



wwPDB EM Validation Summary Report ⓘ

Jan 1, 2025 – 04:07 PM EST

PDB ID : 8WEY
EMDB ID : EMD-37480
Title : PSI-LHCI of the red alga *Cyanidium caldarium* RK-1 (NIES-2137)
Authors : Kato, K.; Hamaguchi, T.; Nakajima, Y.; Kawakami, K.; Yonekura, K.; Shen, J.R.; Nagao, R.
Deposited on : 2023-09-19
Resolution : 1.92 Å(reported)
Based on initial model : .

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
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) : 2.40

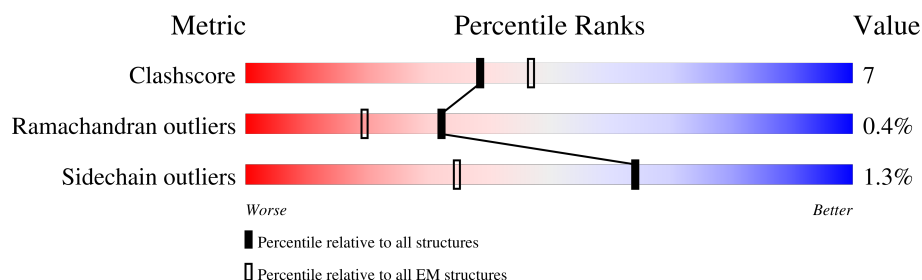
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 1.92 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 ≥ 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	A	748	
2	B	732	
3	C	81	
4	D	139	
5	E	61	
6	F	178	
7	I	32	
8	J	38	

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Mol	Chain	Length	Quality of chain
9	K	68	
10	L	141	
11	M	28	
12	O	155	
13	1	214	
13	4	214	
14	2	222	
14	5	222	
15	3	219	

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
16	CL0	A	801	X	-	-	-
17	CLA	1	301	X	-	-	-
17	CLA	1	302	X	-	-	-
17	CLA	1	304	X	-	-	-
17	CLA	1	305	X	-	-	-
17	CLA	1	306	X	-	-	-
17	CLA	1	307	X	-	-	-
17	CLA	1	308	X	-	-	-
17	CLA	1	309	X	-	-	-
17	CLA	1	310	X	-	-	-
17	CLA	1	311	X	-	-	-
17	CLA	2	304	X	-	-	-
17	CLA	2	305	X	-	-	-
17	CLA	2	306	X	-	-	-
17	CLA	2	308	X	-	-	-
17	CLA	2	309	X	-	-	-
17	CLA	2	310	X	-	-	-
17	CLA	2	311	X	-	-	-
17	CLA	2	312	X	-	-	-
17	CLA	2	313	X	-	-	-
17	CLA	2	314	X	-	-	-
17	CLA	2	315	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	2	316	X	-	-	-
17	CLA	3	305	X	-	-	-
17	CLA	3	306	X	-	-	-
17	CLA	3	307	X	-	-	-
17	CLA	3	308	X	-	-	-
17	CLA	3	309	X	-	-	-
17	CLA	3	310	X	-	-	-
17	CLA	3	311	X	-	-	-
17	CLA	3	312	X	-	-	-
17	CLA	3	313	X	-	-	-
17	CLA	3	314	X	-	-	-
17	CLA	3	315	X	-	-	-
17	CLA	4	303	X	-	-	-
17	CLA	4	304	X	-	-	-
17	CLA	4	305	X	-	-	-
17	CLA	4	306	X	-	-	-
17	CLA	4	307	X	-	-	-
17	CLA	4	308	X	-	-	-
17	CLA	4	309	X	-	-	-
17	CLA	4	310	X	-	-	-
17	CLA	4	311	X	-	-	-
17	CLA	5	302	X	-	-	-
17	CLA	5	303	X	-	-	-
17	CLA	5	304	X	-	-	-
17	CLA	5	305	X	-	-	-
17	CLA	5	306	X	-	-	-
17	CLA	5	307	X	-	-	-
17	CLA	5	308	X	-	-	-
17	CLA	5	309	X	-	-	-
17	CLA	5	310	X	-	-	-
17	CLA	5	311	X	-	-	-
17	CLA	5	312	X	-	-	-
17	CLA	5	313	X	-	-	-
17	CLA	5	314	X	-	-	-
17	CLA	A	802	X	-	-	-
17	CLA	A	803	X	-	-	-
17	CLA	A	804	X	-	-	-
17	CLA	A	805	X	-	-	-
17	CLA	A	806	X	-	-	-
17	CLA	A	808	X	-	-	-
17	CLA	A	809	X	-	-	-
17	CLA	A	811	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	A	812	X	-	-	-
17	CLA	A	813	X	-	-	-
17	CLA	A	816	X	-	-	-
17	CLA	A	817	X	-	-	-
17	CLA	A	818	X	-	-	-
17	CLA	A	819	X	-	-	-
17	CLA	A	821	X	-	-	-
17	CLA	A	822	X	-	-	-
17	CLA	A	823	X	-	-	-
17	CLA	A	824	X	-	-	-
17	CLA	A	825	X	-	-	-
17	CLA	A	826	X	-	-	-
17	CLA	A	827	X	-	-	-
17	CLA	A	828	X	-	-	-
17	CLA	A	829	X	-	-	-
17	CLA	A	830	X	-	-	-
17	CLA	A	831	X	-	-	-
17	CLA	A	832	X	-	-	-
17	CLA	A	833	X	-	-	-
17	CLA	A	834	X	-	-	-
17	CLA	A	835	X	-	-	-
17	CLA	A	836	X	-	-	-
17	CLA	A	837	X	-	-	-
17	CLA	A	838	X	-	-	-
17	CLA	A	839	X	-	-	-
17	CLA	A	852	X	-	-	-
17	CLA	A	853	X	-	-	-
17	CLA	A	854	X	-	-	-
17	CLA	A	855	X	-	-	-
17	CLA	A	856	X	-	-	-
17	CLA	A	859	X	-	-	-
17	CLA	B	801	X	-	-	-
17	CLA	B	802	X	-	-	-
17	CLA	B	804	X	-	-	-
17	CLA	B	805	X	-	-	-
17	CLA	B	806	X	-	-	-
17	CLA	B	807	X	-	-	-
17	CLA	B	808	X	-	-	-
17	CLA	B	809	X	-	-	-
17	CLA	B	810	X	-	-	-
17	CLA	B	811	X	-	-	-
17	CLA	B	812	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	B	813	X	-	-	-
17	CLA	B	814	X	-	-	-
17	CLA	B	815	X	-	-	-
17	CLA	B	816	X	-	-	-
17	CLA	B	818	X	-	-	-
17	CLA	B	819	X	-	-	-
17	CLA	B	820	X	-	-	-
17	CLA	B	821	X	-	-	-
17	CLA	B	823	X	-	-	-
17	CLA	B	824	X	-	-	-
17	CLA	B	825	X	-	-	-
17	CLA	B	826	X	-	-	-
17	CLA	B	827	X	-	-	-
17	CLA	B	828	X	-	-	-
17	CLA	B	829	X	-	-	-
17	CLA	B	830	X	-	-	-
17	CLA	B	832	X	-	-	-
17	CLA	B	833	X	-	-	-
17	CLA	B	834	X	-	-	-
17	CLA	B	835	X	-	-	-
17	CLA	B	836	X	-	-	-
17	CLA	B	837	X	-	-	-
17	CLA	B	838	X	-	-	-
17	CLA	B	839	X	-	-	-
17	CLA	B	840	X	-	-	-
17	CLA	B	841	X	-	-	-
17	CLA	F	203	X	-	-	-
17	CLA	F	204	X	-	-	-
17	CLA	J	103	X	-	-	-
17	CLA	K	103	X	-	-	-
17	CLA	L	202	X	-	-	-
17	CLA	L	203	X	-	-	-
17	CLA	L	204	X	-	-	-
17	CLA	O	203	X	-	-	-
17	CLA	O	204	X	-	-	-
17	CLA	O	205	X	-	-	-
25	5X6	1	312	-	X	-	-
25	5X6	1	313	-	X	-	-
25	5X6	1	314	-	X	-	-
25	5X6	1	315	-	X	-	-
25	5X6	1	316	-	X	-	-
25	5X6	2	317	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	5X6	2	318	-	X	-	-
25	5X6	2	319	-	X	-	-
25	5X6	2	320	-	X	-	-
25	5X6	2	321	-	X	-	-
25	5X6	3	316	-	X	-	-
25	5X6	3	317	-	X	-	-
25	5X6	3	318	-	X	-	-
25	5X6	4	312	-	X	-	-
25	5X6	4	313	-	X	-	-
25	5X6	4	314	-	X	-	-
25	5X6	5	301	-	X	-	-
25	5X6	5	315	-	X	-	-
25	5X6	5	316	-	X	-	-
25	5X6	5	317	-	X	-	-
25	5X6	5	318	-	X	-	-
25	5X6	F	205	-	X	-	-
25	5X6	J	105	-	X	-	-

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 36163 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 Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	741	Total	C	N	O	S	0	0
			5794	3784	996	987	27		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	730	Total	C	N	O	S	0	0
			5818	3829	981	990	18		

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			598	367	104	115	12		

- Molecule 4 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	117	Total	C	N	O	S	0	0
			938	594	165	176	3		

- Molecule 5 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	61	Total	C	N	O	S	0	0
			491	321	77	92	1		

- Molecule 6 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	158	Total	C	N	O	S	0	0
			1296	829	225	238	4		

- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	32	Total	C	N	O	S	0	0
			238	163	33	40	2		

- Molecule 8 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	38	Total	C	N	O	S	0	0
			313	214	46	52	1		

- Molecule 9 is a protein called Photosystem I reaction center subunit X.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	63	Total	C	N	O	S	0	0
			454	294	75	83	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	121	Total	C	N	O	S	0	0
			923	610	146	164	3		

- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	28	Total	C	N	O	S	0	0
			208	138	32	35	3		

- Molecule 12 is a protein called Photosystem I subunit O.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	O	83	Total	C	N	O	0	0
			634	432	97	105		

- Molecule 13 is a protein called Lhcr1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1	172	Total	C	N	O	S	0	0
			1365	892	228	235	10		
13	4	172	Total	C	N	O	S	0	0
			1365	892	228	235	10		

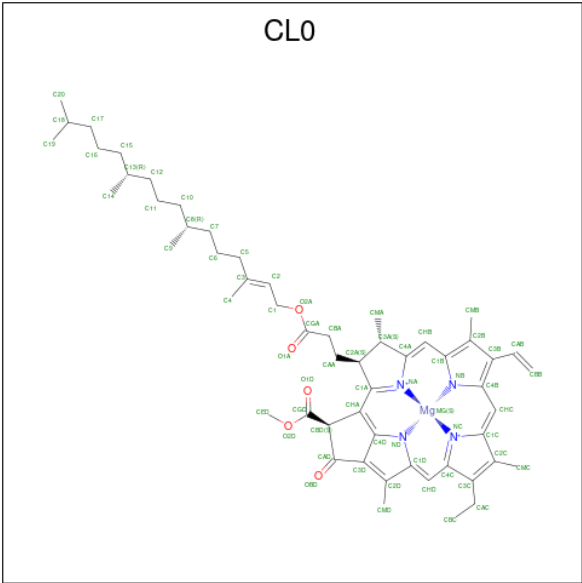
- Molecule 14 is a protein called Lhcr2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	2	183	Total	C	N	O	S	0	0
			1428	926	243	250	9		
14	5	183	Total	C	N	O	S	0	0
			1428	926	243	250	9		

- Molecule 15 is a protein called Lhcr3.

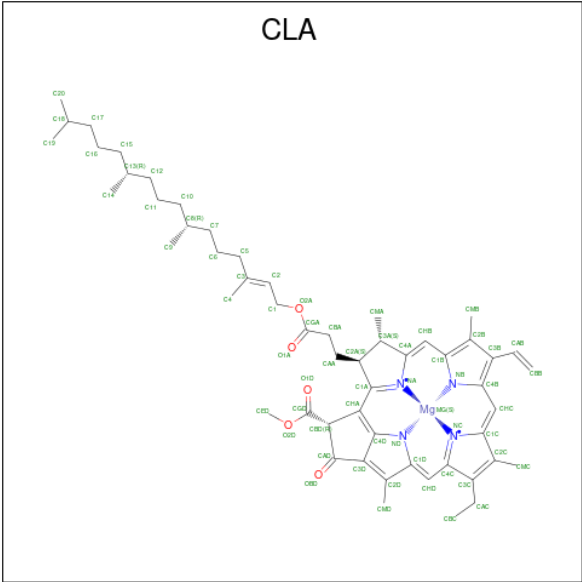
Mol	Chain	Residues	Atoms					AltConf	Trace
15	3	151	Total	C	N	O	S	0	0
			1169	759	198	206	6		

- Molecule 16 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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

- Molecule 17 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
17	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
17	A	1	Total 56	C 46	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 61	C 51	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
17	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
17	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
17	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
17	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	F	1	Total 41	C 33	Mg 1	N 4	O 3	0
17	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	K	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	K	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	L	1	Total 57	C 47	Mg 1	N 4	O 5	0
17	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	O	1	Total 41	C 33	Mg 1	N 4	O 3	0
17	O	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	1	1	Total 59	C 49	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
17	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	1	1	Total 41	C 33	Mg 1	N 4	O 3	0
17	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
17	2	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	2	1	Total 45	C 35	Mg 1	N 4	O 5	0

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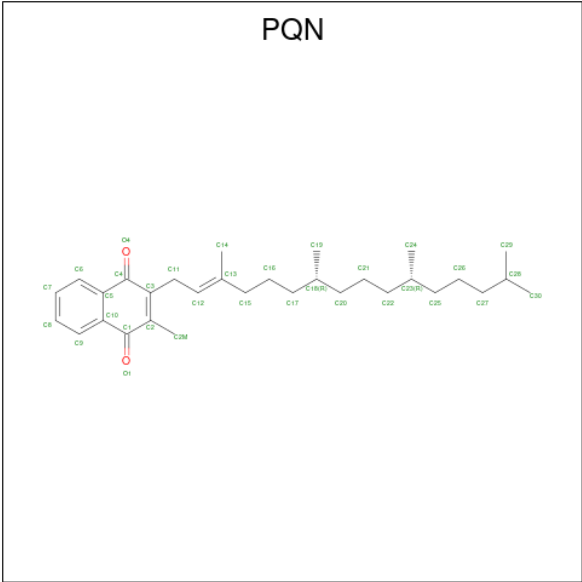
Mol	Chain	Residues	Atoms					AltConf
17	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	3	1	Total 63	C 53	Mg 1	N 4	O 5	0
17	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	3	1	Total 52	C 42	Mg 1	N 4	O 5	0
17	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
17	3	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	3	1	Total 51	C 41	Mg 1	N 4	O 5	0
17	4	1	Total 48	C 38	Mg 1	N 4	O 5	0
17	4	1	Total 59	C 49	Mg 1	N 4	O 5	0
17	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
17	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	4	1	Total 45	C 35	Mg 1	N 4	O 5	0

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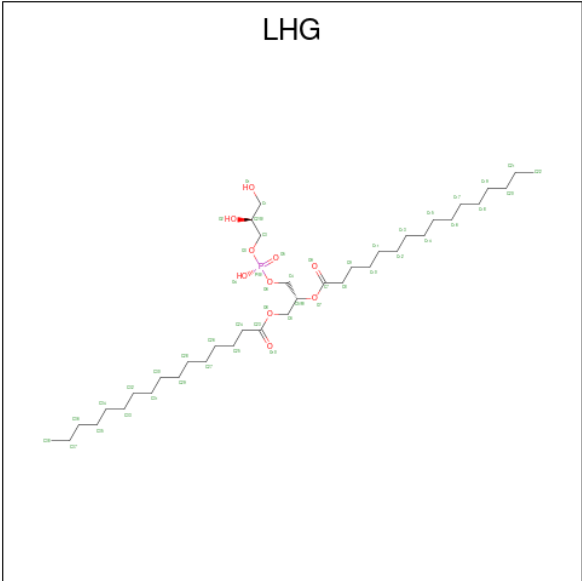
Mol	Chain	Residues	Atoms					AltConf
17	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			44	36	1	4	3	

- Molecule 18 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



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

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



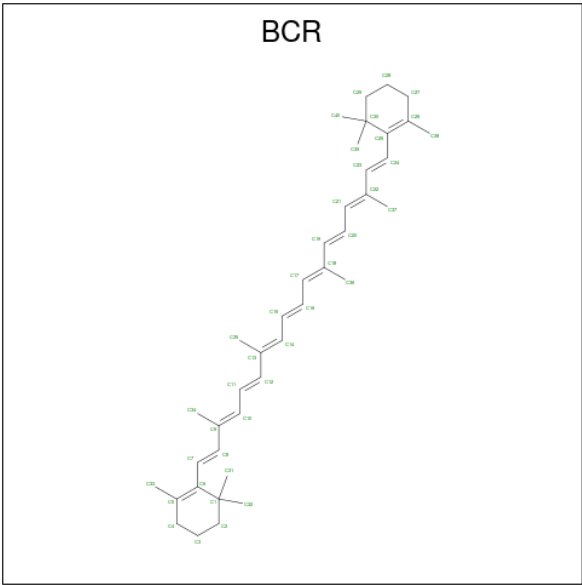
Mol	Chain	Residues	Atoms				AltConf
19	A	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
19	A	1	Total	C	O	P	0
			40	29	10	1	
19	J	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 20 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



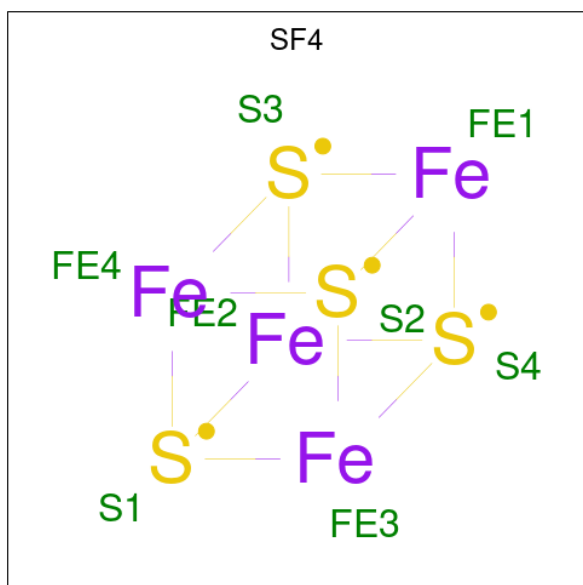
Mol	Chain	Residues	Atoms		AltConf
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	B	1	Total	C	0
			40	40	
20	B	1	Total	C	0
			40	40	
20	B	1	Total	C	0
			40	40	
20	B	1	Total	C	0
			40	40	

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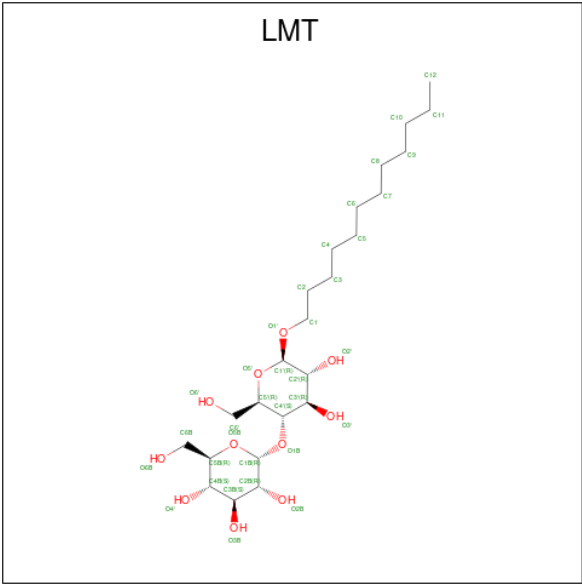
Mol	Chain	Residues	Atoms	AltConf
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	I	1	Total C 40 40	0
20	J	1	Total C 40 40	0
20	K	1	Total C 40 40	0
20	L	1	Total C 40 40	0
20	L	1	Total C 40 40	0
20	L	1	Total C 40 40	0
20	M	1	Total C 40 40	0
20	O	1	Total C 40 40	0

- Molecule 21 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 22 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).

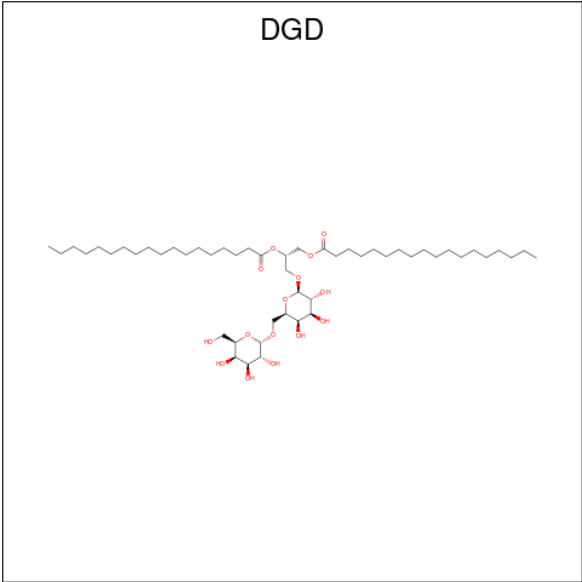


Mol	Chain	Residues	Atoms			AltConf
22	A	1	Total	C	O	0
			35	24	11	
22	B	1	Total	C	O	0
			35	24	11	
22	B	1	Total	C	O	0
			35	24	11	
22	B	1	Total	C	O	0
			35	24	11	
22	F	1	Total	C	O	0
			35	24	11	
22	L	1	Total	C	O	0
			35	24	11	
22	3	1	Total	C	O	0
			35	24	11	

- Molecule 23 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

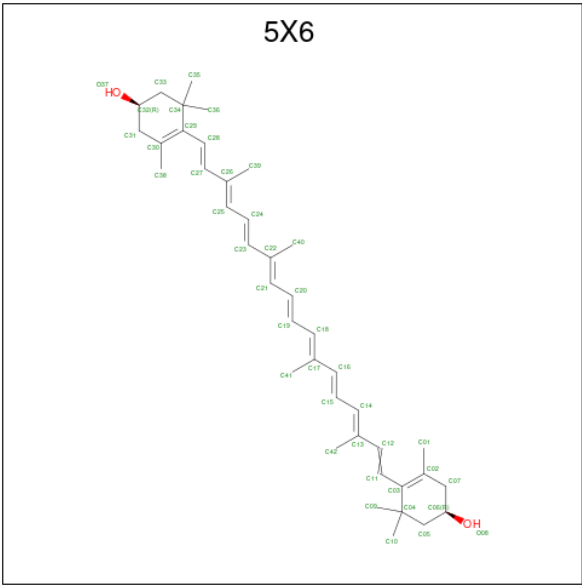
Mol	Chain	Residues	Atoms		AltConf
23	A	4	Total 48	C 48	0
23	B	5	Total 54	C 54	0
23	F	1	Total 9	C 9	0
23	I	1	Total 12	C 12	0
23	J	1	Total 13	C 13	0
23	K	1	Total 13	C 13	0
23	L	1	Total 13	C 13	0
23	O	1	Total 6	C 6	0
23	1	1	Total 8	C 8	0
23	2	3	Total 32	C 32	0
23	3	3	Total 37	C 37	0
23	4	2	Total 24	C 24	0
23	5	1	Total 8	C 8	0

- Molecule 24 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
24	B	1	Total	C	O	0
			66	51	15	

- Molecule 25 is Zeaxanthin (three-letter code: 5X6) (formula: C₄₀H₅₆O₂).



Mol	Chain	Residues	Atoms			AltConf
25	F	1	Total	C	O	0
			42	40	2	
25	J	1	Total	C	O	0
			42	40	2	
25	1	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
25	1	1	Total	C	O	0
			42	40	2	
25	1	1	Total	C	O	0
			42	40	2	
25	1	1	Total	C	O	0
			42	40	2	
25	1	1	Total	C	O	0
			42	40	2	
25	2	1	Total	C	O	0
			42	40	2	
25	2	1	Total	C	O	0
			42	40	2	
25	2	1	Total	C	O	0
			42	40	2	
25	2	1	Total	C	O	0
			42	40	2	
25	2	1	Total	C	O	0
			42	40	2	
25	3	1	Total	C	O	0
			42	40	2	
25	3	1	Total	C	O	0
			42	40	2	
25	3	1	Total	C	O	0
			42	40	2	
25	4	1	Total	C	O	0
			42	40	2	
25	4	1	Total	C	O	0
			42	40	2	
25	4	1	Total	C	O	0
			42	40	2	
25	5	1	Total	C	O	0
			42	40	2	
25	5	1	Total	C	O	0
			42	40	2	
25	5	1	Total	C	O	0
			42	40	2	
25	5	1	Total	C	O	0
			42	40	2	
25	5	1	Total	C	O	0
			42	40	2	

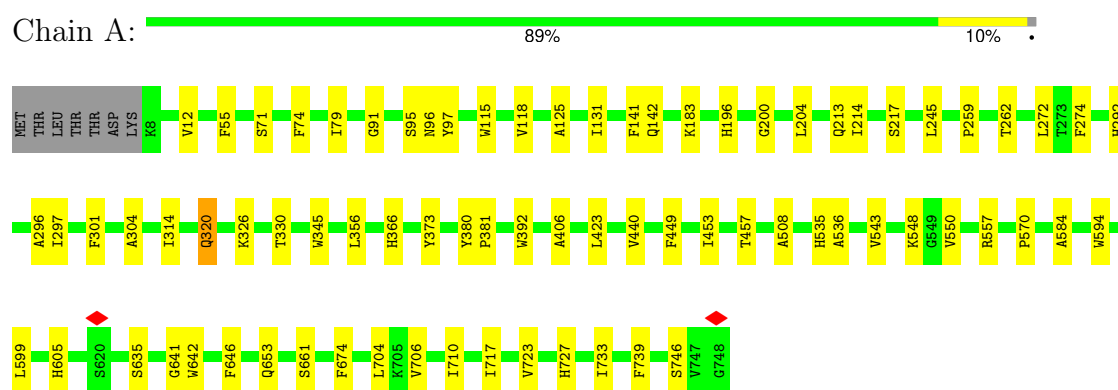
- Molecule 26 is water.

Mol	Chain	Residues	Atoms		AltConf
26	A	203	Total 203	O 203	0
26	B	220	Total 220	O 220	0
26	C	41	Total 41	O 41	0
26	D	18	Total 18	O 18	0
26	E	23	Total 23	O 23	0
26	F	22	Total 22	O 22	0
26	I	2	Total 2	O 2	0
26	J	7	Total 7	O 7	0
26	K	2	Total 2	O 2	0
26	L	7	Total 7	O 7	0
26	M	2	Total 2	O 2	0
26	1	3	Total 3	O 3	0
26	3	1	Total 1	O 1	0
26	4	3	Total 3	O 3	0
26	5	6	Total 6	O 6	0

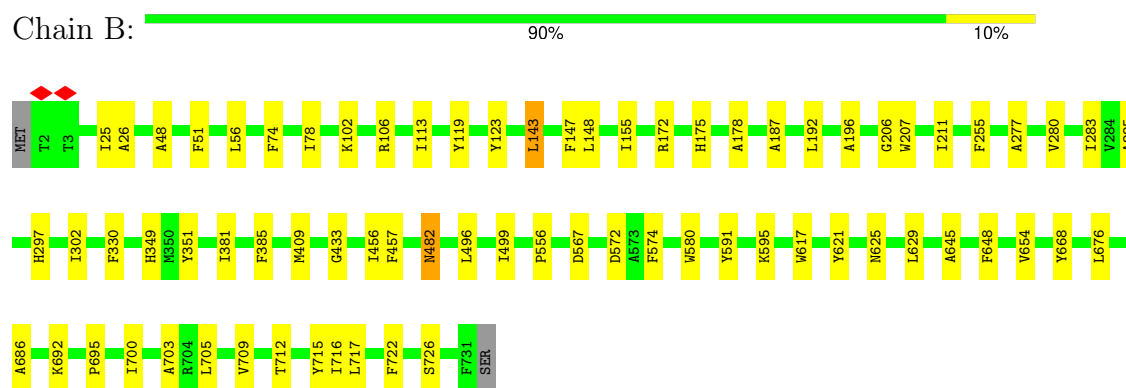
3 Residue-property plots

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

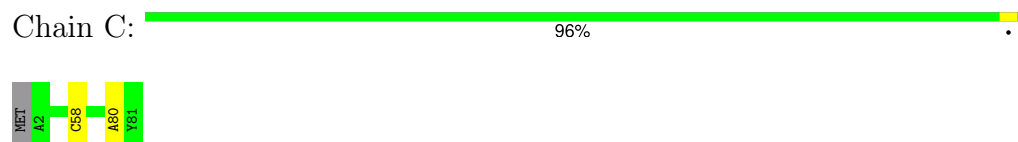
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



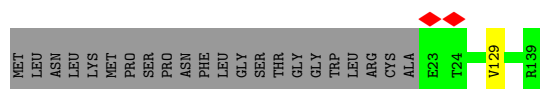
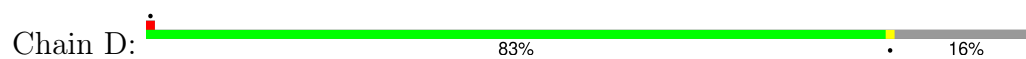
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



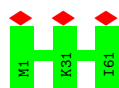
- Molecule 3: Photosystem I iron-sulfur center



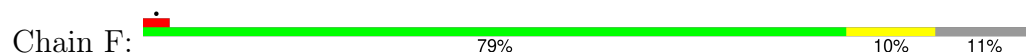
- Molecule 4: Photosystem I reaction center subunit II



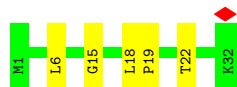
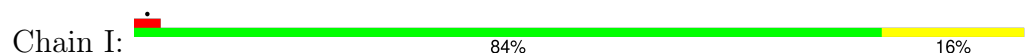
- Molecule 5: Photosystem I reaction center subunit IV



- Molecule 6: Photosystem I reaction center subunit III



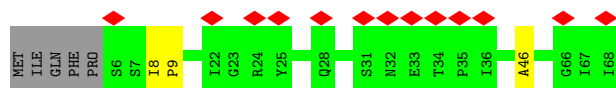
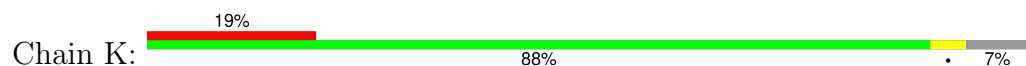
- Molecule 7: Photosystem I reaction center subunit VIII



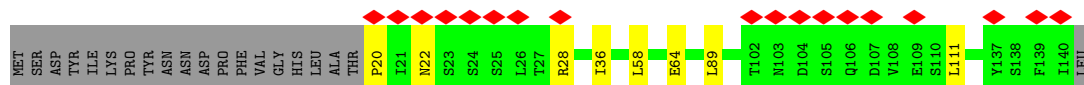
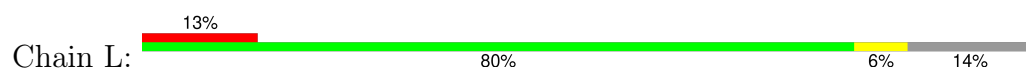
- Molecule 8: Photosystem I reaction center subunit IX

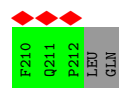


- Molecule 9: Photosystem I reaction center subunit X

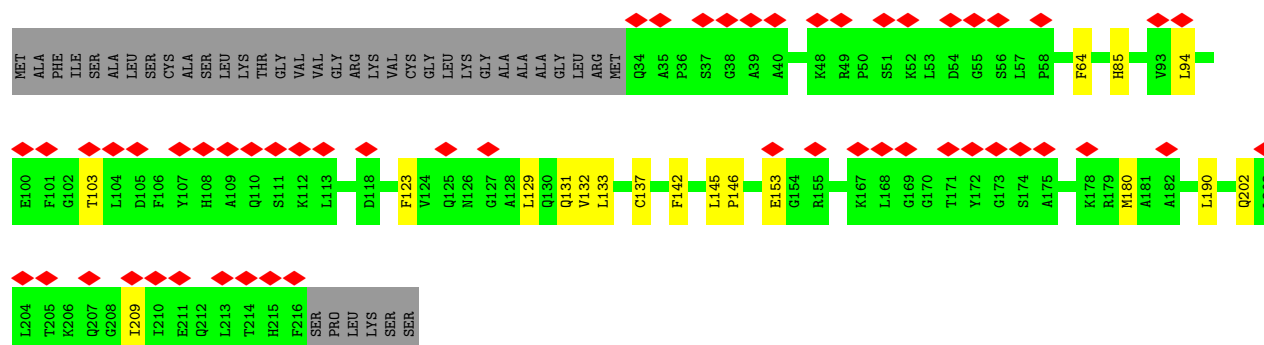
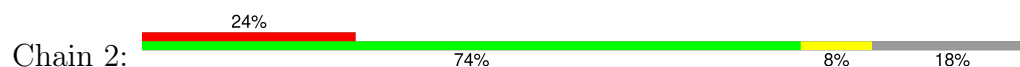


- Molecule 10: Photosystem I reaction center subunit XI

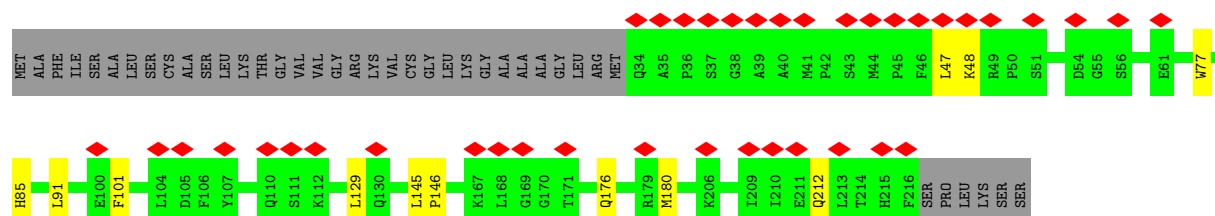
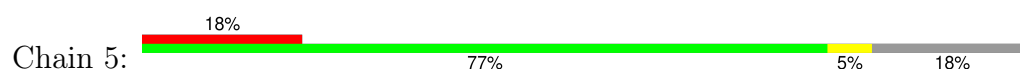




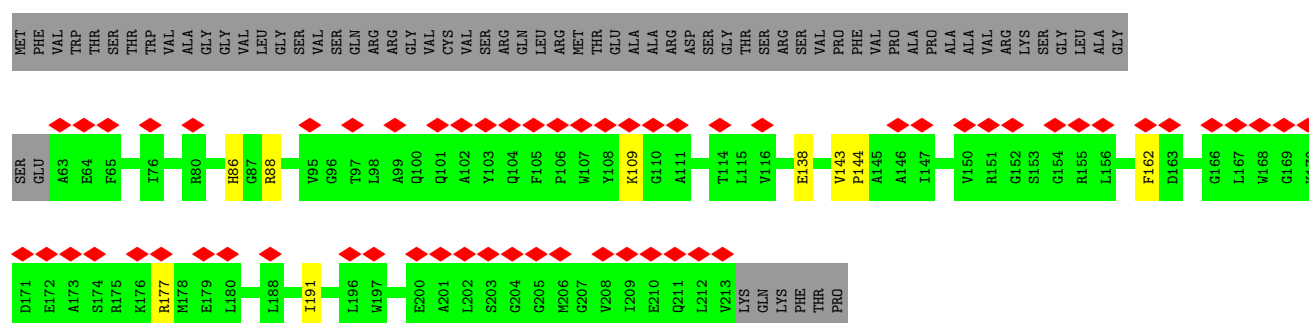
• Molecule 14: Lhcr2



• Molecule 14: Lhcr2



• Molecule 15: Lhcr3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	228449	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	39.8	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.289	Depositor
Minimum map value	-0.106	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	202.752, 202.752, 202.752	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.792, 0.792, 0.792	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL0, LHG, SF4, DGD, BCR, 5X6, CLA, UNL, LMT, PQN

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	A	0.60	0/5979	0.73	0/8148
2	B	0.59	0/6027	0.73	0/8236
3	C	0.61	0/608	0.76	0/822
4	D	0.61	0/957	0.77	0/1292
5	E	0.65	0/500	0.75	0/676
6	F	0.62	0/1329	0.73	0/1799
7	I	0.66	0/243	0.71	0/332
8	J	0.60	0/322	0.65	0/439
9	K	0.70	0/459	0.75	0/627
10	L	0.66	0/945	0.75	0/1281
11	M	0.67	0/209	0.70	0/283
12	O	0.68	0/656	0.74	0/903
13	1	0.66	0/1407	0.76	0/1903
13	4	0.67	0/1407	0.77	0/1903
14	2	0.66	0/1467	0.74	0/1980
14	5	0.66	0/1467	0.74	0/1980
15	3	0.68	0/1199	0.74	0/1627
All	All	0.63	0/25181	0.74	0/34231

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
12	O	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	O	88	ILE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5794	0	5722	66	0
2	B	5818	0	5649	69	0
3	C	598	0	576	2	0
4	D	938	0	933	0	0
5	E	491	0	509	0	0
6	F	1296	0	1263	14	0
7	I	238	0	265	6	0
8	J	313	0	327	1	0
9	K	454	0	490	2	0
10	L	923	0	939	4	0
11	M	208	0	230	5	0
12	O	634	0	644	3	0
13	1	1365	0	1351	12	0
13	4	1365	0	1351	10	0
14	2	1428	0	1406	22	0
14	5	1428	0	1406	9	0
15	3	1169	0	1172	8	0
16	A	65	0	72	3	0
17	1	540	0	442	21	0
17	2	618	0	494	35	0
17	3	530	0	423	15	0
17	4	418	0	321	17	0
17	5	680	0	619	30	0
17	A	2664	0	2743	116	0
17	B	2513	0	2633	137	0
17	F	86	0	62	6	0
17	J	42	0	31	1	0
17	K	97	0	80	3	0
17	L	172	0	164	8	0
17	O	136	0	101	4	0
18	A	33	0	46	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	B	33	0	46	3	0
19	A	89	0	127	1	0
19	J	49	0	74	1	0
20	A	200	0	280	13	0
20	B	280	0	392	10	0
20	I	40	0	56	1	0
20	J	40	0	56	3	0
20	K	40	0	56	1	0
20	L	120	0	168	4	0
20	M	40	0	56	4	0
20	O	40	0	56	0	0
21	A	8	0	0	0	0
21	C	16	0	0	1	0
22	3	35	0	46	0	0
22	A	35	0	46	0	0
22	B	105	0	138	0	0
22	F	35	0	46	0	0
22	L	35	0	46	0	0
23	1	8	0	0	0	0
23	2	32	0	0	0	0
23	3	37	0	0	0	0
23	4	24	0	0	0	0
23	5	8	0	0	0	0
23	A	48	0	0	0	0
23	B	54	0	0	0	0
23	F	9	0	0	0	0
23	I	12	0	0	0	0
23	J	13	0	0	0	0
23	K	13	0	0	0	0
23	L	13	0	0	0	0
23	O	6	0	0	0	0
24	B	66	0	96	3	0
25	1	210	0	0	2	0
25	2	210	0	0	1	0
25	3	126	0	0	2	0
25	4	126	0	0	1	0
25	5	210	0	0	2	0
25	F	42	0	0	0	0
25	J	42	0	0	0	0
26	1	3	0	0	0	0
26	3	1	0	0	0	0
26	4	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	5	6	0	0	0	0
26	A	203	0	0	1	0
26	B	220	0	0	1	0
26	C	41	0	0	0	0
26	D	18	0	0	0	0
26	E	23	0	0	0	0
26	F	22	0	0	0	0
26	I	2	0	0	0	0
26	J	7	0	0	0	0
26	K	2	0	0	0	0
26	L	7	0	0	0	0
26	M	2	0	0	0	0
All	All	36163	0	34249	495	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 7.

The worst 5 of 495 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:LEU:HD21	17:B:807:CLA:HMD2	1.56	0.84
14:2:190:LEU:HD21	17:2:313:CLA:HBC3	1.66	0.77
17:A:834:CLA:HMB1	20:A:845:BCR:H281	1.67	0.77
17:A:859:CLA:HMC1	17:A:859:CLA:HBC2	1.65	0.76
17:B:836:CLA:HBB1	17:B:836:CLA:HMB1	1.68	0.74

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	A	739/748 (99%)	716 (97%)	22 (3%)	1 (0%)	48	40
2	B	728/732 (100%)	712 (98%)	16 (2%)	0	100	100
3	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
4	D	115/139 (83%)	112 (97%)	3 (3%)	0	100	100
5	E	59/61 (97%)	55 (93%)	4 (7%)	0	100	100
6	F	156/178 (88%)	153 (98%)	2 (1%)	1 (1%)	22	10
7	I	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
8	J	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
9	K	61/68 (90%)	58 (95%)	3 (5%)	0	100	100
10	L	119/141 (84%)	113 (95%)	5 (4%)	1 (1%)	16	6
11	M	26/28 (93%)	26 (100%)	0	0	100	100
12	O	81/155 (52%)	70 (86%)	7 (9%)	4 (5%)	2	0
13	1	170/214 (79%)	149 (88%)	19 (11%)	2 (1%)	11	3
13	4	170/214 (79%)	150 (88%)	17 (10%)	3 (2%)	7	1
14	2	181/222 (82%)	171 (94%)	10 (6%)	0	100	100
14	5	181/222 (82%)	171 (94%)	10 (6%)	0	100	100
15	3	149/219 (68%)	137 (92%)	11 (7%)	1 (1%)	19	9
All	All	3079/3492 (88%)	2933 (95%)	133 (4%)	13 (0%)	32	19

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	1	99	THR
12	O	88	ILE
1	A	508	ALA
6	F	53	ALA
10	L	22	ASN

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	A	601/608 (99%)	597 (99%)	4 (1%)	81	77
2	B	596/598 (100%)	588 (99%)	8 (1%)	65	55
3	C	66/67 (98%)	66 (100%)	0	100	100
4	D	98/116 (84%)	97 (99%)	1 (1%)	73	67
5	E	57/57 (100%)	57 (100%)	0	100	100
6	F	136/153 (89%)	134 (98%)	2 (2%)	60	49
7	I	27/27 (100%)	27 (100%)	0	100	100
8	J	34/34 (100%)	34 (100%)	0	100	100
9	K	51/56 (91%)	51 (100%)	0	100	100
10	L	96/114 (84%)	93 (97%)	3 (3%)	35	18
11	M	22/22 (100%)	20 (91%)	2 (9%)	7	1
12	O	63/118 (53%)	61 (97%)	2 (3%)	34	17
13	1	143/178 (80%)	141 (99%)	2 (1%)	62	51
13	4	143/178 (80%)	138 (96%)	5 (4%)	31	15
14	2	146/174 (84%)	145 (99%)	1 (1%)	81	77
14	5	146/174 (84%)	142 (97%)	4 (3%)	40	24
15	3	117/171 (68%)	117 (100%)	0	100	100
All	All	2542/2845 (89%)	2508 (99%)	34 (1%)	64	55

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	4	184	LEU
13	4	209	ASN
14	5	176	GLN
4	D	129	VAL
2	B	692	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	482	ASN
6	F	134	GLN
13	4	194	HIS
14	2	131	GLN
14	2	212	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 238 ligands modelled in this entry, 25 are unknown - leaving 213 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
17	CLA	B	805	-	63,73,73	1.93	15 (23%)	74,113,113	4.19	35 (47%)
17	CLA	3	314	-	44,54,73	2.55	16 (36%)	51,90,113	3.05	25 (49%)
17	CLA	4	307	13	43,53,73	2.53	16 (37%)	50,89,113	3.01	26 (52%)
17	CLA	B	809	-	63,73,73	1.79	16 (25%)	74,113,113	2.79	30 (40%)
17	CLA	A	819	26	63,73,73	1.93	13 (20%)	74,113,113	2.55	26 (35%)
17	CLA	A	806	1	63,73,73	1.81	15 (23%)	74,113,113	2.68	25 (33%)
17	CLA	5	303	14	63,73,73	2.13	16 (25%)	74,113,113	2.67	31 (41%)
25	5X6	4	312	-	43,43,43	4.70	23 (53%)	56,60,60	4.55	28 (50%)
20	BCR	L	201	-	41,41,41	1.30	6 (14%)	56,56,56	1.47	8 (14%)
17	CLA	F	203	26	43,53,73	2.34	16 (37%)	50,89,113	2.94	23 (46%)
25	5X6	4	314	-	43,43,43	4.75	24 (55%)	56,60,60	4.66	32 (57%)
17	CLA	5	307	-	43,53,73	2.39	16 (37%)	50,89,113	3.15	25 (50%)
17	CLA	B	812	-	63,73,73	1.98	15 (23%)	74,113,113	2.48	28 (37%)
17	CLA	B	825	26	63,73,73	1.91	17 (26%)	74,113,113	2.63	25 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	839	26	63,73,73	1.92	16 (25%)	74,113,113	2.70	25 (33%)
17	CLA	B	814	-	63,73,73	1.93	16 (25%)	74,113,113	2.61	25 (33%)
21	SF4	C	102	3	0,12,12	-	-	-		
22	LMT	L	207	-	36,36,36	0.44	0	47,47,47	0.55	0
17	CLA	5	312	14	43,53,73	2.55	16 (37%)	50,89,113	3.04	22 (44%)
17	CLA	B	827	-	63,73,73	1.86	15 (23%)	74,113,113	2.62	30 (40%)
17	CLA	B	808	-	63,73,73	1.90	16 (25%)	74,113,113	2.80	24 (32%)
17	CLA	B	834	26	63,73,73	1.92	15 (23%)	74,113,113	2.61	29 (39%)
17	CLA	5	313	-	43,53,73	2.52	16 (37%)	50,89,113	2.97	26 (52%)
17	CLA	A	856	-	63,73,73	1.88	16 (25%)	74,113,113	2.65	26 (35%)
17	CLA	A	828	-	63,73,73	1.83	14 (22%)	74,113,113	2.74	26 (35%)
17	CLA	A	808	-	53,63,73	2.08	14 (26%)	62,101,113	2.77	28 (45%)
20	BCR	B	846	-	41,41,41	1.38	7 (17%)	56,56,56	1.62	11 (19%)
17	CLA	B	831	-	63,73,73	1.93	15 (23%)	74,113,113	2.62	30 (40%)
17	CLA	2	306	-	43,53,73	2.53	16 (37%)	50,89,113	3.02	25 (50%)
20	BCR	A	846	-	41,41,41	1.35	4 (9%)	56,56,56	1.24	8 (14%)
17	CLA	B	823	-	41,51,73	2.49	16 (39%)	47,86,113	3.14	23 (48%)
17	CLA	A	831	-	63,73,73	1.90	18 (28%)	74,113,113	2.61	26 (35%)
17	CLA	B	839	26	63,73,73	1.88	15 (23%)	74,113,113	2.64	21 (28%)
17	CLA	B	819	-	58,68,73	1.97	14 (24%)	68,107,113	2.90	30 (44%)
17	CLA	B	804	-	63,73,73	1.79	15 (23%)	74,113,113	2.59	26 (35%)
17	CLA	B	826	26	63,73,73	1.92	14 (22%)	74,113,113	2.65	28 (37%)
17	CLA	5	311	14	43,53,73	2.60	17 (39%)	50,89,113	3.06	22 (44%)
17	CLA	A	854	-	63,73,73	1.82	15 (23%)	74,113,113	2.69	25 (33%)
17	CLA	A	818	-	63,73,73	2.02	16 (25%)	74,113,113	2.65	31 (41%)
17	CLA	1	301	13	43,53,73	2.53	16 (37%)	50,89,113	2.90	21 (42%)
17	CLA	A	834	1	63,73,73	2.02	16 (25%)	74,113,113	2.61	29 (39%)
17	CLA	2	304	14	43,53,73	2.54	16 (37%)	50,89,113	3.17	26 (52%)
17	CLA	5	306	14	43,53,73	2.57	17 (39%)	50,89,113	3.04	24 (48%)
20	BCR	B	803	-	41,41,41	1.29	5 (12%)	56,56,56	1.60	10 (17%)
22	LMT	3	301	-	36,36,36	0.48	0	47,47,47	0.52	0
22	LMT	B	850	-	36,36,36	0.41	0	47,47,47	0.67	0
17	CLA	B	820	26	63,73,73	2.02	16 (25%)	74,113,113	2.45	27 (36%)
17	CLA	B	822	-	44,54,73	2.44	15 (34%)	51,90,113	3.16	24 (47%)
17	CLA	A	829	-	48,58,73	2.10	14 (29%)	56,95,113	2.87	30 (53%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	836	-	54,64,73	2.13	17 (31%)	63,102,113	2.81	28 (44%)
17	CLA	B	830	-	63,73,73	1.79	13 (20%)	74,113,113	2.81	29 (39%)
25	5X6	F	205	-	43,43,43	4.02	25 (58%)	56,60,60	5.59	32 (57%)
17	CLA	B	806	-	63,73,73	1.92	15 (23%)	74,113,113	2.71	27 (36%)
17	CLA	2	311	14	53,63,73	2.31	15 (28%)	62,101,113	2.97	25 (40%)
25	5X6	4	313	-	43,43,43	4.79	24 (55%)	56,60,60	4.10	30 (53%)
17	CLA	B	824	-	53,63,73	2.16	15 (28%)	62,101,113	2.92	28 (45%)
17	CLA	5	309	14	63,73,73	2.11	15 (23%)	74,113,113	2.70	30 (40%)
17	CLA	5	314	-	40,52,73	2.54	16 (40%)	50,87,113	2.96	22 (44%)
17	CLA	B	807	-	63,73,73	1.86	15 (23%)	74,113,113	2.54	27 (36%)
25	5X6	1	314	-	43,43,43	4.62	23 (53%)	56,60,60	4.72	33 (58%)
25	5X6	5	315	-	43,43,43	4.62	24 (55%)	56,60,60	4.84	31 (55%)
20	BCR	A	857	-	41,41,41	1.35	7 (17%)	56,56,56	1.36	7 (12%)
17	CLA	5	302	14	43,53,73	2.62	17 (39%)	50,89,113	3.05	21 (42%)
20	BCR	M	101	-	41,41,41	1.37	6 (14%)	56,56,56	1.56	13 (23%)
17	CLA	A	811	-	63,73,73	1.88	16 (25%)	74,113,113	2.58	27 (36%)
17	CLA	A	816	-	63,73,73	1.86	16 (25%)	74,113,113	2.56	23 (31%)
17	CLA	B	857	-	56,66,73	1.94	14 (25%)	65,104,113	2.93	26 (40%)
25	5X6	1	313	-	43,43,43	4.67	24 (55%)	56,60,60	4.70	32 (57%)
17	CLA	A	824	26	53,63,73	2.01	14 (26%)	62,101,113	3.01	29 (46%)
20	BCR	I	101	-	41,41,41	1.33	6 (14%)	56,56,56	1.33	10 (17%)
17	CLA	O	203	-	39,49,73	2.65	16 (41%)	46,84,113	3.25	24 (52%)
20	BCR	B	848	-	41,41,41	1.32	5 (12%)	56,56,56	1.46	8 (14%)
21	SF4	C	101	3	0,12,12	-	-	-	-	-
17	CLA	2	313	14	40,50,73	2.61	15 (37%)	45,85,113	3.23	23 (51%)
24	DGD	B	849	-	67,67,67	0.88	2 (2%)	81,81,81	0.88	4 (4%)
17	CLA	A	812	-	63,73,73	1.95	14 (22%)	74,113,113	2.70	22 (29%)
17	CLA	A	820	-	63,73,73	2.00	15 (23%)	74,113,113	2.65	30 (40%)
22	LMT	A	848	-	36,36,36	0.50	0	47,47,47	1.11	4 (8%)
17	CLA	1	308	-	39,49,73	2.63	15 (38%)	46,84,113	3.19	24 (52%)
17	CLA	A	830	-	54,64,73	2.14	16 (29%)	63,102,113	2.77	26 (41%)
20	BCR	B	843	-	41,41,41	1.33	6 (14%)	56,56,56	1.34	9 (16%)
21	SF4	A	847	2,1	0,12,12	-	-	-	-	-
25	5X6	2	318	-	43,43,43	4.59	24 (55%)	56,60,60	4.43	31 (55%)
17	CLA	A	827	-	63,73,73	1.78	14 (22%)	74,113,113	2.53	25 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	4	309	-	39,49,73	2.65	16 (41%)	46,84,113	3.23	24 (52%)
17	CLA	4	303	13	46,56,73	2.48	16 (34%)	53,92,113	3.02	25 (47%)
17	CLA	A	835	-	49,59,73	2.20	17 (34%)	56,96,113	2.86	25 (44%)
17	CLA	3	311	15	50,60,73	2.38	15 (30%)	57,97,113	3.03	23 (40%)
17	CLA	3	309	-	43,53,73	2.55	16 (37%)	50,89,113	3.09	23 (46%)
17	CLA	A	802	17	53,63,73	2.04	14 (26%)	62,101,113	2.79	26 (41%)
17	CLA	B	829	-	63,73,73	1.85	13 (20%)	74,113,113	2.63	27 (36%)
17	CLA	2	305	14	63,73,73	2.11	15 (23%)	74,113,113	2.65	28 (37%)
17	CLA	O	205	-	43,53,73	2.61	17 (39%)	50,89,113	3.06	24 (48%)
17	CLA	2	309	-	43,53,73	2.51	16 (37%)	50,89,113	3.14	25 (50%)
17	CLA	2	316	-	43,53,73	2.58	17 (39%)	50,89,113	3.08	23 (46%)
17	CLA	3	315	-	49,59,73	2.44	17 (34%)	56,96,113	3.01	25 (44%)
17	CLA	2	308	14	43,53,73	2.61	17 (39%)	50,89,113	3.02	23 (46%)
17	CLA	A	810	-	52,62,73	2.18	18 (34%)	60,99,113	2.88	27 (45%)
17	CLA	B	832	-	63,73,73	1.97	17 (26%)	74,113,113	2.52	26 (35%)
17	CLA	A	814	26	43,53,73	2.43	16 (37%)	50,89,113	3.09	22 (44%)
19	LHG	A	841	-	48,48,48	0.32	0	51,54,54	0.36	0
17	CLA	3	306	-	43,53,73	2.52	16 (37%)	50,89,113	3.07	27 (54%)
17	CLA	A	832	-	63,73,73	1.89	14 (22%)	74,113,113	2.66	27 (36%)
17	CLA	B	835	26	43,53,73	2.36	15 (34%)	50,89,113	3.04	26 (52%)
17	CLA	A	803	-	63,73,73	1.90	16 (25%)	74,113,113	2.70	26 (35%)
17	CLA	A	805	-	48,58,73	2.20	15 (31%)	56,95,113	3.06	26 (46%)
17	CLA	B	811	-	63,73,73	1.92	15 (23%)	74,113,113	2.51	28 (37%)
17	CLA	B	836	-	58,68,73	1.92	14 (24%)	68,107,113	2.65	26 (38%)
25	5X6	1	316	-	43,43,43	4.69	23 (53%)	56,60,60	4.38	28 (50%)
20	BCR	B	844	-	41,41,41	1.34	6 (14%)	56,56,56	1.27	6 (10%)
17	CLA	B	821	-	43,53,73	2.44	16 (37%)	50,89,113	3.08	25 (50%)
22	LMT	B	851	-	36,36,36	0.45	0	47,47,47	0.54	0
25	5X6	3	318	-	43,43,43	4.72	25 (58%)	56,60,60	4.49	31 (55%)
17	CLA	B	810	2	63,73,73	1.85	15 (23%)	74,113,113	2.59	26 (35%)
17	CLA	4	310	-	43,53,73	2.62	17 (39%)	50,89,113	3.04	24 (48%)
25	5X6	2	320	-	43,43,43	4.71	25 (58%)	56,60,60	4.36	31 (55%)
17	CLA	1	309	13	43,53,73	2.58	16 (37%)	50,89,113	3.07	24 (48%)
17	CLA	B	840	-	63,73,73	1.81	17 (26%)	74,113,113	2.73	28 (37%)
17	CLA	A	853	26	63,73,73	1.78	17 (26%)	74,113,113	2.73	30 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	809	17	63,73,73	1.85	18 (28%)	74,113,113	2.64	25 (33%)
17	CLA	5	304	-	63,73,73	2.01	15 (23%)	74,113,113	2.54	29 (39%)
25	5X6	5	301	-	43,43,43	4.72	25 (58%)	56,60,60	4.33	29 (51%)
25	5X6	5	316	-	43,43,43	4.48	24 (55%)	56,60,60	4.72	28 (50%)
25	5X6	3	317	-	43,43,43	4.67	24 (55%)	56,60,60	4.38	27 (48%)
17	CLA	L	203	-	63,73,73	2.02	16 (25%)	74,113,113	2.54	25 (33%)
17	CLA	K	102	26	53,63,73	2.27	16 (30%)	62,101,113	2.83	27 (43%)
17	CLA	A	833	-	63,73,73	1.88	13 (20%)	74,113,113	2.50	30 (40%)
17	CLA	A	807	1	63,73,73	1.94	17 (26%)	74,113,113	2.81	30 (40%)
25	5X6	2	317	-	43,43,43	4.76	24 (55%)	56,60,60	4.32	30 (53%)
17	CLA	3	308	-	43,53,73	2.57	16 (37%)	50,89,113	2.99	22 (44%)
17	CLA	A	823	26	63,73,73	1.92	16 (25%)	74,113,113	2.70	26 (35%)
17	CLA	2	307	14	53,63,73	2.25	17 (32%)	62,101,113	3.07	27 (43%)
17	CLA	A	855	26	59,69,73	1.91	15 (25%)	69,108,113	2.77	26 (37%)
20	BCR	A	843	-	41,41,41	1.35	7 (17%)	56,56,56	1.38	12 (21%)
20	BCR	L	206	-	41,41,41	1.33	7 (17%)	56,56,56	1.41	10 (17%)
25	5X6	5	318	-	43,43,43	4.66	25 (58%)	56,60,60	4.80	32 (57%)
17	CLA	A	817	-	63,73,73	1.89	13 (20%)	74,113,113	2.66	28 (37%)
17	CLA	4	311	-	43,53,73	2.59	17 (39%)	50,89,113	3.13	22 (44%)
17	CLA	4	305	13	43,53,73	2.57	17 (39%)	50,89,113	3.10	24 (48%)
19	LHG	J	102	-	48,48,48	0.27	0	51,54,54	0.36	0
17	CLA	2	314	14	43,53,73	2.58	16 (37%)	50,89,113	3.07	22 (44%)
17	CLA	A	821	-	49,59,73	2.23	17 (34%)	56,96,113	3.07	26 (46%)
17	CLA	L	202	10	55,65,73	2.23	17 (30%)	64,103,113	2.78	26 (40%)
17	CLA	A	852	-	63,73,73	1.86	13 (20%)	74,113,113	2.45	30 (40%)
25	5X6	5	317	-	43,43,43	4.77	24 (55%)	56,60,60	4.66	31 (55%)
17	CLA	1	303	13	53,63,73	2.27	15 (28%)	62,101,113	2.78	25 (40%)
17	CLA	B	841	-	63,73,73	2.04	16 (25%)	74,113,113	2.64	25 (33%)
17	CLA	1	305	-	43,53,73	2.65	17 (39%)	50,89,113	2.99	22 (44%)
17	CLA	4	306	-	43,53,73	2.62	16 (37%)	50,89,113	3.04	22 (44%)
18	PQN	A	840	-	34,34,34	1.54	2 (5%)	43,45,45	1.08	3 (6%)
22	LMT	F	201	-	36,36,36	0.49	1 (2%)	47,47,47	0.56	0
25	5X6	3	316	-	43,43,43	4.74	25 (58%)	56,60,60	4.57	30 (53%)
20	BCR	A	845	-	41,41,41	1.38	7 (17%)	56,56,56	1.43	9 (16%)
17	CLA	1	307	13	58,68,73	2.18	15 (25%)	68,107,113	2.76	25 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	4	304	13	57,67,73	2.23	16 (28%)	66,105,113	2.83	28 (42%)
20	BCR	B	847	-	41,41,41	1.32	7 (17%)	56,56,56	1.39	9 (16%)
17	CLA	F	204	6	39,49,73	2.53	16 (41%)	46,84,113	3.30	26 (56%)
19	LHG	A	842	17	39,39,48	0.28	0	42,45,54	0.37	0
17	CLA	A	859	19	44,54,73	2.38	16 (36%)	51,90,113	3.15	21 (41%)
17	CLA	4	308	13	43,53,73	2.57	16 (37%)	50,89,113	3.11	23 (46%)
20	BCR	A	844	-	41,41,41	1.35	6 (14%)	56,56,56	1.36	7 (12%)
17	CLA	B	818	-	57,67,73	1.97	16 (28%)	66,105,113	2.83	28 (42%)
17	CLA	2	312	-	39,49,73	2.63	16 (41%)	46,84,113	3.29	24 (52%)
25	5X6	2	321	-	43,43,43	4.66	23 (53%)	56,60,60	4.91	28 (50%)
17	CLA	5	310	-	39,49,73	2.67	17 (43%)	46,84,113	3.25	23 (50%)
17	CLA	A	815	-	60,70,73	1.98	15 (25%)	70,109,113	2.63	26 (37%)
17	CLA	B	802	26	63,73,73	1.75	14 (22%)	74,113,113	2.86	32 (43%)
17	CLA	A	837	-	63,73,73	1.81	15 (23%)	74,113,113	2.79	23 (31%)
17	CLA	3	305	15	61,71,73	2.14	15 (24%)	71,110,113	2.68	26 (36%)
17	CLA	O	204	-	48,58,73	2.45	16 (33%)	56,95,113	3.06	26 (46%)
20	BCR	J	104	-	41,41,41	1.36	6 (14%)	56,56,56	1.30	6 (10%)
17	CLA	B	813	-	53,63,73	2.20	17 (32%)	62,101,113	2.88	27 (43%)
17	CLA	A	825	-	63,73,73	1.90	15 (23%)	74,113,113	2.67	27 (36%)
17	CLA	B	817	-	53,63,73	2.14	14 (26%)	62,101,113	2.90	27 (43%)
17	CLA	B	828	-	63,73,73	1.78	14 (22%)	74,113,113	2.69	29 (39%)
16	CL0	A	801	-	63,73,73	1.79	13 (20%)	74,113,113	2.61	31 (41%)
17	CLA	3	307	-	53,63,73	2.34	17 (32%)	62,101,113	2.92	28 (45%)
17	CLA	2	315	-	43,53,73	2.57	16 (37%)	50,89,113	3.04	23 (46%)
17	CLA	A	813	-	40,50,73	2.43	15 (37%)	45,85,113	3.22	27 (60%)
17	CLA	B	833	-	63,73,73	1.83	17 (26%)	74,113,113	2.77	28 (37%)
17	CLA	B	838	-	45,55,73	2.26	16 (35%)	52,91,113	3.21	25 (48%)
17	CLA	1	311	-	43,53,73	2.61	17 (39%)	50,89,113	3.14	24 (48%)
20	BCR	O	202	-	41,41,41	1.37	7 (17%)	56,56,56	1.39	11 (19%)
17	CLA	1	306	13	53,63,73	2.28	16 (30%)	62,101,113	2.65	29 (46%)
17	CLA	2	310	14	43,53,73	2.56	16 (37%)	50,89,113	2.95	21 (42%)
17	CLA	B	816	-	63,73,73	1.98	14 (22%)	74,113,113	2.58	25 (33%)
17	CLA	L	204	26	48,58,73	2.37	16 (33%)	56,95,113	2.88	24 (42%)
25	5X6	1	312	-	43,43,43	4.70	24 (55%)	56,60,60	4.40	30 (53%)
17	CLA	3	313	15	40,50,73	2.60	16 (40%)	45,85,113	3.20	22 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	B	815	-	63,73,73	1.98	15 (23%)	74,113,113	2.63	26 (35%)
20	BCR	L	205	-	41,41,41	1.35	7 (17%)	56,56,56	1.26	6 (10%)
17	CLA	1	310	-	43,53,73	2.60	16 (37%)	50,89,113	3.06	21 (42%)
17	CLA	5	305	14	63,73,73	2.15	15 (23%)	74,113,113	2.89	36 (48%)
17	CLA	K	103	-	40,50,73	2.41	16 (40%)	45,85,113	3.21	25 (55%)
17	CLA	A	838	-	63,73,73	1.83	15 (23%)	74,113,113	2.65	30 (40%)
17	CLA	B	837	-	63,73,73	1.93	16 (25%)	74,113,113	2.72	30 (40%)
25	5X6	J	105	-	43,43,43	4.15	24 (55%)	56,60,60	5.07	28 (50%)
17	CLA	A	804	1	63,73,73	1.86	15 (23%)	74,113,113	2.58	29 (39%)
17	CLA	A	826	-	63,73,73	1.89	15 (23%)	74,113,113	2.63	28 (37%)
25	5X6	1	315	-	43,43,43	4.72	23 (53%)	56,60,60	4.78	30 (53%)
17	CLA	1	304	-	43,53,73	2.55	16 (37%)	50,89,113	3.15	22 (44%)
22	LMT	B	852	-	36,36,36	0.48	0	47,47,47	0.55	0
17	CLA	B	801	-	63,73,73	1.83	14 (22%)	74,113,113	2.34	25 (33%)
17	CLA	1	302	13	57,67,73	2.16	16 (28%)	66,105,113	2.64	27 (40%)
25	5X6	2	319	-	43,43,43	4.84	24 (55%)	56,60,60	4.17	29 (51%)
20	BCR	B	845	-	41,41,41	1.32	7 (17%)	56,56,56	1.33	8 (14%)
17	CLA	A	822	-	53,63,73	2.09	14 (26%)	62,101,113	2.95	22 (35%)
17	CLA	3	312	-	39,49,73	2.66	16 (41%)	46,84,113	3.25	24 (52%)
18	PQN	B	842	-	34,34,34	1.48	2 (5%)	43,45,45	1.16	4 (9%)
17	CLA	3	310	15	43,53,73	2.49	16 (37%)	50,89,113	3.08	25 (50%)
17	CLA	J	103	8	40,50,73	2.35	16 (40%)	45,85,113	3.17	24 (53%)
17	CLA	5	308	14	63,73,73	2.13	16 (25%)	74,113,113	2.56	29 (39%)
20	BCR	K	104	-	41,41,41	1.35	8 (19%)	56,56,56	1.60	15 (26%)

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
17	CLA	B	805	-	1/1/15/20	14/37/115/115	-
17	CLA	3	314	-	1/1/11/20	5/15/93/115	-
17	CLA	4	307	13	1/1/11/20	9/13/91/115	-
17	CLA	B	809	-	1/1/15/20	8/37/115/115	-
17	CLA	A	819	26	1/1/15/20	6/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	806	1	1/1/15/20	10/37/115/115	-
17	CLA	5	303	14	1/1/15/20	9/37/115/115	-
25	5X6	4	312	-	-	22/29/67/67	0/2/2/2
20	BCR	L	201	-	-	8/29/63/63	0/2/2/2
17	CLA	F	203	26	1/1/11/20	0/13/91/115	-
25	5X6	4	314	-	-	22/29/67/67	0/2/2/2
17	CLA	5	307	-	1/1/11/20	5/13/91/115	-
17	CLA	B	812	-	1/1/15/20	13/37/115/115	-
17	CLA	B	825	26	1/1/15/20	5/37/115/115	-
17	CLA	A	839	26	1/1/15/20	8/37/115/115	-
17	CLA	B	814	-	1/1/15/20	9/37/115/115	-
22	LMT	L	207	-	-	8/21/61/61	0/2/2/2
21	SF4	C	102	3	-	-	0/6/5/5
17	CLA	5	312	14	1/1/11/20	5/13/91/115	-
17	CLA	B	827	-	1/1/15/20	6/37/115/115	-
17	CLA	B	808	-	1/1/15/20	7/37/115/115	-
17	CLA	B	834	26	1/1/15/20	9/37/115/115	-
17	CLA	5	313	-	1/1/11/20	6/13/91/115	-
17	CLA	A	856	-	1/1/15/20	5/37/115/115	-
17	CLA	A	828	-	1/1/15/20	8/37/115/115	-
17	CLA	A	808	-	1/1/13/20	7/25/103/115	-
20	BCR	B	846	-	-	6/29/63/63	0/2/2/2
17	CLA	B	831	-	-	10/37/115/115	-
17	CLA	2	306	-	1/1/11/20	4/13/91/115	-
20	BCR	A	846	-	-	4/29/63/63	0/2/2/2
17	CLA	B	823	-	1/1/10/20	3/11/89/115	-
17	CLA	A	831	-	1/1/15/20	9/37/115/115	-
17	CLA	B	839	26	1/1/15/20	7/37/115/115	-
17	CLA	B	819	-	1/1/14/20	4/31/109/115	-
17	CLA	B	804	-	1/1/15/20	6/37/115/115	-
17	CLA	B	826	26	1/1/15/20	13/37/115/115	-
17	CLA	5	311	14	1/1/11/20	7/13/91/115	-
17	CLA	A	854	-	1/1/15/20	3/37/115/115	-
17	CLA	A	818	-	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	1	301	13	1/1/11/20	7/13/91/115	-
17	CLA	A	834	1	1/1/15/20	12/37/115/115	-
17	CLA	2	304	14	1/1/11/20	7/13/91/115	-
17	CLA	5	306	14	1/1/11/20	6/13/91/115	-
20	BCR	B	803	-	-	6/29/63/63	0/2/2/2
22	LMT	3	301	-	-	10/21/61/61	0/2/2/2
22	LMT	B	850	-	-	7/21/61/61	0/2/2/2
17	CLA	B	820	26	1/1/15/20	10/37/115/115	-
17	CLA	B	822	-	-	4/15/93/115	-
17	CLA	A	829	-	1/1/12/20	5/19/97/115	-
17	CLA	A	836	-	1/1/13/20	3/27/105/115	-
17	CLA	B	830	-	1/1/15/20	9/37/115/115	-
25	5X6	F	205	-	-	15/29/67/67	0/2/2/2
17	CLA	B	806	-	1/1/15/20	11/37/115/115	-
17	CLA	2	311	14	1/1/13/20	10/25/103/115	-
25	5X6	4	313	-	-	22/29/67/67	0/2/2/2
17	CLA	B	824	-	1/1/13/20	4/25/103/115	-
17	CLA	5	309	14	1/1/15/20	11/37/115/115	-
17	CLA	5	314	-	1/1/10/20	3/10/88/115	-
17	CLA	B	807	-	1/1/15/20	11/37/115/115	-
25	5X6	1	314	-	-	22/29/67/67	0/2/2/2
25	5X6	5	315	-	-	20/29/67/67	0/2/2/2
20	BCR	A	857	-	-	4/29/63/63	0/2/2/2
17	CLA	5	302	14	1/1/11/20	7/13/91/115	-
20	BCR	M	101	-	-	9/29/63/63	0/2/2/2
17	CLA	A	811	-	1/1/15/20	4/37/115/115	-
17	CLA	A	816	-	1/1/15/20	7/37/115/115	-
17	CLA	B	857	-	-	4/29/107/115	-
25	5X6	1	313	-	-	17/29/67/67	0/2/2/2
17	CLA	A	824	26	1/1/13/20	4/25/103/115	-
20	BCR	I	101	-	-	3/29/63/63	0/2/2/2
17	CLA	O	203	-	1/1/10/20	2/8/86/115	-
20	BCR	B	848	-	-	4/29/63/63	0/2/2/2
21	SF4	C	101	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	2	313	14	1/1/10/20	5/10/88/115	-
24	DGD	B	849	-	-	23/55/95/95	0/2/2/2
17	CLA	A	812	-	1/1/15/20	12/37/115/115	-
17	CLA	A	820	-	-	9/37/115/115	-
22	LMT	A	848	-	-	7/21/61/61	0/2/2/2
17	CLA	1	308	-	1/1/10/20	4/8/86/115	-
17	CLA	A	830	-	1/1/13/20	4/27/105/115	-
20	BCR	B	843	-	-	1/29/63/63	0/2/2/2
25	5X6	2	318	-	-	18/29/67/67	0/2/2/2
21	SF4	A	847	2,1	-	-	0/6/5/5
17	CLA	A	827	-	1/1/15/20	6/37/115/115	-
17	CLA	4	309	-	1/1/10/20	2/8/86/115	-
17	CLA	4	303	13	1/1/11/20	9/17/95/115	-
17	CLA	A	835	-	1/1/12/20	2/21/99/115	-
17	CLA	3	311	15	1/1/12/20	3/22/100/115	-
17	CLA	3	309	-	1/1/11/20	3/13/91/115	-
17	CLA	A	802	17	1/1/13/20	11/25/103/115	-
17	CLA	B	829	-	1/1/15/20	2/37/115/115	-
17	CLA	2	305	14	1/1/15/20	6/37/115/115	-
17	CLA	O	205	-	1/1/11/20	6/13/91/115	-
17	CLA	2	309	-	1/1/11/20	6/13/91/115	-
17	CLA	2	316	-	1/1/11/20	4/13/91/115	-
17	CLA	3	315	-	1/1/12/20	11/21/99/115	-
17	CLA	2	308	14	1/1/11/20	4/13/91/115	-
17	CLA	A	810	-	-	8/24/102/115	-
17	CLA	B	832	-	1/1/15/20	11/37/115/115	-
17	CLA	A	814	26	-	3/13/91/115	-
19	LHG	A	841	-	-	17/53/53/53	-
17	CLA	3	306	-	1/1/11/20	4/13/91/115	-
17	CLA	B	835	26	1/1/11/20	6/13/91/115	-
17	CLA	A	832	-	1/1/15/20	7/37/115/115	-
17	CLA	A	803	-	1/1/15/20	8/37/115/115	-
17	CLA	A	805	-	1/1/12/20	0/19/97/115	-
17	CLA	B	811	-	1/1/15/20	10/37/115/115	-
17	CLA	B	836	-	1/1/14/20	7/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	5X6	1	316	-	-	22/29/67/67	0/2/2/2
20	BCR	B	844	-	-	7/29/63/63	0/2/2/2
17	CLA	B	821	-	1/1/11/20	4/13/91/115	-
22	LMT	B	851	-	-	8/21/61/61	0/2/2/2
25	5X6	3	318	-	-	16/29/67/67	0/2/2/2
17	CLA	B	810	2	1/1/15/20	10/37/115/115	-
17	CLA	4	310	-	1/1/11/20	4/13/91/115	-
25	5X6	2	320	-	-	22/29/67/67	0/2/2/2
17	CLA	1	309	13	1/1/11/20	4/13/91/115	-
17	CLA	B	840	-	1/1/15/20	9/37/115/115	-
17	CLA	A	853	26	1/1/15/20	3/37/115/115	-
17	CLA	A	809	17	1/1/15/20	6/37/115/115	-
17	CLA	5	304	-	1/1/15/20	6/37/115/115	-
25	5X6	5	301	-	-	20/29/67/67	0/2/2/2
25	5X6	5	316	-	-	18/29/67/67	0/2/2/2
25	5X6	3	317	-	-	23/29/67/67	0/2/2/2
17	CLA	L	203	-	1/1/15/20	8/37/115/115	-
17	CLA	K	102	26	-	6/25/103/115	-
17	CLA	A	833	-	1/1/15/20	7/37/115/115	-
17	CLA	A	807	1	-	10/37/115/115	-
25	5X6	2	317	-	-	22/29/67/67	0/2/2/2
17	CLA	3	308	-	1/1/11/20	4/13/91/115	-
17	CLA	A	823	26	1/1/15/20	8/37/115/115	-
17	CLA	2	307	14	-	10/25/103/115	-
17	CLA	A	855	26	1/1/14/20	10/33/111/115	-
20	BCR	A	843	-	-	10/29/63/63	0/2/2/2
20	BCR	L	206	-	-	5/29/63/63	0/2/2/2
25	5X6	5	318	-	-	19/29/67/67	0/2/2/2
17	CLA	A	817	-	1/1/15/20	3/37/115/115	-
17	CLA	4	311	-	1/1/11/20	6/13/91/115	-
17	CLA	4	305	13	1/1/11/20	8/13/91/115	-
19	LHG	J	102	-	-	24/53/53/53	-
17	CLA	2	314	14	1/1/11/20	3/13/91/115	-
17	CLA	A	821	-	1/1/12/20	4/21/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	L	202	10	1/1/13/20	11/28/106/115	-
17	CLA	A	852	-	1/1/15/20	3/37/115/115	-
25	5X6	5	317	-	-	22/29/67/67	0/2/2/2
17	CLA	4	306	-	1/1/11/20	5/13/91/115	-
17	CLA	B	841	-	1/1/15/20	3/37/115/115	-
17	CLA	1	305	-	1/1/11/20	7/13/91/115	-
17	CLA	1	303	13	-	9/25/103/115	-
18	PQN	A	840	-	-	4/23/43/43	0/2/2/2
22	LMT	F	201	-	-	13/21/61/61	0/2/2/2
25	5X6	3	316	-	-	21/29/67/67	0/2/2/2
20	BCR	A	845	-	-	6/29/63/63	0/2/2/2
17	CLA	1	307	13	1/1/14/20	7/31/109/115	-
17	CLA	4	304	13	1/1/13/20	10/30/108/115	-
20	BCR	B	847	-	-	7/29/63/63	0/2/2/2
17	CLA	F	204	6	1/1/10/20	4/8/86/115	-
19	LHG	A	842	17	-	18/44/44/53	-
17	CLA	A	859	19	1/1/11/20	10/15/93/115	-
17	CLA	4	308	13	1/1/11/20	4/13/91/115	-
20	BCR	A	844	-	-	8/29/63/63	0/2/2/2
17	CLA	B	818	-	1/1/13/20	11/30/108/115	-
17	CLA	2	312	-	1/1/10/20	4/8/86/115	-
25	5X6	2	321	-	-	25/29/67/67	0/2/2/2
17	CLA	5	310	-	1/1/10/20	2/8/86/115	-
17	CLA	A	815	-	-	9/34/112/115	-
17	CLA	B	802	26	1/1/15/20	14/37/115/115	-
17	CLA	A	837	-	1/1/15/20	7/37/115/115	-
17	CLA	3	305	15	1/1/14/20	7/35/113/115	-
17	CLA	O	204	-	1/1/12/20	6/19/97/115	-
20	BCR	J	104	-	-	6/29/63/63	0/2/2/2
17	CLA	B	813	-	1/1/13/20	5/25/103/115	-
17	CLA	A	825	-	1/1/15/20	8/37/115/115	-
17	CLA	B	828	-	1/1/15/20	11/37/115/115	-
17	CLA	3	307	-	1/1/13/20	3/25/103/115	-
16	CL0	A	801	-	3/3/20/25	2/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	817	-	-	6/25/103/115	-
17	CLA	2	315	-	1/1/11/20	2/13/91/115	-
17	CLA	A	813	-	1/1/10/20	4/10/88/115	-
17	CLA	B	833	-	1/1/15/20	10/37/115/115	-
17	CLA	B	838	-	1/1/11/20	3/16/94/115	-
17	CLA	1	311	-	1/1/11/20	8/13/91/115	-
20	BCR	O	202	-	-	2/29/63/63	0/2/2/2
17	CLA	1	306	13	1/1/13/20	4/25/103/115	-
17	CLA	2	310	14	1/1/11/20	0/13/91/115	-
17	CLA	B	816	-	1/1/15/20	12/37/115/115	-
17	CLA	L	204	26	1/1/12/20	6/19/97/115	-
25	5X6	1	312	-	-	15/29/67/67	0/2/2/2
17	CLA	3	313	15	1/1/10/20	4/10/88/115	-
17	CLA	B	815	-	1/1/15/20	14/37/115/115	-
20	BCR	L	205	-	-	4/29/63/63	0/2/2/2
17	CLA	1	310	-	1/1/11/20	5/13/91/115	-
17	CLA	5	305	14	1/1/15/20	13/37/115/115	-
17	CLA	K	103	-	1/1/10/20	2/10/88/115	-
17	CLA	A	838	-	1/1/15/20	5/37/115/115	-
17	CLA	B	837	-	1/1/15/20	9/37/115/115	-
25	5X6	J	105	-	-	19/29/67/67	0/2/2/2
17	CLA	A	804	1	1/1/15/20	16/37/115/115	-
17	CLA	A	826	-	1/1/15/20	6/37/115/115	-
25	5X6	1	315	-	-	25/29/67/67	0/2/2/2
17	CLA	1	304	-	1/1/11/20	6/13/91/115	-
22	LMT	B	852	-	-	12/21/61/61	0/2/2/2
17	CLA	B	801	-	1/1/15/20	5/37/115/115	-
17	CLA	1	302	13	1/1/13/20	5/30/108/115	-
25	5X6	2	319	-	-	20/29/67/67	0/2/2/2
20	BCR	B	845	-	-	11/29/63/63	0/2/2/2
17	CLA	A	822	-	1/1/13/20	5/25/103/115	-
17	CLA	3	312	-	1/1/10/20	2/8/86/115	-
18	PQN	B	842	-	-	3/23/43/43	0/2/2/2
17	CLA	3	310	15	1/1/11/20	6/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	J	103	8	1/1/10/20	4/10/88/115	-
17	CLA	5	308	14	1/1/15/20	12/37/115/115	-
20	BCR	K	104	-	-	7/29/63/63	0/2/2/2

