



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 01:56 AM UTC

PDB ID : 6L4T / pdb_00006l4t
EMDB ID : EMD-0834
Title : Structure of the peripheral FCPI from diatom
Authors : Nagao, R.; Kato, K.; Miyazaki, N.; Akita, F.; Shen, J.R.
Deposited on : 2019-10-21
Resolution : 2.60 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:

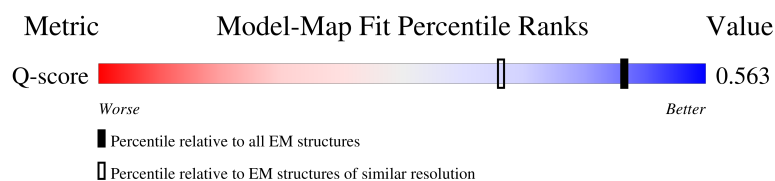
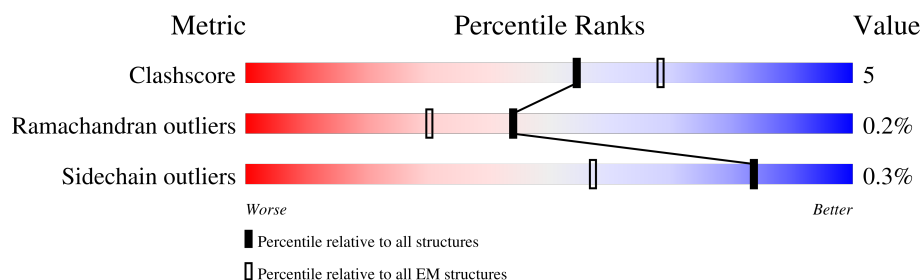
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.60 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.



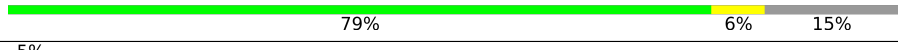
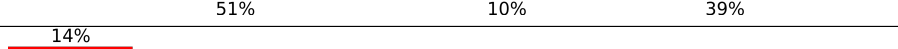
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 (2.10 - 3.10)

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	6	208	
2	7	296	
3	8	270	
4	10	207	

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Mol	Chain	Length	Quality of chain
5	11	229	
6	12	204	
7	13	244	
8	14	249	
9	15	281	
10	16	218	

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
11	CLA	10	304	X	-	-	-
11	CLA	10	305	X	-	-	-
11	CLA	10	307	X	-	-	-
11	CLA	10	308	X	-	-	-
11	CLA	10	309	X	-	-	-
11	CLA	11	305	X	-	-	-
11	CLA	11	307	X	-	-	-
11	CLA	11	309	X	-	-	-
11	CLA	12	303	X	-	-	-
11	CLA	12	304	X	-	-	-
11	CLA	12	306	X	-	-	-
11	CLA	12	307	X	-	-	-
11	CLA	12	308	X	-	-	-
11	CLA	12	312	X	-	-	-
11	CLA	12	321	X	-	-	-
11	CLA	13	302	X	-	-	-
11	CLA	13	307	X	-	-	-
11	CLA	13	309	X	-	-	-
11	CLA	14	302	X	-	-	-
11	CLA	14	303	X	-	-	-
11	CLA	14	304	X	-	-	-
11	CLA	14	305	X	-	-	-
11	CLA	14	309	X	-	-	-
11	CLA	14	310	X	-	-	-
11	CLA	14	313	X	-	-	-
11	CLA	15	303	X	-	-	-
11	CLA	15	304	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	15	305	X	-	-	-
11	CLA	15	306	X	-	-	-
11	CLA	15	307	X	-	-	-
11	CLA	15	308	X	-	-	-
11	CLA	15	309	X	-	-	-
11	CLA	15	310	X	-	-	-
11	CLA	15	311	X	-	-	-
11	CLA	15	312	X	-	-	-
11	CLA	16	302	X	-	-	-
11	CLA	16	303	X	-	-	-
11	CLA	16	305	X	-	-	-
11	CLA	16	306	X	-	-	-
11	CLA	16	307	X	-	-	-
11	CLA	16	308	X	-	-	-
11	CLA	16	310	X	-	-	-
11	CLA	6	301	X	-	-	-
11	CLA	6	302	X	-	-	-
11	CLA	6	303	X	-	-	-
11	CLA	6	304	X	-	-	-
11	CLA	6	306	X	-	-	-
11	CLA	6	307	X	-	-	-
11	CLA	6	312	X	-	-	-
11	CLA	6	313	X	-	-	-
11	CLA	6	314	X	-	-	-
11	CLA	7	302	X	-	-	-
11	CLA	7	303	X	-	-	-
11	CLA	7	304	X	-	-	-
11	CLA	7	305	X	-	-	-
11	CLA	7	308	X	-	-	-
11	CLA	7	309	X	-	-	-
11	CLA	7	310	X	-	-	-
11	CLA	8	301	X	-	-	-
11	CLA	8	302	X	-	-	-
11	CLA	8	303	X	-	-	-
11	CLA	8	304	X	-	-	-
11	CLA	8	308	X	-	-	-

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 23863 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 Fucoxanthin chlorophyll a/c-binding protein Lhcr12.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	6	174	Total	C	N	O	S	0	0
			1354	884	216	246	8		

- Molecule 2 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr10.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	7	188	Total	C	N	O	S	0	0
			1416	894	240	266	16		

- Molecule 3 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	8	213	Total	C	N	O	S	0	0
			1660	1075	274	302	9		

- Molecule 4 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	10	169	Total	C	N	O	S	0	0
			1302	849	212	233	8		

- Molecule 5 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq13.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	11	191	Total	C	N	O	S	0	0
			1479	958	243	270	8		

- Molecule 6 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	12	173	Total	C	N	O	S	0	0
			1274	814	209	243	8		

- Molecule 7 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq11.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	13	150	Total	C	N	O	S	0	0
			1148	736	203	204	5		

- Molecule 8 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	14	208	Total	C	N	O	S	0	0
			1609	1049	262	292	6		

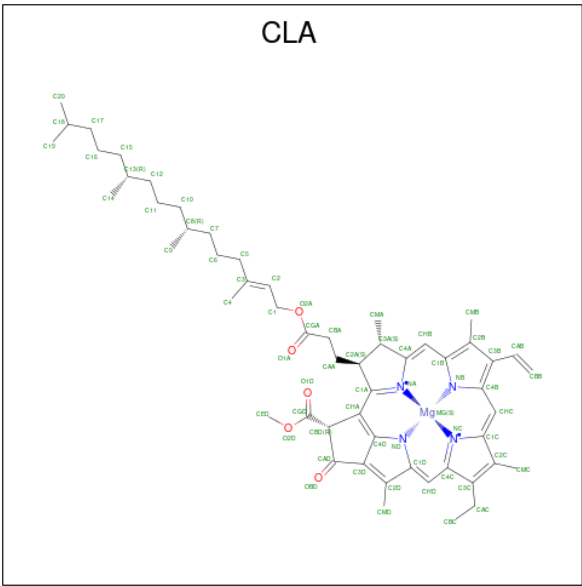
- Molecule 9 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	15	211	Total	C	N	O	S	0	0
			1654	1077	273	298	6		

- Molecule 10 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	16	174	Total	C	N	O	S	0	0
			1313	846	217	242	8		

- Molecule 11 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
11	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
11	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
11	8	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
11	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	8	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
11	10	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	10	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	10	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	10	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	10	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	10	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	11	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	11	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	11	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	11	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	11	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	12	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
11	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	13	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	13	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	13	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	14	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	14	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
11	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	14	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
11	14	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	14	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
11	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	14	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
11	15	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	15	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
11	15	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	15	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
11	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	15	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	15	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	16	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	16	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	16	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	16	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
11	16	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
11	16	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
11	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 12 is Chlorophyll c1 (CCD ID: KC1) (formula: $C_{35}H_{30}MgN_4O_5$).

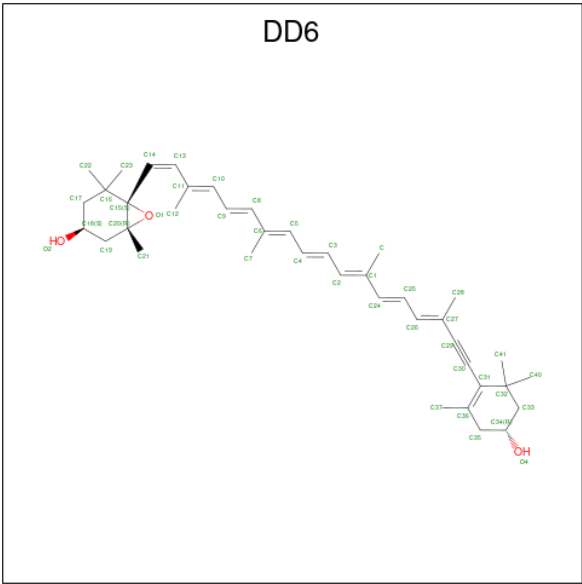


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Mol	Chain	Residues	Atoms					AltConf
12	10	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	10	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	16	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	16	1	Total 45	C 35	Mg 1	N 4	O 5	0

- Molecule 13 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene -3,3'-diol (CCD ID: DD6) (formula: C₄₀H₅₄O₃).



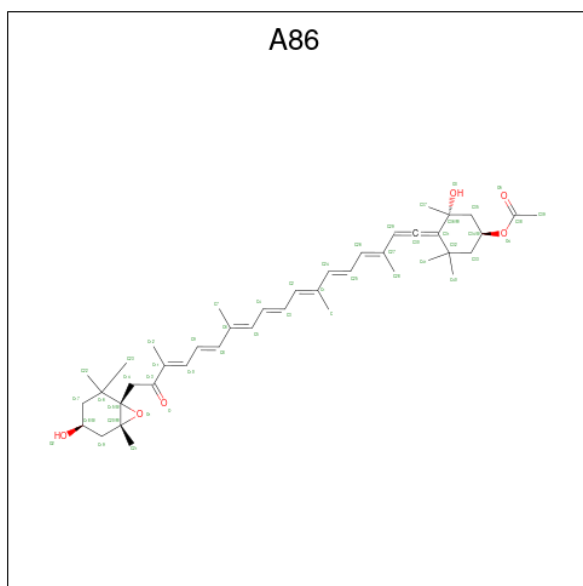
Mol	Chain	Residues	Atoms			AltConf
13	6	1	Total	C	O	0
			43	40	3	
13	6	1	Total	C	O	0
			43	40	3	
13	6	1	Total	C	O	0
			43	40	3	
13	7	1	Total	C	O	0
			43	40	3	
13	7	1	Total	C	O	0
			43	40	3	
13	7	1	Total	C	O	0
			43	40	3	
13	7	1	Total	C	O	0
			43	40	3	
13	8	1	Total	C	O	0
			43	40	3	
13	8	1	Total	C	O	0
			43	40	3	
13	10	1	Total	C	O	0
			43	40	3	
13	10	1	Total	C	O	0
			43	40	3	
13	11	1	Total	C	O	0
			43	40	3	

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Mol	Chain	Residues	Atoms			AltConf
13	12	1	Total	C	O	0
			43	40	3	
13	12	1	Total	C	O	0
			43	40	3	
13	13	1	Total	C	O	0
			43	40	3	
13	15	1	Total	C	O	0
			43	40	3	
13	15	1	Total	C	O	0
			43	40	3	
13	16	1	Total	C	O	0
			43	40	3	

- Molecule 14 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'-yl acetate (CCD ID: A86) (formula: C₄₂H₅₈O₆).



Mol	Chain	Residues	Atoms			AltConf
14	6	1	Total	C	O	0
			48	42	6	
14	7	1	Total	C	O	0
			48	42	6	
14	7	1	Total	C	O	0
			48	42	6	
14	7	1	Total	C	O	0
			48	42	6	
14	8	1	Total	C	O	0
			48	42	6	

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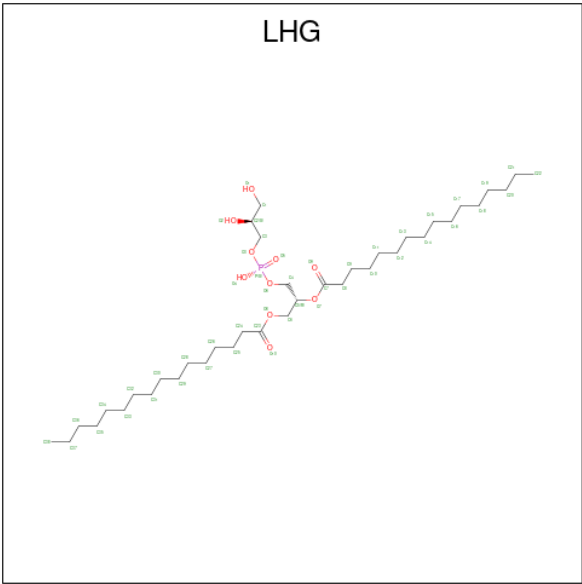
Mol	Chain	Residues	Atoms			AltConf
14	8	1	Total	C	O	0
			48	42	6	
14	10	1	Total	C	O	0
			48	42	6	
14	10	1	Total	C	O	0
			48	42	6	
14	10	1	Total	C	O	0
			48	42	6	
14	10	1	Total	C	O	0
			48	42	6	
14	10	1	Total	C	O	0
			48	42	6	
14	11	1	Total	C	O	0
			48	42	6	
14	11	1	Total	C	O	0
			48	42	6	
14	11	1	Total	C	O	0
			48	42	6	
14	11	1	Total	C	O	0
			48	42	6	
14	12	1	Total	C	O	0
			48	42	6	
14	12	1	Total	C	O	0
			48	42	6	
14	13	1	Total	C	O	0
			45	40	5	
14	13	1	Total	C	O	0
			48	42	6	
14	14	1	Total	C	O	0
			48	42	6	
14	14	1	Total	C	O	0
			48	42	6	
14	14	1	Total	C	O	0
			48	42	6	
14	14	1	Total	C	O	0
			48	42	6	
14	14	1	Total	C	O	0
			48	42	6	
14	14	1	Total	C	O	0
			48	42	6	

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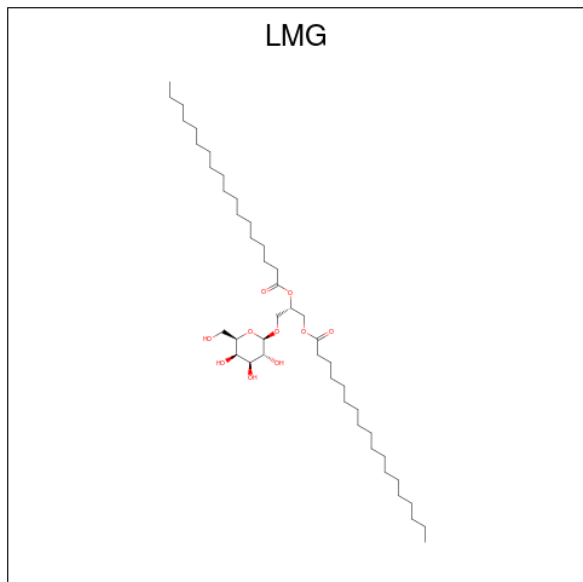
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
14	14	1	48	42	6	0
14	14	1	48	42	6	0
14	15	1	48	42	6	0
14	15	1	48	42	6	0
14	15	1	48	42	6	0
14	15	1	48	42	6	0
14	15	1	48	42	6	0
14	15	1	48	42	6	0
14	16	1	48	42	6	0
14	16	1	48	42	6	0

- Molecule 15 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



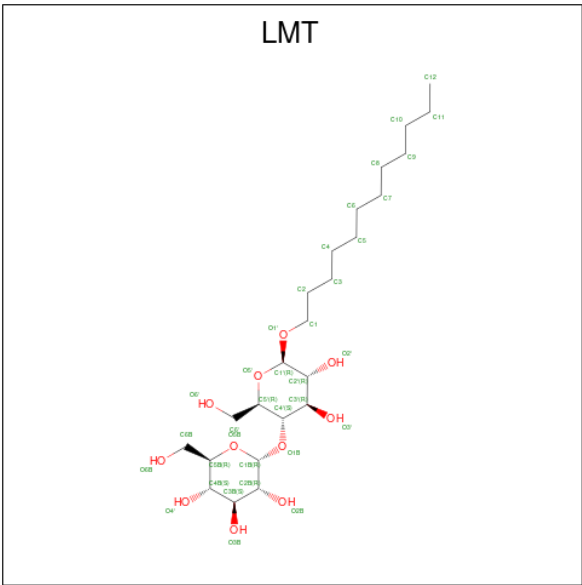
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
15	6	1	27	16	10	1	0

- Molecule 16 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
16	7	1	Total	C	O	0
			37	27	10	
16	8	1	Total	C	O	0
			37	27	10	
16	8	1	Total	C	O	0
			42	32	10	
16	8	1	Total	C	O	0
			29	19	10	
16	14	1	Total	C	O	0
			38	28	10	

- Molecule 17 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
17	7	1	Total	C	O	0
			35	24	11	
17	8	1	Total	C	O	0
			35	24	11	
17	8	1	Total	C	O	0
			35	24	11	
17	8	1	Total	C	O	0
			35	24	11	
17	11	1	Total	C	O	0
			35	24	11	
17	11	1	Total	C	O	0
			35	24	11	
17	12	1	Total	C	O	0
			35	24	11	
17	12	1	Total	C	O	0
			35	24	11	
17	12	1	Total	C	O	0
			35	24	11	
17	12	1	Total	C	O	0
			35	24	11	
17	12	1	Total	C	O	0
			35	24	11	
17	15	1	Total	C	O	0
			35	24	11	
17	16	1	Total	C	O	0
			35	24	11	

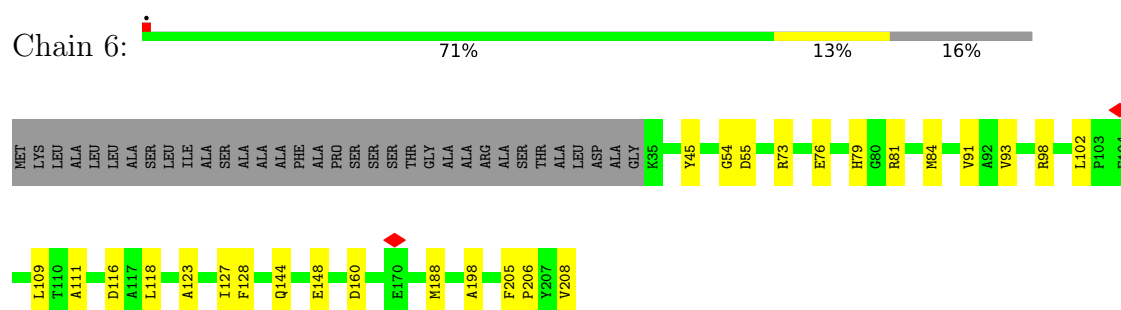
- Molecule 18 is water.

Mol	Chain	Residues	Atoms		AltConf
18	6	2	Total 2	O 2	0
18	7	2	Total 2	O 2	0
18	8	4	Total 4	O 4	0
18	10	1	Total 1	O 1	0
18	11	1	Total 1	O 1	0
18	12	2	Total 2	O 2	0

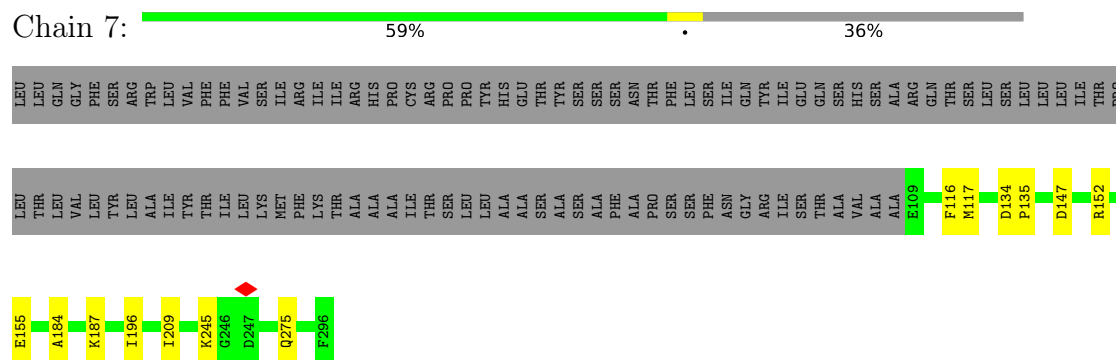
3 Residue-property plots

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.

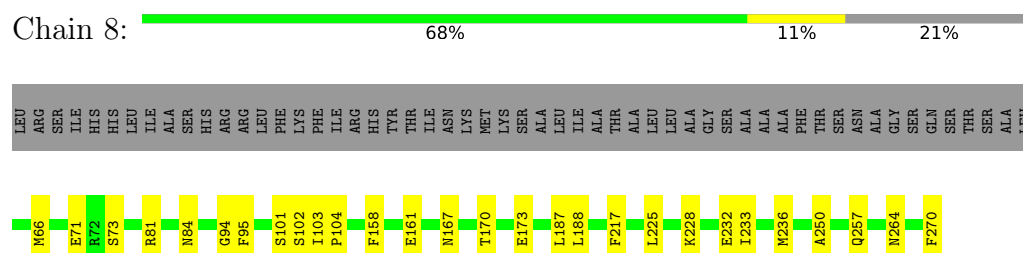
- Molecule 1: Fucoxanthin chlorophyll a/c-binding protein Lhcr12



- Molecule 2: Fucoxanthin chlorophyll a/c-binding protein Lhcr10

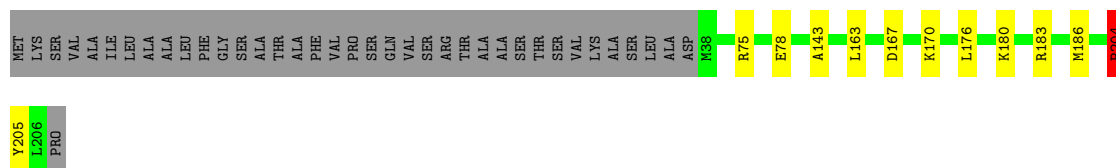


- Molecule 3: Fucoxanthin chlorophyll a/c-binding protein Lhcr4



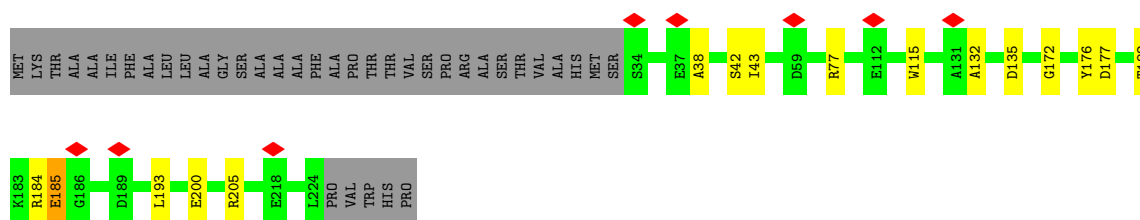
- Molecule 4: Fucoxanthin chlorophyll a/c-binding protein Lhcr3

Chain 10:  76% 5% 18%



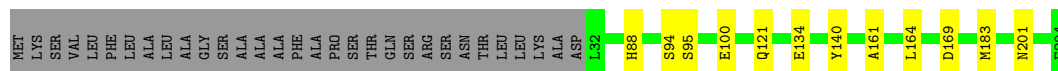
- Molecule 5: Fucoxanthin chlorophyll a/c-binding protein Lhcq13

Chain 11:  76% 7% 17%



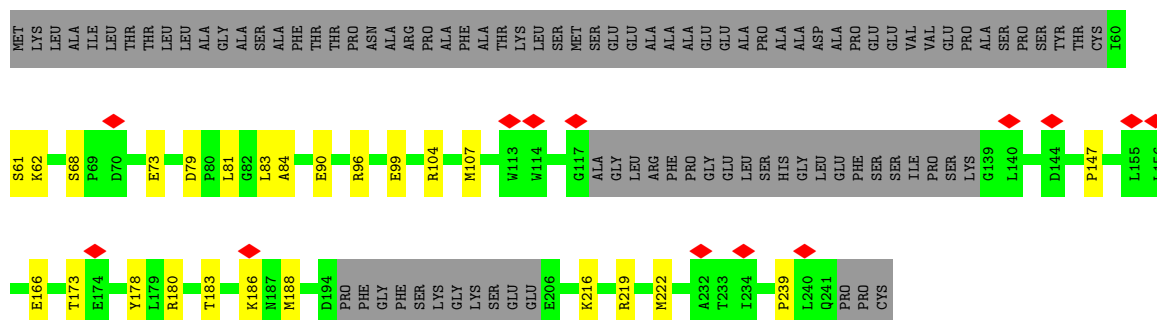
- Molecule 6: Fucoxanthin chlorophyll a/c-binding protein Lhcq3

Chain 12:  79% 6% 15%



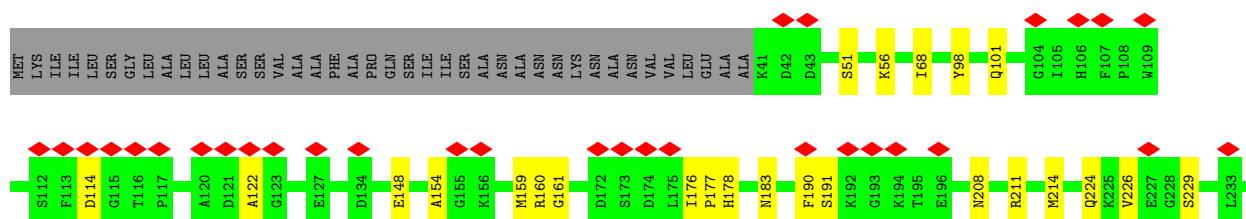
- Molecule 7: Fucoxanthin chlorophyll a/c-binding protein Lhcq11

Chain 13:  5% 51% 10% 39%



- Molecule 8: Fucoxanthin chlorophyll a/c-binding protein Lhcq10

Chain 14:  14% 73% 10% 16%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	470801	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.322	Depositor
Minimum map value	-0.132	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.045	Depositor
Map size ($\text{\AA}$)	560.952, 560.952, 560.952	wwPDB
Map dimensions	504, 504, 504	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.113, 1.113, 1.113	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, DD6, LMT, LHG, LMG, KC1, A86

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	6	0.29	0/1391	0.45	0/1886
2	7	0.28	0/1445	0.45	0/1952
3	8	0.32	0/1706	0.45	0/2310
4	10	0.28	0/1344	0.51	0/1824
5	11	0.25	0/1522	0.48	2/2070 (0.1%)
6	12	0.31	0/1305	0.47	0/1776
7	13	0.22	0/1177	0.53	2/1592 (0.1%)
8	14	0.25	0/1660	0.66	4/2255 (0.2%)
9	15	0.28	0/1705	0.78	10/2319 (0.4%)
10	16	0.23	0/1347	0.55	0/1833
All	All	0.27	0/14602	0.55	18/19817 (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
4	10	0	1
8	14	0	2
9	15	0	3
All	All	0	6

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	15	152	ILE	CA-C-N	6.81	143.34	127.00
9	15	152	ILE	C-N-CA	6.81	143.34	127.00
8	14	122	ALA	CA-C-N	6.41	133.24	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	14	122	ALA	C-N-CA	6.41	133.24	121.70
9	15	141	ALA	CA-C-N	6.38	133.19	121.70

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	10	204	PRO	Peptide
8	14	154	ALA	Peptide
8	14	161	GLY	Peptide
9	15	136	ALA	Peptide
9	15	264	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	6	1354	0	1328	18	0
2	7	1416	0	1379	10	0
3	8	1660	0	1625	21	0
4	10	1302	0	1274	8	0
5	11	1479	0	1452	11	0
6	12	1274	0	1267	8	0
7	13	1148	0	1130	17	0
8	14	1609	0	1568	18	0
9	15	1654	0	1613	19	0
10	16	1313	0	1310	21	0
11	10	435	0	465	8	0
11	11	315	0	337	7	0
11	12	566	0	604	13	0
11	13	350	0	354	8	0
11	14	468	0	400	9	0
11	15	685	0	589	14	0
11	16	478	0	429	14	0
11	6	620	0	658	13	0
11	7	566	0	609	12	0
11	8	420	0	427	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	10	135	0	0	0	0
12	11	180	0	0	0	0
12	12	180	0	0	0	0
12	13	270	0	0	1	0
12	14	135	0	0	0	0
12	16	90	0	0	1	0
12	6	180	0	0	0	0
12	7	90	0	0	0	0
12	8	315	0	0	1	0
13	10	86	0	0	1	0
13	11	43	0	0	1	0
13	12	86	0	0	0	0
13	13	43	0	0	1	0
13	15	86	0	0	0	0
13	16	43	0	0	0	0
13	6	129	0	0	4	0
13	7	172	0	0	1	0
13	8	86	0	0	0	0
14	10	240	0	0	0	0
14	11	192	0	0	2	0
14	12	96	0	0	0	0
14	13	93	0	0	0	0
14	14	432	0	0	2	0
14	15	288	0	0	0	0
14	16	96	0	0	0	0
14	6	48	0	0	0	0
14	7	144	0	0	1	0
14	8	96	0	0	1	0
15	6	27	0	24	0	0
16	14	38	0	46	1	0
16	7	37	0	44	1	0
16	8	108	0	123	2	0
17	11	70	0	92	2	0
17	12	175	0	230	5	0
17	15	35	0	46	0	0
17	16	35	0	46	0	0
17	7	35	0	46	0	0
17	8	105	0	138	1	0
18	10	1	0	0	0	0
18	11	1	0	0	0	0
18	12	2	0	0	0	0
18	6	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	7	2	0	0	0	0
18	8	4	0	0	0	0
All	All	23863	0	19653	222	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 5.

The worst 5 of 222 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)
8:14:101:GLN:OE1	11:14:303:CLA:NA	2.01	0.94
9:15:105:GLU:OE1	11:15:302:CLA:NB	2.22	0.72
7:13:73:GLU:OE1	11:13:307:CLA:NC	2.23	0.71
1:6:127:ILE:HB	11:6:311:CLA:HBC1	1.77	0.66
9:15:127:PHE:O	9:15:138:HIS:NE2	2.33	0.62

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	6	172/208 (83%)	170 (99%)	2 (1%)	0	100	100
2	7	186/296 (63%)	178 (96%)	8 (4%)	0	100	100
3	8	211/270 (78%)	205 (97%)	6 (3%)	0	100	100
4	10	167/207 (81%)	152 (91%)	13 (8%)	2 (1%)	10	23
5	11	189/229 (82%)	171 (90%)	18 (10%)	0	100	100
6	12	171/204 (84%)	160 (94%)	11 (6%)	0	100	100
7	13	144/244 (59%)	136 (94%)	8 (6%)	0	100	100
8	14	206/249 (83%)	177 (86%)	29 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	15	209/281 (74%)	173 (83%)	35 (17%)	1 (0%)	24	46
10	16	172/218 (79%)	156 (91%)	16 (9%)	0	100	100
All	All	1827/2406 (76%)	1678 (92%)	146 (8%)	3 (0%)	44	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	15	250	PRO
4	10	205	TYR
4	10	204	PRO

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	6	140/160 (88%)	140 (100%)	0	100	100
2	7	143/236 (61%)	143 (100%)	0	100	100
3	8	171/215 (80%)	171 (100%)	0	100	100
4	10	133/161 (83%)	133 (100%)	0	100	100
5	11	154/181 (85%)	154 (100%)	0	100	100
6	12	136/159 (86%)	136 (100%)	0	100	100
7	13	112/184 (61%)	112 (100%)	0	100	100
8	14	166/196 (85%)	166 (100%)	0	100	100
9	15	171/231 (74%)	169 (99%)	2 (1%)	63	83
10	16	139/174 (80%)	137 (99%)	2 (1%)	59	81
All	All	1465/1897 (77%)	1461 (100%)	4 (0%)	84	94

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	15	138	HIS

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Mol	Chain	Res	Type
9	15	253	VAL
10	16	168	ILE
10	16	209	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
10	16	177	GLN
9	15	200	ASN
8	14	73	ASN
9	15	94	ASN
6	12	201	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

192 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	CLA	7	311	2	50,54,73	2.36	20 (40%)	59,90,113	3.00	27 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	A86	14	317	-	47,50,50	4.28	25 (53%)	51,76,76	7.30	18 (35%)
11	CLA	15	302	11,9	69,73,73	2.03	19 (27%)	82,113,113	2.81	32 (39%)
12	KC1	13	305	7	49,53,53	3.04	24 (48%)	61,89,89	3.82	34 (55%)
12	KC1	8	306	18	49,53,53	2.96	24 (48%)	61,89,89	3.82	38 (62%)
11	CLA	12	306	6	69,73,73	1.95	19 (27%)	82,113,113	2.54	29 (35%)
12	KC1	11	306	5	49,53,53	3.05	25 (51%)	61,89,89	3.88	34 (55%)
16	LMG	7	319	-	37,37,55	0.98	2 (5%)	45,45,63	1.28	5 (11%)
16	LMG	8	321	-	42,42,55	0.93	3 (7%)	50,50,63	1.34	4 (8%)
11	CLA	13	304	7	49,53,73	2.43	20 (40%)	58,89,113	3.06	28 (48%)
11	CLA	12	303	6	69,73,73	2.00	19 (27%)	82,113,113	2.56	30 (36%)
13	DD6	12	317	-	40,45,45	5.41	23 (57%)	51,67,67	6.14	27 (52%)
11	CLA	12	302	6	69,73,73	1.94	20 (28%)	82,113,113	2.73	32 (39%)
13	DD6	10	314	-	40,45,45	5.38	23 (57%)	51,67,67	5.86	29 (56%)
11	CLA	6	304	1	69,73,73	2.02	20 (28%)	82,113,113	2.61	30 (36%)
11	CLA	8	304	3	62,66,73	2.05	18 (29%)	73,104,113	2.91	34 (46%)
12	KC1	16	304	10	49,53,53	3.07	23 (46%)	61,89,89	3.64	32 (52%)
11	CLA	6	303	18	69,73,73	1.99	21 (30%)	82,113,113	2.65	29 (35%)
12	KC1	12	305	6	49,53,53	3.01	23 (46%)	61,89,89	3.86	34 (55%)
14	A86	11	315	-	47,50,50	4.19	23 (48%)	51,76,76	6.99	19 (37%)
17	LMT	8	319	-	36,36,36	0.39	0	47,47,47	0.86	1 (2%)
14	A86	16	312	-	47,50,50	4.28	24 (51%)	51,76,76	6.88	22 (43%)
11	CLA	6	312	1	49,53,73	2.42	19 (38%)	58,89,113	3.01	26 (44%)
11	CLA	15	311	14	49,53,73	2.42	20 (40%)	58,89,113	3.04	27 (46%)
11	CLA	16	301	10	69,73,73	1.96	18 (26%)	82,113,113	2.64	31 (37%)
17	LMT	12	318	-	36,36,36	0.40	0	47,47,47	0.80	1 (2%)
11	CLA	12	321	8	69,73,73	2.00	21 (30%)	82,113,113	2.57	30 (36%)
12	KC1	6	305	1	49,53,53	3.01	24 (48%)	61,89,89	3.85	32 (52%)
14	A86	14	321	-	47,50,50	4.42	25 (53%)	51,76,76	6.97	16 (31%)
12	KC1	10	312	4	49,53,53	3.02	24 (48%)	61,89,89	3.95	34 (55%)
14	A86	10	302	-	47,50,50	4.35	23 (48%)	51,76,76	7.17	19 (37%)
14	A86	15	321	-	47,50,50	4.32	26 (55%)	51,76,76	7.20	18 (35%)
12	KC1	16	311	10	49,53,53	3.07	24 (48%)	61,89,89	3.73	32 (52%)
12	KC1	8	311	18	49,53,53	3.00	24 (48%)	61,89,89	3.90	34 (55%)
11	CLA	11	305	18	59,63,73	2.18	20 (33%)	70,101,113	2.94	31 (44%)
11	CLA	15	308	11,9	49,53,73	2.39	20 (40%)	58,89,113	3.01	31 (53%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	KC1	8	312	12	49,53,53	3.01	24 (48%)	61,89,89	3.61	34 (55%)
11	CLA	10	307	4	69,73,73	1.95	21 (30%)	82,113,113	2.57	33 (40%)
14	A86	14	315	-	47,50,50	4.19	24 (51%)	51,76,76	7.41	19 (37%)
11	CLA	15	305	9,14	49,53,73	2.40	20 (40%)	58,89,113	3.05	29 (50%)
11	CLA	14	307	12	69,73,73	2.03	20 (28%)	82,113,113	2.68	27 (32%)
14	A86	15	320	-	47,50,50	4.48	23 (48%)	51,76,76	6.80	18 (35%)
11	CLA	15	309	-	69,73,73	2.05	20 (28%)	82,113,113	2.64	28 (34%)
14	A86	7	315	-	47,50,50	4.02	20 (42%)	51,76,76	6.39	25 (49%)
11	CLA	14	312	8,14	49,53,73	2.40	20 (40%)	58,89,113	3.02	28 (48%)
14	A86	13	313	-	44,47,50	4.46	24 (54%)	48,72,76	7.11	13 (27%)
11	CLA	7	303	2	69,73,73	1.94	19 (27%)	82,113,113	2.62	30 (36%)
13	DD6	7	316	-	40,45,45	5.48	21 (52%)	51,67,67	5.86	29 (56%)
14	A86	8	318	-	47,50,50	4.20	24 (51%)	51,76,76	9.47	23 (45%)
14	A86	7	314	-	47,50,50	4.03	23 (48%)	51,76,76	6.53	18 (35%)
17	LMT	11	302	-	36,36,36	0.32	0	47,47,47	0.80	2 (4%)
11	CLA	7	306	2	69,73,73	1.97	17 (24%)	82,113,113	2.66	29 (35%)
11	CLA	14	310	-	54,58,73	2.27	20 (37%)	64,95,113	2.99	31 (48%)
11	CLA	14	305	8	54,58,73	2.27	20 (37%)	64,95,113	2.94	30 (46%)
16	LMG	8	323	16	29,29,55	1.13	3 (10%)	37,37,63	1.27	6 (16%)
11	CLA	6	311	1	69,73,73	1.96	18 (26%)	82,113,113	2.71	32 (39%)
11	CLA	12	308	18	69,73,73	1.98	21 (30%)	82,113,113	2.53	27 (32%)
11	CLA	10	303	4	69,73,73	1.96	19 (27%)	82,113,113	2.62	30 (36%)
12	KC1	8	307	3	49,53,53	2.93	23 (46%)	61,89,89	3.92	36 (59%)
14	A86	14	320	-	47,50,50	4.37	25 (53%)	51,76,76	5.95	19 (37%)
15	LHG	6	319	11	26,26,48	0.92	1 (3%)	29,32,54	1.38	3 (10%)
11	CLA	15	313	9	69,73,73	2.02	20 (28%)	82,113,113	2.64	32 (39%)
17	LMT	12	320	-	36,36,36	0.35	0	47,47,47	0.71	0
14	A86	7	318	-	47,50,50	4.27	23 (48%)	51,76,76	6.53	23 (45%)
14	A86	14	319	11	47,50,50	4.30	25 (53%)	51,76,76	6.92	17 (33%)
14	A86	14	318	-	47,50,50	4.34	24 (51%)	51,76,76	7.06	16 (31%)
14	A86	11	314	-	47,50,50	4.24	23 (48%)	51,76,76	6.27	22 (43%)
14	A86	15	316	11	47,50,50	4.32	24 (51%)	51,76,76	6.49	17 (33%)
14	A86	15	315	-	47,50,50	4.51	24 (51%)	51,76,76	6.92	27 (52%)
14	A86	10	317	-	47,50,50	4.43	24 (51%)	51,76,76	6.78	16 (31%)
11	CLA	12	310	18	69,73,73	1.96	20 (28%)	82,113,113	2.64	29 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	KC1	11	311	-	49,53,53	3.03	24 (48%)	61,89,89	3.63	34 (55%)
11	CLA	13	307	7	69,73,73	2.02	22 (31%)	82,113,113	2.62	32 (39%)
12	KC1	14	306	8	49,53,53	3.04	24 (48%)	61,89,89	3.89	38 (62%)
14	A86	6	317	-	47,50,50	4.26	25 (53%)	51,76,76	5.71	21 (41%)
12	KC1	13	312	7	49,53,53	3.09	25 (51%)	61,89,89	3.86	35 (57%)
13	DD6	15	318	-	40,45,45	5.57	22 (55%)	51,67,67	6.05	30 (58%)
12	KC1	14	308	8,11	49,53,53	3.06	24 (48%)	61,89,89	3.75	32 (52%)
13	DD6	6	316	-	40,45,45	5.47	24 (60%)	51,67,67	5.57	29 (56%)
14	A86	10	315	-	47,50,50	4.37	23 (48%)	51,76,76	6.79	17 (33%)
13	DD6	10	313	-	40,45,45	5.51	23 (57%)	51,67,67	6.12	28 (54%)
12	KC1	8	313	3	49,53,53	2.96	21 (42%)	61,89,89	3.96	34 (55%)
14	A86	10	316	-	47,50,50	4.16	23 (48%)	51,76,76	6.65	20 (39%)
11	CLA	15	307	9	54,58,73	2.25	20 (37%)	64,95,113	2.88	30 (46%)
14	A86	8	315	-	47,50,50	3.91	21 (44%)	51,76,76	6.82	20 (39%)
12	KC1	12	309	6	49,53,53	3.00	23 (46%)	61,89,89	3.78	36 (59%)
17	LMT	8	322	-	36,36,36	0.37	0	47,47,47	0.72	0
12	KC1	10	306	4	49,53,53	2.95	24 (48%)	61,89,89	3.97	36 (59%)
12	KC1	8	314	12,18	49,53,53	3.00	24 (48%)	61,89,89	3.75	34 (55%)
13	DD6	15	319	11	40,45,45	5.64	23 (57%)	51,67,67	6.12	29 (56%)
11	CLA	8	305	3	69,73,73	1.94	20 (28%)	82,113,113	4.42	34 (41%)
11	CLA	12	304	13,6	69,73,73	2.00	19 (27%)	82,113,113	2.82	32 (39%)
14	A86	15	322	11	47,50,50	4.51	24 (51%)	51,76,76	6.98	20 (39%)
12	KC1	7	312	-	49,53,53	2.97	21 (42%)	61,89,89	3.91	34 (55%)
13	DD6	12	315	11	40,45,45	5.41	23 (57%)	51,67,67	6.01	26 (50%)
17	LMT	8	324	-	36,36,36	0.40	0	47,47,47	0.70	0
11	CLA	16	307	-	50,54,73	2.36	20 (40%)	59,90,113	2.99	28 (47%)
11	CLA	6	307	15	69,73,73	1.99	20 (28%)	82,113,113	2.50	30 (36%)
17	LMT	11	316	-	36,36,36	0.40	0	47,47,47	1.00	5 (10%)
11	CLA	8	301	3	69,73,73	1.95	18 (26%)	82,113,113	2.67	30 (36%)
11	CLA	13	302	7	69,73,73	2.00	21 (30%)	82,113,113	2.54	32 (39%)
12	KC1	8	310	3	49,53,53	2.92	21 (42%)	61,89,89	3.86	34 (55%)
11	CLA	8	308	3	59,63,73	2.13	19 (32%)	70,101,113	2.83	31 (44%)
12	KC1	12	313	6	49,53,53	3.03	24 (48%)	61,89,89	4.50	33 (54%)
11	CLA	7	309	2	69,73,73	1.99	20 (28%)	82,113,113	2.59	31 (37%)
13	DD6	7	313	-	40,45,45	5.37	22 (55%)	51,67,67	6.30	29 (56%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	A86	10	301	-	47,50,50	4.11	23 (48%)	51,76,76	5.99	22 (43%)
14	A86	12	314	-	47,50,50	4.18	24 (51%)	51,76,76	6.76	19 (37%)
11	CLA	15	304	13,11,9	69,73,73	2.04	20 (28%)	82,113,113	2.67	30 (36%)
11	CLA	7	304	18	69,73,73	2.07	19 (27%)	82,113,113	2.76	30 (36%)
11	CLA	15	303	11,14,9	64,68,73	2.08	21 (32%)	76,107,113	2.79	31 (40%)
12	KC1	13	310	7	49,53,53	3.05	24 (48%)	61,89,89	3.85	35 (57%)
11	CLA	7	310	2	69,73,73	1.97	17 (24%)	82,113,113	2.51	29 (35%)
11	CLA	16	306	10	56,60,73	2.21	21 (37%)	65,97,113	2.86	31 (47%)
12	KC1	13	308	7	49,53,53	3.04	25 (51%)	61,89,89	3.90	34 (55%)
17	LMT	12	322	-	36,36,36	0.43	0	47,47,47	0.89	1 (2%)
12	KC1	12	311	6	49,53,53	3.03	23 (46%)	61,89,89	3.95	37 (60%)
11	CLA	10	309	4	69,73,73	2.02	20 (28%)	82,113,113	2.58	30 (36%)
11	CLA	14	303	8	61,65,73	2.15	20 (32%)	72,103,113	2.82	32 (44%)
11	CLA	11	307	5	69,73,73	1.99	19 (27%)	82,113,113	2.62	31 (37%)
11	CLA	6	306	1	69,73,73	1.98	18 (26%)	82,113,113	2.64	35 (42%)
11	CLA	15	306	-	49,53,73	2.39	20 (40%)	58,89,113	3.16	27 (46%)
17	LMT	15	301	-	36,36,36	0.44	0	47,47,47	1.05	3 (6%)
11	CLA	10	304	4	69,73,73	1.99	20 (28%)	82,113,113	2.57	28 (34%)
13	DD6	8	317	-	40,45,45	5.47	24 (60%)	51,67,67	6.03	29 (56%)
14	A86	11	313	-	47,50,50	4.22	24 (51%)	51,76,76	6.95	19 (37%)
11	CLA	8	303	18	69,73,73	1.94	18 (26%)	82,113,113	2.56	30 (36%)
11	CLA	16	309	10	49,53,73	2.40	20 (40%)	58,89,113	3.13	27 (46%)
11	CLA	14	302	8	69,73,73	2.01	20 (28%)	82,113,113	2.68	35 (42%)
13	DD6	16	313	-	40,45,45	5.58	23 (57%)	51,67,67	6.27	30 (58%)
11	CLA	8	309	3	51,55,73	2.30	20 (39%)	60,91,113	2.94	27 (45%)
13	DD6	11	312	-	40,45,45	5.46	23 (57%)	51,67,67	6.07	28 (54%)
12	KC1	13	311	7	49,53,53	3.04	25 (51%)	61,89,89	3.64	34 (55%)
11	CLA	6	314	-	69,73,73	2.04	20 (28%)	82,113,113	2.58	30 (36%)
11	CLA	12	312	6	69,73,73	1.99	20 (28%)	82,113,113	2.63	30 (36%)
11	CLA	15	312	9	49,53,73	2.40	19 (38%)	58,89,113	3.19	31 (53%)
11	CLA	7	302	2	69,73,73	1.94	20 (28%)	82,113,113	2.63	31 (37%)
14	A86	11	301	-	47,50,50	4.24	23 (48%)	51,76,76	6.95	19 (37%)
12	KC1	13	306	7	49,53,53	3.00	24 (48%)	61,89,89	3.82	36 (59%)
12	KC1	11	310	5	49,53,53	3.05	24 (48%)	61,89,89	3.88	34 (55%)
12	KC1	6	310	1	49,53,53	2.99	24 (48%)	61,89,89	3.84	35 (57%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	DD6	6	318	-	40,45,45	5.38	23 (57%)	51,67,67	5.89	27 (52%)
14	A86	14	314	-	47,50,50	4.30	24 (51%)	51,76,76	6.90	22 (43%)
11	CLA	11	309	5	69,73,73	2.03	20 (28%)	82,113,113	2.59	29 (35%)
12	KC1	7	307	18	49,53,53	3.01	23 (46%)	61,89,89	3.74	33 (54%)
11	CLA	6	301	1	69,73,73	1.98	19 (27%)	82,113,113	2.65	32 (39%)
14	A86	15	317	11	47,50,50	4.40	24 (51%)	51,76,76	7.01	14 (27%)
11	CLA	16	305	10	54,58,73	2.21	21 (38%)	64,95,113	2.89	30 (46%)
14	A86	14	301	-	47,50,50	4.31	24 (51%)	51,76,76	6.74	18 (35%)
17	LMT	12	301	-	36,36,36	0.39	0	47,47,47	0.80	0
13	DD6	6	315	-	40,45,45	5.44	25 (62%)	51,67,67	5.75	27 (52%)
11	CLA	7	308	2	69,73,73	1.93	20 (28%)	82,113,113	2.59	28 (34%)
11	CLA	15	314	11	49,53,73	2.35	20 (40%)	58,89,113	3.16	28 (48%)
17	LMT	7	320	-	36,36,36	0.30	0	47,47,47	0.71	1 (2%)
11	CLA	14	309	8	49,53,73	2.43	19 (38%)	58,89,113	2.98	27 (46%)
12	KC1	6	308	1	49,53,53	2.98	24 (48%)	61,89,89	4.02	32 (52%)
12	KC1	6	309	1	49,53,53	3.01	24 (48%)	61,89,89	3.89	36 (59%)
16	LMG	14	322	-	38,38,55	0.97	3 (7%)	46,46,63	1.21	3 (6%)
11	CLA	11	303	5	69,73,73	1.99	19 (27%)	82,113,113	2.64	29 (35%)
17	LMT	12	319	-	36,36,36	0.37	0	47,47,47	0.80	0
11	CLA	8	302	3	69,73,73	1.98	20 (28%)	82,113,113	2.68	29 (35%)
11	CLA	13	301	7	69,73,73	1.96	18 (26%)	82,113,113	2.66	32 (39%)
17	LMT	16	315	-	36,36,36	0.41	0	47,47,47	0.65	0
11	CLA	13	309	-	49,53,73	2.42	21 (42%)	58,89,113	3.02	29 (50%)
11	CLA	7	305	2	69,73,73	1.96	21 (30%)	82,113,113	2.55	31 (37%)
16	LMG	8	320	16	37,37,55	0.97	1 (2%)	45,45,63	1.25	4 (8%)
14	A86	12	316	-	47,50,50	4.26	23 (48%)	51,76,76	6.91	17 (33%)
12	KC1	14	311	8	49,53,53	3.02	25 (51%)	61,89,89	3.87	34 (55%)
11	CLA	13	303	-	69,73,73	2.04	20 (28%)	82,113,113	2.70	33 (40%)
13	DD6	7	317	-	40,45,45	5.53	22 (55%)	51,67,67	6.05	29 (56%)
11	CLA	16	310	10	49,53,73	2.40	22 (44%)	58,89,113	3.06	29 (50%)
11	CLA	11	308	5	69,73,73	1.97	18 (26%)	82,113,113	2.65	32 (39%)
11	CLA	16	308	10	49,53,73	2.40	20 (40%)	58,89,113	3.09	28 (48%)
11	CLA	16	302	10	69,73,73	1.96	21 (30%)	82,113,113	2.61	30 (36%)
11	CLA	12	307	6	50,54,73	2.29	19 (38%)	59,90,113	3.04	30 (50%)
11	CLA	6	313	18	59,63,73	2.15	18 (30%)	70,101,113	2.76	29 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	14	313	8	50,54,73	2.36	20 (40%)	59,90,113	3.12	29 (49%)
11	CLA	15	310	9	49,53,73	2.42	20 (40%)	58,89,113	3.08	27 (46%)
11	CLA	10	305	18	69,73,73	1.98	17 (24%)	82,113,113	2.72	32 (39%)
11	CLA	10	311	-	49,53,73	2.39	20 (40%)	58,89,113	3.02	26 (44%)
11	CLA	16	303	10	69,73,73	1.99	18 (26%)	82,113,113	2.76	31 (37%)
14	A86	14	316	-	47,50,50	4.25	23 (48%)	51,76,76	6.78	16 (31%)
14	A86	16	314	-	47,50,50	4.34	24 (51%)	51,76,76	7.09	20 (39%)
12	KC1	11	304	5	49,53,53	2.99	25 (51%)	61,89,89	3.89	35 (57%)
13	DD6	7	301	-	40,45,45	5.49	25 (62%)	51,67,67	5.83	28 (54%)
14	A86	13	315	-	47,50,50	4.41	24 (51%)	51,76,76	7.07	17 (33%)
13	DD6	8	316	-	40,45,45	5.39	23 (57%)	51,67,67	5.86	27 (52%)
12	KC1	10	310	4	49,53,53	3.02	24 (48%)	61,89,89	3.96	36 (59%)
11	CLA	10	308	4	69,73,73	2.00	18 (26%)	82,113,113	2.66	32 (39%)
13	DD6	13	314	-	40,45,45	5.54	23 (57%)	51,67,67	6.16	31 (60%)
11	CLA	14	304	8	49,53,73	2.40	20 (40%)	58,89,113	3.04	26 (44%)
11	CLA	6	302	1	69,73,73	1.99	19 (27%)	82,113,113	2.58	31 (37%)

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
11	CLA	7	311	2	-	7/17/93/115	-
14	A86	14	317	-	-	15/34/90/90	0/3/3/3
11	CLA	15	302	11,9	-	16/39/115/115	-
12	KC1	13	305	7	-	11/15/71/71	-
12	KC1	8	306	18	-	5/15/71/71	-
11	CLA	12	306	6	1/1/15/20	5/39/115/115	-
12	KC1	11	306	5	-	10/15/71/71	-
16	LMG	7	319	-	-	12/32/52/70	0/1/1/1
16	LMG	8	321	-	-	21/37/57/70	0/1/1/1
11	CLA	13	304	7	-	7/15/91/115	-
11	CLA	12	303	6	1/1/15/20	8/39/115/115	-
13	DD6	12	317	-	-	12/26/80/80	0/3/3/3
11	CLA	12	302	6	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	DD6	10	314	-	-	9/26/80/80	0/3/3/3
11	CLA	6	304	1	1/1/15/20	19/39/115/115	-
11	CLA	8	304	3	1/1/13/20	13/31/107/115	-
12	KC1	16	304	10	-	8/15/71/71	-
11	CLA	6	303	18	1/1/15/20	8/39/115/115	-
12	KC1	12	305	6	-	6/15/71/71	-
14	A86	11	315	-	-	14/34/90/90	0/3/3/3
17	LMT	8	319	-	-	10/21/61/61	0/2/2/2
14	A86	16	312	-	-	13/34/90/90	0/3/3/3
11	CLA	6	312	1	1/1/11/20	5/15/91/115	-
11	CLA	15	311	14	1/1/11/20	7/15/91/115	-
11	CLA	16	301	10	-	15/39/115/115	-
17	LMT	12	318	-	-	1/21/61/61	0/2/2/2
11	CLA	12	321	8	1/1/15/20	3/39/115/115	-
12	KC1	6	305	1	-	6/15/71/71	-
14	A86	14	321	-	-	16/34/90/90	0/3/3/3
12	KC1	10	312	4	-	4/15/71/71	-
14	A86	10	302	-	-	12/34/90/90	0/3/3/3
14	A86	15	321	-	-	12/34/90/90	0/3/3/3
12	KC1	16	311	10	-	6/15/71/71	-
12	KC1	8	311	18	-	8/15/71/71	-
11	CLA	11	305	18	1/1/13/20	9/27/103/115	-
11	CLA	15	308	11,9	1/1/11/20	9/15/91/115	-
12	KC1	8	312	12	-	6/15/71/71	-
11	CLA	10	307	4	1/1/15/20	12/39/115/115	-
14	A86	14	315	-	-	10/34/90/90	0/3/3/3
11	CLA	15	305	9,14	1/1/11/20	10/15/91/115	-
11	CLA	14	307	12	-	8/39/115/115	-
14	A86	15	320	-	-	15/34/90/90	0/3/3/3
11	CLA	15	309	-	1/1/15/20	12/39/115/115	-
14	A86	7	315	-	-	8/34/90/90	0/3/3/3
11	CLA	14	312	8,14	-	8/15/91/115	-
14	A86	13	313	-	-	10/30/86/90	0/3/3/3
11	CLA	7	303	2	1/1/15/20	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	DD6	7	316	-	-	10/26/80/80	0/3/3/3
14	A86	8	318	-	-	11/34/90/90	0/3/3/3
14	A86	7	314	-	-	16/34/90/90	0/3/3/3
17	LMT	11	302	-	-	0/21/61/61	0/2/2/2
11	CLA	7	306	2	-	22/39/115/115	-
11	CLA	14	310	-	1/1/12/20	6/21/97/115	-
11	CLA	14	305	8	1/1/12/20	3/21/97/115	-
16	LMG	8	323	16	-	5/24/44/70	0/1/1/1
11	CLA	6	311	1	-	16/39/115/115	-
11	CLA	12	308	18	1/1/15/20	8/39/115/115	-
11	CLA	10	303	4	-	9/39/115/115	-
12	KC1	8	307	3	-	8/15/71/71	-
14	A86	14	320	-	-	10/34/90/90	0/3/3/3
15	LHG	6	319	11	-	12/31/31/53	-
11	CLA	15	313	9	-	10/39/115/115	-
17	LMT	12	320	-	-	1/21/61/61	0/2/2/2
14	A86	7	318	-	-	9/34/90/90	0/3/3/3
14	A86	14	319	11	-	10/34/90/90	0/3/3/3
14	A86	14	318	-	-	15/34/90/90	0/3/3/3
14	A86	11	314	-	-	18/34/90/90	0/3/3/3
14	A86	15	316	11	-	13/34/90/90	0/3/3/3
14	A86	15	315	-	-	8/34/90/90	0/3/3/3
14	A86	10	317	-	-	10/34/90/90	0/3/3/3
11	CLA	12	310	18	-	10/39/115/115	-
12	KC1	11	311	-	-	9/15/71/71	-
11	CLA	13	307	7	1/1/15/20	8/39/115/115	-
12	KC1	14	306	8	-	8/15/71/71	-
14	A86	6	317	-	-	8/34/90/90	0/3/3/3
12	KC1	13	312	7	-	6/15/71/71	-
13	DD6	15	318	-	-	13/26/80/80	0/3/3/3
12	KC1	14	308	8,11	-	9/15/71/71	-
13	DD6	6	316	-	-	12/26/80/80	0/3/3/3
14	A86	10	315	-	-	13/34/90/90	0/3/3/3
13	DD6	10	313	-	-	11/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	KC1	8	313	3	-	5/15/71/71	-
14	A86	10	316	-	-	11/34/90/90	0/3/3/3
11	CLA	15	307	9	1/1/12/20	6/21/97/115	-
14	A86	8	315	-	-	7/34/90/90	0/3/3/3
12	KC1	12	309	6	-	8/15/71/71	-
17	LMT	8	322	-	-	1/21/61/61	0/2/2/2
12	KC1	10	306	4	-	8/15/71/71	-
12	KC1	8	314	12,18	-	6/15/71/71	-
13	DD6	15	319	11	-	13/26/80/80	0/3/3/3
11	CLA	8	305	3	-	12/39/115/115	-
11	CLA	12	304	13,6	1/1/15/20	13/39/115/115	-
14	A86	15	322	11	-	15/34/90/90	0/3/3/3
12	KC1	7	312	-	-	4/15/71/71	-
13	DD6	12	315	11	-	10/26/80/80	0/3/3/3
17	LMT	8	324	-	-	5/21/61/61	0/2/2/2
11	CLA	16	307	-	1/1/11/20	5/17/93/115	-
11	CLA	6	307	15	1/1/15/20	9/39/115/115	-
17	LMT	11	316	-	-	1/21/61/61	0/2/2/2
11	CLA	8	301	3	1/1/15/20	15/39/115/115	-
11	CLA	13	302	7	1/1/15/20	13/39/115/115	-
12	KC1	8	310	3	-	7/15/71/71	-
11	CLA	8	308	3	1/1/13/20	10/27/103/115	-
12	KC1	12	313	6	-	7/15/71/71	-
11	CLA	7	309	2	1/1/15/20	16/39/115/115	-
13	DD6	7	313	-	-	10/26/80/80	0/3/3/3
14	A86	10	301	-	-	8/34/90/90	0/3/3/3
14	A86	12	314	-	-	10/34/90/90	0/3/3/3
11	CLA	15	304	13,11,9	1/1/15/20	20/39/115/115	-
11	CLA	7	304	18	1/1/15/20	9/39/115/115	-
11	CLA	15	303	11,14,9	1/1/14/20	8/33/109/115	-
12	KC1	13	310	7	-	5/15/71/71	-
11	CLA	7	310	2	1/1/15/20	14/39/115/115	-
11	CLA	16	306	10	1/1/12/20	14/24/100/115	-
12	KC1	13	308	7	-	10/15/71/71	-
17	LMT	12	322	-	-	1/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	KC1	12	311	6	-	5/15/71/71	-
11	CLA	10	309	4	1/1/15/20	13/39/115/115	-
11	CLA	14	303	8	1/1/13/20	10/30/106/115	-
11	CLA	11	307	5	1/1/15/20	12/39/115/115	-
11	CLA	6	306	1	1/1/15/20	11/39/115/115	-
11	CLA	15	306	-	1/1/11/20	8/15/91/115	-
17	LMT	15	301	-	-	8/21/61/61	0/2/2/2
11	CLA	10	304	4	1/1/15/20	3/39/115/115	-
13	DD6	8	317	-	-	11/26/80/80	0/3/3/3
14	A86	11	313	-	-	12/34/90/90	0/3/3/3
11	CLA	8	303	18	1/1/15/20	9/39/115/115	-
11	CLA	16	309	10	-	7/15/91/115	-
11	CLA	14	302	8	1/1/15/20	13/39/115/115	-
13	DD6	16	313	-	-	13/26/80/80	0/3/3/3
11	CLA	8	309	3	-	4/18/94/115	-
13	DD6	11	312	-	-	11/26/80/80	0/3/3/3
12	KC1	13	311	7	-	5/15/71/71	-
11	CLA	6	314	-	1/1/15/20	7/39/115/115	-
11	CLA	12	312	6	1/1/15/20	14/39/115/115	-
11	CLA	15	312	9	1/1/11/20	8/15/91/115	-
11	CLA	7	302	2	1/1/15/20	15/39/115/115	-
14	A86	11	301	-	-	11/34/90/90	0/3/3/3
12	KC1	13	306	7	-	11/15/71/71	-
12	KC1	11	310	5	-	7/15/71/71	-
12	KC1	6	310	1	-	6/15/71/71	-
13	DD6	6	318	-	-	9/26/80/80	0/3/3/3
14	A86	14	314	-	-	10/34/90/90	0/3/3/3
11	CLA	11	309	5	1/1/15/20	17/39/115/115	-
12	KC1	7	307	18	-	7/15/71/71	-
11	CLA	6	301	1	1/1/15/20	14/39/115/115	-
14	A86	15	317	11	-	15/34/90/90	0/3/3/3
11	CLA	16	305	10	1/1/12/20	2/21/97/115	-
14	A86	14	301	-	-	9/34/90/90	0/3/3/3
17	LMT	12	301	-	-	3/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	DD6	6	315	-	-	9/26/80/80	0/3/3/3
11	CLA	7	308	2	1/1/15/20	10/39/115/115	-
11	CLA	15	314	11	-	6/15/91/115	-
17	LMT	7	320	-	-	4/21/61/61	0/2/2/2
11	CLA	14	309	8	1/1/11/20	3/15/91/115	-
12	KC1	6	308	1	-	8/15/71/71	-
12	KC1	6	309	1	-	4/15/71/71	-
16	LMG	14	322	-	-	14/33/53/70	0/1/1/1
11	CLA	11	303	5	-	12/39/115/115	-
17	LMT	12	319	-	-	0/21/61/61	0/2/2/2
11	CLA	8	302	3	1/1/15/20	6/39/115/115	-
11	CLA	13	301	7	-	18/39/115/115	-
17	LMT	16	315	-	-	5/21/61/61	0/2/2/2
11	CLA	13	309	-	1/1/11/20	7/15/91/115	-
11	CLA	7	305	2	1/1/15/20	6/39/115/115	-
16	LMG	8	320	16	-	17/32/52/70	0/1/1/1
14	A86	12	316	-	-	13/34/90/90	0/3/3/3
12	KC1	14	311	8	-	5/15/71/71	-
11	CLA	13	303	-	-	17/39/115/115	-
13	DD6	7	317	-	-	16/26/80/80	0/3/3/3
11	CLA	16	310	10	1/1/11/20	8/15/91/115	-
11	CLA	11	308	5	-	16/39/115/115	-
11	CLA	16	308	10	1/1/11/20	6/15/91/115	-
11	CLA	16	302	10	1/1/15/20	10/39/115/115	-
11	CLA	12	307	6	1/1/11/20	8/17/93/115	-
11	CLA	6	313	18	1/1/13/20	7/27/103/115	-
11	CLA	14	313	8	1/1/11/20	4/17/93/115	-
11	CLA	15	310	9	1/1/11/20	6/15/91/115	-
11	CLA	10	305	18	1/1/15/20	10/39/115/115	-
11	CLA	10	311	-	-	7/15/91/115	-
11	CLA	16	303	10	1/1/15/20	20/39/115/115	-
14	A86	14	316	-	-	10/34/90/90	0/3/3/3
14	A86	16	314	-	-	10/34/90/90	0/3/3/3
12	KC1	11	304	5	-	7/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	DD6	7	301	-	-	11/26/80/80	0/3/3/3
14	A86	13	315	-	-	15/34/90/90	0/3/3/3
13	DD6	8	316	-	-	11/26/80/80	0/3/3/3
12	KC1	10	310	4	-	7/15/71/71	-
11	CLA	10	308	4	1/1/15/20	11/39/115/115	-
13	DD6	13	314	-	-	13/26/80/80	0/3/3/3
11	CLA	14	304	8	1/1/11/20	6/15/91/115	-
11	CLA	6	302	1	1/1/15/20	4/39/115/115	-

The worst 5 of 3759 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	15	322	A86	C14-C13	16.36	1.69	1.51
14	10	317	A86	C14-C13	16.06	1.69	1.51
14	15	315	A86	C14-C13	15.85	1.68	1.51
14	16	314	A86	C14-C13	15.69	1.68	1.51
14	15	320	A86	C14-C13	15.56	1.68	1.51

The worst 5 of 4958 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	14	315	A86	O1-C20-C19	46.52	157.09	113.49
14	14	317	A86	O1-C20-C19	45.75	156.37	113.49
14	15	321	A86	O1-C20-C19	45.66	156.29	113.49
14	8	318	A86	O1-C20-C19	45.43	156.07	113.49
14	16	314	A86	O1-C20-C19	44.92	155.59	113.49

5 of 63 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	6	301	CLA	ND
11	6	302	CLA	ND
11	6	303	CLA	ND
11	6	304	CLA	ND
11	6	306	CLA	ND

5 of 1824 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	6	301	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
11	6	301	CLA	C3A-C2A-CAA-CBA
11	6	303	CLA	C4B-C3B-CAB-CBB
11	6	304	CLA	C2B-C3B-CAB-CBB
11	6	304	CLA	C4B-C3B-CAB-CBB

There are no ring outliers.

