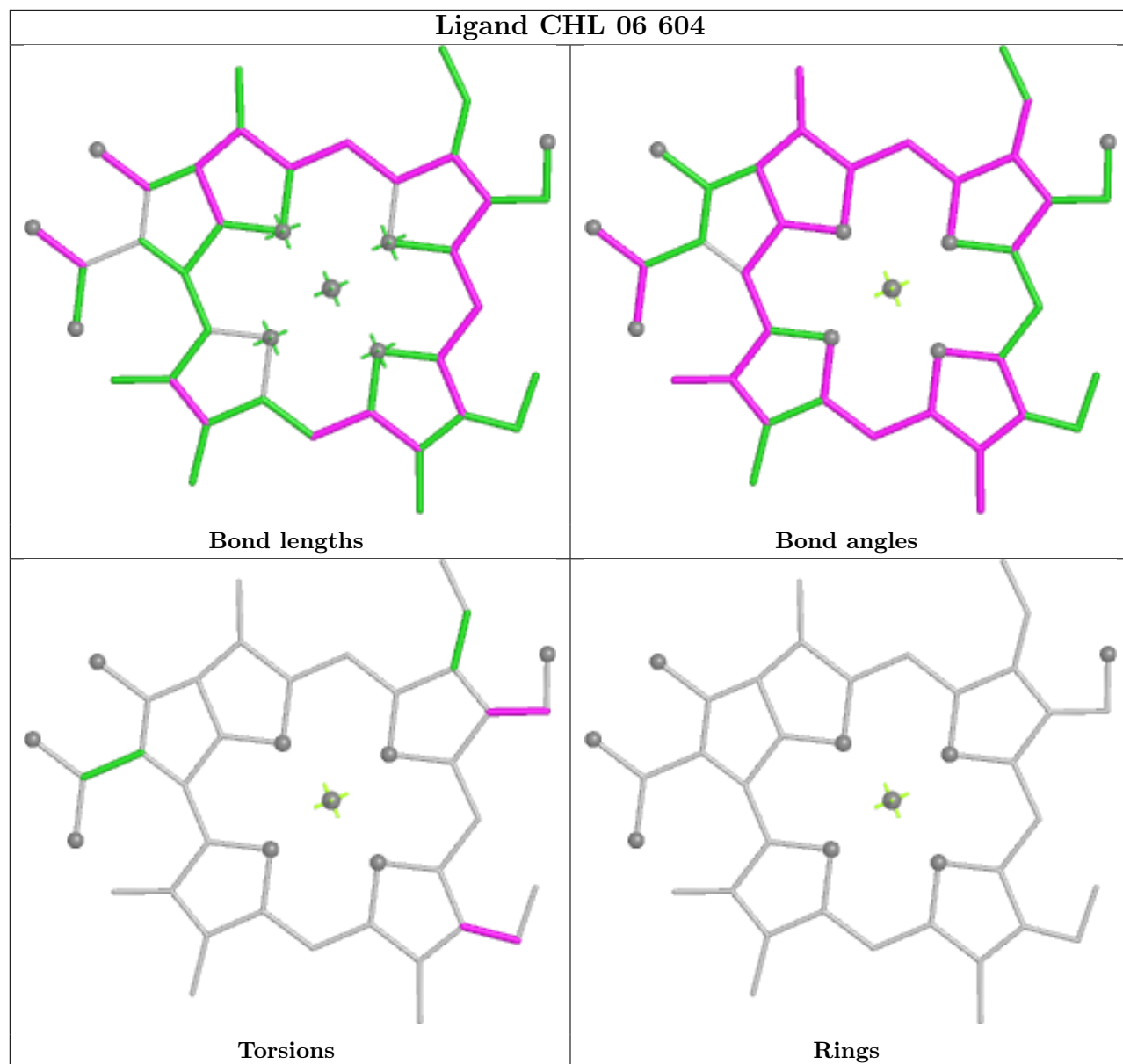


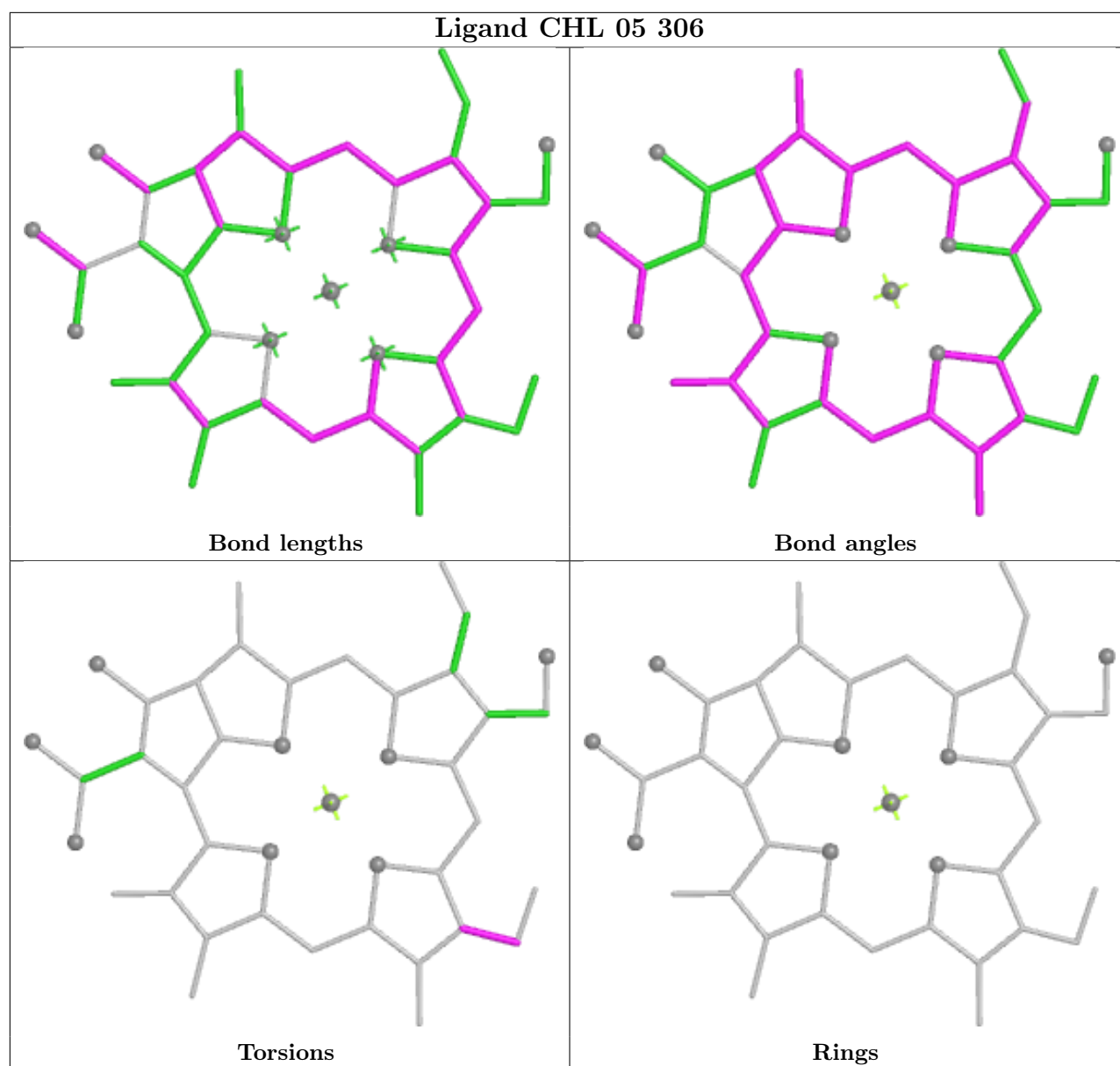


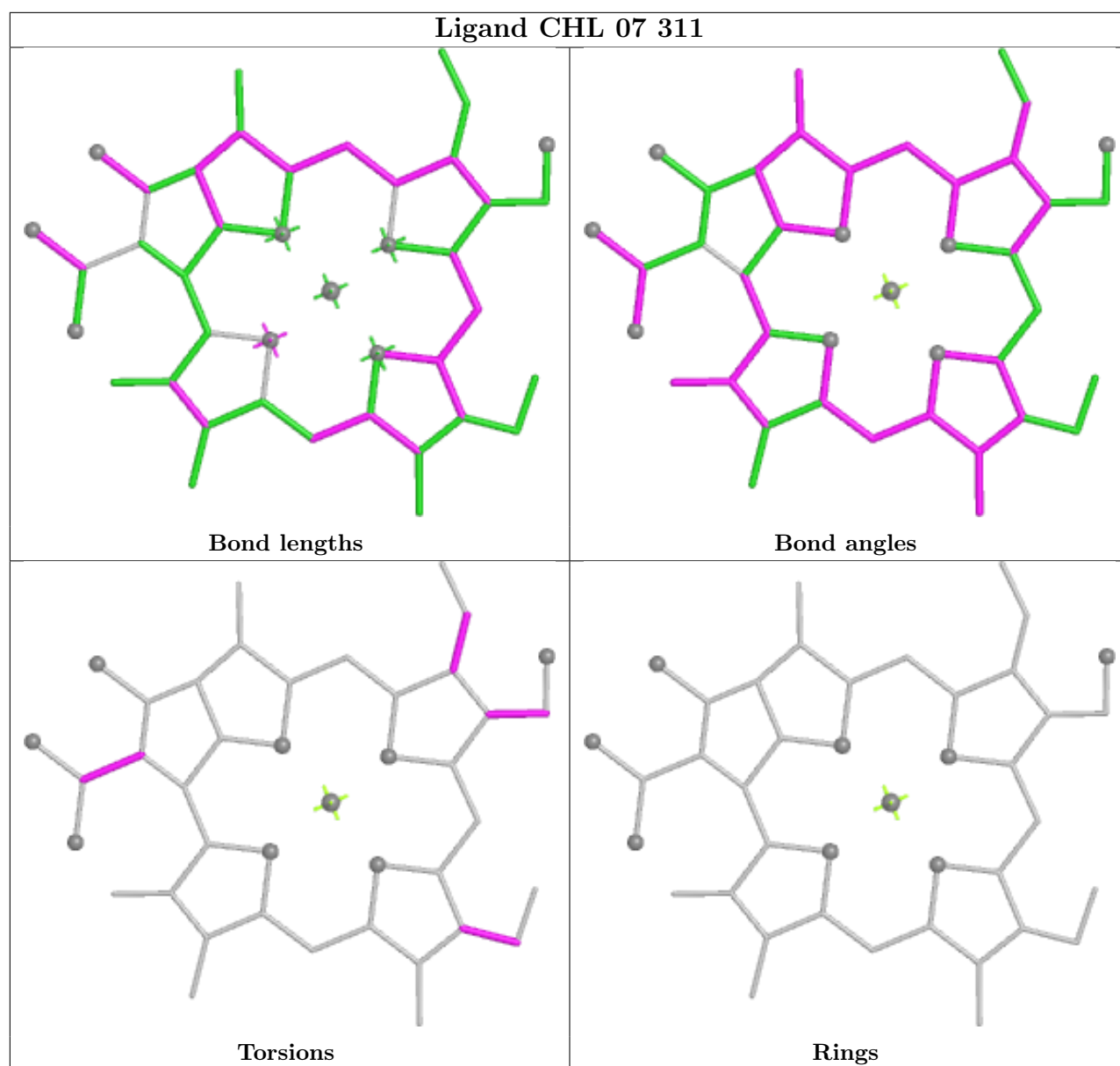


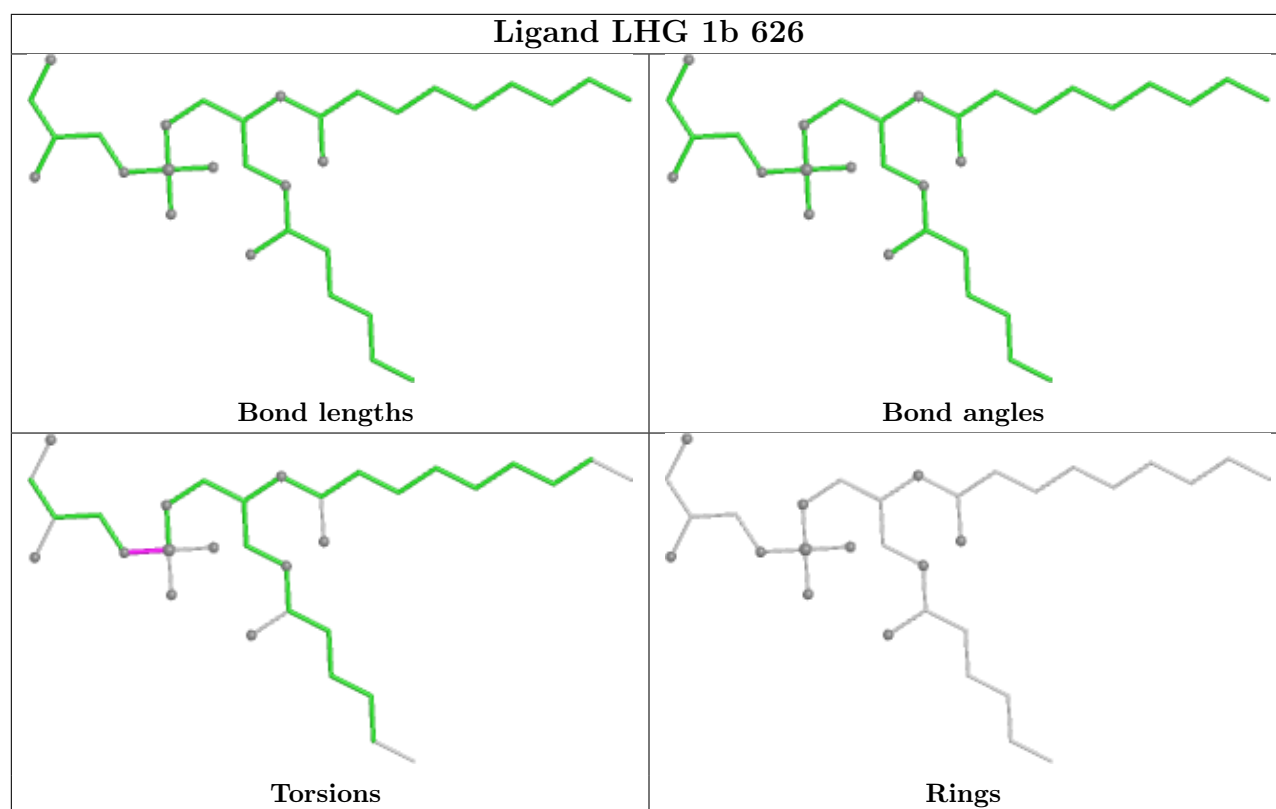


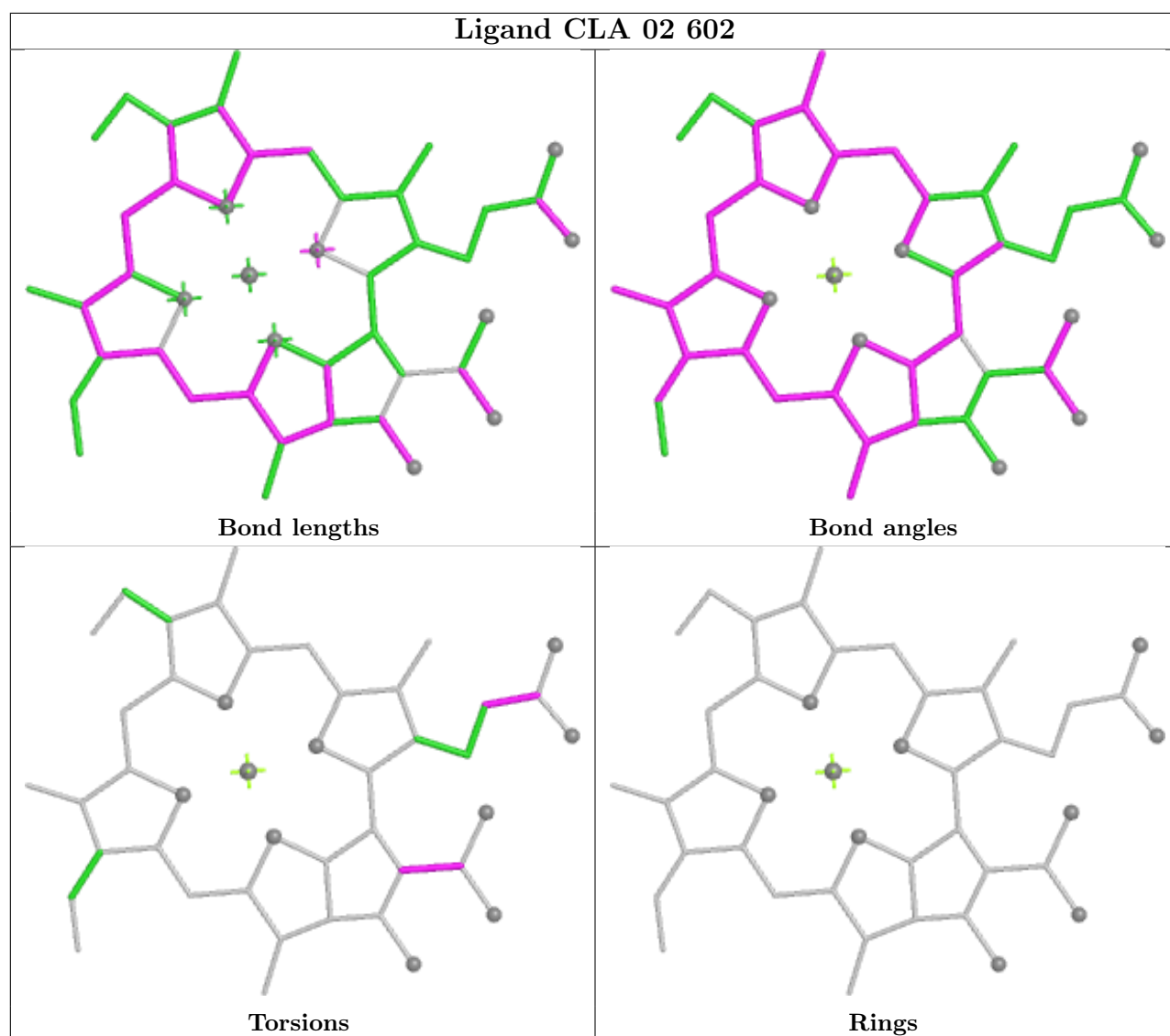


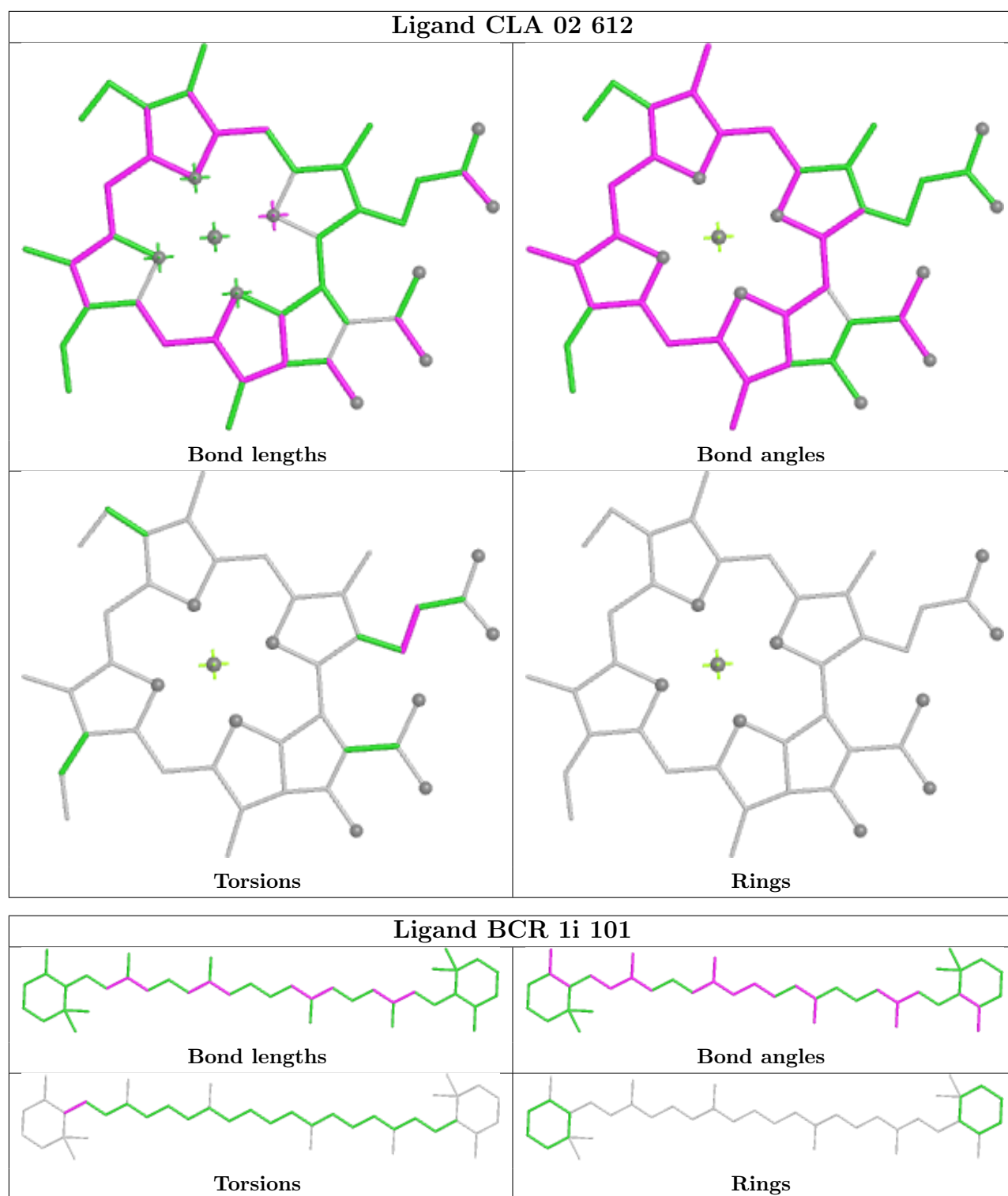


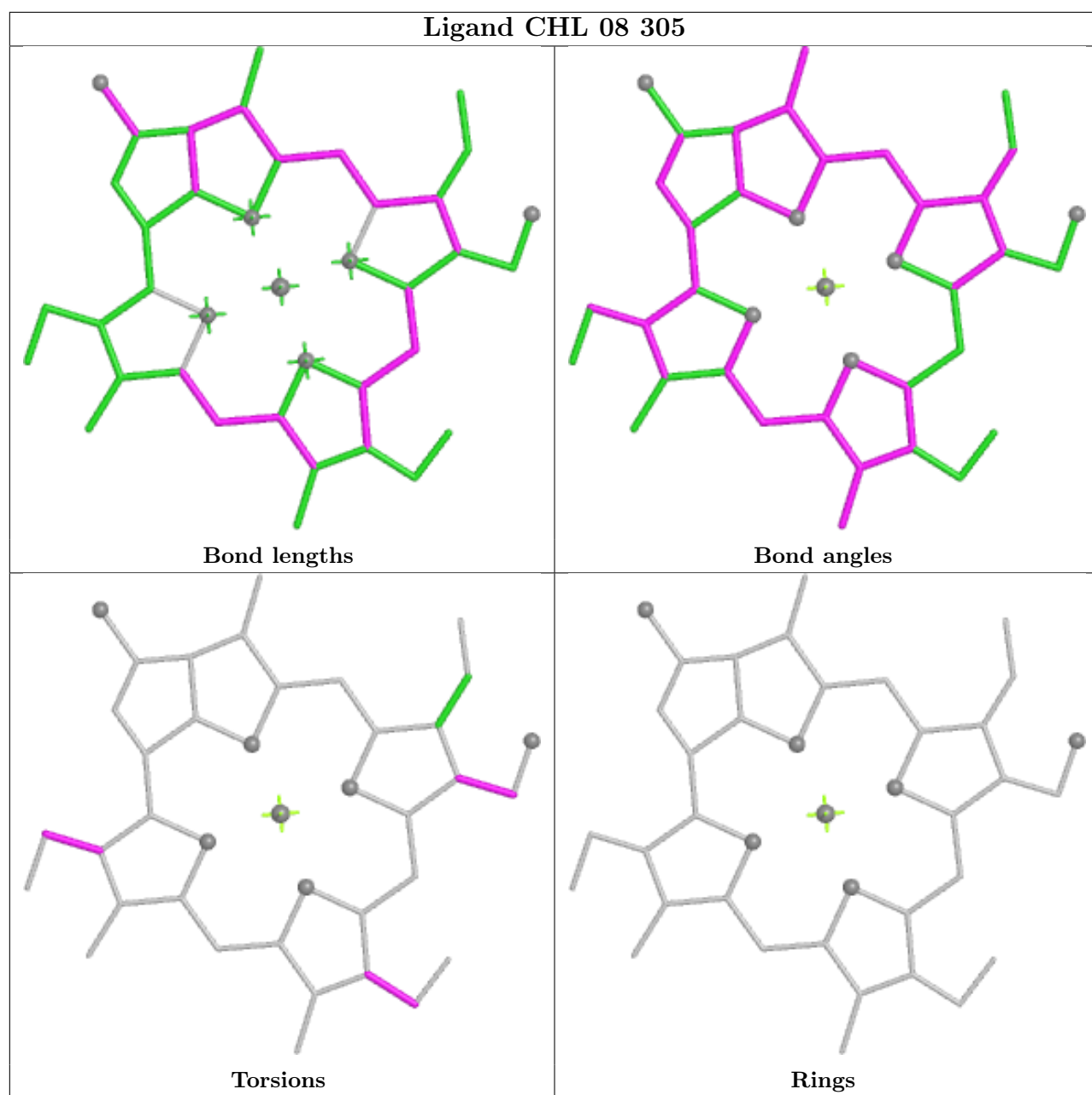


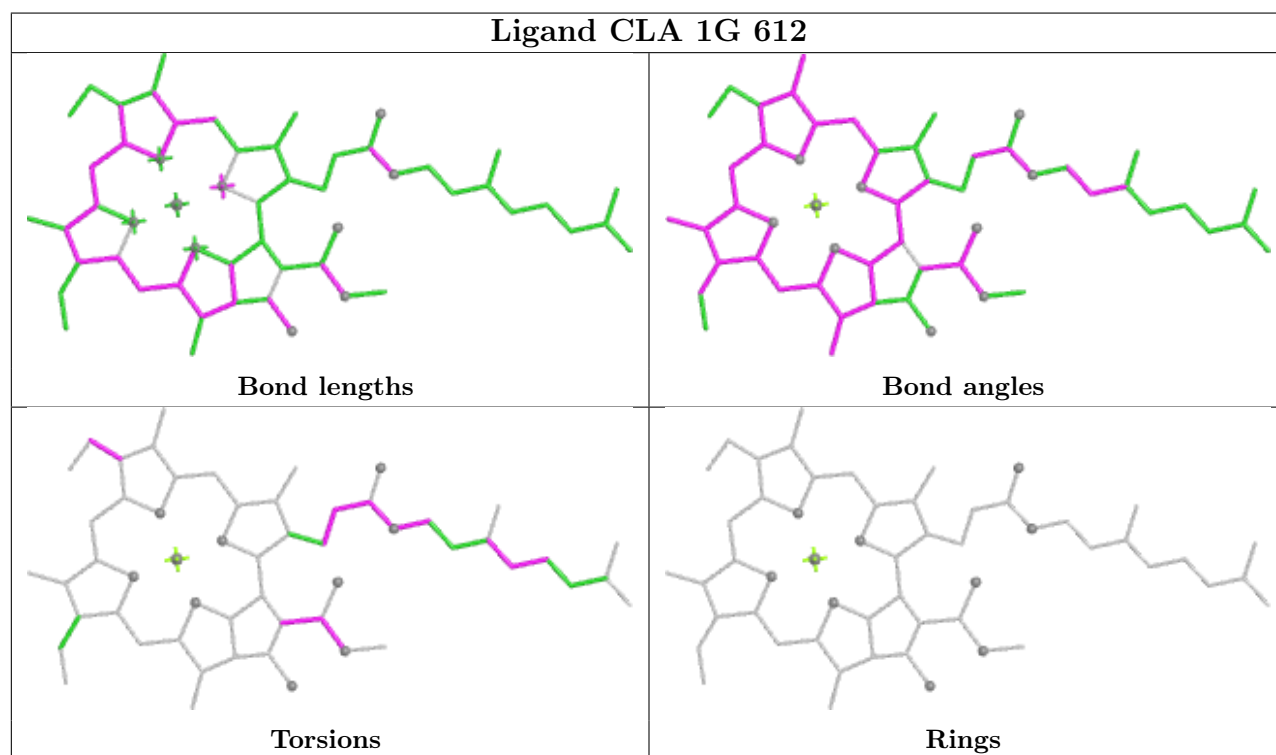
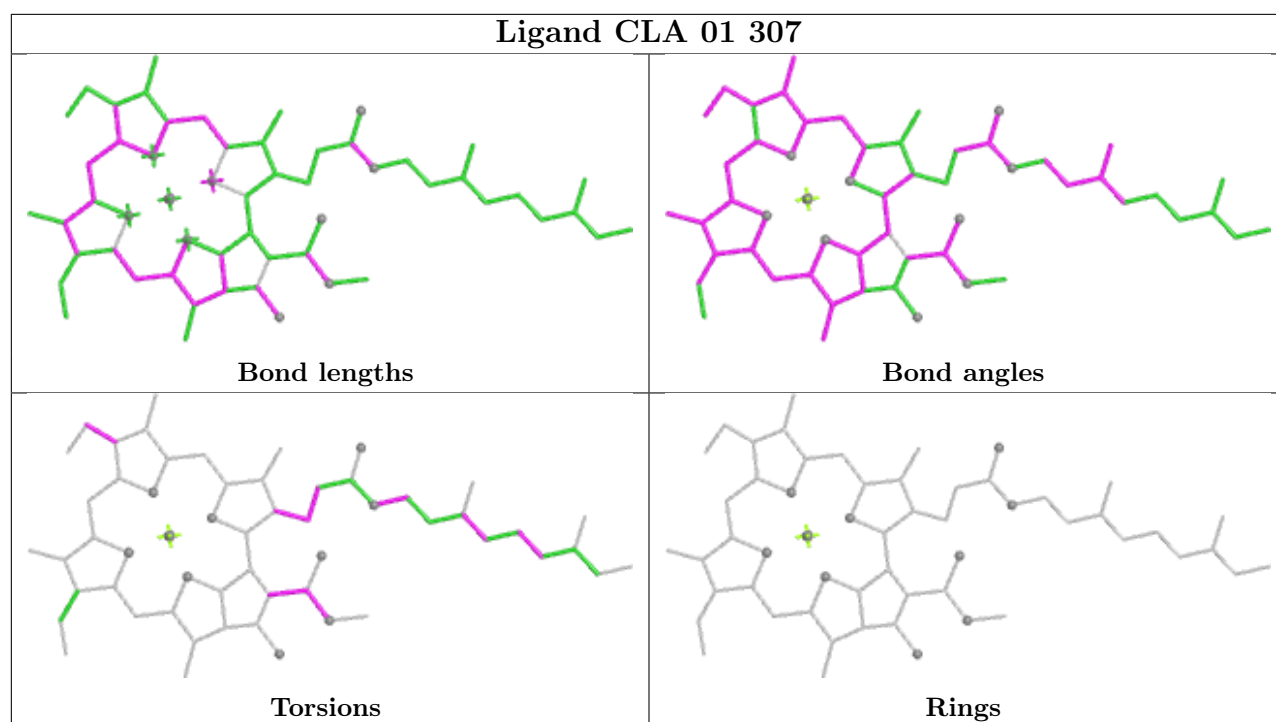


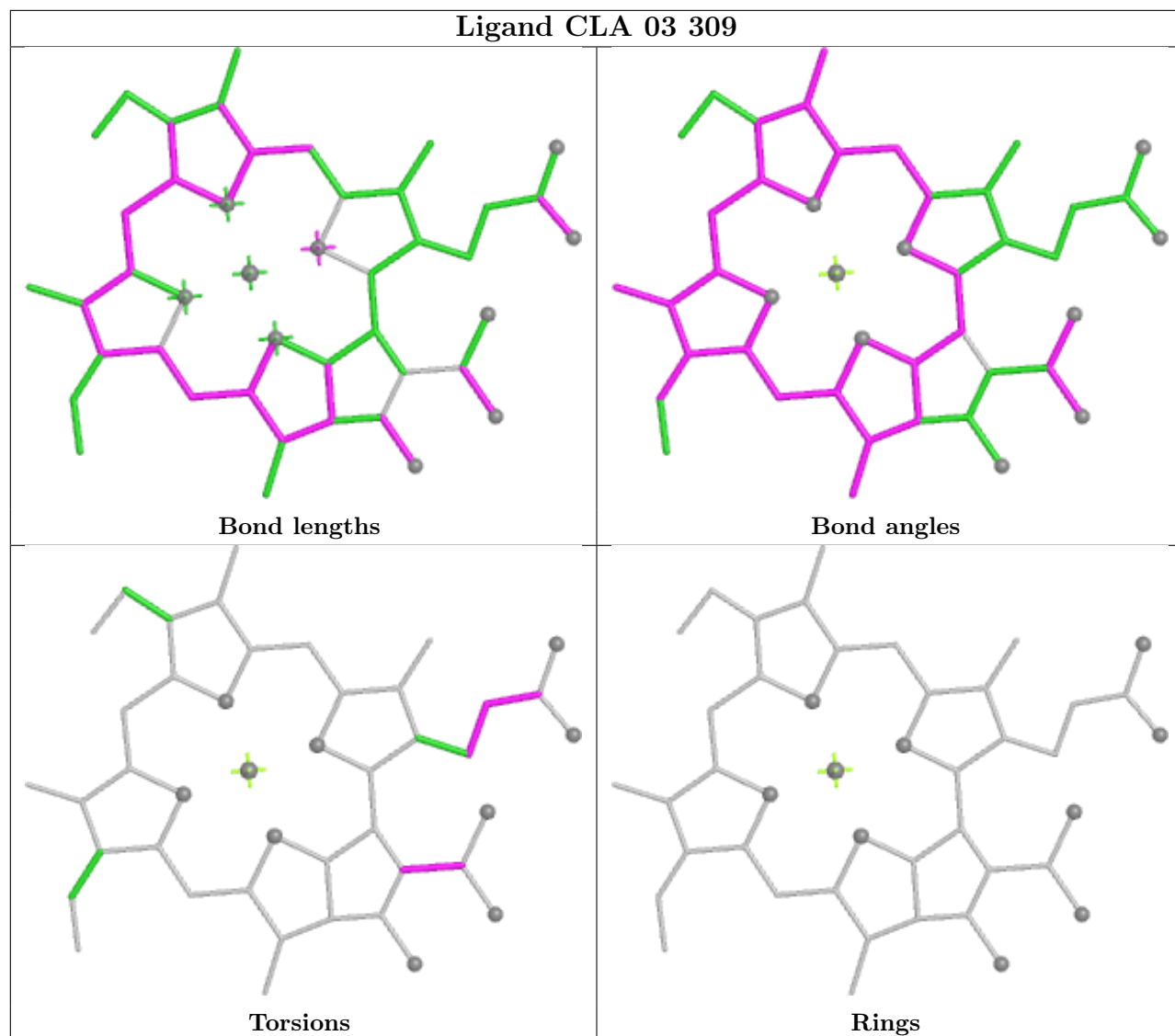


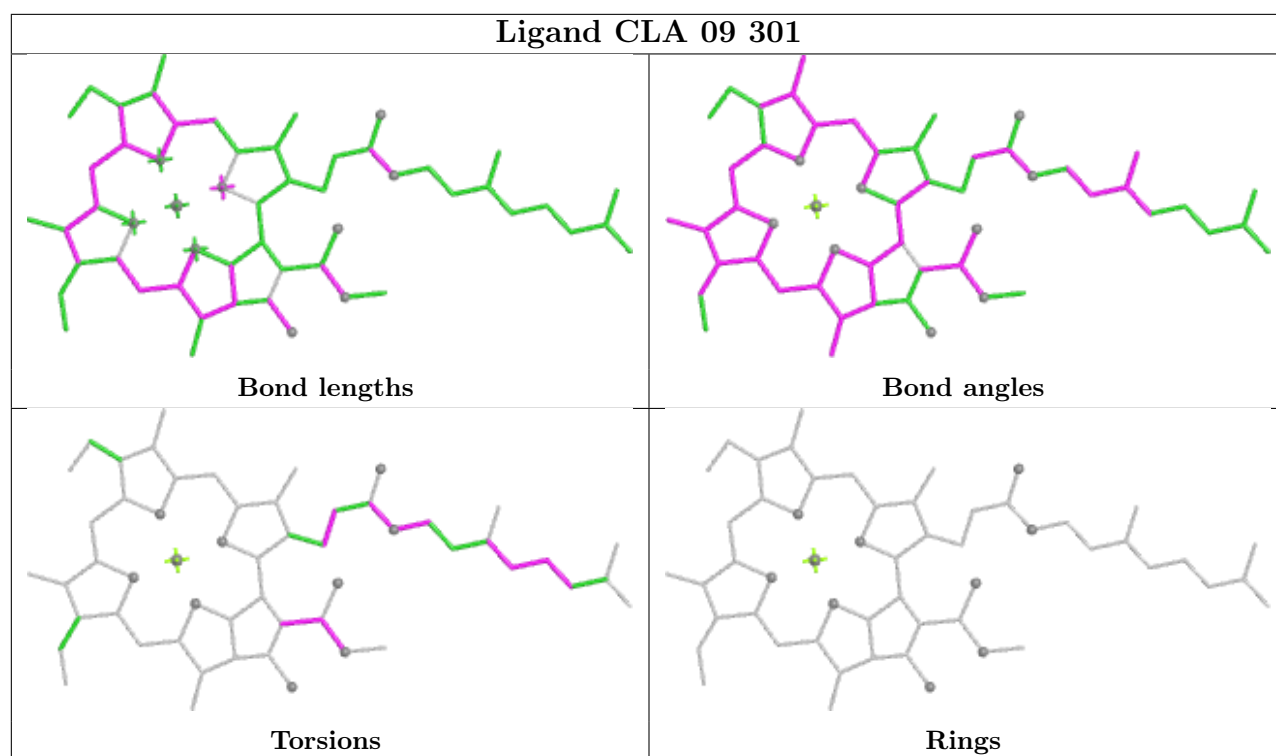


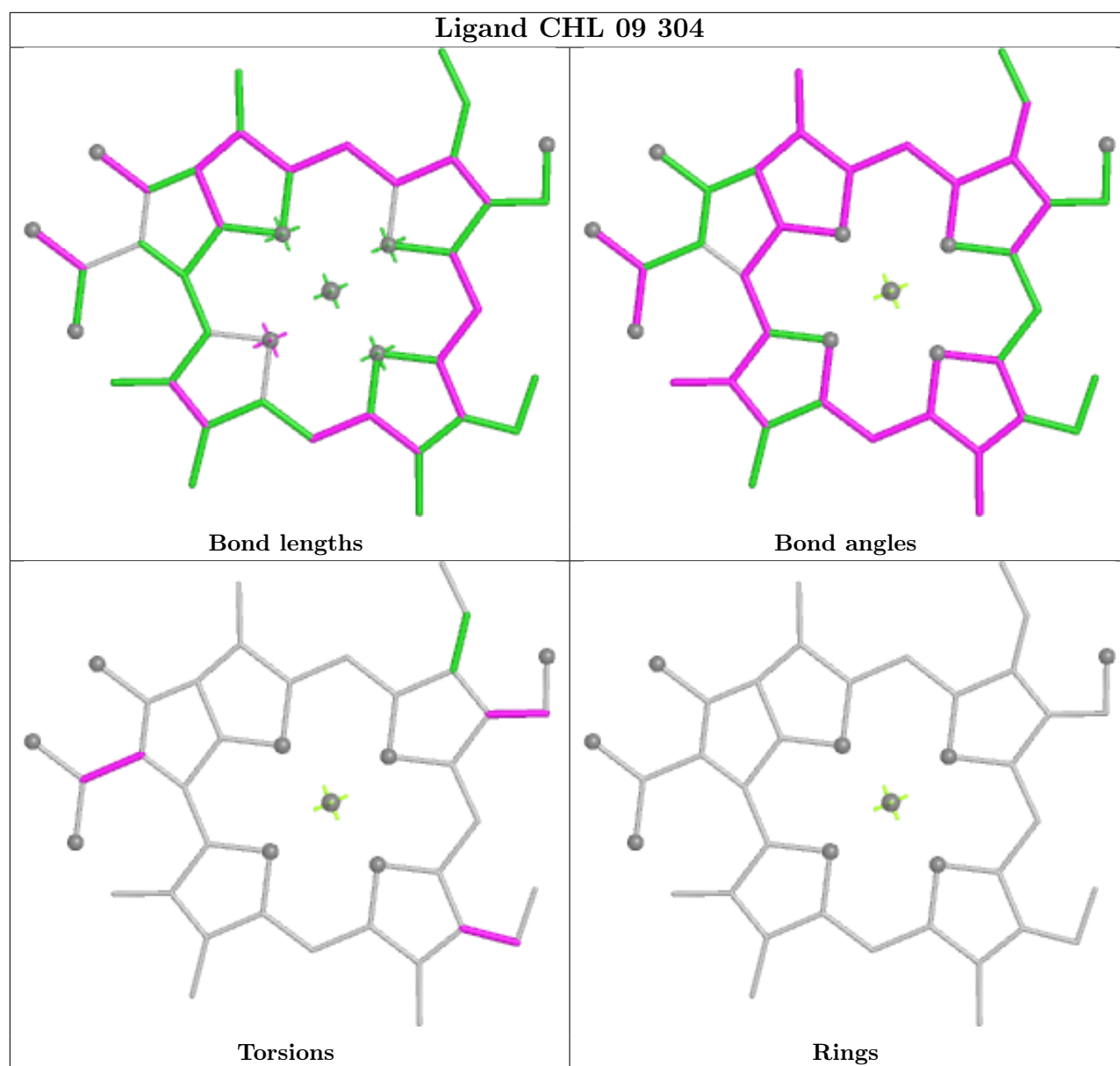


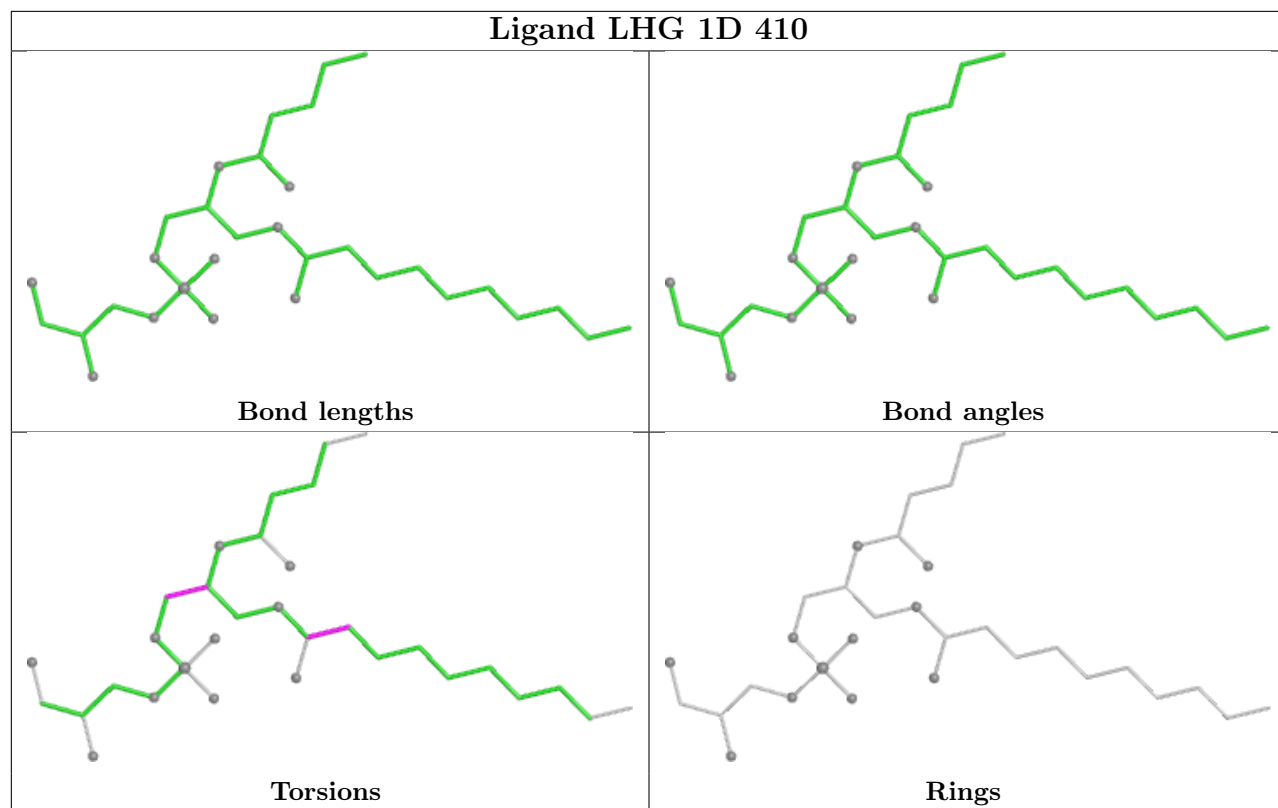


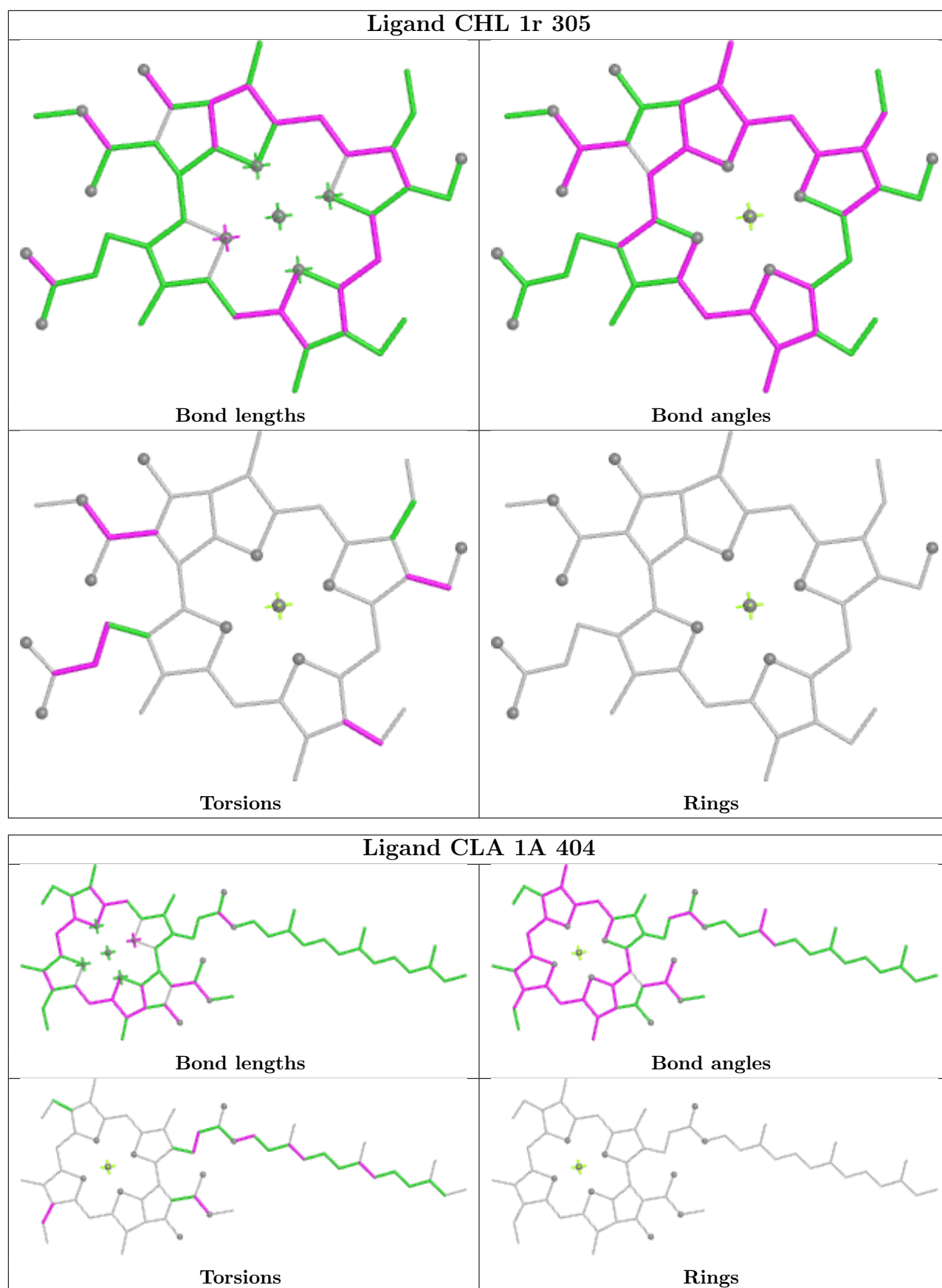


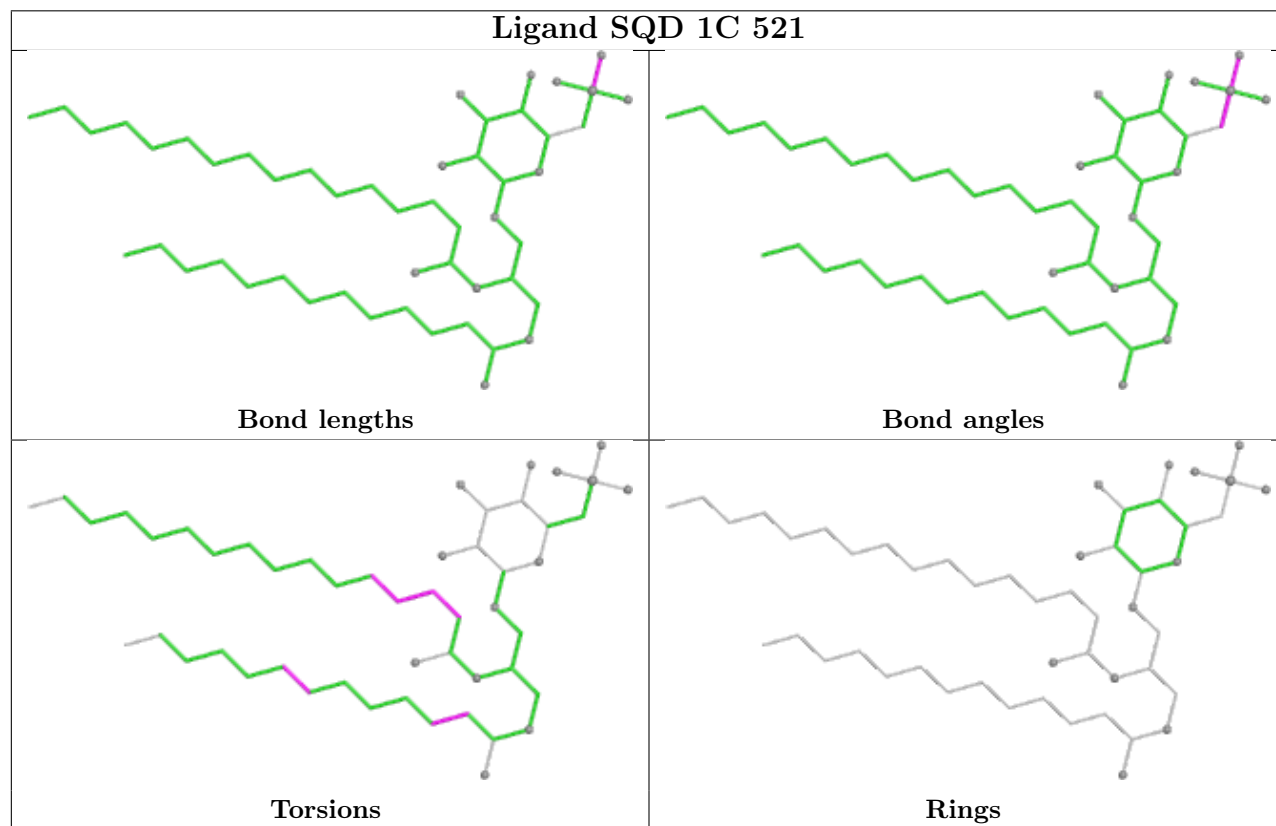
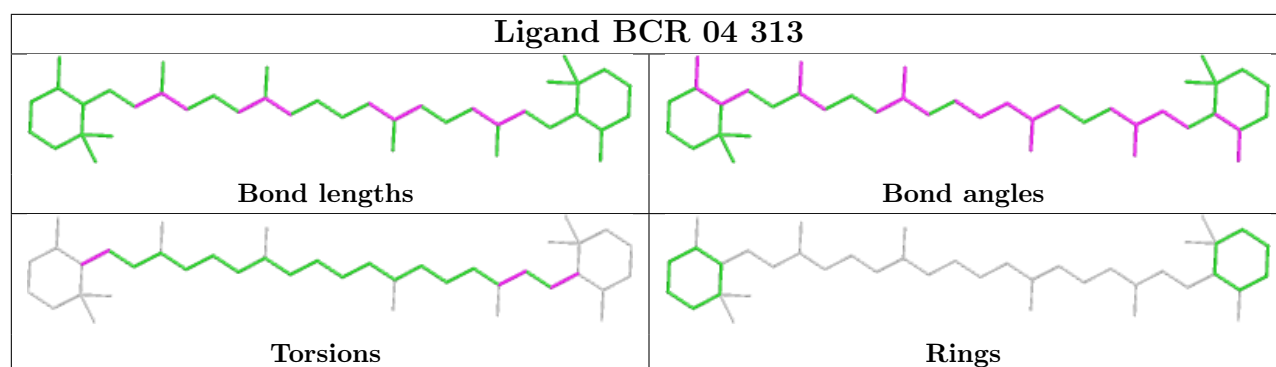


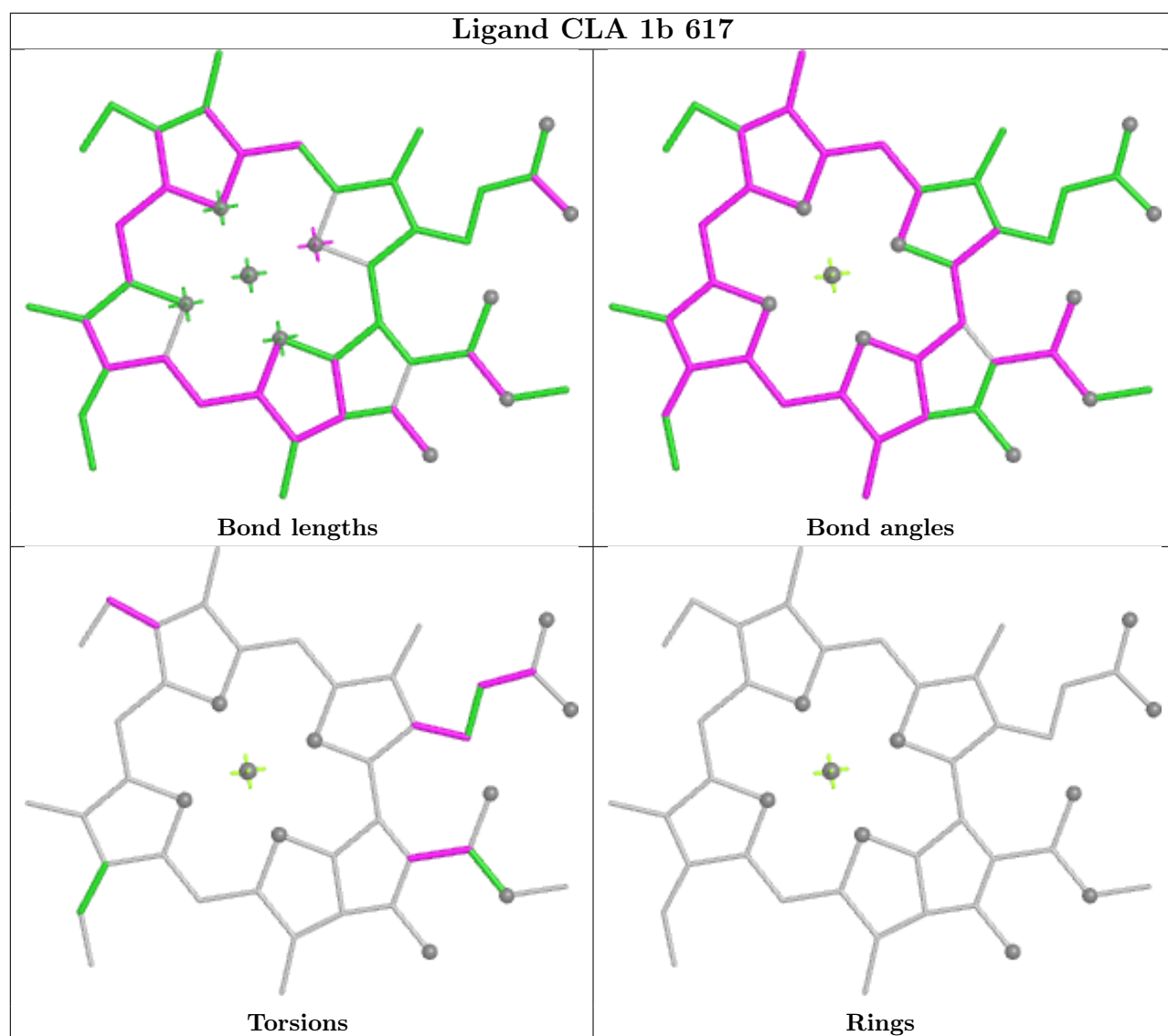


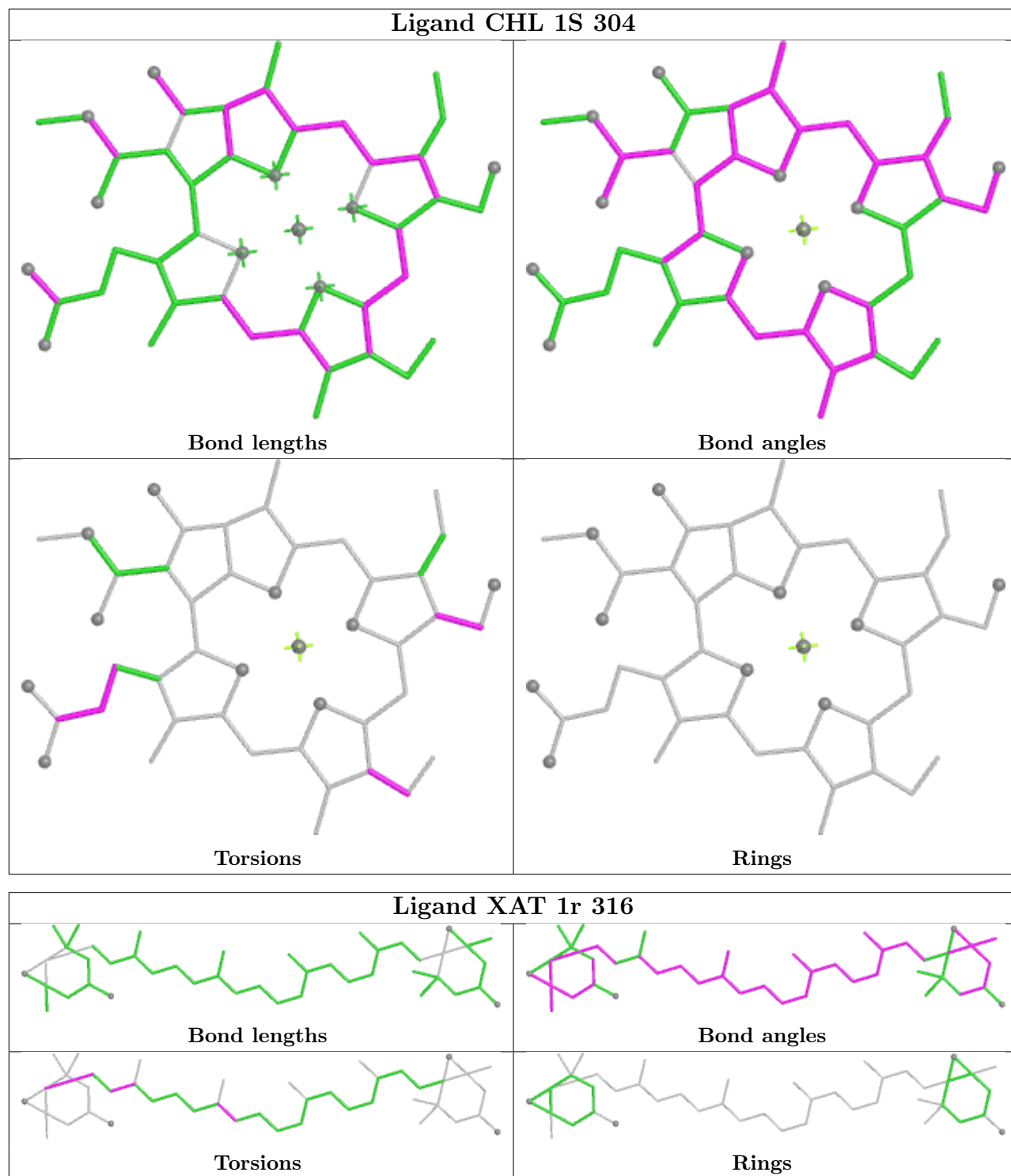


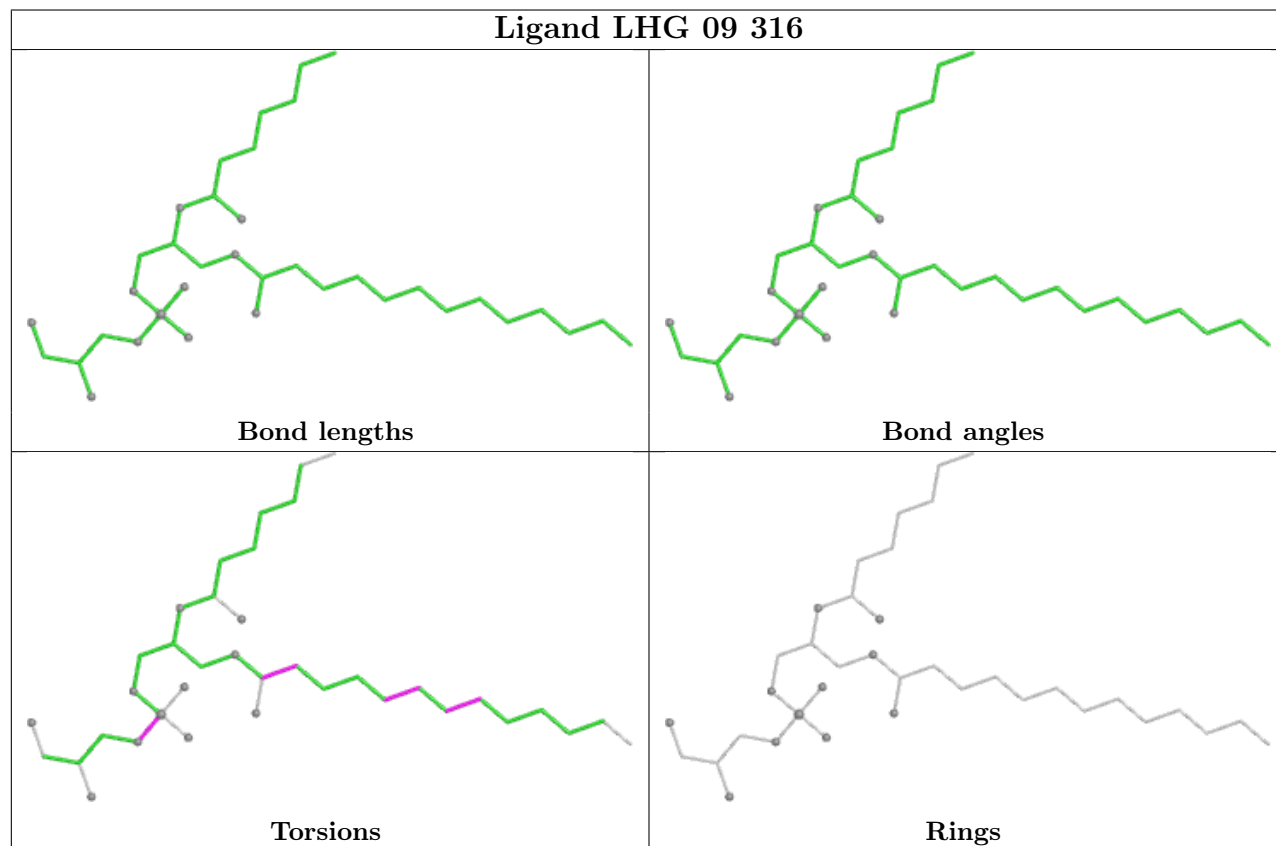
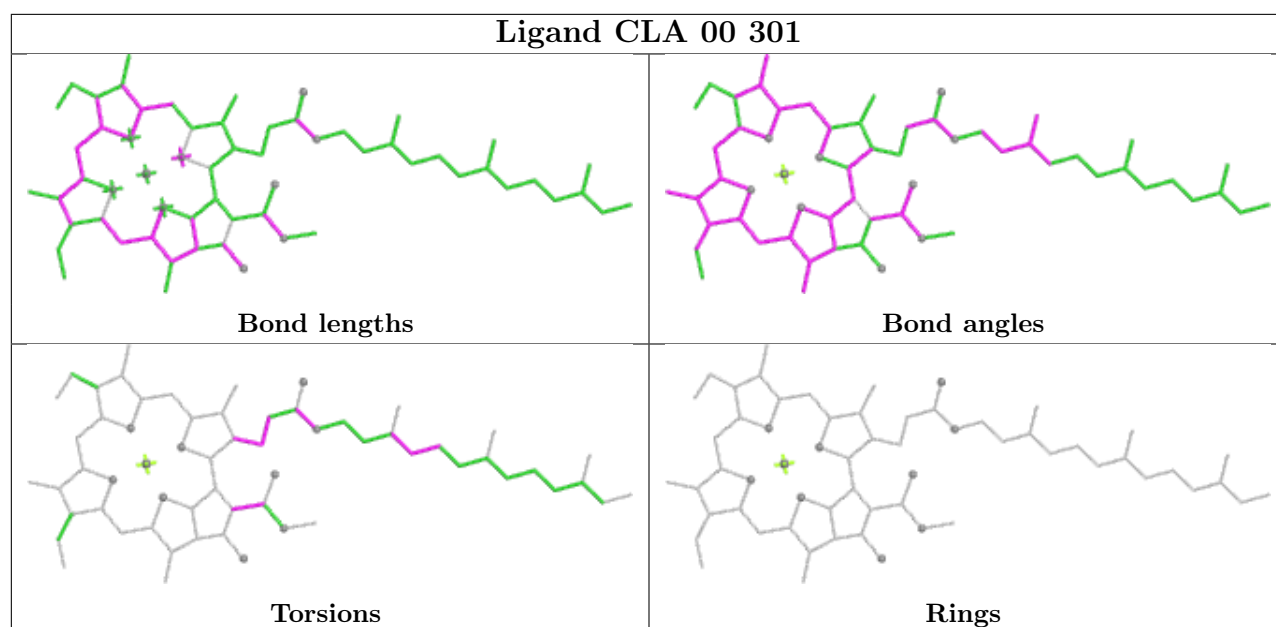


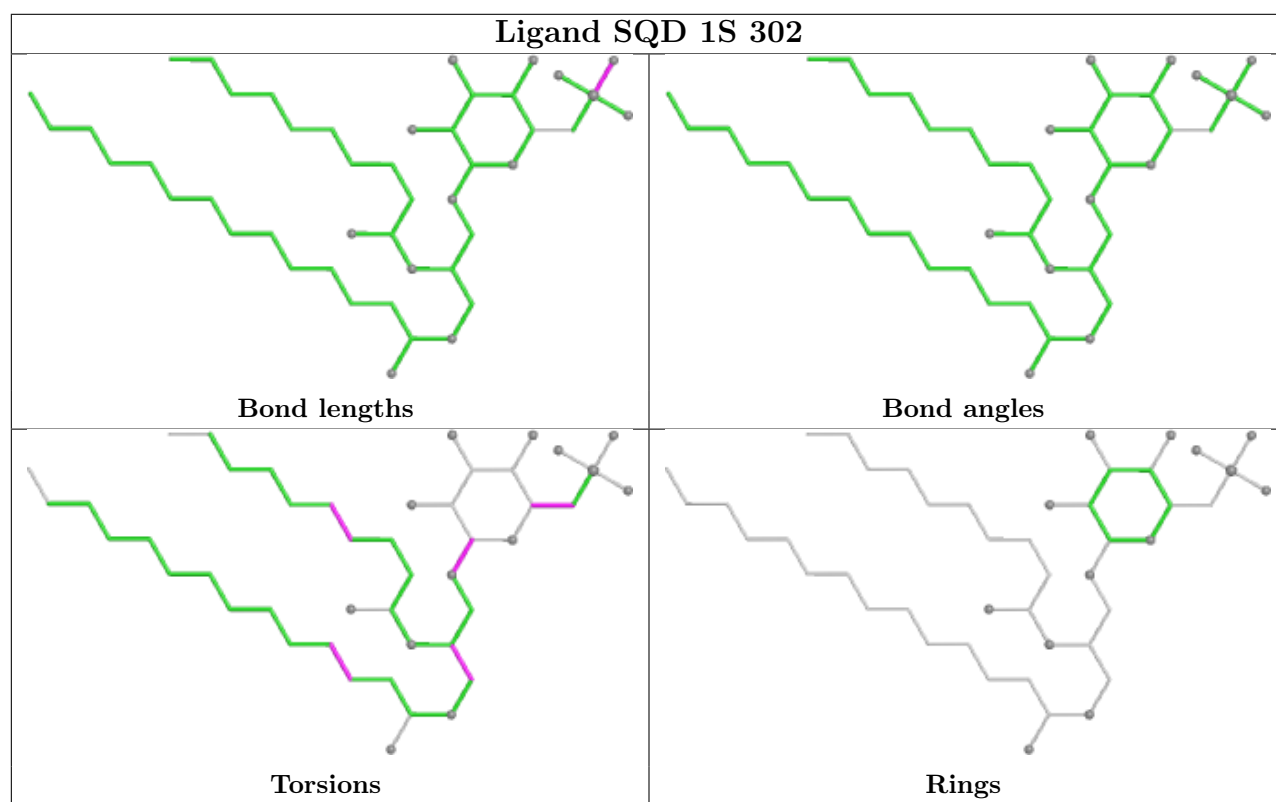
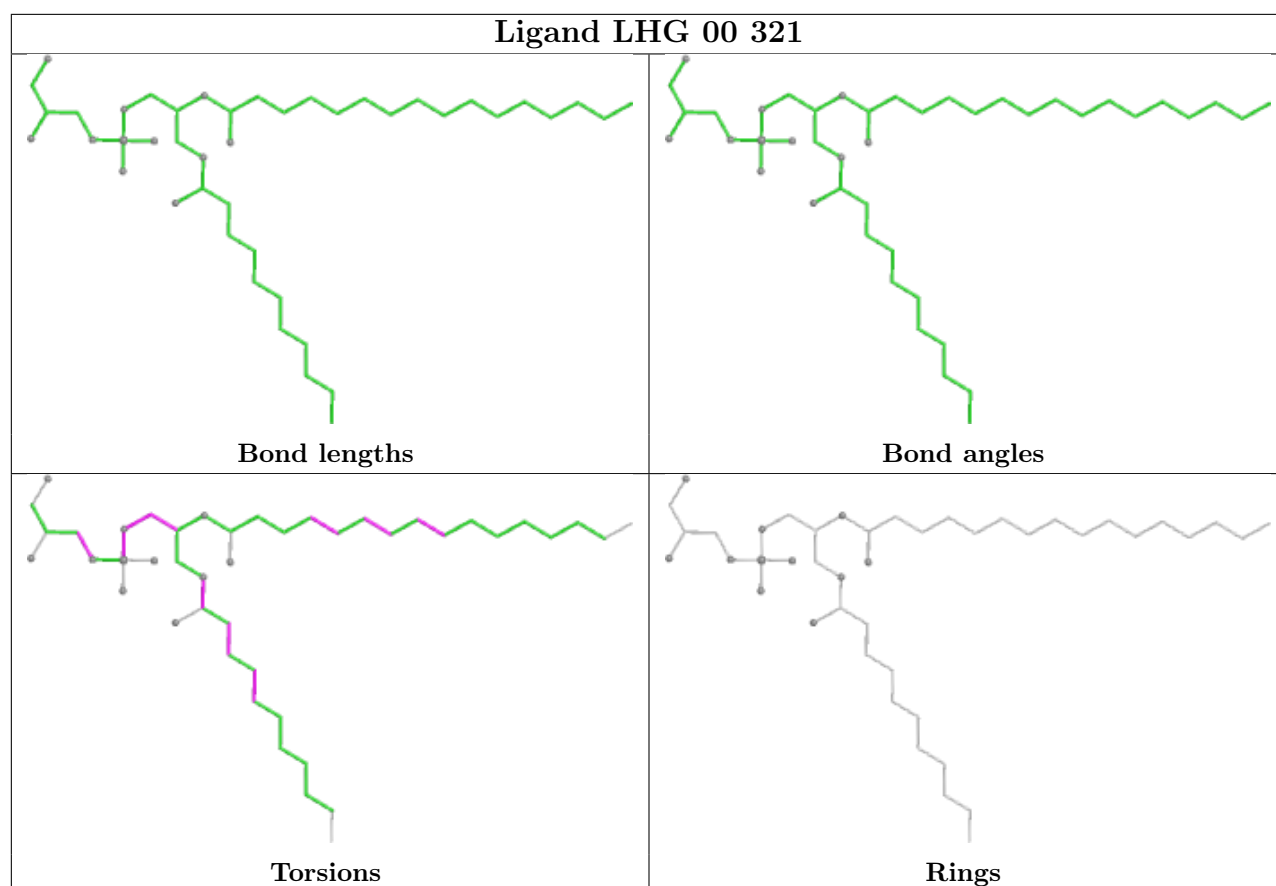


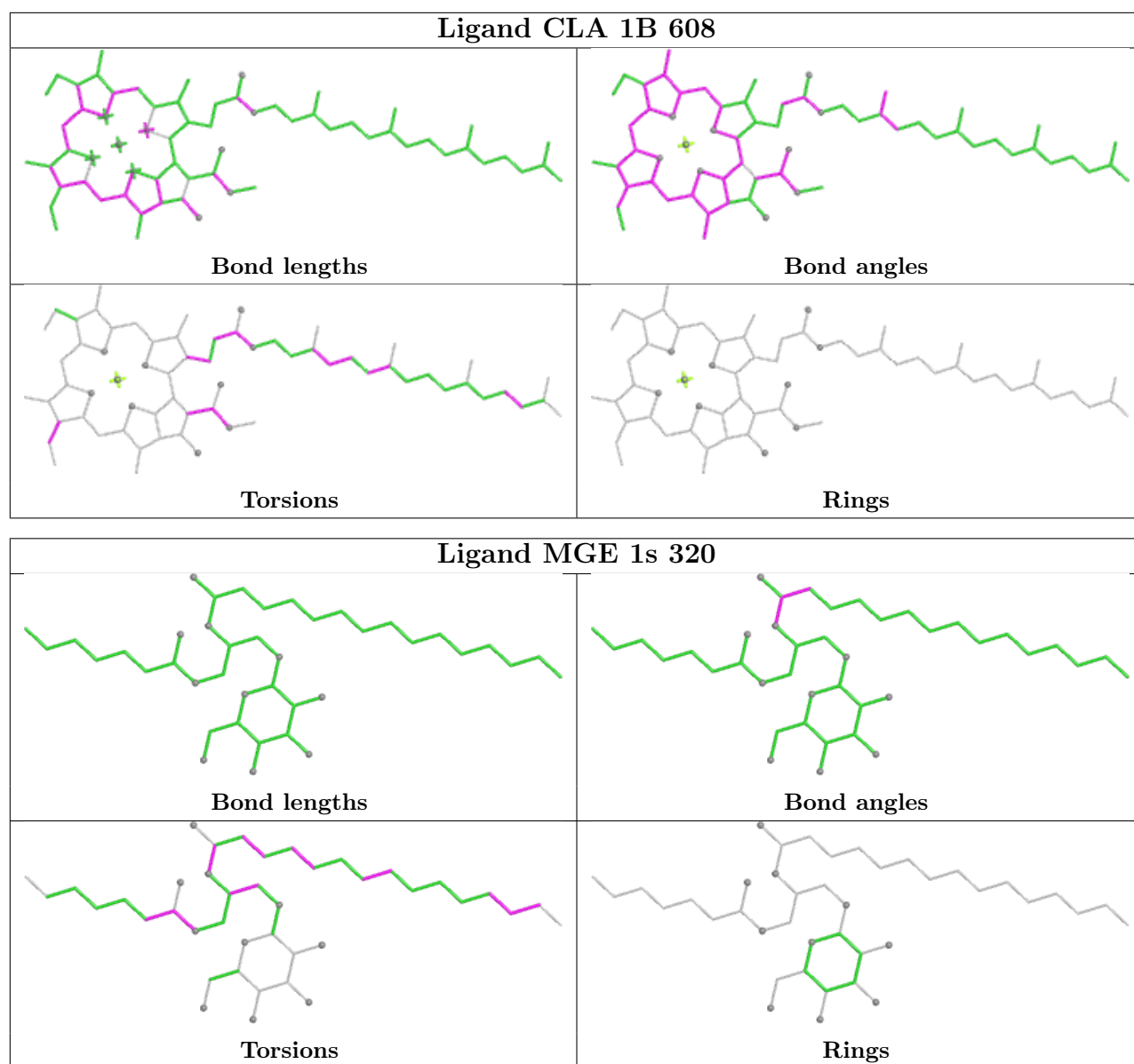


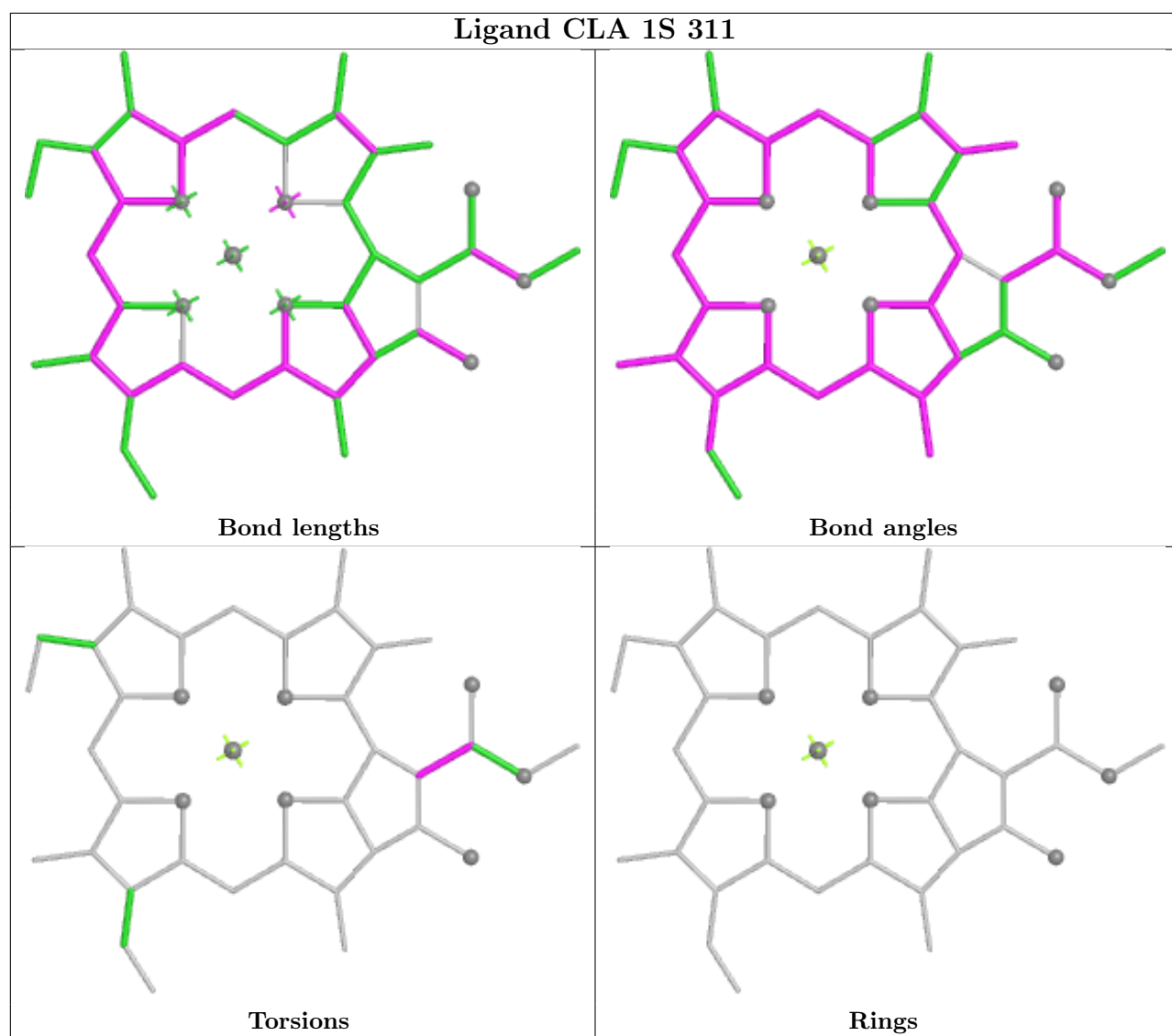


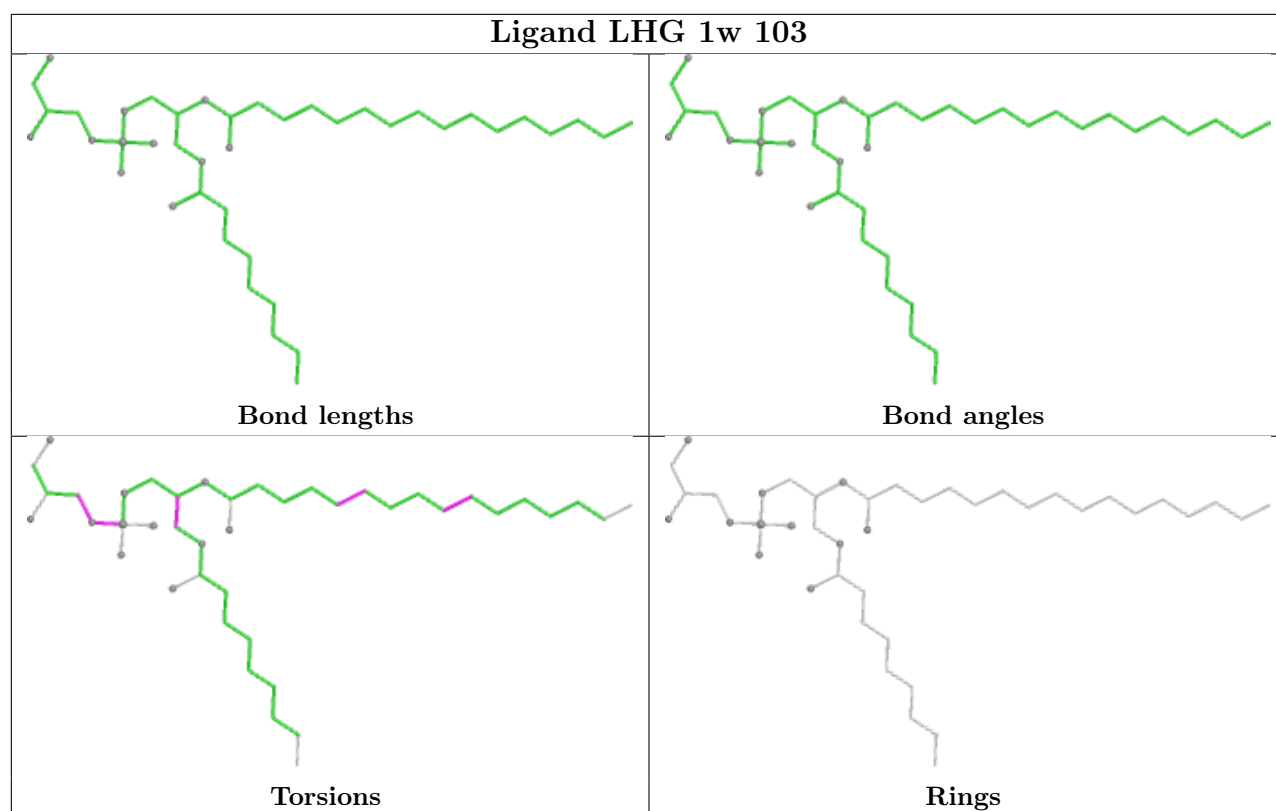


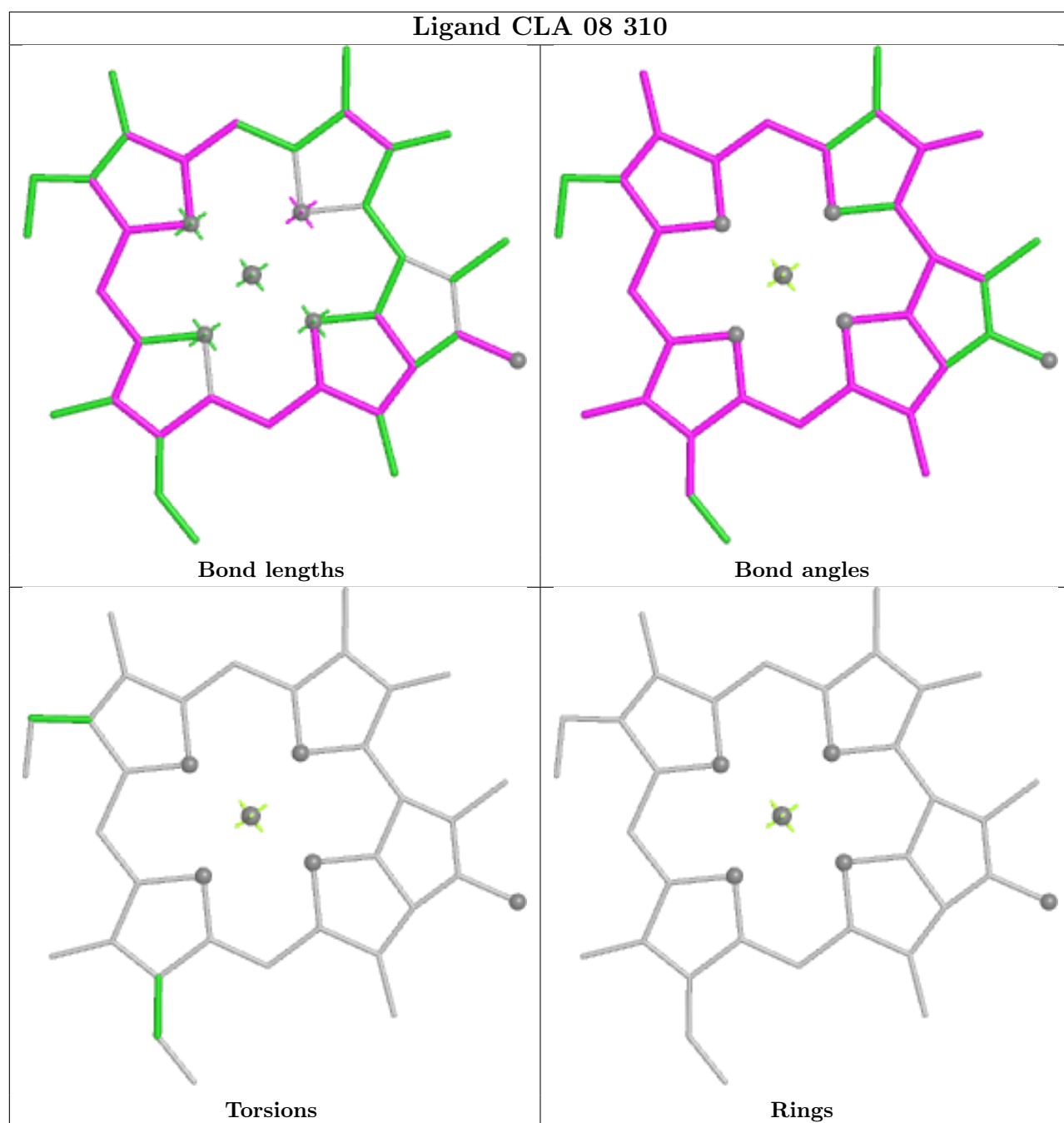


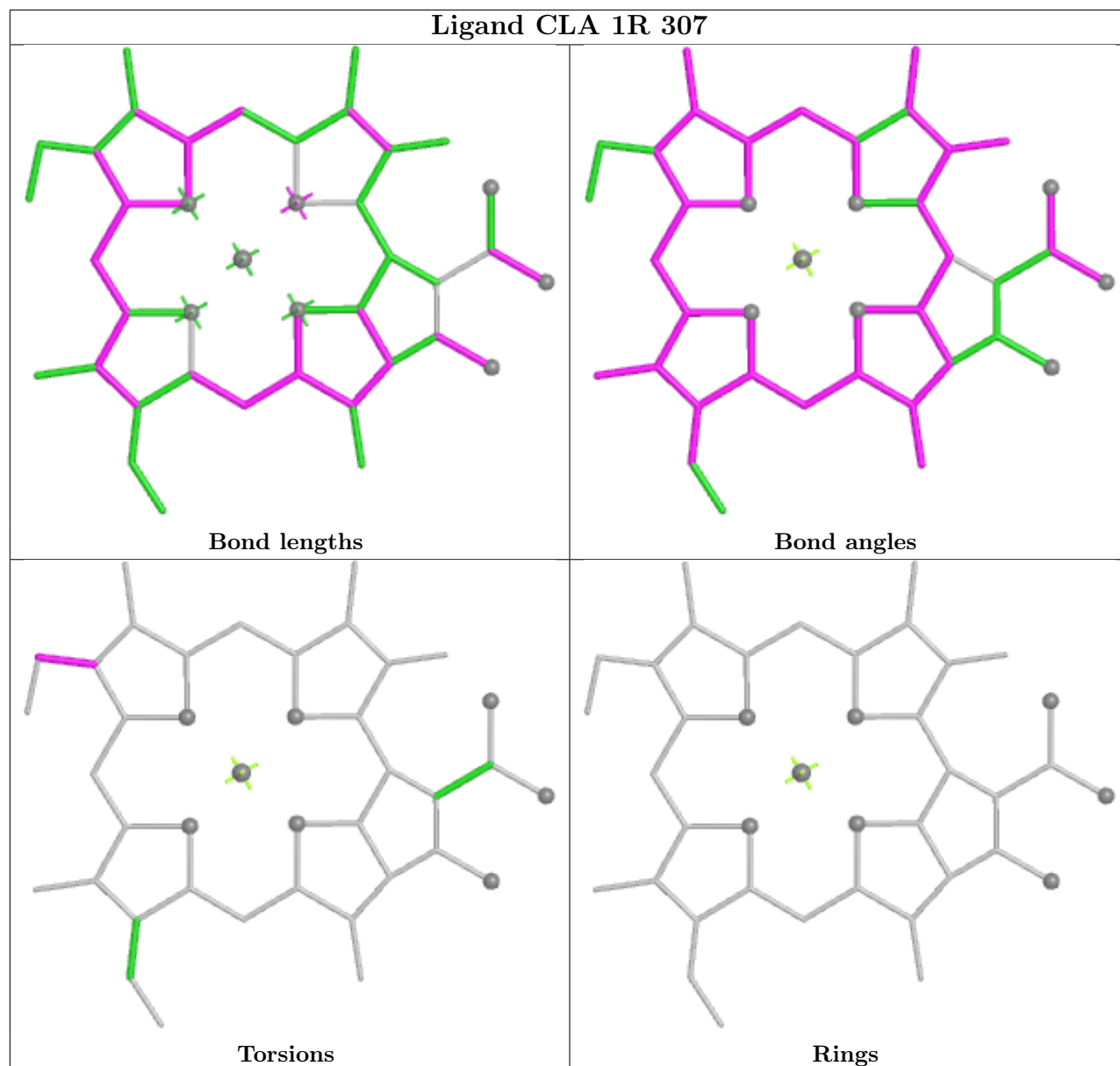


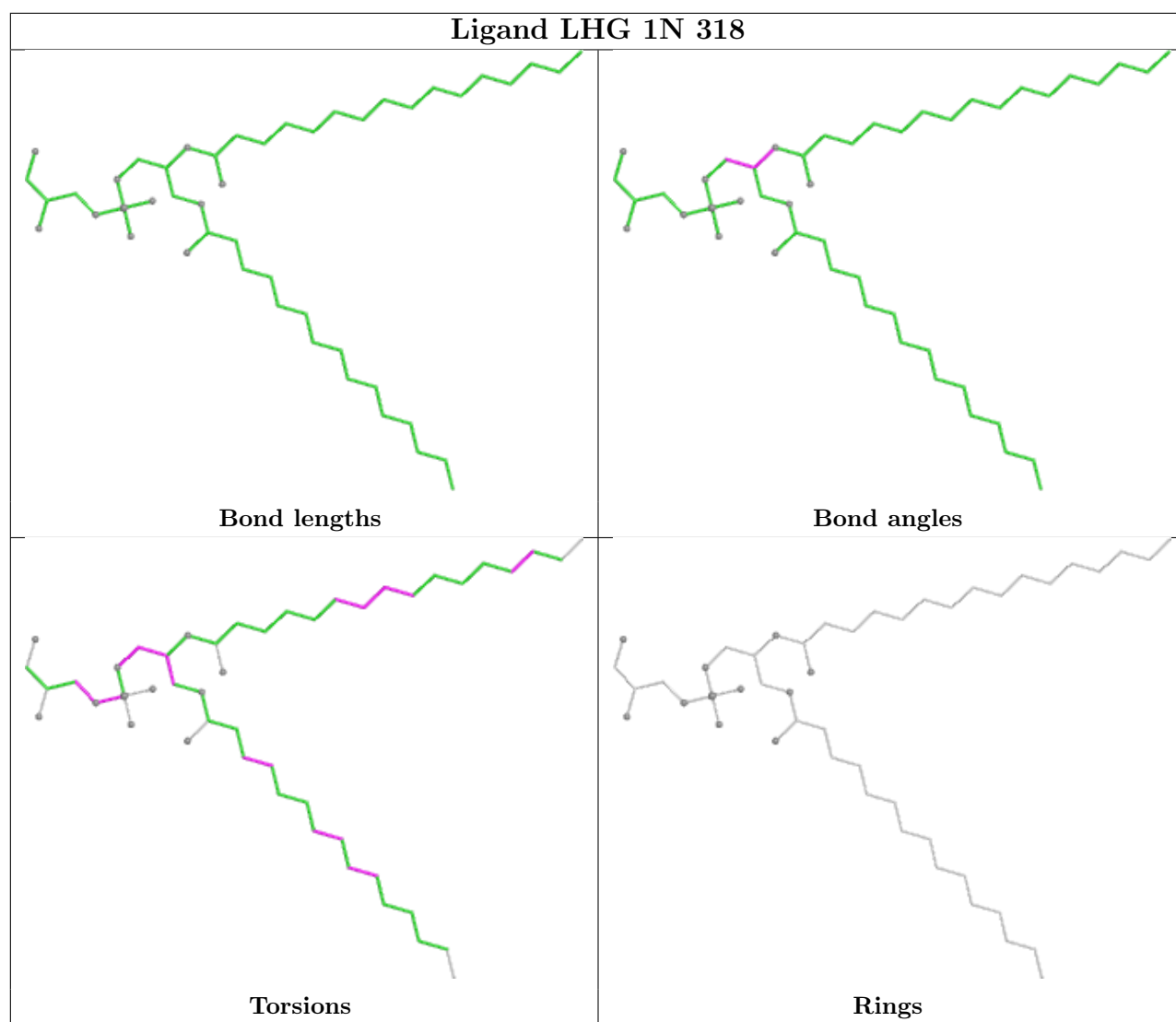


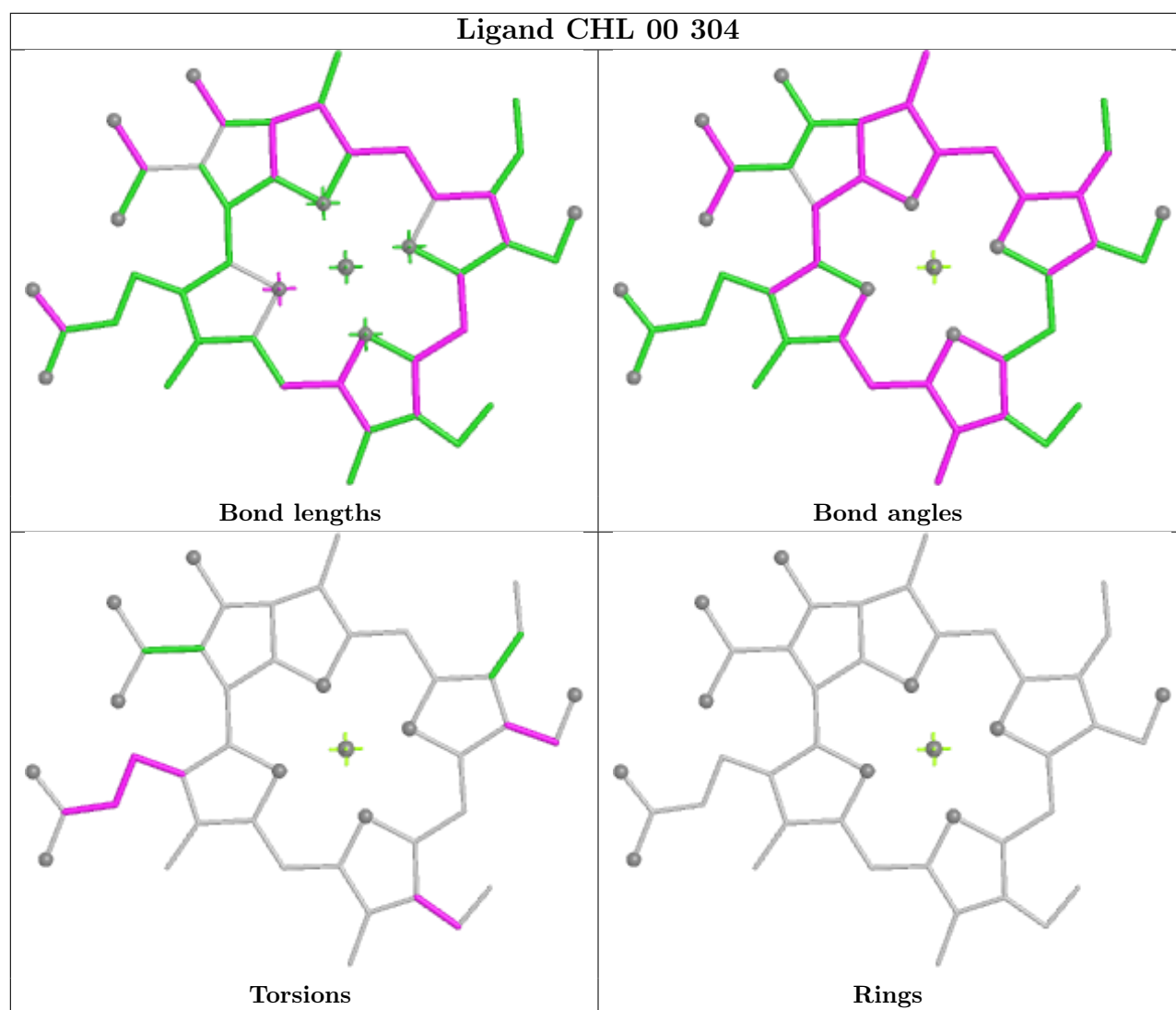


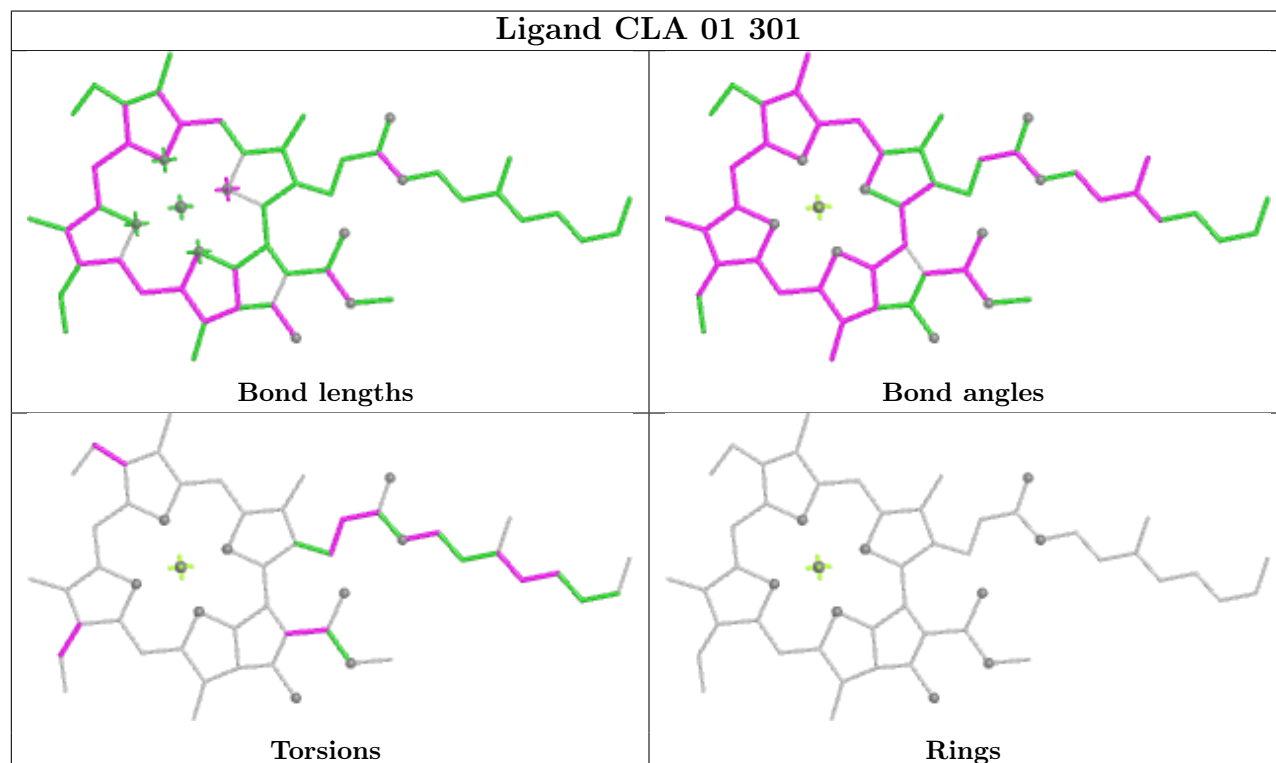
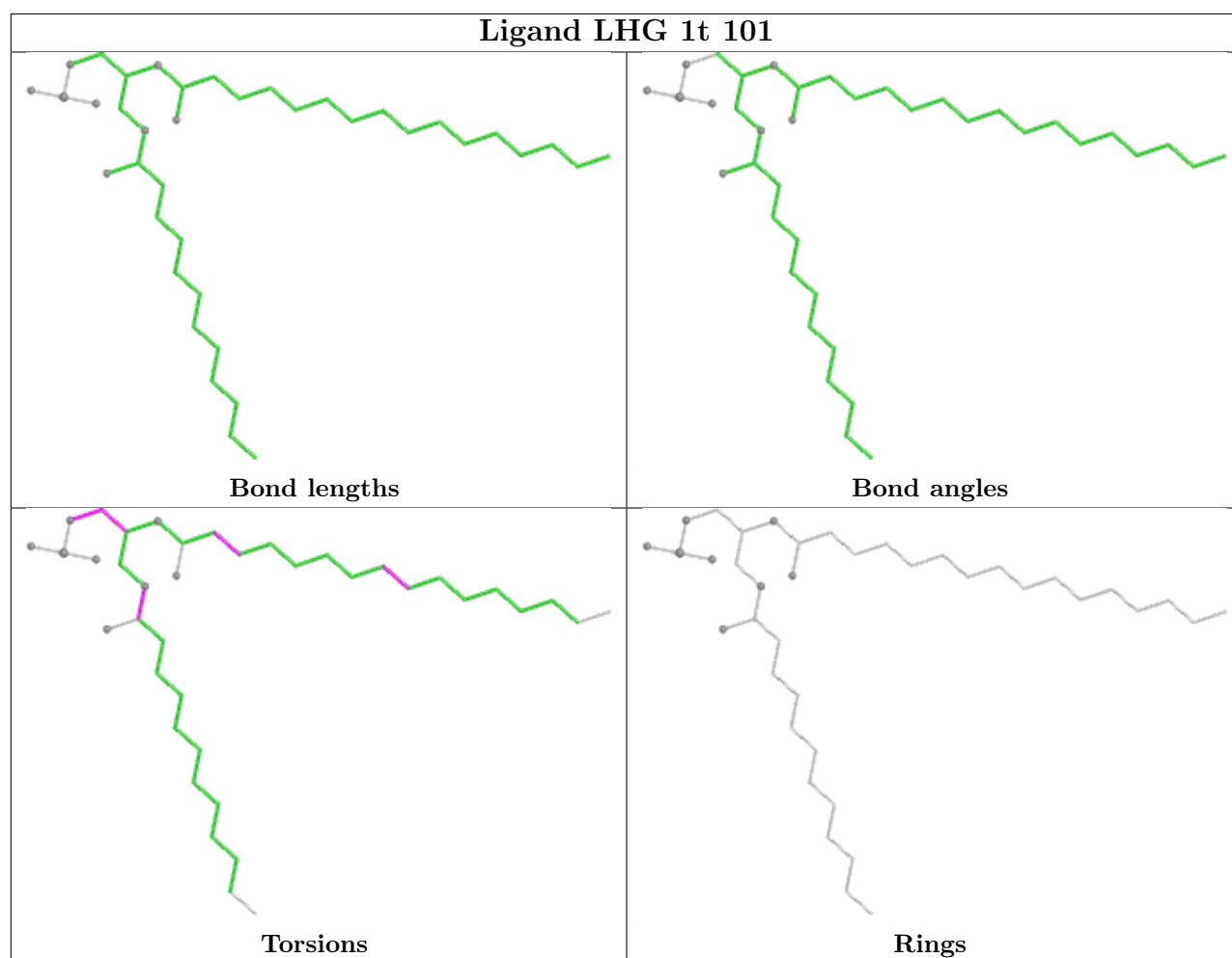




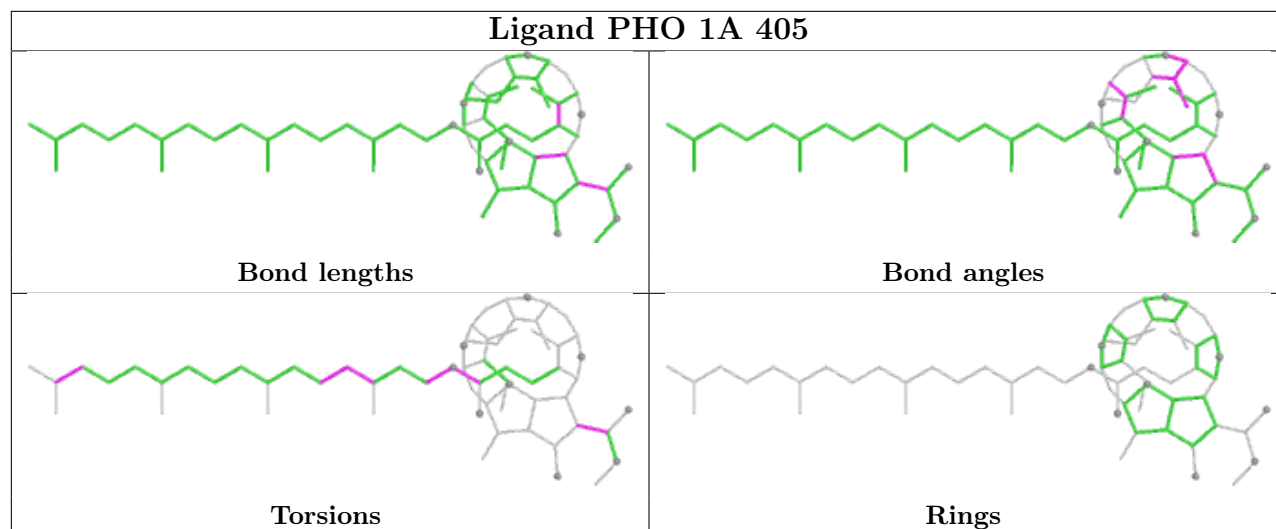




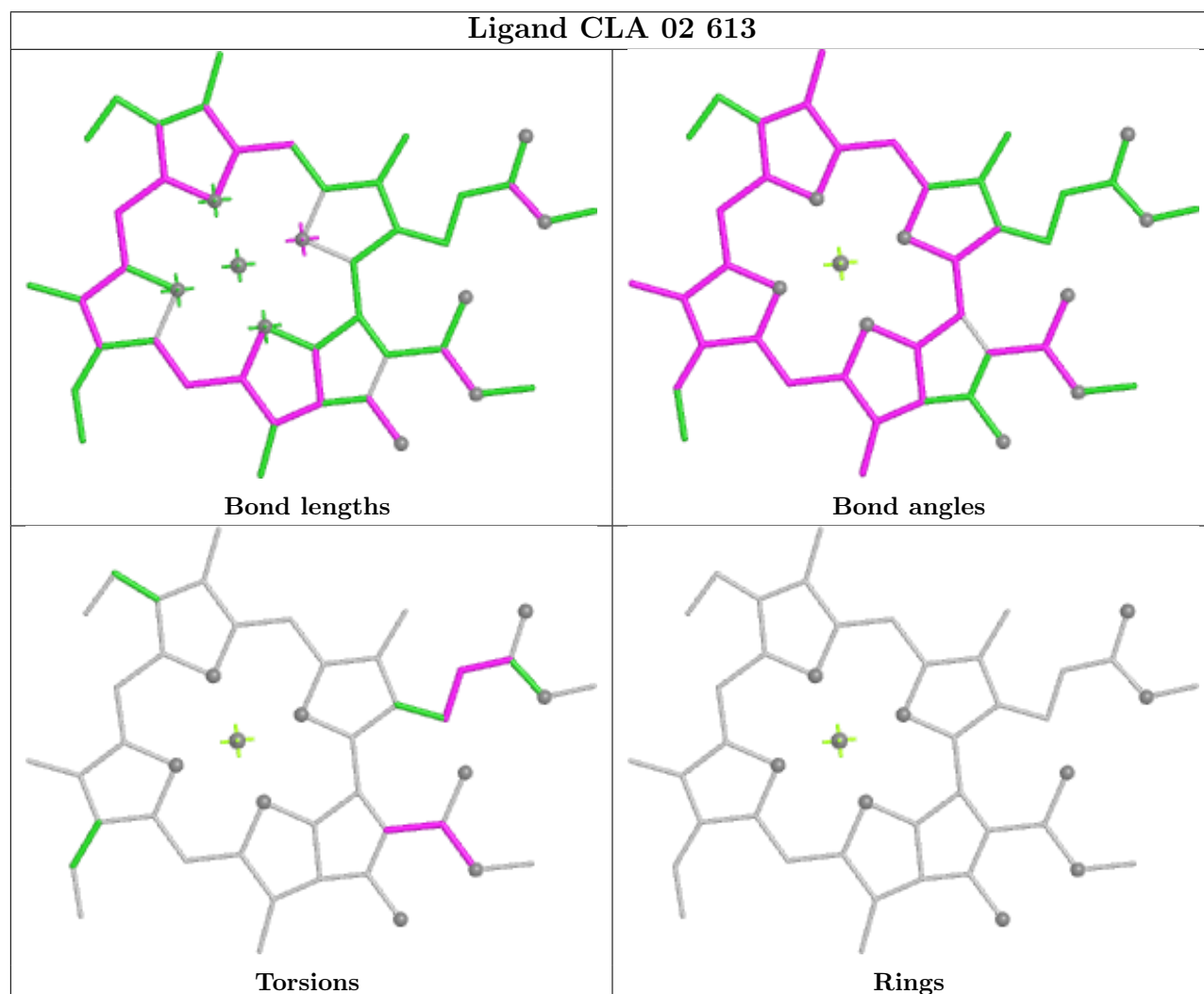


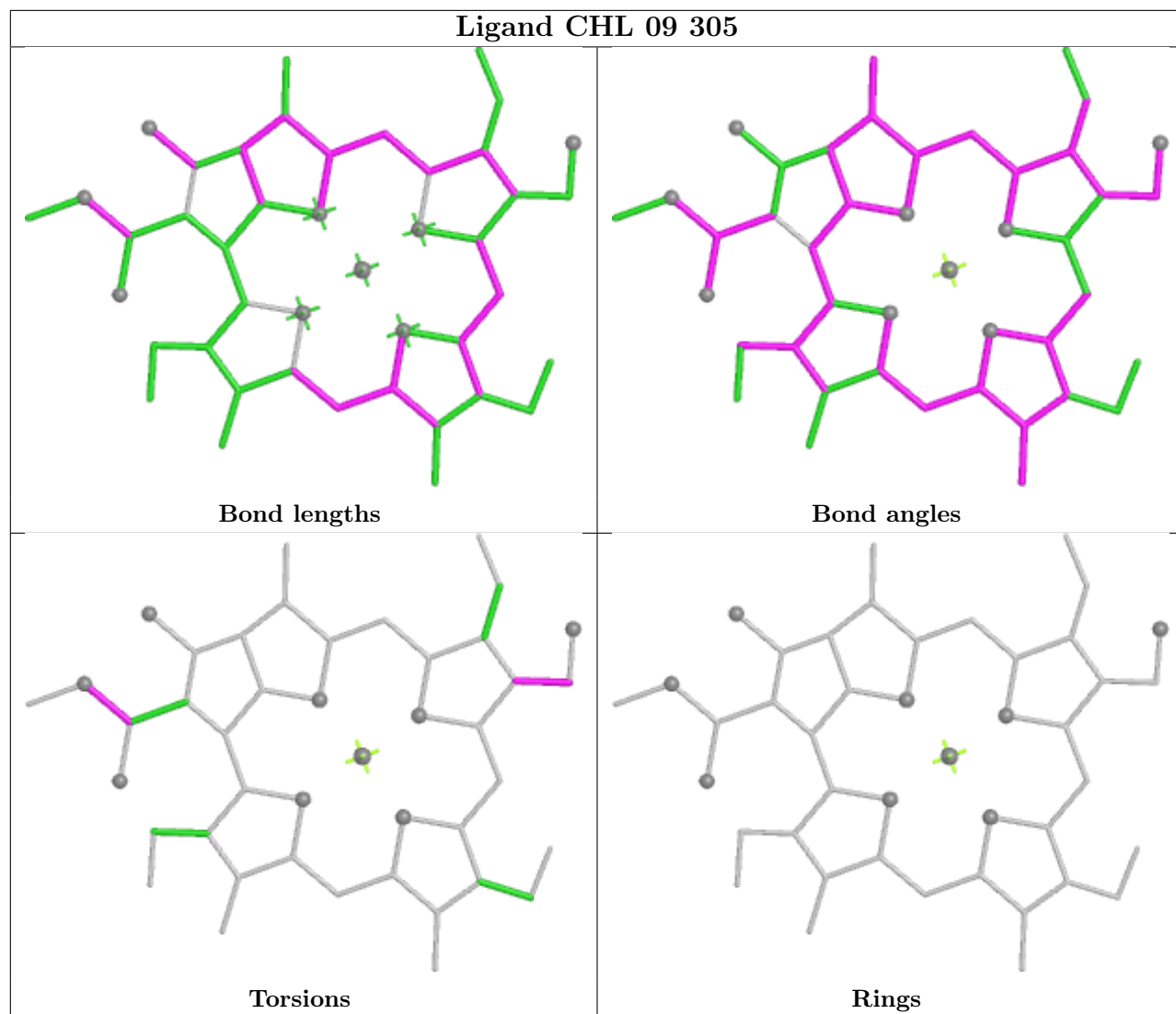


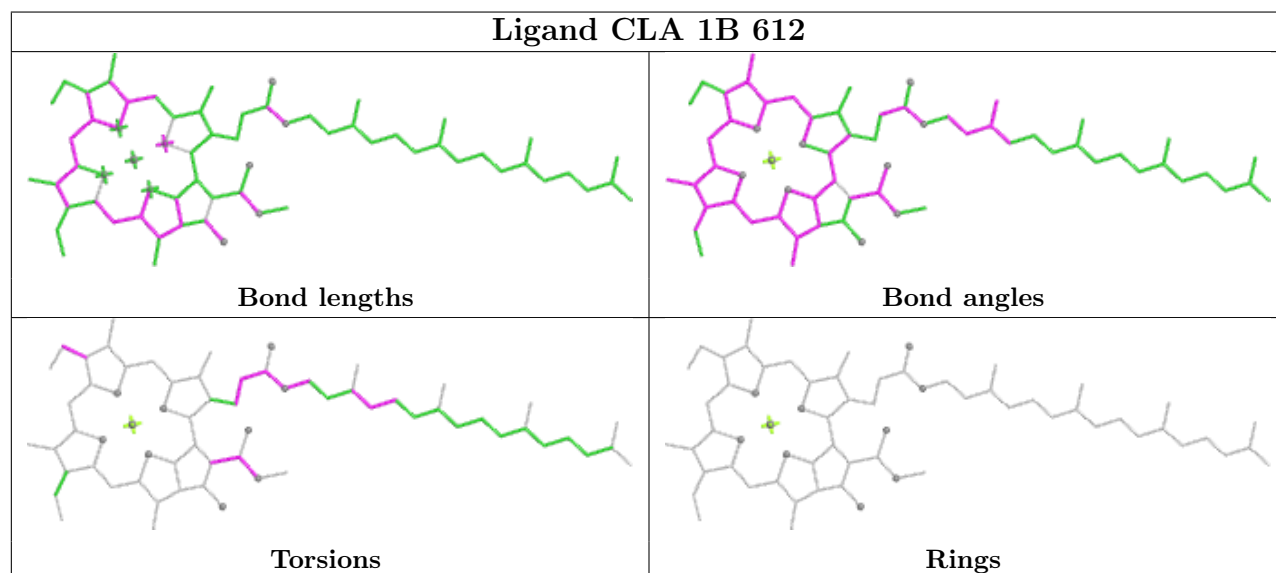
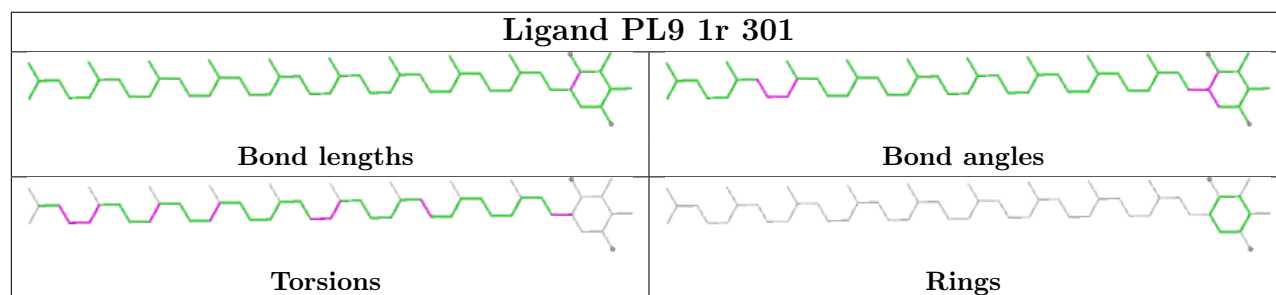
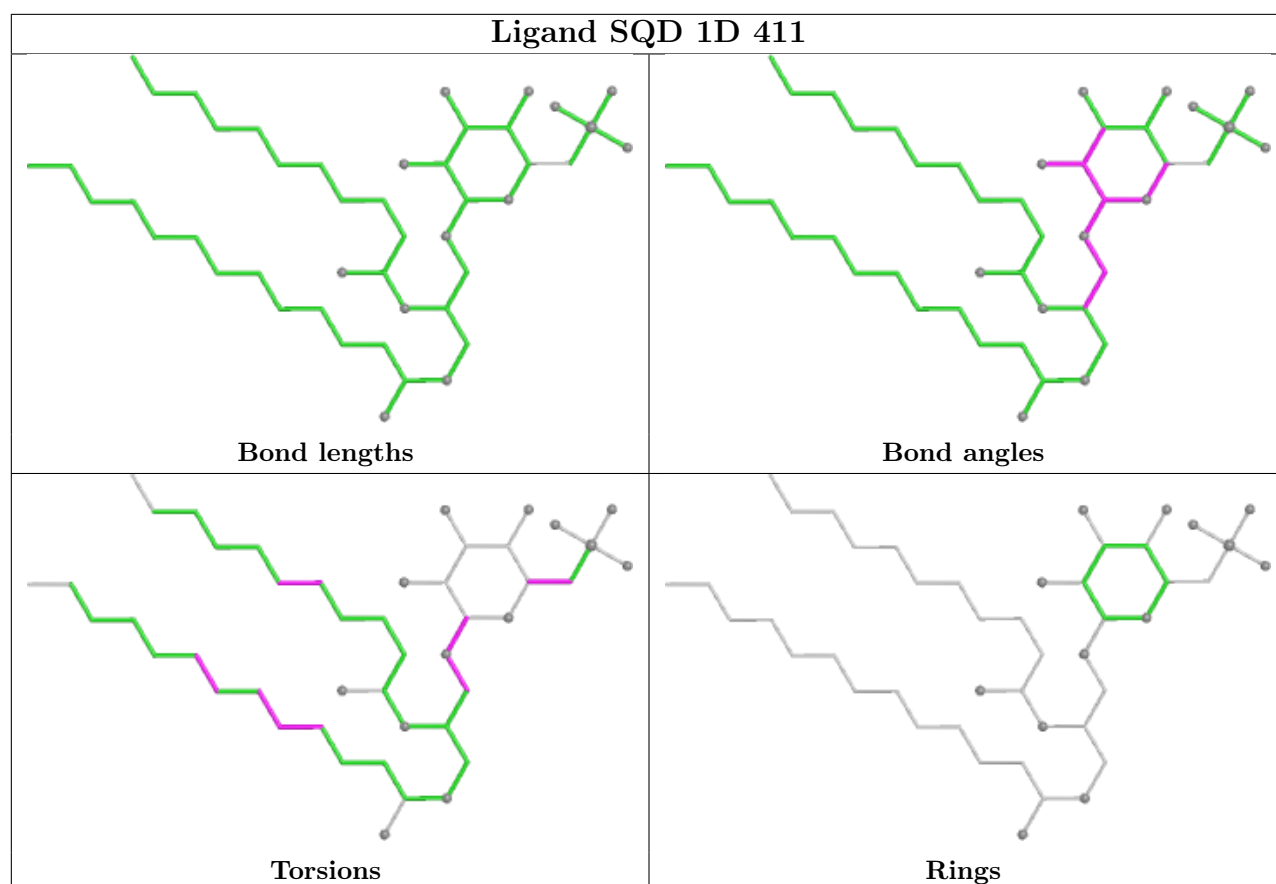
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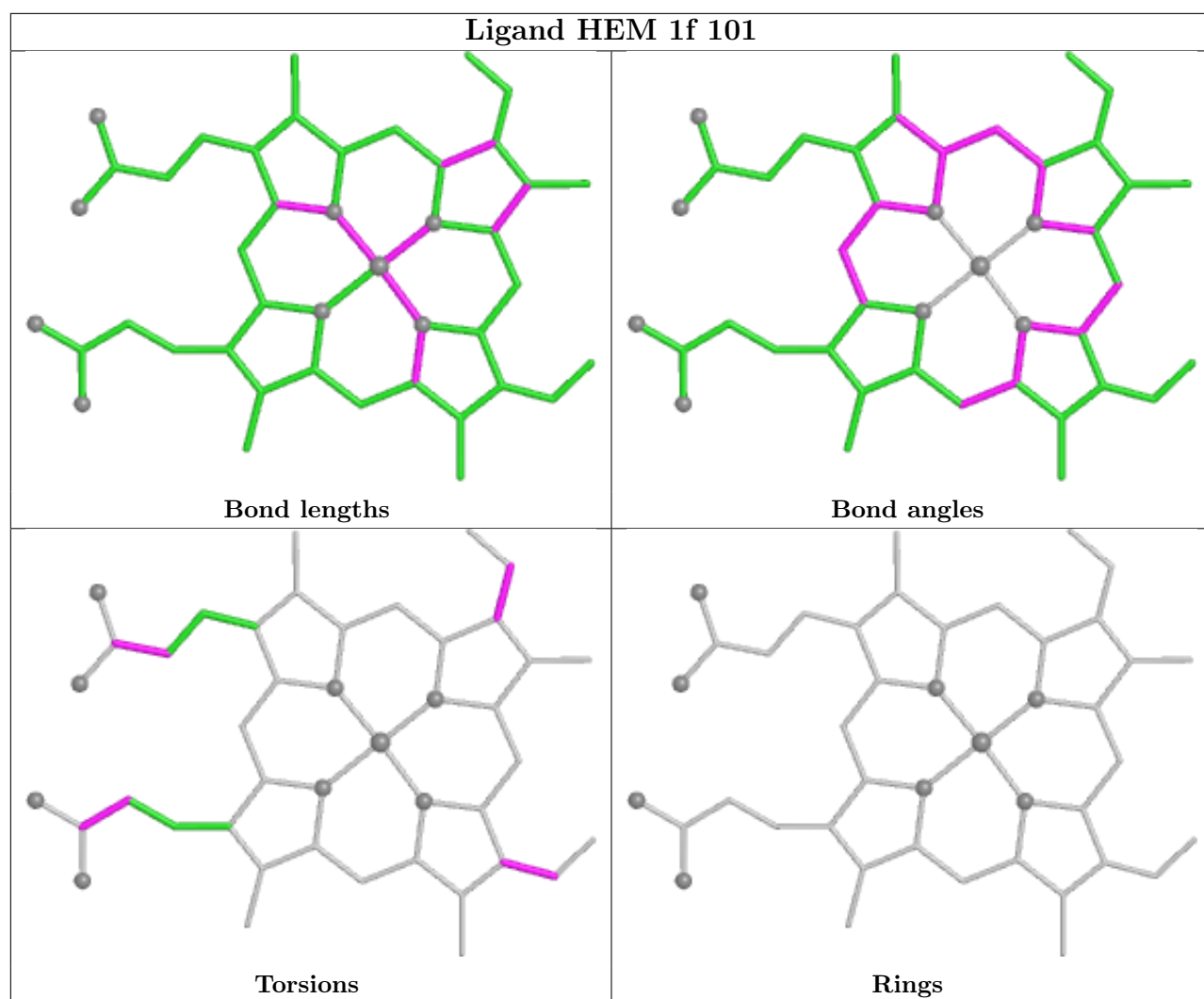


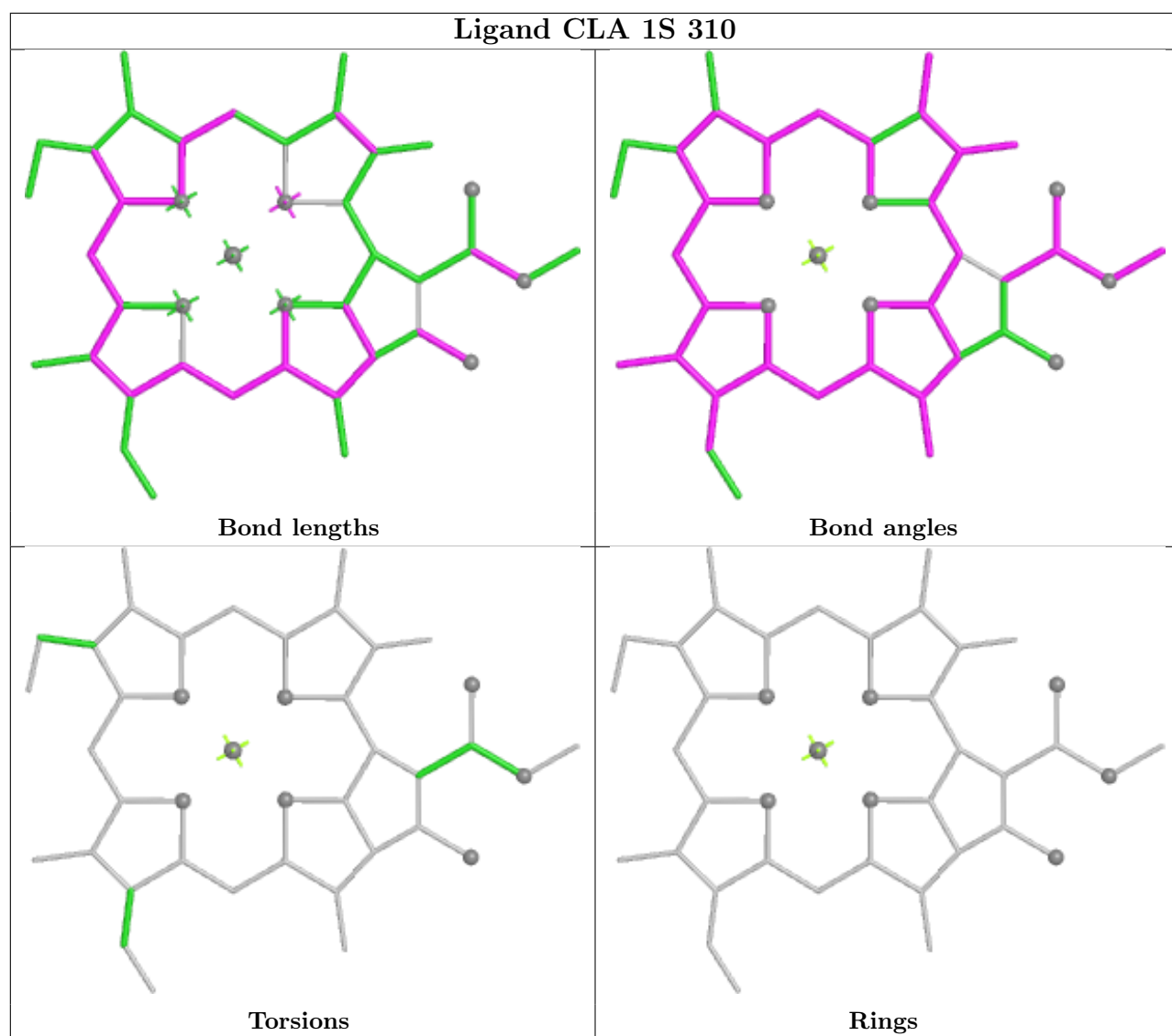
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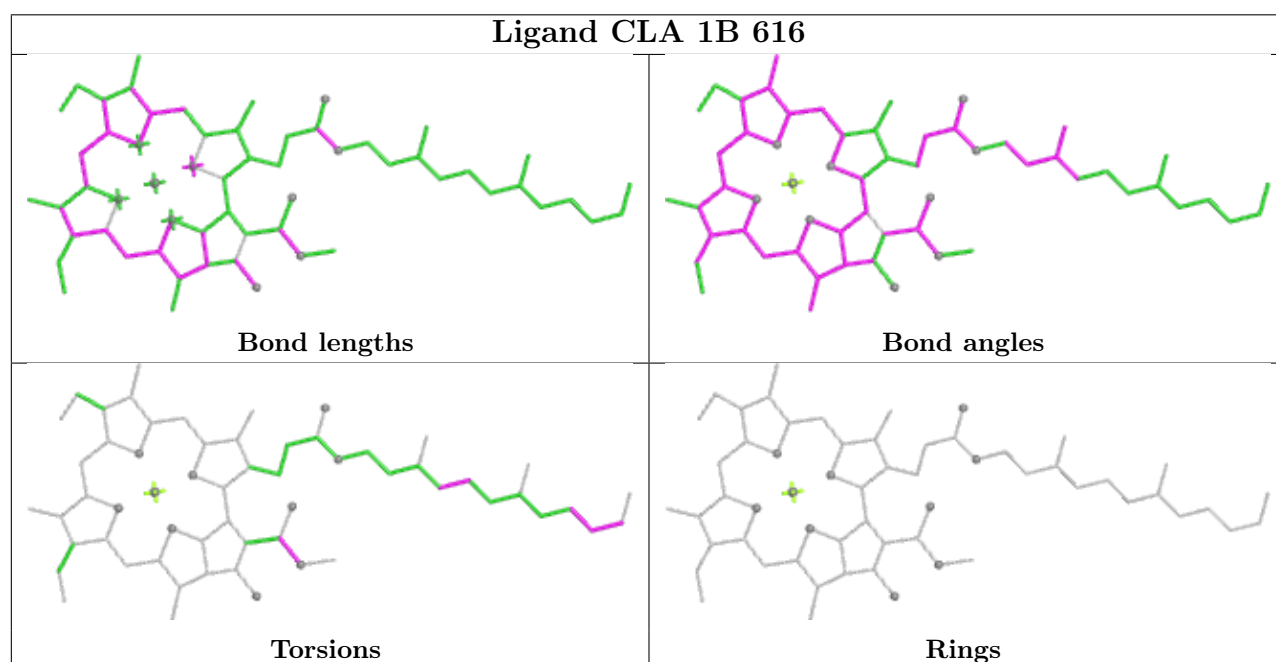
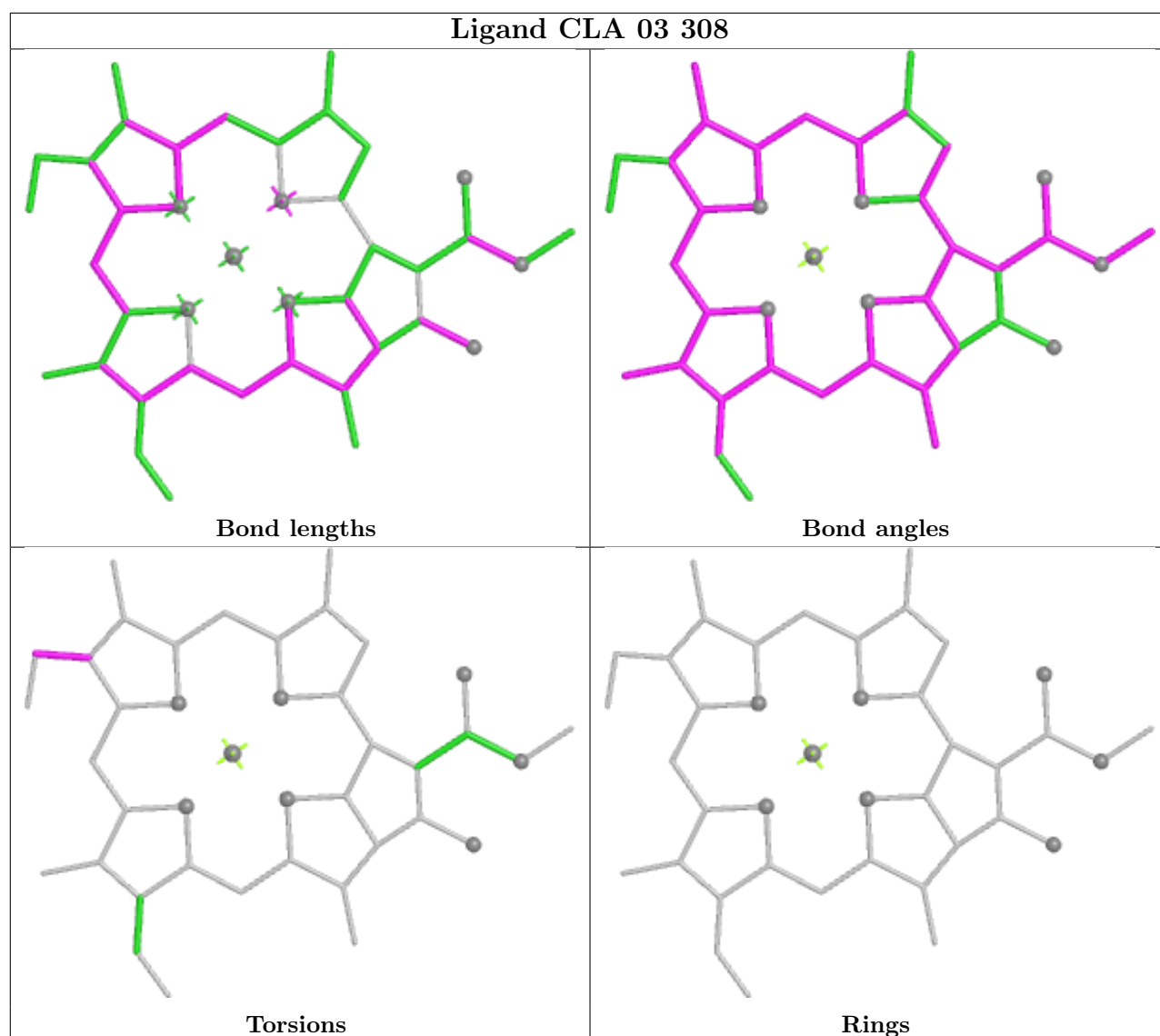


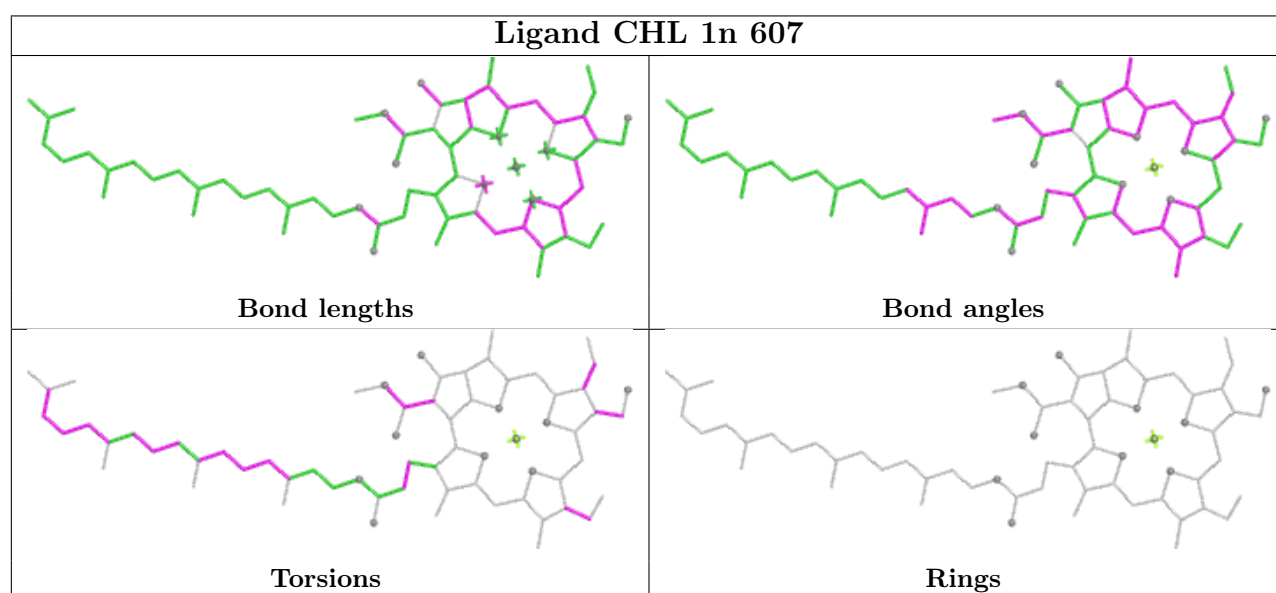
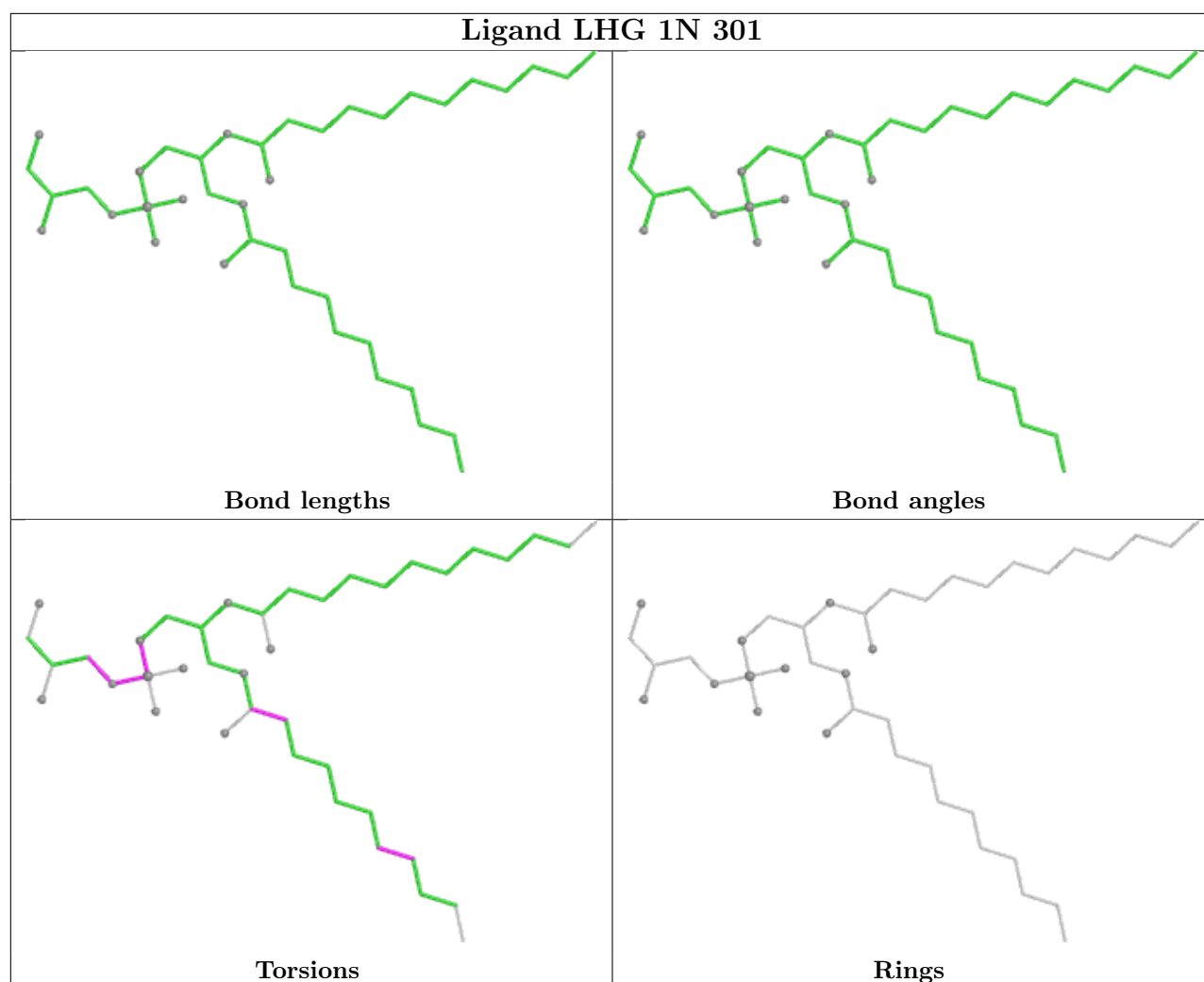