The worst 5 of 3088 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	319	5X6	C18-C17	9.30	1.57	1.35
25	4	313	5X6	C18-C17	9.15	1.57	1.35
25	1	313	5X6	C18-C17	9.09	1.56	1.35
25	5	318	5X6	C18-C17	9.01	1.56	1.35
25	2	320	5X6	C18-C17	9.00	1.56	1.35

The worst 5 of 4882 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	805	CLA	O2A-CGA-O1A	-18.10	78.34	123.63
17	B	805	CLA	O2A-CGA-CBA	17.05	163.81	111.83
25	2	321	5X6	C01-C02-C03	-15.02	108.10	124.48
25	F	205	5X6	C28-C27-C26	-14.47	104.83	126.23
25	1	316	5X6	C01-C02-C03	-13.95	109.26	124.48

5 of 144 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	A	801	CL0	NA
16	A	801	CL0	ND
16	A	801	CL0	NC
17	A	802	CLA	ND
17	A	803	CLA	ND

5 of 1751 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	804	CLA	C11-C10-C8-C9
17	A	806	CLA	CHA-CBD-CGD-O1D
17	A	806	CLA	CHA-CBD-CGD-O2D
17	A	809	CLA	CHA-CBD-CGD-O1D
17	A	809	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

183 monomers are involved in 416 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	805	CLA	5	0
17	3	314	CLA	1	0
17	4	307	CLA	4	0
17	B	809	CLA	1	0
17	A	819	CLA	6	0
17	A	806	CLA	1	0
17	5	303	CLA	1	0
20	L	201	BCR	2	0
17	F	203	CLA	3	0
25	4	314	5X6	1	0
17	5	307	CLA	2	0
17	B	812	CLA	6	0
17	B	825	CLA	5	0
17	A	839	CLA	5	0
17	B	814	CLA	6	0
21	C	102	SF4	1	0
17	5	312	CLA	2	0
17	B	827	CLA	2	0
17	B	808	CLA	2	0
17	B	834	CLA	4	0
17	5	313	CLA	5	0
17	A	856	CLA	1	0
17	A	828	CLA	1	0
17	A	808	CLA	1	0
17	B	831	CLA	4	0
17	2	306	CLA	2	0
20	A	846	BCR	4	0
17	B	823	CLA	5	0
17	A	831	CLA	5	0
17	B	839	CLA	7	0
17	B	819	CLA	1	0
17	B	804	CLA	3	0
17	B	826	CLA	5	0
17	5	311	CLA	1	0
17	A	854	CLA	6	0
17	A	818	CLA	3	0
17	1	301	CLA	2	0
17	A	834	CLA	3	0
17	2	304	CLA	4	0
17	5	306	CLA	1	0
20	B	803	BCR	3	0
17	B	820	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	822	CLA	1	0
17	A	829	CLA	2	0
17	A	836	CLA	3	0
17	B	830	CLA	5	0
17	B	806	CLA	1	0
17	2	311	CLA	1	0
17	B	824	CLA	2	0
17	5	309	CLA	3	0
17	5	314	CLA	2	0
17	B	807	CLA	6	0
25	1	314	5X6	1	0
20	A	857	BCR	2	0
17	5	302	CLA	2	0
20	M	101	BCR	4	0
17	A	811	CLA	7	0
17	A	816	CLA	7	0
17	B	857	CLA	4	0
17	A	824	CLA	1	0
20	I	101	BCR	1	0
17	O	203	CLA	2	0
20	B	848	BCR	1	0
17	2	313	CLA	3	0
24	B	849	DGD	3	0
17	A	812	CLA	2	0
17	A	820	CLA	2	0
17	1	308	CLA	3	0
17	A	830	CLA	2	0
20	B	843	BCR	1	0
25	2	318	5X6	1	0
17	A	827	CLA	1	0
17	4	309	CLA	2	0
17	4	303	CLA	2	0
17	A	835	CLA	1	0
17	3	311	CLA	1	0
17	3	309	CLA	1	0
17	A	802	CLA	1	0
17	B	829	CLA	2	0
17	2	305	CLA	1	0
17	O	205	CLA	1	0
17	2	309	CLA	7	0
17	2	316	CLA	2	0
17	3	315	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	2	308	CLA	2	0
17	A	810	CLA	3	0
17	B	832	CLA	2	0
17	A	814	CLA	2	0
17	3	306	CLA	2	0
17	A	832	CLA	3	0
17	B	835	CLA	4	0
17	A	803	CLA	4	0
17	A	805	CLA	1	0
17	B	811	CLA	5	0
17	B	836	CLA	8	0
20	B	844	BCR	1	0
17	B	821	CLA	1	0
17	B	810	CLA	5	0
17	4	310	CLA	2	0
17	1	309	CLA	2	0
17	B	840	CLA	4	0
17	A	853	CLA	5	0
17	A	809	CLA	2	0
17	5	304	CLA	3	0
25	3	317	5X6	2	0
17	L	203	CLA	3	0
17	K	102	CLA	1	0
17	A	833	CLA	1	0
17	A	807	CLA	2	0
17	3	308	CLA	1	0
17	A	823	CLA	5	0
17	2	307	CLA	10	0
17	A	855	CLA	4	0
20	A	843	BCR	3	0
20	L	206	BCR	1	0
25	5	318	5X6	2	0
17	A	817	CLA	2	0
17	4	311	CLA	3	0
17	4	305	CLA	2	0
19	J	102	LHG	1	0
17	2	314	CLA	1	0
17	A	821	CLA	2	0
17	L	202	CLA	1	0
17	A	852	CLA	4	0
17	1	303	CLA	1	0
17	B	841	CLA	6	0

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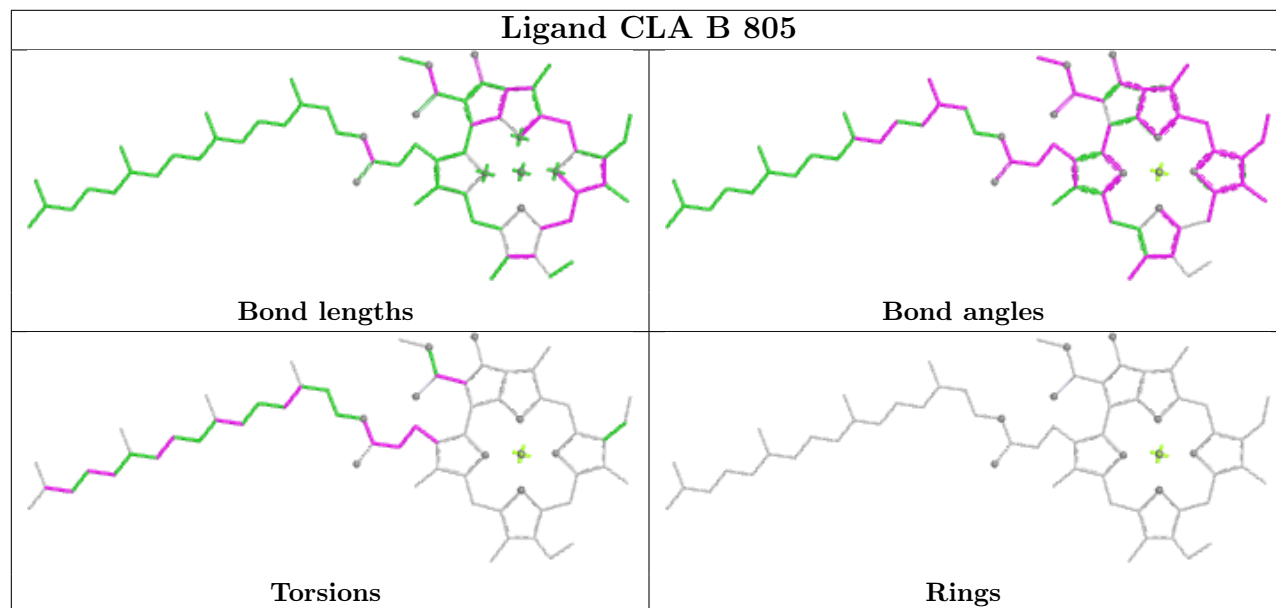
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	1	305	CLA	3	0
17	4	306	CLA	3	0
18	A	840	PQN	1	0
20	A	845	BCR	2	0
17	1	307	CLA	1	0
20	B	847	BCR	3	0
17	F	204	CLA	3	0
19	A	842	LHG	1	0
17	A	859	CLA	5	0
17	4	308	CLA	1	0
20	A	844	BCR	3	0
17	B	818	CLA	4	0
17	2	312	CLA	1	0
17	5	310	CLA	1	0
17	A	815	CLA	5	0
17	B	802	CLA	7	0
17	A	837	CLA	4	0
17	3	305	CLA	2	0
17	O	204	CLA	2	0
20	J	104	BCR	3	0
17	B	813	CLA	5	0
17	A	825	CLA	2	0
17	B	817	CLA	5	0
17	B	828	CLA	6	0
16	A	801	CL0	3	0
17	3	307	CLA	1	0
17	2	315	CLA	1	0
17	A	813	CLA	3	0
17	B	833	CLA	4	0
17	B	838	CLA	3	0
17	1	311	CLA	1	0
17	1	306	CLA	3	0
17	2	310	CLA	3	0
17	B	816	CLA	2	0
17	L	204	CLA	5	0
25	1	312	5X6	1	0
17	3	313	CLA	1	0
17	B	815	CLA	4	0
20	L	205	BCR	1	0
17	1	310	CLA	3	0
17	5	305	CLA	4	0
17	K	103	CLA	2	0

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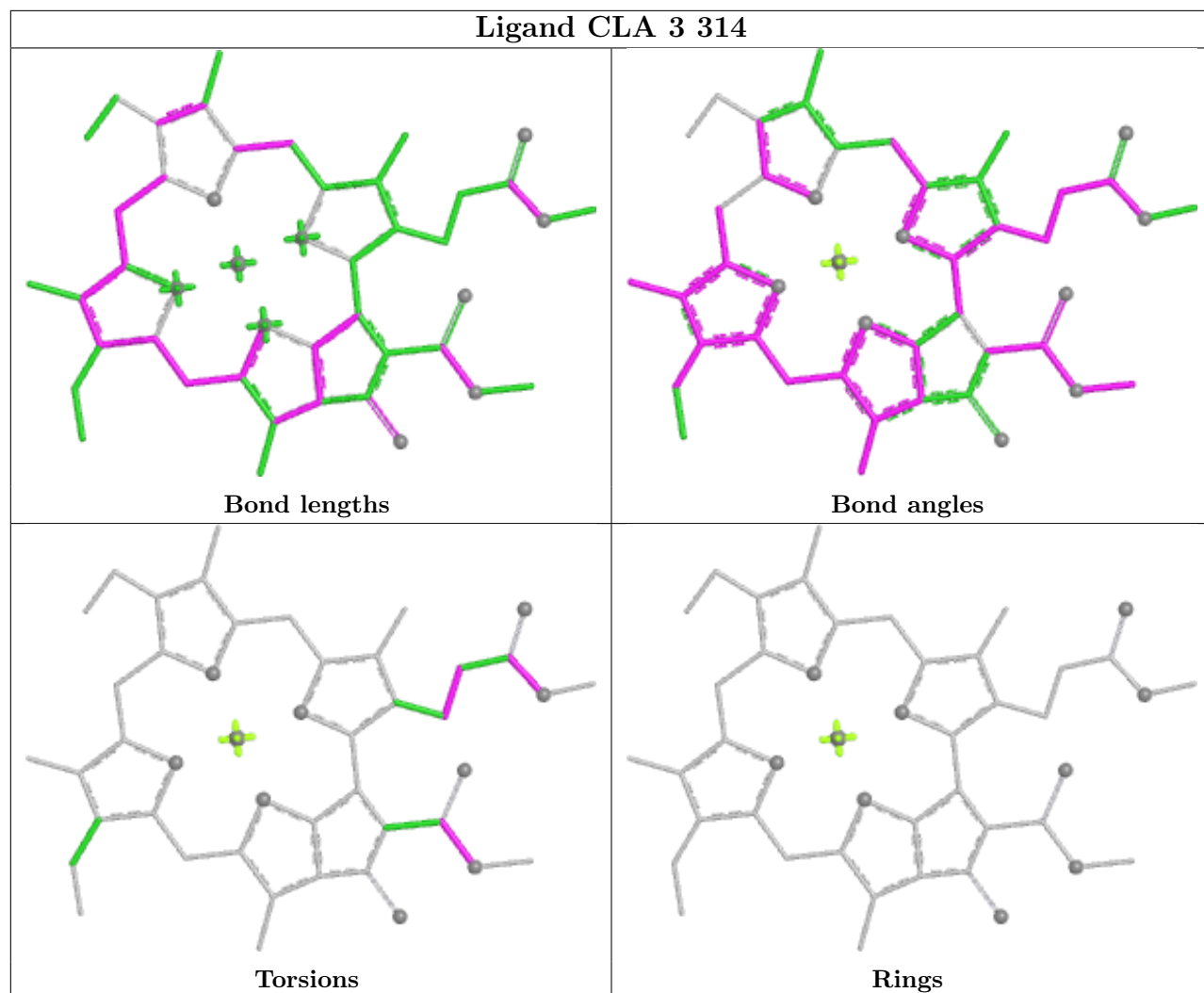
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	838	CLA	1	0
17	B	837	CLA	5	0
17	A	804	CLA	3	0
17	A	826	CLA	5	0
17	1	304	CLA	3	0
17	B	801	CLA	3	0
17	1	302	CLA	1	0
20	B	845	BCR	1	0
17	A	822	CLA	2	0
17	3	312	CLA	2	0
18	B	842	PQN	3	0
17	3	310	CLA	2	0
17	J	103	CLA	1	0
17	5	308	CLA	5	0
20	K	104	BCR	1	0

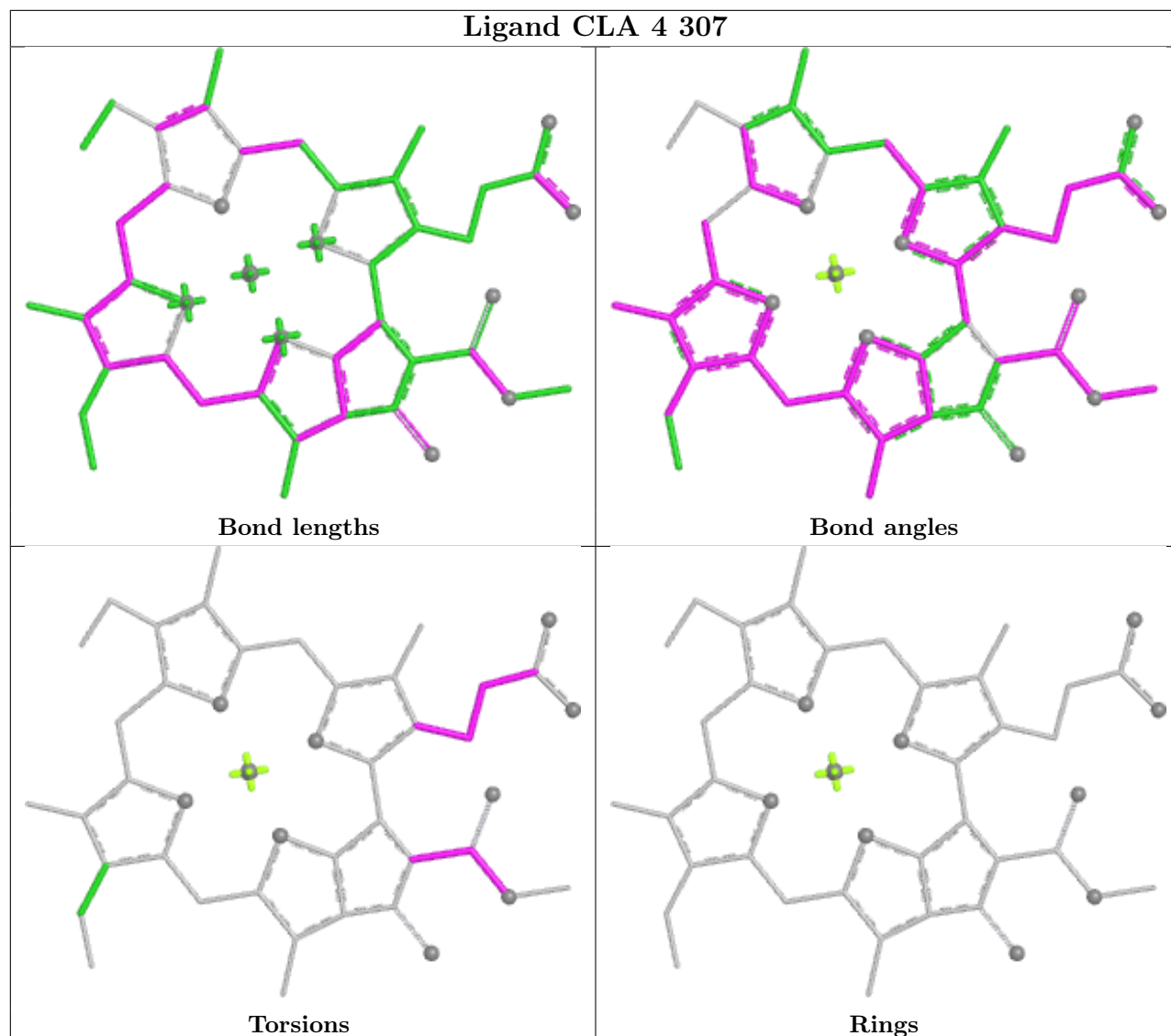
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



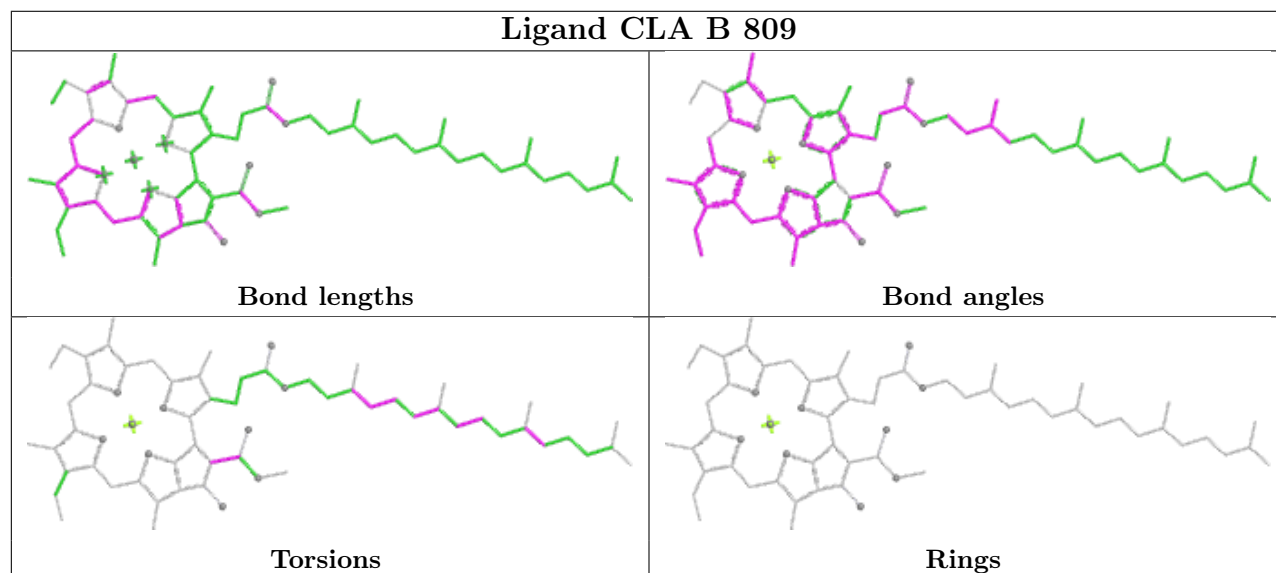
Ligand CLA 3 314

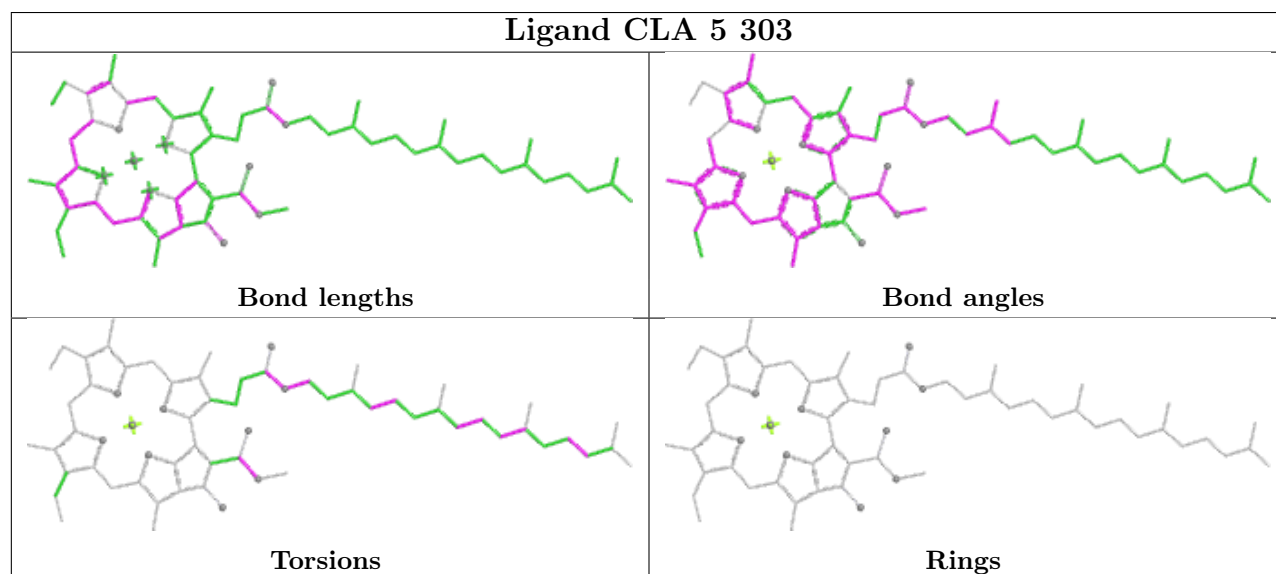
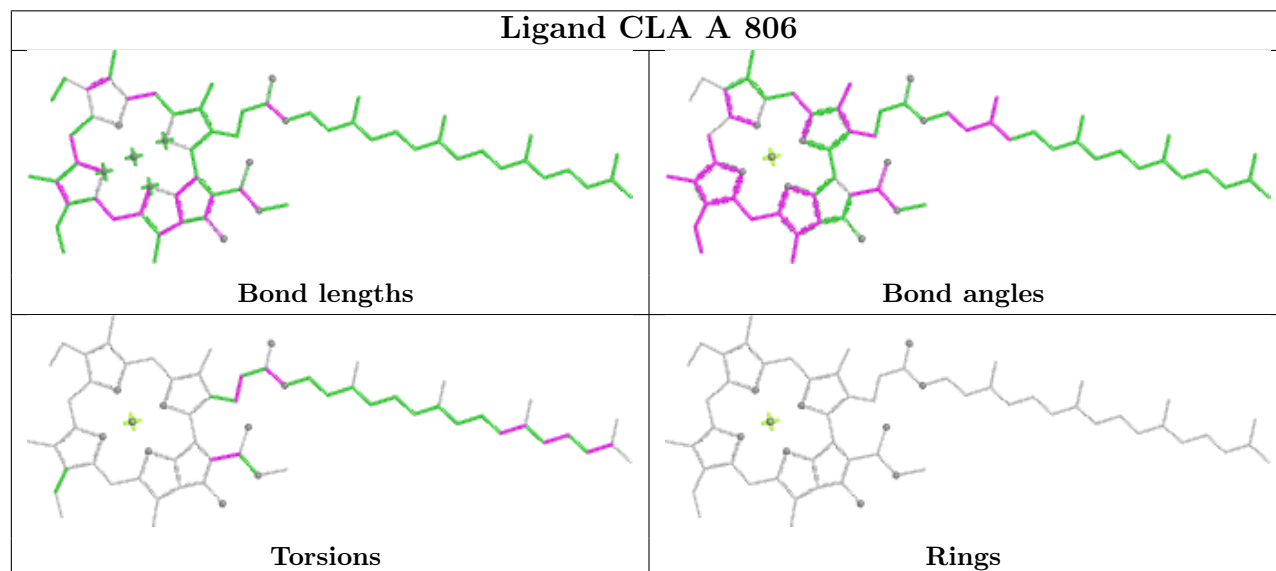
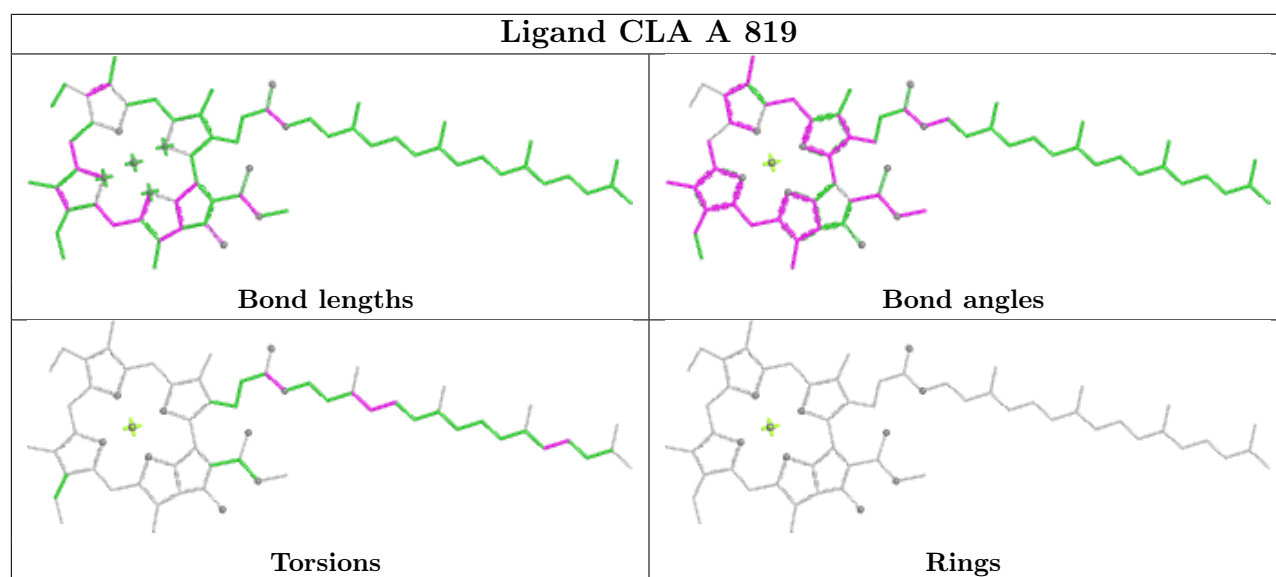


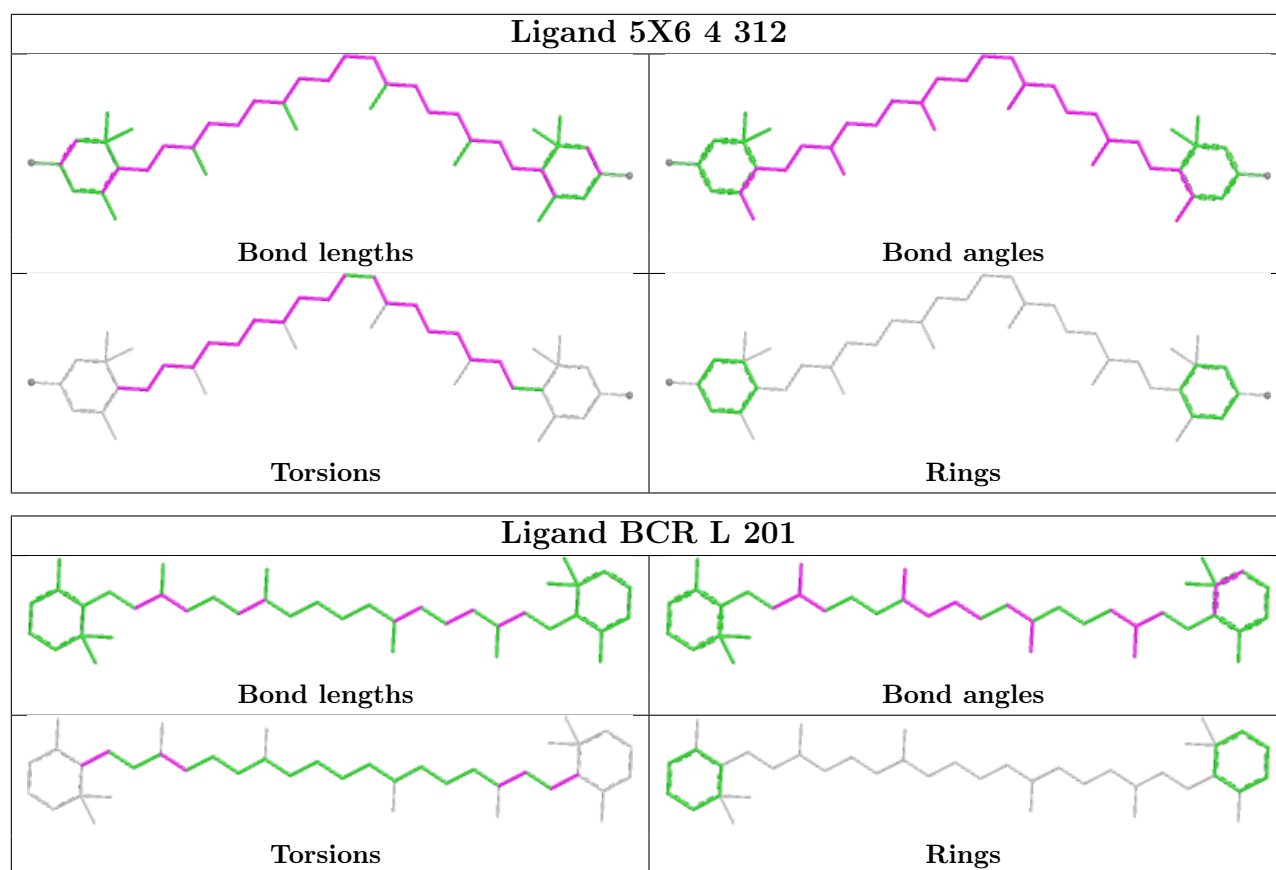
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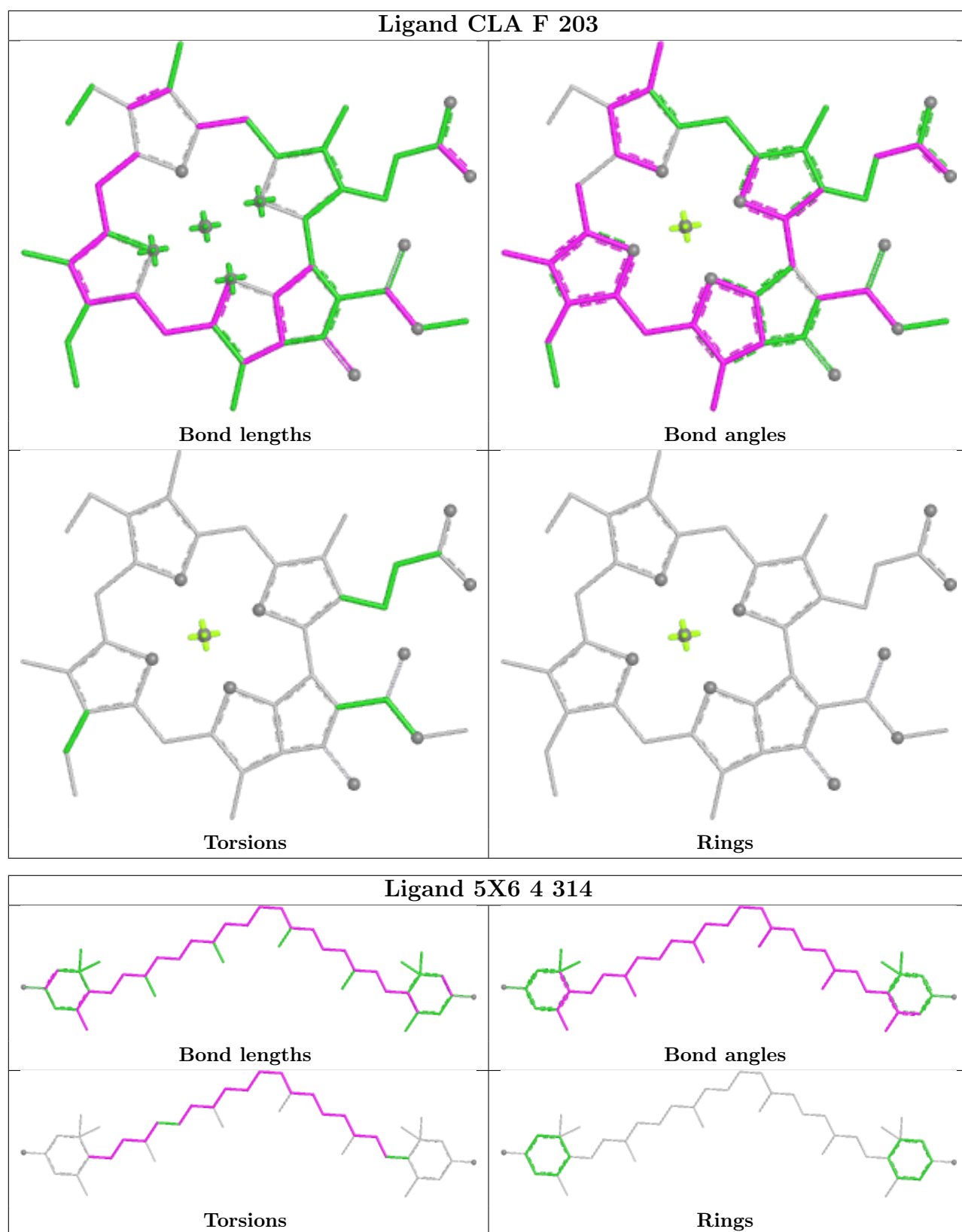


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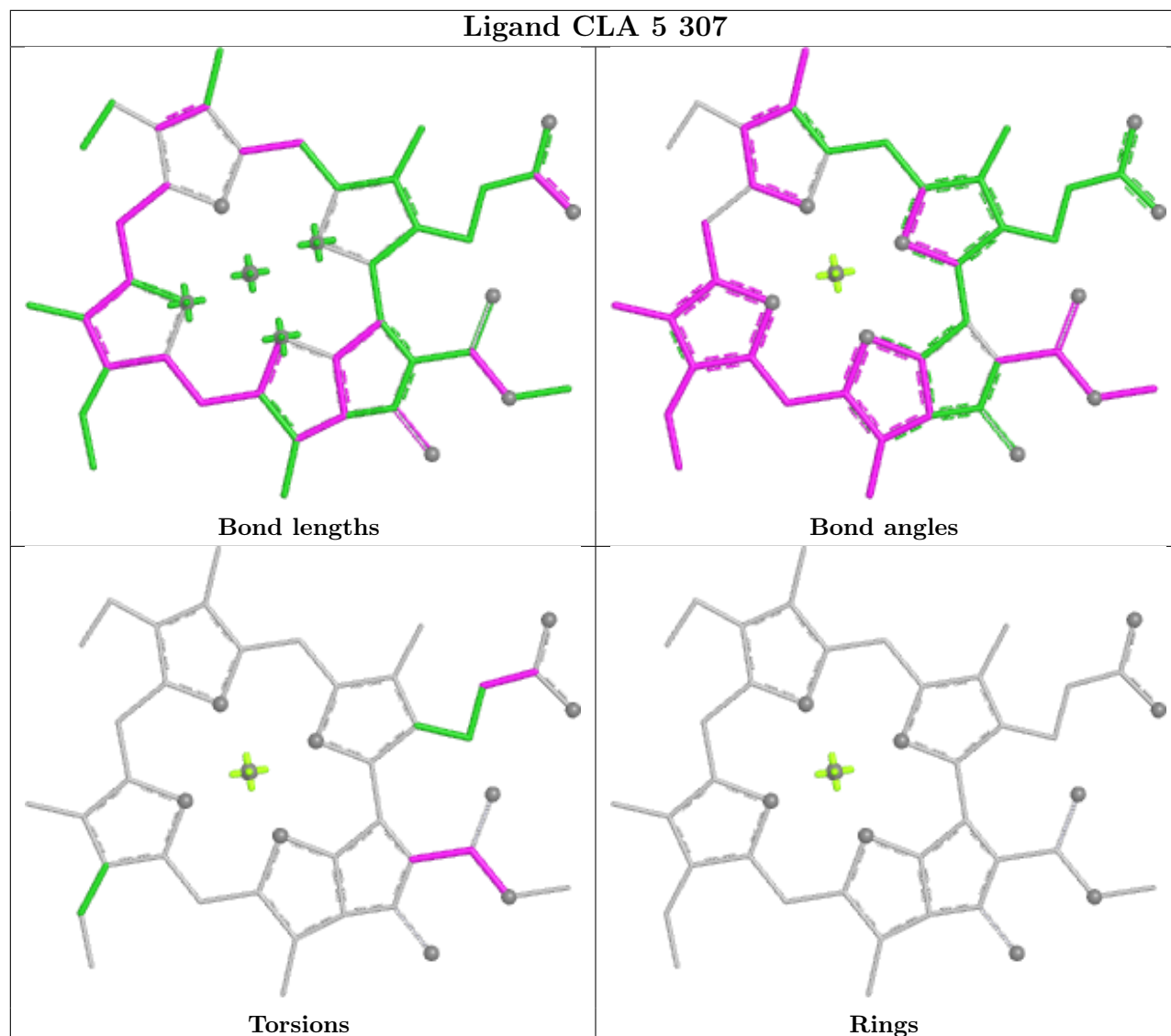




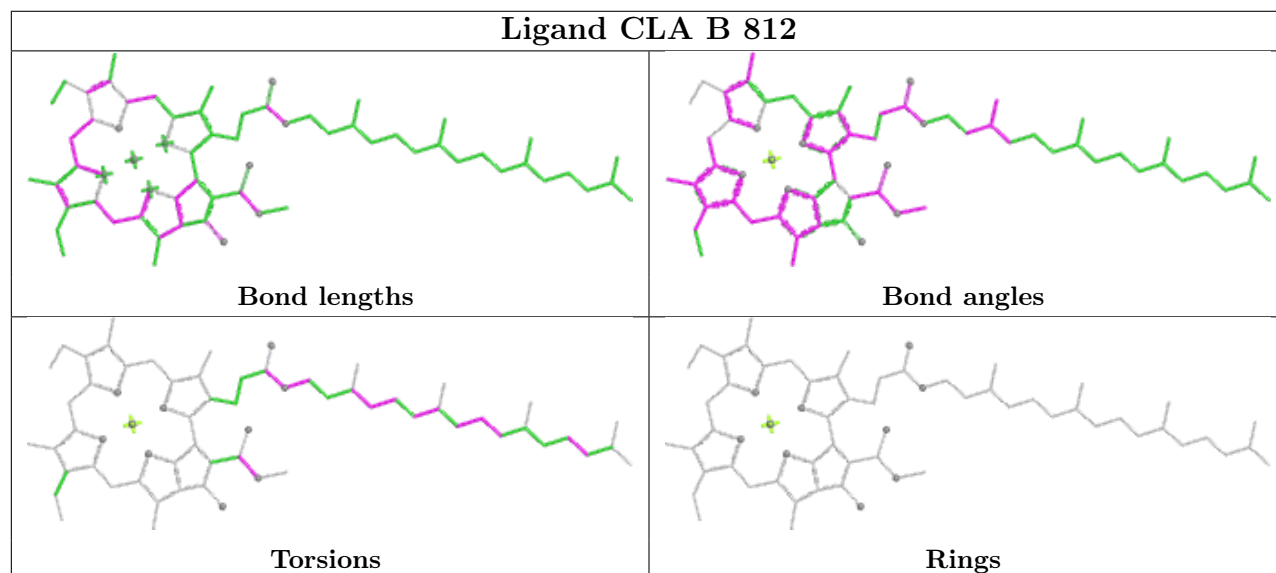


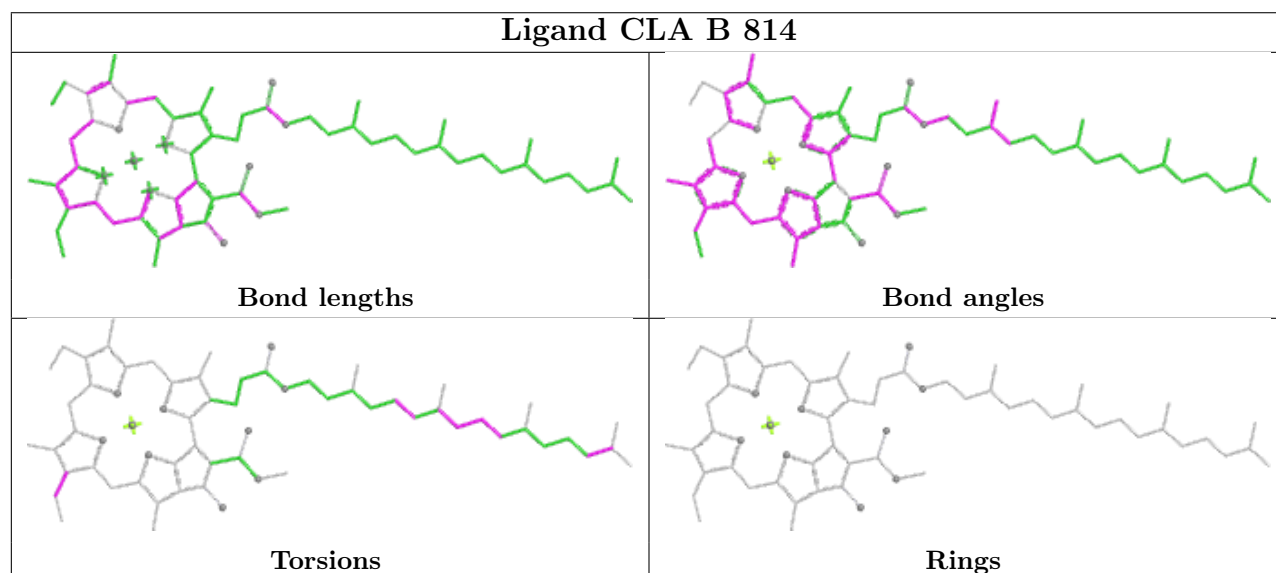
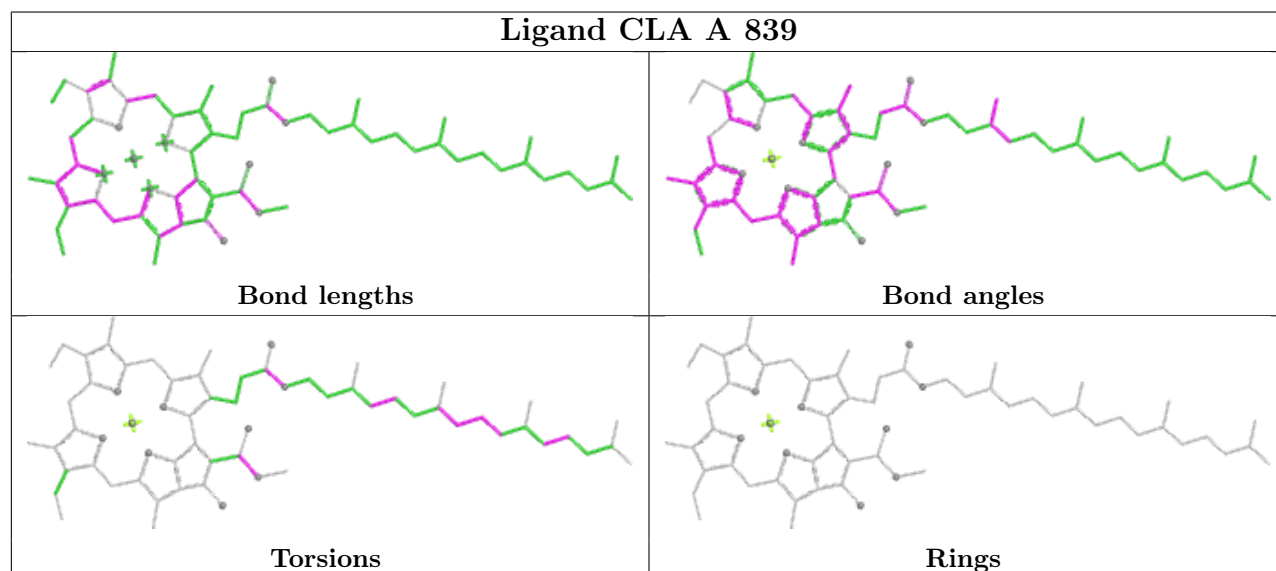
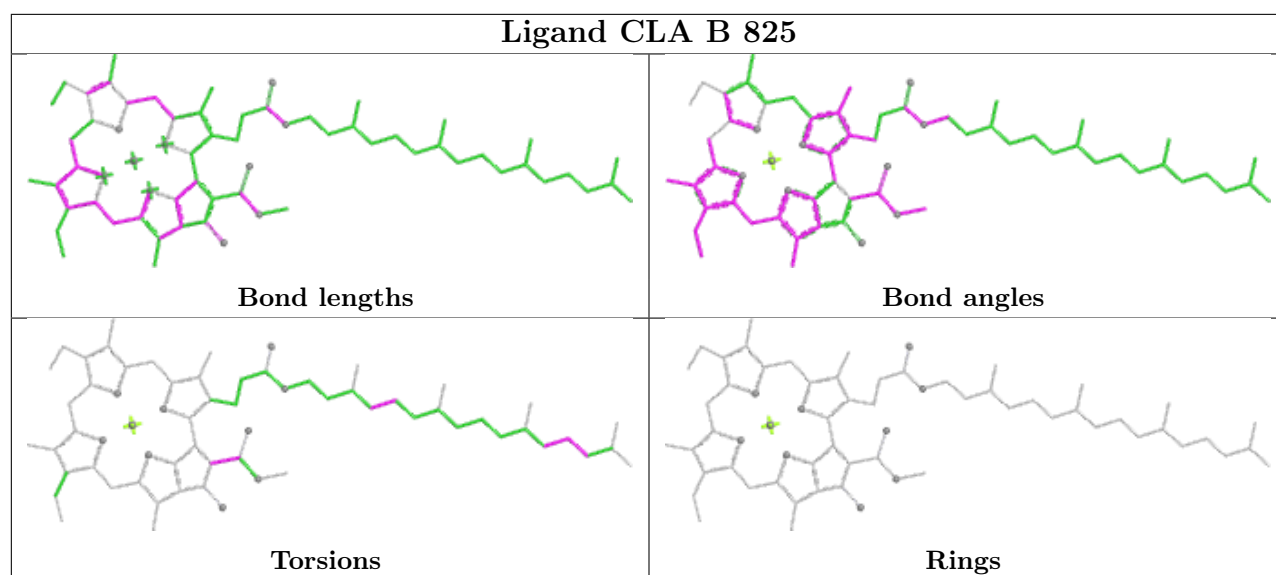


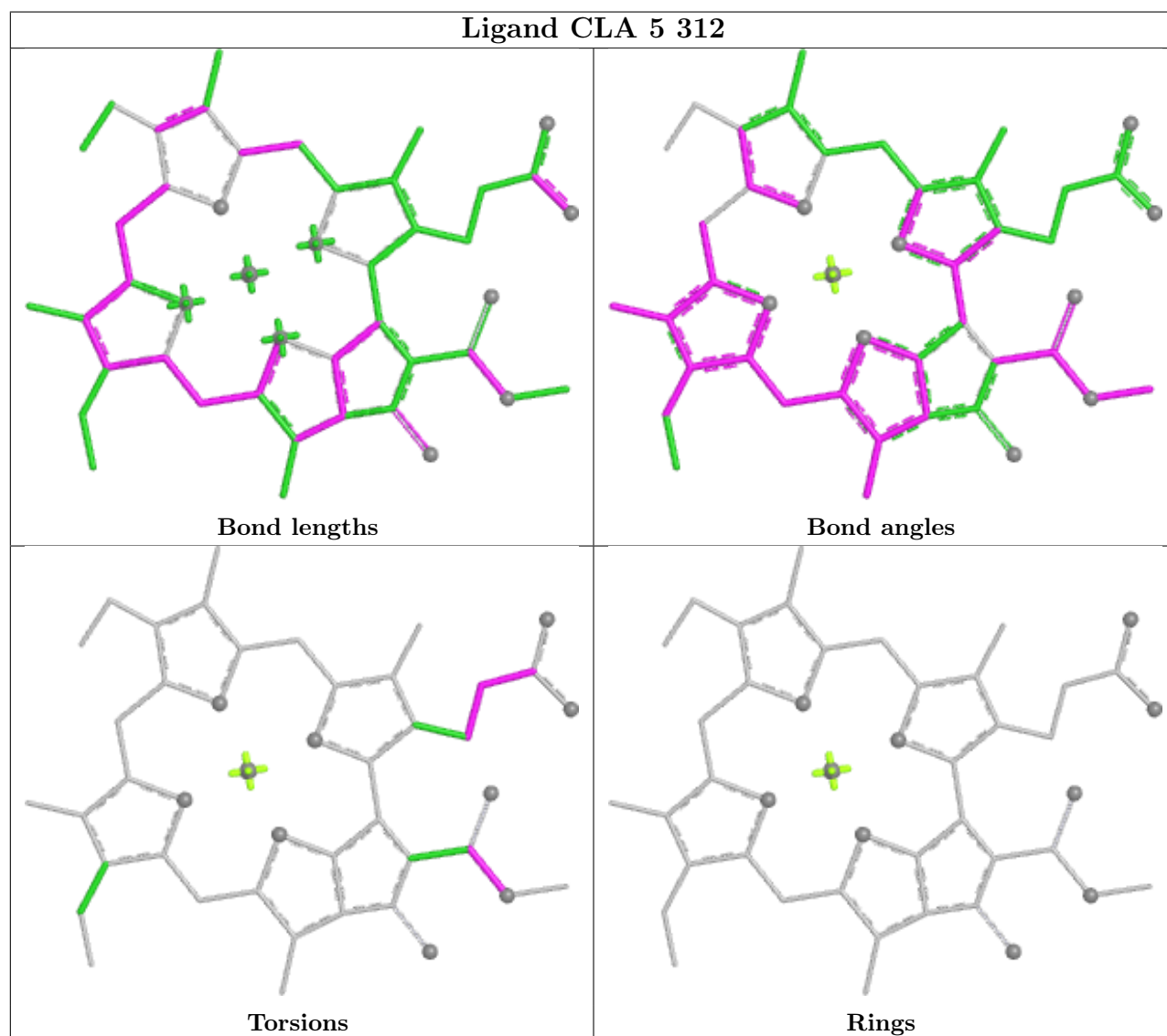
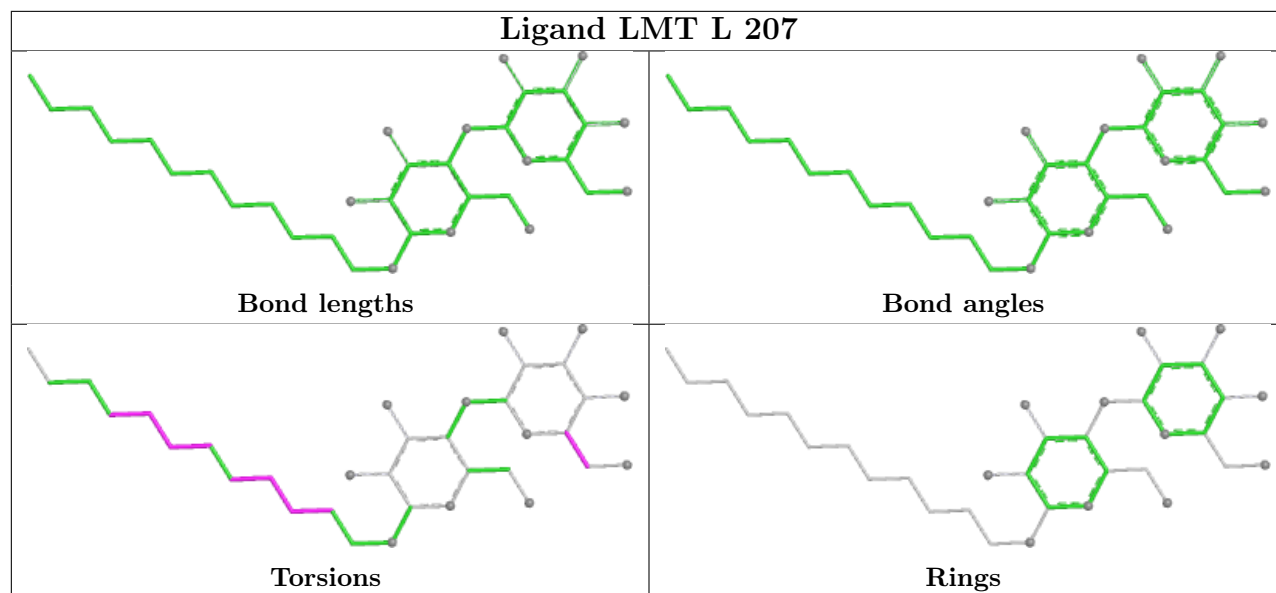
Ligand CLA 5 307

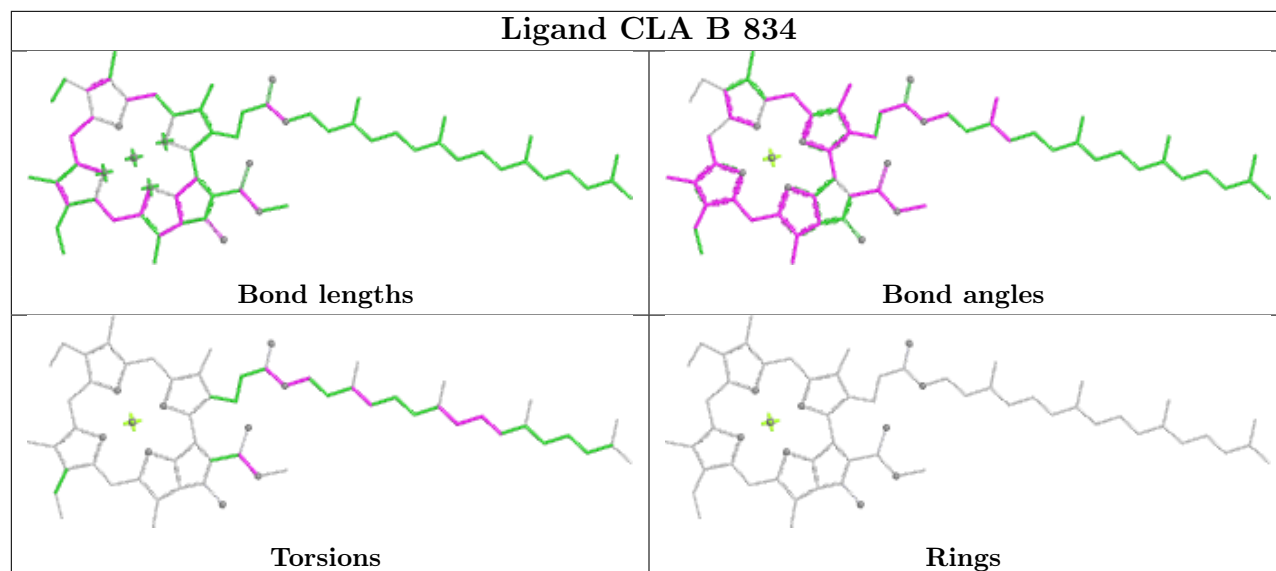
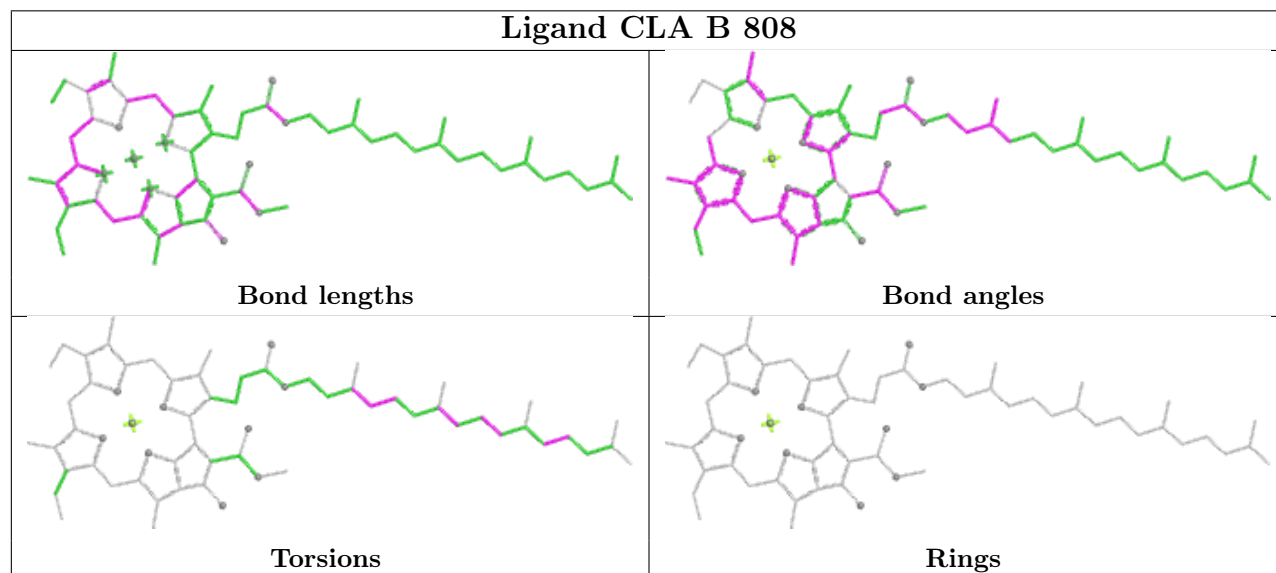
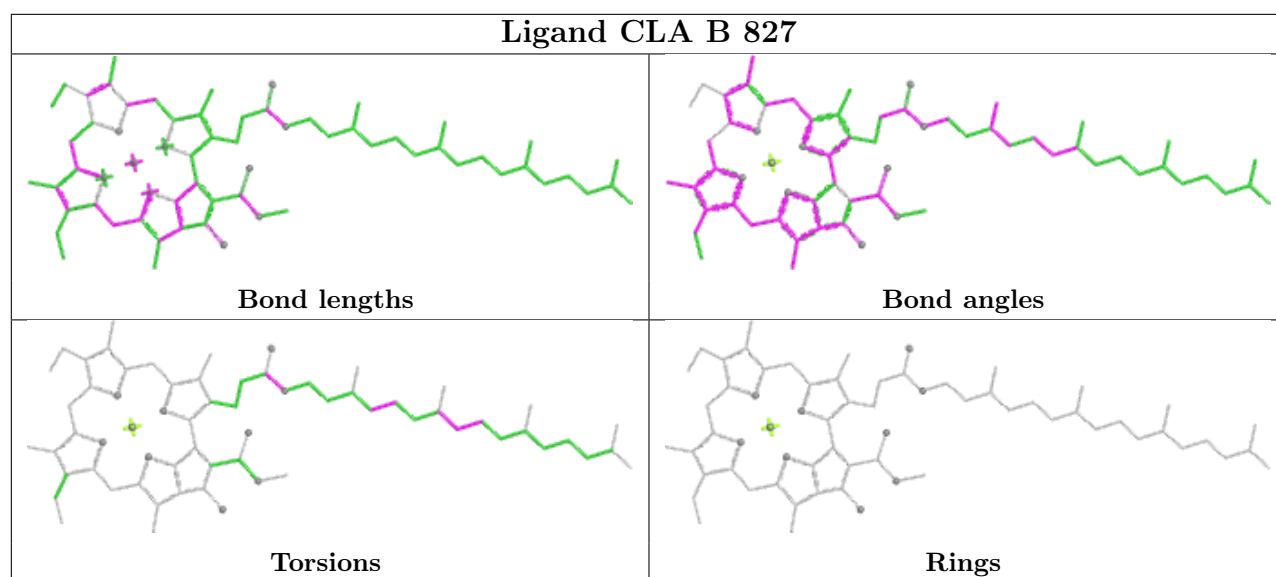


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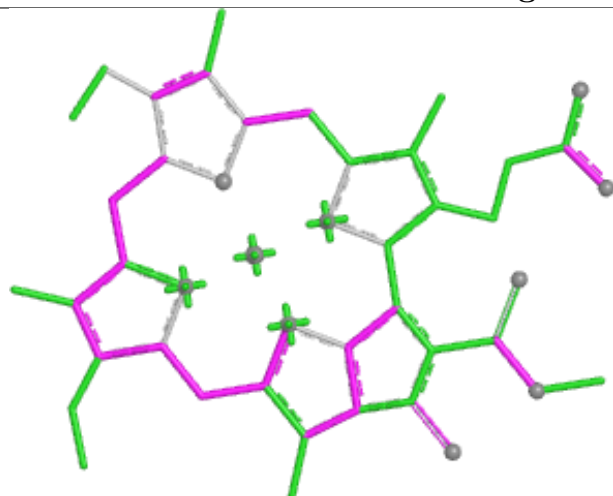




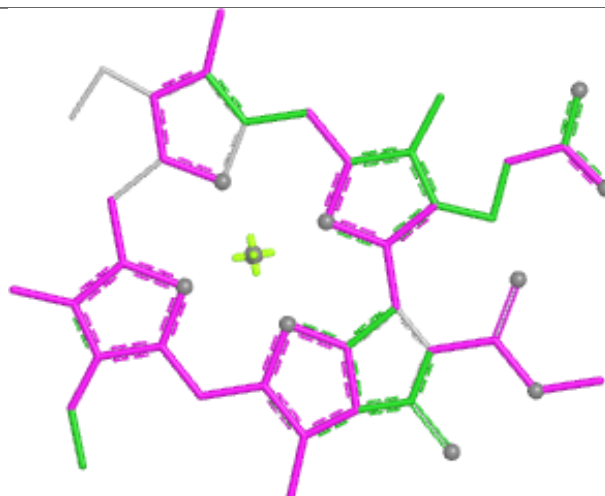




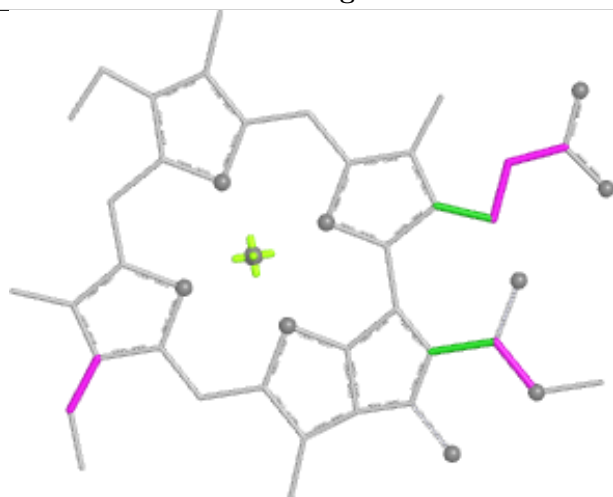
Ligand CLA 5 313



Bond lengths



Bond angles

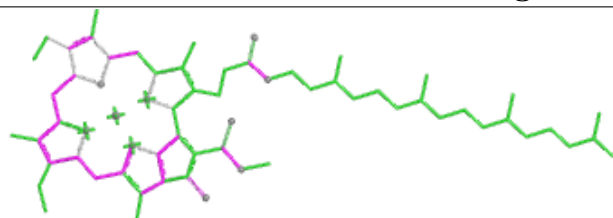


Torsions

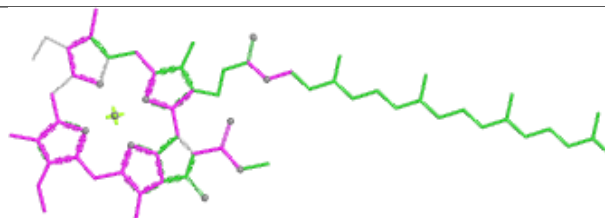


Rings

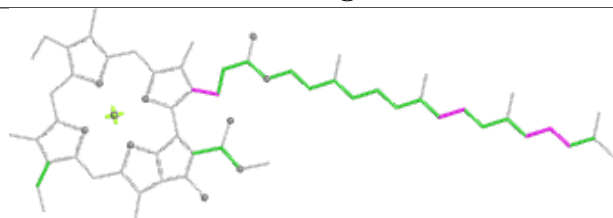
Ligand CLA A 856



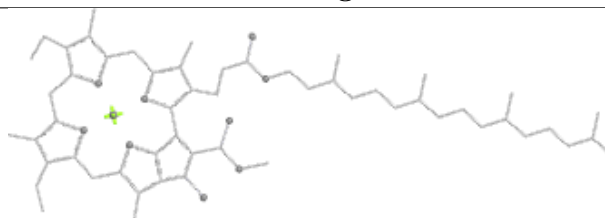
Bond lengths



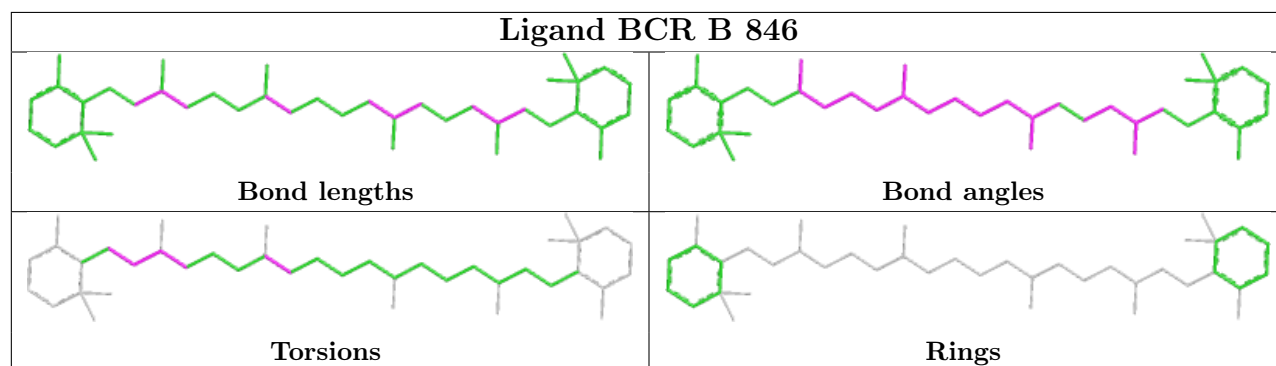
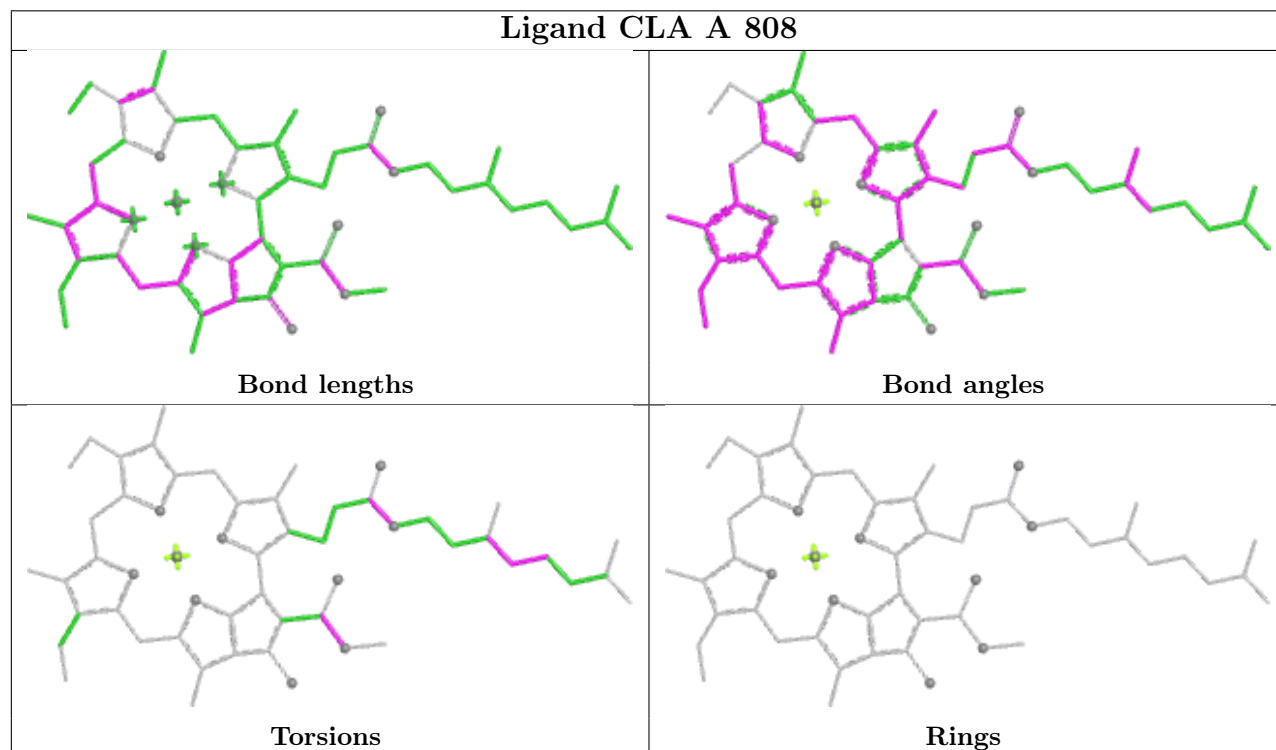
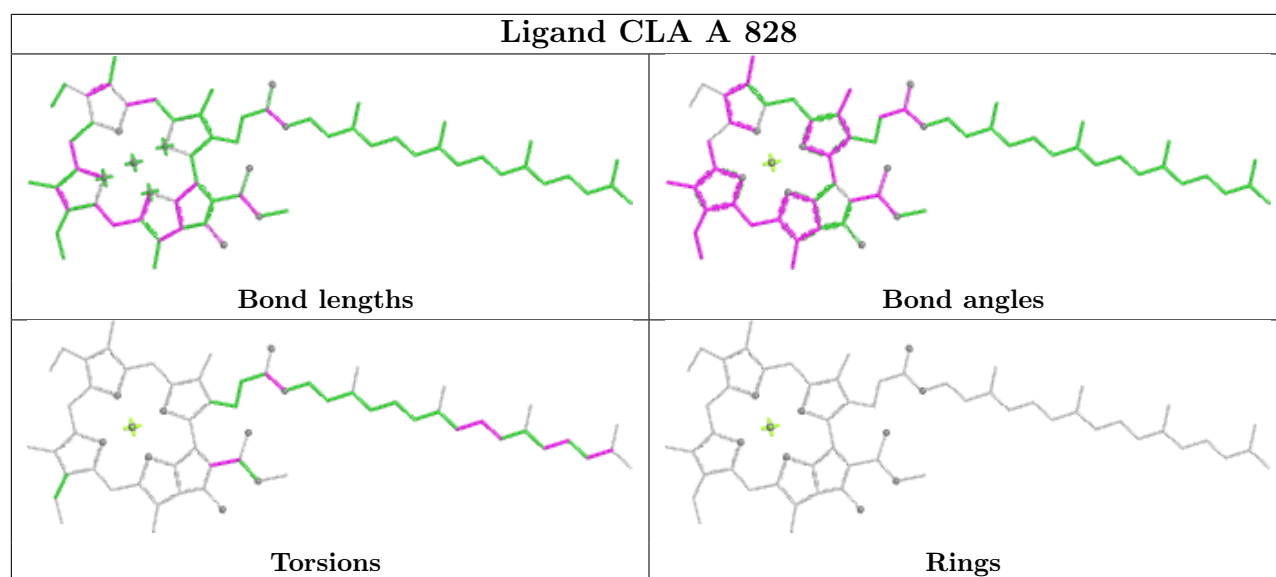
Bond angles

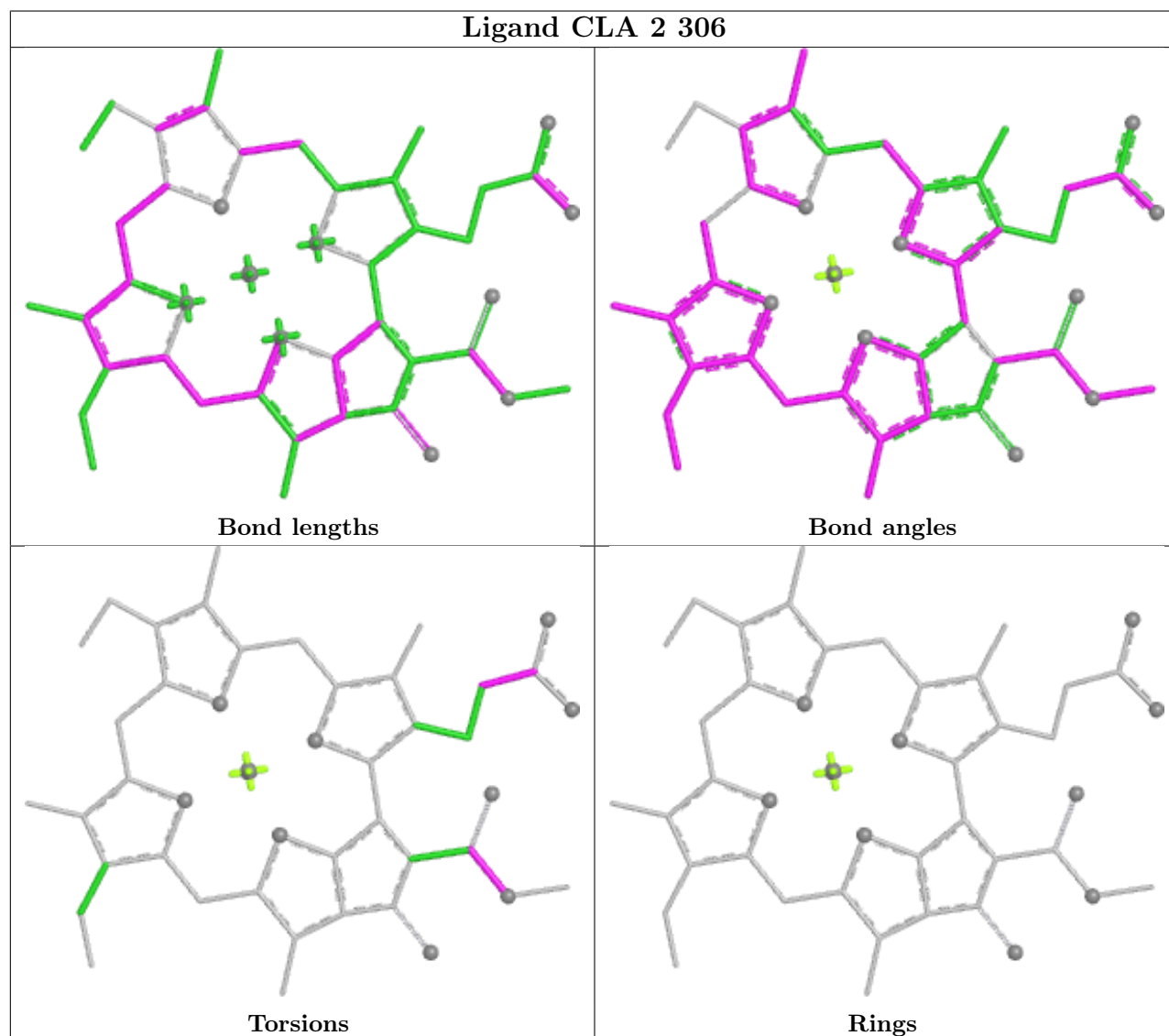
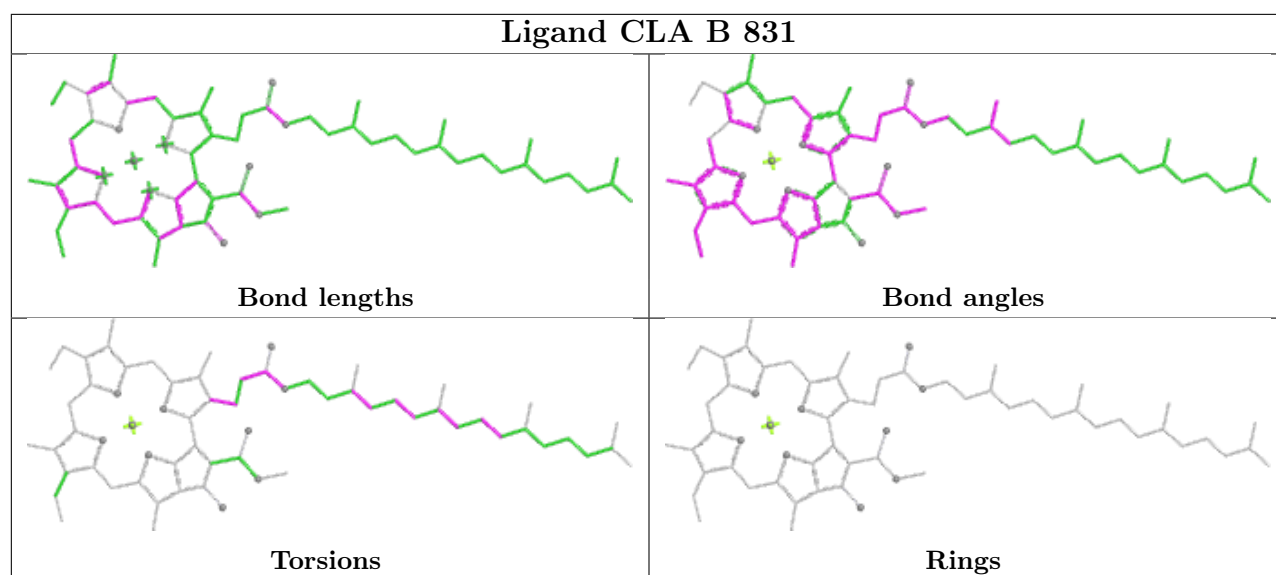