87 monomers are involved in 131 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	14	317	A86	1	0
11	15	302	CLA	5	0
11	12	306	CLA	2	0
16	7	319	LMG	1	0
16	8	321	LMG	1	0
11	13	304	CLA	1	0
11	12	303	CLA	4	0
11	12	302	CLA	1	0
11	6	304	CLA	2	0
11	8	304	CLA	1	0
12	16	304	KC1	1	0
11	6	303	CLA	1	0
14	11	315	A86	1	0
11	16	301	CLA	7	0
11	12	321	CLA	1	0
11	10	307	CLA	2	0
11	14	307	CLA	2	0
11	15	309	CLA	2	0
11	14	312	CLA	1	0
11	7	303	CLA	1	0
14	7	314	A86	1	0
11	7	306	CLA	2	0
11	14	305	CLA	1	0
16	8	323	LMG	1	0
11	6	311	CLA	3	0
11	12	308	CLA	2	0
11	10	303	CLA	3	0
14	14	320	A86	1	0
11	15	313	CLA	3	0
17	12	320	LMT	2	0
14	11	314	A86	1	0
11	12	310	CLA	2	0
11	13	307	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	6	316	DD6	1	0
13	10	313	DD6	1	0
12	8	313	KC1	1	0
11	15	307	CLA	1	0
14	8	315	A86	1	0
11	8	305	CLA	2	0
11	12	304	CLA	2	0
17	8	324	LMT	1	0
11	16	307	CLA	2	0
17	11	316	LMT	2	0
11	8	301	CLA	1	0
11	13	302	CLA	1	0
11	8	308	CLA	2	0
11	7	309	CLA	1	0
13	7	313	DD6	1	0
11	15	304	CLA	1	0
11	15	303	CLA	3	0
12	13	310	KC1	1	0
11	7	310	CLA	2	0
11	16	306	CLA	1	0
17	12	322	LMT	2	0
11	10	309	CLA	1	0
11	14	303	CLA	3	0
11	11	307	CLA	1	0
11	6	306	CLA	2	0
11	10	304	CLA	3	0
11	8	303	CLA	5	0
11	14	302	CLA	2	0
11	8	309	CLA	1	0
13	11	312	DD6	1	0
11	12	312	CLA	1	0
11	7	302	CLA	1	0
13	6	318	DD6	1	0
11	6	301	CLA	2	0
17	12	301	LMT	1	0
13	6	315	DD6	2	0
11	7	308	CLA	4	0
16	14	322	LMG	1	0
11	11	303	CLA	4	0
17	12	319	LMT	1	0
11	8	302	CLA	1	0
11	13	301	CLA	1	0

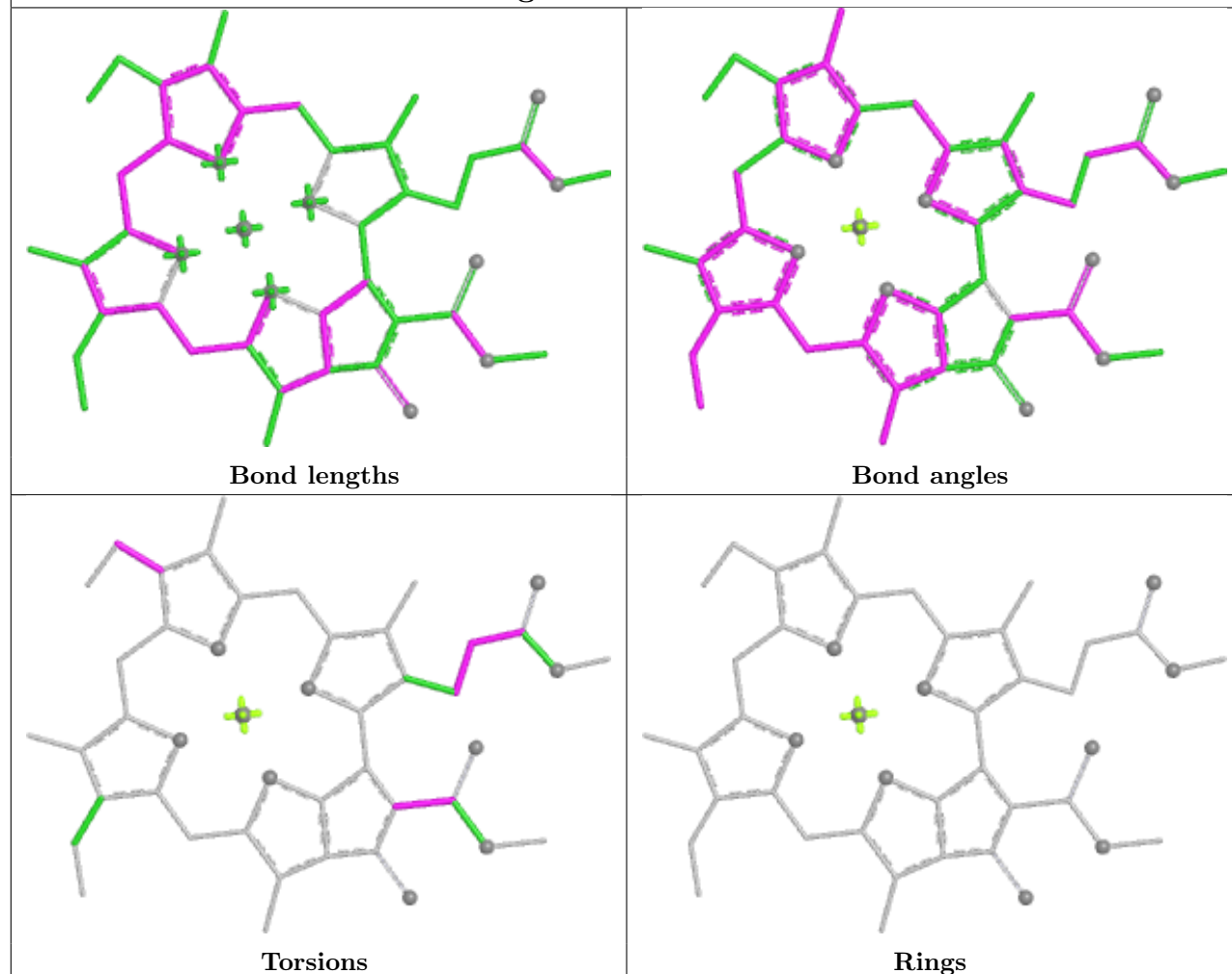
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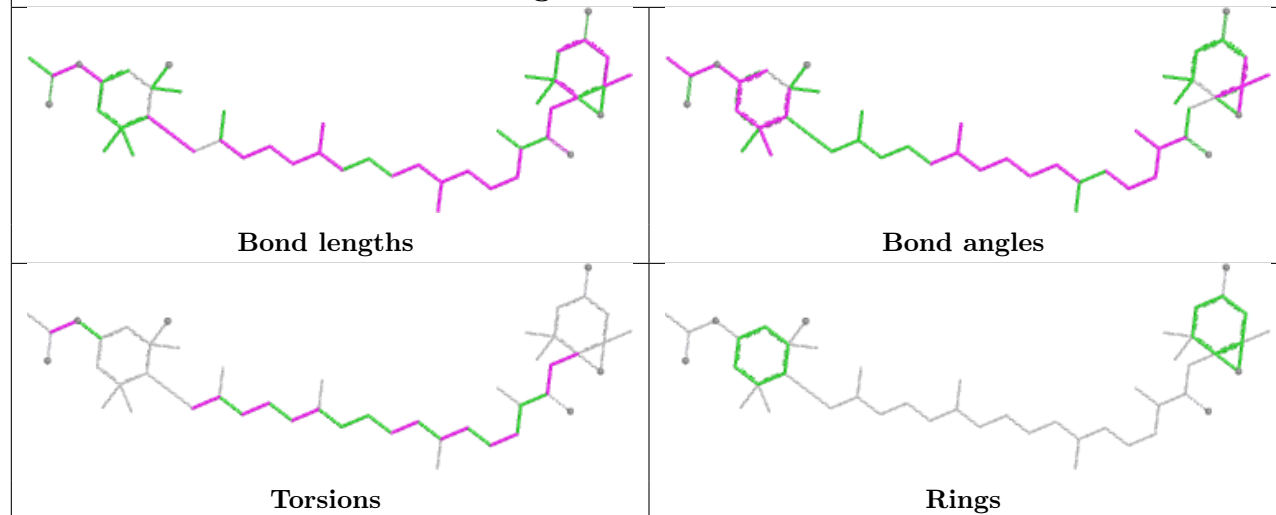
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	7	305	CLA	1	0
16	8	320	LMG	1	0
11	13	303	CLA	1	0
11	16	310	CLA	1	0
11	11	308	CLA	2	0
11	16	302	CLA	1	0
11	6	313	CLA	2	0
11	10	305	CLA	1	0
11	16	303	CLA	2	0
11	10	308	CLA	2	0
13	13	314	DD6	1	0
11	6	302	CLA	1	0

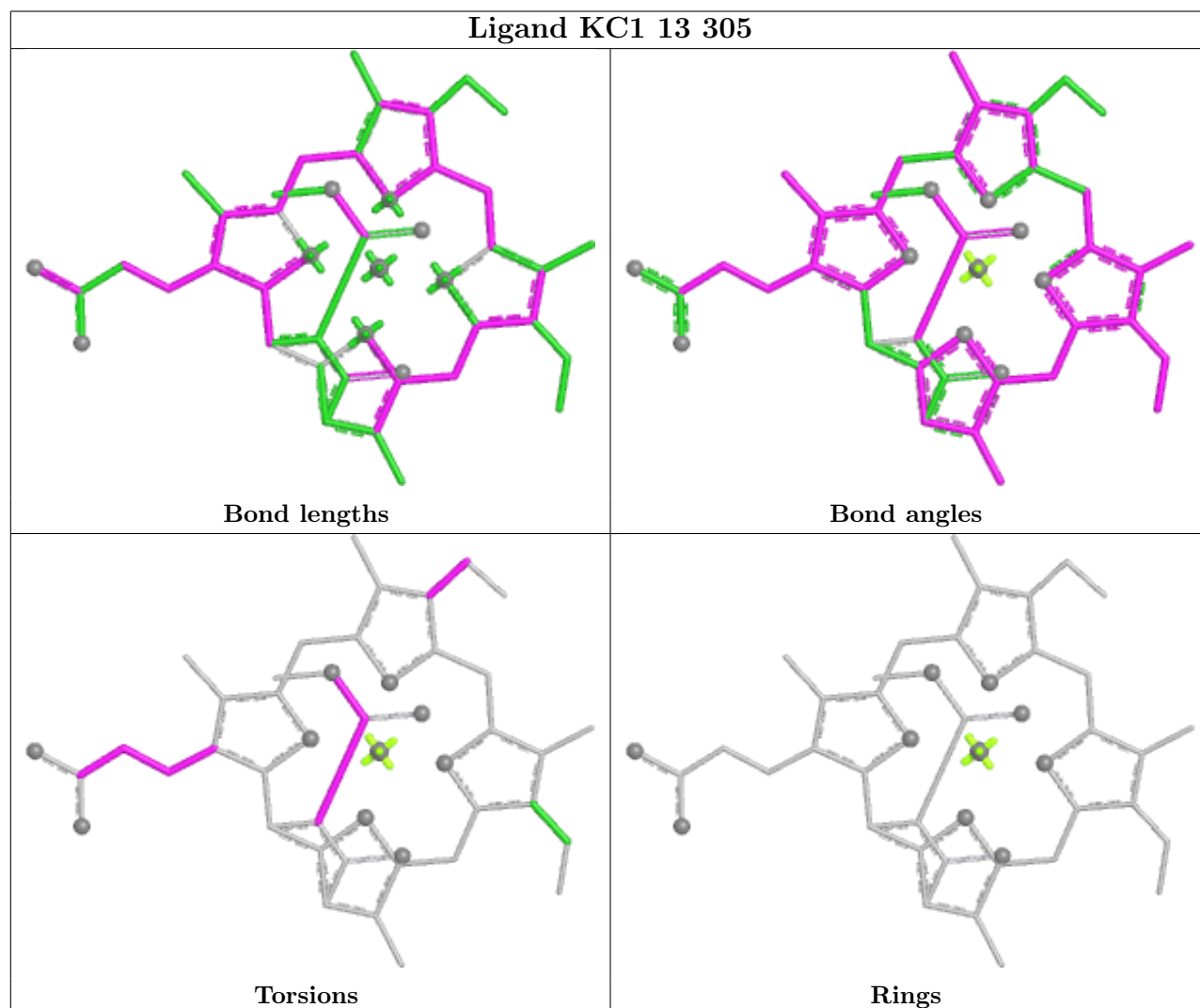
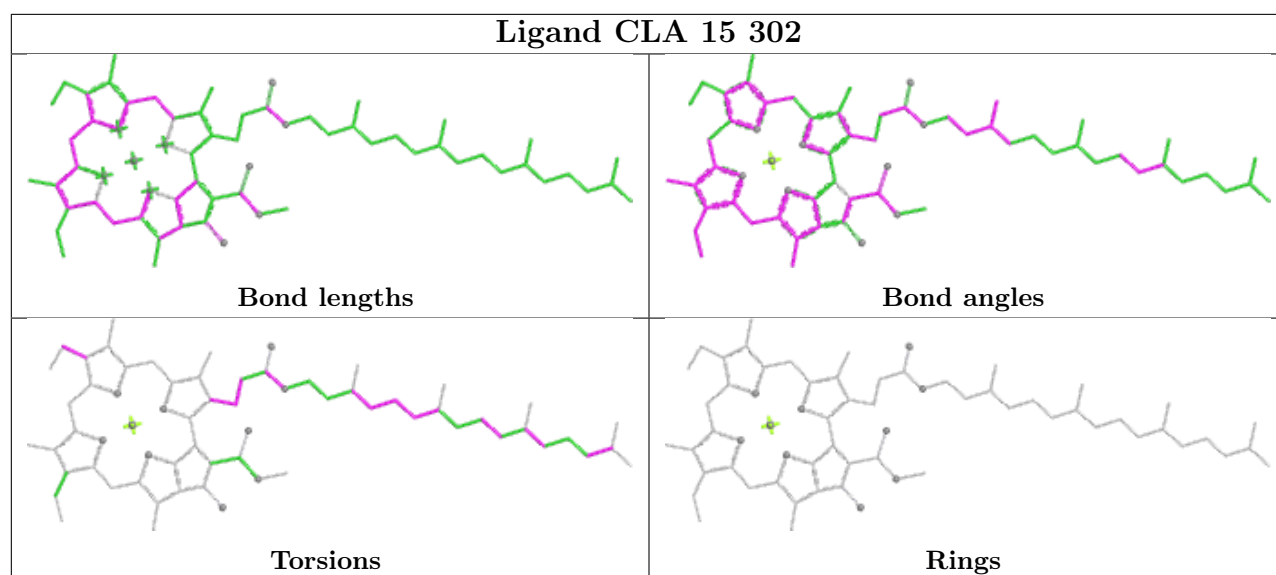
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand CLA 7 311

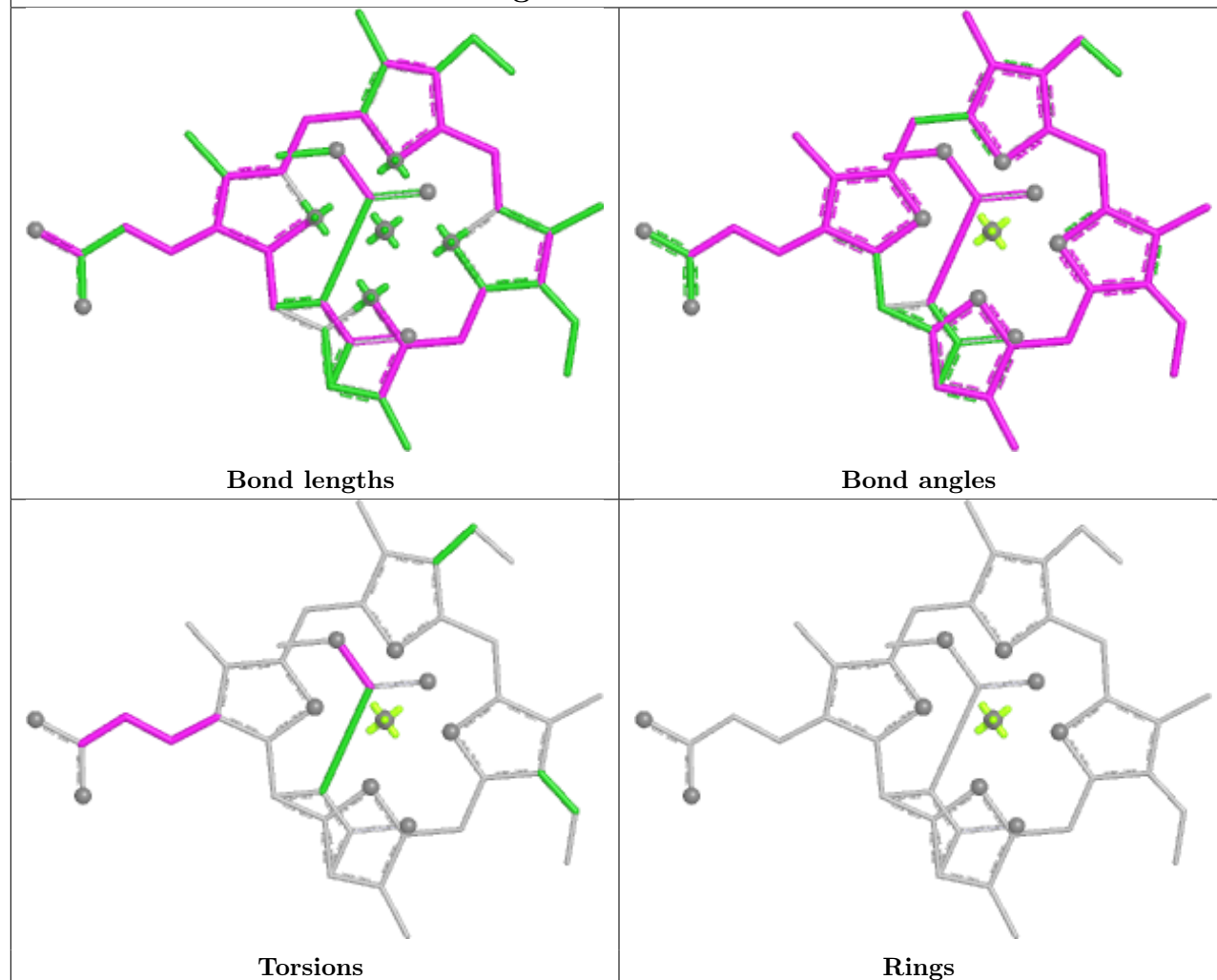


Ligand A86 14 317

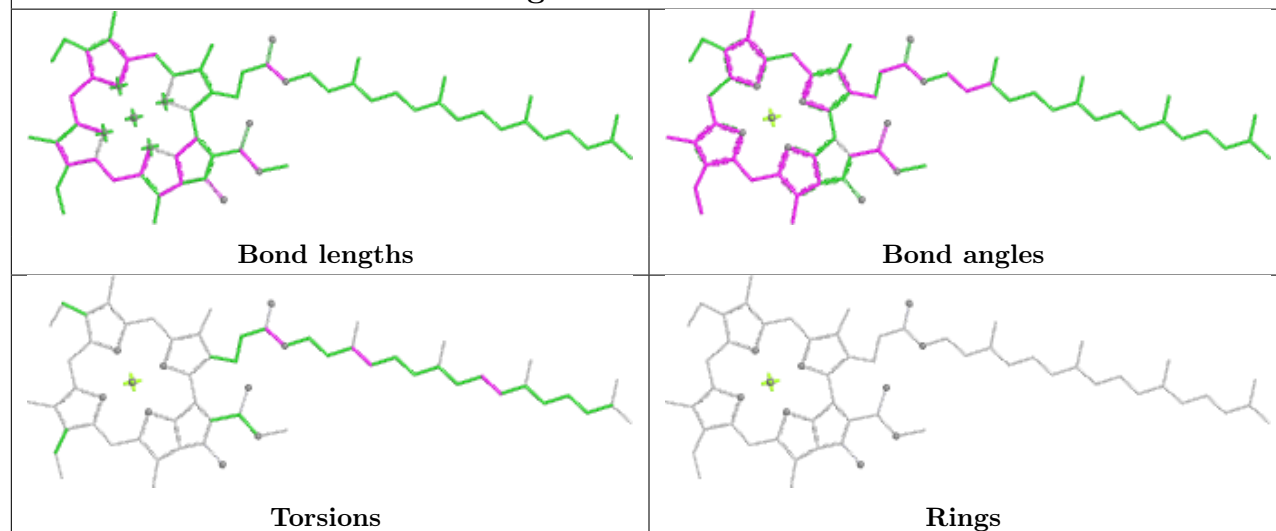


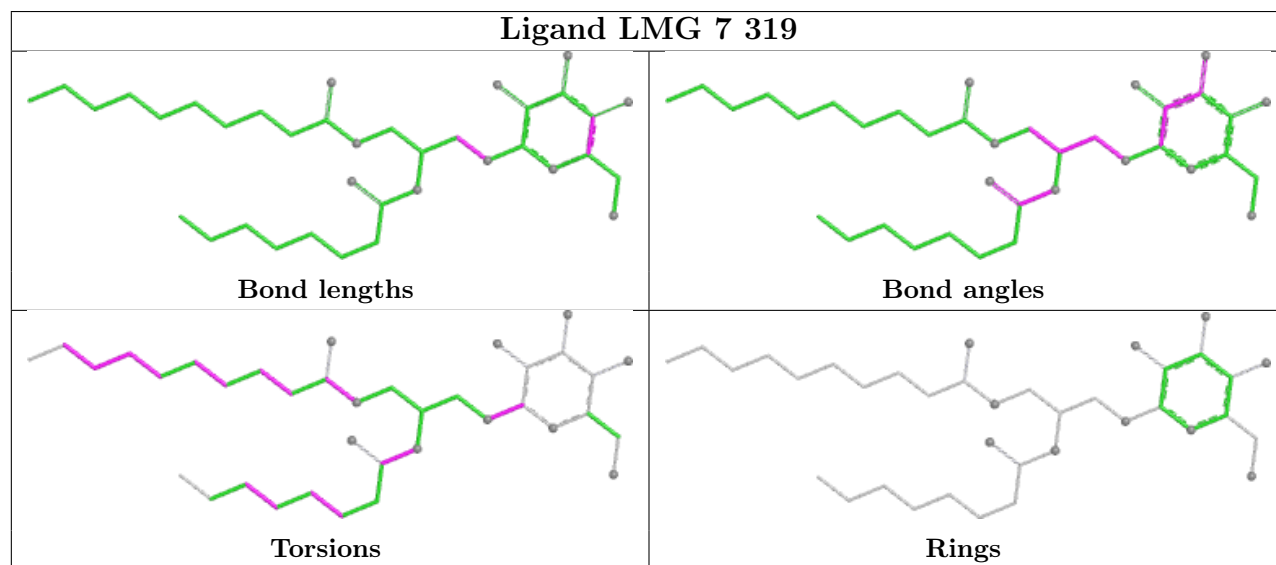
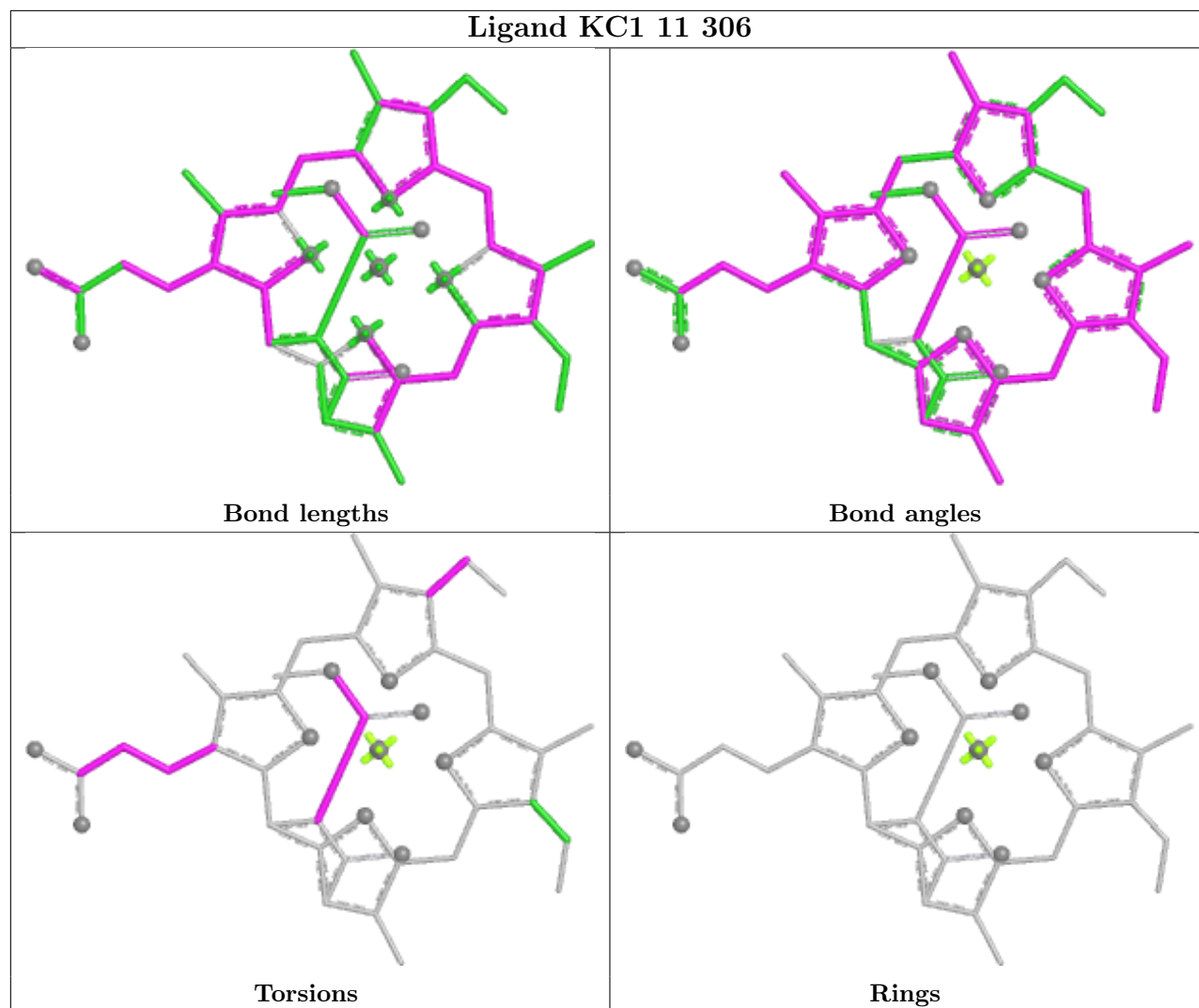


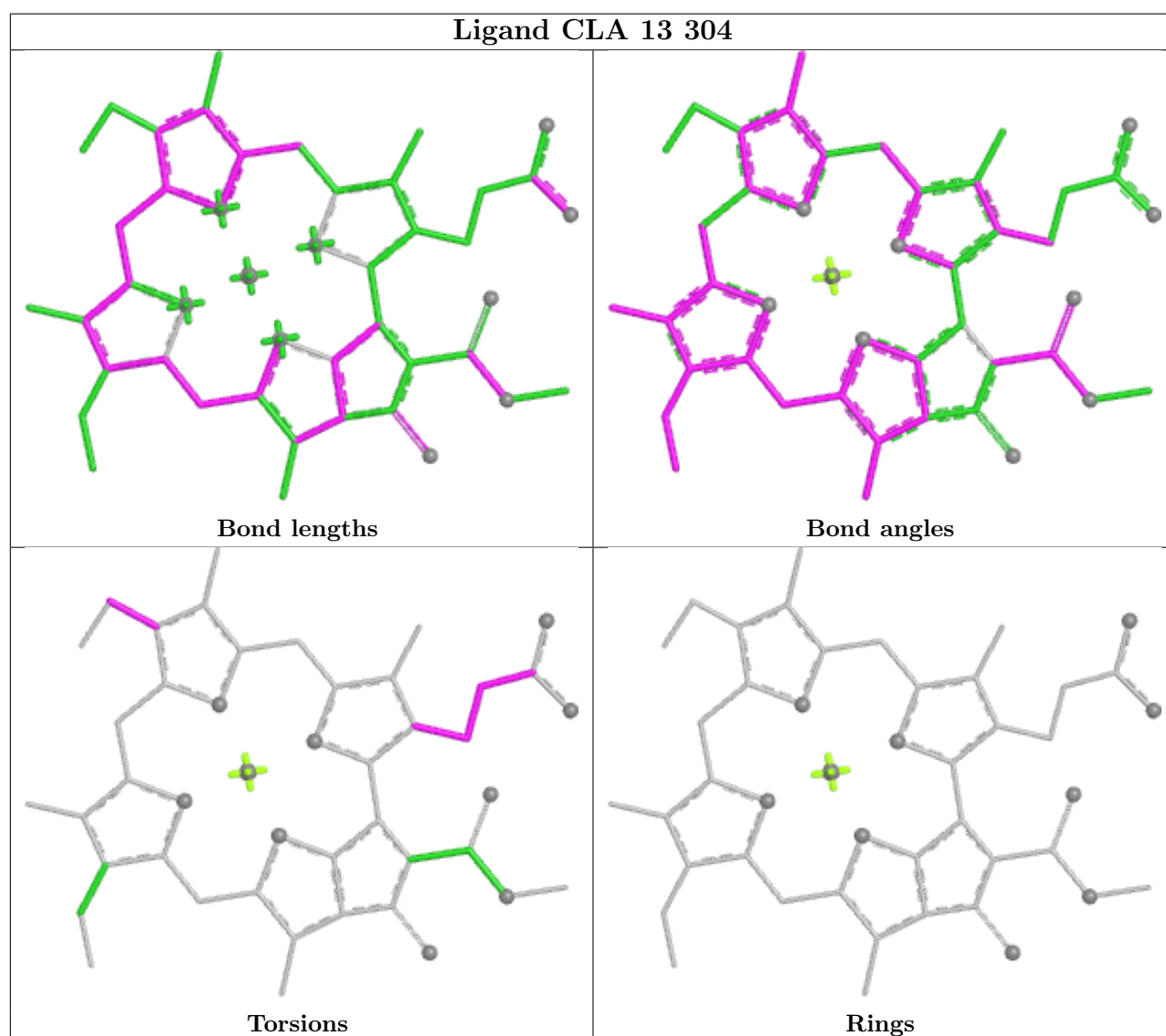
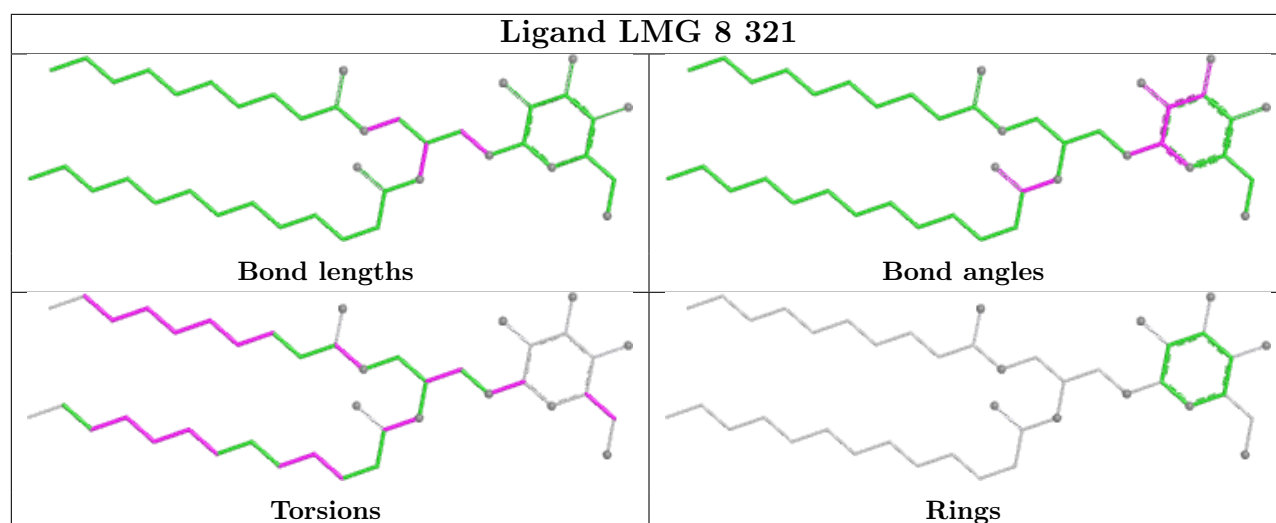
Ligand KC1 8 306

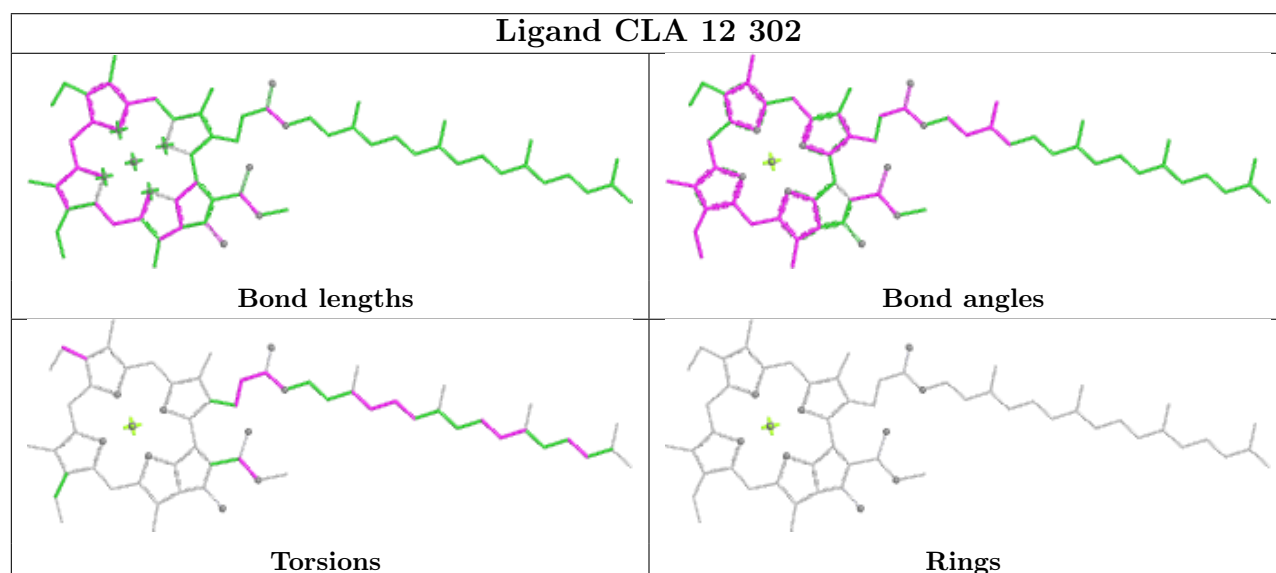
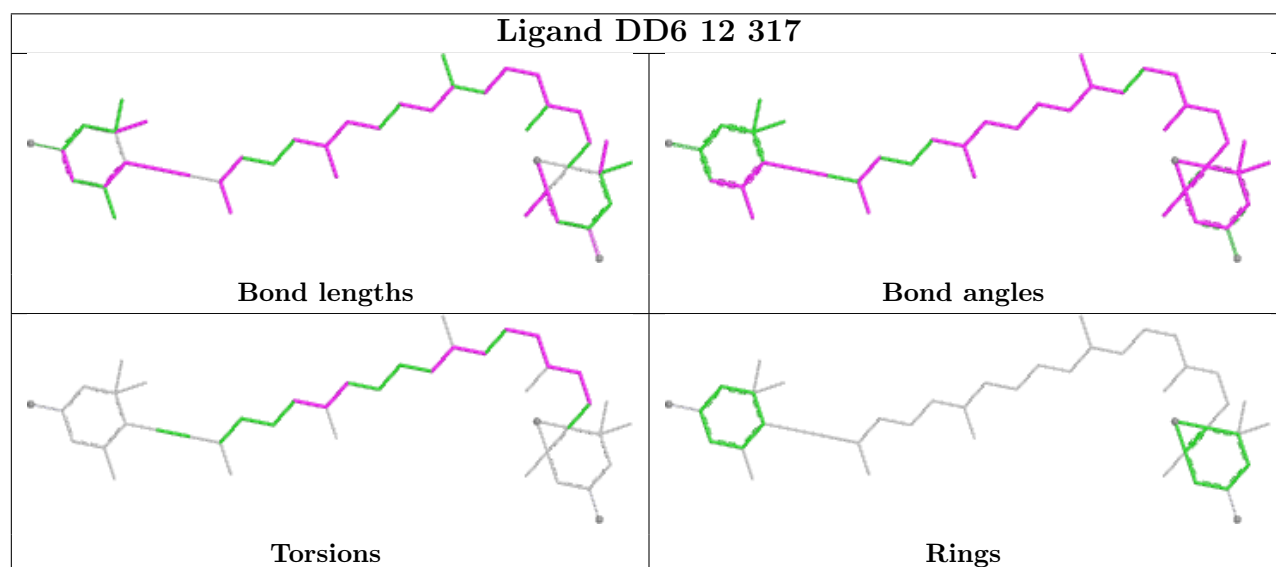
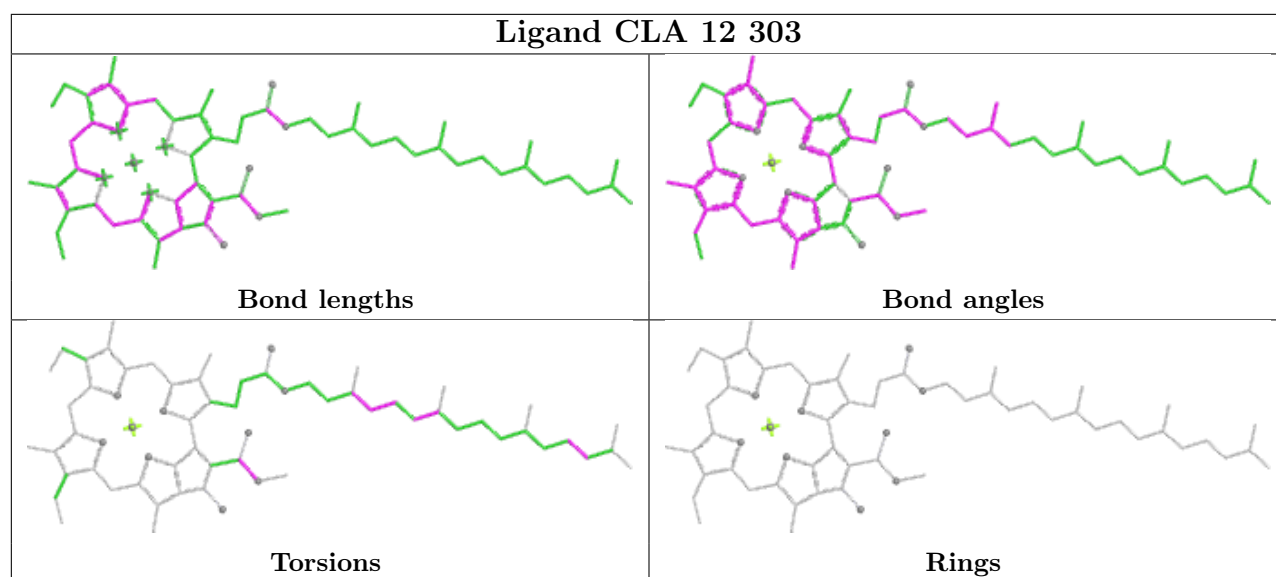


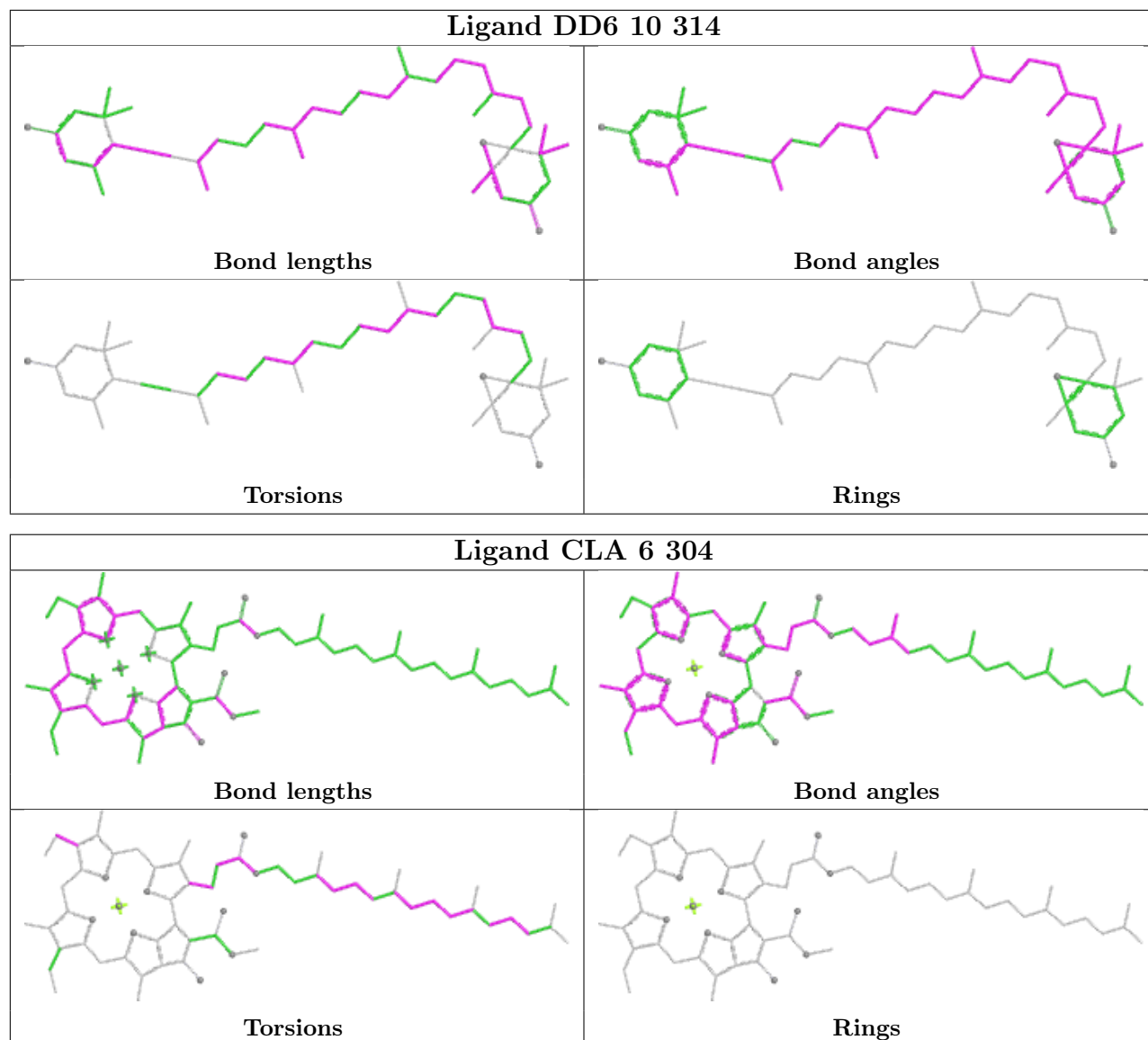
Ligand CLA 12 306



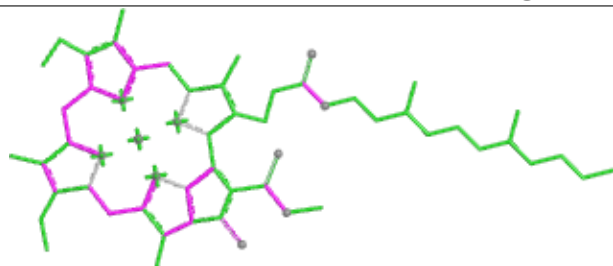




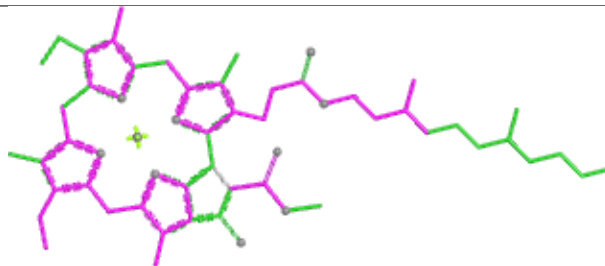




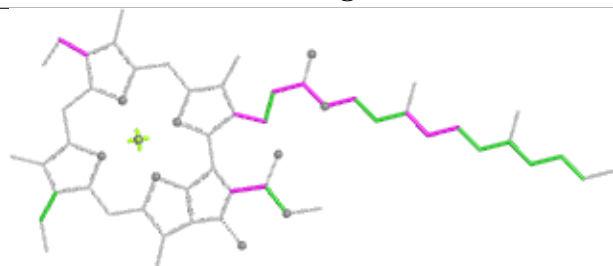
Ligand CLA 8 304



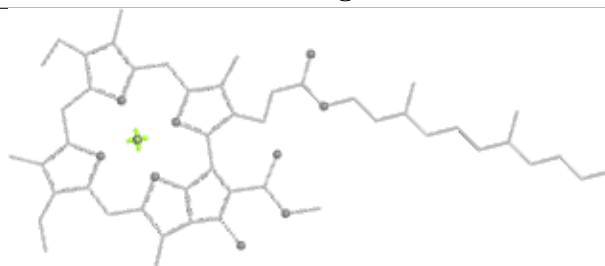
Bond lengths



Bond angles

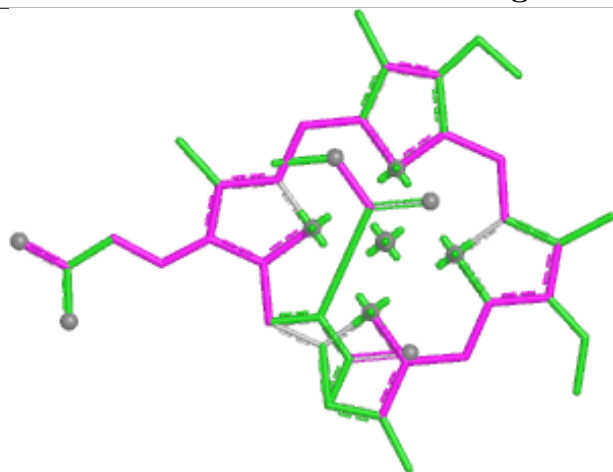


Torsions

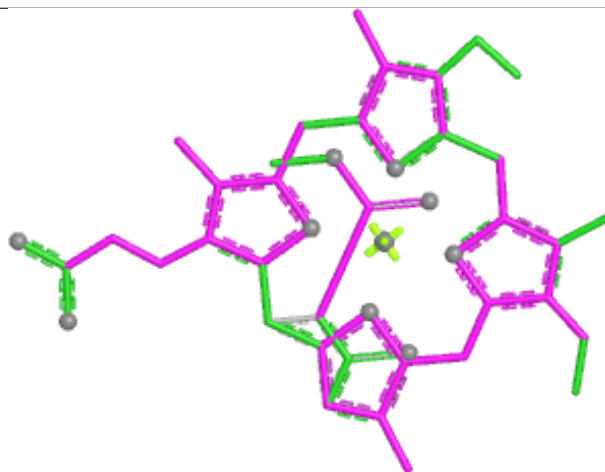


Rings

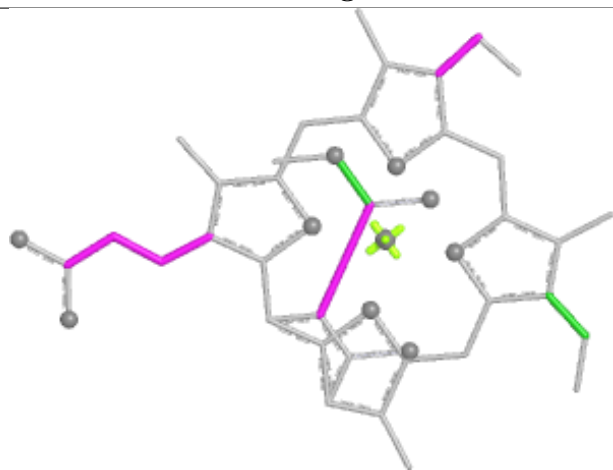
Ligand KC1 16 304



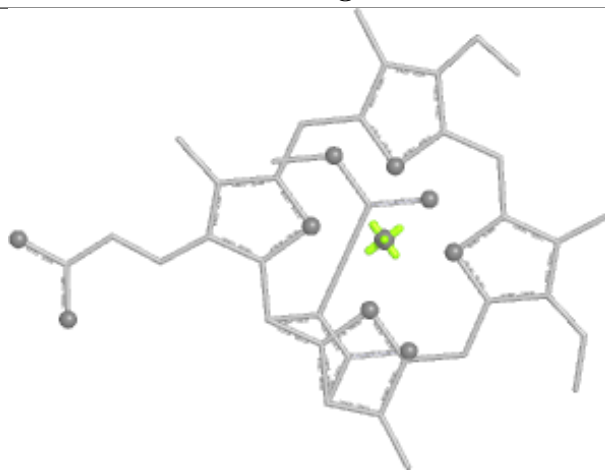
Bond lengths



Bond angles

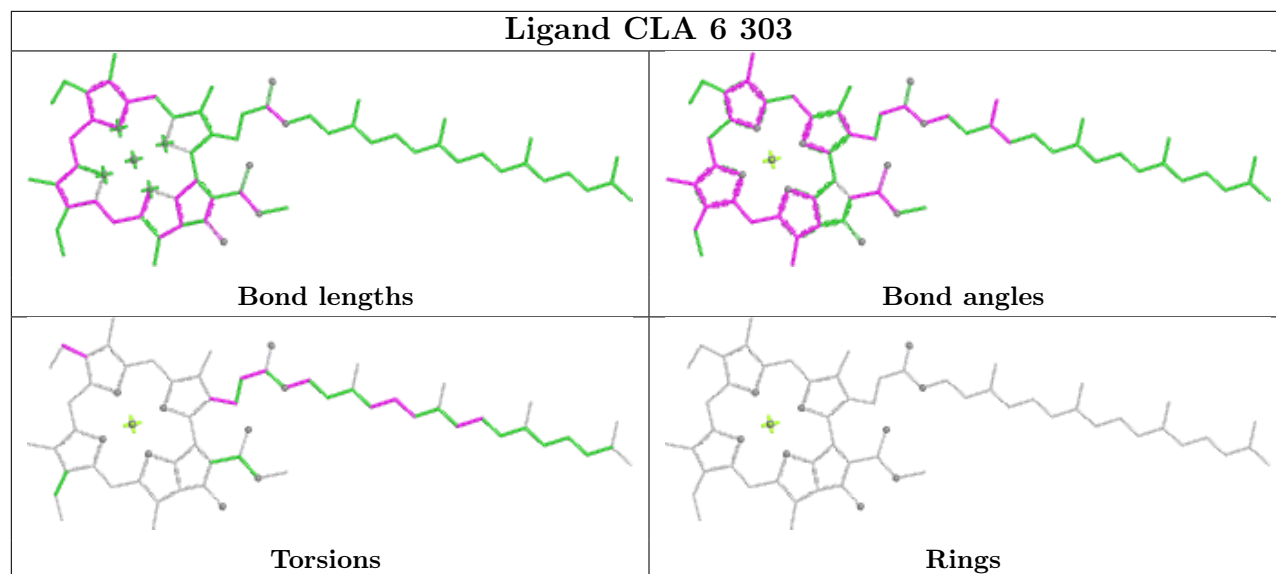


Torsions

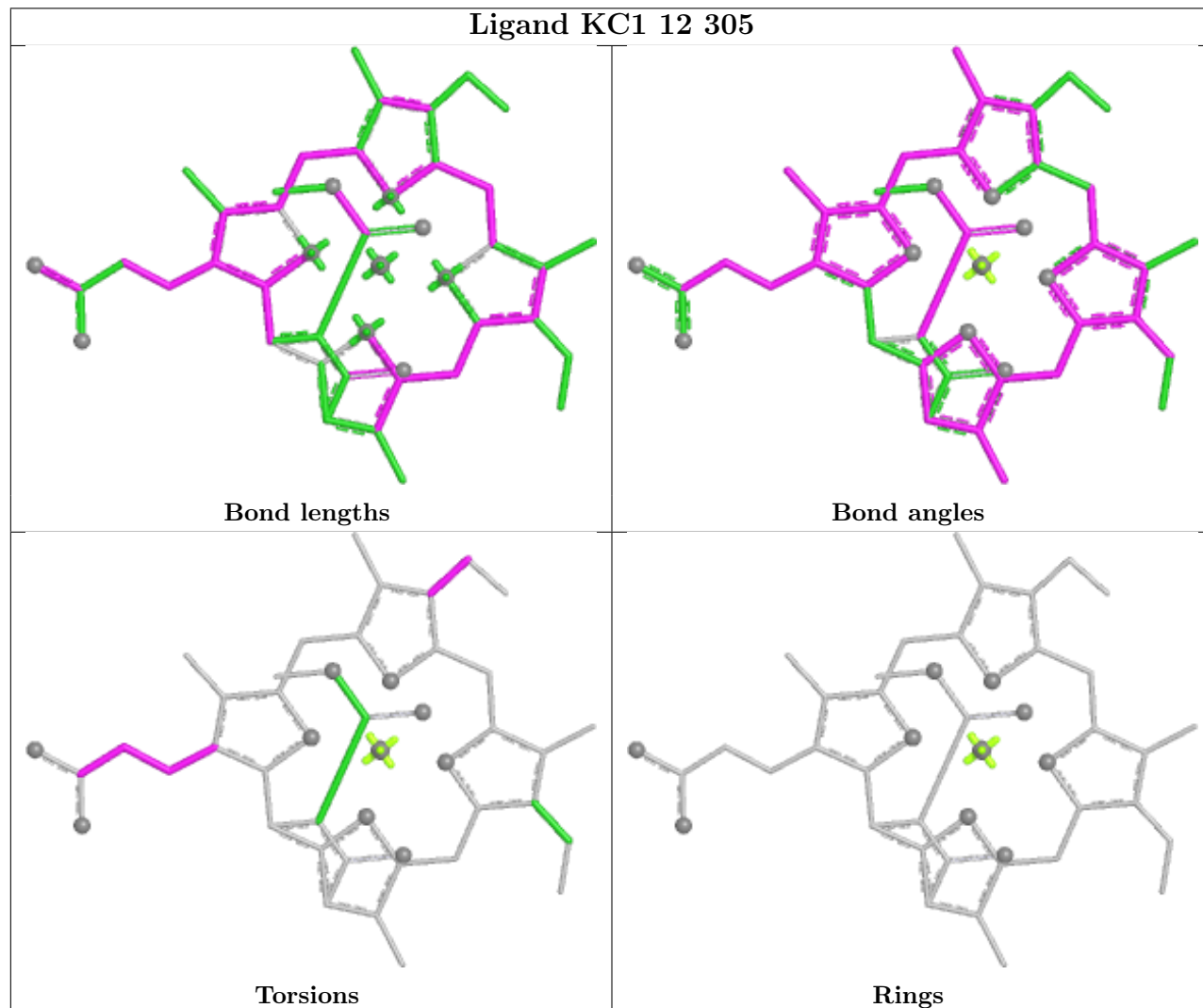


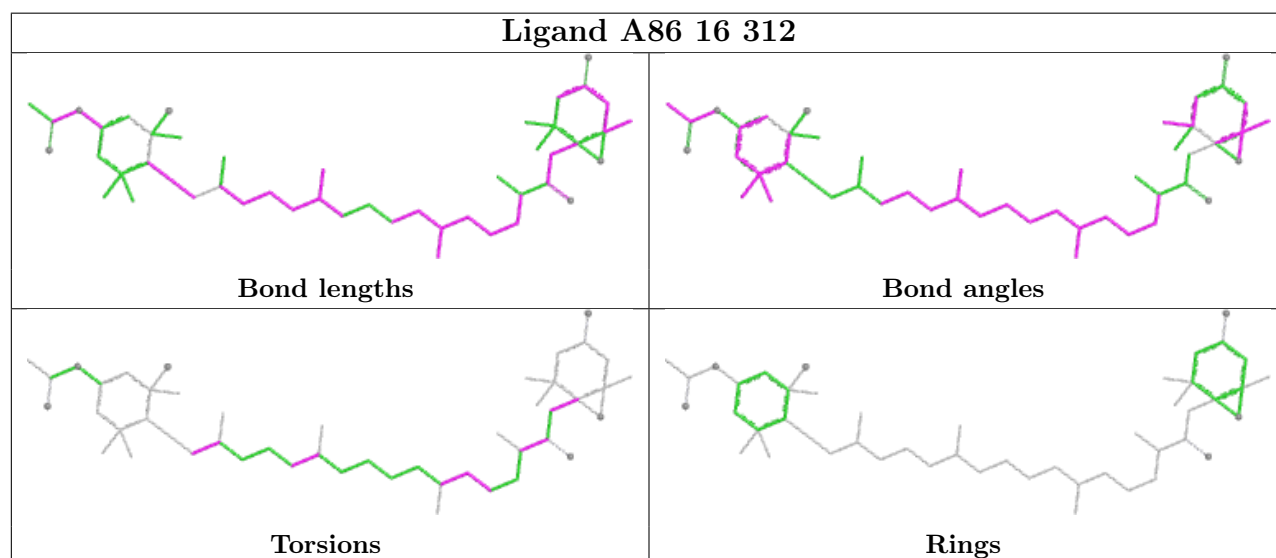
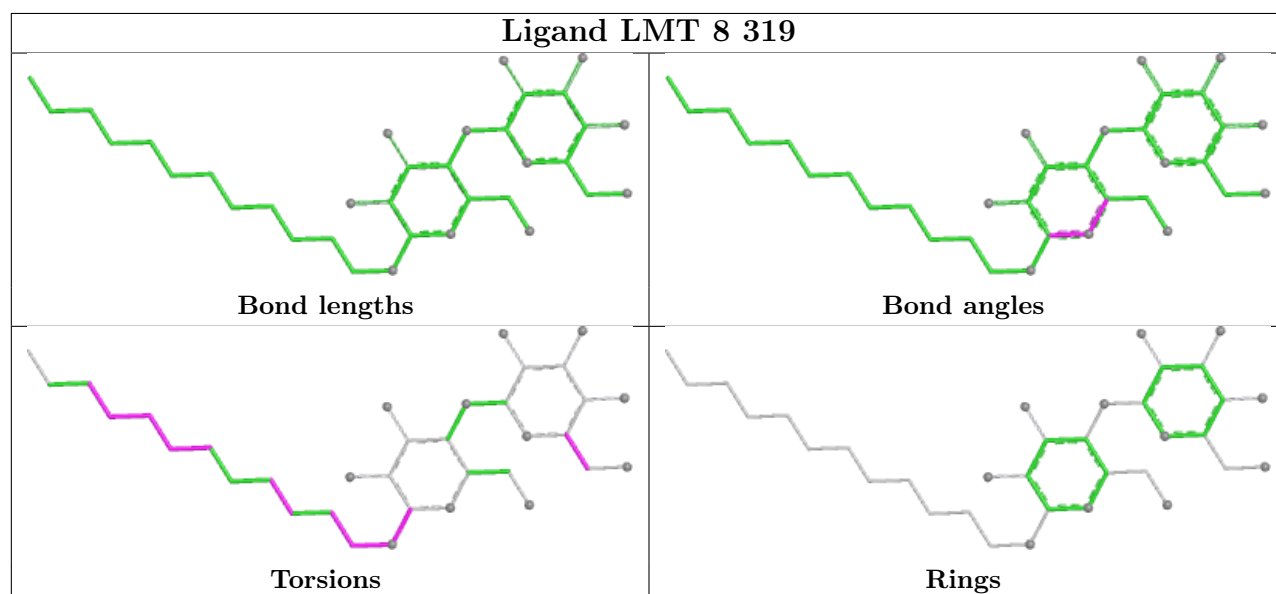
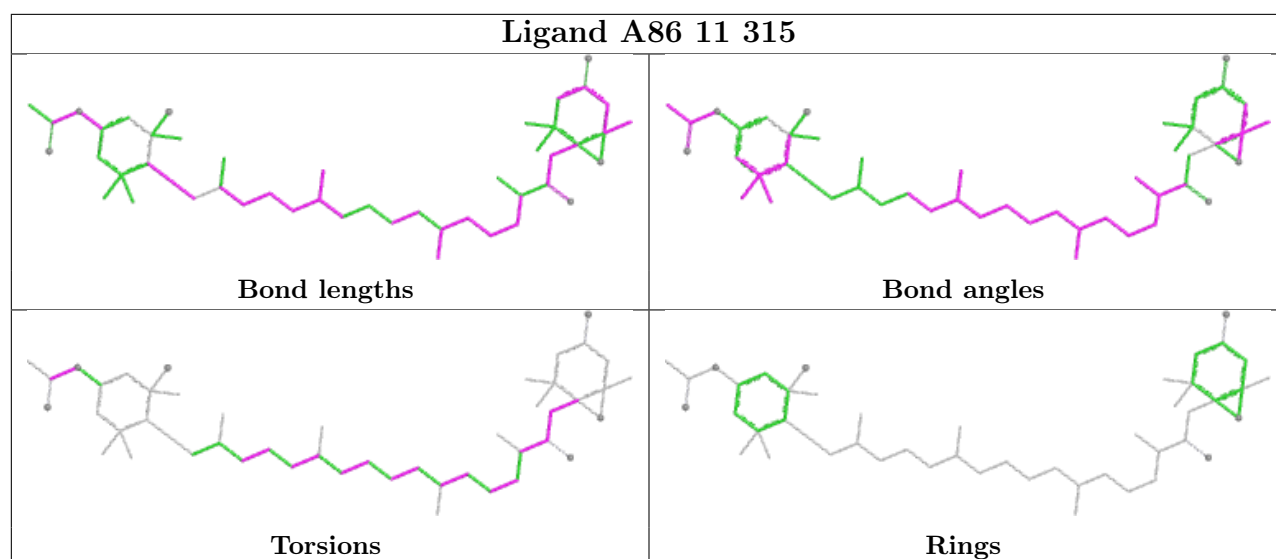
Rings

Ligand CLA 6 303

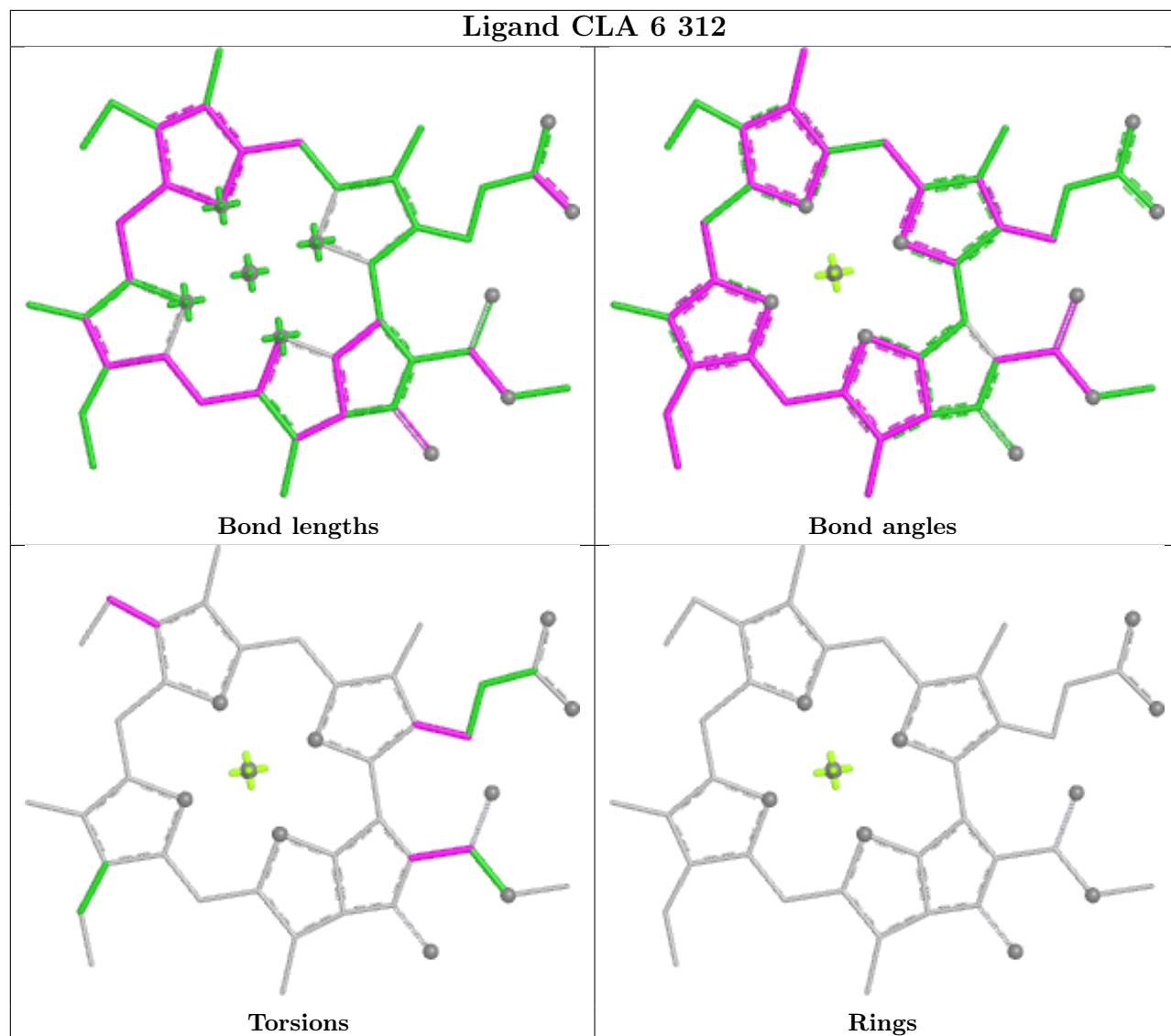


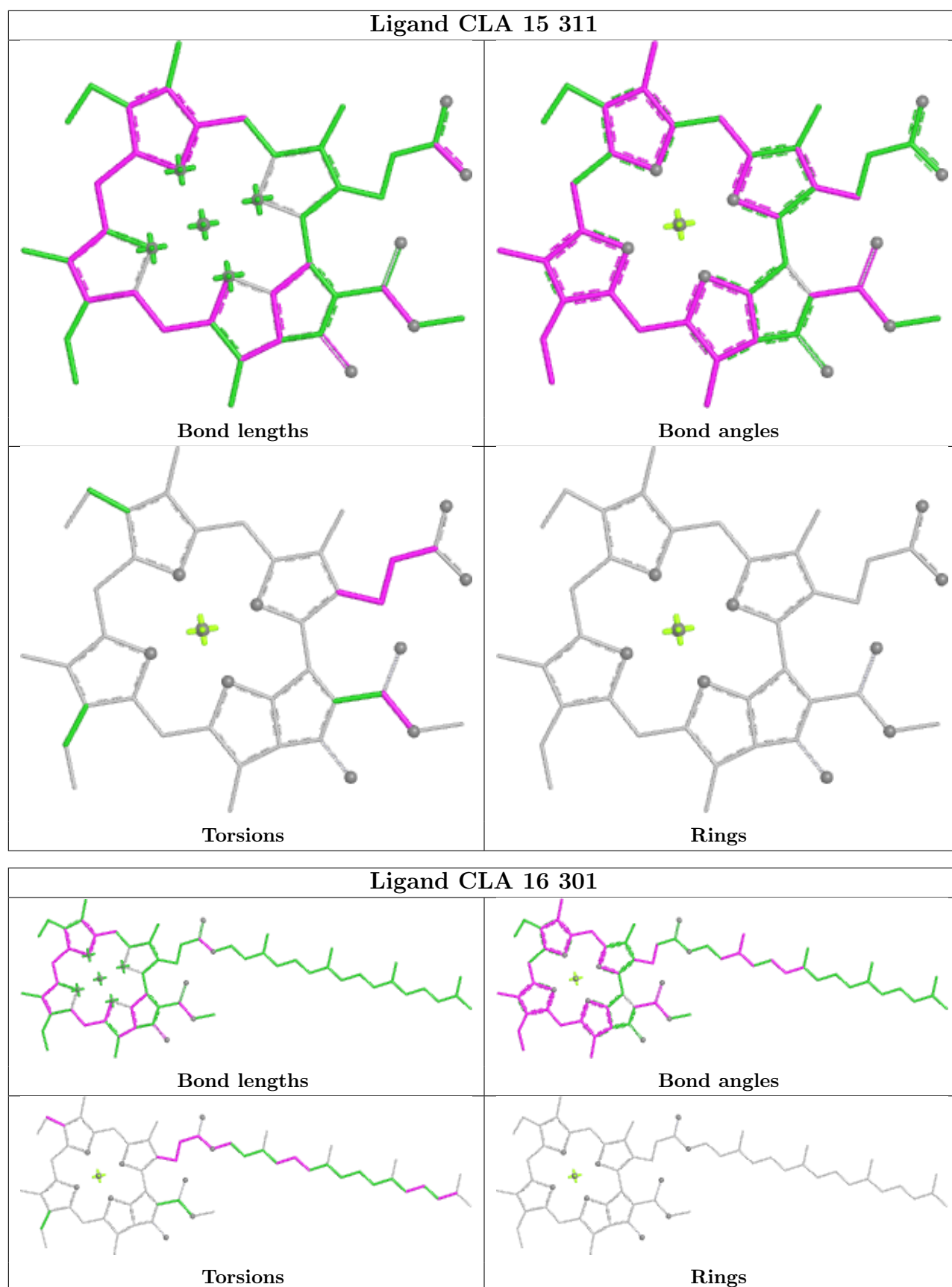
Ligand KC1 12 305

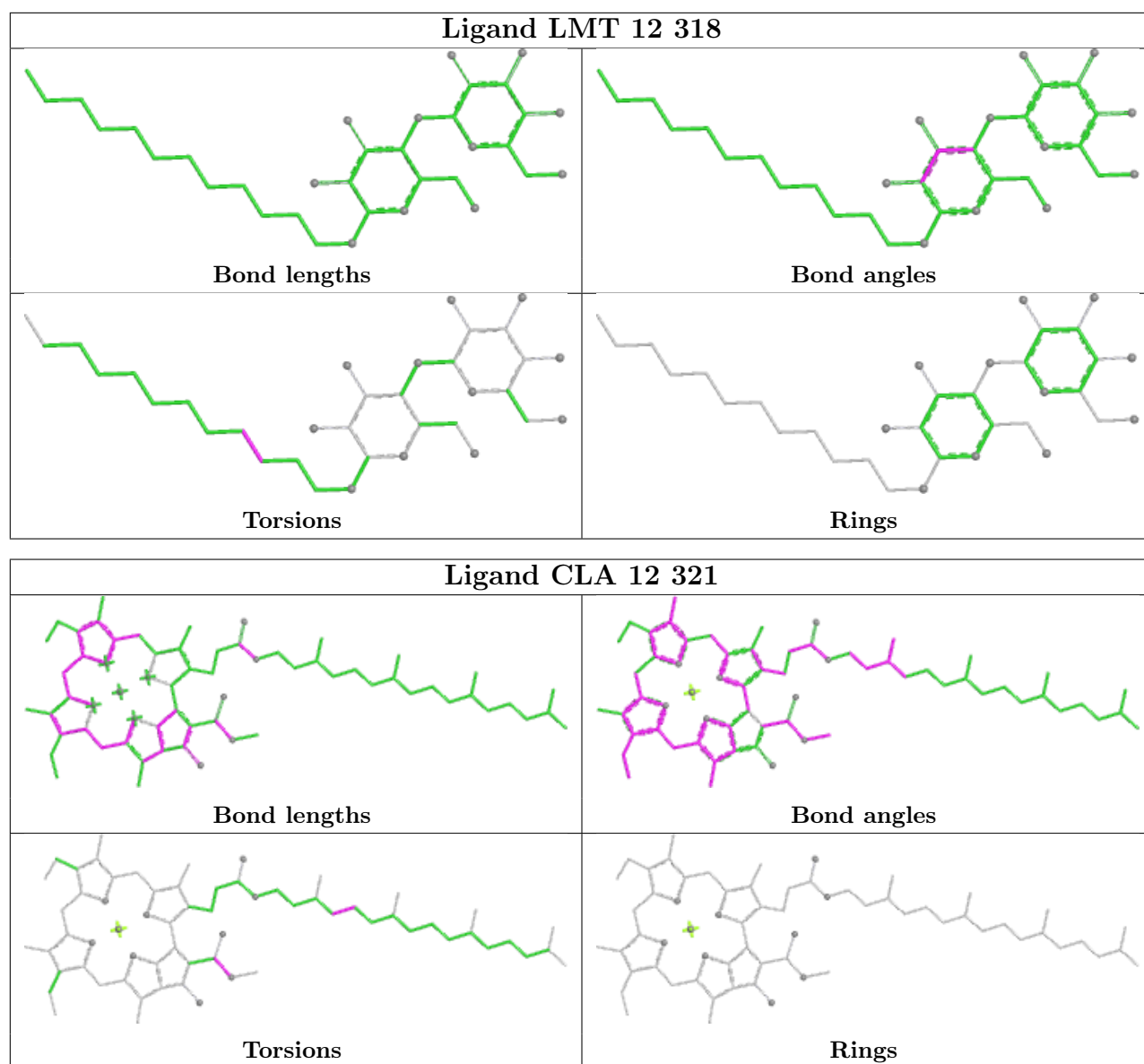




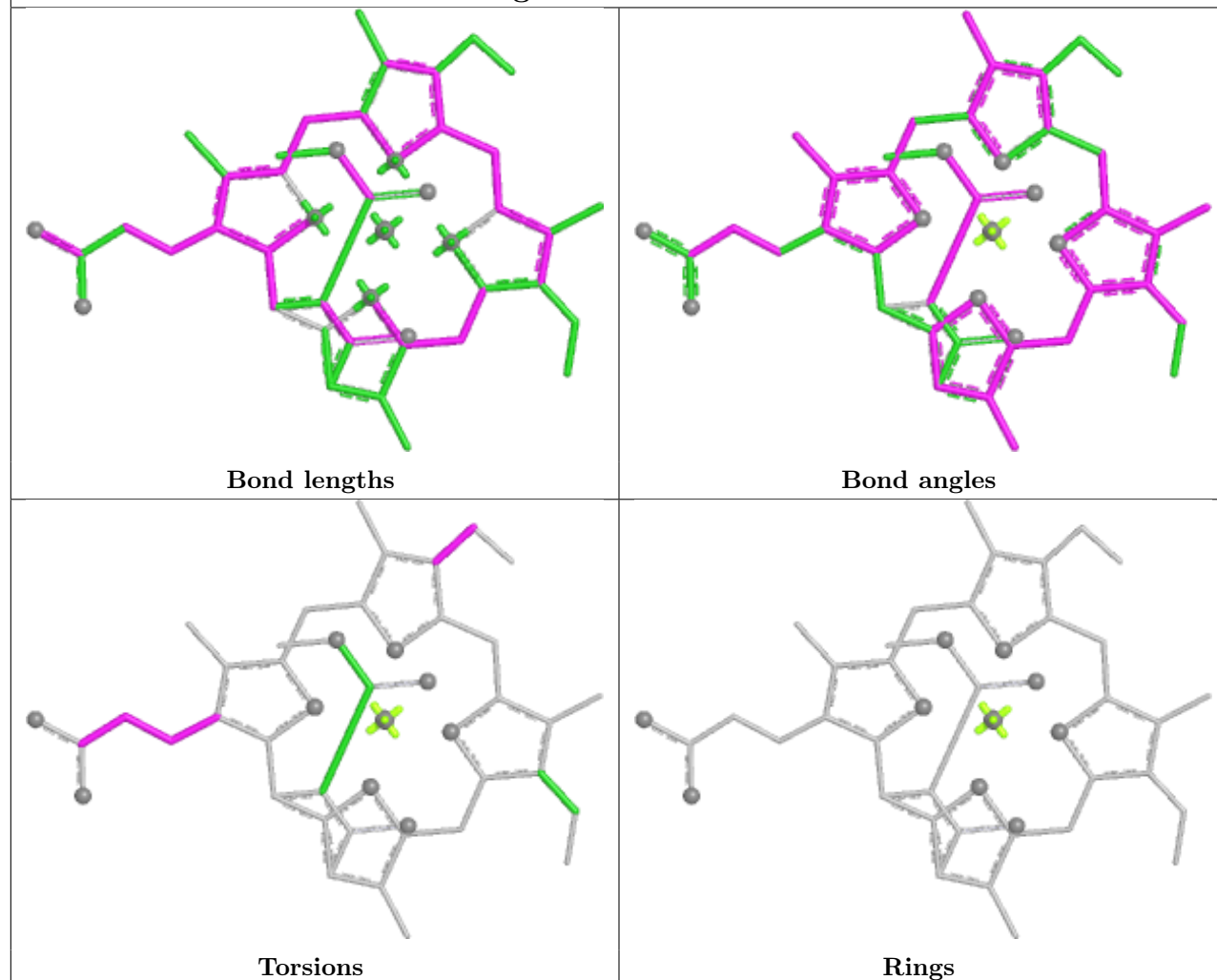
Ligand CLA 6 312



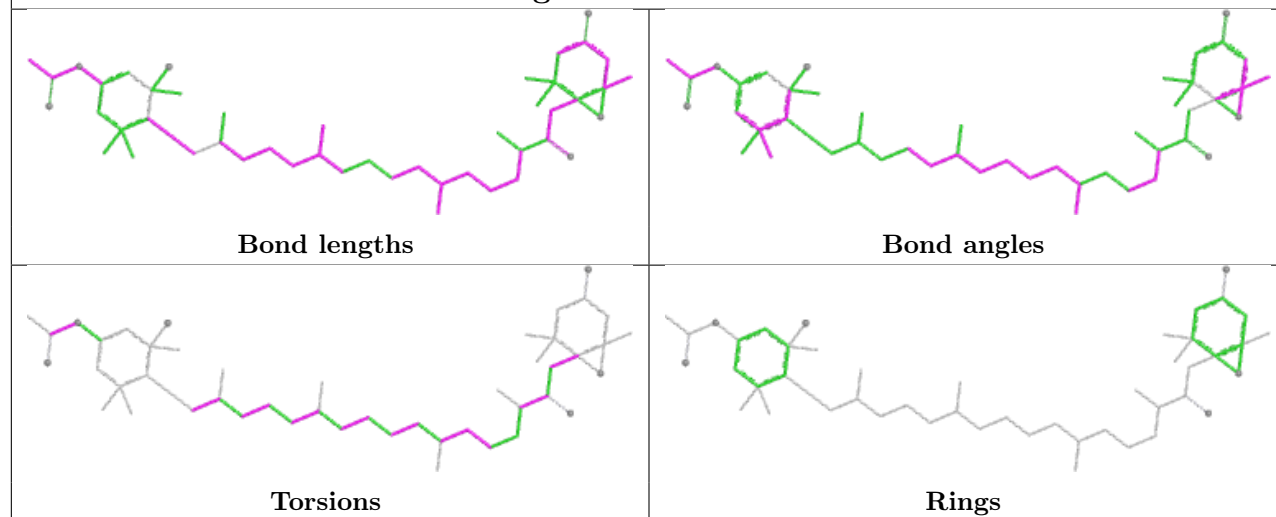


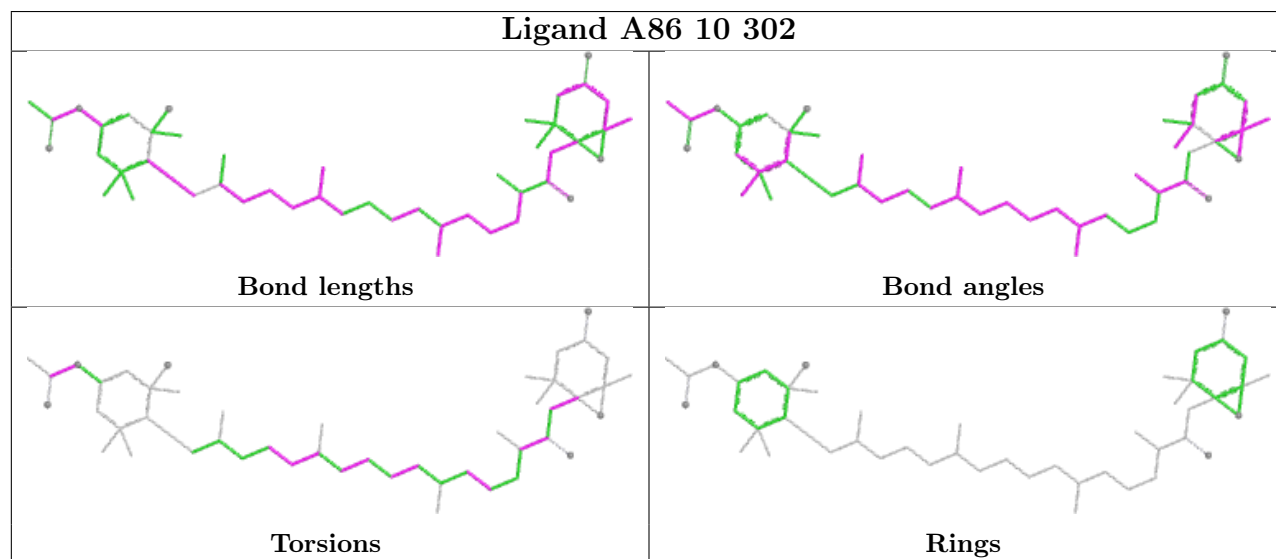
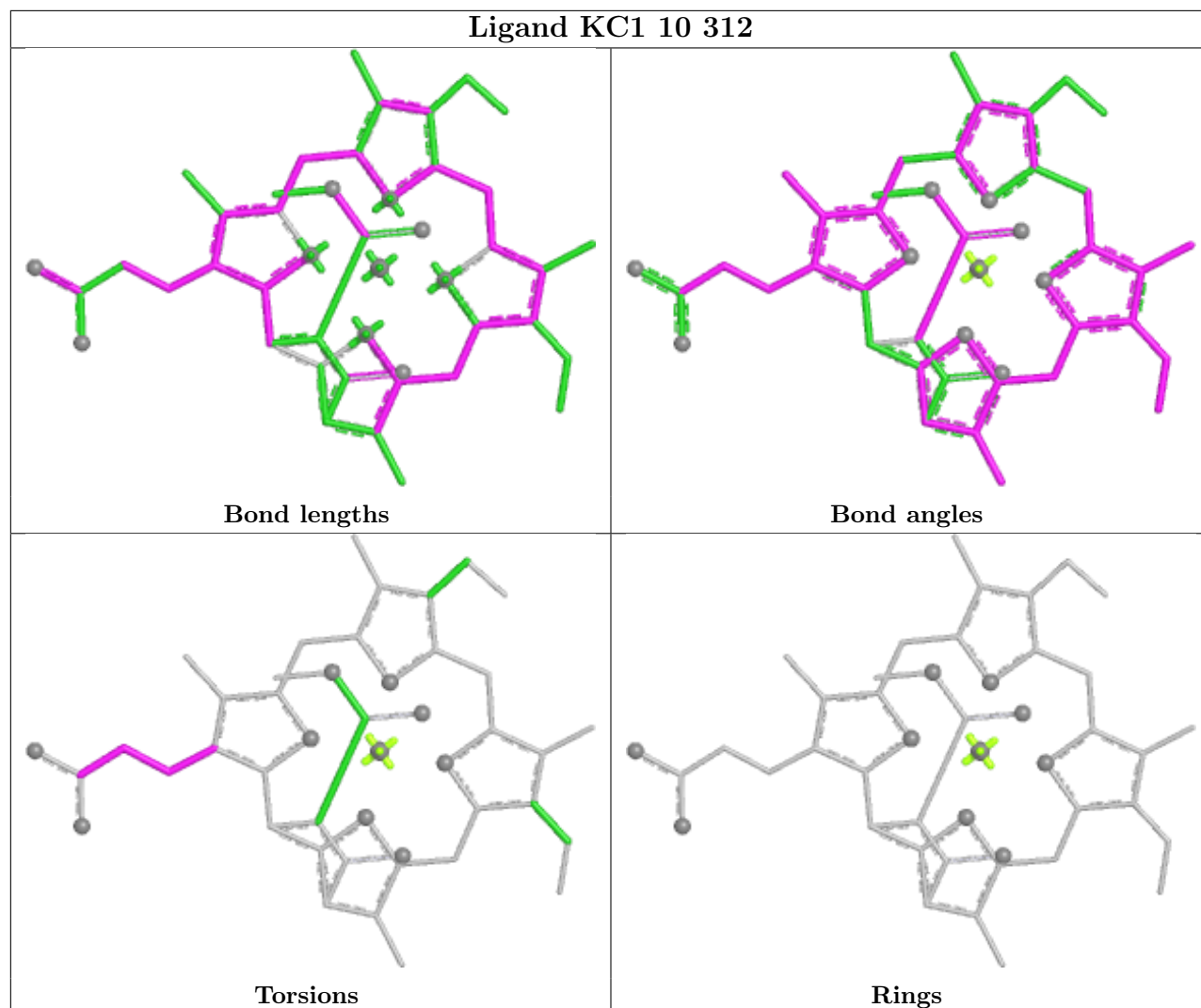