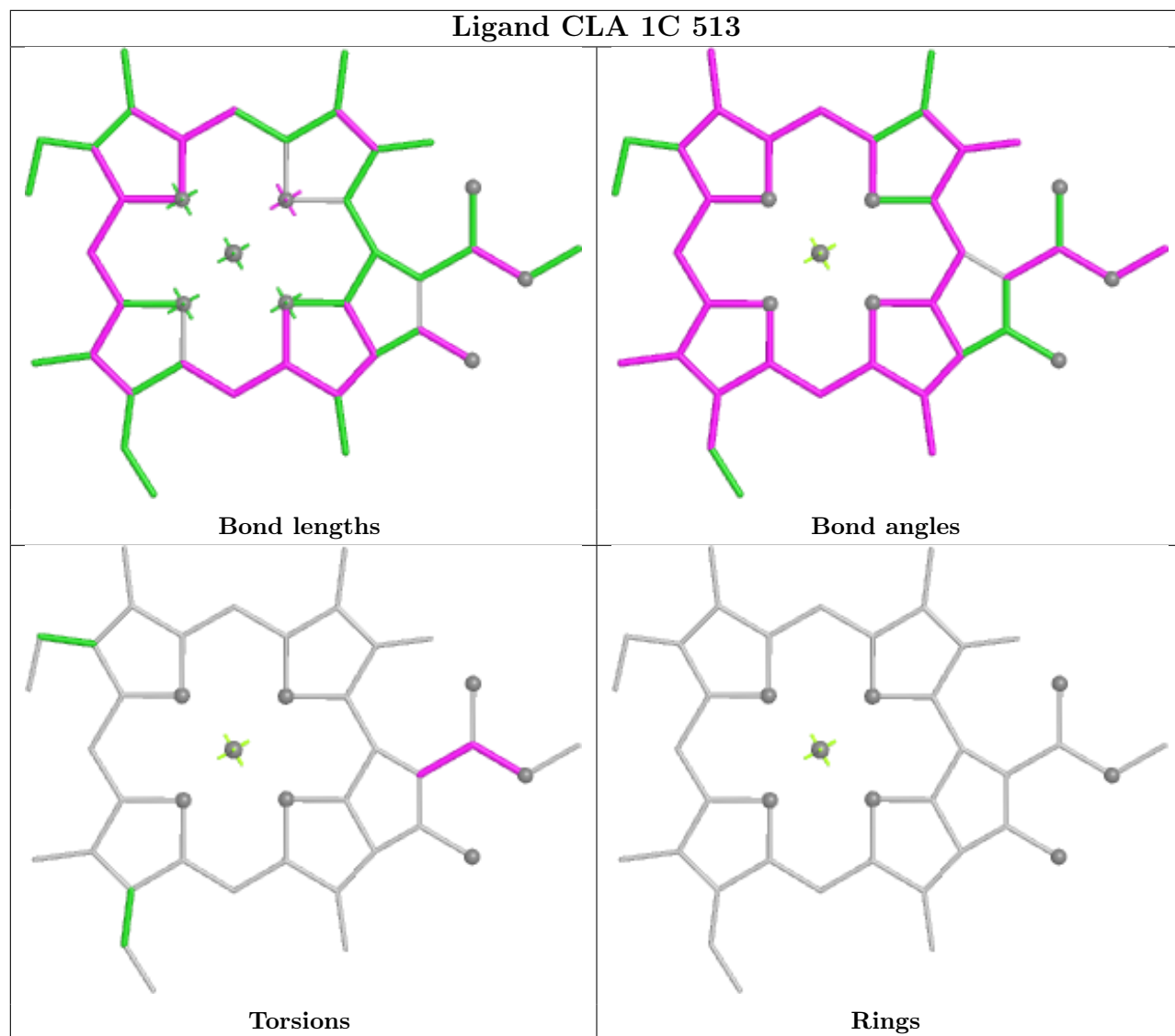


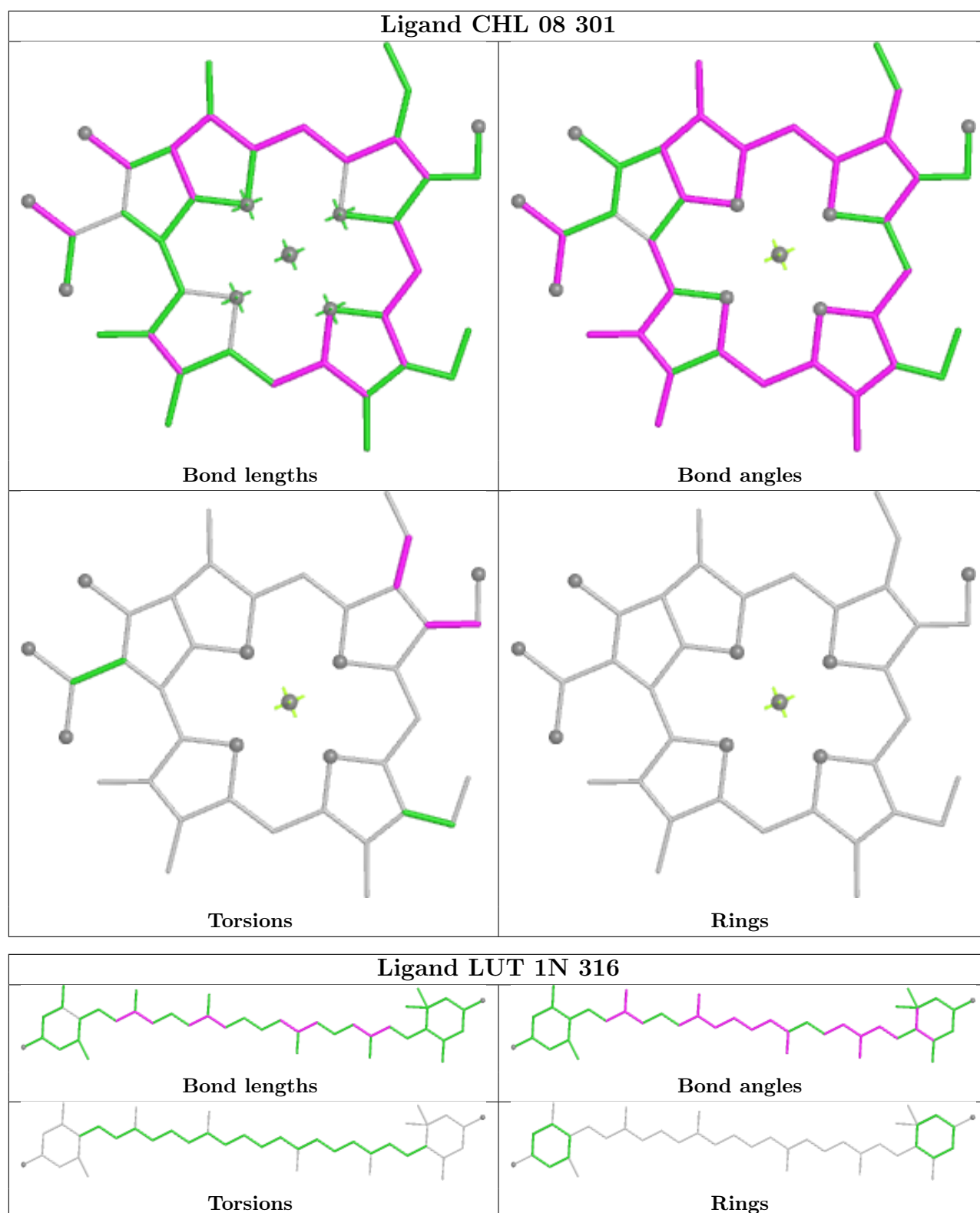


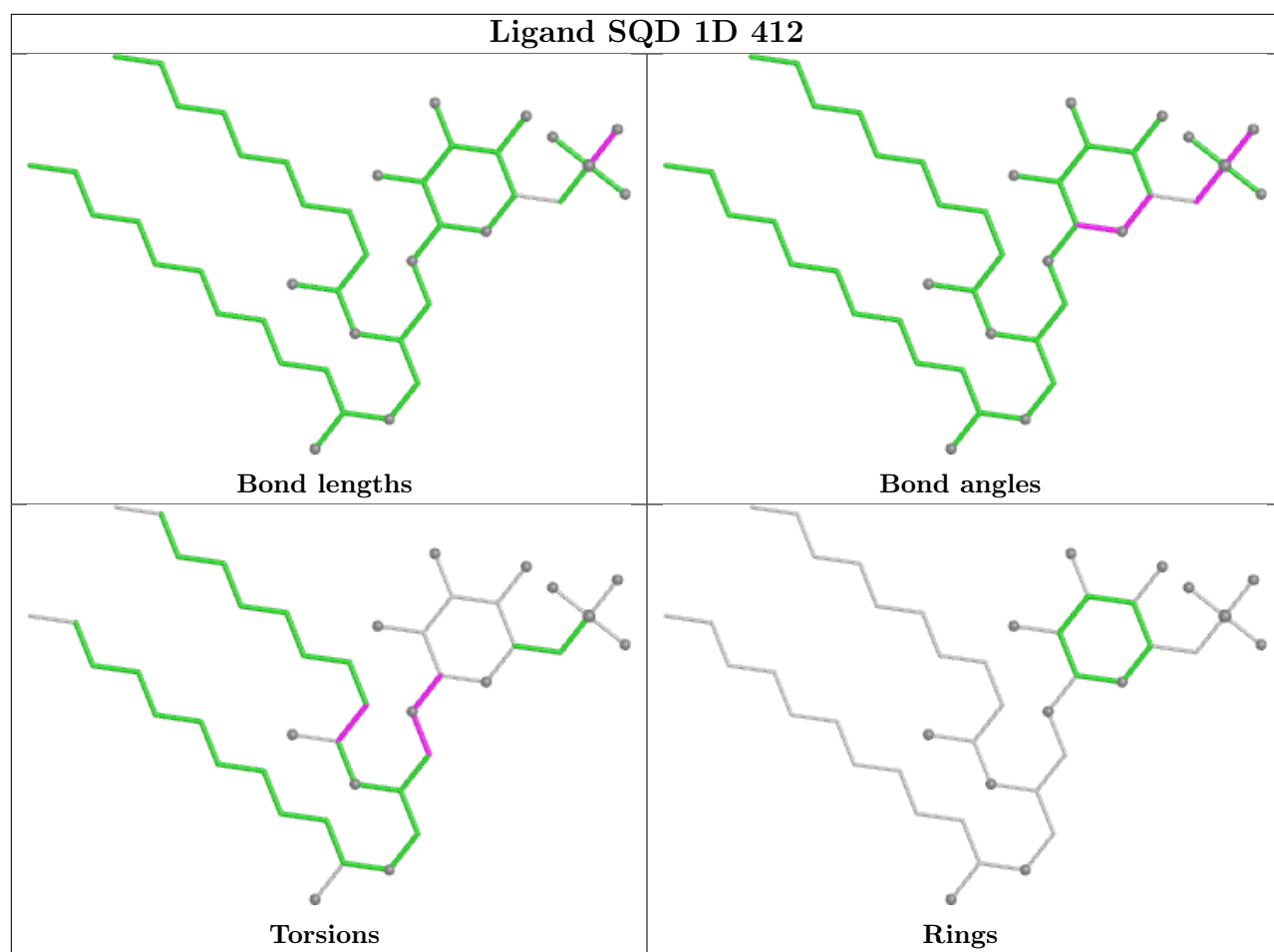


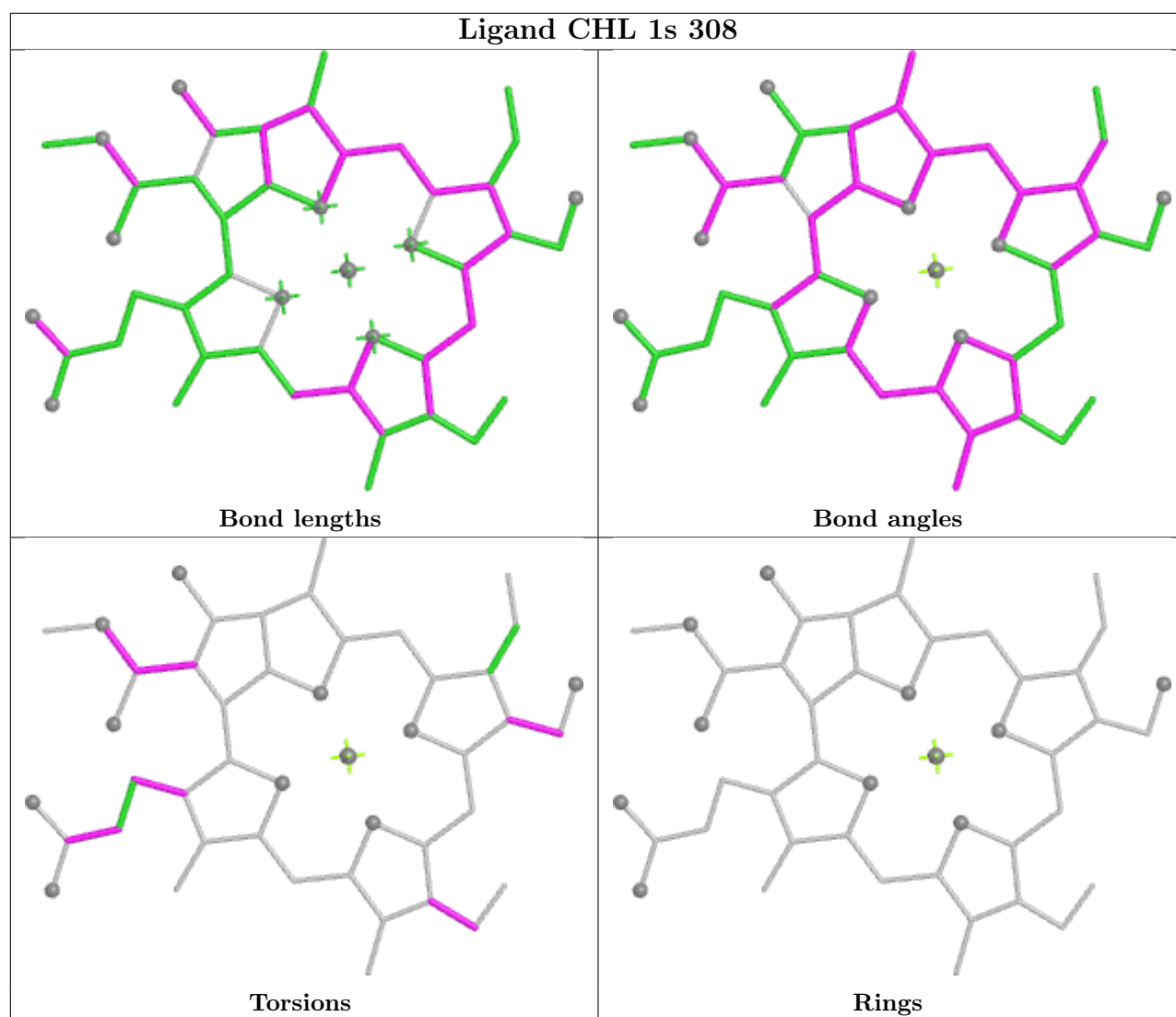


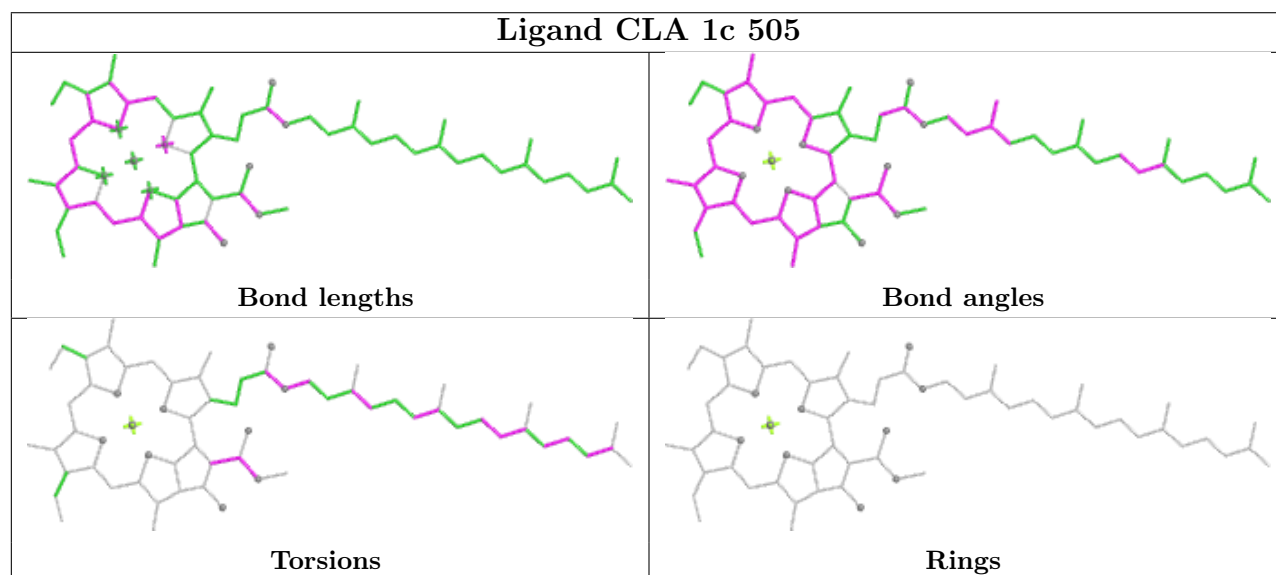
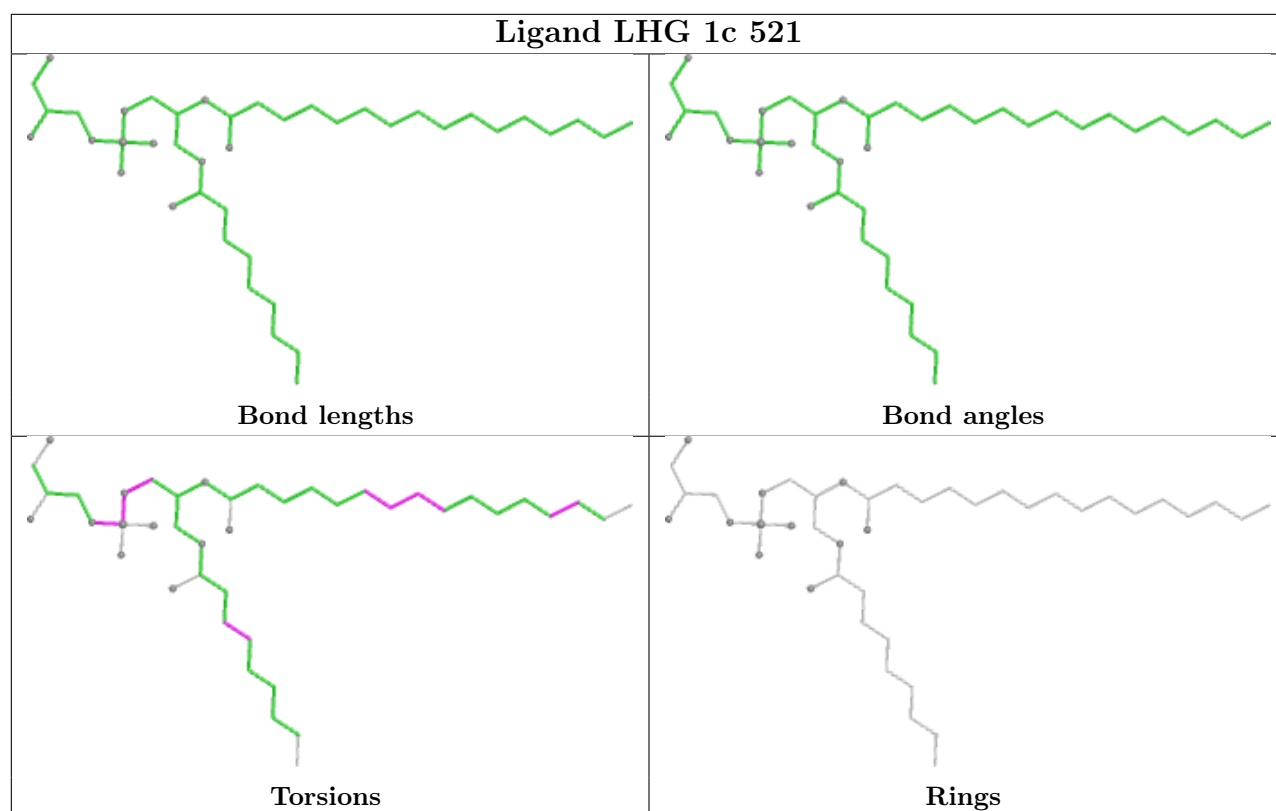


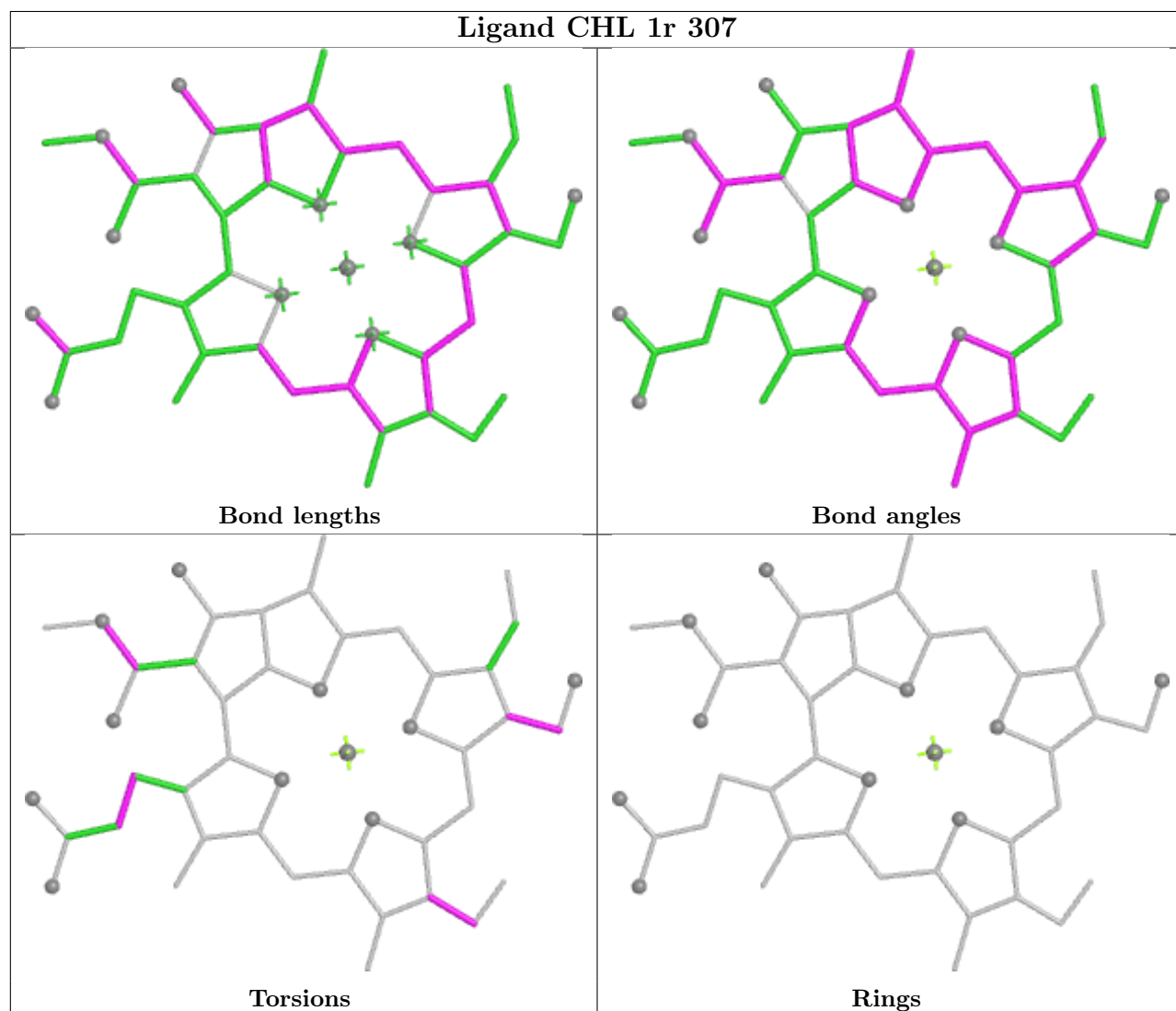
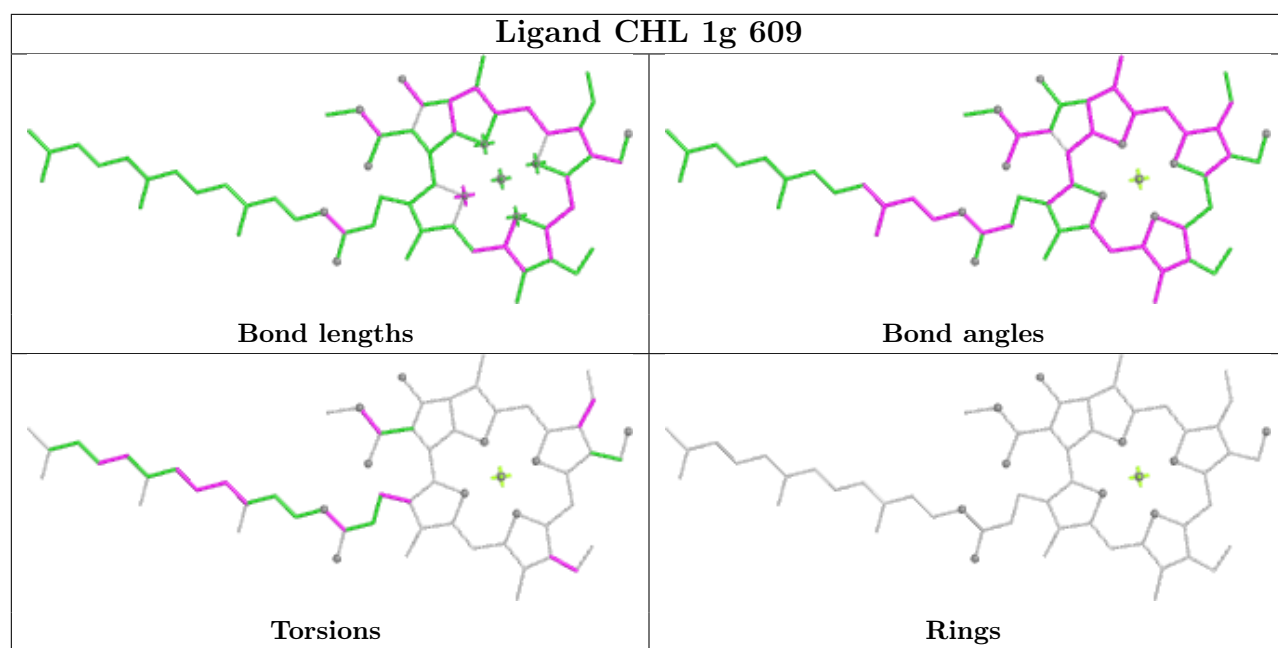


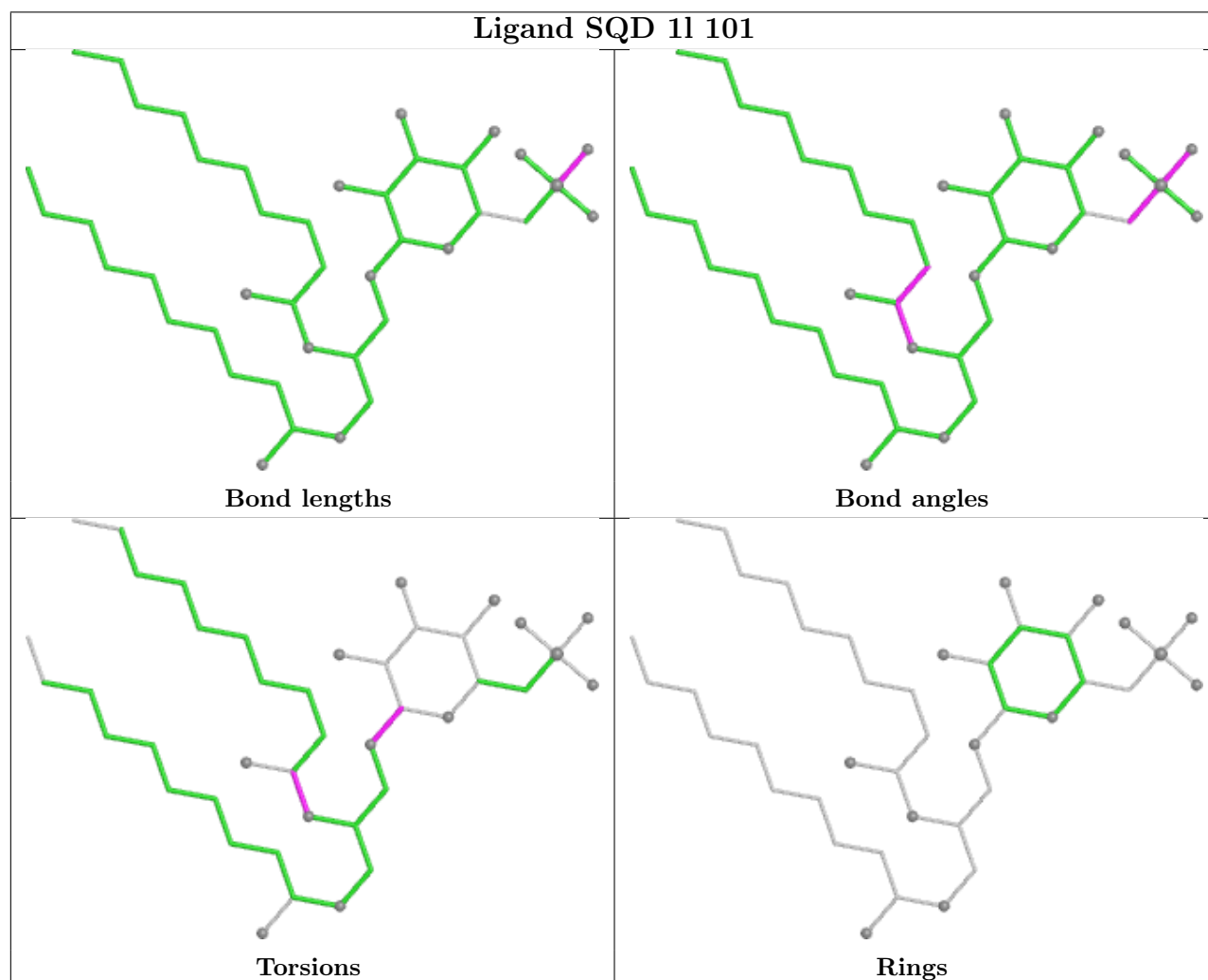
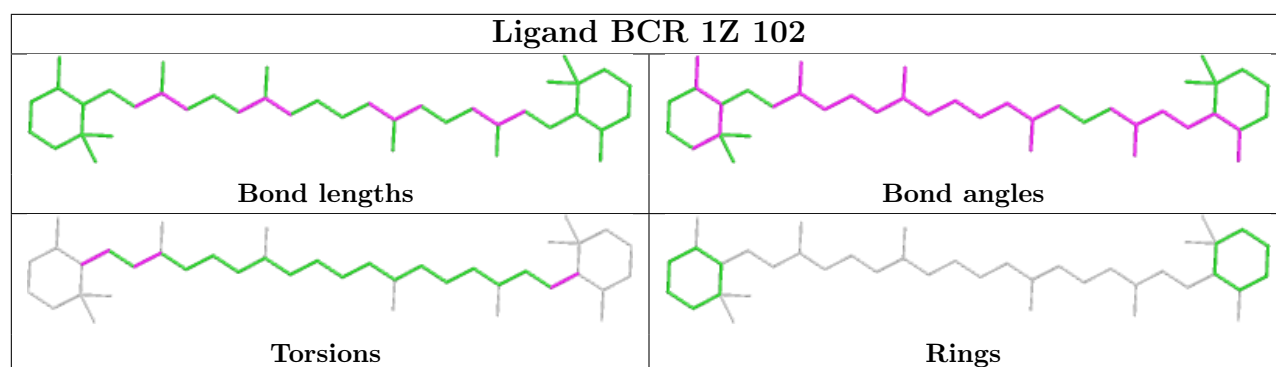


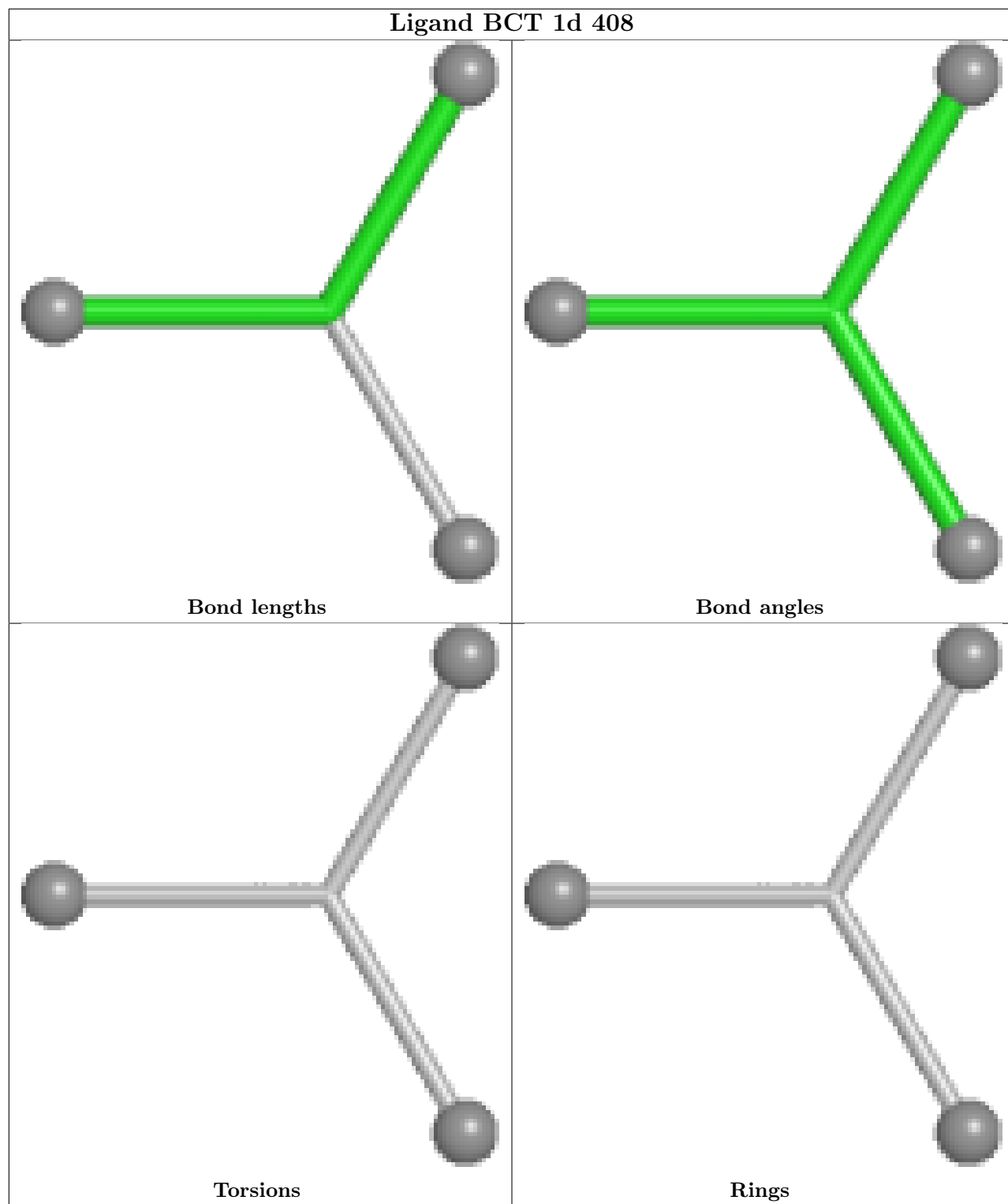


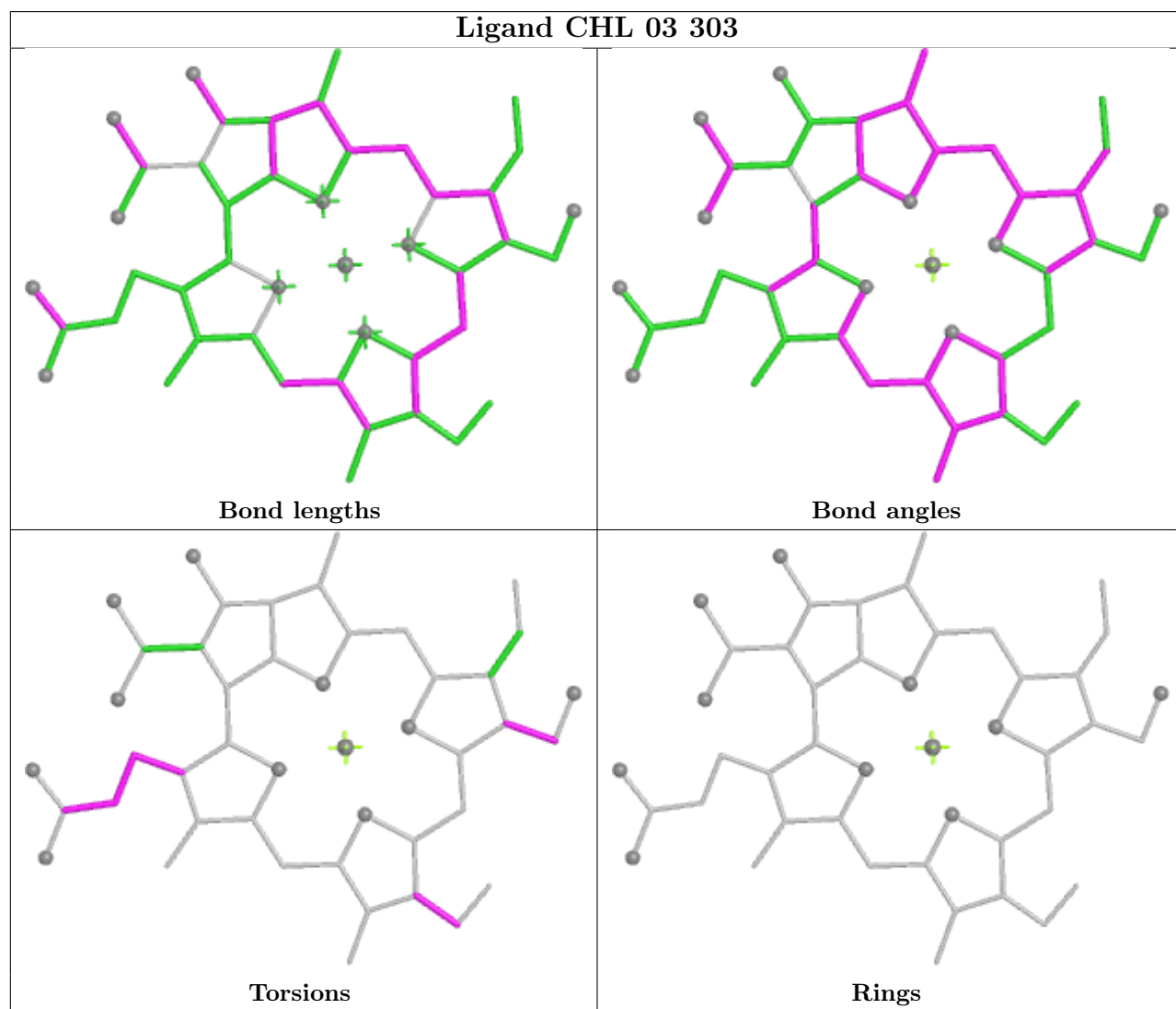
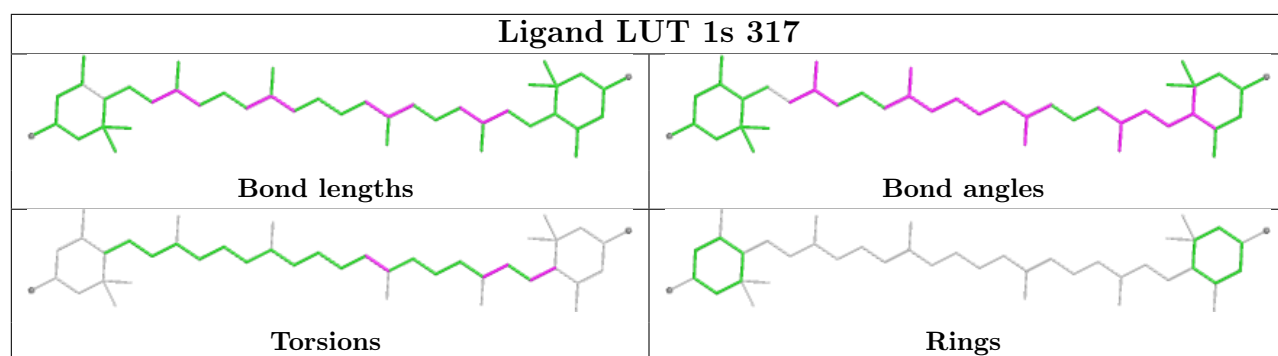


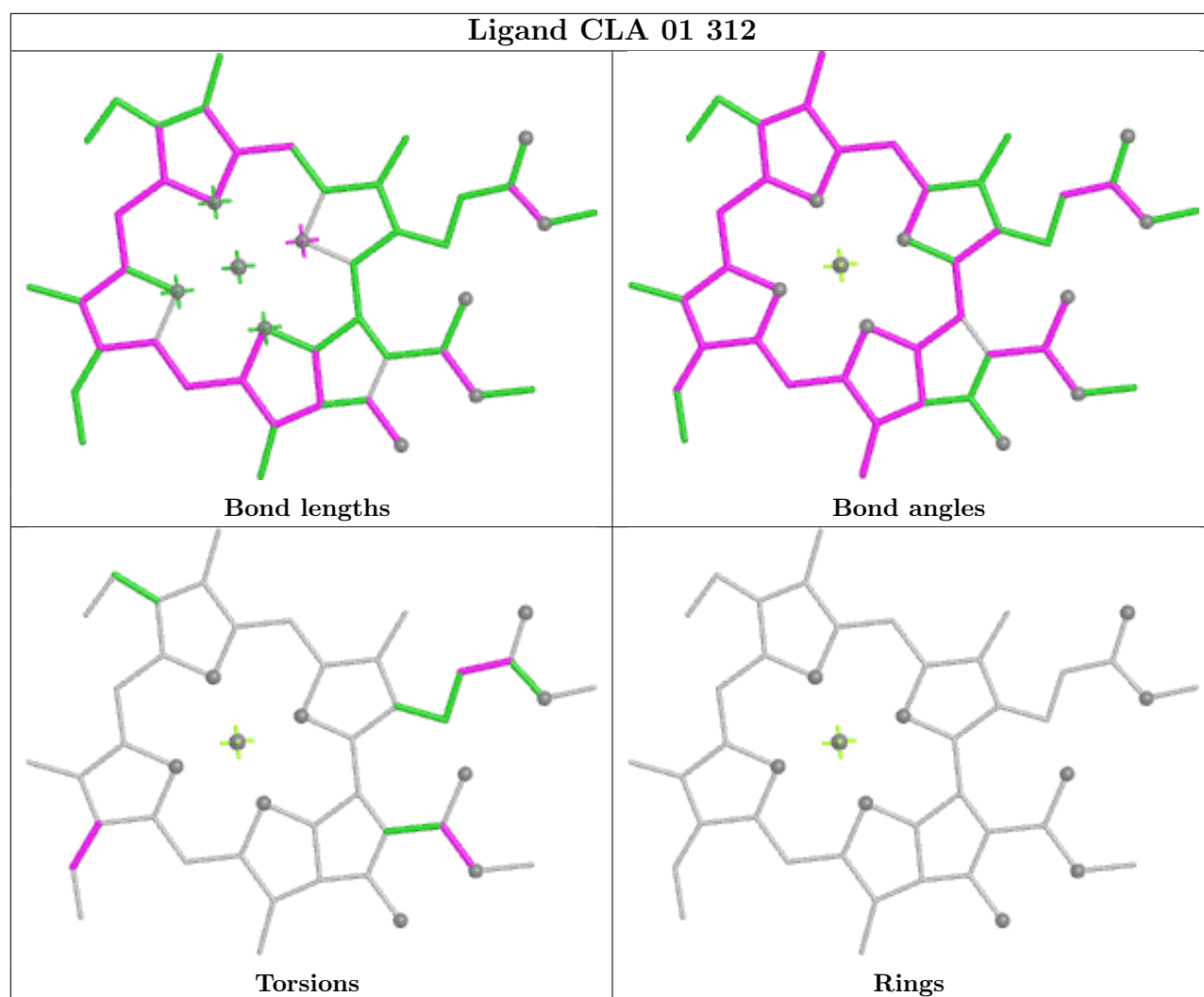


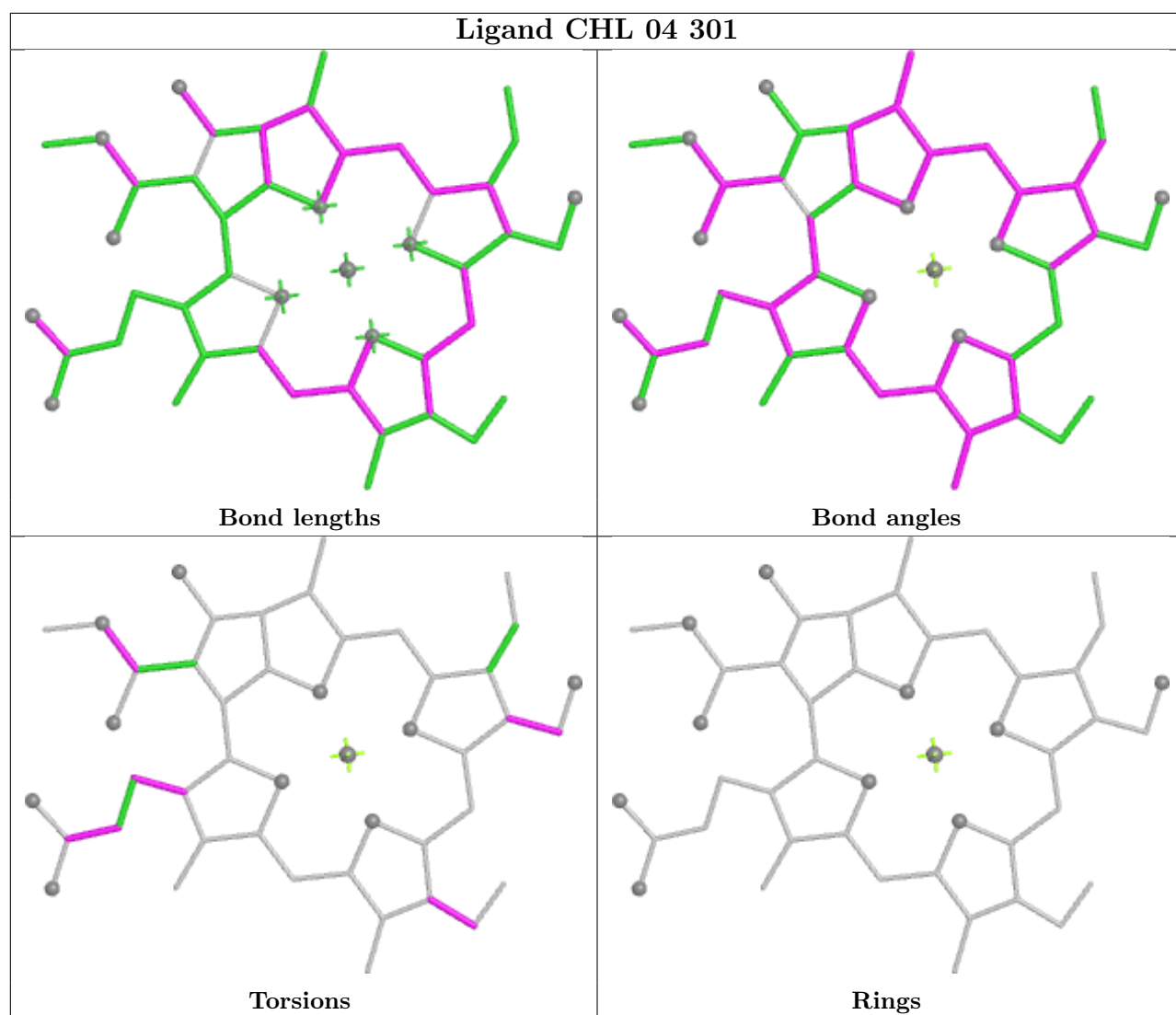


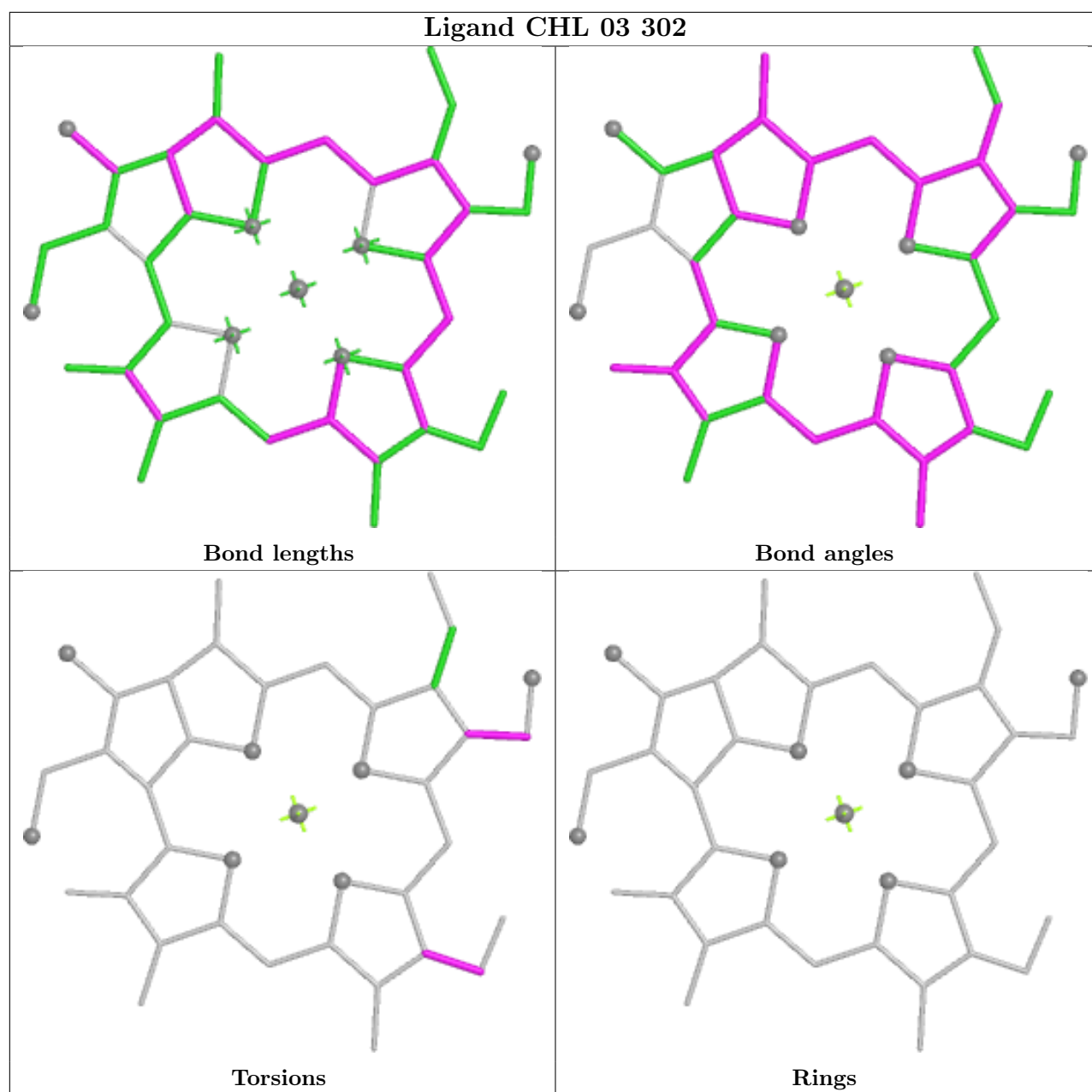


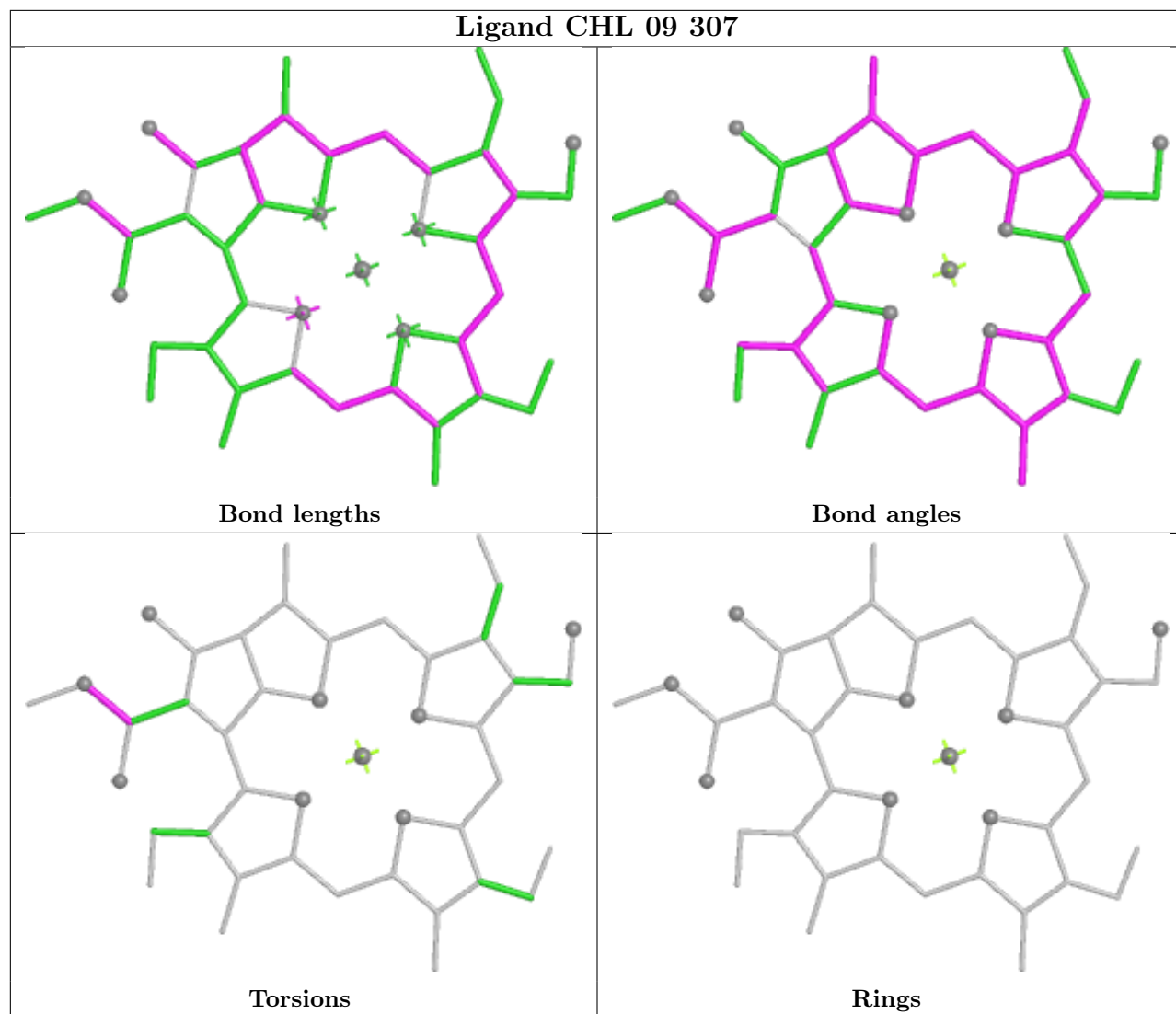


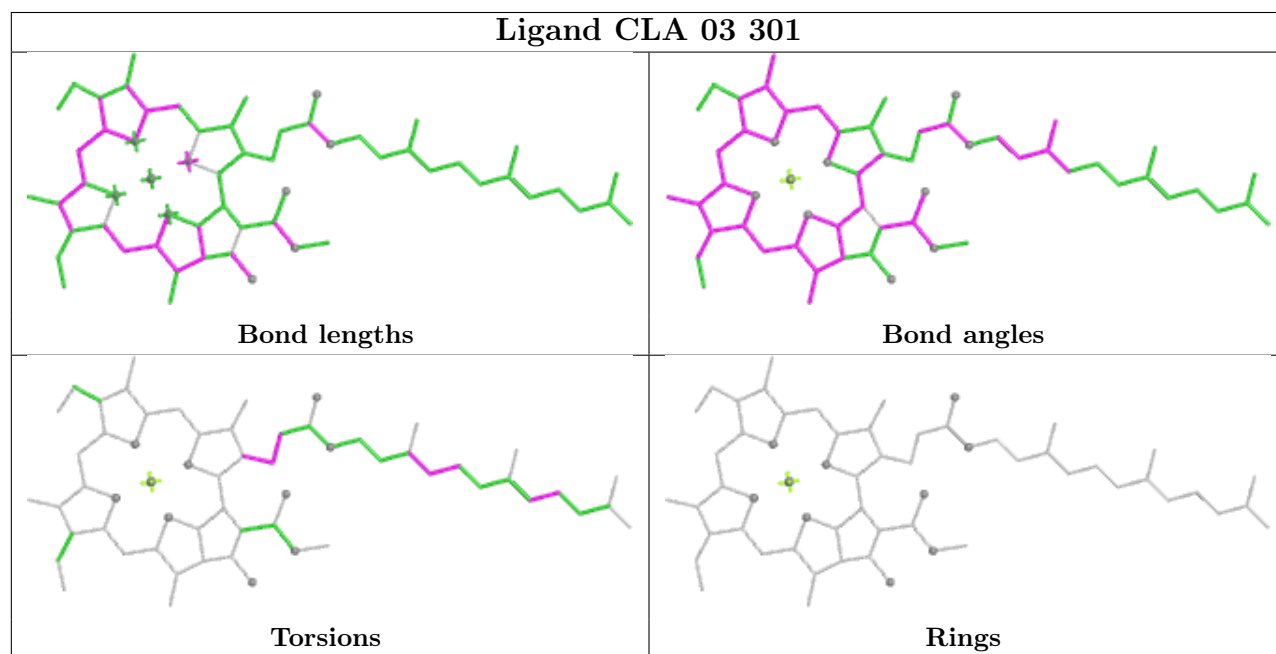
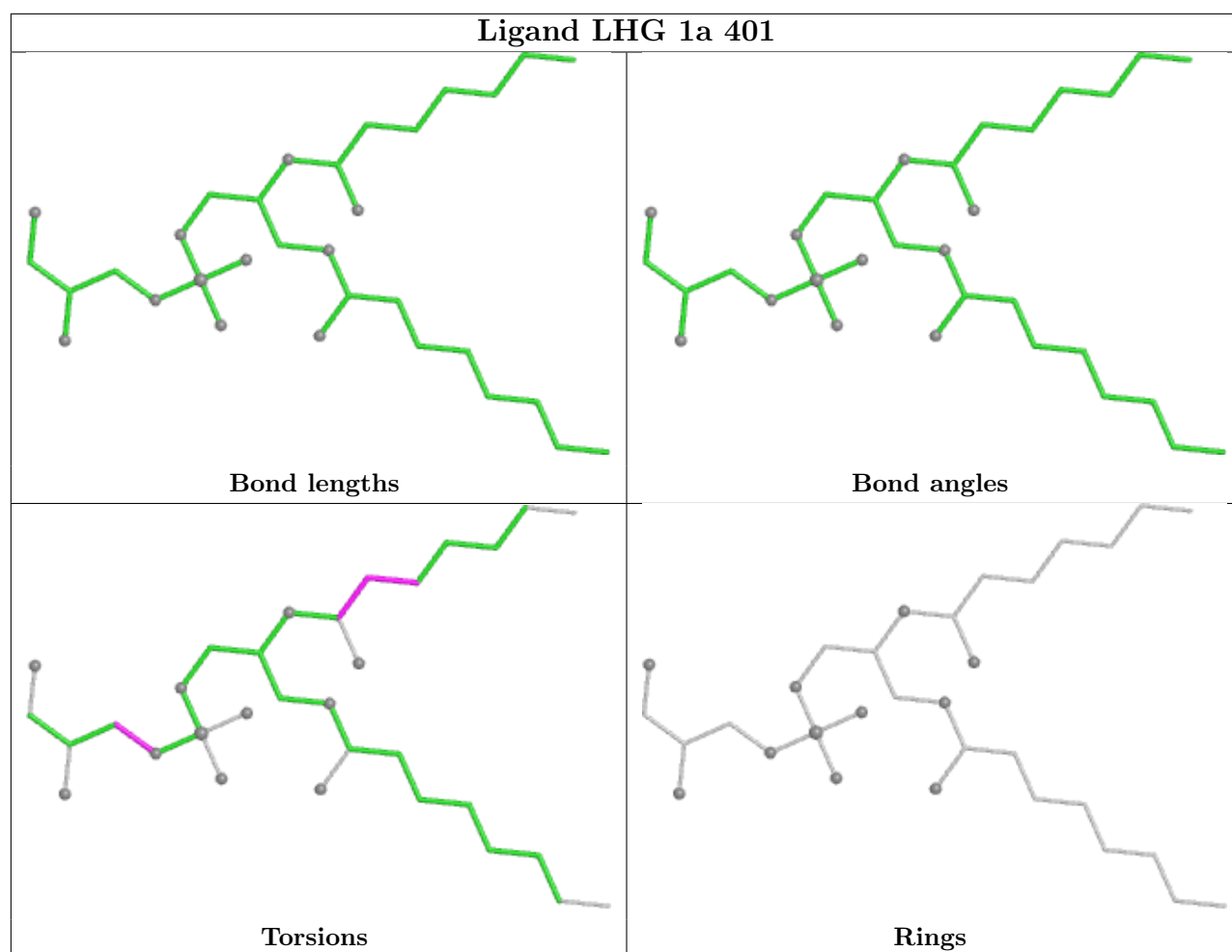


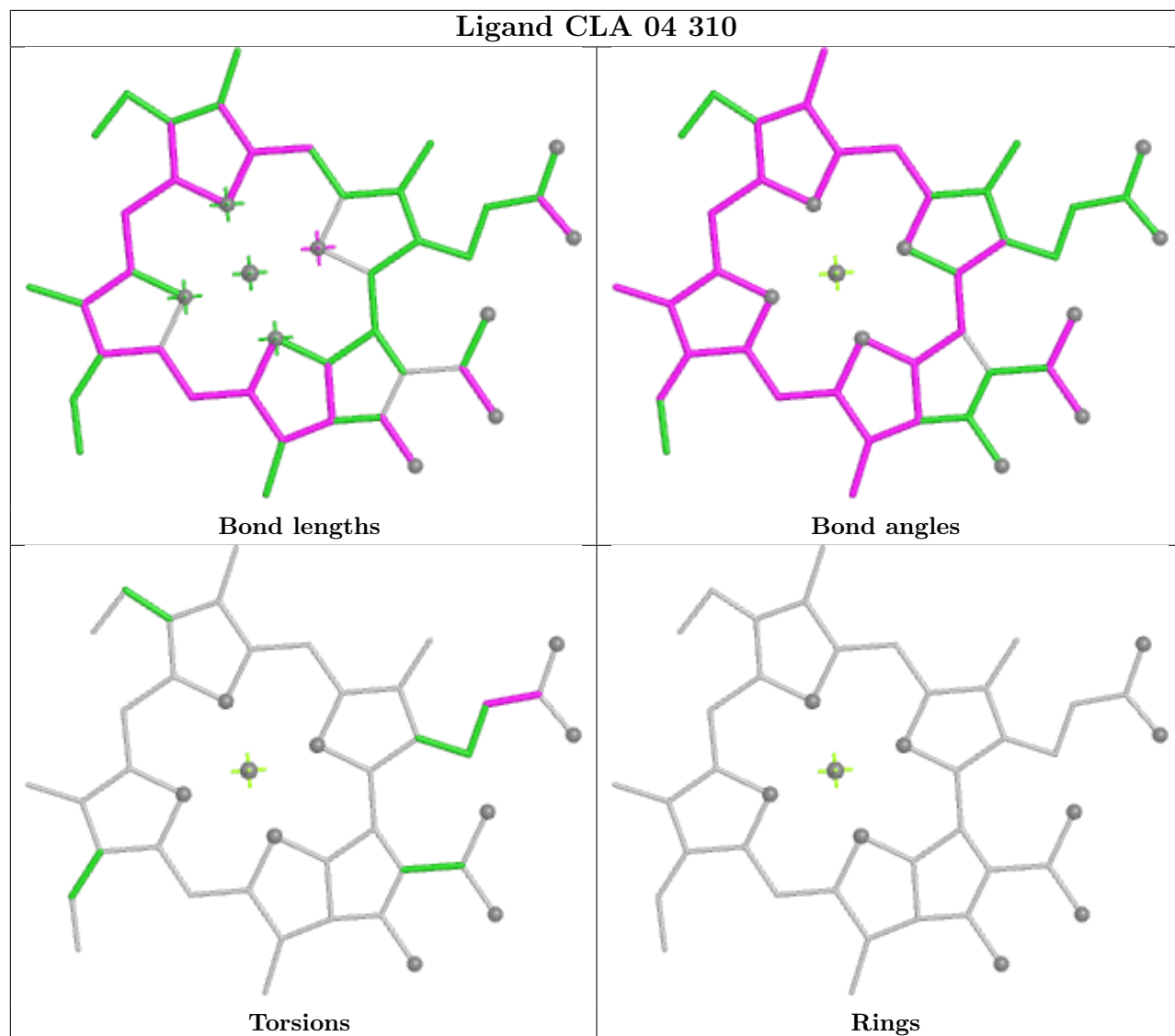


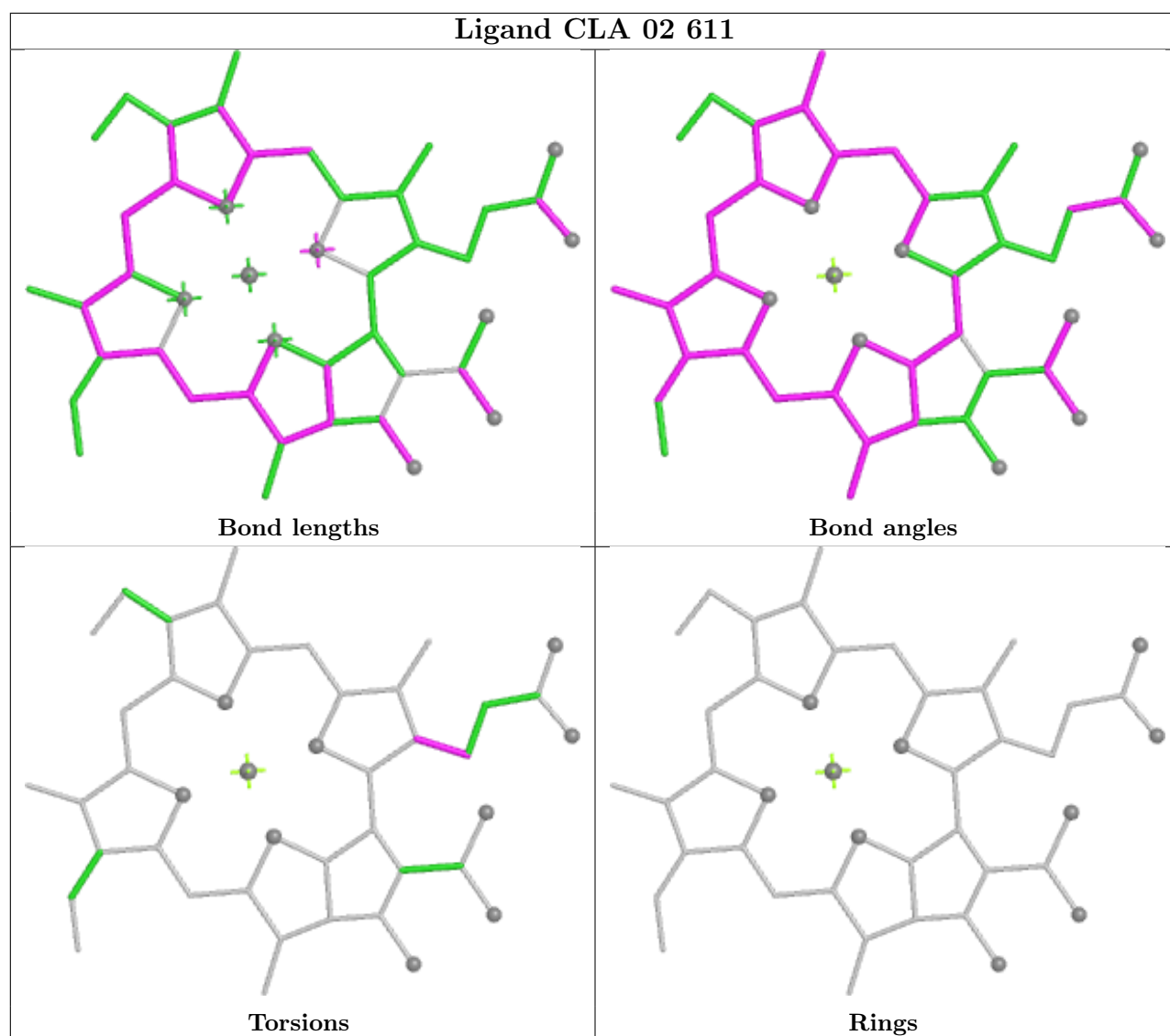


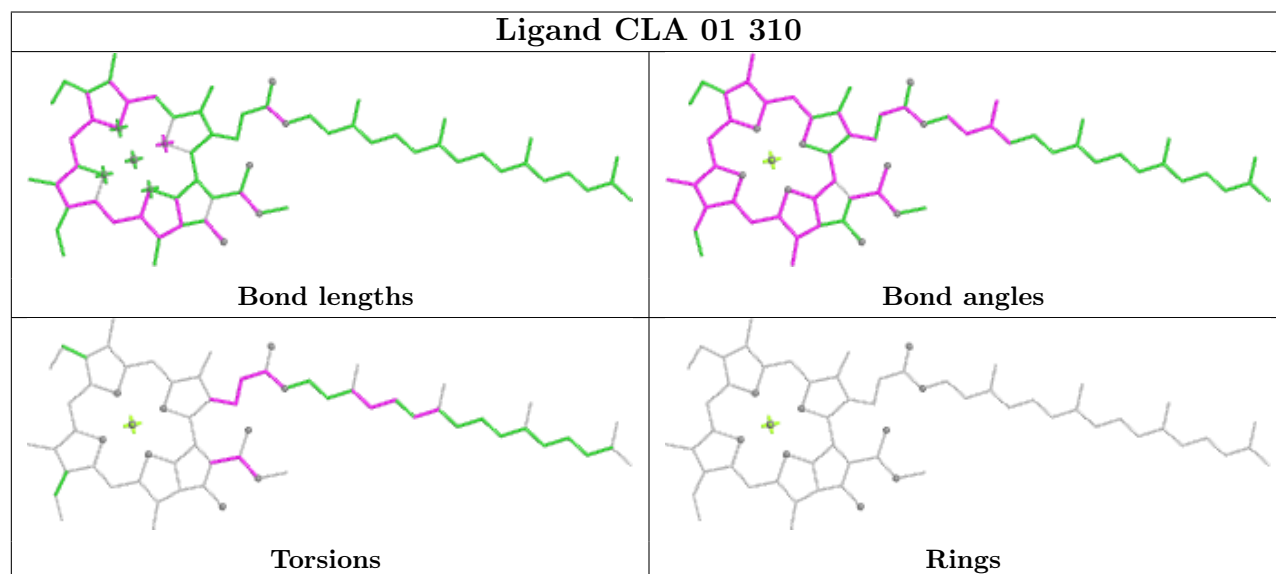
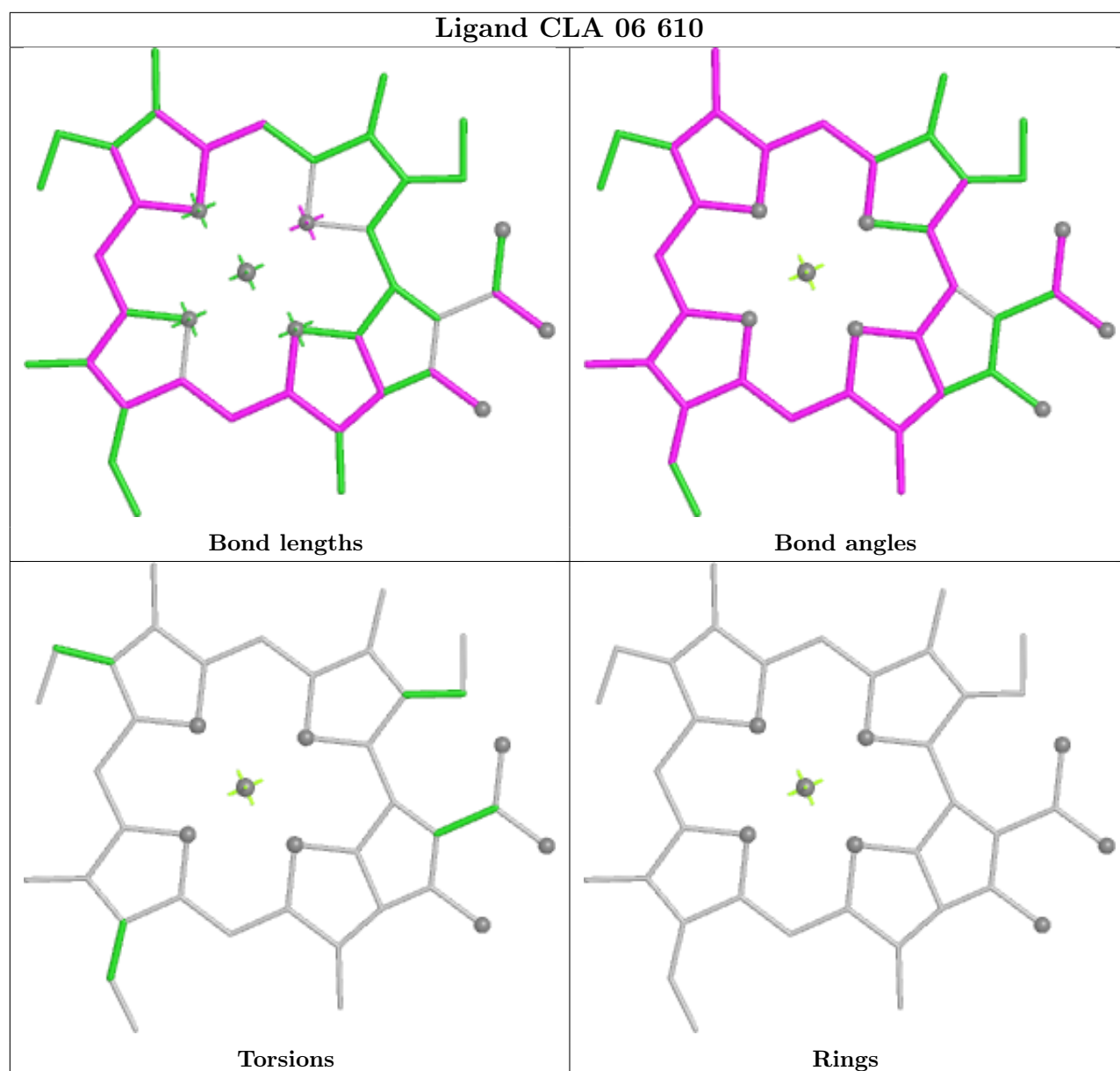


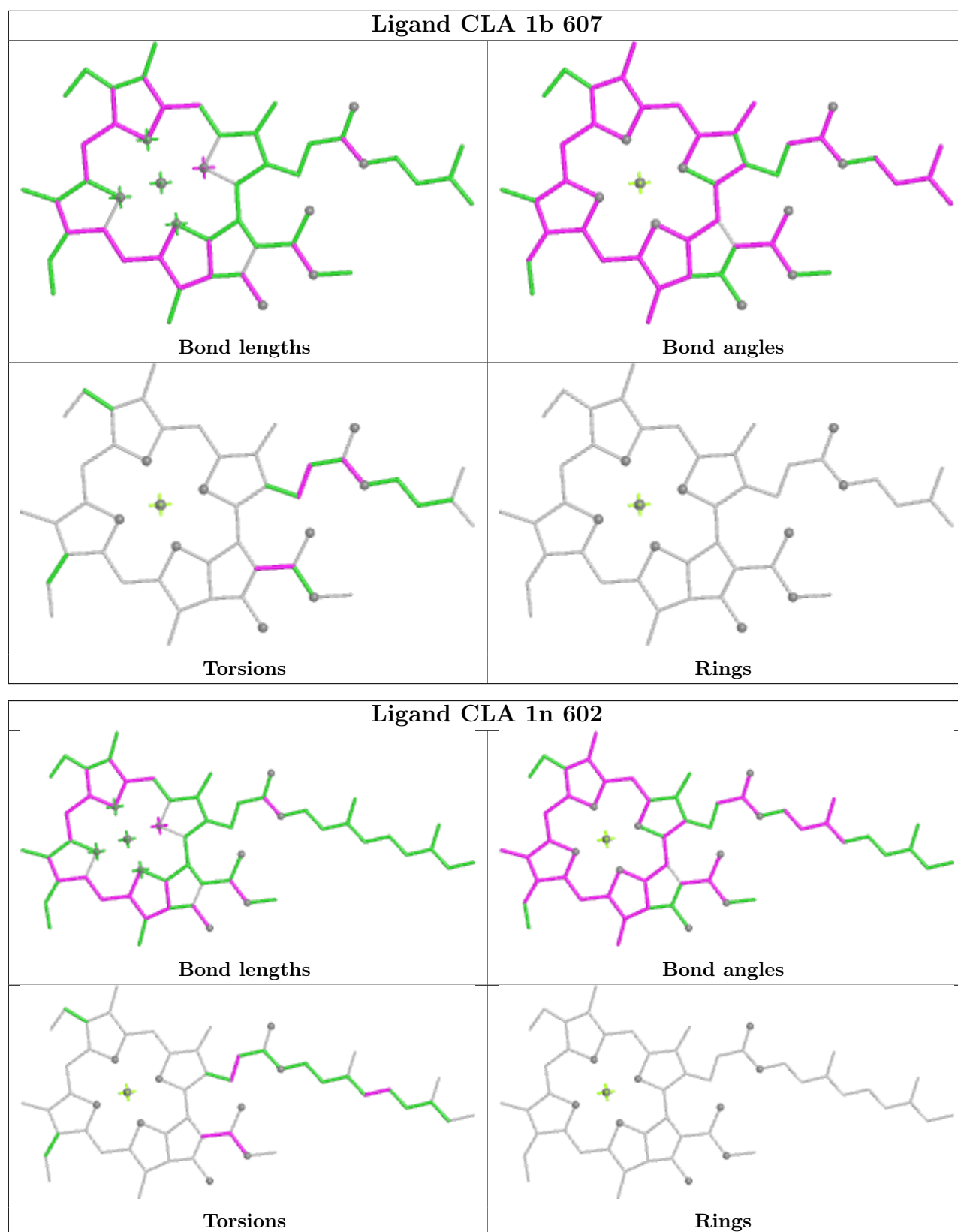


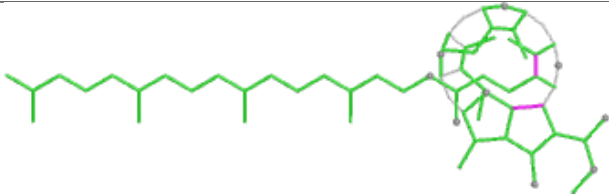
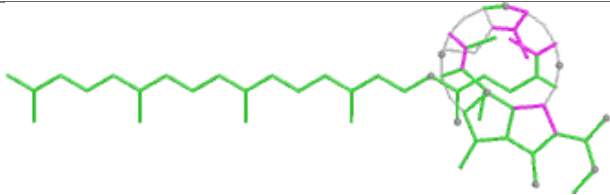
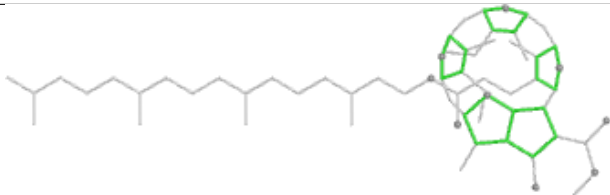


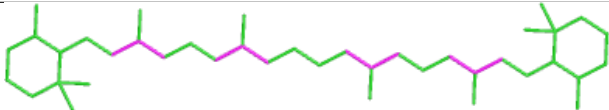
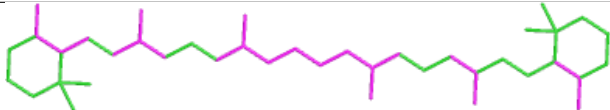
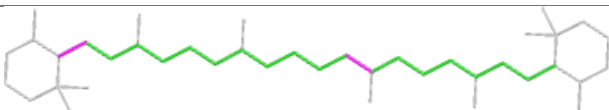
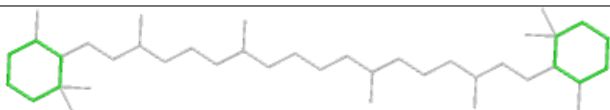


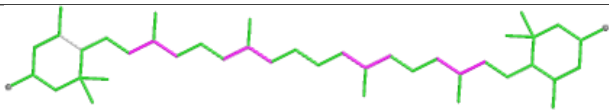
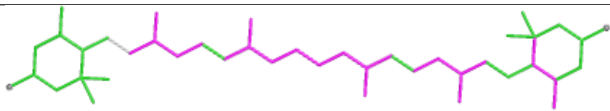
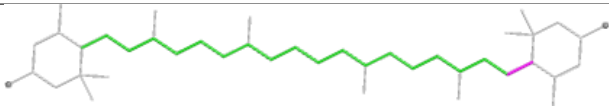
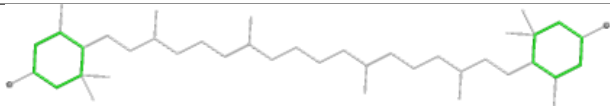


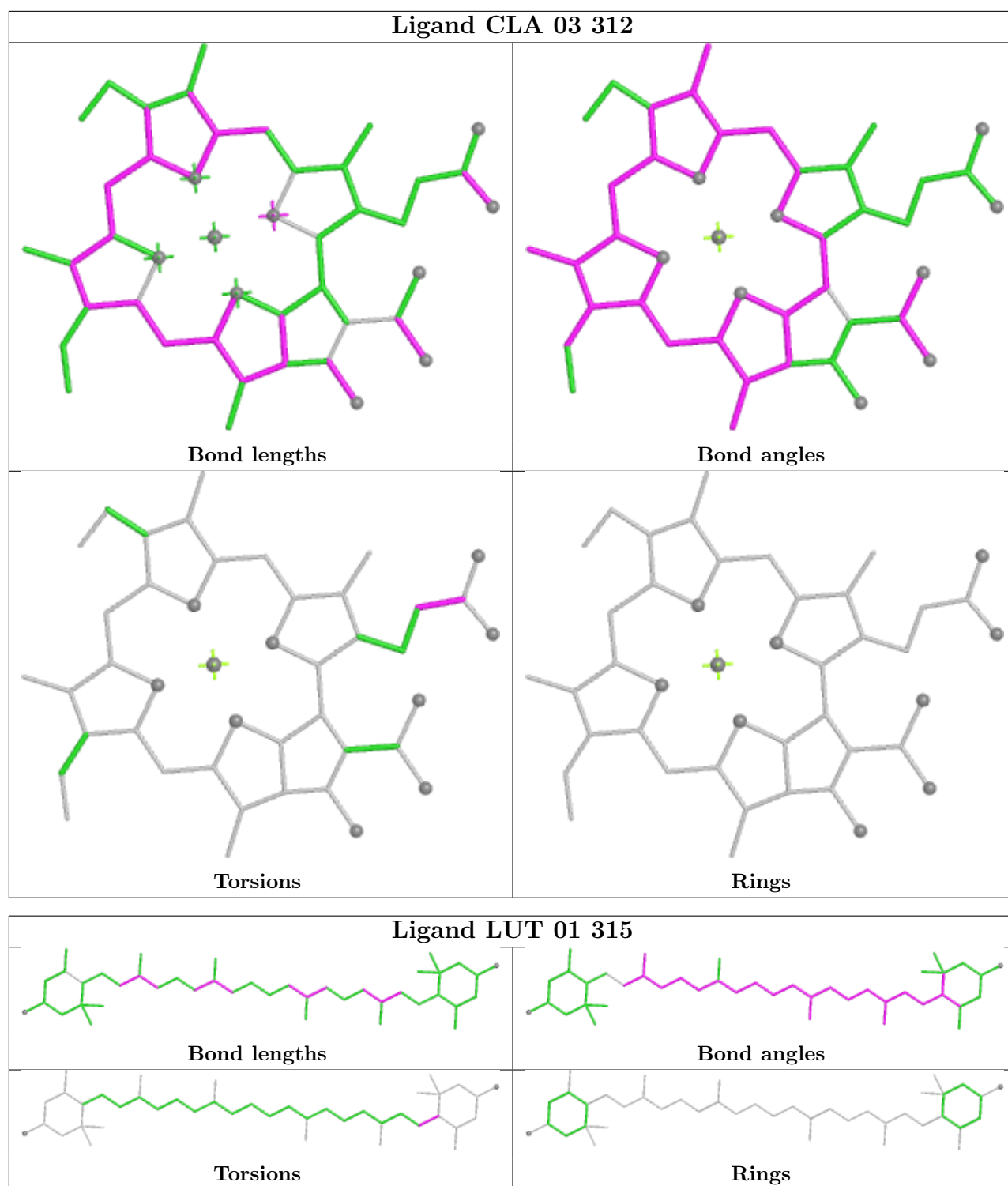


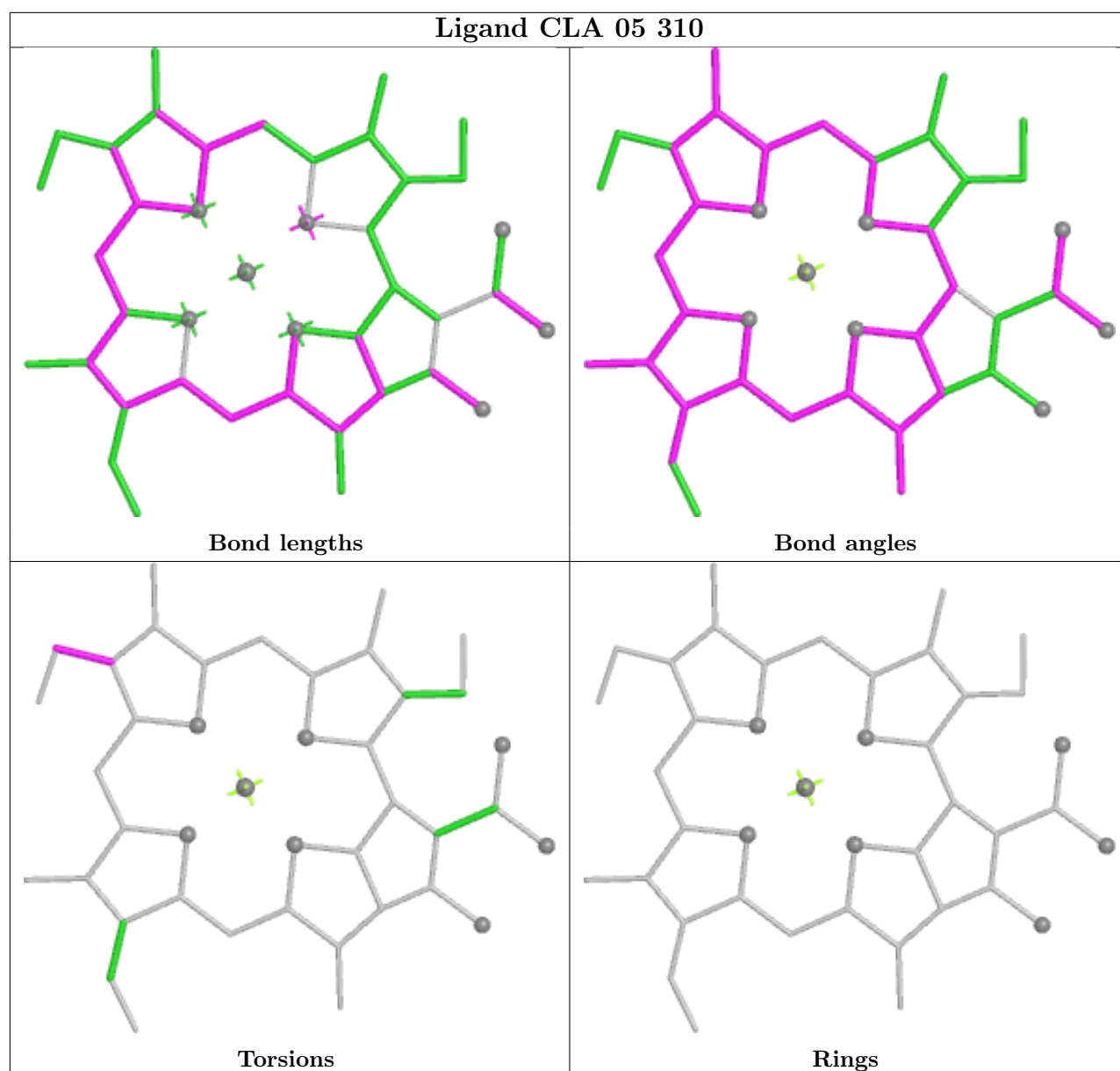


Ligand PHO 1d 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

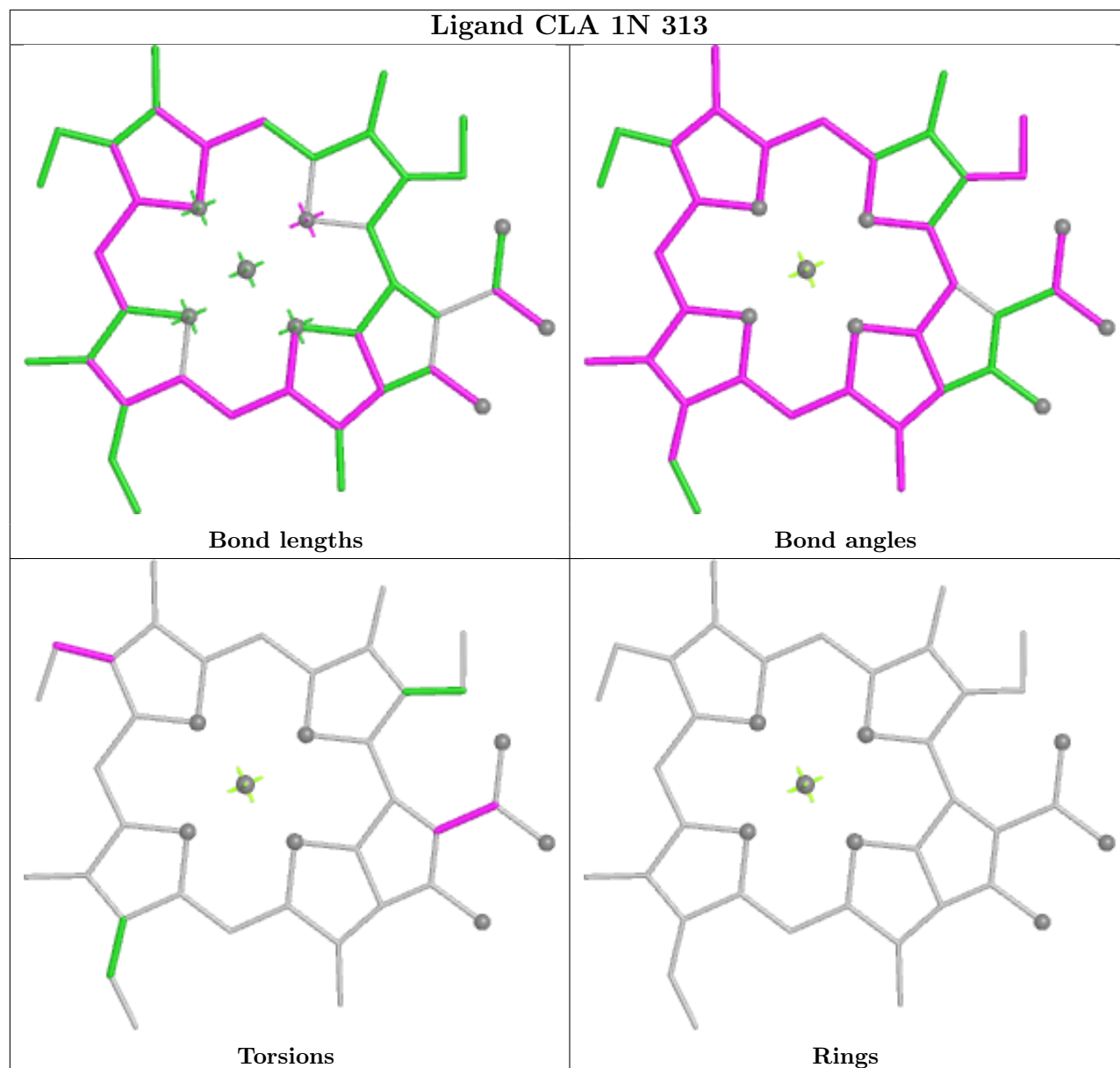
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Bond lengths	Bond angles
	
Torsions	Rings

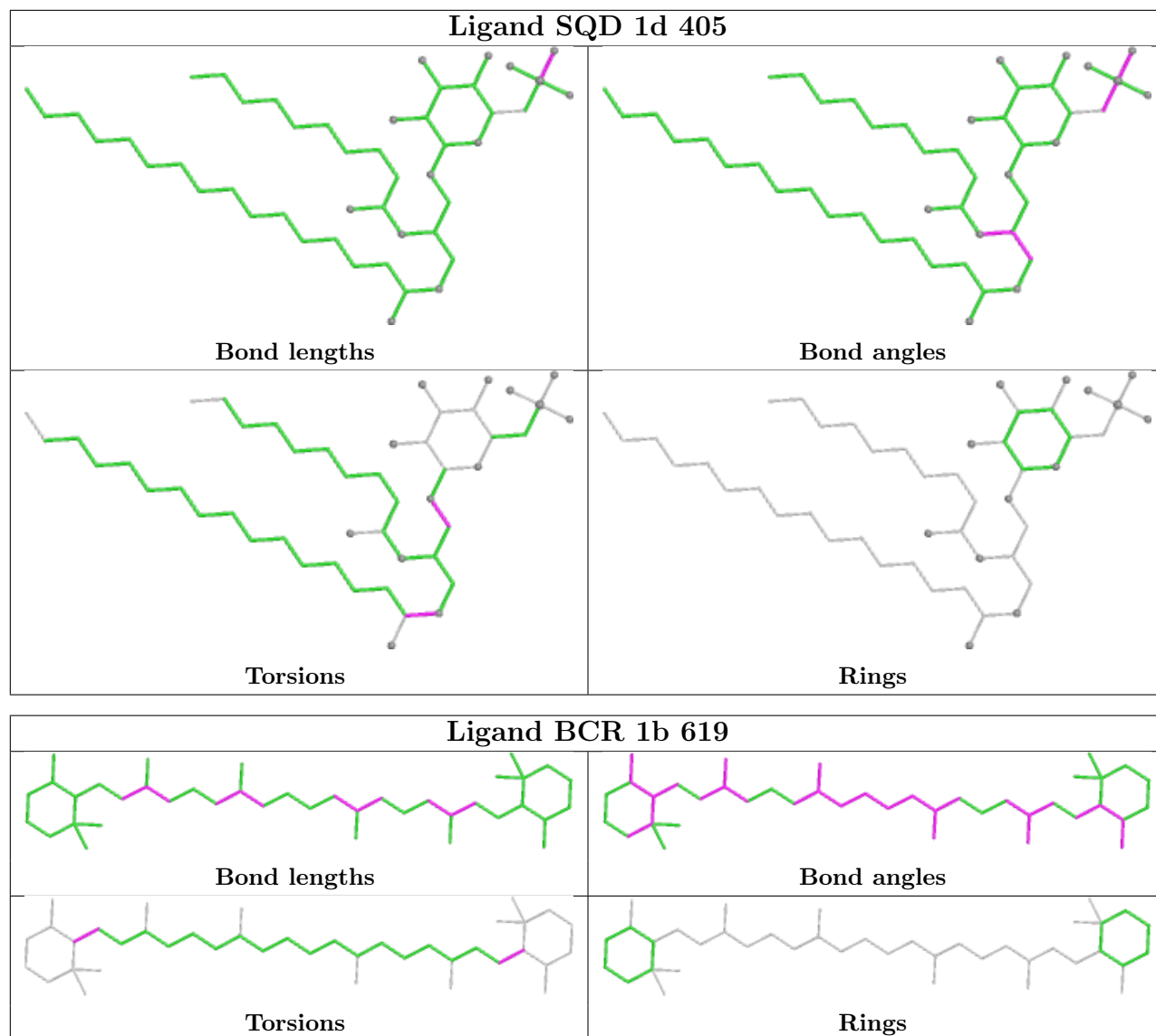
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Bond lengths	Bond angles
	
Torsions	Rings



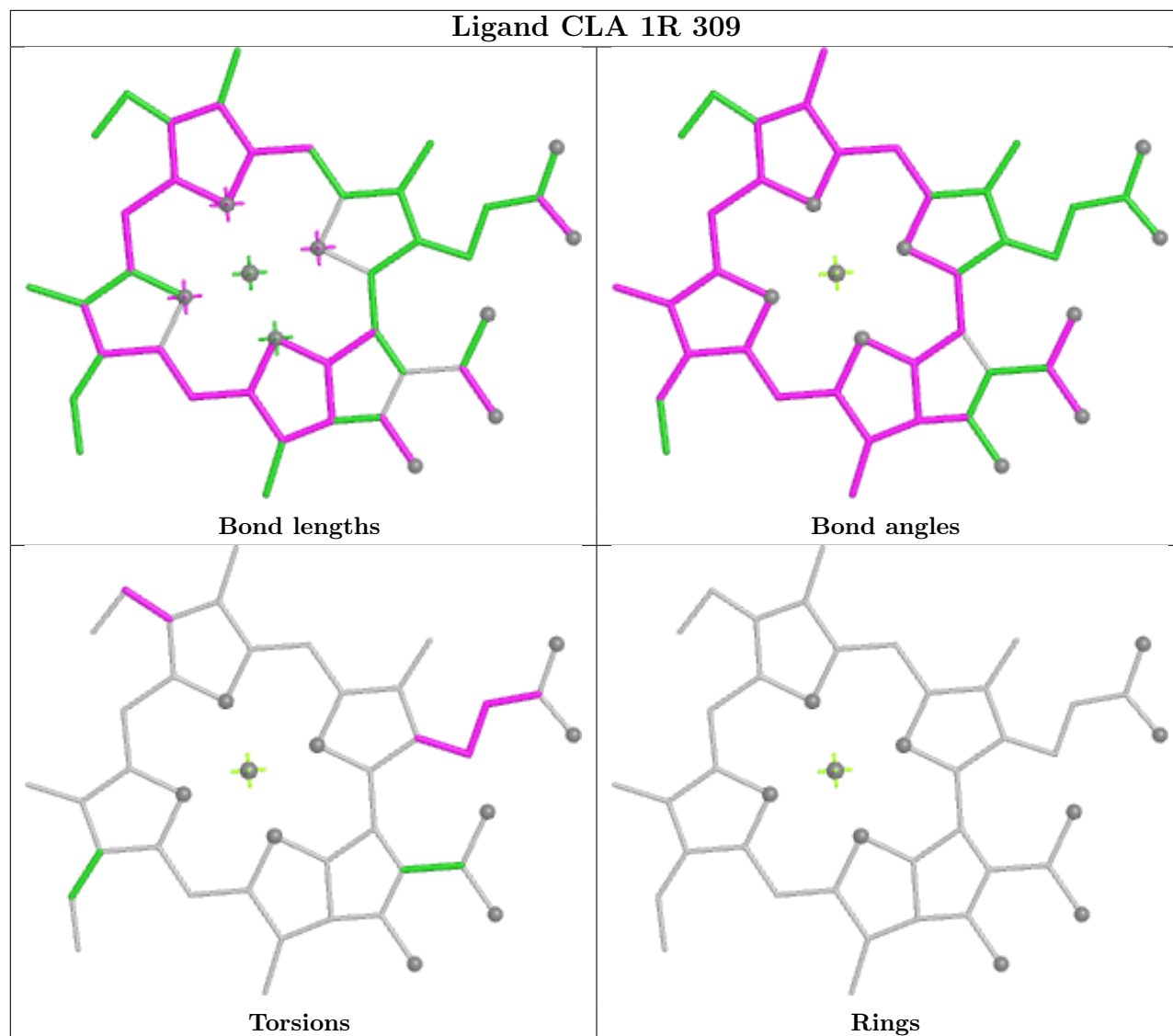


Ligand CLA 1N 313

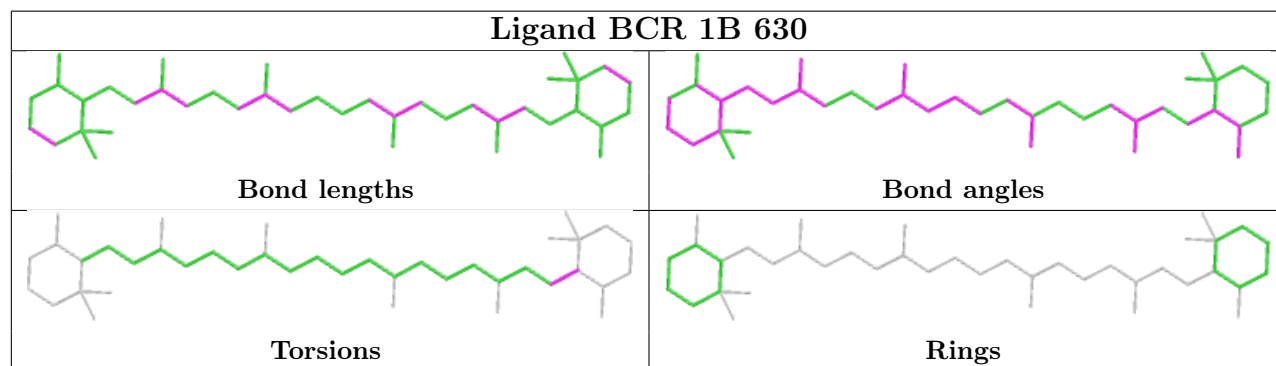


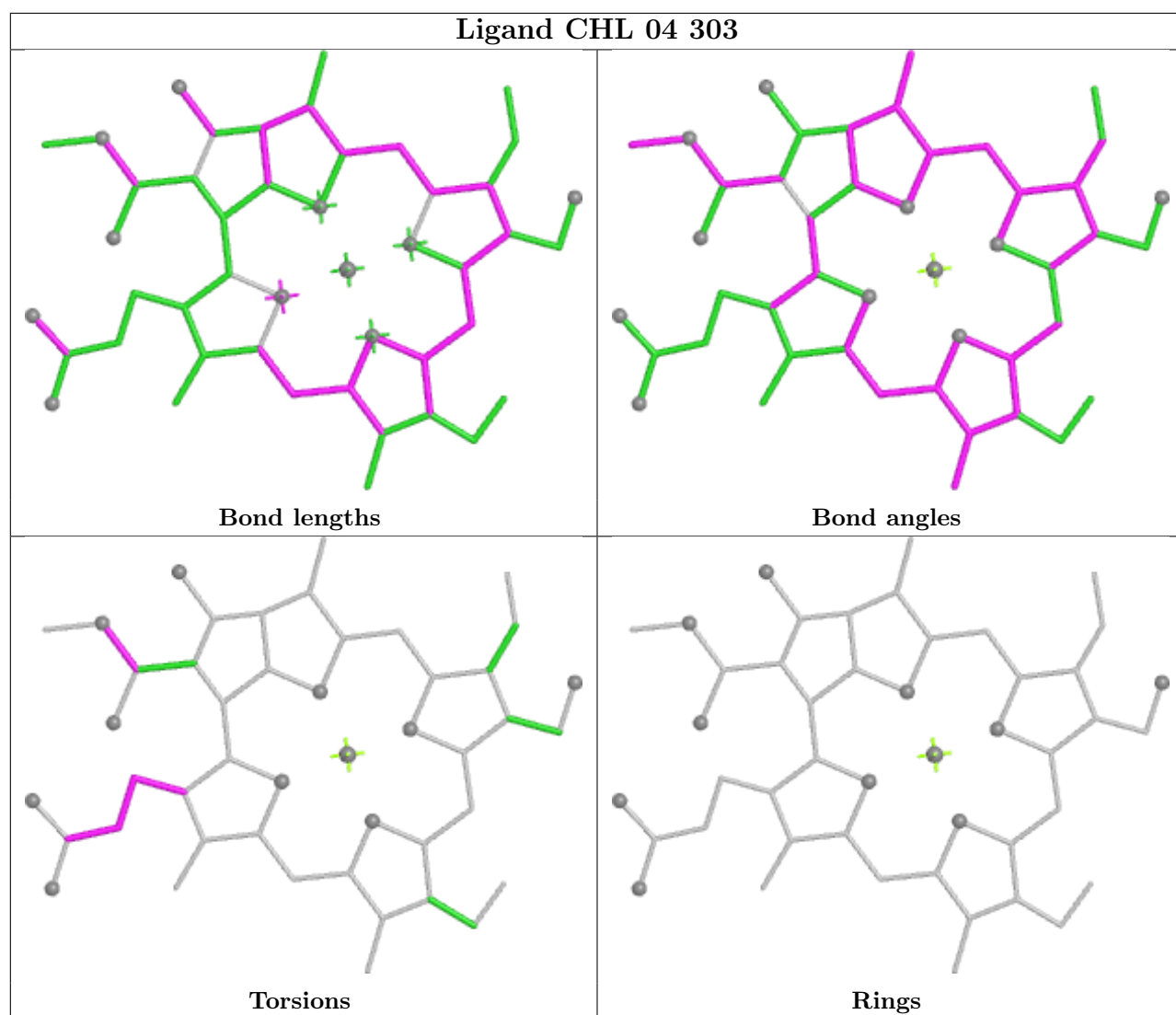


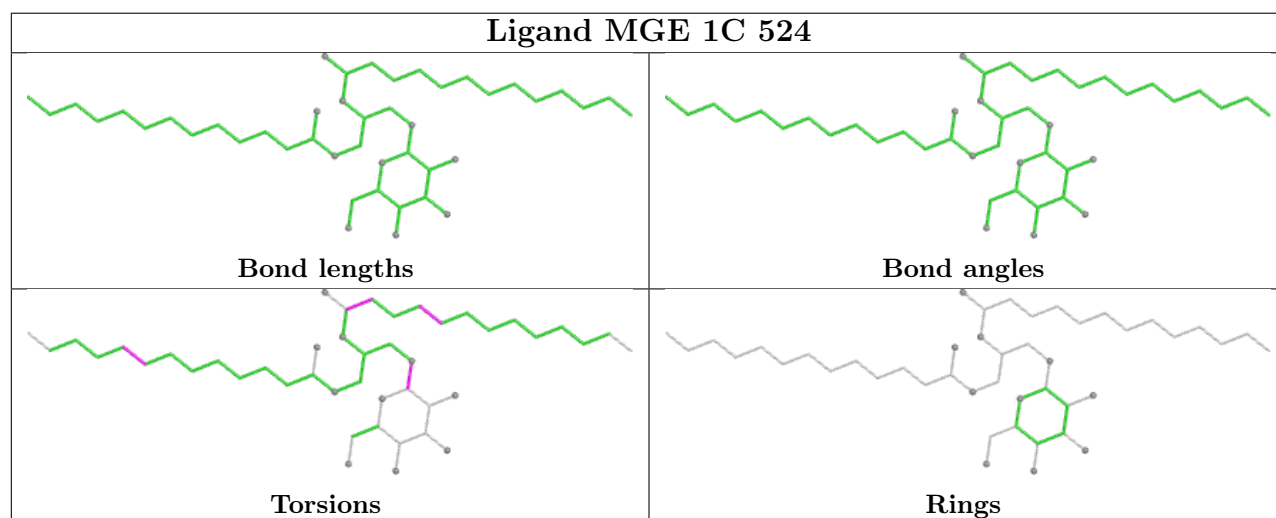
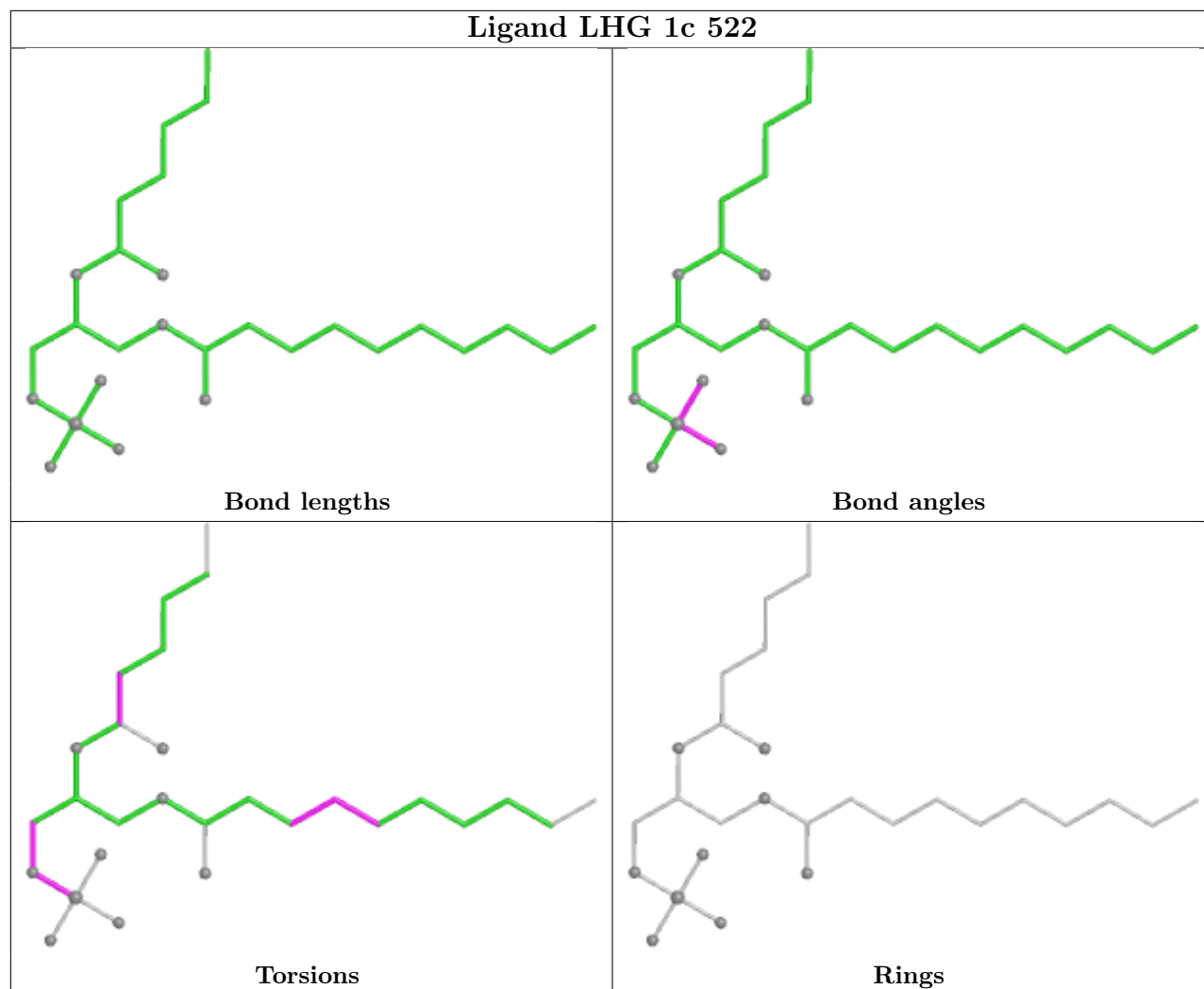
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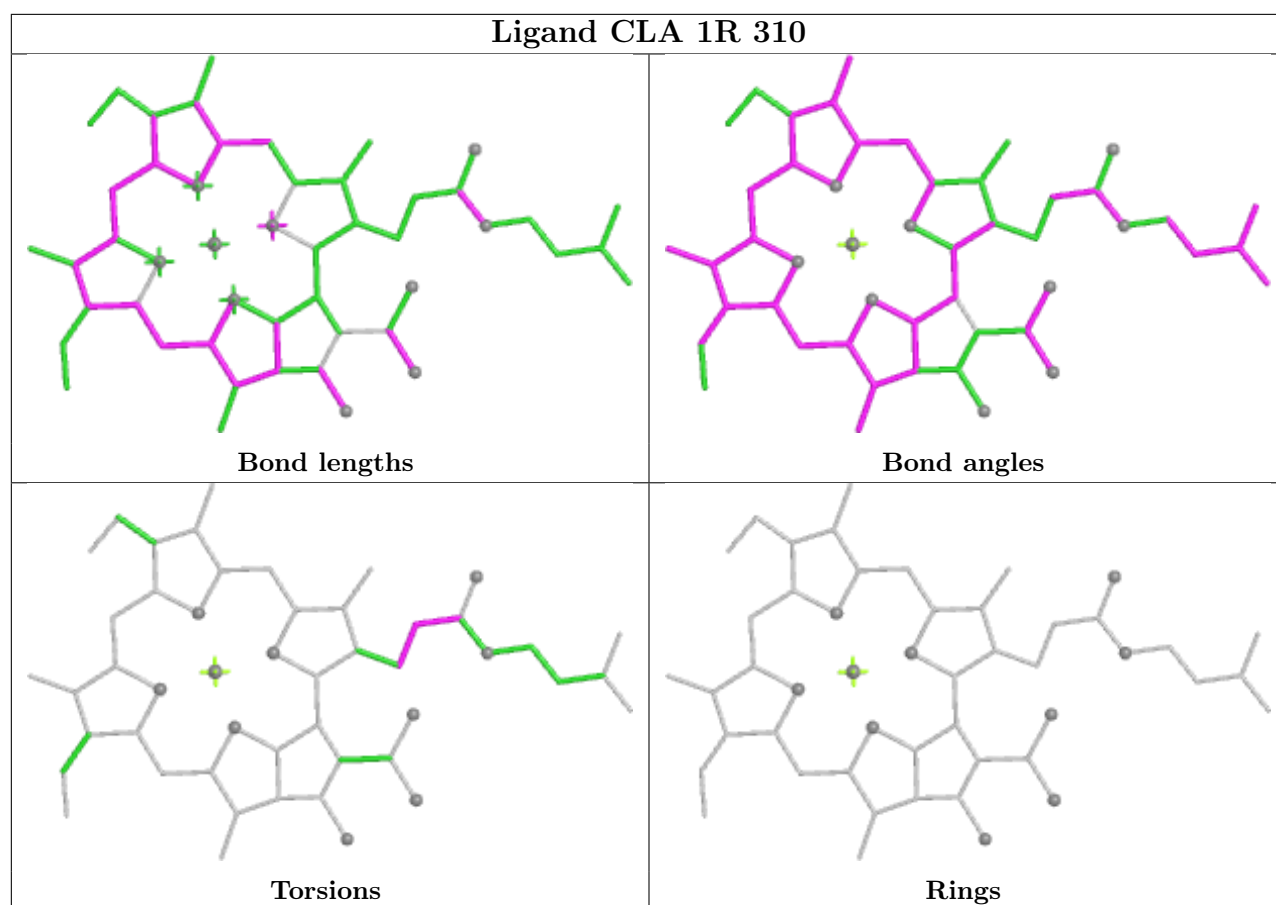


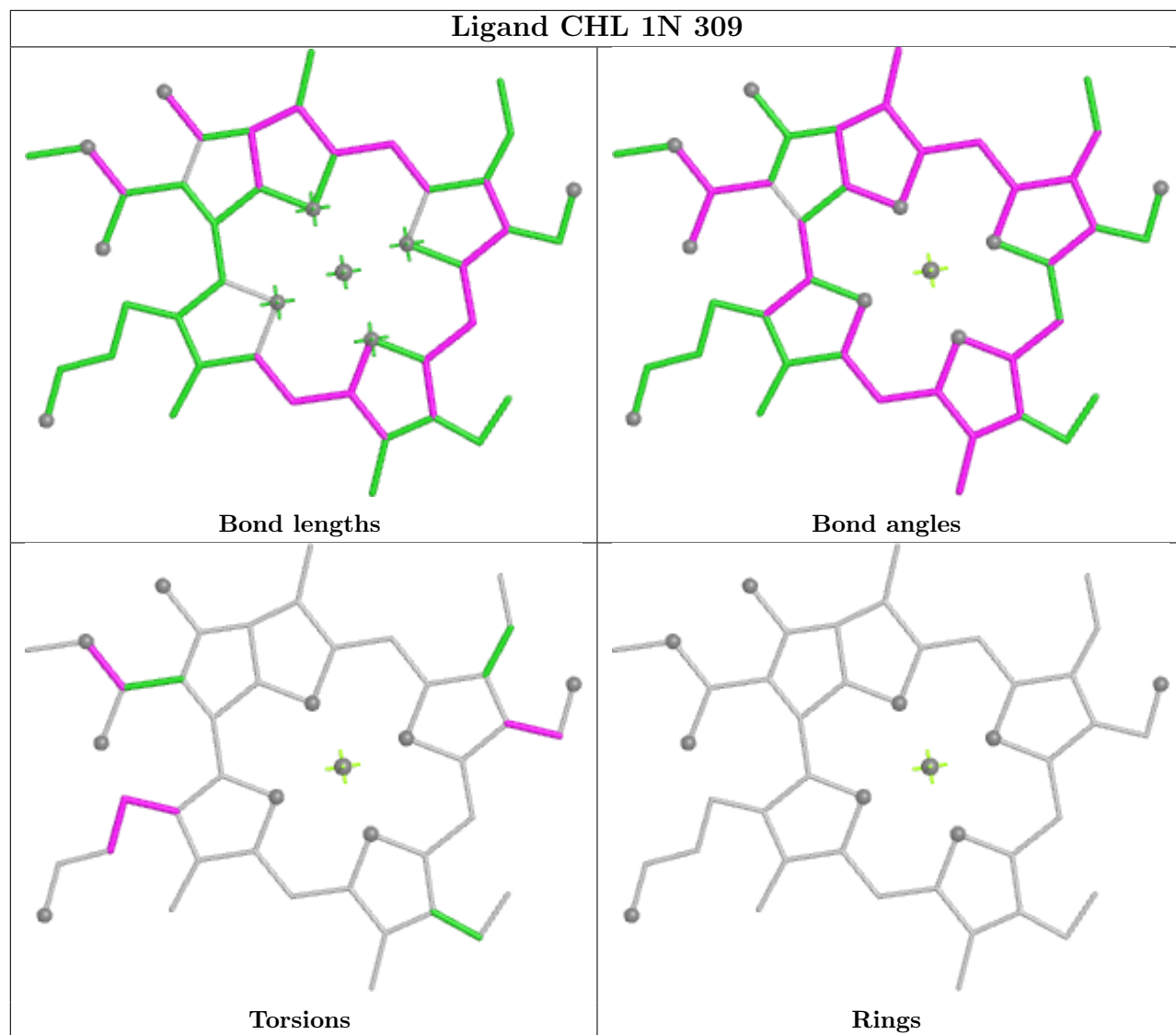
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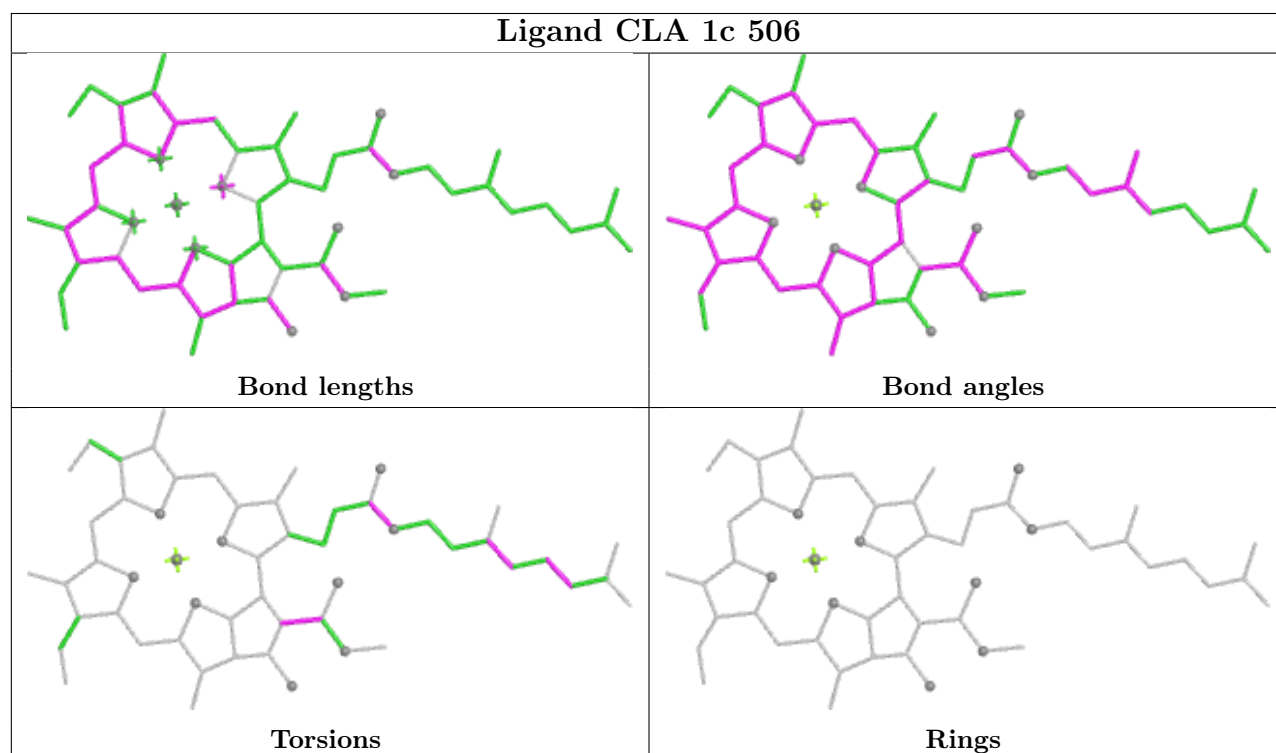
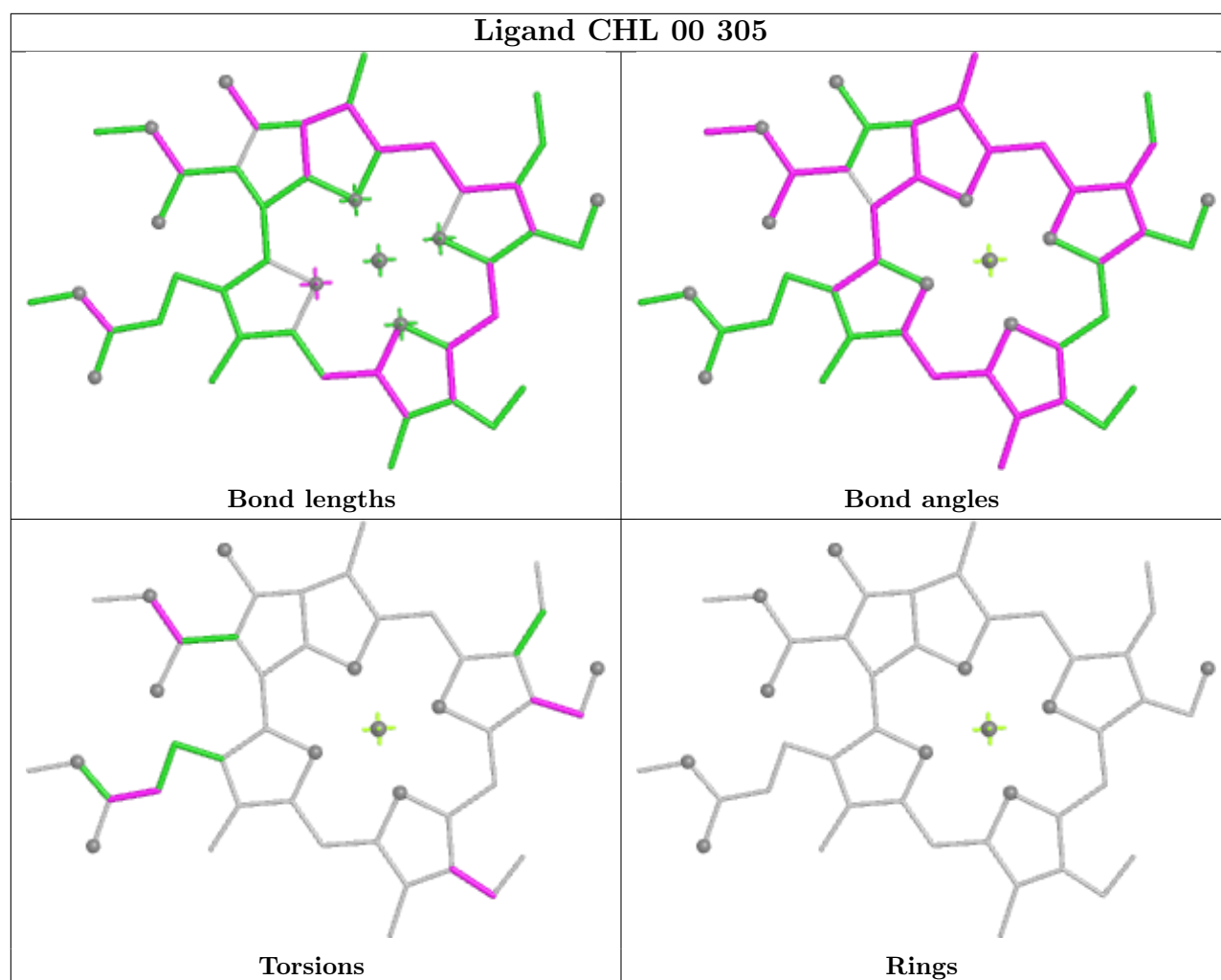


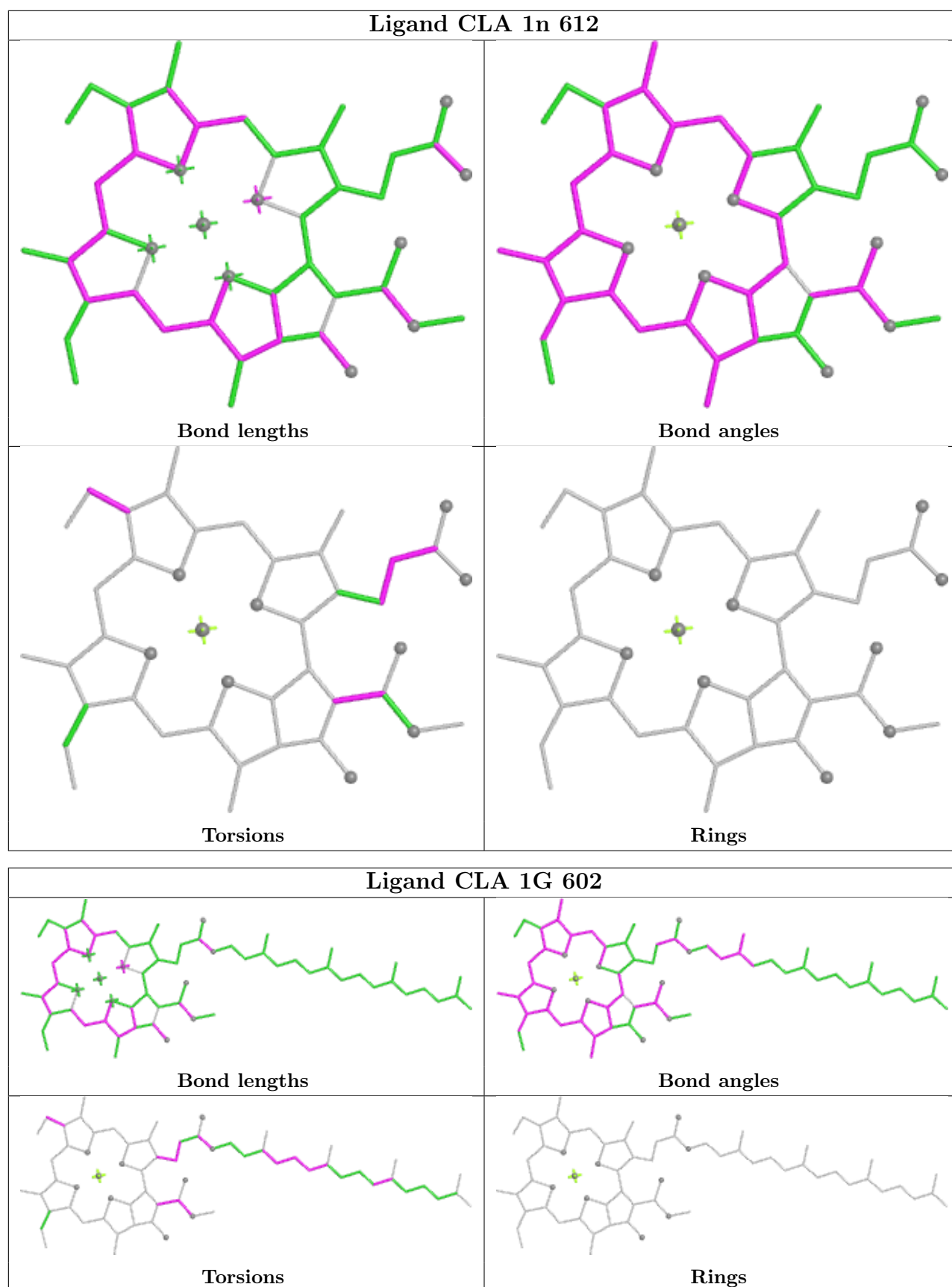


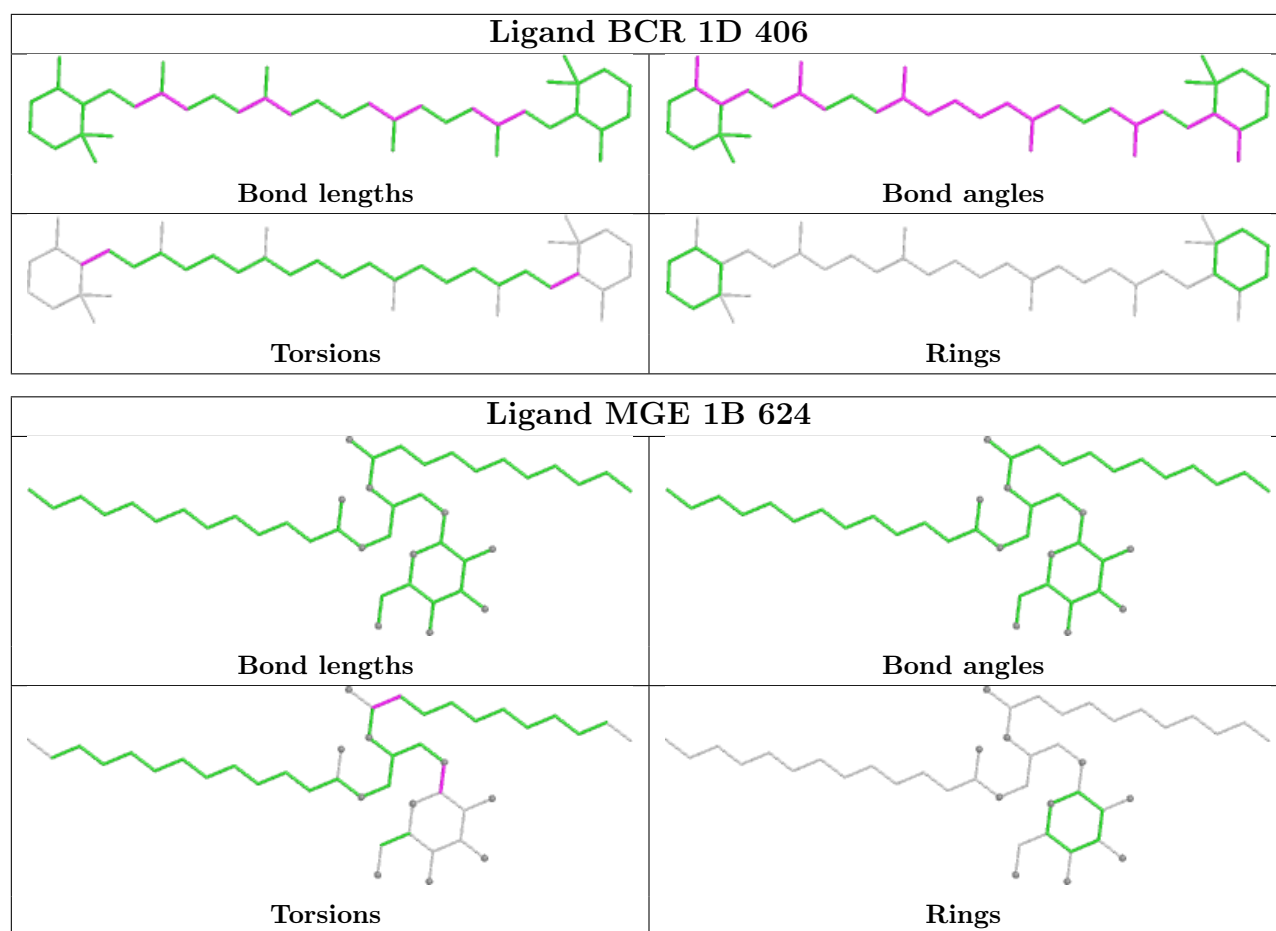


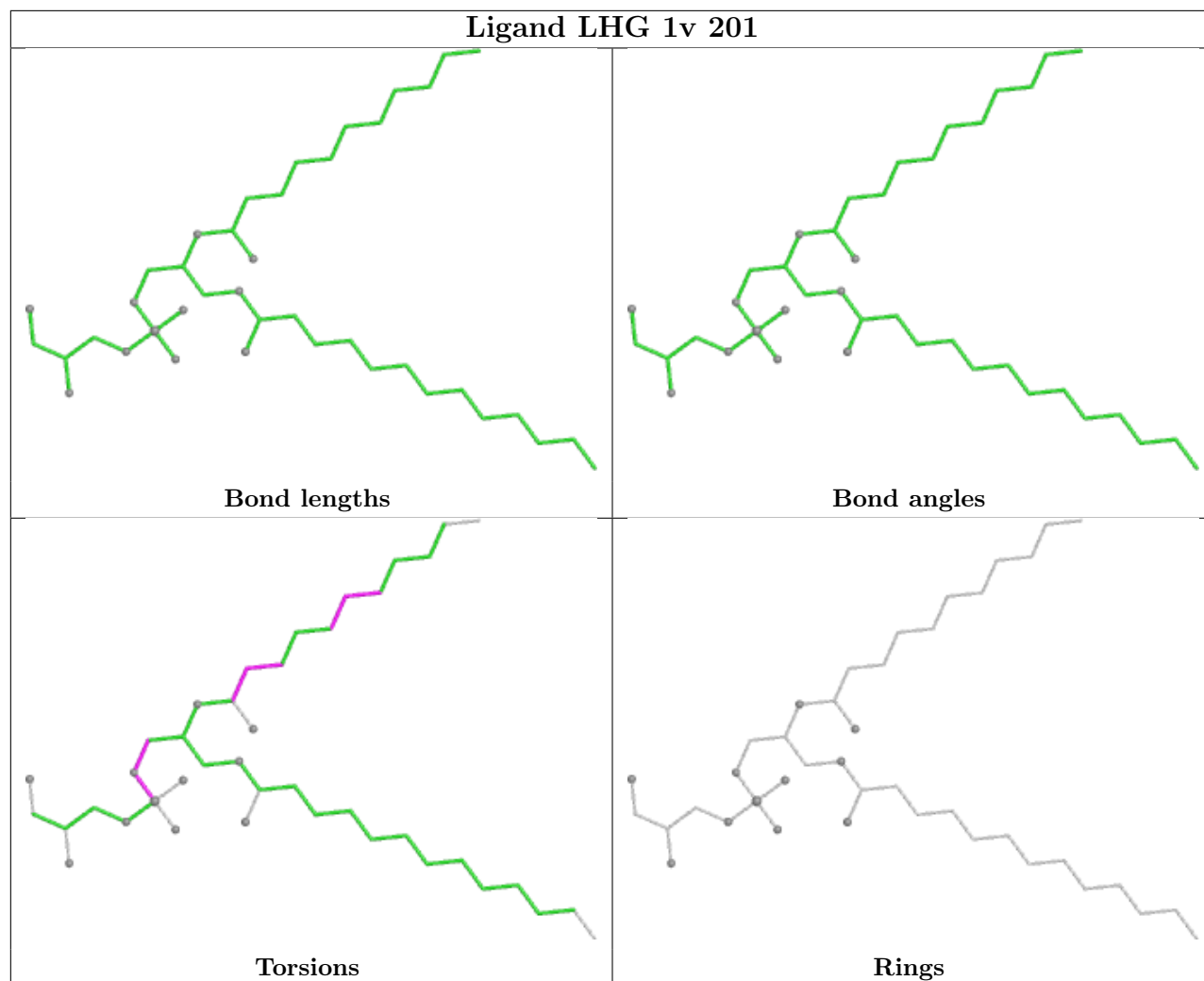


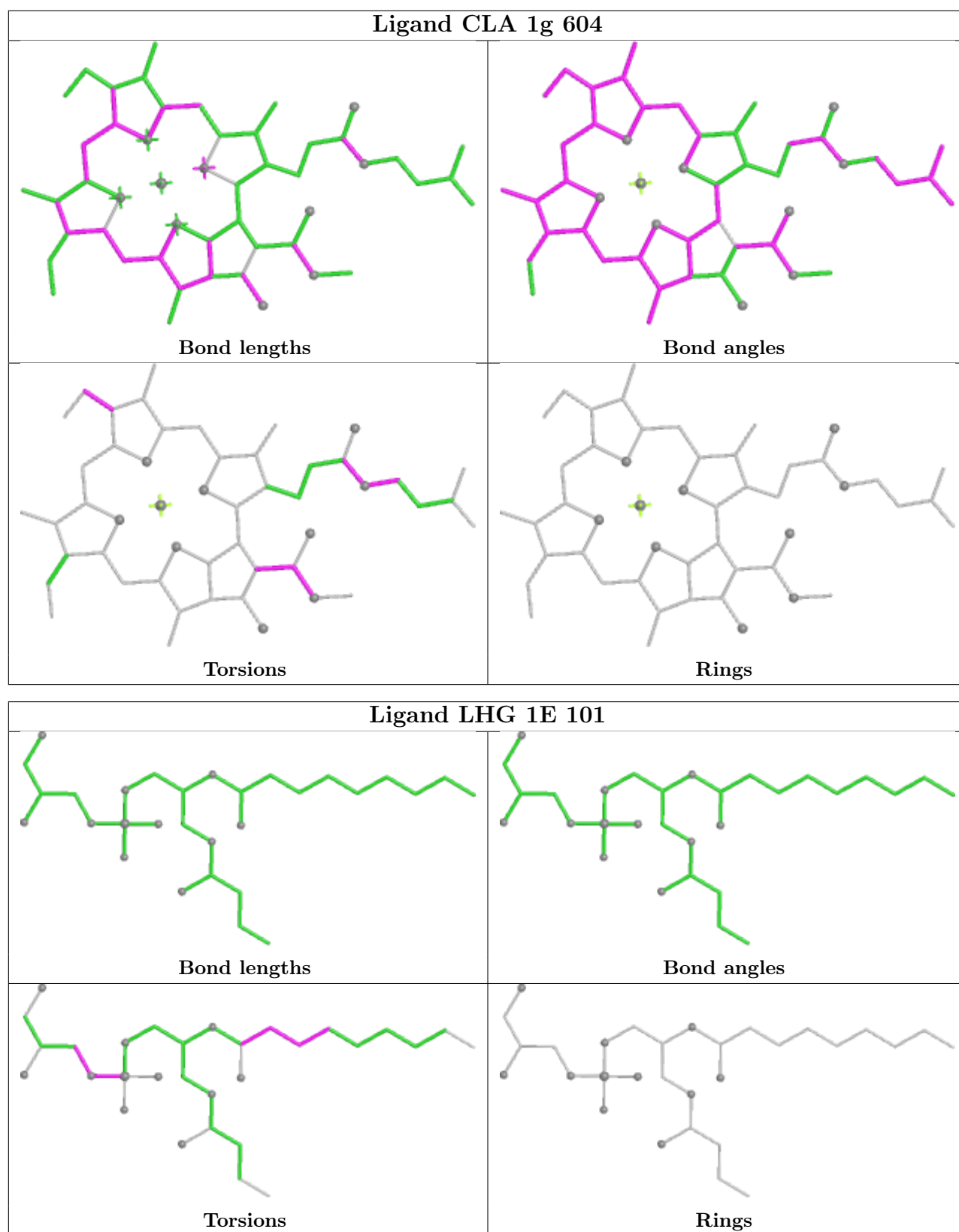


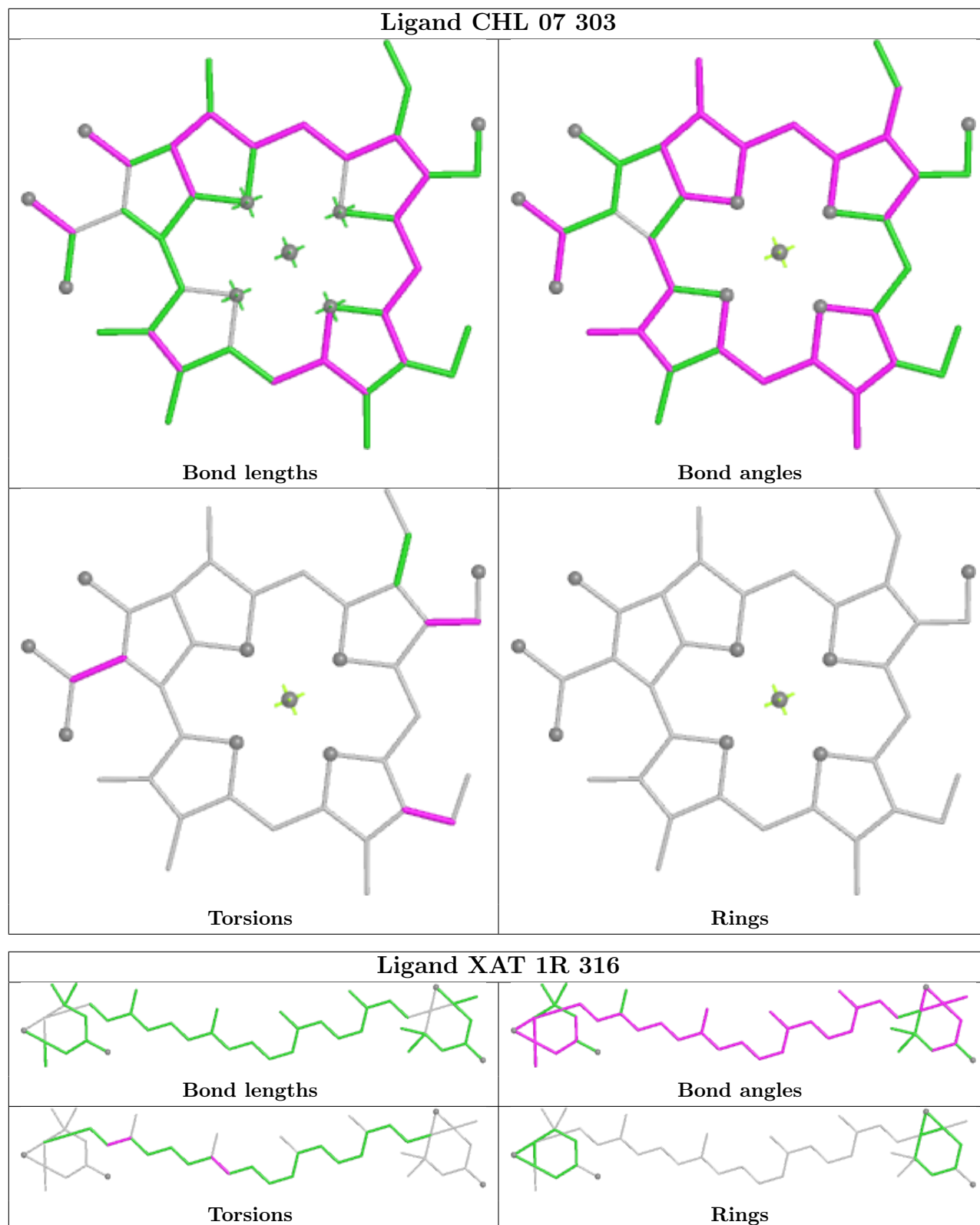


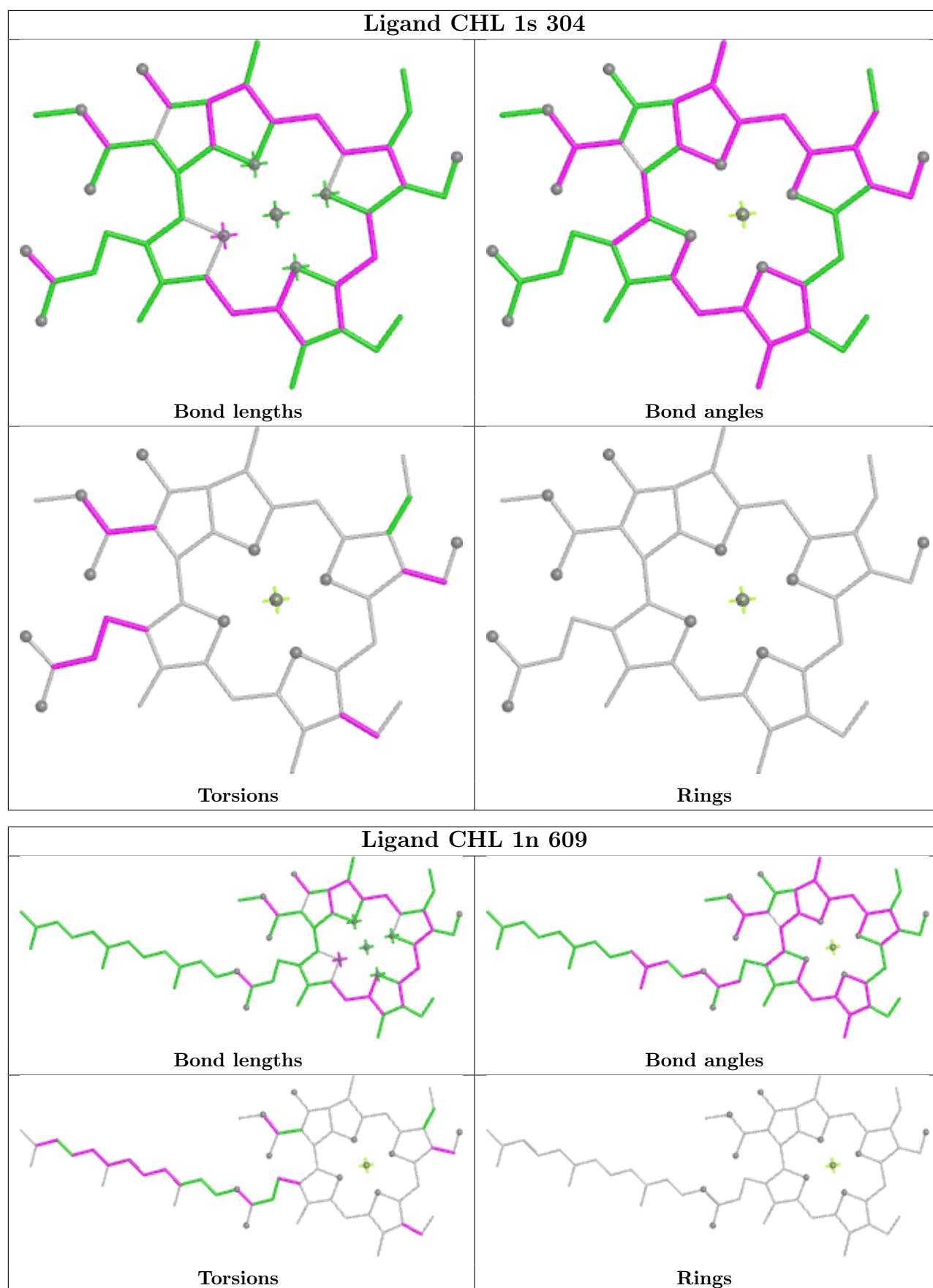


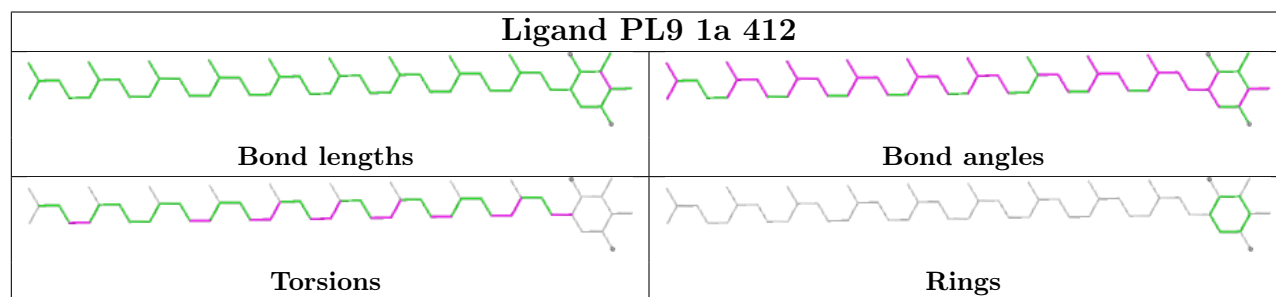
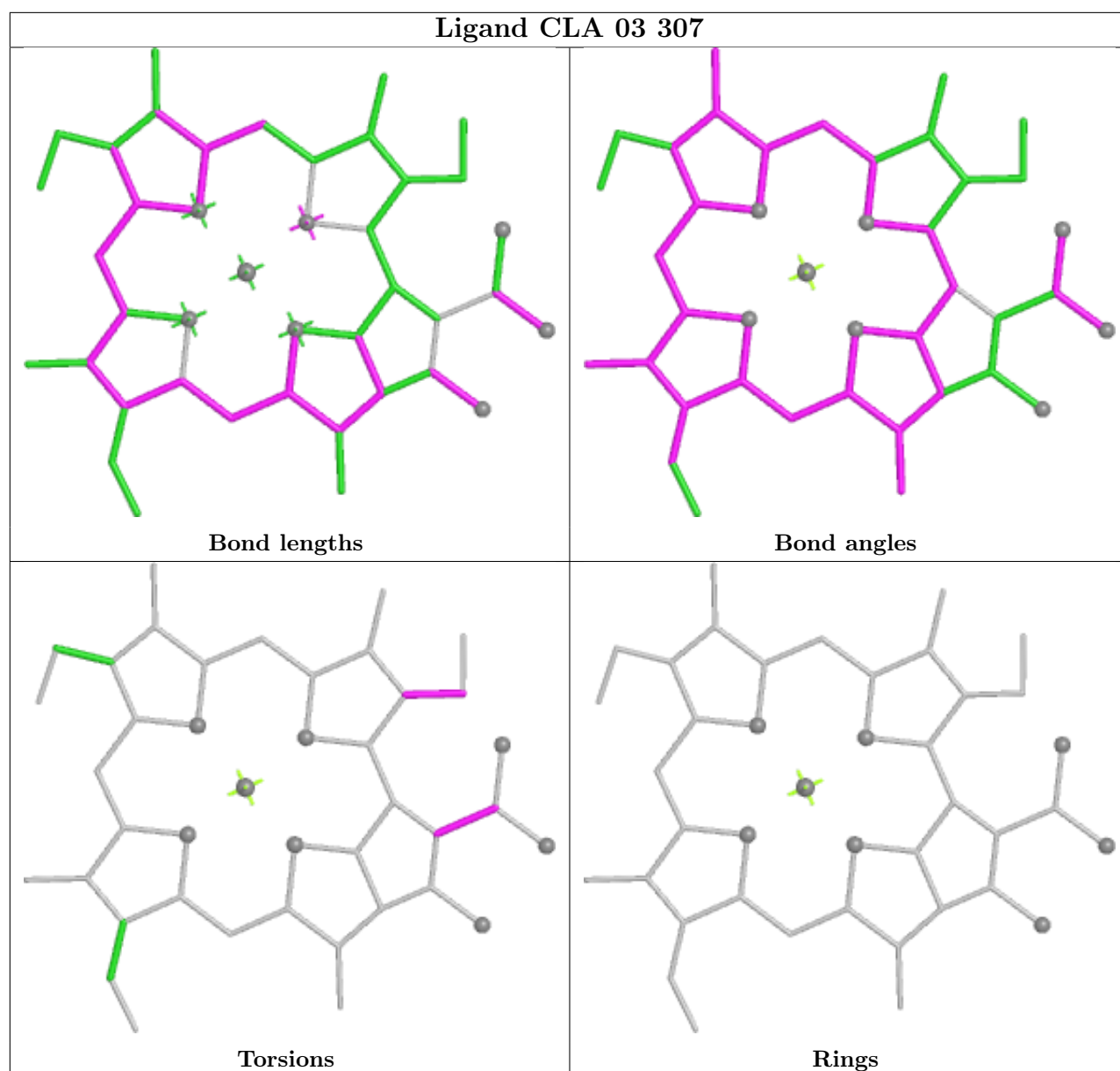


