



## wwPDB EM Validation Summary Report ⓘ

Jun 17, 2025 – 11:20 AM EDT

PDB ID : 9MH1 / pdb\_00009mh1  
EMDB ID : EMD-48266  
Title : Dunaliella tertiolecta PSI-LHCI supercomplex  
Authors : Liu, H.W.; Khera, R.; Iwai, M.; Merchant, S.S.  
Deposited on : 2024-12-11  
Resolution : 2.10 Å(reported)  
Based on initial model : 6SL5

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

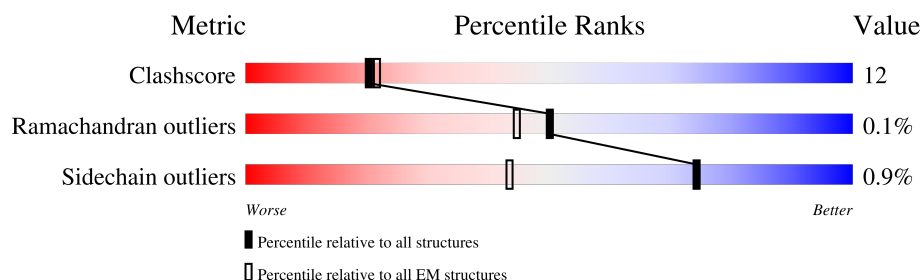
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.10 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.





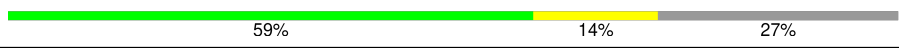



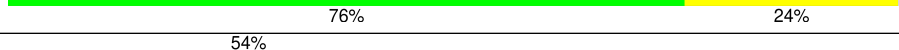


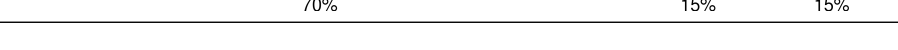
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	228	
2	3	286	
3	7	255	
4	8	254	
5	9	222	
6	A	751	
7	B	735	
8	C	81	

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Mol	Chain	Length	Quality of chain
9	D	193	
10	E	111	
11	F	227	
12	G	141	
13	H	134	
14	I	109	
15	J	41	
16	K	123	
17	L	198	
18	2	261	

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
19	CHL	1	601	X	-	-	-
19	CHL	1	606	X	-	-	-
19	CHL	2	302	X	-	-	-
19	CHL	2	306	X	-	-	-
19	CHL	3	301	X	-	-	-
19	CHL	3	323	X	-	-	-
19	CHL	7	306	X	-	-	-
19	CHL	7	307	X	-	-	-
19	CHL	7	308	X	-	-	-
19	CHL	8	304	X	-	-	-
19	CHL	8	305	X	-	-	-
19	CHL	8	306	X	-	-	-
19	CHL	9	606	X	-	-	-
20	CLA	1	602	X	-	-	-
20	CLA	1	603	X	-	-	-
20	CLA	1	604	X	-	-	-
20	CLA	1	605	X	-	-	-
20	CLA	1	607	X	-	-	-
20	CLA	1	608	X	-	-	-
20	CLA	1	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	1	610	X	-	-	-
20	CLA	1	611	X	-	-	-
20	CLA	1	612	X	-	-	-
20	CLA	1	613	X	-	-	-
20	CLA	1	614	X	-	-	-
20	CLA	2	301	X	-	-	-
20	CLA	2	303	X	-	-	-
20	CLA	2	304	X	-	-	-
20	CLA	2	305	X	-	-	-
20	CLA	2	307	X	-	-	-
20	CLA	2	308	X	-	-	-
20	CLA	2	309	X	-	-	-
20	CLA	2	310	X	-	-	-
20	CLA	2	311	X	-	-	-
20	CLA	2	312	X	-	-	-
20	CLA	2	313	X	-	-	-
20	CLA	3	302	X	-	-	-
20	CLA	3	303	X	-	-	-
20	CLA	3	304	X	-	-	-
20	CLA	3	305	X	-	-	-
20	CLA	3	306	X	-	-	-
20	CLA	3	307	X	-	-	-
20	CLA	3	308	X	-	-	-
20	CLA	3	309	X	-	-	-
20	CLA	3	310	X	-	-	-
20	CLA	3	311	X	-	-	-
20	CLA	3	312	X	-	-	-
20	CLA	3	313	X	-	-	-
20	CLA	3	314	X	-	-	-
20	CLA	3	324	X	-	-	-
20	CLA	3	325	X	-	-	-
20	CLA	7	303	X	-	-	-
20	CLA	7	304	X	-	-	-
20	CLA	7	305	X	-	-	-
20	CLA	7	309	X	-	-	-
20	CLA	7	310	X	-	-	-
20	CLA	7	311	X	-	-	-
20	CLA	7	312	X	-	-	-
20	CLA	7	313	X	-	-	-
20	CLA	7	314	X	-	-	-
20	CLA	7	315	X	-	-	-
20	CLA	7	323	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	8	301	X	-	-	-
20	CLA	8	302	X	-	-	-
20	CLA	8	303	X	-	-	-
20	CLA	8	307	X	-	-	-
20	CLA	8	308	X	-	-	-
20	CLA	8	309	X	-	-	-
20	CLA	8	310	X	-	-	-
20	CLA	8	311	X	-	-	-
20	CLA	8	312	X	-	-	-
20	CLA	8	313	X	-	-	-
20	CLA	9	601	X	-	-	-
20	CLA	9	602	X	-	-	-
20	CLA	9	603	X	-	-	-
20	CLA	9	604	X	-	-	-
20	CLA	9	605	X	-	-	-
20	CLA	9	607	X	-	-	-
20	CLA	9	608	X	-	-	-
20	CLA	9	609	X	-	-	-
20	CLA	9	610	X	-	-	-
20	CLA	9	611	X	-	-	-
20	CLA	9	612	X	-	-	-
20	CLA	A	5004	X	-	-	-
20	CLA	A	5005	X	-	-	-
20	CLA	A	5006	X	-	-	-
20	CLA	A	5007	X	-	-	-
20	CLA	A	5008	X	-	-	-
20	CLA	A	5009	X	-	-	-
20	CLA	A	5010	X	-	-	-
20	CLA	A	5011	X	-	-	-
20	CLA	A	5012	X	-	-	-
20	CLA	A	5013	X	-	-	-
20	CLA	A	5015	X	-	-	-
20	CLA	A	5016	X	-	-	-
20	CLA	A	5017	X	-	-	-
20	CLA	A	5018	X	-	-	-
20	CLA	A	5019	X	-	-	-
20	CLA	A	5020	X	-	-	-
20	CLA	A	5021	X	-	-	-
20	CLA	A	5022	X	-	-	-
20	CLA	A	5023	X	-	-	-
20	CLA	A	5024	X	-	-	-
20	CLA	A	5025	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	A	5026	X	-	-	-
20	CLA	A	5027	X	-	-	-
20	CLA	A	5028	X	-	-	-
20	CLA	A	5029	X	-	-	-
20	CLA	A	5030	X	-	-	-
20	CLA	A	5031	X	-	-	-
20	CLA	A	5032	X	-	-	-
20	CLA	A	5033	X	-	-	-
20	CLA	A	5034	X	-	-	-
20	CLA	A	5035	X	-	-	-
20	CLA	A	5036	X	-	-	-
20	CLA	A	5037	X	-	-	-
20	CLA	A	5038	X	-	-	-
20	CLA	A	5039	X	-	-	-
20	CLA	A	5040	X	-	-	-
20	CLA	A	5041	X	-	-	-
20	CLA	A	5042	X	-	-	-
20	CLA	A	5043	X	-	-	-
20	CLA	A	5044	X	-	-	-
20	CLA	B	804	X	-	-	-
20	CLA	B	805	X	-	-	-
20	CLA	B	806	X	-	-	-
20	CLA	B	807	X	-	-	-
20	CLA	B	808	X	-	-	-
20	CLA	B	809	X	-	-	-
20	CLA	B	810	X	-	-	-
20	CLA	B	811	X	-	-	-
20	CLA	B	812	X	-	-	-
20	CLA	B	813	X	-	-	-
20	CLA	B	814	X	-	-	-
20	CLA	B	815	X	-	-	-
20	CLA	B	816	X	-	-	-
20	CLA	B	817	X	-	-	-
20	CLA	B	818	X	-	-	-
20	CLA	B	819	X	-	-	-
20	CLA	B	820	X	-	-	-
20	CLA	B	821	X	-	-	-
20	CLA	B	822	X	-	-	-
20	CLA	B	823	X	-	-	-
20	CLA	B	824	X	-	-	-
20	CLA	B	825	X	-	-	-
20	CLA	B	826	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	B	827	X	-	-	-
20	CLA	B	828	X	-	-	-
20	CLA	B	829	X	-	-	-
20	CLA	B	830	X	-	-	-
20	CLA	B	831	X	-	-	-
20	CLA	B	832	X	-	-	-
20	CLA	B	833	X	-	-	-
20	CLA	B	834	X	-	-	-
20	CLA	B	835	X	-	-	-
20	CLA	B	836	X	-	-	-
20	CLA	B	838	X	-	-	-
20	CLA	B	839	X	-	-	-
20	CLA	B	840	X	-	-	-
20	CLA	F	303	X	-	-	-
20	CLA	F	306	X	-	-	-
20	CLA	F	307	X	-	-	-
20	CLA	F	308	X	-	-	-
20	CLA	G	201	X	-	-	-
20	CLA	G	202	X	-	-	-
20	CLA	G	203	X	-	-	-
20	CLA	G	204	X	-	-	-
20	CLA	H	201	X	-	-	-
20	CLA	J	104	X	-	-	-
20	CLA	K	4002	X	-	-	-
20	CLA	K	4003	X	-	-	-
20	CLA	K	4004	X	-	-	-
20	CLA	K	4005	X	-	-	-
20	CLA	L	201	X	-	-	-
20	CLA	L	202	X	-	-	-
20	CLA	L	204	X	-	-	-
20	CLA	L	205	X	-	-	-
21	LUT	1	615	X	-	-	-
21	LUT	2	314	X	-	-	-
21	LUT	2	315	X	-	-	-
21	LUT	3	315	X	-	-	-
21	LUT	7	316	X	-	-	-
21	LUT	8	314	X	-	-	-
21	LUT	9	613	X	-	-	-
30	CL0	A	5003	X	-	-	-

## 2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 41548 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	197	Total	C	N	O	S	0	0
			1505	965	255	278	7		

- Molecule 2 is a protein called LHCA3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	226	Total	C	N	O	S	0	0
			1719	1120	282	312	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	7	217	Total	C	N	O	S	0	0
			1669	1078	281	304	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	8	226	Total	C	N	O	S	0	0
			1721	1108	286	320	7		

- Molecule 5 is a protein called LHCA9.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	9	187	Total	C	N	O	S	0	0
			1453	945	244	259	5		

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	740	Total	C	N	O	S	0	0
			5808	3795	993	1002	18		

- Molecule 7 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	734	Total	C	N	O	S	0	0
			5814	3816	975	1010	13		

- Molecule 8 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	80	Total	C	N	O	S	0	0
			600	370	104	115	11		

- Molecule 9 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	143	Total	C	N	O	S	0	0
			1133	727	193	207	6		

- Molecule 10 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	68	Total	C	N	O	S	0	0
			540	343	95	102			

- Molecule 11 is a protein called PSAF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	165	Total	C	N	O	S	0	0
			1300	836	225	237	2		

- Molecule 12 is a protein called PSAG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	105	Total	C	N	O	S	0	0
			794	515	134	142	3		

- Molecule 13 is a protein called PSAH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	47	Total	C	N	O	S	0	0
			349	223	60	66			

- Molecule 14 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	35	Total	C	N	O	S	0	0
			274	191	40	42	1		

- Molecule 15 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	41	Total	C	N	O	S	0	0
			327	223	47	56	1		

- Molecule 16 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	83	Total	C	N	O	S	0	0
			579	370	101	105	3		

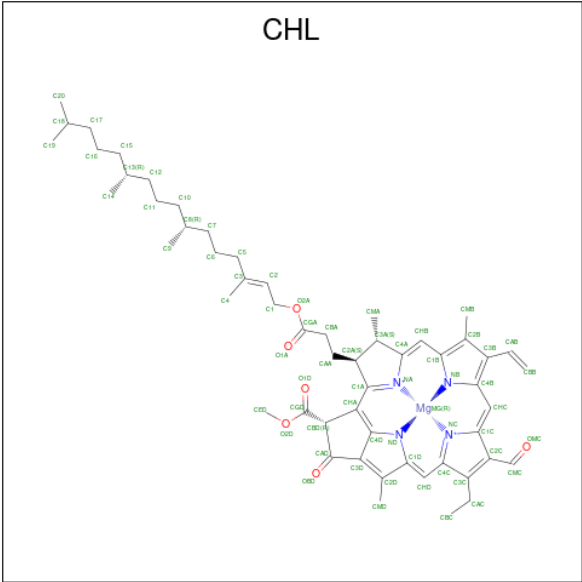
- Molecule 17 is a protein called PSAL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	124	Total	C	N	O	S	0	0
			891	580	146	160	5		

- Molecule 18 is a protein called LHCA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	2	222	Total	C	N	O	S	0	0
			1728	1125	284	311	8		

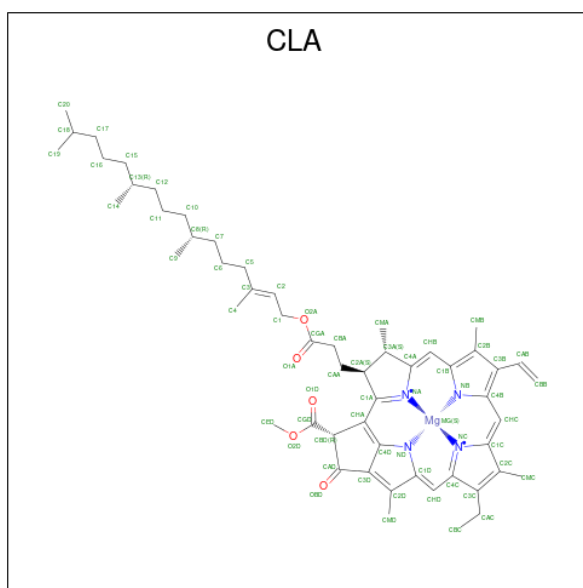
- Molecule 19 is CHLOROPHYLL B (CCD ID: CHL) (formula: C<sub>55</sub>H<sub>70</sub>MgN<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
19	1	1	Total 47	C 36	Mg 1	N 4	O 6	0
19	1	1	Total 47	C 36	Mg 1	N 4	O 6	0
19	3	1	Total 62	C 51	Mg 1	N 4	O 6	0
19	3	1	Total 61	C 50	Mg 1	N 4	O 6	0
19	7	1	Total 46	C 35	Mg 1	N 4	O 6	0
19	7	1	Total 47	C 36	Mg 1	N 4	O 6	0
19	7	1	Total 48	C 37	Mg 1	N 4	O 6	0
19	8	1	Total 47	C 36	Mg 1	N 4	O 6	0
19	8	1	Total 47	C 36	Mg 1	N 4	O 6	0
19	8	1	Total 51	C 40	Mg 1	N 4	O 6	0
19	9	1	Total 47	C 36	Mg 1	N 4	O 6	0
19	2	1	Total 61	C 50	Mg 1	N 4	O 6	0
19	2	1	Total 47	C 36	Mg 1	N 4	O 6	0

- Molecule 20 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as

"Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
20	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	1	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	1	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	1	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	3	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
20	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	7	1	Total 47	C 37	Mg 1	N 4	O 5	0
20	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	8	1	Total 47	C 37	Mg 1	N 4	O 5	0
20	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	9	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	9	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	9	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	9	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	9	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	A	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	A	1	Total 49	C 40	Mg 1	N 4	O 4	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 48	C 38	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	B	1	Total 51	C 41	Mg 1	N 4	O 5	0
20	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	F	1	Total 65	C 55	Mg 1	N 4	O 5	0

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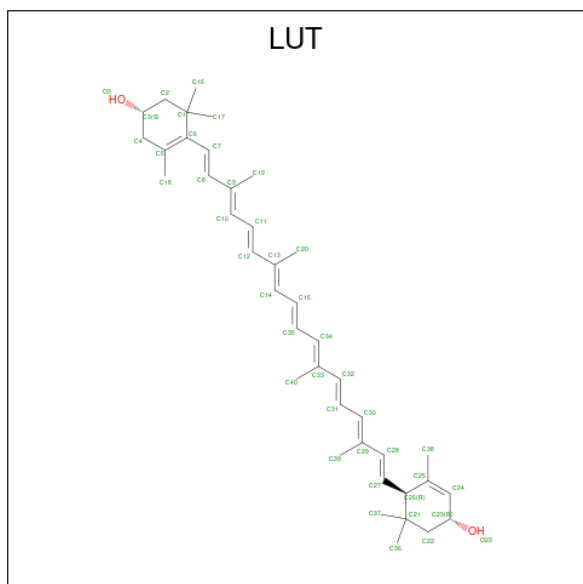
Mol	Chain	Residues	Atoms					AltConf
20	F	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	F	1	Total 47	C 37	Mg 1	N 4	O 5	0
20	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	G	1	Total 47	C 37	Mg 1	N 4	O 5	0
20	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	J	1	Total 49	C 39	Mg 1	N 4	O 5	0
20	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	K	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	K	1	Total 48	C 38	Mg 1	N 4	O 5	0
20	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	2	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

- Molecule 21 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula:  $C_{40}H_{56}O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
21	1	1	Total	C	O	0
			42	40	2	
21	3	1	Total	C	O	0
			42	40	2	
21	7	1	Total	C	O	0
			42	40	2	

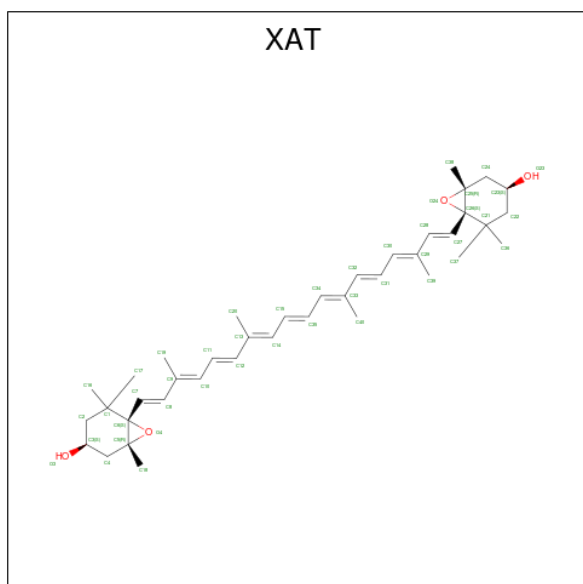
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Mol	Chain	Residues	Atoms			AltConf
21	8	1	Total	C	O	0
			42	40	2	
21	9	1	Total	C	O	0
			42	40	2	
21	2	1	Total	C	O	0
			42	40	2	
21	2	1	Total	C	O	0
			42	40	2	

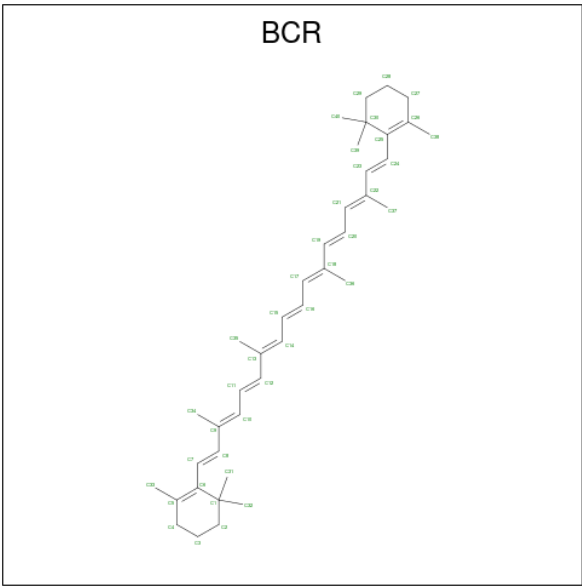
- Molecule 22 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'-TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			AltConf
22	1	1	Total	C	O	0
			44	40	4	
22	3	1	Total	C	O	0
			44	40	4	
22	7	1	Total	C	O	0
			44	40	4	
22	8	1	Total	C	O	0
			44	40	4	
22	9	1	Total	C	O	0
			44	40	4	
22	9	1	Total	C	O	0
			44	40	4	

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>) (labeled as "Ligand

of Interest" by depositor).



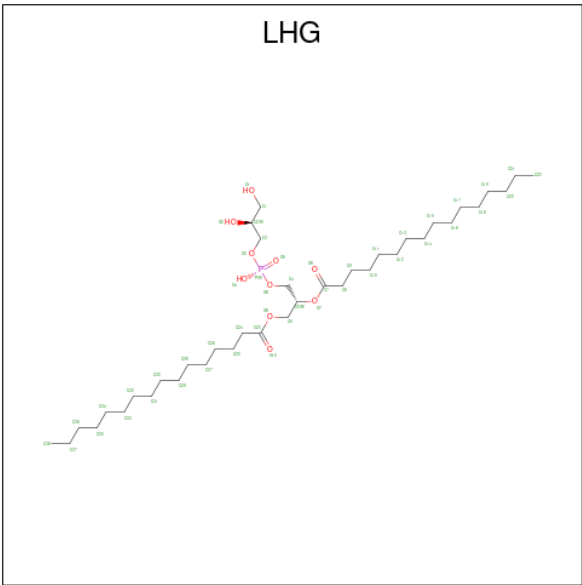
Mol	Chain	Residues	Atoms	AltConf
23	1	1	Total C 40 40	0
23	3	1	Total C 40 40	0
23	3	1	Total C 40 40	0
23	3	1	Total C 40 40	0
23	7	1	Total C 40 40	0
23	8	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 39 39	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	F	1	Total C 40 40	0
23	F	1	Total C 40 40	0
23	G	1	Total C 40 40	0
23	I	1	Total C 40 40	0
23	J	1	Total C 40 40	0
23	J	1	Total C 40 40	0
23	J	1	Total C 40 40	0
23	K	1	Total C 40 40	0
23	K	1	Total C 40 40	0
23	L	1	Total C 40 40	0
23	L	1	Total C 40 40	0

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P) (labeled as "Ligand of Interest" by depositor).



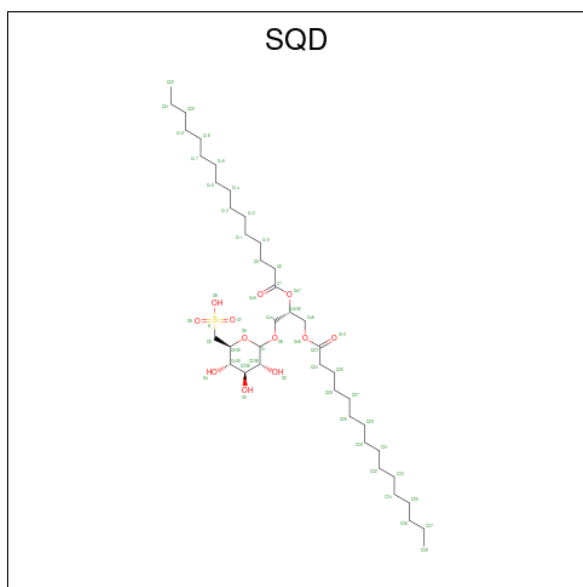
Mol	Chain	Residues	Atoms				AltConf
24	1	1	Total	C	O	P	0
			26	15	10	1	
24	1	1	Total	C	O	P	0
			46	35	10	1	
24	7	1	Total	C	O	P	0
			22	11	10	1	
24	7	1	Total	C	O	P	0
			34	23	10	1	
24	8	1	Total	C	O	P	0
			29	18	10	1	
24	8	1	Total	C	O	P	0
			38	27	10	1	
24	8	1	Total	C	O	P	0
			43	32	10	1	
24	9	1	Total	C	O	P	0
			36	25	10	1	
24	A	1	Total	C	O	P	0
			36	25	10	1	
24	A	1	Total	C	O	P	0
			49	38	10	1	
24	A	1	Total	C	O	P	0
			28	17	10	1	
24	A	1	Total	C	O	P	0
			34	25	8	1	
24	B	1	Total	C	O	P	0
			32	21	10	1	
24	B	1	Total	C	O	P	0
			30	19	10	1	

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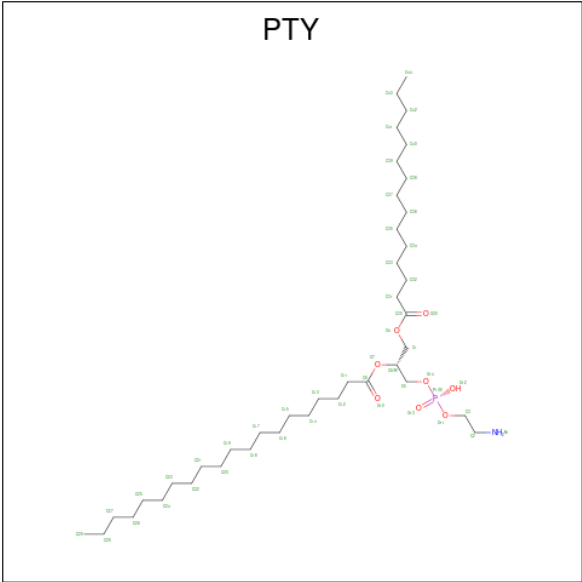
Mol	Chain	Residues	Atoms				AltConf
24	I	1	Total	C	O	P	0
			28	17	10	1	
24	2	1	Total	C	O	P	0
			25	16	8	1	

- Molecule 25 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ) (labeled as "Ligand of Interest" by depositor).



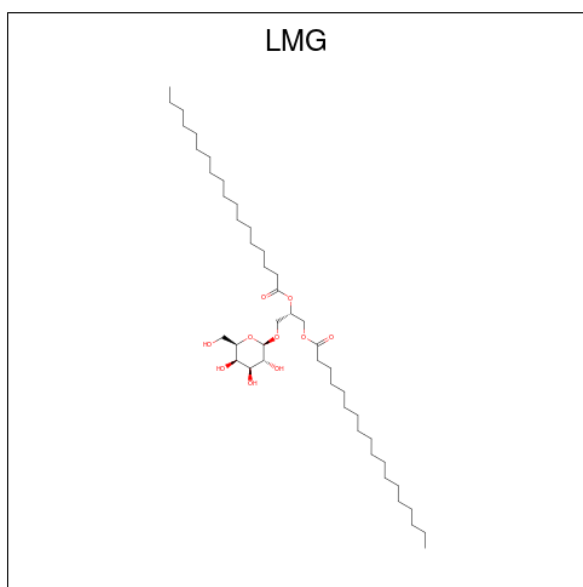
Mol	Chain	Residues	Atoms				AltConf
25	1	1	Total	C	O	S	0
			38	25	12	1	
25	3	1	Total	C	O	S	0
			35	22	12	1	
25	3	1	Total	C	O	S	0
			41	28	12	1	
25	7	1	Total	C	O	S	0
			39	26	12	1	
25	B	1	Total	C	O	S	0
			31	18	12	1	
25	F	1	Total	C	O	S	0
			39	26	12	1	

- Molecule 26 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula:  $C_{40}H_{80}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).



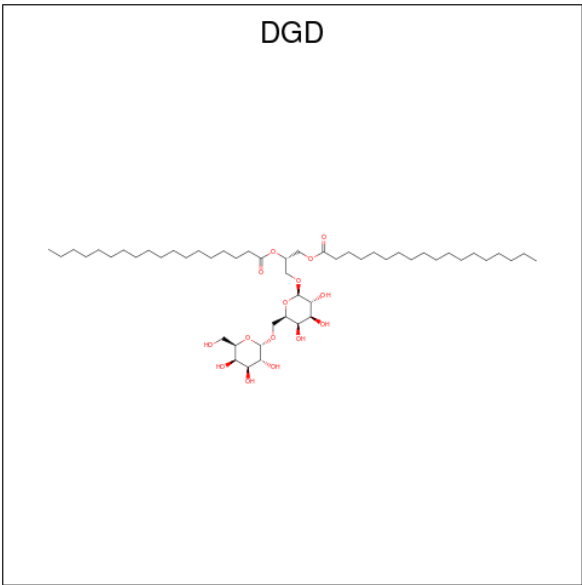
Mol	Chain	Residues	Atoms					AltConf
26	3	1	Total	C	N	O	P	0
			50	40	1	8	1	
26	7	1	Total	C	O	P		0
			15	6	8	1		
26	B	1	Total	C	N	O	P	0
			27	17	1	8	1	
26	F	1	Total	C	N	O	P	0
			29	19	1	8	1	
26	F	1	Total	C	N	O	P	0
			32	22	1	8	1	
26	F	1	Total	C	N	O	P	0
			31	21	1	8	1	

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>) (labeled as "Ligand of Interest" by depositor).



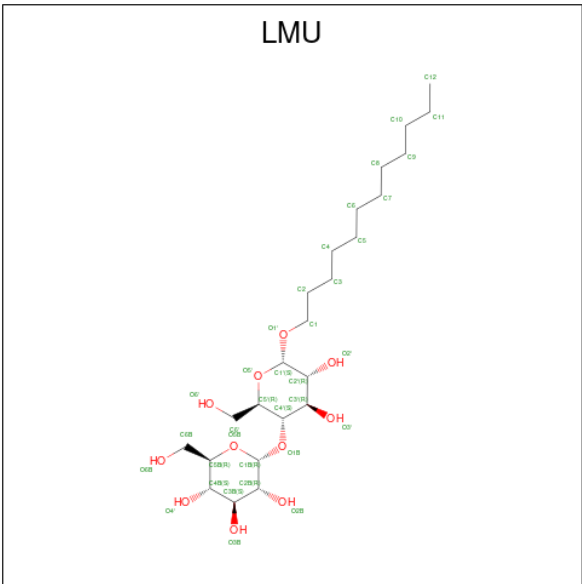
Mol	Chain	Residues	Atoms			AltConf
27	7	1	Total	C	O	0
			50	40	10	
27	7	1	Total	C	O	0
			30	20	10	
27	A	1	Total	C	O	0
			32	22	10	
27	G	1	Total	C	O	0
			43	34	9	
27	J	1	Total	C	O	0
			29	19	10	

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
28	7	1	Total	C	O	0
			39	24	15	
28	B	1	Total	C	O	0
			61	46	15	

- Molecule 29 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
29	7	1	Total	C	O	0
			32	21	11	

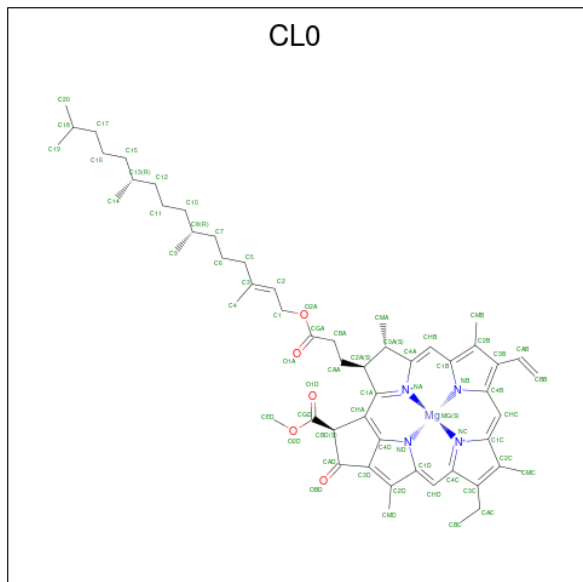
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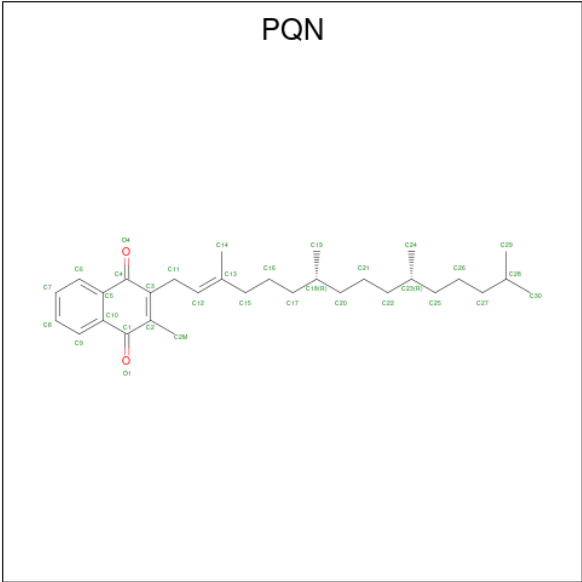
Mol	Chain	Residues	Atoms			AltConf
29	8	1	Total	C	O	0
			33	22	11	
29	8	1	Total	C	O	0
			35	24	11	
29	9	1	Total	C	O	0
			29	18	11	
29	A	1	Total	C	O	0
			35	24	11	
29	F	1	Total	C	O	0
			32	21	11	

- Molecule 30 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



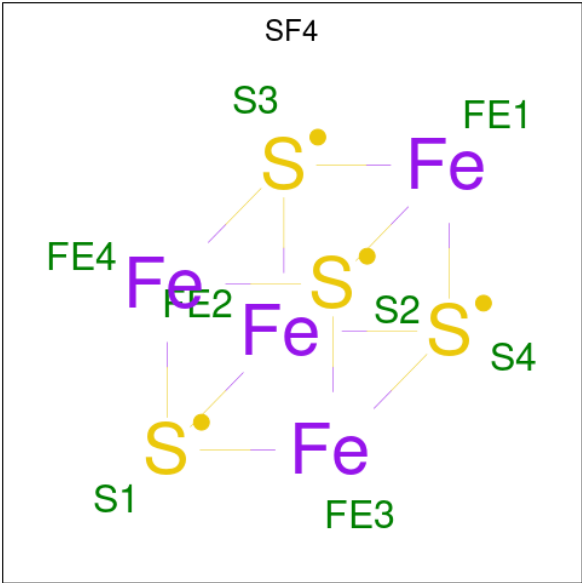
Mol	Chain	Residues	Atoms					AltConf
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 31 is PHYLLOQUINONE (CCD ID: PQN) (formula:  $C_{31}H_{46}O_2$ ).



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

- Molecule 32 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



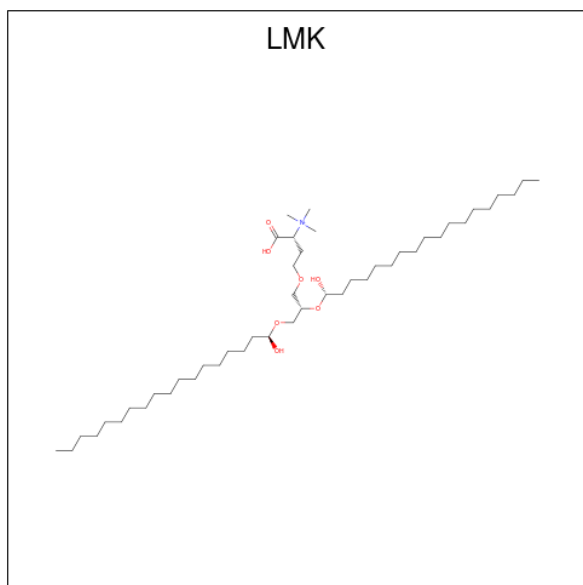
Mol	Chain	Residues	Atoms			AltConf
32	A	1	Total	Fe	S	0
			8	4	4	
32	C	1	Total	Fe	S	0
			8	4	4	

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

- Molecule 33 is trimethyl-[(2 {R})-1-oxidanyl-1-oxidanylidene-4-[(2 {S})-2-[(1 {S})-1-oxidanyloctadecoxy]-3-[(1 {R})-1-oxidanyloctadecoxy]propoxy]butan-2-yl]azanium (CCD ID: LMK) (formula: C<sub>46</sub>H<sub>94</sub>NO<sub>7</sub>) (labeled as "Ligand of Interest" by depositor).

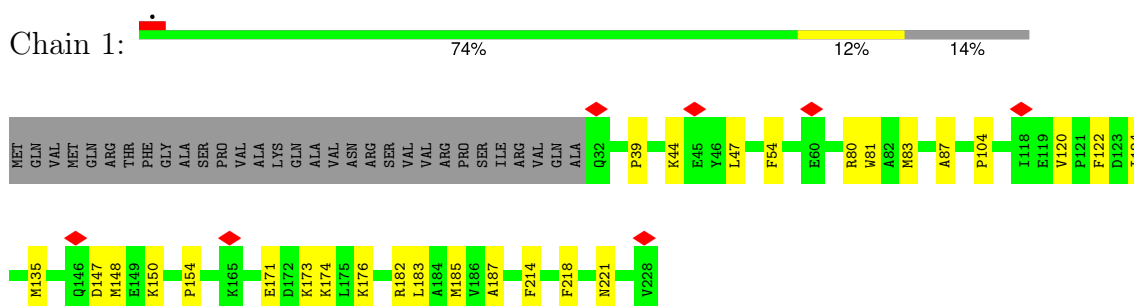


Mol	Chain	Residues	Atoms				AltConf
33	J	1	Total	C	N	O	0
			35	27	1	7	

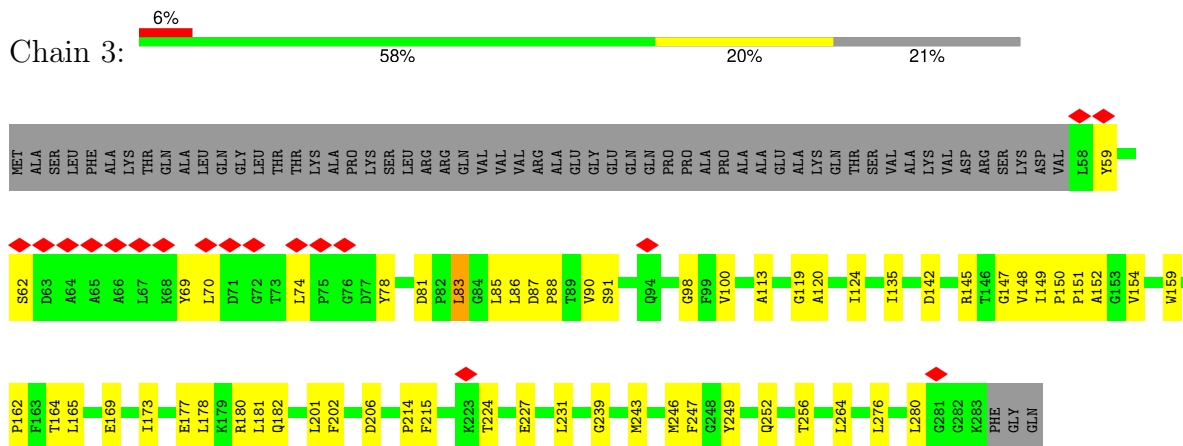
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

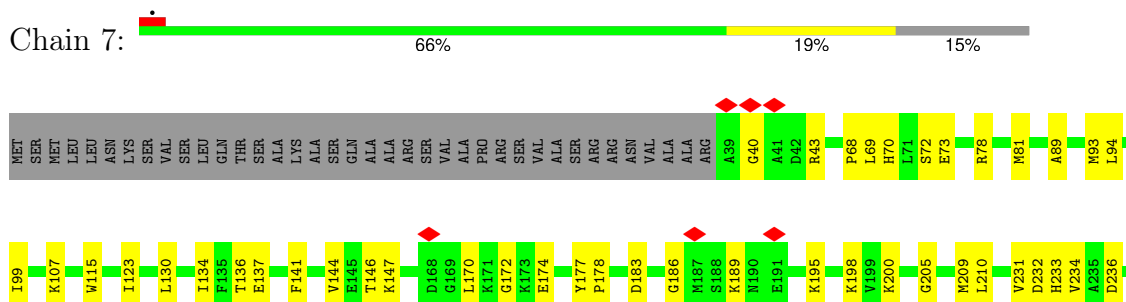
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



- Molecule 2: LHCA3

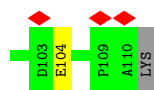


- Molecule 3: Chlorophyll a-b binding protein, chloroplastic



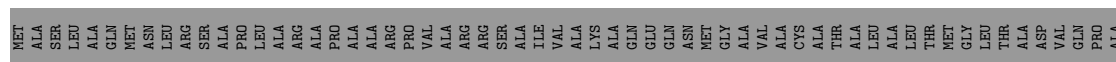






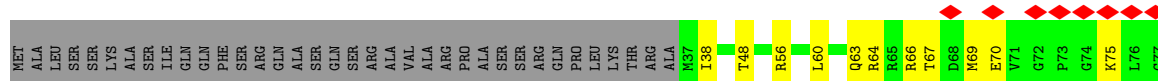
- Molecule 11: PSAF1

Chain F: 59% 14% 27%



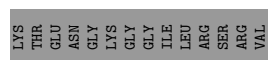
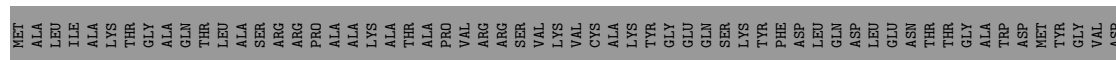
- Molecule 12: PSAG1

Chain G: 21% 60% 14% 26%



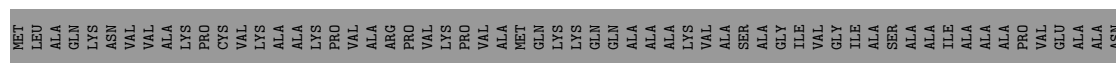
- Molecule 13: PSAH1

Chain H: 34% 19% 16% 65%

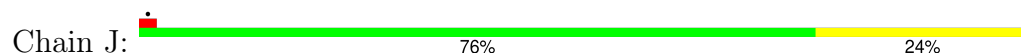


- Molecule 14: Photosystem I reaction center subunit VIII

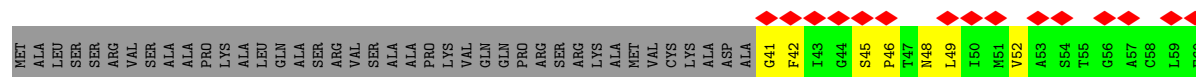
Chain I: 24% 8% 68%



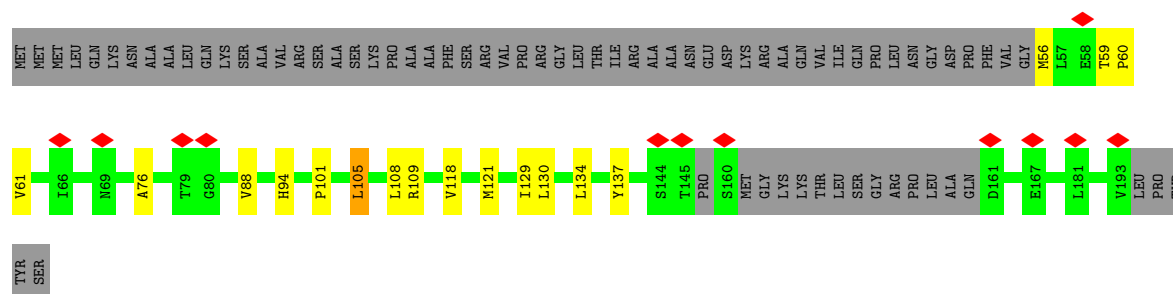
- Molecule 15: Photosystem I reaction center subunit IX



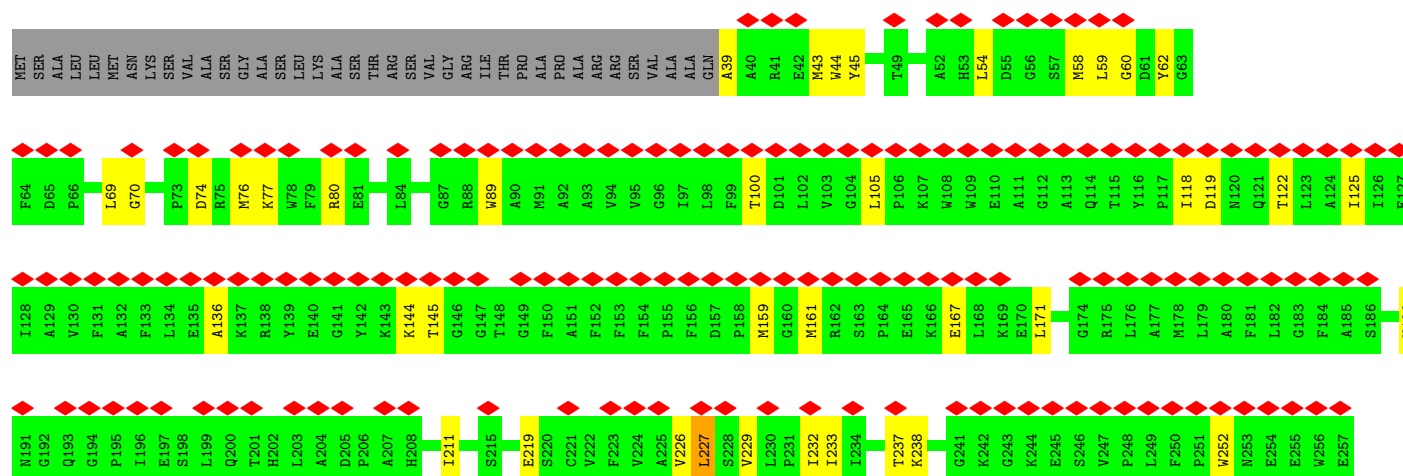
• Molecule 16: PSI-K



• Molecule 17: PSAL1



• Molecule 18: LHCA2







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	126839	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.091	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0172	Depositor
Map size (Å)	503.99997, 503.99997, 503.99997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CHL, BCR, SF4, DGD, PTY, LMG, PQN, LUT, XAT, SQD, LMK, LMU, CLA, LHG, CL0

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	1	0.18	0/1544	0.38	0/2093
2	3	0.16	0/1768	0.40	0/2402
3	7	0.15	0/1722	0.39	0/2339
4	8	0.17	0/1770	0.37	0/2401
5	9	0.20	0/1496	0.46	0/2038
6	A	0.14	0/6004	0.33	0/8190
7	B	0.14	0/6026	0.35	1/8235 (0.0%)
8	C	0.12	0/610	0.33	0/828
9	D	0.14	0/1163	0.40	0/1571
10	E	0.10	0/552	0.28	0/750
11	F	0.17	0/1329	0.42	0/1797
12	G	0.17	0/814	0.41	0/1100
13	H	0.18	0/353	0.45	0/474
14	I	0.23	0/286	0.57	0/394
15	J	0.16	0/338	0.43	0/461
16	K	0.22	0/587	0.54	0/795
17	L	0.15	0/911	0.35	0/1244
18	2	0.16	0/1779	0.40	0/2417
All	All	0.16	0/29052	0.38	1/39529 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	54	GLN	CA-CB-CG	6.45	127.00	114.10

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1505	0	1468	25	0
2	3	1719	0	1676	60	0
3	7	1669	0	1612	42	0
4	8	1721	0	1661	35	0
5	9	1453	0	1437	34	0
6	A	5808	0	5638	135	0
7	B	5814	0	5556	141	0
8	C	600	0	582	10	0
9	D	1133	0	1138	23	0
10	E	540	0	539	7	0
11	F	1300	0	1322	25	0
12	G	794	0	796	20	0
13	H	349	0	357	18	0
14	I	274	0	282	8	0
15	J	327	0	328	9	0
16	K	579	0	608	19	0
17	L	891	0	908	22	0
18	2	1728	0	1697	59	0
19	1	94	0	62	7	0
19	2	108	0	88	10	0
19	3	123	0	115	22	0
19	7	141	0	95	12	0
19	8	145	0	95	18	0
19	9	47	0	30	2	0
20	1	604	0	486	28	0
20	2	517	0	381	20	0
20	3	769	0	649	36	0
20	7	595	0	533	22	0
20	8	606	0	552	29	0
20	9	563	0	462	29	0
20	A	2475	0	2517	137	0
20	B	2260	0	2330	140	0
20	F	217	0	197	11	0
20	G	203	0	170	17	0
20	H	60	0	57	2	0
20	J	49	0	39	2	0
20	K	193	0	151	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	L	245	0	249	11	0
21	1	42	0	56	7	0
21	2	84	0	112	2	0
21	3	42	0	56	2	0
21	7	42	0	56	2	0
21	8	42	0	56	4	0
21	9	42	0	56	2	0
22	1	44	0	56	0	0
22	3	44	0	56	7	0
22	7	44	0	56	4	0
22	8	44	0	54	1	0
22	9	88	0	112	2	0
23	1	40	0	56	5	0
23	3	120	0	168	18	0
23	7	40	0	56	3	0
23	8	40	0	56	10	0
23	A	200	0	280	22	0
23	B	279	0	388	23	0
23	F	80	0	112	10	0
23	G	40	0	56	1	0
23	I	40	0	53	1	0
23	J	120	0	168	15	0
23	K	80	0	112	6	0
23	L	80	0	110	5	0
24	1	72	0	87	6	0
24	2	25	0	23	1	0
24	7	56	0	52	6	0
24	8	110	0	132	3	0
24	9	36	0	45	0	0
24	A	147	0	181	8	0
24	B	62	0	63	1	0
24	I	28	0	26	2	0
25	1	38	0	40	2	0
25	3	76	0	78	3	0
25	7	39	0	42	1	0
25	B	31	0	25	0	0
25	F	39	0	42	3	0
26	3	50	0	79	1	0
26	7	15	0	5	1	0
26	B	27	0	27	0	0
26	F	92	0	99	3	0
27	7	80	0	102	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	A	32	0	34	2	0
27	G	43	0	55	6	0
27	J	29	0	28	0	0
28	7	39	0	36	0	0
28	B	61	0	83	9	0
29	7	32	0	37	0	0
29	8	68	0	85	5	0
29	9	29	0	30	0	0
29	A	35	0	45	2	0
29	F	32	0	37	0	0
30	A	65	0	72	10	0
31	A	33	0	46	3	0
31	B	33	0	46	8	0
32	A	8	0	0	1	0
32	C	16	0	0	1	0
33	J	35	0	0	0	0
All	All	41548	0	40986	992	0

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

The worst 5 of 992 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)
20:9:607:CLA:CMB	18:2:232:ILE:HD13	1.11	1.58
20:9:607:CLA:HMB1	18:2:232:ILE:CD1	0.97	1.43
20:9:607:CLA:HMB1	18:2:232:ILE:CG1	1.58	1.31
18:2:161:MET:HG2	20:2:308:CLA:O1A	1.31	1.31
20:9:607:CLA:CMB	18:2:232:ILE:CD1	1.84	1.19

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	195/228 (86%)	185 (95%)	10 (5%)	0	100	100
2	3	224/286 (78%)	212 (95%)	12 (5%)	0	100	100
3	7	215/255 (84%)	206 (96%)	9 (4%)	0	100	100
4	8	224/254 (88%)	221 (99%)	3 (1%)	0	100	100
5	9	185/222 (83%)	173 (94%)	12 (6%)	0	100	100
6	A	738/751 (98%)	711 (96%)	27 (4%)	0	100	100
7	B	732/735 (100%)	710 (97%)	22 (3%)	0	100	100
8	C	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
9	D	141/193 (73%)	129 (92%)	12 (8%)	0	100	100
10	E	66/111 (60%)	64 (97%)	2 (3%)	0	100	100
11	F	163/227 (72%)	155 (95%)	8 (5%)	0	100	100
12	G	103/141 (73%)	97 (94%)	5 (5%)	1 (1%)	13	9
13	H	45/134 (34%)	42 (93%)	3 (7%)	0	100	100
14	I	33/109 (30%)	33 (100%)	0	0	100	100
15	J	39/41 (95%)	36 (92%)	3 (8%)	0	100	100
16	K	81/123 (66%)	65 (80%)	14 (17%)	2 (2%)	4	2
17	L	120/198 (61%)	117 (98%)	3 (2%)	0	100	100
18	2	220/261 (84%)	211 (96%)	8 (4%)	1 (0%)	25	23
All	All	3602/4350 (83%)	3442 (96%)	156 (4%)	4 (0%)	50	51

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	K	74	ALA
16	K	66	LEU
18	2	118	ILE
12	G	38	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	153/179 (86%)	153 (100%)	0	100	100
2	3	170/217 (78%)	169 (99%)	1 (1%)	84	89
3	7	171/201 (85%)	171 (100%)	0	100	100
4	8	173/197 (88%)	171 (99%)	2 (1%)	67	74
5	9	152/180 (84%)	149 (98%)	3 (2%)	50	57
6	A	599/609 (98%)	594 (99%)	5 (1%)	79	84
7	B	595/596 (100%)	586 (98%)	9 (2%)	60	67
8	C	68/69 (99%)	66 (97%)	2 (3%)	37	41
9	D	123/156 (79%)	122 (99%)	1 (1%)	79	84
10	E	60/93 (64%)	60 (100%)	0	100	100
11	F	136/177 (77%)	136 (100%)	0	100	100
12	G	82/111 (74%)	81 (99%)	1 (1%)	67	74
13	H	35/103 (34%)	35 (100%)	0	100	100
14	I	28/77 (36%)	28 (100%)	0	100	100
15	J	36/36 (100%)	35 (97%)	1 (3%)	38	43
16	K	58/88 (66%)	58 (100%)	0	100	100
17	L	91/150 (61%)	90 (99%)	1 (1%)	70	77
18	2	176/205 (86%)	175 (99%)	1 (1%)	84	89
All	All	2906/3444 (84%)	2879 (99%)	27 (1%)	74	82

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	B	283	VAL
7	B	569	CYS
15	J	5	THR
7	B	526	LEU
7	B	578	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
6	A	421	ASN

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Mol	Chain	Res	Type
6	A	659	GLN
14	I	105	GLN
6	A	637	GLN
7	B	11	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

270 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	$\# Z  > 2$
20	CLA	B	819	7	63,73,73	1.33	5 (7%)	74,113,113	1.33	7 (9%)
20	CLA	3	305	2	48,58,73	1.47	5 (10%)	56,95,113	1.46	8 (14%)
20	CLA	A	5035	6	63,73,73	1.35	5 (7%)	74,113,113	1.27	6 (8%)
32	SF4	C	102	8	0,12,12	-	-	-	-	-
29	LMU	8	322	-	36,36,36	0.12	0	47,47,47	0.20	0
20	CLA	3	309	2	44,54,73	1.58	5 (11%)	51,90,113	1.38	6 (11%)
31	PQN	B	841	-	34,34,34	0.29	0	43,45,45	0.55	1 (2%)
20	CLA	B	837	7	53,63,73	1.42	5 (9%)	62,101,113	1.43	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	LUT	1	615	-	42,43,43	0.19	0	51,60,60	1.43	7 (13%)
31	PQN	A	5045	-	34,34,34	0.27	0	43,45,45	0.56	1 (2%)
22	XAT	8	315	-	41,47,47	0.16	0	54,74,74	0.83	1 (1%)
23	BCR	L	203	-	41,41,41	0.14	0	56,56,56	0.25	0
20	CLA	B	810	7	63,73,73	1.31	7 (11%)	74,113,113	1.26	8 (10%)
20	CLA	9	612	5	44,54,73	1.60	5 (11%)	51,90,113	1.37	6 (11%)
20	CLA	A	5040	-	58,68,73	1.40	5 (8%)	68,107,113	1.28	6 (8%)
27	LMG	7	324	-	30,30,55	0.24	0	38,38,63	0.24	0
20	CLA	B	829	7	63,73,73	1.39	5 (7%)	74,113,113	1.28	8 (10%)
20	CLA	K	4005	-	46,56,73	1.67	6 (13%)	53,92,113	1.56	7 (13%)
20	CLA	K	4002	-	43,53,73	1.70	4 (9%)	50,89,113	1.50	6 (12%)
20	CLA	F	303	7	63,73,73	1.41	7 (11%)	74,113,113	1.69	13 (17%)
20	CLA	A	5017	-	53,63,73	1.48	5 (9%)	62,101,113	1.44	7 (11%)
20	CLA	8	308	4	58,68,73	1.36	5 (8%)	68,107,113	1.22	6 (8%)
25	SQD	3	322	-	39,41,54	0.22	0	49,52,65	0.26	0
20	CLA	1	614	1	44,54,73	1.58	4 (9%)	51,90,113	1.51	6 (11%)
20	CLA	2	312	18	40,52,73	1.66	5 (12%)	45,87,113	1.50	6 (13%)
20	CLA	A	5014	-	63,73,73	1.33	6 (9%)	74,113,113	1.39	8 (10%)
20	CLA	7	314	3	48,58,73	1.54	5 (10%)	56,95,113	1.43	8 (14%)
20	CLA	9	605	5	43,53,73	1.65	5 (11%)	50,89,113	1.62	5 (10%)
23	BCR	A	5049	-	41,41,41	0.27	0	56,56,56	1.03	5 (8%)
23	BCR	3	319	-	41,41,41	1.38	8 (19%)	56,56,56	1.53	12 (21%)
27	LMG	G	206	-	43,43,55	0.19	0	51,51,63	0.18	0
23	BCR	L	206	-	41,41,41	0.17	0	56,56,56	0.48	0
20	CLA	1	607	-	48,58,73	1.54	5 (10%)	56,95,113	1.38	8 (14%)
20	CLA	3	325	6	53,63,73	1.48	5 (9%)	62,101,113	1.37	6 (9%)
19	CHL	1	601	-	45,55,74	1.53	4 (8%)	48,91,114	1.66	9 (18%)
26	PTY	3	321	-	49,49,49	0.44	0	52,54,54	0.78	2 (3%)
23	BCR	K	4006	-	41,41,41	0.17	0	56,56,56	0.32	0
23	BCR	A	5051	-	41,41,41	0.14	0	56,56,56	0.25	0
23	BCR	J	106	-	41,41,41	0.17	0	56,56,56	0.36	0
27	LMG	J	103	-	29,29,55	0.20	0	37,37,63	0.14	0
20	CLA	7	303	3	58,68,73	1.39	6 (10%)	68,107,113	1.22	7 (10%)
20	CLA	3	311	-	53,63,73	1.46	5 (9%)	62,101,113	1.39	7 (11%)
28	DGD	7	321	-	40,40,67	0.24	0	54,54,81	0.34	0
20	CLA	8	307	4	45,55,73	1.81	9 (20%)	52,91,113	2.04	13 (25%)
19	CHL	1	606	-	45,55,74	1.61	4 (8%)	48,91,114	1.99	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	2	313	-	48,58,73	1.53	5 (10%)	56,95,113	1.47	8 (14%)
20	CLA	1	603	1	53,63,73	1.49	6 (11%)	62,101,113	1.39	7 (11%)
20	CLA	B	833	7	58,68,73	1.41	5 (8%)	68,107,113	1.39	6 (8%)
24	LHG	9	617	20	35,35,48	0.35	0	38,41,54	0.36	0
20	CLA	B	815	-	63,73,73	1.30	6 (9%)	74,113,113	1.27	7 (9%)
23	BCR	J	105	-	41,41,41	0.15	0	56,56,56	0.27	0
24	LHG	A	5052	-	48,48,48	0.29	0	51,54,54	0.28	0
20	CLA	B	821	-	53,63,73	1.46	5 (9%)	62,101,113	1.38	7 (11%)
20	CLA	B	840	-	63,73,73	1.32	5 (7%)	74,113,113	1.21	7 (9%)
20	CLA	3	310	2	44,54,73	1.62	7 (15%)	51,90,113	1.58	6 (11%)
20	CLA	2	309	-	43,53,73	1.62	5 (11%)	50,89,113	1.45	6 (12%)
22	XAT	9	614	-	41,47,47	0.14	0	54,74,74	0.75	3 (5%)
20	CLA	A	5025	6	58,68,73	1.40	6 (10%)	68,107,113	1.26	4 (5%)
24	LHG	7	319	-	21,21,48	0.41	0	24,27,54	0.45	0
26	PTY	B	802	-	26,26,49	0.61	0	29,31,54	0.50	0
26	PTY	F	302	-	31,31,49	0.56	0	34,36,54	0.46	0
20	CLA	H	201	18	58,68,73	1.54	6 (10%)	68,107,113	1.33	9 (13%)
20	CLA	L	204	17	63,73,73	1.33	5 (7%)	74,113,113	1.19	7 (9%)
29	LMU	8	318	-	34,34,36	0.13	0	45,45,47	0.14	0
20	CLA	1	604	-	48,58,73	1.45	5 (10%)	56,95,113	1.46	8 (14%)
19	CHL	2	306	-	45,55,74	1.16	5 (11%)	48,91,114	2.14	12 (25%)
20	CLA	8	310	4	44,54,73	1.64	8 (18%)	51,90,113	1.57	7 (13%)
20	CLA	8	301	4	58,68,73	1.38	5 (8%)	68,107,113	1.29	8 (11%)
24	LHG	2	316	-	24,24,48	0.55	0	27,29,54	0.84	2 (7%)
20	CLA	A	5021	6	48,58,73	1.53	6 (12%)	56,95,113	1.39	8 (14%)
20	CLA	B	825	-	63,73,73	1.33	7 (11%)	74,113,113	1.19	7 (9%)
20	CLA	7	323	4	45,55,73	1.59	6 (13%)	52,91,113	1.45	8 (15%)
23	BCR	B	847	-	41,41,41	0.17	0	56,56,56	0.56	2 (3%)
20	CLA	A	5034	6	63,73,73	1.35	5 (7%)	74,113,113	1.34	8 (10%)
20	CLA	1	612	-	58,68,73	1.43	5 (8%)	68,107,113	1.32	6 (8%)
20	CLA	8	313	4	44,54,73	1.60	6 (13%)	51,90,113	1.39	6 (11%)
21	LUT	2	315	-	42,43,43	0.20	0	51,60,60	0.74	2 (3%)
20	CLA	G	204	-	43,53,73	1.86	7 (16%)	50,89,113	1.48	5 (10%)
20	CLA	B	832	7	63,73,73	1.35	6 (9%)	74,113,113	1.25	7 (9%)
20	CLA	3	303	-	44,54,73	1.59	5 (11%)	51,90,113	1.50	6 (11%)
20	CLA	A	5019	6	53,63,73	1.48	7 (13%)	62,101,113	1.36	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	7	309	3	44,54,73	1.59	5 (11%)	51,90,113	1.46	6 (11%)
20	CLA	B	818	7	63,73,73	1.32	6 (9%)	74,113,113	1.27	6 (8%)
20	CLA	A	5033	6	53,63,73	1.44	5 (9%)	62,101,113	1.33	7 (11%)
23	BCR	B	846	-	41,41,41	0.13	0	56,56,56	0.37	0
20	CLA	B	823	7	53,63,73	1.45	6 (11%)	62,101,113	1.25	8 (12%)
29	LMU	9	616	-	30,30,36	0.19	0	41,41,47	0.86	2 (4%)
20	CLA	2	301	-	44,54,73	1.57	5 (11%)	51,90,113	1.40	6 (11%)
20	CLA	8	303	-	63,73,73	1.37	7 (11%)	74,113,113	1.15	6 (8%)
20	CLA	A	5007	6,20	63,73,73	1.31	6 (9%)	74,113,113	1.20	7 (9%)
20	CLA	3	314	2	44,54,73	1.60	5 (11%)	51,90,113	1.44	6 (11%)
20	CLA	7	313	3	63,73,73	1.42	6 (9%)	74,113,113	1.32	7 (9%)
20	CLA	B	812	7	53,63,73	1.48	5 (9%)	62,101,113	1.33	6 (9%)
20	CLA	B	813	7	44,54,73	1.60	6 (13%)	51,90,113	1.42	6 (11%)
21	LUT	2	314	-	42,43,43	0.29	0	51,60,60	1.04	3 (5%)
20	CLA	A	5042	6	58,68,73	1.41	6 (10%)	68,107,113	1.32	8 (11%)
20	CLA	1	605	-	43,53,73	1.63	6 (13%)	50,89,113	1.58	6 (12%)
29	LMU	F	305	-	33,33,36	0.16	0	44,44,47	0.48	0
19	CHL	3	301	2	60,70,74	1.21	4 (6%)	66,109,114	1.95	8 (12%)
19	CHL	7	307	-	45,55,74	1.27	4 (8%)	48,91,114	2.47	9 (18%)
20	CLA	A	5008	6	63,73,73	1.32	6 (9%)	74,113,113	1.27	7 (9%)
20	CLA	9	610	5	48,58,73	1.59	7 (14%)	56,95,113	1.56	9 (16%)
20	CLA	3	324	6	53,63,73	1.47	5 (9%)	62,101,113	1.37	7 (11%)
20	CLA	F	307	-	45,55,73	1.57	5 (11%)	52,91,113	1.40	7 (13%)
23	BCR	3	318	-	41,41,41	0.14	0	56,56,56	0.34	0
23	BCR	A	5047	-	41,41,41	0.29	0	56,56,56	0.54	0
24	LHG	I	4002	-	27,27,48	0.38	0	30,33,54	0.36	0
25	SQD	7	322	-	37,39,54	0.23	0	47,50,65	0.24	0
20	CLA	B	811	7	63,73,73	1.35	6 (9%)	74,113,113	1.33	7 (9%)
20	CLA	A	5028	6	63,73,73	1.37	7 (11%)	74,113,113	1.37	7 (9%)
20	CLA	L	202	-	63,73,73	1.34	5 (7%)	74,113,113	1.24	7 (9%)
28	DGD	B	848	-	62,62,67	0.18	0	76,76,81	0.19	0
20	CLA	L	201	7	63,73,73	1.35	5 (7%)	74,113,113	1.33	8 (10%)
20	CLA	B	809	7	63,73,73	1.32	5 (7%)	74,113,113	1.29	7 (9%)
22	XAT	3	316	-	41,47,47	0.14	0	54,74,74	0.81	2 (3%)
20	CLA	8	311	4	63,73,73	1.38	6 (9%)	74,113,113	1.25	7 (9%)
20	CLA	G	203	12	44,54,73	1.62	5 (11%)	51,90,113	1.45	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	LHG	A	5055	-	33,33,48	0.45	0	36,38,54	0.65	2 (5%)
20	CLA	F	306	-	58,68,73	1.37	5 (8%)	68,107,113	1.25	7 (10%)
19	CHL	2	302	18	59,69,74	1.19	4 (6%)	65,108,114	1.91	8 (12%)
20	CLA	A	5032	6	48,58,73	1.63	7 (14%)	56,95,113	1.44	8 (14%)
20	CLA	B	836	7	58,68,73	1.37	5 (8%)	68,107,113	1.27	8 (11%)
23	BCR	A	5050	-	41,41,41	0.13	0	56,56,56	0.39	0
24	LHG	8	319	-	37,37,48	0.33	0	40,43,54	0.31	0
20	CLA	7	304	3	53,63,73	1.50	6 (11%)	62,101,113	1.37	7 (11%)
23	BCR	J	102	-	41,41,41	0.24	0	56,56,56	0.93	4 (7%)
19	CHL	8	306	-	49,59,74	1.65	4 (8%)	53,96,114	2.07	8 (15%)
26	PTY	F	310	-	30,30,49	0.56	0	33,35,54	0.55	0
20	CLA	7	310	3	63,73,73	1.29	5 (7%)	74,113,113	1.20	7 (9%)
20	CLA	B	824	-	63,73,73	1.32	7 (11%)	74,113,113	1.41	9 (12%)
30	CL0	A	5003	6	63,73,73	1.14	4 (6%)	74,113,113	1.84	7 (9%)
24	LHG	1	620	-	45,45,48	0.31	0	48,51,54	0.34	0
20	CLA	A	5010	-	49,59,73	1.53	5 (10%)	56,96,113	1.47	8 (14%)
20	CLA	2	308	-	43,53,73	1.62	5 (11%)	50,89,113	1.42	8 (16%)
19	CHL	3	323	-	59,69,74	1.30	4 (6%)	65,108,114	2.18	8 (12%)
19	CHL	7	306	-	44,54,74	1.40	5 (11%)	47,90,114	2.16	6 (12%)
20	CLA	A	5018	6	58,68,73	1.39	6 (10%)	68,107,113	1.32	6 (8%)
20	CLA	A	5023	6	48,58,73	1.52	5 (10%)	56,95,113	1.57	9 (16%)
23	BCR	K	4001	-	41,41,41	0.18	0	56,56,56	0.35	0
26	PTY	F	301	-	28,28,49	0.59	0	31,33,54	0.50	0
20	CLA	A	5020	6	63,73,73	1.33	5 (7%)	74,113,113	1.30	9 (12%)
20	CLA	8	309	24	58,68,73	1.43	7 (12%)	68,107,113	1.31	7 (10%)
20	CLA	A	5027	-	54,64,73	1.51	7 (12%)	63,102,113	1.34	8 (12%)
20	CLA	A	5039	6	53,63,73	1.45	6 (11%)	62,101,113	1.35	8 (12%)
20	CLA	2	304	-	48,58,73	1.50	5 (10%)	56,95,113	1.38	8 (14%)
20	CLA	B	830	7	63,73,73	1.37	5 (7%)	74,113,113	1.29	8 (10%)
20	CLA	1	602	1	53,63,73	1.47	5 (9%)	62,101,113	1.41	8 (12%)
24	LHG	1	618	20	25,25,48	0.41	0	28,31,54	0.40	0
24	LHG	8	320	-	42,42,48	0.31	0	45,48,54	0.30	0
25	SQD	3	320	-	33,35,54	0.27	0	43,46,65	0.39	0
20	CLA	8	312	4	44,54,73	1.59	5 (11%)	51,90,113	1.49	6 (11%)
20	CLA	8	321	-	44,54,73	1.64	5 (11%)	51,90,113	1.56	8 (15%)
20	CLA	B	827	-	63,73,73	1.32	5 (7%)	74,113,113	1.28	7 (9%)
23	BCR	F	304	-	41,41,41	0.17	0	56,56,56	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	9	602	5	58,68,73	1.35	5 (8%)	68,107,113	1.27	8 (11%)
25	SQD	1	619	-	36,38,54	0.27	0	46,49,65	0.52	1 (2%)
20	CLA	A	5016	6	63,73,73	1.34	6 (9%)	74,113,113	1.33	7 (9%)
20	CLA	B	820	-	63,73,73	1.38	8 (12%)	74,113,113	1.39	6 (8%)
20	CLA	A	5005	-	63,73,73	1.34	6 (9%)	74,113,113	1.27	5 (6%)
19	CHL	8	305	-	45,55,74	1.50	4 (8%)	48,91,114	2.43	6 (12%)
20	CLA	G	201	7	63,73,73	1.35	5 (7%)	74,113,113	1.21	6 (8%)
20	CLA	2	303	18	48,58,73	1.59	7 (14%)	56,95,113	1.51	10 (17%)
20	CLA	J	104	15	47,57,73	1.55	5 (10%)	53,93,113	1.45	6 (11%)
20	CLA	9	611	-	53,63,73	1.48	6 (11%)	62,101,113	1.45	7 (11%)
24	LHG	7	320	20	33,33,48	0.34	0	36,39,54	0.33	0
20	CLA	2	305	-	43,53,73	1.64	5 (11%)	50,89,113	1.45	6 (12%)
32	SF4	A	5046	7,6	0,12,12	-	-	-	-	-
20	CLA	7	312	3	50,60,73	1.52	7 (14%)	57,97,113	1.52	8 (14%)
20	CLA	A	5041	6	63,73,73	1.32	6 (9%)	74,113,113	1.29	8 (10%)
20	CLA	A	5038	6	48,58,73	1.52	6 (12%)	56,95,113	1.53	7 (12%)
23	BCR	B	845	-	40,40,41	0.17	0	54,54,56	0.48	1 (1%)
20	CLA	B	839	7	63,73,73	1.33	6 (9%)	74,113,113	1.21	8 (10%)
20	CLA	B	805	-	63,73,73	1.33	7 (11%)	74,113,113	1.40	9 (12%)
23	BCR	7	318	-	41,41,41	0.14	0	56,56,56	0.38	0
23	BCR	B	844	-	41,41,41	0.34	0	56,56,56	1.11	6 (10%)
20	CLA	K	4003	-	53,63,73	1.48	5 (9%)	62,101,113	1.31	7 (11%)
20	CLA	L	205	-	48,58,73	1.50	5 (10%)	56,95,113	1.43	8 (14%)
21	LUT	9	613	-	42,43,43	0.26	0	51,60,60	0.30	0
26	PTY	7	302	-	14,14,49	1.11	2 (14%)	15,18,54	1.70	2 (13%)
20	CLA	7	305	-	48,58,73	1.57	6 (12%)	56,95,113	1.45	7 (12%)
23	BCR	F	309	-	41,41,41	0.17	0	56,56,56	0.40	0
20	CLA	B	816	-	53,63,73	1.45	5 (9%)	62,101,113	1.43	8 (12%)
20	CLA	B	828	-	63,73,73	1.39	7 (11%)	74,113,113	1.31	6 (8%)
29	LMU	7	325	-	33,33,36	0.13	0	44,44,47	0.15	0
20	CLA	B	834	-	48,58,73	1.52	5 (10%)	56,95,113	1.47	9 (16%)
24	LHG	A	5054	20	27,27,48	0.42	0	30,33,54	0.49	0
20	CLA	9	601	5	44,54,73	1.58	5 (11%)	51,90,113	1.36	7 (13%)
23	BCR	B	803	-	41,41,41	0.26	0	56,56,56	0.63	1 (1%)
22	XAT	1	616	-	41,47,47	0.14	0	54,74,74	0.84	2 (3%)
22	XAT	9	615	-	41,47,47	0.18	0	54,74,74	0.79	3 (5%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	A	5036	6	62,72,73	1.33	5 (8%)	72,111,113	1.33	6 (8%)
21	LUT	7	316	-	42,43,43	0.35	0	51,60,60	0.53	1 (1%)
20	CLA	B	838	-	53,63,73	1.52	7 (13%)	62,101,113	1.43	7 (11%)
25	SQD	F	311	-	37,39,54	0.26	0	47,50,65	0.49	1 (2%)
20	CLA	8	302	4	63,73,73	1.38	6 (9%)	74,113,113	1.35	7 (9%)
20	CLA	1	611	1	44,54,73	1.63	6 (13%)	51,90,113	1.58	9 (17%)
27	LMG	A	5001	-	32,32,55	0.20	0	40,40,63	0.31	0
20	CLA	3	312	2	44,54,73	1.59	5 (11%)	51,90,113	1.37	6 (11%)
20	CLA	9	604	5	48,58,73	1.54	5 (10%)	56,95,113	1.33	7 (12%)
20	CLA	1	610	24	44,54,73	1.57	5 (11%)	51,90,113	1.38	6 (11%)
29	LMU	A	5053	-	36,36,36	0.13	0	47,47,47	0.15	0
20	CLA	9	603	-	53,63,73	1.51	6 (11%)	62,101,113	1.49	7 (11%)
20	CLA	1	613	1	48,58,73	1.56	6 (12%)	56,95,113	1.52	7 (12%)
20	CLA	B	817	-	58,68,73	1.42	7 (12%)	68,107,113	1.36	6 (8%)
20	CLA	1	609	1	53,63,73	1.45	6 (11%)	62,101,113	1.32	6 (9%)
21	LUT	8	314	-	42,43,43	0.27	0	51,60,60	0.42	0
20	CLA	A	5043	24	47,57,73	1.52	5 (10%)	54,93,113	1.44	7 (12%)
24	LHG	B	801	-	31,31,48	0.36	0	34,37,54	0.33	0
23	BCR	A	5048	-	41,41,41	0.17	0	56,56,56	0.24	0
20	CLA	9	608	5	48,58,73	1.52	6 (12%)	56,95,113	1.35	7 (12%)
20	CLA	A	5012	6	63,73,73	1.34	6 (9%)	74,113,113	1.17	7 (9%)
24	LHG	8	317	20	28,28,48	0.38	0	31,34,54	0.34	0
19	CHL	7	308	-	46,56,74	1.51	4 (8%)	49,92,114	1.96	8 (16%)
20	CLA	A	5029	6	63,73,73	1.31	6 (9%)	74,113,113	1.28	8 (10%)
20	CLA	A	5006	6	63,73,73	1.32	6 (9%)	74,113,113	1.32	8 (10%)
19	CHL	8	304	4	45,55,74	2.22	4 (8%)	48,91,114	2.67	10 (20%)
23	BCR	G	205	-	41,41,41	0.21	0	56,56,56	0.49	0
23	BCR	B	843	-	41,41,41	0.22	0	56,56,56	0.40	0
20	CLA	B	814	7	63,73,73	1.37	6 (9%)	74,113,113	1.31	7 (9%)
20	CLA	K	4004	16	43,53,73	1.67	7 (16%)	50,89,113	1.56	6 (12%)
22	XAT	7	317	-	41,47,47	0.17	0	54,74,74	0.86	3 (5%)
20	CLA	A	5013	6,20	63,73,73	1.33	5 (7%)	74,113,113	1.25	7 (9%)
23	BCR	1	617	-	41,41,41	0.18	0	56,56,56	0.26	0
25	SQD	B	850	-	29,31,54	0.21	0	39,42,65	0.25	0
20	CLA	B	826	7	63,73,73	1.39	7 (11%)	74,113,113	1.37	8 (10%)
20	CLA	3	302	2	63,73,73	1.35	6 (9%)	74,113,113	1.32	7 (9%)
24	LHG	A	5002	-	35,35,48	0.36	0	38,41,54	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	3	308	2	53,63,73	1.44	5 (9%)	62,101,113	1.27	7 (11%)
20	CLA	A	5009	6	63,73,73	1.35	6 (9%)	74,113,113	1.38	8 (10%)
24	LHG	B	849	-	29,29,48	0.40	0	32,35,54	0.42	0
20	CLA	A	5011	6	63,73,73	1.32	5 (7%)	74,113,113	1.24	6 (8%)
20	CLA	A	5031	6	63,73,73	1.38	5 (7%)	74,113,113	1.29	7 (9%)
23	BCR	3	317	-	41,41,41	0.16	0	56,56,56	0.32	0
20	CLA	G	202	12	45,55,73	1.60	6 (13%)	52,91,113	1.58	7 (13%)
27	LMG	7	301	-	50,50,55	0.18	0	58,58,63	0.15	0
20	CLA	3	313	-	40,50,73	1.68	6 (15%)	45,85,113	1.40	6 (13%)
20	CLA	3	304	-	44,54,73	1.57	6 (13%)	51,90,113	1.43	6 (11%)
33	LMK	J	101	-	34,34,53	0.42	0	34,41,60	0.52	1 (2%)
23	BCR	8	316	-	41,41,41	0.16	0	56,56,56	0.40	0
32	SF4	C	101	8	0,12,12	-	-	-	-	-
20	CLA	A	5030	-	63,73,73	1.35	6 (9%)	74,113,113	1.37	8 (10%)
20	CLA	2	307	18	44,54,73	1.61	5 (11%)	51,90,113	1.36	6 (11%)
20	CLA	7	315	3	43,53,73	1.61	5 (11%)	50,89,113	1.52	6 (12%)
20	CLA	2	310	18	44,54,73	1.64	6 (13%)	51,90,113	1.60	8 (15%)
20	CLA	9	609	24	44,54,73	1.58	5 (11%)	51,90,113	1.42	6 (11%)
20	CLA	7	311	24	58,68,73	1.42	7 (12%)	68,107,113	1.33	8 (11%)
20	CLA	3	306	-	49,59,73	1.50	5 (10%)	56,96,113	1.41	8 (14%)
20	CLA	9	607	5	58,68,73	1.33	6 (10%)	68,107,113	1.25	6 (8%)
20	CLA	A	5004	-	63,73,73	1.34	6 (9%)	74,113,113	1.26	7 (9%)
23	BCR	B	842	-	41,41,41	0.19	0	56,56,56	0.33	0
20	CLA	B	835	7	49,59,73	1.52	5 (10%)	56,96,113	1.61	6 (10%)
20	CLA	A	5024	6	58,68,73	1.39	5 (8%)	68,107,113	1.22	7 (10%)
20	CLA	A	5037	6	48,58,73	1.54	5 (10%)	56,95,113	1.41	9 (16%)
20	CLA	B	807	-	63,73,73	1.32	6 (9%)	74,113,113	1.33	7 (9%)
20	CLA	A	5022	-	63,73,73	1.32	6 (9%)	74,113,113	1.30	6 (8%)
20	CLA	2	311	-	48,58,73	1.56	4 (8%)	56,95,113	1.52	8 (14%)
20	CLA	B	808	7	63,73,73	1.97	6 (9%)	74,113,113	1.22	10 (13%)
20	CLA	B	804	7	63,73,73	1.37	7 (11%)	74,113,113	1.14	6 (8%)
20	CLA	1	608	1	44,54,73	1.57	5 (11%)	51,90,113	1.47	7 (13%)
19	CHL	9	606	-	45,55,74	1.50	4 (8%)	48,91,114	2.07	8 (16%)
20	CLA	A	5044	-	63,73,73	1.32	6 (9%)	74,113,113	1.38	8 (10%)
20	CLA	B	806	7	46,56,73	1.52	5 (10%)	53,92,113	1.48	8 (15%)
20	CLA	A	5015	-	53,63,73	1.44	5 (9%)	62,101,113	1.45	7 (11%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	3	307	2	63,73,73	1.35	5 (7%)	74,113,113	1.26	8 (10%)
20	CLA	A	5026	-	63,73,73	1.37	6 (9%)	74,113,113	1.44	6 (8%)
20	CLA	B	822	7	63,73,73	1.33	5 (7%)	74,113,113	1.32	7 (9%)
20	CLA	F	308	11	43,53,73	1.62	5 (11%)	50,89,113	1.49	6 (12%)
20	CLA	B	831	7	58,68,73	1.39	6 (10%)	68,107,113	1.33	7 (10%)
21	LUT	3	315	-	42,43,43	0.31	0	51,60,60	0.38	0
23	BCR	I	4001	-	41,41,41	0.17	0	56,56,56	0.29	0

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
20	CLA	B	819	7	1/1/15/20	11/37/115/115	-
20	CLA	3	305	2	1/1/12/20	5/19/97/115	-
20	CLA	A	5035	6	1/1/15/20	15/37/115/115	-
32	SF4	C	102	8	-	-	0/6/5/5
29	LMU	8	322	-	-	6/21/61/61	0/2/2/2
20	CLA	3	309	2	1/1/11/20	8/15/93/115	-
31	PQN	B	841	-	-	5/23/43/43	0/2/2/2
21	LUT	1	615	-	3/3/12/27	8/29/67/67	0/2/2/2
20	CLA	B	837	7	-	1/25/103/115	-
31	PQN	A	5045	-	-	2/23/43/43	0/2/2/2
22	XAT	8	315	-	-	1/31/93/93	0/4/4/4
23	BCR	L	203	-	-	4/29/63/63	0/2/2/2
20	CLA	B	810	7	1/1/15/20	11/37/115/115	-
20	CLA	9	612	5	1/1/11/20	6/15/93/115	-
20	CLA	A	5040	-	1/1/14/20	7/31/109/115	-
27	LMG	7	324	-	-	10/25/45/70	0/1/1/1
20	CLA	B	829	7	1/1/15/20	16/37/115/115	-
20	CLA	K	4005	-	1/1/11/20	9/17/95/115	-
20	CLA	K	4002	-	1/1/11/20	6/13/91/115	-
20	CLA	F	303	7	1/1/15/20	12/37/115/115	-
20	CLA	A	5017	-	1/1/13/20	11/25/103/115	-
20	CLA	8	308	4	1/1/14/20	11/31/109/115	-
25	SQD	3	322	-	-	14/36/56/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	1	614	1	1/1/11/20	8/15/93/115	-
20	CLA	2	312	18	1/1/11/20	5/13/91/115	-
20	CLA	A	5014	-	-	11/37/115/115	-
20	CLA	7	314	3	1/1/12/20	5/19/97/115	-
20	CLA	9	605	5	1/1/11/20	4/13/91/115	-
23	BCR	A	5049	-	-	4/29/63/63	0/2/2/2
23	BCR	3	319	-	-	23/29/63/63	0/2/2/2
27	LMG	G	206	-	-	6/37/57/70	0/1/1/1
23	BCR	L	206	-	-	6/29/63/63	0/2/2/2
20	CLA	1	607	-	1/1/12/20	7/19/97/115	-
20	CLA	3	325	6	1/1/13/20	4/25/103/115	-
19	CHL	1	601	-	1/1/16/26	6/17/115/137	-
26	PTY	3	321	-	-	24/53/53/53	-
23	BCR	K	4006	-	-	4/29/63/63	0/2/2/2
23	BCR	A	5051	-	-	4/29/63/63	0/2/2/2
23	BCR	J	106	-	-	2/29/63/63	0/2/2/2
27	LMG	J	103	-	-	3/24/44/70	0/1/1/1
20	CLA	7	303	3	1/1/14/20	11/31/109/115	-
20	CLA	3	311	-	1/1/13/20	8/25/103/115	-
28	DGD	7	321	-	-	8/28/68/95	0/2/2/2
20	CLA	8	307	4	1/1/11/20	6/16/94/115	-
19	CHL	1	606	-	1/1/16/26	10/17/115/137	-
20	CLA	2	313	-	1/1/12/20	5/19/97/115	-
20	CLA	1	603	1	1/1/13/20	11/25/103/115	-
20	CLA	B	833	7	1/1/14/20	10/31/109/115	-
24	LHG	9	617	20	-	15/40/40/53	-
20	CLA	B	815	-	1/1/15/20	10/37/115/115	-
23	BCR	J	105	-	-	4/29/63/63	0/2/2/2
24	LHG	A	5052	-	-	12/53/53/53	-
20	CLA	B	821	-	1/1/13/20	8/25/103/115	-
20	CLA	B	840	-	1/1/15/20	9/37/115/115	-
20	CLA	3	310	2	1/1/11/20	5/15/93/115	-
20	CLA	2	309	-	1/1/11/20	2/13/91/115	-
22	XAT	9	614	-	-	0/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	5025	6	1/1/14/20	11/31/109/115	-
24	LHG	7	319	-	-	7/25/25/53	-
26	PTY	B	802	-	-	12/30/30/53	-
26	PTY	F	302	-	-	16/35/35/53	-
20	CLA	H	201	18	1/1/14/20	17/31/109/115	-
20	CLA	L	204	17	1/1/15/20	10/37/115/115	-
29	LMU	8	318	-	-	2/19/59/61	0/2/2/2
20	CLA	1	604	-	1/1/12/20	5/19/97/115	-
19	CHL	2	306	-	2/2/16/26	7/17/115/137	-
20	CLA	8	310	4	1/1/11/20	7/15/93/115	-
20	CLA	8	301	4	1/1/14/20	9/31/109/115	-
24	LHG	2	316	-	-	4/26/26/53	-
20	CLA	A	5021	6	1/1/12/20	6/19/97/115	-
20	CLA	B	825	-	1/1/15/20	9/37/115/115	-
20	CLA	7	323	4	1/1/11/20	8/16/94/115	-
23	BCR	B	847	-	-	5/29/63/63	0/2/2/2
20	CLA	A	5034	6	1/1/15/20	2/37/115/115	-
20	CLA	1	612	-	1/1/14/20	11/31/109/115	-
20	CLA	8	313	4	1/1/11/20	5/15/93/115	-
21	LUT	2	315	-	3/3/12/27	12/29/67/67	0/2/2/2
20	CLA	G	204	-	1/1/11/20	5/13/91/115	-
20	CLA	B	832	7	1/1/15/20	12/37/115/115	-
20	CLA	3	303	-	1/1/11/20	4/15/93/115	-
20	CLA	A	5019	6	1/1/13/20	9/25/103/115	-
20	CLA	7	309	3	1/1/11/20	4/15/93/115	-
20	CLA	B	818	7	1/1/15/20	15/37/115/115	-
20	CLA	A	5033	6	1/1/13/20	1/25/103/115	-
23	BCR	B	846	-	-	0/29/63/63	0/2/2/2
20	CLA	B	823	7	1/1/13/20	10/25/103/115	-
29	LMU	9	616	-	-	5/15/55/61	0/2/2/2
20	CLA	2	301	-	1/1/11/20	4/15/93/115	-
20	CLA	8	303	-	1/1/15/20	13/37/115/115	-
20	CLA	A	5007	6,20	1/1/15/20	8/37/115/115	-
20	CLA	3	314	2	1/1/11/20	5/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	7	313	3	1/1/15/20	11/37/115/115	-
20	CLA	B	812	7	1/1/13/20	4/25/103/115	-
20	CLA	B	813	7	1/1/11/20	2/15/93/115	-
21	LUT	2	314	-	3/3/12/27	4/29/67/67	0/2/2/2
20	CLA	A	5042	6	1/1/14/20	6/31/109/115	-
20	CLA	1	605	-	1/1/11/20	4/13/91/115	-
29	LMU	F	305	-	-	7/18/58/61	0/2/2/2
19	CHL	3	301	2	2/2/19/26	20/35/133/137	-
19	CHL	7	307	-	2/2/16/26	5/17/115/137	-
20	CLA	A	5008	6	1/1/15/20	11/37/115/115	-
20	CLA	9	610	5	1/1/12/20	10/19/97/115	-
20	CLA	3	324	6	1/1/13/20	10/25/103/115	-
20	CLA	F	307	-	1/1/11/20	5/16/94/115	-
23	BCR	3	318	-	-	3/29/63/63	0/2/2/2
23	BCR	A	5047	-	-	5/29/63/63	0/2/2/2
24	LHG	I	4002	-	-	6/32/32/53	-
25	SQD	7	322	-	-	4/34/54/69	0/1/1/1
20	CLA	B	811	7	1/1/15/20	7/37/115/115	-
20	CLA	A	5028	6	1/1/15/20	15/37/115/115	-
20	CLA	L	202	-	1/1/15/20	14/37/115/115	-
28	DGD	B	848	-	-	12/50/90/95	0/2/2/2
20	CLA	L	201	7	1/1/15/20	13/37/115/115	-
20	CLA	B	809	7	1/1/15/20	14/37/115/115	-
22	XAT	3	316	-	-	3/31/93/93	0/4/4/4
20	CLA	8	311	4	1/1/15/20	17/37/115/115	-
20	CLA	G	203	12	1/1/11/20	6/15/93/115	-
24	LHG	A	5055	-	-	4/35/35/53	-
20	CLA	F	306	-	1/1/14/20	10/31/109/115	-
19	CHL	2	302	18	2/2/19/26	16/33/131/137	-
20	CLA	A	5032	6	1/1/12/20	2/19/97/115	-
20	CLA	B	836	7	1/1/14/20	4/31/109/115	-
23	BCR	A	5050	-	-	3/29/63/63	0/2/2/2
24	LHG	8	319	-	-	8/42/42/53	-
20	CLA	7	304	3	1/1/13/20	2/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	J	102	-	-	8/29/63/63	0/2/2/2
19	CHL	8	306	-	2/2/17/26	8/21/119/137	-
26	PTY	F	310	-	-	13/34/34/53	-
20	CLA	7	310	3	1/1/15/20	14/37/115/115	-
20	CLA	B	824	-	1/1/15/20	10/37/115/115	-
30	CL0	A	5003	6	1/1/20/25	21/37/135/135	-
24	LHG	1	620	-	-	13/50/50/53	-
20	CLA	A	5010	-	1/1/12/20	2/21/99/115	-
20	CLA	2	308	-	1/1/11/20	3/13/91/115	-
19	CHL	3	323	-	3/3/19/26	16/33/131/137	-
19	CHL	7	306	-	1/1/16/26	2/15/113/137	-
20	CLA	A	5018	6	1/1/14/20	9/31/109/115	-
20	CLA	A	5023	6	1/1/12/20	5/19/97/115	-
23	BCR	K	4001	-	-	4/29/63/63	0/2/2/2
26	PTY	F	301	-	-	14/32/32/53	-
20	CLA	A	5020	6	1/1/15/20	13/37/115/115	-
20	CLA	8	309	24	1/1/14/20	10/31/109/115	-
20	CLA	A	5027	-	1/1/13/20	8/27/105/115	-
20	CLA	A	5039	6	1/1/13/20	3/25/103/115	-
20	CLA	2	304	-	1/1/12/20	8/19/97/115	-
20	CLA	B	830	7	1/1/15/20	14/37/115/115	-
20	CLA	1	602	1	1/1/13/20	11/25/103/115	-
24	LHG	1	618	20	-	5/30/30/53	-
24	LHG	8	320	-	-	6/47/47/53	-
25	SQD	3	320	-	-	4/30/50/69	0/1/1/1
20	CLA	8	312	4	1/1/11/20	7/15/93/115	-
20	CLA	B	827	-	1/1/15/20	10/37/115/115	-
20	CLA	8	321	-	-	9/15/93/115	-
23	BCR	F	304	-	-	0/29/63/63	0/2/2/2
20	CLA	9	602	5	1/1/14/20	10/31/109/115	-
25	SQD	1	619	-	-	14/33/53/69	0/1/1/1
20	CLA	A	5016	6	1/1/15/20	15/37/115/115	-
20	CLA	B	820	-	1/1/15/20	11/37/115/115	-
20	CLA	A	5005	-	1/1/15/20	6/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CHL	8	305	-	1/1/16/26	4/17/115/137	-
20	CLA	G	201	7	1/1/15/20	13/37/115/115	-
20	CLA	2	303	18	1/1/12/20	4/19/97/115	-
20	CLA	J	104	15	1/1/11/20	4/18/96/115	-
20	CLA	9	611	-	1/1/13/20	5/25/103/115	-
24	LHG	7	320	20	-	9/38/38/53	-
20	CLA	2	305	-	1/1/11/20	6/13/91/115	-
32	SF4	A	5046	7,6	-	-	0/6/5/5
20	CLA	7	312	3	1/1/12/20	5/22/100/115	-
20	CLA	A	5041	6	1/1/15/20	6/37/115/115	-
20	CLA	A	5038	6	1/1/12/20	5/19/97/115	-
23	BCR	B	845	-	-	2/27/61/63	0/2/2/2
20	CLA	B	839	7	1/1/15/20	8/37/115/115	-
20	CLA	B	805	-	1/1/15/20	14/37/115/115	-
23	BCR	7	318	-	-	2/29/63/63	0/2/2/2
23	BCR	B	844	-	-	10/29/63/63	0/2/2/2
20	CLA	K	4003	-	1/1/13/20	11/25/103/115	-
20	CLA	L	205	-	1/1/12/20	6/19/97/115	-
21	LUT	9	613	-	3/3/12/27	2/29/67/67	0/2/2/2
26	PTY	7	302	-	-	8/14/14/53	-
20	CLA	7	305	-	1/1/12/20	4/19/97/115	-
23	BCR	F	309	-	-	4/29/63/63	0/2/2/2
20	CLA	B	816	-	1/1/13/20	9/25/103/115	-
20	CLA	B	828	-	1/1/15/20	16/37/115/115	-
29	LMU	7	325	-	-	4/18/58/61	0/2/2/2
20	CLA	B	834	-	1/1/12/20	11/19/97/115	-
24	LHG	A	5054	20	-	9/32/32/53	-
20	CLA	9	601	5	1/1/11/20	9/15/93/115	-
23	BCR	B	803	-	-	3/29/63/63	0/2/2/2
22	XAT	1	616	-	-	2/31/93/93	0/4/4/4
22	XAT	9	615	-	-	5/31/93/93	0/4/4/4
20	CLA	A	5036	6	1/1/15/20	6/37/115/115	-
21	LUT	7	316	-	3/3/12/27	2/29/67/67	0/2/2/2
20	CLA	B	838	-	1/1/13/20	5/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	SQD	F	311	-	-	6/34/54/69	0/1/1/1
20	CLA	8	302	4	1/1/15/20	11/37/115/115	-
20	CLA	1	611	1	1/1/11/20	6/15/93/115	-
27	LMG	A	5001	-	-	6/26/46/70	0/1/1/1
20	CLA	3	312	2	1/1/11/20	7/15/93/115	-
20	CLA	9	604	5	1/1/12/20	4/19/97/115	-
20	CLA	1	610	24	1/1/11/20	7/15/93/115	-
29	LMU	A	5053	-	-	3/21/61/61	0/2/2/2
20	CLA	9	603	-	1/1/13/20	10/25/103/115	-
20	CLA	1	613	1	1/1/12/20	6/19/97/115	-
20	CLA	B	817	-	1/1/14/20	7/31/109/115	-
20	CLA	1	609	1	1/1/13/20	6/25/103/115	-
21	LUT	8	314	-	3/3/12/27	2/29/67/67	0/2/2/2
20	CLA	A	5043	24	1/1/11/20	5/17/95/115	-
24	LHG	B	801	-	-	8/36/36/53	-
23	BCR	A	5048	-	-	0/29/63/63	0/2/2/2
20	CLA	9	608	5	1/1/12/20	6/19/97/115	-
20	CLA	A	5012	6	1/1/15/20	10/37/115/115	-
24	LHG	8	317	20	-	5/33/33/53	-
19	CHL	7	308	-	2/2/16/26	6/18/116/137	-
20	CLA	A	5029	6	1/1/15/20	16/37/115/115	-
20	CLA	A	5006	6	1/1/15/20	14/37/115/115	-
19	CHL	8	304	4	1/1/16/26	7/17/115/137	-
23	BCR	G	205	-	-	6/29/63/63	0/2/2/2
23	BCR	B	843	-	-	0/29/63/63	0/2/2/2
20	CLA	B	814	7	1/1/15/20	15/37/115/115	-
20	CLA	K	4004	16	1/1/11/20	6/13/91/115	-
22	XAT	7	317	-	-	3/31/93/93	0/4/4/4
20	CLA	A	5013	6,20	1/1/15/20	11/37/115/115	-
23	BCR	1	617	-	-	0/29/63/63	0/2/2/2
25	SQD	B	850	-	-	10/25/45/69	0/1/1/1
20	CLA	B	826	7	1/1/15/20	9/37/115/115	-
20	CLA	3	302	2	1/1/15/20	10/37/115/115	-
24	LHG	A	5002	-	-	10/40/40/53	-
20	CLA	3	308	2	1/1/13/20	8/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	5009	6	1/1/15/20	14/37/115/115	-
24	LHG	B	849	-	-	8/34/34/53	-
20	CLA	A	5011	6	1/1/15/20	11/37/115/115	-
20	CLA	A	5031	6	1/1/15/20	7/37/115/115	-
23	BCR	3	317	-	-	4/29/63/63	0/2/2/2
20	CLA	G	202	12	1/1/11/20	5/16/94/115	-
27	LMG	7	301	-	-	10/45/65/70	0/1/1/1
20	CLA	3	313	-	1/1/10/20	0/10/88/115	-
20	CLA	3	304	-	1/1/11/20	6/15/93/115	-
33	LMK	J	101	-	-	5/41/41/60	-
23	BCR	8	316	-	-	2/29/63/63	0/2/2/2
32	SF4	C	101	8	-	-	0/6/5/5
20	CLA	A	5030	-	1/1/15/20	12/37/115/115	-
20	CLA	2	307	18	1/1/11/20	9/15/93/115	-
20	CLA	7	315	3	1/1/11/20	4/13/91/115	-
20	CLA	2	310	18	1/1/11/20	8/15/93/115	-
20	CLA	9	609	24	1/1/11/20	8/15/93/115	-
20	CLA	7	311	24	1/1/14/20	8/31/109/115	-
20	CLA	3	306	-	1/1/12/20	6/21/99/115	-
20	CLA	9	607	5	1/1/14/20	13/31/109/115	-
20	CLA	A	5004	-	1/1/15/20	13/37/115/115	-
23	BCR	B	842	-	-	2/29/63/63	0/2/2/2
20	CLA	B	835	7	1/1/12/20	5/21/99/115	-
20	CLA	A	5024	6	1/1/14/20	14/31/109/115	-
20	CLA	A	5037	6	1/1/12/20	7/19/97/115	-
20	CLA	B	807	-	1/1/15/20	12/37/115/115	-
20	CLA	A	5022	-	1/1/15/20	6/37/115/115	-
20	CLA	2	311	-	1/1/12/20	8/19/97/115	-
20	CLA	B	808	7	1/1/15/20	11/37/115/115	-
20	CLA	B	804	7	1/1/15/20	17/37/115/115	-
20	CLA	1	608	1	1/1/11/20	6/15/93/115	-
19	CHL	9	606	-	2/2/16/26	11/17/115/137	-
20	CLA	A	5044	-	1/1/15/20	10/37/115/115	-
20	CLA	B	806	7	1/1/11/20	9/17/95/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	5015	-	1/1/13/20	8/25/103/115	-
20	CLA	3	307	2	1/1/15/20	13/37/115/115	-
20	CLA	A	5026	-	1/1/15/20	10/37/115/115	-
20	CLA	B	822	7	1/1/15/20	13/37/115/115	-
20	CLA	F	308	11	1/1/11/20	3/13/91/115	-
20	CLA	B	831	7	1/1/14/20	8/31/109/115	-
21	LUT	3	315	-	3/3/12/27	2/29/67/67	0/2/2/2
23	BCR	I	4001	-	-	4/29/63/63	0/2/2/2

The worst 5 of 1012 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	808	CLA	MG-NA	11.87	2.34	2.06
19	8	304	CHL	MG-NC	11.84	2.34	2.06
19	1	606	CHL	MG-NA	8.23	2.25	2.06
20	G	204	CLA	CHB-C4A	7.79	1.40	1.33
19	8	306	CHL	MG-NA	7.43	2.23	2.06

The worst 5 of 1380 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	8	304	CHL	C4A-NA-C1A	15.46	113.73	106.68
19	7	307	CHL	C4A-NA-C1A	14.62	113.35	106.68
19	3	323	CHL	C4A-NA-C1A	14.54	113.31	106.68
19	8	305	CHL	C4A-NA-C1A	14.54	113.31	106.68
30	A	5003	CL0	C4A-NA-C1A	12.73	112.49	106.68

5 of 208 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	1	601	CHL	ND
19	1	606	CHL	ND
19	3	301	CHL	C8
19	3	301	CHL	NC
19	3	323	CHL	C8

5 of 2063 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	1	601	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	1	601	CHL	CHA-CBD-CGD-O1D
19	1	601	CHL	CHA-CBD-CGD-O2D
19	1	601	CHL	CBD-CGD-O2D-CED
19	1	606	CHL	C1C-C2C-CMC-OMC

There are no ring outliers.