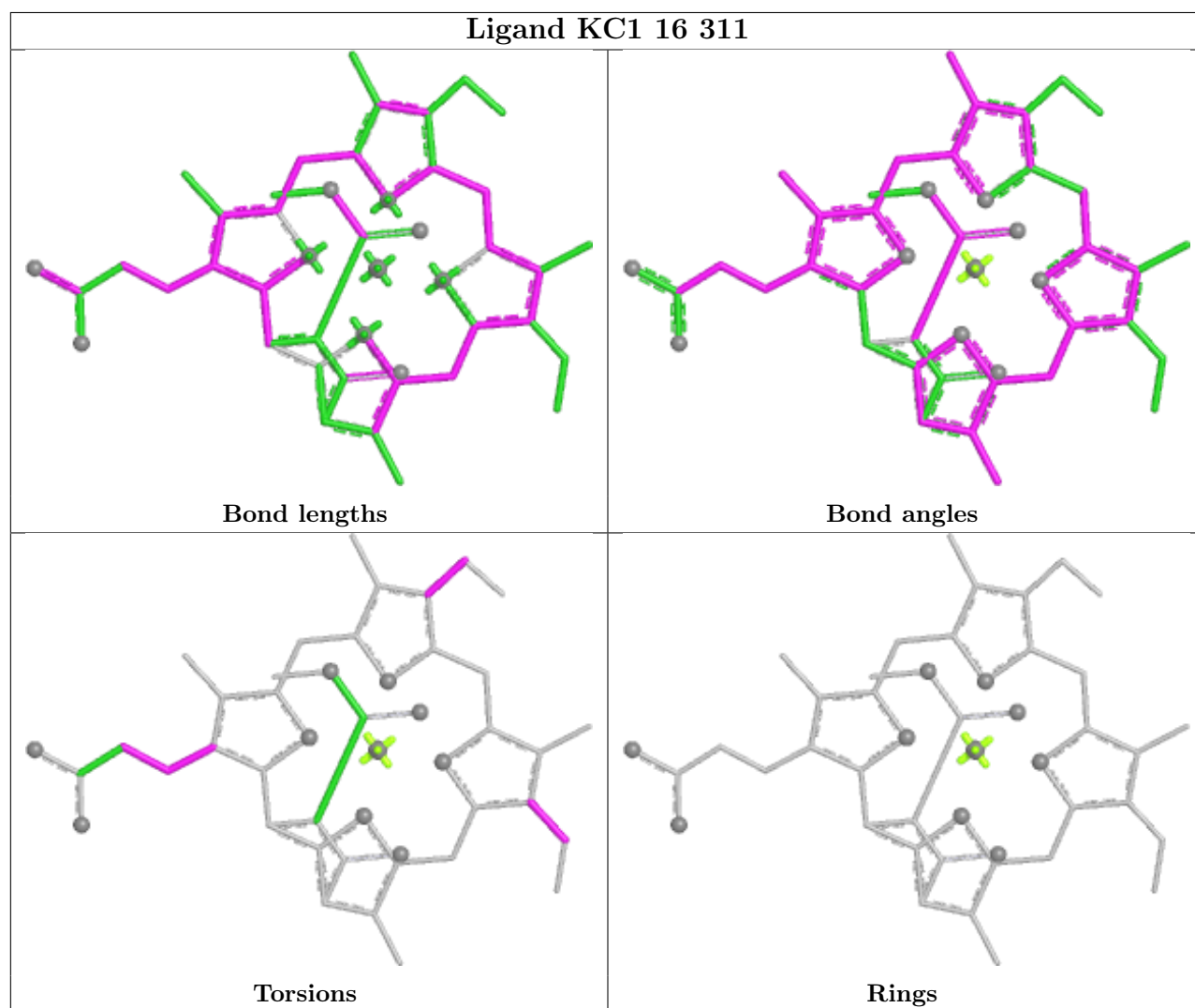
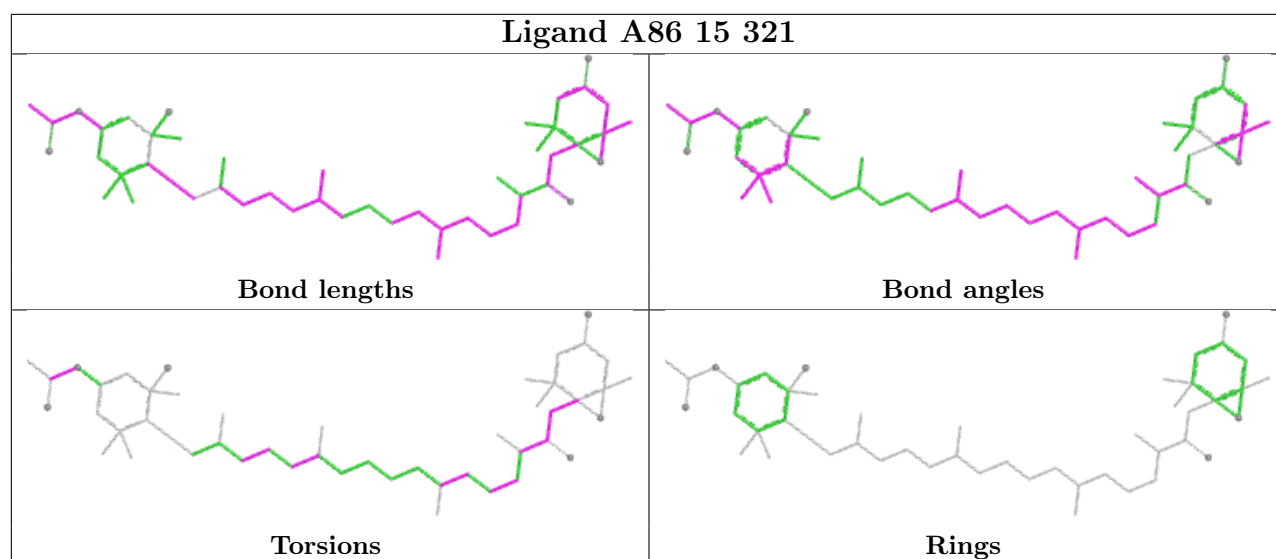
Ligand KC1 6 305



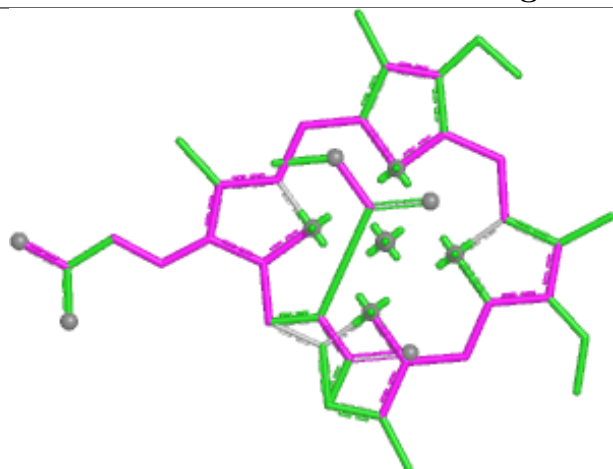
Ligand A86 14 321



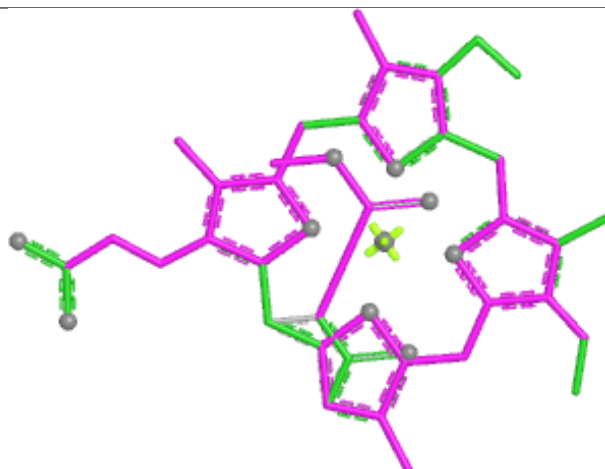




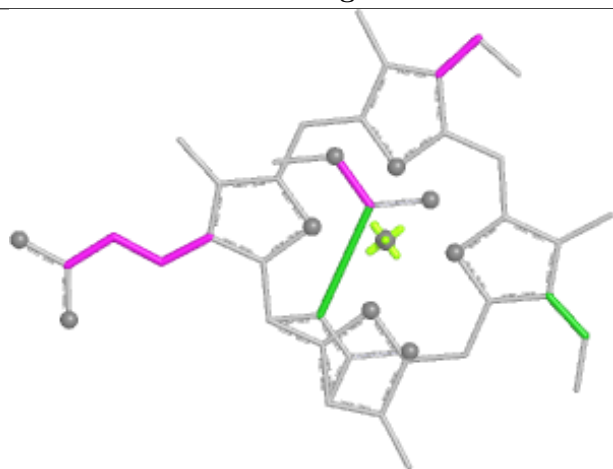
Ligand KC1 8 311



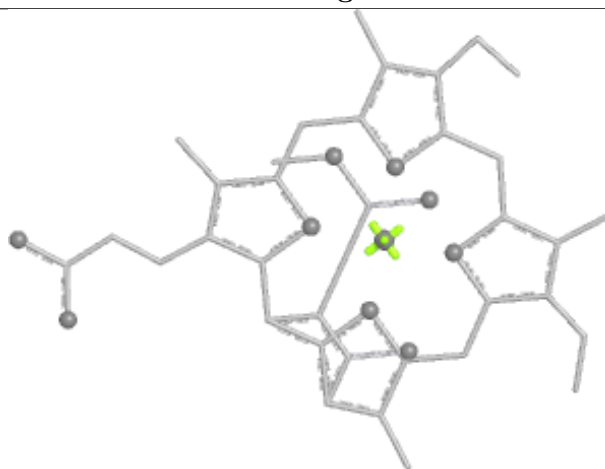
Bond lengths



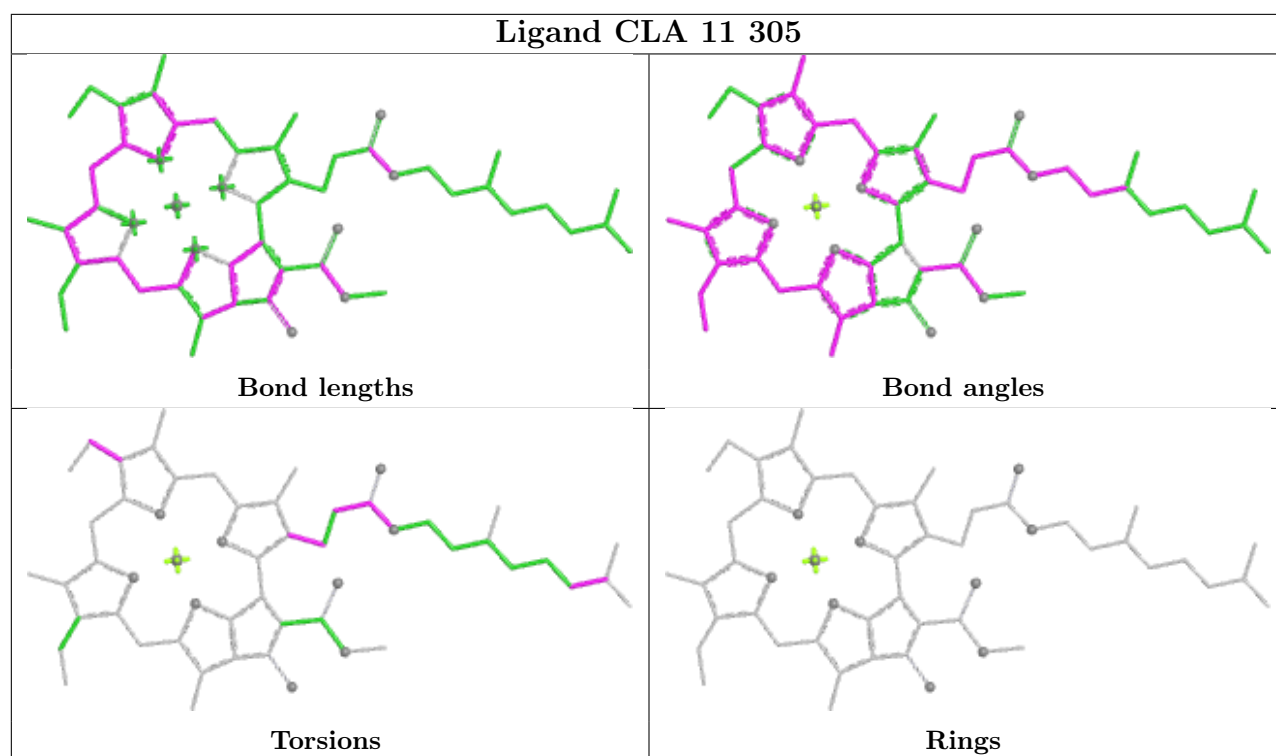
Bond angles

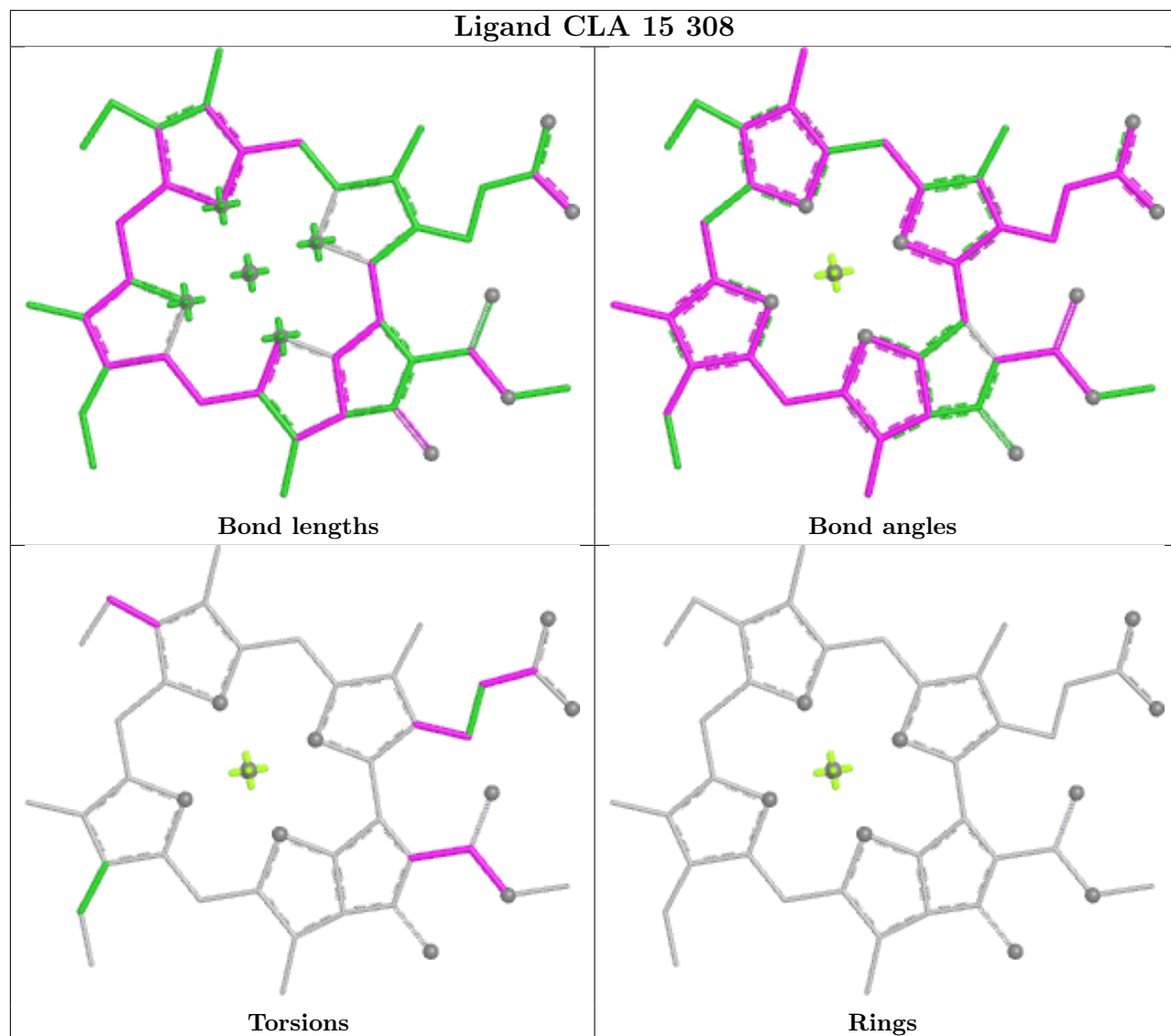


Torsions

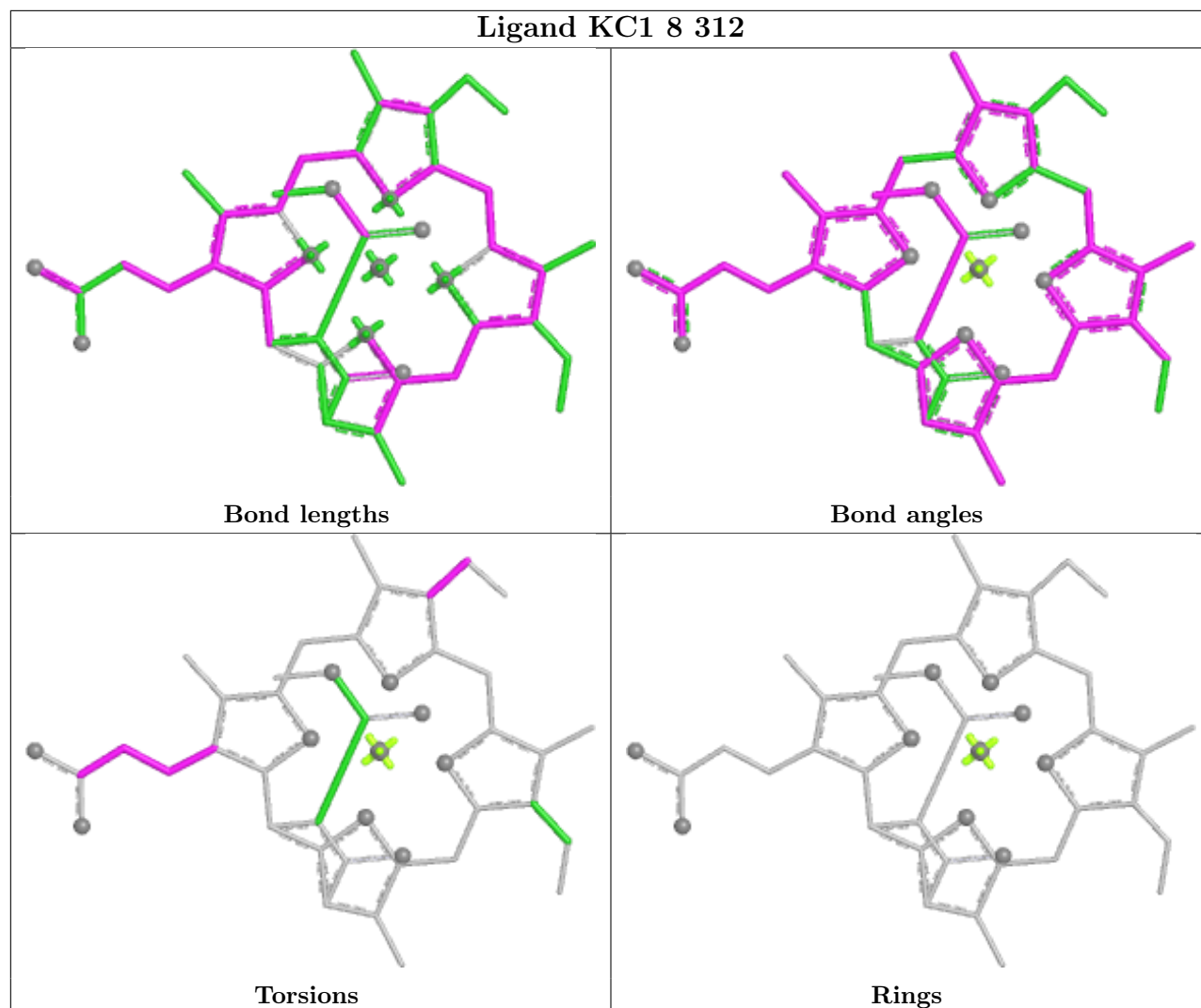


Rings

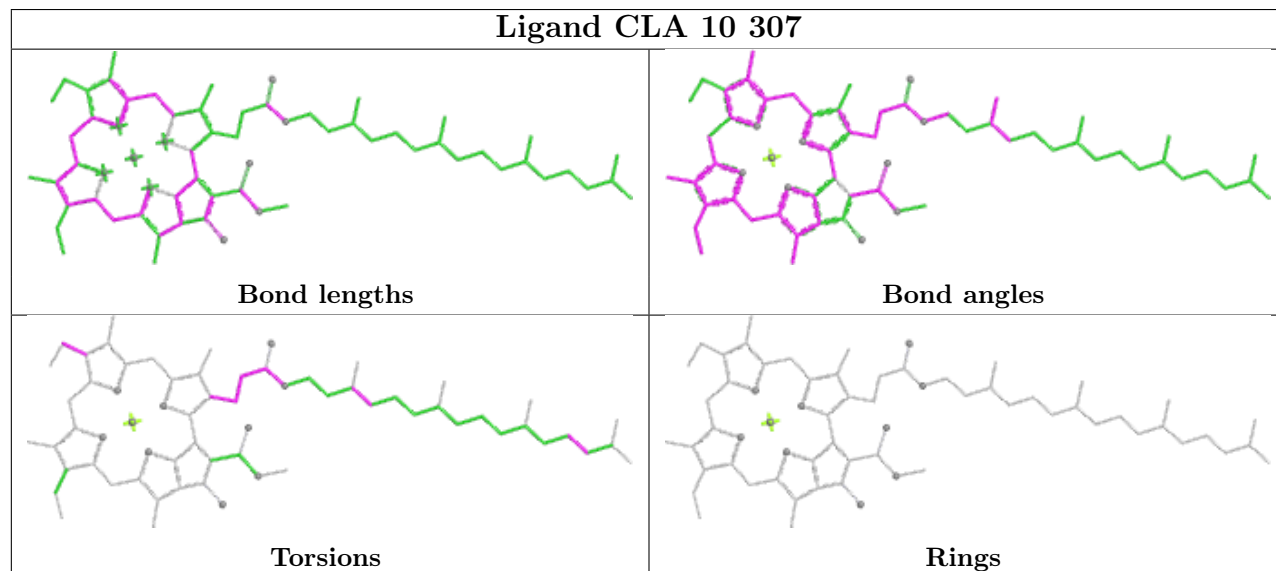


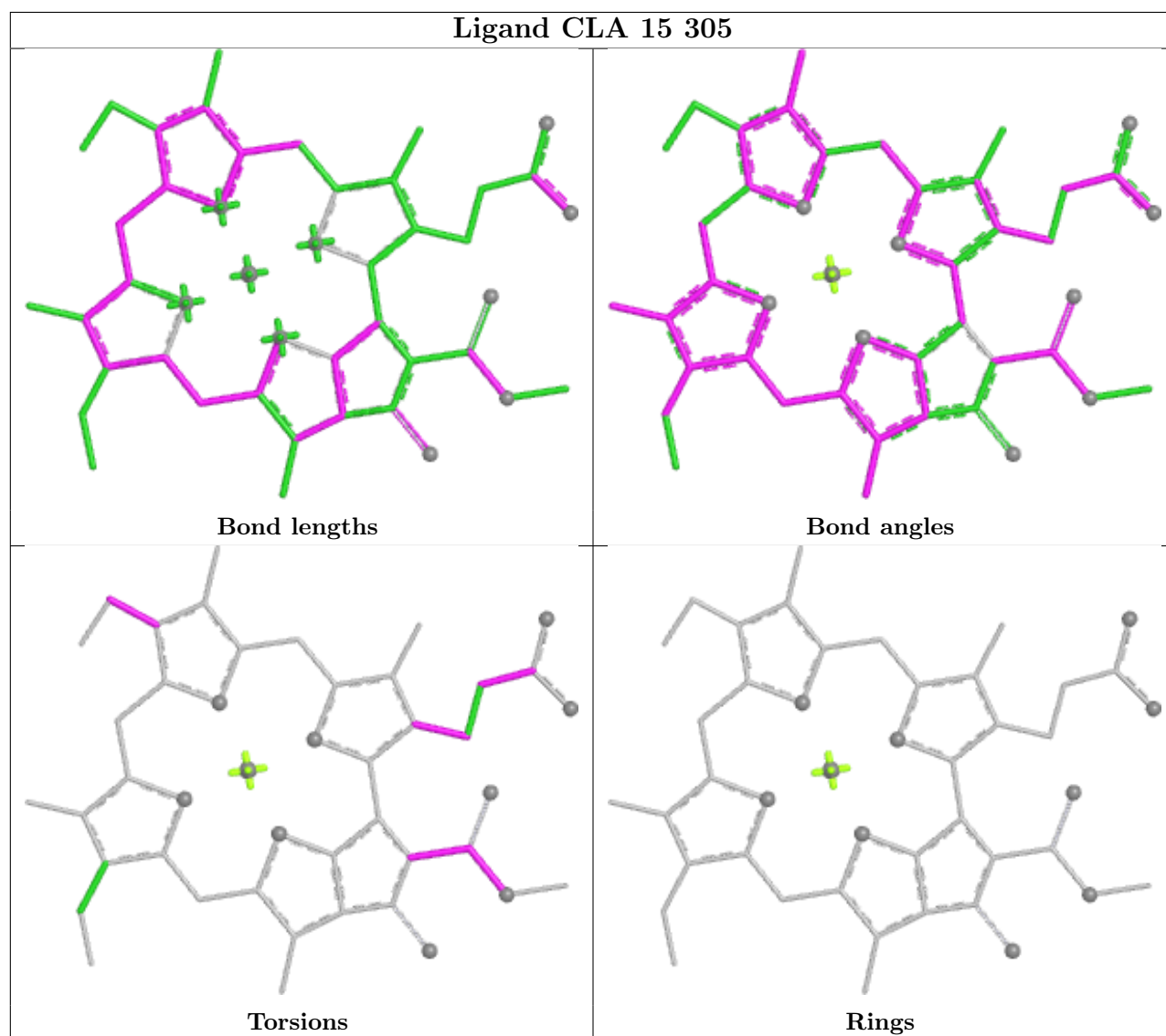
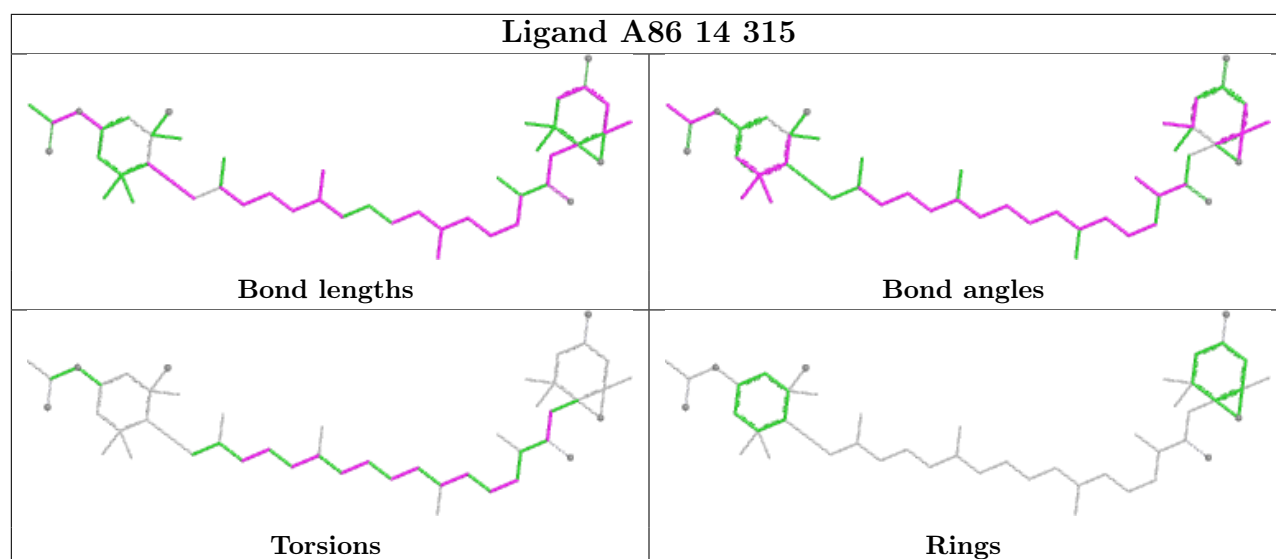


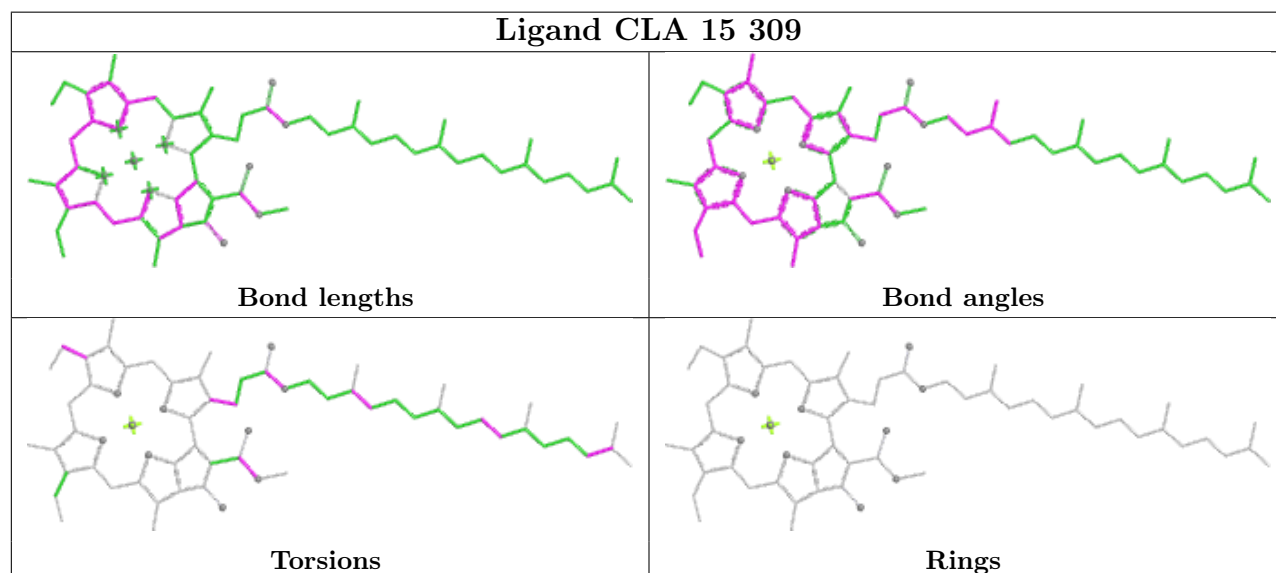
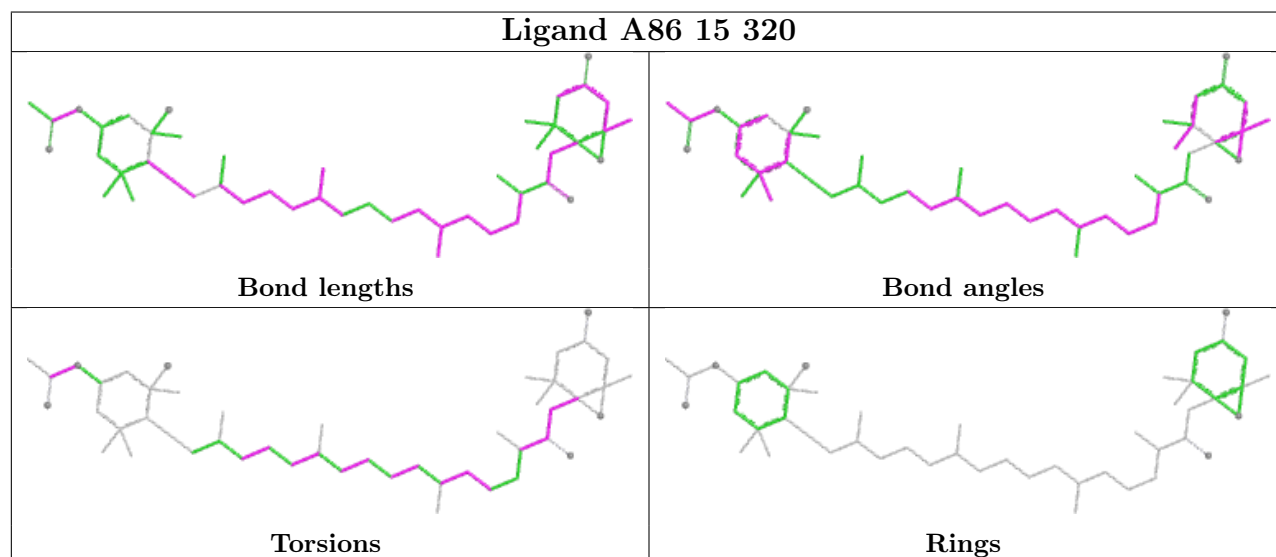
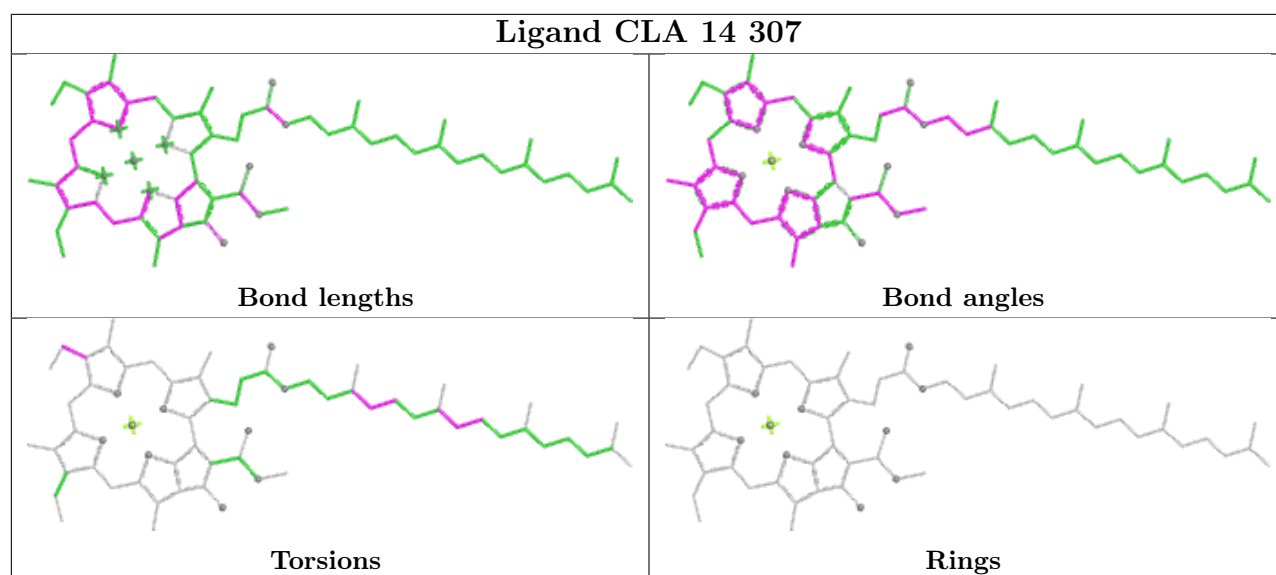
Ligand KC1 8 312

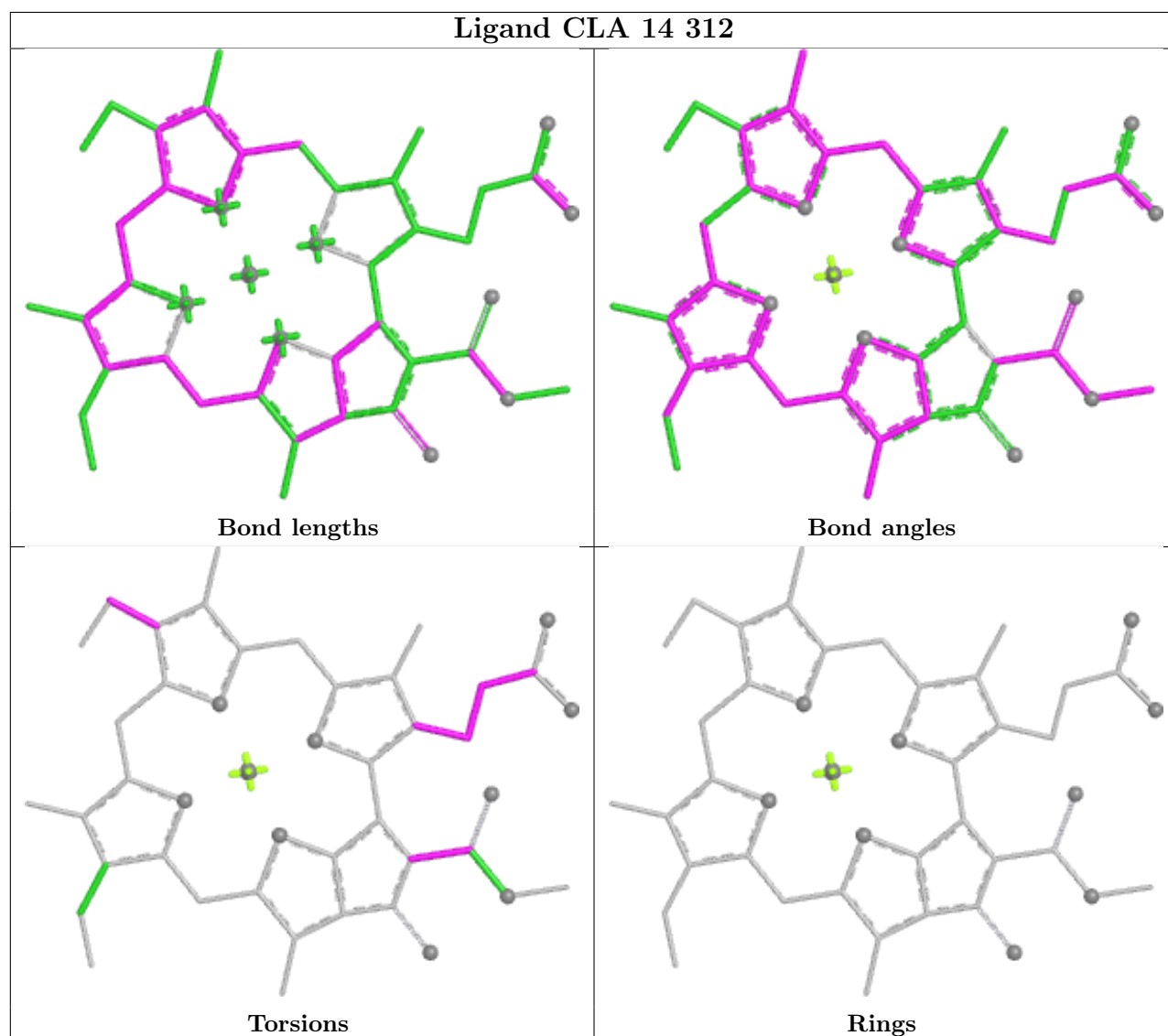
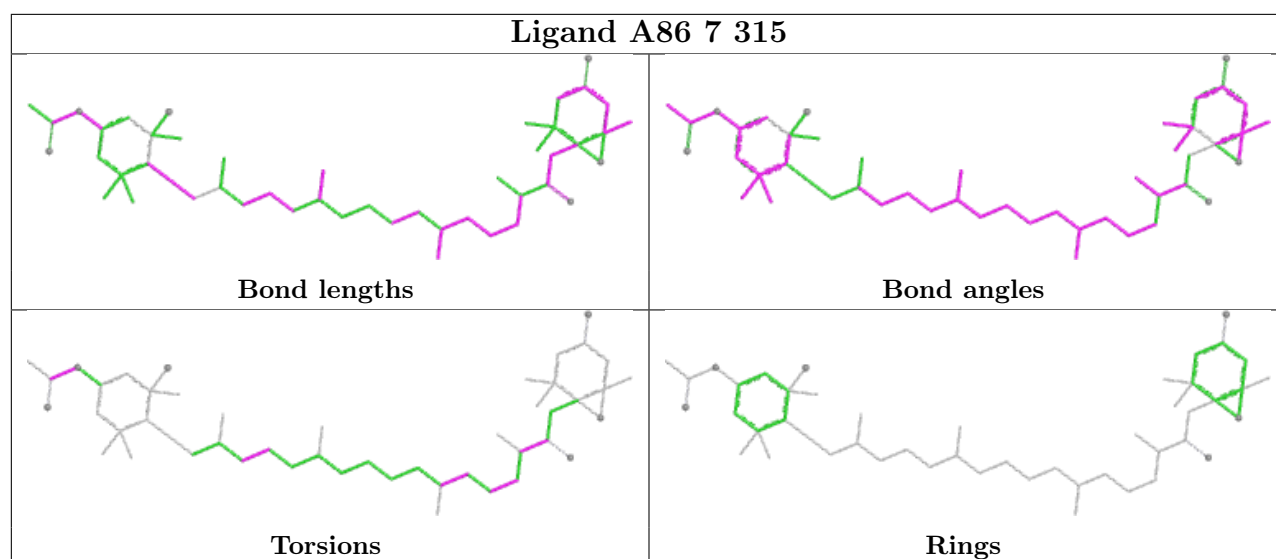


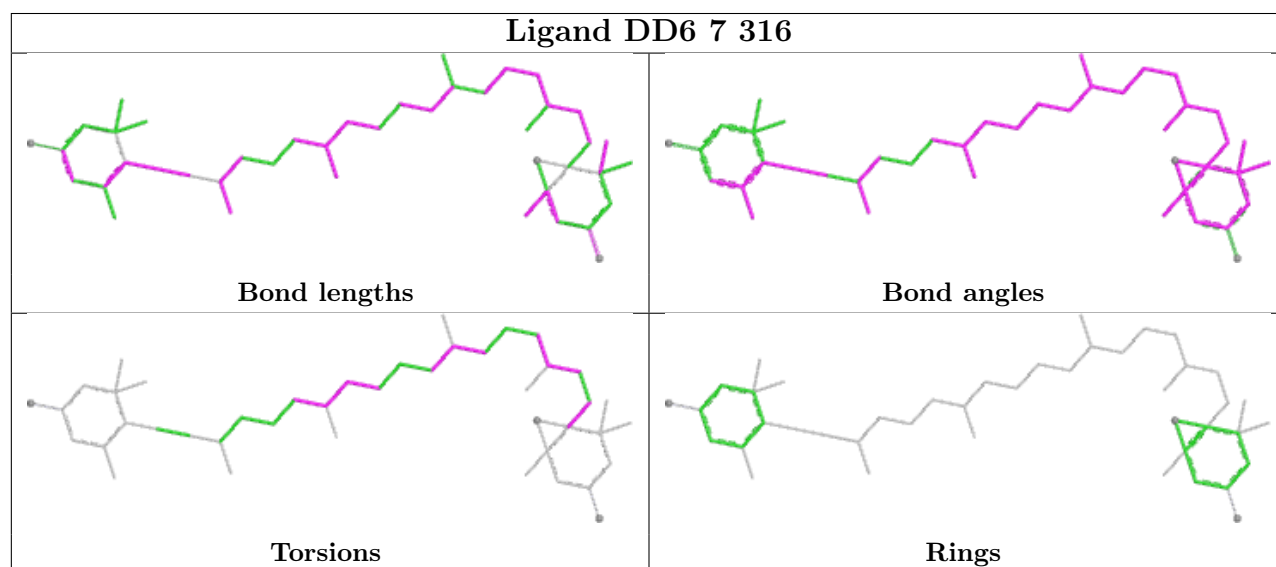
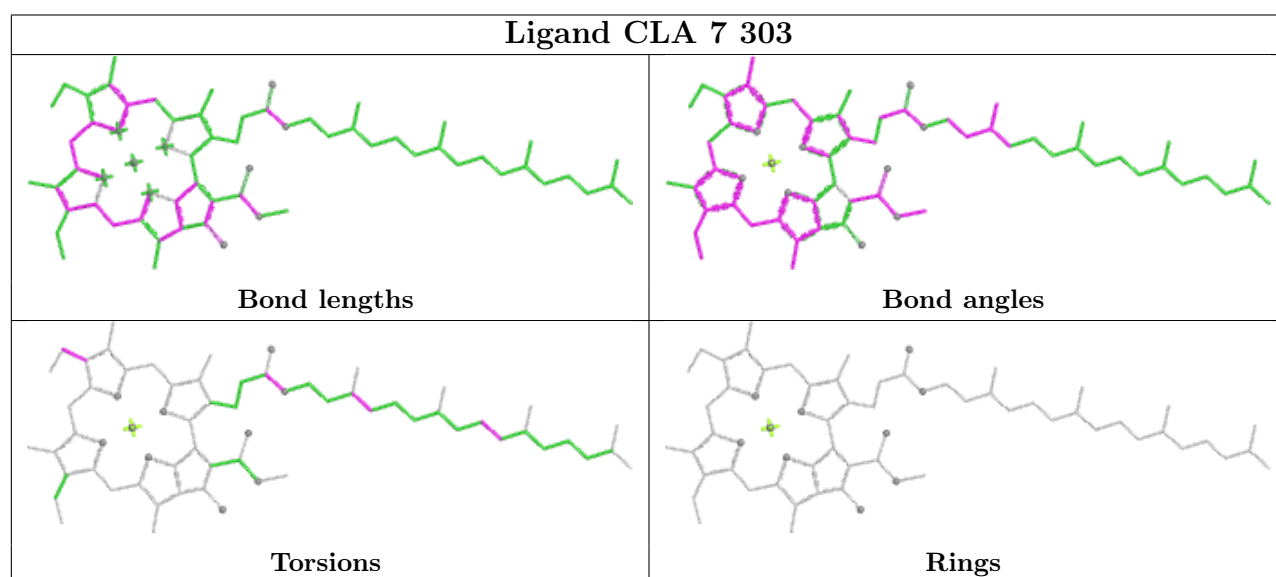
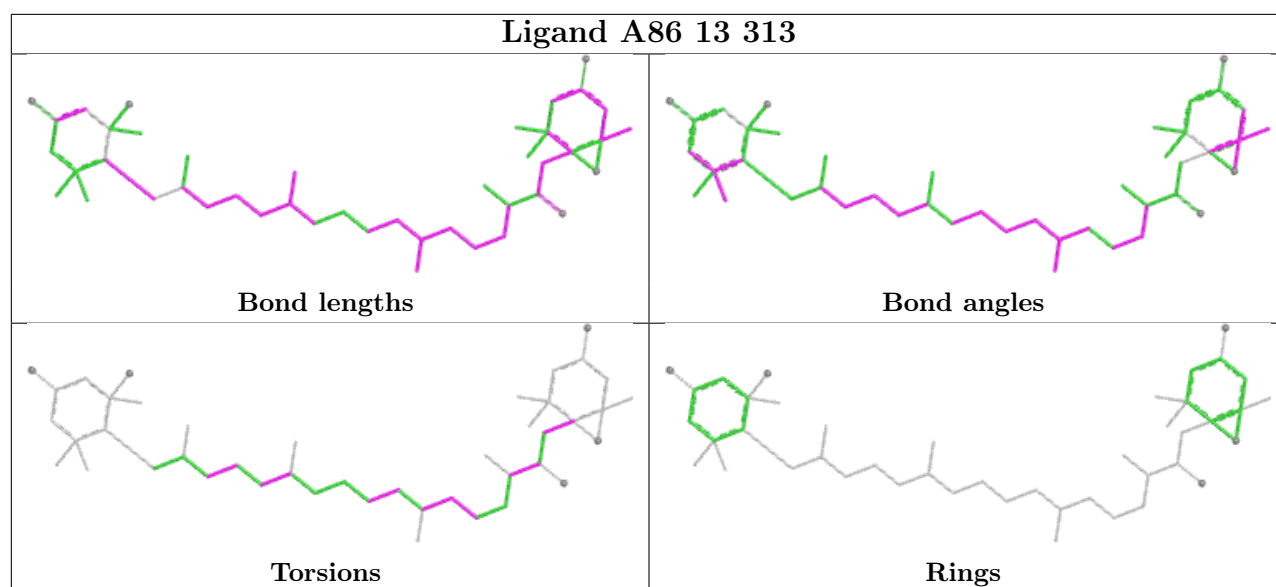
Ligand CLA 10 307

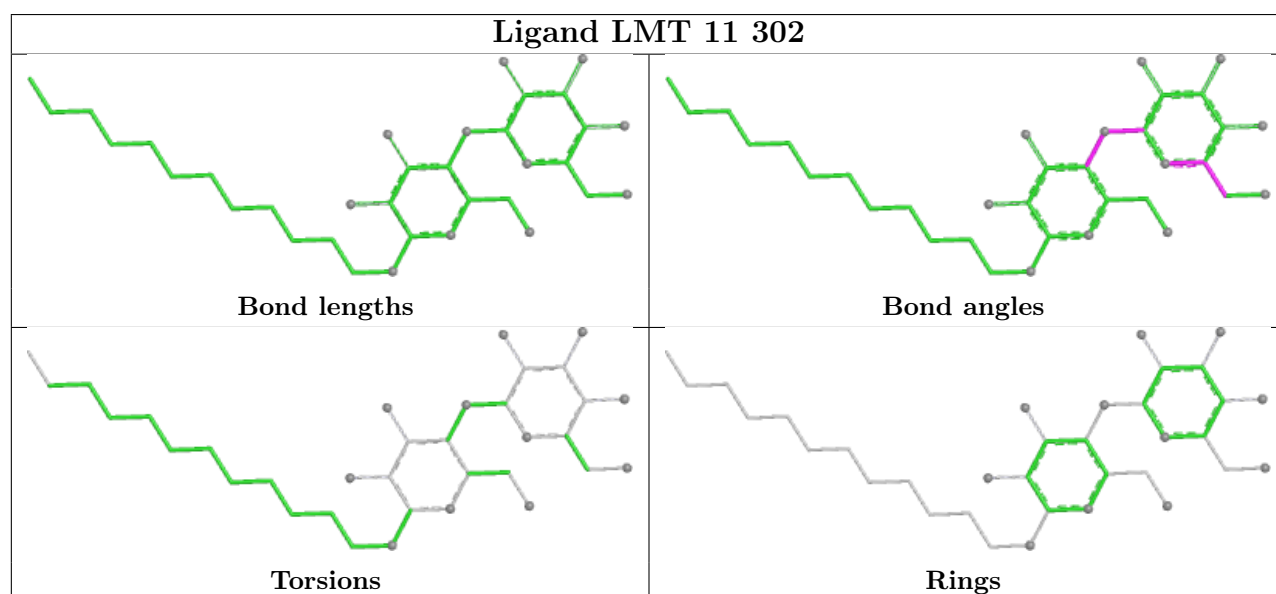
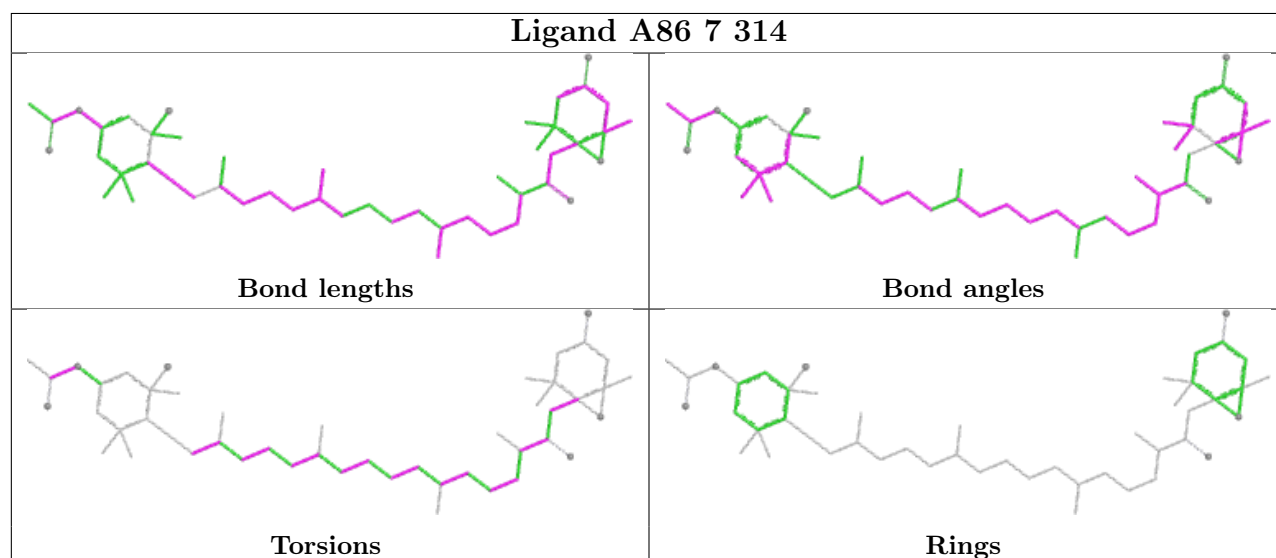
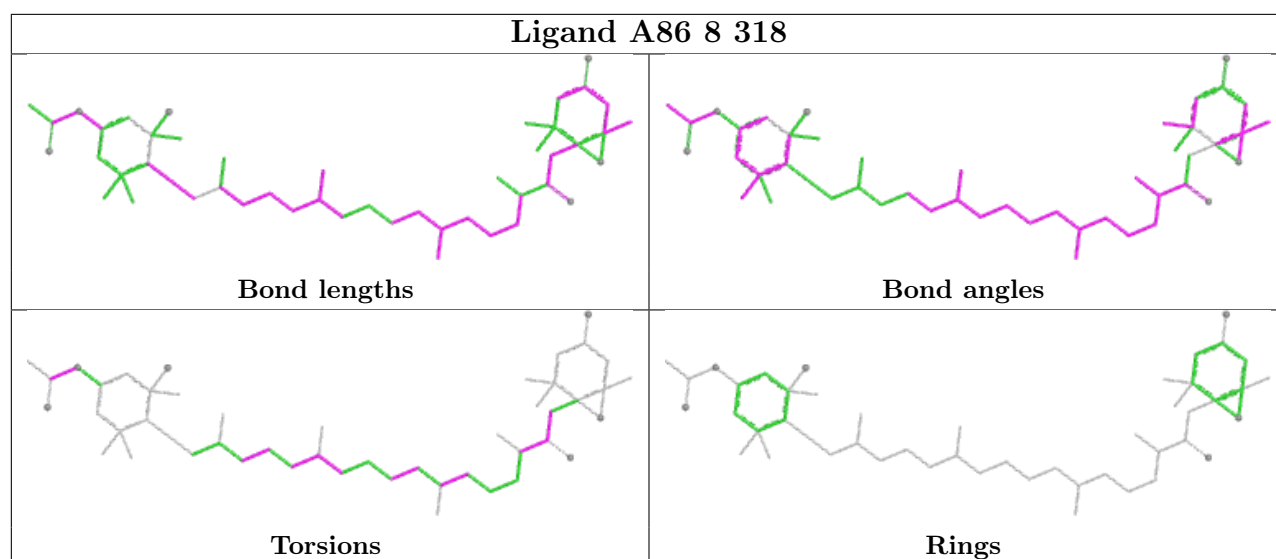