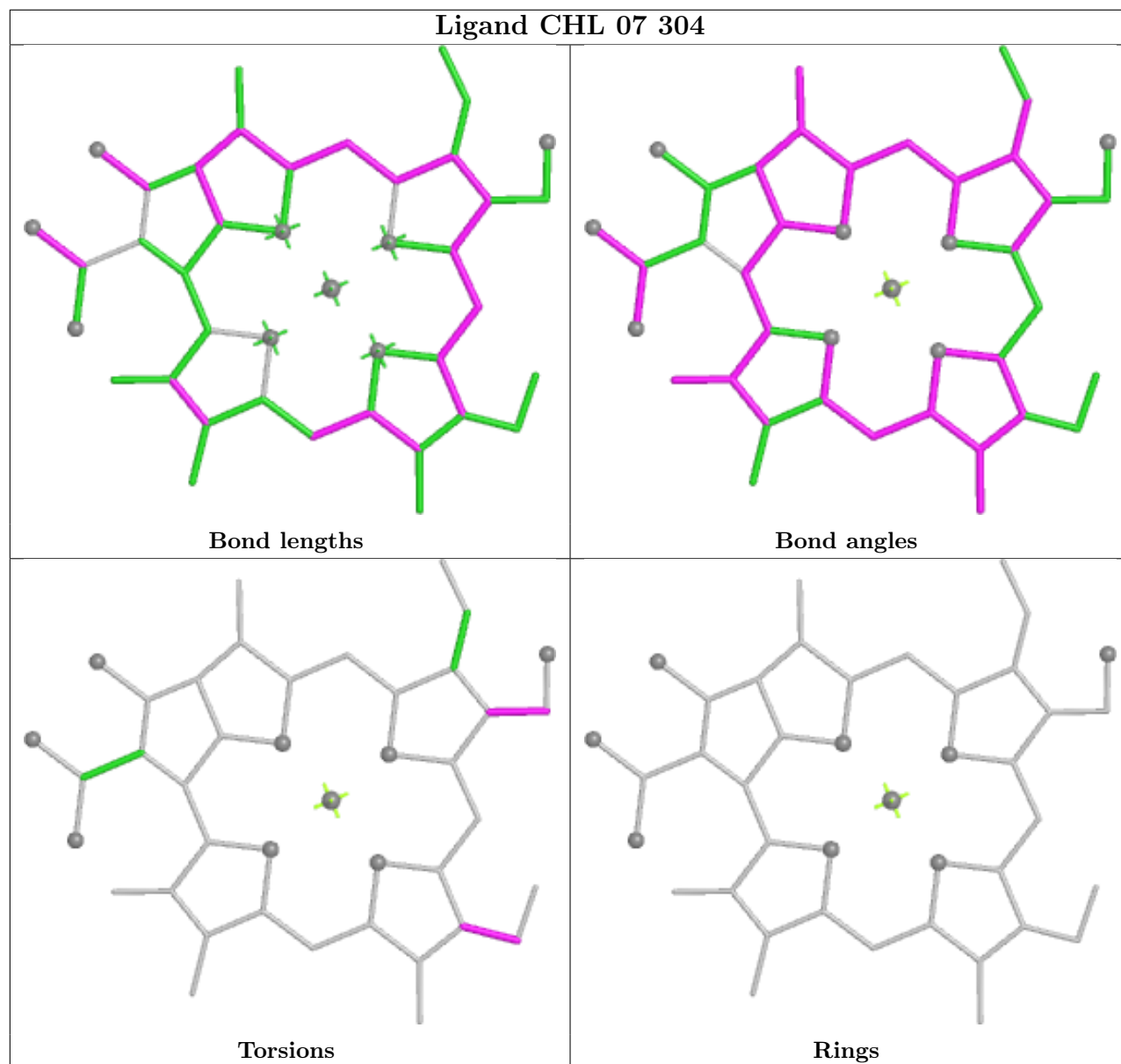


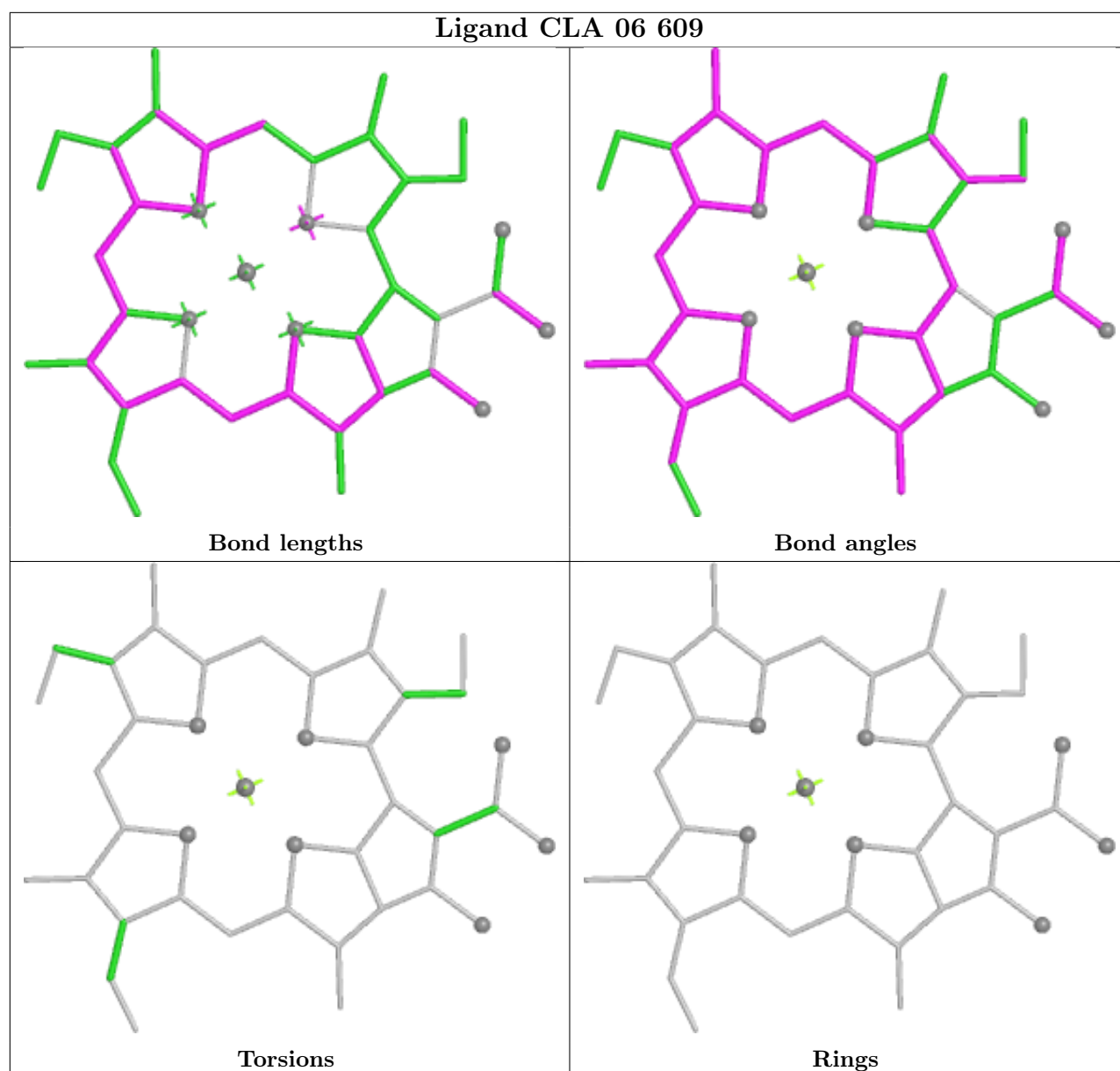


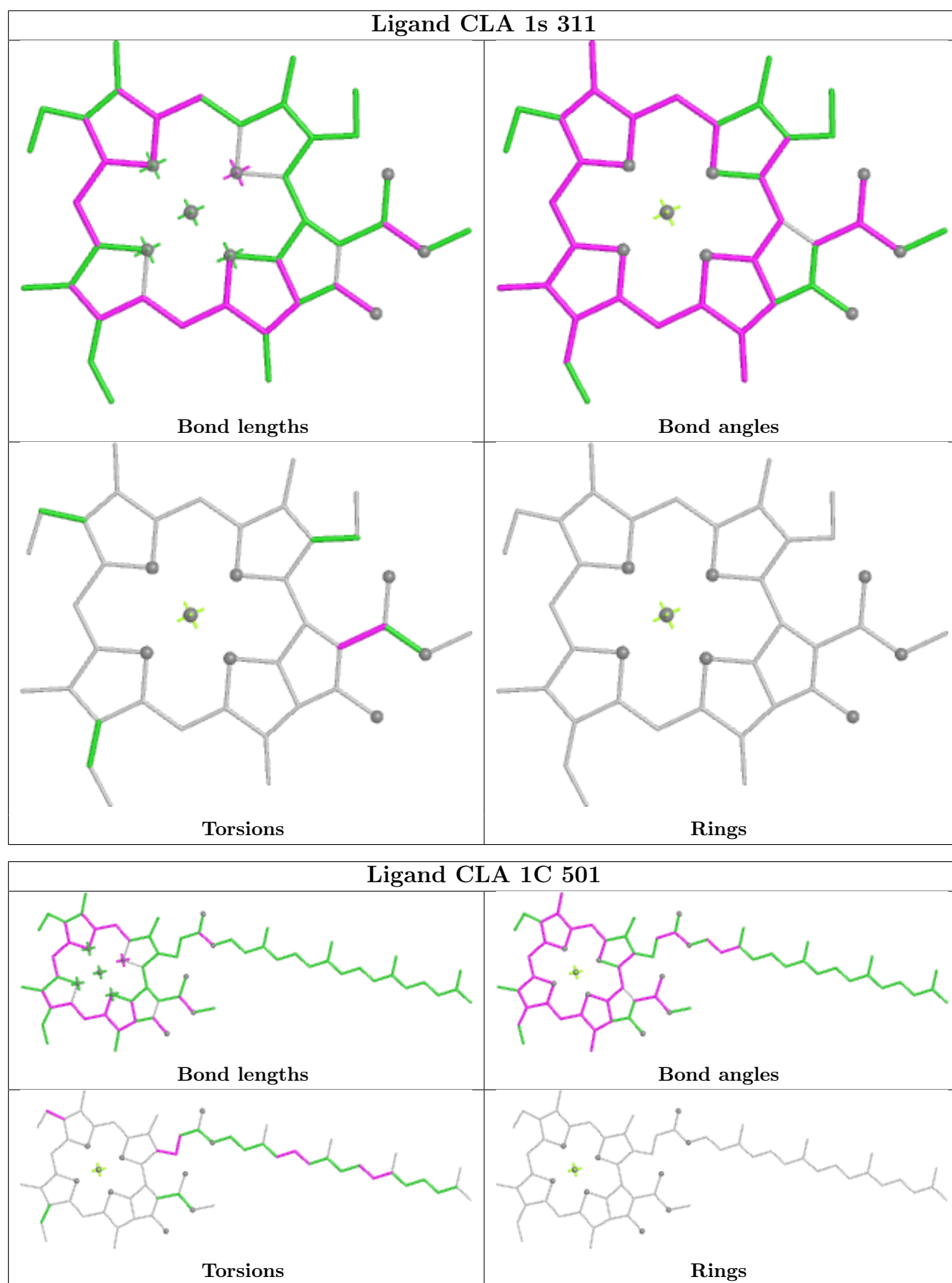


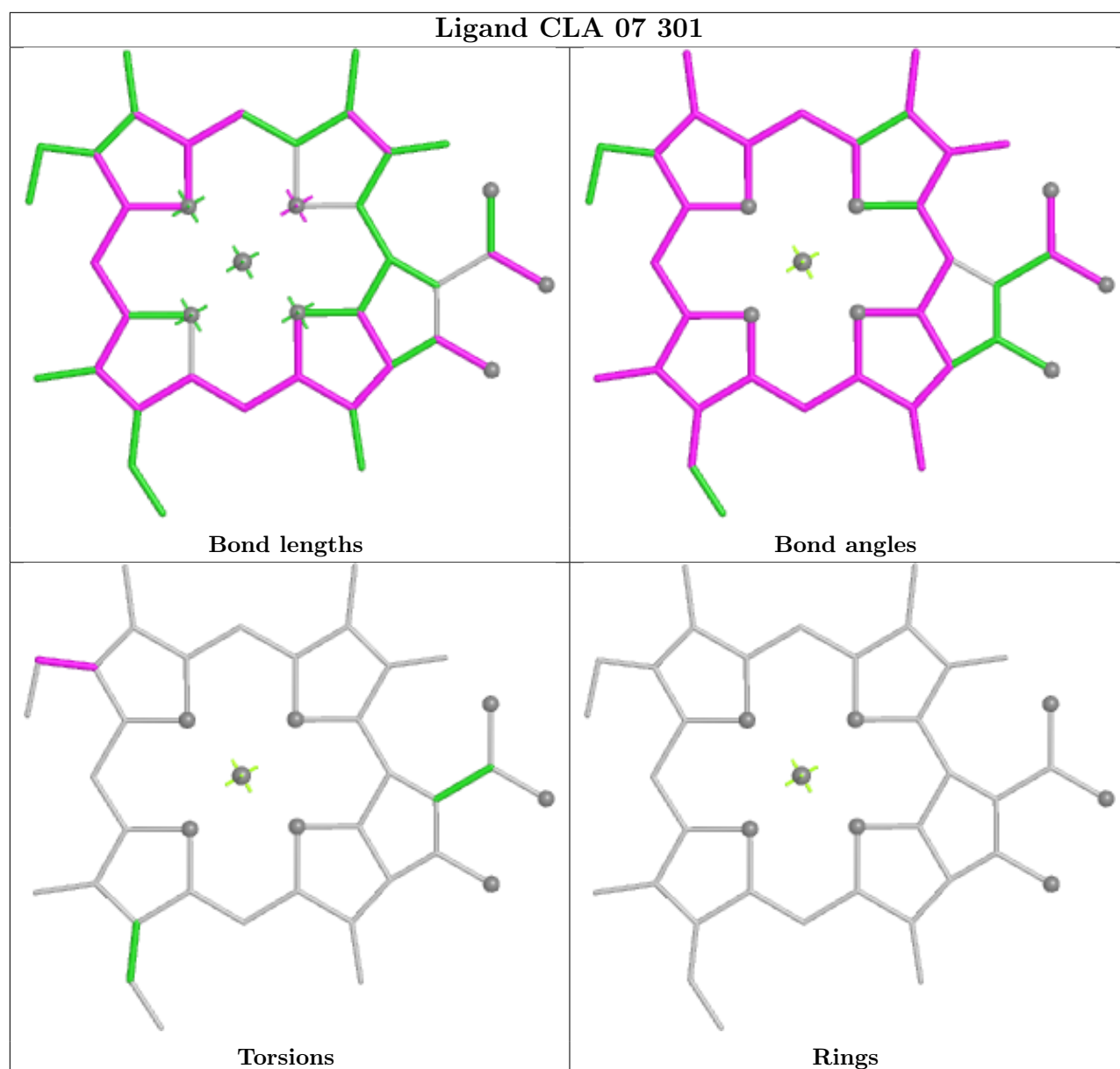


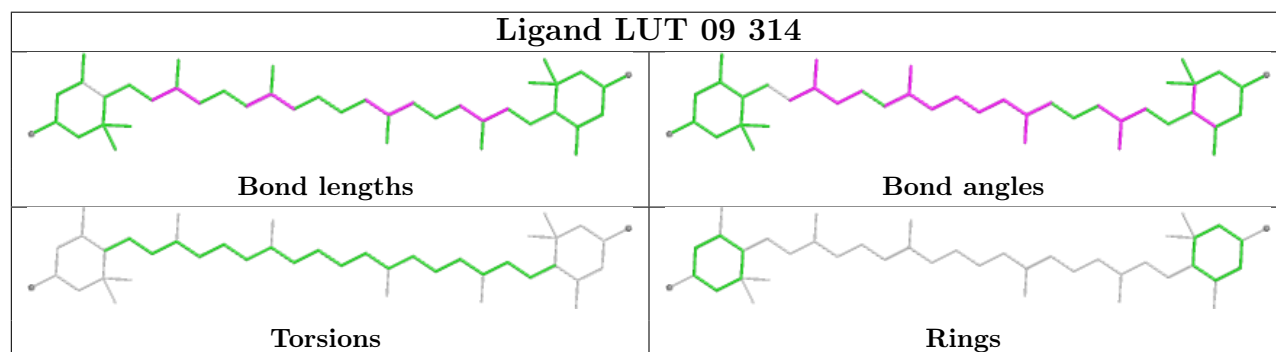
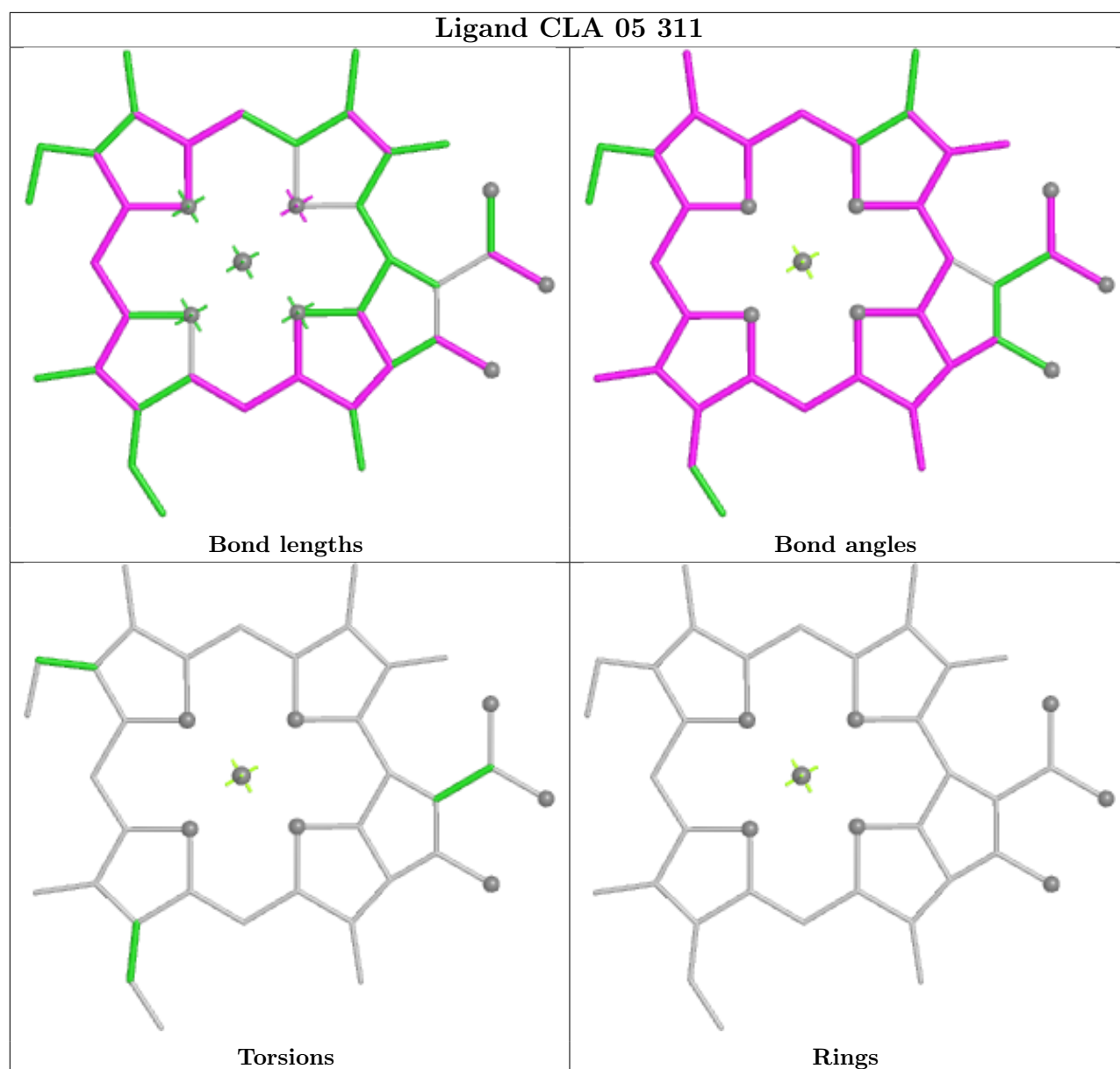




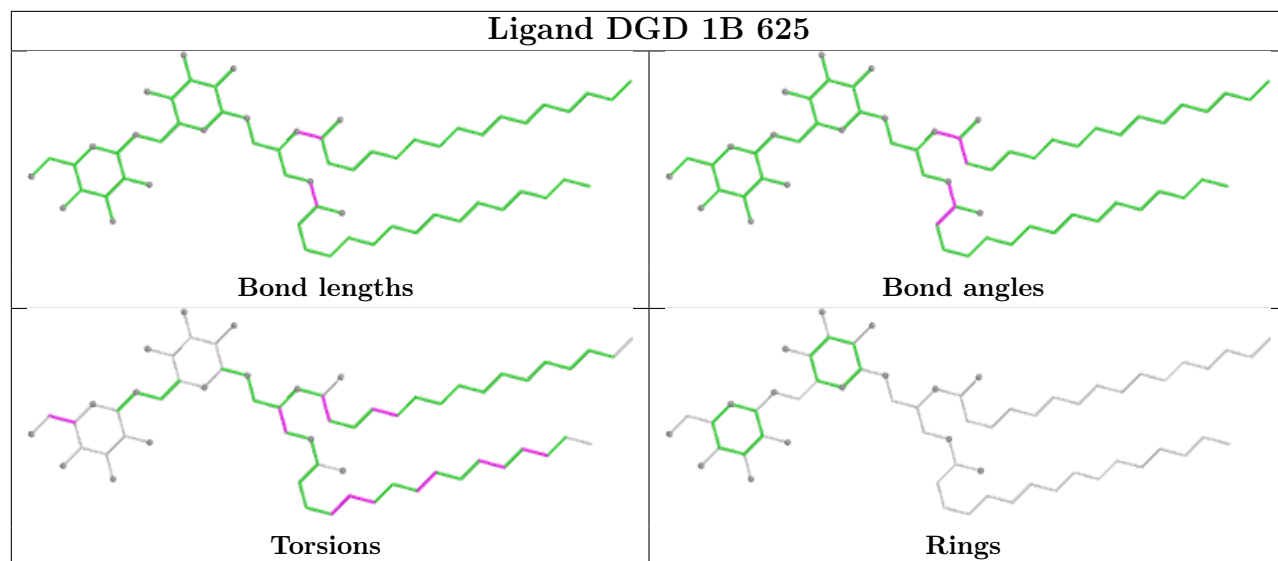




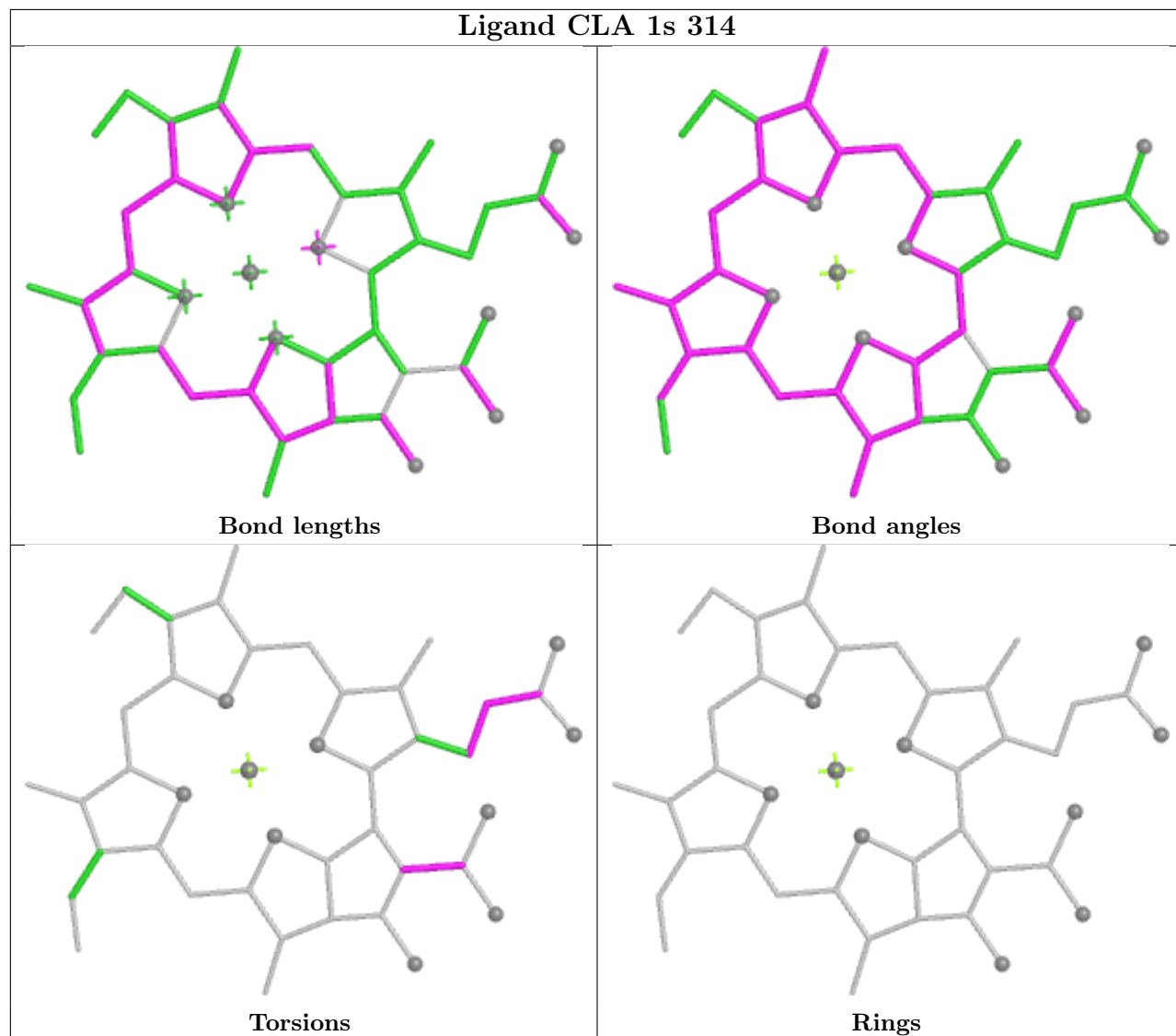


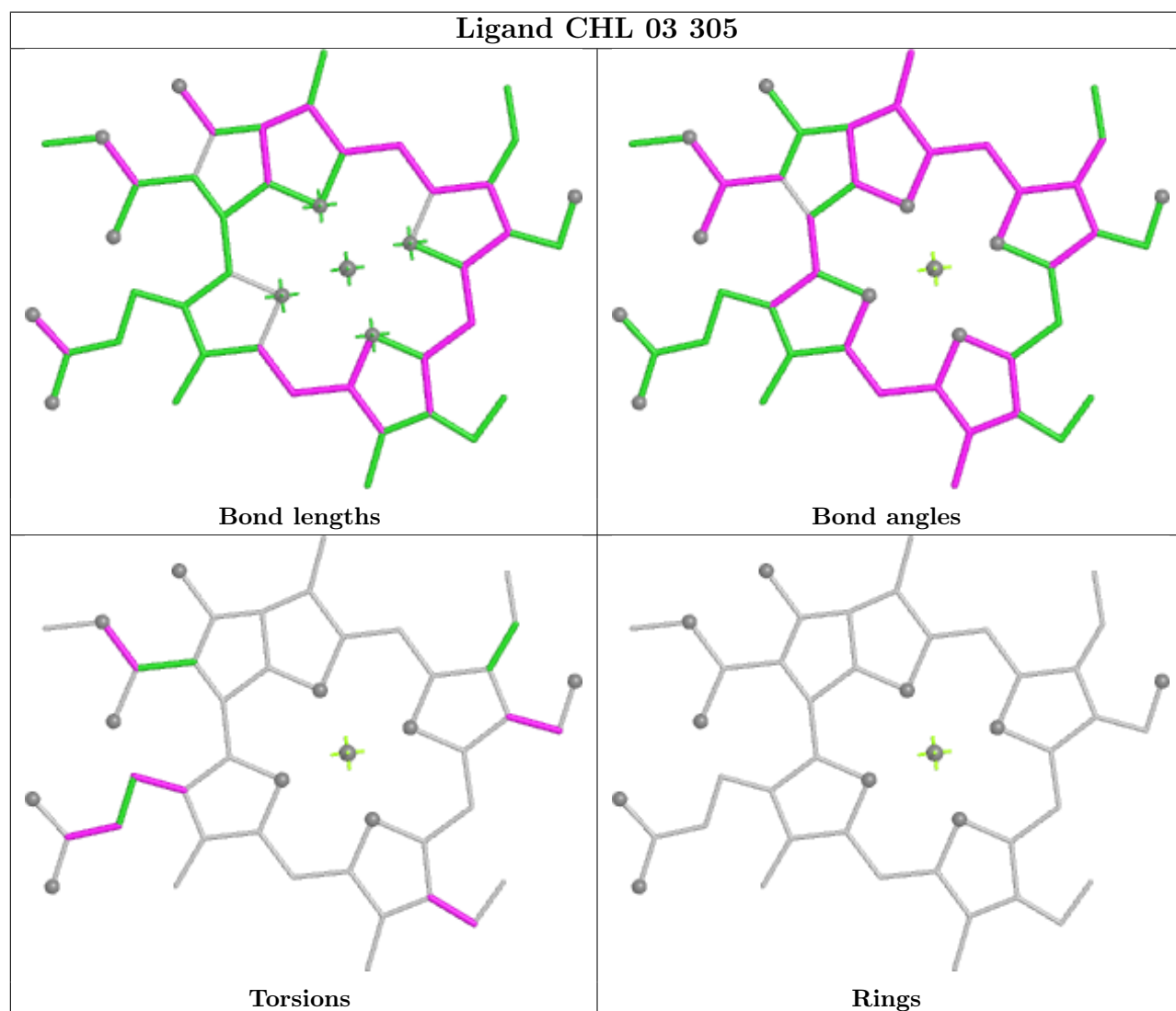
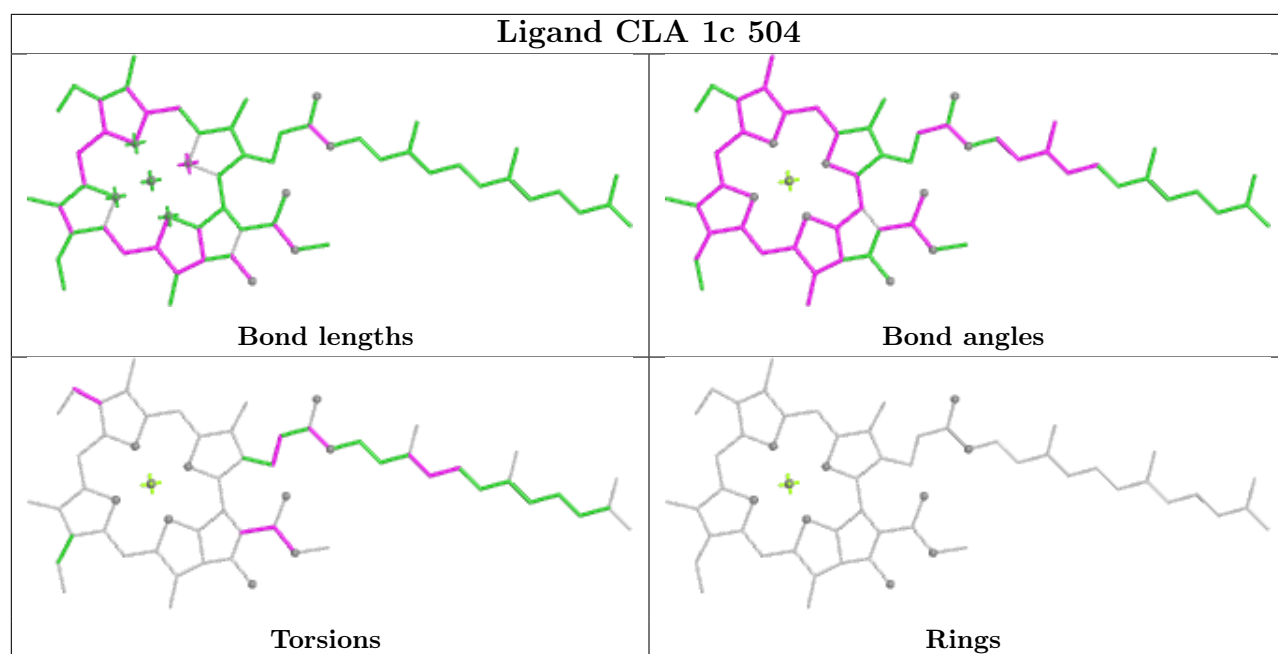


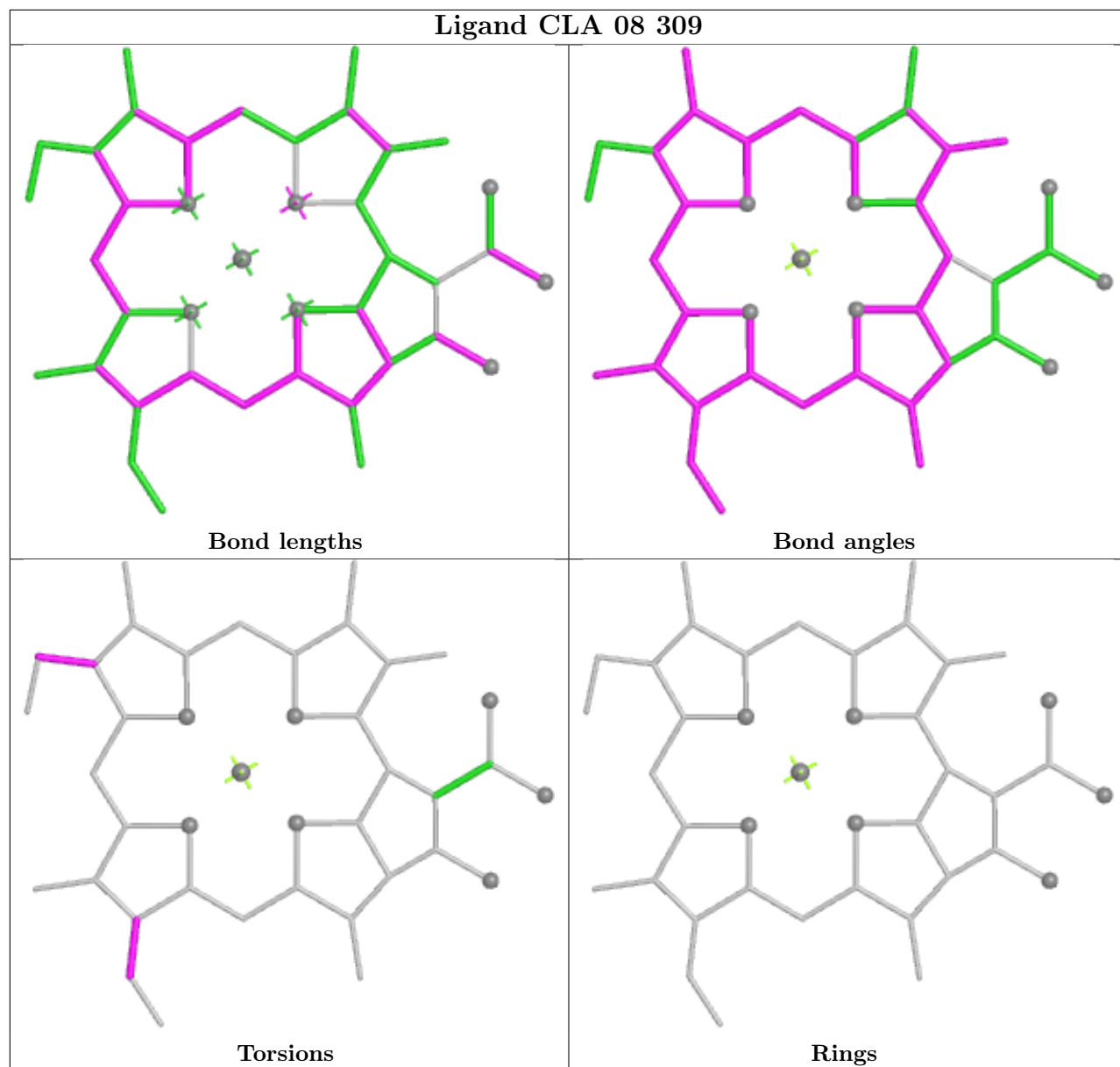
Ligand DGD 1B 625

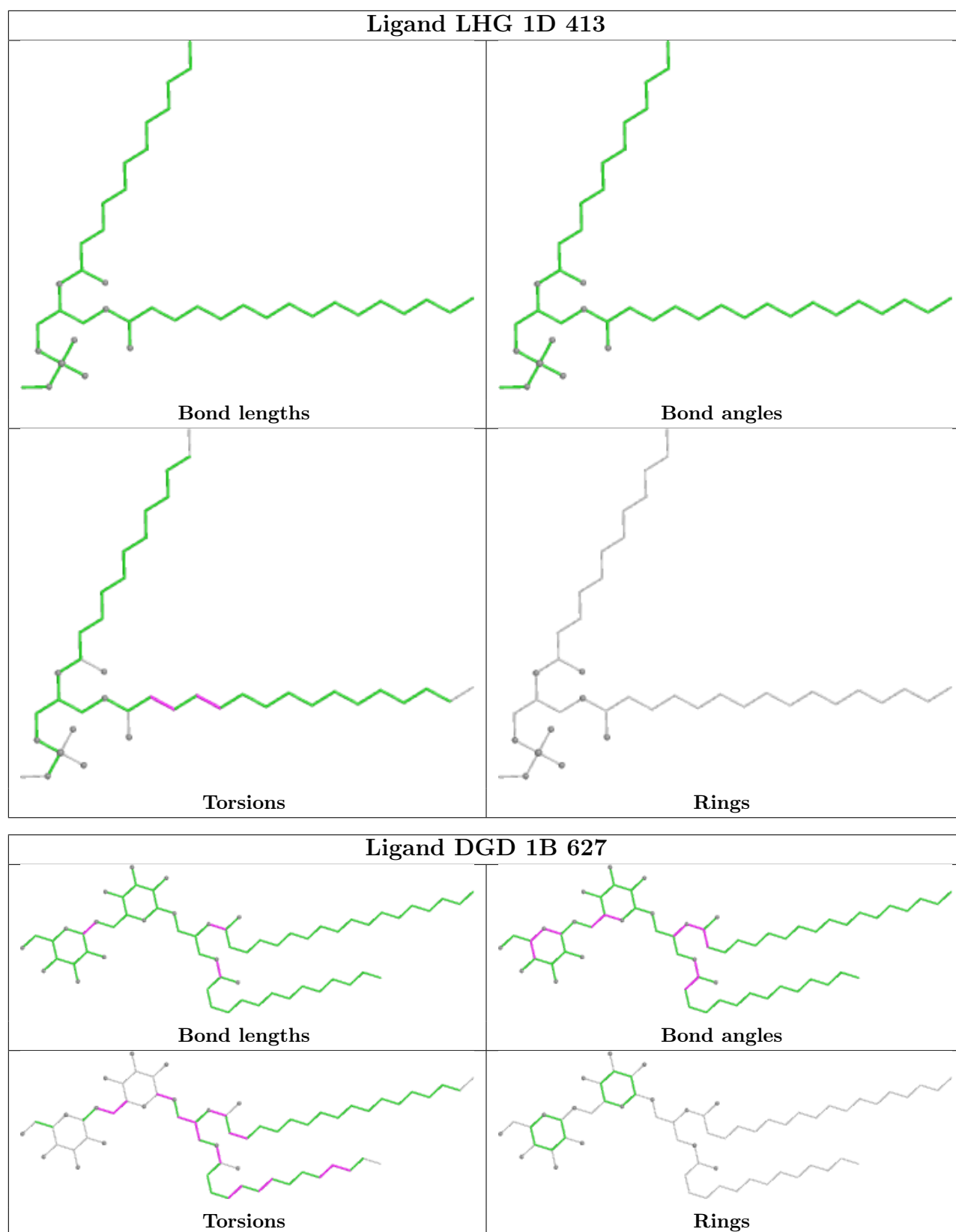


Ligand CLA 1s 314

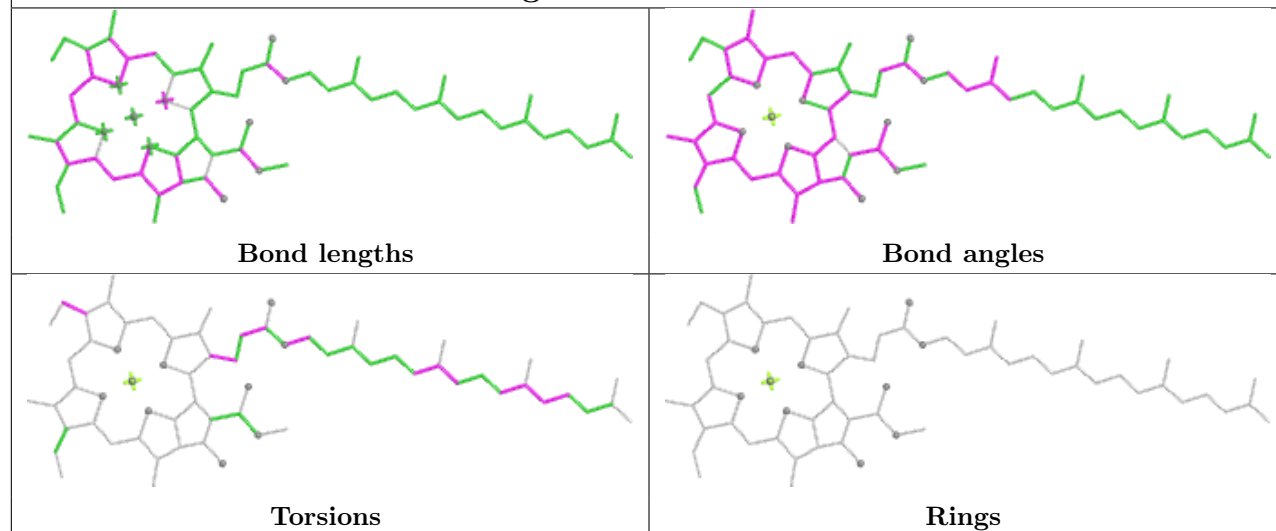




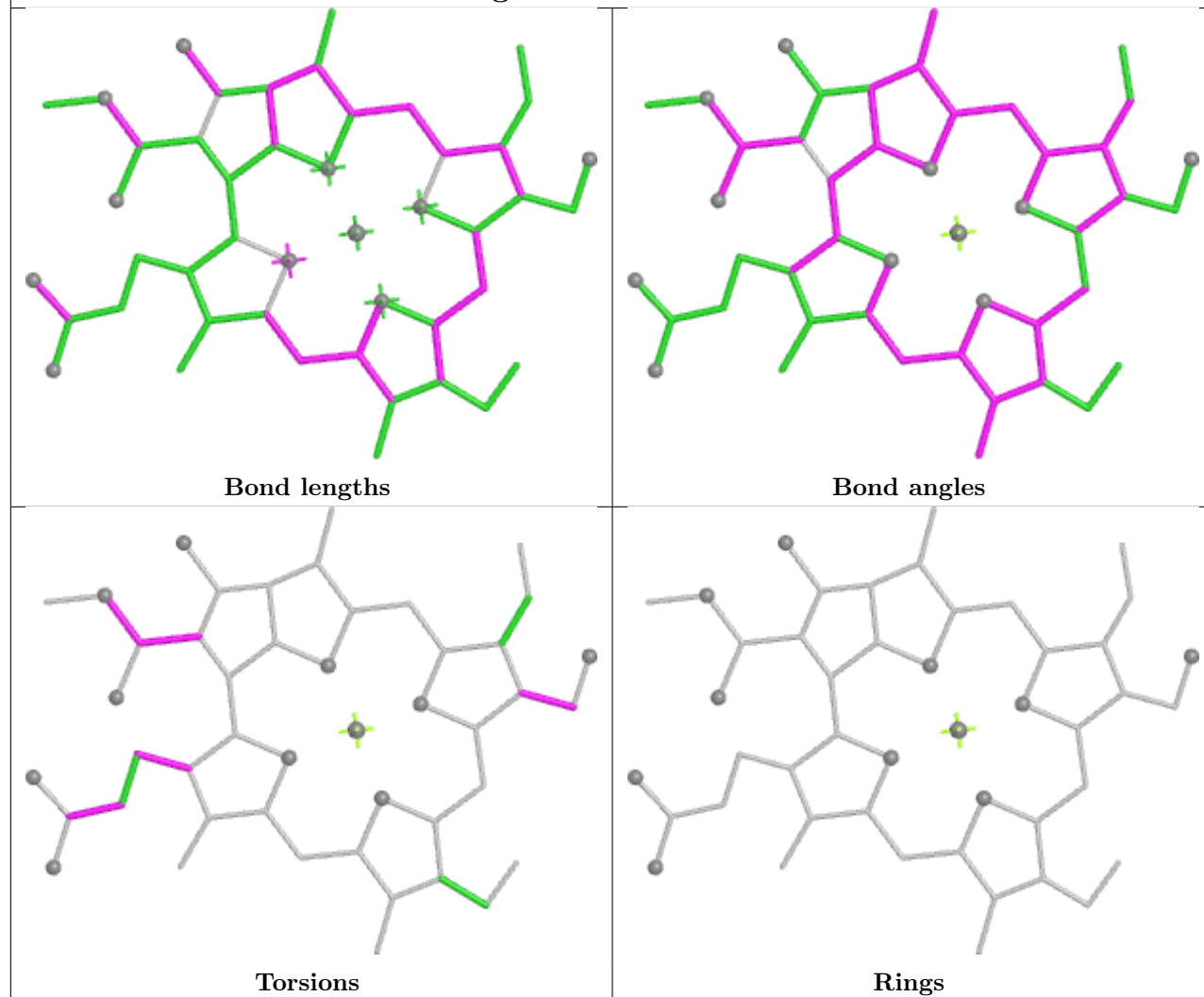


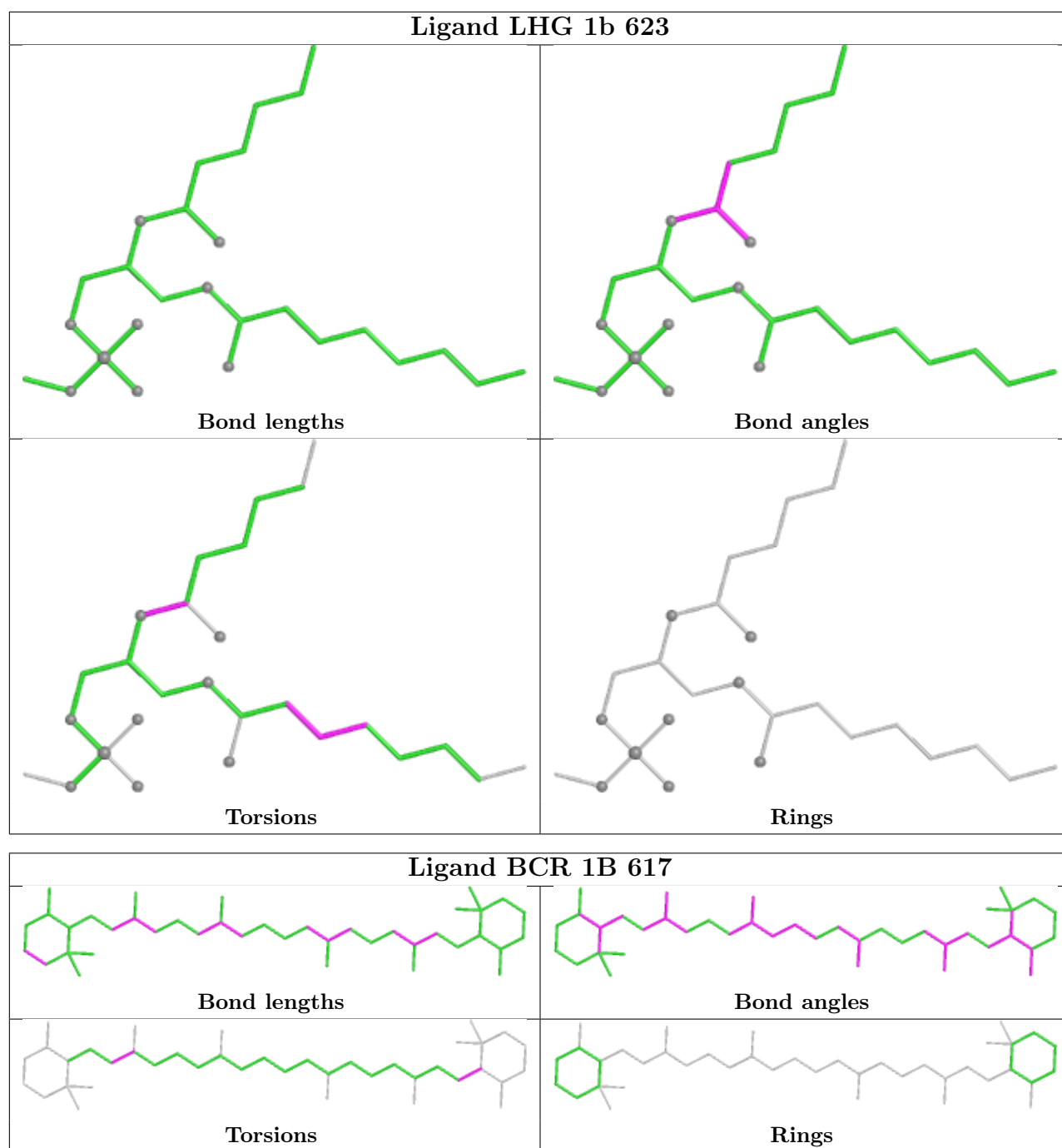


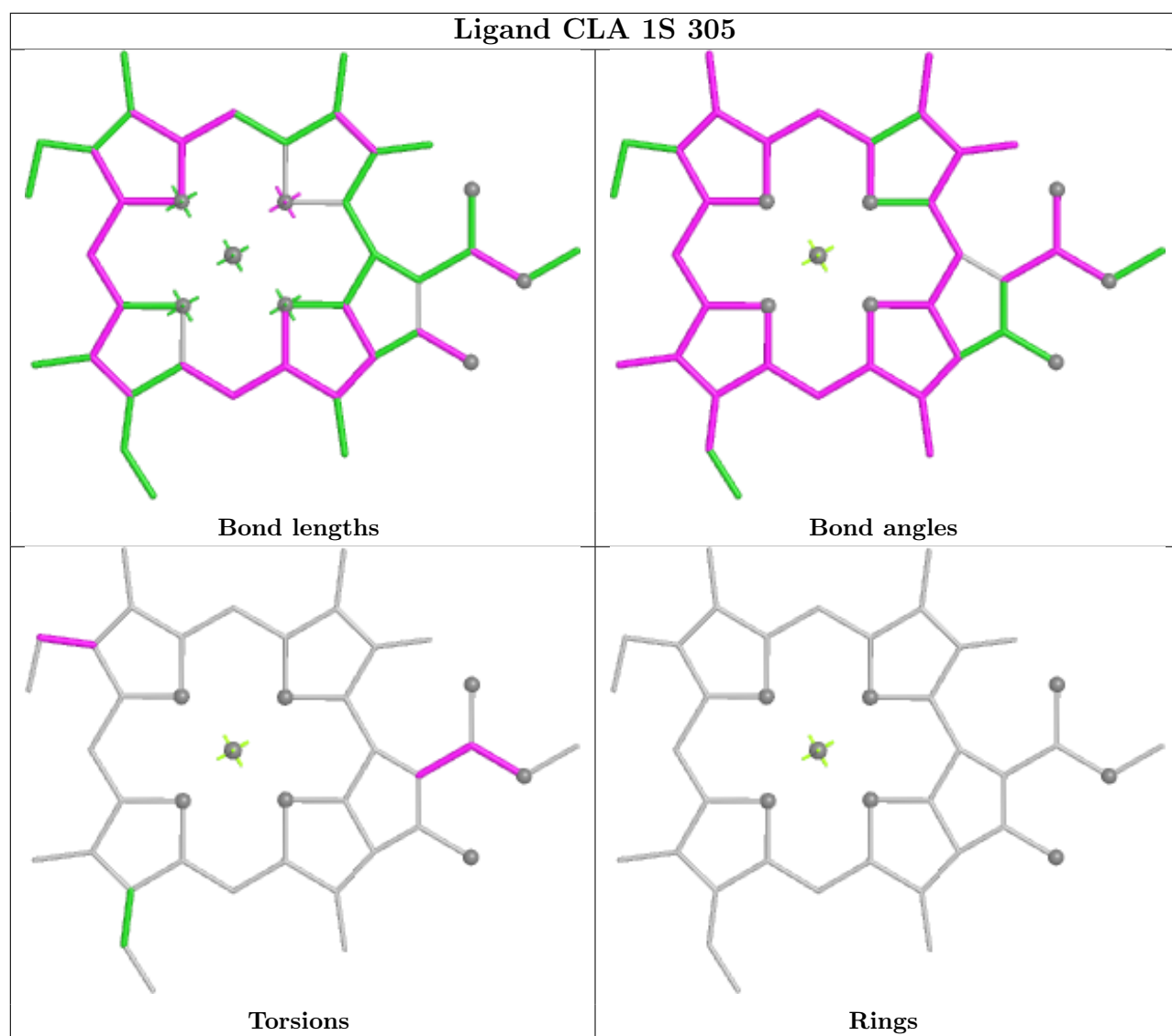
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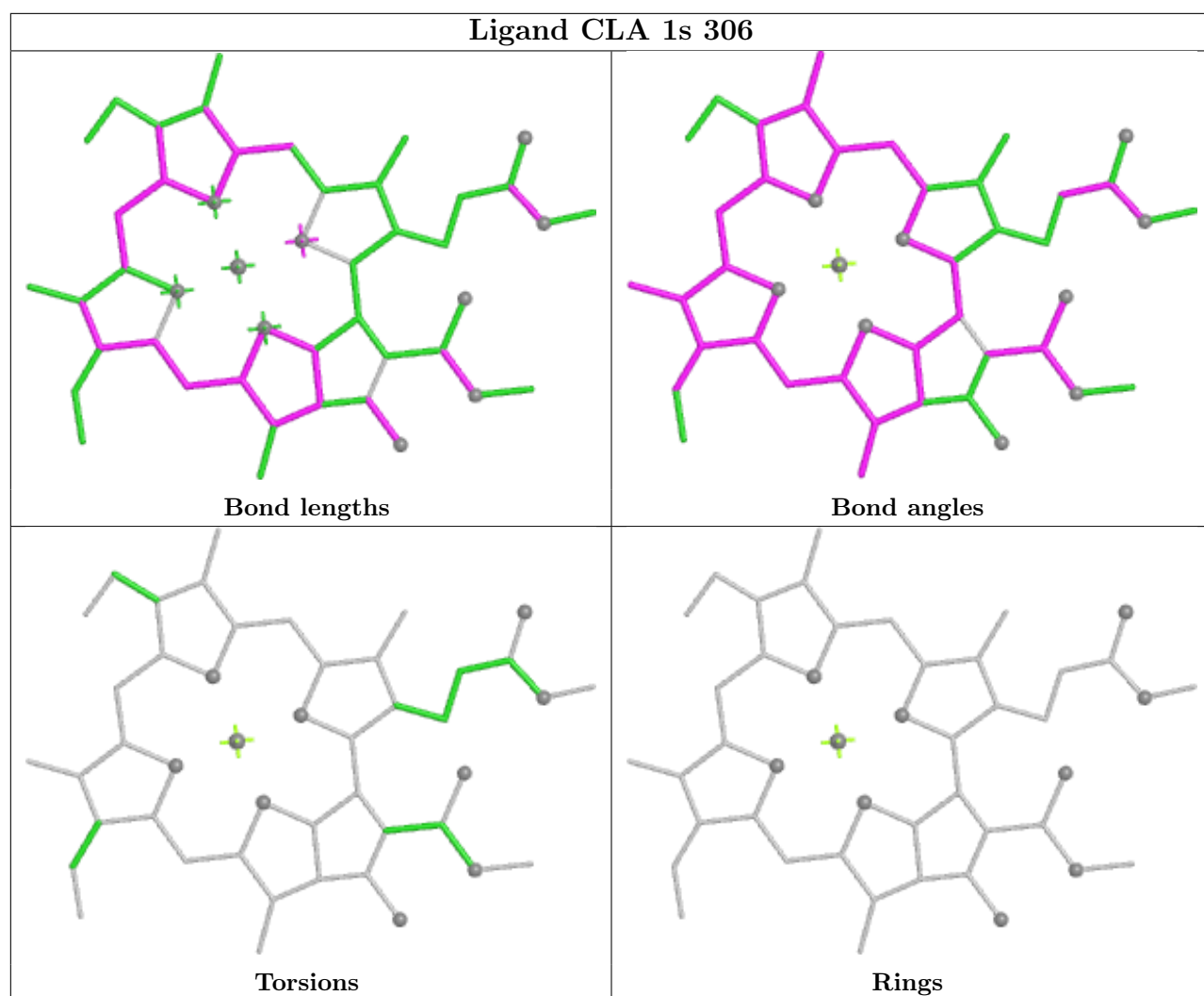


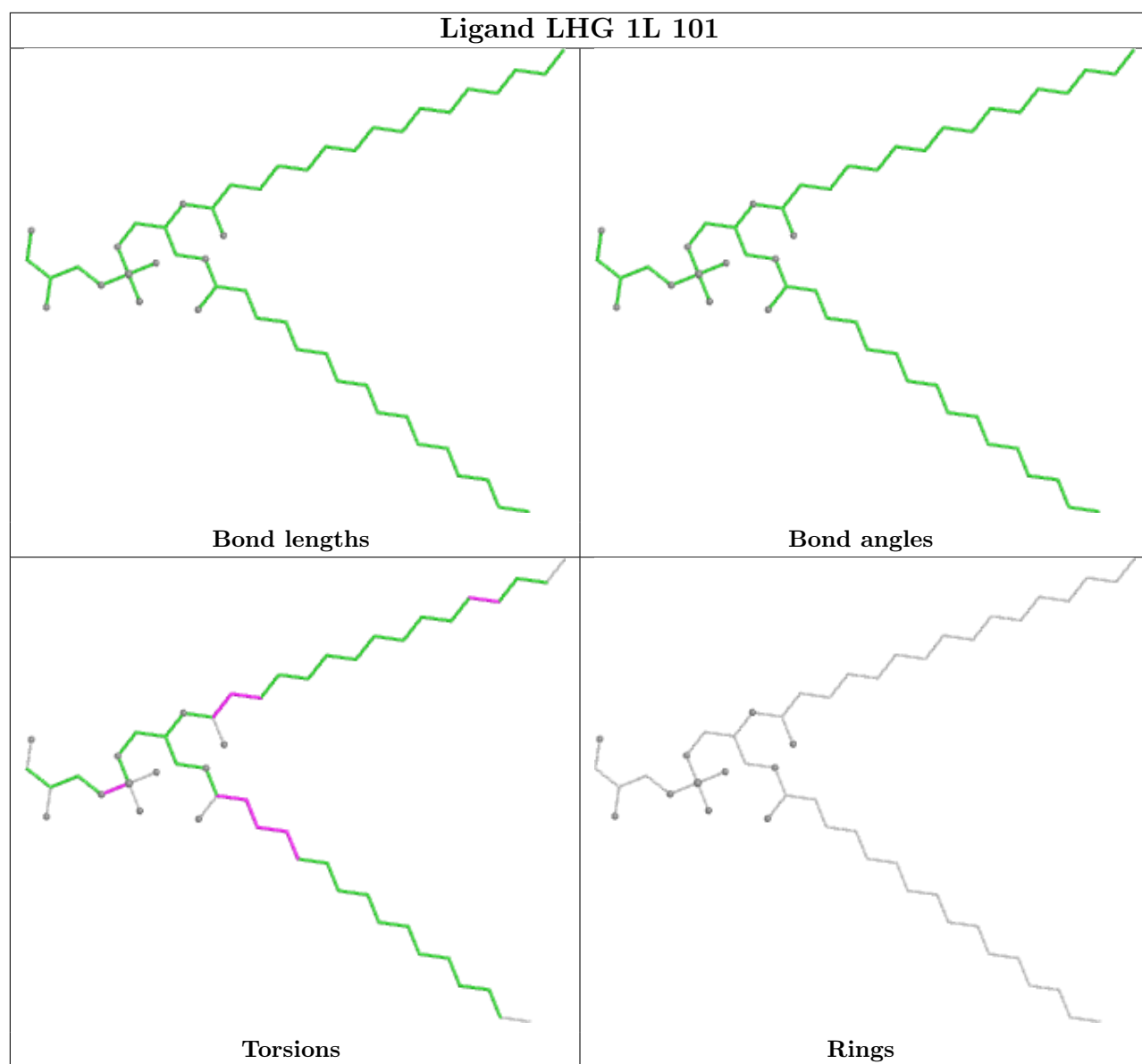
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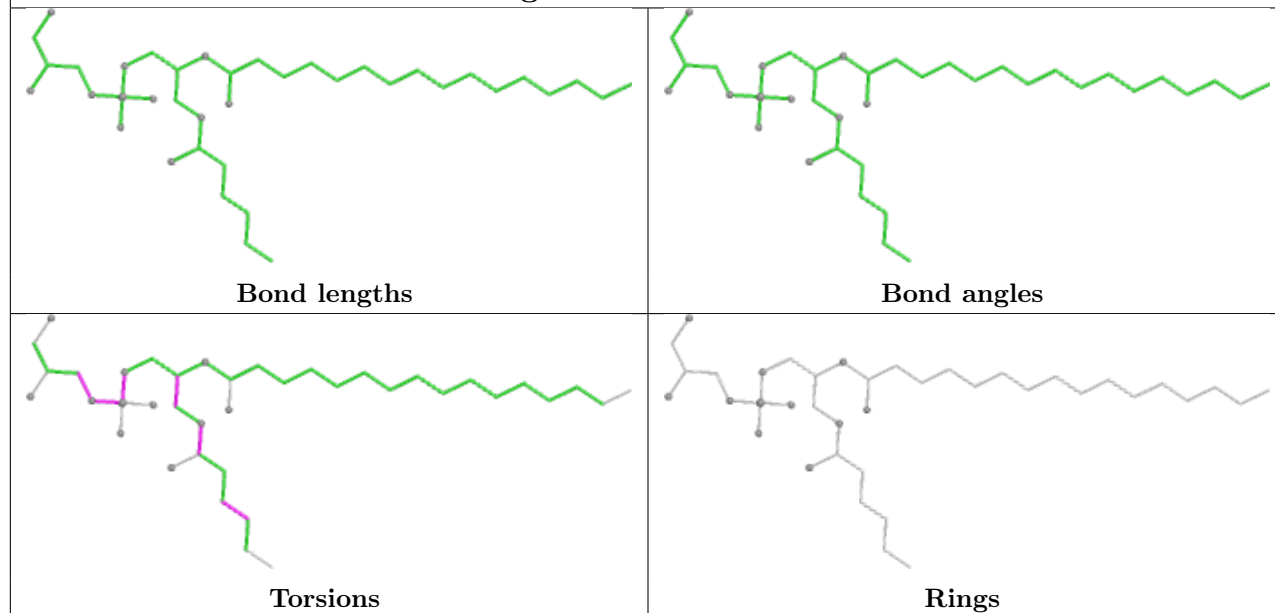




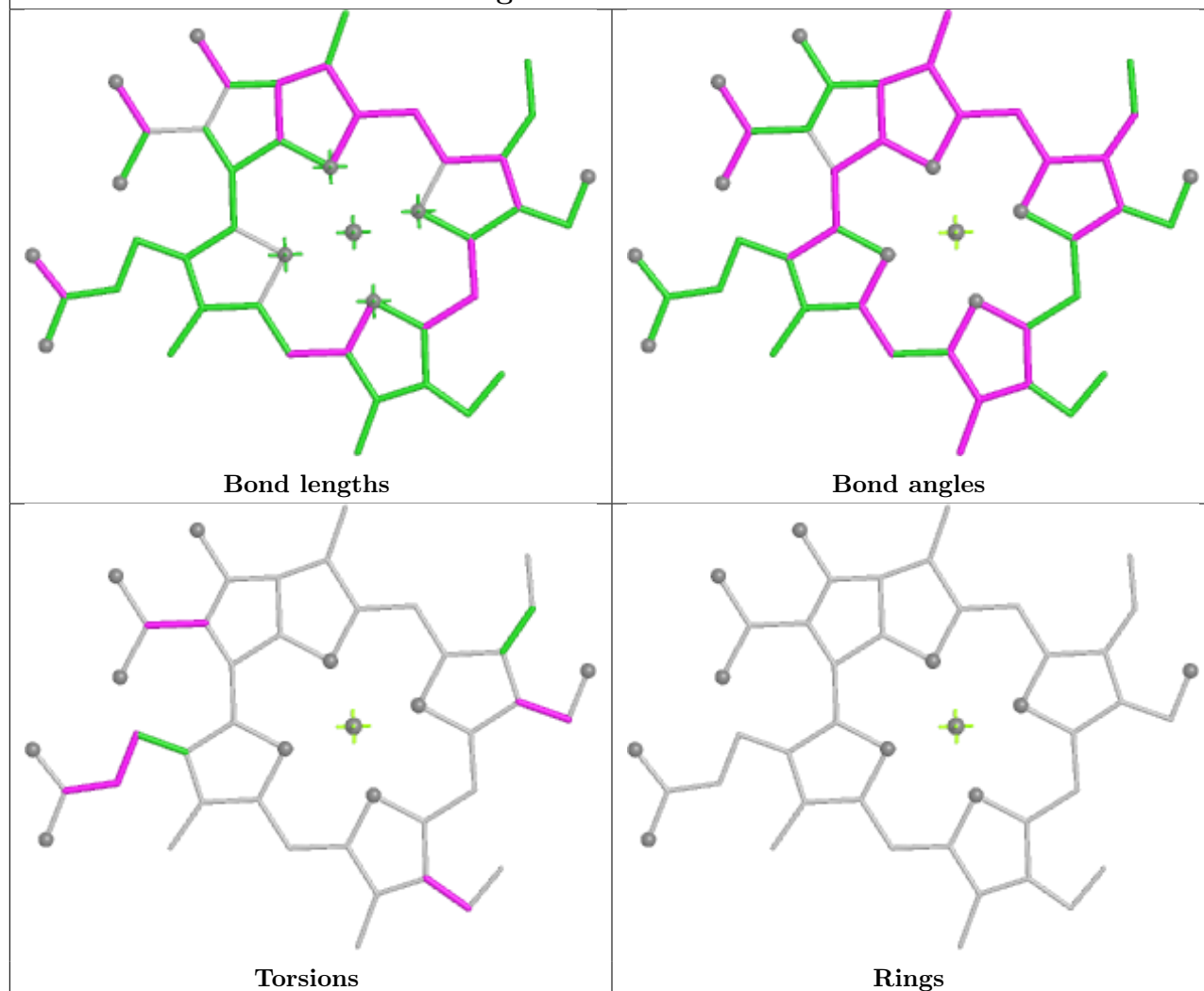


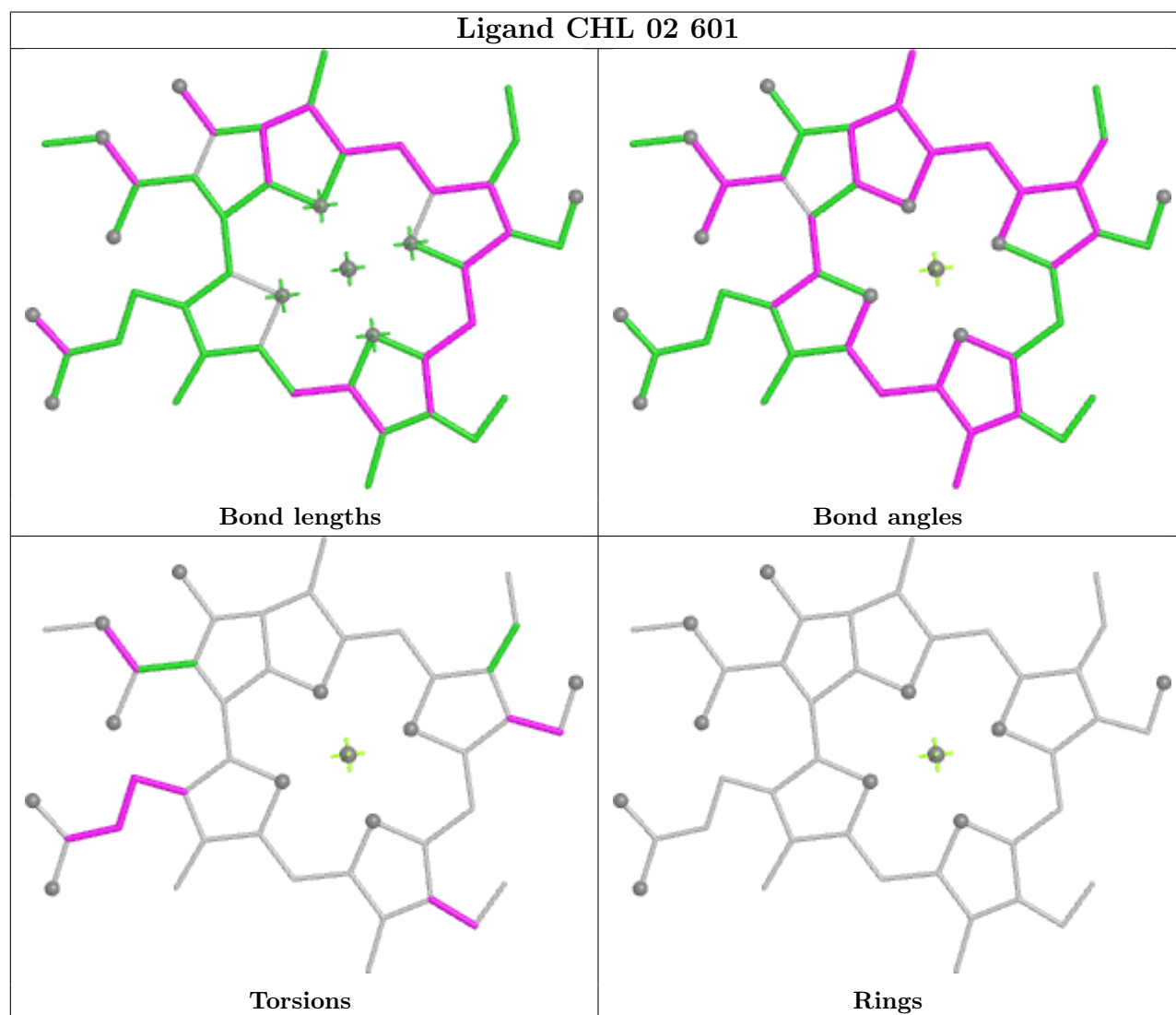
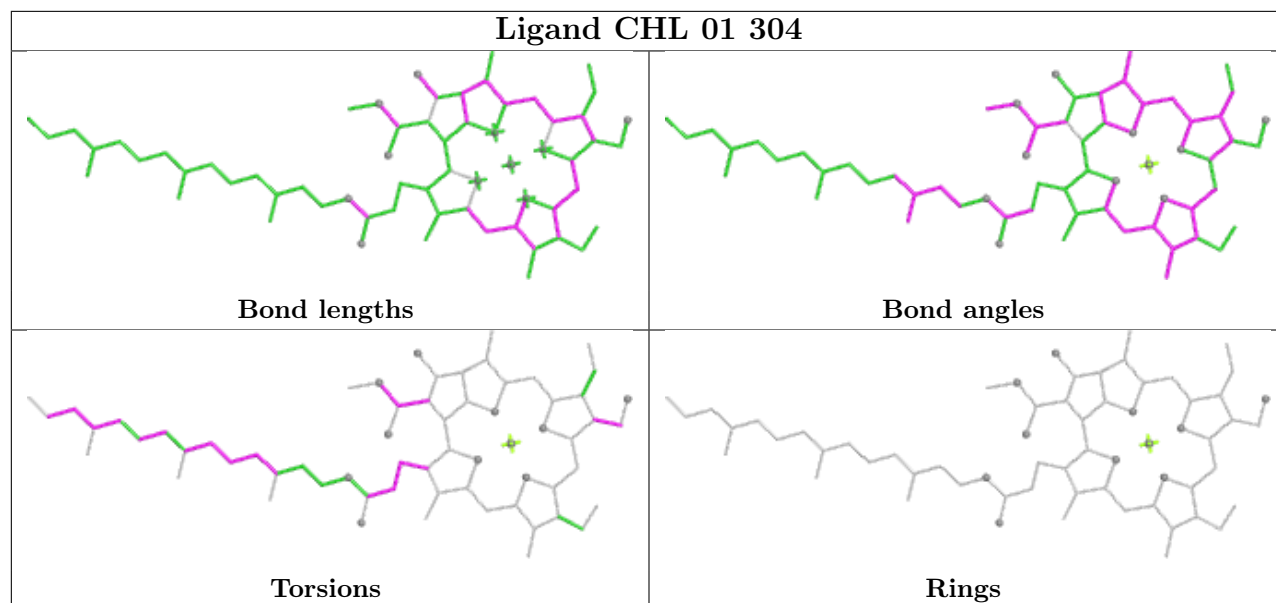


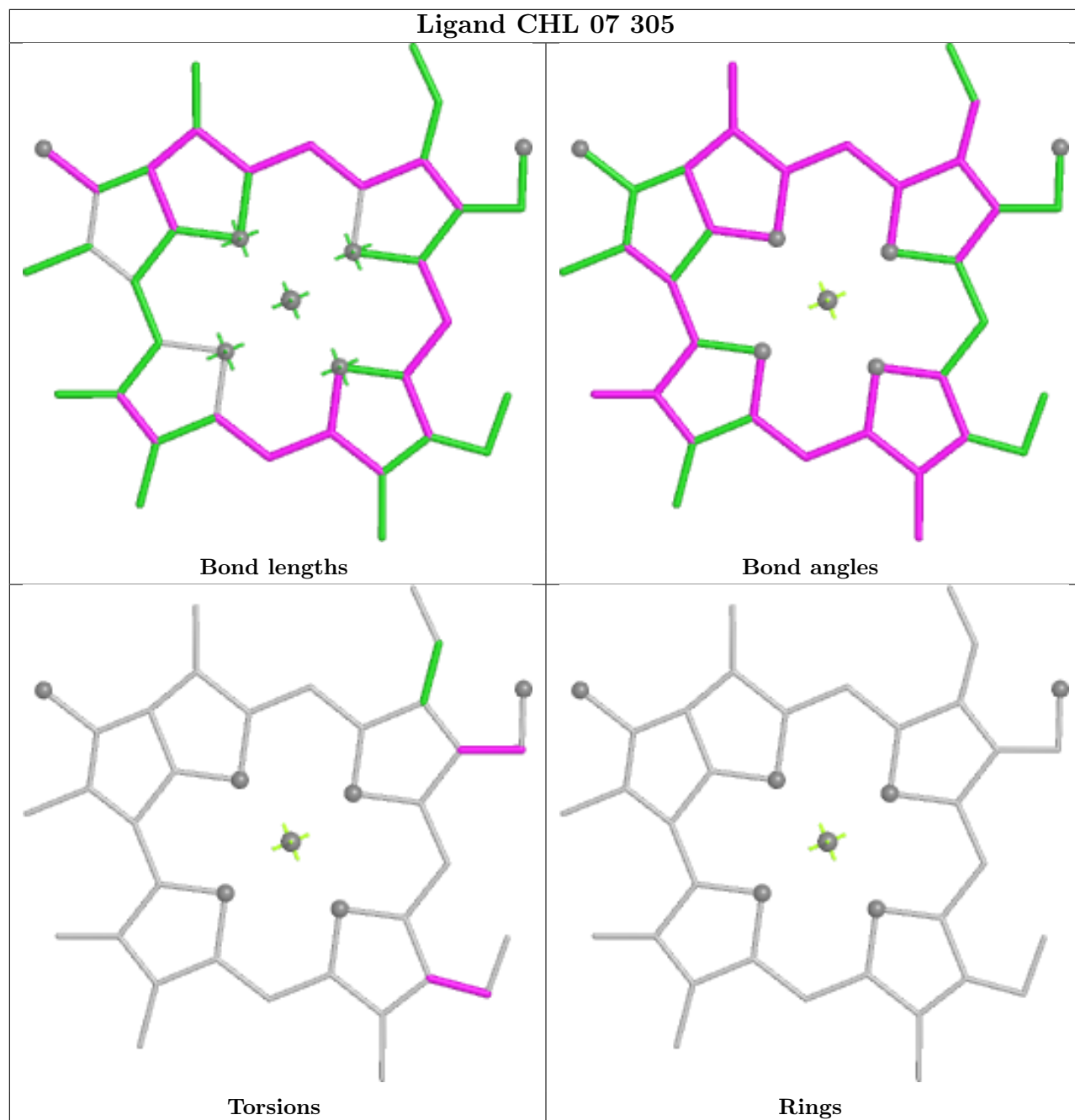
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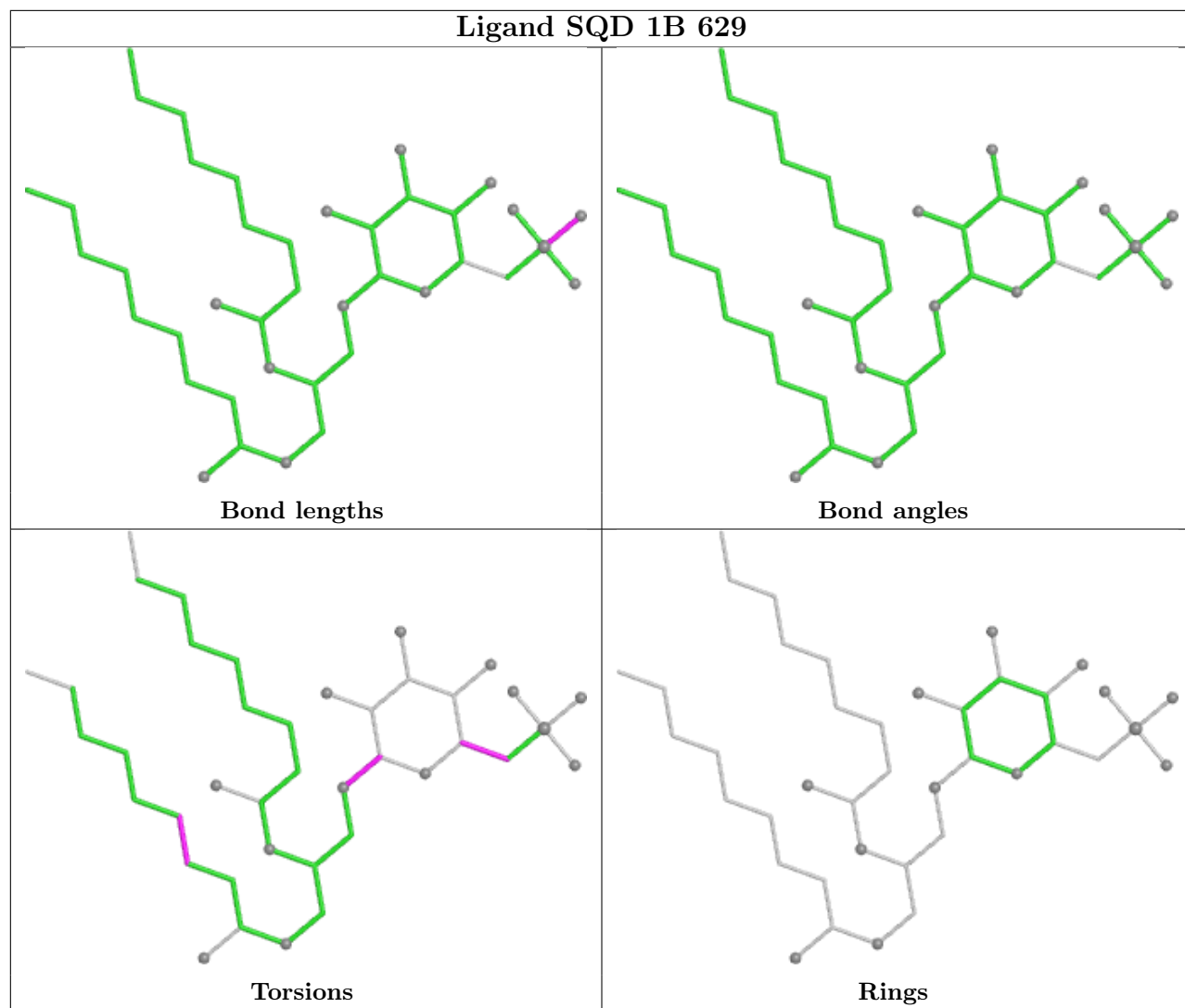


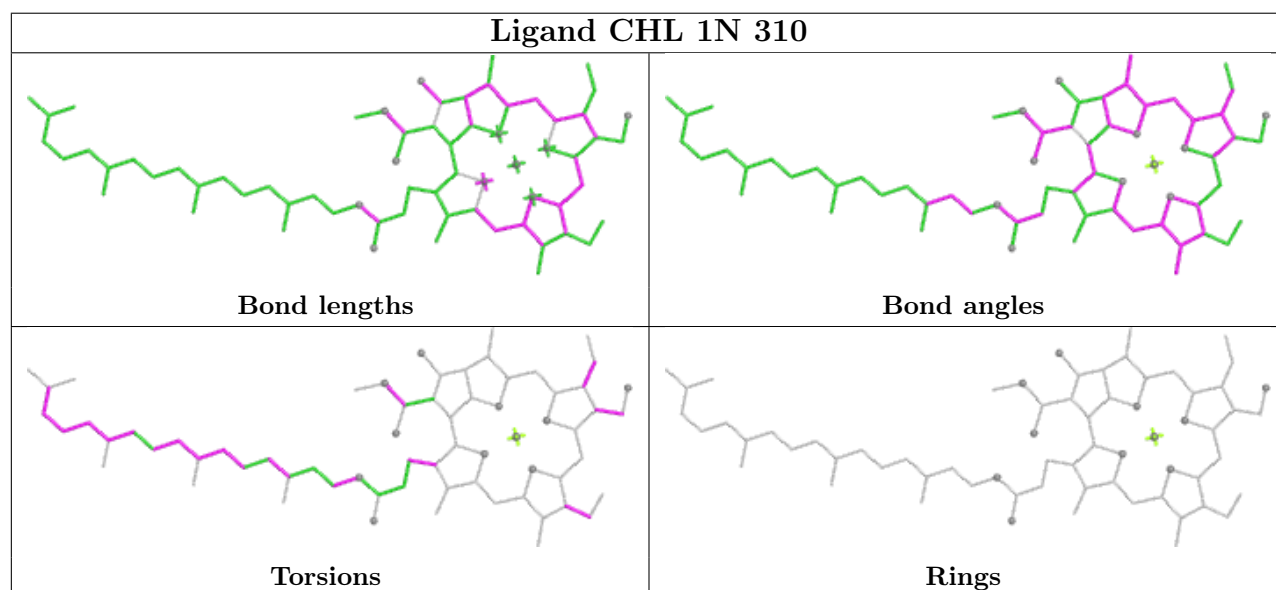
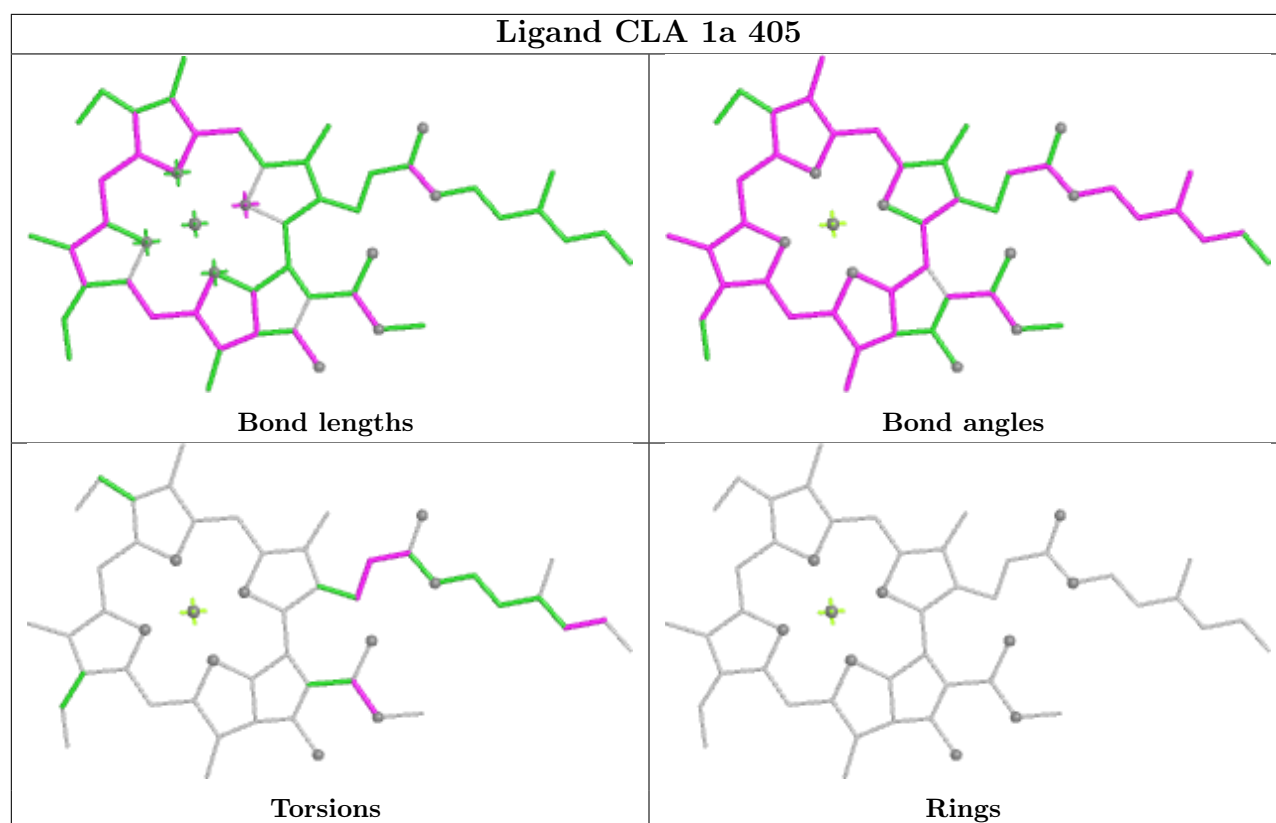
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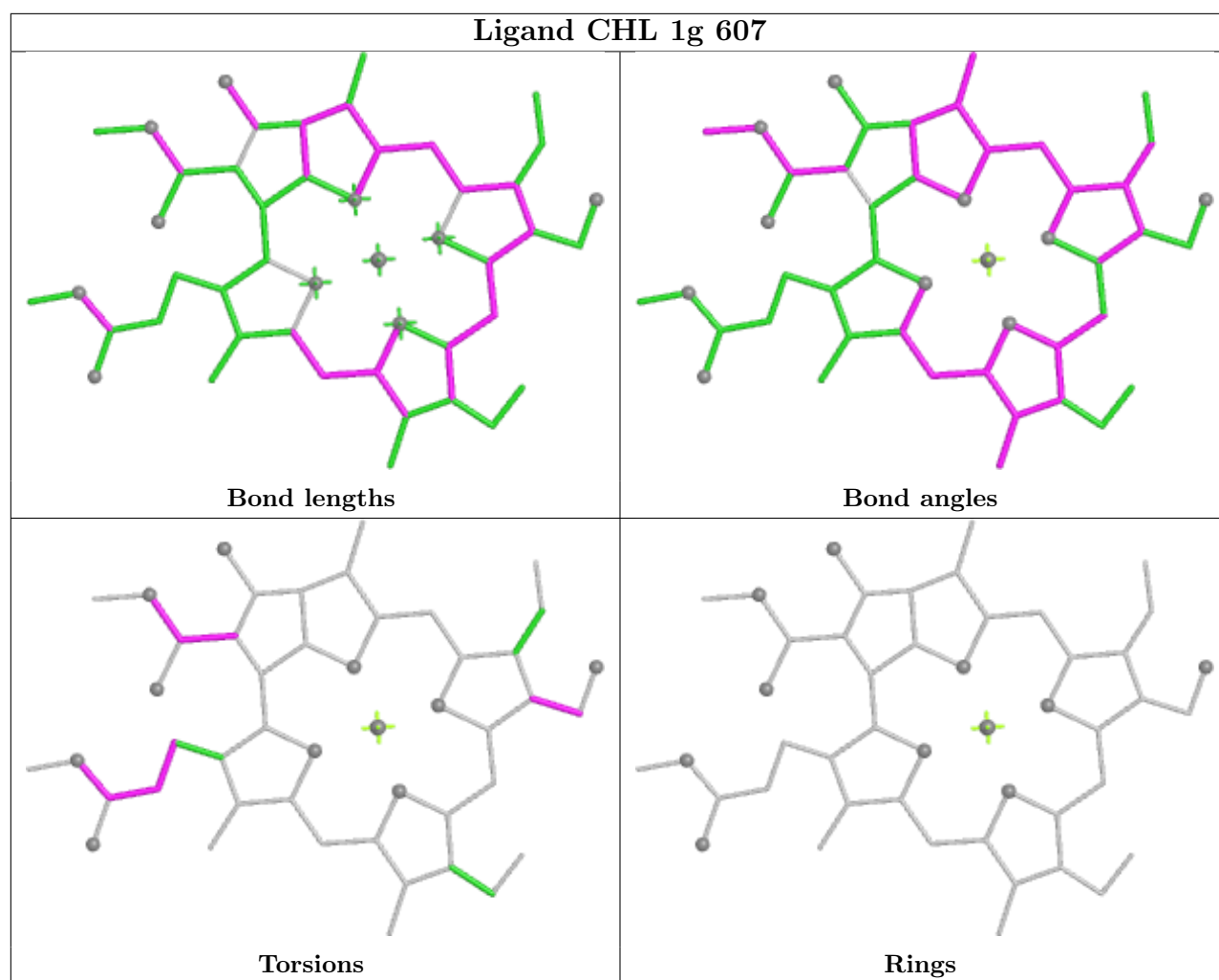


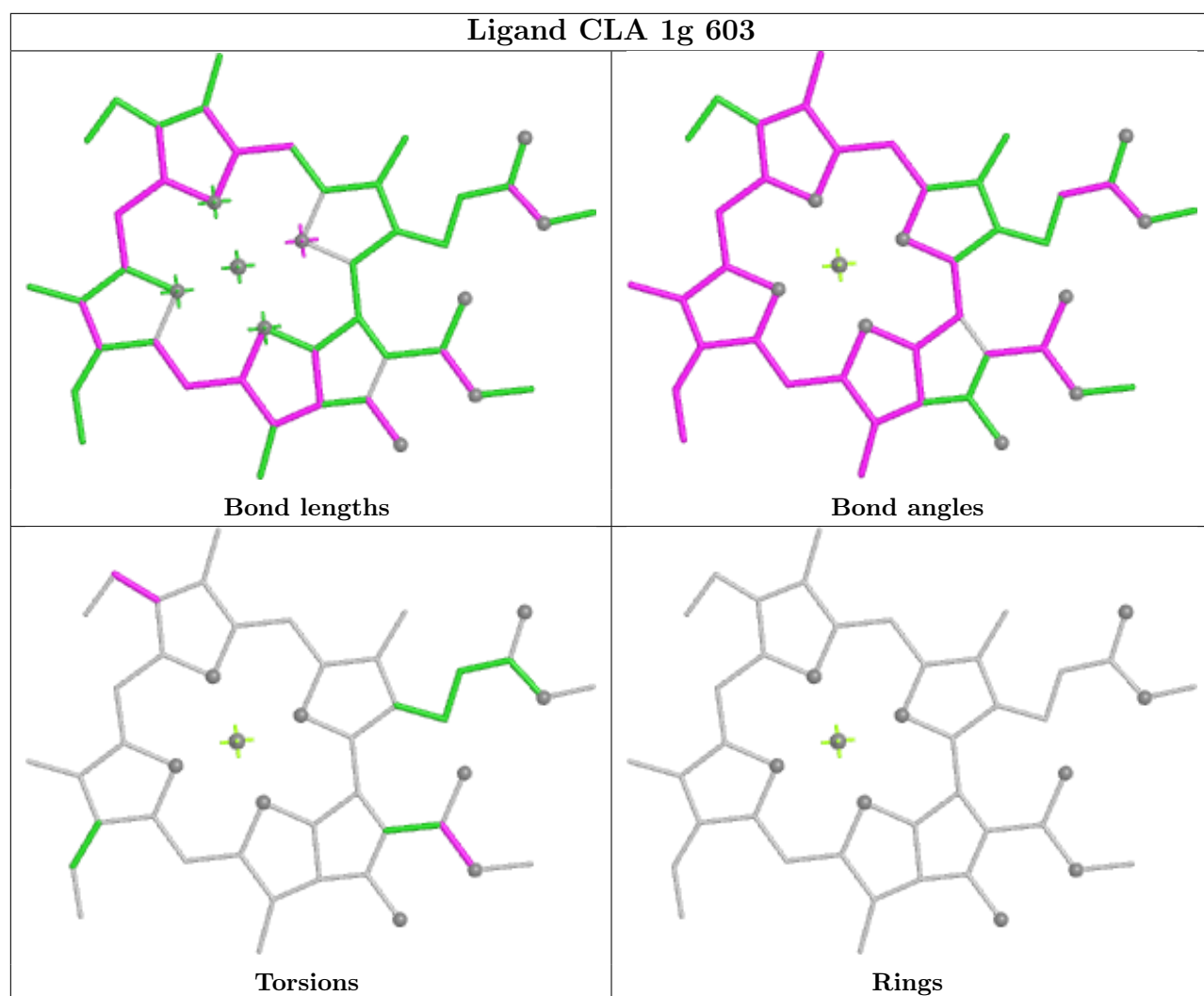


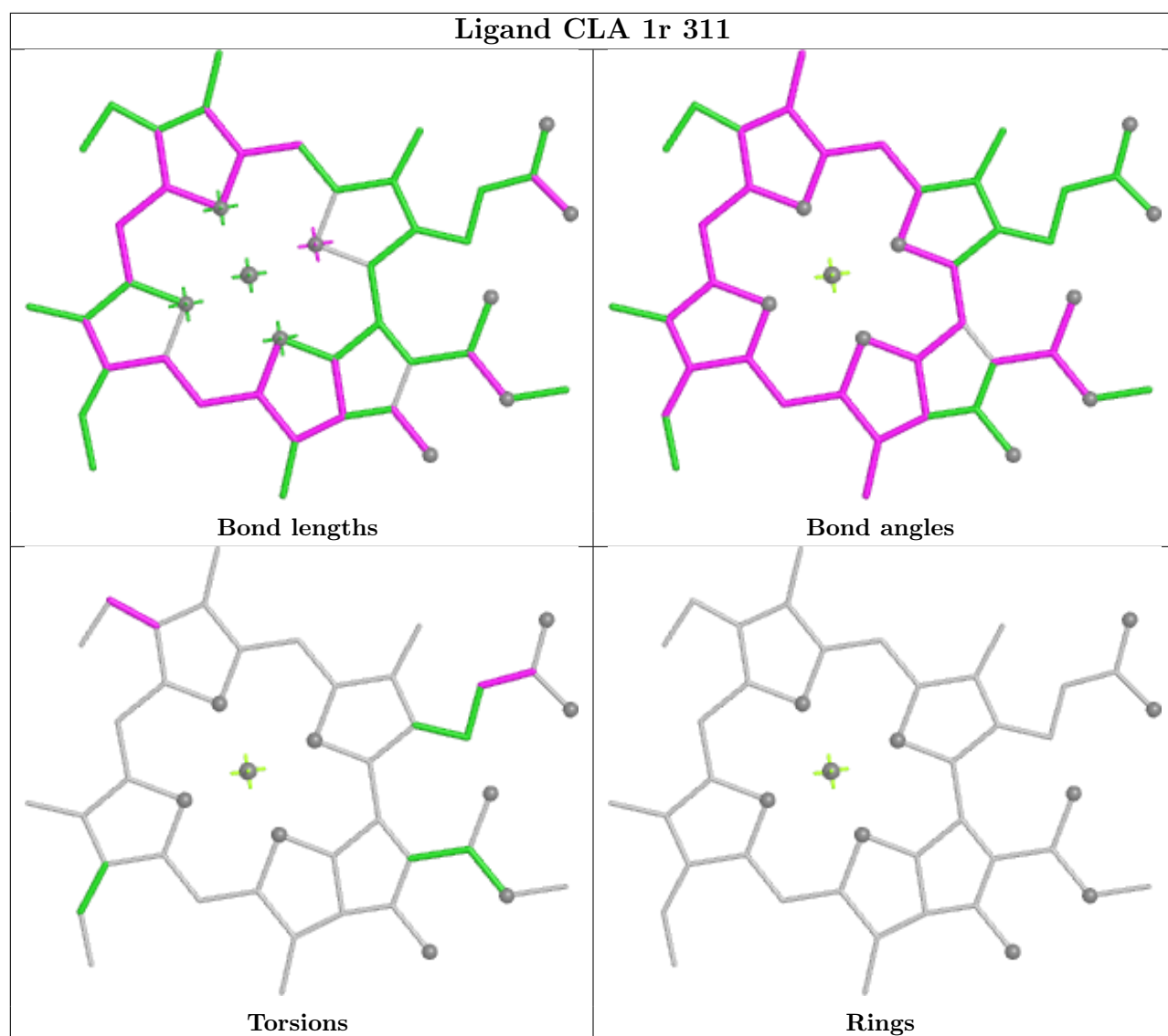


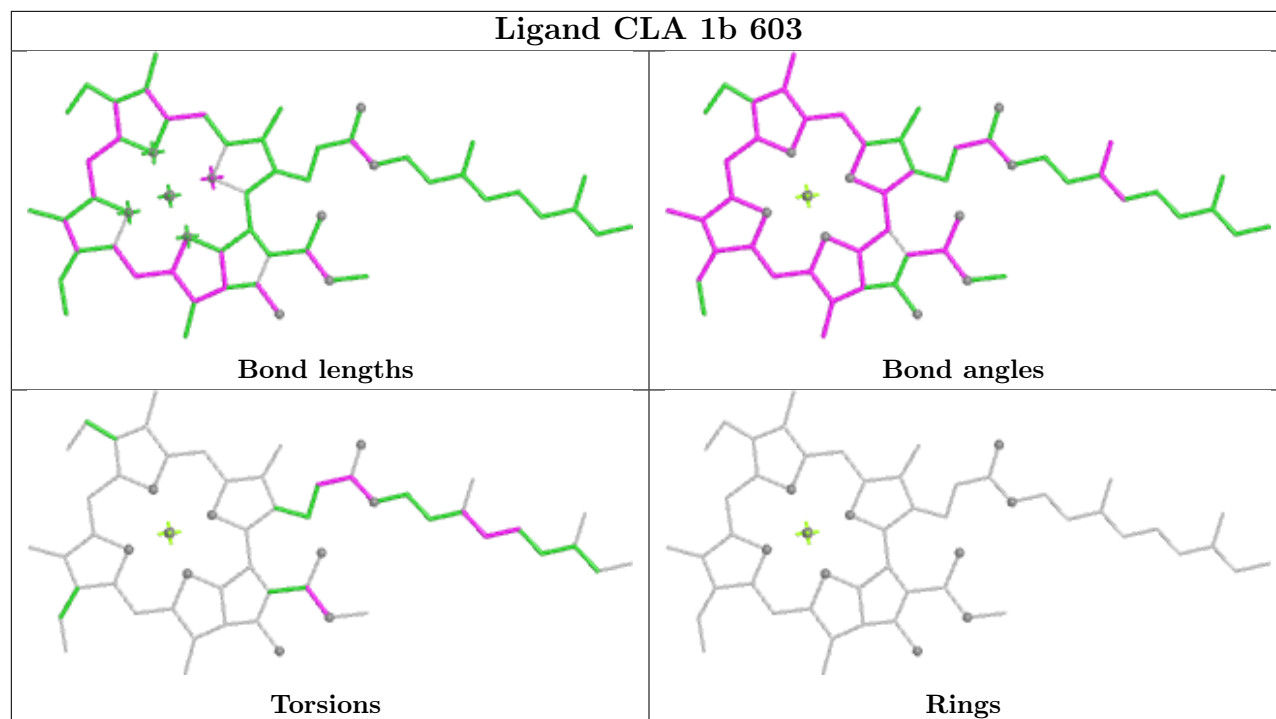


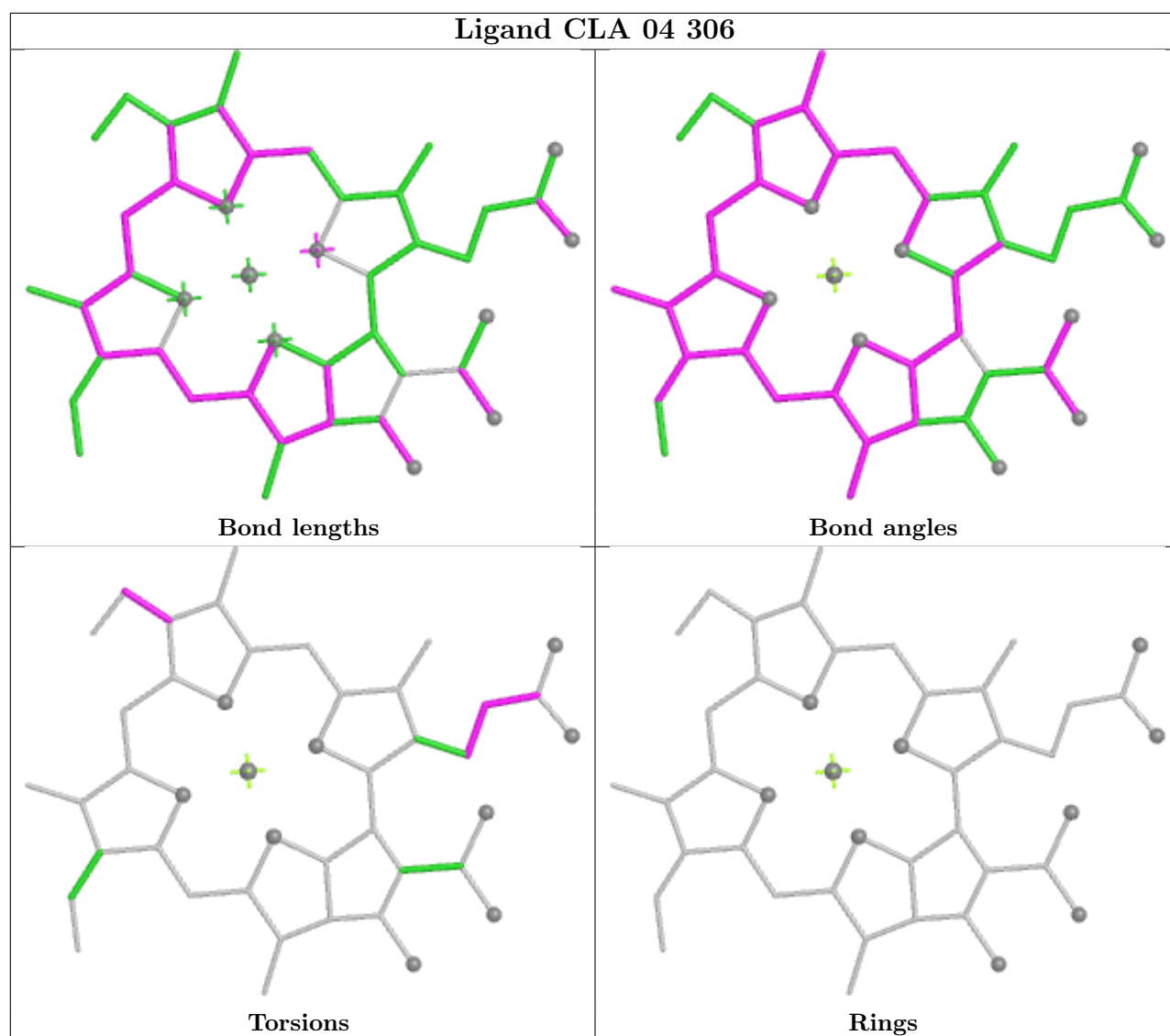


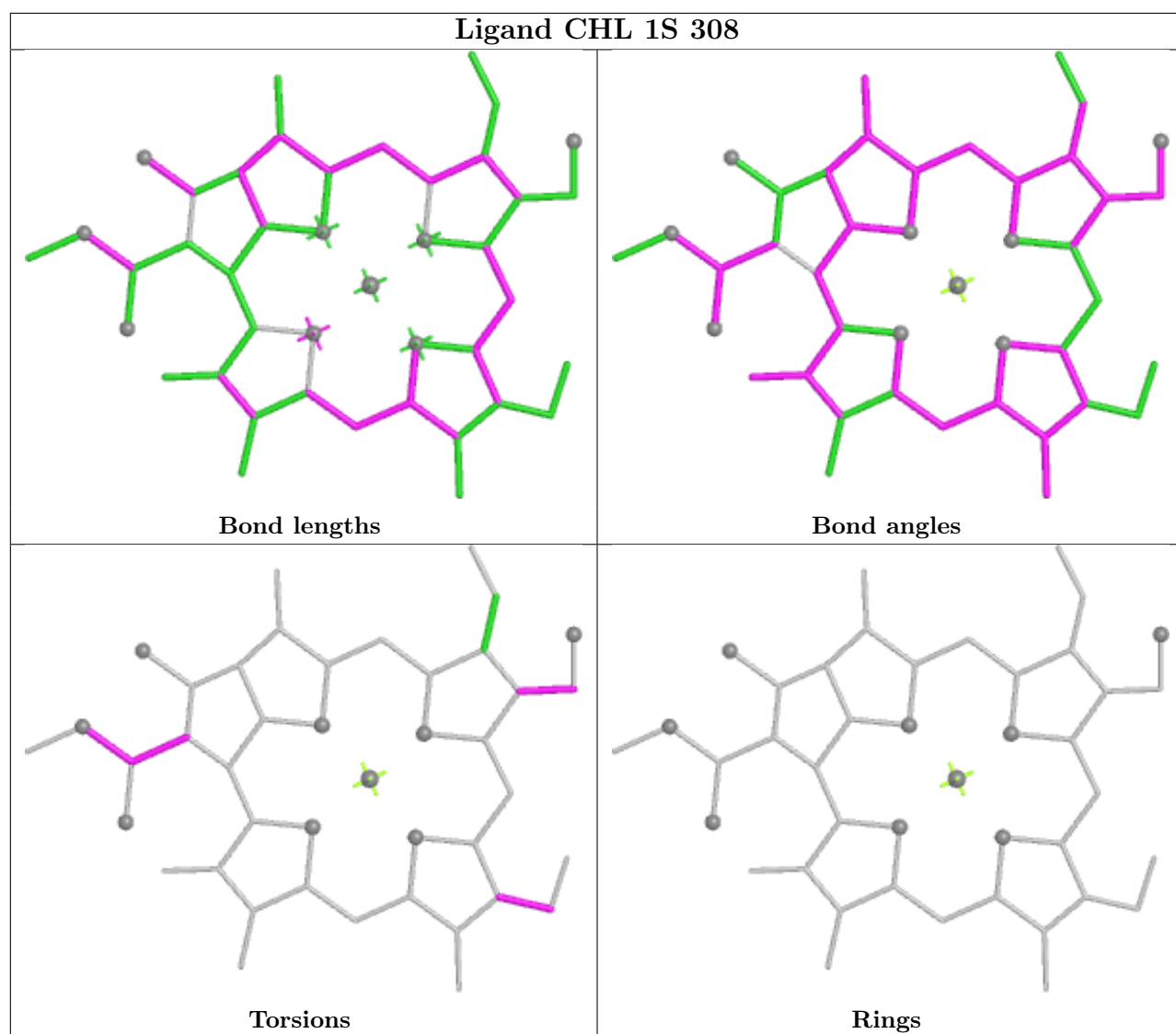


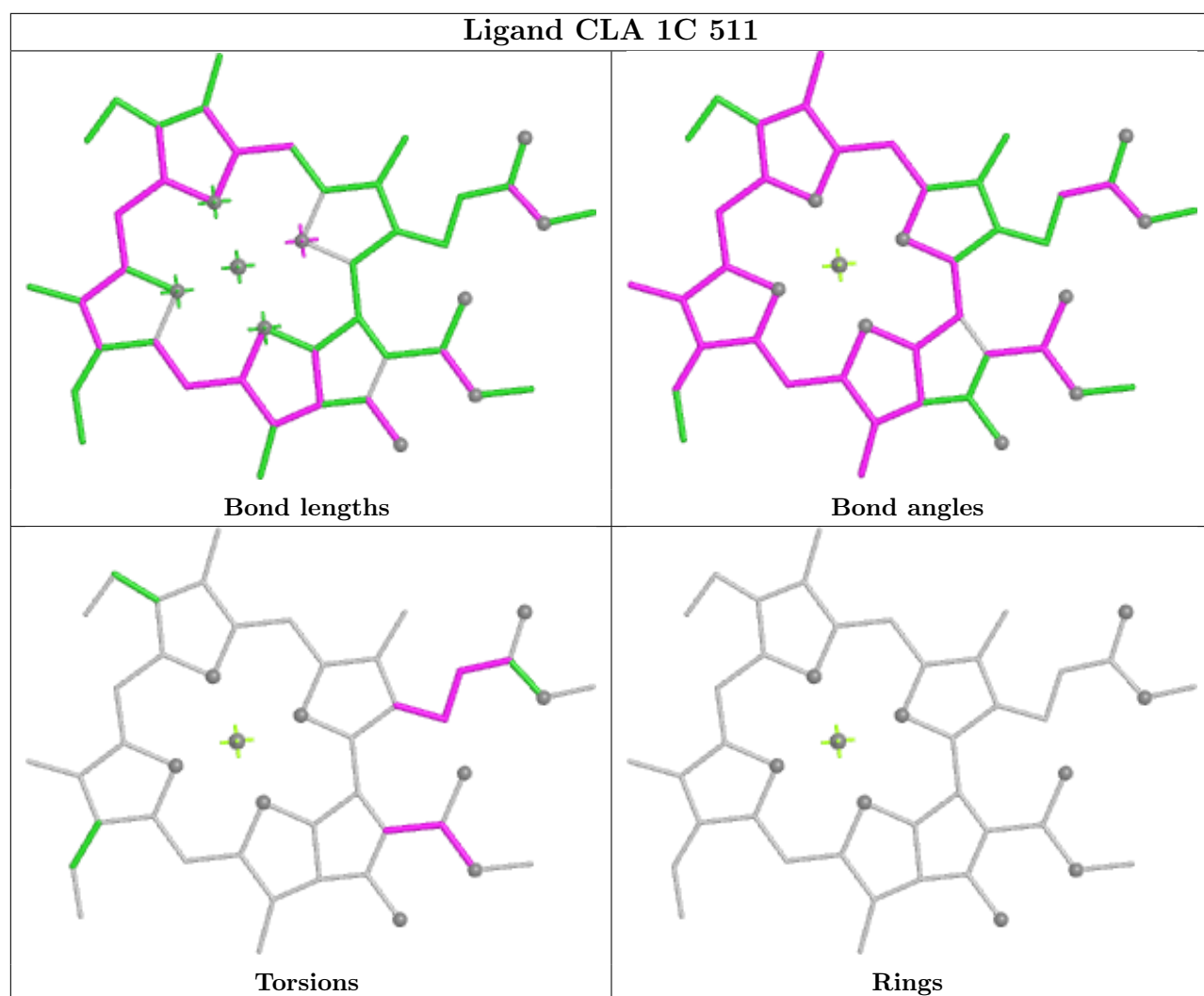


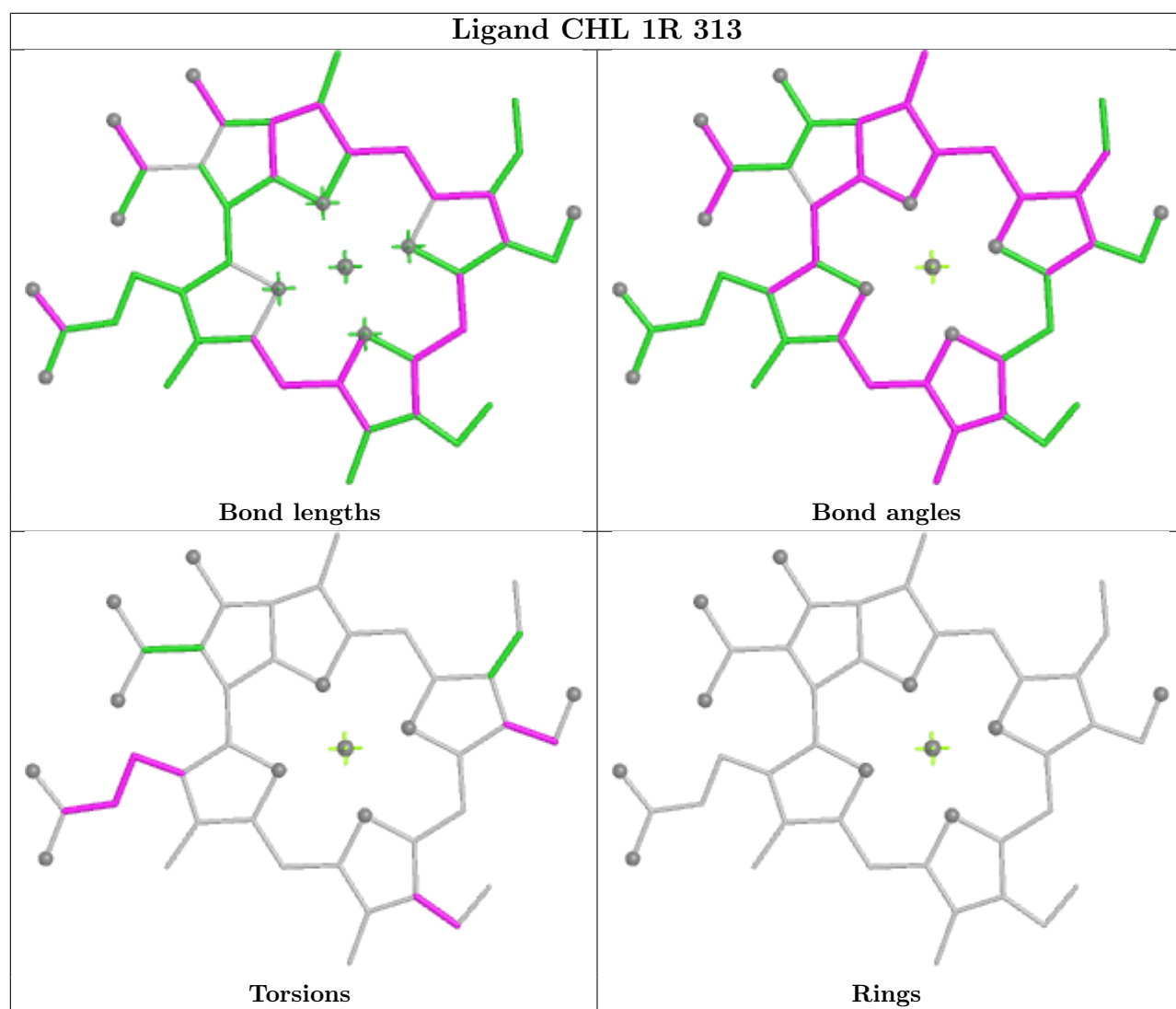


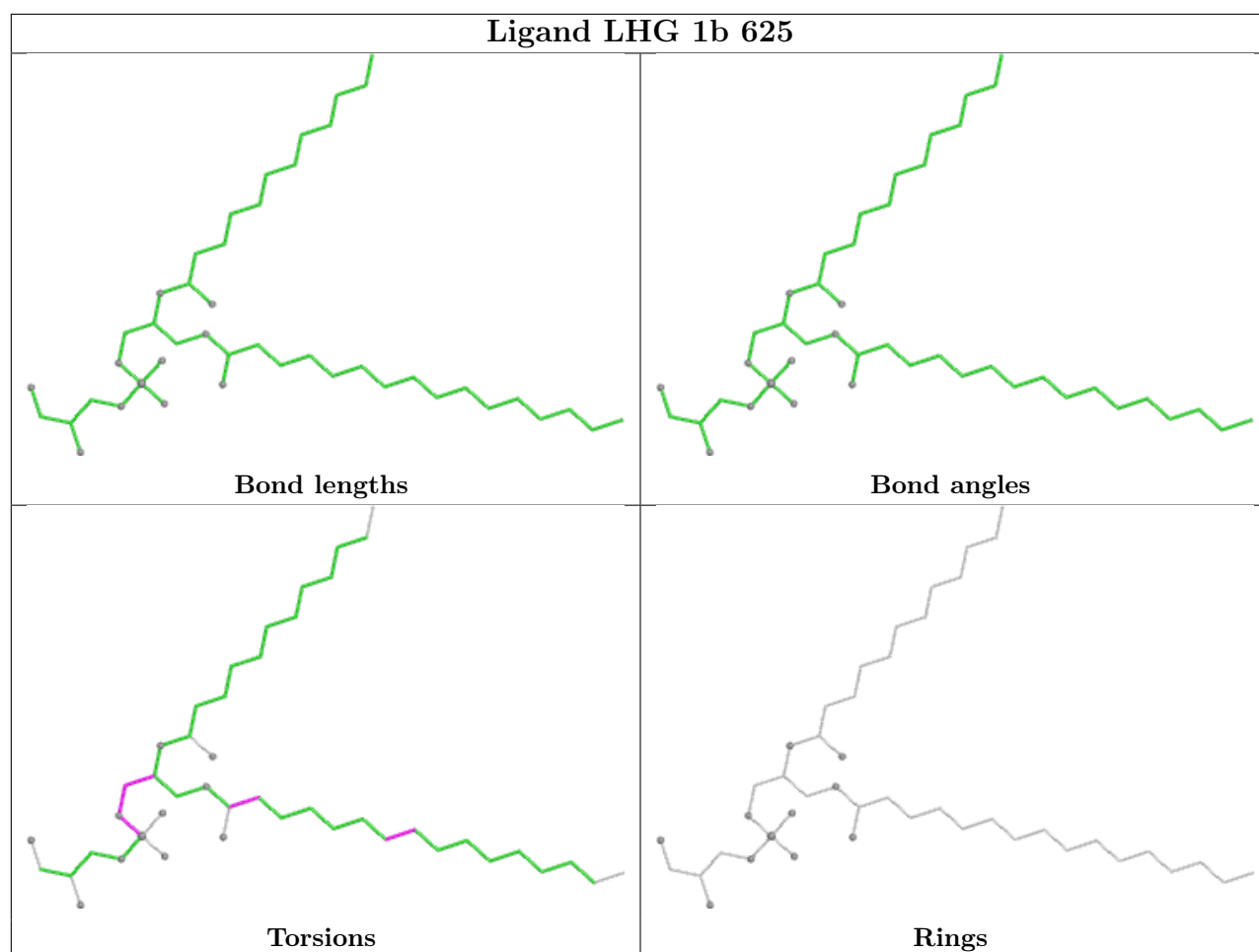


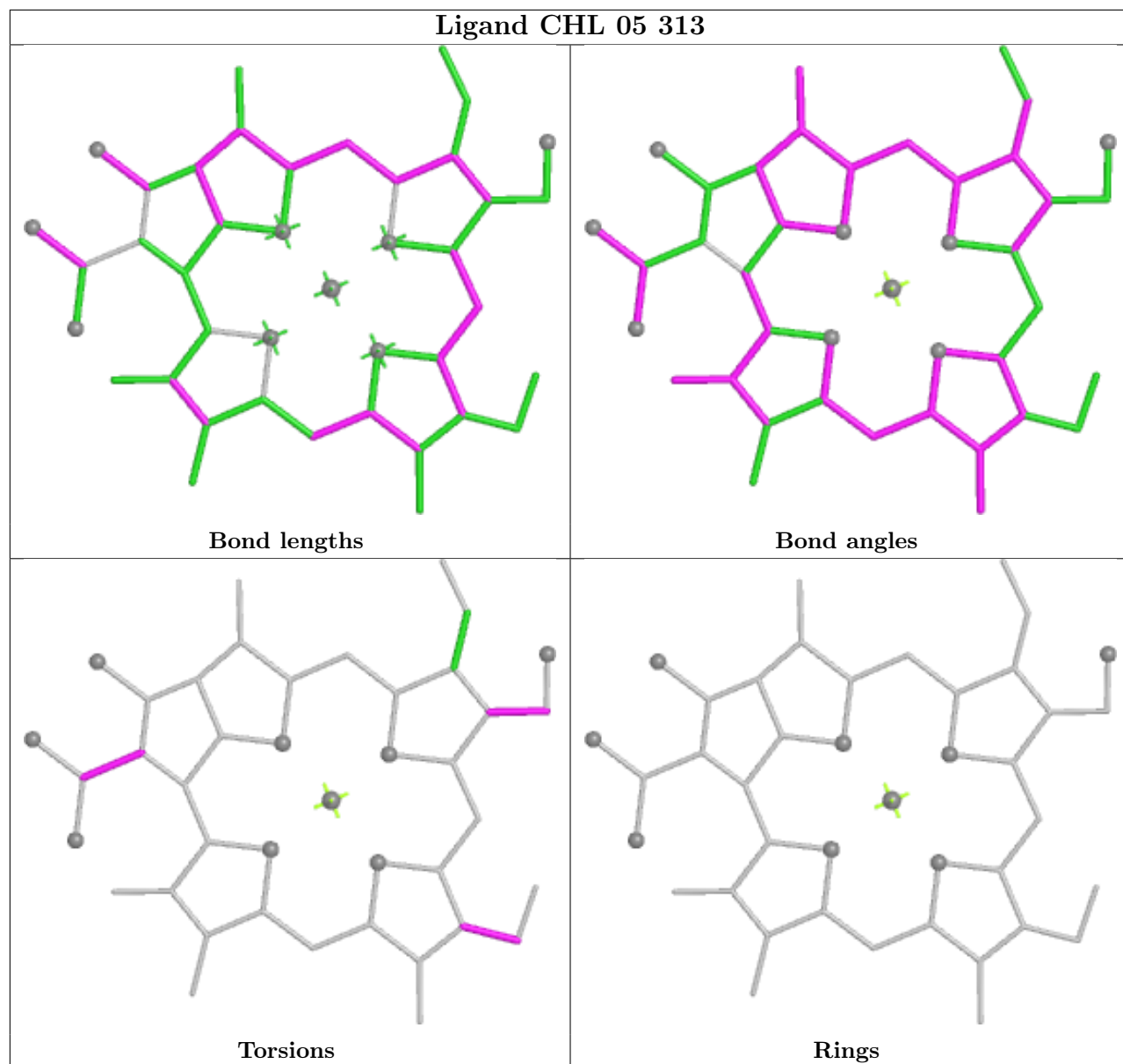


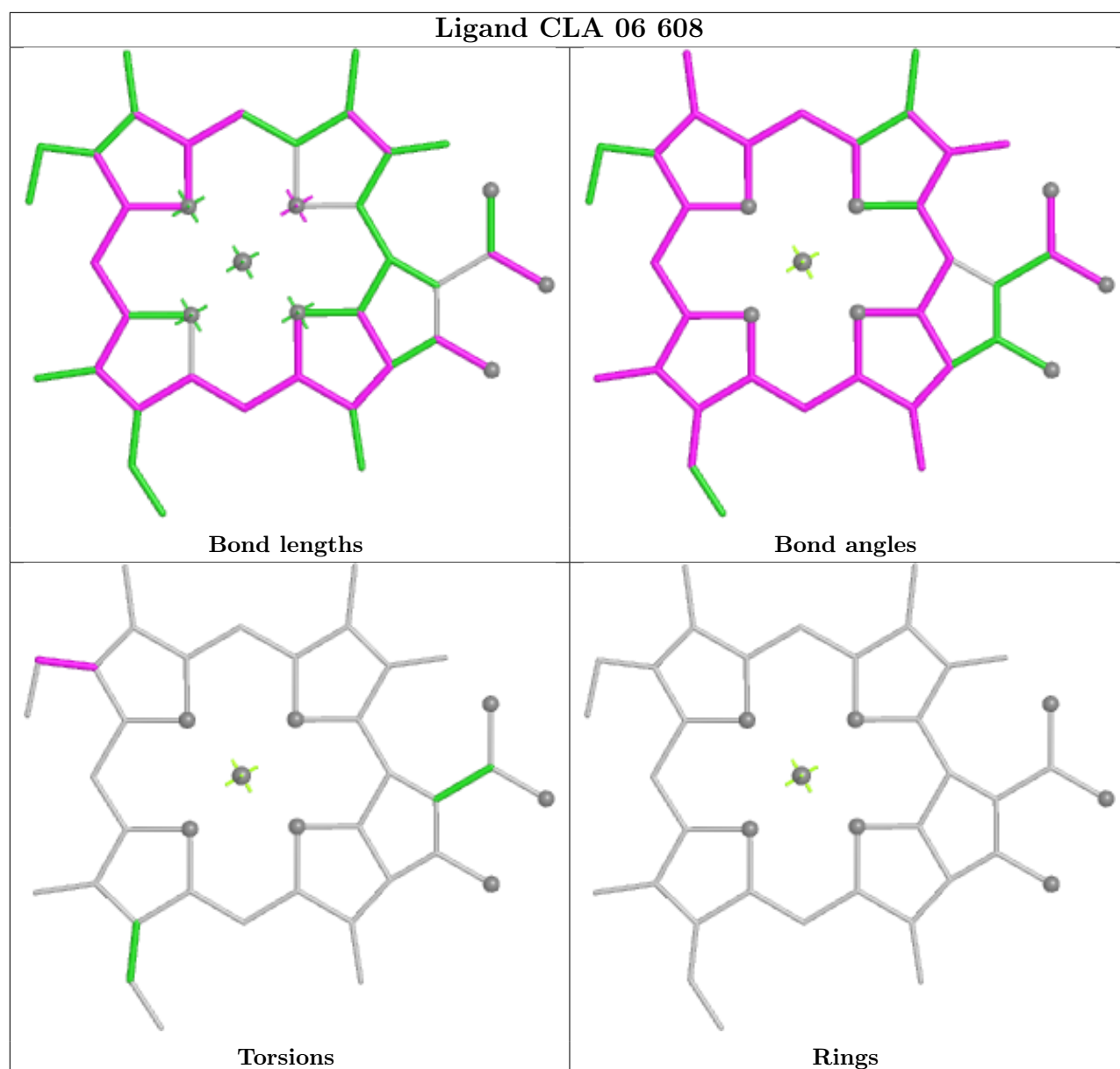


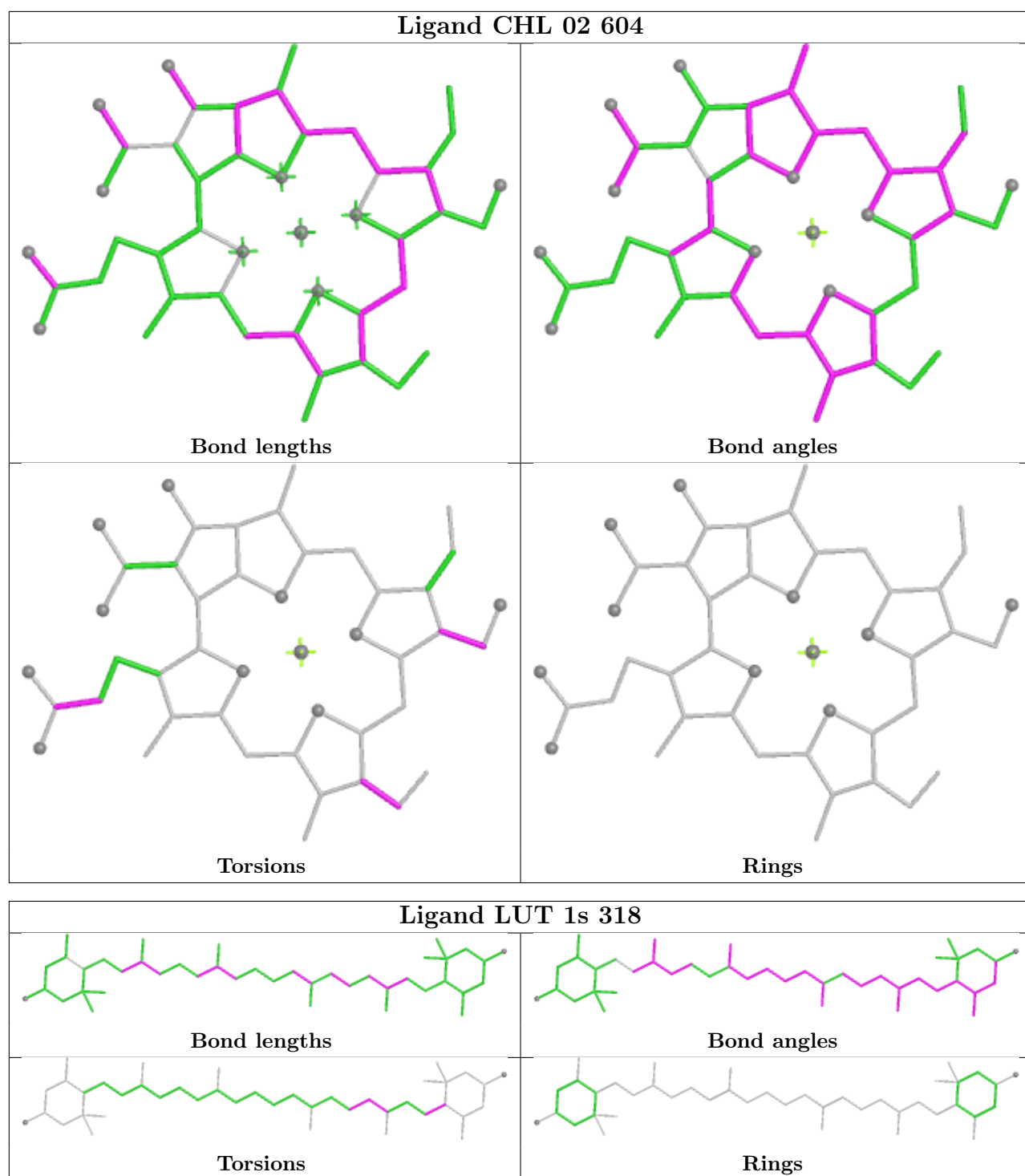


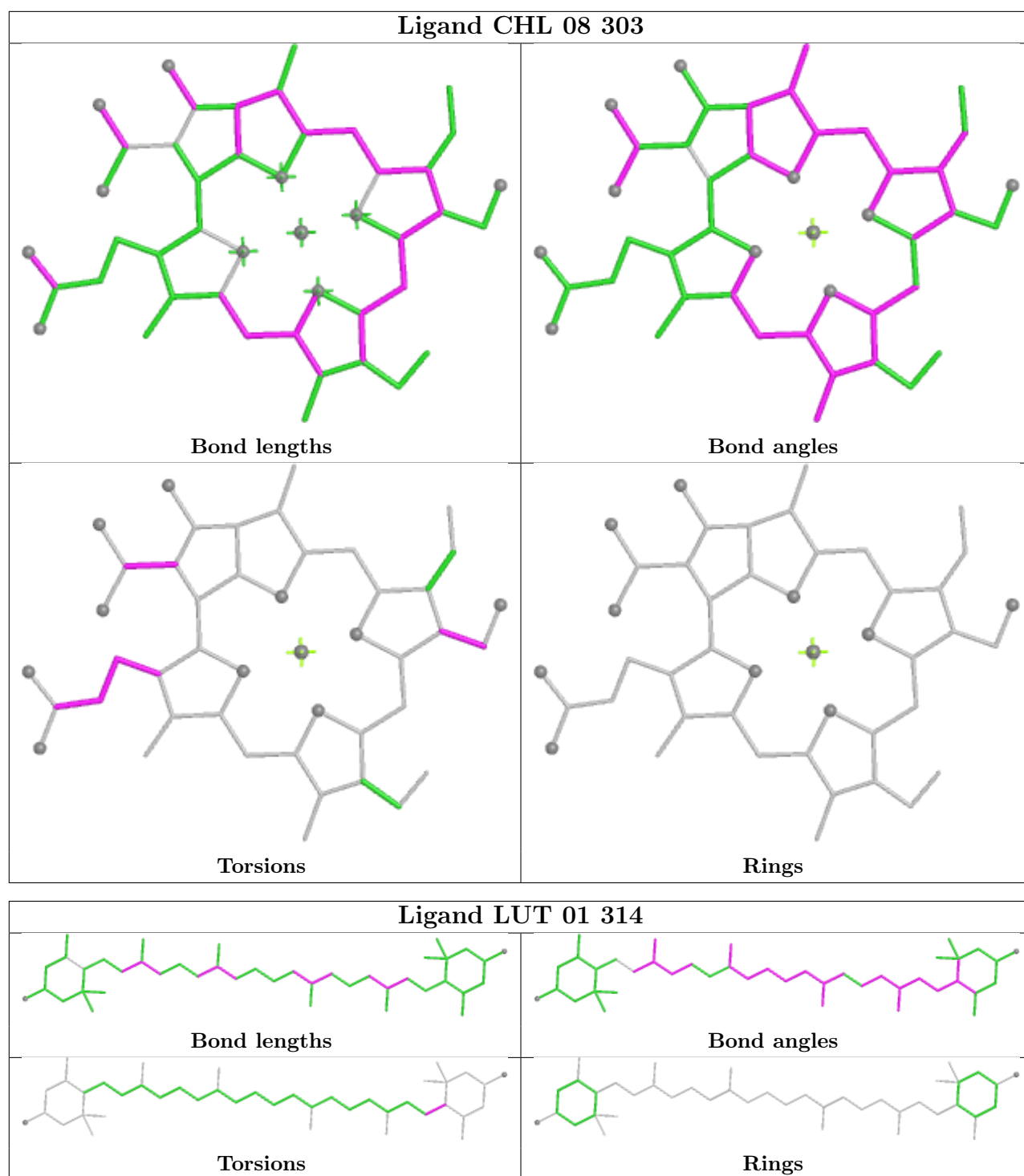


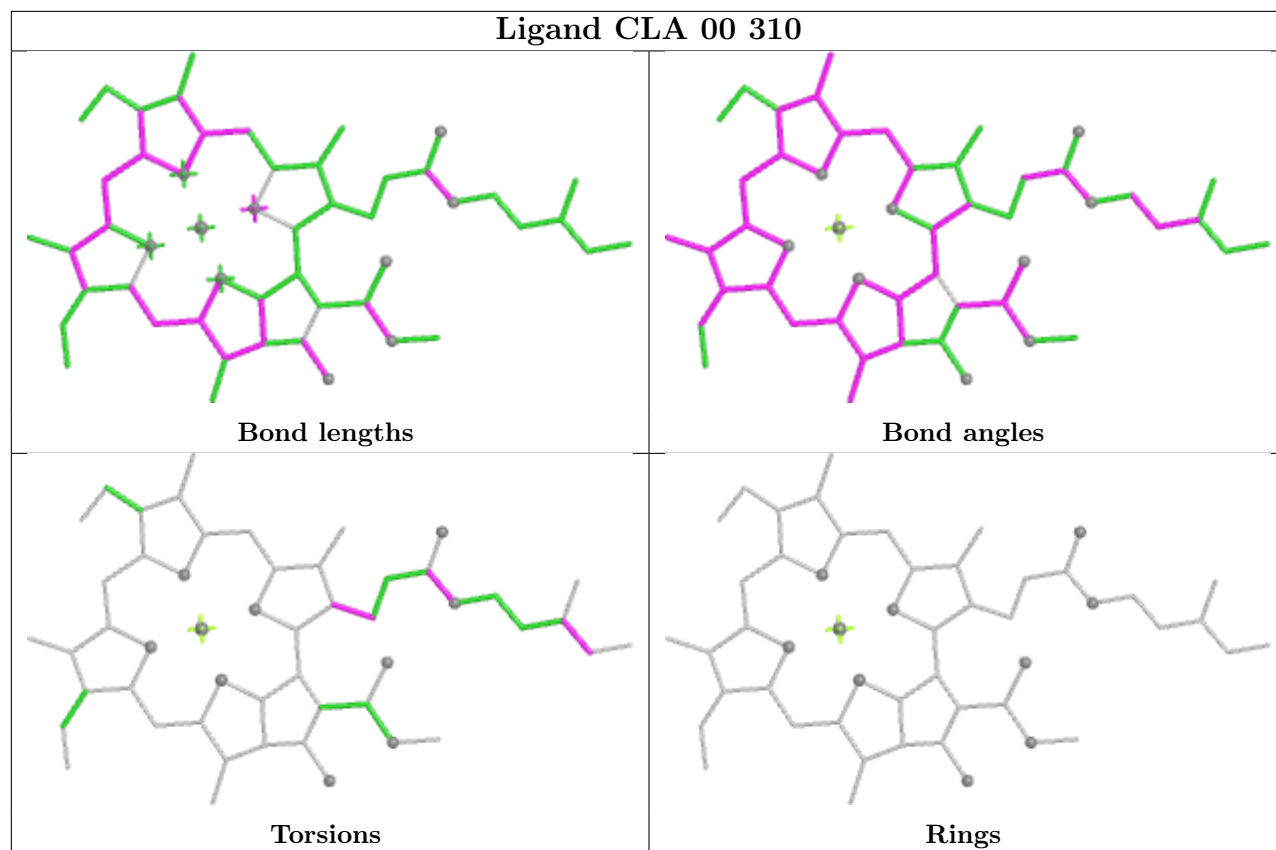


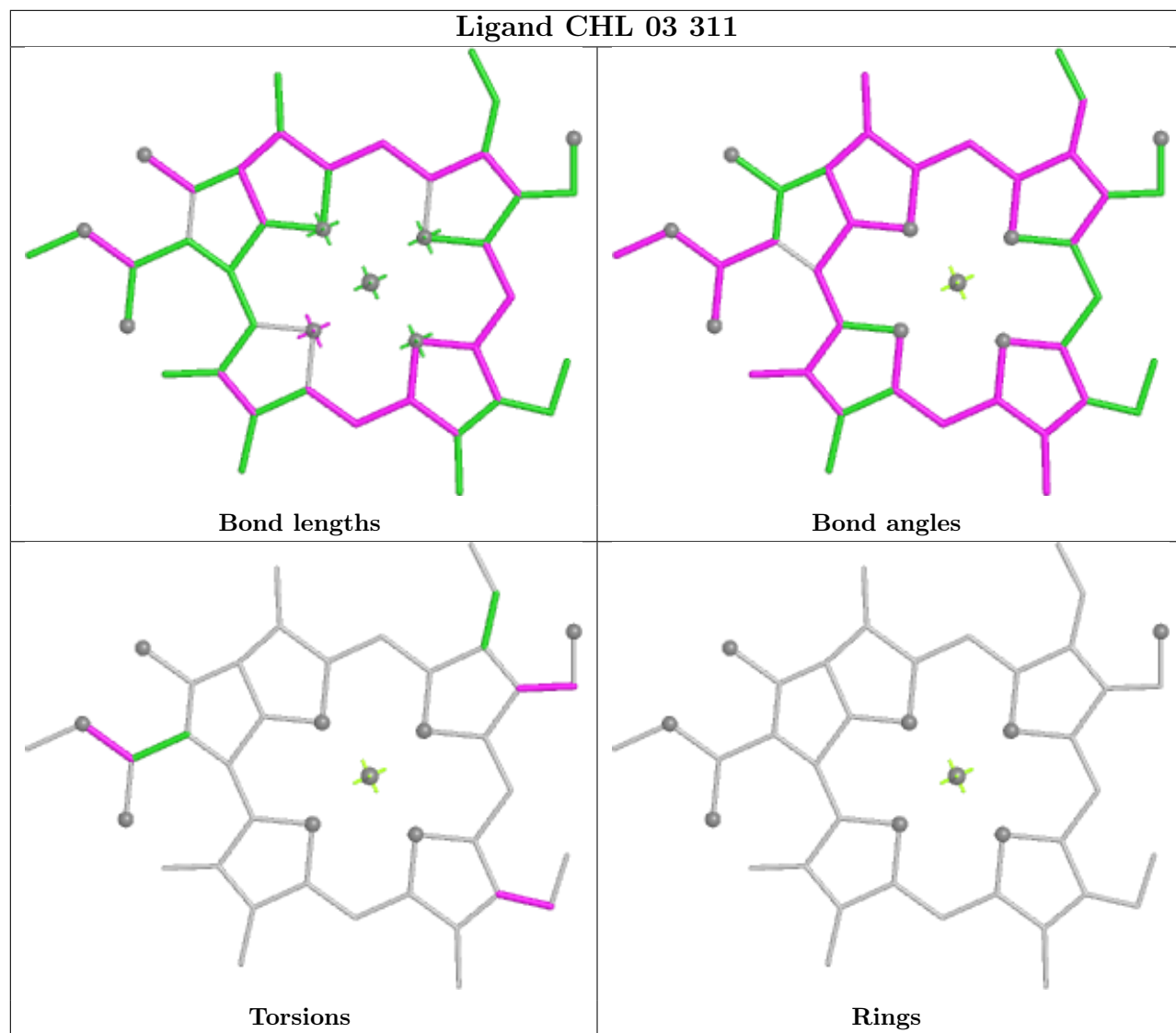


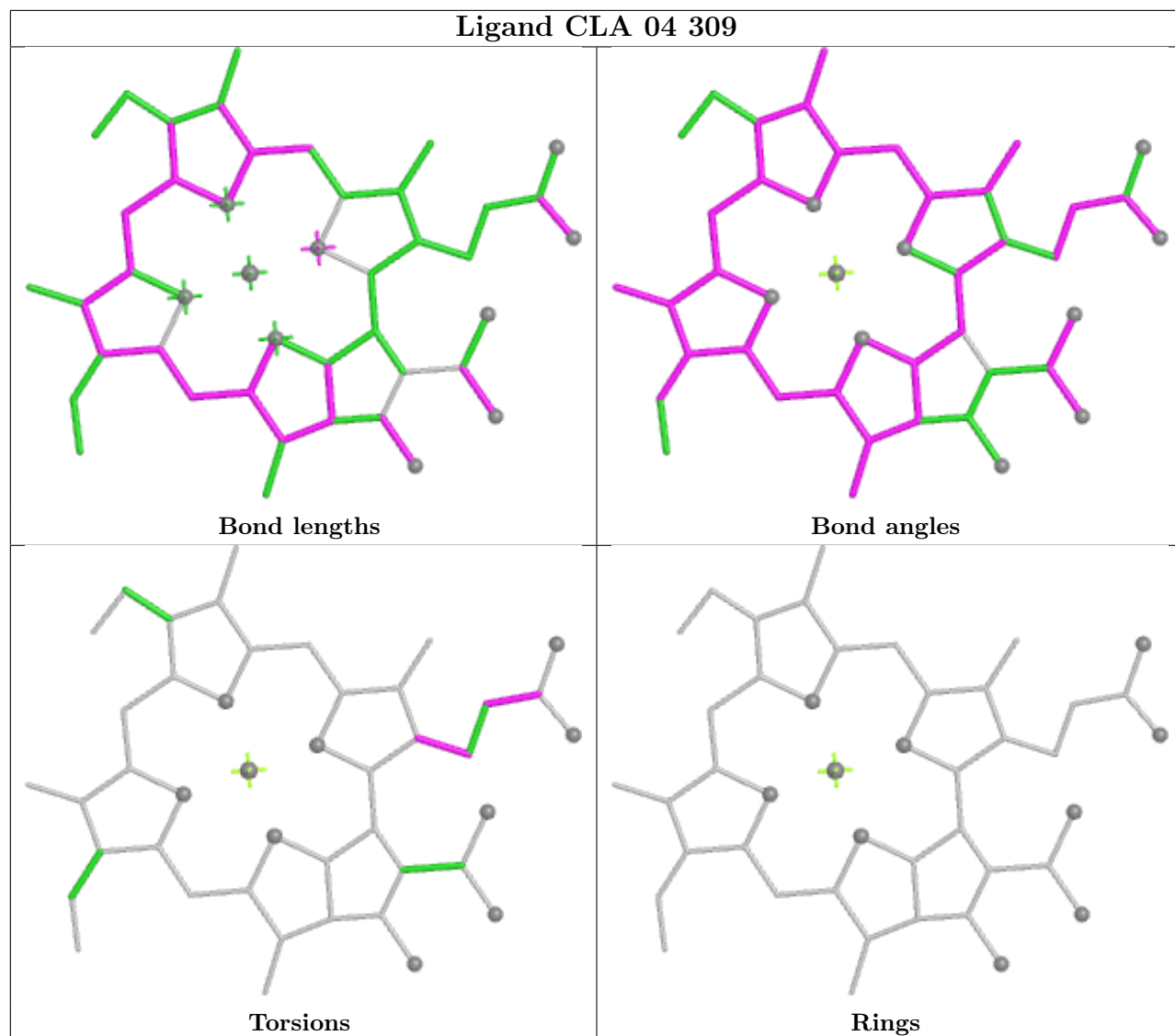


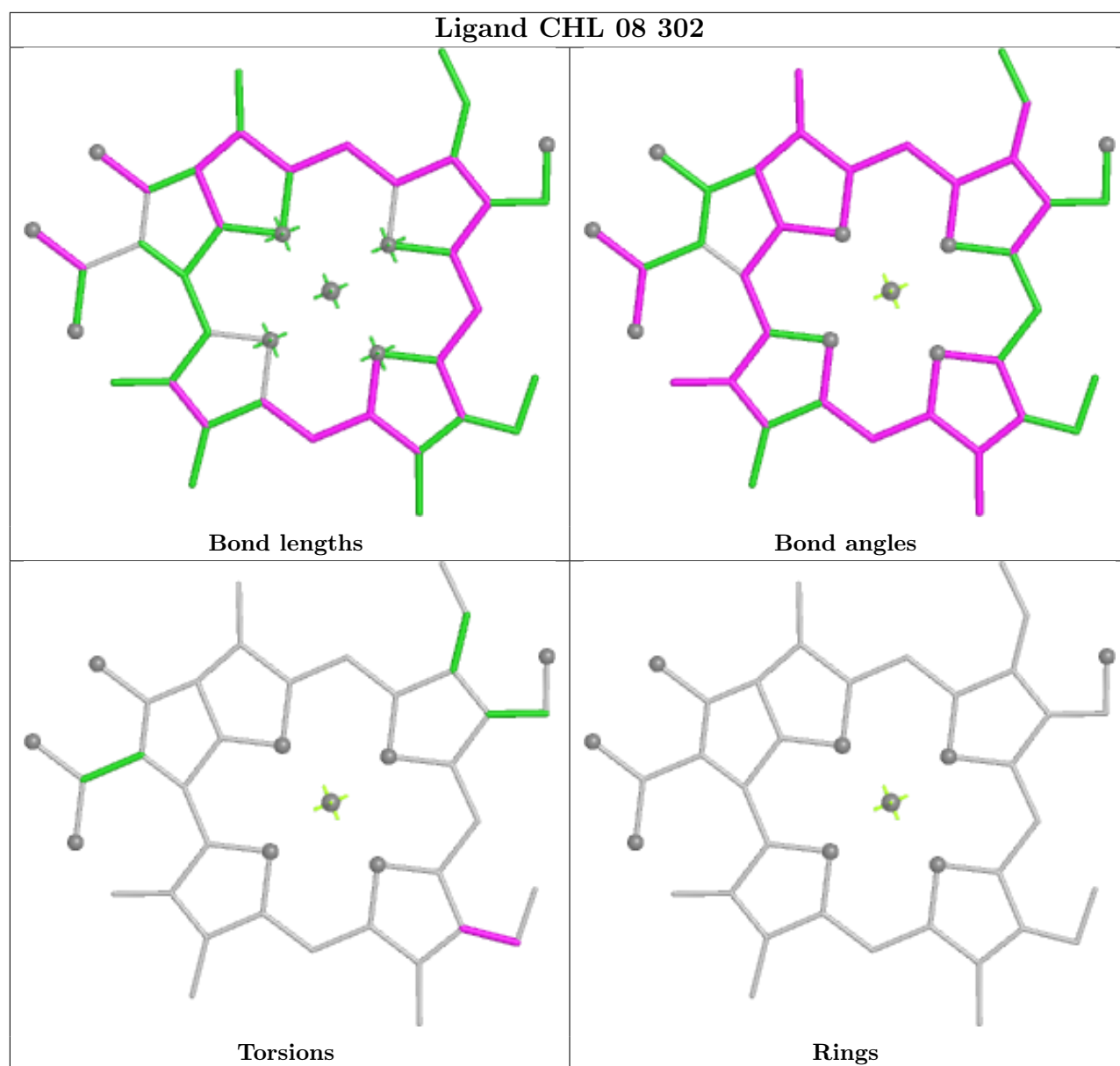


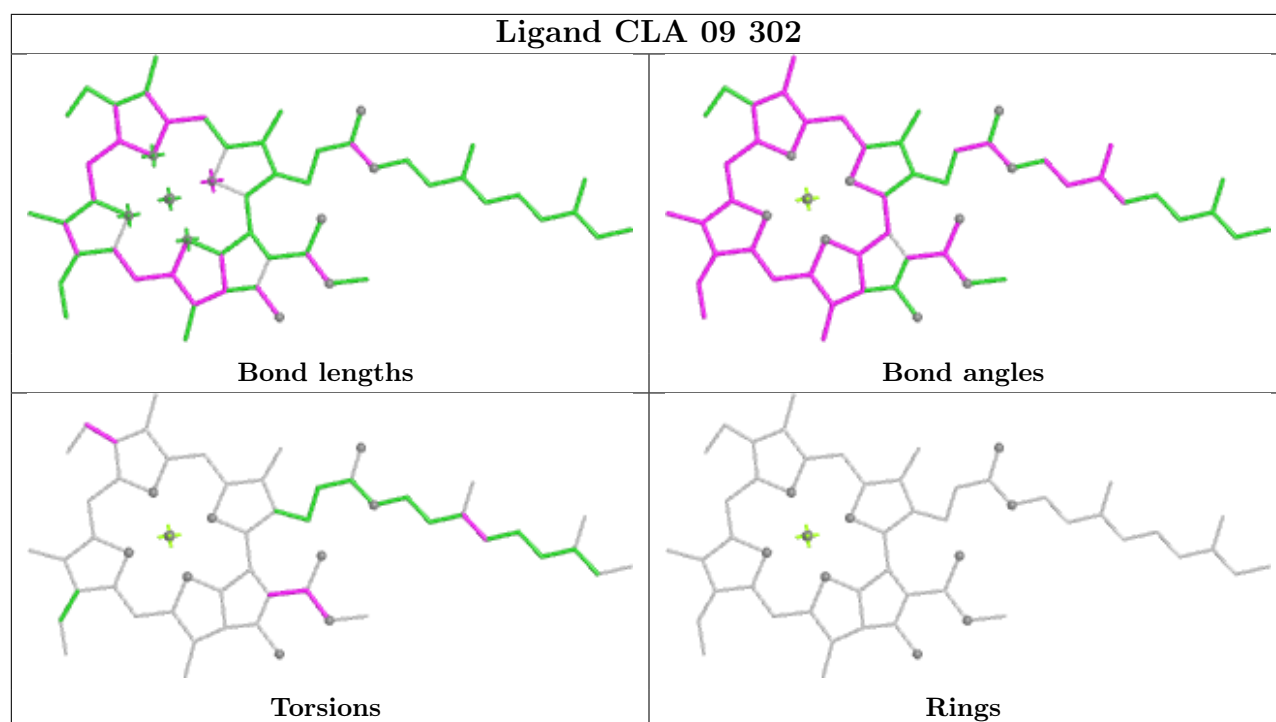


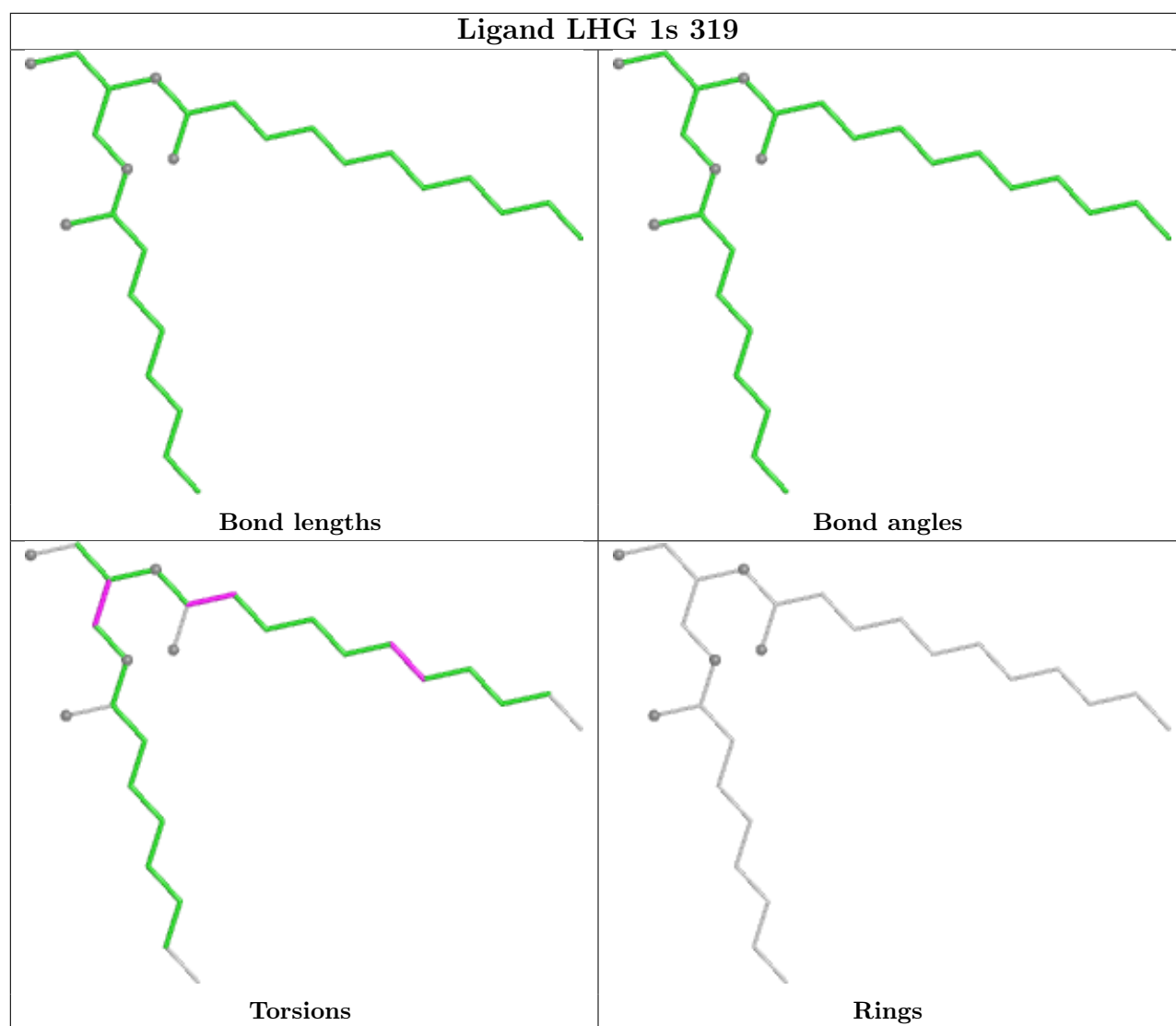


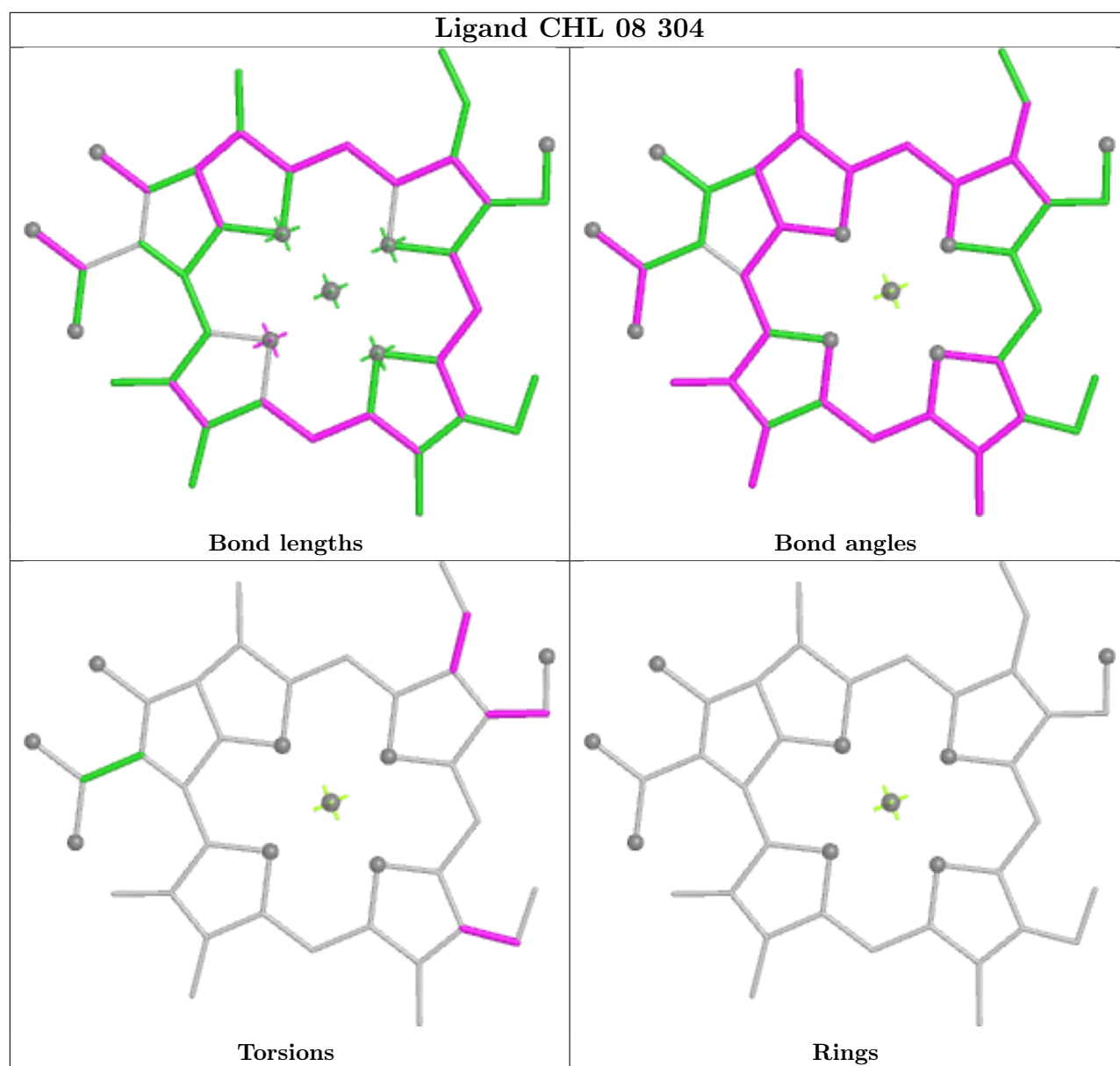


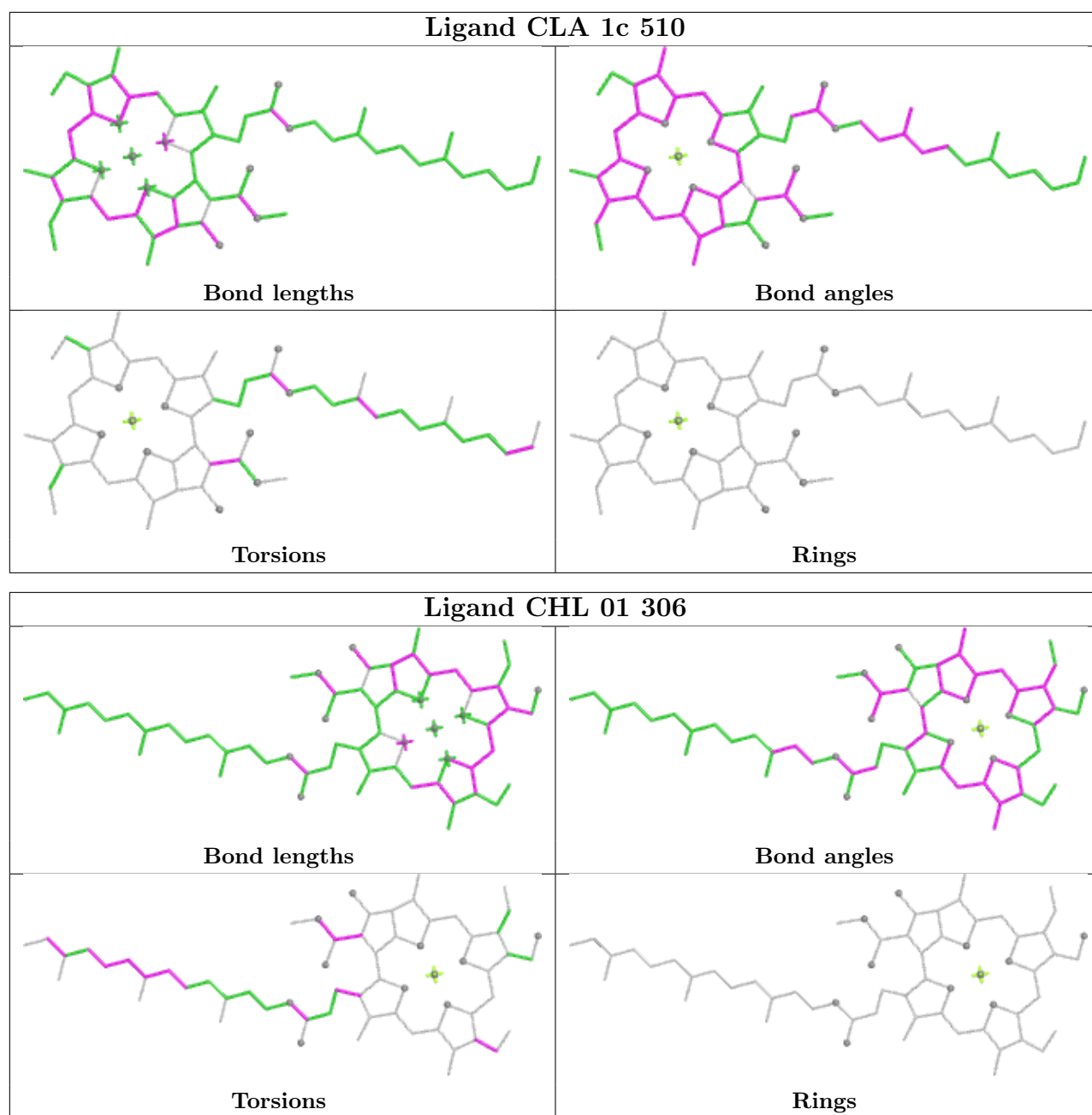


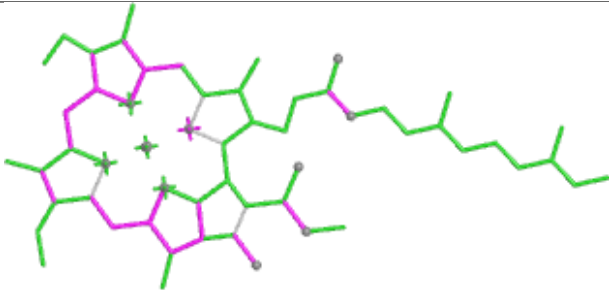
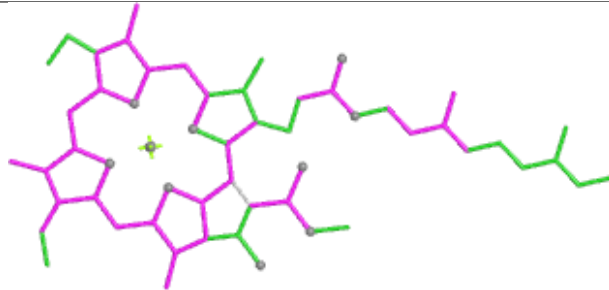
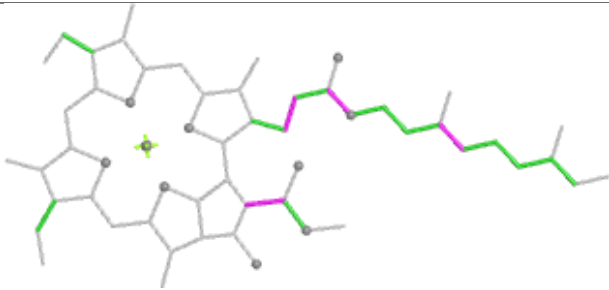
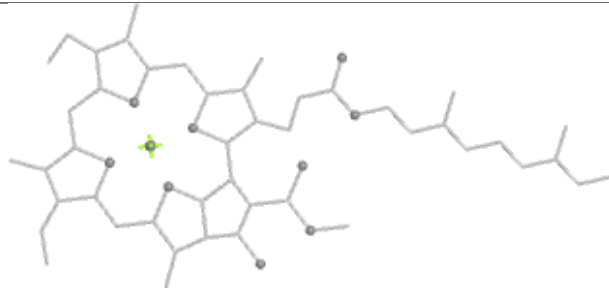
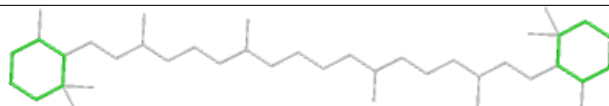