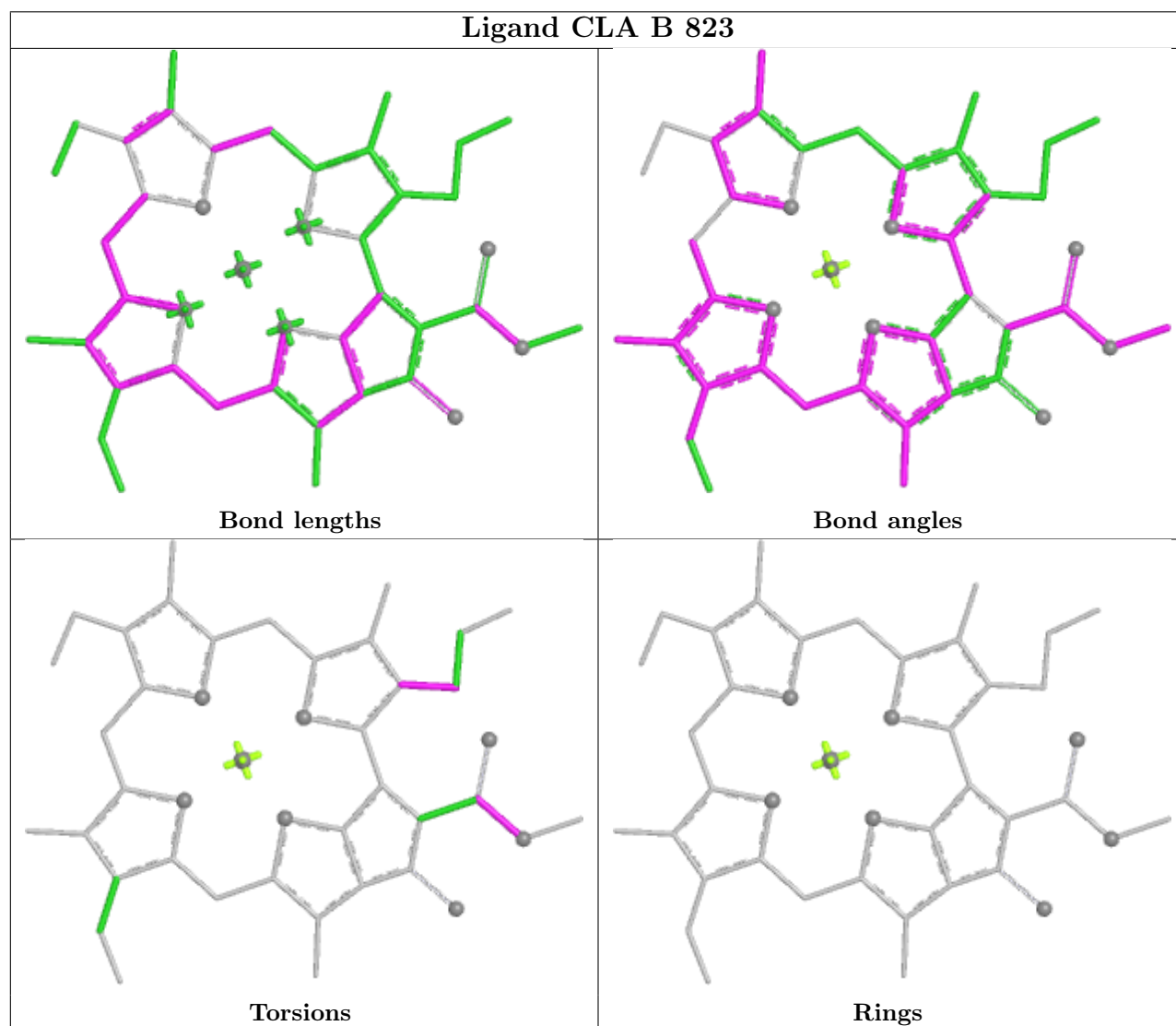
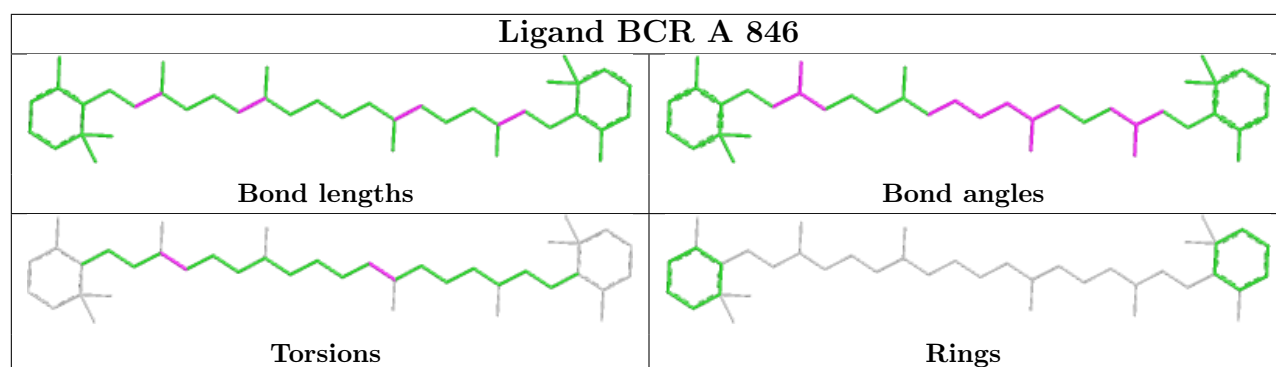
Torsions

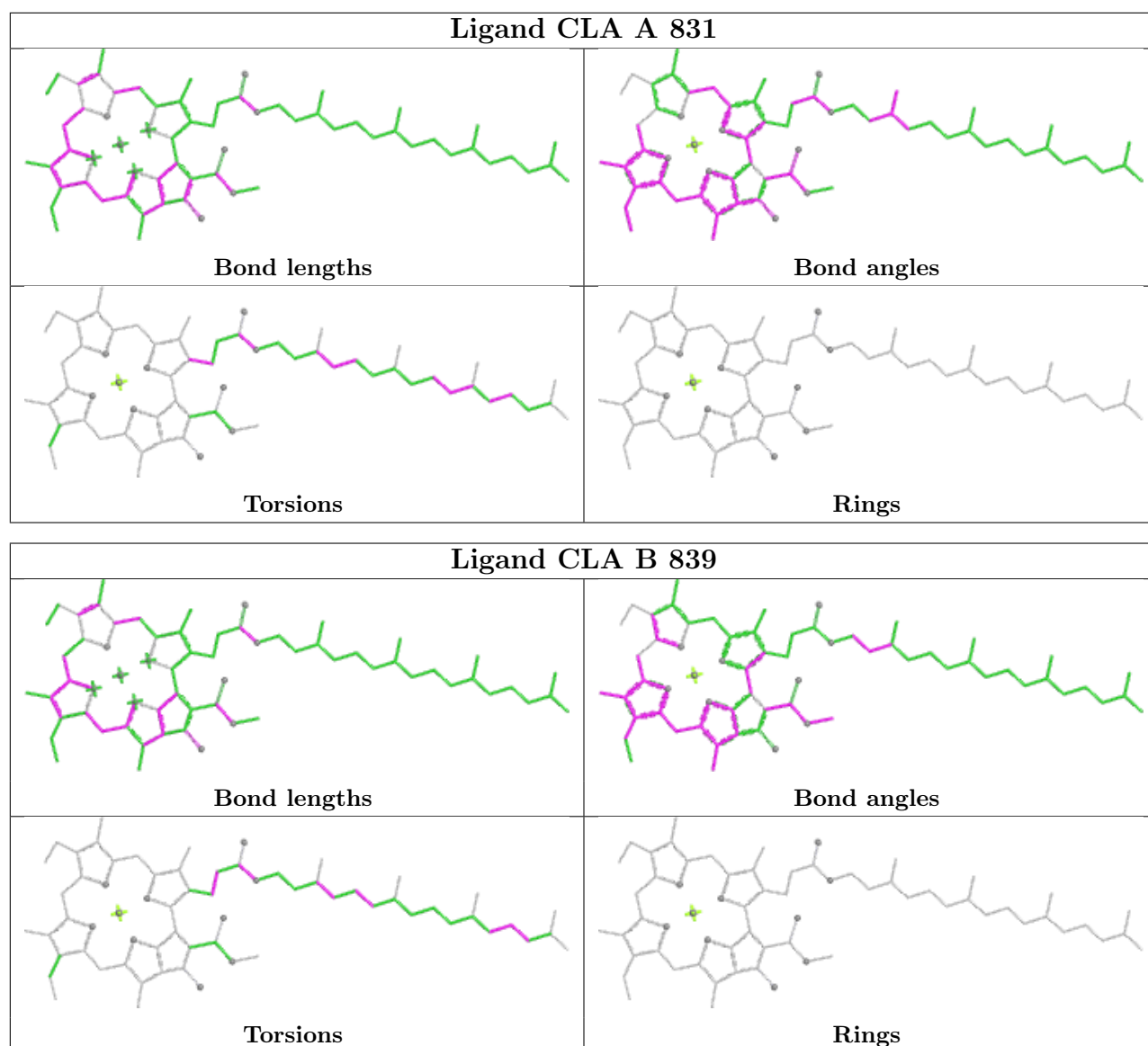


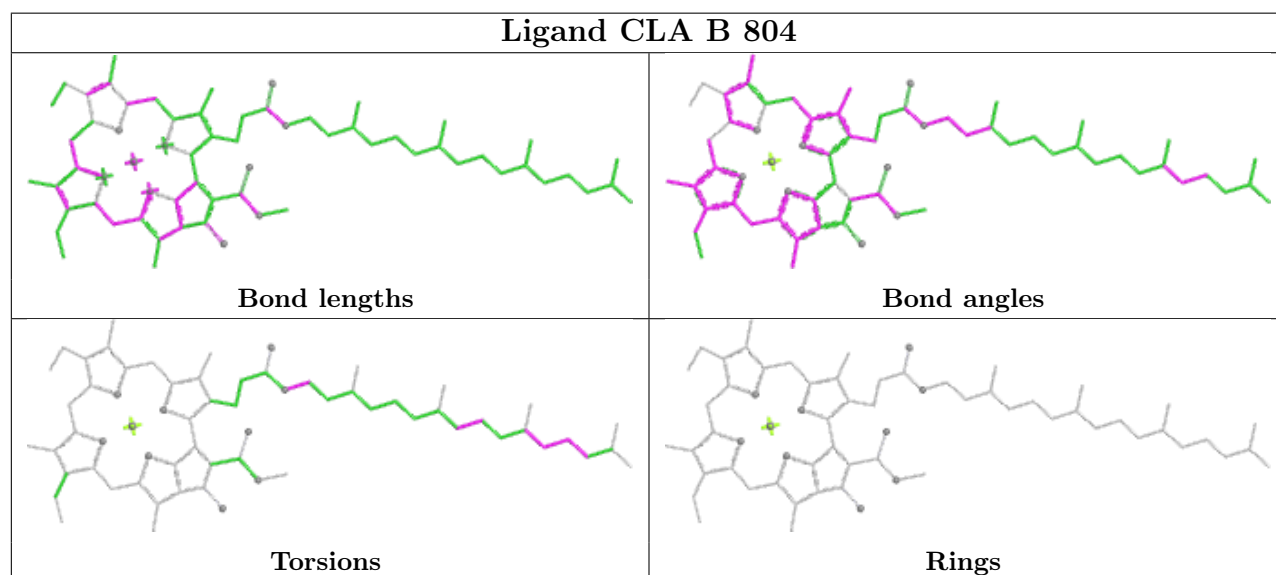
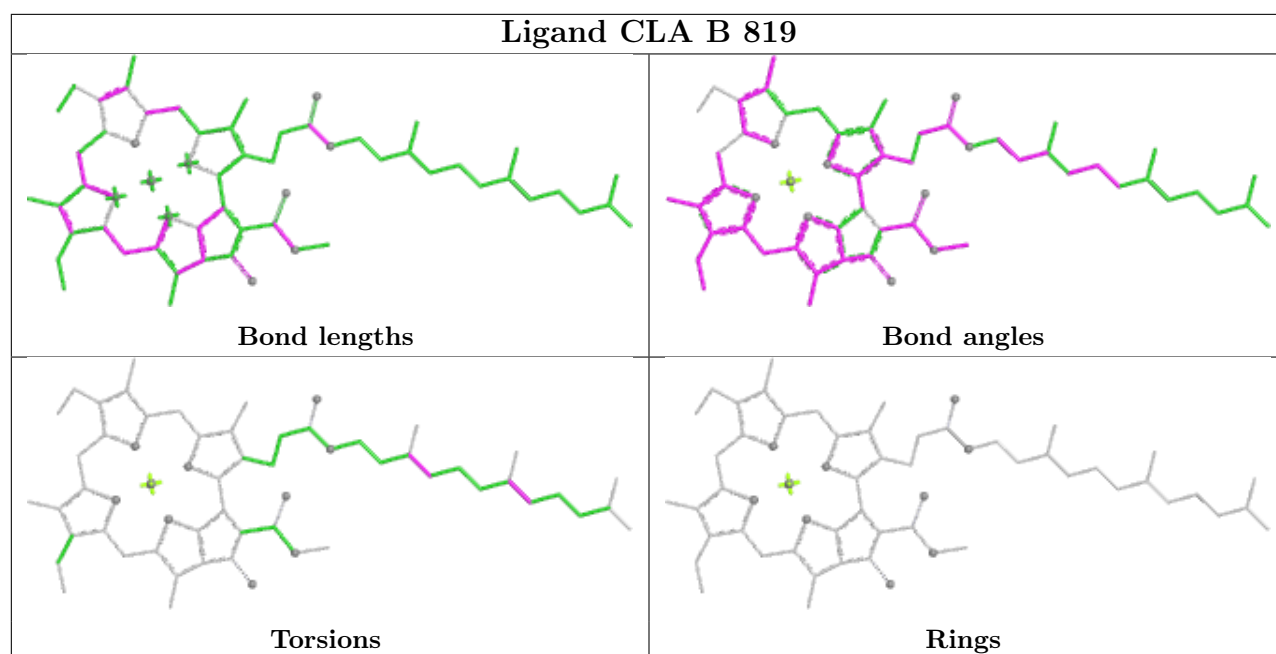
Rings

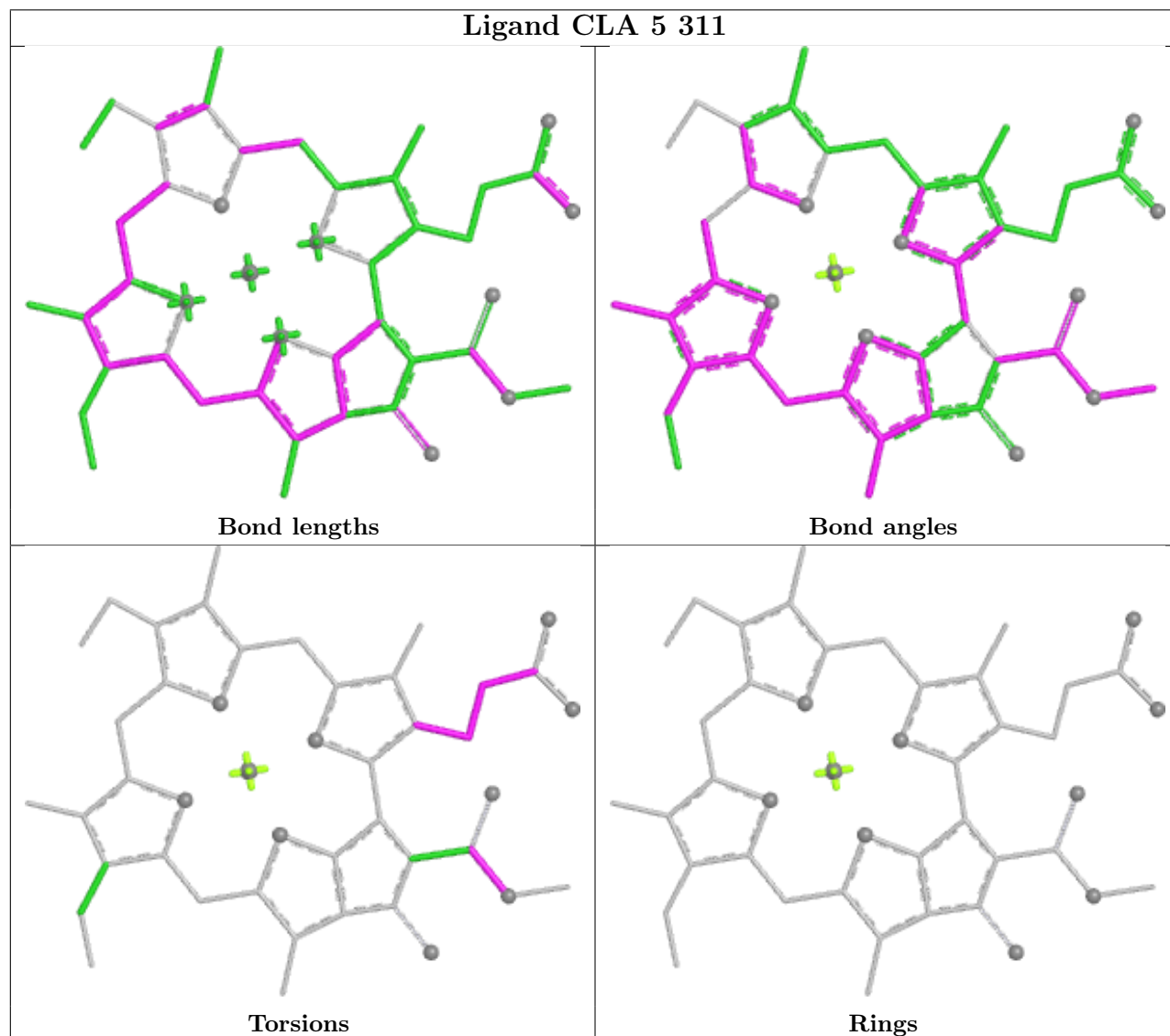
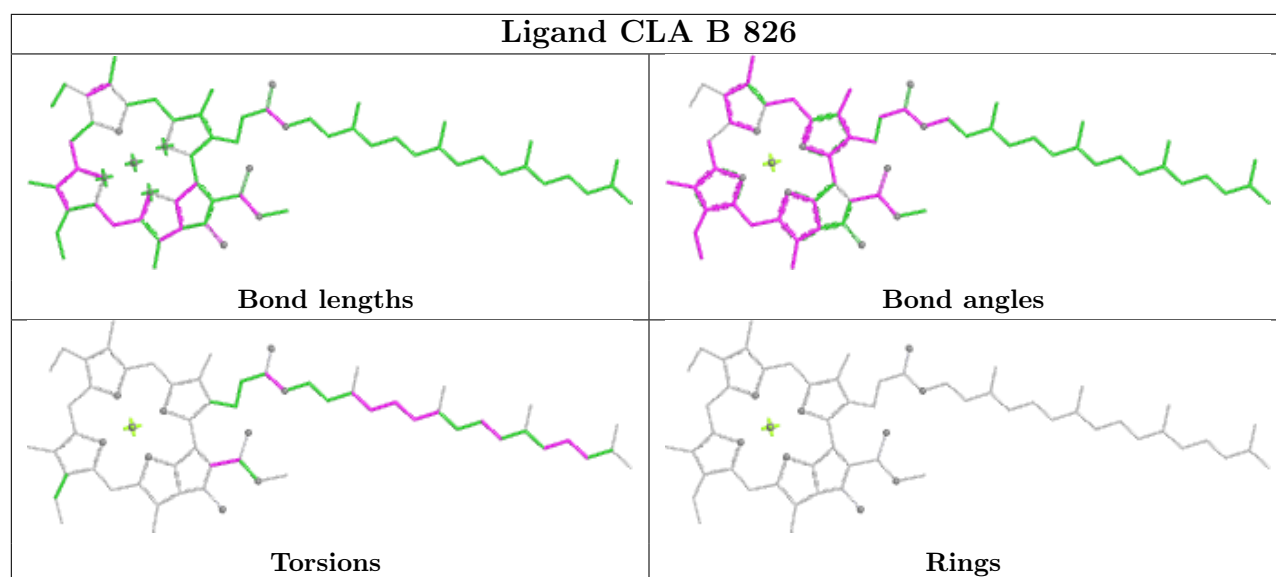


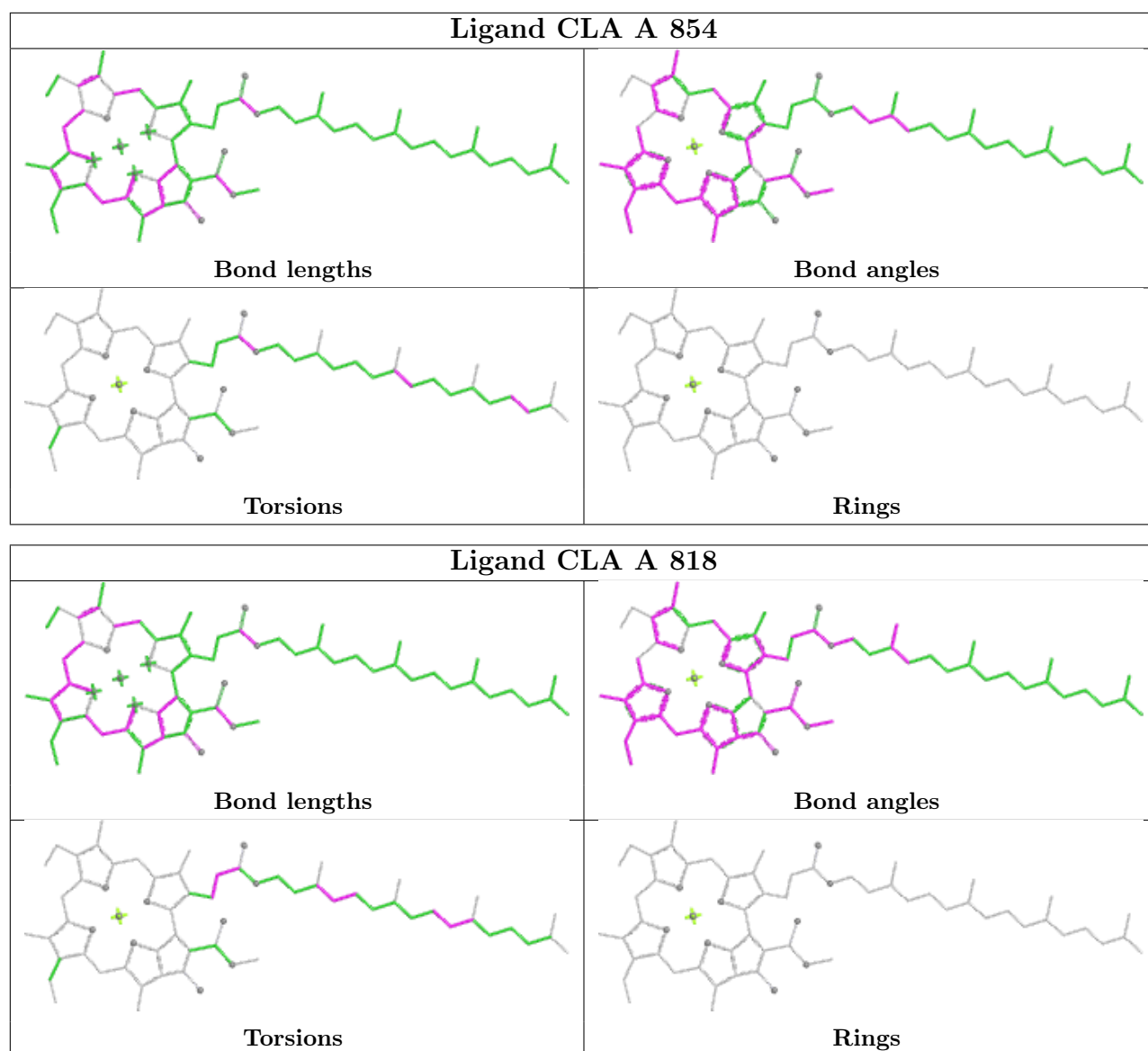


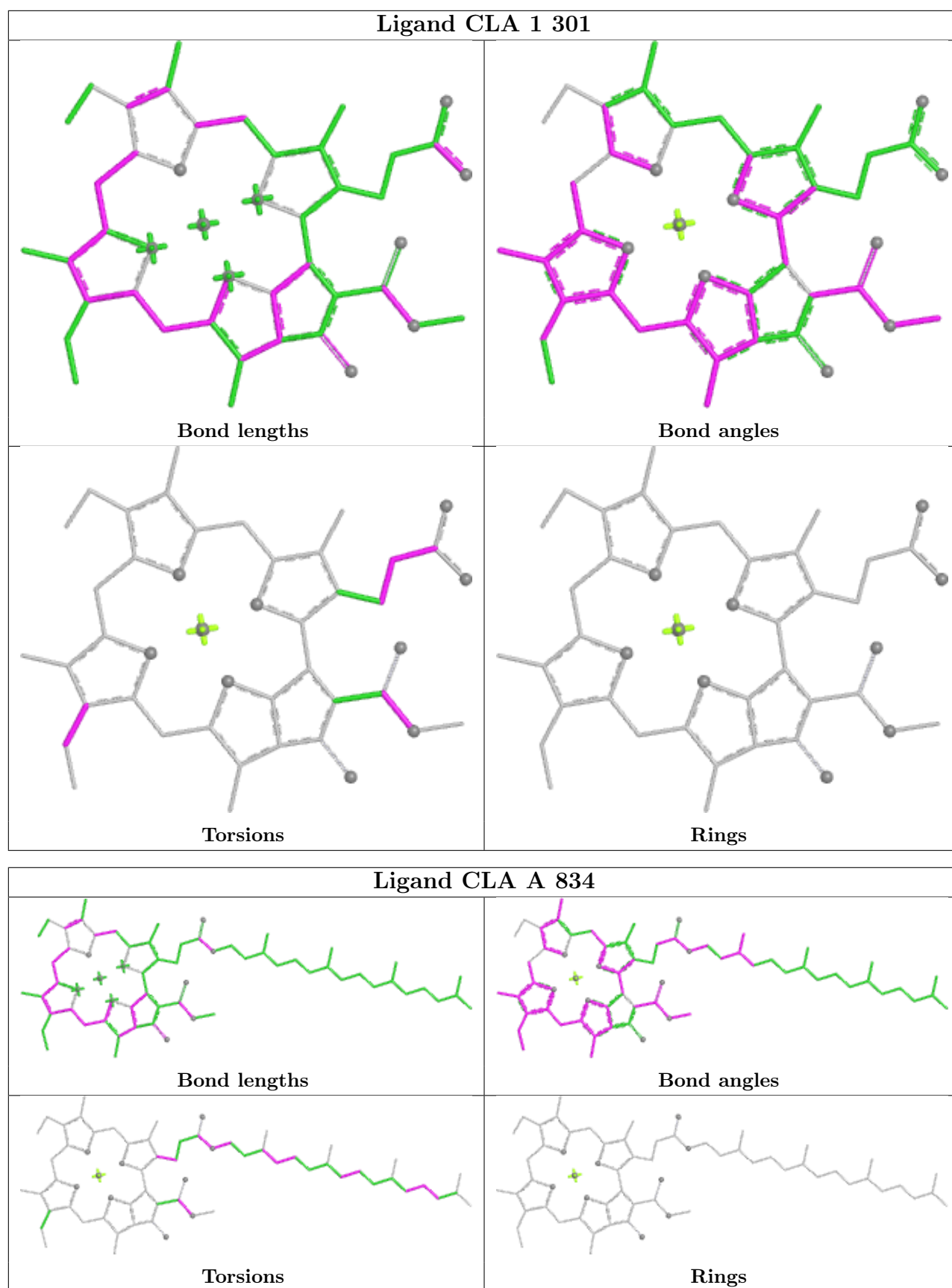




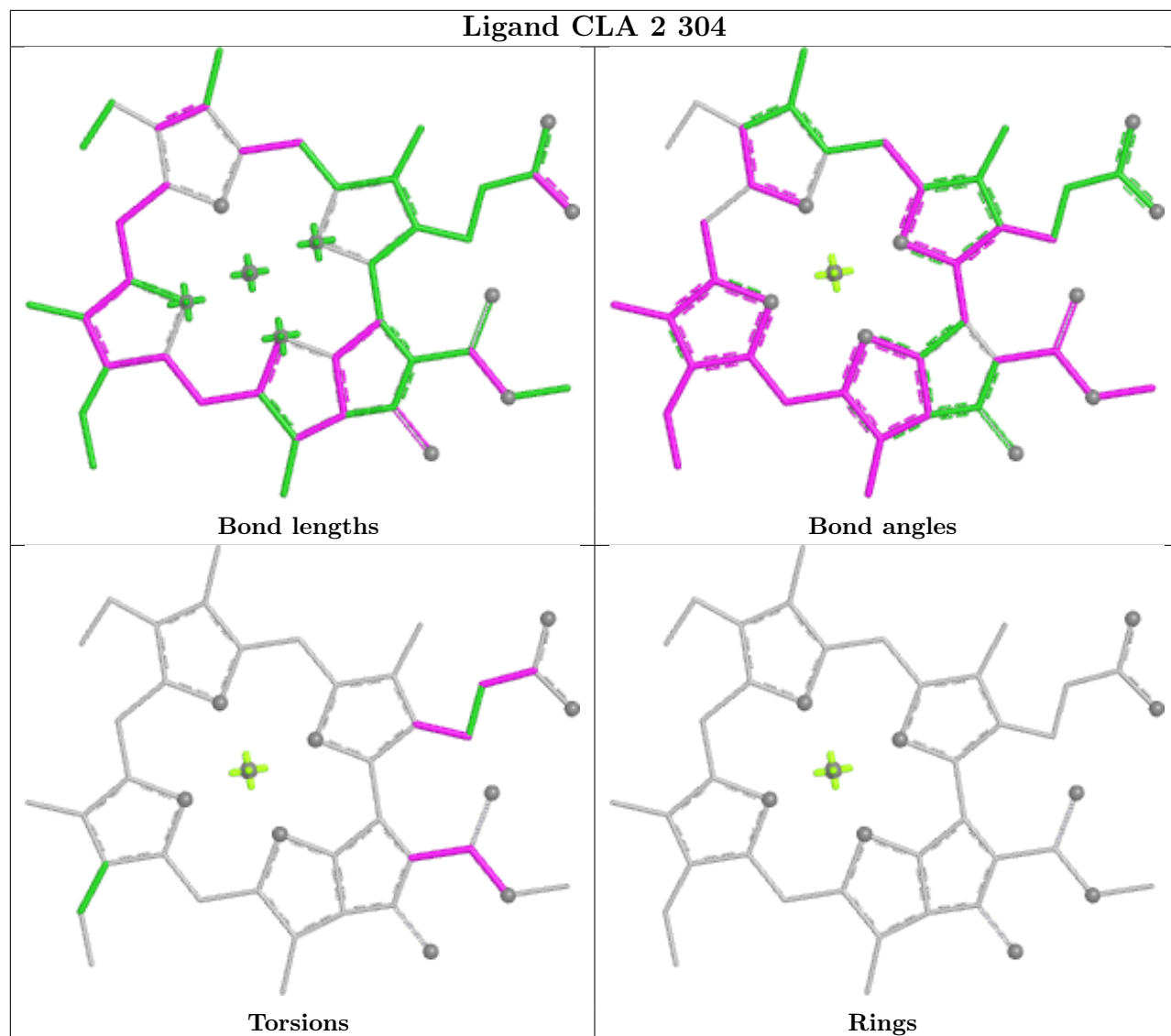




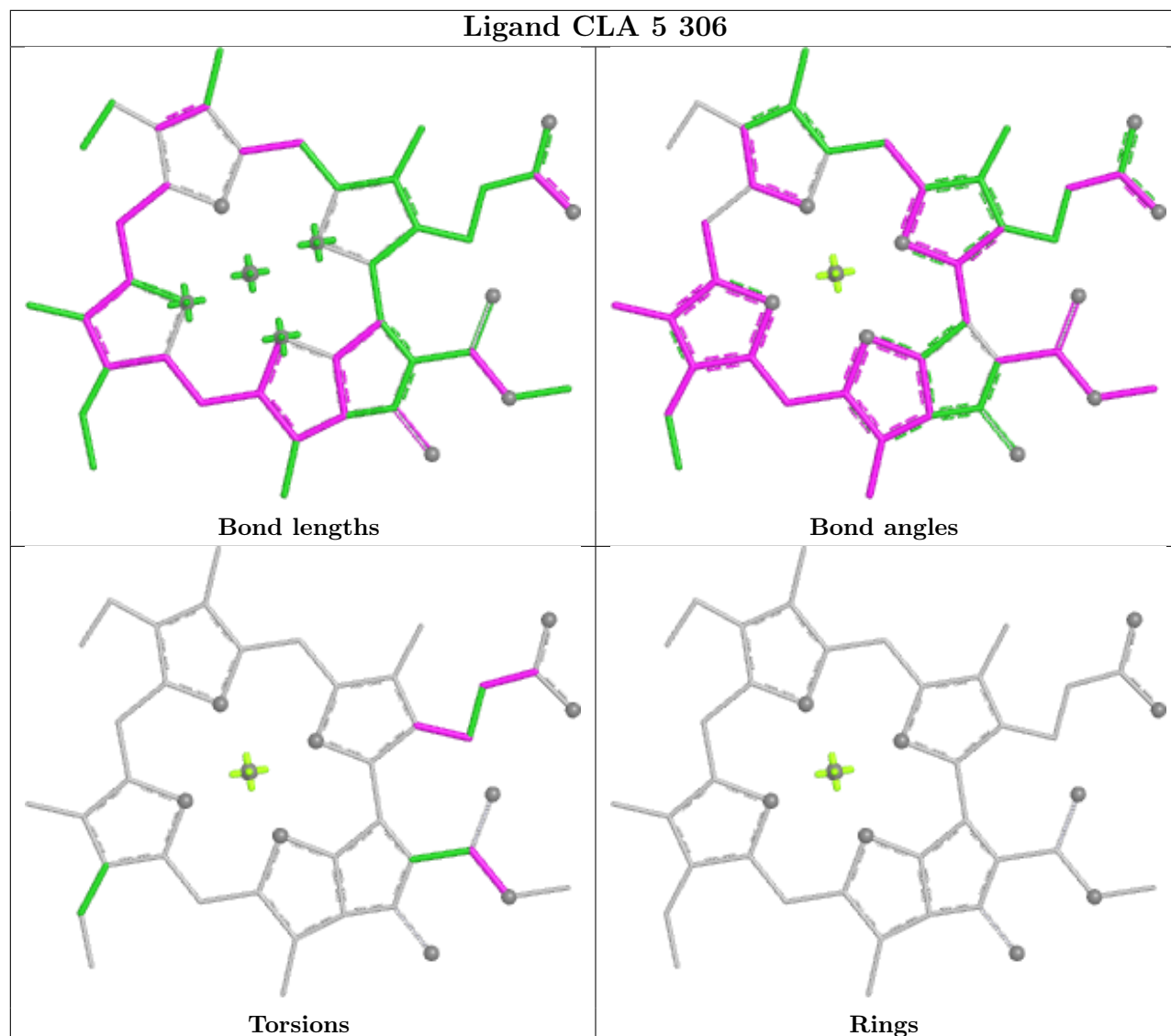




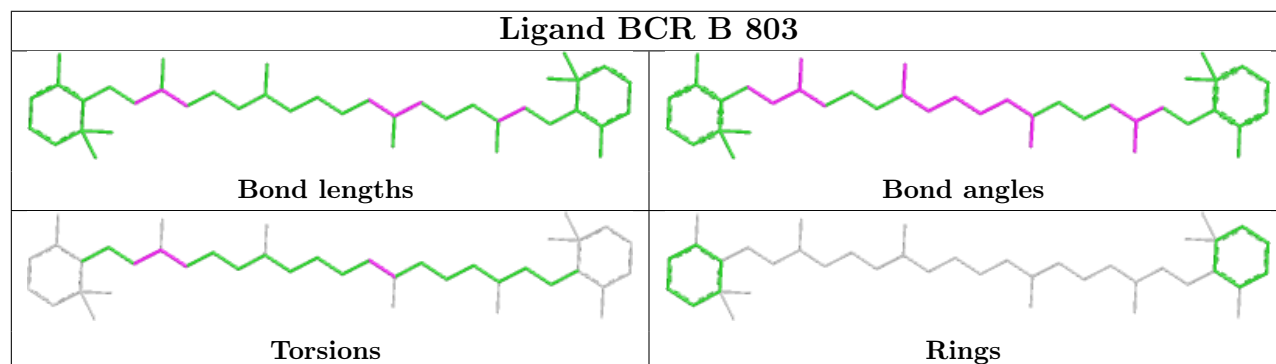
Ligand CLA 2 304

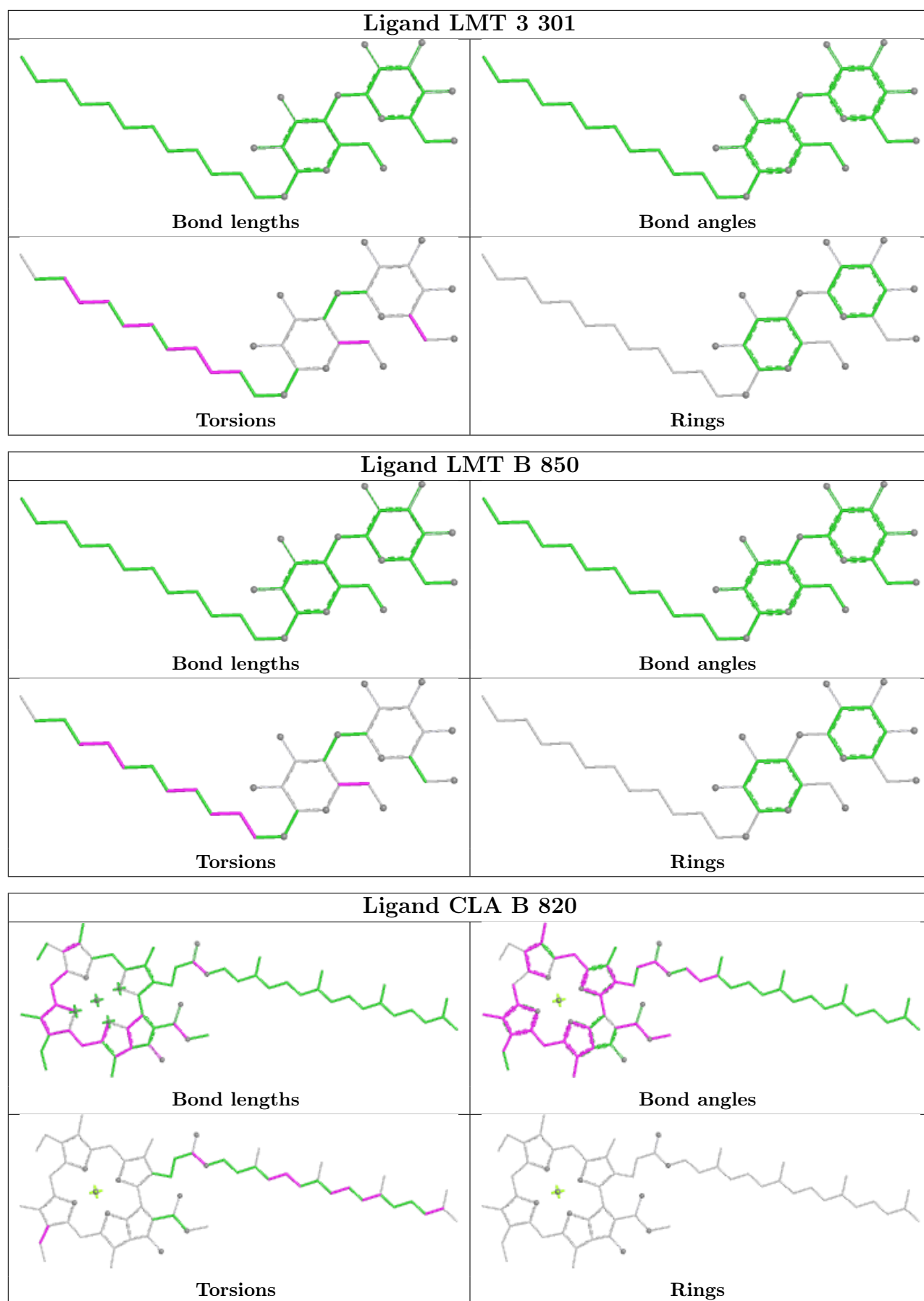


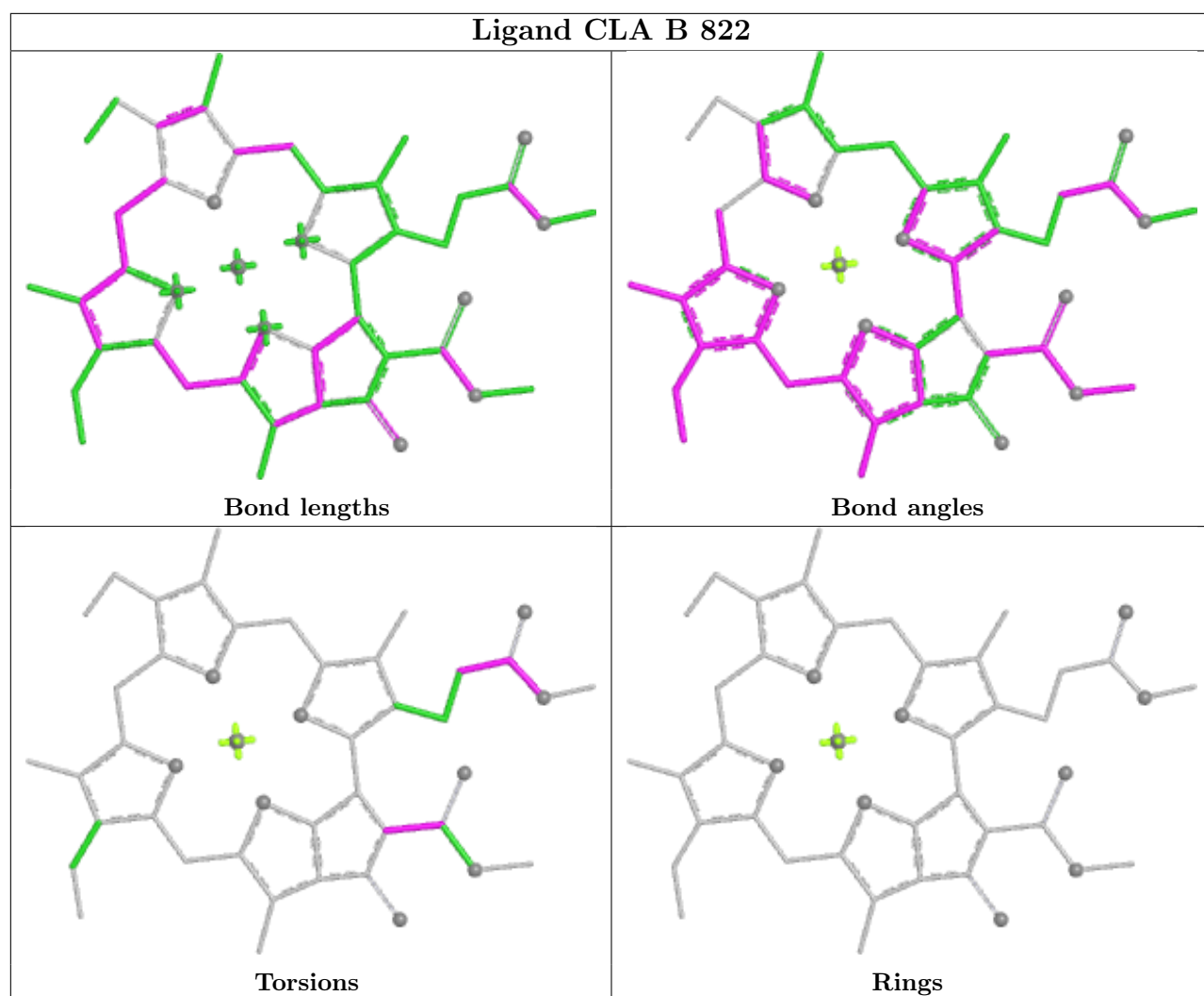
Ligand CLA 5 306



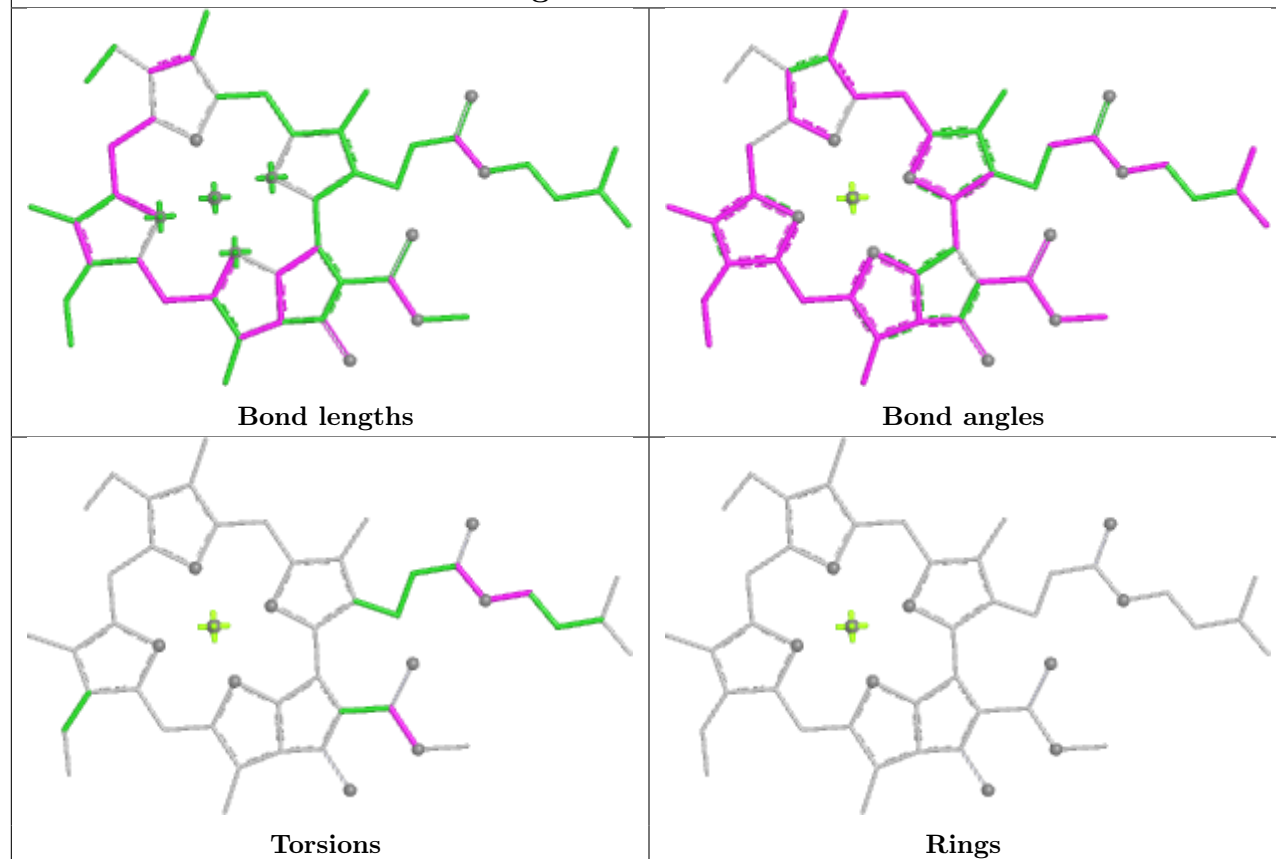
Ligand BCR B 803



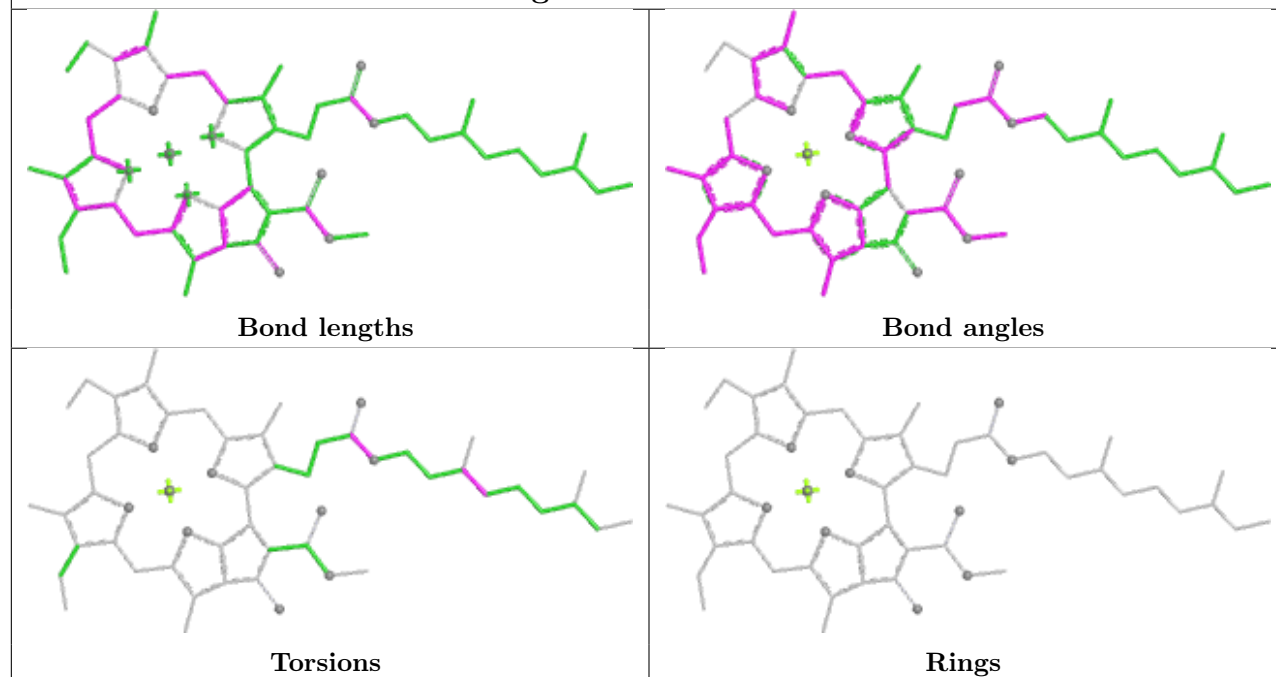


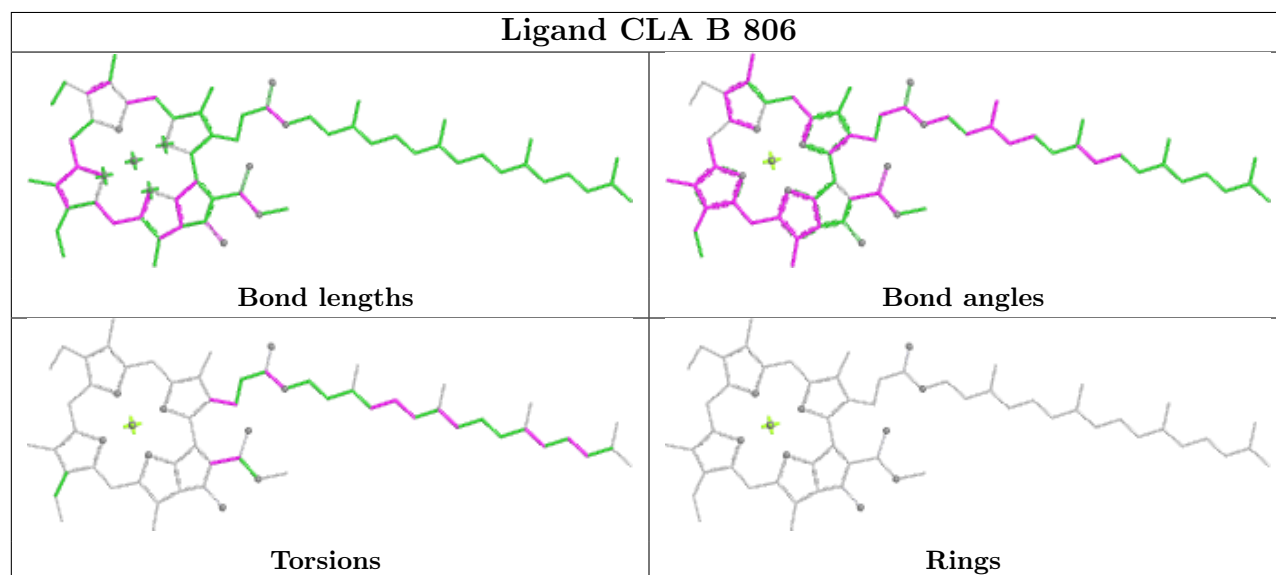
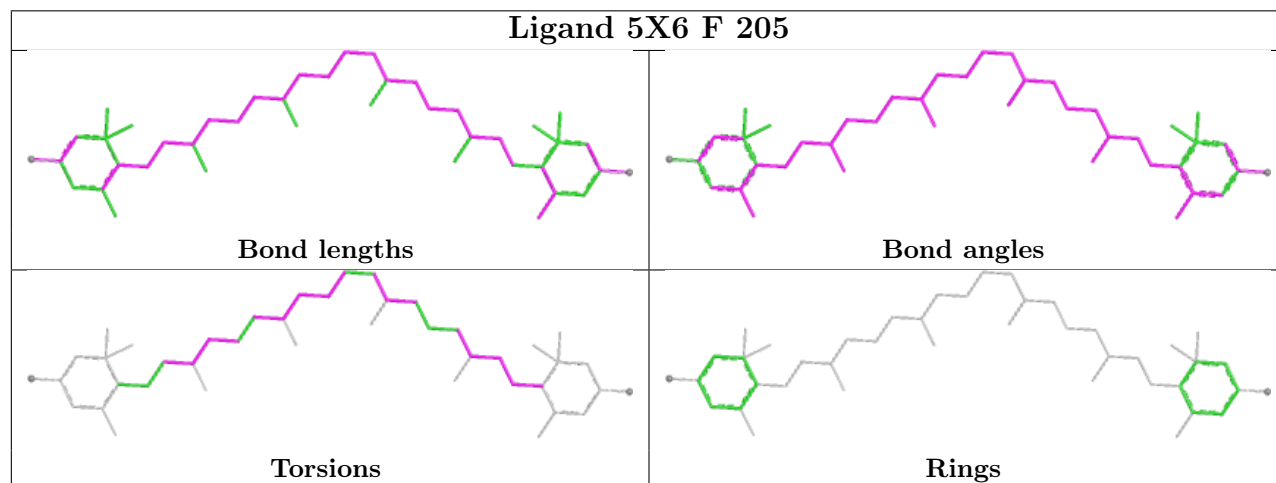
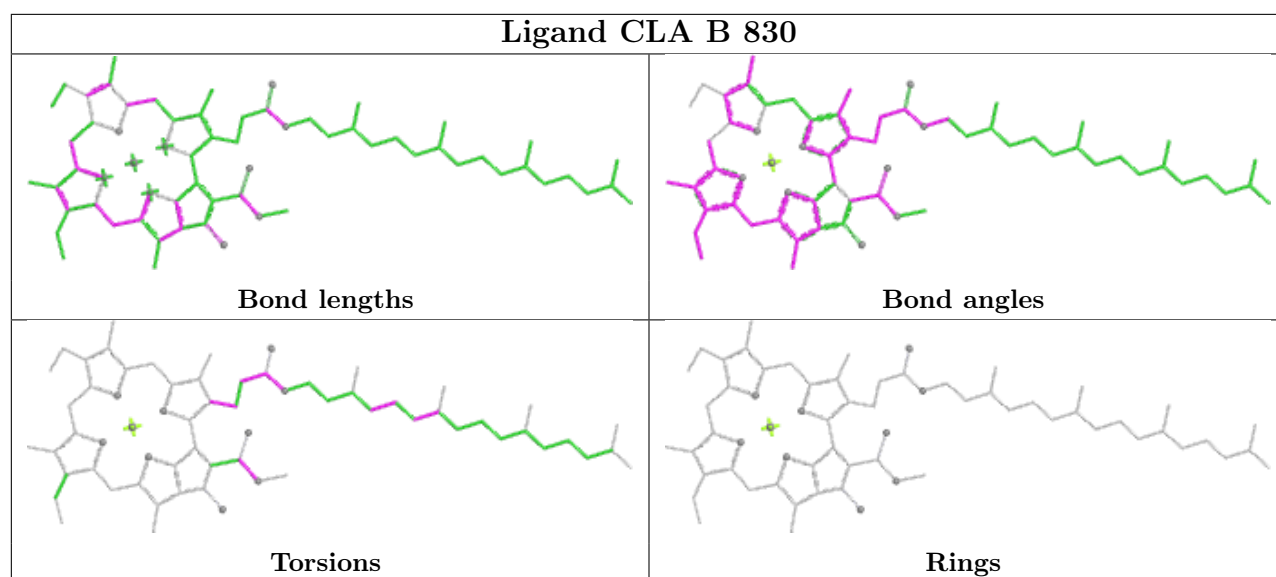