229 monomers are involved in 645 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	819	CLA	6	0
20	3	305	CLA	4	0
20	A	5035	CLA	6	0
32	C	102	SF4	1	0
29	8	322	LMU	4	0
31	B	841	PQN	8	0
20	B	837	CLA	1	0
21	1	615	LUT	7	0
31	A	5045	PQN	3	0
22	8	315	XAT	1	0
23	L	203	BCR	2	0
20	B	810	CLA	6	0
20	A	5040	CLA	5	0
27	7	324	LMG	2	0
20	B	829	CLA	5	0
20	K	4005	CLA	4	0
20	K	4002	CLA	2	0
20	F	303	CLA	3	0
20	A	5017	CLA	2	0
20	8	308	CLA	3	0
25	3	322	SQD	2	0
20	1	614	CLA	1	0
20	A	5014	CLA	4	0
20	7	314	CLA	2	0
23	A	5049	BCR	5	0
23	3	319	BCR	10	0
27	G	206	LMG	6	0
23	L	206	BCR	3	0
20	1	607	CLA	3	0
20	3	325	CLA	2	0
19	1	601	CHL	4	0
26	3	321	PTY	1	0
23	K	4006	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	5051	BCR	4	0
23	J	106	BCR	3	0
20	7	303	CLA	5	0
20	3	311	CLA	4	0
20	8	307	CLA	3	0
19	1	606	CHL	3	0
20	2	313	CLA	1	0
20	1	603	CLA	1	0
20	B	833	CLA	2	0
20	B	815	CLA	3	0
23	J	105	BCR	3	0
24	A	5052	LHG	2	0
20	B	821	CLA	2	0
20	B	840	CLA	4	0
22	9	614	XAT	1	0
20	A	5025	CLA	5	0
24	7	319	LHG	1	0
26	F	302	PTY	1	0
20	H	201	CLA	2	0
20	L	204	CLA	4	0
29	8	318	LMU	1	0
20	1	604	CLA	1	0
19	2	306	CHL	5	0
20	8	310	CLA	2	0
20	8	301	CLA	6	0
24	2	316	LHG	1	0
20	A	5021	CLA	3	0
20	B	825	CLA	5	0
20	7	323	CLA	2	0
23	B	847	BCR	4	0
20	A	5034	CLA	1	0
20	1	612	CLA	5	0
21	2	315	LUT	2	0
20	G	204	CLA	5	0
20	B	832	CLA	8	0
20	A	5019	CLA	2	0
20	B	818	CLA	1	0
20	A	5033	CLA	5	0
23	B	846	BCR	3	0
20	B	823	CLA	3	0
20	2	301	CLA	1	0
20	8	303	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	5007	CLA	2	0
20	3	314	CLA	2	0
20	7	313	CLA	5	0
20	B	812	CLA	3	0
20	A	5042	CLA	6	0
20	1	605	CLA	7	0
19	3	301	CHL	13	0
19	7	307	CHL	7	0
20	A	5008	CLA	1	0
20	3	324	CLA	2	0
20	F	307	CLA	6	0
23	3	318	BCR	7	0
23	A	5047	BCR	5	0
24	I	4002	LHG	2	0
25	7	322	SQD	1	0
20	B	811	CLA	4	0
20	A	5028	CLA	4	0
20	L	202	CLA	2	0
28	B	848	DGD	9	0
20	L	201	CLA	4	0
20	B	809	CLA	4	0
22	3	316	XAT	7	0
20	8	311	CLA	1	0
20	G	203	CLA	8	0
24	A	5055	LHG	2	0
20	F	306	CLA	2	0
19	2	302	CHL	5	0
20	A	5032	CLA	3	0
20	B	836	CLA	5	0
23	A	5050	BCR	4	0
24	8	319	LHG	2	0
20	7	304	CLA	1	0
23	J	102	BCR	9	0
19	8	306	CHL	5	0
20	7	310	CLA	3	0
20	B	824	CLA	5	0
30	A	5003	CL0	10	0
24	1	620	LHG	3	0
20	A	5010	CLA	4	0
20	2	308	CLA	5	0
19	3	323	CHL	9	0
19	7	306	CHL	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	5018	CLA	5	0
20	A	5023	CLA	3	0
23	K	4001	BCR	3	0
26	F	301	PTY	2	0
20	A	5020	CLA	6	0
20	8	309	CLA	4	0
20	A	5027	CLA	2	0
20	B	830	CLA	2	0
20	1	602	CLA	1	0
24	1	618	LHG	3	0
25	3	320	SQD	1	0
20	8	312	CLA	1	0
20	8	321	CLA	2	0
20	B	827	CLA	6	0
23	F	304	BCR	4	0
20	9	602	CLA	2	0
25	1	619	SQD	2	0
20	A	5016	CLA	7	0
20	B	820	CLA	4	0
20	A	5005	CLA	13	0
19	8	305	CHL	7	0
20	G	201	CLA	4	0
20	2	303	CLA	3	0
20	J	104	CLA	2	0
20	9	611	CLA	3	0
24	7	320	LHG	5	0
20	2	305	CLA	1	0
32	A	5046	SF4	1	0
20	7	312	CLA	1	0
20	A	5041	CLA	7	0
23	B	845	BCR	2	0
20	B	839	CLA	9	0
20	B	805	CLA	12	0
23	7	318	BCR	3	0
23	B	844	BCR	5	0
20	L	205	CLA	1	0
21	9	613	LUT	2	0
26	7	302	PTY	1	0
20	7	305	CLA	2	0
23	F	309	BCR	6	0
20	B	816	CLA	3	0
20	B	828	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	834	CLA	2	0
24	A	5054	LHG	2	0
23	B	803	BCR	4	0
22	9	615	XAT	1	0
20	A	5036	CLA	3	0
21	7	316	LUT	2	0
20	B	838	CLA	2	0
25	F	311	SQD	3	0
20	8	302	CLA	2	0
20	1	611	CLA	3	0
27	A	5001	LMG	2	0
20	9	604	CLA	1	0
20	1	610	CLA	3	0
29	A	5053	LMU	2	0
20	9	603	CLA	4	0
20	B	817	CLA	2	0
20	1	609	CLA	2	0
21	8	314	LUT	4	0
20	A	5043	CLA	3	0
23	A	5048	BCR	4	0
20	9	608	CLA	1	0
20	A	5012	CLA	5	0
24	8	317	LHG	1	0
19	7	308	CHL	3	0
20	A	5029	CLA	8	0
20	A	5006	CLA	3	0
19	8	304	CHL	9	0
23	G	205	BCR	1	0
23	B	843	BCR	4	0
20	B	814	CLA	8	0
20	K	4004	CLA	3	0
22	7	317	XAT	4	0
20	A	5013	CLA	3	0
23	1	617	BCR	5	0
20	B	826	CLA	8	0
20	3	302	CLA	6	0
24	A	5002	LHG	2	0
20	3	308	CLA	1	0
20	A	5009	CLA	1	0
24	B	849	LHG	1	0
20	A	5011	CLA	6	0
20	A	5031	CLA	3	0

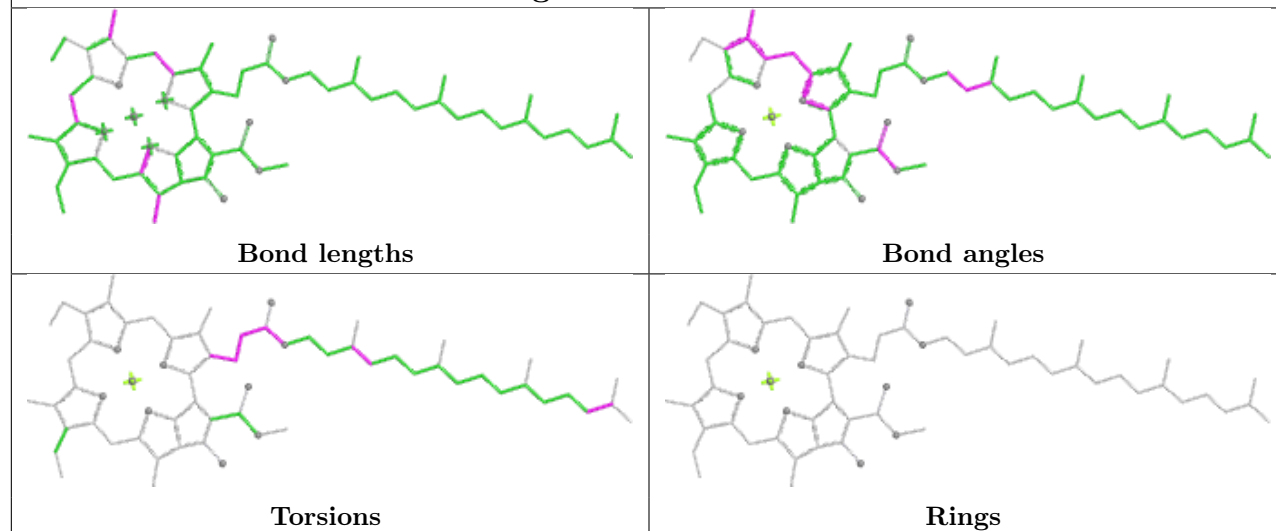
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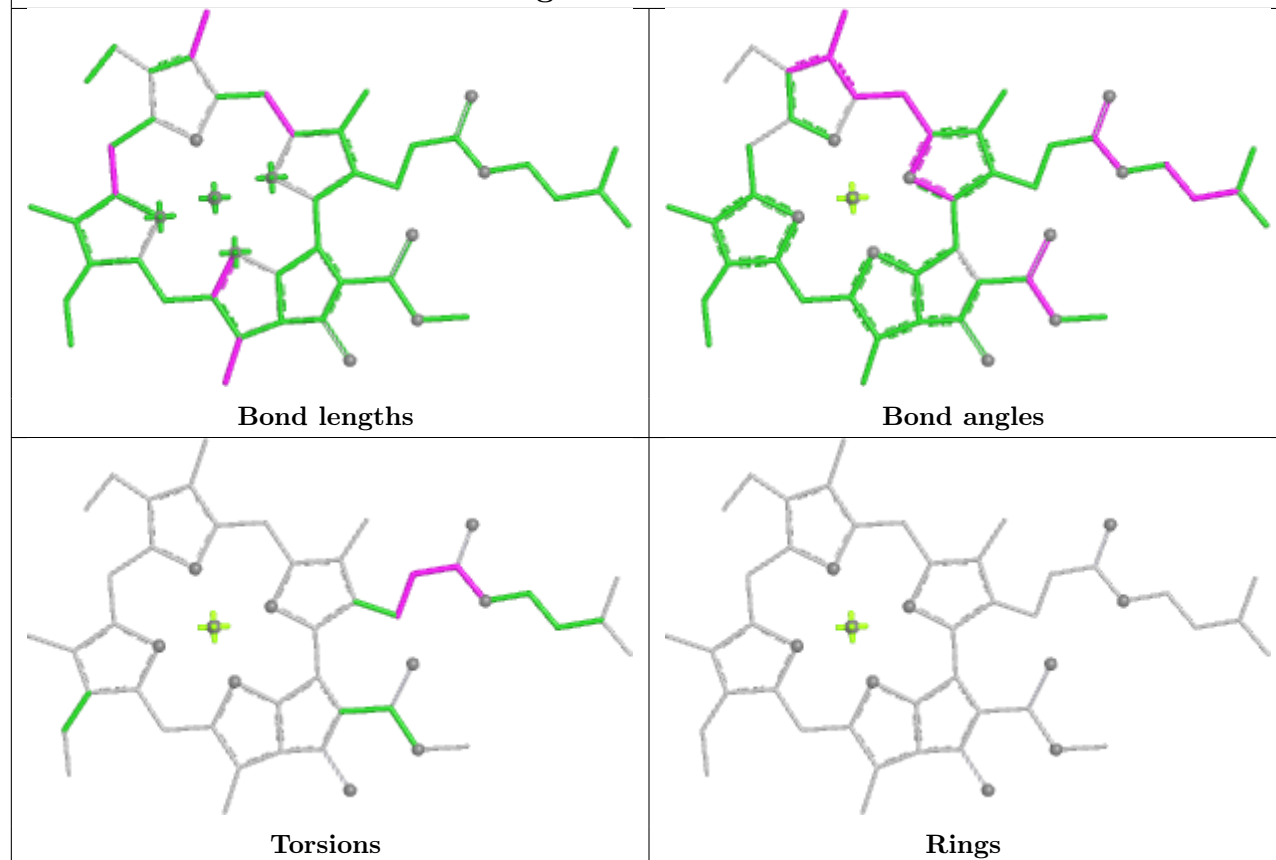
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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27	7	301	LMG	5	0
20	3	313	CLA	2	0
20	3	304	CLA	1	0
23	8	316	BCR	10	0
20	A	5030	CLA	4	0
20	2	307	CLA	1	0
20	7	311	CLA	1	0
20	3	306	CLA	5	0
20	9	607	CLA	19	0
20	A	5004	CLA	7	0
23	B	842	BCR	1	0
20	B	835	CLA	1	0
20	B	807	CLA	8	0
20	A	5022	CLA	1	0
20	2	311	CLA	8	0
20	B	808	CLA	5	0
20	B	804	CLA	5	0
20	1	608	CLA	4	0
19	9	606	CHL	2	0
20	A	5044	CLA	7	0
20	B	806	CLA	2	0
20	3	307	CLA	8	0
20	A	5026	CLA	4	0
20	B	822	CLA	4	0
20	B	831	CLA	6	0
21	3	315	LUT	2	0
23	I	4001	BCR	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.

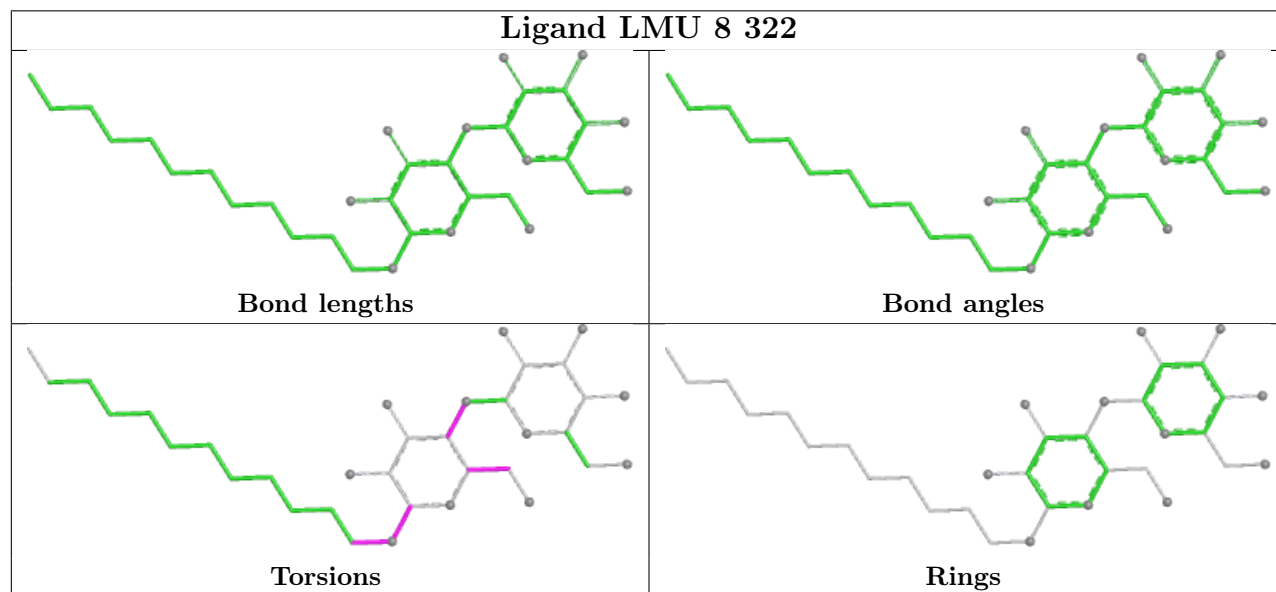
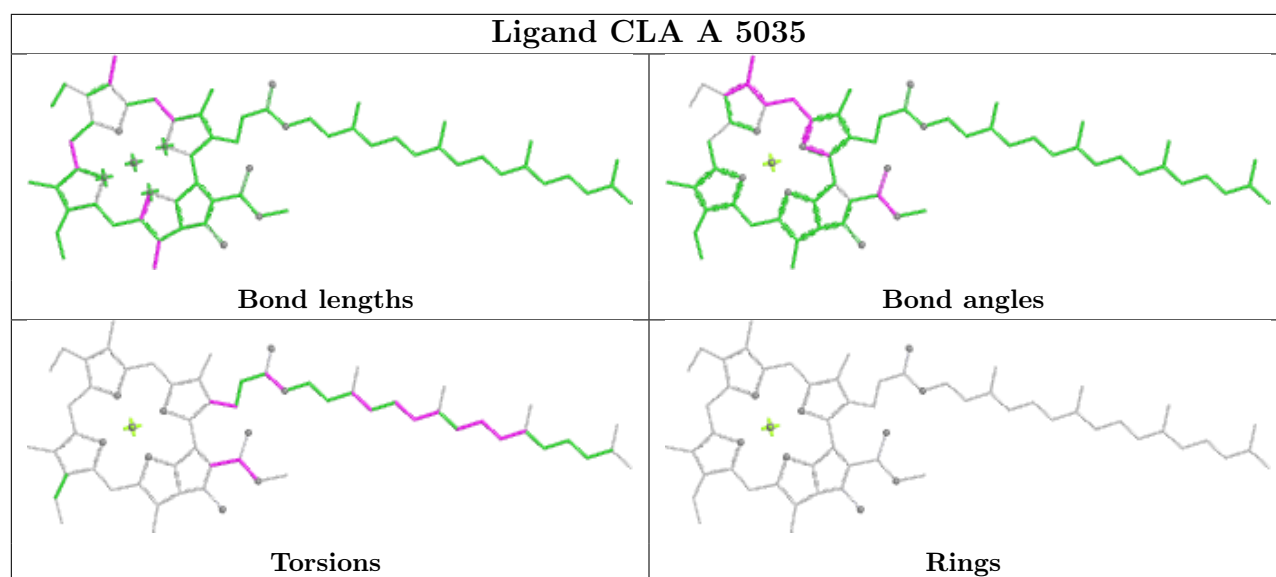
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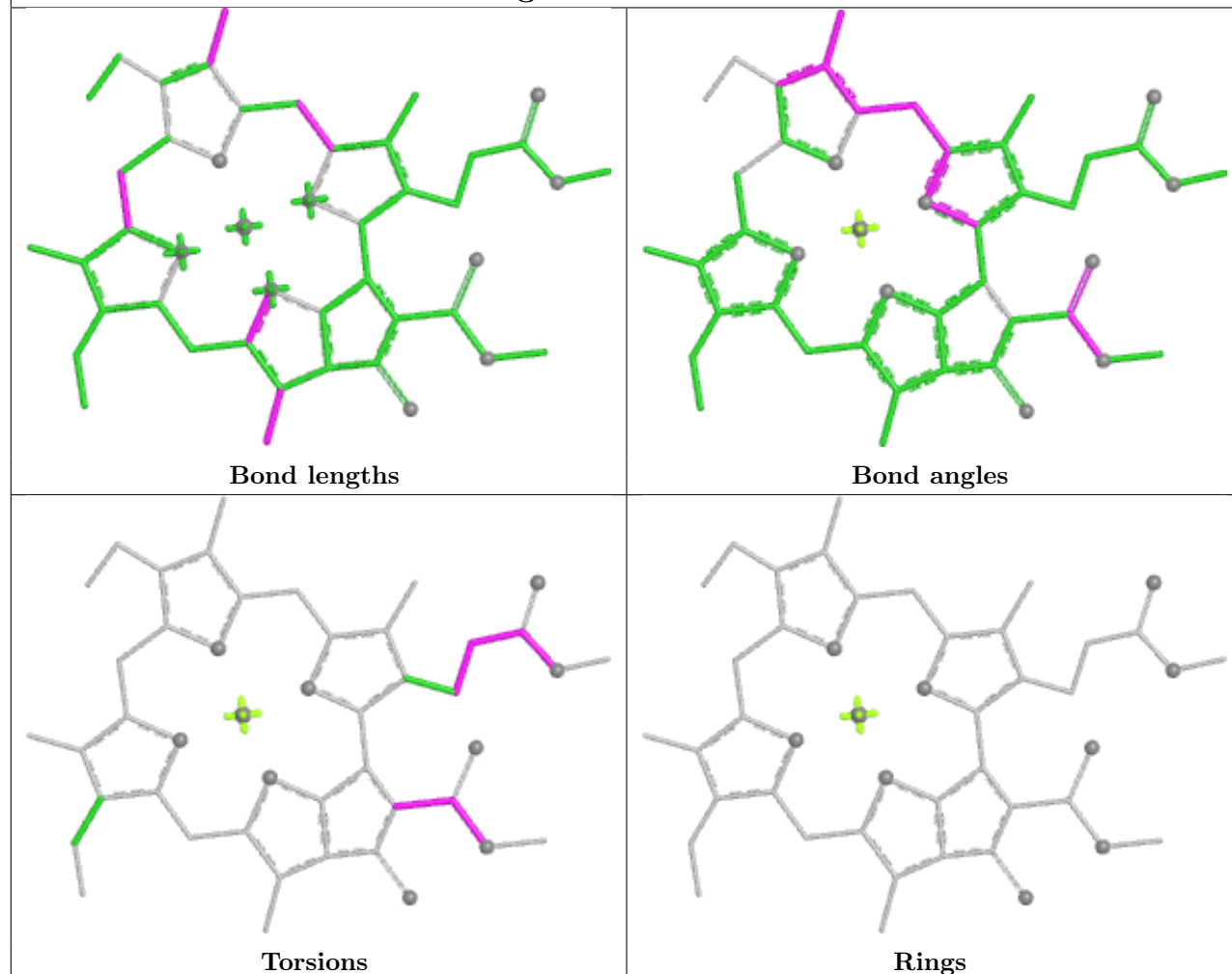
## Ligand CLA 3 305



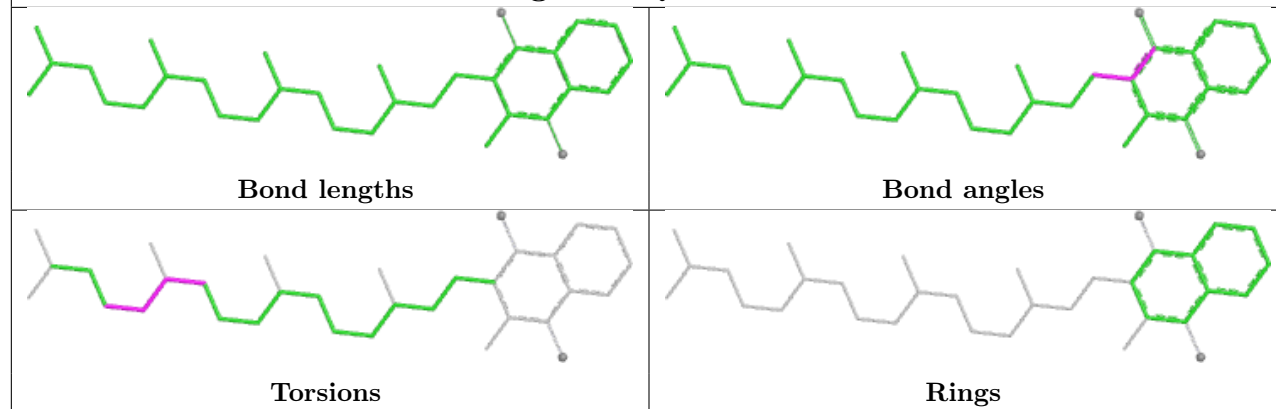


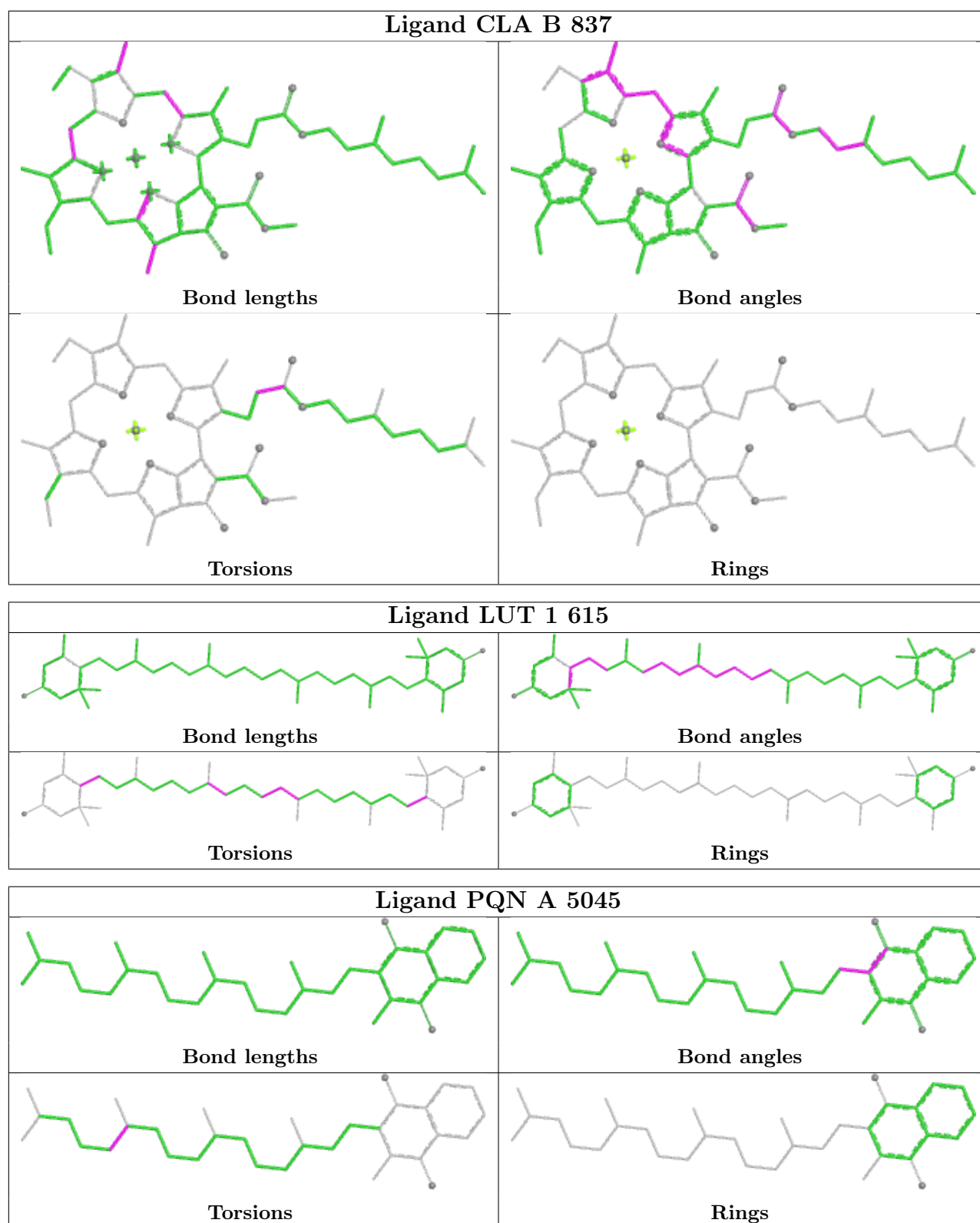


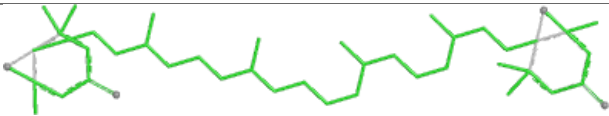
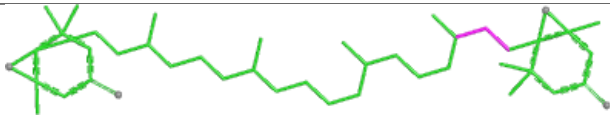
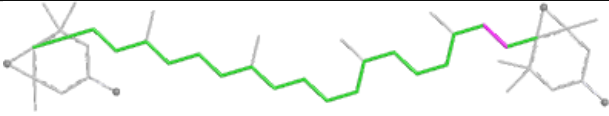
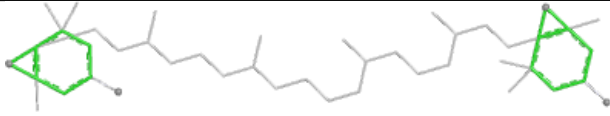
## Ligand CLA 3 309

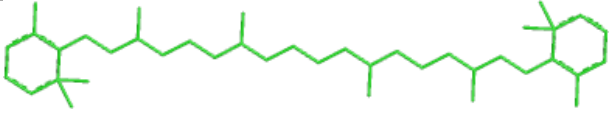
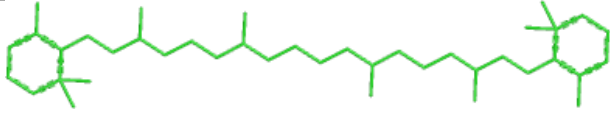
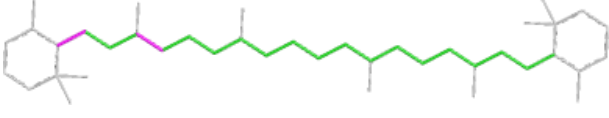
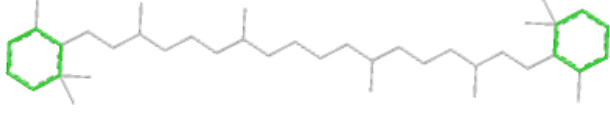


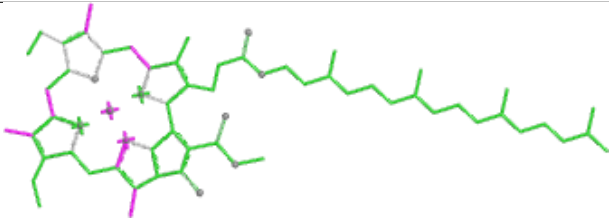
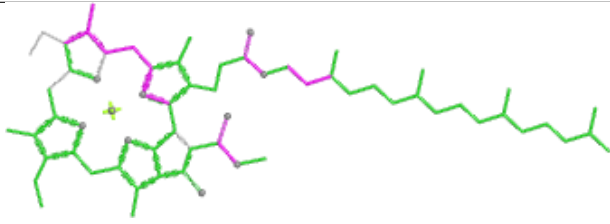
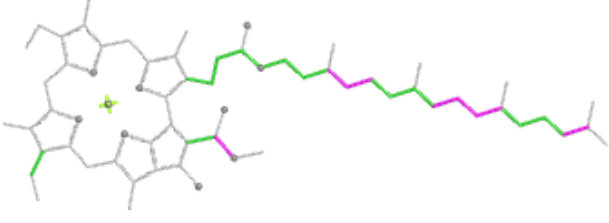
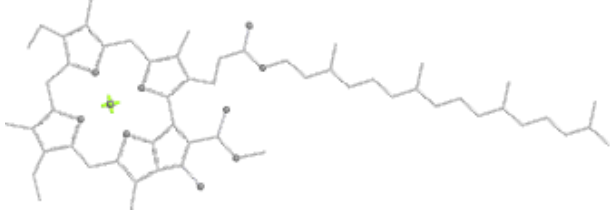
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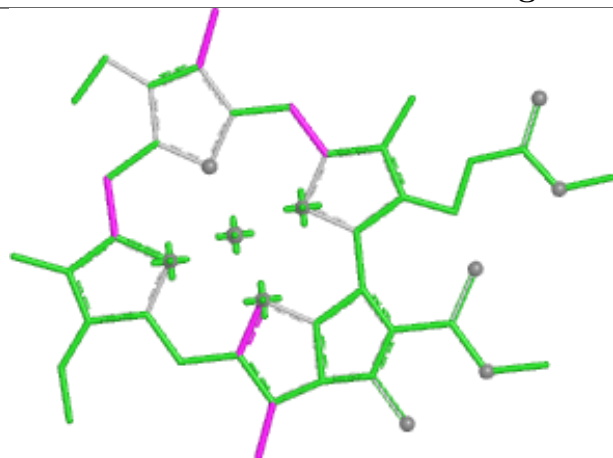


Ligand XAT 8 315	
	
Bond lengths	Bond angles
	
Torsions	Rings

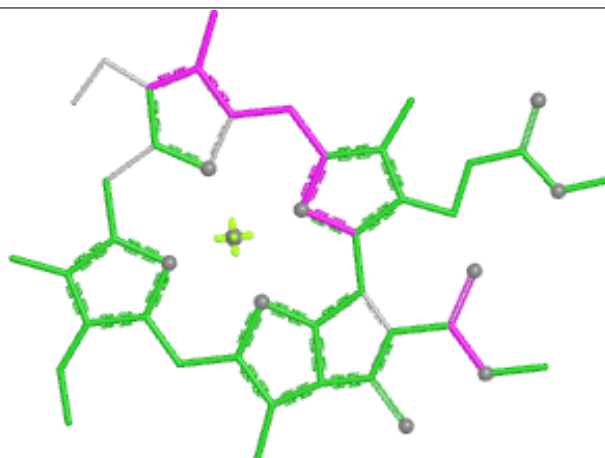
Ligand BCR L 203	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 810	
	
Bond lengths	Bond angles
	
Torsions	Rings

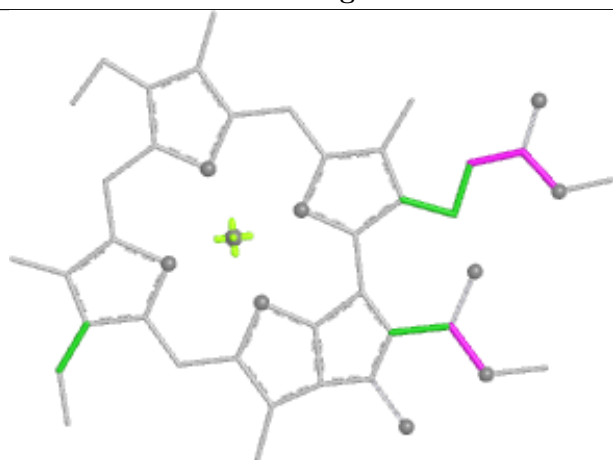
## Ligand CLA 9 612



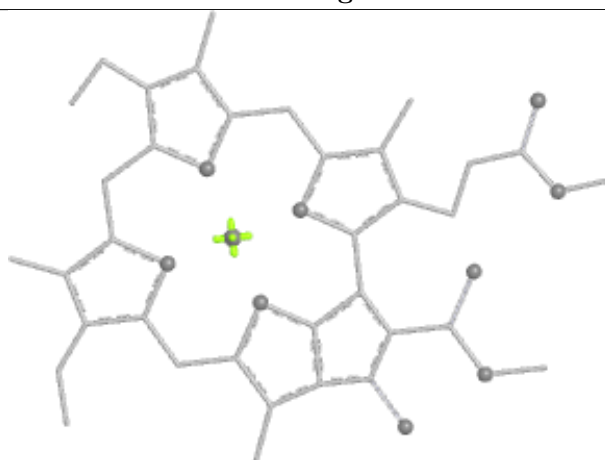
Bond lengths



Bond angles

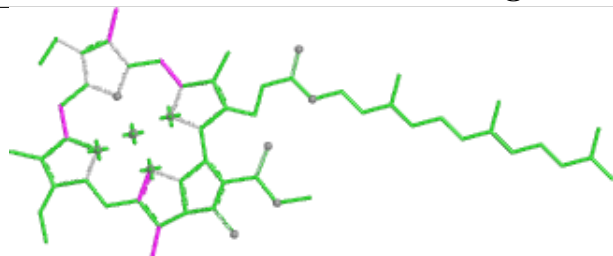


Torsions

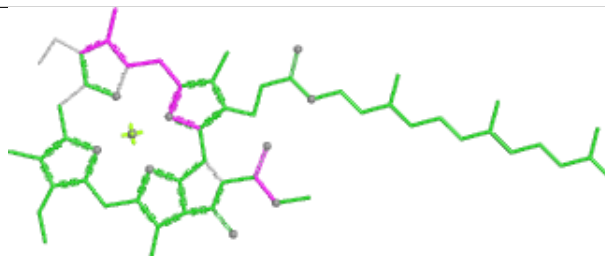


Rings

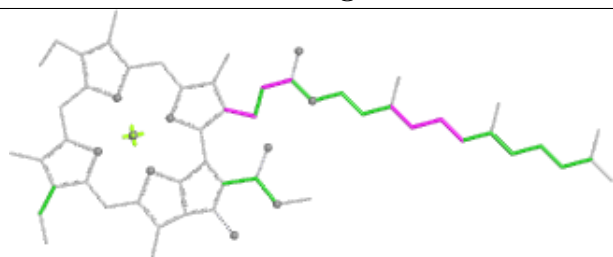
## Ligand CLA A 5040



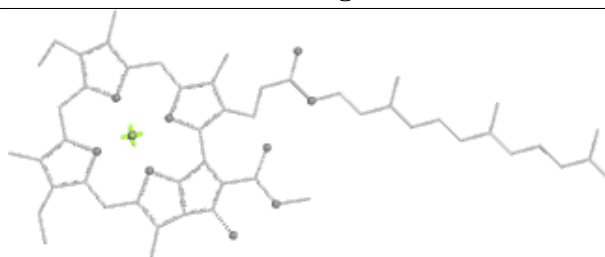
Bond lengths



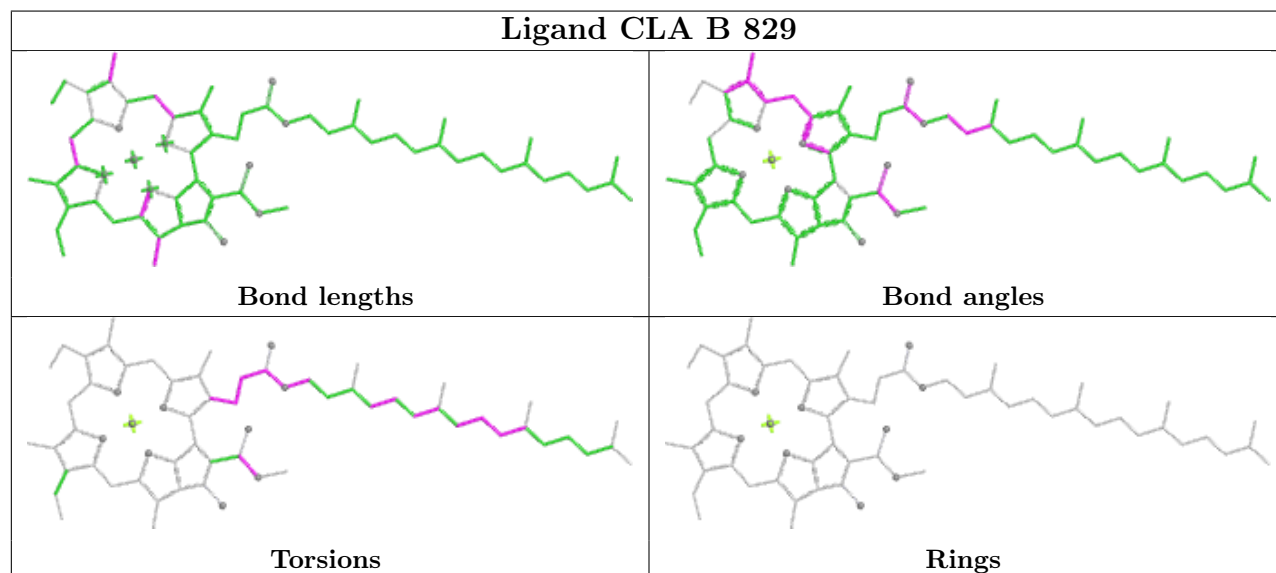
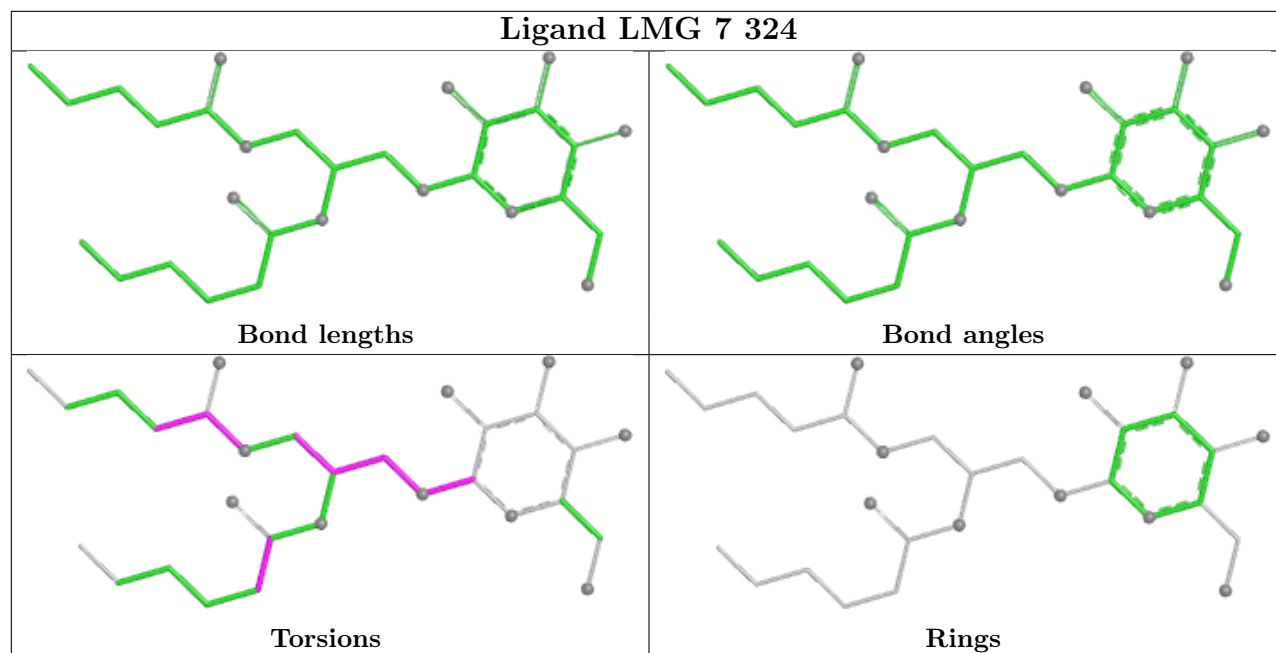
Bond angles

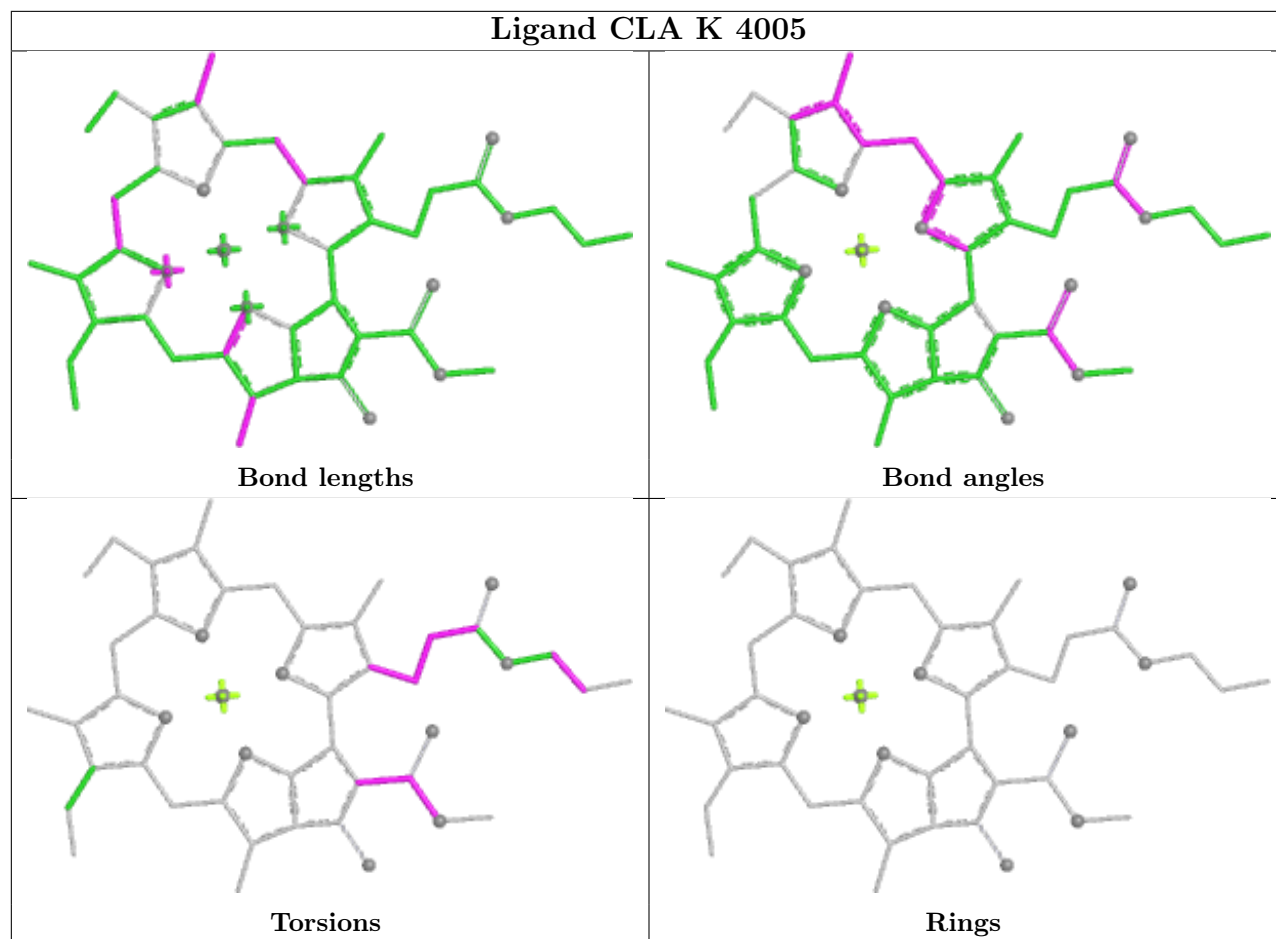


Torsions

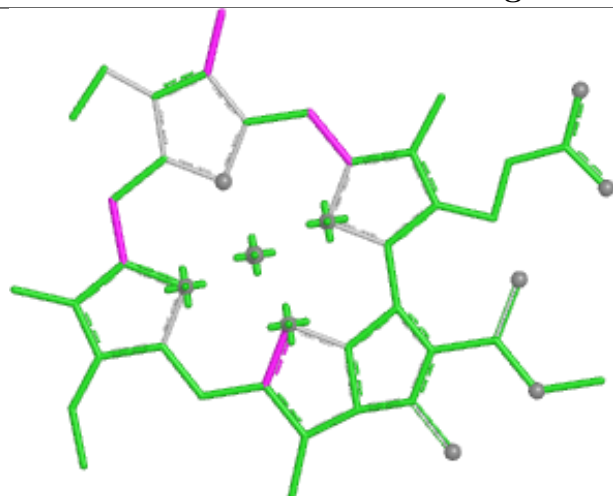


Rings

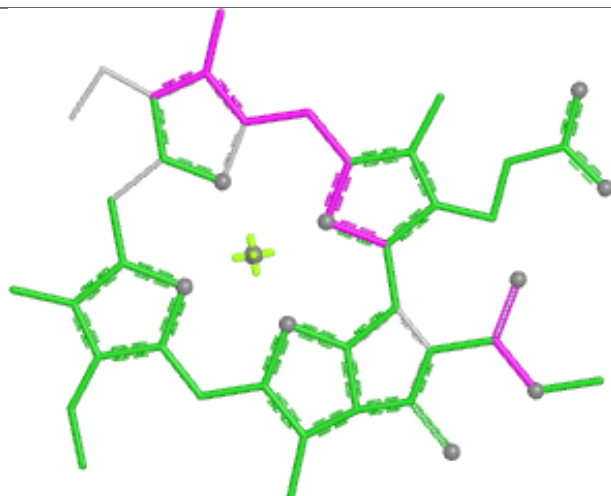




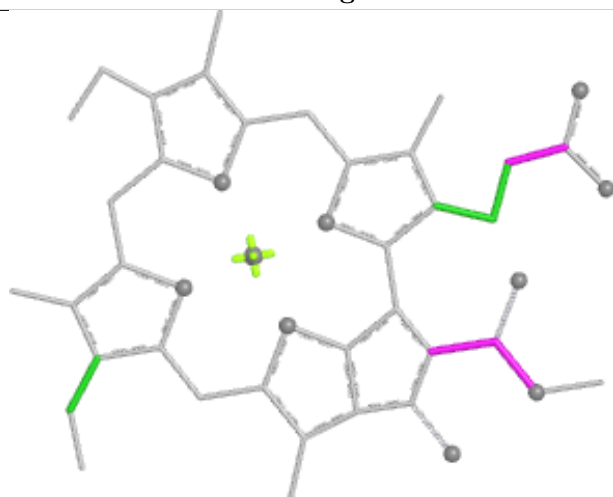
## Ligand CLA K 4002



Bond lengths



Bond angles

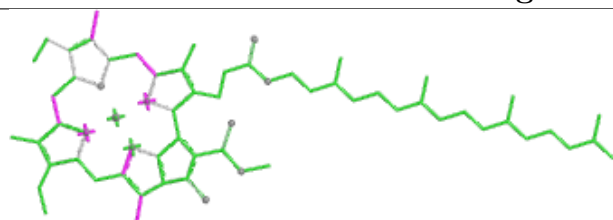


Torsions

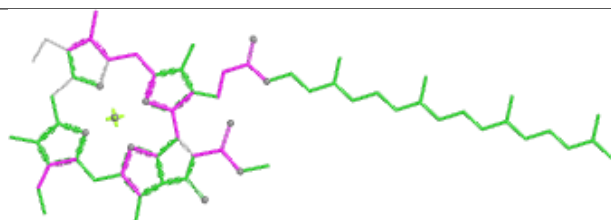


Rings

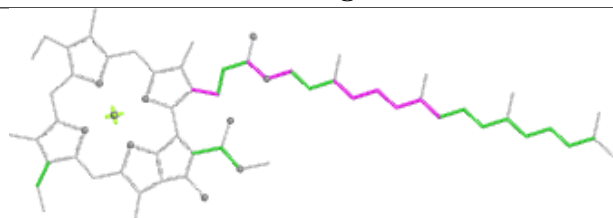
## Ligand CLA F 303



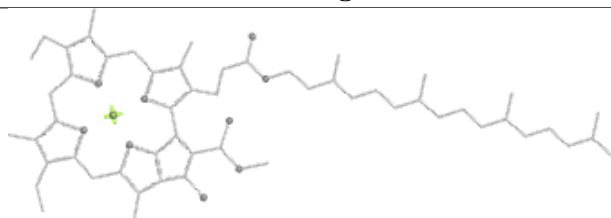
Bond lengths



Bond angles



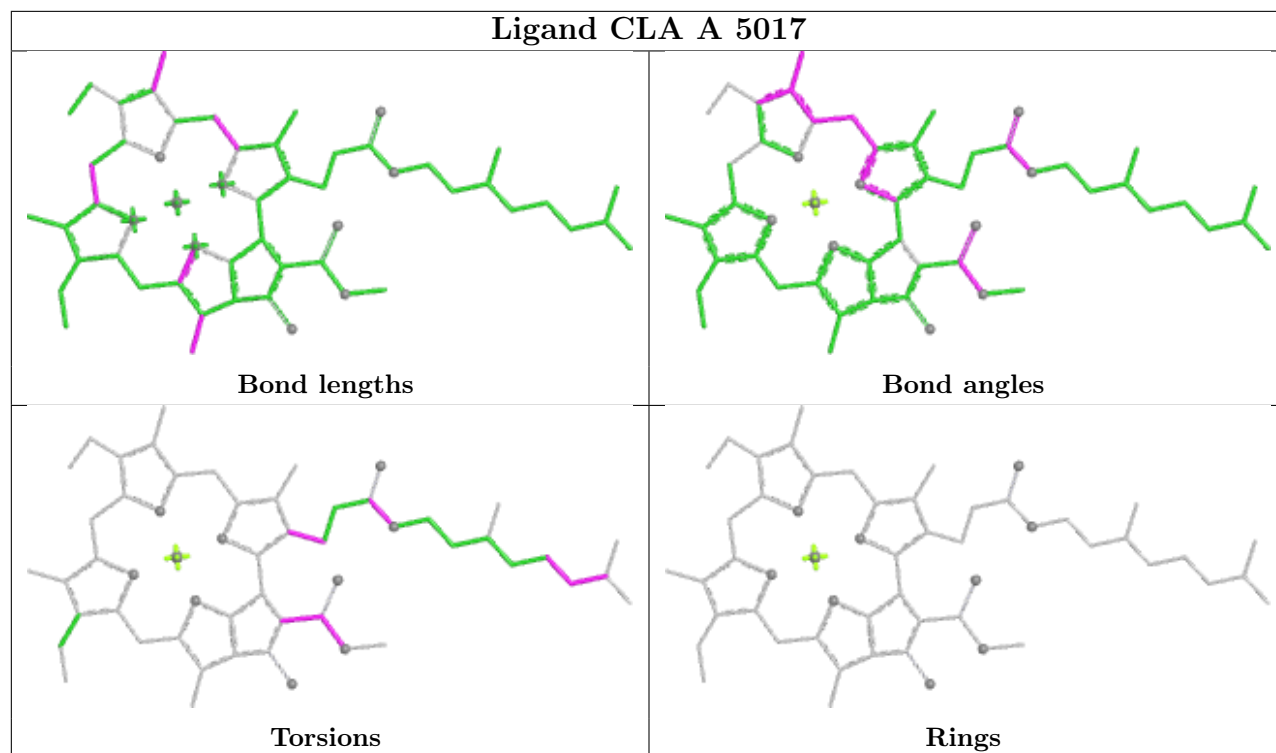
Torsions



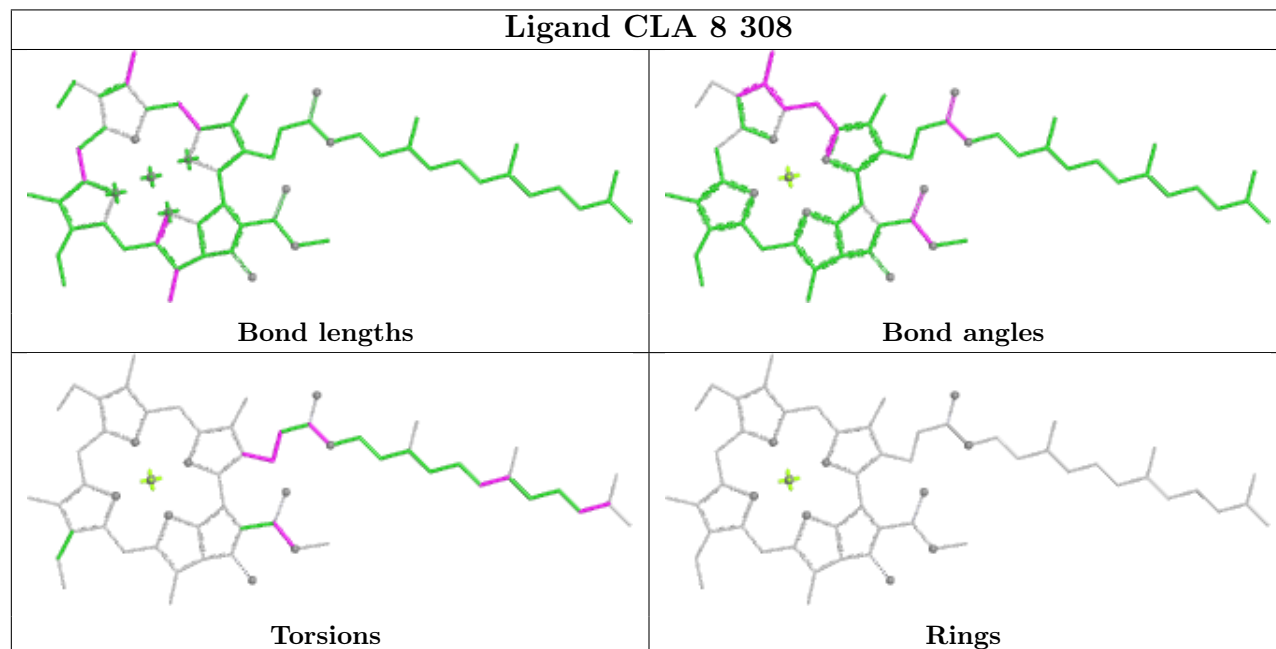
Rings

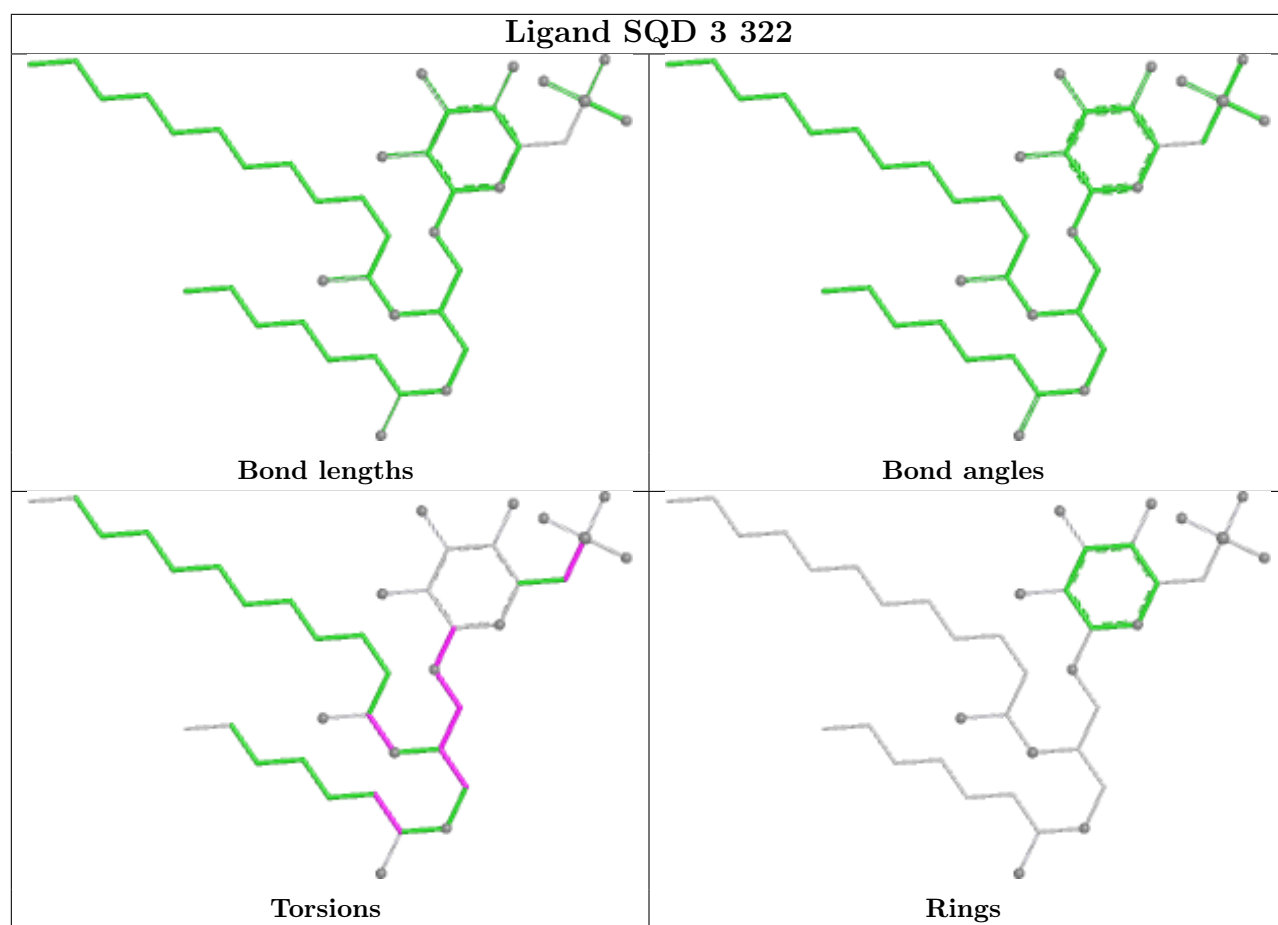


## Ligand CLA A 5017

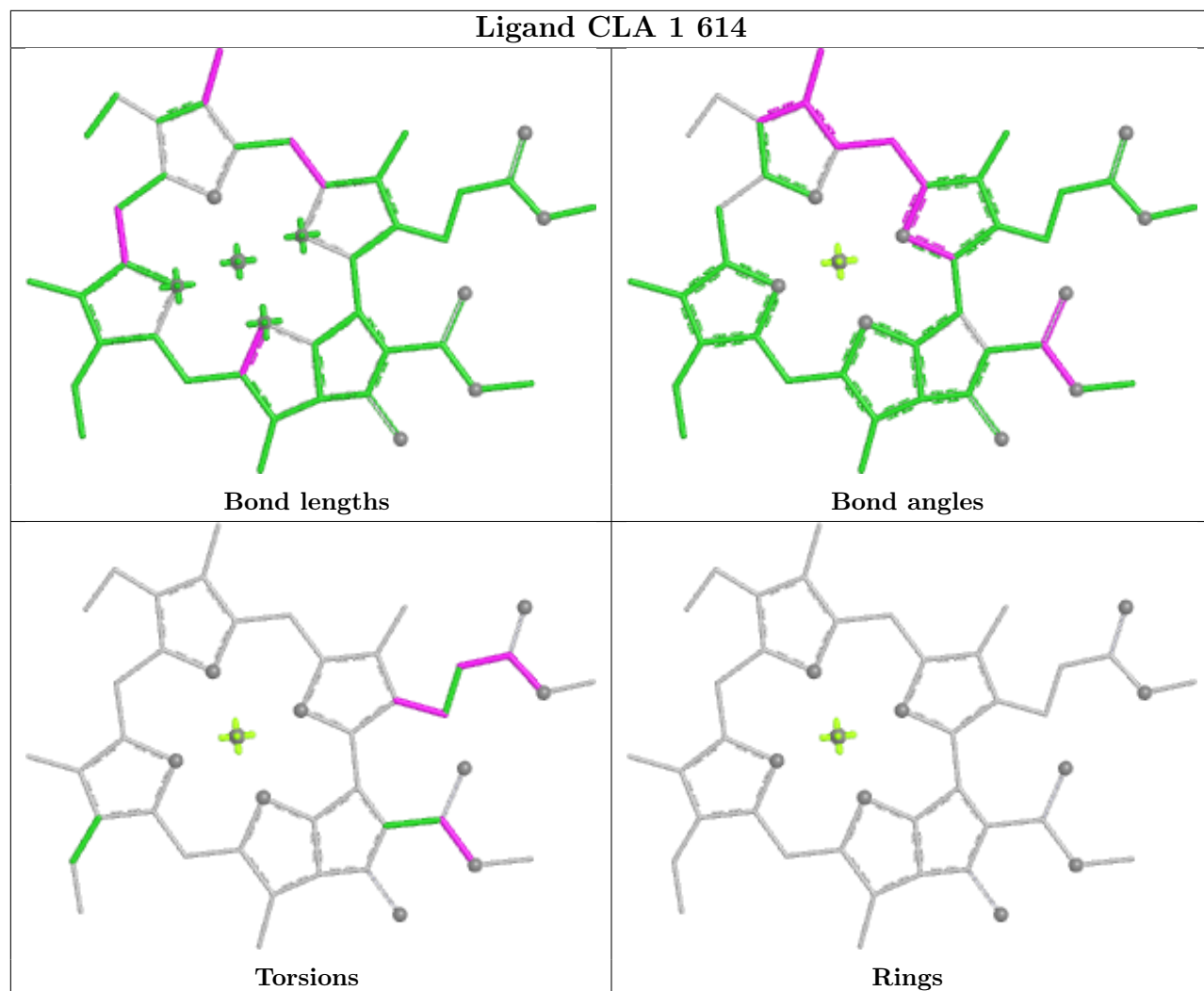


## Ligand CLA 8 308

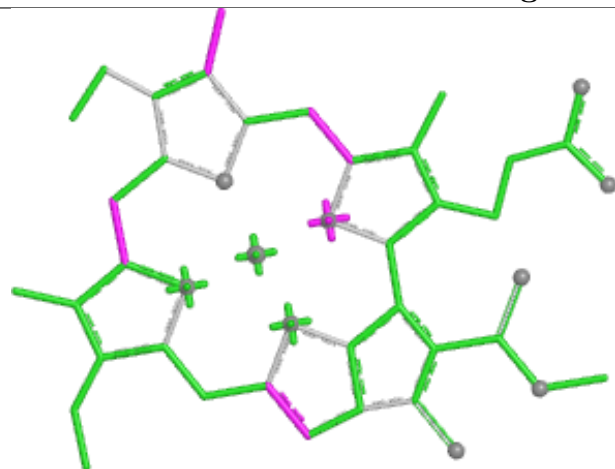




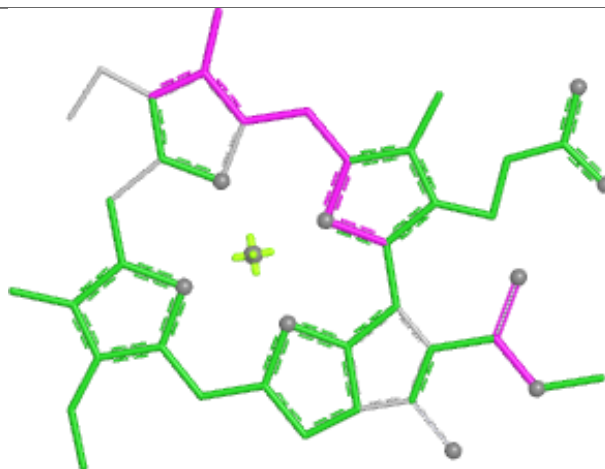
## Ligand CLA 1 614



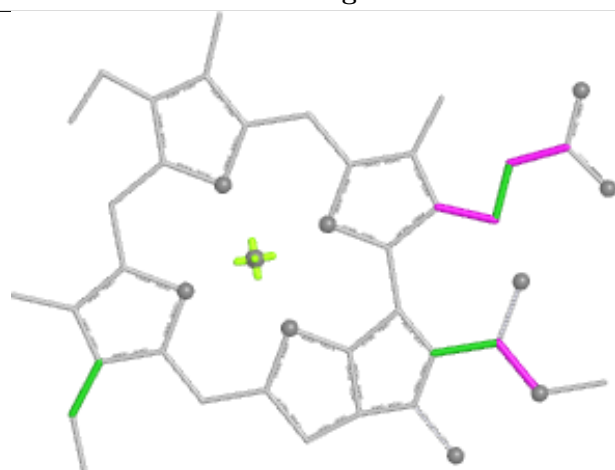
## Ligand CLA 2 312



Bond lengths



Bond angles

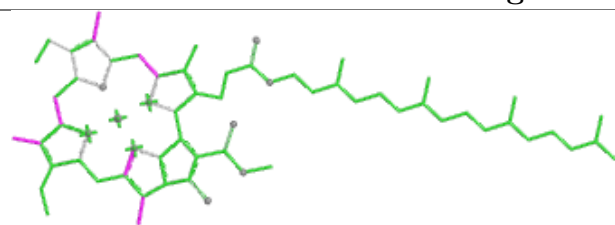


Torsions

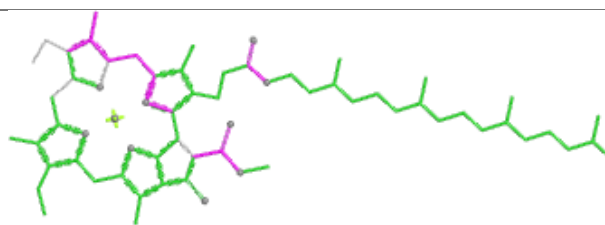


Rings

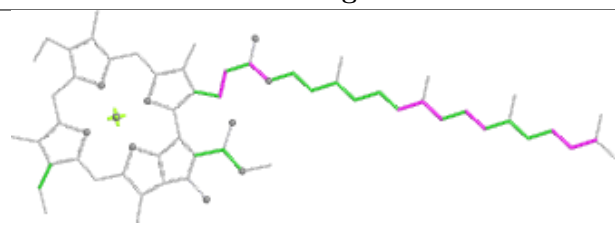
## Ligand CLA A 5014



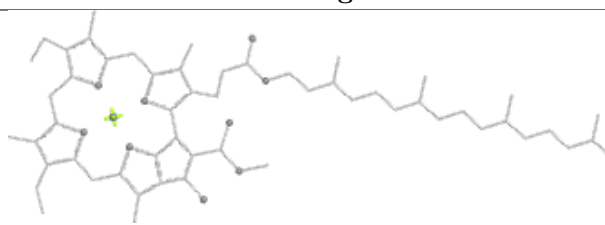
Bond lengths



Bond angles

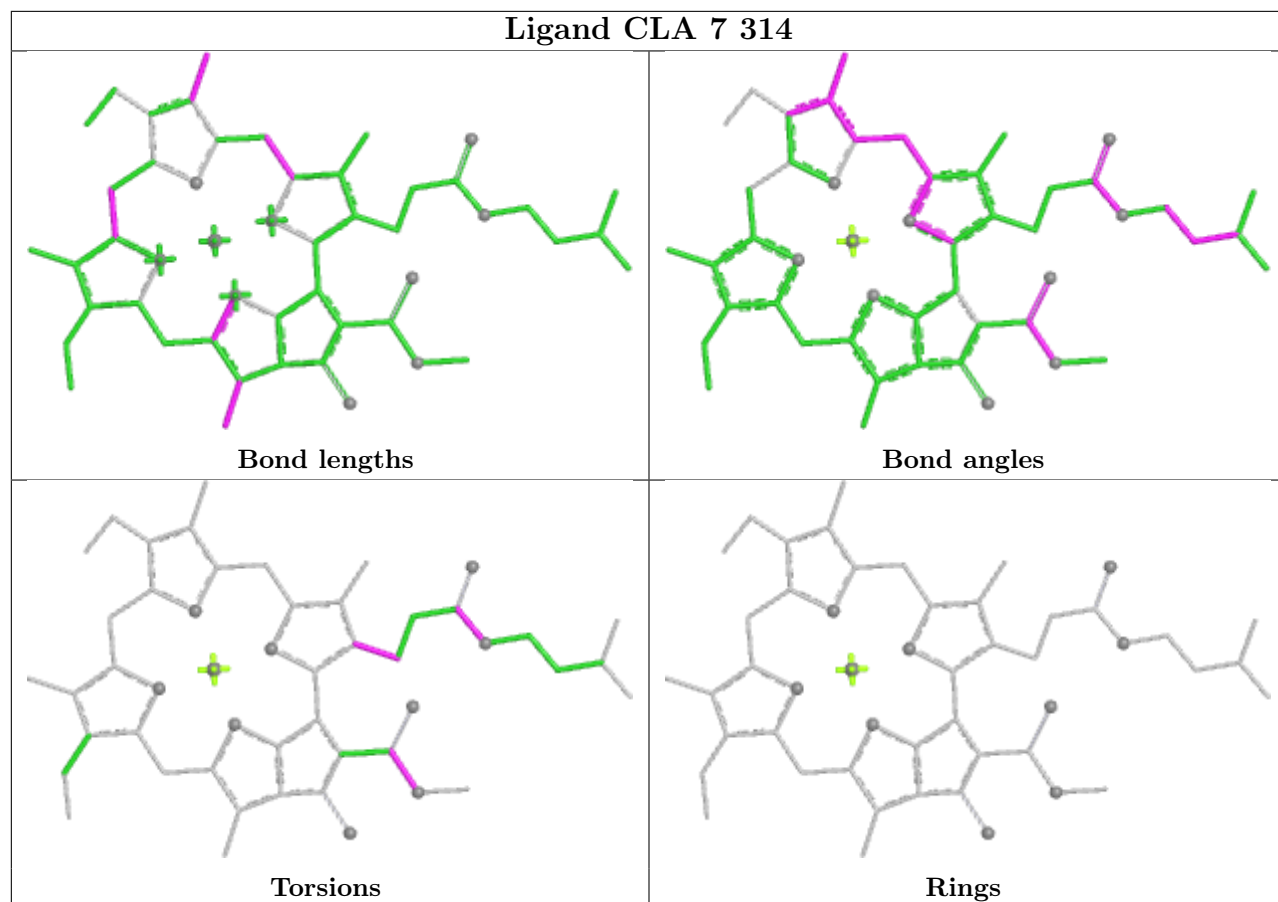


Torsions

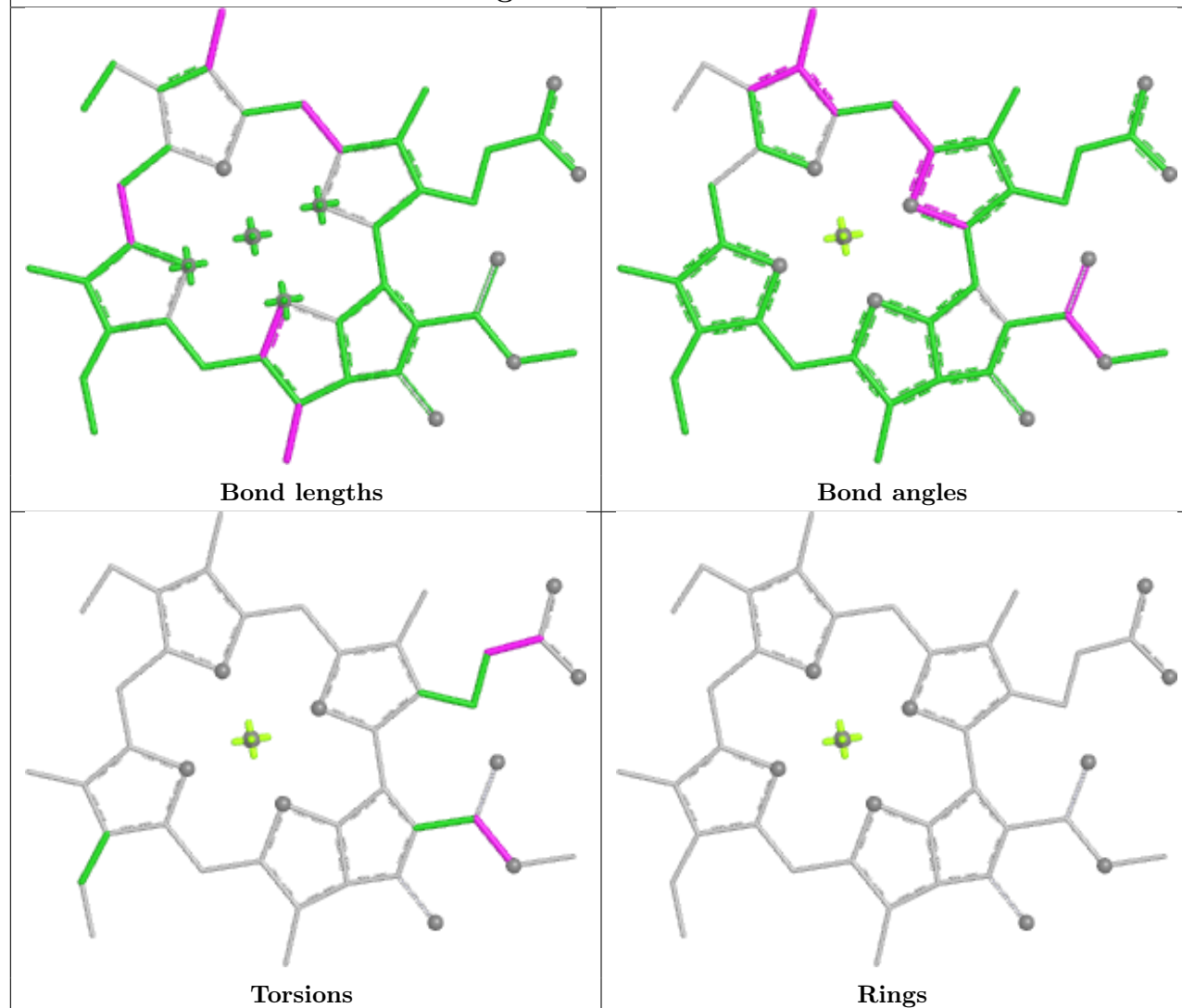


Rings

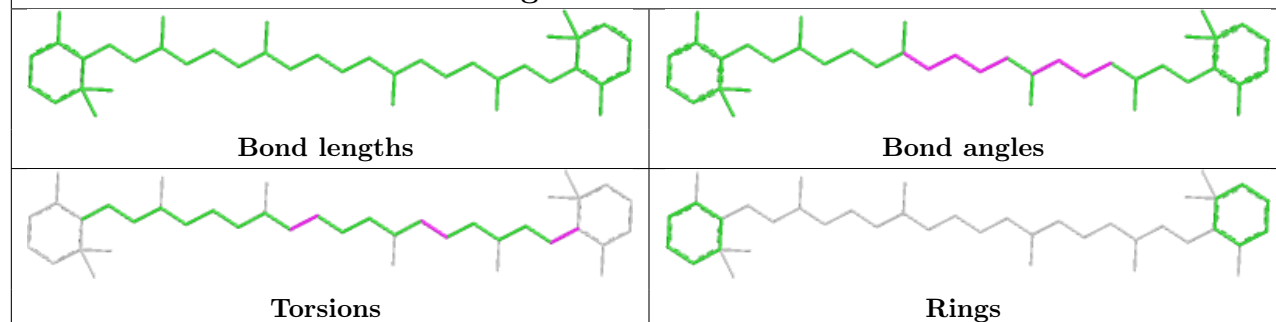
## Ligand CLA 7 314

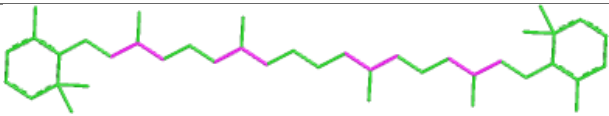
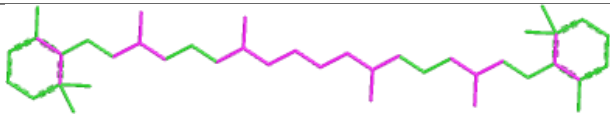
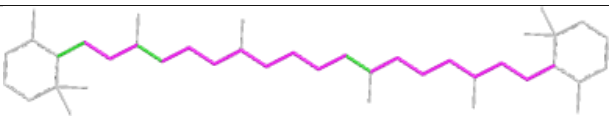
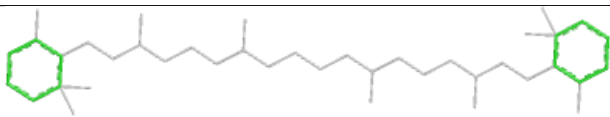



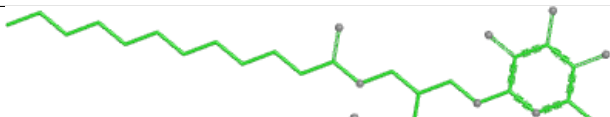
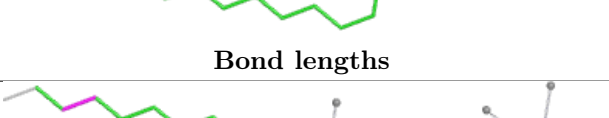
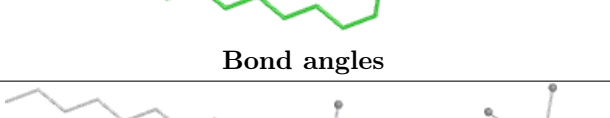
## Ligand CLA 9 605

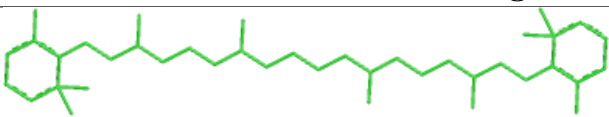
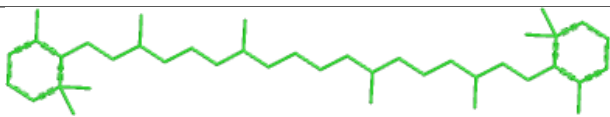
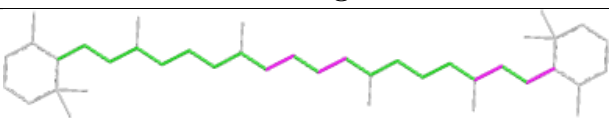
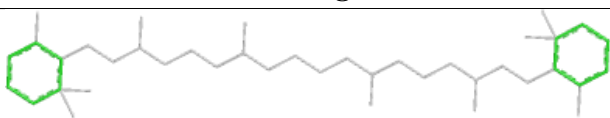


## Ligand BCR A 5049

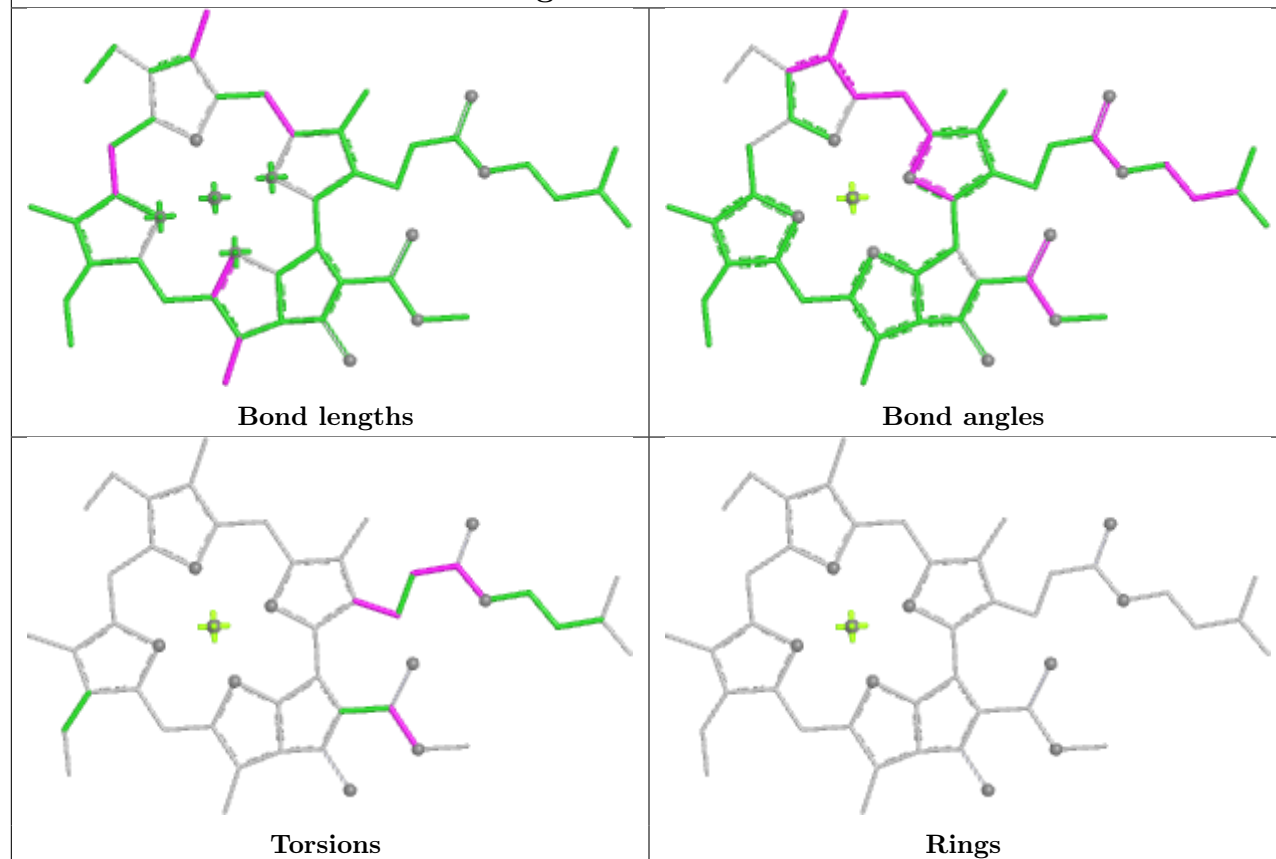


Ligand BCR 3 319	
	
Bond lengths	Bond angles
	
Torsions	Rings

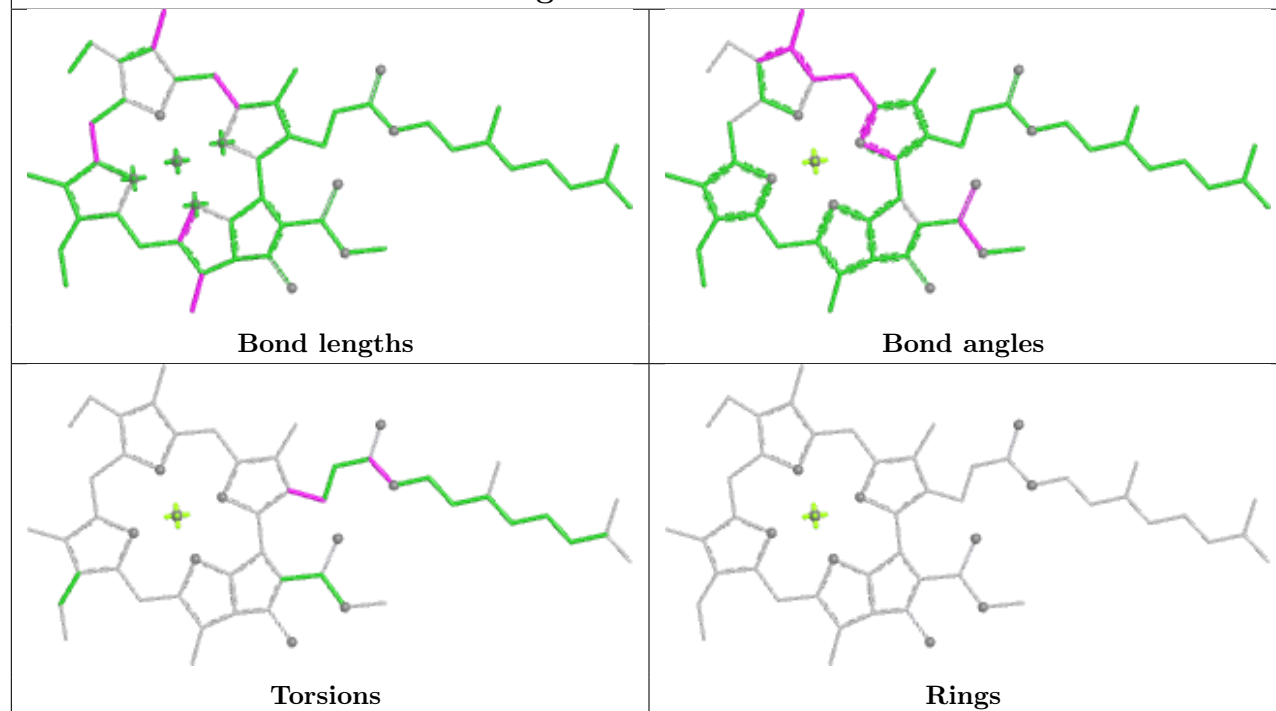
Ligand LMG G 206	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR L 206	
	
Bond lengths	Bond angles
	
Torsions	Rings

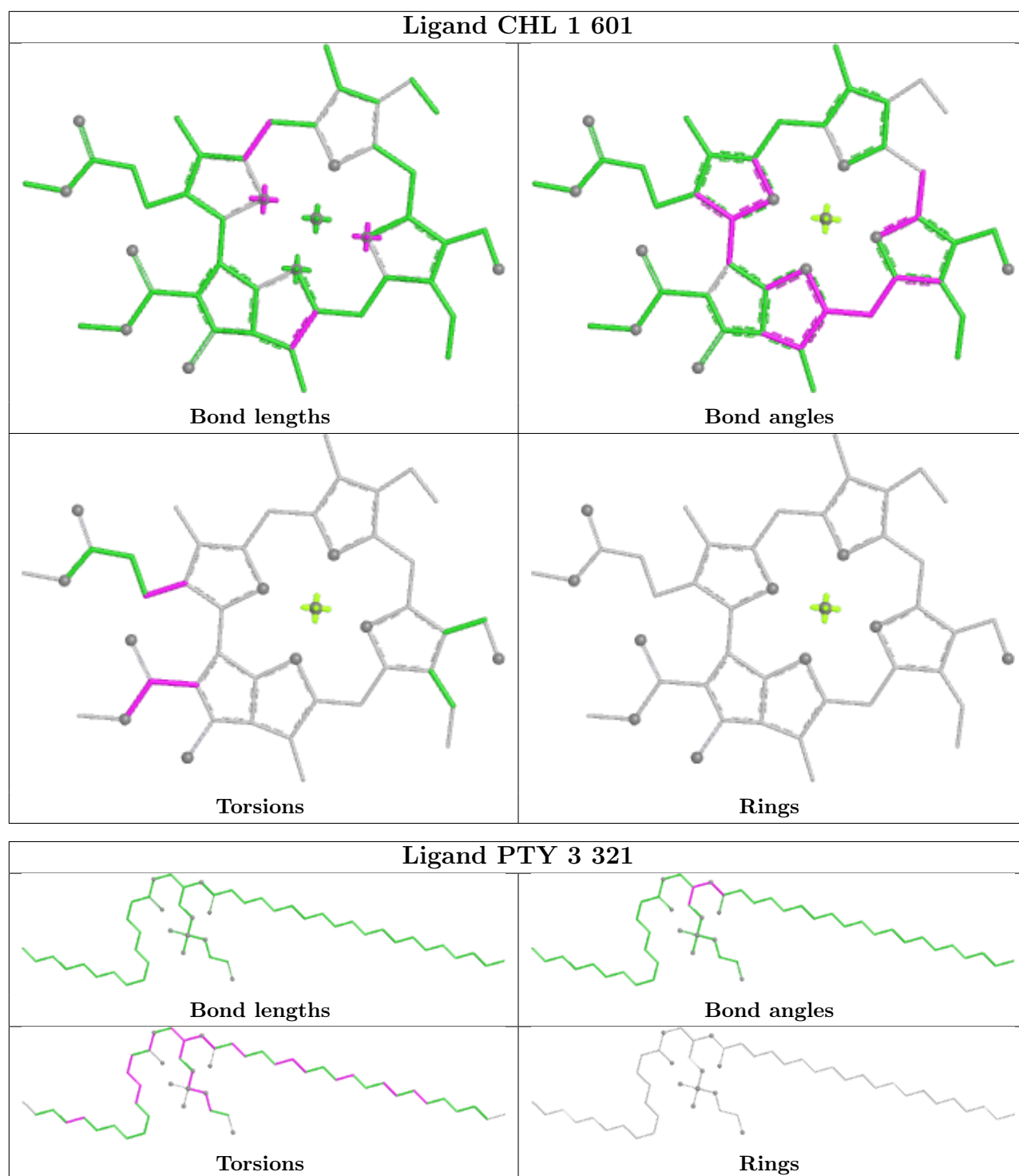
## Ligand CLA 1 607

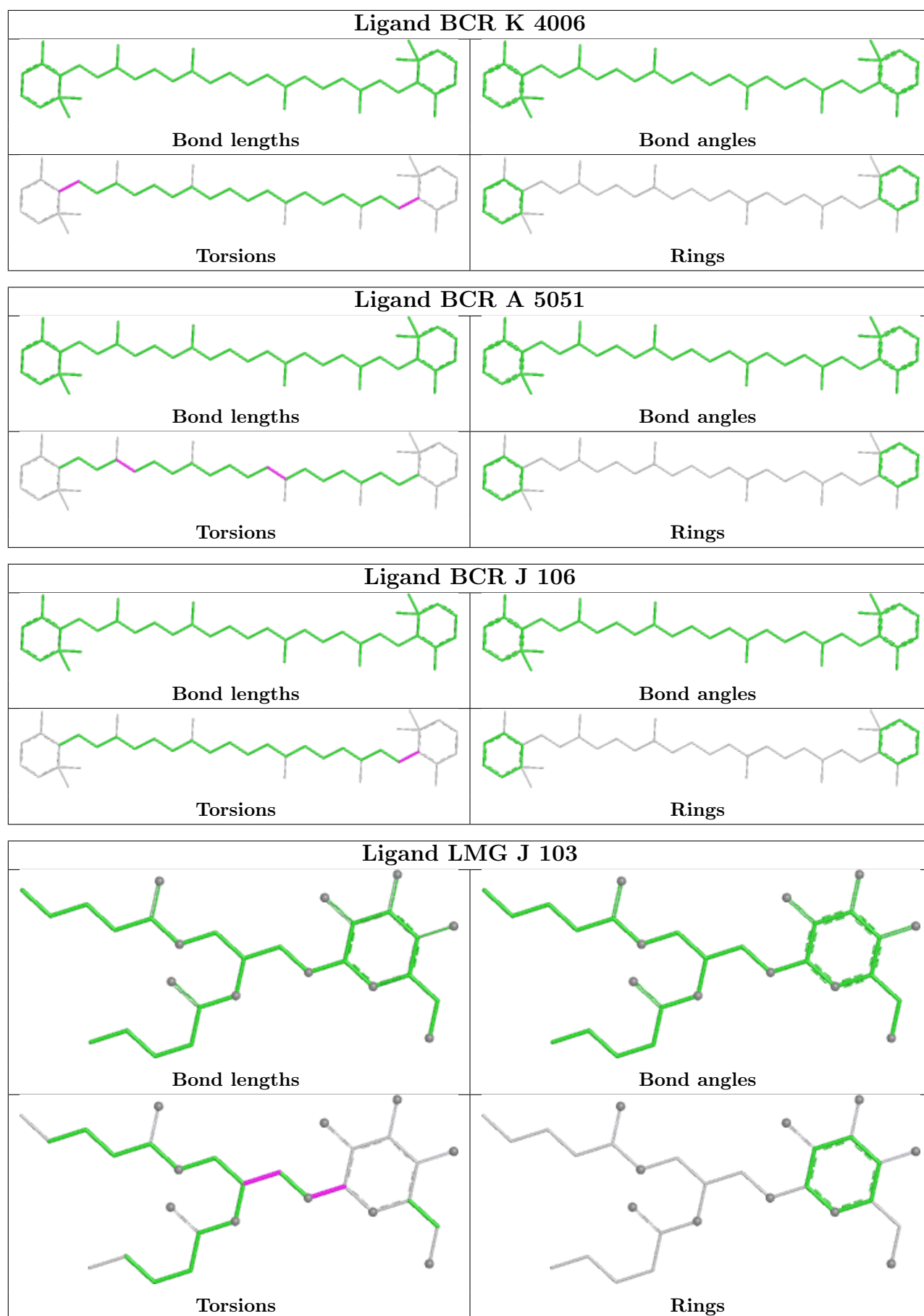


## Ligand CLA 3 325

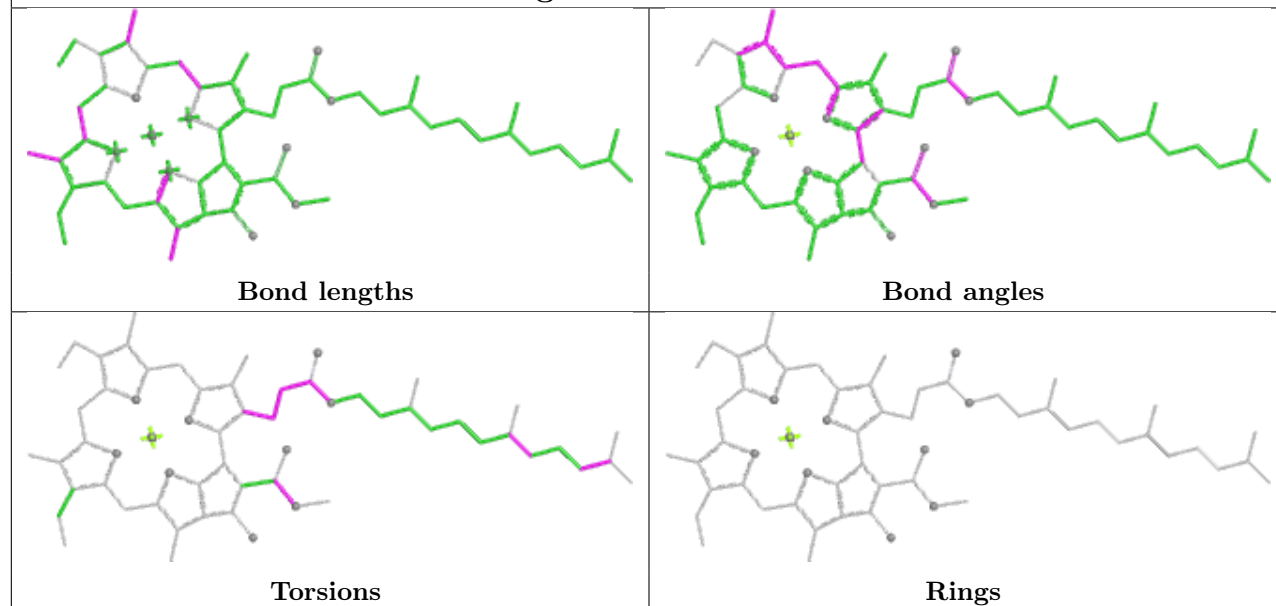




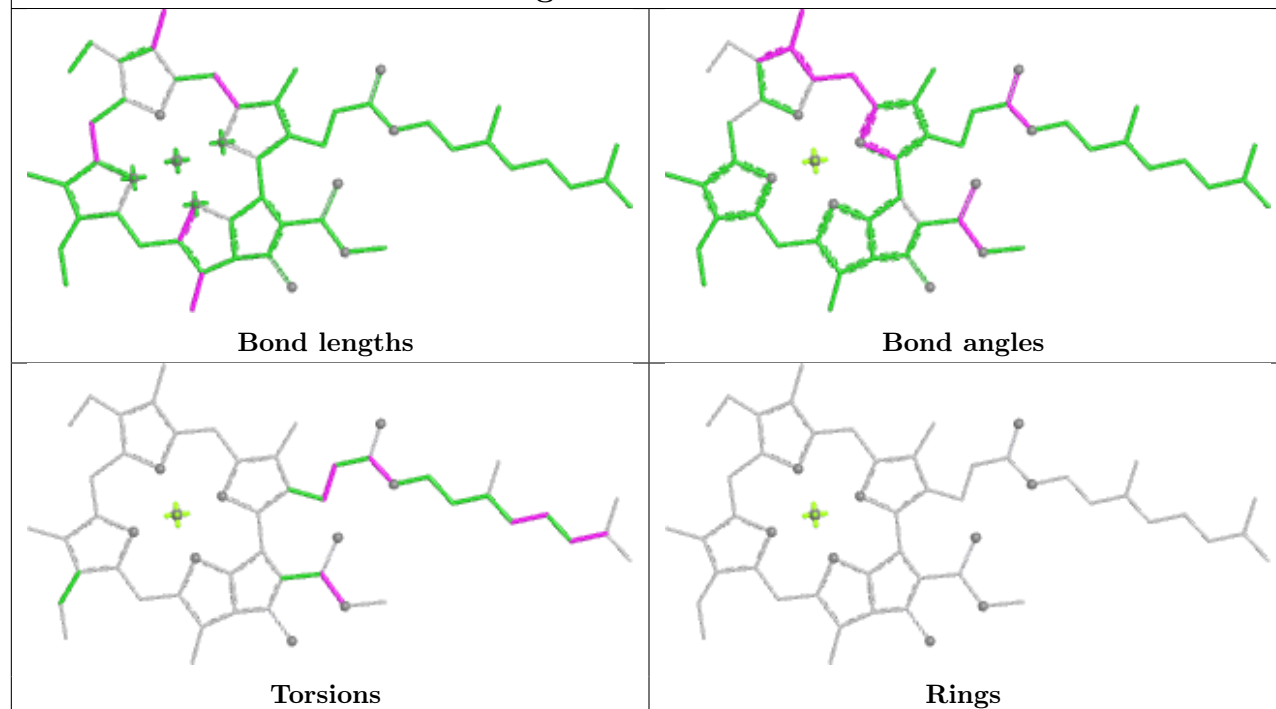


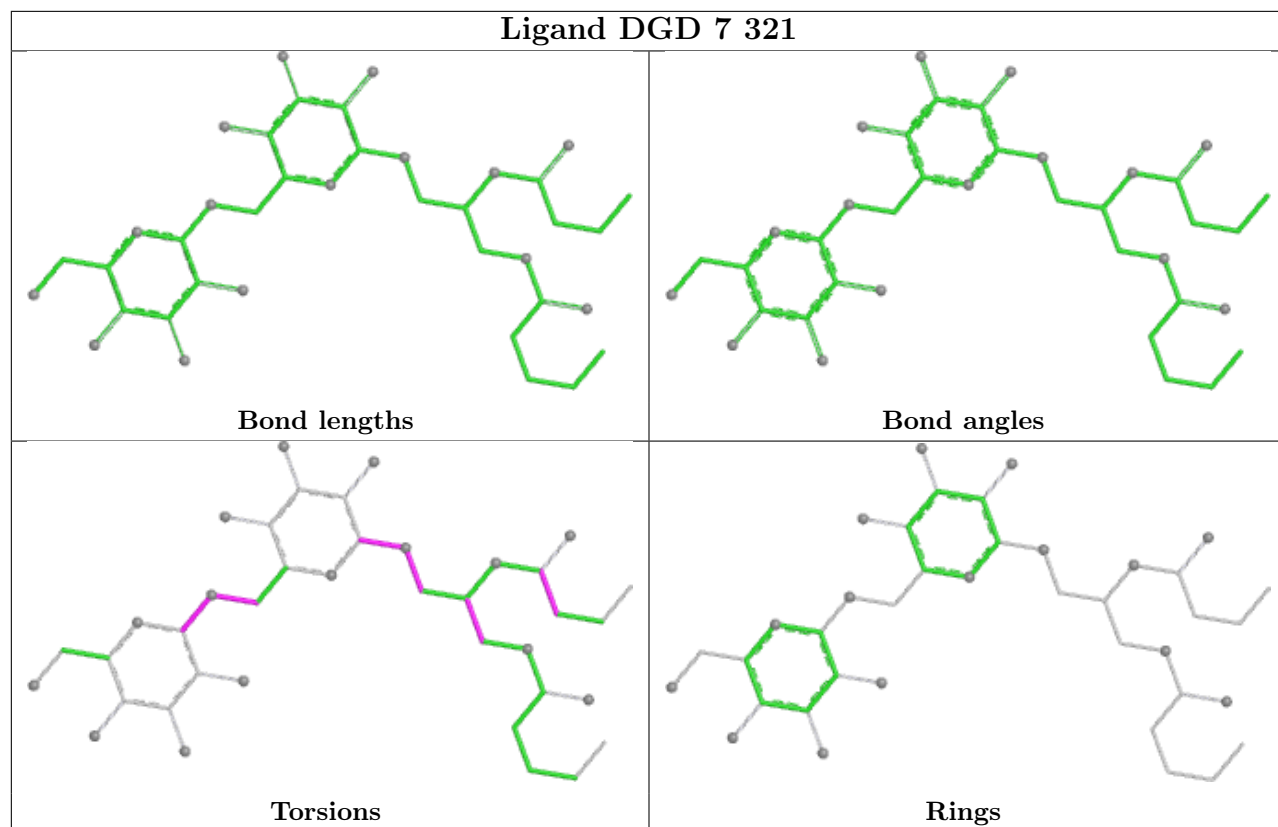


## Ligand CLA 7 303

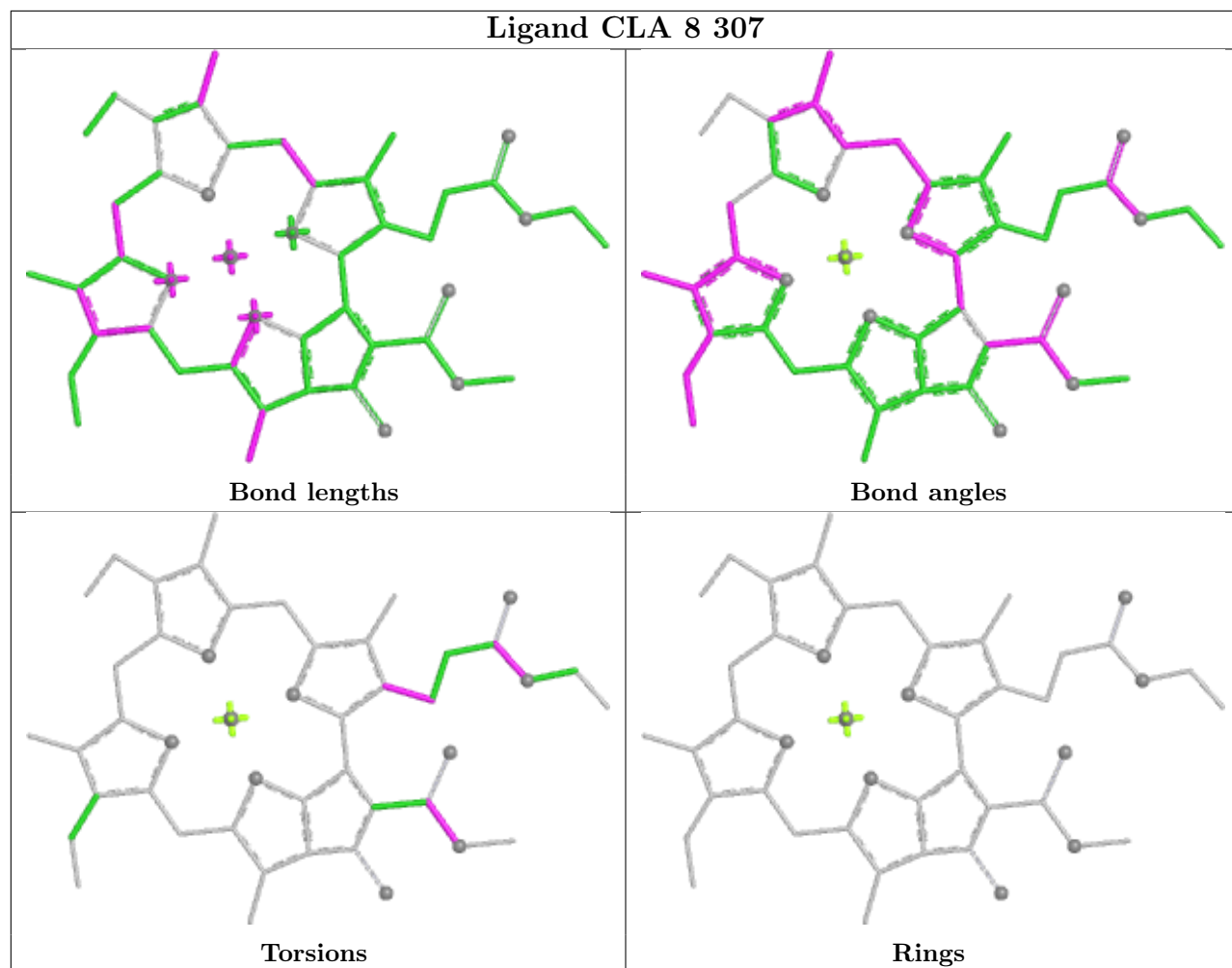


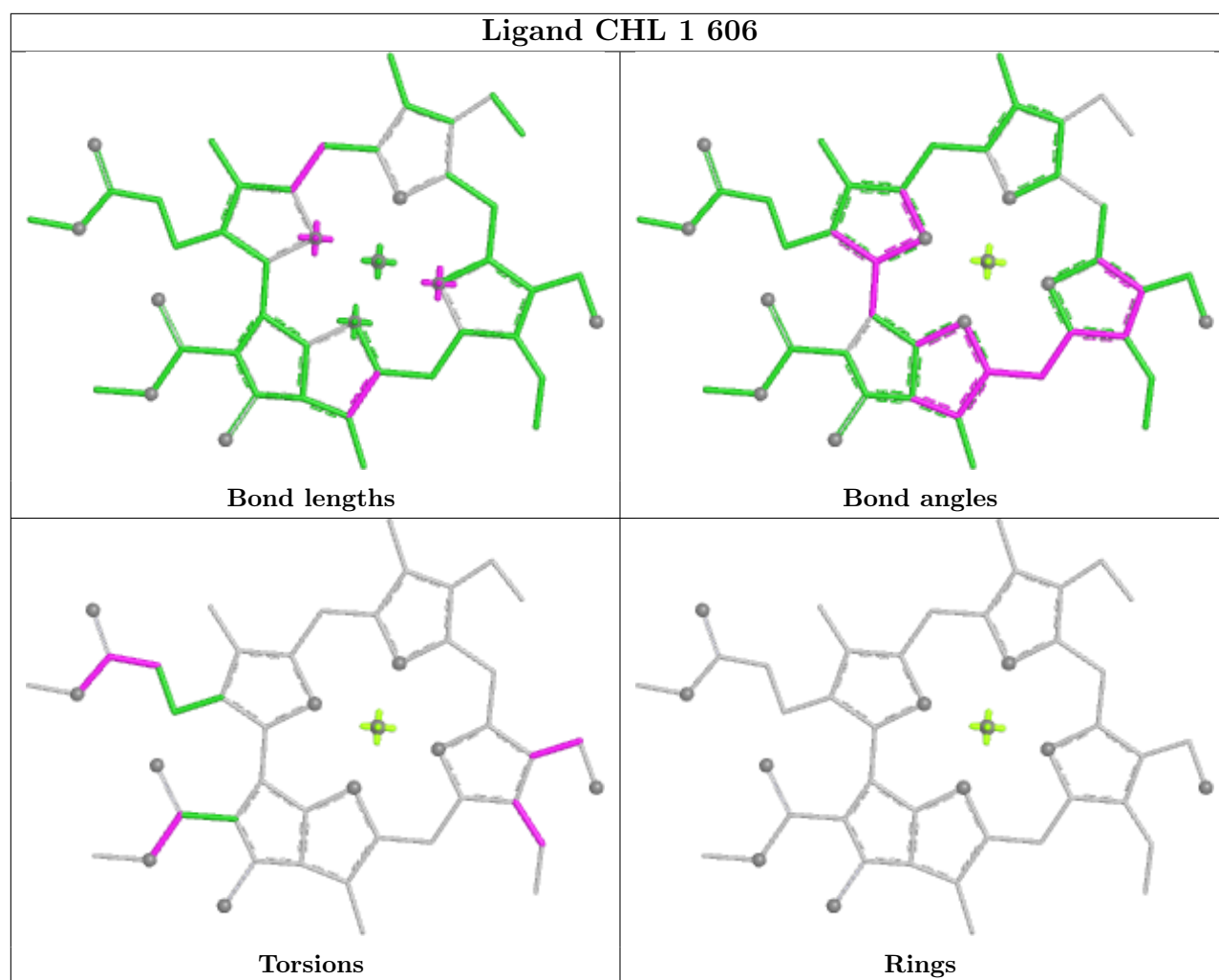
## Ligand CLA 3 311



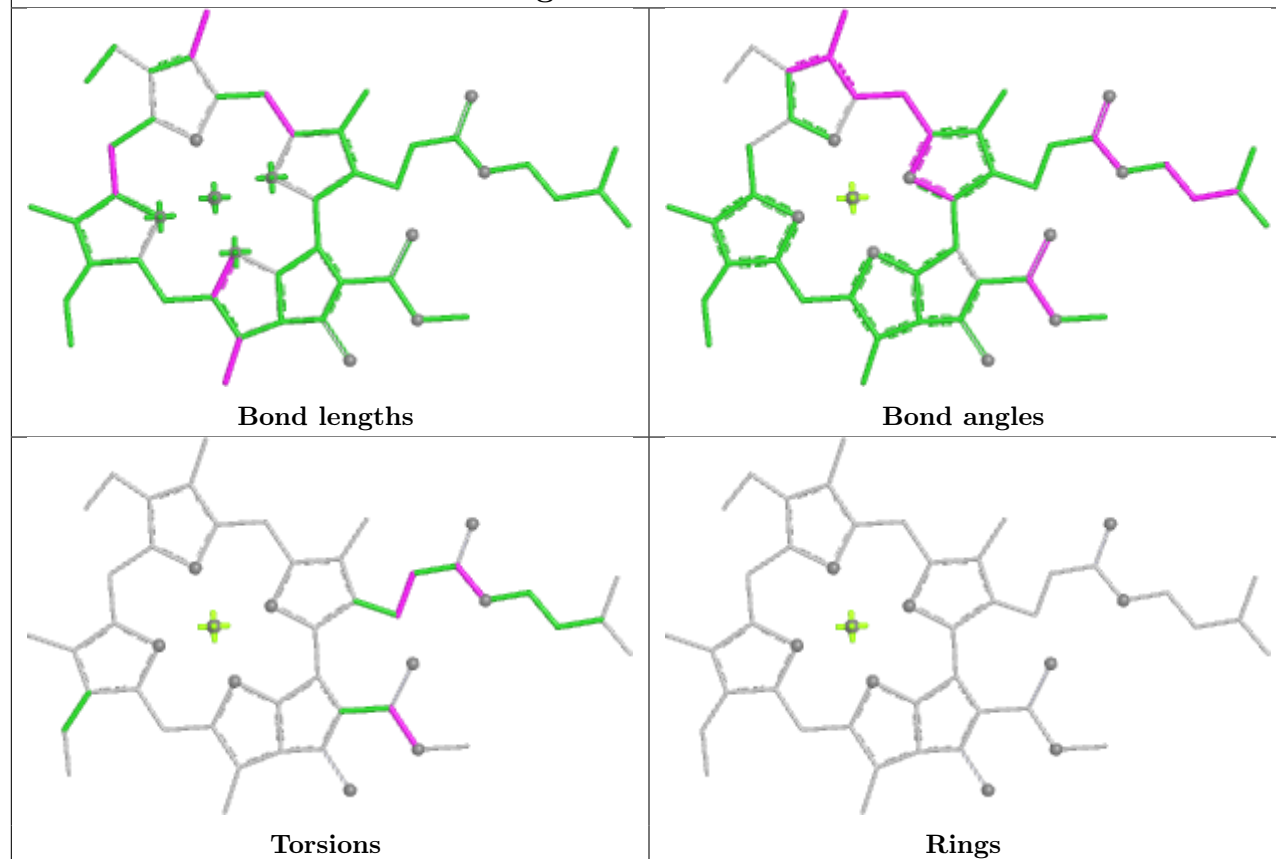


## Ligand CLA 8 307

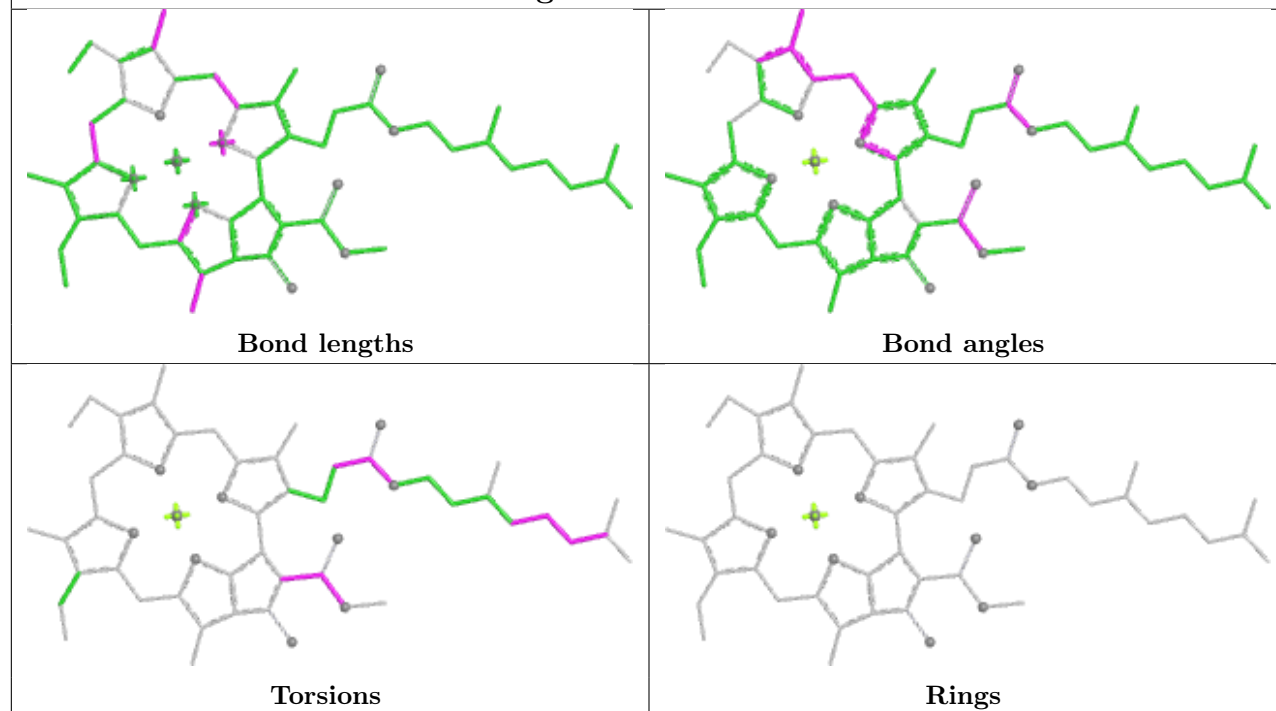


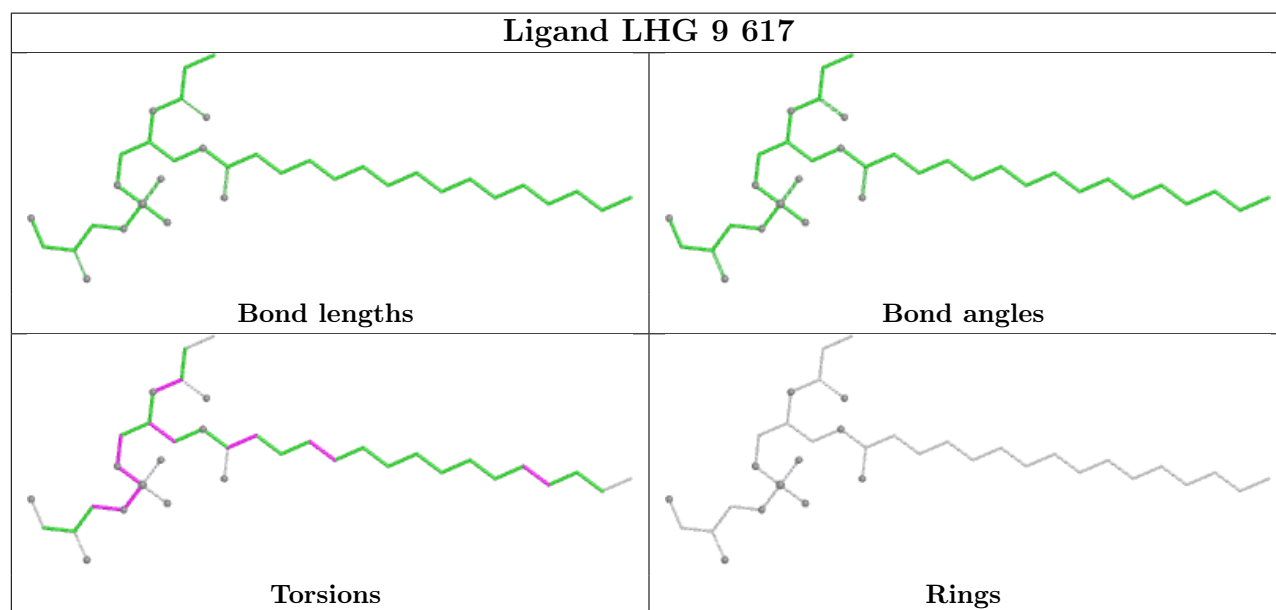
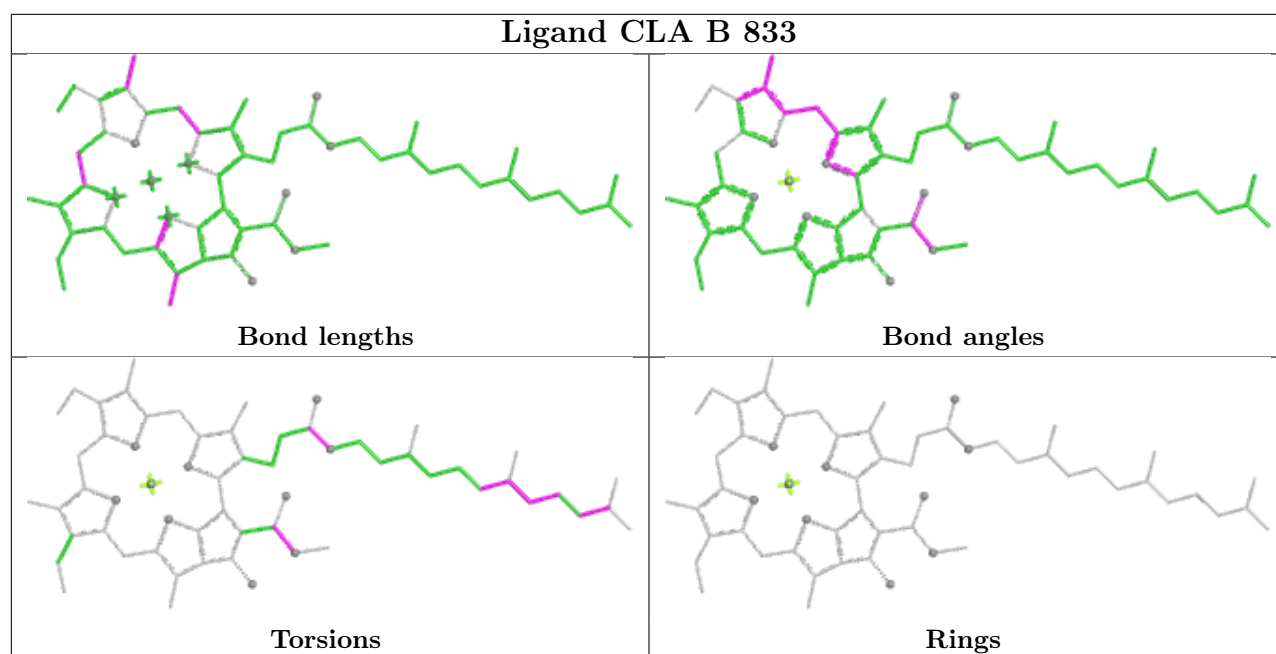