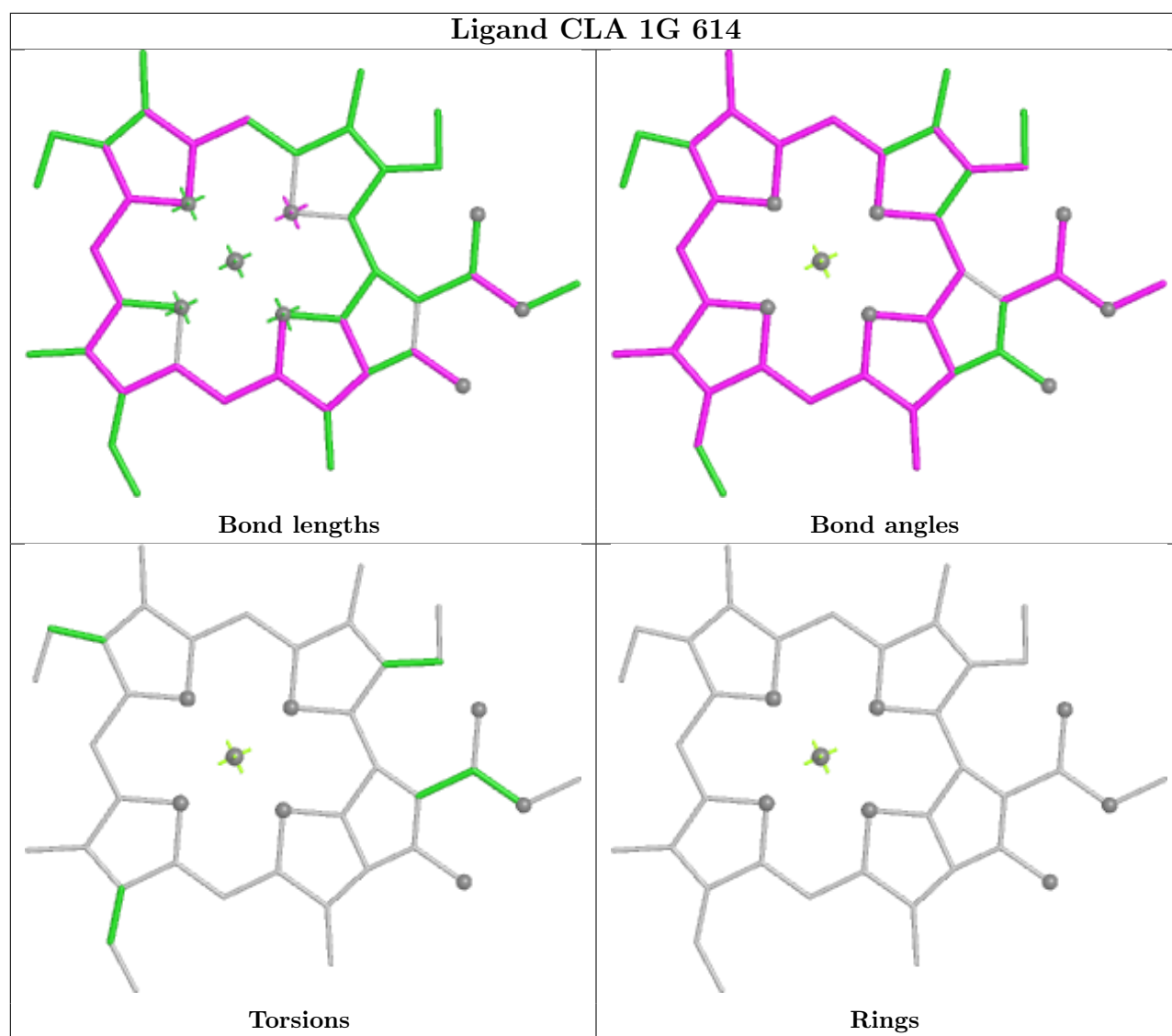


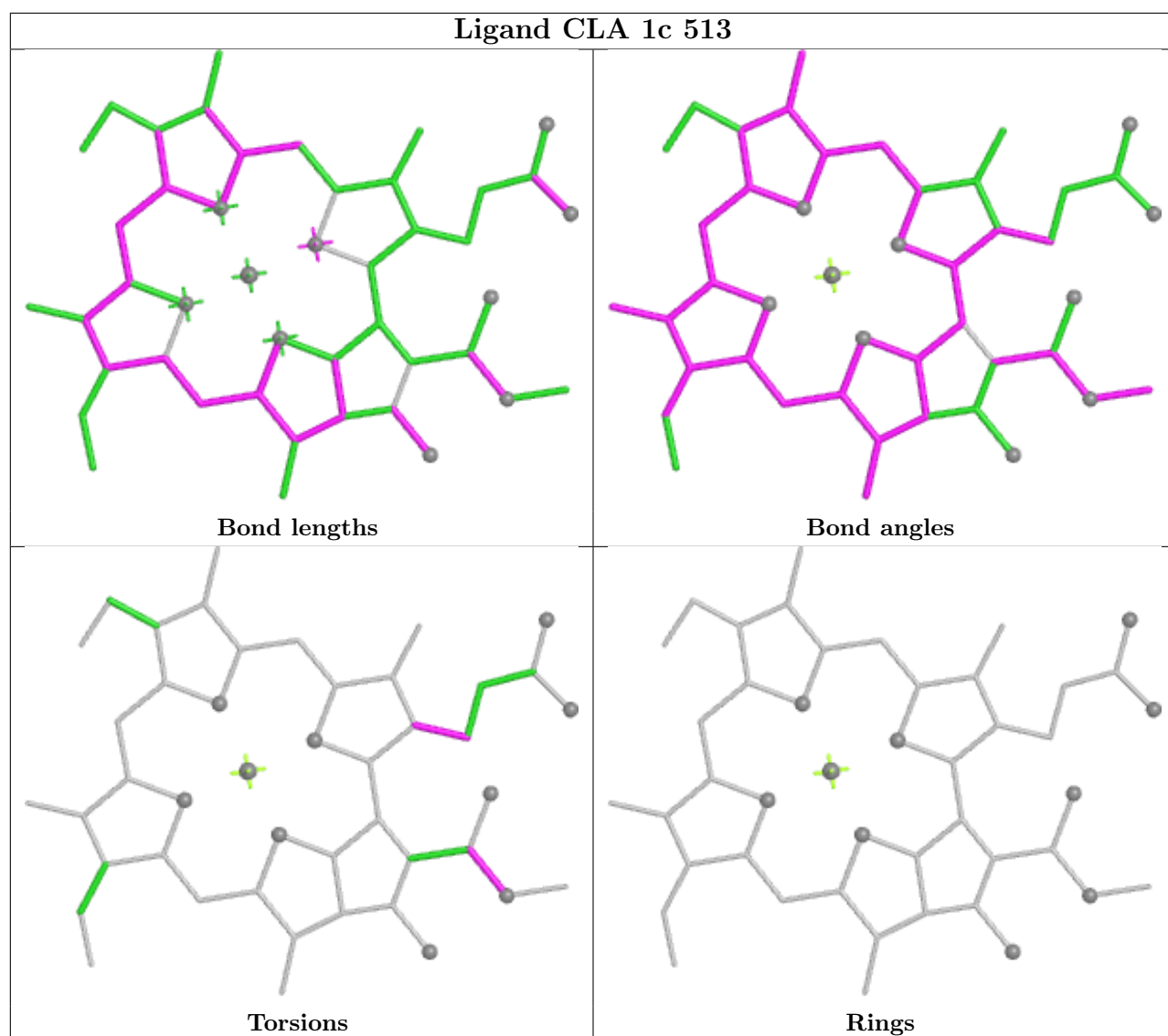


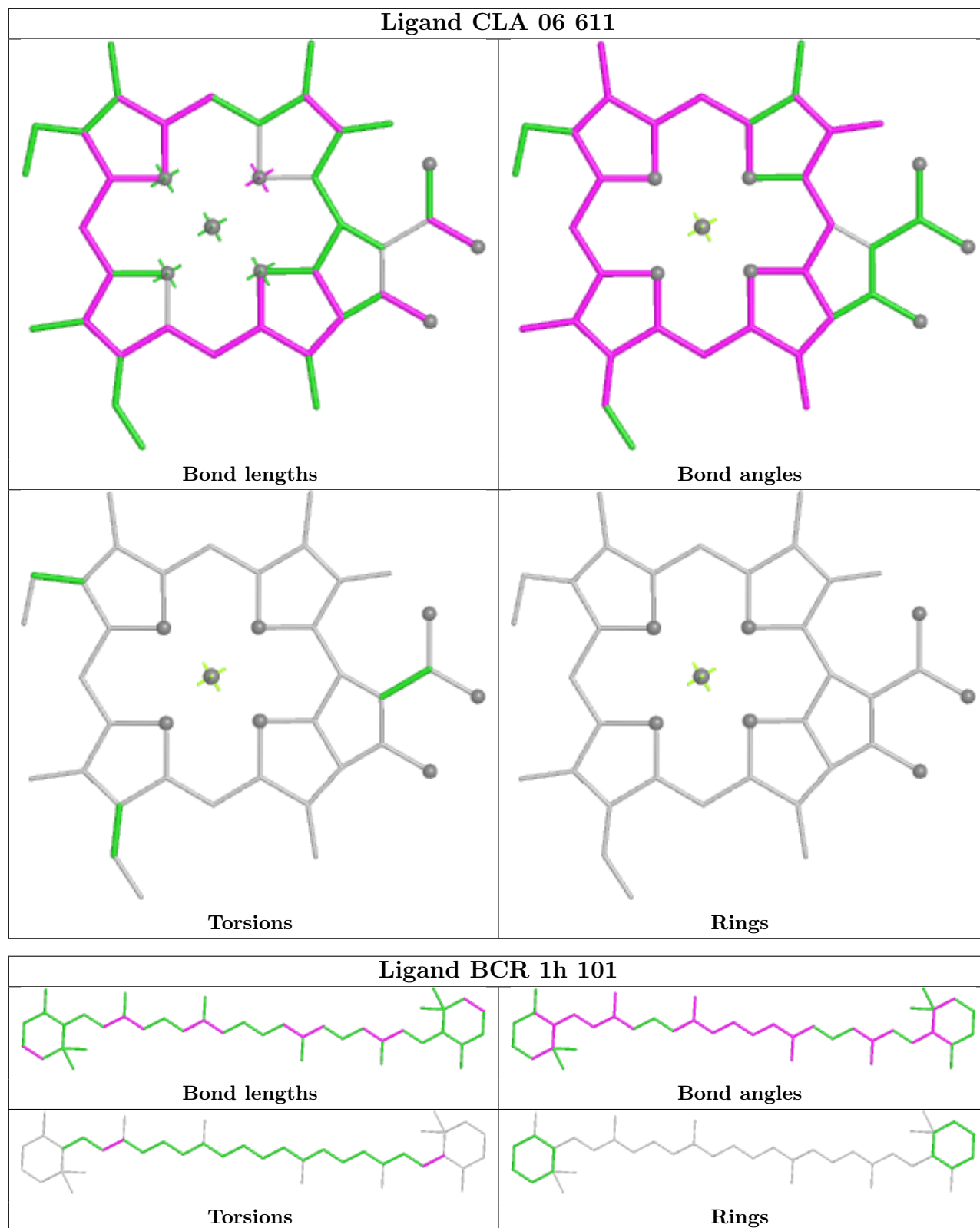


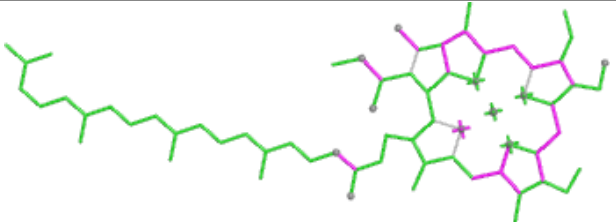
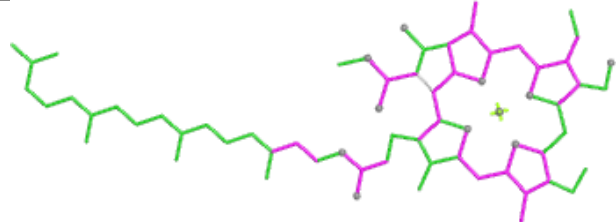
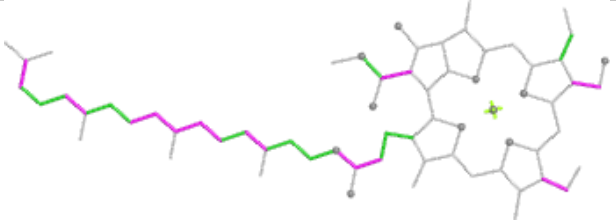
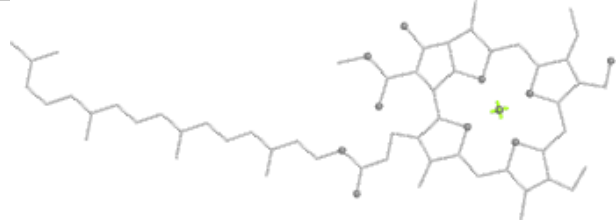
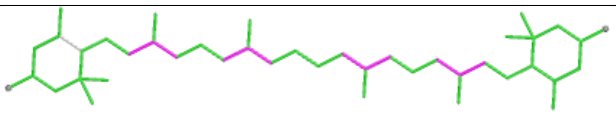
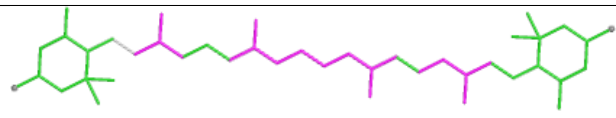
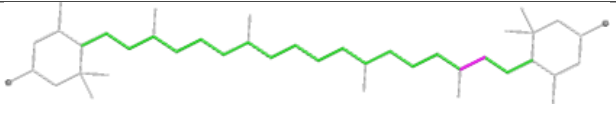
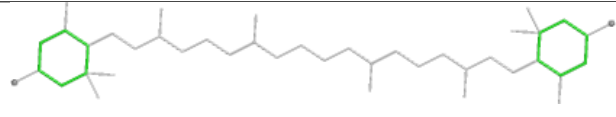


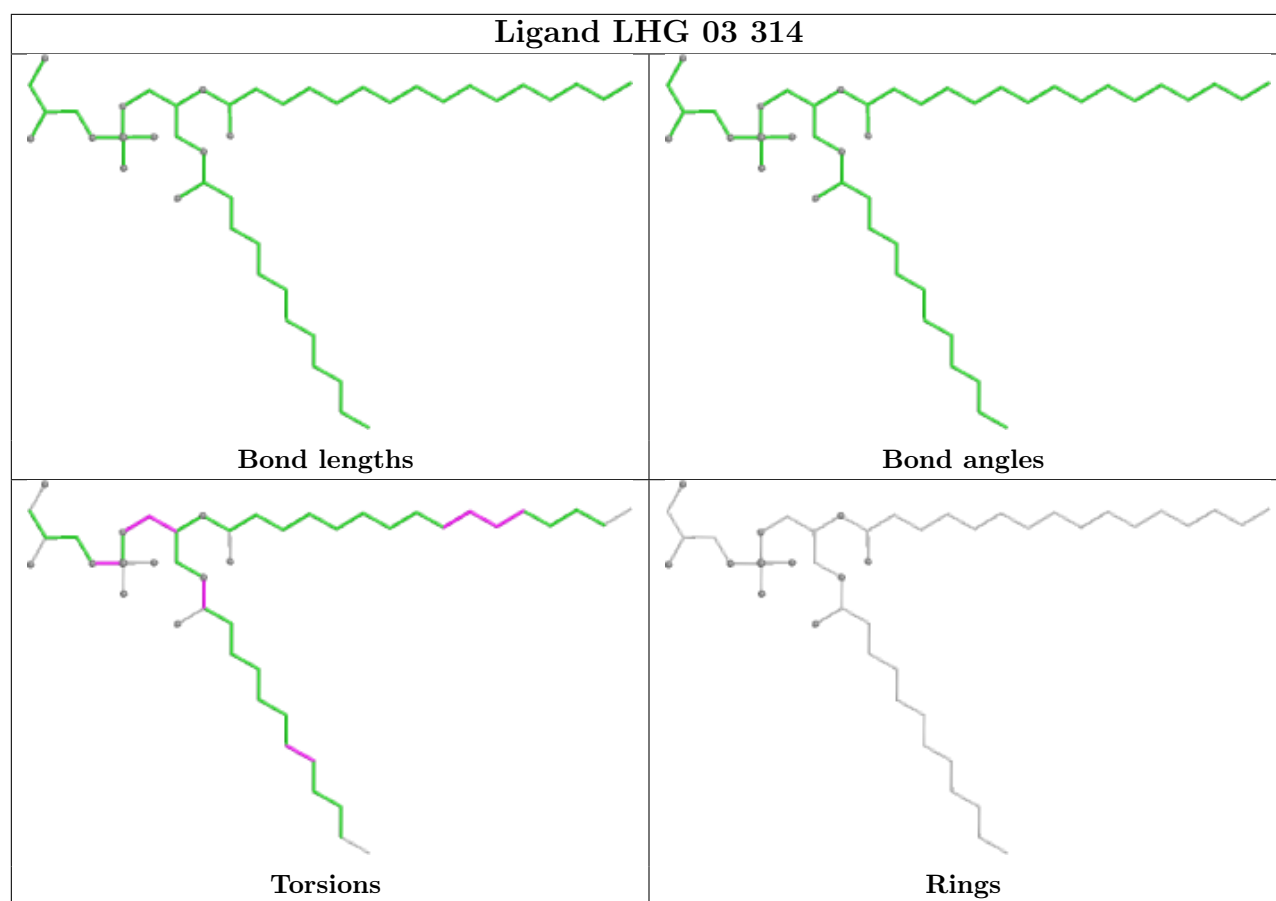
Ligand CLA 1B 604	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR 1J 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

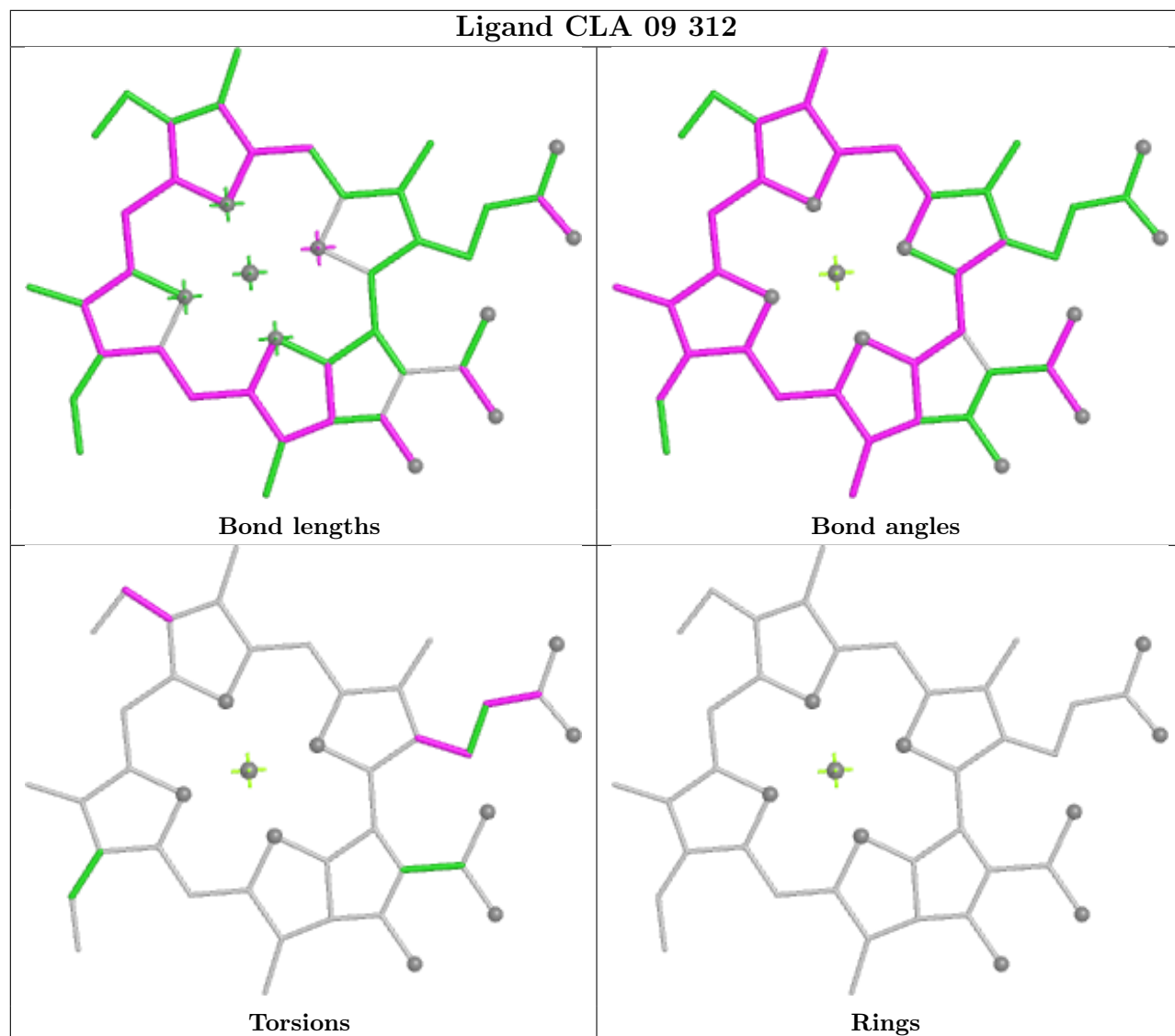


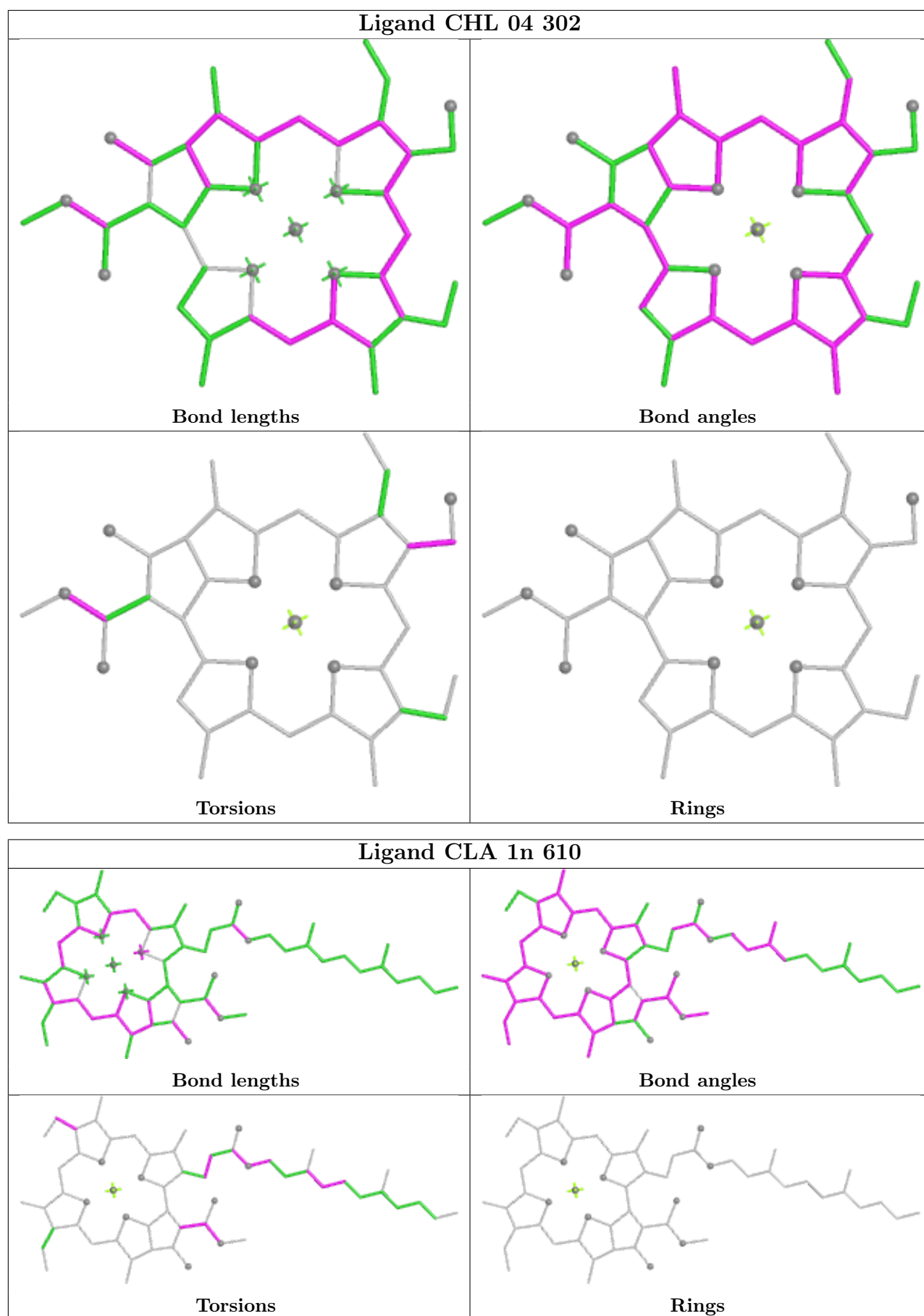


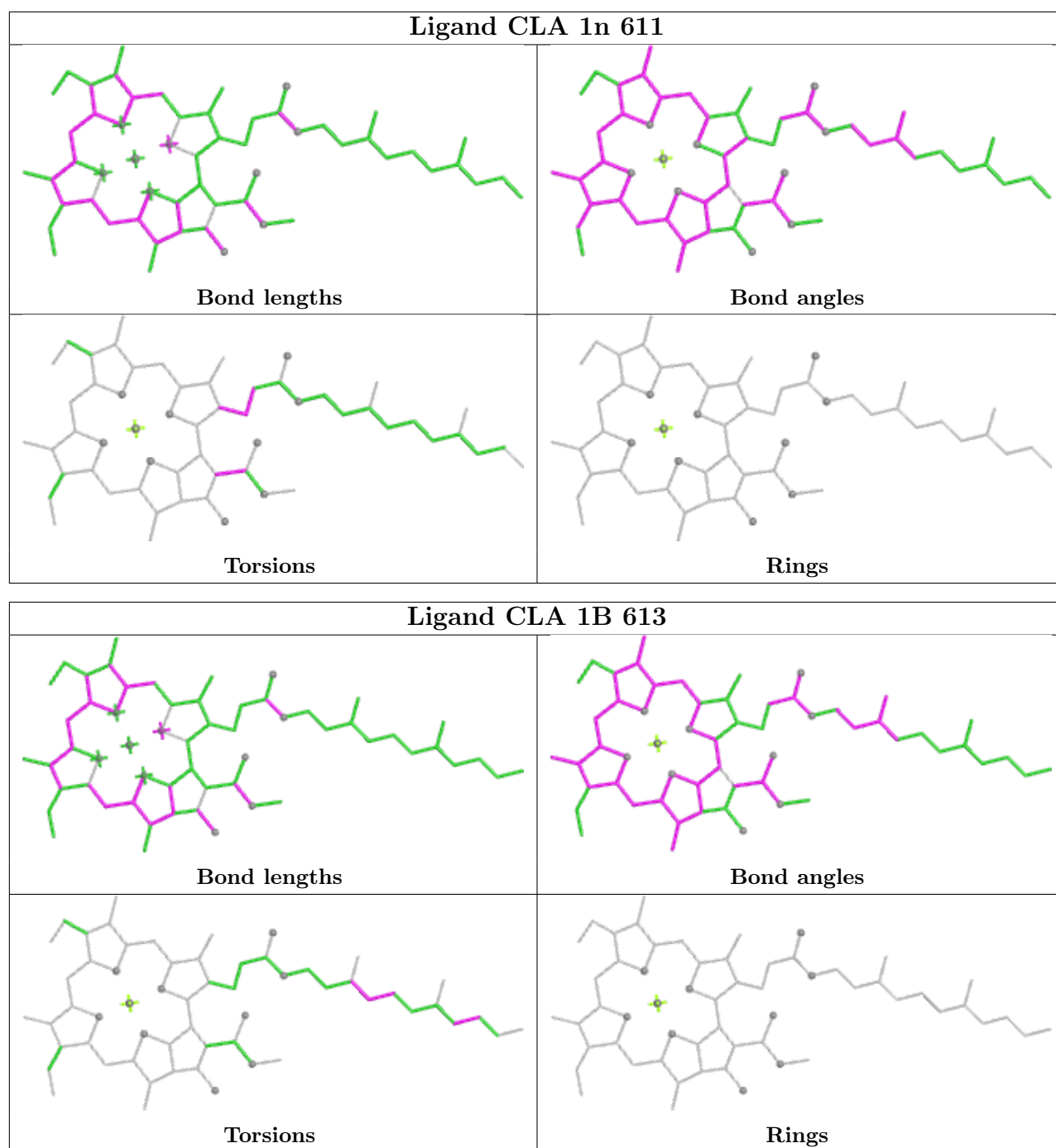


Ligand CHL 1G 601	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LUT 1G 615	
 Bond lengths	 Bond angles
 Torsions	 Rings

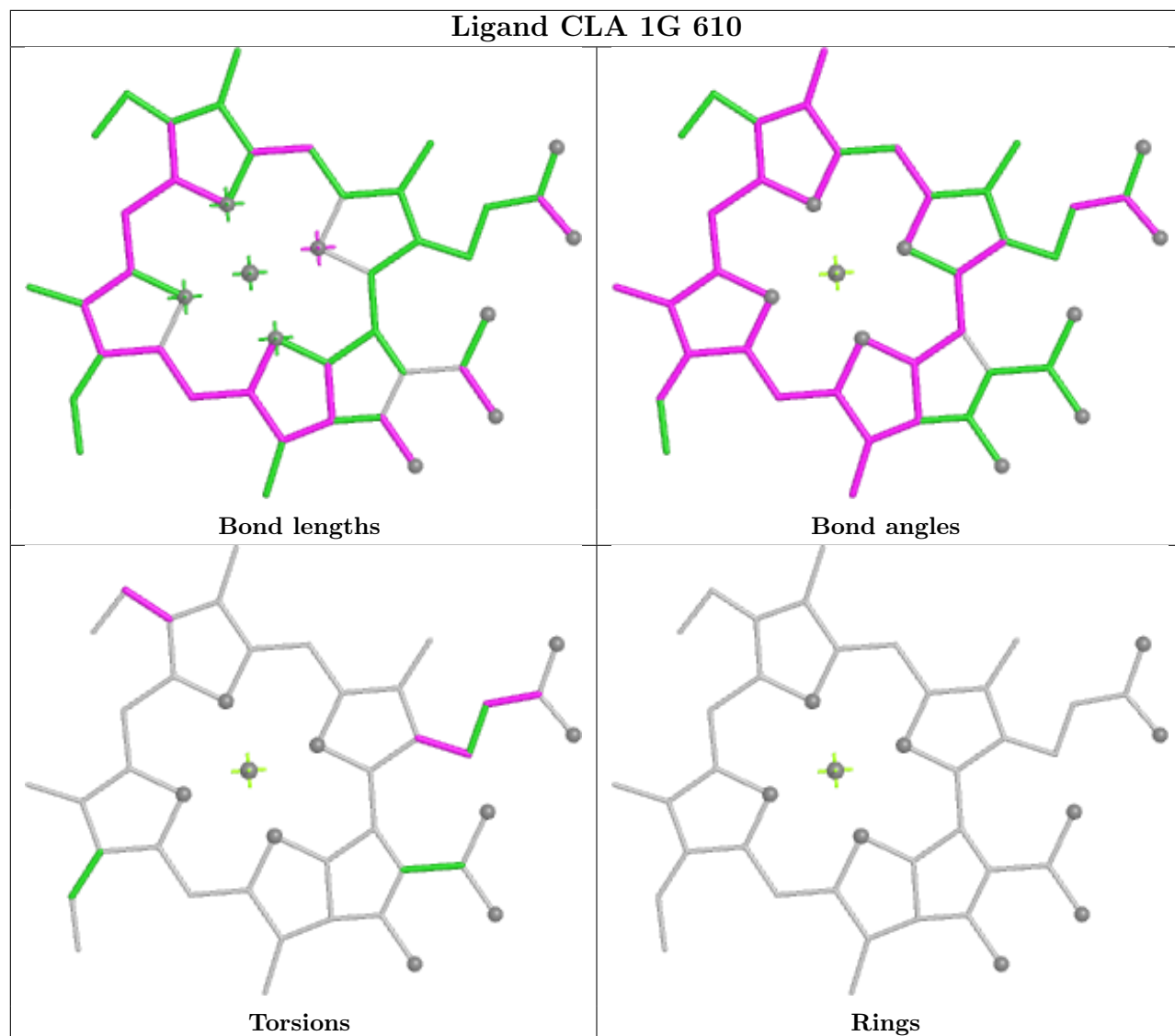


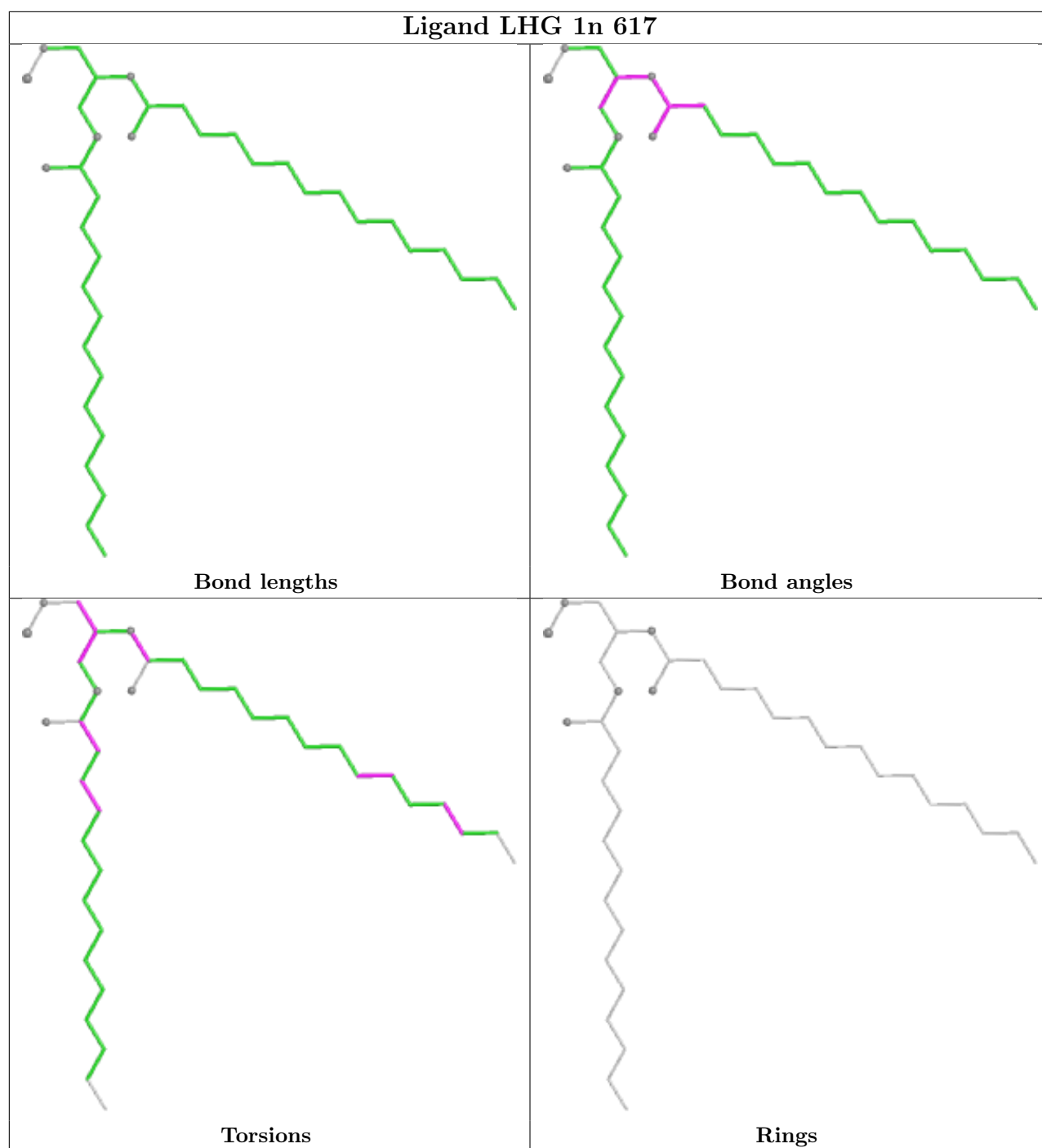


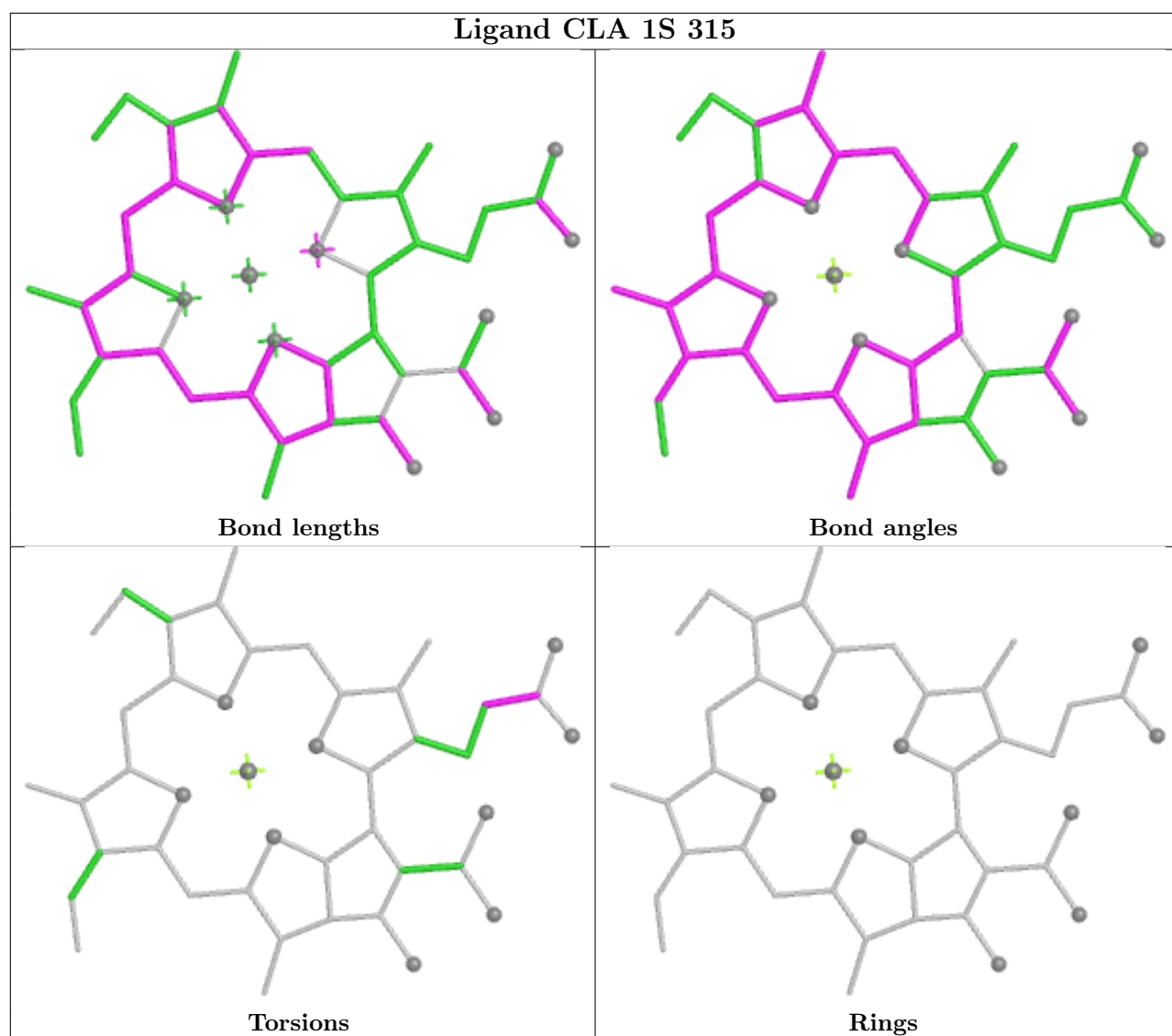


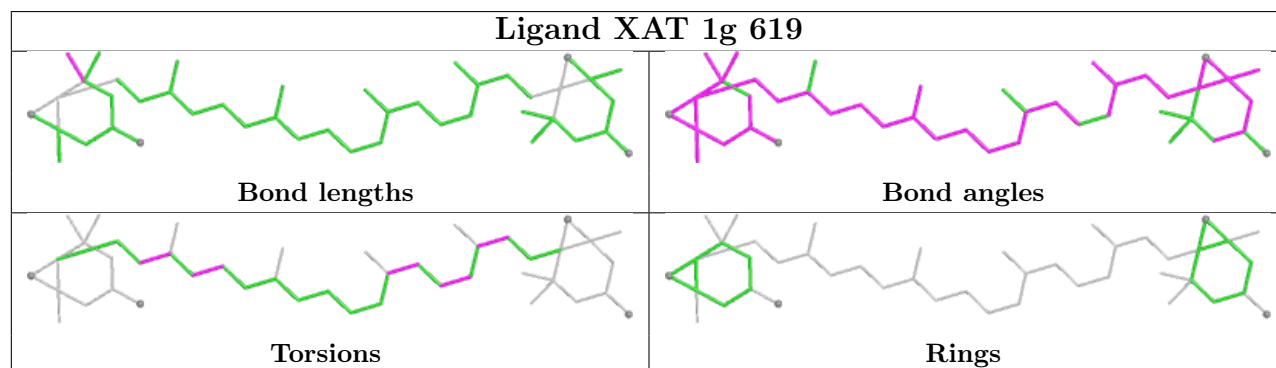
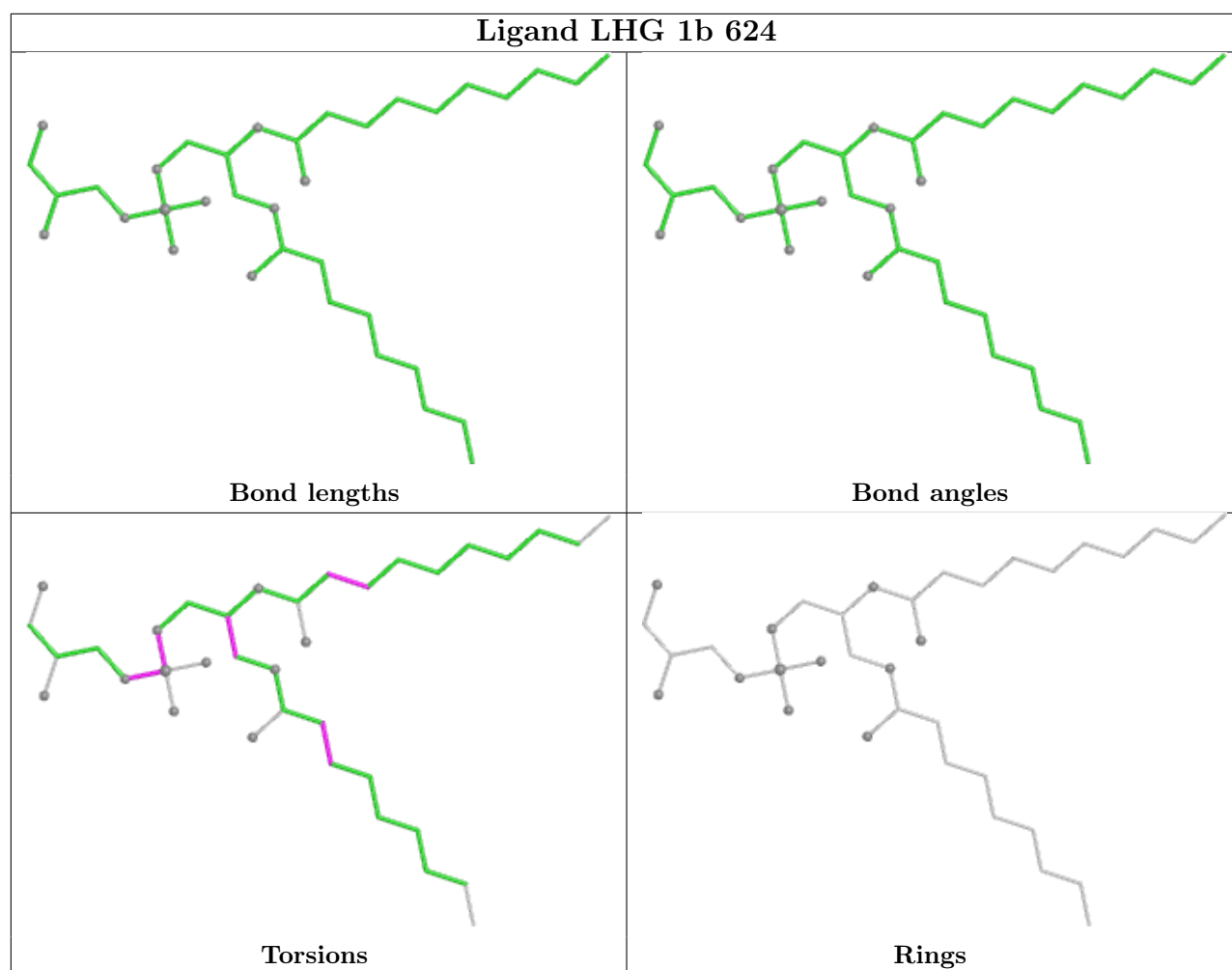


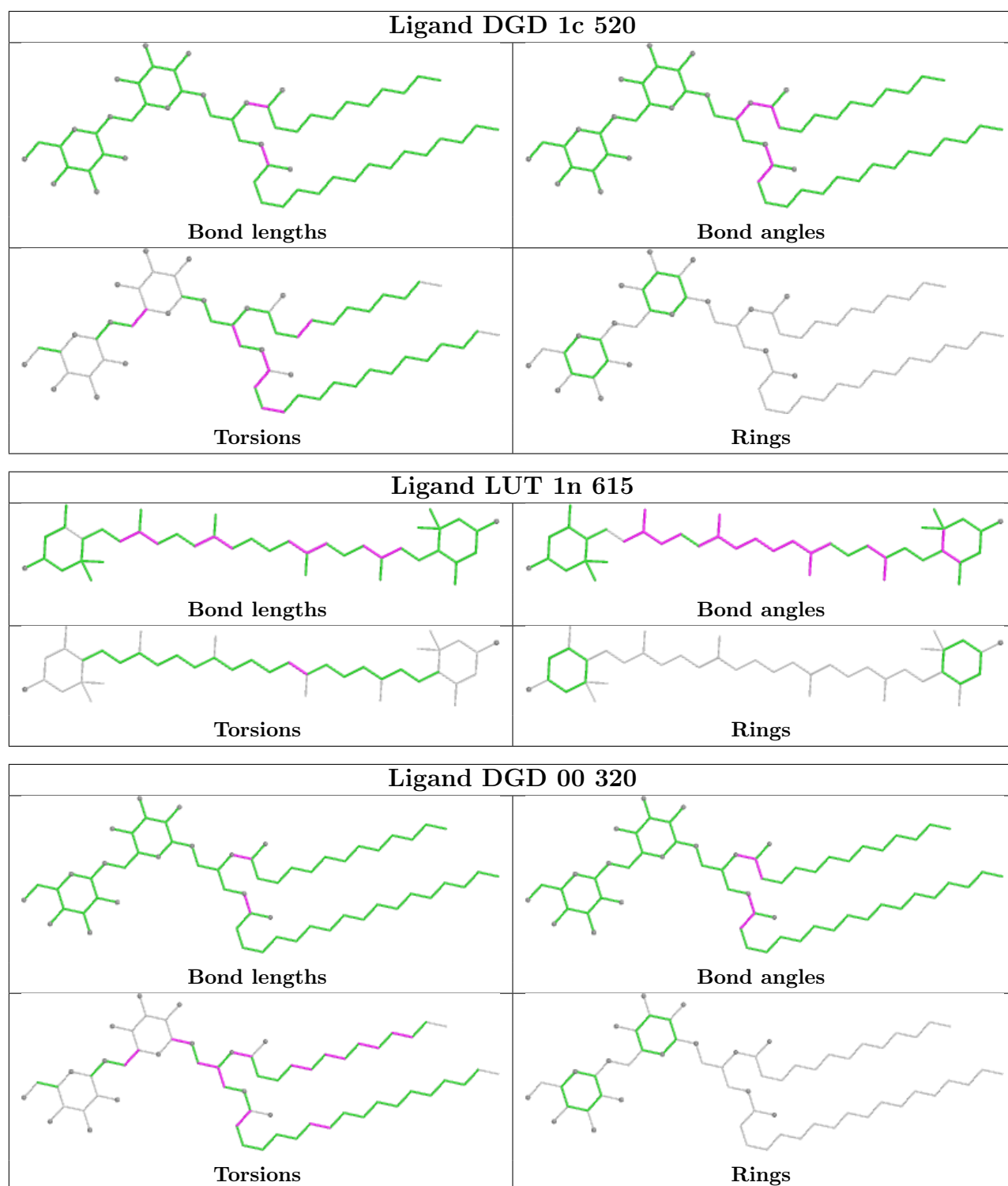
Ligand CLA 1G 610

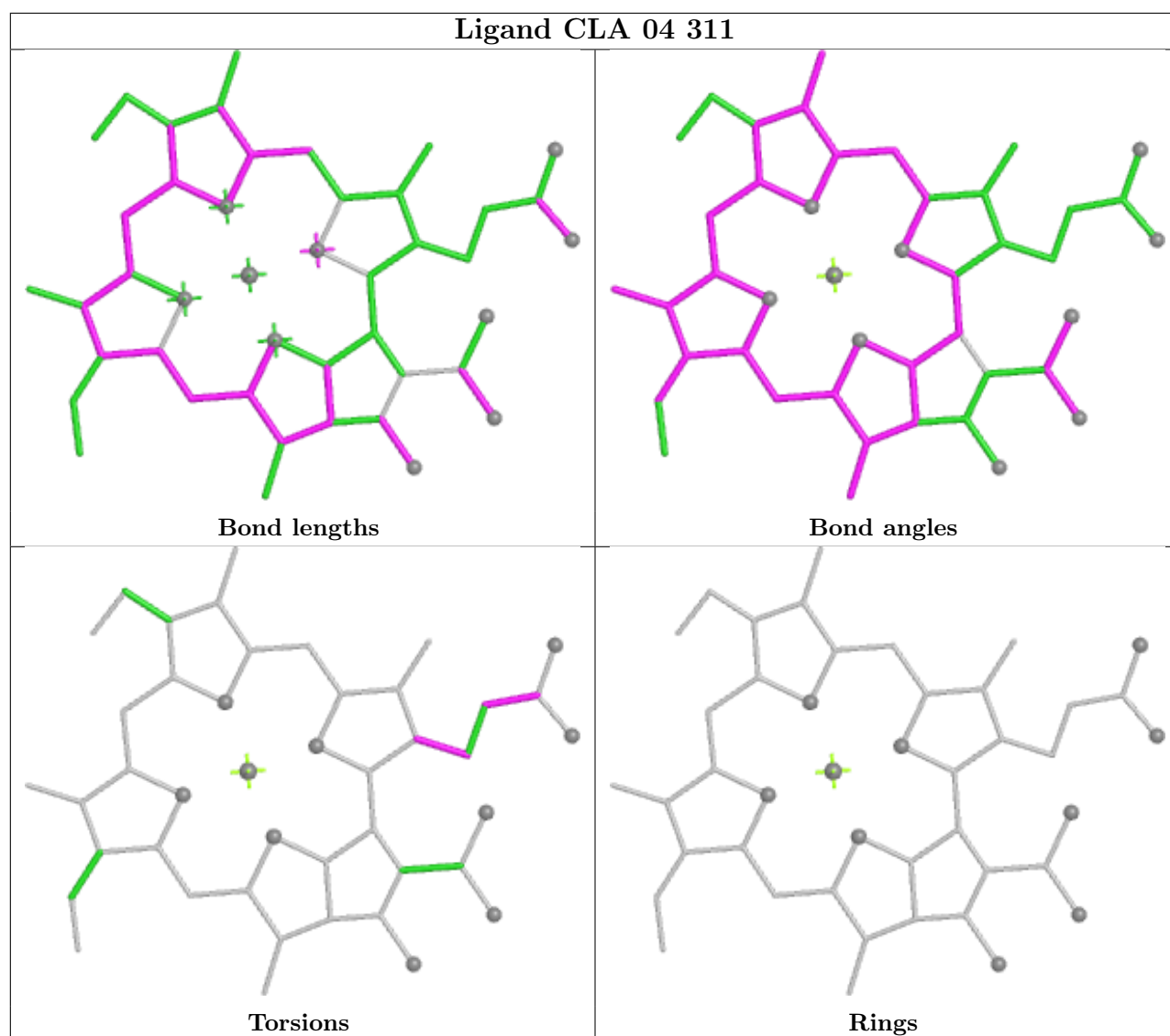


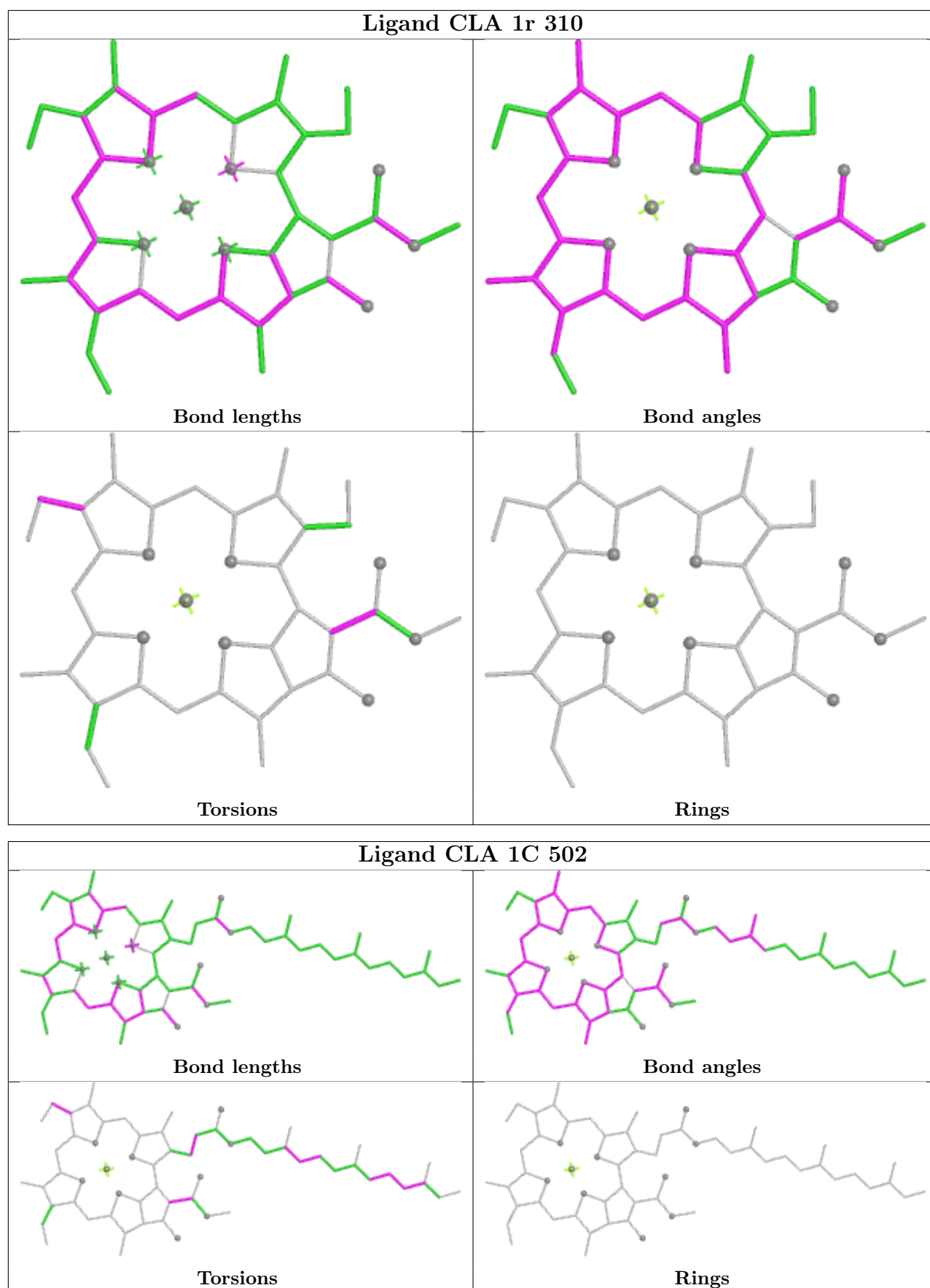


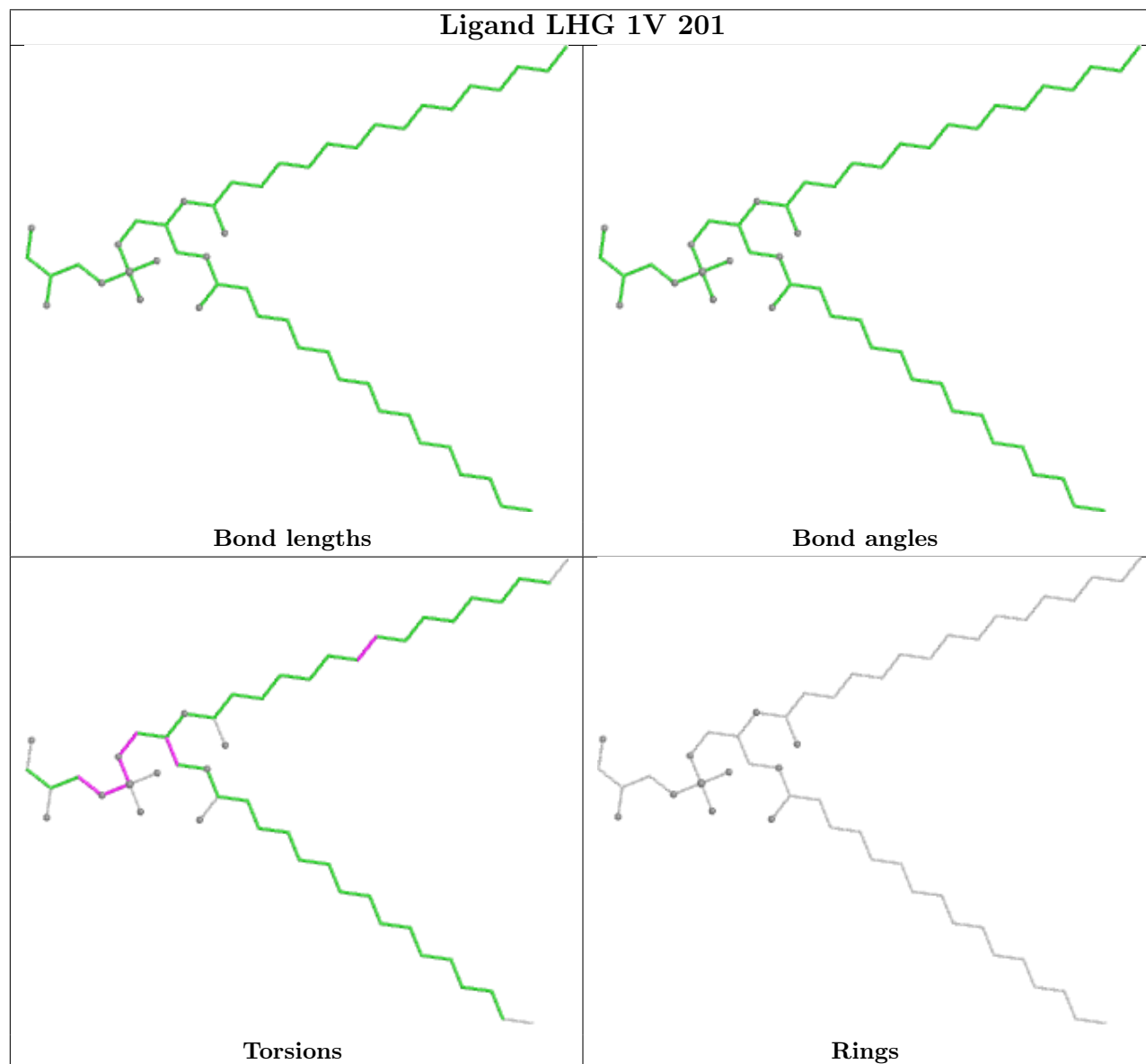
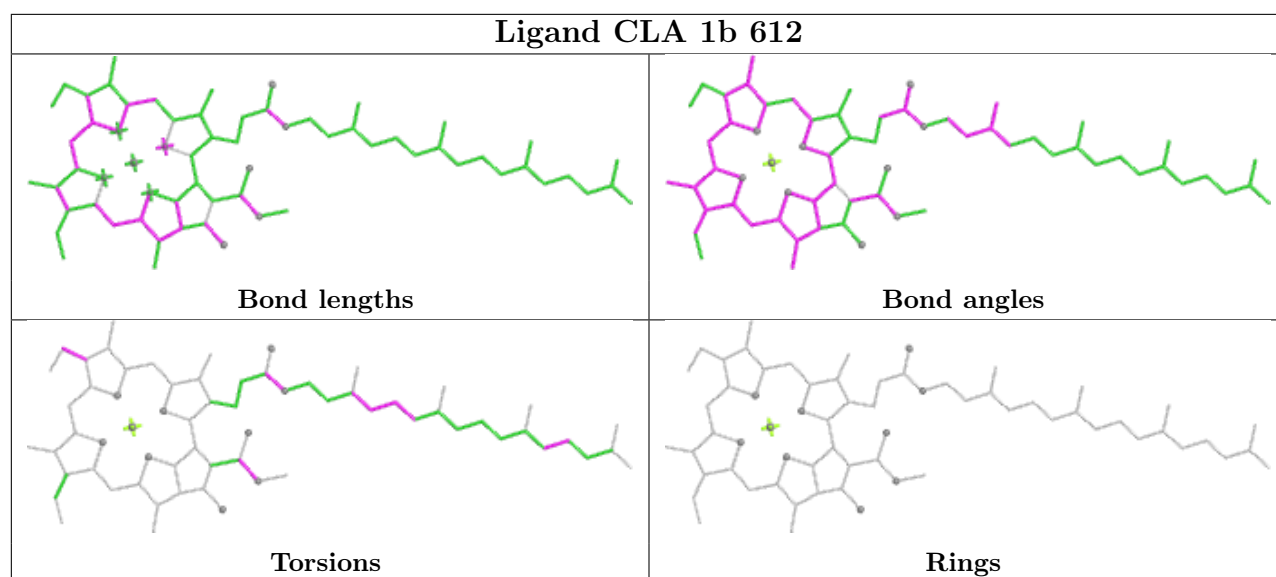


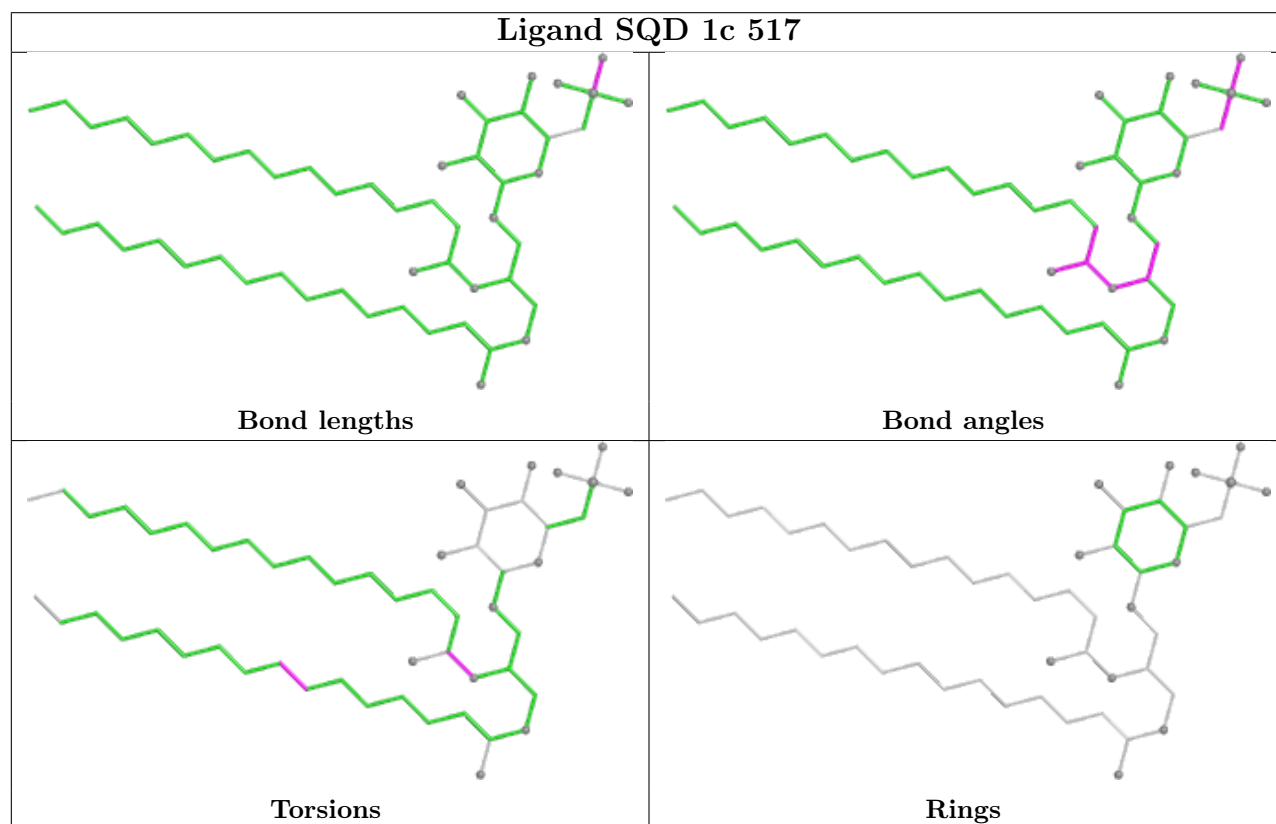
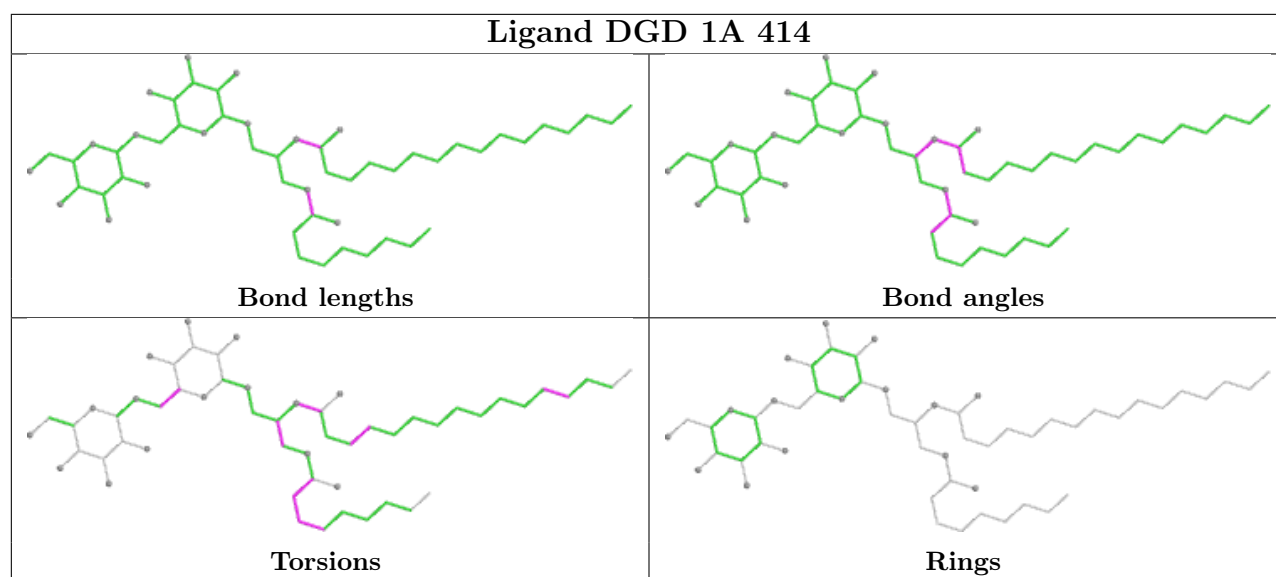


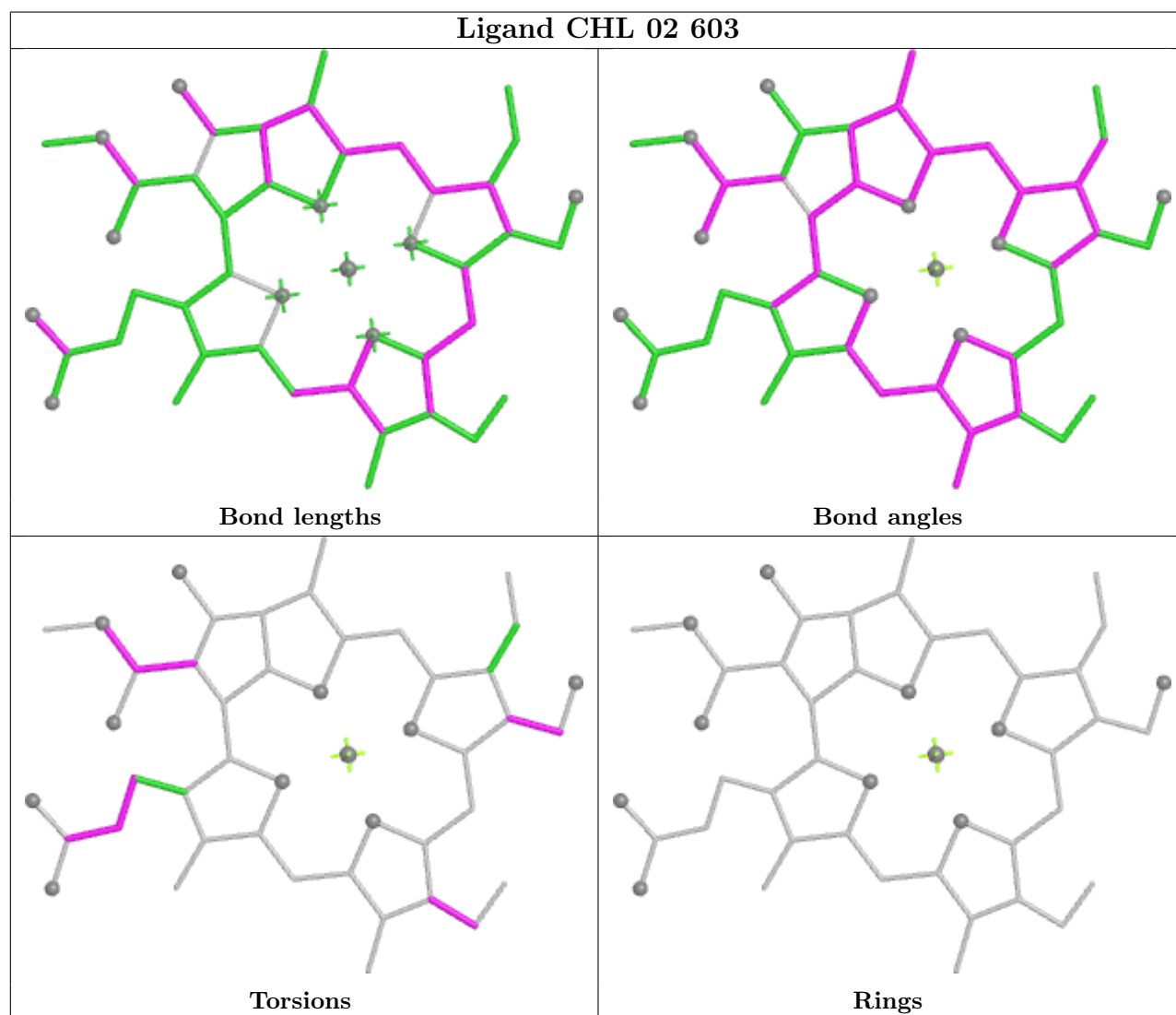
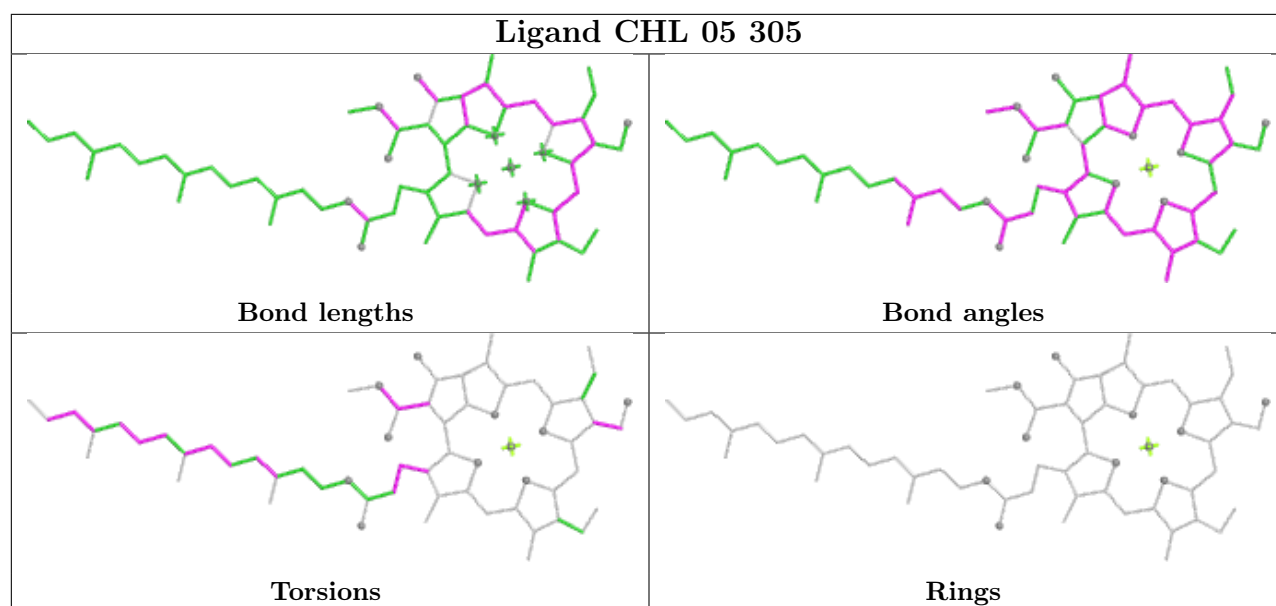


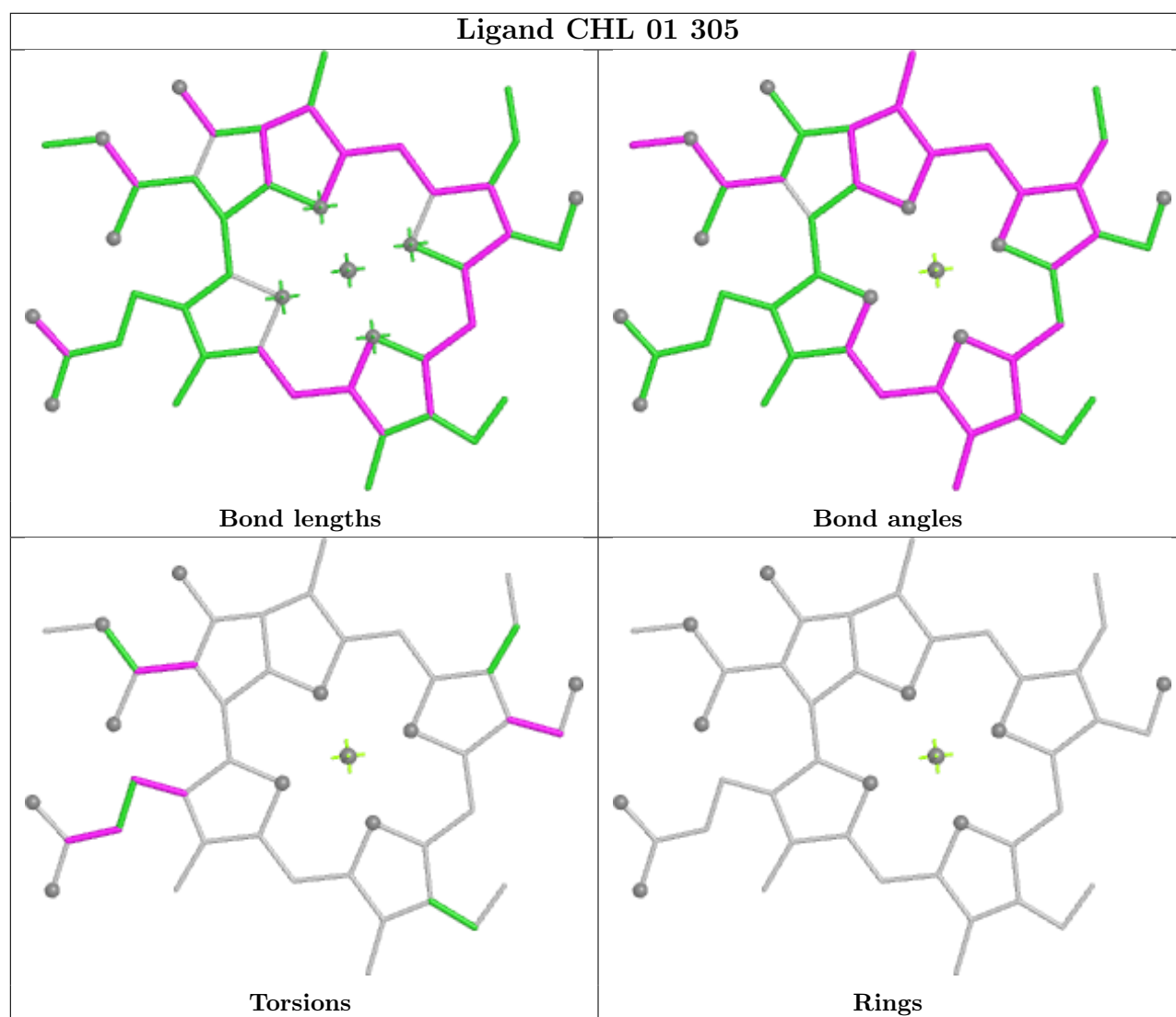


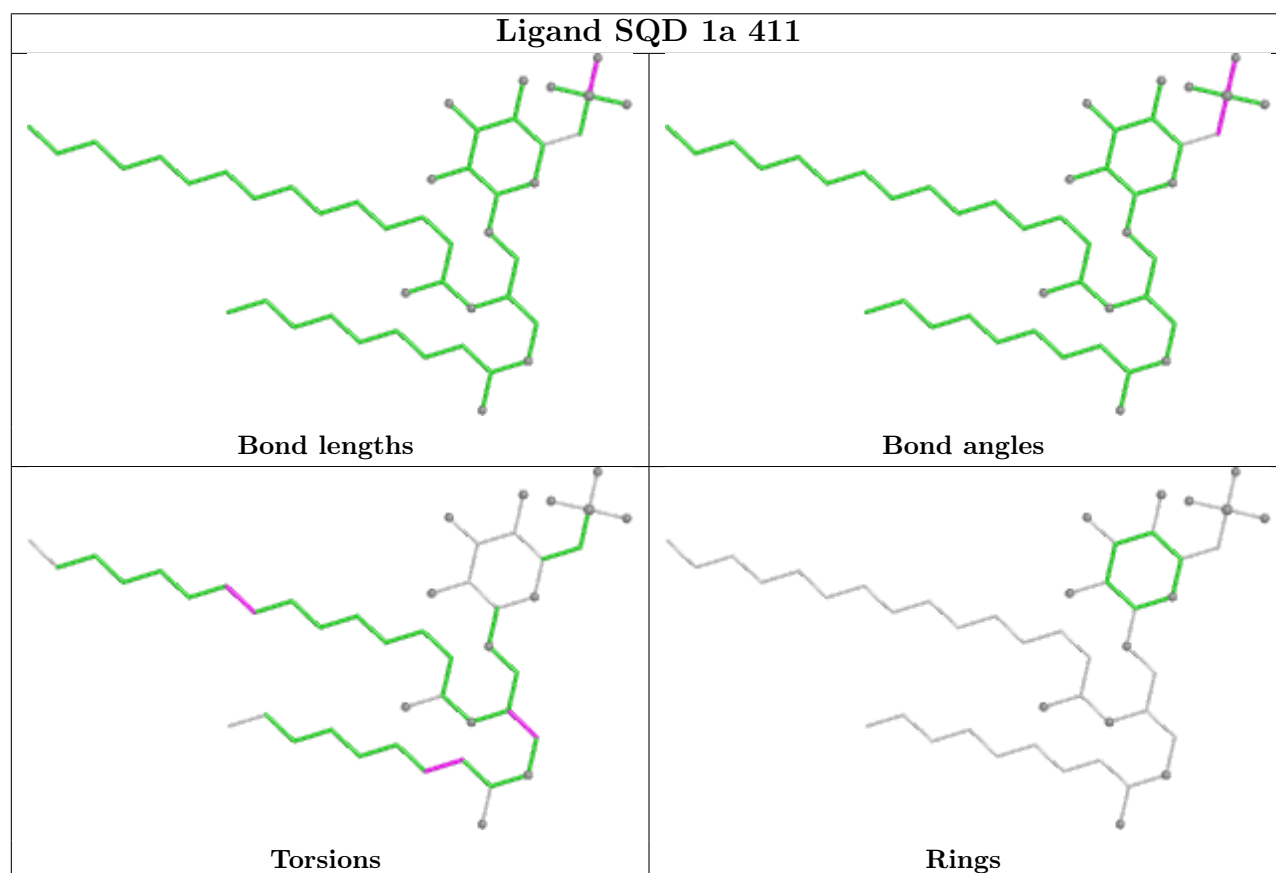
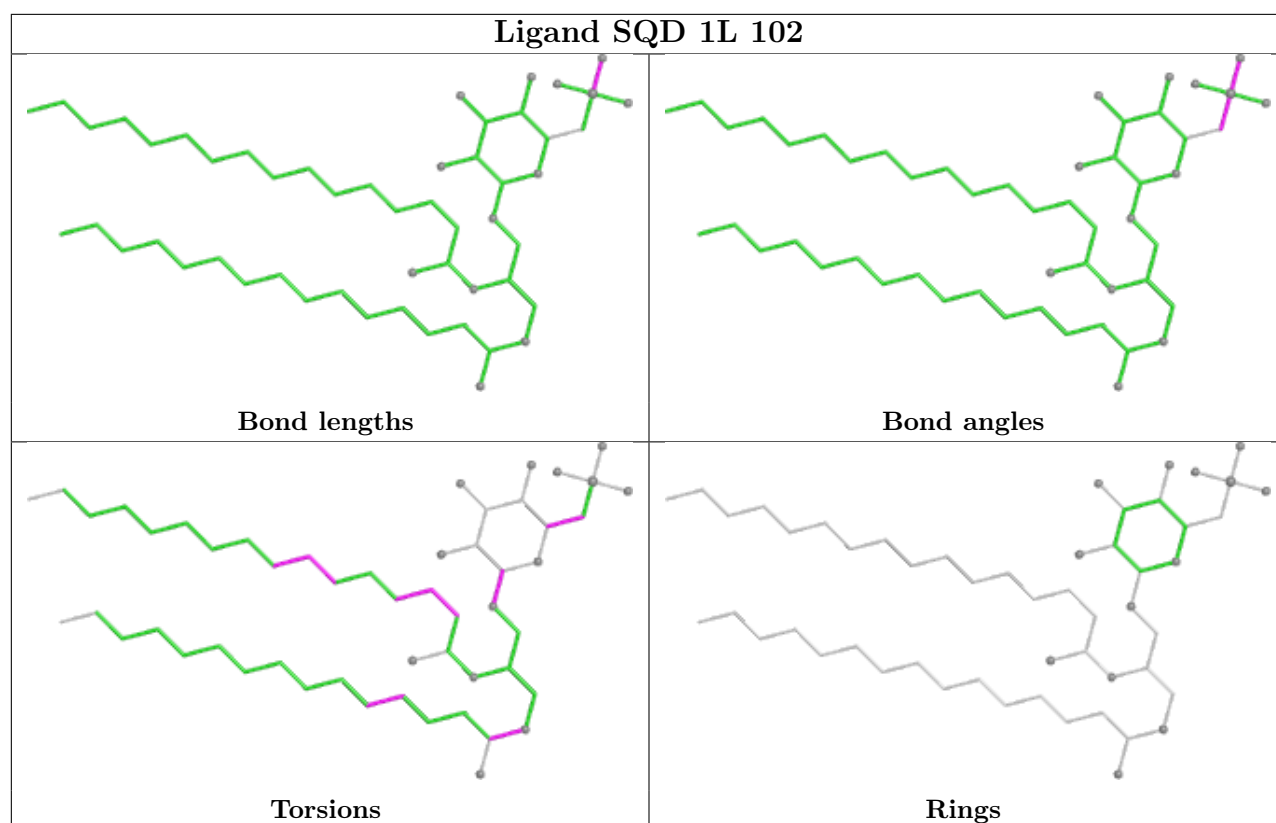


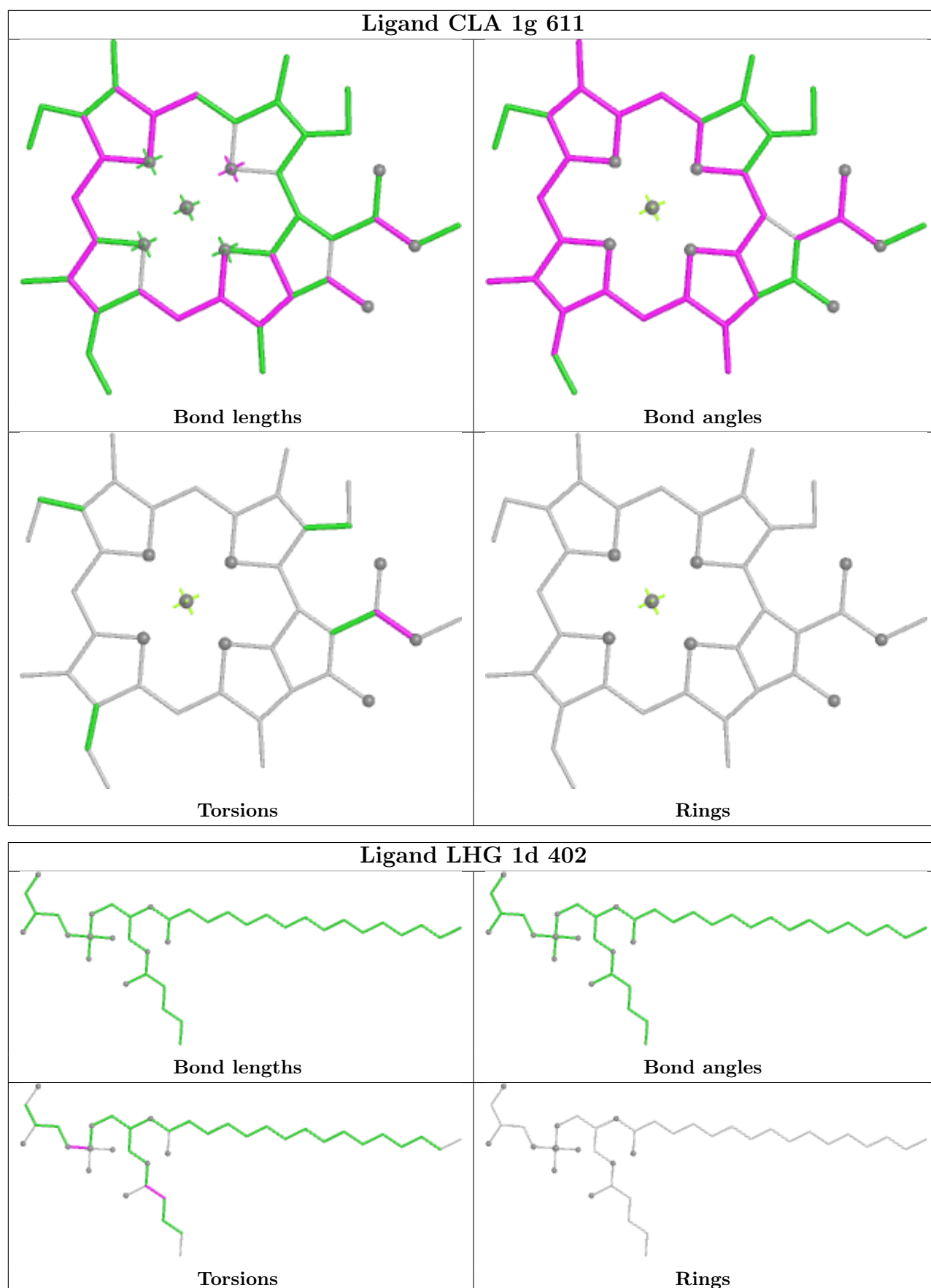


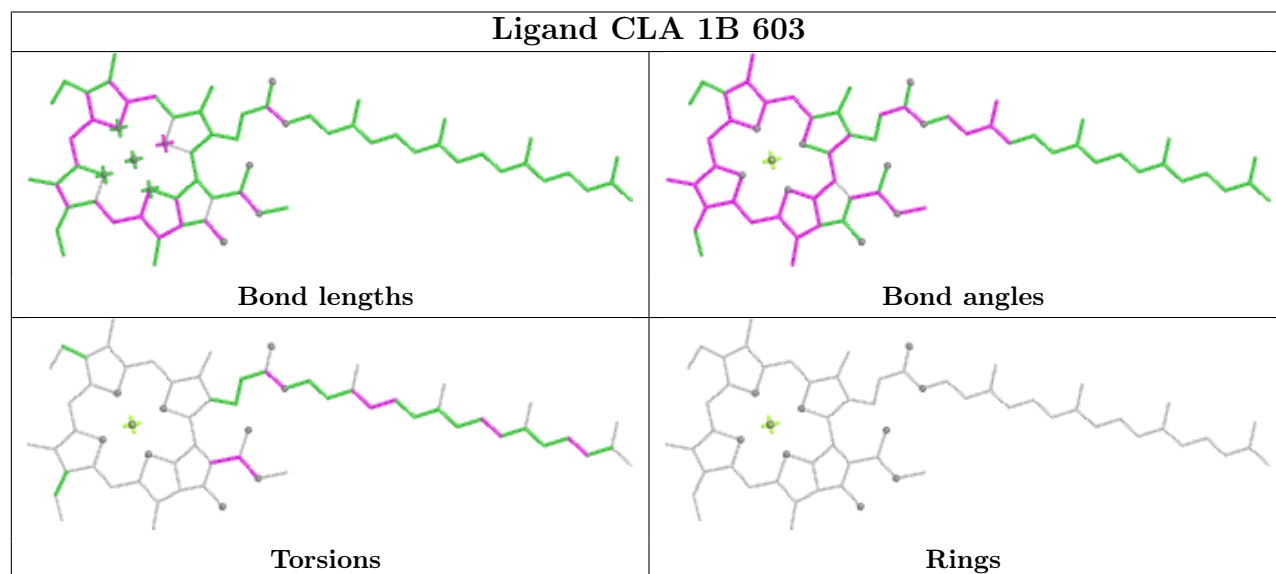
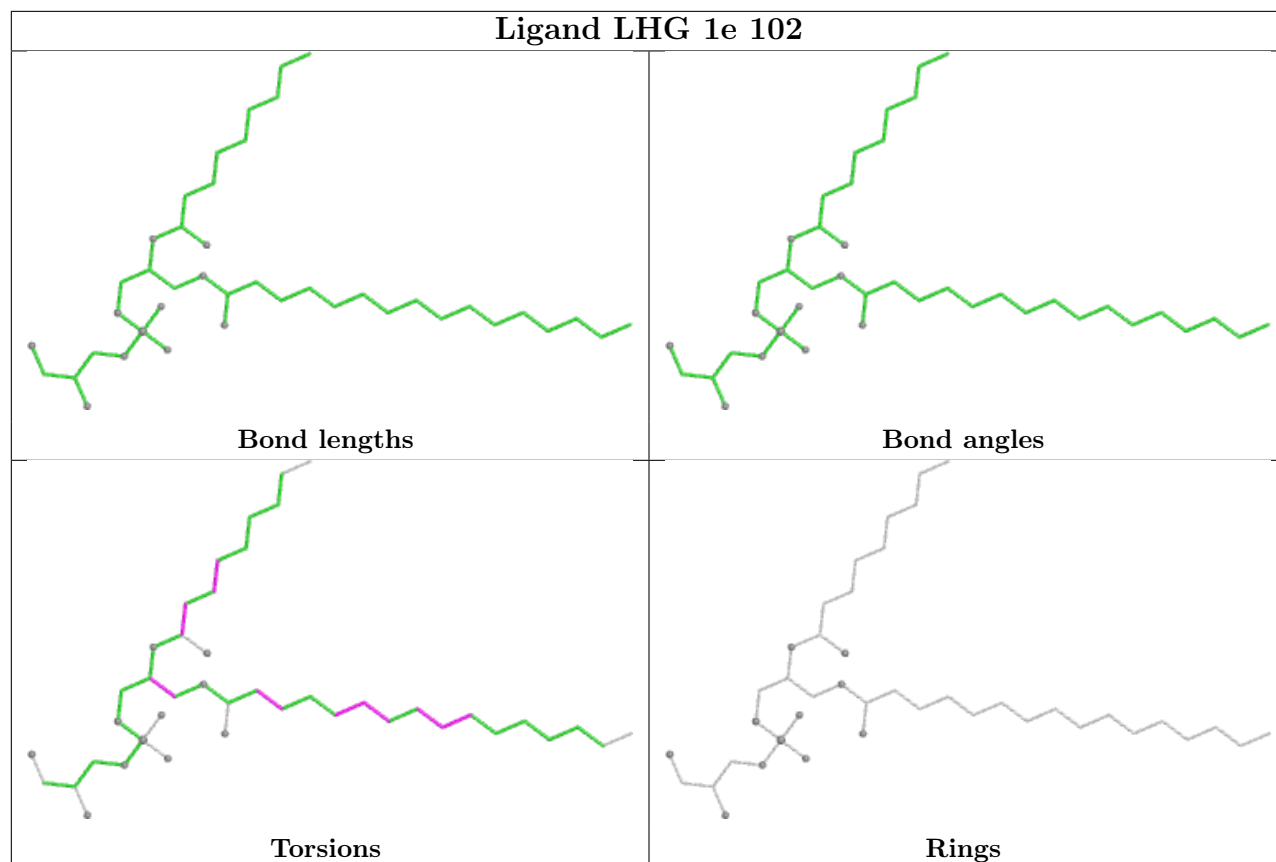


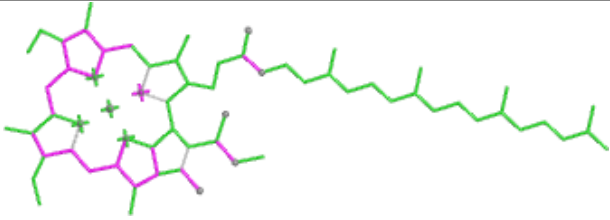
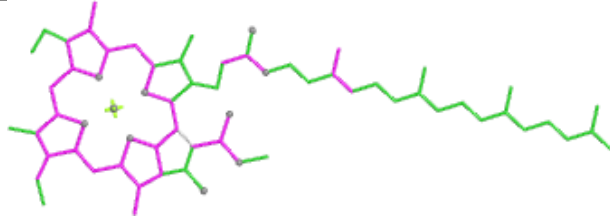
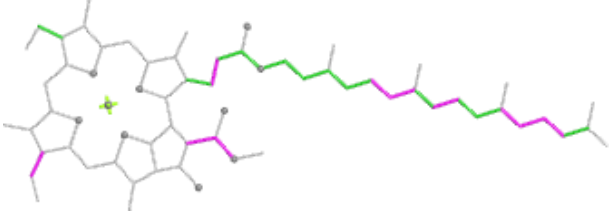
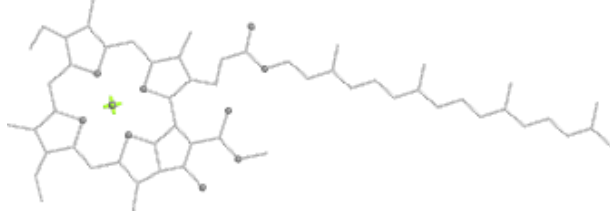
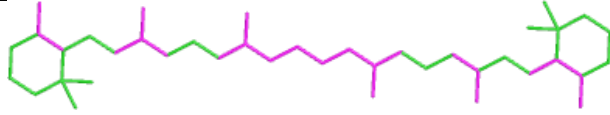
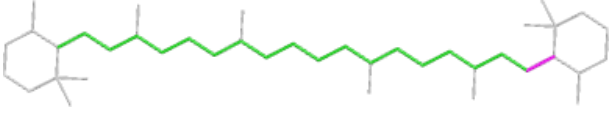
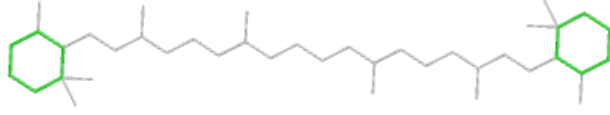
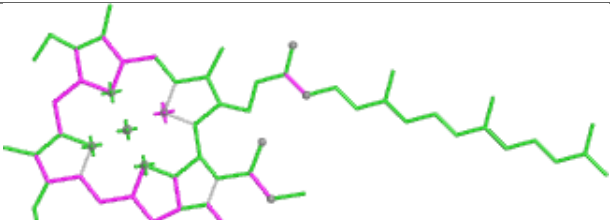
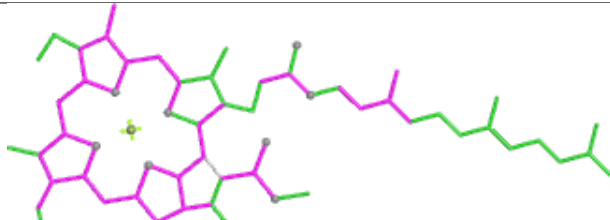
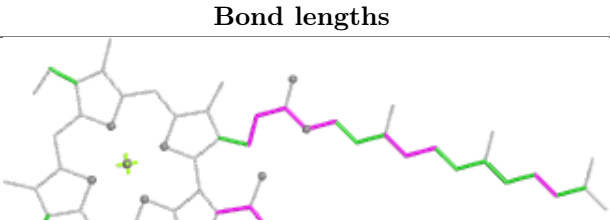
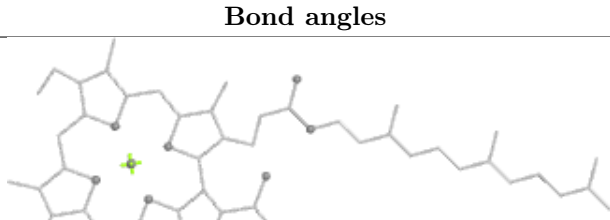


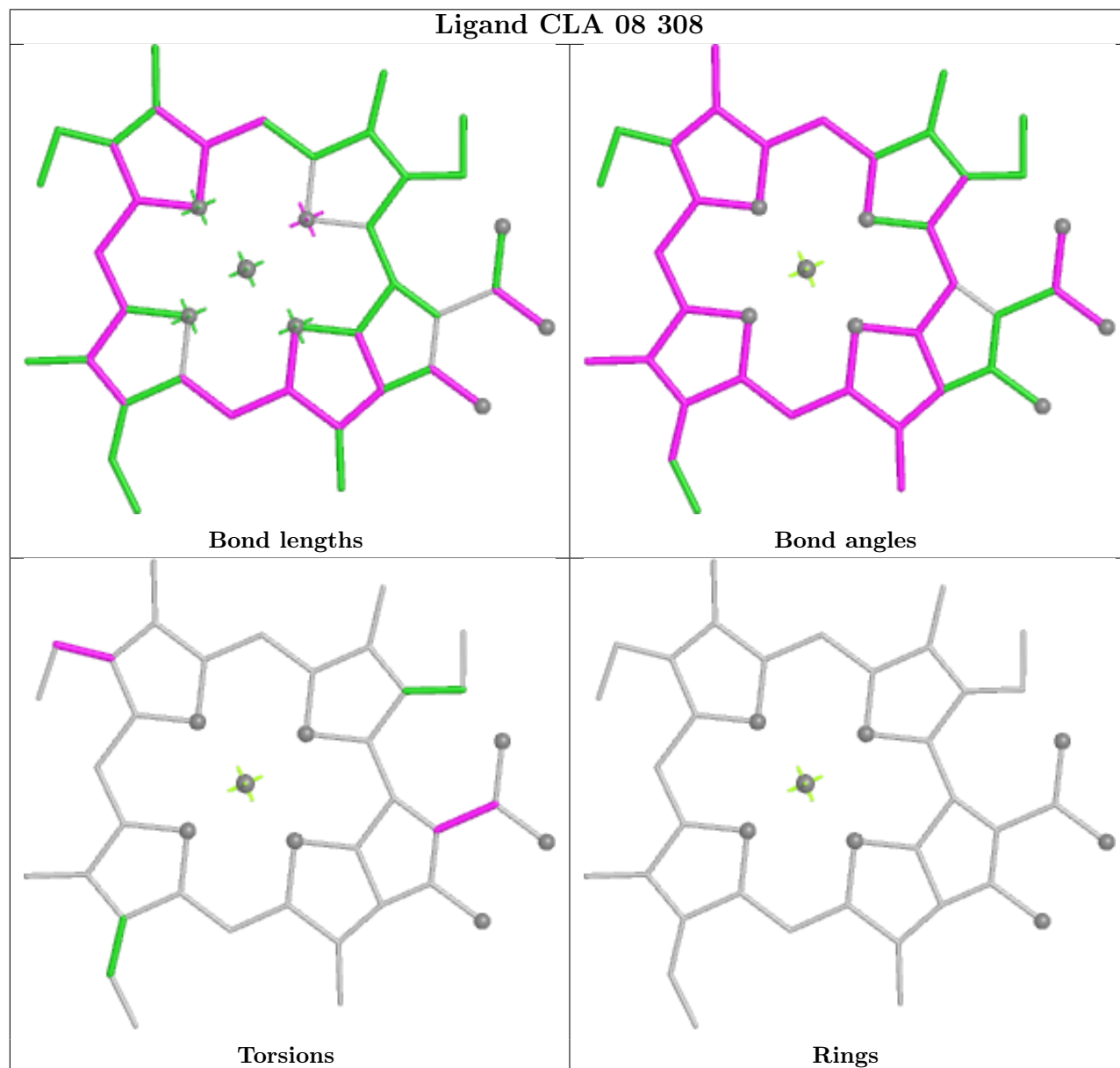
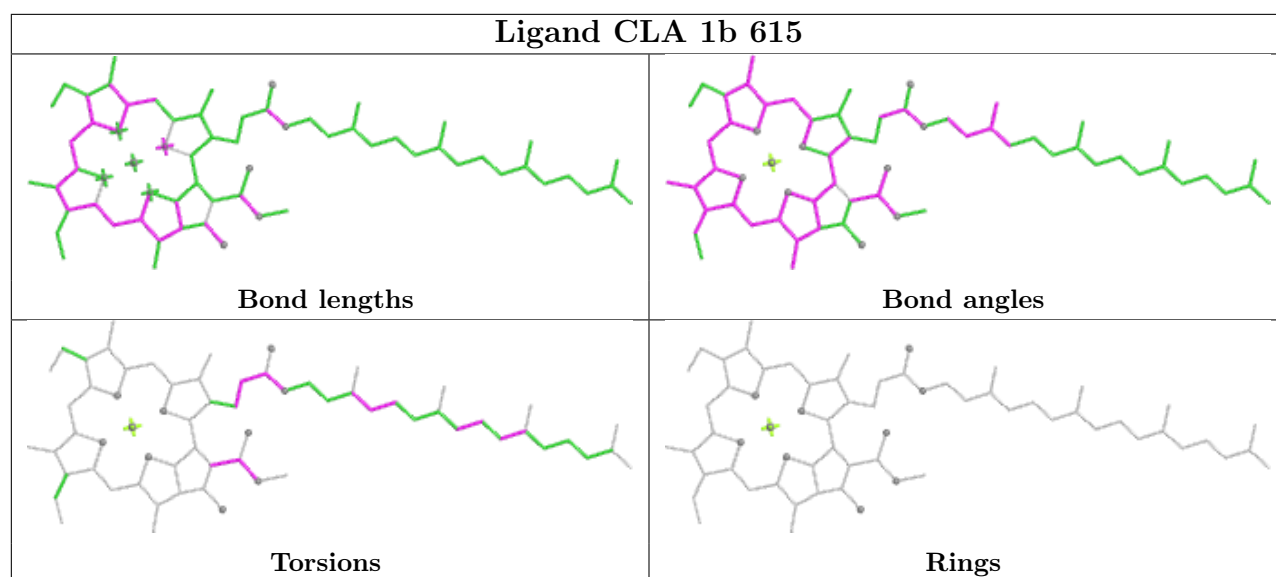


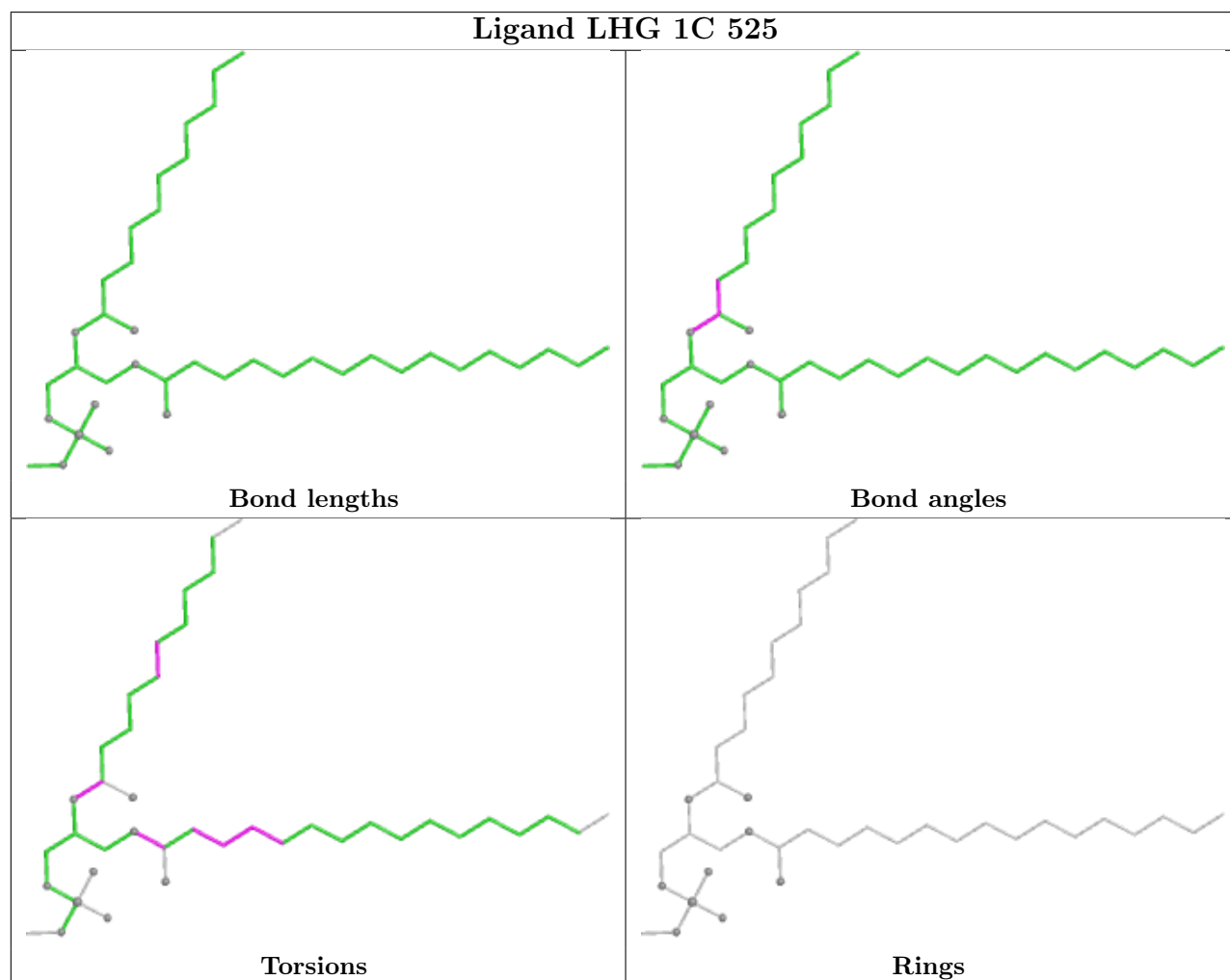
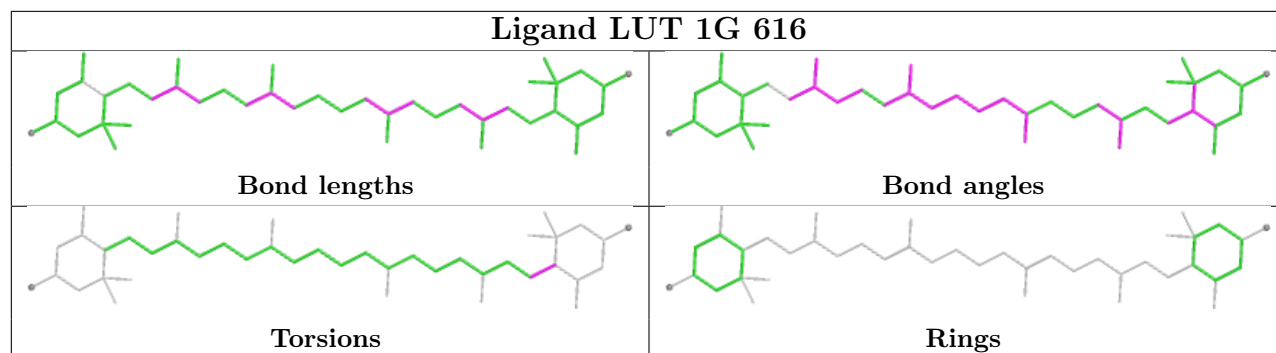


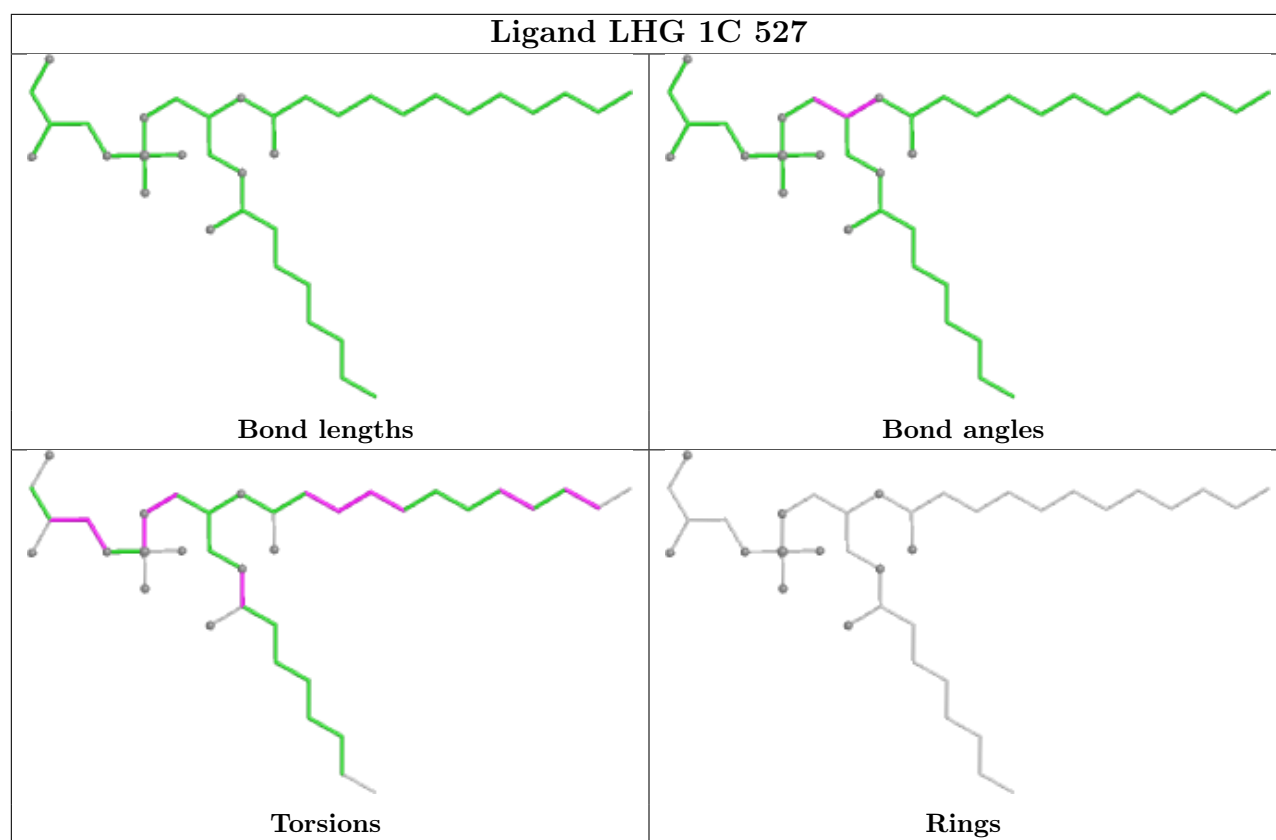


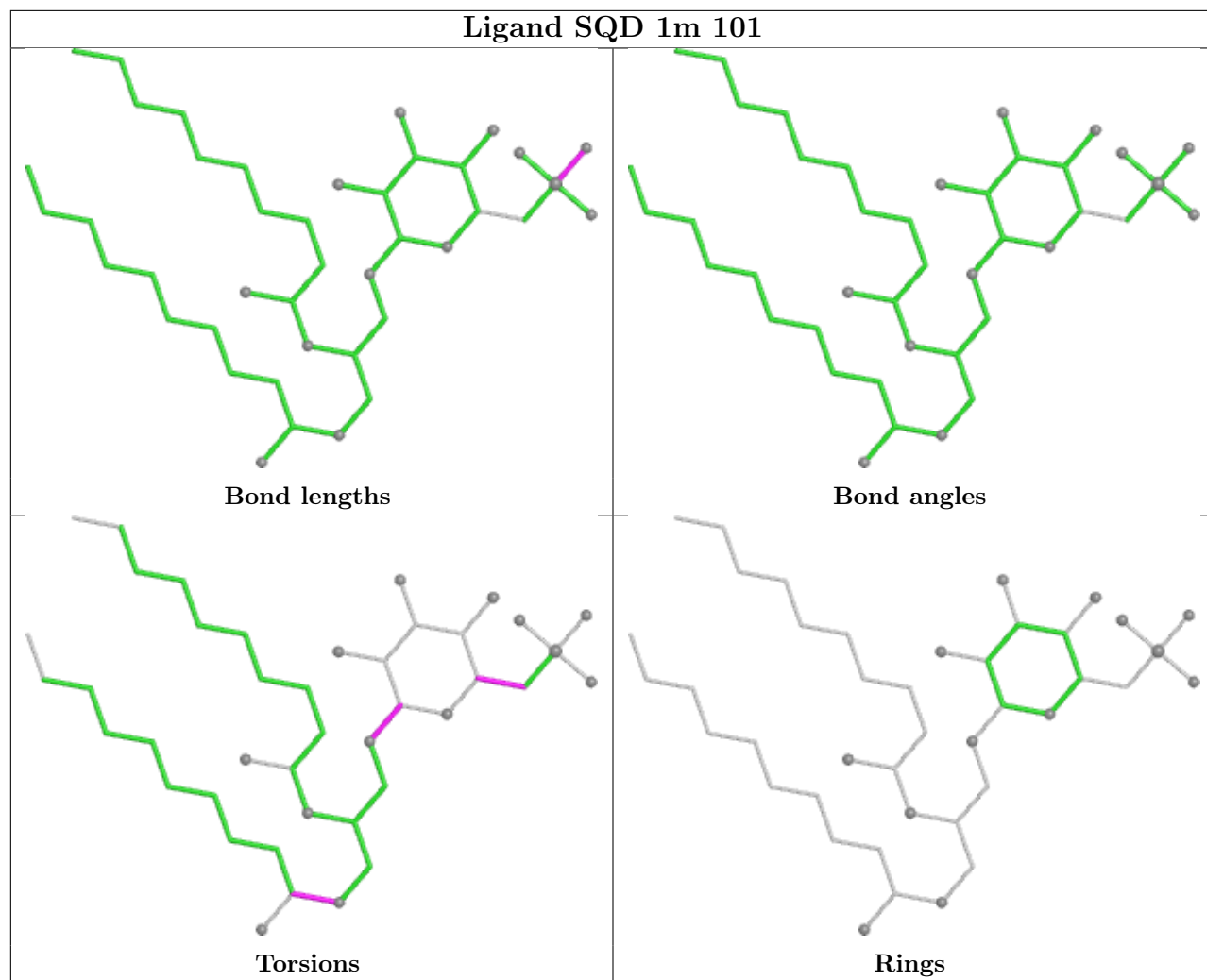


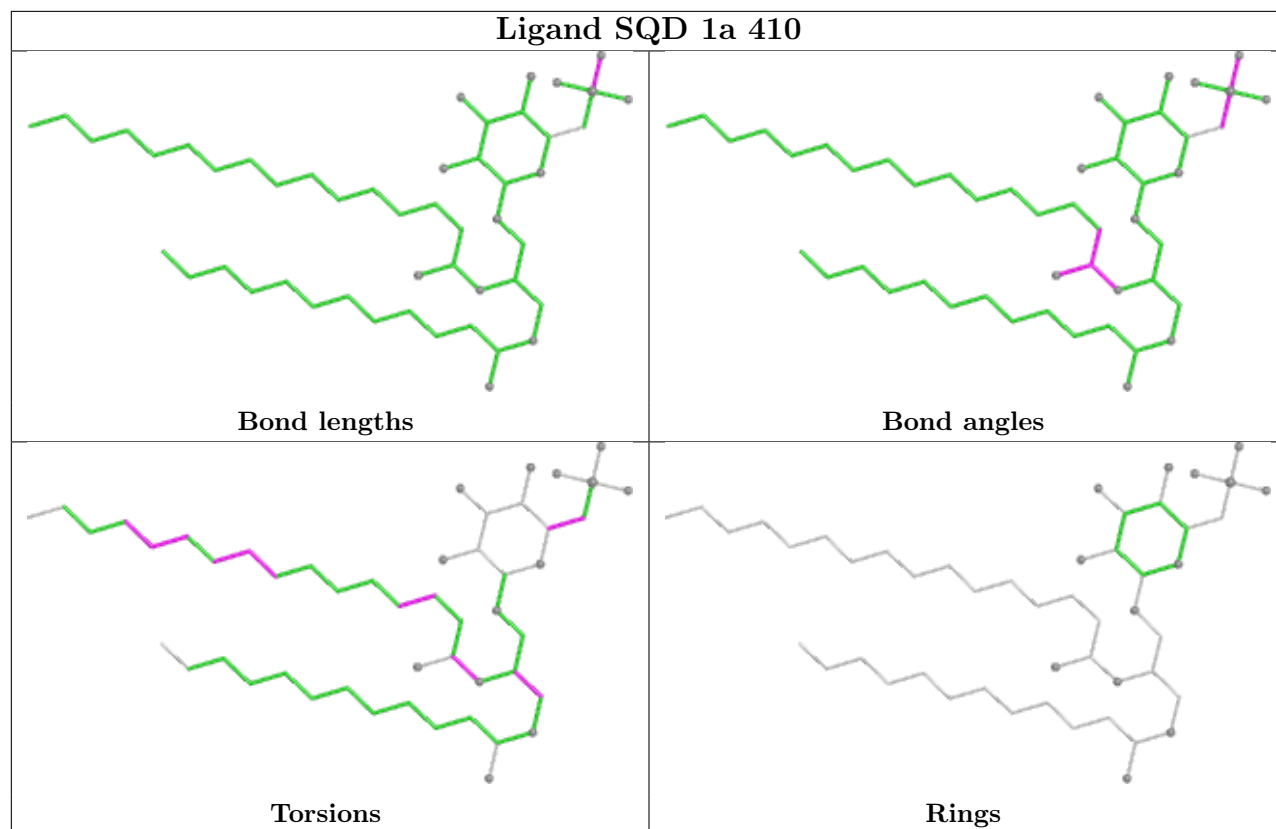
Ligand CLA 1b 611	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR 1Z 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA 1C 505	
 Bond lengths	 Bond angles
 Torsions	 Rings

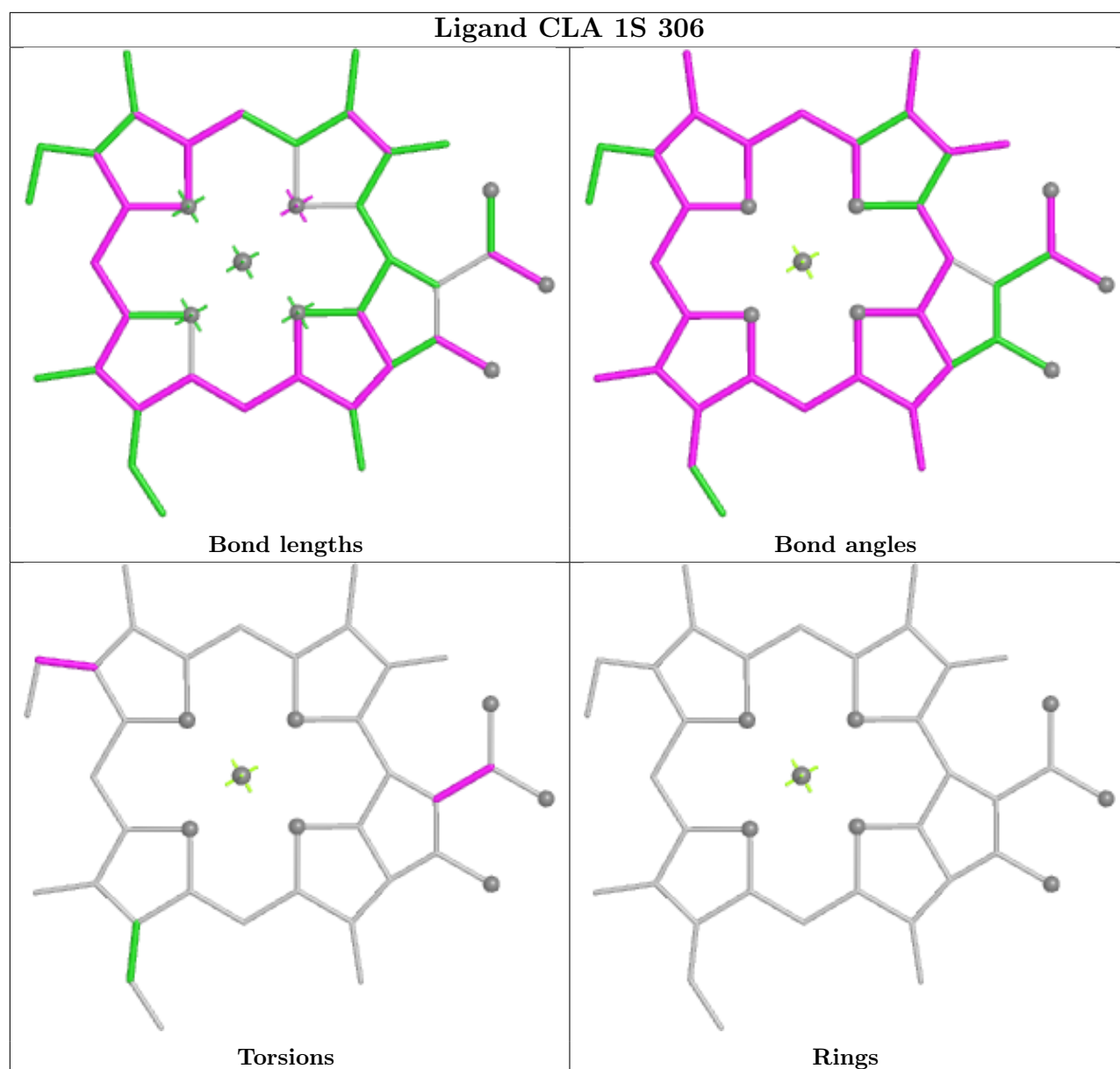


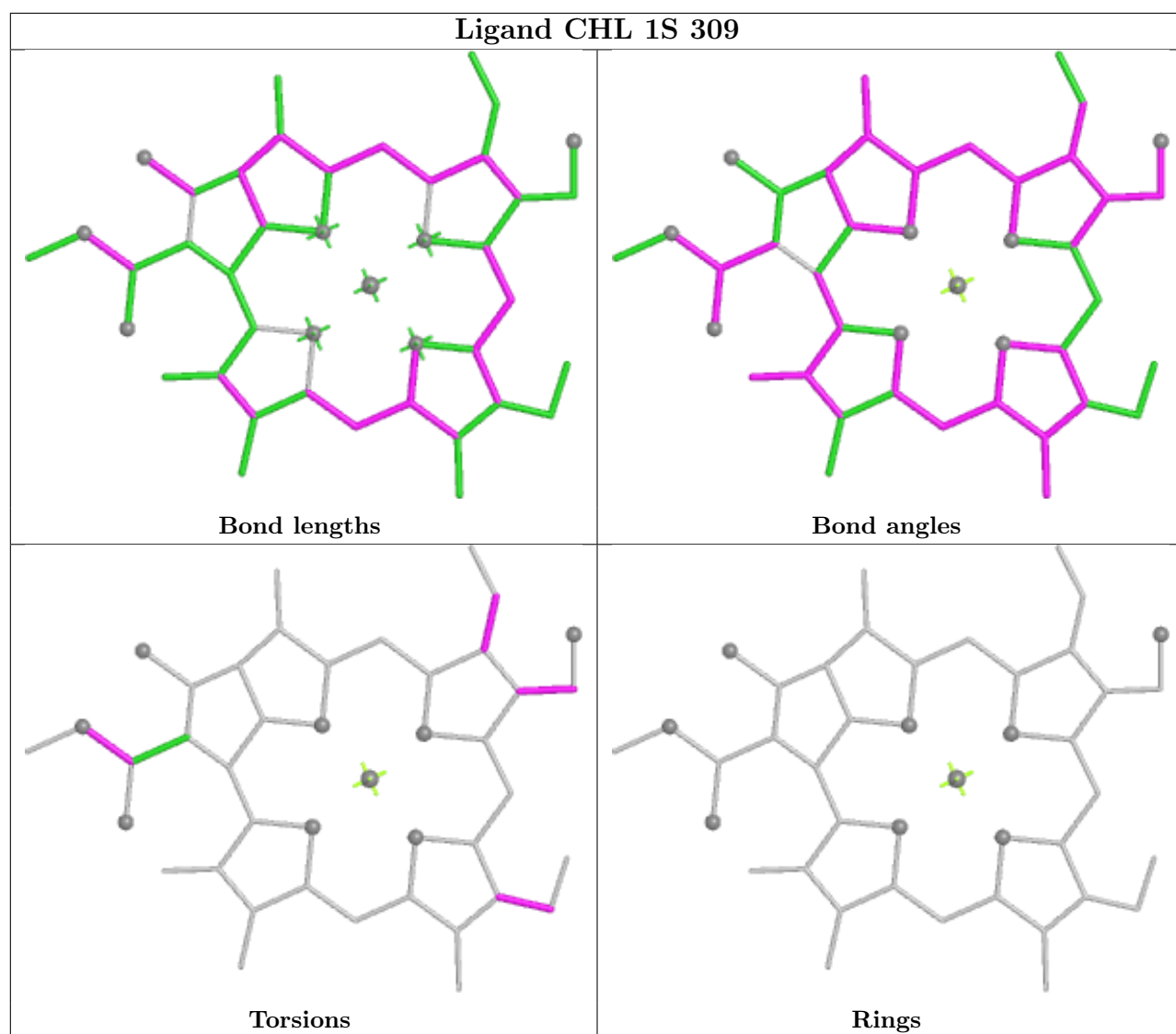


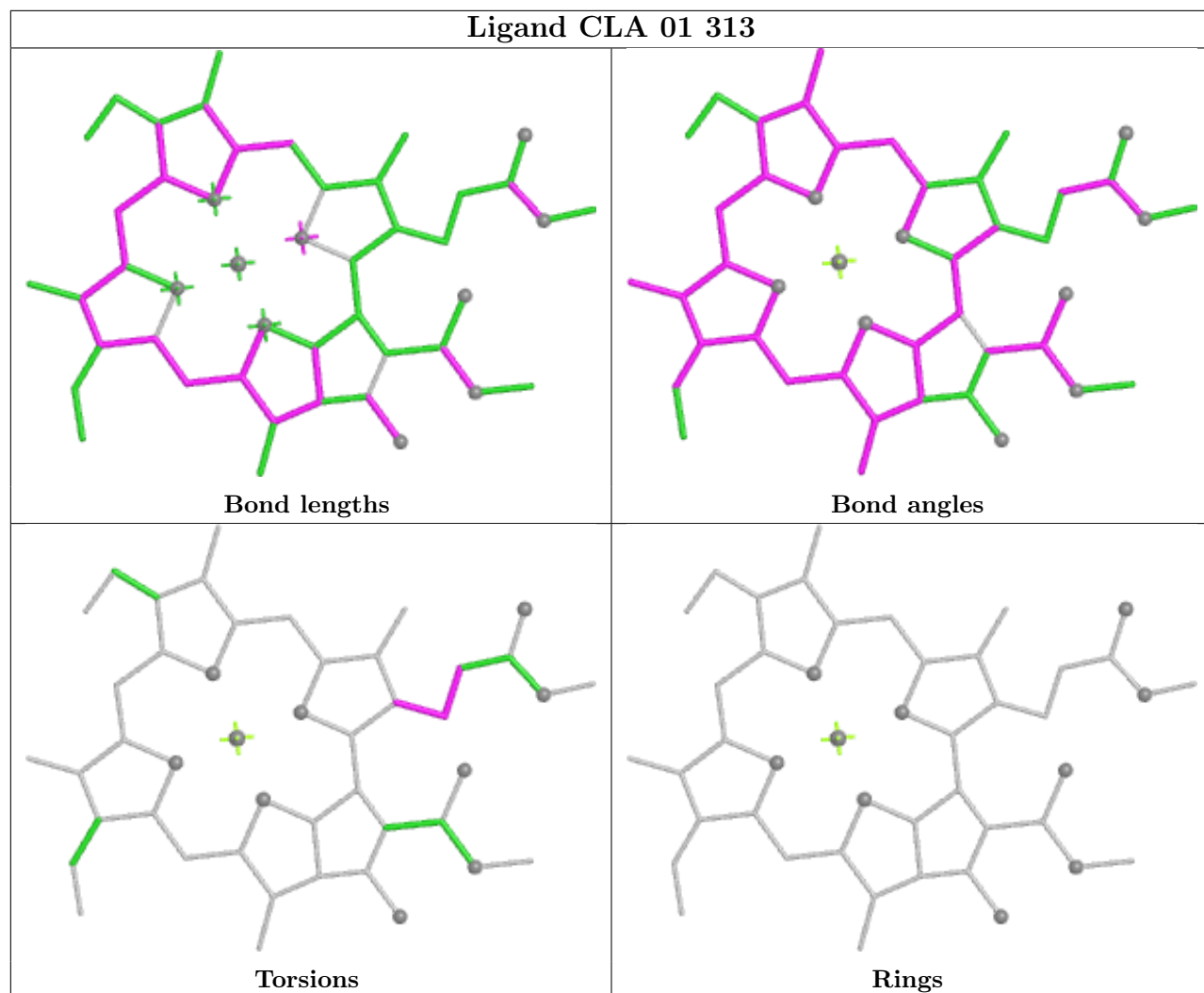


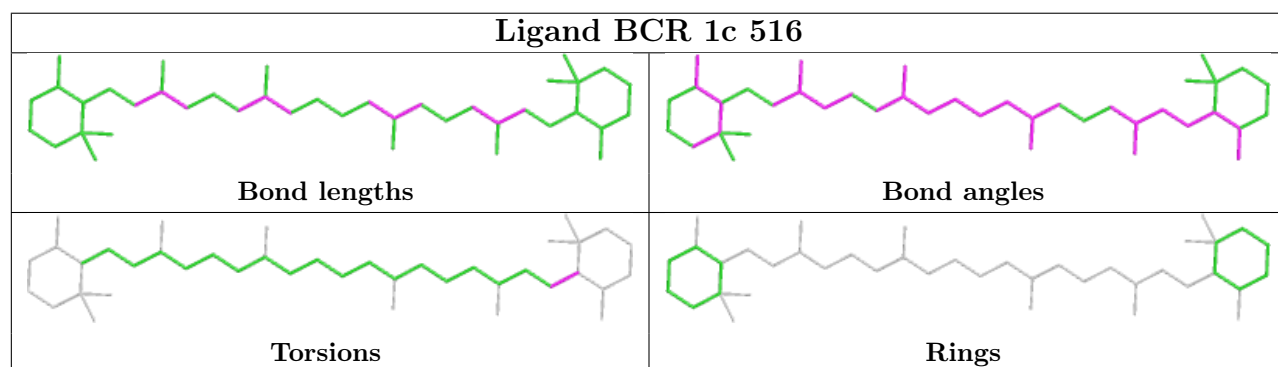
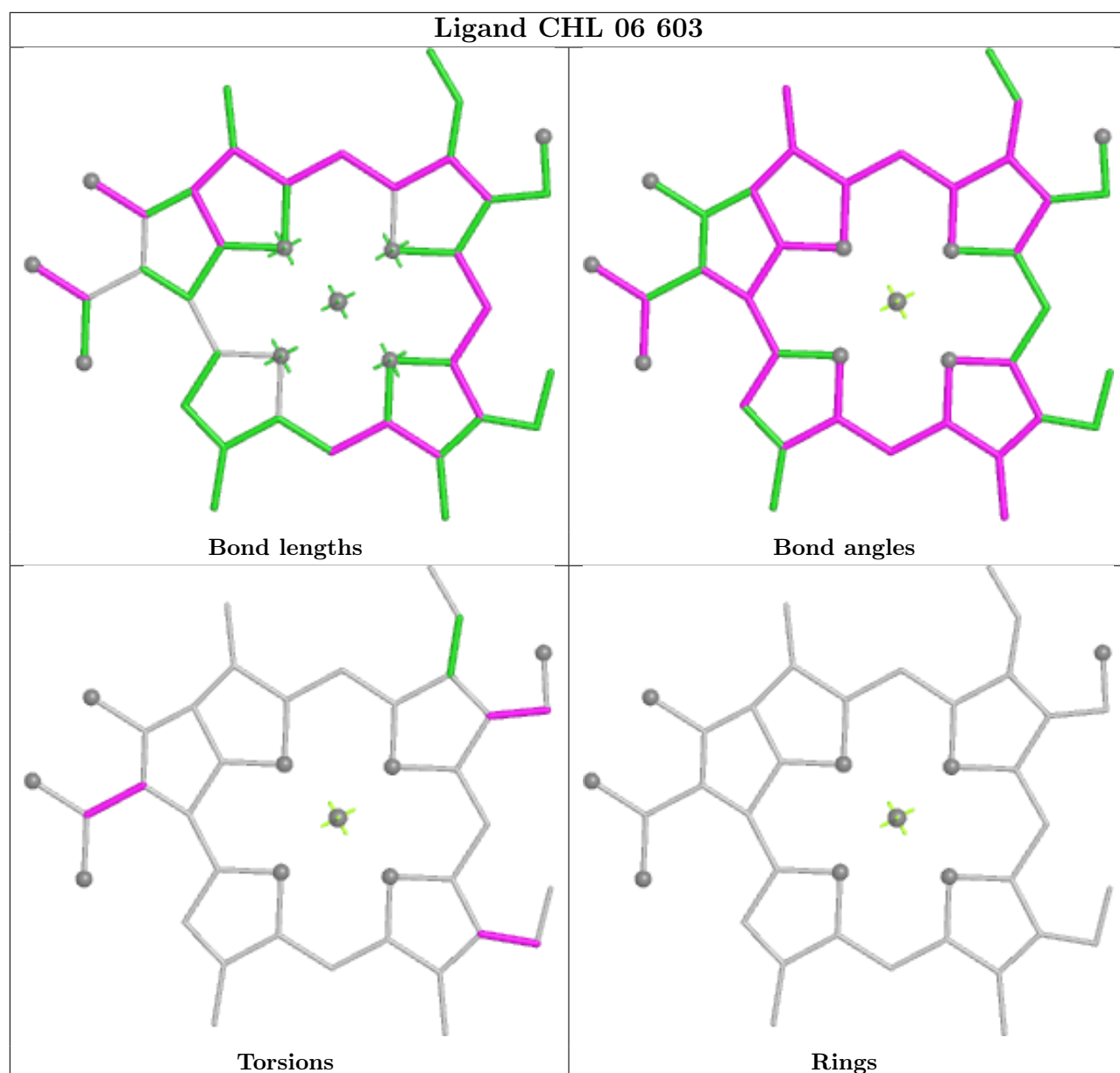