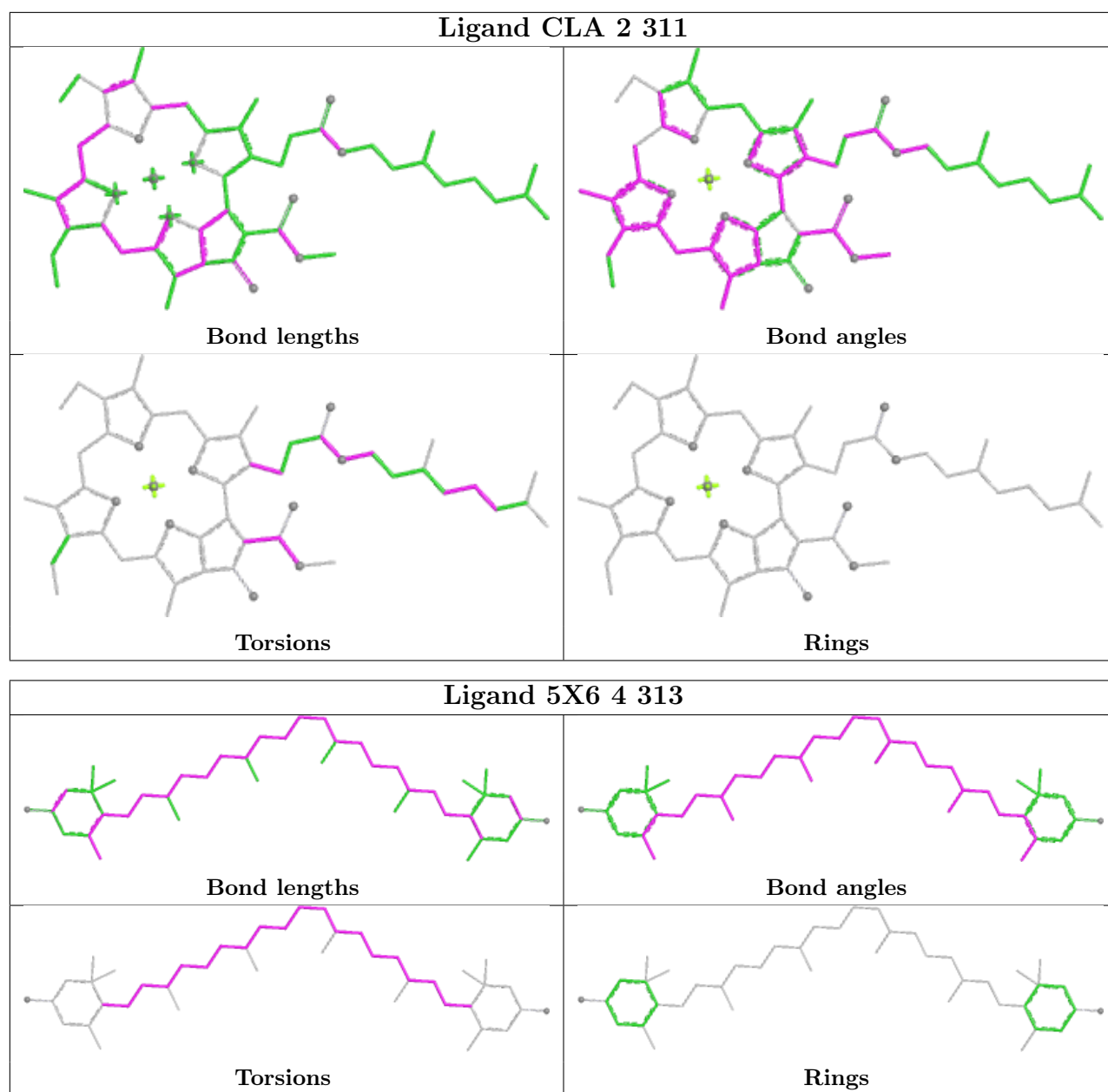
Ligand CLA A 829



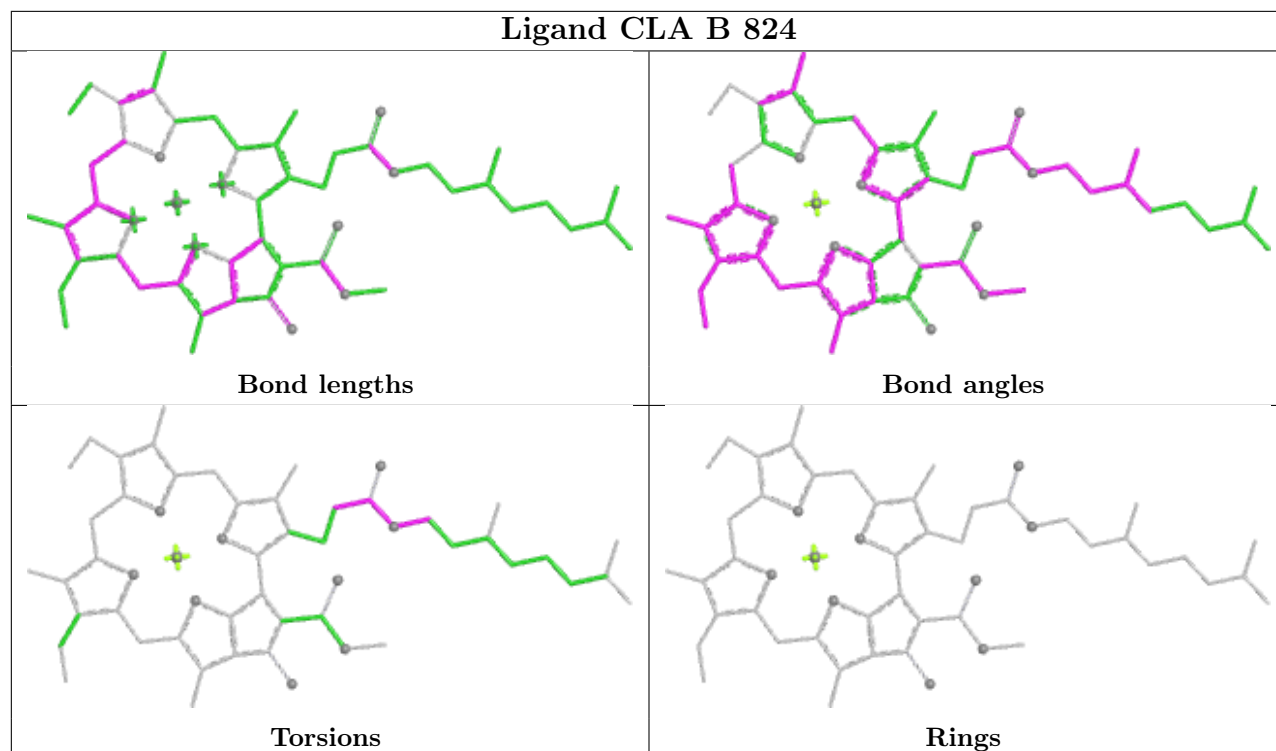
Ligand CLA A 836



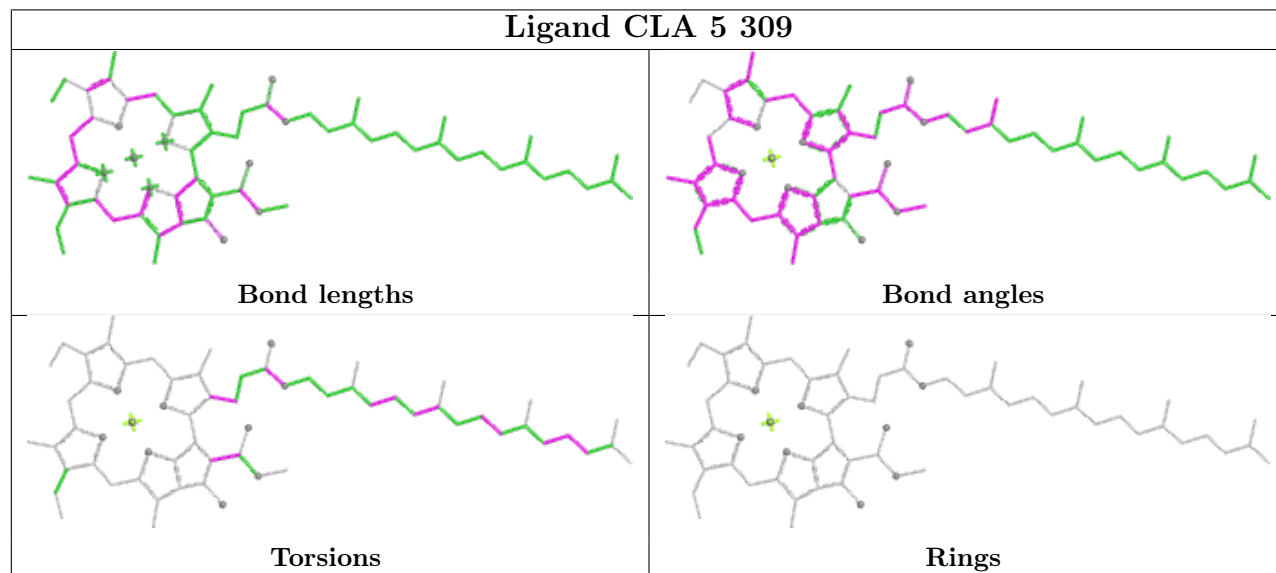




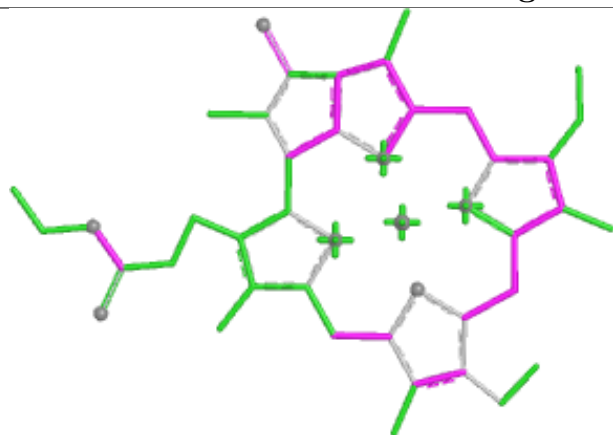
Ligand CLA B 824



Ligand CLA 5 309



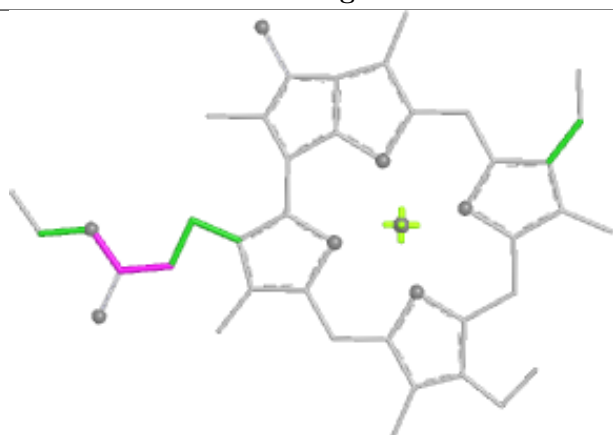
Ligand CLA 5 314



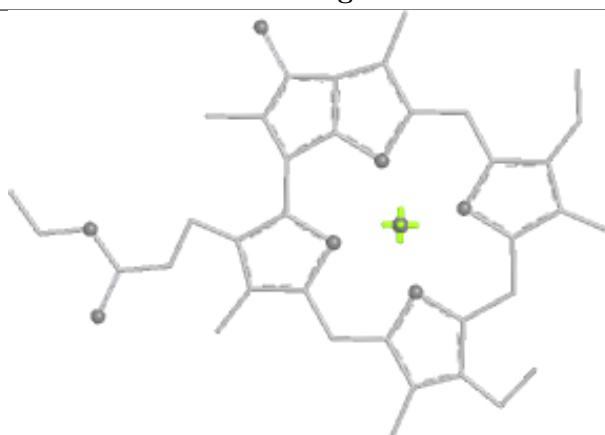
Bond lengths



Bond angles

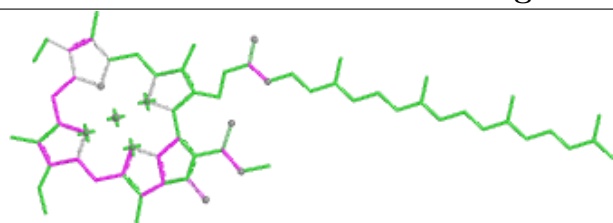


Torsions

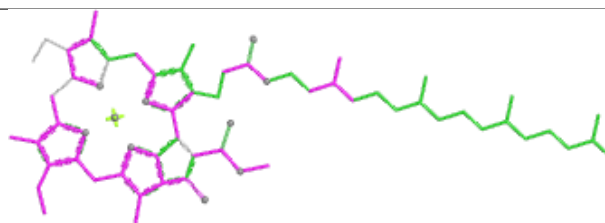


Rings

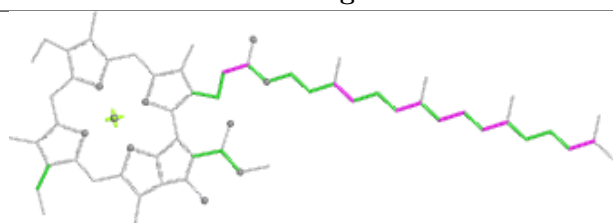
Ligand CLA B 807



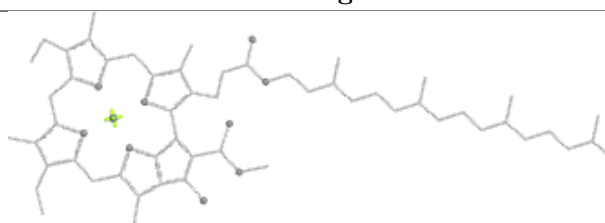
Bond lengths



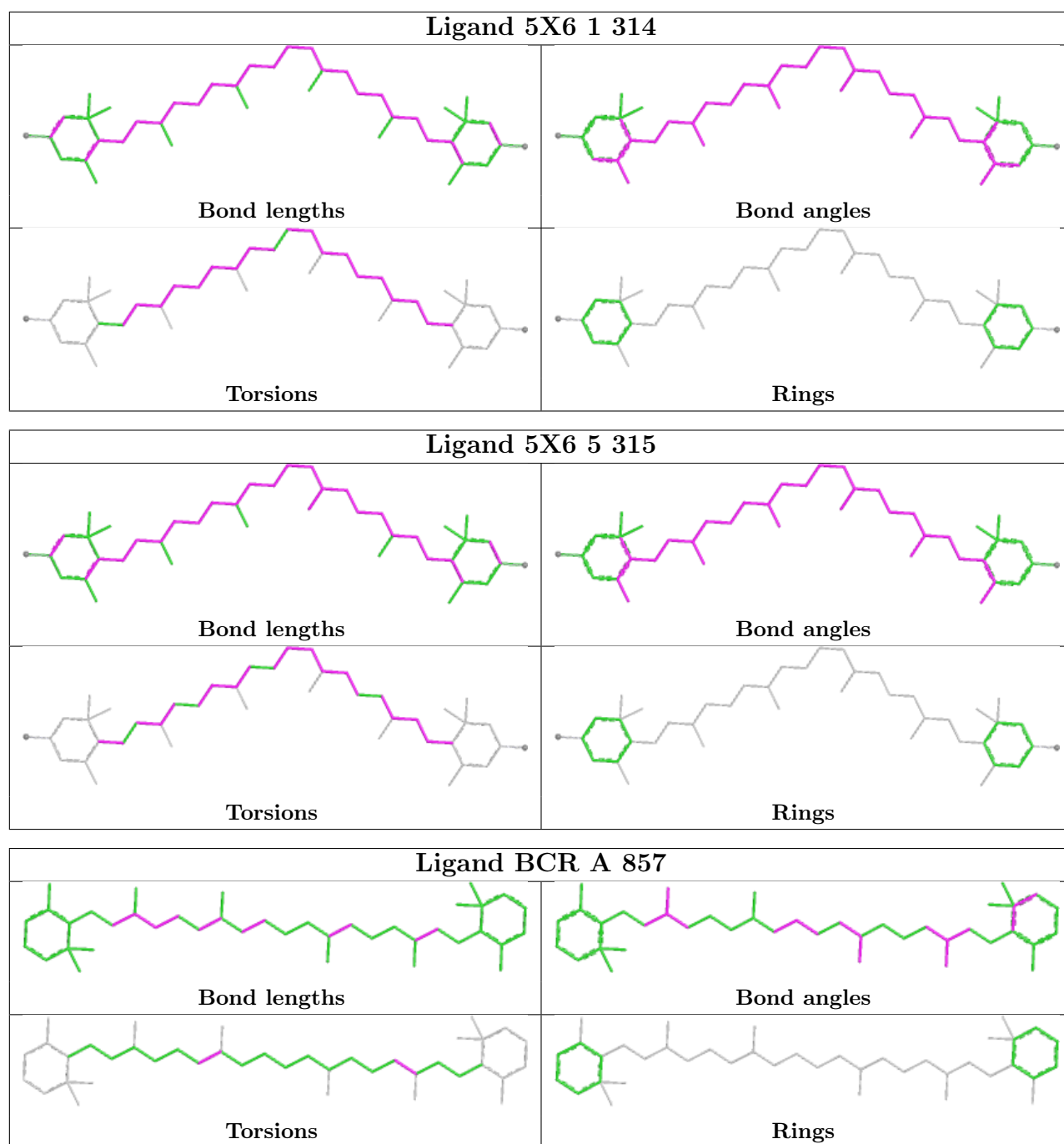
Bond angles



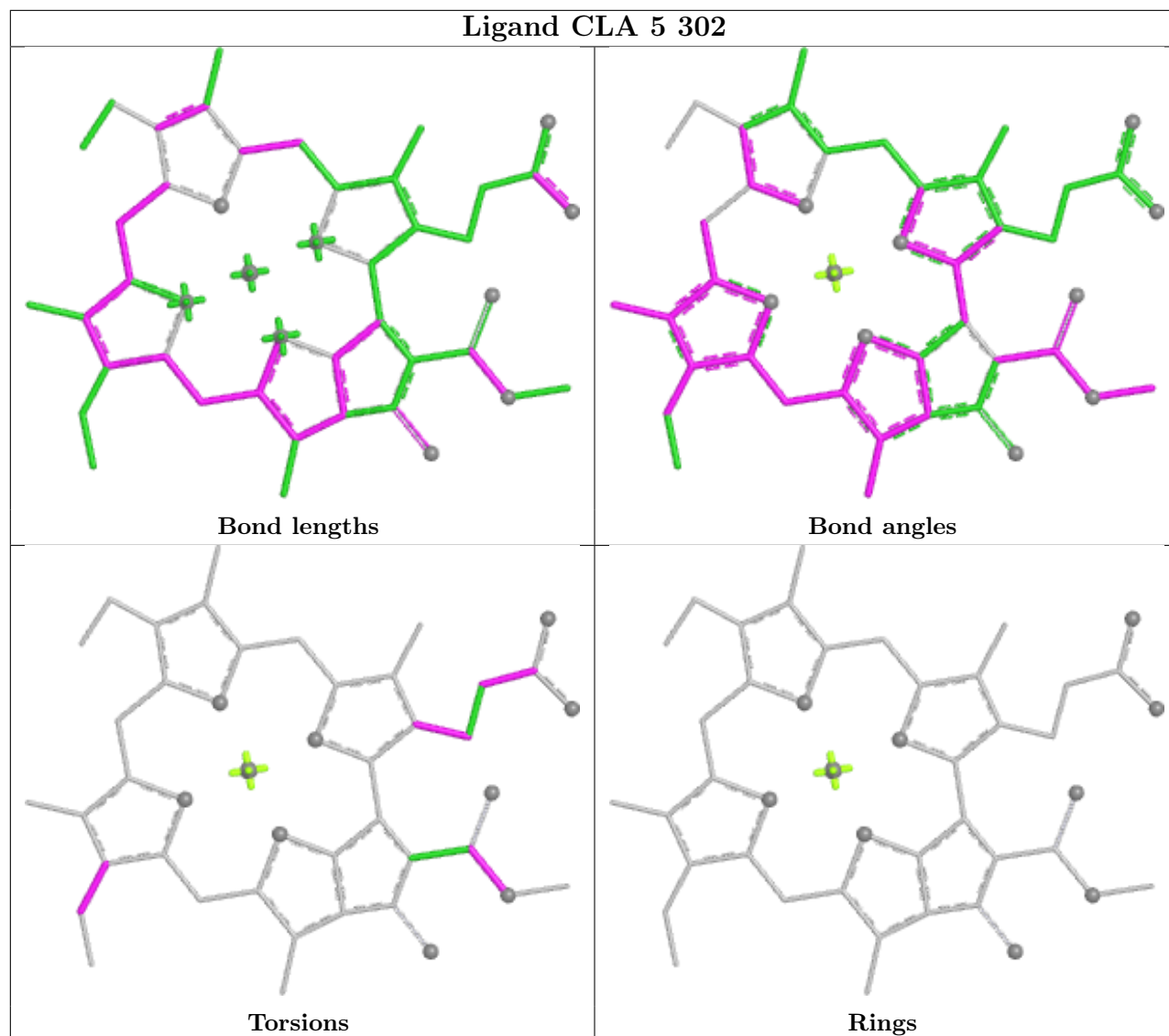
Torsions



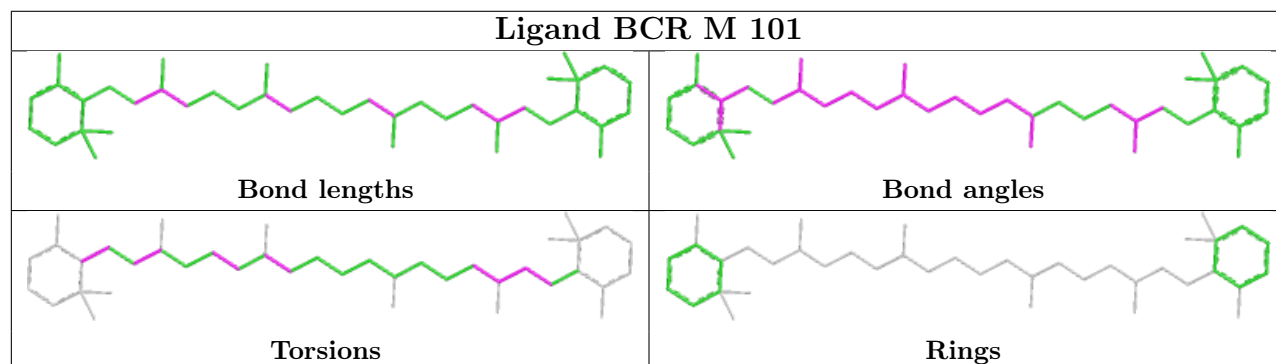
Rings

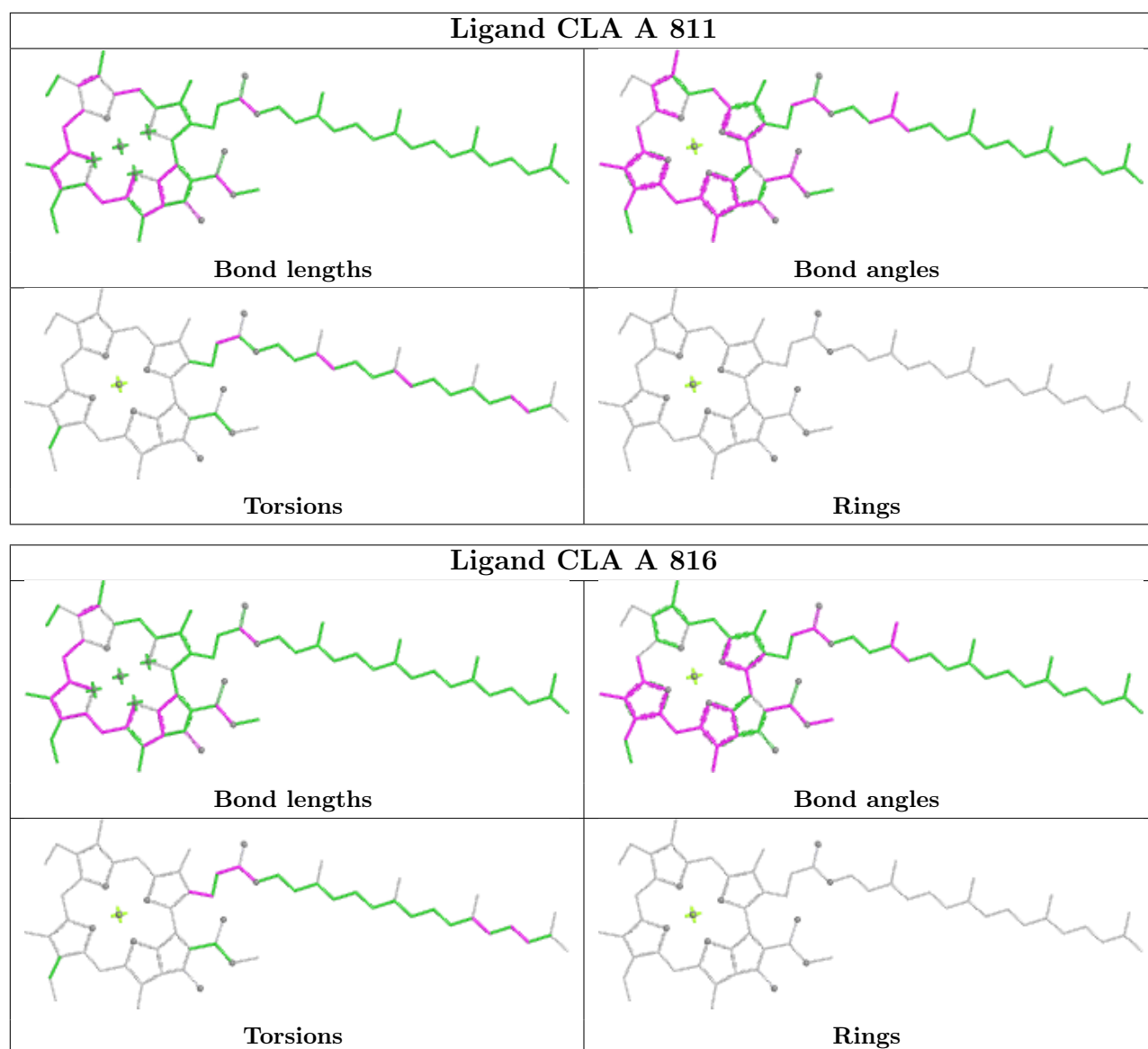


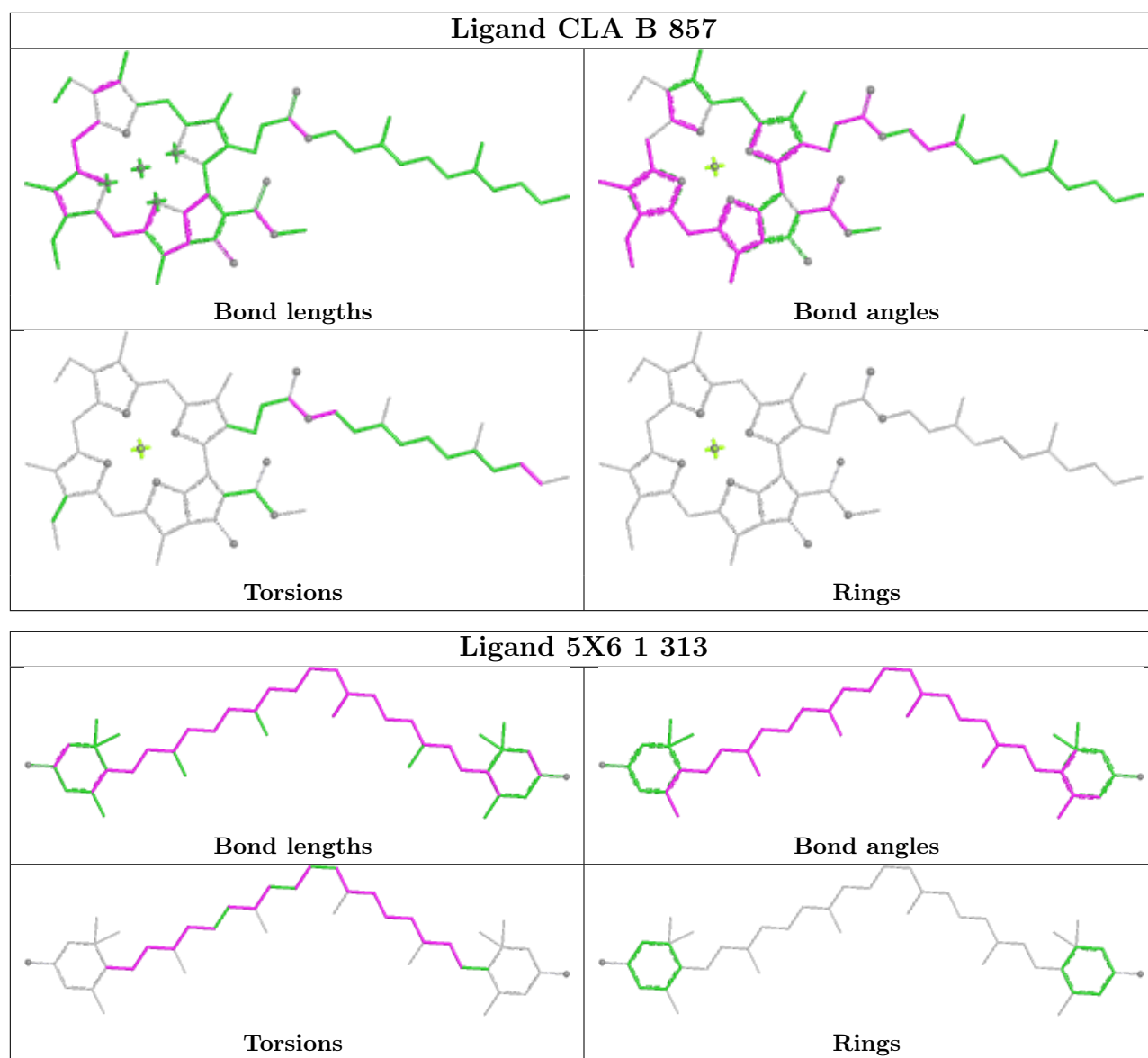
Ligand CLA 5 302

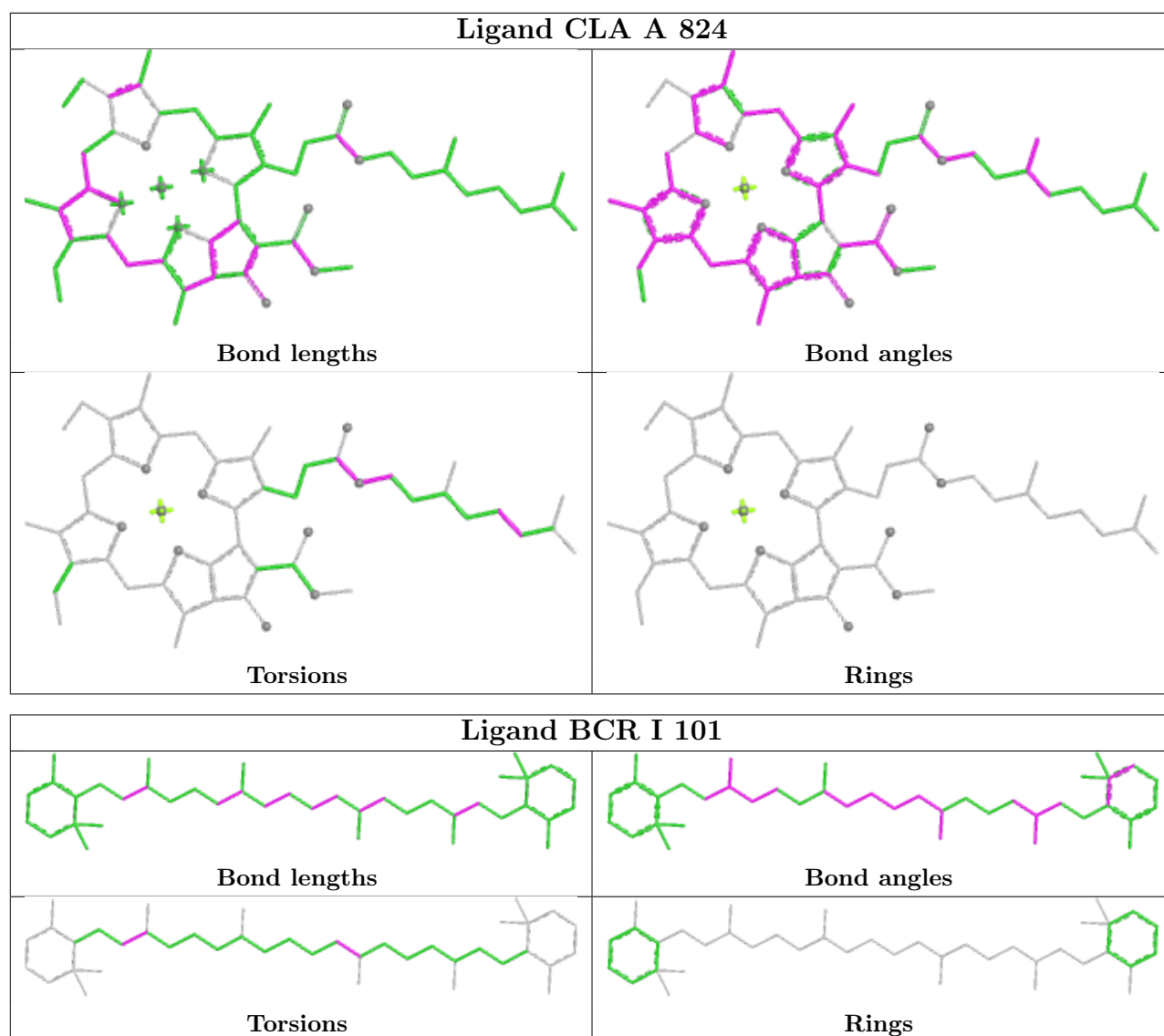


Ligand BCR M 101

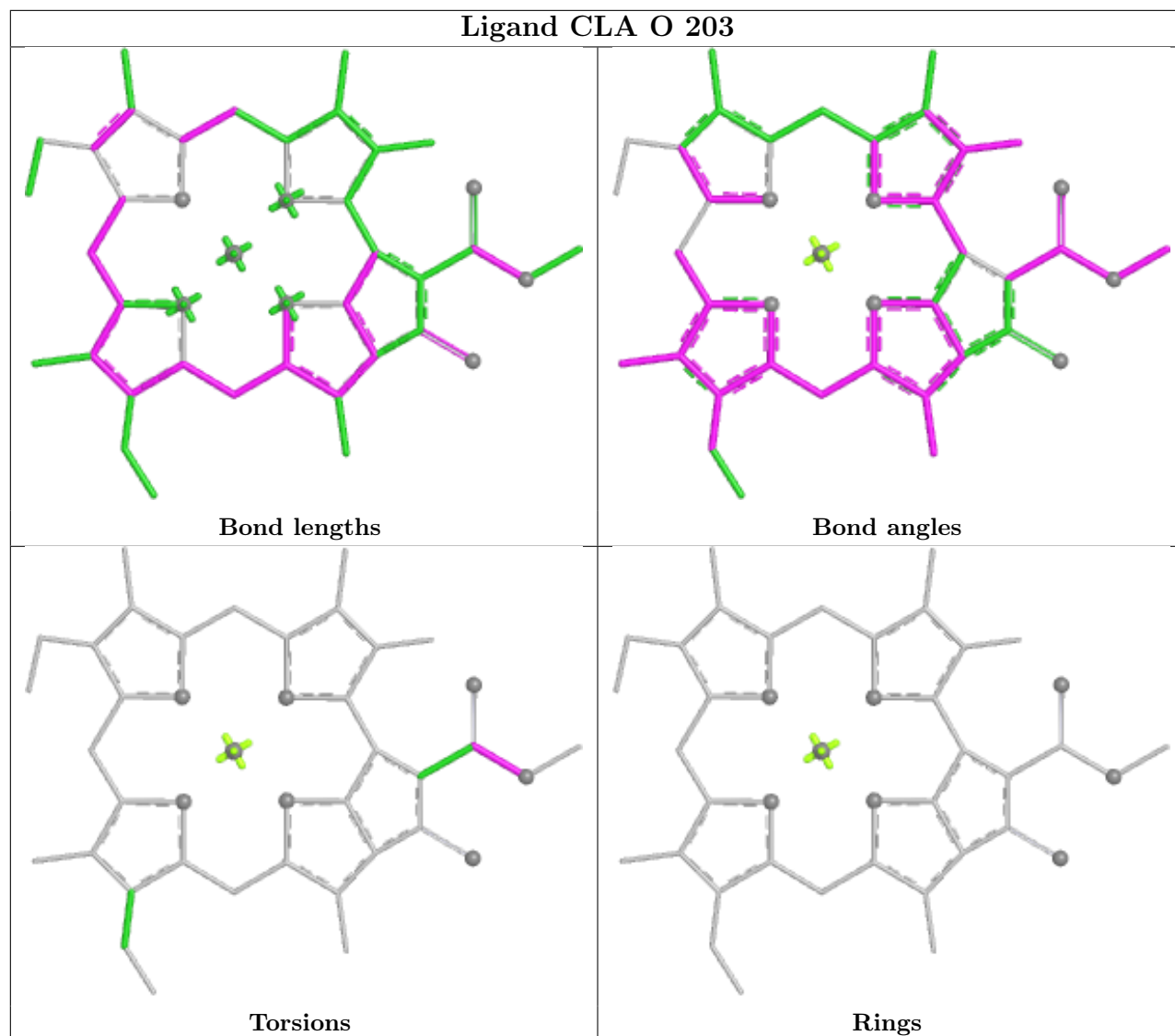




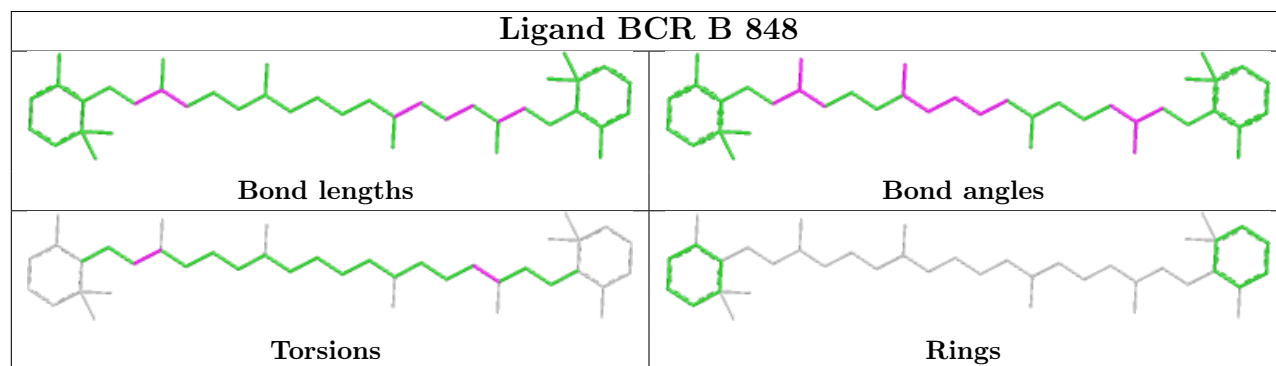




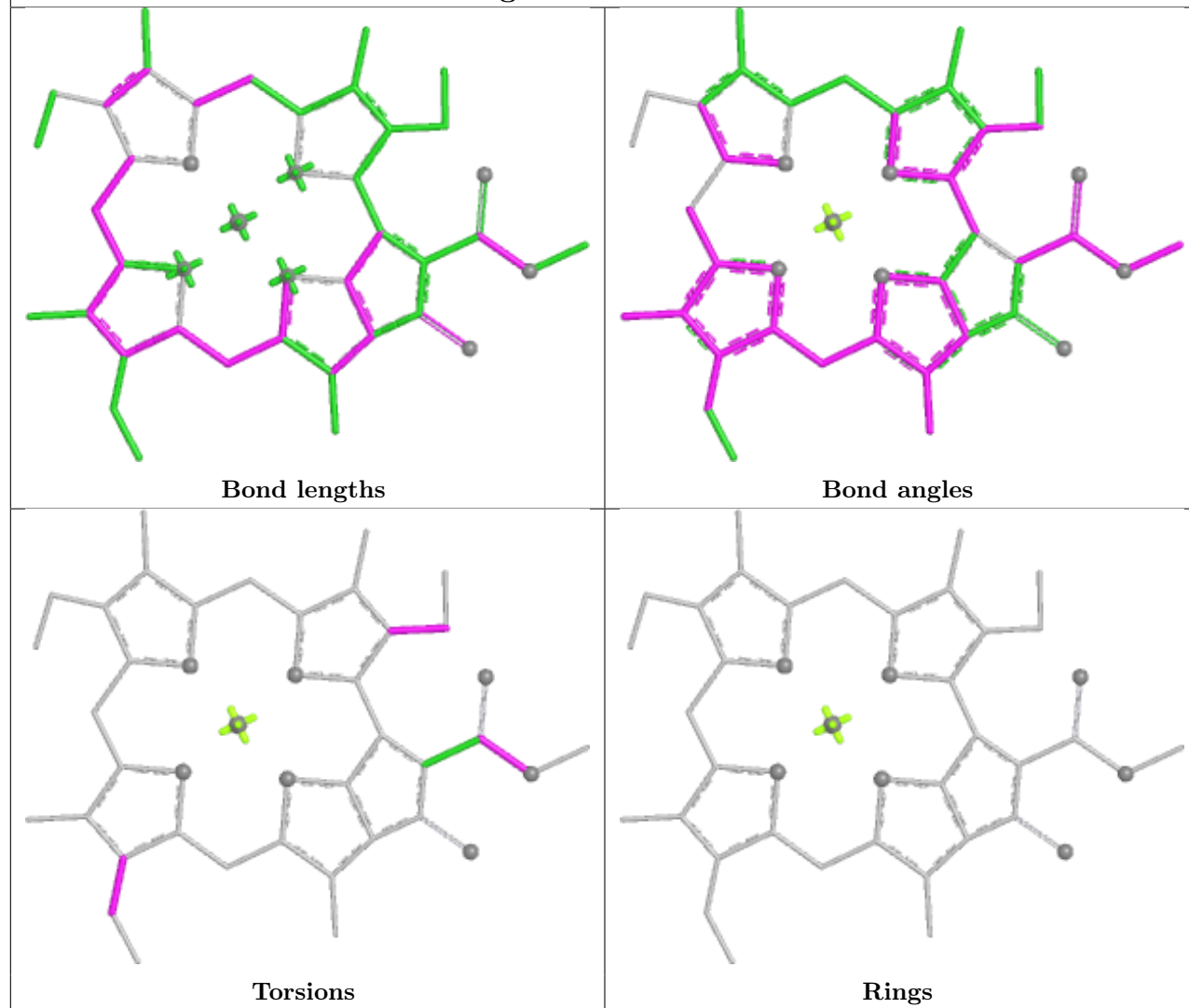
Ligand CLA O 203



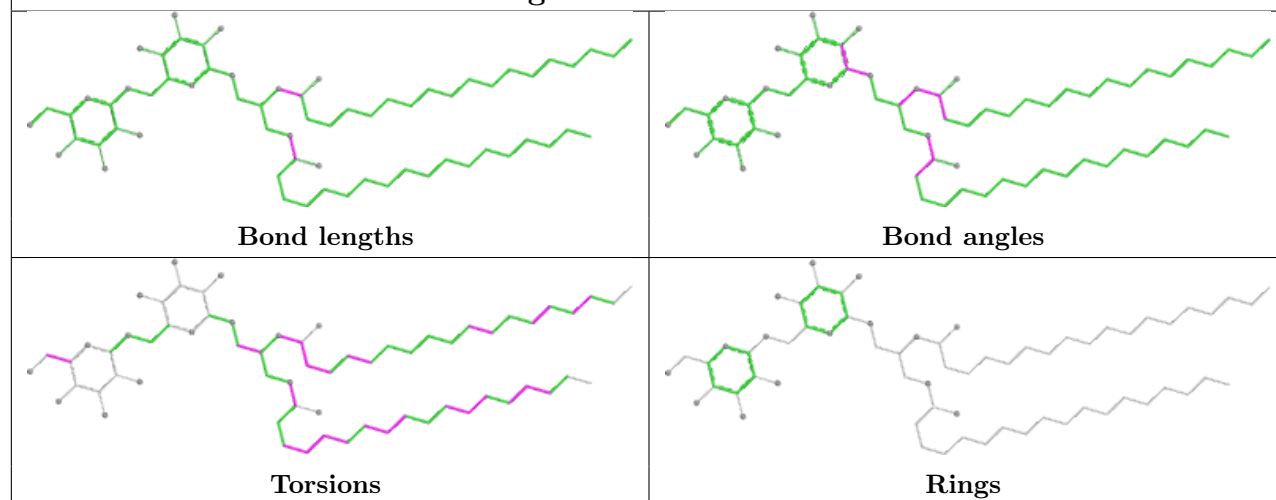
Ligand BCR B 848

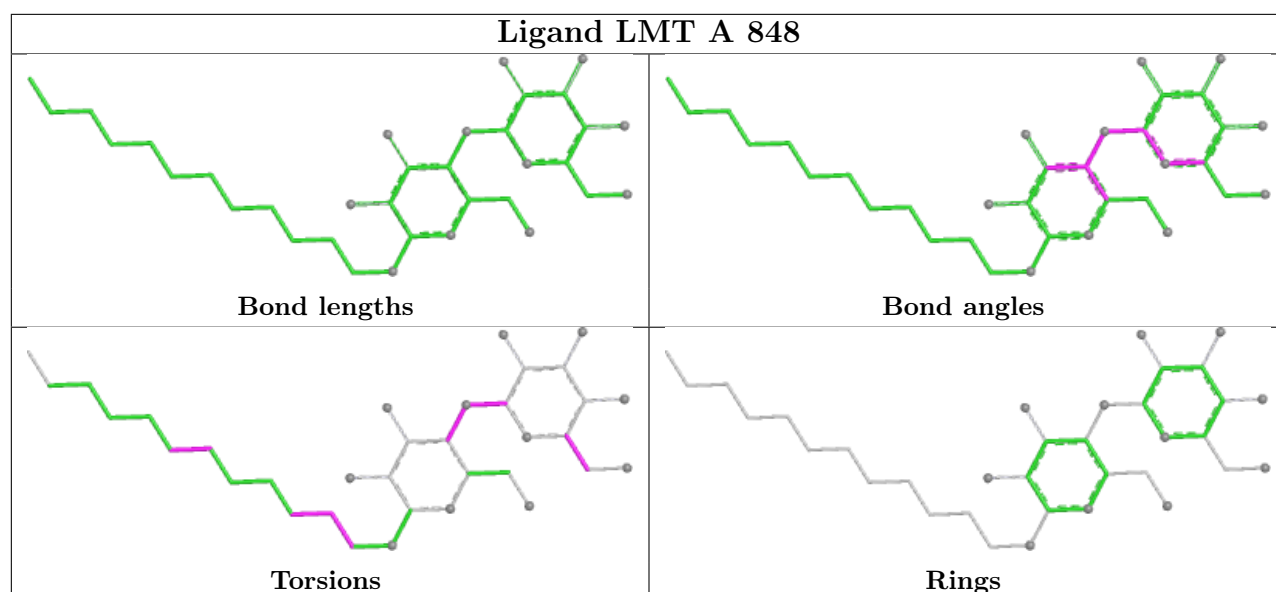
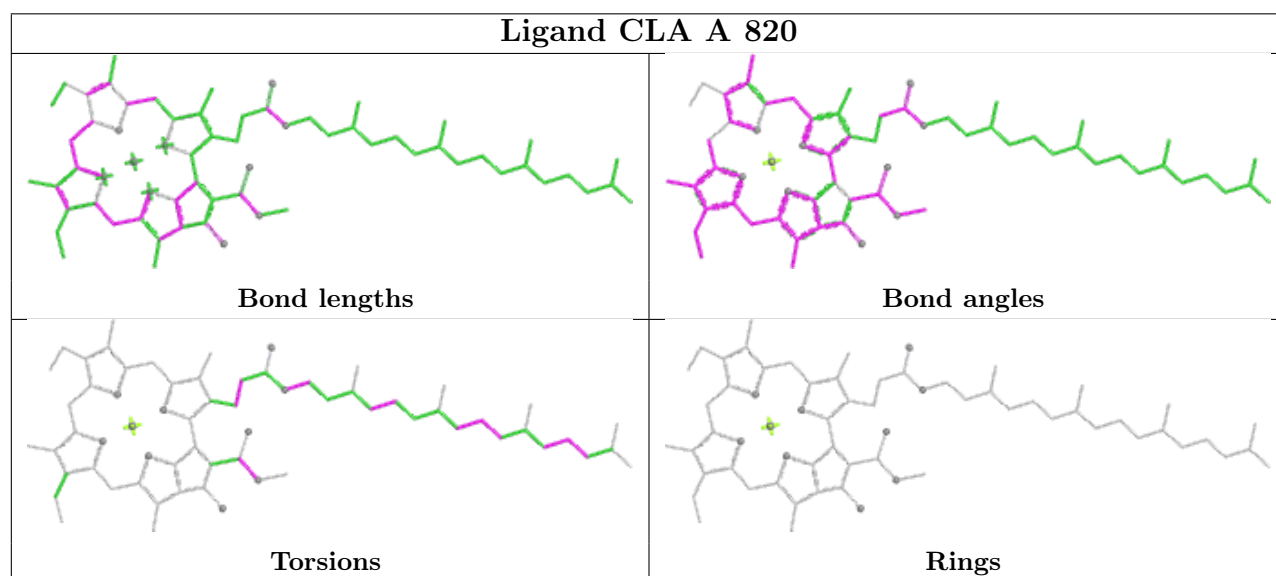
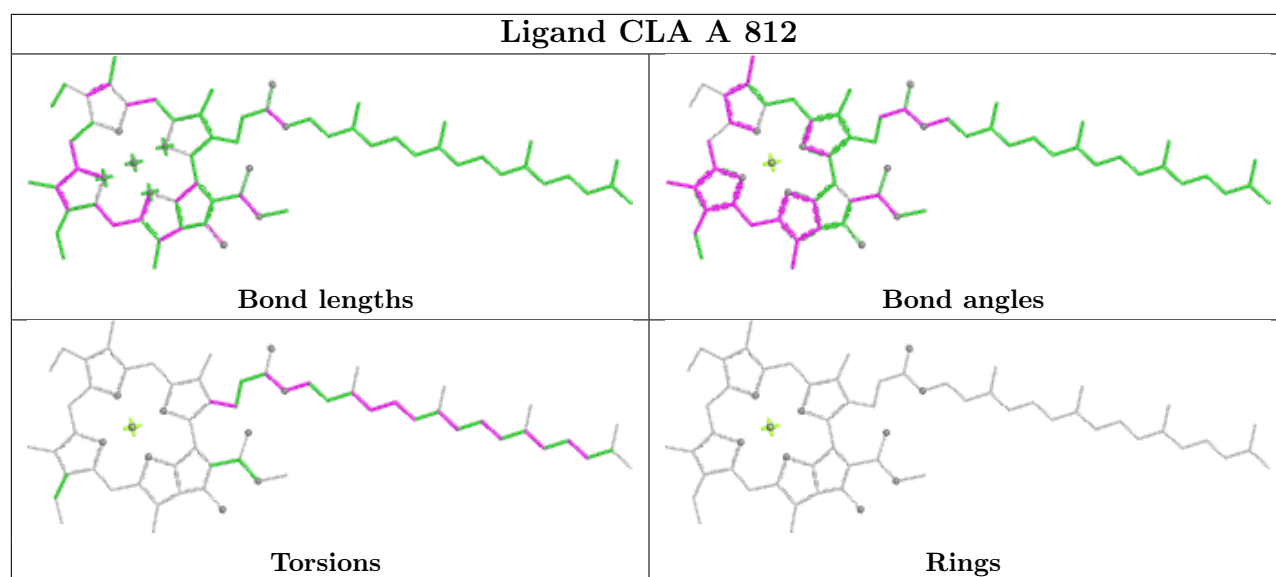


Ligand CLA 2 313

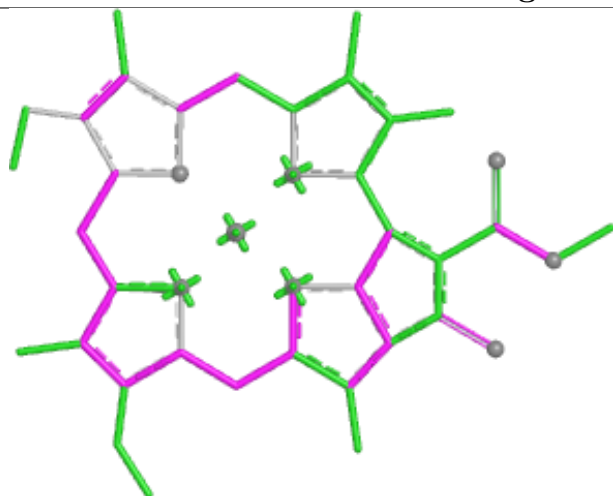


Ligand DGD B 849

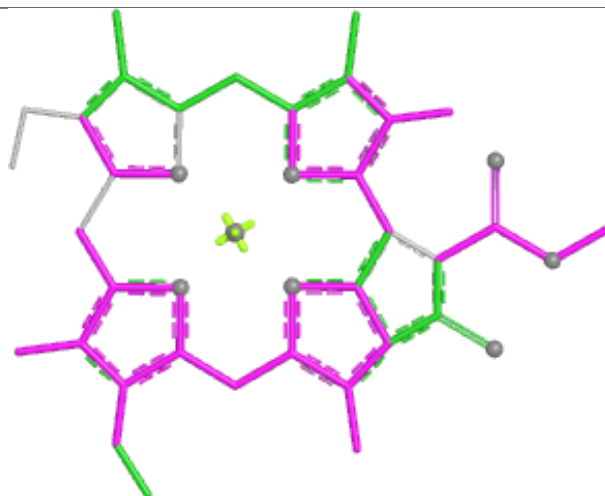




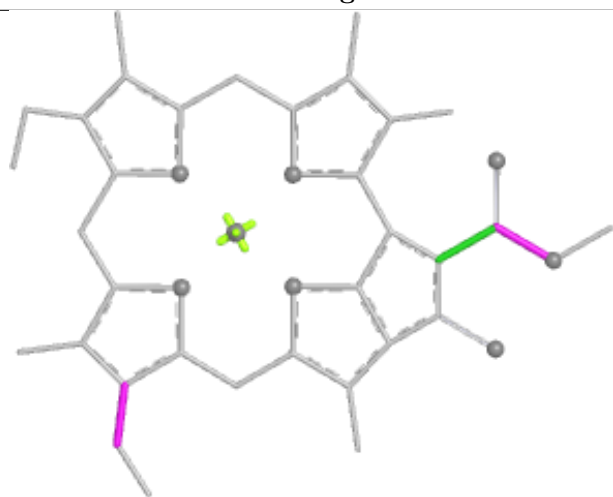
Ligand CLA 1 308



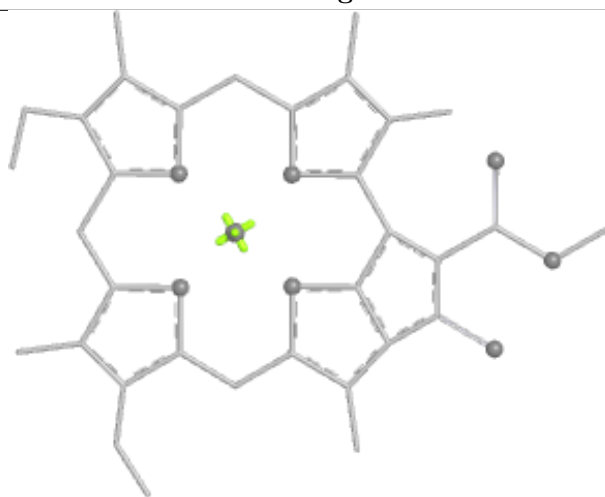
Bond lengths



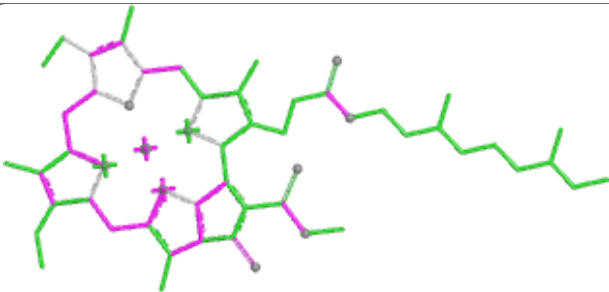
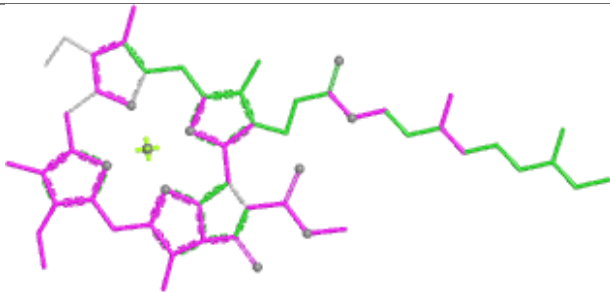
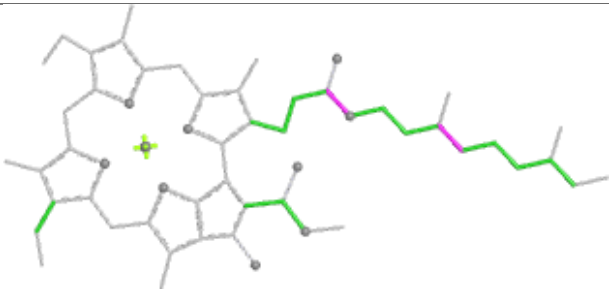
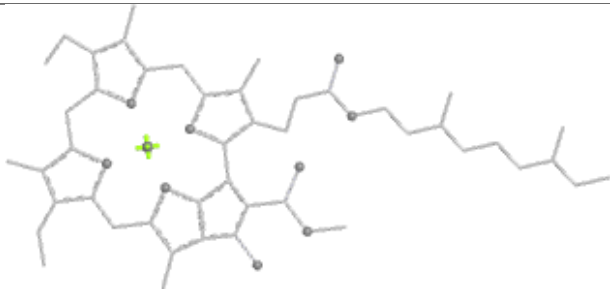
Bond angles

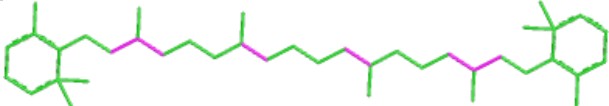


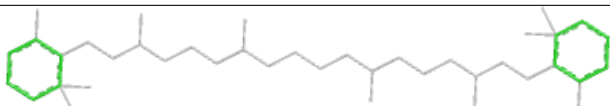


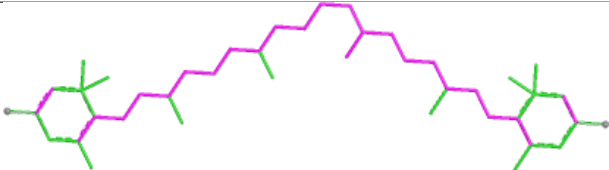
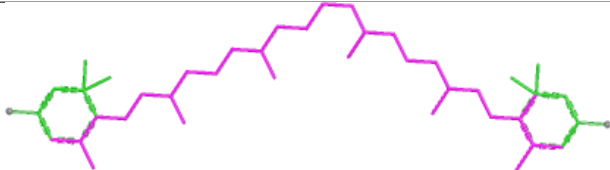
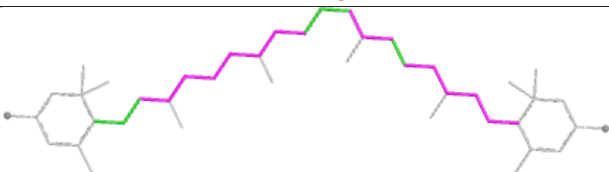
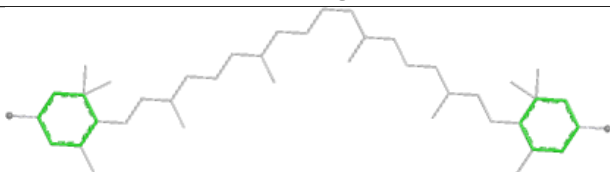
Torsions

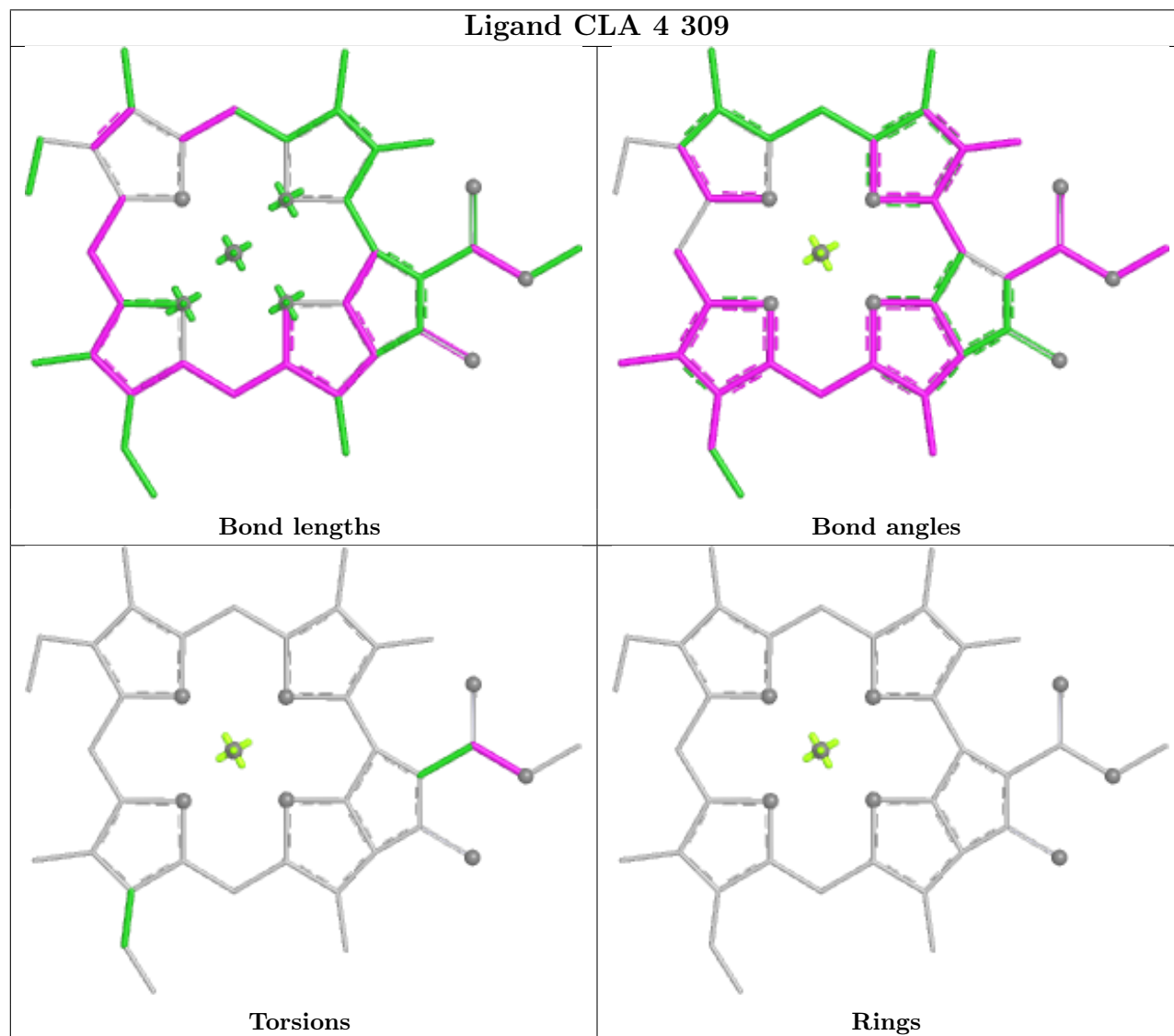
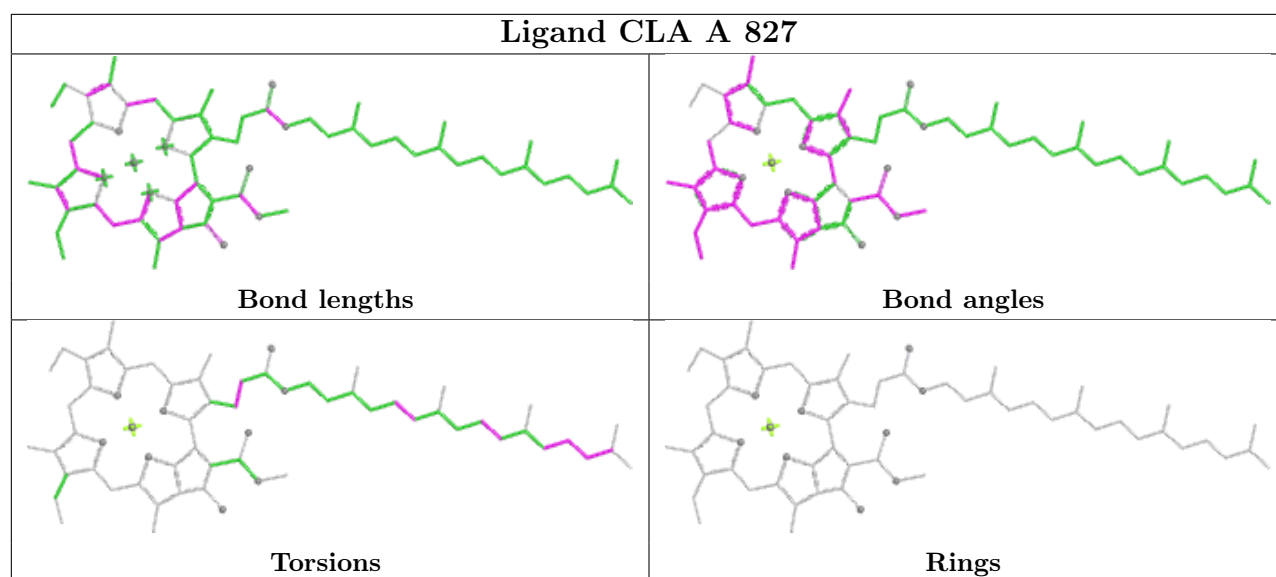


Rings

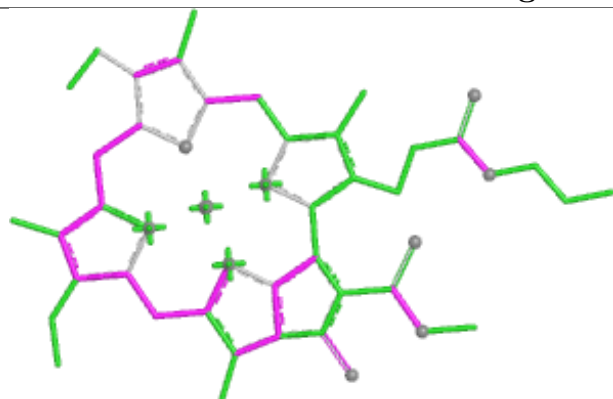
Ligand CLA A 830	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 843	
	
Bond lengths	Bond angles
	
Torsions	Rings

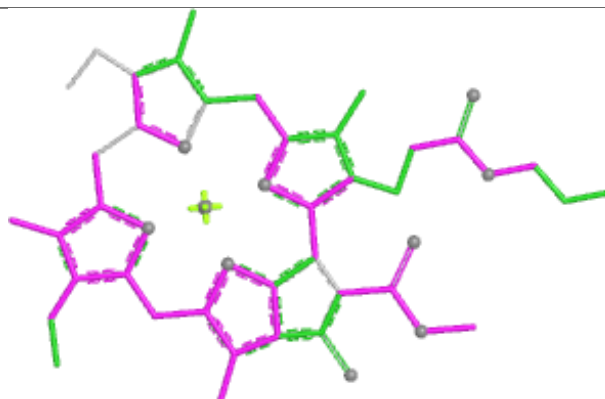
Ligand 5X6 2 318	
	
Bond lengths	Bond angles
	
Torsions	Rings



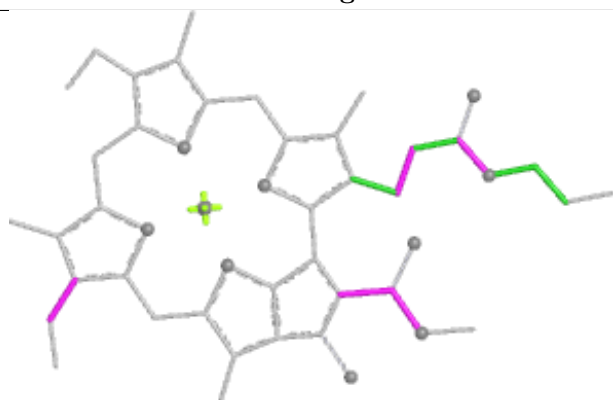
Ligand CLA 4 303



Bond lengths



Bond angles

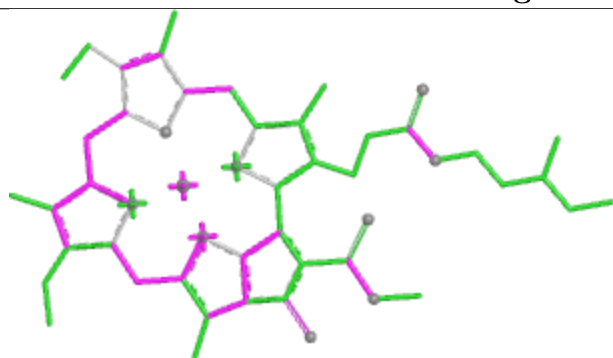


Torsions

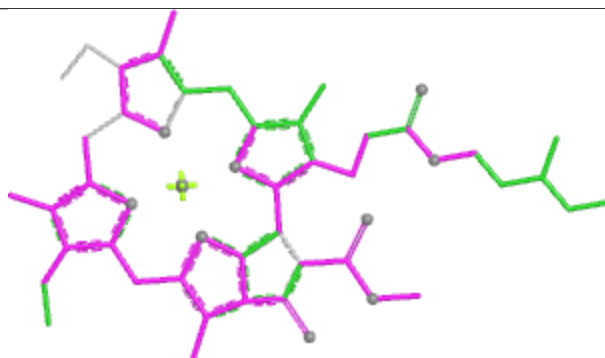


Rings

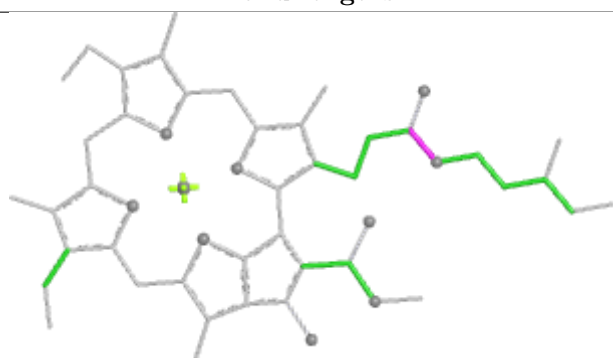
Ligand CLA A 835



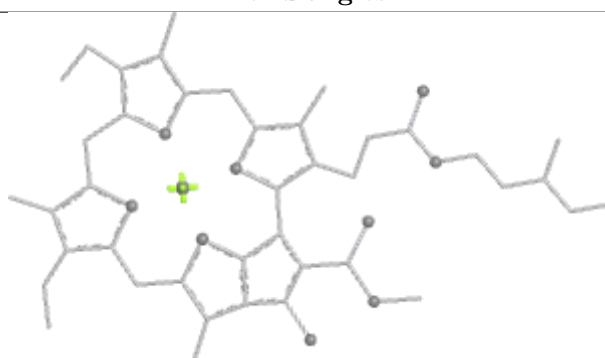
Bond lengths



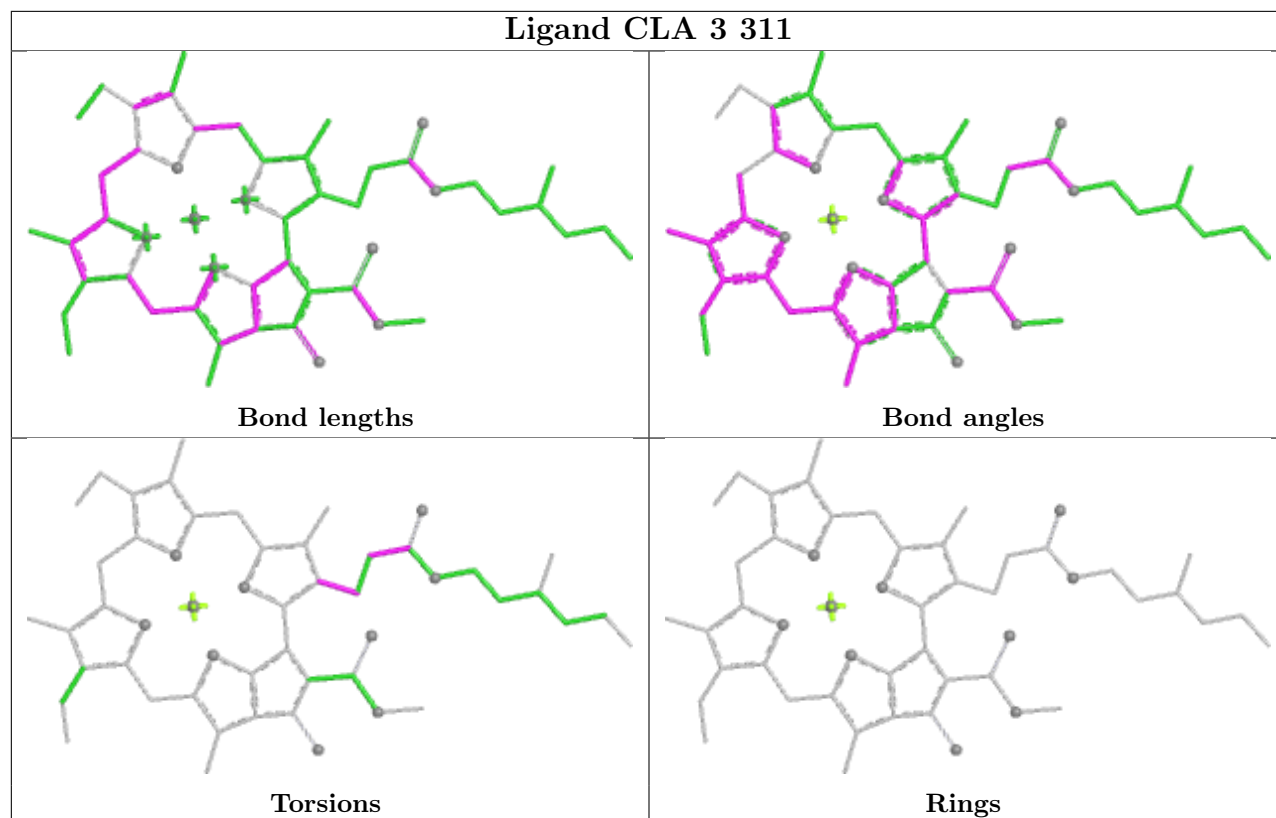
Bond angles



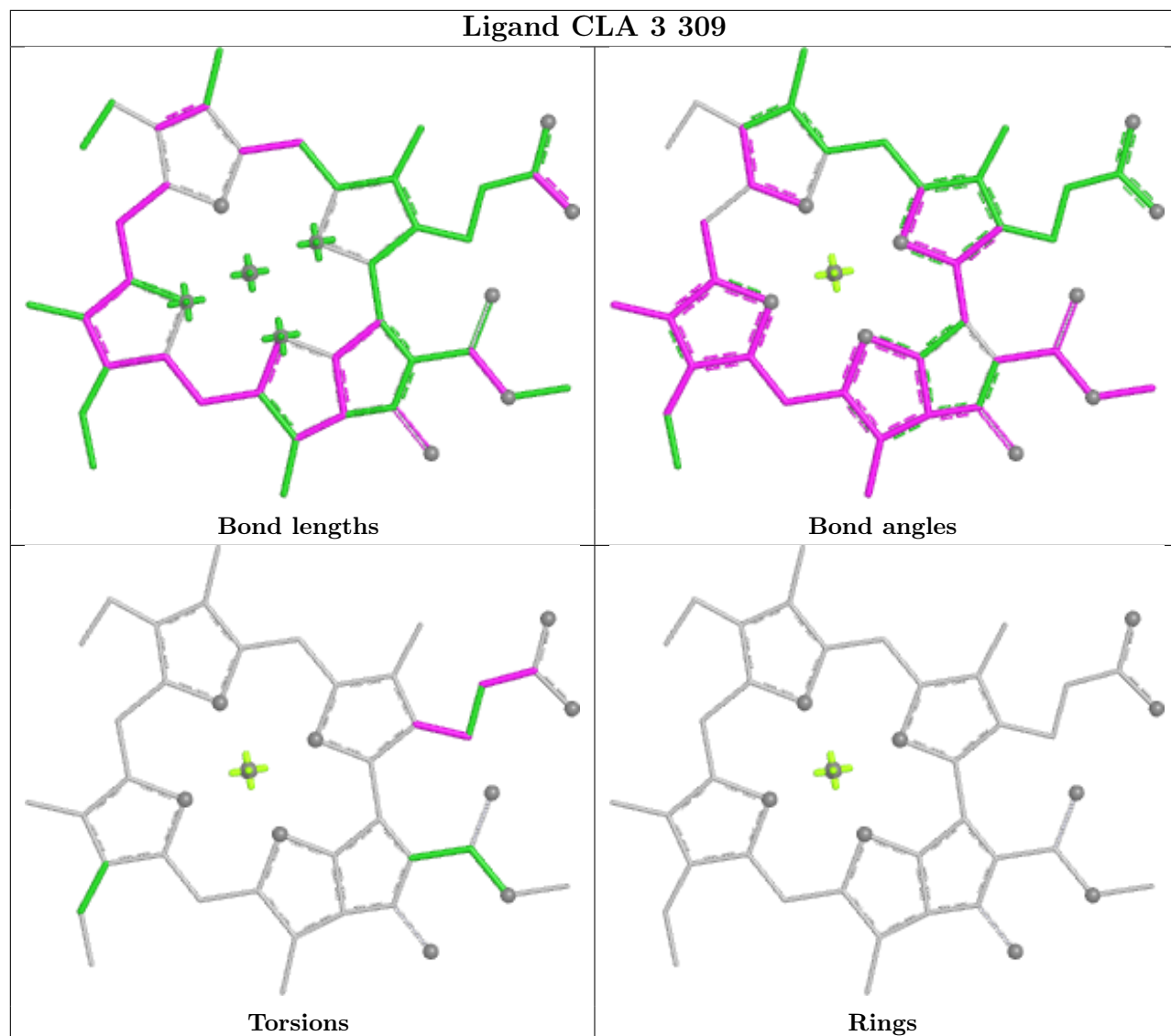
Torsions

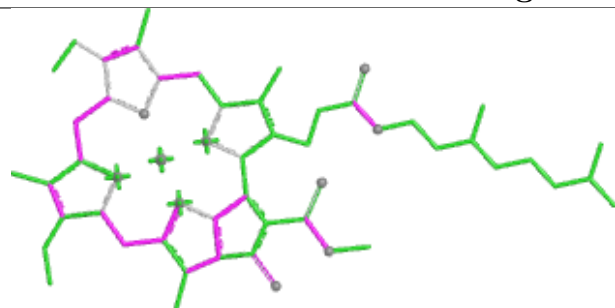


Rings

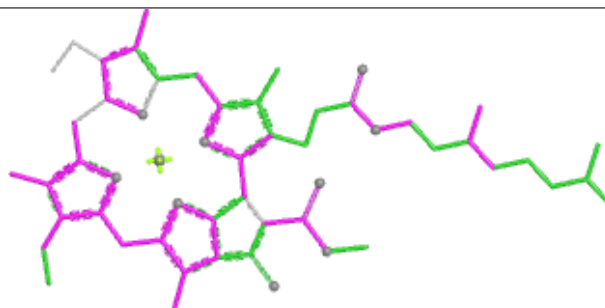


Ligand CLA 3 309

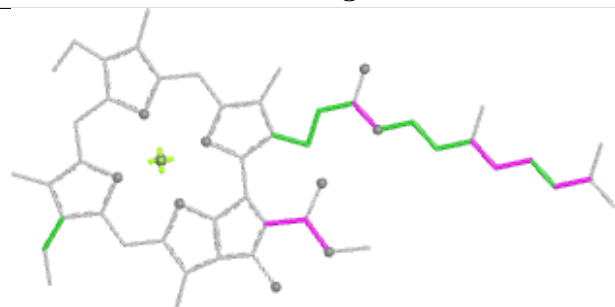


Ligand CLA A 802

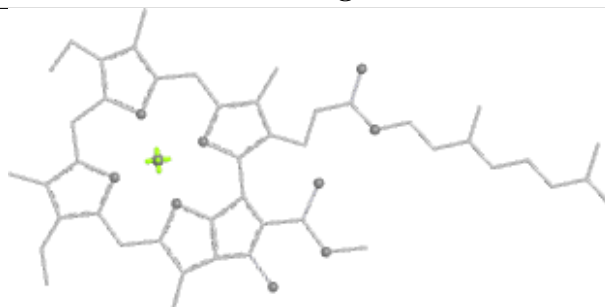
Bond lengths



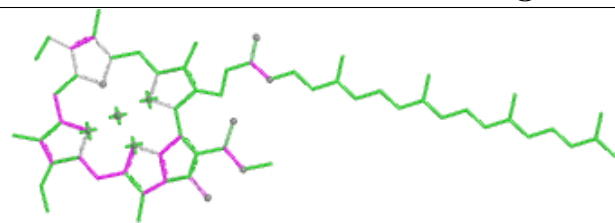
Bond angles



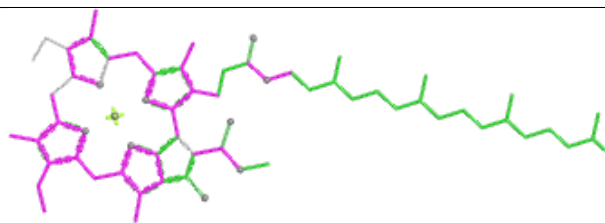
Torsions



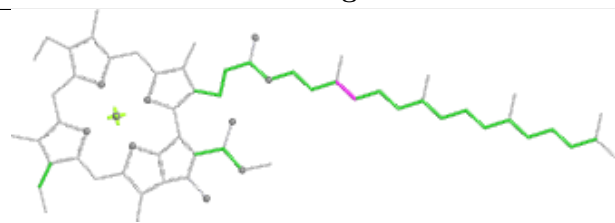
Rings

Ligand CLA B 829

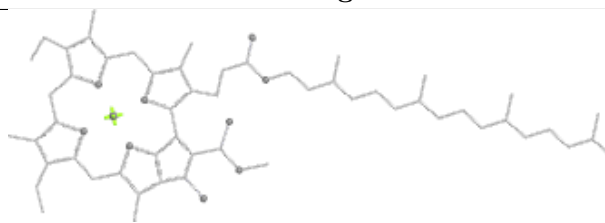
Bond lengths



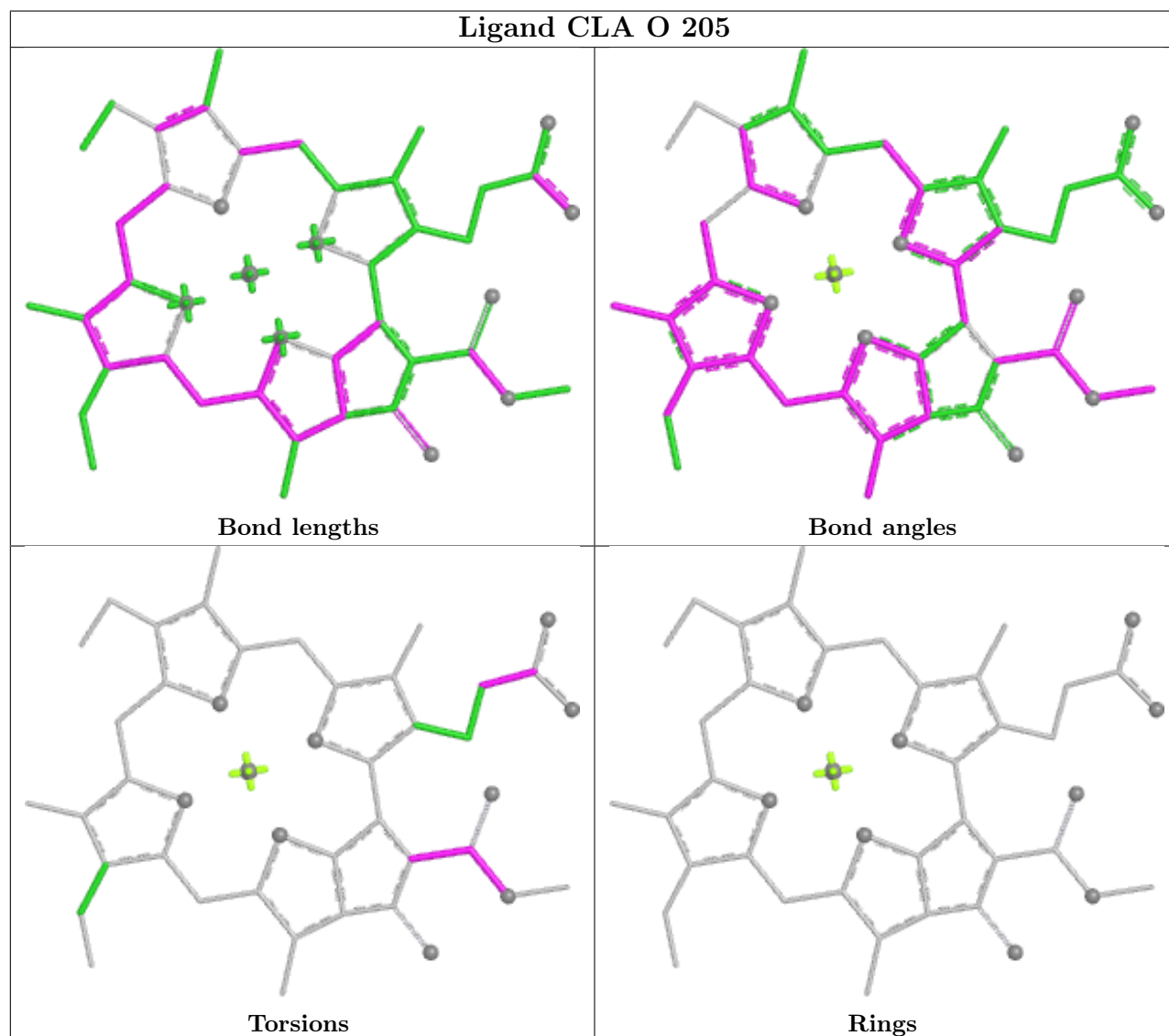
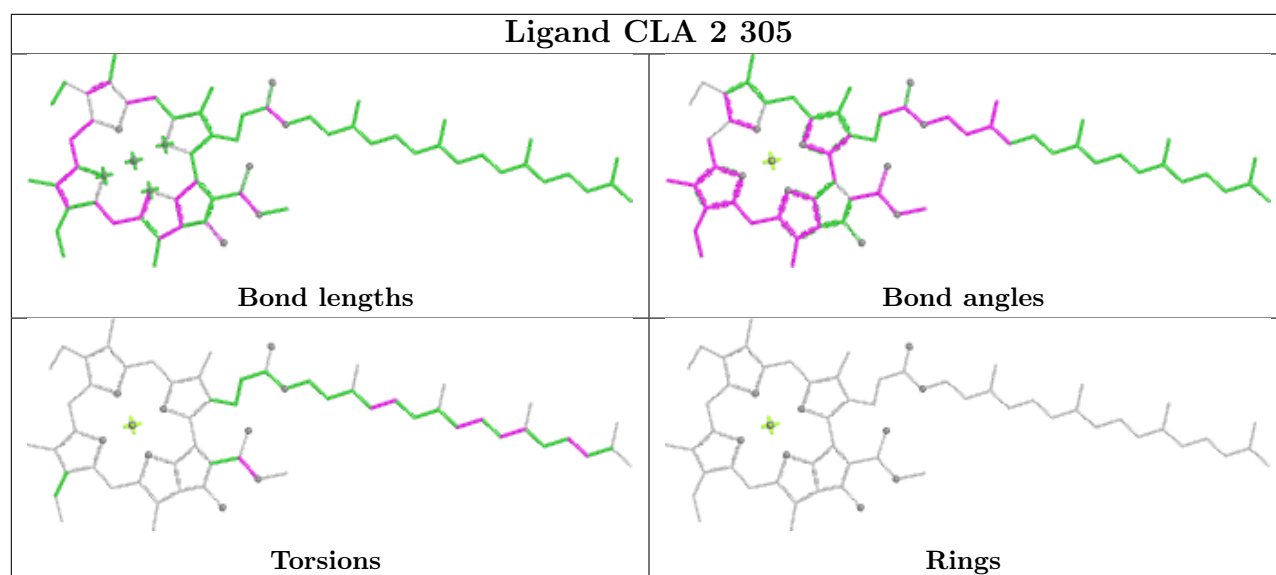
Bond angles



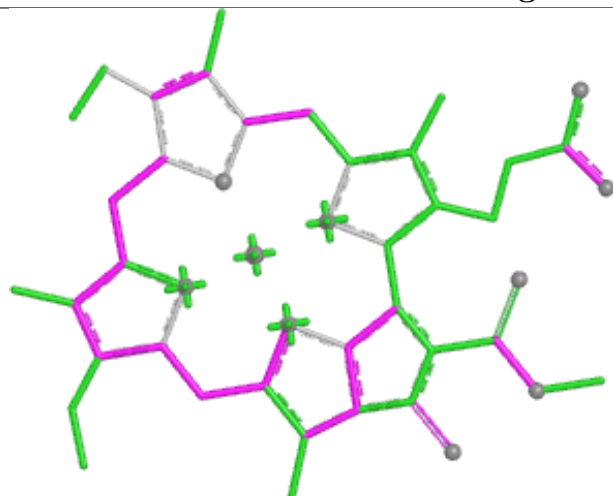
Torsions



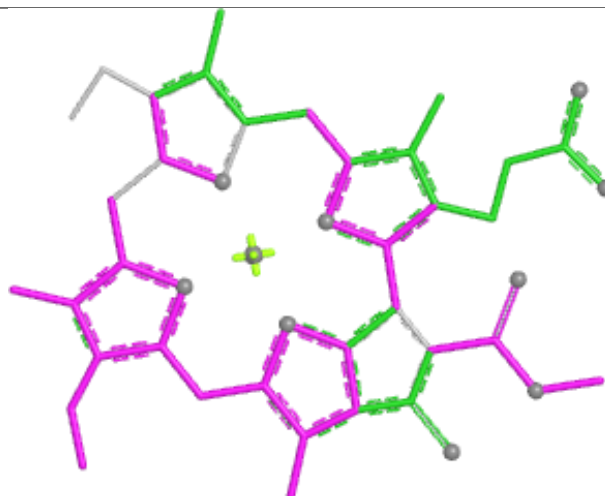
Rings



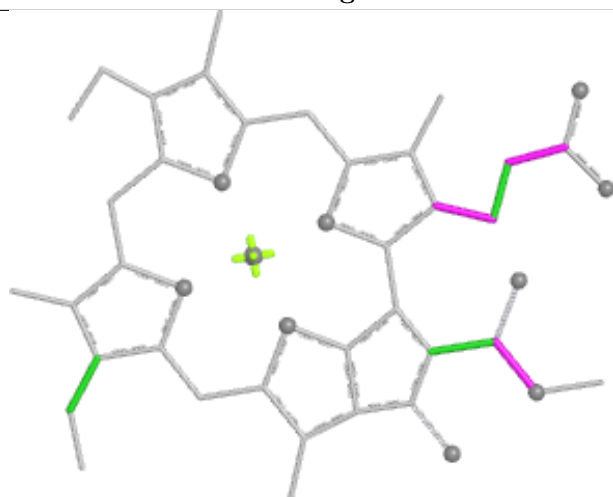
Ligand CLA 2 309



Bond lengths



Bond angles

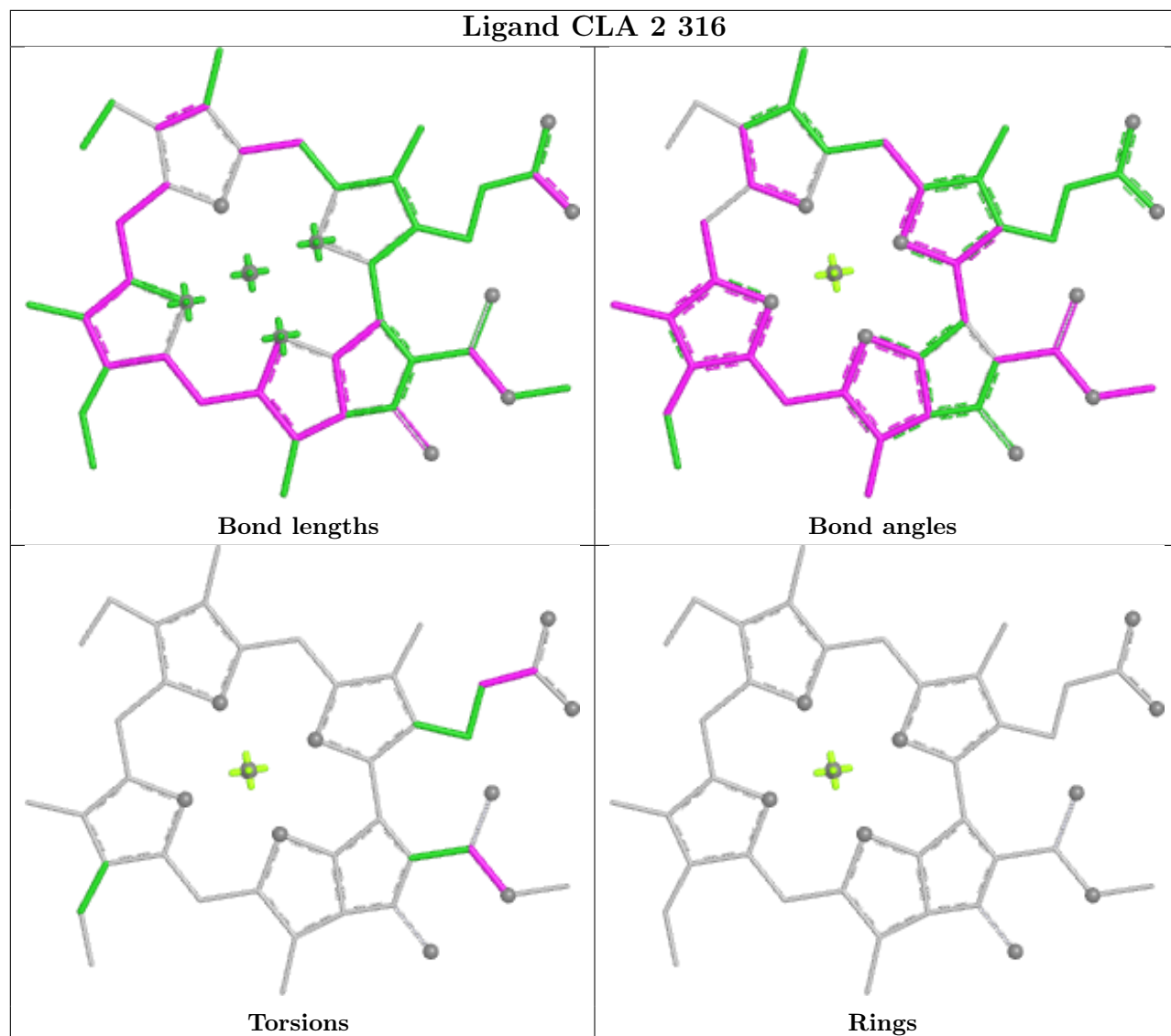


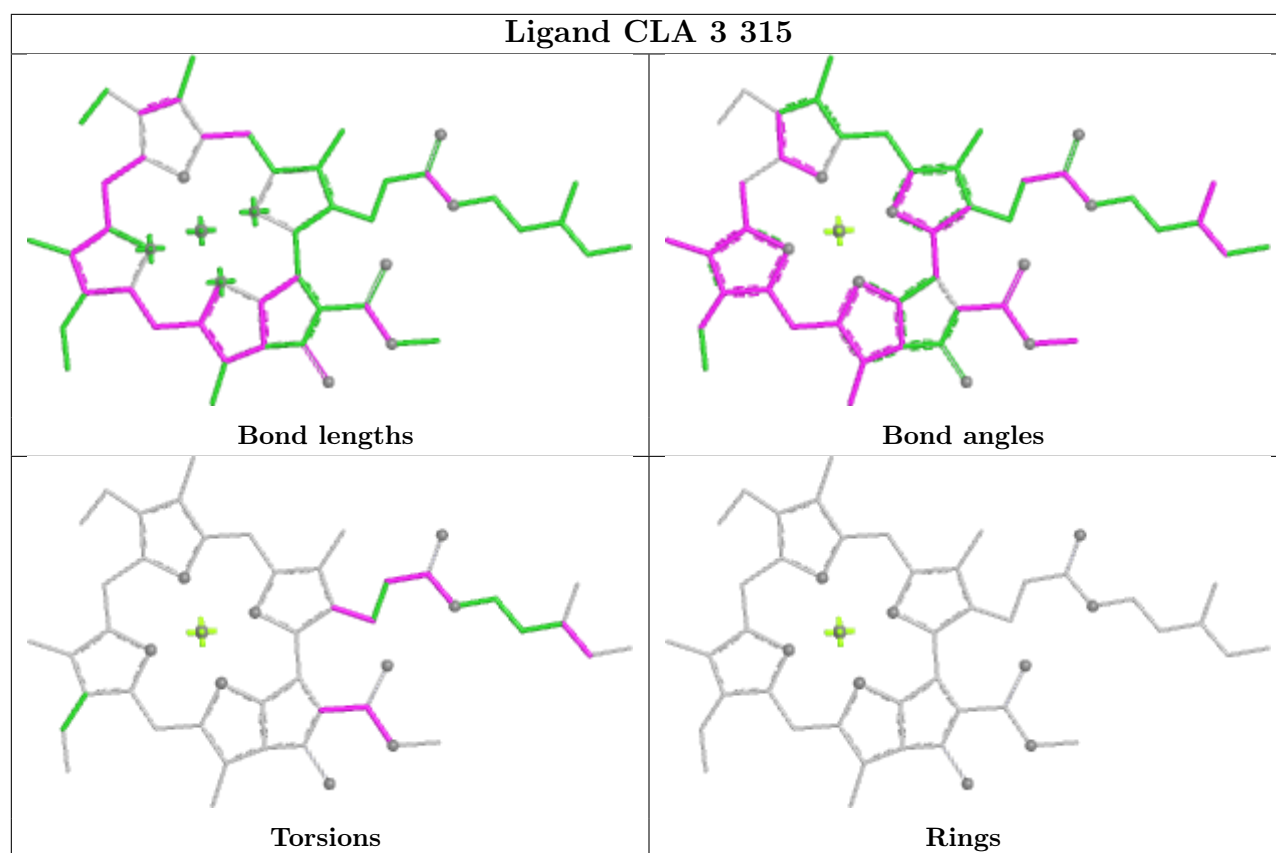
Torsions



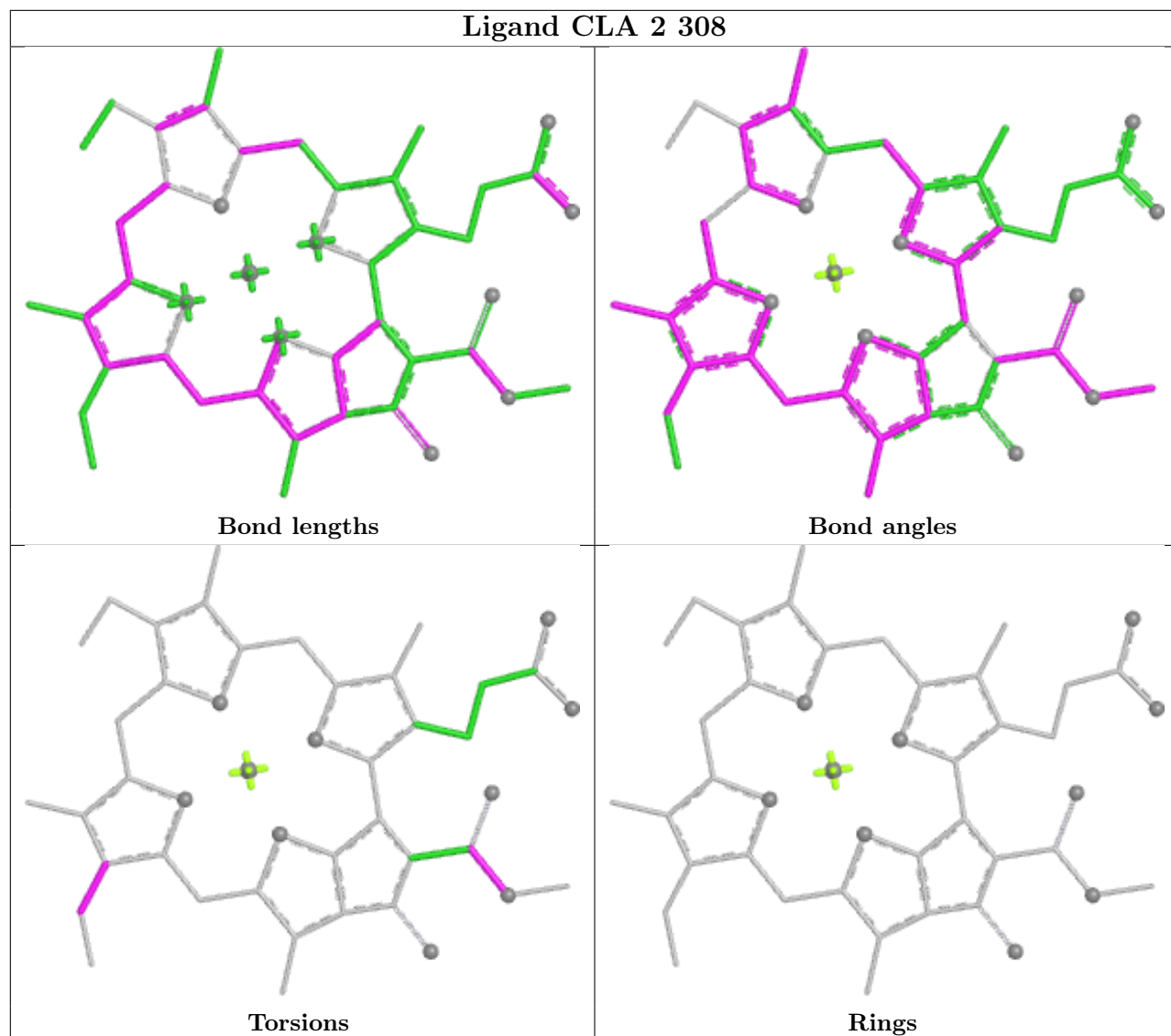
Rings

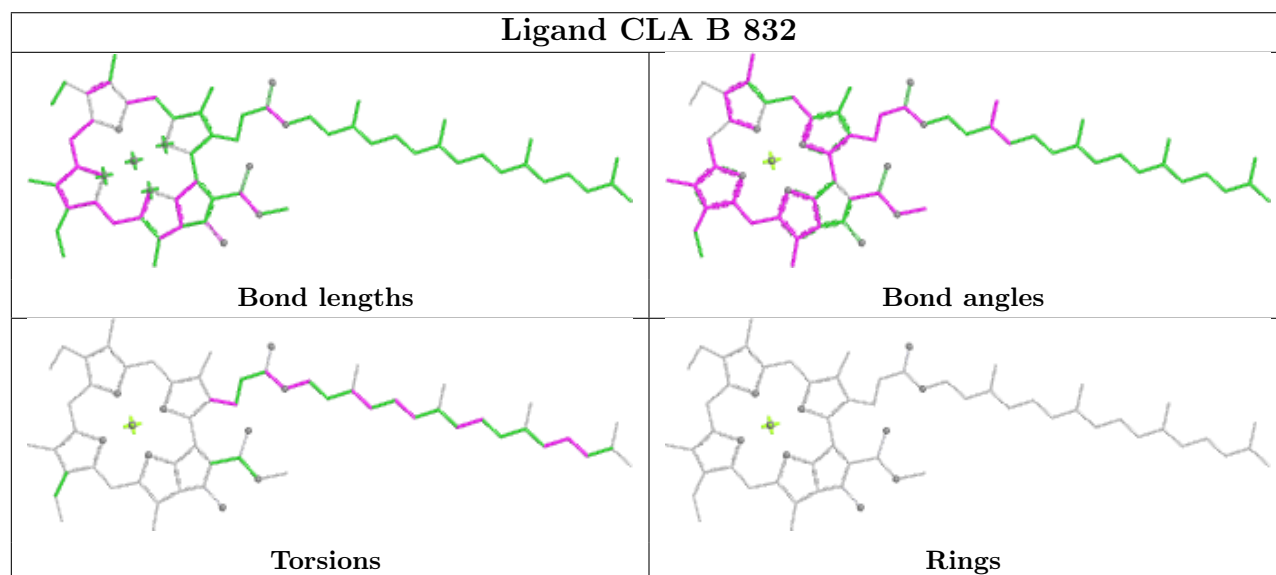
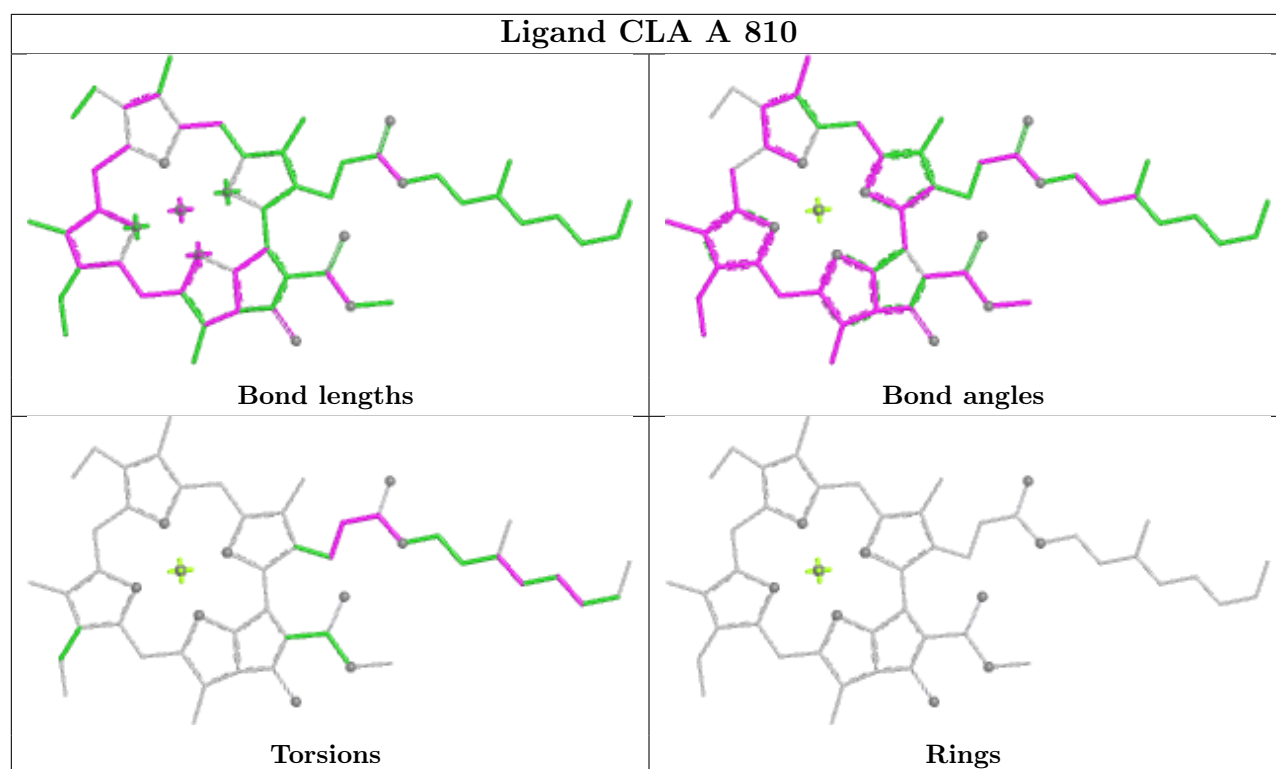
Ligand CLA 2 316



