



wwPDB EM Validation Summary Report ⓘ

Oct 27, 2024 – 12:21 PM JST

PDB ID : 5ZGB
EMDB ID : EMD-6929
Title : Cryo-EM structure of the red algal PSI-LHCR
Authors : Pi, X.
Deposited on : 2018-03-08
Resolution : 3.63 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.39

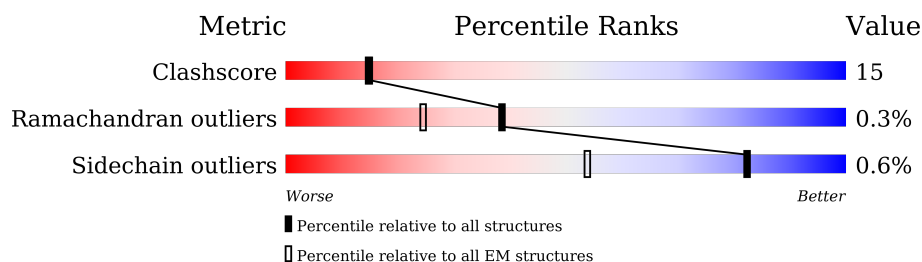
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.63 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	 71% 27% .
2	B	732	 75% 24% .
3	C	81	 70% 28% .
4	D	139	 59% 24% .. 14%
5	E	94	 5% 56% 9% 35%
6	F	185	 74% 9% 17%
7	I	32	 66% 31% .
8	J	38	 71% 29%

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Mol	Chain	Length	Quality of chain
9	K	60	
10	L	140	
11	M	29	
12	O	155	
13	1	175	
13	4	175	
14	2	199	
14	5	199	
15	3	188	

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	-	X	-
17	CLA	1	601	X	-	-	-
17	CLA	1	602	X	-	-	-
17	CLA	1	603	X	-	-	-
17	CLA	1	604	X	-	-	-
17	CLA	1	605	X	-	-	-
17	CLA	1	606	X	-	-	-
17	CLA	1	607	X	-	-	-
17	CLA	1	608	X	-	-	-
17	CLA	1	609	X	-	-	-
17	CLA	1	610	X	-	-	-
17	CLA	1	611	X	-	-	-
17	CLA	1	612	X	-	-	-
17	CLA	2	601	X	-	-	-
17	CLA	2	602	X	-	-	-
17	CLA	2	603	X	-	-	-
17	CLA	2	604	X	-	-	-
17	CLA	2	605	X	-	-	-
17	CLA	2	606	X	-	-	-
17	CLA	2	607	X	-	-	-
17	CLA	2	608	X	-	-	-
17	CLA	2	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	2	610	X	-	-	-
17	CLA	2	611	X	-	-	-
17	CLA	2	612	X	-	-	-
17	CLA	2	613	X	-	-	-
17	CLA	3	202	X	-	-	-
17	CLA	3	203	X	-	-	-
17	CLA	3	204	X	-	-	-
17	CLA	3	205	X	-	-	-
17	CLA	3	206	X	-	-	-
17	CLA	3	207	X	-	-	-
17	CLA	3	208	X	-	-	-
17	CLA	3	209	X	-	-	-
17	CLA	3	210	X	-	-	-
17	CLA	3	211	X	-	-	-
17	CLA	3	212	X	-	-	-
17	CLA	3	213	X	-	-	-
17	CLA	4	601	X	-	-	-
17	CLA	4	602	X	-	-	-
17	CLA	4	603	X	-	-	-
17	CLA	4	604	X	-	-	-
17	CLA	4	605	X	-	-	-
17	CLA	4	606	X	-	-	-
17	CLA	4	607	X	-	-	-
17	CLA	4	608	X	-	-	-
17	CLA	4	609	X	-	-	-
17	CLA	4	610	X	-	-	-
17	CLA	4	611	X	-	-	-
17	CLA	5	601	X	-	-	-
17	CLA	5	602	X	-	-	-
17	CLA	5	603	X	-	-	-
17	CLA	5	604	X	-	-	-
17	CLA	5	605	X	-	-	-
17	CLA	5	606	X	-	-	-
17	CLA	5	607	X	-	-	-
17	CLA	5	608	X	-	-	-
17	CLA	5	609	X	-	-	-
17	CLA	5	610	X	-	-	-
17	CLA	5	611	X	-	-	-
17	CLA	5	612	X	-	-	-
17	CLA	5	613	X	-	-	-
17	CLA	A	802	X	-	-	-
17	CLA	A	803	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	A	804	X	-	-	-
17	CLA	A	805	X	-	-	-
17	CLA	A	806	X	-	-	-
17	CLA	A	807	X	-	-	-
17	CLA	A	808	X	-	-	-
17	CLA	A	809	X	-	-	-
17	CLA	A	810	X	-	-	-
17	CLA	A	811	X	-	-	-
17	CLA	A	812	X	-	-	-
17	CLA	A	813	X	-	-	-
17	CLA	A	814	X	-	-	-
17	CLA	A	815	X	-	-	-
17	CLA	A	816	X	-	-	-
17	CLA	A	817	X	-	-	-
17	CLA	A	818	X	-	-	-
17	CLA	A	819	X	-	-	-
17	CLA	A	820	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	848	X	-	-	-
17	CLA	B	801	X	-	-	-
17	CLA	B	802	X	-	-	-
17	CLA	B	803	X	-	-	-
17	CLA	B	804	X	-	-	-
17	CLA	B	806	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
17	CLA	B	813	X	-	-	-
17	CLA	B	814	X	-	-	-
17	CLA	B	815	X	-	-	-
17	CLA	B	816	X	-	-	-
17	CLA	B	817	X	-	-	-
17	CLA	B	818	X	-	-	-
17	CLA	B	819	X	-	-	-
17	CLA	B	820	X	-	-	-
17	CLA	B	821	X	-	-	-
17	CLA	B	822	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	831	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	B	842	X	-	-	-
17	CLA	B	843	X	-	-	-
17	CLA	F	301	X	-	-	-
17	CLA	F	302	X	-	-	-
17	CLA	F	303	X	-	-	-
17	CLA	J	101	X	-	-	-
17	CLA	J	102	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	J	103	X	-	-	-
17	CLA	K	102	X	-	-	-
17	CLA	K	103	X	-	-	-
17	CLA	L	202	X	-	-	-
17	CLA	L	203	X	-	-	-
17	CLA	L	204	X	-	-	-
17	CLA	O	201	X	-	-	-
17	CLA	O	203	X	-	-	-
17	CLA	O	204	X	-	-	-
17	CLA	O	205	X	-	-	-
25	ZEX	1	615	-	X	-	-
25	ZEX	1	616	-	X	-	-
25	ZEX	2	614	-	X	-	-
25	ZEX	3	216	-	X	-	-
25	ZEX	3	218	-	X	-	-
25	ZEX	4	612	-	X	-	-
25	ZEX	5	614	-	X	-	-
25	ZEX	5	615	-	X	-	-

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 35011 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 PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	741	Total	C	N	O	S	0	0
			5798	3792	996	983	27		

- Molecule 2 is a protein called PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	731	Total	C	N	O	S	0	0
			5819	3827	982	991	19		

- Molecule 3 is a protein called PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			597	367	104	114	12		

- Molecule 4 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	119	Total	C	N	O	S	0	0
			950	600	167	179	4		

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	61	Total	C	N	O	0	0
			493	322	79	92		

- Molecule 6 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	154	Total	C	N	O	S	0	0
			1263	811	214	234	4		

- Molecule 7 is a protein called PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	31	Total	C	N	O	S	0	0
			230	158	32	39	1		

- Molecule 8 is a protein called PsaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	38	Total	C	N	O	S	0	0
			312	214	46	51	1		

- Molecule 9 is a protein called PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	59	Total	C	N	O	S	0	0
			428	279	70	74	5		

- Molecule 10 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	119	Total	C	N	O	S	0	0
			900	591	148	159	2		

- Molecule 11 is a protein called PsaM.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	27	Total	C	N	O	S	0	0
			204	136	32	34	2		

- Molecule 12 is a protein called PsaO.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	O	83	Total	C	N	O	0	0
			641	439	97	105		

- Molecule 13 is a protein called Lhcr1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1	169	Total	C	N	O	S	0	0
			1351	887	227	229	8		
13	4	170	Total	C	N	O	S	0	0
			1358	892	228	230	8		

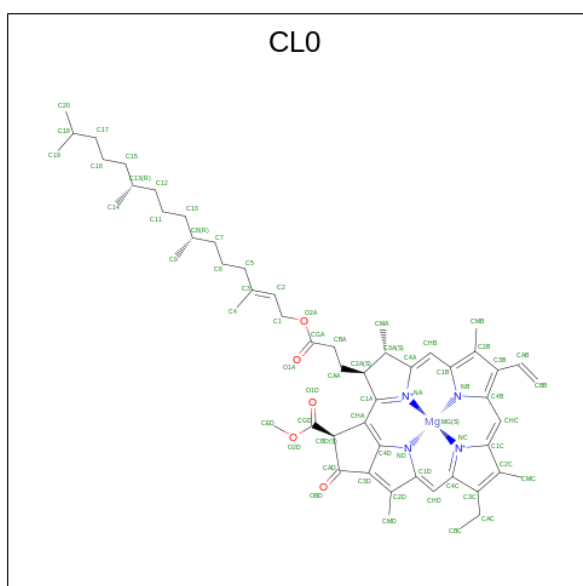
- Molecule 14 is a protein called Lhcr2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	2	175	Total	C	N	O	S	0	0
			1371	892	233	239	7		
14	5	175	Total	C	N	O	S	0	0
			1371	892	233	239	7		

- Molecule 15 is a protein called Lhcr3.

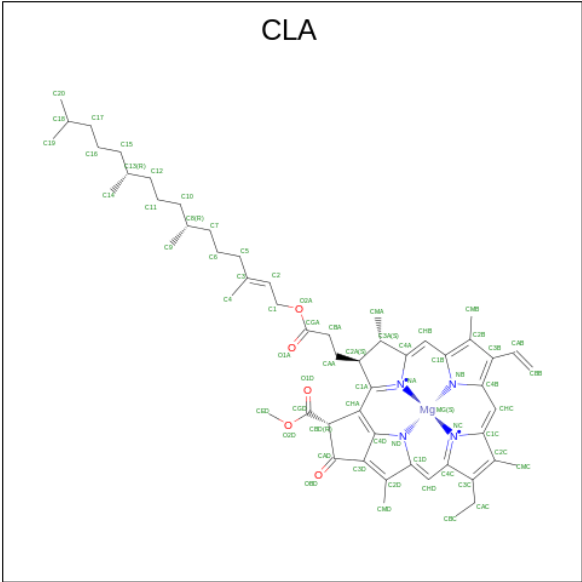
Mol	Chain	Residues	Atoms					AltConf	Trace
15	3	170	Total	C	N	O	S	0	0
			1303	845	219	232	7		

- Molecule 16 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			62	52	1	4	5	

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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 45	C 35	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 49	C 39	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 45	C 35	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 65	C 55	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	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 45	C 35	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 54	C 44	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 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 42	C 34	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
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 45	C 35	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 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 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

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Mol	Chain	Residues	Atoms					AltConf
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	F	1	Total 61	C 51	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 65	C 55	Mg 1	N 4	O 5	0
17	J	1	Total 58	C 48	Mg 1	N 4	O 5	0
17	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	K	1	Total 45	C 35	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 52	C 42	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 48	C 38	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 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 42	C 34	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 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 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
17	2	1	Total 50	C 40	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

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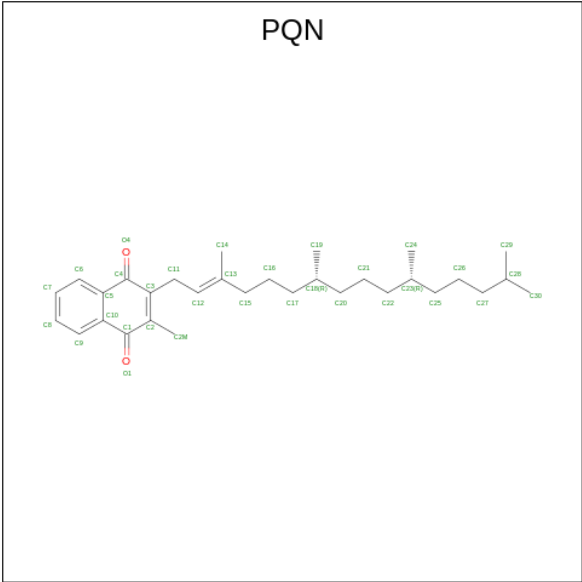
Mol	Chain	Residues	Atoms					AltConf
17	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	3	1	Total 63	C 53	Mg 1	N 4	O 5	0
17	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	3	1	Total 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 42	C 34	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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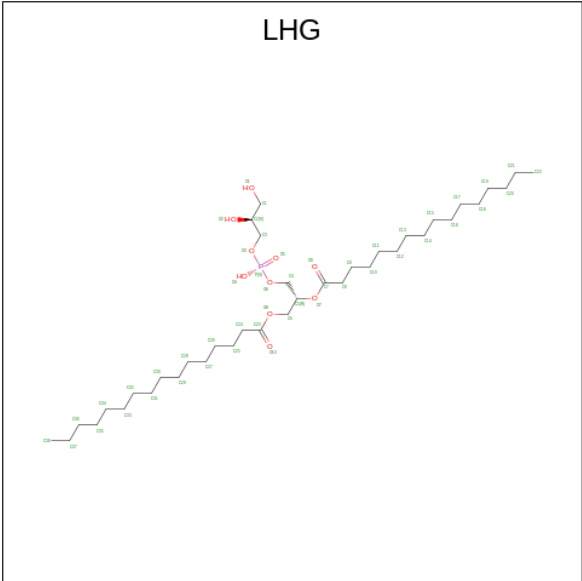
Mol	Chain	Residues	Atoms					AltConf
17	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			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
			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
			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	

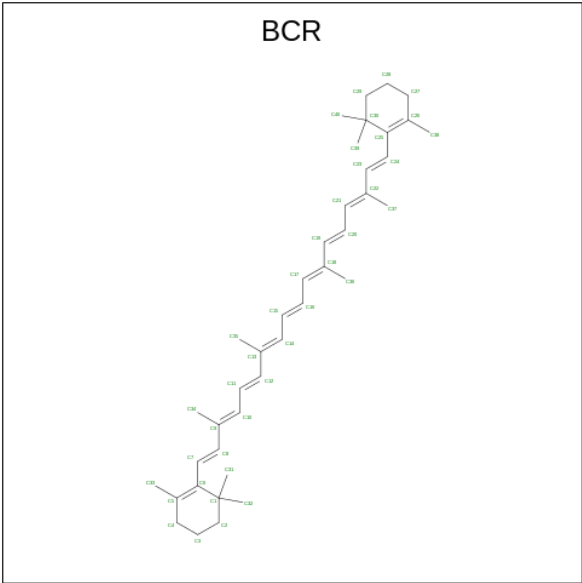
- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



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

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



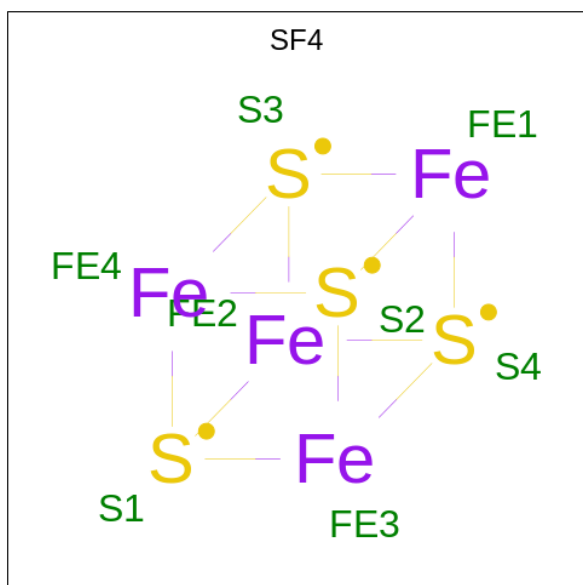
Mol	Chain	Residues	Atoms		AltConf
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	B	1	Total	C	0
			40	40	
20	B	1	Total	C	0
			40	40	
20	B	1	Total	C	0
			40	40	
20	B	1	Total	C	0
			40	40	
20	B	1	Total	C	0
			40	40	

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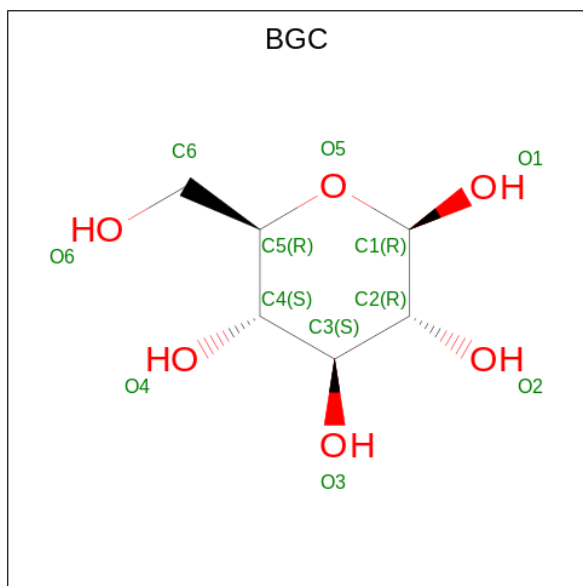
Mol	Chain	Residues	Atoms	AltConf
20	B	1	Total C 40 40	0
20	F	1	Total C 40 40	0
20	I	1	Total C 40 40	0
20	J	1	Total C 40 40	0
20	J	1	Total C 40 40	0
20	K	1	Total C 40 40	0
20	K	1	Total C 40 40	0
20	L	1	Total C 40 40	0
20	L	1	Total C 40 40	0
20	L	1	Total C 40 40	0
20	O	1	Total C 40 40	0

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



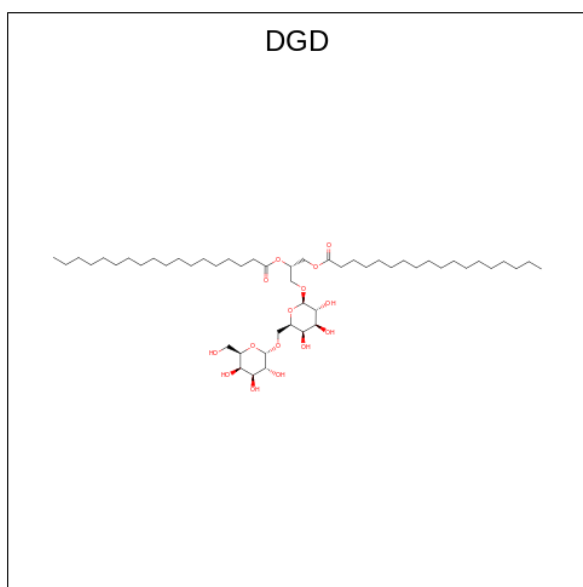
Mol	Chain	Residues	Atoms			AltConf
21	A	1	Total	Fe	S	0
			8	4	4	
21	C	1	Total	Fe	S	0
			8	4	4	
21	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 22 is beta-D-glucopyranose (three-letter code: BGC) (formula: C₆H₁₂O₆).



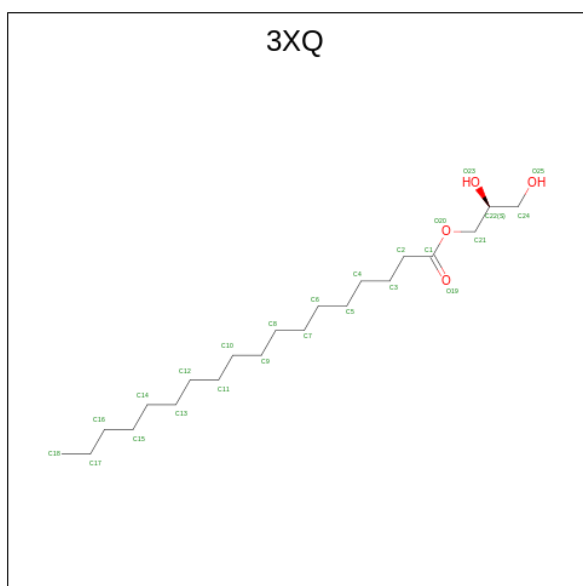
Mol	Chain	Residues	Atoms			AltConf
22	A	1	Total	C	O	0
			11	6	5	

- Molecule 23 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



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

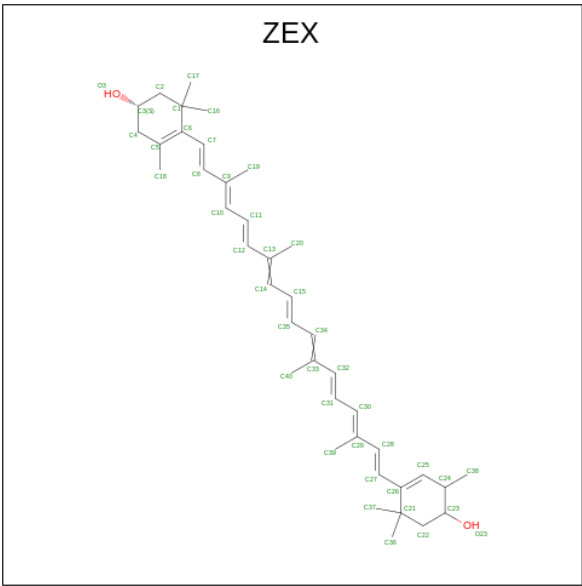
- Molecule 24 is (2S)-2,3-dihydroxypropyl octadecanoate (three-letter code: 3XQ) (formula: $C_{21}H_{42}O_4$).



Mol	Chain	Residues	Atoms			AltConf
24	J	1	Total	C	O	0
			25	21	4	

- Molecule 25 is (1R,2S)-4-{(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(4S)-4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl}-

2,5,5-trimethylcyclohex-3-en-1-ol (three-letter code: ZEX) (formula: C₄₀H₅₆O₂).



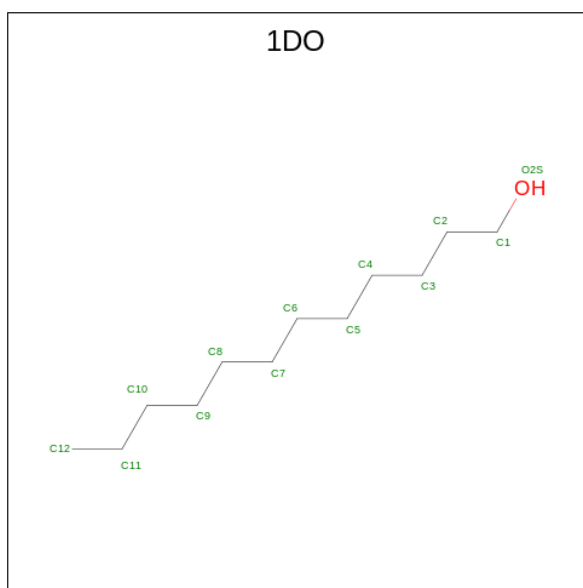
Mol	Chain	Residues	Atoms			AltConf
25	1	1	Total	C	O	0
			42	40	2	
25	1	1	Total	C	O	0
			42	40	2	
25	1	1	Total	C	O	0
			42	40	2	
25	1	1	Total	C	O	0
			42	40	2	
25	1	1	Total	C	O	0
			42	40	2	
25	2	1	Total	C	O	0
			42	40	2	
25	2	1	Total	C	O	0
			42	40	2	
25	2	1	Total	C	O	0
			42	40	2	
25	2	1	Total	C	O	0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

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Mol	Chain	Residues	Atoms			AltConf
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	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	

- Molecule 26 is 1-DODECANOL (three-letter code: 1DO) (formula: $C_{12}H_{26}O$).