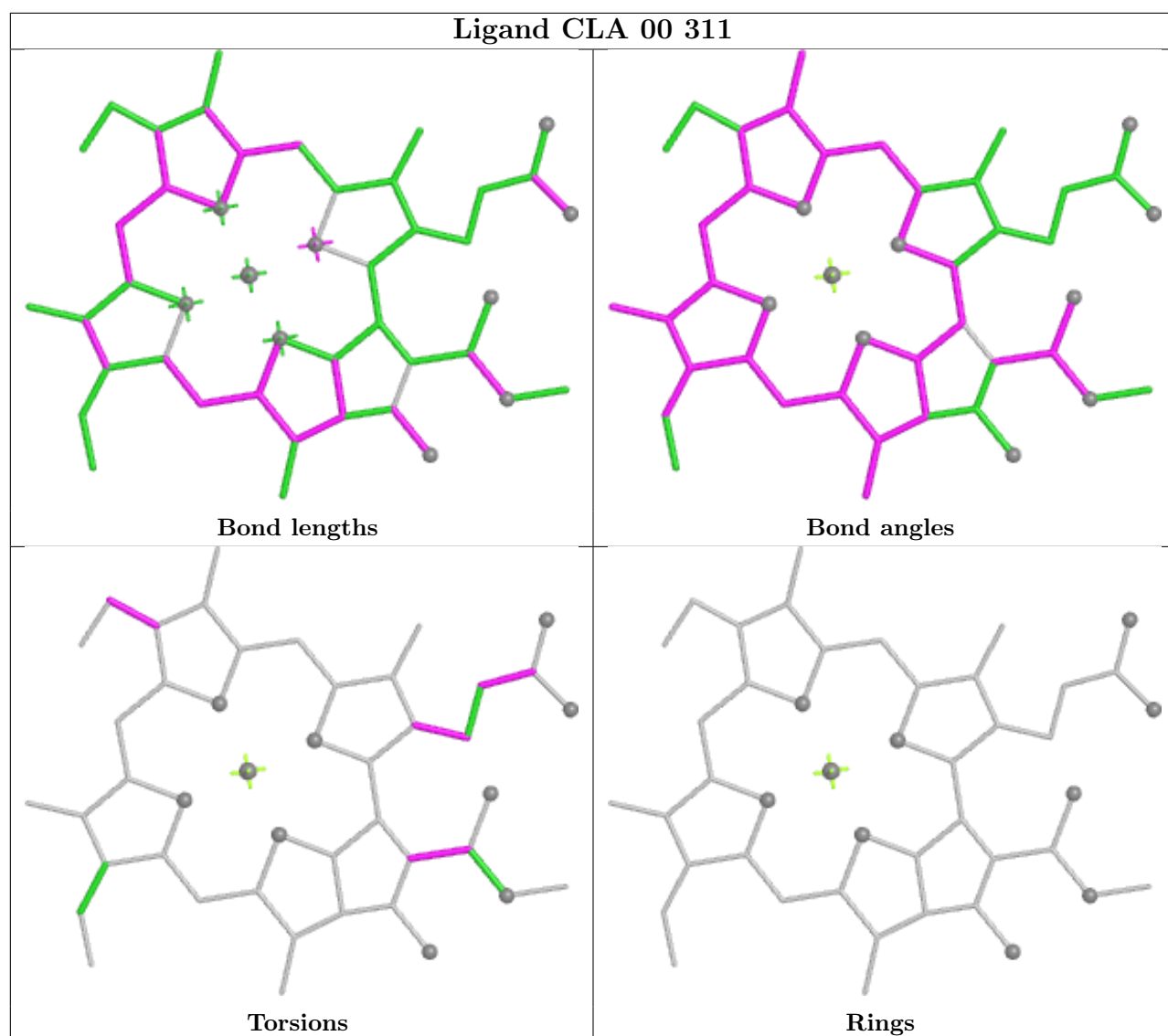


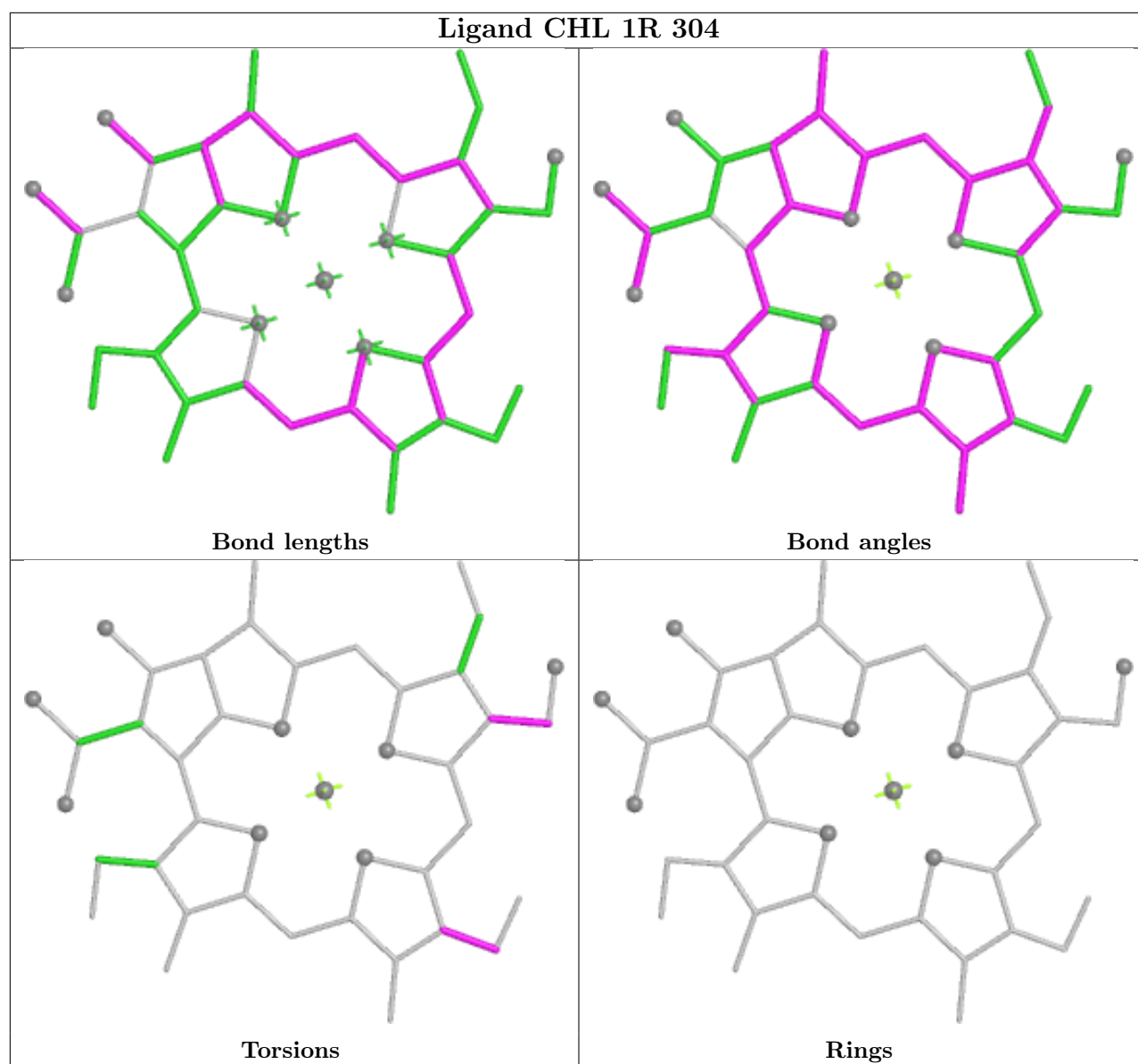


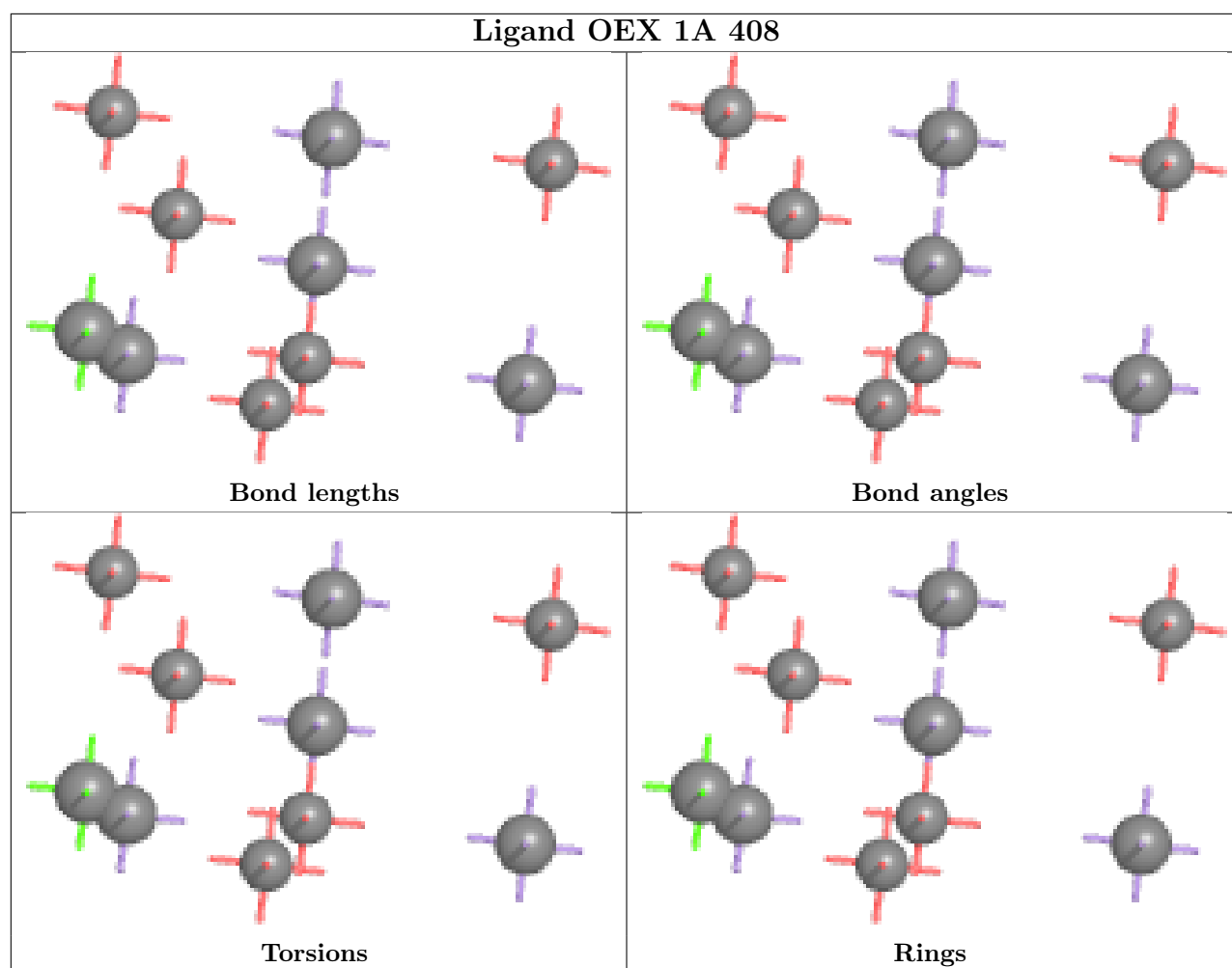


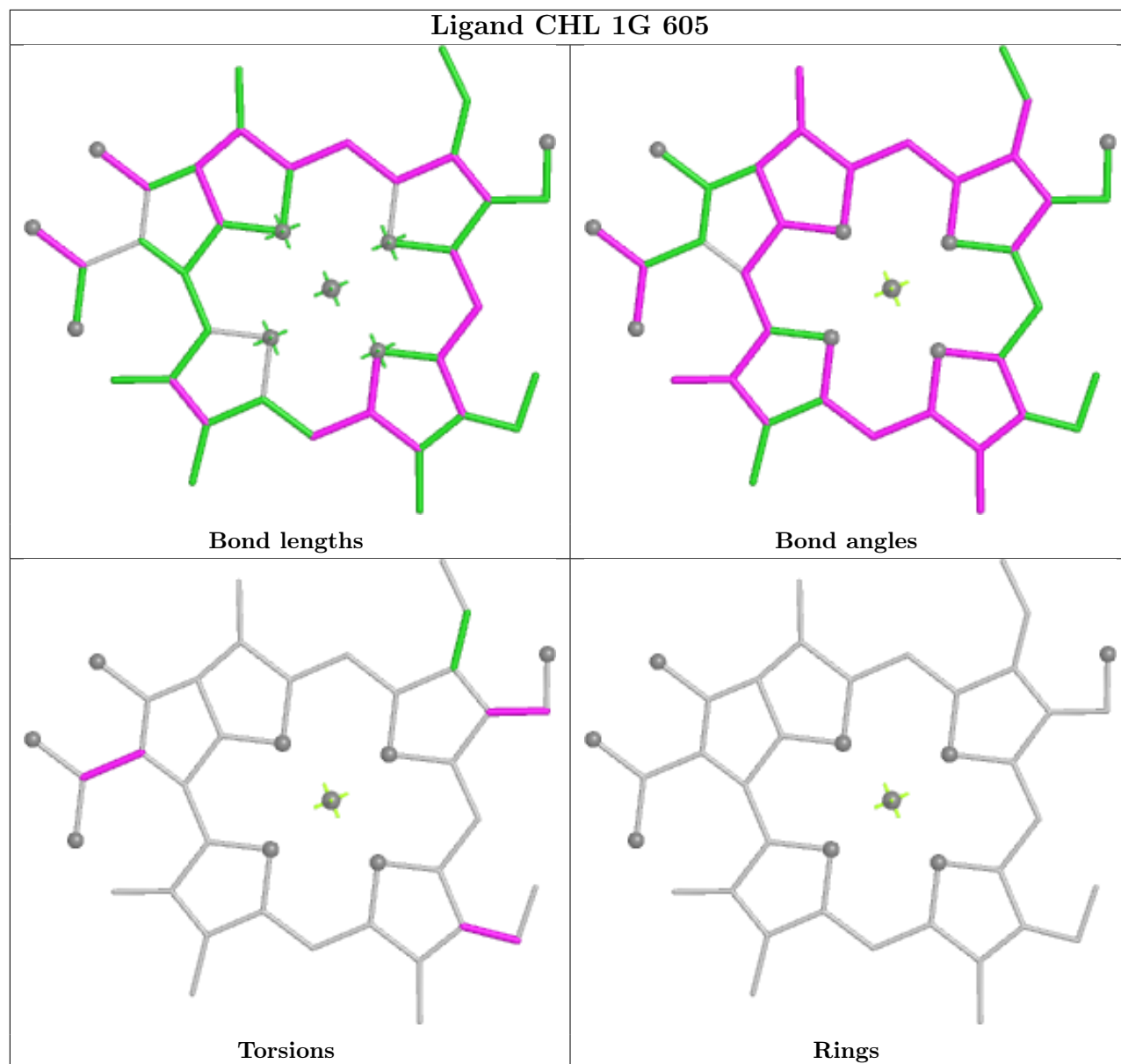


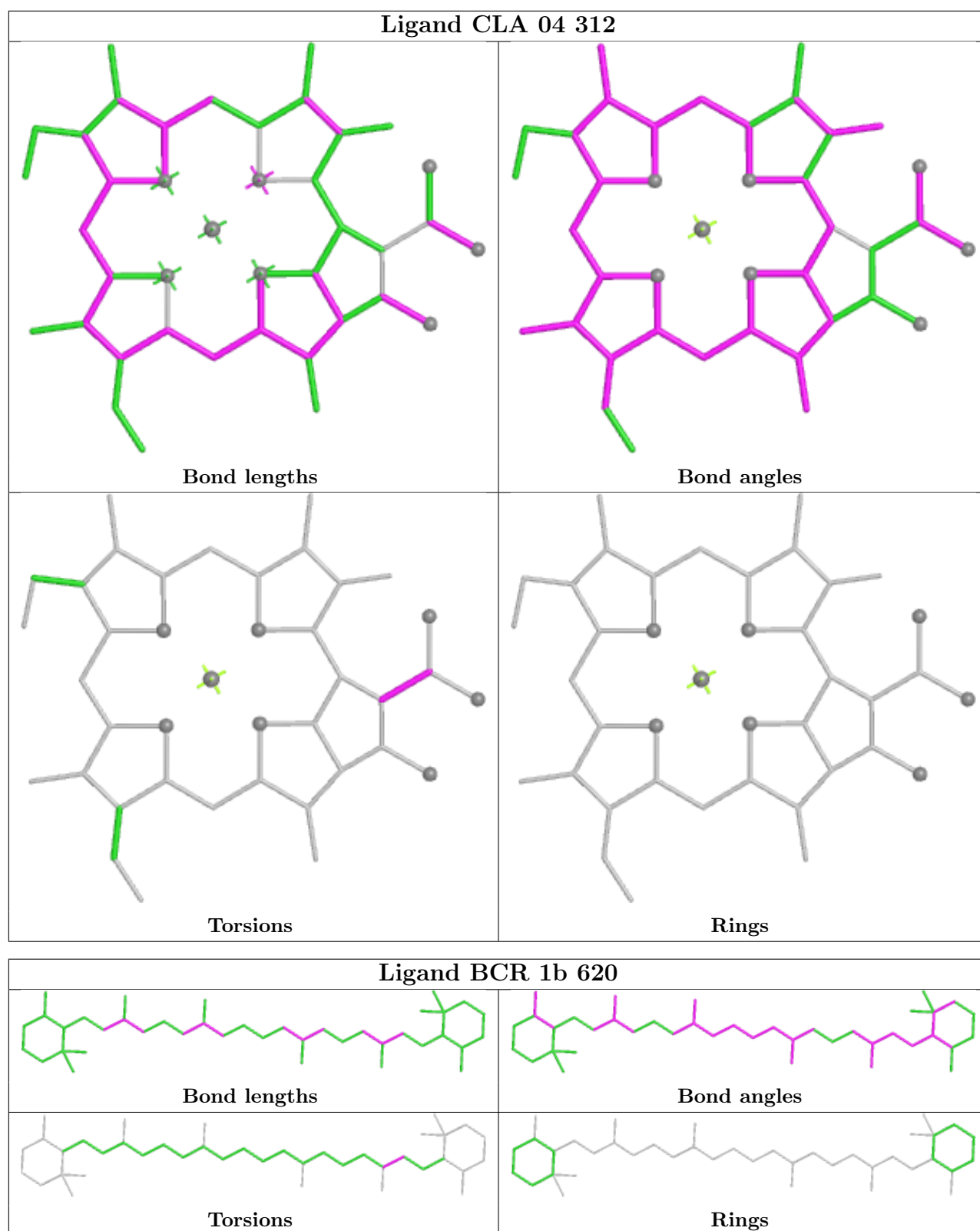


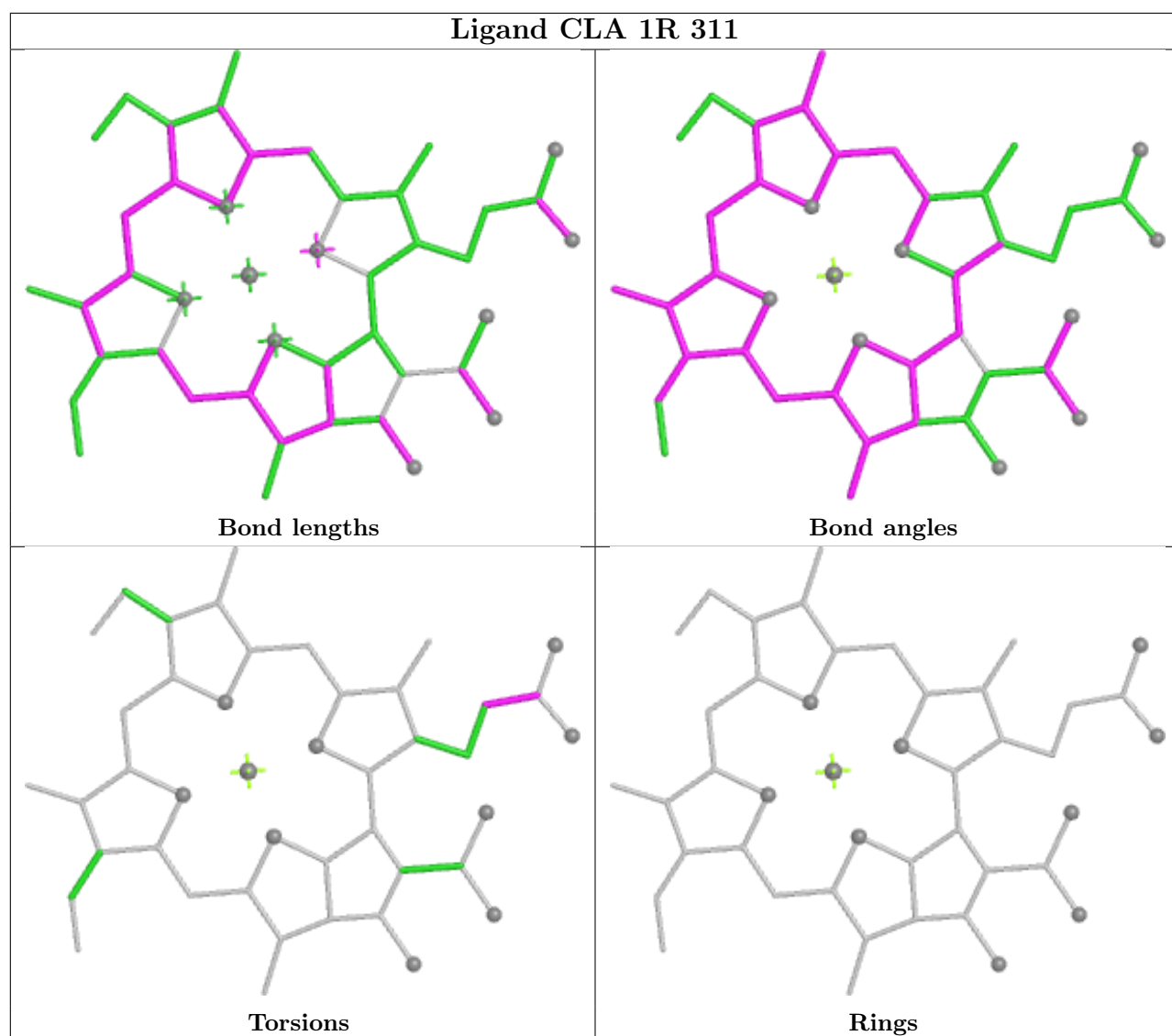


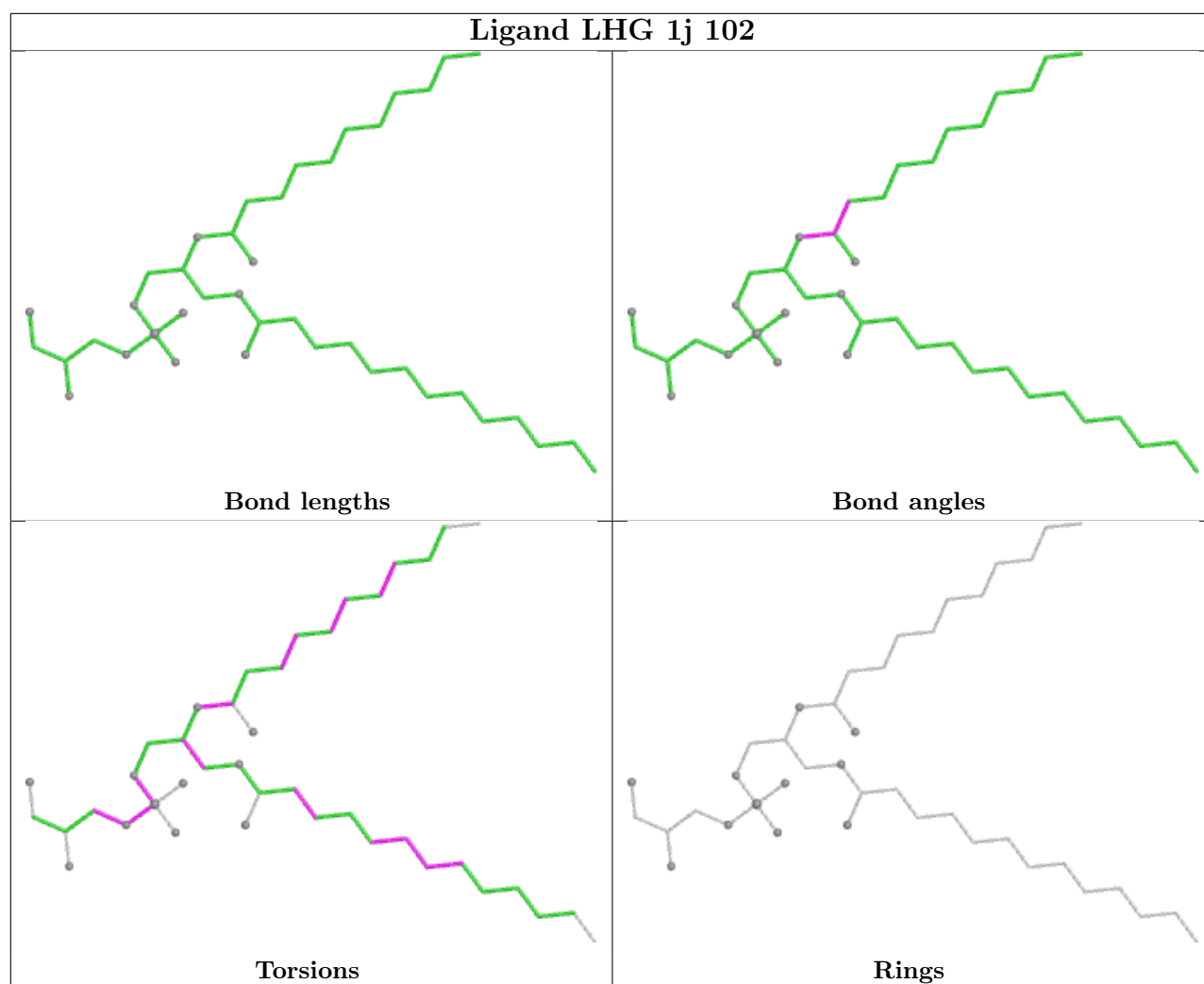


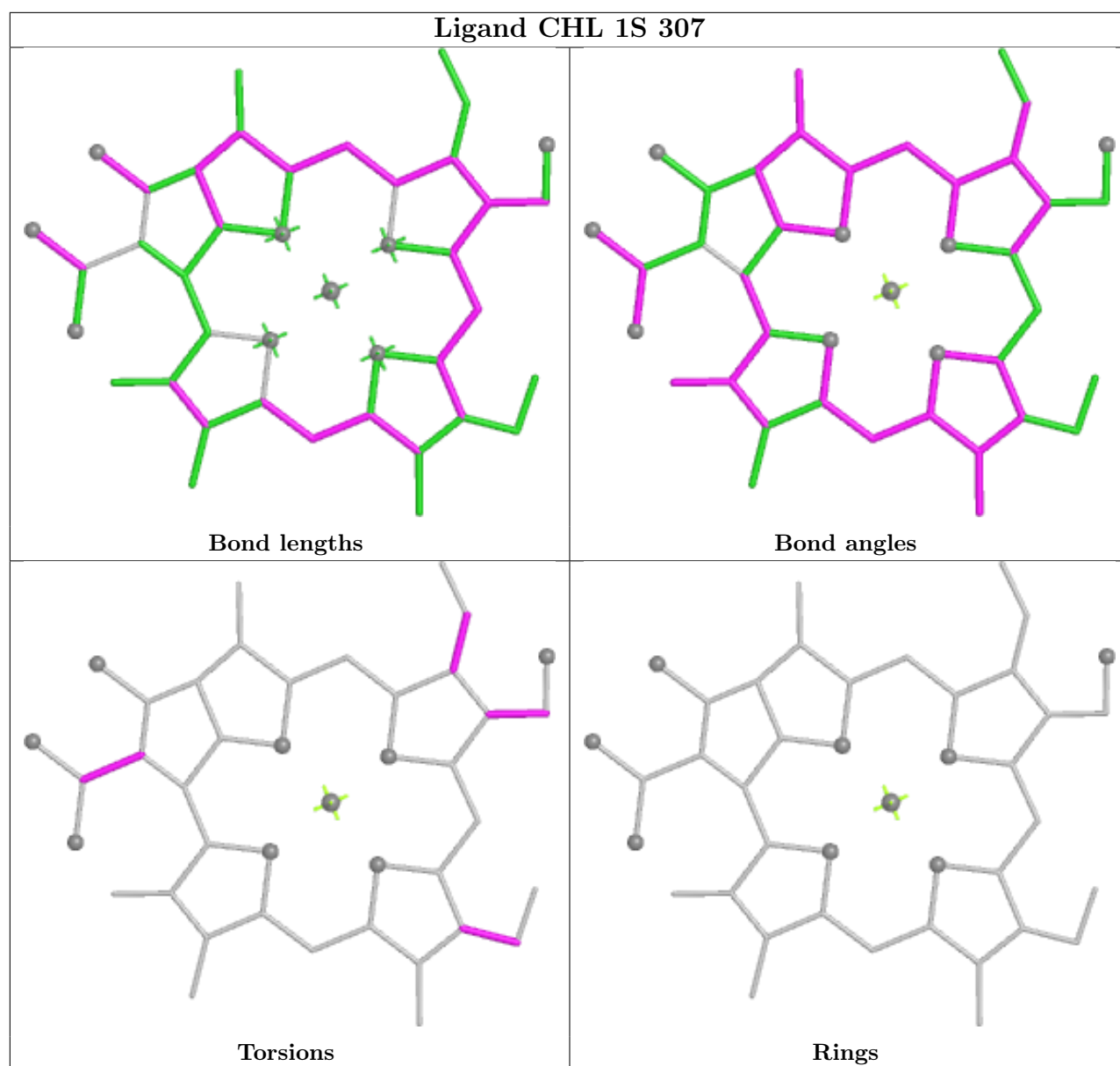


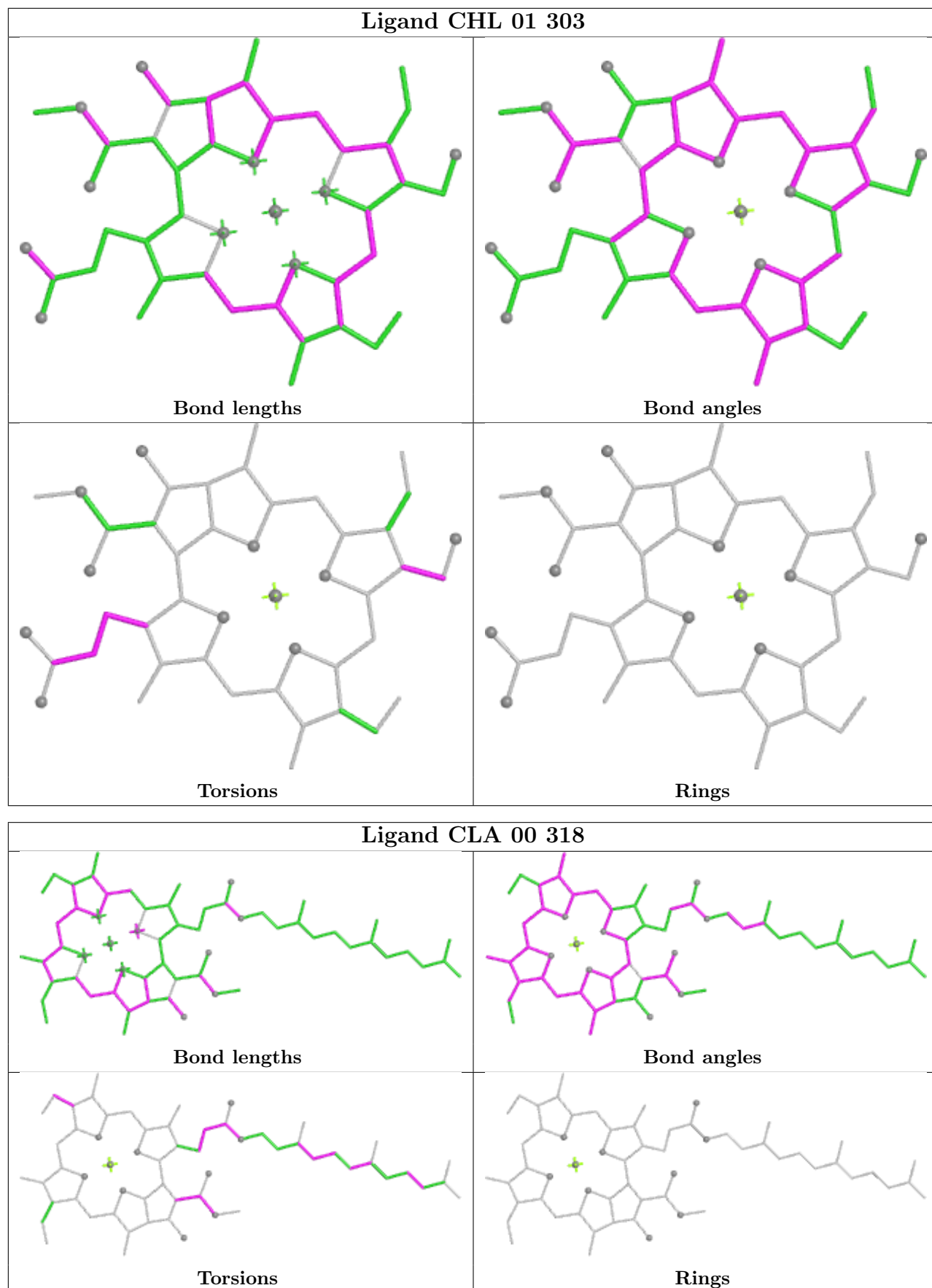


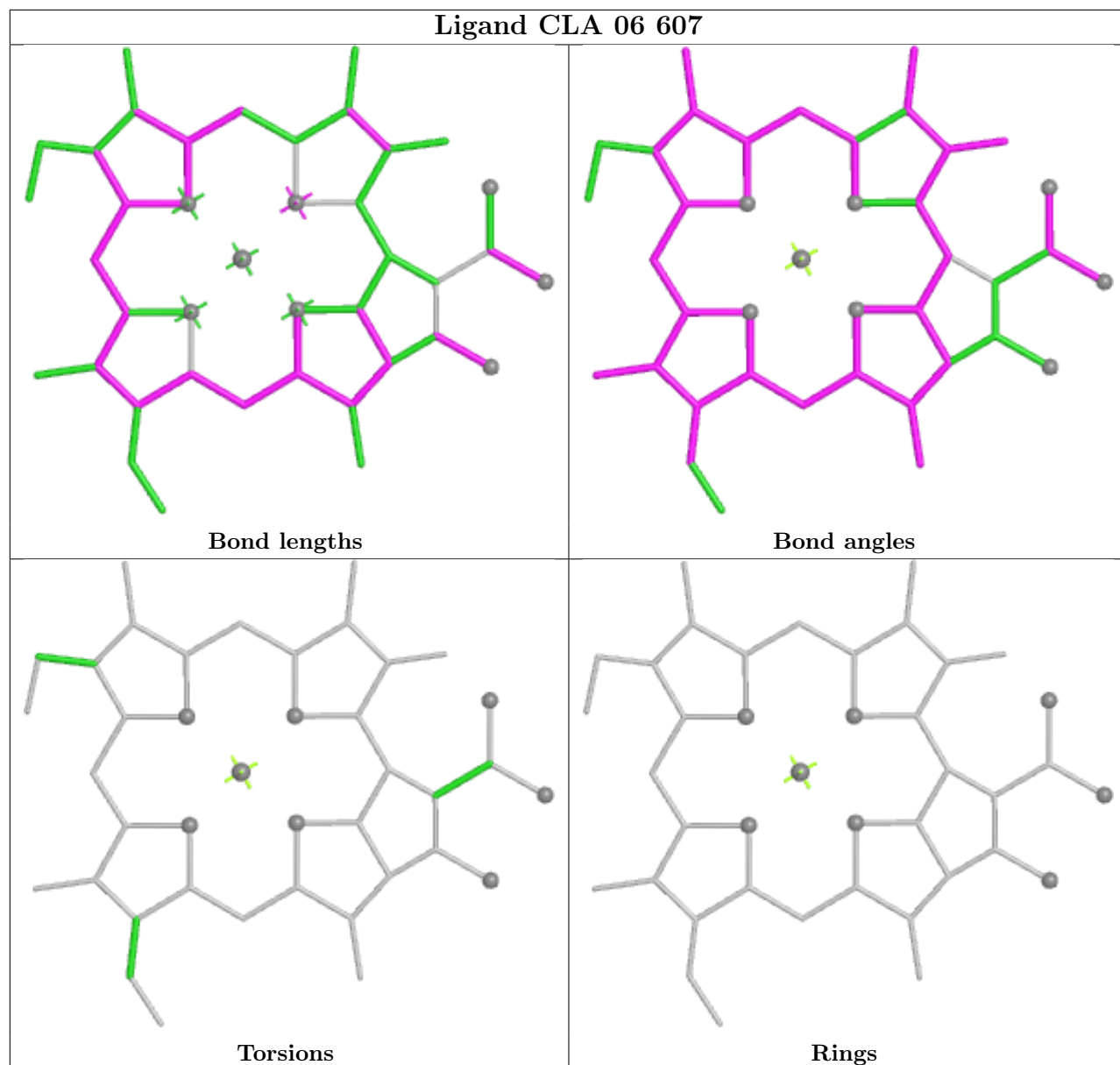


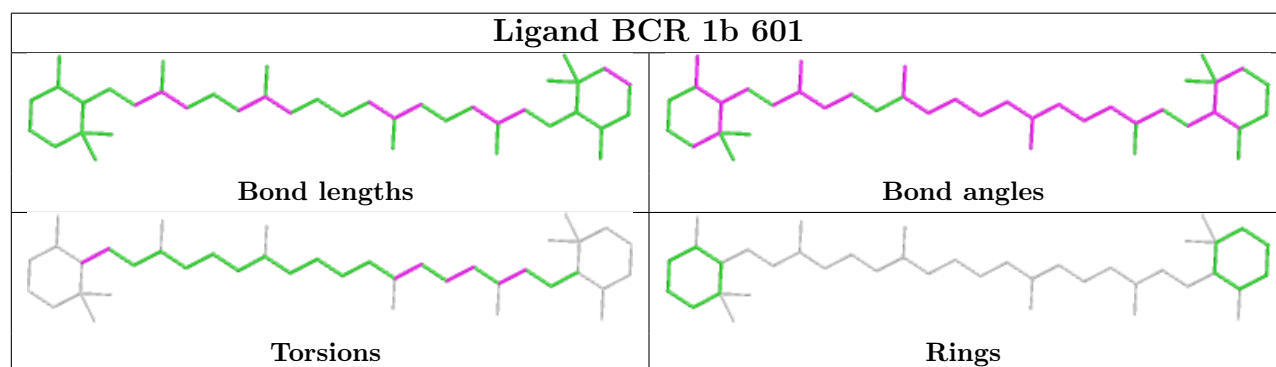
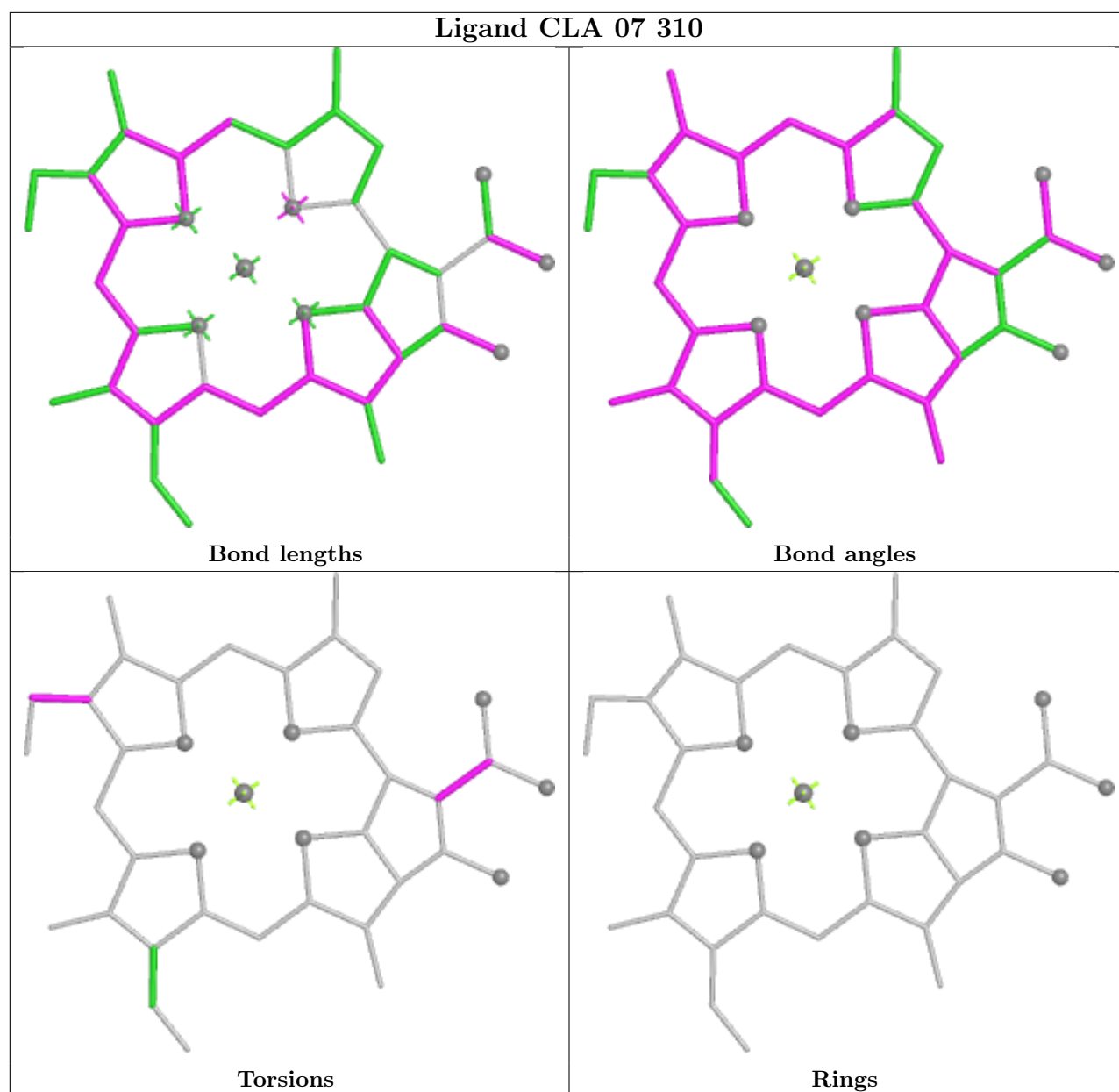


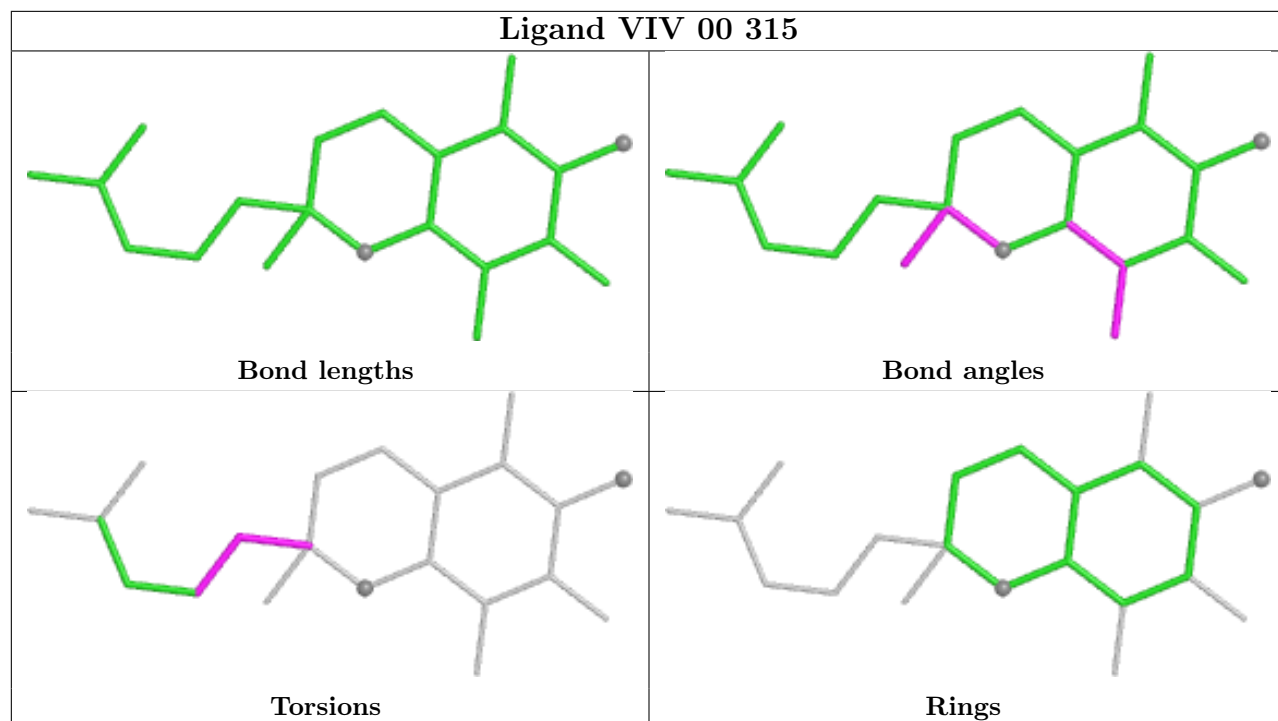


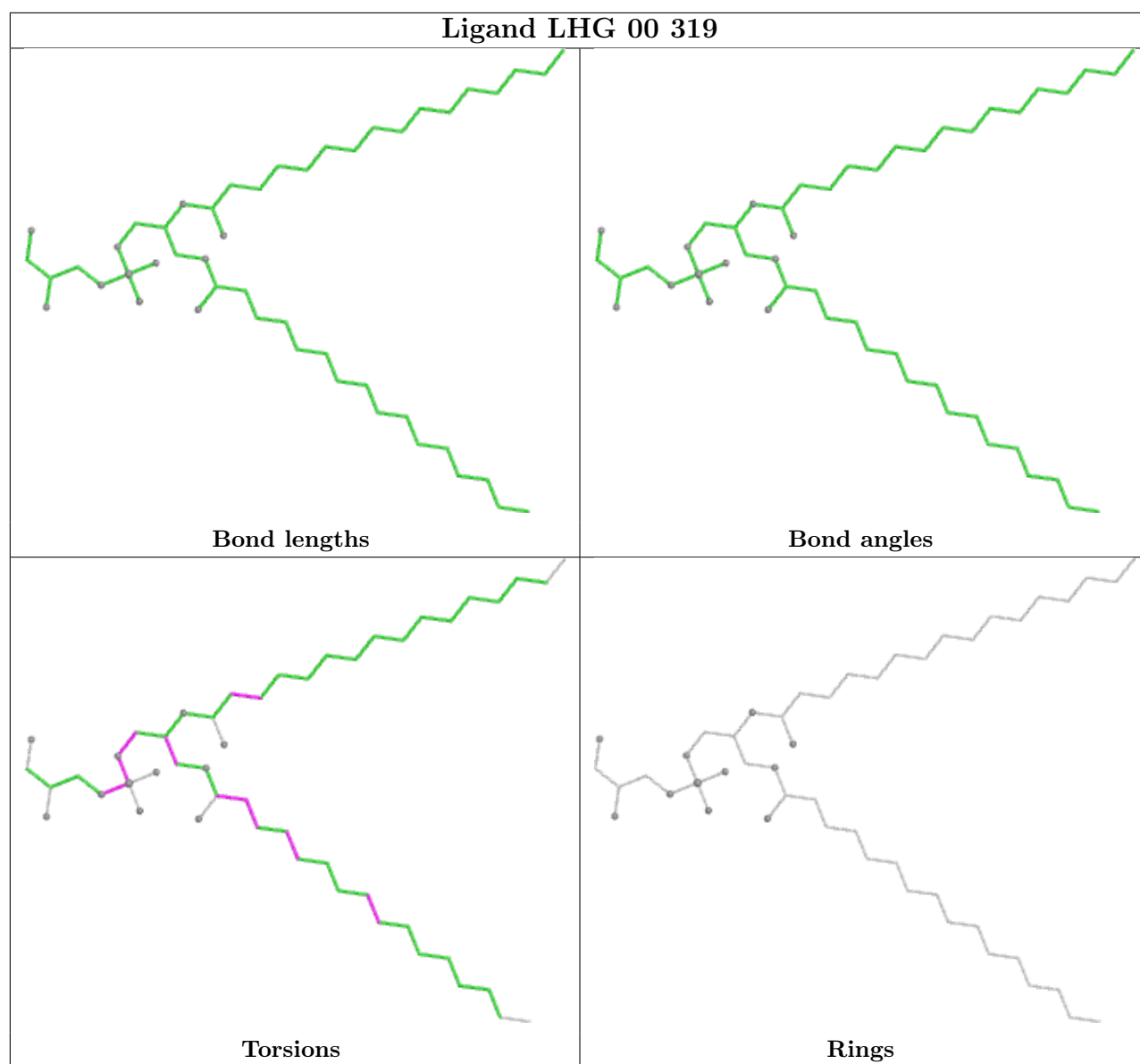


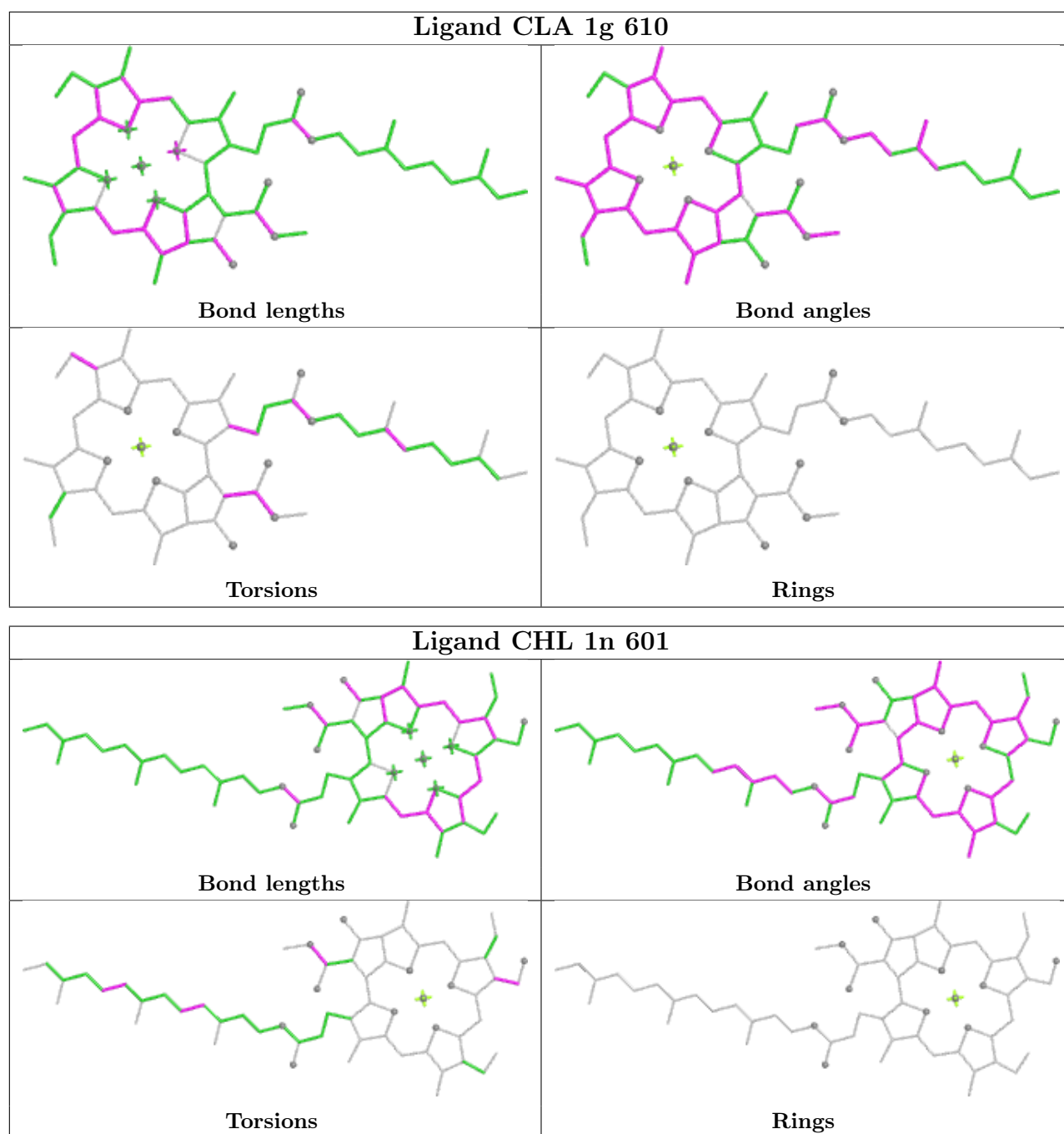


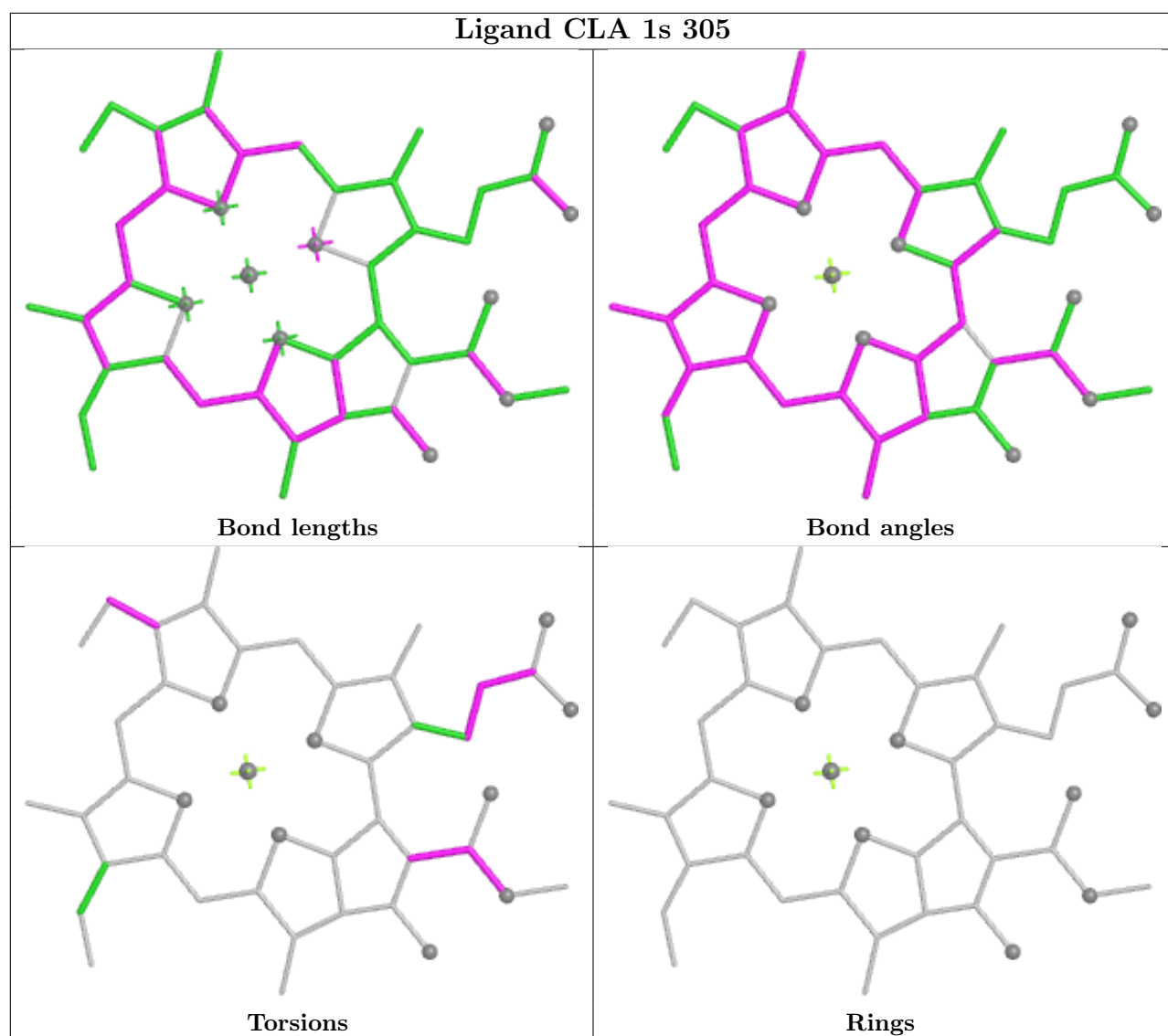


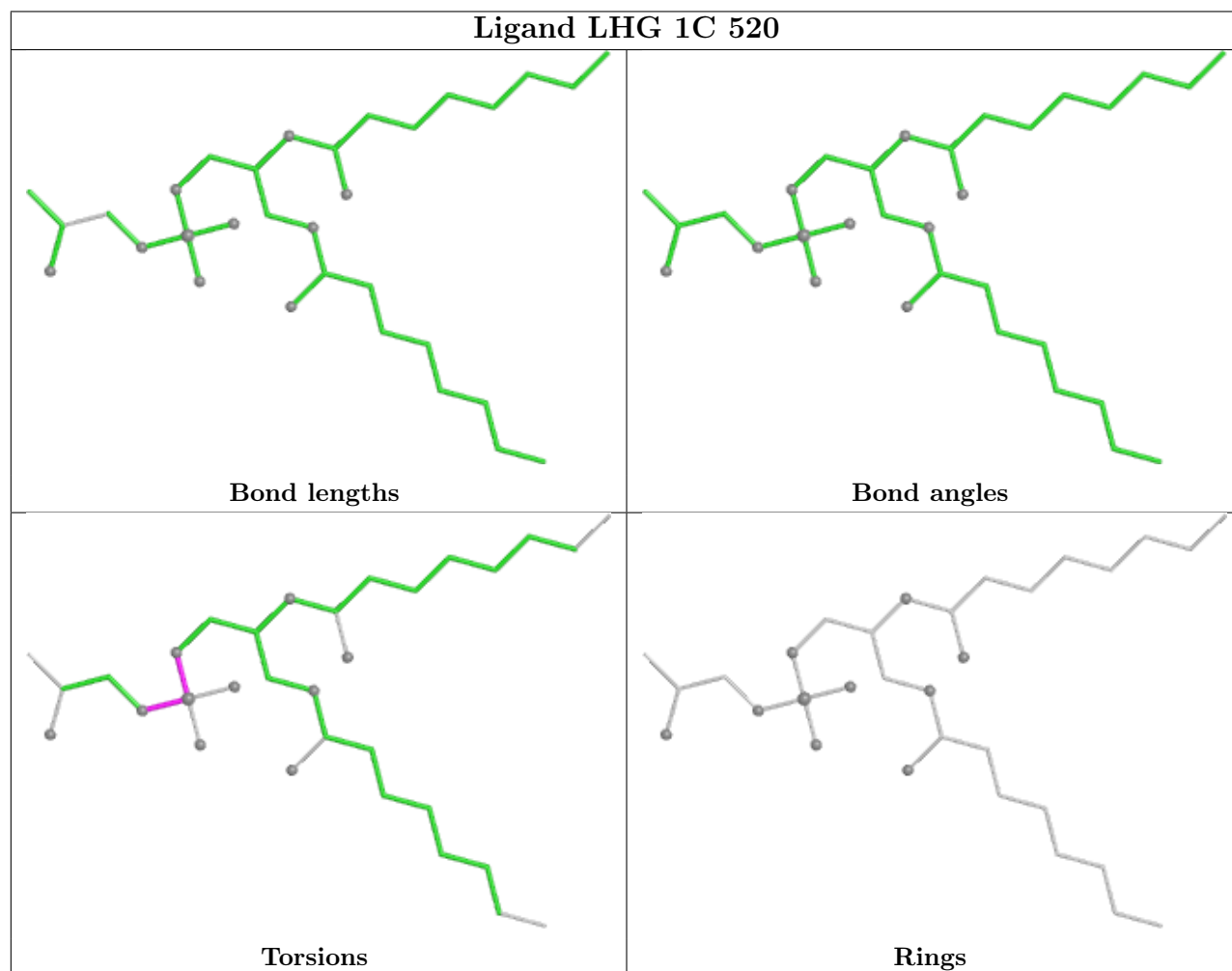
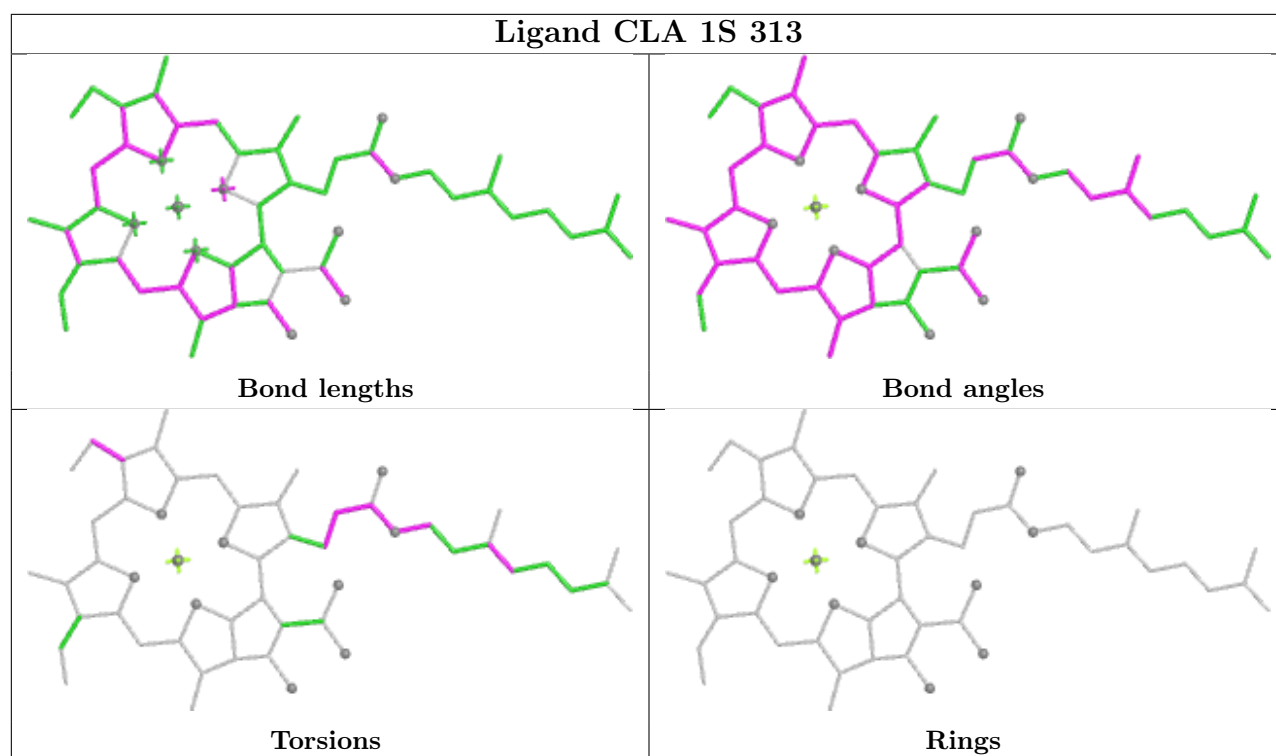


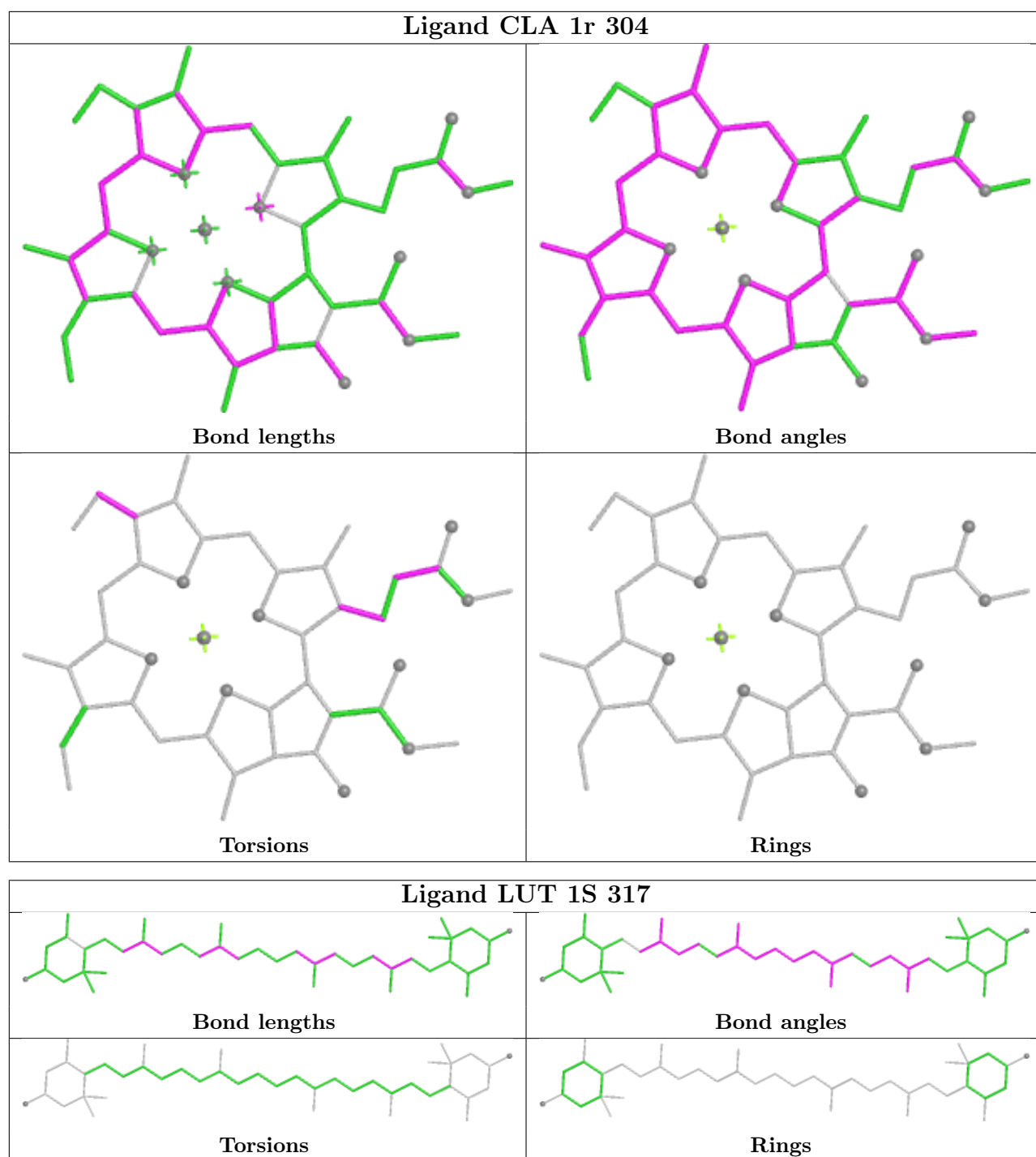


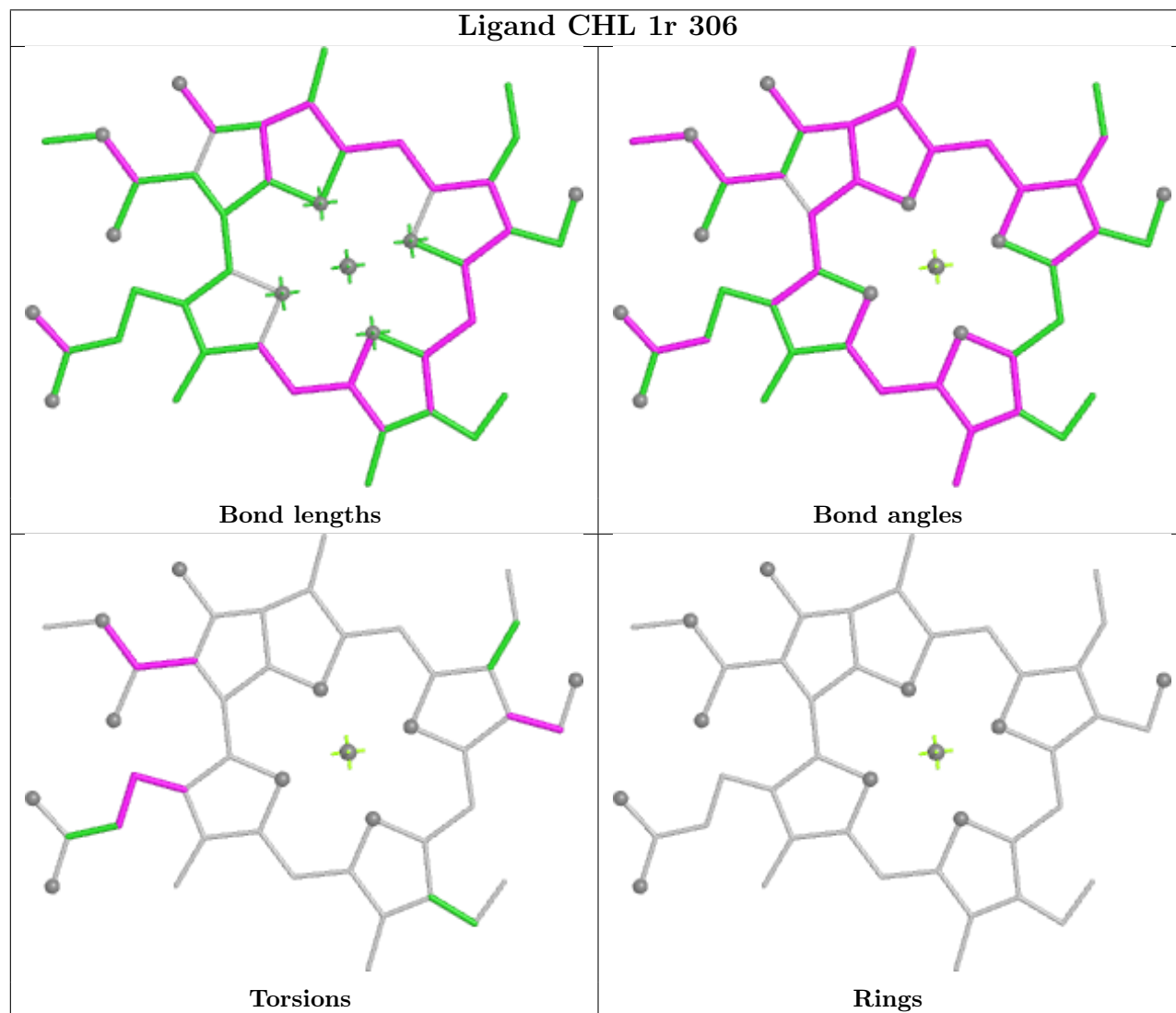
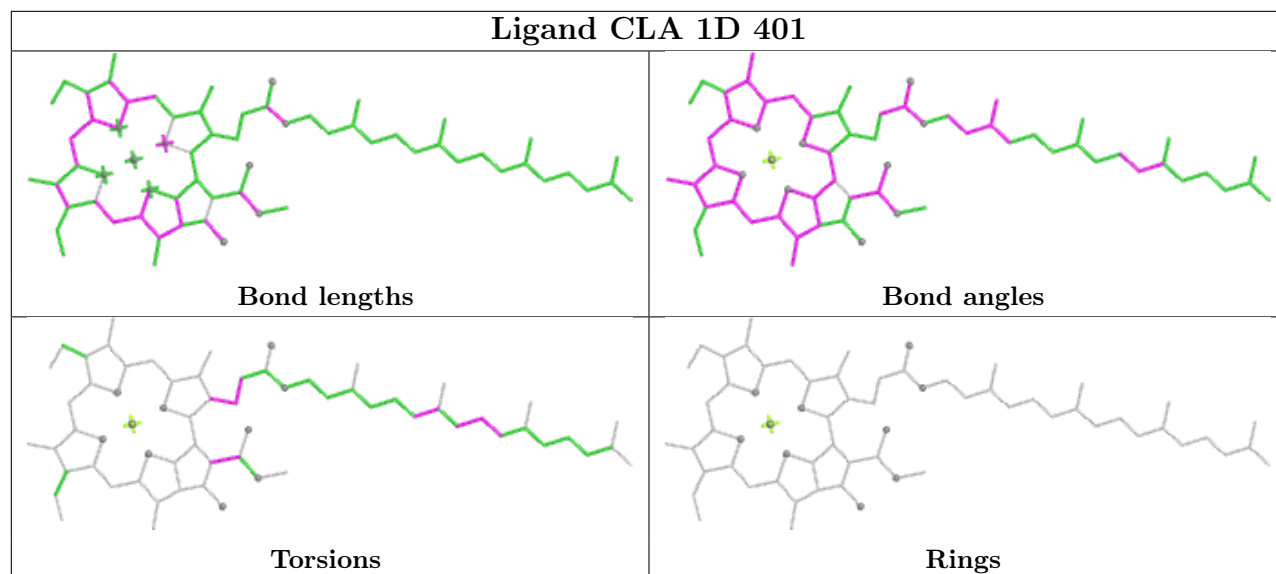


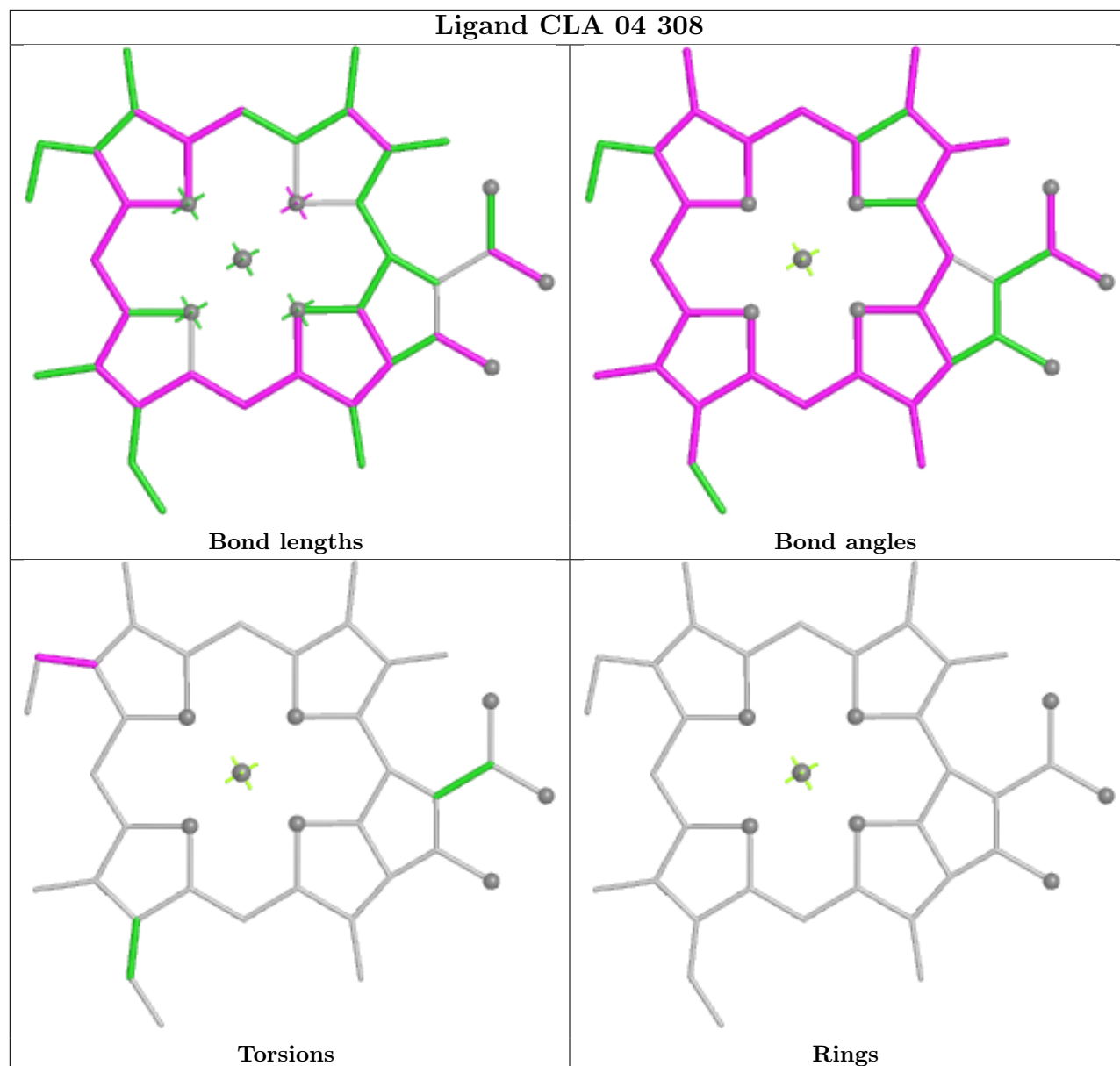


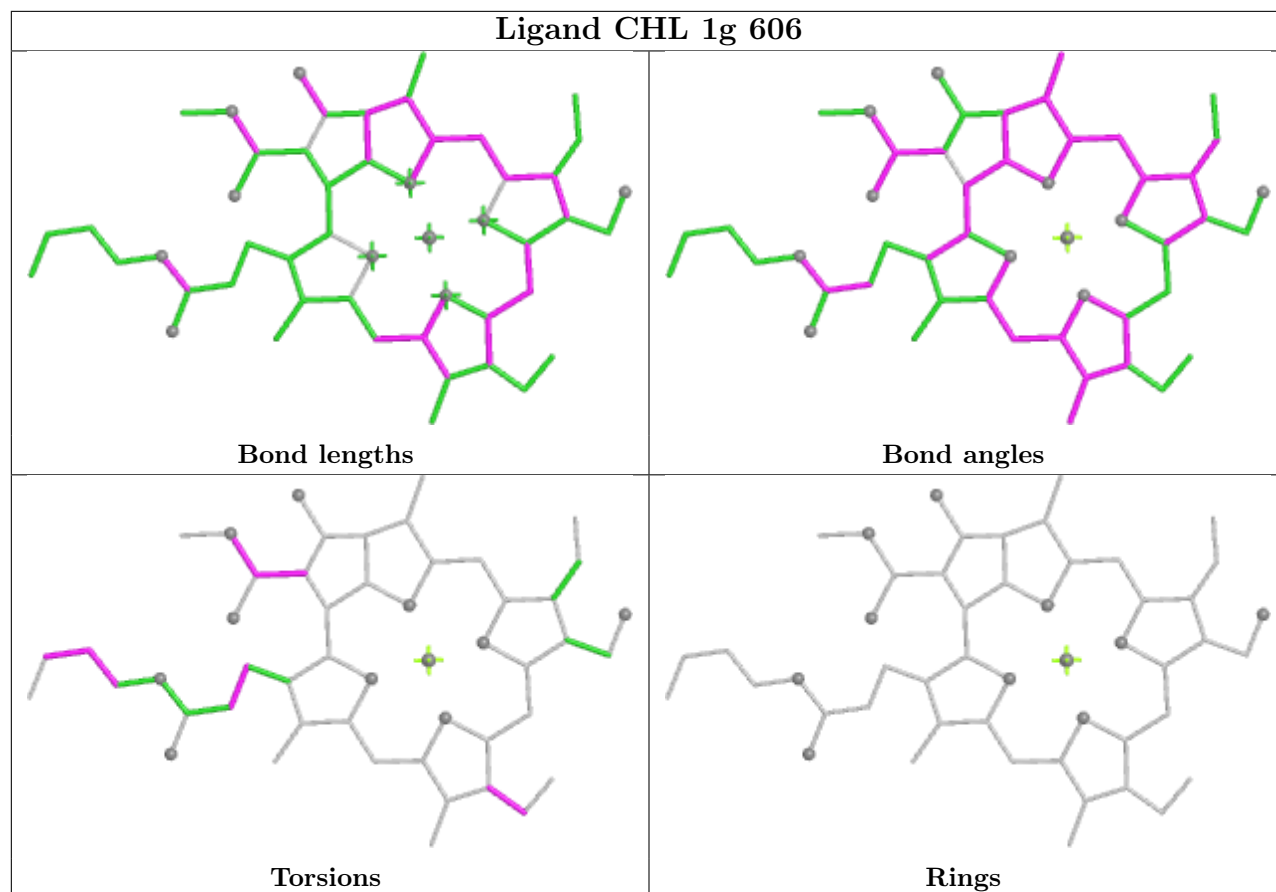


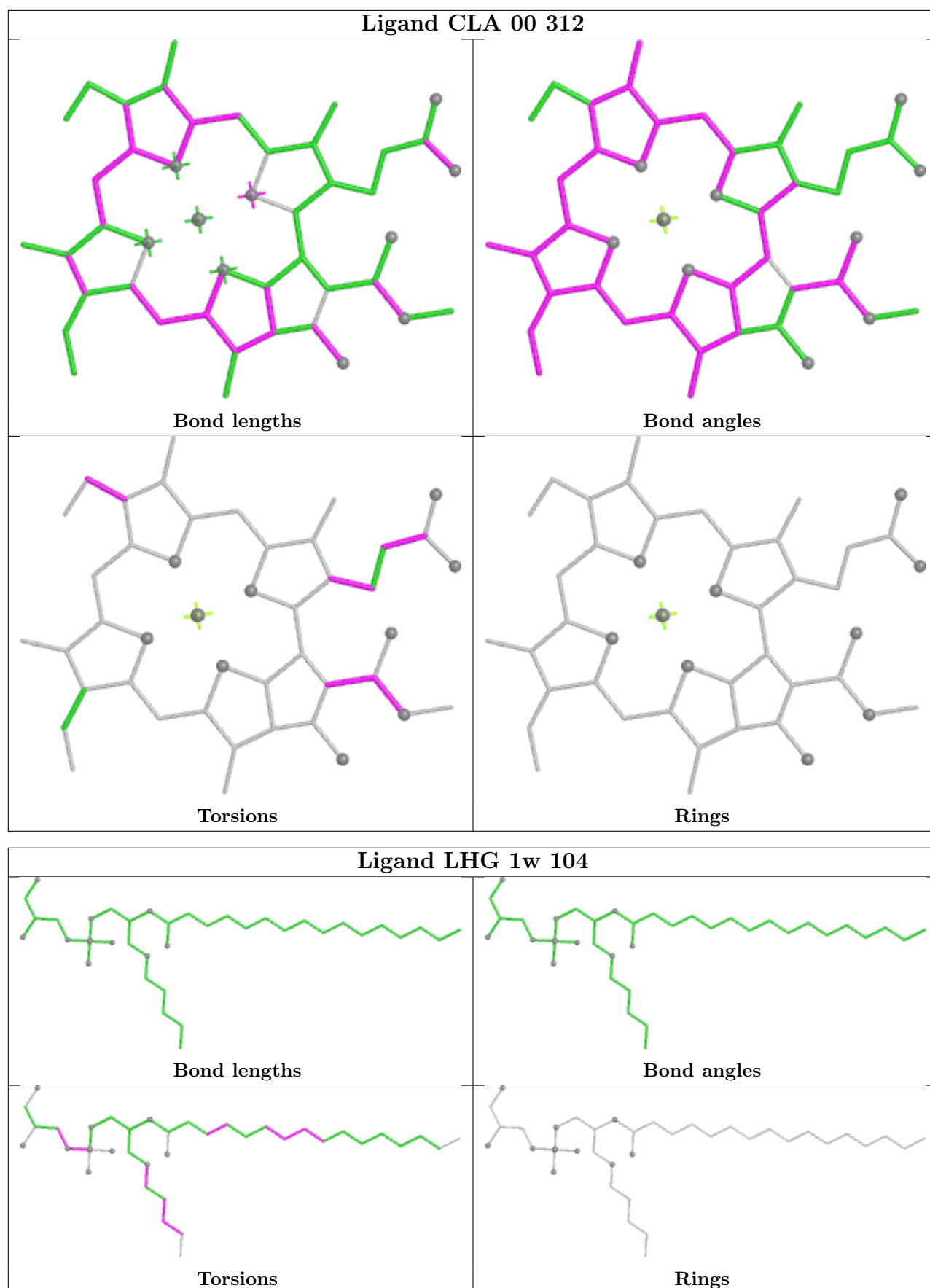


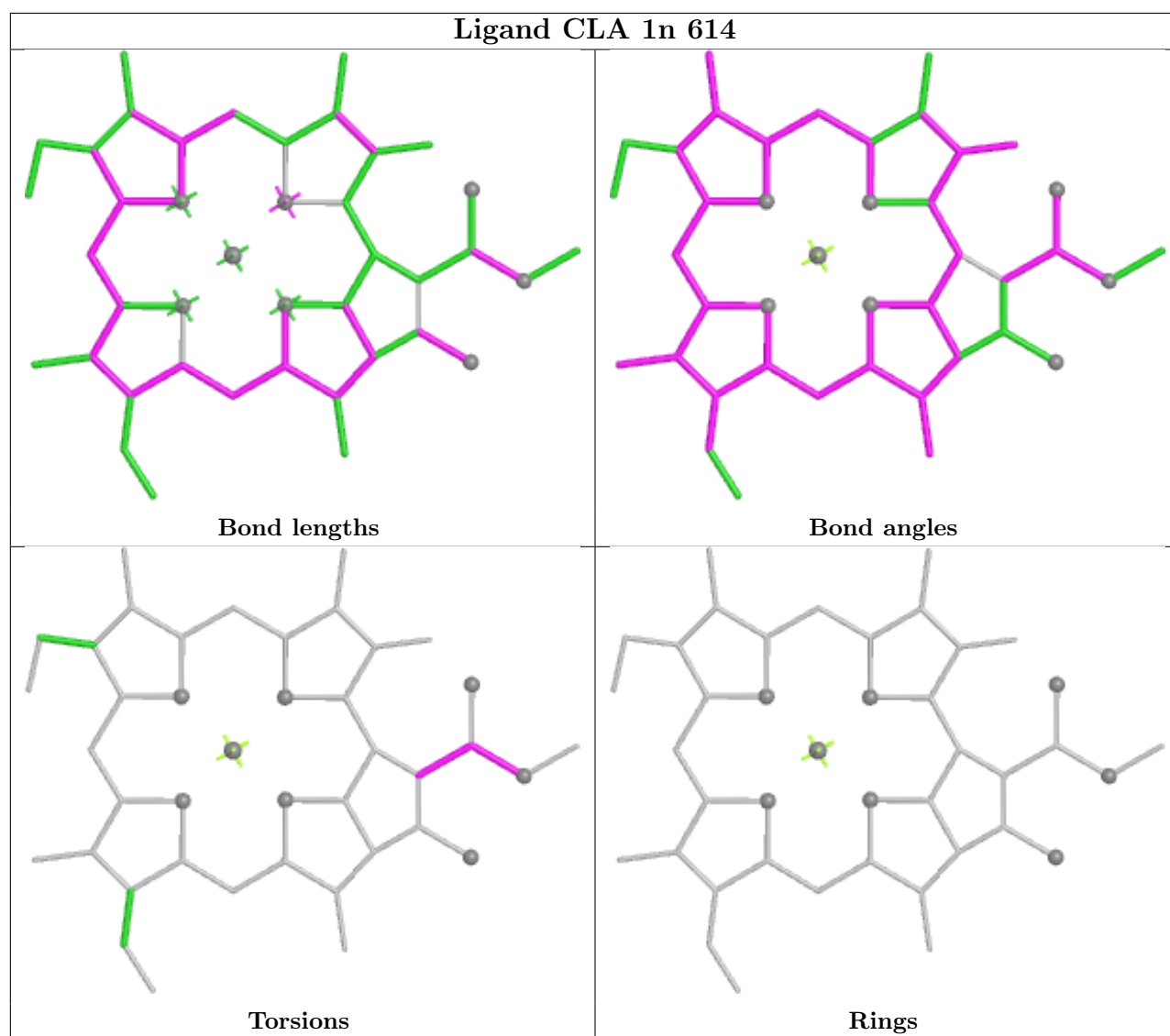


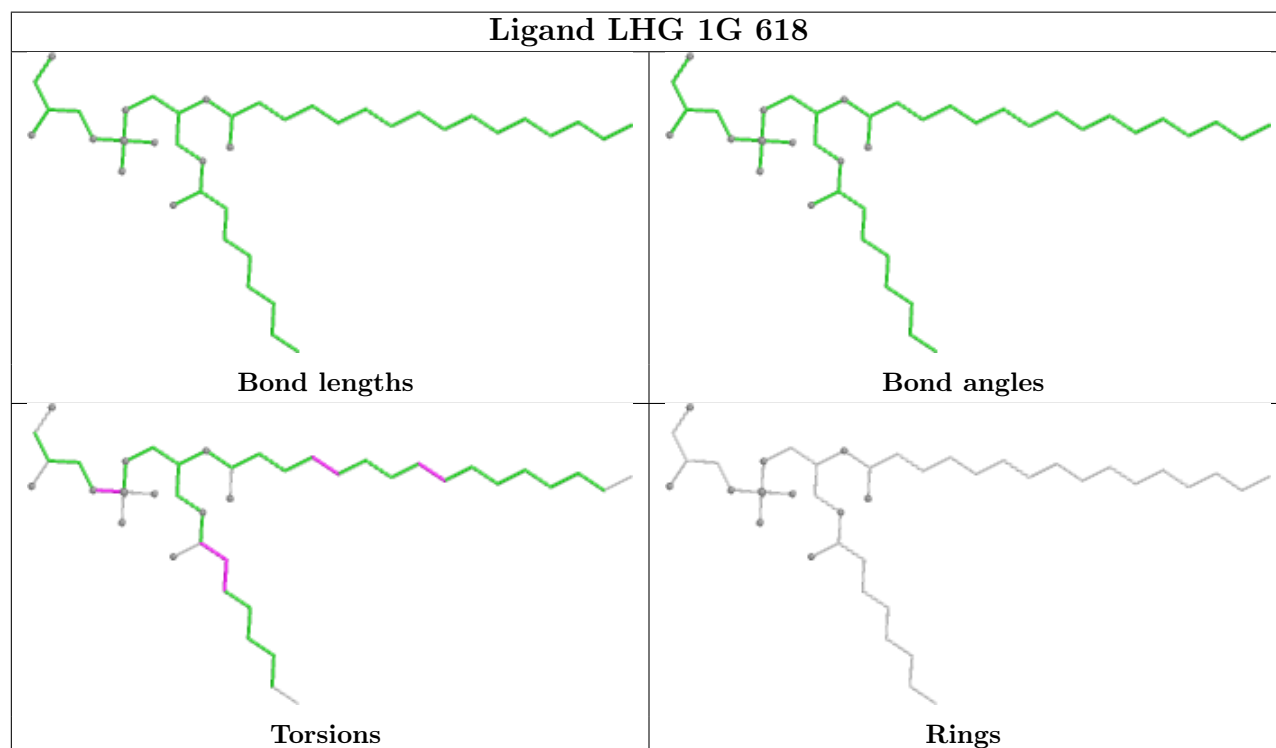
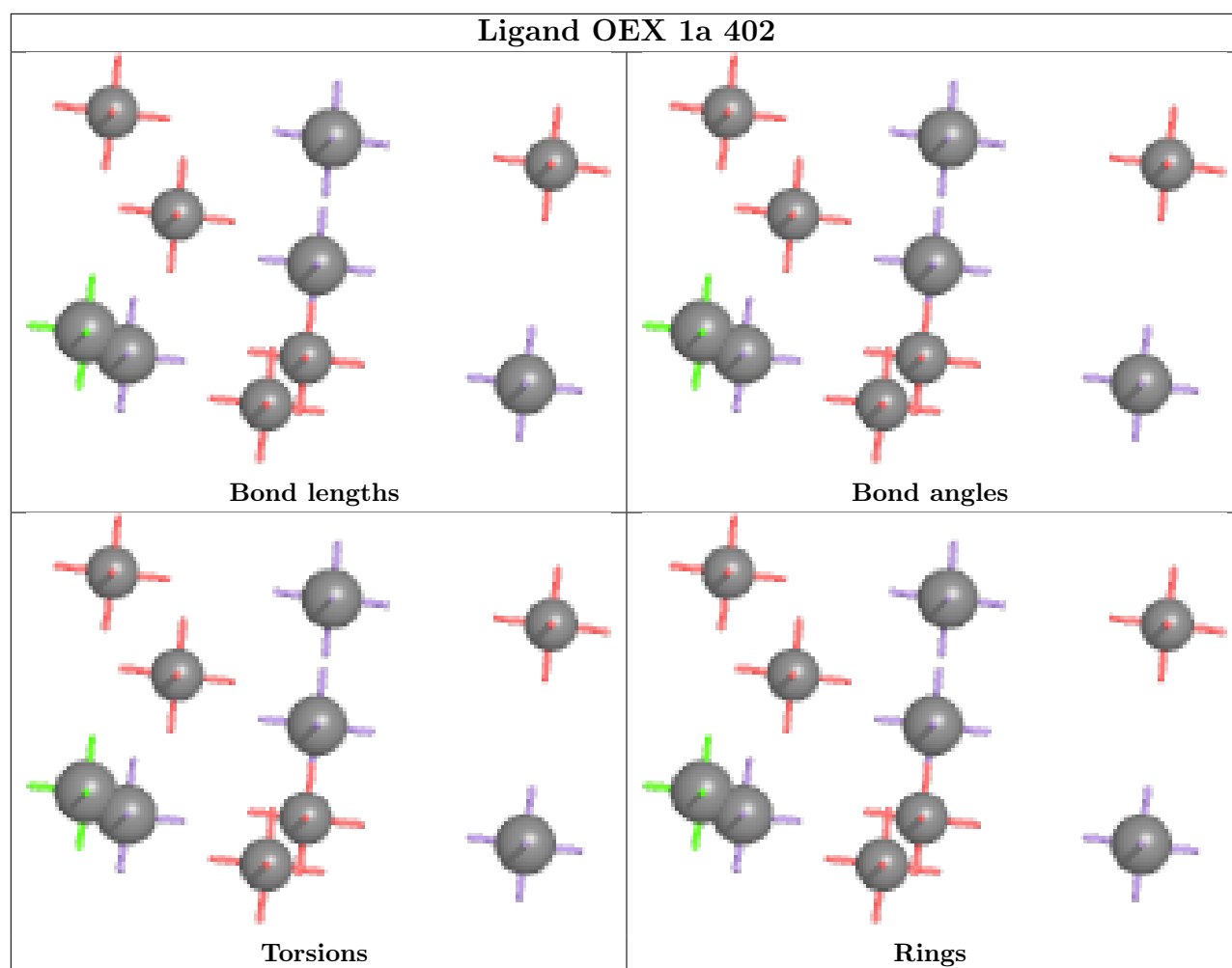


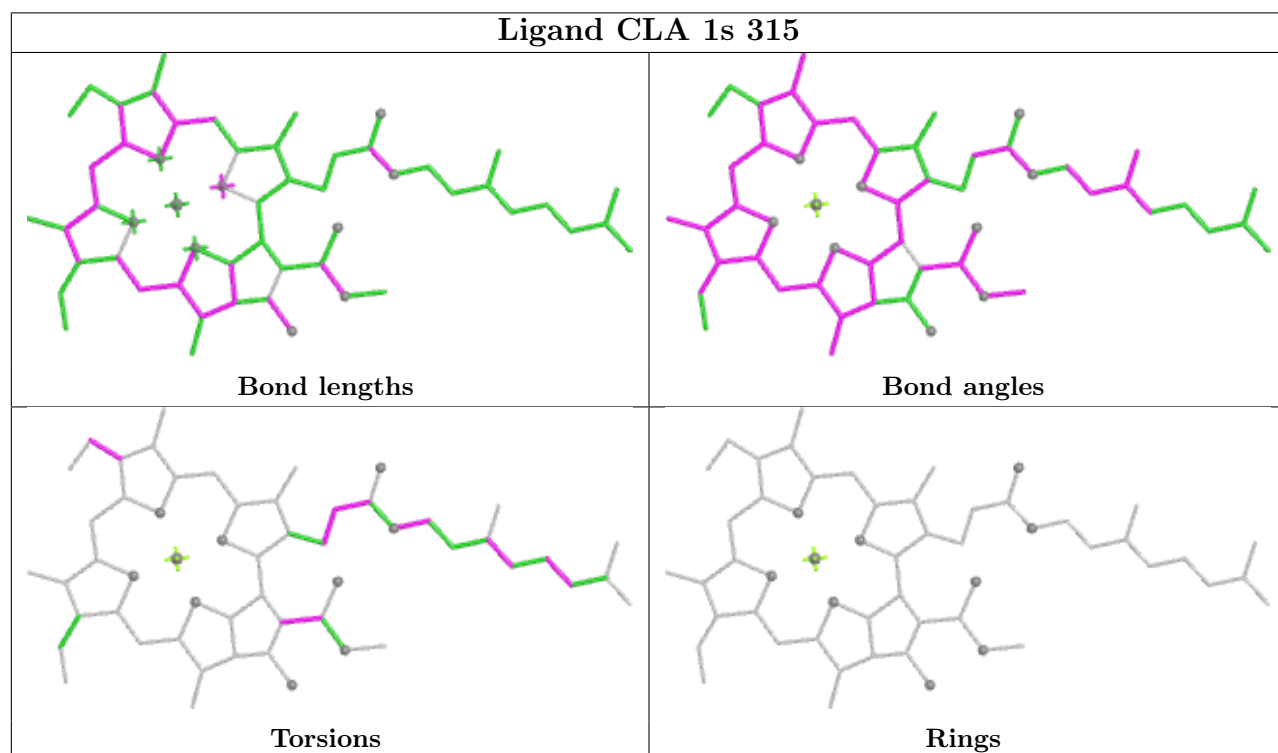
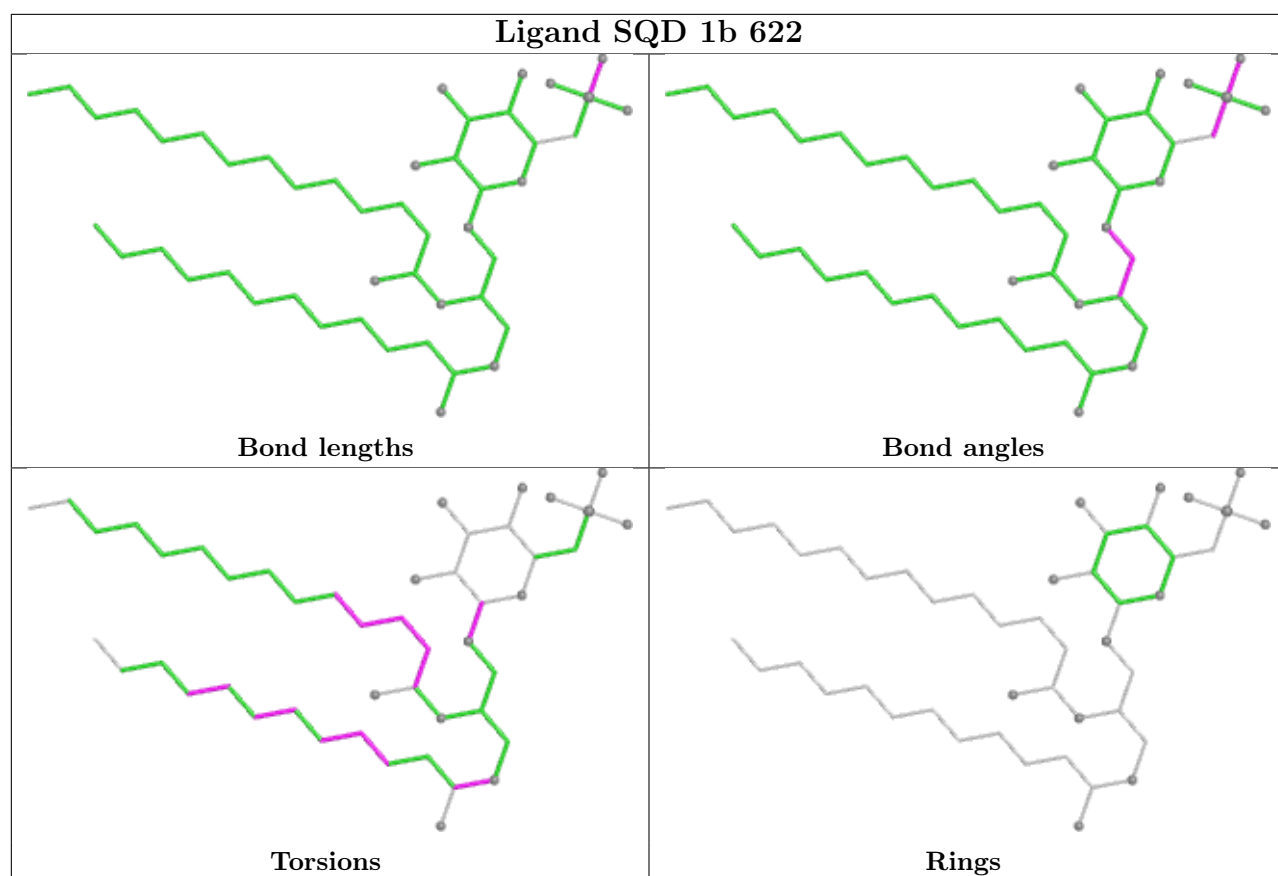


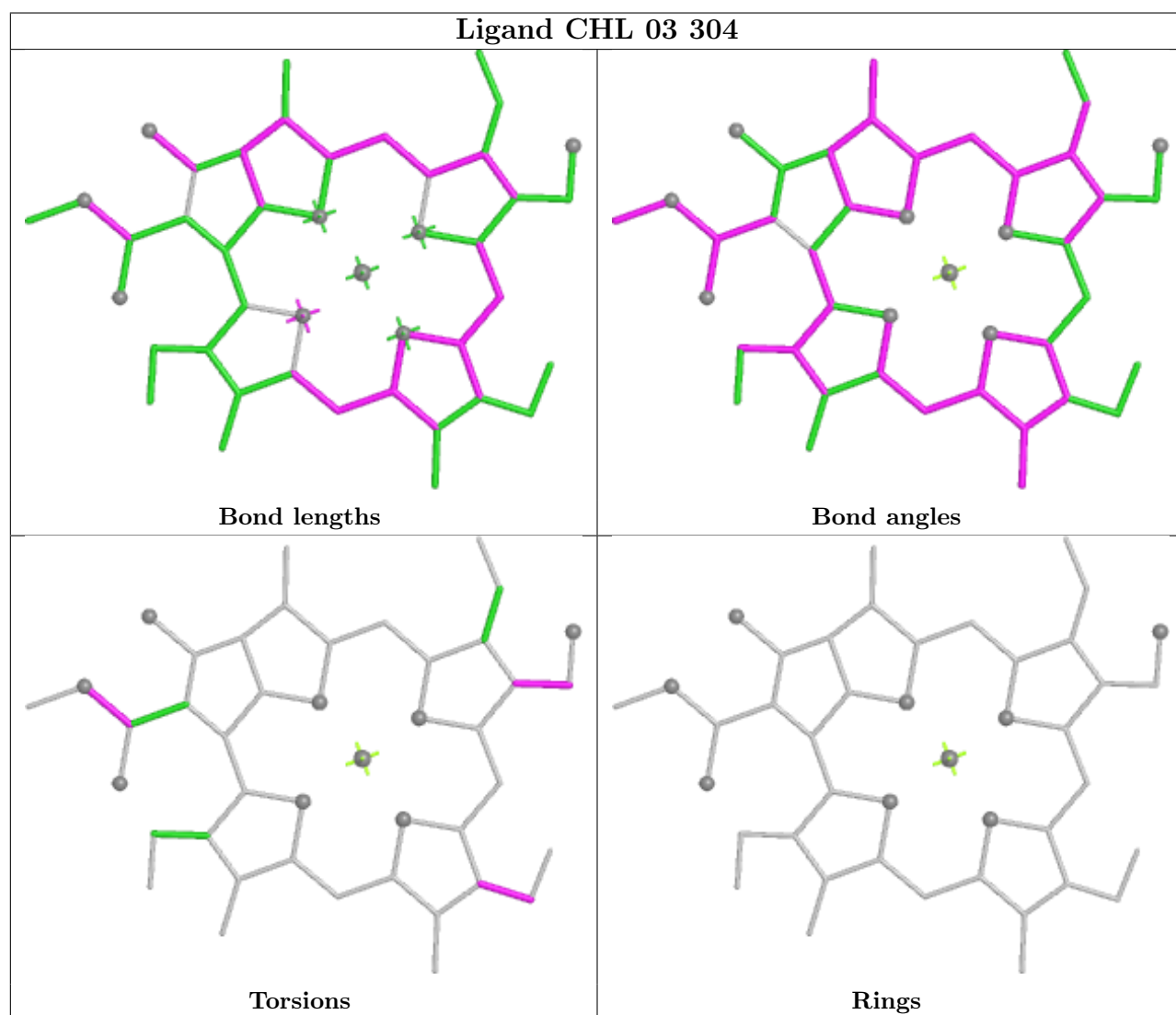
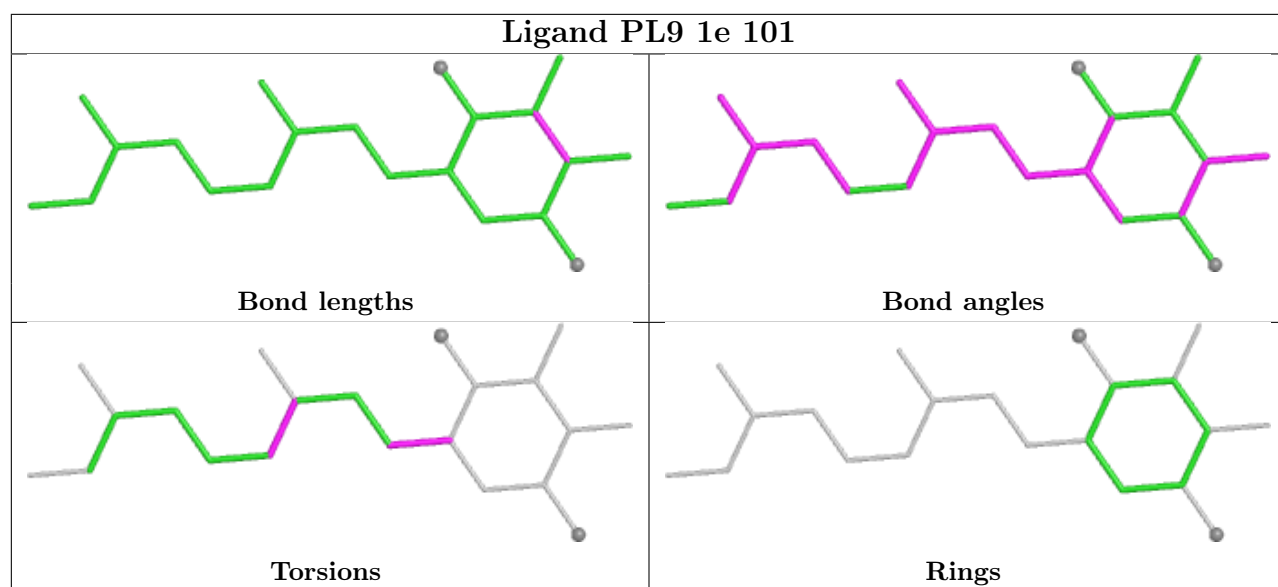


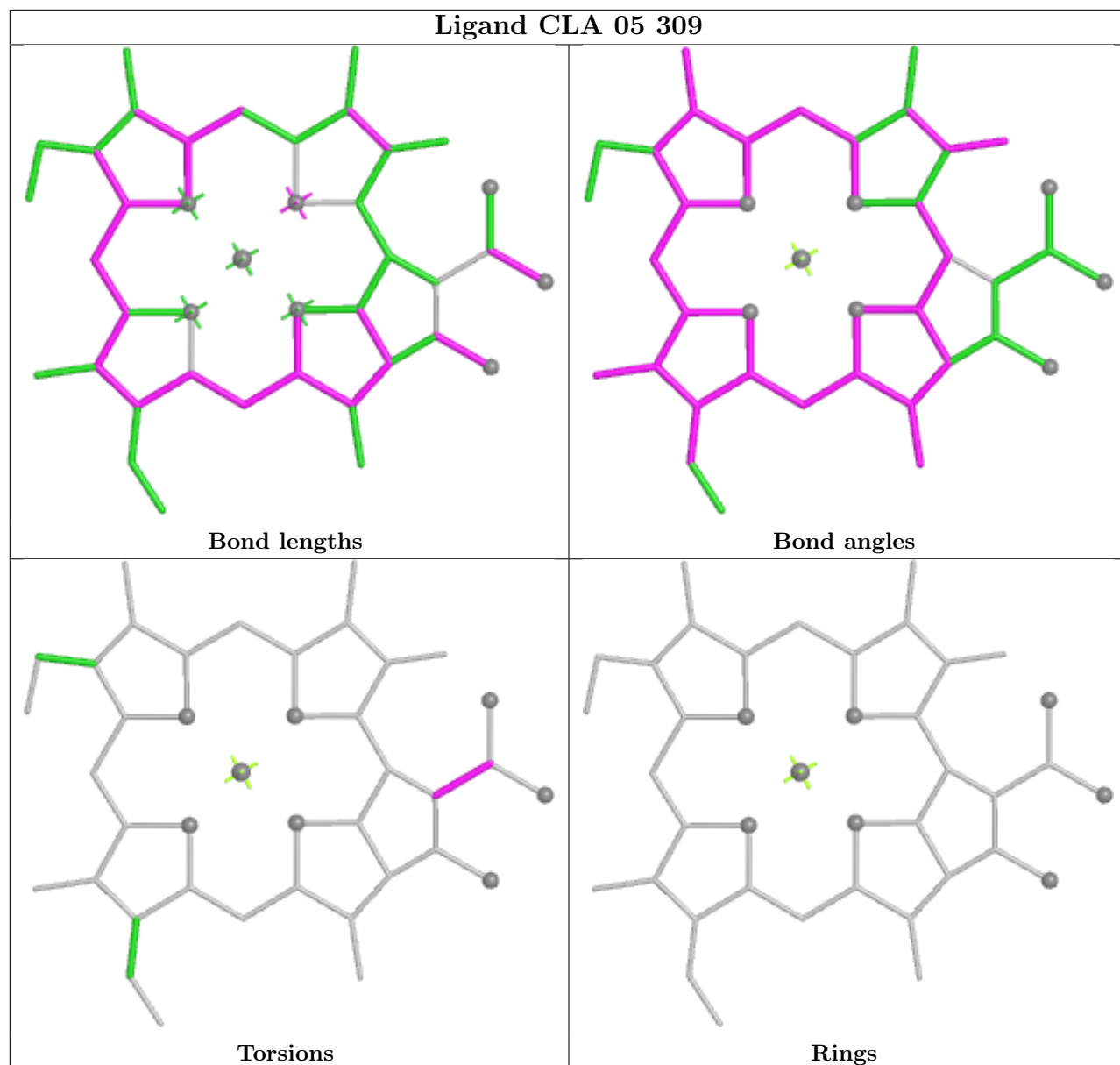


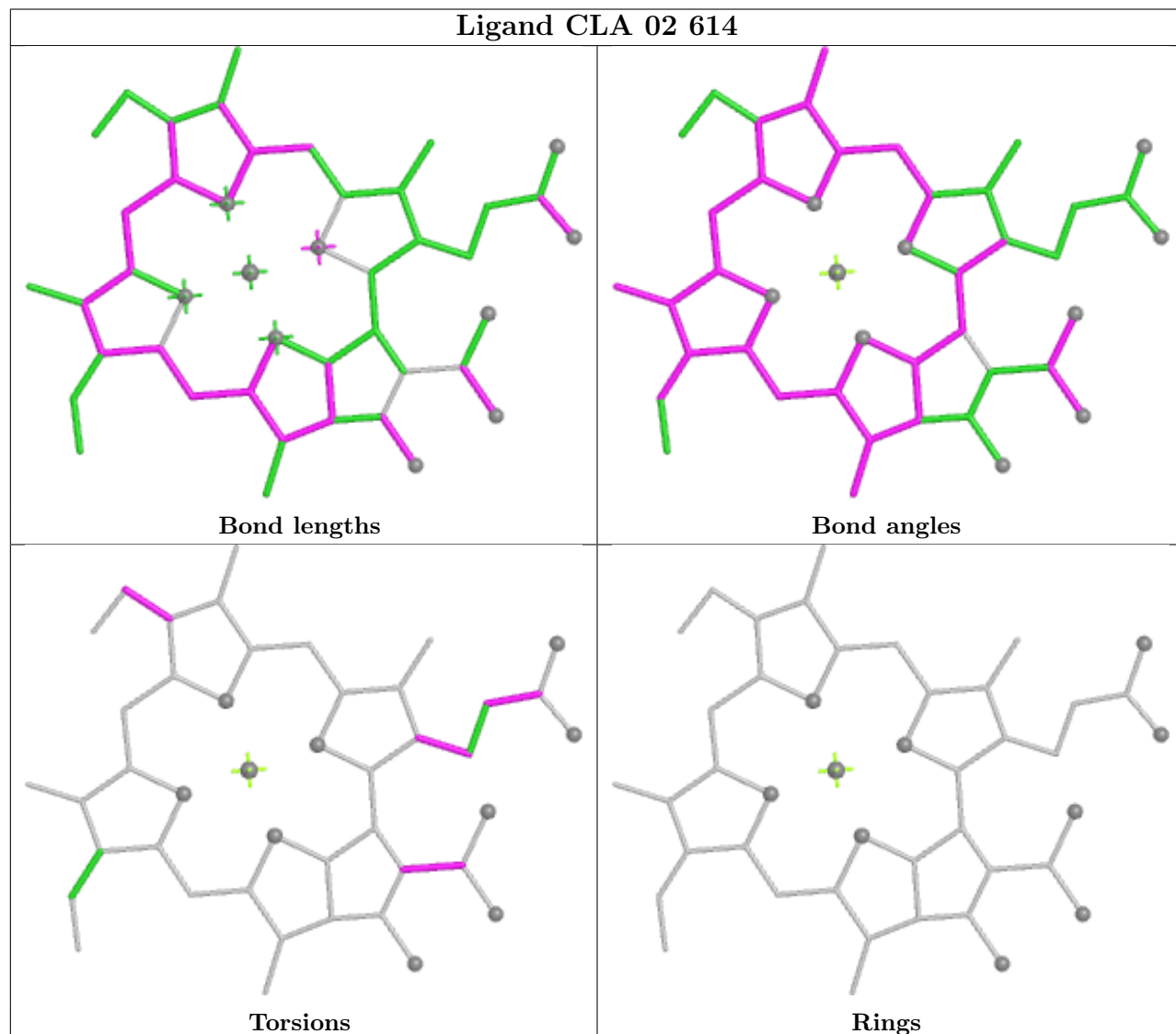
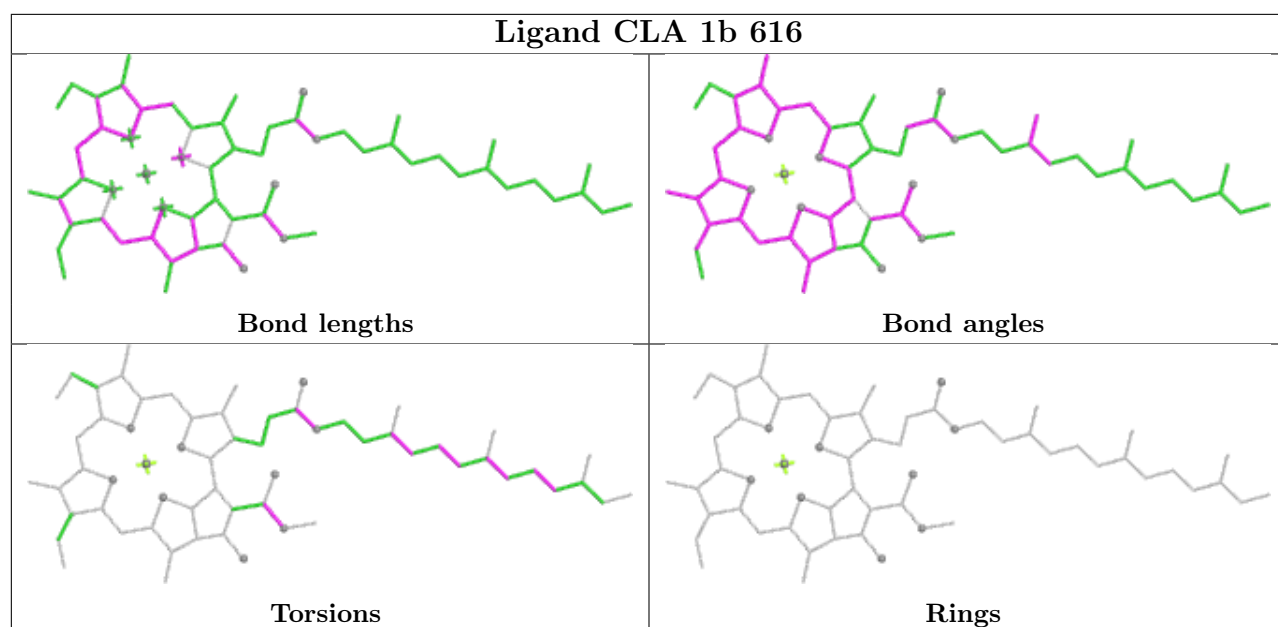


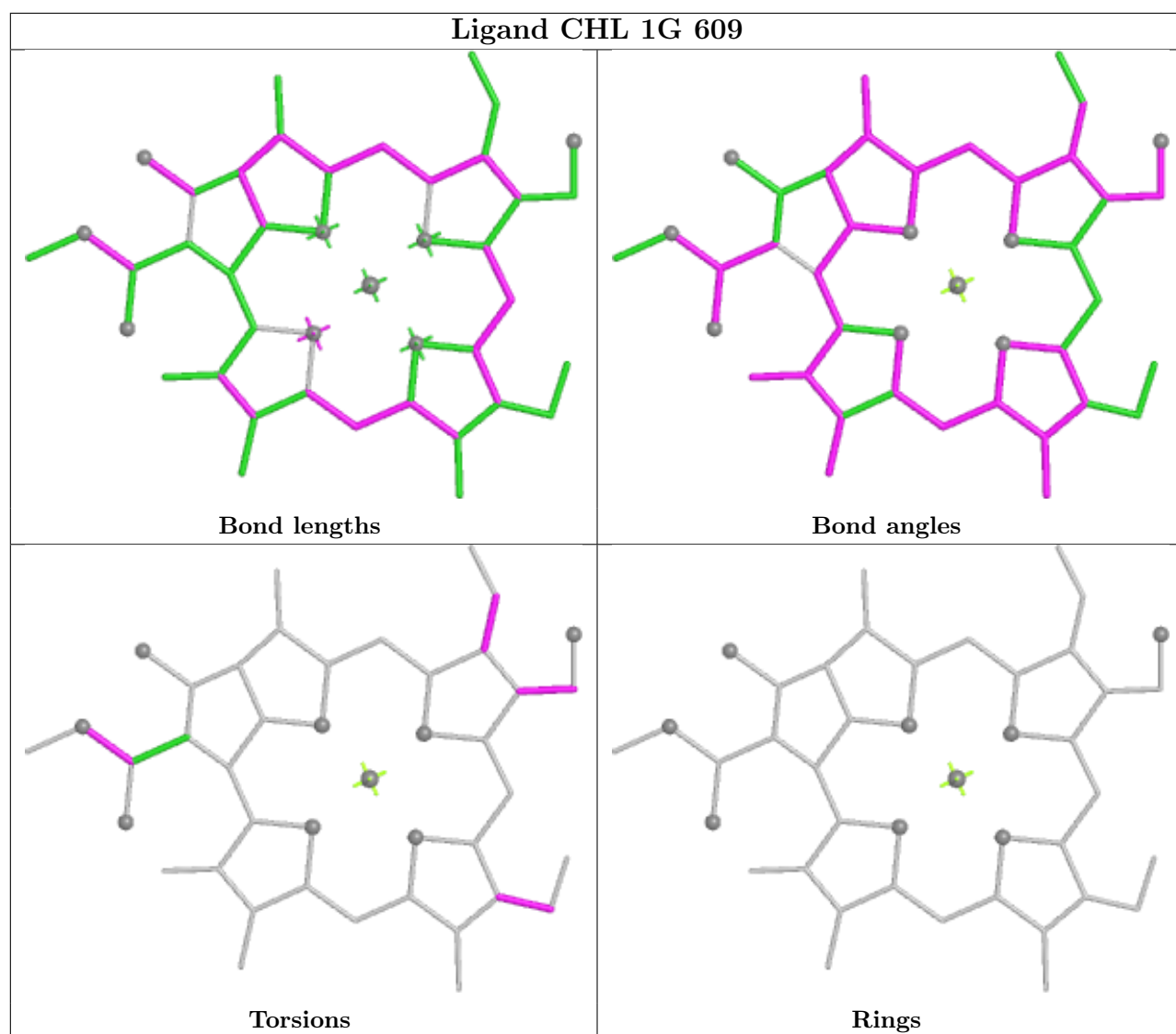


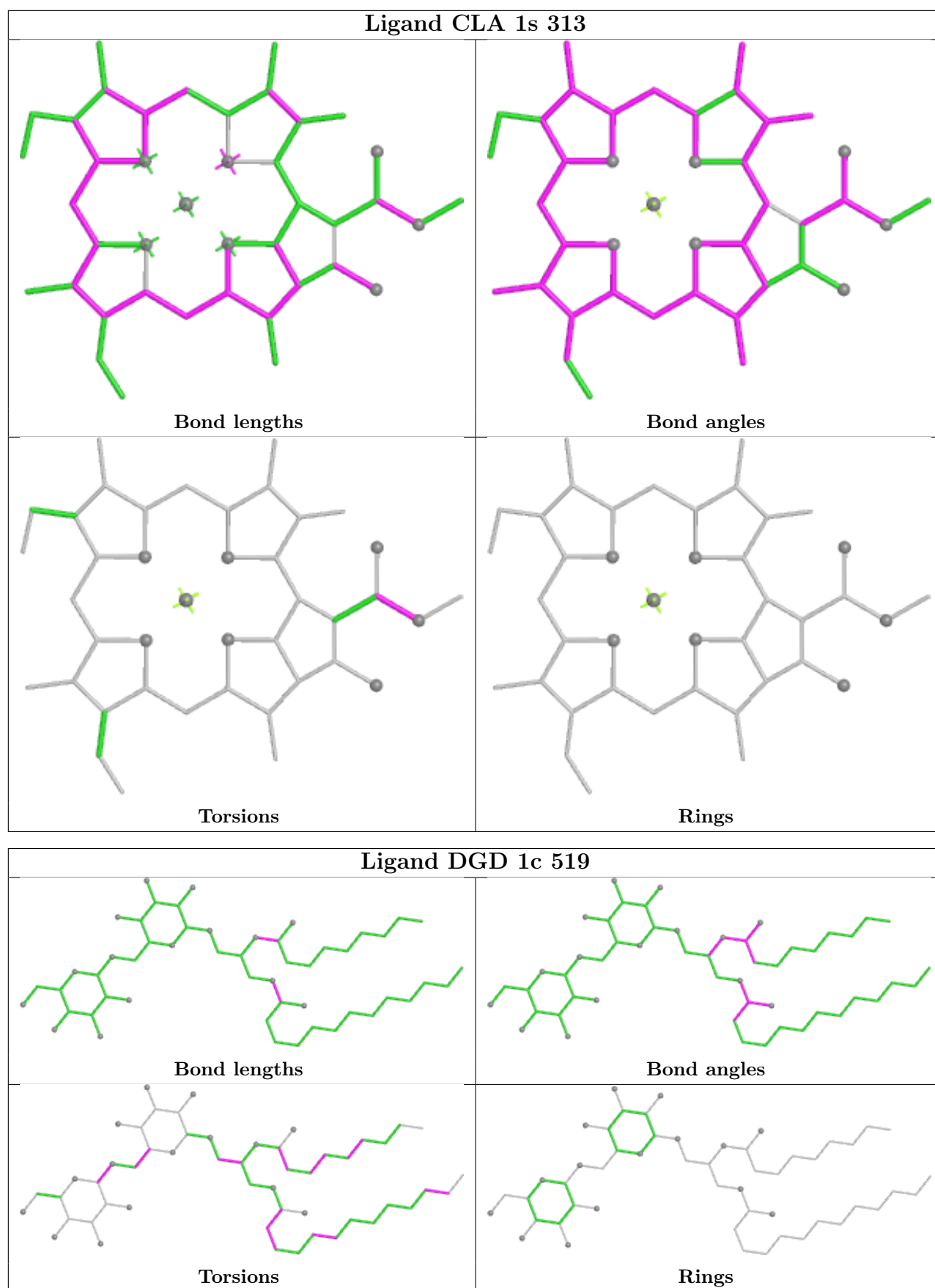


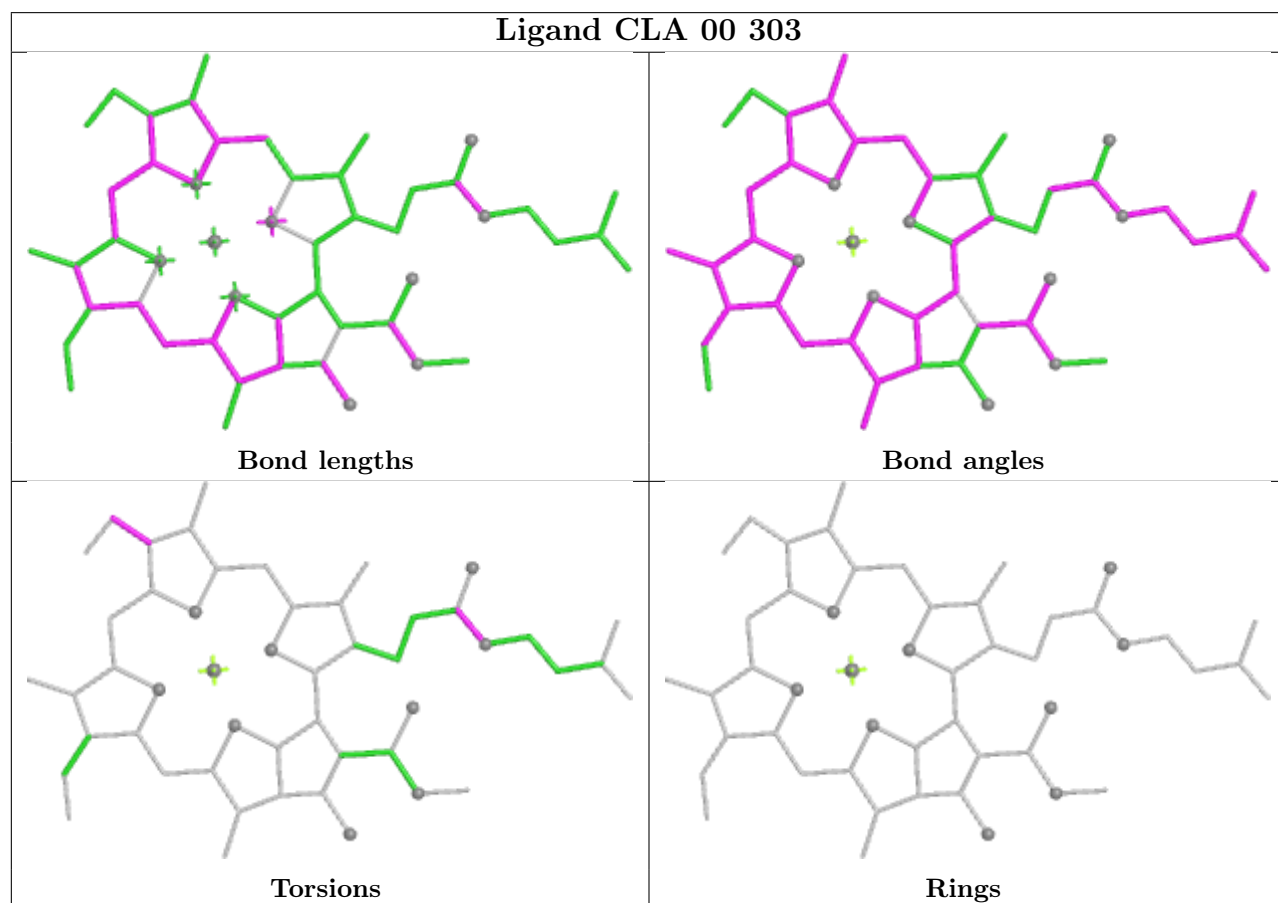
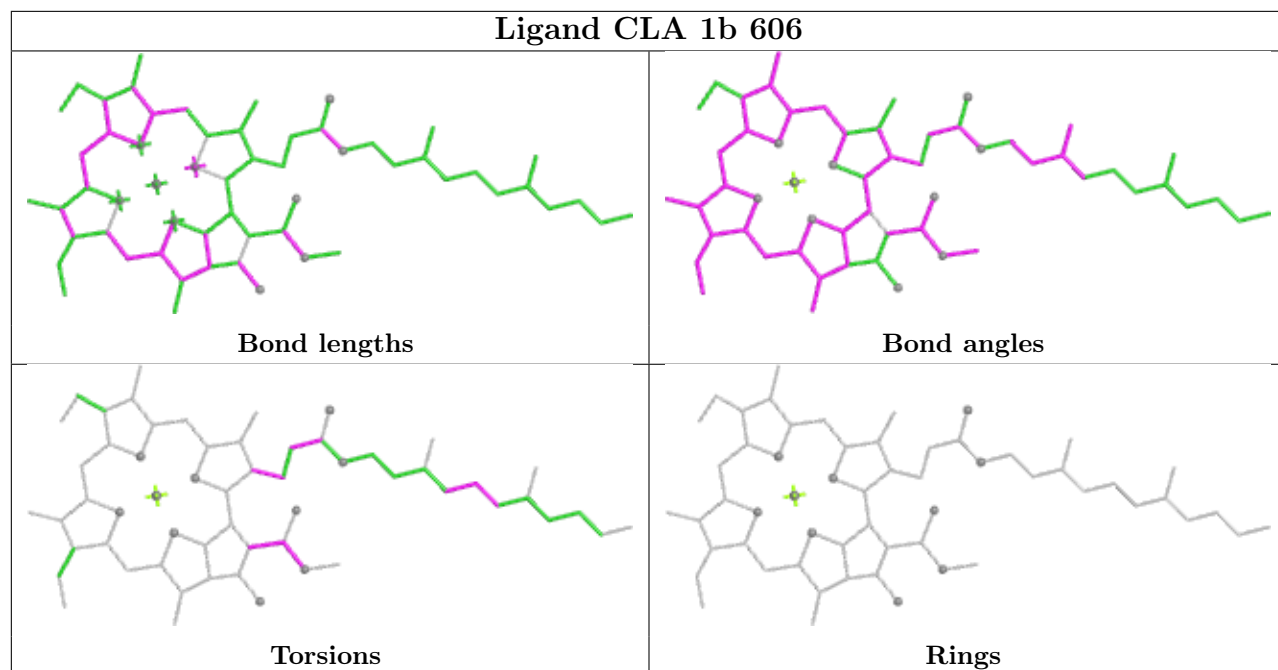


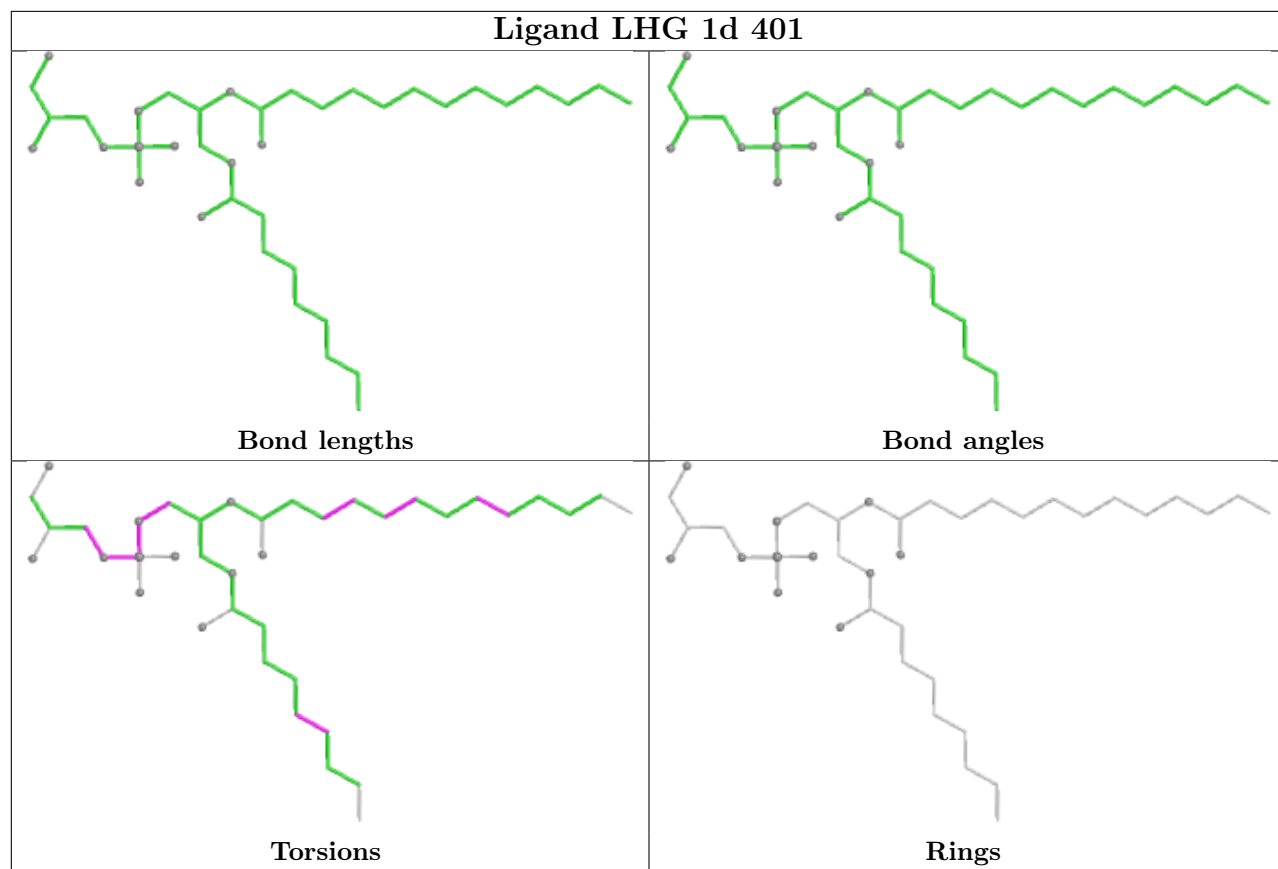


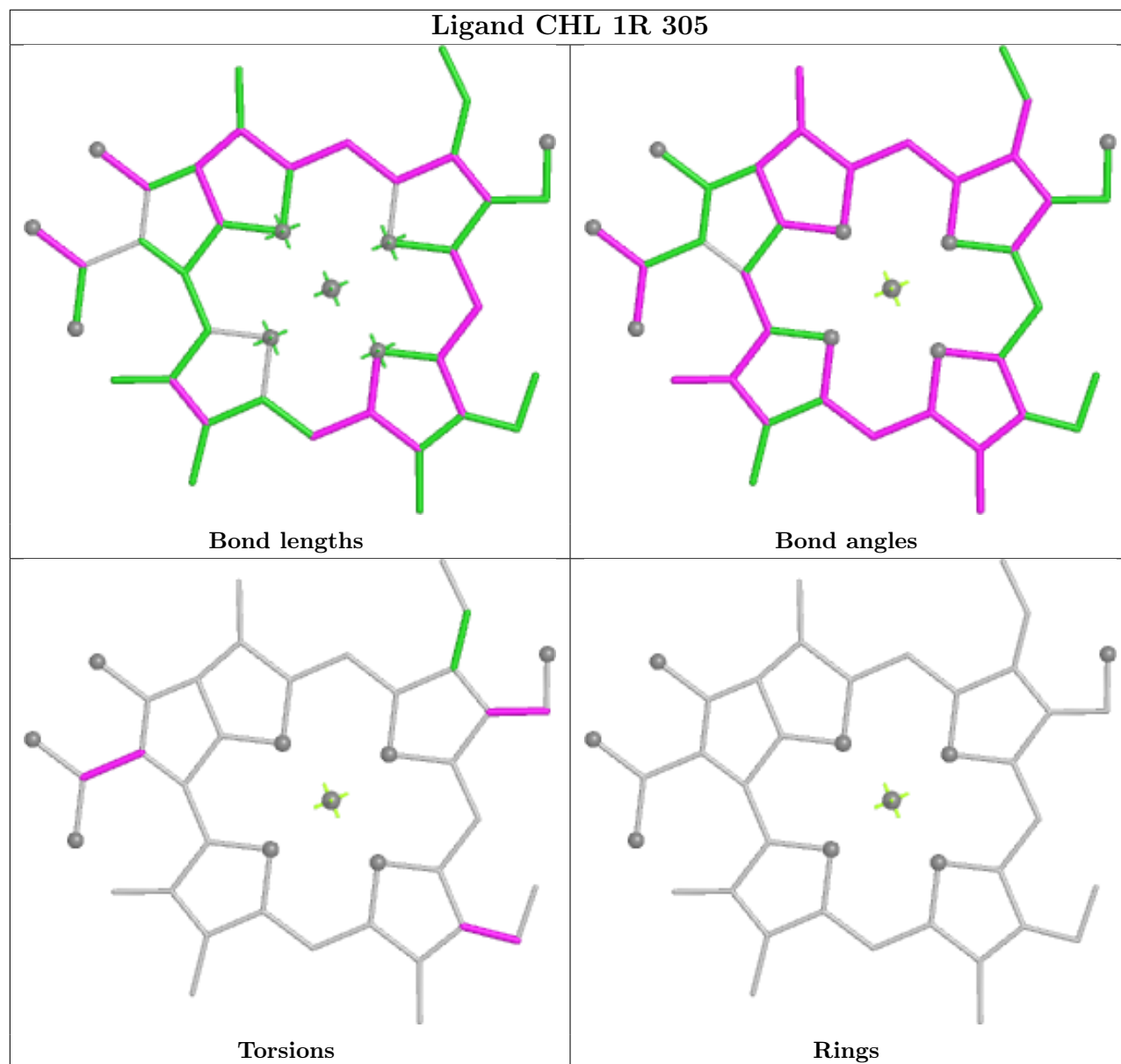


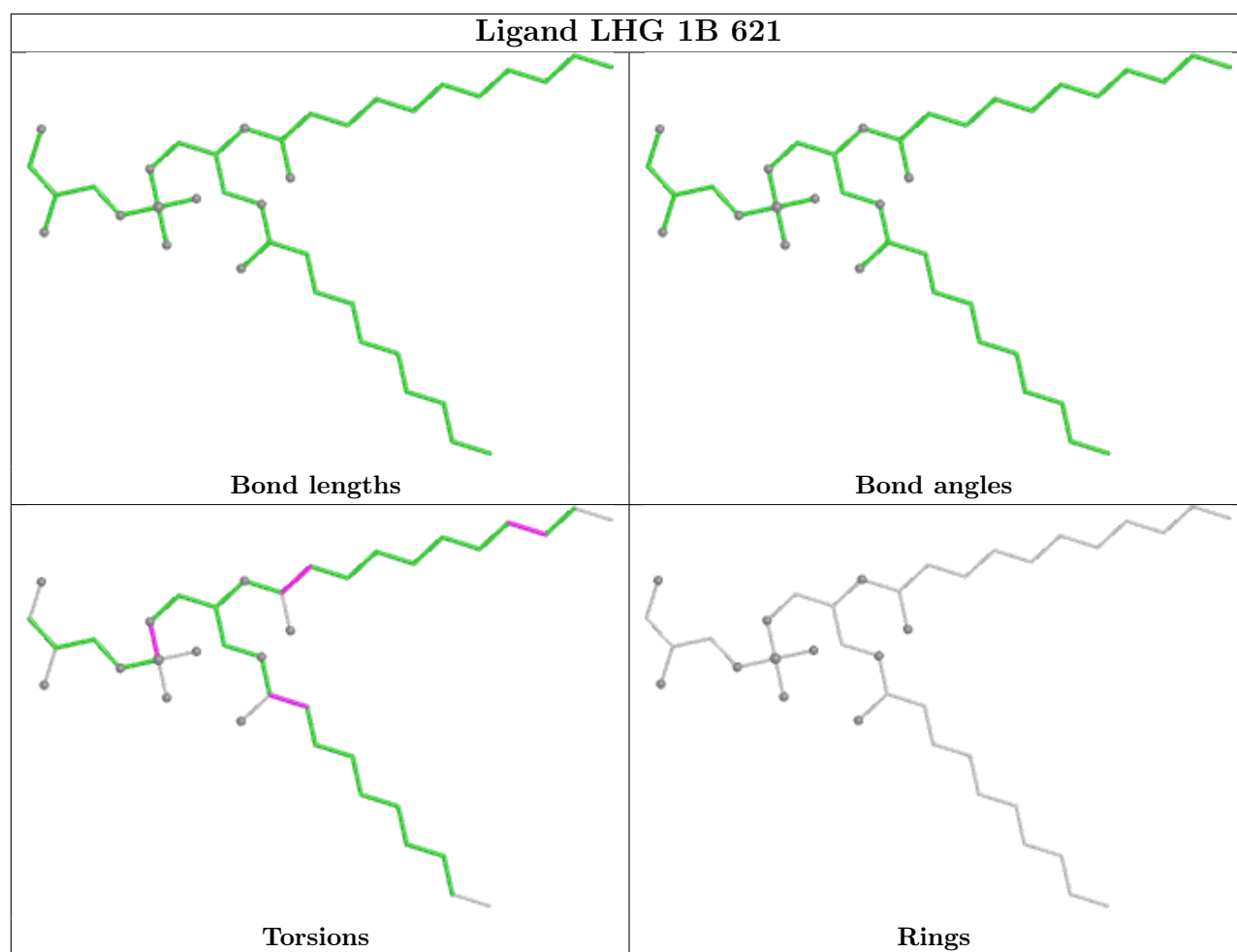


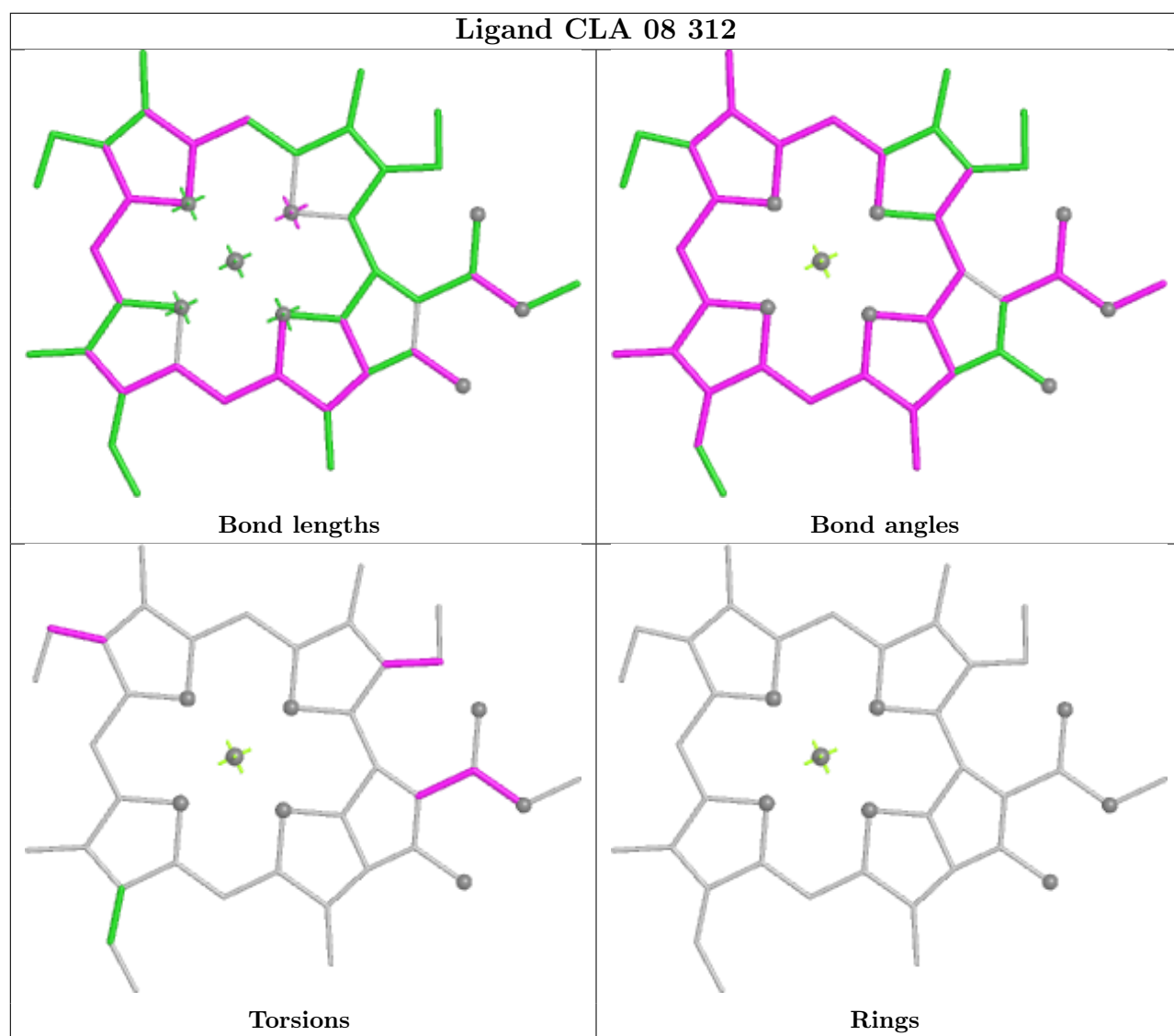


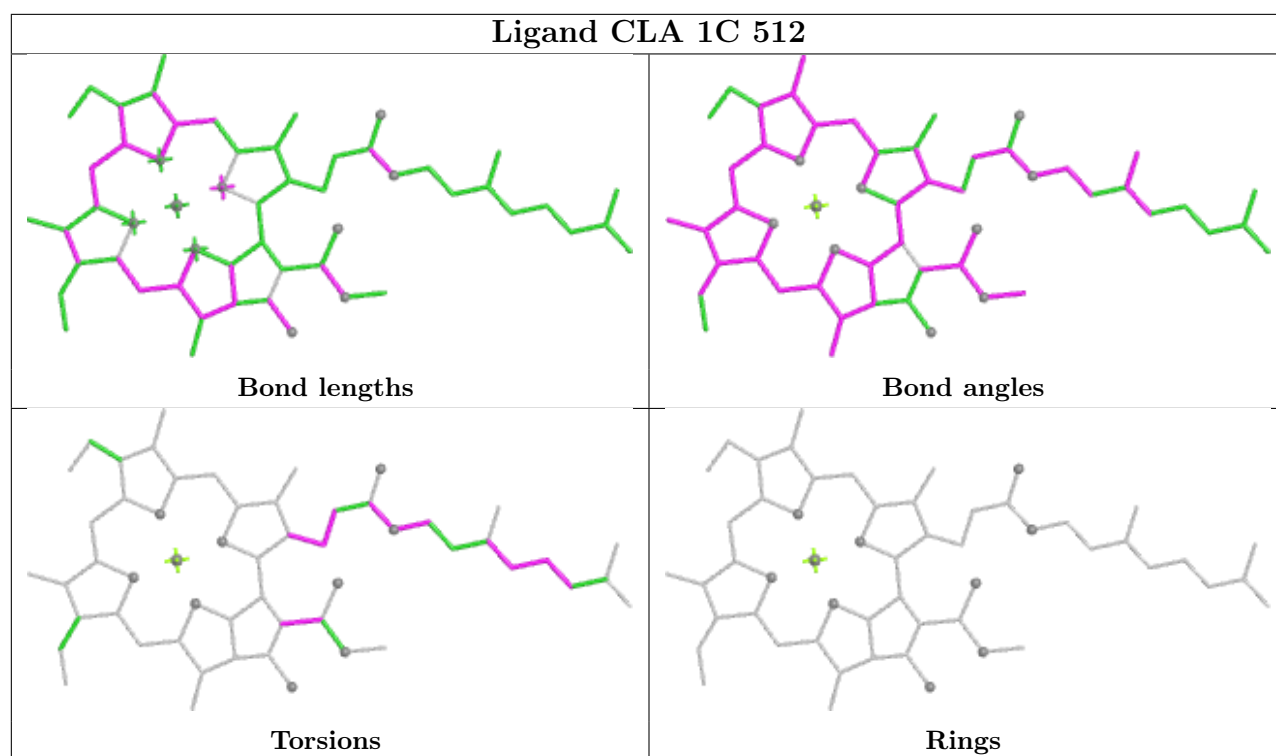


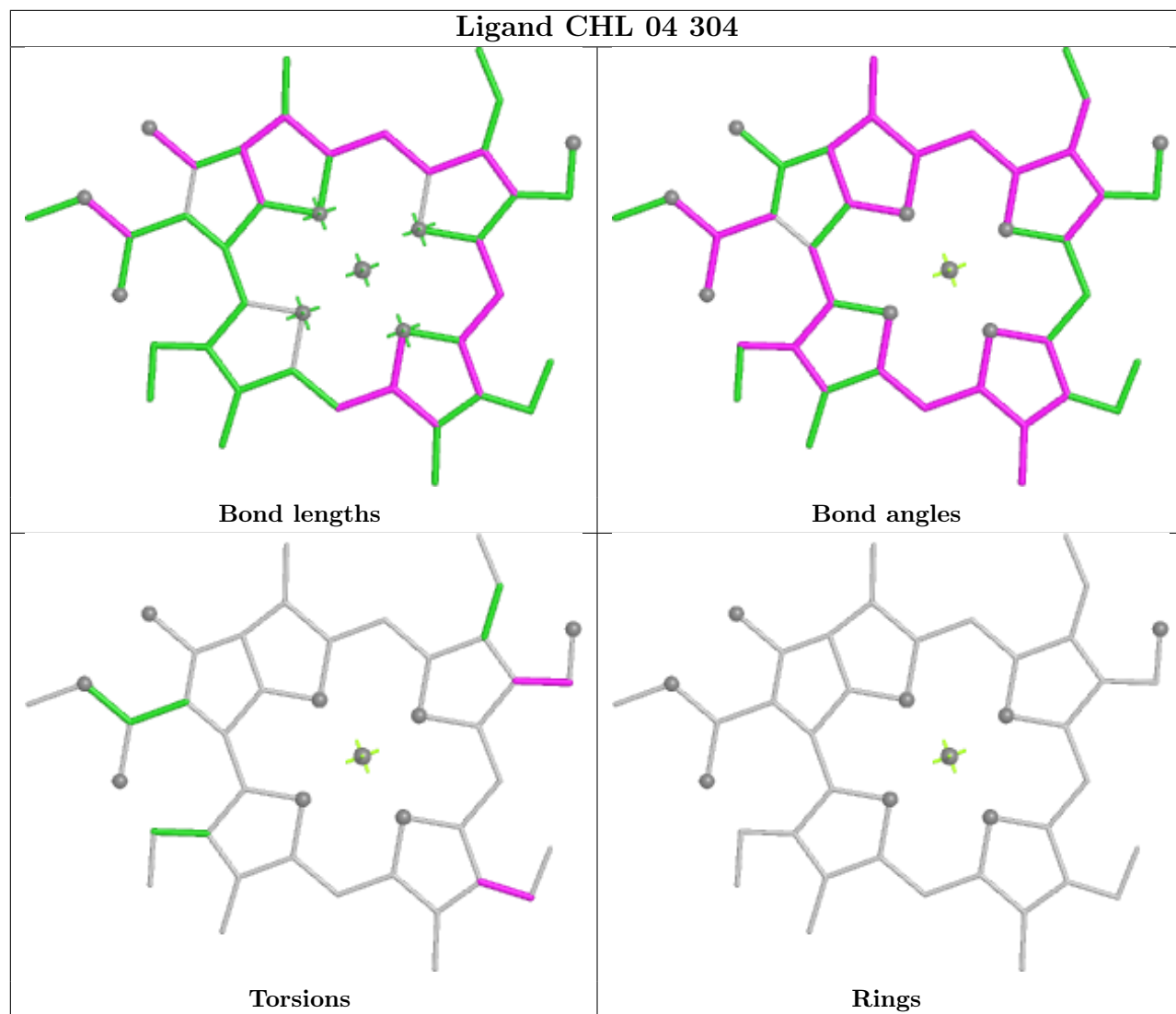


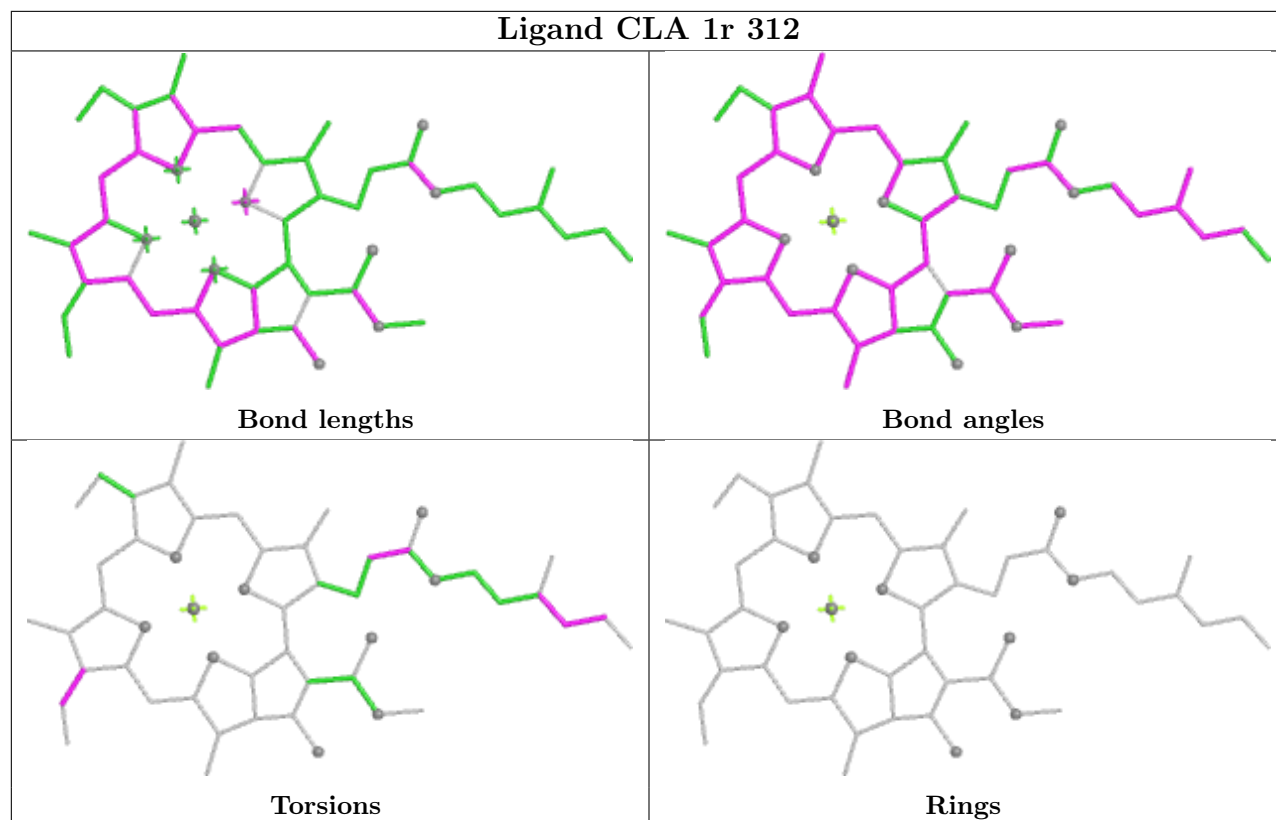


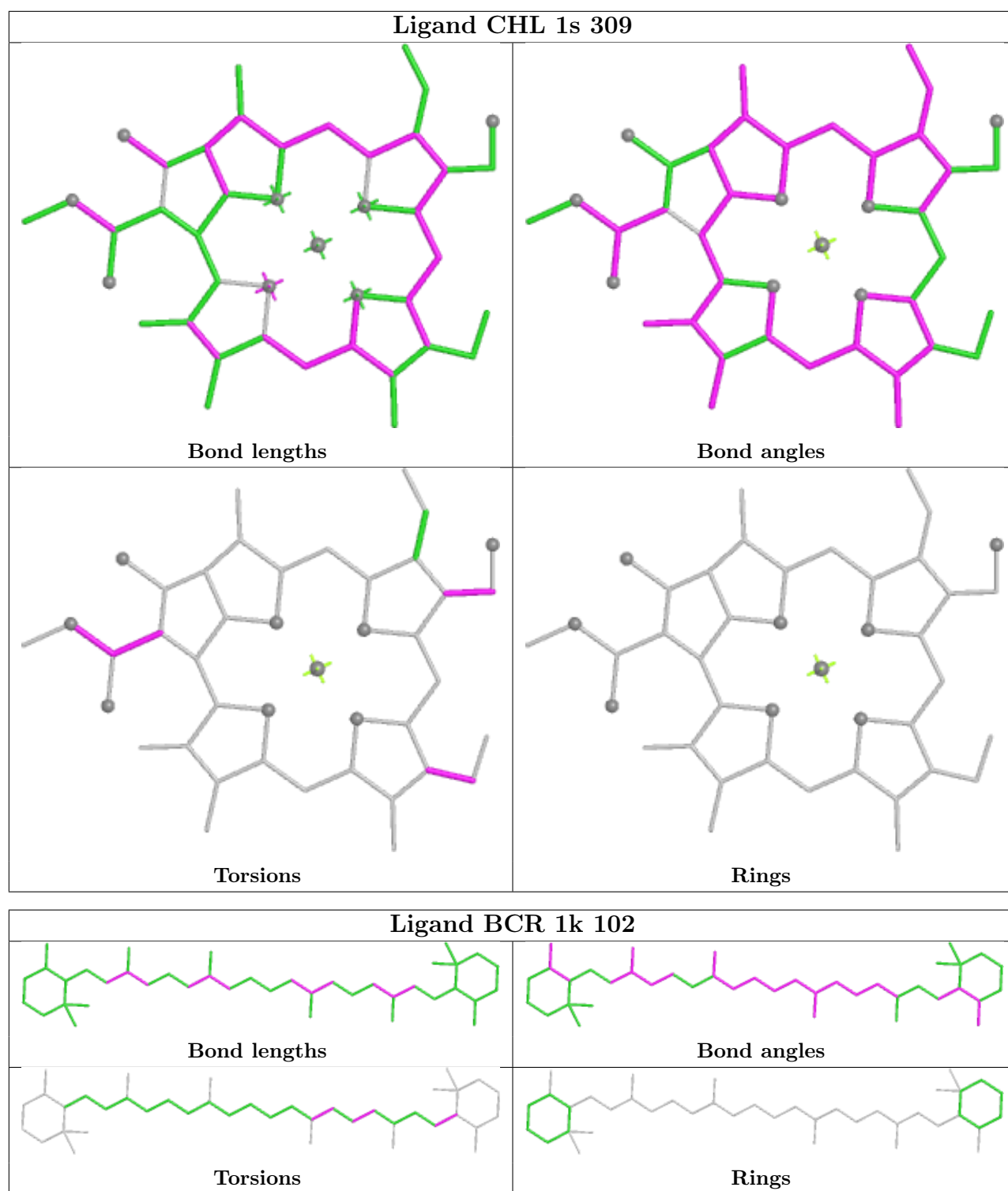


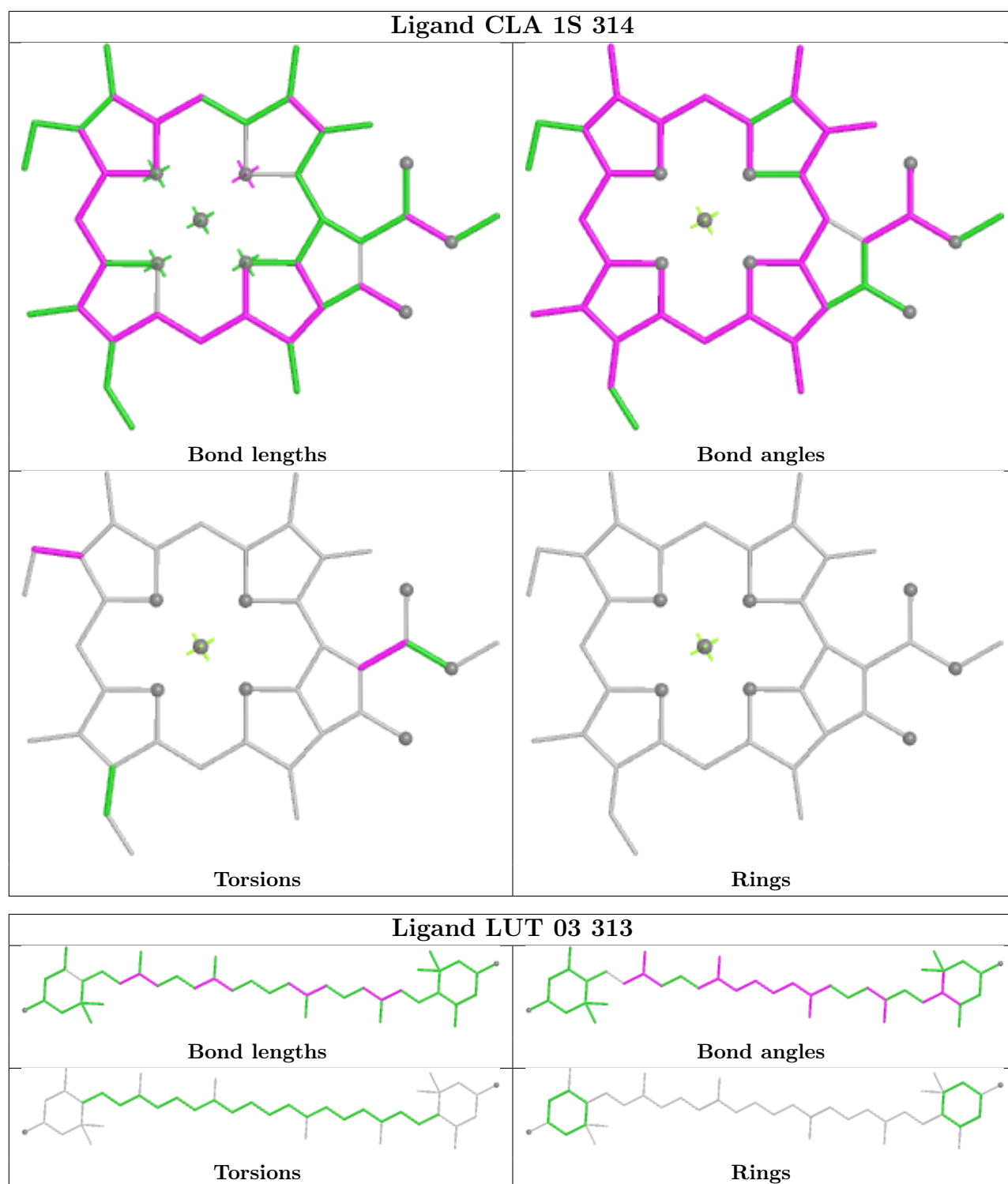


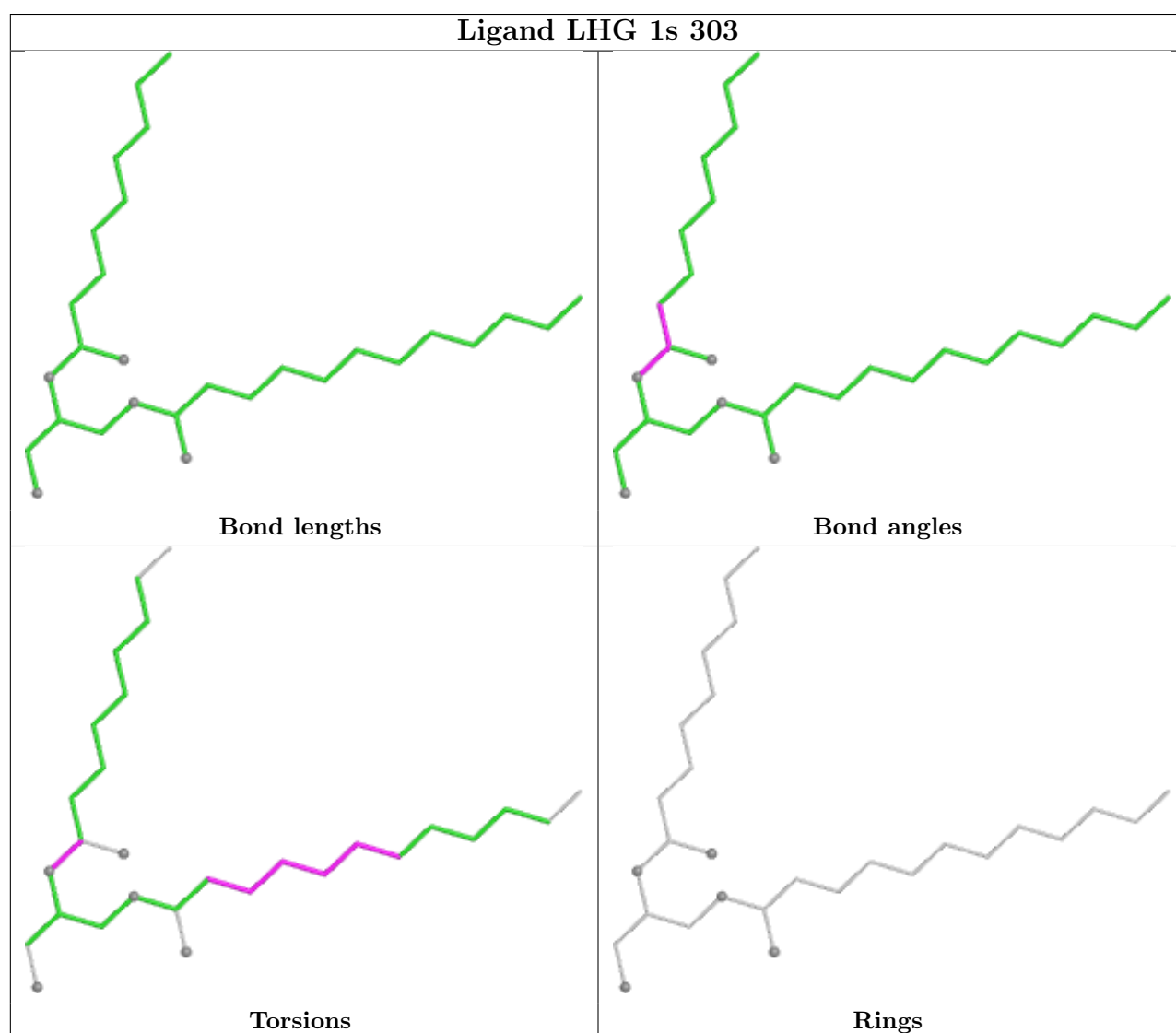
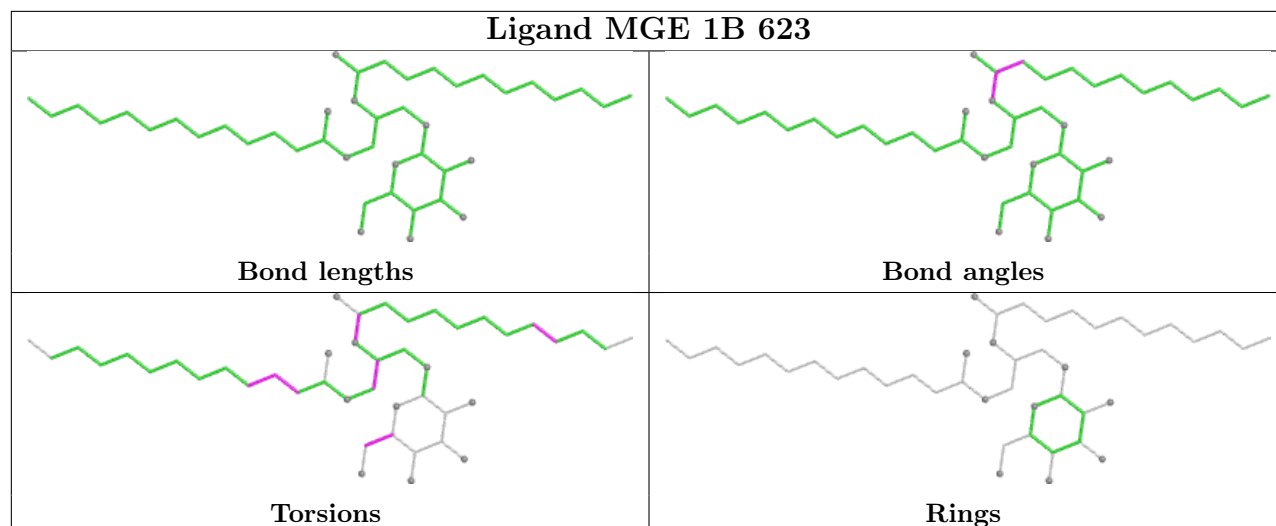