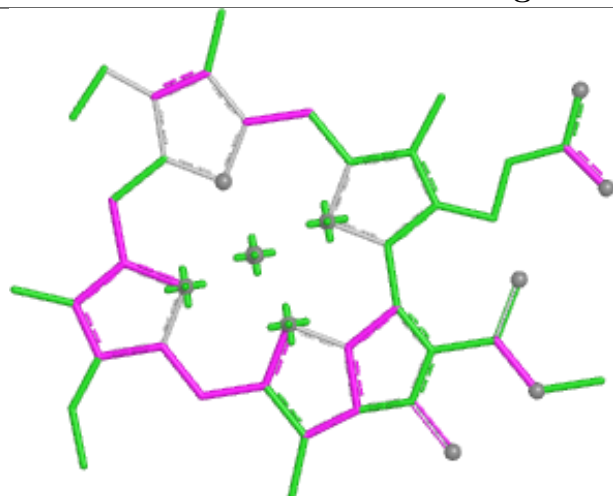


Ligand CLA 2 308

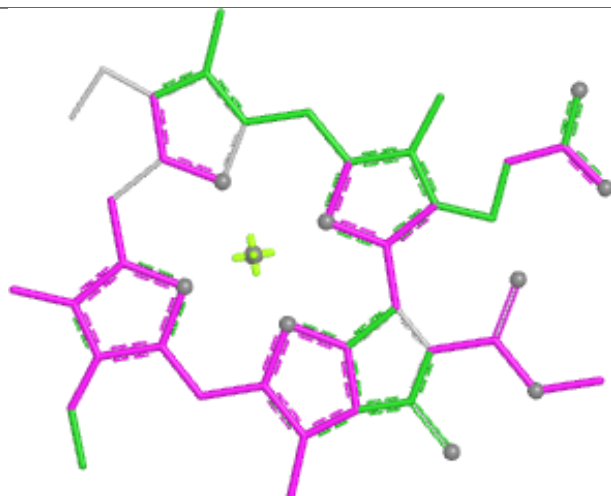




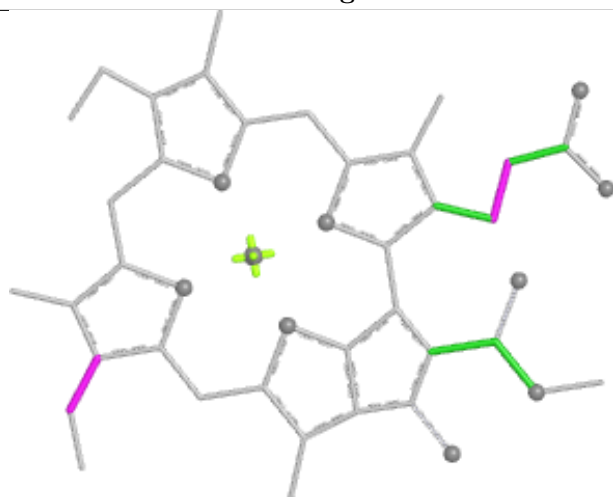
Ligand CLA A 814



Bond lengths



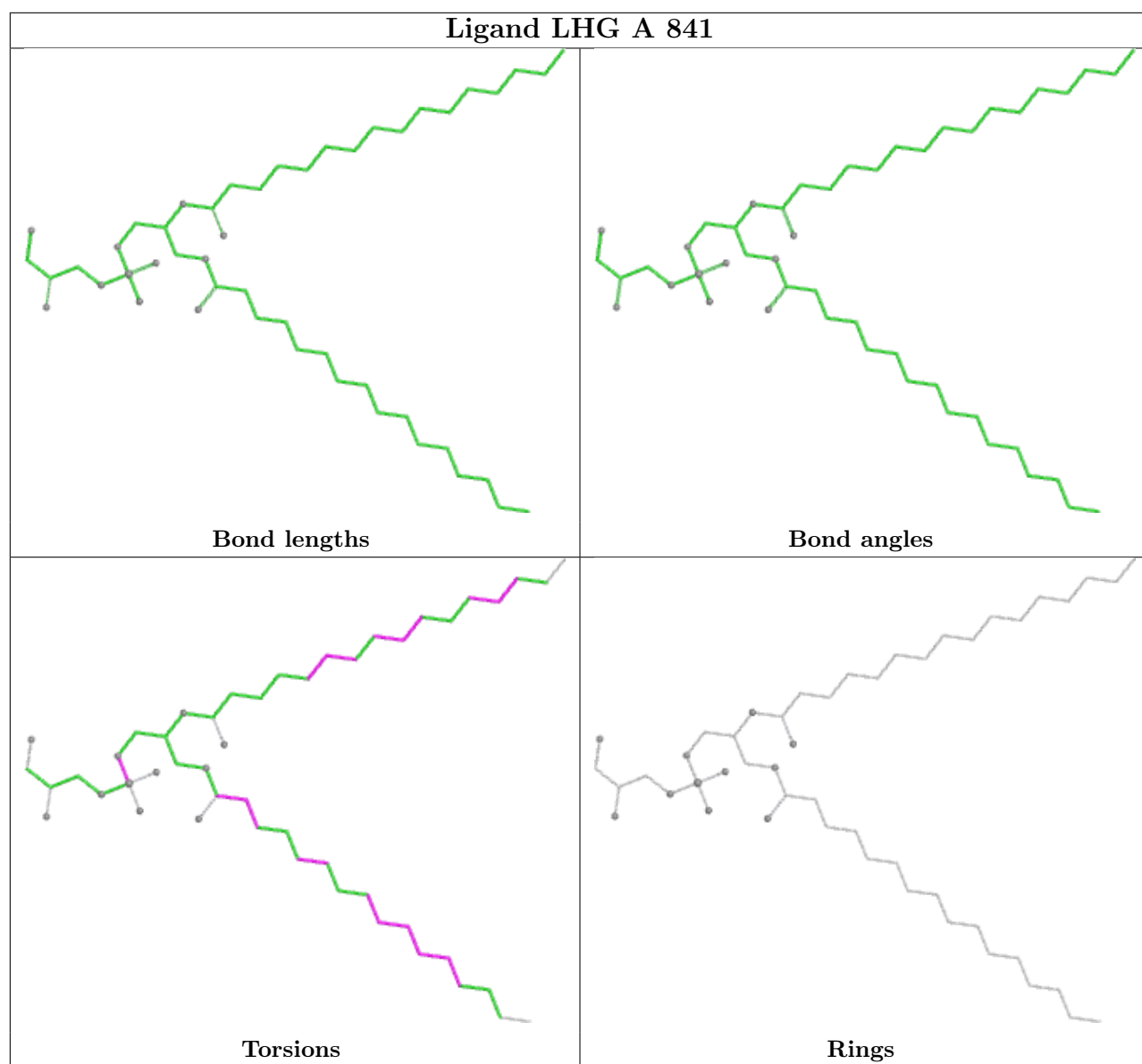
Bond angles



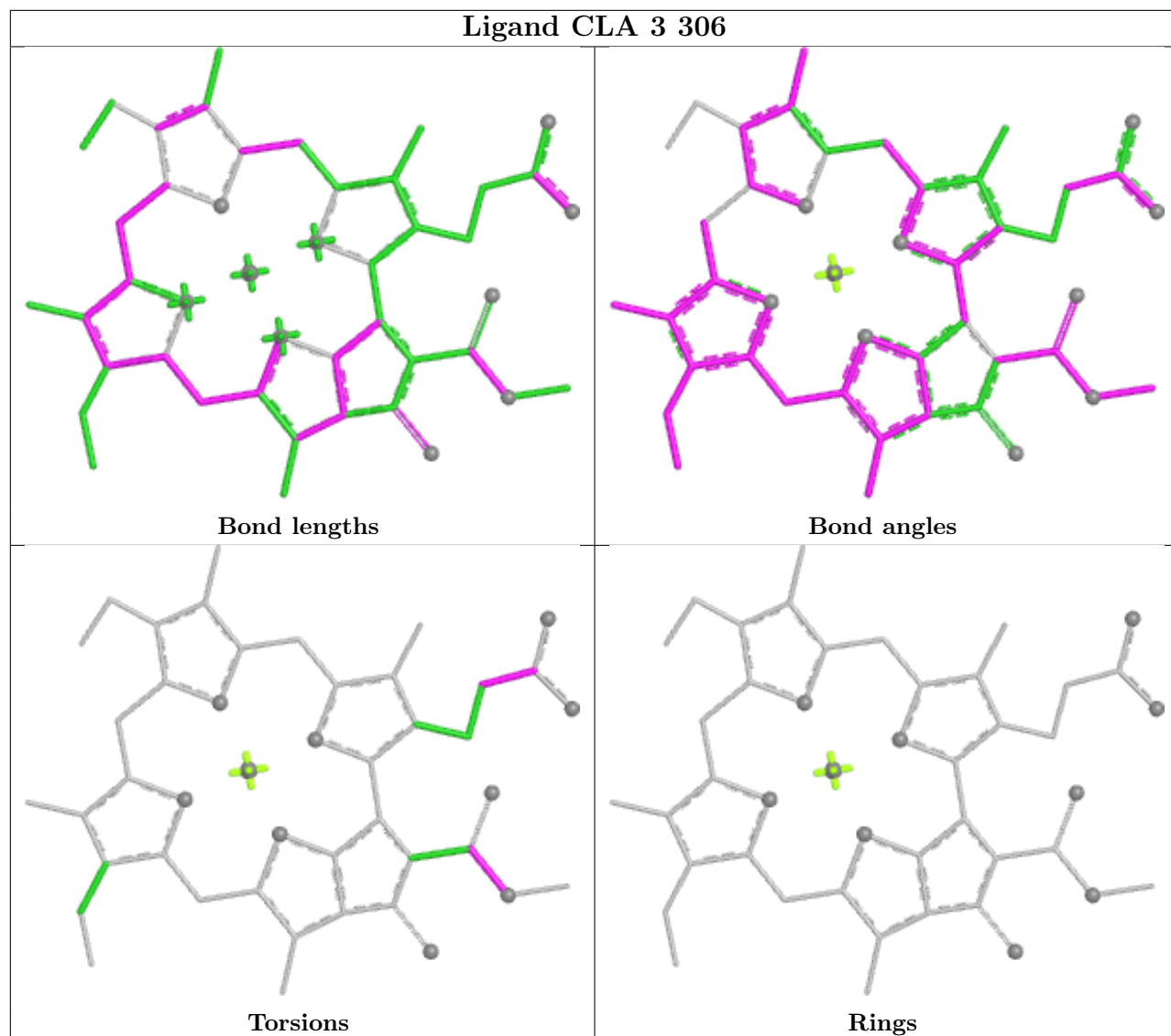
Torsions



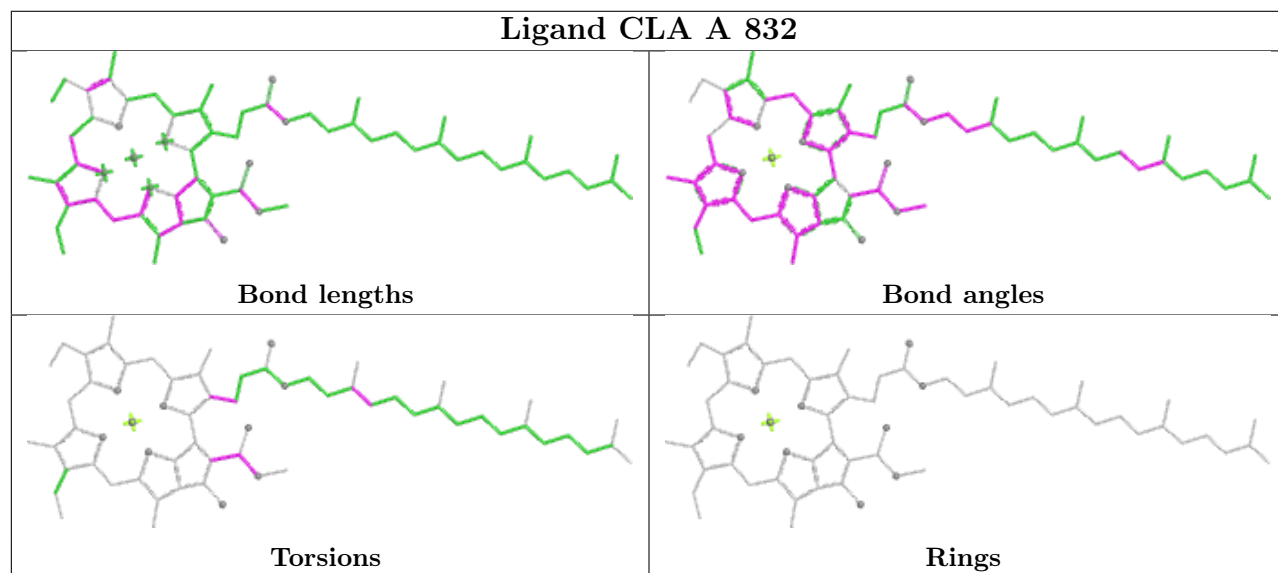
Rings



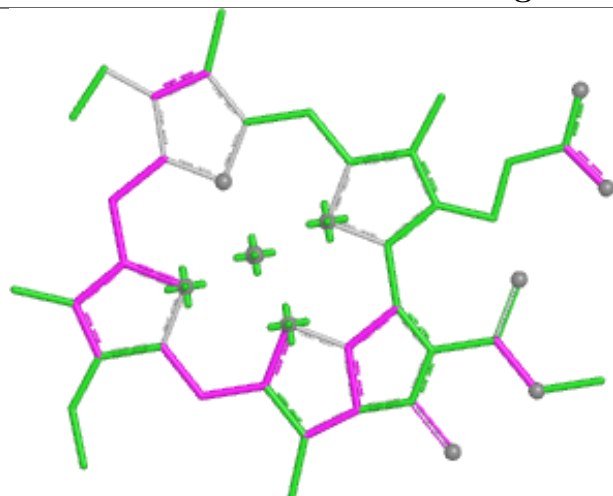
Ligand CLA 3 306



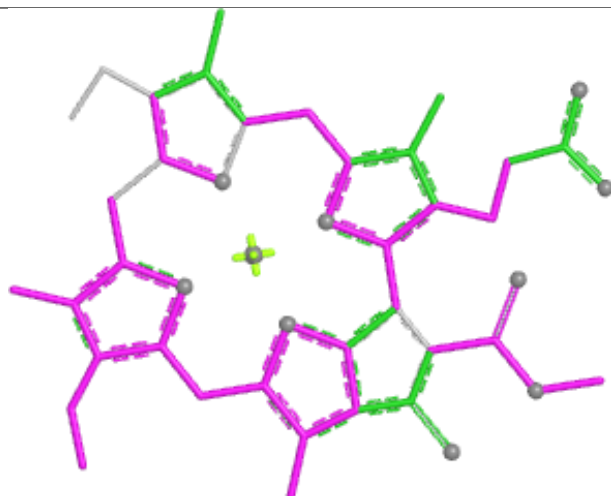
Ligand CLA A 832



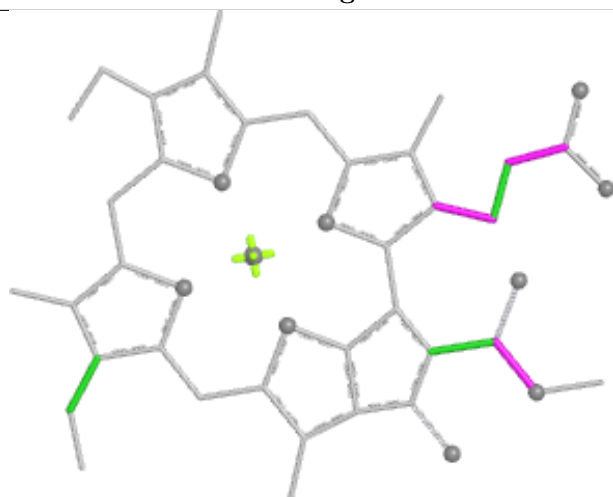
Ligand CLA B 835



Bond lengths



Bond angles

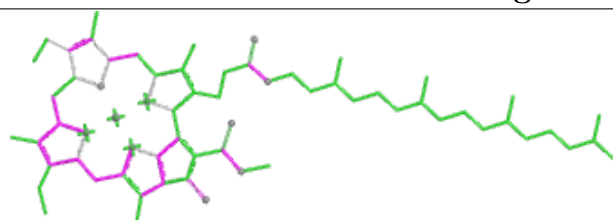


Torsions

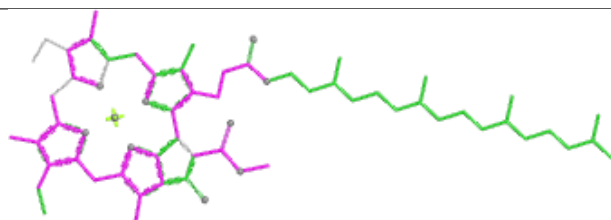


Rings

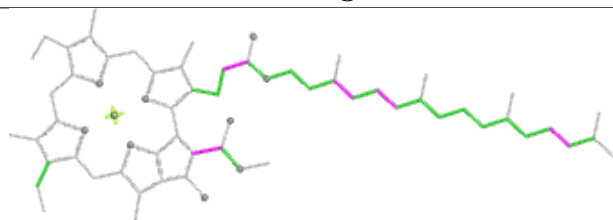
Ligand CLA A 803



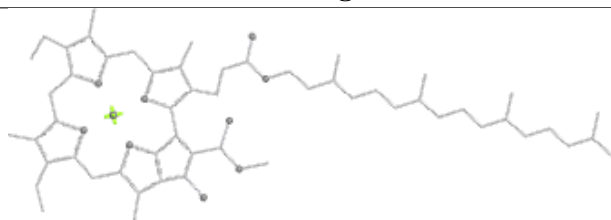
Bond lengths



Bond angles

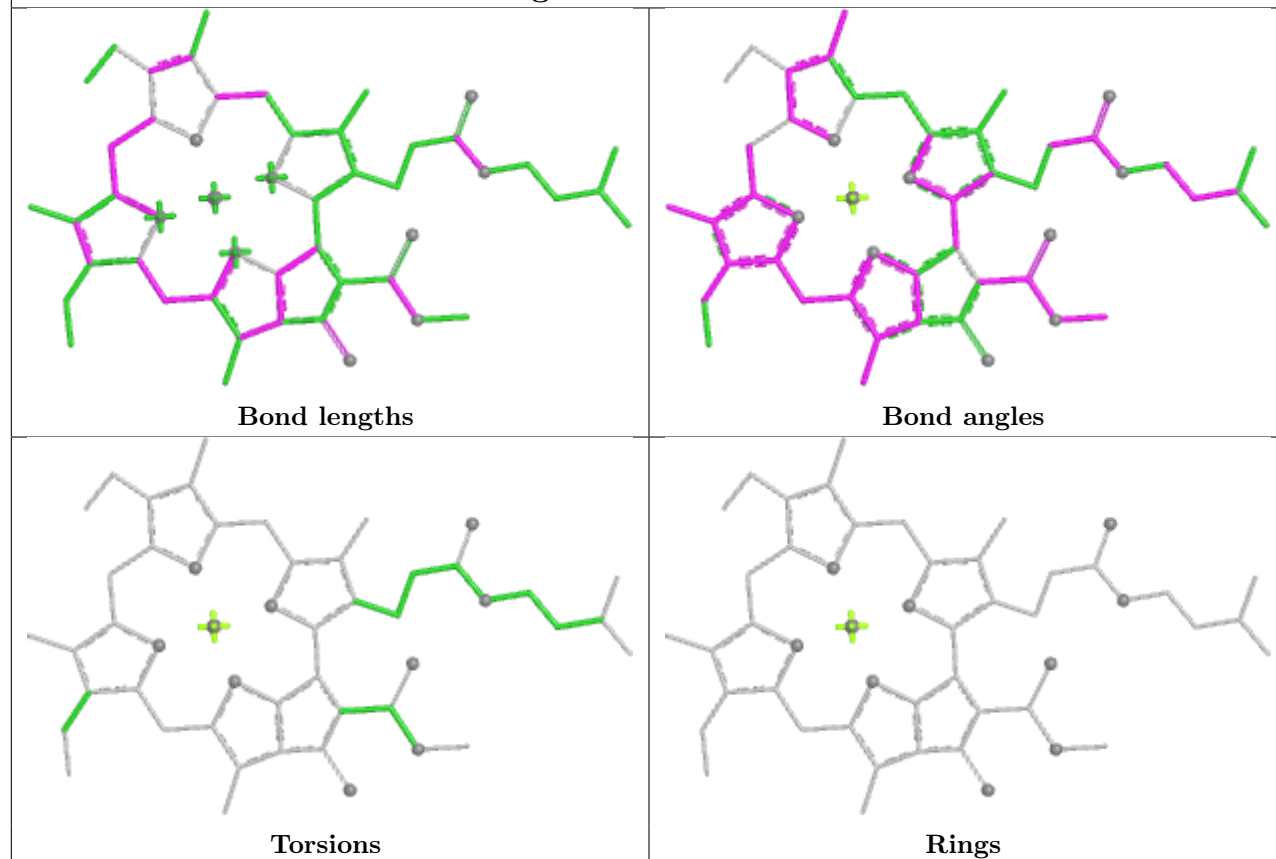


Torsions

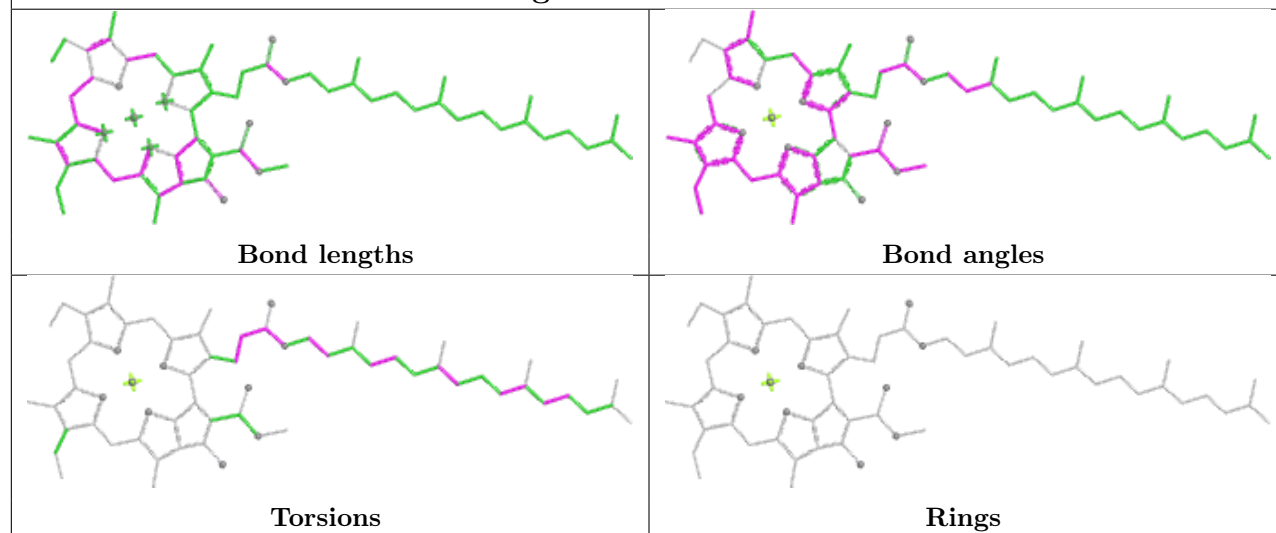


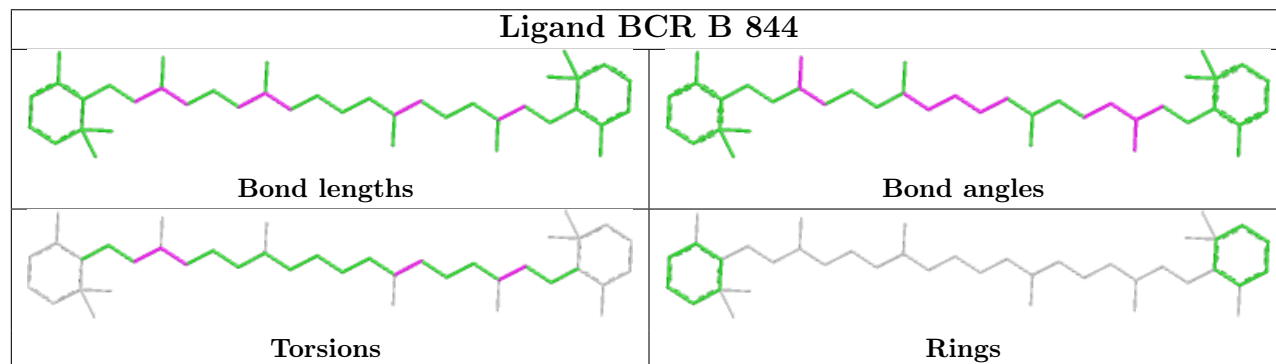
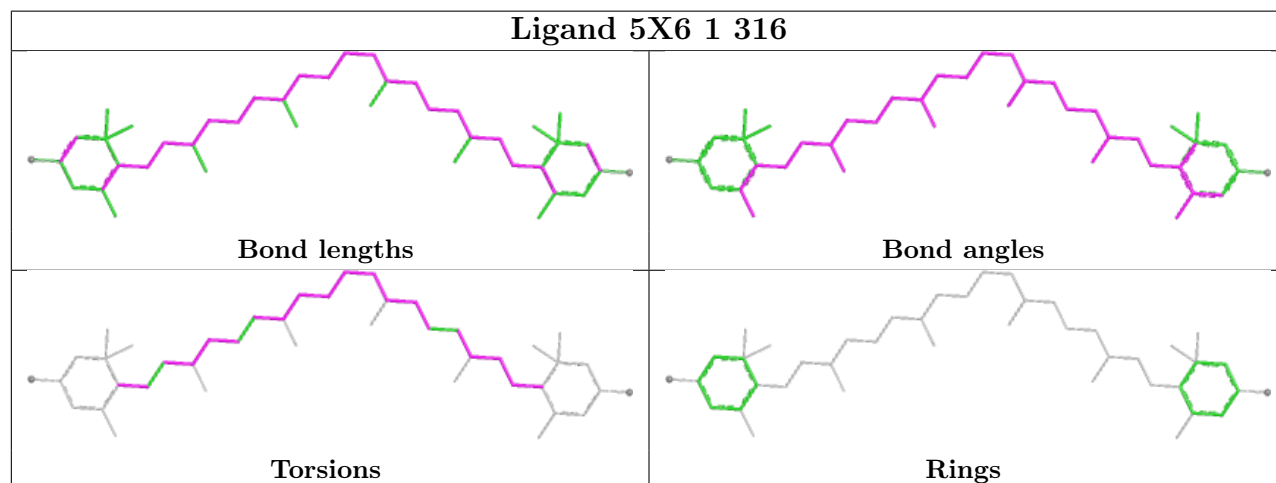
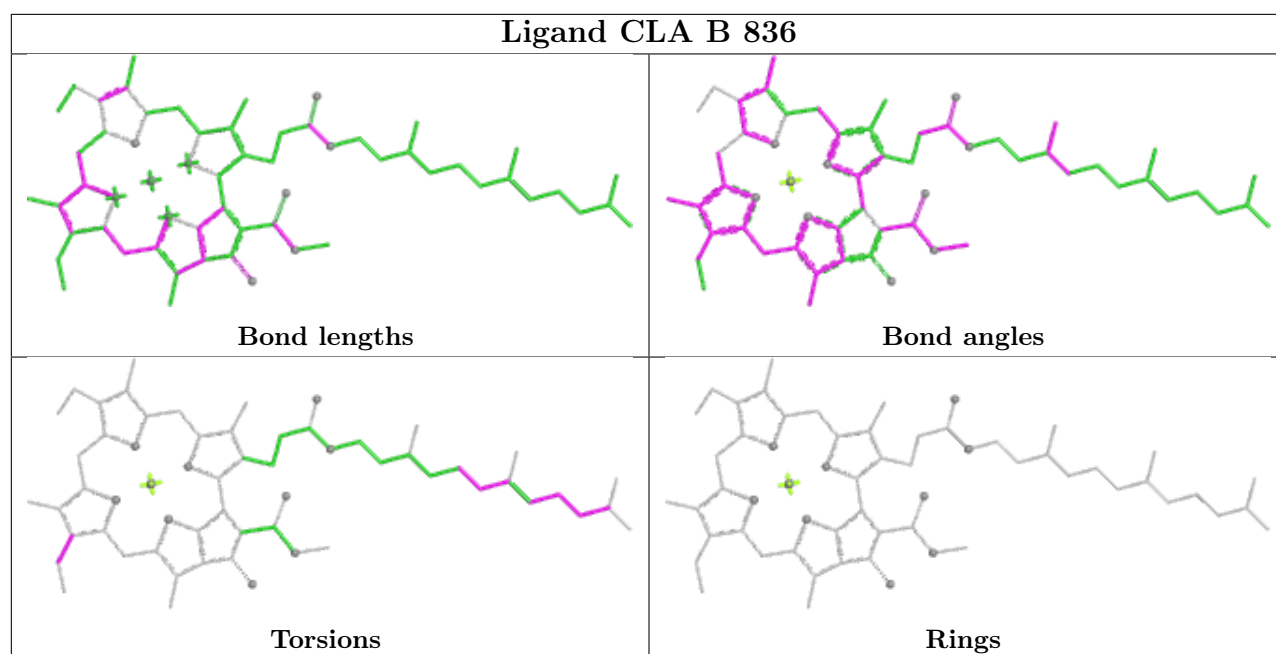
Rings

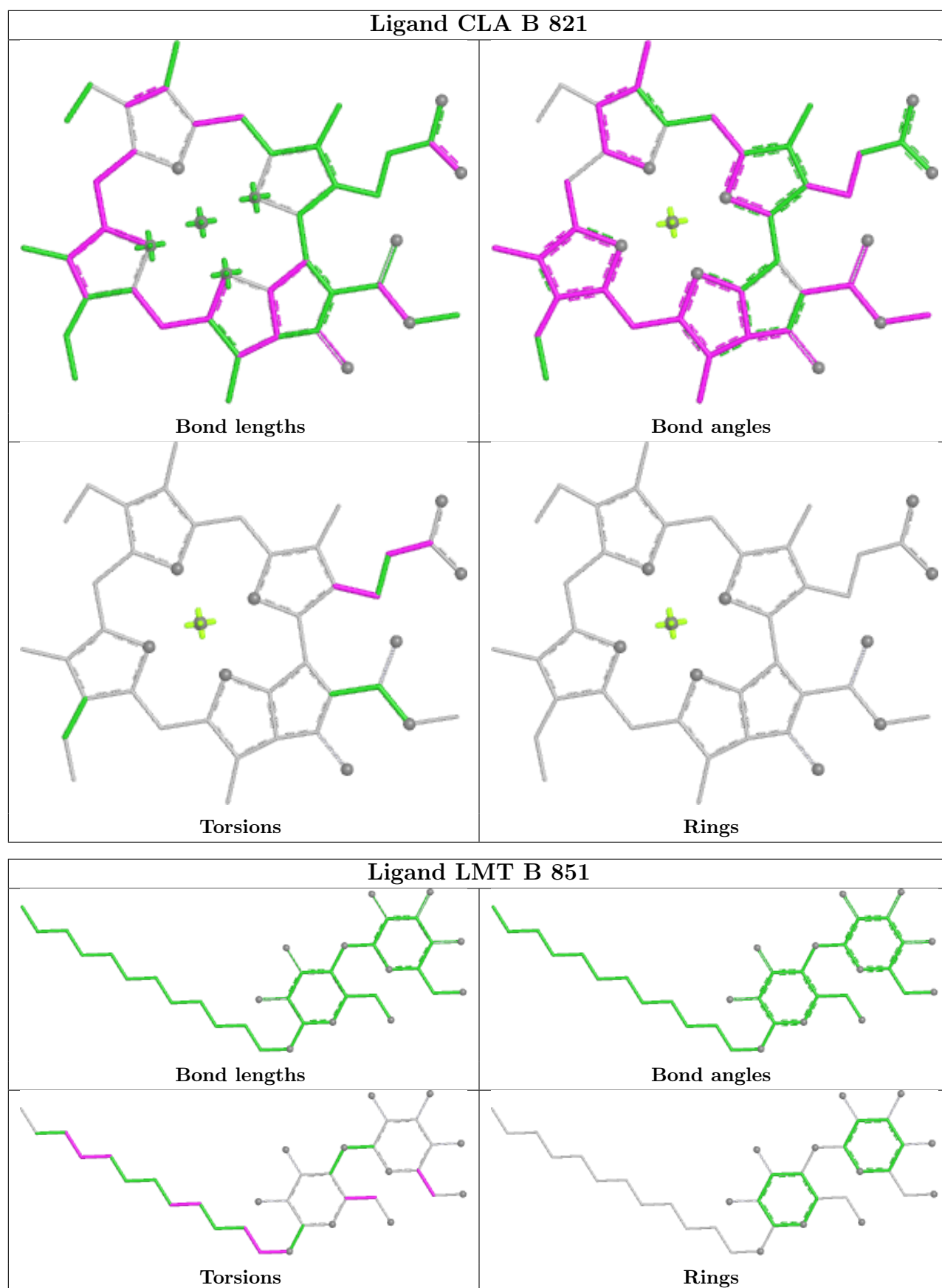
Ligand CLA A 805

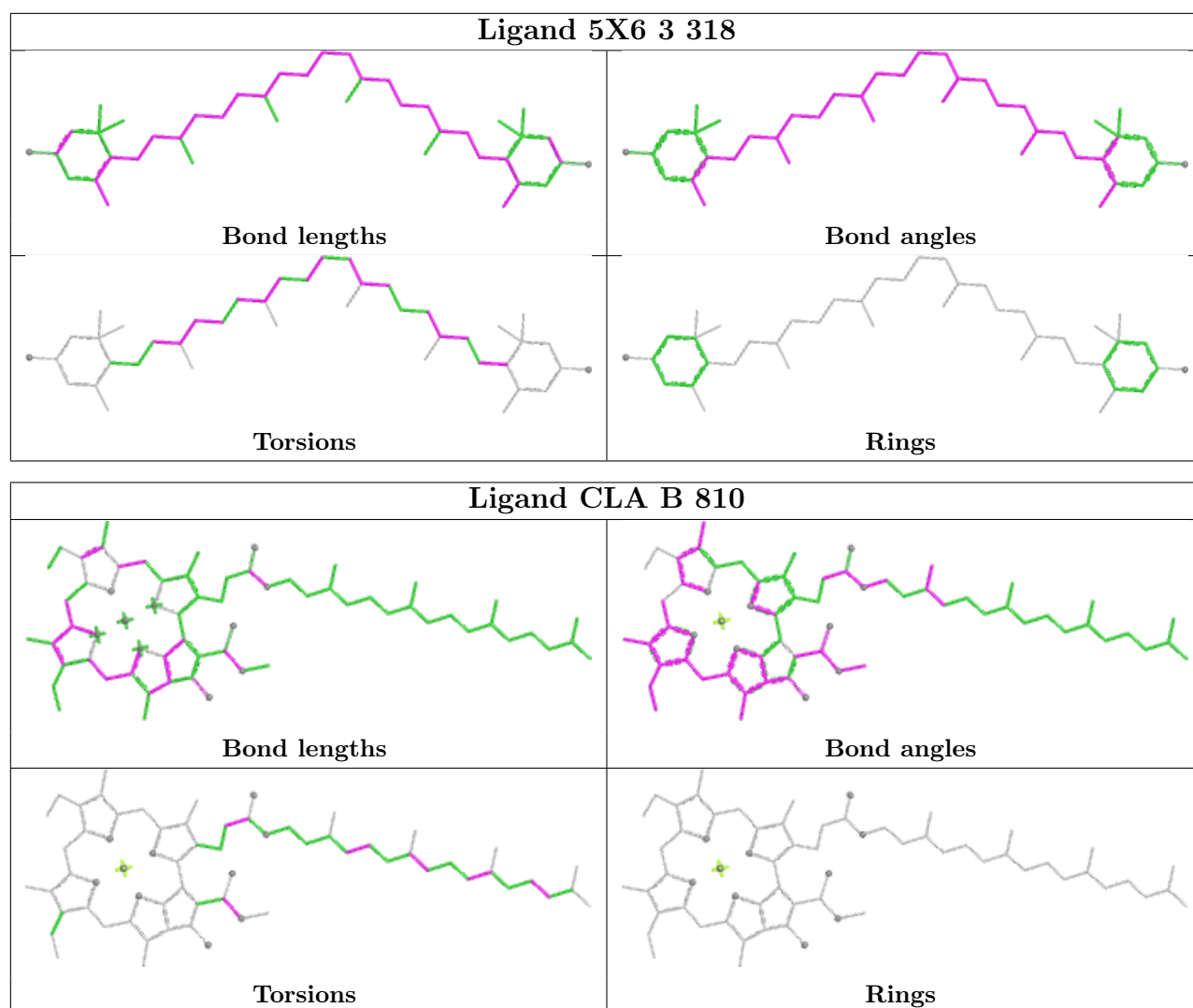


Ligand CLA B 811

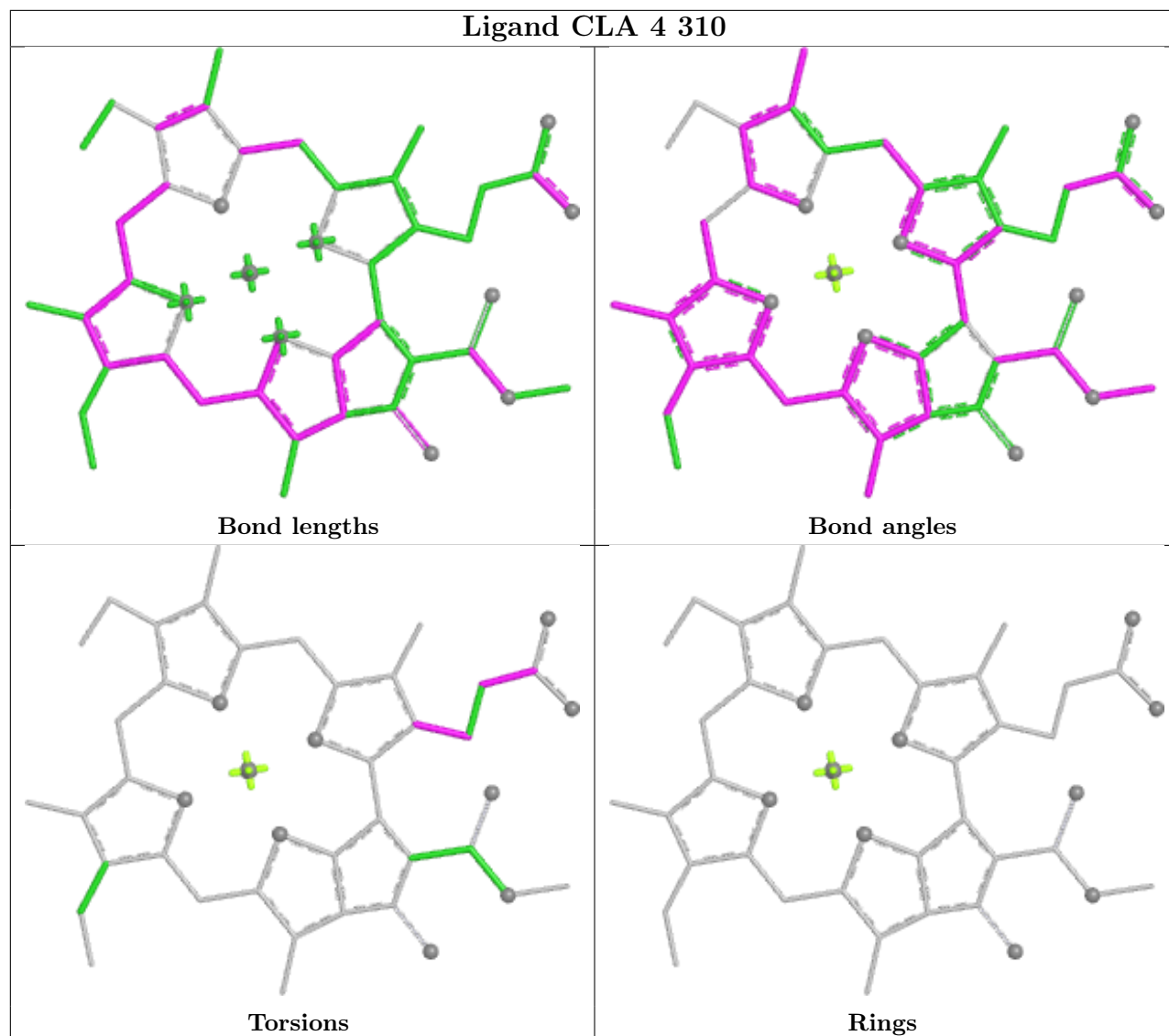




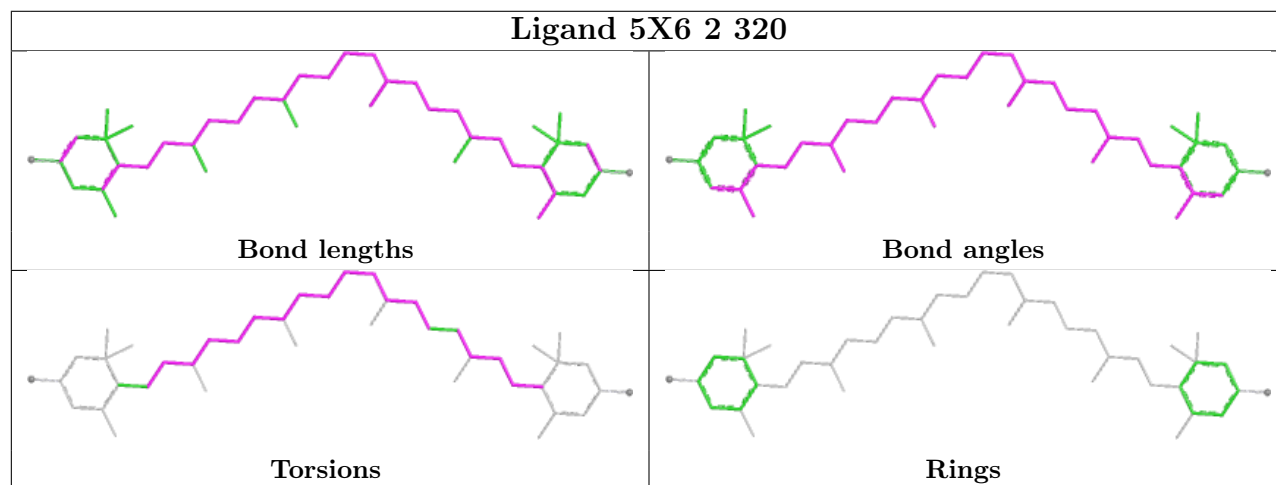




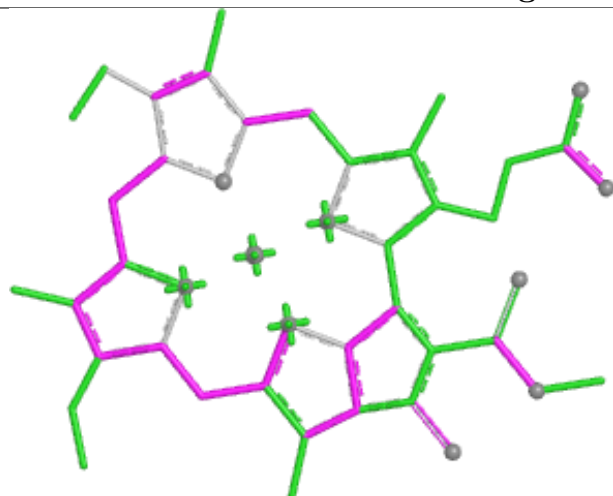
Ligand CLA 4 310



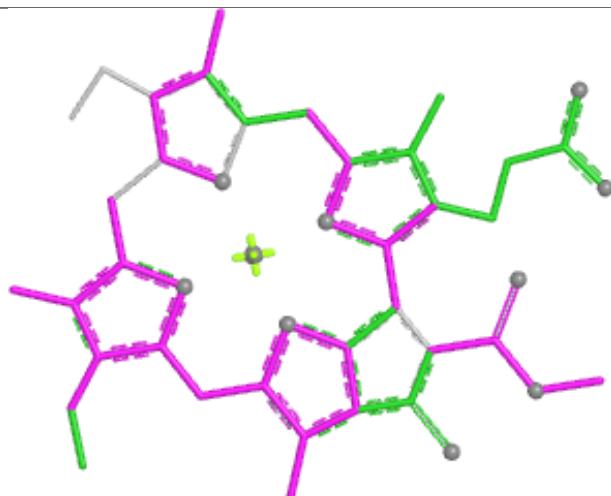
Ligand 5X6 2 320



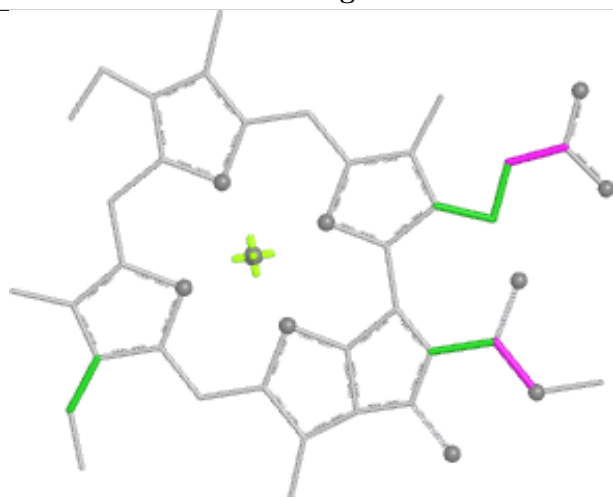
Ligand CLA 1 309



Bond lengths



Bond angles

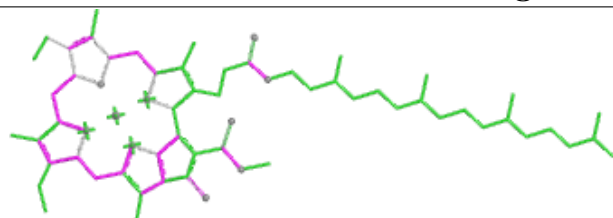


Torsions

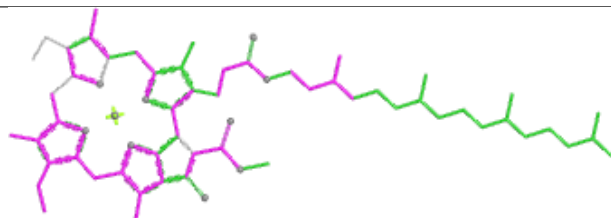


Rings

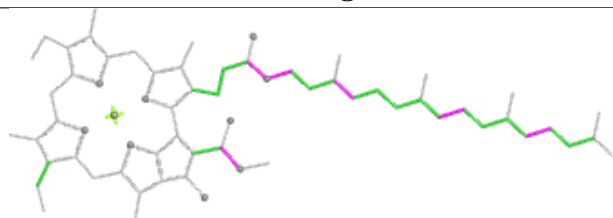
Ligand CLA B 840



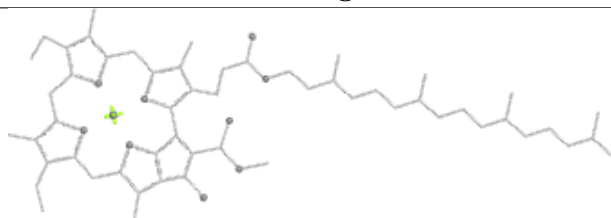
Bond lengths



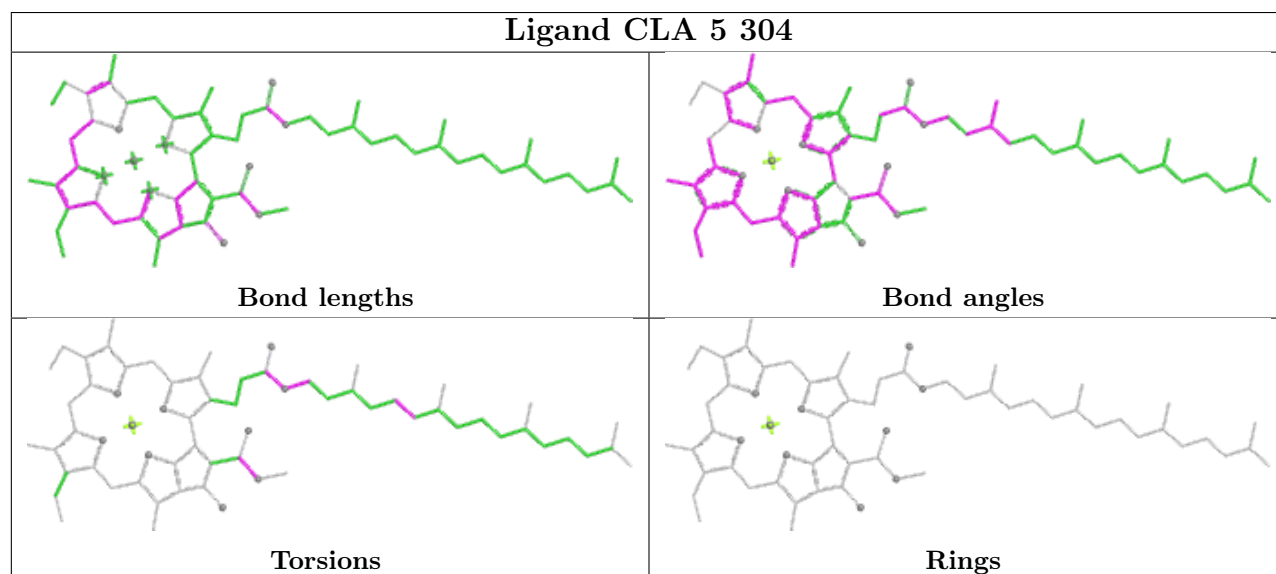
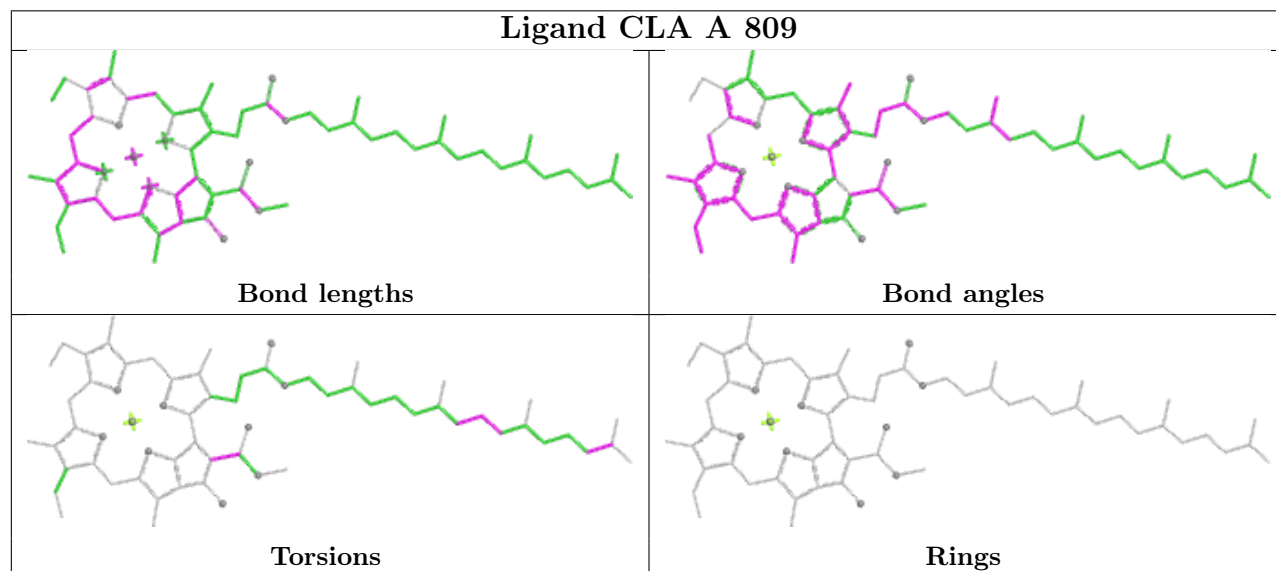
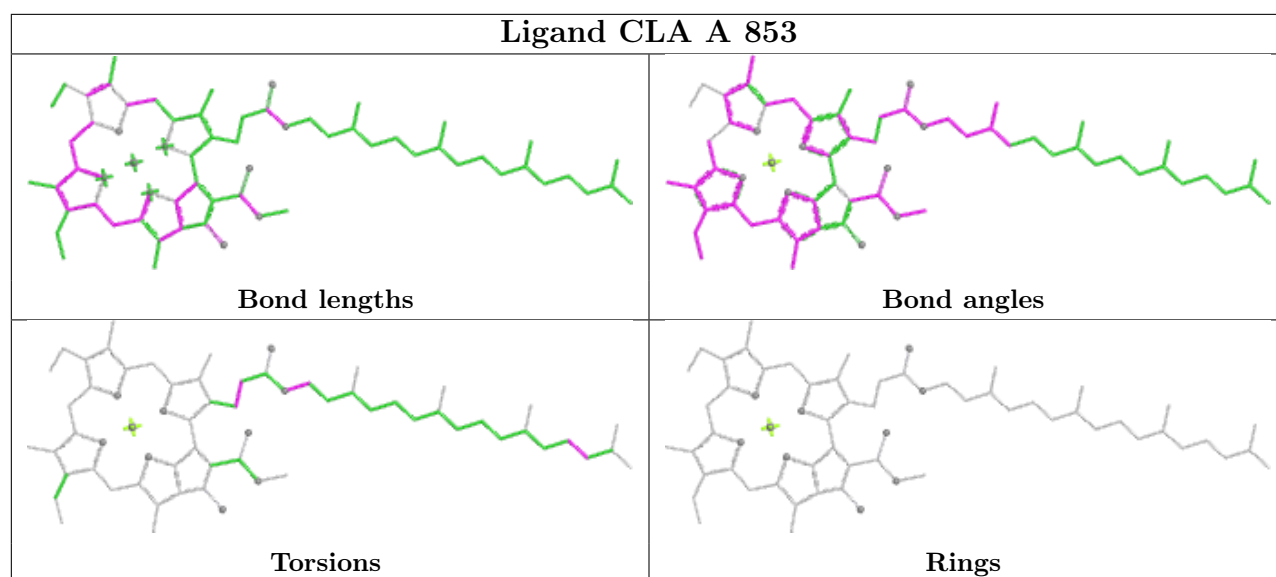
Bond angles

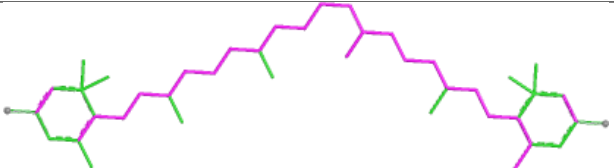
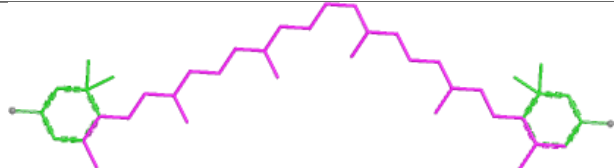
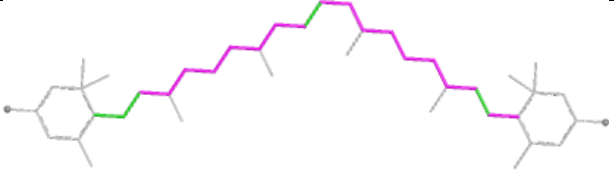
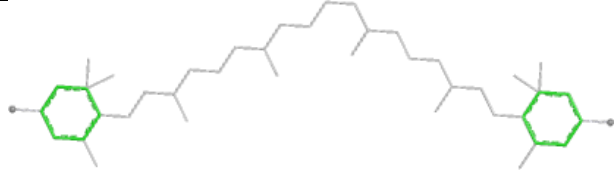


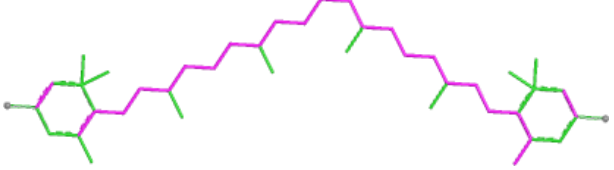

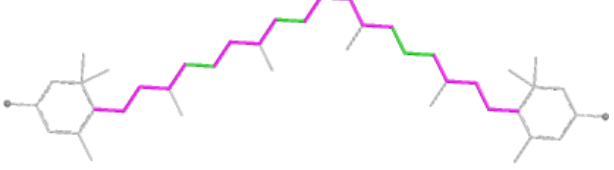
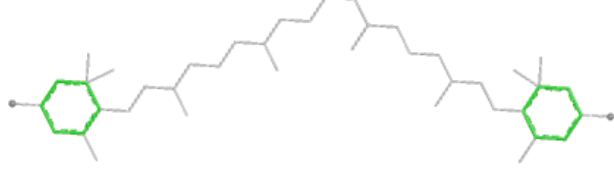
Torsions

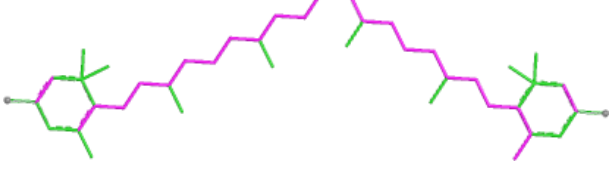
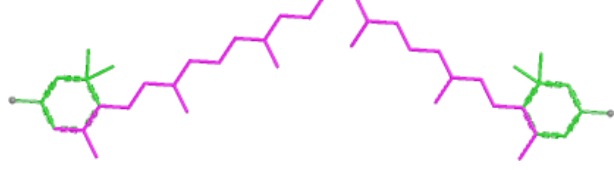
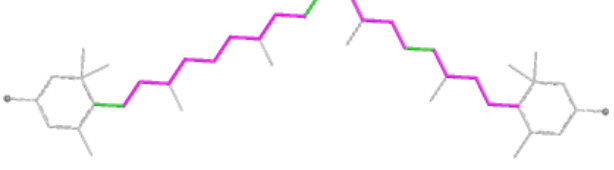
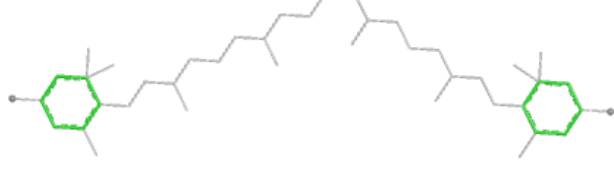


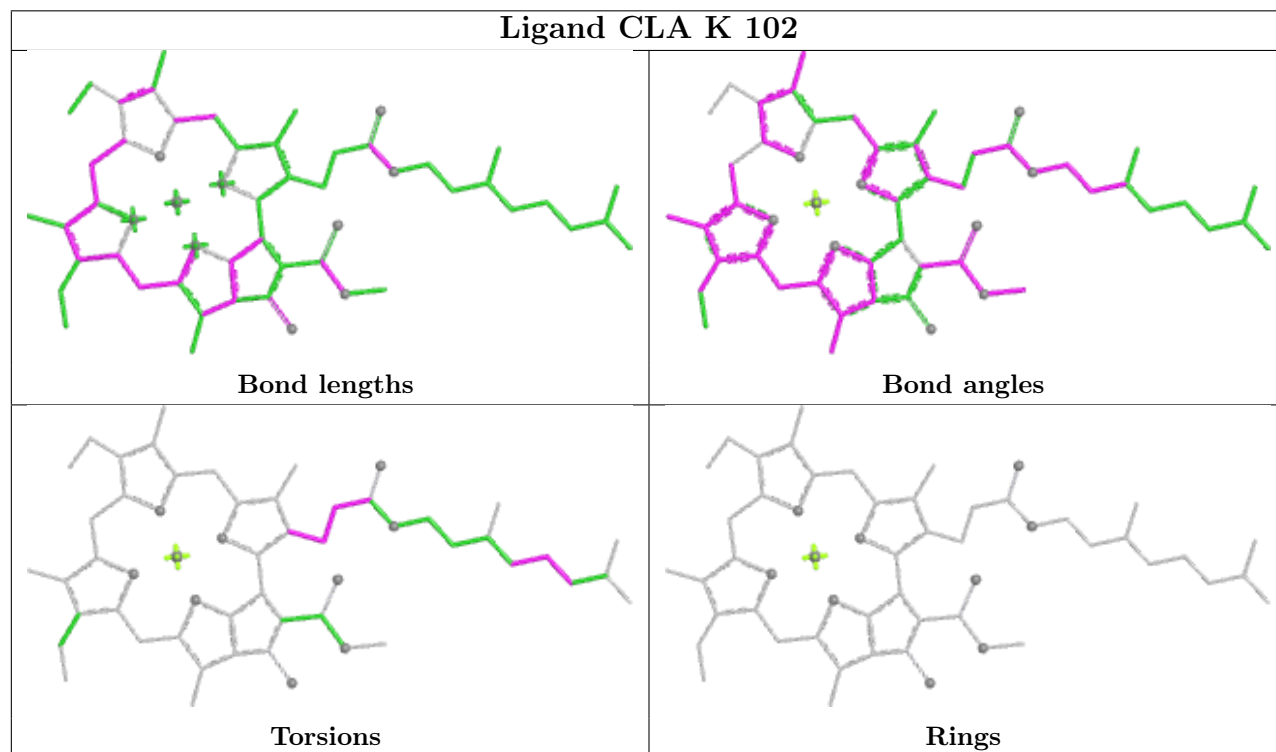
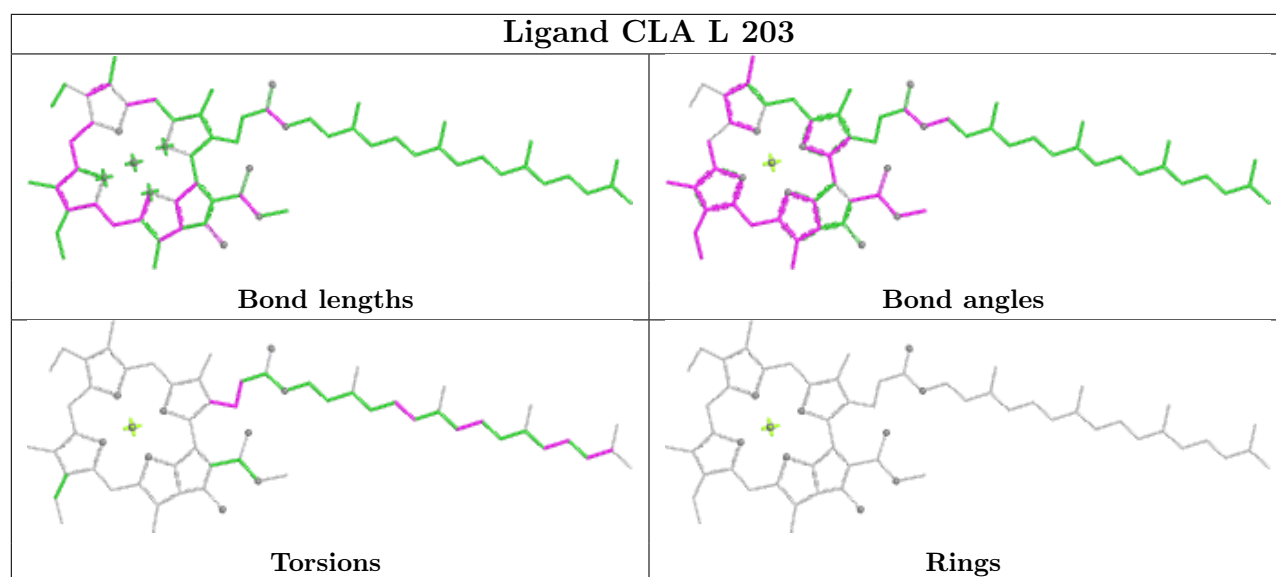
Rings

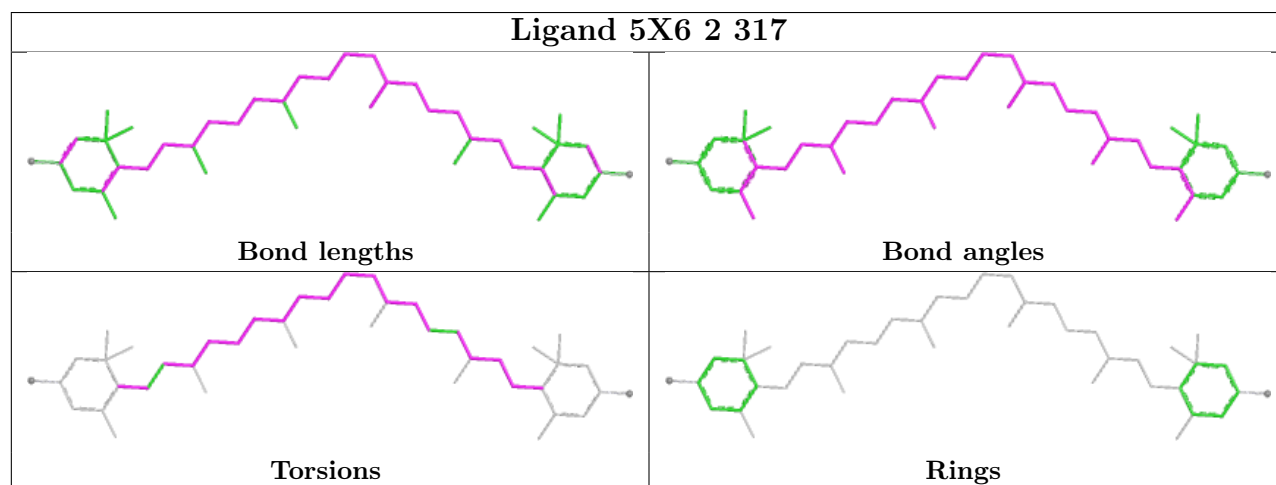
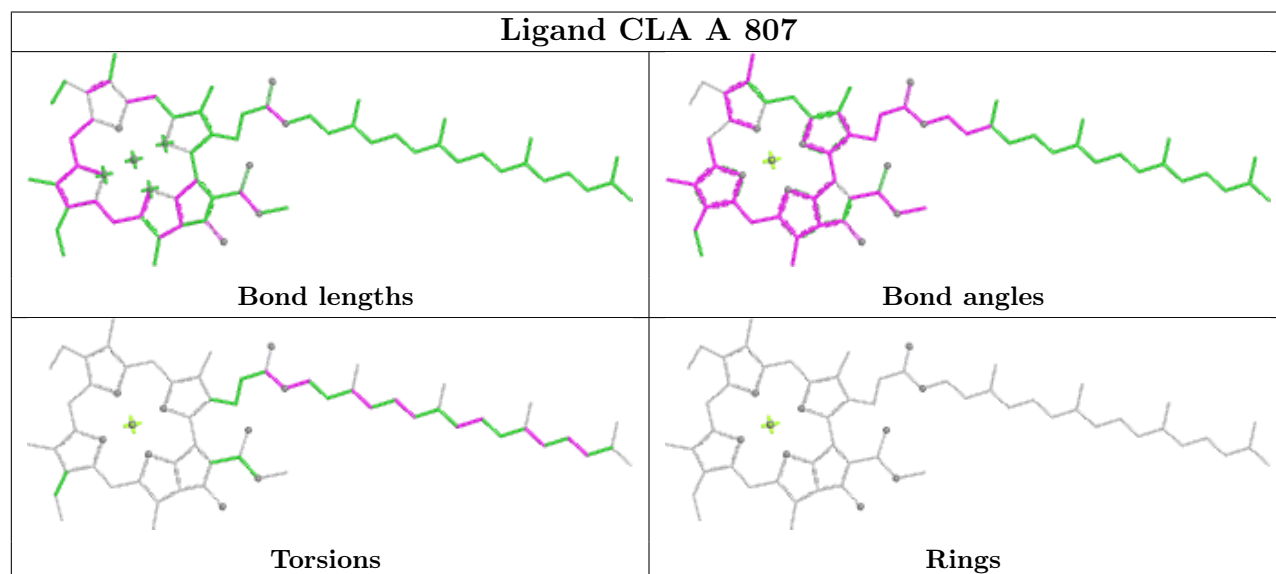
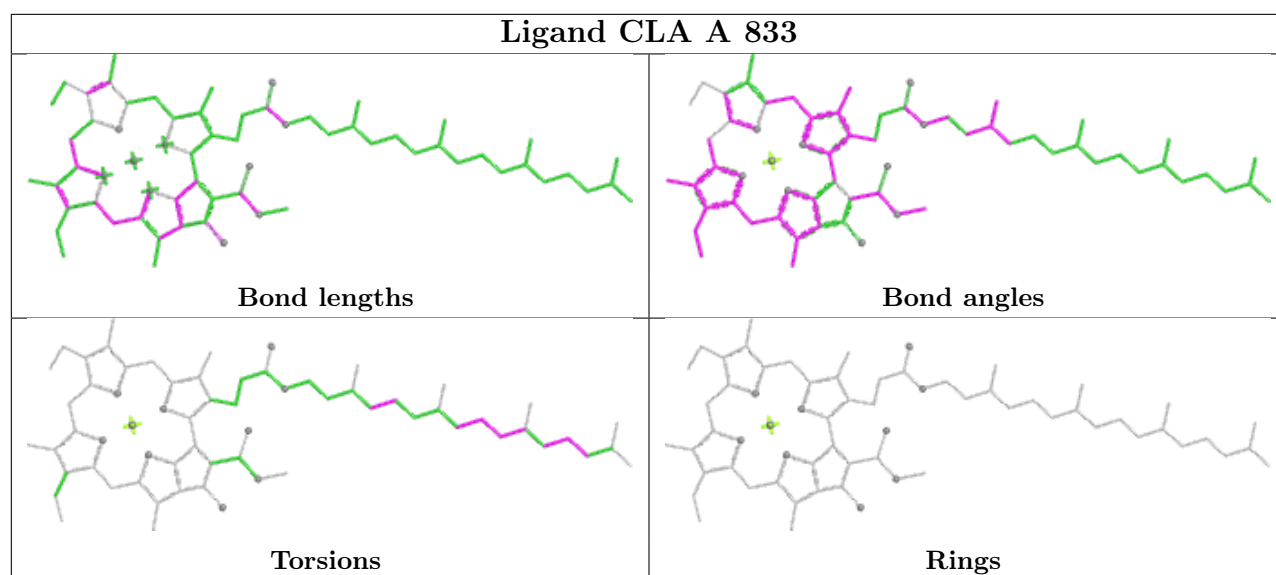


Ligand 5X6 5 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

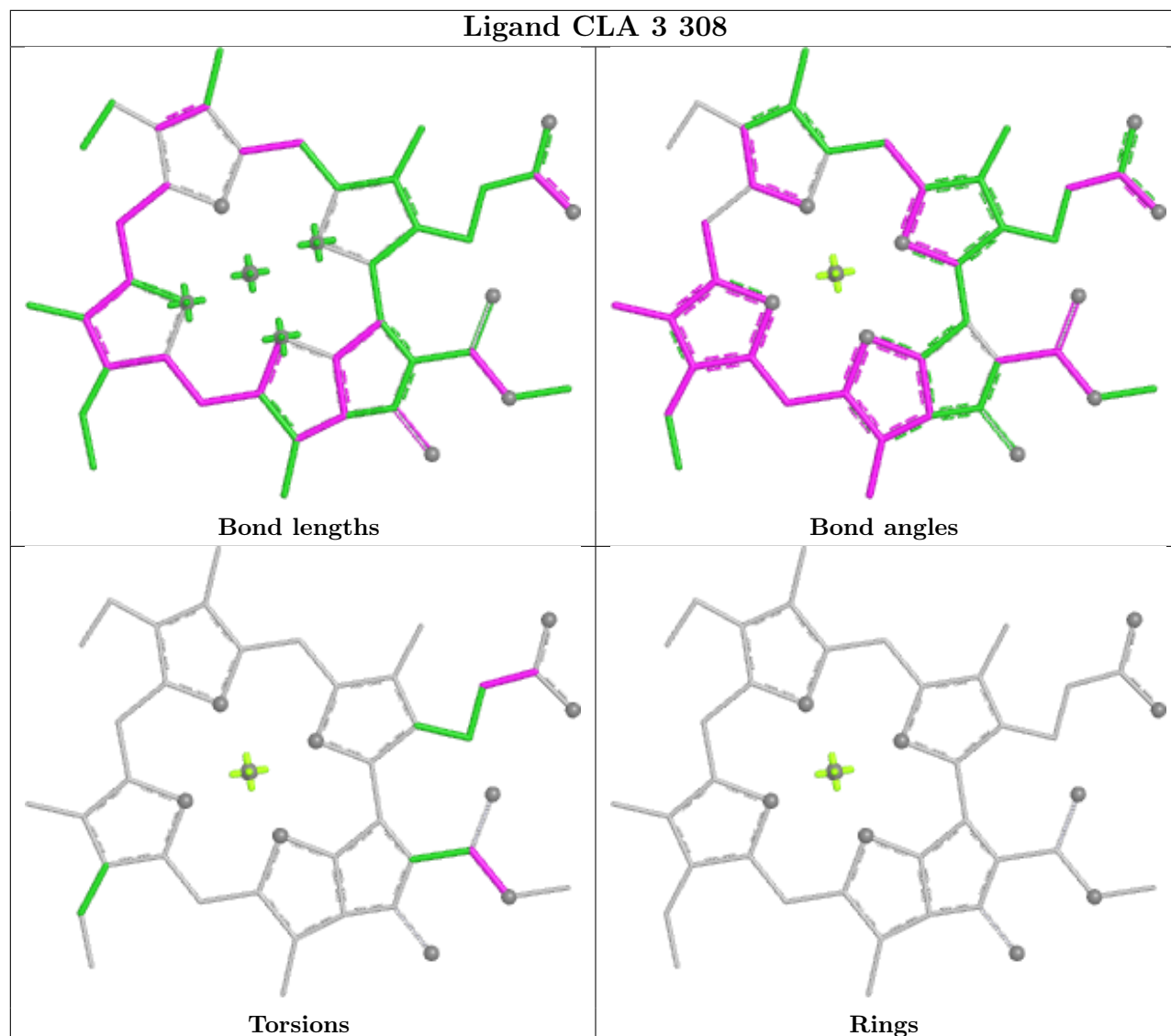
Ligand 5X6 5 316	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand 5X6 3 317	
	