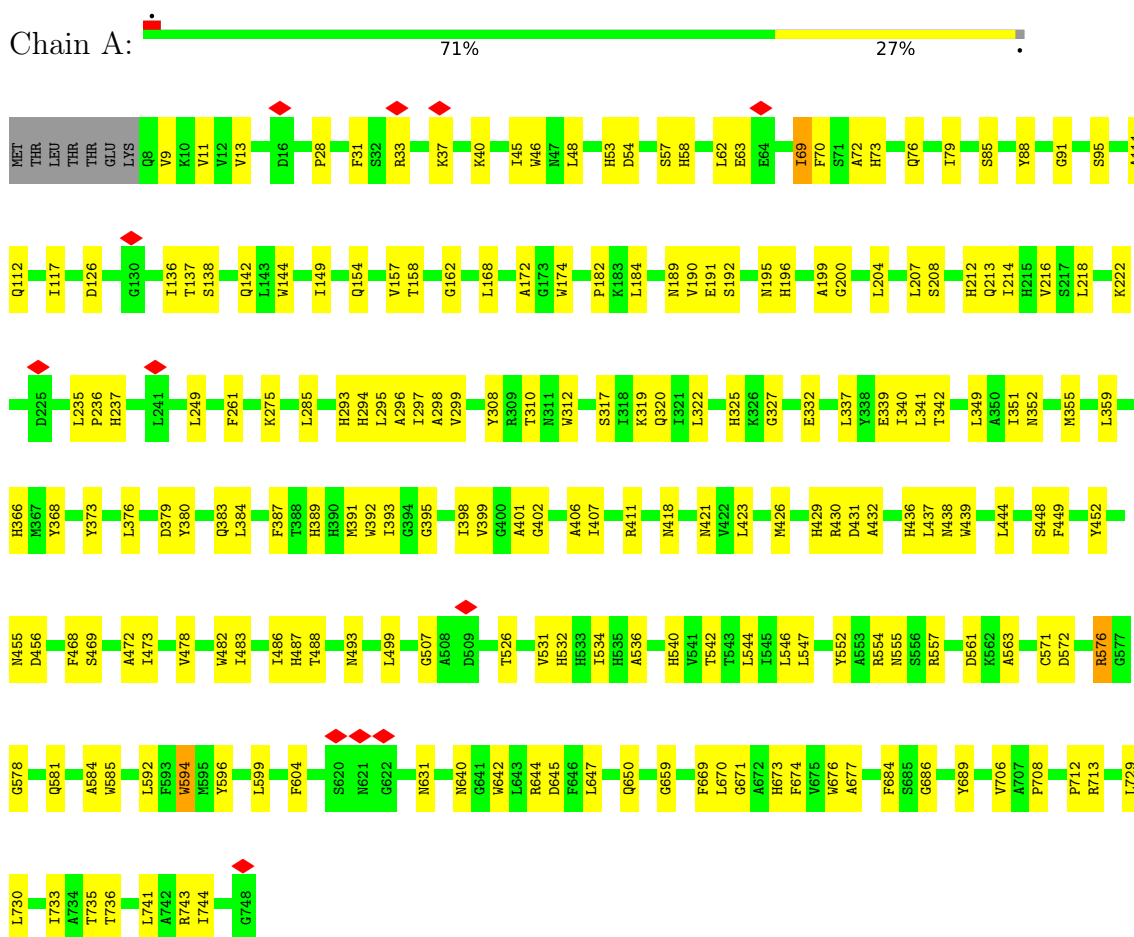


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
26	3	1	13	12	1	0

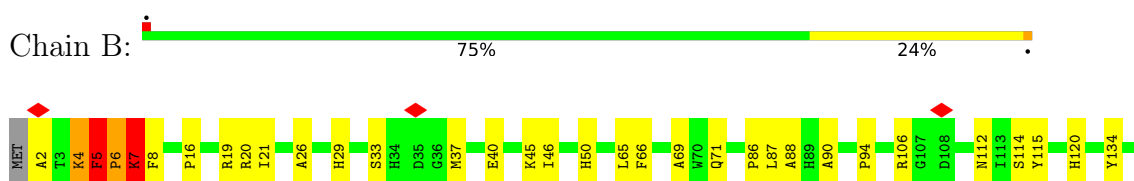
3 Residue-property plots

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

• Molecule 1: PsaA



• Molecule 2: PsaB

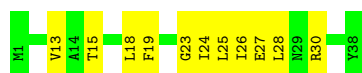




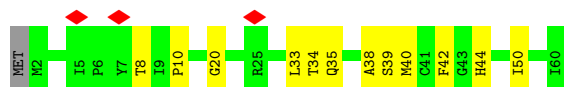
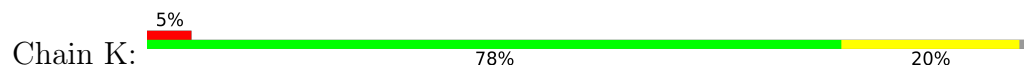
- Molecule 7: PsaI



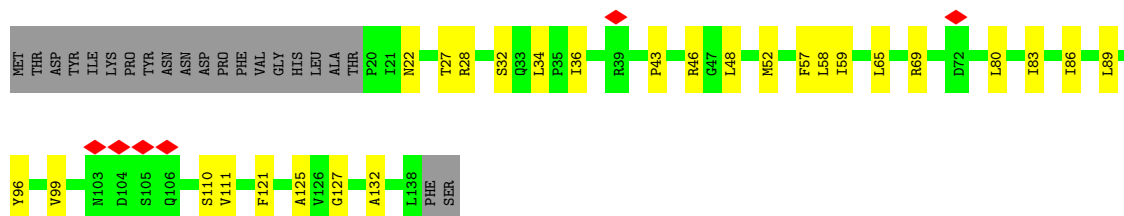
- Molecule 8: PsaJ



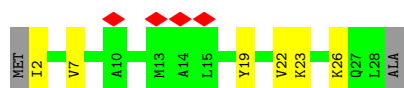
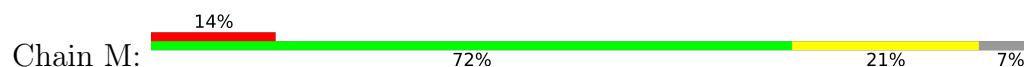
- Molecule 9: PsaK



- Molecule 10: PsaL

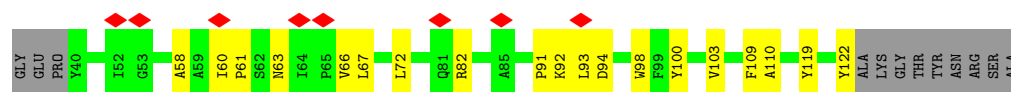


- Molecule 11: PsaM

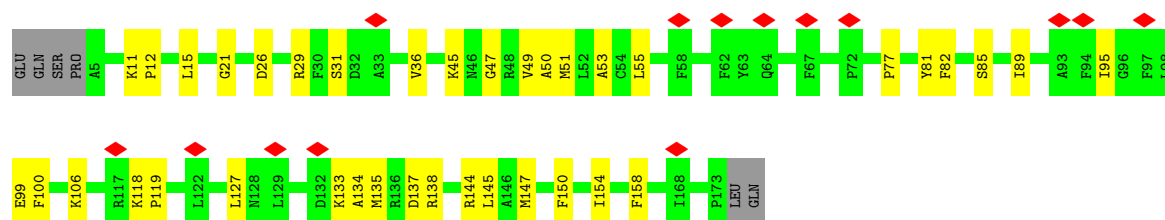
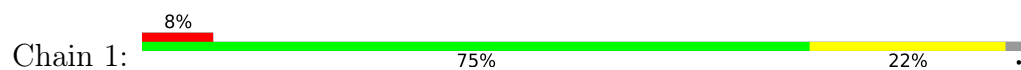


- Molecule 12: PsaO

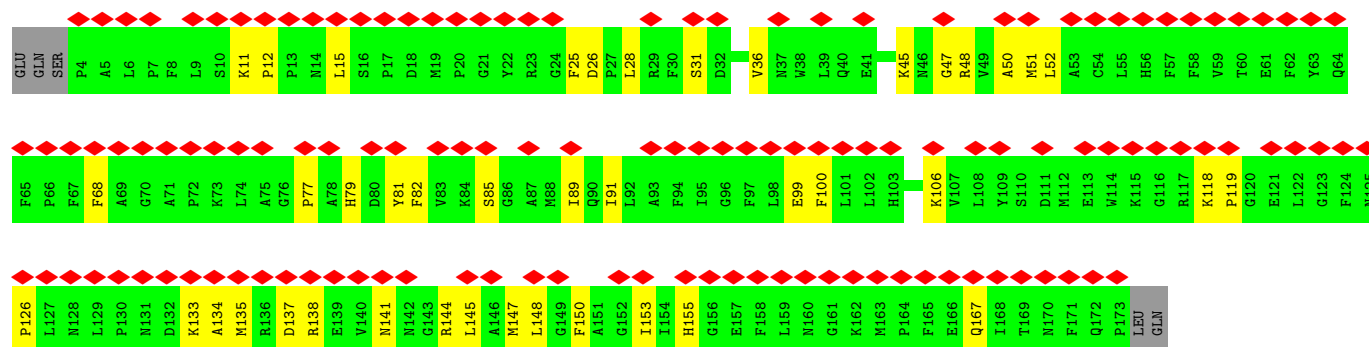


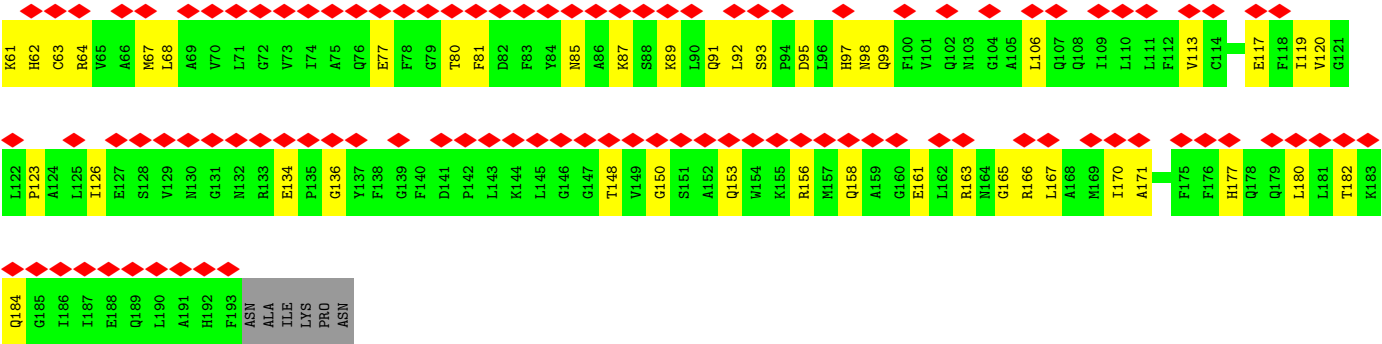


• Molecule 13: Lhcr1

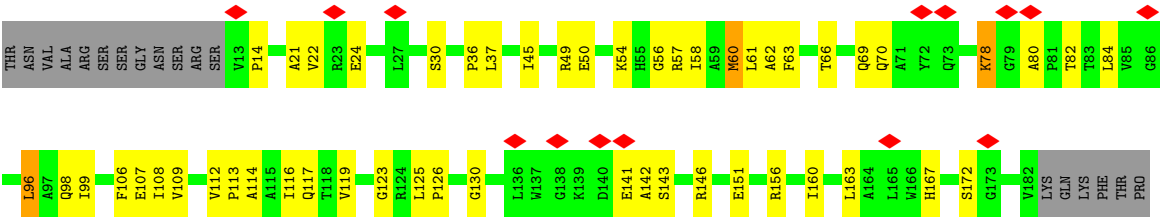


• Molecule 13: Lhcr1





• Molecule 15: Lhcr3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	124279	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.17	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.653	Depositor
Minimum map value	-0.170	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.0562	Depositor
Map size (\AA)	294.0, 294.0, 294.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, 3XQ, BGC, BCR, ZEX, PQN, DGD, CLA, 1DO, CL0, SF4

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	0.58	1/5985 (0.0%)	0.64	1/8158 (0.0%)
2	B	0.56	1/6028 (0.0%)	0.66	3/8236 (0.0%)
3	C	0.54	0/607	0.60	0/822
4	D	0.40	0/969	0.59	0/1307
5	E	0.49	0/502	0.56	0/680
6	F	0.44	0/1296	0.63	0/1760
7	I	0.40	0/235	0.73	1/321 (0.3%)
8	J	0.48	0/321	0.62	0/437
9	K	0.35	0/433	0.63	0/588
10	L	0.36	0/919	0.57	0/1247
11	M	0.29	0/205	0.60	0/277
12	O	0.36	0/664	0.66	0/913
13	1	0.36	0/1395	0.65	0/1884
13	4	0.36	0/1403	0.65	0/1895
14	2	0.38	0/1407	0.67	0/1898
14	5	0.38	0/1407	0.67	0/1898
15	3	0.41	1/1337 (0.1%)	0.69	2/1817 (0.1%)
All	All	0.49	3/25113 (0.0%)	0.64	7/34138 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
14	2	0	2
14	5	0	2
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	594	TRP	CB-CG	-6.51	1.38	1.50
2	B	580	TRP	CB-CG	-5.68	1.40	1.50
15	3	80	ALA	C-N	5.42	1.44	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	572	ASP	CB-CG-OD1	8.16	125.64	118.30
2	B	514	ASP	CB-CG-OD1	7.40	124.96	118.30
1	A	571	CYS	CA-CB-SG	-6.53	102.25	114.00
7	I	16	LEU	CA-CB-CG	5.66	128.31	115.30
15	3	96	LEU	CA-CB-CG	5.59	128.16	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	2	136	GLY	Peptide
14	2	98	ASN	Peptide
14	5	136	GLY	Peptide
14	5	98	ASN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5798	0	5727	206	0
2	B	5819	0	5648	166	0
3	C	597	0	584	21	0
4	D	950	0	943	91	0
5	E	493	0	509	5	0
6	F	1263	0	1236	13	0
7	I	230	0	253	8	0
8	J	312	0	327	15	0
9	K	428	0	464	11	0
10	L	900	0	931	21	0
11	M	204	0	226	5	0
12	O	641	0	650	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	1	1351	0	1322	28	0
13	4	1358	0	1330	33	0
14	2	1371	0	1362	43	0
14	5	1371	0	1362	41	0
15	3	1303	0	1305	46	0
16	A	65	0	71	59	0
17	1	565	0	443	19	0
17	2	600	0	466	26	0
17	3	565	0	440	27	0
17	4	505	0	384	23	0
17	5	600	0	463	26	0
17	A	2310	0	2337	152	0
17	B	2469	0	2499	158	0
17	F	147	0	123	4	0
17	J	165	0	158	11	0
17	K	87	0	64	2	0
17	L	172	0	164	6	0
17	O	188	0	144	4	0
18	A	33	0	46	4	0
18	B	33	0	46	3	0
19	A	89	0	127	6	0
20	A	160	0	224	15	0
20	B	280	0	392	24	0
20	F	40	0	56	2	0
20	I	40	0	56	4	0
20	J	80	0	112	6	0
20	K	80	0	112	10	0
20	L	120	0	168	11	0
20	O	40	0	56	5	0
21	A	8	0	0	0	0
21	C	16	0	0	2	0
22	A	11	0	9	0	0
23	B	66	0	96	5	0
24	J	25	0	0	0	0
25	1	210	0	280	19	0
25	2	168	0	224	11	0
25	3	252	0	336	20	0
25	4	252	0	336	18	0
25	5	168	0	224	16	0
26	3	13	0	25	1	0
All	All	35011	0	34860	1041	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 15.

The worst 5 of 1041 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:TRP:CD2	16:A:801:CL0:H56	1.25	1.63
4:D:82:LYS:HE3	4:D:95:LEU:CA	1.36	1.50
1:A:642:TRP:CE2	16:A:801:CL0:H56	1.50	1.45
4:D:82:LYS:NZ	4:D:95:LEU:HB2	1.26	1.44
4:D:82:LYS:CE	4:D:95:LEU:C	1.87	1.43

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%)	681 (92%)	57 (8%)	1 (0%)	48	78
2	B	729/732 (100%)	654 (90%)	72 (10%)	3 (0%)	30	61
3	C	78/81 (96%)	68 (87%)	10 (13%)	0	100	100
4	D	117/139 (84%)	102 (87%)	12 (10%)	3 (3%)	4	25
5	E	59/94 (63%)	52 (88%)	7 (12%)	0	100	100
6	F	152/185 (82%)	134 (88%)	18 (12%)	0	100	100
7	I	29/32 (91%)	26 (90%)	3 (10%)	0	100	100
8	J	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
9	K	57/60 (95%)	51 (90%)	6 (10%)	0	100	100
10	L	117/140 (84%)	106 (91%)	11 (9%)	0	100	100
11	M	25/29 (86%)	23 (92%)	2 (8%)	0	100	100
12	O	81/155 (52%)	67 (83%)	14 (17%)	0	100	100
13	1	167/175 (95%)	130 (78%)	36 (22%)	1 (1%)	22	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	4	168/175 (96%)	131 (78%)	36 (21%)	1 (1%)	22	53
14	2	173/199 (87%)	130 (75%)	43 (25%)	0	100	100
14	5	173/199 (87%)	130 (75%)	43 (25%)	0	100	100
15	3	168/188 (89%)	143 (85%)	25 (15%)	0	100	100
All	All	3068/3369 (91%)	2663 (87%)	396 (13%)	9 (0%)	38	66

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	5	PHE
2	B	7	LYS
4	D	96	HIS
4	D	100	GLY
2	B	6	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	598/605 (99%)	595 (100%)	3 (0%)	86	92
2	B	598/599 (100%)	595 (100%)	3 (0%)	86	92
3	C	66/67 (98%)	66 (100%)	0	100	100
4	D	101/118 (86%)	99 (98%)	2 (2%)	50	69
5	E	58/87 (67%)	58 (100%)	0	100	100
6	F	136/162 (84%)	136 (100%)	0	100	100
7	I	26/27 (96%)	26 (100%)	0	100	100
8	J	34/34 (100%)	34 (100%)	0	100	100
9	K	48/49 (98%)	48 (100%)	0	100	100
10	L	94/113 (83%)	93 (99%)	1 (1%)	70	81
11	M	22/23 (96%)	22 (100%)	0	100	100
12	O	64/121 (53%)	63 (98%)	1 (2%)	58	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	1	139/145 (96%)	138 (99%)	1 (1%)	81	89
13	4	140/145 (97%)	139 (99%)	1 (1%)	81	89
14	2	142/160 (89%)	141 (99%)	1 (1%)	81	89
14	5	142/160 (89%)	141 (99%)	1 (1%)	81	89
15	3	132/148 (89%)	131 (99%)	1 (1%)	79	87
All	All	2540/2763 (92%)	2525 (99%)	15 (1%)	82	91

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	98	LYS
13	4	11	LYS
10	L	22	ASN
14	5	85	ASN
14	2	85	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
14	2	85	ASN
15	3	98	GLN
14	5	164	ASN
14	5	85	ASN
10	L	22	ASN