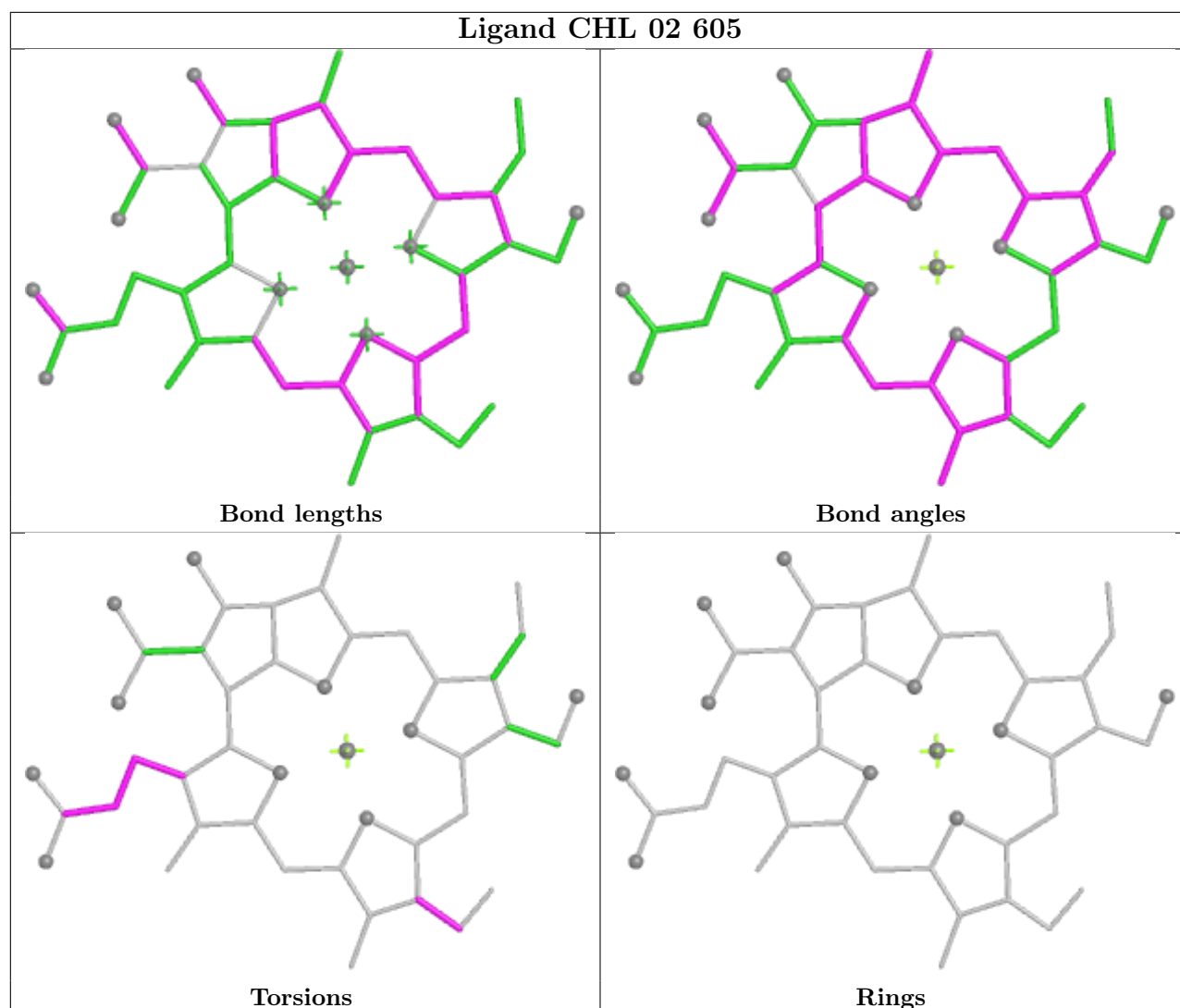
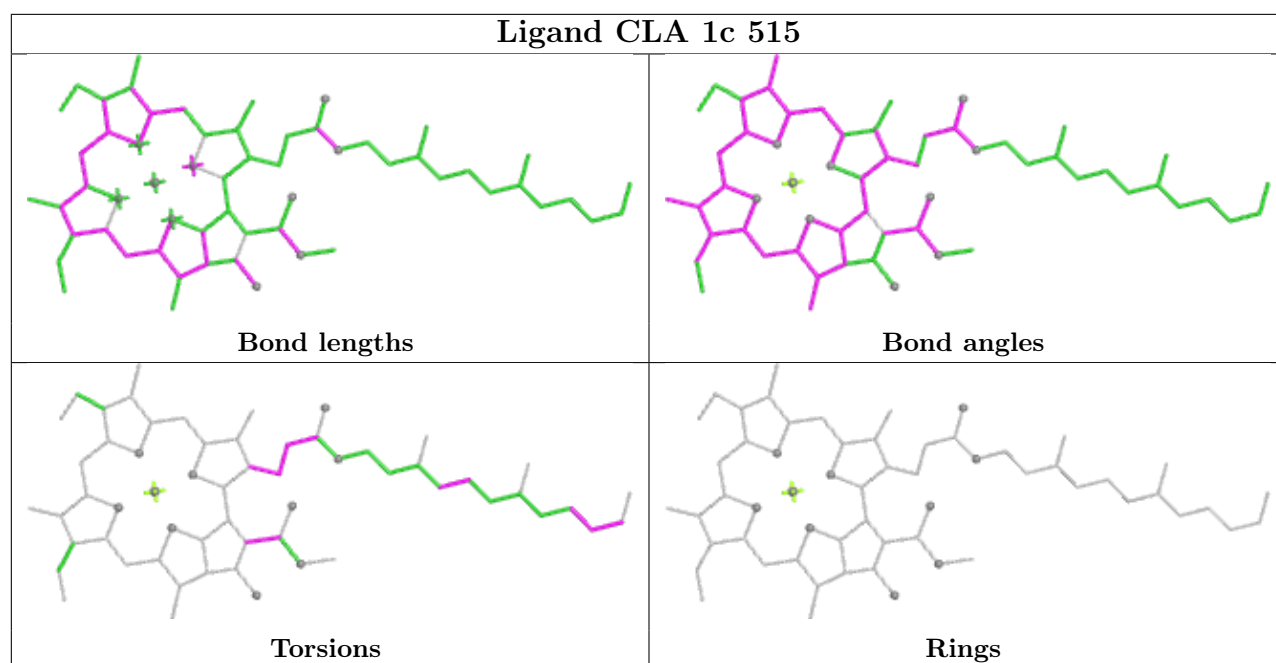




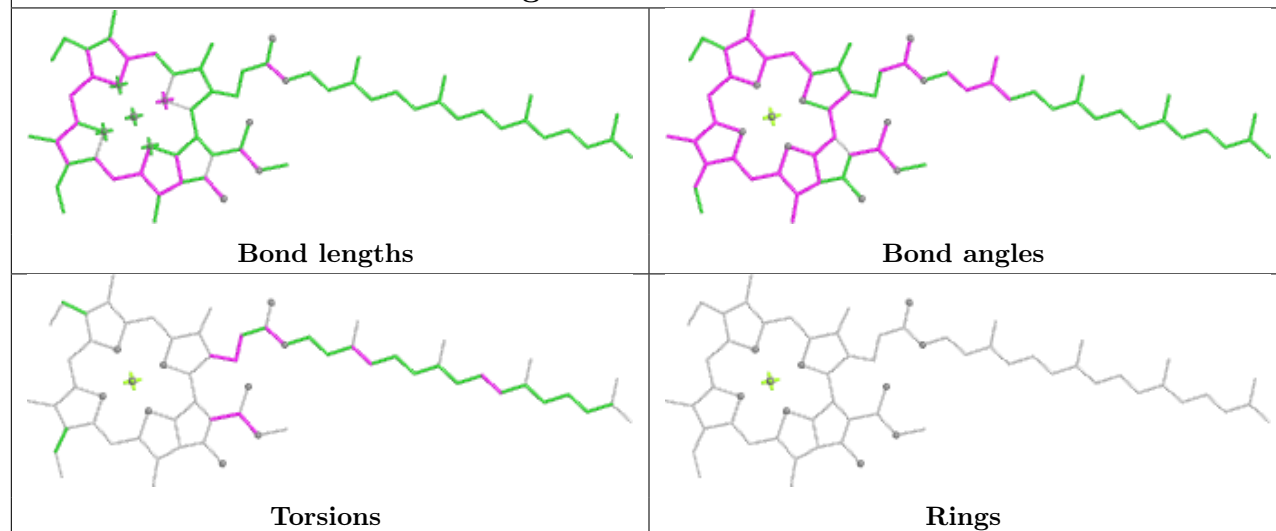




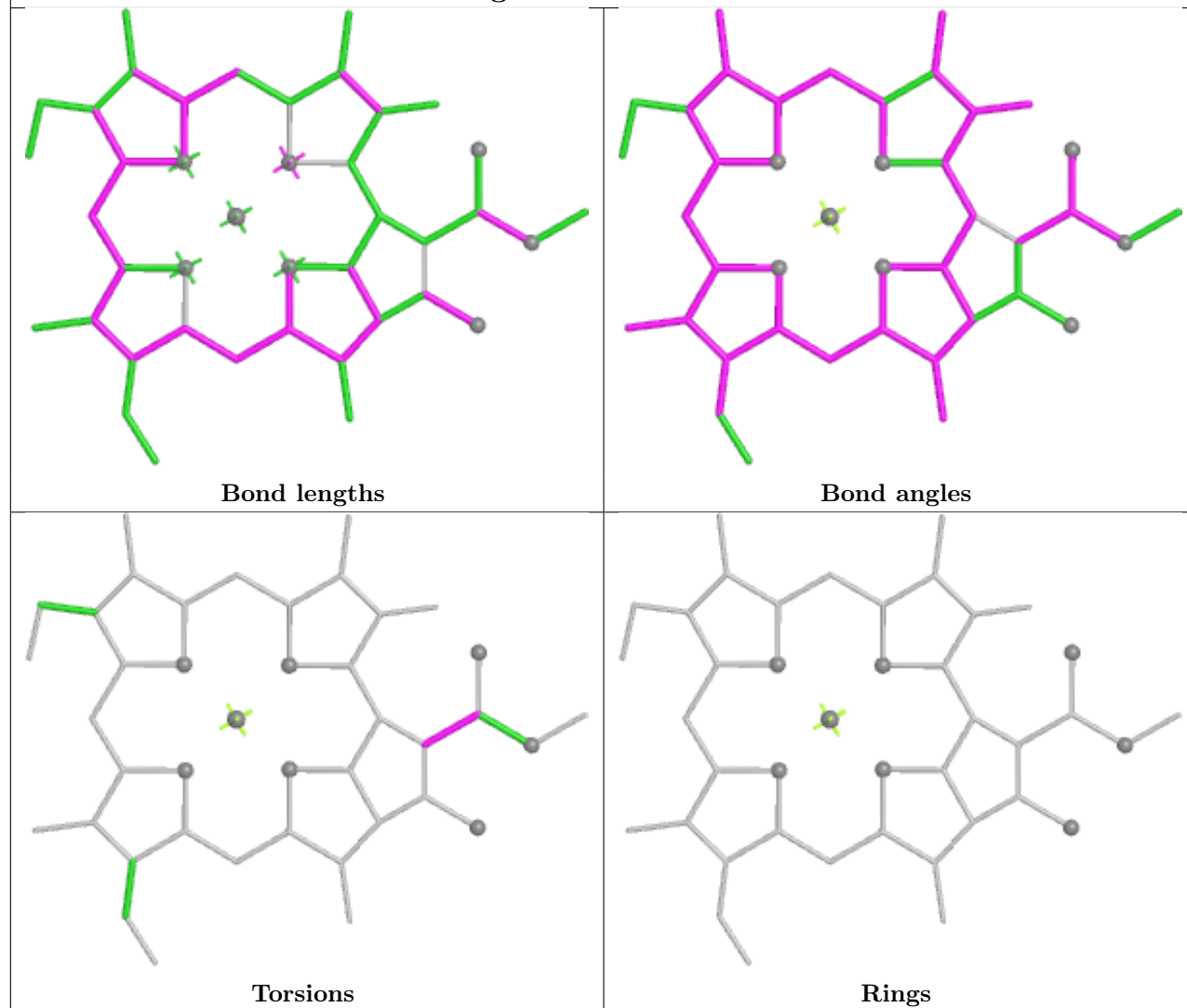


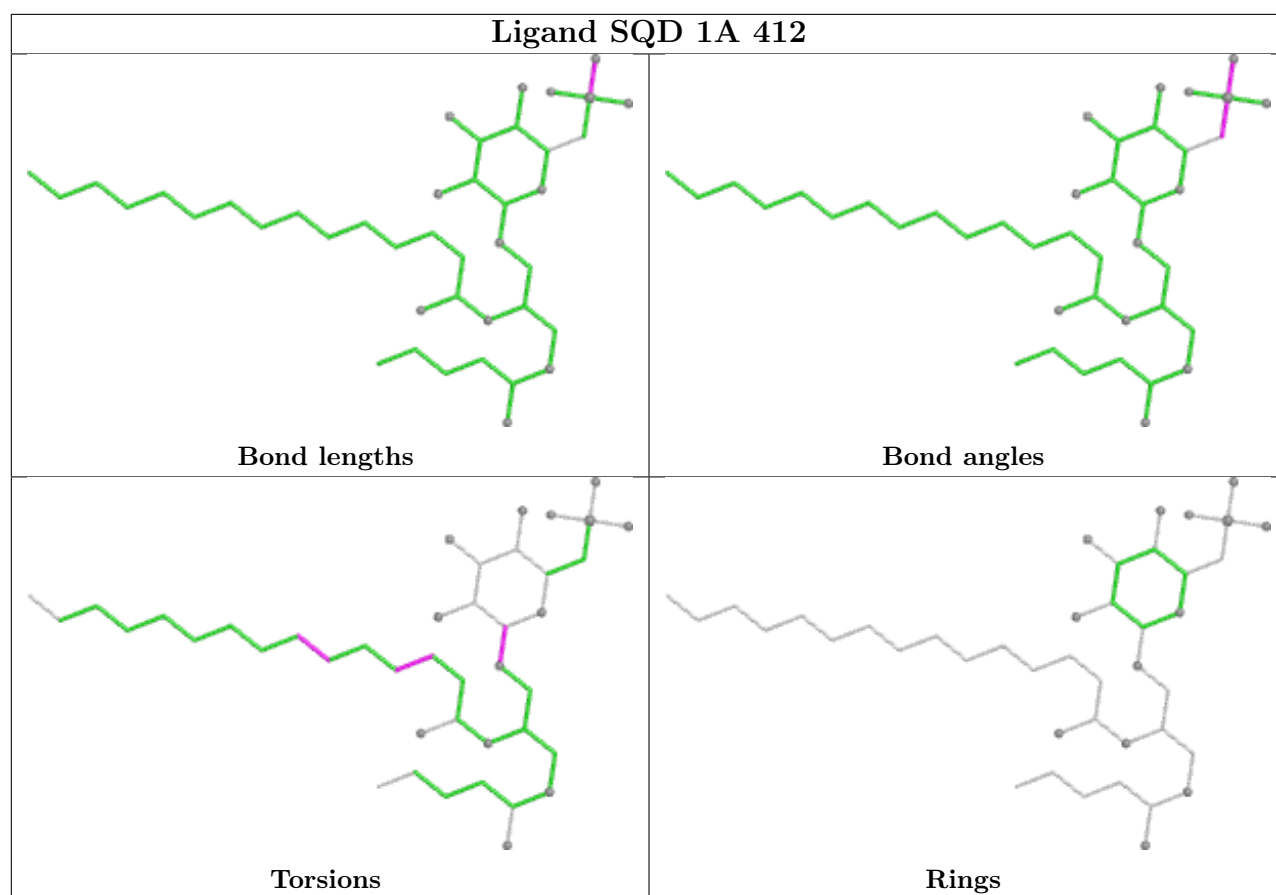


Ligand CLA 1N 303

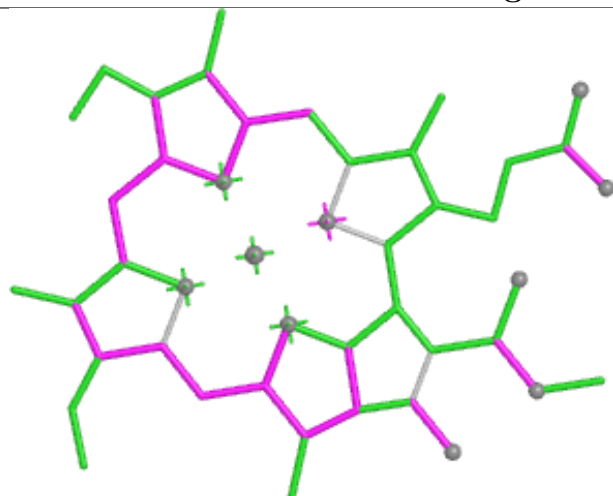


Ligand CLA 04 314

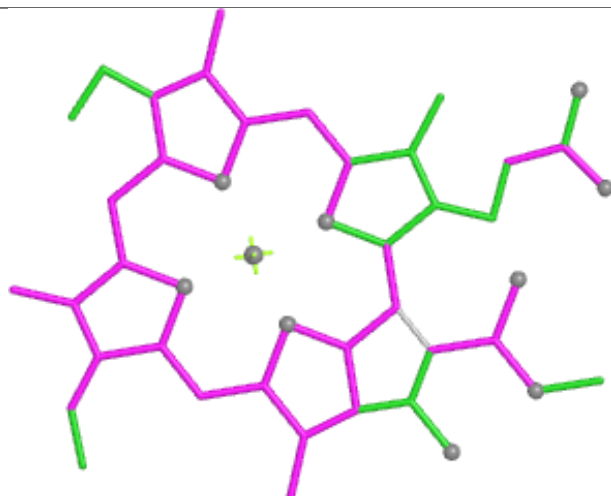




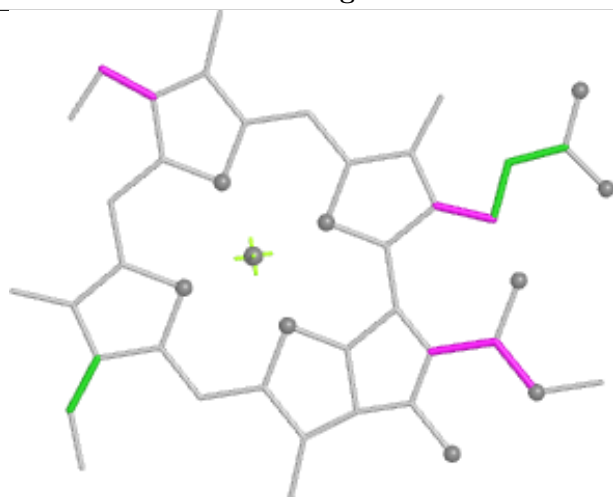
Ligand CLA 1N 304



Bond lengths



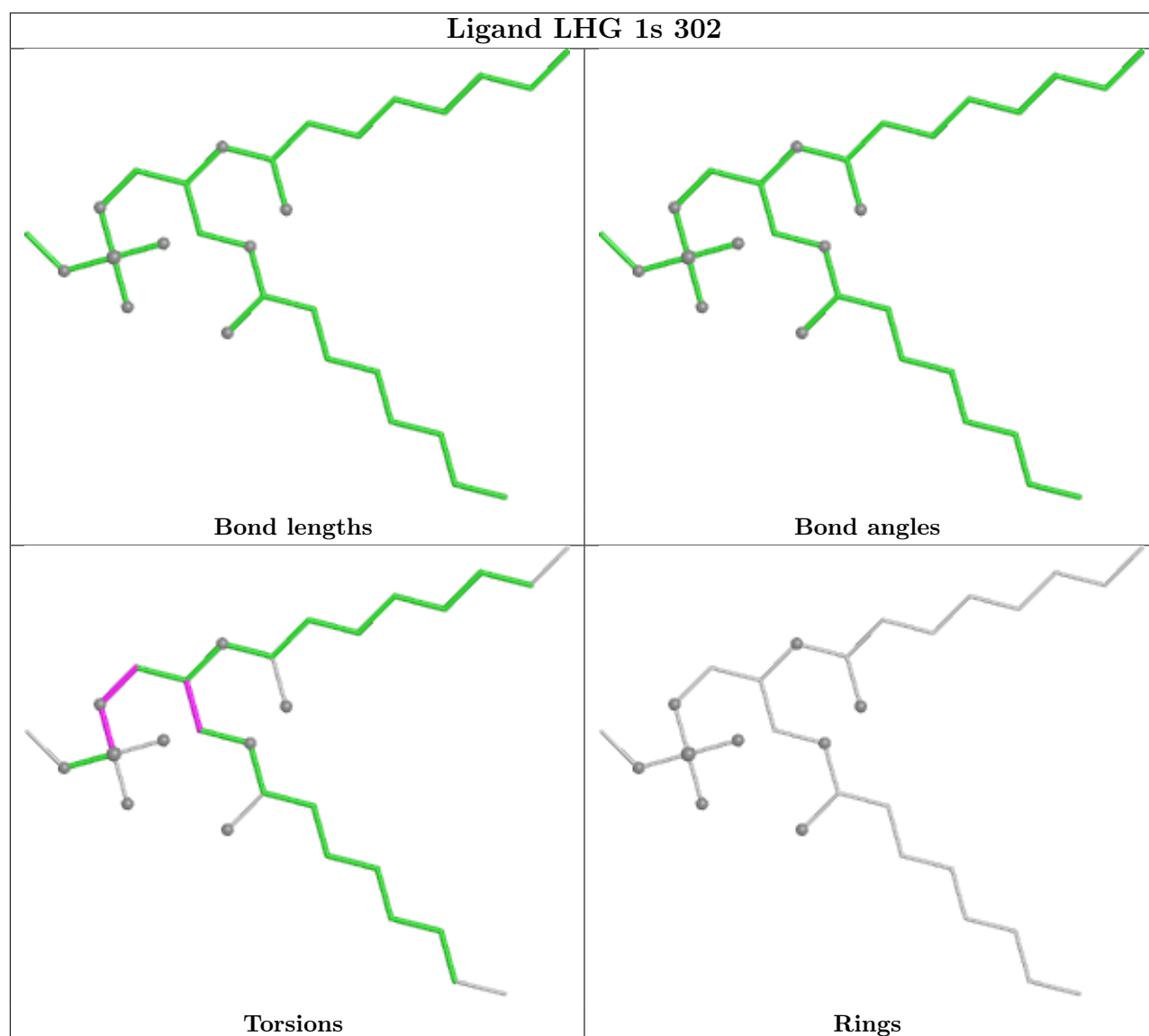
Bond angles

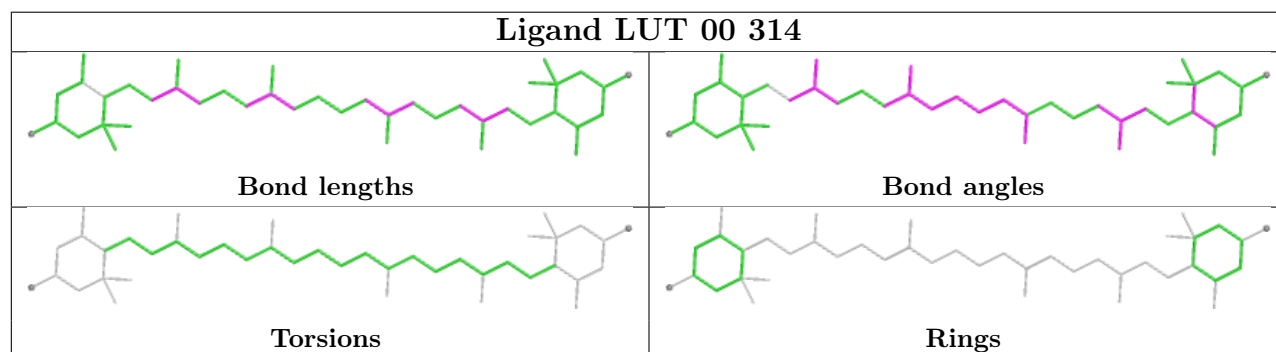
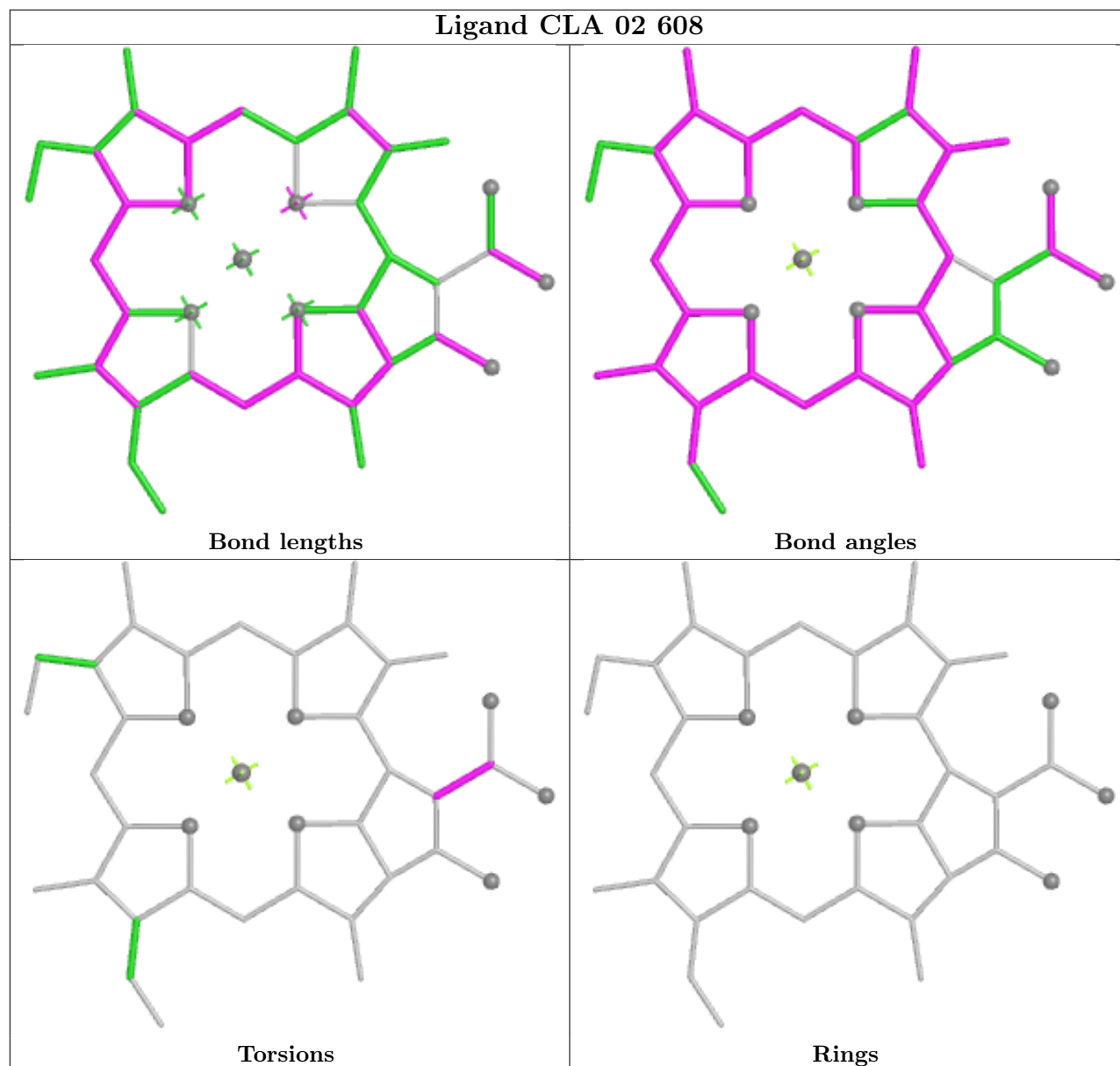


Torsions

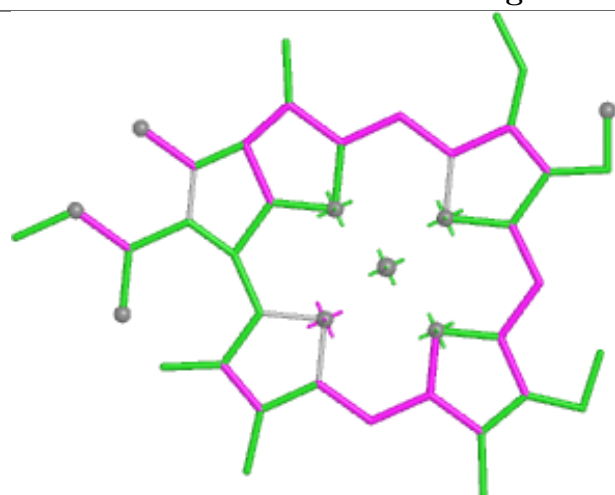


Rings





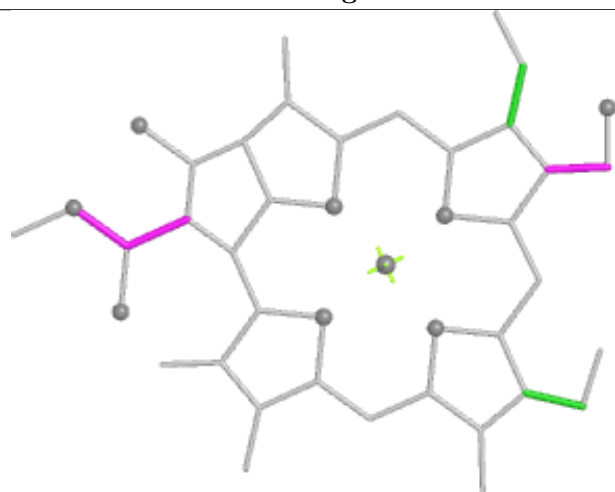
Ligand CHL 1N 306



Bond lengths



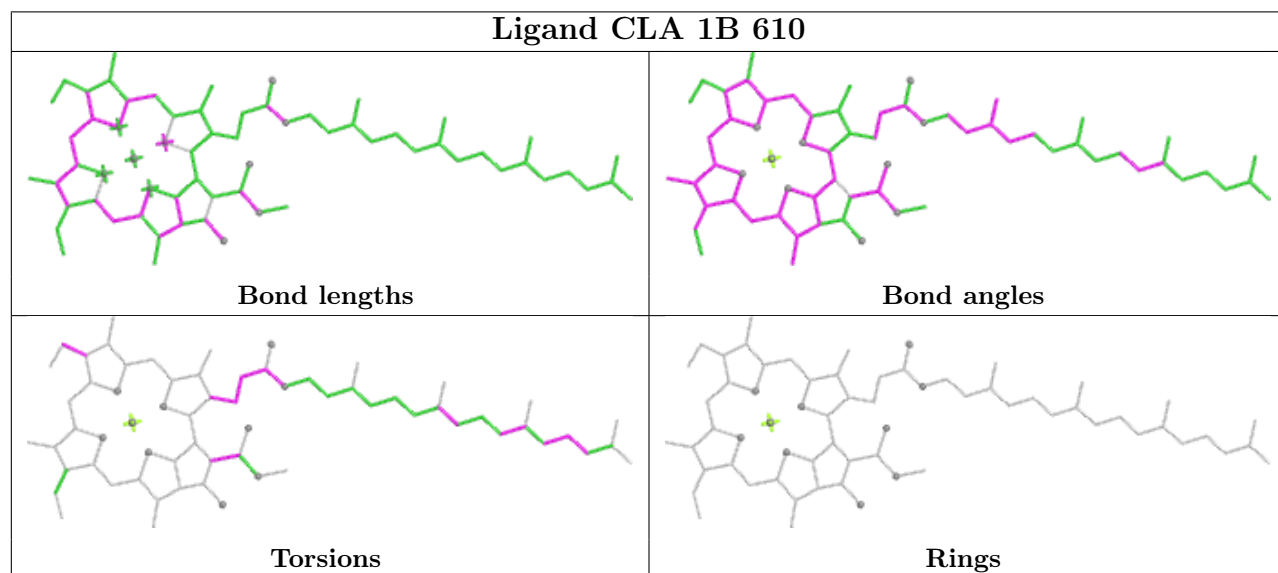
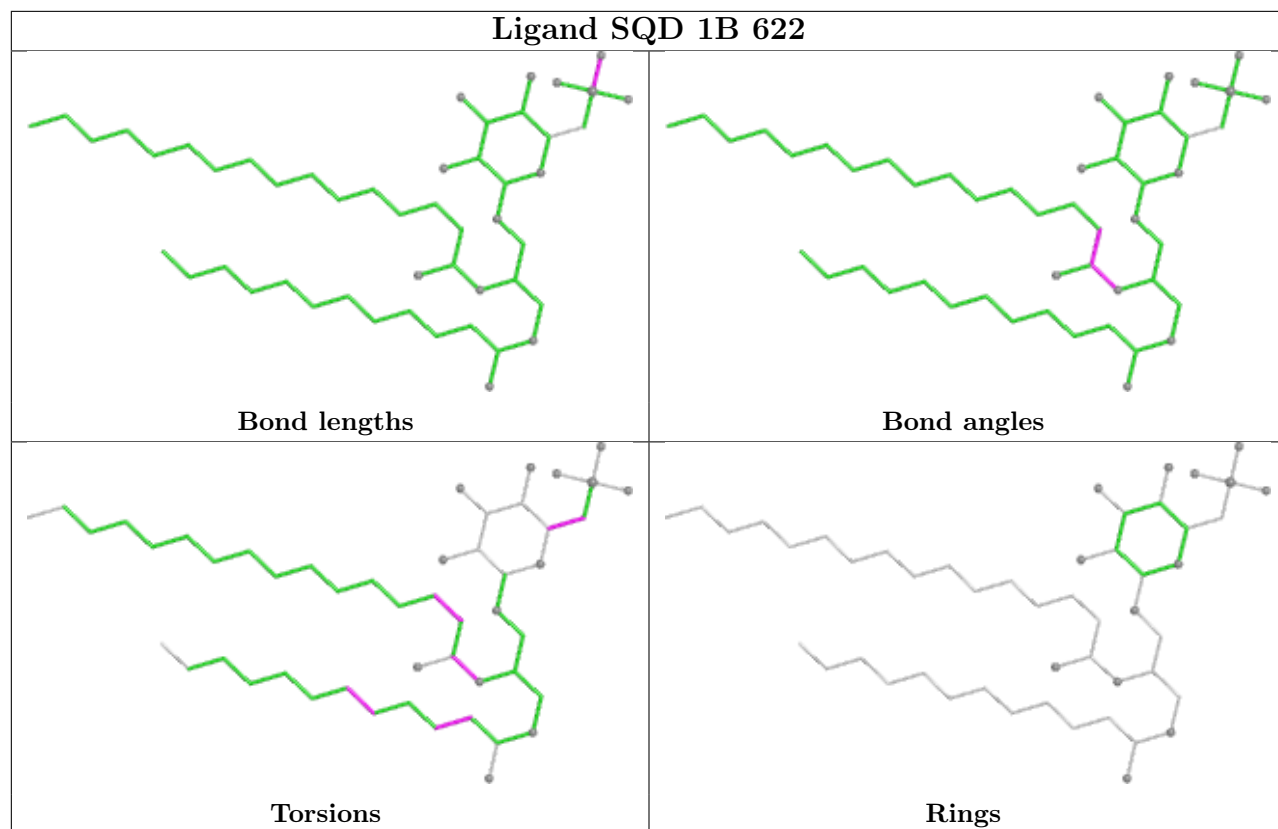
Bond angles

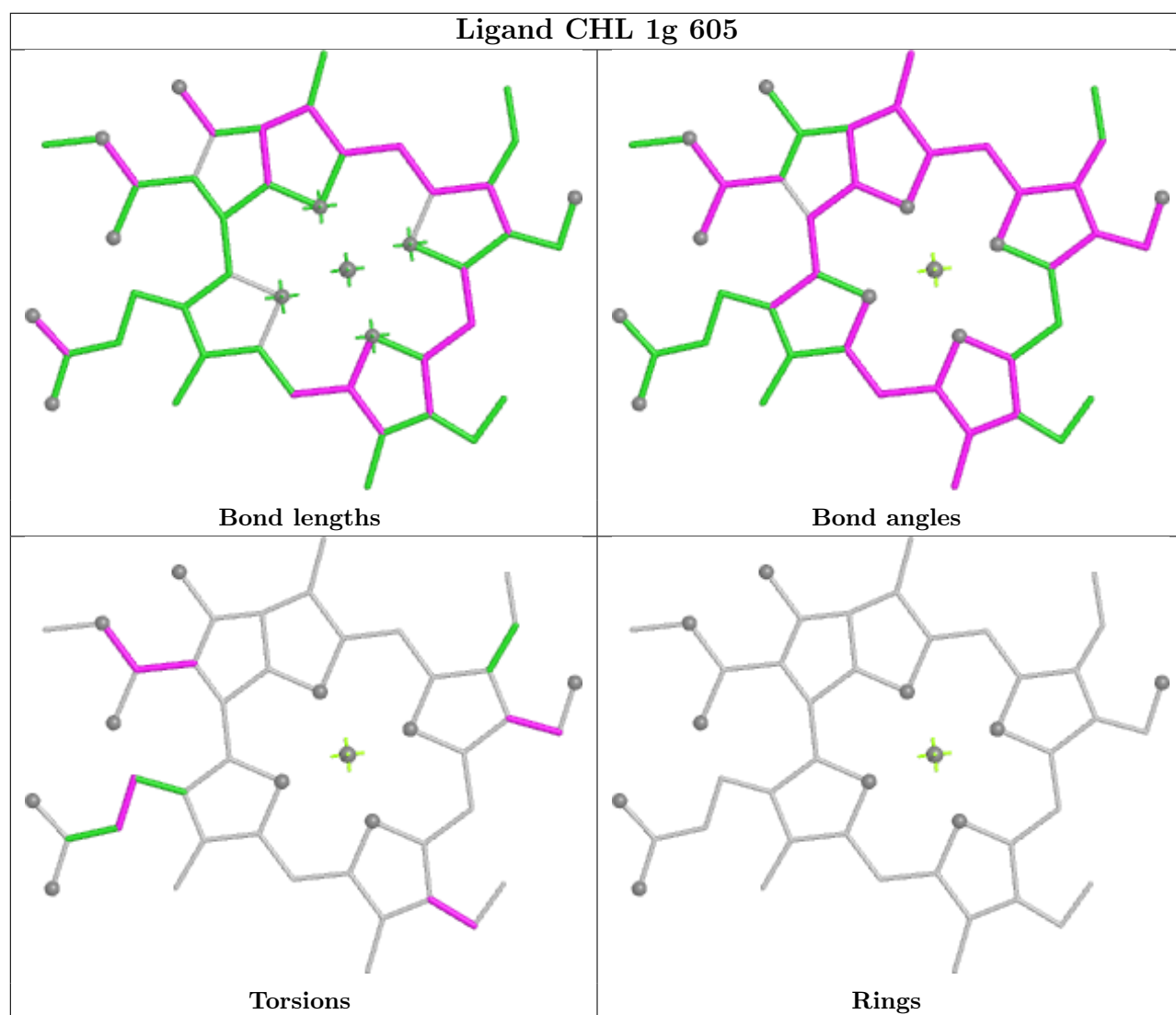


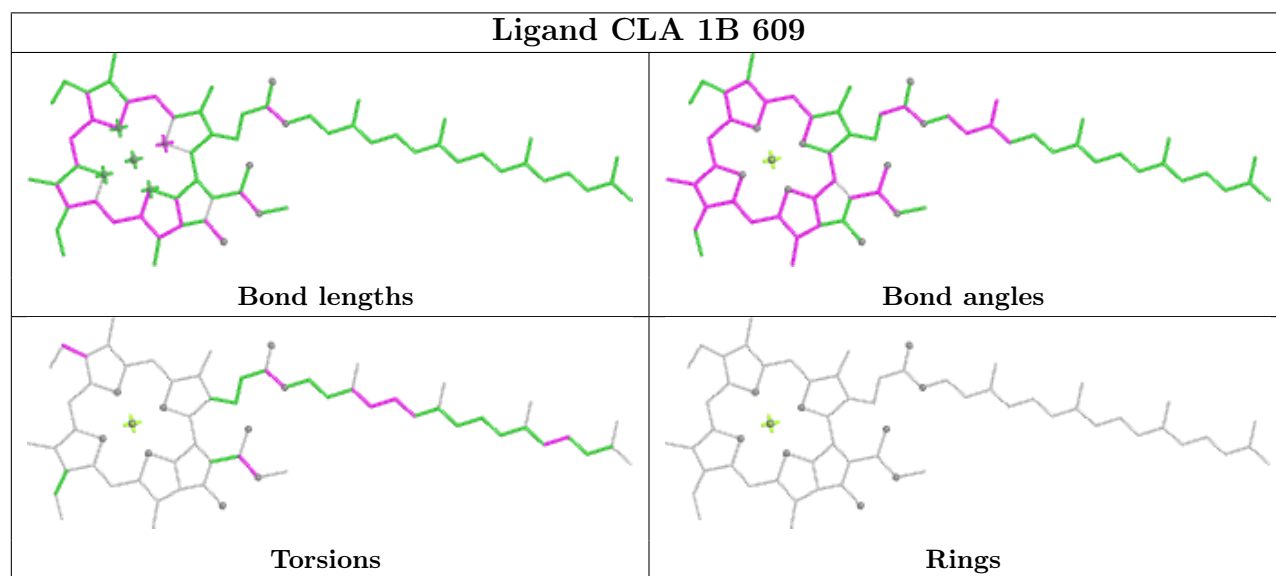
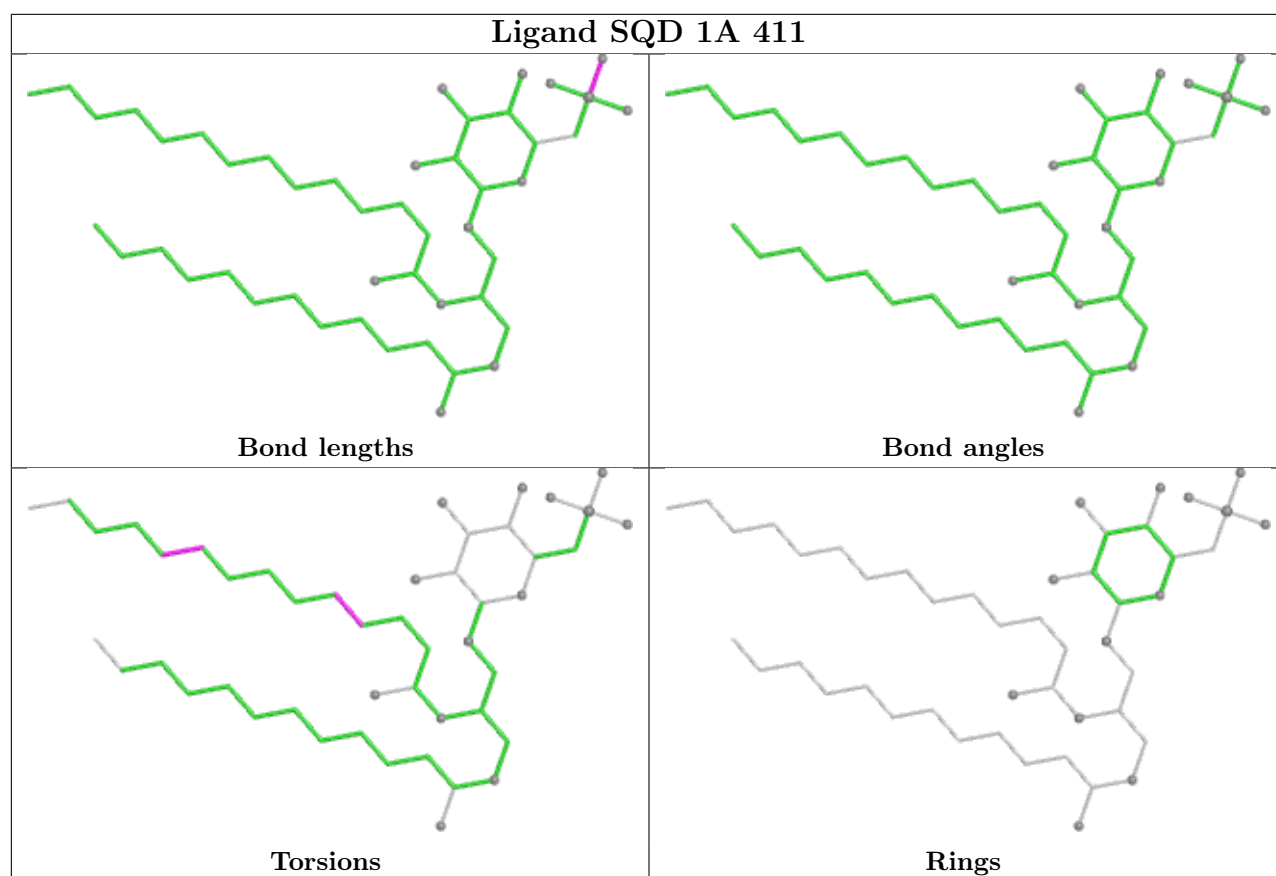
Torsions

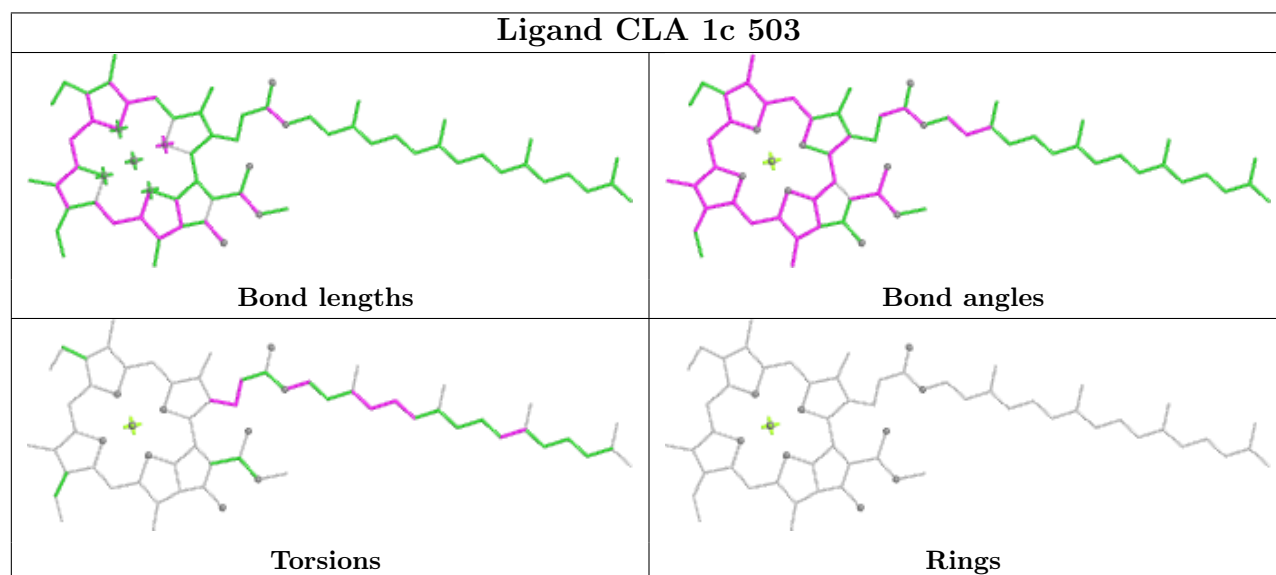
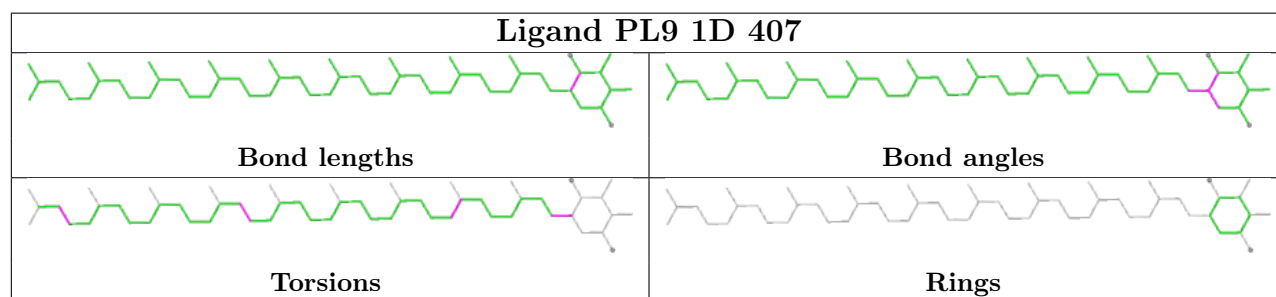
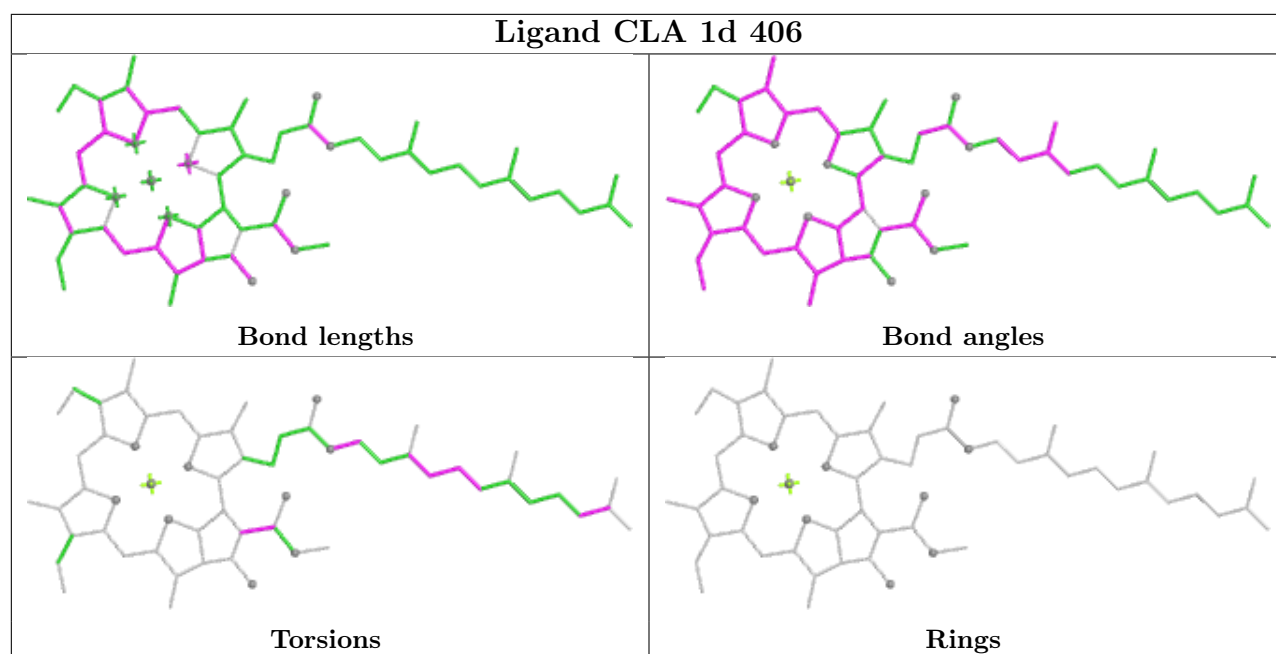


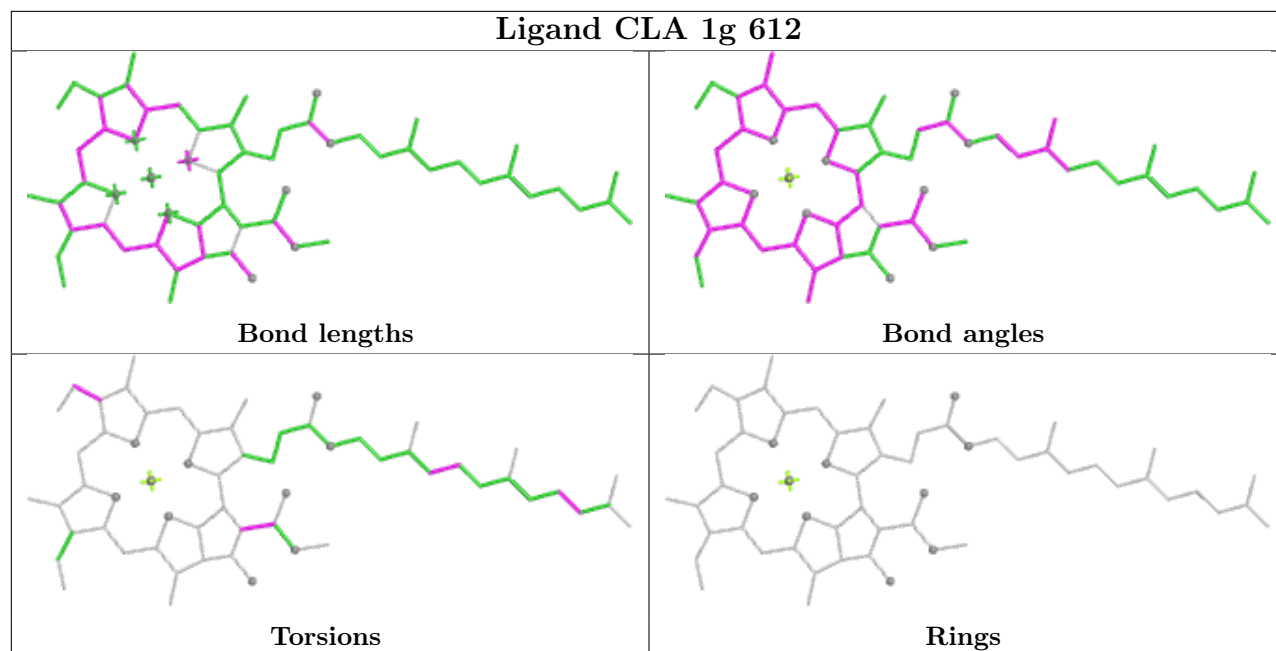
Rings

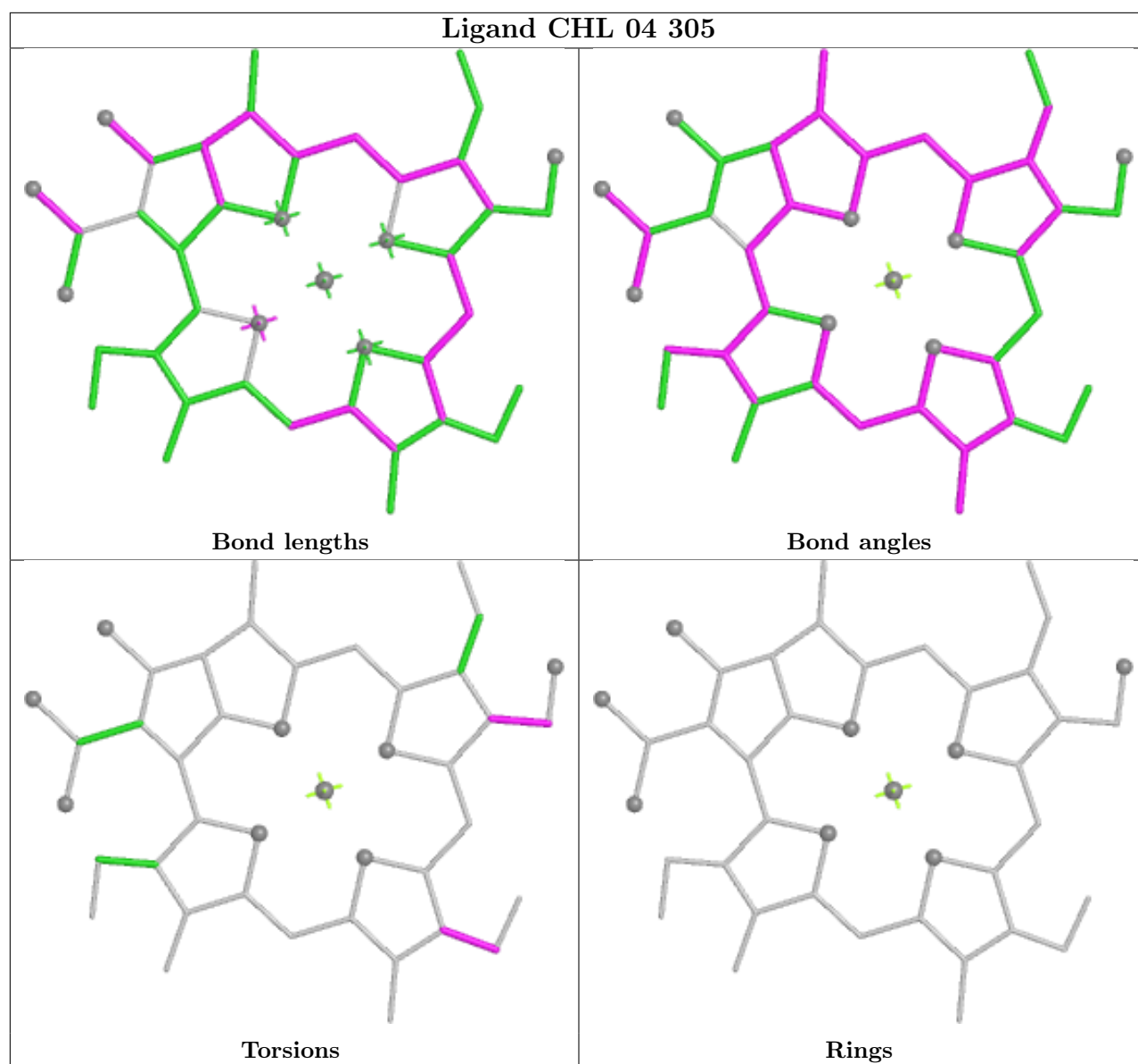


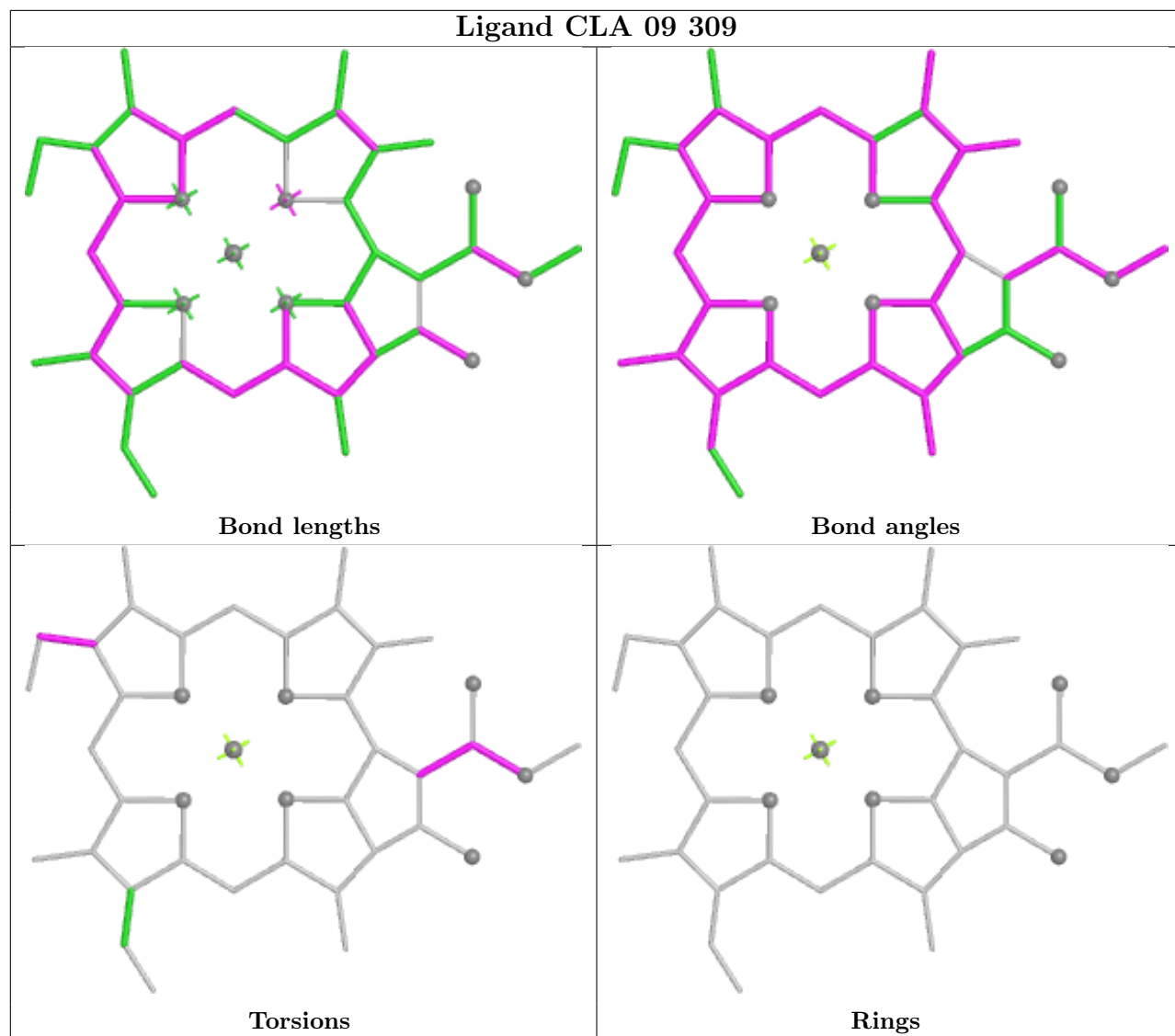


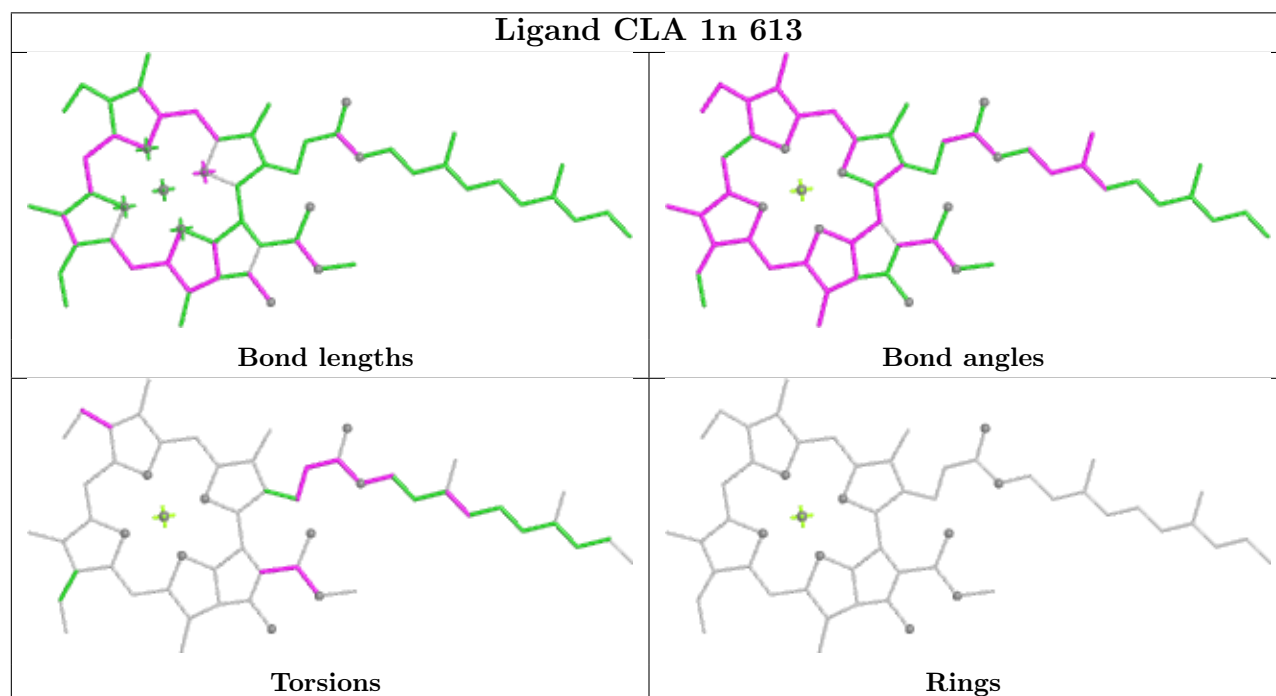
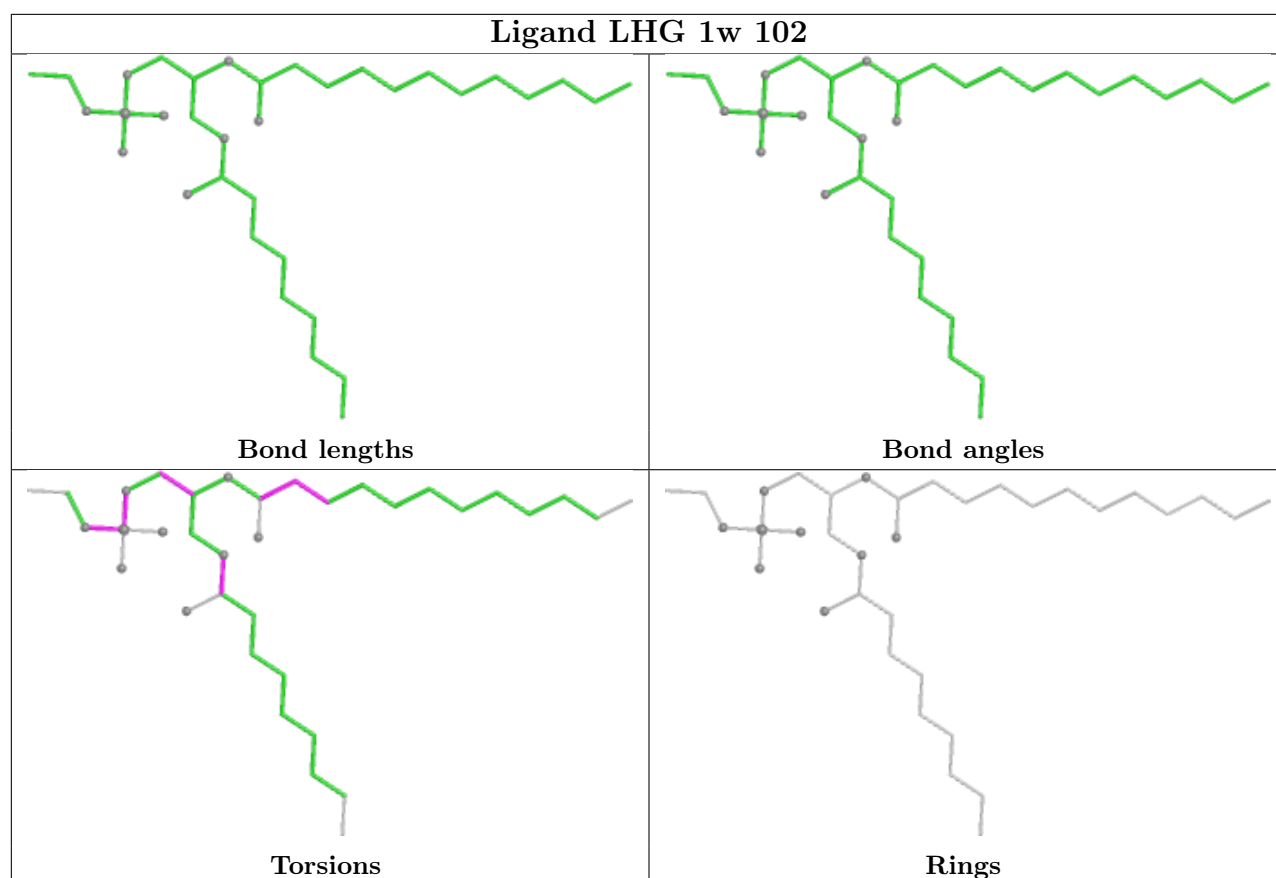


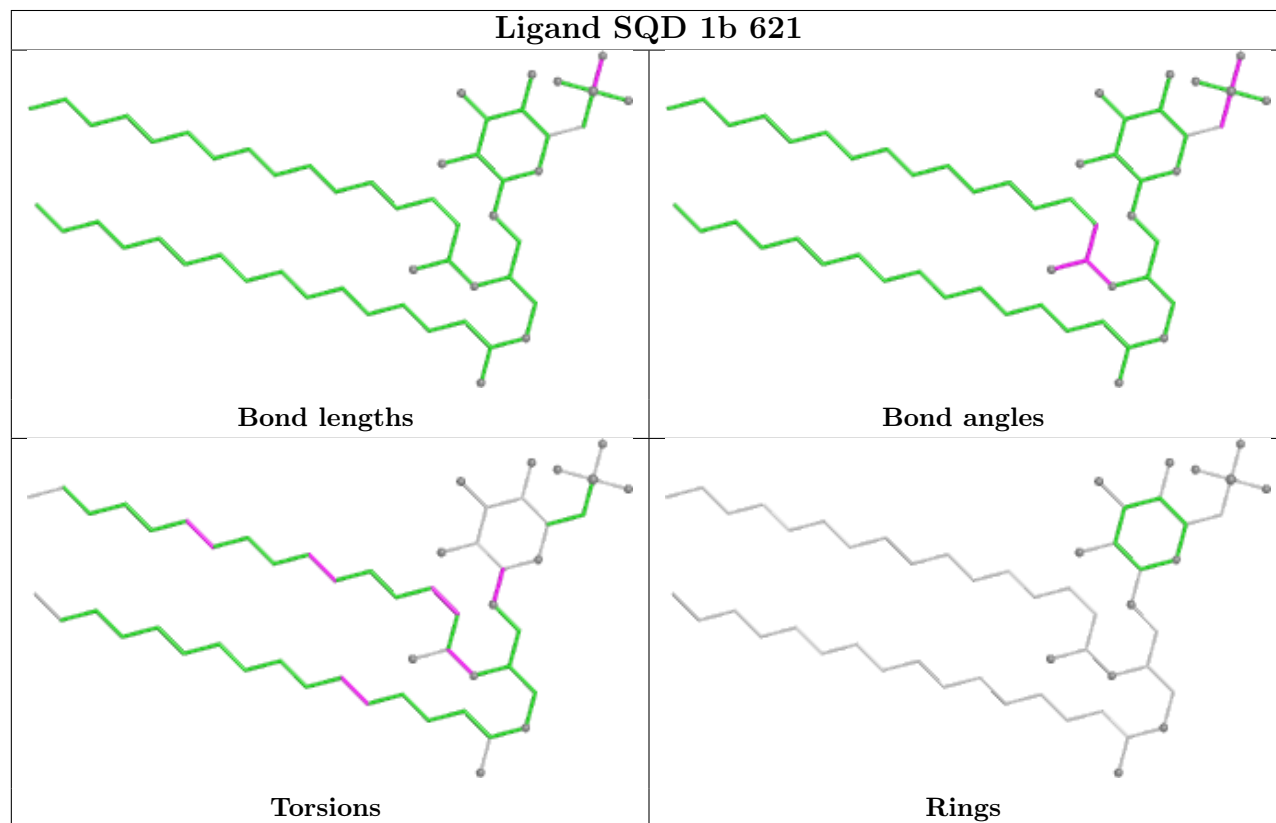
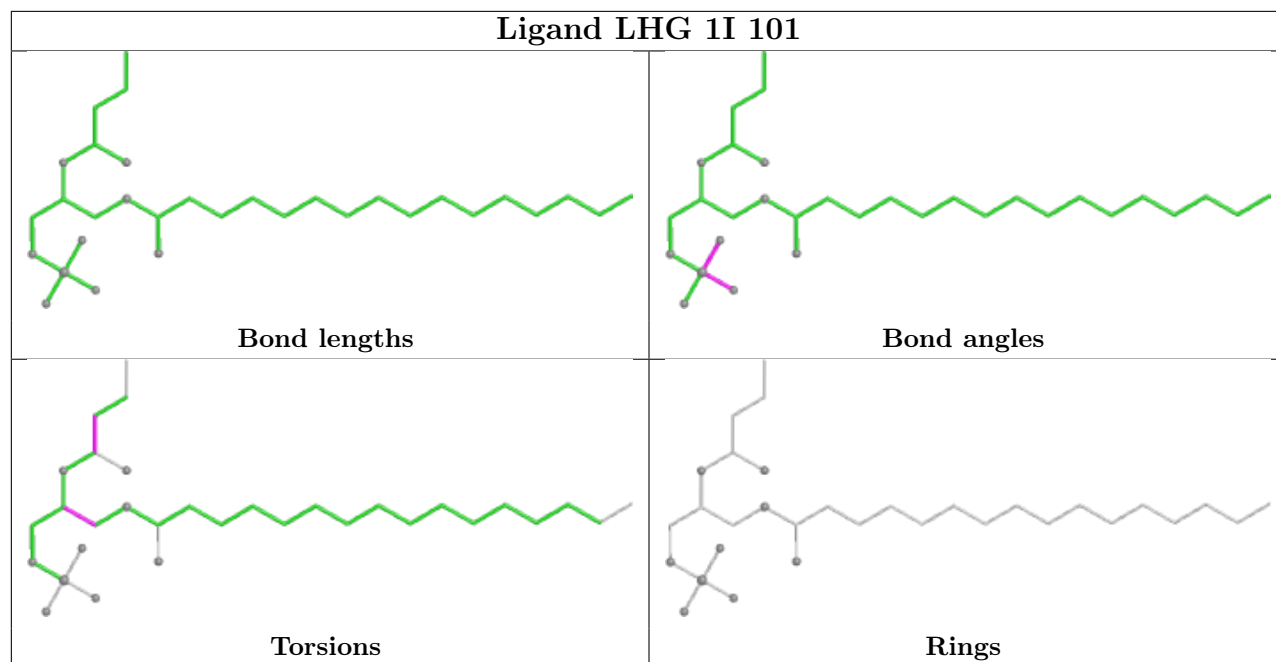


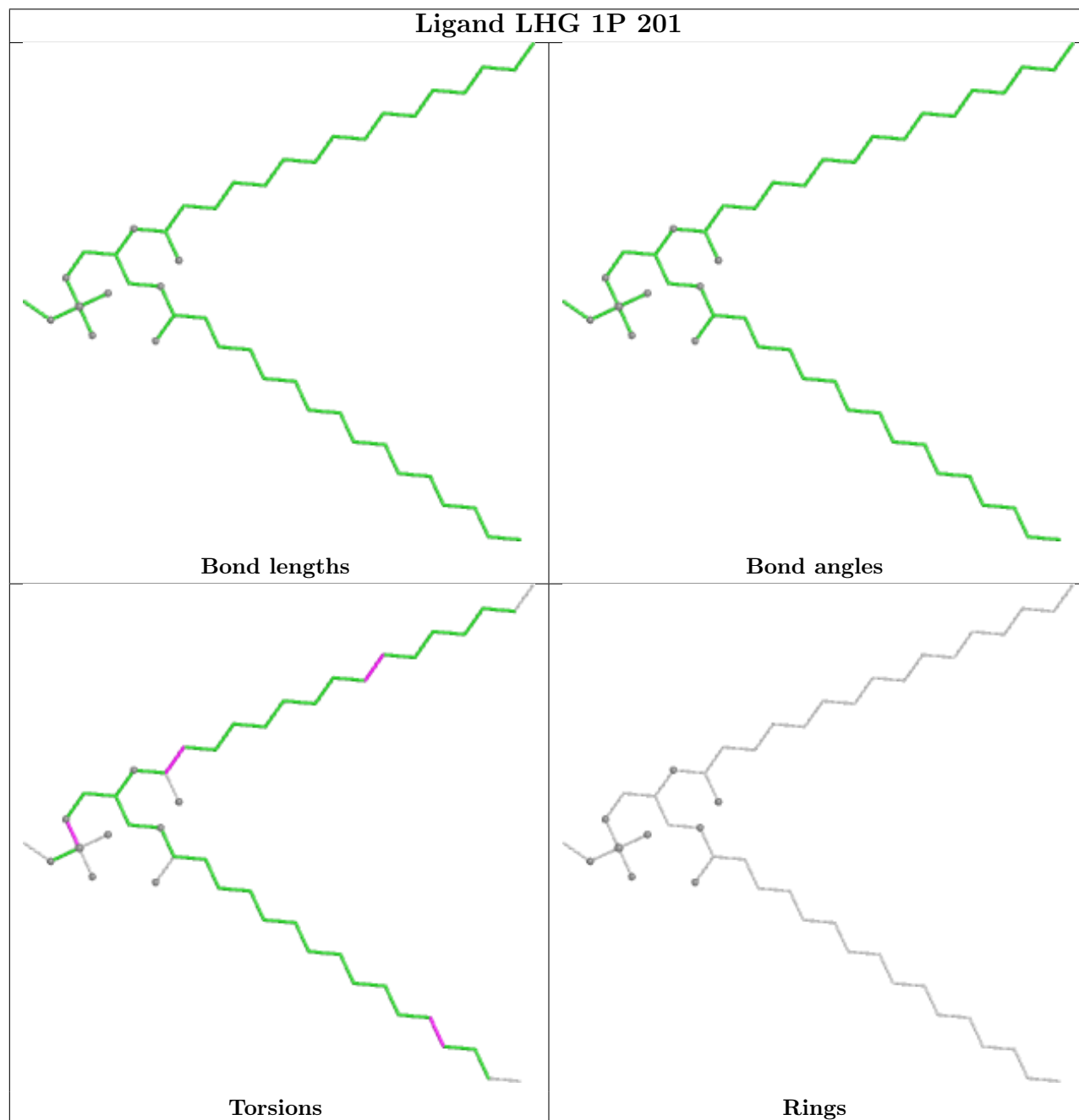
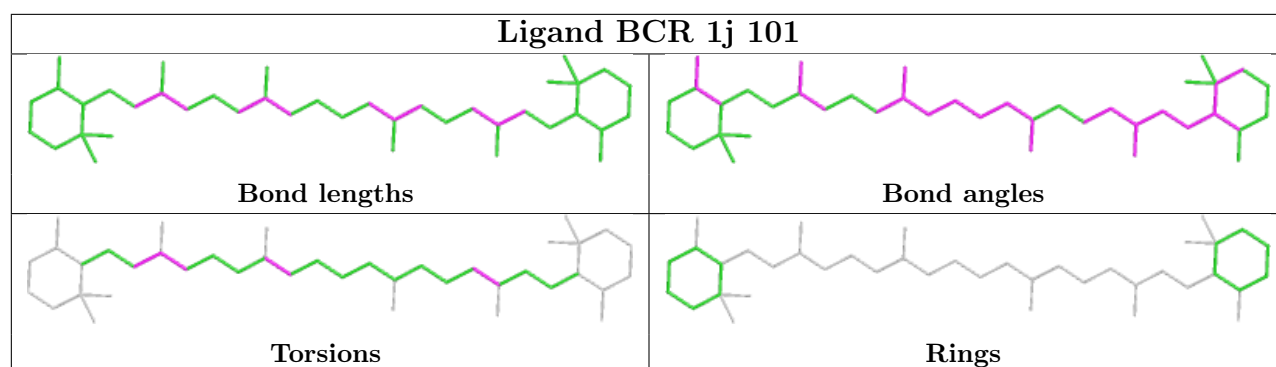


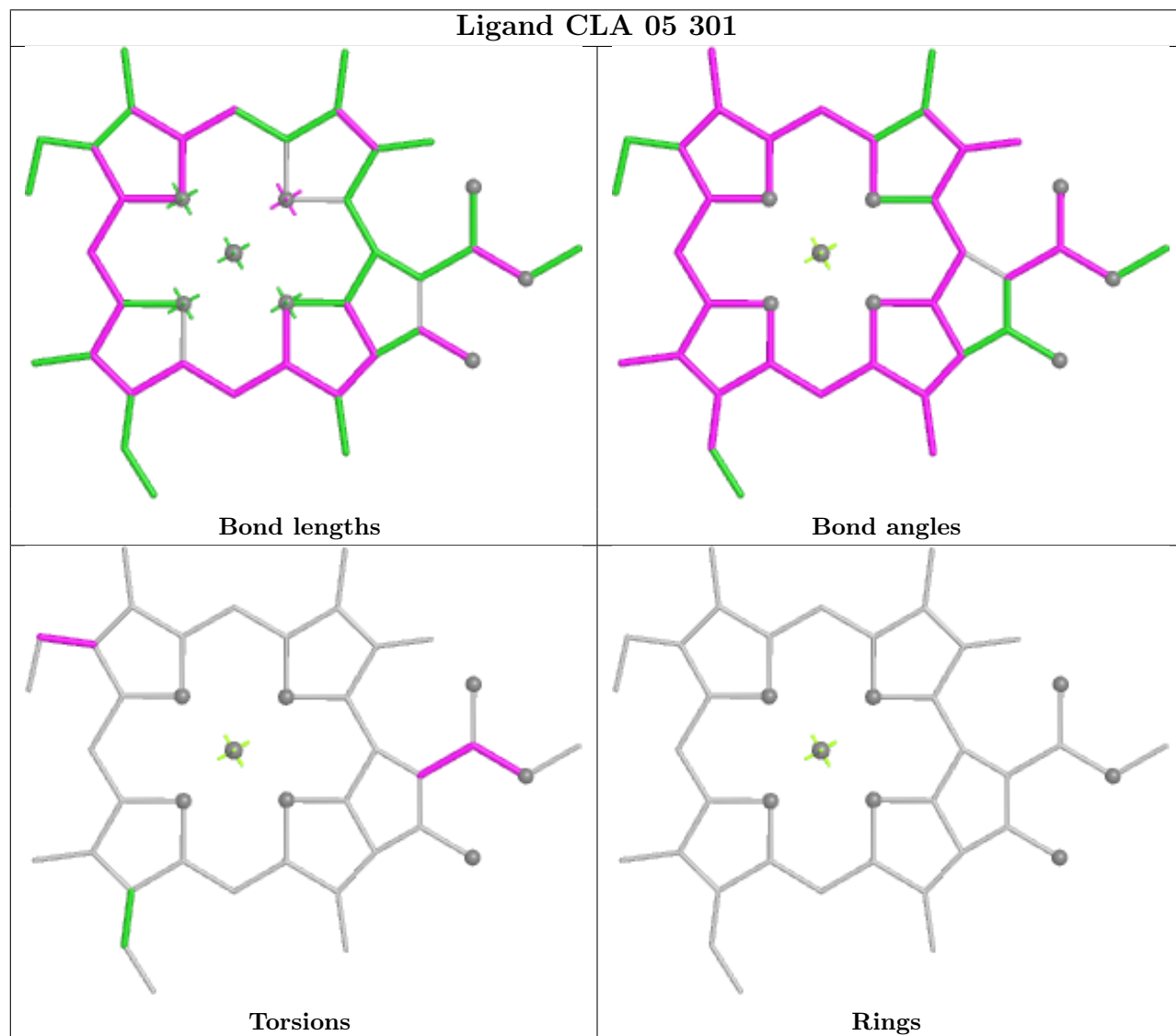
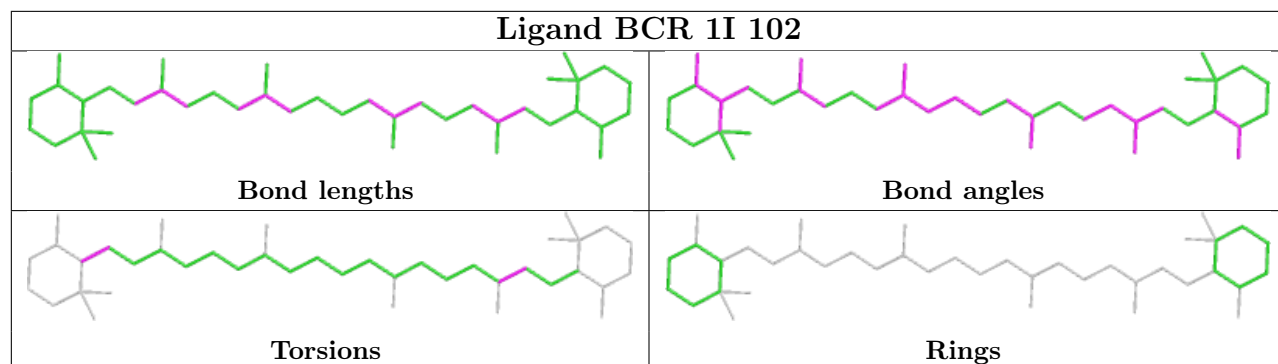


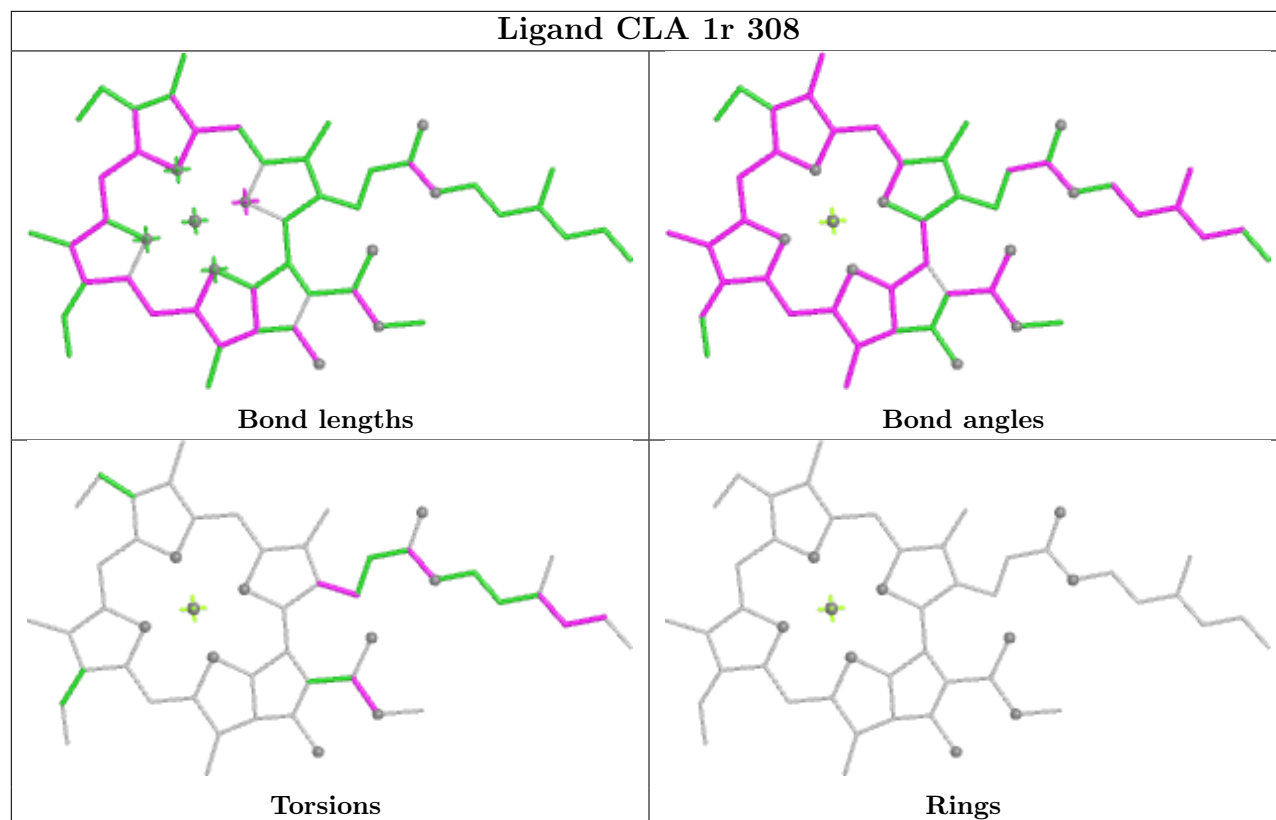




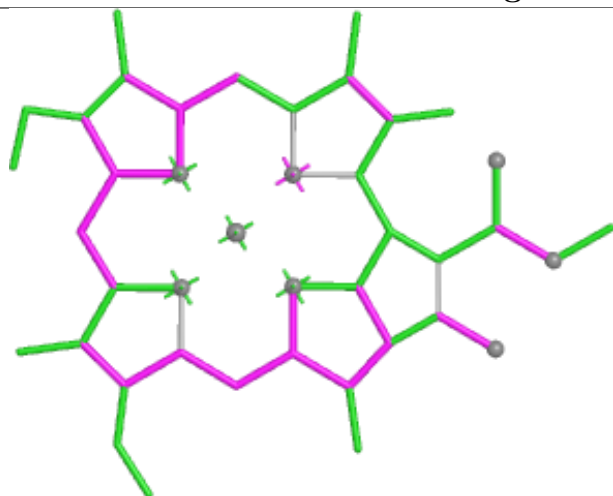




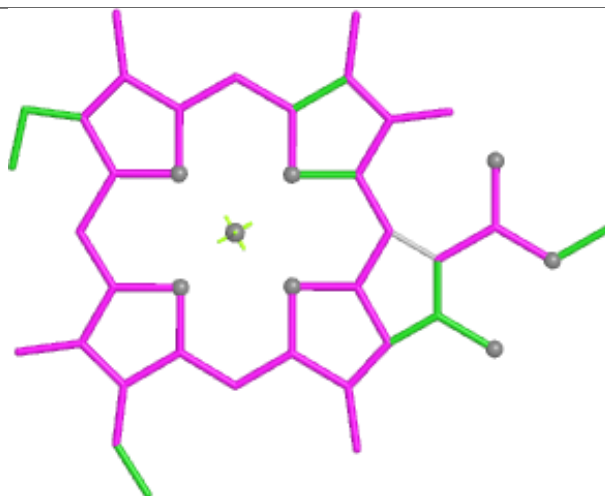




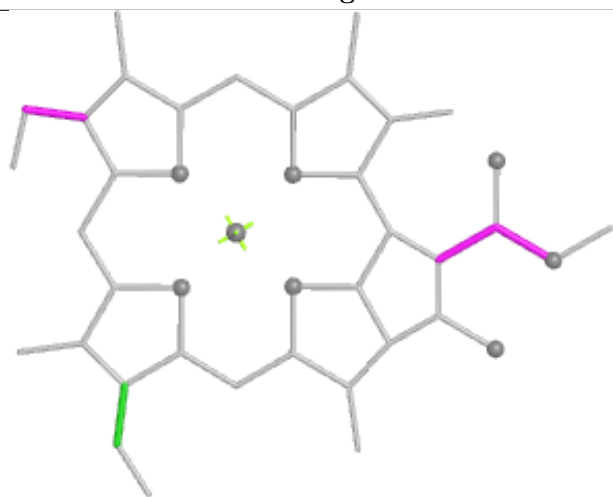
Ligand CLA 1G 604



Bond lengths



Bond angles

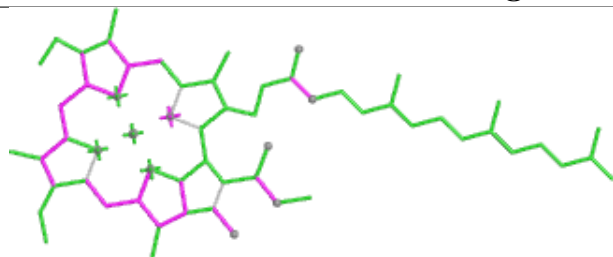


Torsions

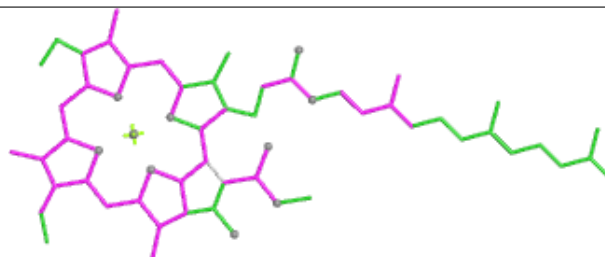


Rings

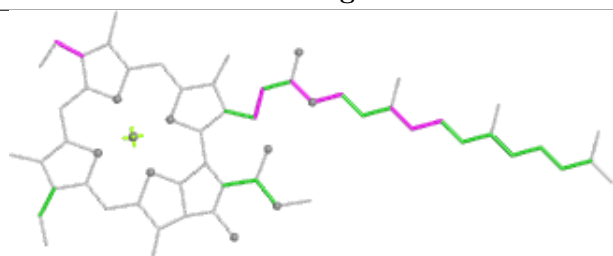
Ligand CLA 1R 302



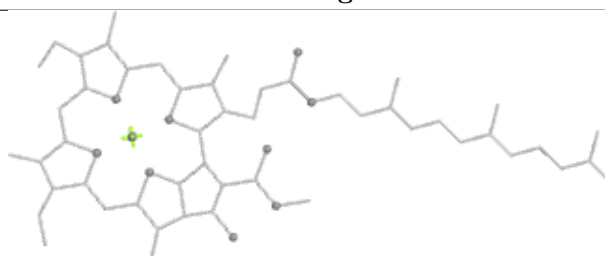
Bond lengths



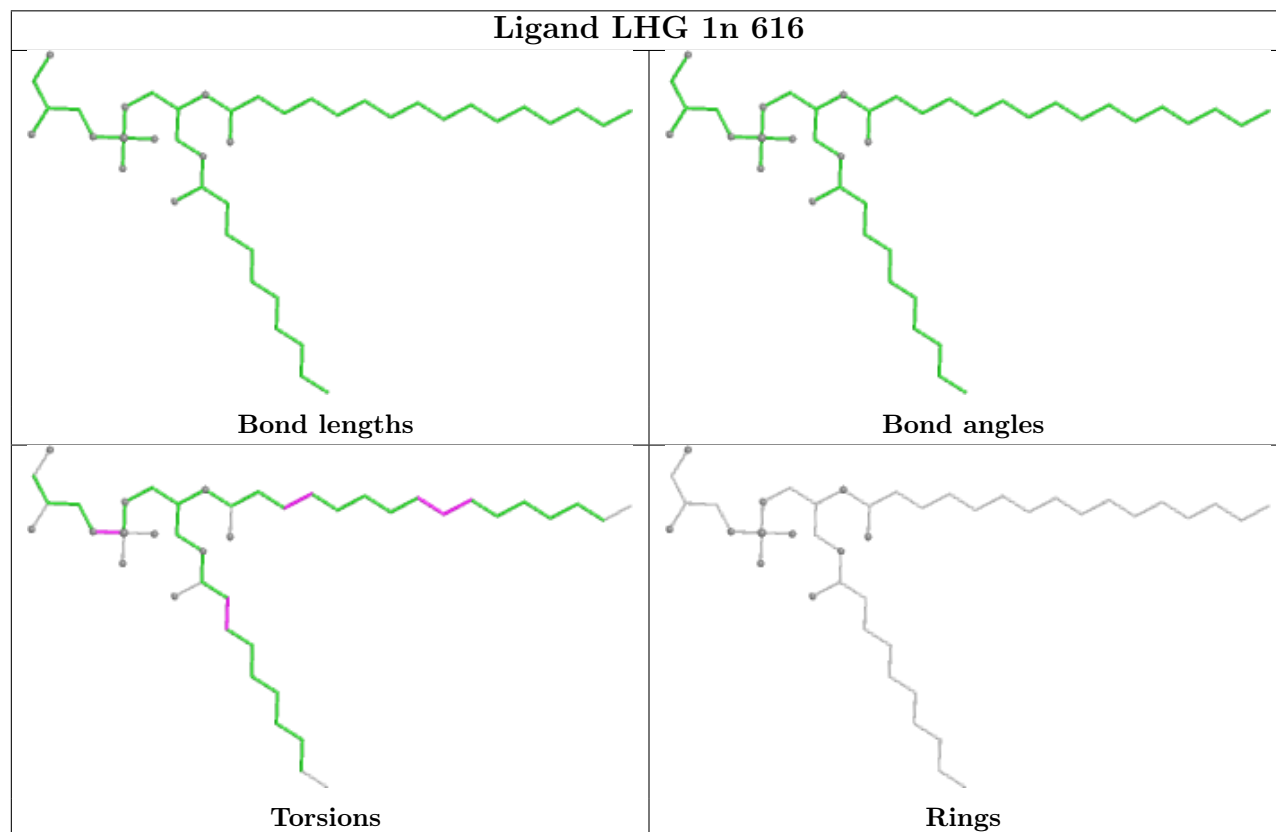
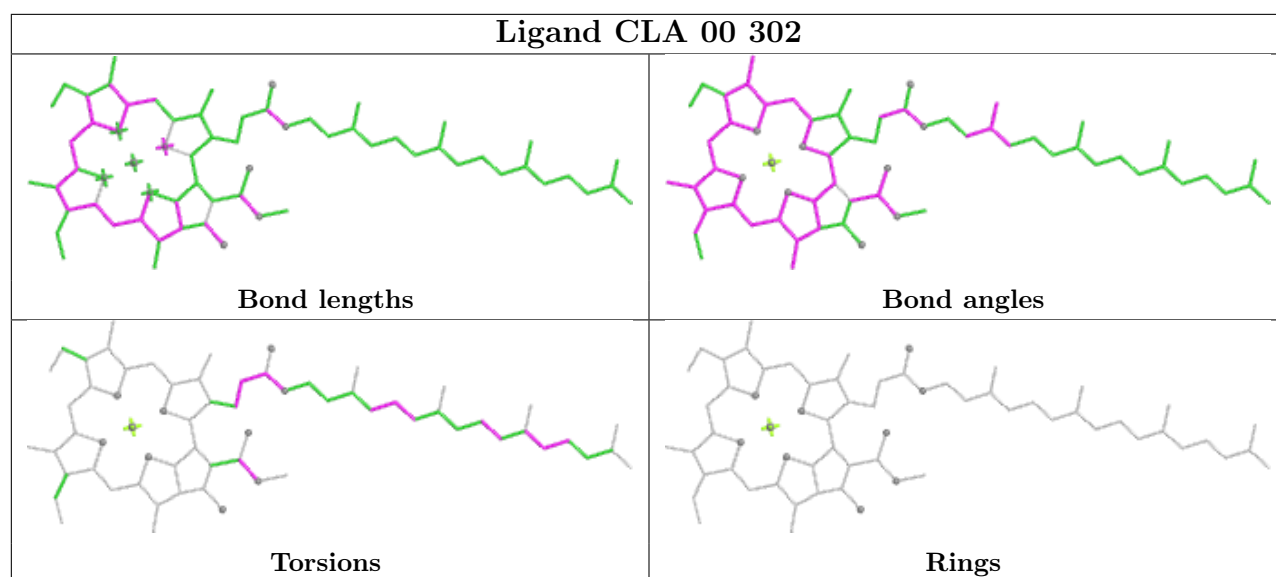
Bond angles

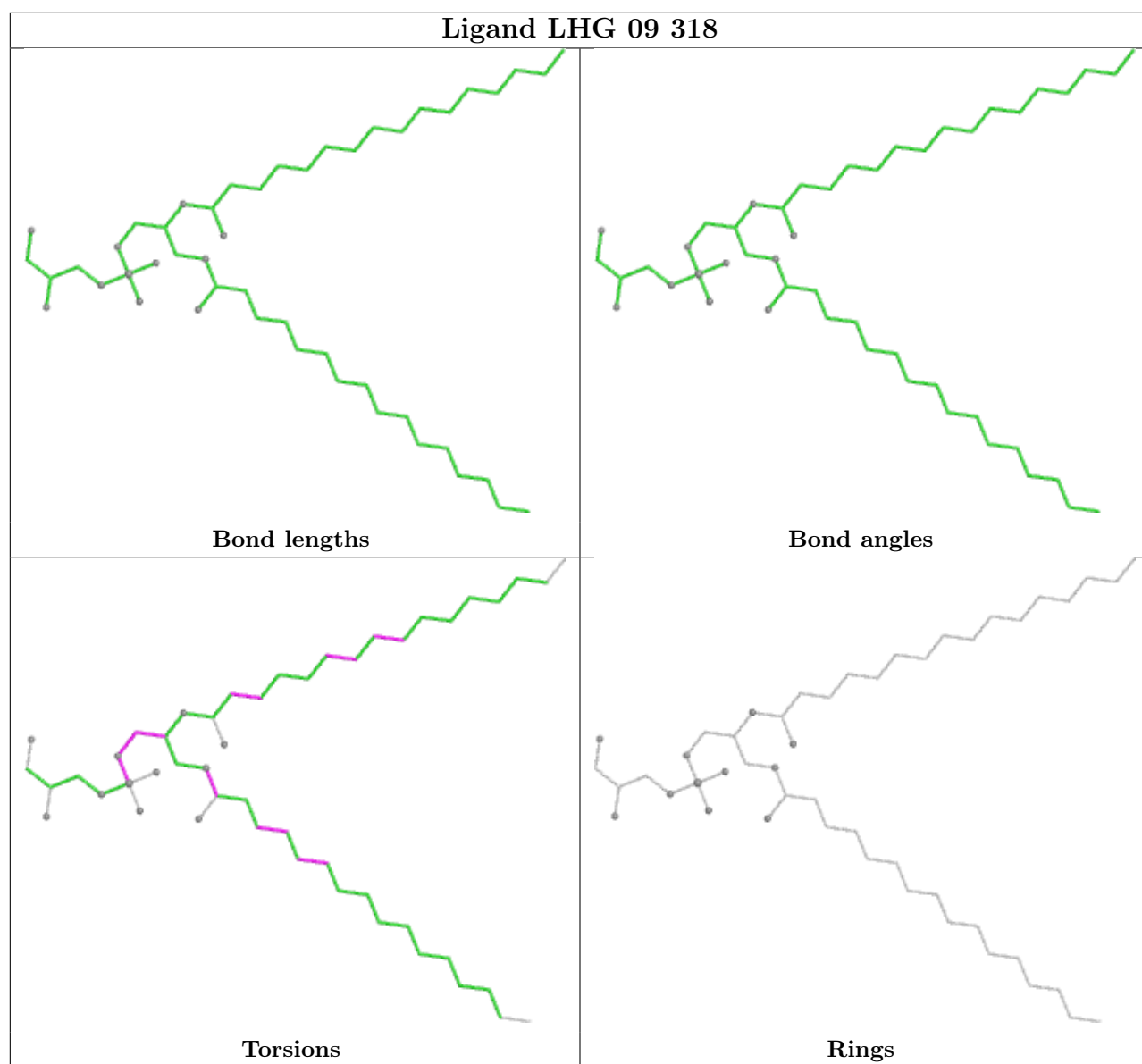


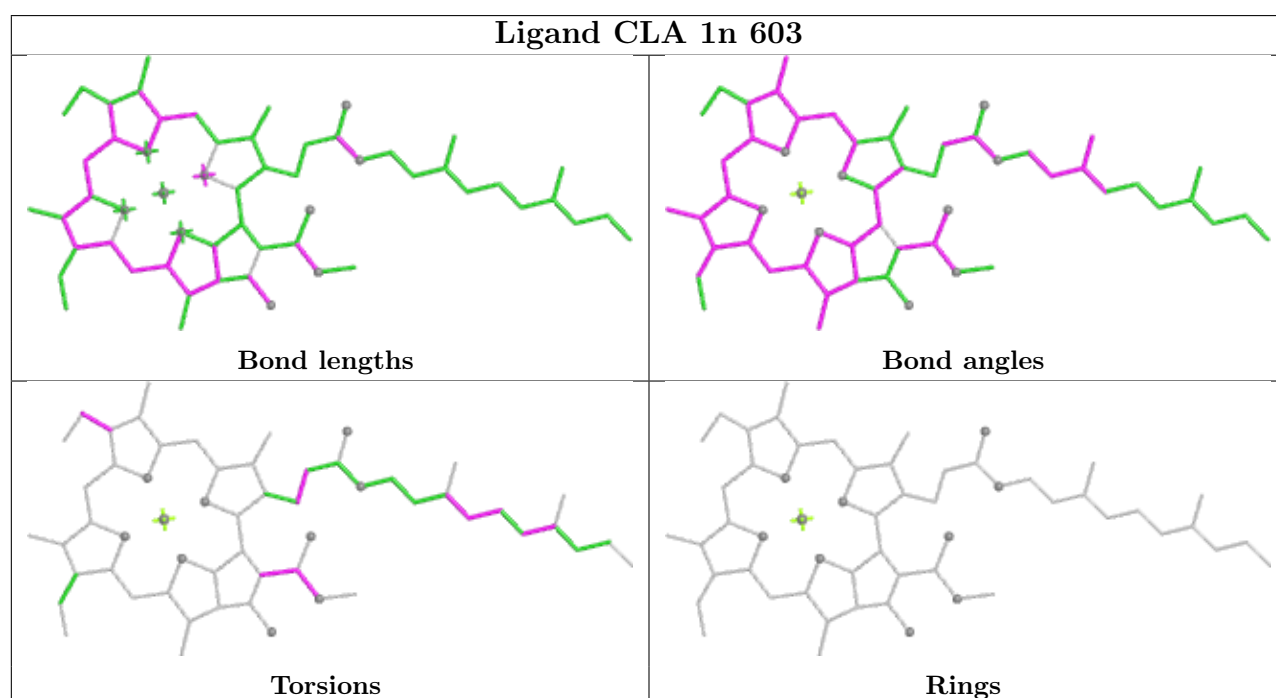
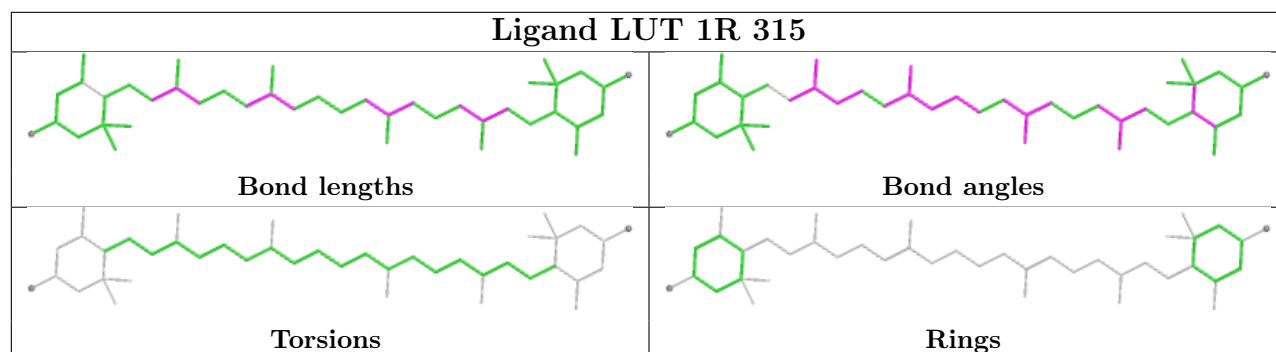
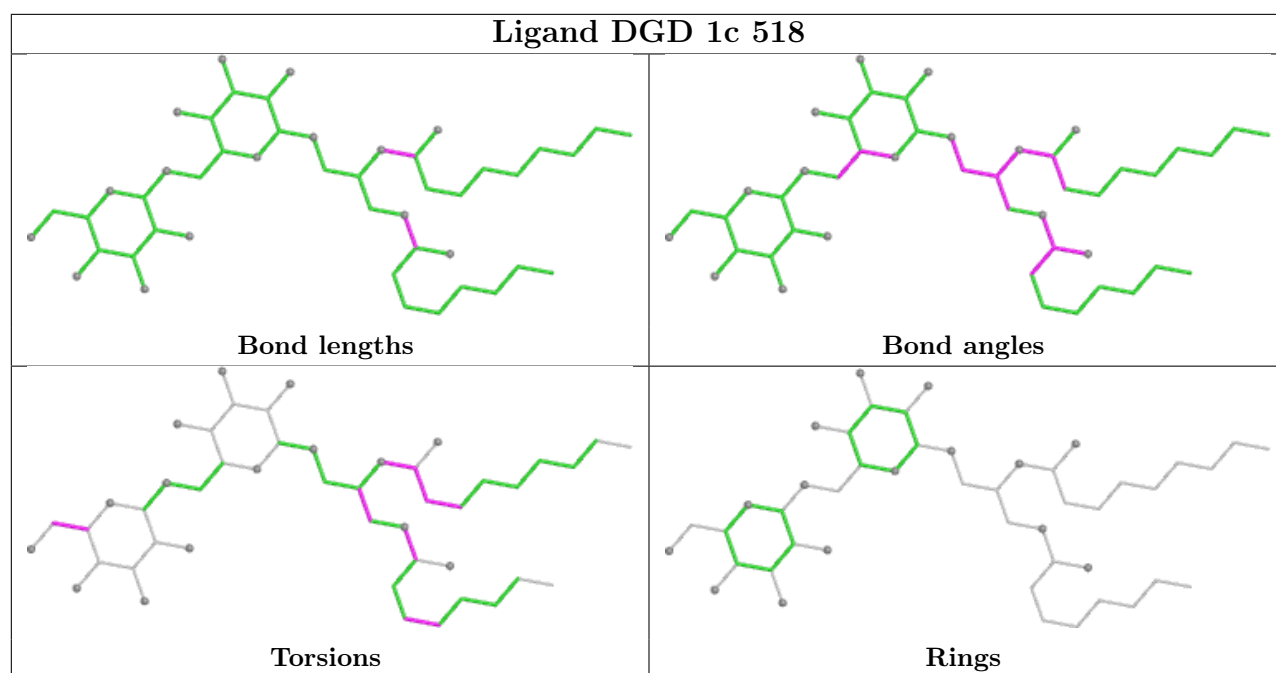
Torsions

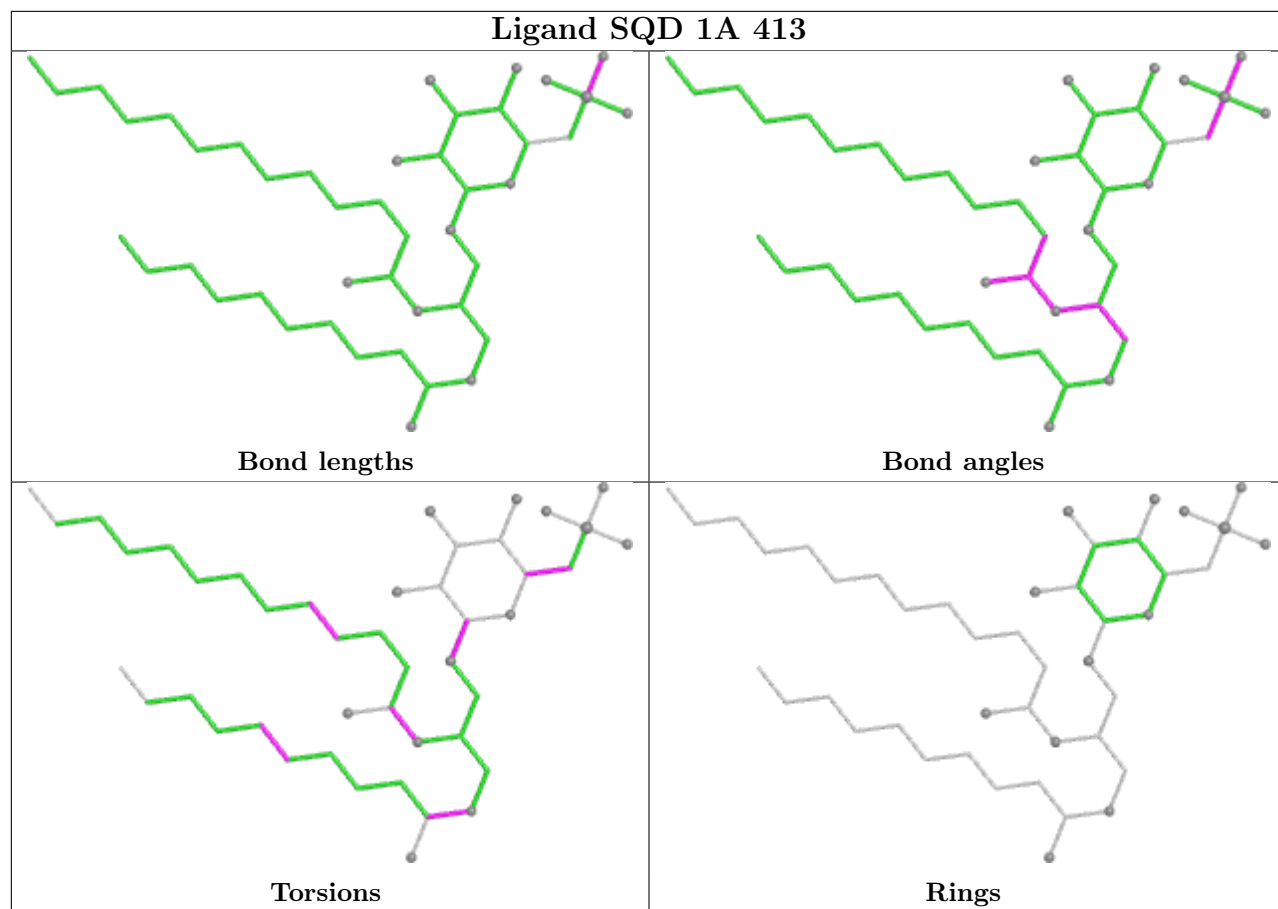


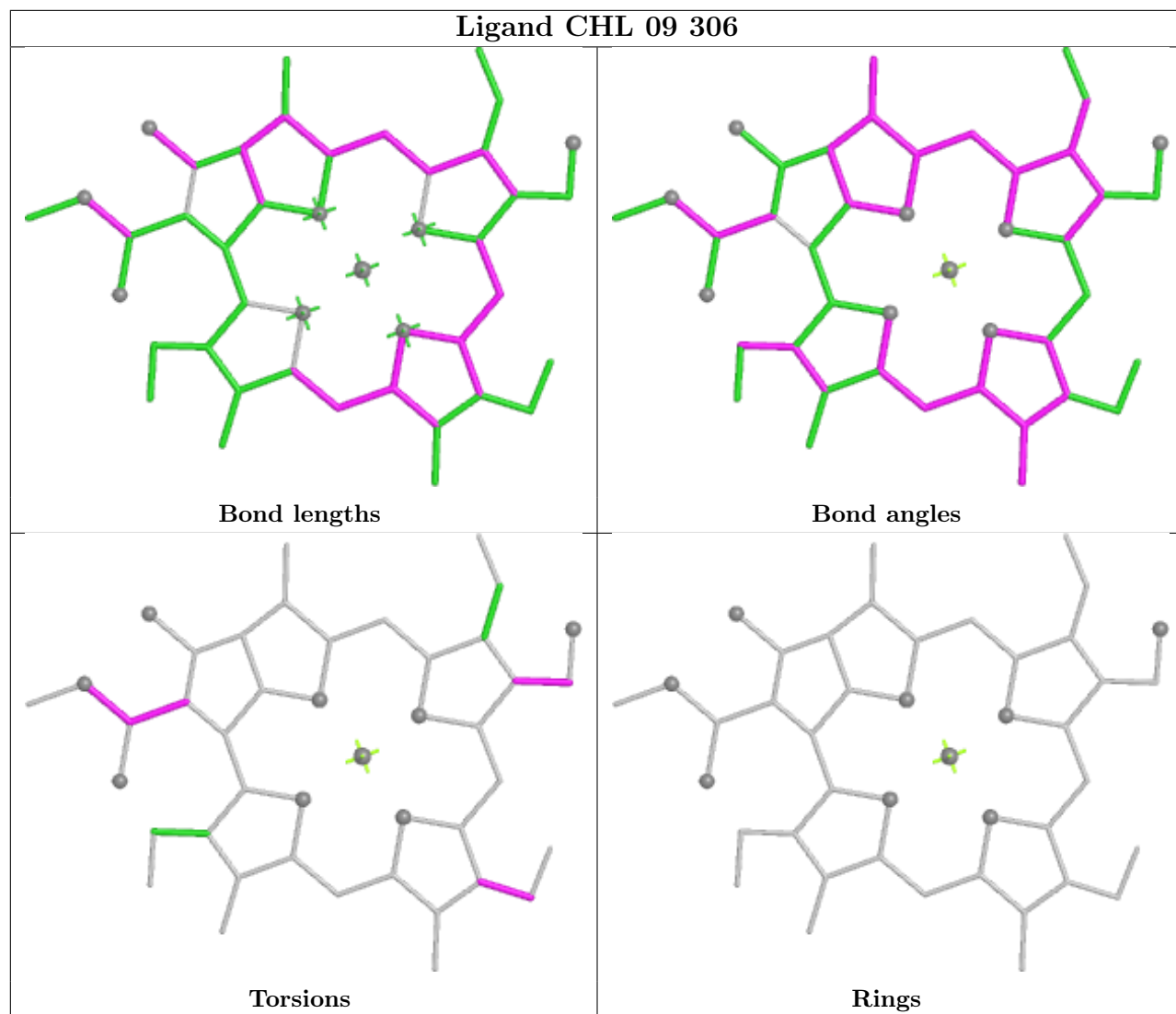
Rings

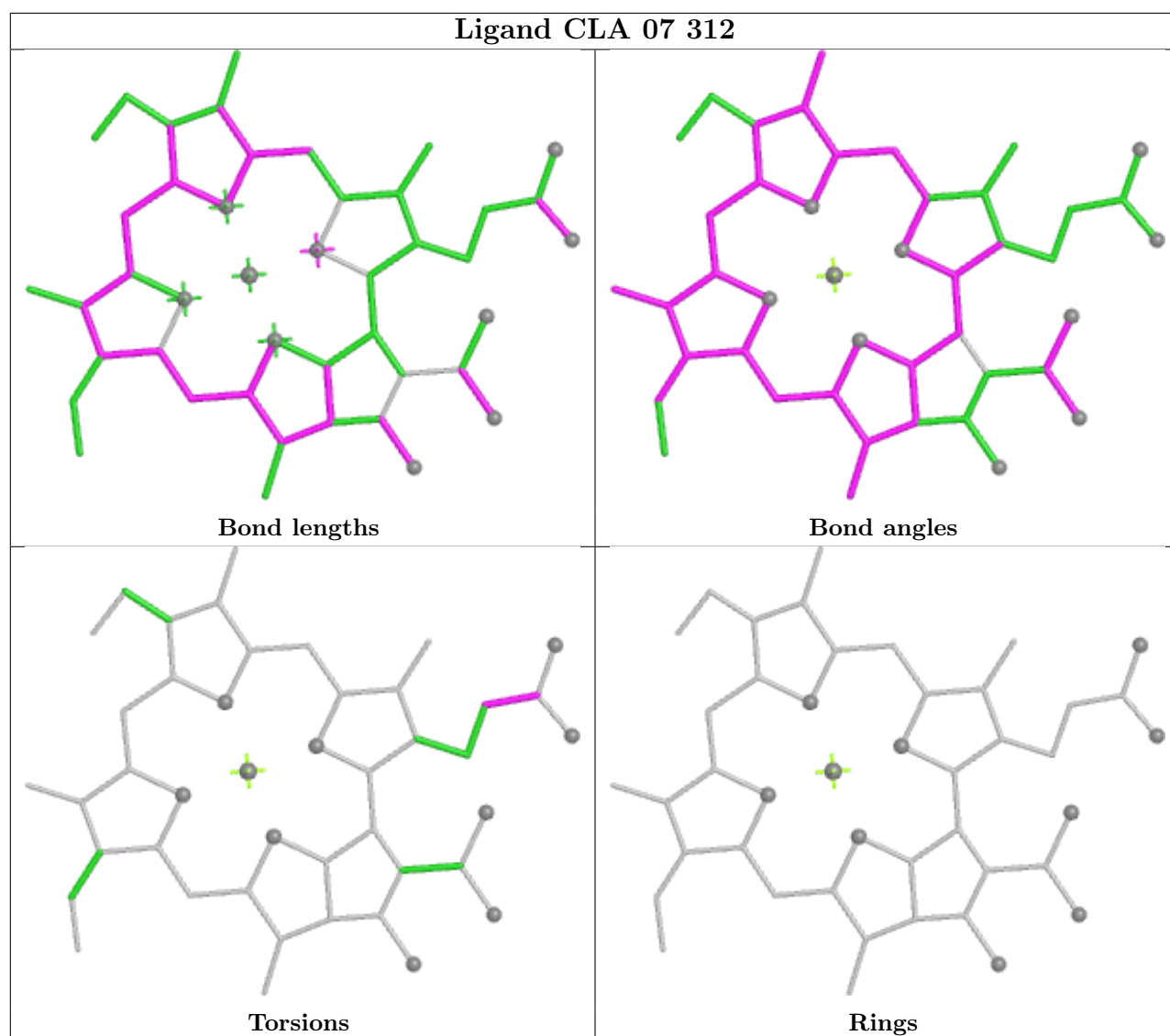


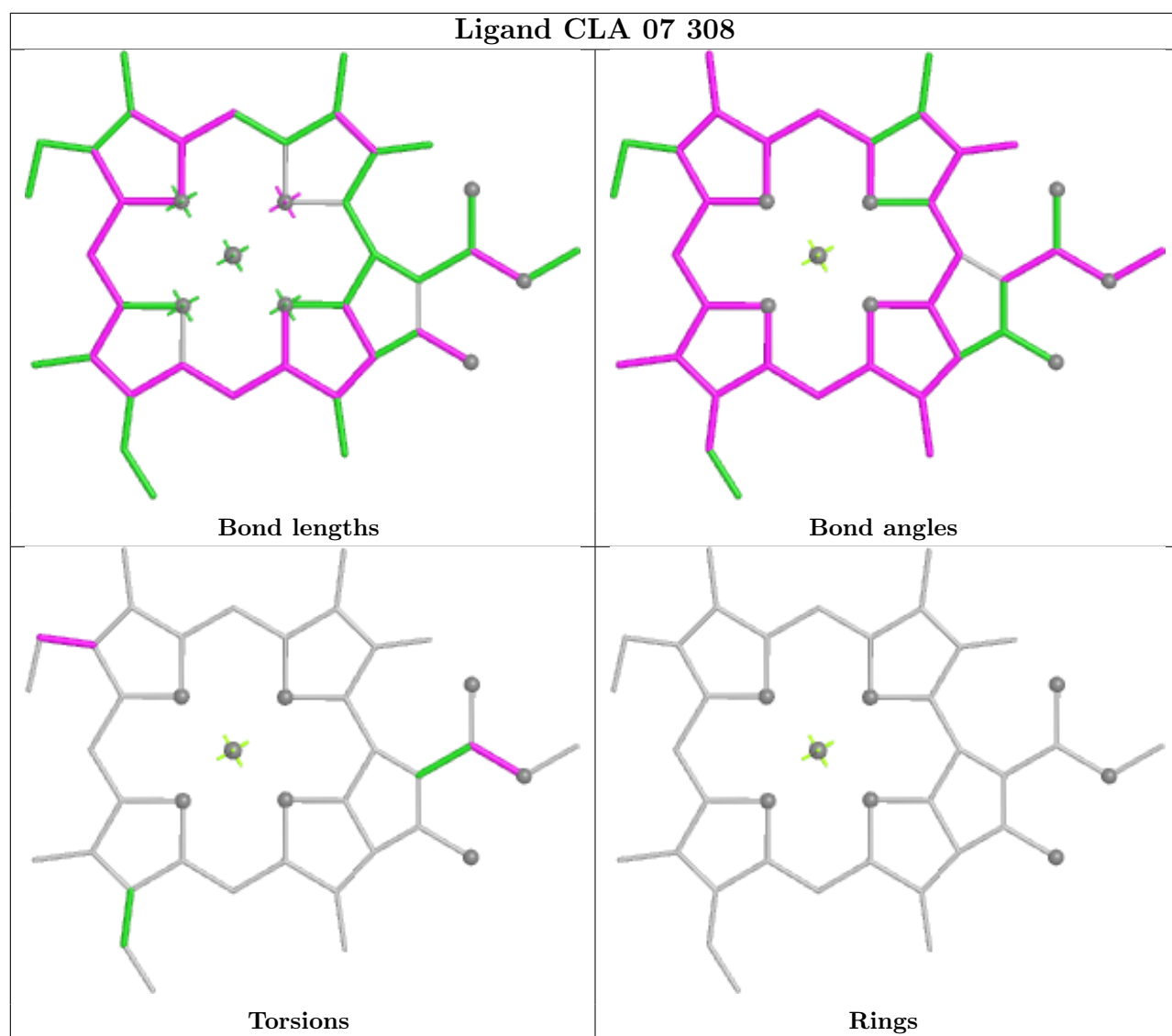




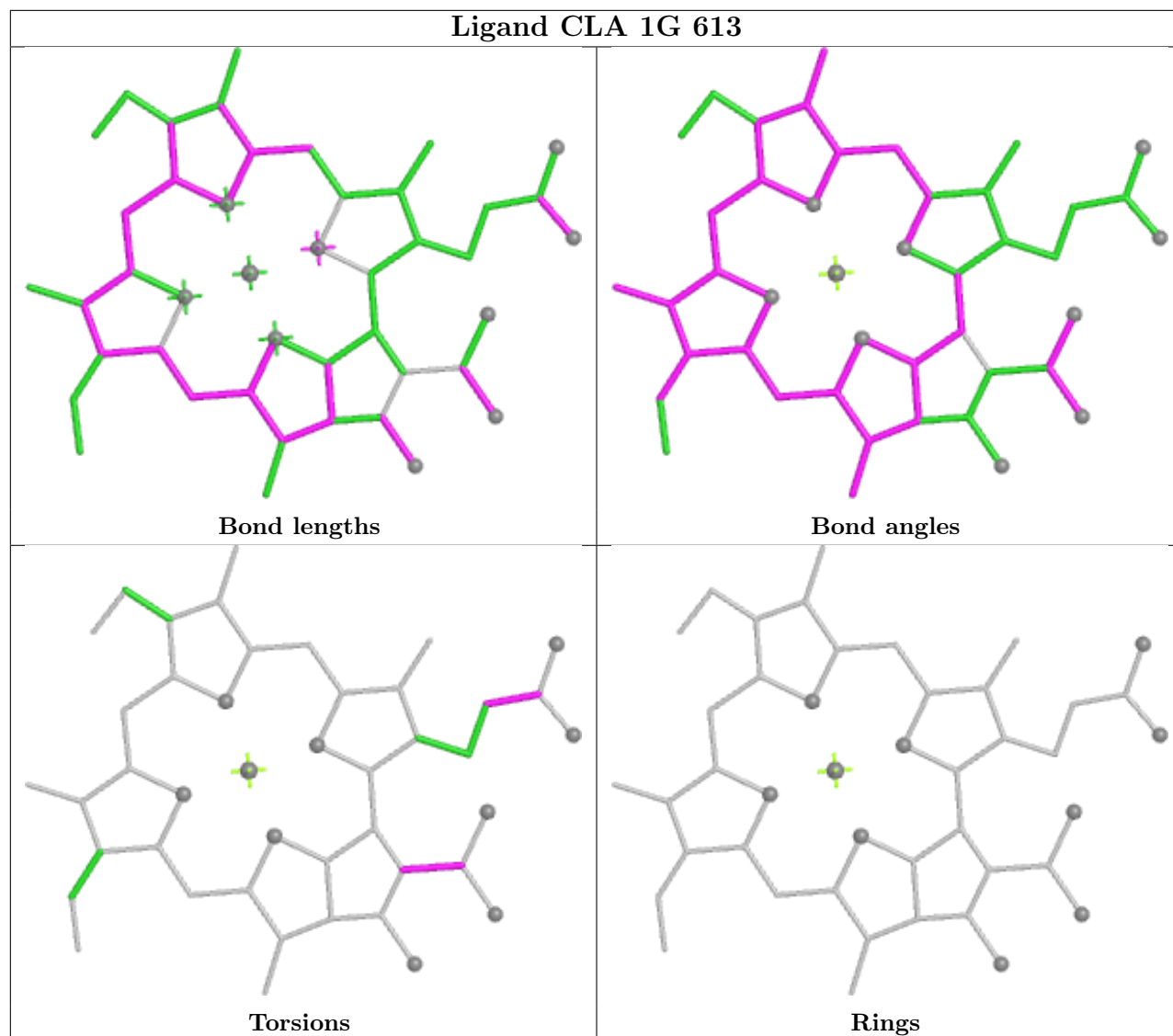


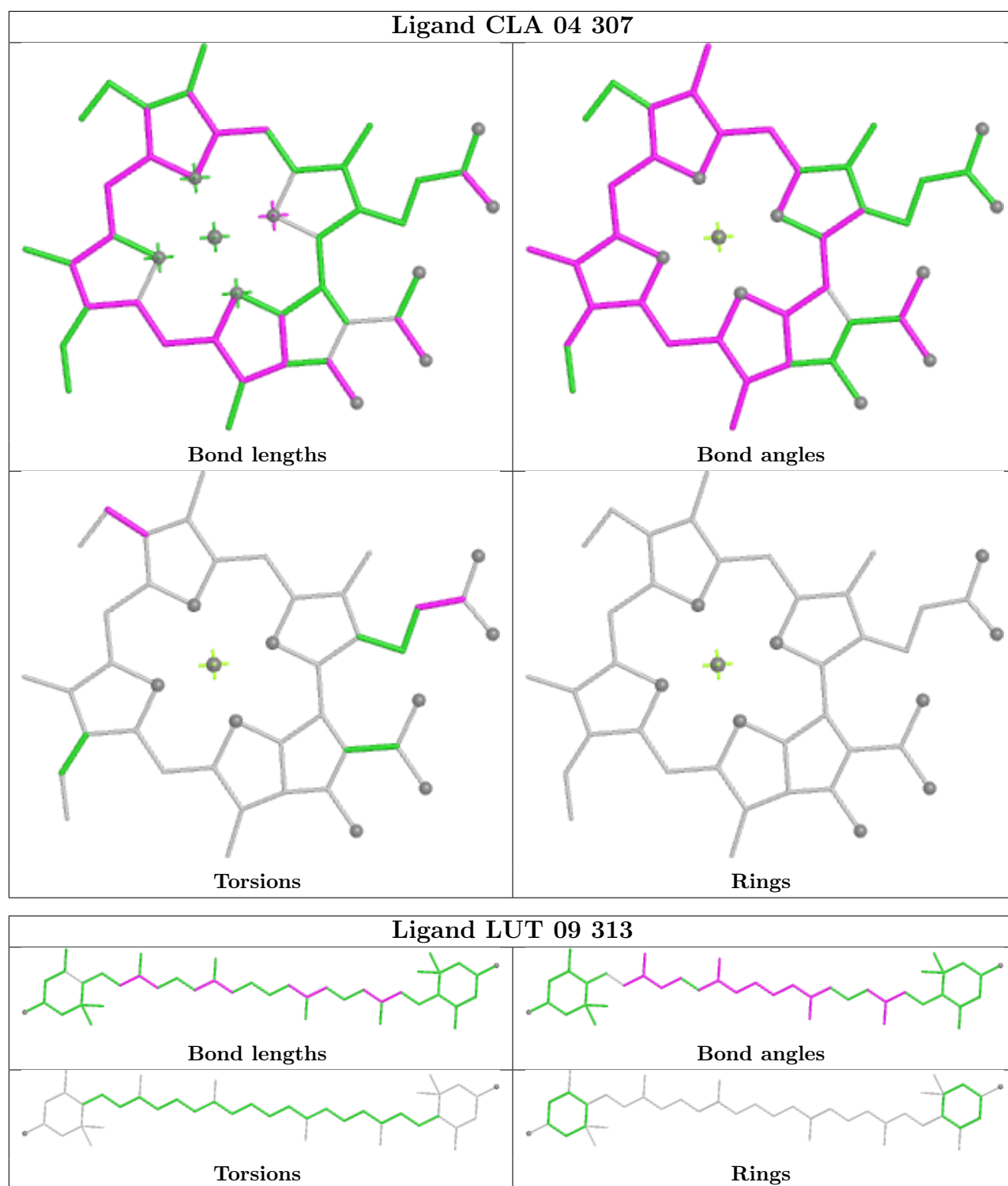


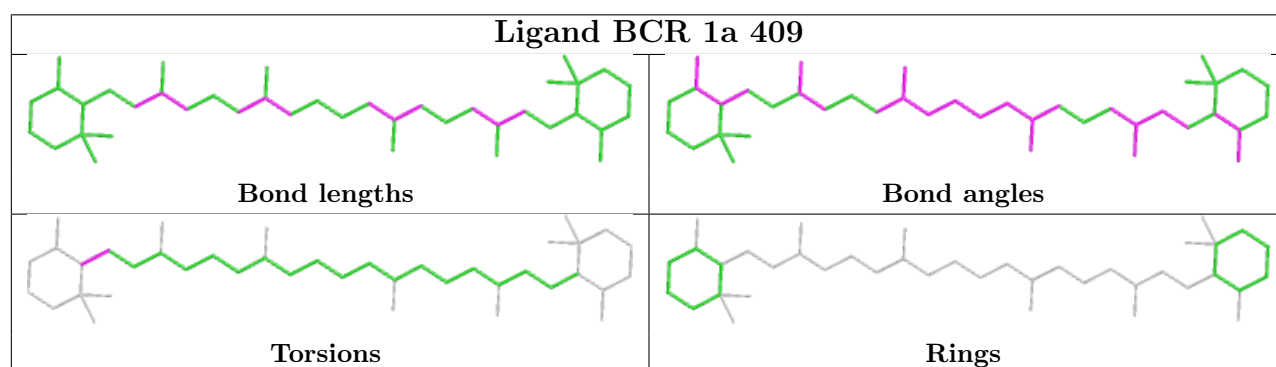
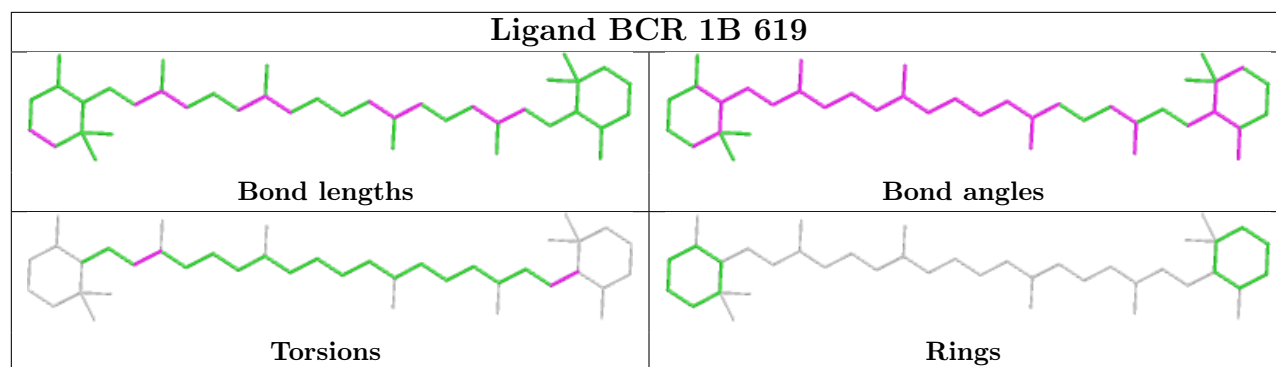
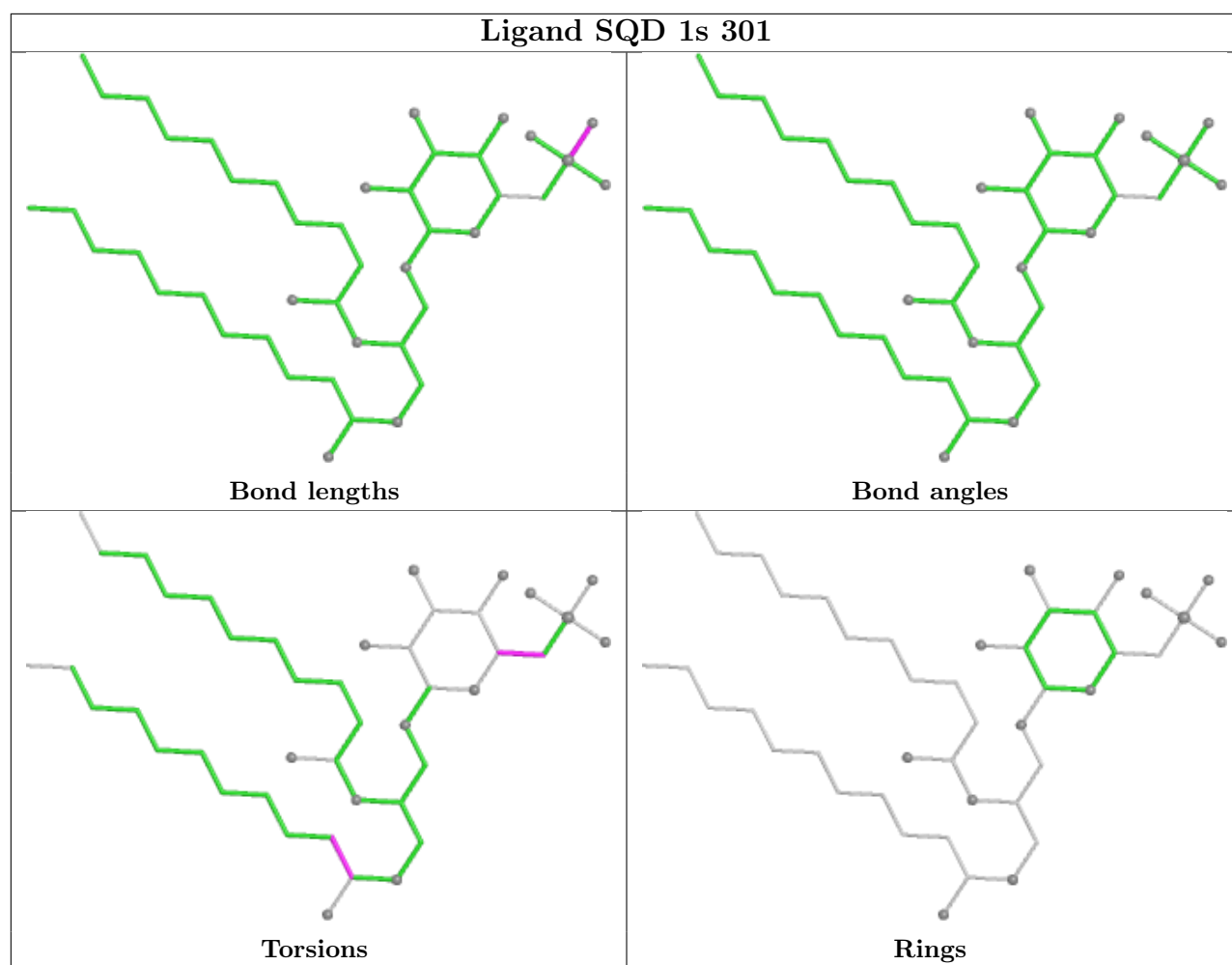