Bond lengths	Bond angles
	
Torsions	Rings

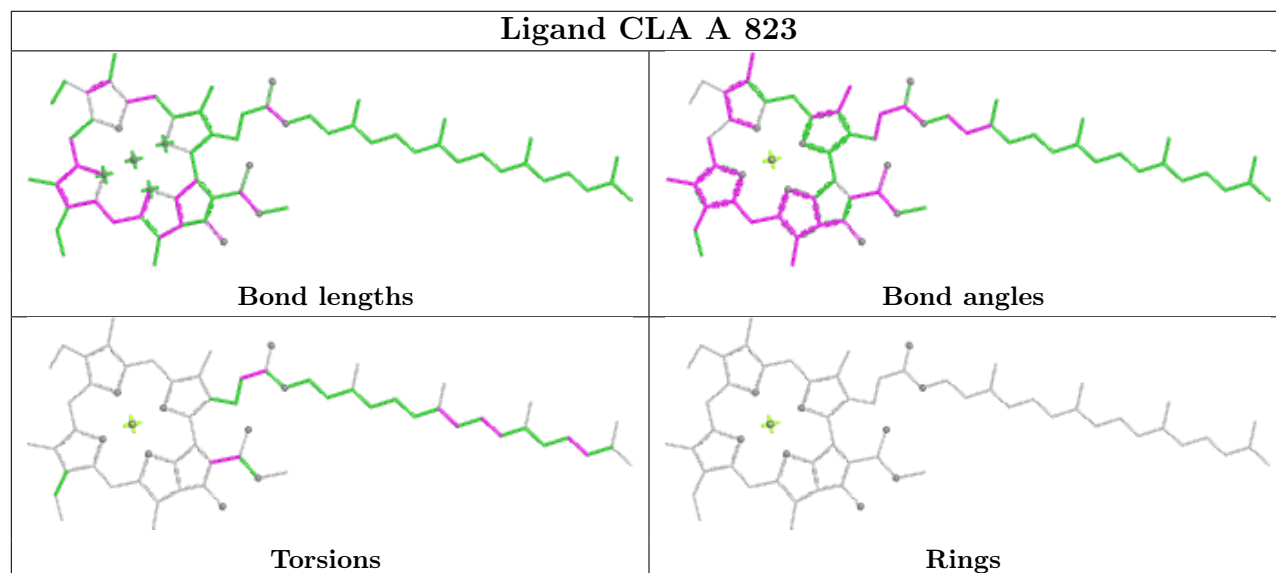




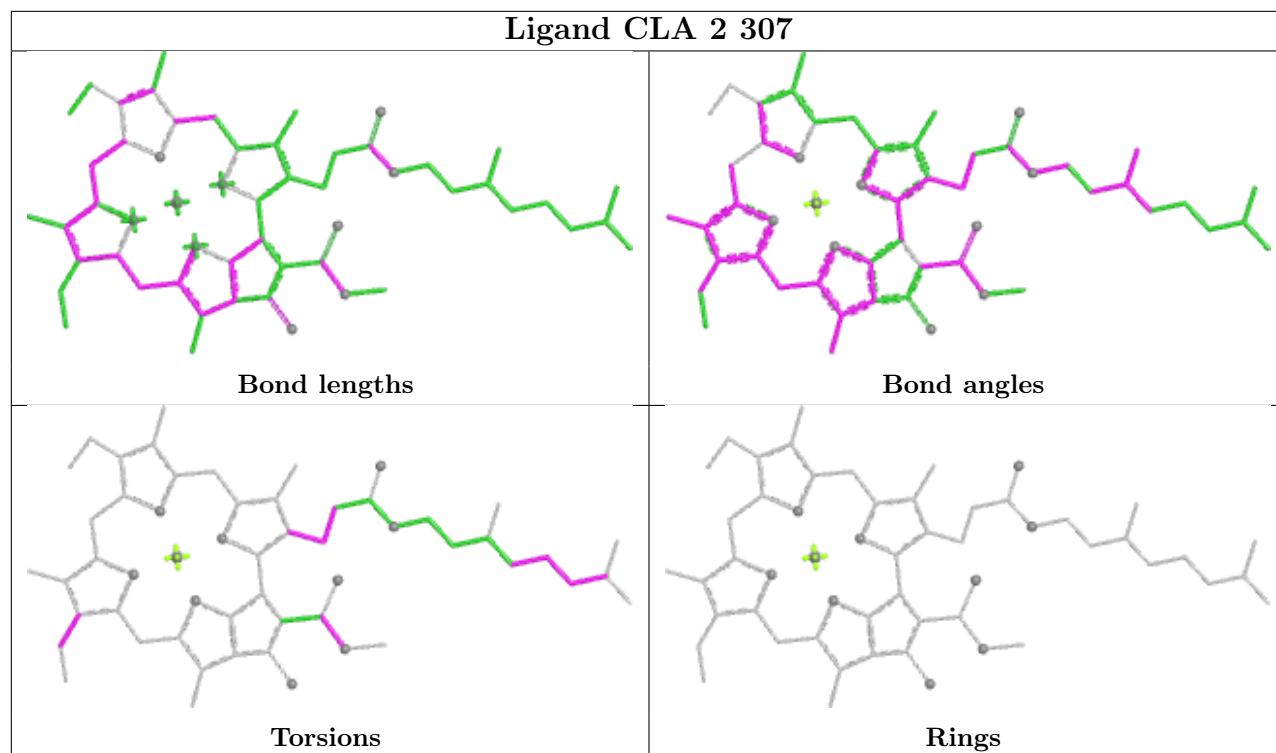
Ligand CLA 3 308



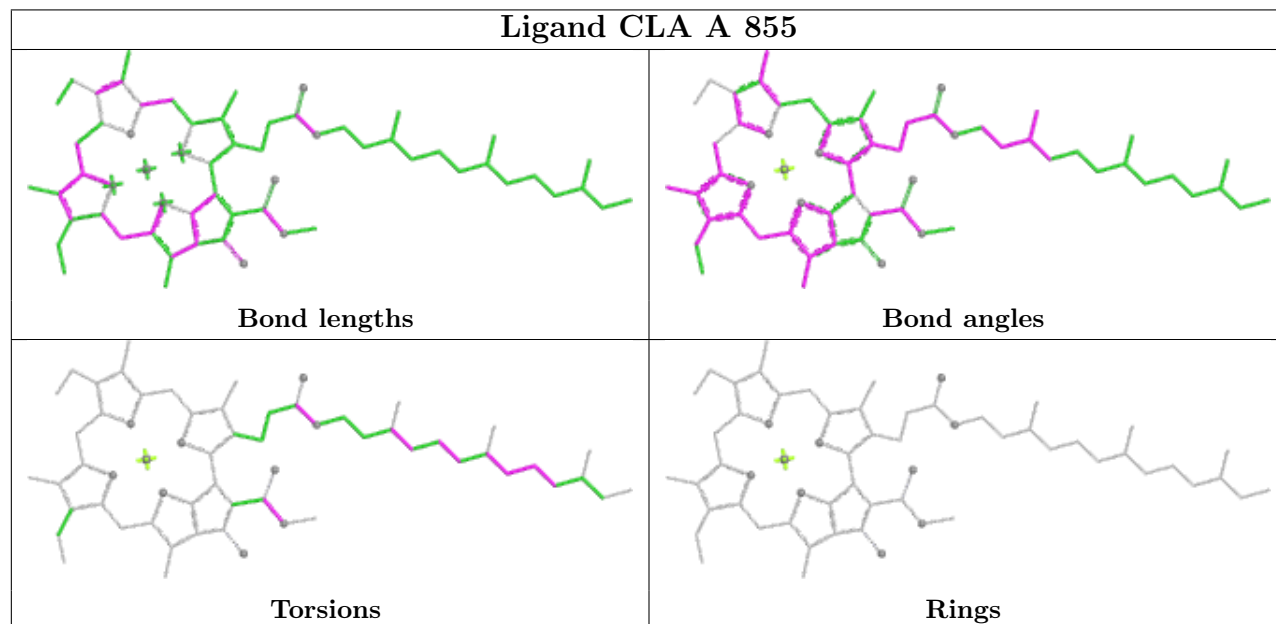
Ligand CLA A 823



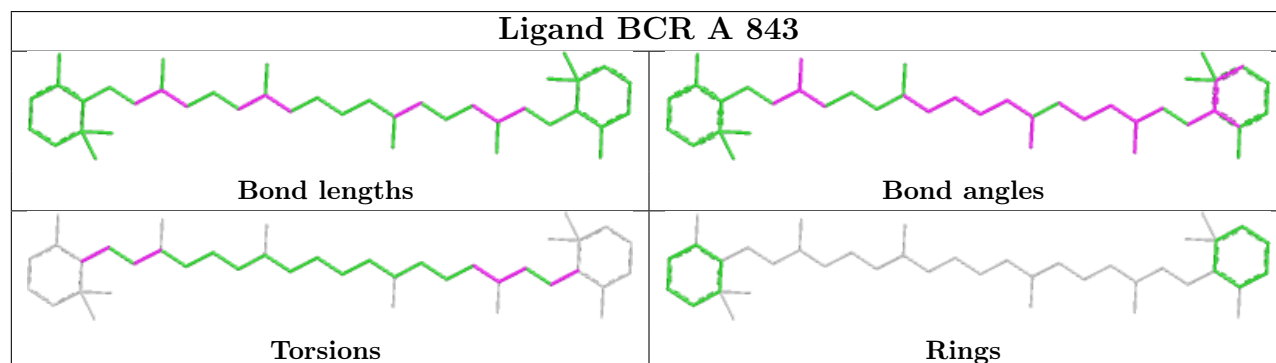
Ligand CLA 2 307

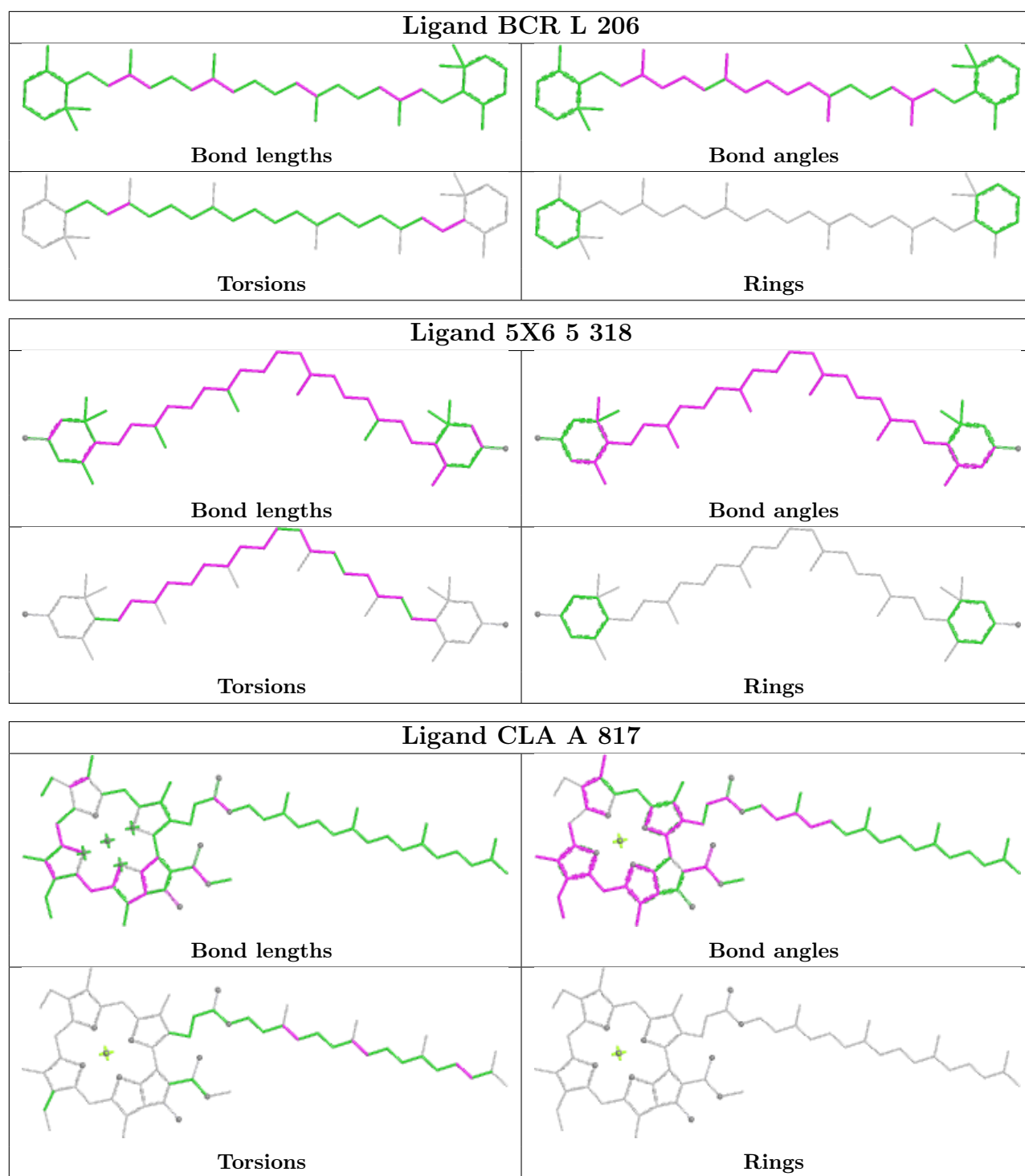


Ligand CLA A 855

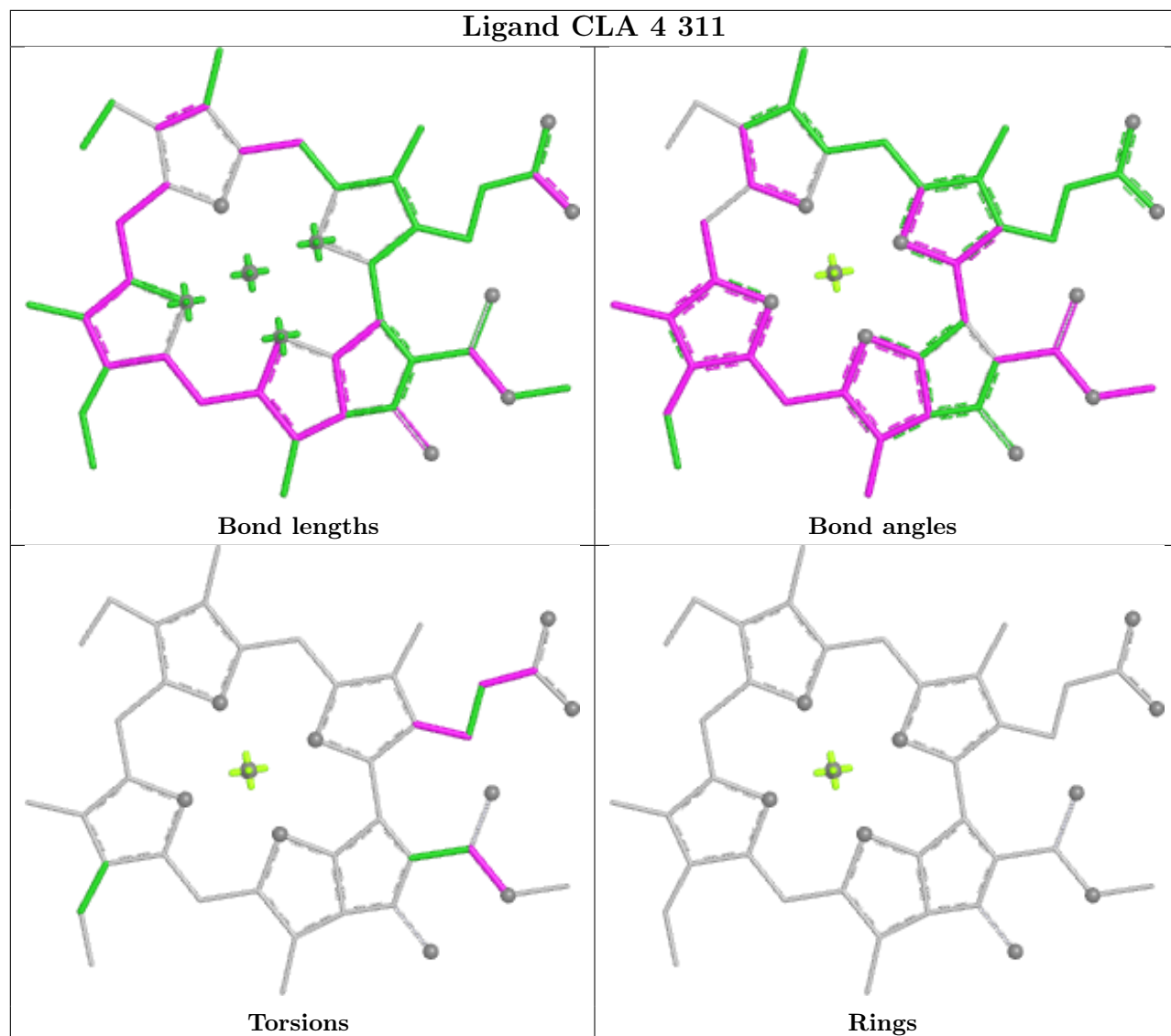


Ligand BCR A 843

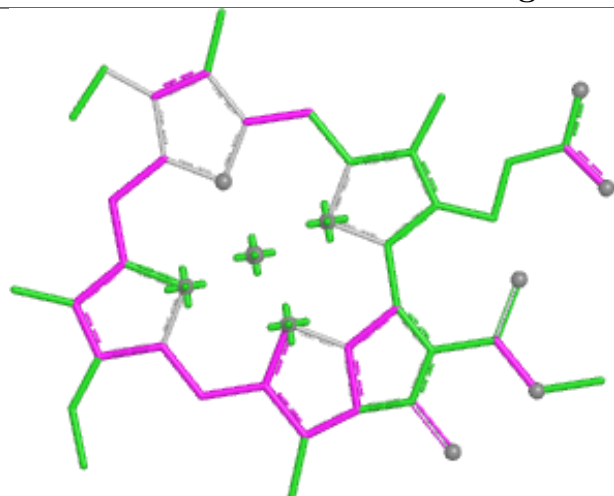




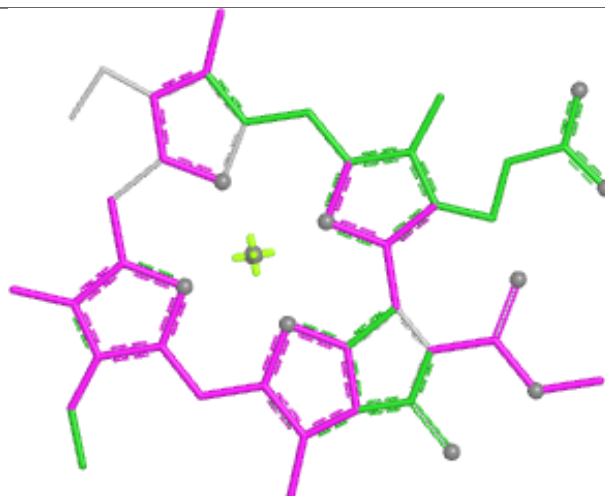
Ligand CLA 4 311



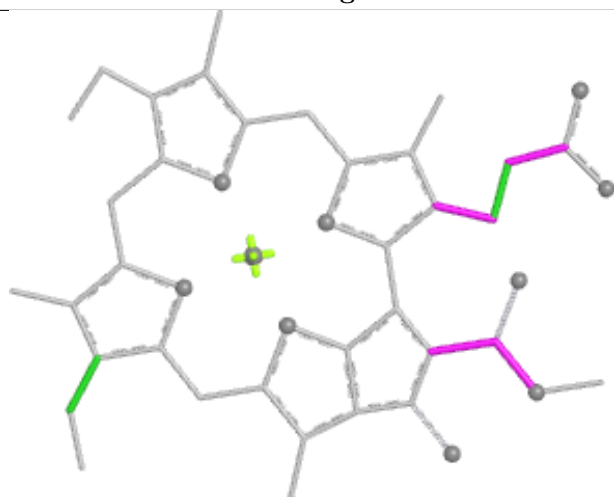
Ligand CLA 4 305



Bond lengths



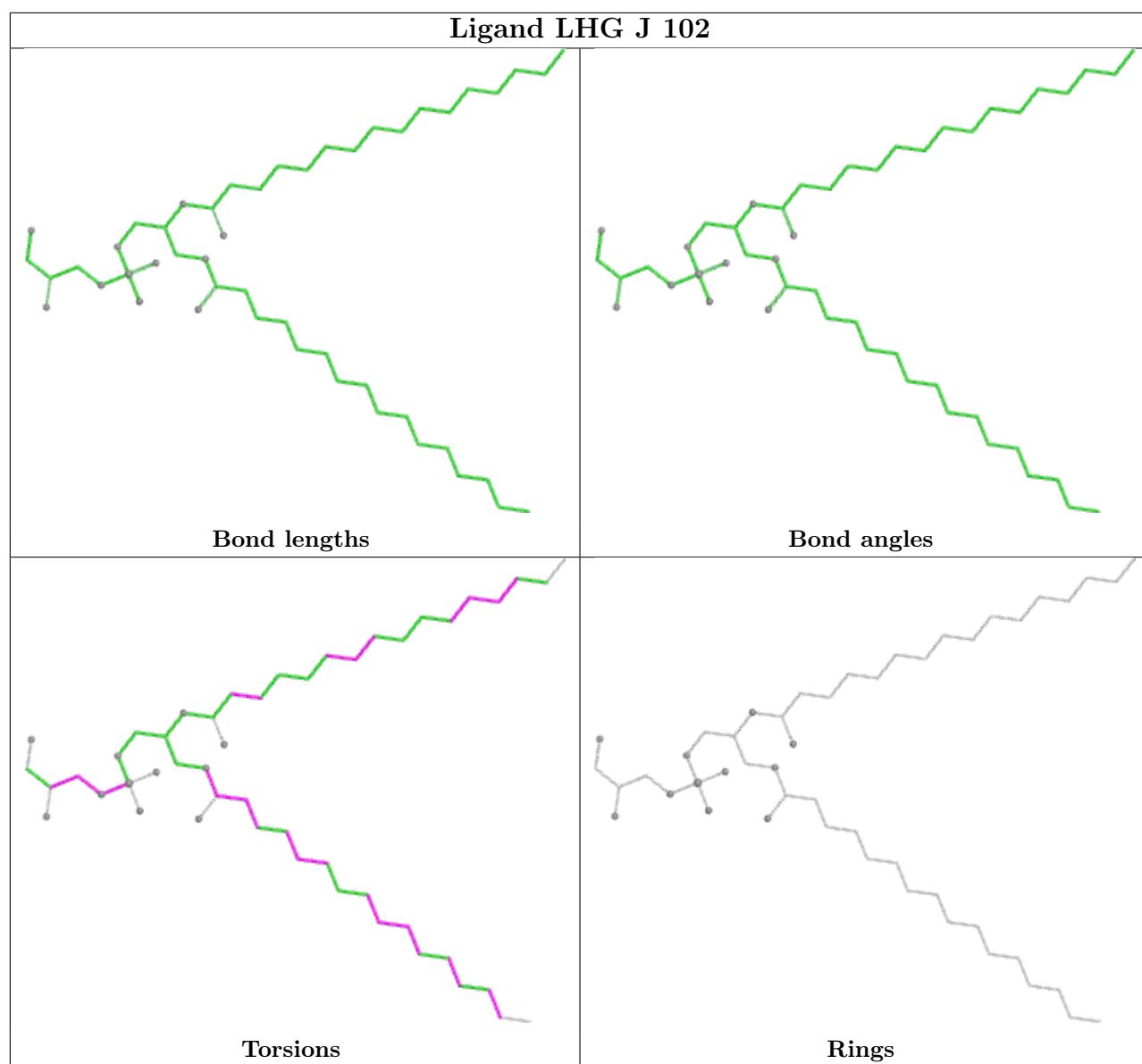
Bond angles



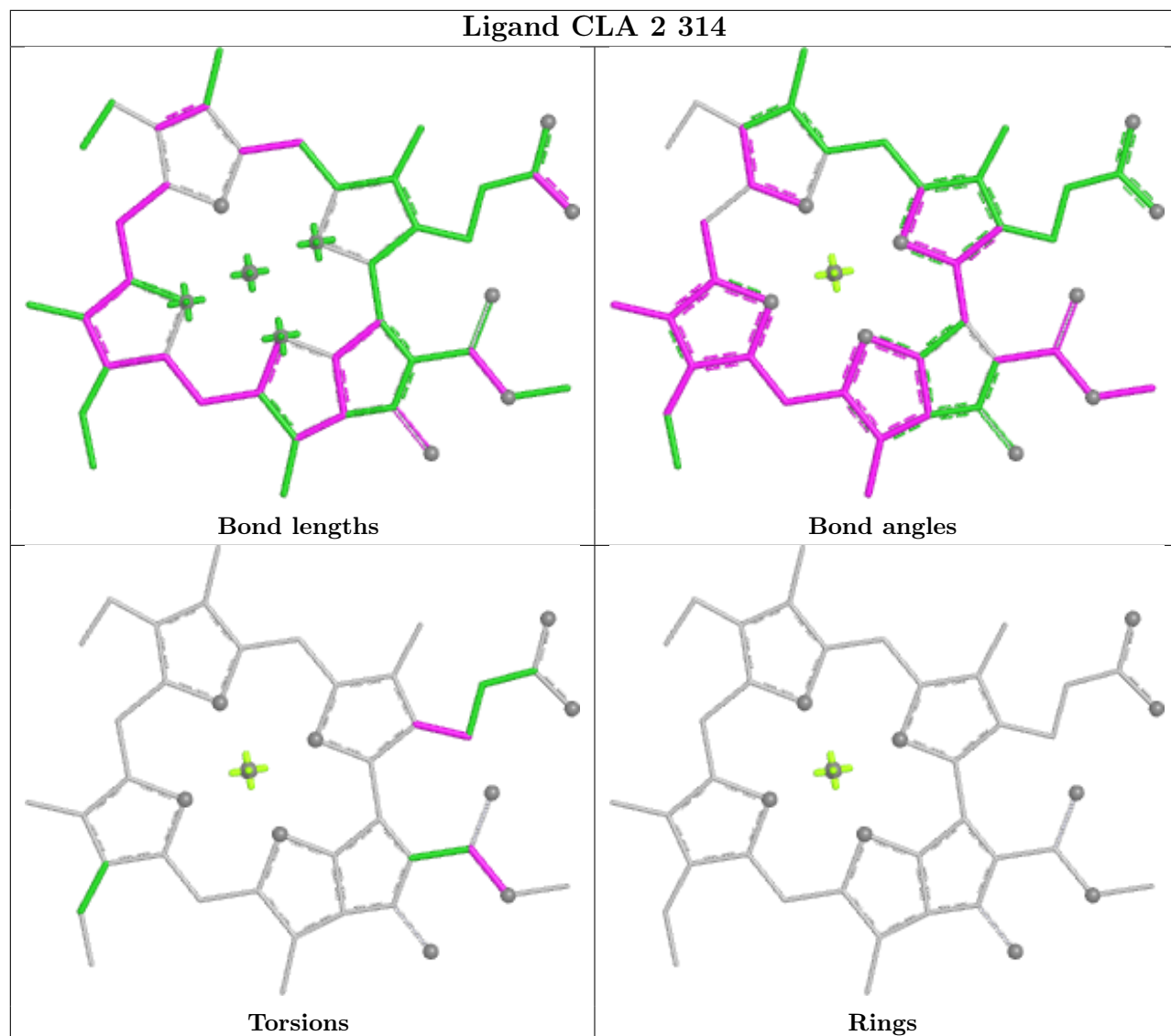
Torsions



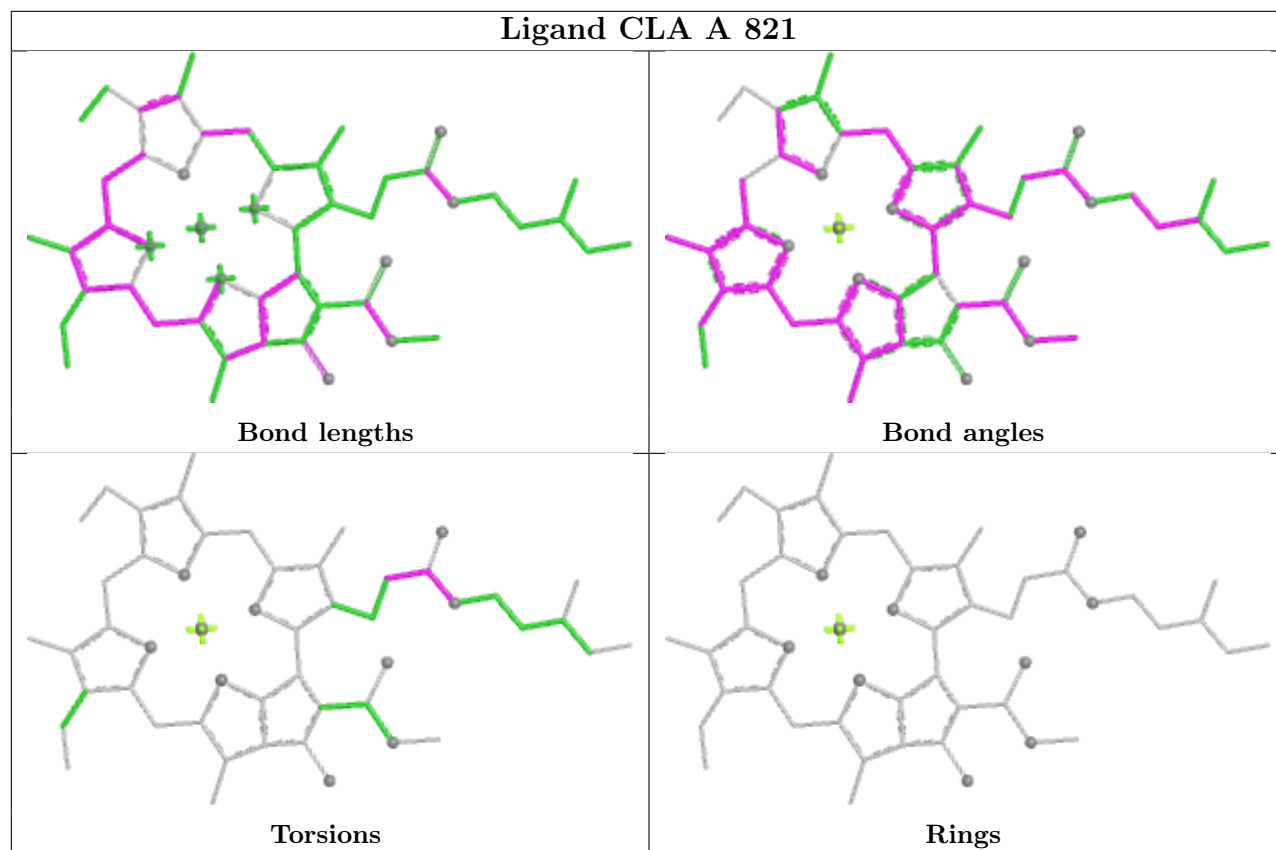
Rings



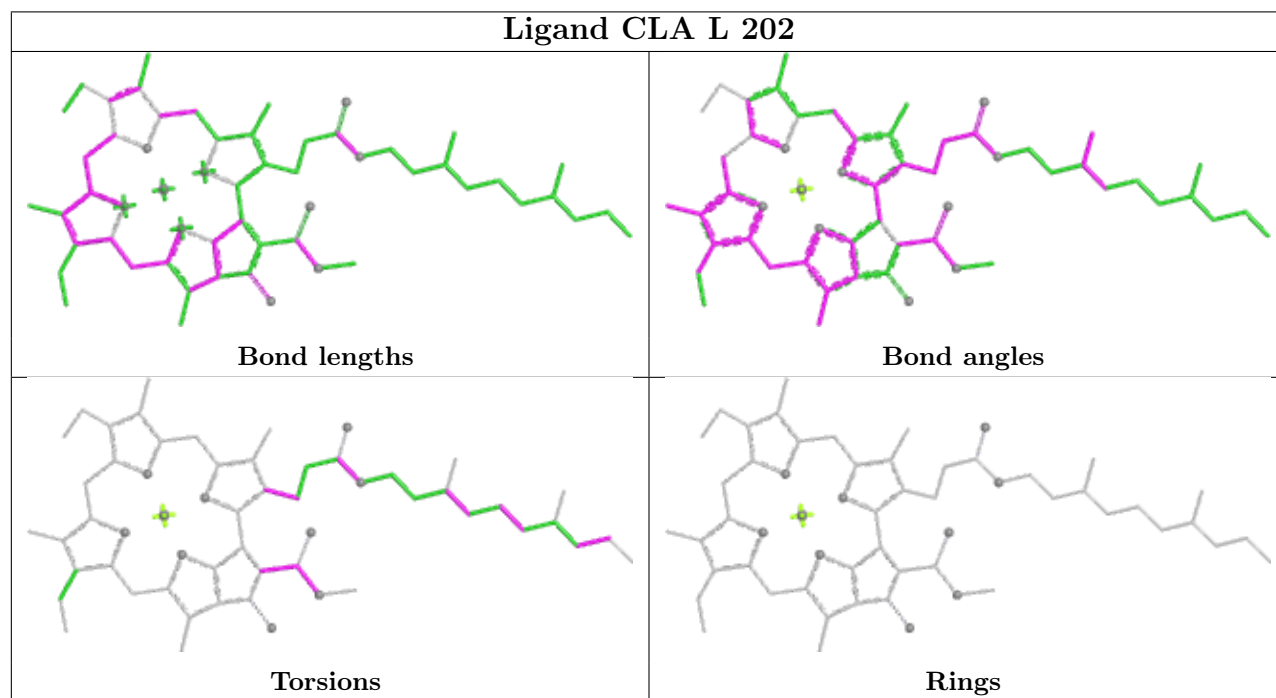
Ligand CLA 2 314

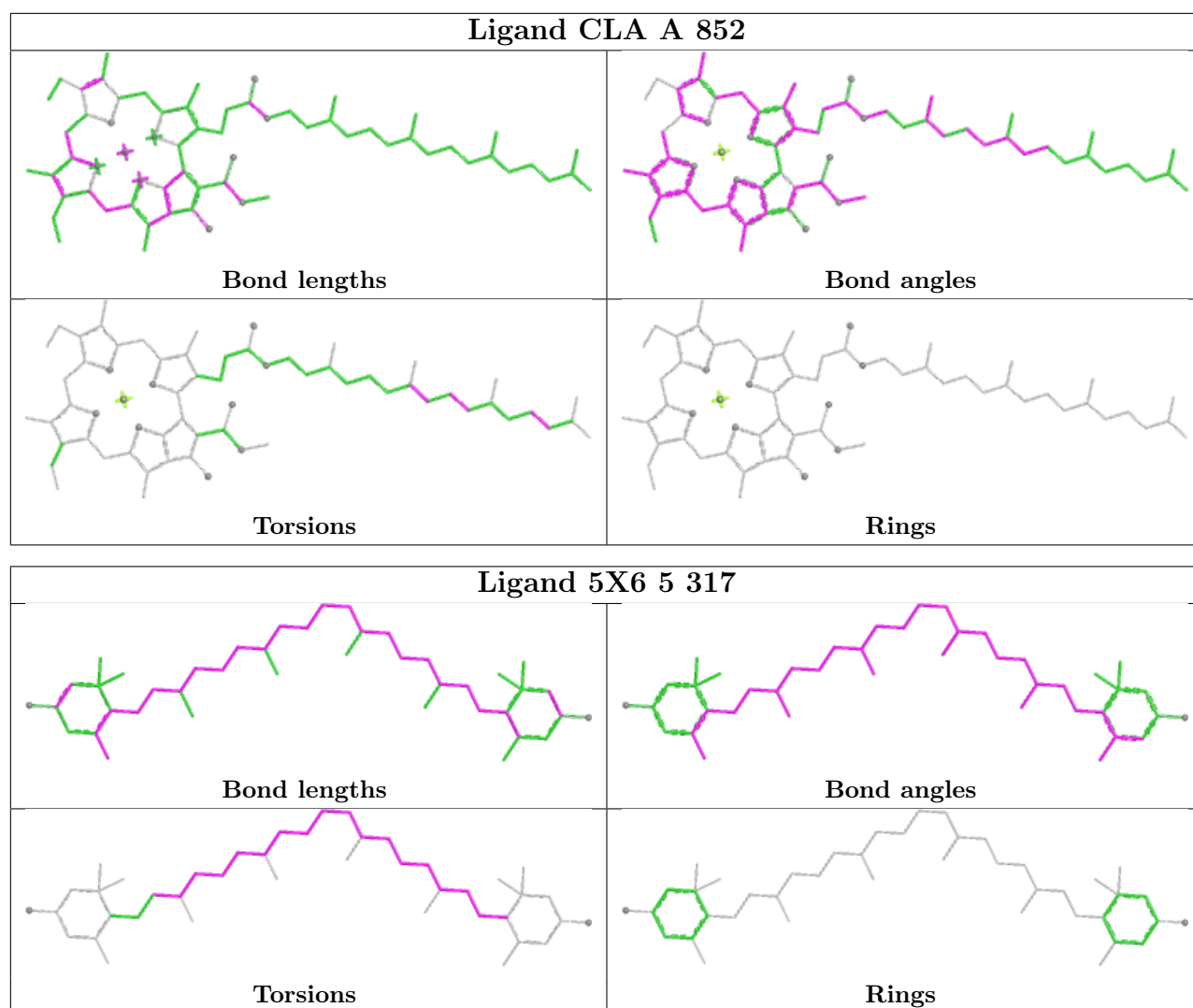


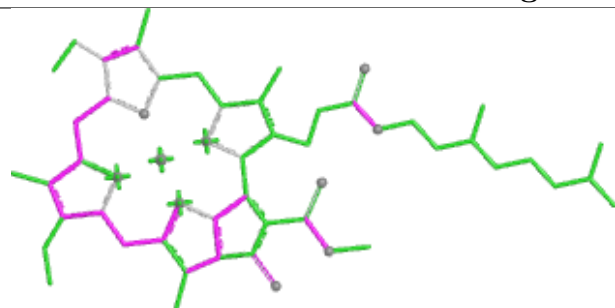
Ligand CLA A 821



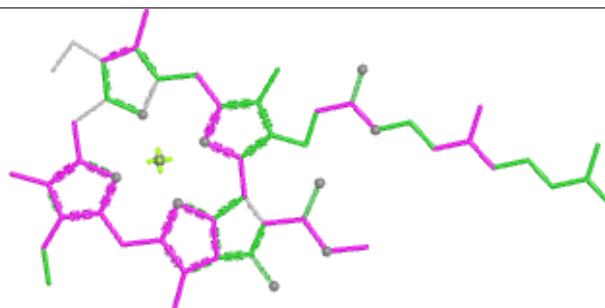
Ligand CLA L 202



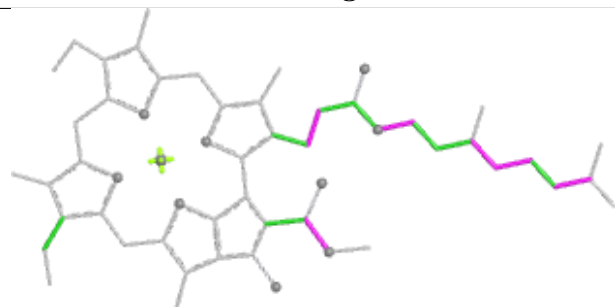


Ligand CLA 1 303

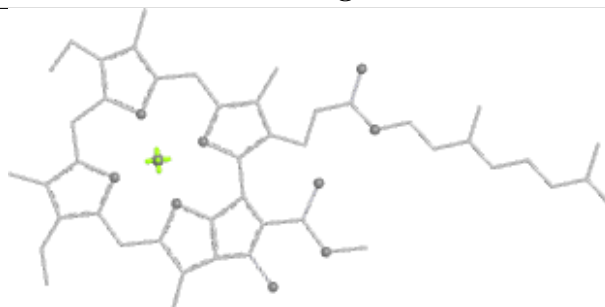
Bond lengths



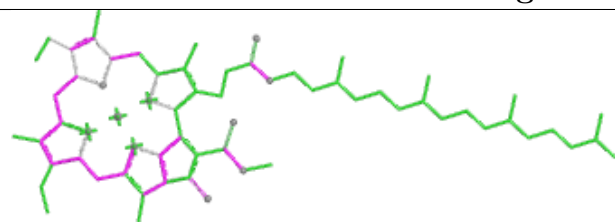
Bond angles



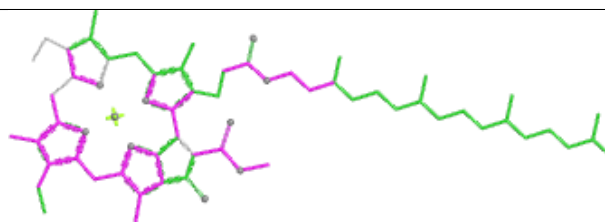
Torsions



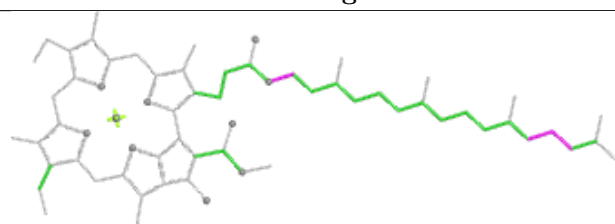
Rings

Ligand CLA B 841

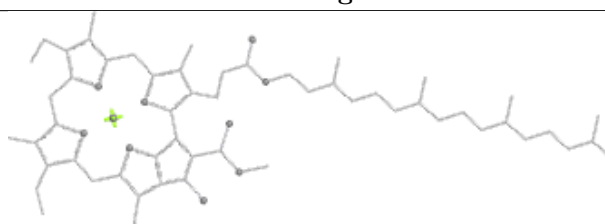
Bond lengths



Bond angles

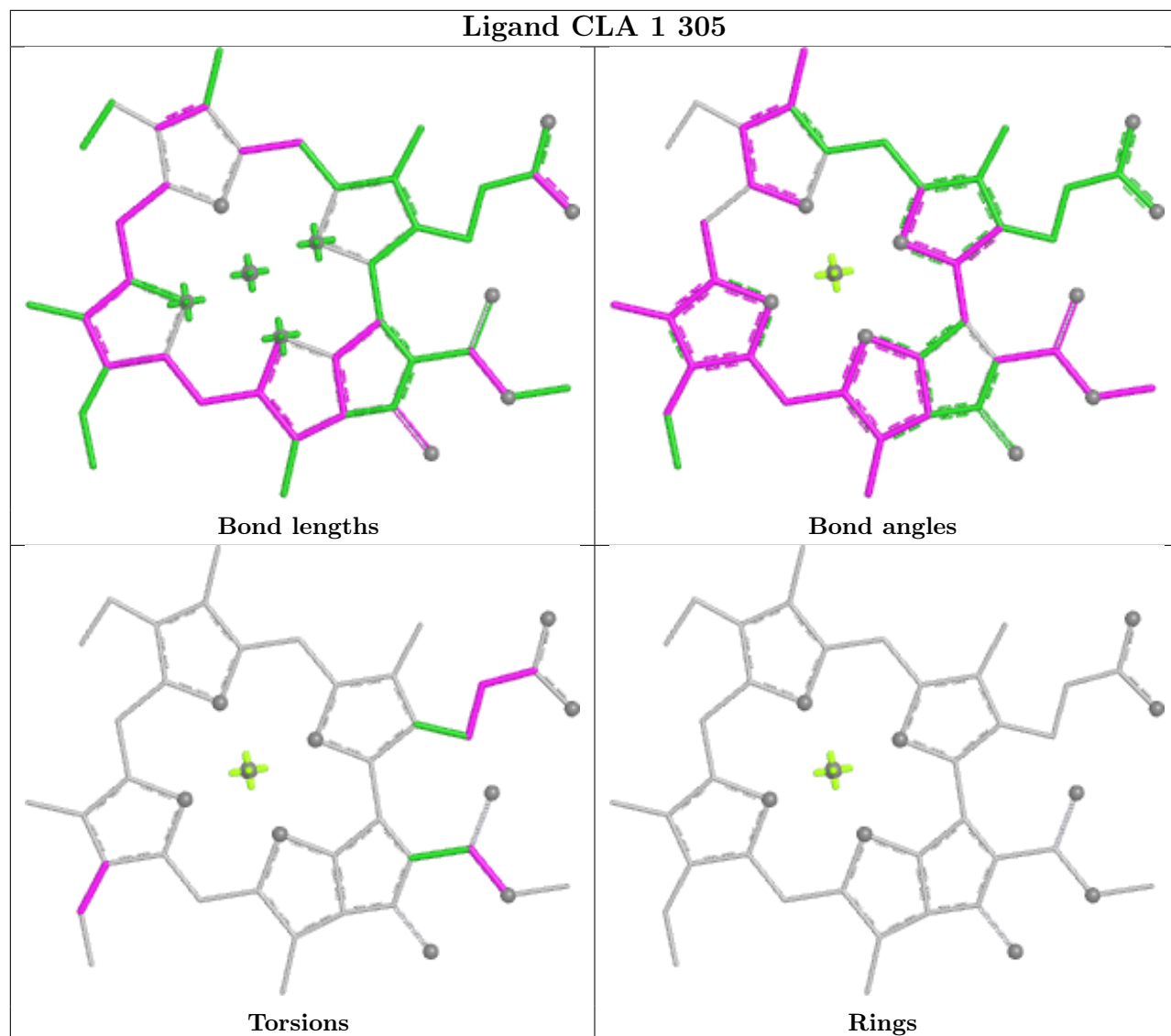


Torsions

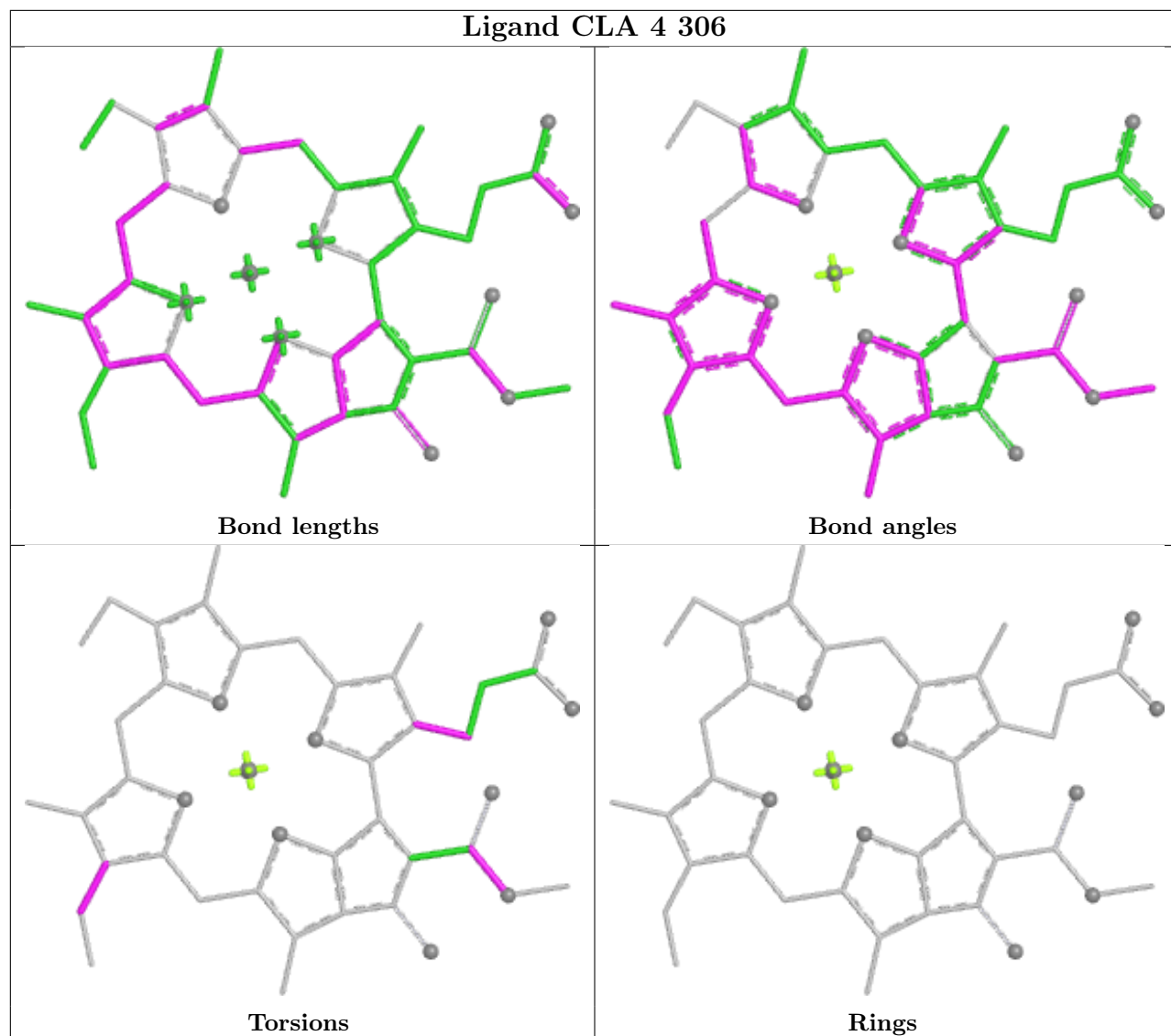


Rings

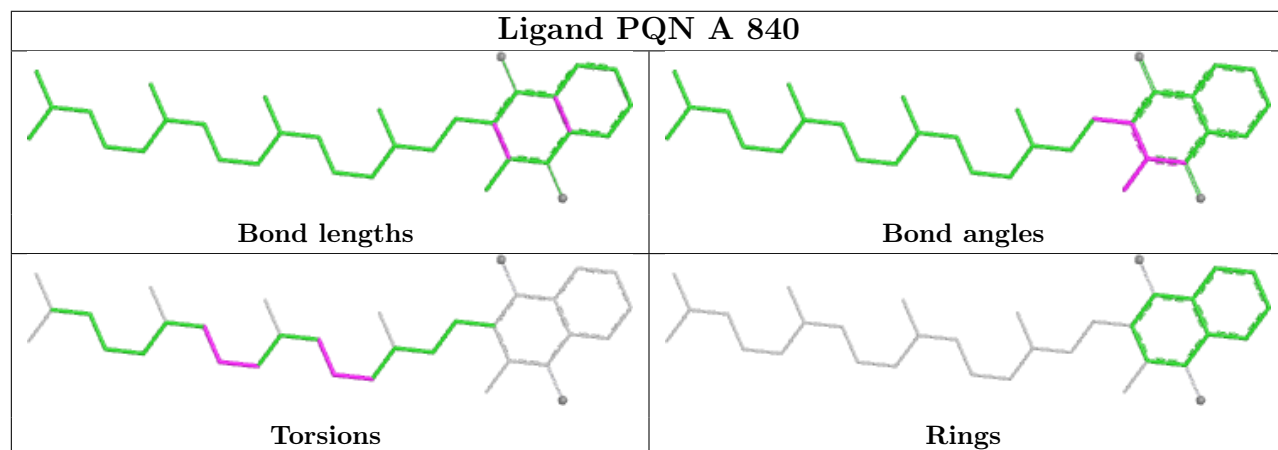
Ligand CLA 1 305

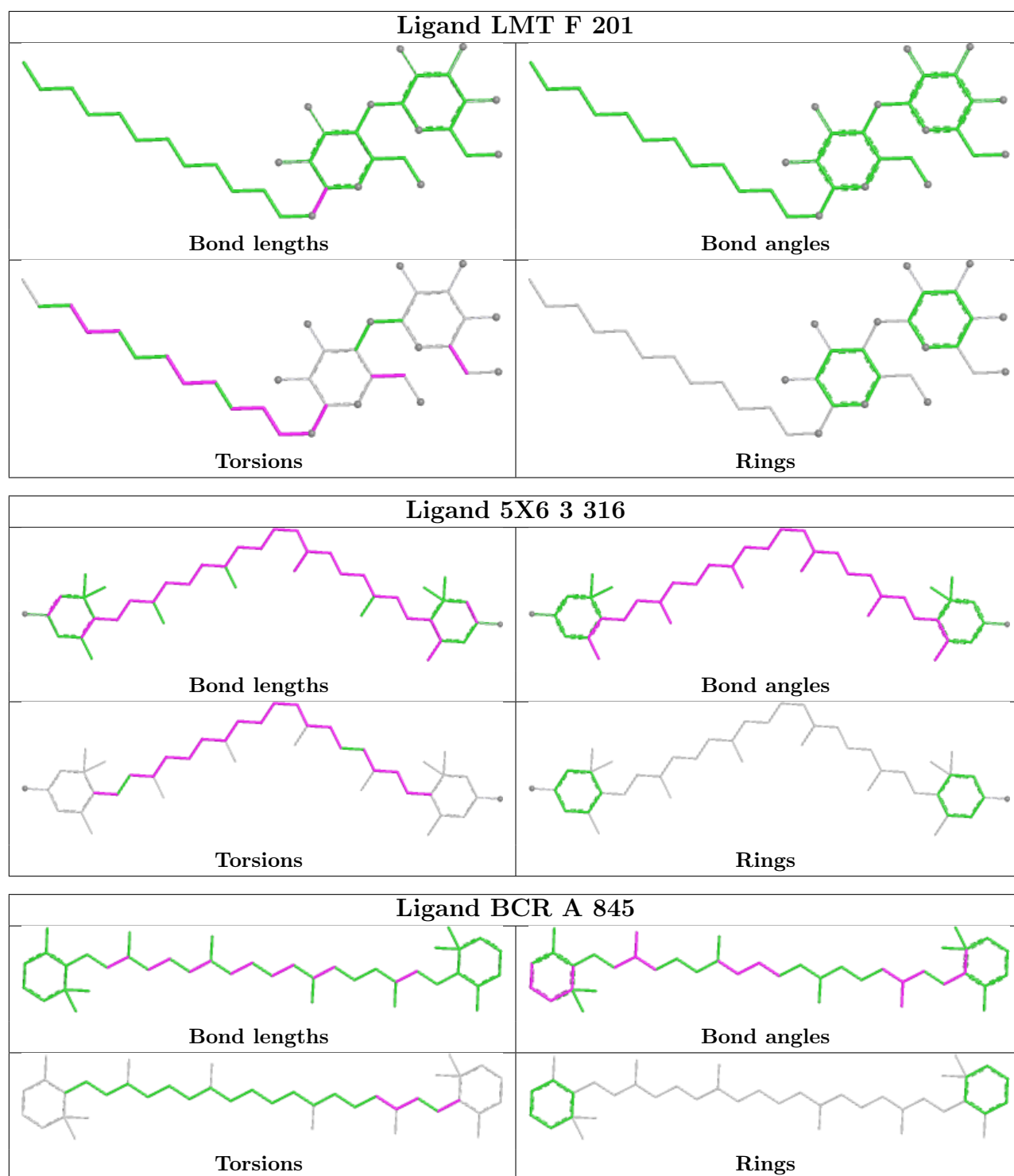


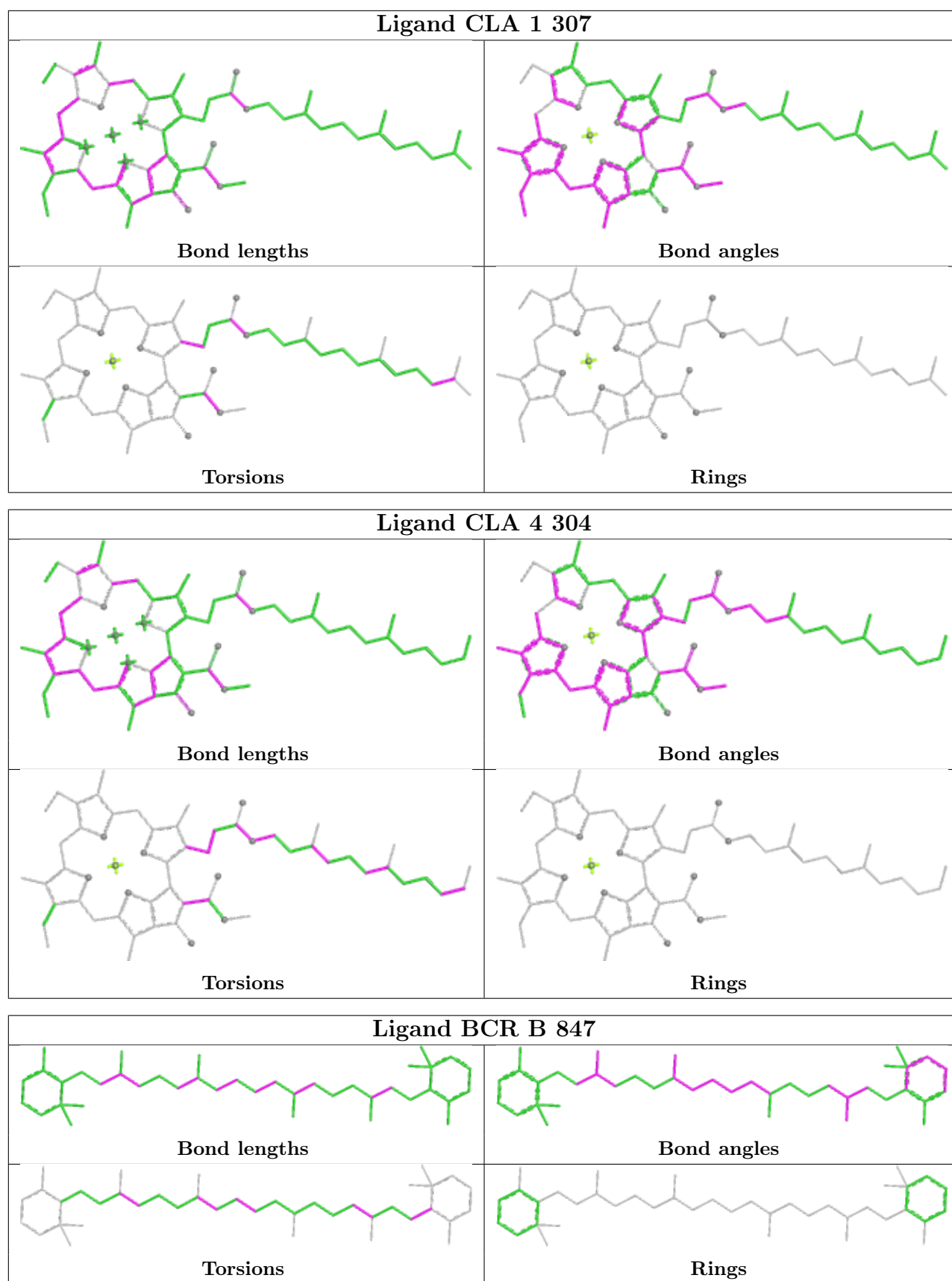
Ligand CLA 4 306



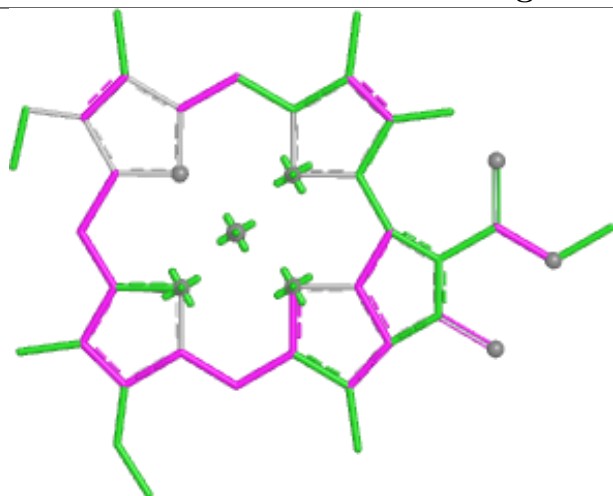
Ligand PQN A 840



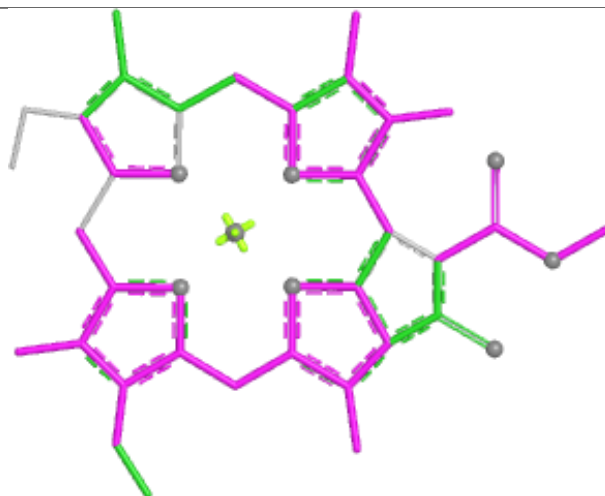




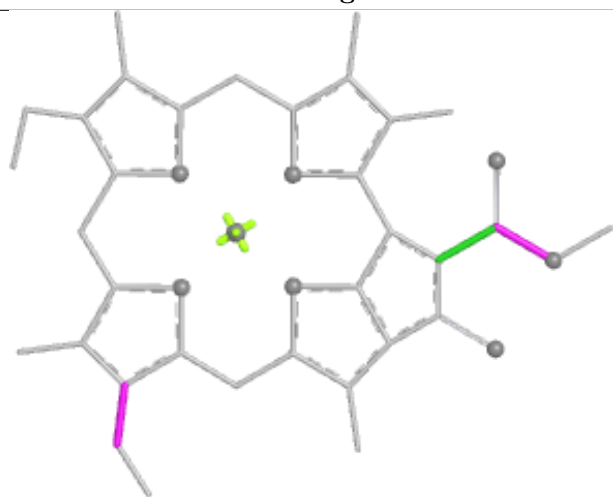
Ligand CLA F 204



Bond lengths



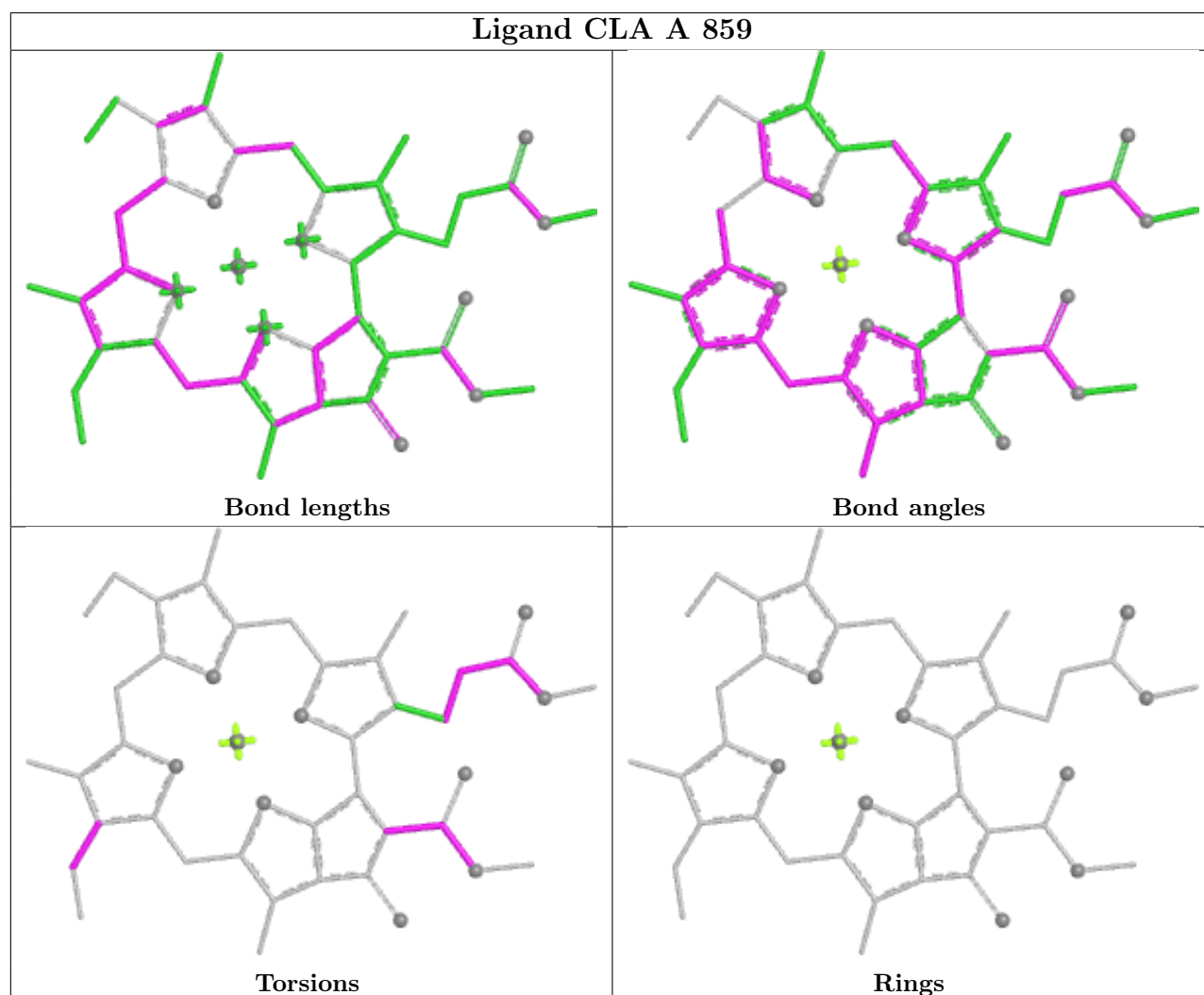
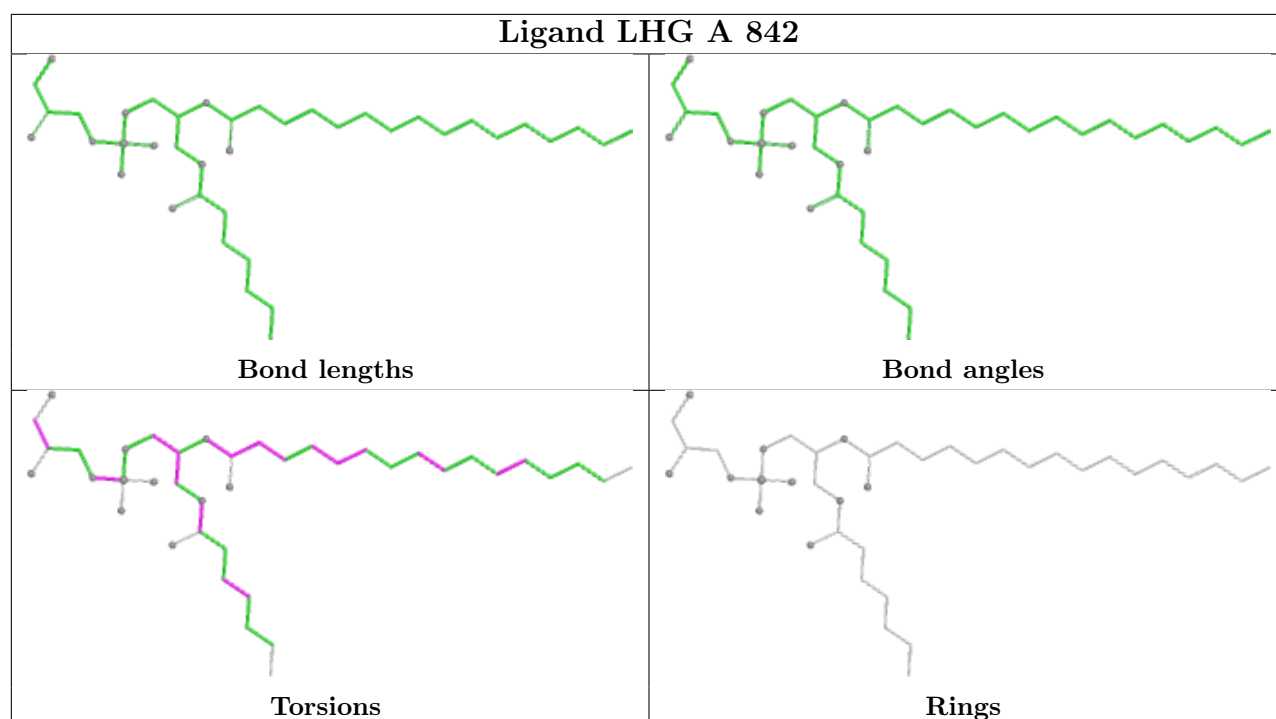
Bond angles



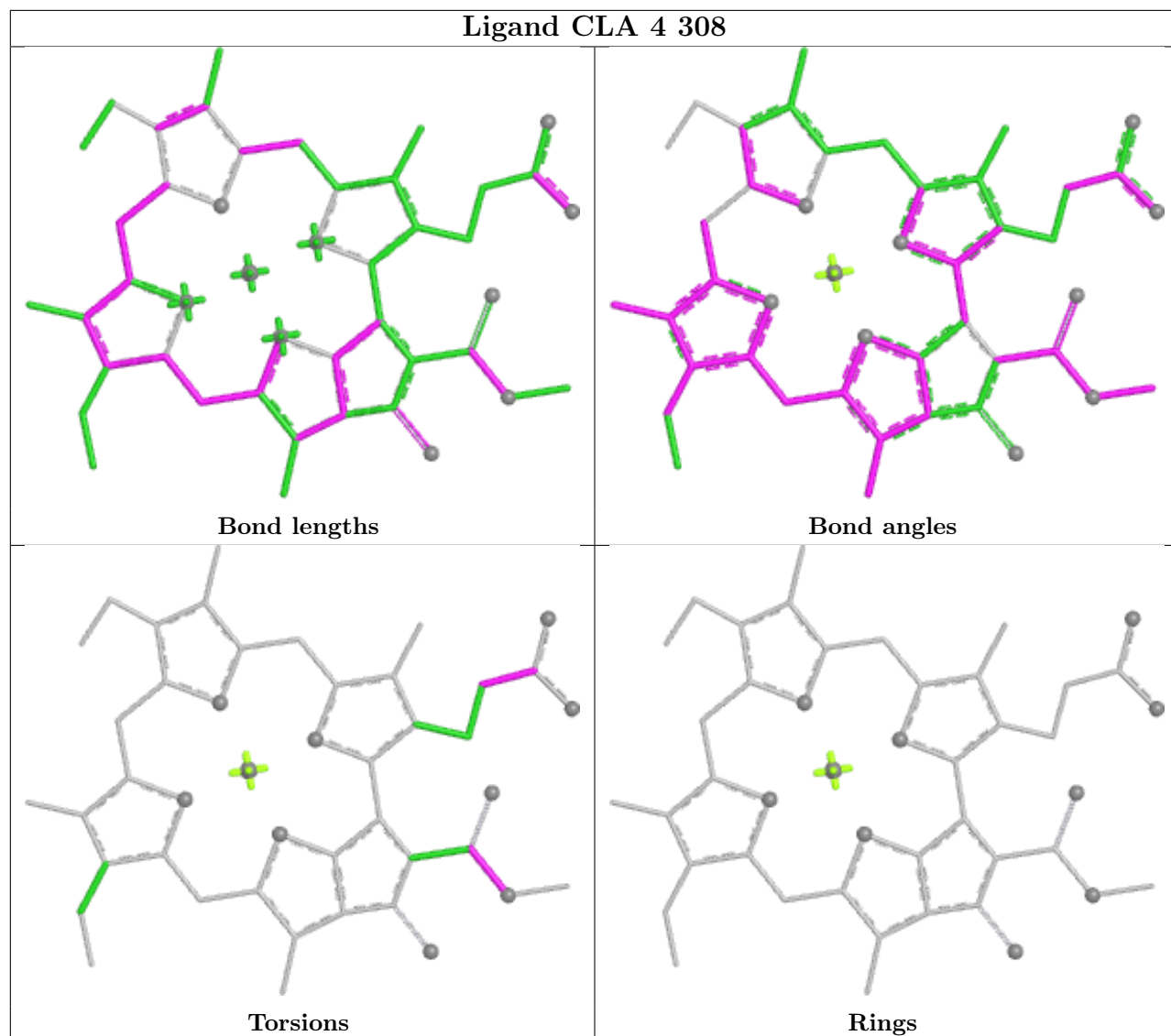
Torsions



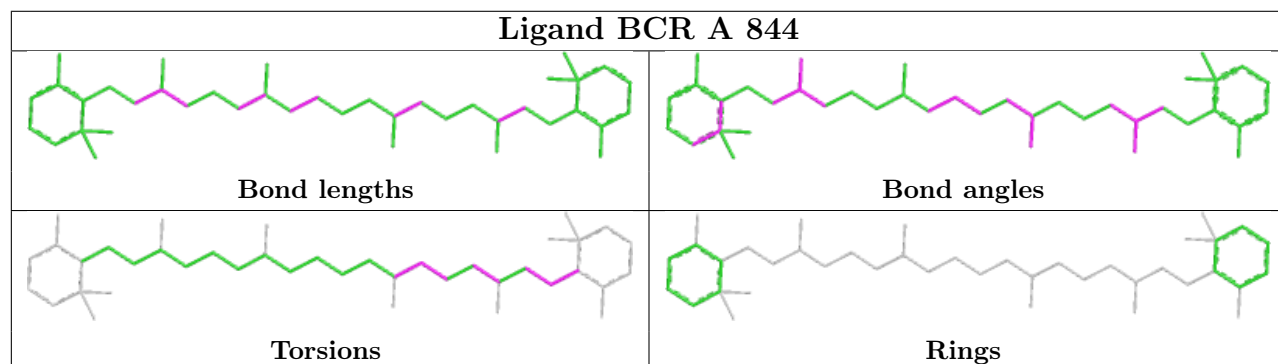
Rings



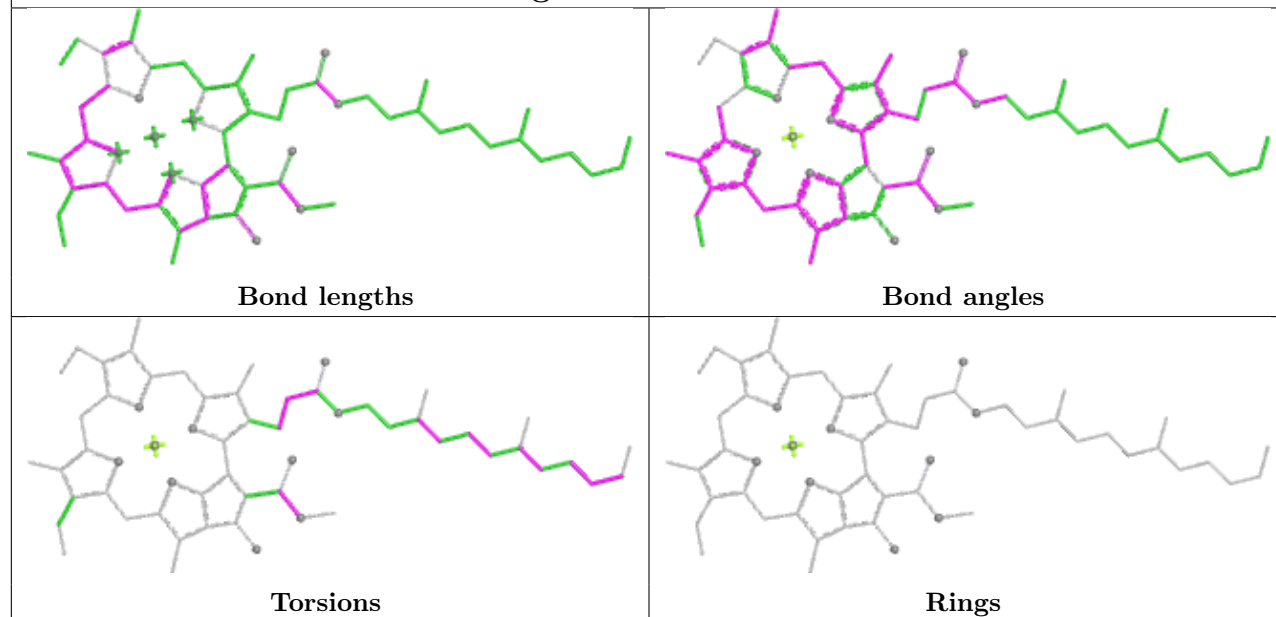
Ligand CLA 4 308



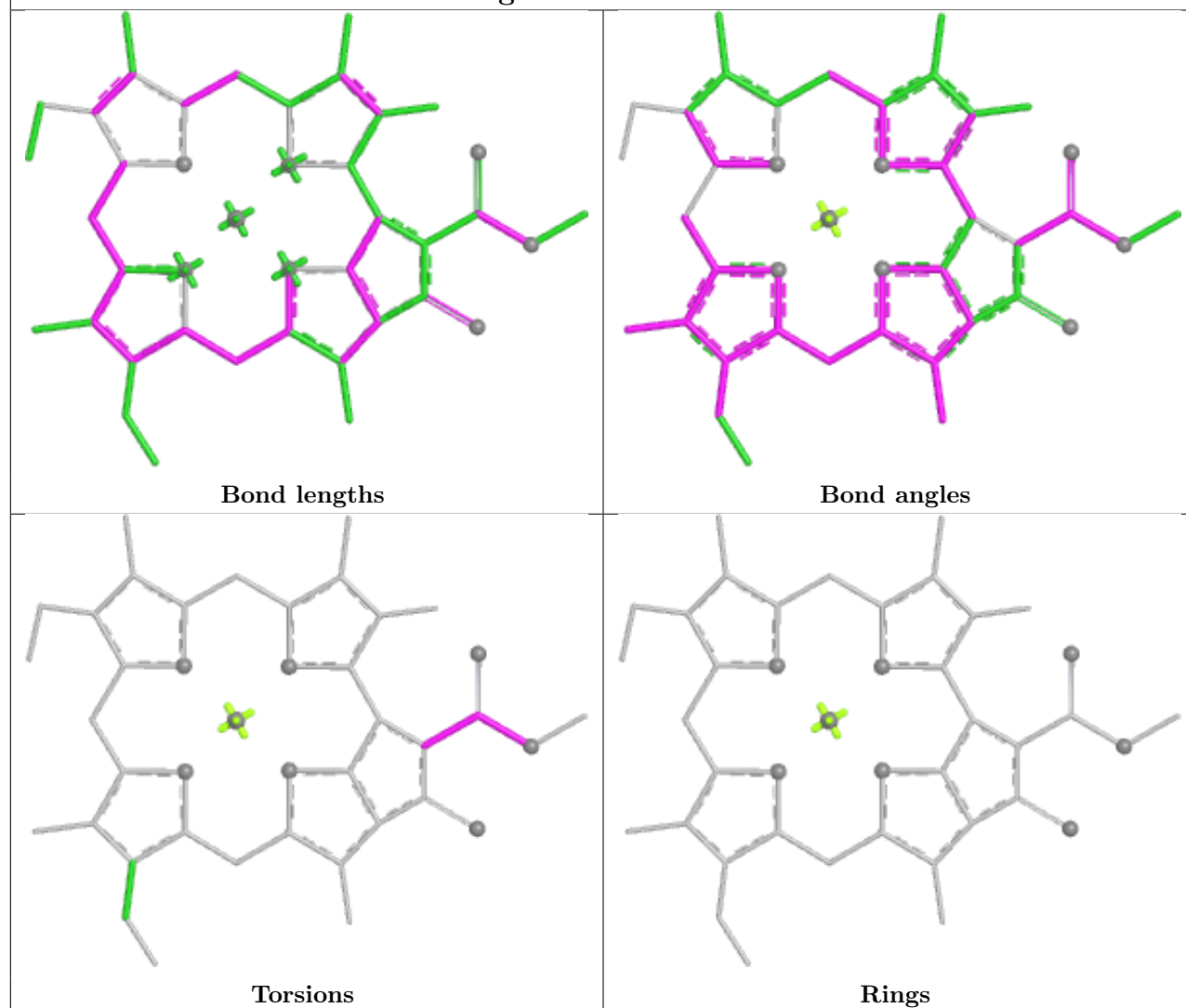
Ligand BCR A 844

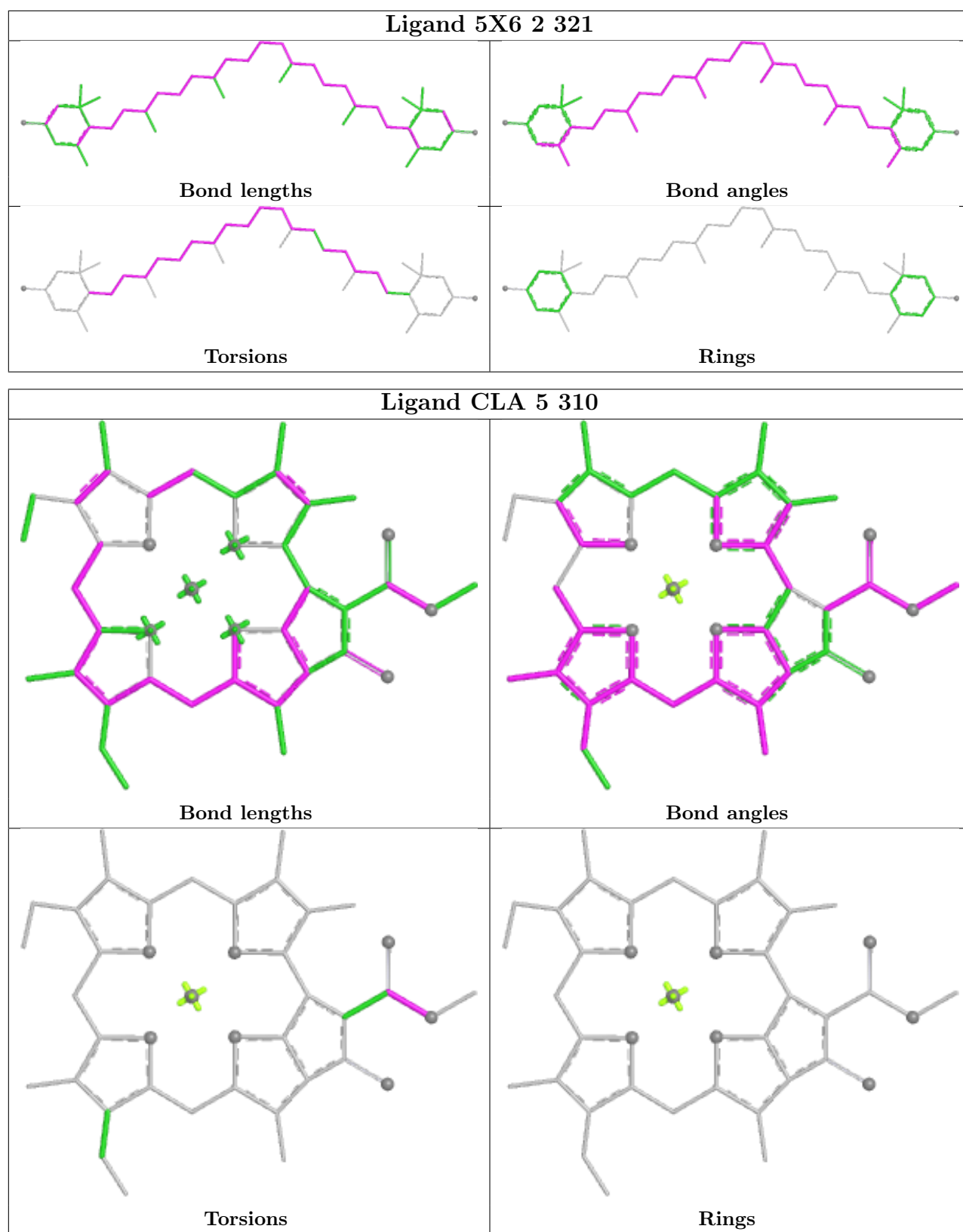


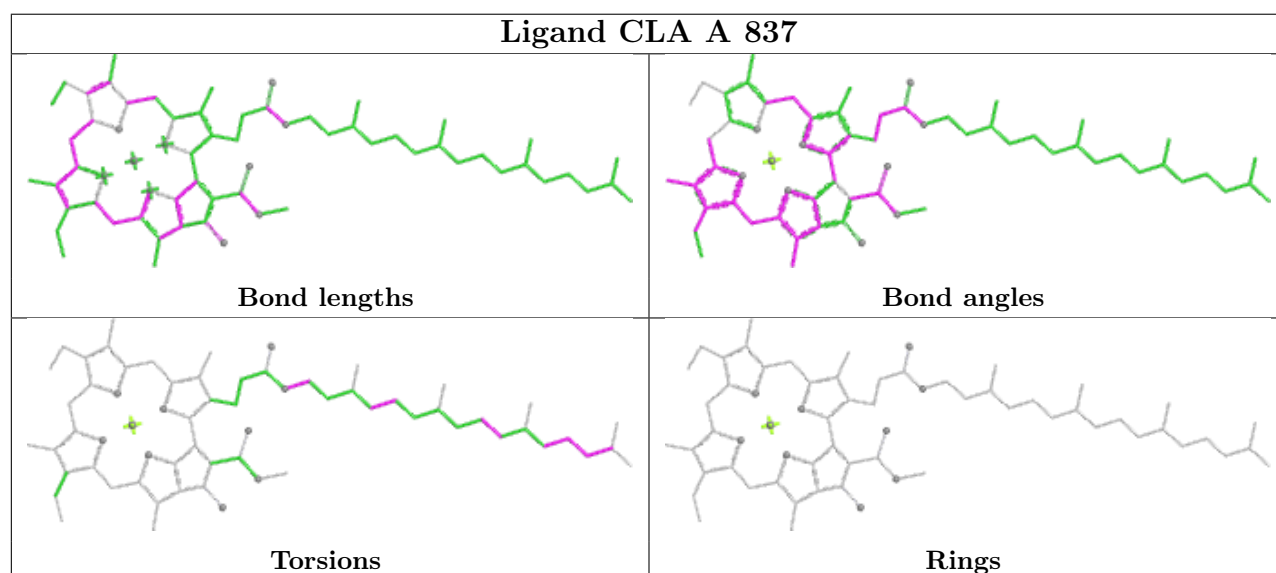
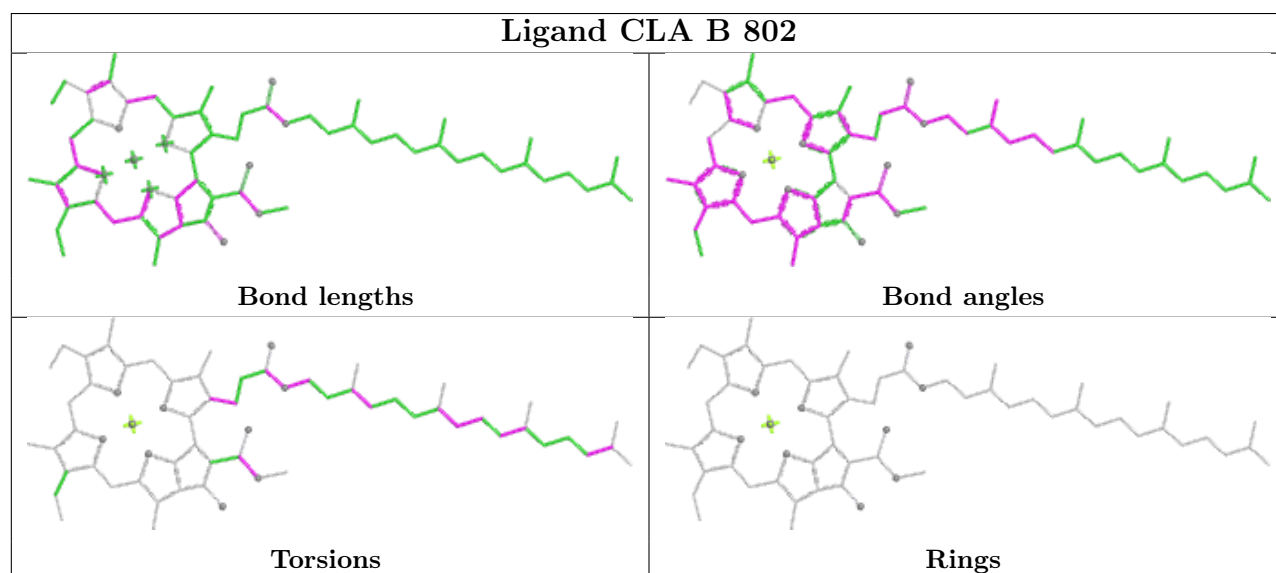
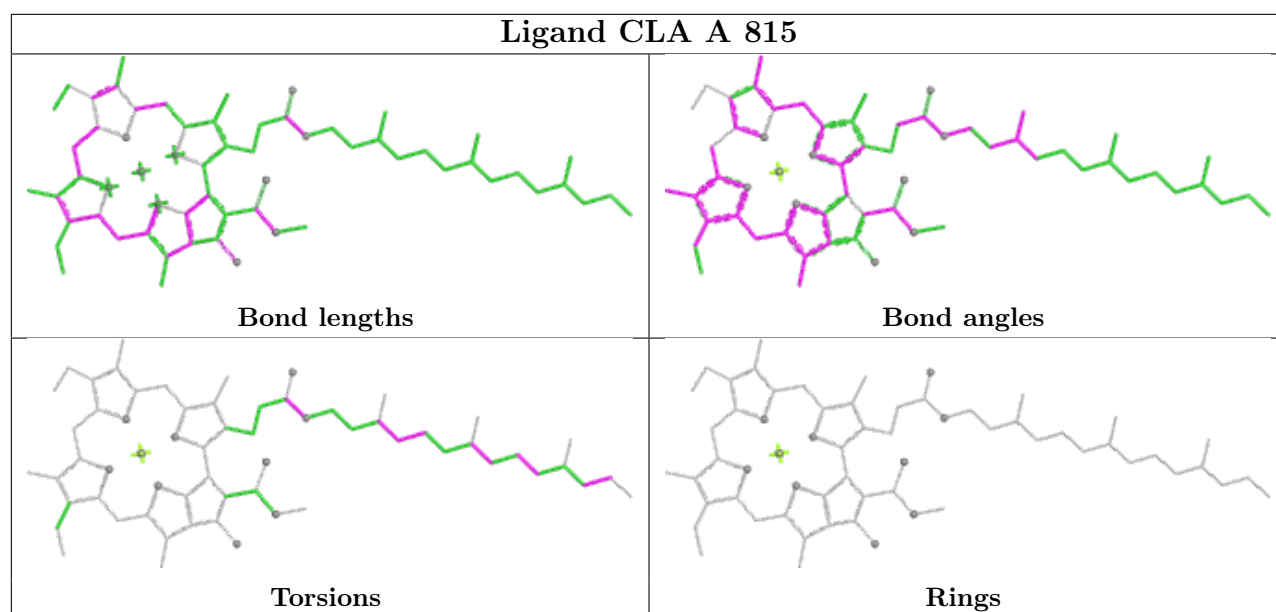
Ligand CLA B 818