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

215 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	B	836	-	65,73,73	1.48	10 (15%)	76,113,113	1.54	11 (14%)
17	CLA	A	808	-	55,63,73	1.57	11 (20%)	64,101,113	1.58	10 (15%)
17	CLA	3	213	-	51,59,73	1.61	9 (17%)	59,96,113	1.61	8 (13%)
17	CLA	A	830	-	56,64,73	1.52	9 (16%)	65,102,113	1.61	8 (12%)
20	BCR	B	846	-	41,41,41	1.18	2 (4%)	56,56,56	1.32	6 (10%)
17	CLA	J	103	-	42,50,73	1.73	10 (23%)	48,85,113	1.77	8 (16%)
16	CL0	A	801	-	65,73,73	2.87	24 (36%)	76,113,113	3.22	39 (51%)
20	BCR	B	805	-	41,41,41	1.27	3 (7%)	56,56,56	1.48	10 (17%)
25	ZEX	5	614	-	42,43,43	5.17	20 (47%)	55,60,60	5.13	32 (58%)
17	CLA	B	803	-	65,73,73	1.44	10 (15%)	76,113,113	1.64	10 (13%)
17	CLA	L	202	10	57,65,73	1.58	10 (17%)	66,103,113	1.47	6 (9%)
17	CLA	2	608	-	50,58,73	1.64	8 (16%)	58,95,113	1.90	11 (18%)
17	CLA	4	606	-	45,53,73	1.74	8 (17%)	52,89,113	1.76	6 (11%)
17	CLA	B	808	-	65,73,73	1.46	10 (15%)	76,113,113	1.64	17 (22%)
17	CLA	A	807	1	65,73,73	1.48	12 (18%)	76,113,113	1.68	15 (19%)
17	CLA	B	833	-	45,53,73	1.77	10 (22%)	52,89,113	1.71	11 (21%)
17	CLA	A	831	-	65,73,73	1.44	10 (15%)	76,113,113	1.59	10 (13%)
17	CLA	O	204	-	50,58,73	1.65	7 (14%)	58,95,113	1.61	10 (17%)
17	CLA	1	601	-	48,56,73	1.67	10 (20%)	55,92,113	2.27	13 (23%)
17	CLA	5	603	-	65,73,73	1.47	10 (15%)	76,113,113	1.59	13 (17%)
25	ZEX	4	614	-	42,43,43	5.17	19 (45%)	55,60,60	4.78	29 (52%)
17	CLA	4	605	-	41,50,73	1.83	5 (12%)	46,85,113	1.77	7 (15%)
17	CLA	A	809	-	65,73,73	1.43	11 (16%)	76,113,113	1.60	11 (14%)
20	BCR	A	843	-	41,41,41	1.23	3 (7%)	56,56,56	1.35	7 (12%)
17	CLA	A	815	-	62,70,73	1.46	10 (16%)	72,109,113	1.55	8 (11%)
17	CLA	5	610	-	45,53,73	1.71	7 (15%)	52,89,113	1.75	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	4	603	-	45,53,73	1.69	8 (17%)	52,89,113	1.79	9 (17%)
20	BCR	L	206	-	41,41,41	1.12	2 (4%)	56,56,56	1.25	6 (10%)
25	ZEX	3	201	-	42,43,43	5.19	19 (45%)	55,60,60	5.28	30 (54%)
25	ZEX	3	217	-	42,43,43	5.10	20 (47%)	55,60,60	4.94	27 (49%)
17	CLA	B	842	-	65,73,73	1.47	11 (16%)	76,113,113	1.52	7 (9%)
17	CLA	3	211	-	42,50,73	1.78	9 (21%)	48,85,113	1.76	9 (18%)
17	CLA	5	613	-	43,52,73	1.77	5 (11%)	51,87,113	1.67	9 (17%)
17	CLA	A	838	-	65,73,73	1.43	10 (15%)	76,113,113	1.55	9 (11%)
19	LHG	A	842	-	39,39,48	0.76	1 (2%)	42,45,54	1.32	6 (14%)
17	CLA	A	818	-	45,53,73	1.73	10 (22%)	52,89,113	1.98	12 (23%)
25	ZEX	3	216	-	42,43,43	5.09	19 (45%)	55,60,60	5.10	31 (56%)
17	CLA	2	605	-	45,53,73	1.73	10 (22%)	52,89,113	1.83	10 (19%)
17	CLA	4	609	-	41,49,73	1.83	5 (12%)	47,84,113	1.79	8 (17%)
20	BCR	J	105	-	41,41,41	1.32	3 (7%)	56,56,56	1.33	7 (12%)
17	CLA	1	604	-	45,53,73	1.66	8 (17%)	52,89,113	1.72	8 (15%)
17	CLA	B	823	-	45,53,73	1.74	10 (22%)	52,89,113	1.70	8 (15%)
17	CLA	1	603	-	45,53,73	1.77	10 (22%)	52,89,113	1.65	8 (15%)
17	CLA	A	827	-	65,73,73	1.57	10 (15%)	76,113,113	1.58	14 (18%)
17	CLA	B	801	-	65,73,73	1.41	9 (13%)	76,113,113	2.03	14 (18%)
17	CLA	2	609	-	41,49,73	1.78	9 (21%)	47,84,113	1.81	9 (19%)
20	BCR	J	104	-	41,41,41	1.28	3 (7%)	56,56,56	1.42	9 (16%)
17	CLA	B	839	-	65,73,73	1.53	11 (16%)	76,113,113	1.51	9 (11%)
17	CLA	1	610	-	45,53,73	1.76	8 (17%)	52,89,113	1.74	10 (19%)
17	CLA	B	817	-	45,53,73	1.67	10 (22%)	52,89,113	1.78	7 (13%)
17	CLA	3	209	-	52,60,73	1.56	8 (15%)	60,97,113	1.70	9 (15%)
17	CLA	4	607	-	45,53,73	1.71	7 (15%)	52,89,113	1.83	10 (19%)
17	CLA	5	608	-	45,53,73	1.74	9 (20%)	52,89,113	1.88	10 (19%)
17	CLA	O	201	-	52,60,73	1.59	8 (15%)	60,97,113	1.67	9 (15%)
17	CLA	1	605	-	41,50,73	1.83	6 (14%)	46,85,113	1.67	8 (17%)
17	CLA	B	843	-	65,73,73	1.44	8 (12%)	76,113,113	1.47	11 (14%)
17	CLA	B	810	-	65,73,73	1.41	10 (15%)	76,113,113	1.50	10 (13%)
17	CLA	L	204	-	50,58,73	1.63	10 (20%)	58,95,113	1.63	9 (15%)
17	CLA	B	835	-	65,73,73	1.54	10 (15%)	76,113,113	1.54	8 (10%)
17	CLA	A	848	-	65,73,73	1.46	11 (16%)	76,113,113	2.11	18 (23%)
17	CLA	B	821	-	60,68,73	1.47	11 (18%)	70,107,113	1.71	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	4	604	-	45,53,73	1.77	7 (15%)	52,89,113	1.63	9 (17%)
17	CLA	K	103	-	42,50,73	1.77	9 (21%)	48,85,113	1.81	8 (16%)
17	CLA	3	204	-	45,53,73	1.73	8 (17%)	52,89,113	1.71	9 (17%)
17	CLA	F	301	-	61,69,73	1.48	10 (16%)	71,108,113	1.53	8 (11%)
25	ZEX	4	616	-	42,43,43	5.04	19 (45%)	55,60,60	5.19	32 (58%)
17	CLA	A	821	-	51,59,73	1.65	9 (17%)	59,96,113	1.60	8 (13%)
17	CLA	3	203	-	63,71,73	1.45	9 (14%)	73,110,113	1.74	9 (12%)
17	CLA	5	607	-	45,53,73	1.96	9 (20%)	52,89,113	1.74	12 (23%)
17	CLA	5	612	-	45,53,73	1.74	6 (13%)	52,89,113	1.84	9 (17%)
17	CLA	A	805	-	65,73,73	1.44	9 (13%)	76,113,113	1.70	13 (17%)
17	CLA	A	828	-	65,73,73	1.62	13 (20%)	76,113,113	1.86	19 (25%)
17	CLA	A	817	-	65,73,73	1.51	11 (16%)	76,113,113	1.56	11 (14%)
25	ZEX	1	614	-	42,43,43	5.03	19 (45%)	55,60,60	5.77	30 (54%)
17	CLA	1	609	-	41,49,73	1.75	8 (19%)	47,84,113	1.88	9 (19%)
17	CLA	2	601	-	45,53,73	1.72	8 (17%)	52,89,113	1.81	9 (17%)
20	BCR	K	104	-	41,41,41	1.15	2 (4%)	56,56,56	1.35	7 (12%)
17	CLA	A	829	-	50,58,73	1.70	10 (20%)	58,95,113	1.53	10 (17%)
20	BCR	I	101	-	41,41,41	1.19	2 (4%)	56,56,56	1.40	8 (14%)
21	SF4	C	101	3	0,12,12	-	-	-	-	-
20	BCR	B	849	-	41,41,41	1.27	3 (7%)	56,56,56	1.57	10 (17%)
25	ZEX	2	616	-	42,43,43	5.27	20 (47%)	55,60,60	4.77	29 (52%)
25	ZEX	2	617	-	42,43,43	4.80	19 (45%)	55,60,60	5.29	29 (52%)
25	ZEX	3	218	-	42,43,43	5.43	20 (47%)	55,60,60	4.52	33 (60%)
25	ZEX	1	616	-	42,43,43	5.05	19 (45%)	55,60,60	5.10	32 (58%)
25	ZEX	3	215	-	42,43,43	4.97	19 (45%)	55,60,60	5.27	33 (60%)
17	CLA	2	604	-	42,50,73	1.71	10 (23%)	48,85,113	1.90	7 (14%)
21	SF4	C	102	-	0,12,12	-	-	-	-	-
17	CLA	B	819	-	55,63,73	1.50	9 (16%)	64,101,113	1.65	8 (12%)
17	CLA	B	825	-	43,51,73	1.77	11 (25%)	49,86,113	1.67	9 (18%)
17	CLA	A	814	-	45,53,73	1.75	8 (17%)	52,89,113	1.79	12 (23%)
17	CLA	B	806	-	65,73,73	1.52	12 (18%)	76,113,113	1.87	14 (18%)
17	CLA	A	803	-	65,73,73	1.49	12 (18%)	76,113,113	1.77	13 (17%)
17	CLA	A	837	-	65,73,73	1.41	8 (12%)	76,113,113	1.56	9 (11%)
17	CLA	1	606	-	45,53,73	1.72	10 (22%)	52,89,113	1.67	9 (17%)
17	CLA	1	602	-	59,67,73	1.45	10 (16%)	68,105,113	1.70	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	BCR	F	304	-	41,41,41	1.18	2 (4%)	56,56,56	1.39	10 (17%)
17	CLA	B	816	-	65,73,73	1.41	10 (15%)	76,113,113	1.56	12 (15%)
17	CLA	B	809	-	65,73,73	1.50	11 (16%)	76,113,113	1.55	10 (13%)
17	CLA	B	829	-	65,73,73	1.46	10 (15%)	76,113,113	1.54	9 (11%)
17	CLA	A	812	-	45,53,73	1.65	9 (20%)	52,89,113	1.88	10 (19%)
20	BCR	A	845	-	41,41,41	1.34	3 (7%)	56,56,56	1.43	9 (16%)
25	ZEX	5	617	-	42,43,43	4.98	19 (45%)	55,60,60	5.31	26 (47%)
17	CLA	A	823	-	65,73,73	1.46	10 (15%)	76,113,113	1.51	14 (18%)
25	ZEX	2	615	-	42,43,43	4.79	18 (42%)	55,60,60	5.10	31 (56%)
17	CLA	1	612	-	45,53,73	1.75	9 (20%)	52,89,113	1.73	9 (17%)
17	CLA	B	822	-	65,73,73	1.49	11 (16%)	76,113,113	1.49	7 (9%)
17	CLA	4	601	-	48,56,73	1.68	7 (14%)	55,92,113	1.84	11 (20%)
17	CLA	B	811	-	65,73,73	1.43	12 (18%)	76,113,113	1.83	15 (19%)
24	3XQ	J	106	-	24,24,24	0.60	1 (4%)	25,25,25	1.13	0
26	1DO	3	219	22	12,12,12	0.26	0	11,11,11	0.85	0
17	CLA	A	832	-	65,73,73	1.40	10 (15%)	76,113,113	1.73	13 (17%)
17	CLA	A	839	-	65,73,73	1.46	12 (18%)	76,113,113	1.59	9 (11%)
25	ZEX	1	613	-	42,43,43	4.99	18 (42%)	55,60,60	5.22	32 (58%)
17	CLA	B	812	-	65,73,73	1.50	12 (18%)	76,113,113	1.55	12 (15%)
17	CLA	B	826	-	55,63,73	1.60	10 (18%)	64,101,113	1.50	9 (14%)
18	PQN	B	844	-	34,34,34	2.78	9 (26%)	42,45,45	2.32	7 (16%)
20	BCR	B	847	-	41,41,41	1.17	3 (7%)	56,56,56	1.34	8 (14%)
25	ZEX	1	615	-	42,43,43	4.86	19 (45%)	55,60,60	5.26	33 (60%)
17	CLA	A	833	-	65,73,73	1.44	10 (15%)	76,113,113	1.58	10 (13%)
17	CLA	A	836	-	65,73,73	1.48	11 (16%)	76,113,113	1.64	13 (17%)
17	CLA	B	827	-	65,73,73	1.47	11 (16%)	76,113,113	1.66	12 (15%)
17	CLA	B	824	-	46,54,73	1.70	10 (21%)	53,90,113	1.68	8 (15%)
17	CLA	4	611	-	45,53,73	1.81	7 (15%)	52,89,113	1.65	9 (17%)
17	CLA	B	820	-	59,67,73	1.57	10 (16%)	68,105,113	1.60	11 (16%)
17	CLA	F	303	-	41,49,73	1.74	9 (21%)	47,84,113	1.82	8 (17%)
17	CLA	5	605	-	45,53,73	1.75	6 (13%)	52,89,113	1.69	8 (15%)
25	ZEX	1	617	-	42,43,43	4.91	18 (42%)	55,60,60	5.13	29 (52%)
20	BCR	O	202	-	41,41,41	1.34	3 (7%)	56,56,56	1.53	11 (19%)
17	CLA	L	203	-	65,73,73	1.43	10 (15%)	76,113,113	1.45	7 (9%)
17	CLA	5	604	-	45,53,73	1.74	7 (15%)	52,89,113	1.72	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	802	-	55,63,73	1.55	10 (18%)	64,101,113	1.86	10 (15%)
17	CLA	1	608	-	60,68,73	1.51	10 (16%)	70,107,113	1.54	9 (12%)
17	CLA	2	603	-	45,53,73	1.67	9 (20%)	52,89,113	1.80	7 (13%)
20	BCR	B	845	-	41,41,41	1.06	2 (4%)	56,56,56	1.25	8 (14%)
21	SF4	A	847	-	0,12,12	-	-	-	-	-
17	CLA	A	825	-	65,73,73	1.48	10 (15%)	76,113,113	1.62	10 (13%)
20	BCR	K	101	-	41,41,41	1.23	3 (7%)	56,56,56	1.36	9 (16%)
17	CLA	B	804	-	65,73,73	1.55	10 (15%)	76,113,113	1.69	19 (25%)
17	CLA	K	102	-	45,53,73	1.69	10 (22%)	52,89,113	1.70	9 (17%)
17	CLA	3	212	-	46,54,73	1.68	7 (15%)	53,90,113	1.65	7 (13%)
19	LHG	A	841	-	48,48,48	0.69	1 (2%)	51,54,54	1.27	6 (11%)
25	ZEX	5	615	-	42,43,43	5.32	20 (47%)	55,60,60	4.94	31 (56%)
17	CLA	A	804	-	65,73,73	1.44	9 (13%)	76,113,113	1.68	9 (11%)
17	CLA	A	820	-	49,57,73	1.64	11 (22%)	55,93,113	1.77	9 (16%)
17	CLA	B	818	-	42,50,73	1.81	10 (23%)	48,85,113	1.83	9 (18%)
17	CLA	J	102	-	58,66,73	1.52	11 (18%)	67,104,113	1.61	8 (11%)
17	CLA	B	838	-	60,68,73	1.56	10 (16%)	70,107,113	1.62	11 (15%)
17	CLA	2	611	-	45,53,73	1.72	10 (22%)	52,89,113	1.88	10 (19%)
17	CLA	3	208	-	45,53,73	1.78	10 (22%)	52,89,113	1.67	8 (15%)
20	BCR	L	205	-	41,41,41	1.12	2 (4%)	56,56,56	1.56	9 (16%)
17	CLA	2	602	-	65,73,73	1.50	10 (15%)	76,113,113	1.53	8 (10%)
17	CLA	A	822	-	55,63,73	1.58	11 (20%)	64,101,113	1.65	9 (14%)
17	CLA	A	811	-	65,73,73	1.46	11 (16%)	76,113,113	1.53	10 (13%)
17	CLA	3	205	-	45,53,73	1.78	10 (22%)	52,89,113	1.79	9 (17%)
17	CLA	4	610	-	45,53,73	1.78	6 (13%)	52,89,113	1.72	8 (15%)
20	BCR	A	846	-	41,41,41	1.33	2 (4%)	56,56,56	1.39	9 (16%)
23	DGD	B	851	-	67,67,67	1.03	3 (4%)	81,81,81	1.47	11 (13%)
25	ZEX	4	613	-	42,43,43	5.05	20 (47%)	55,60,60	5.08	31 (56%)
25	ZEX	4	612	-	42,43,43	5.10	19 (45%)	55,60,60	5.09	31 (56%)
17	CLA	5	606	-	45,53,73	1.81	10 (22%)	52,89,113	2.45	22 (42%)
17	CLA	2	607	-	45,53,73	1.71	10 (22%)	52,89,113	1.77	9 (17%)
17	CLA	5	601	-	45,53,73	1.76	6 (13%)	52,89,113	1.71	8 (15%)
25	ZEX	4	615	-	42,43,43	5.16	19 (45%)	55,60,60	4.81	28 (50%)
17	CLA	A	806	1	65,73,73	1.41	11 (16%)	76,113,113	1.56	10 (13%)
17	CLA	F	302	-	45,53,73	1.72	9 (20%)	52,89,113	1.75	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	BCR	L	201	-	41,41,41	1.30	3 (7%)	56,56,56	1.35	9 (16%)
20	BCR	B	850	-	41,41,41	1.26	3 (7%)	56,56,56	1.53	9 (16%)
17	CLA	B	840	-	47,55,73	1.62	9 (19%)	54,91,113	1.81	8 (14%)
17	CLA	1	607	-	45,53,73	1.69	8 (17%)	52,89,113	1.97	10 (19%)
17	CLA	B	814	-	54,62,73	1.66	9 (16%)	67,100,113	1.90	12 (17%)
17	CLA	B	830	-	65,73,73	1.43	11 (16%)	76,113,113	1.49	11 (14%)
17	CLA	A	834	-	45,53,73	1.77	9 (20%)	52,89,113	1.72	8 (15%)
17	CLA	A	835	-	51,59,73	1.56	9 (17%)	59,96,113	1.81	9 (15%)
17	CLA	B	807	-	45,53,73	1.70	10 (22%)	52,89,113	1.81	8 (15%)
17	CLA	3	207	-	45,53,73	1.70	9 (20%)	52,89,113	1.79	9 (17%)
17	CLA	5	602	-	45,53,73	1.78	6 (13%)	52,89,113	1.82	10 (19%)
17	CLA	5	609	-	41,49,73	1.88	8 (19%)	47,84,113	2.11	16 (34%)
17	CLA	2	610	-	42,50,73	1.77	10 (23%)	48,85,113	1.84	8 (16%)
17	CLA	3	206	-	45,53,73	1.84	9 (20%)	52,89,113	1.81	12 (23%)
25	ZEX	3	214	-	42,43,43	5.06	19 (45%)	55,60,60	5.27	30 (54%)
17	CLA	2	606	-	45,53,73	1.72	10 (22%)	52,89,113	1.68	9 (17%)
20	BCR	A	844	-	41,41,41	1.18	2 (4%)	56,56,56	1.42	10 (17%)
25	ZEX	5	616	-	42,43,43	5.23	20 (47%)	55,60,60	5.04	28 (50%)
17	CLA	2	613	-	45,53,73	1.75	9 (20%)	52,89,113	1.66	9 (17%)
17	CLA	3	210	-	41,49,73	1.77	7 (17%)	47,84,113	1.87	10 (21%)
17	CLA	1	611	-	45,53,73	1.70	10 (22%)	52,89,113	2.13	10 (19%)
17	CLA	4	608	-	45,53,73	1.79	9 (20%)	52,89,113	1.80	9 (17%)
20	BCR	B	848	-	41,41,41	1.19	2 (4%)	56,56,56	1.41	9 (16%)
17	CLA	4	602	-	59,67,73	1.51	9 (15%)	68,105,113	1.70	10 (14%)
17	CLA	B	837	-	45,53,73	1.78	10 (22%)	52,89,113	1.69	7 (13%)
17	CLA	A	824	-	55,63,73	1.55	11 (20%)	64,101,113	1.76	12 (18%)
17	CLA	O	205	-	45,53,73	1.76	8 (17%)	52,89,113	1.62	9 (17%)
17	CLA	3	202	-	45,53,73	1.71	7 (15%)	52,89,113	1.70	9 (17%)
17	CLA	2	612	-	45,53,73	1.74	10 (22%)	52,89,113	1.74	7 (13%)
17	CLA	B	832	-	65,73,73	1.54	12 (18%)	76,113,113	1.91	14 (18%)
17	CLA	B	831	-	65,73,73	1.56	9 (13%)	76,113,113	1.52	10 (13%)
17	CLA	B	834	-	43,51,73	1.77	10 (23%)	49,86,113	1.80	10 (20%)
17	CLA	J	101	-	65,73,73	1.44	10 (15%)	76,113,113	1.64	10 (13%)
17	CLA	B	815	-	55,63,73	1.56	9 (16%)	64,101,113	1.56	8 (12%)
18	PQN	A	840	-	34,34,34	2.77	10 (29%)	42,45,45	2.16	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	819	-	65,73,73	1.51	11 (16%)	76,113,113	1.71	9 (11%)
25	ZEX	4	617	-	42,43,43	5.16	19 (45%)	55,60,60	5.04	30 (54%)
17	CLA	B	828	-	65,73,73	1.45	10 (15%)	76,113,113	1.62	10 (13%)
25	ZEX	2	614	-	42,43,43	4.94	19 (45%)	55,60,60	5.25	33 (60%)
17	CLA	B	841	-	65,73,73	1.44	10 (15%)	76,113,113	1.56	9 (11%)
17	CLA	A	826	-	65,73,73	1.46	10 (15%)	76,113,113	1.70	10 (13%)
17	CLA	A	810	-	54,62,73	1.58	10 (18%)	62,99,113	1.53	7 (11%)
17	CLA	O	203	-	41,49,73	1.80	6 (14%)	47,84,113	1.79	9 (19%)
17	CLA	B	813	-	65,73,73	1.49	10 (15%)	76,113,113	1.46	11 (14%)
17	CLA	5	611	-	45,53,73	1.76	5 (11%)	52,89,113	1.68	8 (15%)
22	BGC	A	849	26	11,11,12	1.66	3 (27%)	15,15,17	1.04	0
17	CLA	B	802	-	65,73,73	1.57	11 (16%)	76,113,113	1.75	24 (31%)
17	CLA	A	816	-	65,73,73	1.48	11 (16%)	76,113,113	1.56	10 (13%)
17	CLA	A	813	-	42,50,73	1.74	9 (21%)	48,85,113	1.93	7 (14%)

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	836	-	1/1/15/20	16/37/115/115	-
17	CLA	A	808	-	1/1/13/20	8/25/103/115	-
17	CLA	3	213	-	1/1/12/20	8/21/99/115	-
17	CLA	A	830	-	1/1/13/20	6/27/105/115	-
20	BCR	B	846	-	-	11/29/63/63	0/2/2/2
17	CLA	J	103	-	1/1/10/20	6/10/88/115	-
16	CL0	A	801	-	3/3/20/25	10/37/135/135	-
20	BCR	B	805	-	-	15/29/63/63	0/2/2/2
25	ZEX	5	614	-	-	18/29/67/67	0/2/2/2
17	CLA	B	803	-	1/1/15/20	22/37/115/115	-
17	CLA	L	202	10	1/1/13/20	14/28/106/115	-
17	CLA	2	608	-	1/1/12/20	8/19/97/115	-
17	CLA	4	606	-	1/1/11/20	4/13/91/115	-
17	CLA	B	808	-	1/1/15/20	16/37/115/115	-
17	CLA	A	807	1	1/1/15/20	19/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	833	-	1/1/11/20	5/13/91/115	-
17	CLA	A	831	-	1/1/15/20	18/37/115/115	-
17	CLA	O	204	-	1/1/12/20	6/19/97/115	-
17	CLA	1	601	-	1/1/11/20	6/17/95/115	-
17	CLA	5	603	-	1/1/15/20	20/37/115/115	-
25	ZEX	4	614	-	-	17/29/67/67	0/2/2/2
17	CLA	4	605	-	1/1/10/20	2/9/87/115	-
17	CLA	A	809	-	1/1/15/20	13/37/115/115	-
20	BCR	A	843	-	-	16/29/63/63	0/2/2/2
17	CLA	A	815	-	1/1/14/20	13/34/112/115	-
17	CLA	5	610	-	1/1/11/20	8/13/91/115	-
17	CLA	4	603	-	1/1/11/20	10/13/91/115	-
20	BCR	L	206	-	-	15/29/63/63	0/2/2/2
25	ZEX	3	201	-	-	16/29/67/67	0/2/2/2
25	ZEX	3	217	-	-	15/29/67/67	0/2/2/2
17	CLA	B	842	-	1/1/15/20	14/37/115/115	-
17	CLA	3	211	-	1/1/10/20	1/10/88/115	-
17	CLA	5	613	-	1/1/10/20	4/10/88/115	-
17	CLA	A	838	-	1/1/15/20	11/37/115/115	-
19	LHG	A	842	-	-	19/44/44/53	-
17	CLA	A	818	-	1/1/11/20	7/13/91/115	-
25	ZEX	3	216	-	-	19/29/67/67	0/2/2/2
17	CLA	2	605	-	1/1/11/20	7/13/91/115	-
17	CLA	4	609	-	1/1/10/20	5/8/86/115	-
20	BCR	J	105	-	-	14/29/63/63	0/2/2/2
17	CLA	1	604	-	1/1/11/20	7/13/91/115	-
17	CLA	B	823	-	1/1/11/20	2/13/91/115	-
17	CLA	1	603	-	1/1/11/20	7/13/91/115	-
17	CLA	A	827	-	1/1/15/20	18/37/115/115	-
17	CLA	B	801	-	1/1/15/20	14/37/115/115	-
17	CLA	2	609	-	1/1/10/20	3/8/86/115	-
20	BCR	J	104	-	-	16/29/63/63	0/2/2/2
17	CLA	B	839	-	1/1/15/20	10/37/115/115	-
17	CLA	1	610	-	1/1/11/20	4/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	817	-	1/1/11/20	3/13/91/115	-
17	CLA	3	209	-	1/1/12/20	7/22/100/115	-
17	CLA	4	607	-	1/1/11/20	7/13/91/115	-
17	CLA	5	608	-	1/1/11/20	5/13/91/115	-
17	CLA	O	201	-	1/1/12/20	7/22/100/115	-
17	CLA	1	605	-	1/1/10/20	3/9/87/115	-
17	CLA	B	843	-	1/1/15/20	16/37/115/115	-
17	CLA	B	810	-	1/1/15/20	17/37/115/115	-
17	CLA	L	204	-	1/1/12/20	6/19/97/115	-
17	CLA	B	835	-	1/1/15/20	17/37/115/115	-
17	CLA	A	848	-	1/1/15/20	9/37/115/115	-
17	CLA	B	821	-	1/1/14/20	16/31/109/115	-
17	CLA	4	604	-	1/1/11/20	7/13/91/115	-
17	CLA	K	103	-	1/1/10/20	5/10/88/115	-
17	CLA	3	204	-	1/1/11/20	6/13/91/115	-
17	CLA	F	301	-	1/1/14/20	14/33/111/115	-
25	ZEX	4	616	-	-	17/29/67/67	0/2/2/2
17	CLA	A	821	-	1/1/12/20	12/21/99/115	-
17	CLA	3	203	-	1/1/14/20	20/35/113/115	-
17	CLA	5	607	-	1/1/11/20	7/13/91/115	-
17	CLA	5	612	-	1/1/11/20	5/13/91/115	-
17	CLA	A	805	-	1/1/15/20	16/37/115/115	-
17	CLA	A	828	-	1/1/15/20	10/37/115/115	-
17	CLA	A	817	-	1/1/15/20	15/37/115/115	-
25	ZEX	1	614	-	-	16/29/67/67	0/2/2/2
17	CLA	1	609	-	1/1/10/20	0/8/86/115	-
17	CLA	2	601	-	1/1/11/20	6/13/91/115	-
20	BCR	K	104	-	-	19/29/63/63	0/2/2/2
17	CLA	A	829	-	1/1/12/20	4/19/97/115	-
20	BCR	I	101	-	-	18/29/63/63	0/2/2/2
25	ZEX	3	218	-	-	17/29/67/67	0/2/2/2
20	BCR	B	849	-	-	23/29/63/63	0/2/2/2
25	ZEX	2	616	-	-	19/29/67/67	0/2/2/2
25	ZEX	2	617	-	-	19/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	SF4	C	101	3	-	-	0/6/5/5
25	ZEX	1	616	-	-	20/29/67/67	0/2/2/2
25	ZEX	3	215	-	-	16/29/67/67	0/2/2/2
17	CLA	2	604	-	1/1/10/20	3/10/88/115	-
21	SF4	C	102	-	-	-	0/6/5/5
17	CLA	B	819	-	1/1/13/20	12/25/103/115	-
17	CLA	B	825	-	1/1/10/20	5/11/89/115	-
17	CLA	A	814	-	1/1/11/20	4/13/91/115	-
17	CLA	B	806	-	1/1/15/20	16/37/115/115	-
17	CLA	A	803	-	1/1/15/20	2/37/115/115	-
17	CLA	A	837	-	1/1/15/20	12/37/115/115	-
17	CLA	1	606	-	1/1/11/20	6/13/91/115	-
17	CLA	1	602	-	1/1/13/20	10/30/108/115	-
20	BCR	F	304	-	-	18/29/63/63	0/2/2/2
17	CLA	B	816	-	1/1/15/20	19/37/115/115	-
17	CLA	B	809	-	1/1/15/20	15/37/115/115	-
17	CLA	B	829	-	1/1/15/20	17/37/115/115	-
17	CLA	A	812	-	1/1/11/20	6/13/91/115	-
20	BCR	A	845	-	-	18/29/63/63	0/2/2/2
25	ZEX	5	617	-	-	18/29/67/67	0/2/2/2
17	CLA	A	823	-	1/1/15/20	16/37/115/115	-
25	ZEX	2	615	-	-	16/29/67/67	0/2/2/2
17	CLA	1	612	-	1/1/11/20	7/13/91/115	-
17	CLA	B	822	-	1/1/15/20	17/37/115/115	-
17	CLA	4	601	-	1/1/11/20	7/17/95/115	-
17	CLA	B	811	-	1/1/15/20	6/37/115/115	-
24	3XQ	J	106	-	-	17/24/24/24	-
26	1DO	3	219	22	-	3/10/10/10	-
17	CLA	A	832	-	1/1/15/20	18/37/115/115	-
17	CLA	A	839	-	1/1/15/20	17/37/115/115	-
25	ZEX	1	613	-	-	16/29/67/67	0/2/2/2
17	CLA	B	812	-	1/1/15/20	18/37/115/115	-
17	CLA	B	826	-	1/1/13/20	7/25/103/115	-
18	PQN	B	844	-	-	7/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	BCR	B	847	-	-	23/29/63/63	0/2/2/2
25	ZEX	1	615	-	-	20/29/67/67	0/2/2/2
17	CLA	A	833	-	1/1/15/20	16/37/115/115	-
17	CLA	A	836	-	1/1/15/20	13/37/115/115	-
17	CLA	B	827	-	1/1/15/20	11/37/115/115	-
17	CLA	B	824	-	1/1/11/20	6/15/93/115	-
17	CLA	4	611	-	1/1/11/20	8/13/91/115	-
17	CLA	B	820	-	1/1/13/20	16/30/108/115	-
17	CLA	F	303	-	1/1/10/20	3/8/86/115	-
17	CLA	5	605	-	1/1/11/20	8/13/91/115	-
25	ZEX	1	617	-	-	18/29/67/67	0/2/2/2
20	BCR	O	202	-	-	14/29/63/63	0/2/2/2
17	CLA	L	203	-	1/1/15/20	14/37/115/115	-
17	CLA	5	604	-	1/1/11/20	6/13/91/115	-
17	CLA	A	802	-	1/1/13/20	7/25/103/115	-
17	CLA	1	608	-	1/1/14/20	9/31/109/115	-
17	CLA	2	603	-	1/1/11/20	2/13/91/115	-
20	BCR	B	845	-	-	16/29/63/63	0/2/2/2
21	SF4	A	847	-	-	-	0/6/5/5
17	CLA	A	825	-	1/1/15/20	9/37/115/115	-
20	BCR	K	101	-	-	11/29/63/63	0/2/2/2
17	CLA	B	804	-	1/1/15/20	17/37/115/115	-
17	CLA	K	102	-	1/1/11/20	5/13/91/115	-
17	CLA	3	212	-	1/1/11/20	8/15/93/115	-
19	LHG	A	841	-	-	27/53/53/53	-
25	ZEX	5	615	-	-	19/29/67/67	0/2/2/2
17	CLA	A	804	-	1/1/15/20	14/37/115/115	-
17	CLA	A	820	-	1/1/11/20	5/18/96/115	-
17	CLA	B	818	-	1/1/10/20	4/10/88/115	-
17	CLA	J	102	-	1/1/13/20	8/29/107/115	-
17	CLA	B	838	-	1/1/14/20	18/31/109/115	-
17	CLA	2	611	-	1/1/11/20	5/13/91/115	-
17	CLA	3	208	-	1/1/11/20	8/13/91/115	-
20	BCR	L	205	-	-	15/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	2	602	-	1/1/15/20	12/37/115/115	-
17	CLA	A	822	-	1/1/13/20	7/25/103/115	-
17	CLA	A	811	-	1/1/15/20	13/37/115/115	-
17	CLA	3	205	-	1/1/11/20	7/13/91/115	-
17	CLA	4	610	-	1/1/11/20	4/13/91/115	-
20	BCR	A	846	-	-	18/29/63/63	0/2/2/2
23	DGD	B	851	-	-	30/55/95/95	0/2/2/2
25	ZEX	4	613	-	-	16/29/67/67	0/2/2/2
25	ZEX	4	612	-	-	19/29/67/67	0/2/2/2
17	CLA	5	606	-	1/1/11/20	3/13/91/115	-
17	CLA	2	607	-	1/1/11/20	3/13/91/115	-
17	CLA	5	601	-	1/1/11/20	6/13/91/115	-
25	ZEX	4	615	-	-	16/29/67/67	0/2/2/2
17	CLA	A	806	1	1/1/15/20	16/37/115/115	-
17	CLA	F	302	-	1/1/11/20	4/13/91/115	-
20	BCR	L	201	-	-	18/29/63/63	0/2/2/2
20	BCR	B	850	-	-	15/29/63/63	0/2/2/2
17	CLA	B	840	-	1/1/11/20	4/16/94/115	-
17	CLA	1	607	-	1/1/11/20	7/13/91/115	-
17	CLA	B	814	-	1/1/13/20	10/25/101/115	-
17	CLA	B	830	-	1/1/15/20	21/37/115/115	-
17	CLA	A	834	-	1/1/11/20	8/13/91/115	-
17	CLA	A	835	-	1/1/12/20	10/21/99/115	-
17	CLA	B	807	-	1/1/11/20	7/13/91/115	-
17	CLA	3	207	-	1/1/11/20	5/13/91/115	-
17	CLA	5	602	-	1/1/11/20	7/13/91/115	-
17	CLA	5	609	-	1/1/10/20	5/8/86/115	-
17	CLA	2	610	-	1/1/10/20	5/10/88/115	-
17	CLA	3	206	-	1/1/11/20	4/13/91/115	-
25	ZEX	3	214	-	-	14/29/67/67	0/2/2/2
17	CLA	2	606	-	1/1/11/20	7/13/91/115	-
20	BCR	A	844	-	-	17/29/63/63	0/2/2/2
25	ZEX	5	616	-	-	16/29/67/67	0/2/2/2
17	CLA	2	613	-	1/1/11/20	5/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	3	210	-	1/1/10/20	5/8/86/115	-
17	CLA	1	611	-	1/1/11/20	10/13/91/115	-
17	CLA	4	608	-	1/1/11/20	6/13/91/115	-
20	BCR	B	848	-	-	19/29/63/63	0/2/2/2
17	CLA	4	602	-	1/1/13/20	14/30/108/115	-
17	CLA	B	837	-	1/1/11/20	6/13/91/115	-
17	CLA	A	824	-	1/1/13/20	5/25/103/115	-
17	CLA	O	205	-	1/1/11/20	6/13/91/115	-
17	CLA	3	202	-	1/1/11/20	5/13/91/115	-
17	CLA	2	612	-	1/1/11/20	3/13/91/115	-
17	CLA	B	832	-	1/1/15/20	10/37/115/115	-
17	CLA	B	831	-	1/1/15/20	14/37/115/115	-
17	CLA	B	834	-	1/1/10/20	3/11/89/115	-
17	CLA	J	101	-	1/1/15/20	18/37/115/115	-
17	CLA	B	815	-	1/1/13/20	6/25/103/115	-
18	PQN	A	840	-	-	11/23/43/43	0/2/2/2
17	CLA	A	819	-	1/1/15/20	13/37/115/115	-
25	ZEX	4	617	-	-	18/29/67/67	0/2/2/2
17	CLA	B	828	-	1/1/15/20	4/37/115/115	-
25	ZEX	2	614	-	-	18/29/67/67	0/2/2/2
17	CLA	B	841	-	1/1/15/20	14/37/115/115	-
17	CLA	A	826	-	1/1/15/20	12/37/115/115	-
17	CLA	A	810	-	1/1/12/20	8/24/102/115	-
17	CLA	O	203	-	1/1/10/20	3/8/86/115	-
17	CLA	B	813	-	1/1/15/20	15/37/115/115	-
17	CLA	5	611	-	1/1/11/20	7/13/91/115	-
22	BGC	A	849	26	-	2/2/19/22	0/1/1/1
17	CLA	B	802	-	1/1/15/20	12/37/115/115	-
17	CLA	A	816	-	1/1/15/20	11/37/115/115	-
17	CLA	A	813	-	1/1/10/20	5/10/88/115	-

The worst 5 of 2053 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	218	ZEX	C14-C13	15.85	1.56	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	616	ZEX	C14-C13	14.96	1.55	1.35
25	1	616	ZEX	C14-C13	14.67	1.55	1.35
25	3	201	ZEX	C14-C13	14.51	1.55	1.35
25	3	216	ZEX	C14-C13	14.50	1.55	1.35

The worst 5 of 2576 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	614	ZEX	C31-C30-C29	-16.44	103.84	127.31
25	1	614	ZEX	C39-C29-C28	-14.08	95.90	118.08
25	5	617	ZEX	C15-C14-C13	-13.48	108.07	127.31
25	3	201	ZEX	C31-C30-C29	-13.33	108.28	127.31
16	A	801	CL0	C4A-NA-C1A	13.29	112.68	106.71

5 of 160 chirality outliers are listed below:

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

5 of 2345 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	802	CLA	CHA-CBD-CGD-O1D
17	A	802	CLA	CHA-CBD-CGD-O2D
17	A	804	CLA	C1A-C2A-CAA-CBA
17	A	805	CLA	CHA-CBD-CGD-O1D
17	A	805	CLA	CAD-CBD-CGD-O1D

There are no ring outliers.