## Ligand CLA 2 313

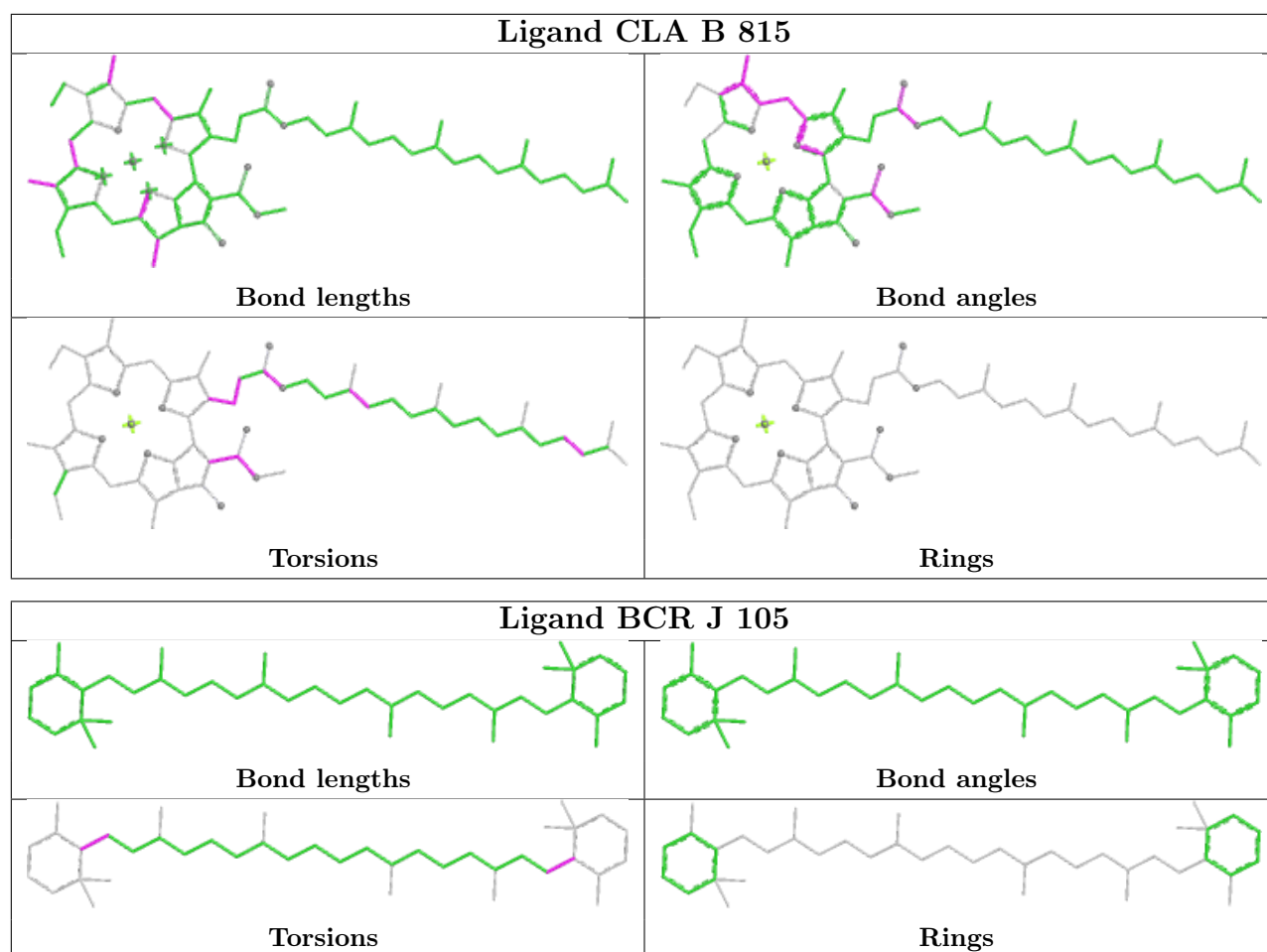


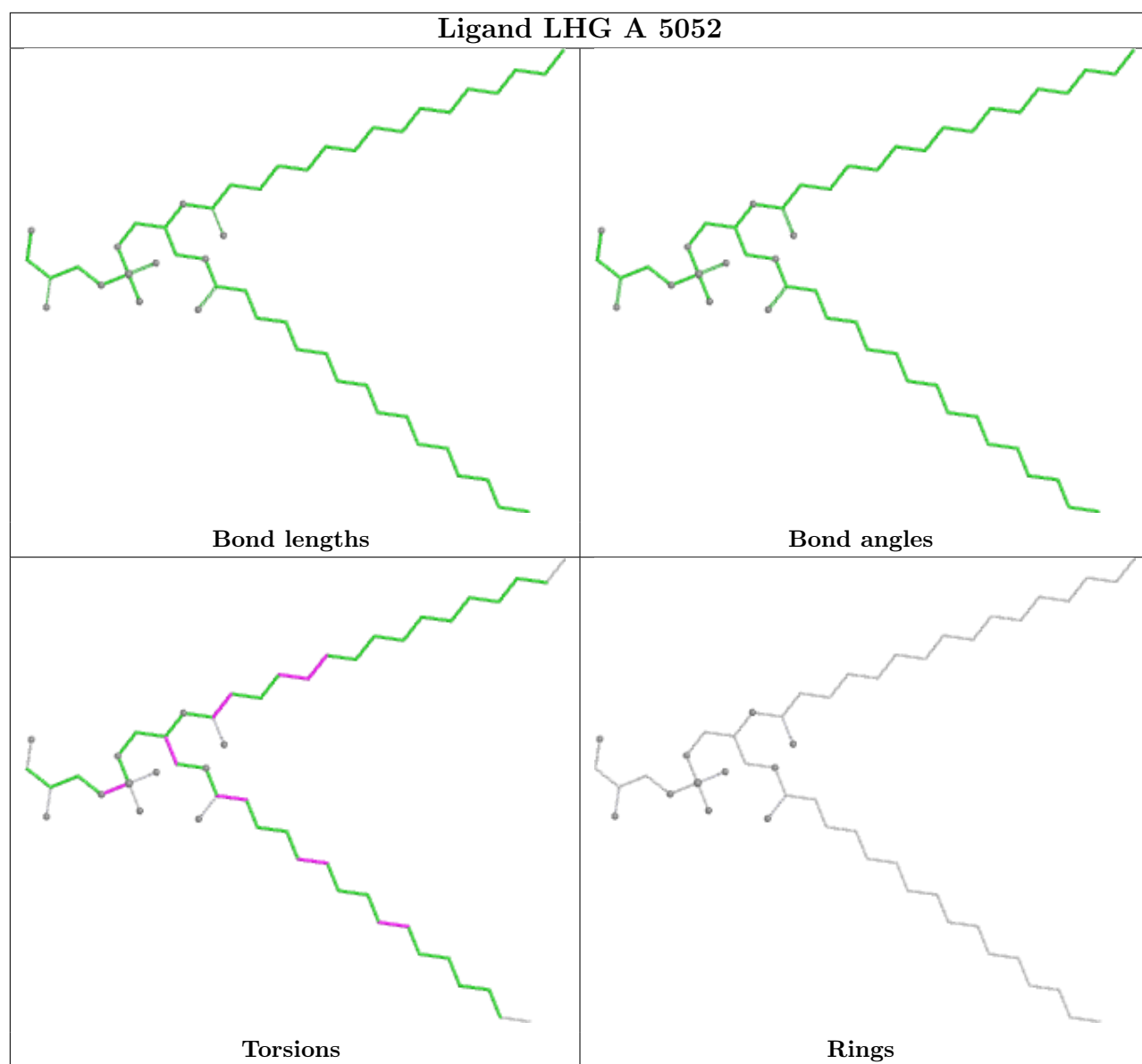
## Ligand CLA 1 603



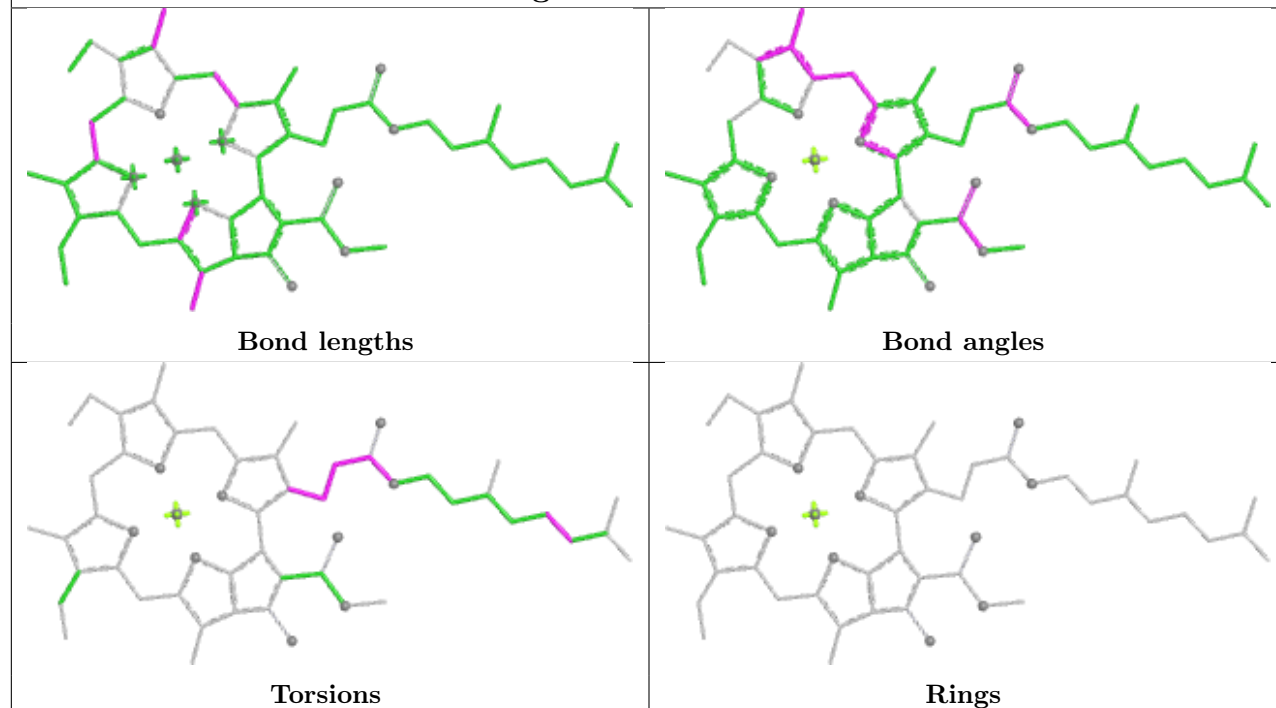




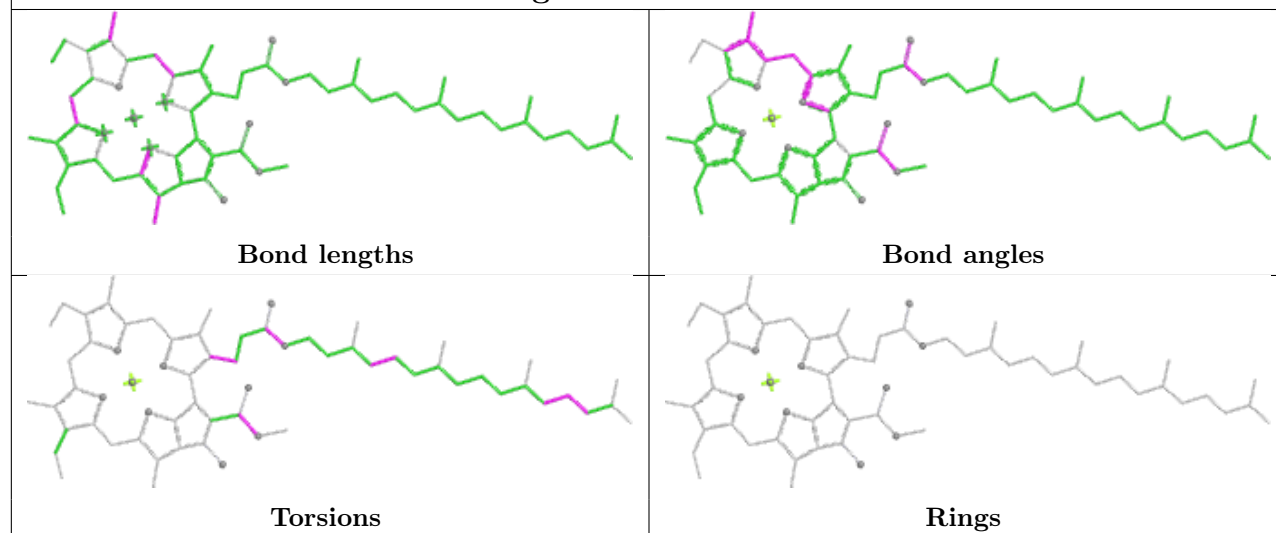




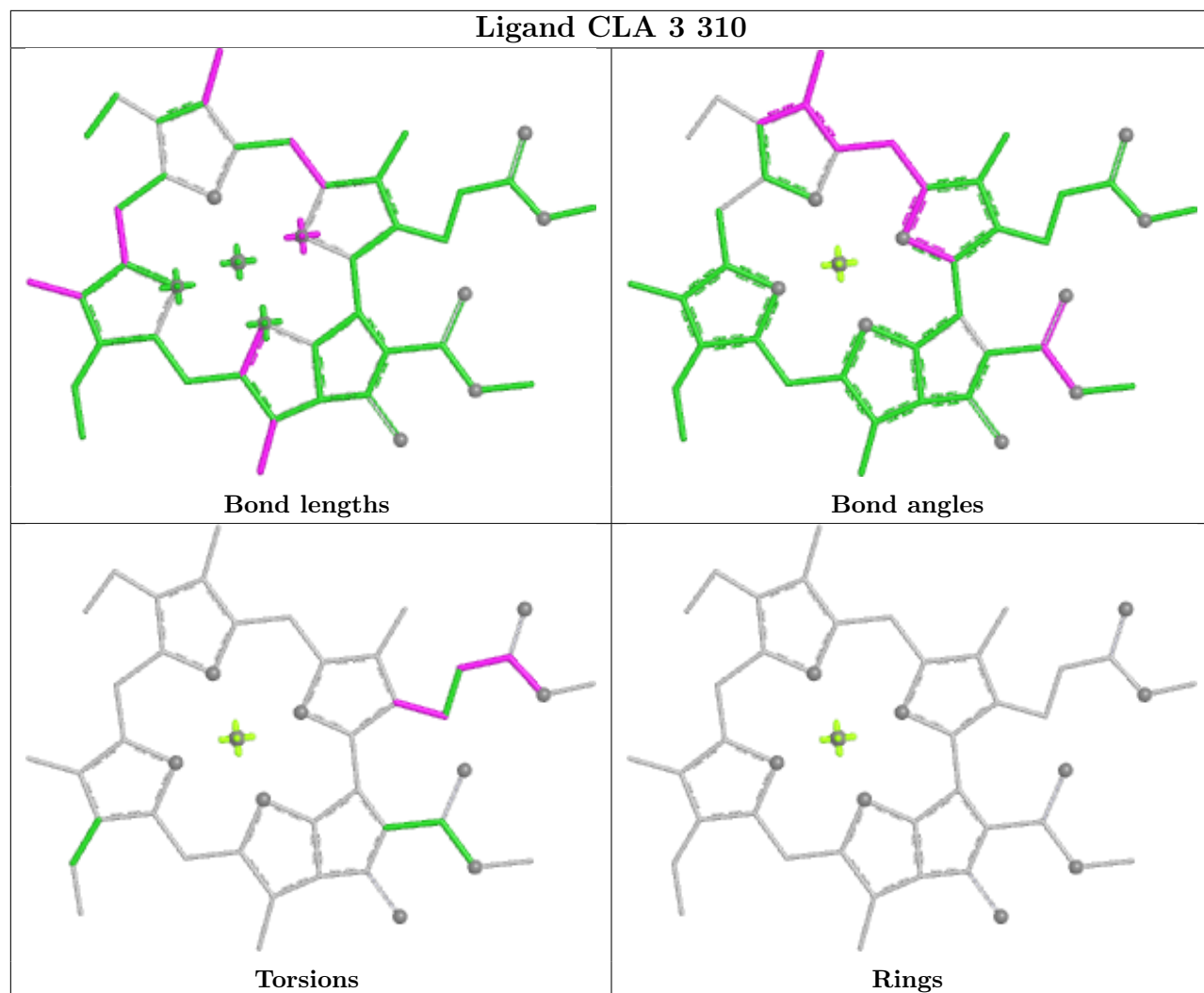
## Ligand CLA B 821



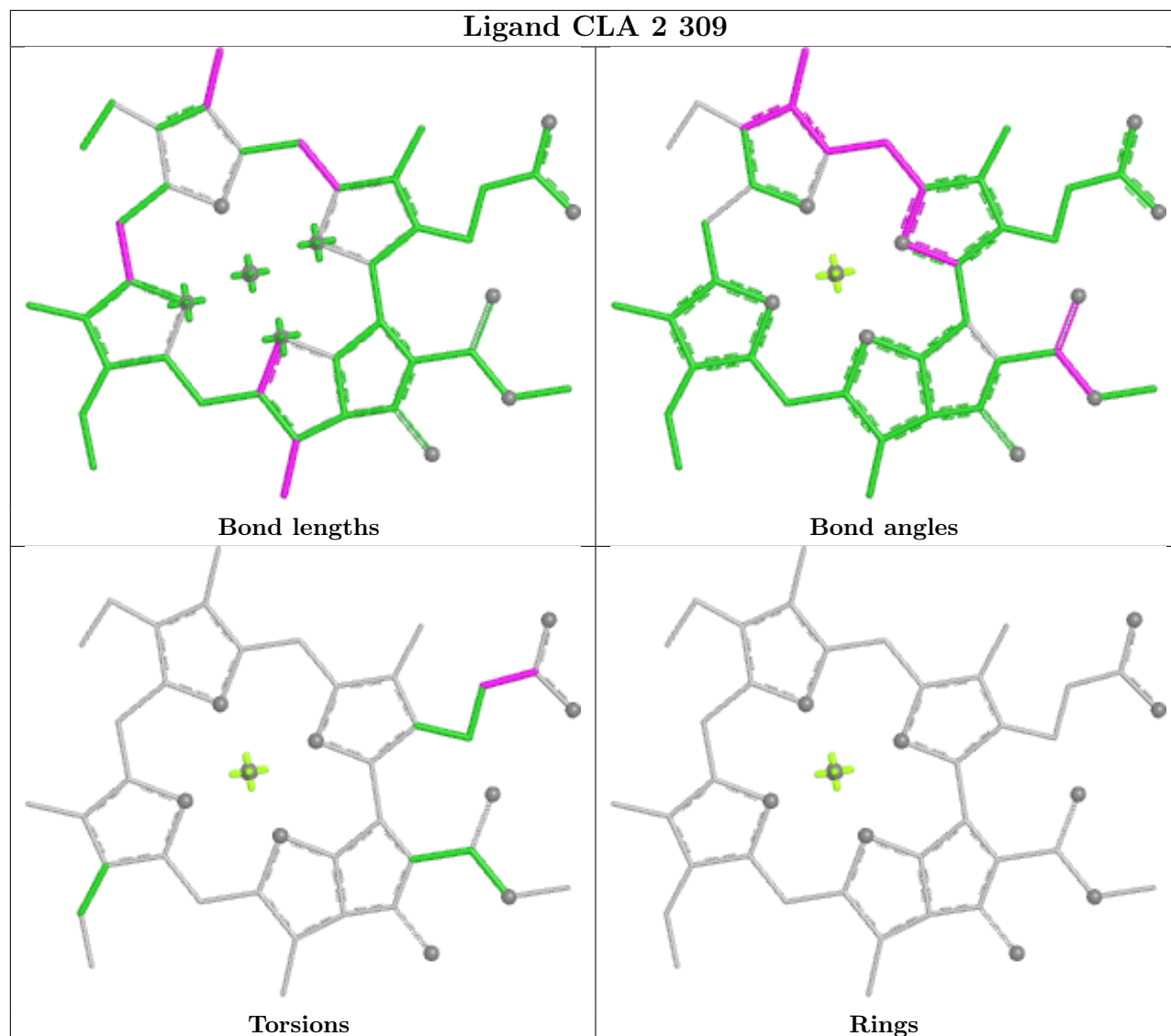
## Ligand CLA B 840



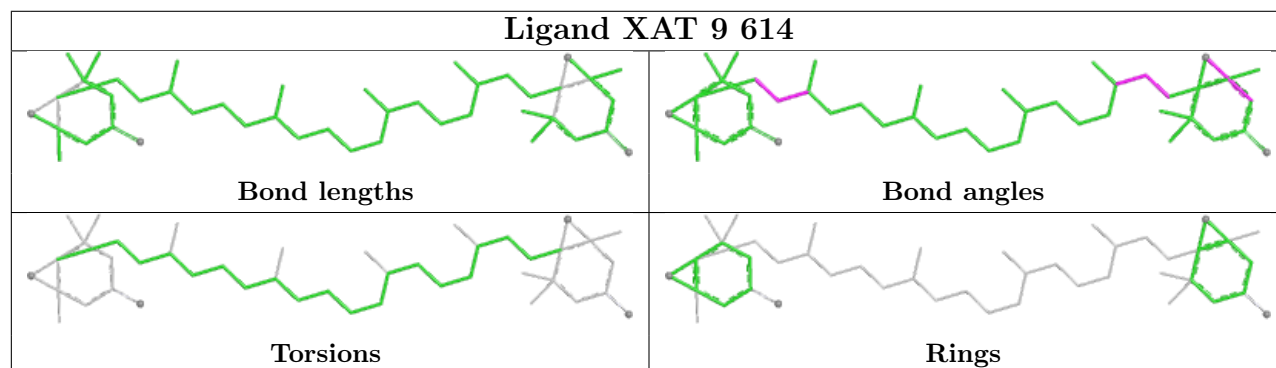
## Ligand CLA 3 310



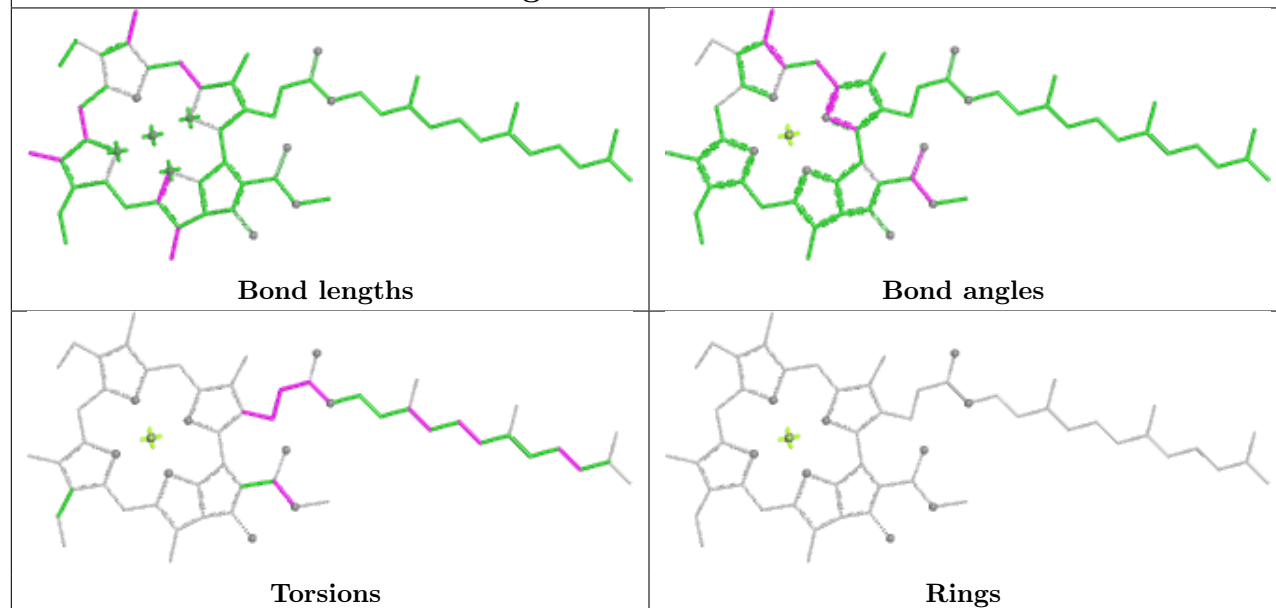
## Ligand CLA 2 309



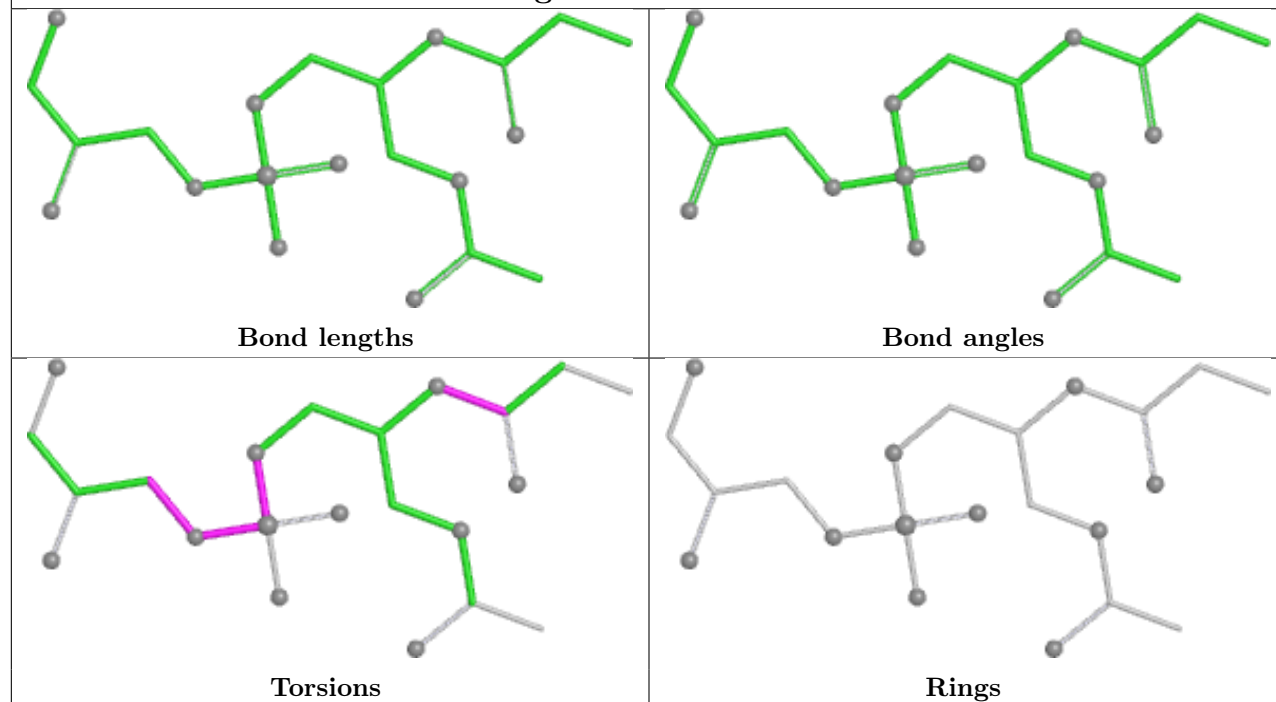
## Ligand XAT 9 614

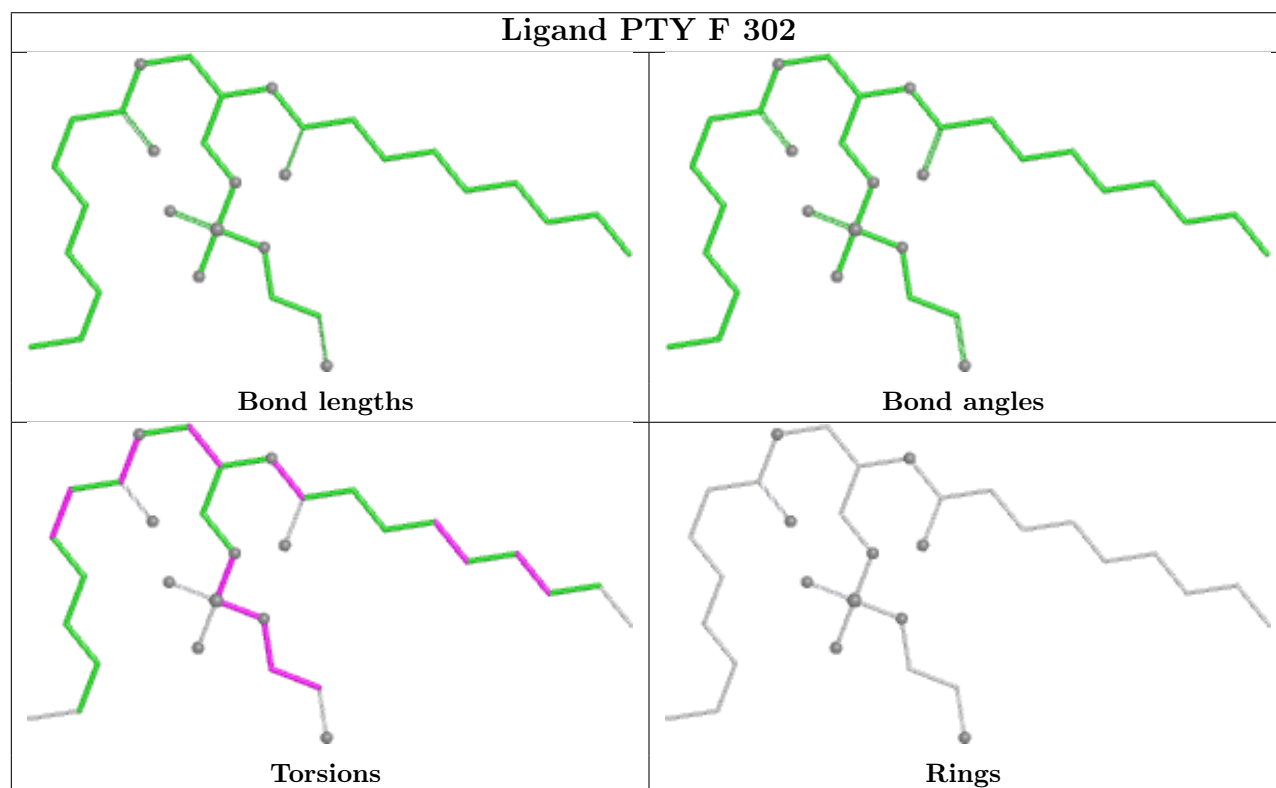
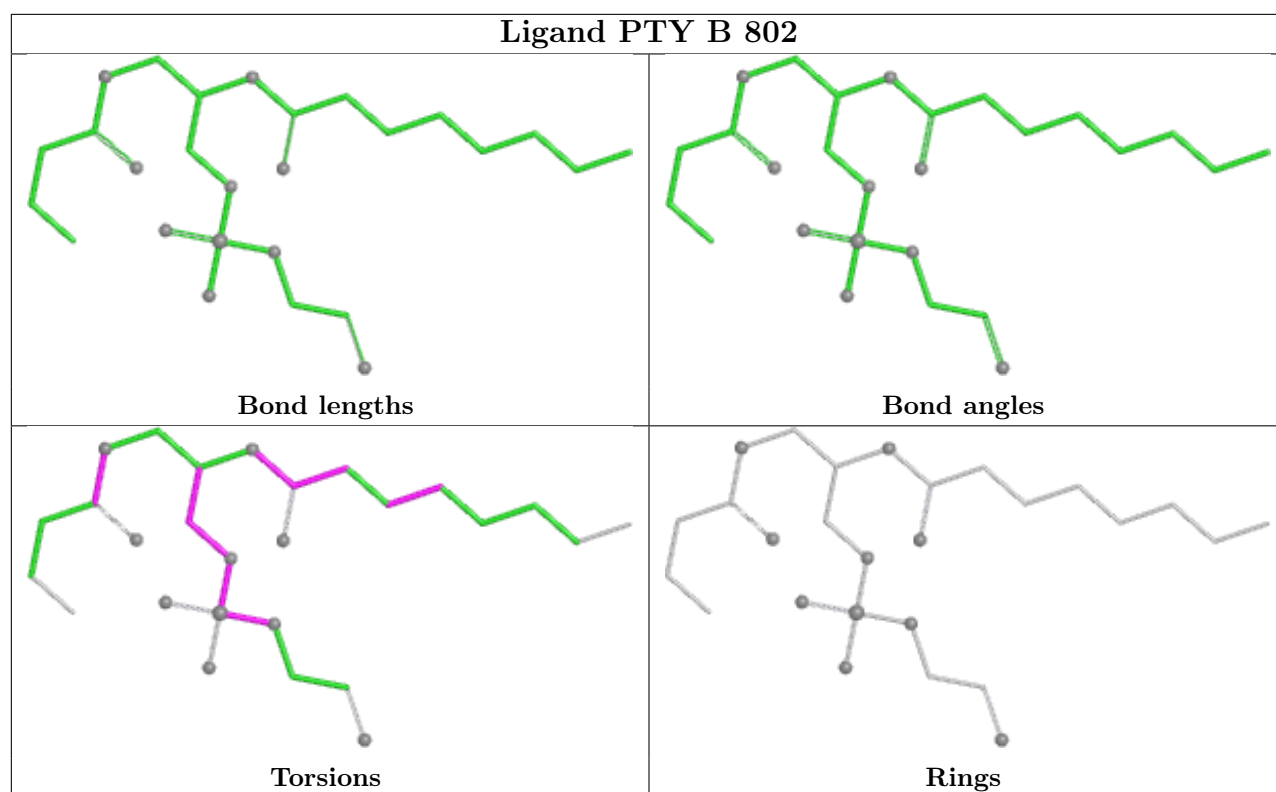


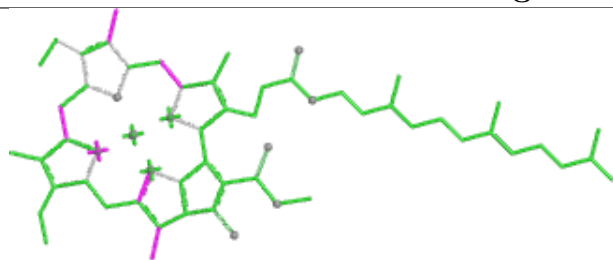
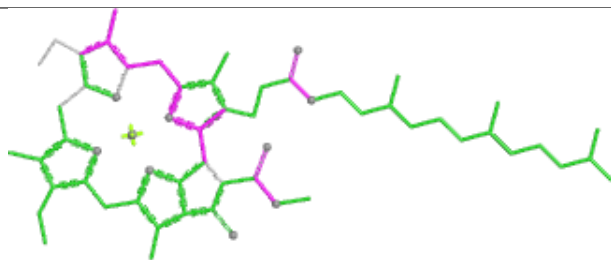
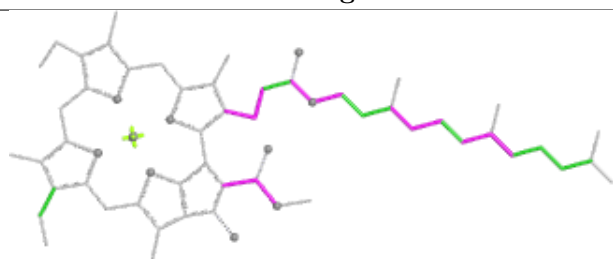
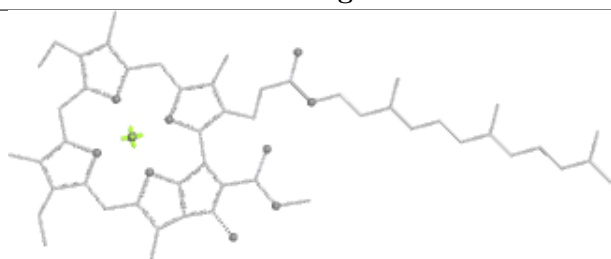
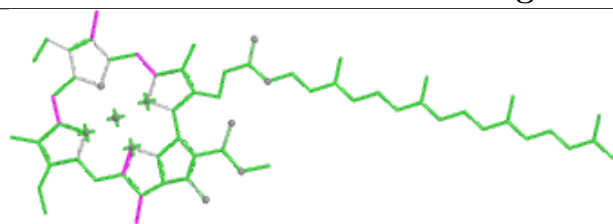
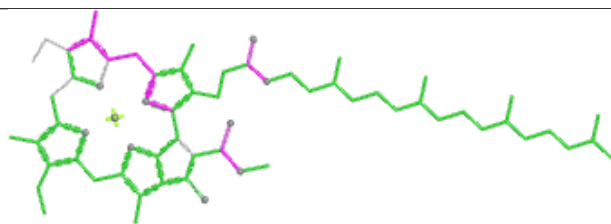
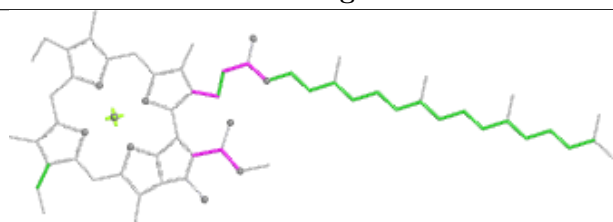
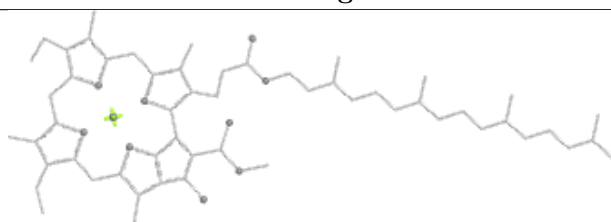
## Ligand CLA A 5025



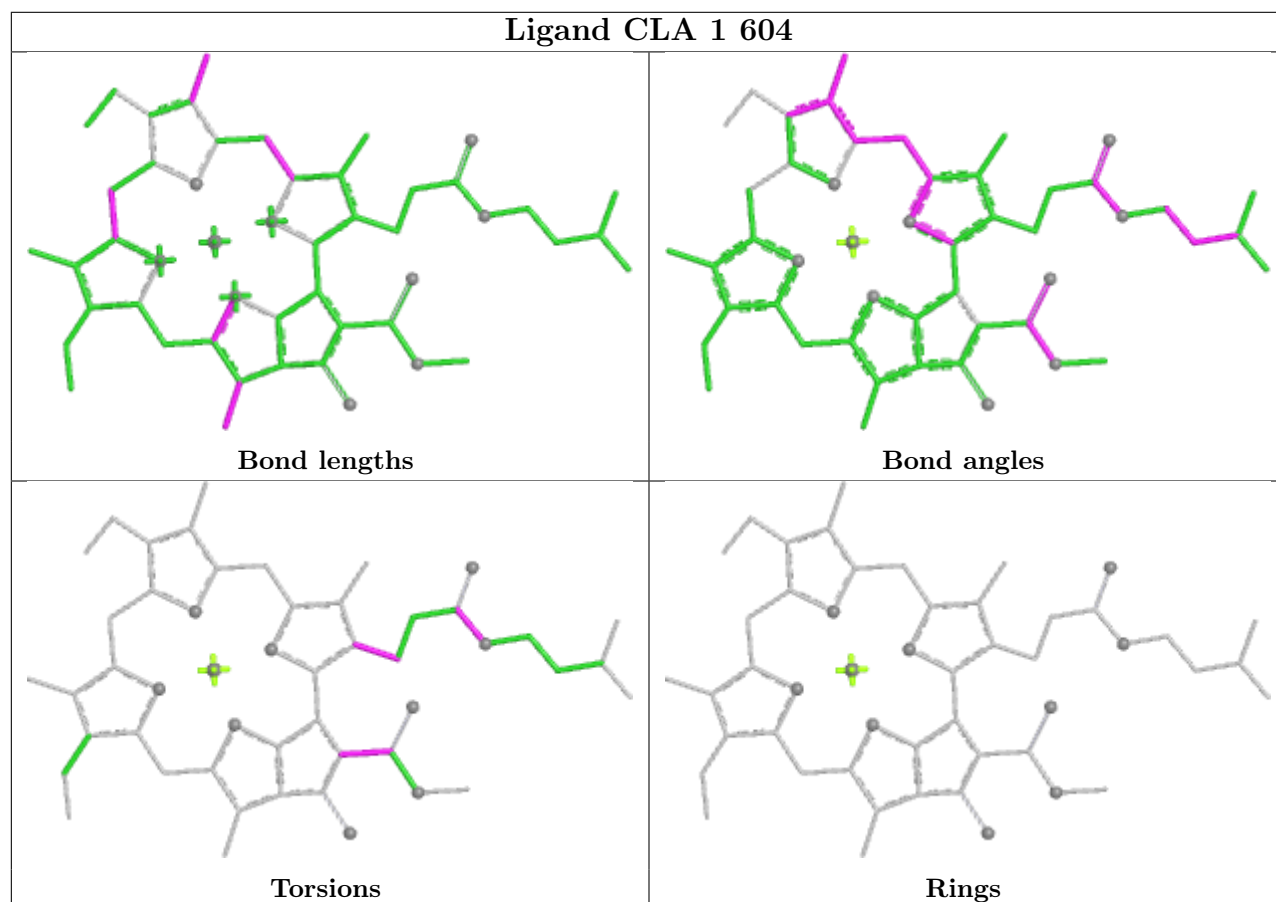
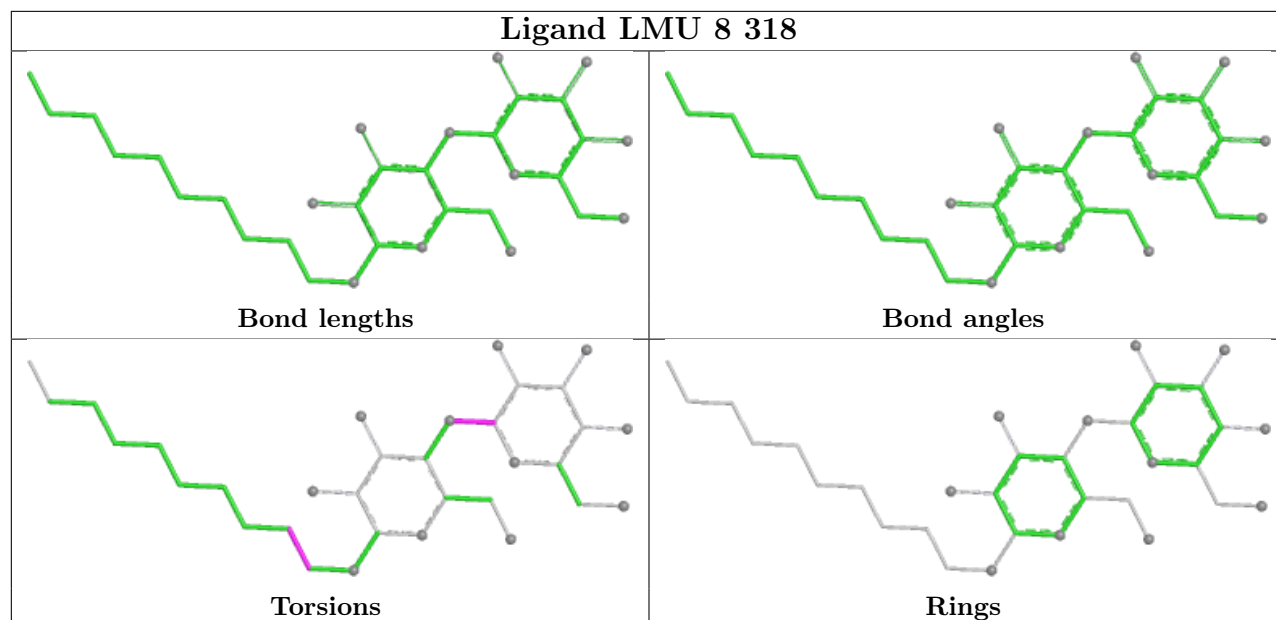
## Ligand LHG 7 319



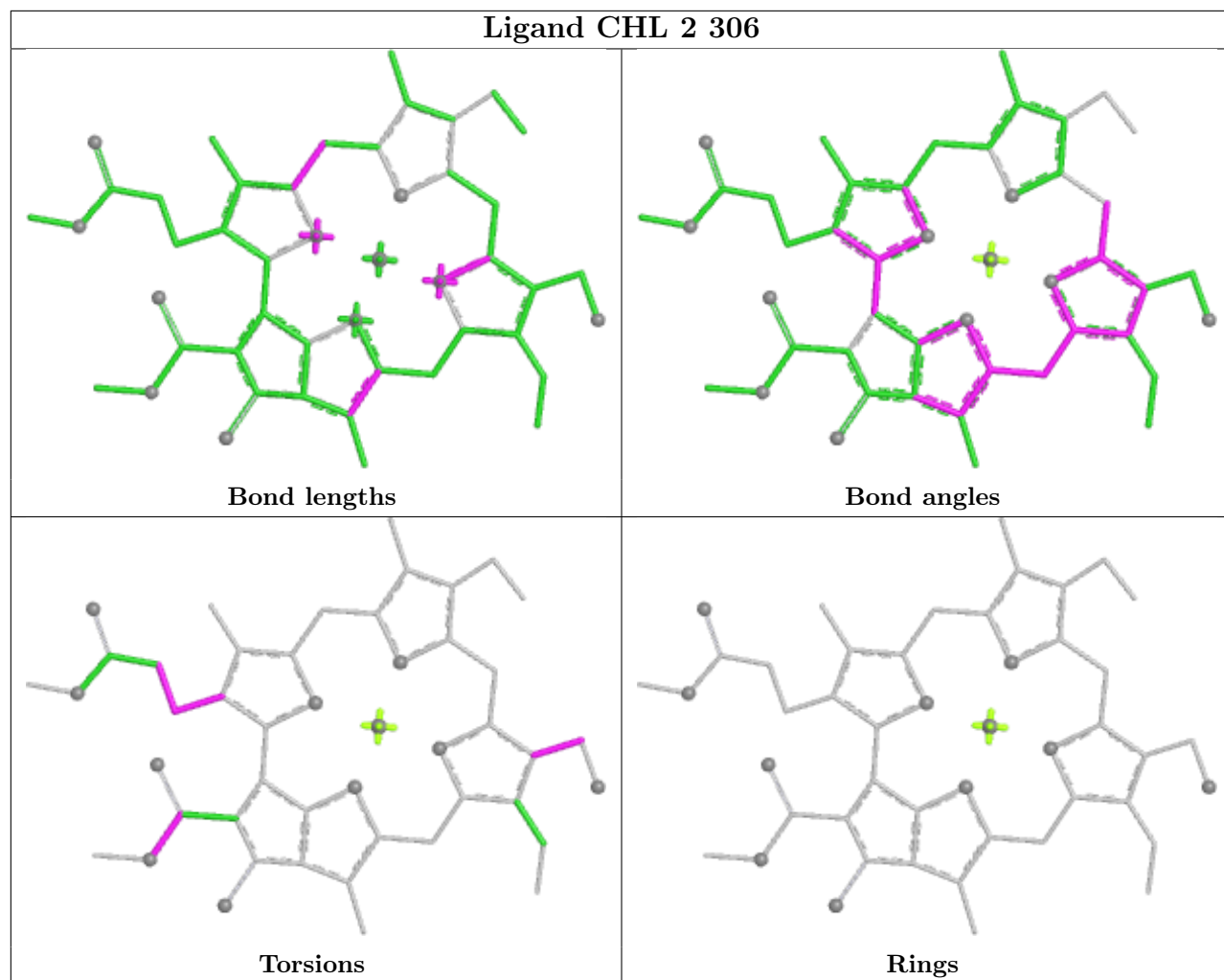


**Ligand CLA H 201****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA L 204****Bond lengths****Bond angles****Torsions****Rings**

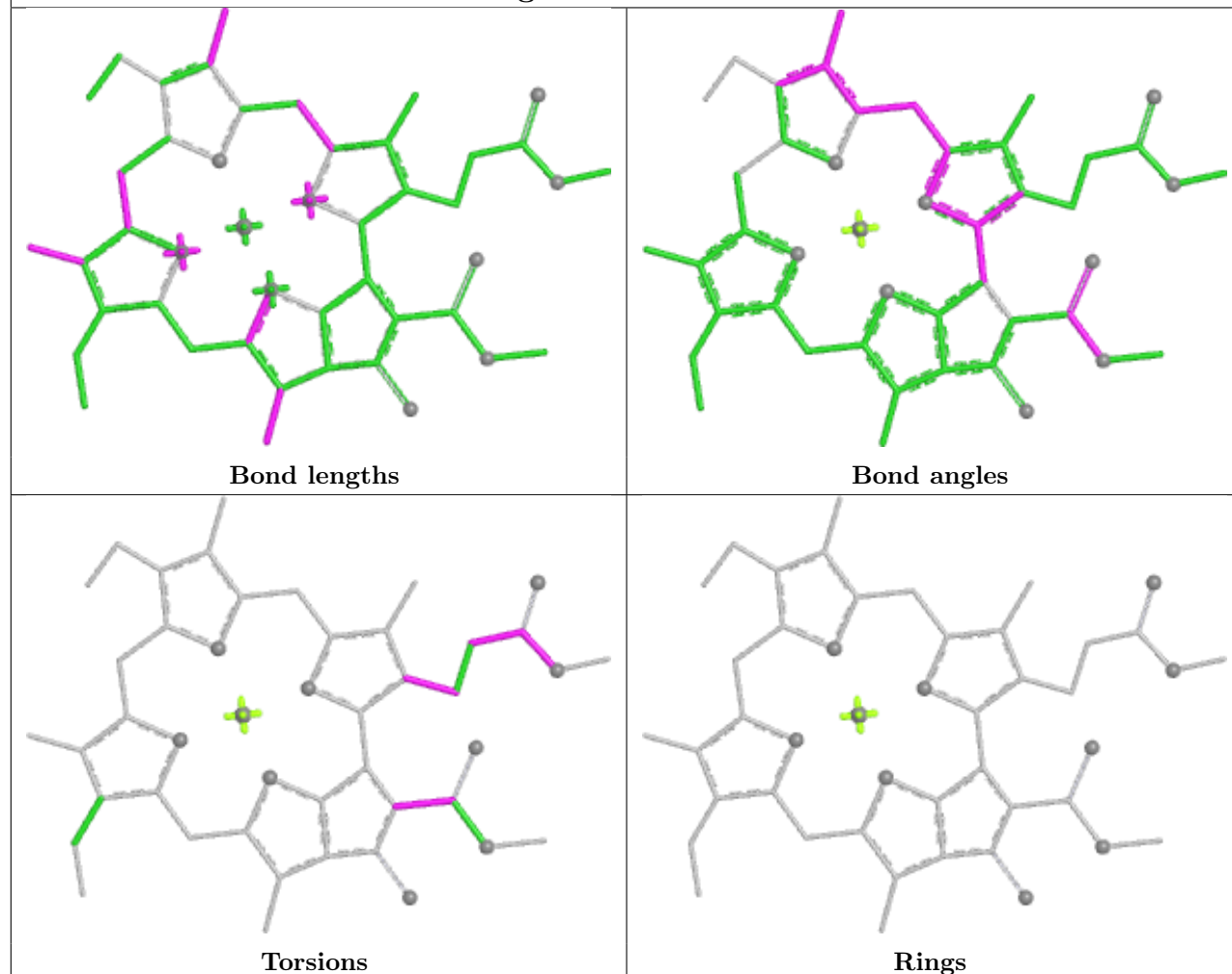




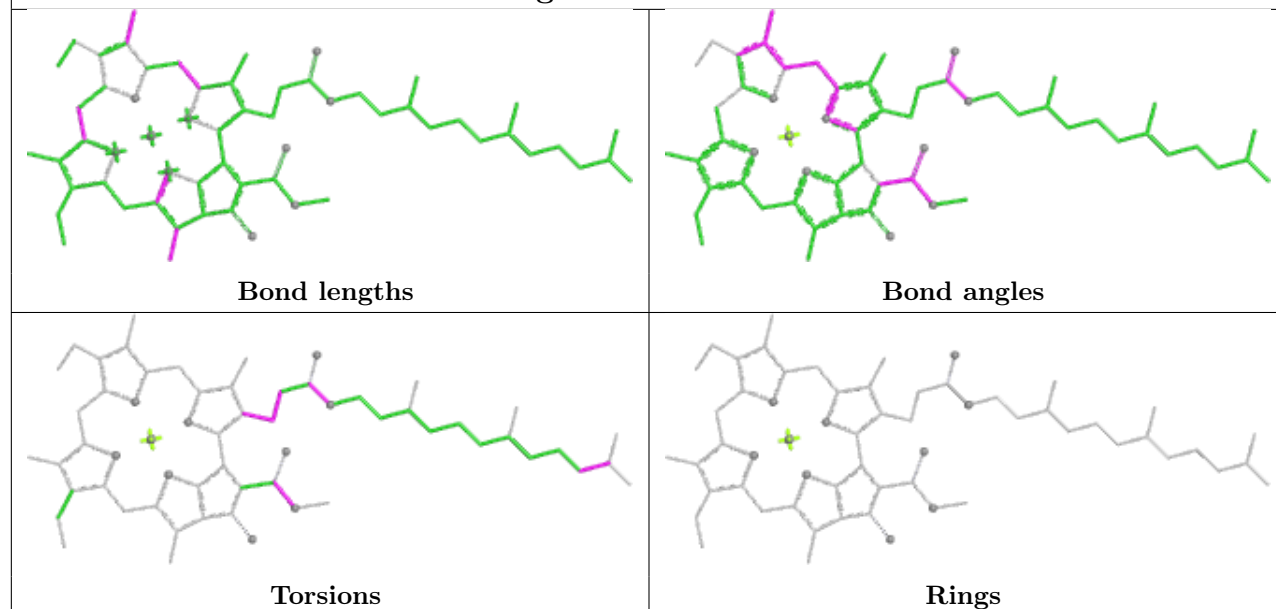
## Ligand CHL 2 306

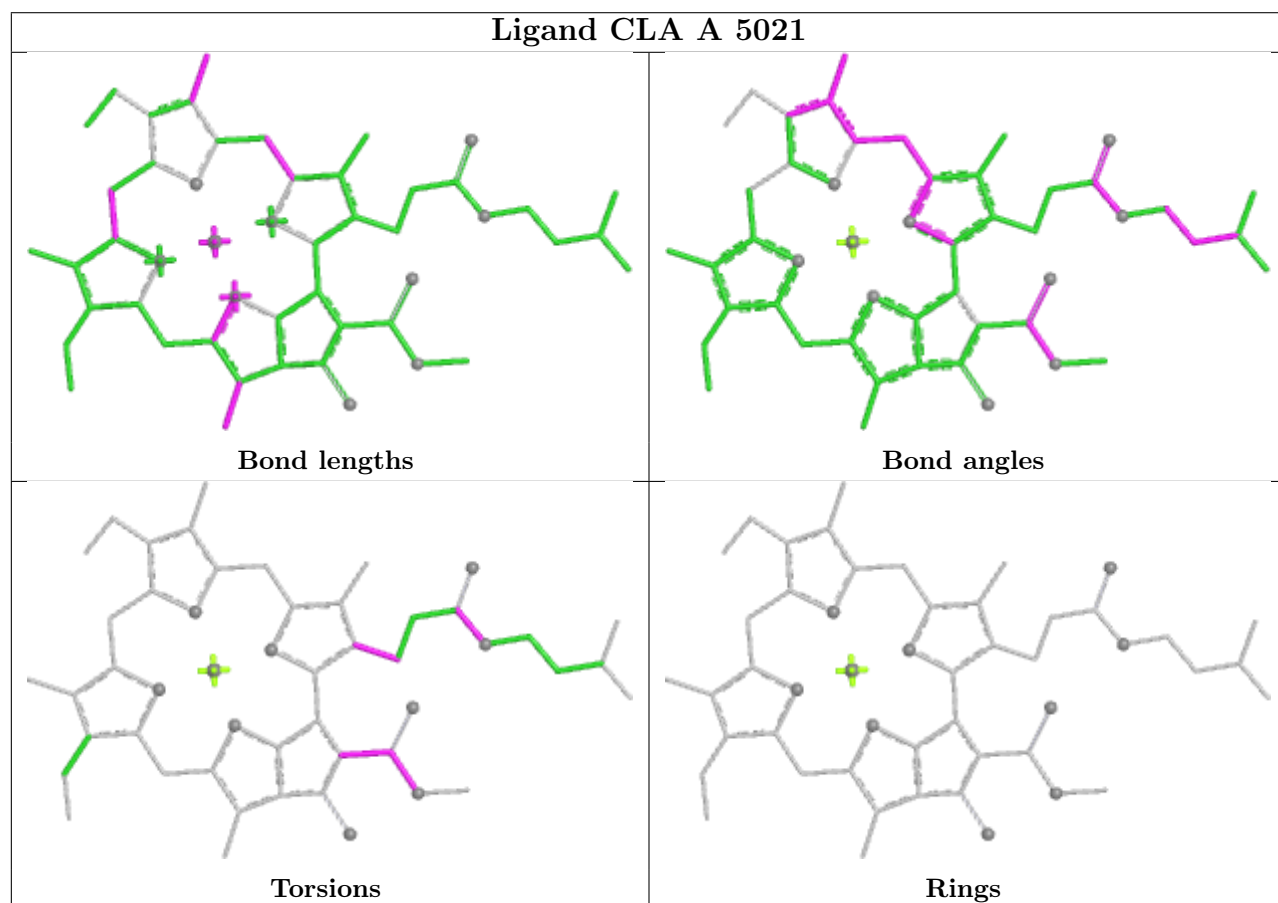
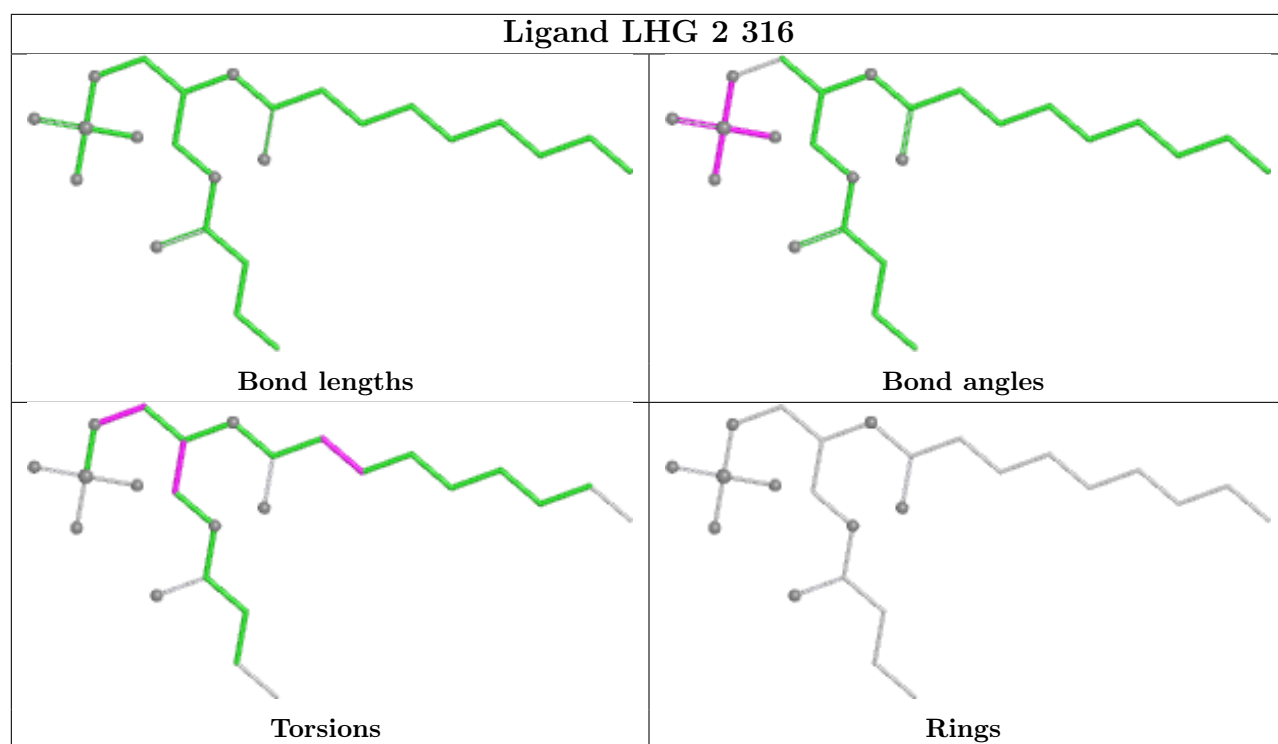


## Ligand CLA 8 310

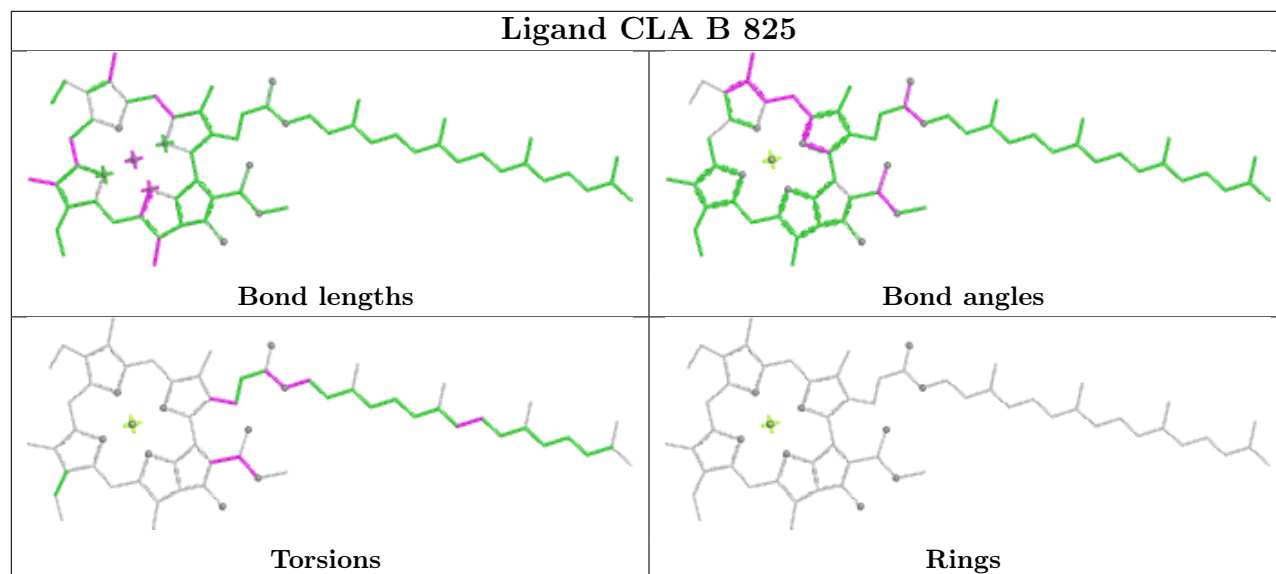


## Ligand CLA 8 301

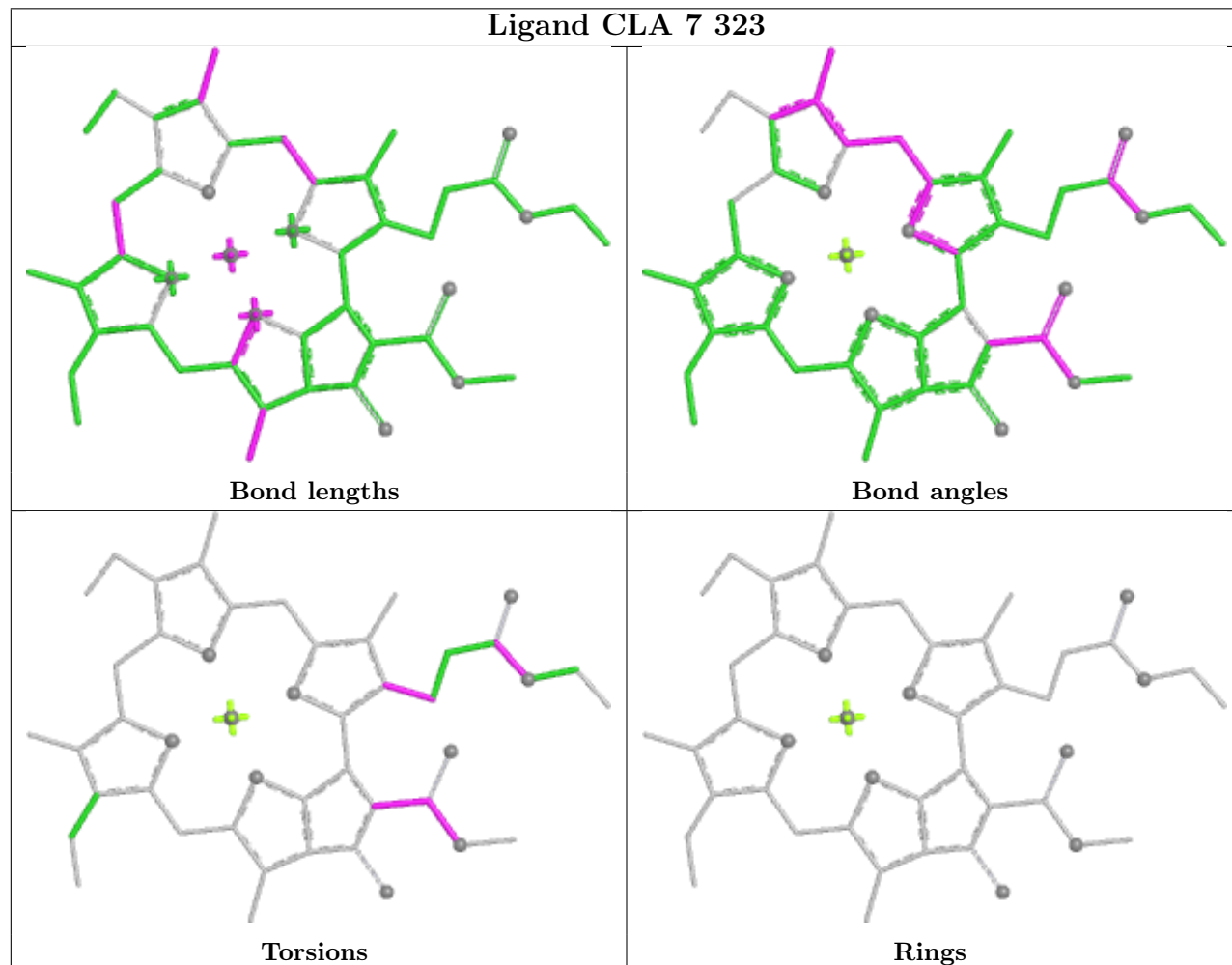


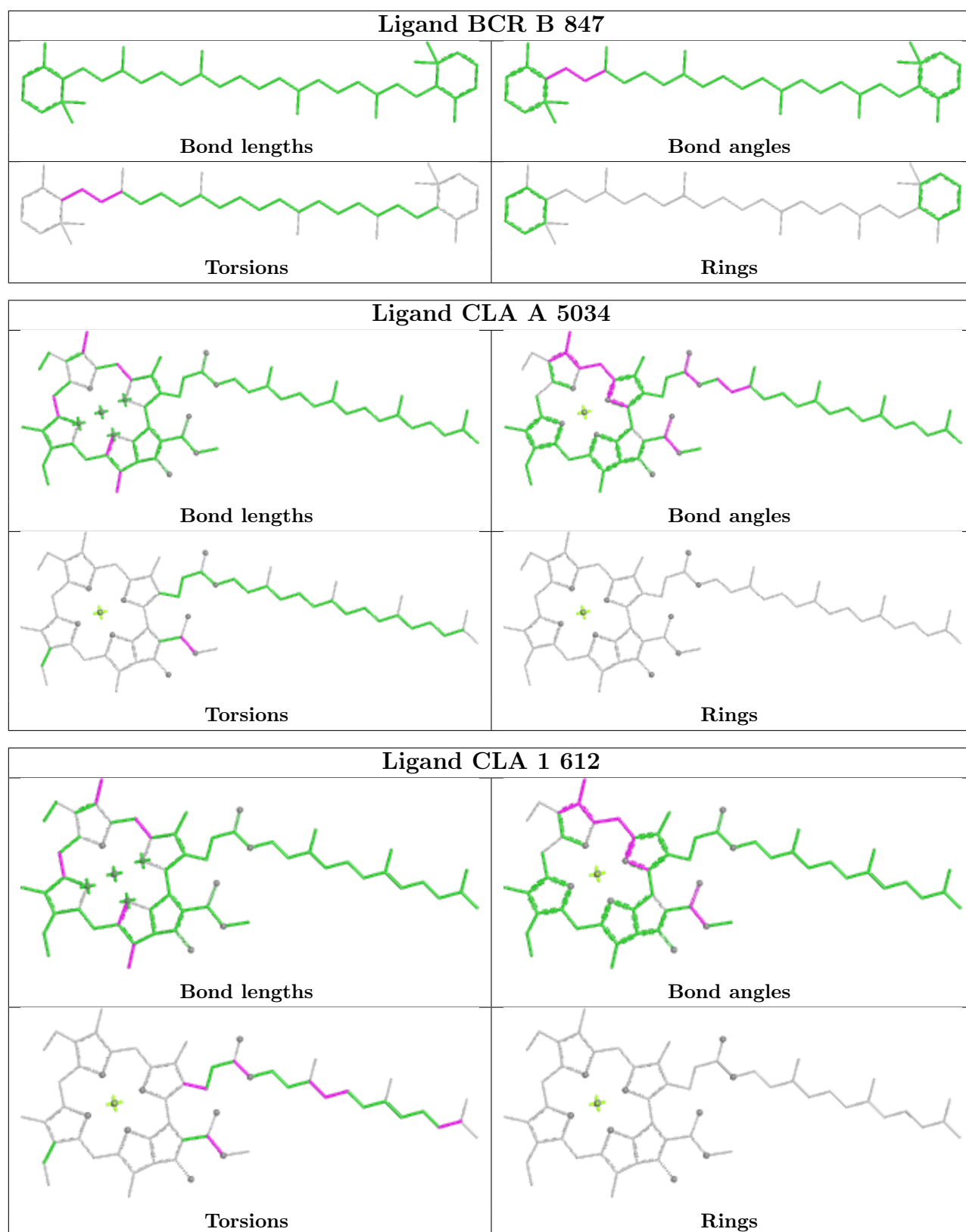


## Ligand CLA B 825

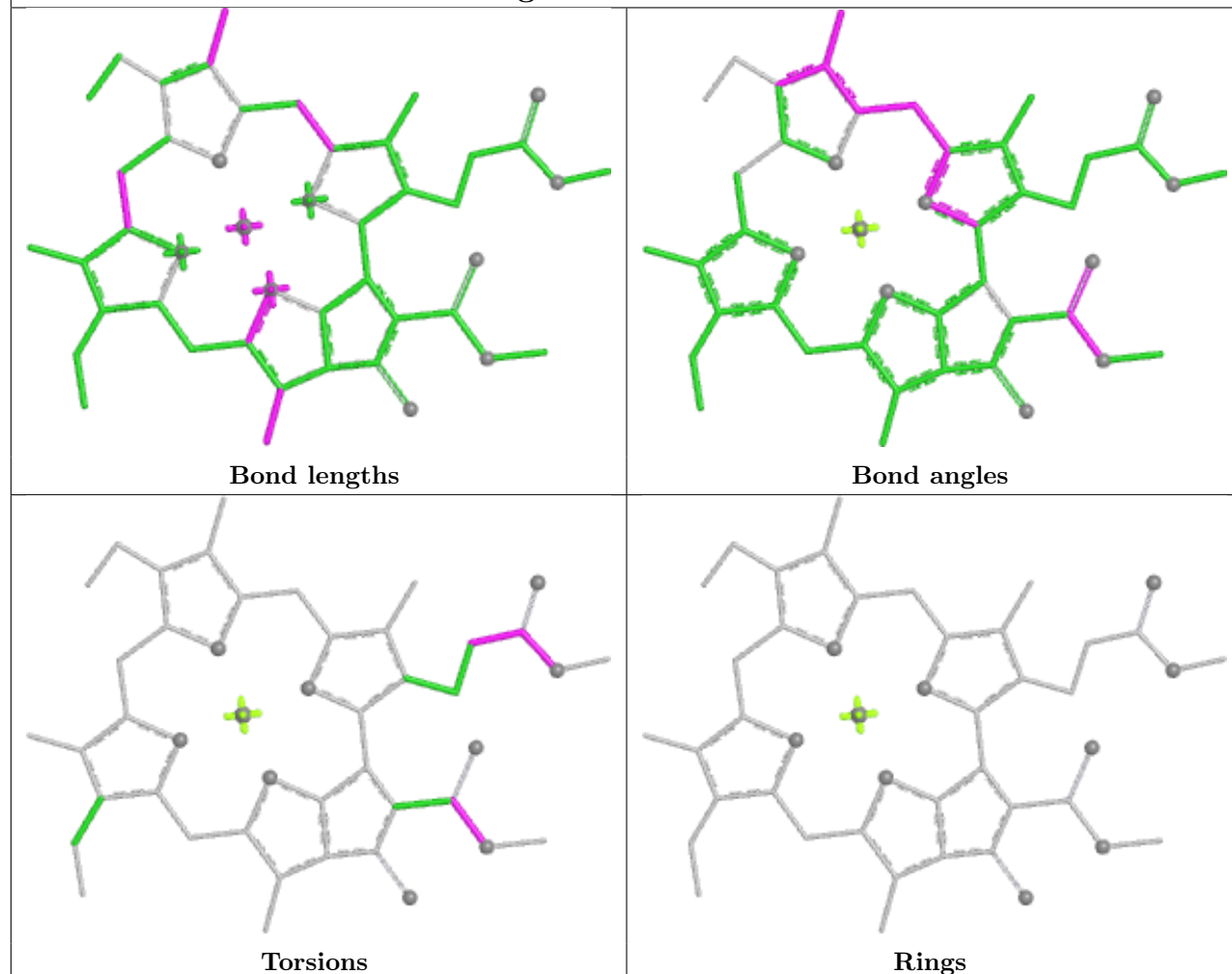


## Ligand CLA 7 323

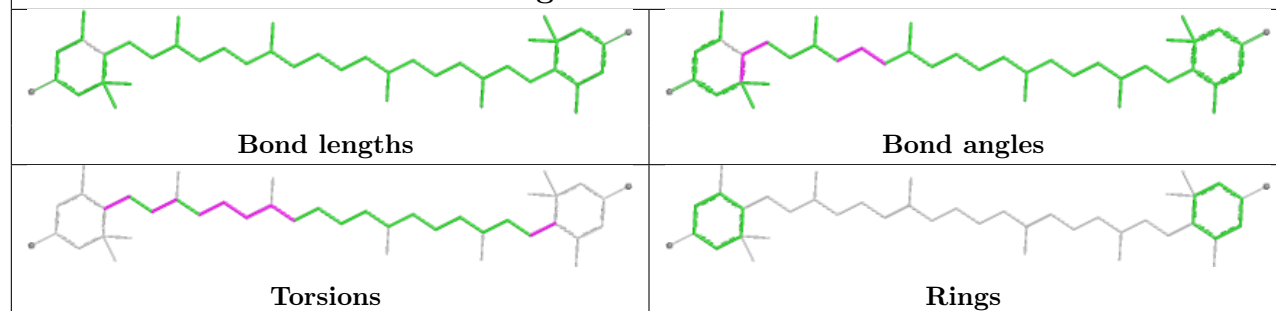




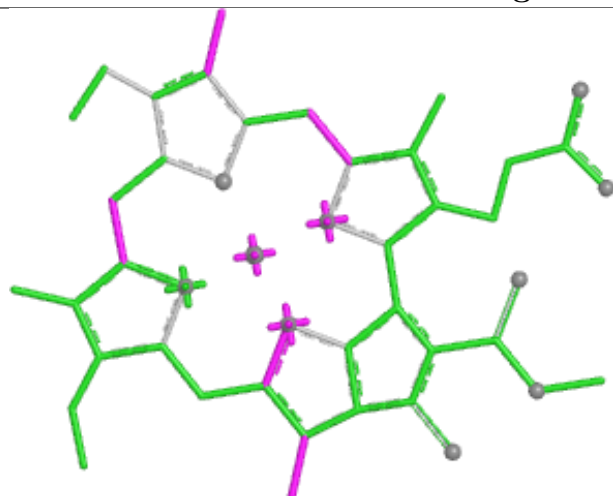
## Ligand CLA 8 313



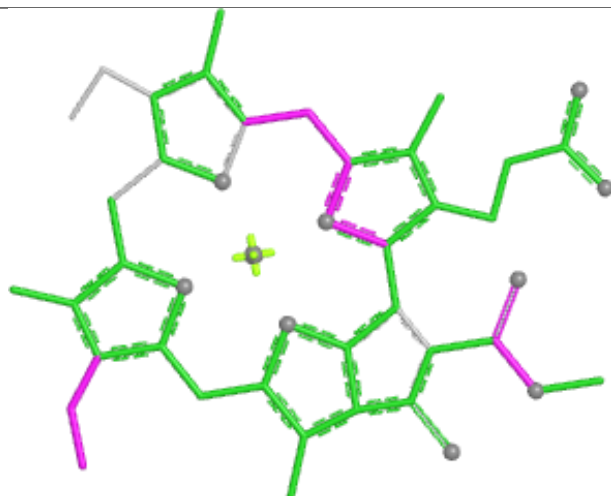
## Ligand LUT 2 315



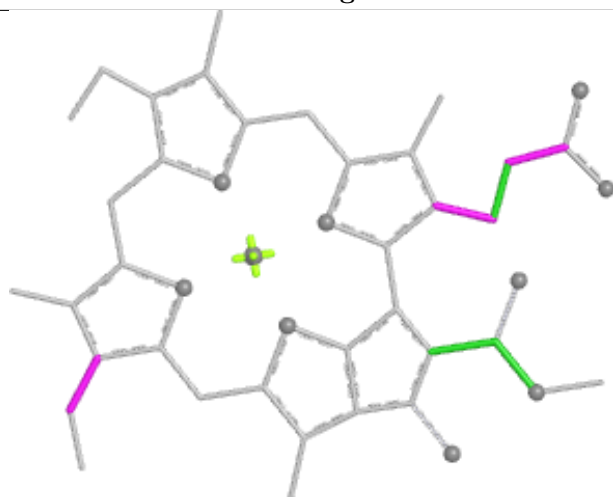
## Ligand CLA G 204



Bond lengths



Bond angles

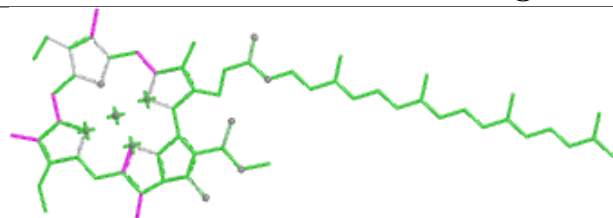


Torsions

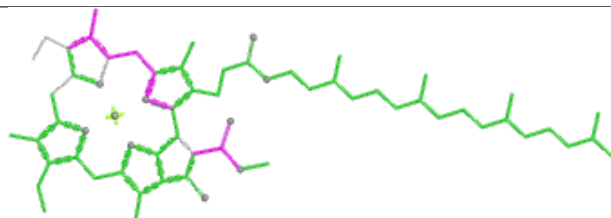


Rings

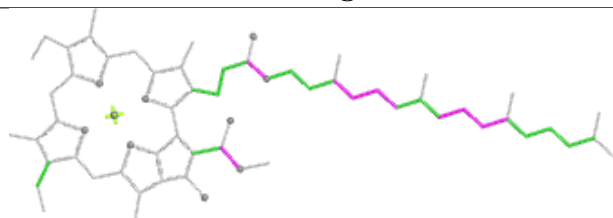
## Ligand CLA B 832



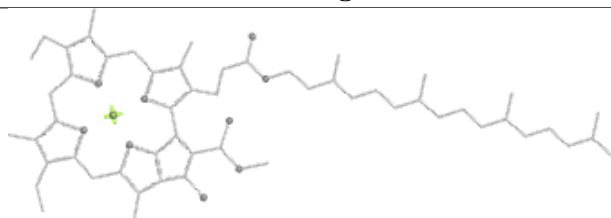
Bond lengths



Bond angles



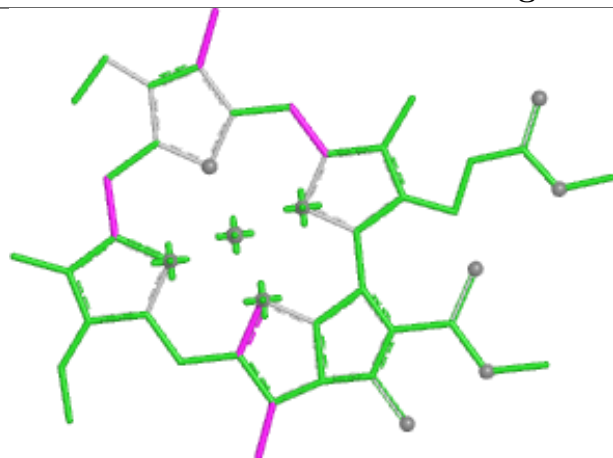
Torsions



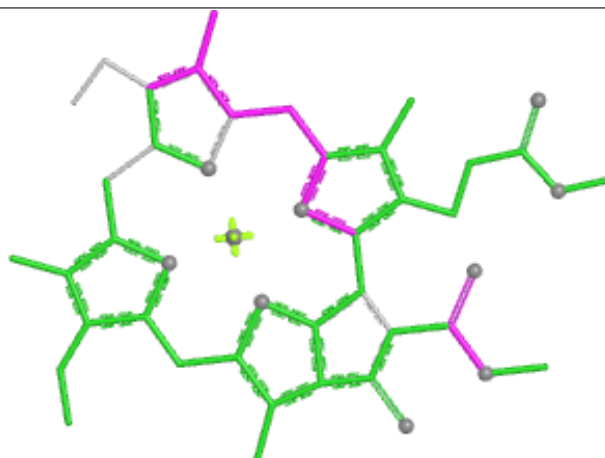
Rings



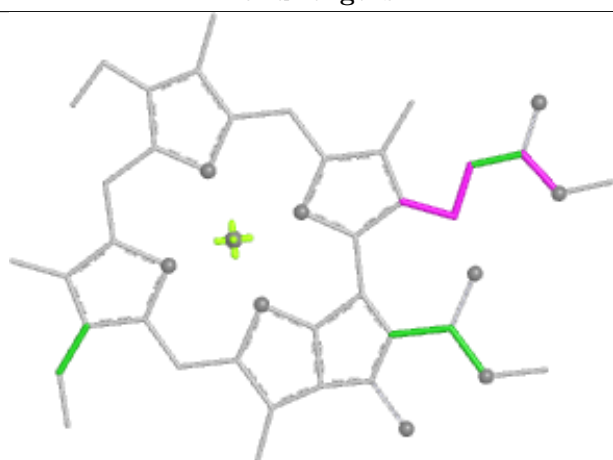
## Ligand CLA 3 303



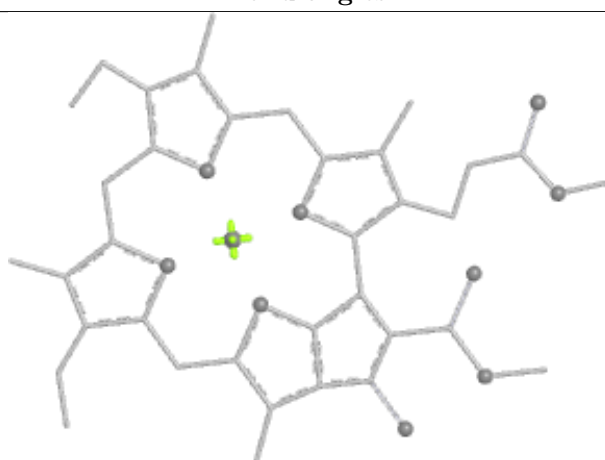
Bond lengths



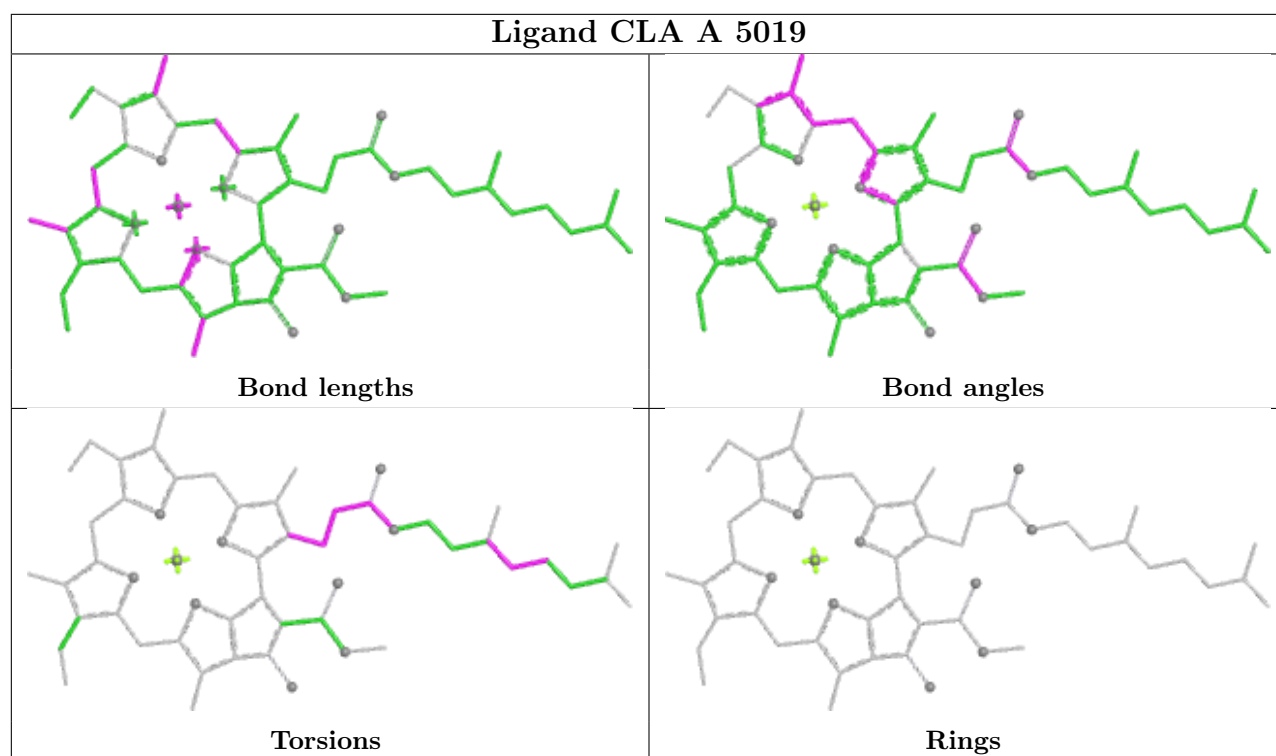
Bond angles



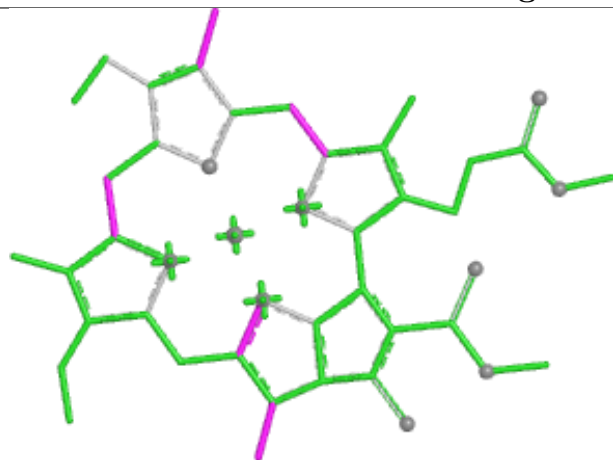
Torsions



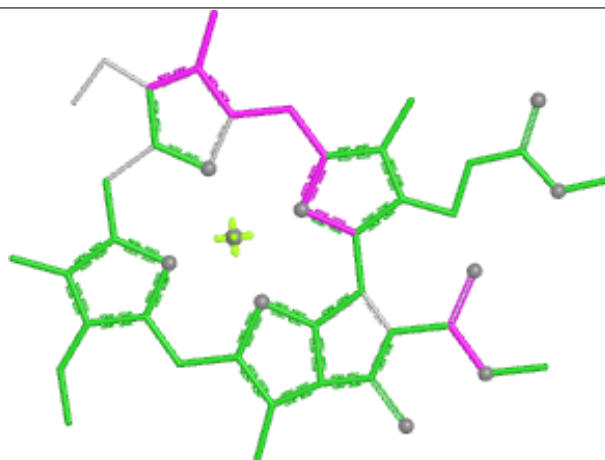
Rings



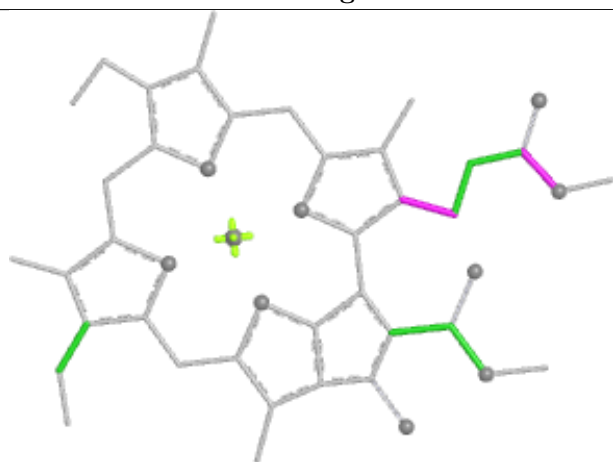
## Ligand CLA 7 309



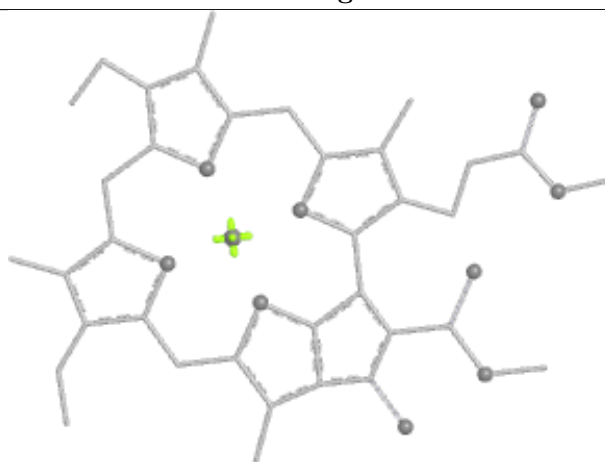
Bond lengths



Bond angles

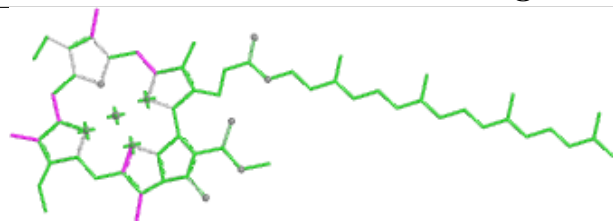


Torsions

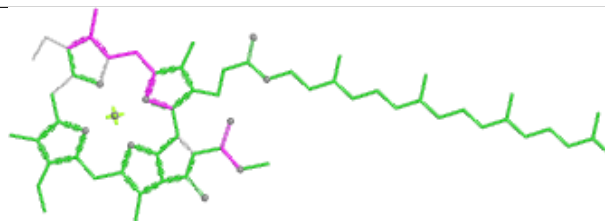


Rings

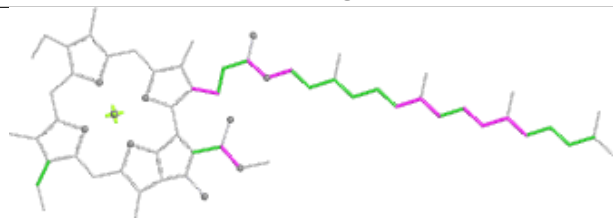
## Ligand CLA B 818



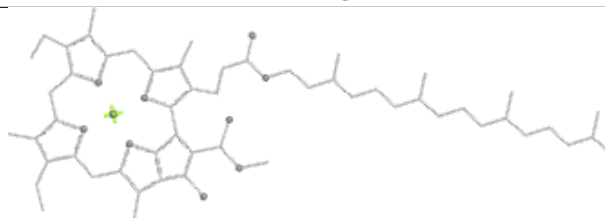
Bond lengths



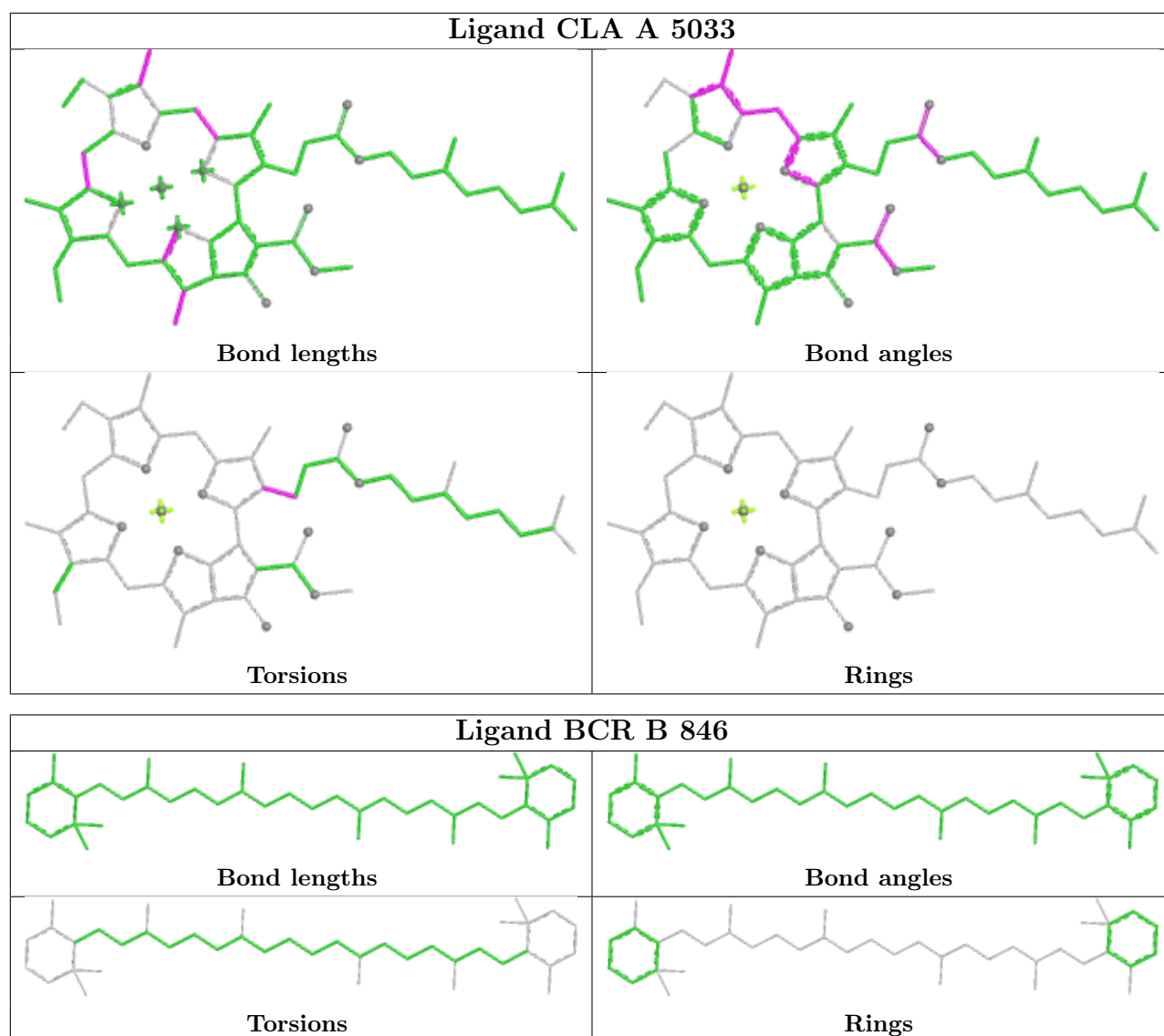
Bond angles

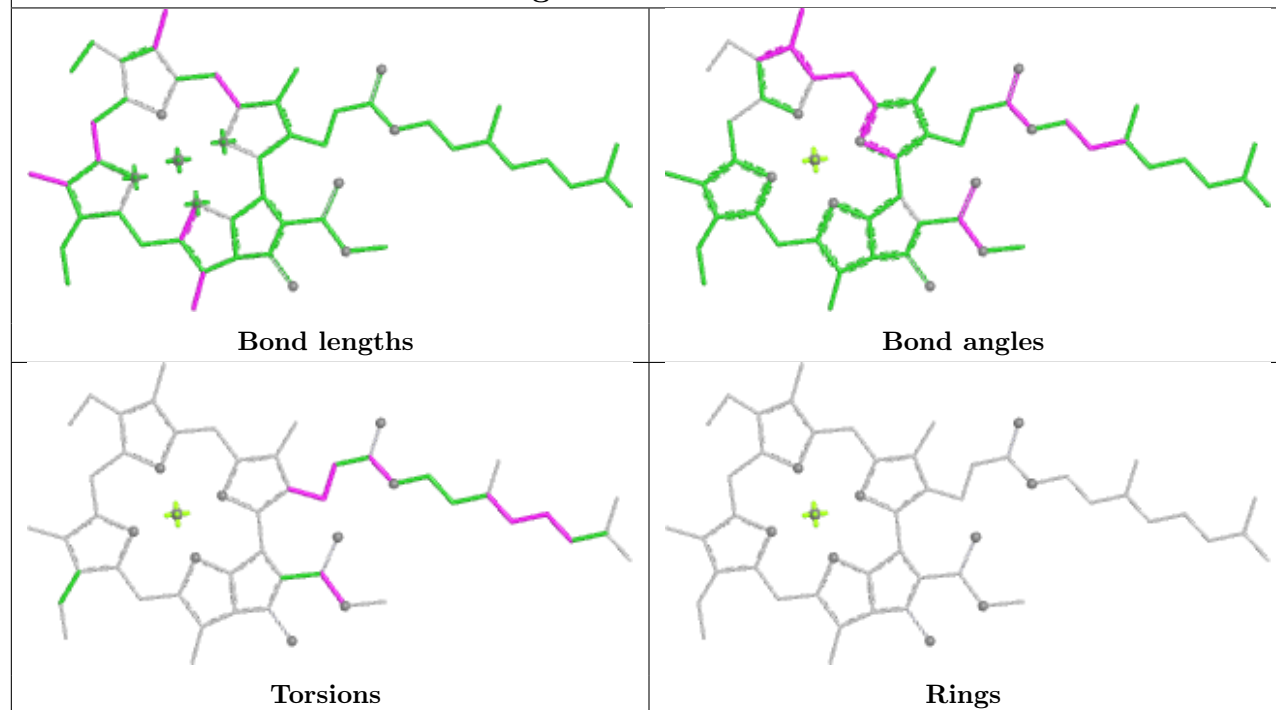
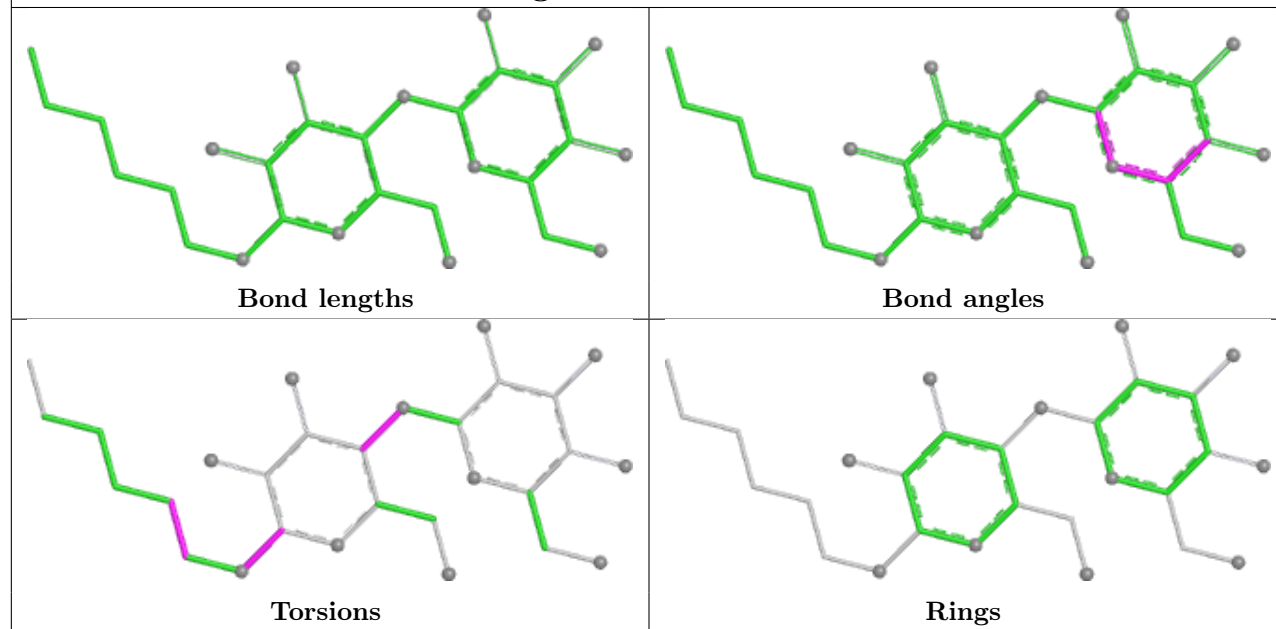