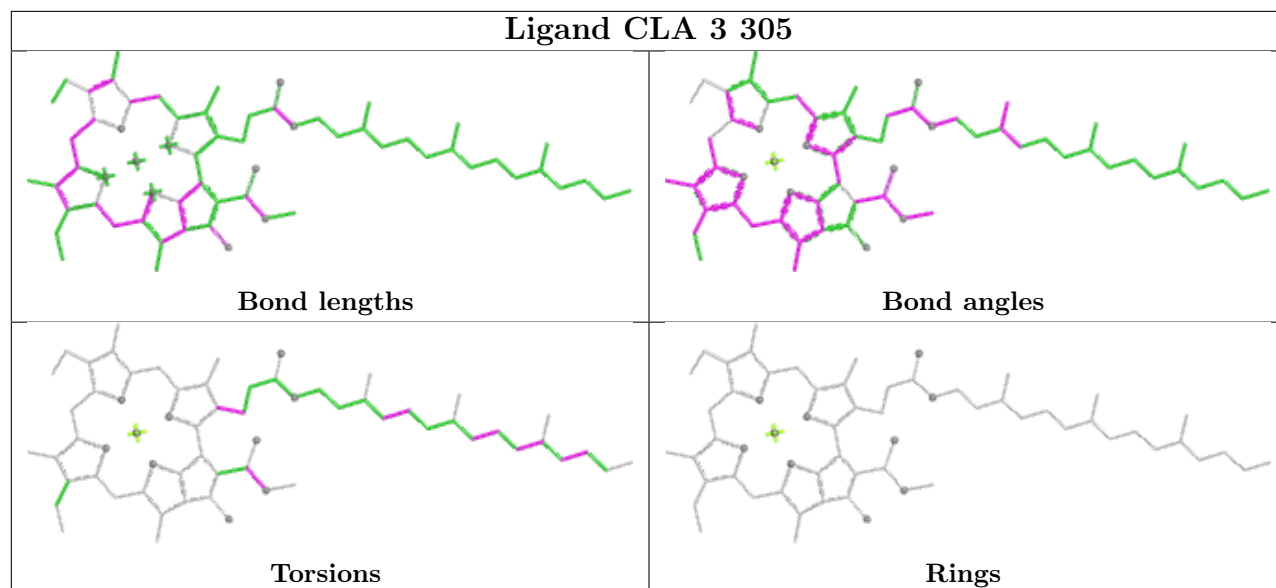
Ligand CLA 2 312



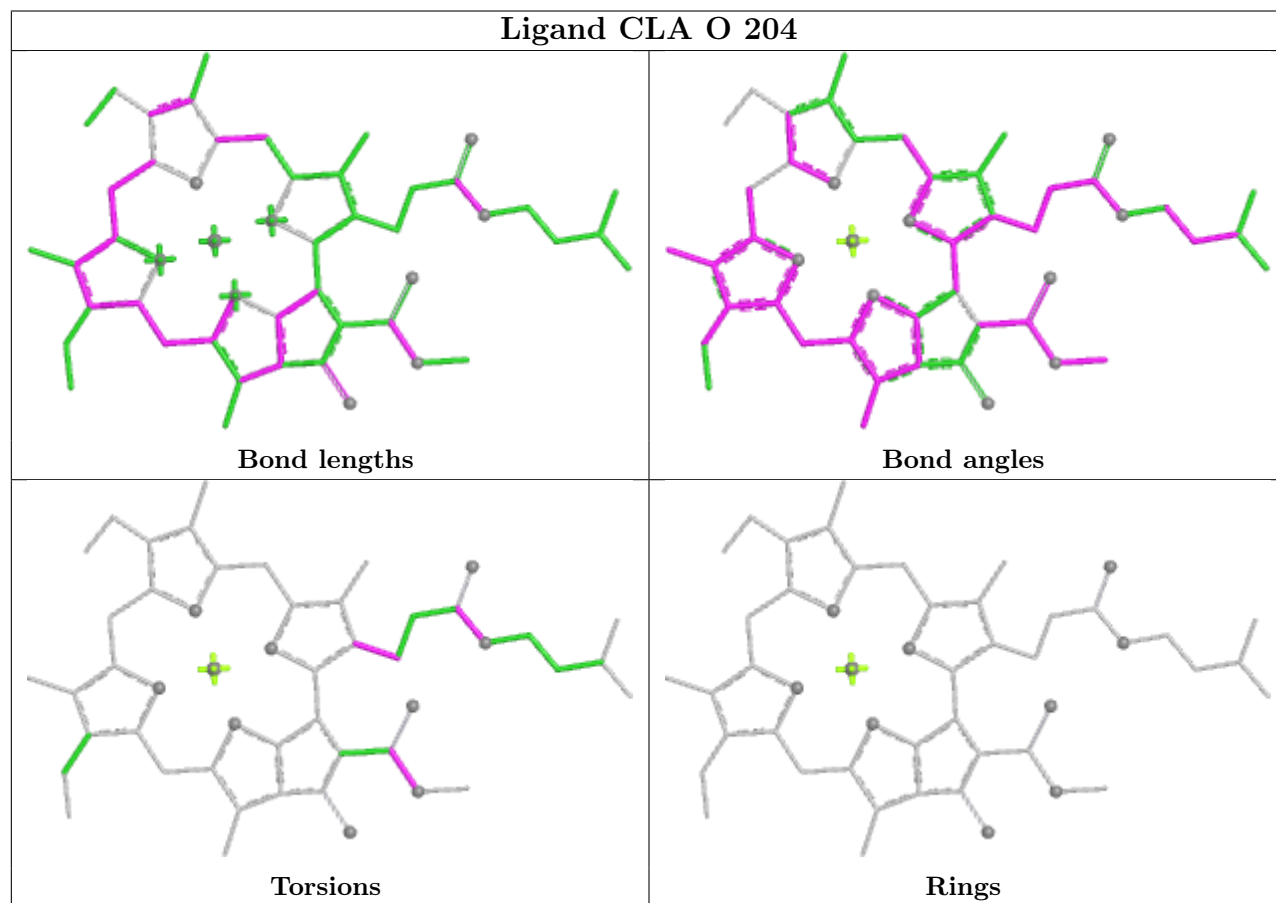


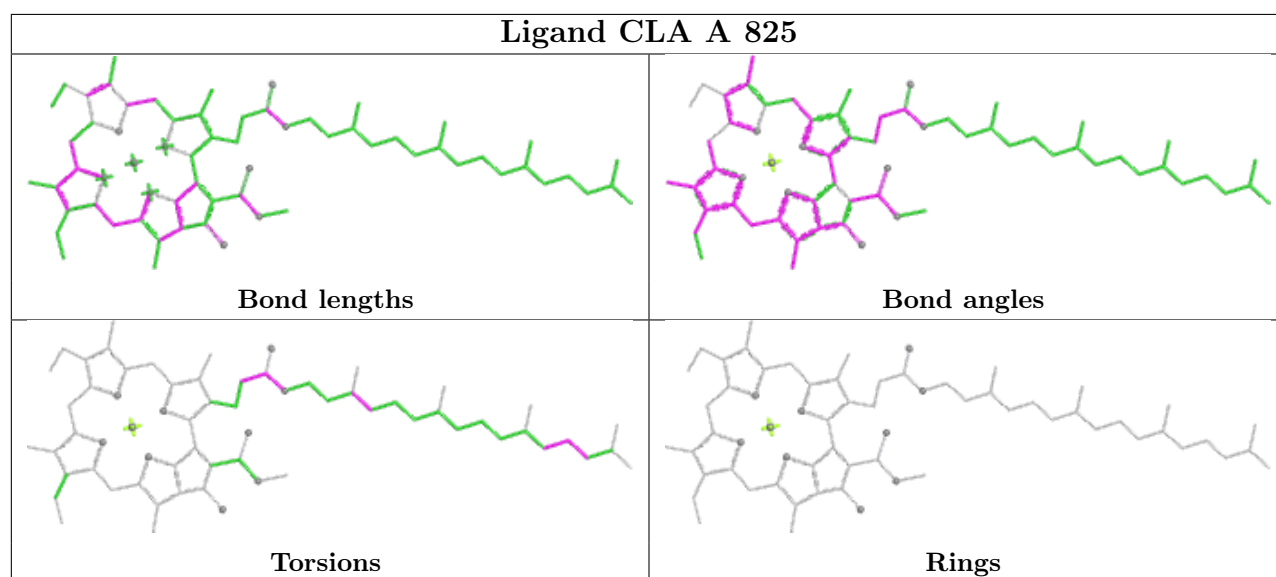
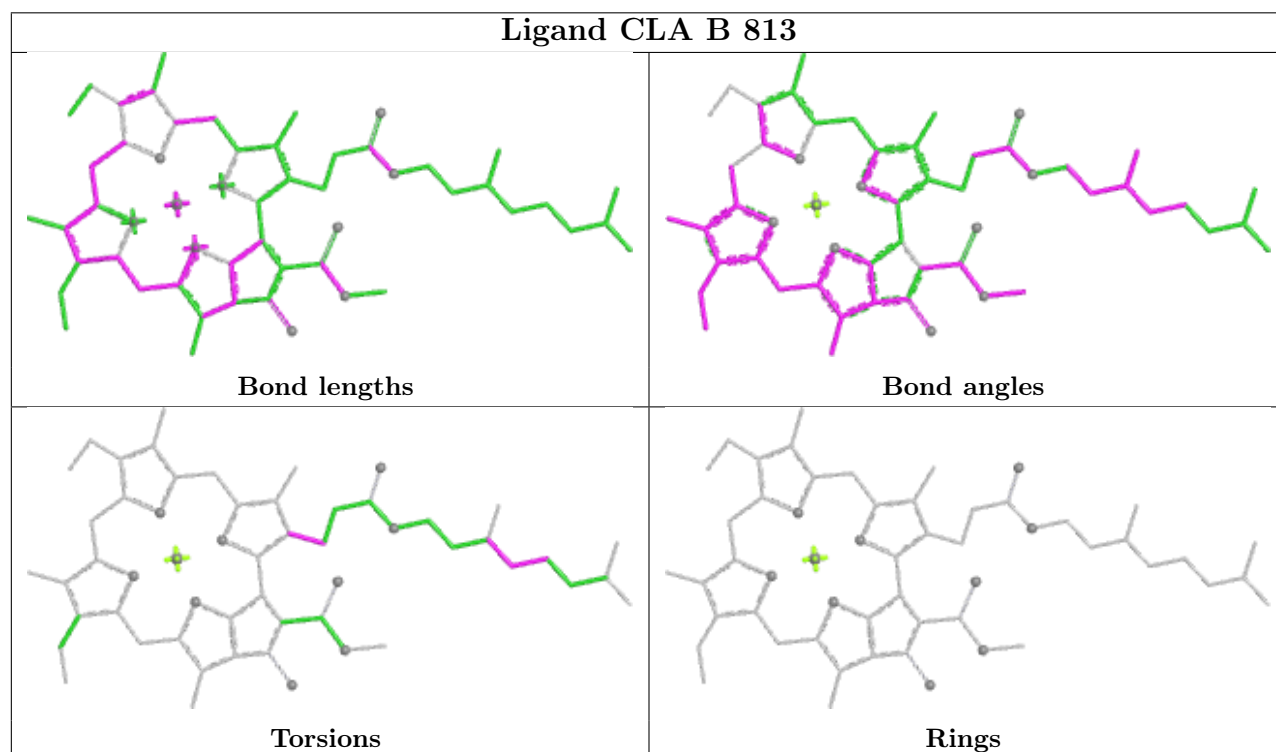
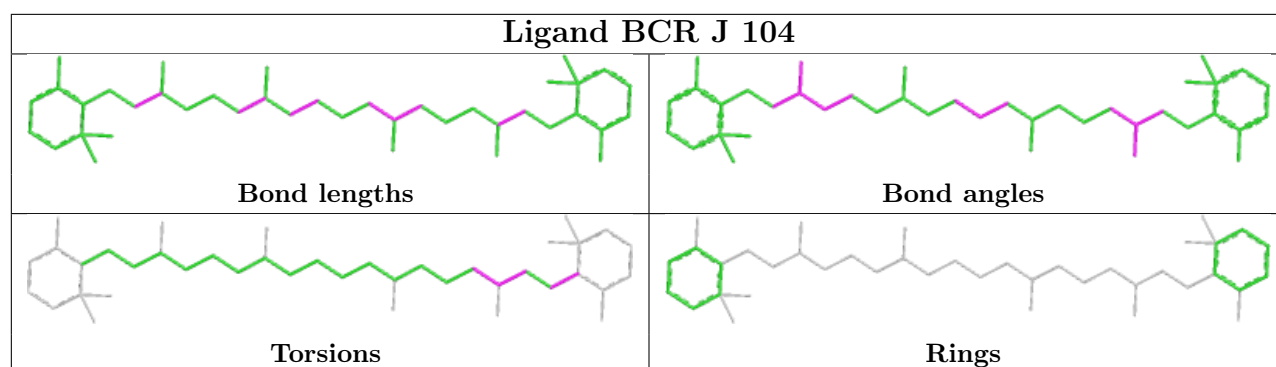


Ligand CLA 3 305

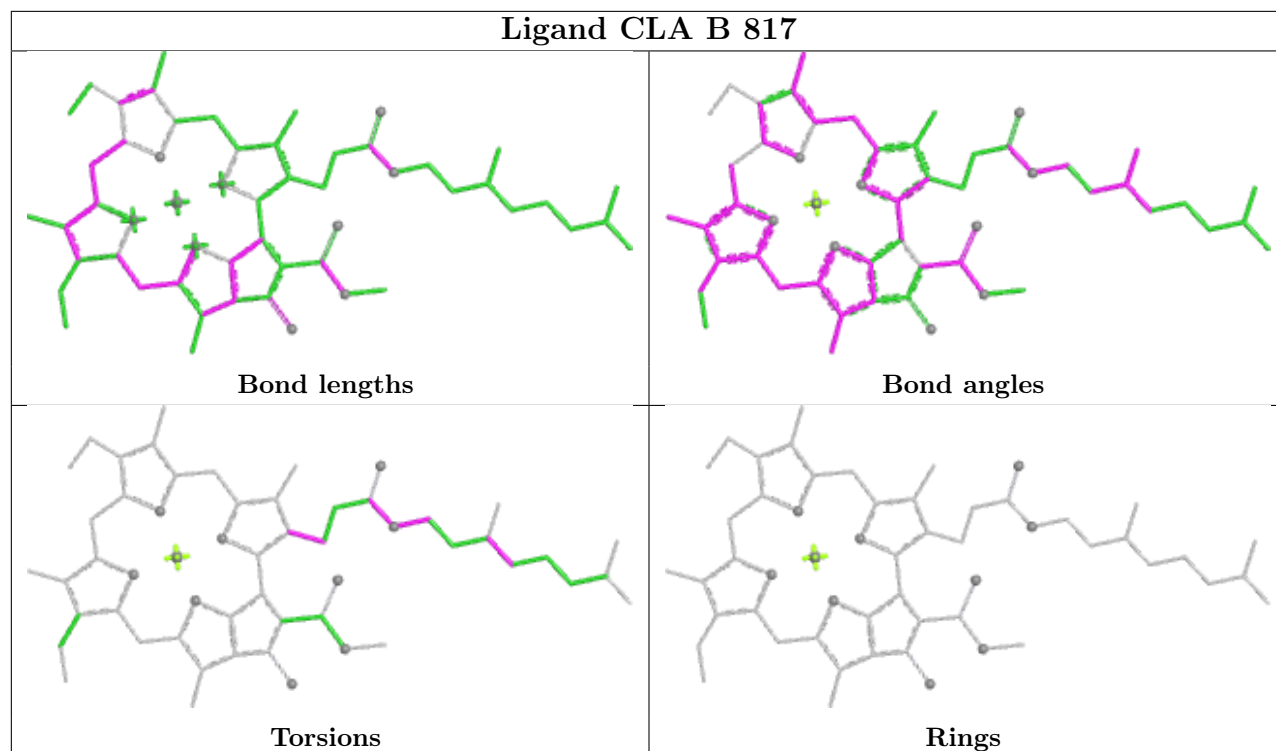


Ligand CLA O 204

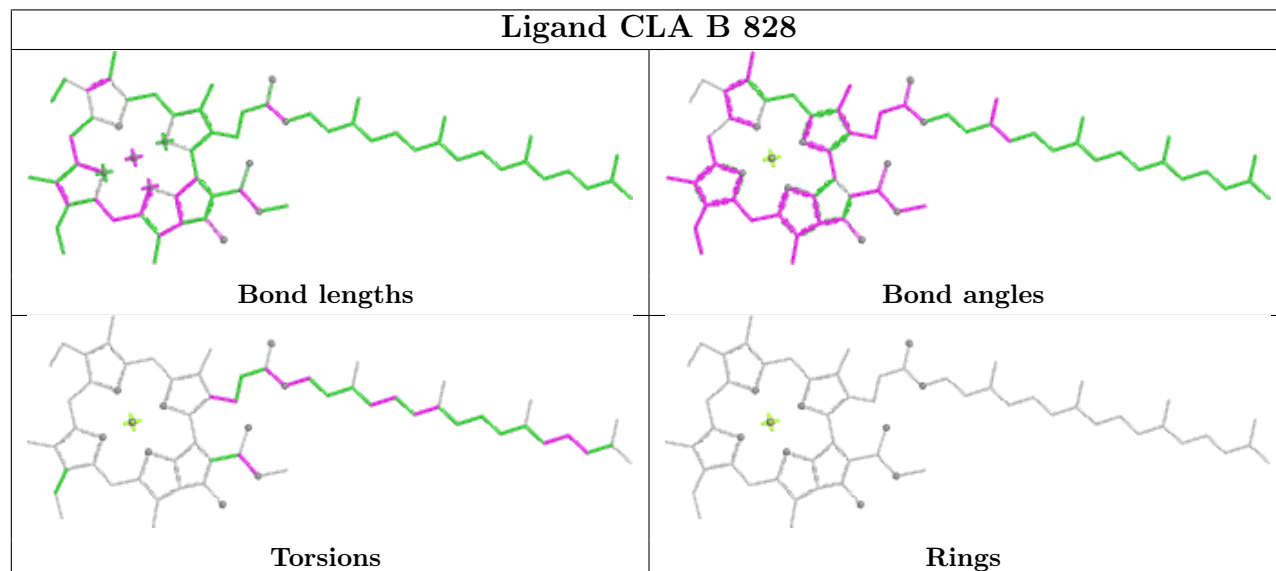


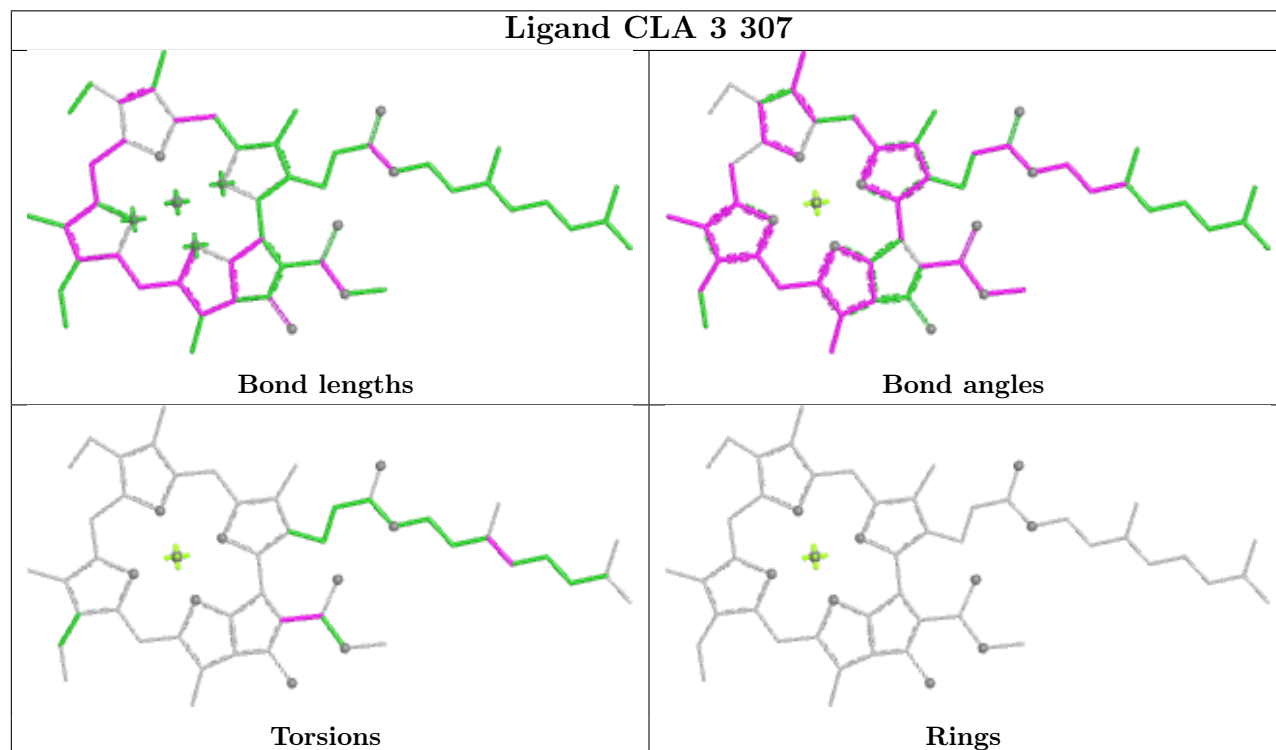
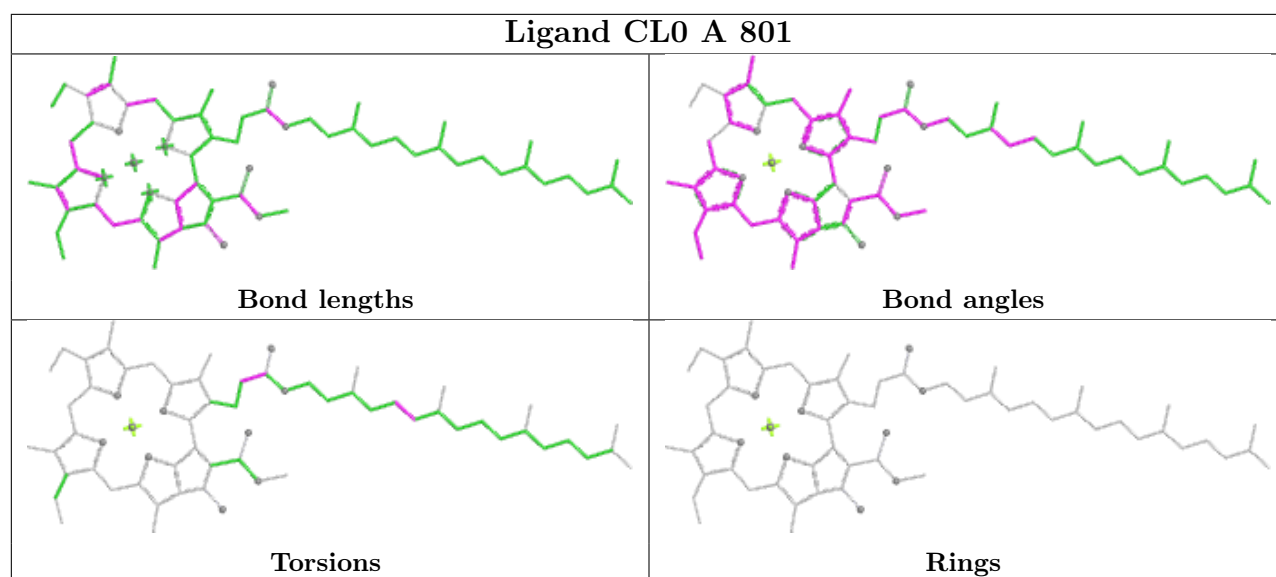


Ligand CLA B 817

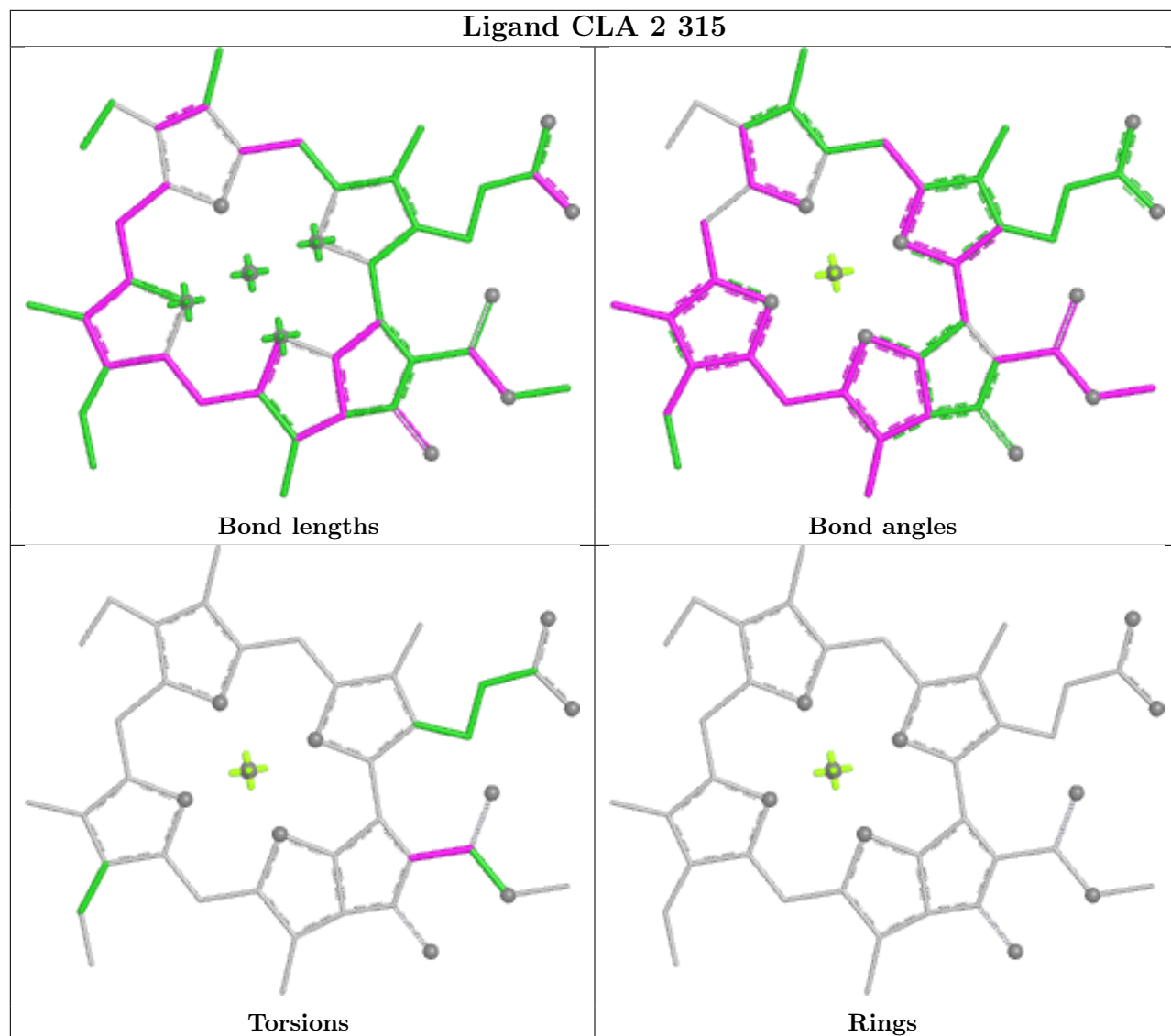


Ligand CLA B 828

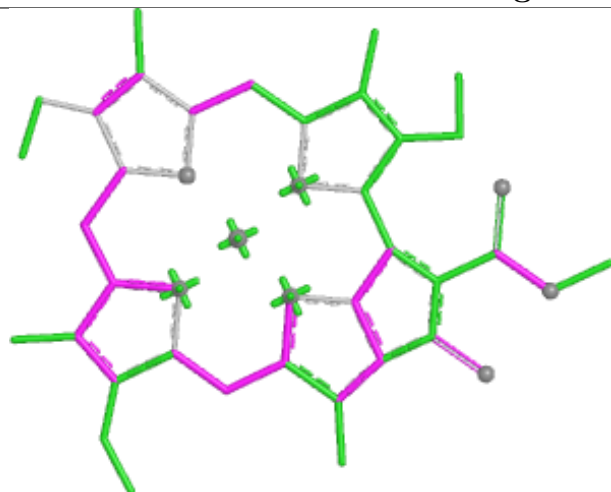




Ligand CLA 2 315



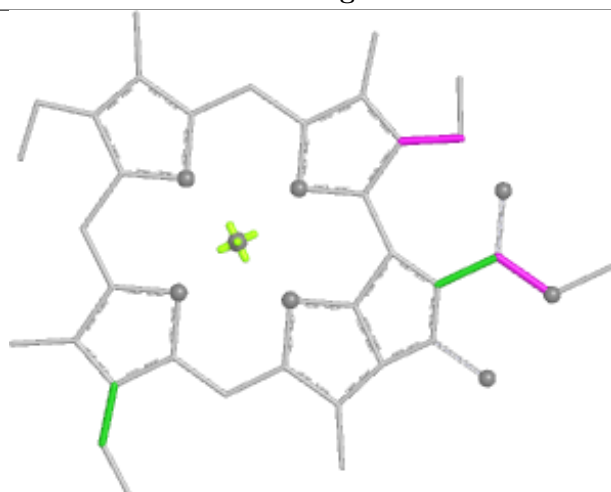
Ligand CLA A 813



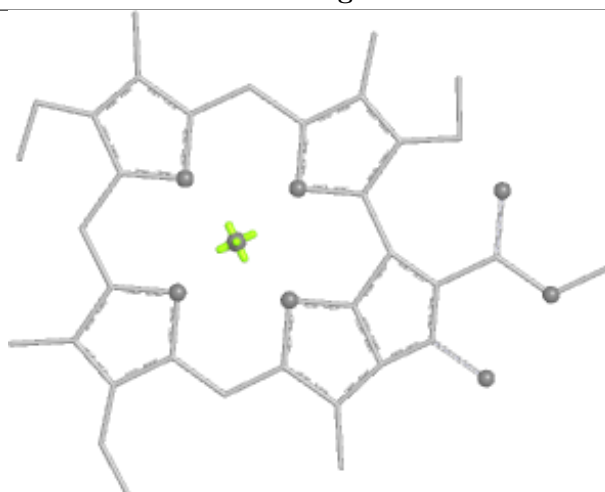
Bond lengths



Bond angles

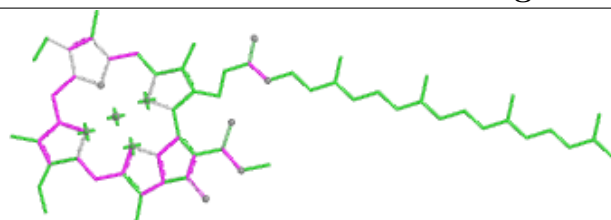


Torsions

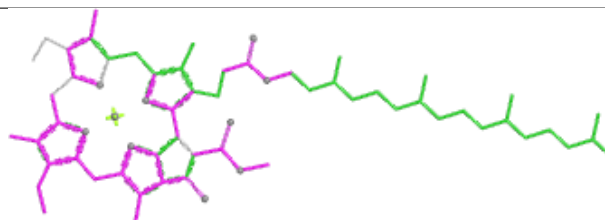


Rings

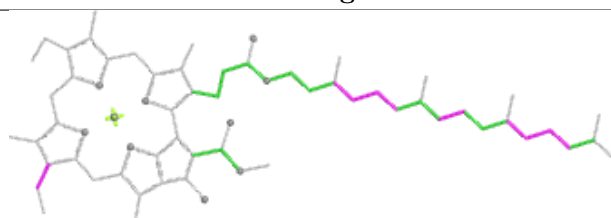
Ligand CLA B 833



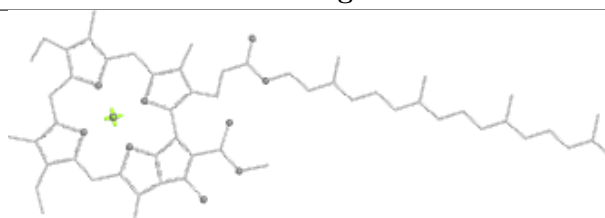
Bond lengths



Bond angles

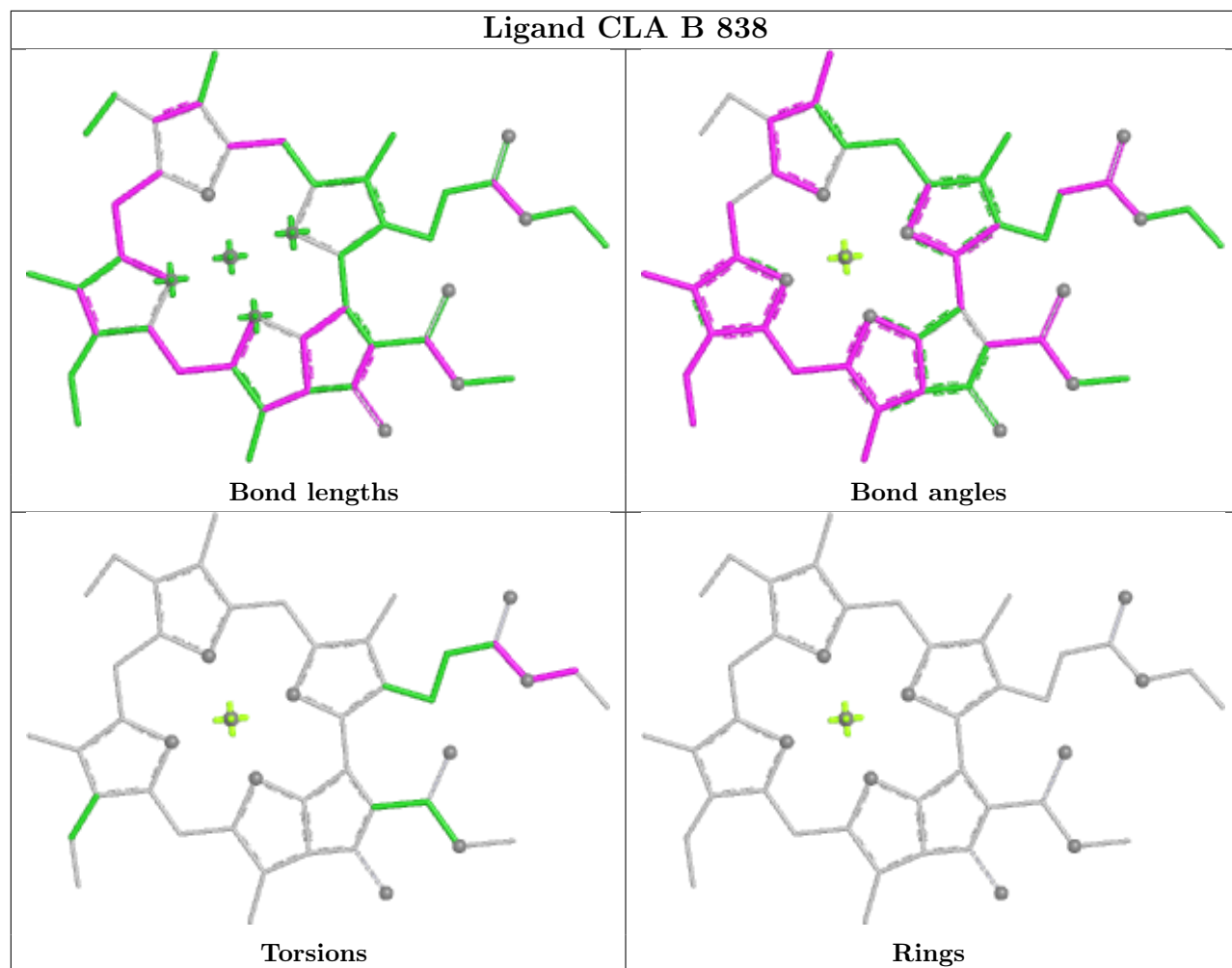


Torsions

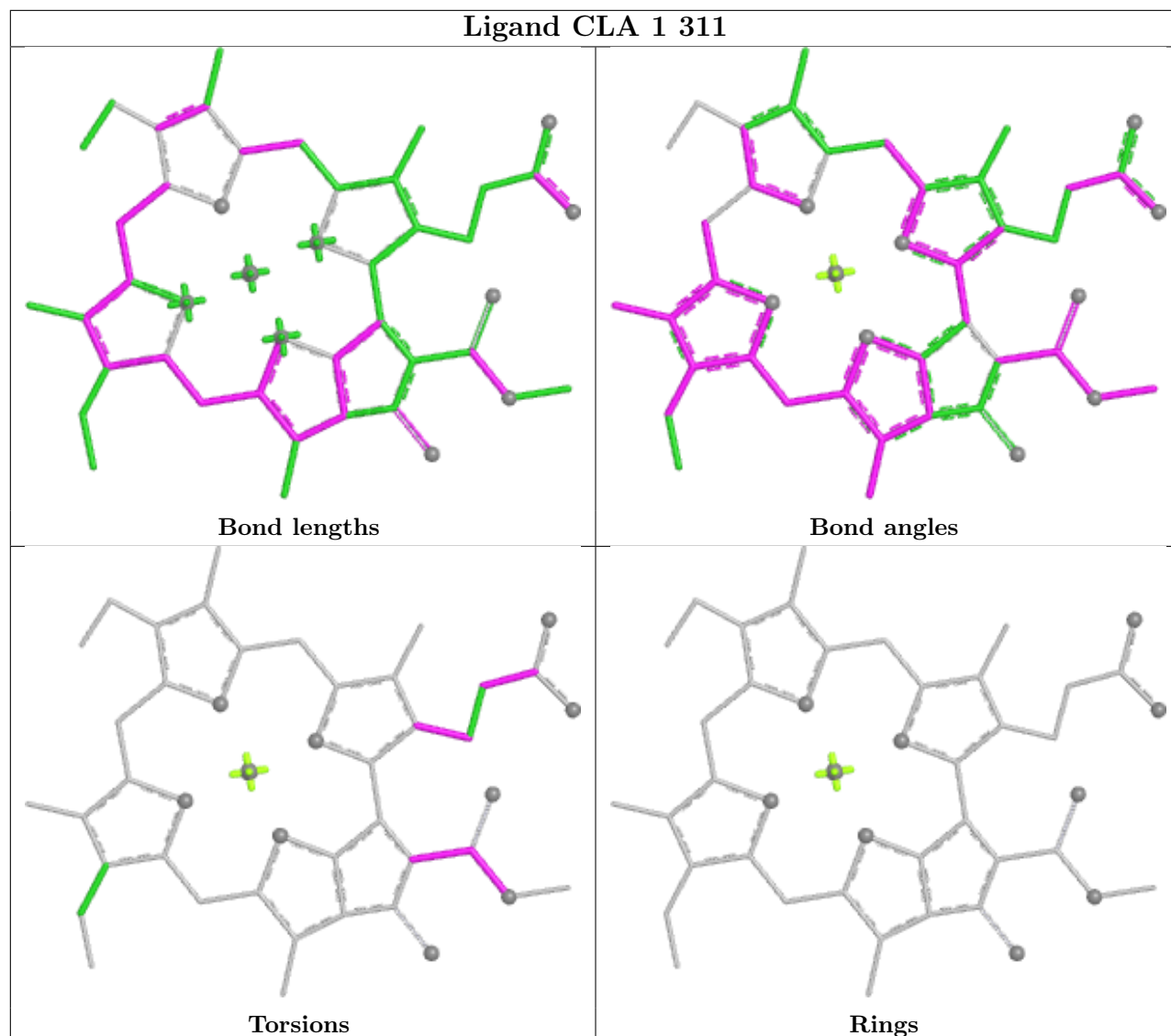


Rings

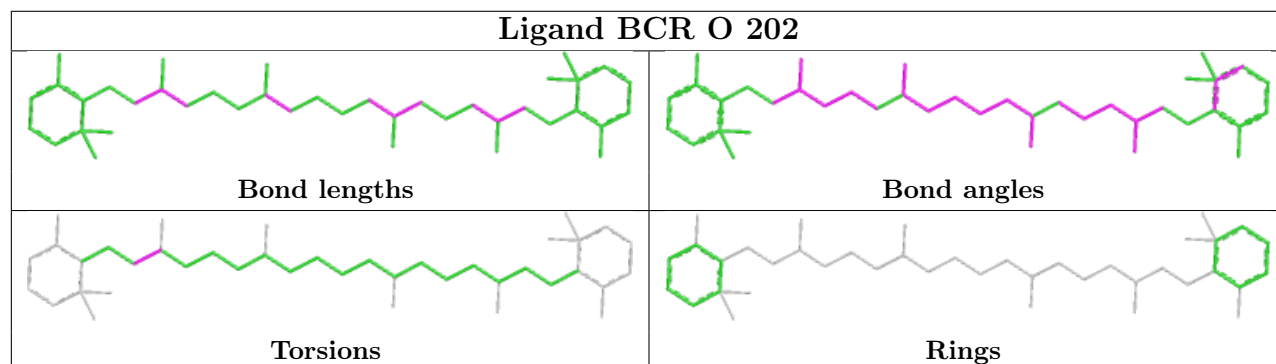
Ligand CLA B 838

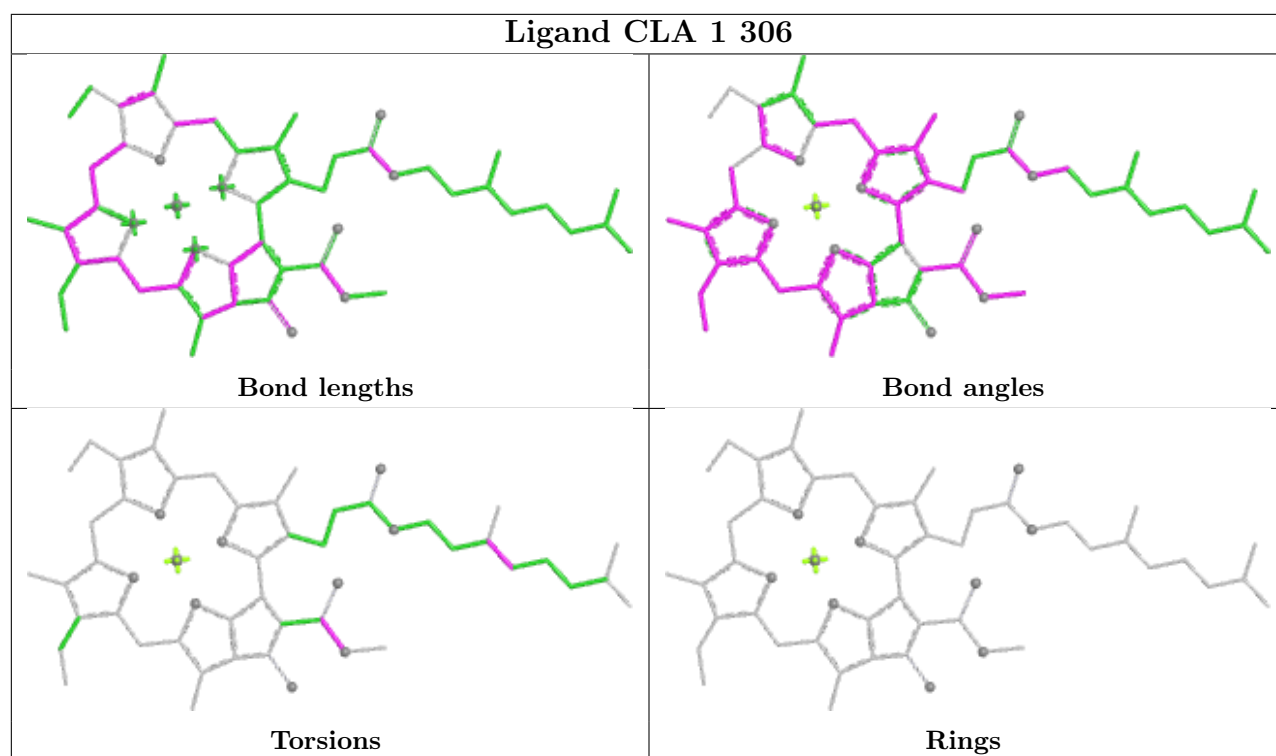


Ligand CLA 1 311

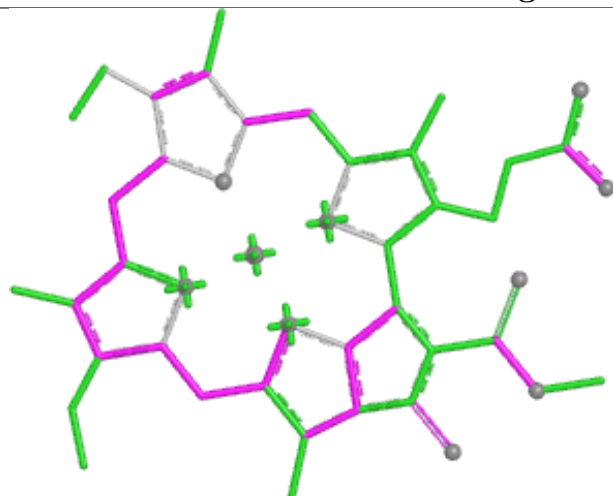


Ligand BCR O 202

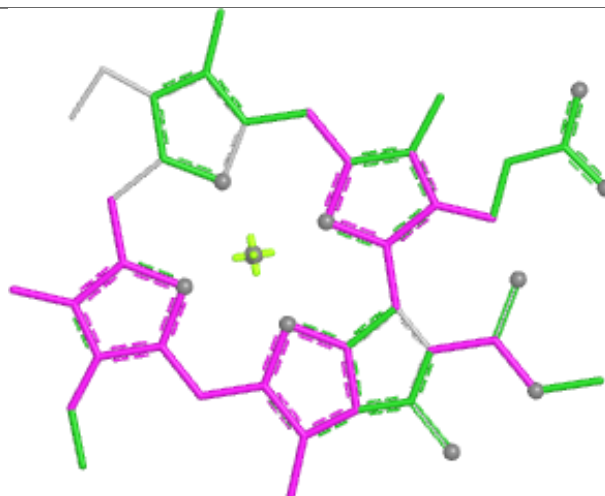




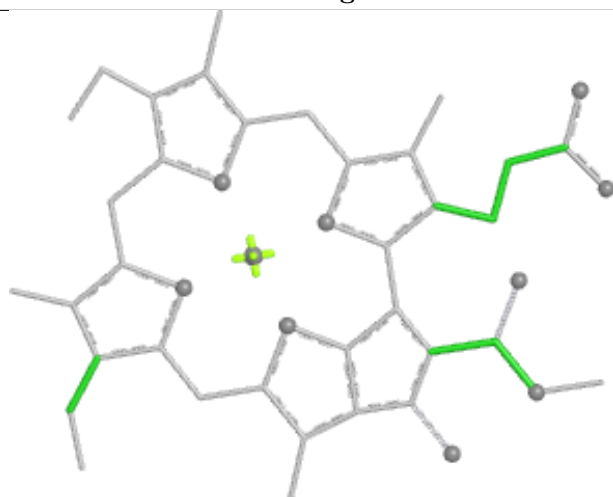
Ligand CLA 2 310



Bond lengths



Bond angles

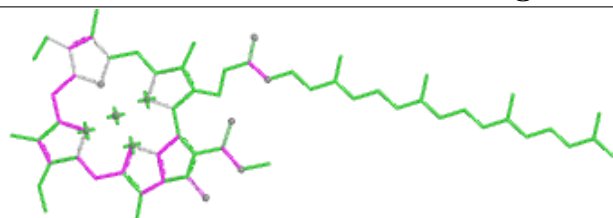


Torsions

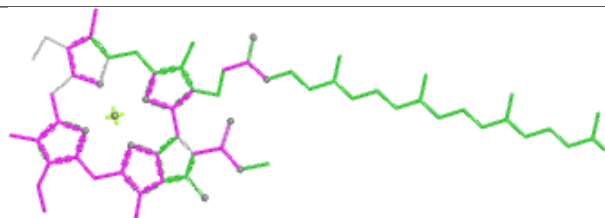


Rings

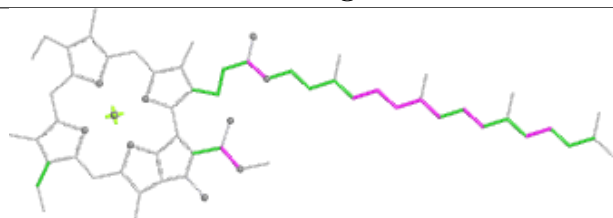
Ligand CLA B 816



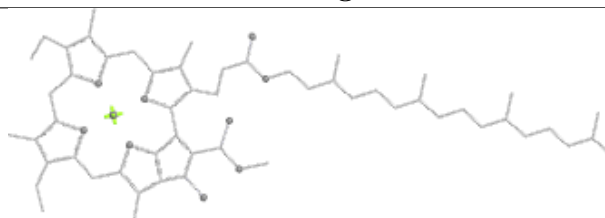
Bond lengths



Bond angles

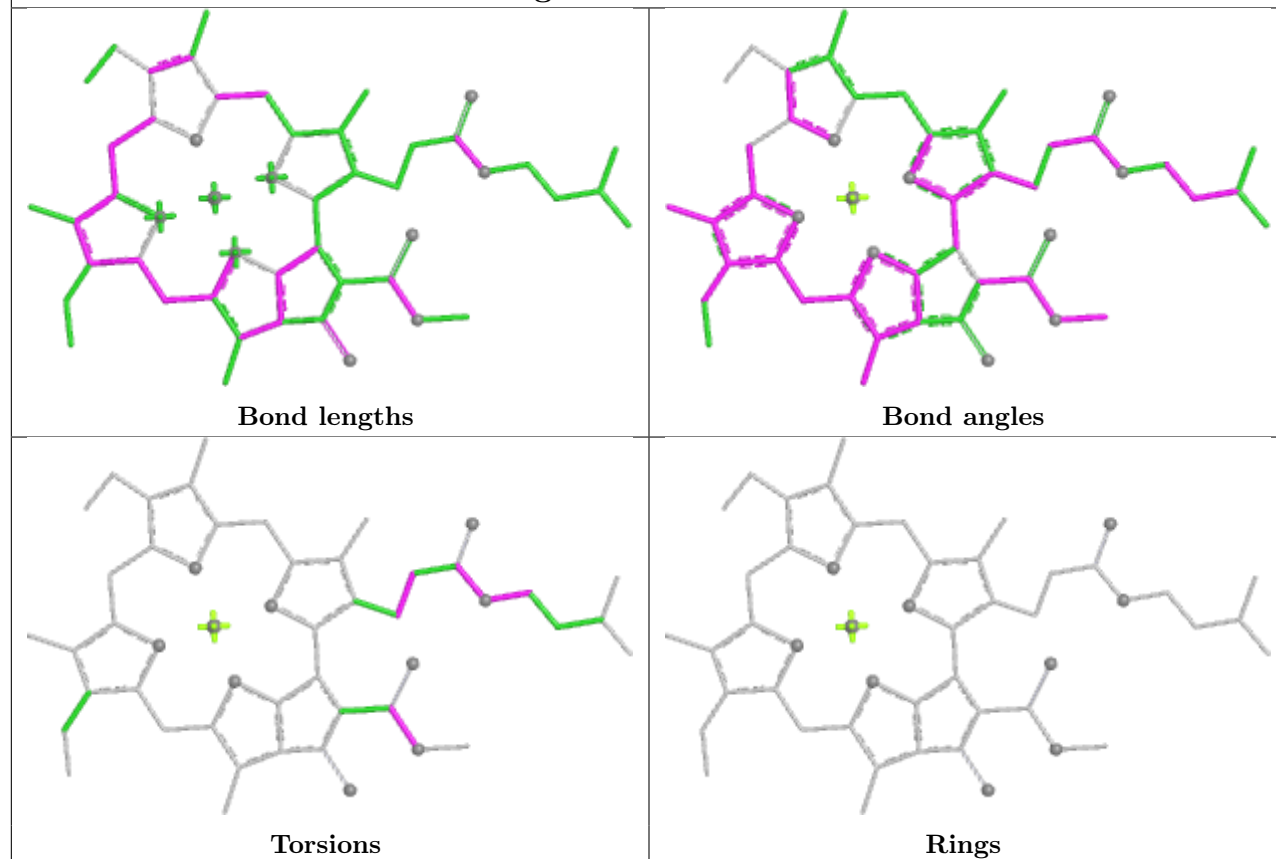


Torsions

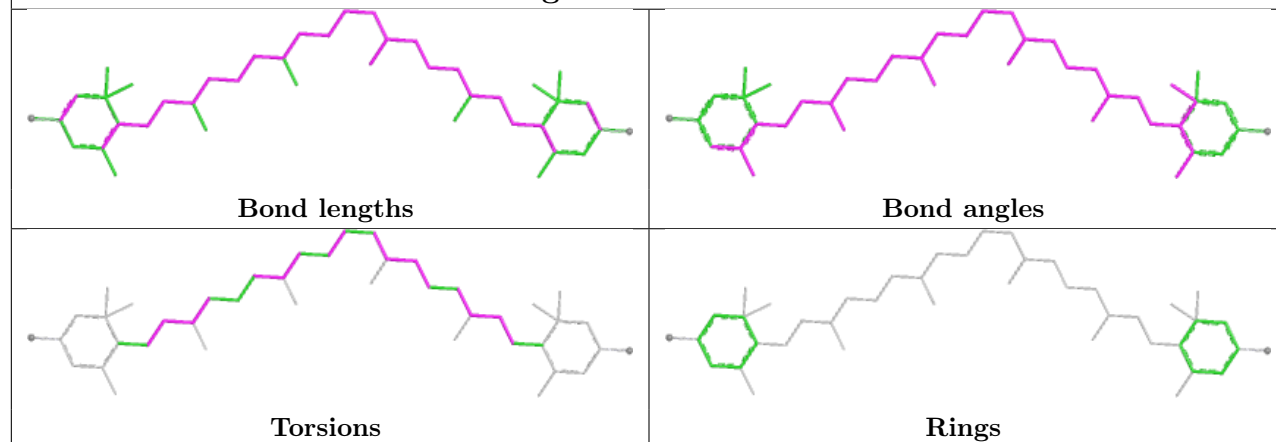


Rings

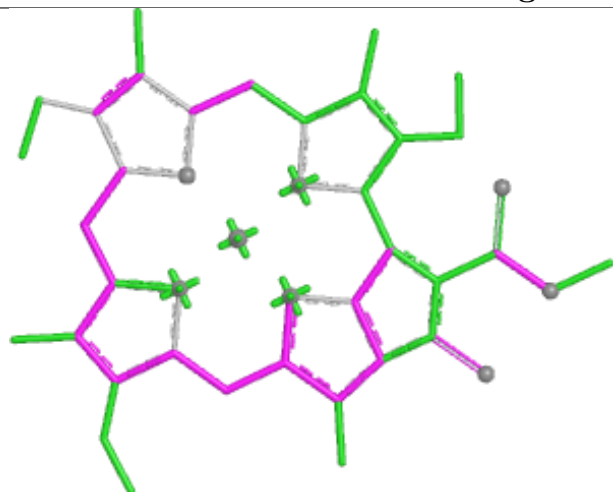
Ligand CLA L 204



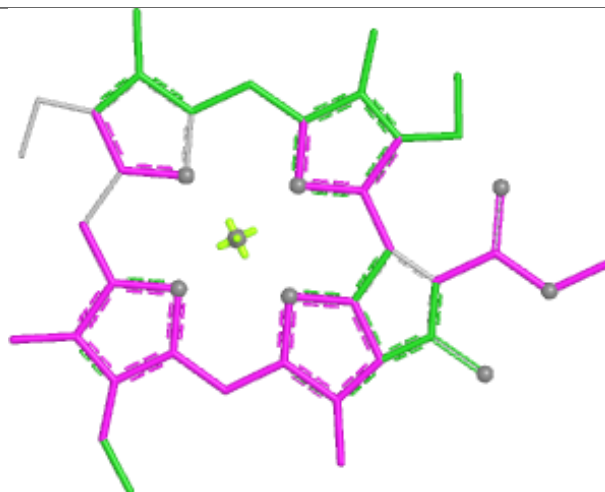
Ligand 5X6 1 312



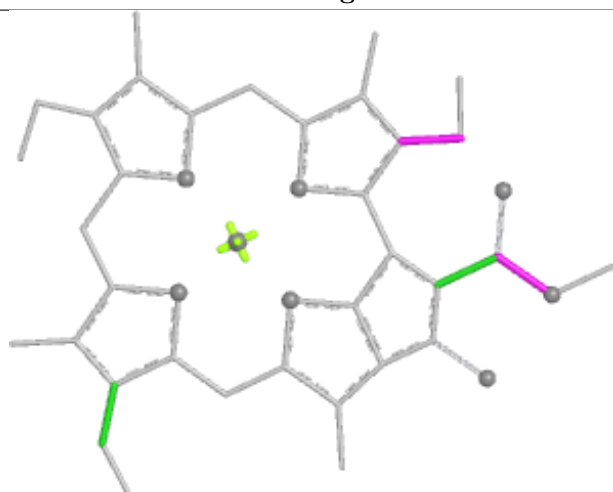
Ligand CLA 3 313



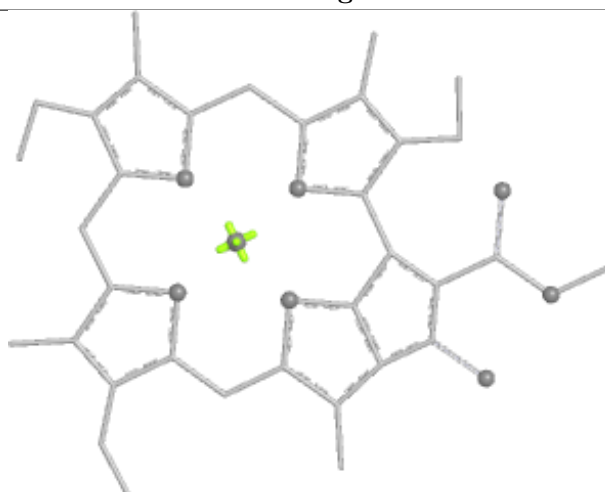
Bond lengths



Bond angles

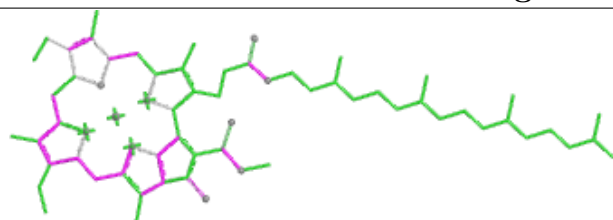


Torsions

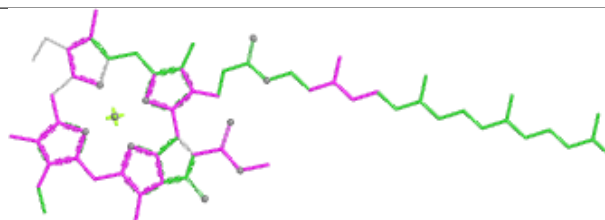


Rings

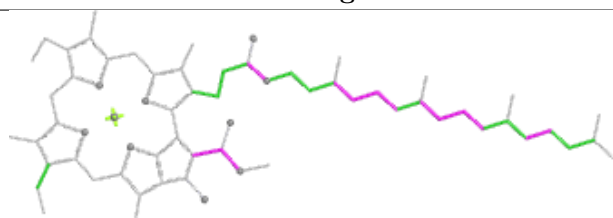
Ligand CLA B 815



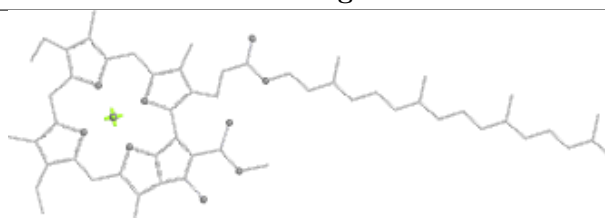
Bond lengths



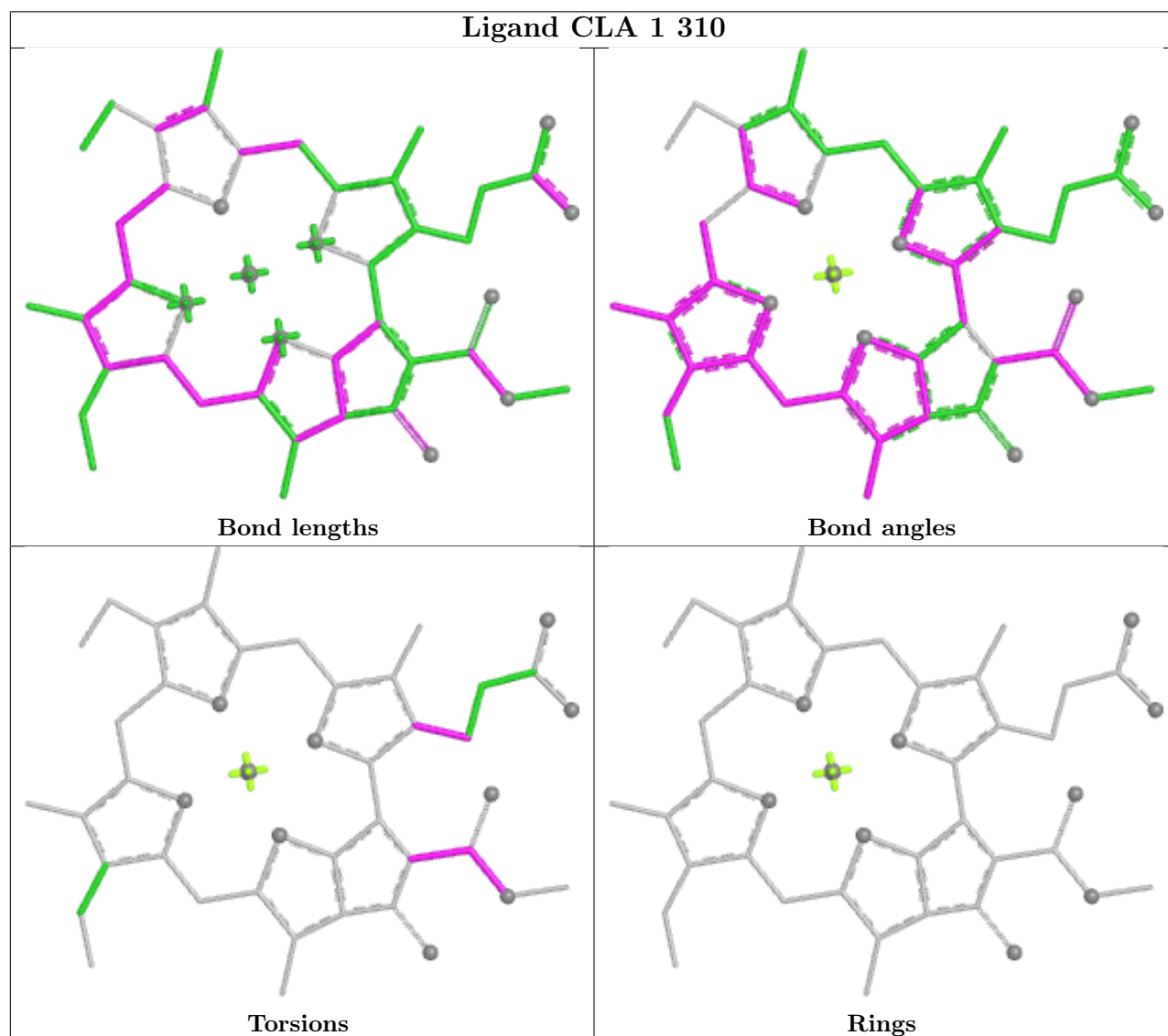
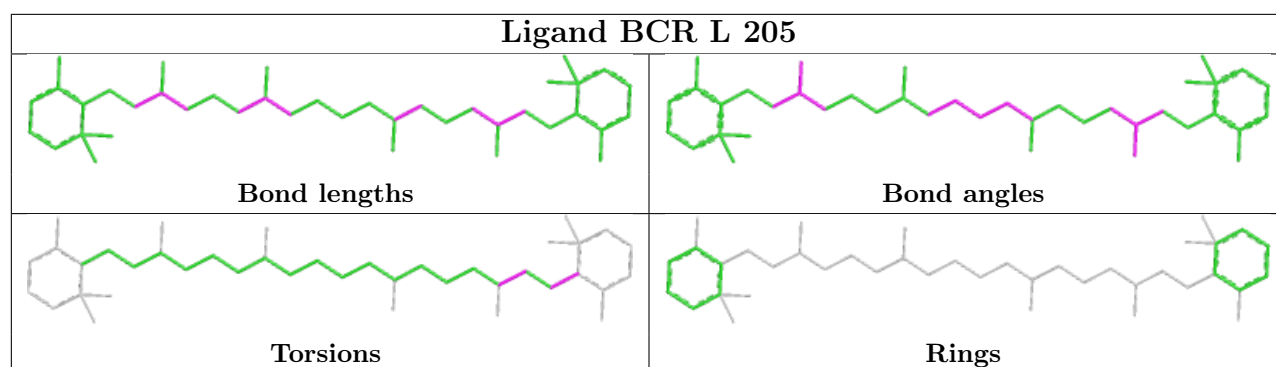
Bond angles



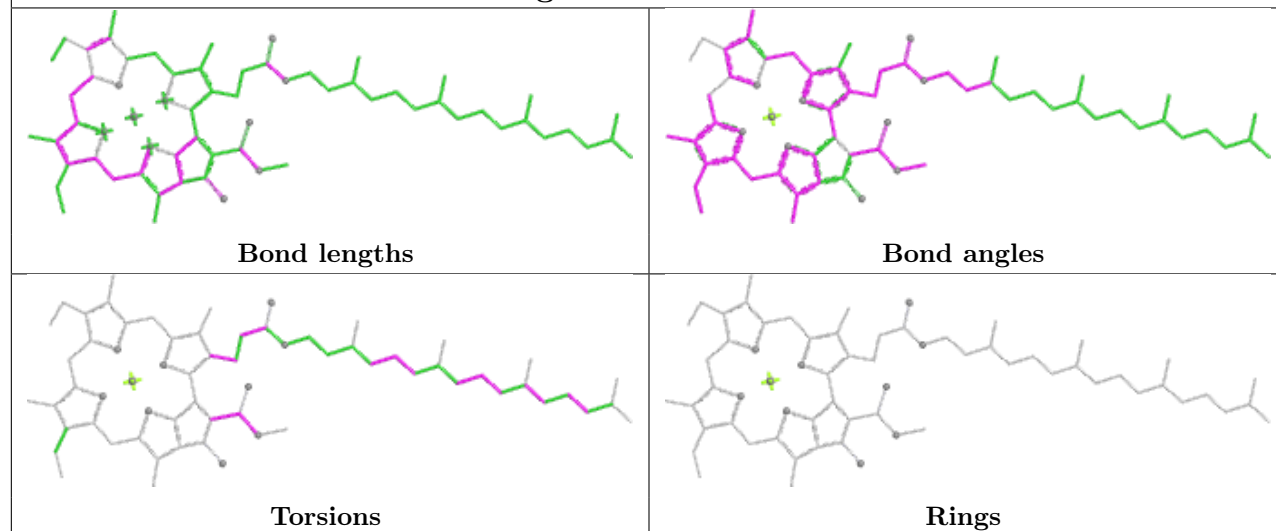
Torsions



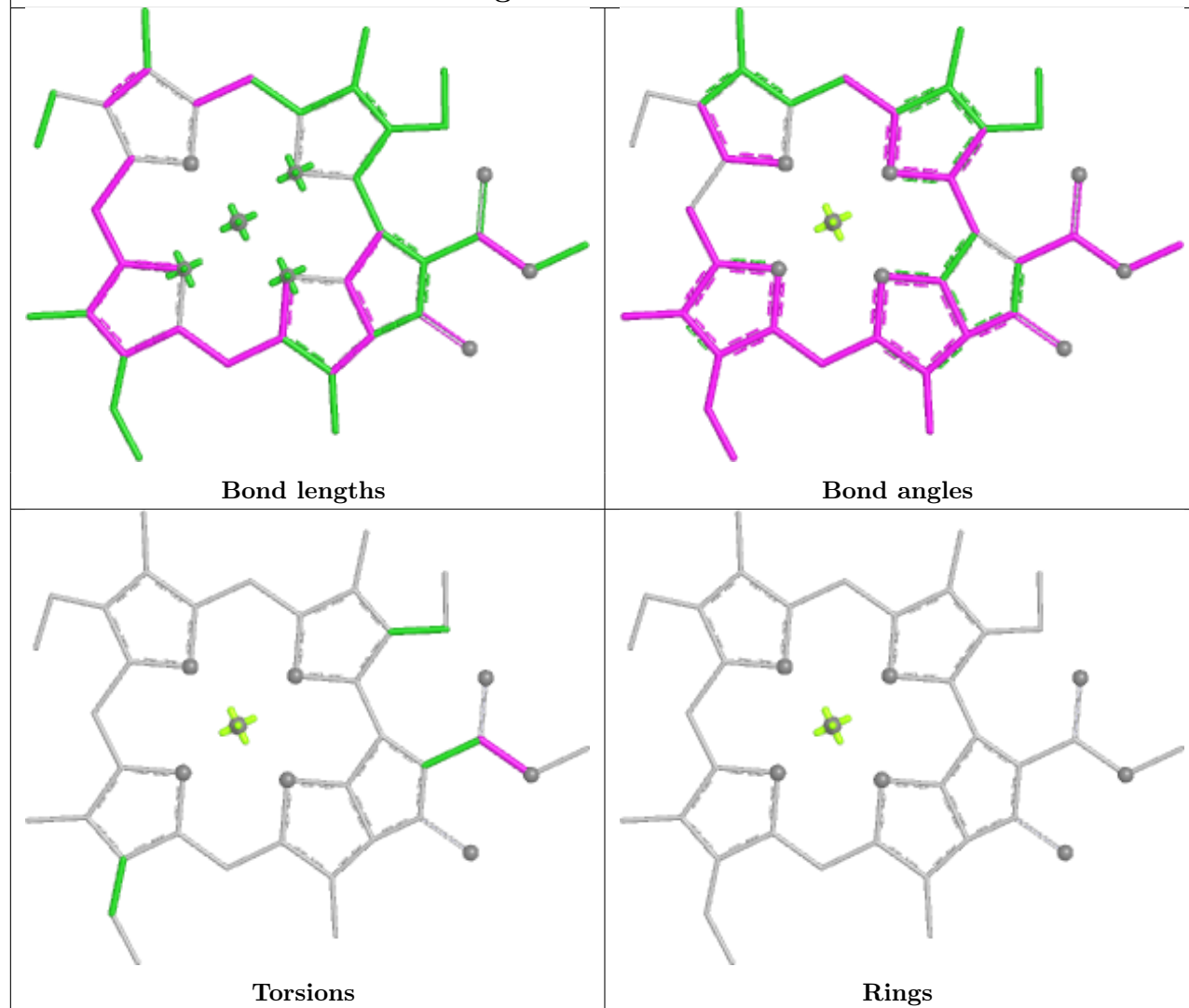
Rings

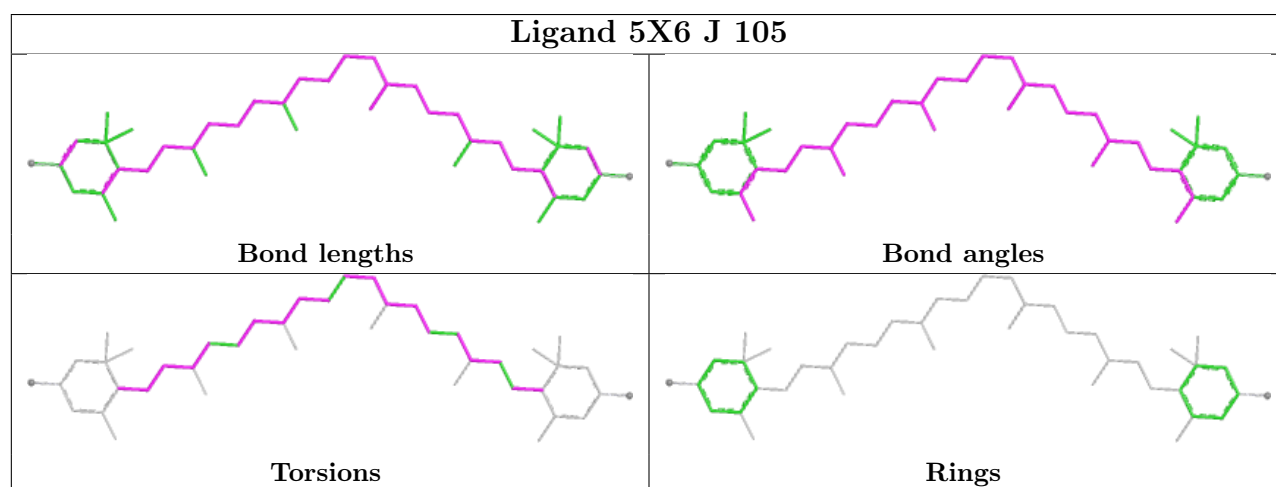
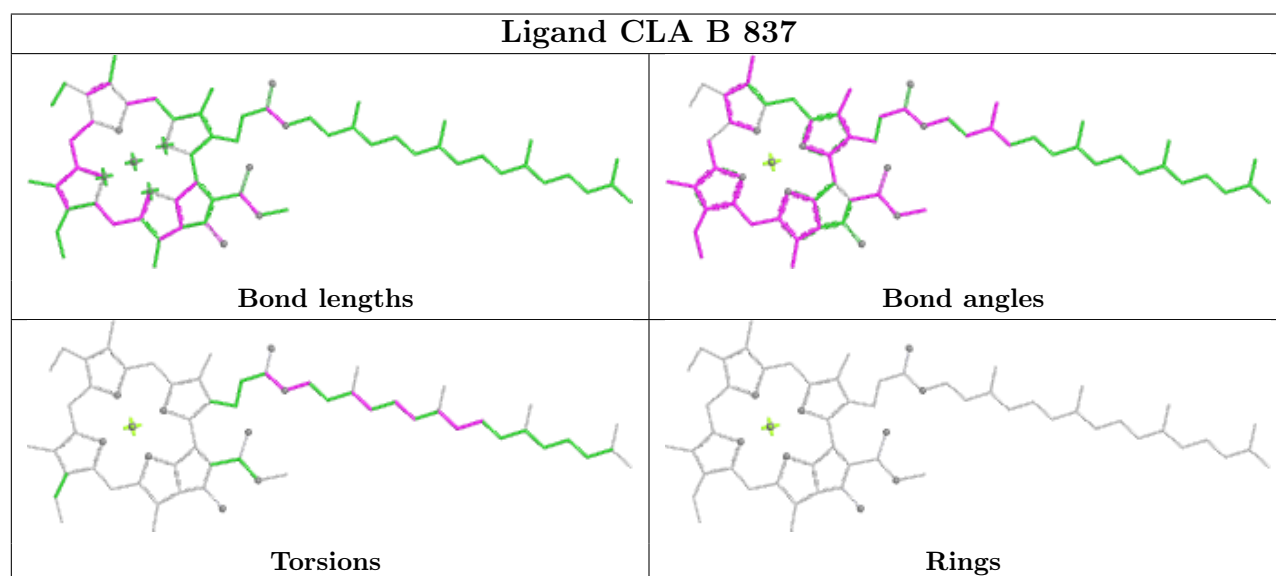
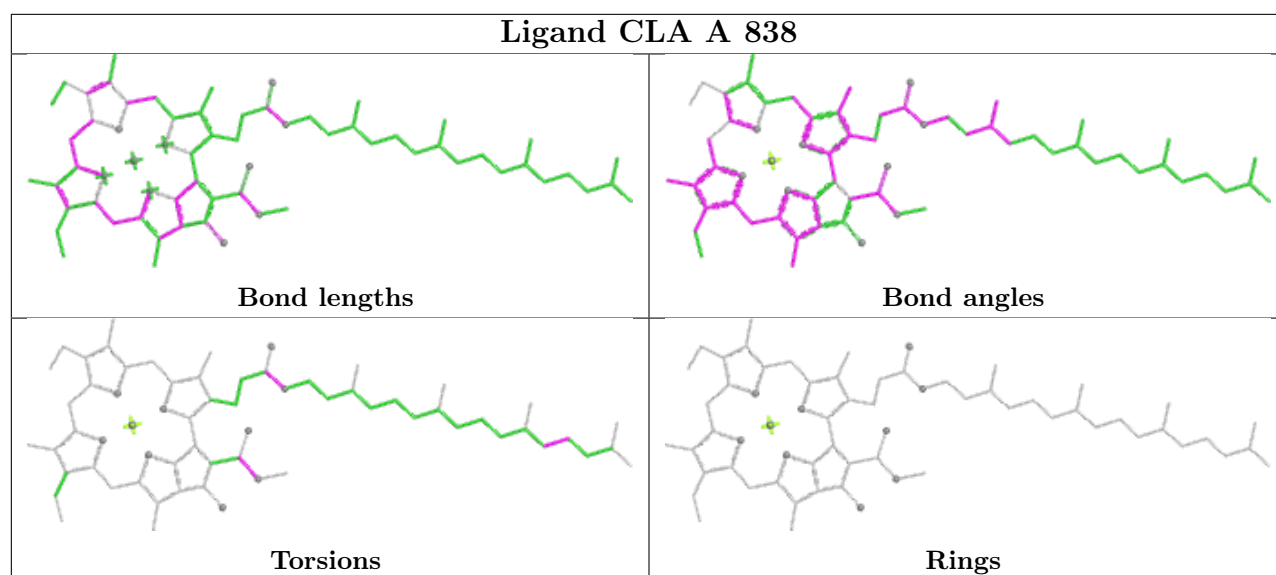