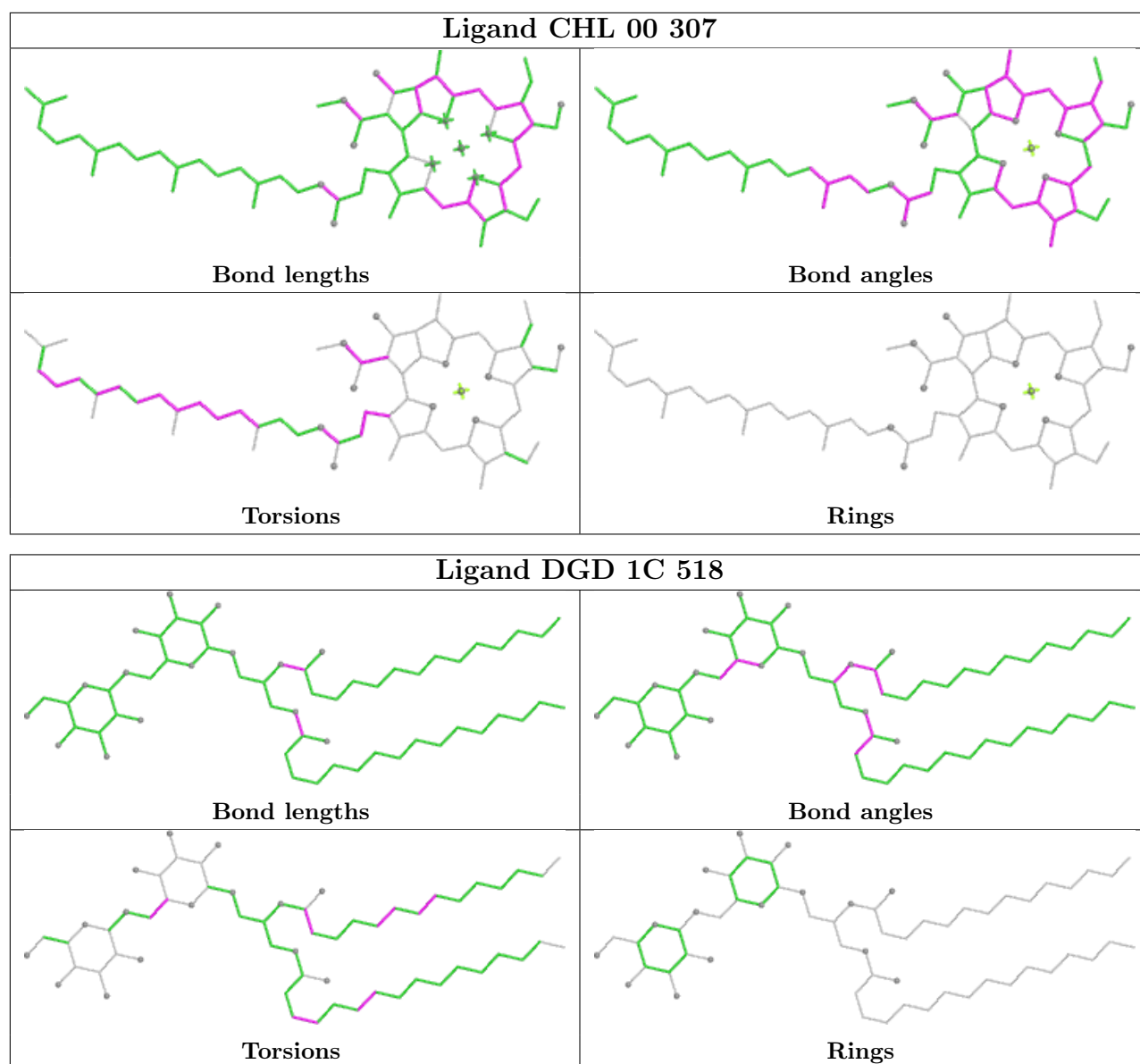


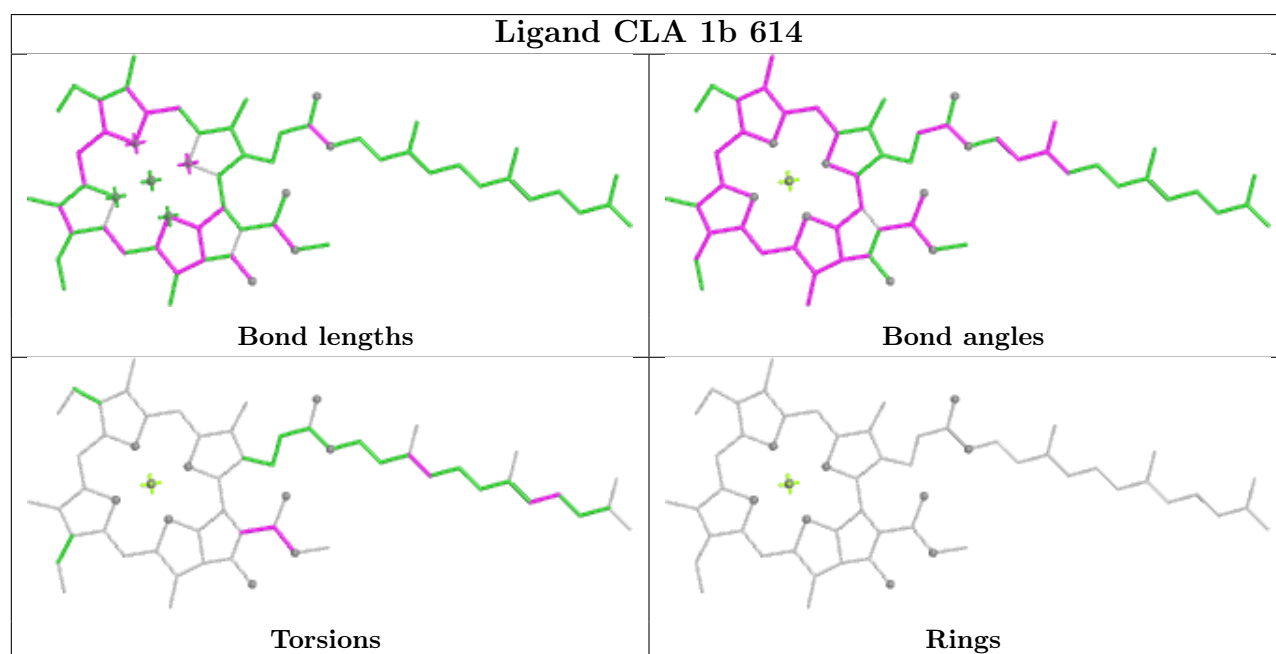
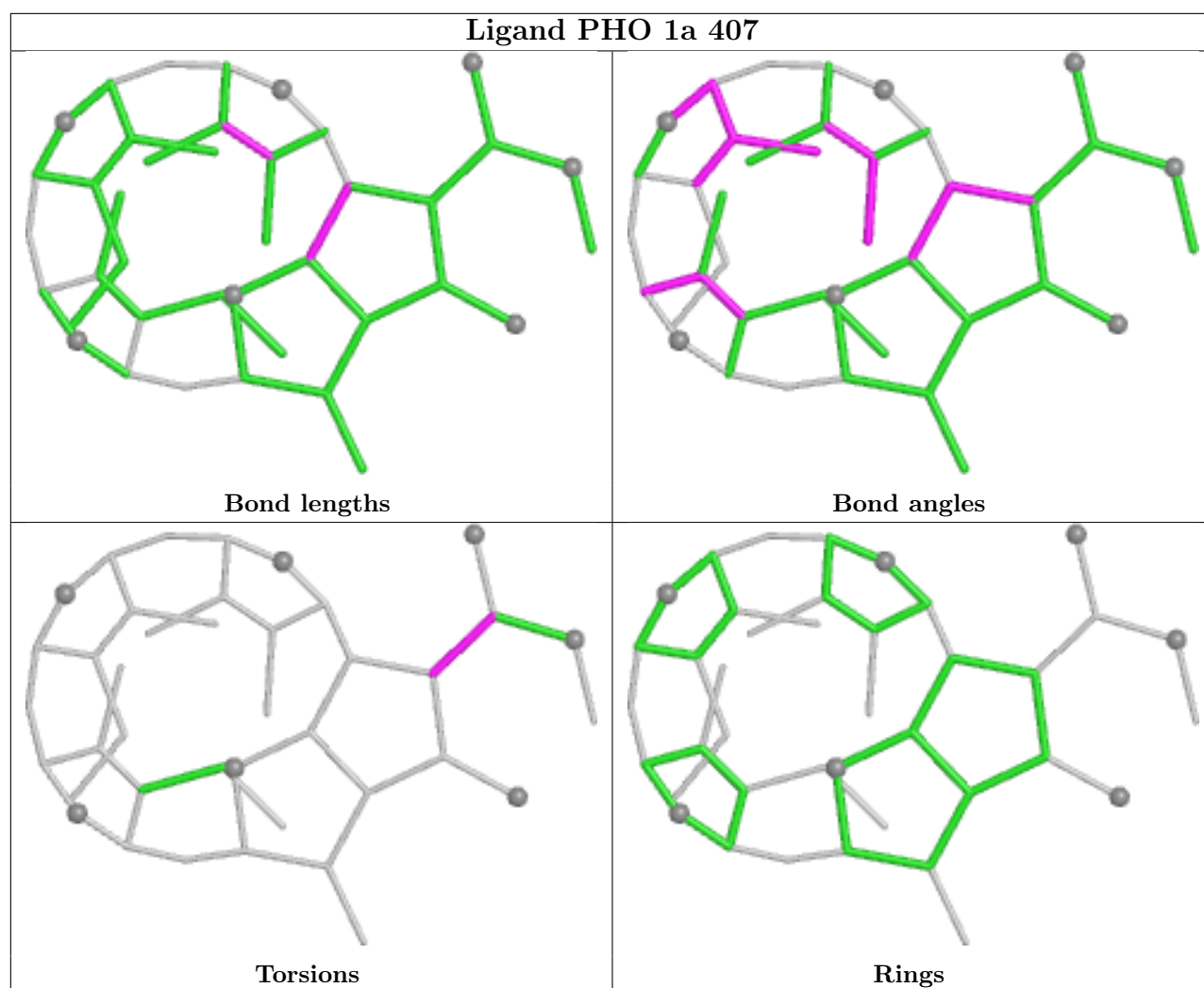
Ligand CLA 1G 613

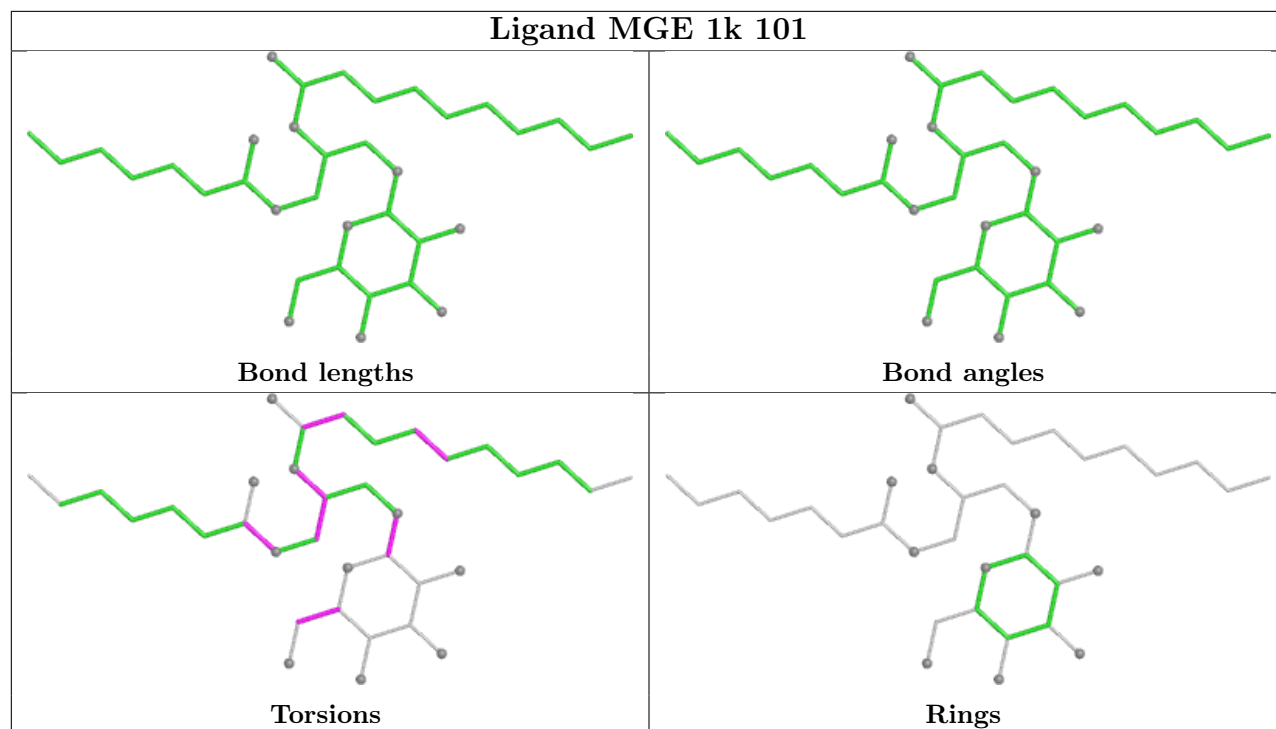


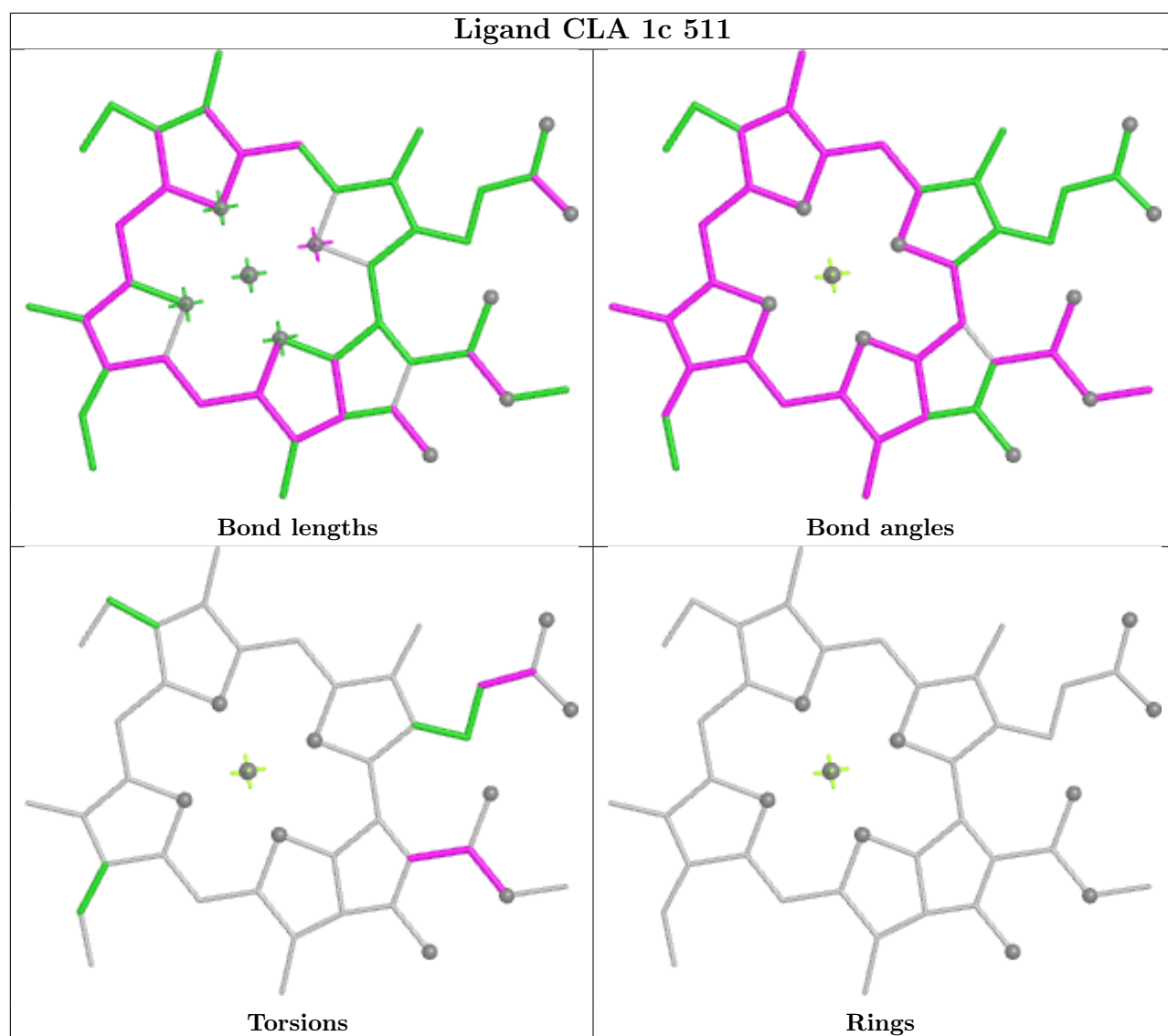




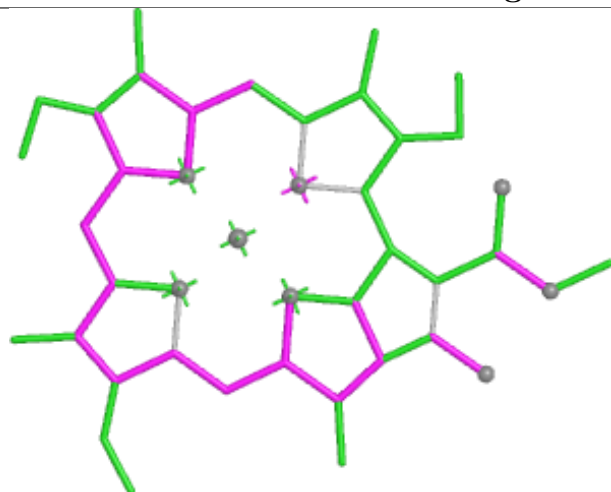




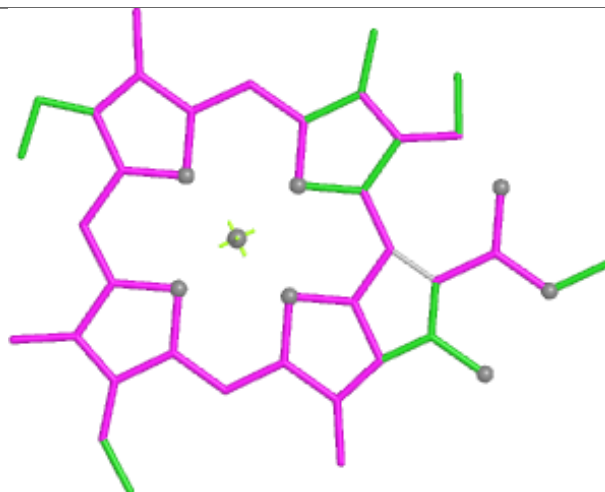




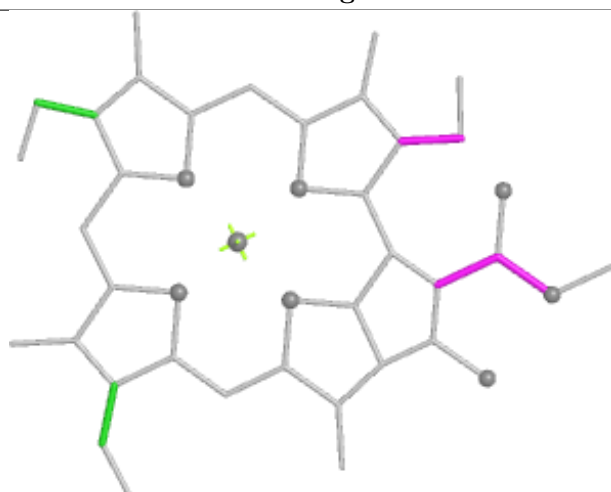
Ligand CLA 1D 405



Bond lengths



Bond angles

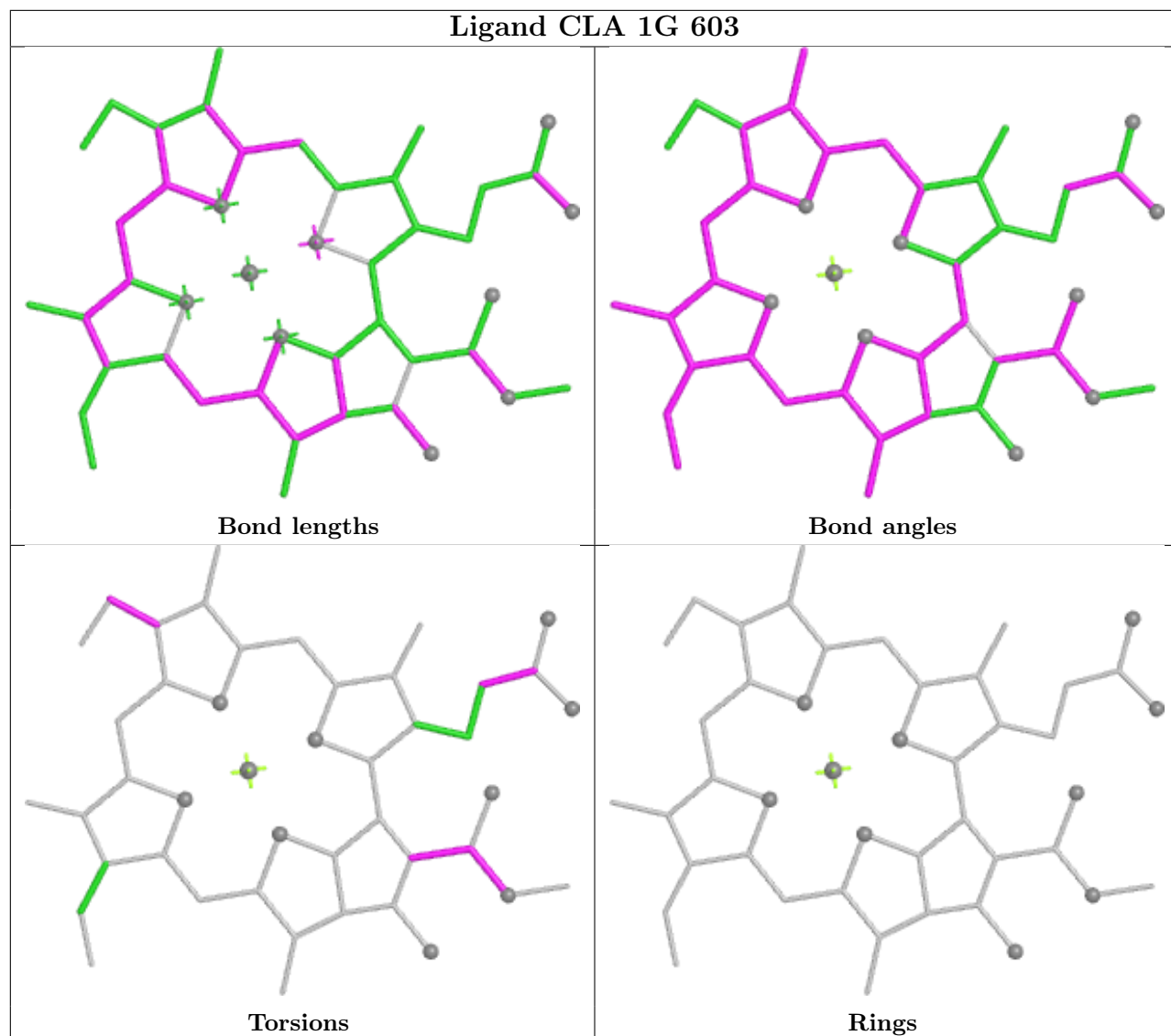


Torsions

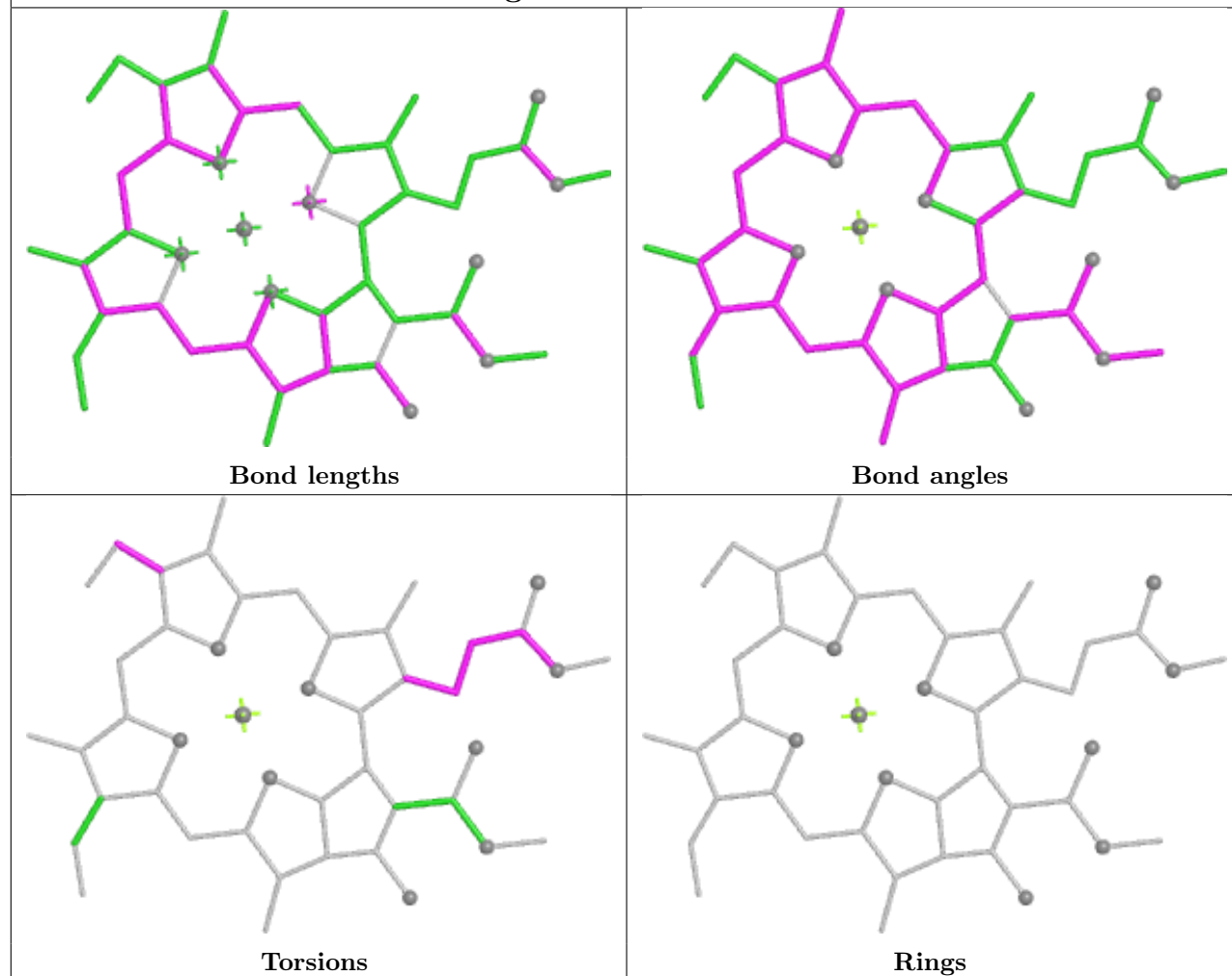


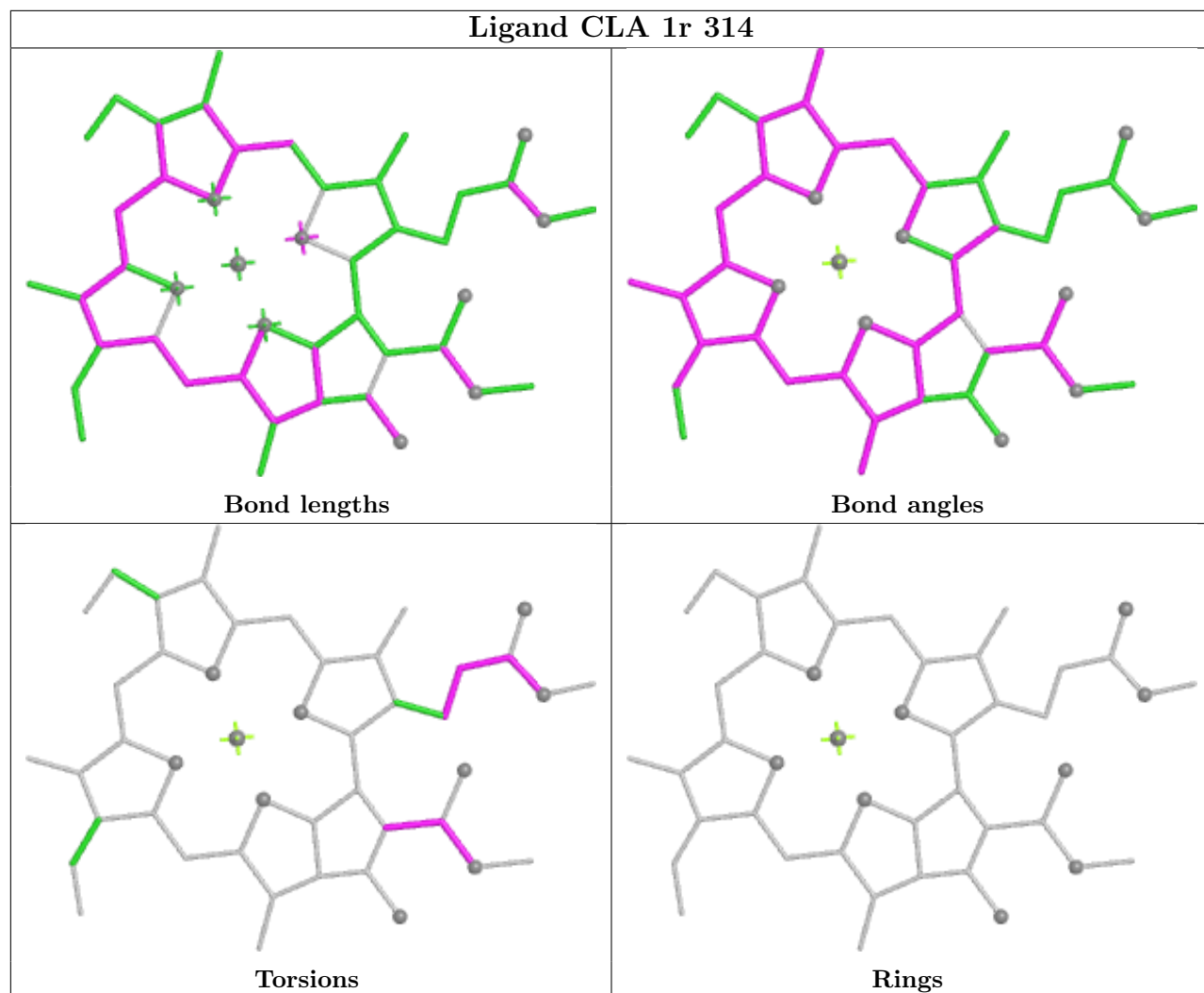
Rings

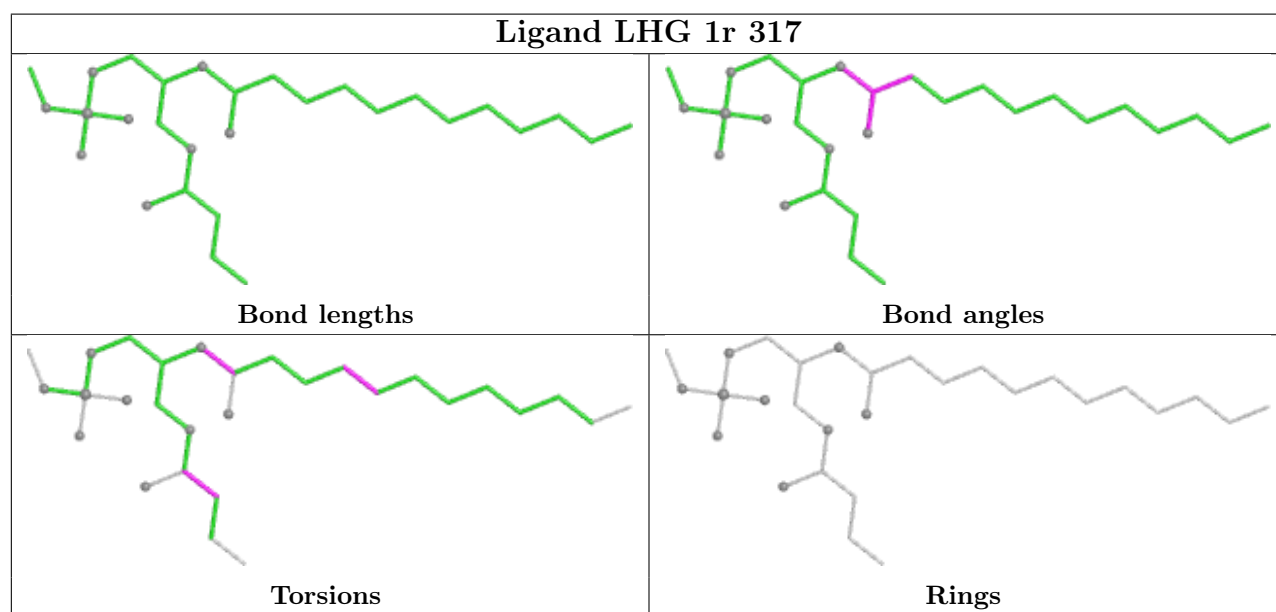
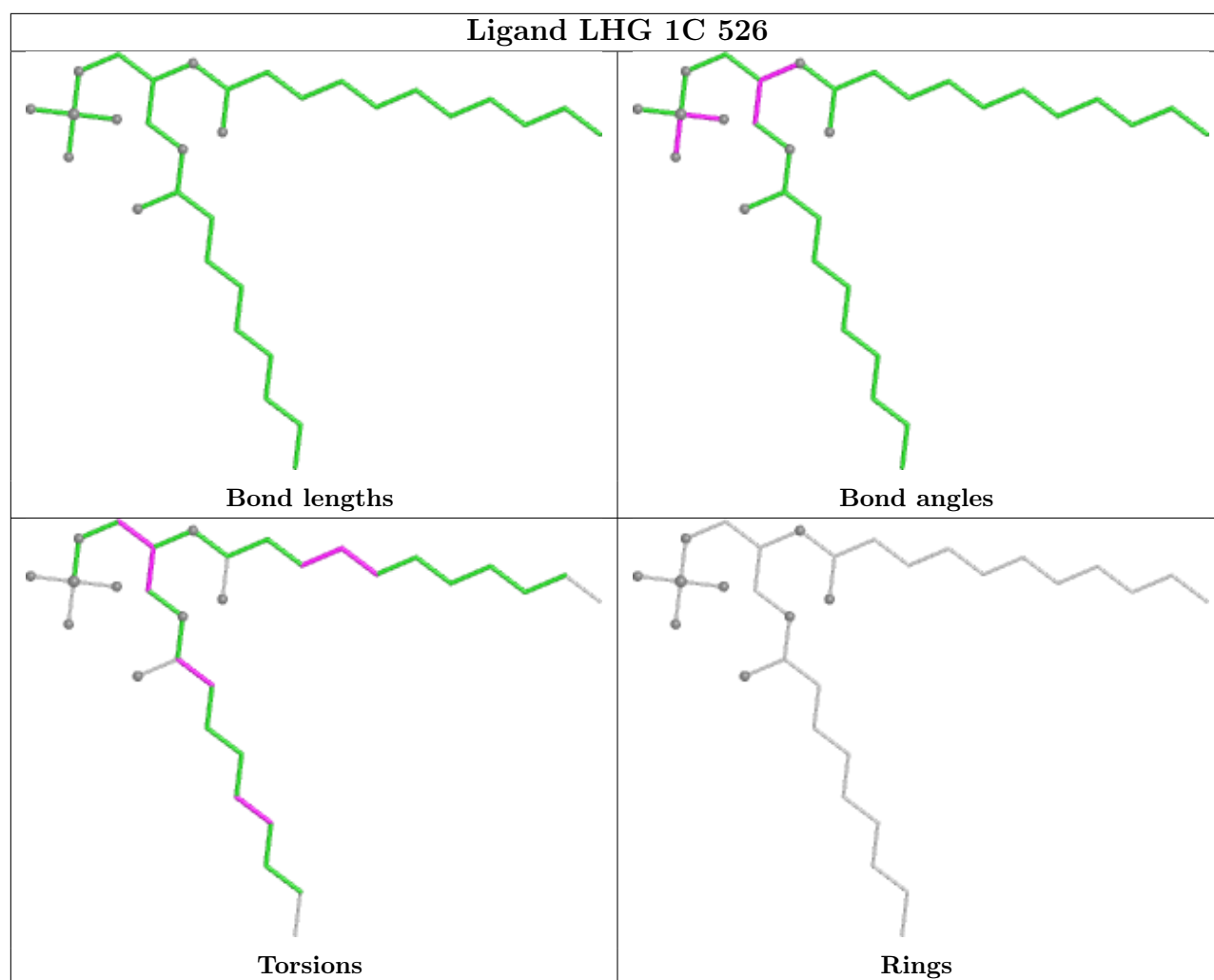
Ligand CLA 1G 603

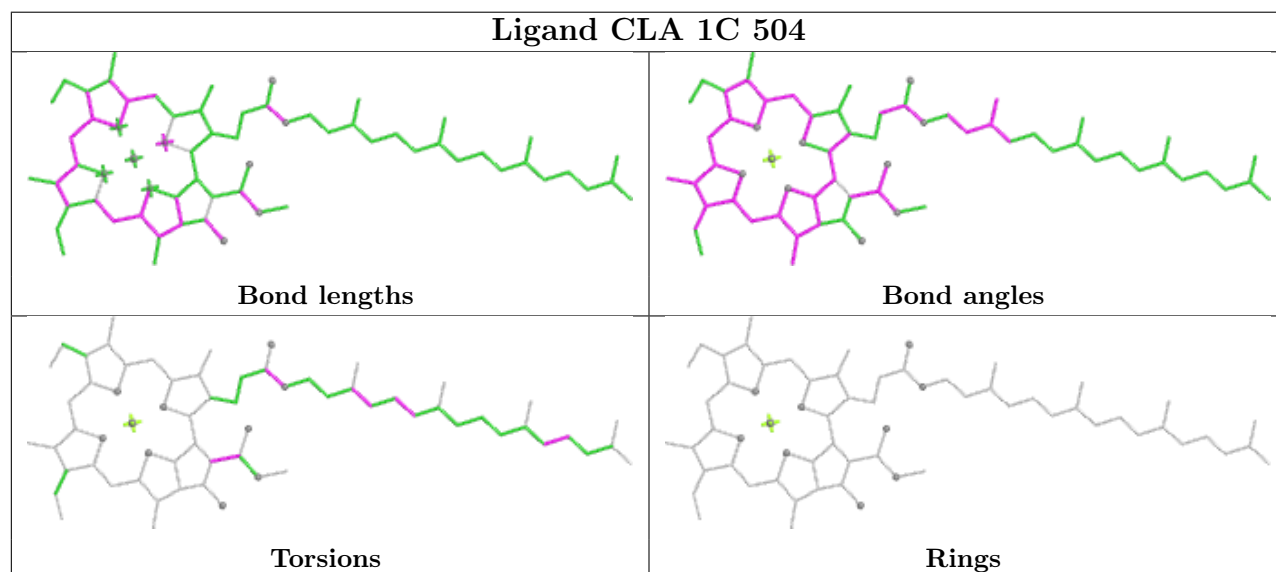
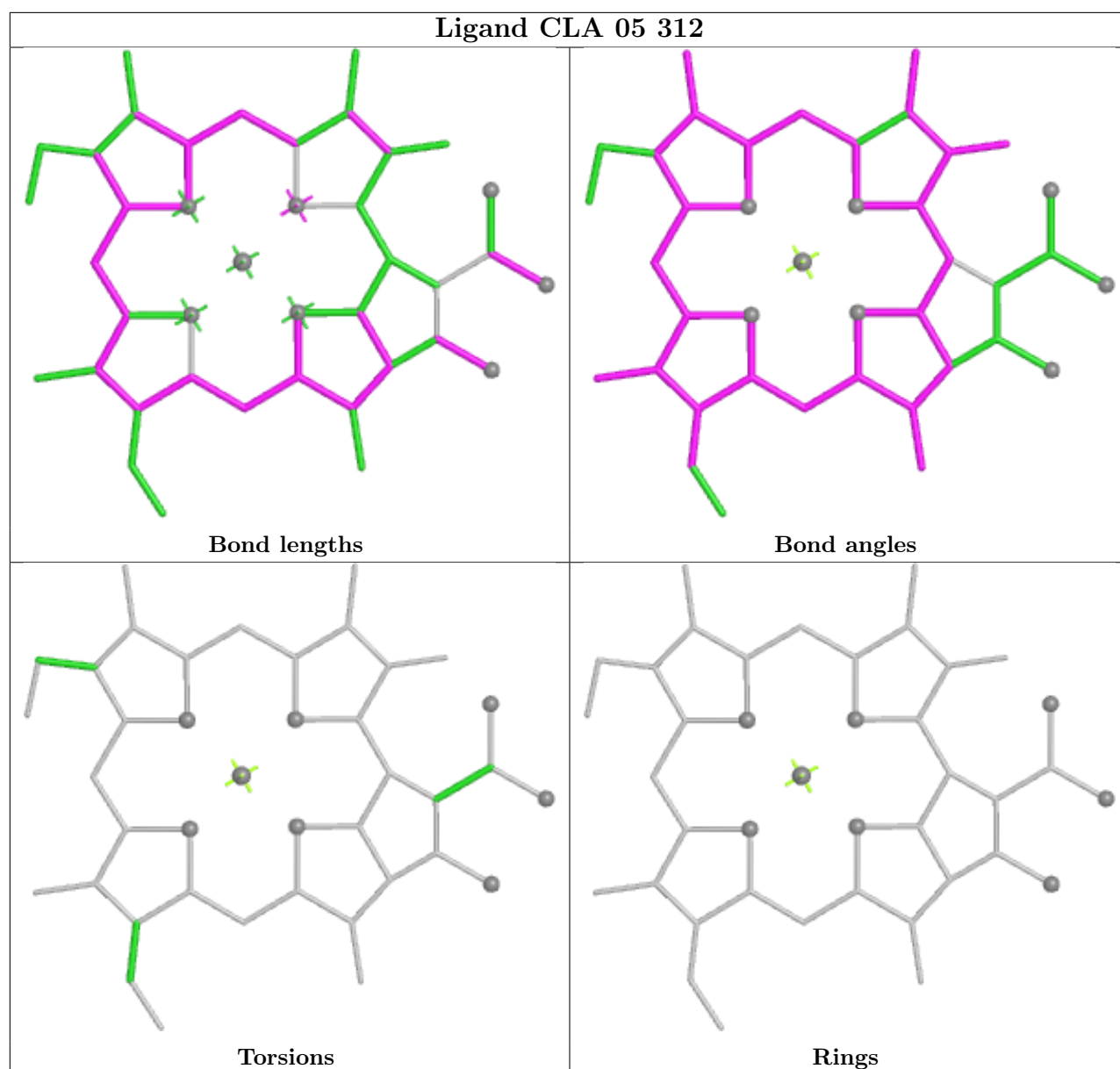


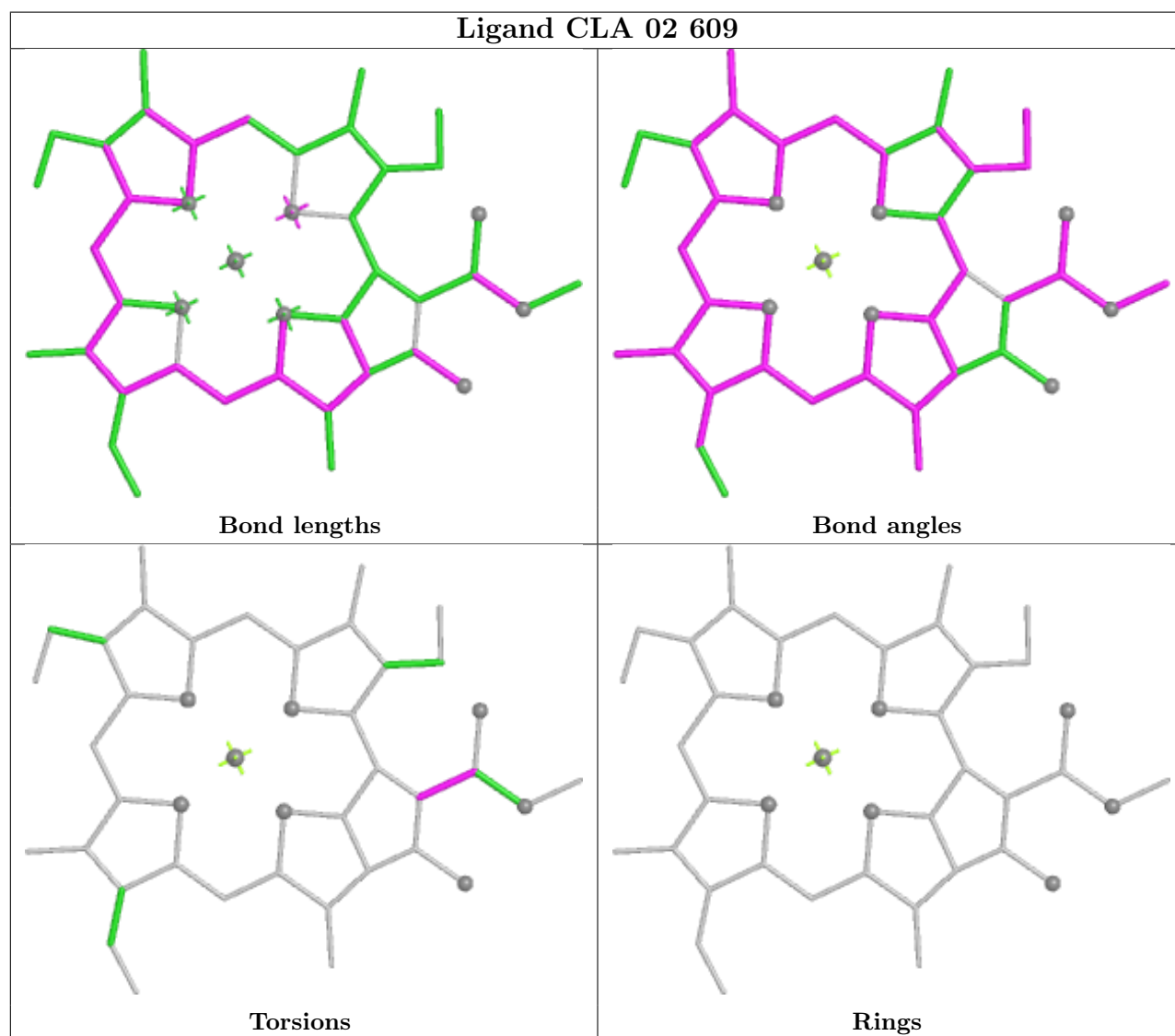
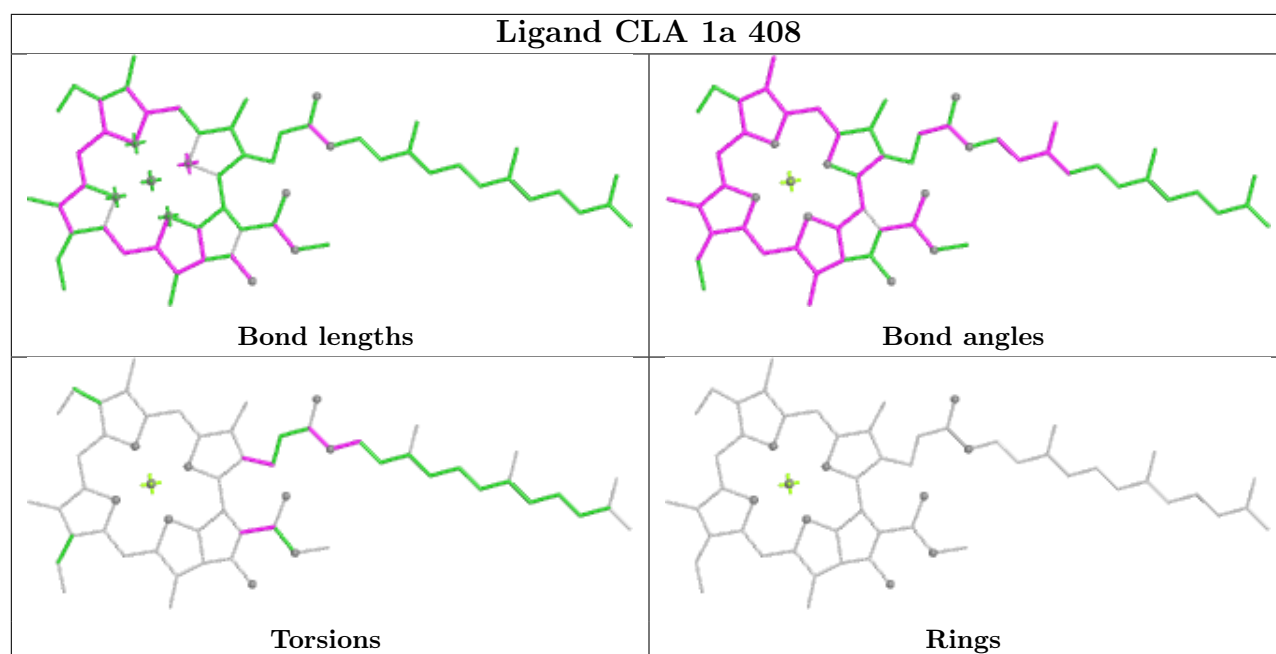
Ligand CLA 1R 312

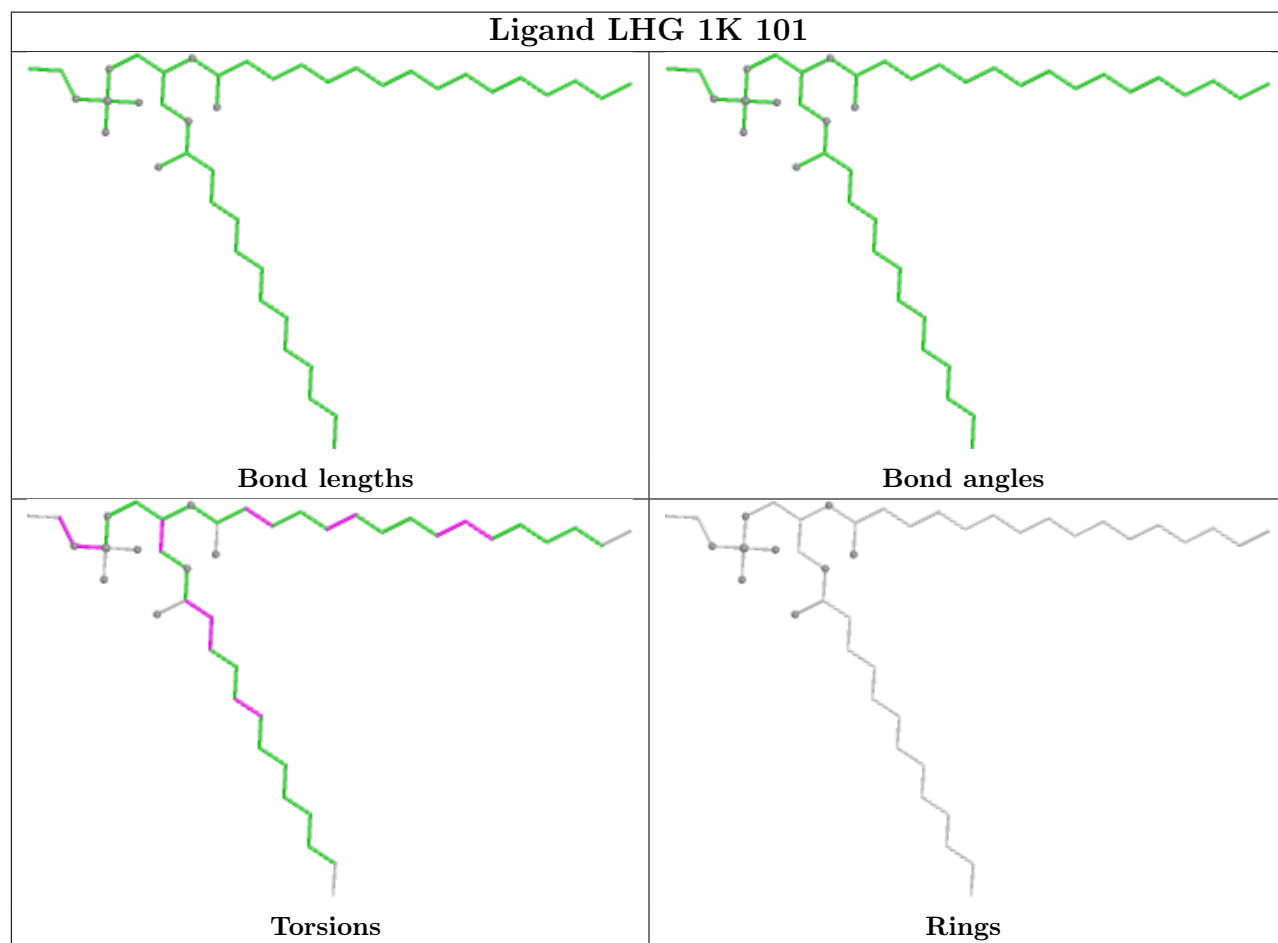
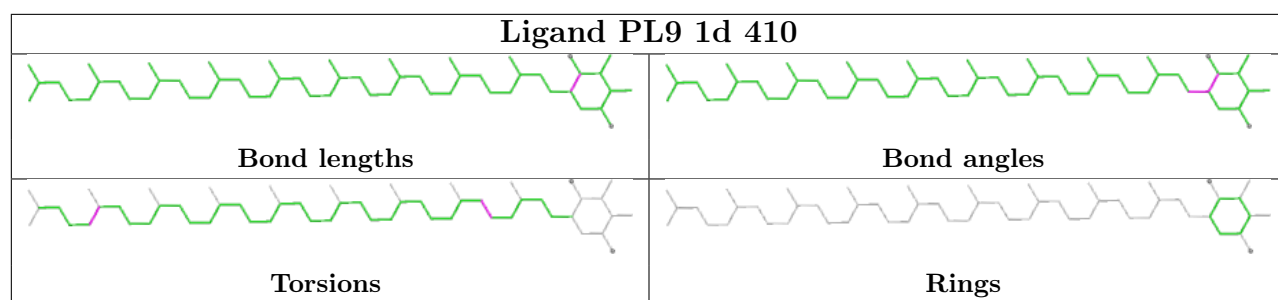


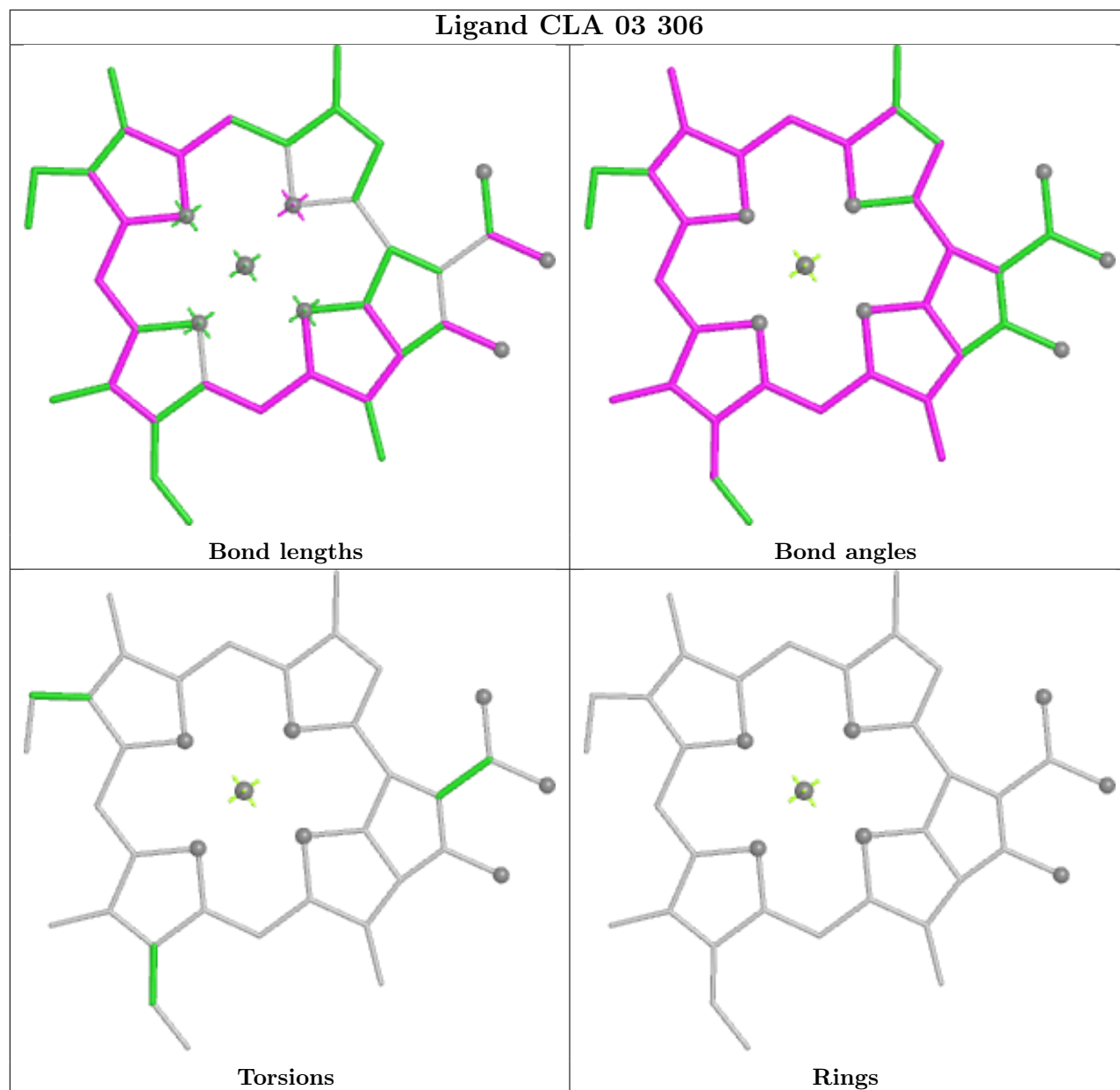


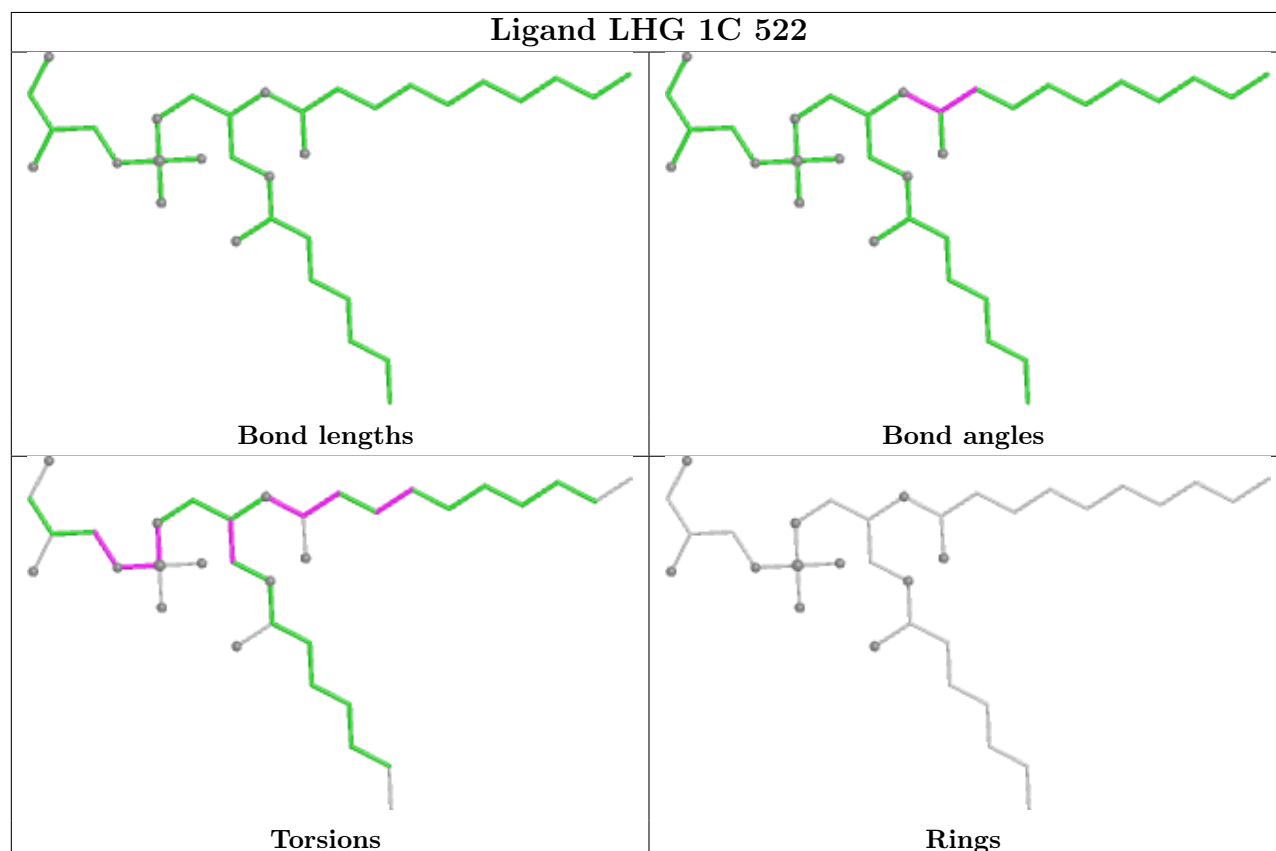
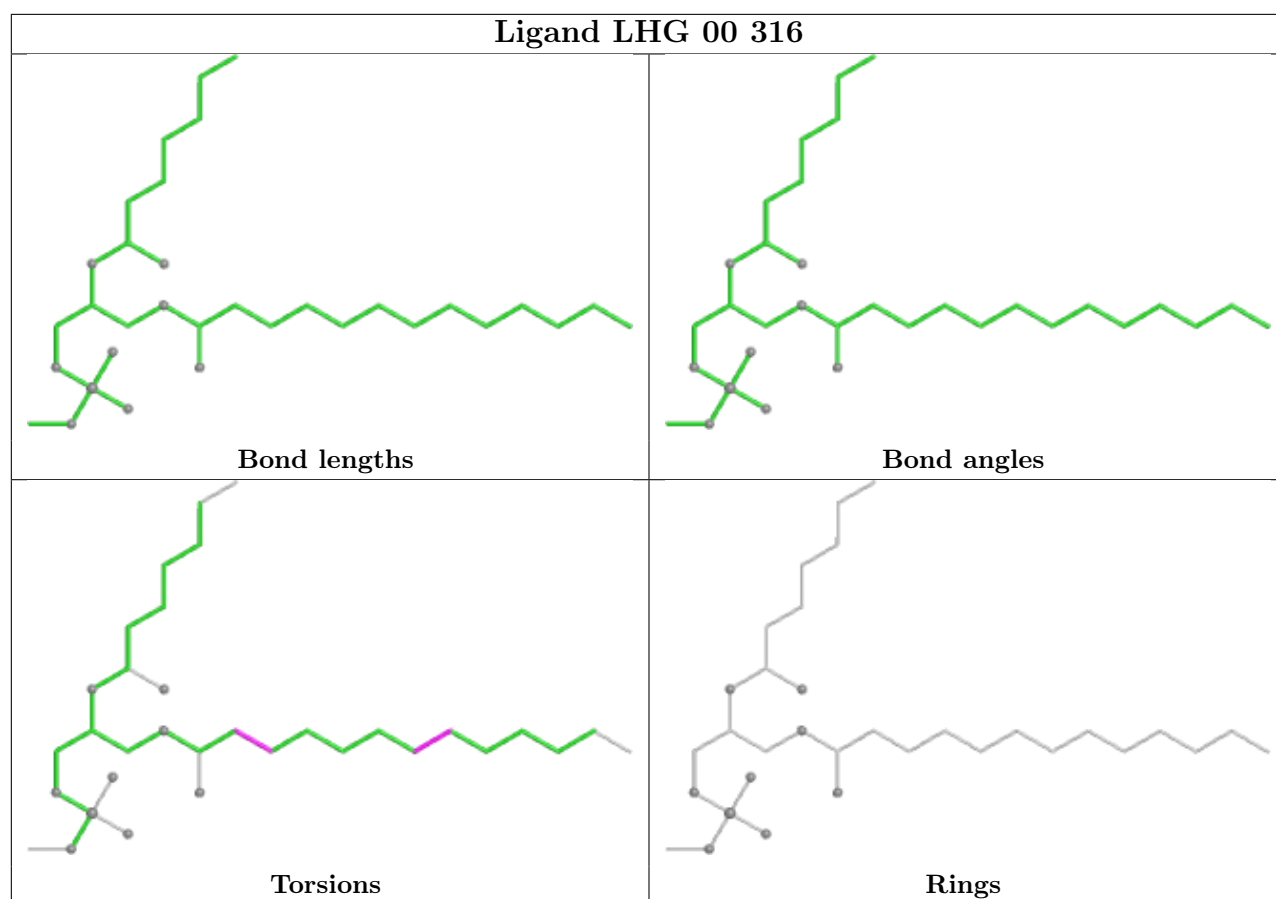


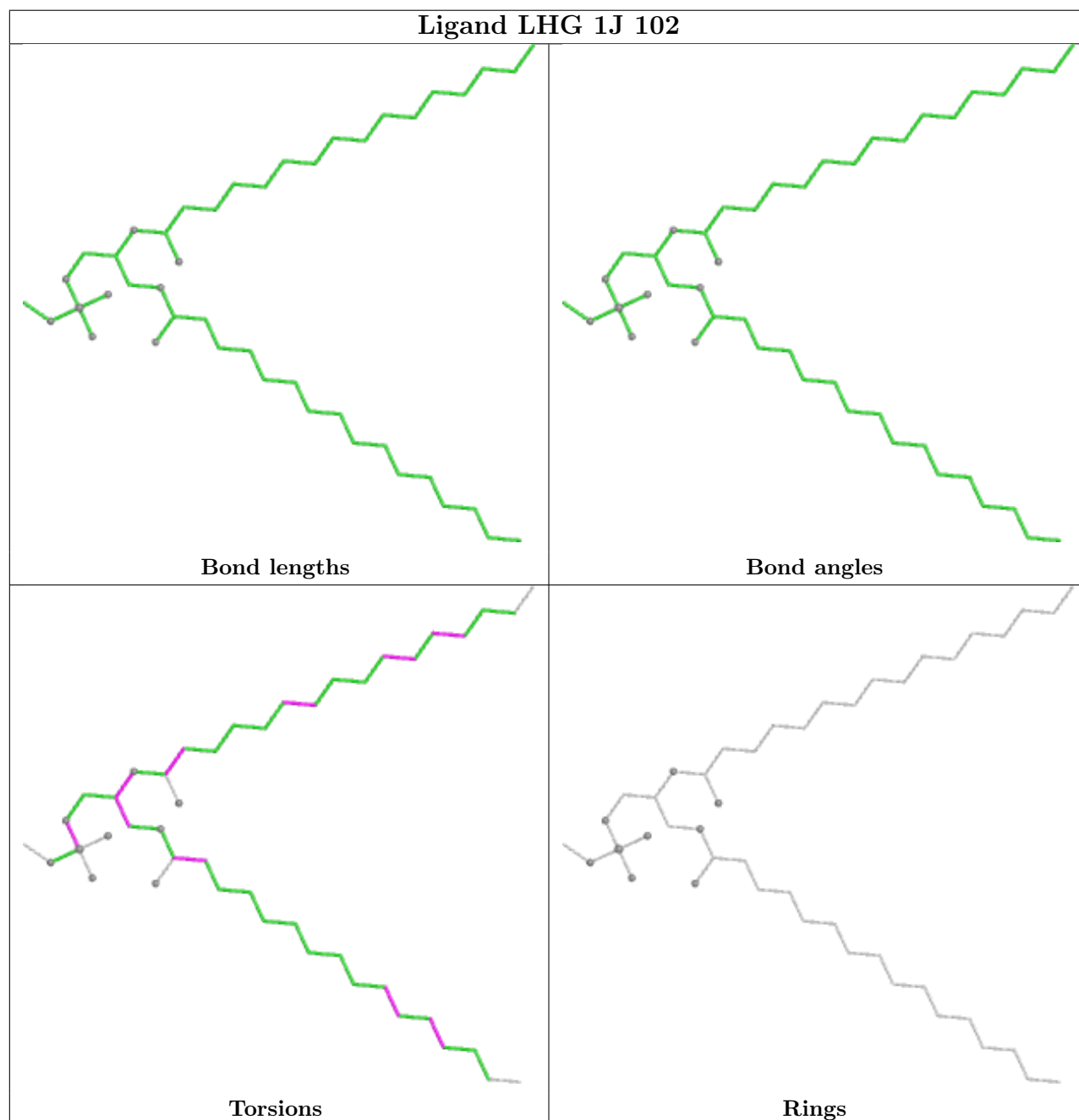
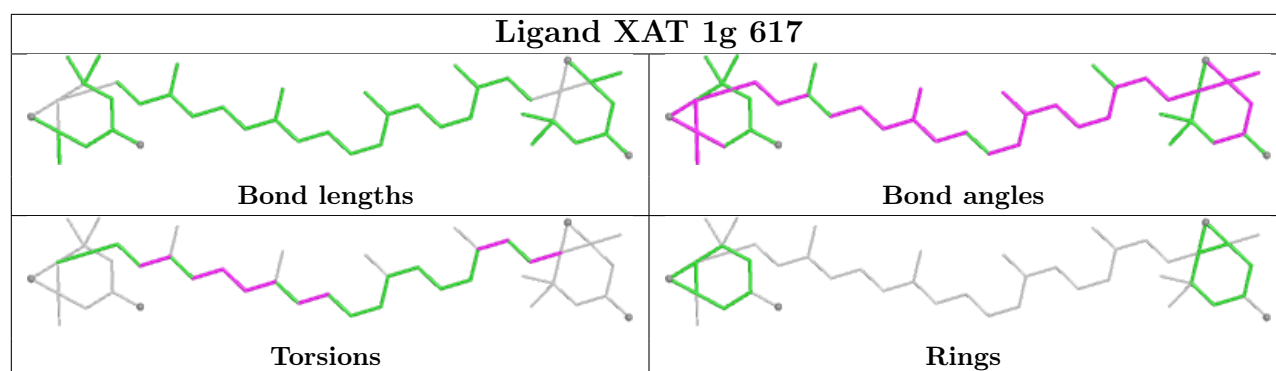


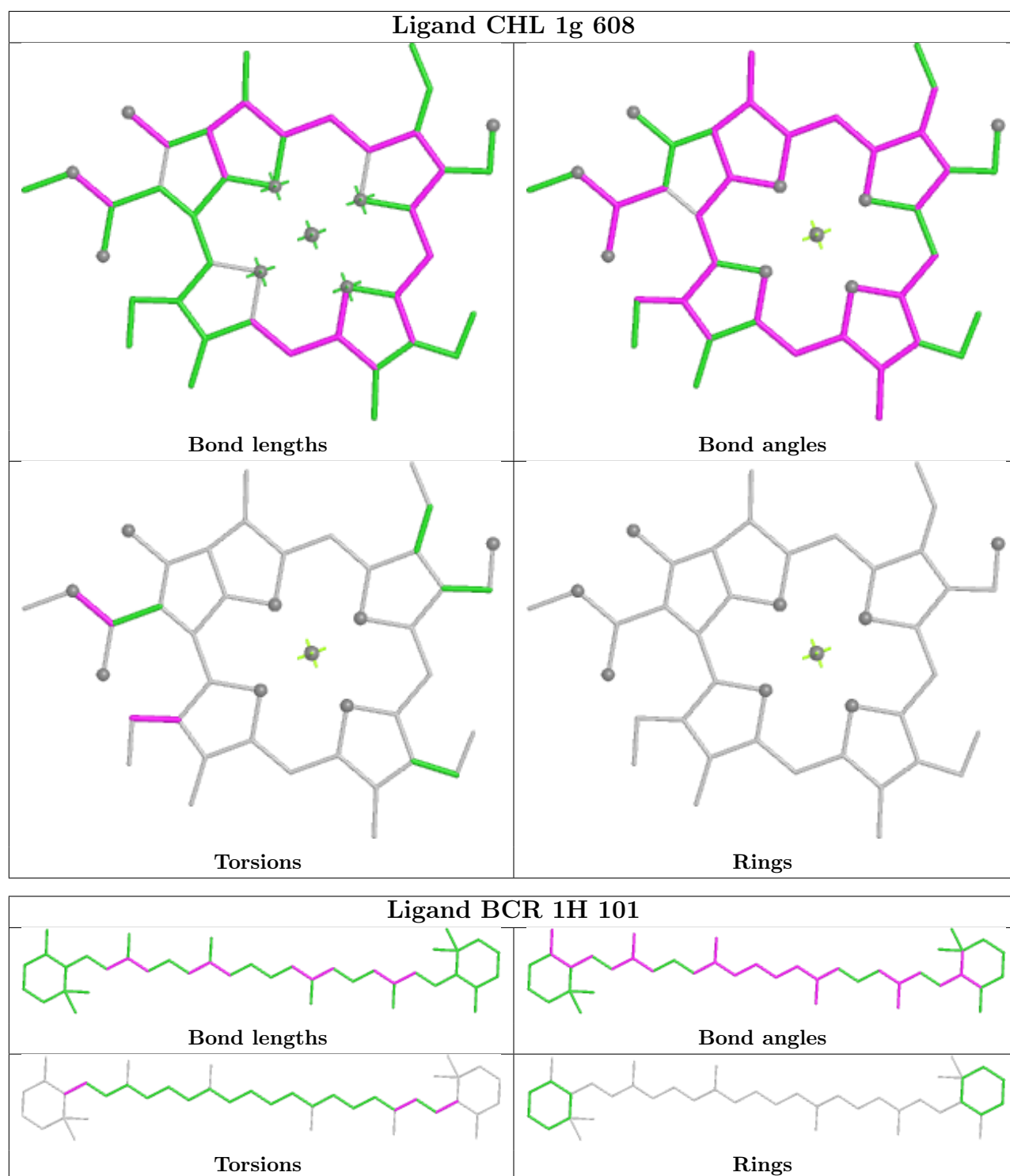


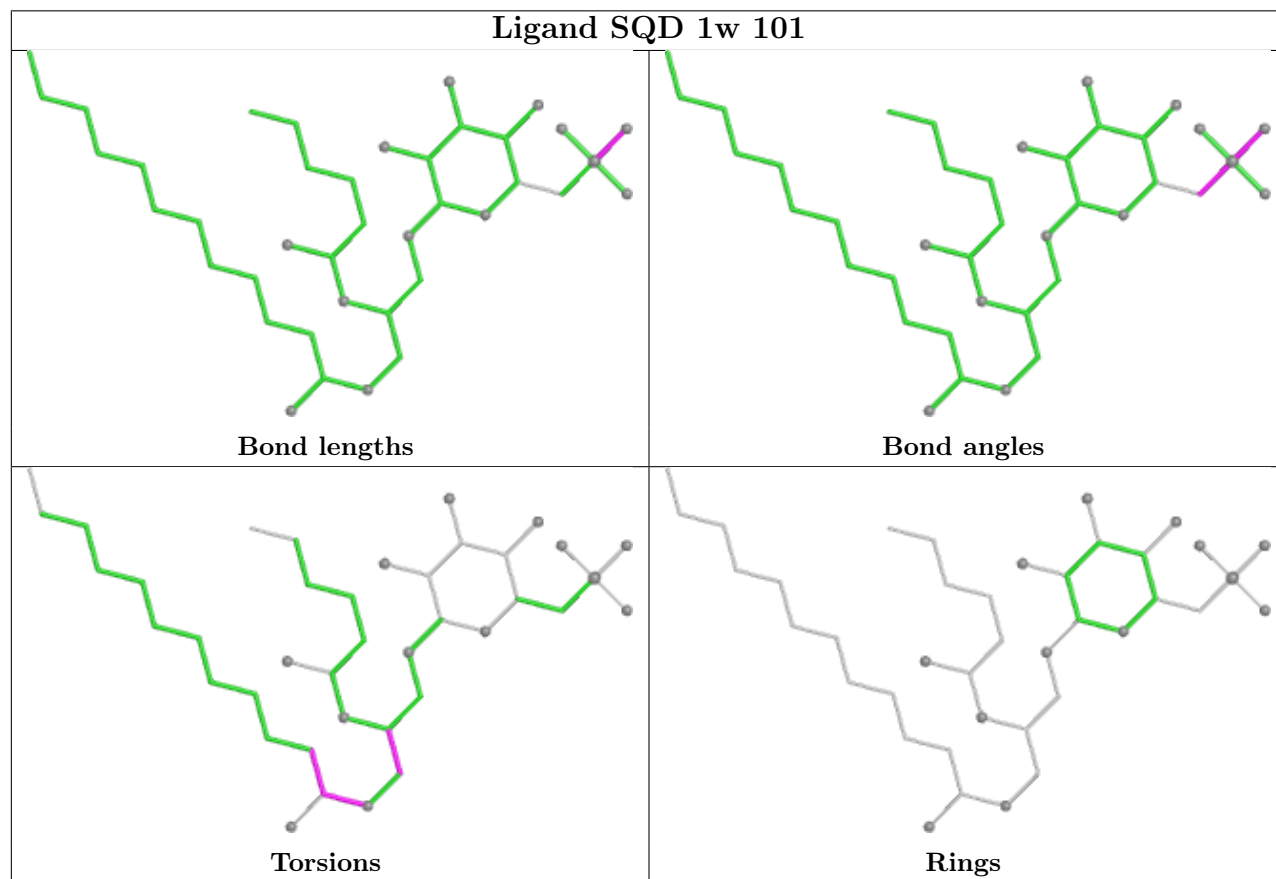
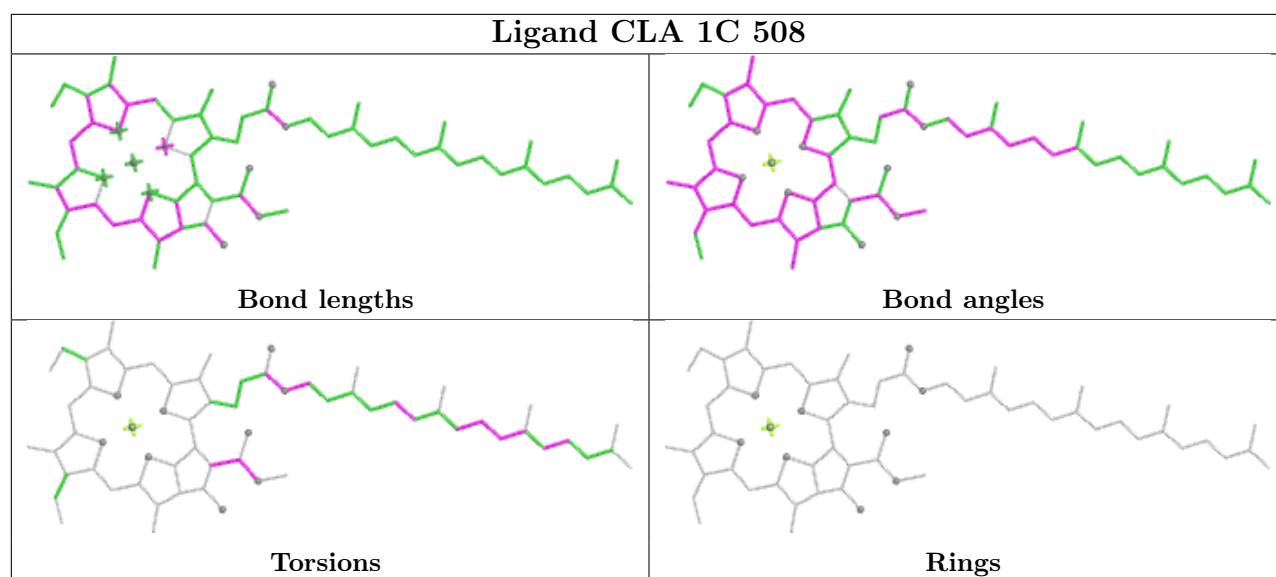


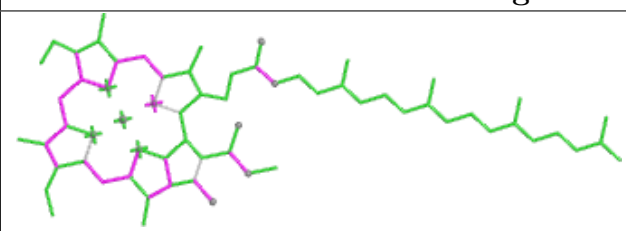
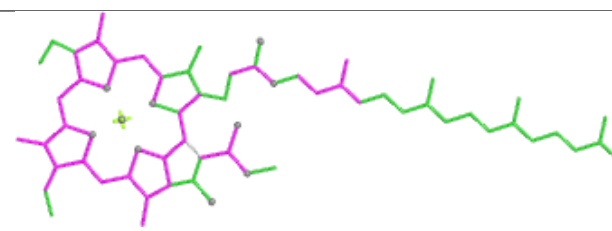
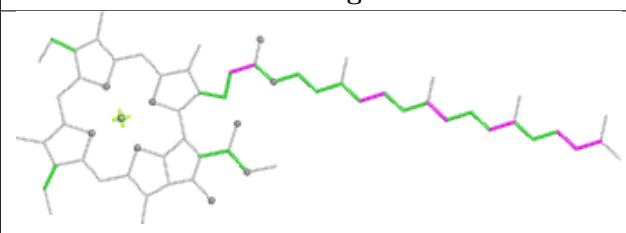
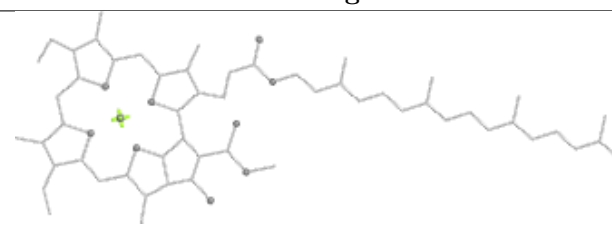


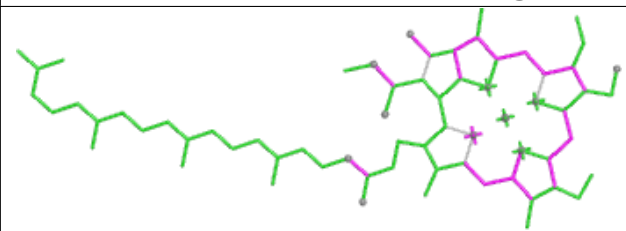
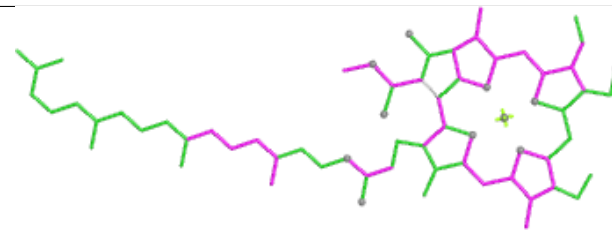
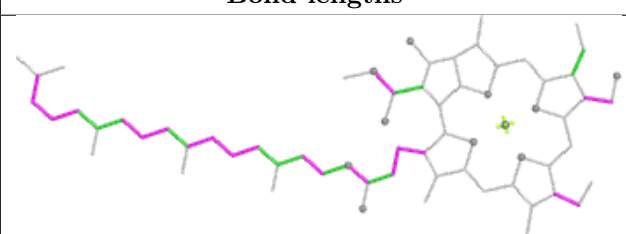
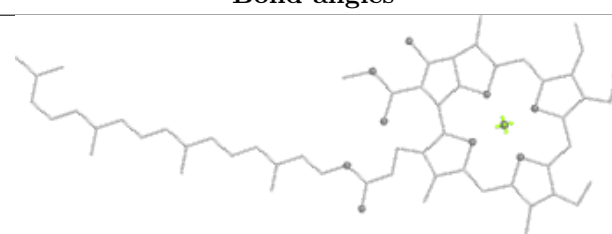


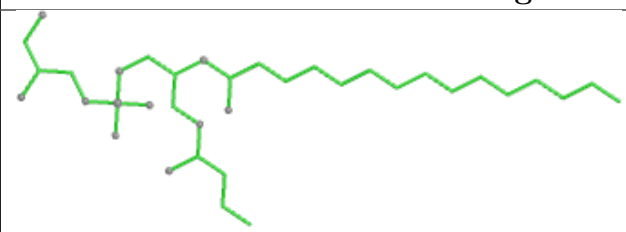
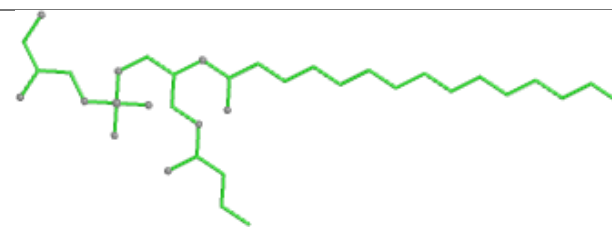
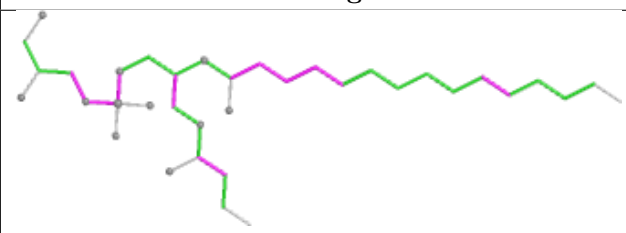
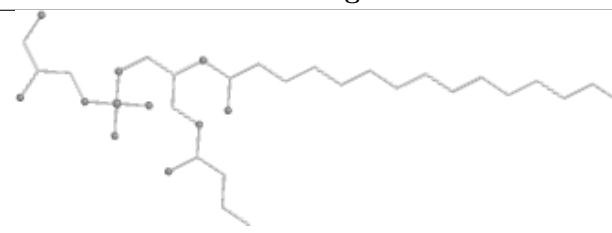


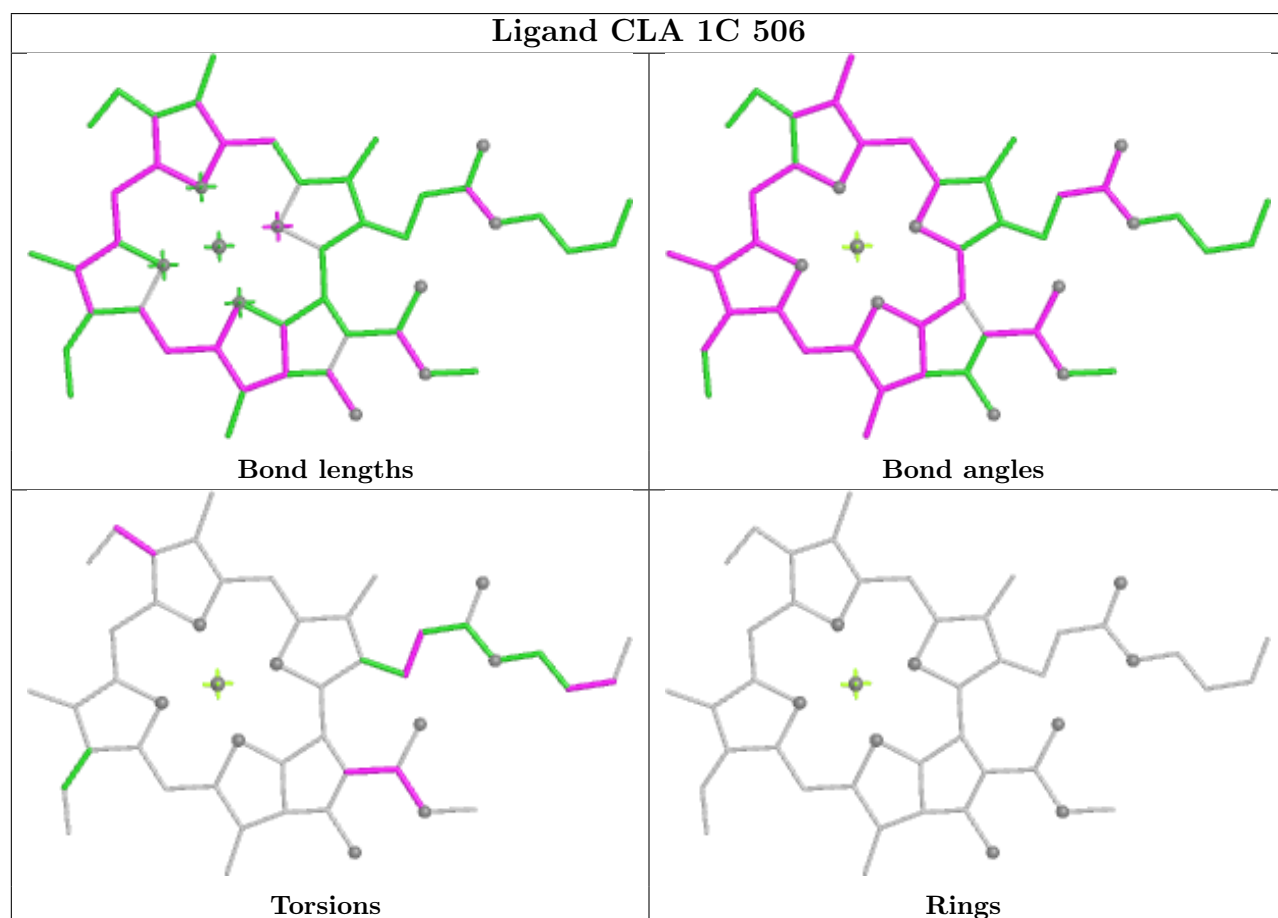
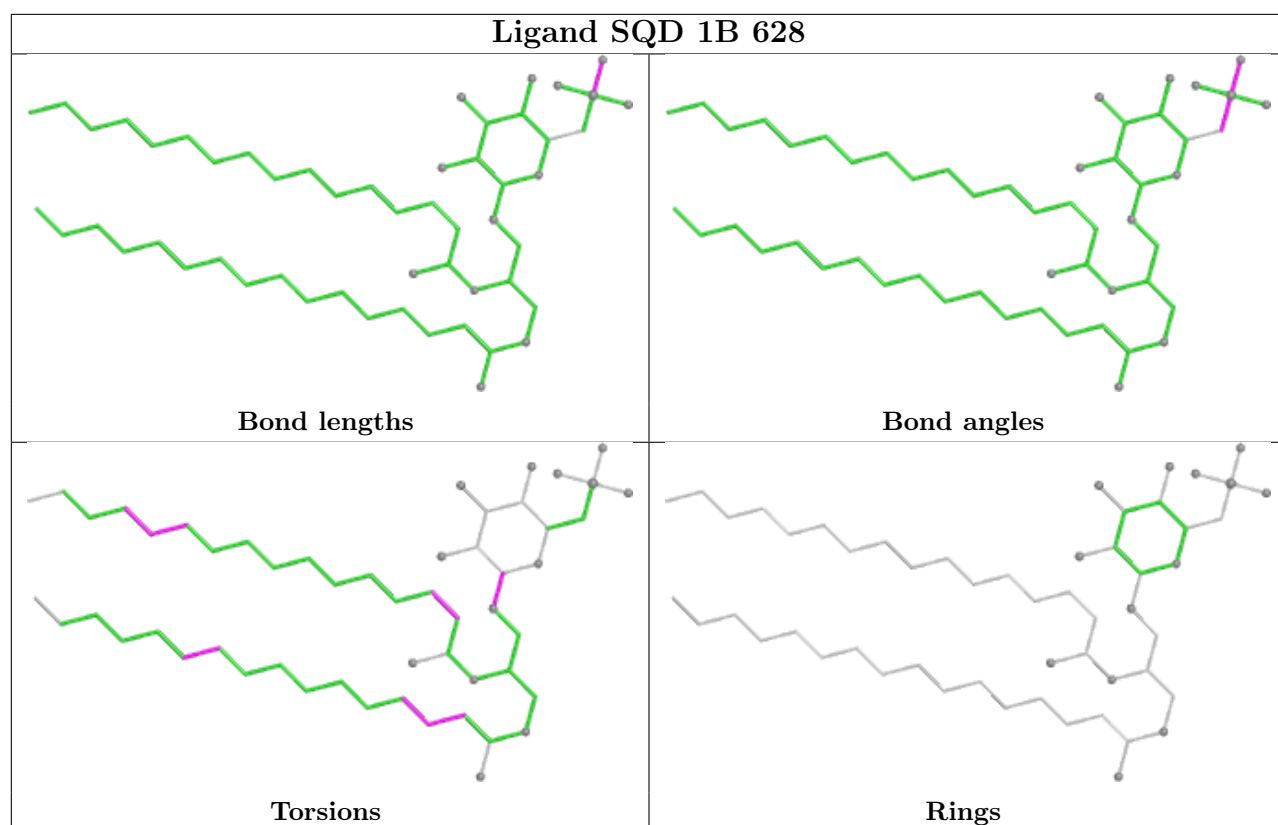


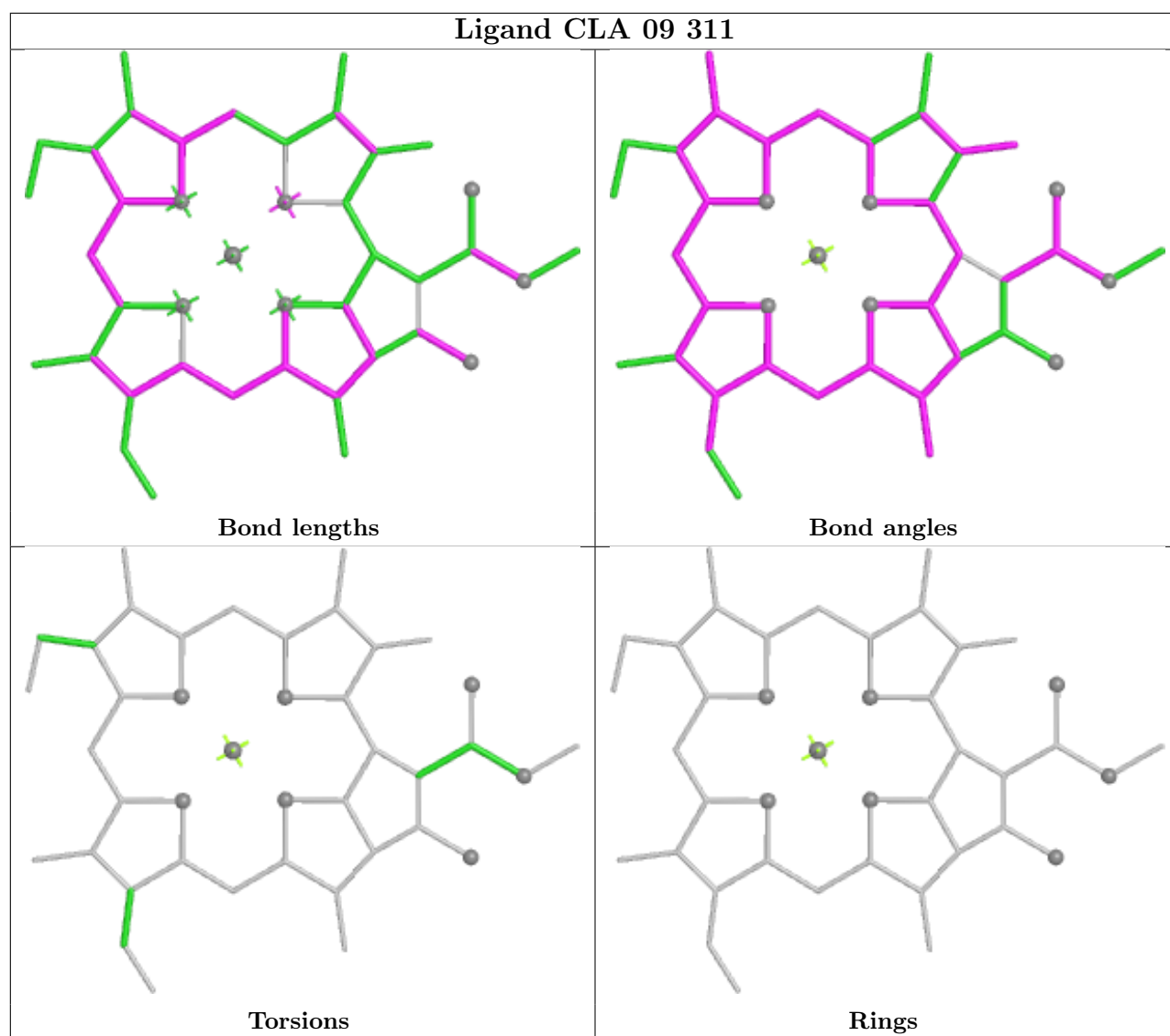


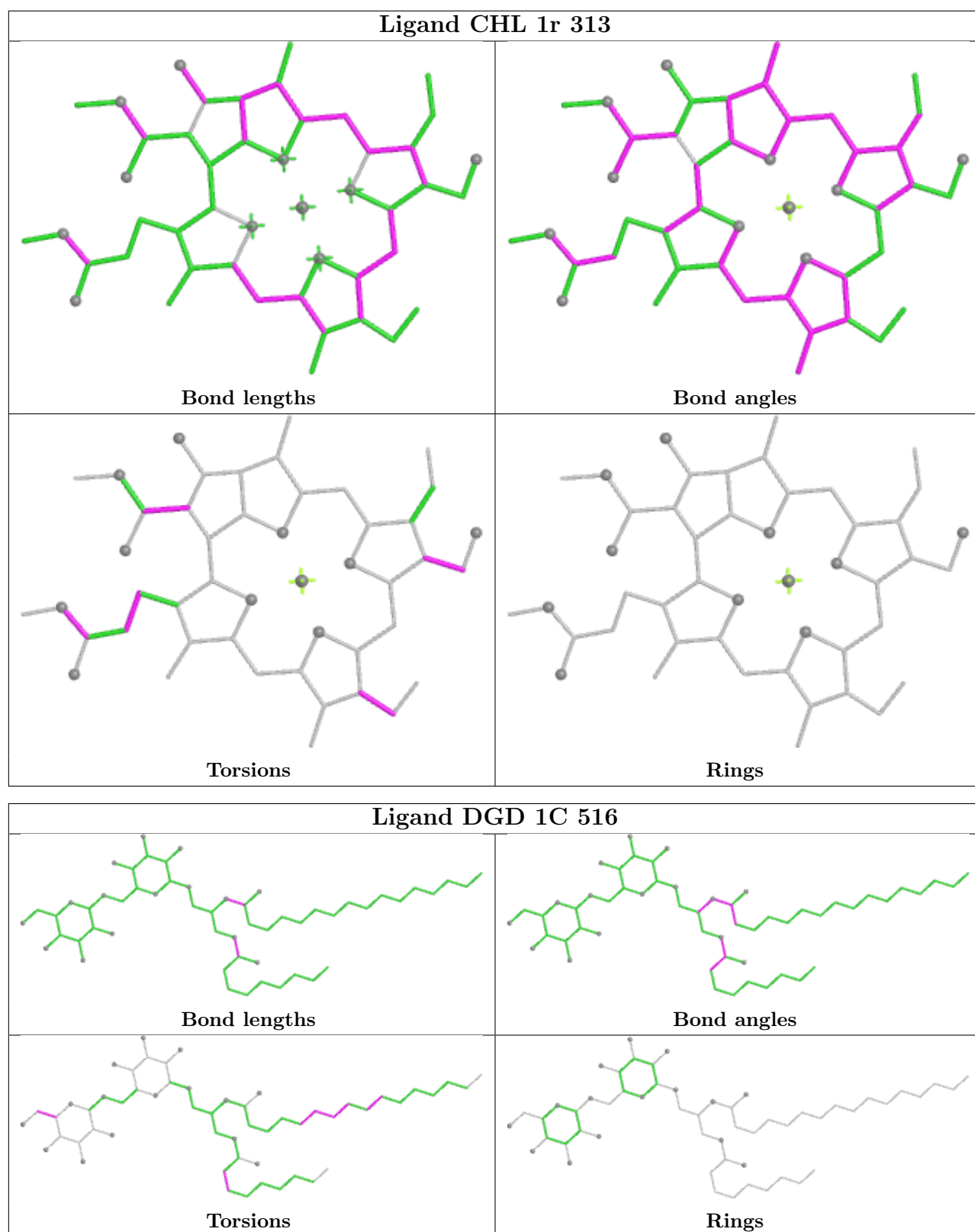
Ligand CLA 1B 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

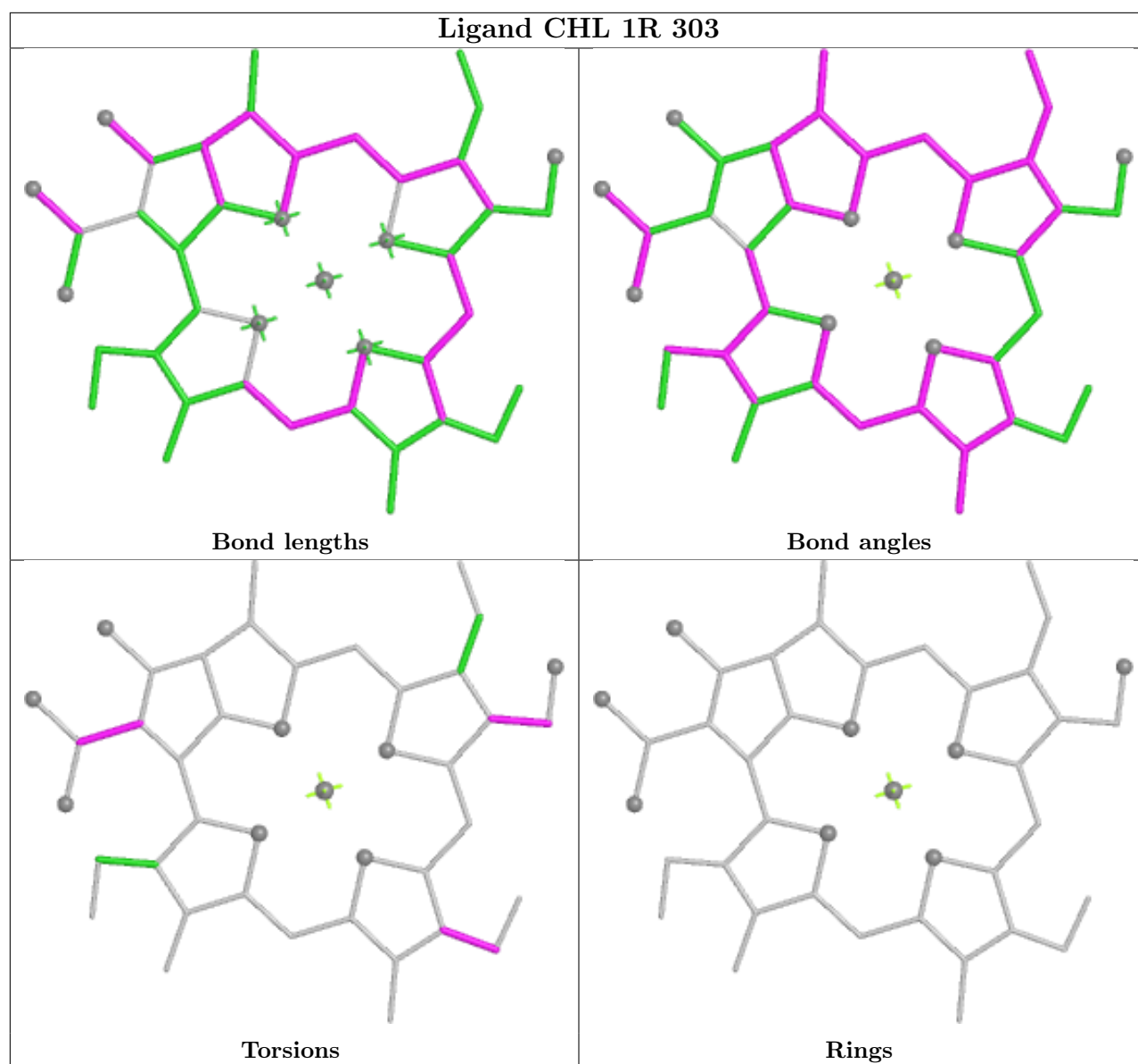
Ligand CHL 1N 308	
	
Bond lengths	Bond angles
	
Torsions	Rings

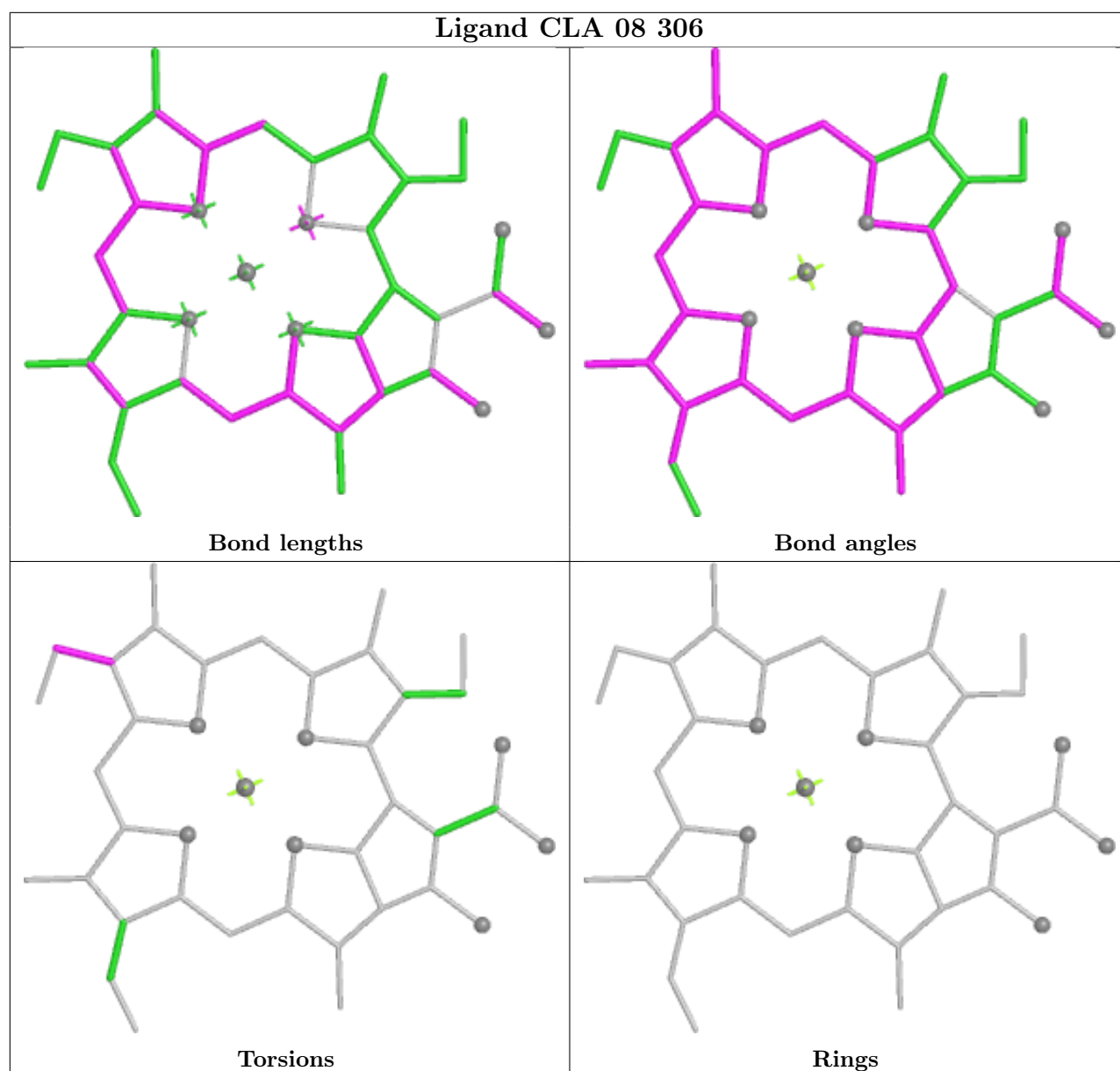
Ligand LHG 01 316	
	
Bond lengths	Bond angles
	
Torsions	Rings

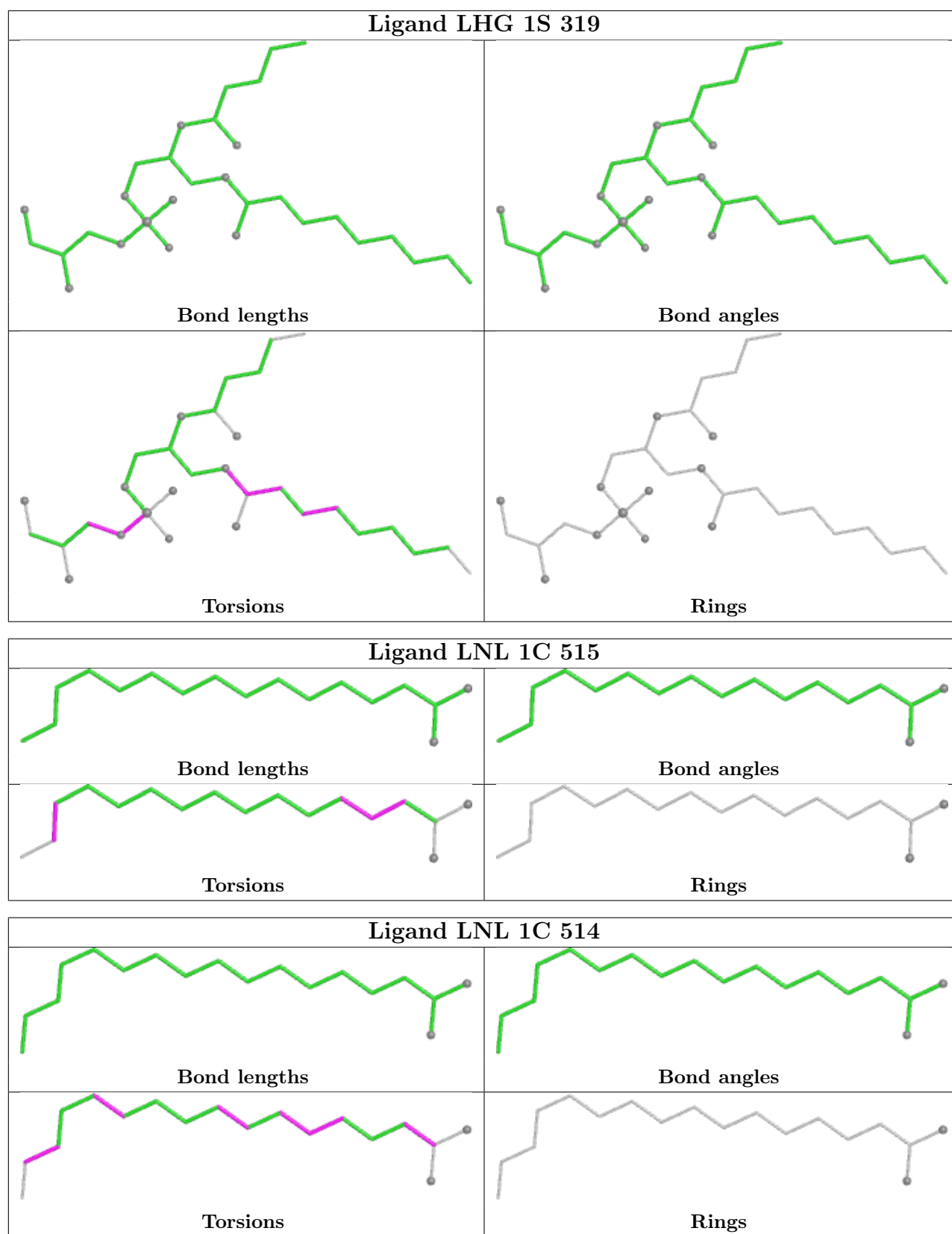


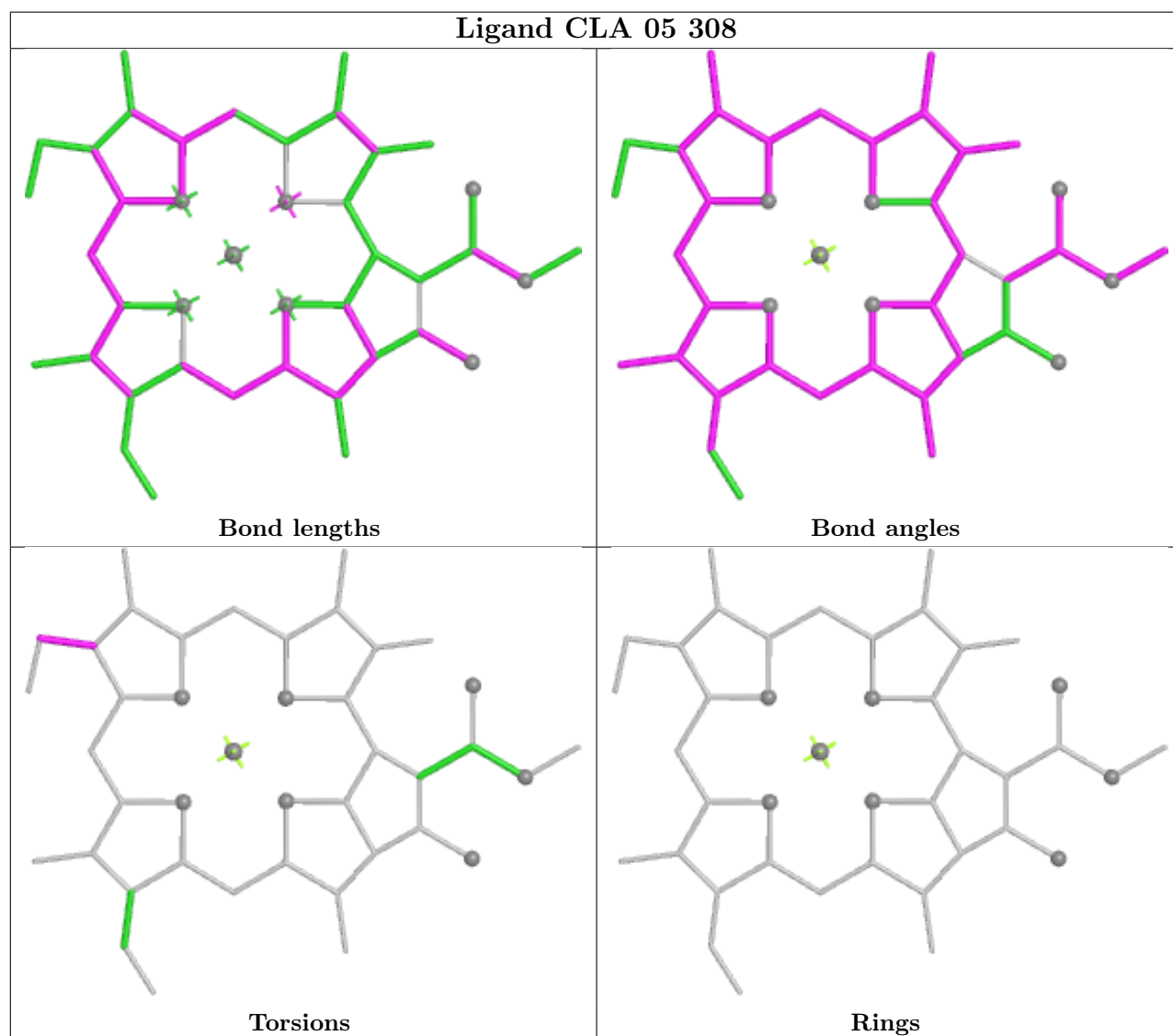
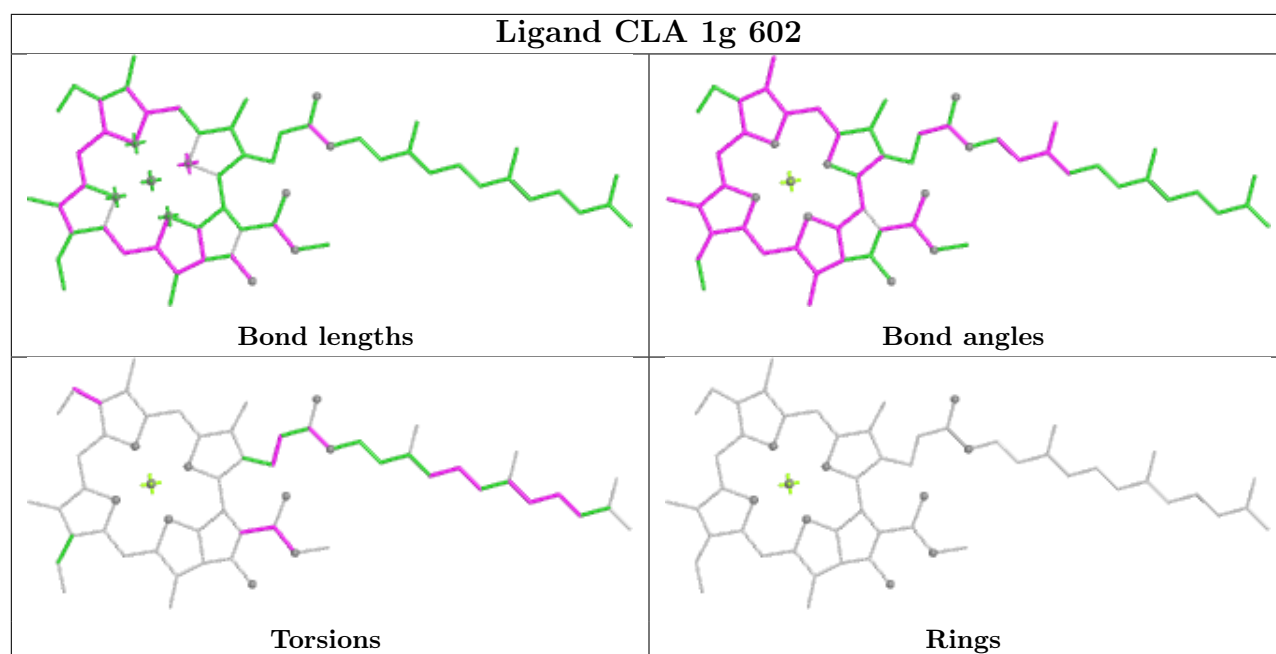


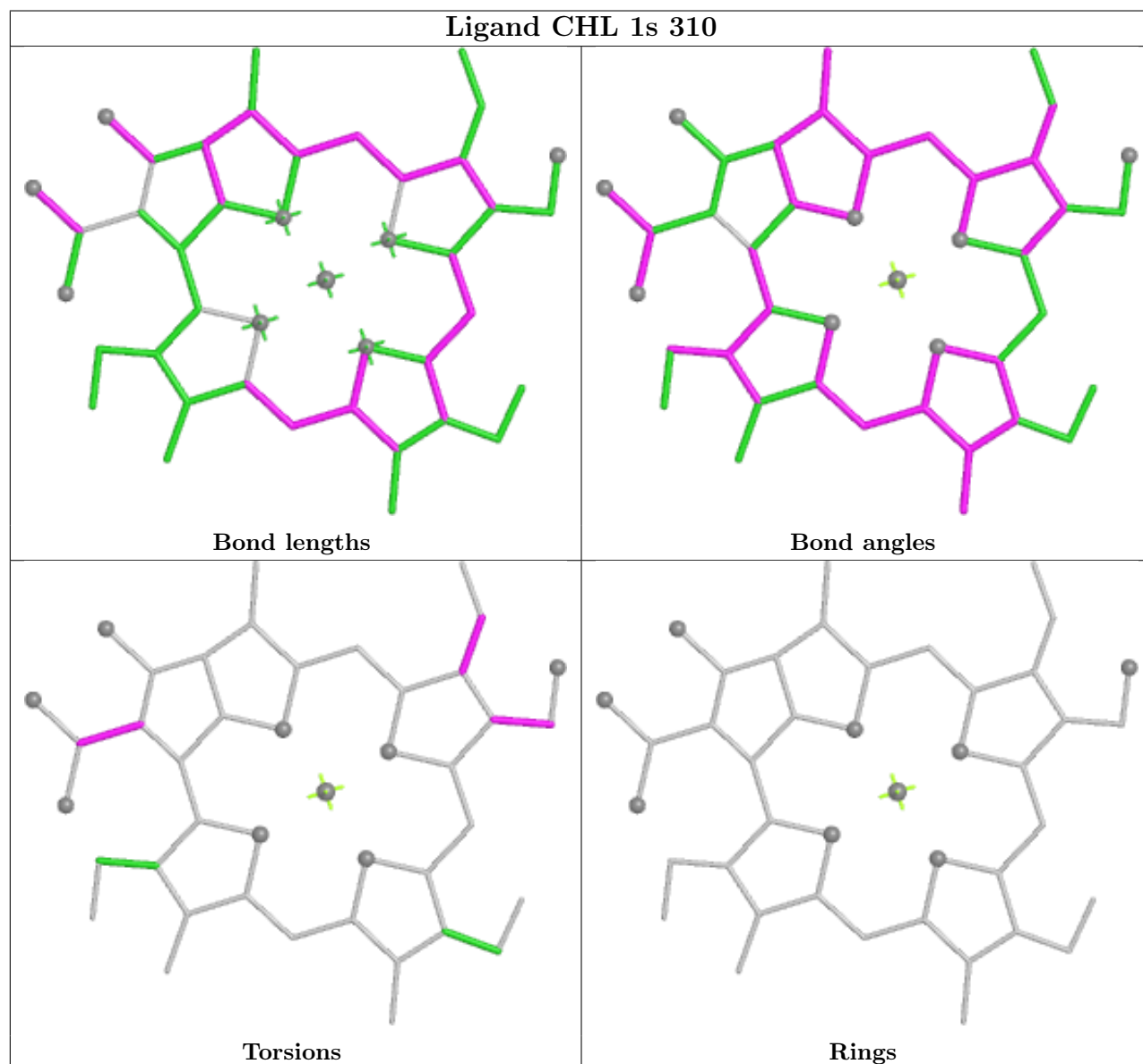
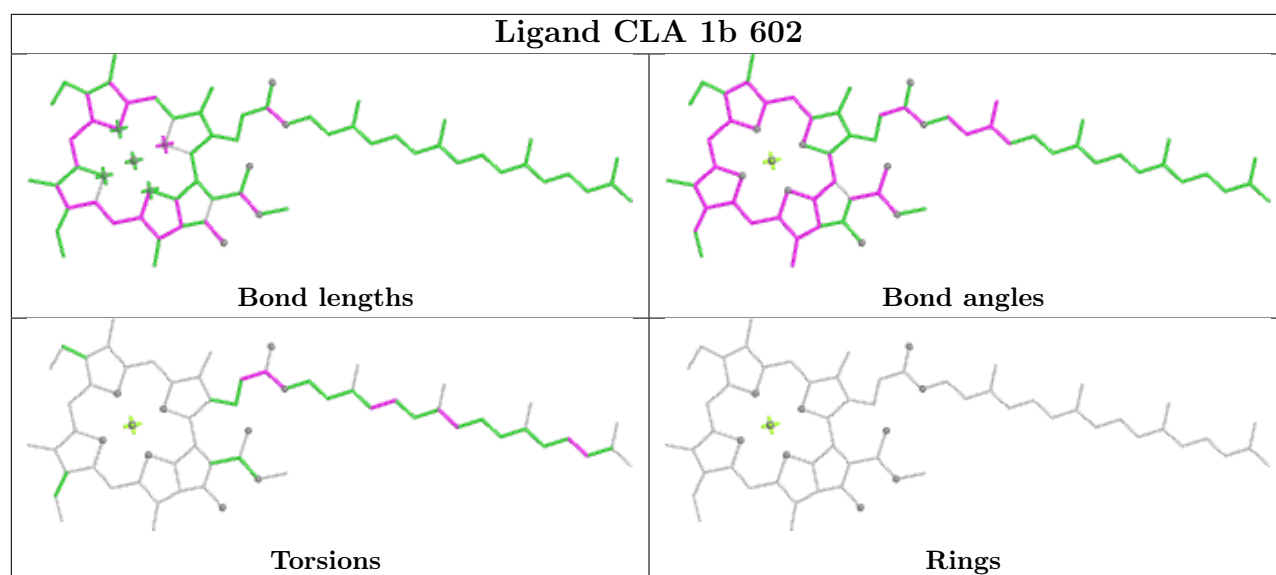


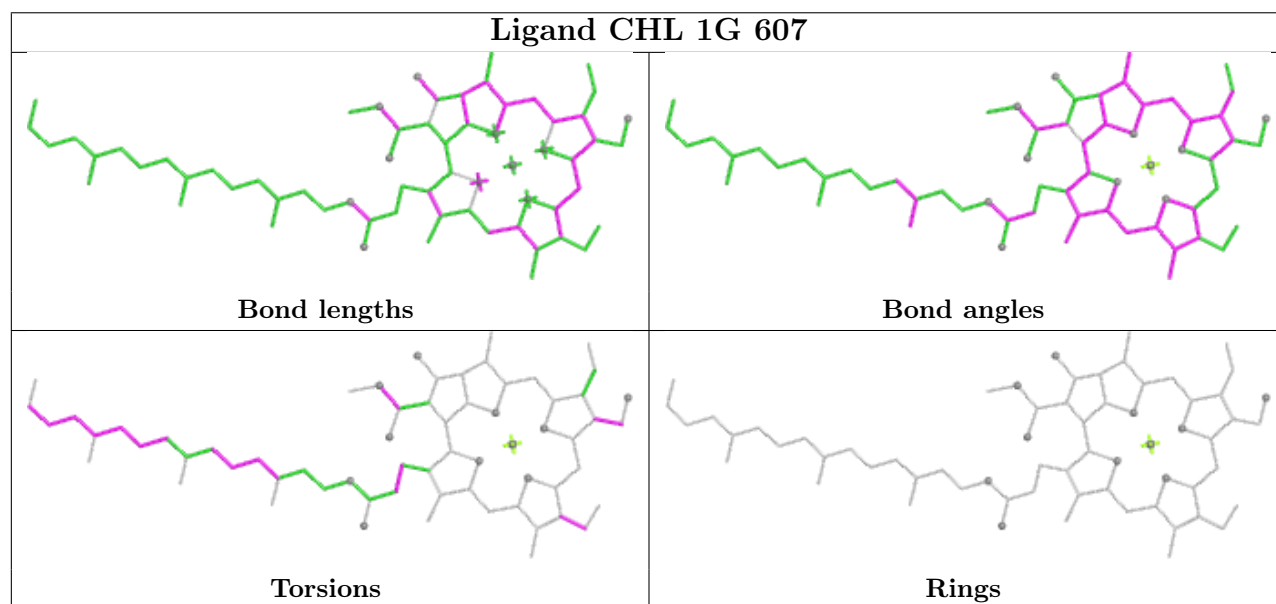
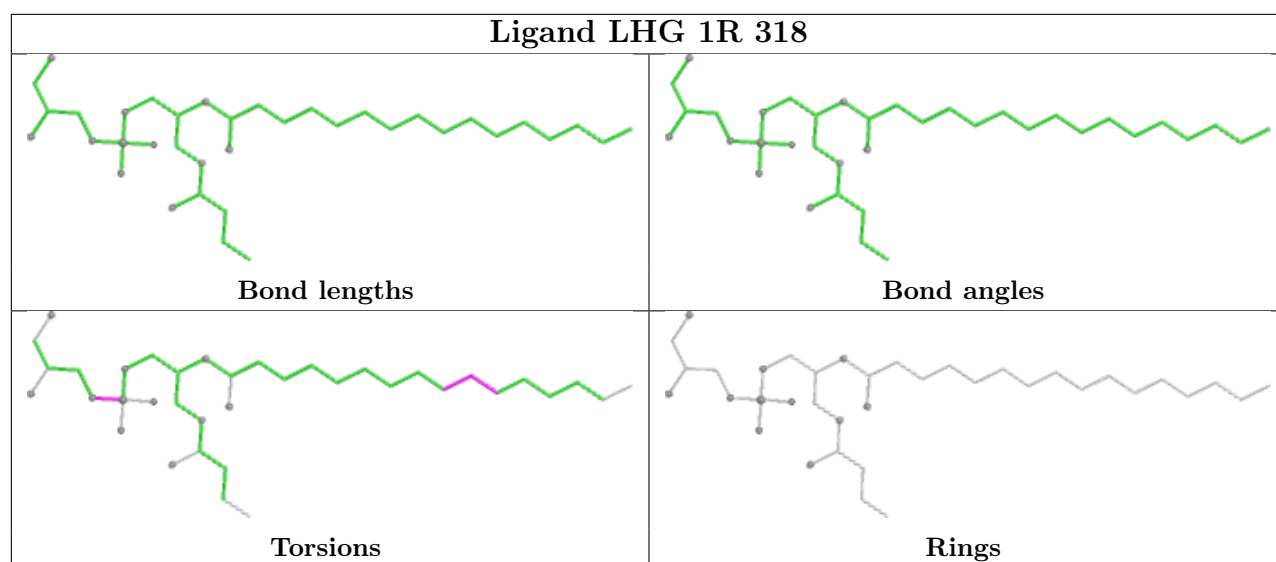


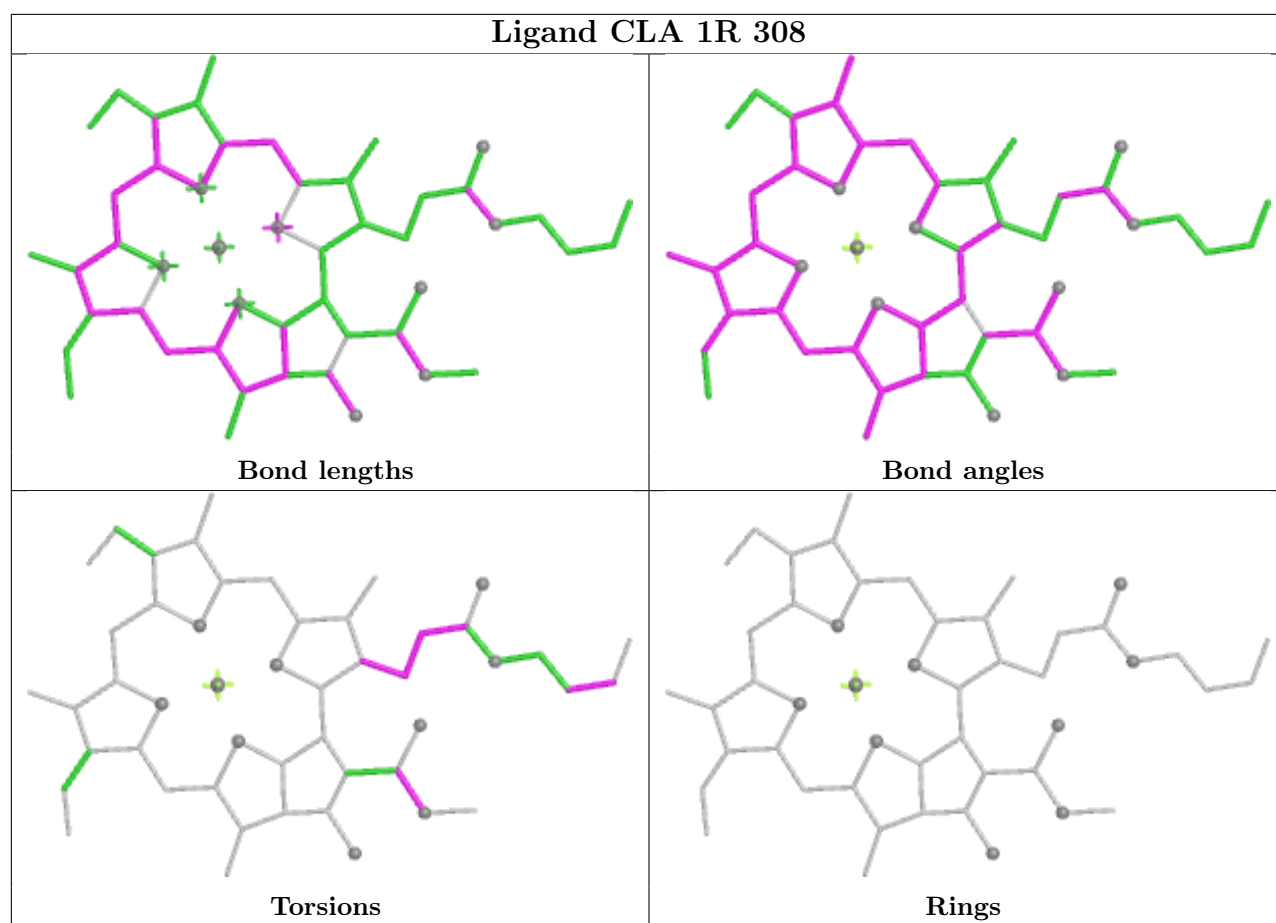


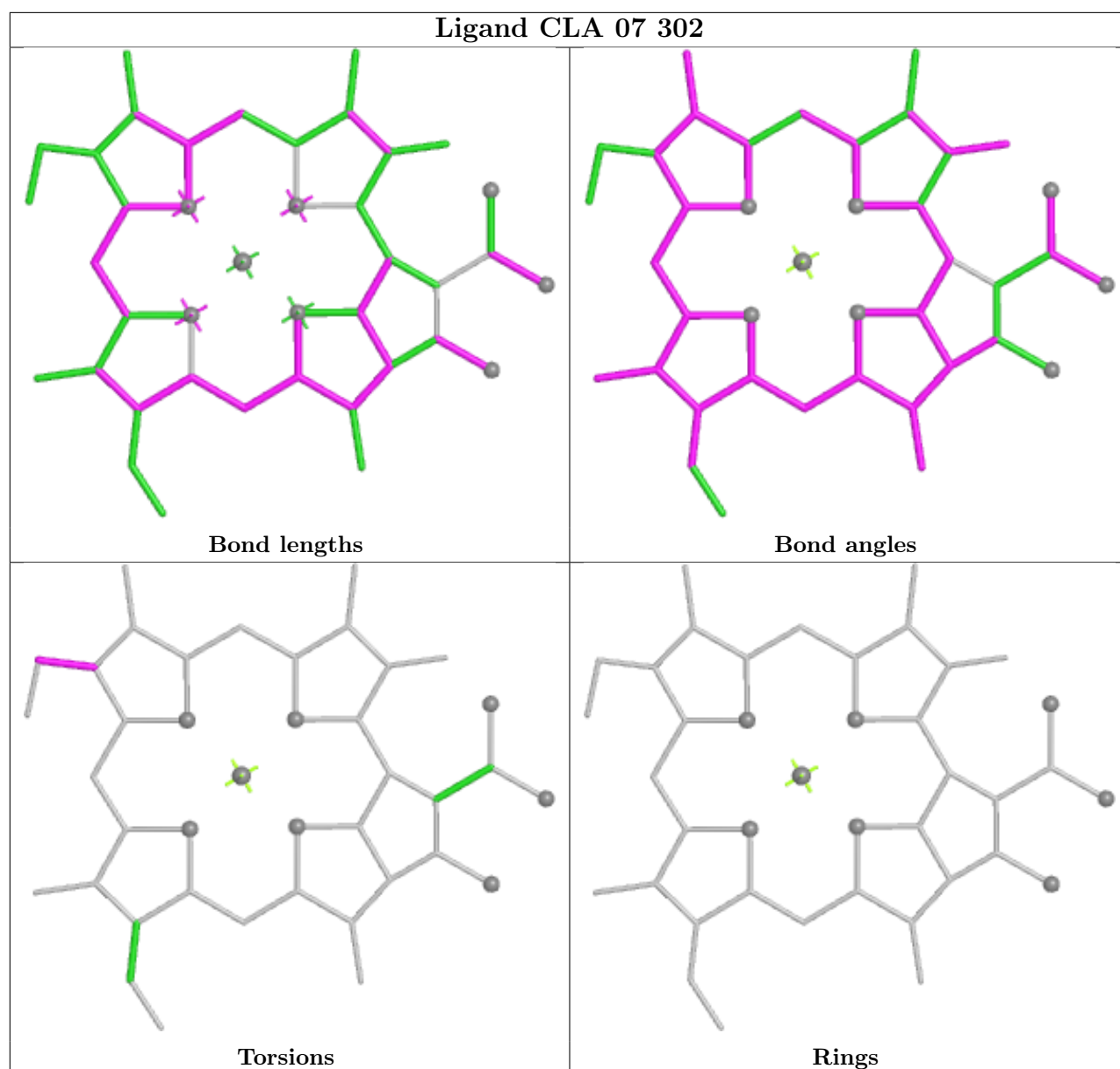


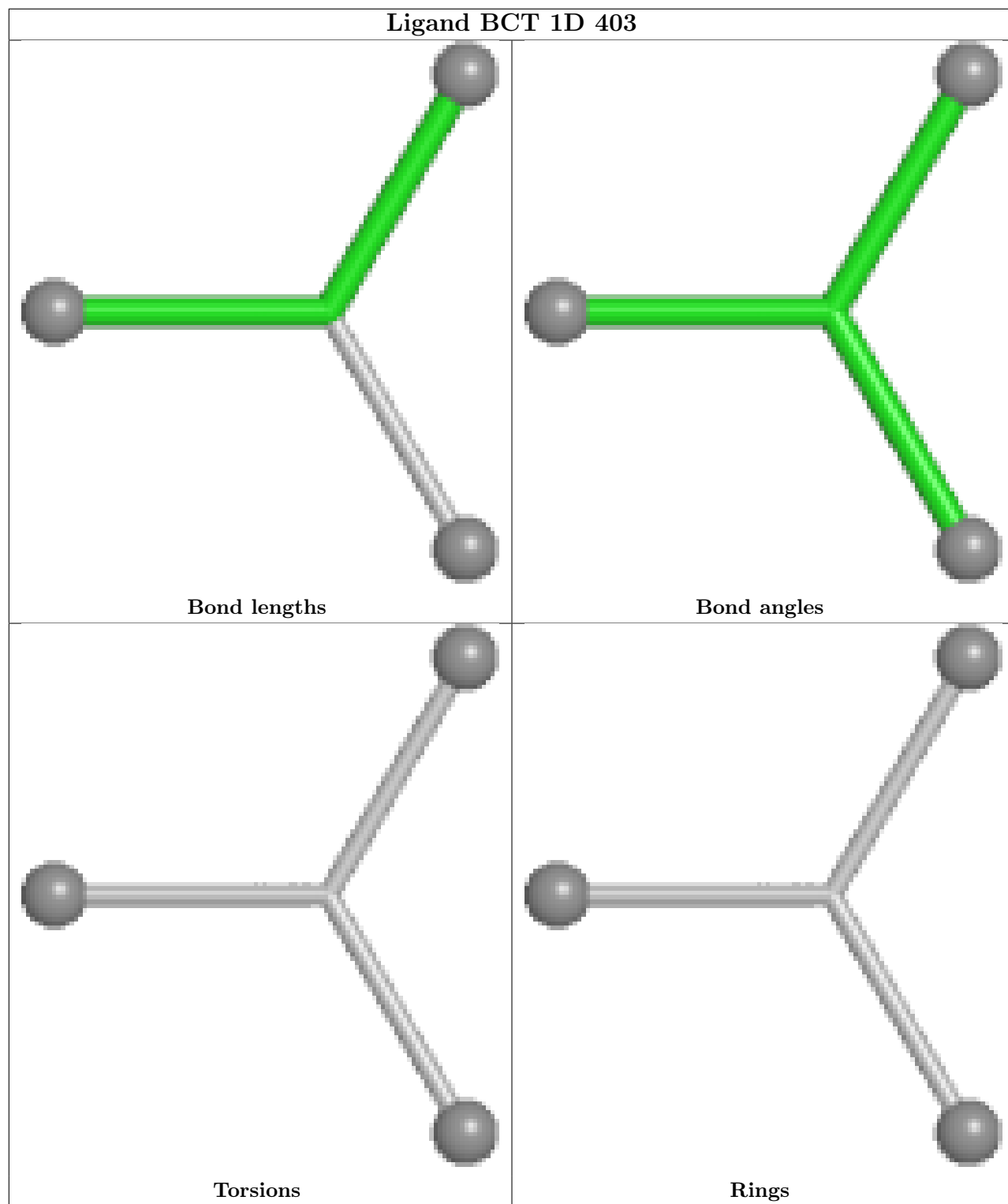


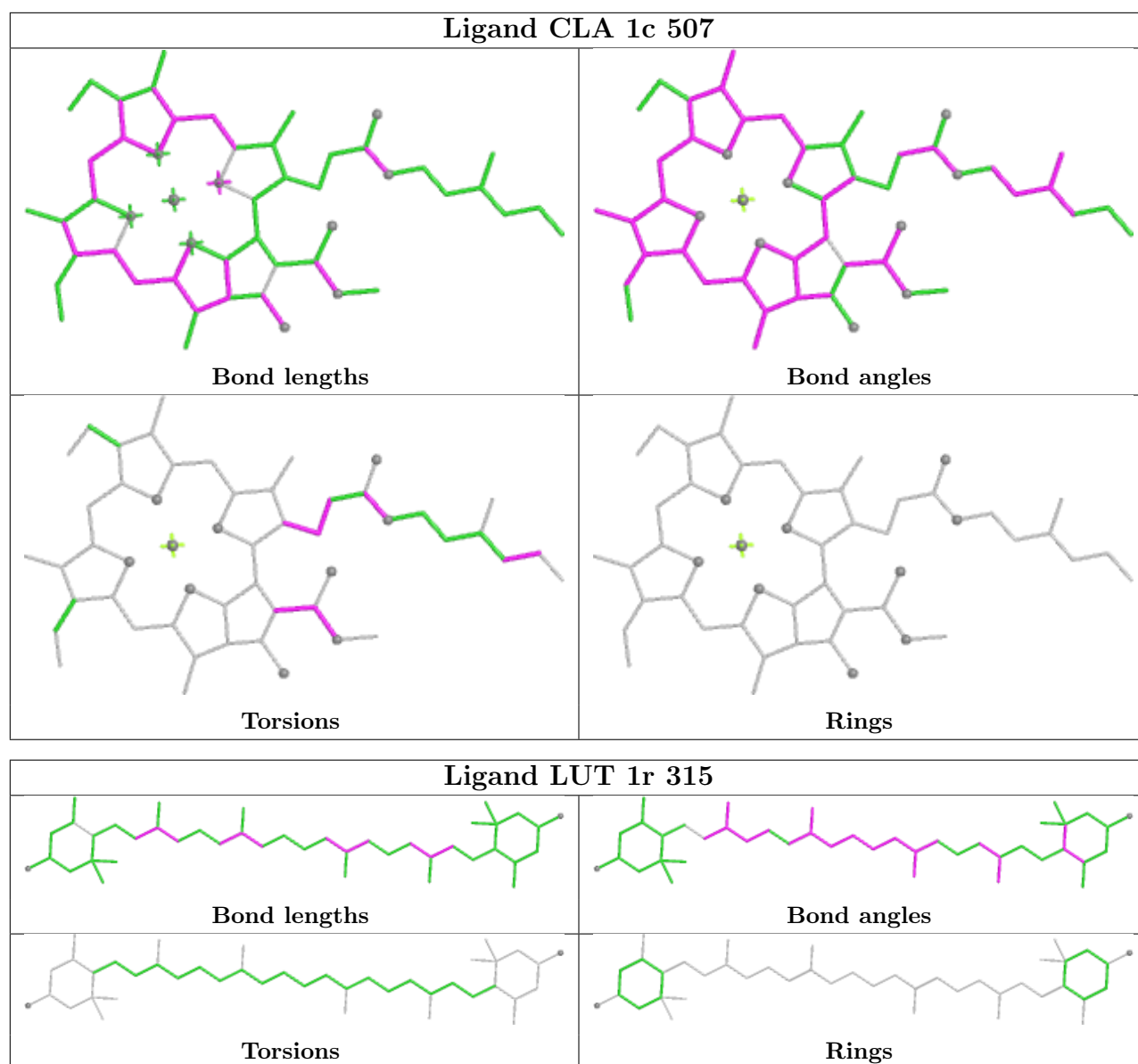


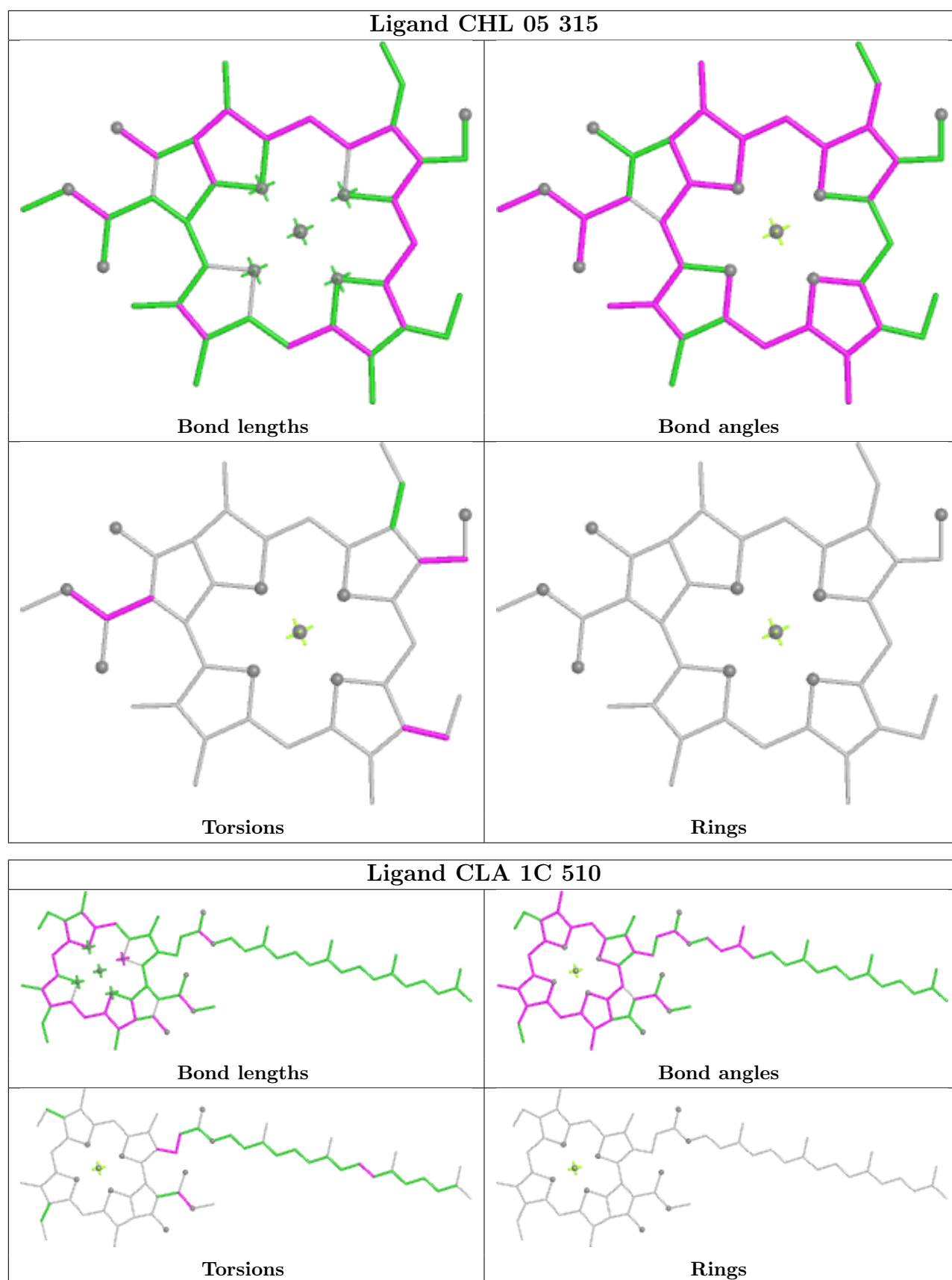




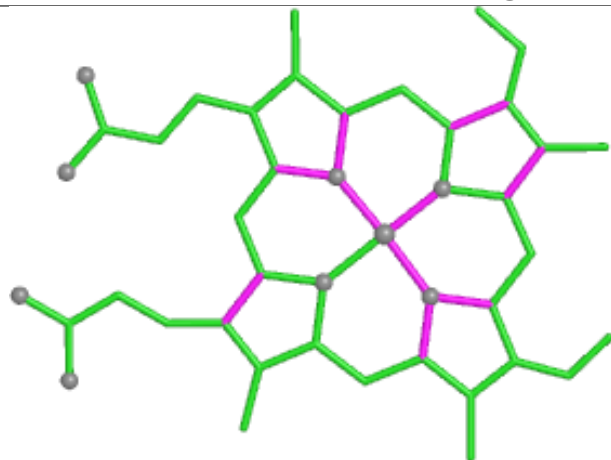




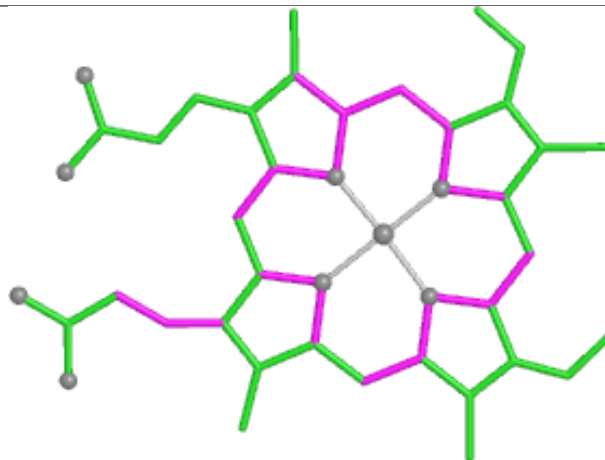




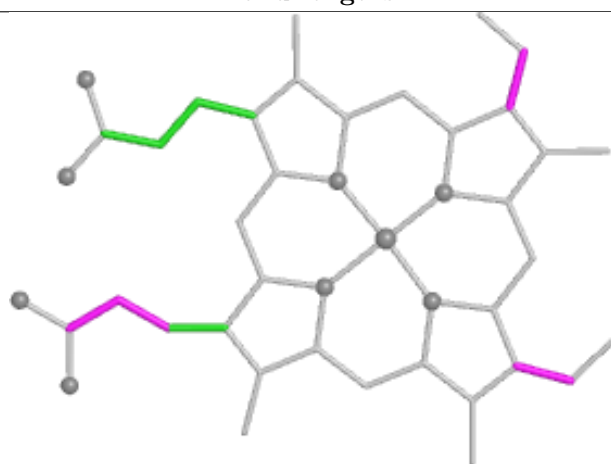
Ligand HEM 1E 103



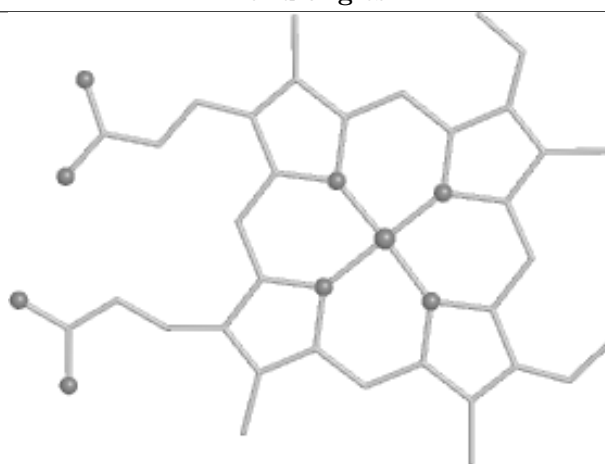
Bond lengths



Bond angles

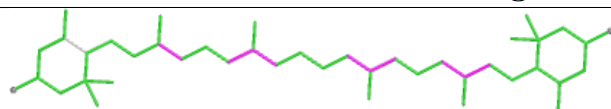


Torsions

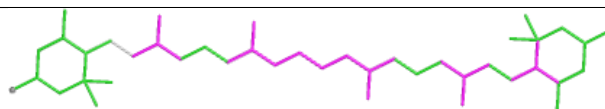


Rings

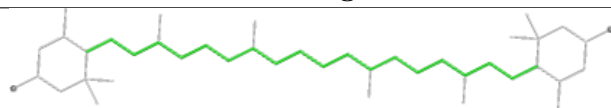
Ligand LUT 07 313



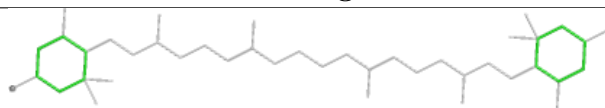
Bond lengths



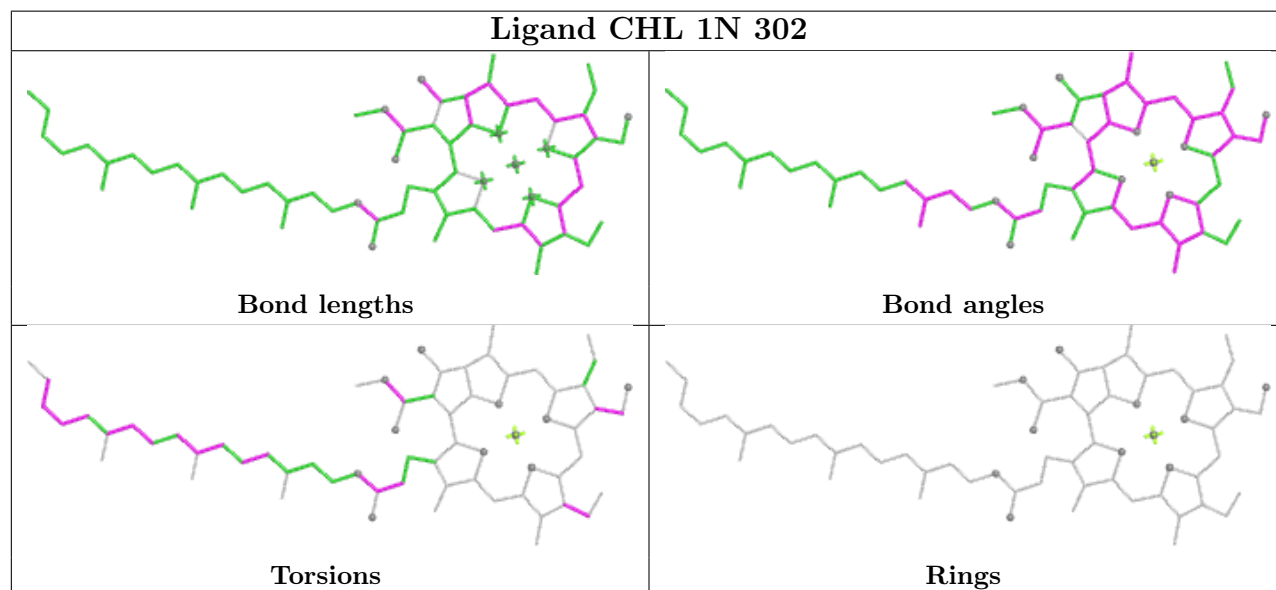
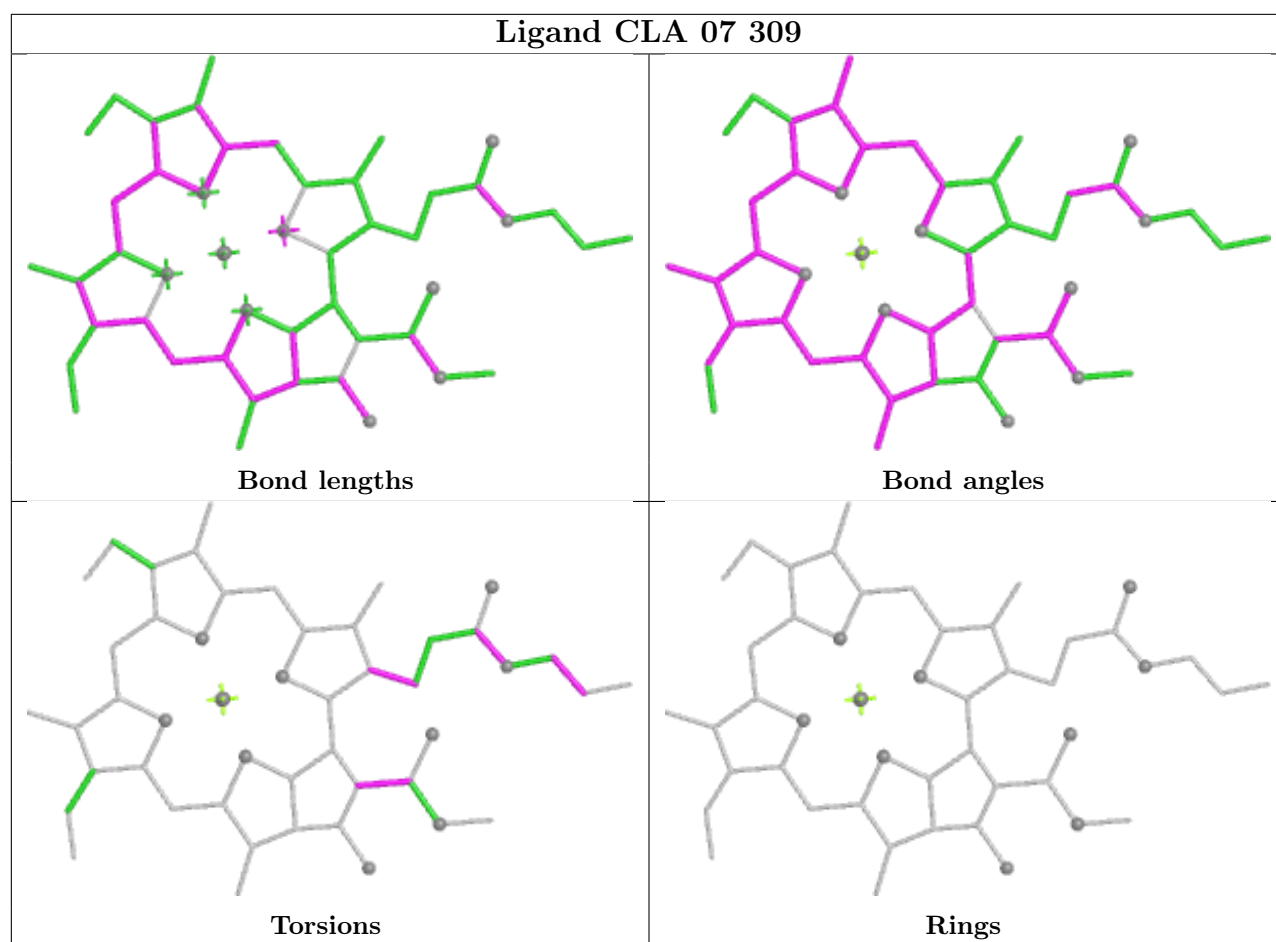
Bond angles