Torsions

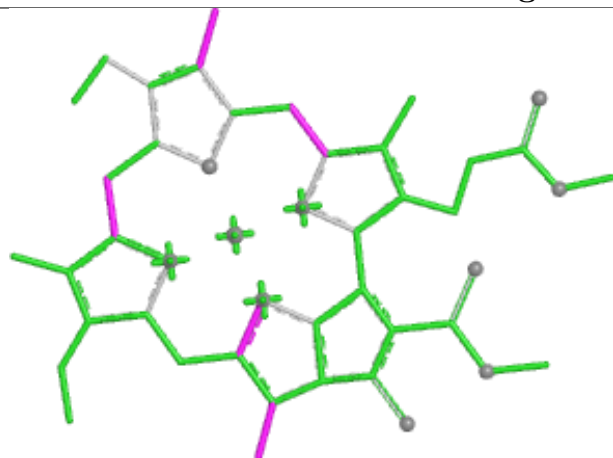


Rings

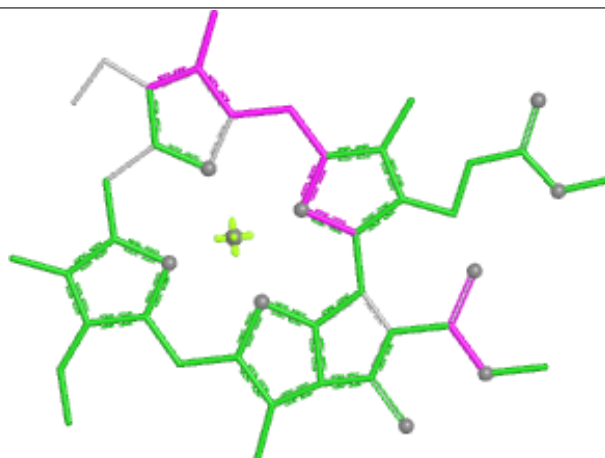


**Ligand CLA B 823****Ligand LMU 9 616**

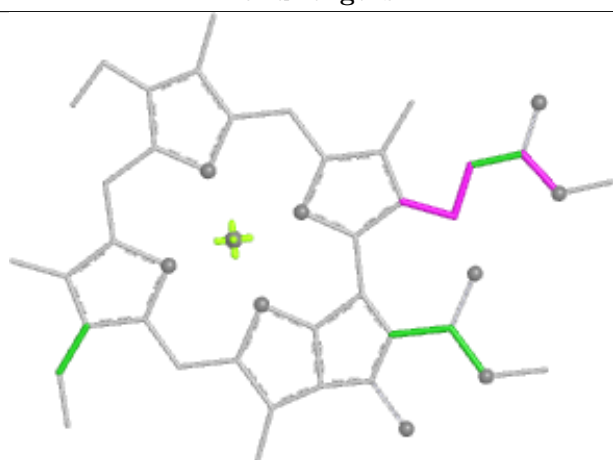
## Ligand CLA 2 301



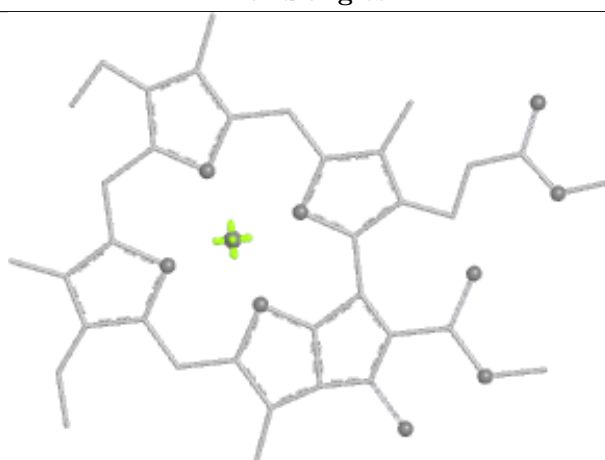
Bond lengths



Bond angles

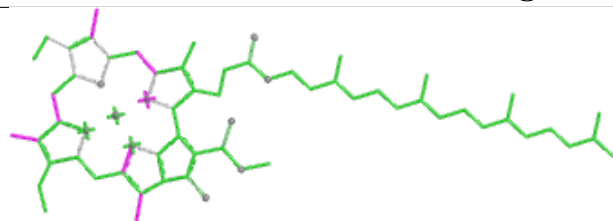


Torsions

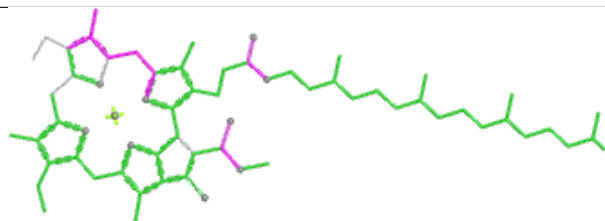


Rings

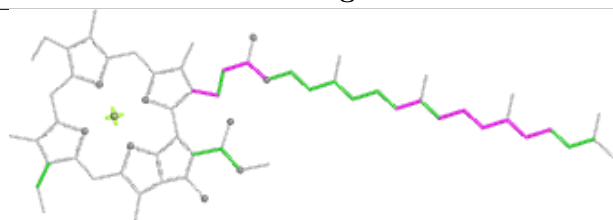
## Ligand CLA 8 303



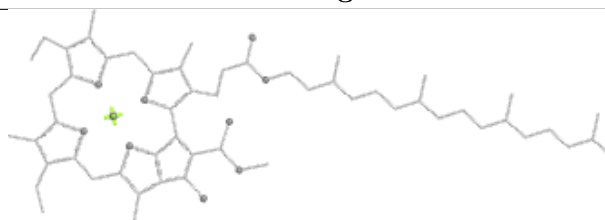
Bond lengths



Bond angles

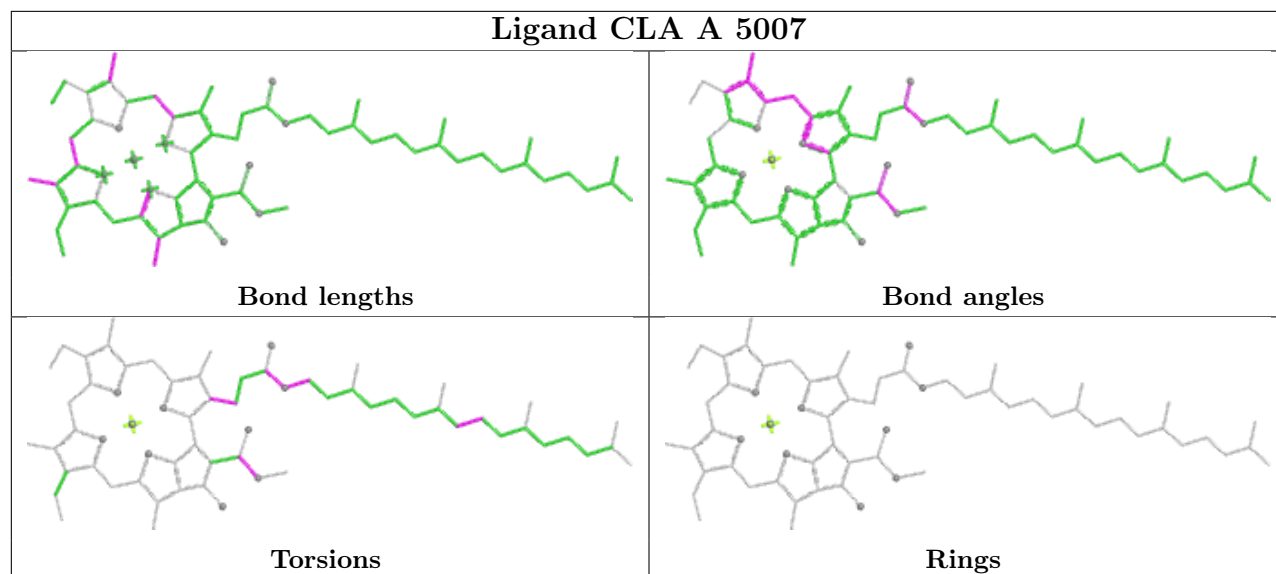


Torsions

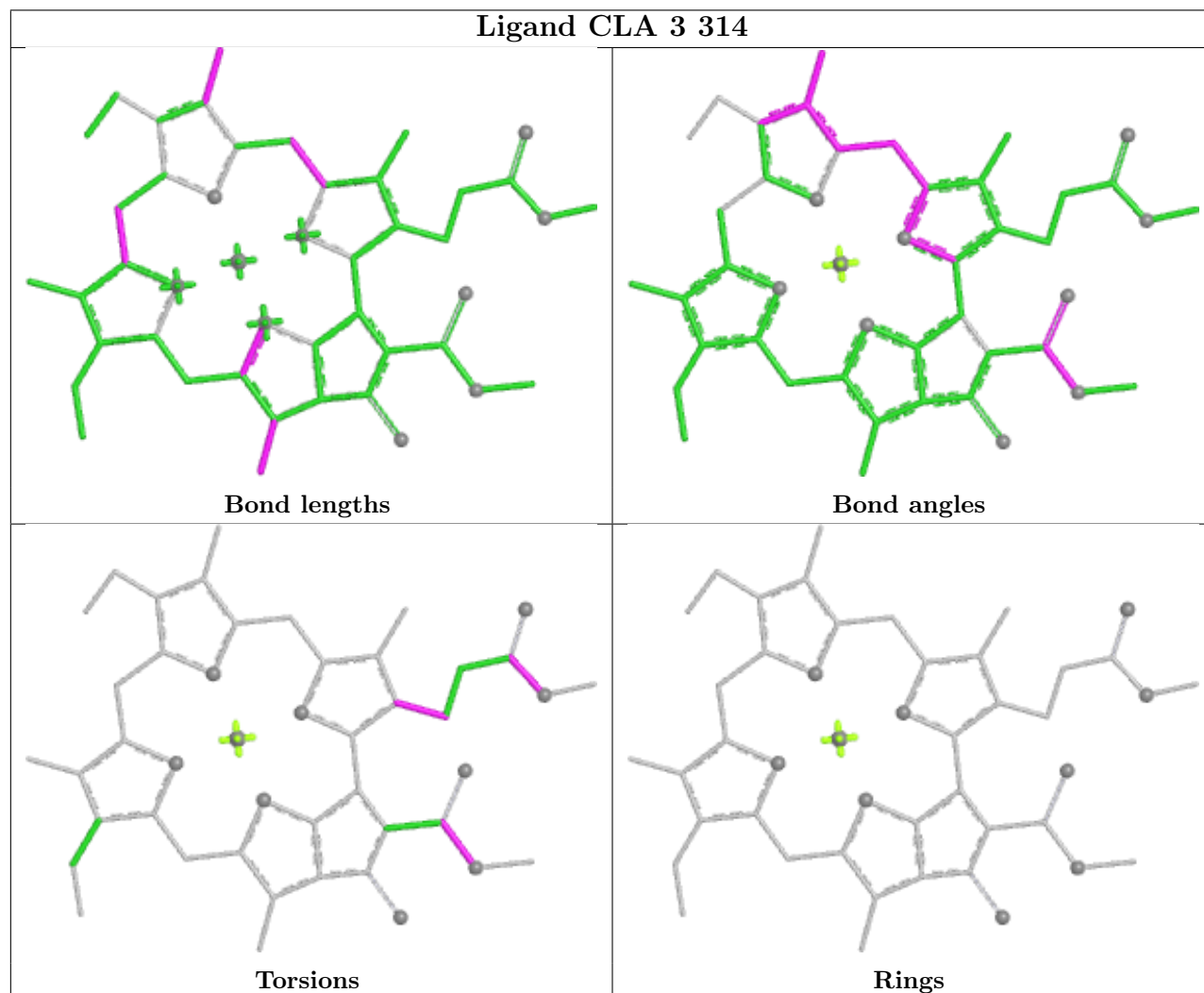


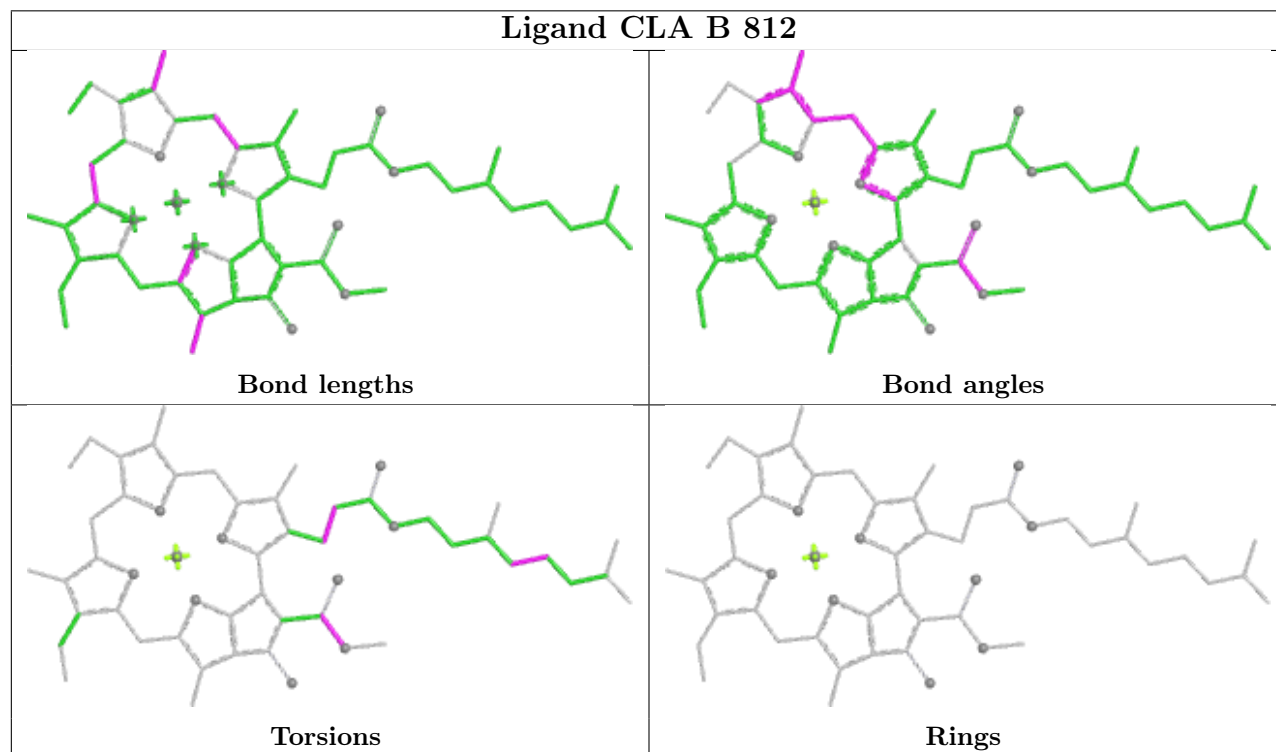
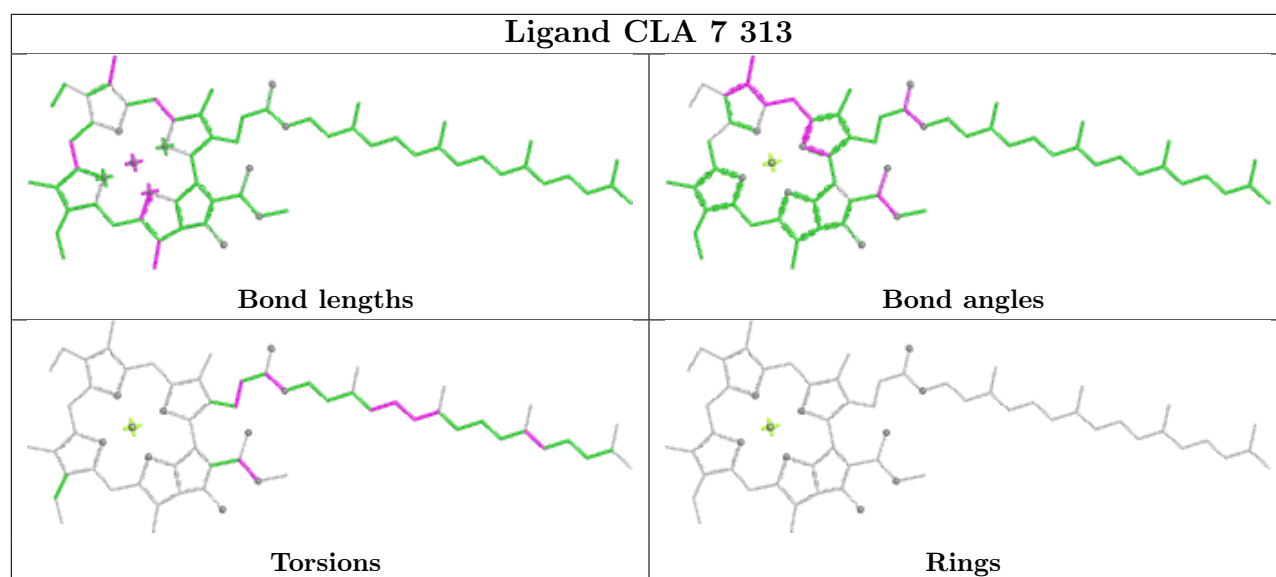
Rings

## Ligand CLA A 5007



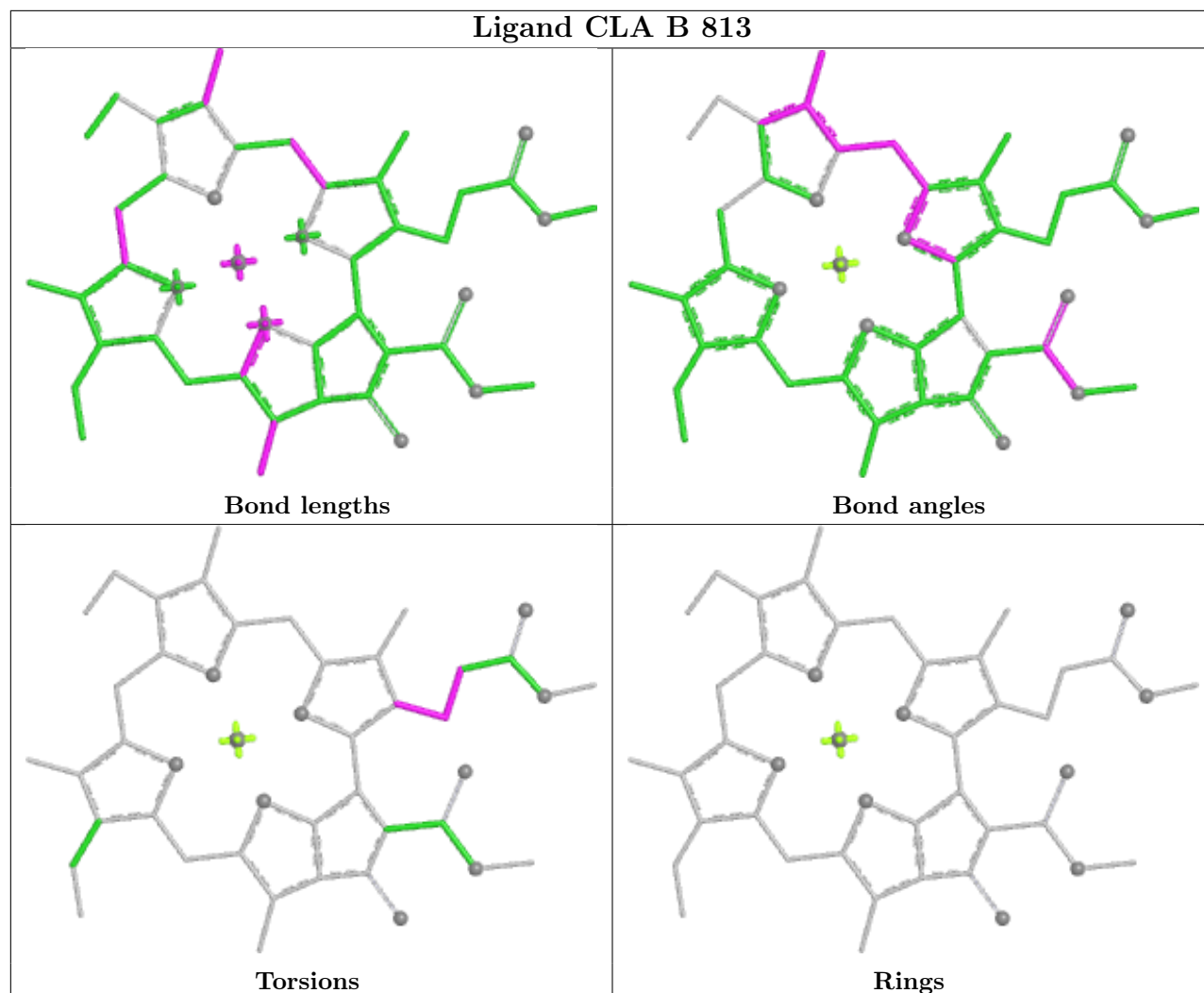
## Ligand CLA 3 314



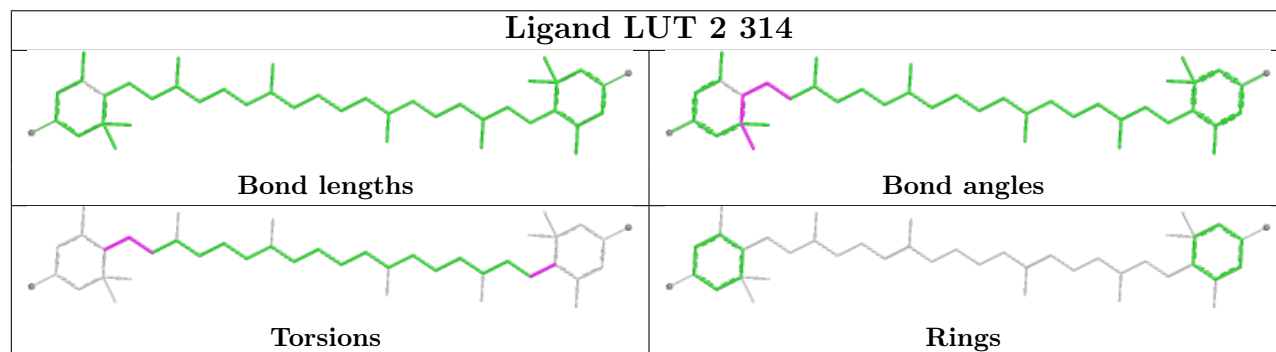




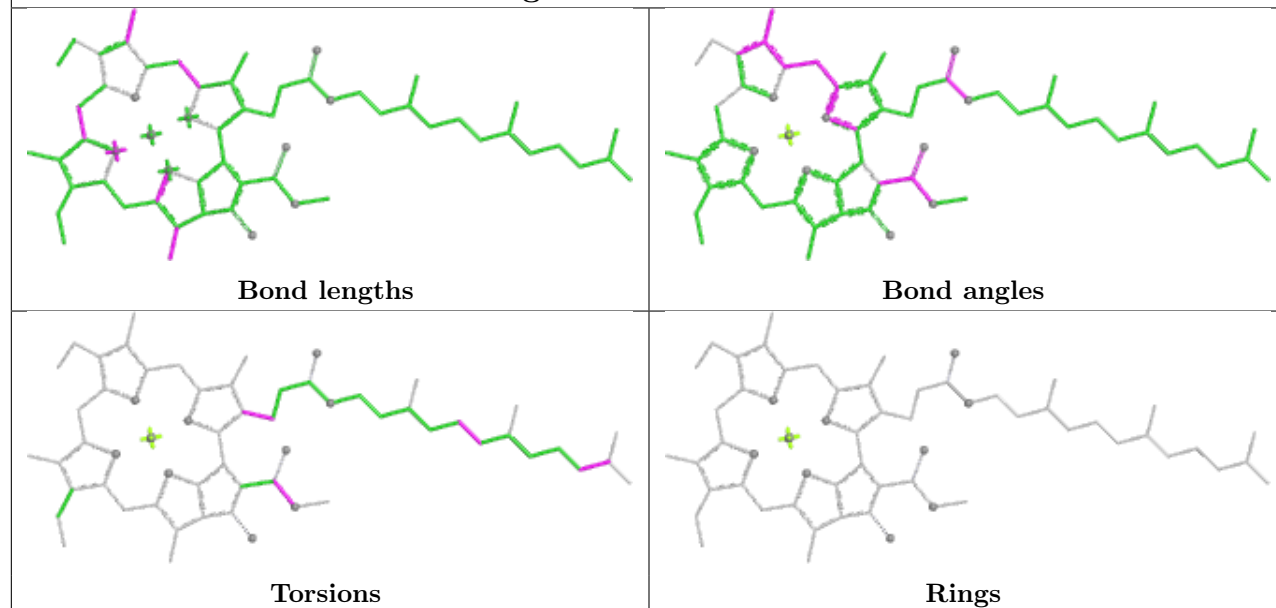
## Ligand CLA B 813



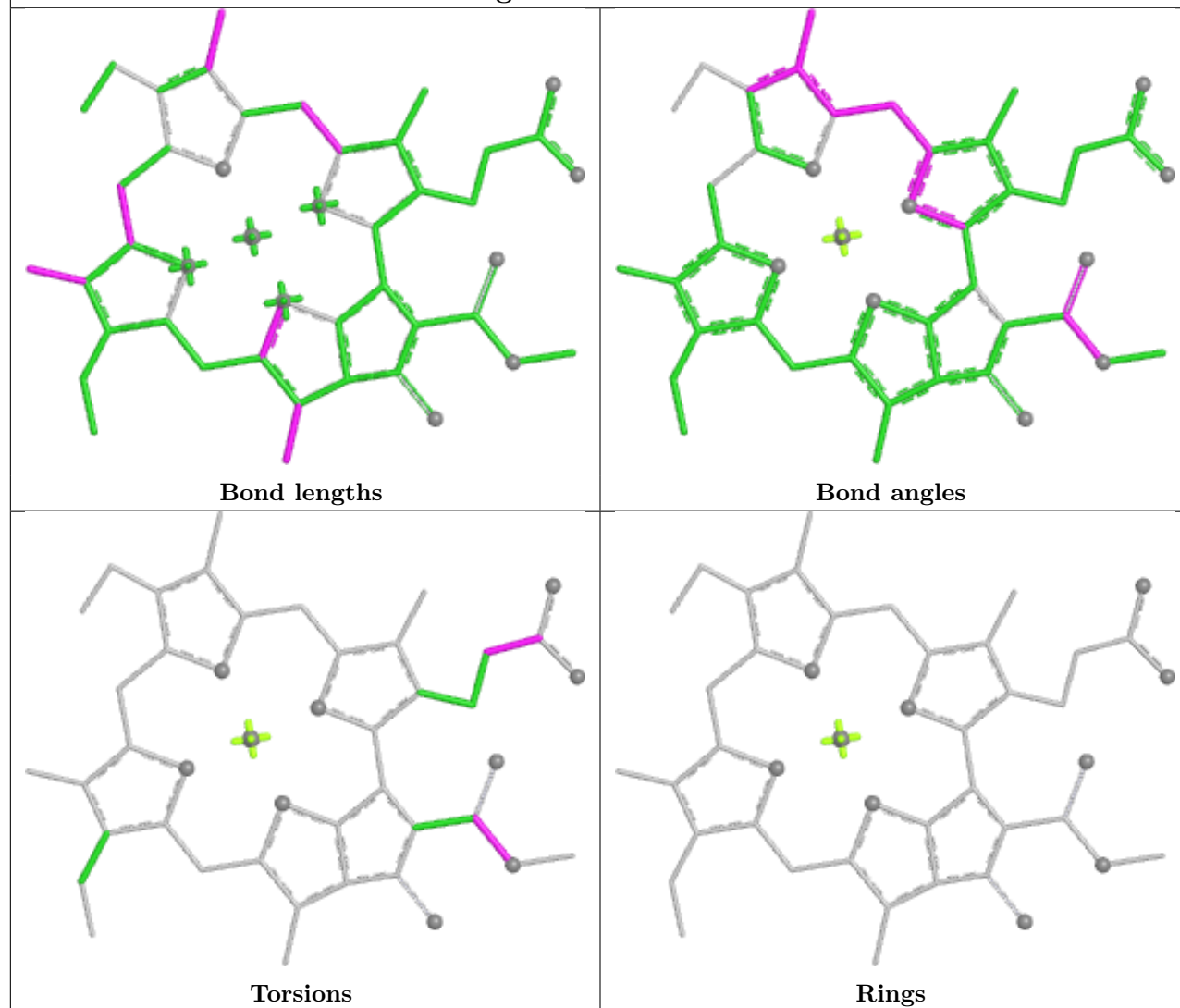
## Ligand LUT 2 314

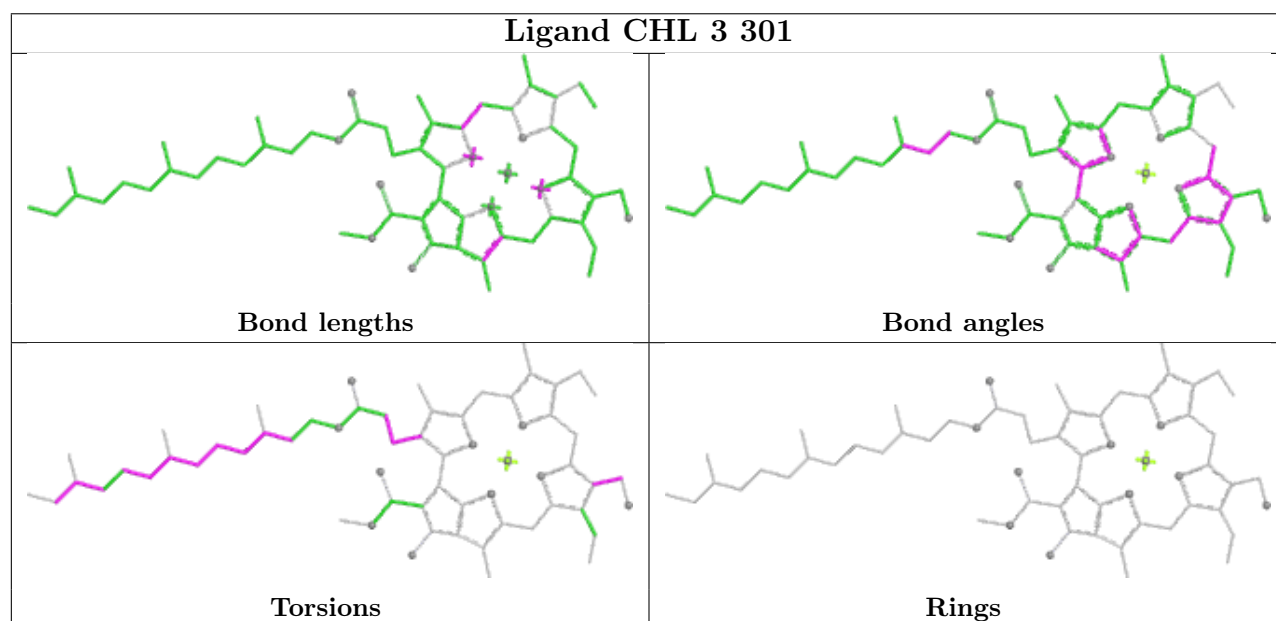
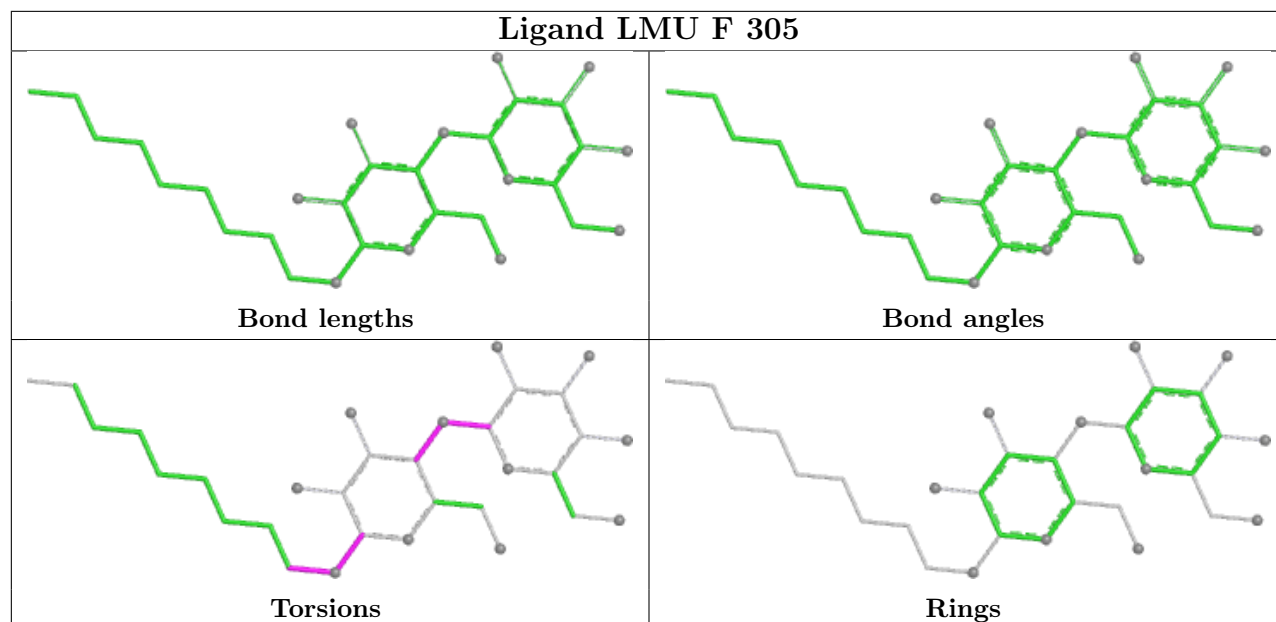


## Ligand CLA A 5042

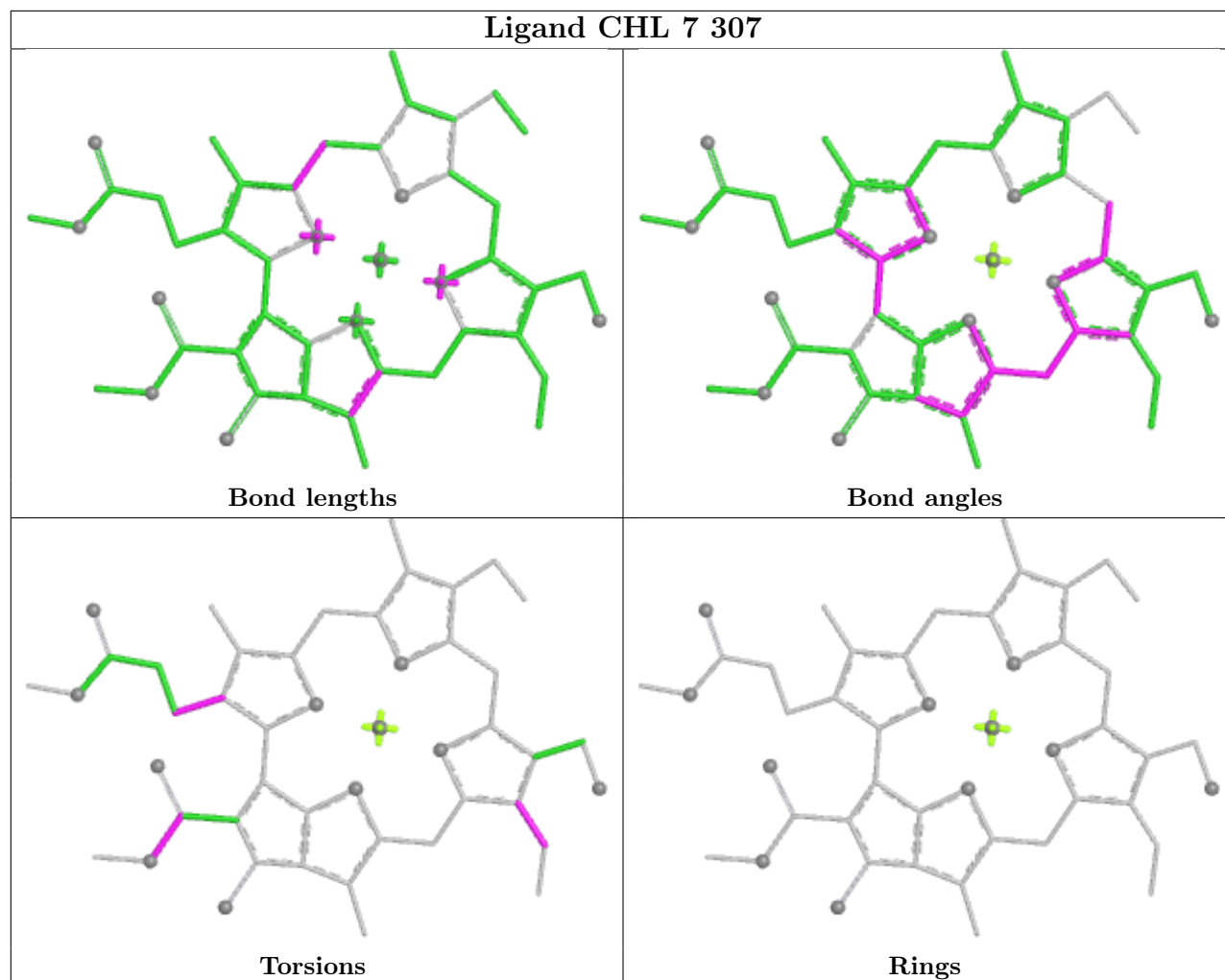


## Ligand CLA 1 605

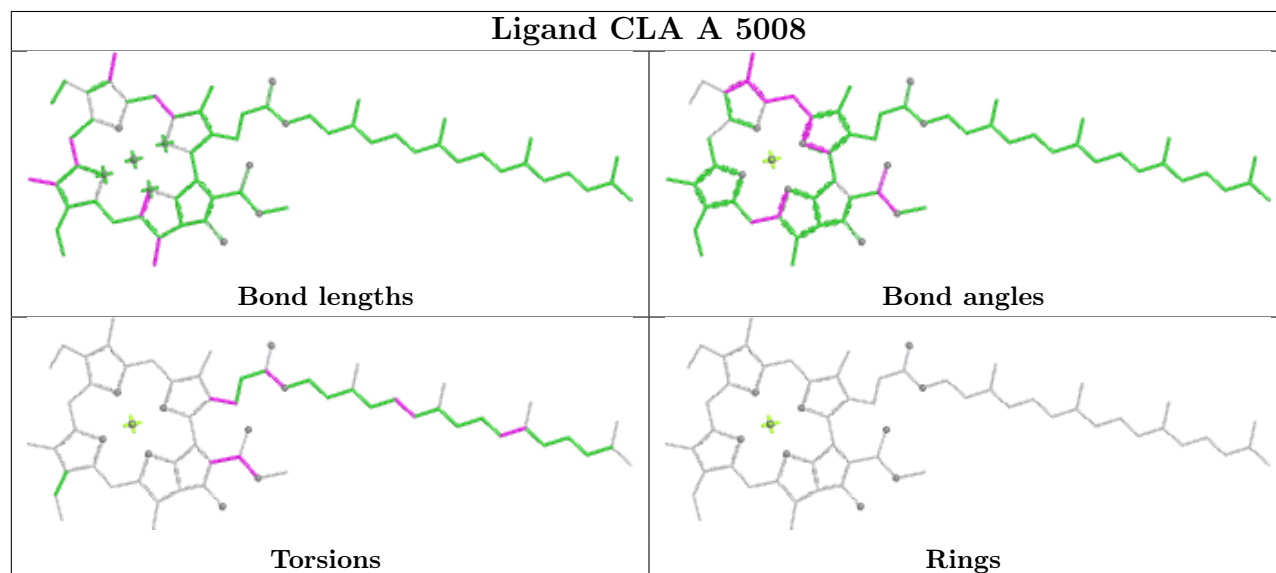




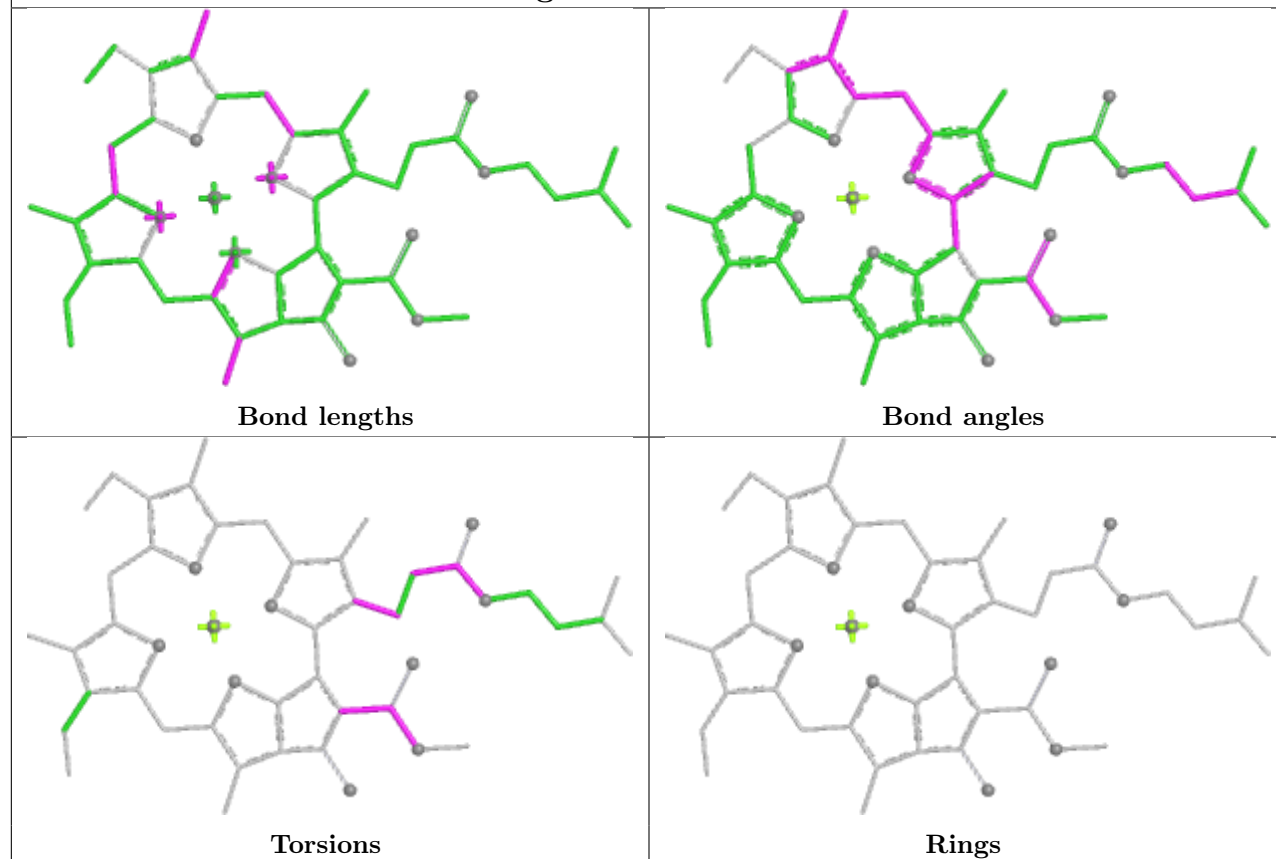
## Ligand CHL 7 307



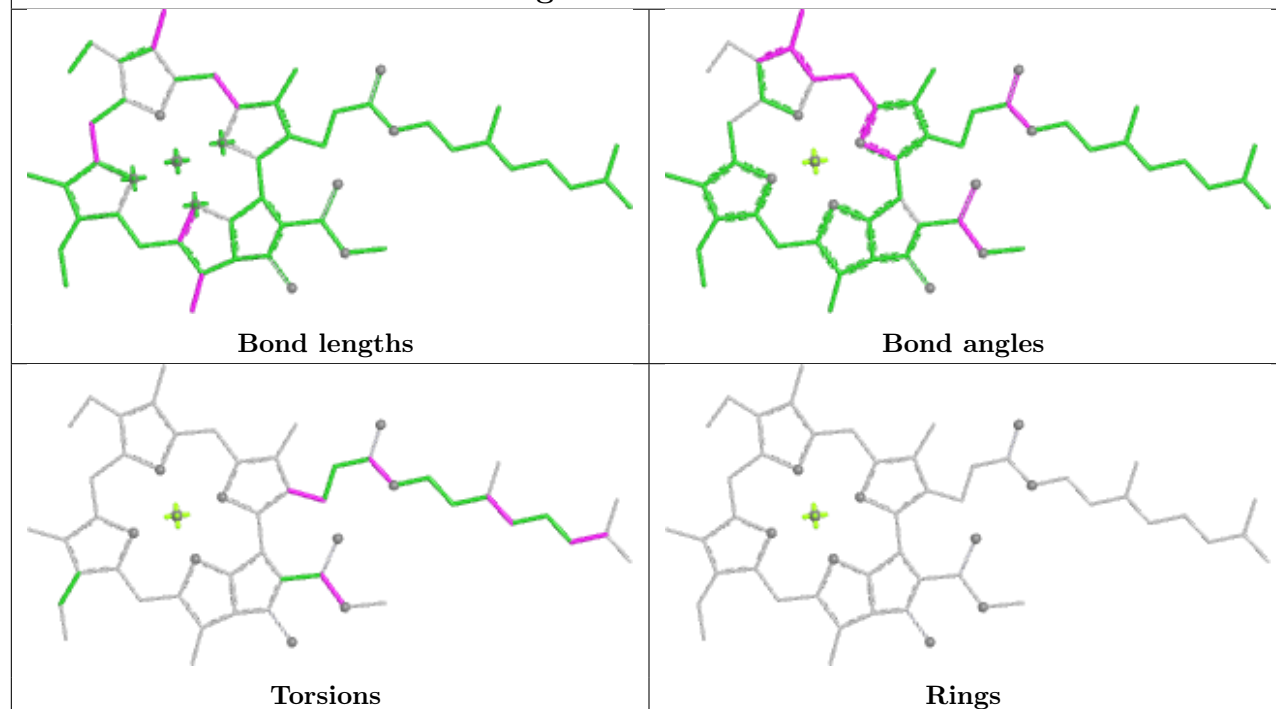
## Ligand CLA A 5008

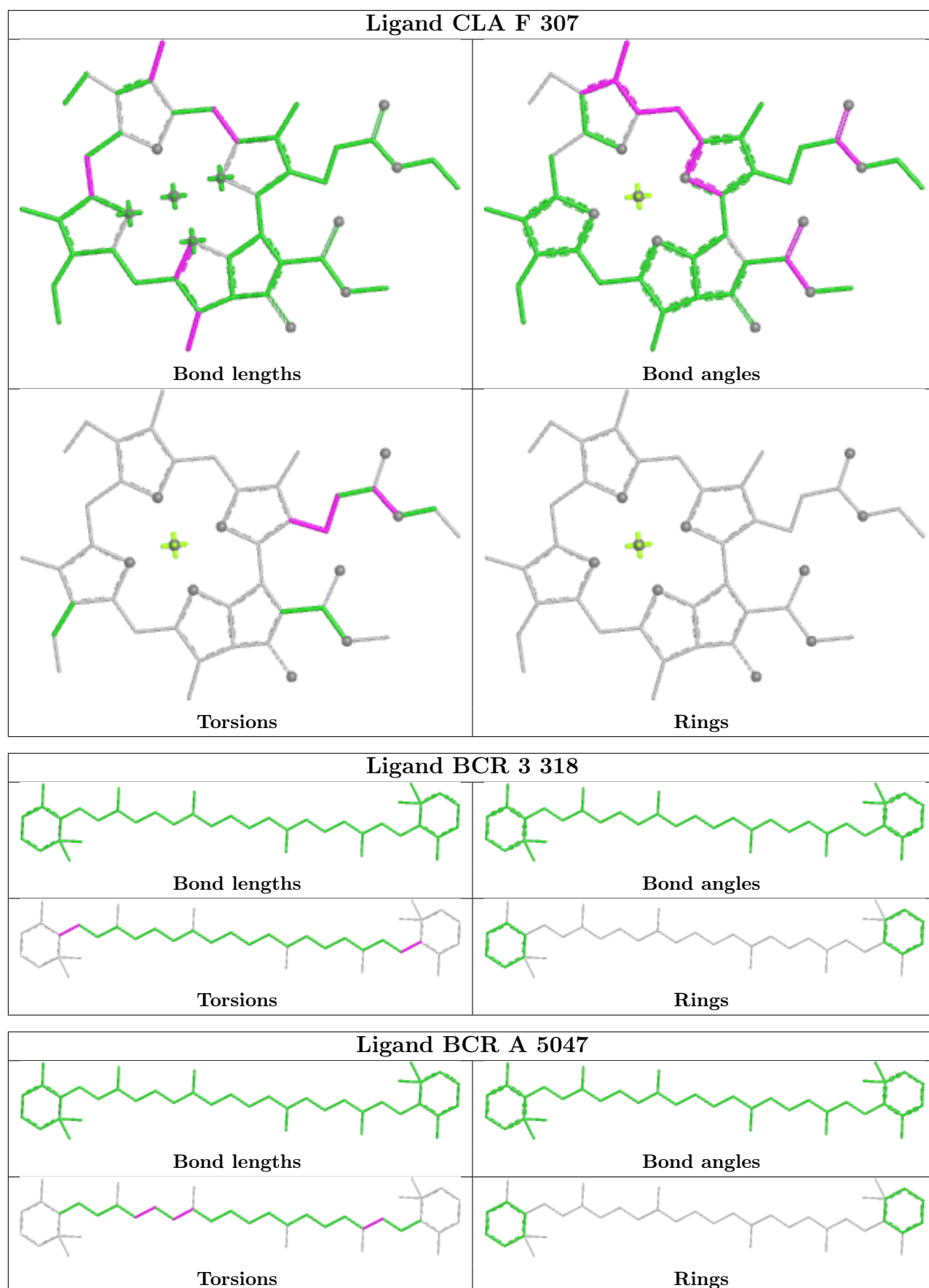


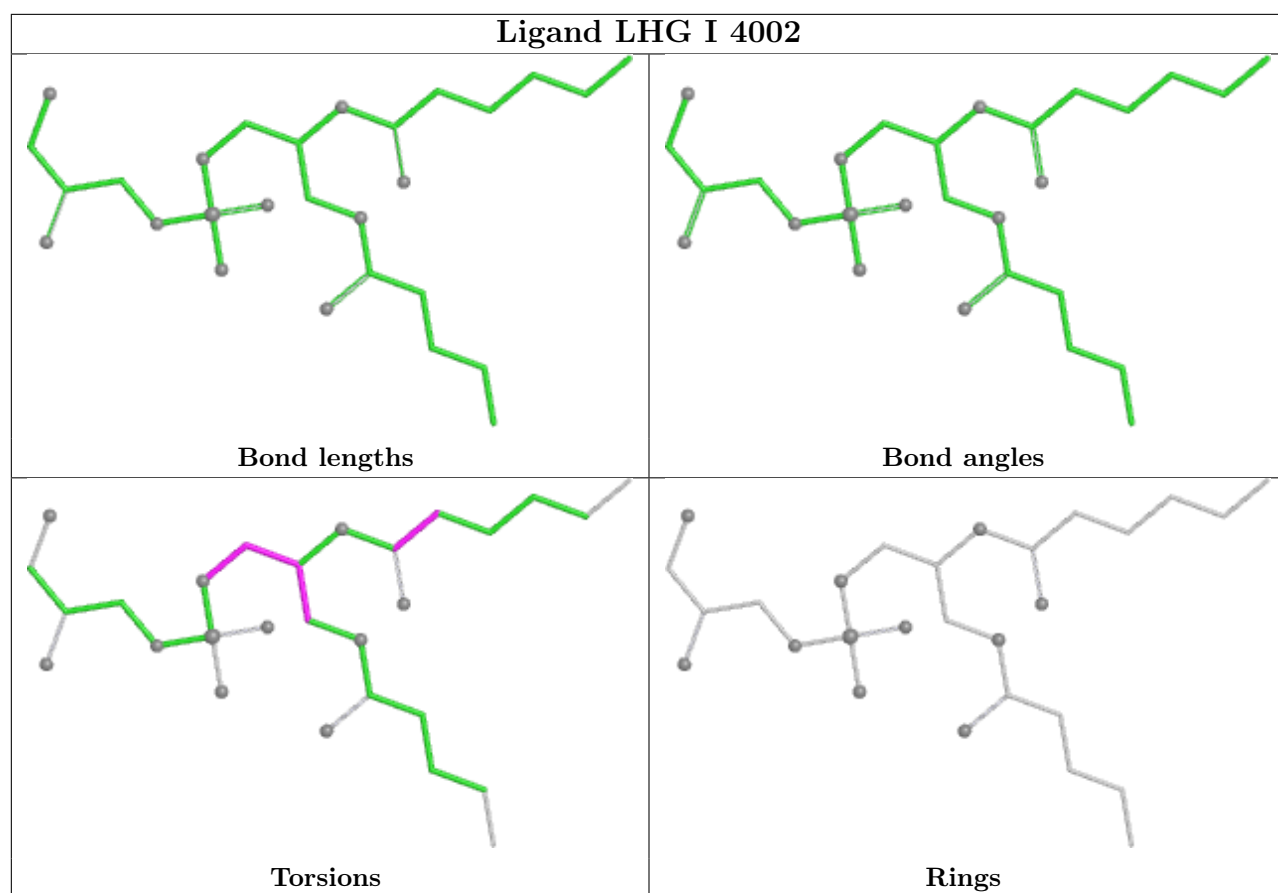
## Ligand CLA 9 610

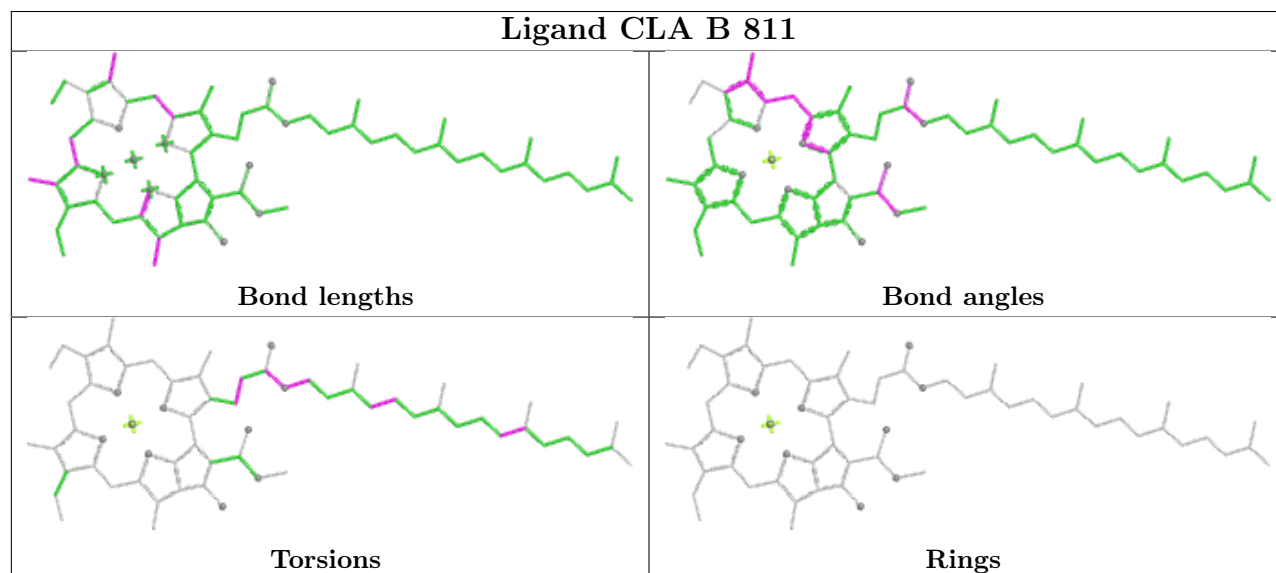
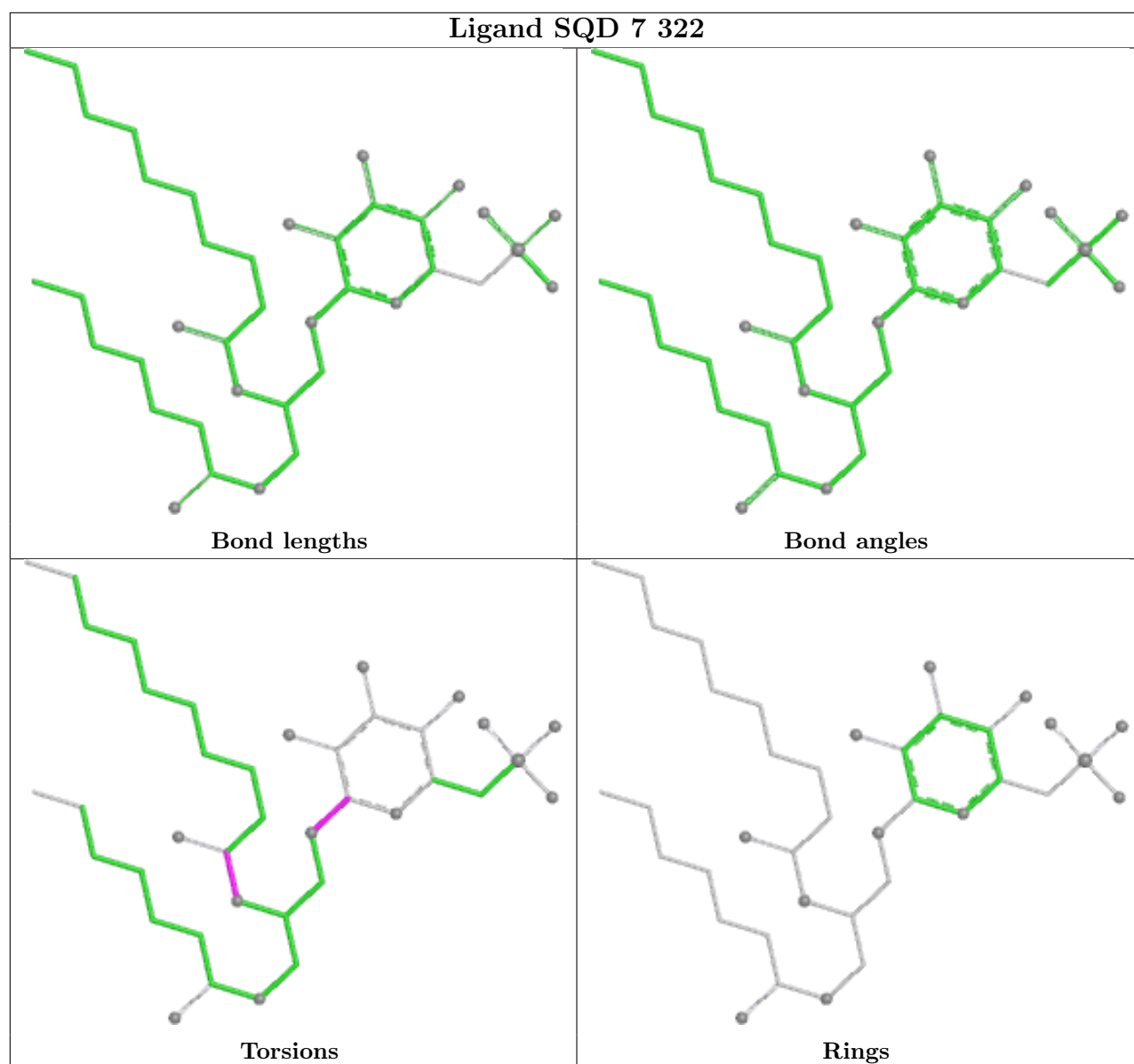


## Ligand CLA 3 324

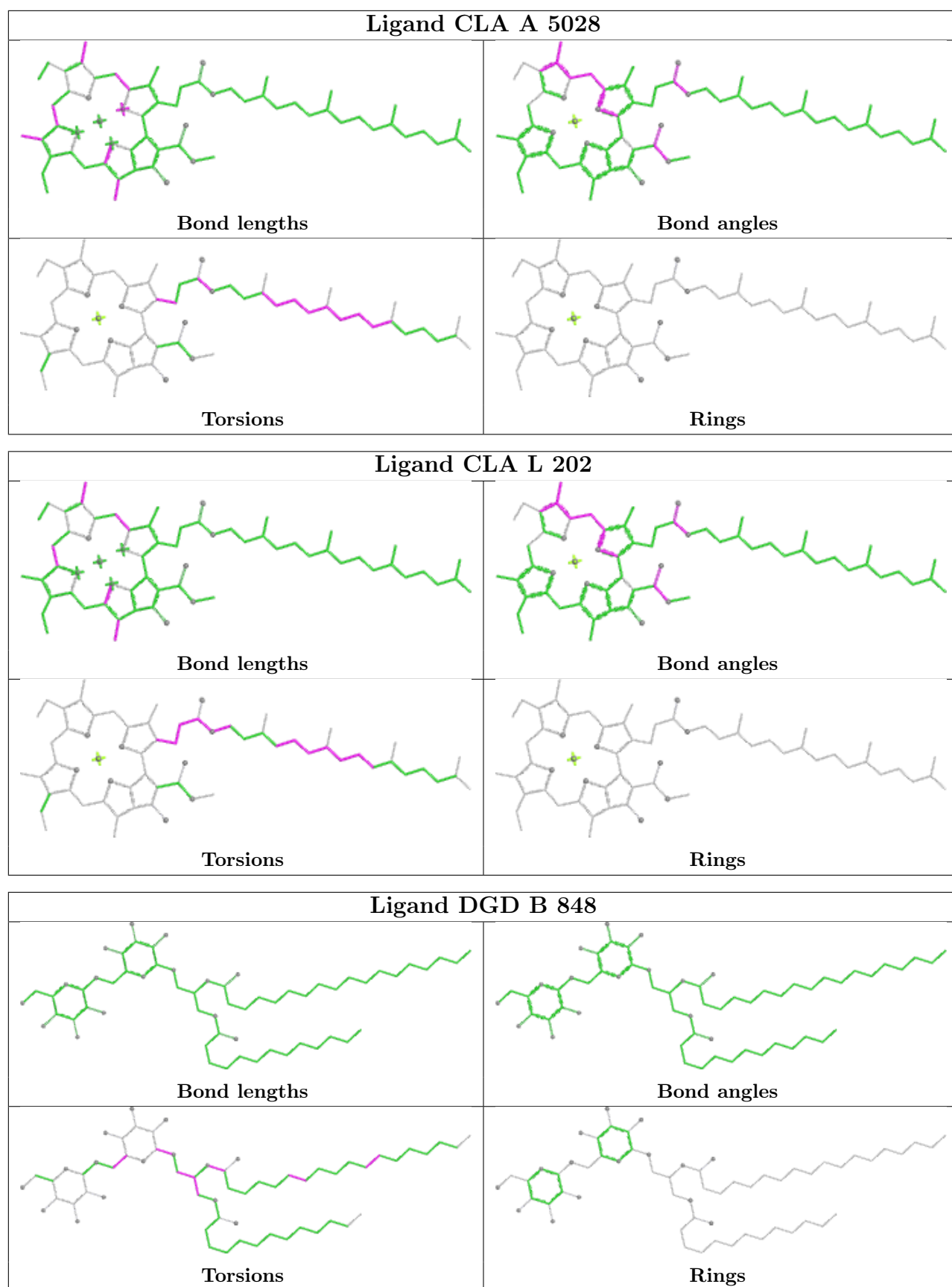




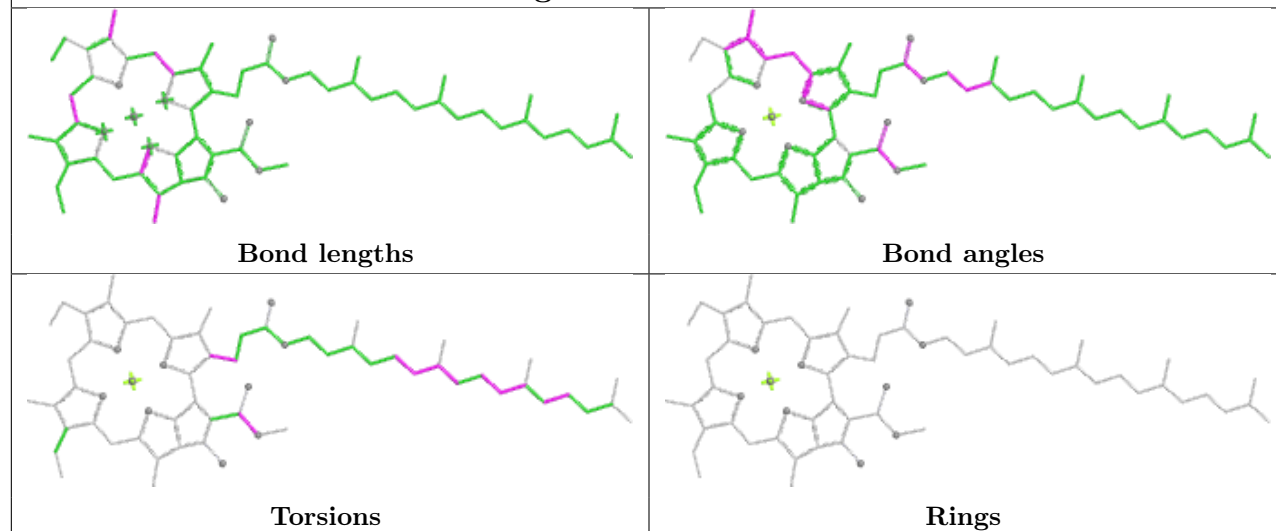




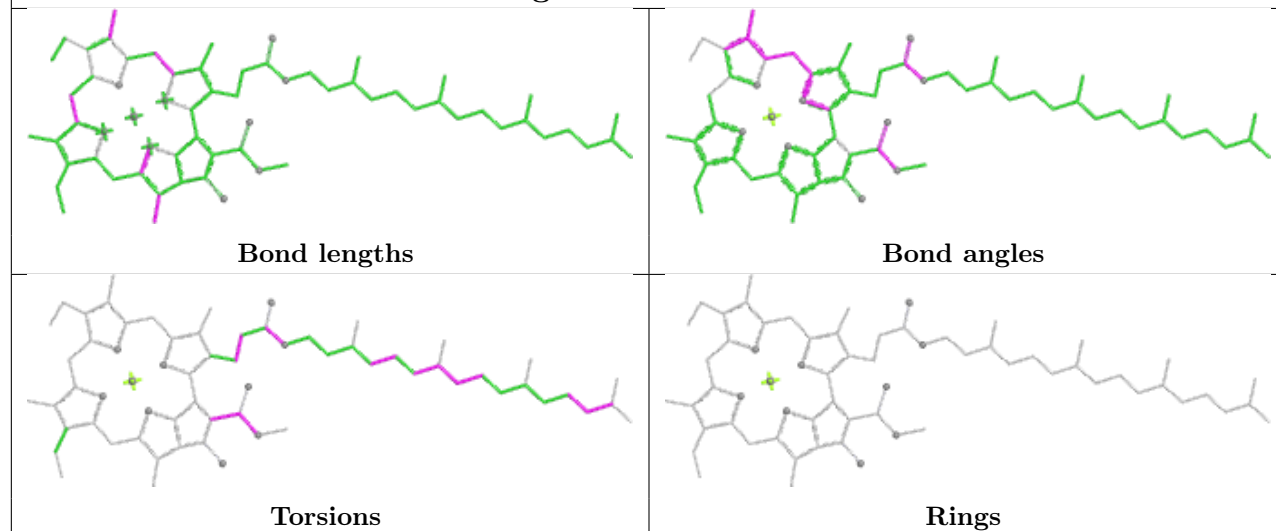




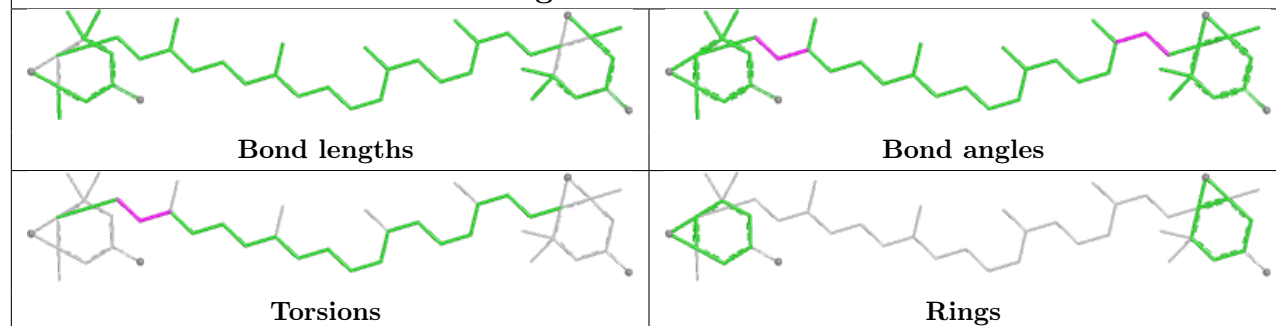
## Ligand CLA L 201



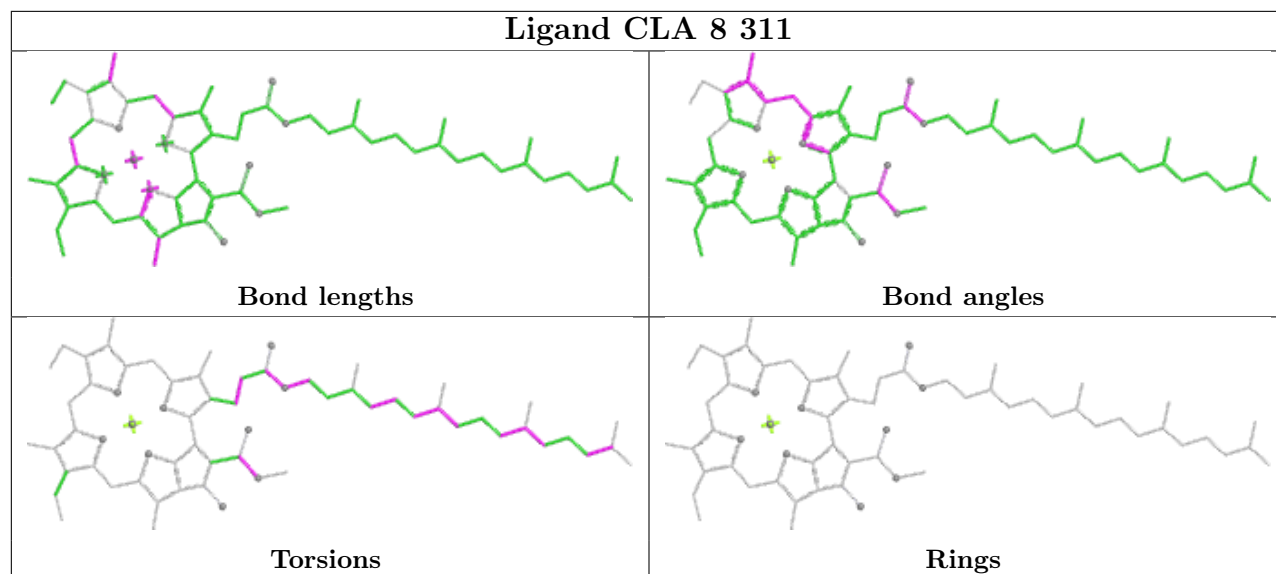
## Ligand CLA B 809



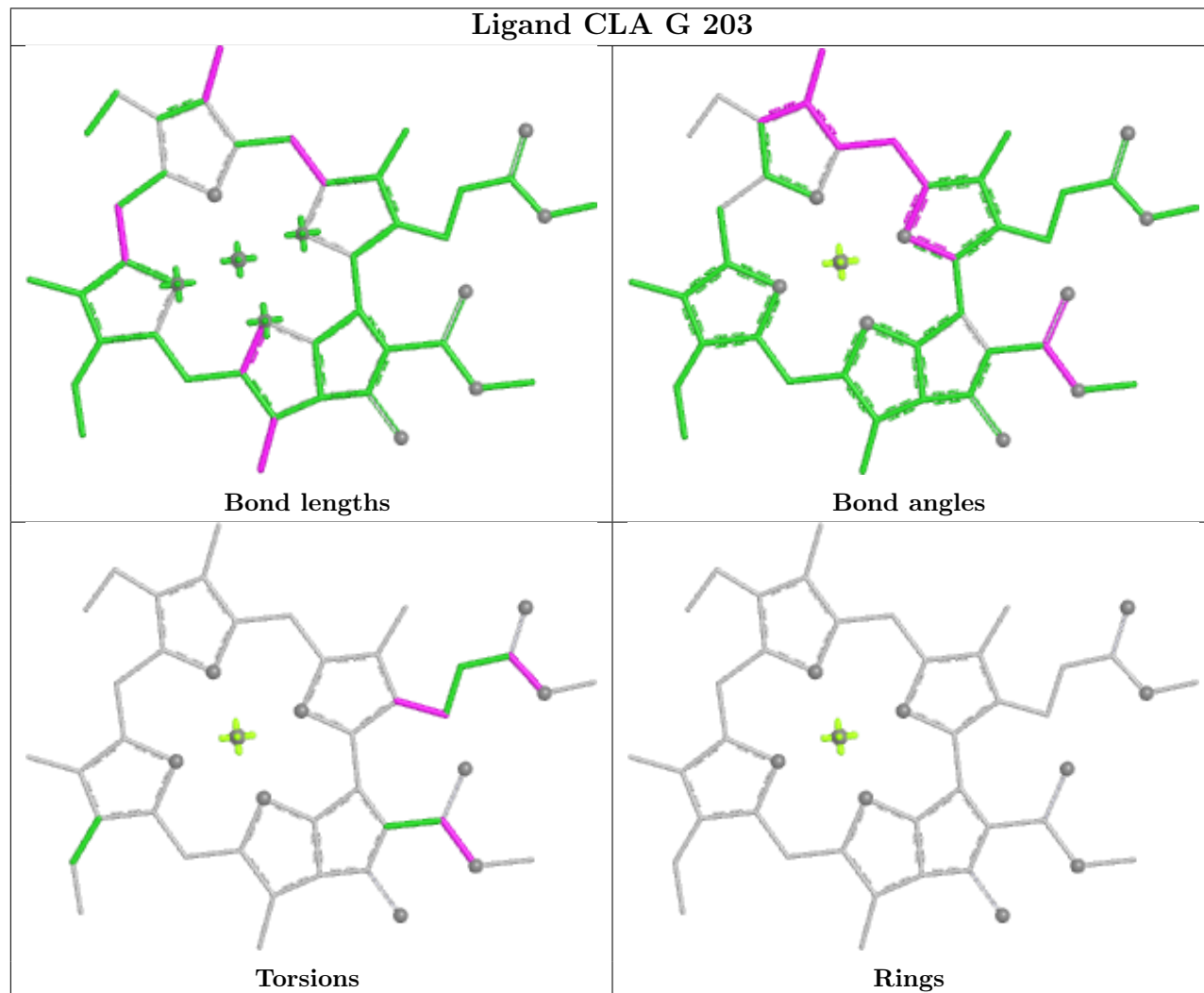
## Ligand XAT 3 316

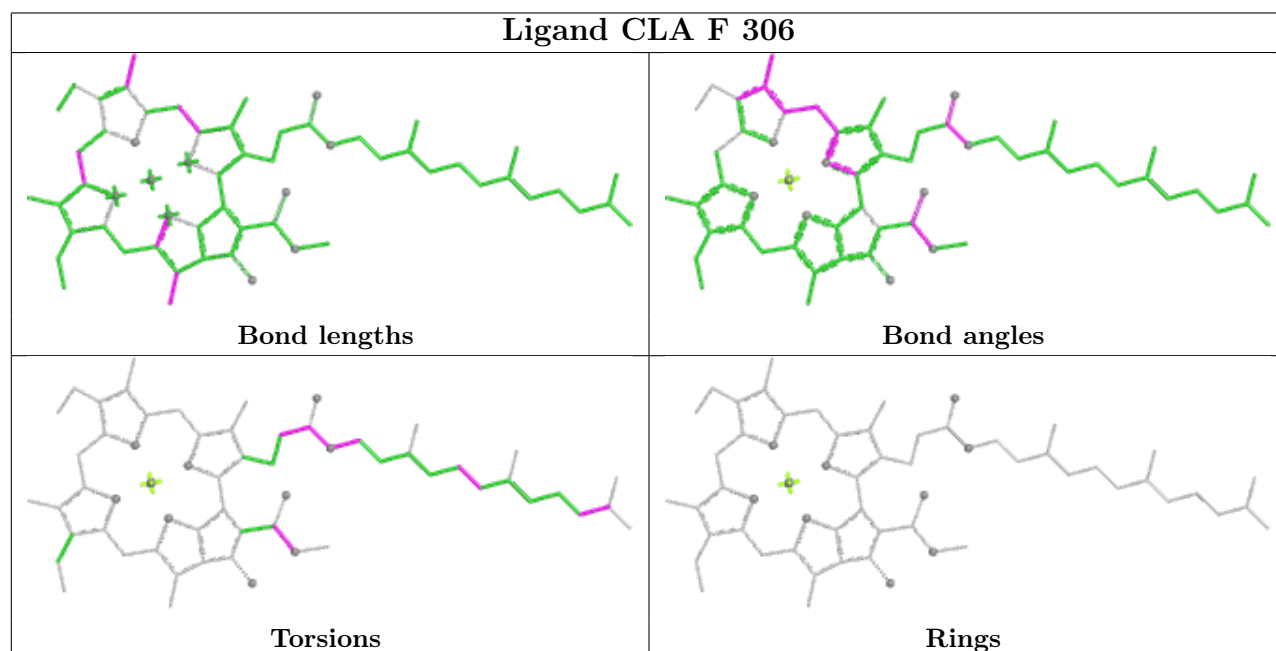
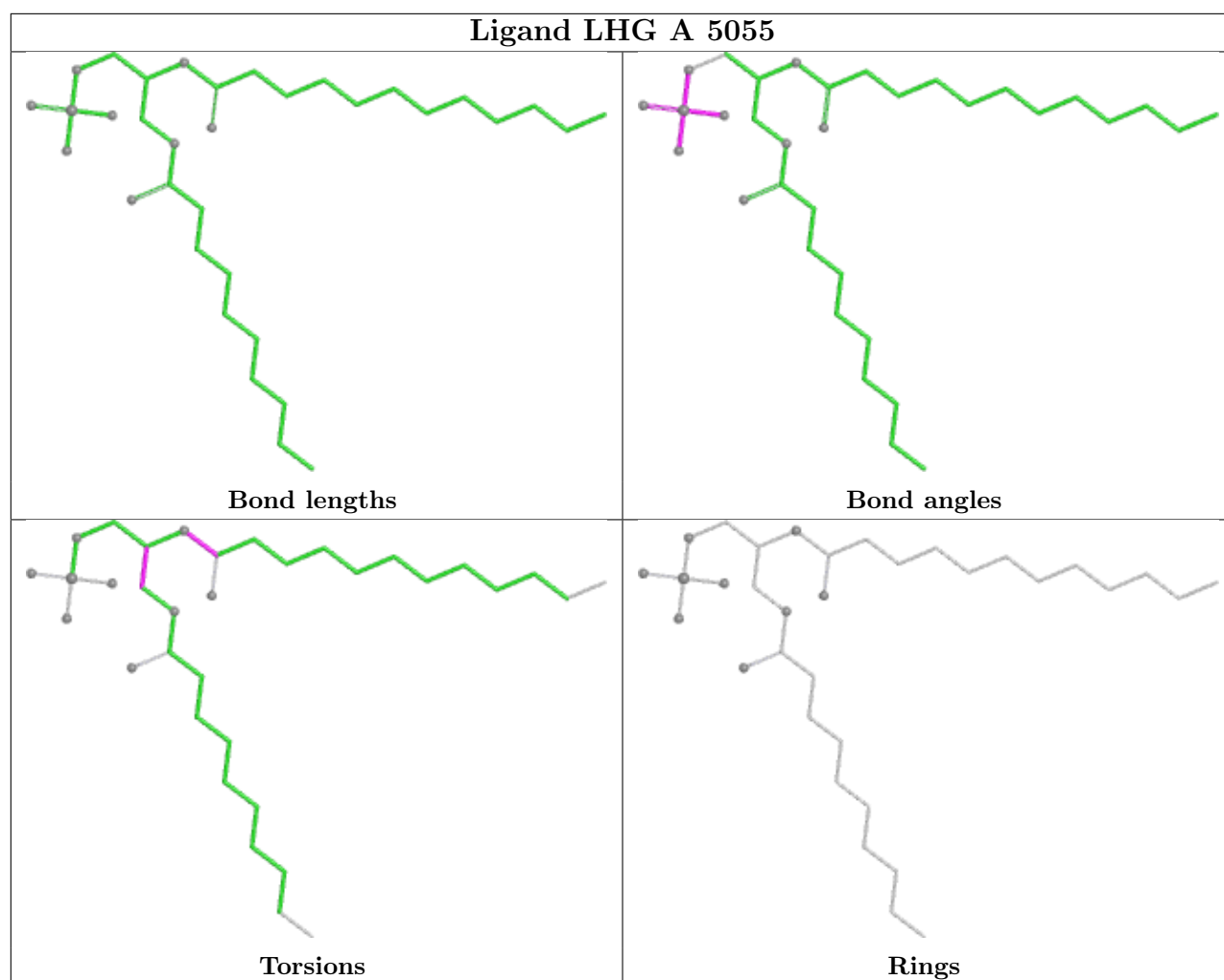


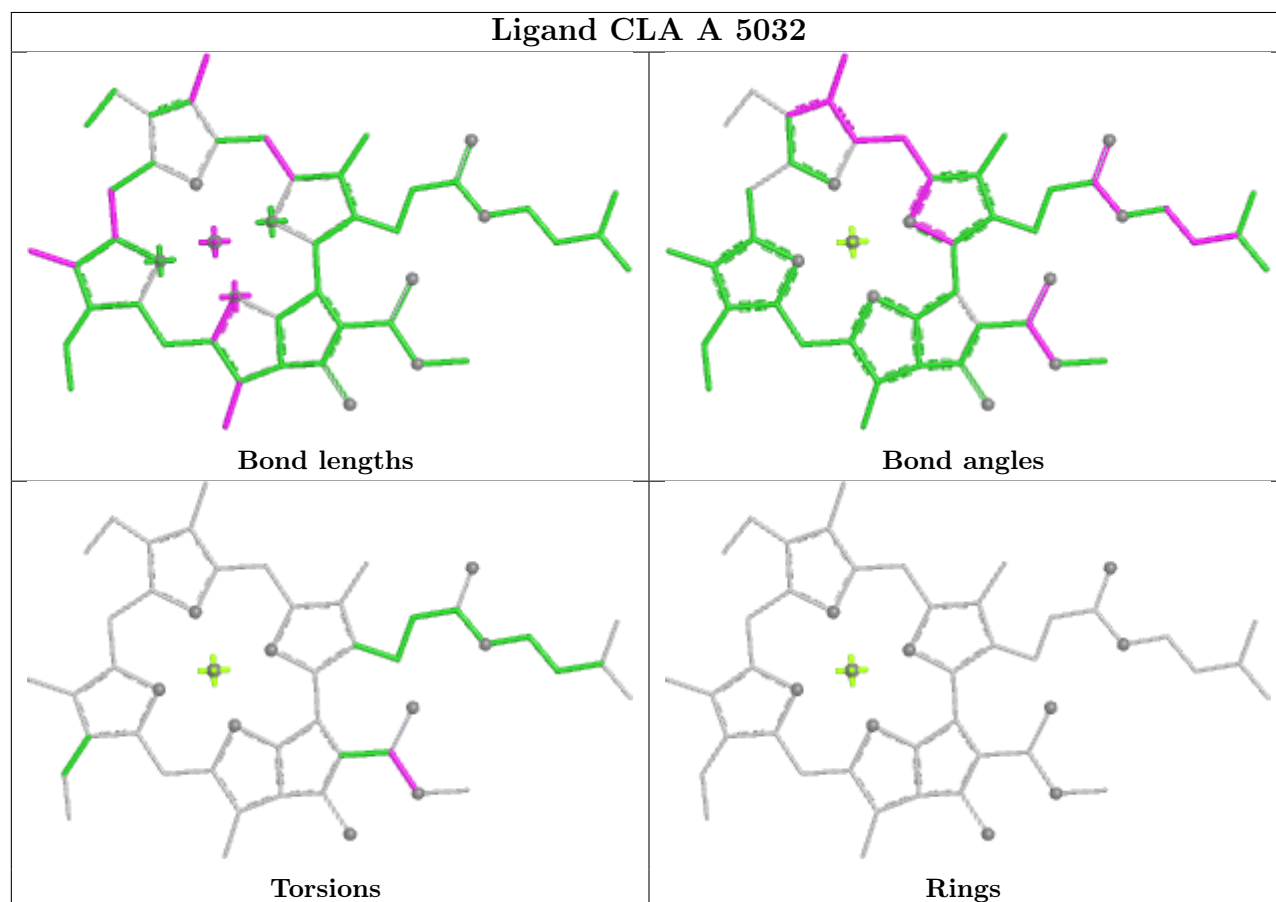
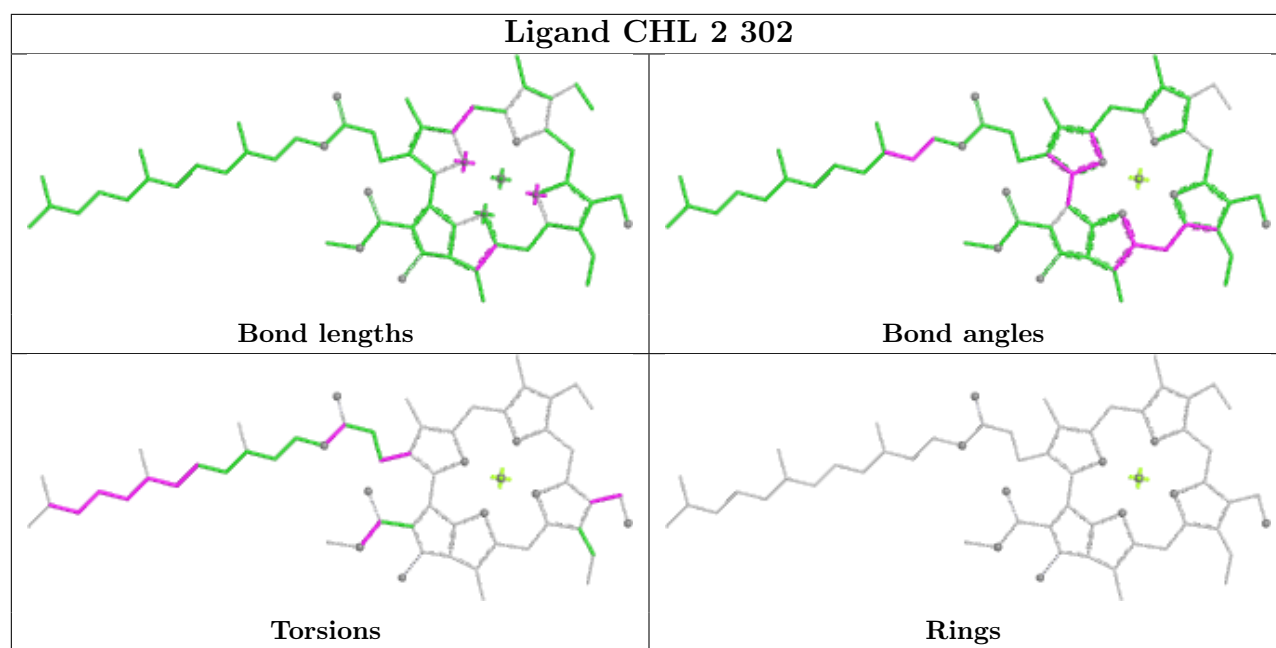
## Ligand CLA 8 311

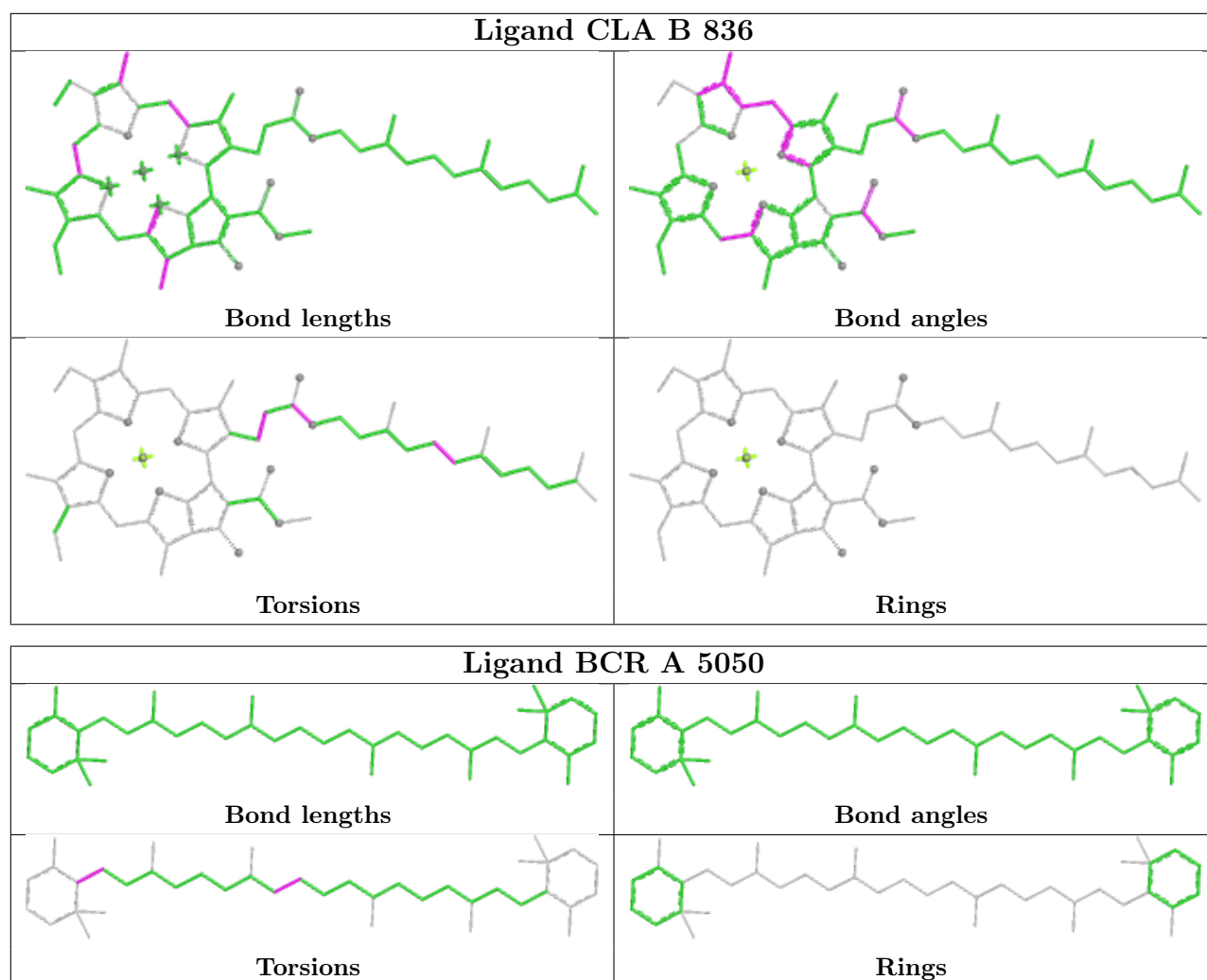


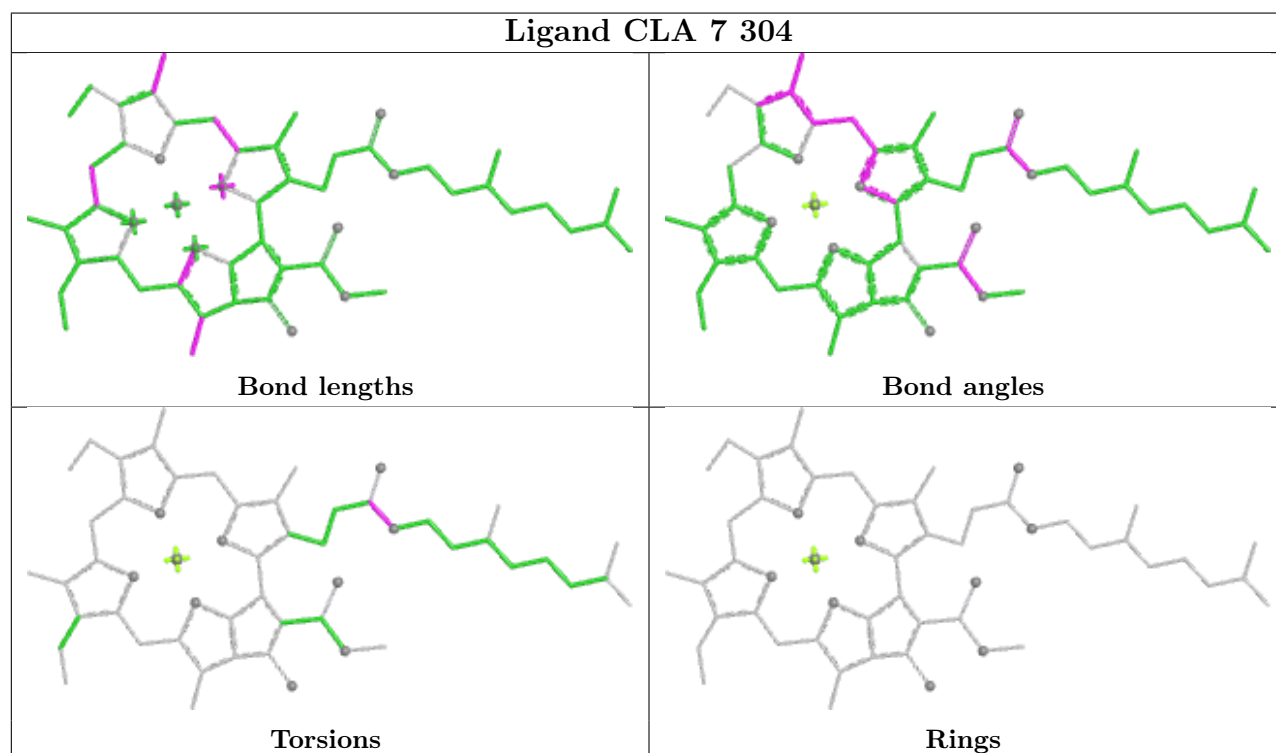
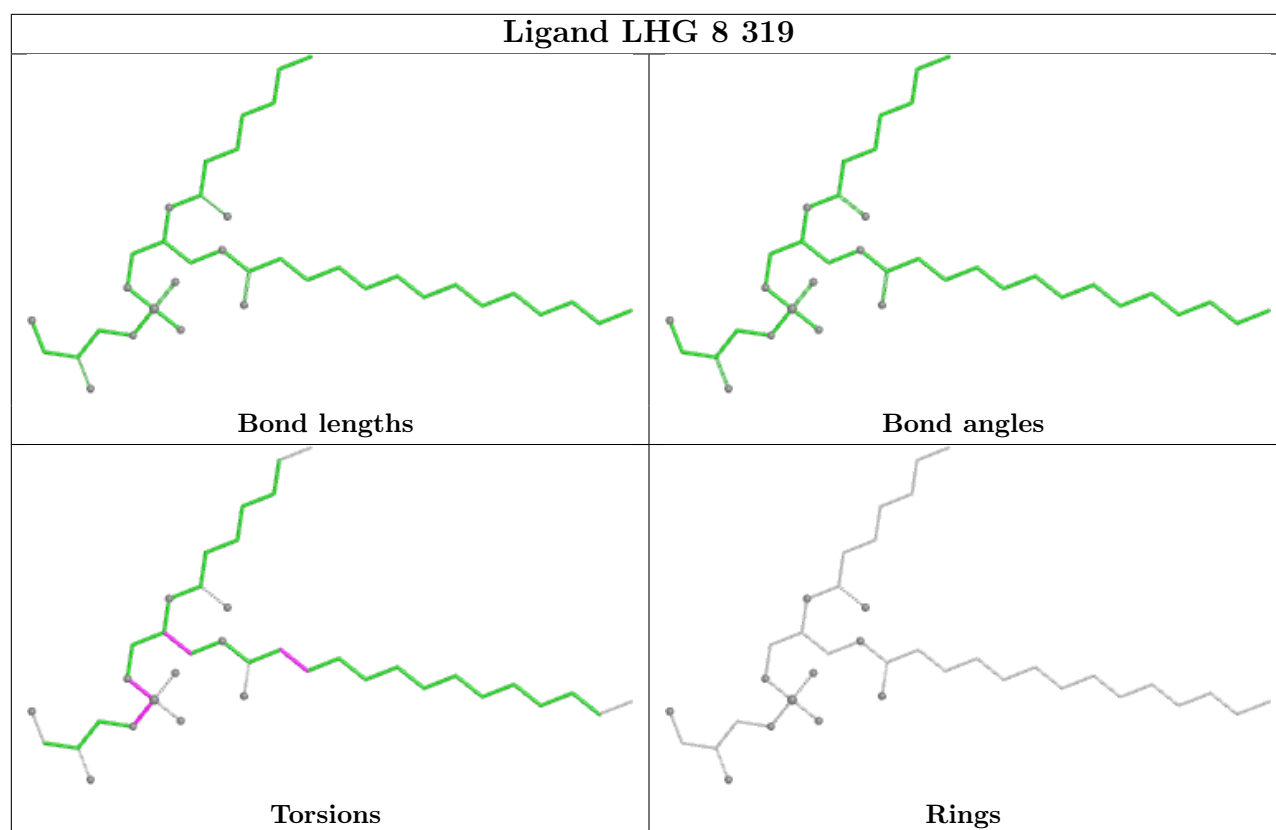
## Ligand CLA G 203