196 monomers are involved in 583 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	836	CLA	5	0
17	A	808	CLA	3	0
17	A	830	CLA	3	0
20	B	846	BCR	2	0
17	J	103	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	801	CL0	59	0
20	B	805	BCR	6	0
25	5	614	ZEX	4	0
17	B	803	CLA	2	0
17	L	202	CLA	1	0
17	2	608	CLA	2	0
17	4	606	CLA	3	0
17	B	808	CLA	3	0
17	A	807	CLA	5	0
17	B	833	CLA	3	0
17	A	831	CLA	11	0
17	O	204	CLA	2	0
17	1	601	CLA	3	0
17	5	603	CLA	7	0
25	4	614	ZEX	6	0
17	A	809	CLA	3	0
20	A	843	BCR	5	0
17	A	815	CLA	4	0
20	L	206	BCR	2	0
25	3	201	ZEX	4	0
25	3	217	ZEX	1	0
17	B	842	CLA	14	0
17	A	838	CLA	9	0
19	A	842	LHG	3	0
17	A	818	CLA	4	0
25	3	216	ZEX	1	0
17	2	605	CLA	2	0
17	4	609	CLA	3	0
20	J	105	BCR	2	0
17	1	604	CLA	1	0
17	1	603	CLA	2	0
17	A	827	CLA	5	0
17	B	801	CLA	11	0
17	2	609	CLA	2	0
20	J	104	BCR	4	0
17	B	839	CLA	5	0
17	1	610	CLA	1	0
17	B	817	CLA	2	0
17	3	209	CLA	2	0
17	4	607	CLA	1	0
17	5	608	CLA	2	0
17	O	201	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	843	CLA	4	0
17	B	810	CLA	4	0
17	L	204	CLA	1	0
17	B	835	CLA	7	0
17	A	848	CLA	9	0
17	B	821	CLA	5	0
17	4	604	CLA	3	0
17	K	103	CLA	1	0
17	3	204	CLA	3	0
17	F	301	CLA	1	0
25	4	616	ZEX	2	0
17	A	821	CLA	1	0
17	3	203	CLA	8	0
17	5	607	CLA	3	0
17	5	612	CLA	2	0
17	A	805	CLA	5	0
17	A	828	CLA	5	0
17	A	817	CLA	8	0
25	1	614	ZEX	8	0
17	1	609	CLA	1	0
17	2	601	CLA	4	0
20	K	104	BCR	5	0
17	A	829	CLA	2	0
20	I	101	BCR	4	0
21	C	101	SF4	1	0
20	B	849	BCR	2	0
25	2	616	ZEX	1	0
25	2	617	ZEX	2	0
25	3	218	ZEX	6	0
25	1	616	ZEX	2	0
25	3	215	ZEX	6	0
17	2	604	CLA	2	0
21	C	102	SF4	1	0
17	B	819	CLA	3	0
17	B	825	CLA	1	0
17	A	814	CLA	1	0
17	B	806	CLA	11	0
17	A	803	CLA	7	0
17	A	837	CLA	4	0
17	1	606	CLA	4	0
17	1	602	CLA	2	0
20	F	304	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	816	CLA	7	0
17	B	809	CLA	6	0
17	B	829	CLA	6	0
17	A	812	CLA	1	0
20	A	845	BCR	3	0
25	5	617	ZEX	8	0
17	A	823	CLA	5	0
25	2	615	ZEX	4	0
17	1	612	CLA	2	0
17	B	822	CLA	4	0
17	4	601	CLA	3	0
17	B	811	CLA	4	0
26	3	219	1DO	1	0
17	A	832	CLA	4	0
17	A	839	CLA	5	0
25	1	613	ZEX	3	0
17	B	812	CLA	7	0
17	B	826	CLA	2	0
18	B	844	PQN	3	0
20	B	847	BCR	6	0
25	1	615	ZEX	2	0
17	A	833	CLA	4	0
17	A	836	CLA	8	0
17	B	827	CLA	6	0
17	B	824	CLA	3	0
17	4	611	CLA	5	0
17	B	820	CLA	4	0
17	5	605	CLA	2	0
25	1	617	ZEX	4	0
20	O	202	BCR	5	0
17	L	203	CLA	4	0
17	5	604	CLA	2	0
17	A	802	CLA	1	0
17	2	603	CLA	2	0
20	B	845	BCR	1	0
17	A	825	CLA	5	0
20	K	101	BCR	6	0
17	B	804	CLA	9	0
17	K	102	CLA	1	0
17	3	212	CLA	3	0
19	A	841	LHG	3	0
25	5	615	ZEX	1	0

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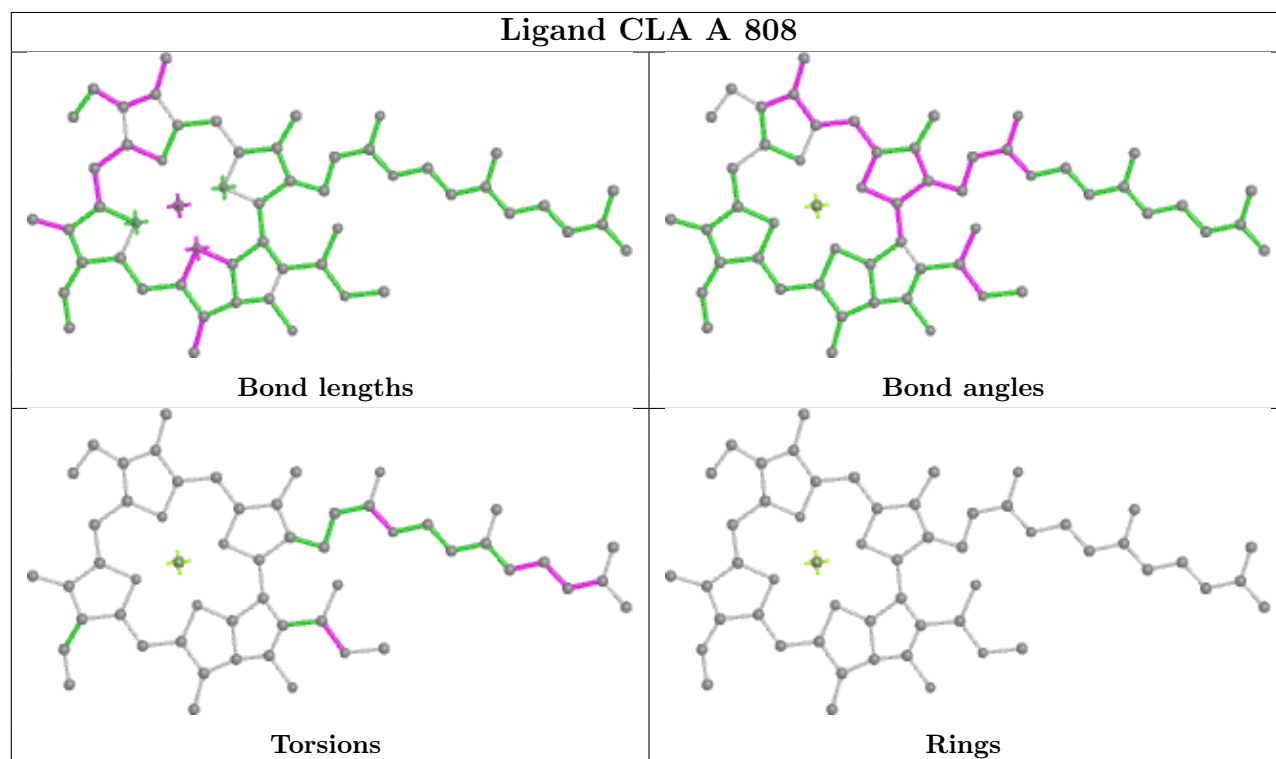
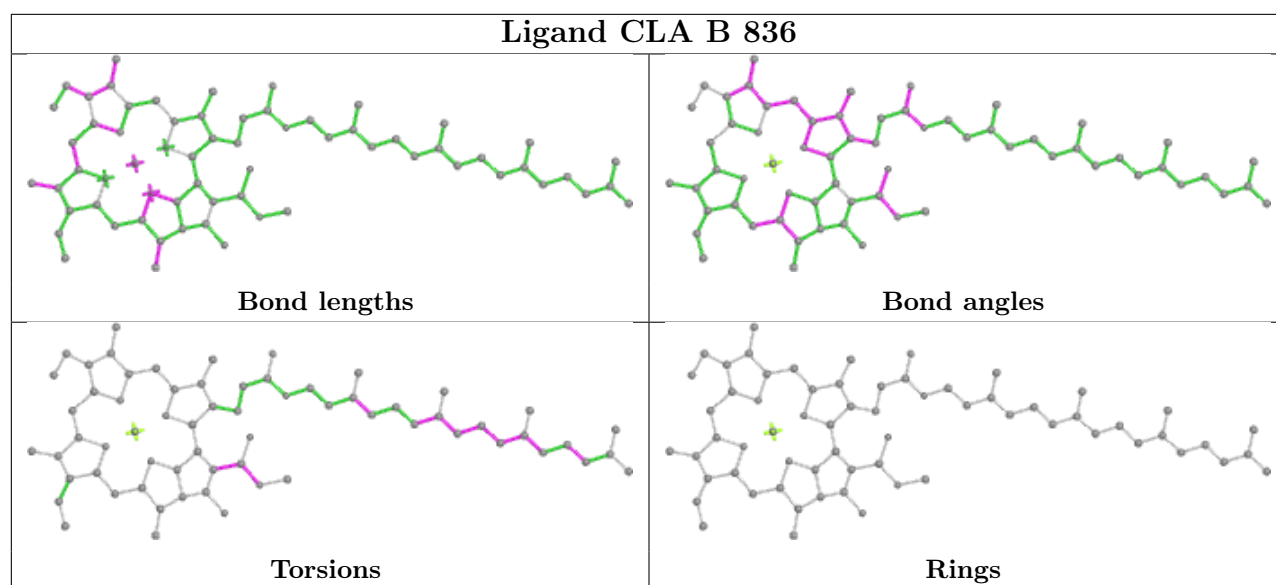
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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17	A	820	CLA	1	0
17	B	818	CLA	3	0
17	J	102	CLA	4	0
17	B	838	CLA	4	0
17	3	208	CLA	2	0
20	L	205	BCR	6	0
17	2	602	CLA	6	0
17	A	822	CLA	2	0
17	A	811	CLA	4	0
17	3	205	CLA	2	0
20	A	846	BCR	6	0
23	B	851	DGD	5	0
25	4	613	ZEX	4	0
25	4	612	ZEX	3	0
17	5	606	CLA	4	0
17	2	607	CLA	1	0
17	5	601	CLA	2	0
25	4	615	ZEX	2	0
17	A	806	CLA	8	0
17	F	302	CLA	3	0
20	L	201	BCR	3	0
20	B	850	BCR	4	0
17	B	840	CLA	3	0
17	1	607	CLA	2	0
17	B	814	CLA	2	0
17	B	830	CLA	7	0
17	A	834	CLA	6	0
17	A	835	CLA	1	0
17	3	207	CLA	4	0
17	5	602	CLA	2	0
17	5	609	CLA	1	0
17	2	610	CLA	2	0
17	3	206	CLA	5	0
25	3	214	ZEX	3	0
17	2	606	CLA	3	0
20	A	844	BCR	1	0
25	5	616	ZEX	3	0
17	2	613	CLA	1	0
17	3	210	CLA	1	0
17	1	611	CLA	1	0
17	4	608	CLA	4	0

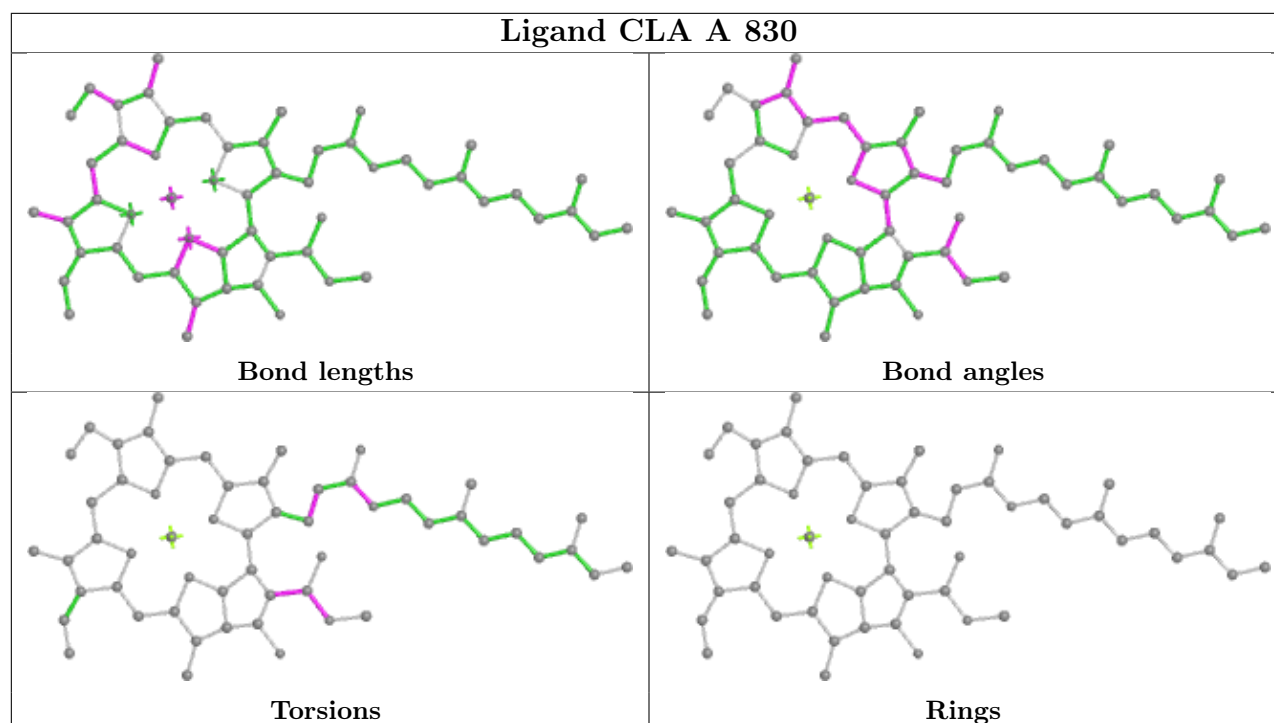
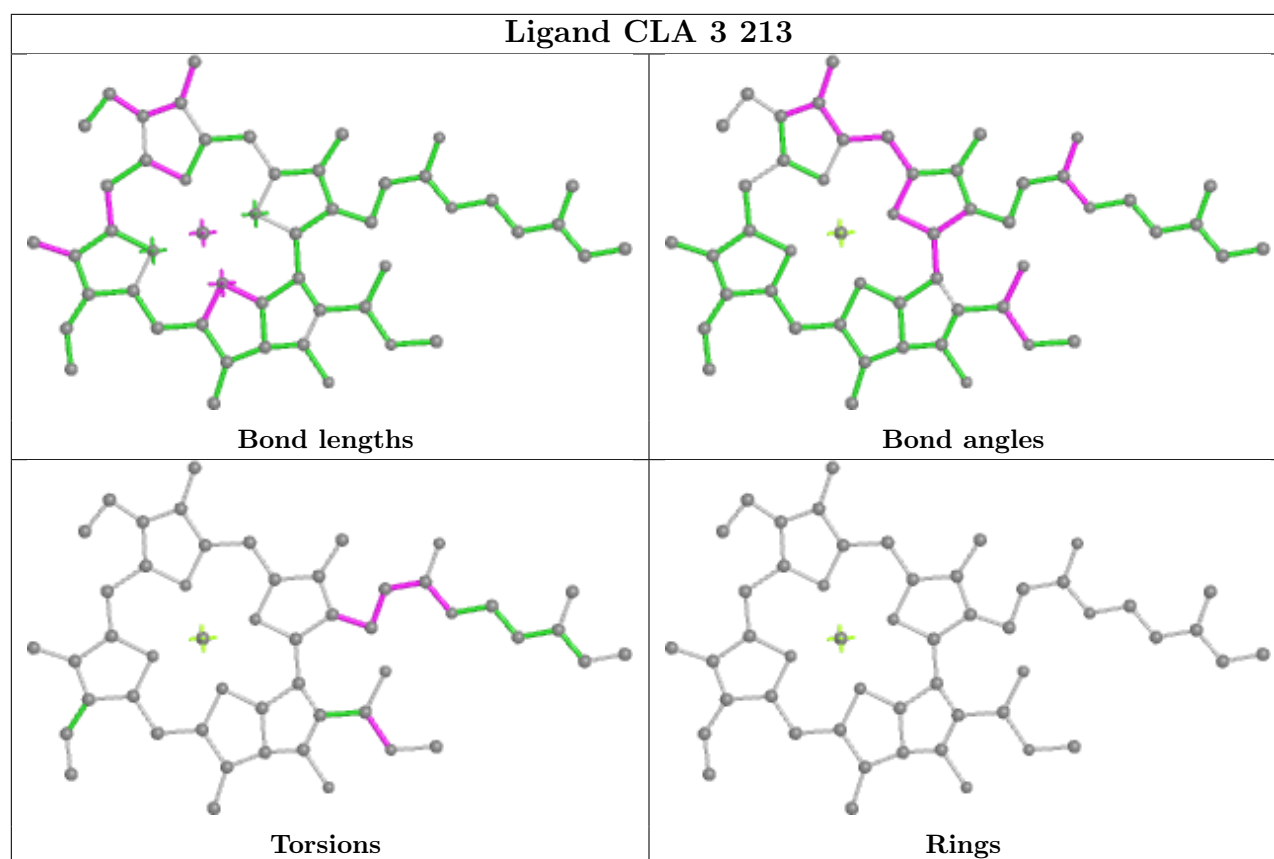
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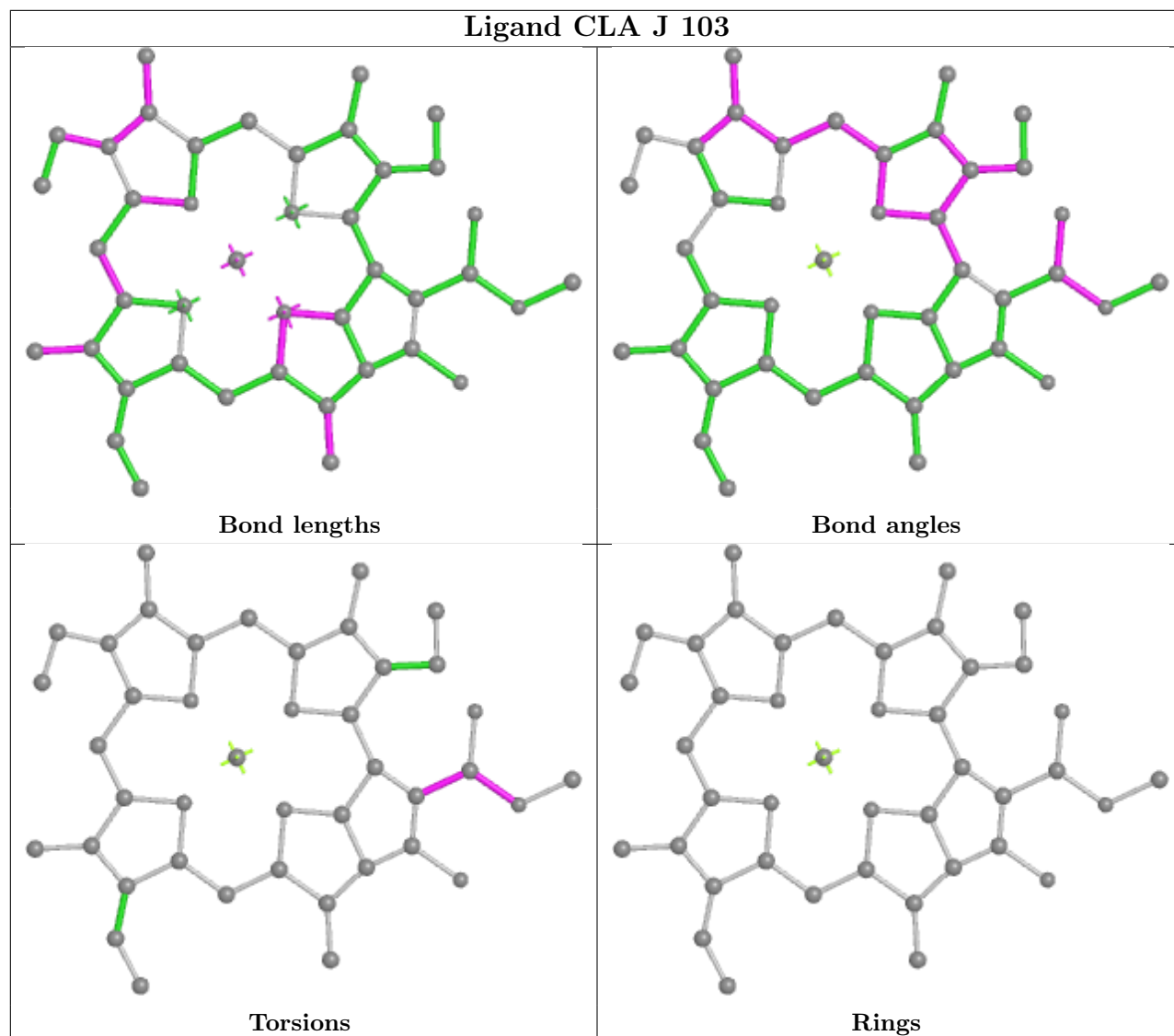
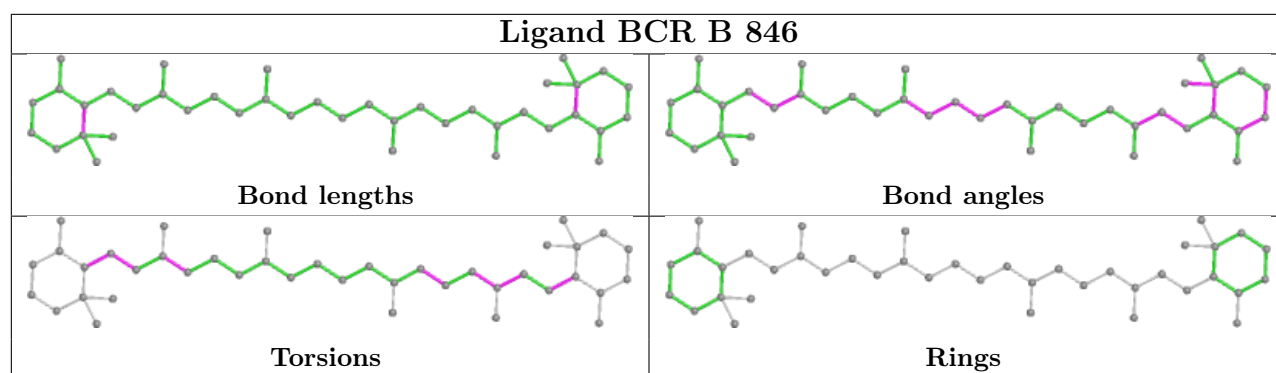
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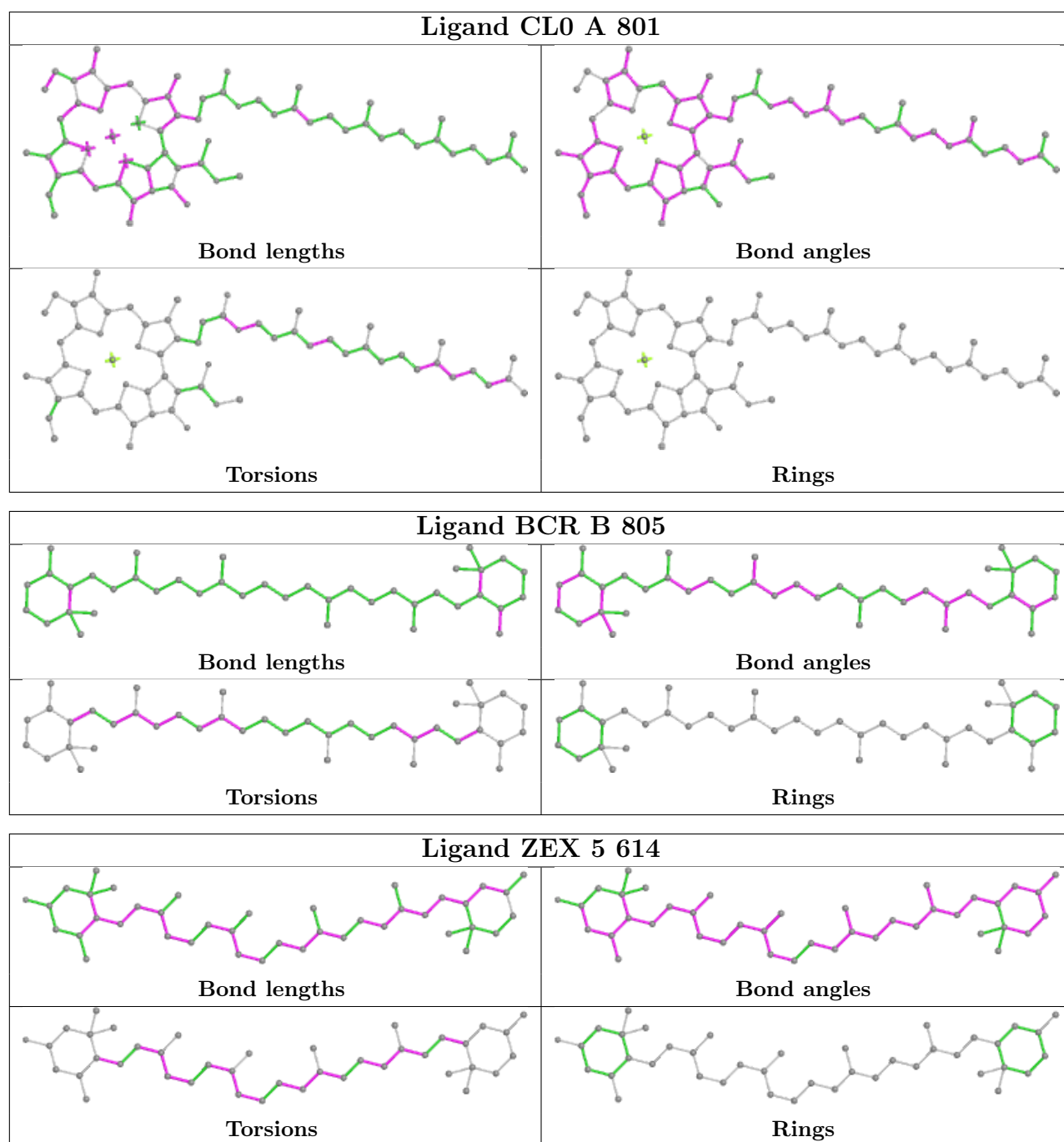
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	848	BCR	4	0
17	4	602	CLA	2	0
17	B	837	CLA	2	0
17	A	824	CLA	3	0
17	O	205	CLA	1	0
17	2	612	CLA	1	0
17	B	832	CLA	5	0
17	B	831	CLA	9	0
17	B	834	CLA	1	0
17	J	101	CLA	6	0
18	A	840	PQN	4	0
17	A	819	CLA	5	0
25	4	617	ZEX	1	0
17	B	828	CLA	4	0
25	2	614	ZEX	4	0
17	B	841	CLA	9	0
17	A	826	CLA	10	0
17	A	810	CLA	3	0
17	B	813	CLA	4	0
17	5	611	CLA	1	0
17	B	802	CLA	8	0
17	A	816	CLA	5	0
17	A	813	CLA	2	0