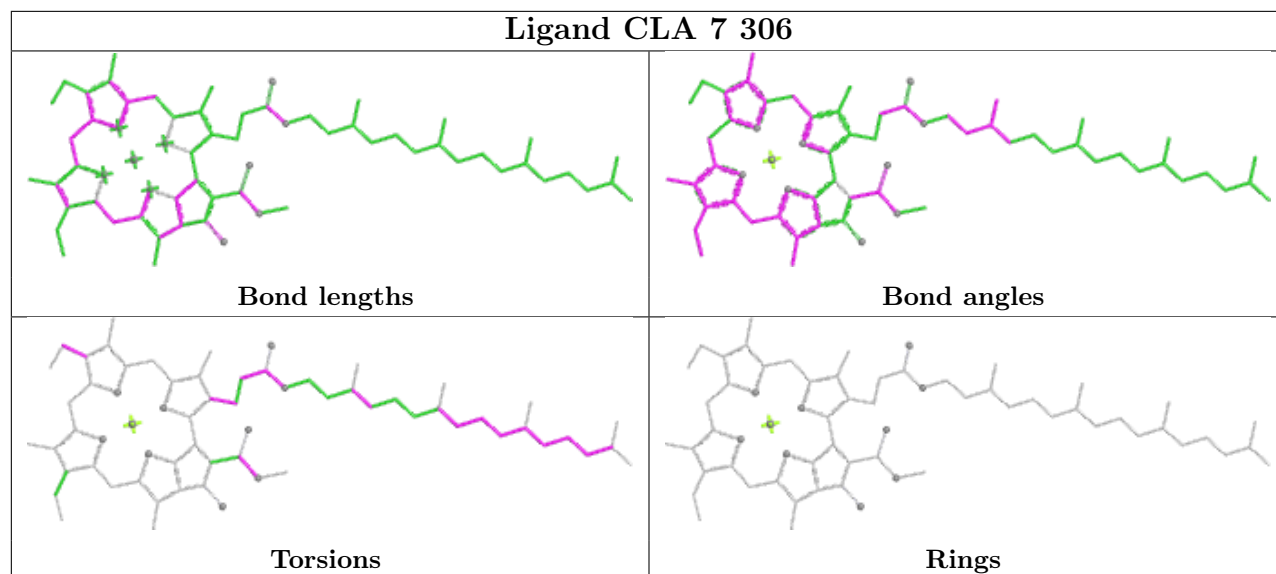




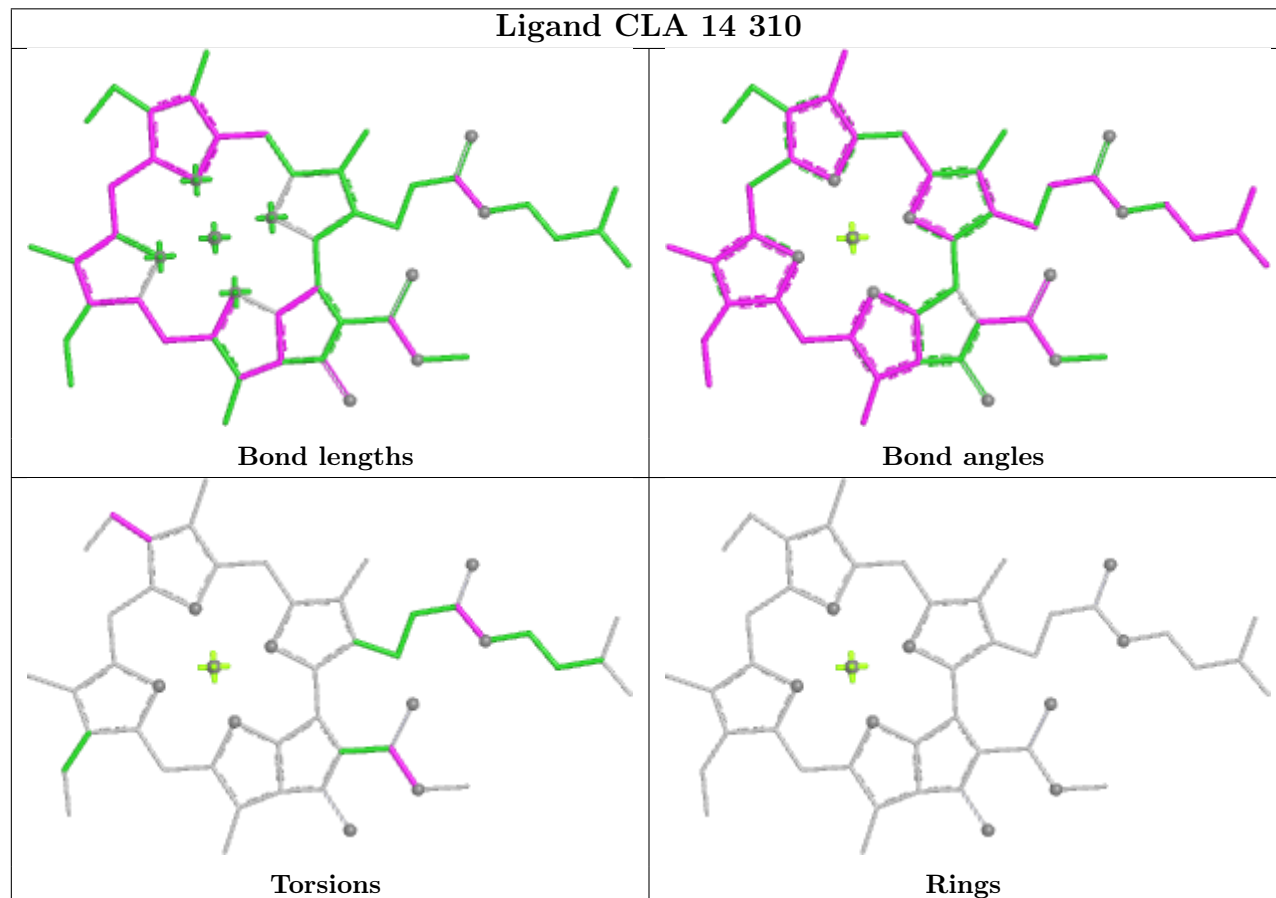


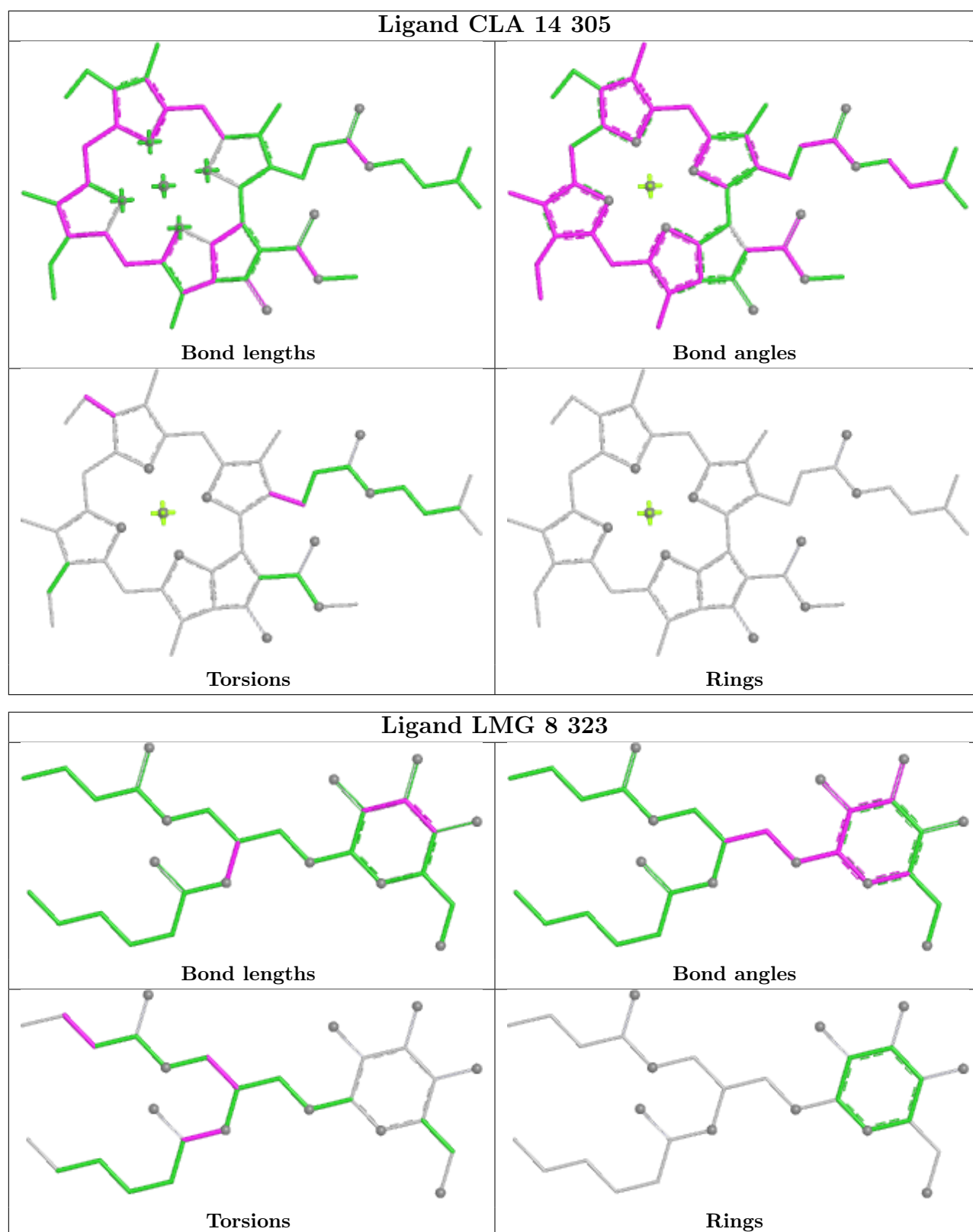


Ligand CLA 7 306

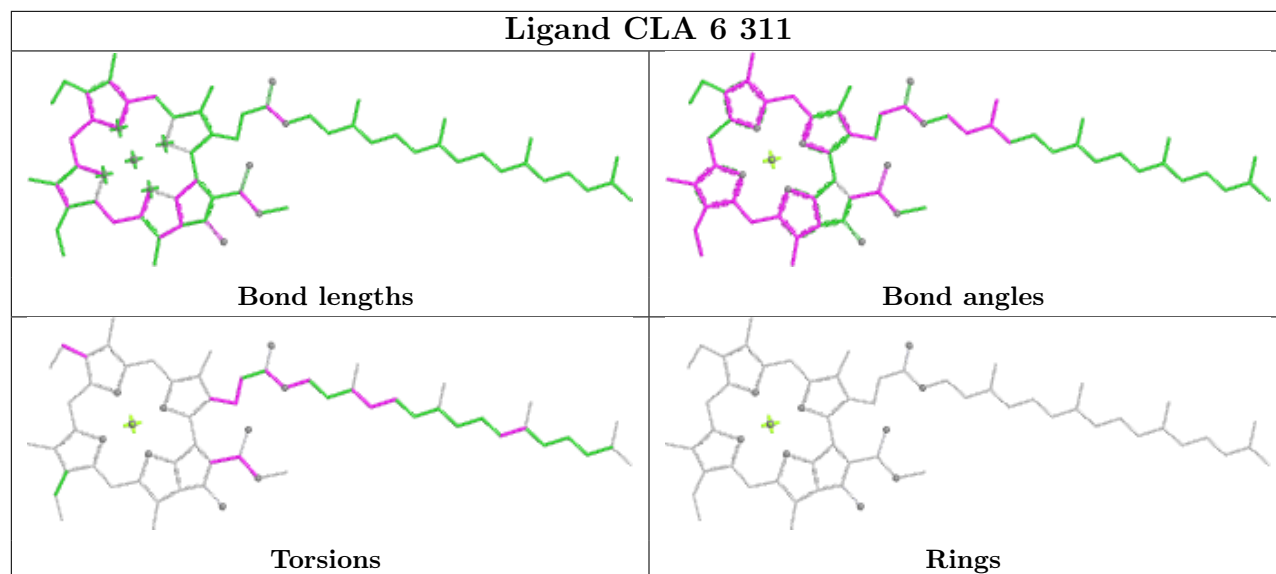


Ligand CLA 14 310

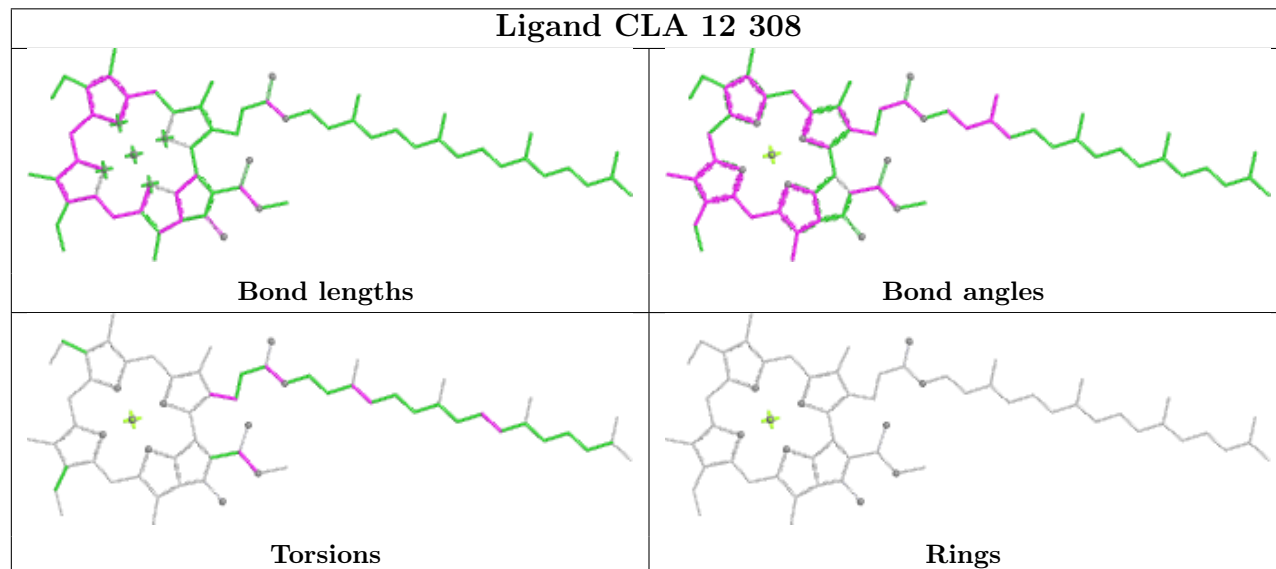




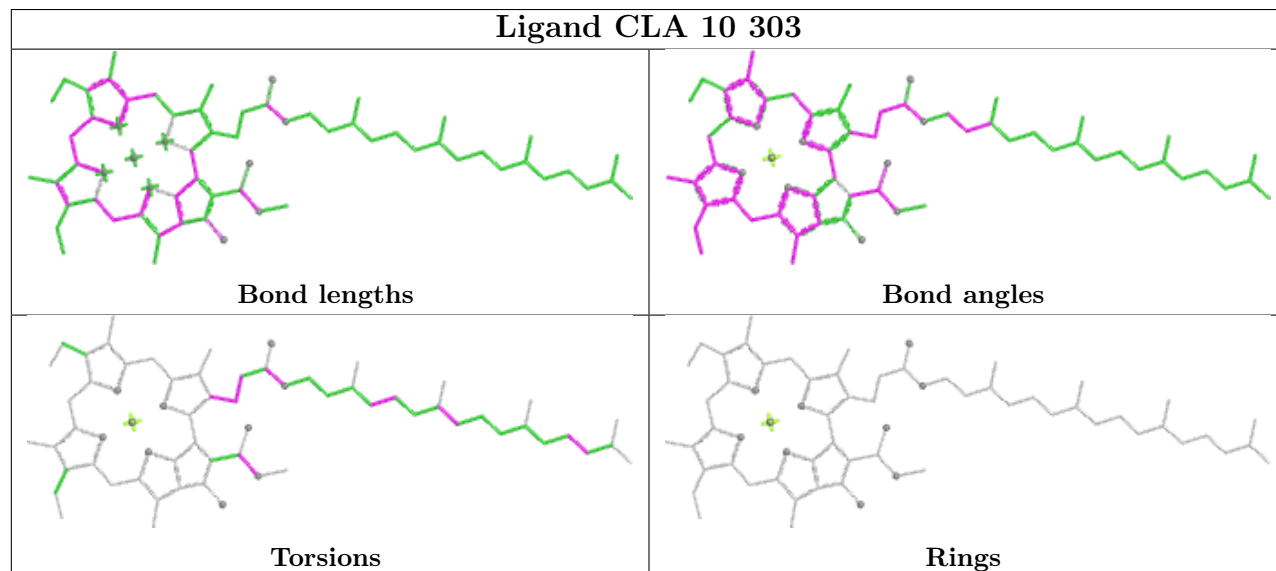
Ligand CLA 6 311



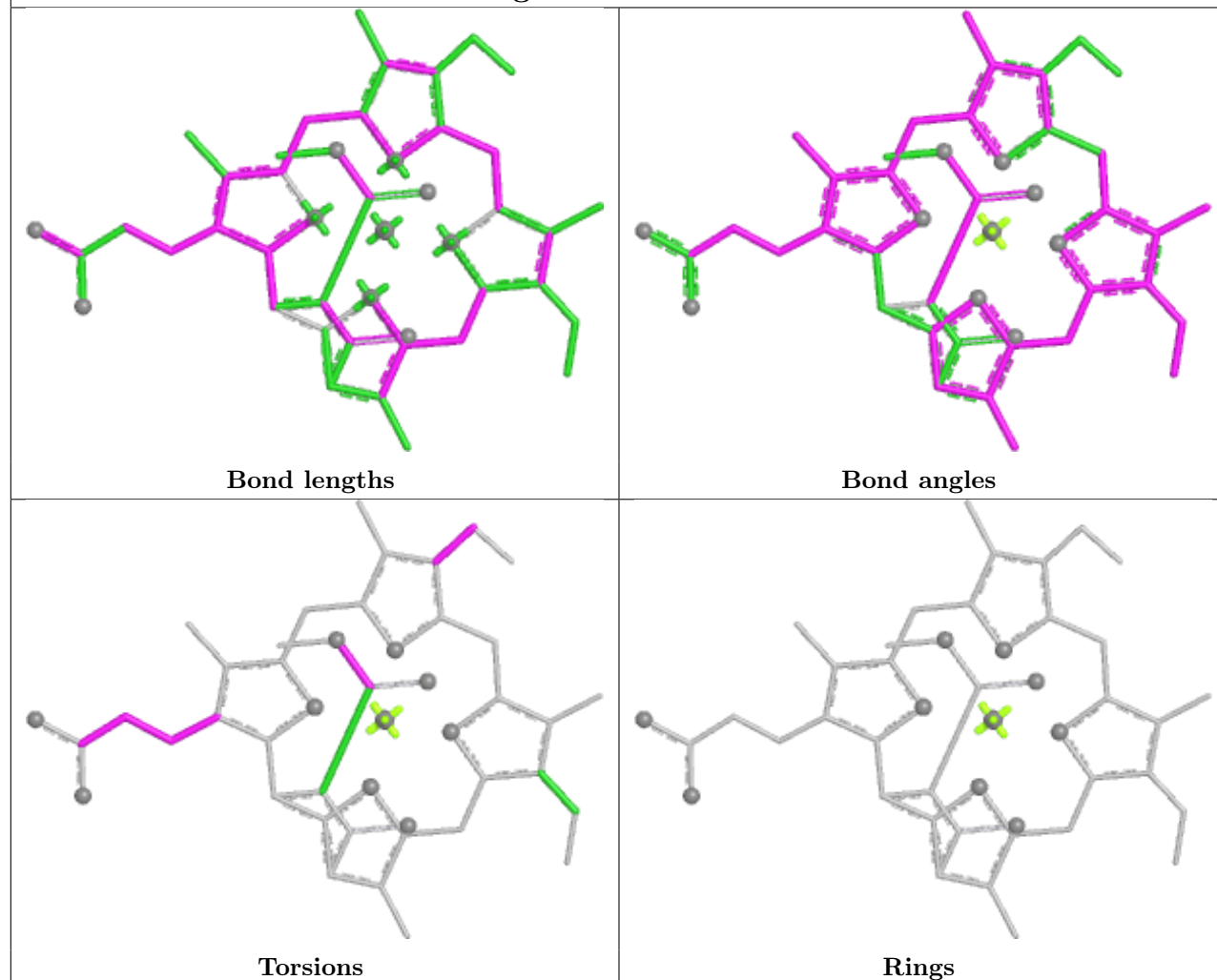
Ligand CLA 12 308



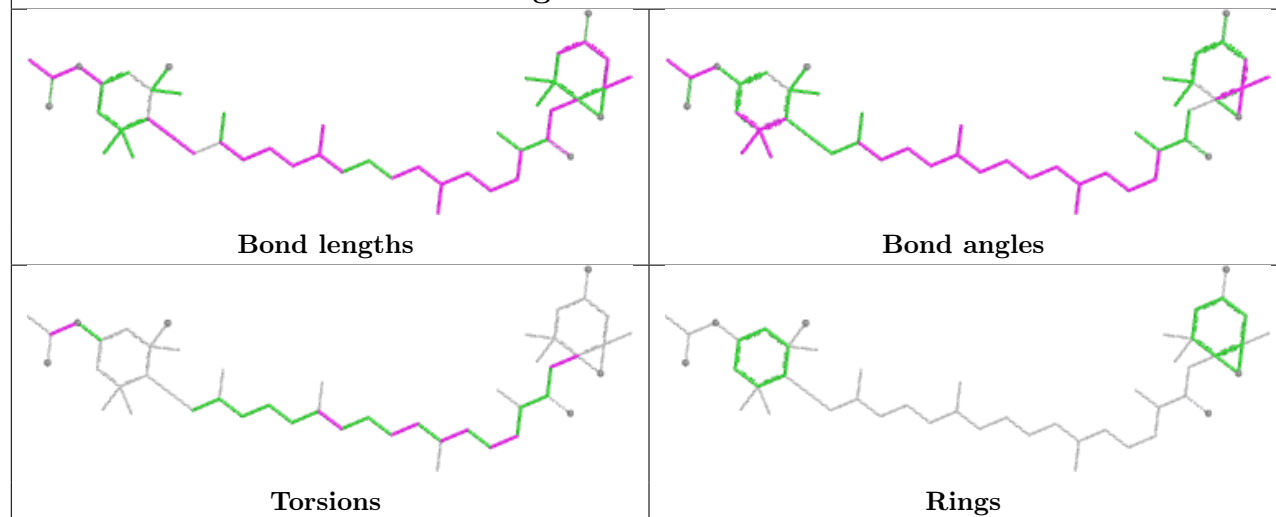
Ligand CLA 10 303

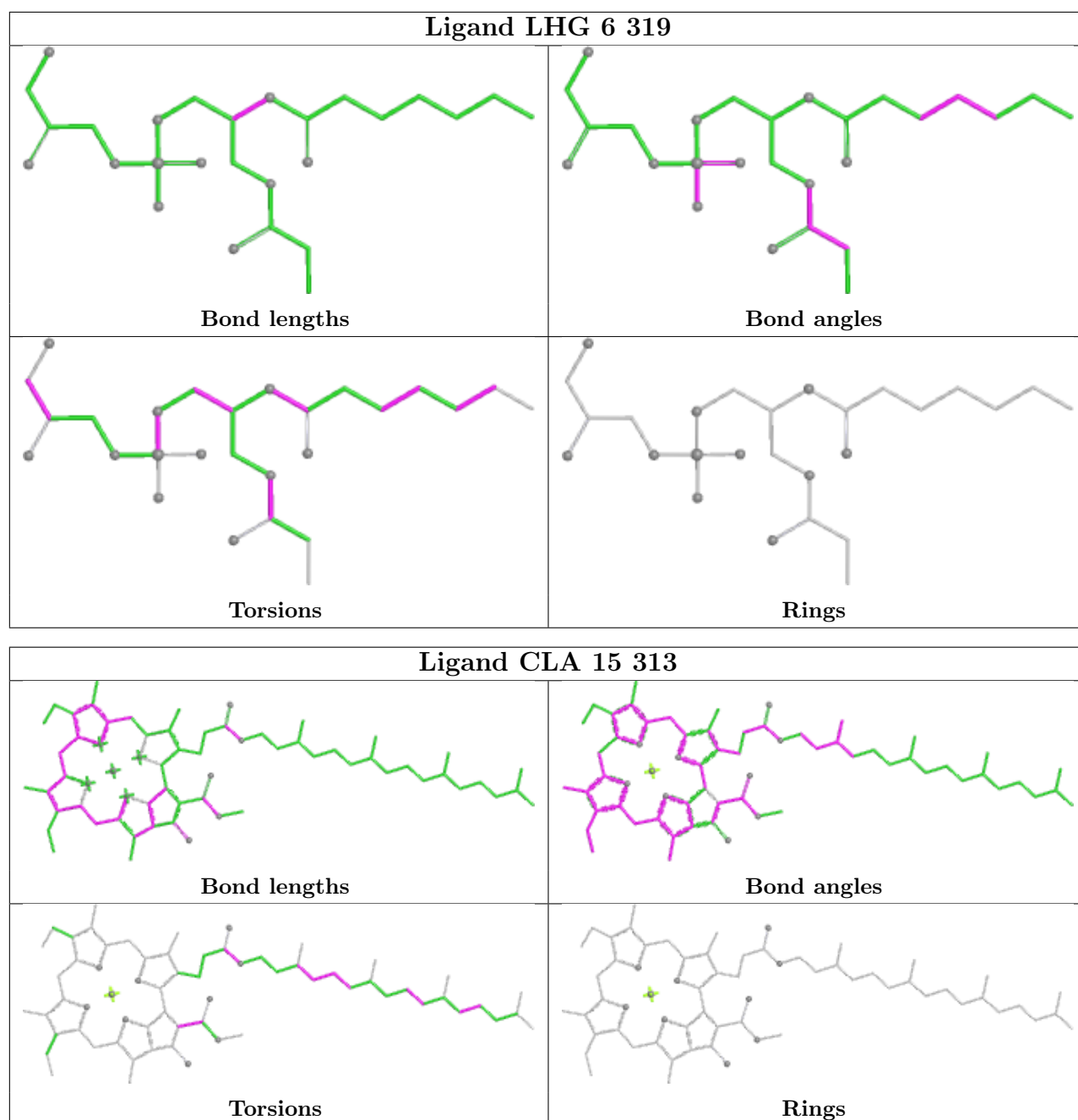


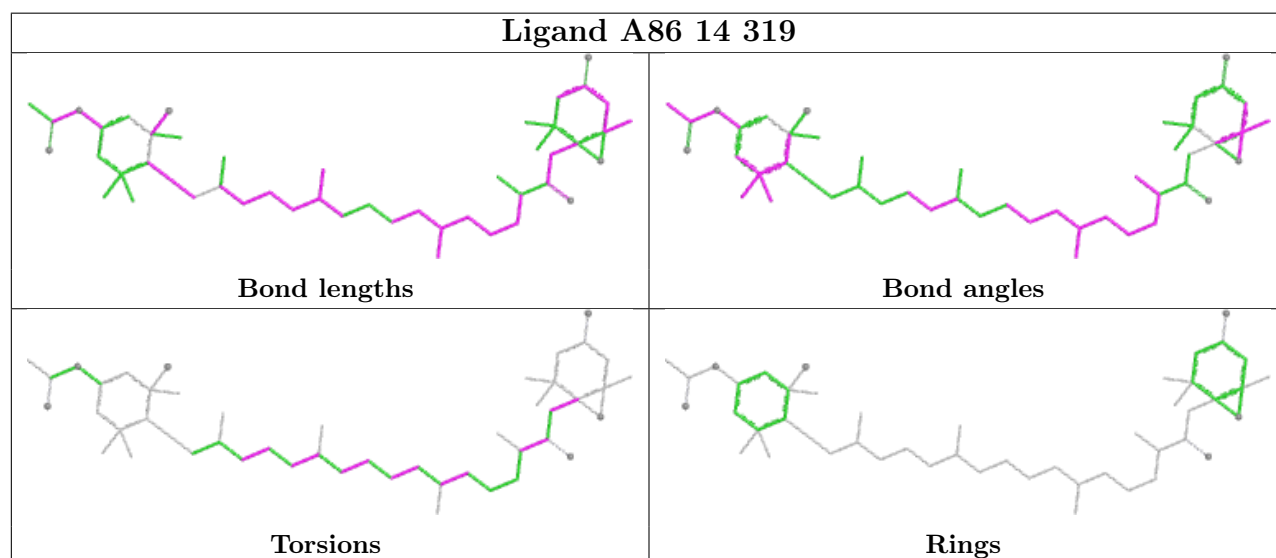
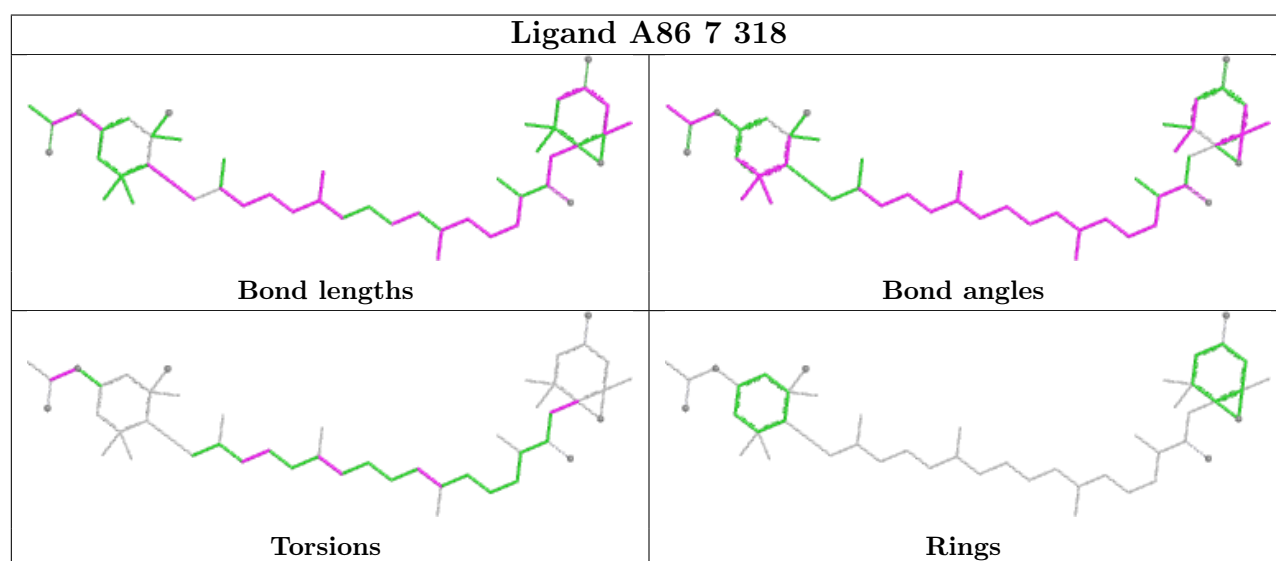
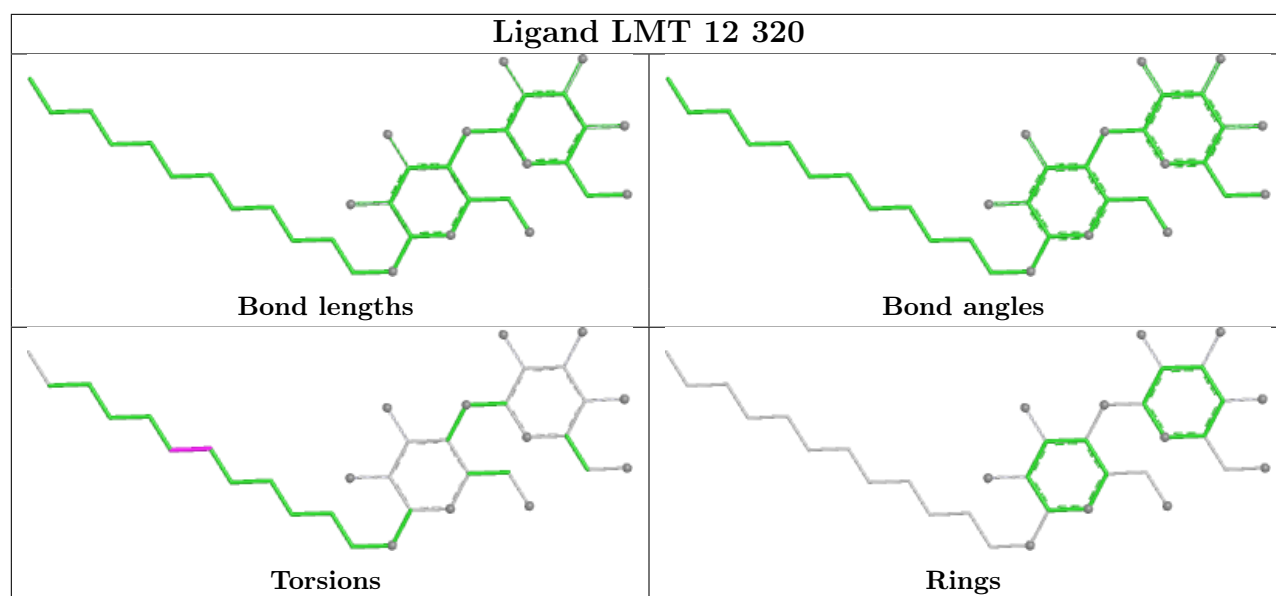
Ligand KC1 8 307

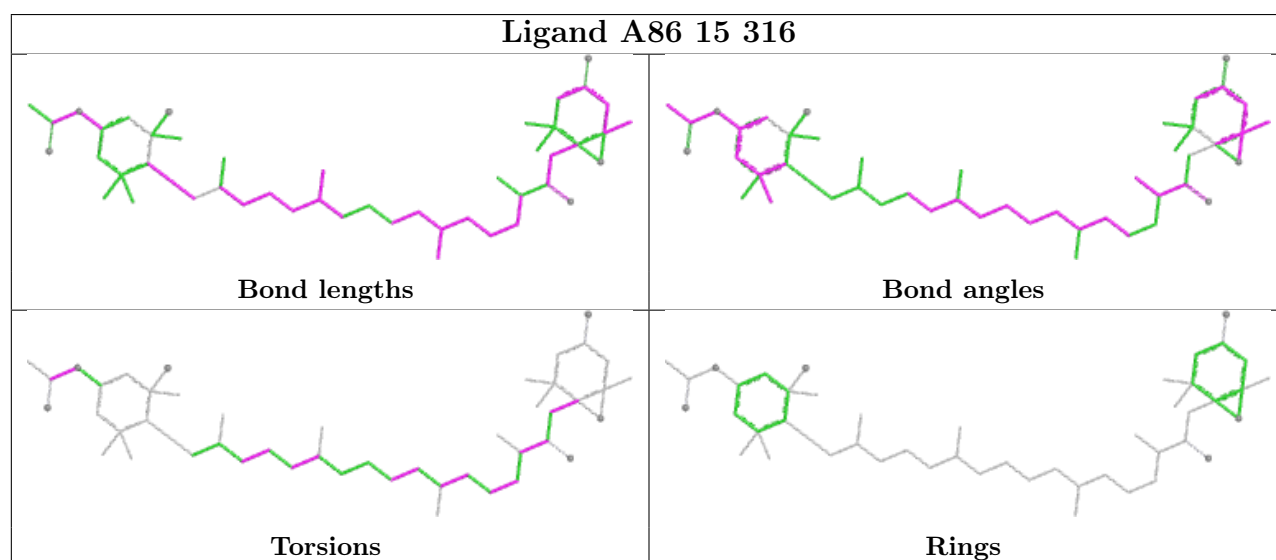
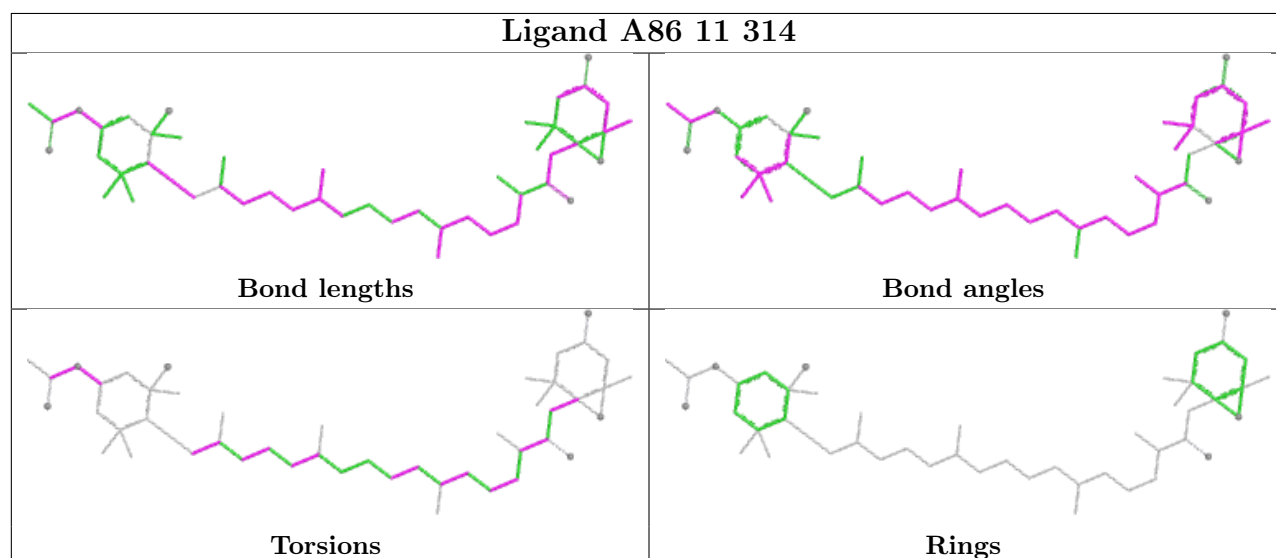
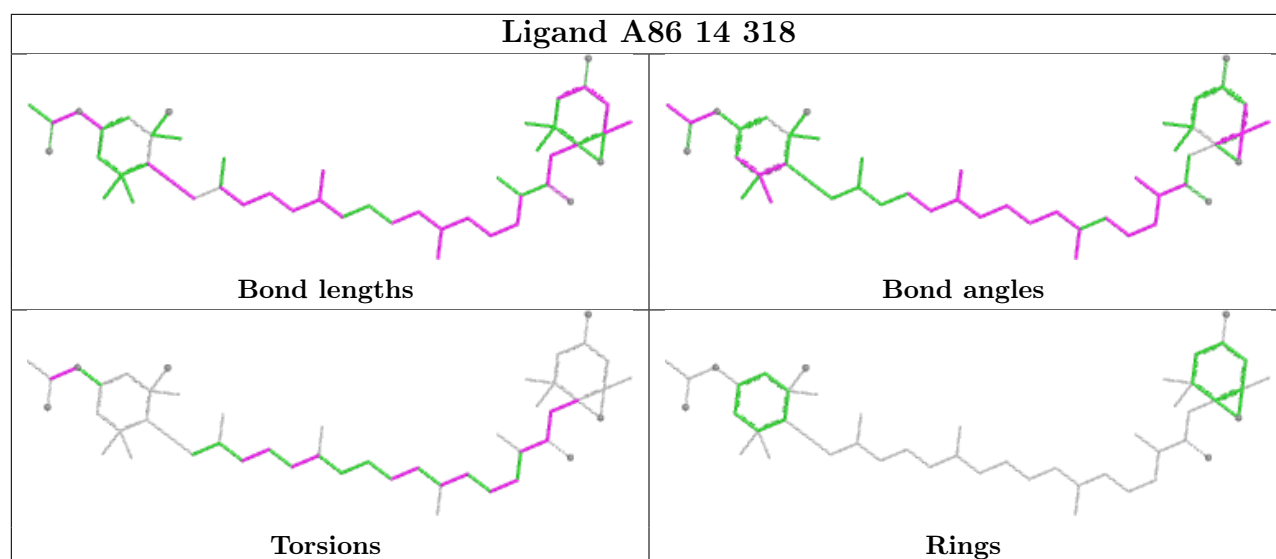


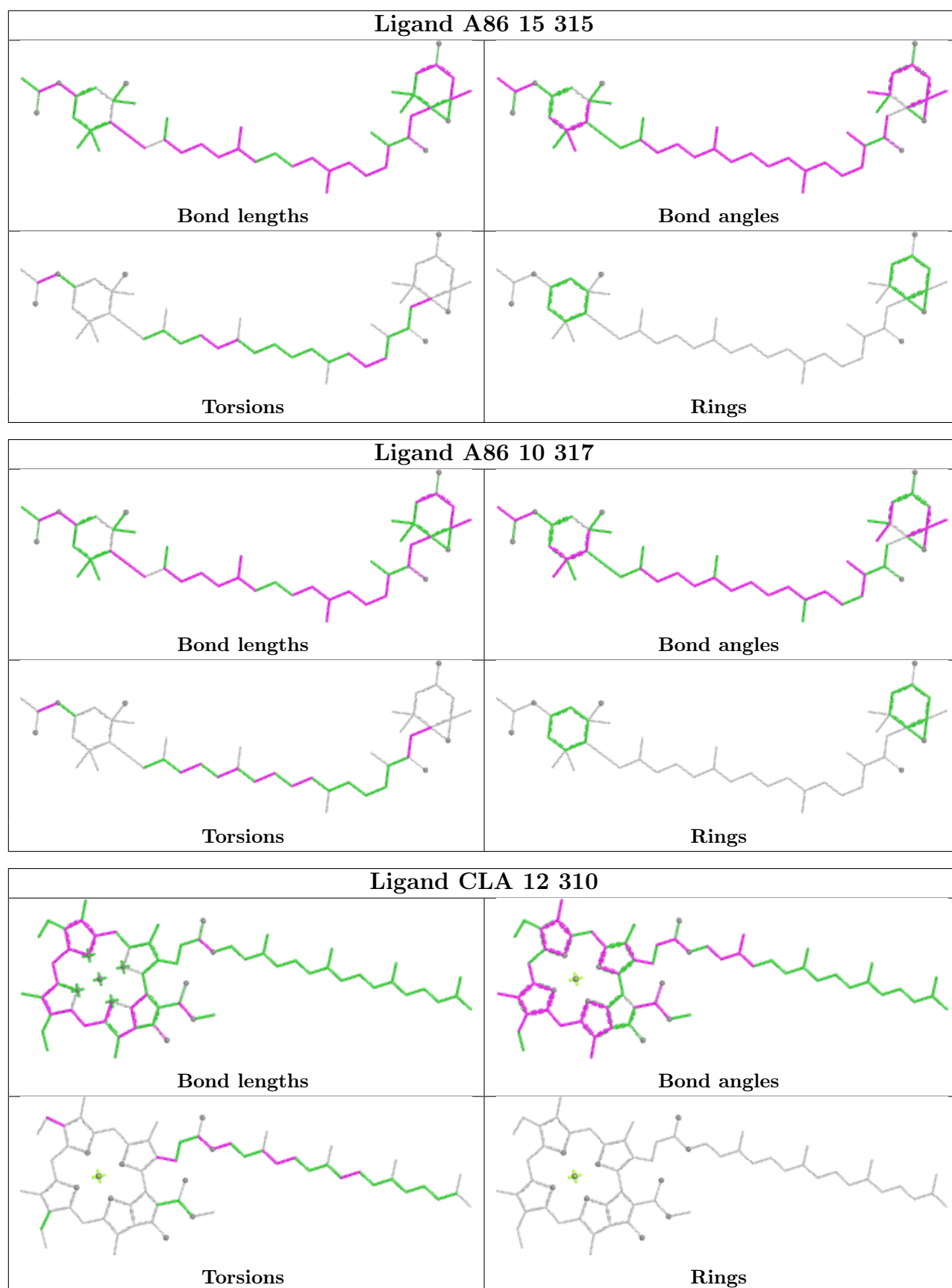
Ligand A86 14 320

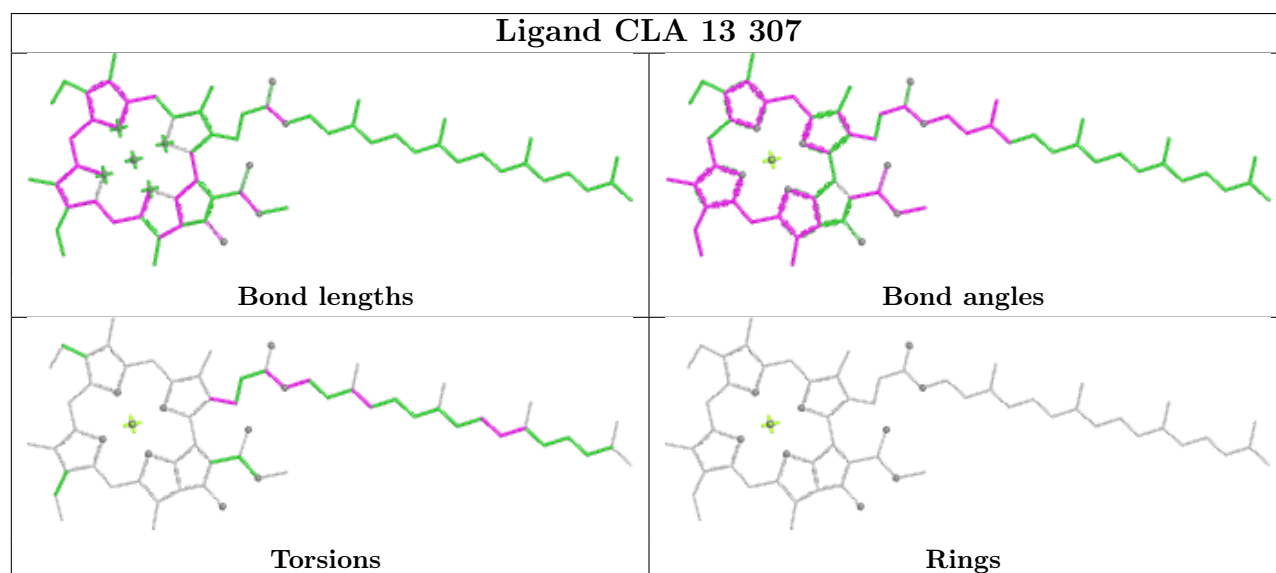
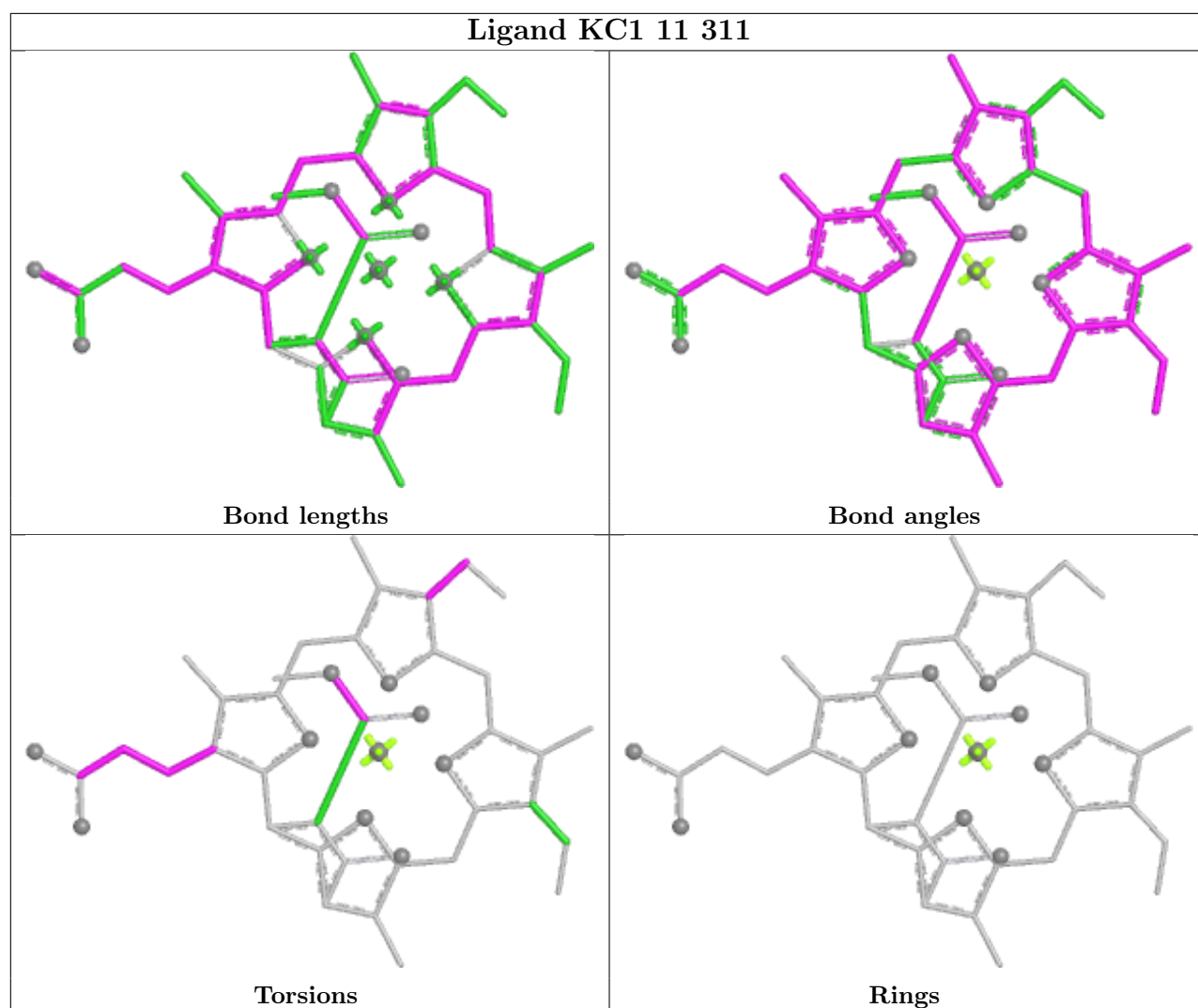


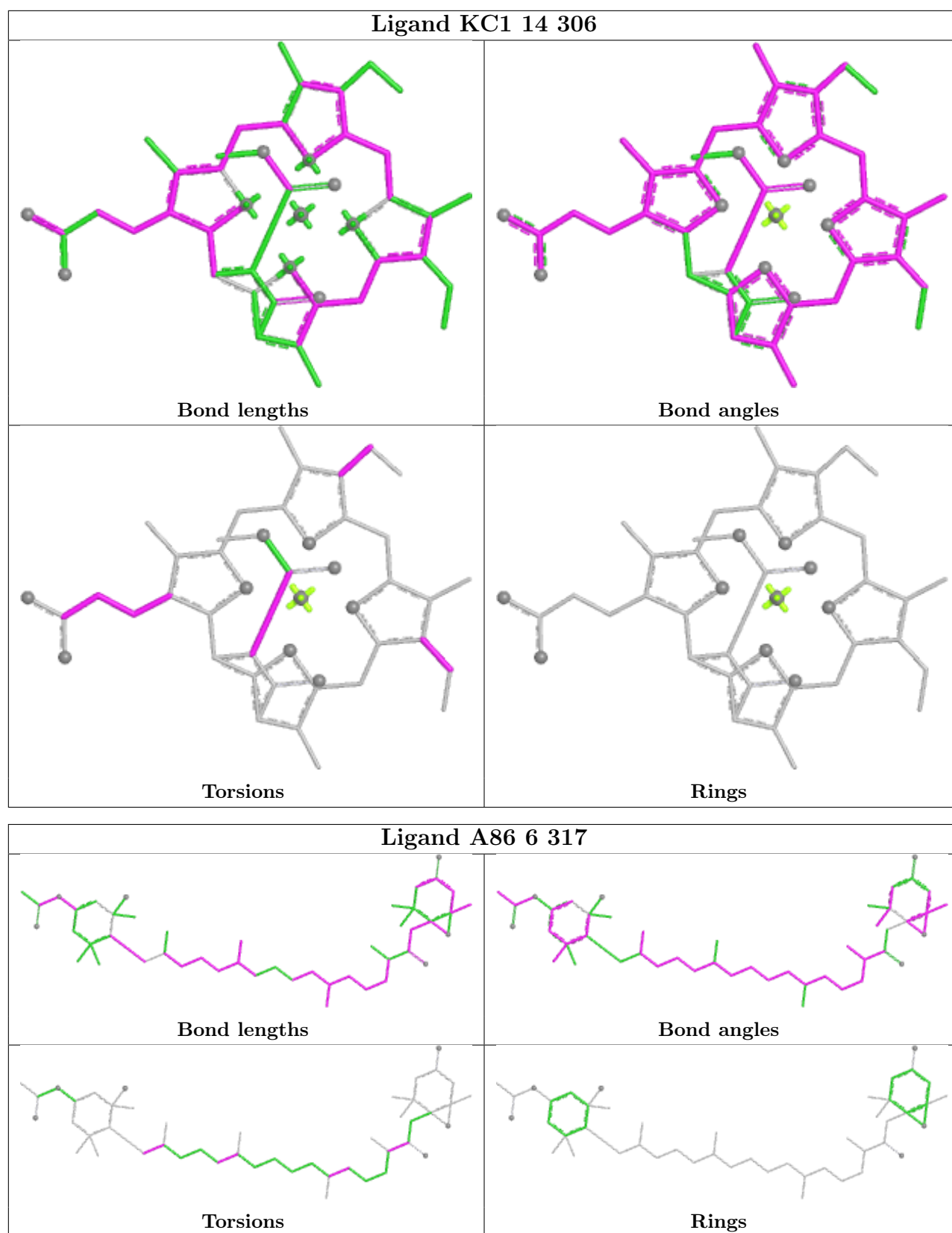


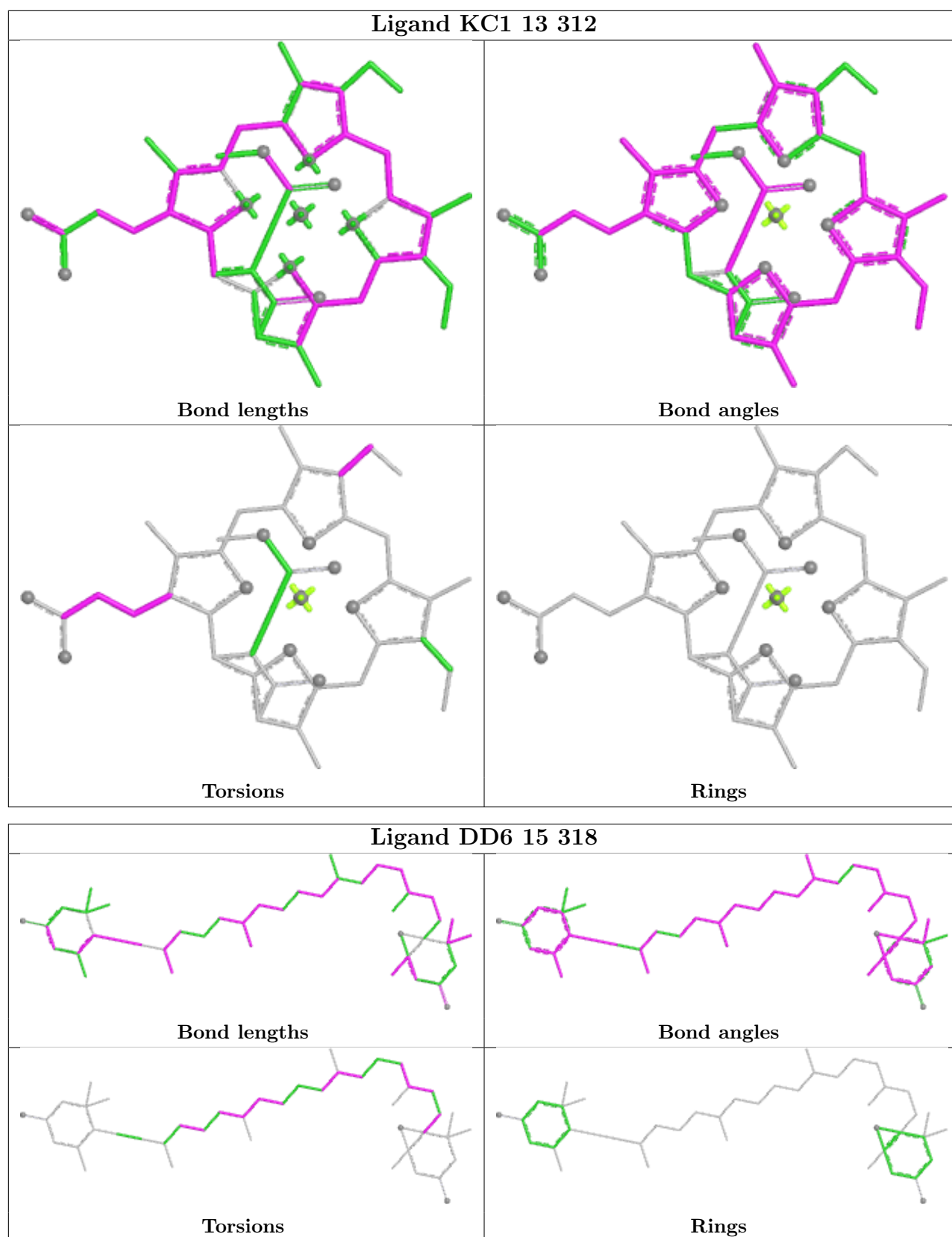


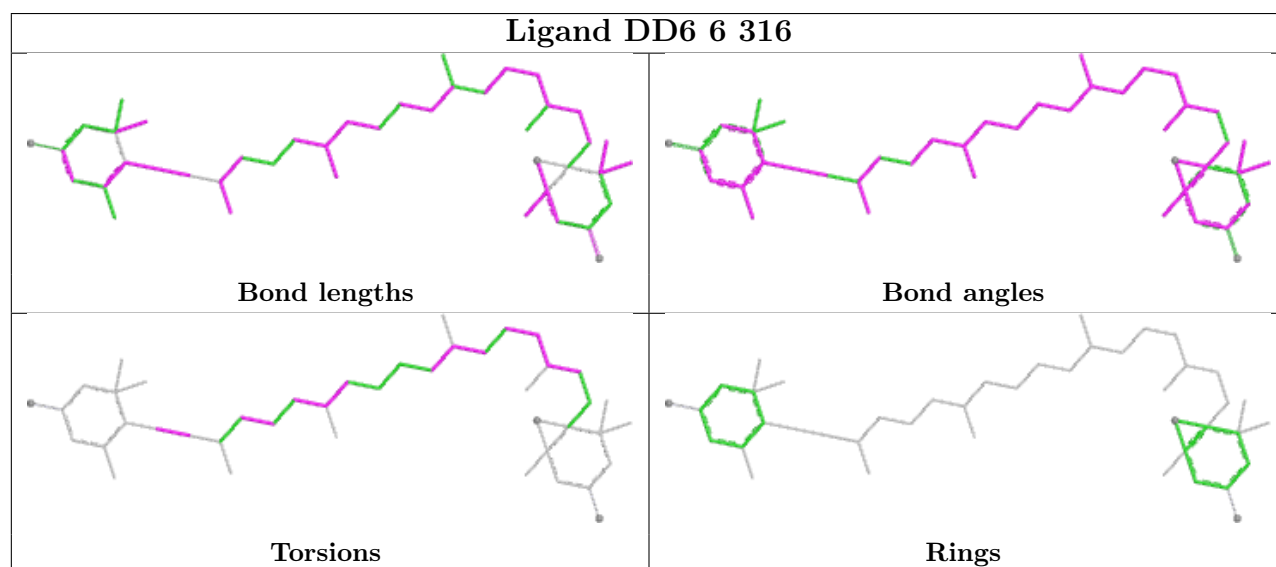
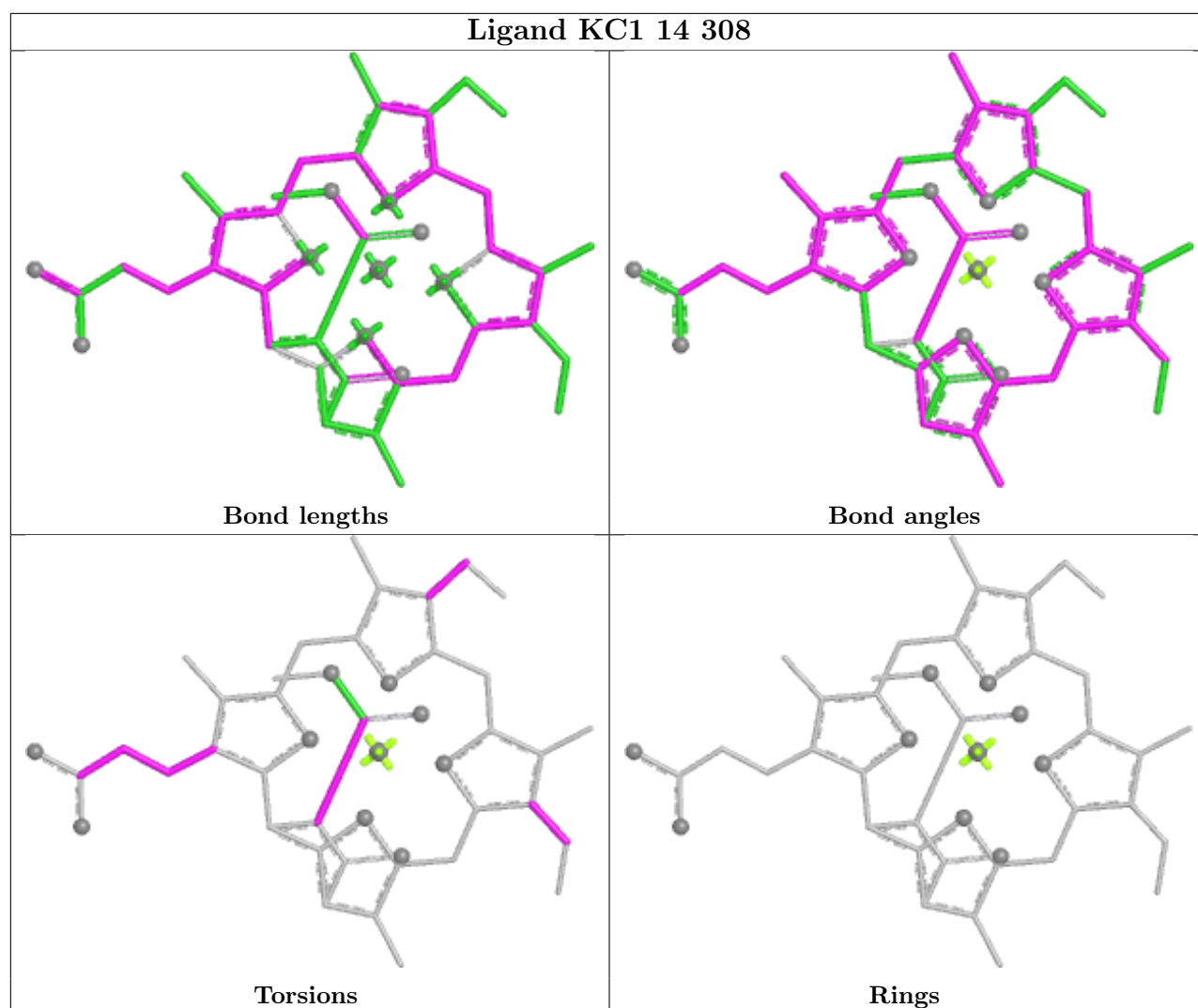


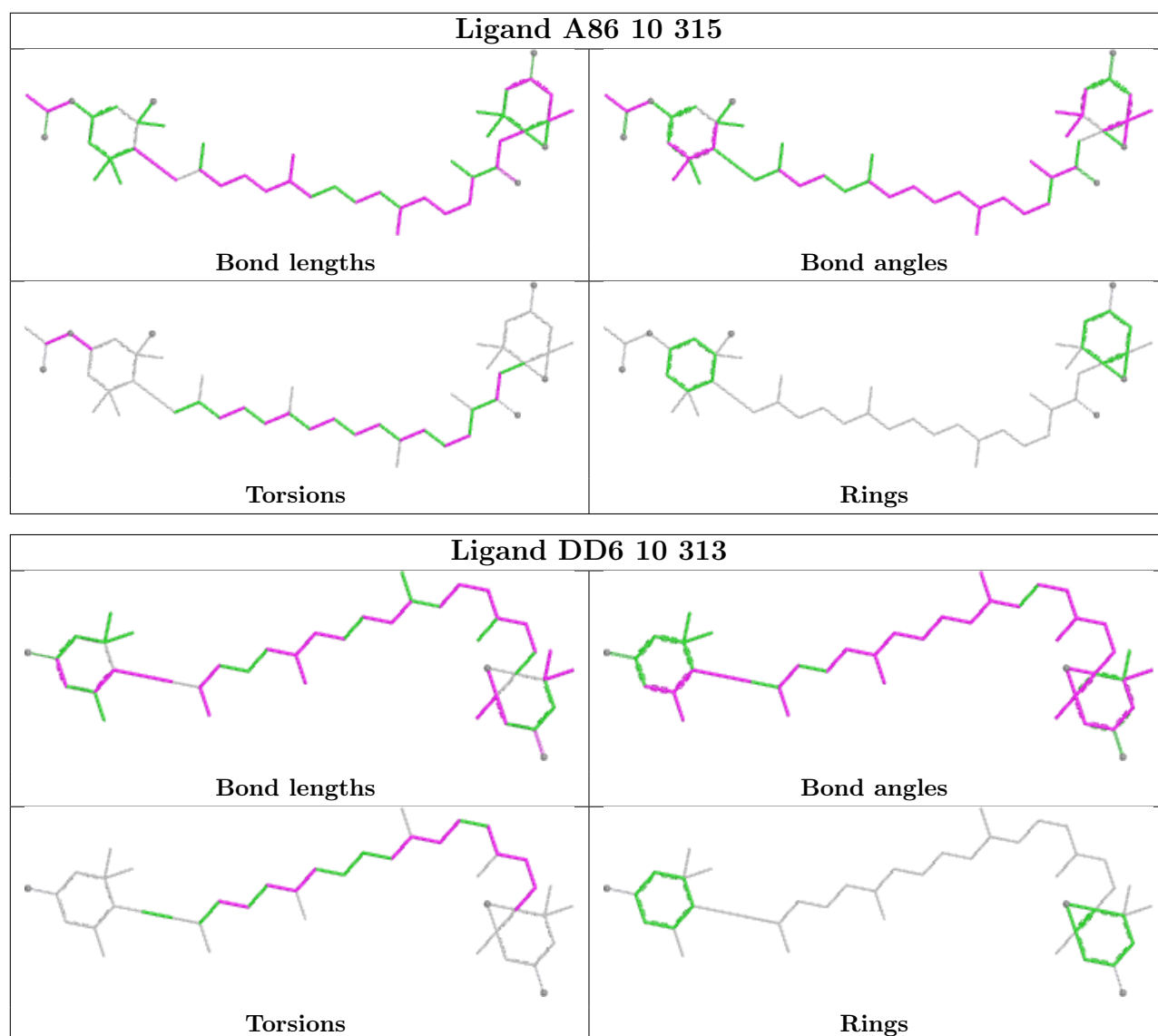




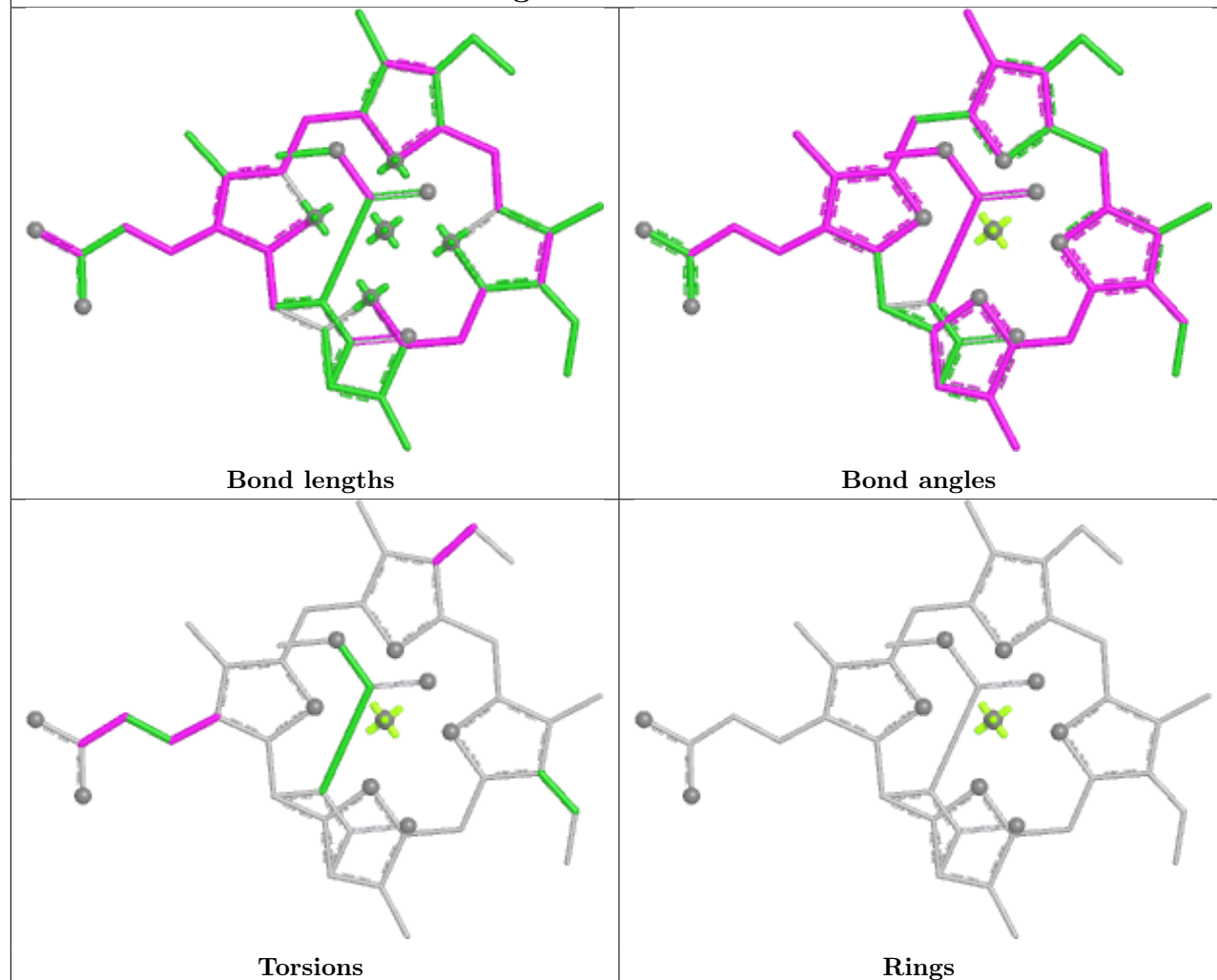




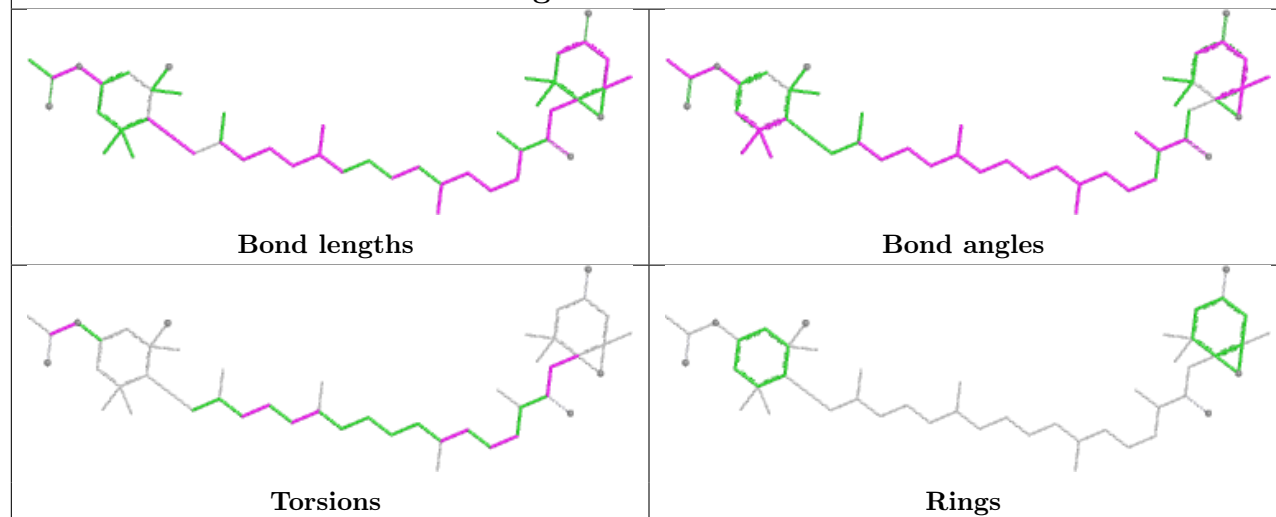




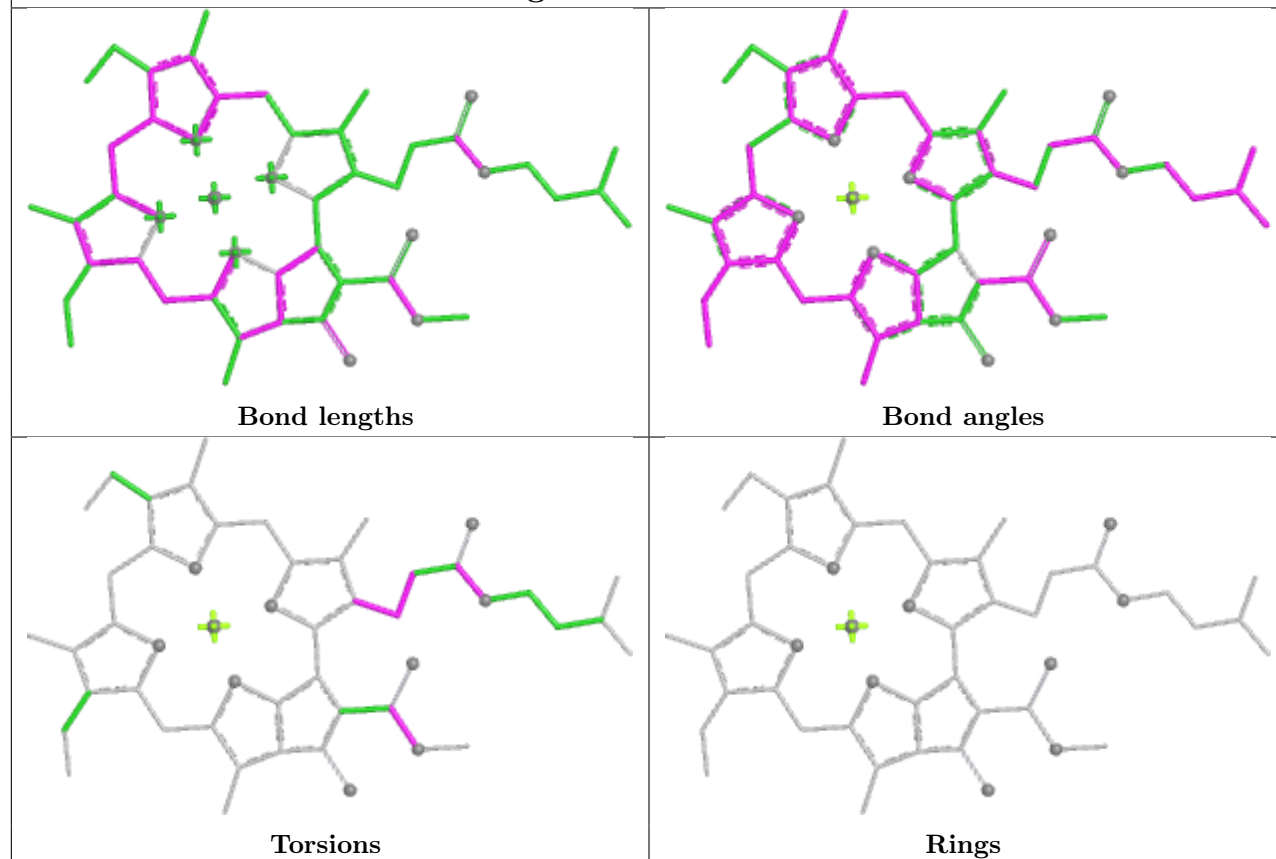
Ligand KC1 8 313



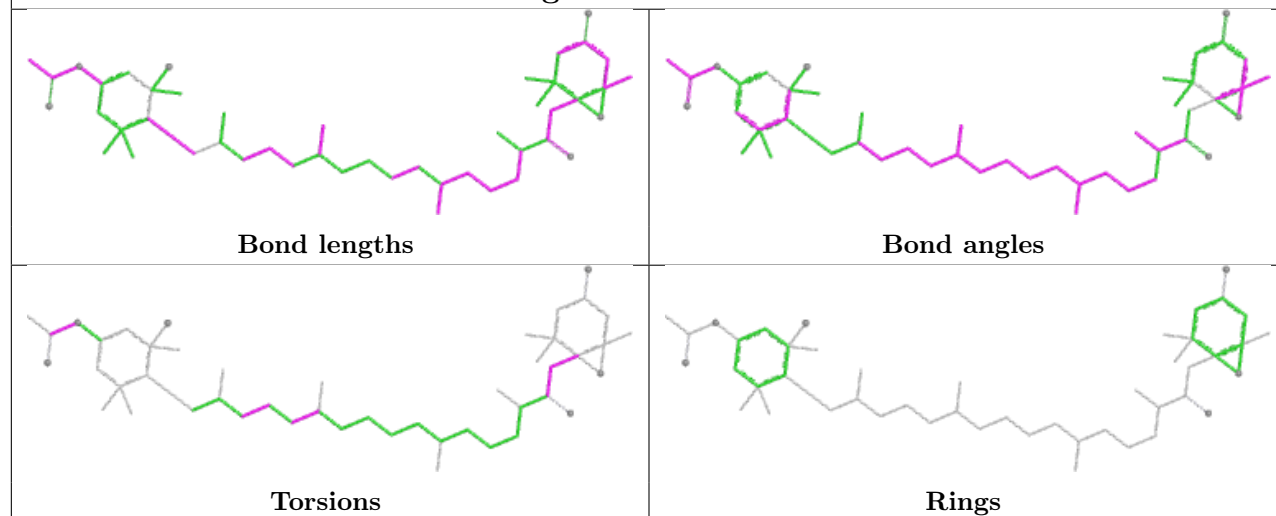
Ligand A86 10 316

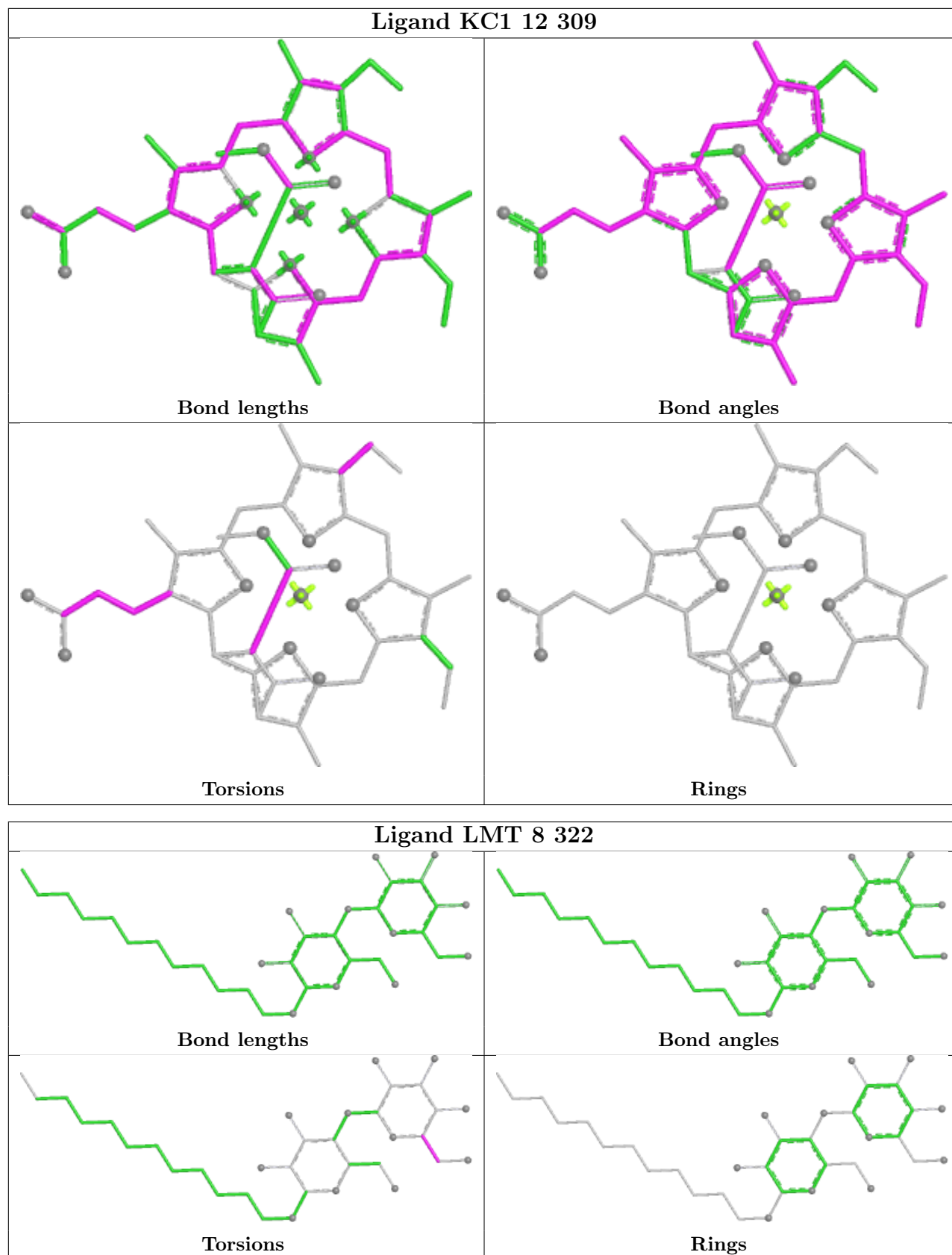


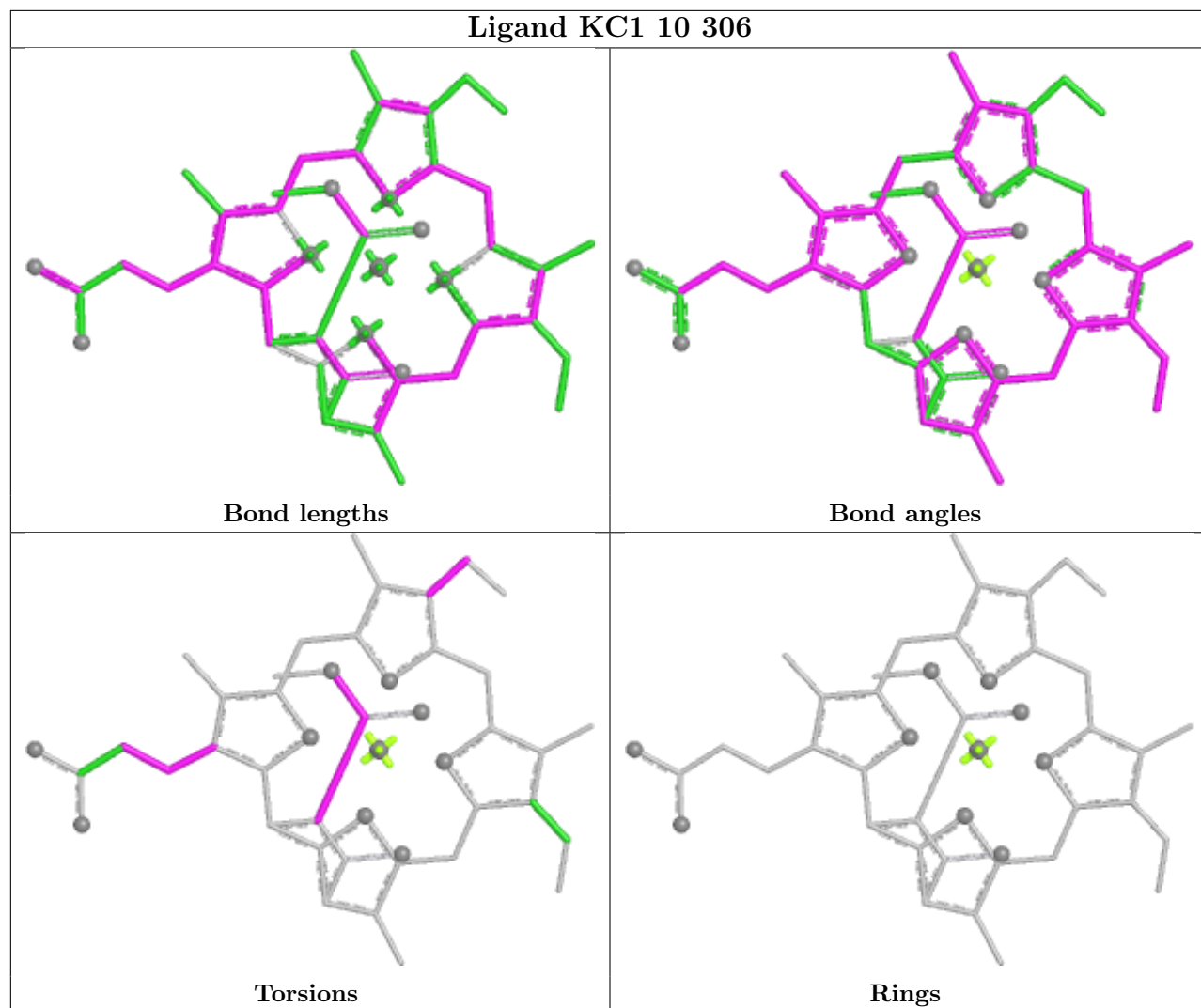
Ligand CLA 15 307



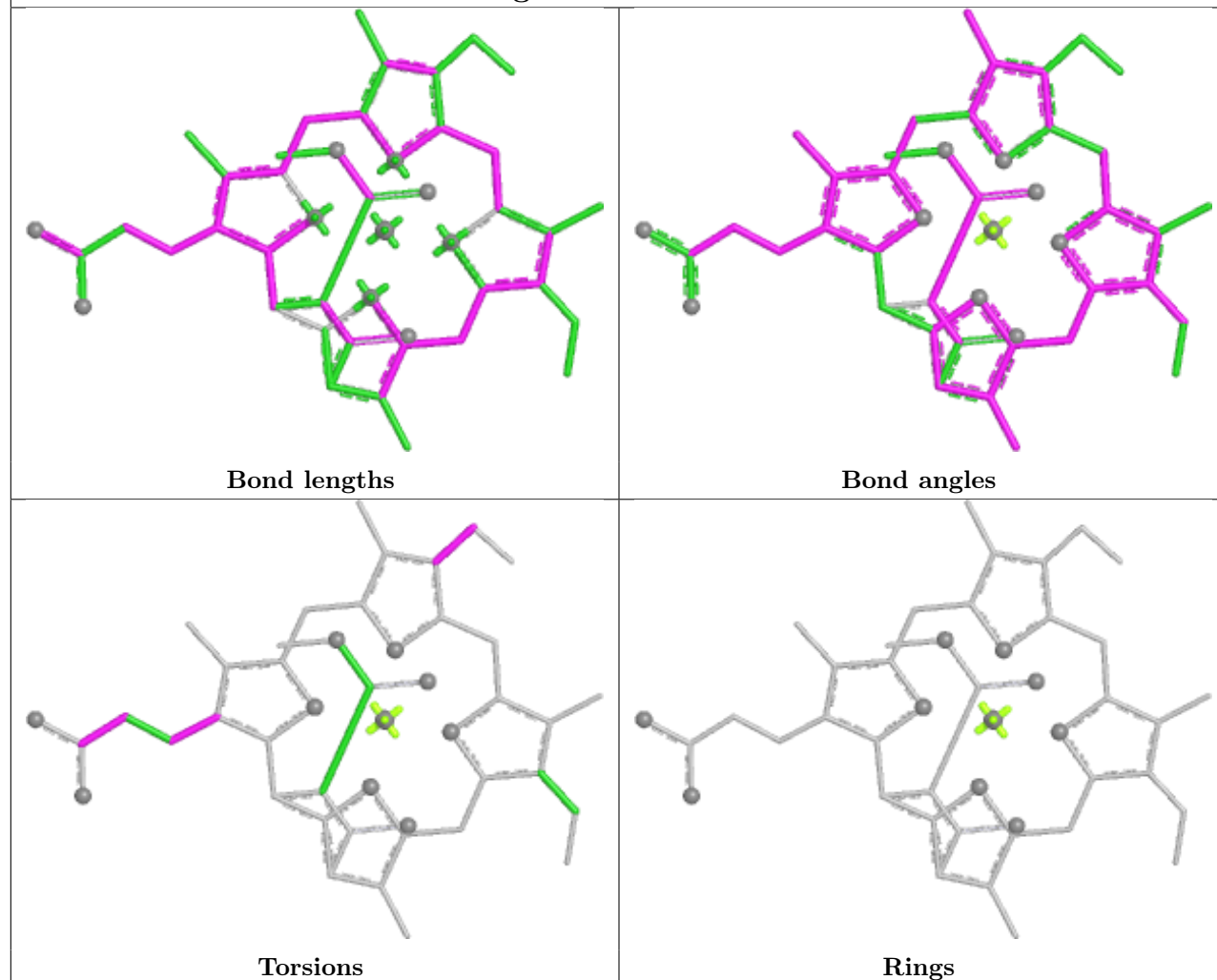
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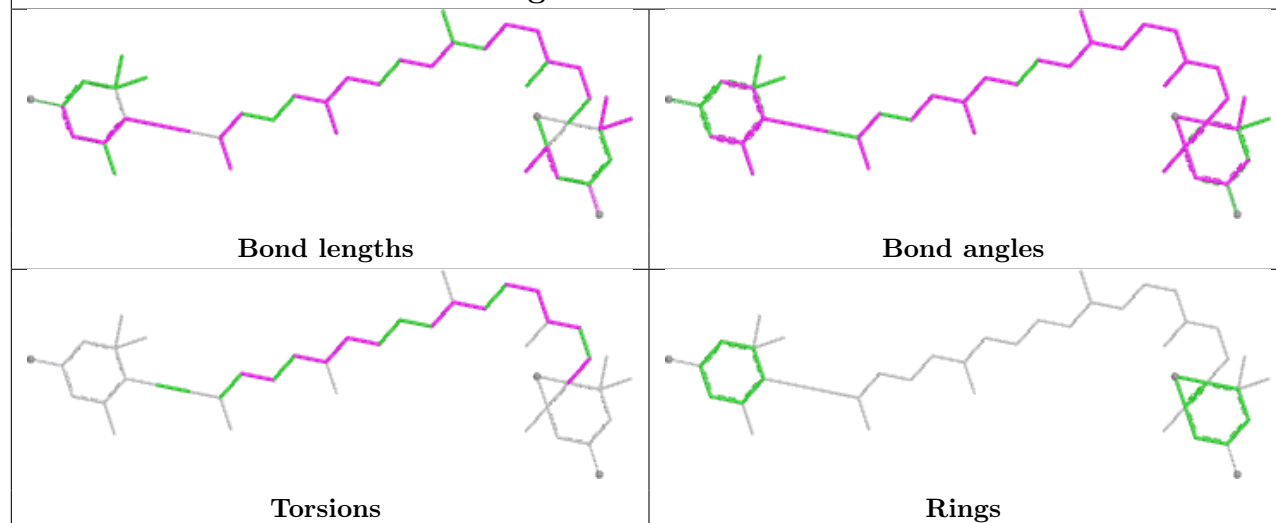