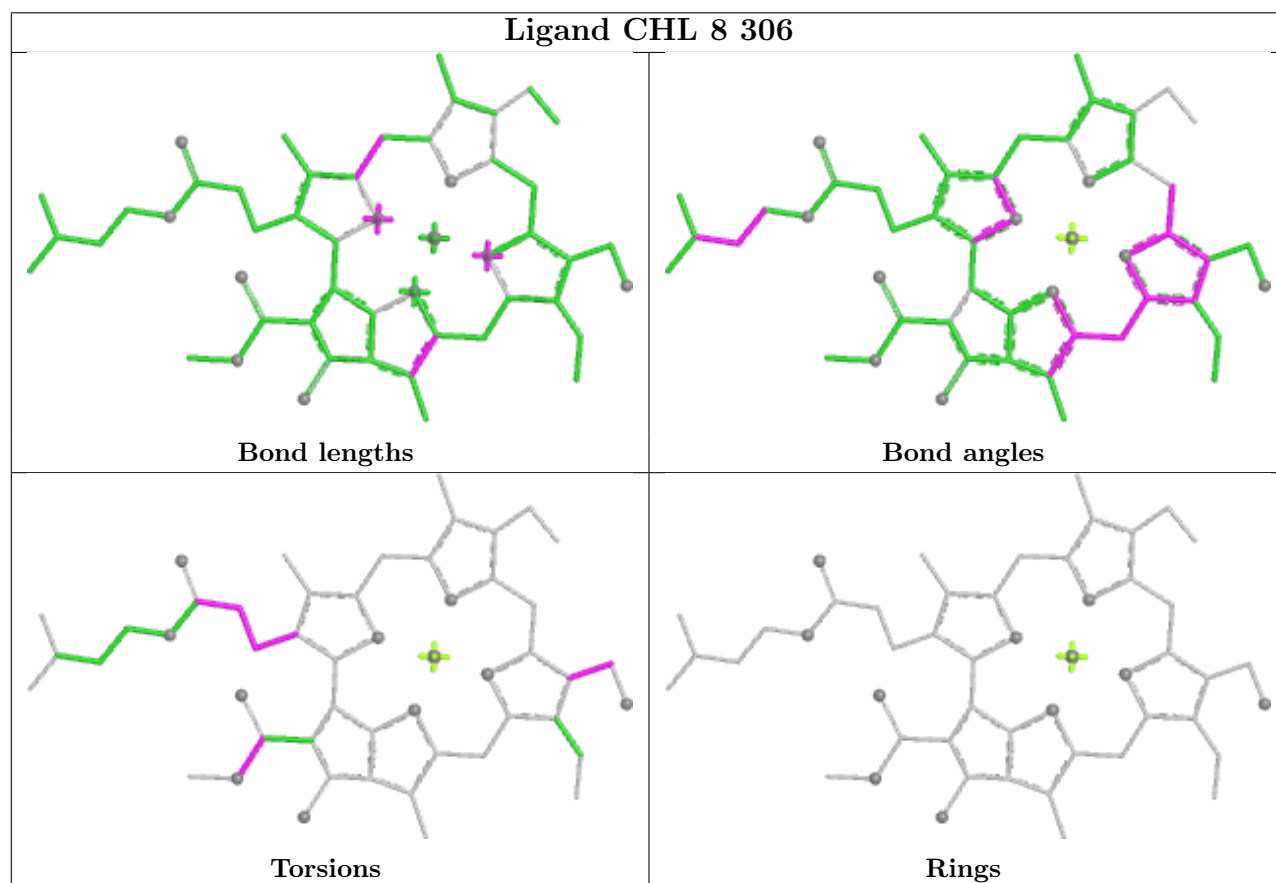
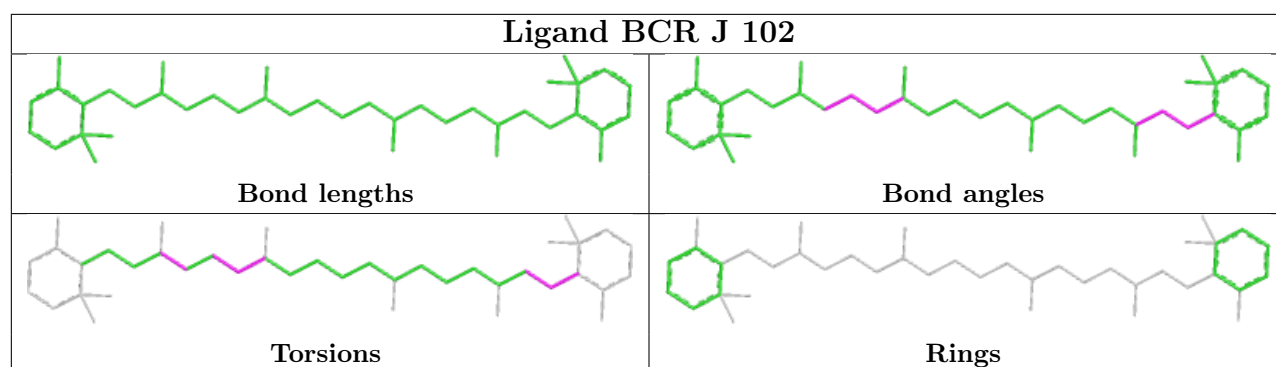




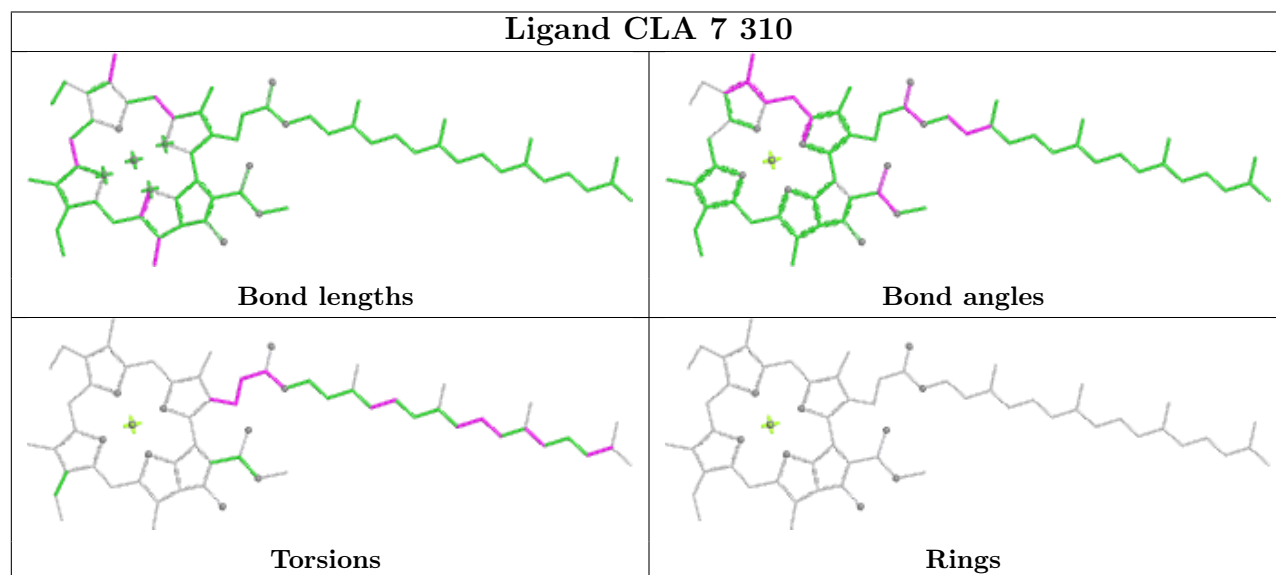
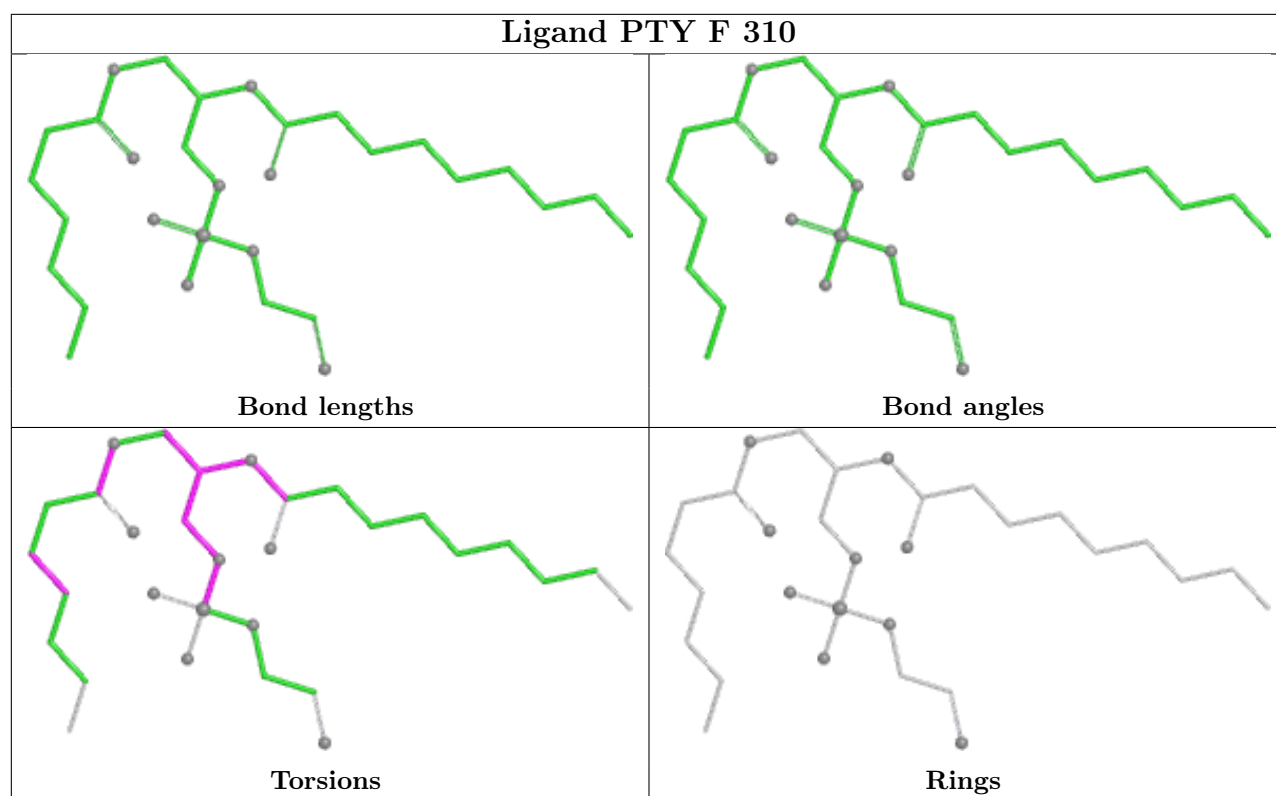


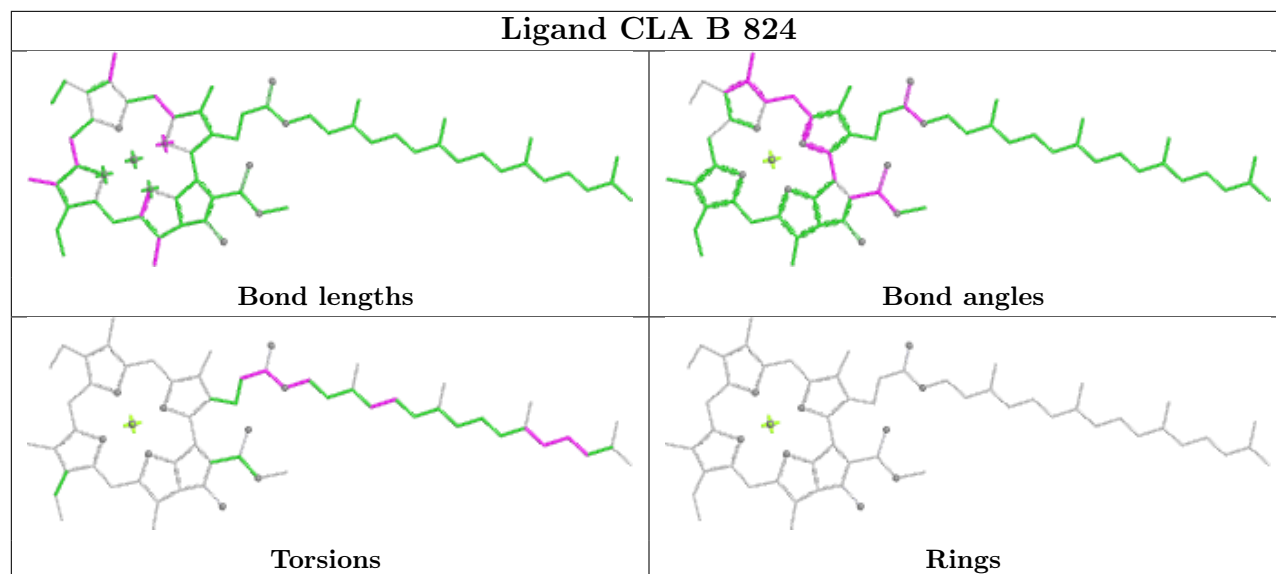
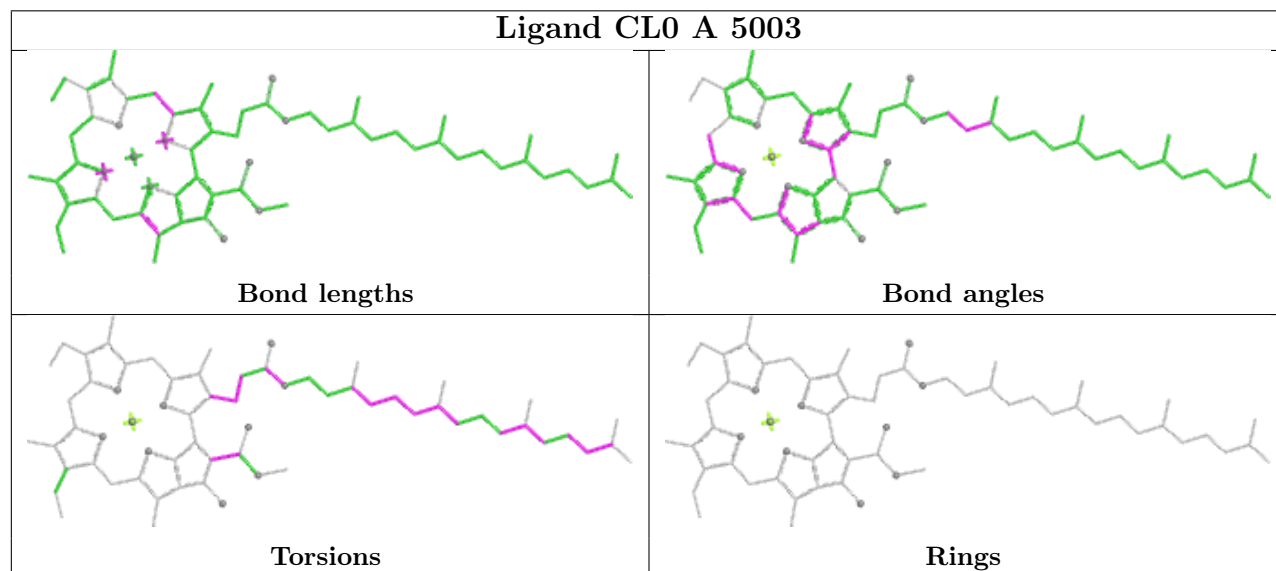


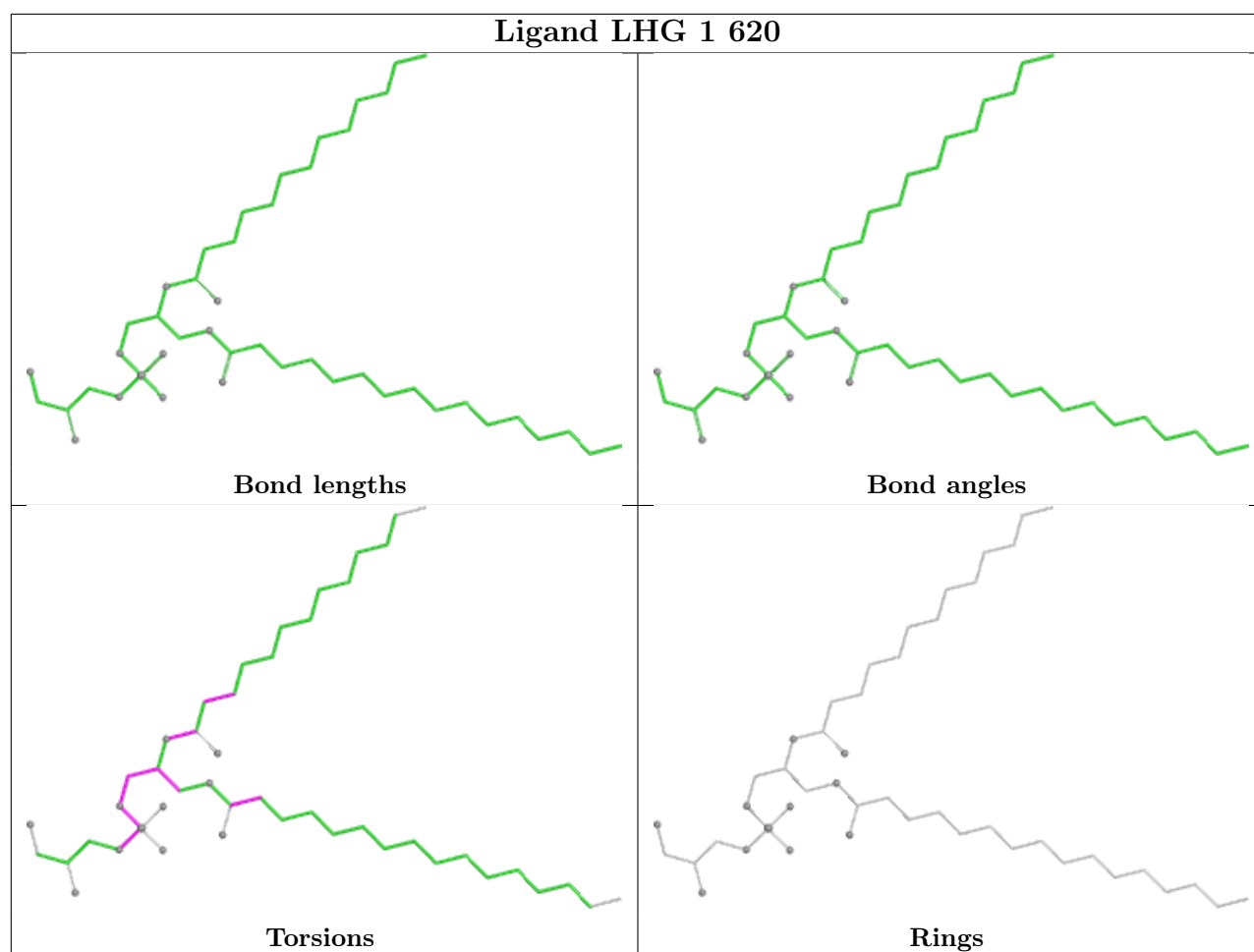


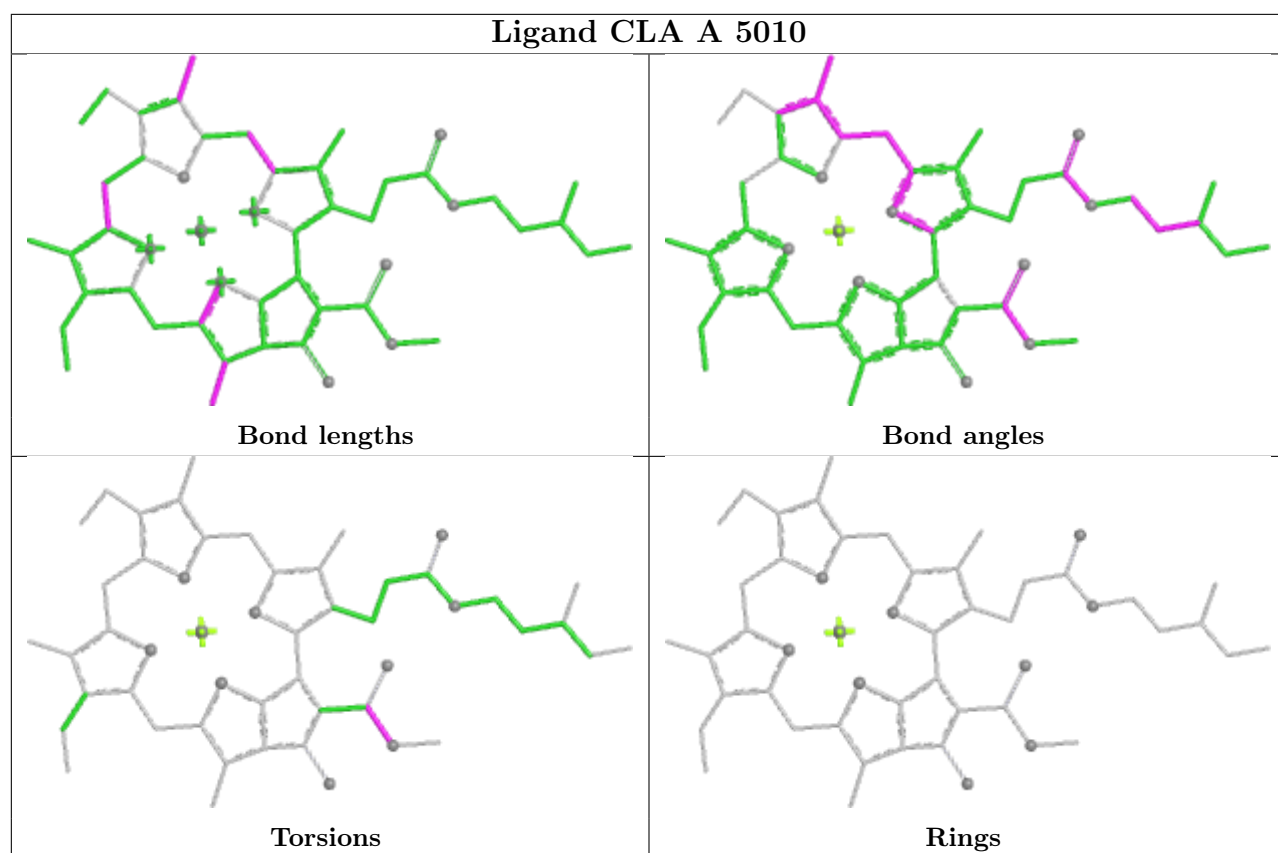




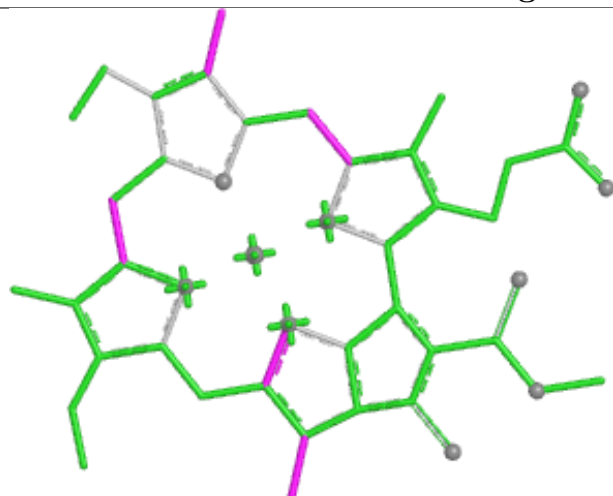


**Ligand CLA B 824****Ligand CL0 A 5003**

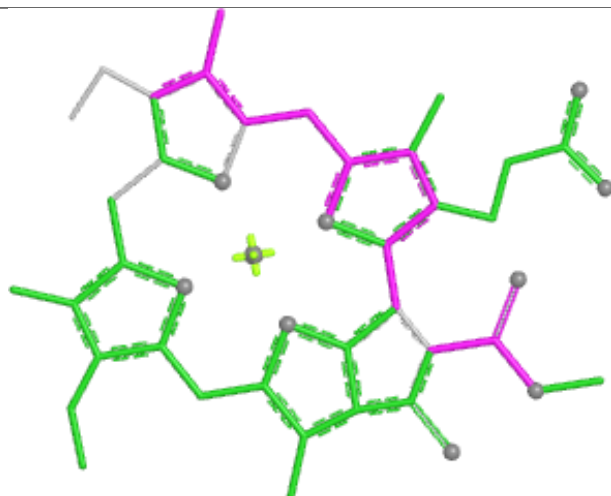




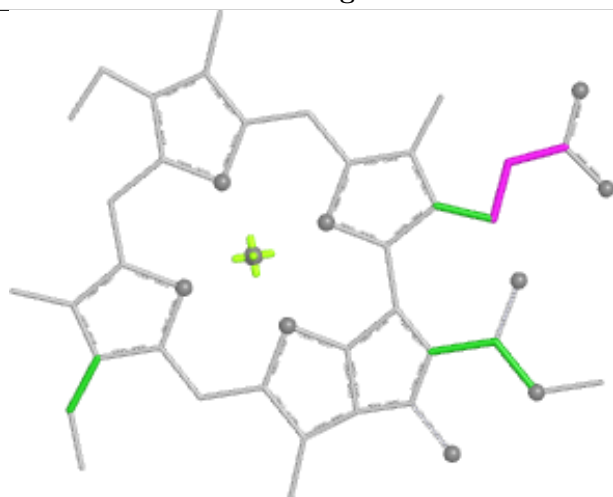
## Ligand CLA 2 308



Bond lengths



Bond angles

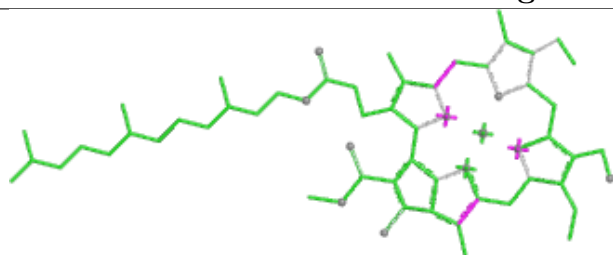


Torsions

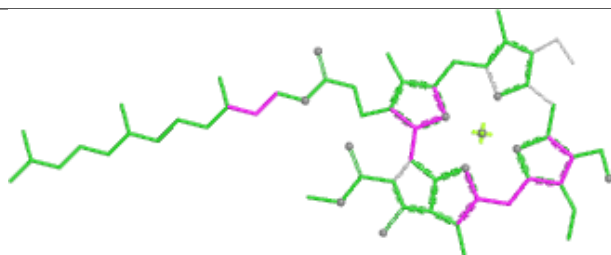


Rings

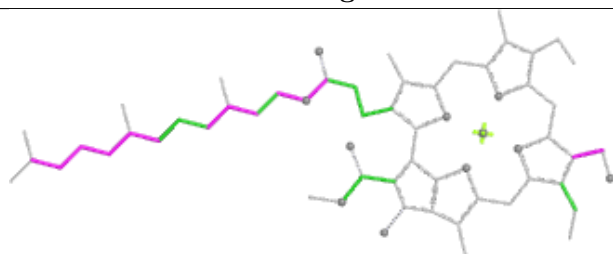
## Ligand CHL 3 323



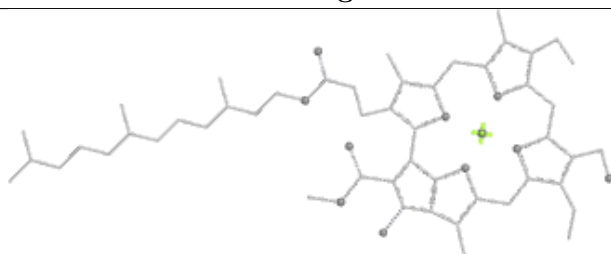
Bond lengths



Bond angles

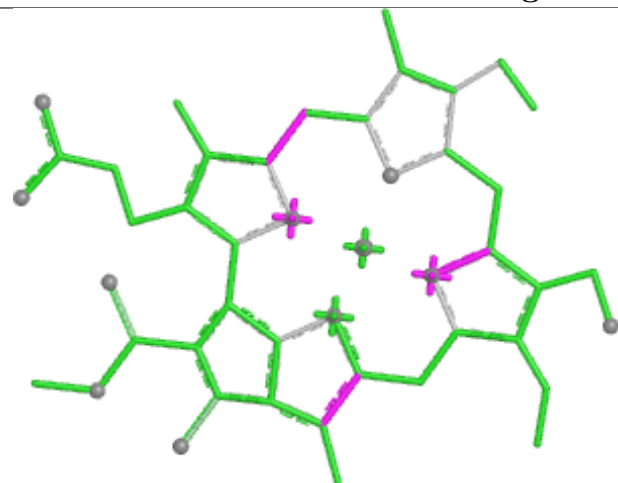


Torsions

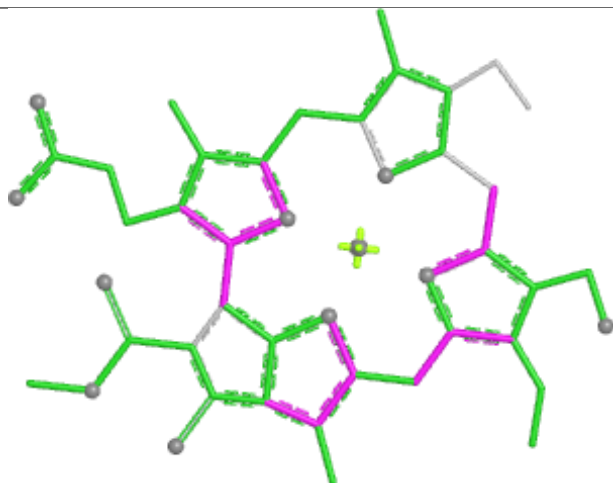


Rings

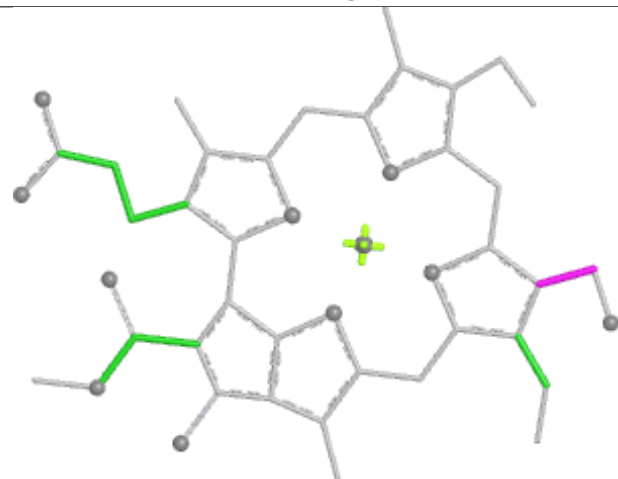
## Ligand CHL 7 306



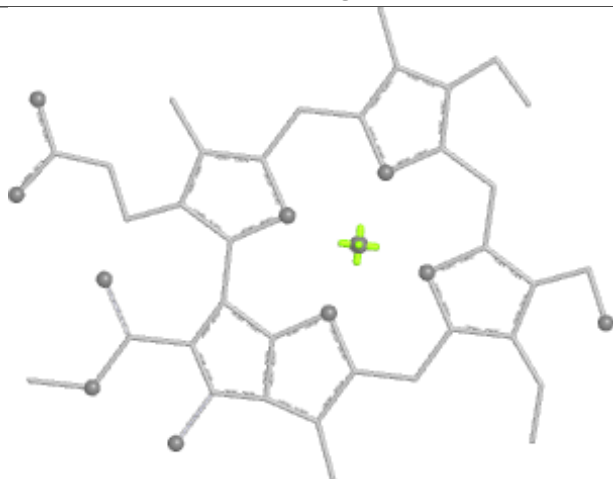
Bond lengths



Bond angles

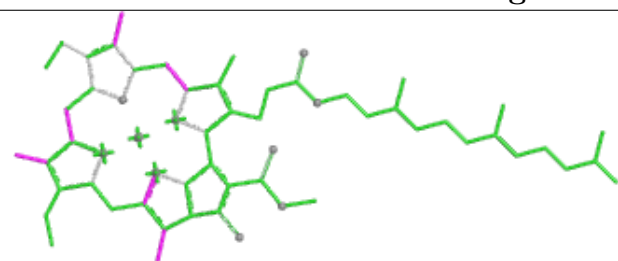


Torsions

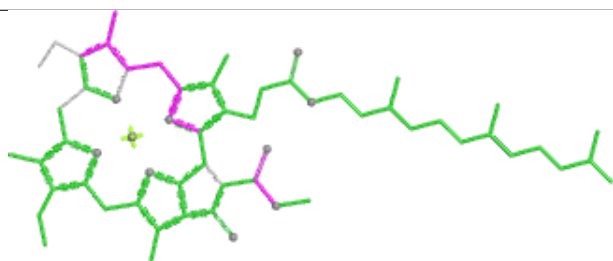


Rings

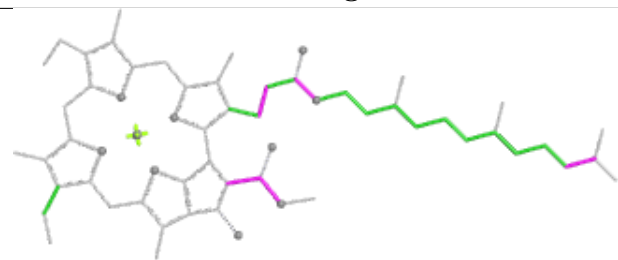
## Ligand CLA A 5018



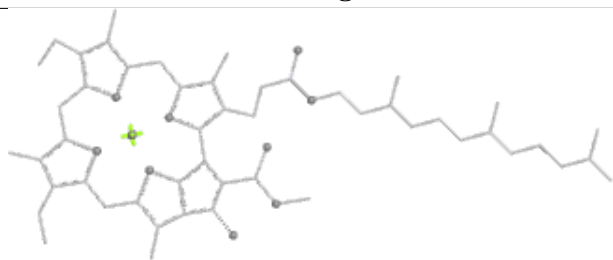
Bond lengths



Bond angles

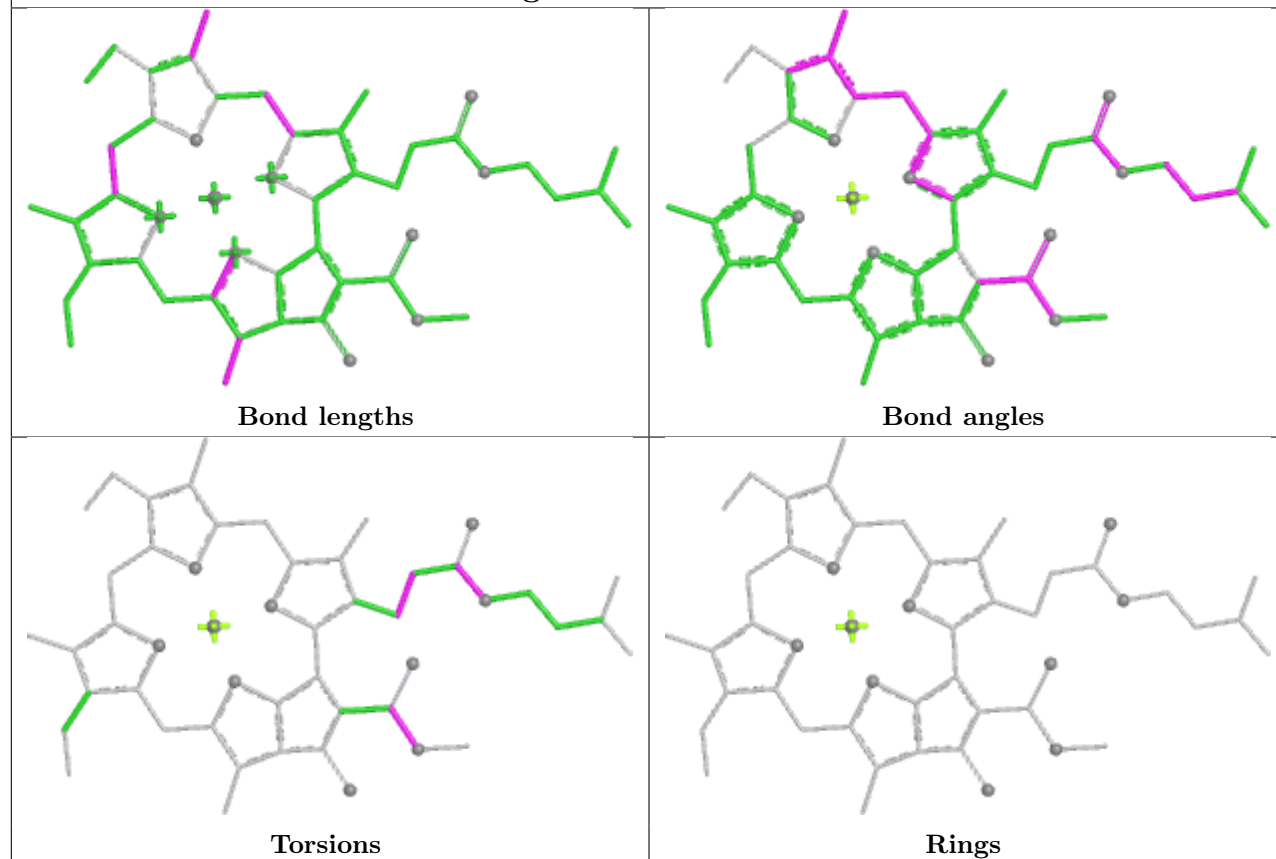


Torsions

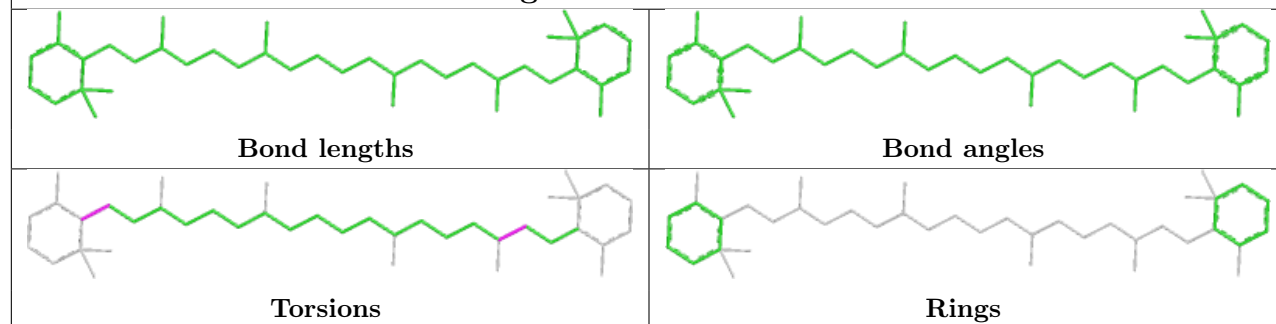


Rings

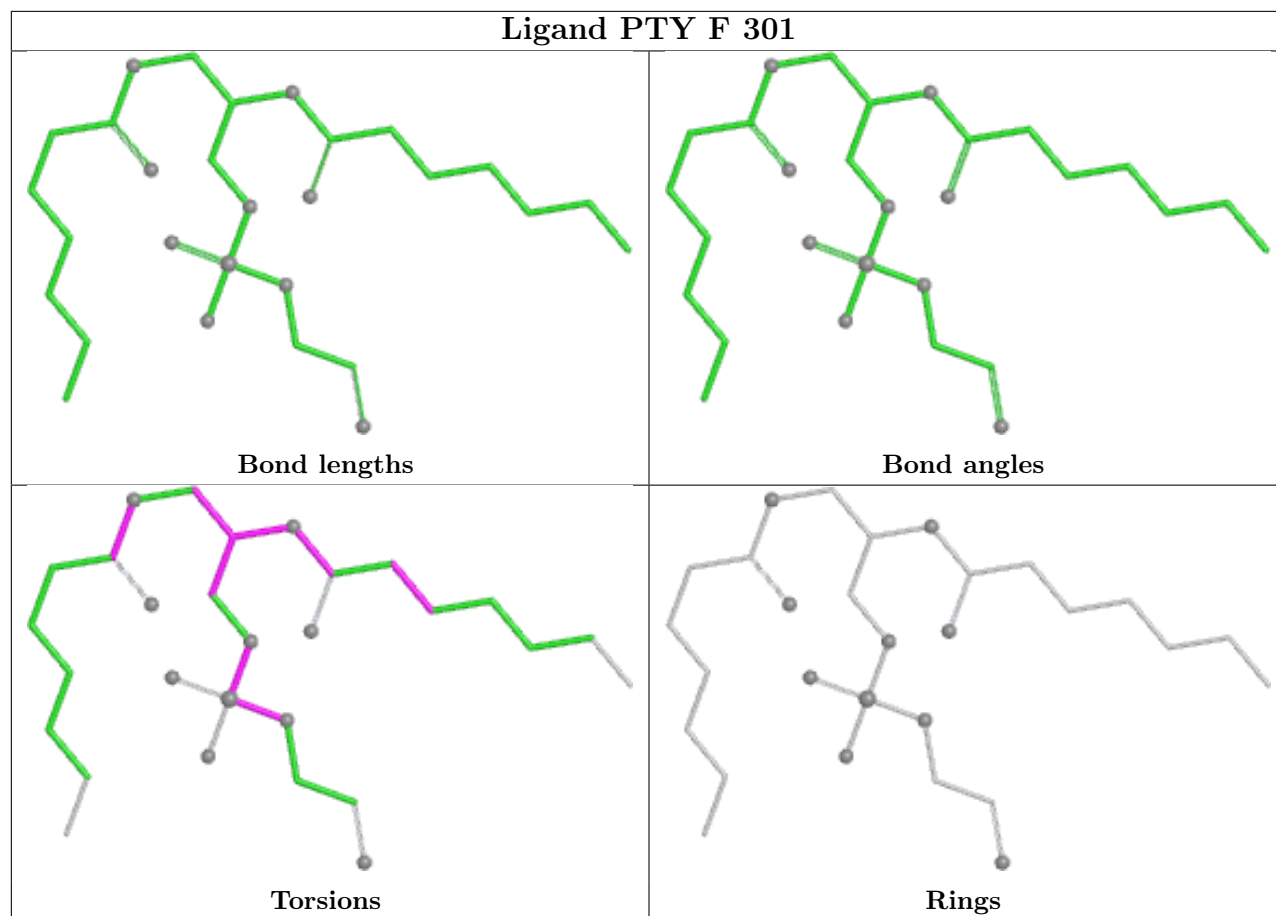
## Ligand CLA A 5023



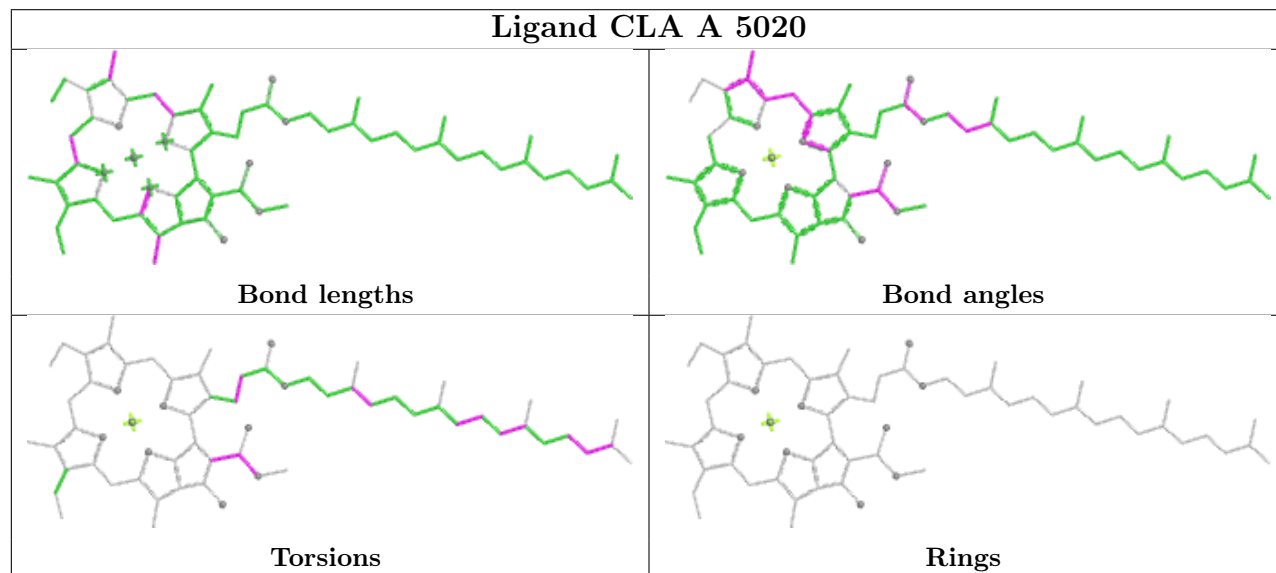
## Ligand BCR K 4001



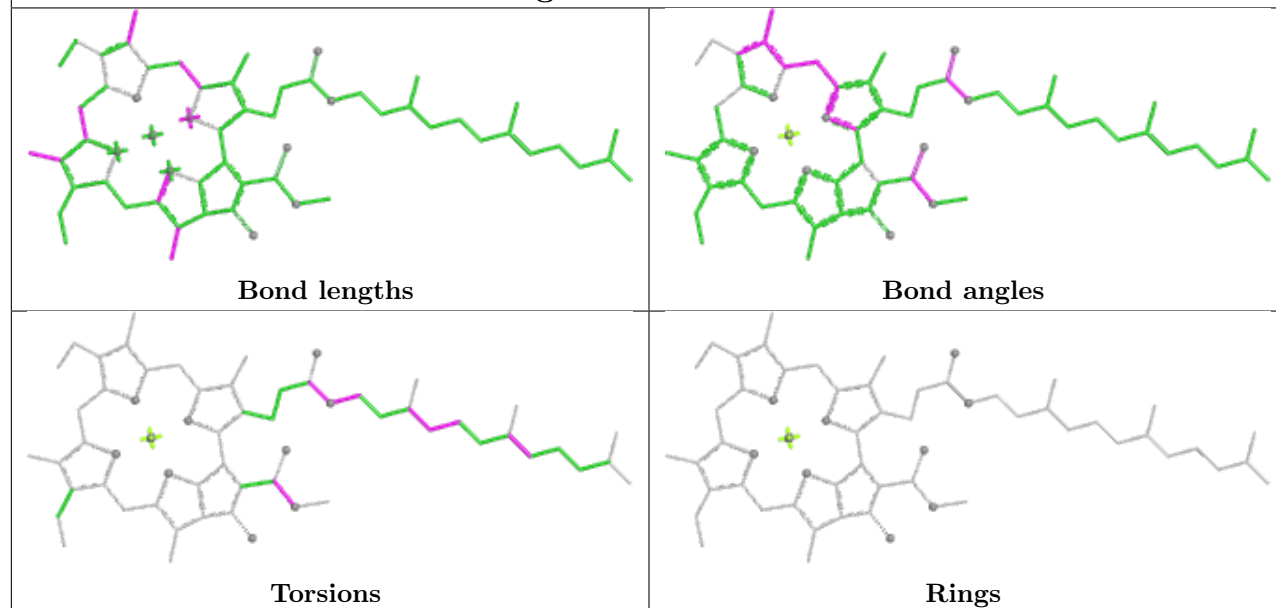
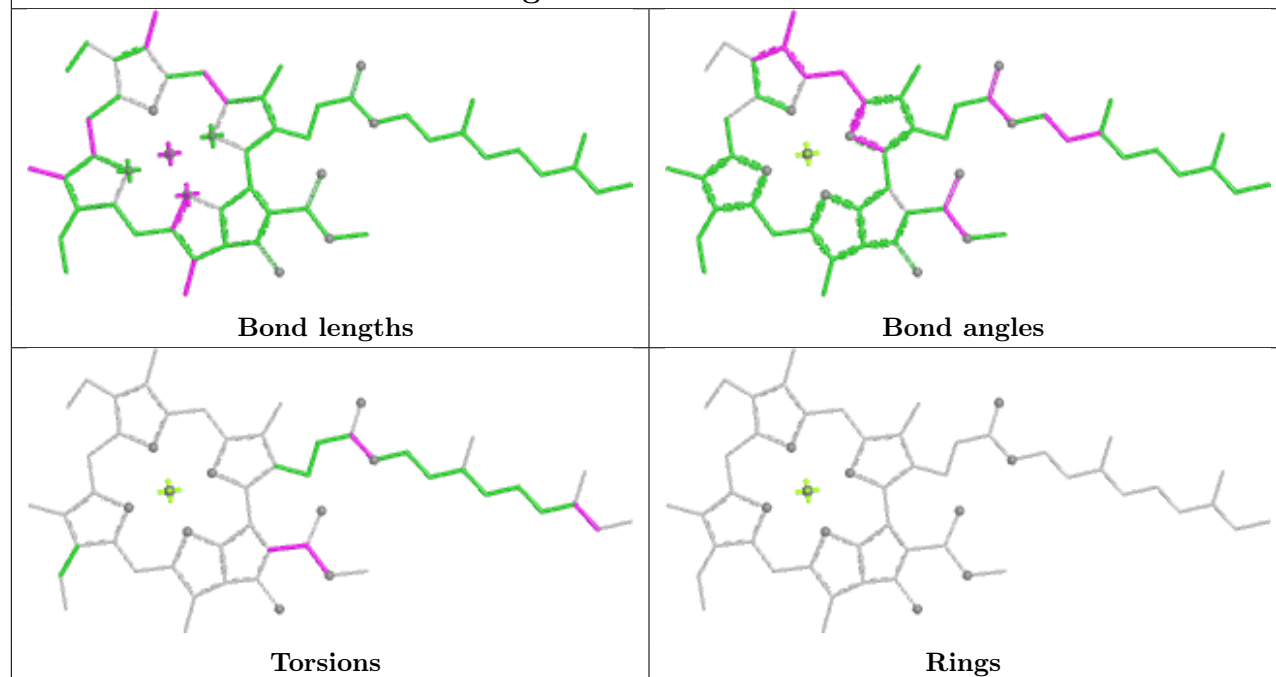
## Ligand PTY F 301



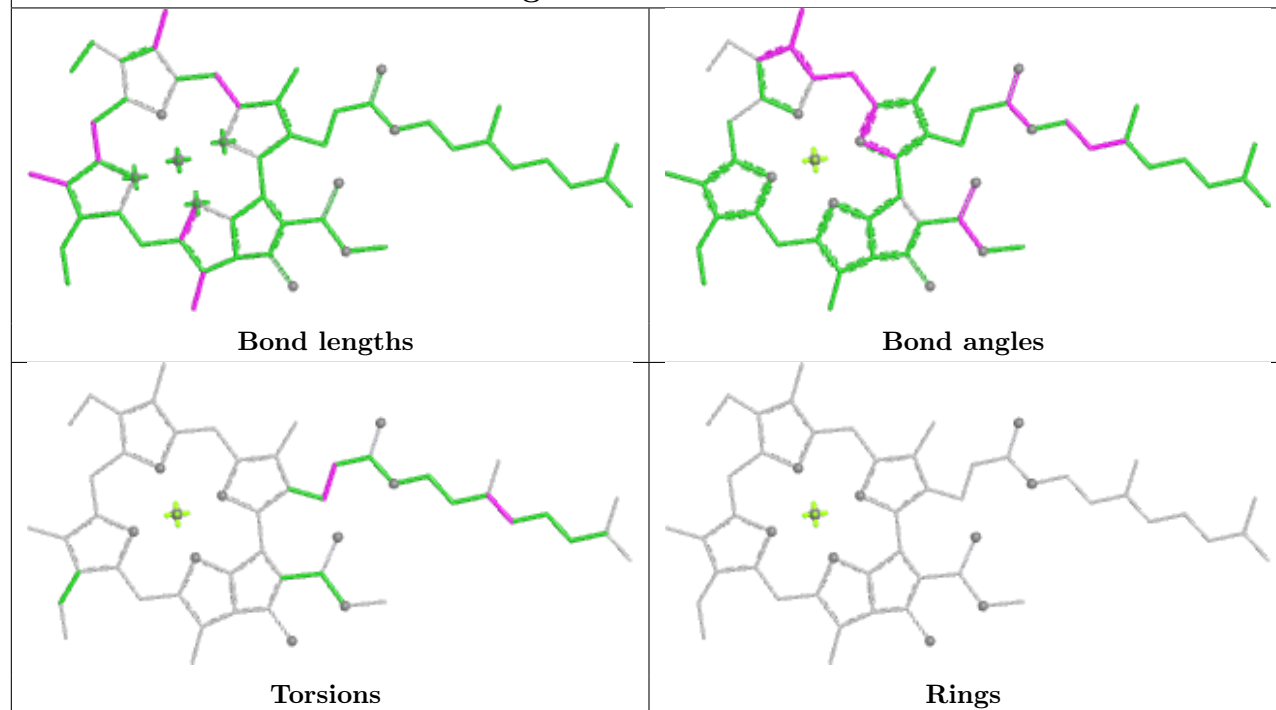
## Ligand CLA A 5020



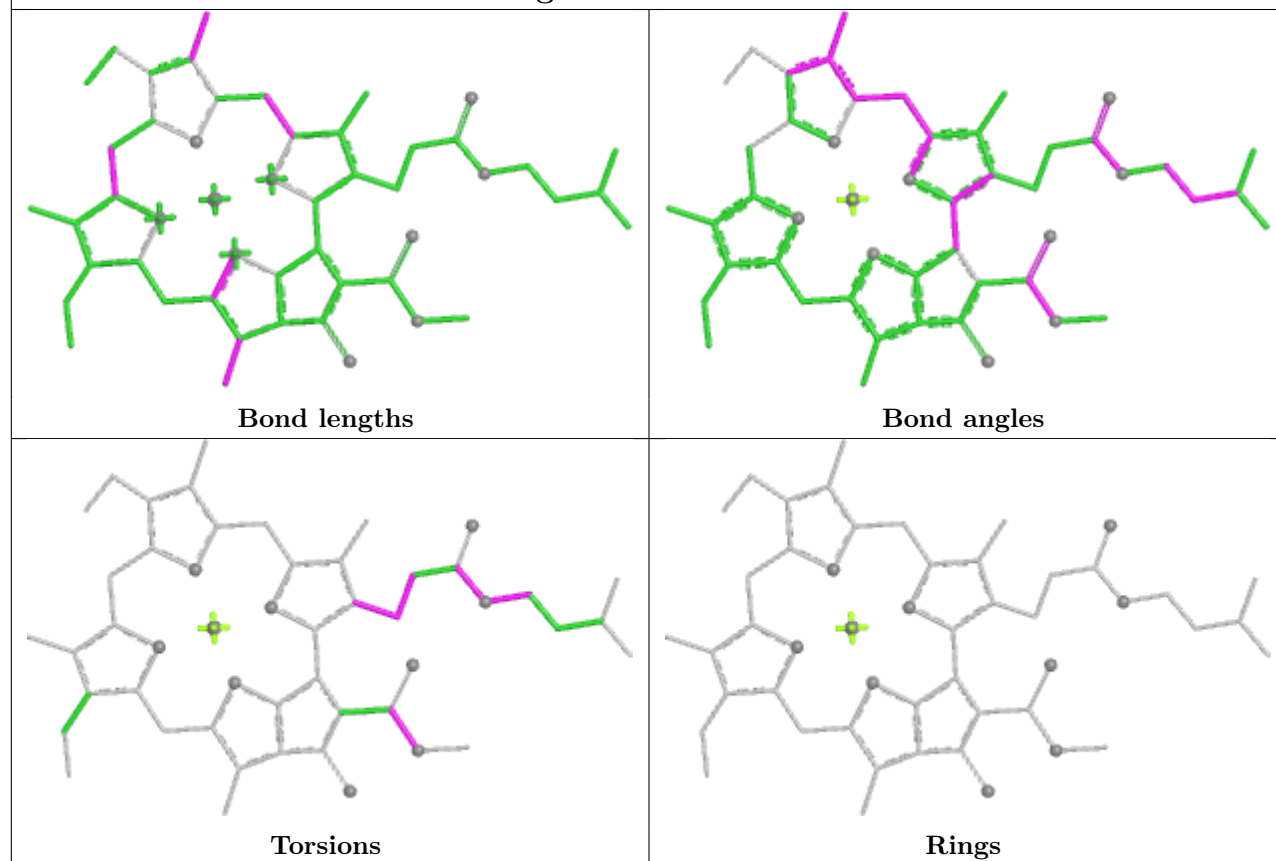


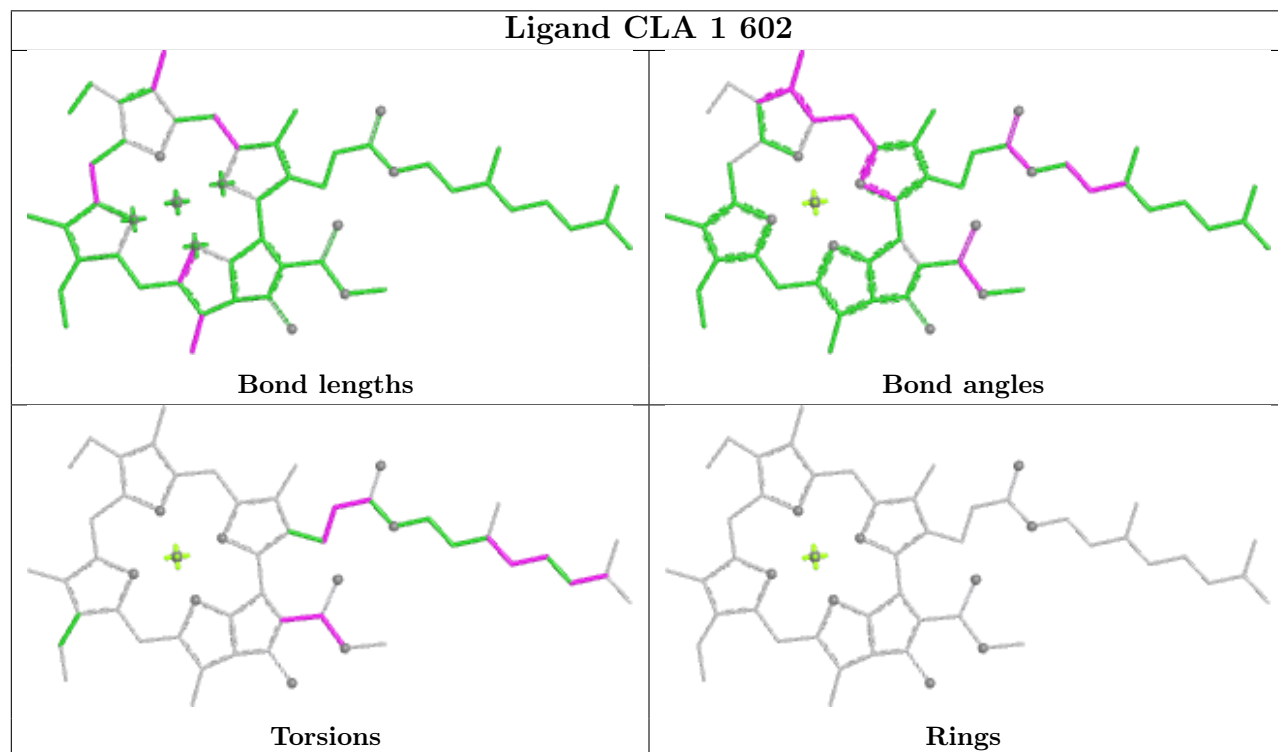
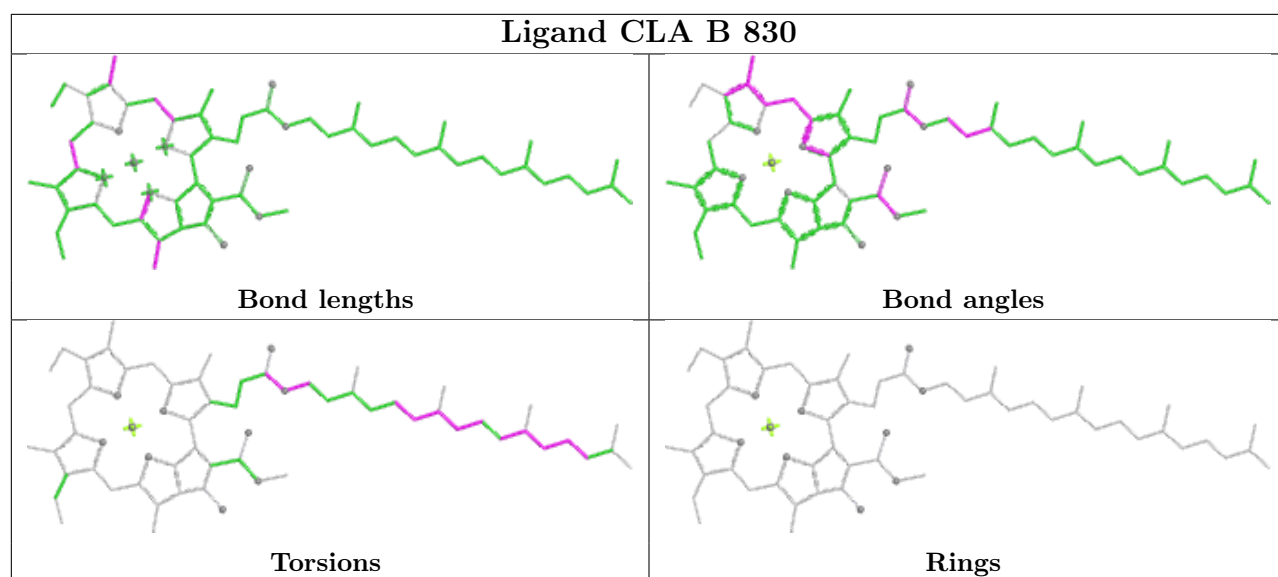
**Ligand CLA 8 309****Ligand CLA A 5027**

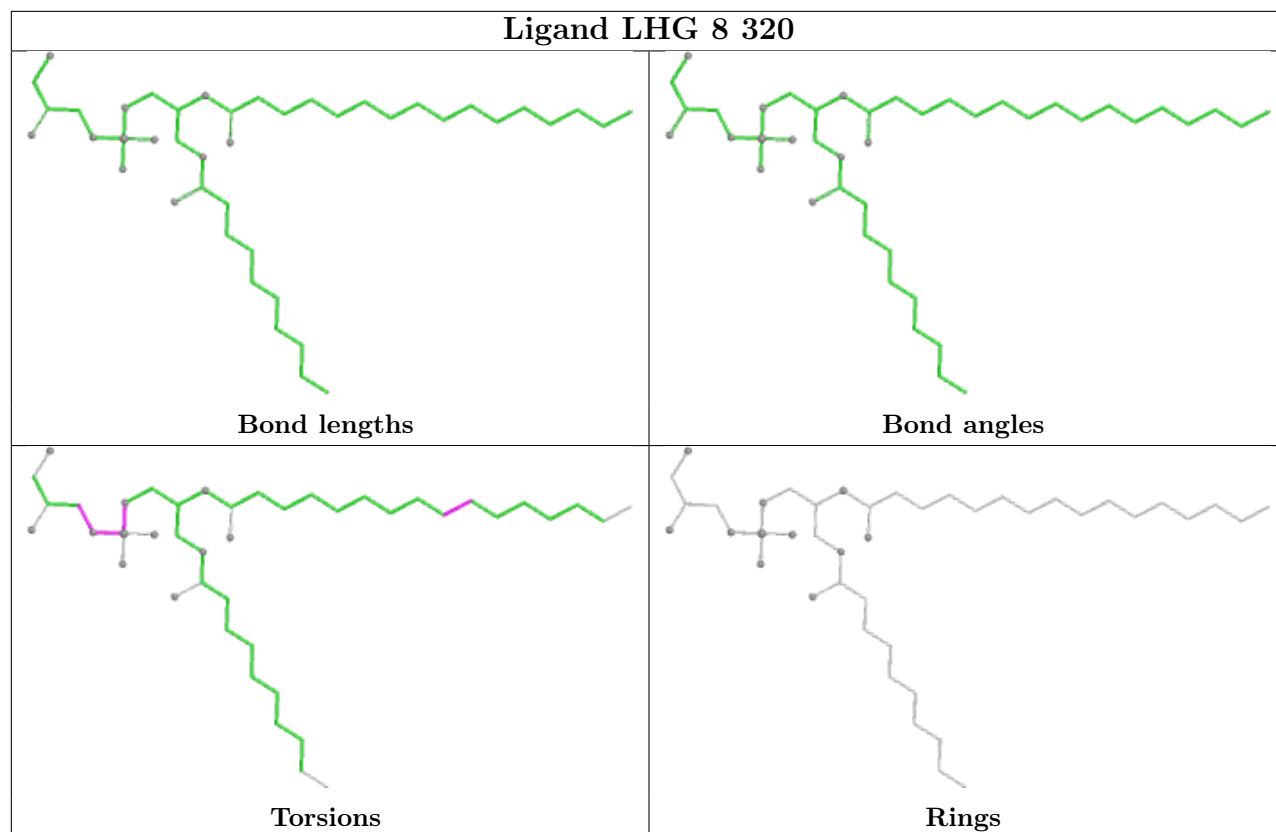
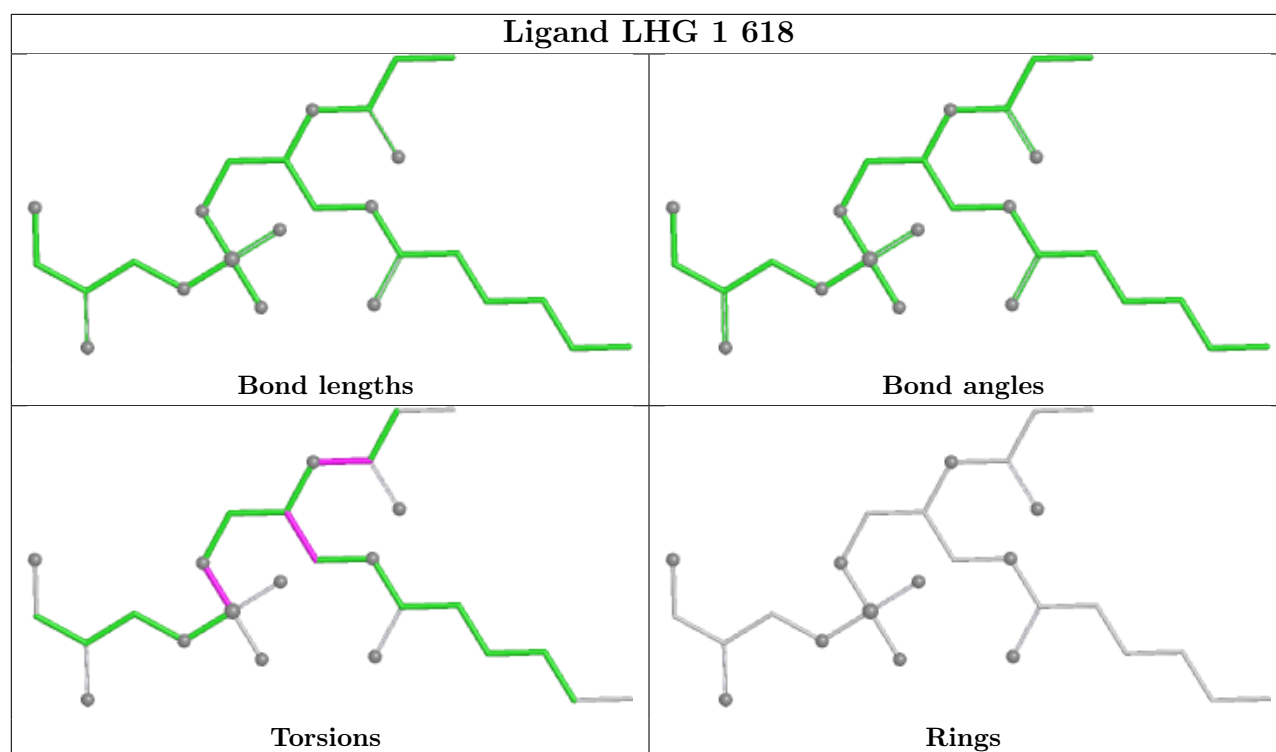
## Ligand CLA A 5039

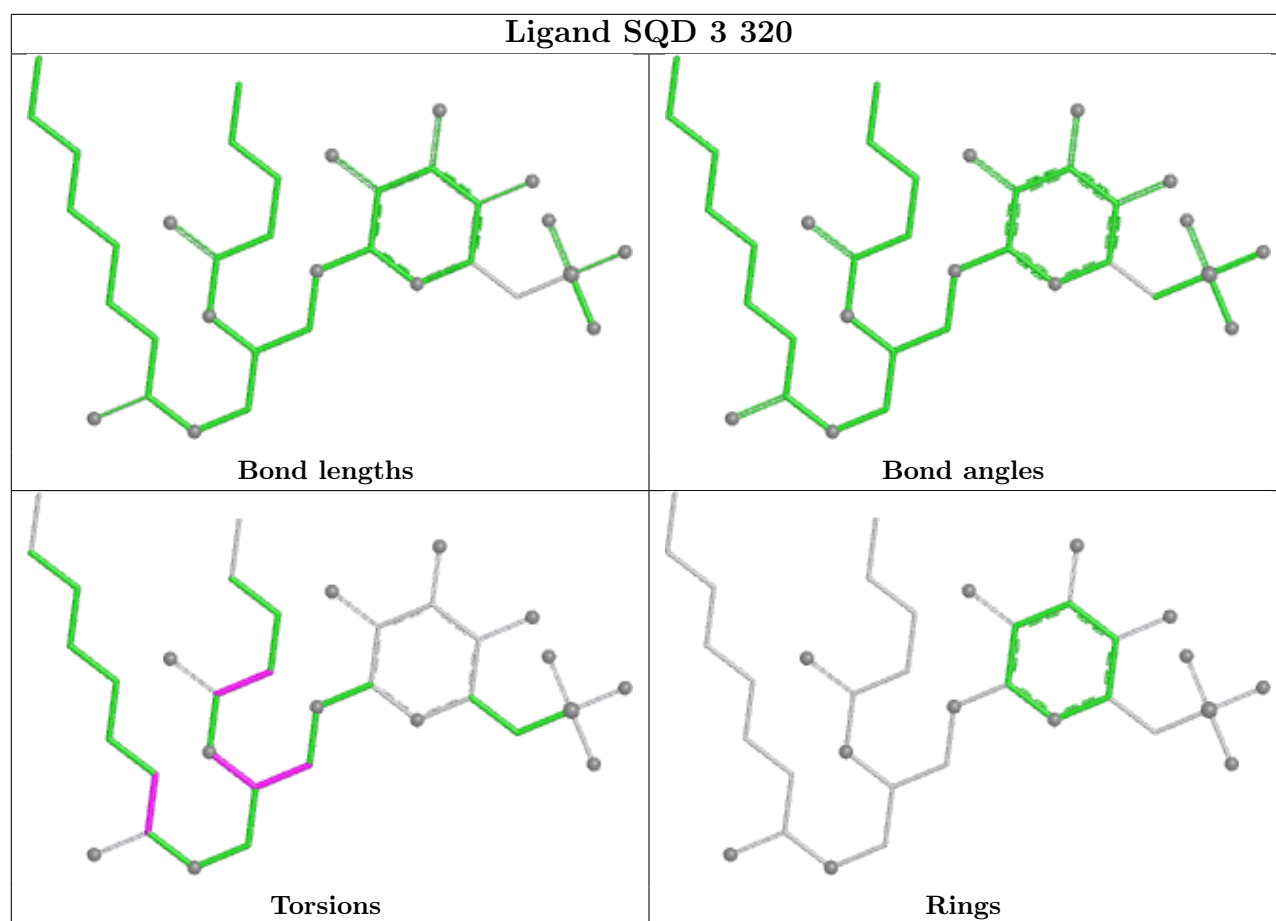


## Ligand CLA 2 304

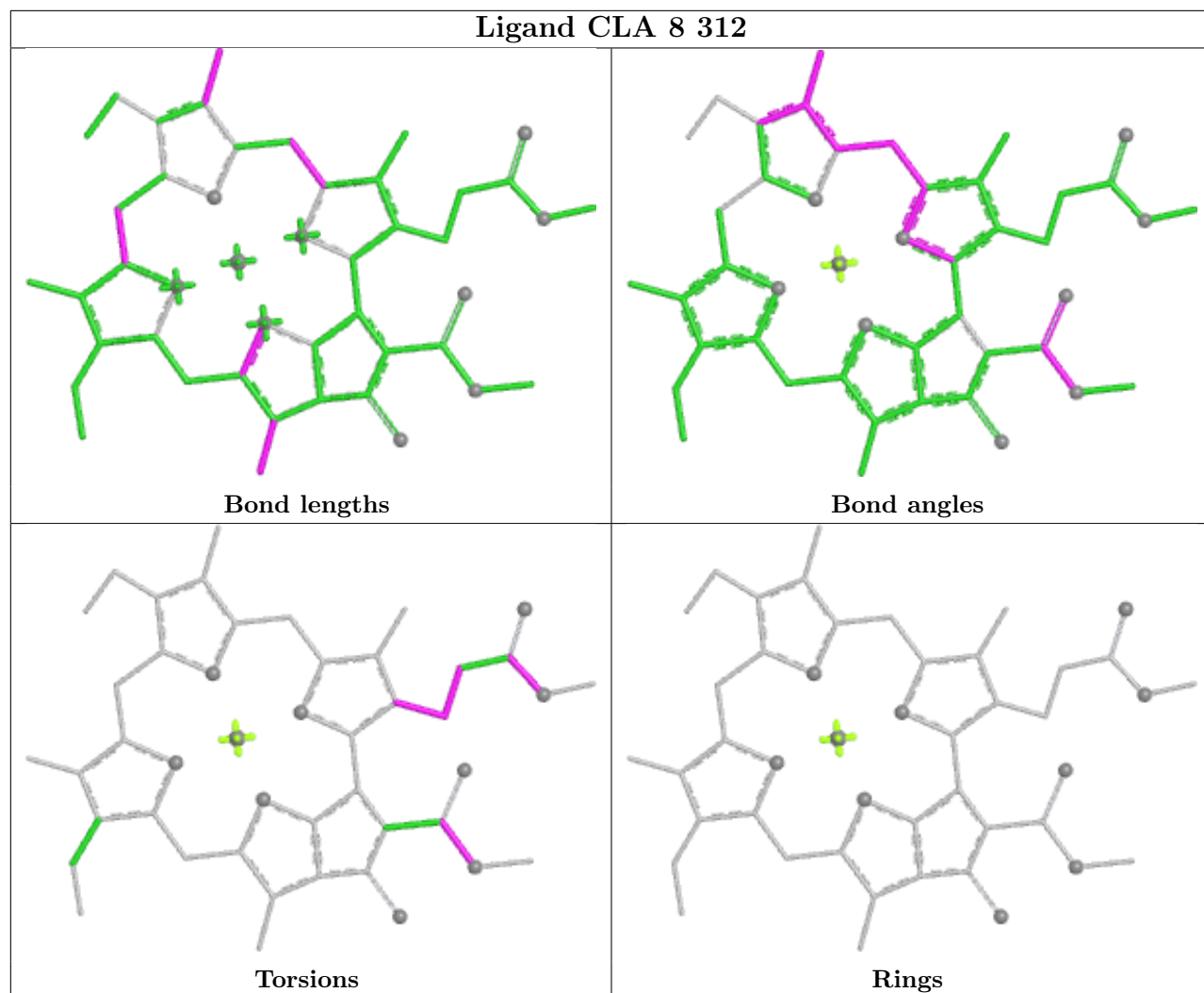




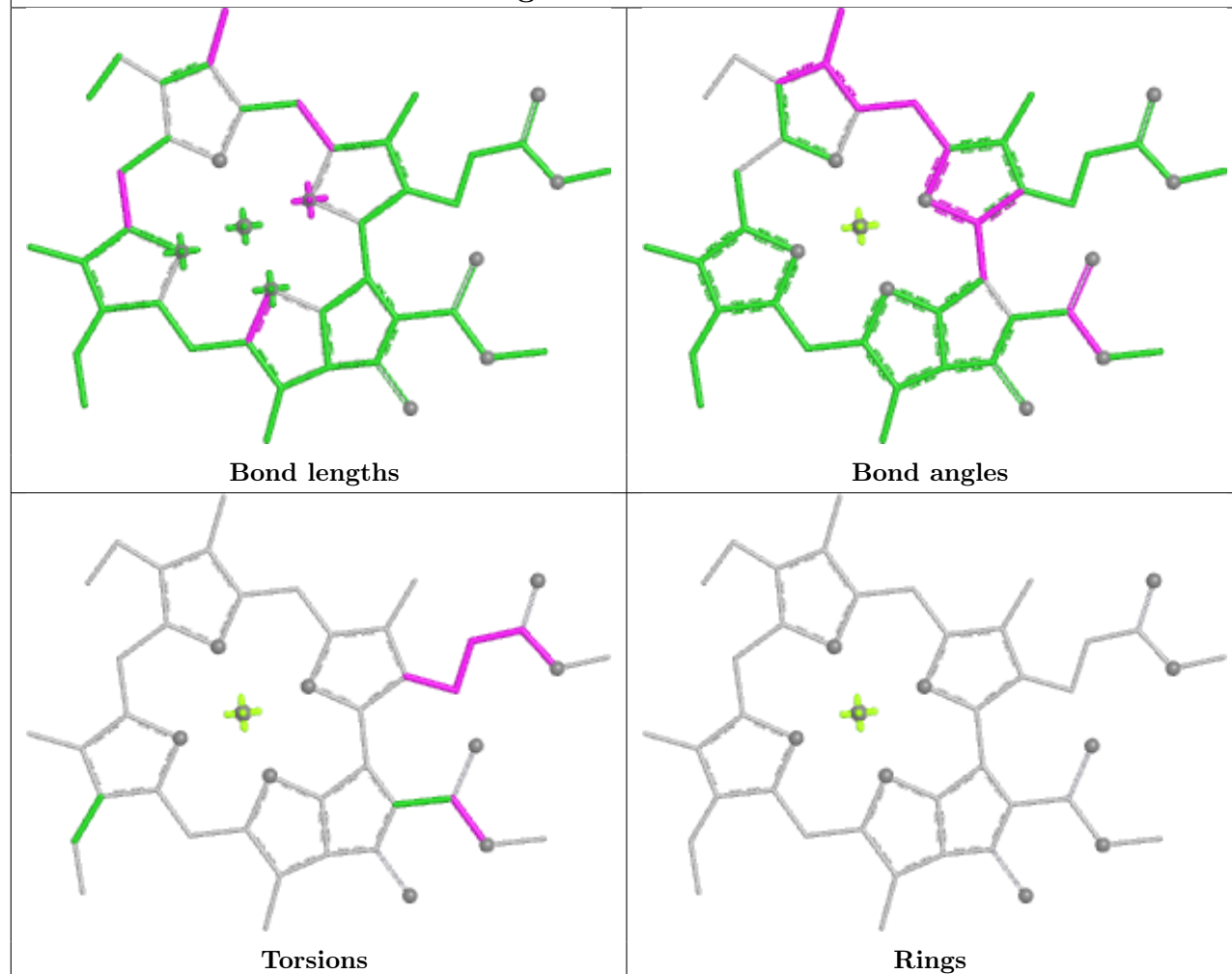




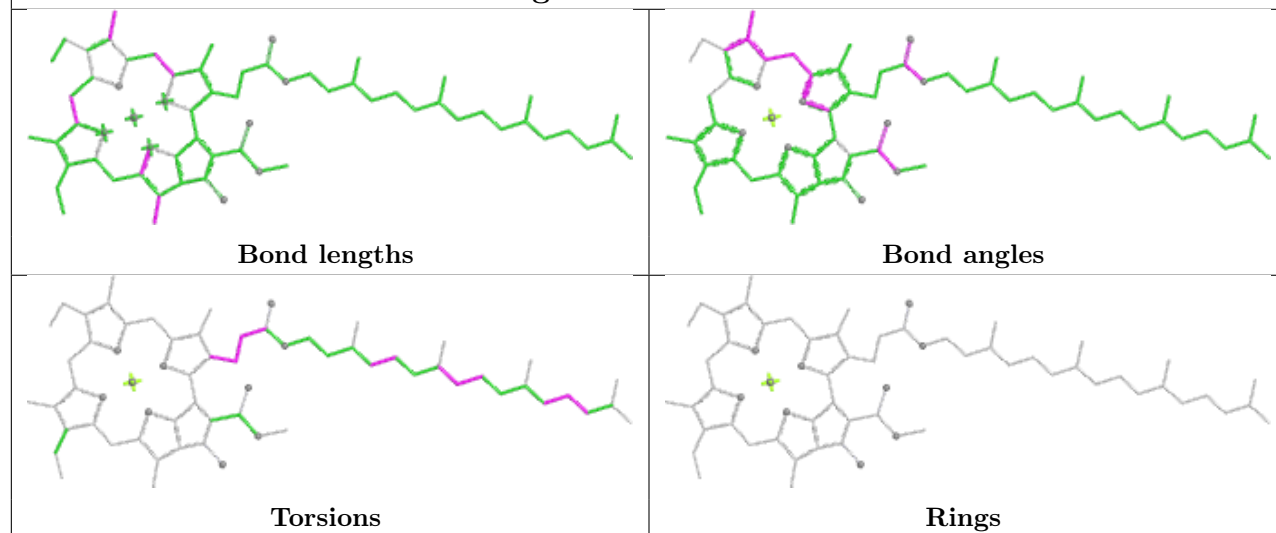
## Ligand CLA 8 312

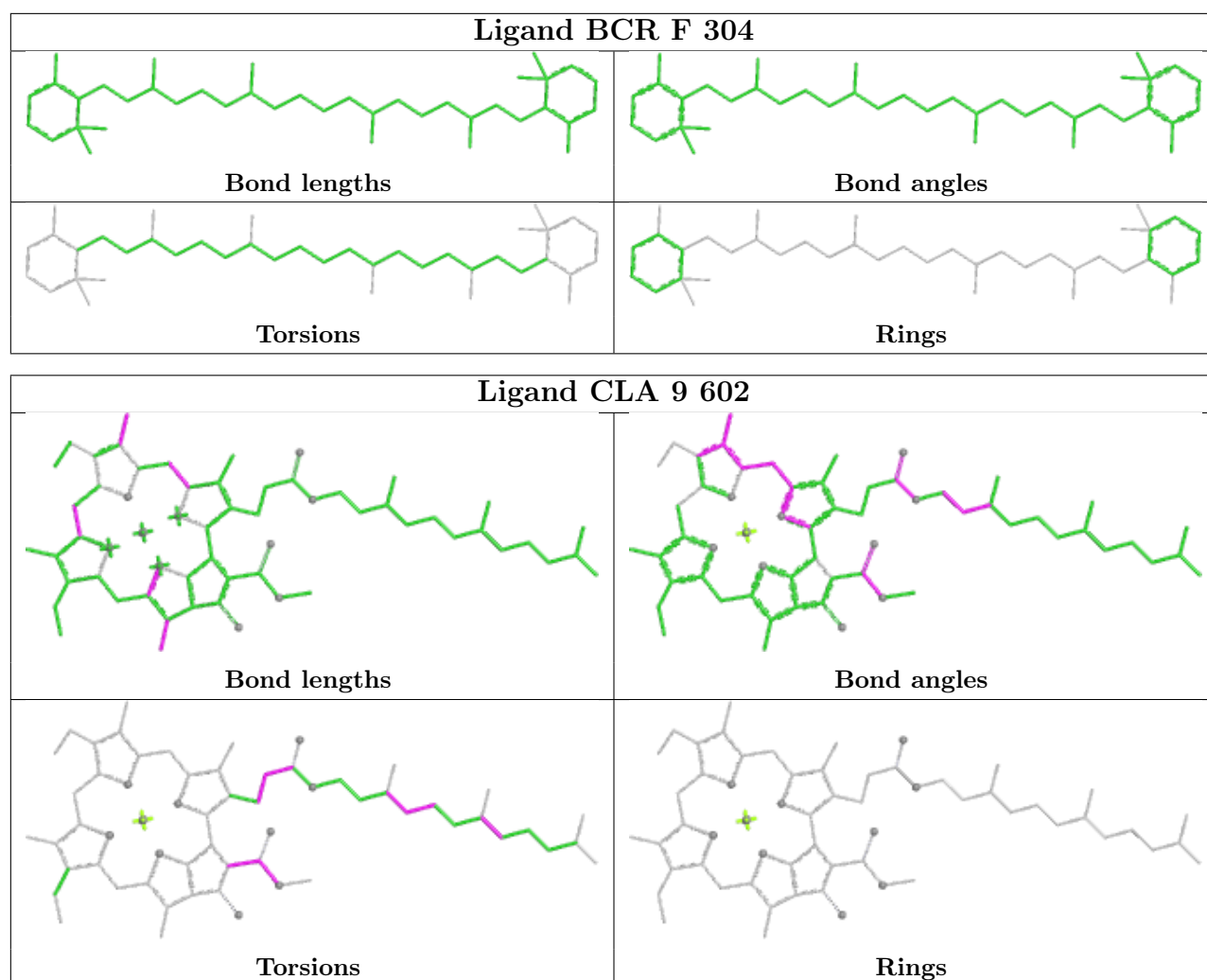


## Ligand CLA 8 321

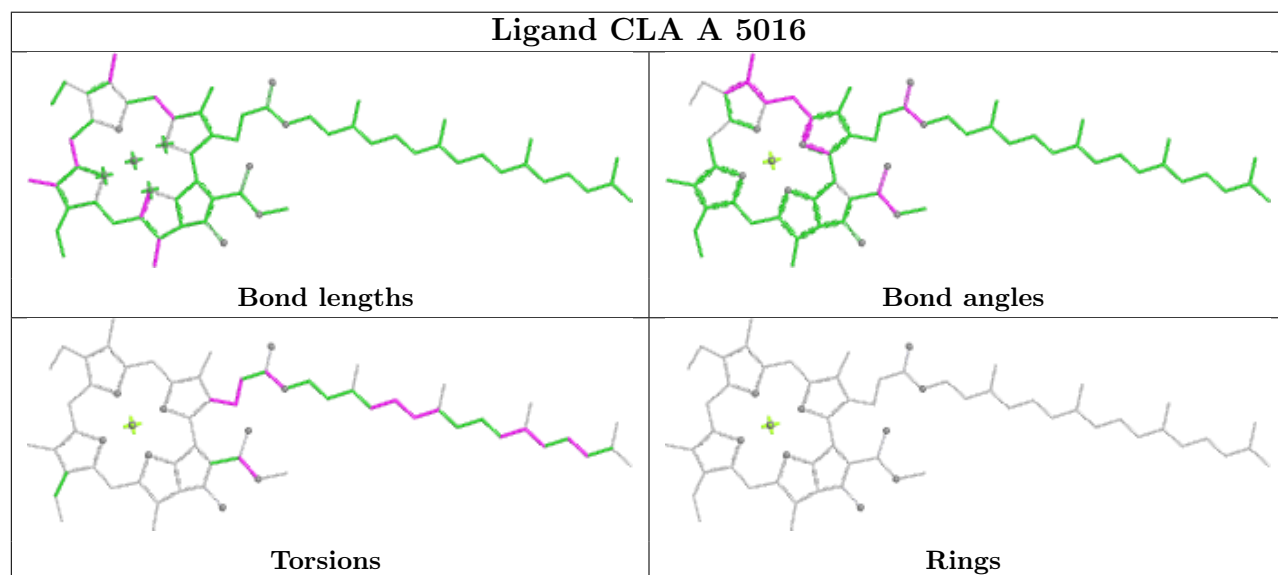
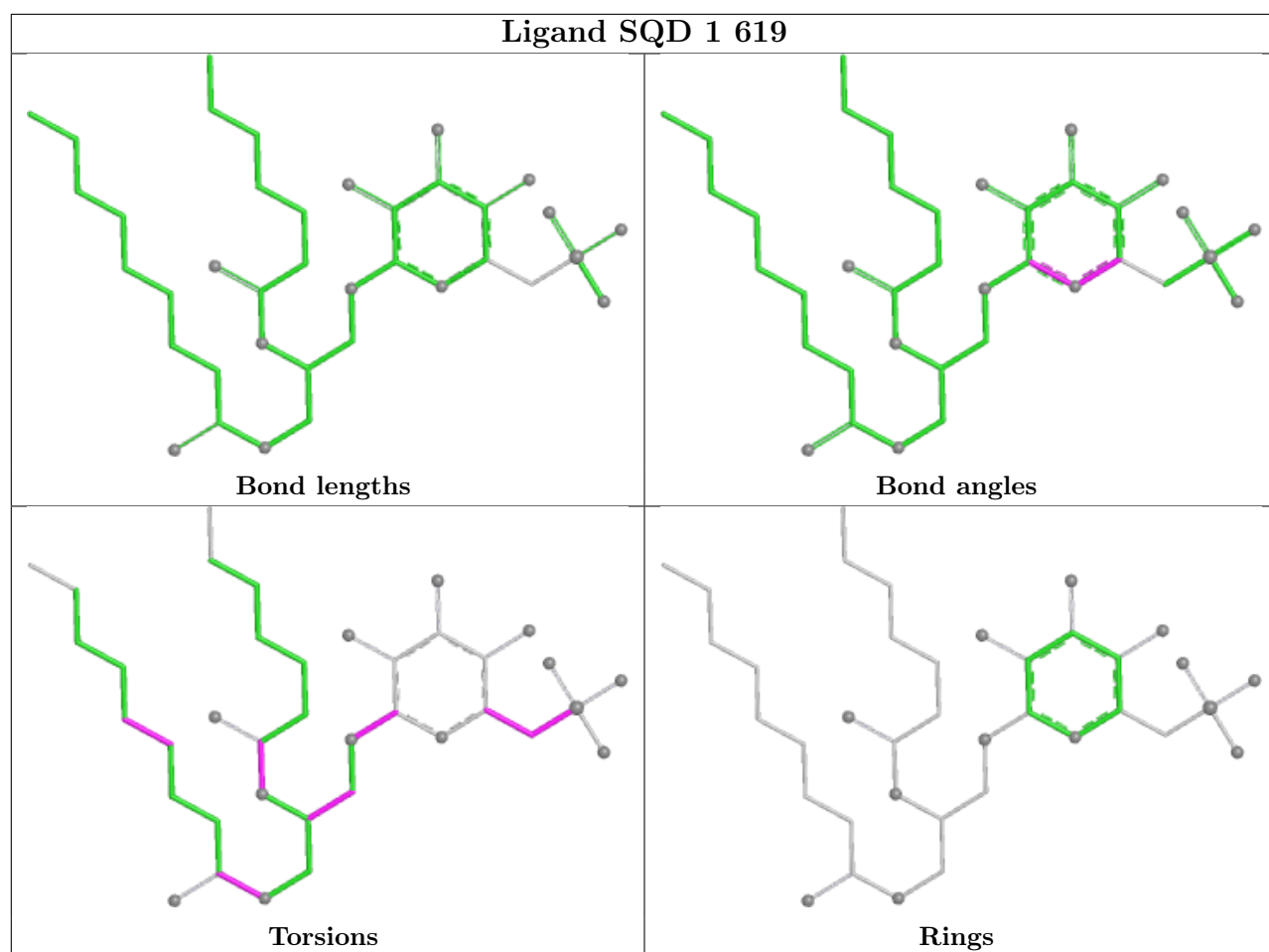