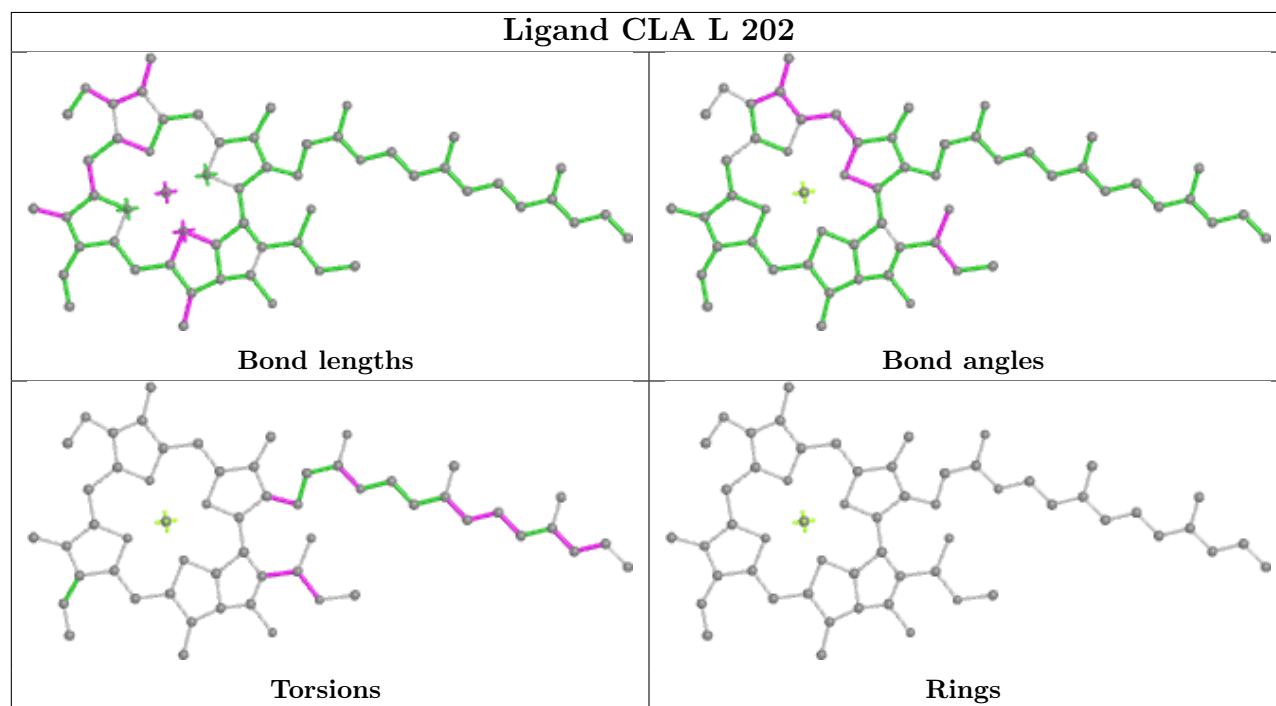
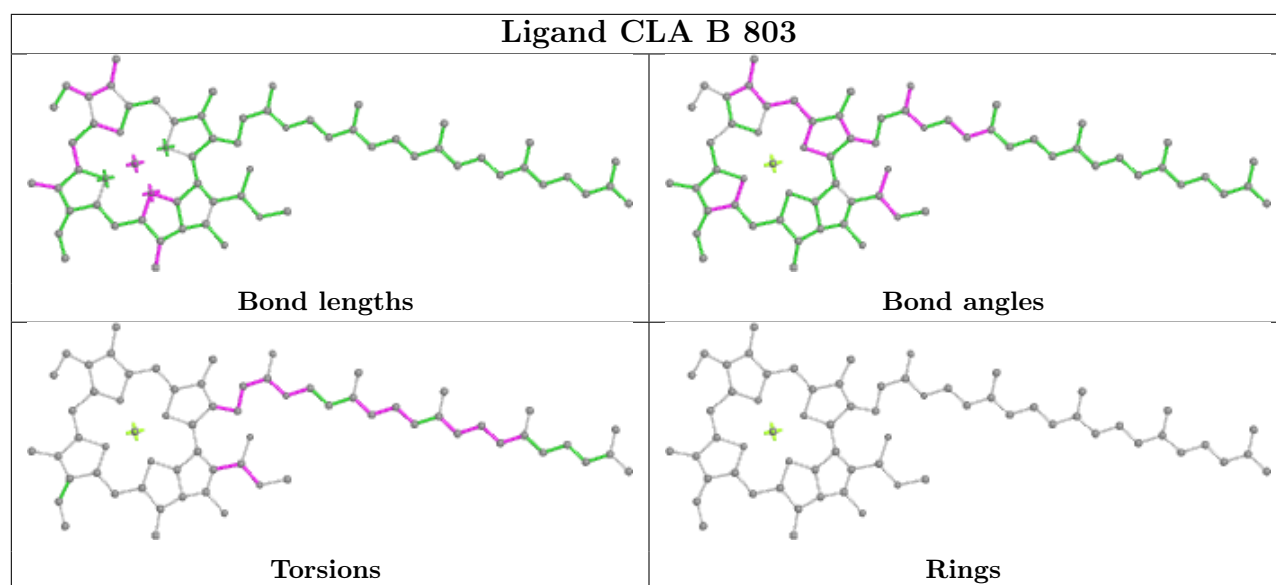
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



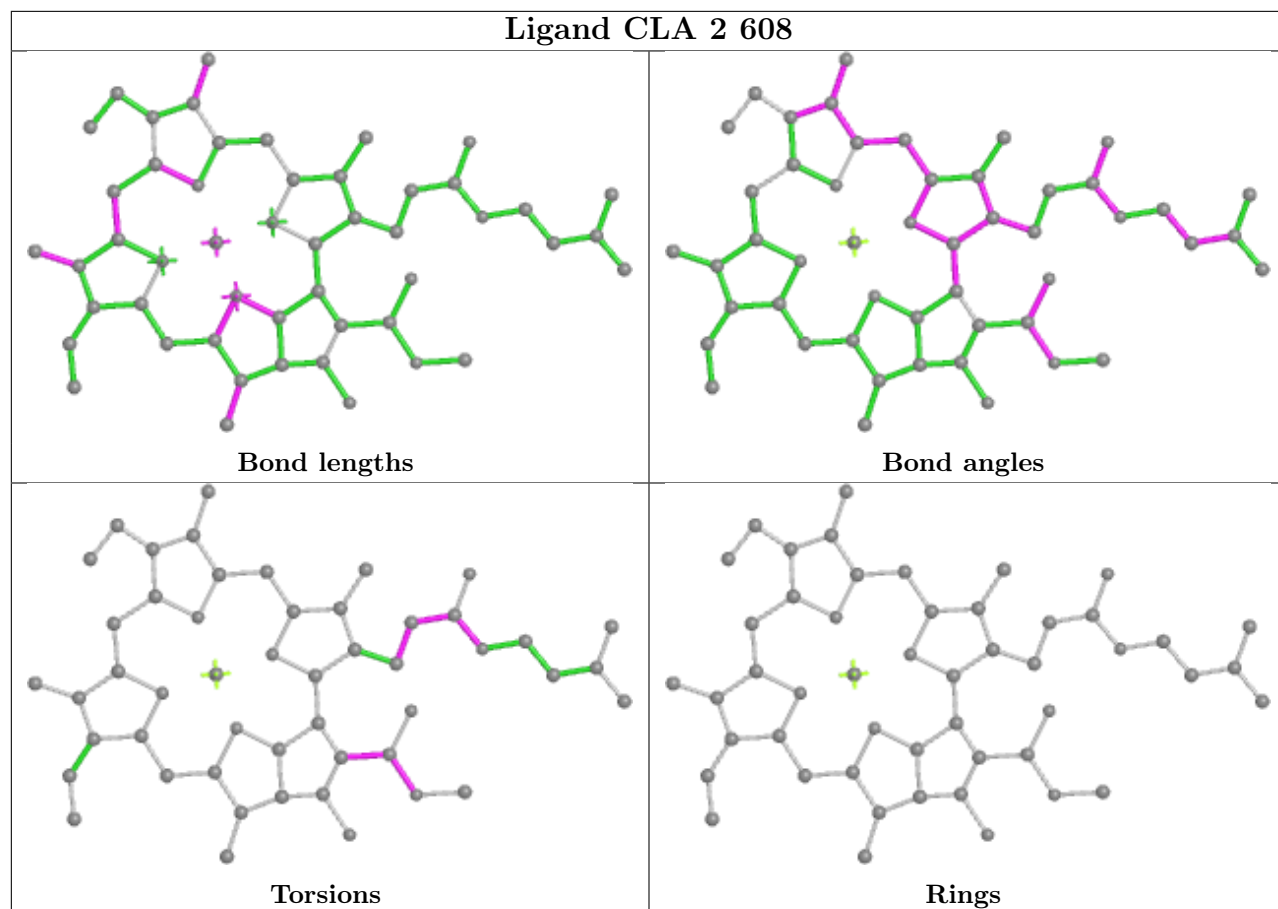




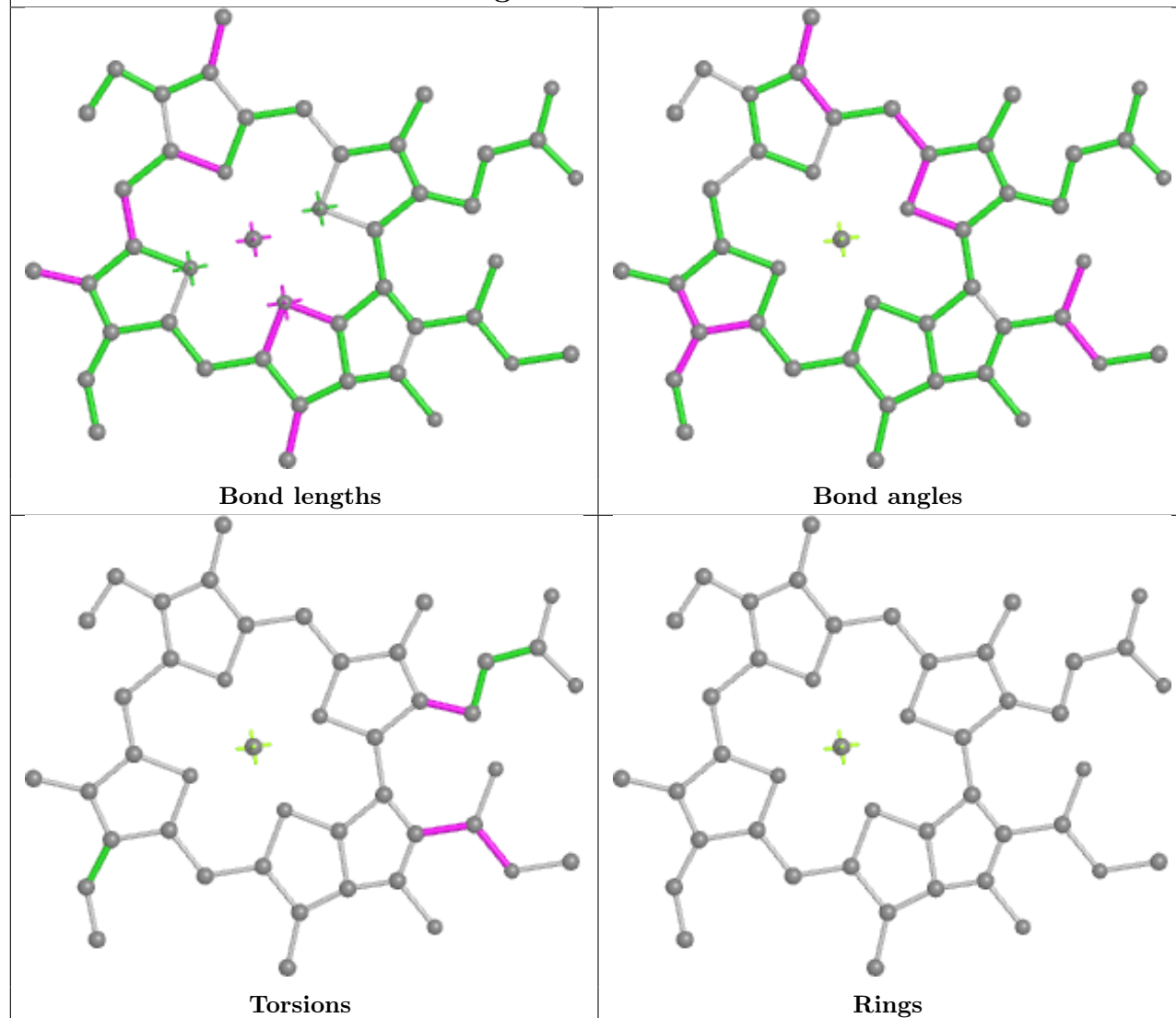




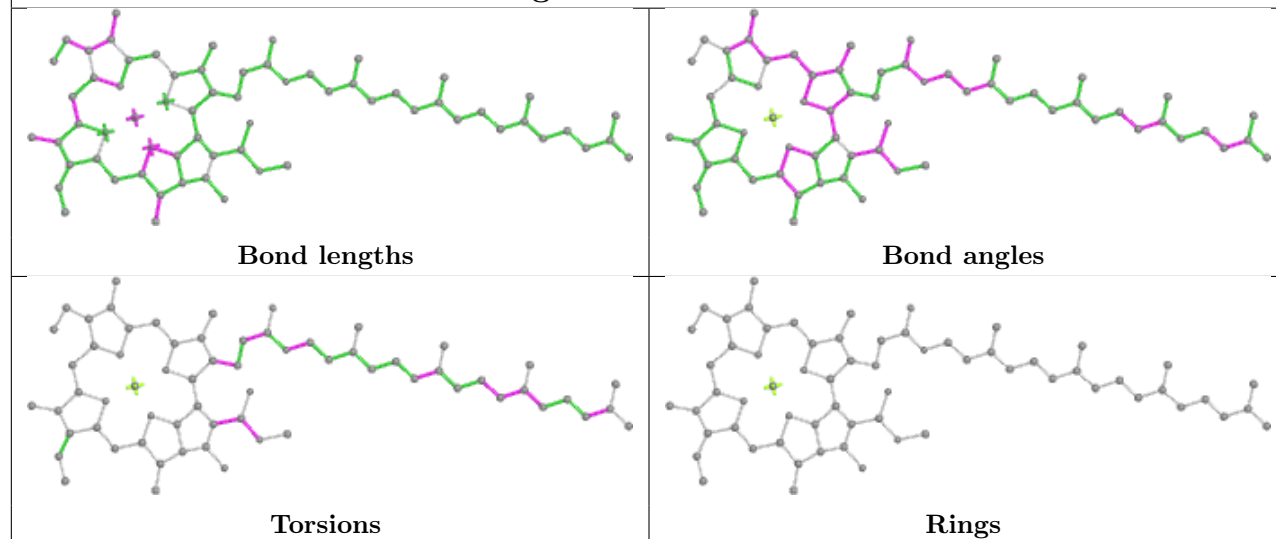
Ligand CLA 2 608



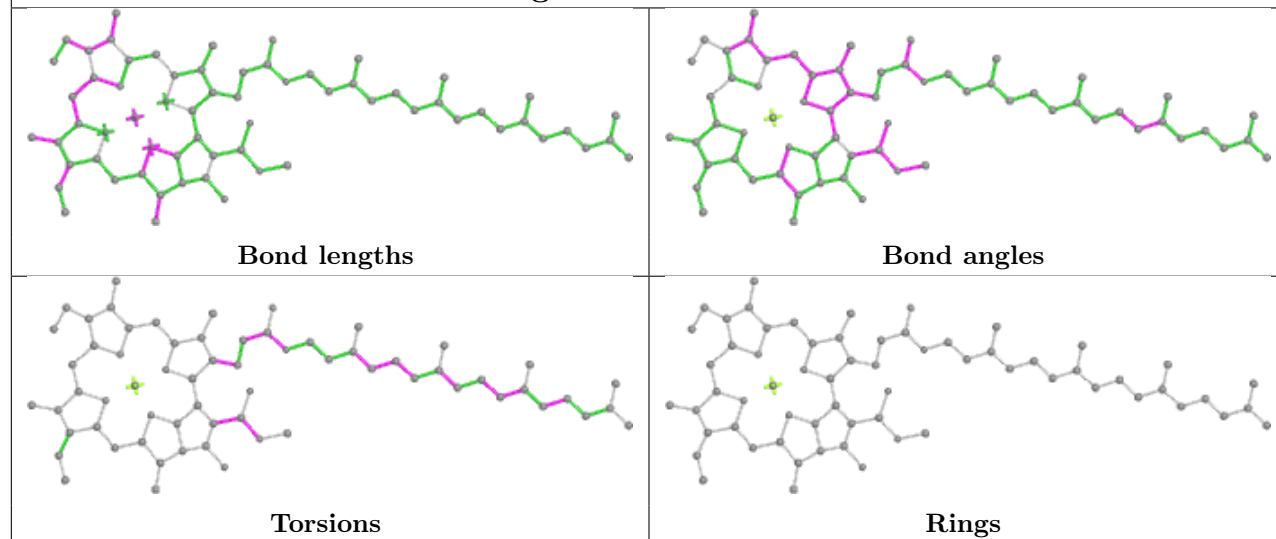
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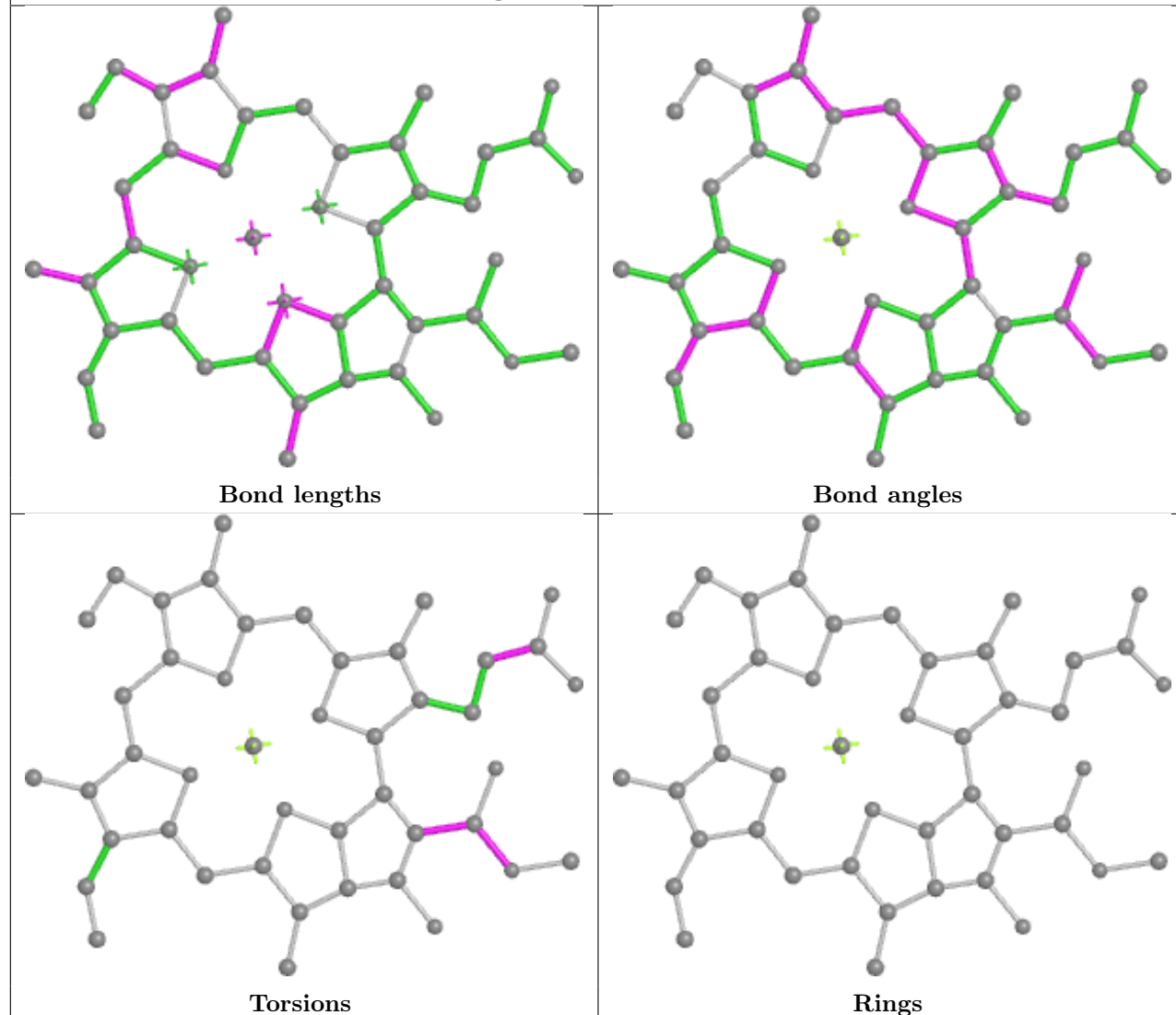
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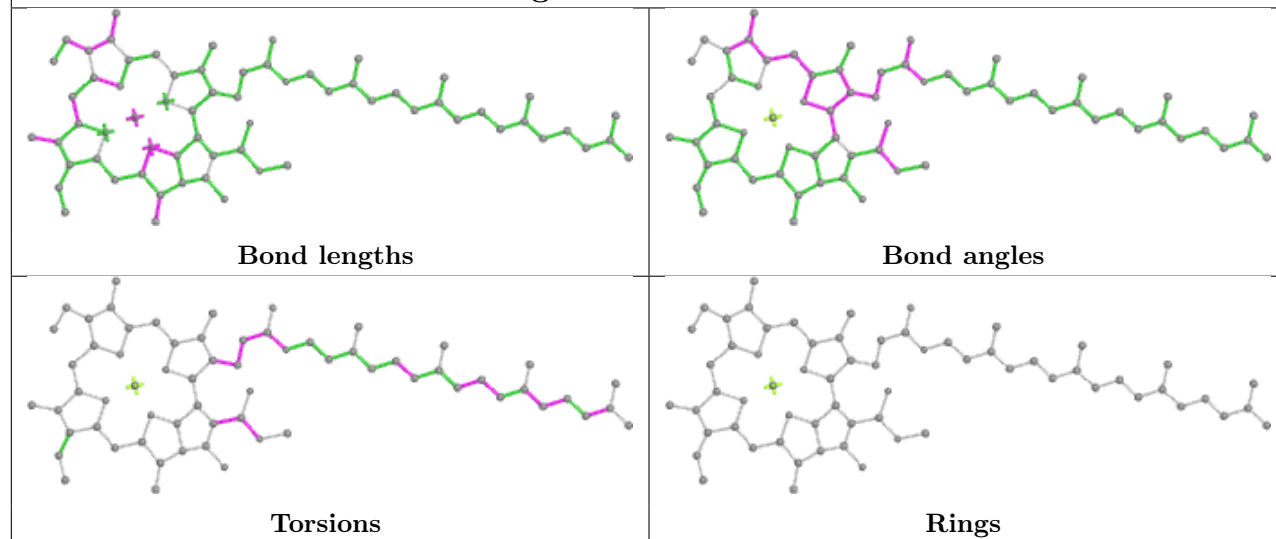
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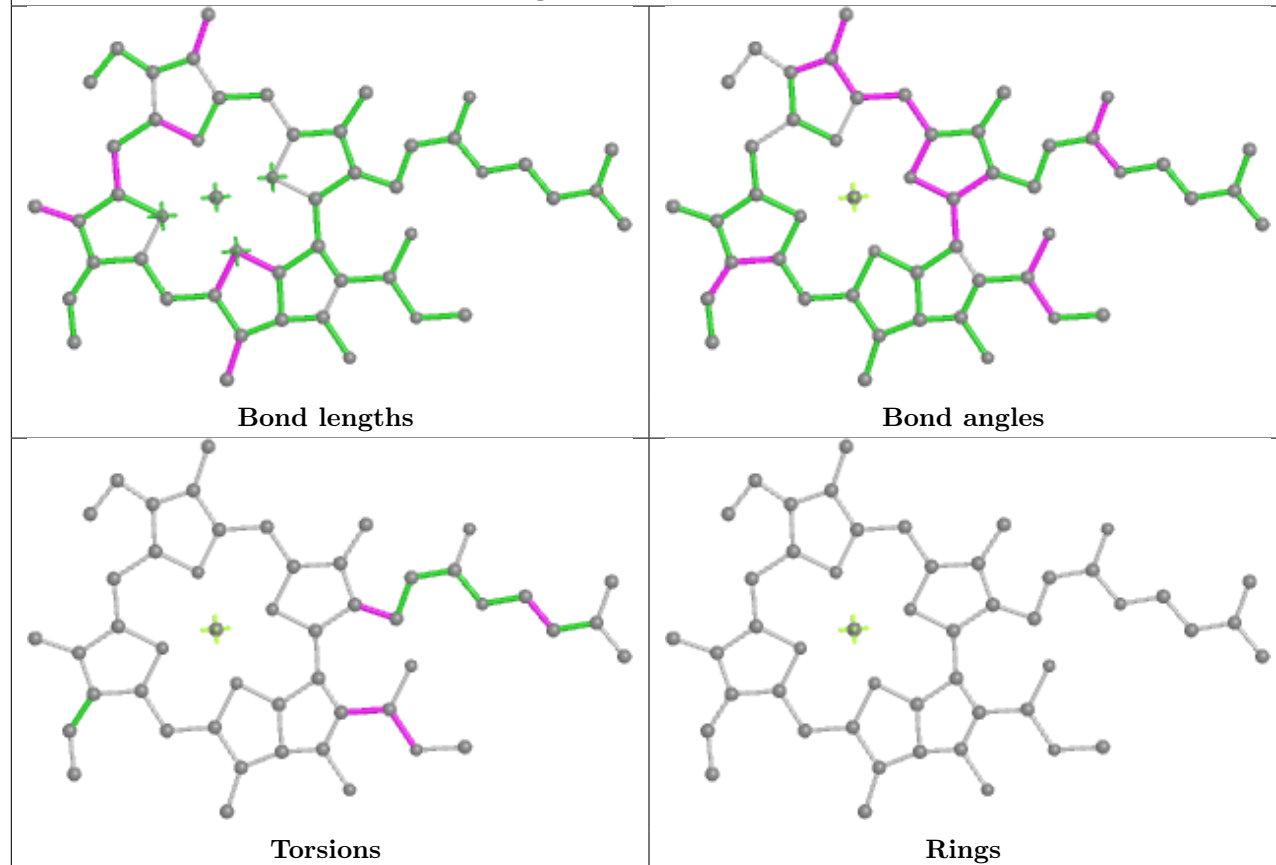
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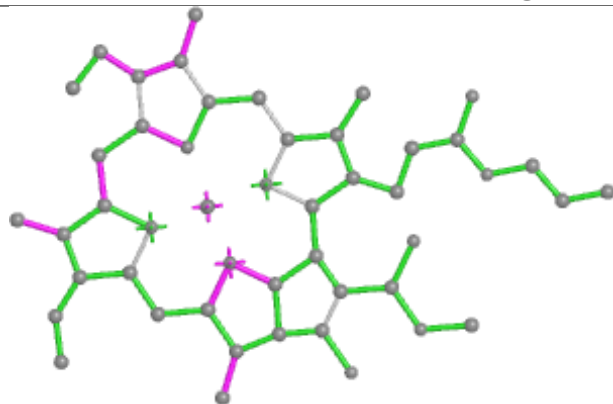
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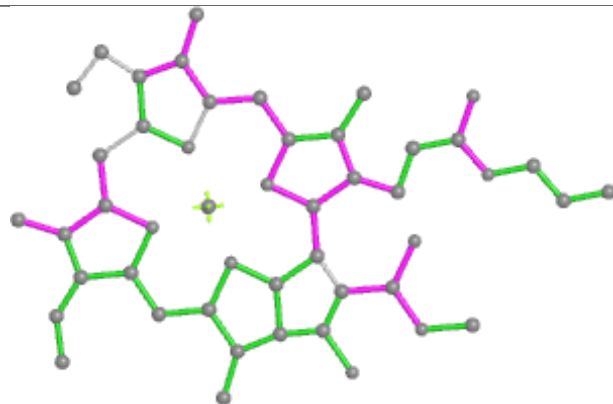
Ligand CLA O 204