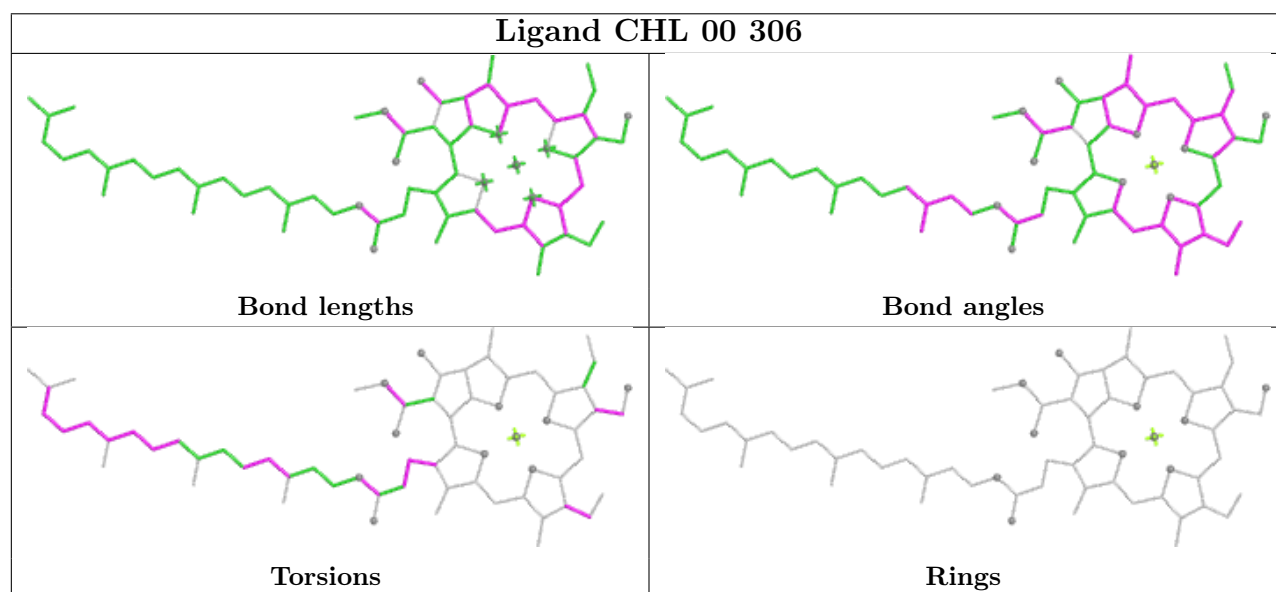
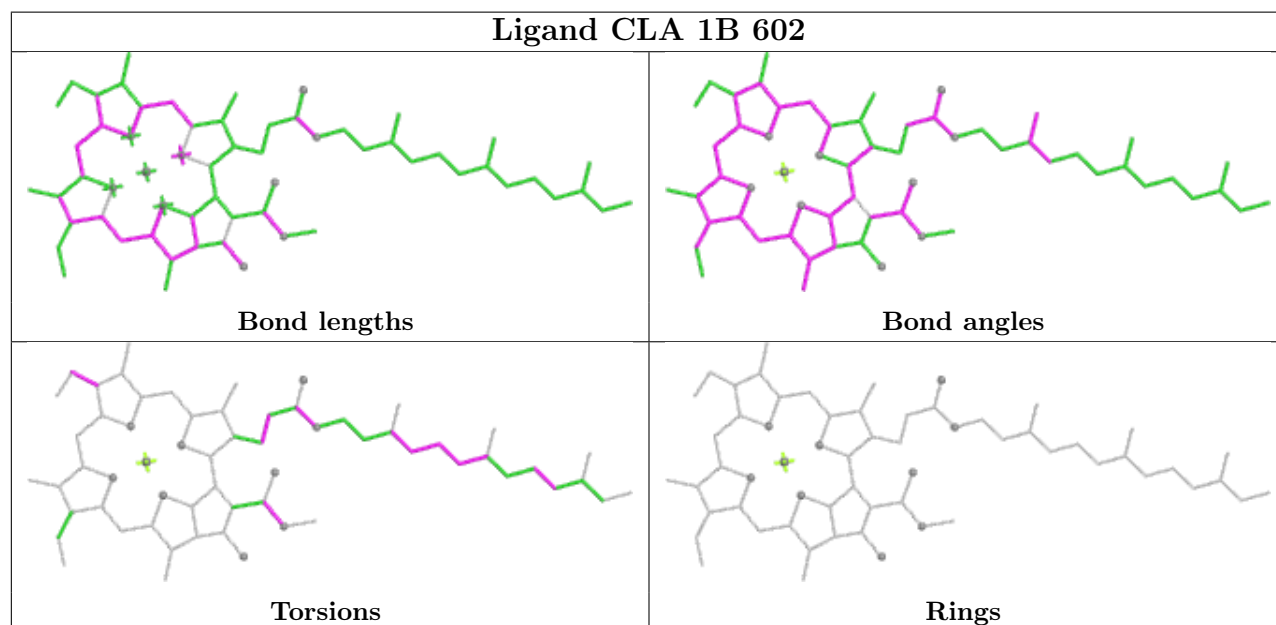
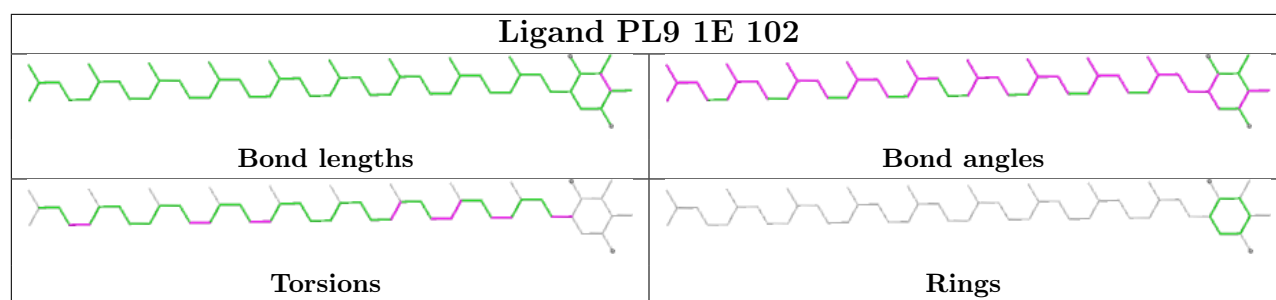


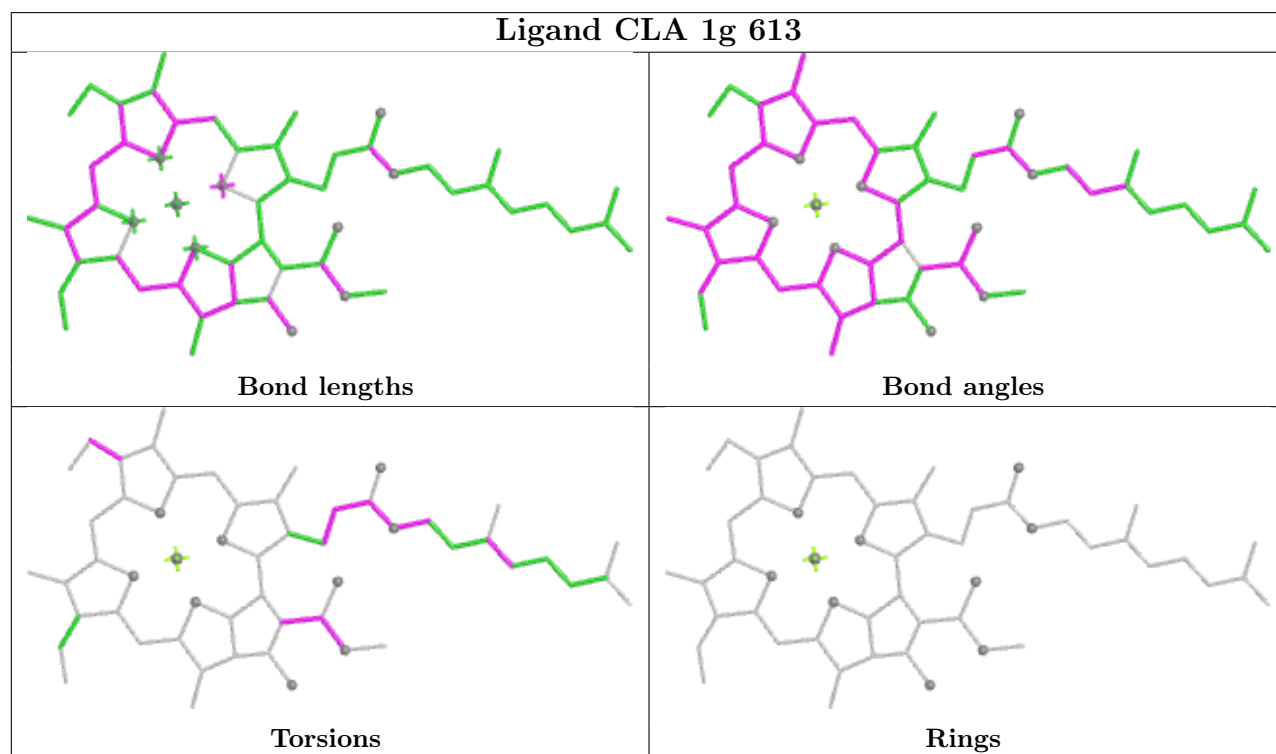
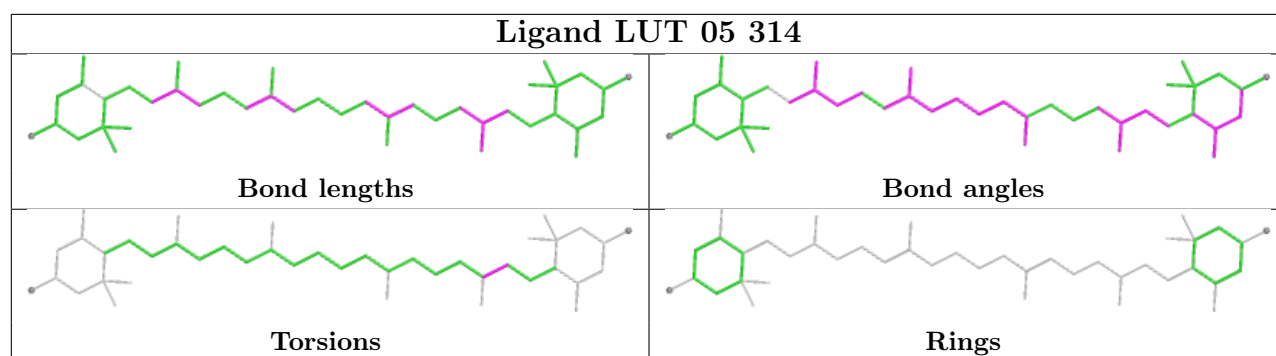
Torsions

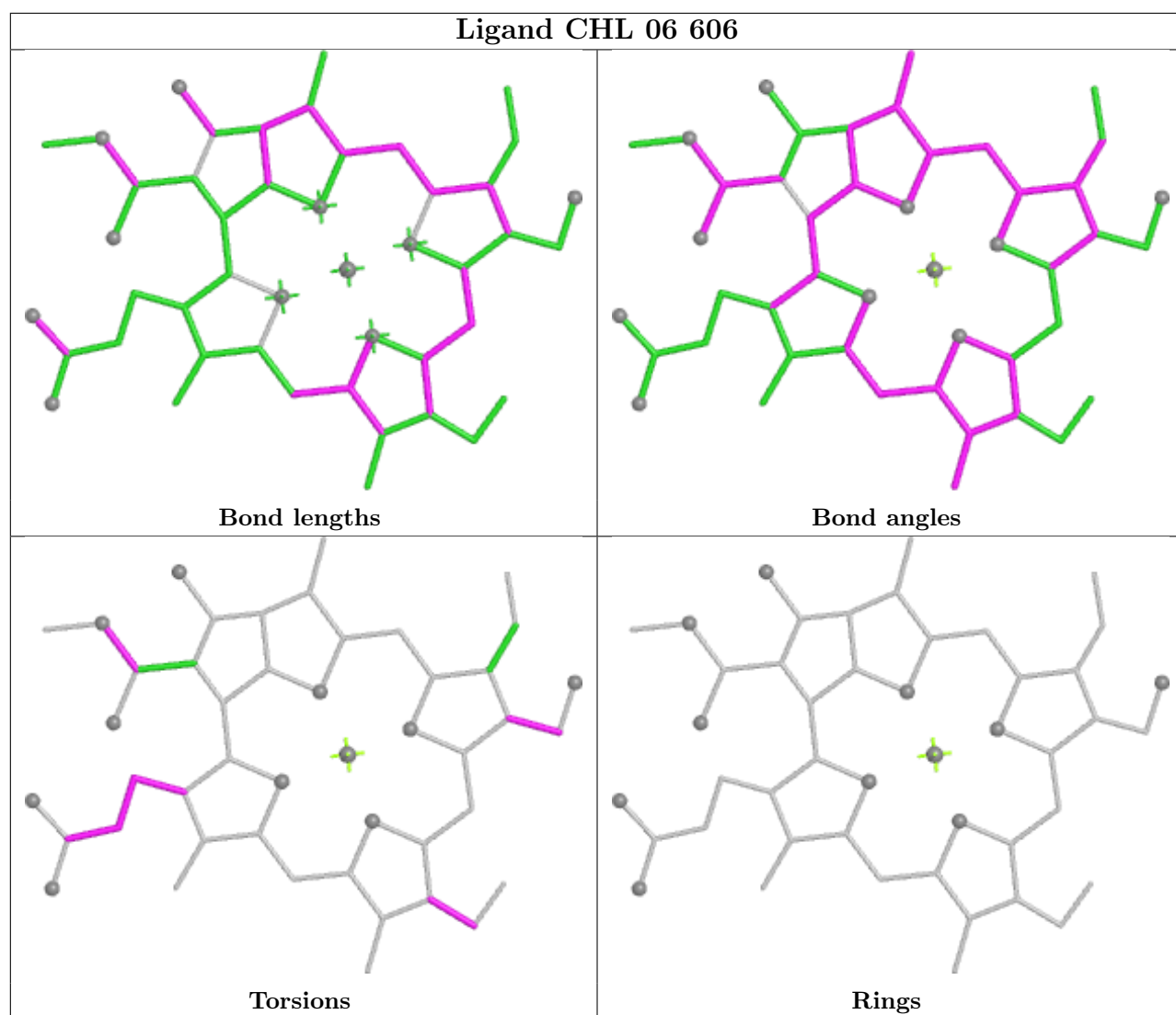


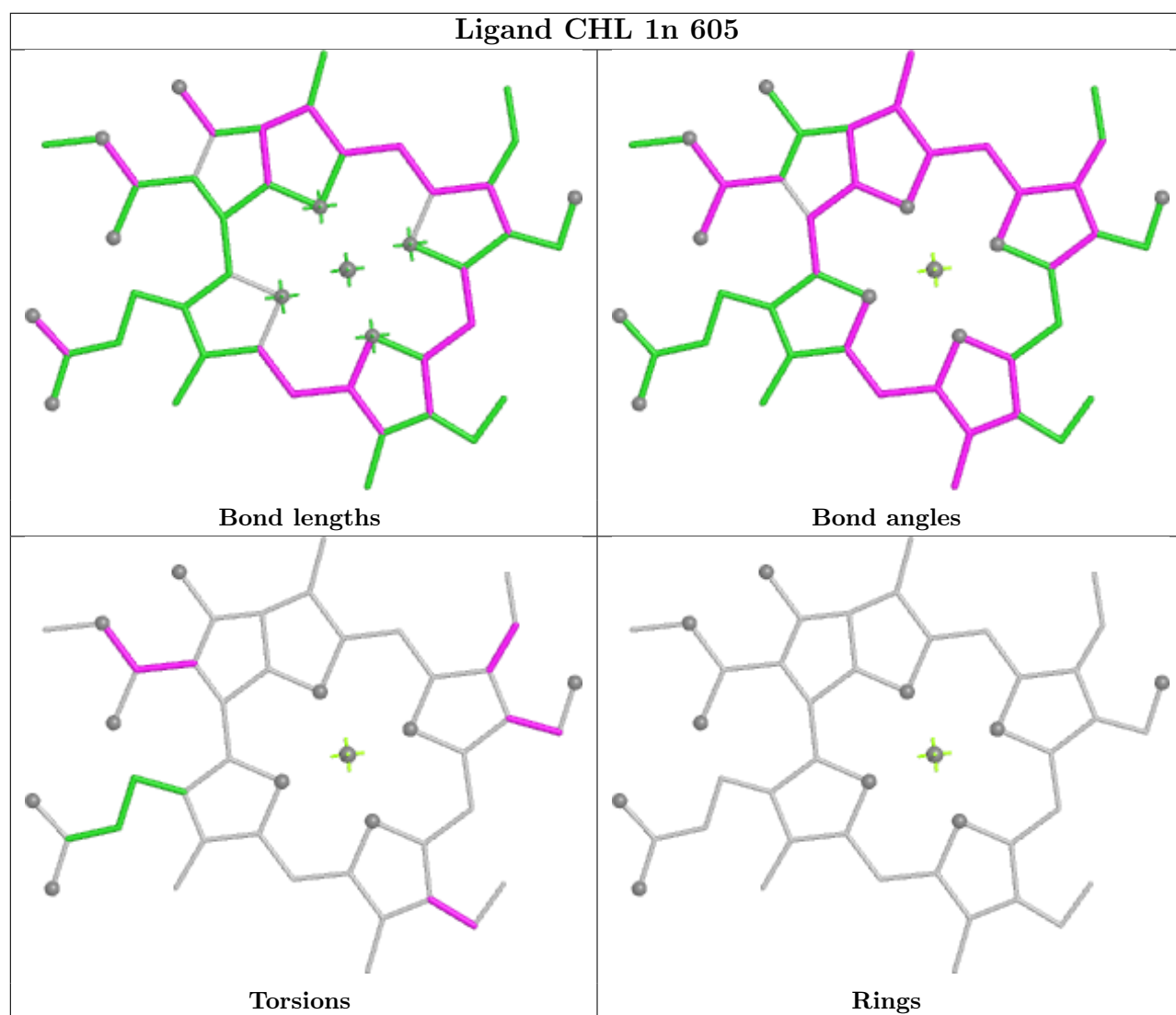
Rings

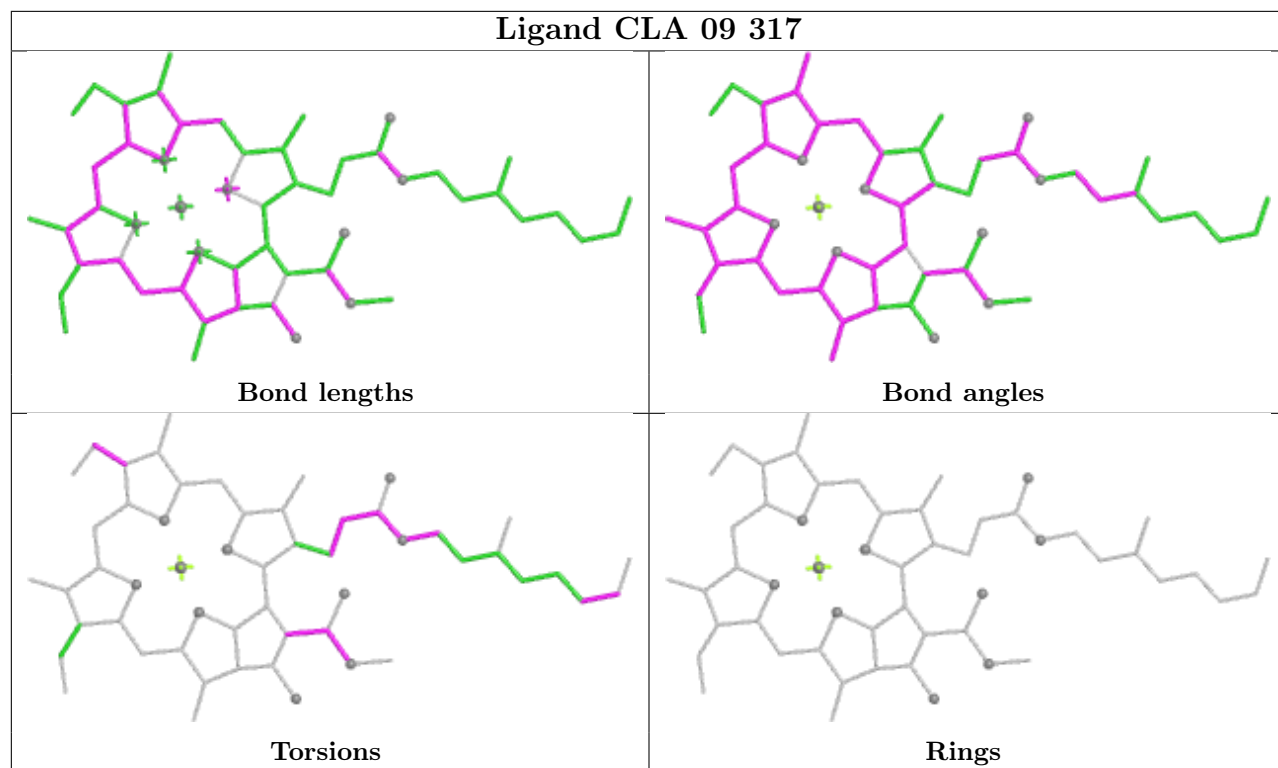


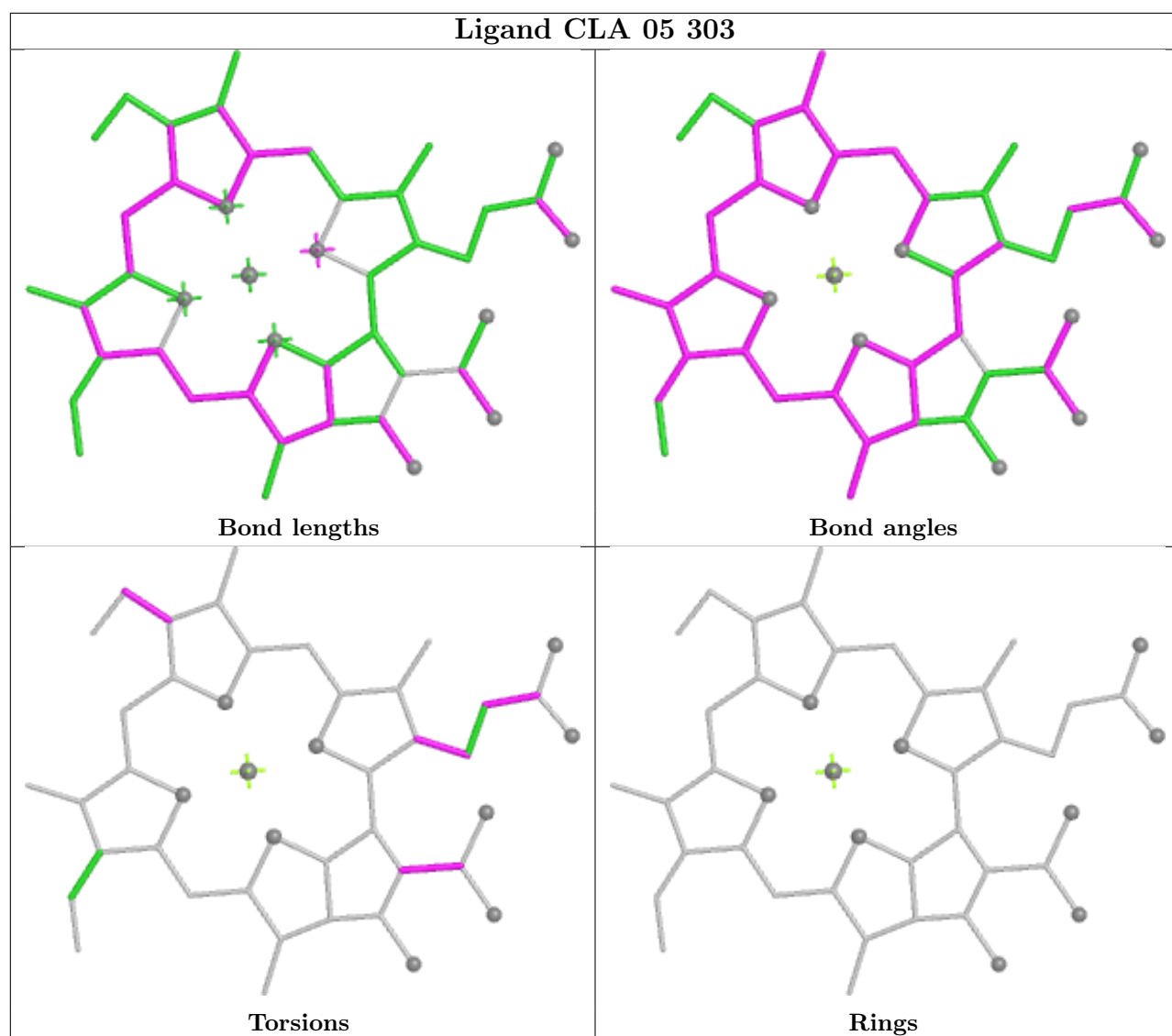


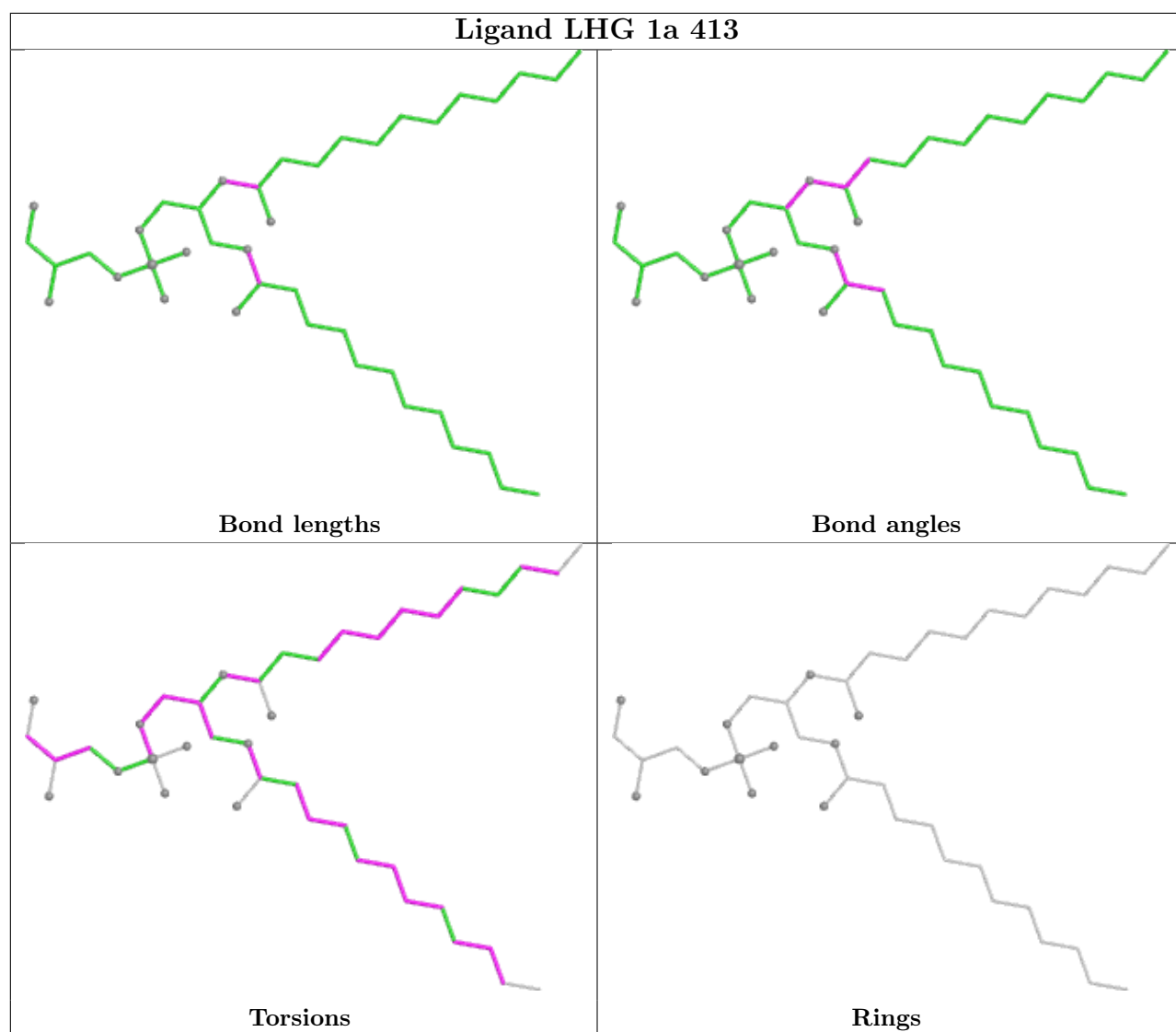


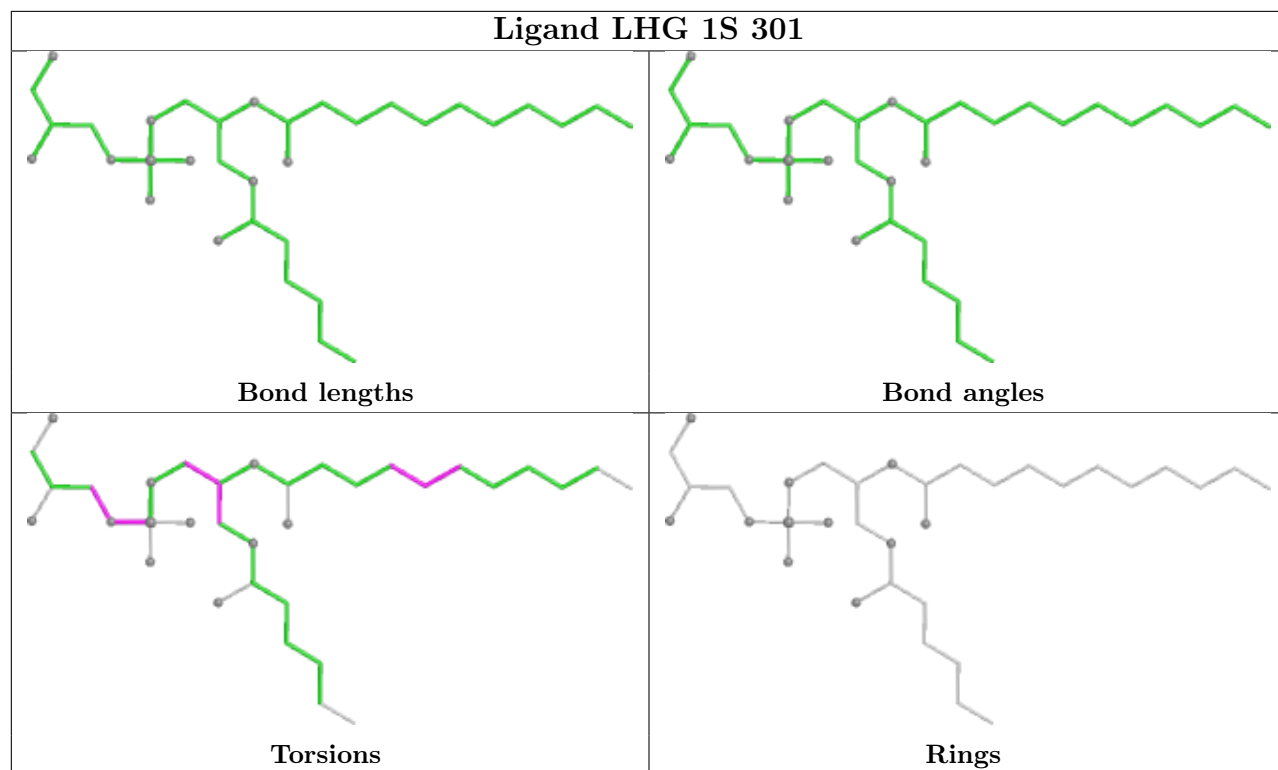


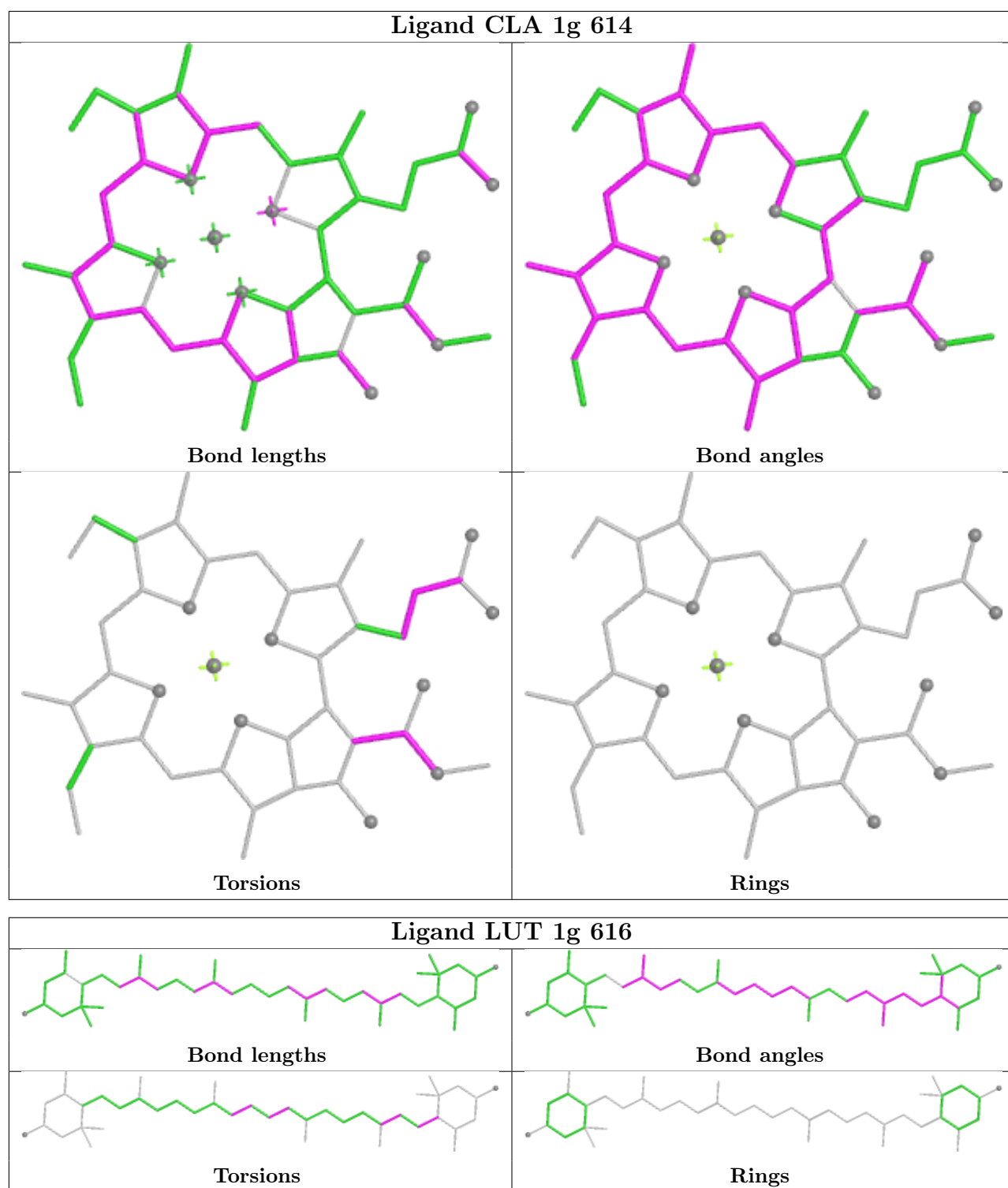


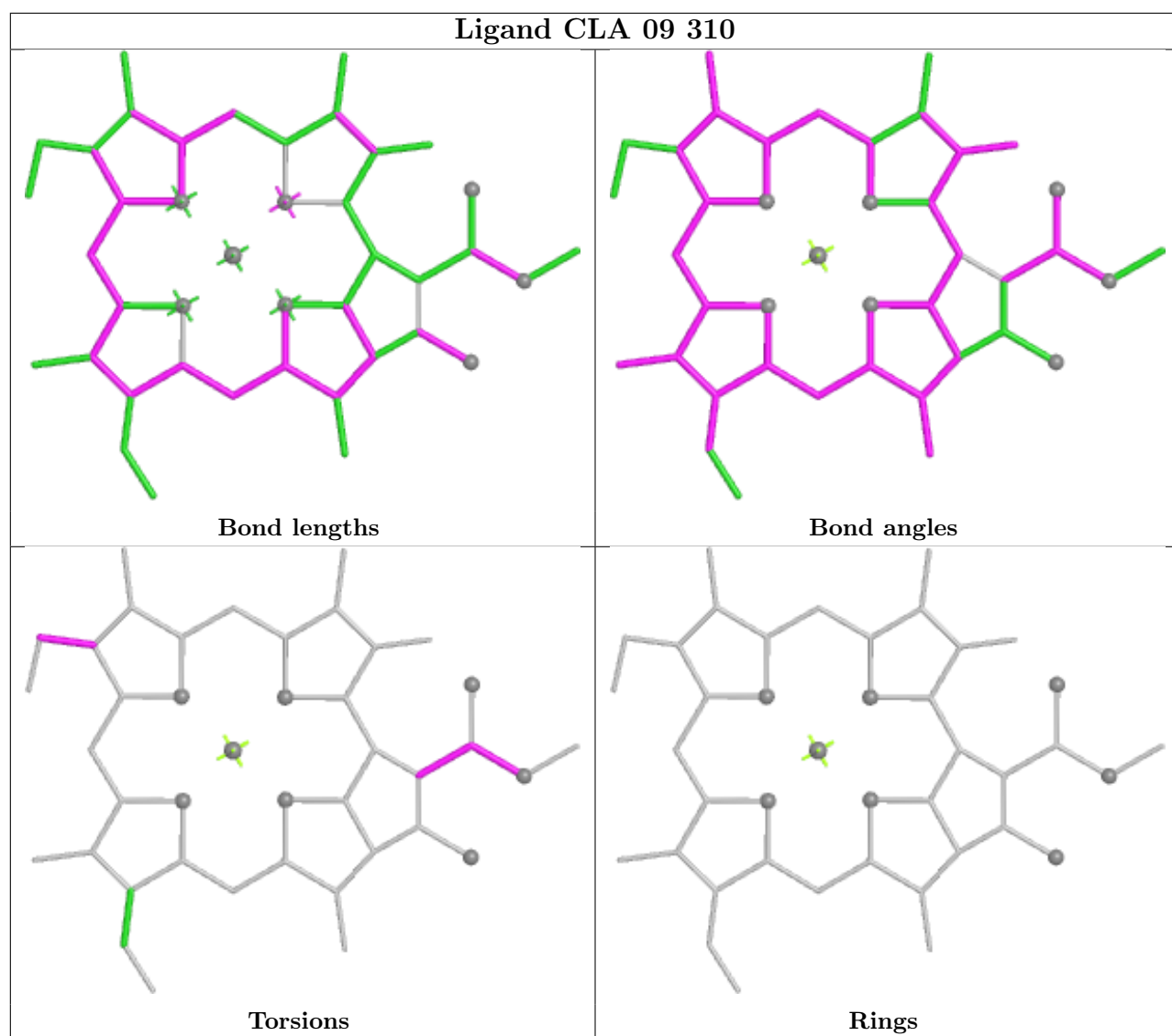


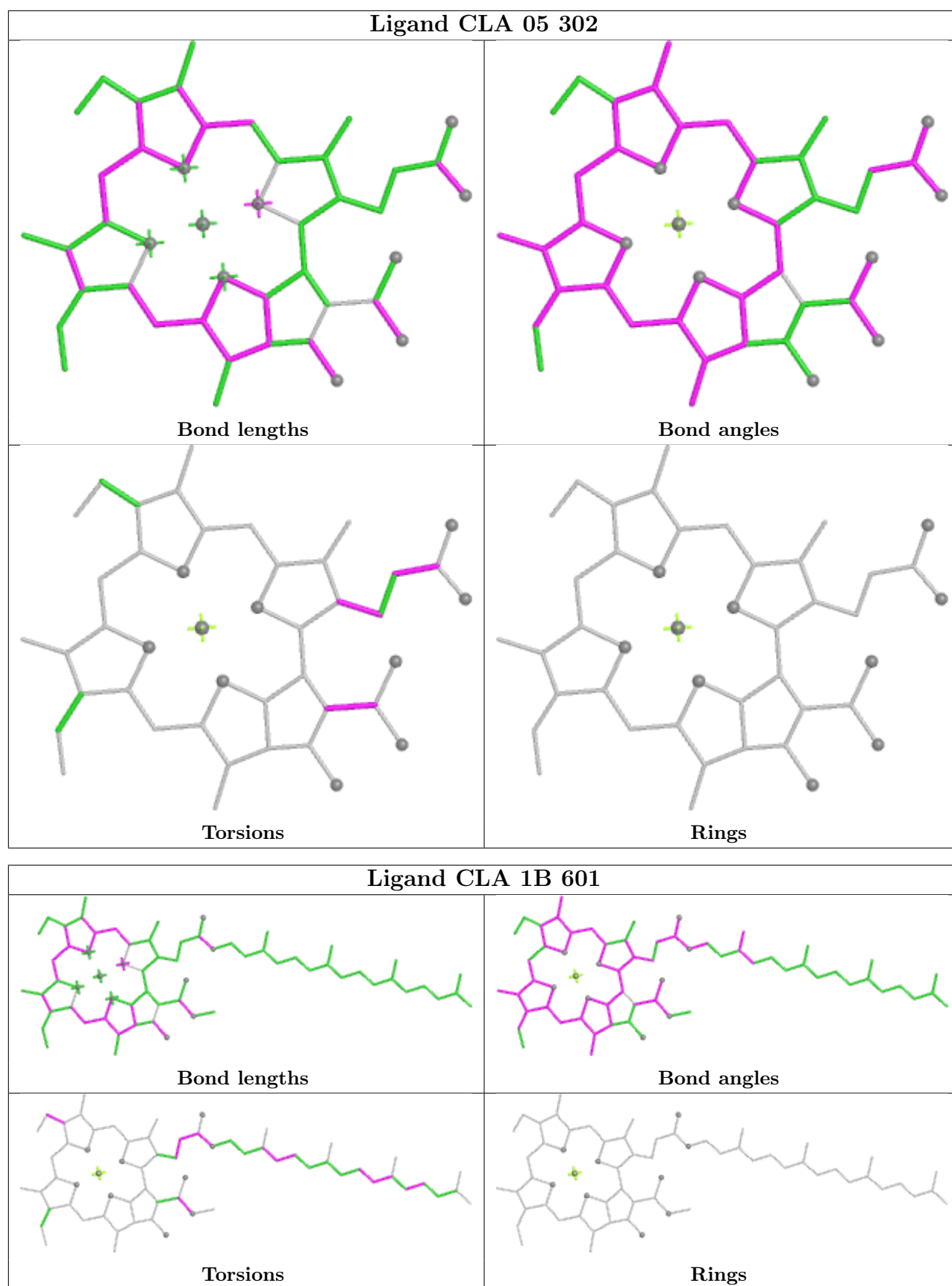


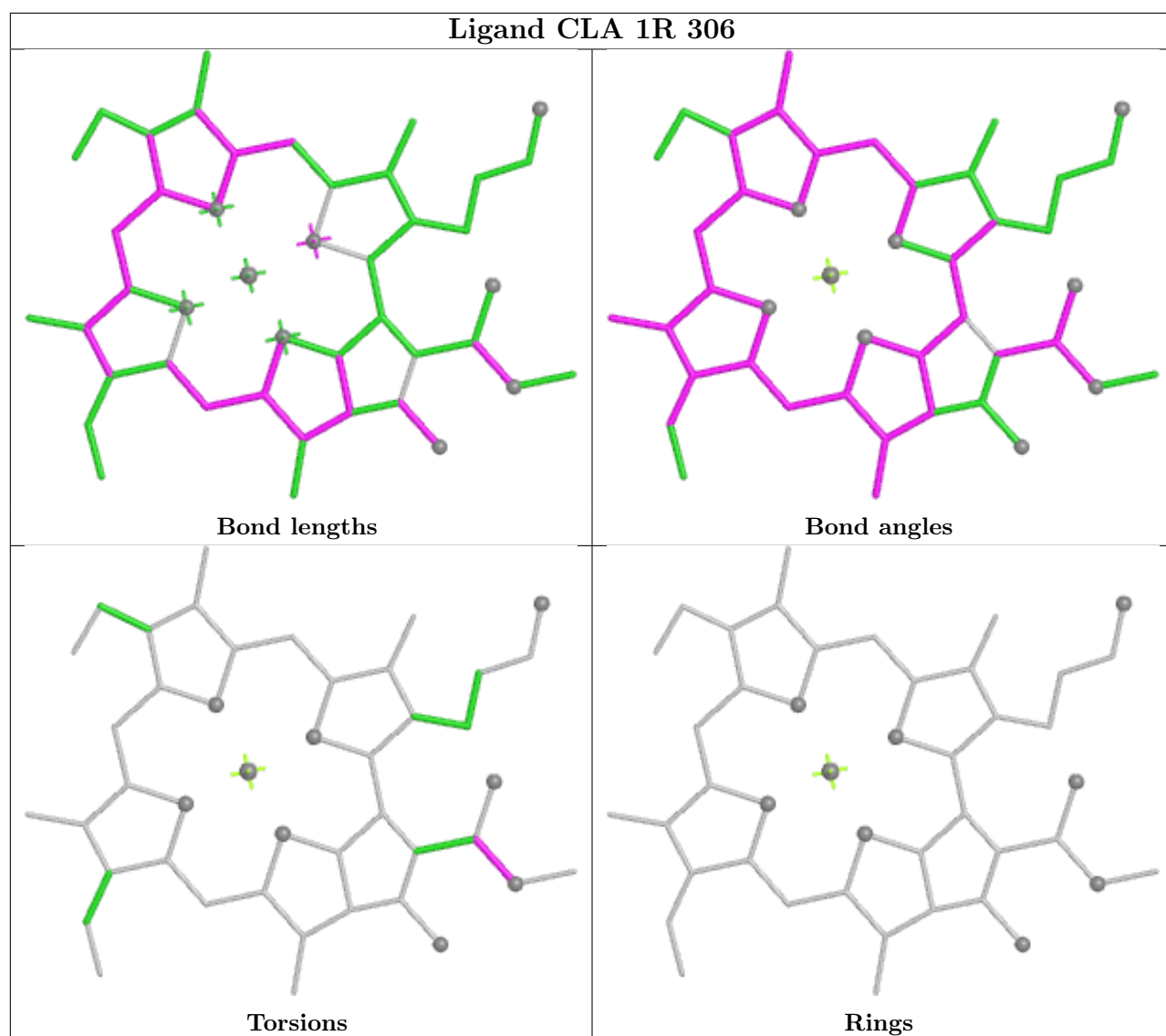


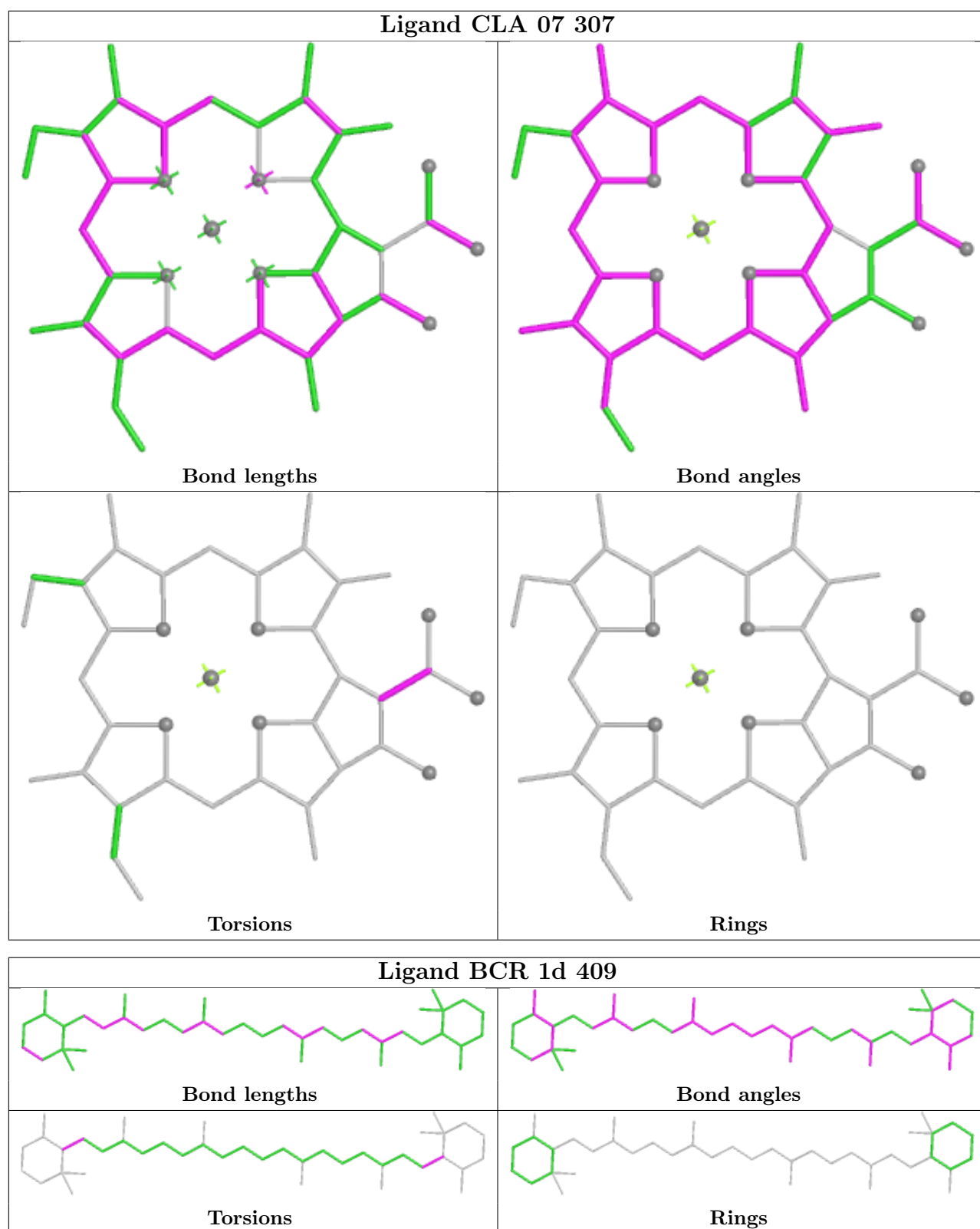


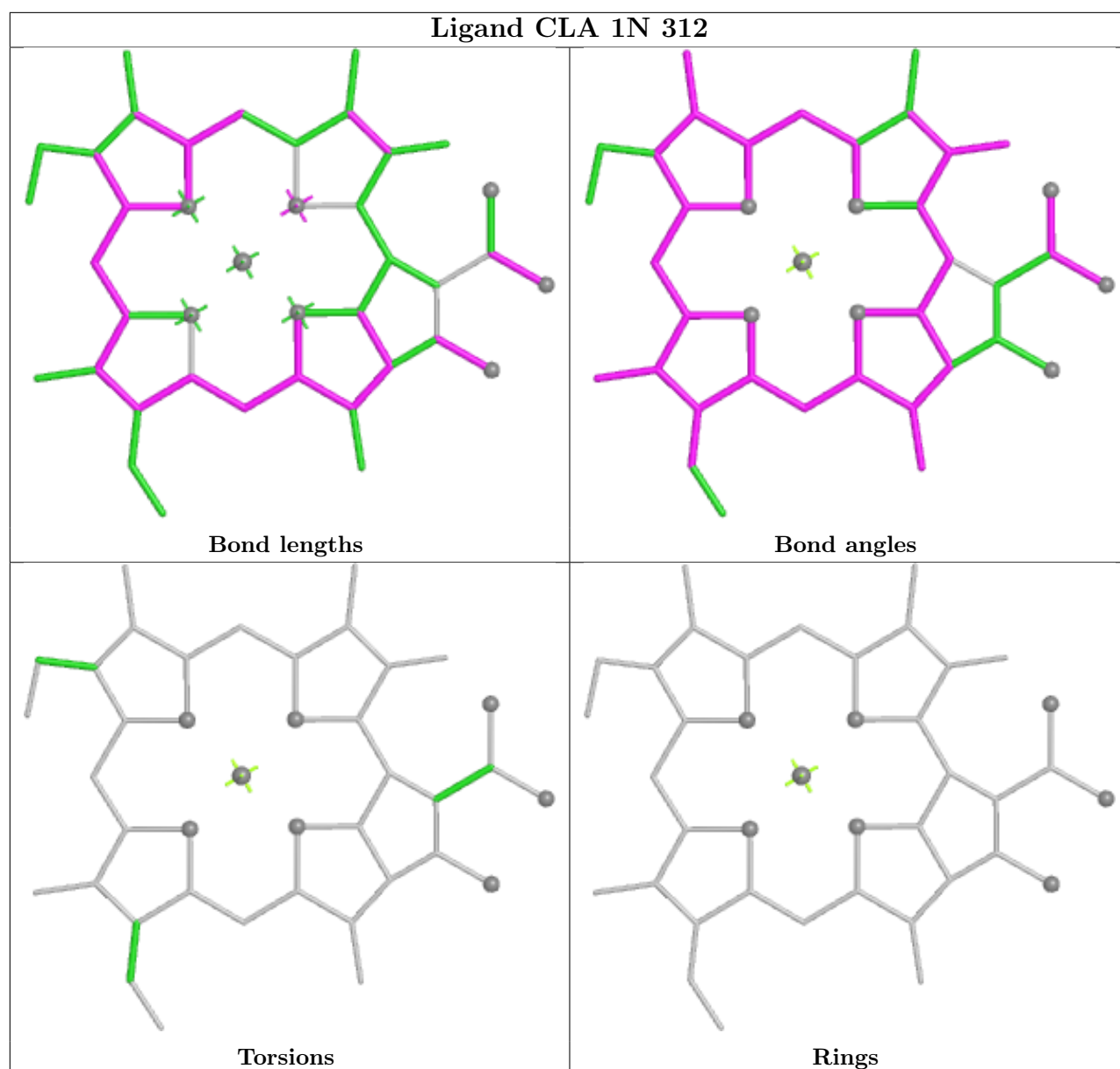




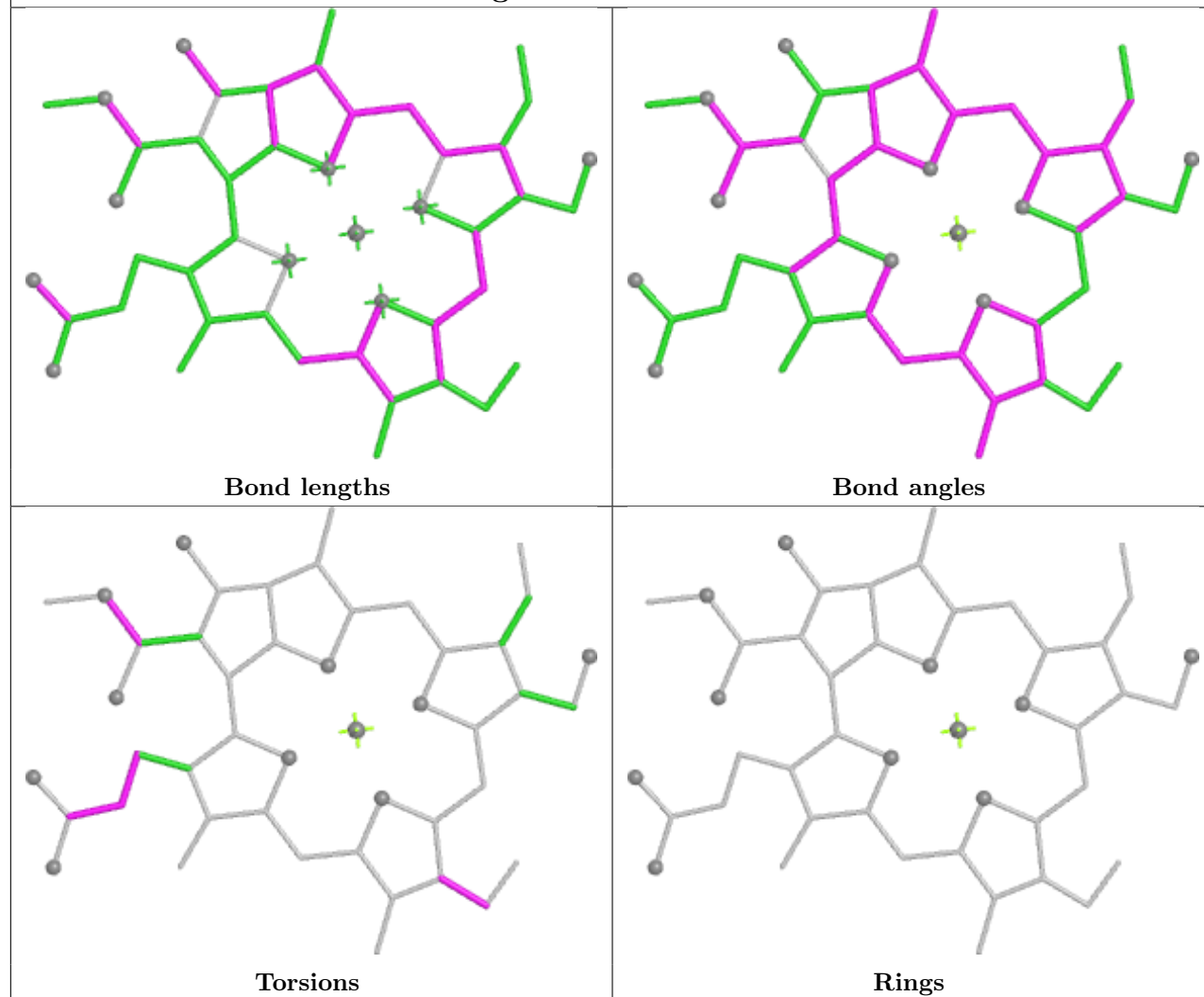




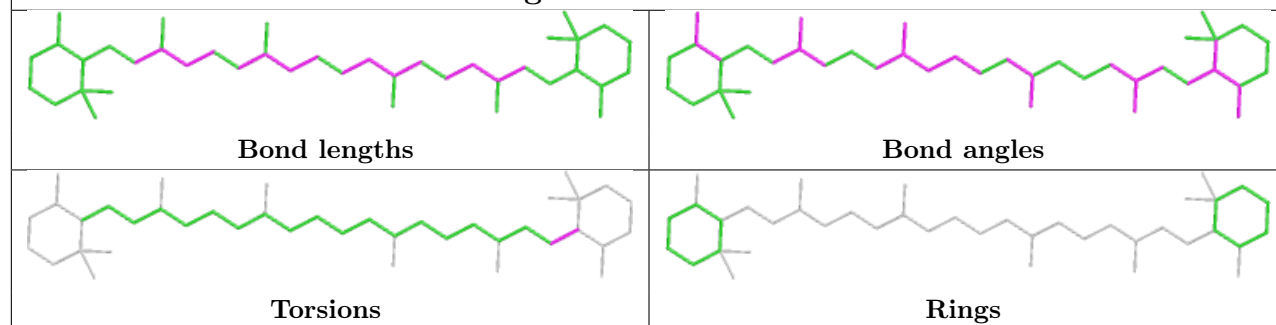


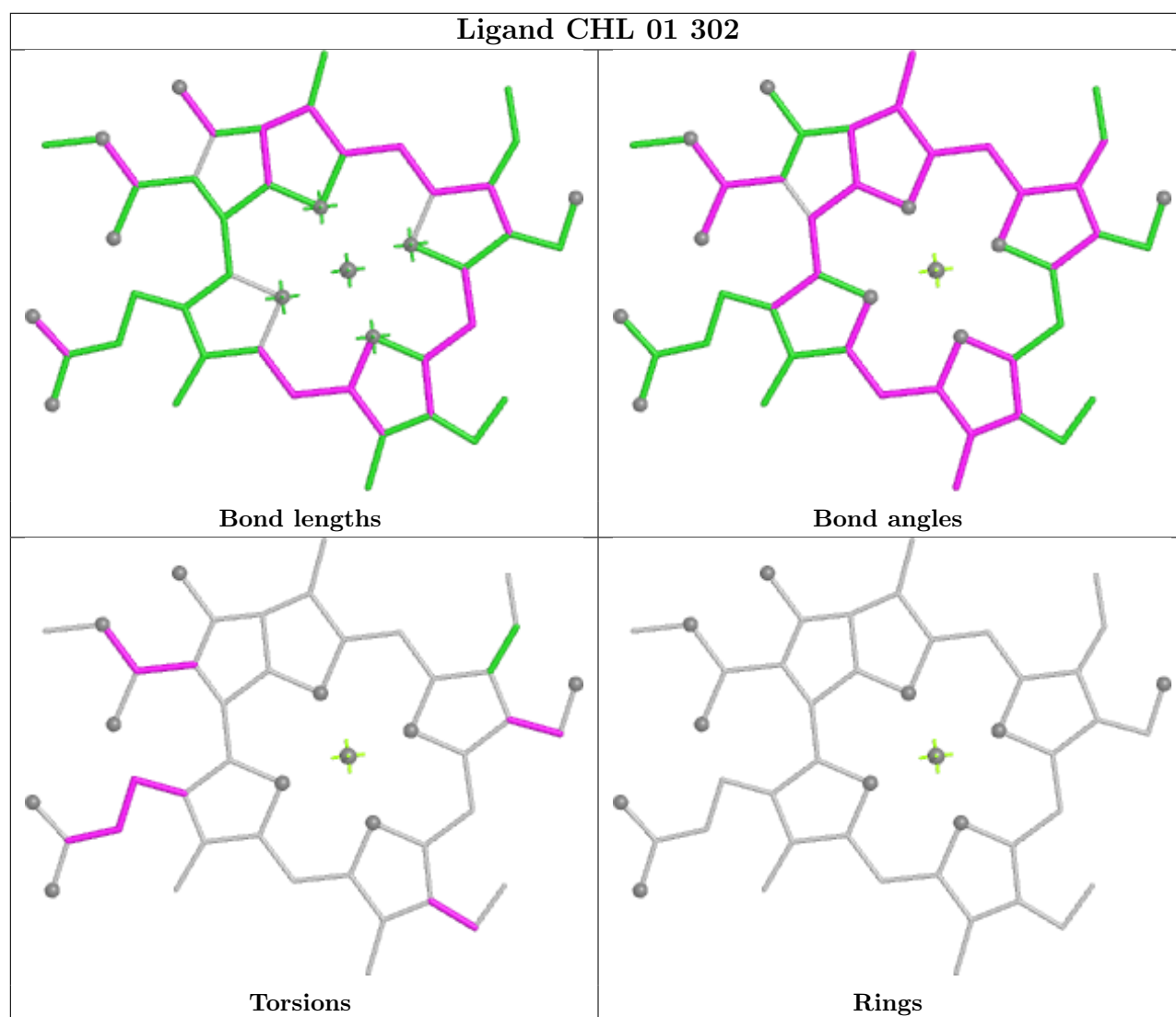


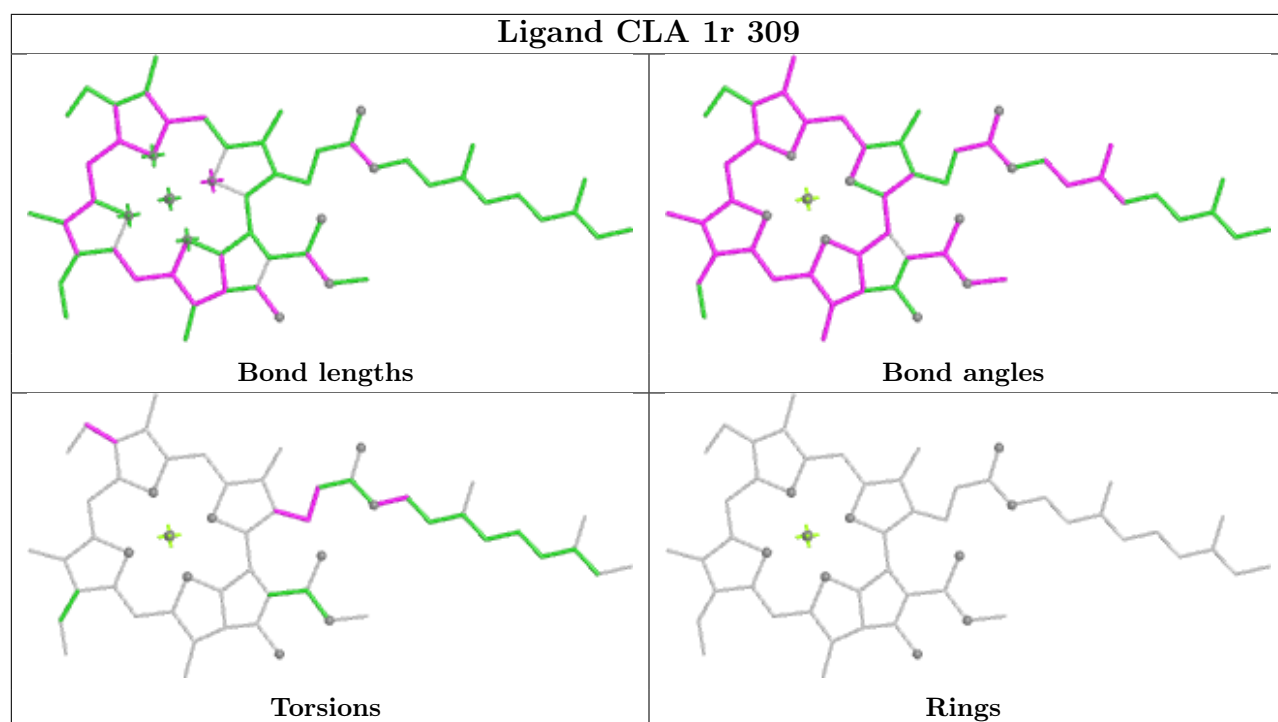
Ligand CHL 1N 307

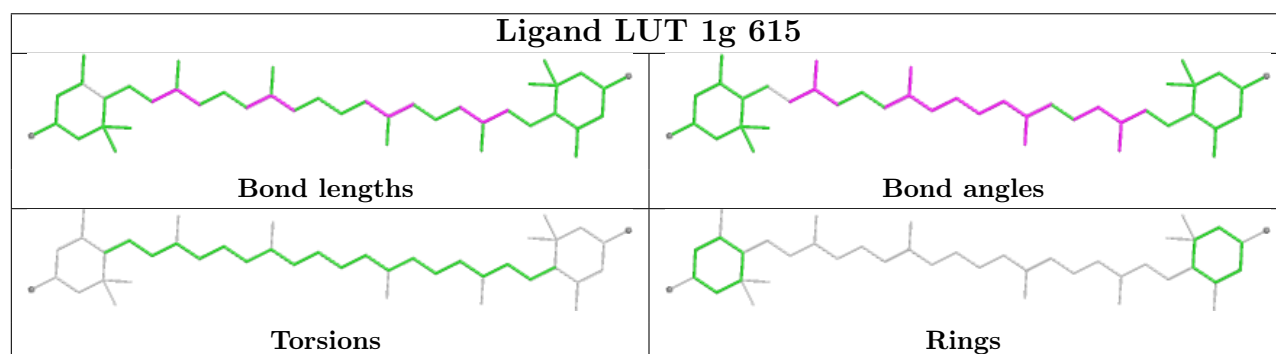
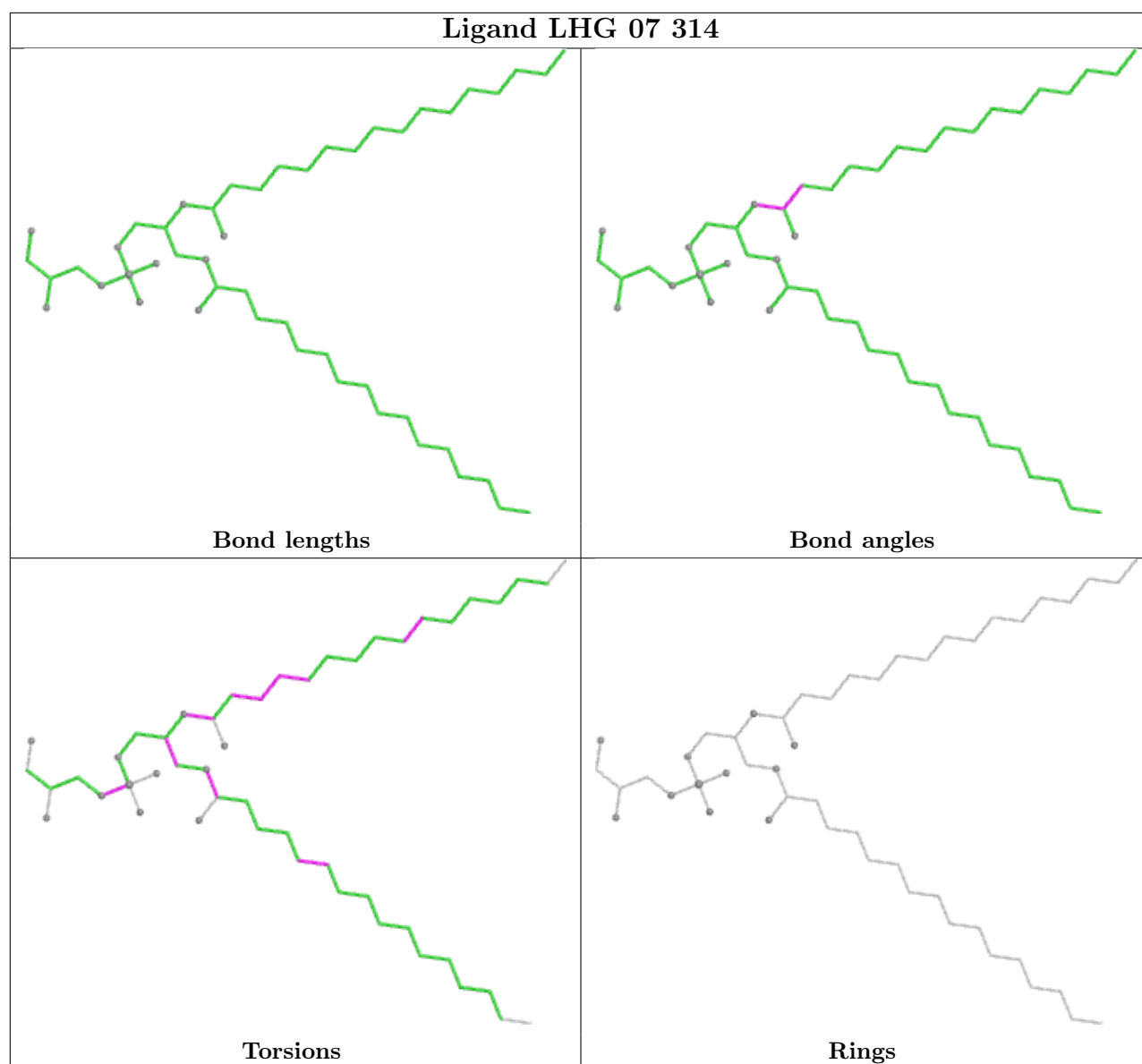


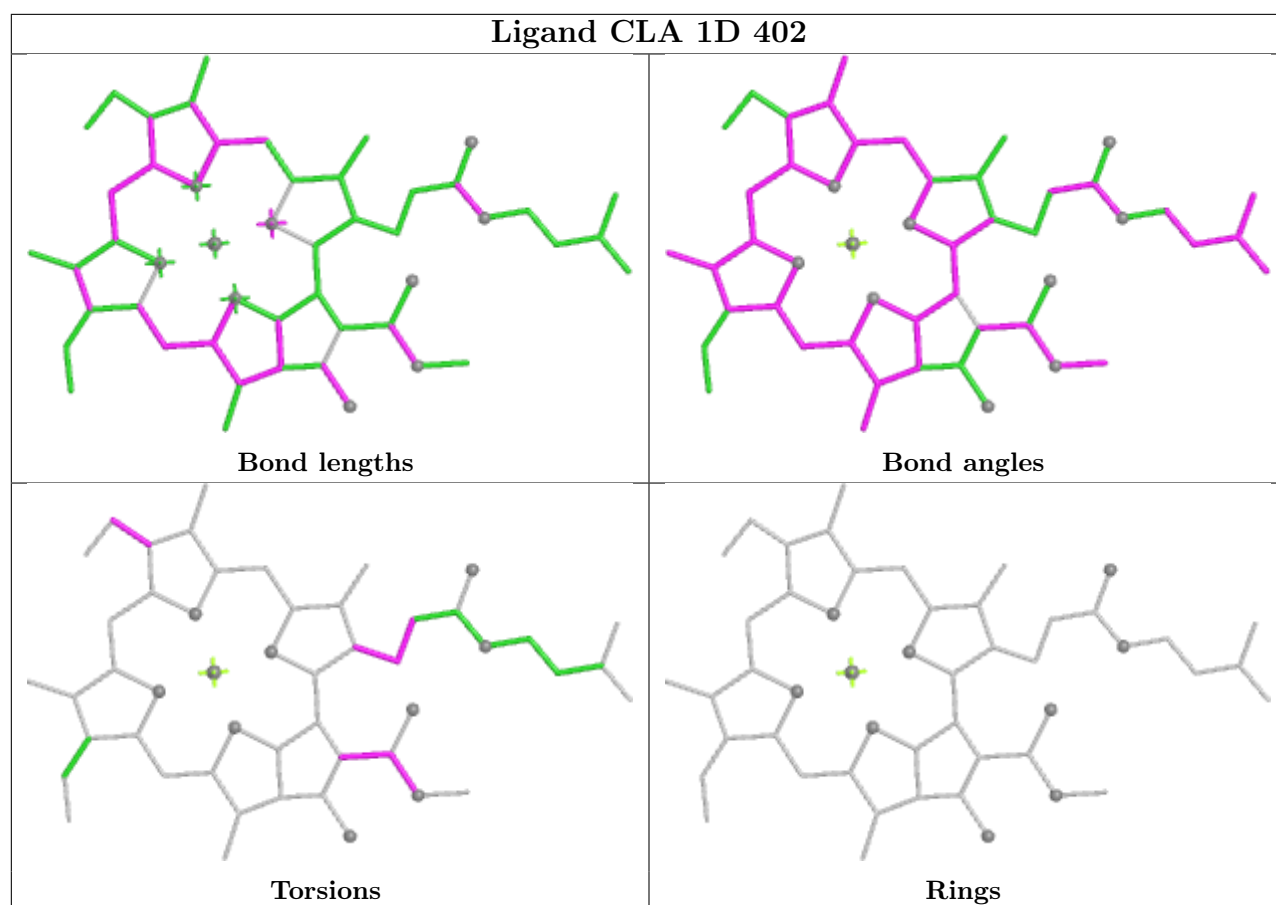
Ligand BCR 1b 618

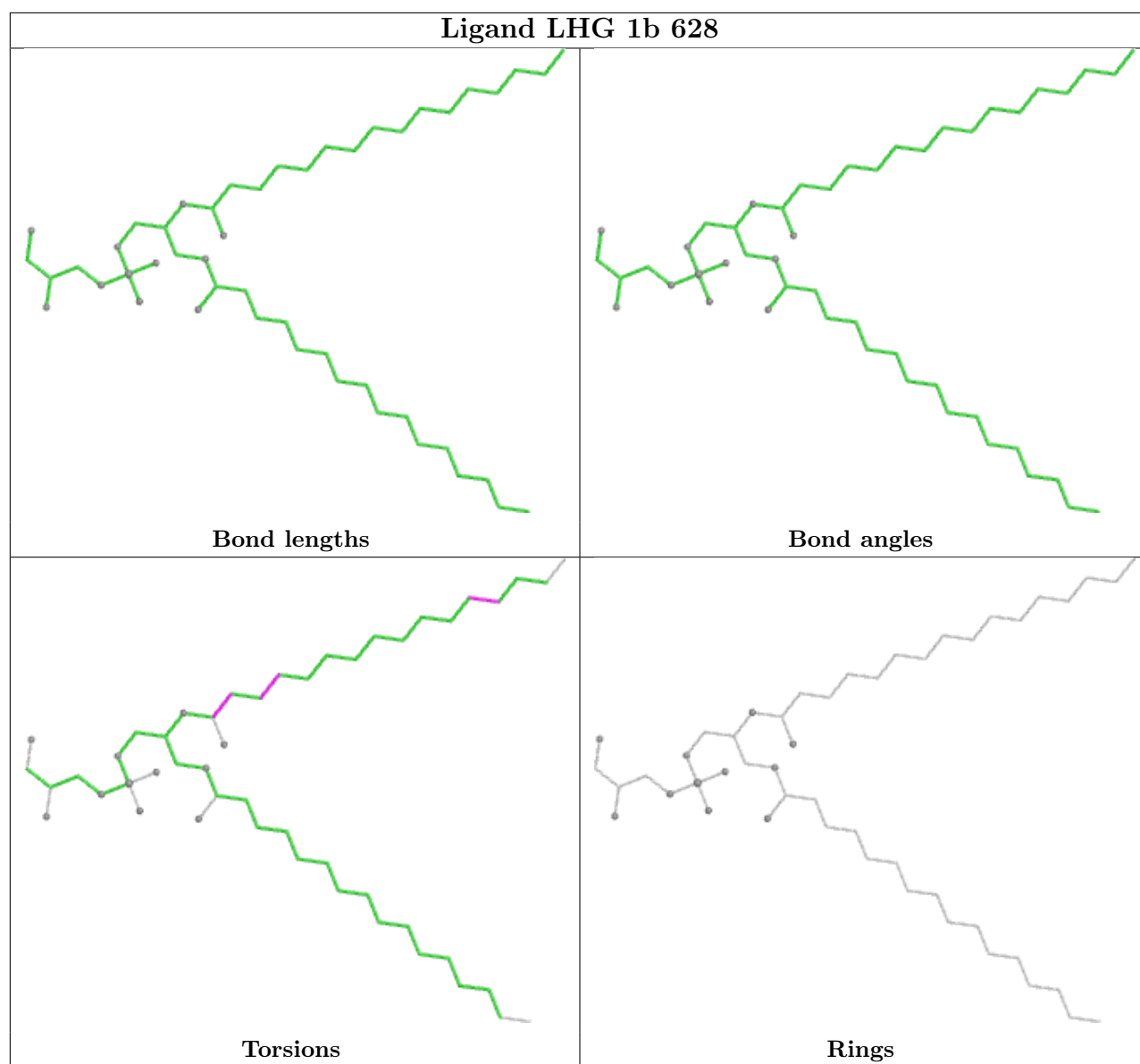


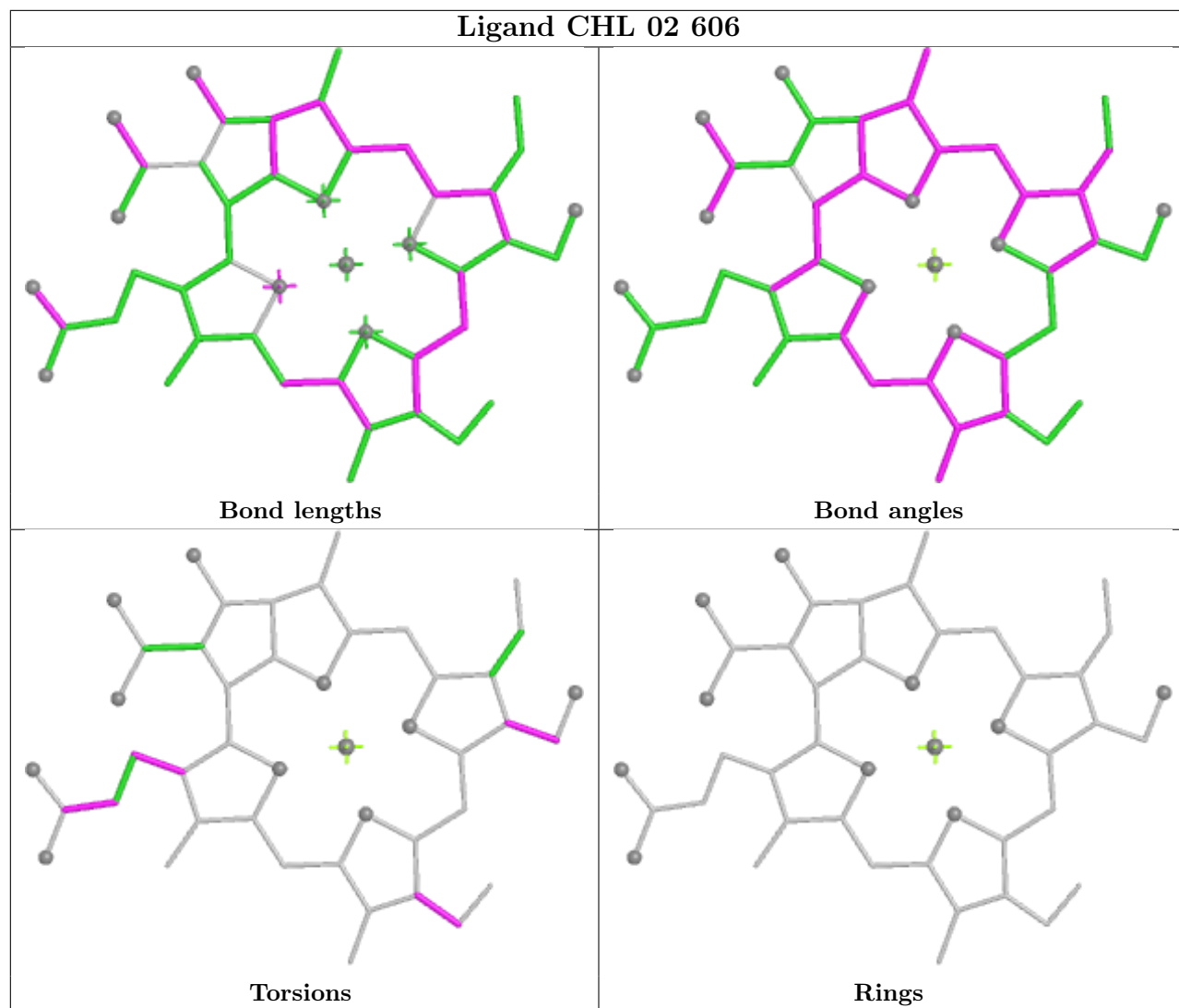




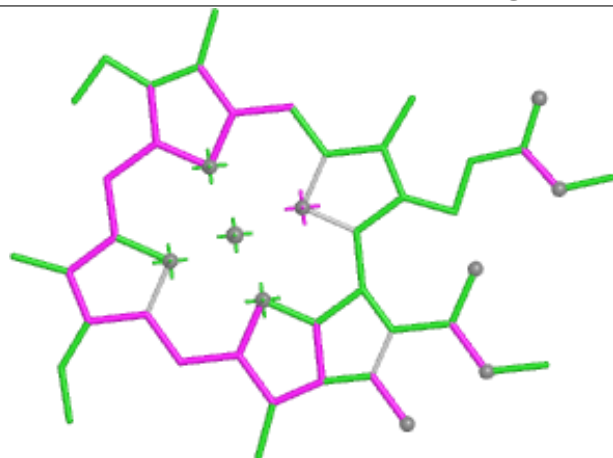




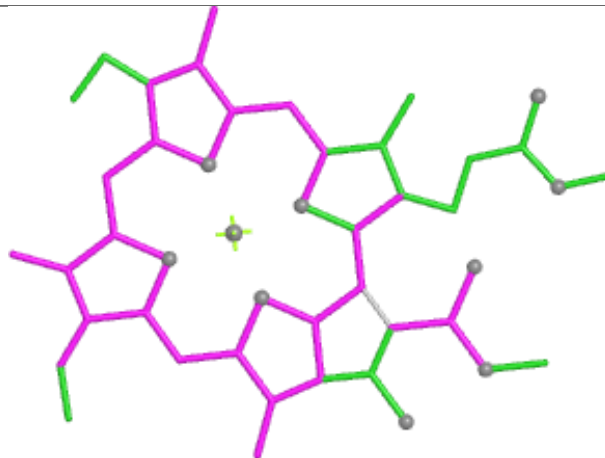




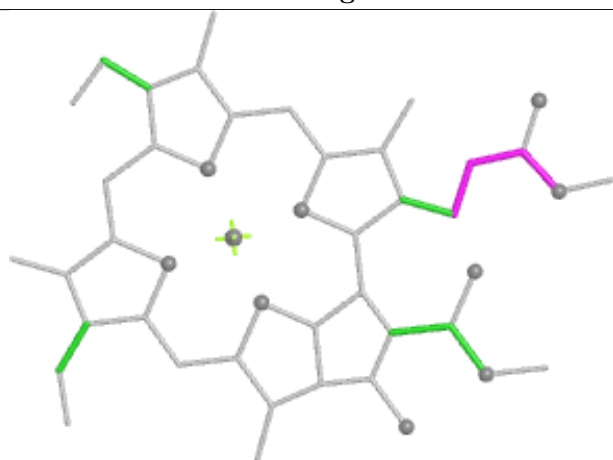
Ligand CLA 1R 314



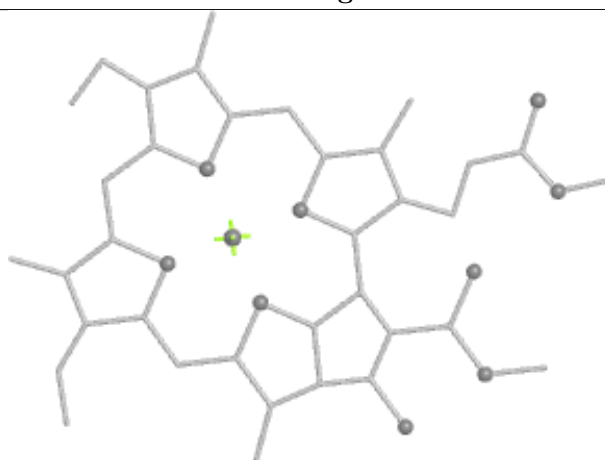
Bond lengths



Bond angles

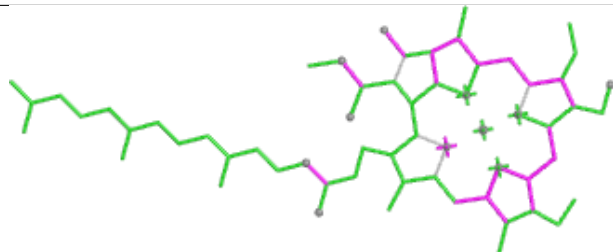


Torsions

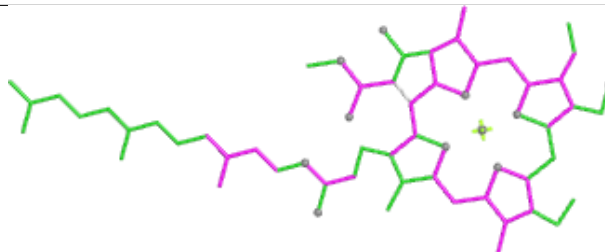


Rings

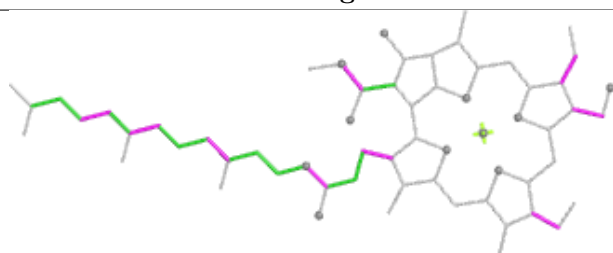
Ligand CHL 09 308



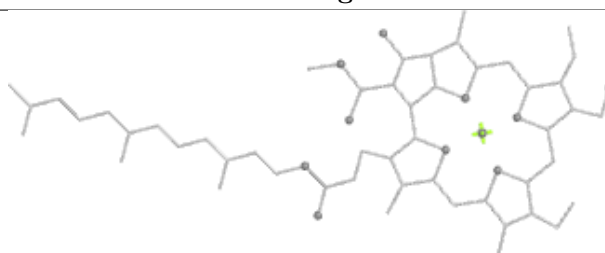
Bond lengths



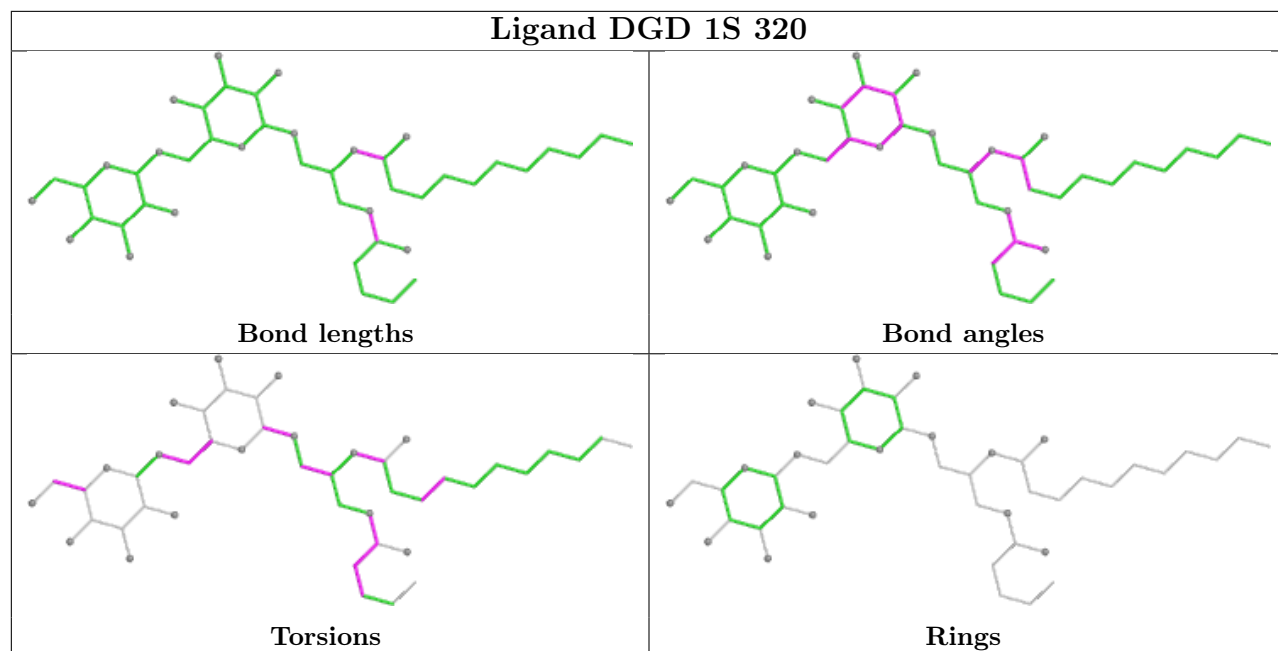
Bond angles

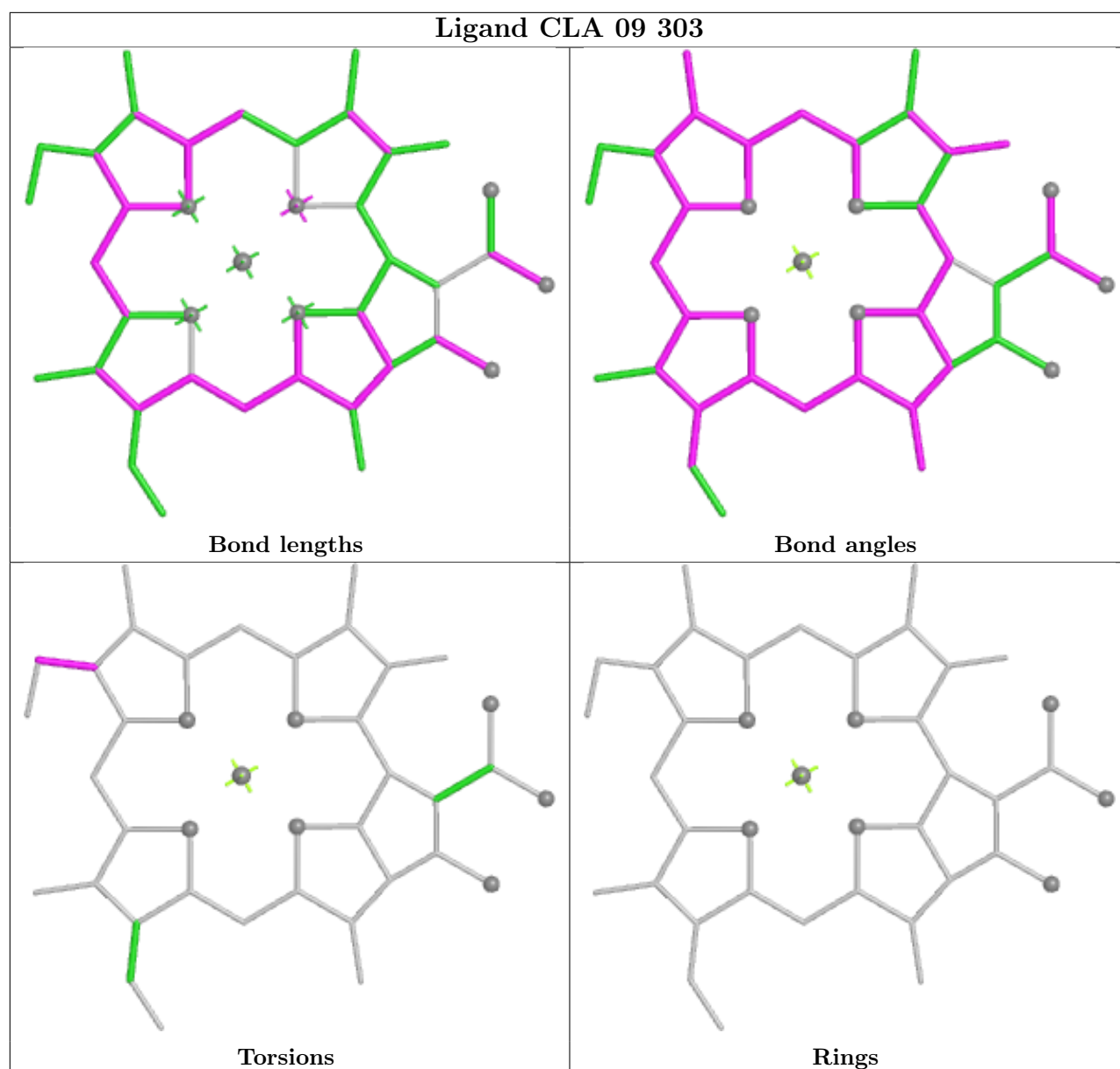


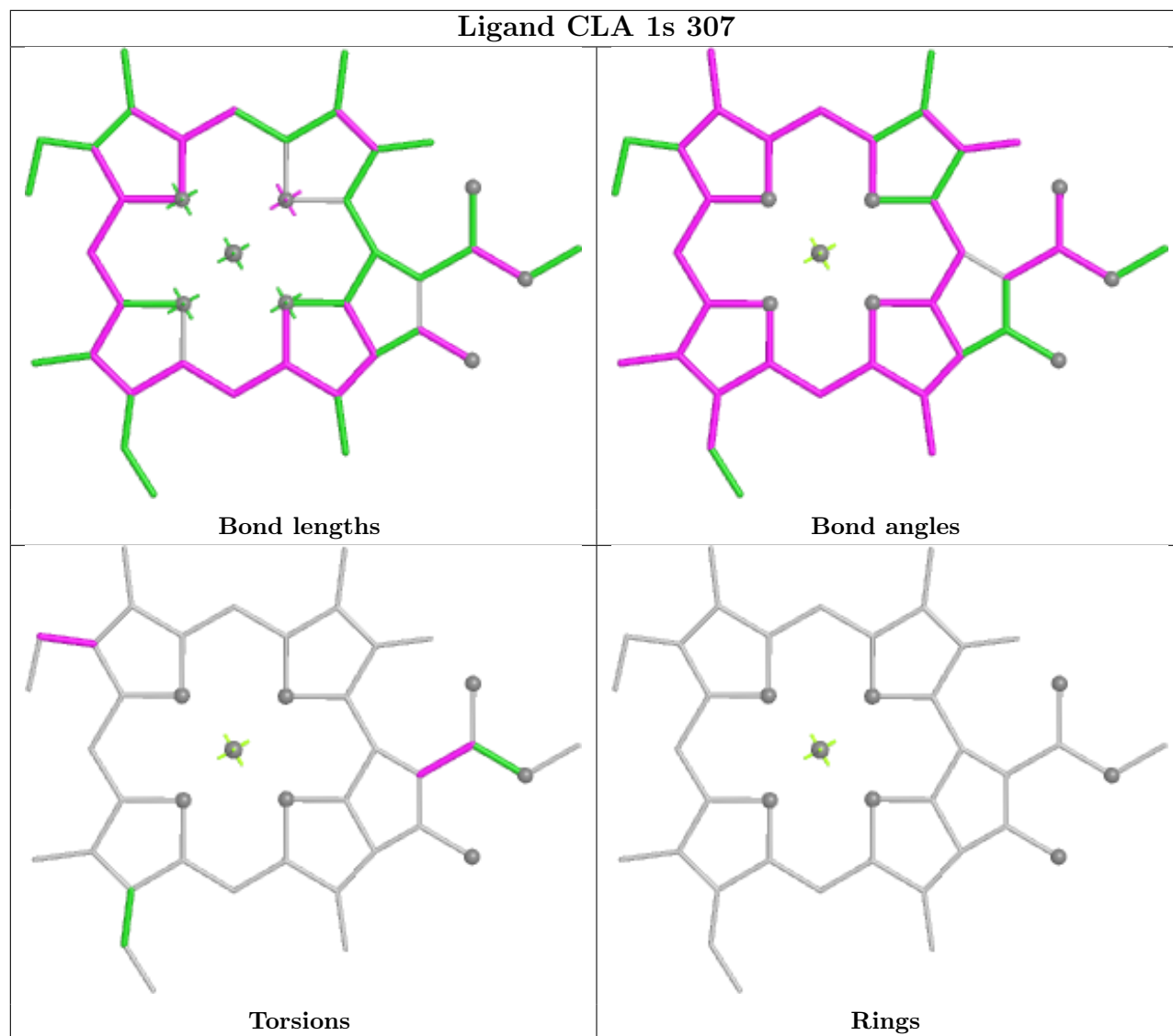
Torsions

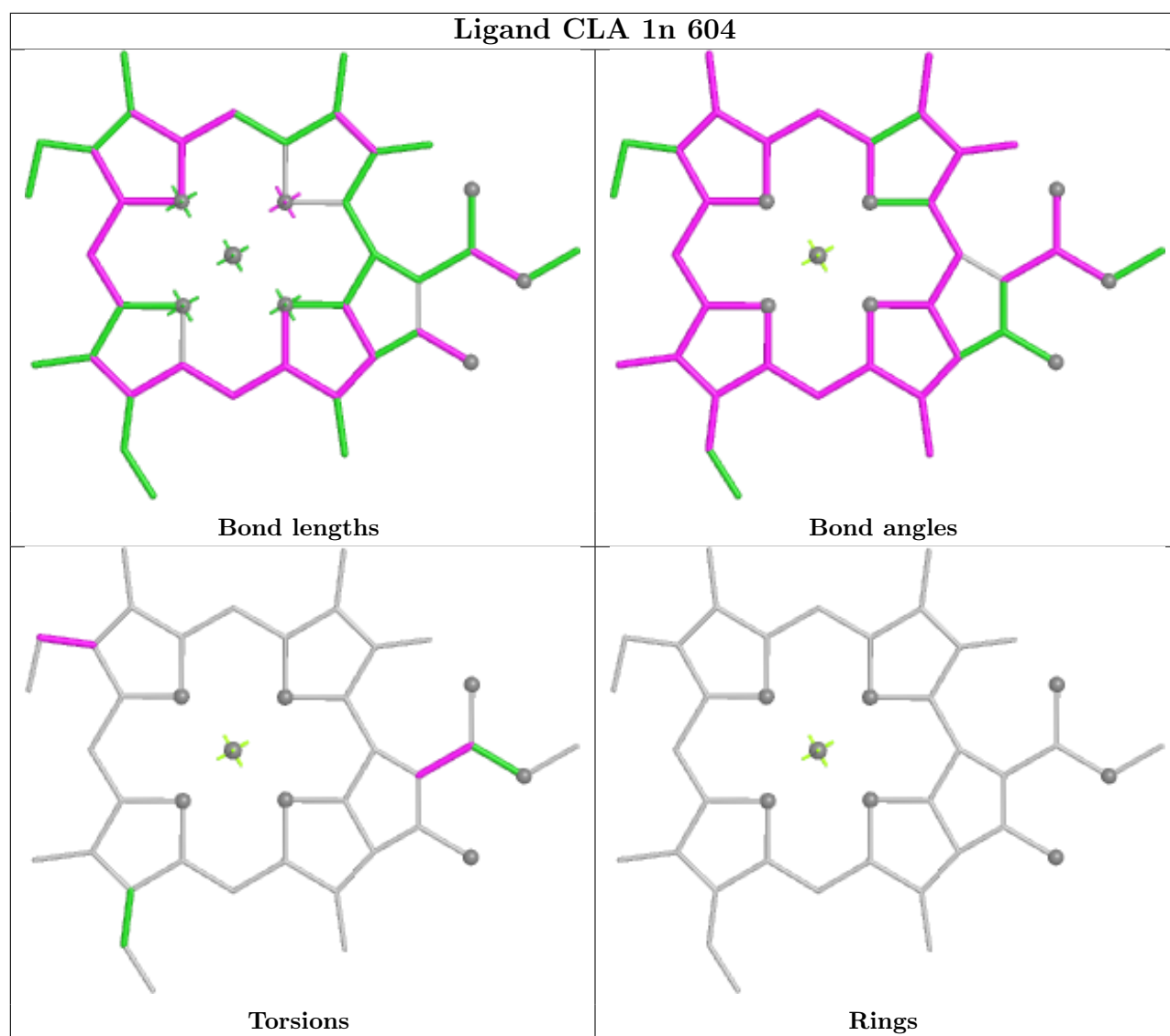


Rings









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.

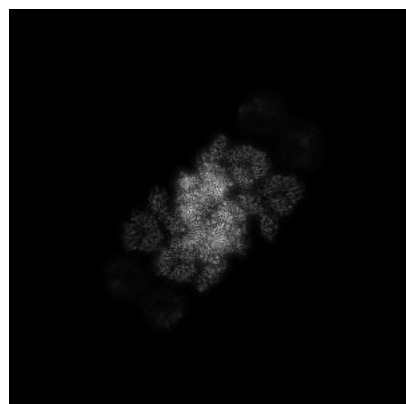
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-68060. These allow visual inspection of the internal detail of the map and identification of artifacts.

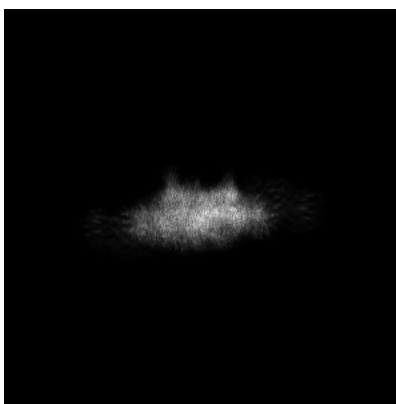
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

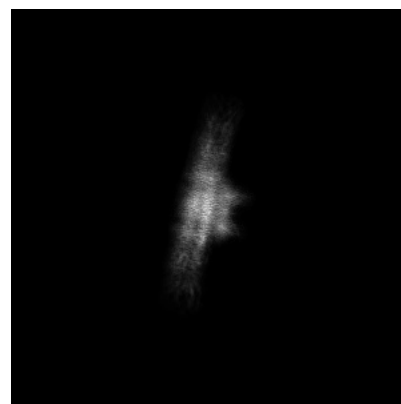
6.1.1 Primary map



X

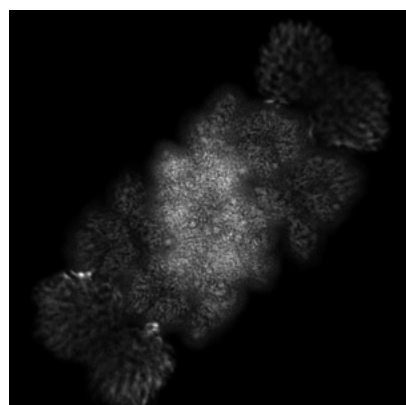


Y

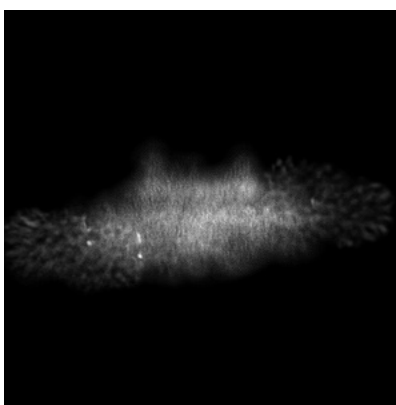


Z

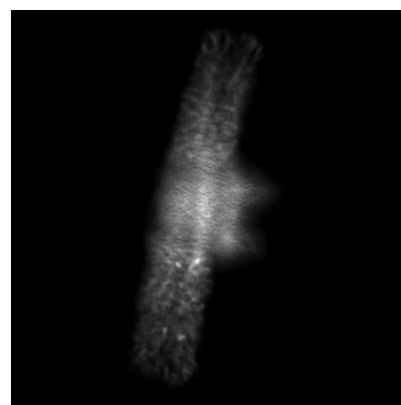
6.1.2 Raw map



X



Y

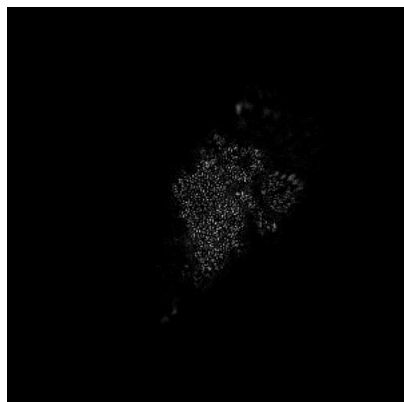


Z

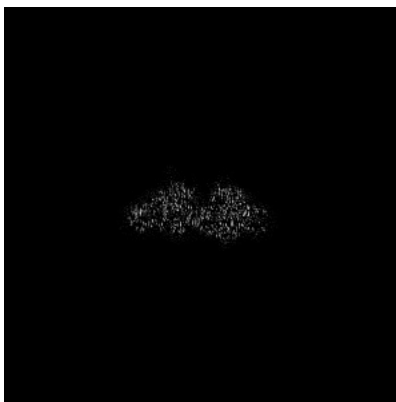
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

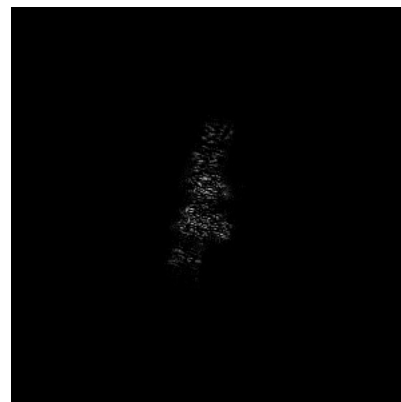
6.2.1 Primary map



X Index: 400

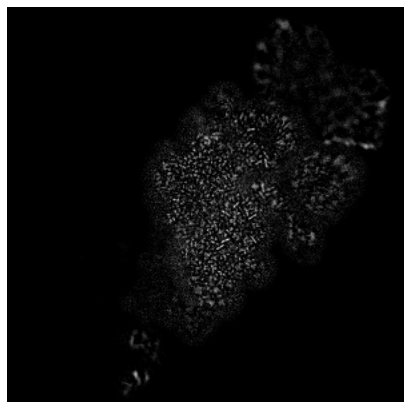


Y Index: 400

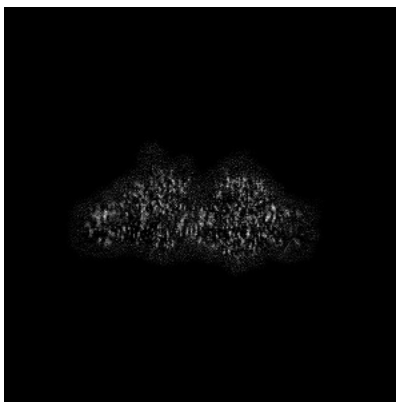


Z Index: 400

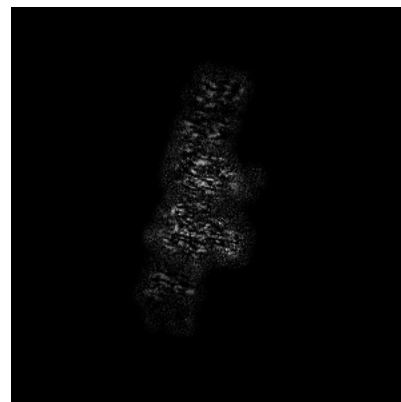
6.2.2 Raw map



X Index: 256



Y Index: 256

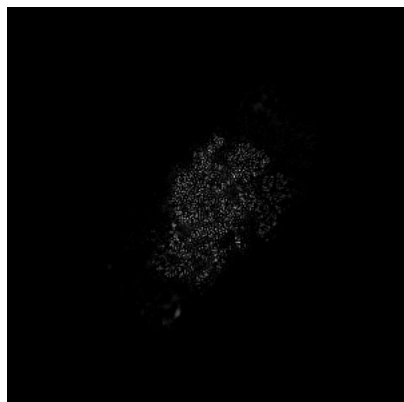


Z Index: 256

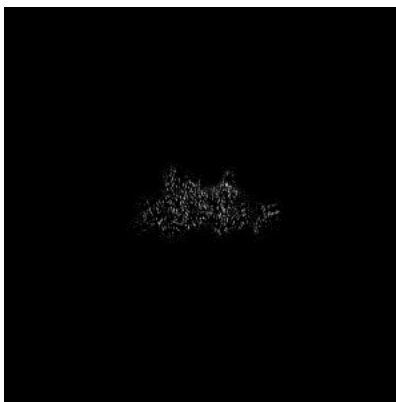
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

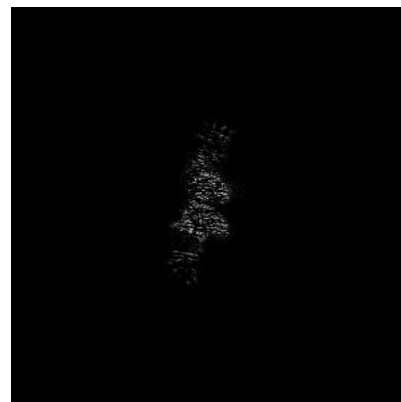
6.3.1 Primary map



X Index: 384

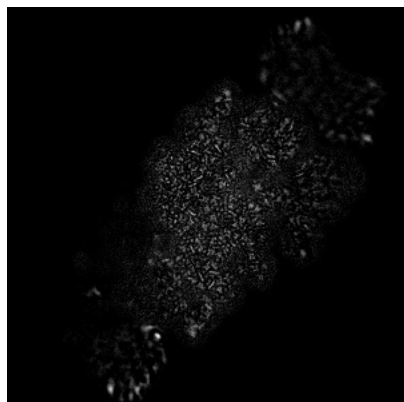


Y Index: 424

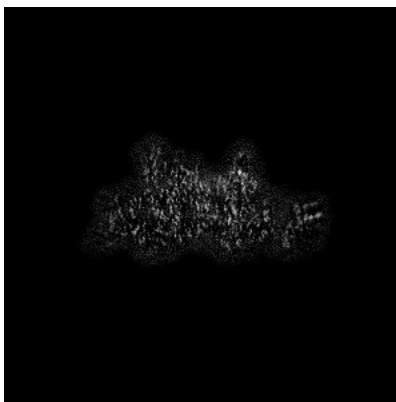


Z Index: 395

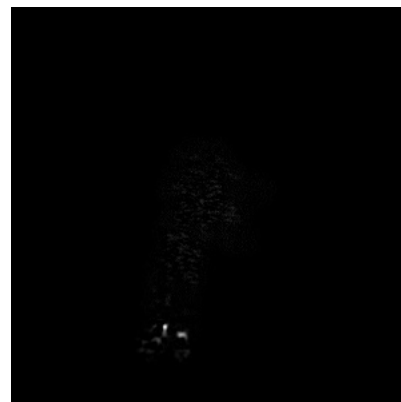
6.3.2 Raw map



X Index: 245



Y Index: 280

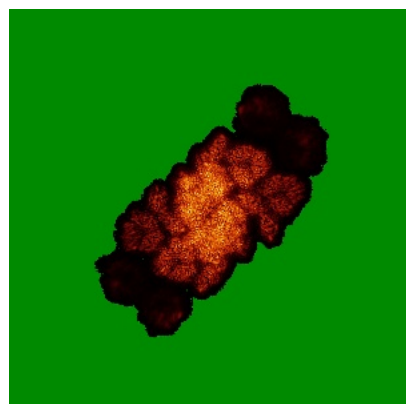


Z Index: 173

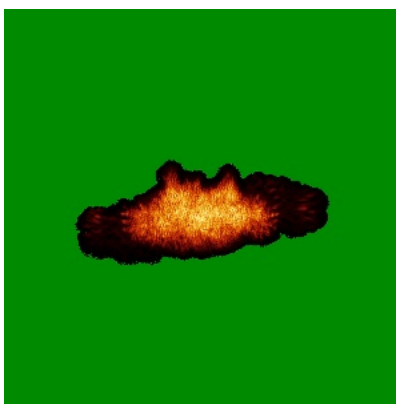
The images above show the largest variance slices of the map in three orthogonal directions.

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

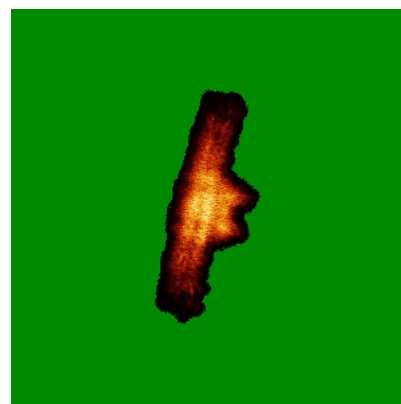
6.4.1 Primary map



X

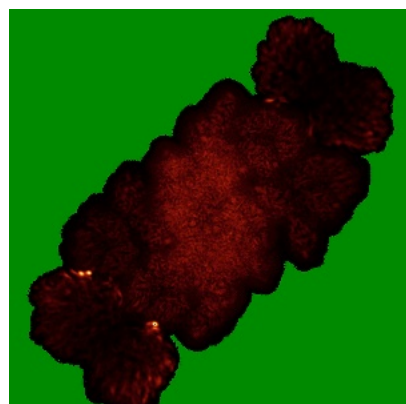


Y

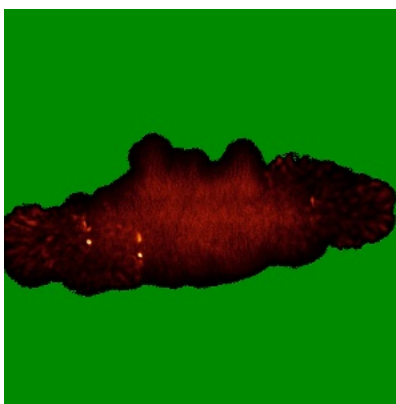


Z

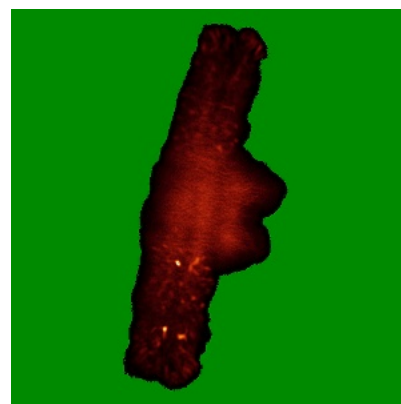
6.4.2 Raw map



X



Y

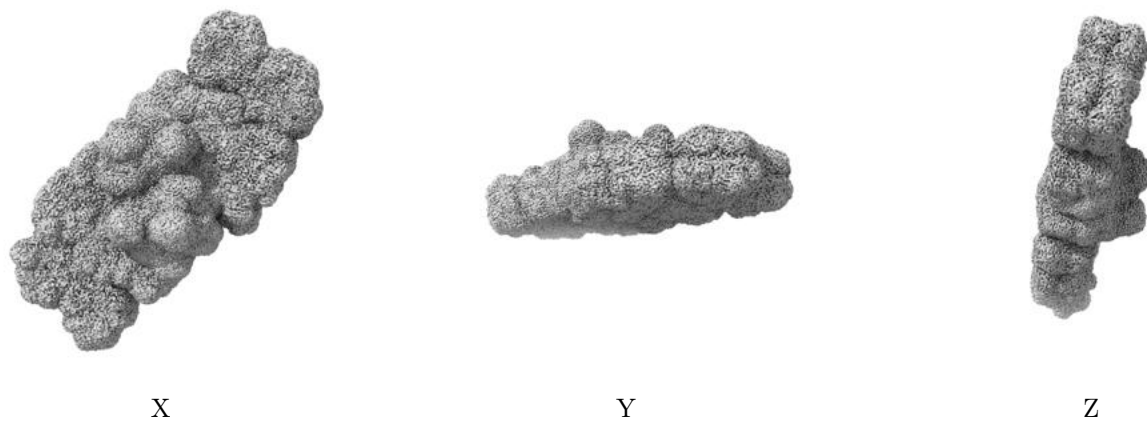


Z

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.

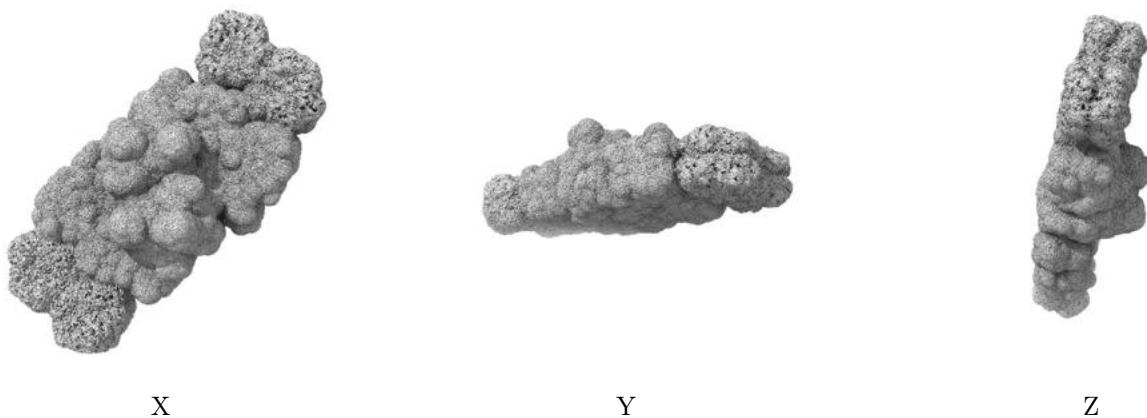
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0004. 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.

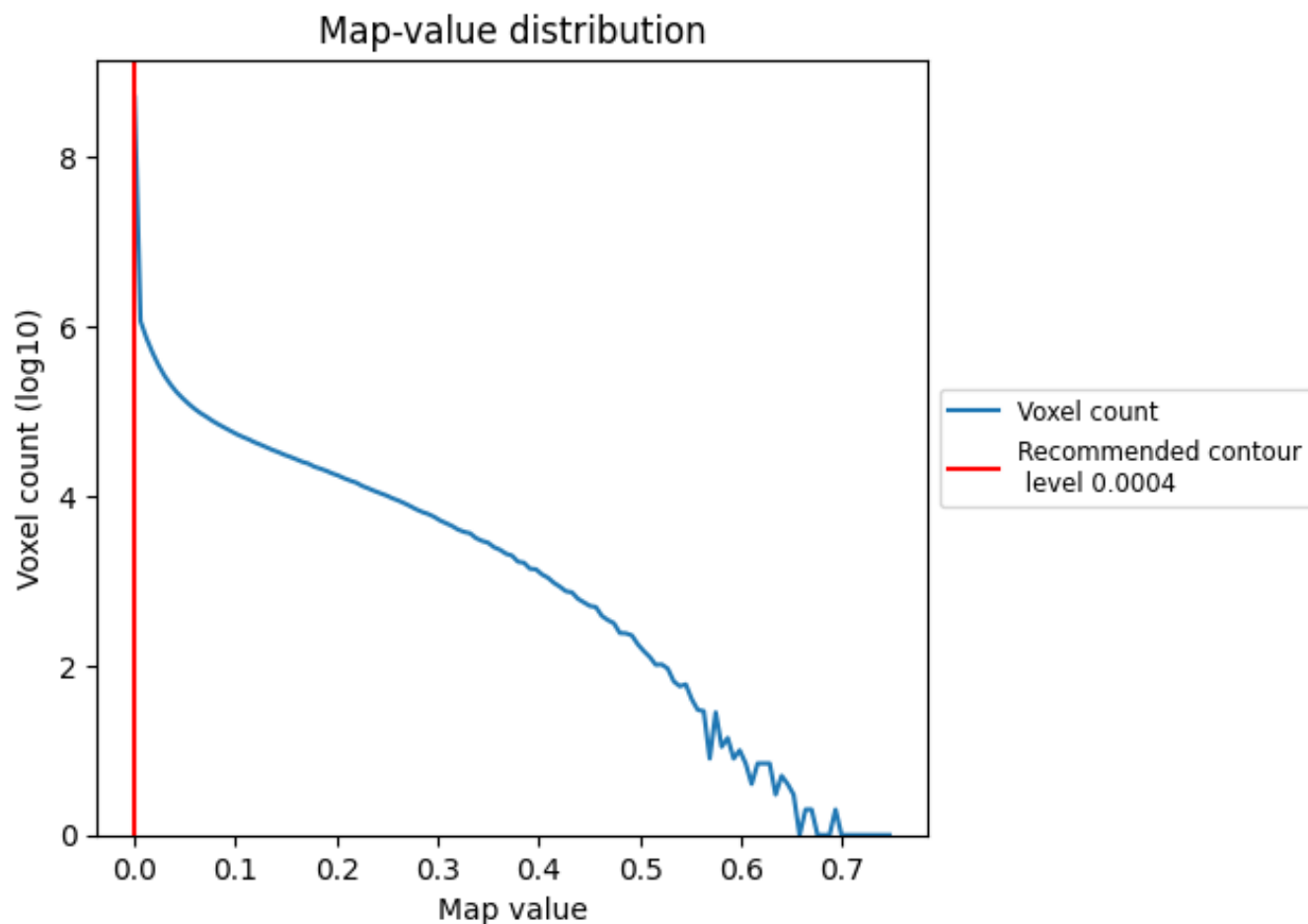
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

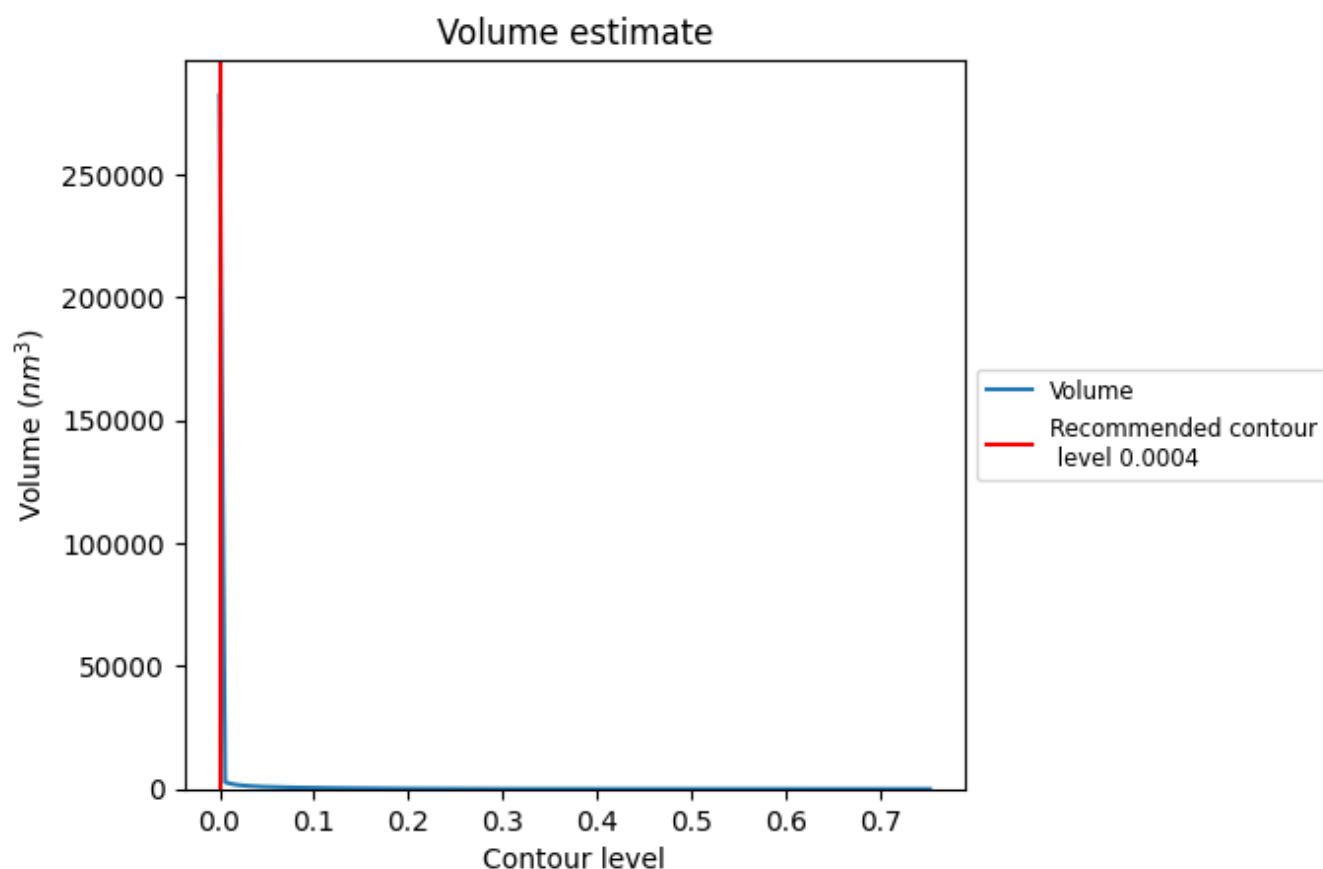
This section contains the results of statistical analysis of the map.

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.

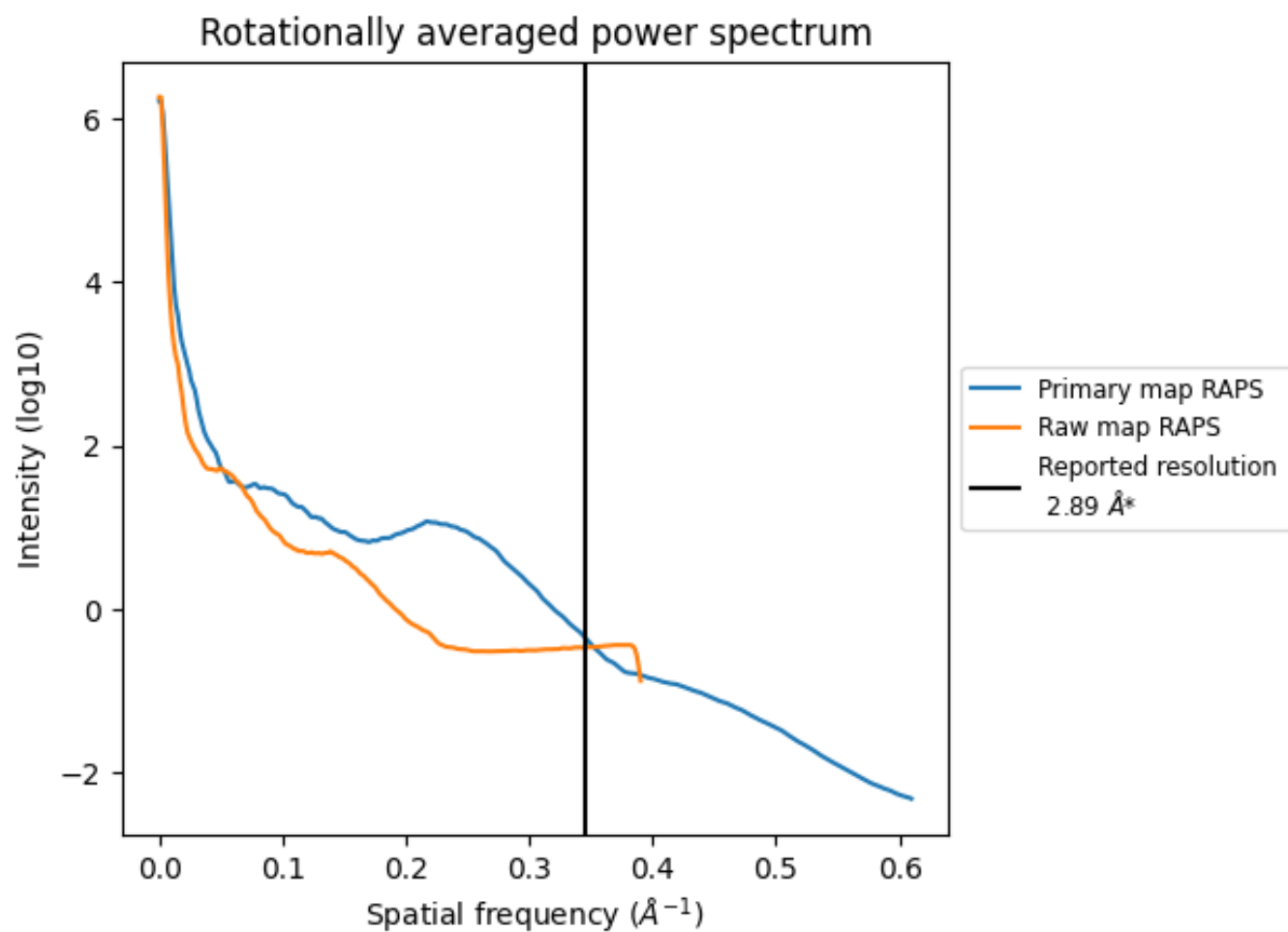
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 263293 nm^3 ; this corresponds to an approximate mass of 237839 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 ⓘ

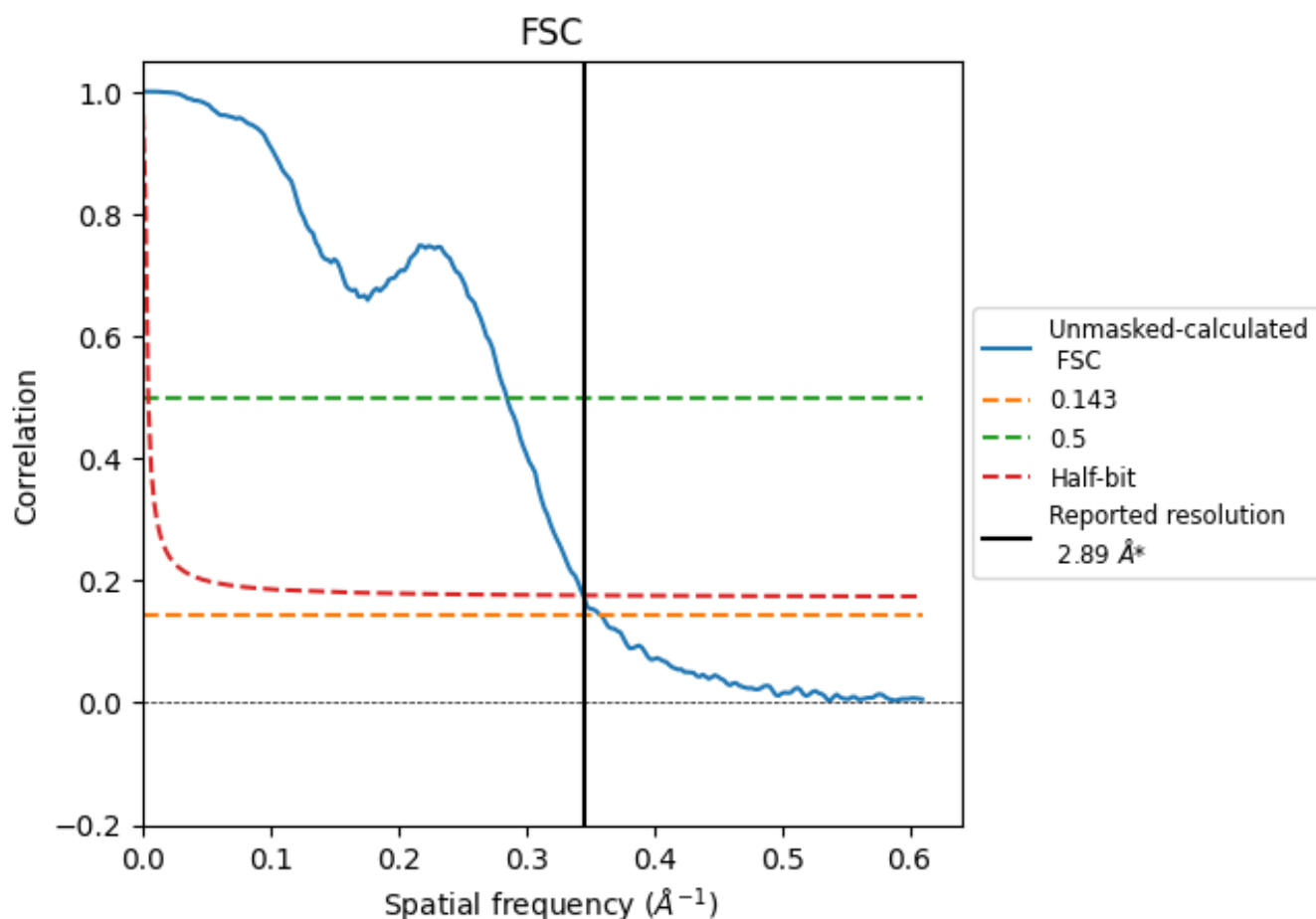


*Reported resolution corresponds to spatial frequency of 0.346 Å⁻¹

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 0.346 Å⁻¹

8.2 Resolution estimates [i](#)

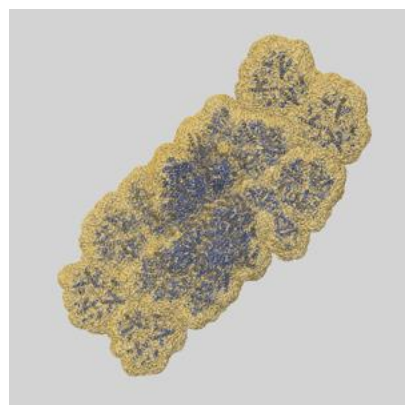
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.89	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.79	3.51	2.90

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

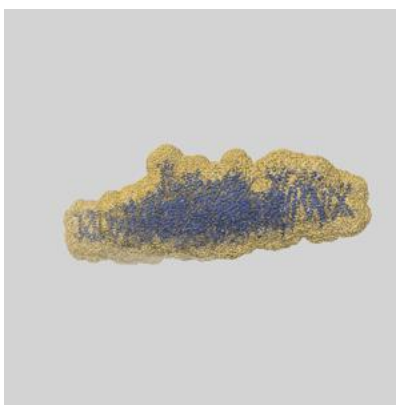
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-68060 and PDB model 21WV. Per-residue inclusion information can be found in [section 3](#) on [page 48](#).

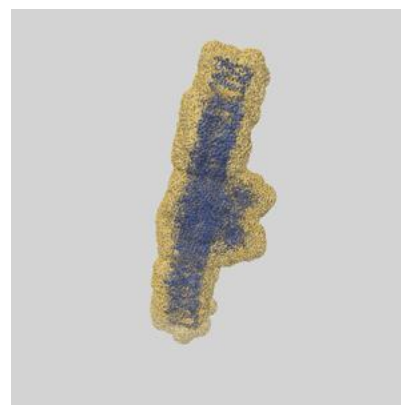
9.1 Map-model overlay [i](#)



X



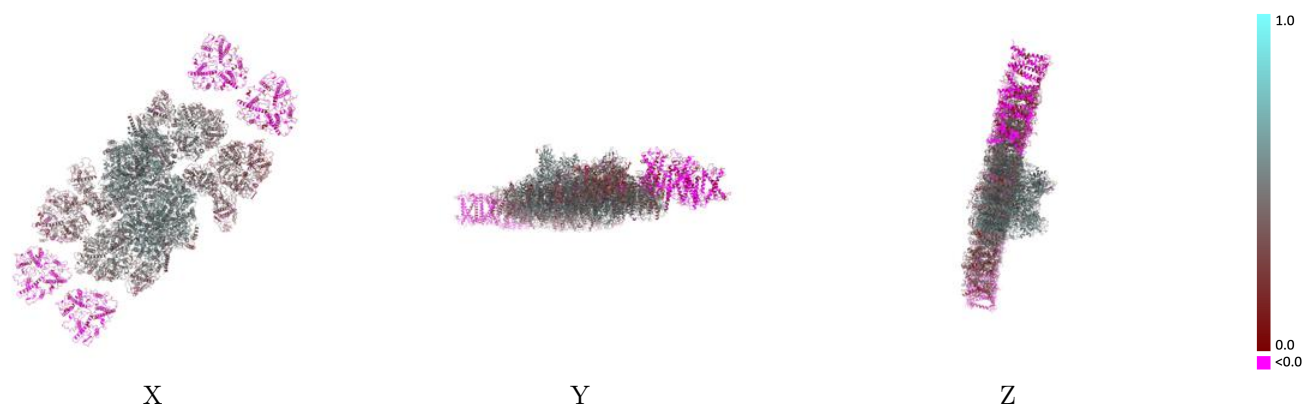
Y



Z

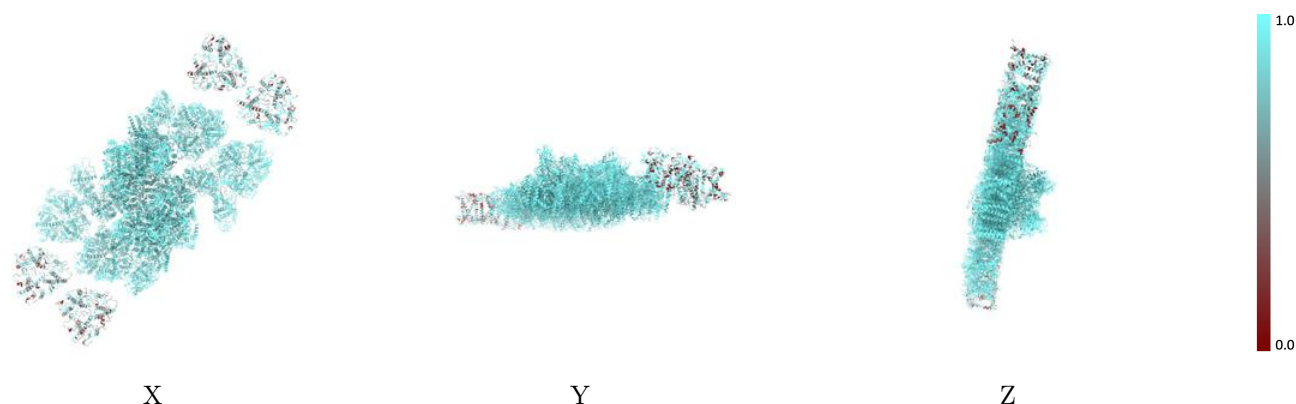
The images above show the 3D surface view of the map at the recommended contour level 0.0004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



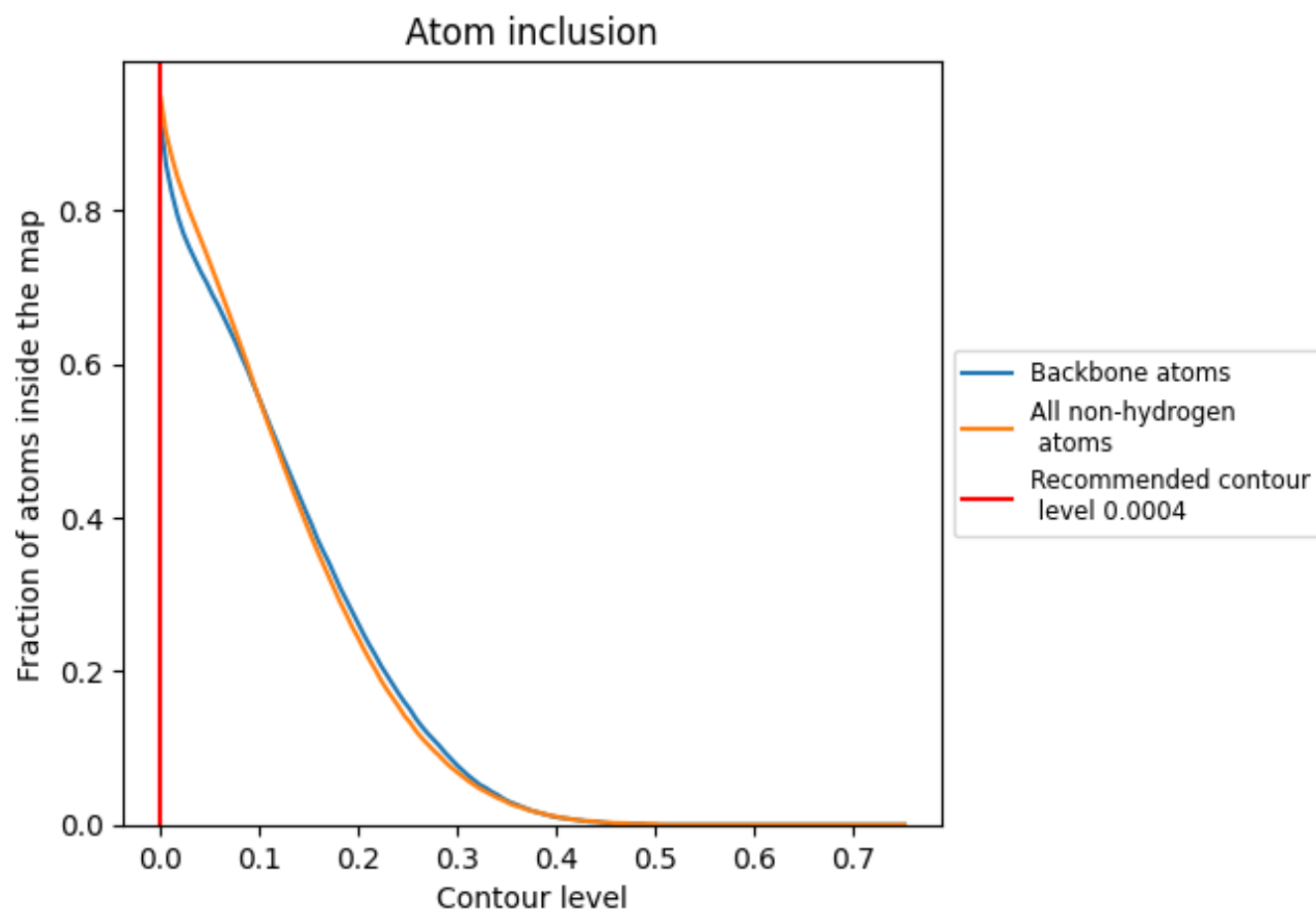
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0004).

9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 95% 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 (0.0004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9470	 0.3800
00	 0.9970	 0.4430
01	 0.9800	 0.3150
02	 0.9720	 0.2450
03	 0.9810	 0.3180
04	 0.9650	 0.2730
05	 0.9740	 0.3000
06	 0.9610	 0.2300
07	 0.9630	 0.2850
08	 0.9710	 0.2990
09	 0.9950	 0.4360
11	 0.5760	 -0.0760
12	 0.5830	 -0.0680
13	 0.6250	 -0.0570
14	 0.6740	 -0.0620
15	 0.6350	 -0.0590
16	 0.6030	 -0.0450
17	 0.6470	 -0.0370
18	 0.6310	 -0.0240
19	 0.6320	 -0.0630
1A	 0.9980	 0.5250
1B	 1.0000	 0.5300
1C	 0.9990	 0.5330
1D	 0.9990	 0.5480
1E	 0.9990	 0.5150
1F	 1.0000	 0.5250
1G	 0.9900	 0.3870
1H	 0.9980	 0.4890
1I	 1.0000	 0.5140
1J	 0.9970	 0.5010
1K	 0.9970	 0.5020
1L	 1.0000	 0.5260
1M	 1.0000	 0.5010
1N	 0.9930	 0.4150
1O	 1.0000	 0.4690



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Chain	Atom inclusion	Q-score
1P	 1.0000	 0.5030
1R	 0.9930	 0.3970
1S	 0.9840	 0.3590
1T	 1.0000	 0.5470
1U	 1.0000	 0.5070
1V	 0.9890	 0.3880
1W	 0.9960	 0.4520
1X	 0.9940	 0.4850
1Y	 0.9920	 0.4170
1Z	 0.9950	 0.3940
1a	 1.0000	 0.5350
1b	 1.0000	 0.5250
1c	 1.0000	 0.5340
1d	 0.9990	 0.5430
1e	 1.0000	 0.5310
1f	 1.0000	 0.5390
1g	 0.9920	 0.3950
1h	 1.0000	 0.5080
1i	 1.0000	 0.5150
1j	 1.0000	 0.4970
1k	 0.9950	 0.5150
1l	 1.0000	 0.5380
1m	 1.0000	 0.5010
1n	 0.9920	 0.4040
1o	 0.9970	 0.4850
1p	 1.0000	 0.4930
1r	 0.9930	 0.3660
1s	 0.9800	 0.3510
1t	 1.0000	 0.5370
1u	 1.0000	 0.4780
1v	 0.9890	 0.3480
1w	 0.9940	 0.4680
1x	 1.0000	 0.4910
1y	 0.9920	 0.4020
1z	 0.9940	 0.3900
20	 0.6930	 -0.0220
21	 0.6490	 -0.0440
22	 0.7030	 -0.0350