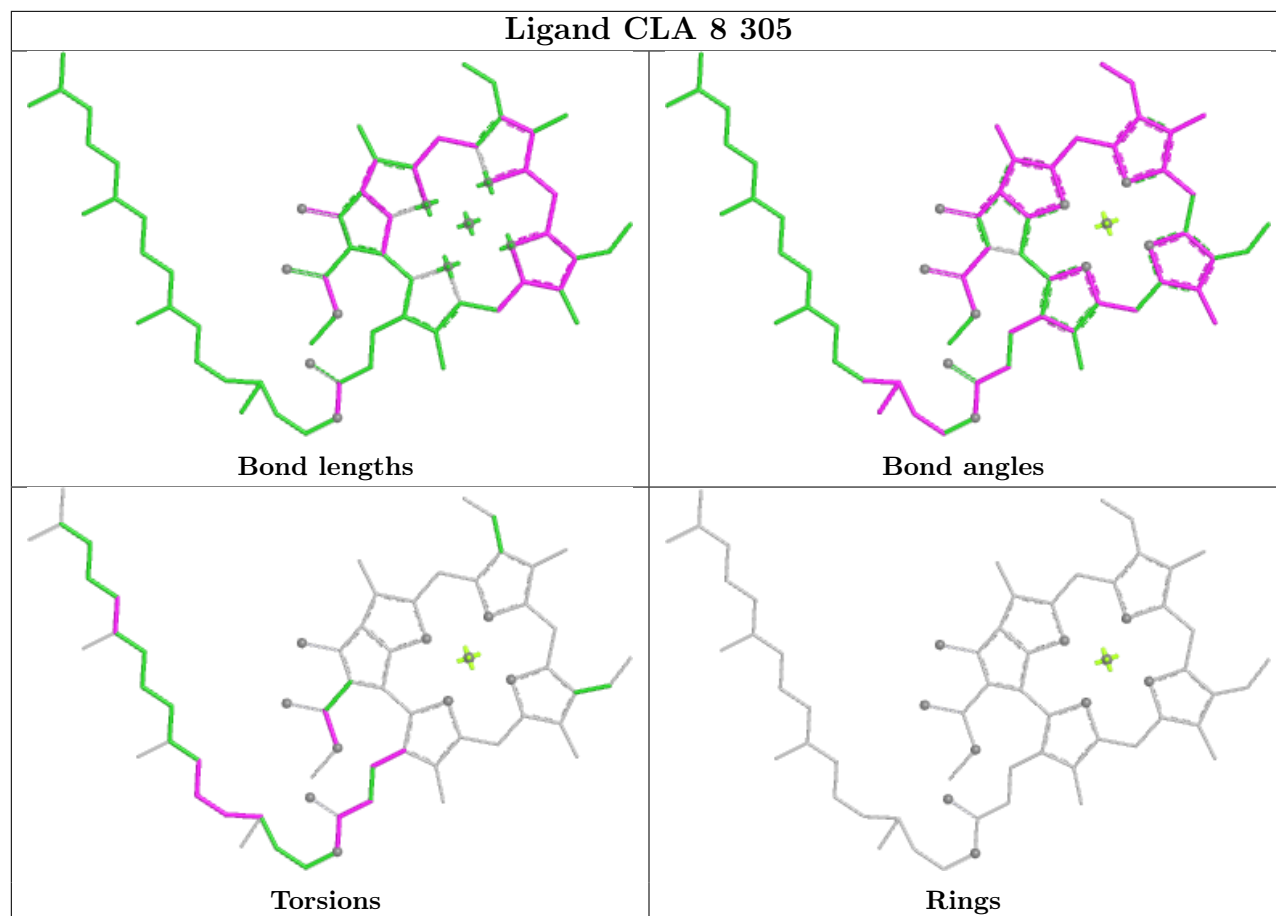
Ligand KC1 8 314



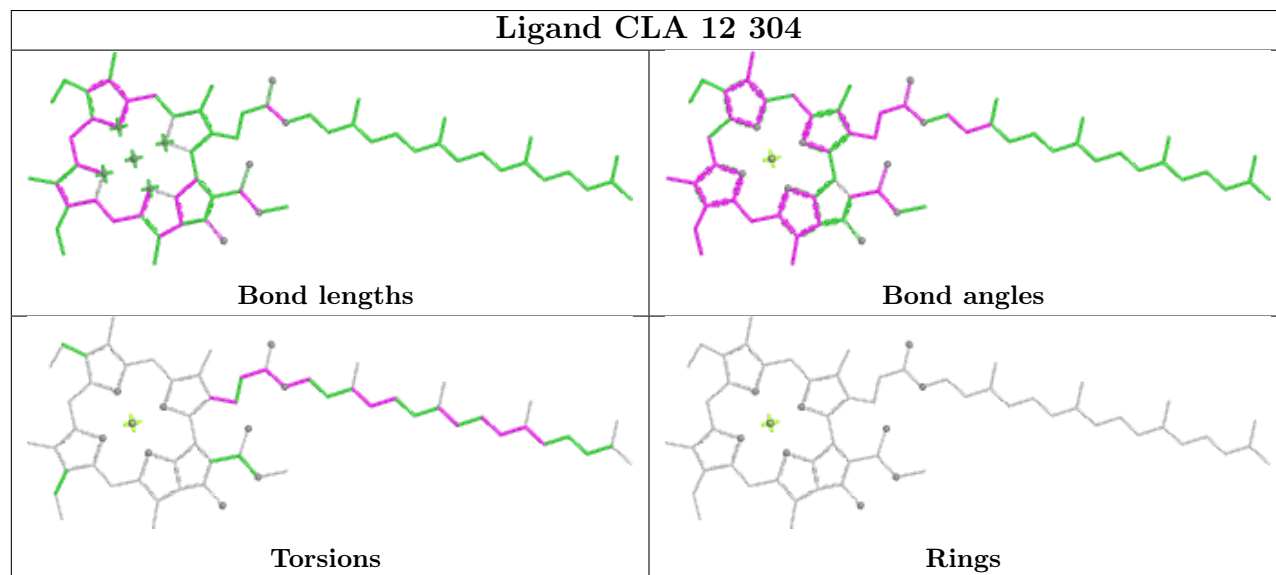
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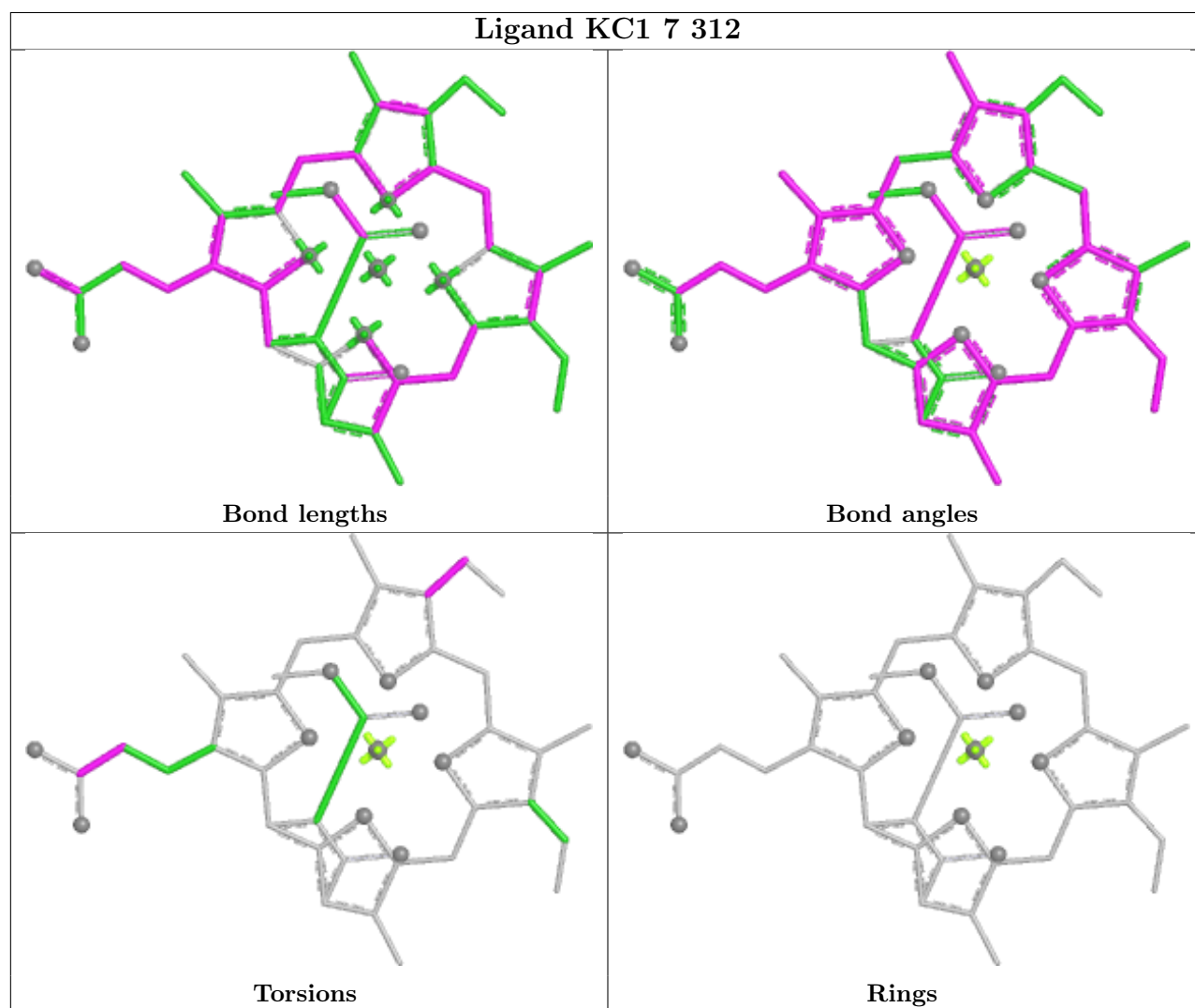
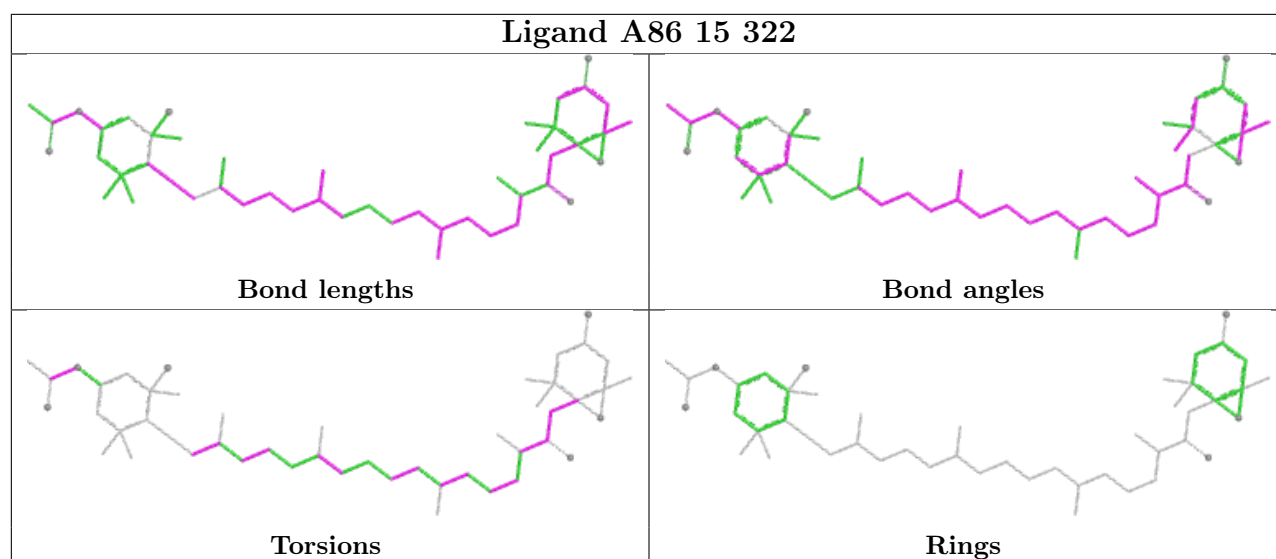


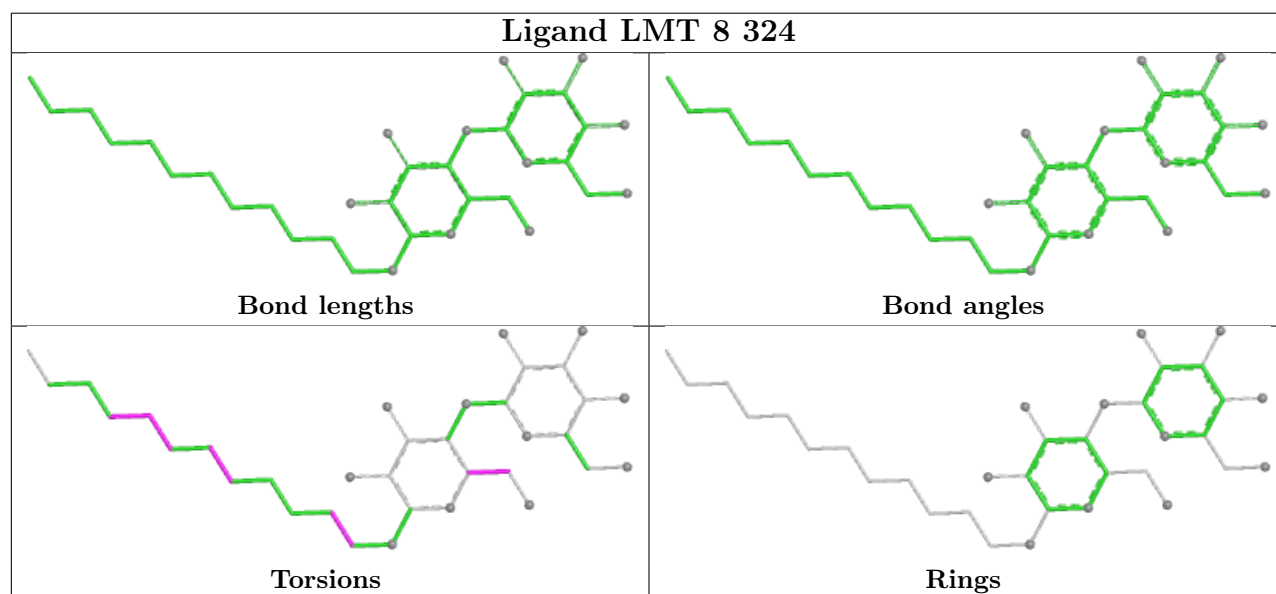
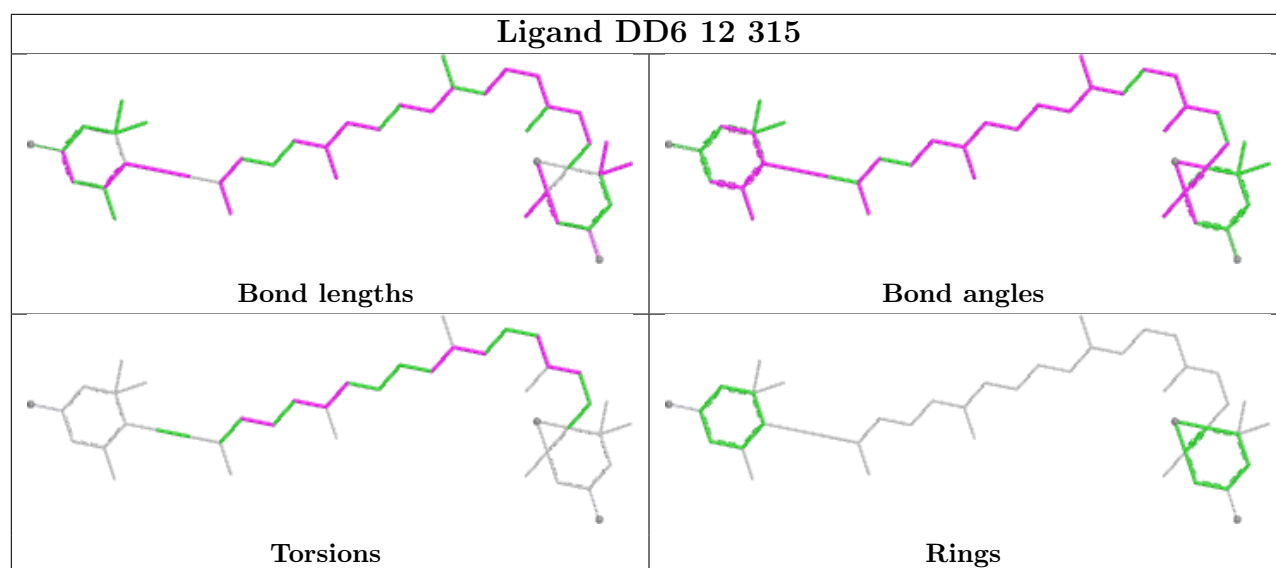
Ligand CLA 8 305

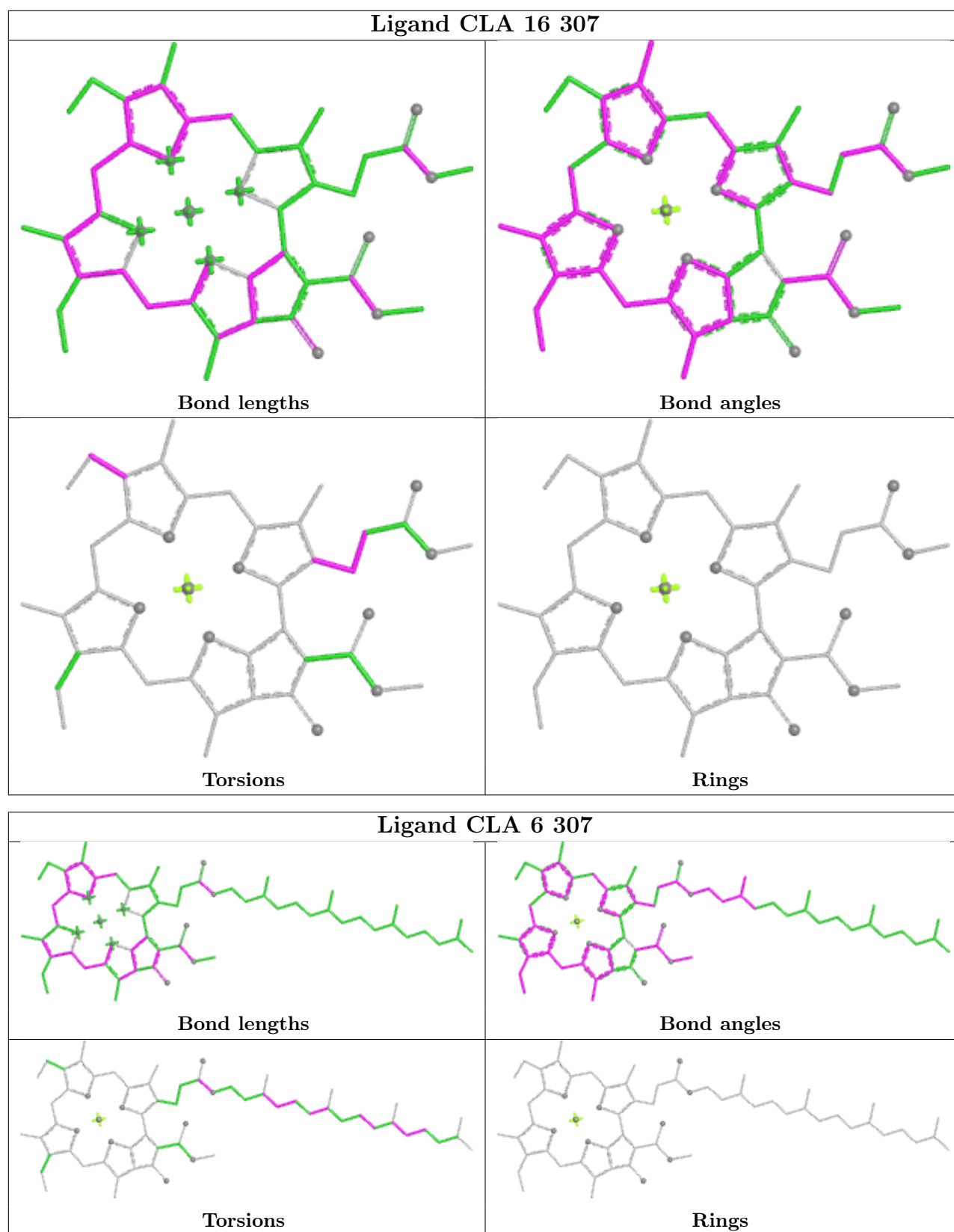


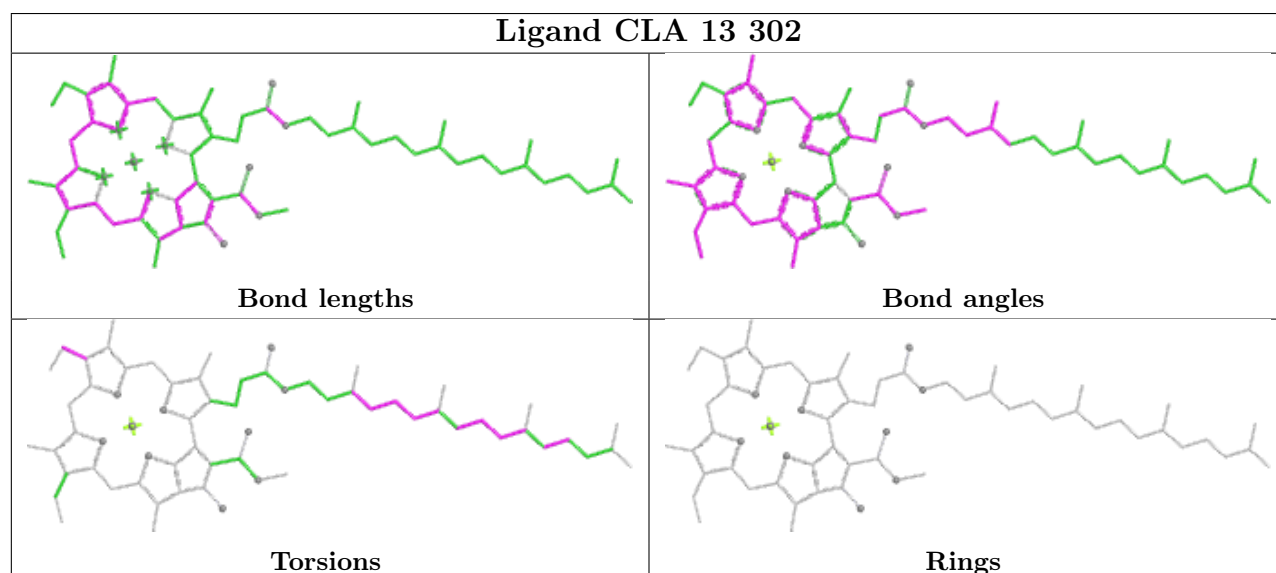
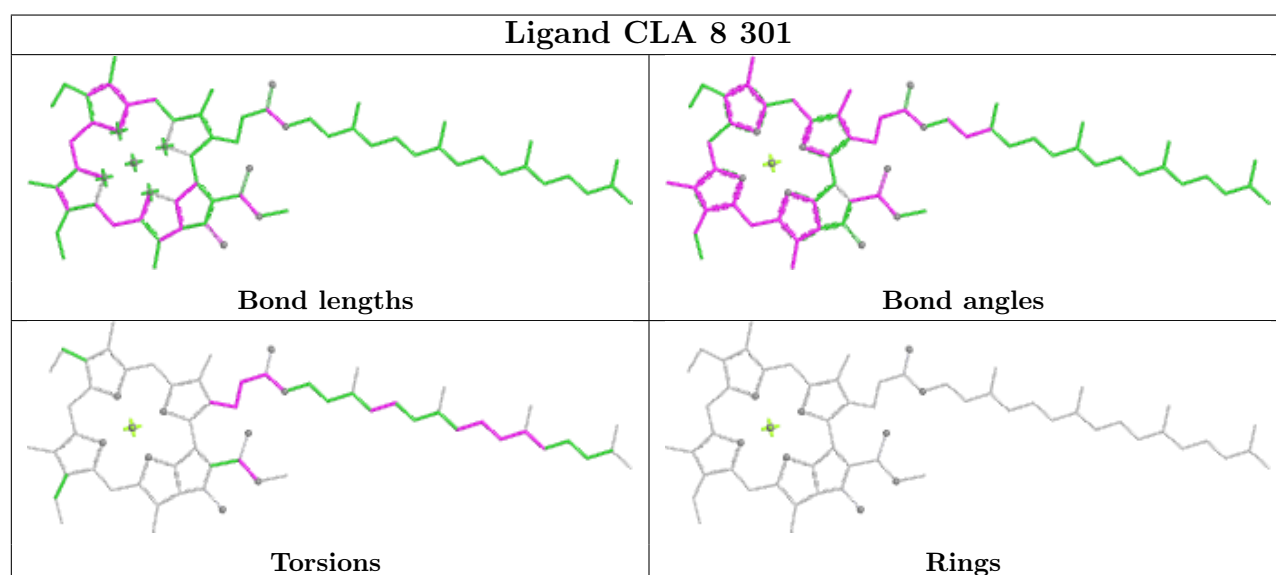
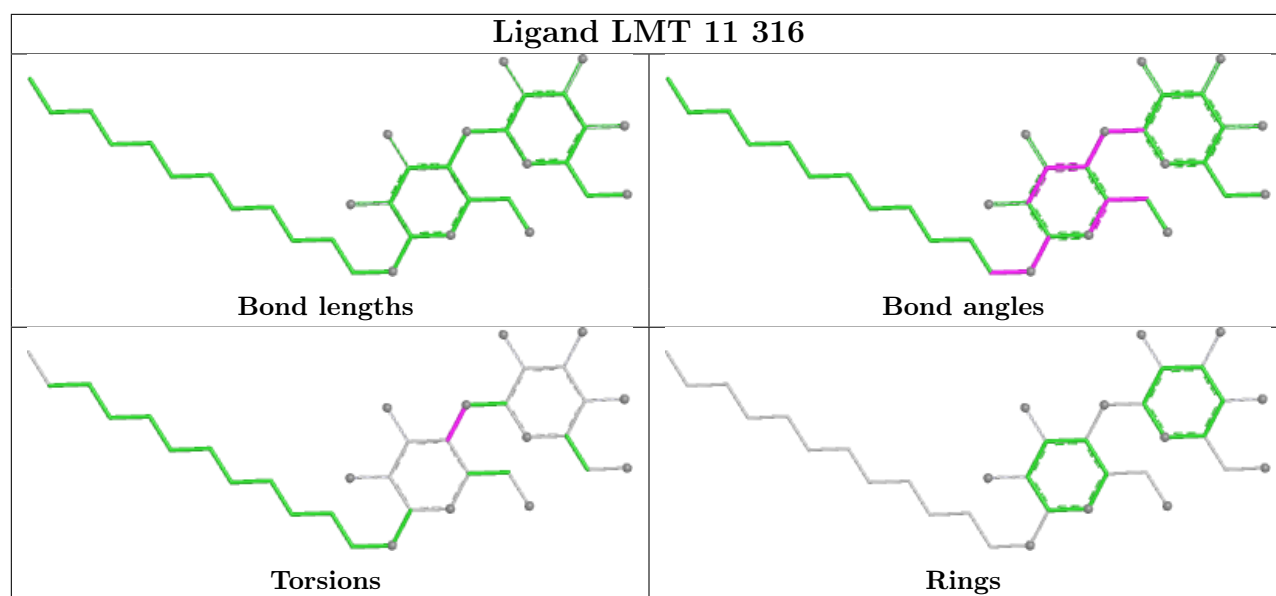
Ligand CLA 12 304



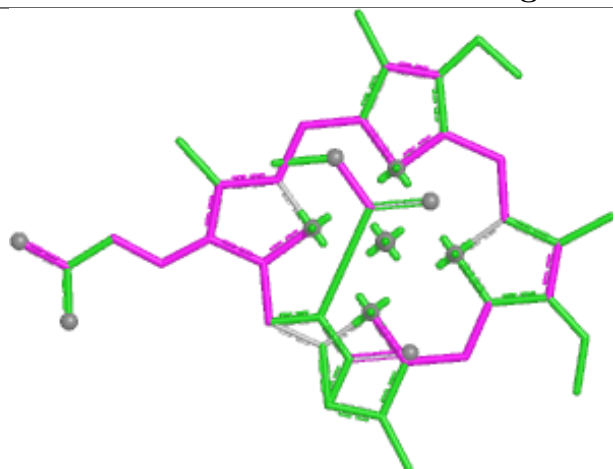




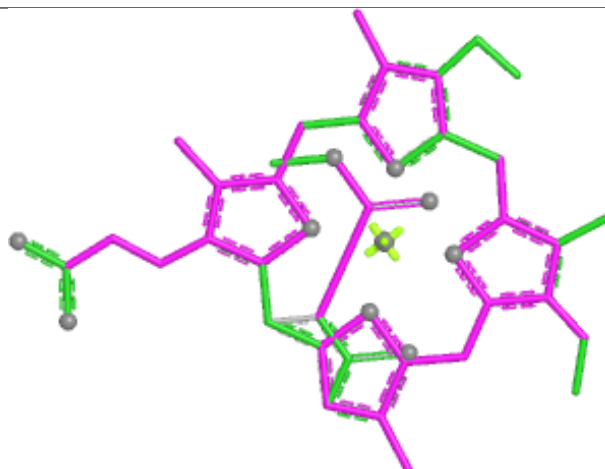




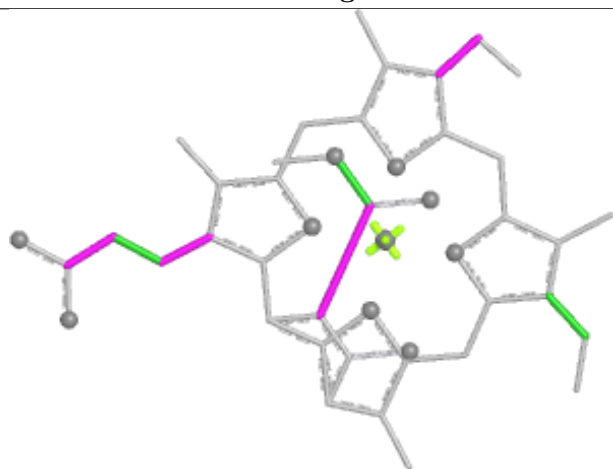
Ligand KC1 8 310



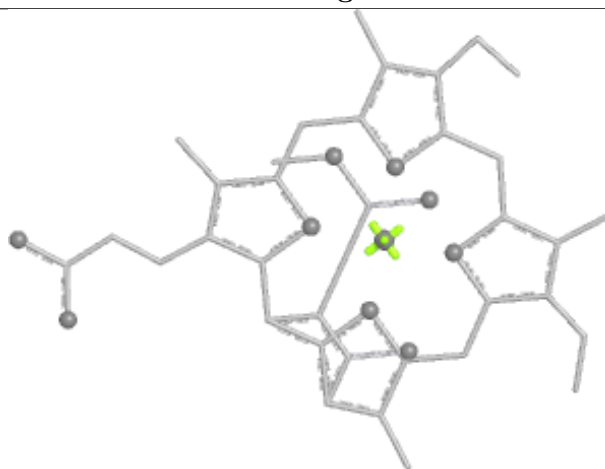
Bond lengths



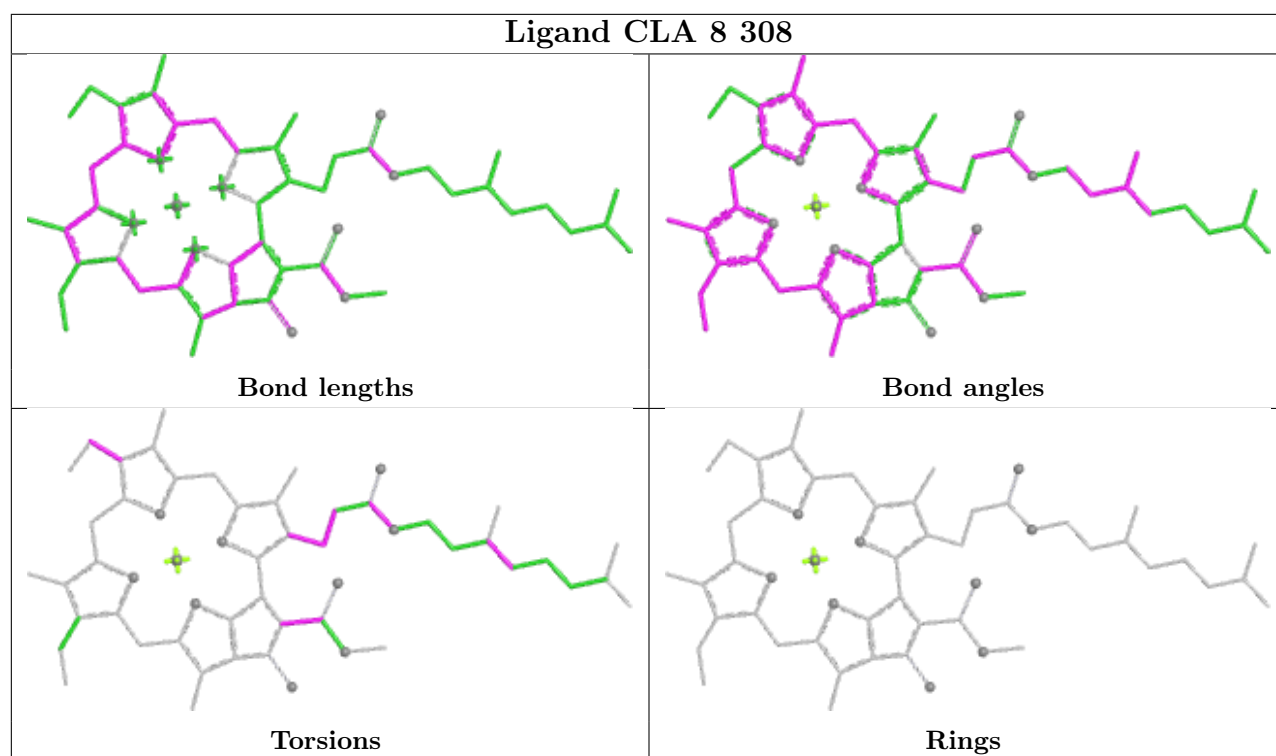
Bond angles

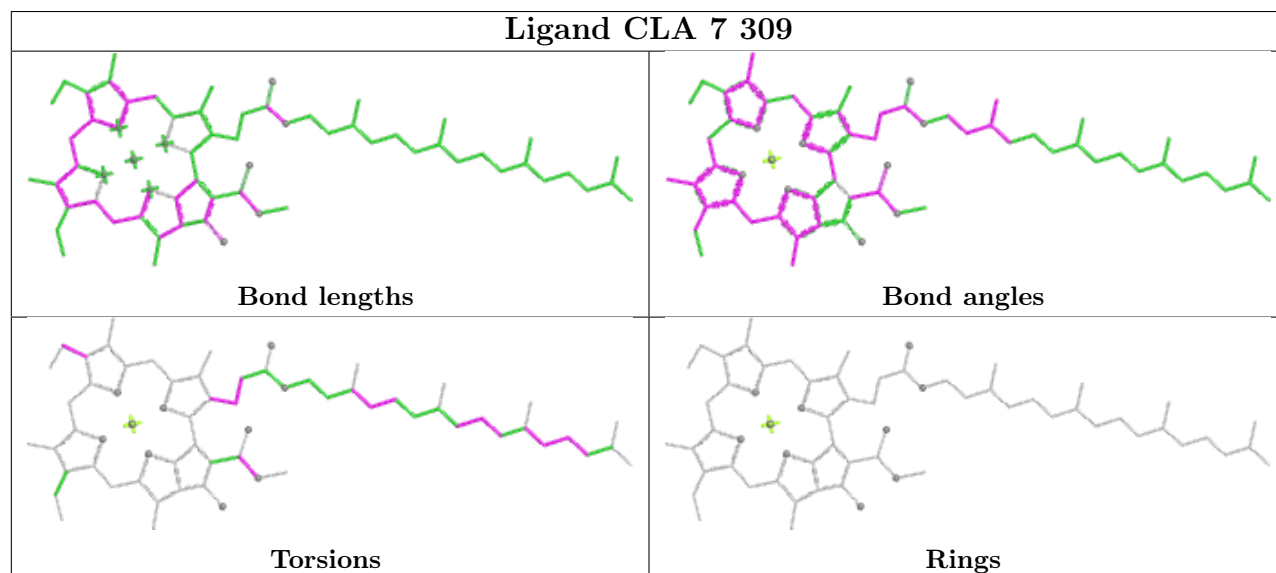
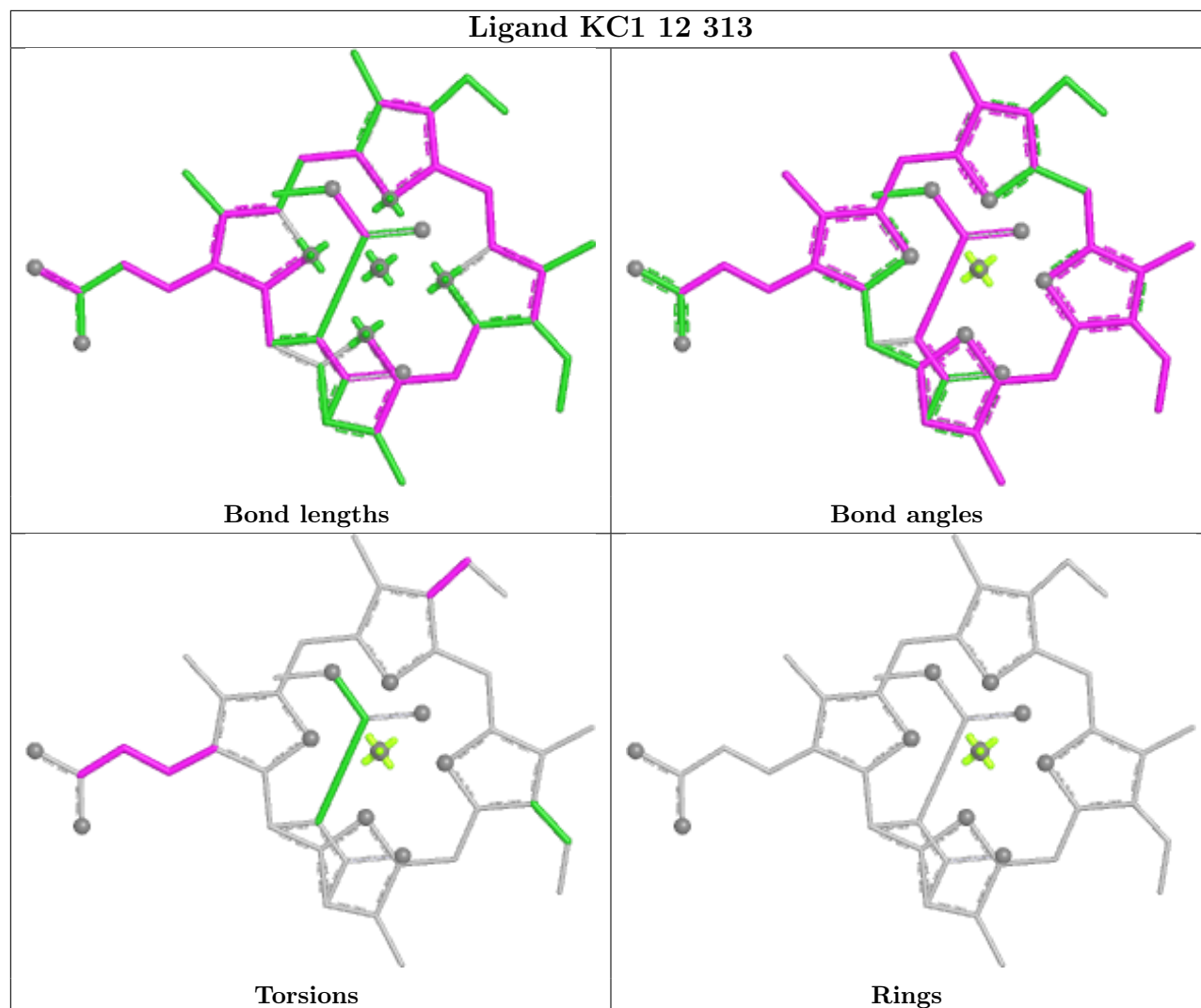


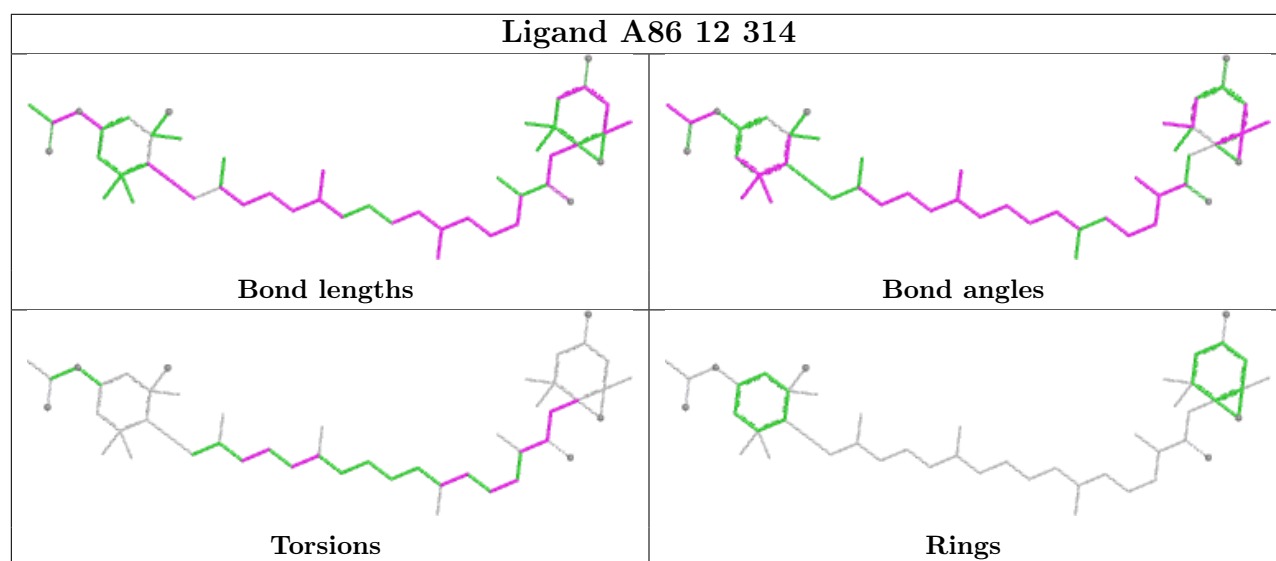
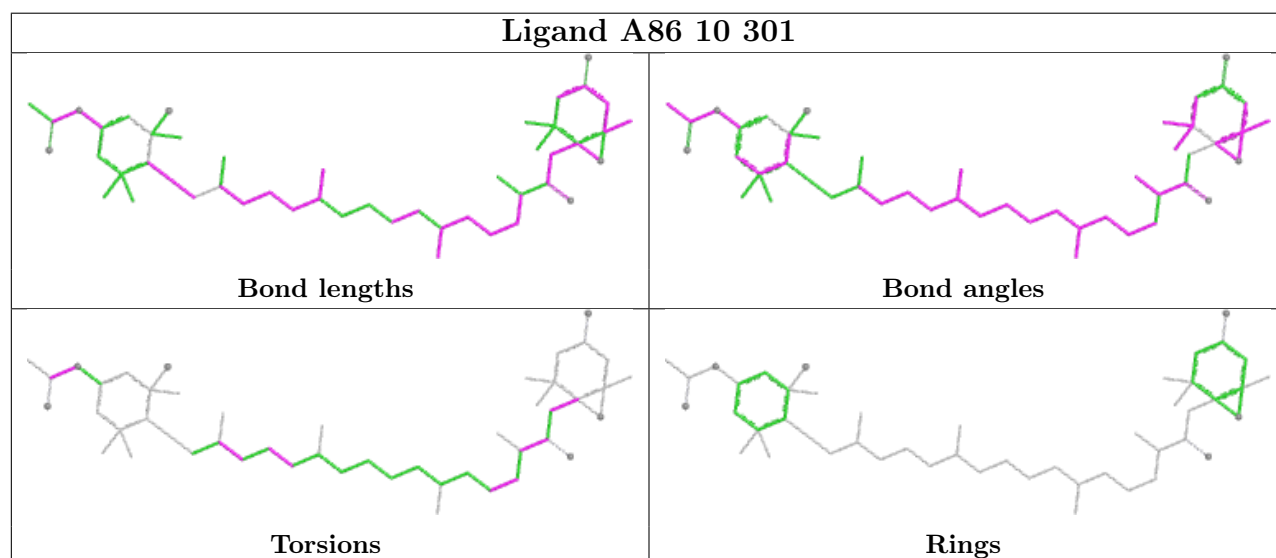
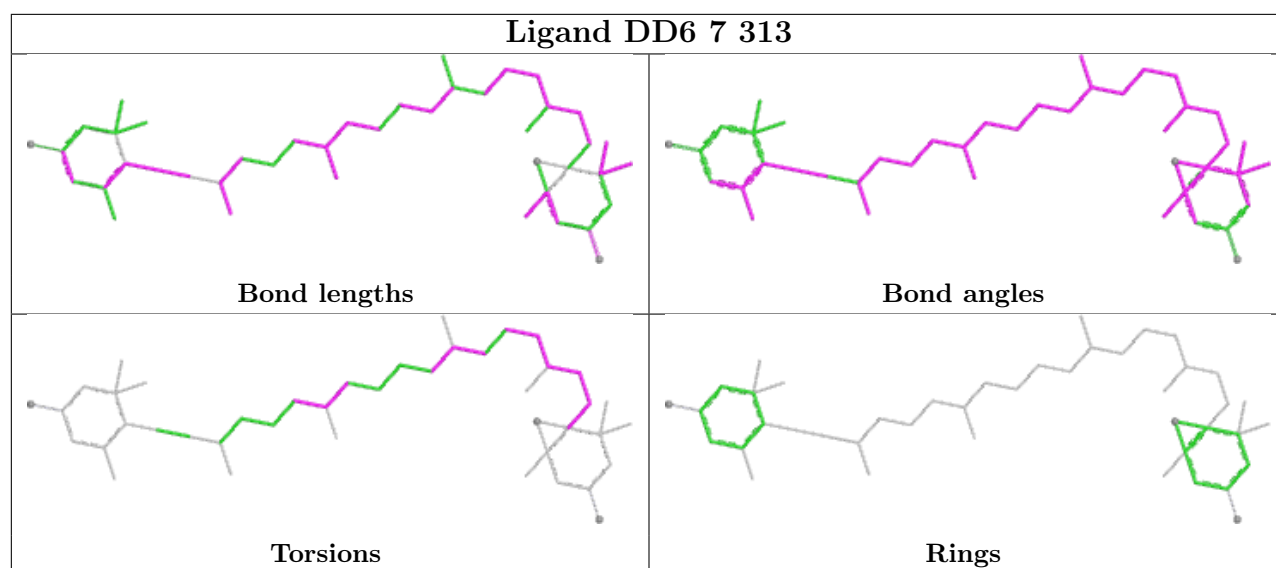
Torsions

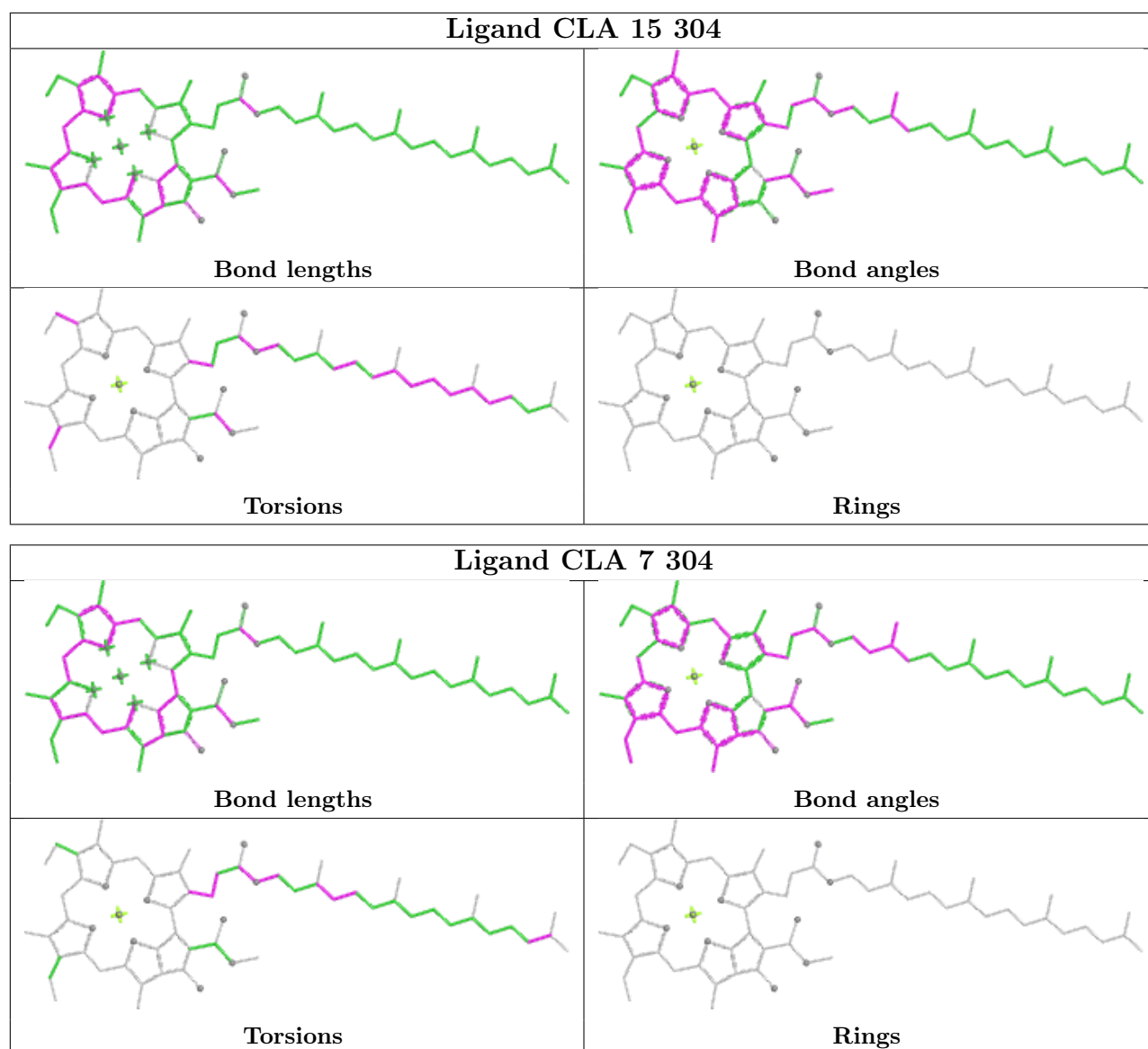


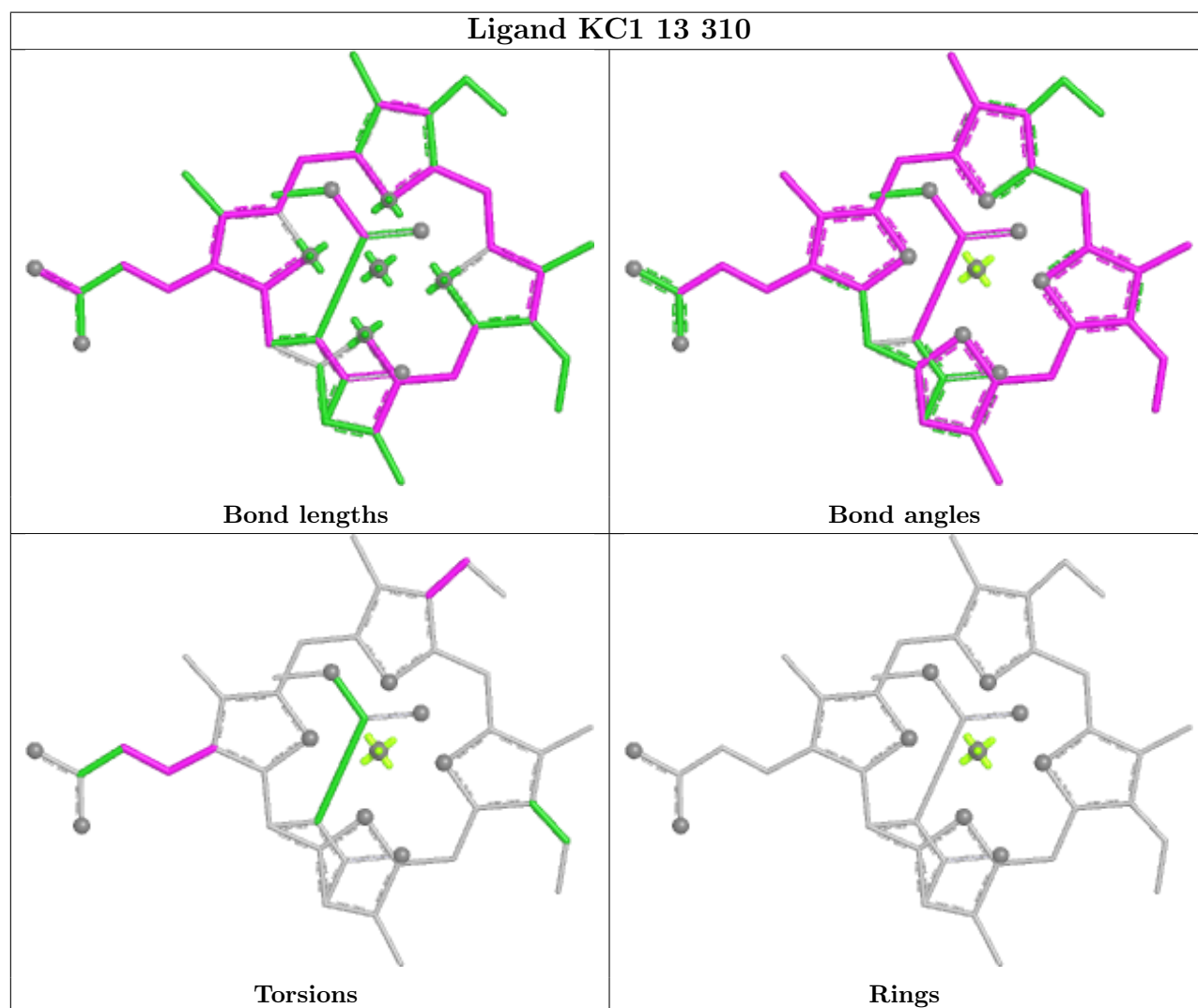
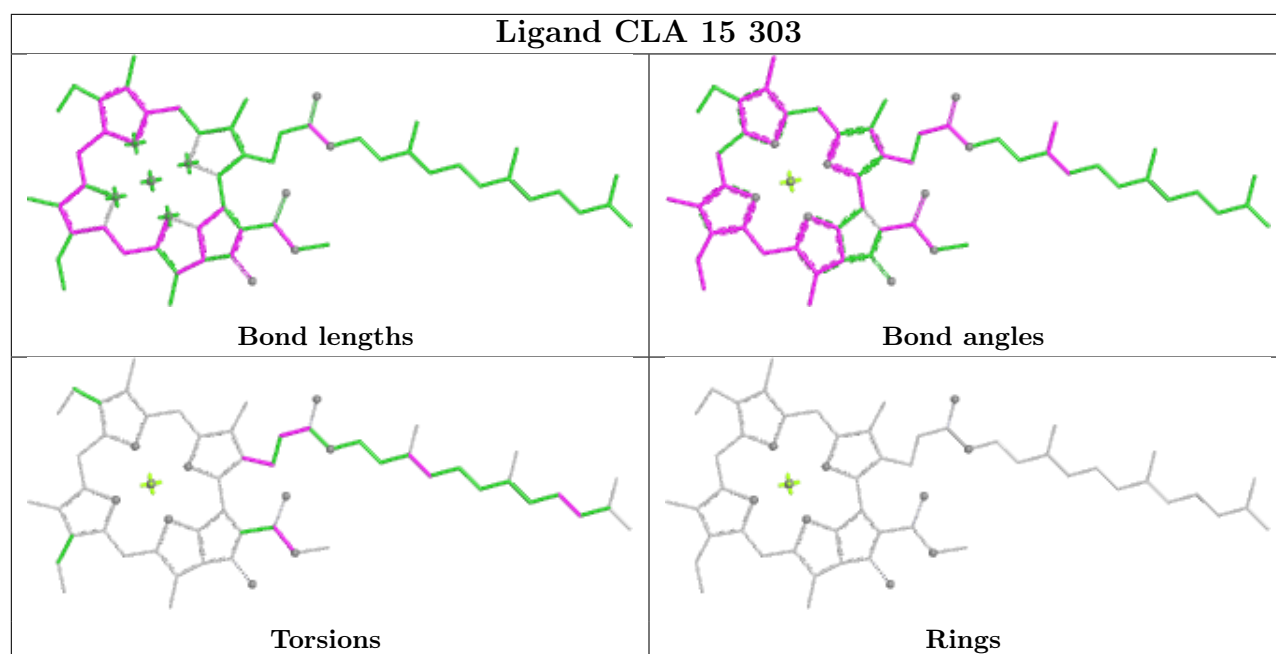
Rings

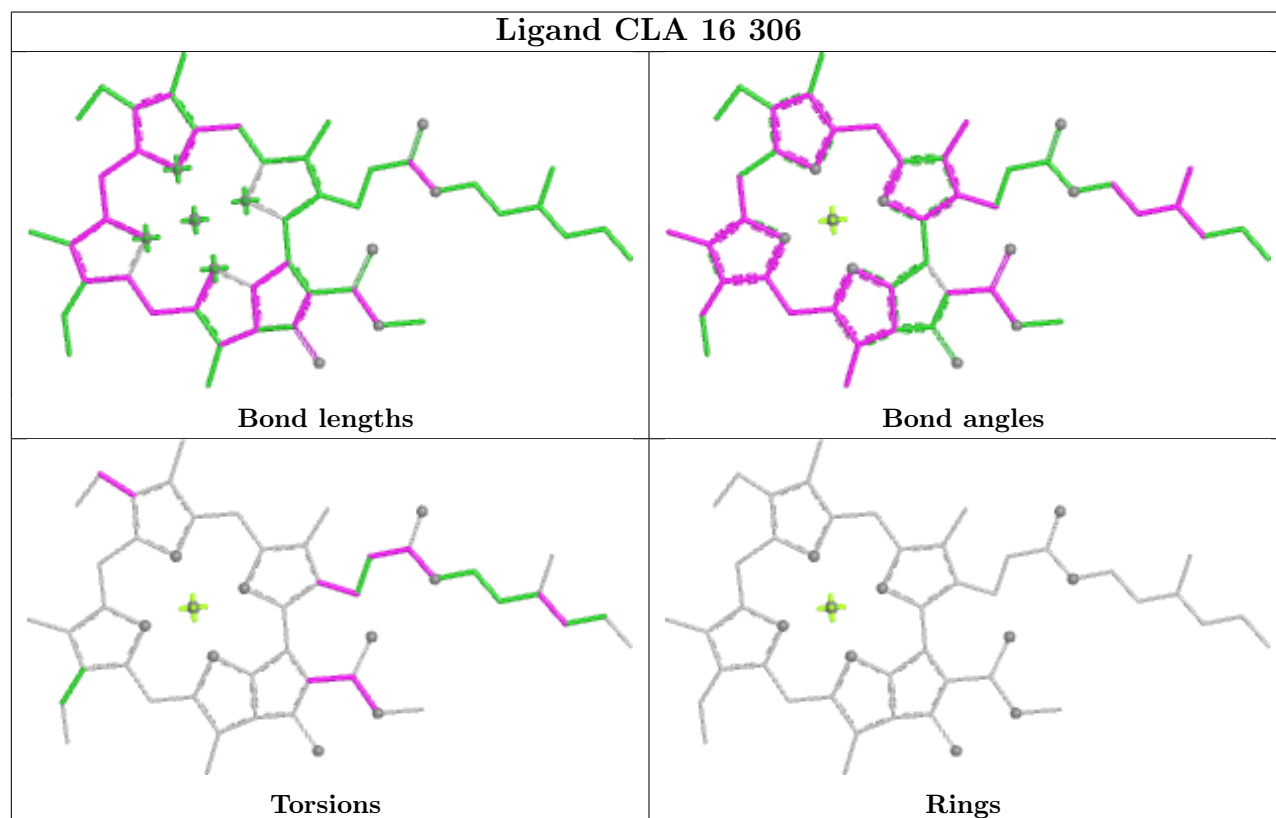
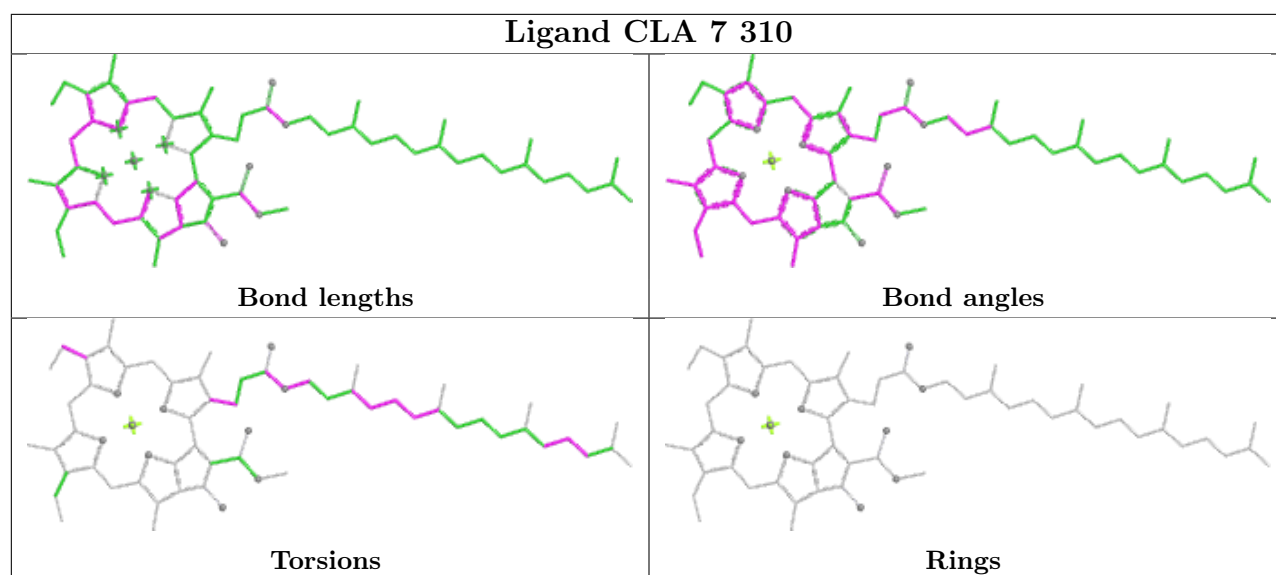


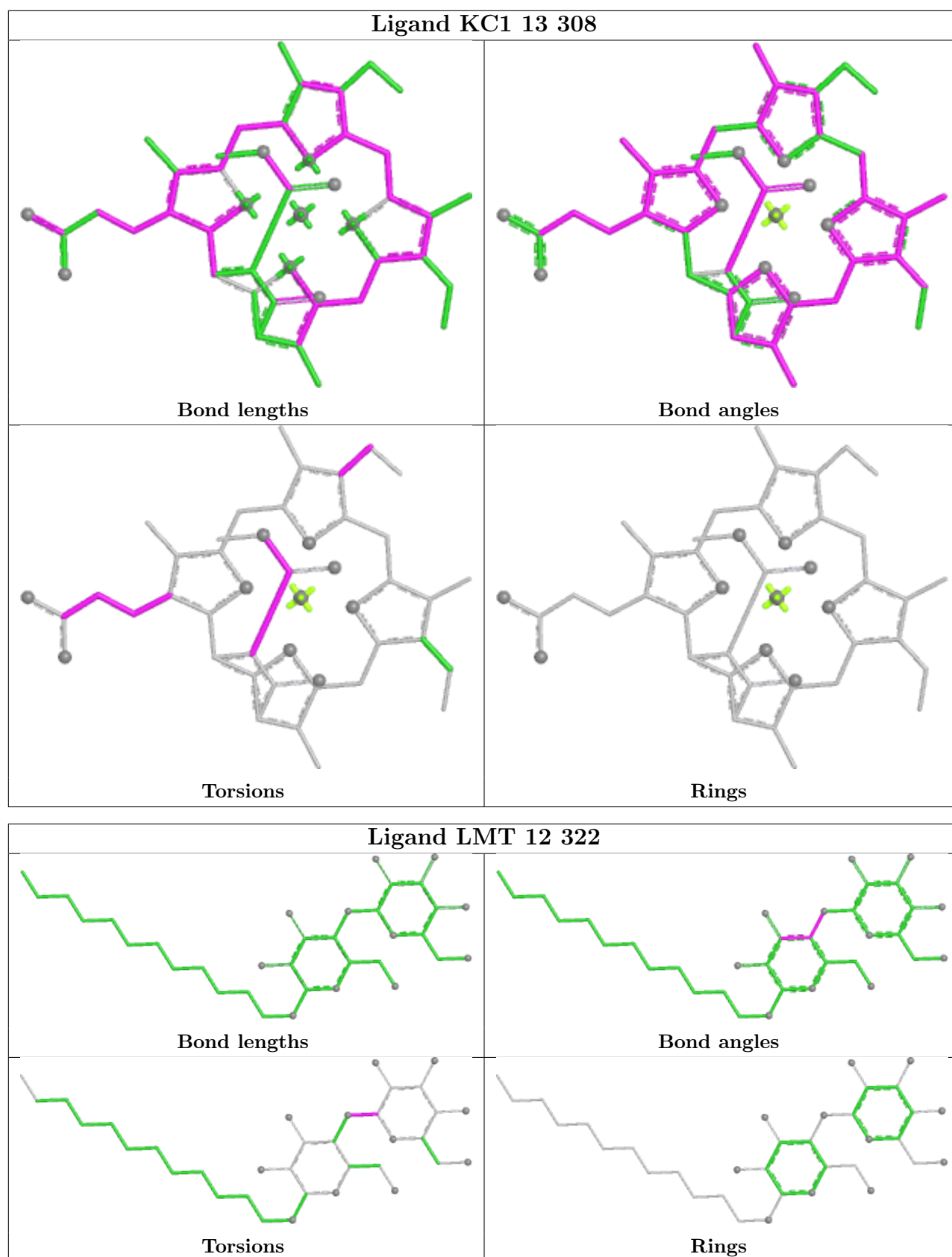


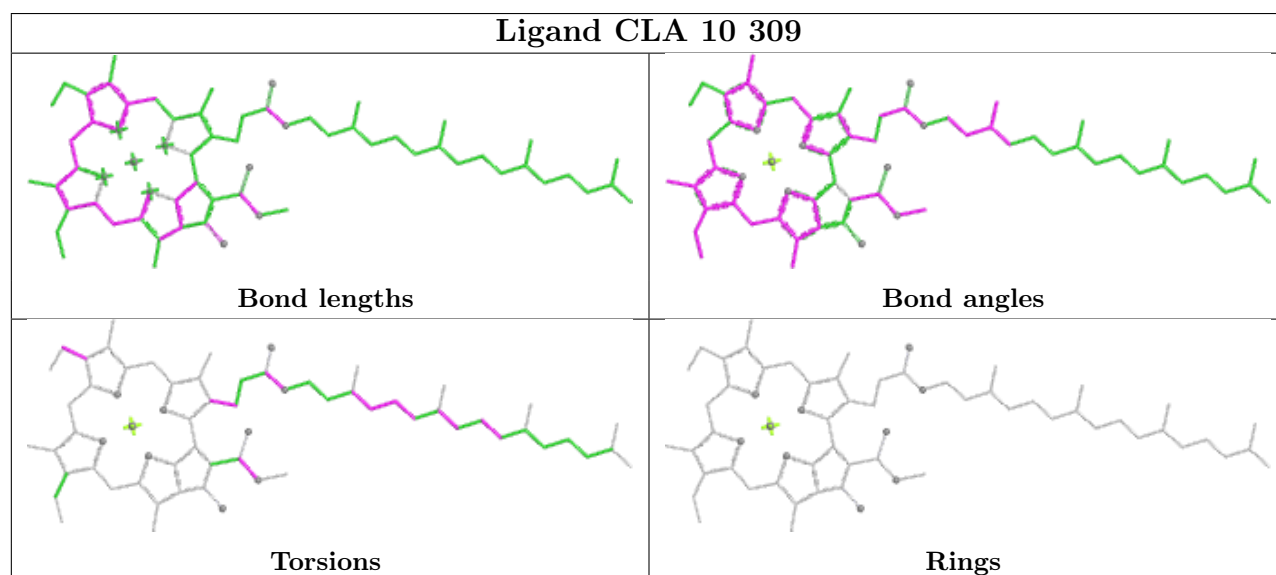
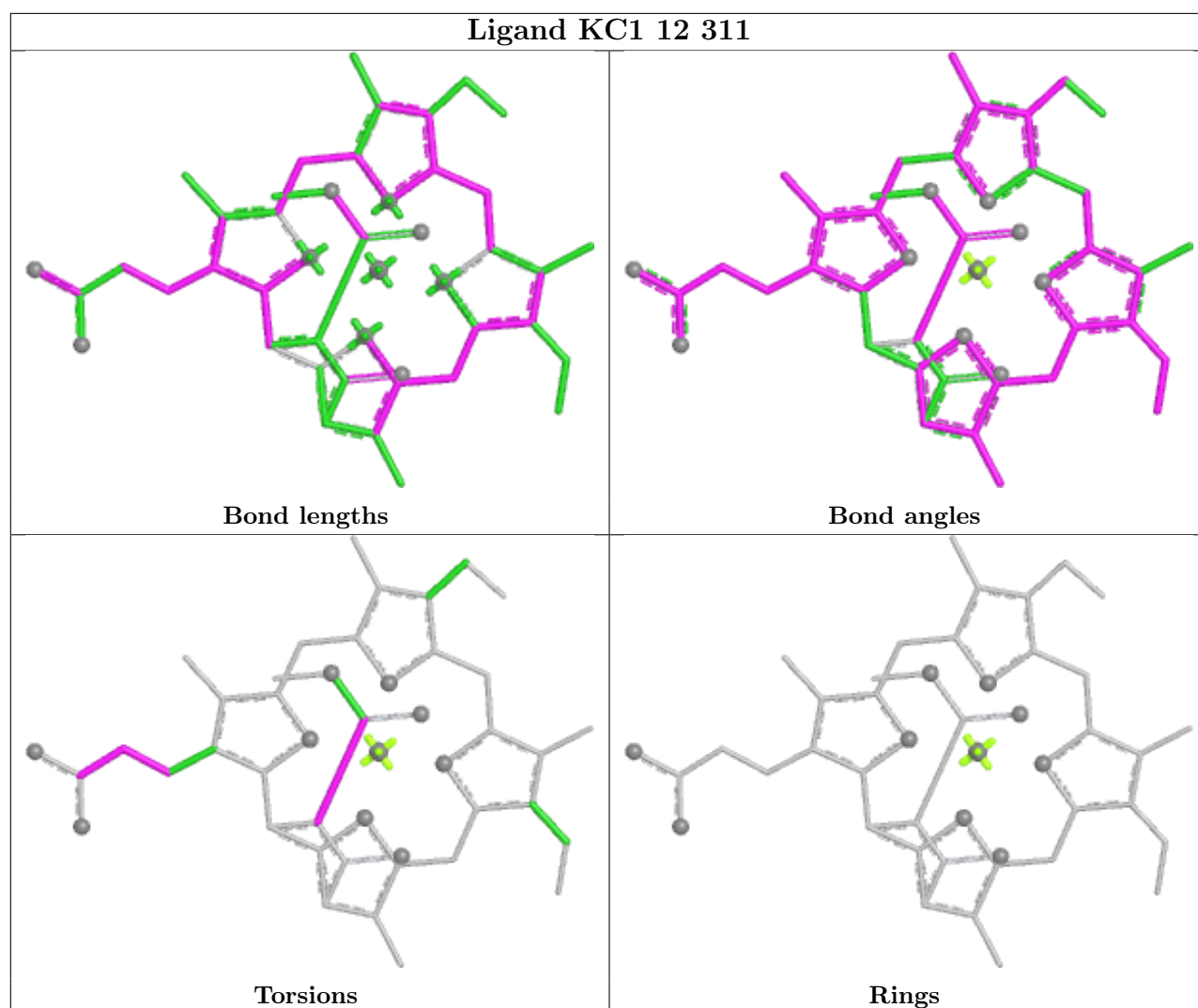