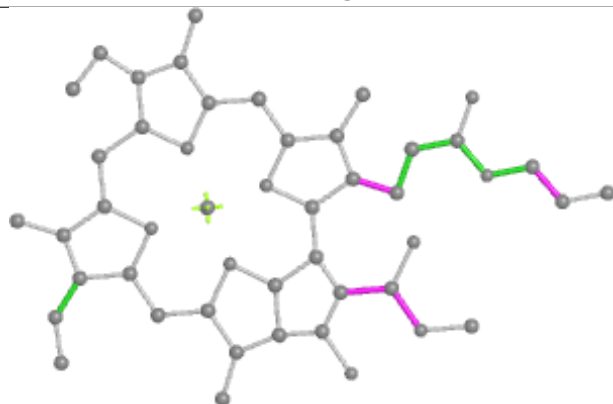
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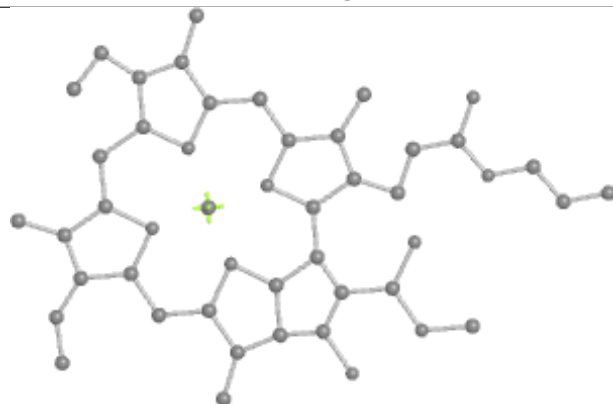
Bond lengths



Bond angles

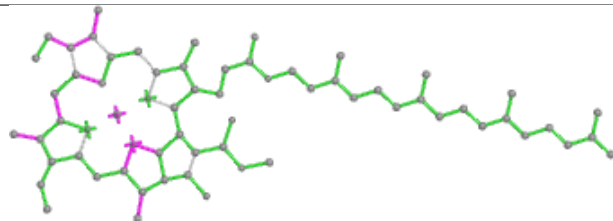


Torsions

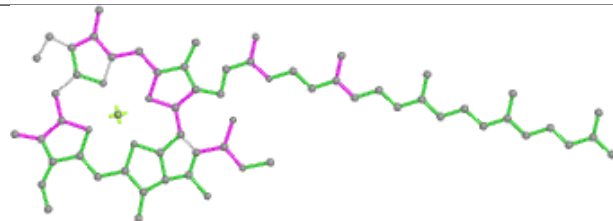


Rings

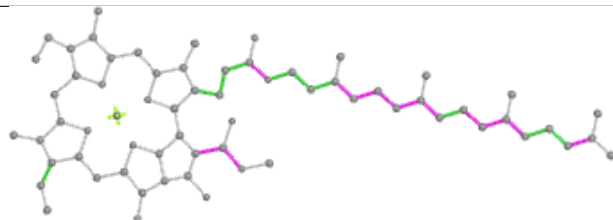
Ligand CLA 5 603



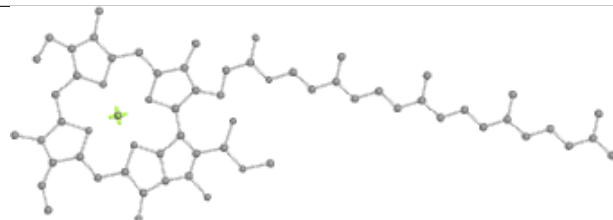
Bond lengths



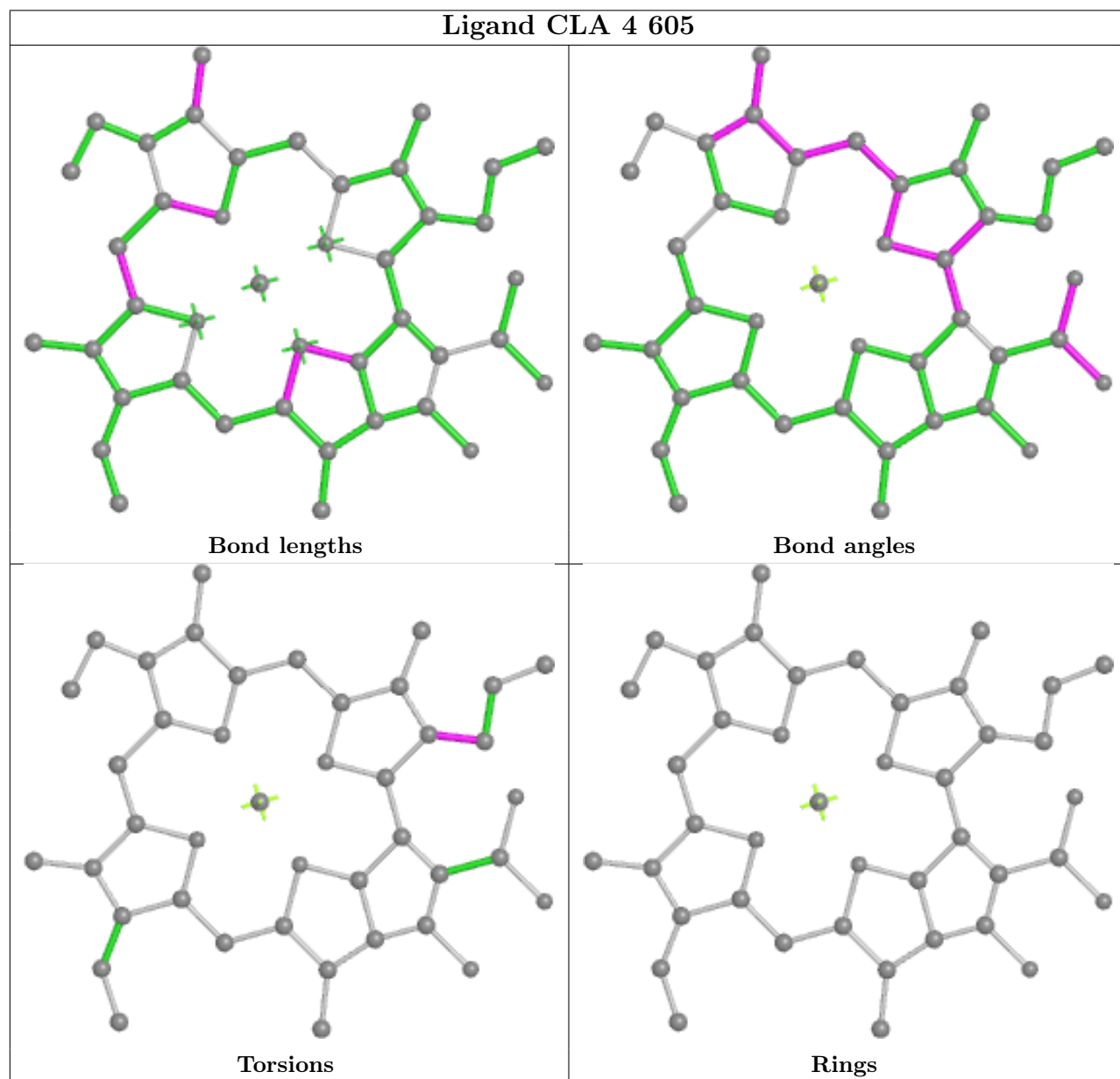
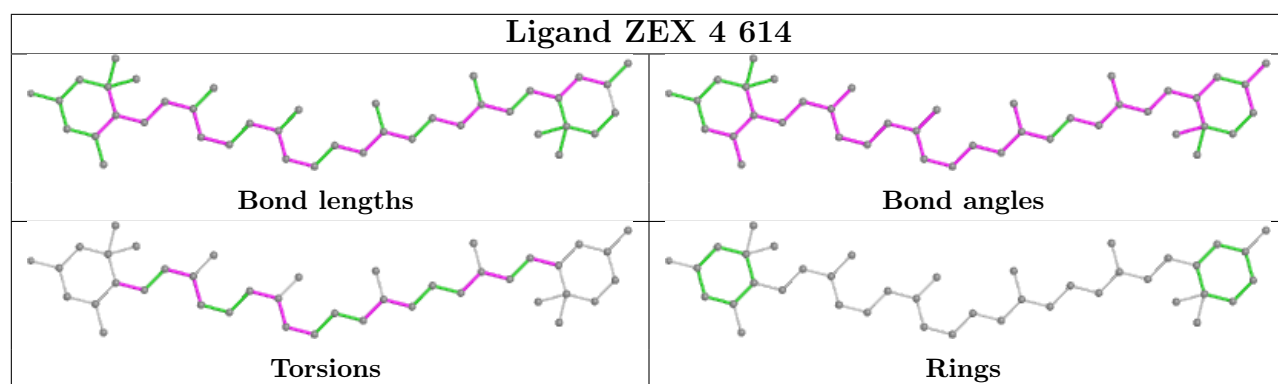
Bond angles

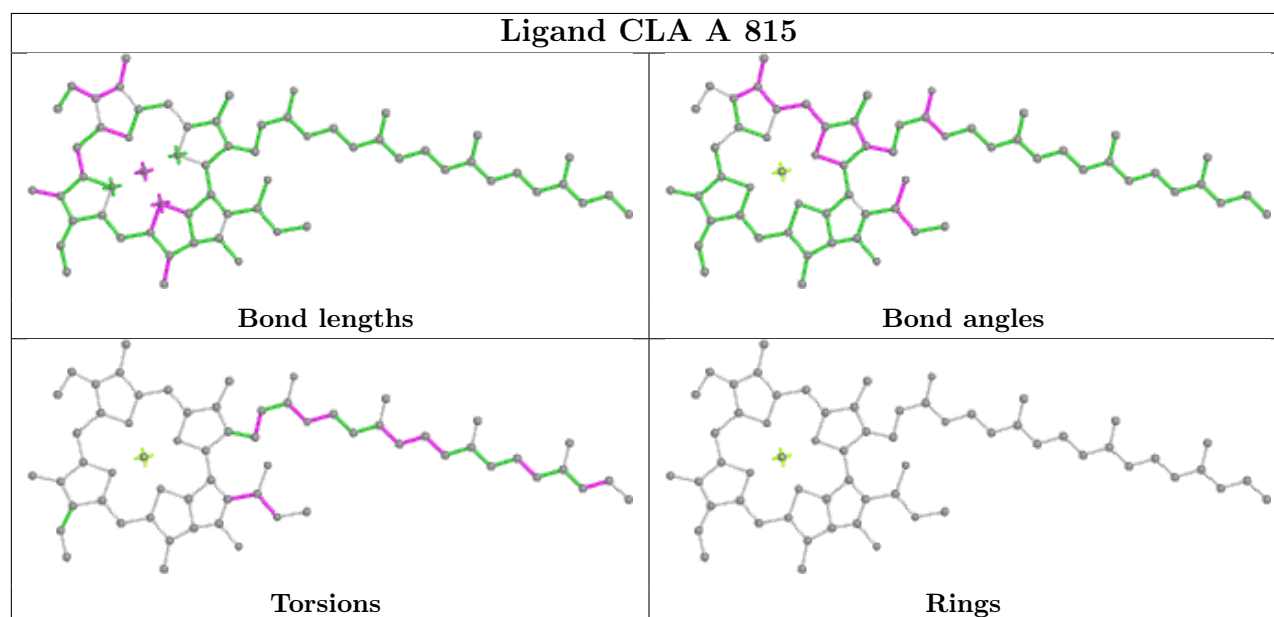
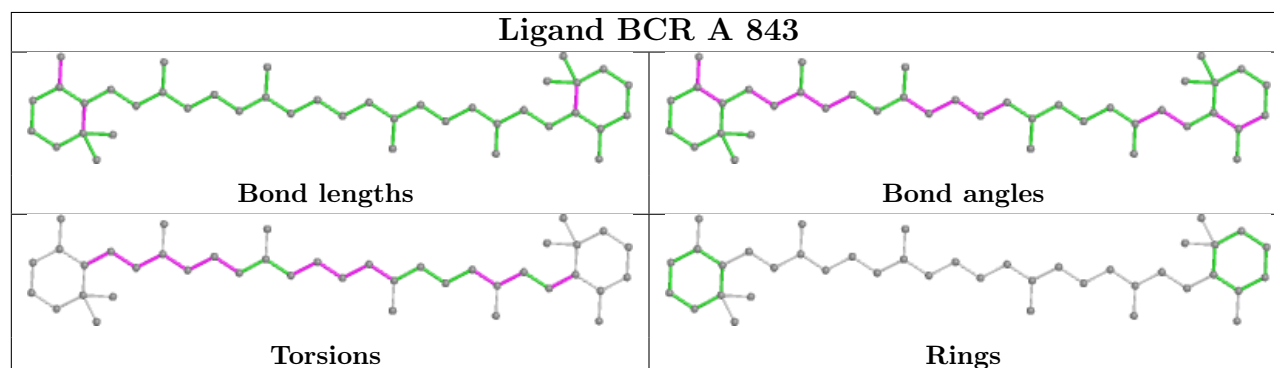
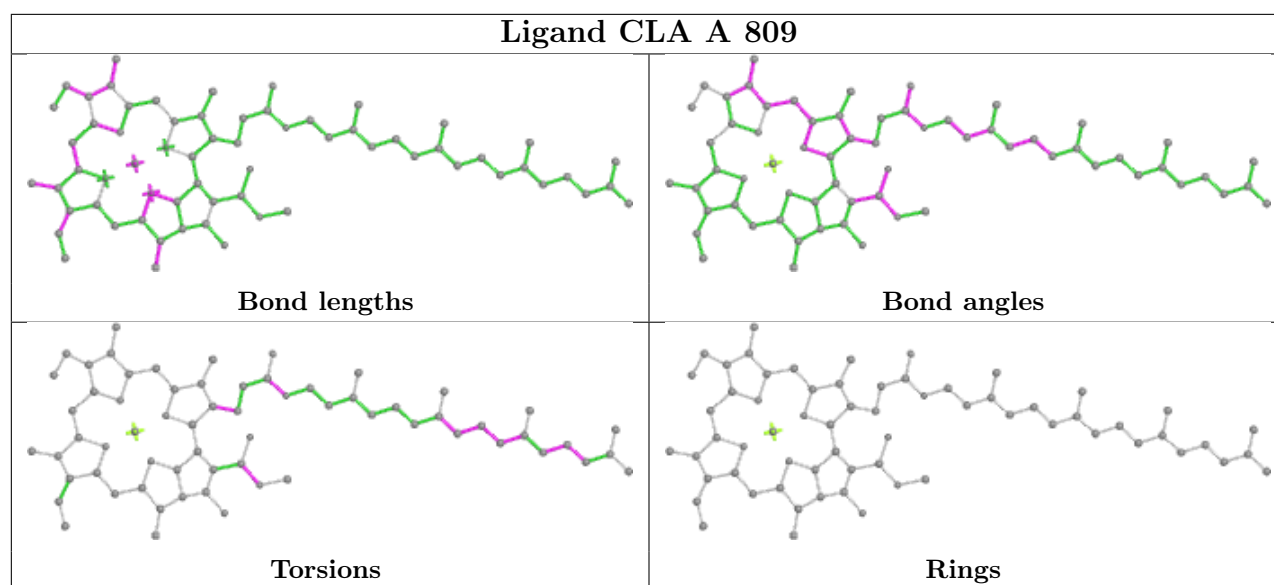