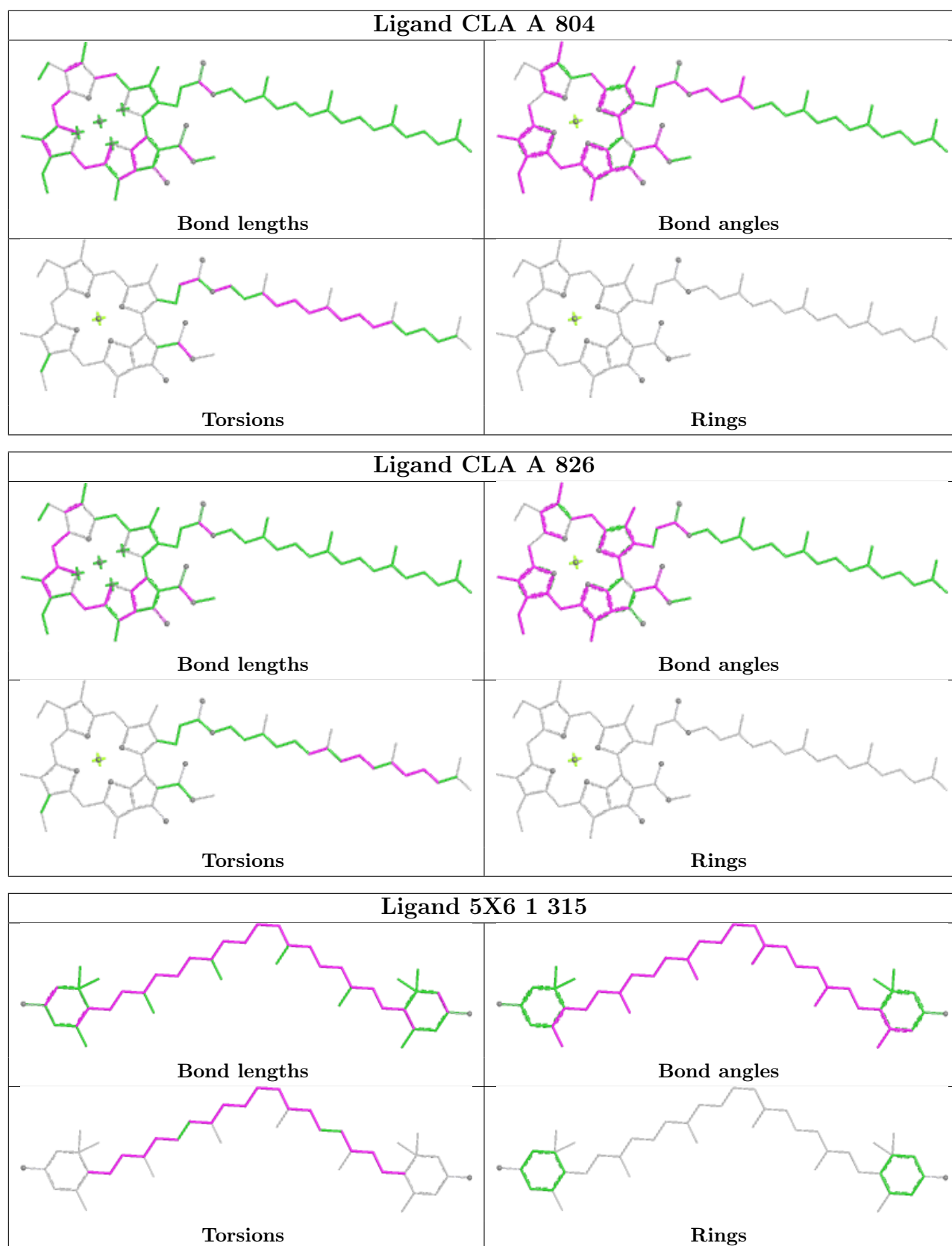
Ligand CLA 5 305



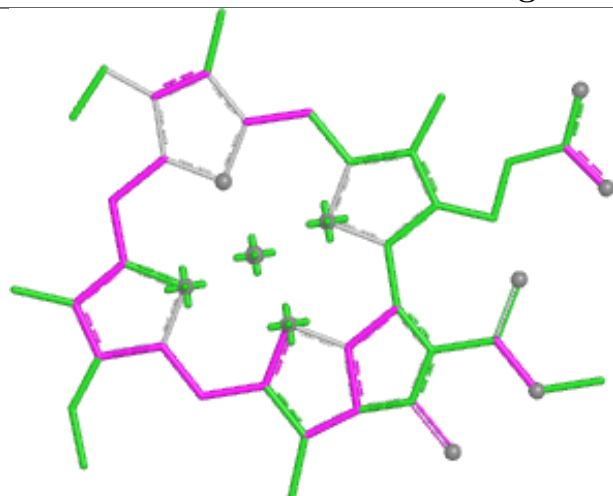
Ligand CLA K 103



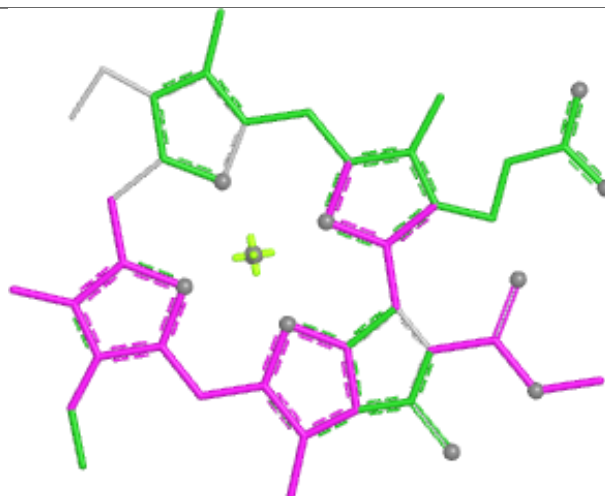




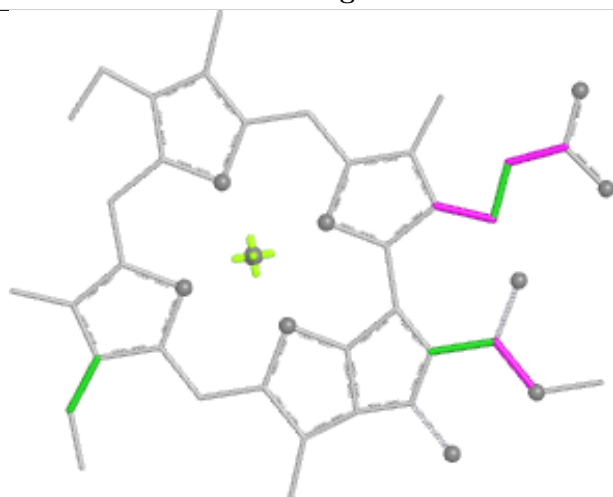
Ligand CLA 1 304



Bond lengths



Bond angles

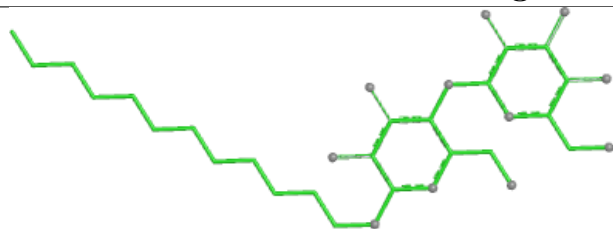


Torsions

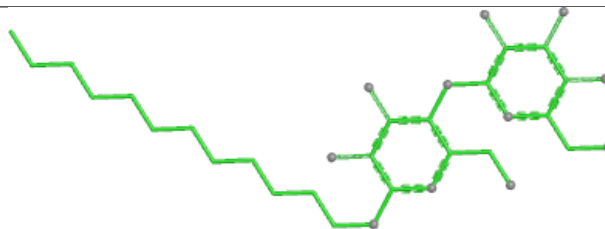


Rings

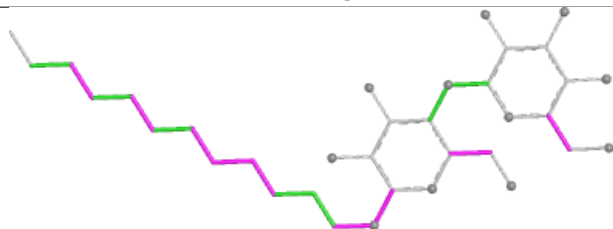
Ligand LMT B 852



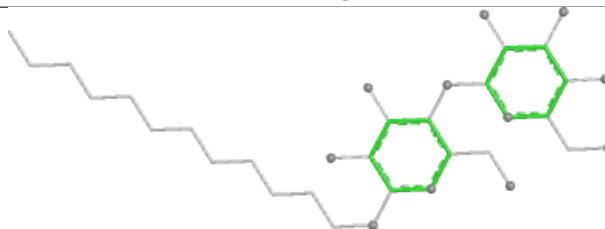
Bond lengths



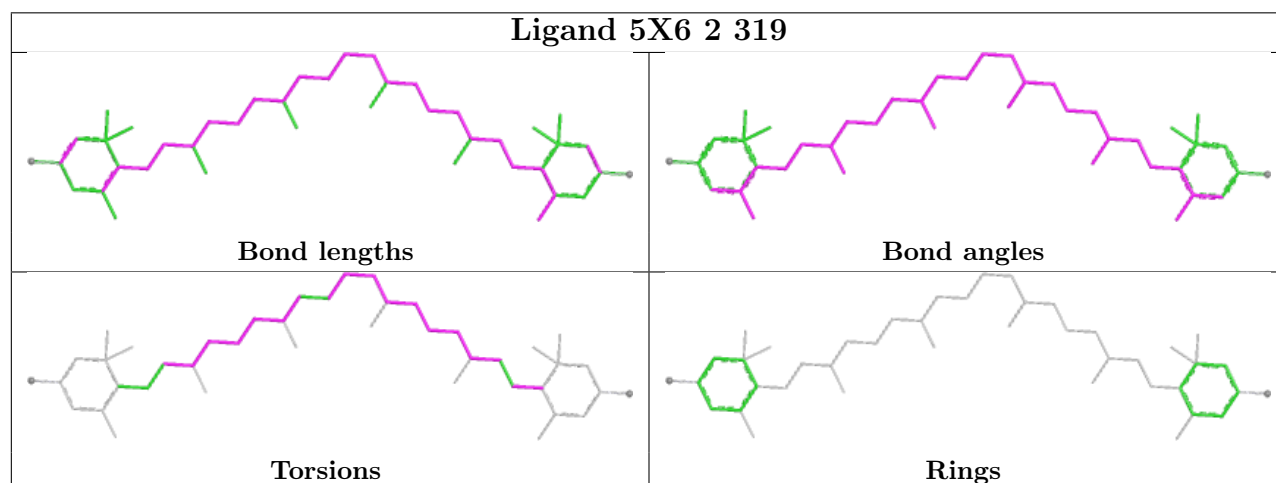
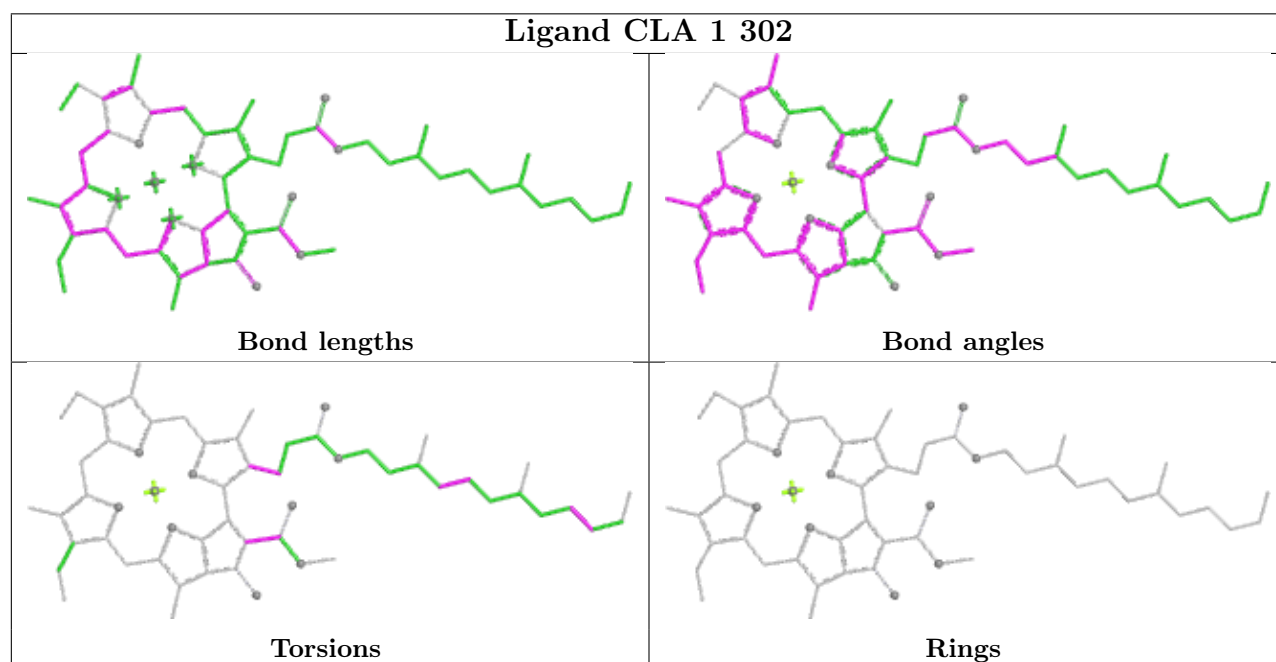
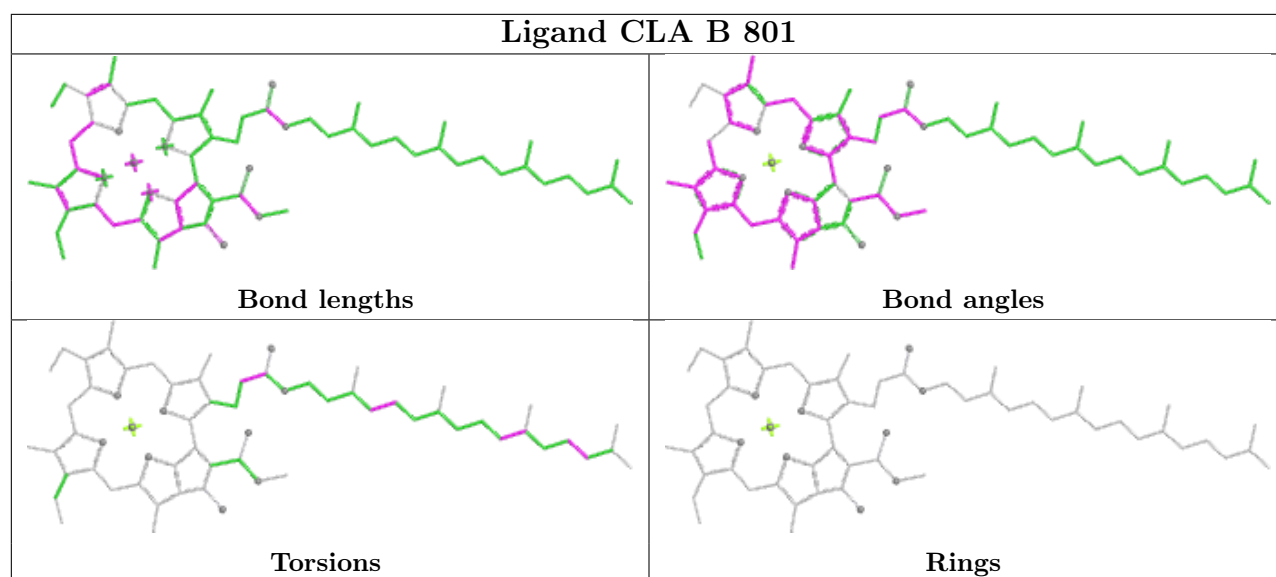
Bond angles

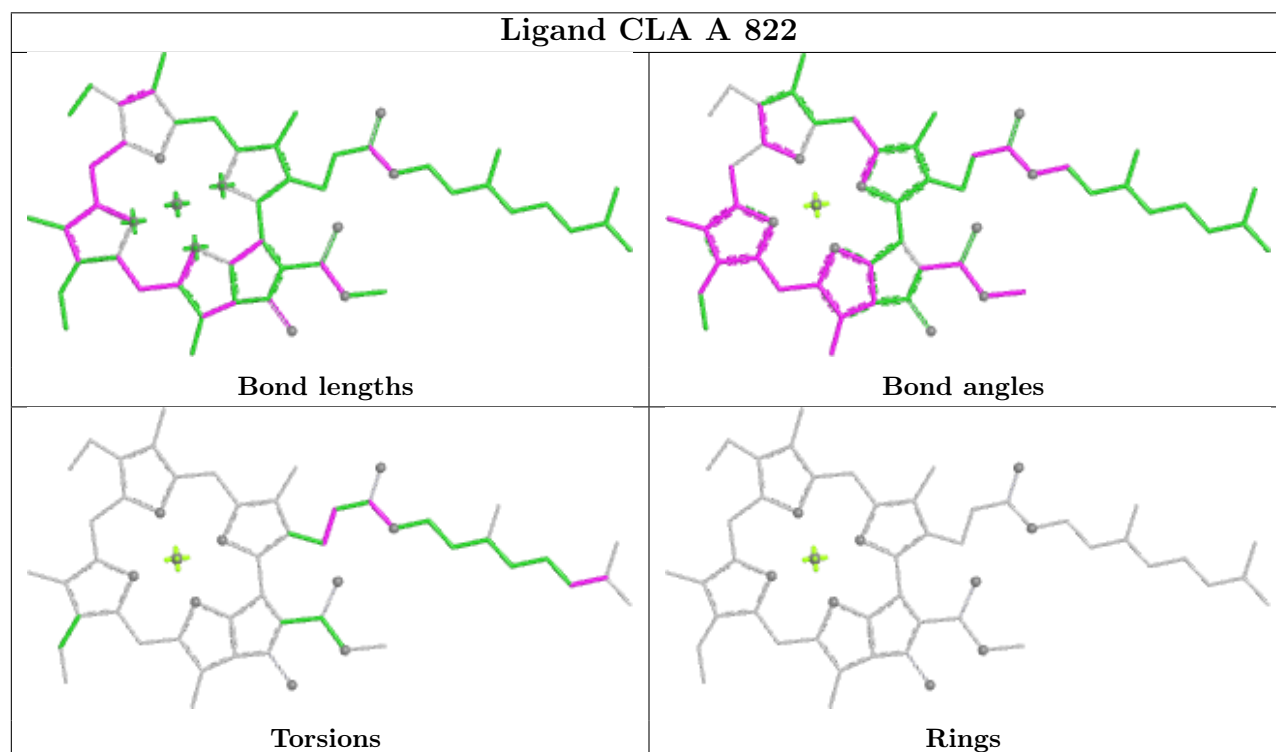
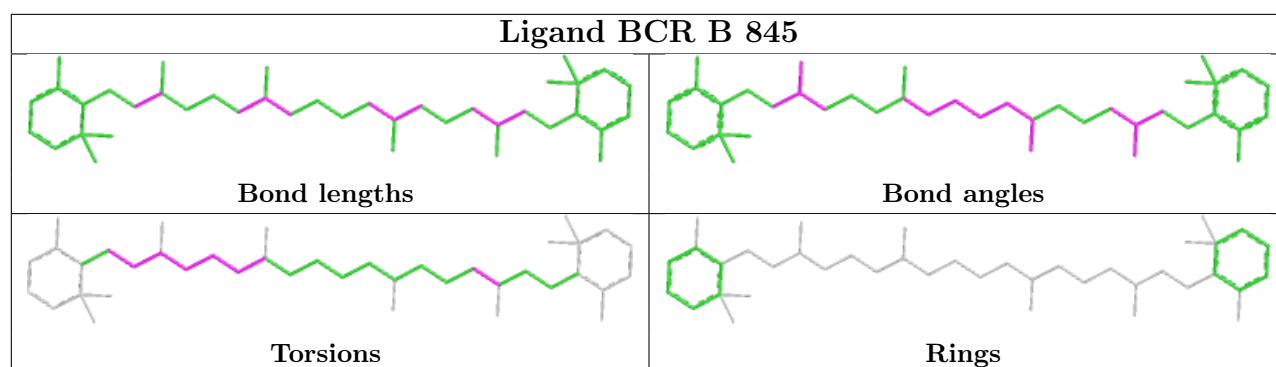


Torsions

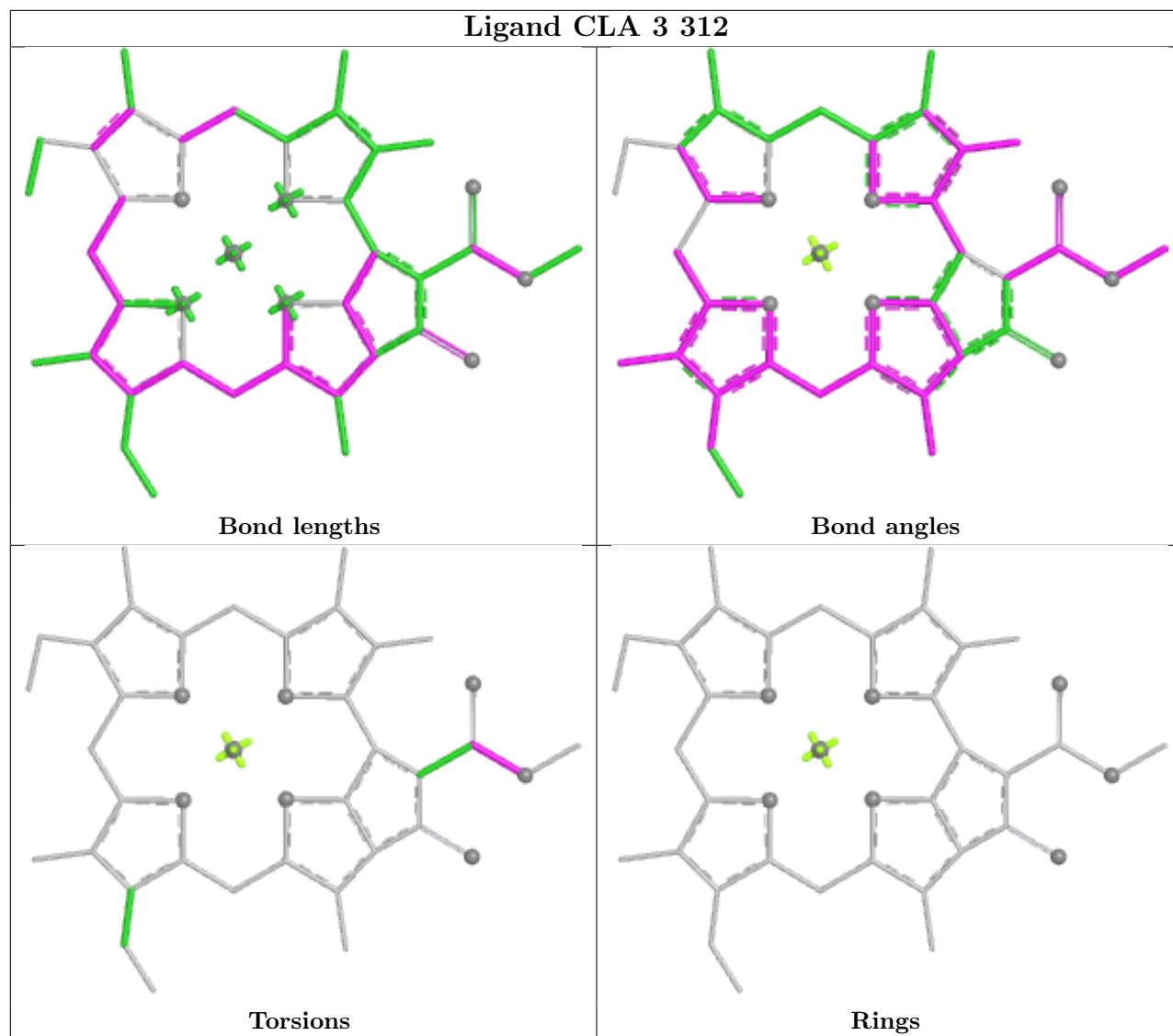


Rings

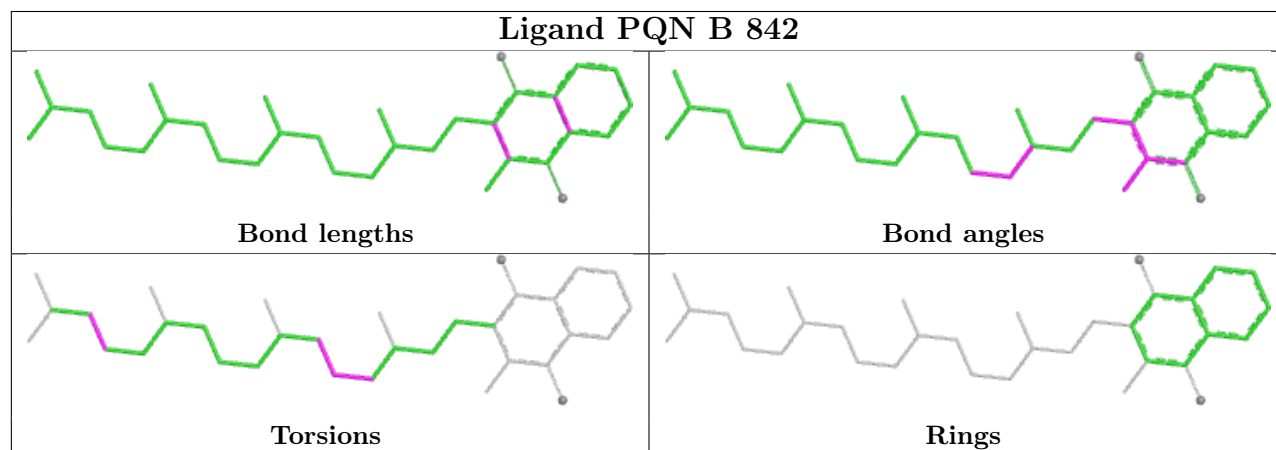




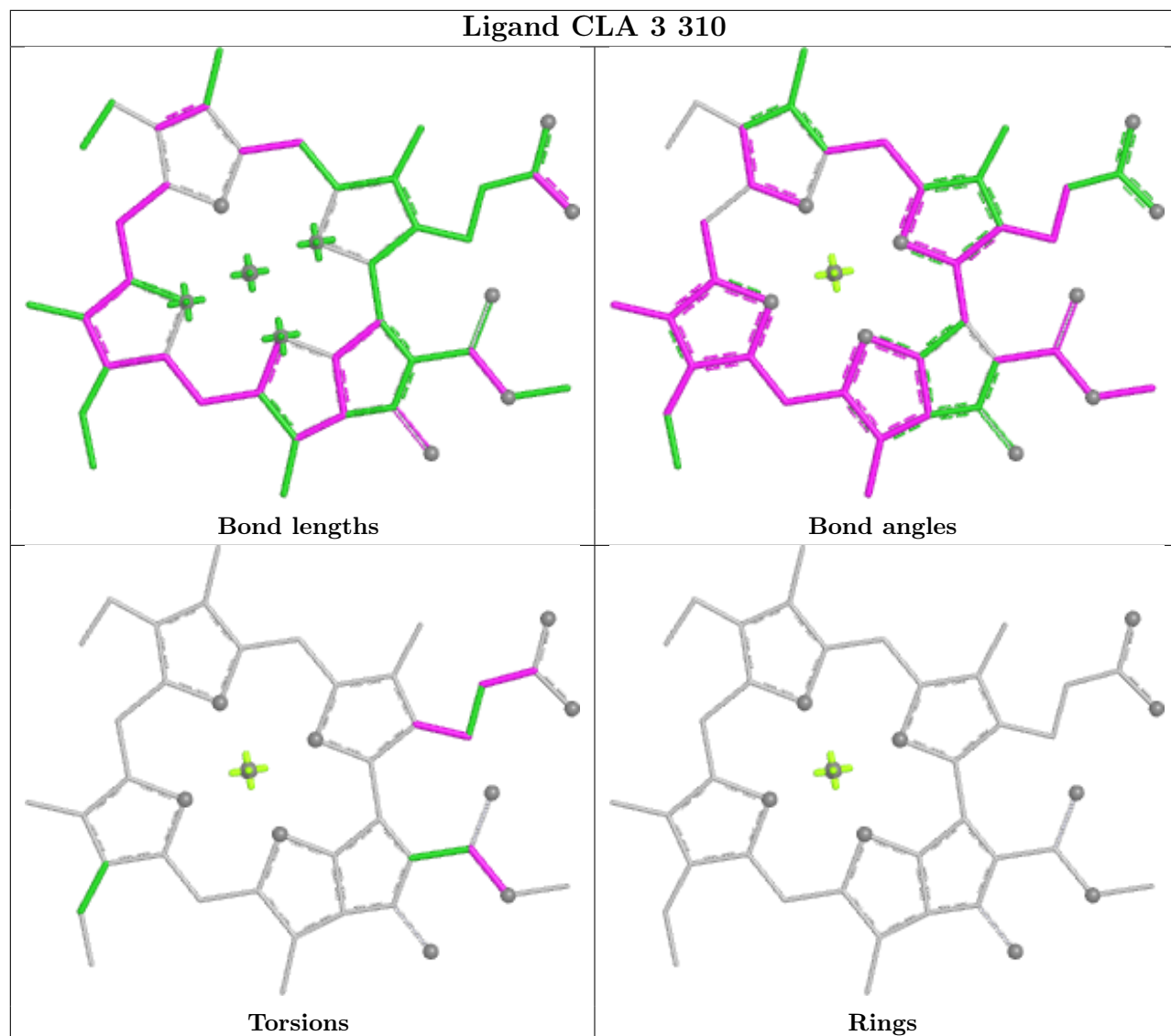
Ligand CLA 3 312



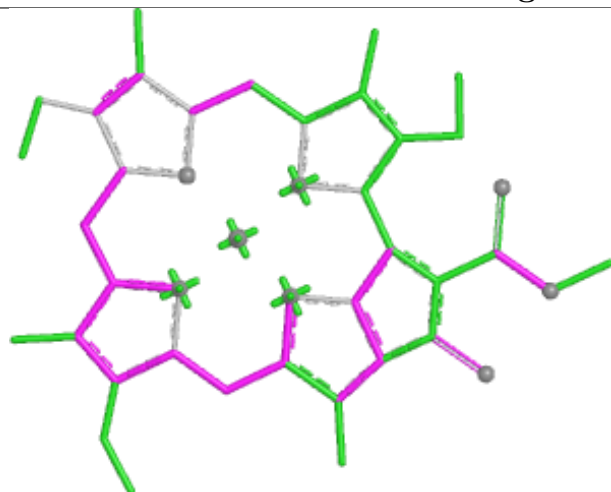
Ligand PQN B 842



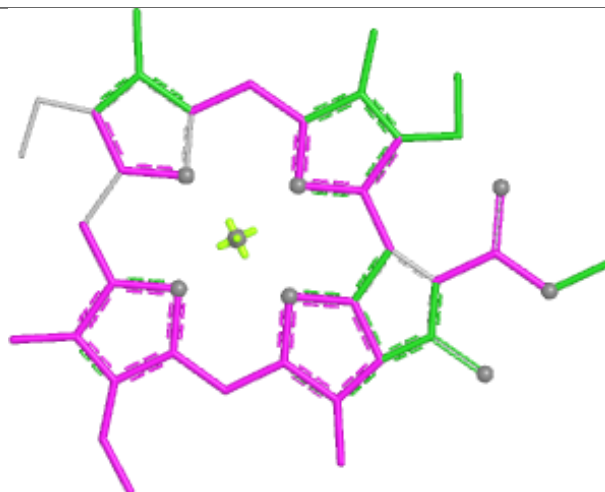
Ligand CLA 3 310



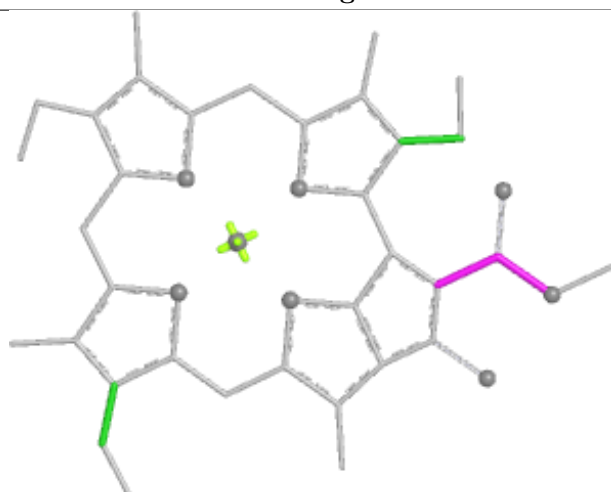
Ligand CLA J 103



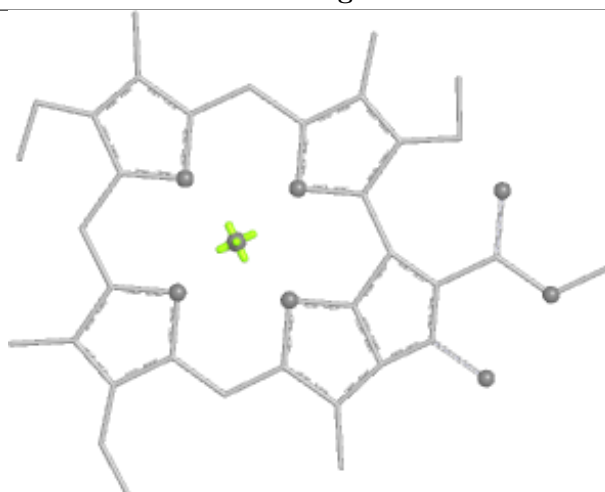
Bond lengths



Bond angles

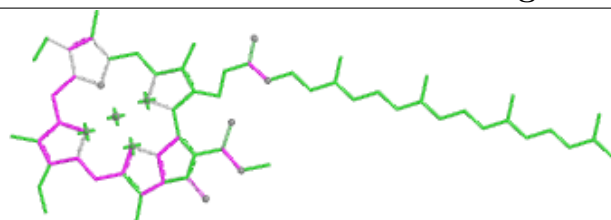


Torsions

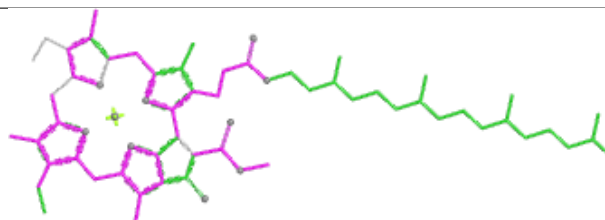


Rings

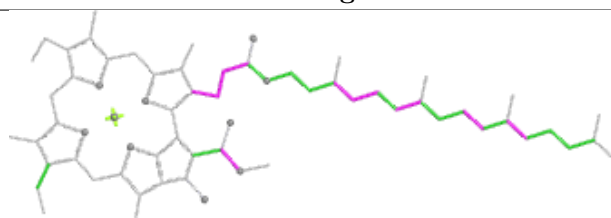
Ligand CLA 5 308



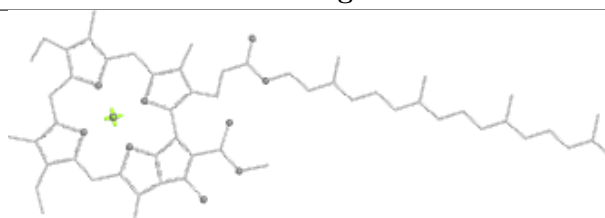
Bond lengths



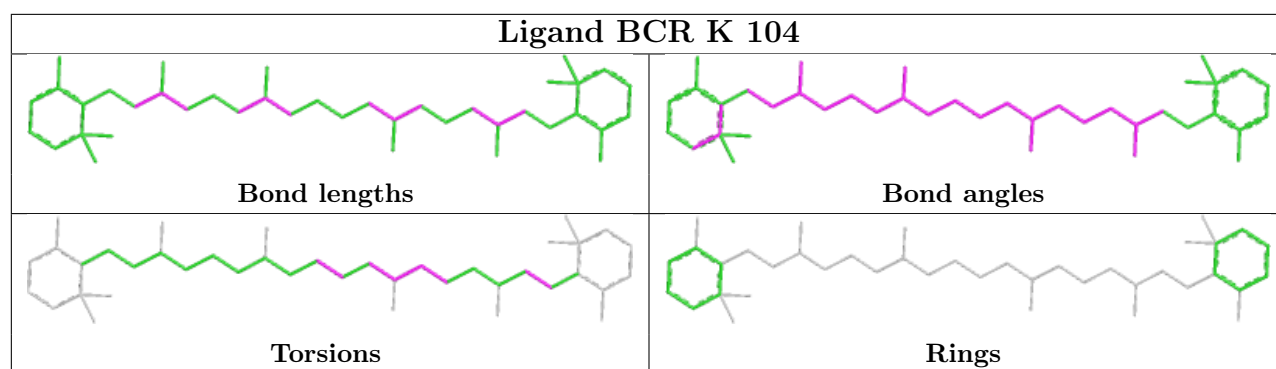
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

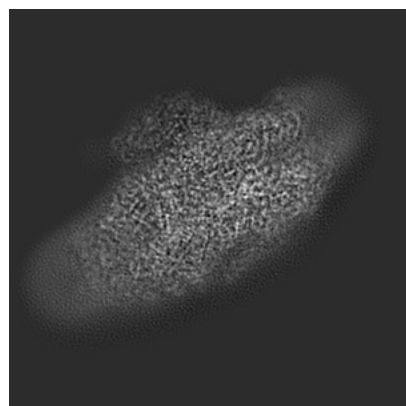
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37480. These allow visual inspection of the internal detail of the map and identification of artifacts.

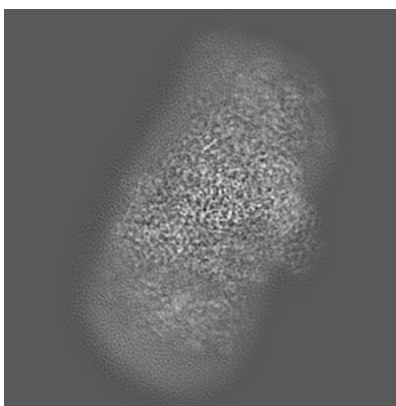
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

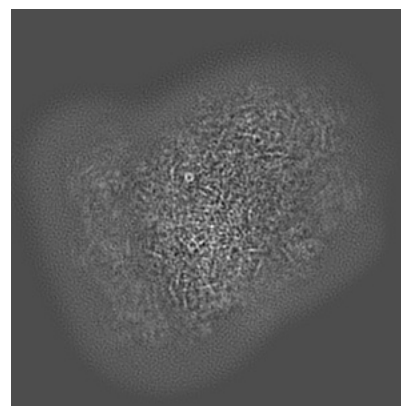
6.1.1 Primary map



X

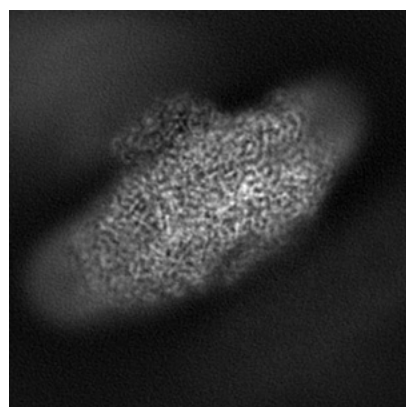


Y

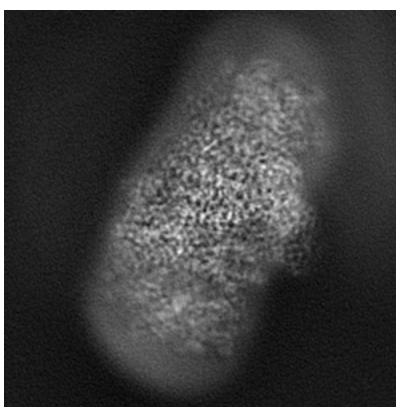


Z

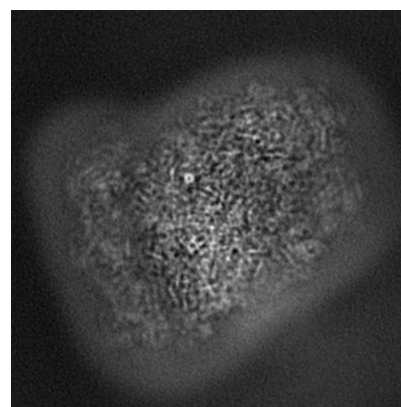
6.1.2 Raw map



X



Y

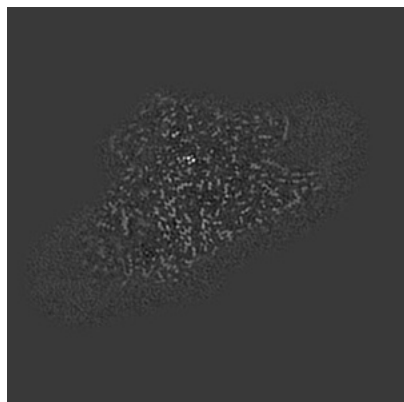


Z

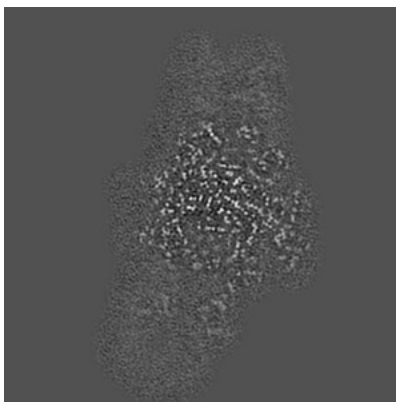
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

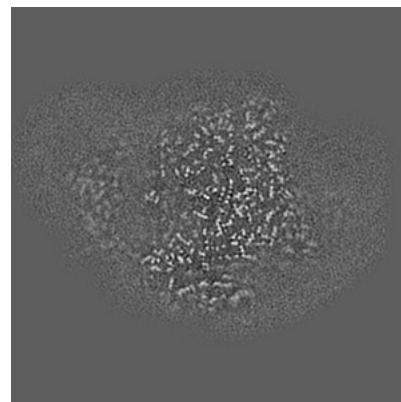
6.2.1 Primary map



X Index: 128

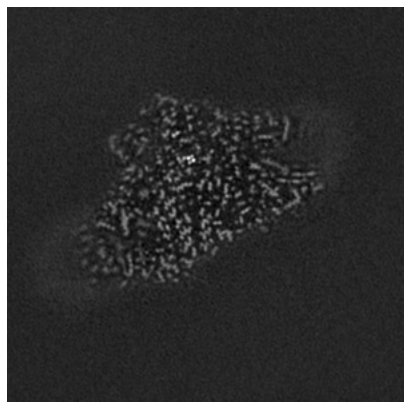


Y Index: 128

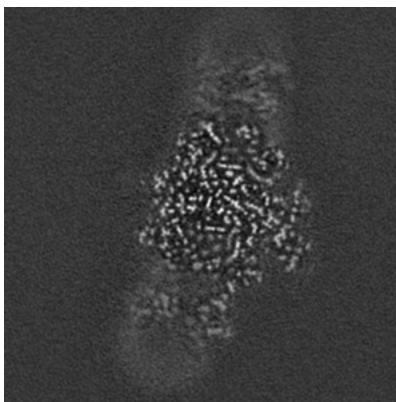


Z Index: 128

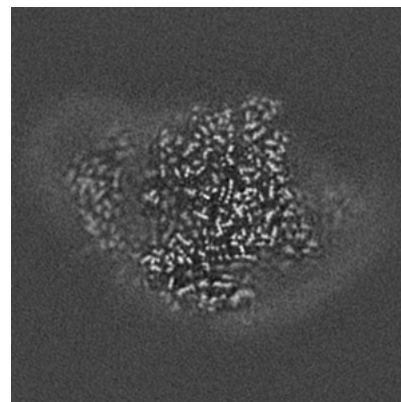
6.2.2 Raw map



X Index: 128



Y Index: 128

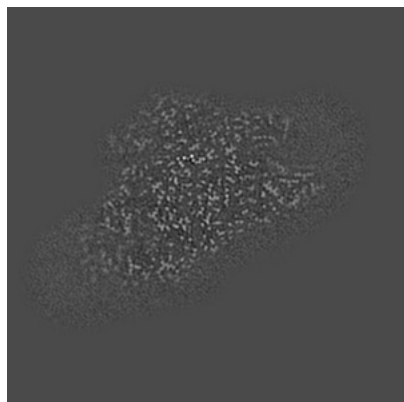


Z Index: 128

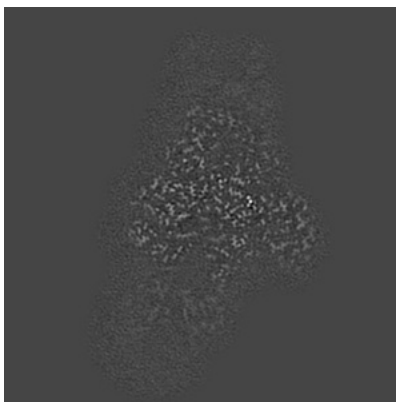
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

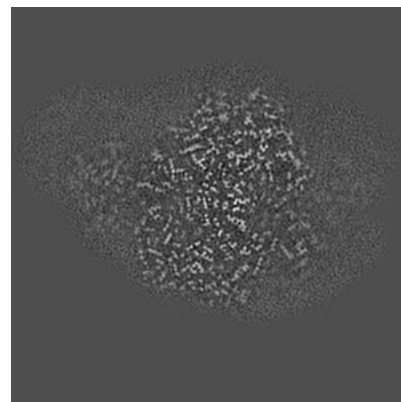
6.3.1 Primary map



X Index: 127

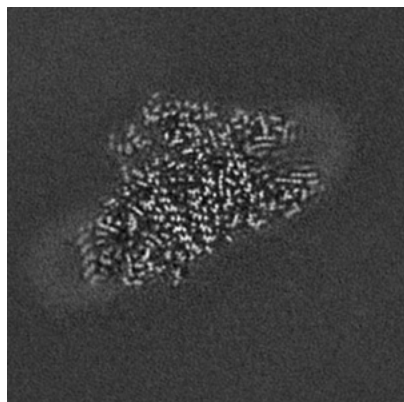


Y Index: 117

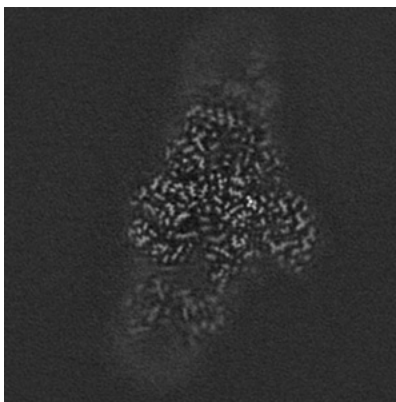


Z Index: 137

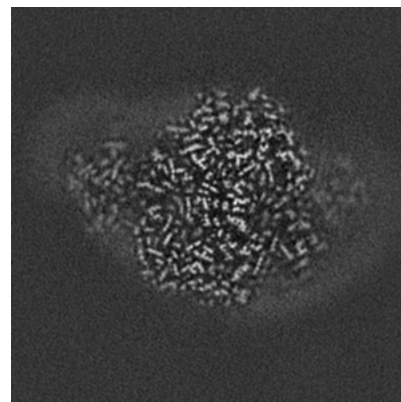
6.3.2 Raw map



X Index: 125



Y Index: 117

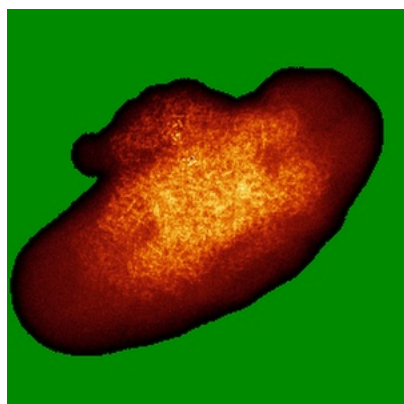


Z Index: 137

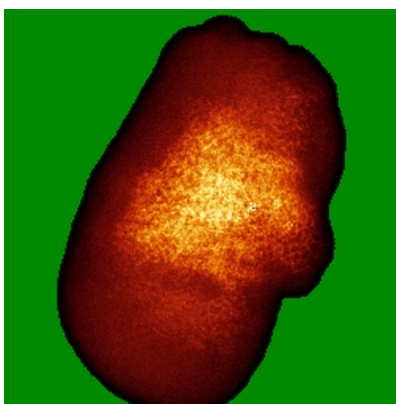
The images above show the largest variance slices of the map in three orthogonal directions.

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

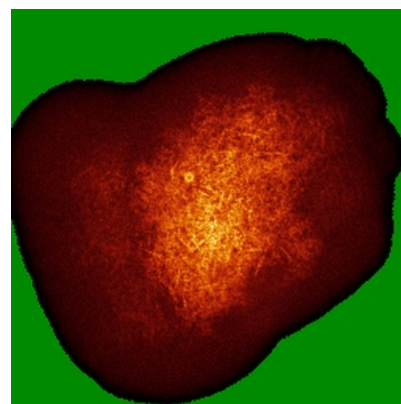
6.4.1 Primary map



X

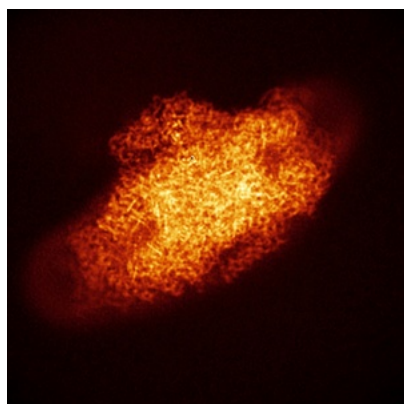


Y

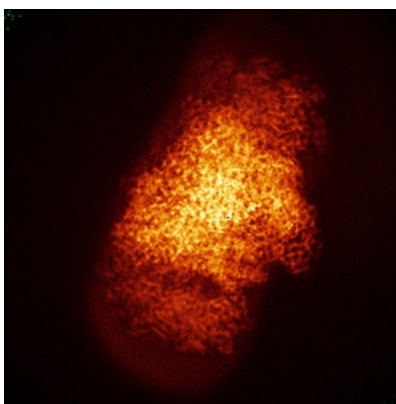


Z

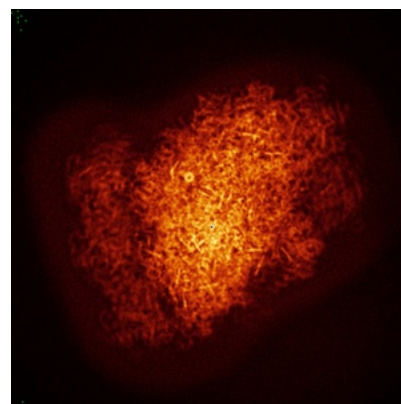
6.4.2 Raw map



X



Y

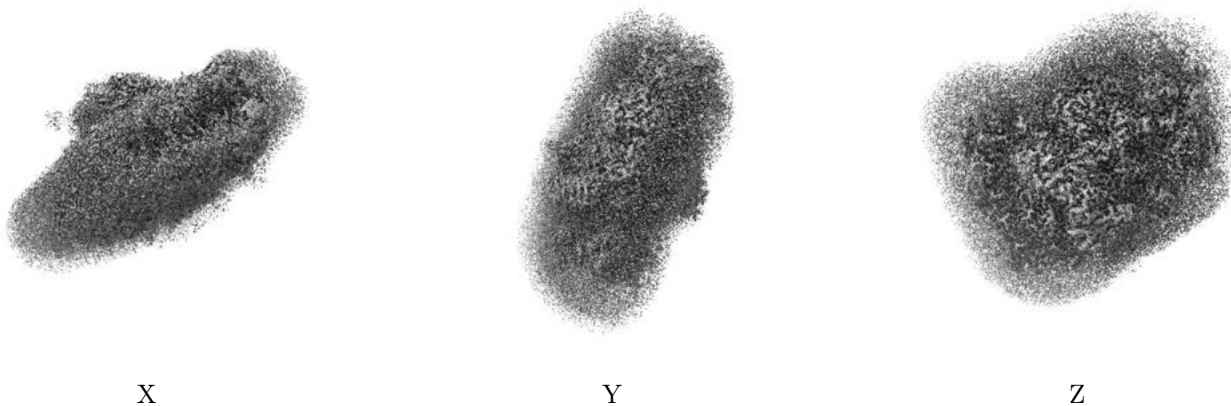


Z

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 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

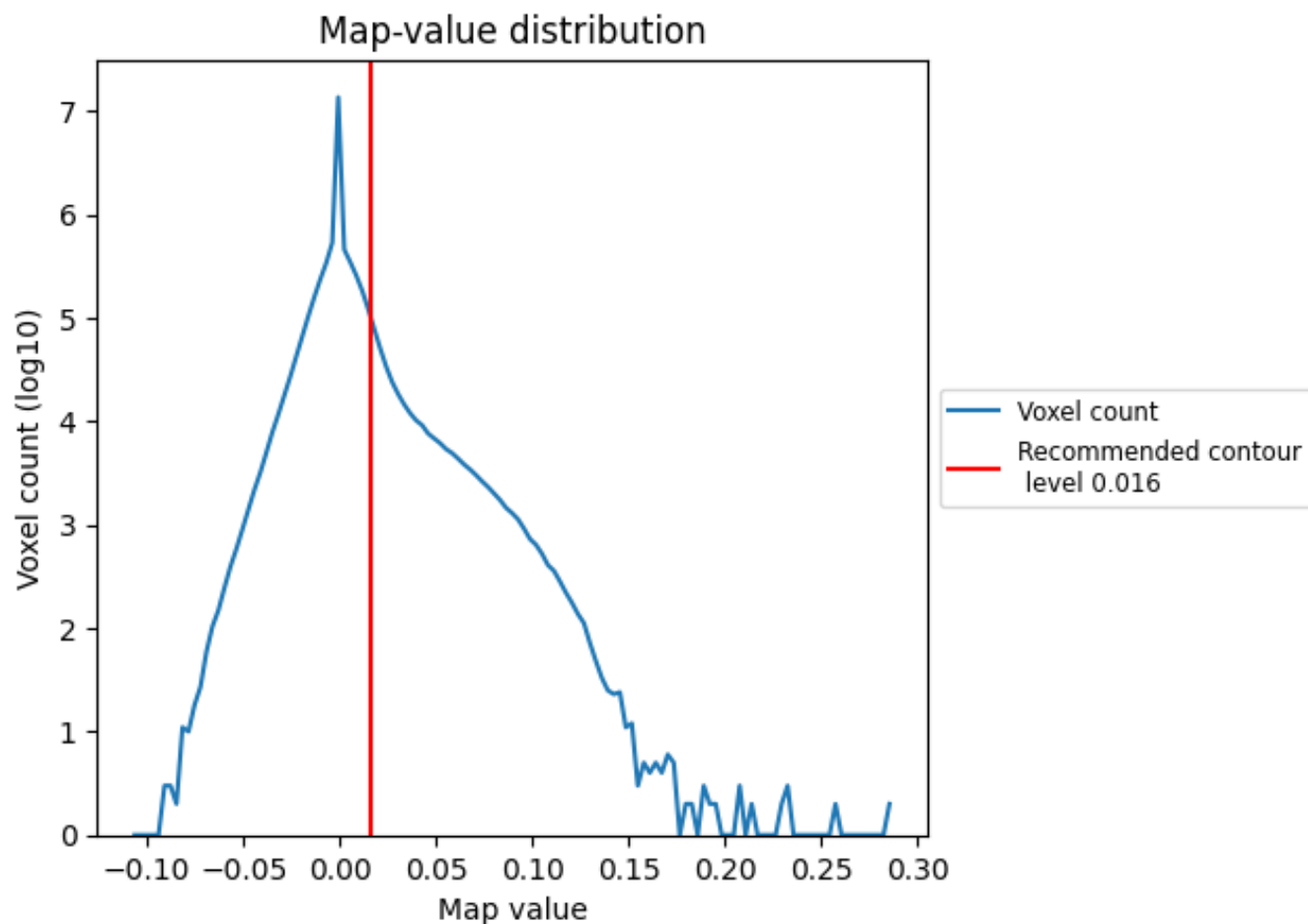
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

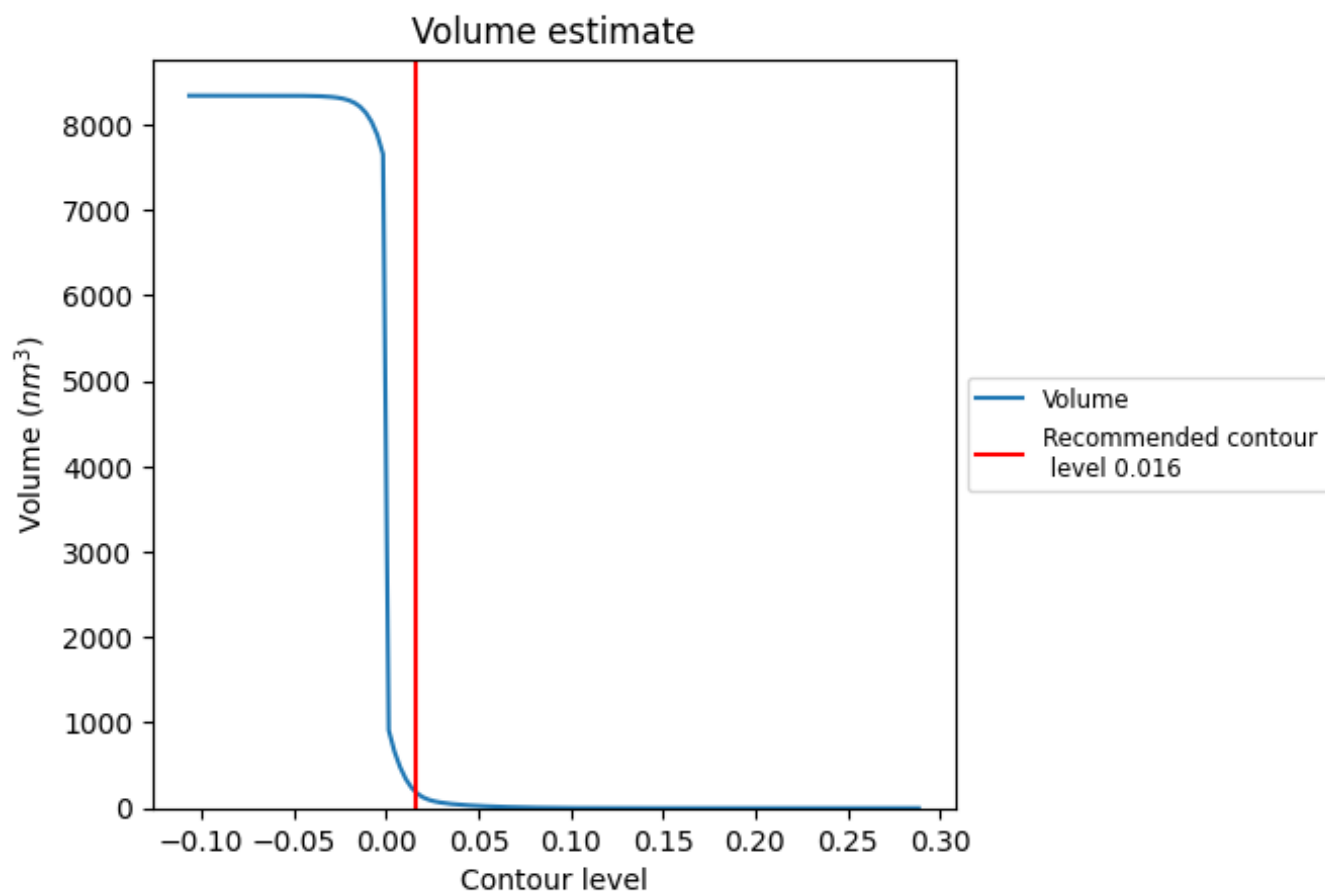
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

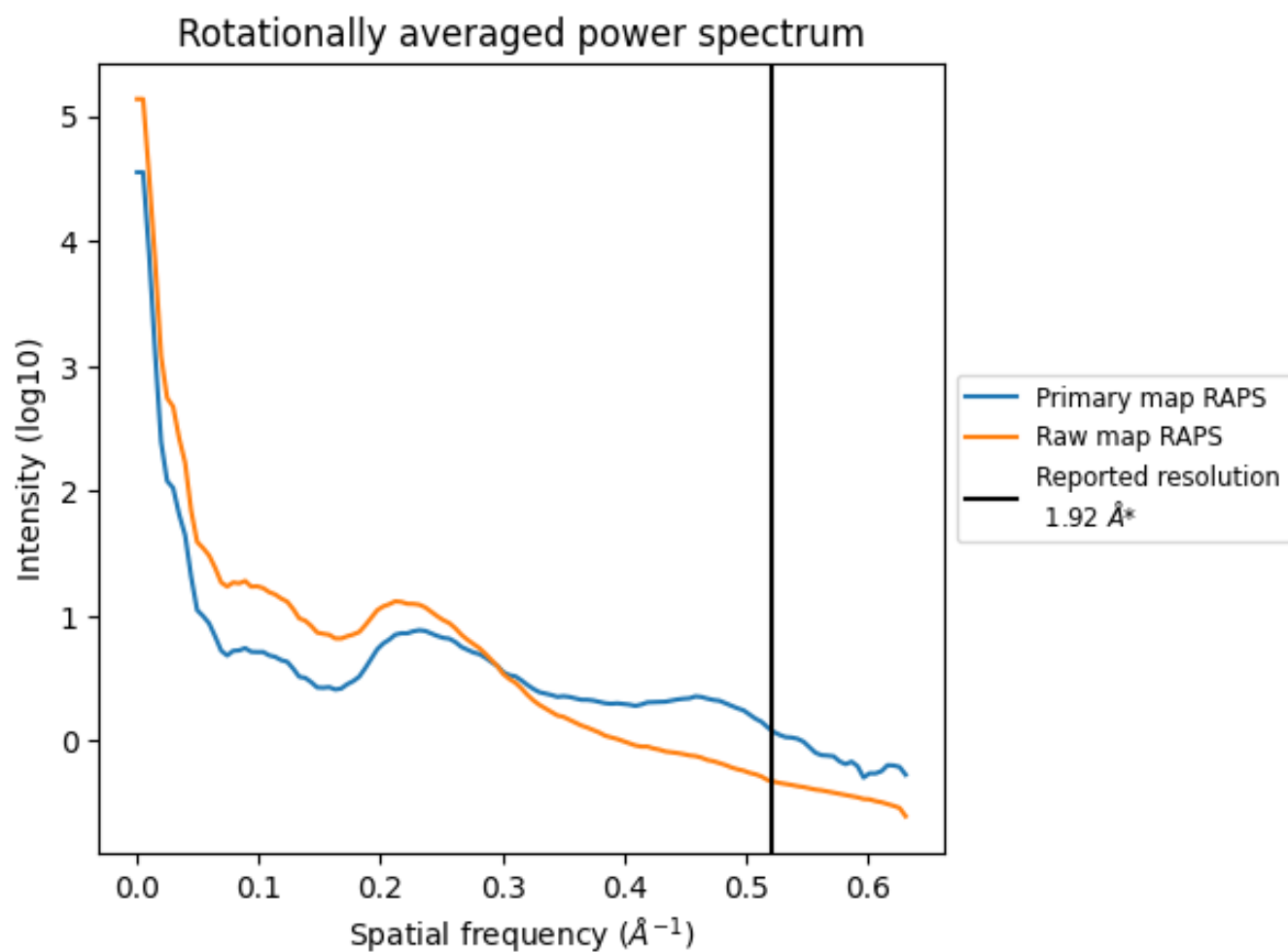
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 193 nm^3 ; this corresponds to an approximate mass of 174 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 ⓘ

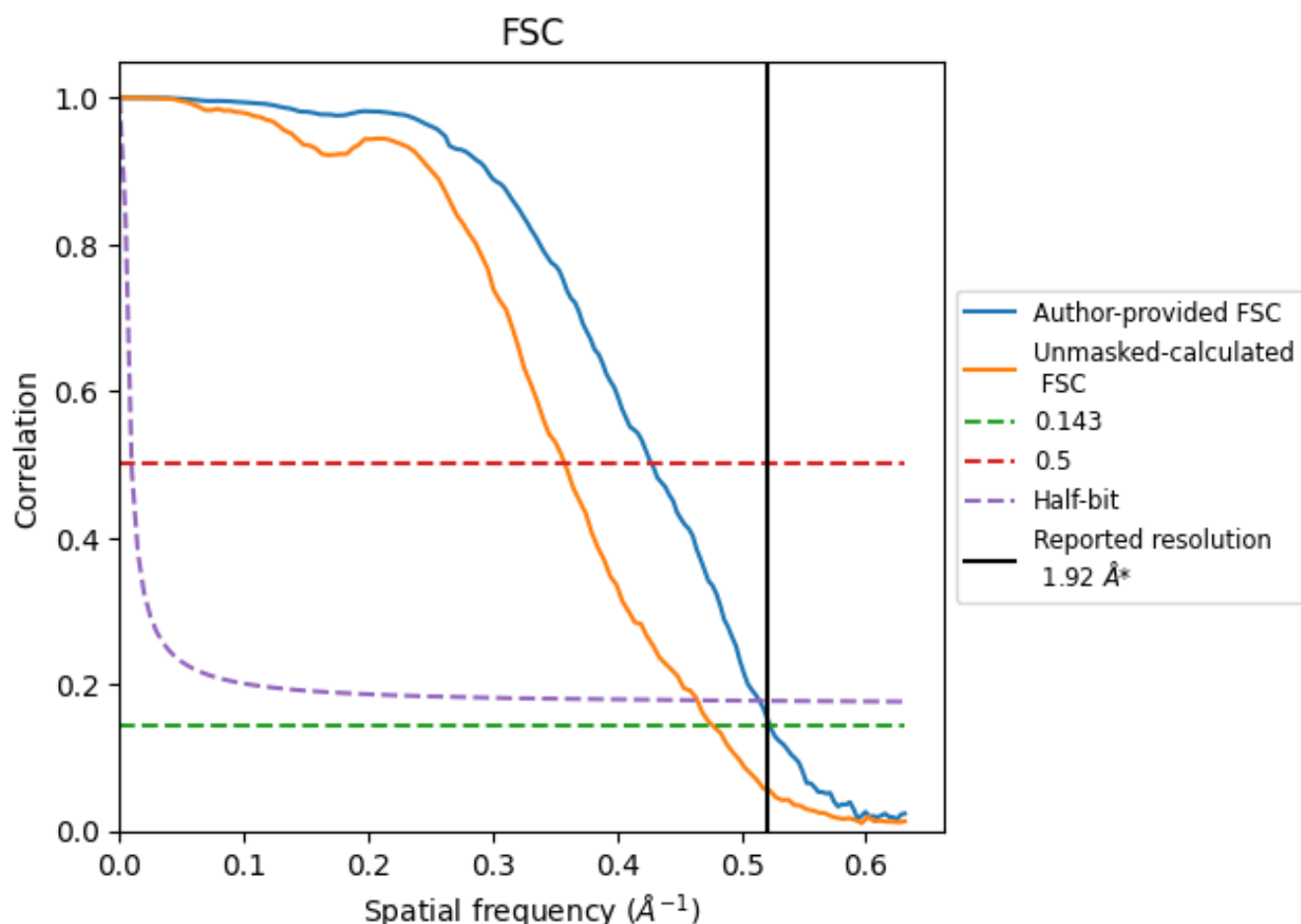


*Reported resolution corresponds to spatial frequency of 0.521 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.521 \AA^{-1}

8.2 Resolution estimates [i](#)

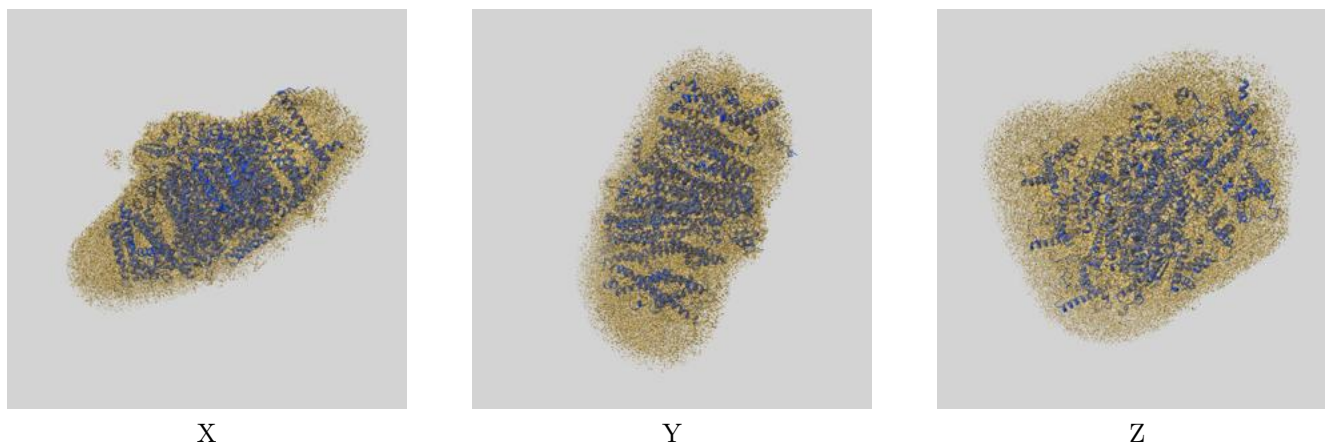
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.92	-	-
Author-provided FSC curve	1.91	2.34	1.94
Unmasked-calculated*	2.10	2.79	2.15

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

9 Map-model fit [i](#)

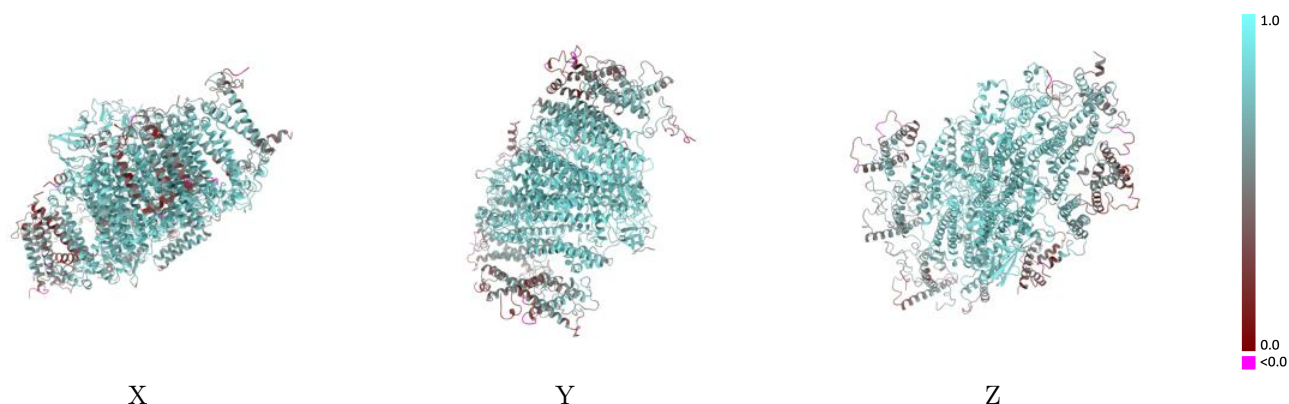
This section contains information regarding the fit between EMDB map EMD-37480 and PDB model 8WEY. Per-residue inclusion information can be found in section [3](#) on page [27](#).

9.1 Map-model overlay [i](#)



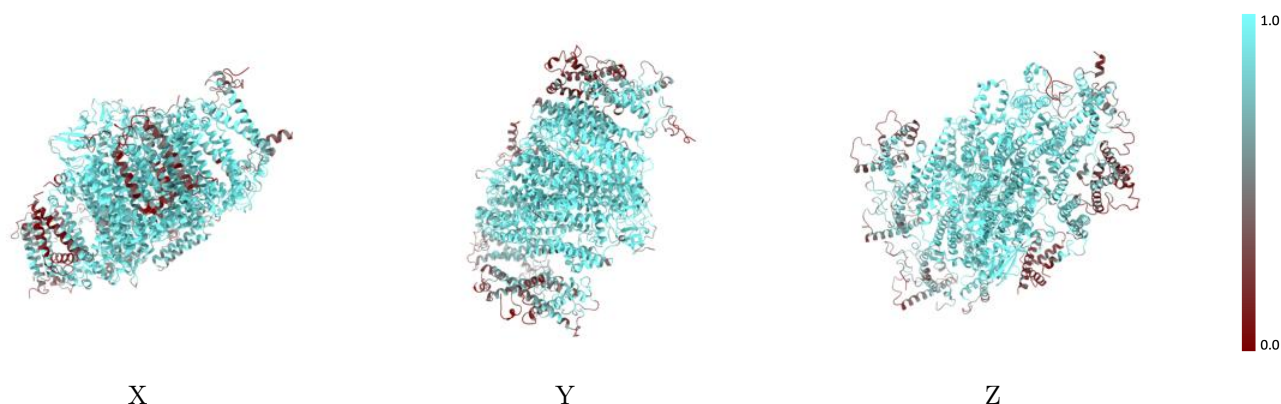
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



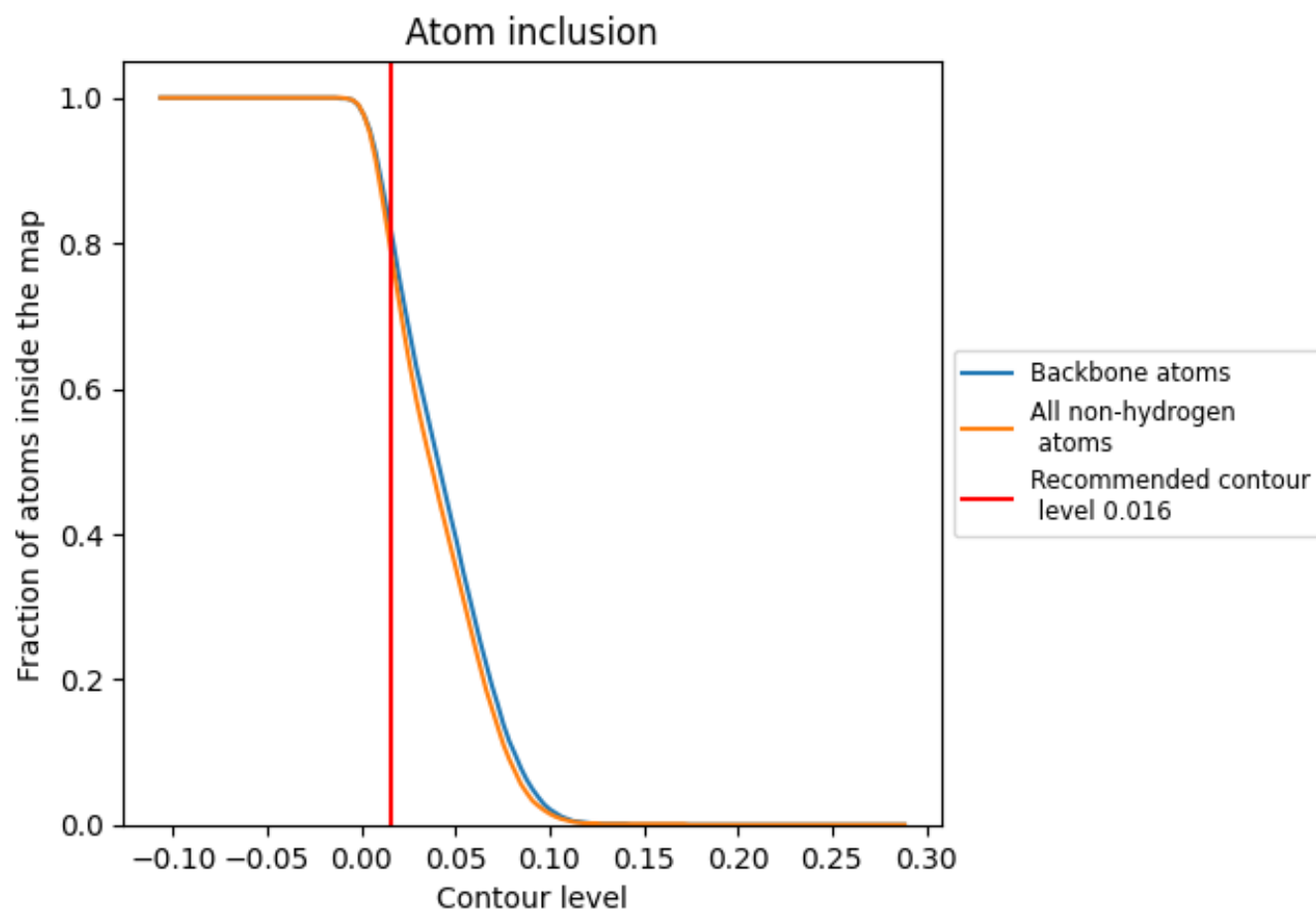
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.016).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 78% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7850	<div></div> 0.6620
1	<div></div> 0.5470	<div></div> 0.4670
2	<div></div> 0.5650	<div></div> 0.4990
3	<div></div> 0.4990	<div></div> 0.4530
4	<div></div> 0.3480	<div></div> 0.3730
5	<div></div> 0.6250	<div></div> 0.5340
A	<div></div> 0.9480	<div></div> 0.7870
B	<div></div> 0.9320	<div></div> 0.7720
C	<div></div> 0.9780	<div></div> 0.8100
D	<div></div> 0.8930	<div></div> 0.7170
E	<div></div> 0.8800	<div></div> 0.7220
F	<div></div> 0.8730	<div></div> 0.7150
I	<div></div> 0.8930	<div></div> 0.7250
J	<div></div> 0.8960	<div></div> 0.7440
K	<div></div> 0.7180	<div></div> 0.5880
L	<div></div> 0.7930	<div></div> 0.6310
M	<div></div> 0.8300	<div></div> 0.6850
O	<div></div> 0.2150	<div></div> 0.3110