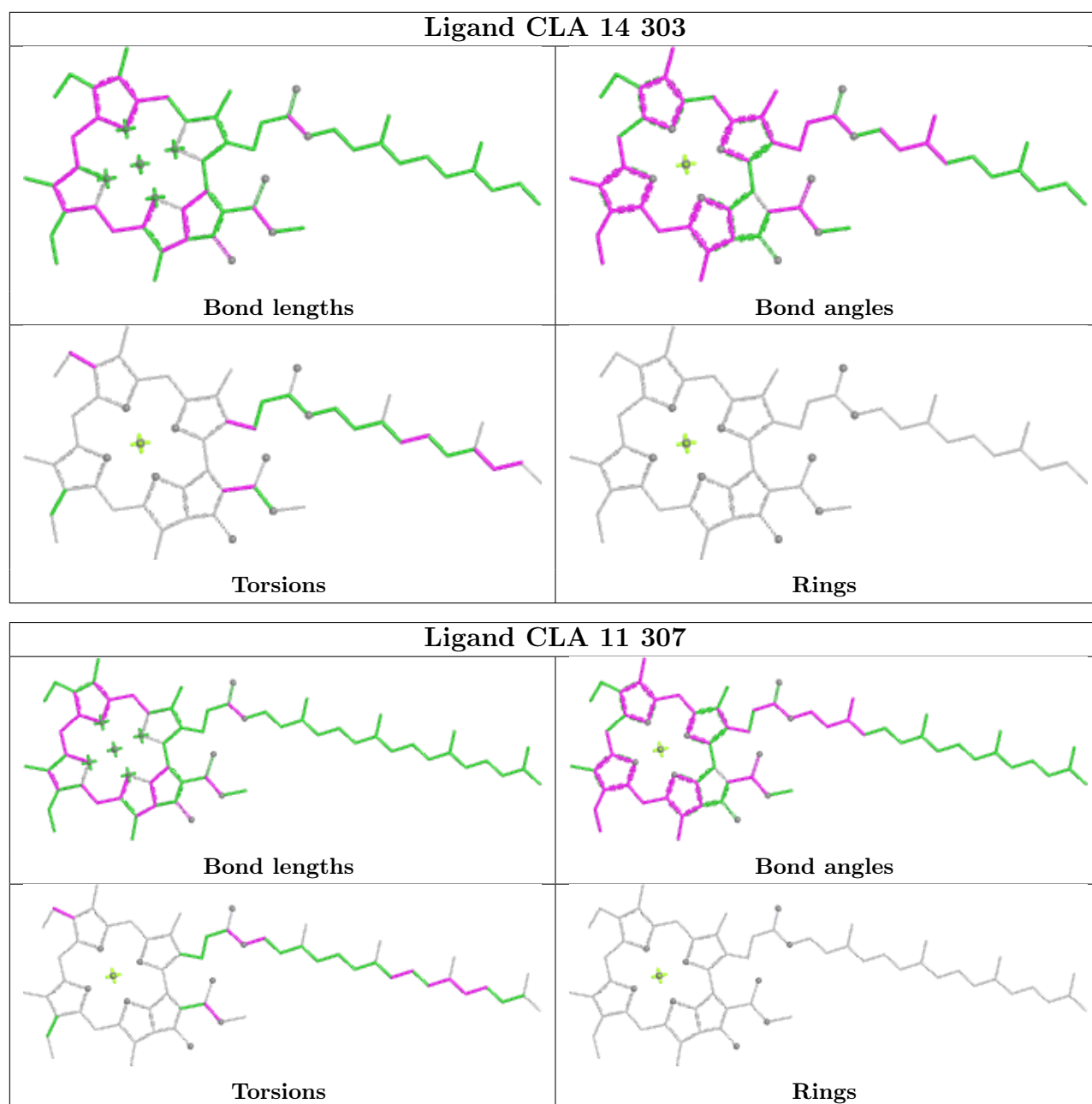




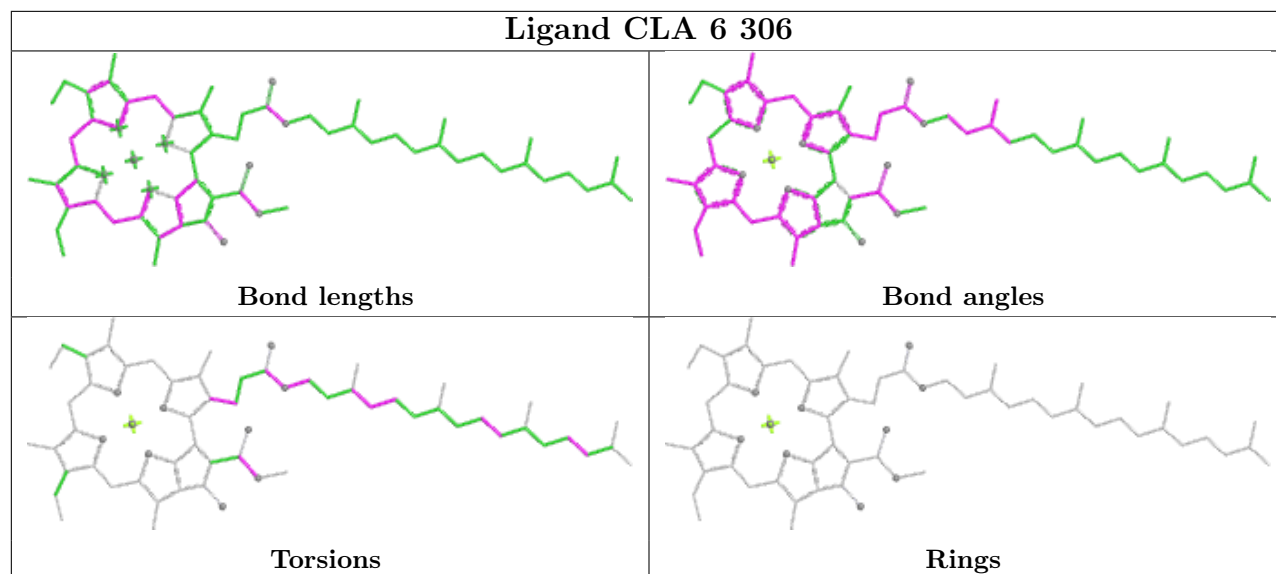




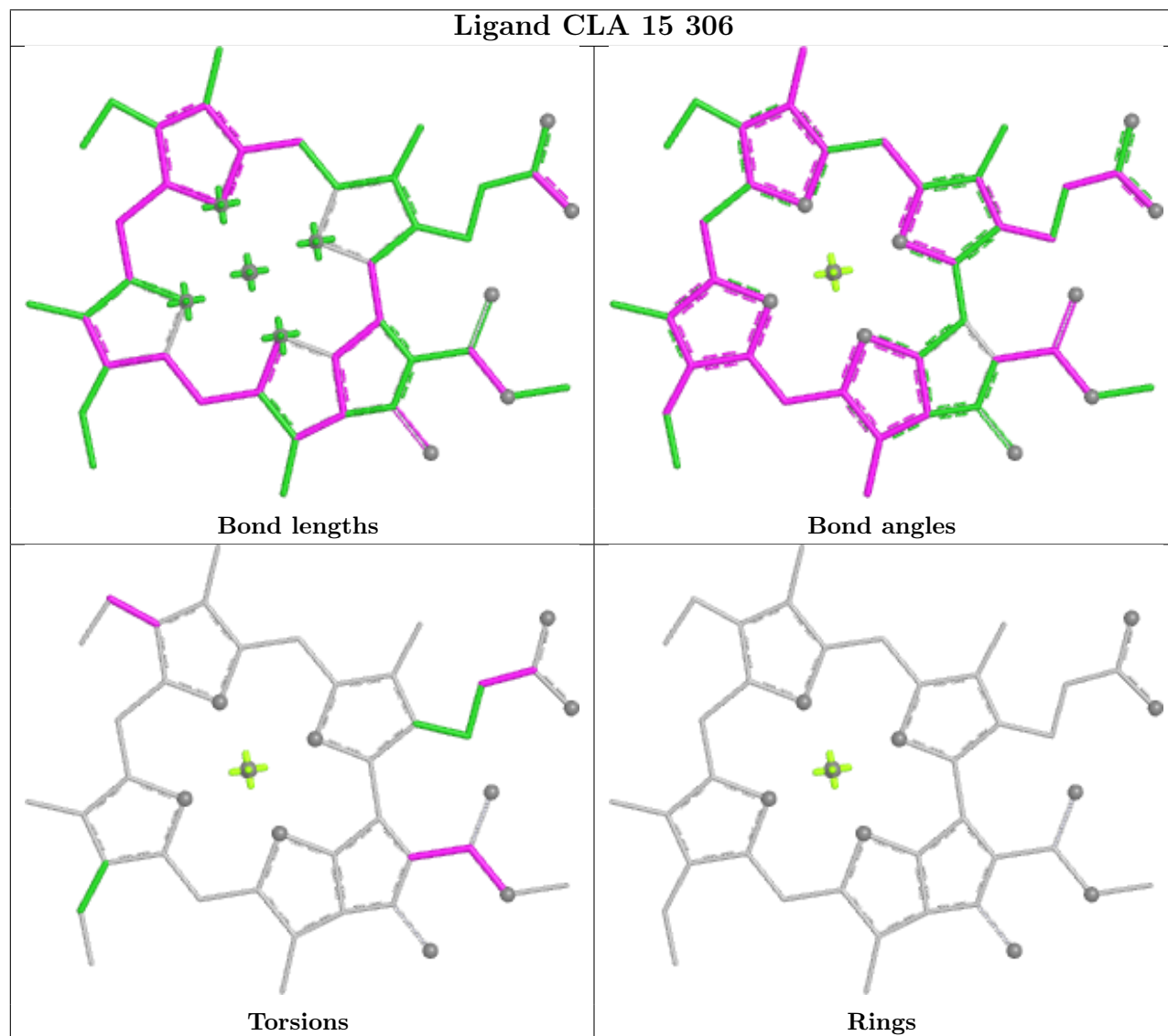


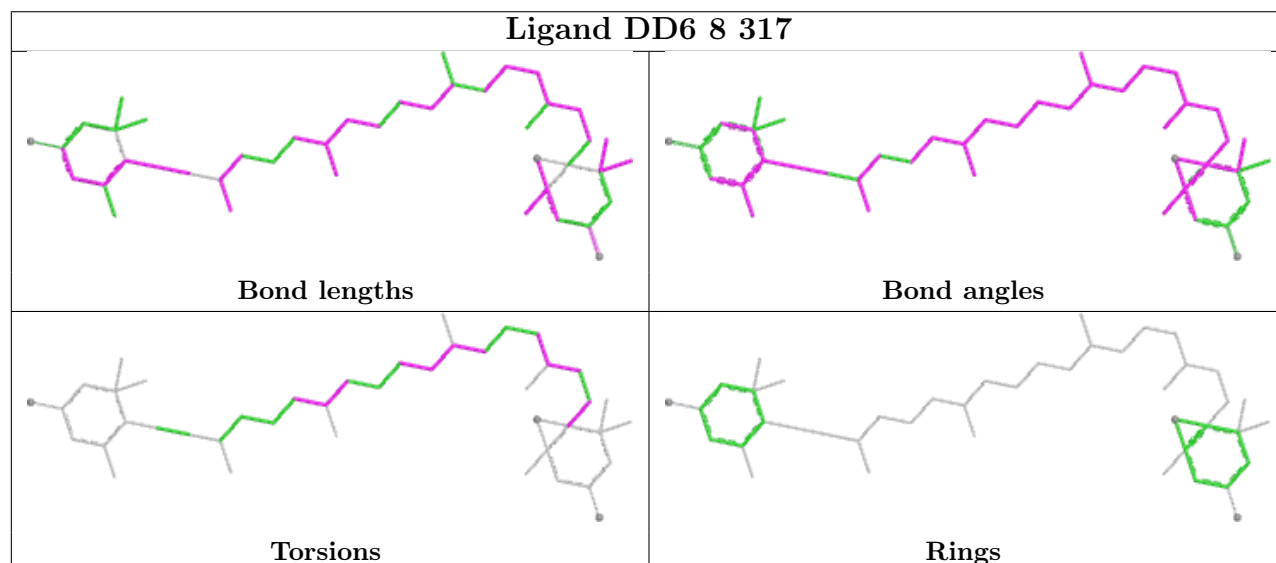
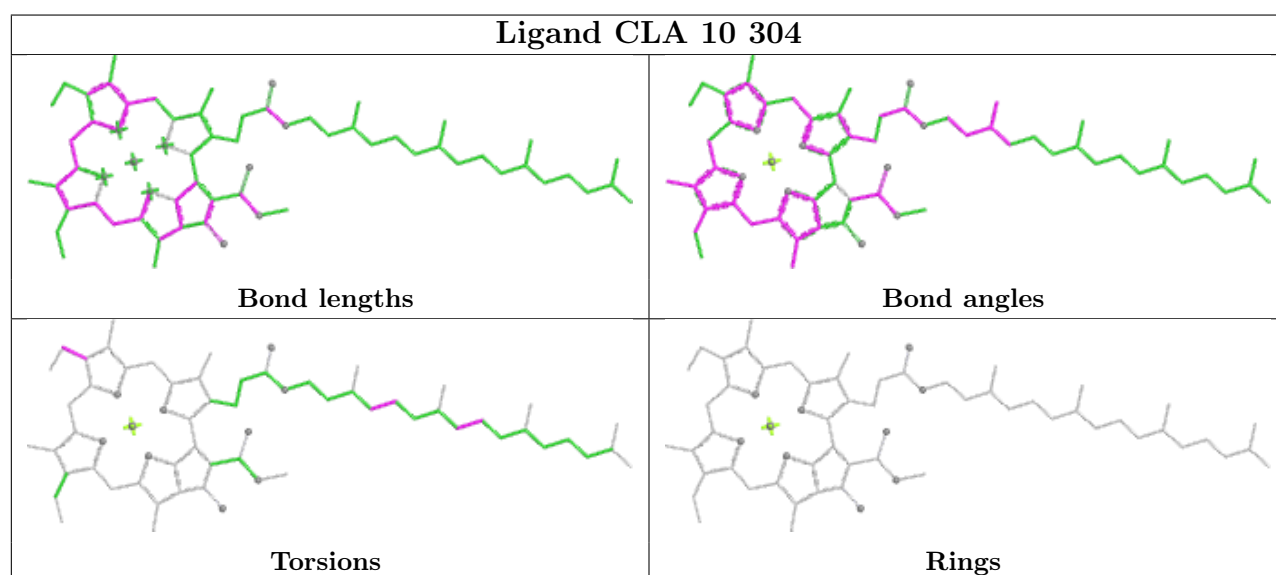
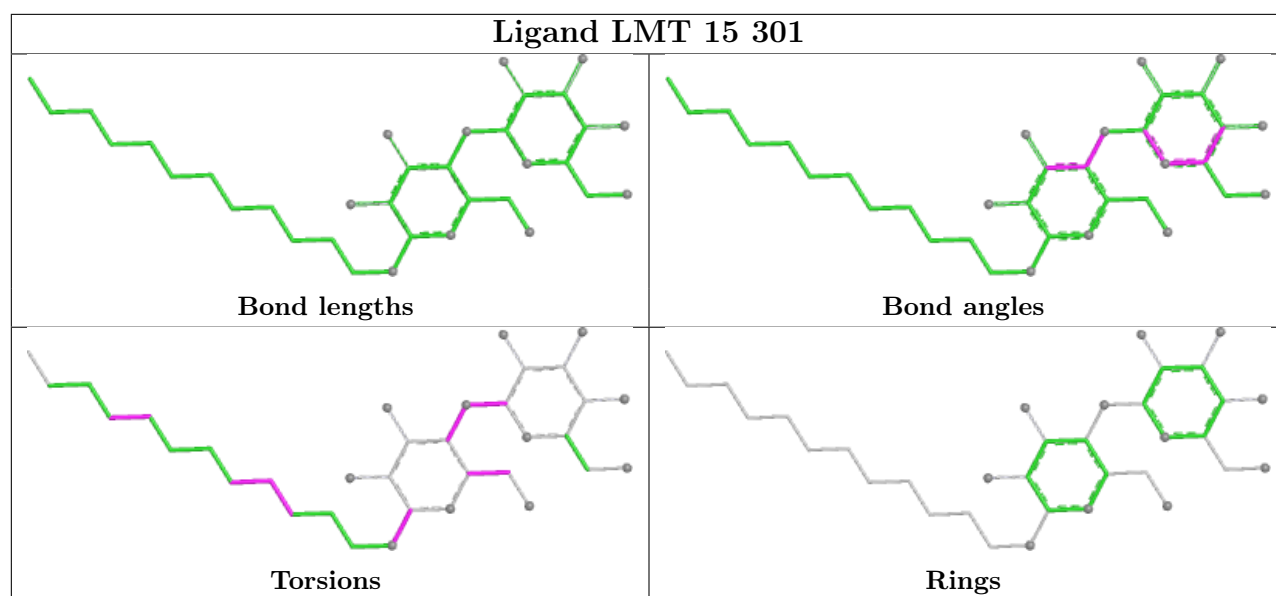


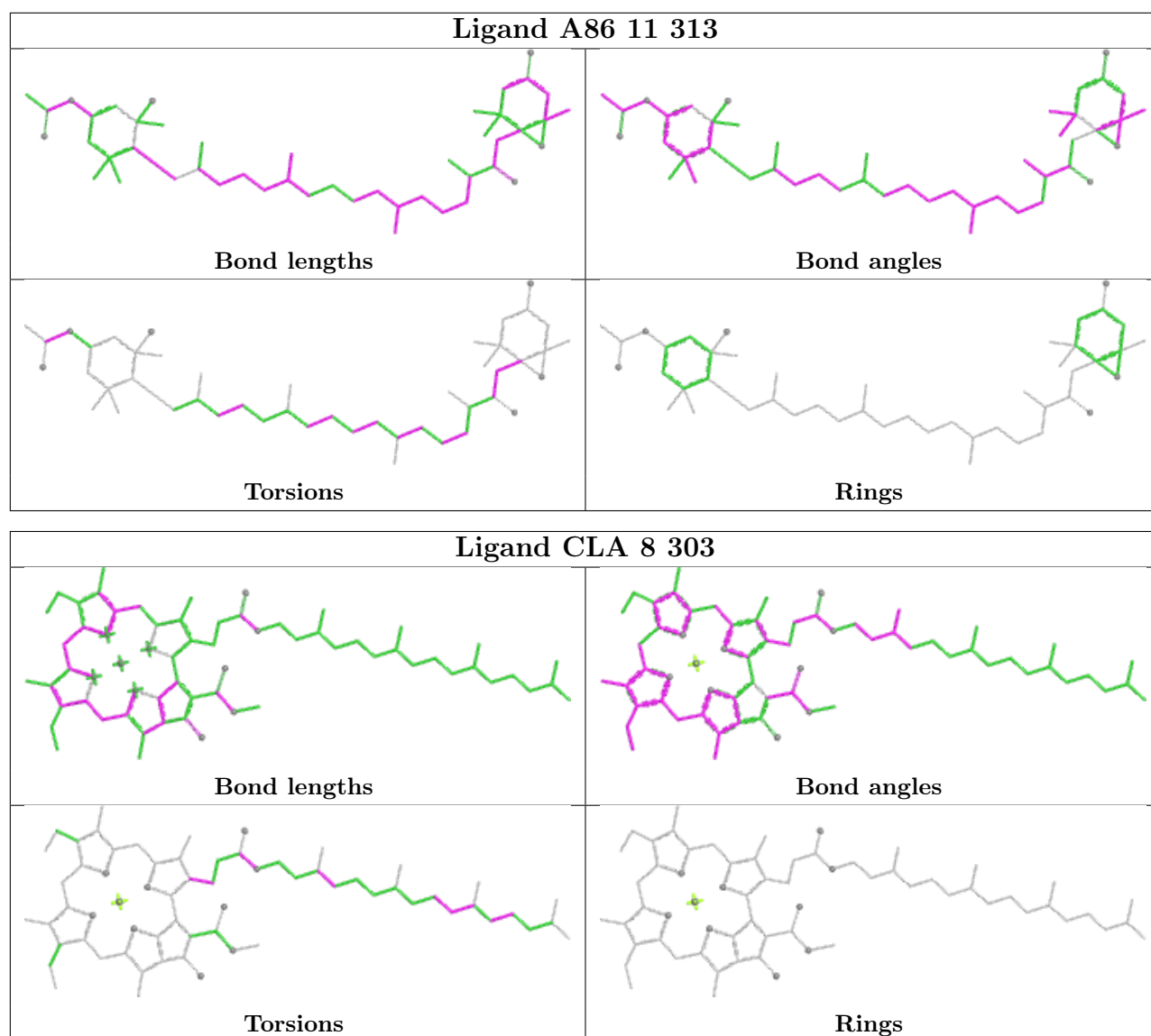
Ligand CLA 6 306



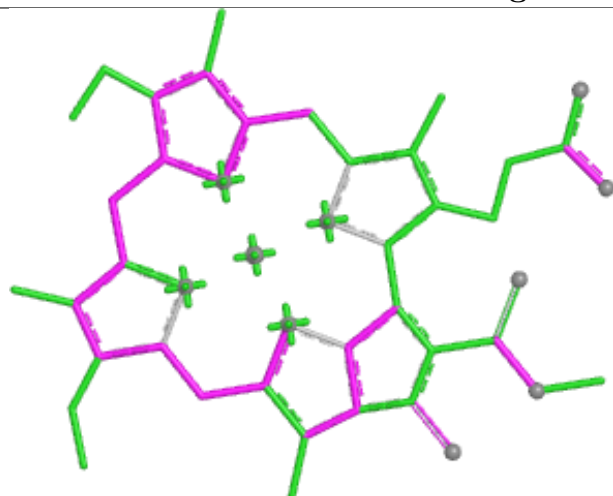
Ligand CLA 15 306



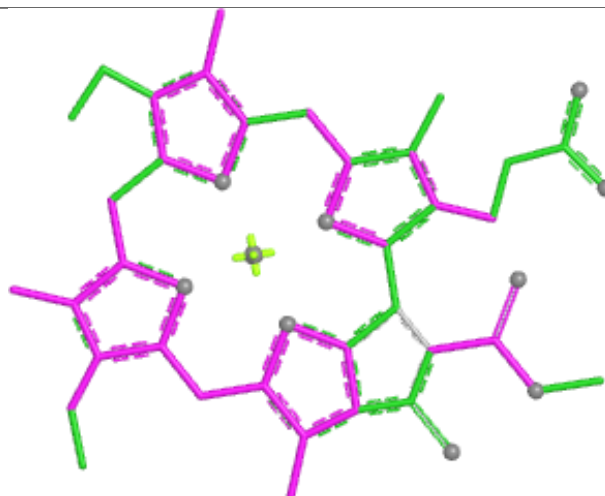




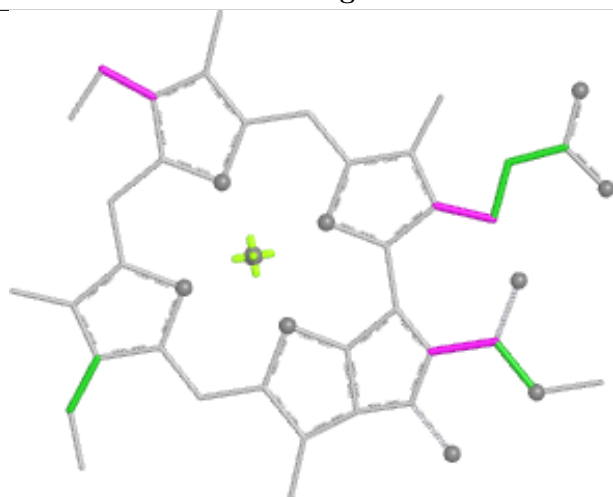
Ligand CLA 16 309



Bond lengths



Bond angles

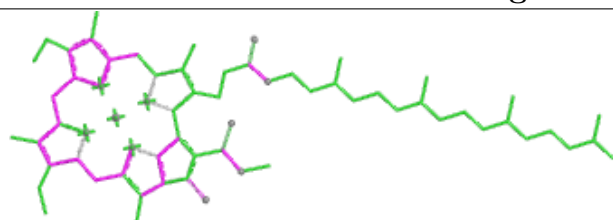


Torsions

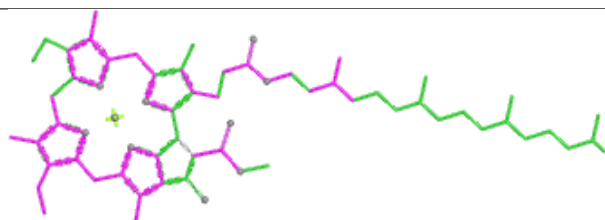


Rings

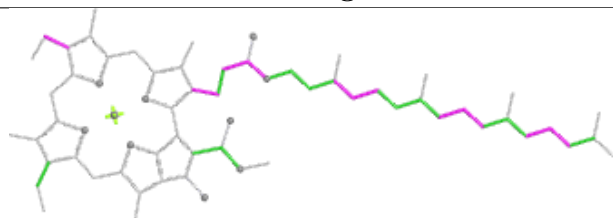
Ligand CLA 14 302



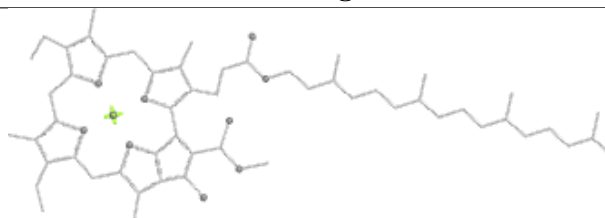
Bond lengths



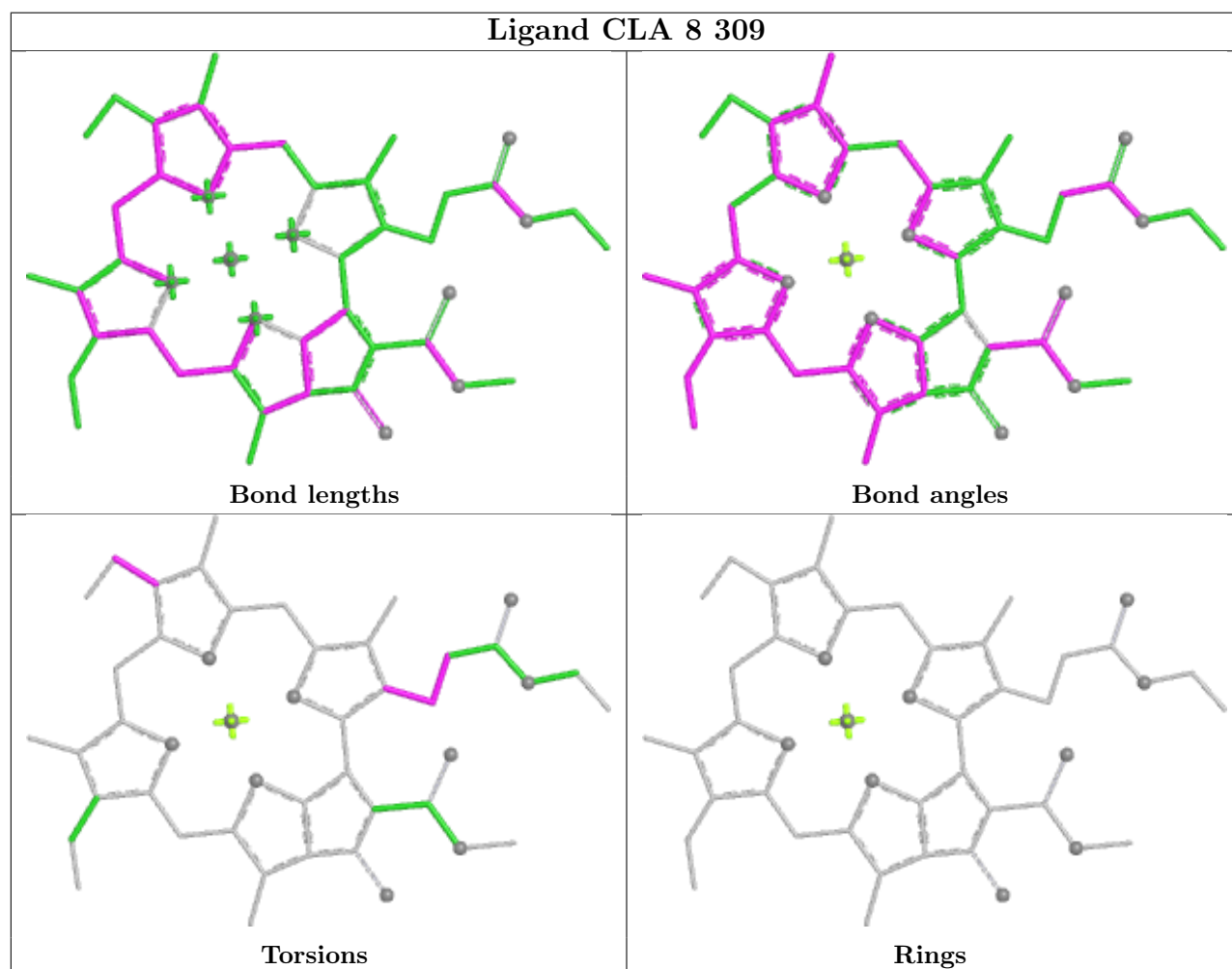
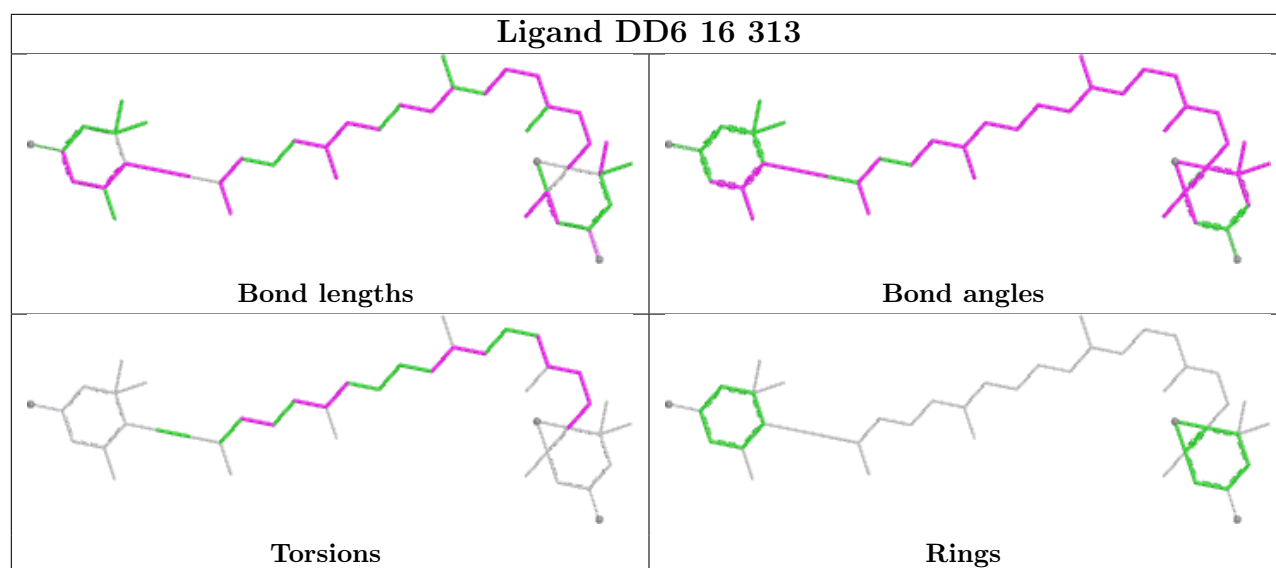
Bond angles

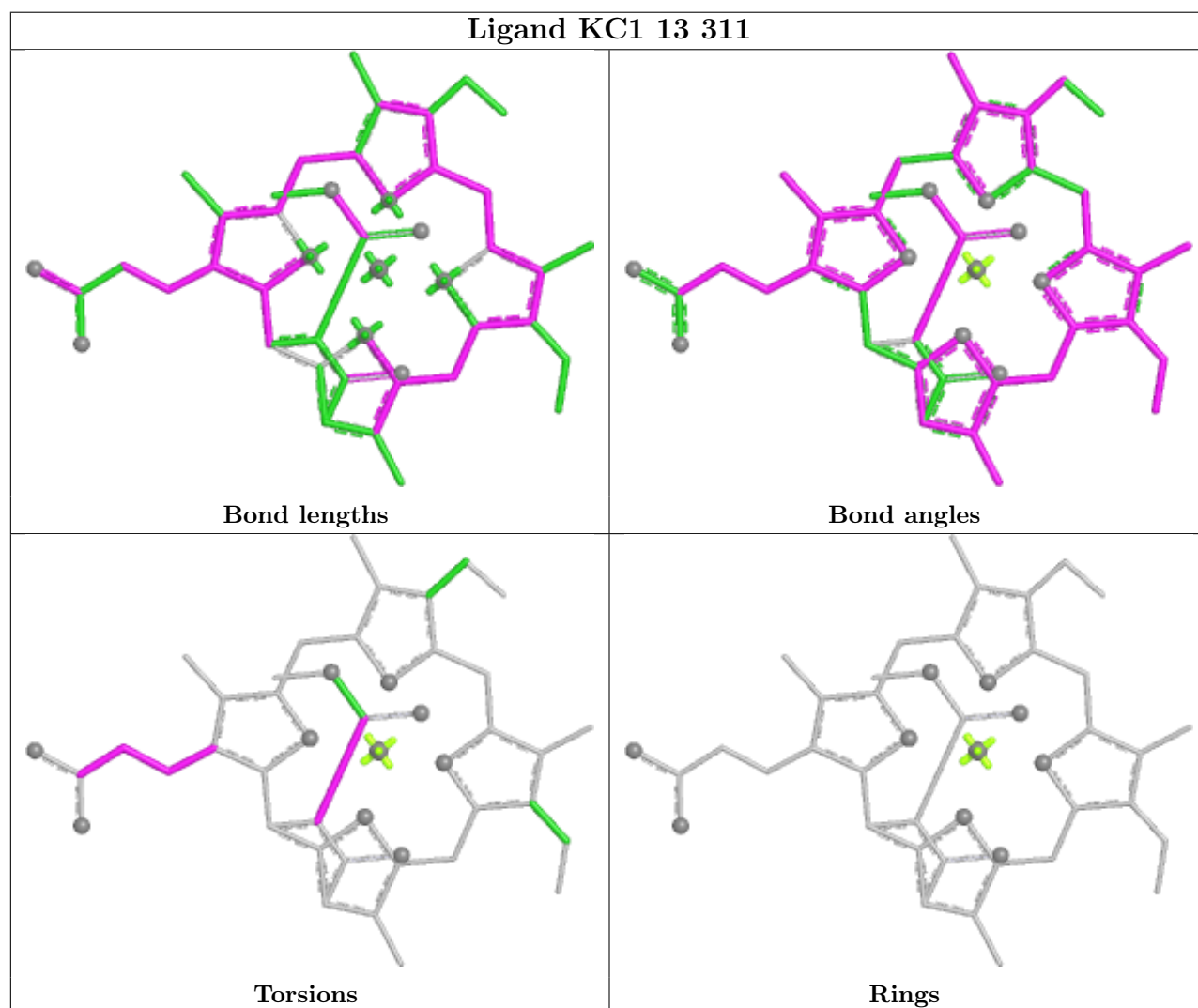
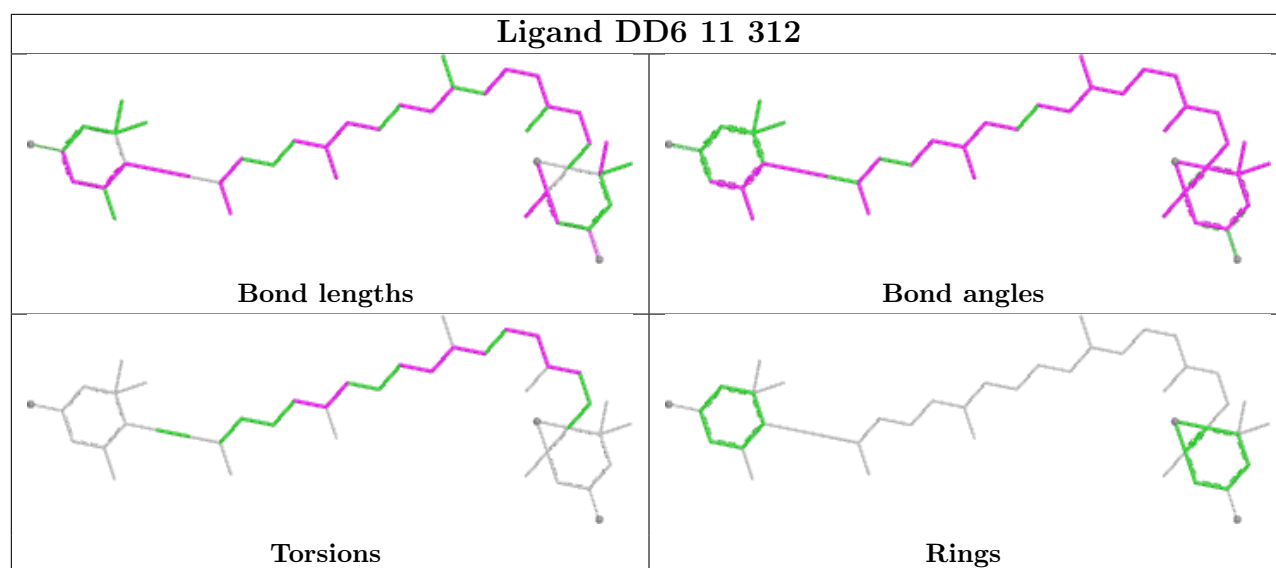


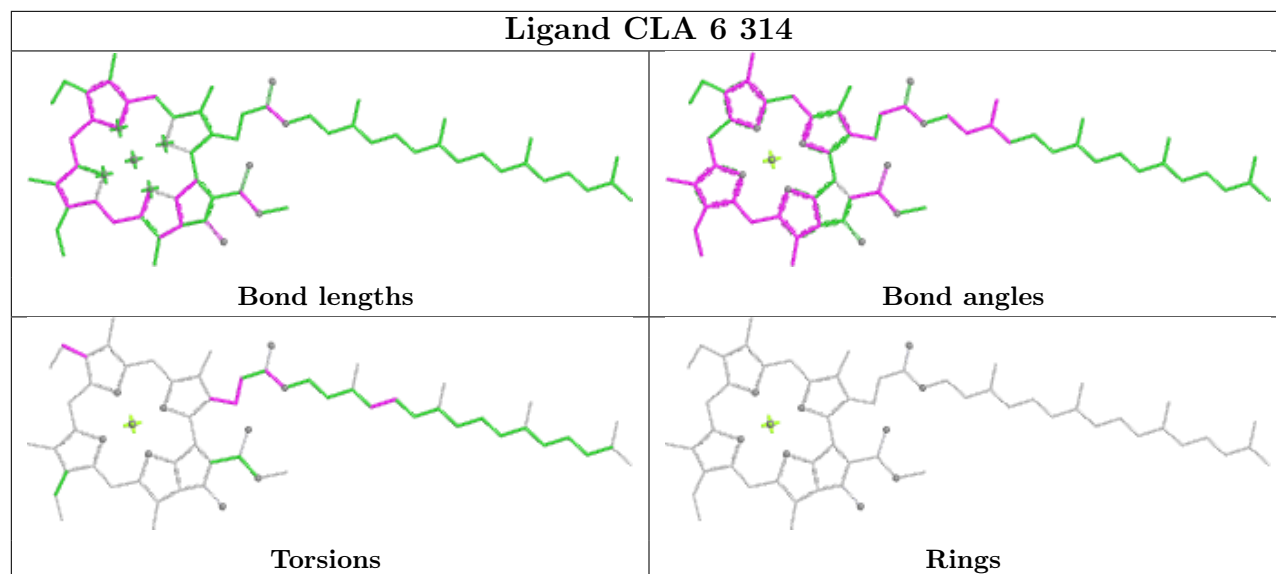
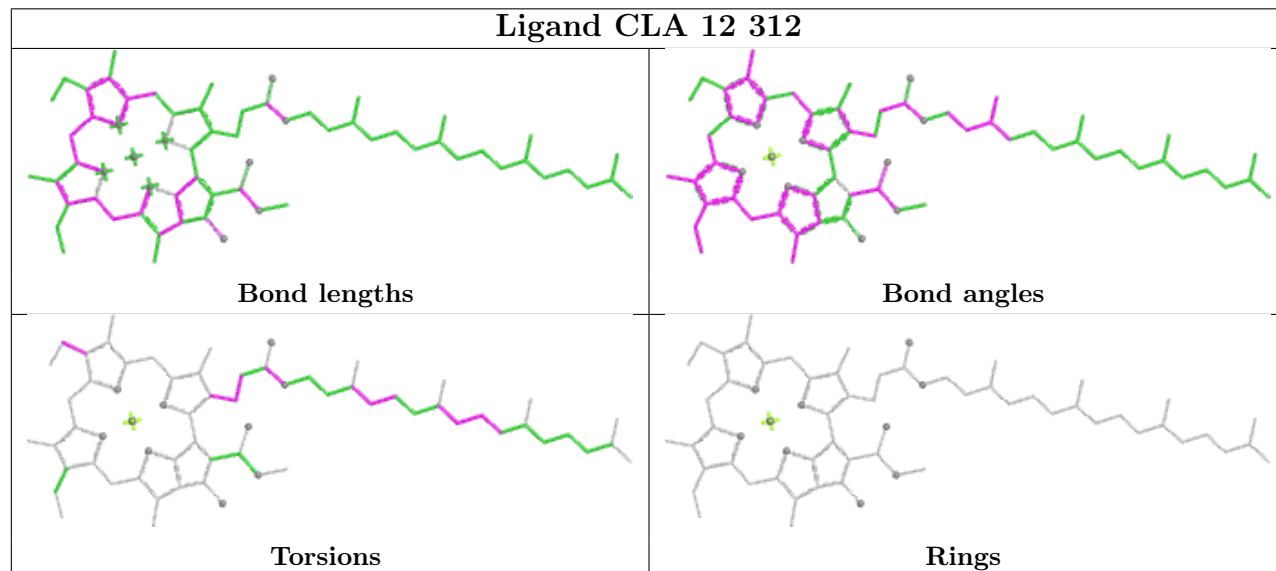
Torsions

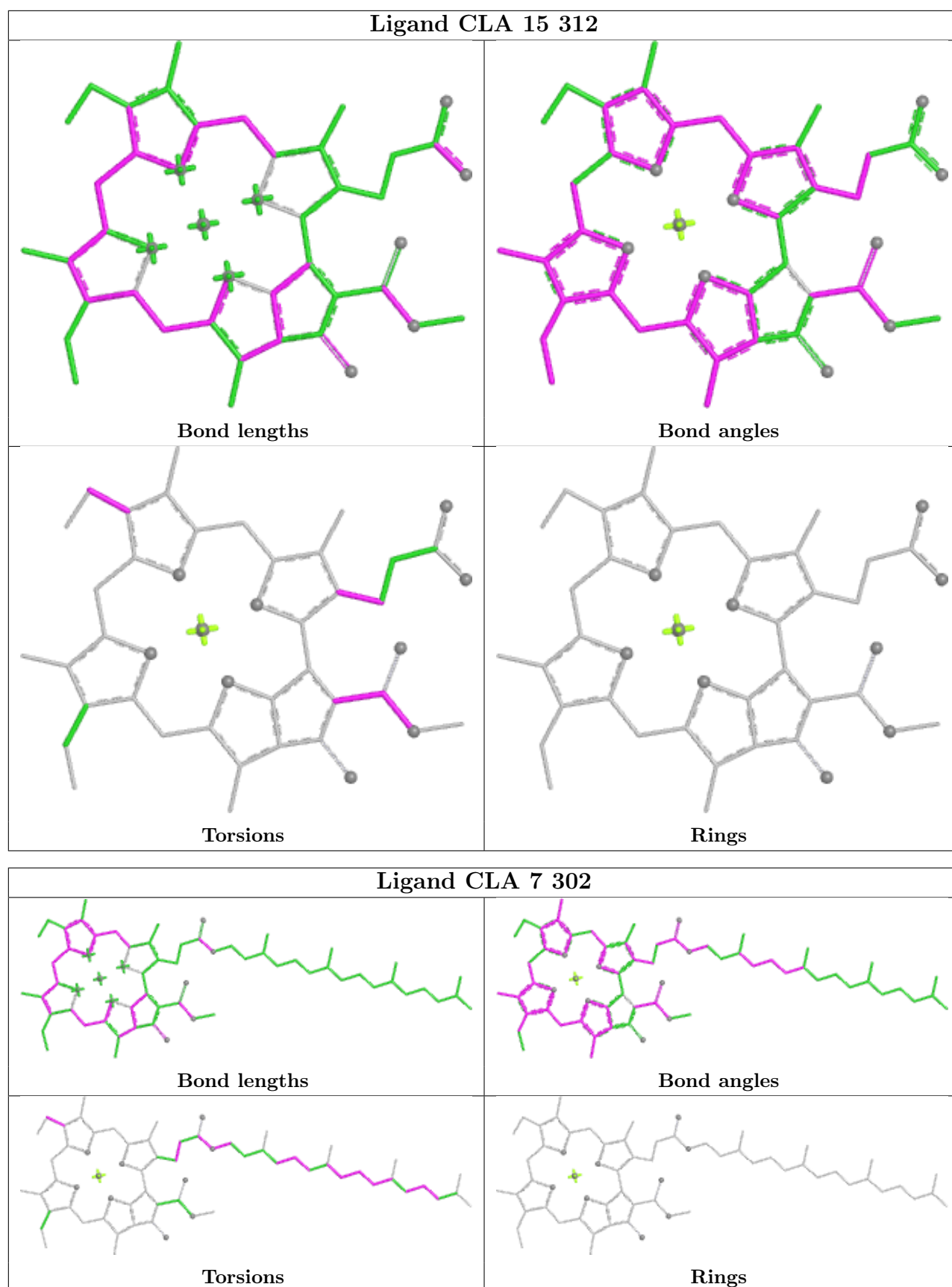


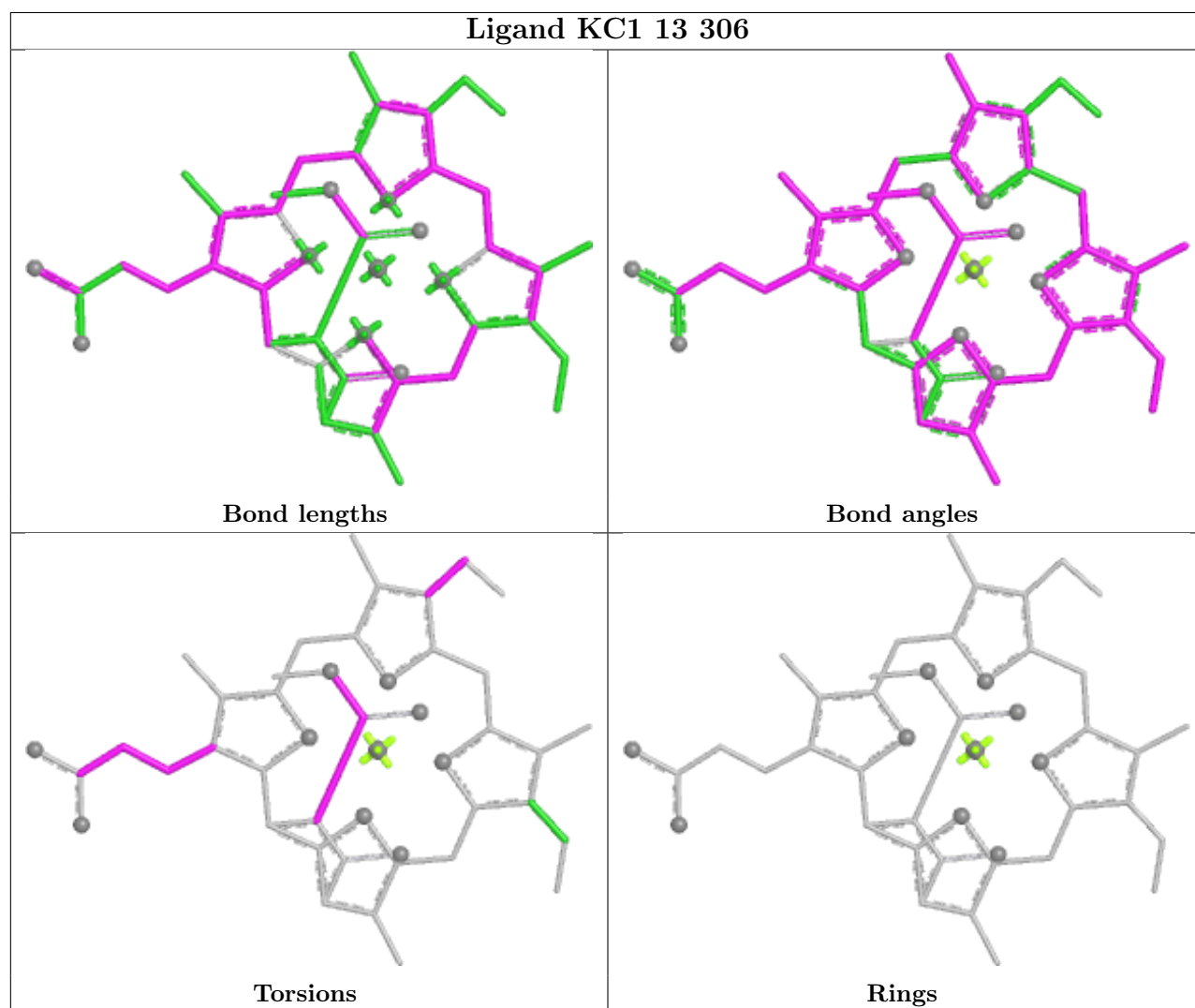
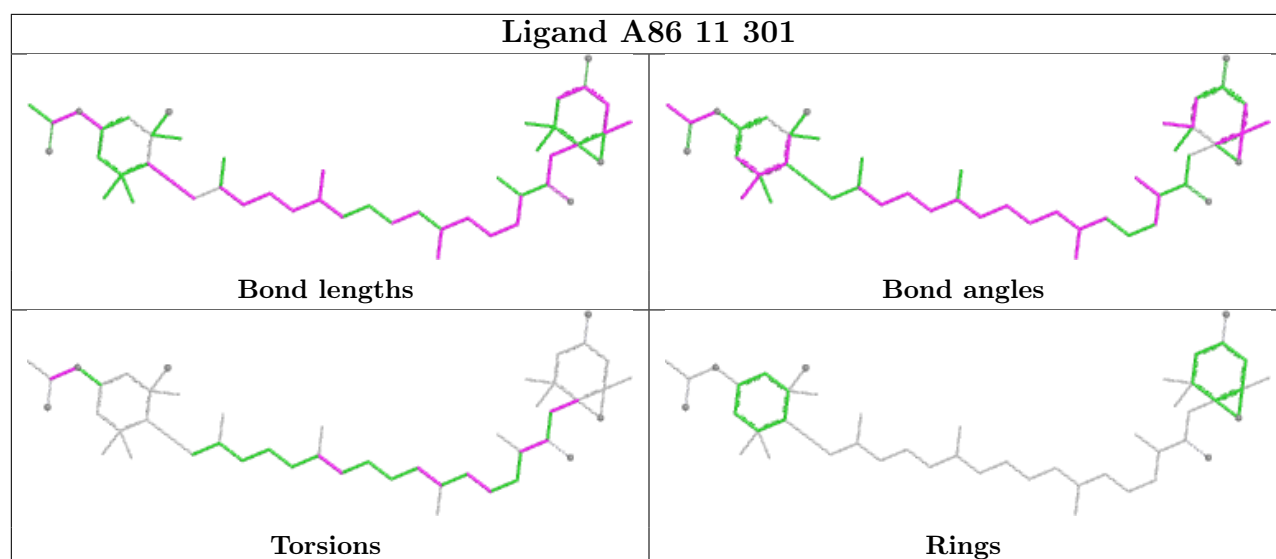
Rings

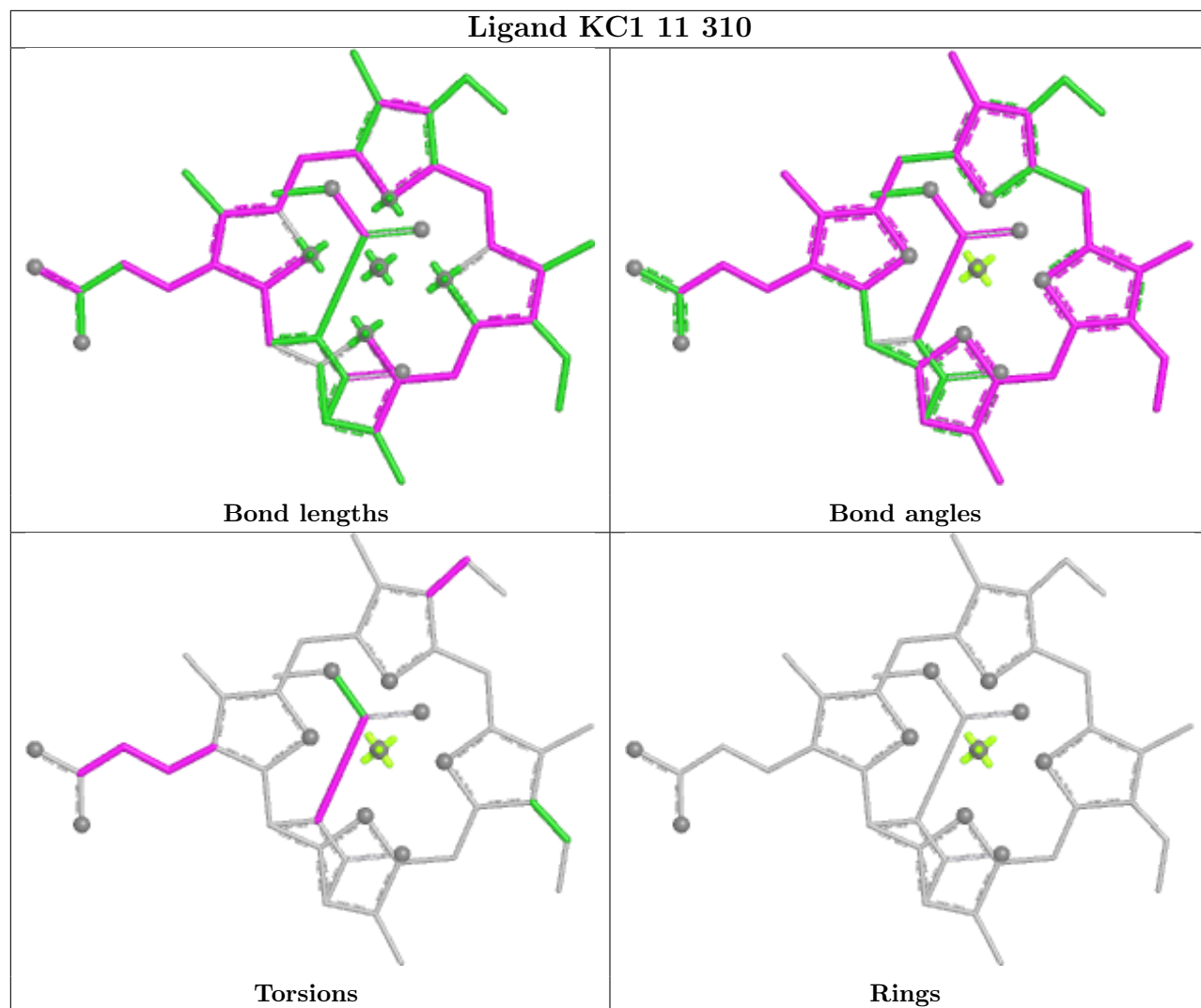




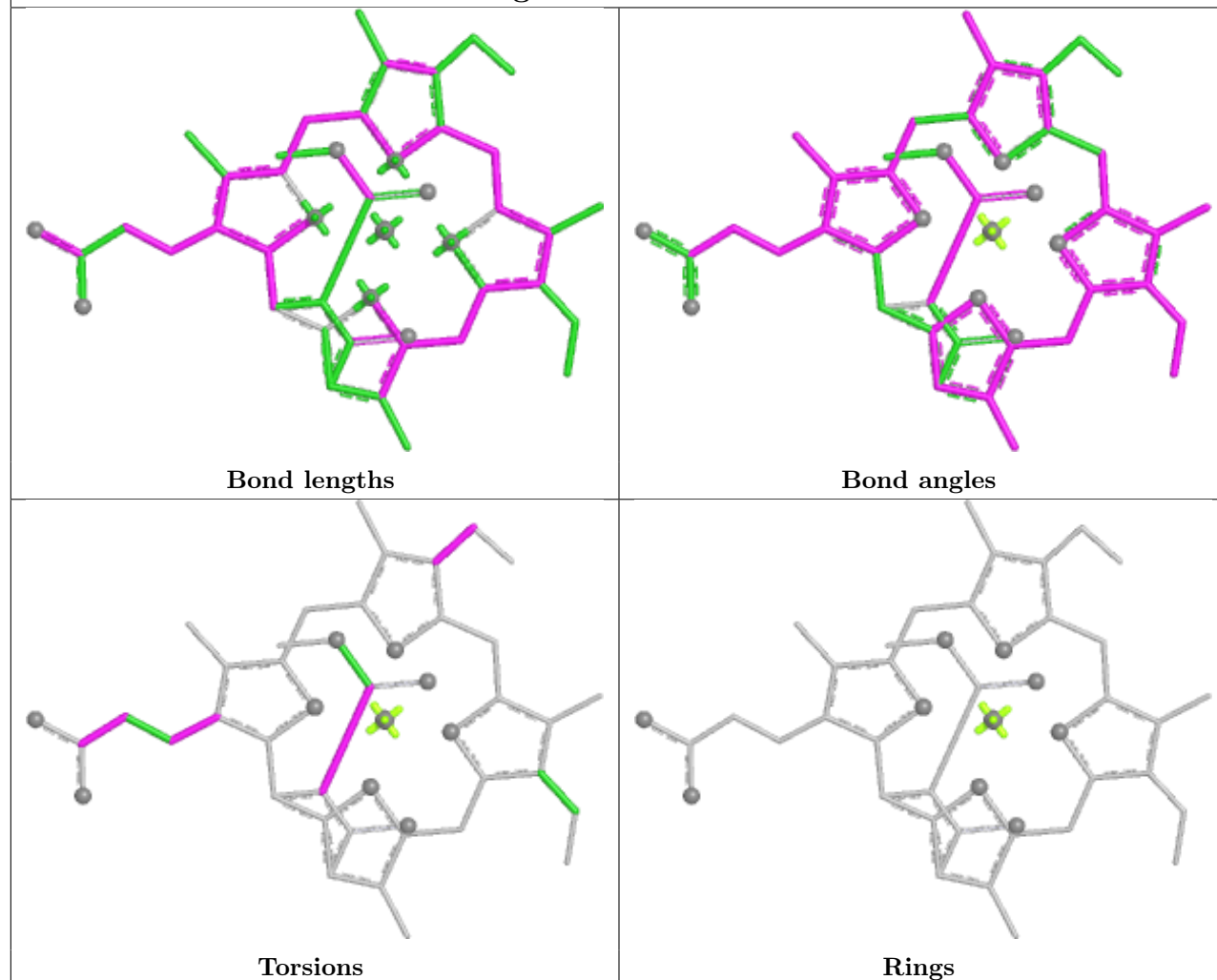
Ligand CLA 6 314**Ligand CLA 12 312**



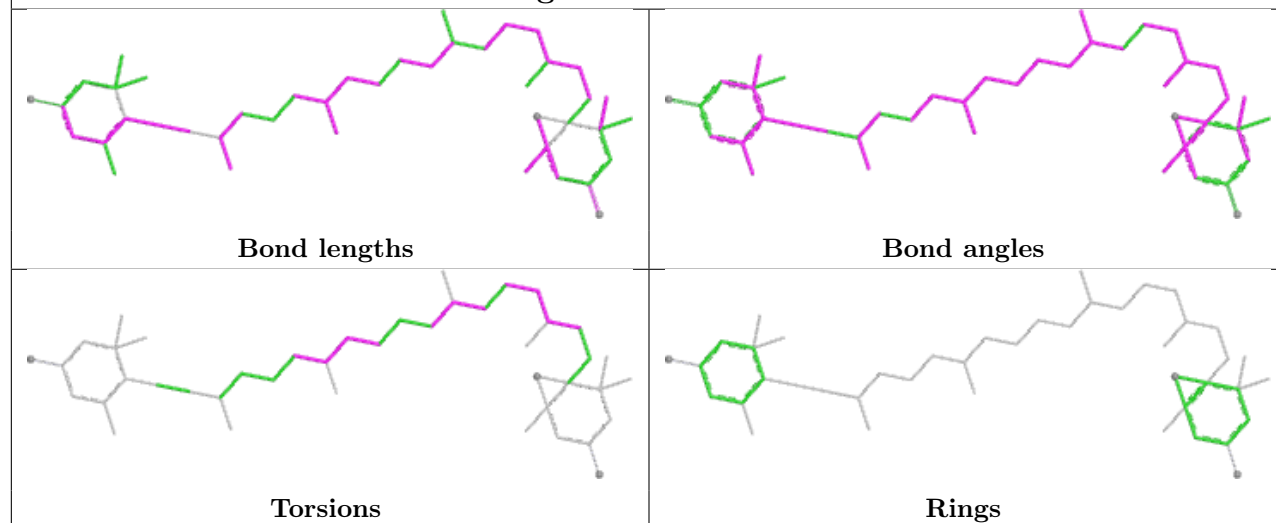


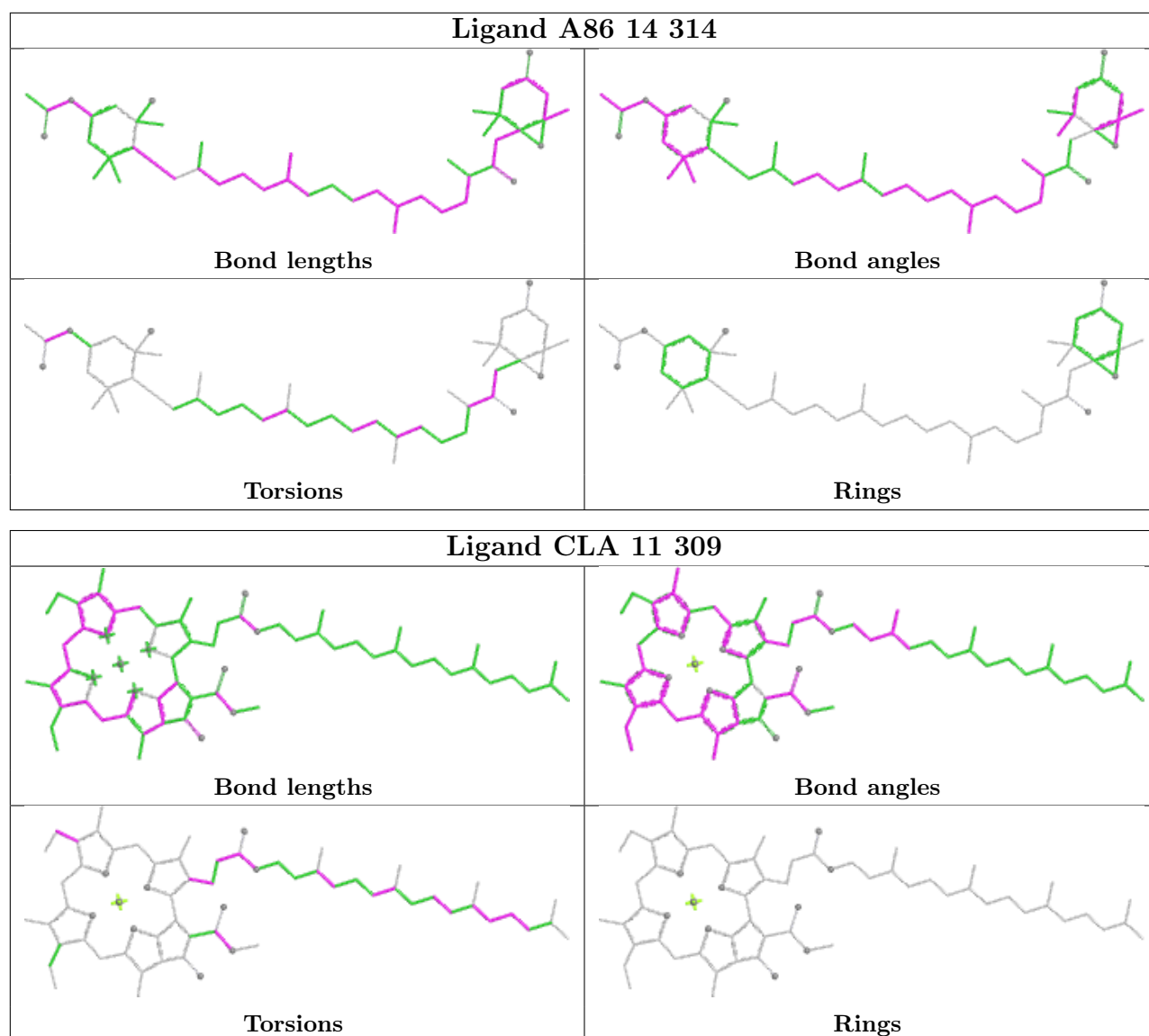


Ligand KC1 6 310

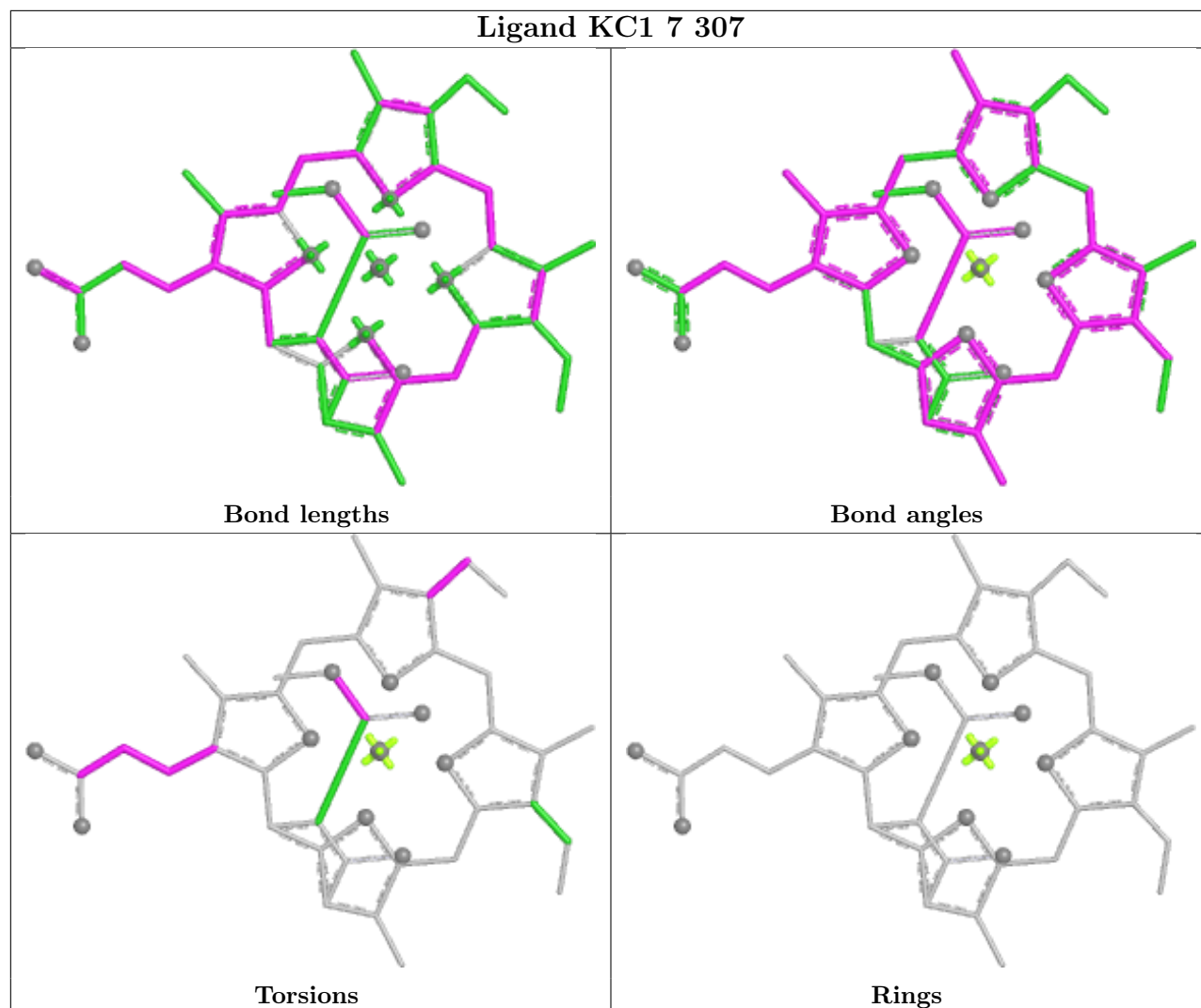


Ligand DD6 6 318

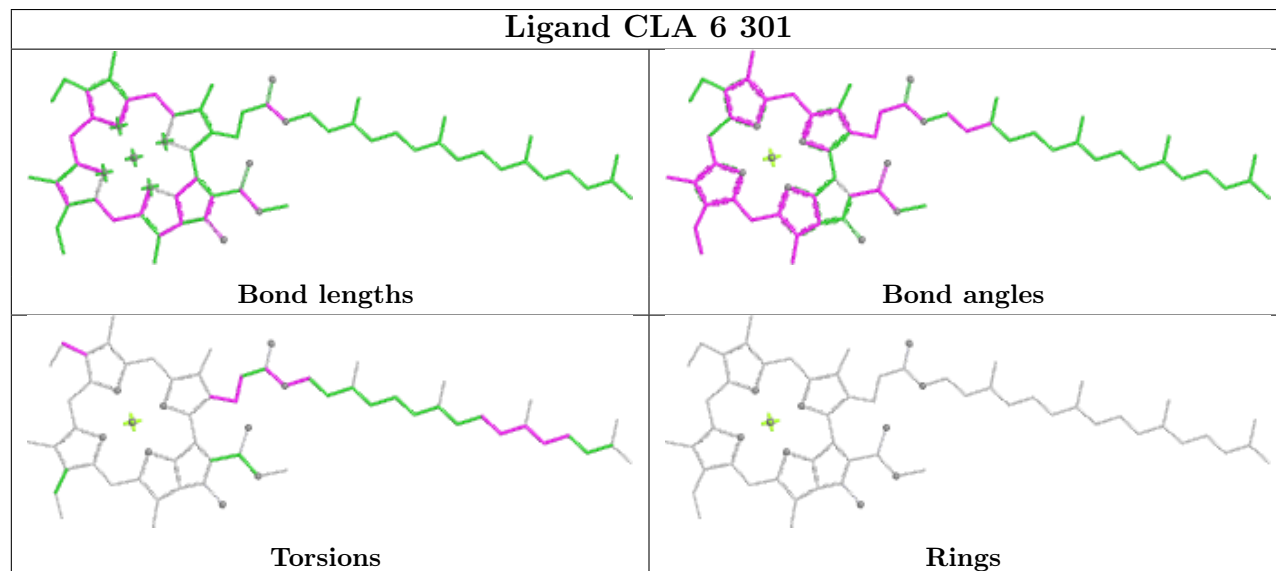


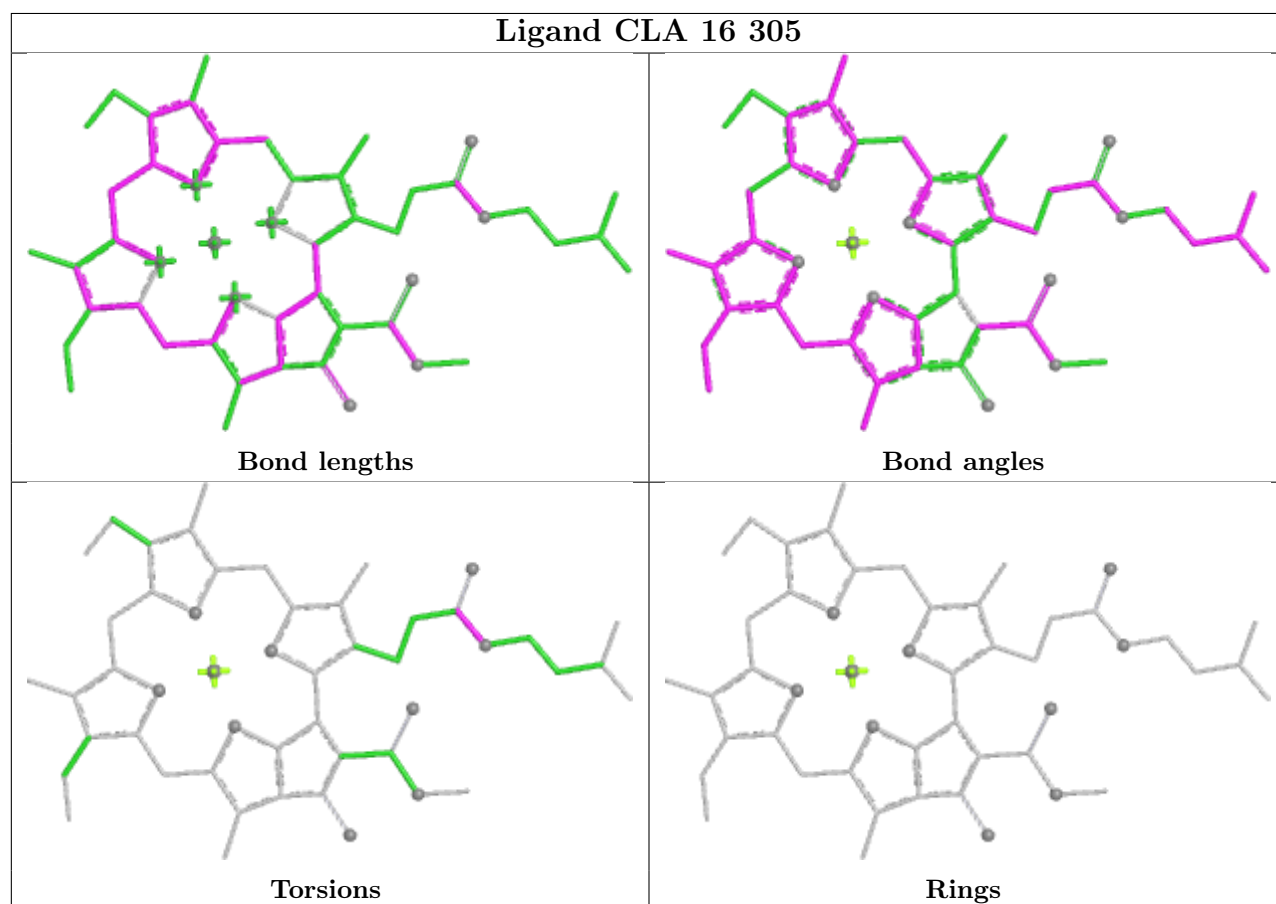
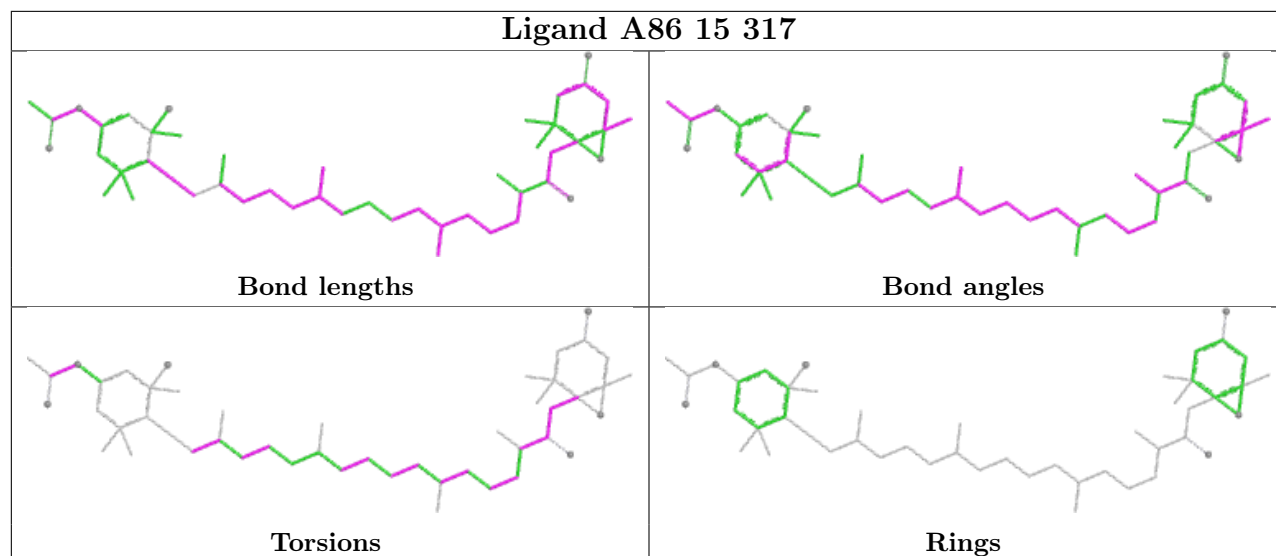