Torsions

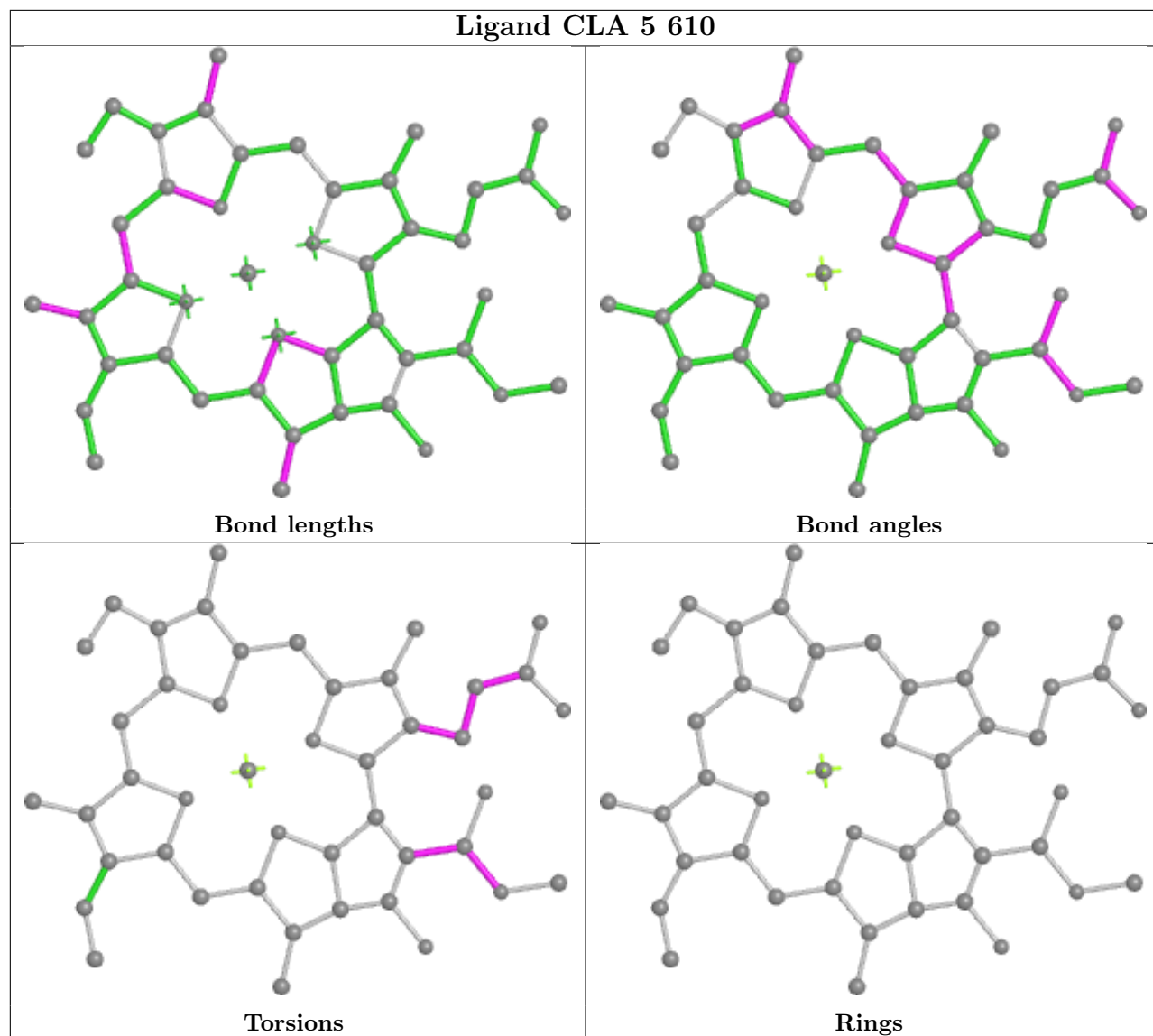


Rings

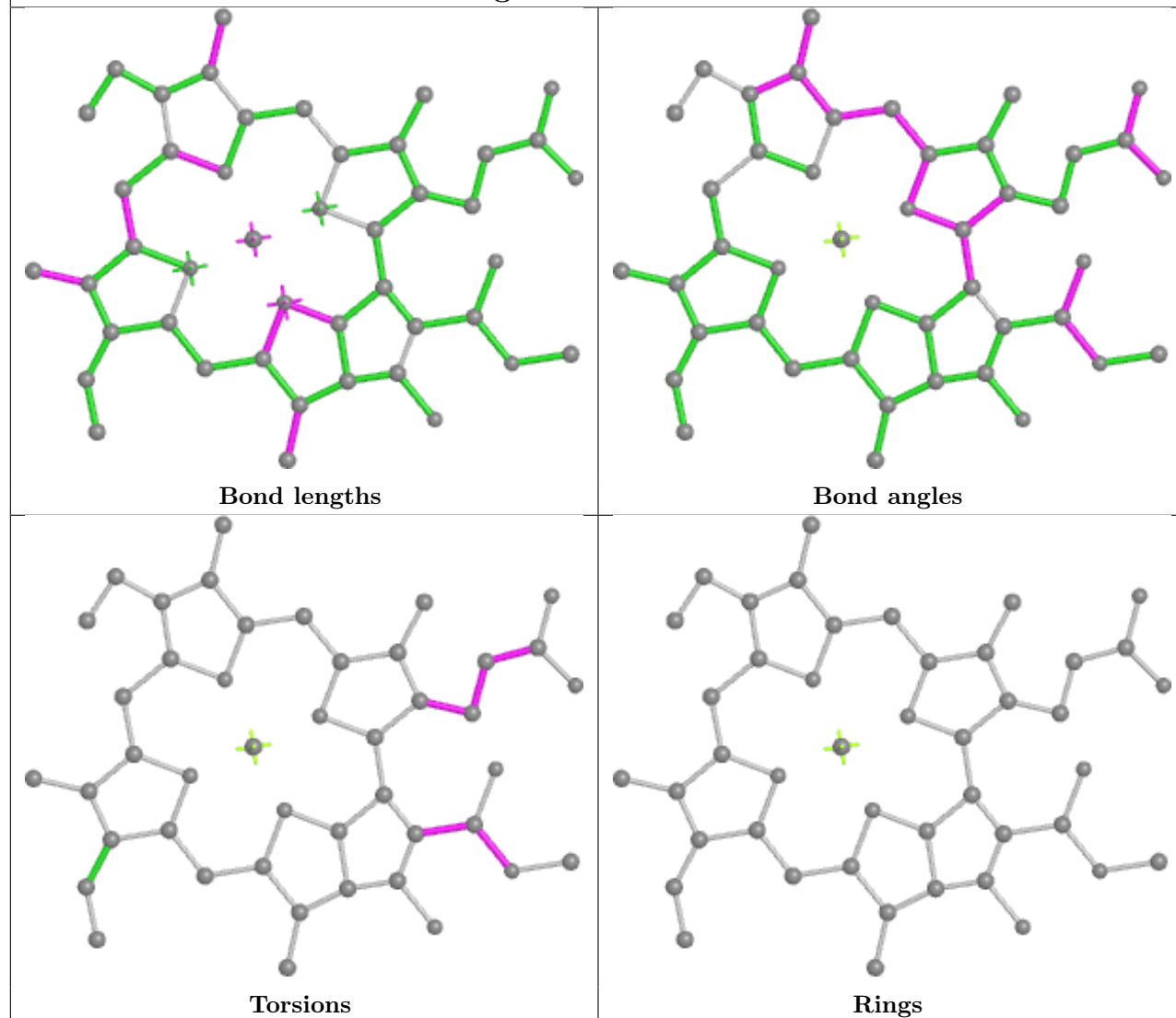




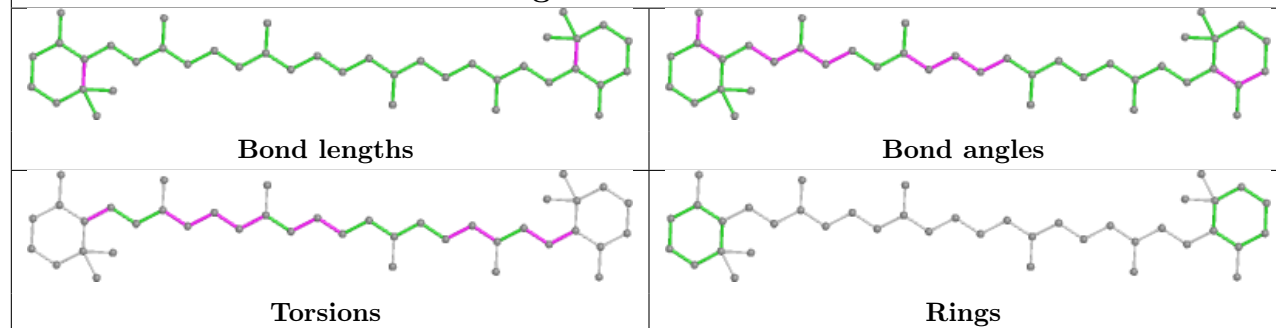
Ligand CLA 5 610

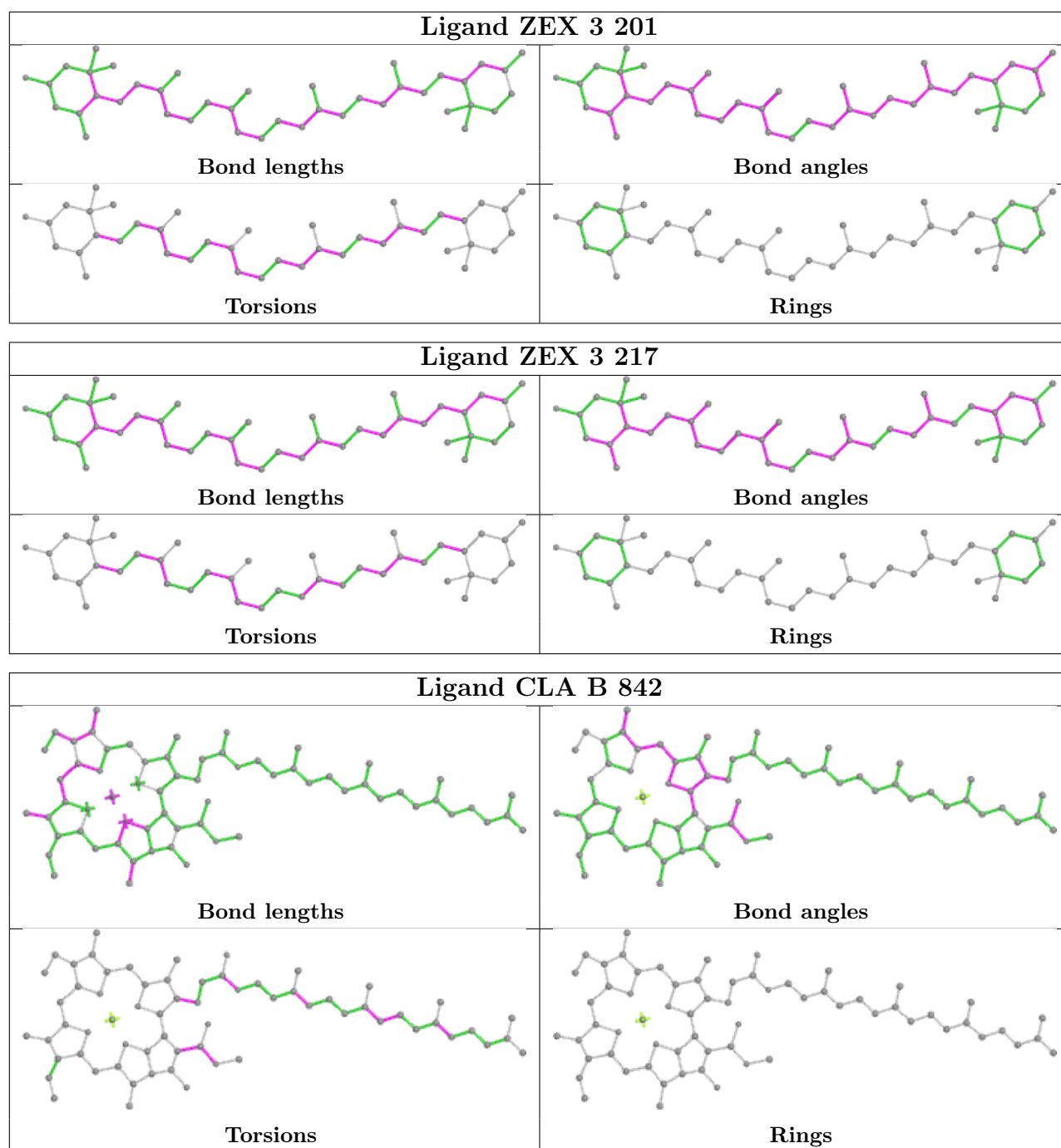


Ligand CLA 4 603

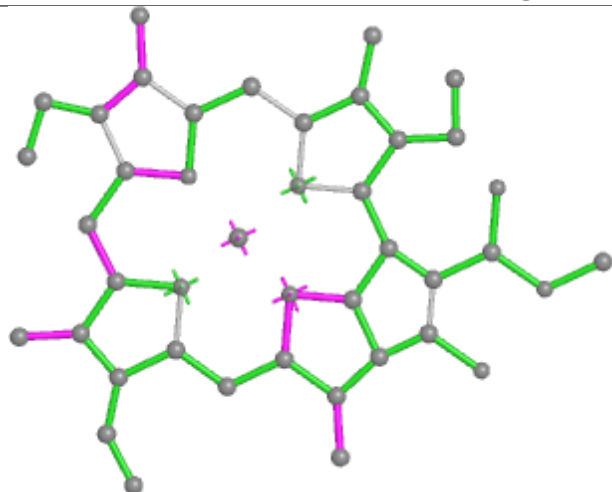


Ligand BCR L 206

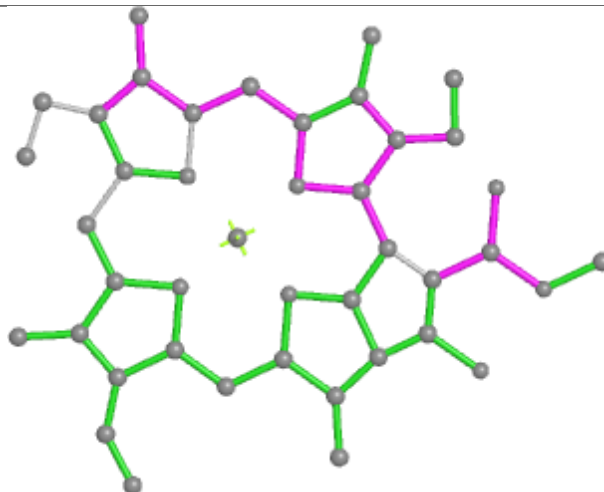




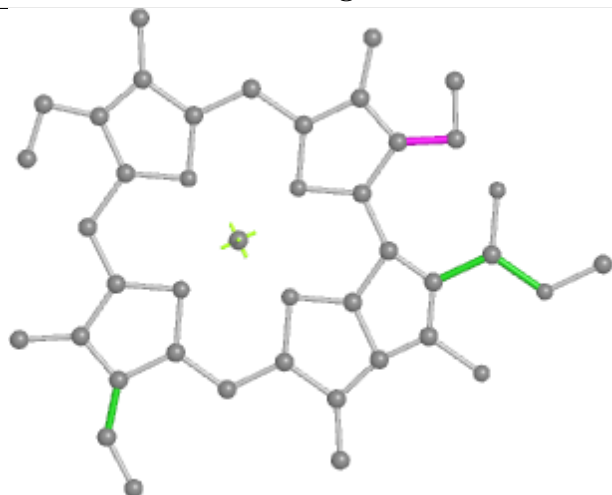
Ligand CLA 3 211



Bond lengths



Bond angles

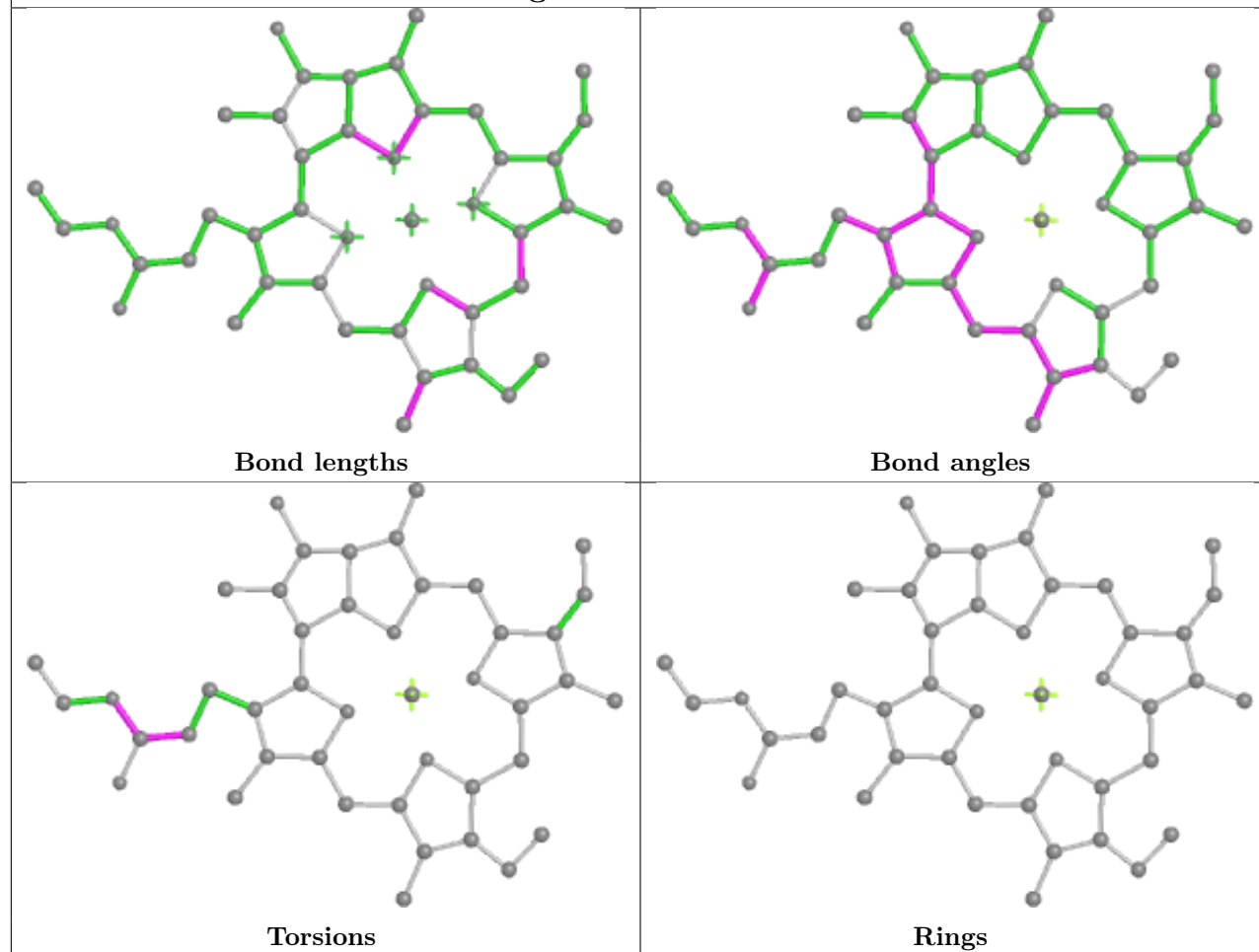


Torsions

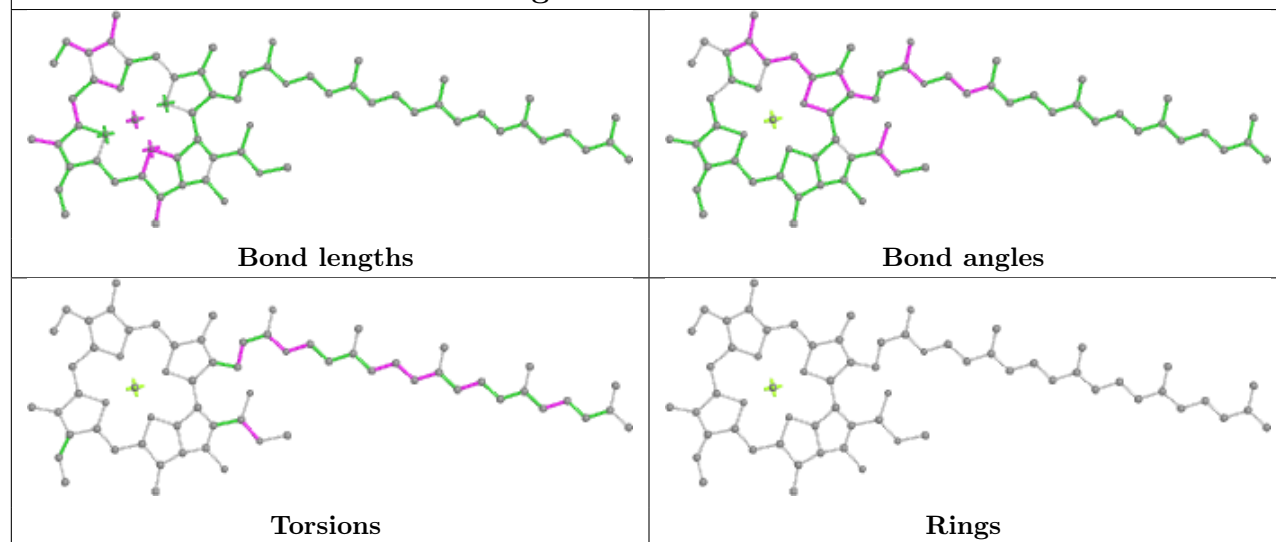


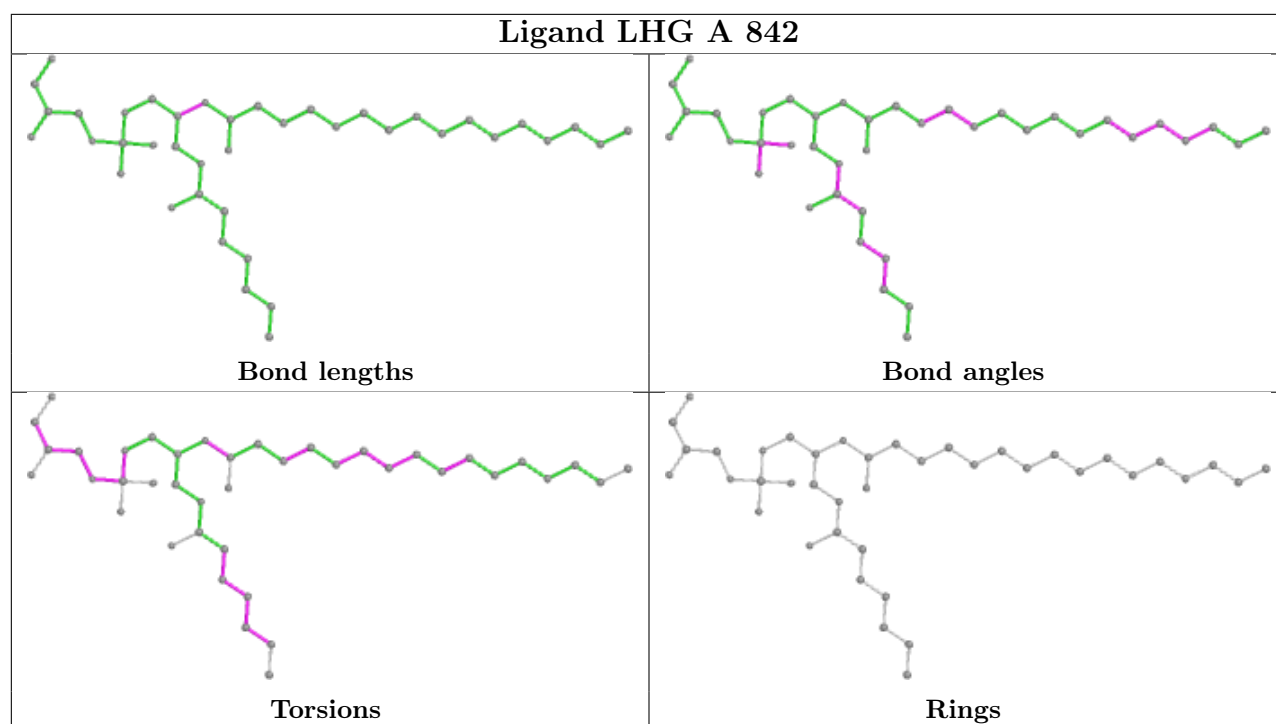
Rings

Ligand CLA 5 613

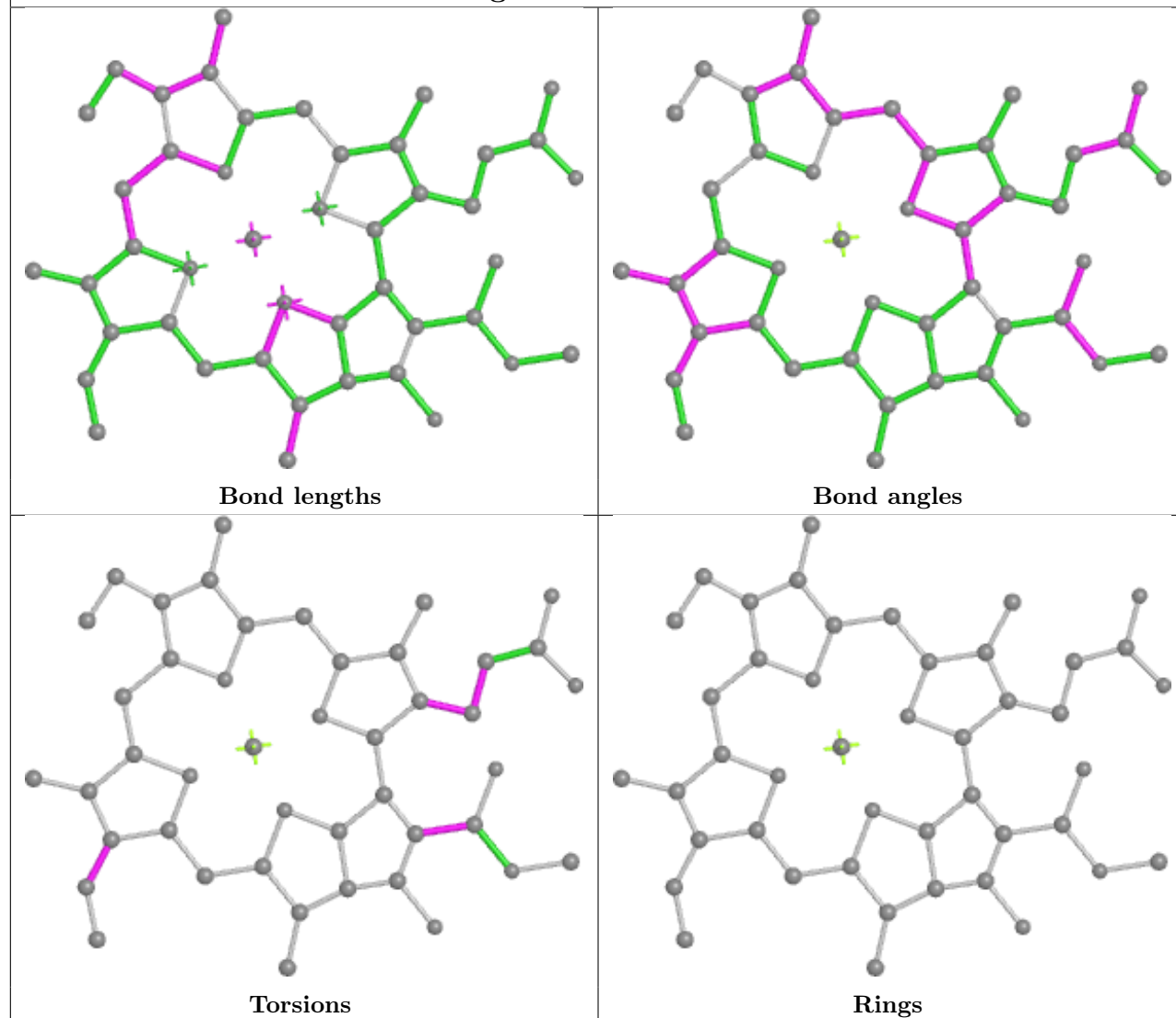


Ligand CLA A 838

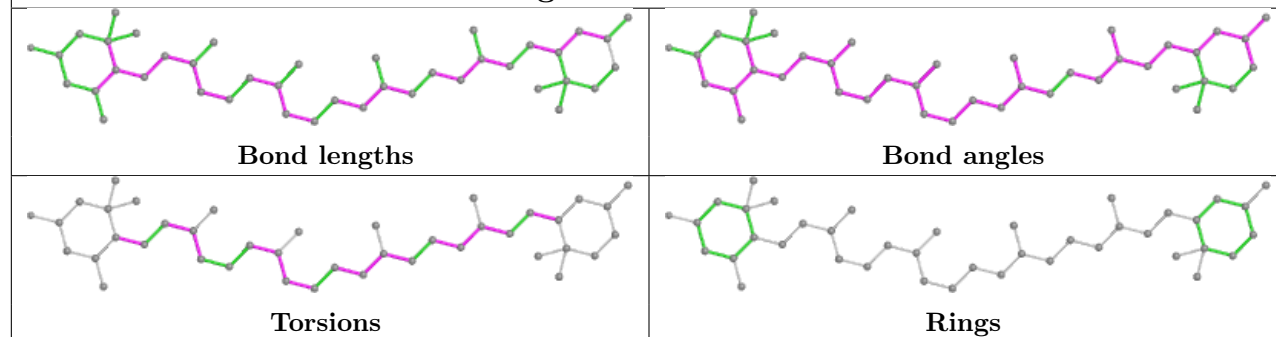




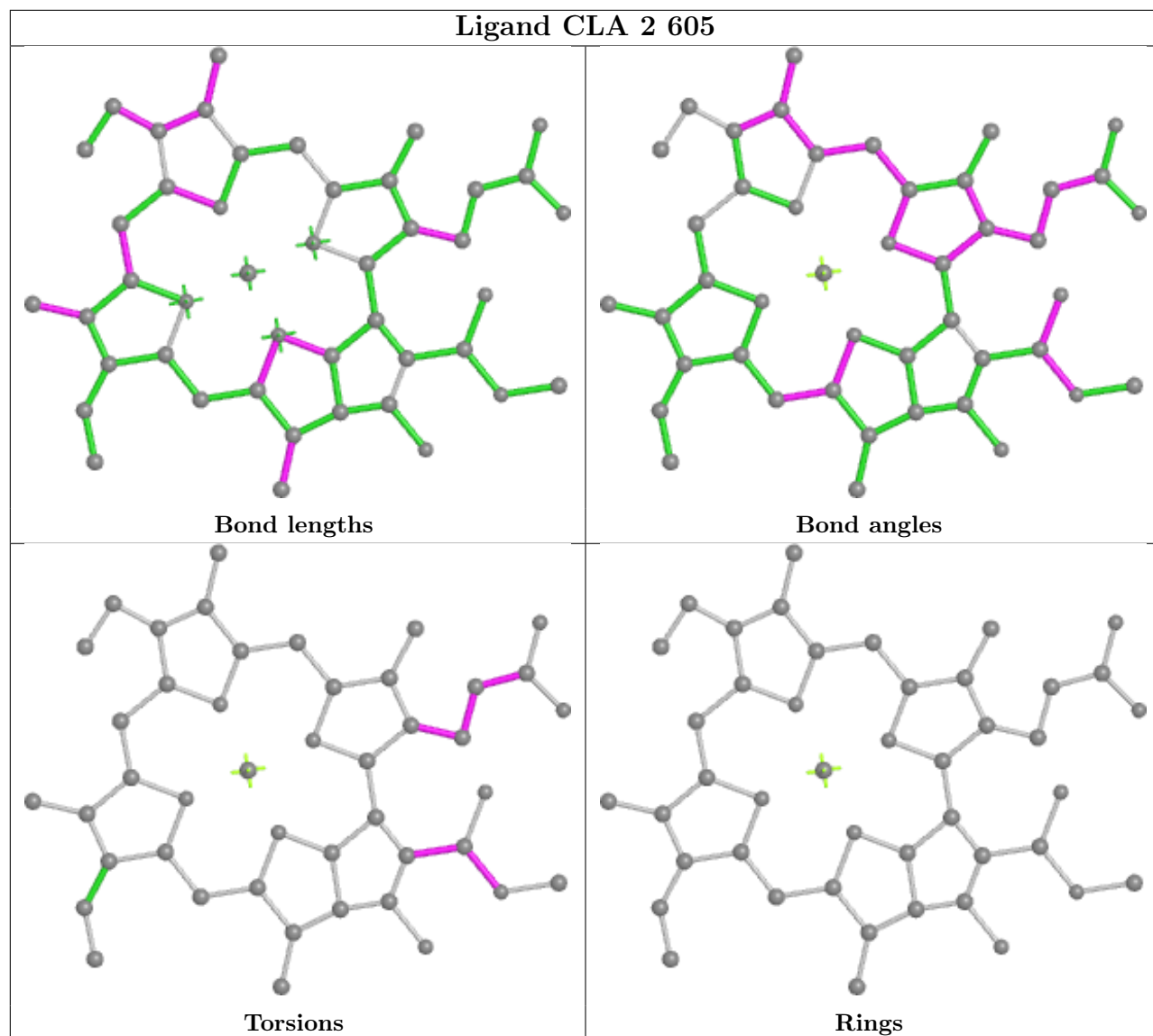
Ligand CLA A 818



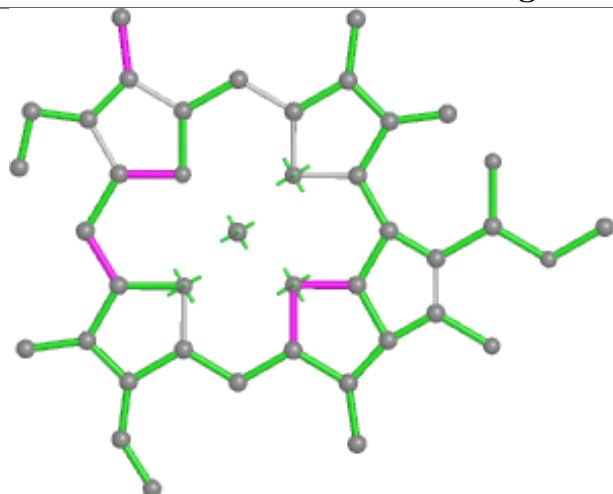
Ligand ZEX 3 216