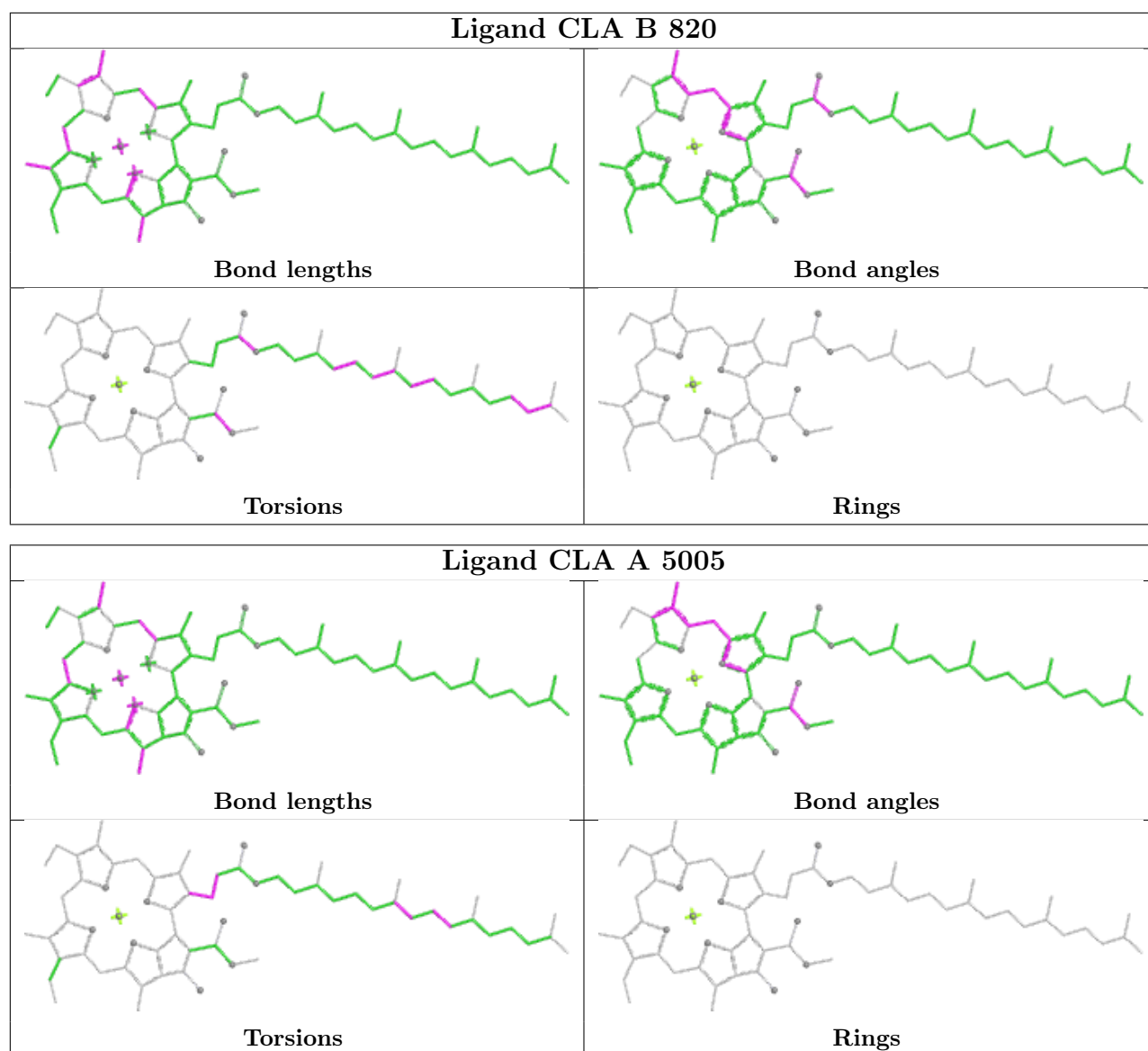
## Ligand CLA B 827



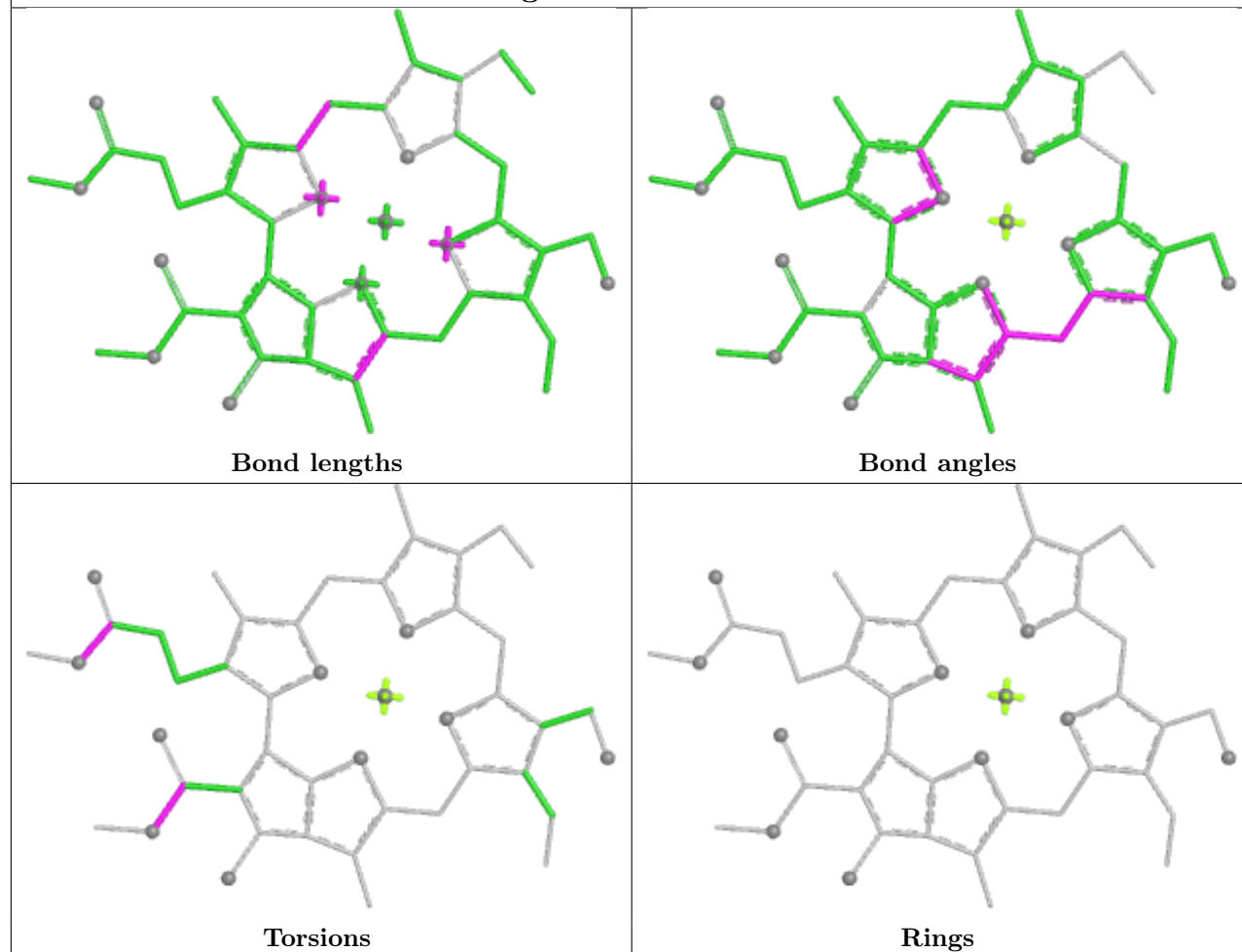




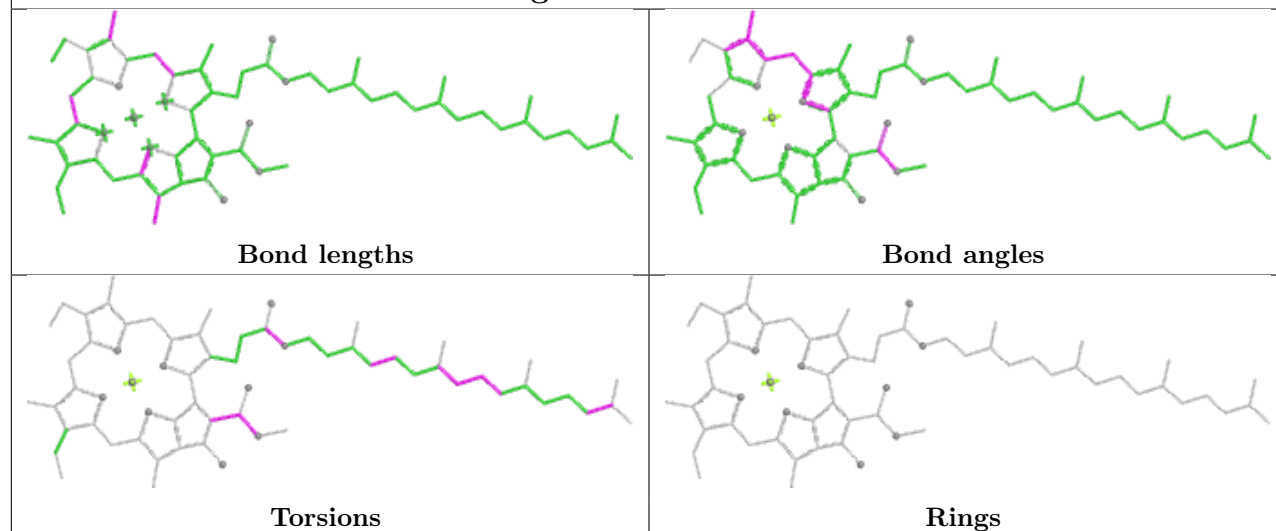




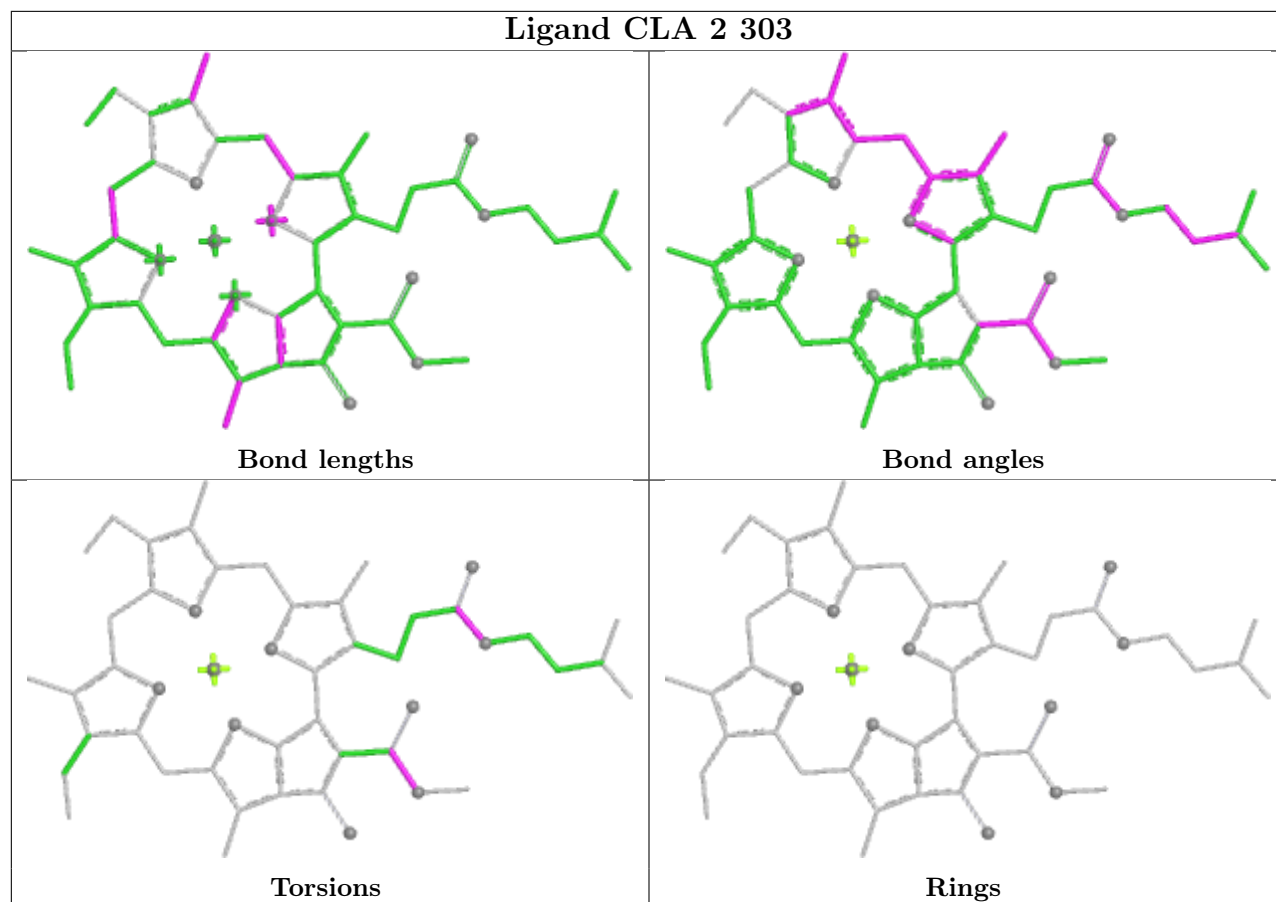
## Ligand CHL 8 305



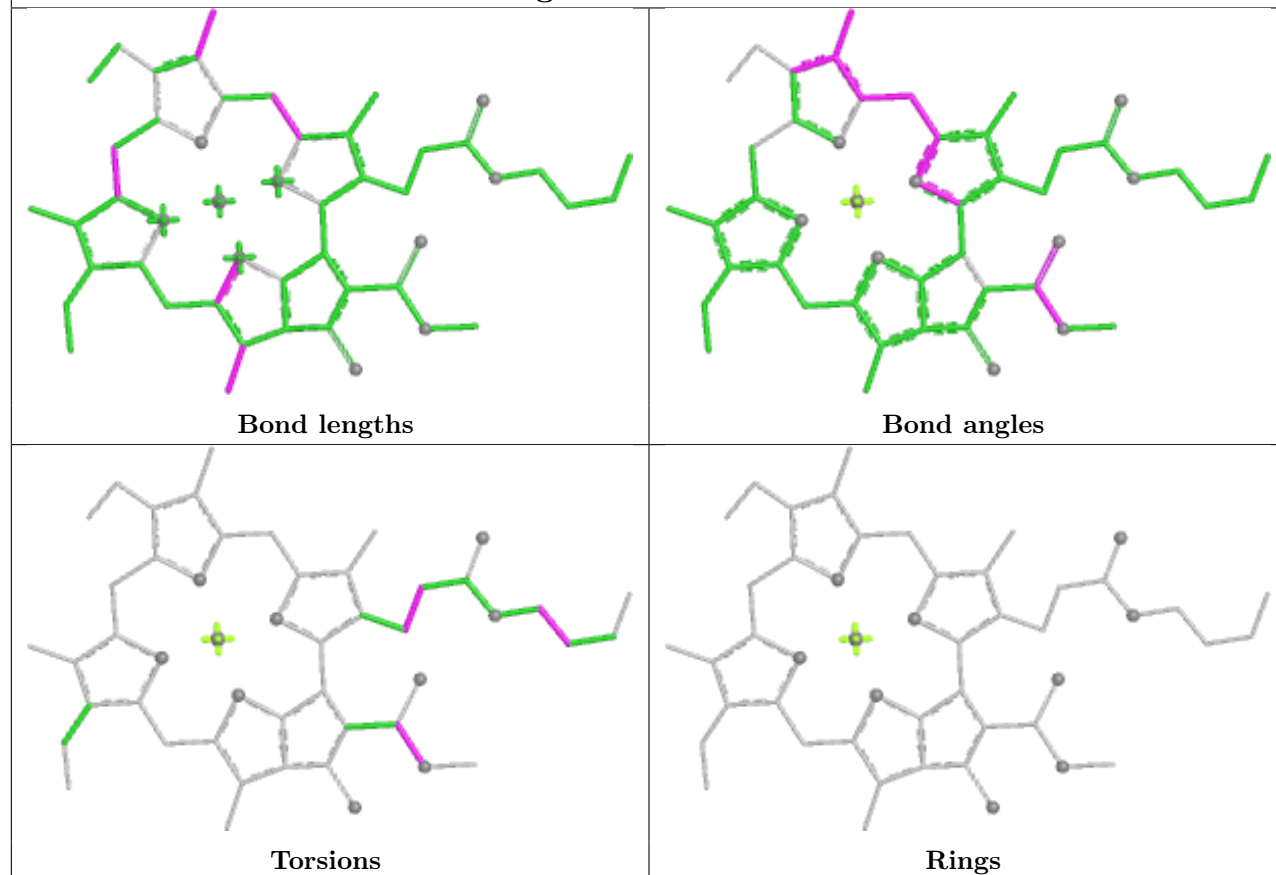
## Ligand CLA G 201



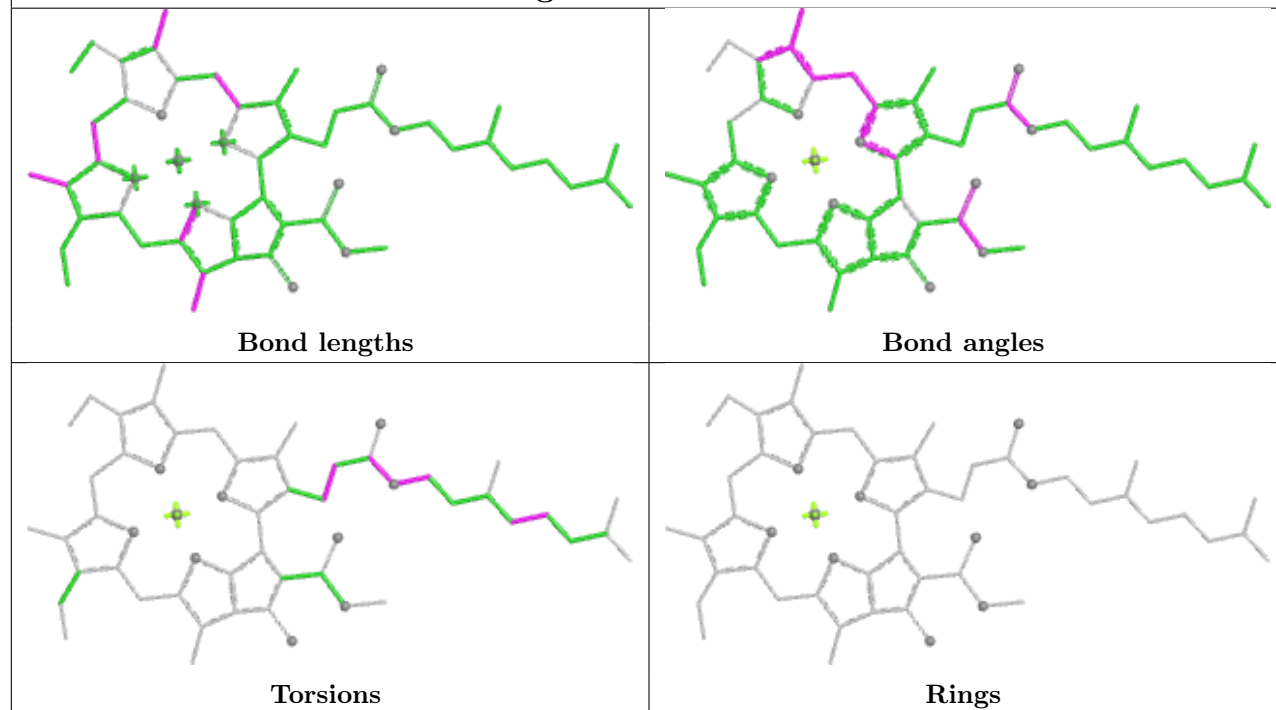
## Ligand CLA 2 303

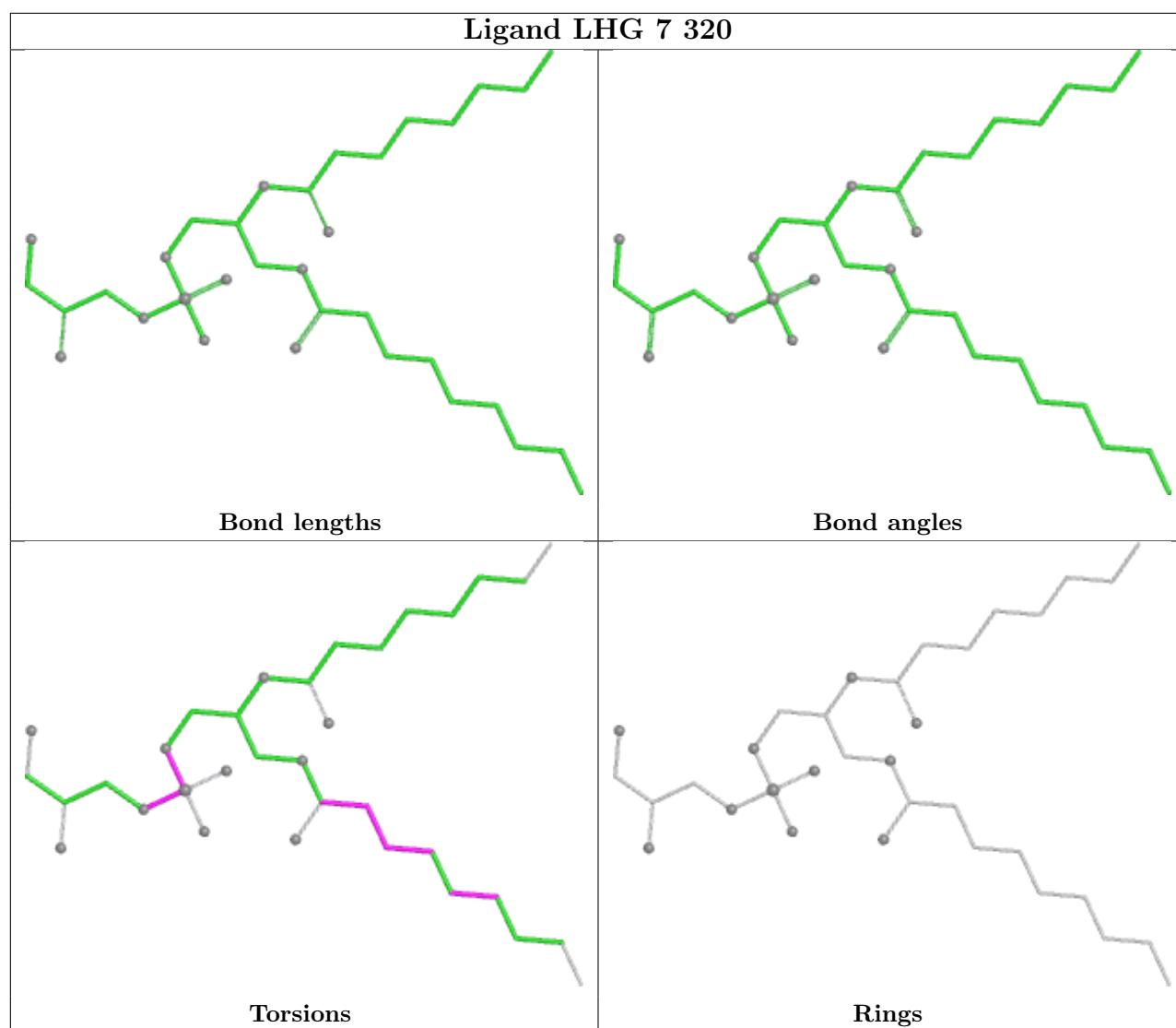


## Ligand CLA J 104

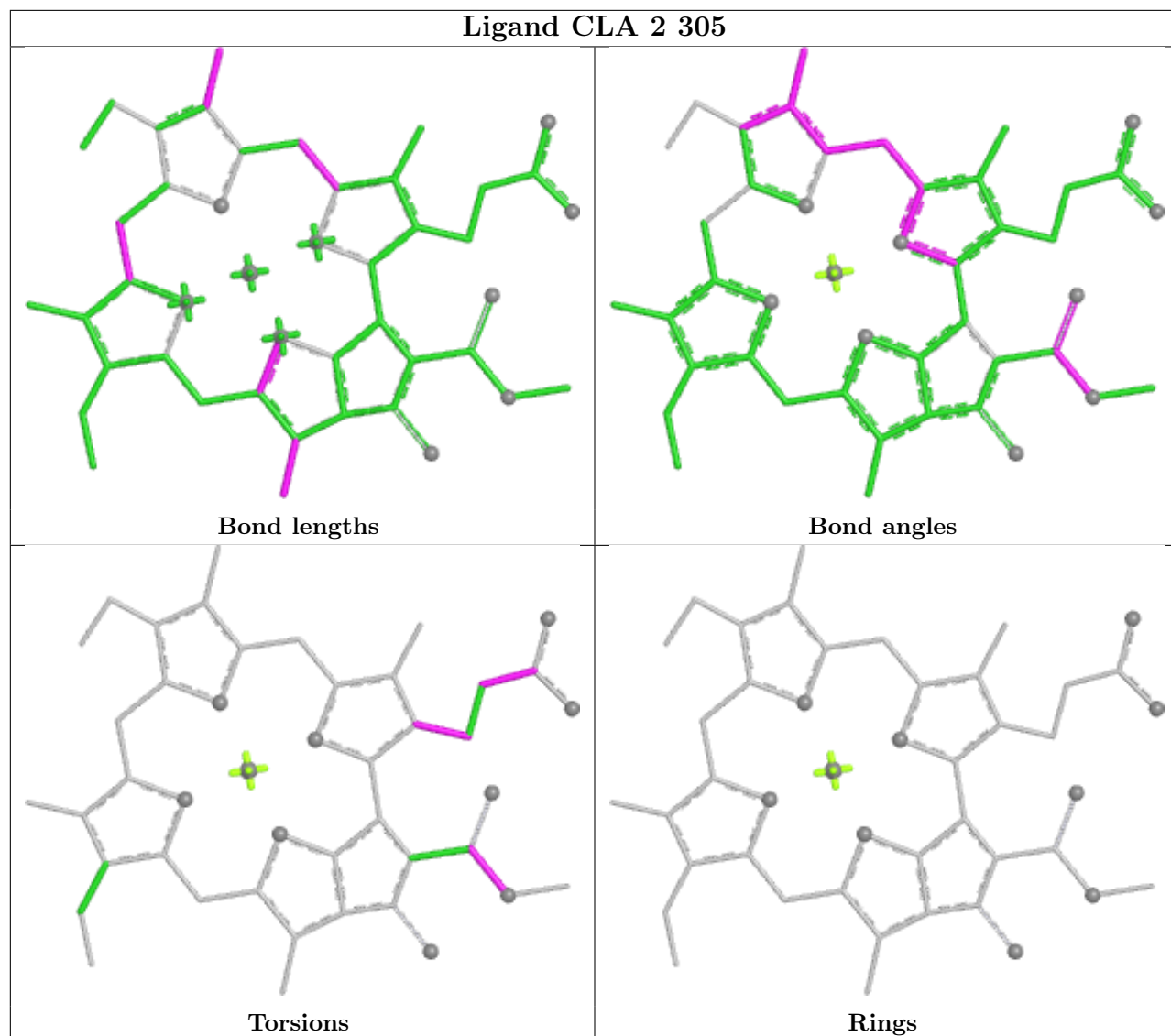


## Ligand CLA 9 611

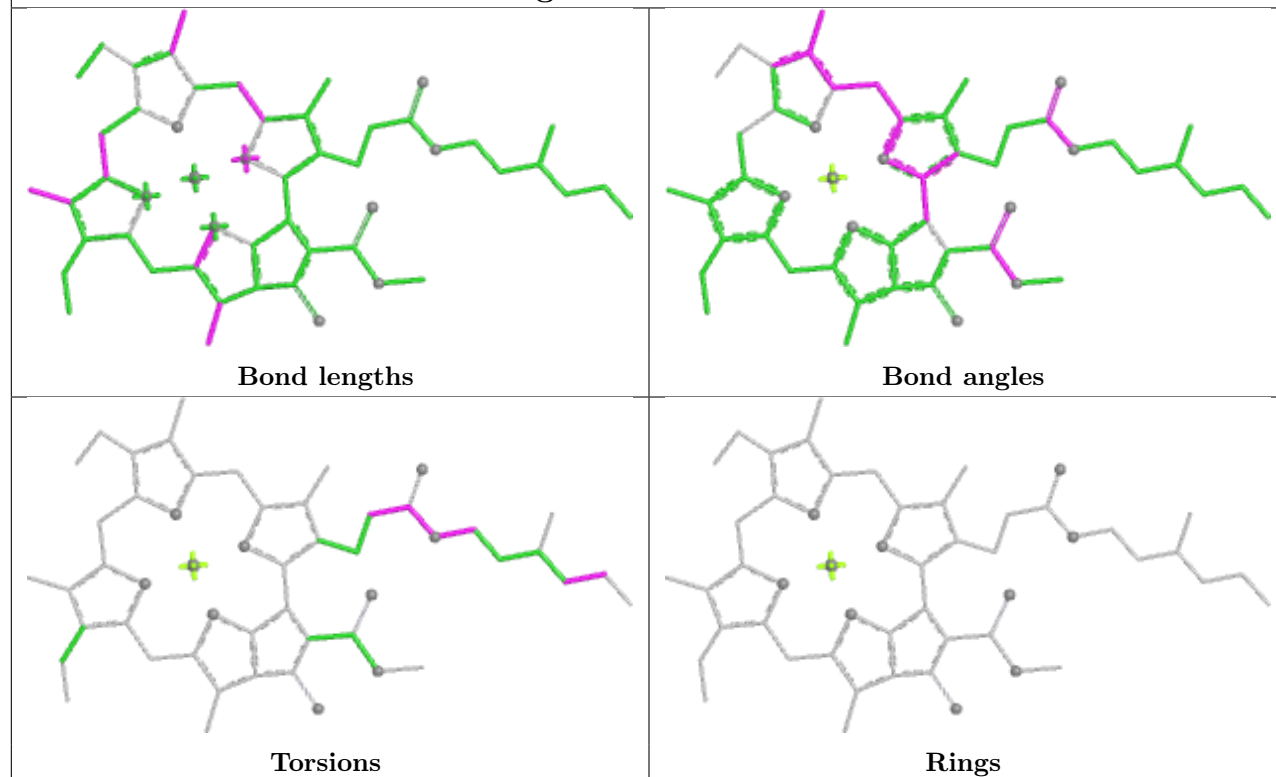




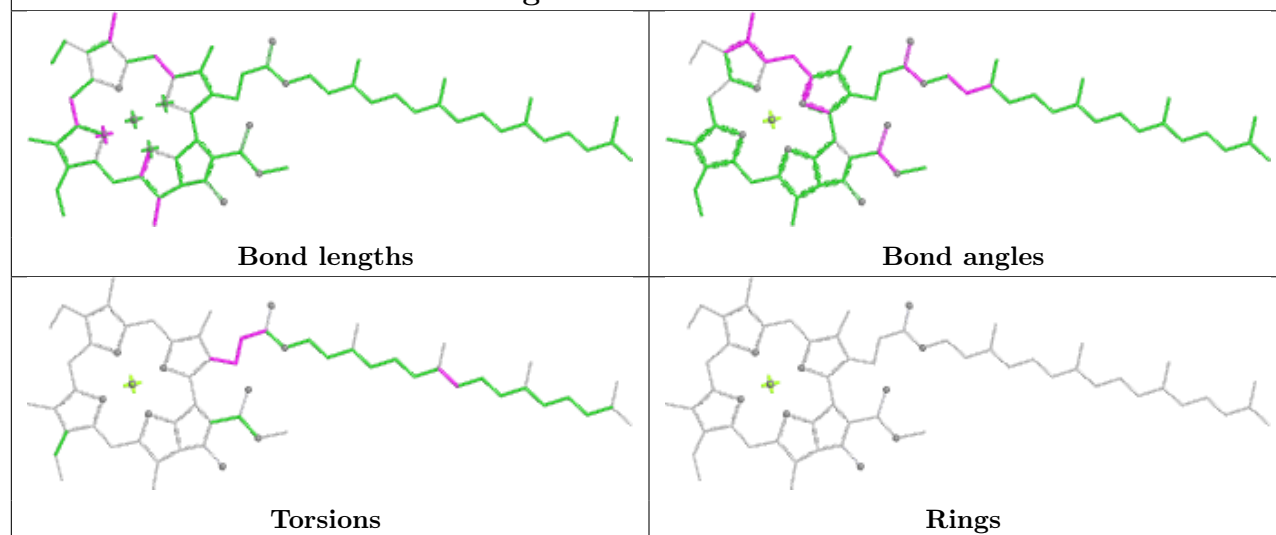
## Ligand CLA 2 305



## Ligand CLA 7 312

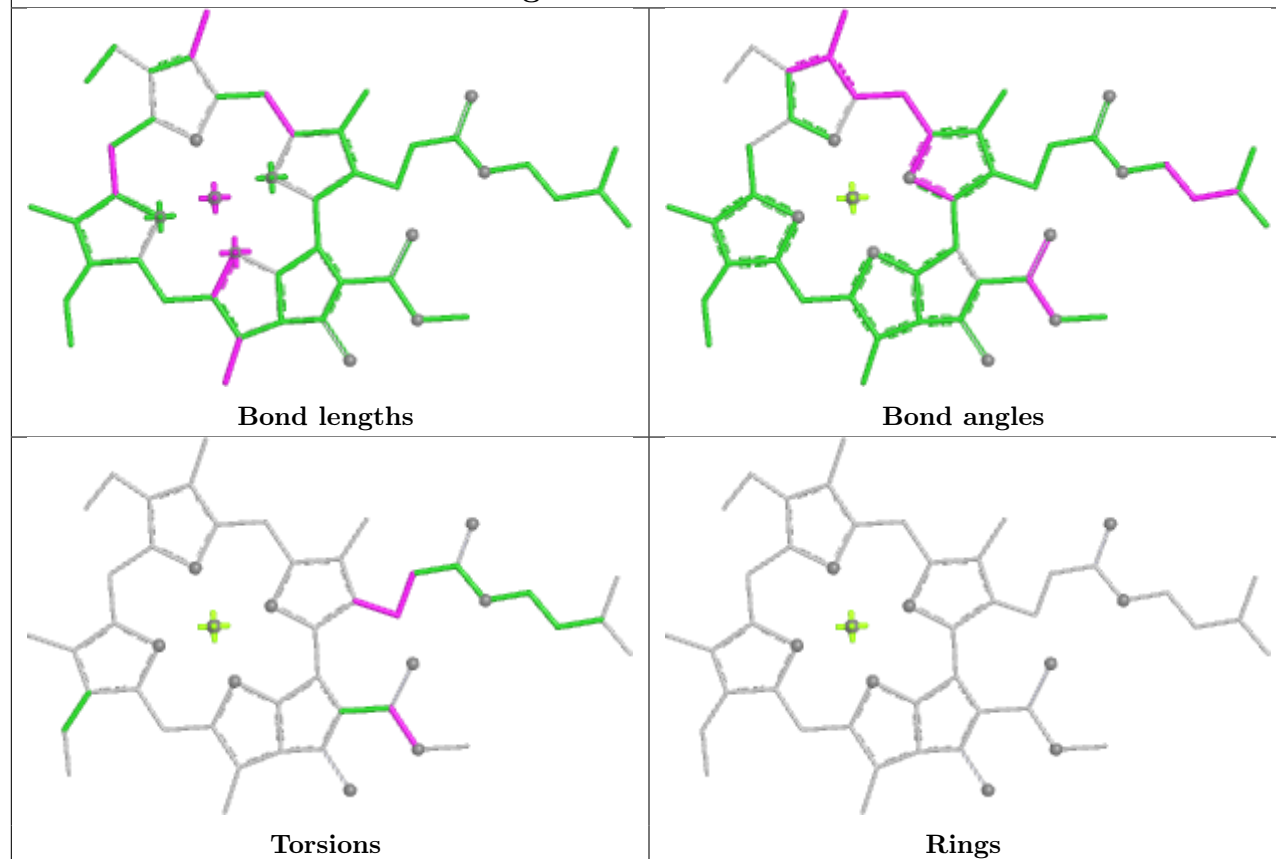


## Ligand CLA A 5041

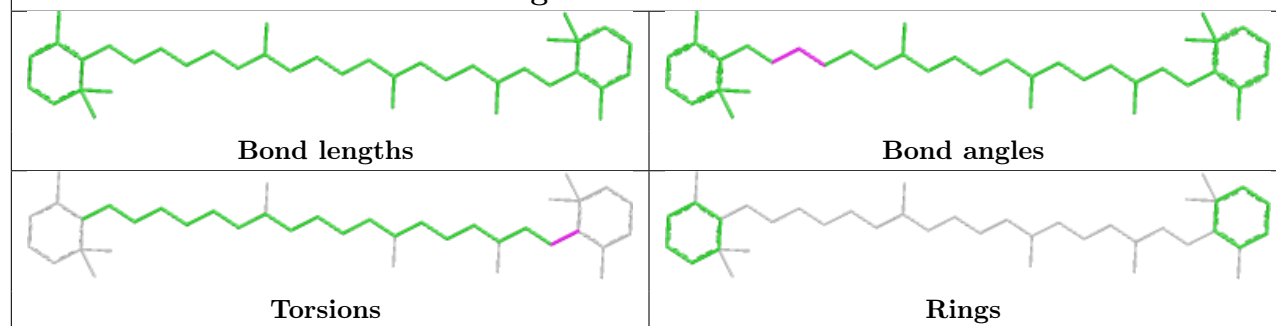


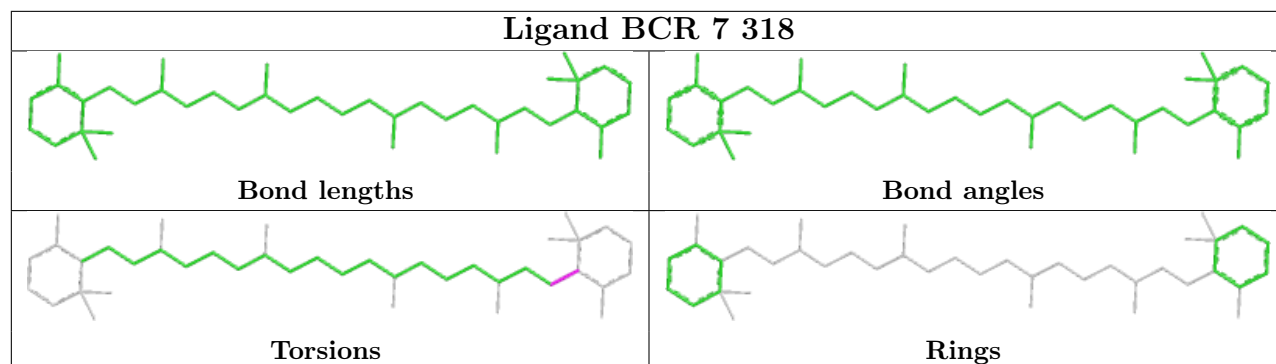
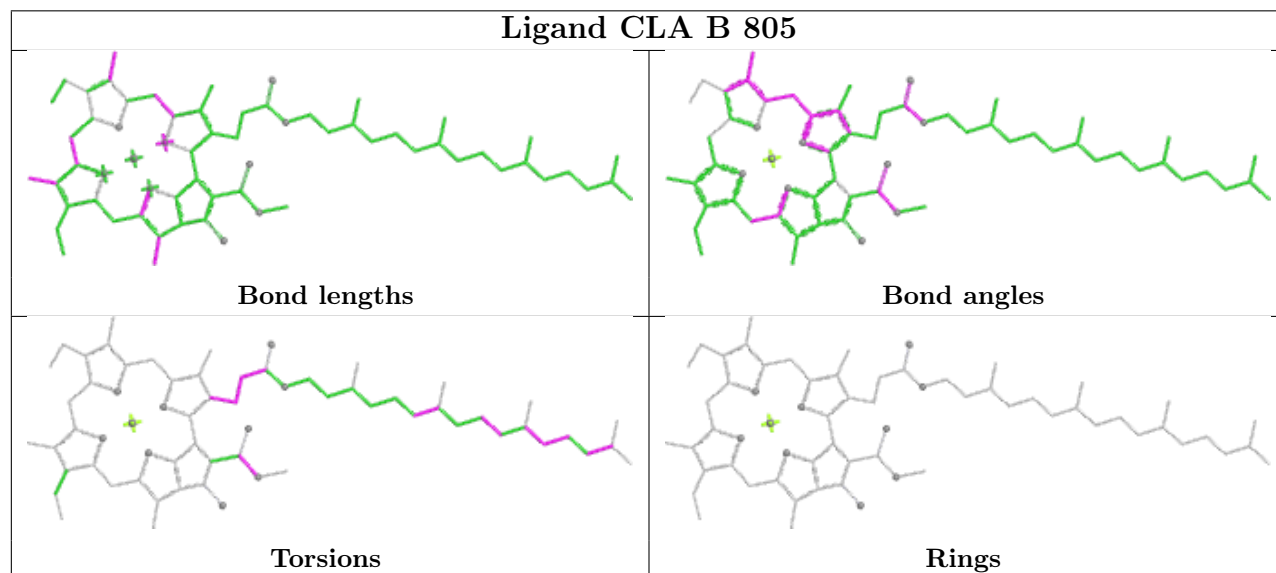
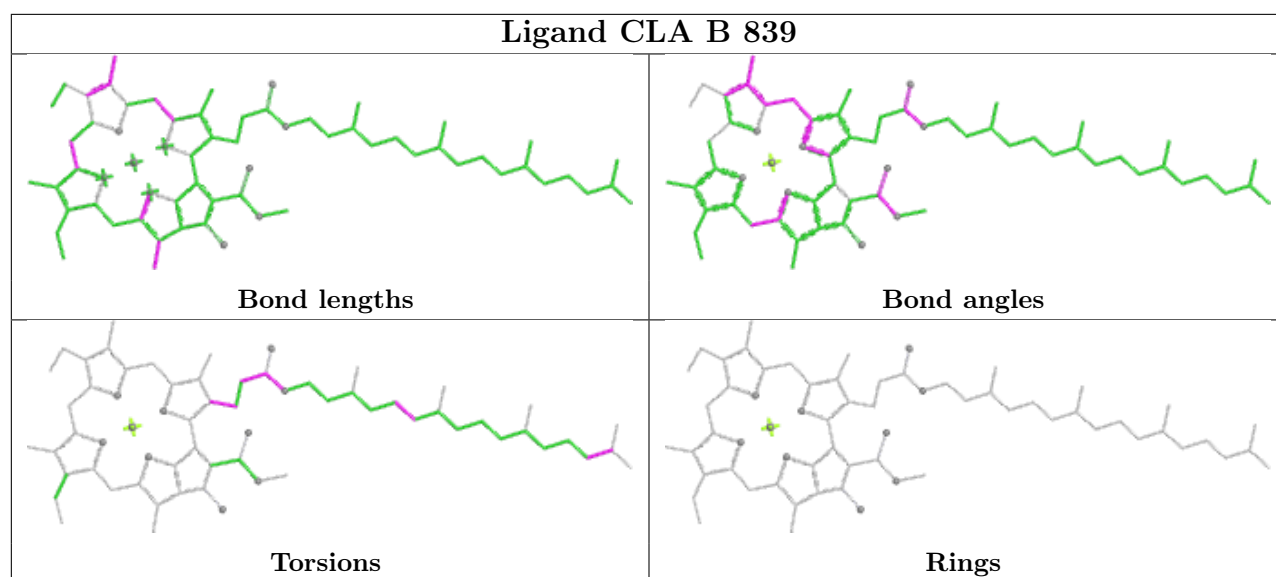


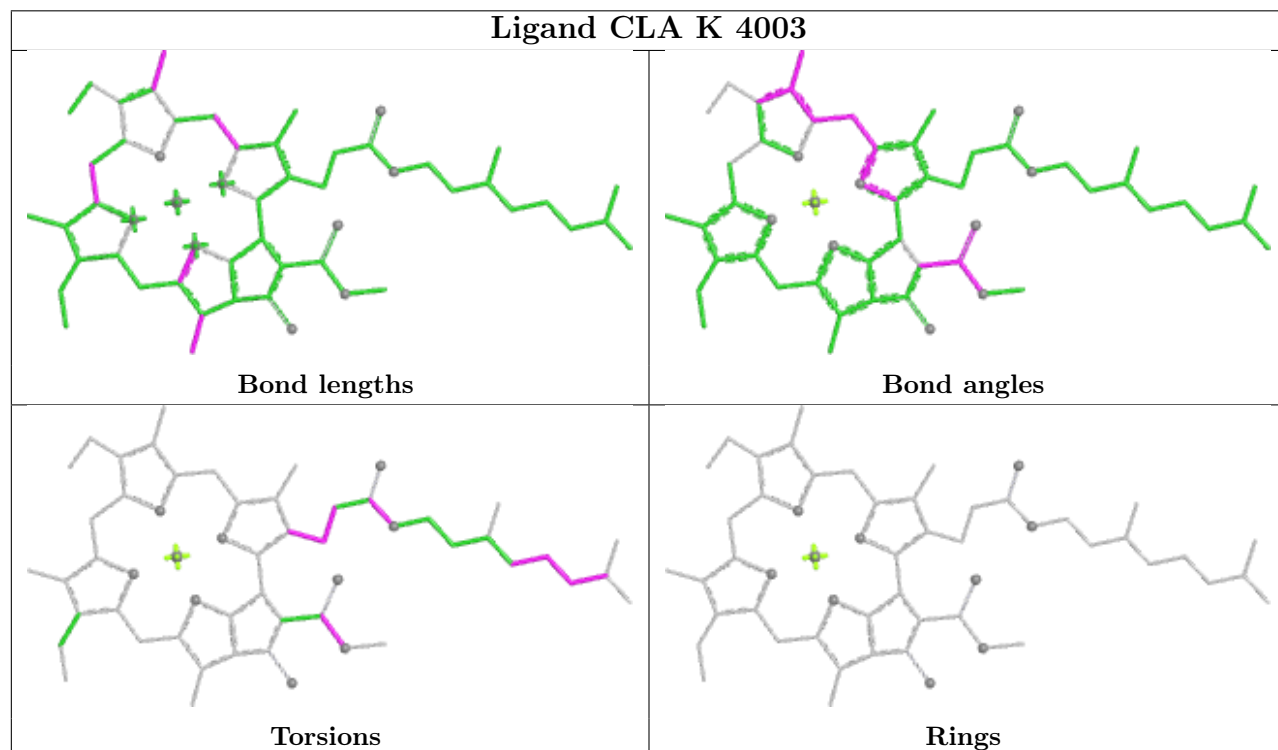
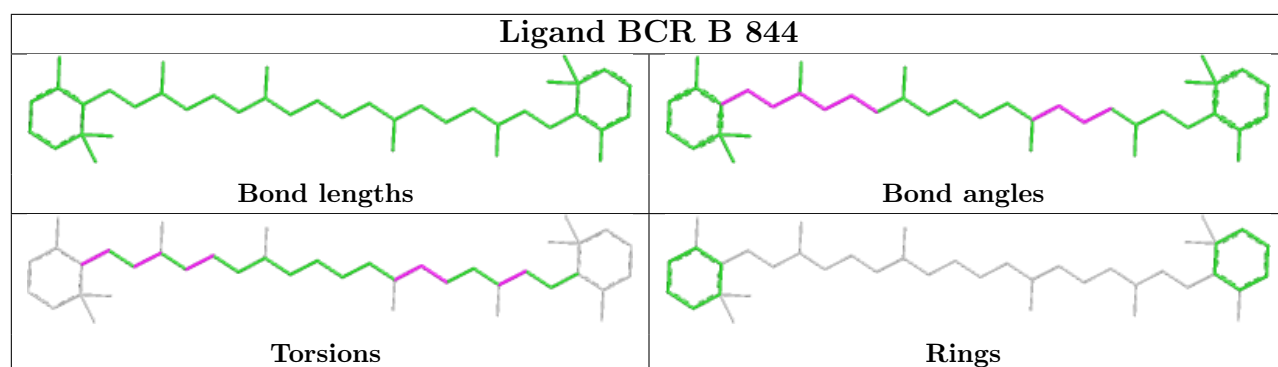
## Ligand CLA A 5038



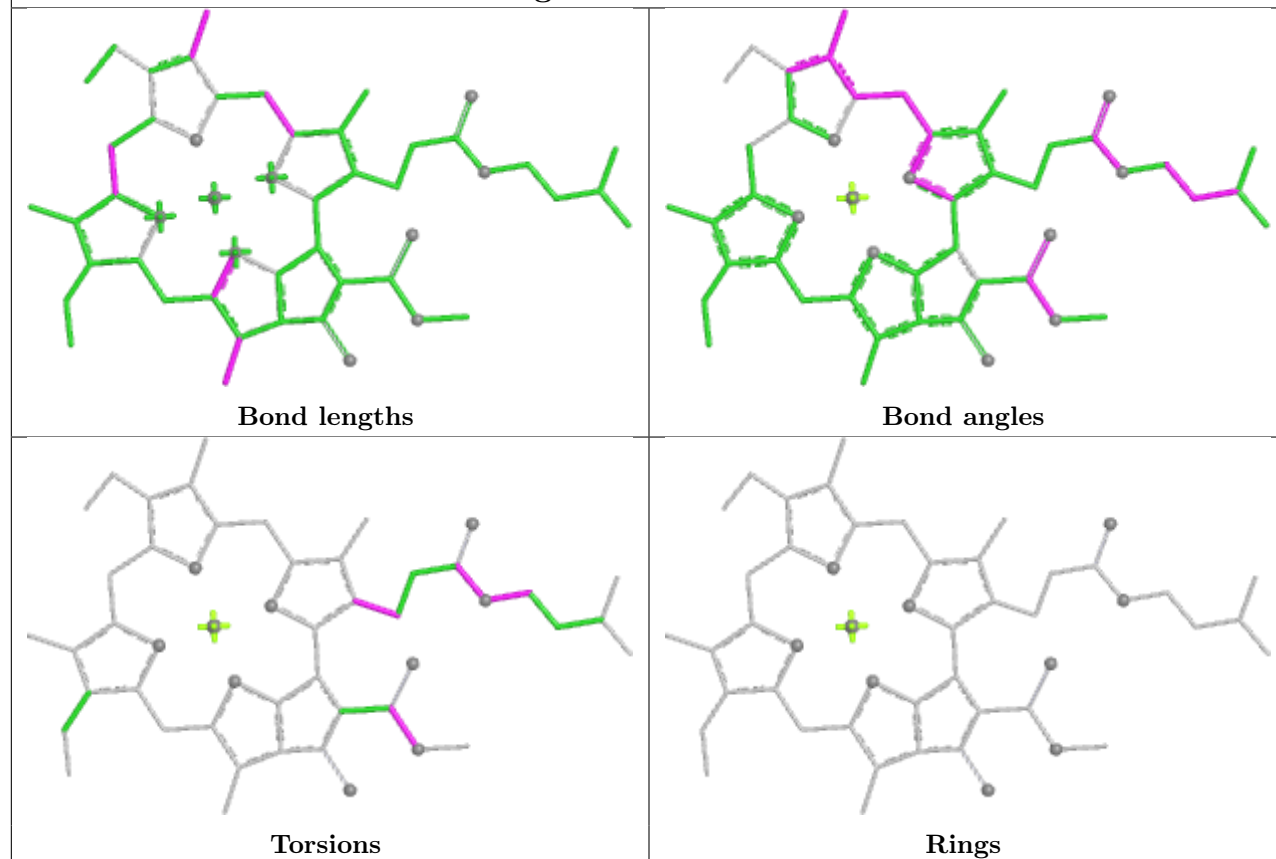
## Ligand BCR B 845



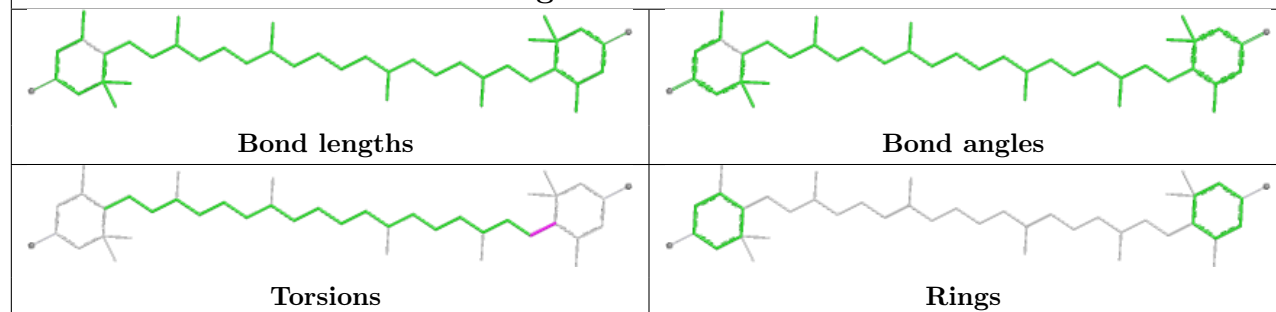


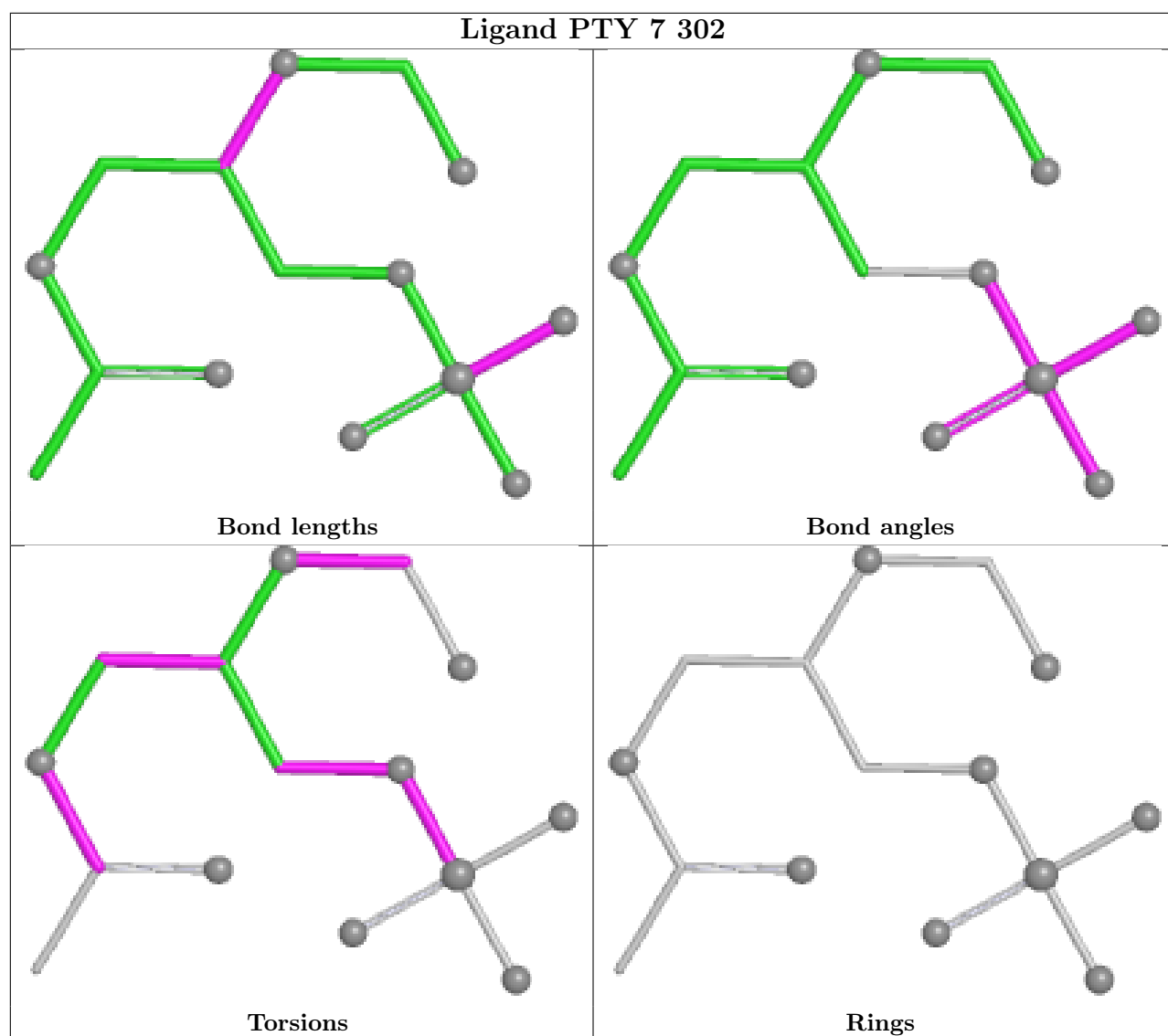


## Ligand CLA L 205

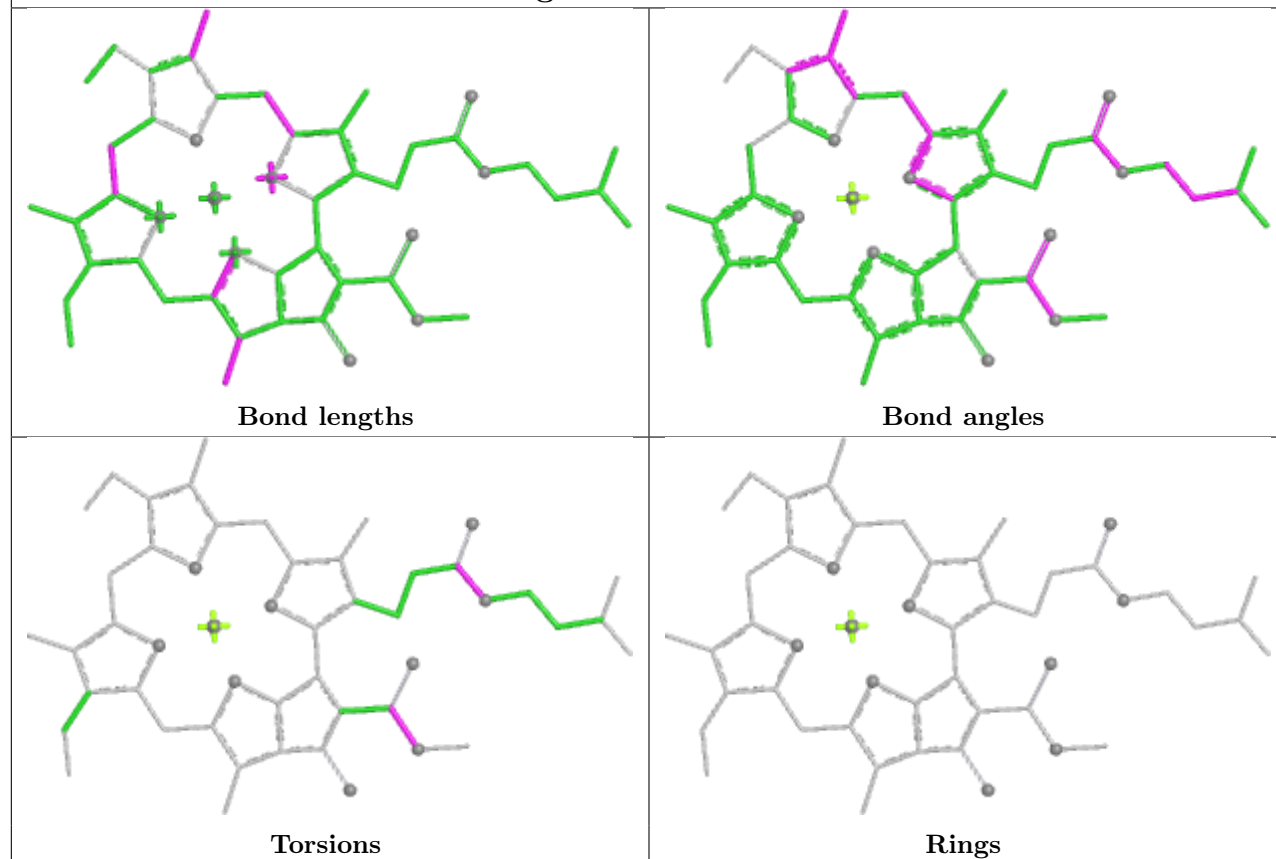


## Ligand LUT 9 613

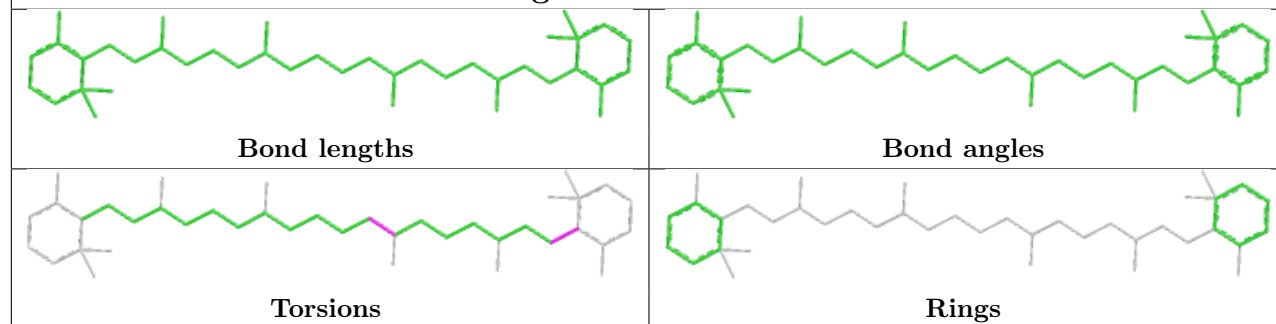


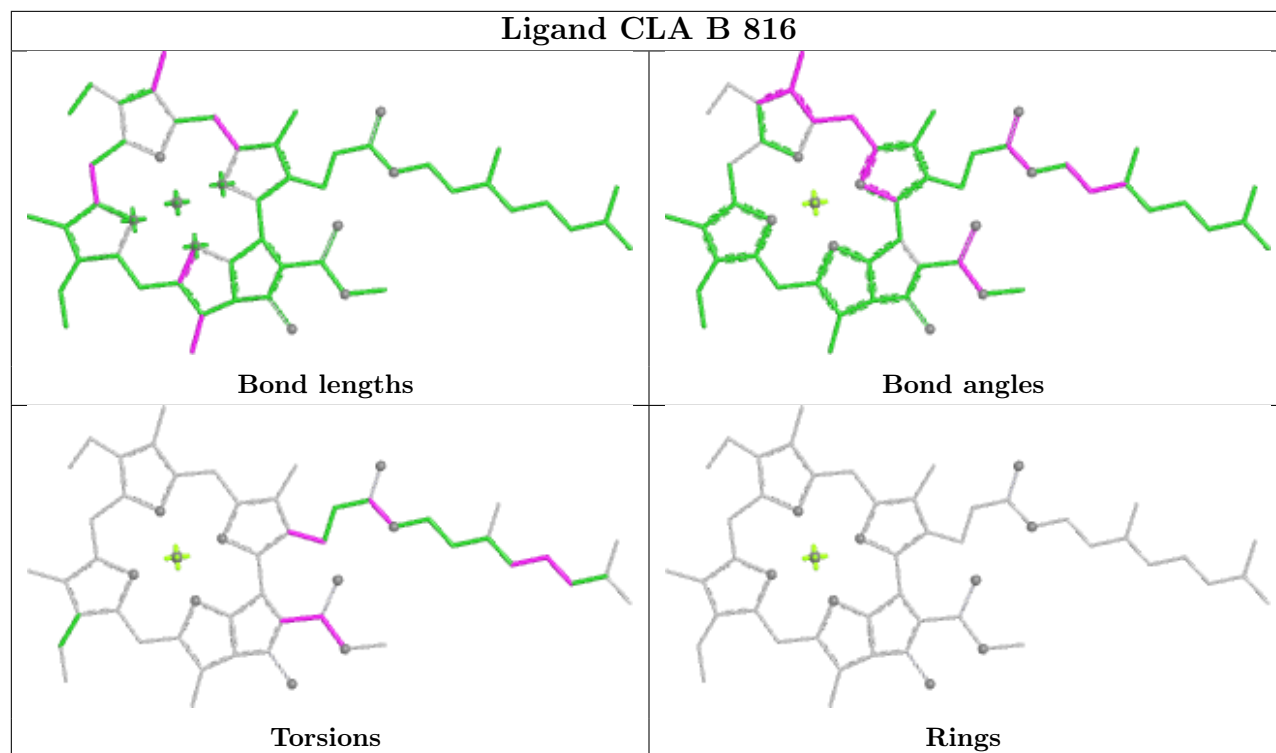
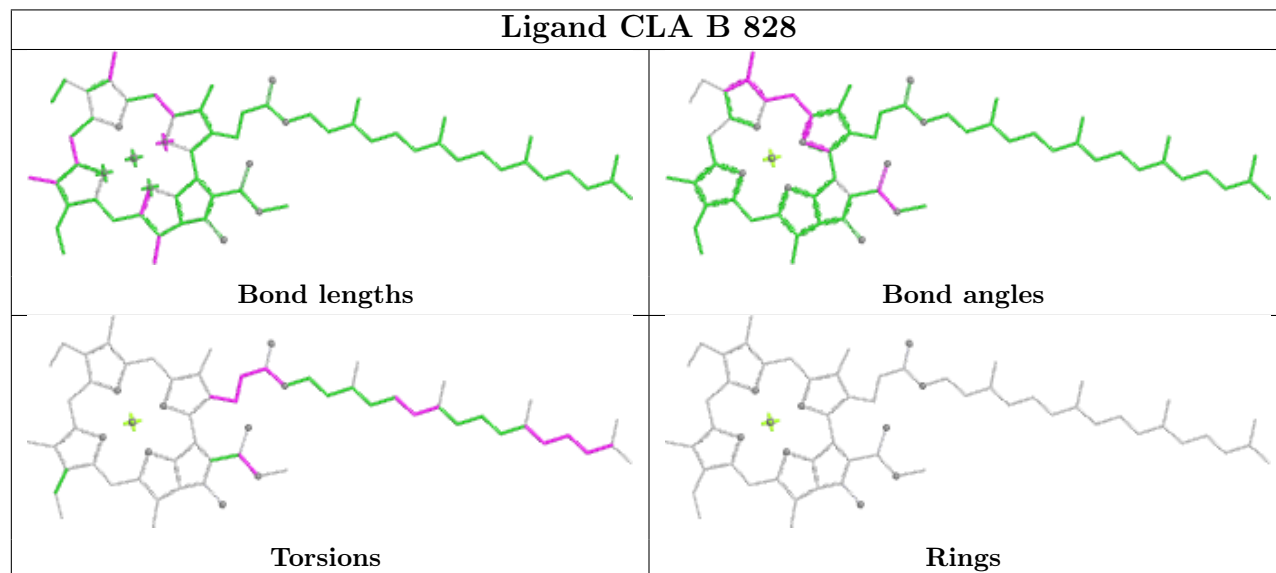


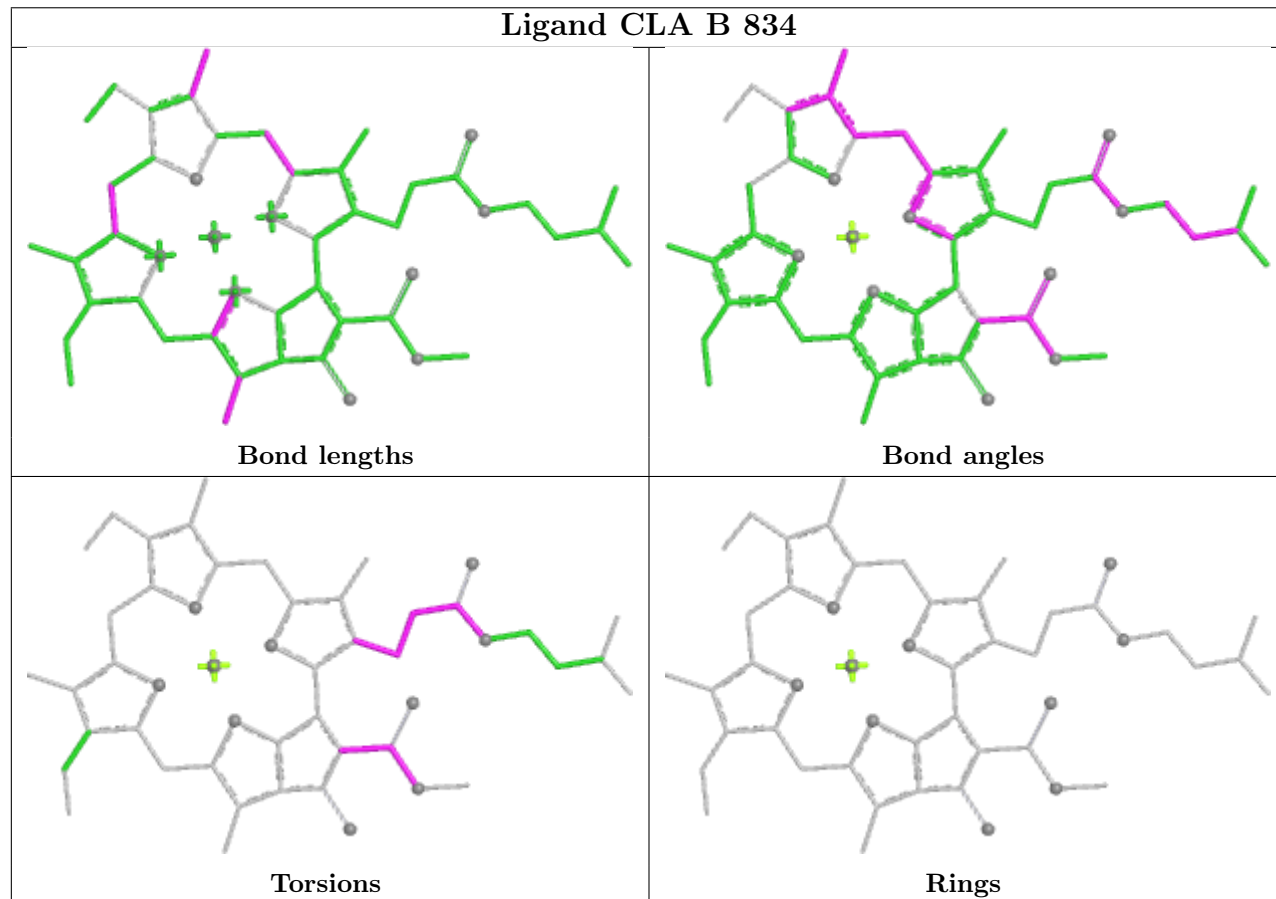
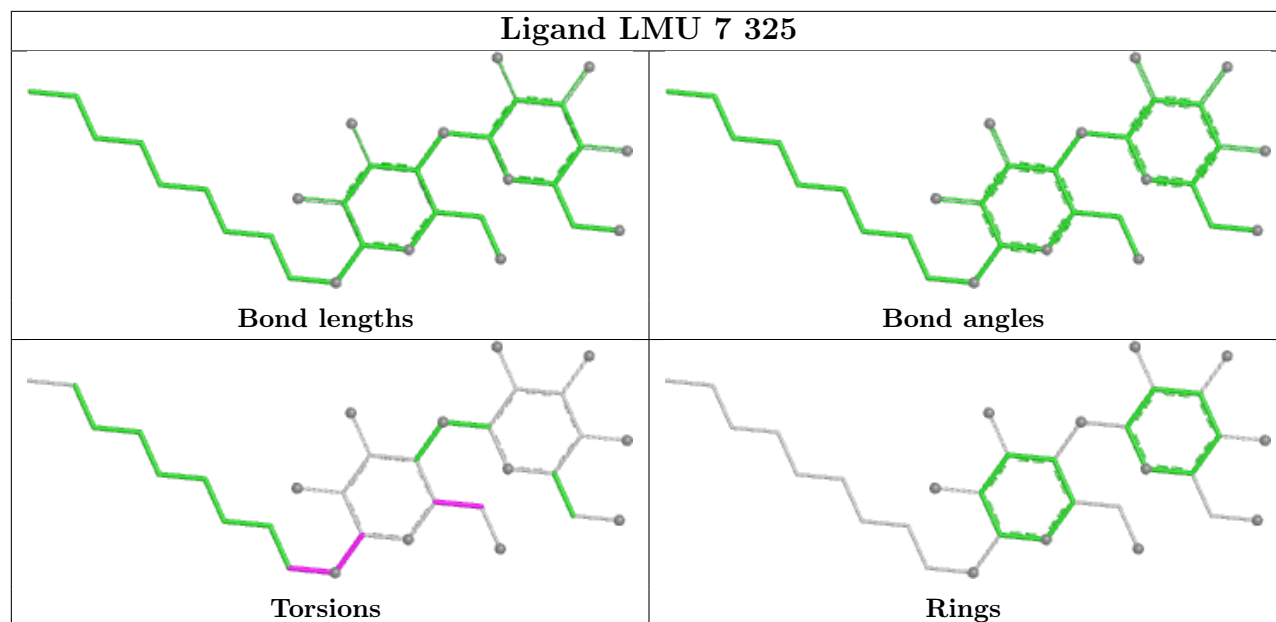
## Ligand CLA 7 305



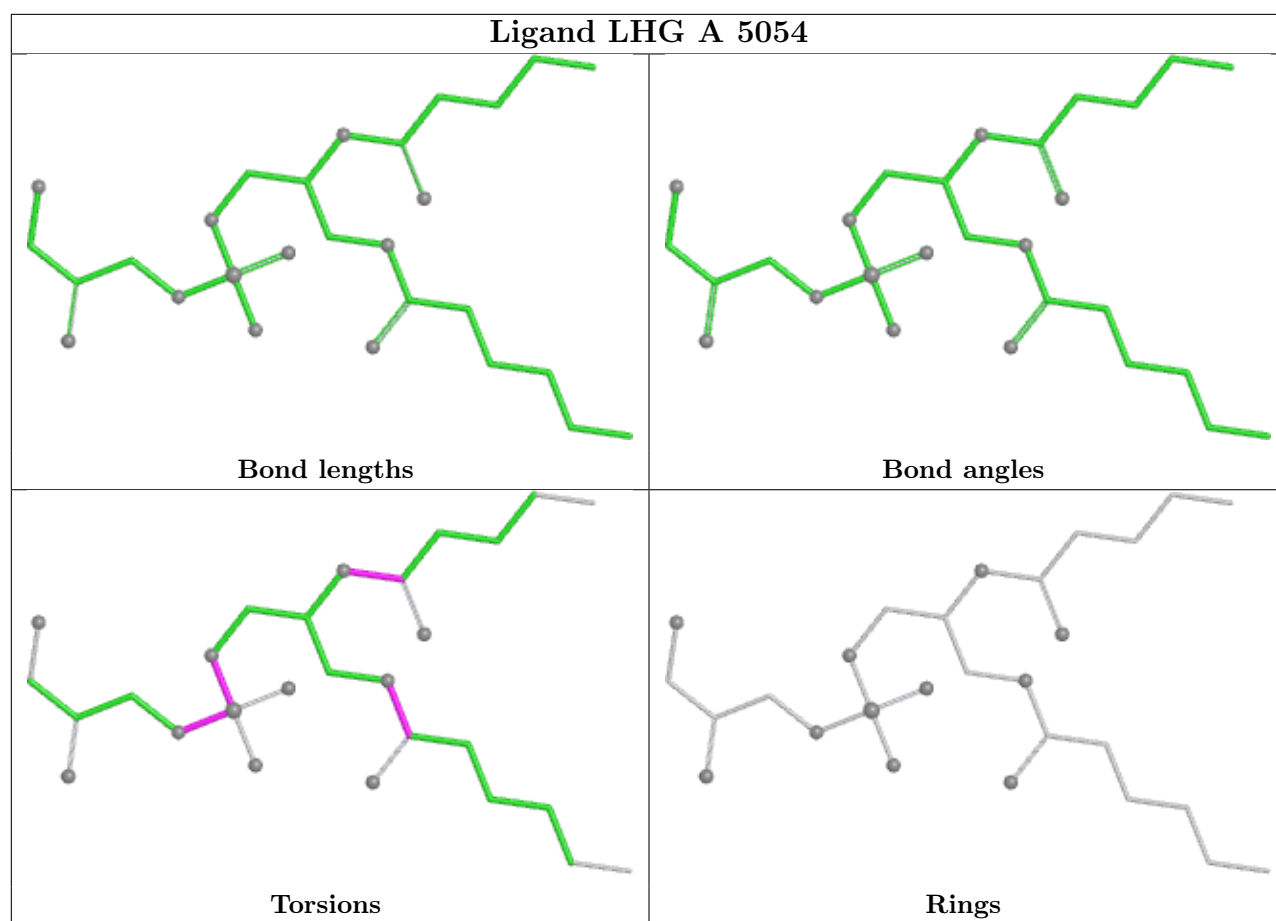
## Ligand BCR F 309



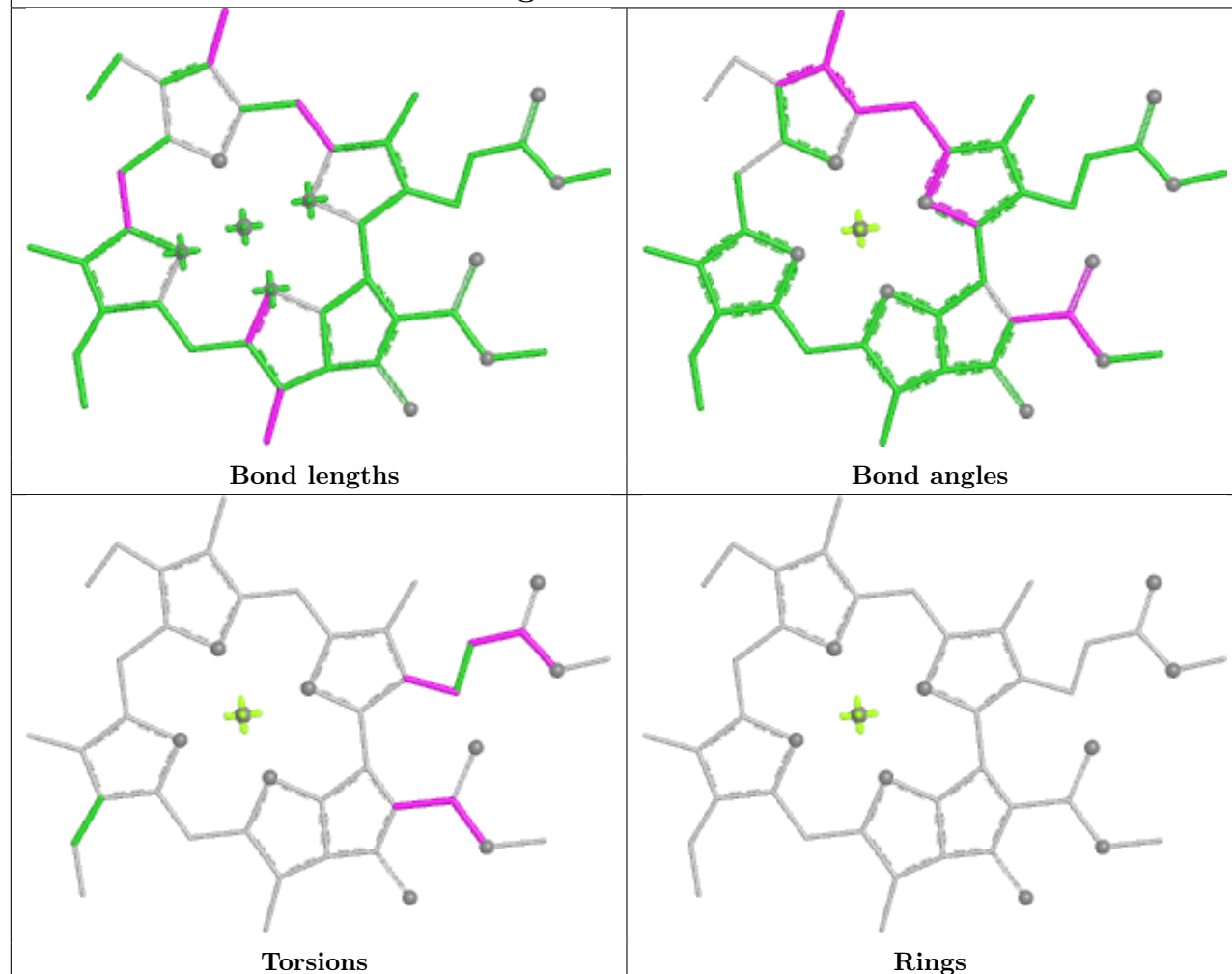
**Ligand CLA B 816****Ligand CLA B 828**



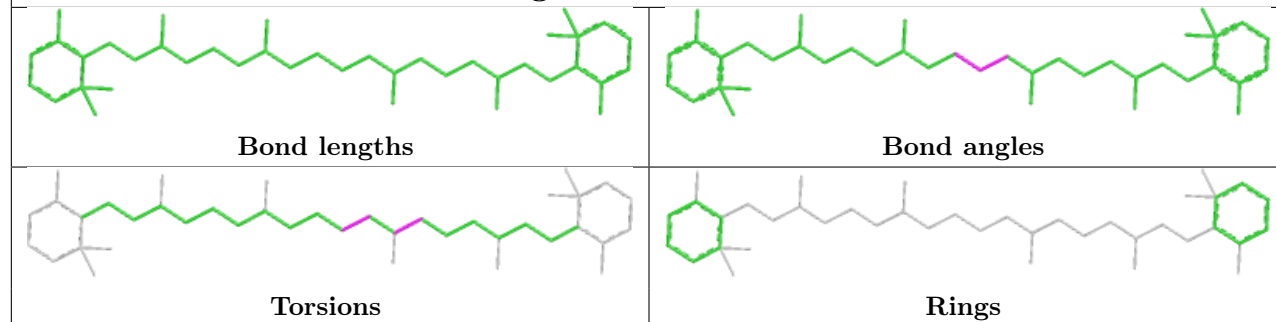


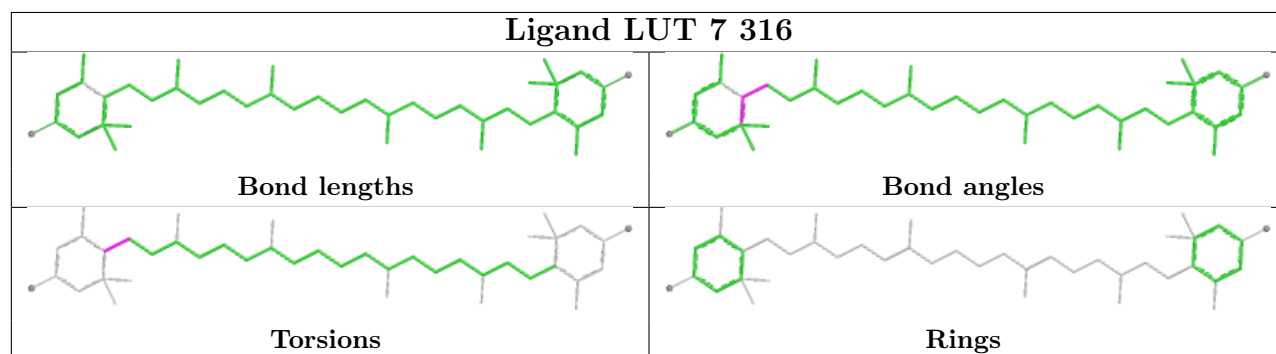
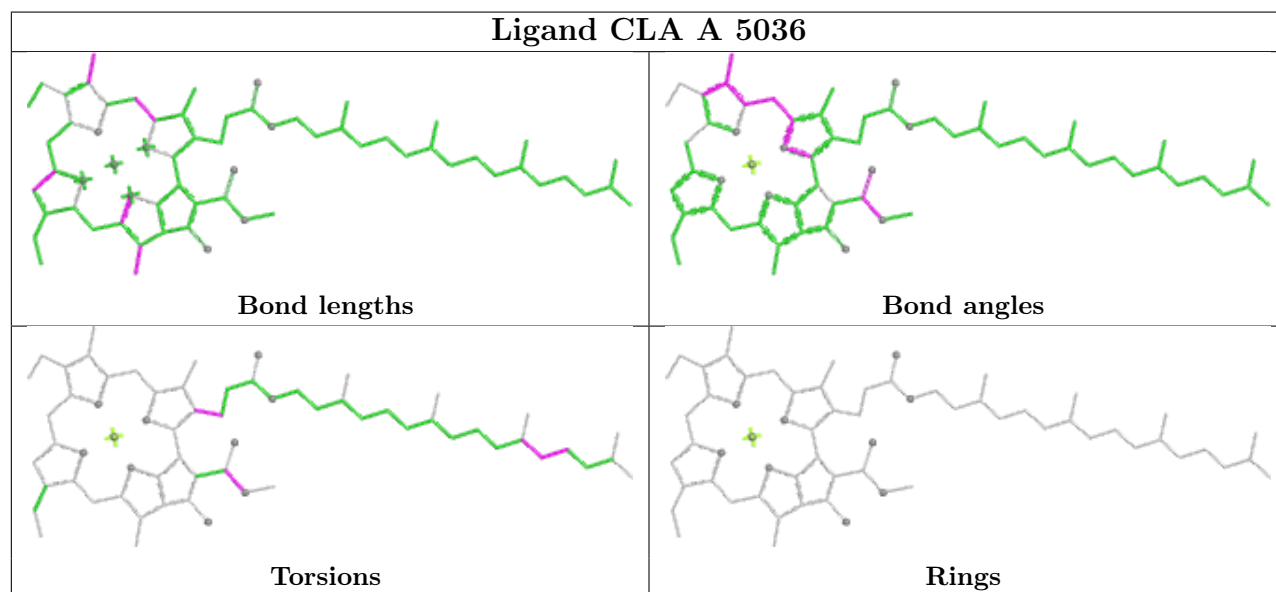
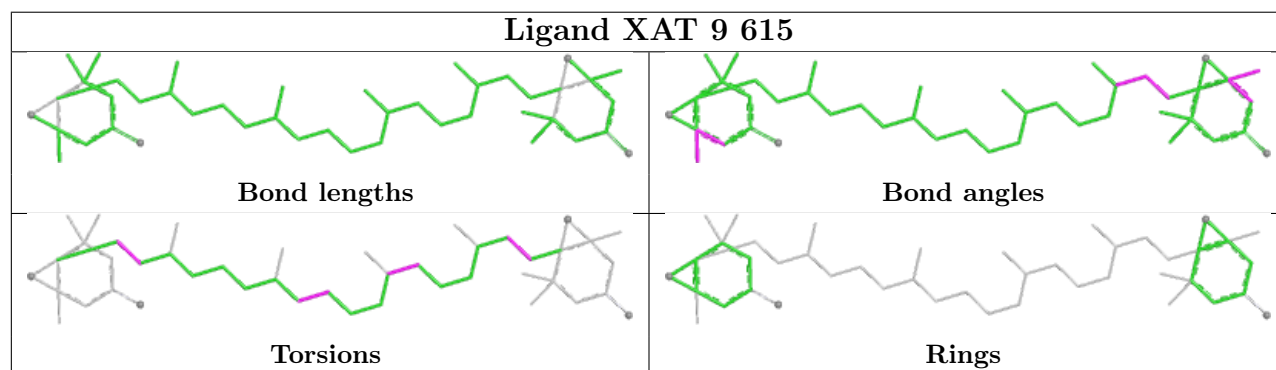
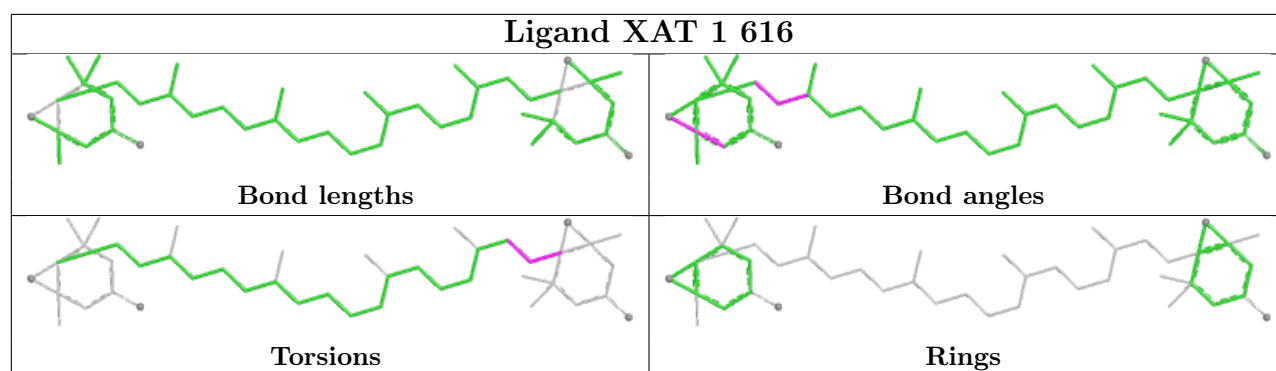


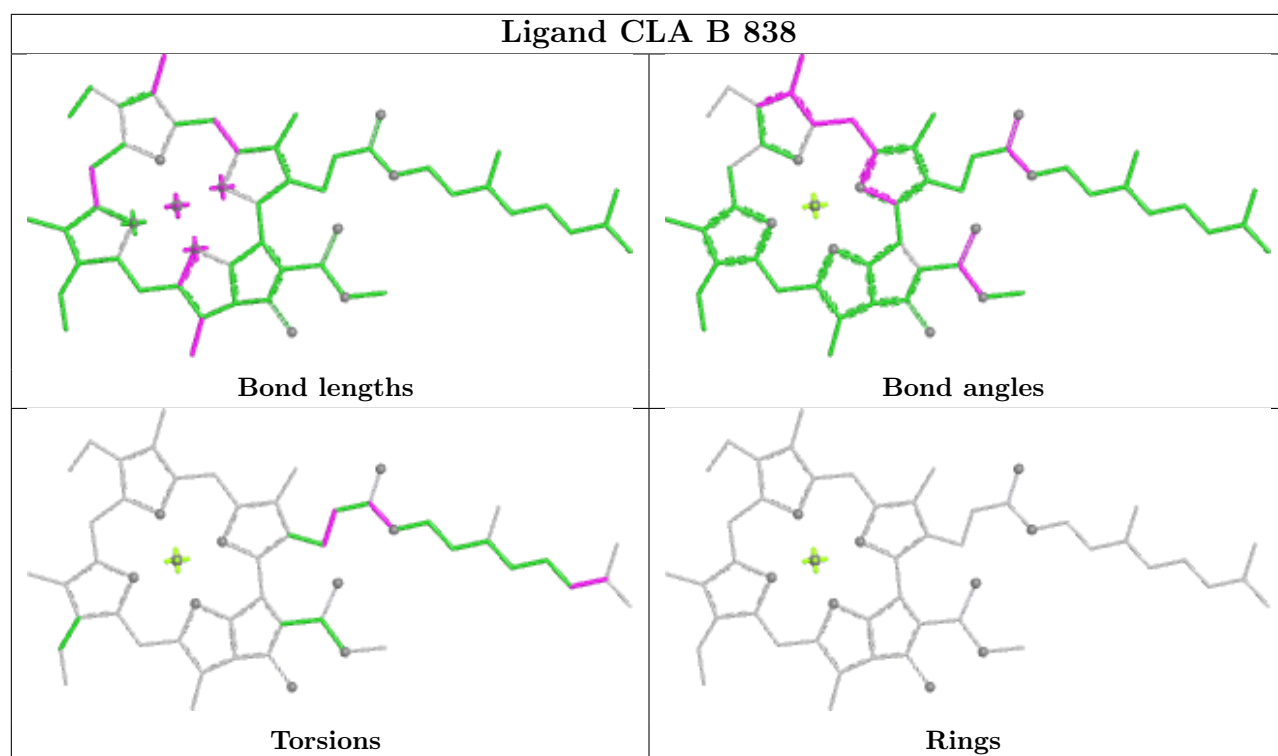
## Ligand CLA 9 601



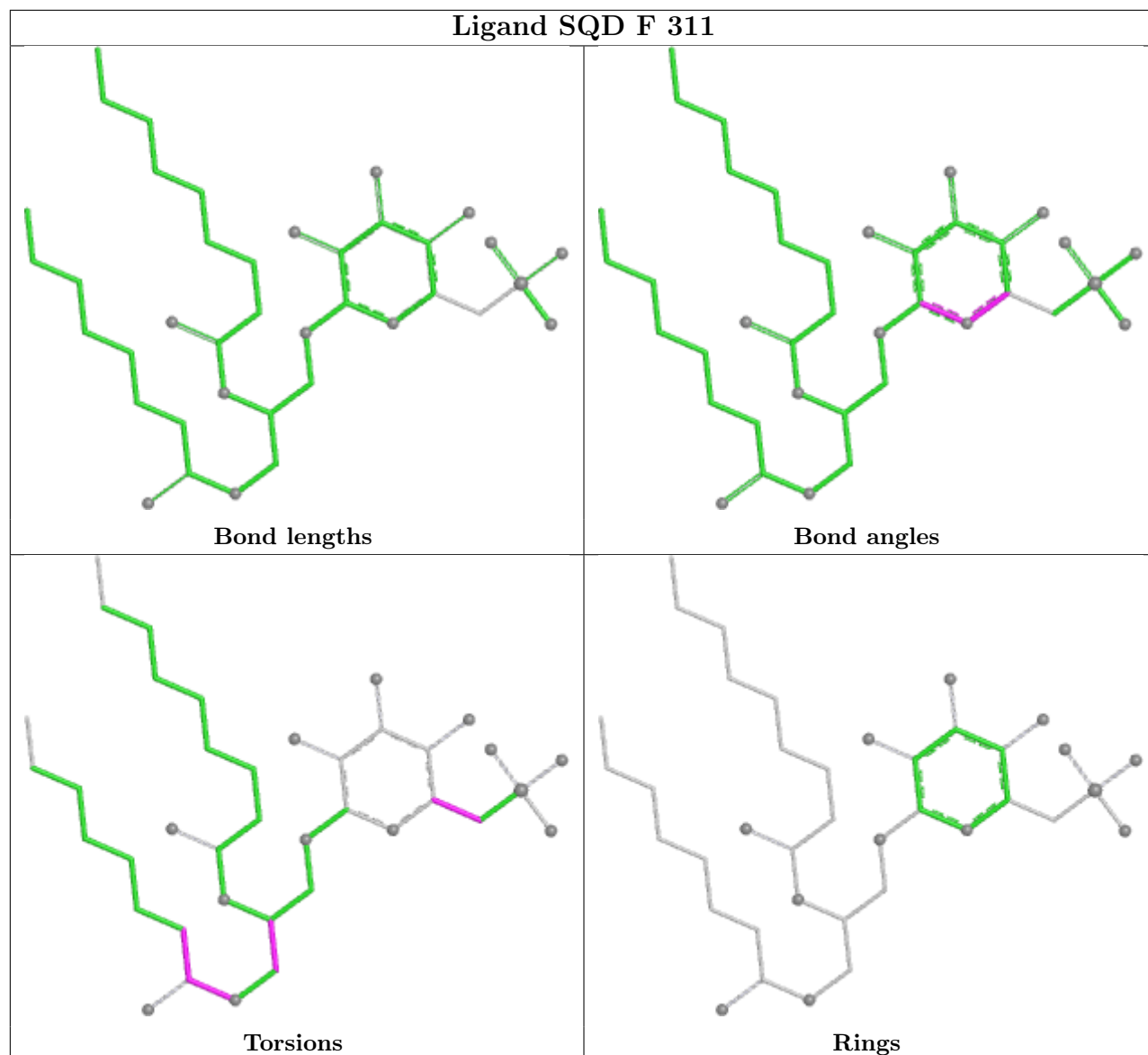
## Ligand BCR B 803



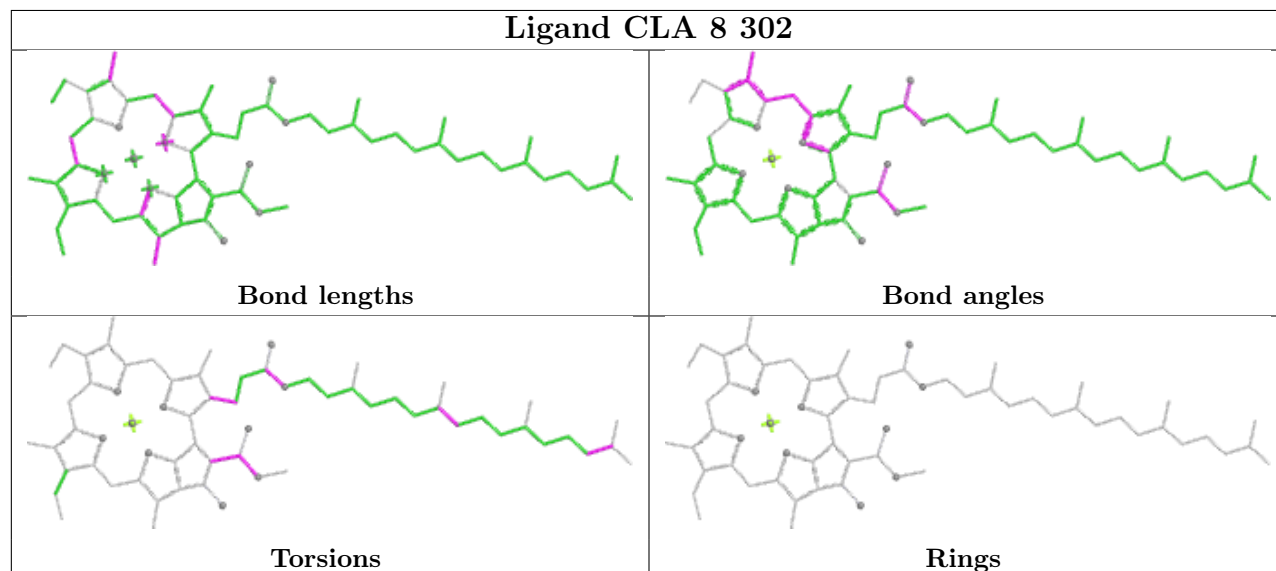




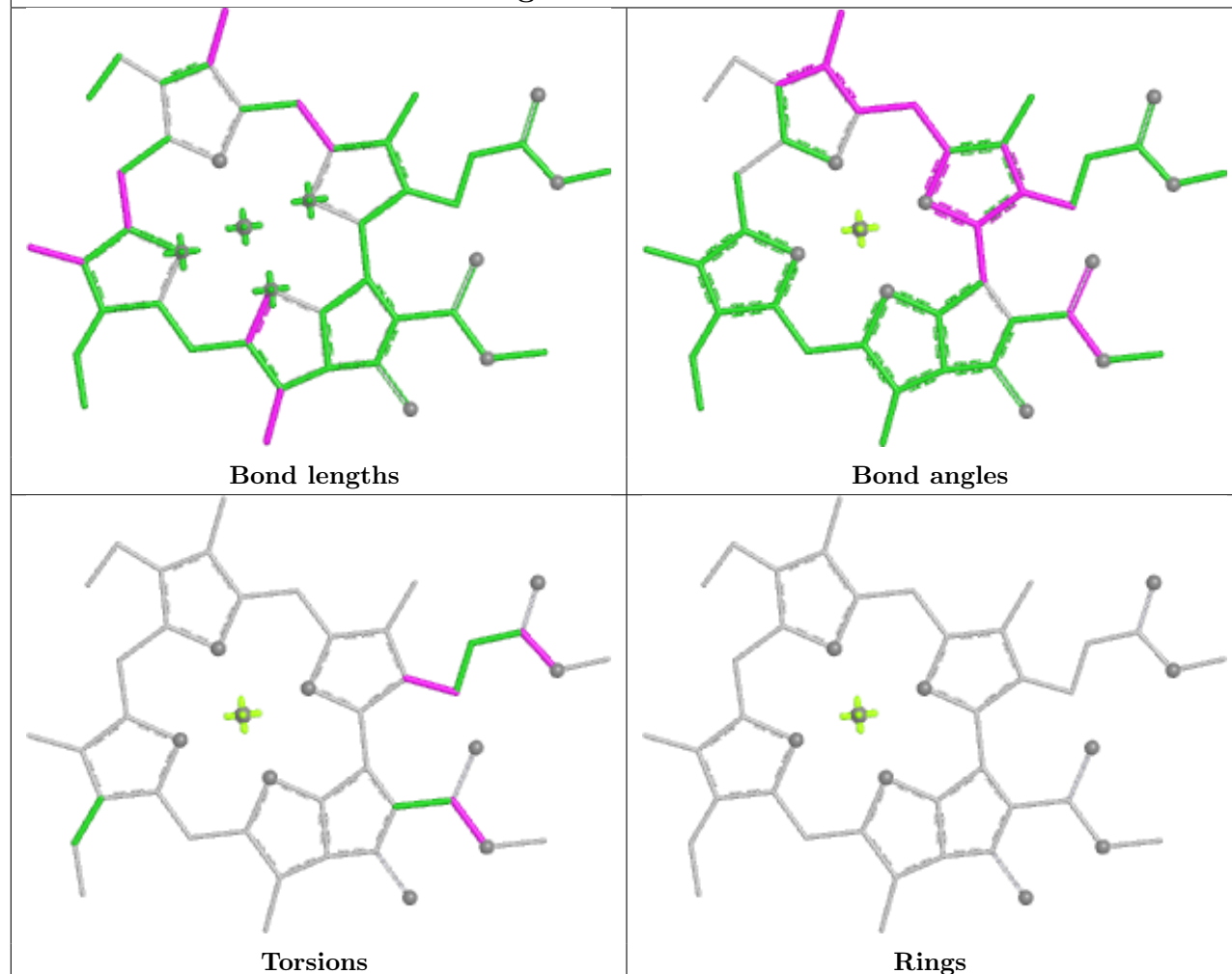
## Ligand SQD F 311



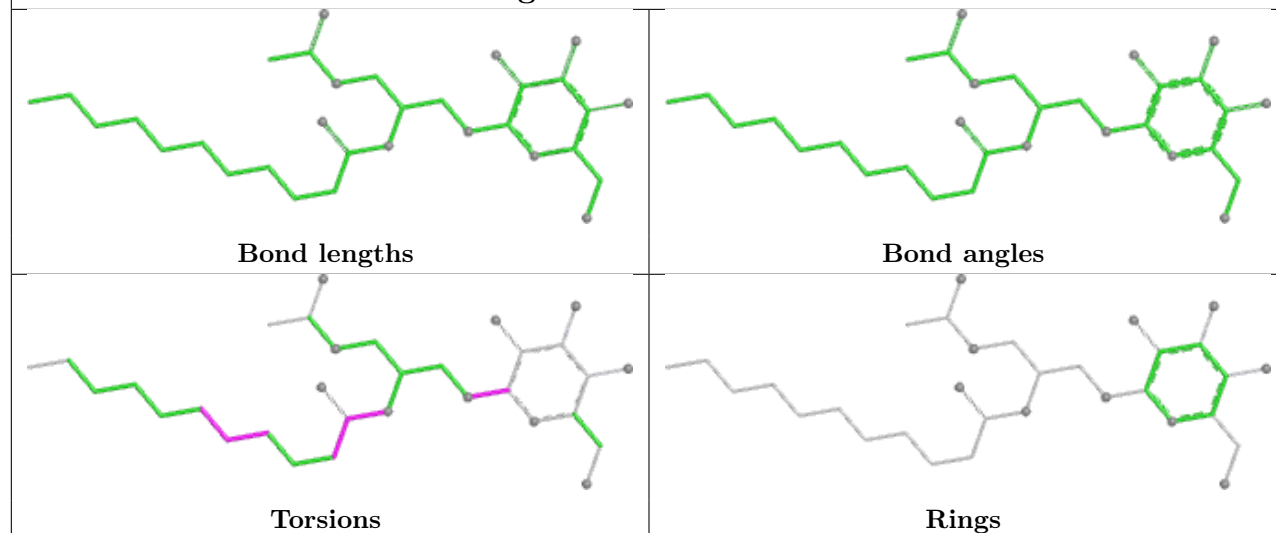
## Ligand CLA 8 302



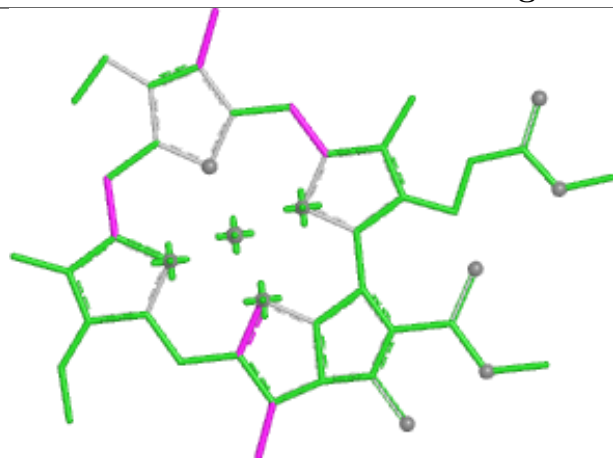
## Ligand CLA 1 611



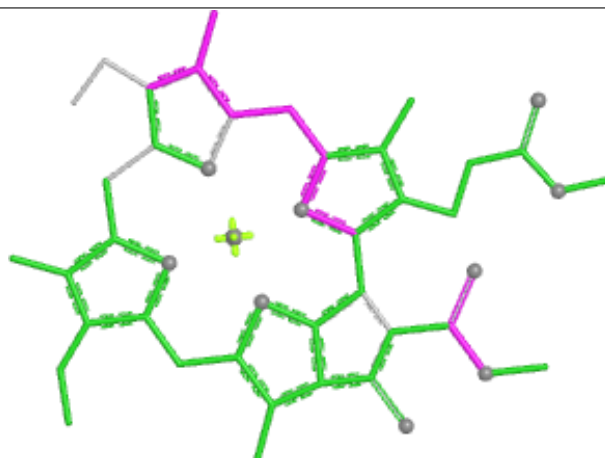
## Ligand LMG A 5001



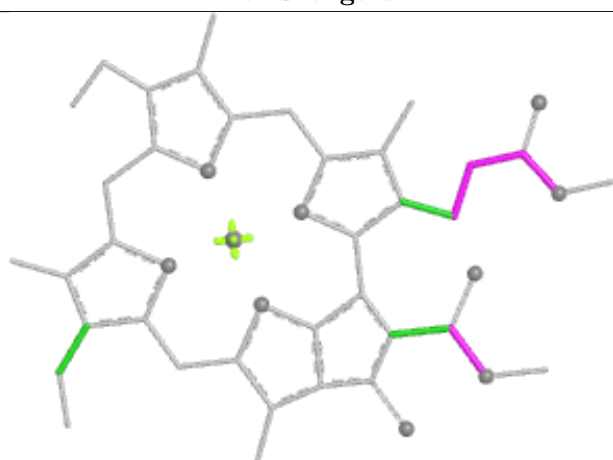
## Ligand CLA 3 312



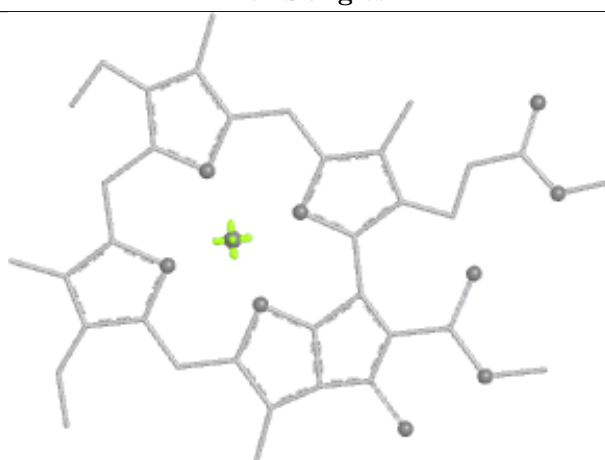
Bond lengths



Bond angles

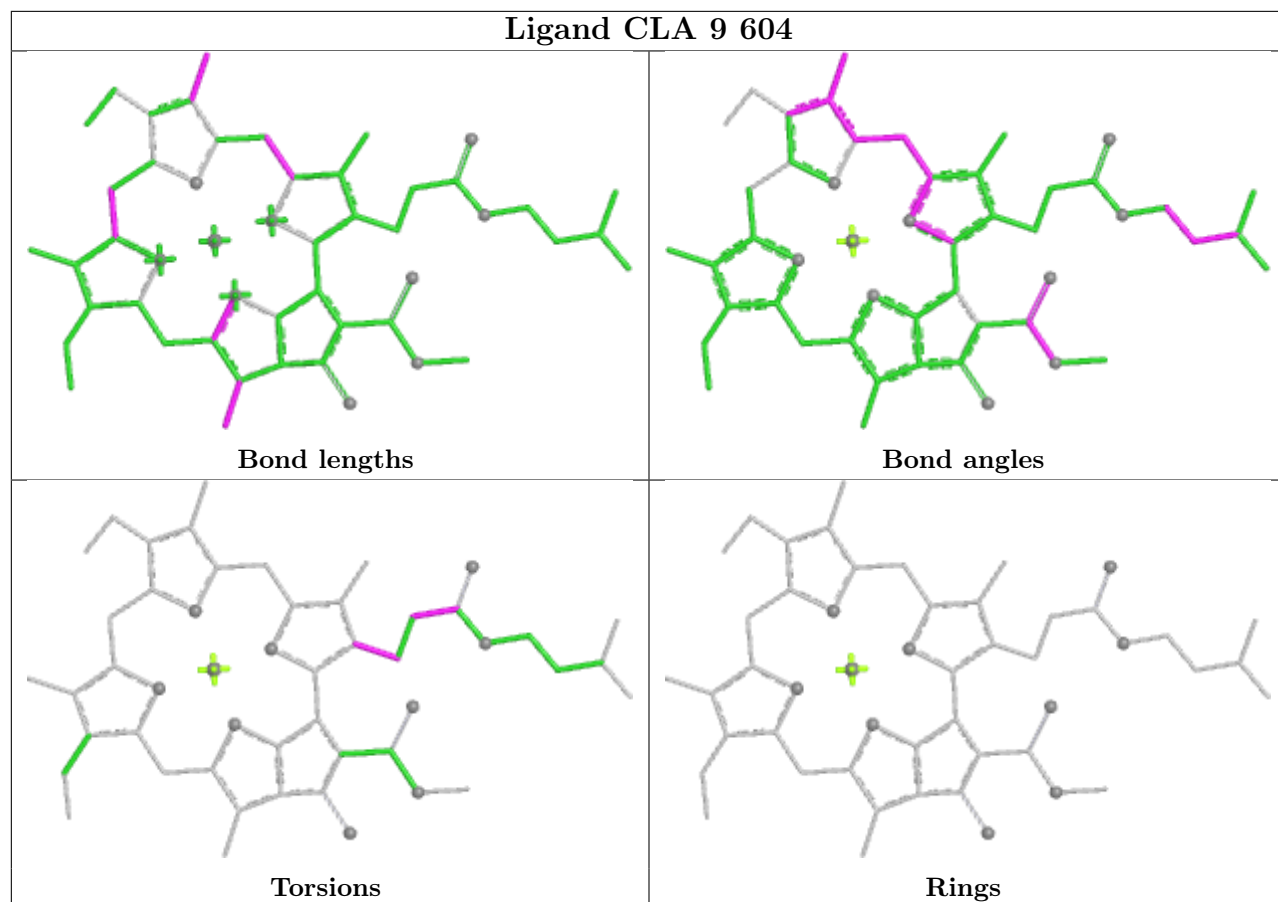


Torsions



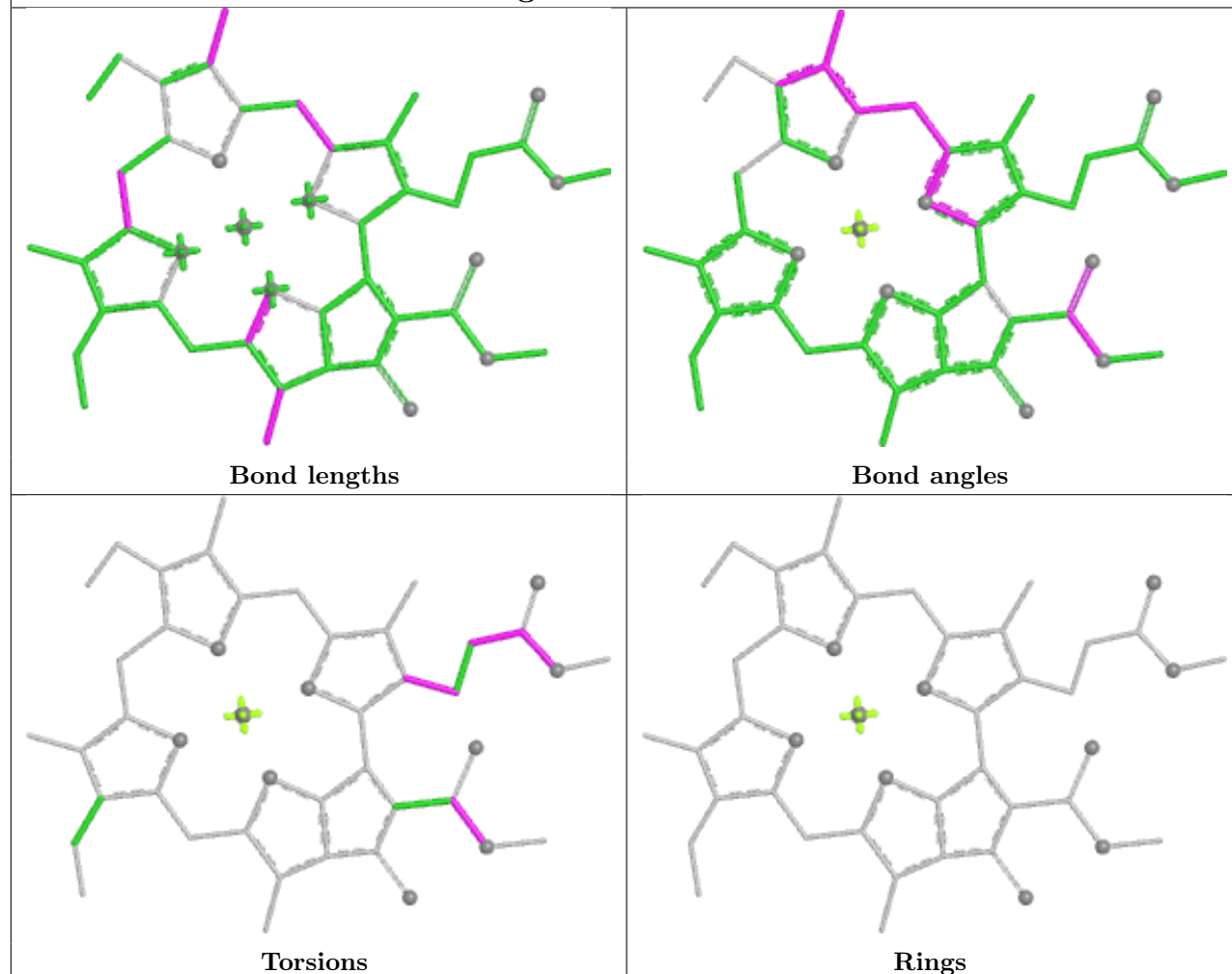
Rings

## Ligand CLA 9 604

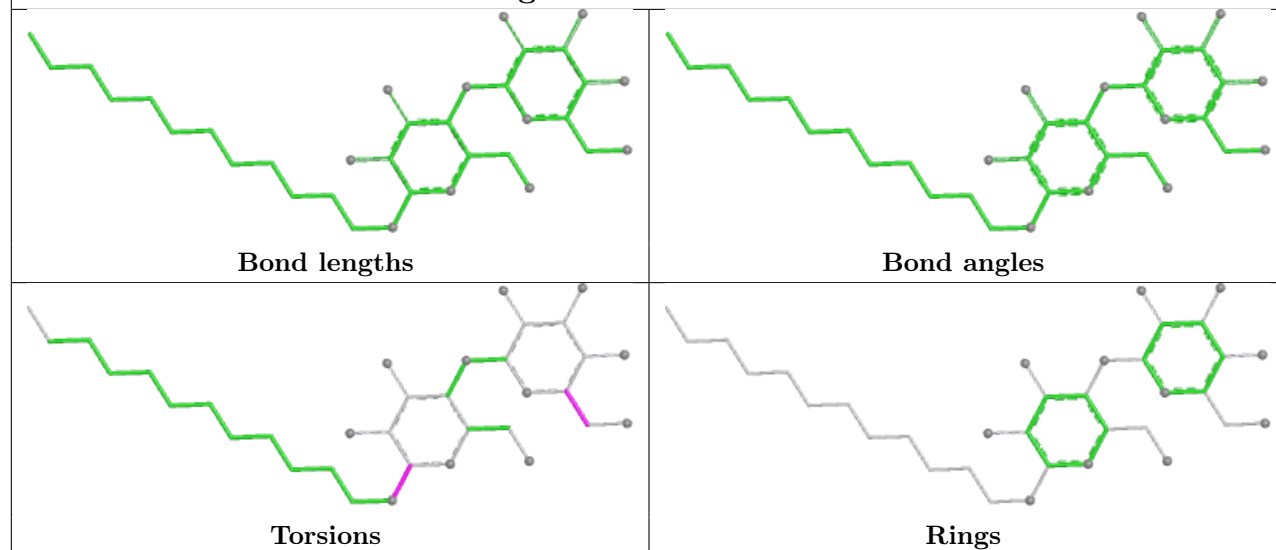




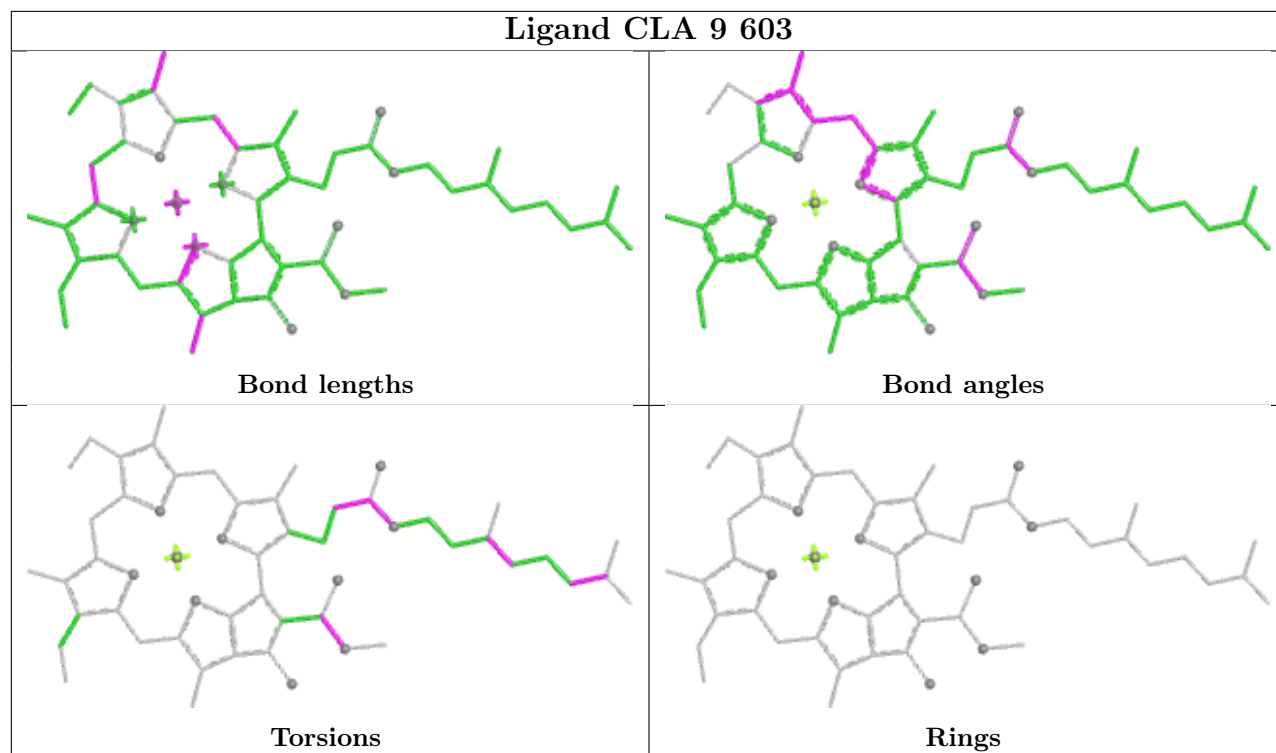
## Ligand CLA 1 610



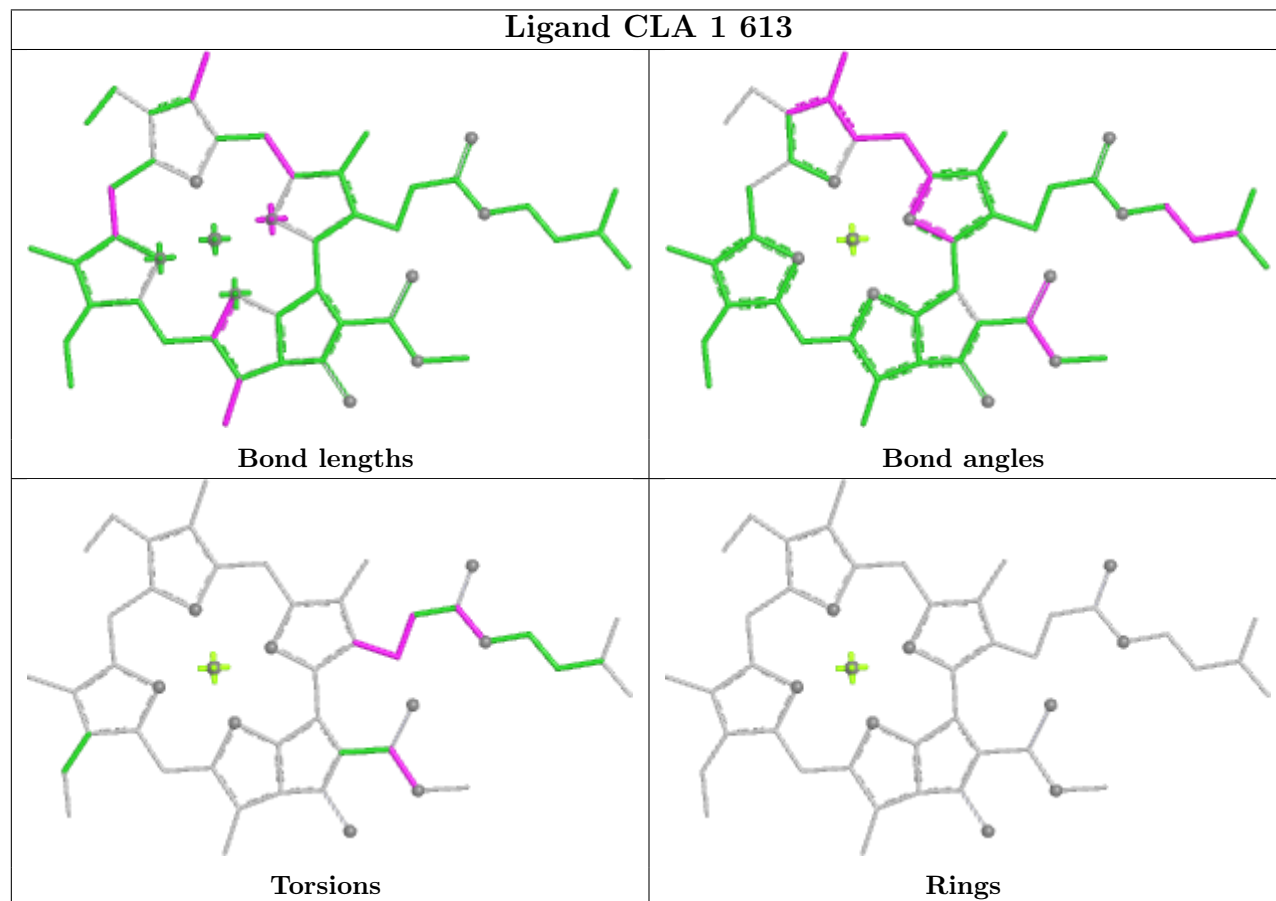
## Ligand LMU A 5053

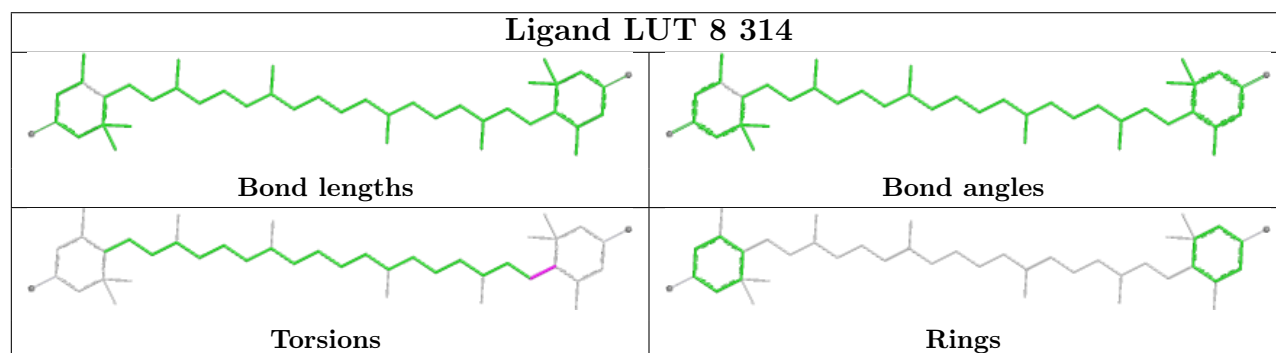
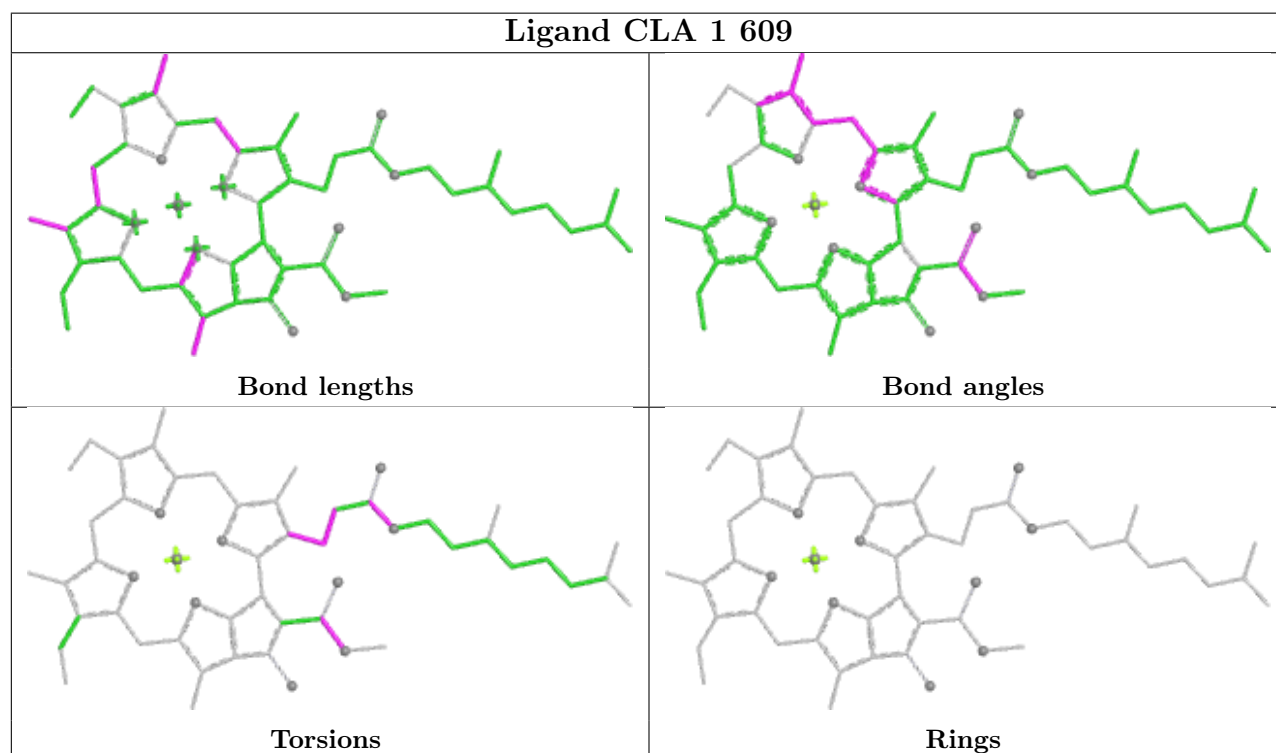
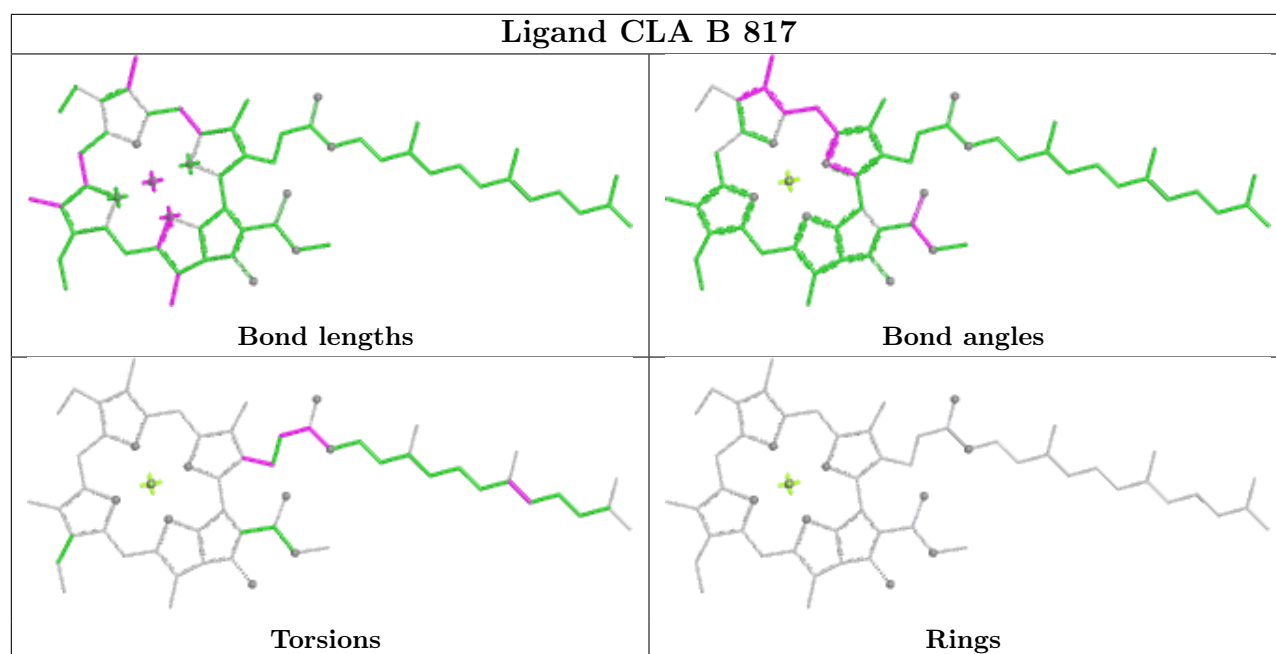