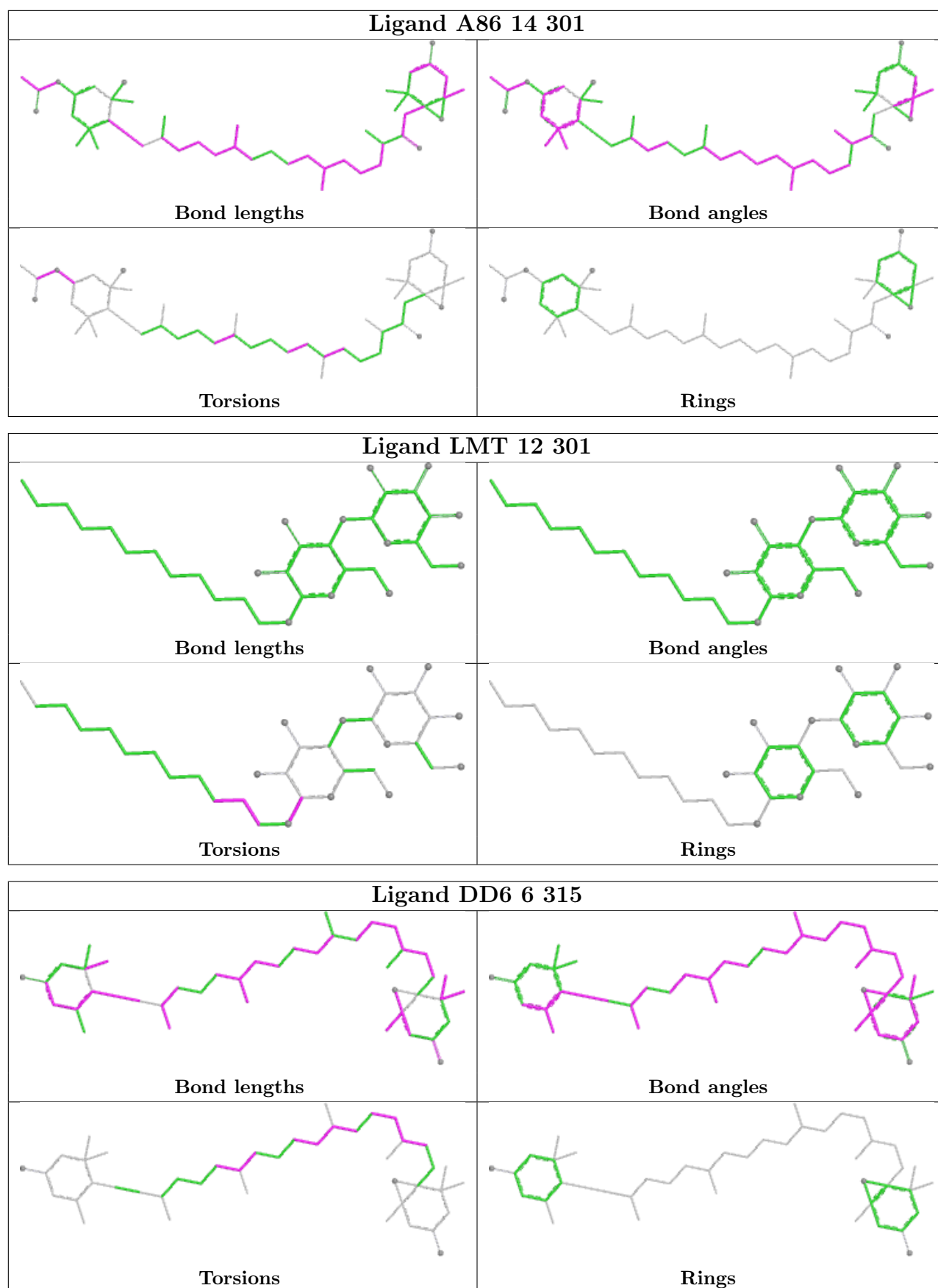
Ligand KC1 7 307



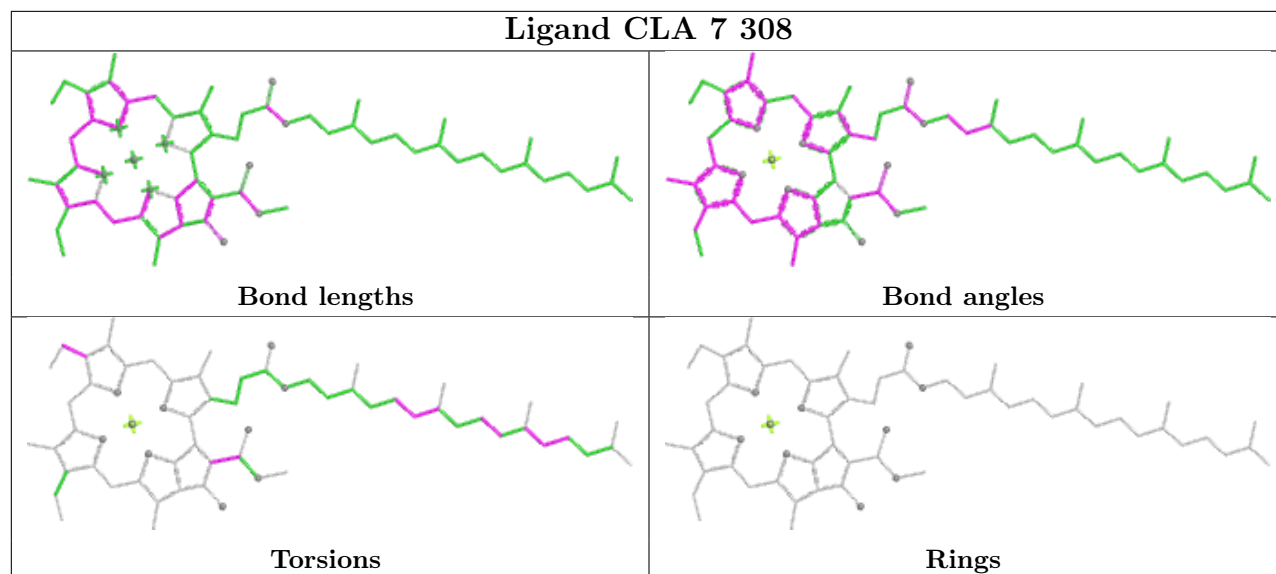
Ligand CLA 6 301



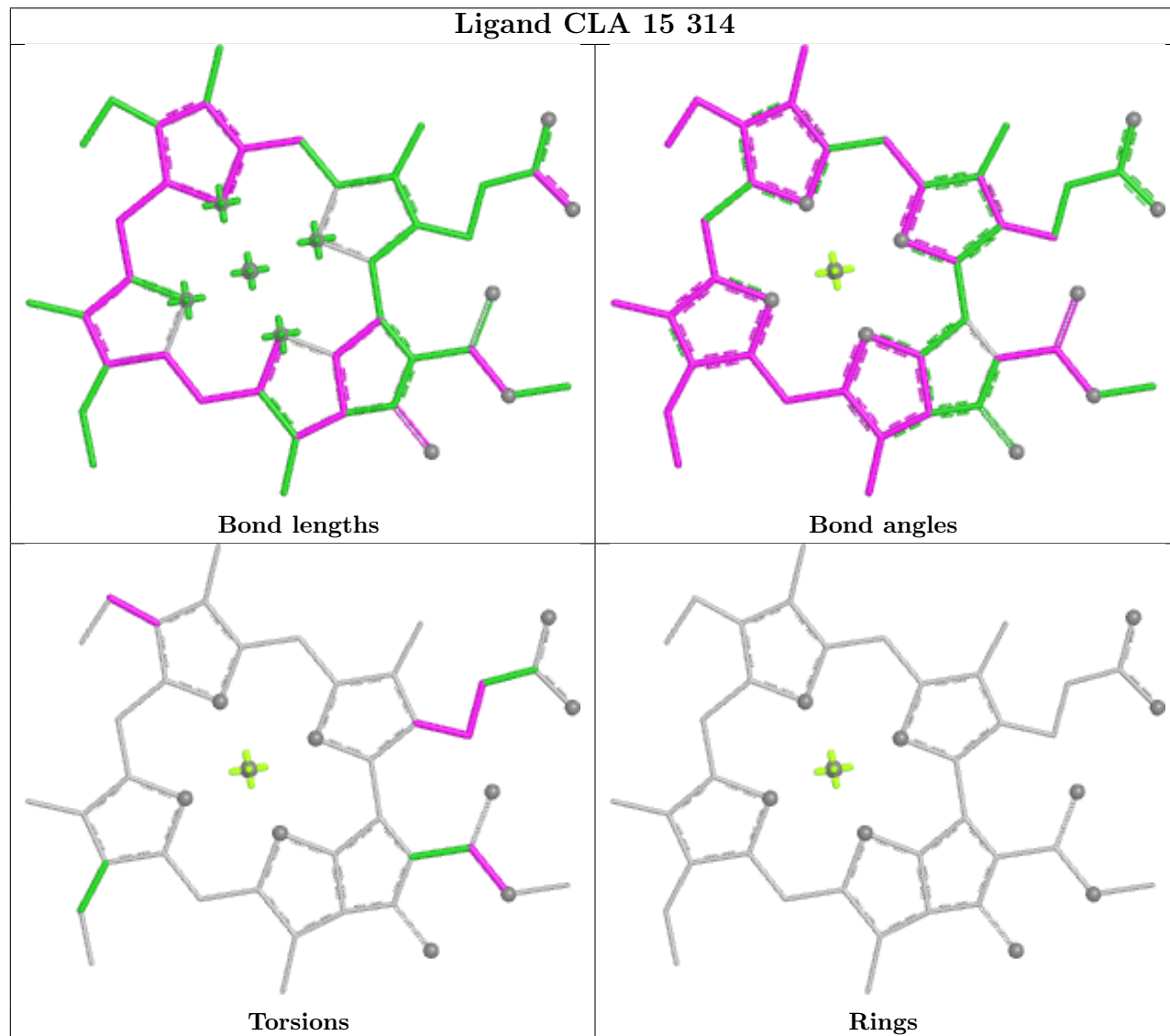


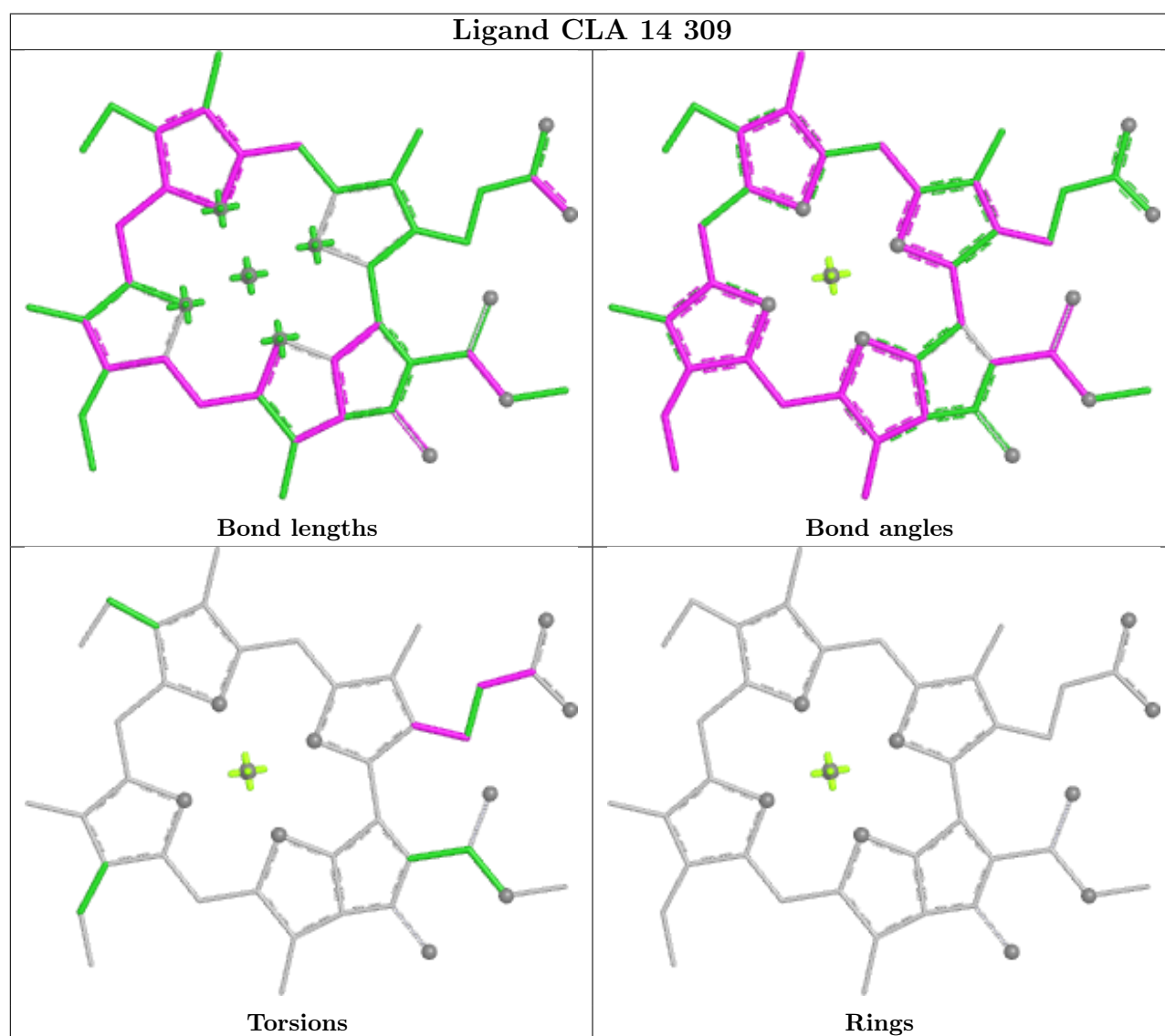
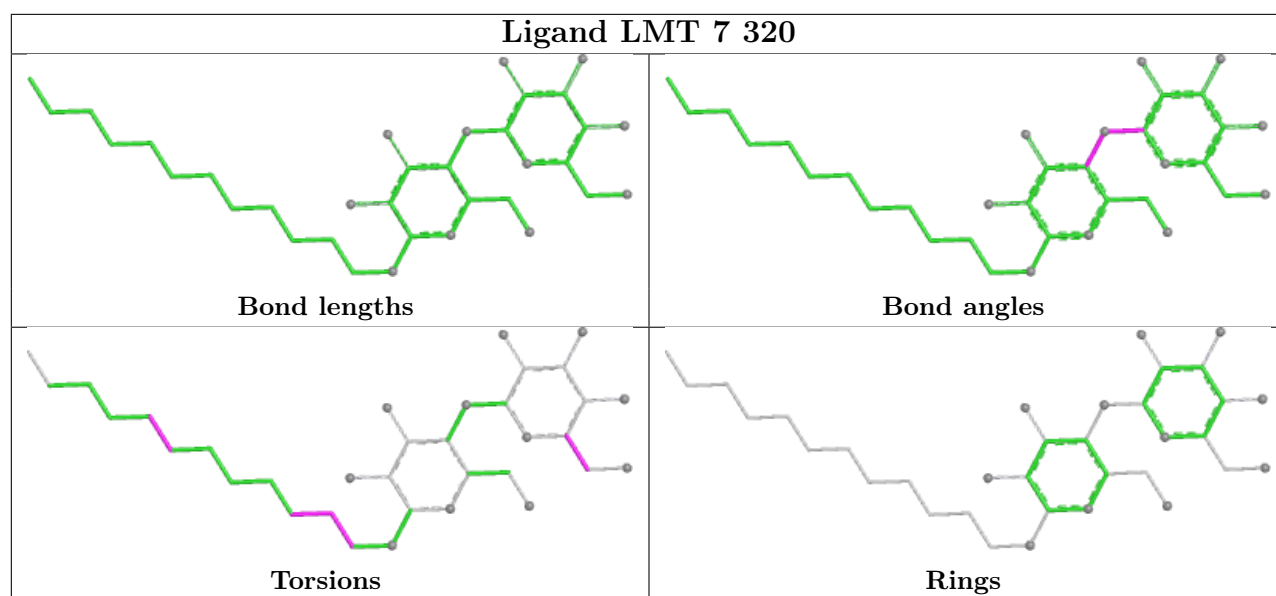


Ligand CLA 7 308

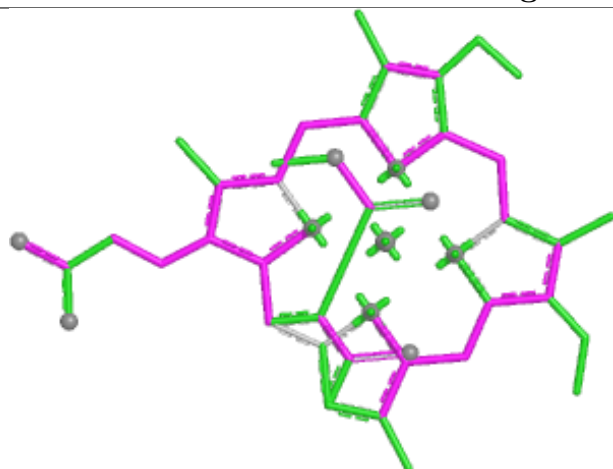


Ligand CLA 15 314

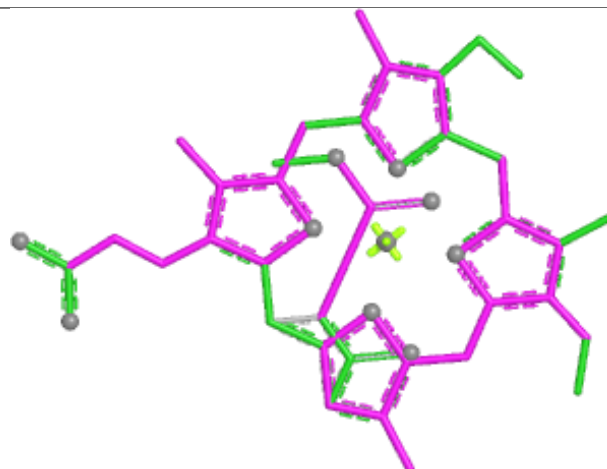




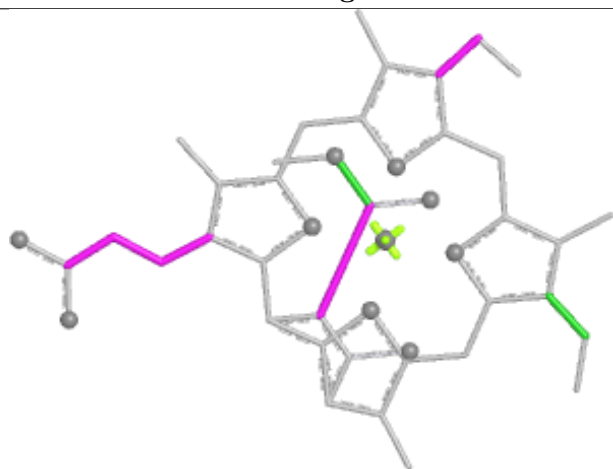
Ligand KC1 6 308



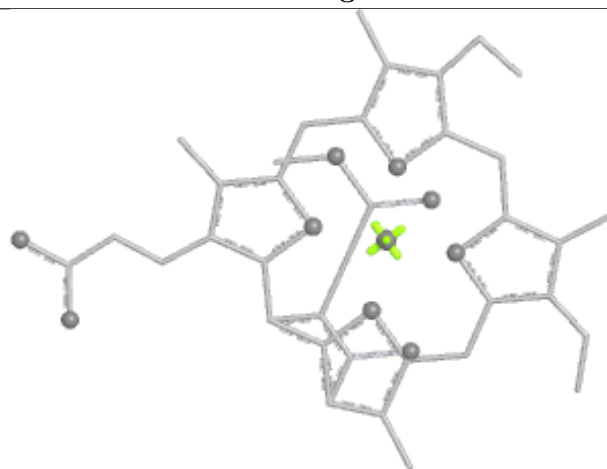
Bond lengths



Bond angles

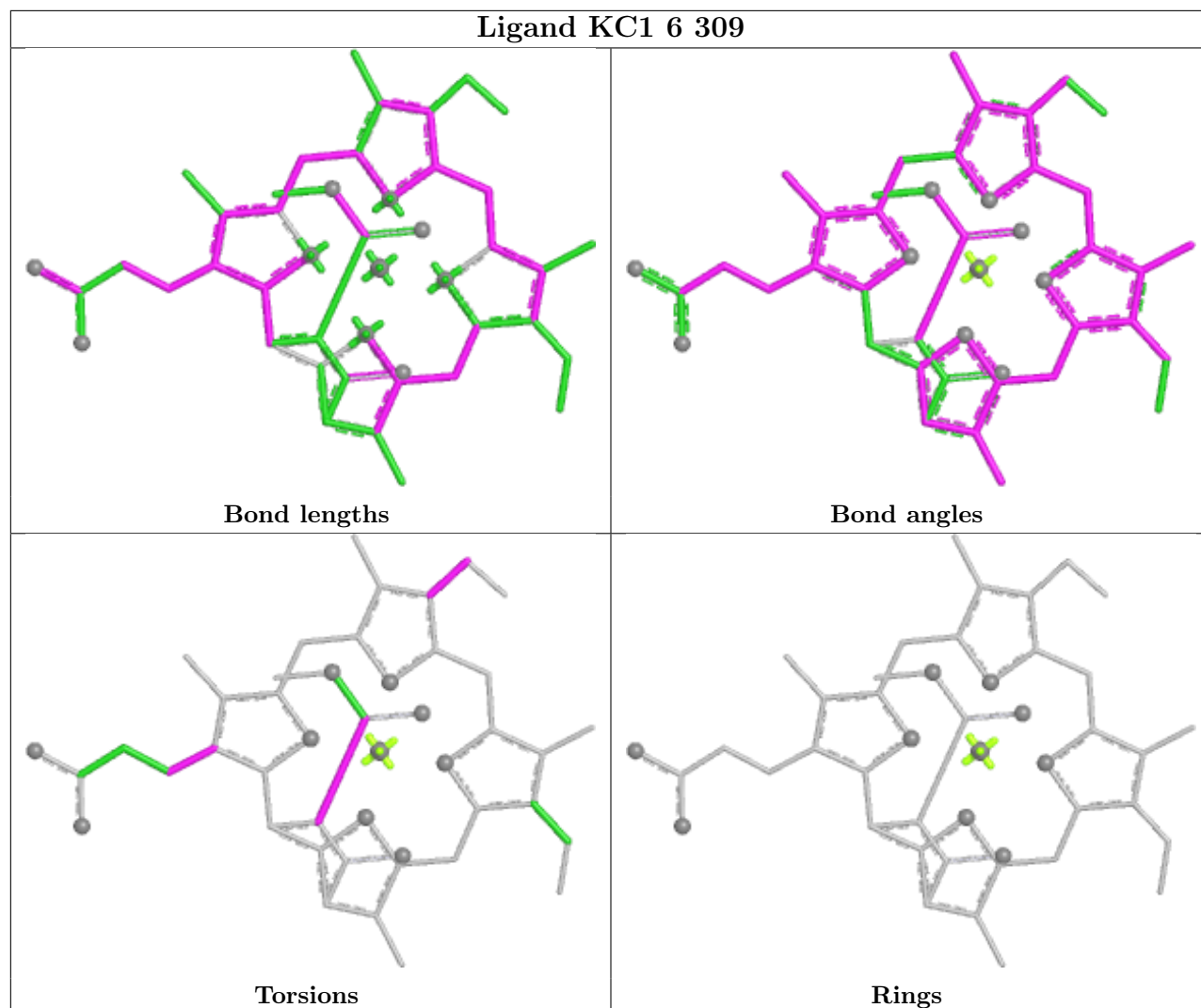


Torsions

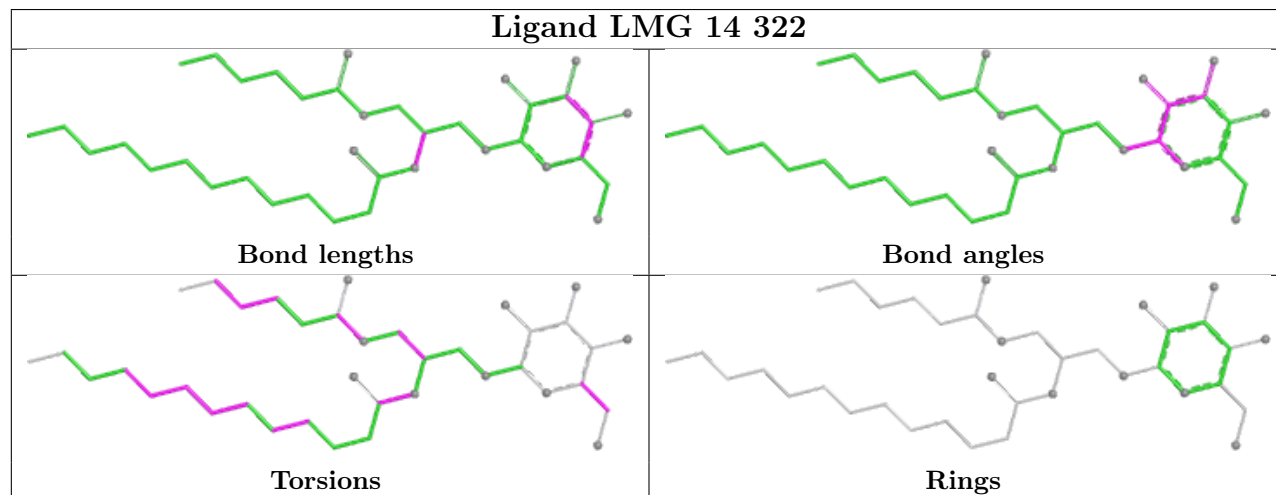


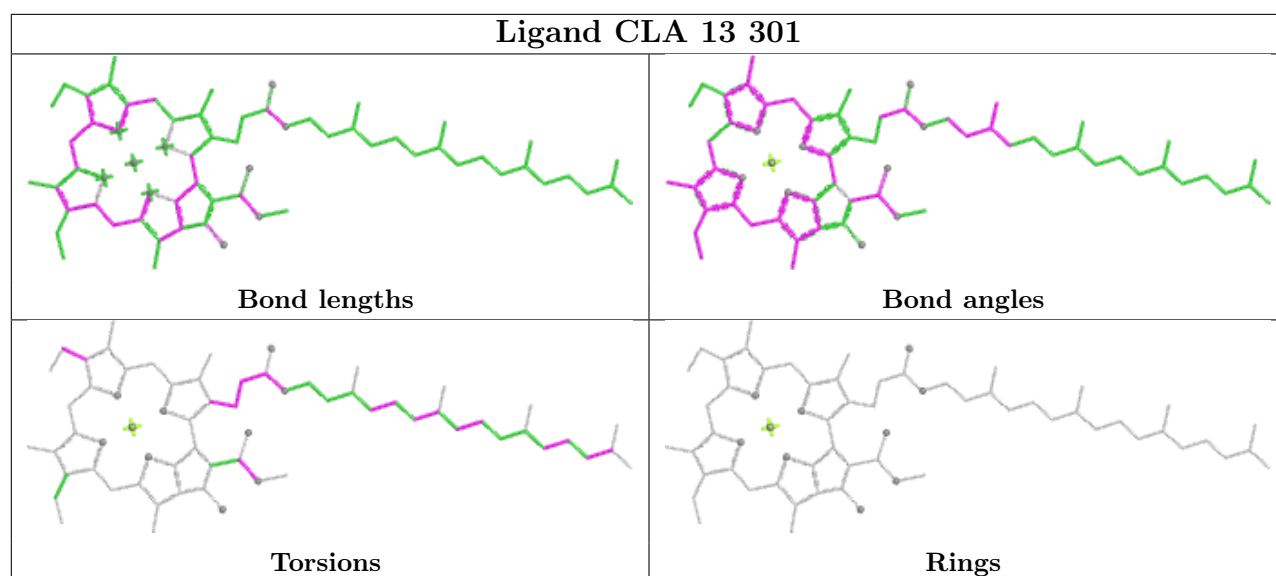
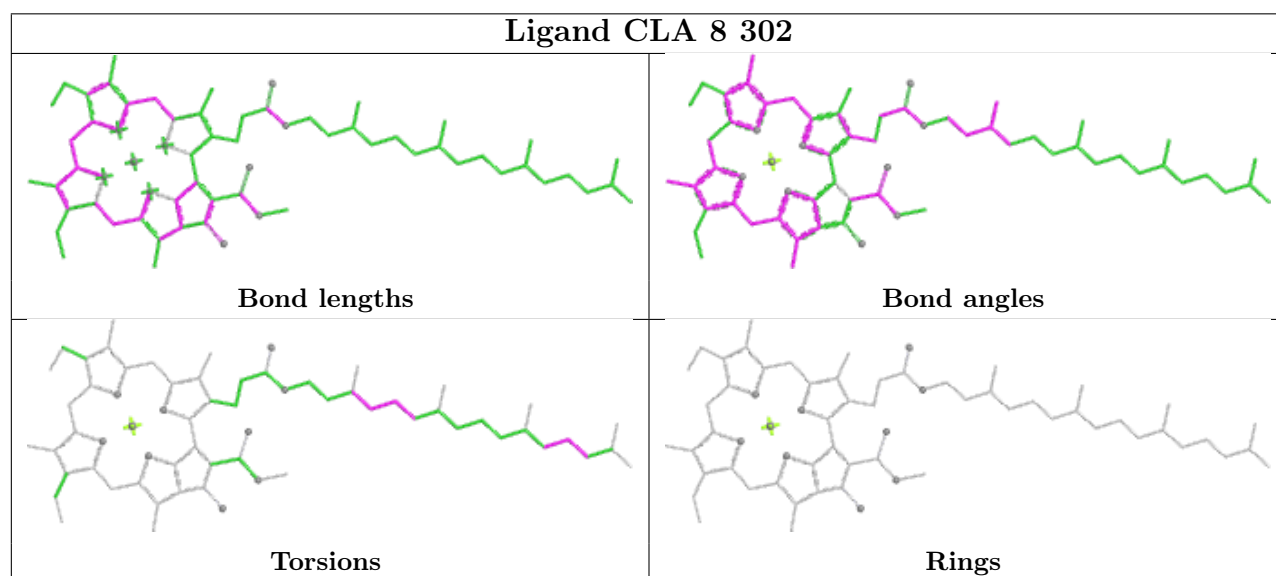
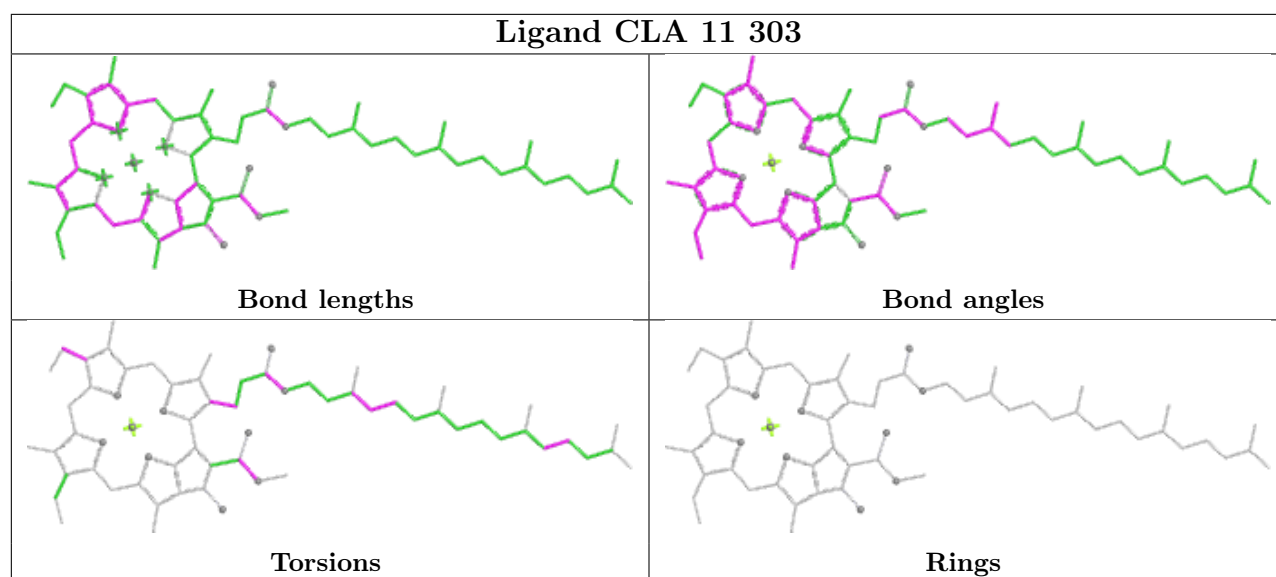
Rings

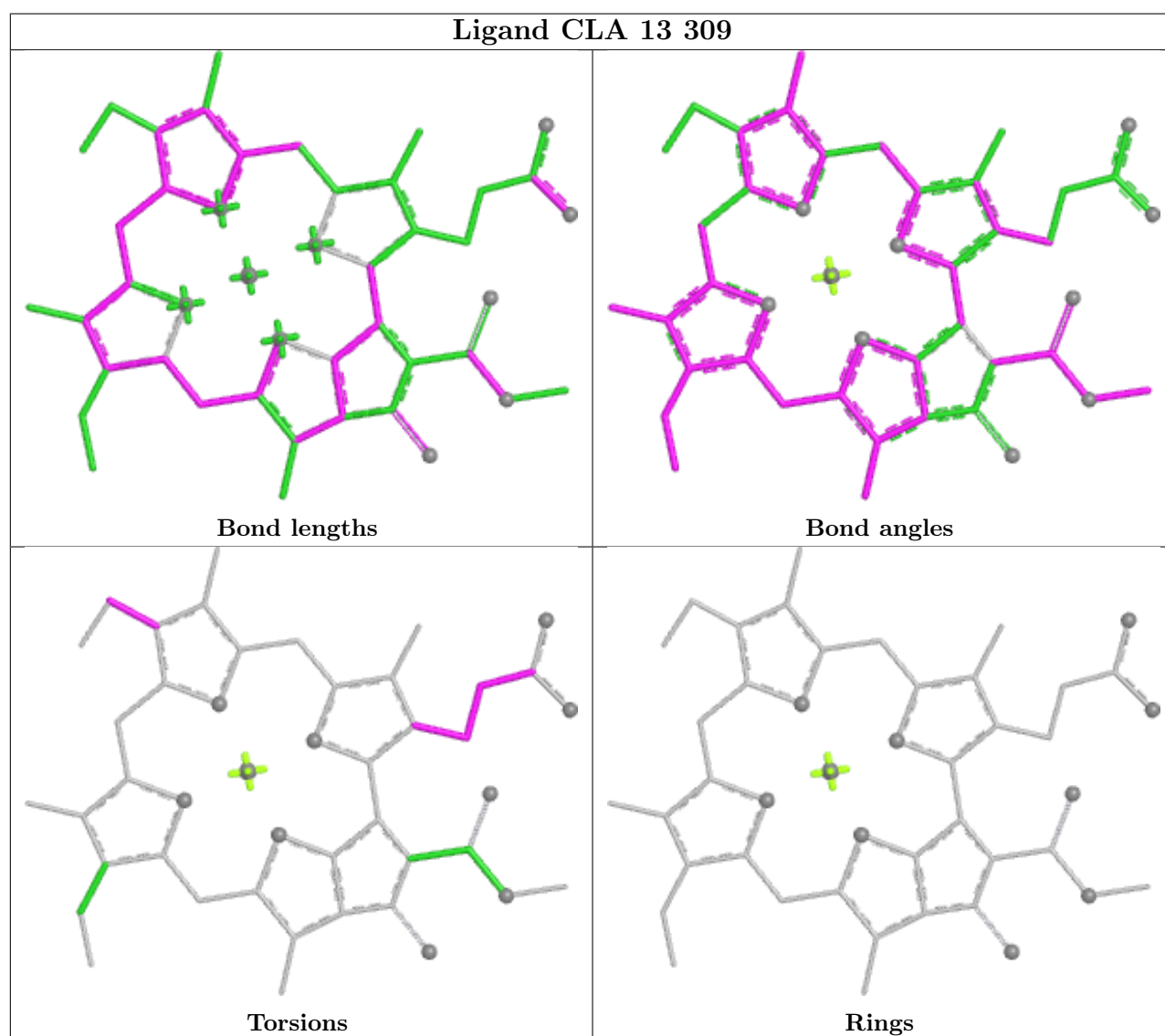
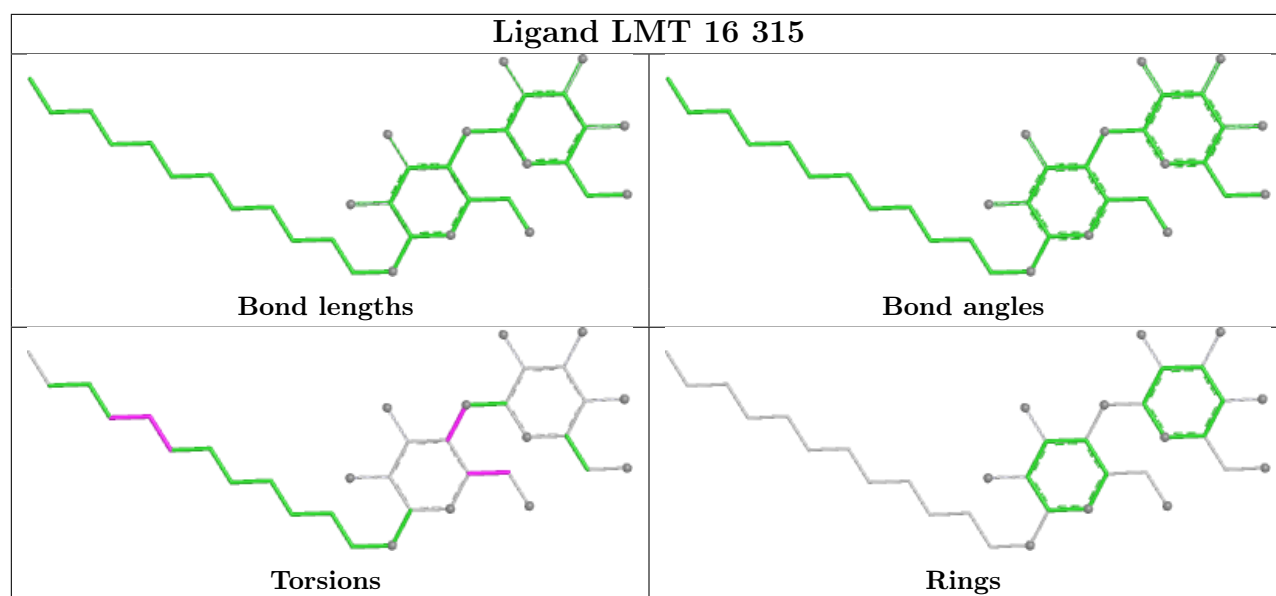
Ligand KC1 6 309

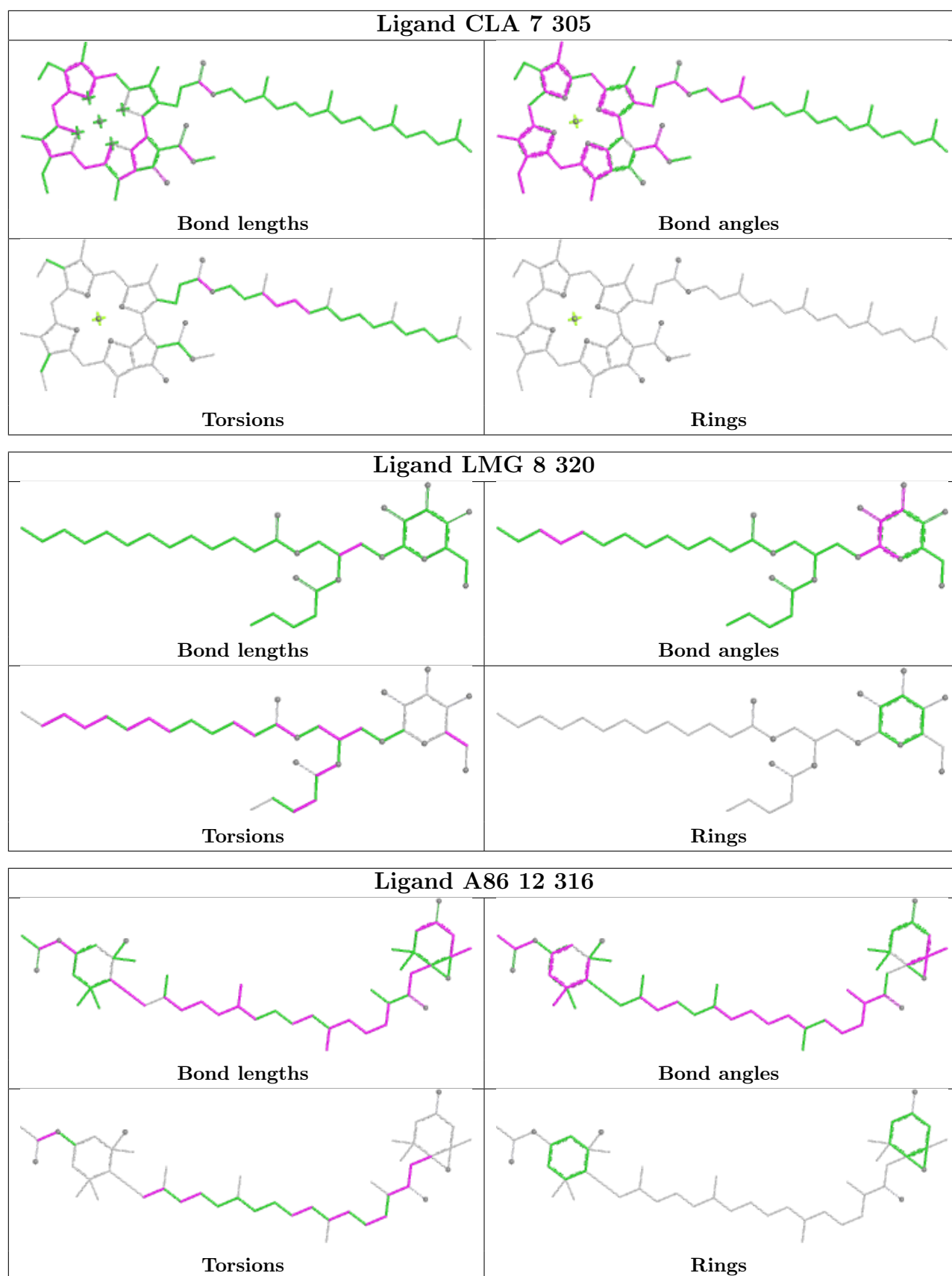


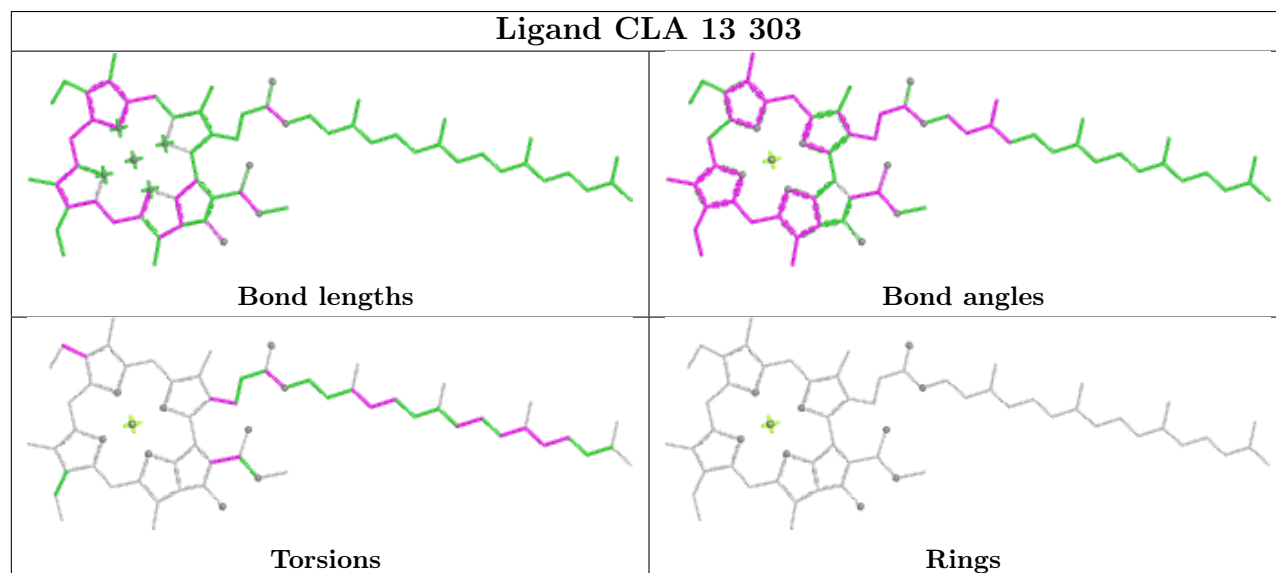
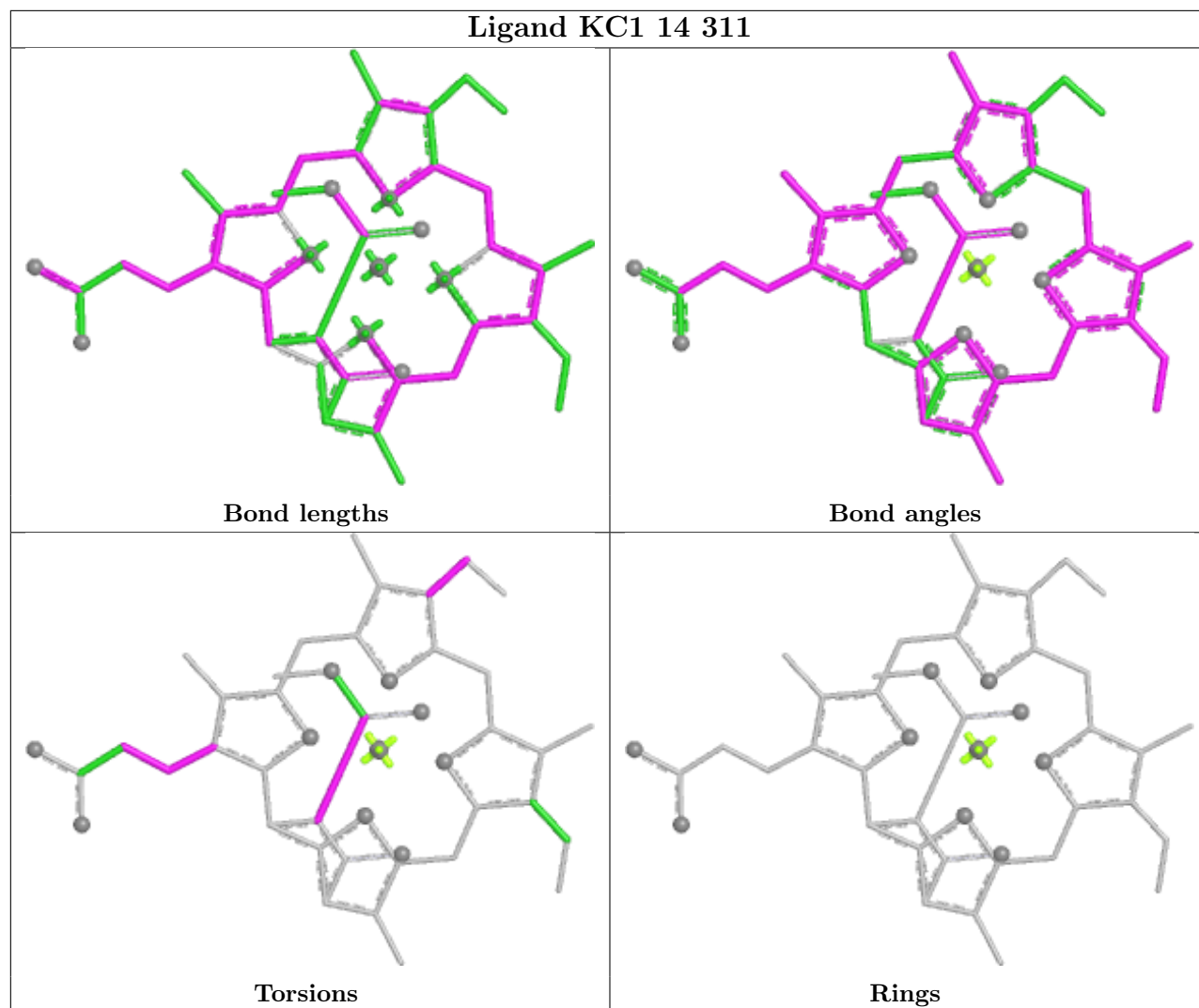
Ligand LMG 14 322



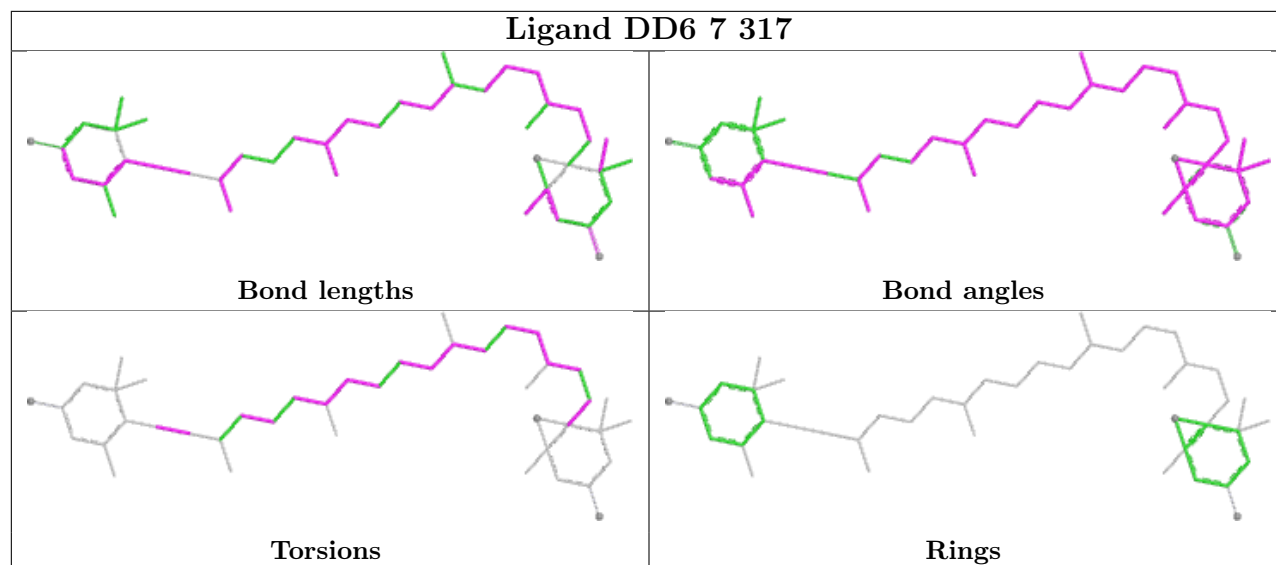




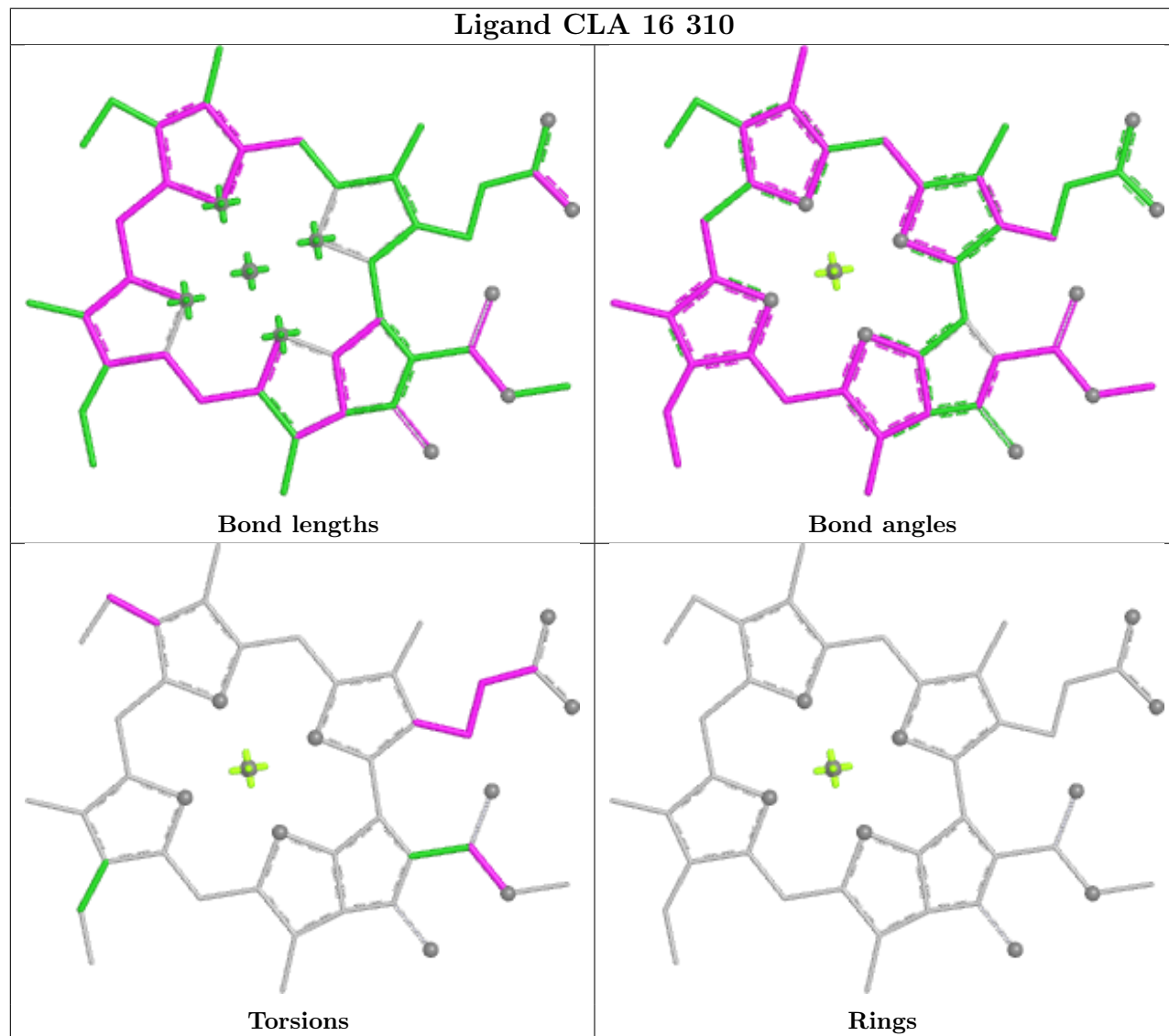


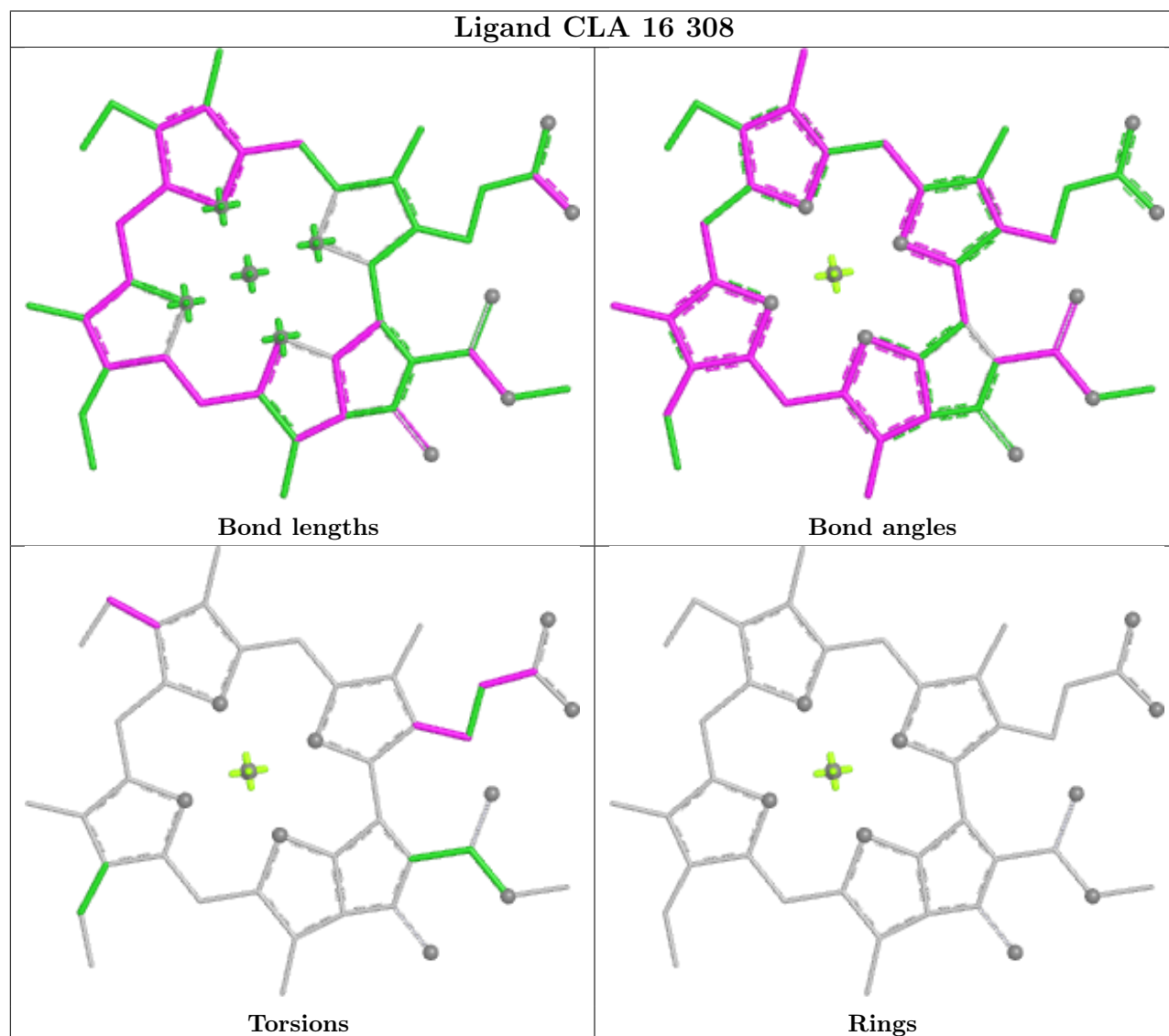
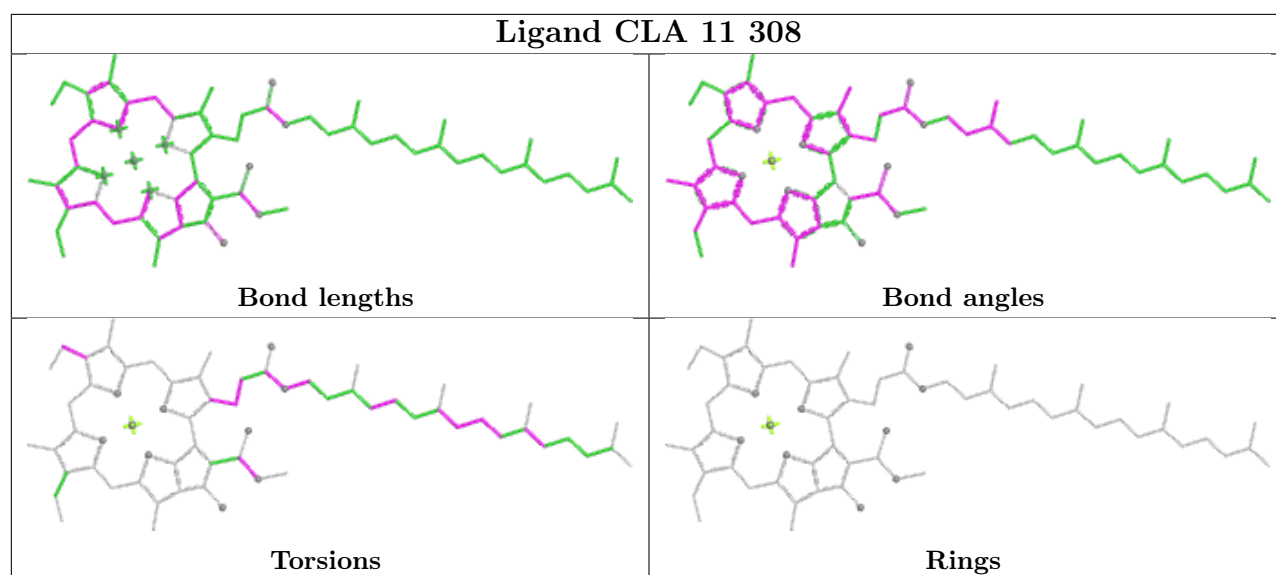


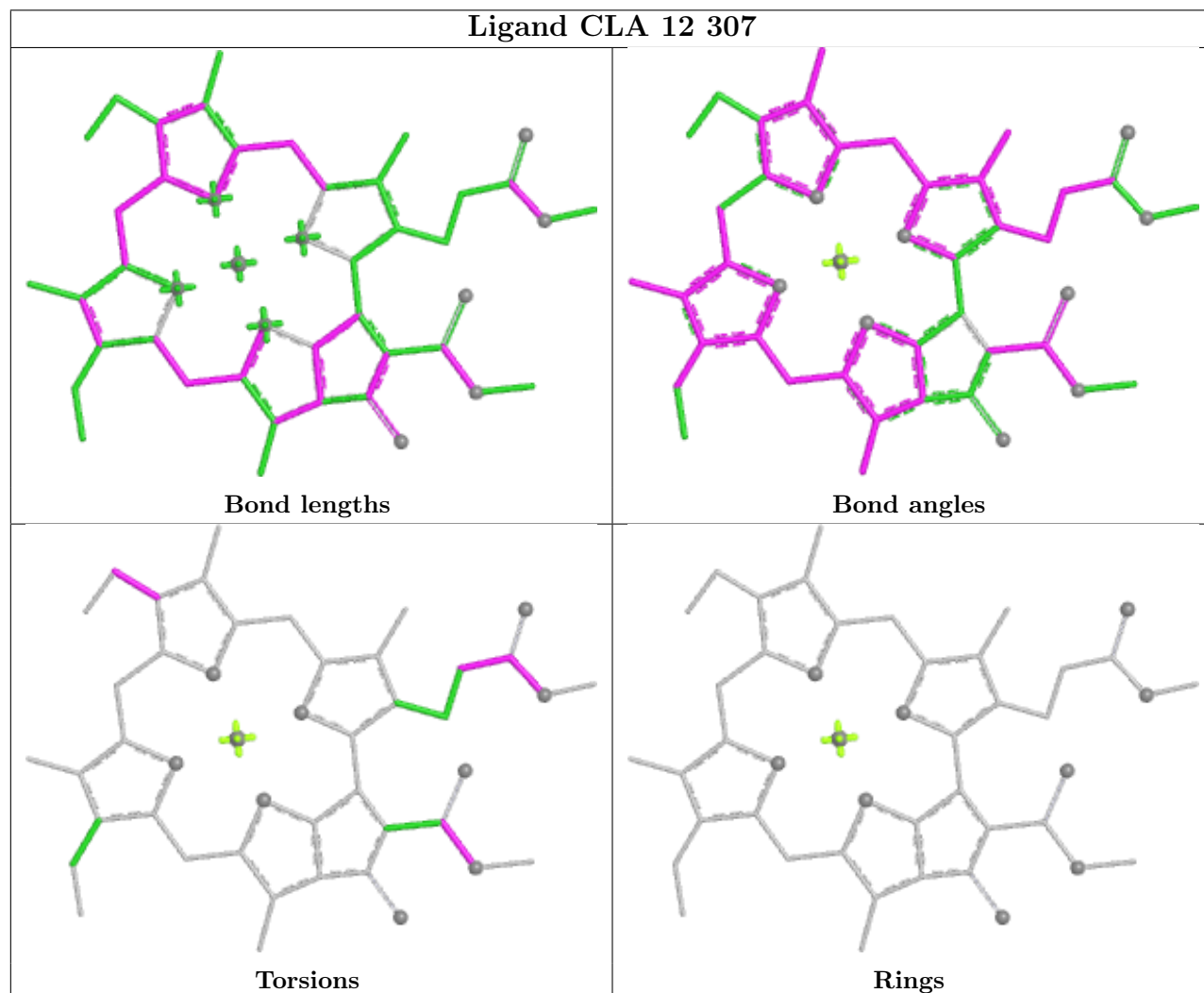
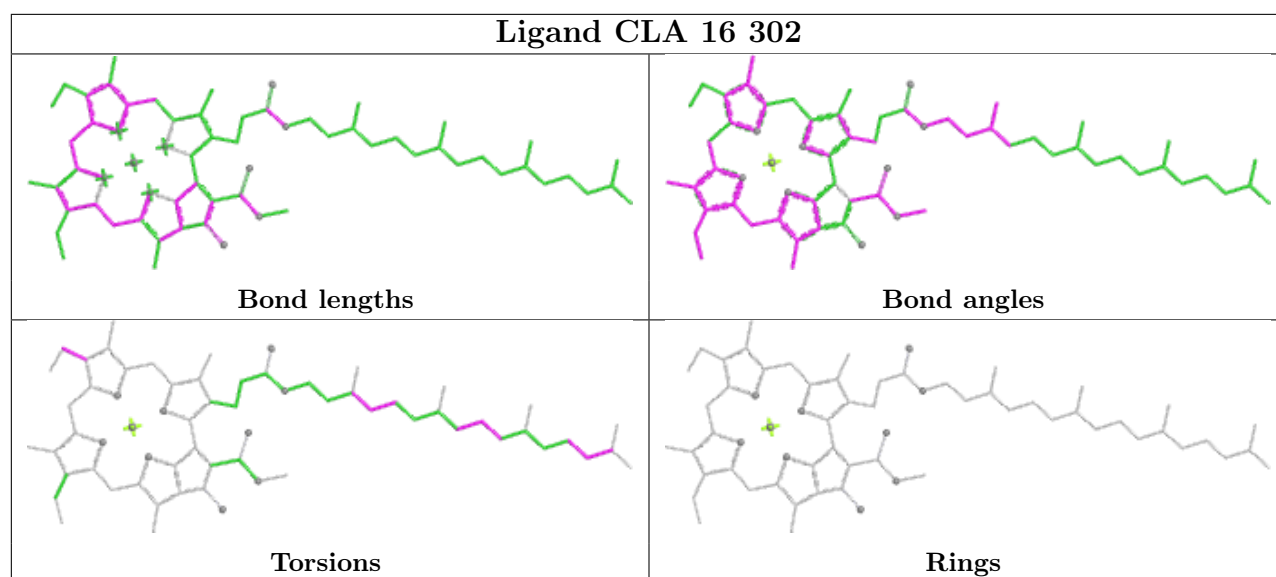
Ligand DD6 7 317

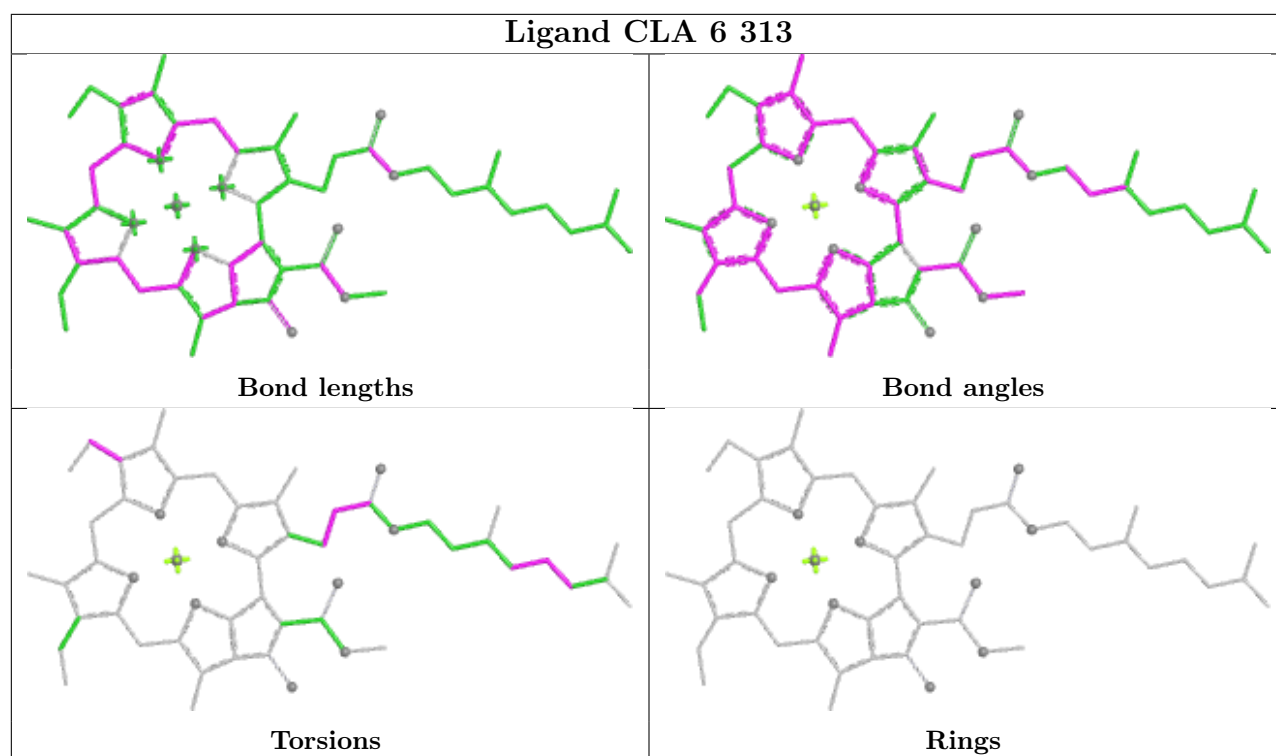


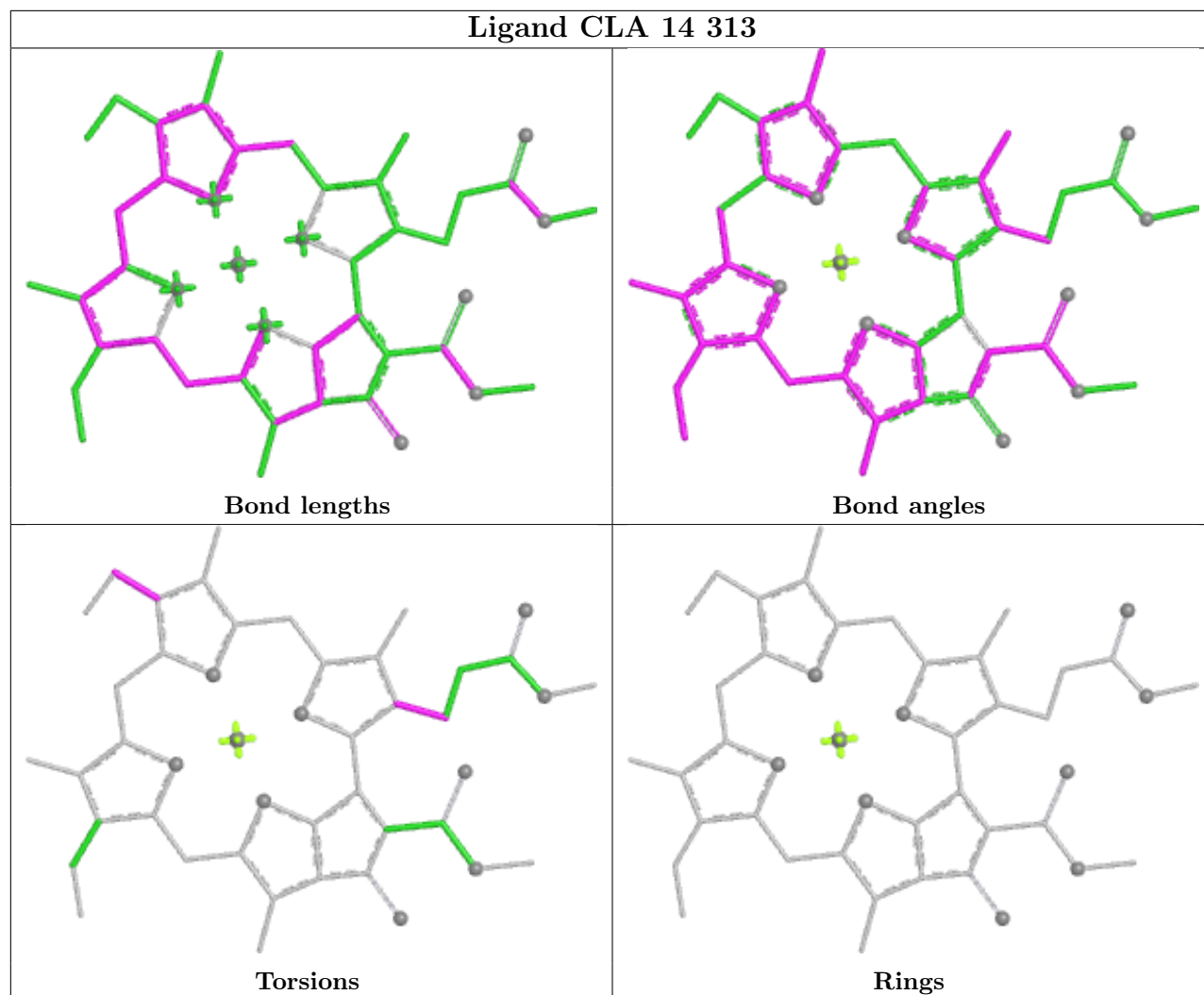
Ligand CLA 16 310

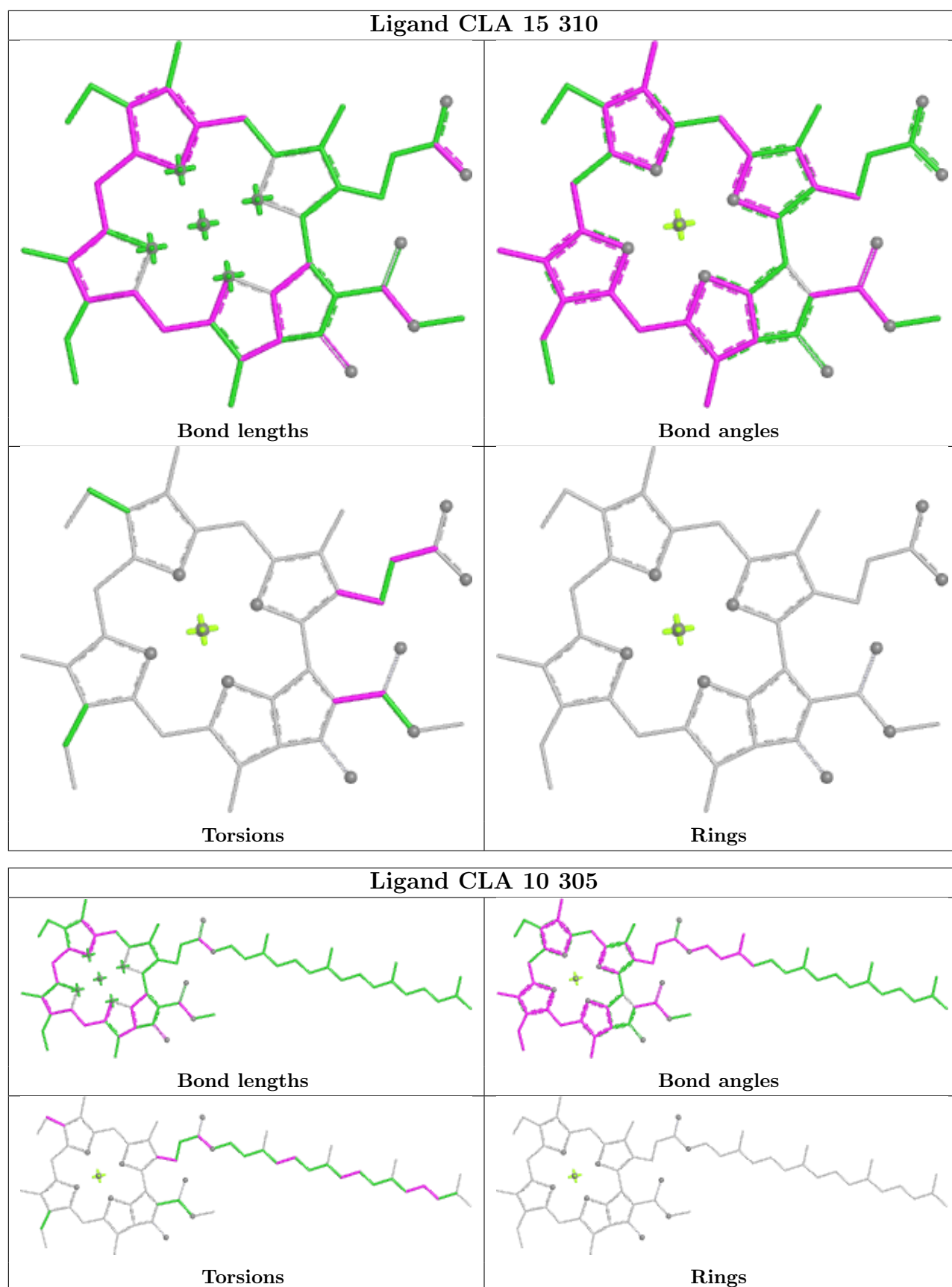


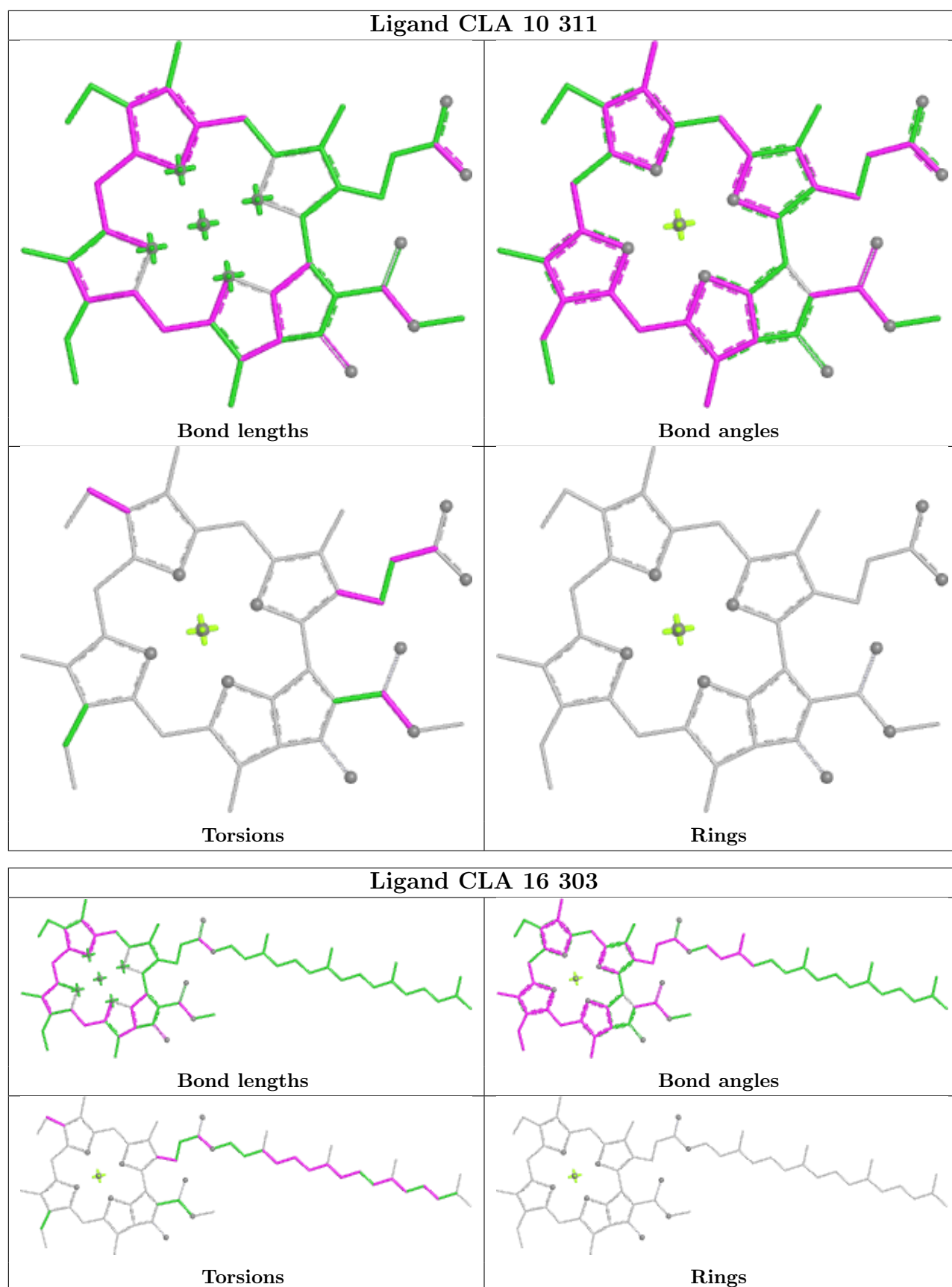


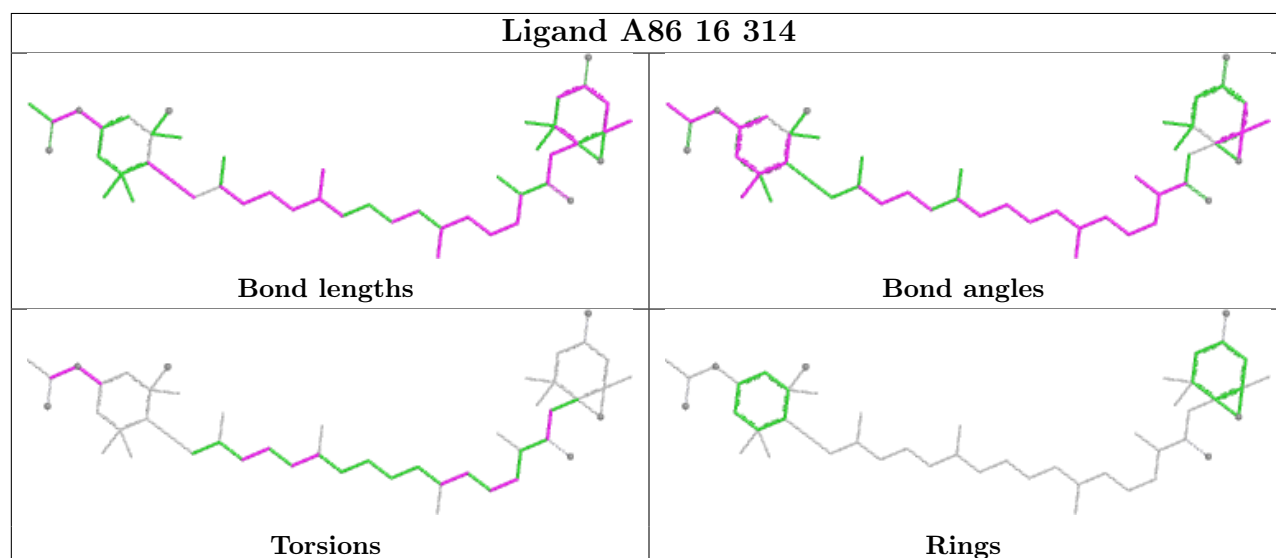
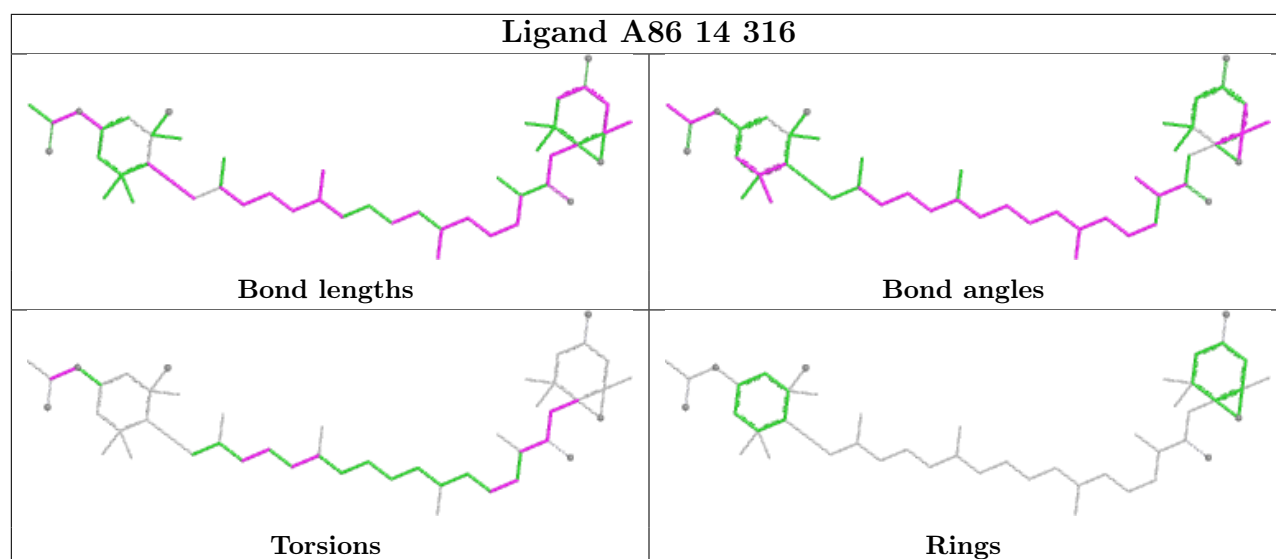


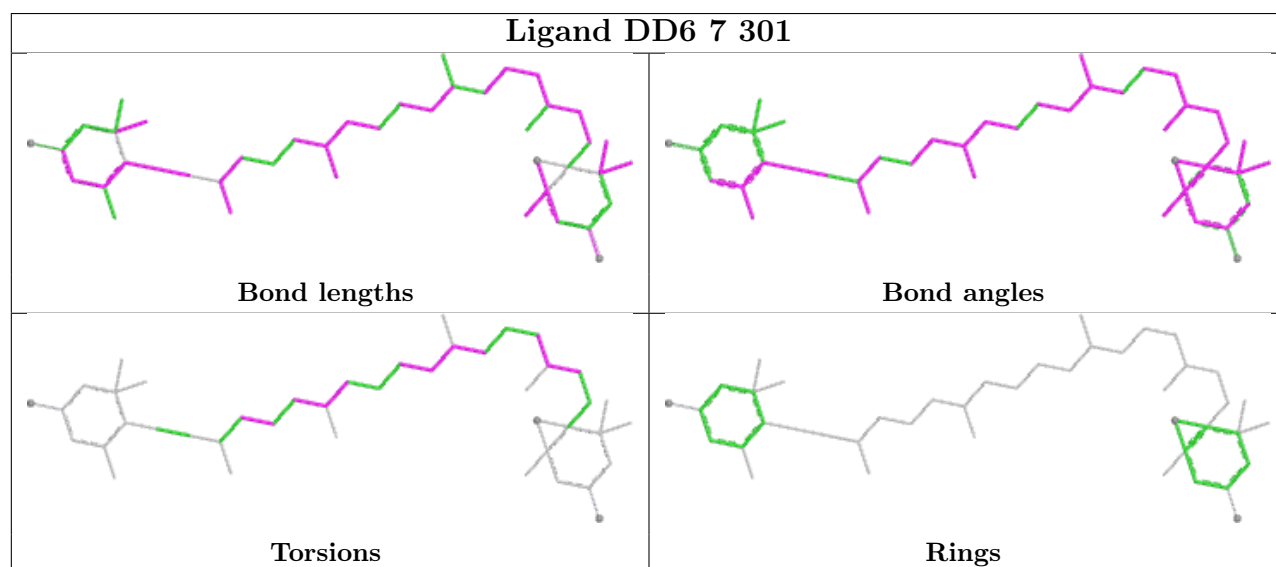
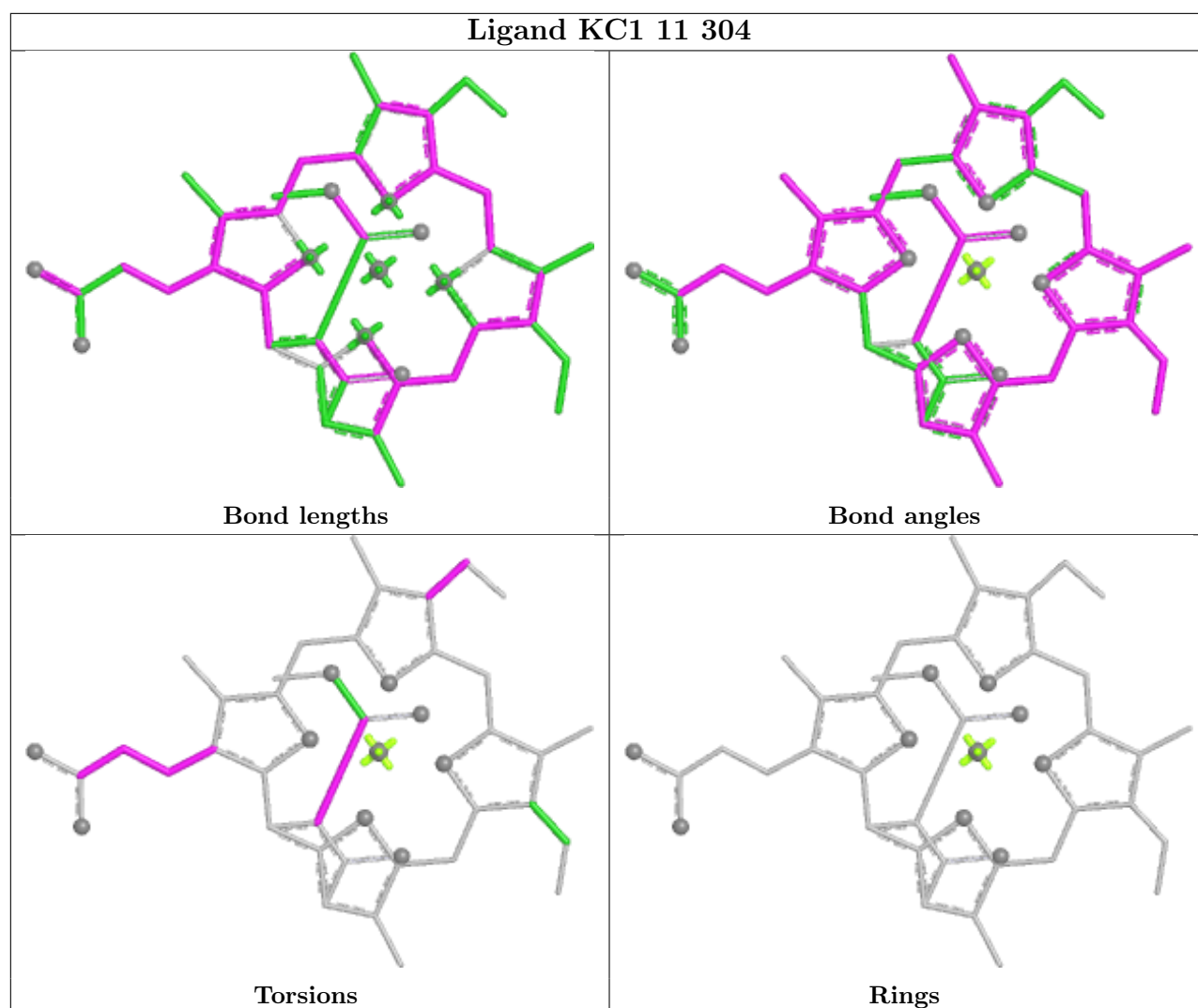


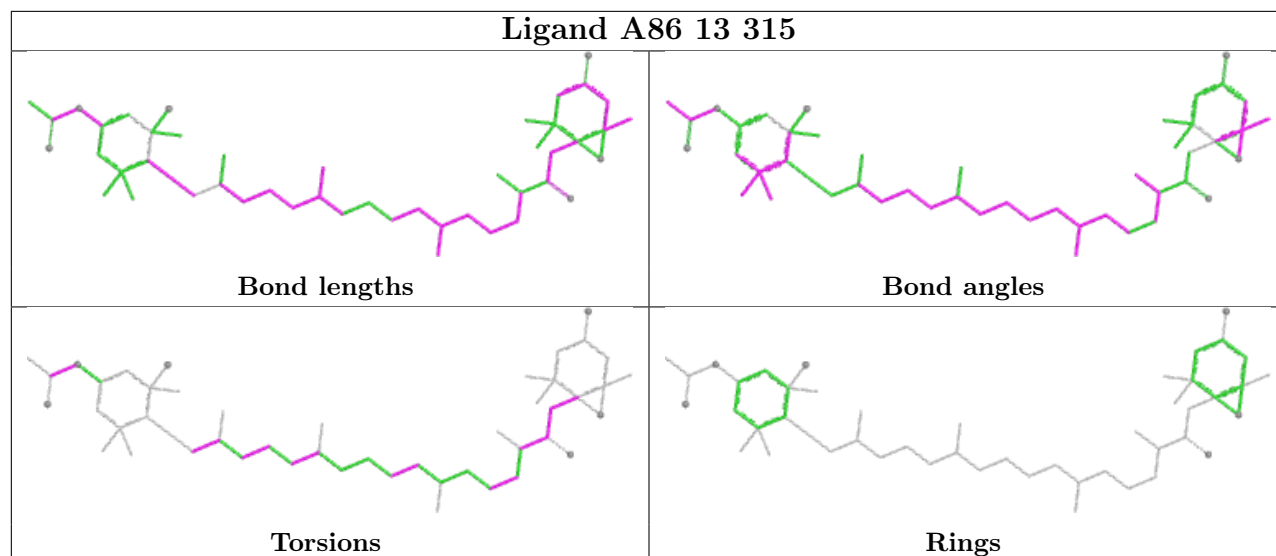
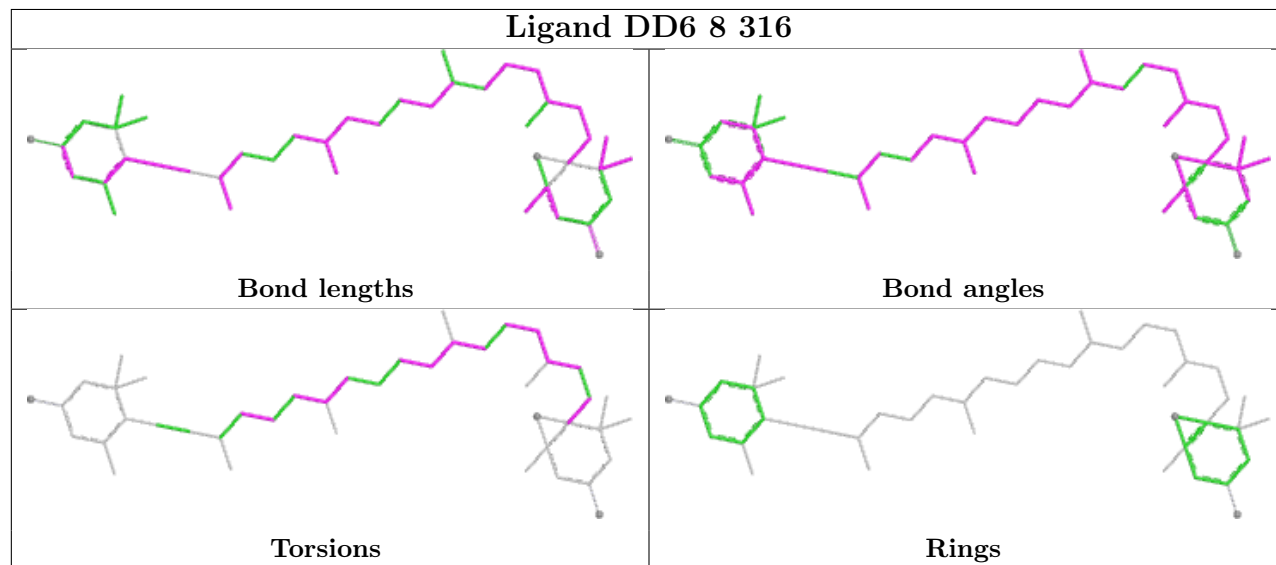


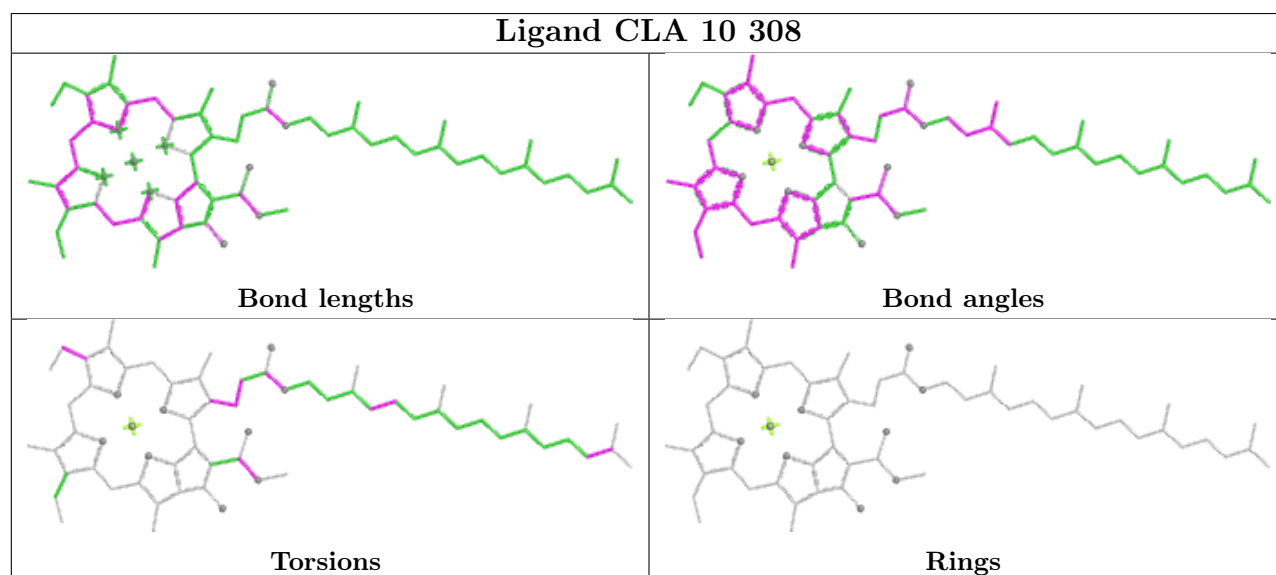
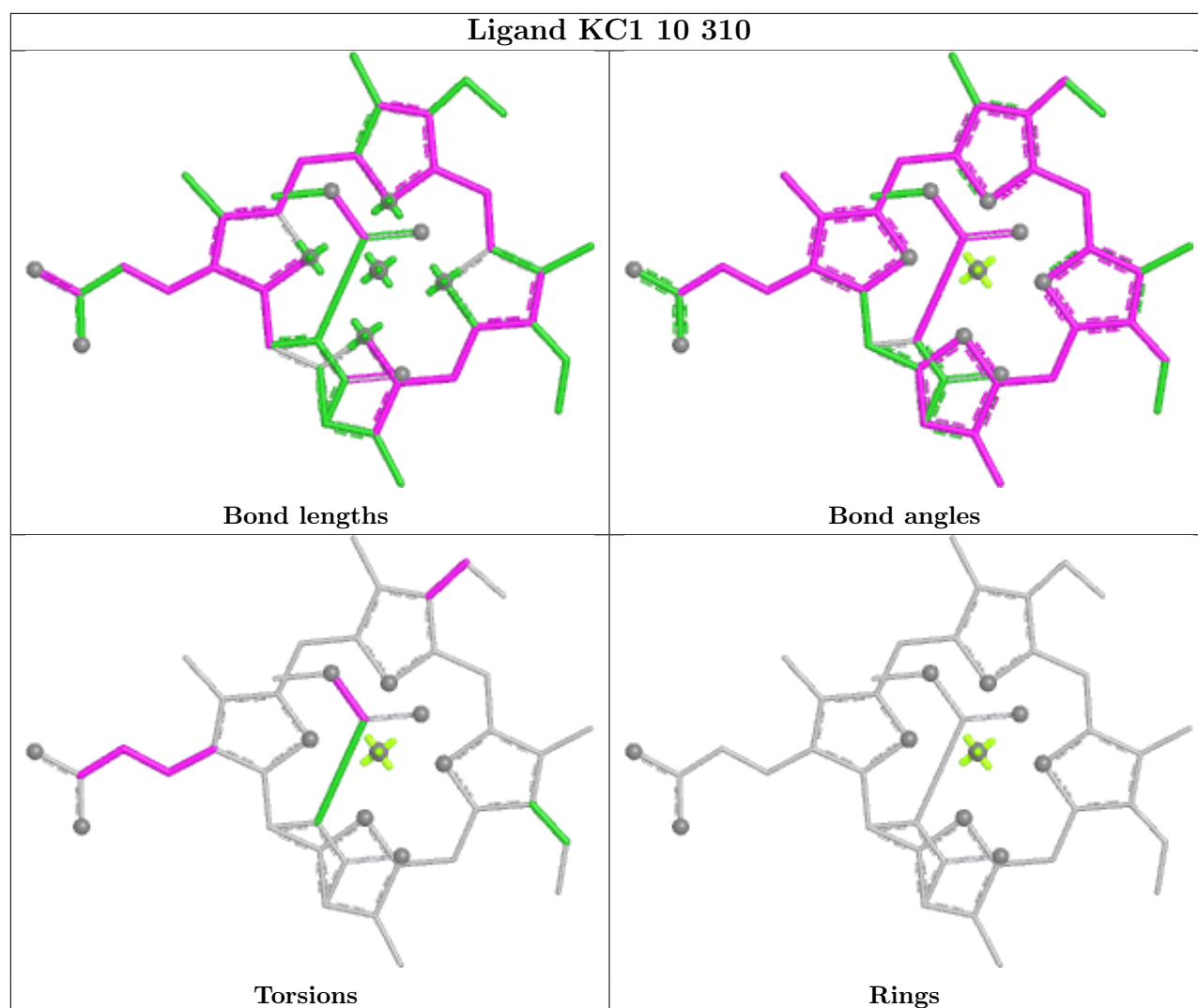


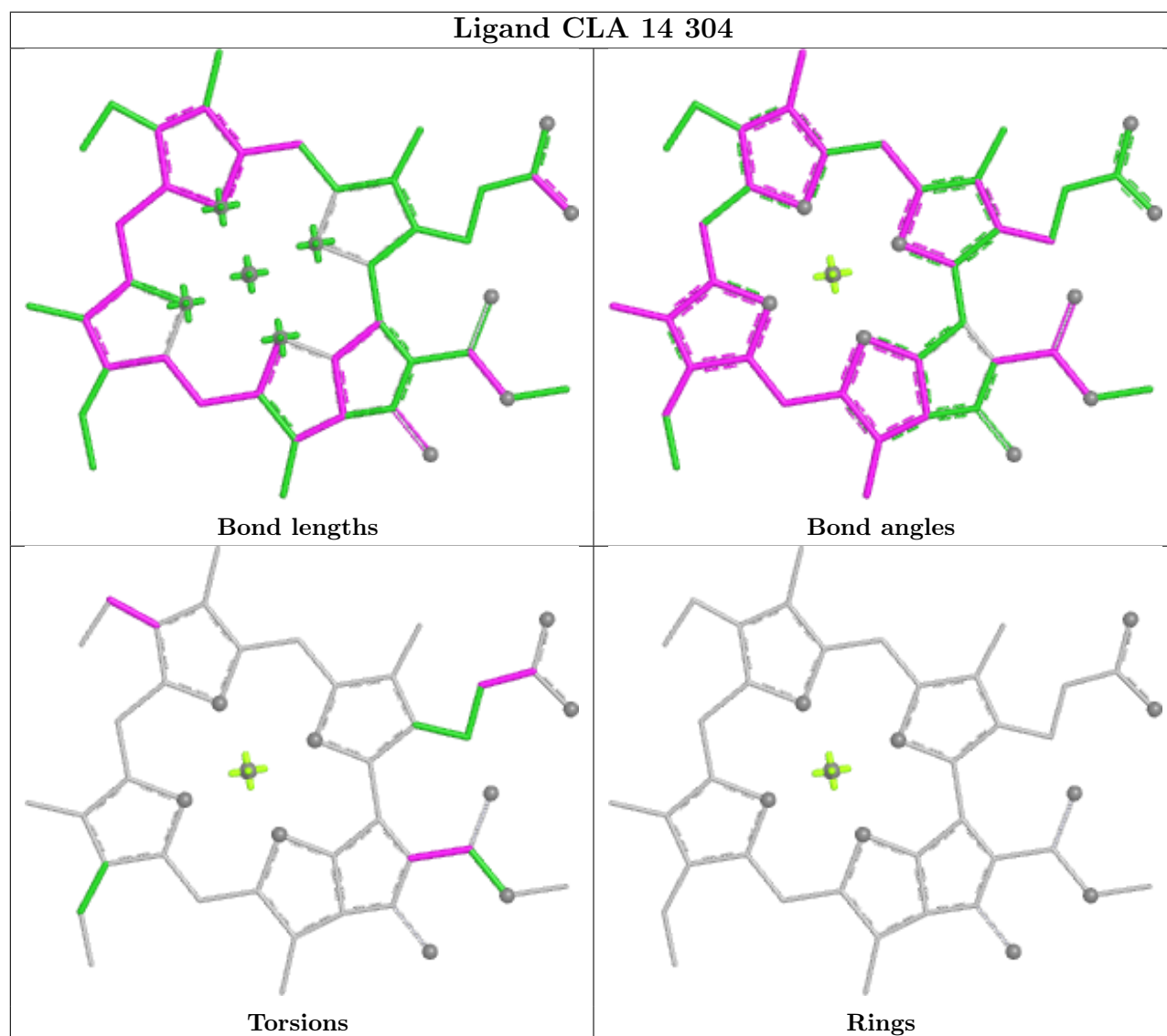
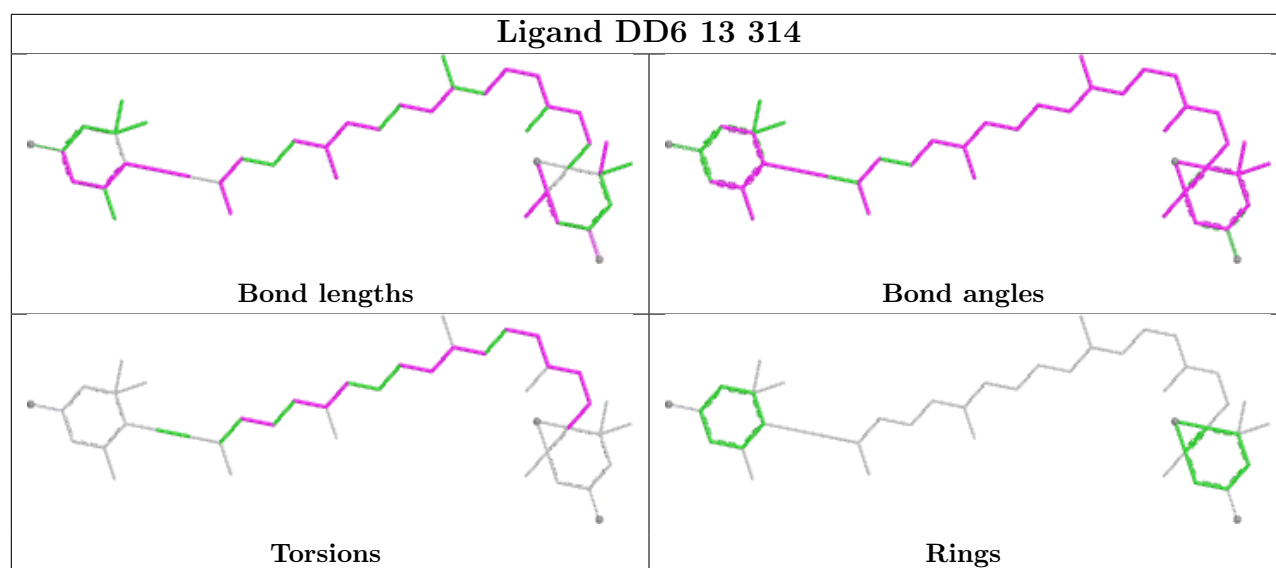


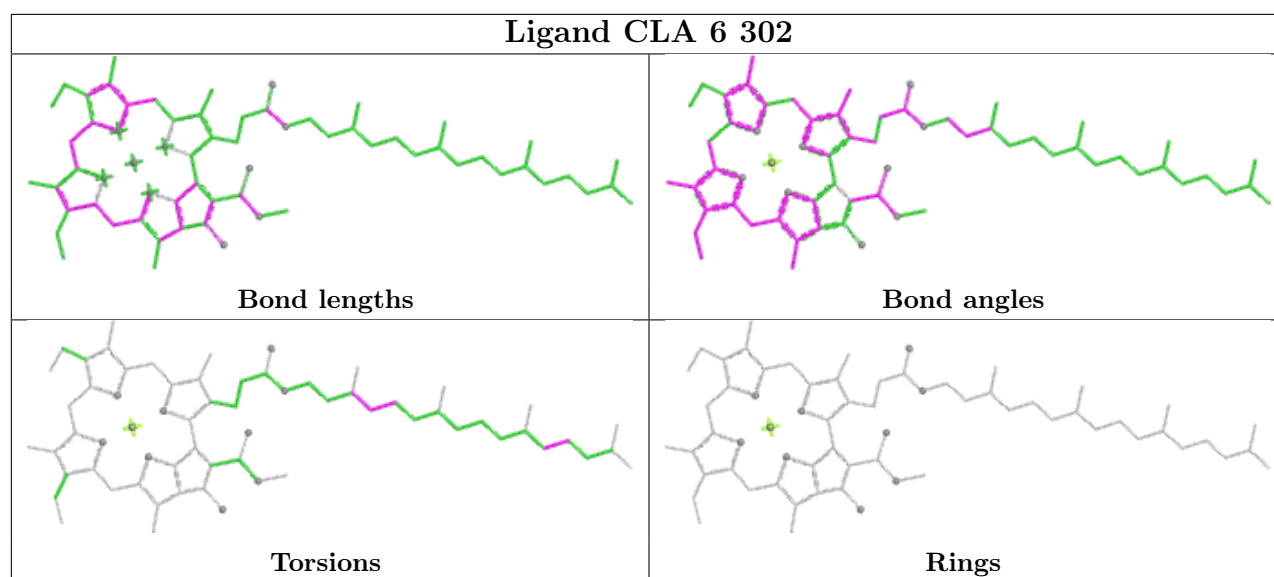




Ligand A86 13 315**Ligand DD6 8 316**







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.

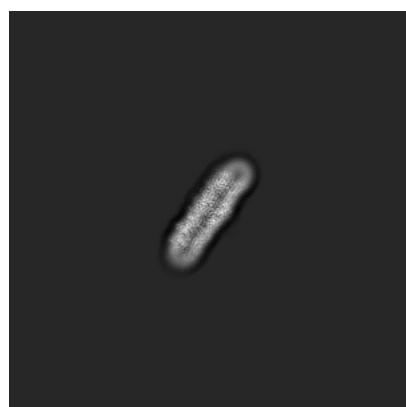
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0834. These allow visual inspection of the internal detail of the map and identification of artifacts.

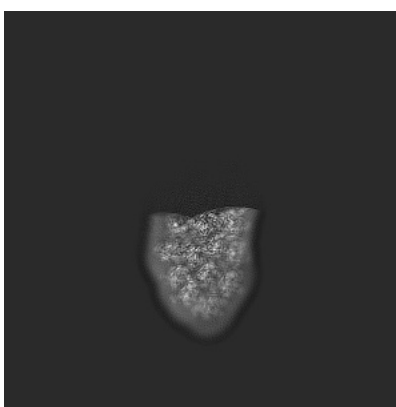
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

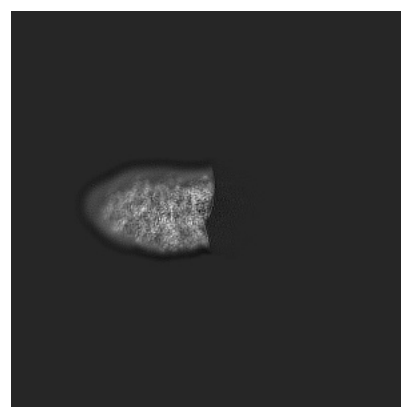
6.1.1 Primary map



X



Y

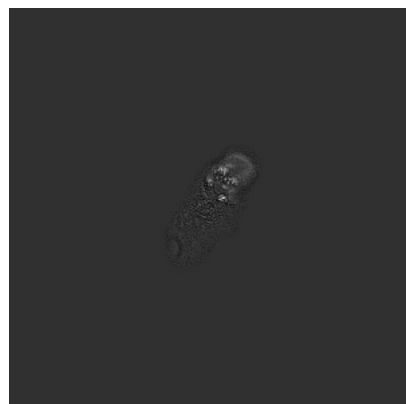


Z

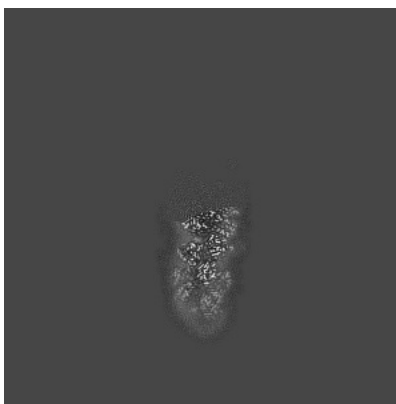
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

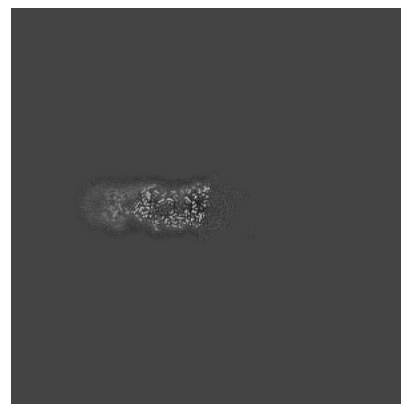
6.2.1 Primary map



X Index: 252



Y Index: 252



Z Index: 252

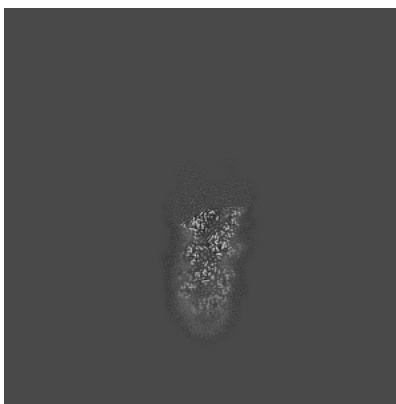
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

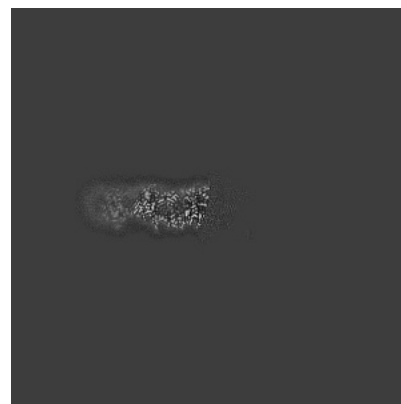
6.3.1 Primary map



X Index: 202



Y Index: 256

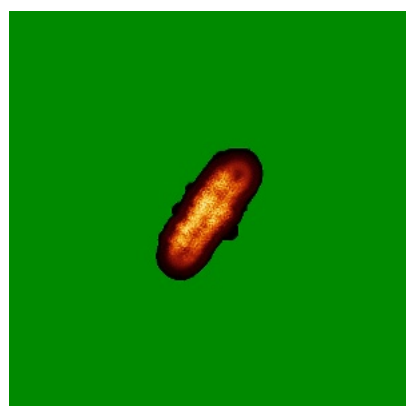


Z Index: 253

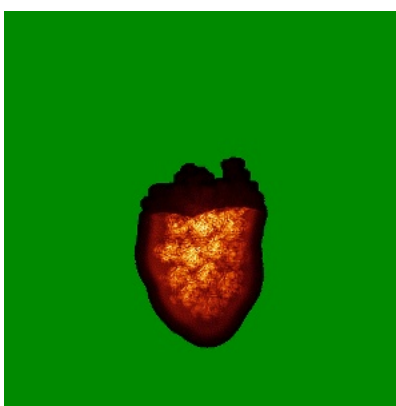
The images above show the largest variance slices of the map in three orthogonal directions.

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

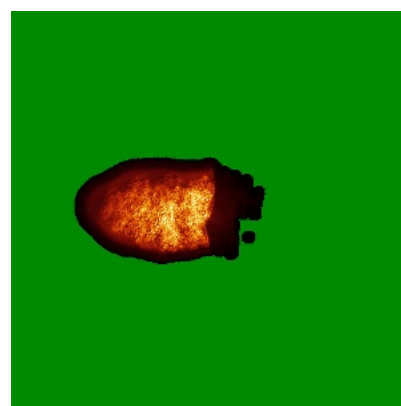
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

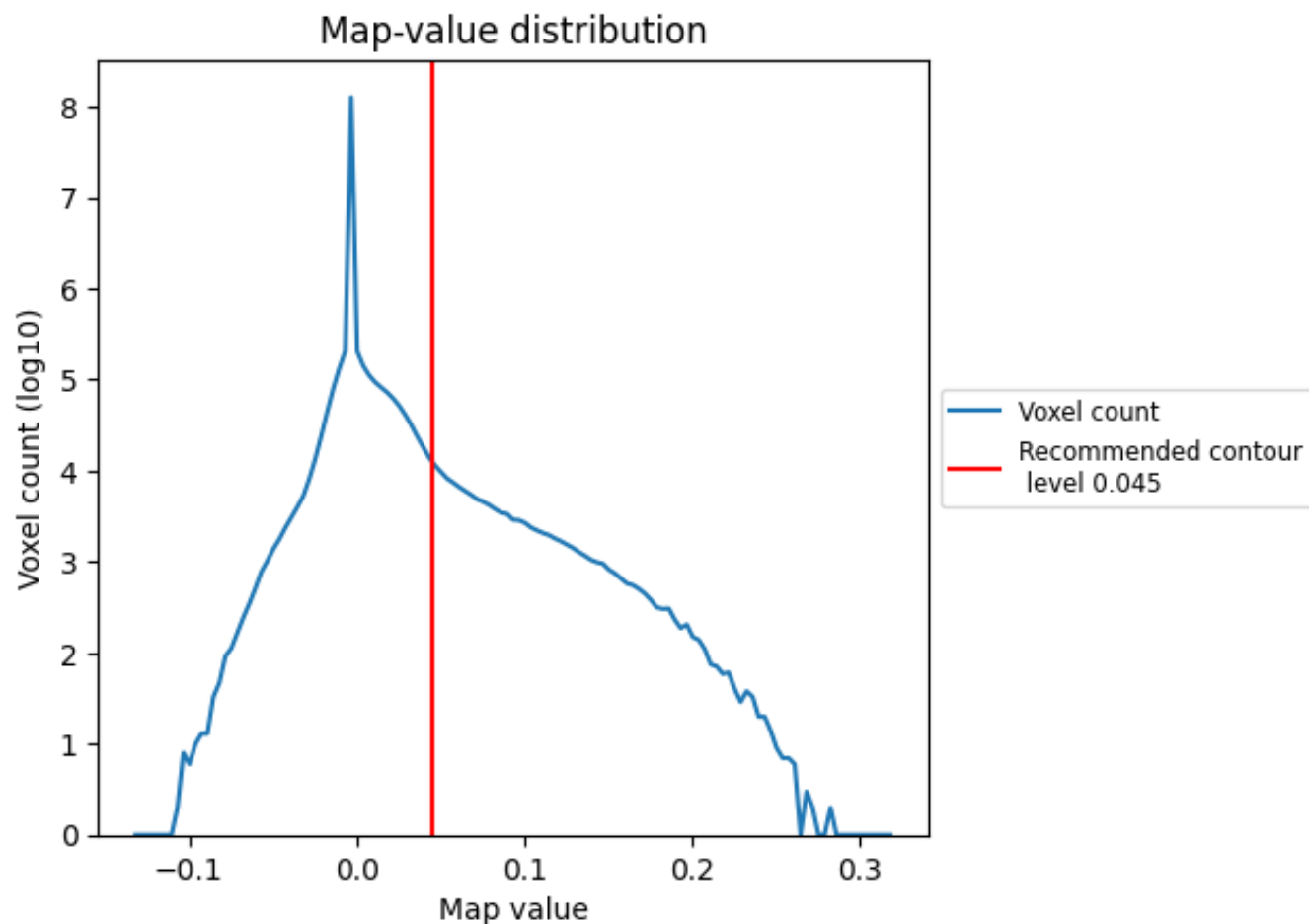
6.6 Mask visualisation

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

7 Map analysis [i](#)

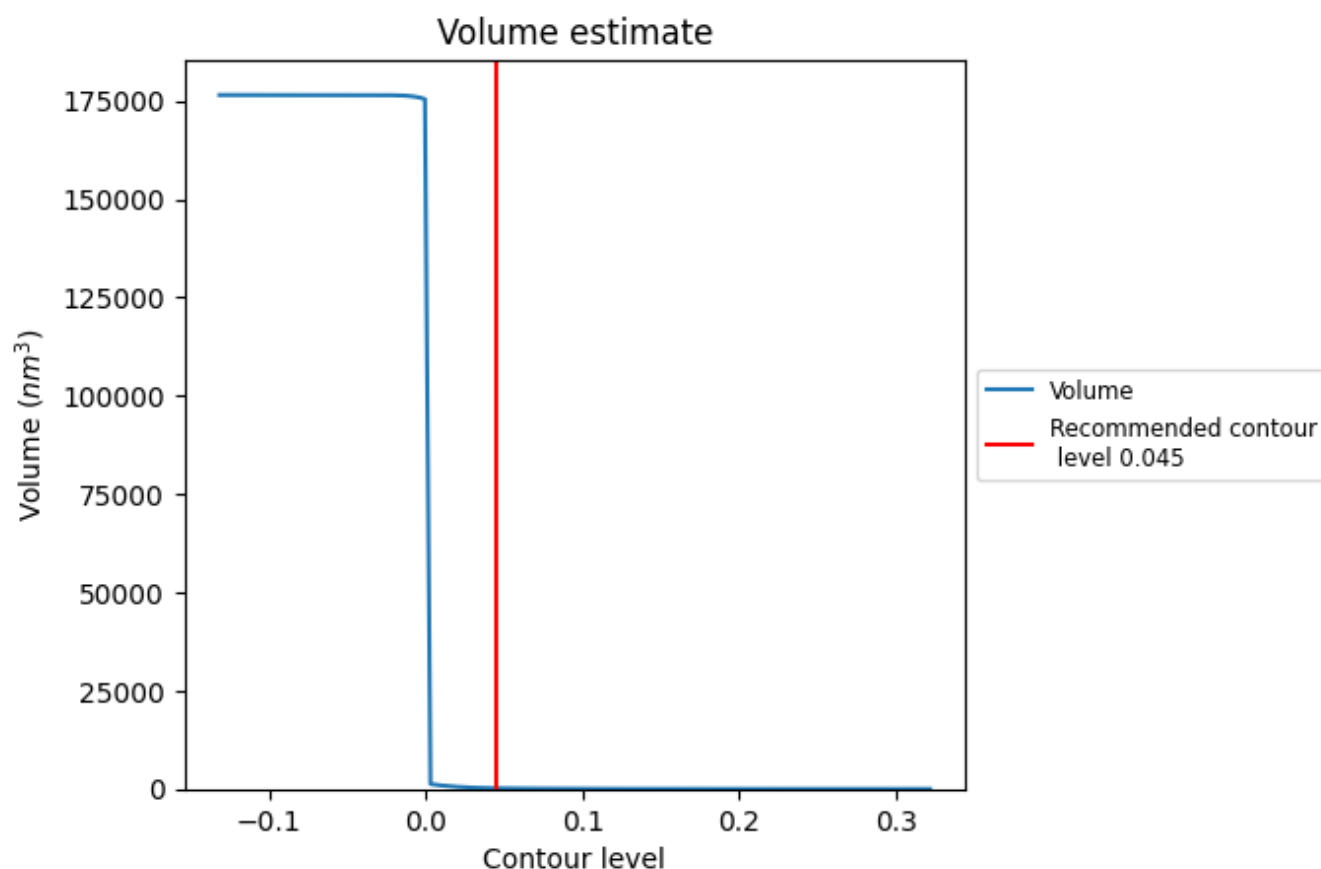
This section contains the results of statistical analysis of the map.

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.

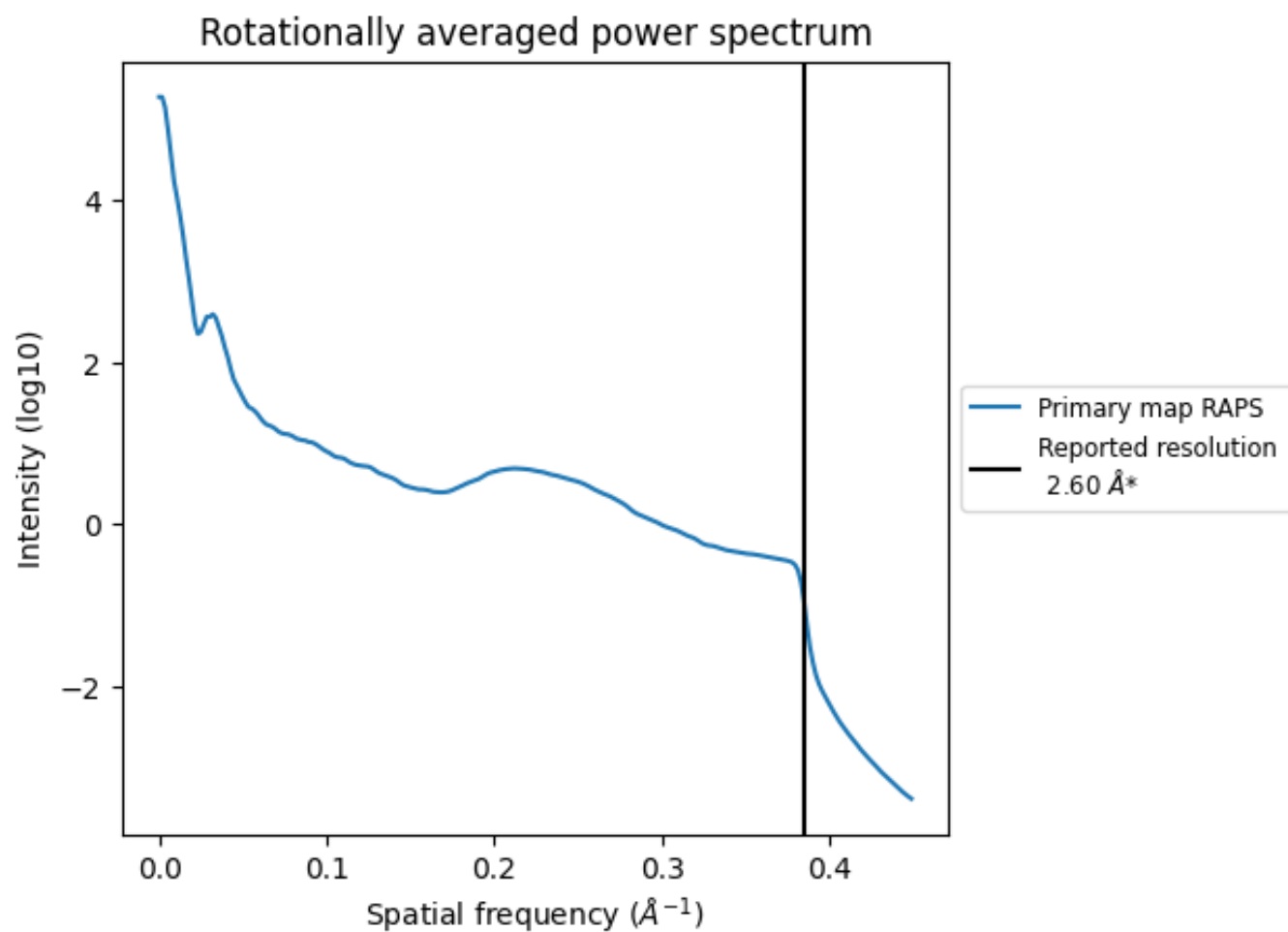
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 169 nm³; this corresponds to an approximate mass of 153 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 ⓘ

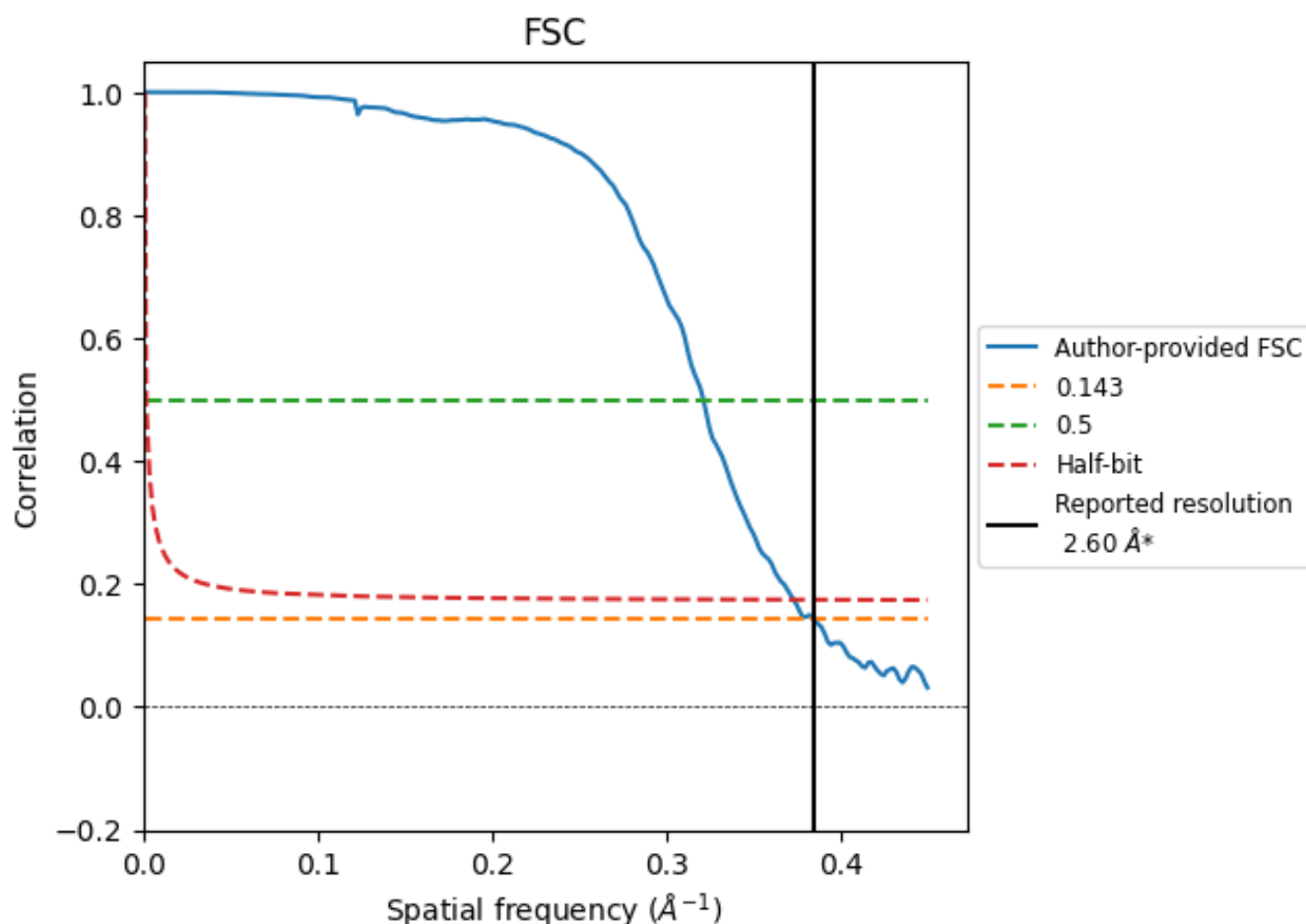


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 0.385 Å⁻¹

8.2 Resolution estimates [i](#)

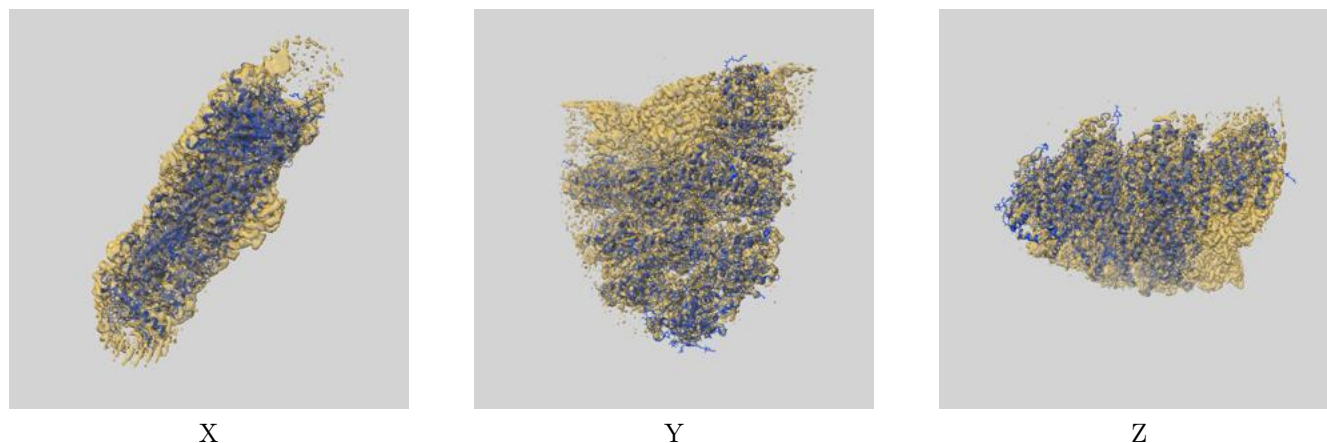
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.60	3.12	2.68
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

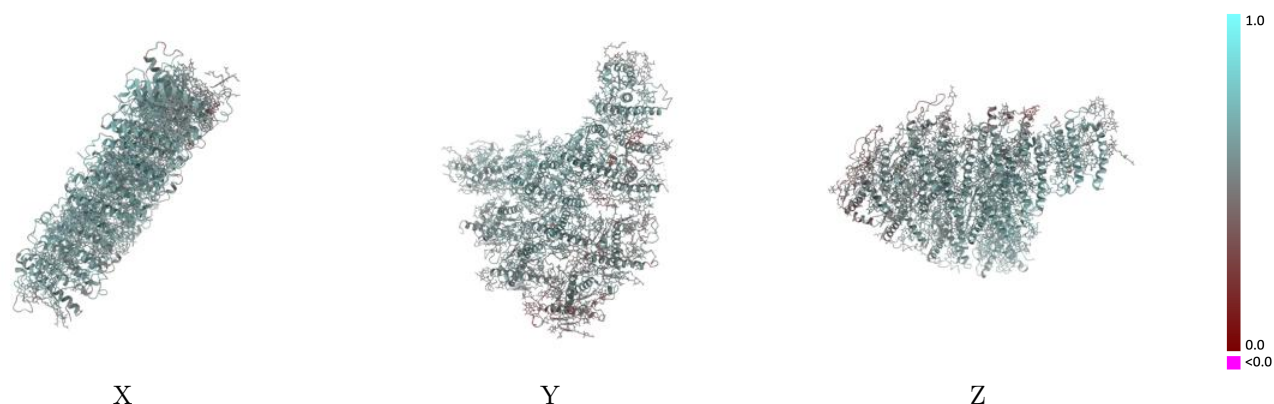
This section contains information regarding the fit between EMDB map EMD-0834 and PDB model 6L4T. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

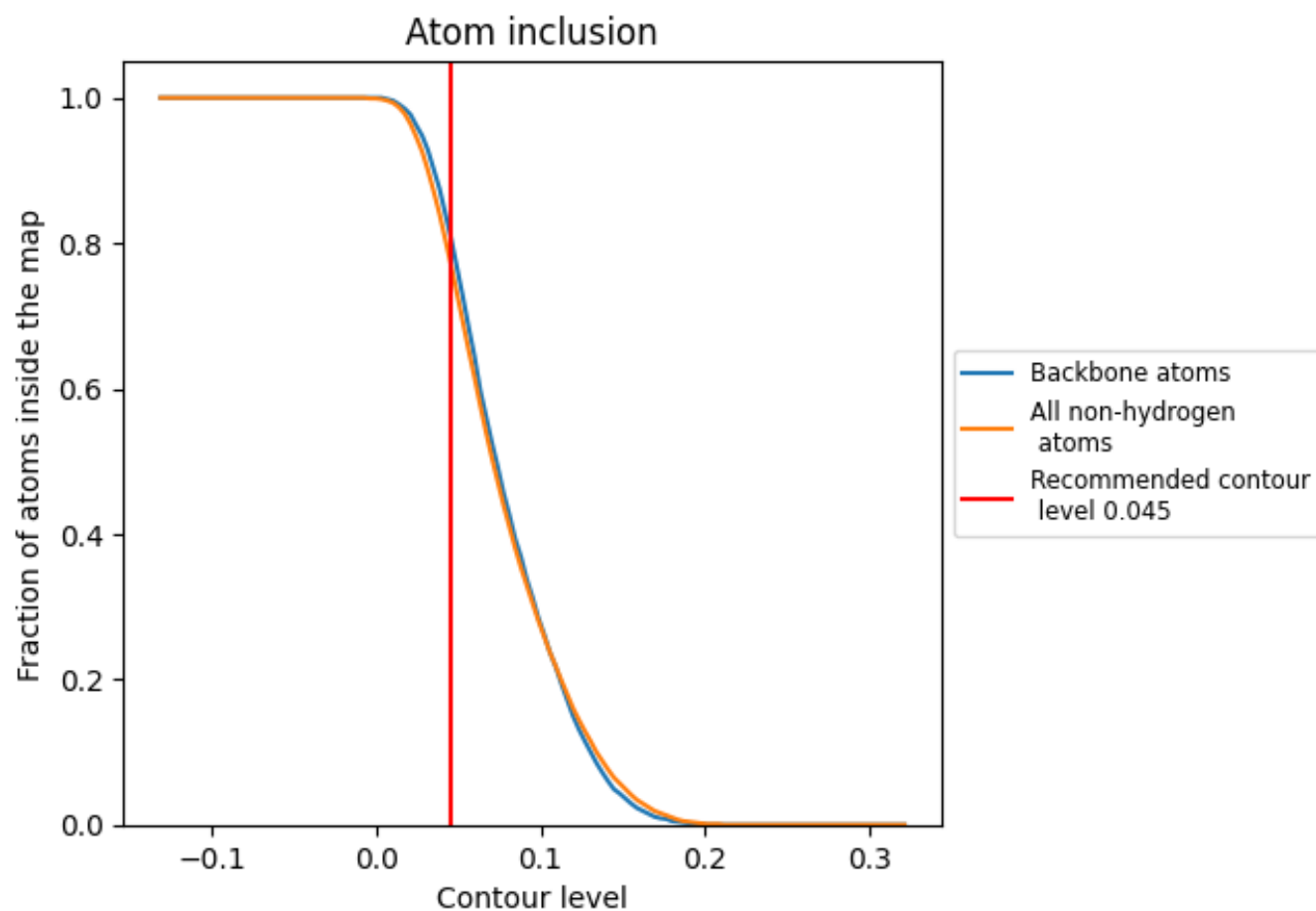


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 77% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7740	0.5630
10	0.8430	0.5780
11	0.8120	0.5720
12	0.8320	0.5990
13	0.6760	0.5130
14	0.6570	0.5180
15	0.4780	0.4670
16	0.7820	0.5480
6	0.8430	0.5800
7	0.8880	0.6240
8	0.9000	0.6310

1.0
0.0
<0.0