## Ligand CLA 9 603

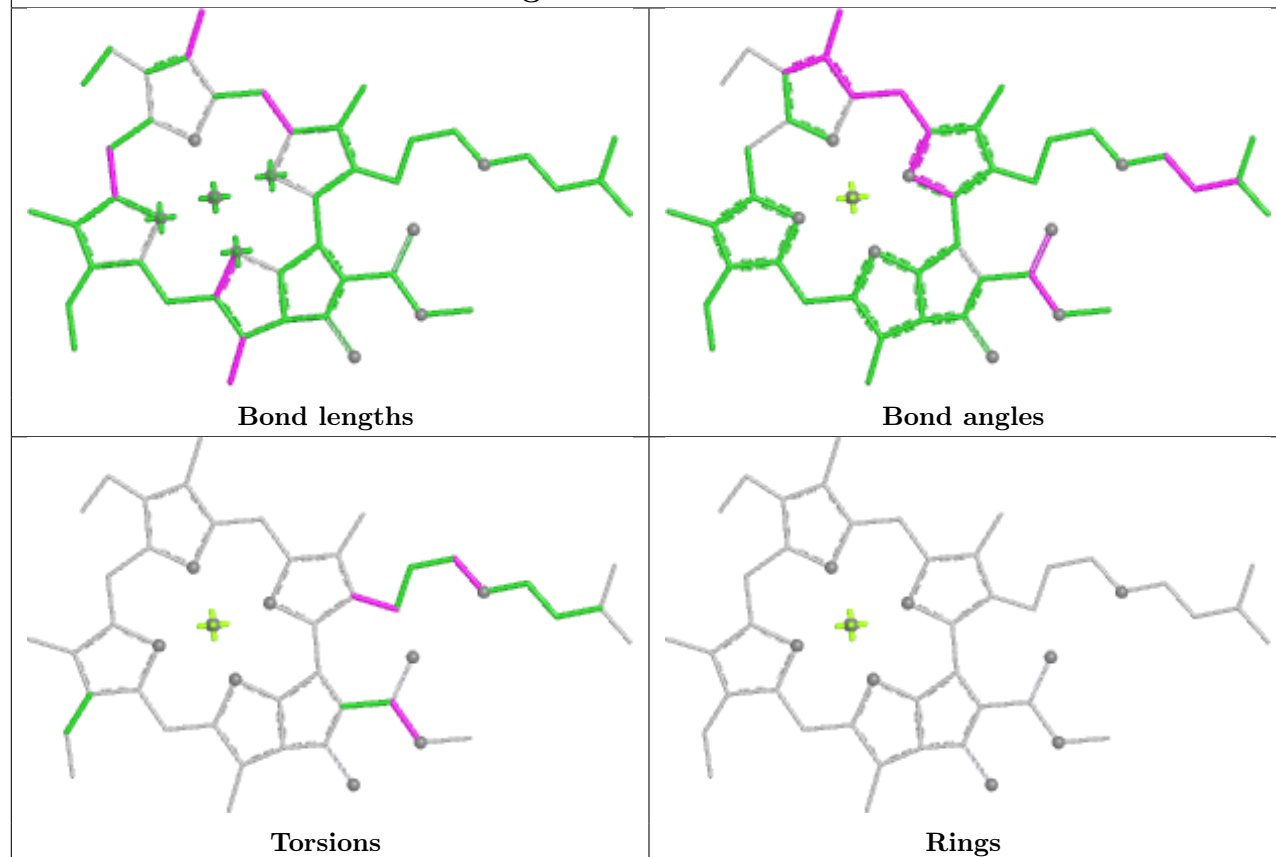


## Ligand CLA 1 613

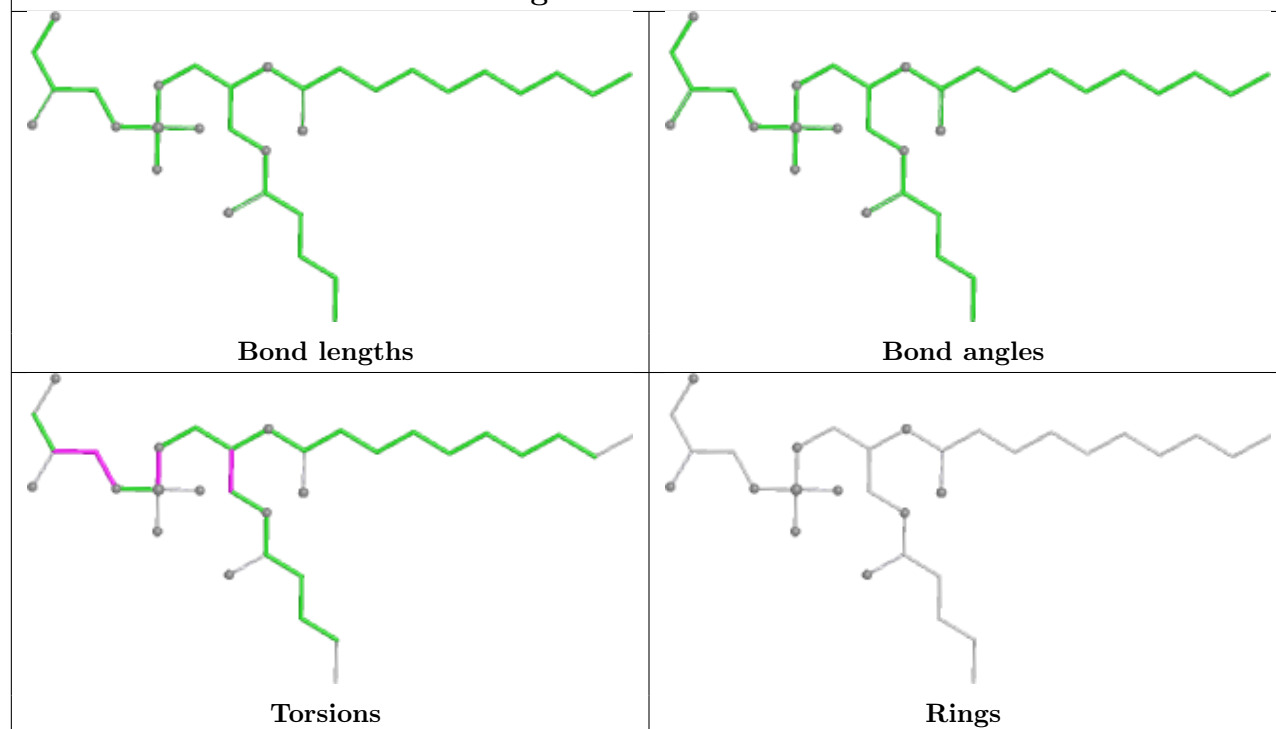


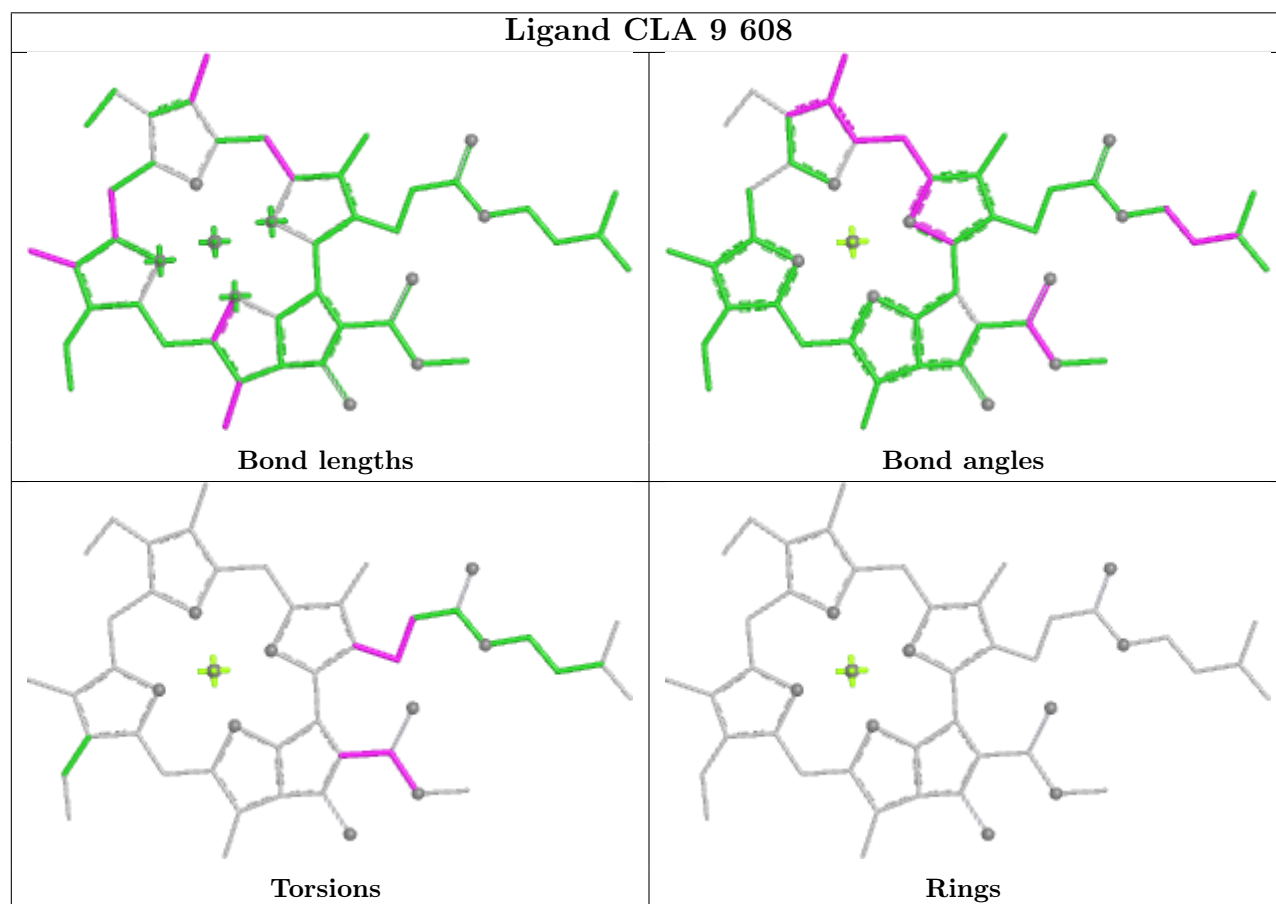
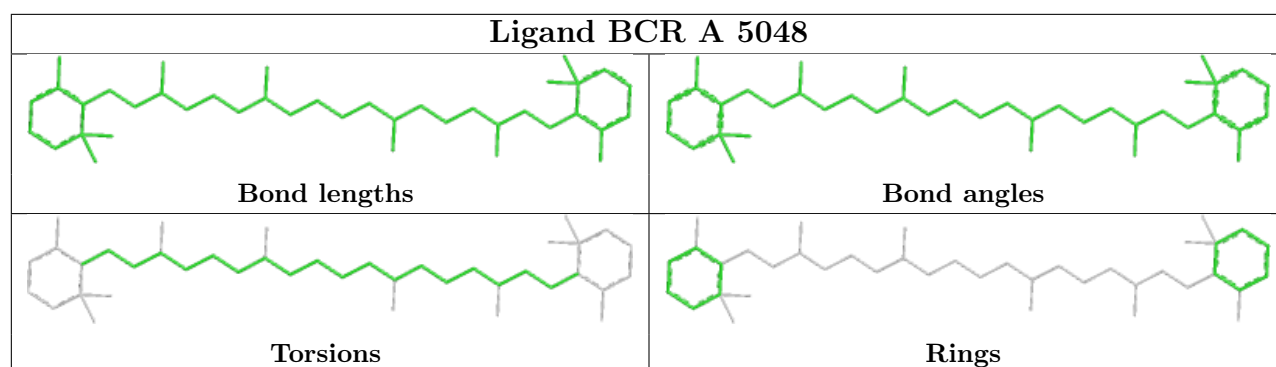


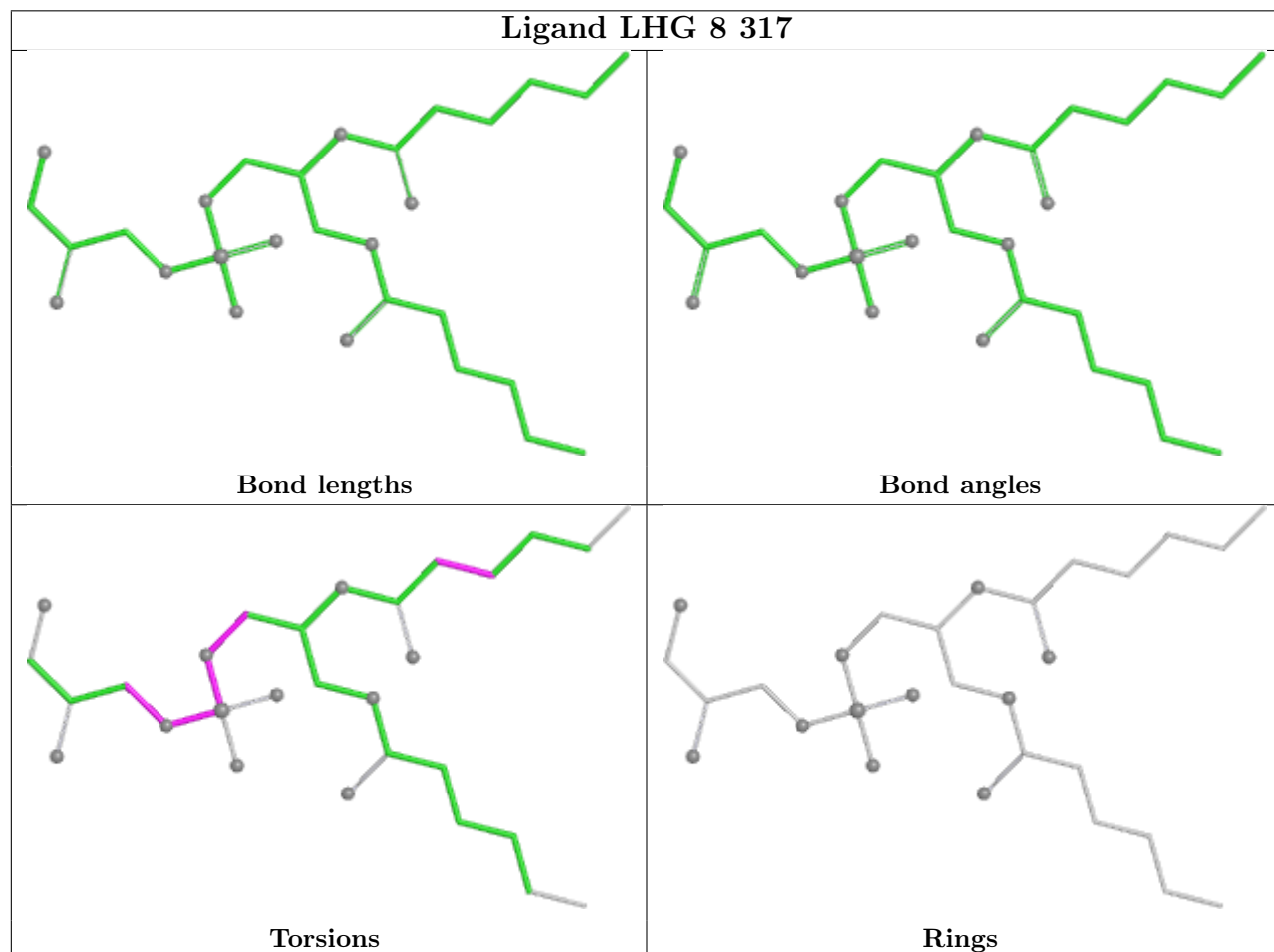
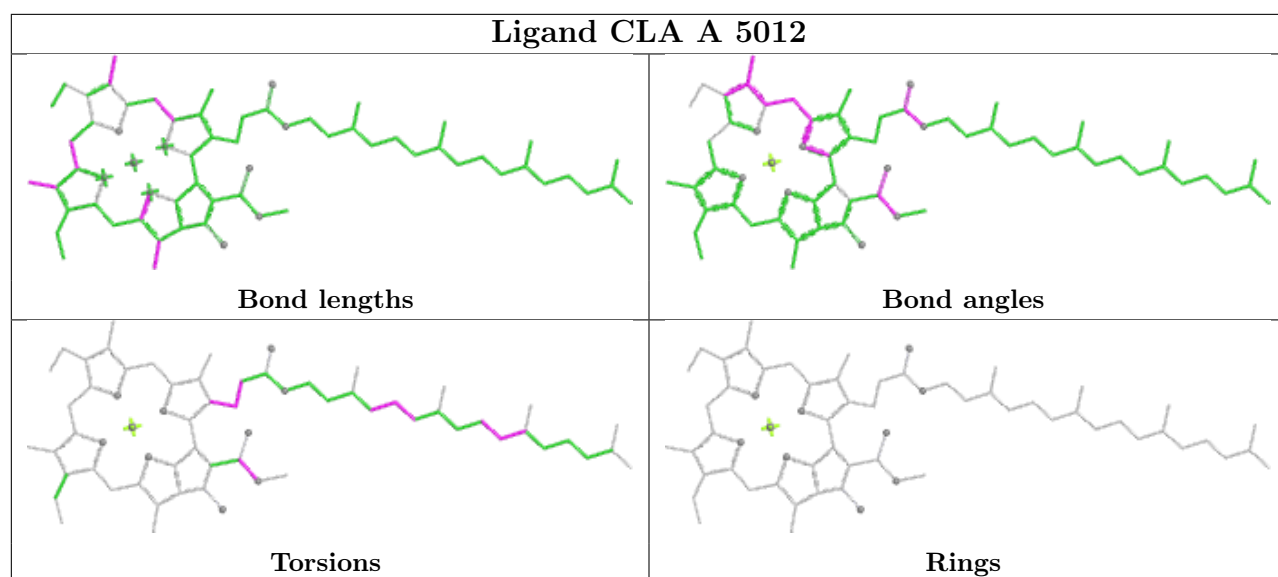
## Ligand CLA A 5043



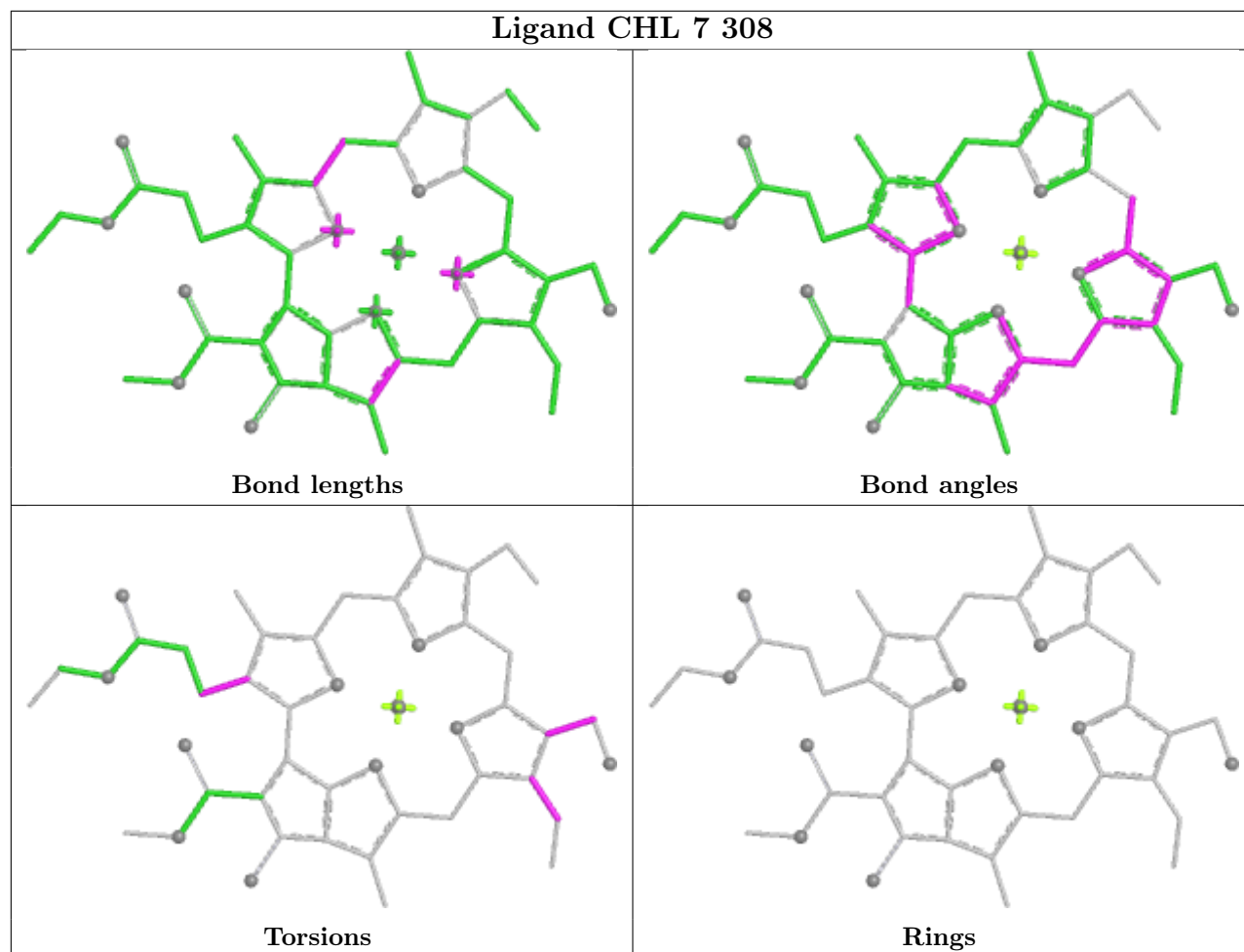
## Ligand LHG B 801



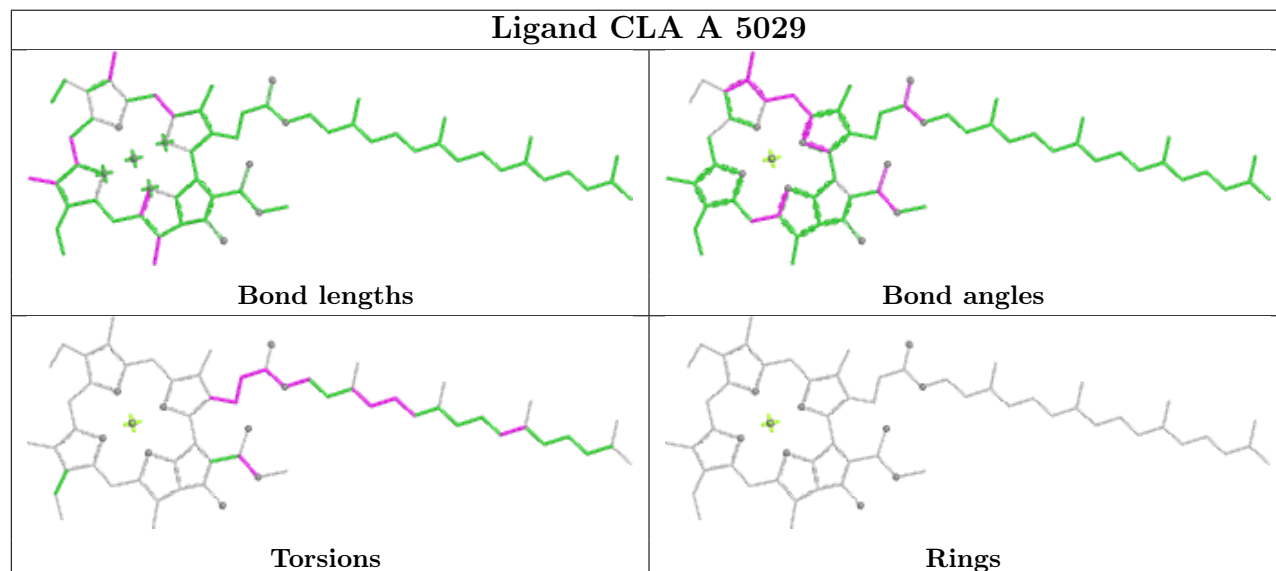


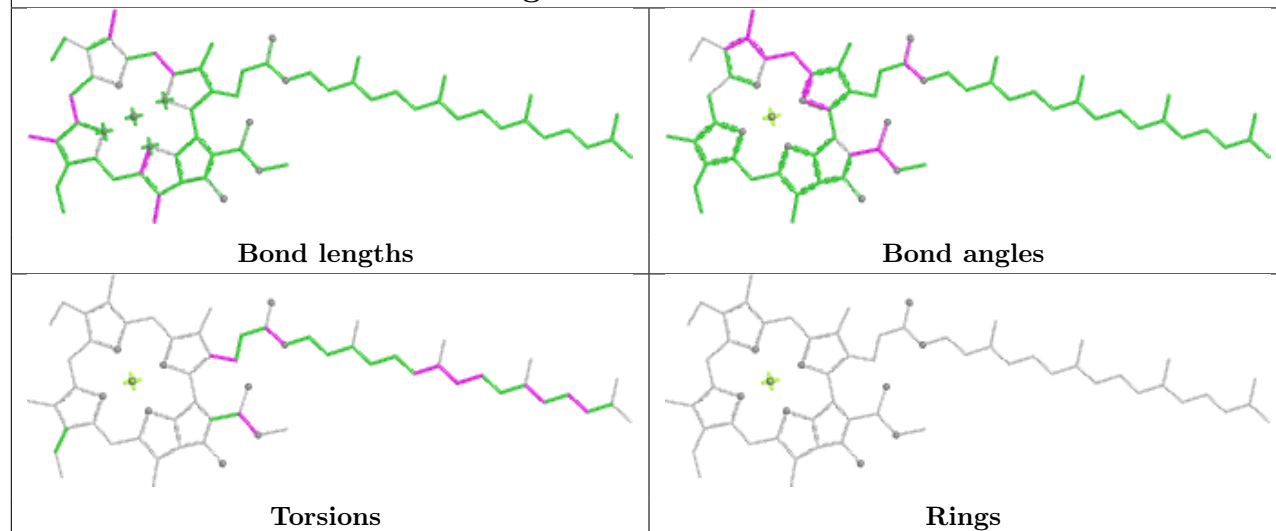
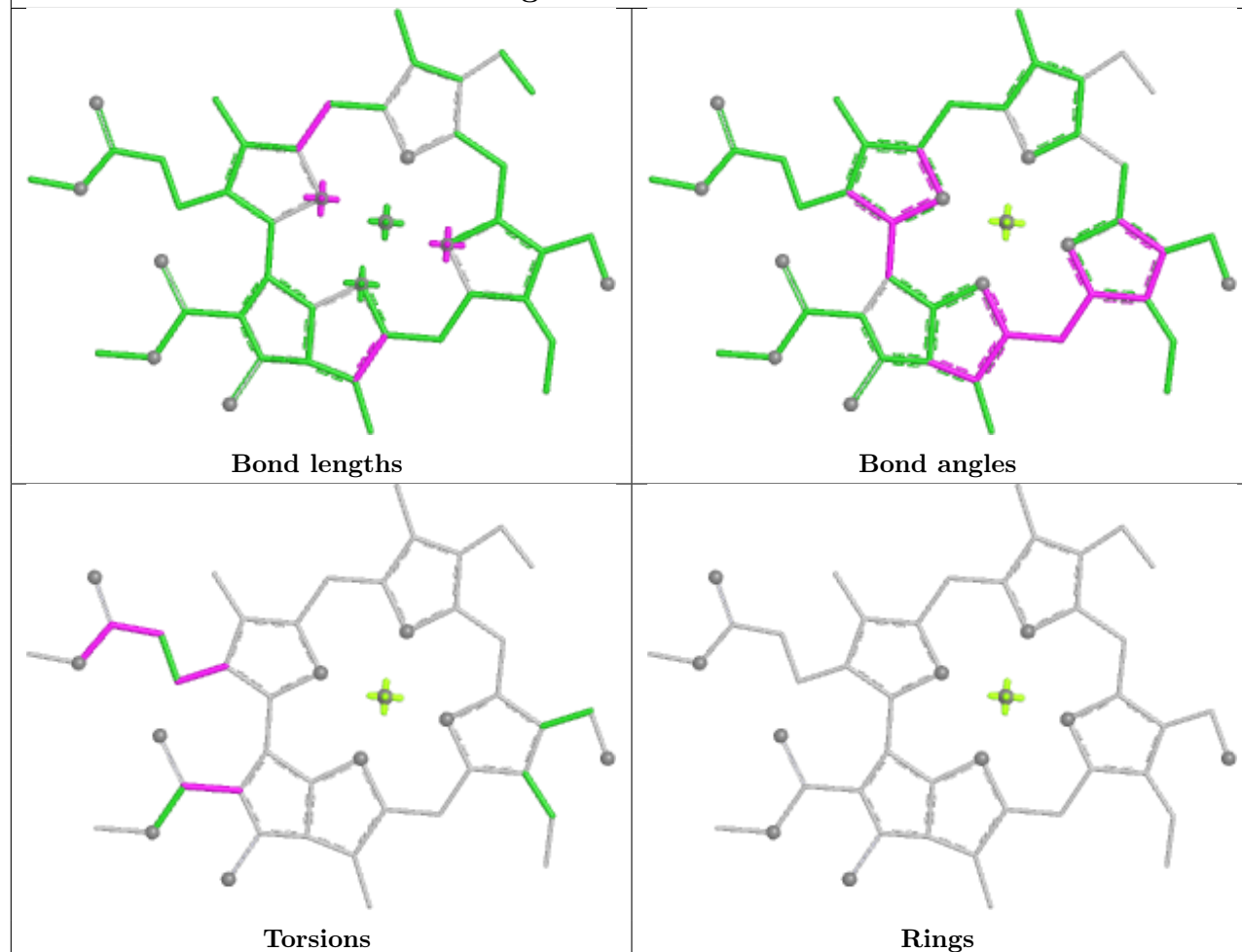


## Ligand CHL 7 308

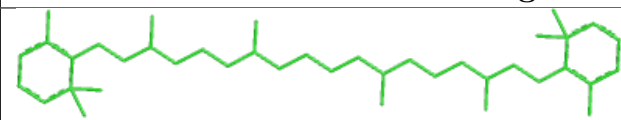
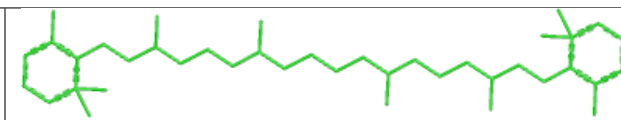
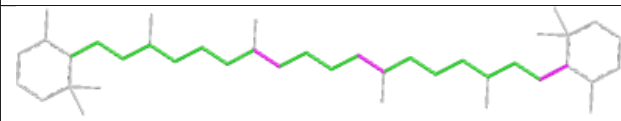
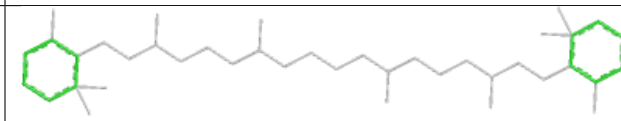


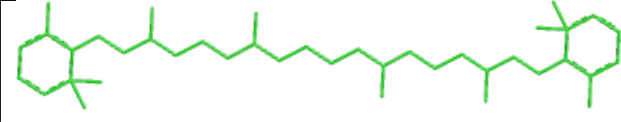
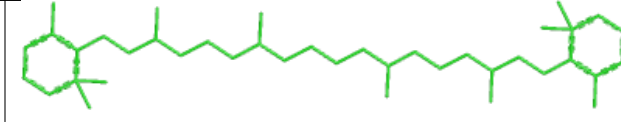
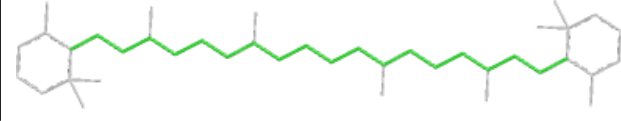
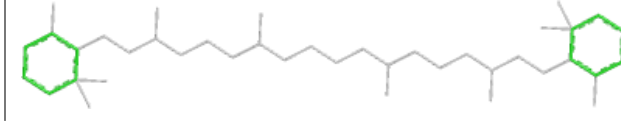
## Ligand CLA A 5029

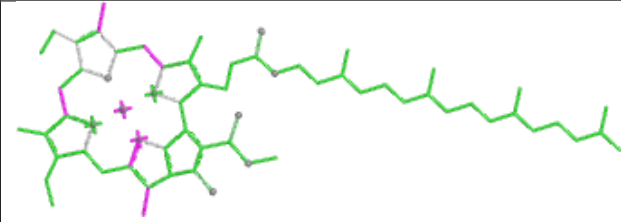
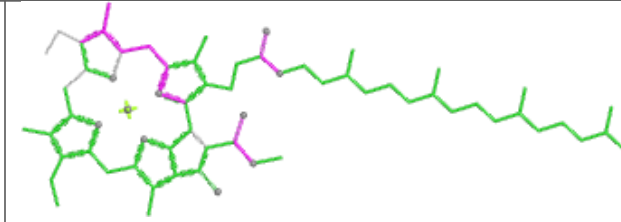
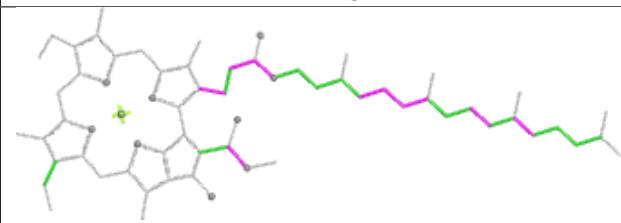
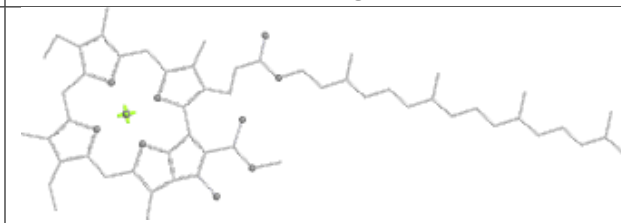


**Ligand CLA A 5006****Ligand CHL 8 304**

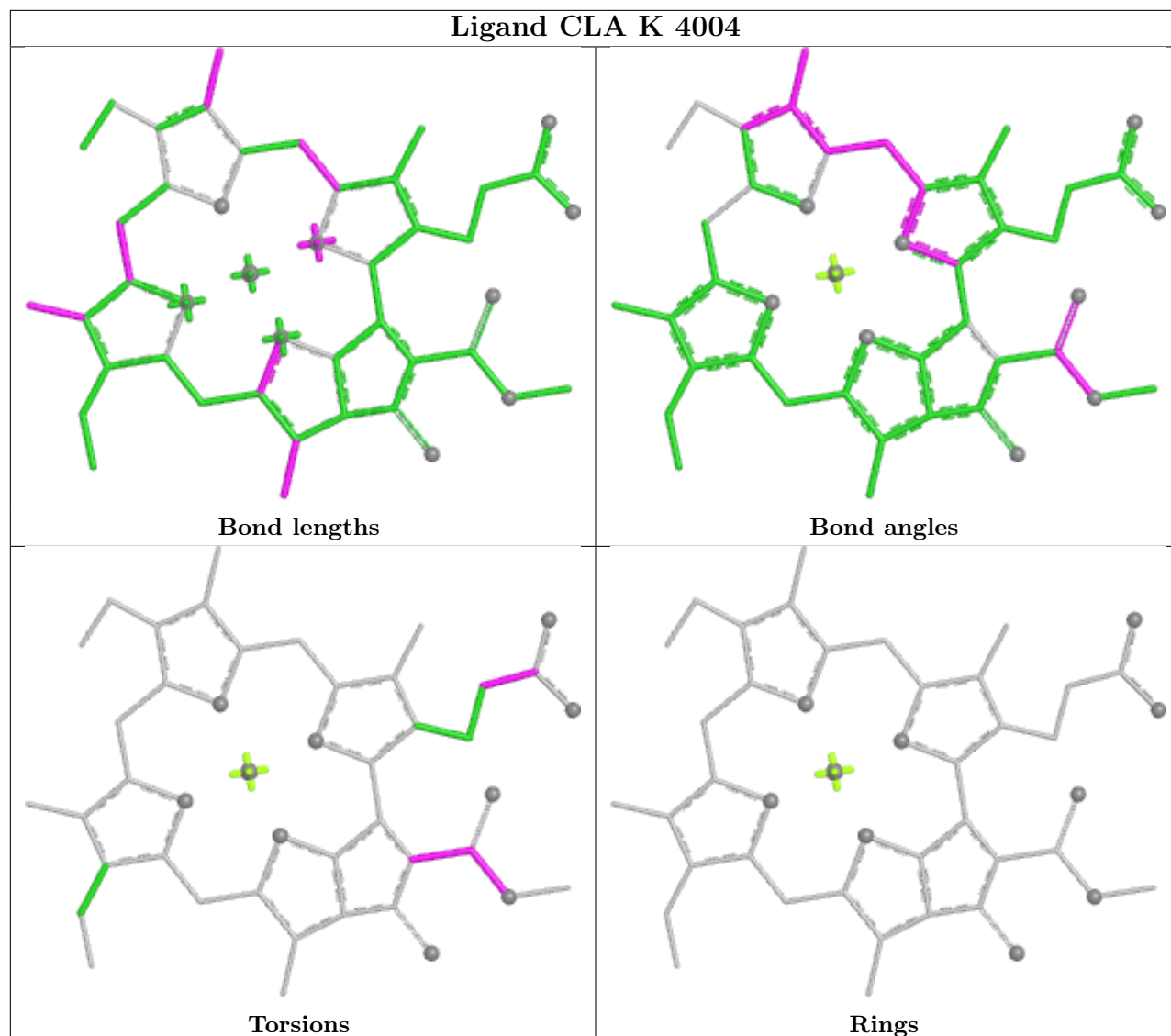


Ligand BCR G 205	
	
Bond lengths	Bond angles
	
Torsions	Rings

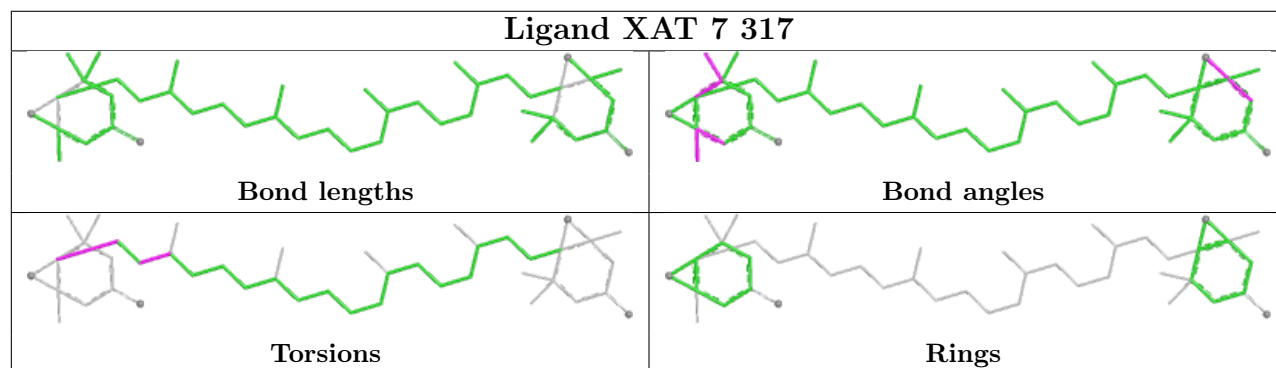
Ligand BCR B 843	
	
Bond lengths	Bond angles
	
Torsions	Rings

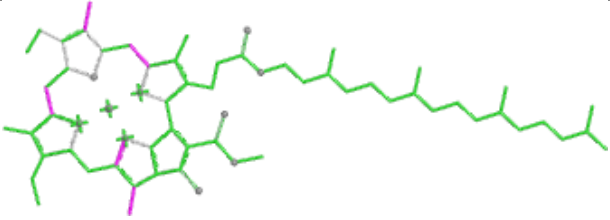
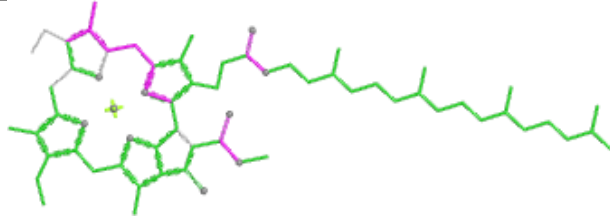
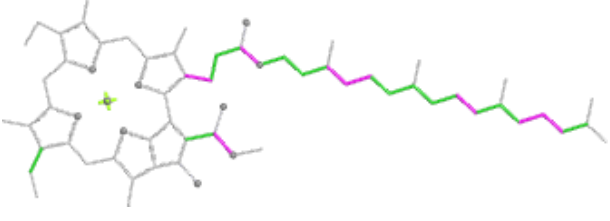
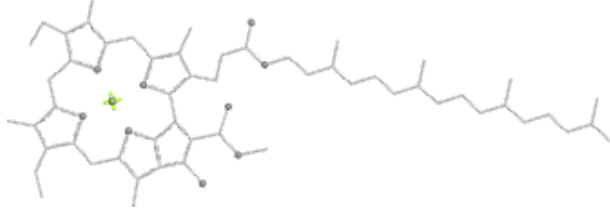
Ligand CLA B 814	
	
Bond lengths	Bond angles
	
Torsions	Rings

## Ligand CLA K 4004



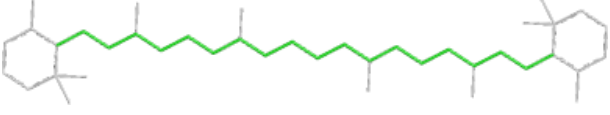
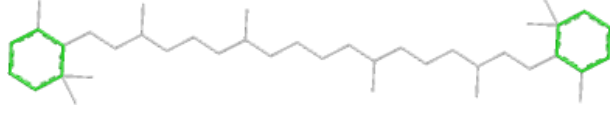


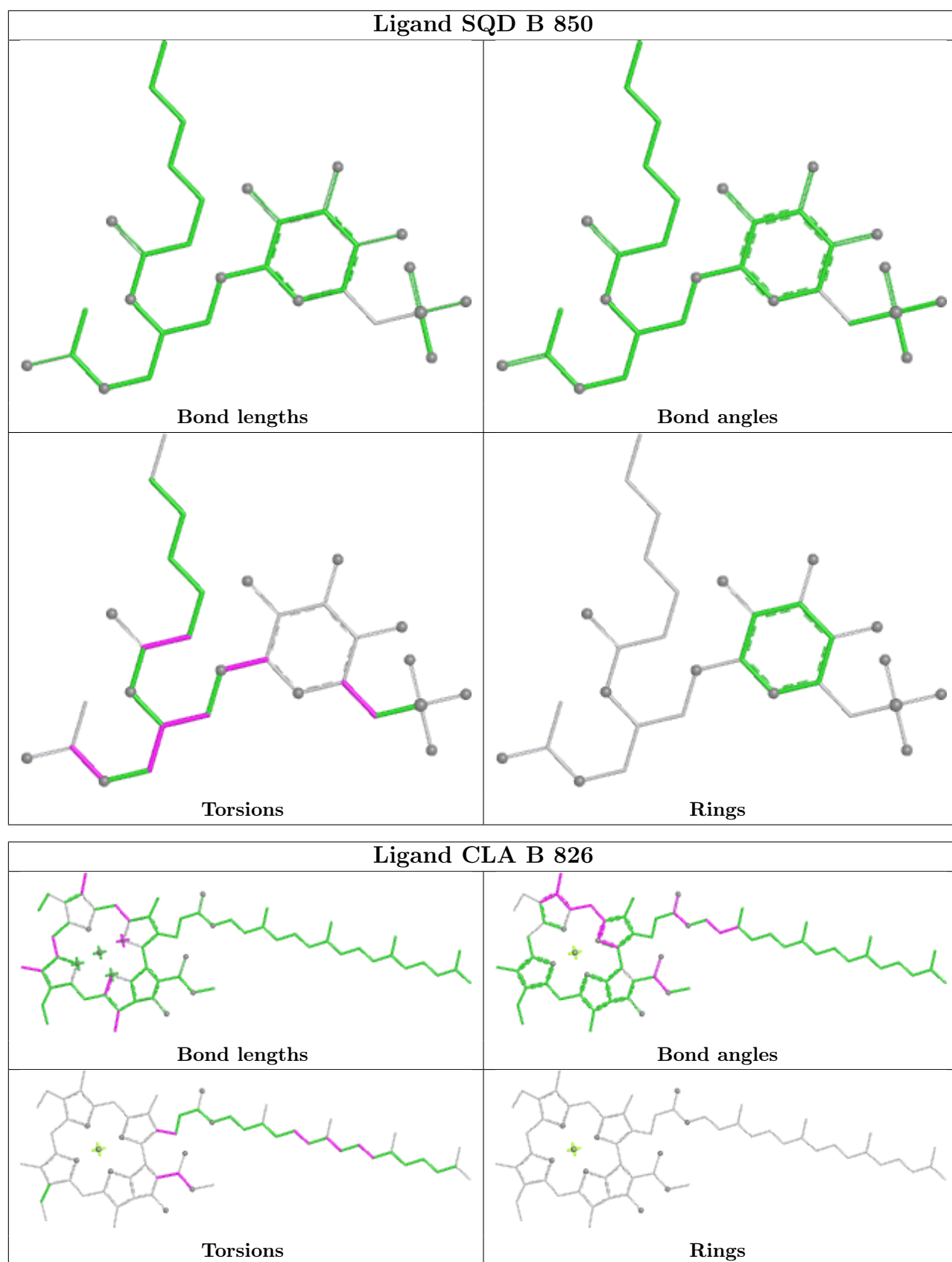
## Ligand XAT 7 317

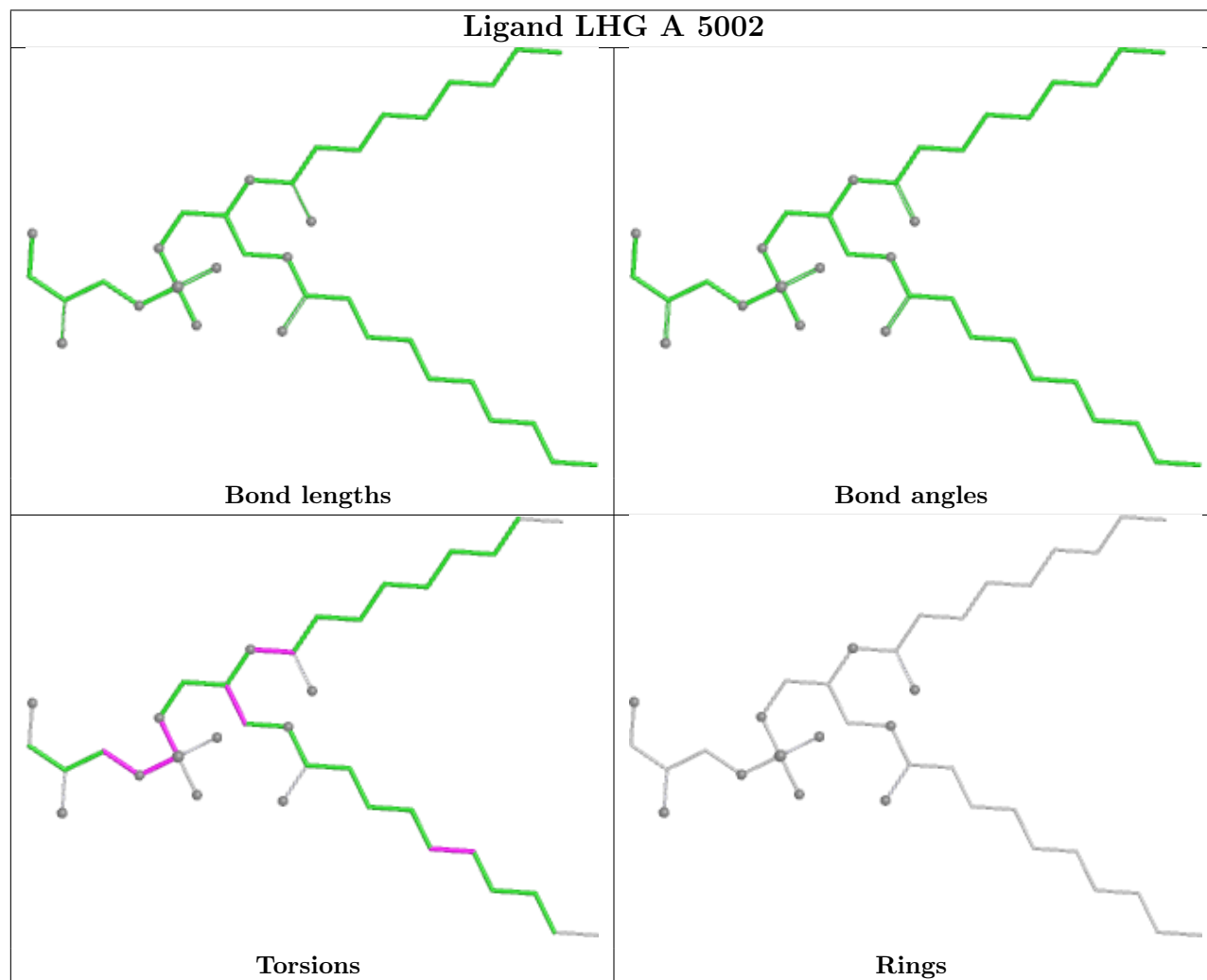
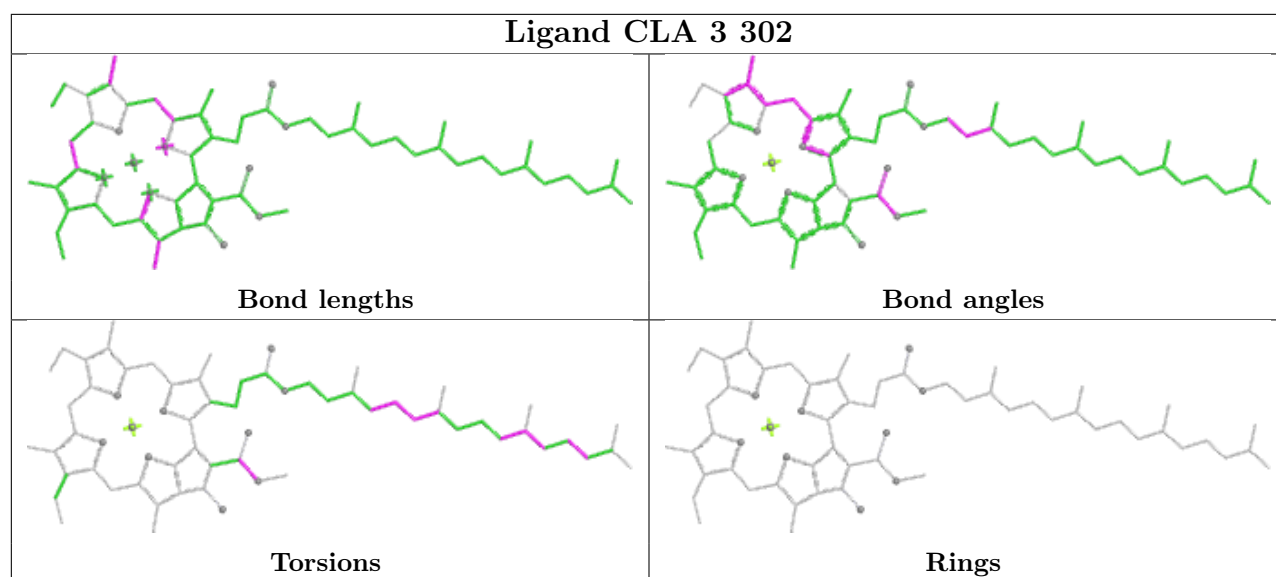


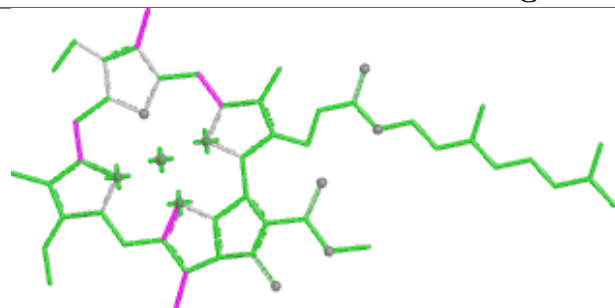
Ligand CLA A 5013			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

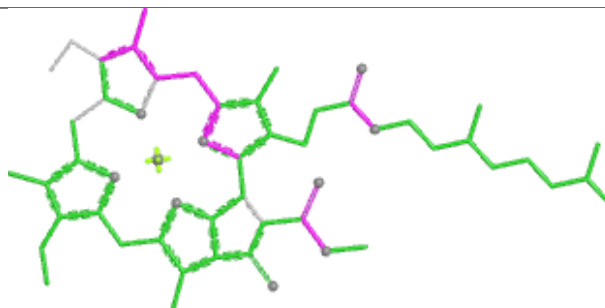
Ligand BCR 1 617			
			
Bond lengths	Bond angles		
			
Torsions	Rings		



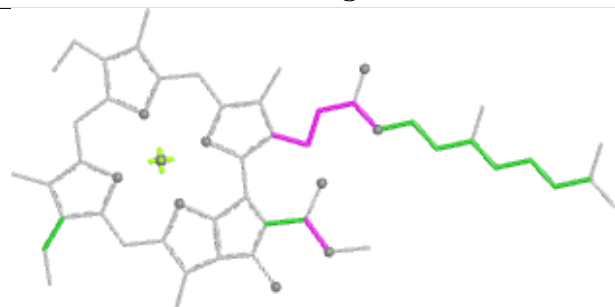


**Ligand CLA 3 308**

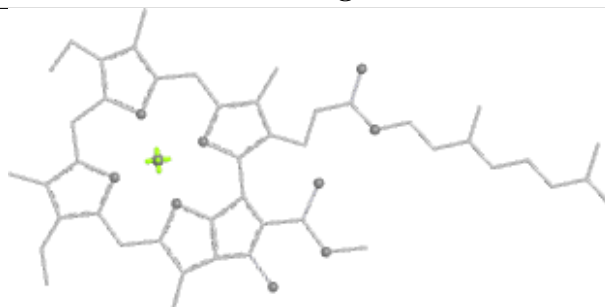
Bond lengths



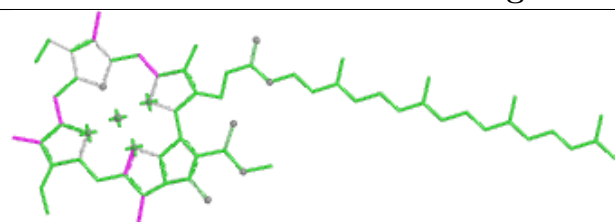
Bond angles



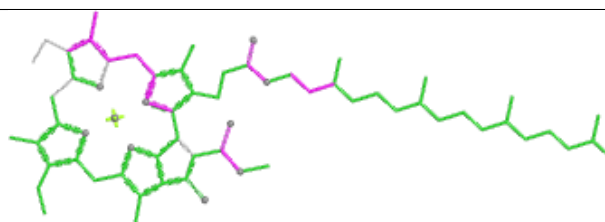
Torsions



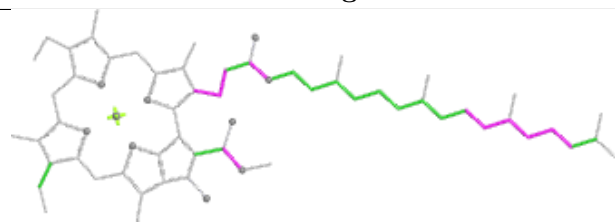
Rings

**Ligand CLA A 5009**

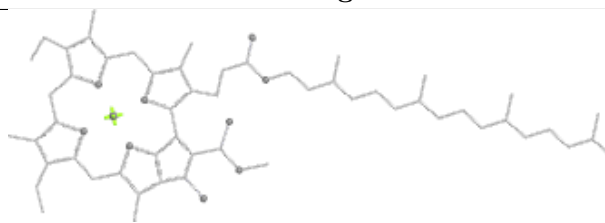
Bond lengths



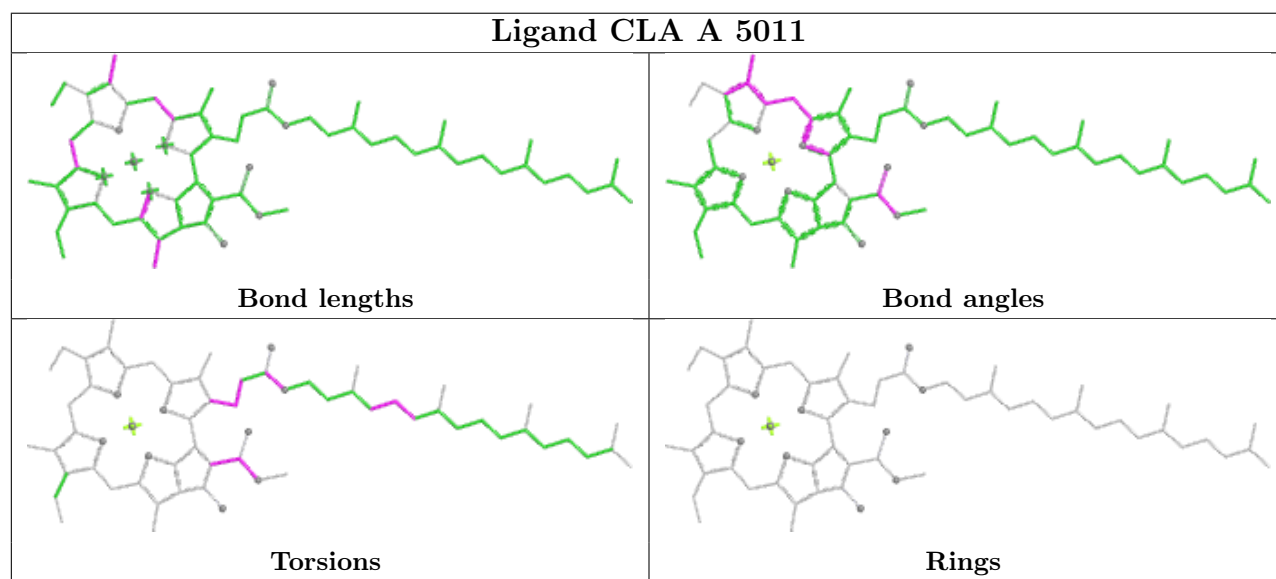
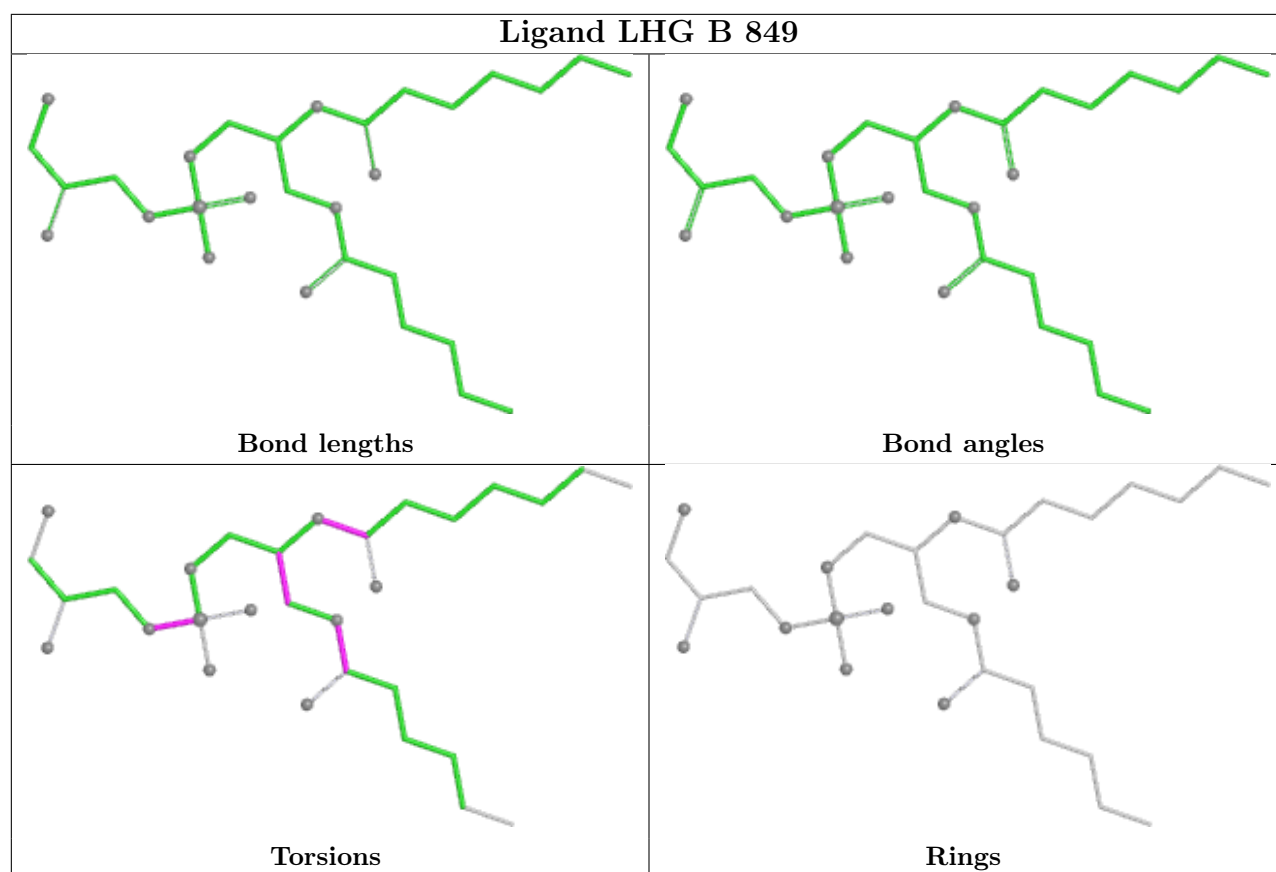
Bond angles

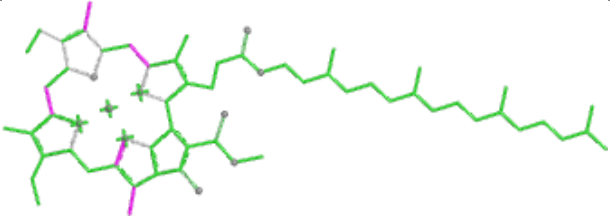
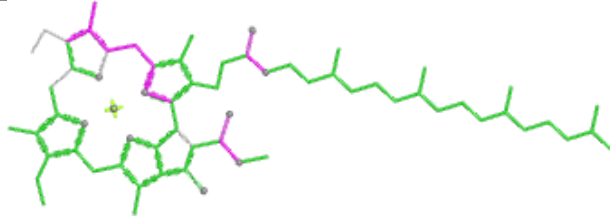
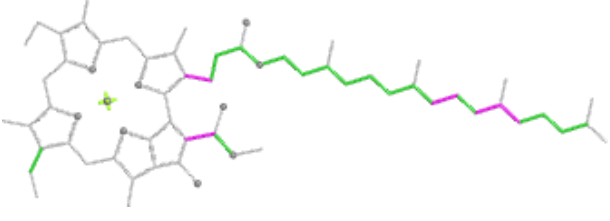
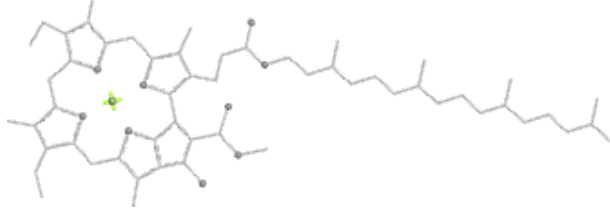


Torsions

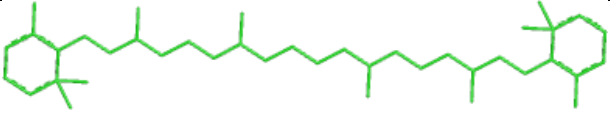
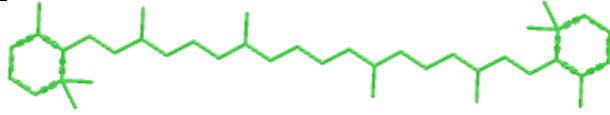
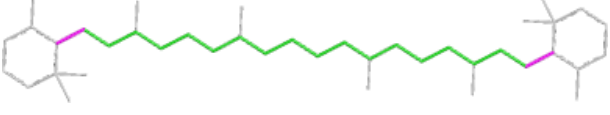
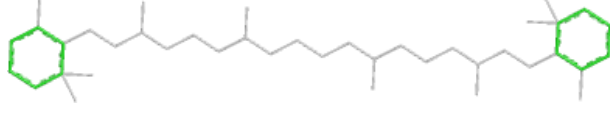


Rings



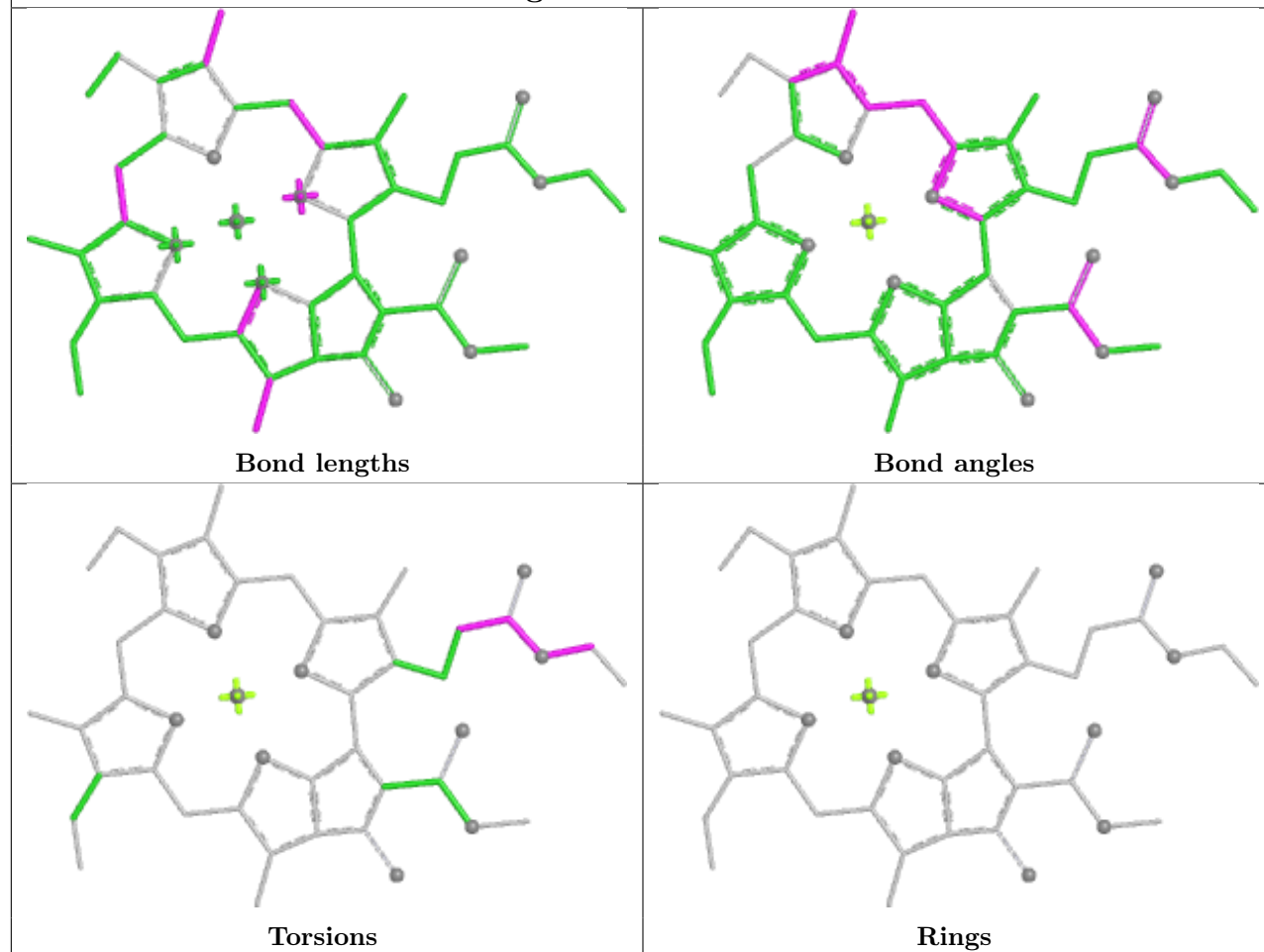
Ligand CLA A 5031			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

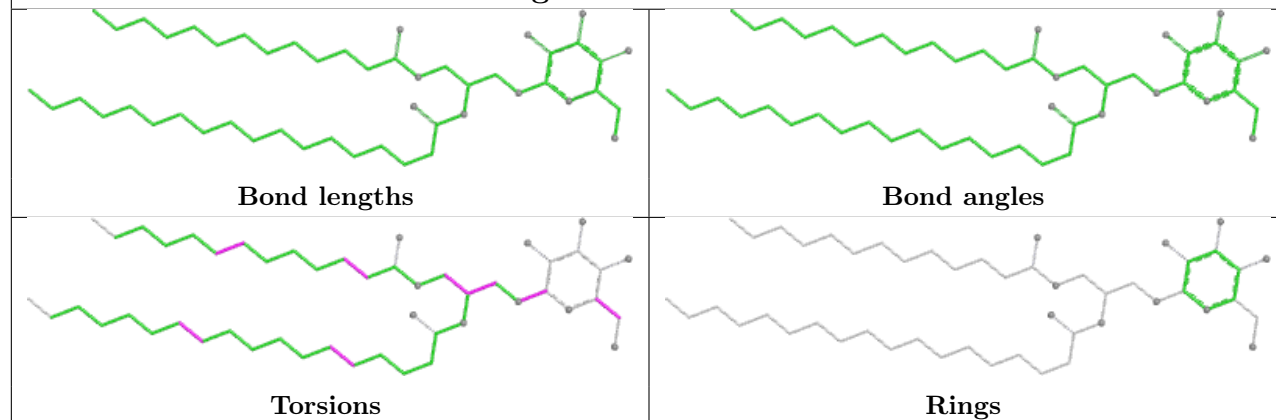
Ligand BCR 3 317			
			
Bond lengths	Bond angles		
			
Torsions	Rings		



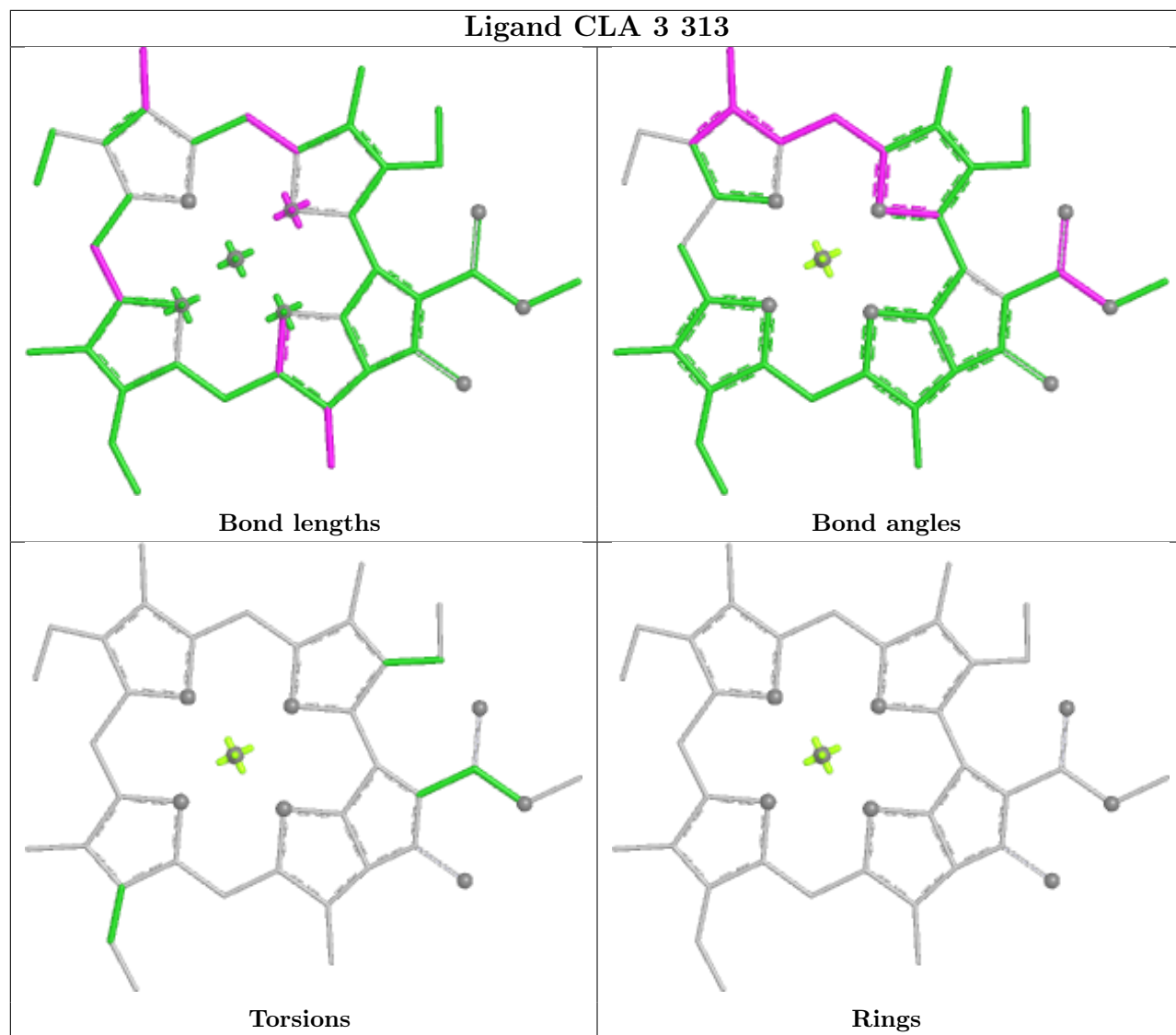
## Ligand CLA G 202



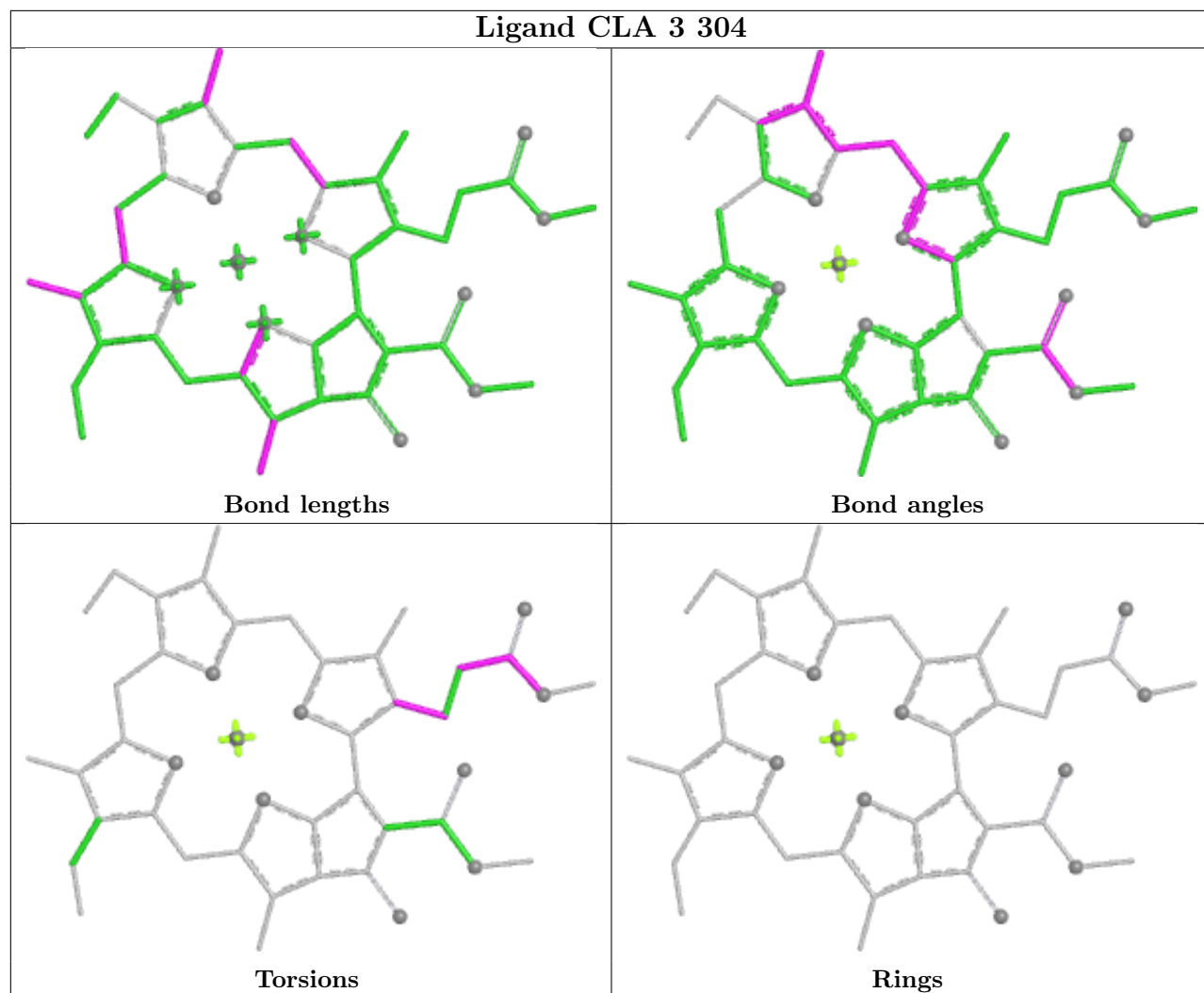
## Ligand LMG 7 301

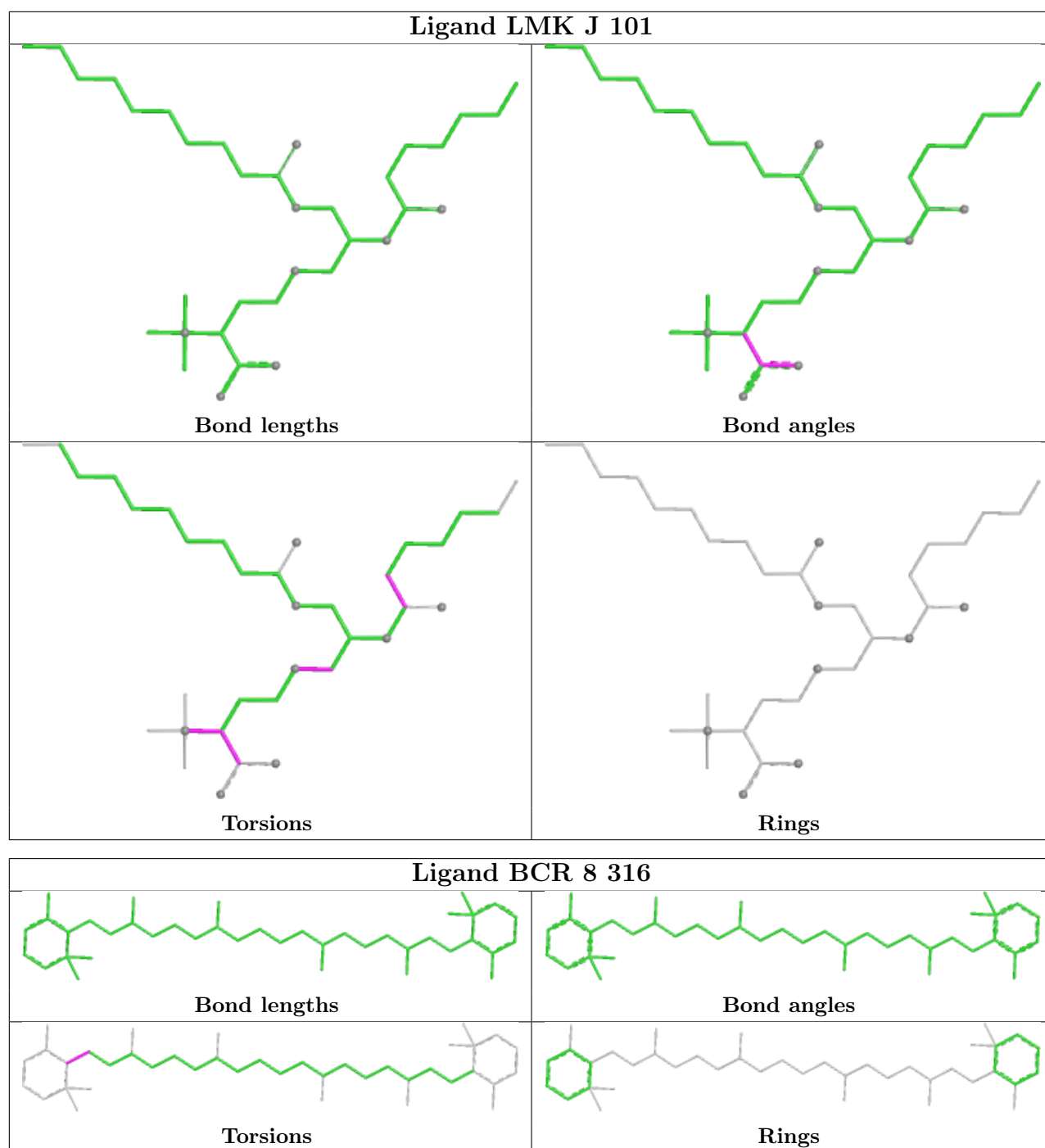


## Ligand CLA 3 313

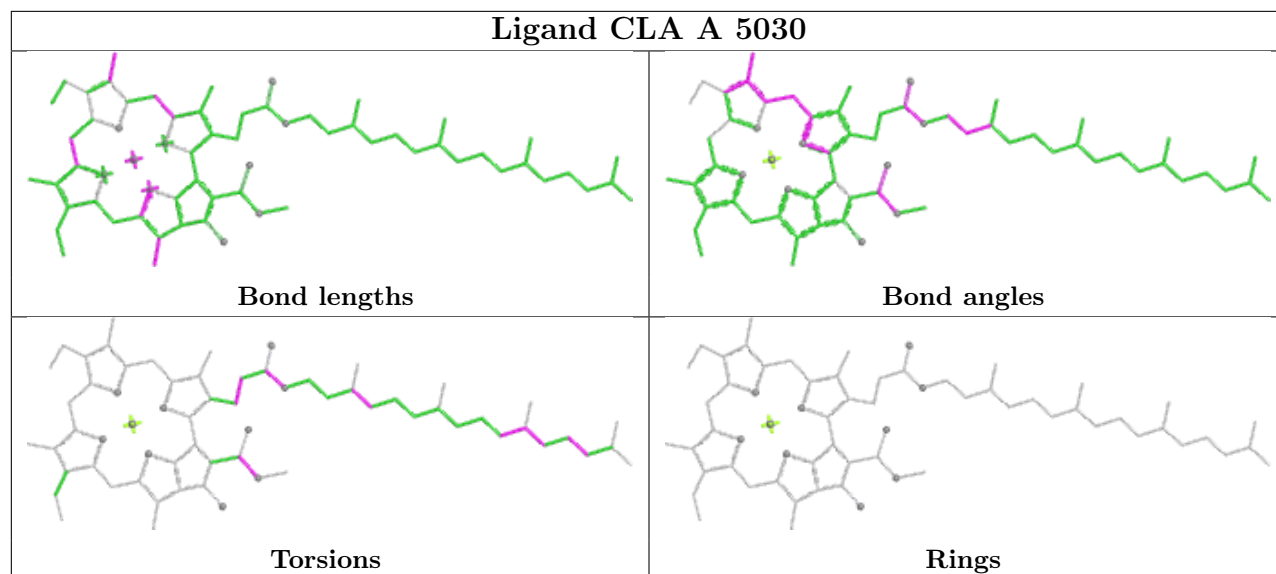


## Ligand CLA 3 304

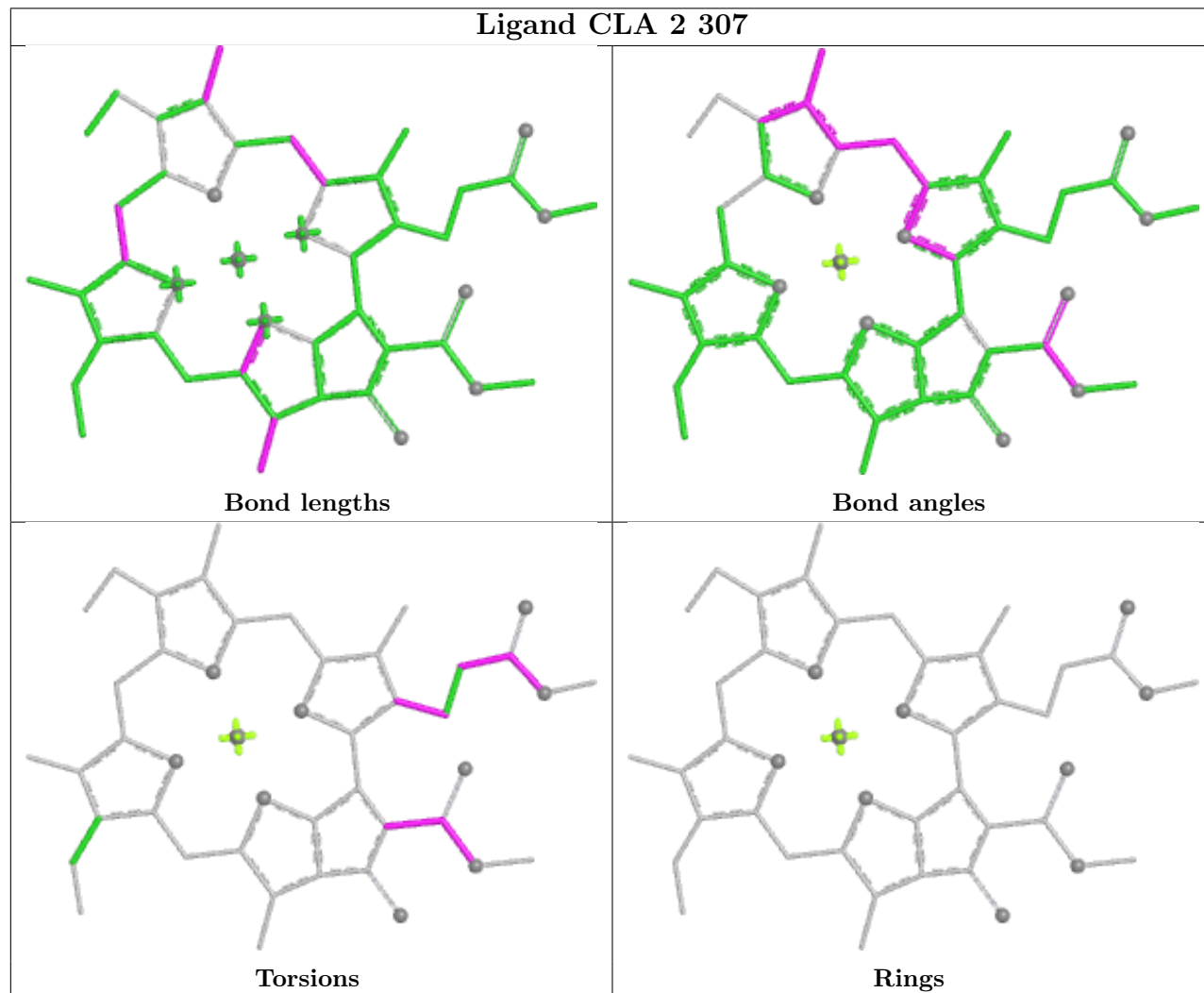




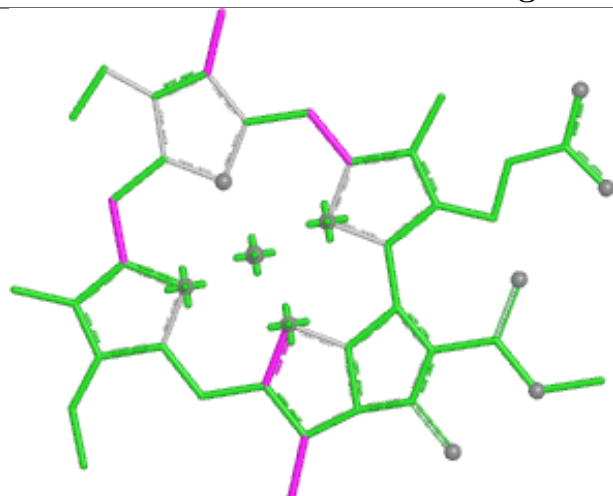
## Ligand CLA A 5030



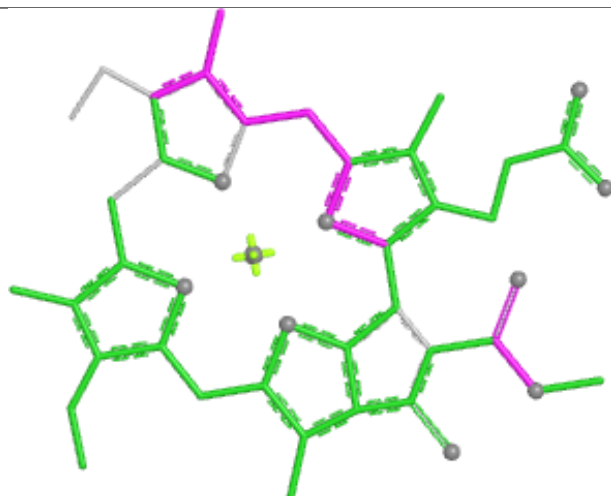
## Ligand CLA 2 307



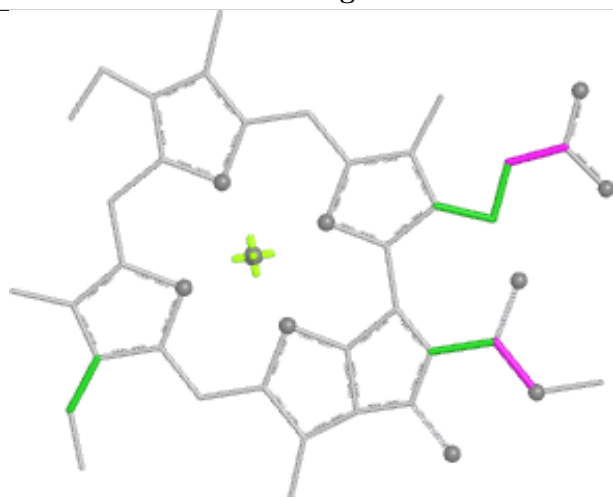
## Ligand CLA 7 315



Bond lengths



Bond angles

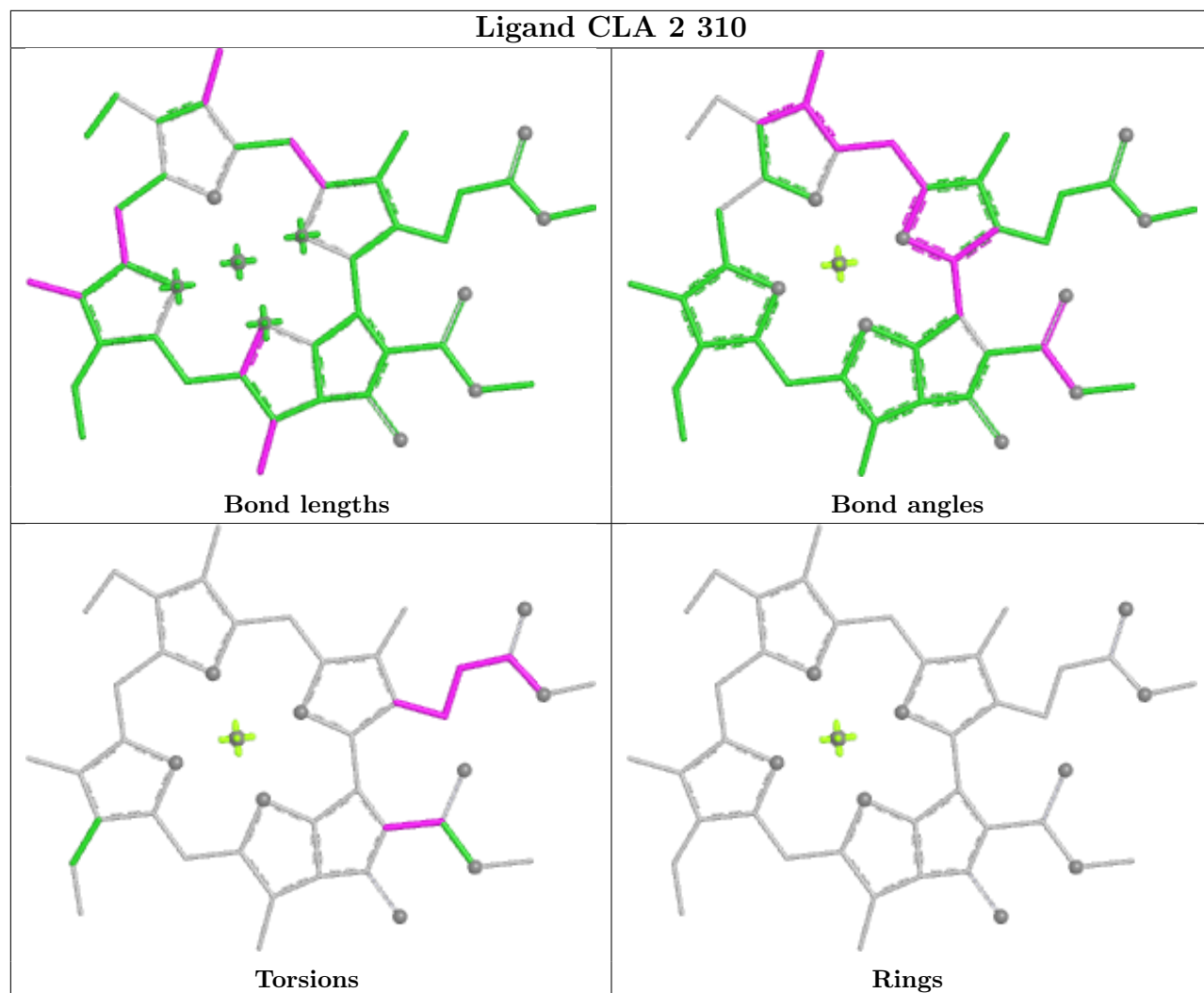


Torsions

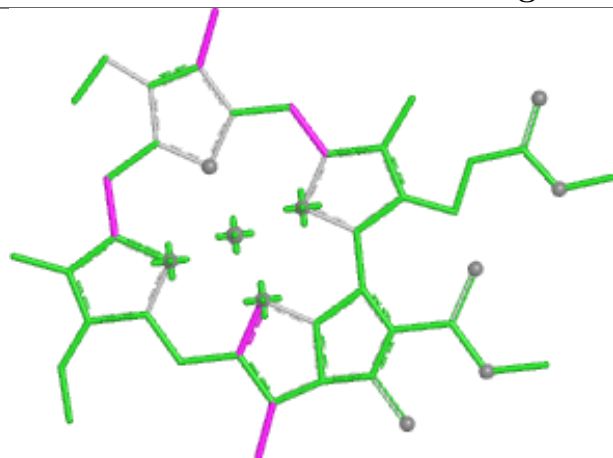


Rings

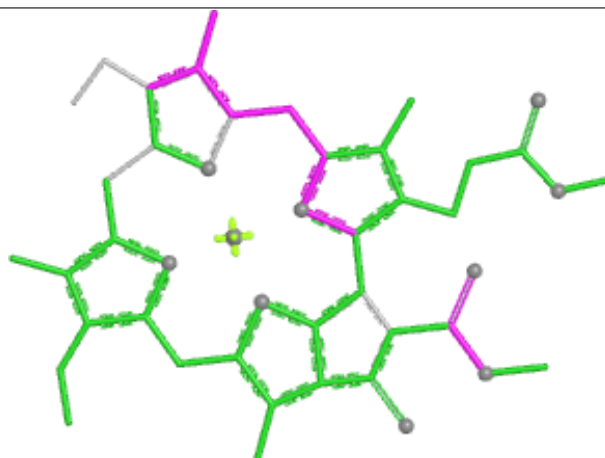
## Ligand CLA 2 310



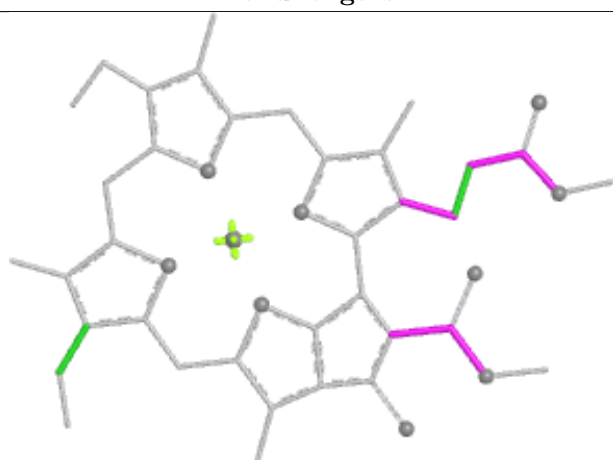
## Ligand CLA 9 609



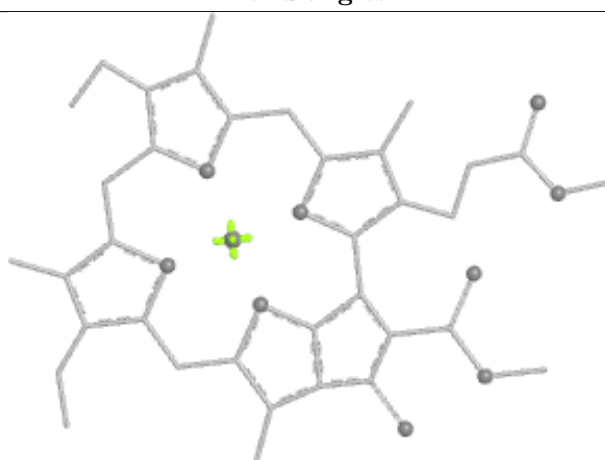
Bond lengths



Bond angles

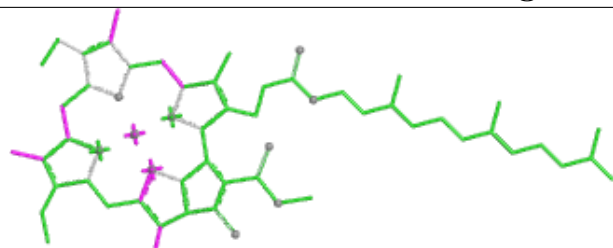


Torsions

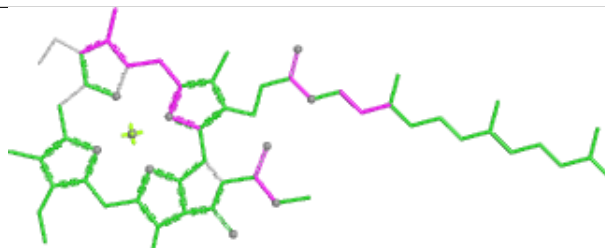


Rings

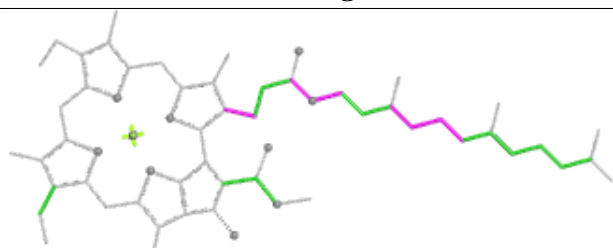
## Ligand CLA 7 311



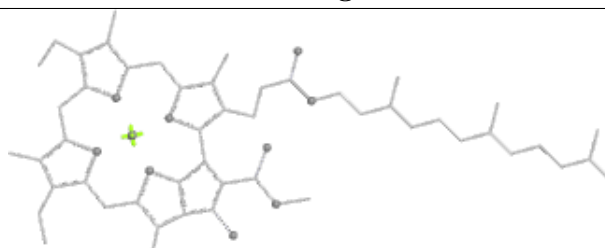
Bond lengths



Bond angles

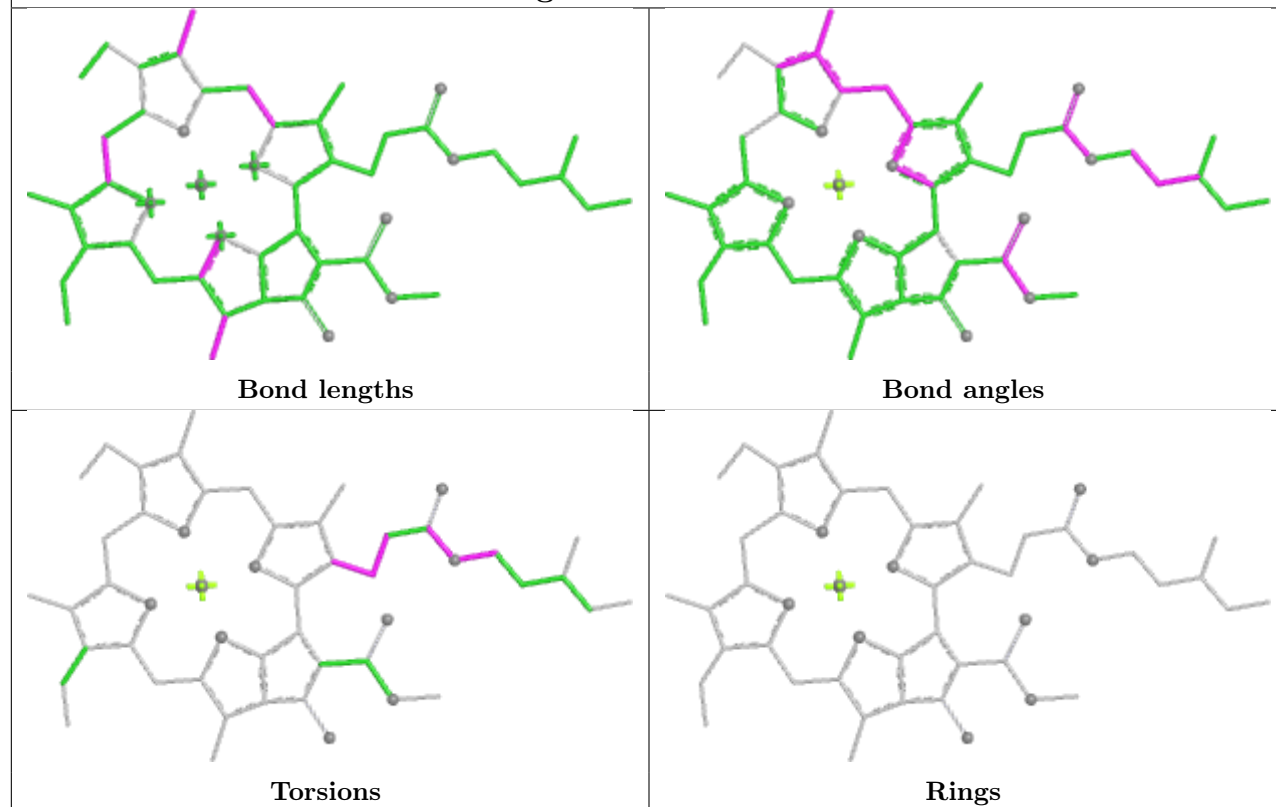
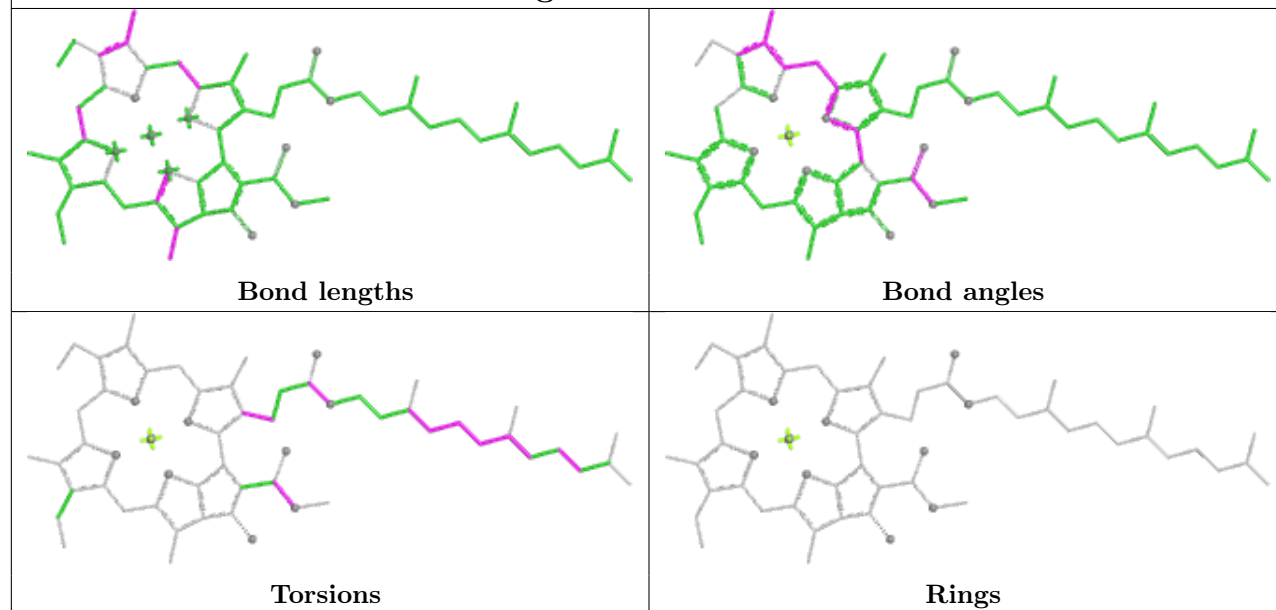


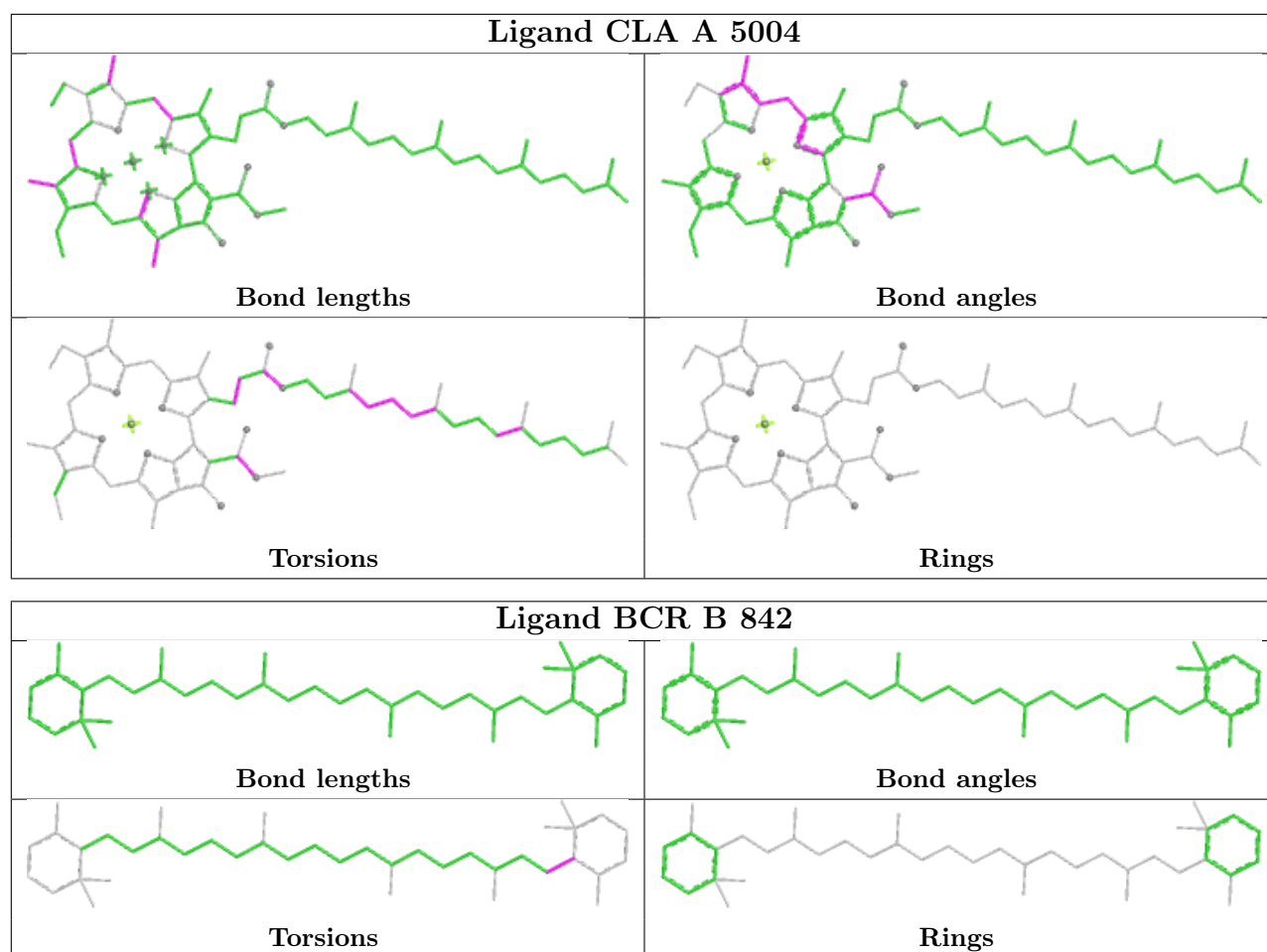
Torsions



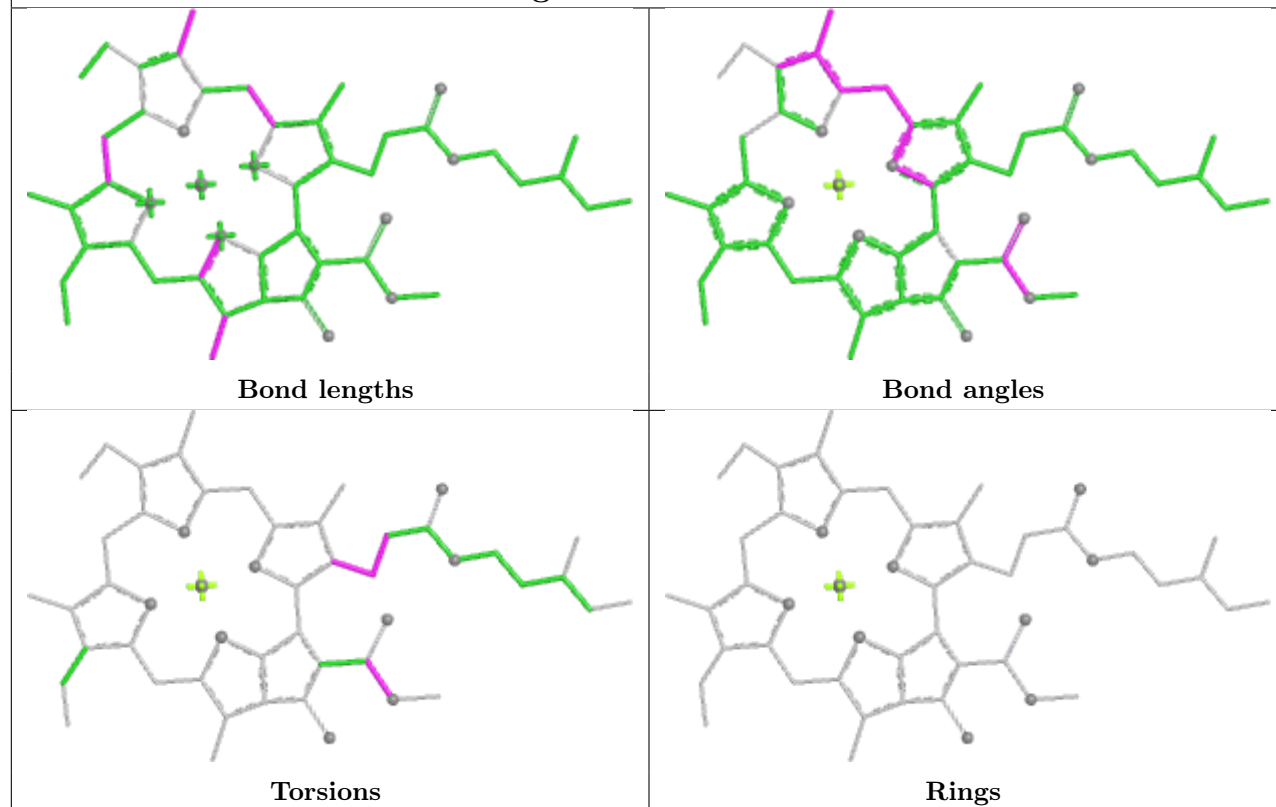
Rings



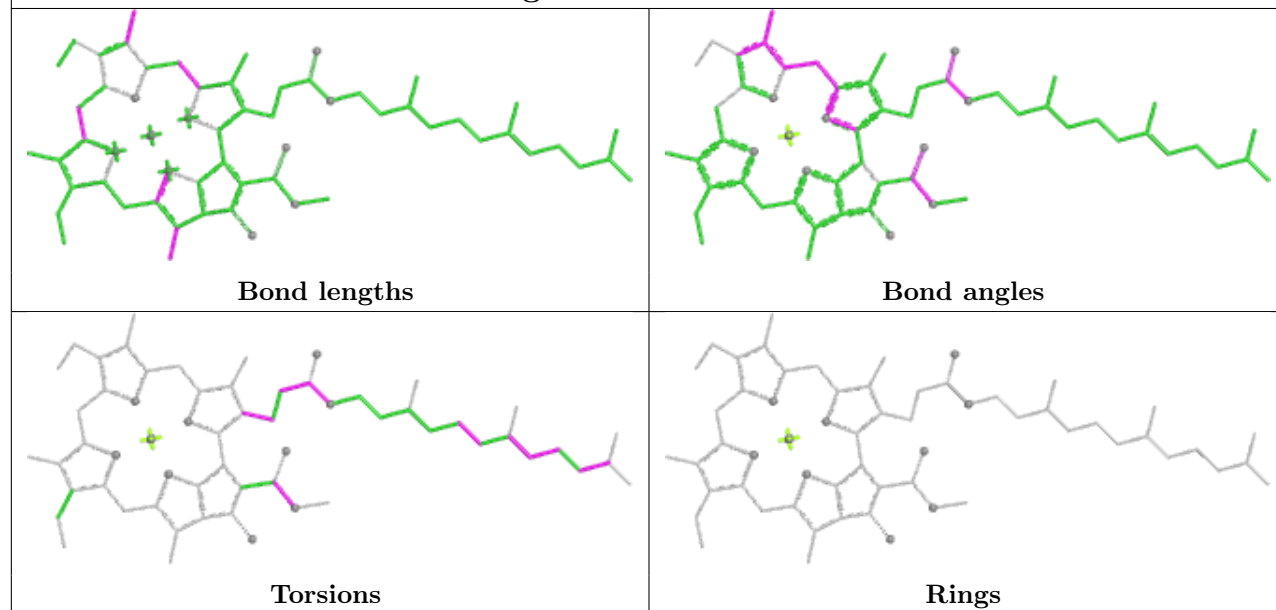
**Ligand CLA 3 306****Ligand CLA 9 607**



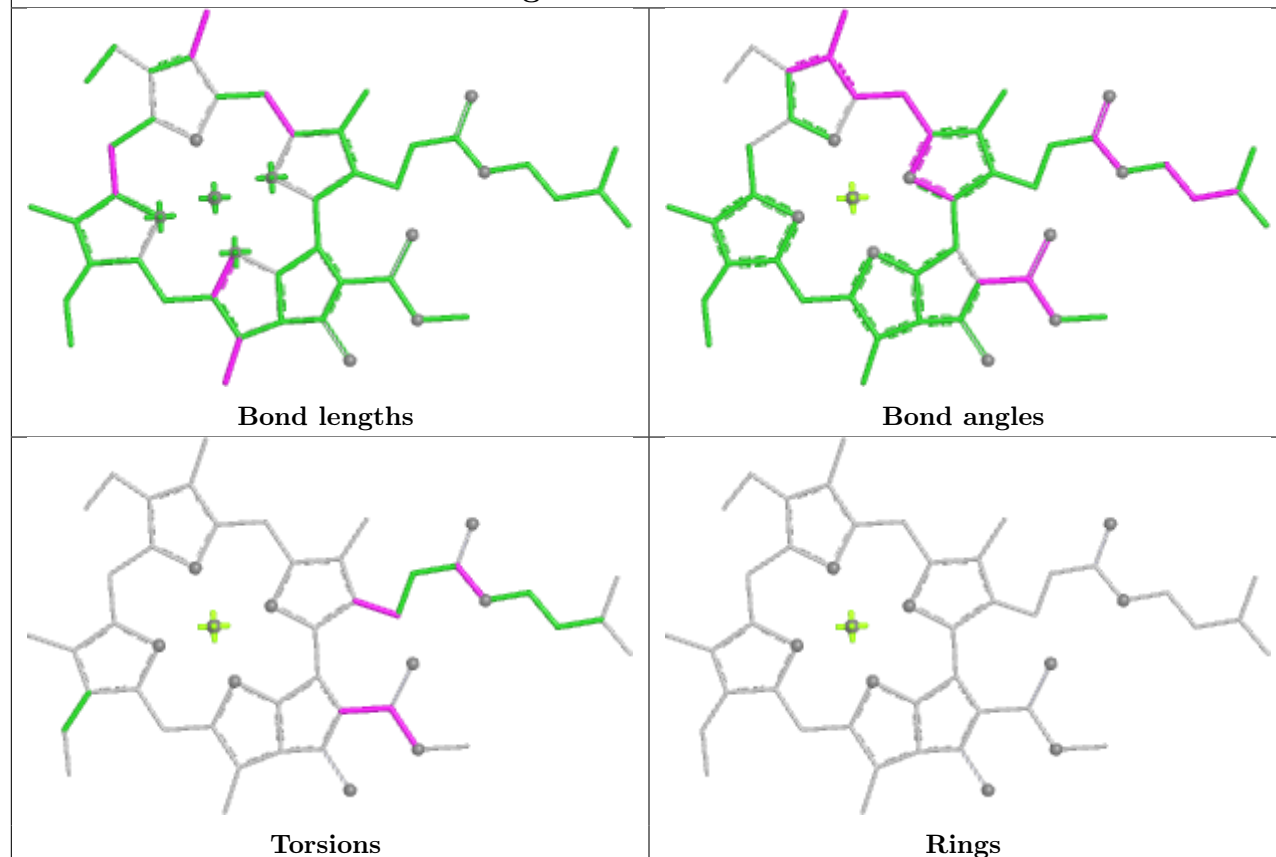
## Ligand CLA B 835



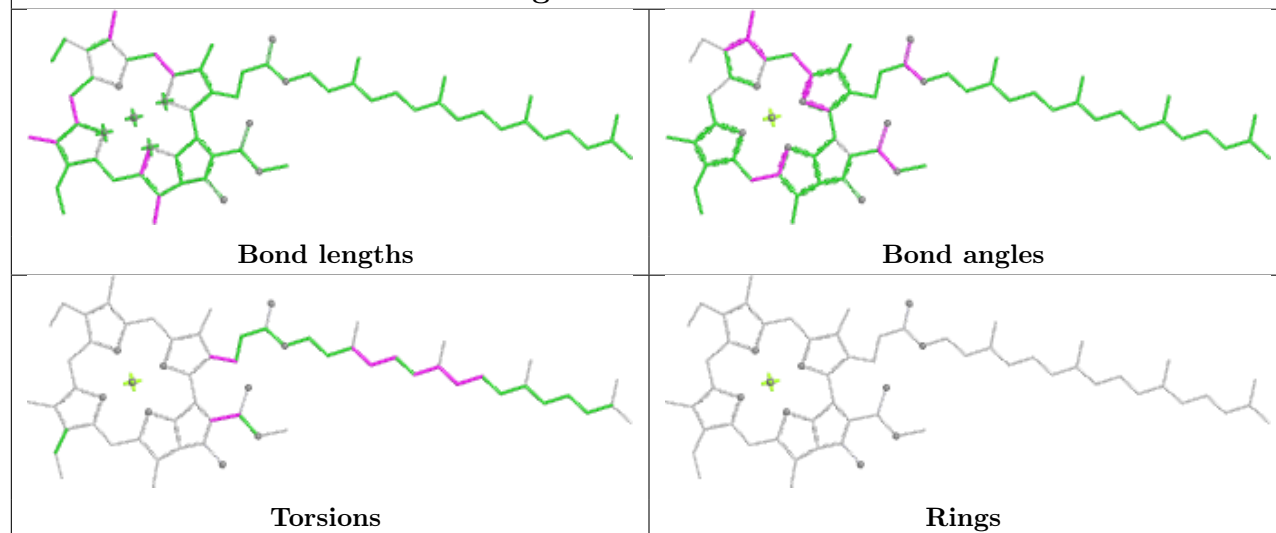
## Ligand CLA A 5024

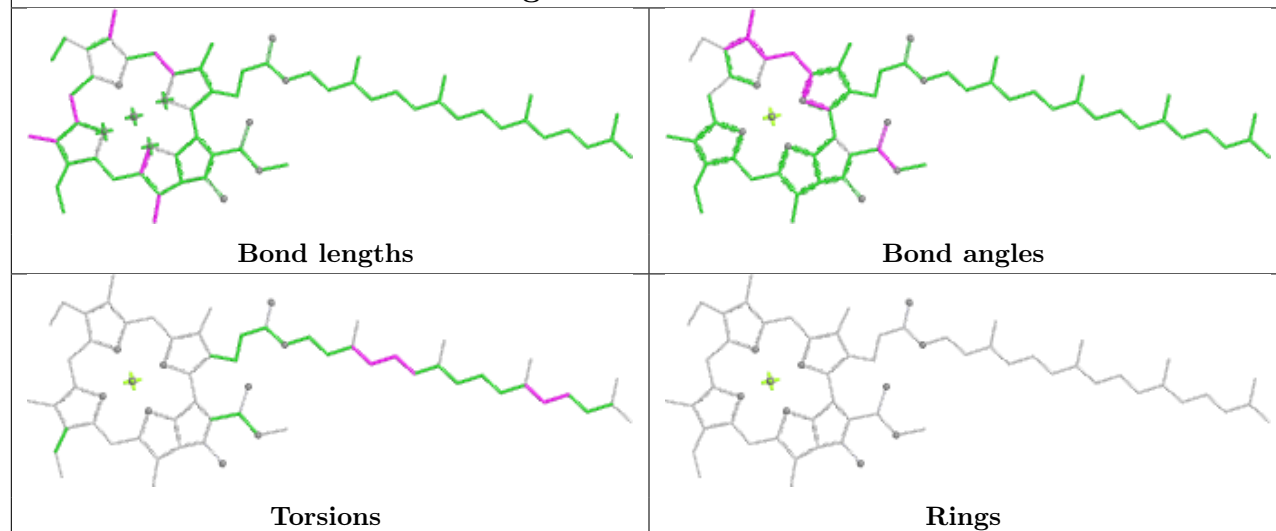
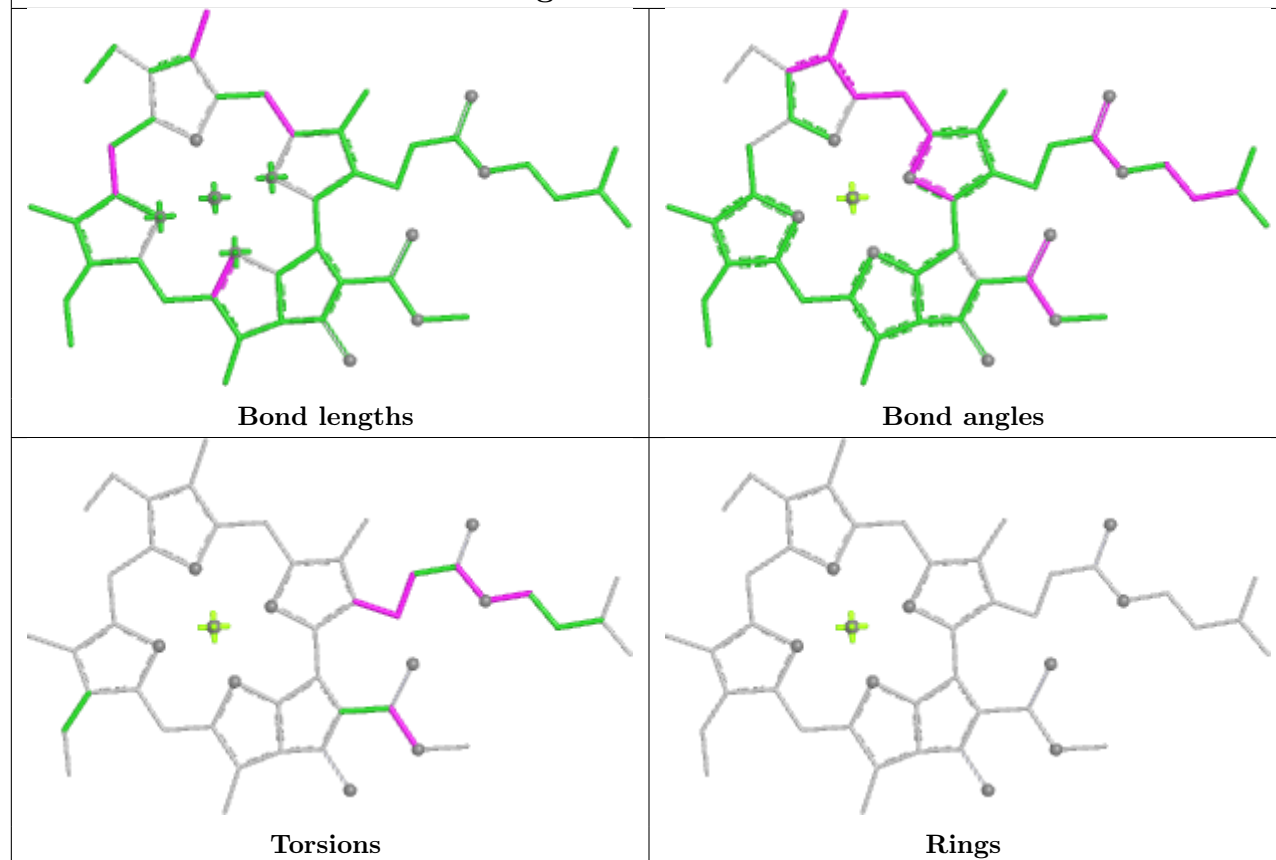


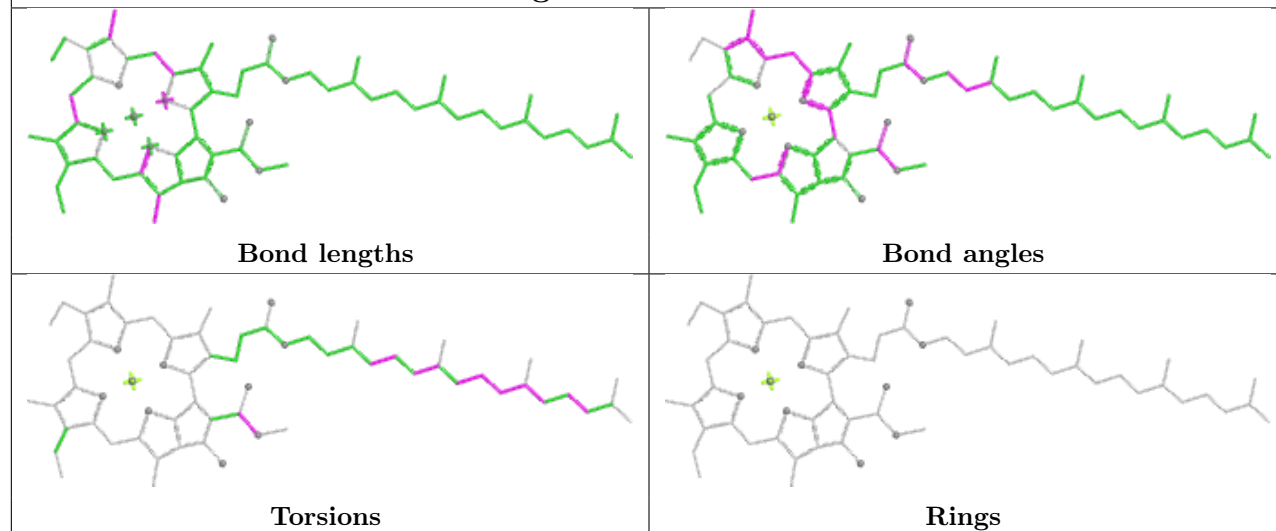
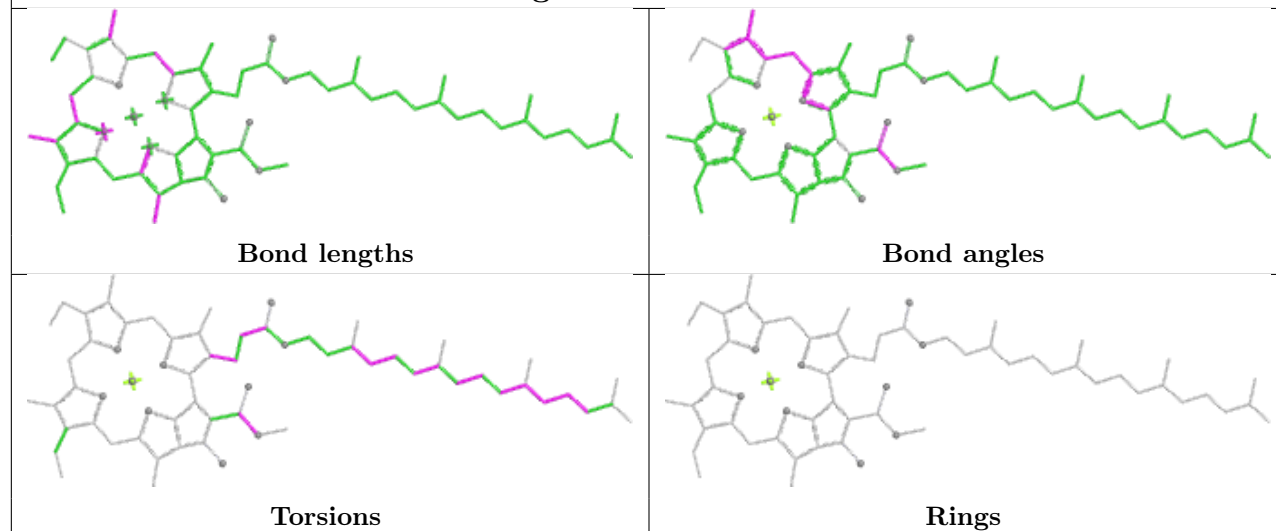
## Ligand CLA A 5037



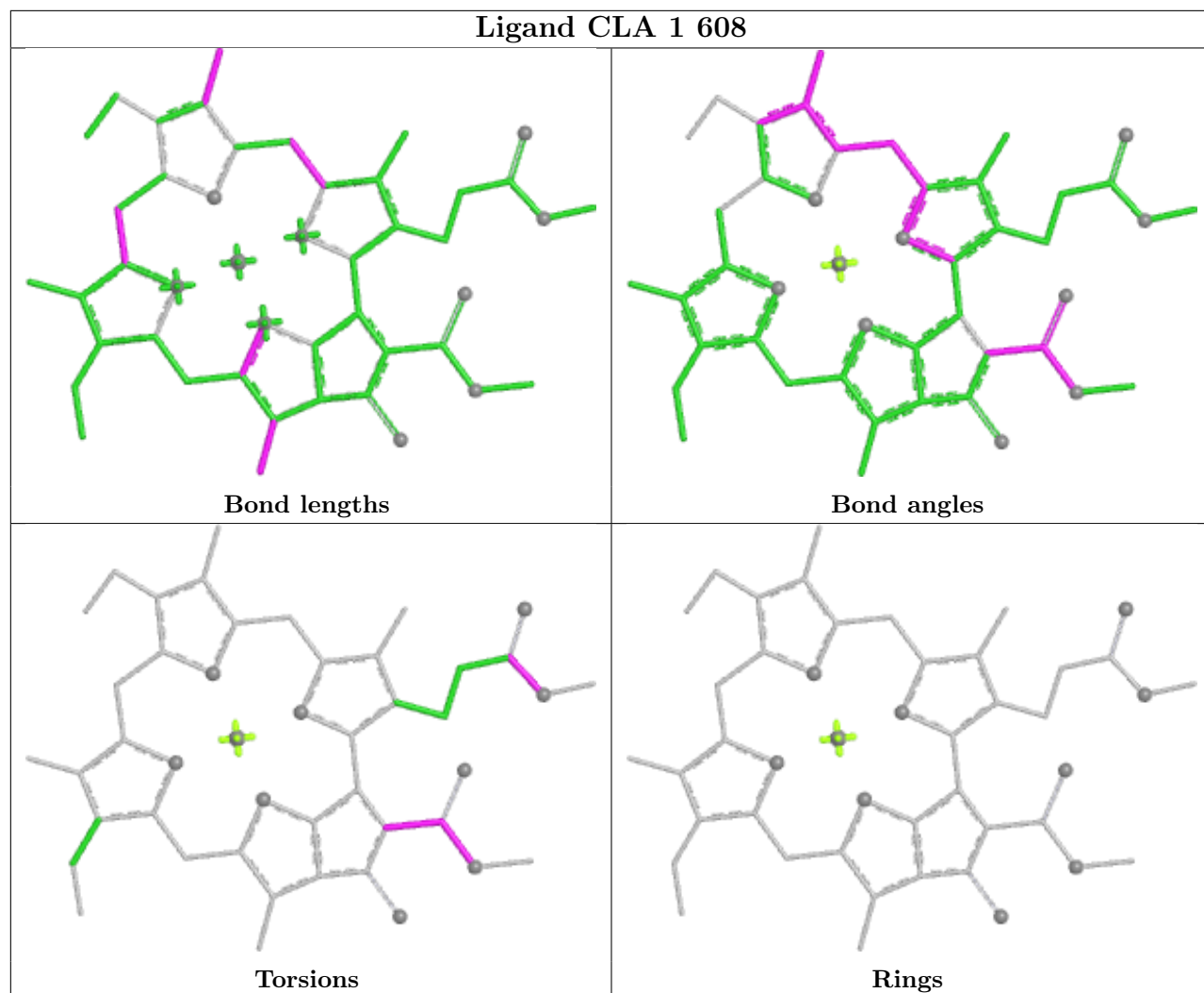
## Ligand CLA B 807



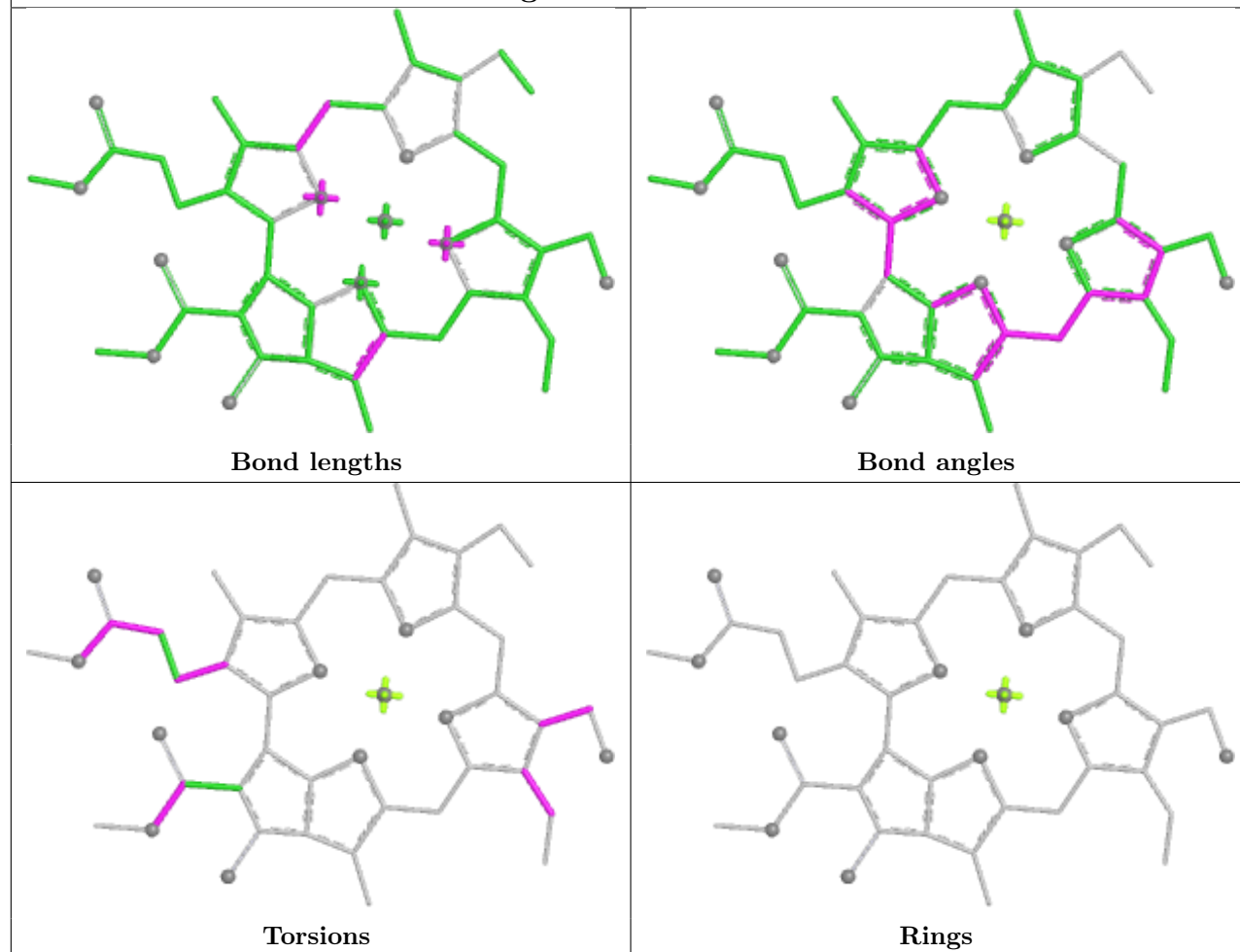
**Ligand CLA A 5022****Ligand CLA 2 311**

**Ligand CLA B 808****Ligand CLA B 804**

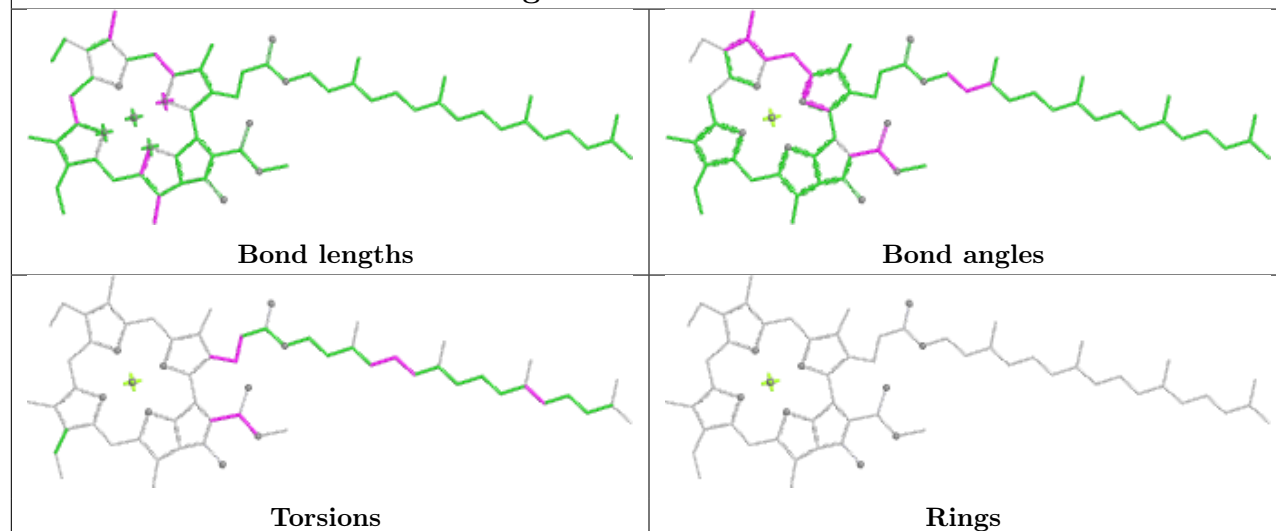
## Ligand CLA 1 608



## Ligand CHL 9 606

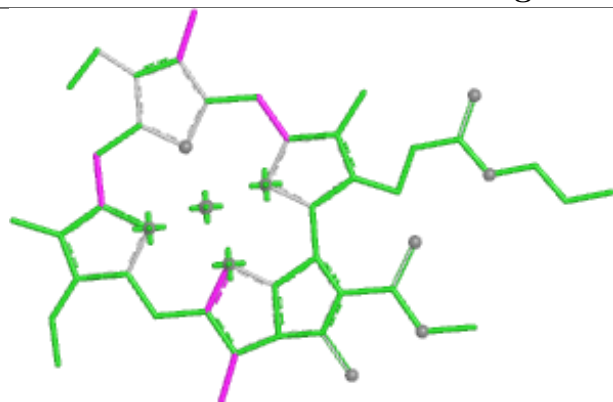


## Ligand CLA A 5044

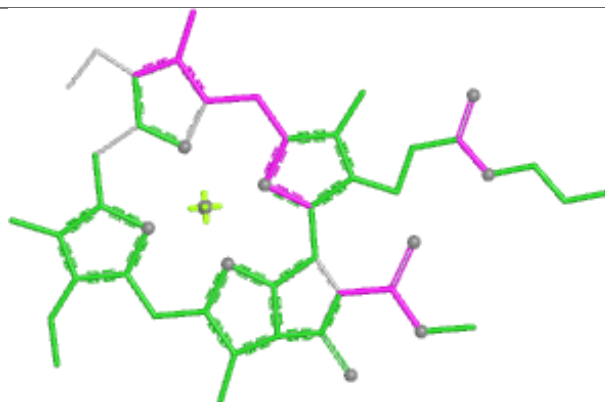




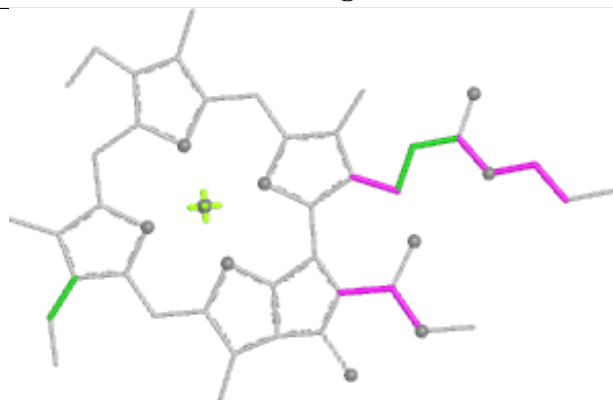
## Ligand CLA B 806



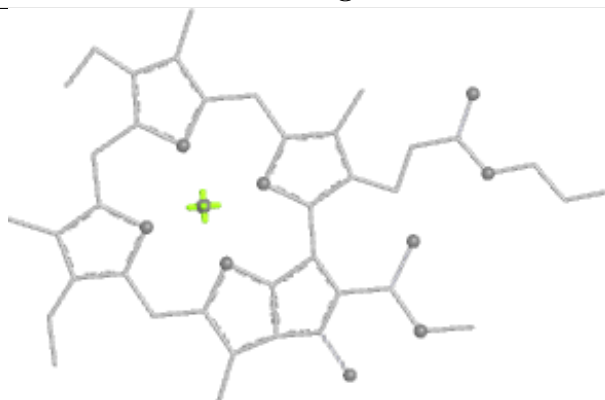
Bond lengths



Bond angles

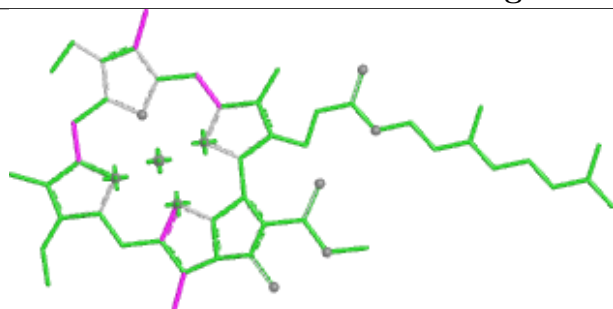


Torsions

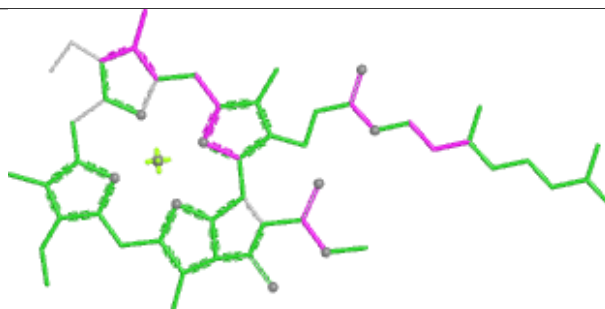


Rings

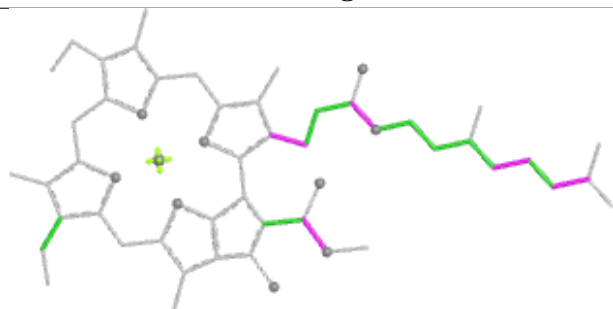
## Ligand CLA A 5015



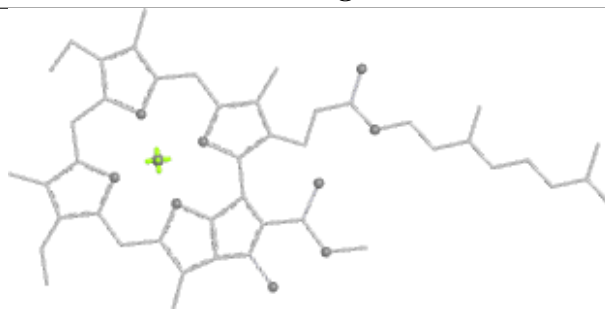
Bond lengths



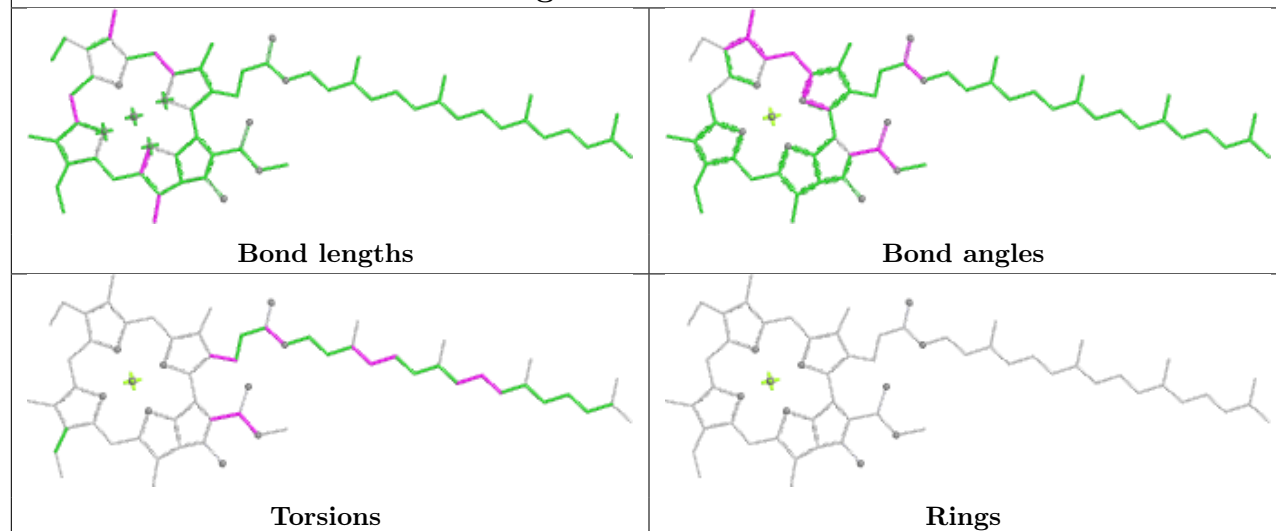
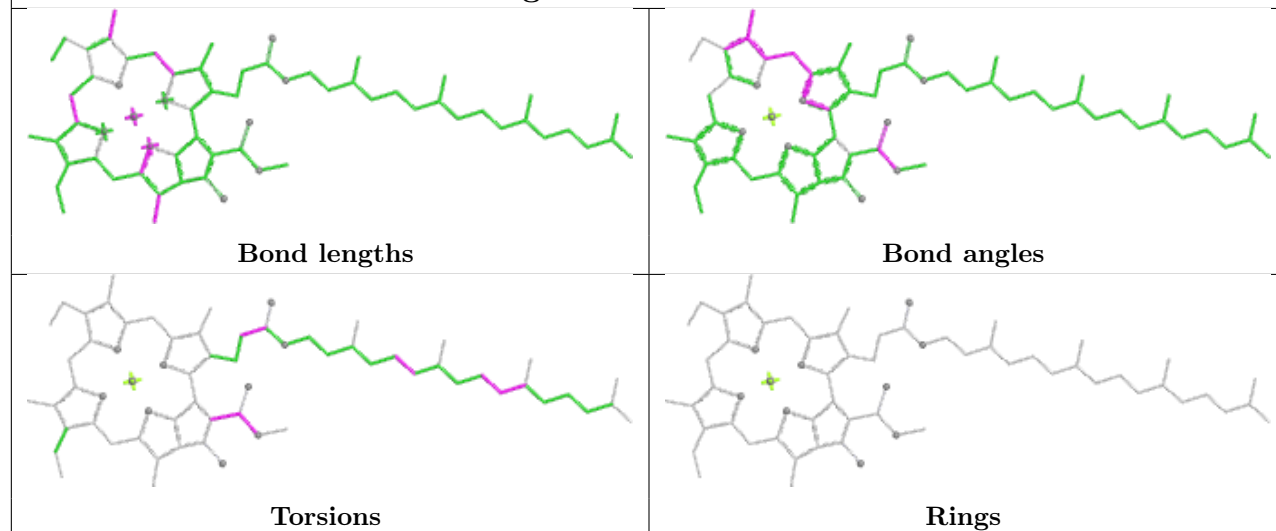
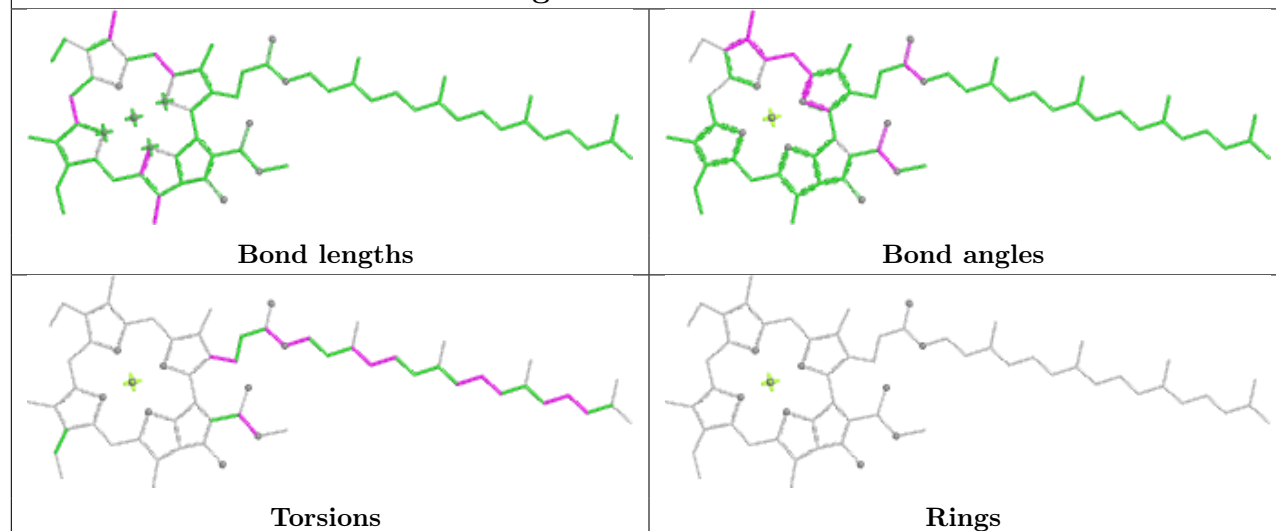
Bond angles



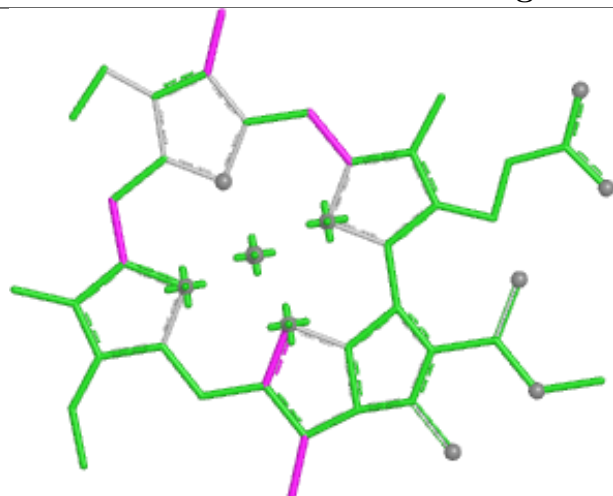
Torsions



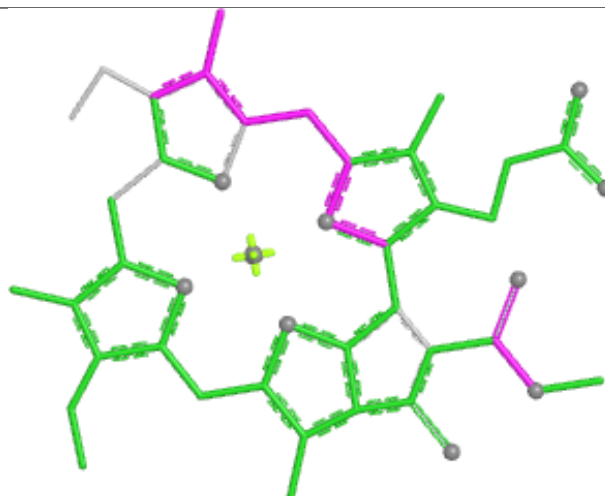
Rings

**Ligand CLA 3 307****Ligand CLA A 5026****Ligand CLA B 822**

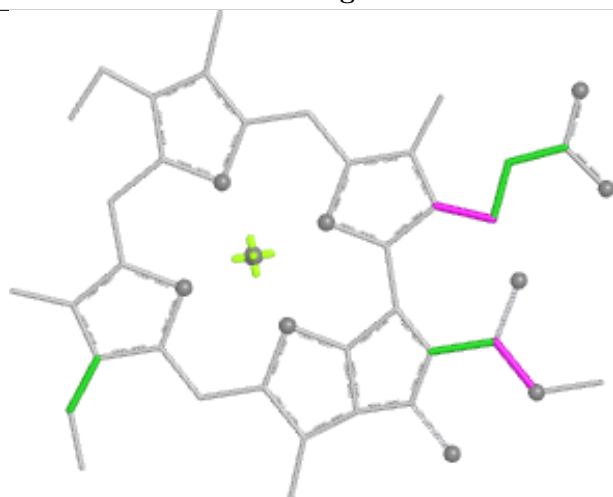
## Ligand CLA F 308



Bond lengths



Bond angles

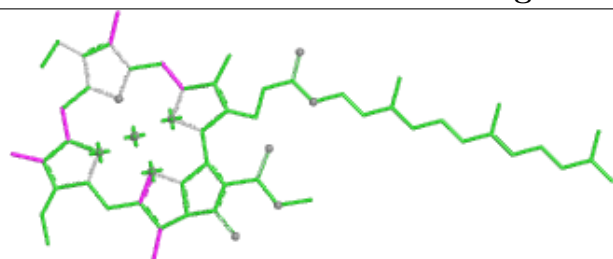


Torsions

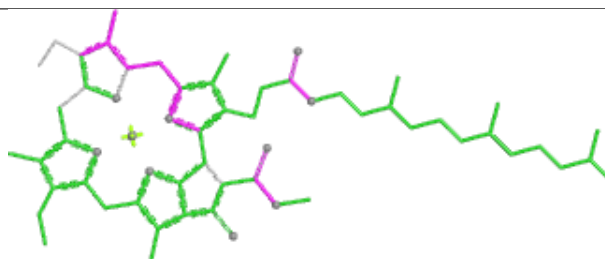


Rings

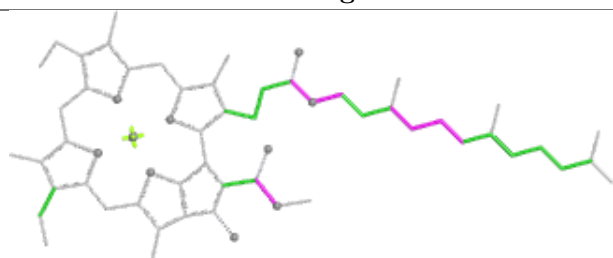
## Ligand CLA B 831



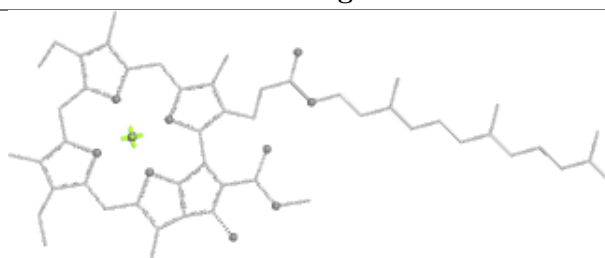
Bond lengths



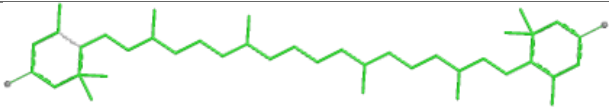
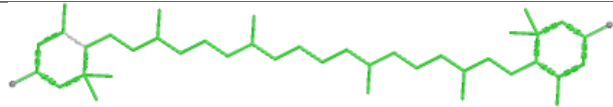

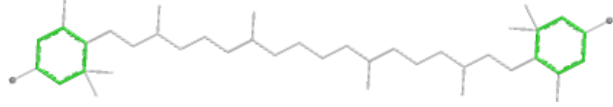
Bond angles

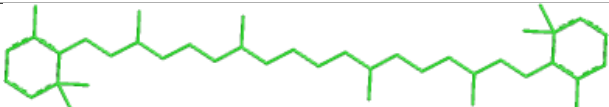
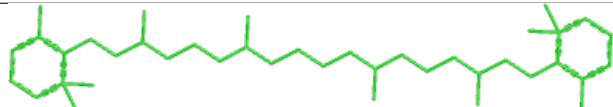
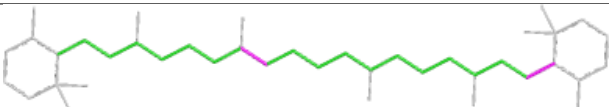
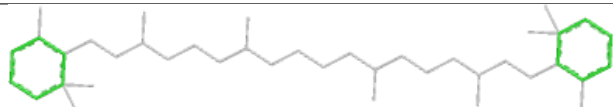


Torsions



Rings

Ligand LUT 3 315	
	Bond lengths
	Bond angles
	Torsions
	Rings

Ligand BCR I 4001	
	Bond lengths
	Bond angles
	Torsions
	Rings

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

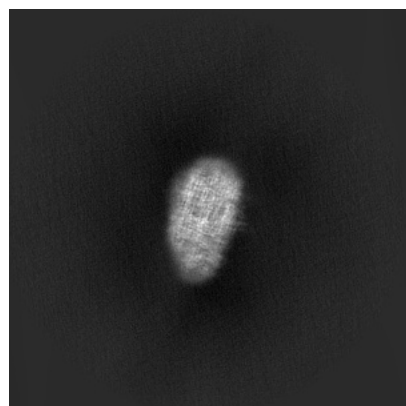
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48266. These allow visual inspection of the internal detail of the map and identification of artifacts.

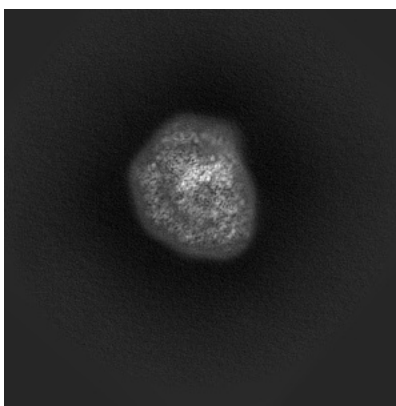
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

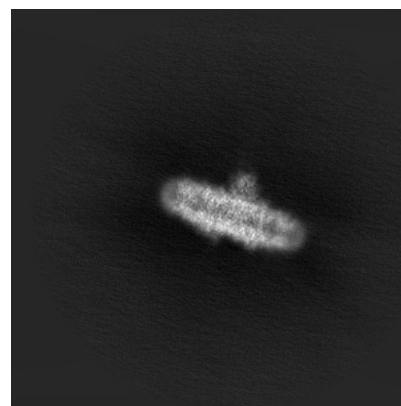
#### 6.1.1 Primary map



X

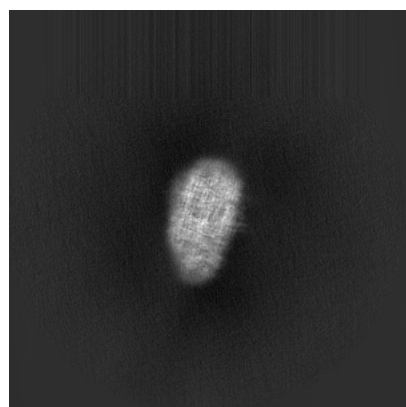


Y

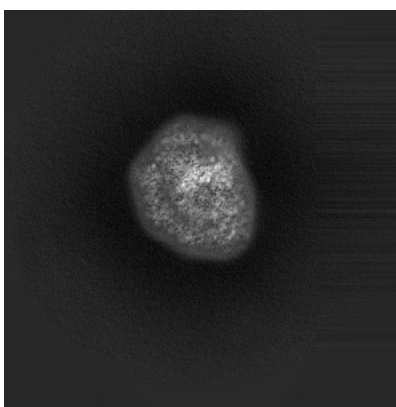


Z

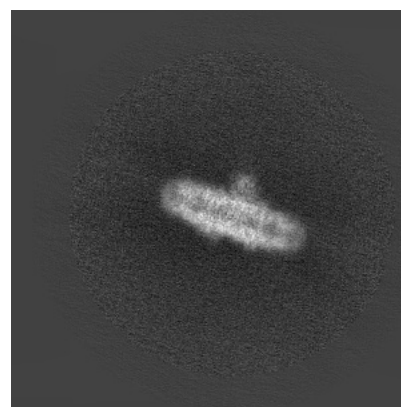
#### 6.1.2 Raw map



X



Y

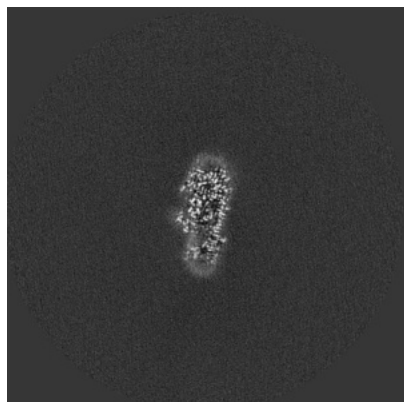


Z

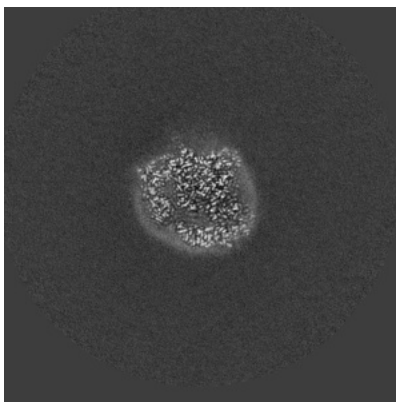
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

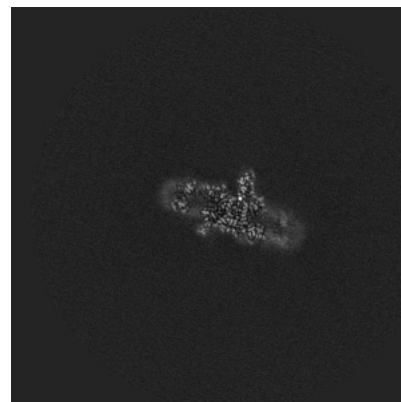
### 6.2.1 Primary map



X Index: 240

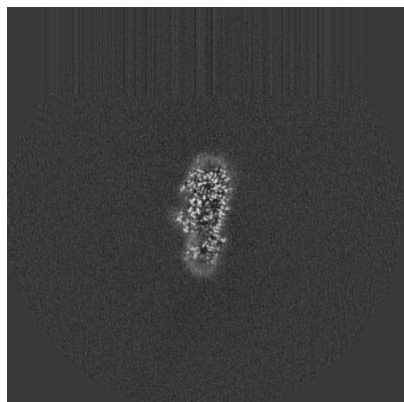


Y Index: 240

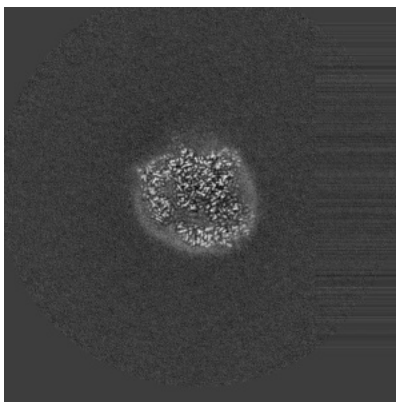


Z Index: 240

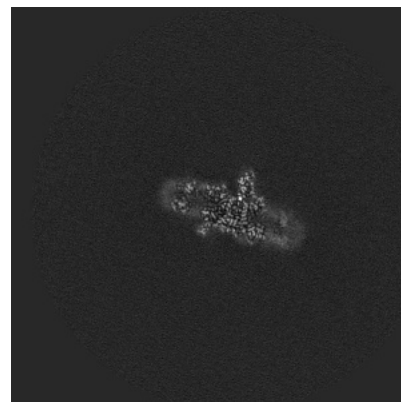
### 6.2.2 Raw map



X Index: 240



Y Index: 240

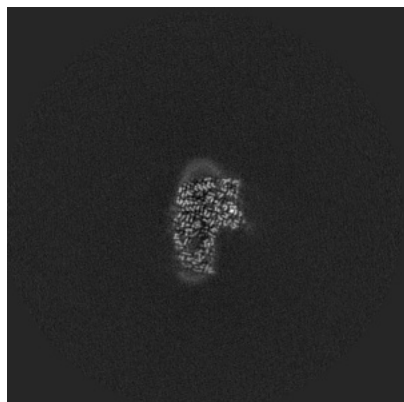


Z Index: 240

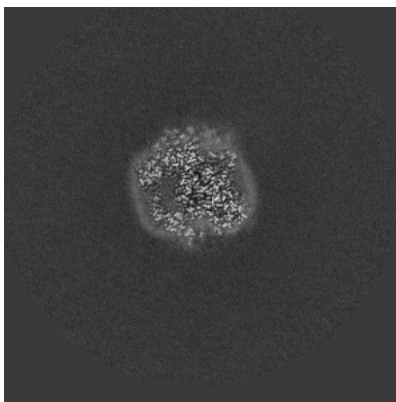
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

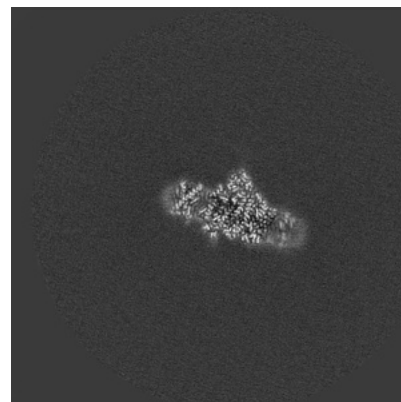
### 6.3.1 Primary map



X Index: 277

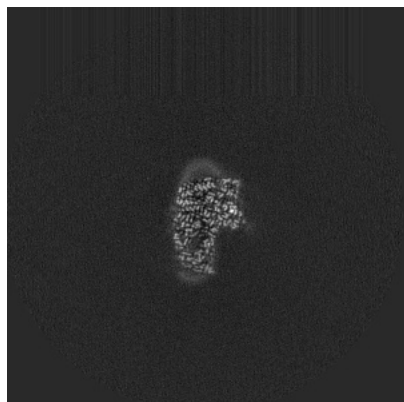


Y Index: 231

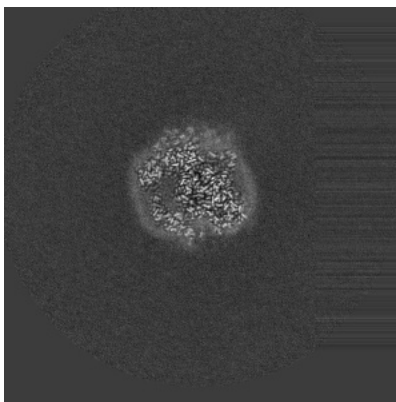


Z Index: 224

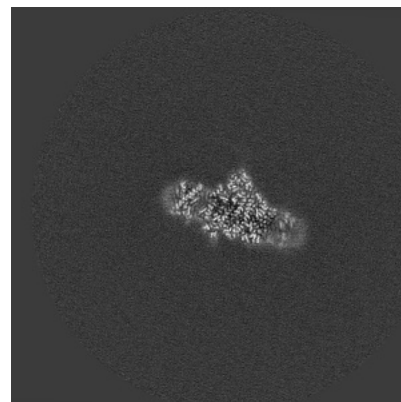
### 6.3.2 Raw map



X Index: 277



Y Index: 231



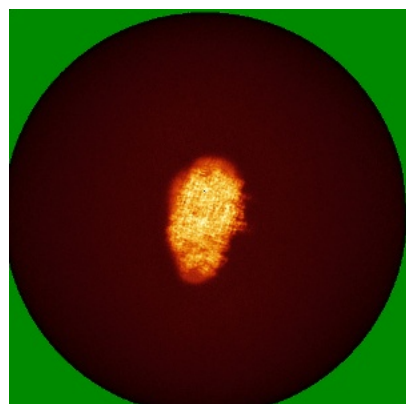
Z Index: 224

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

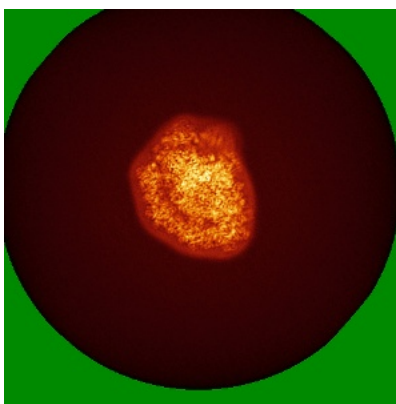


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 6.4.1 Primary map



X

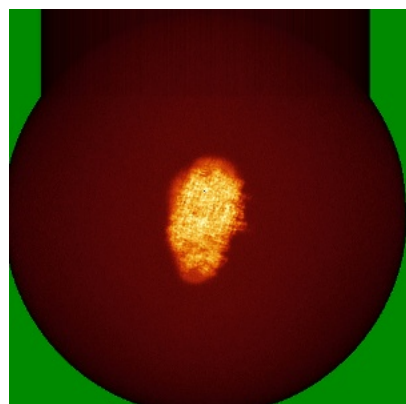


Y

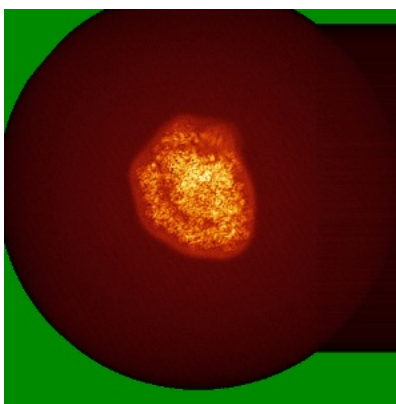


Z

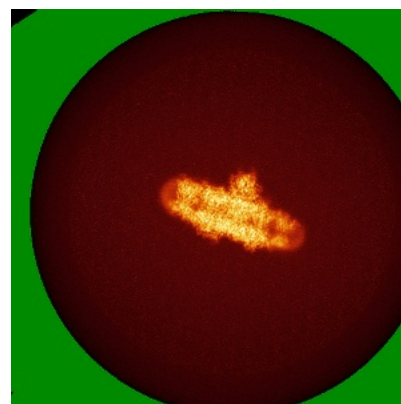
### 6.4.2 Raw map



X



Y



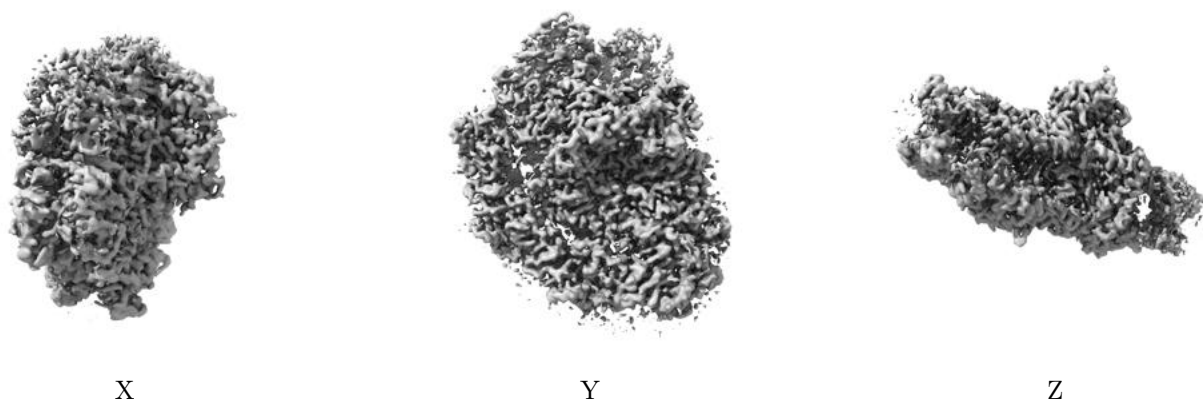
Z

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



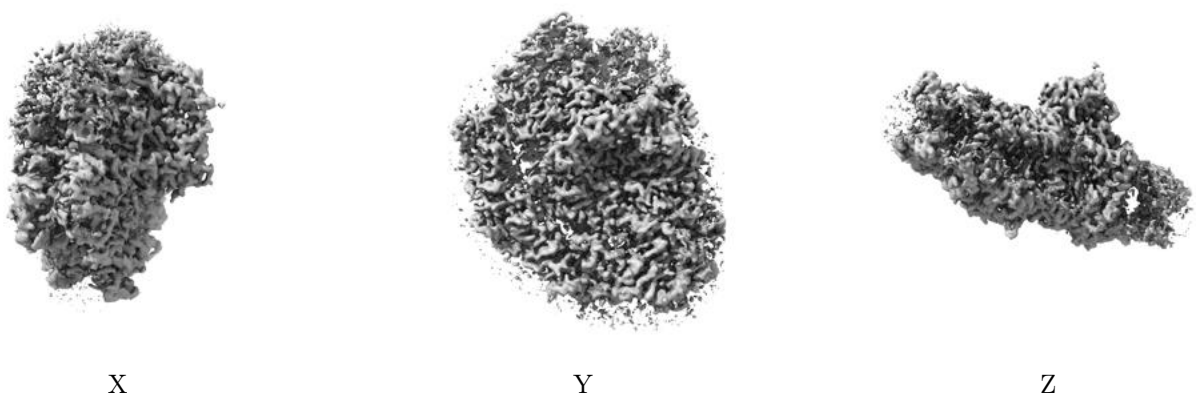
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0172. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

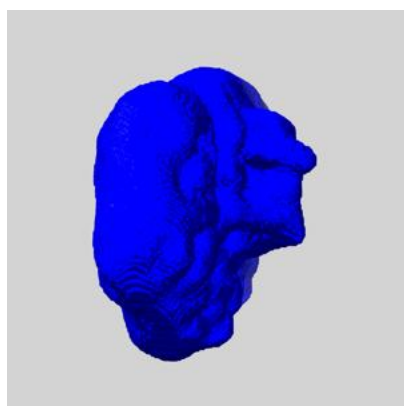
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

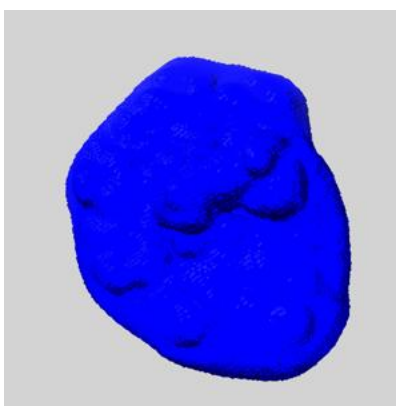
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

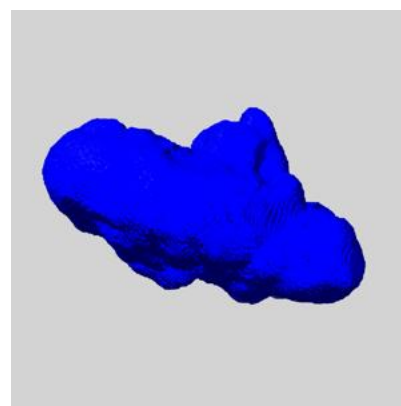
### 6.6.1 emd\_48266\_msk\_1.map [i](#)



X



Y

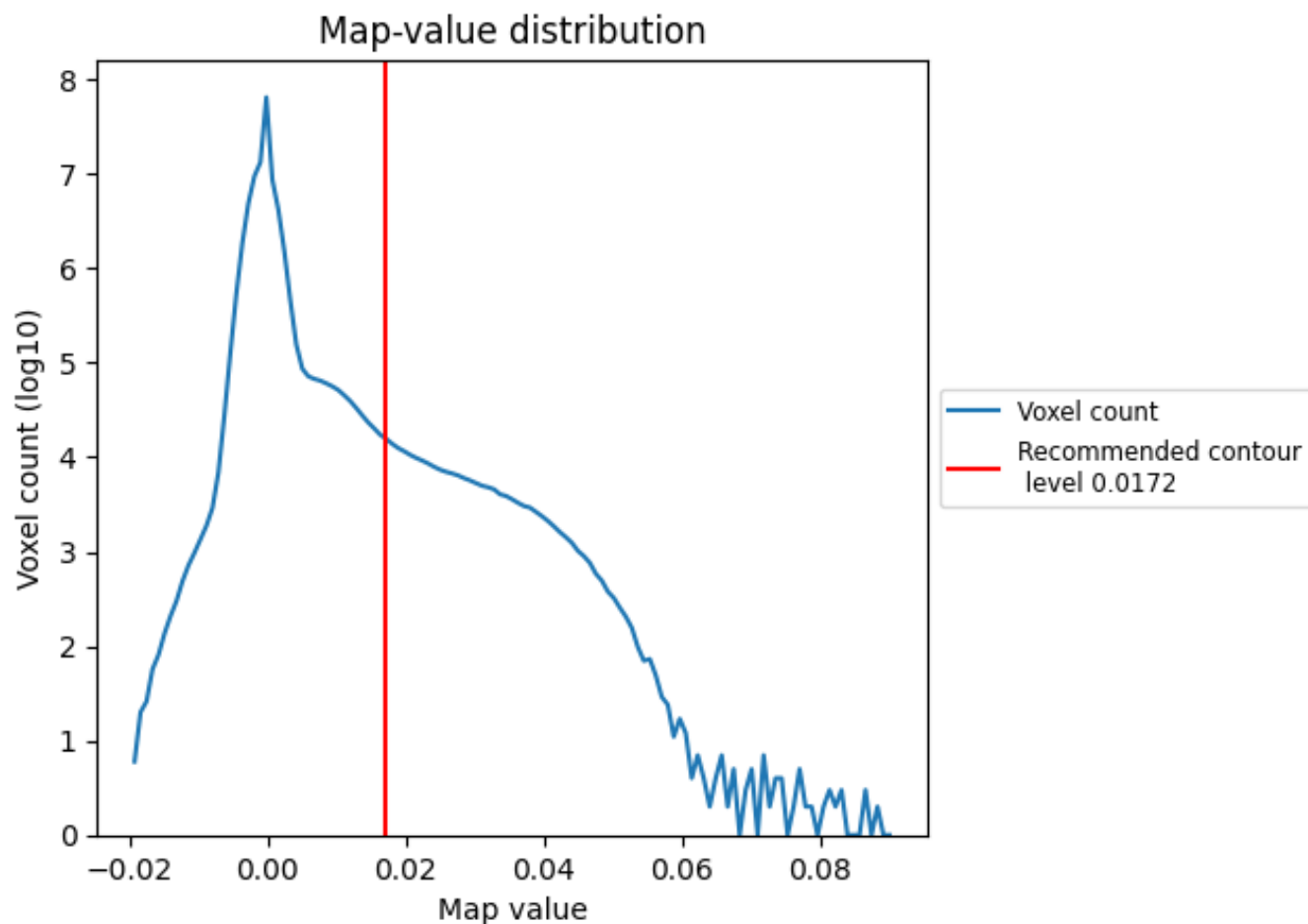


Z

## 7 Map analysis [i](#)

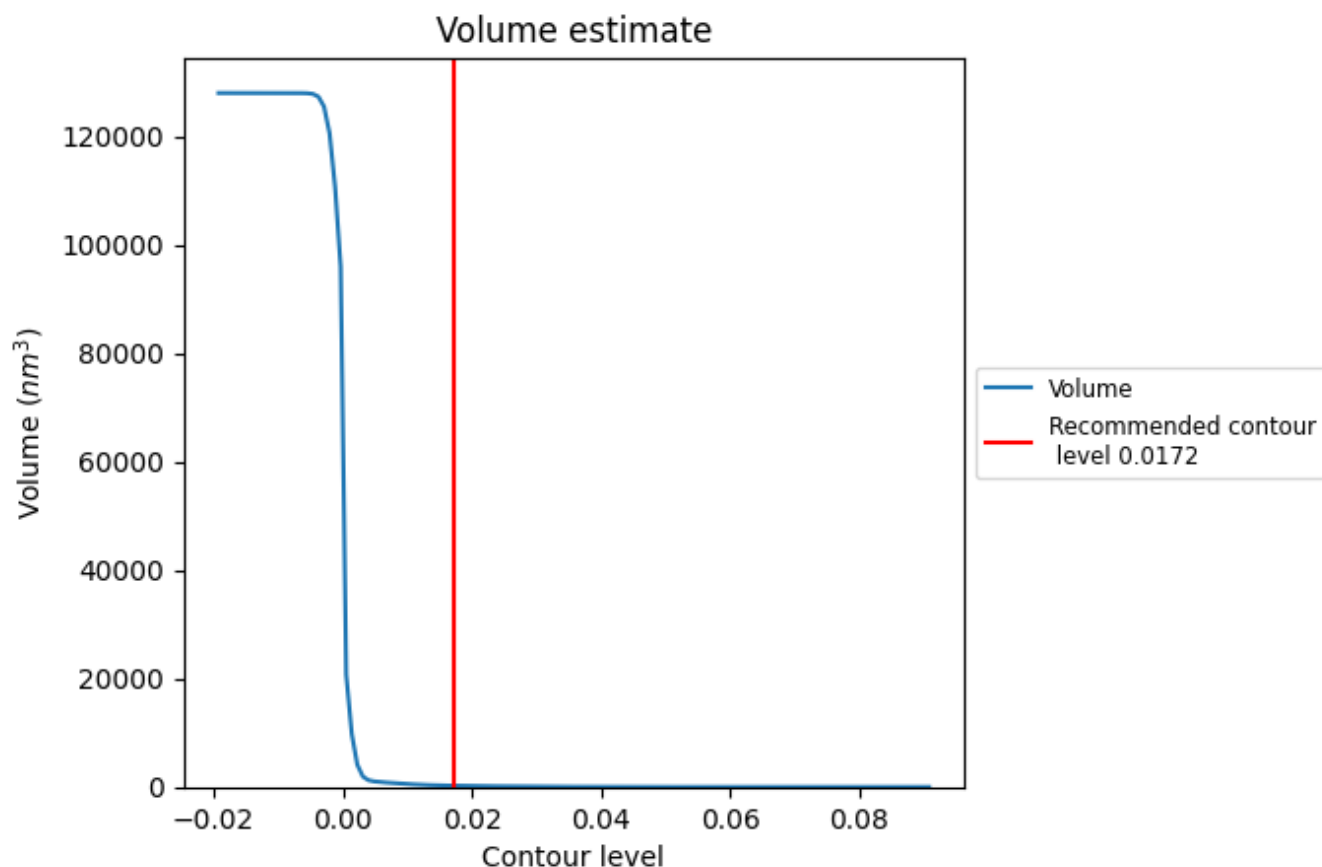
This section contains the results of statistical analysis of the map.

### 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.

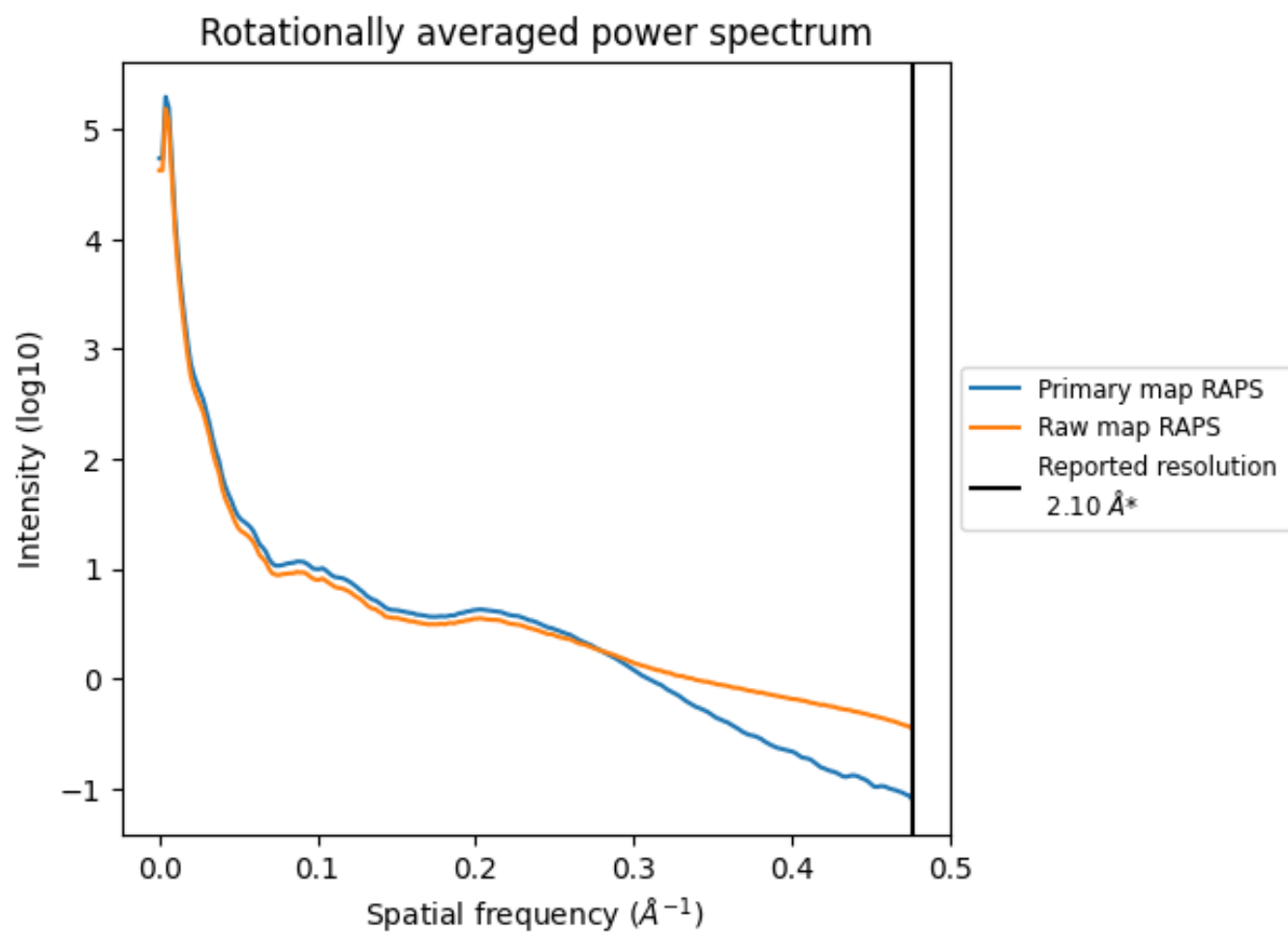
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 229 nm<sup>3</sup>; this corresponds to an approximate mass of 207 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 ⓘ

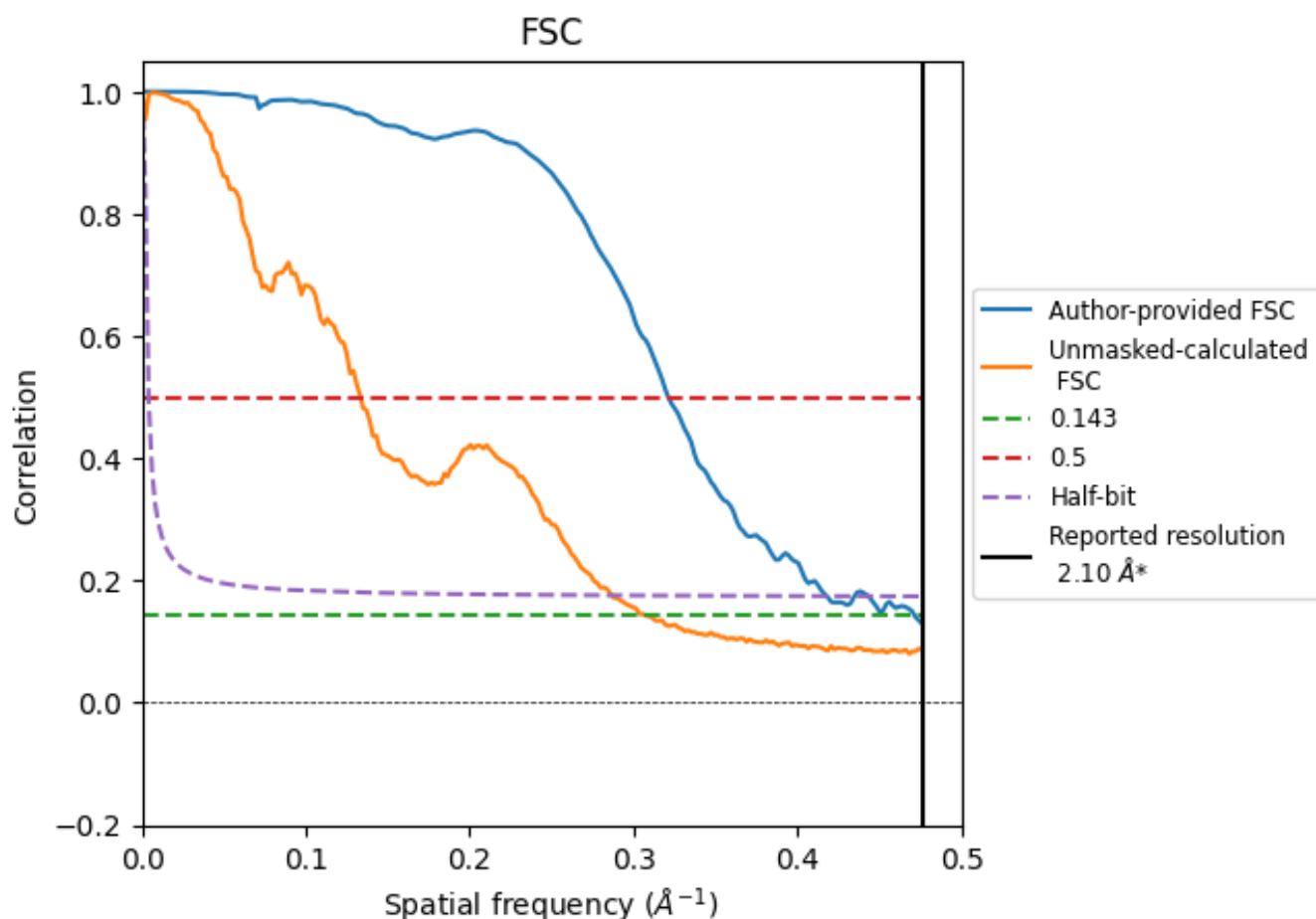


\*Reported resolution corresponds to spatial frequency of 0.476 Å<sup>-1</sup>

## 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 0.476 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

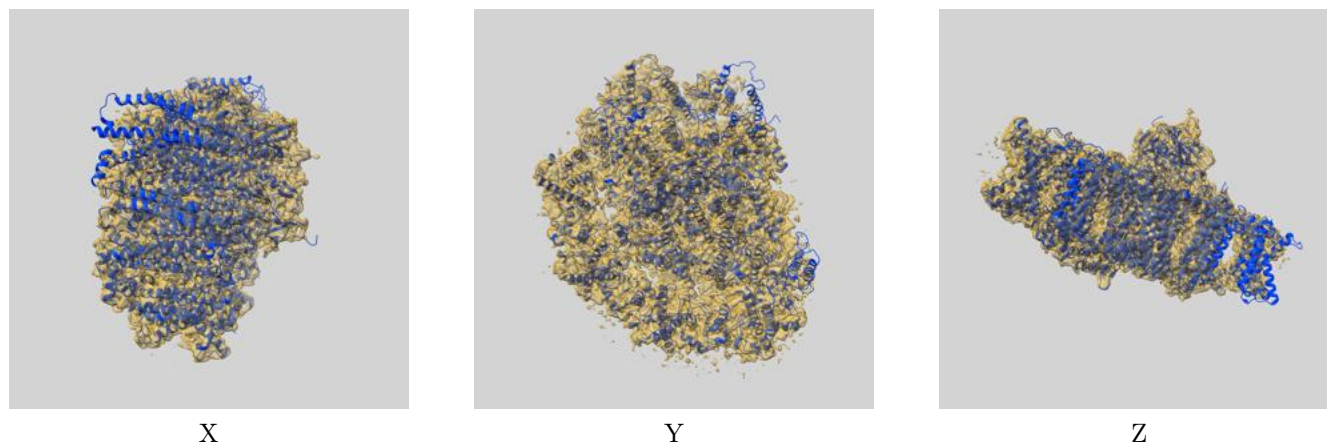
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.10	-	-
Author-provided FSC curve	2.12	3.11	2.39
Unmasked-calculated*	3.26	7.50	3.49

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.26 differs from the reported value 2.1 by more than 10 %

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-48266 and PDB model 9MH1. Per-residue inclusion information can be found in section [3](#) on page [32](#).

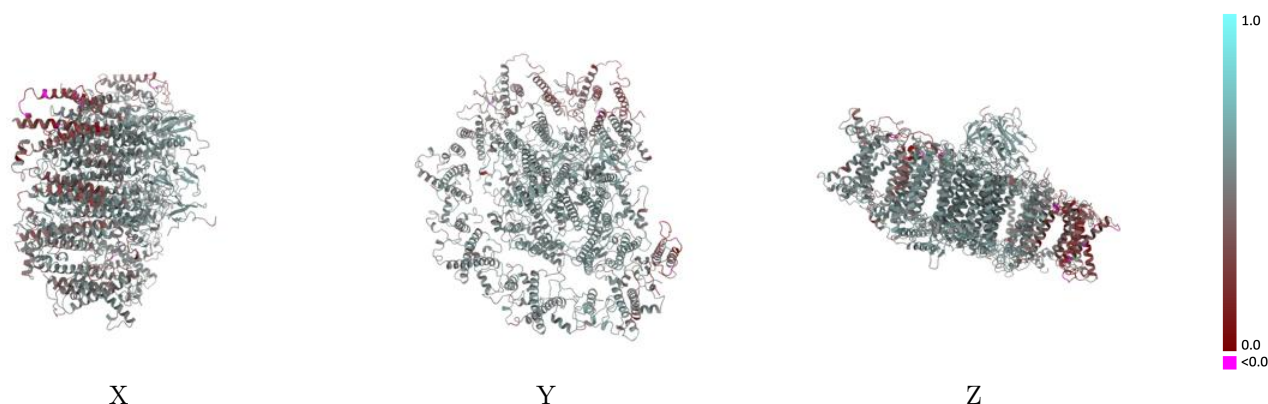
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0172 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

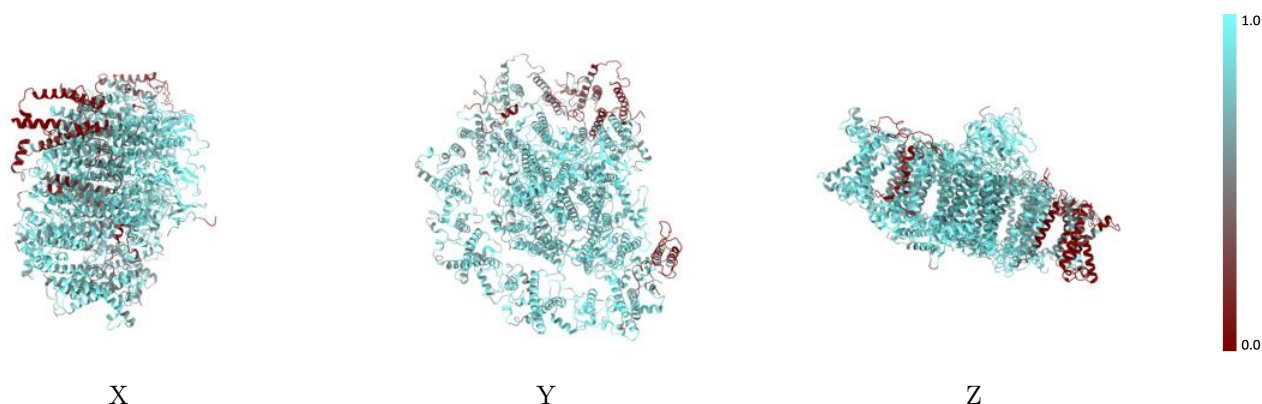


## 9.2 Q-score mapped to coordinate model [i](#)



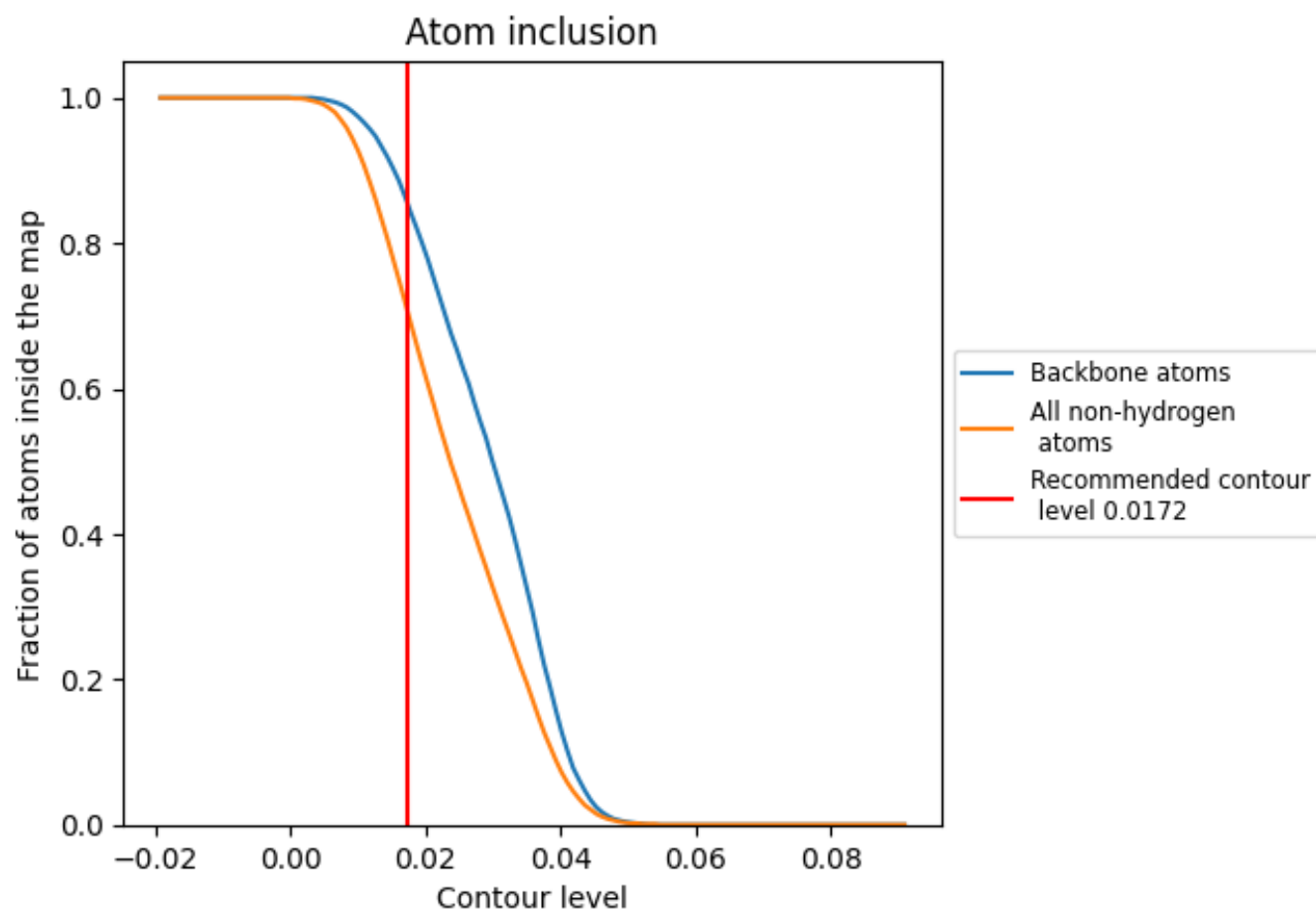
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0172).







































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 71% 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 (0.0172) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7100	 0.4980
1	 0.7310	 0.4860
2	 0.2090	 0.2700
3	 0.7210	 0.5040
7	 0.7580	 0.5100
8	 0.7130	 0.4890
9	 0.5830	 0.4050
A	 0.8190	 0.5560
B	 0.8060	 0.5480
C	 0.9350	 0.5560
D	 0.8560	 0.5350
E	 0.7870	 0.5370
F	 0.7380	 0.5230
G	 0.5650	 0.4550
H	 0.0980	 0.2690
I	 0.7050	 0.4850
J	 0.7390	 0.5190
K	 0.2050	 0.3020
L	 0.6460	 0.4800