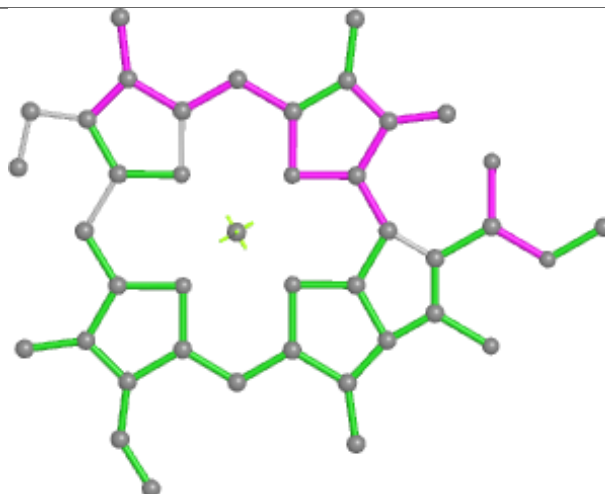
Ligand CLA 2 605



Ligand CLA 4 609



Bond lengths



Bond angles

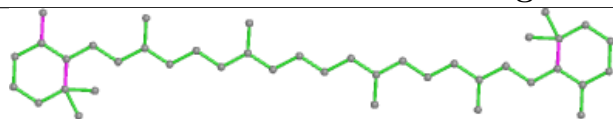


Torsions

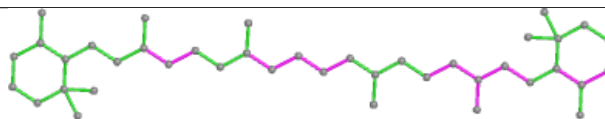


Rings

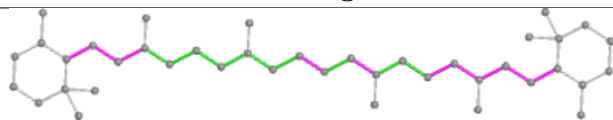
Ligand BCR J 105



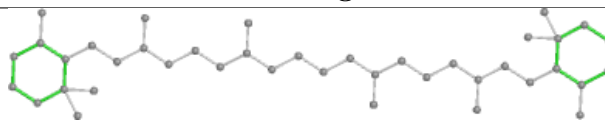
Bond lengths



Bond angles

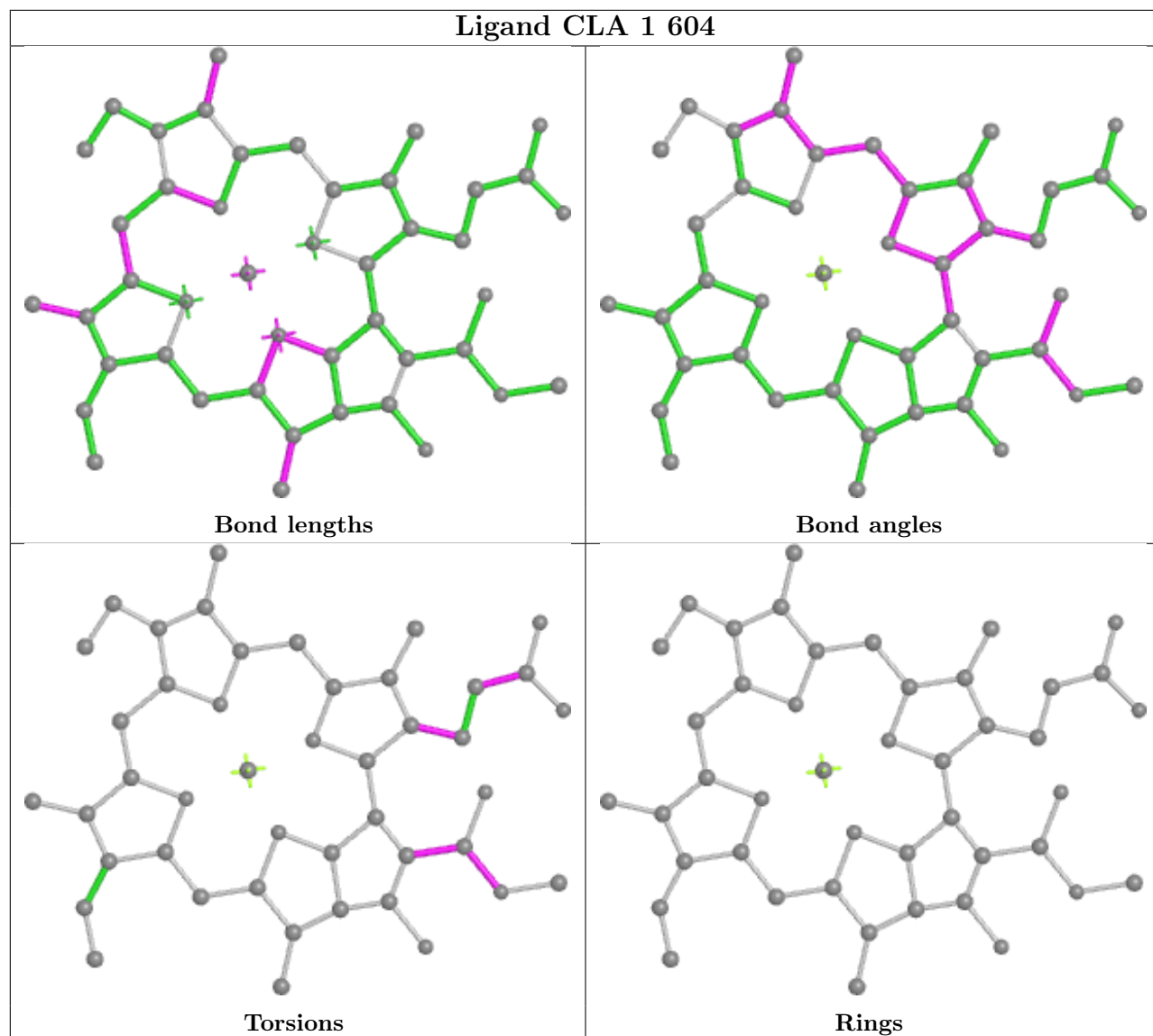


Torsions

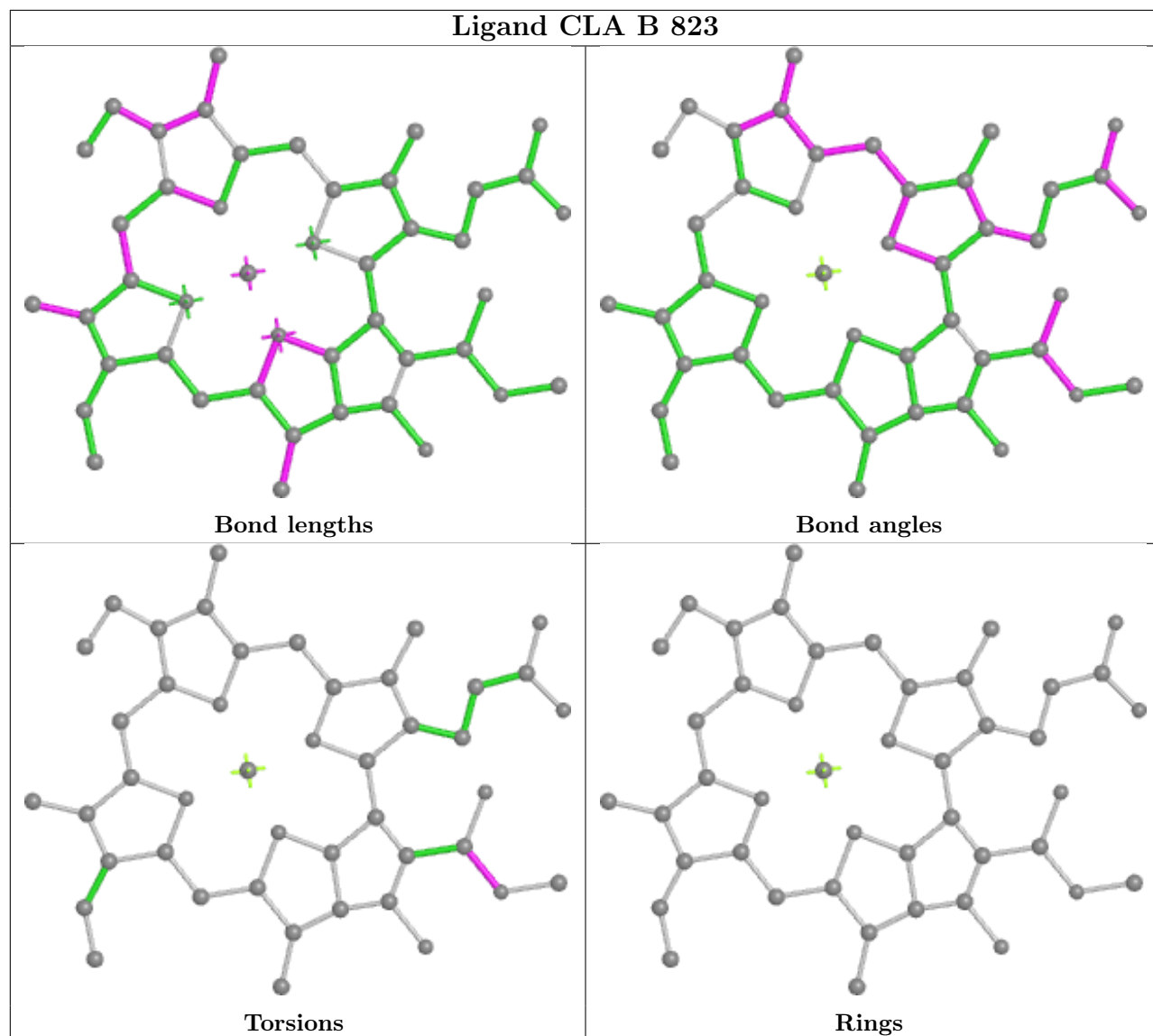


Rings

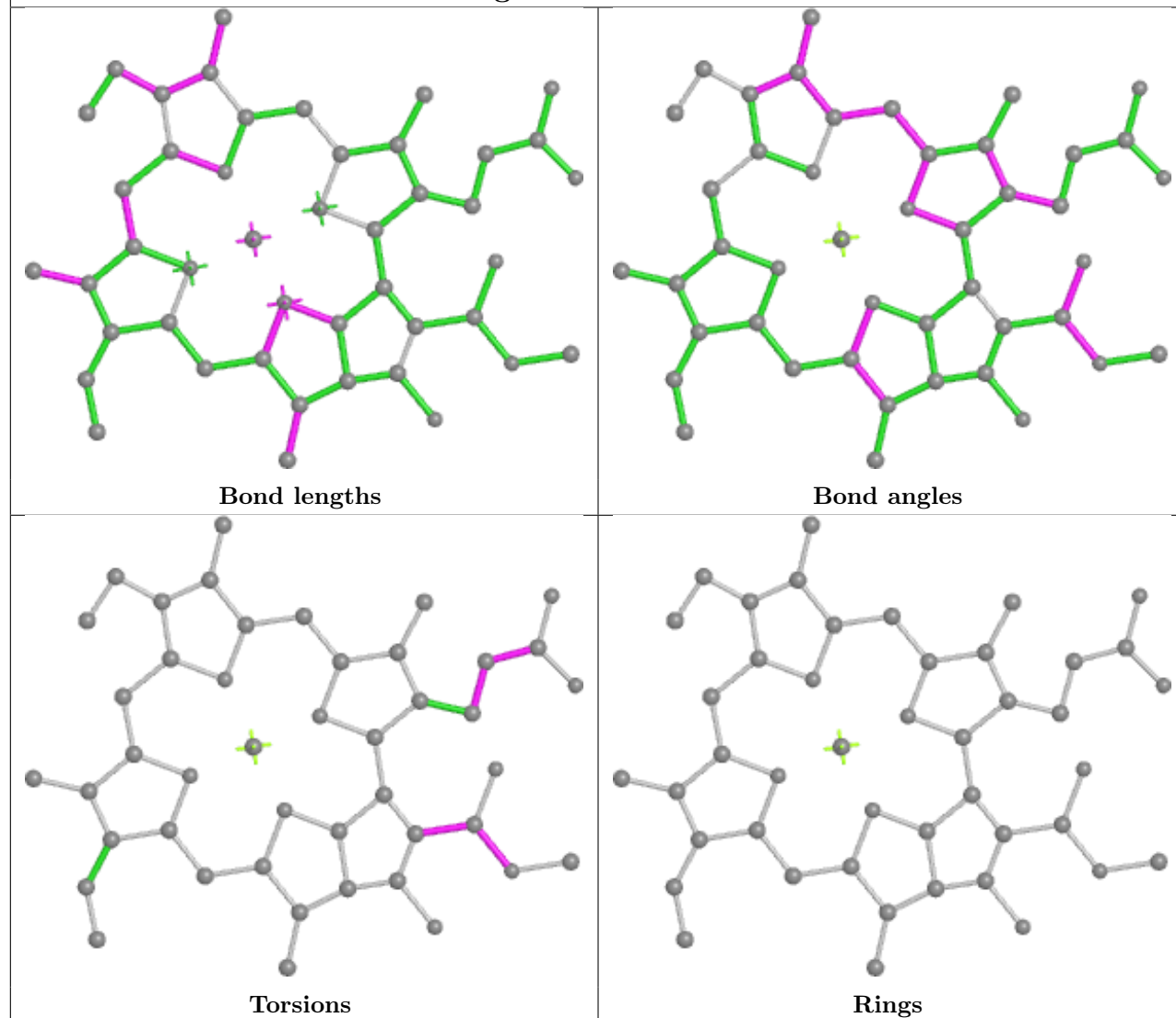
Ligand CLA 1 604



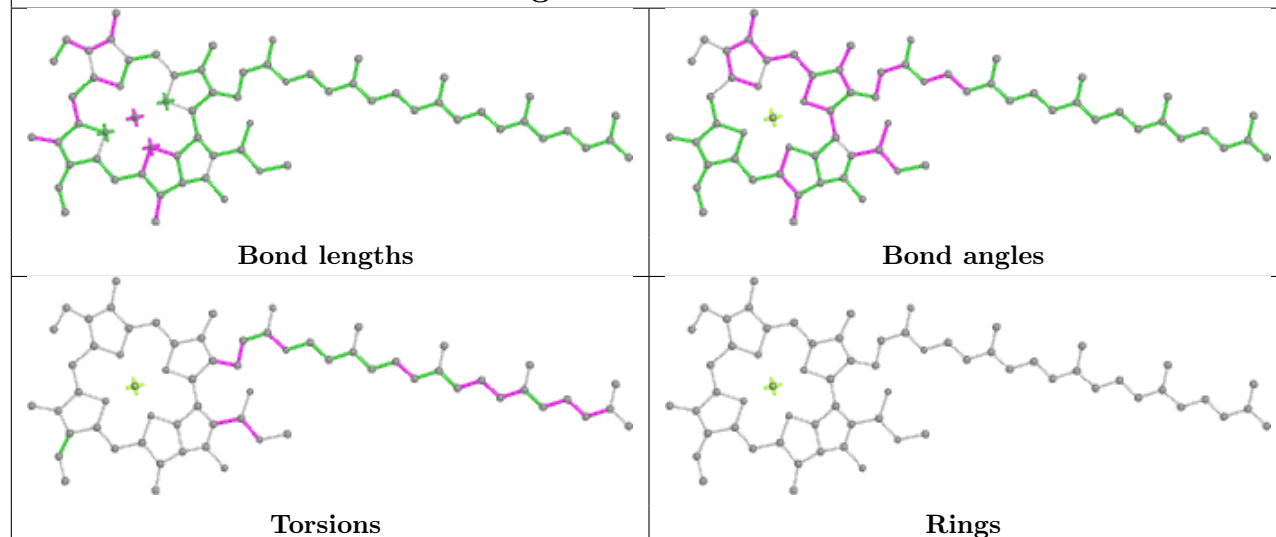
Ligand CLA B 823



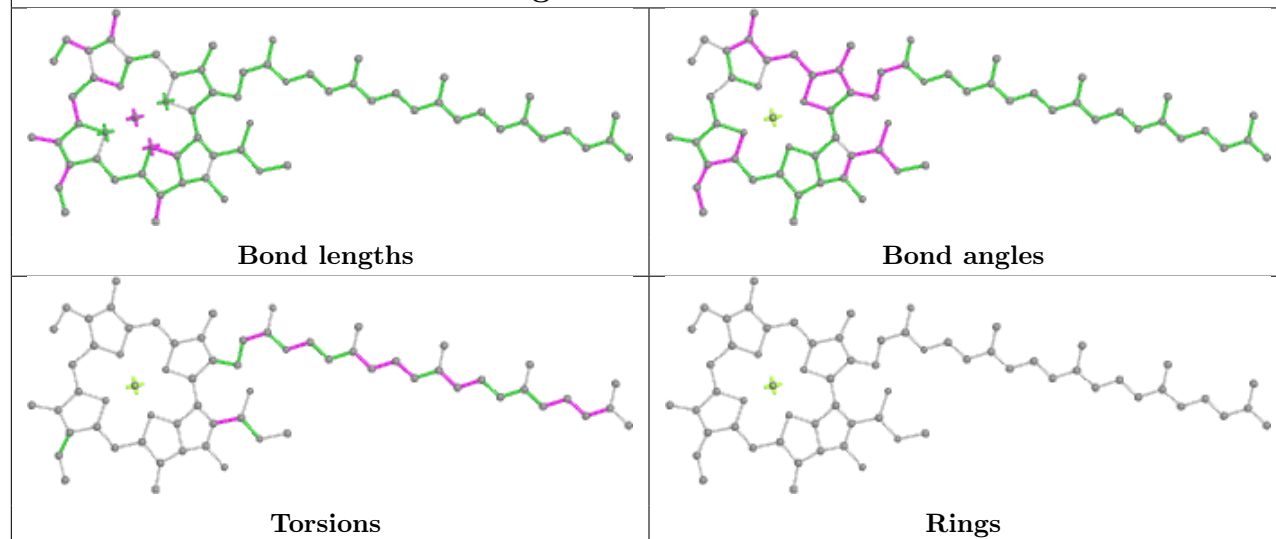
Ligand CLA 1 603



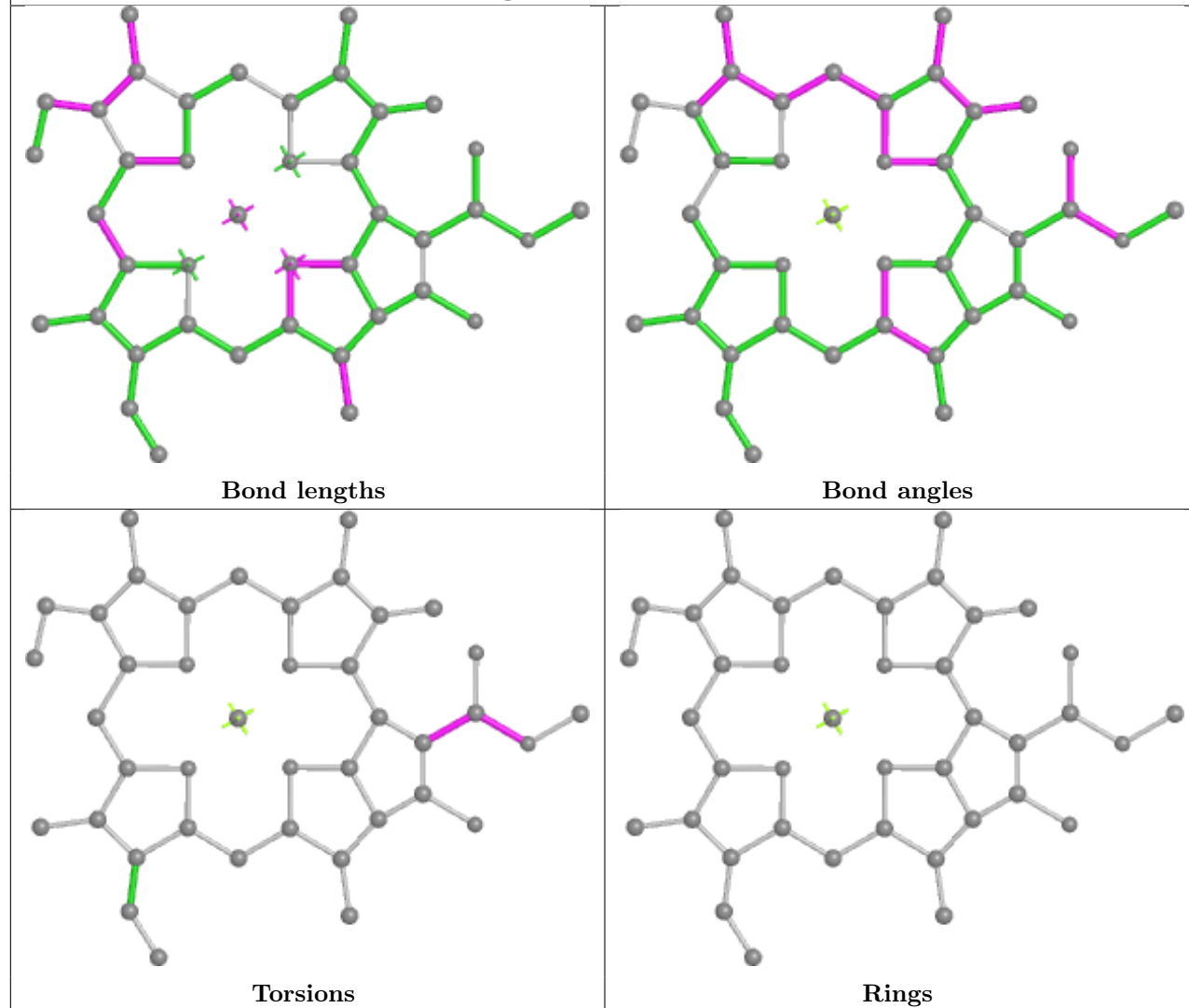
Ligand CLA A 827

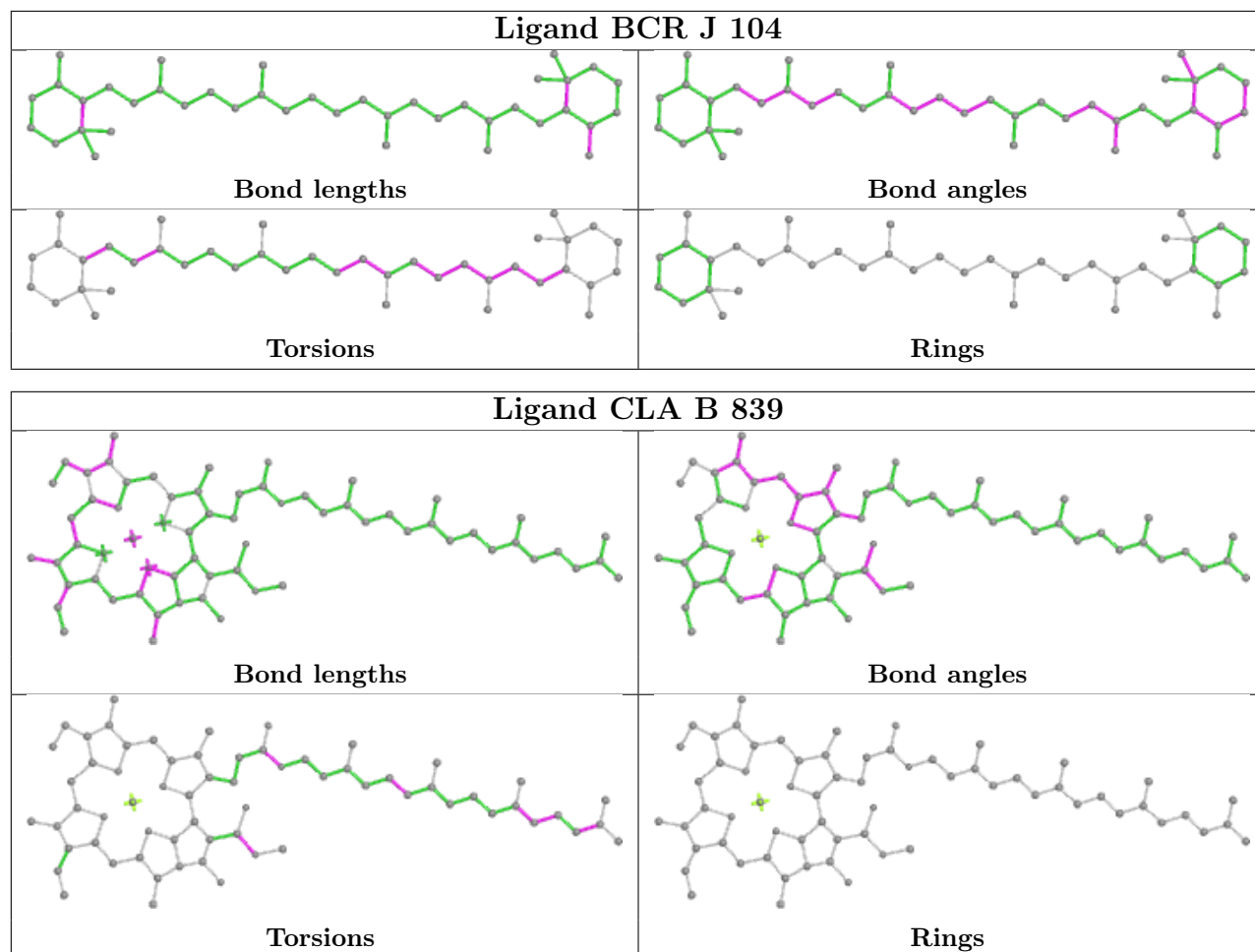


Ligand CLA B 801

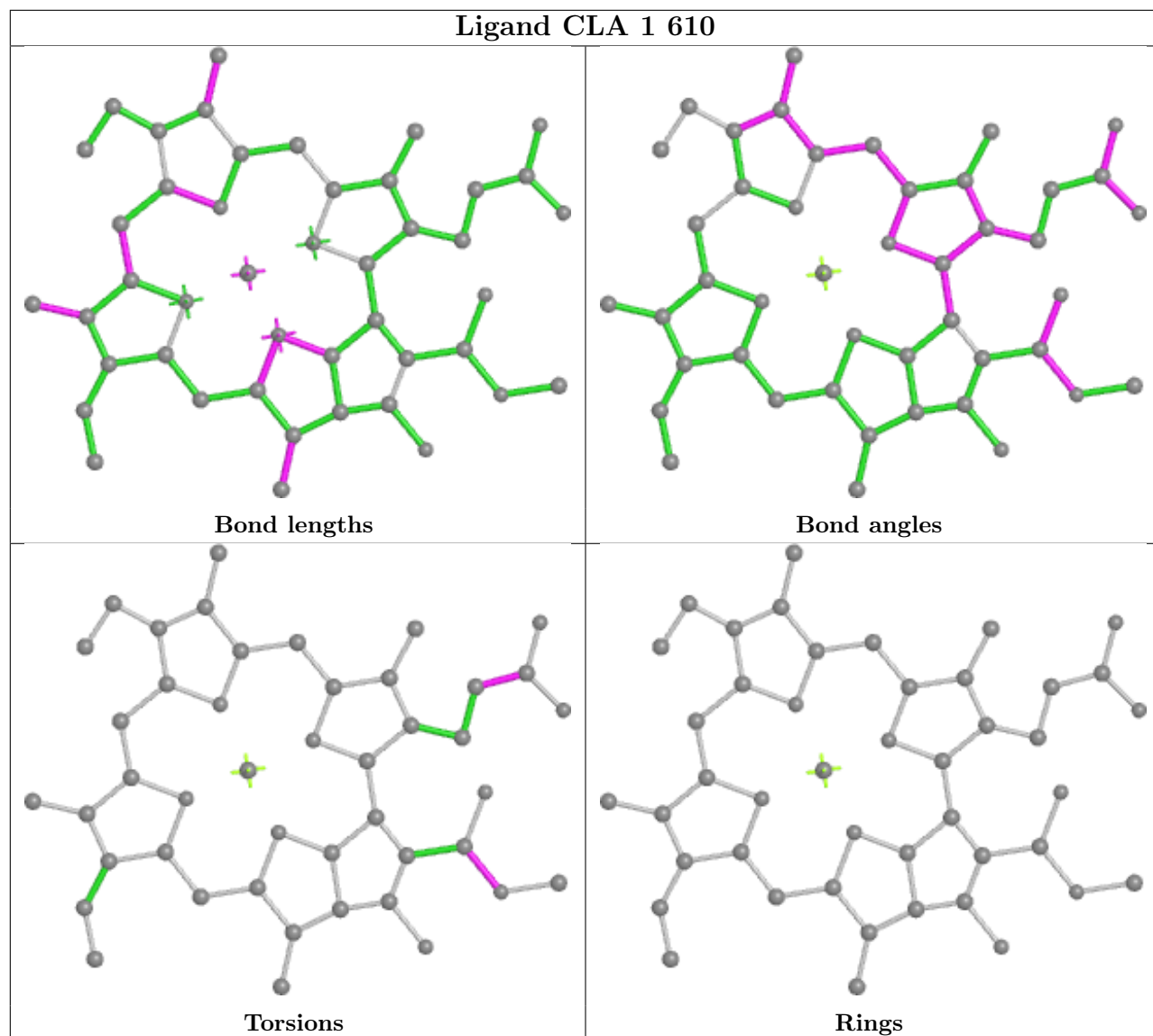


Ligand CLA 2 609

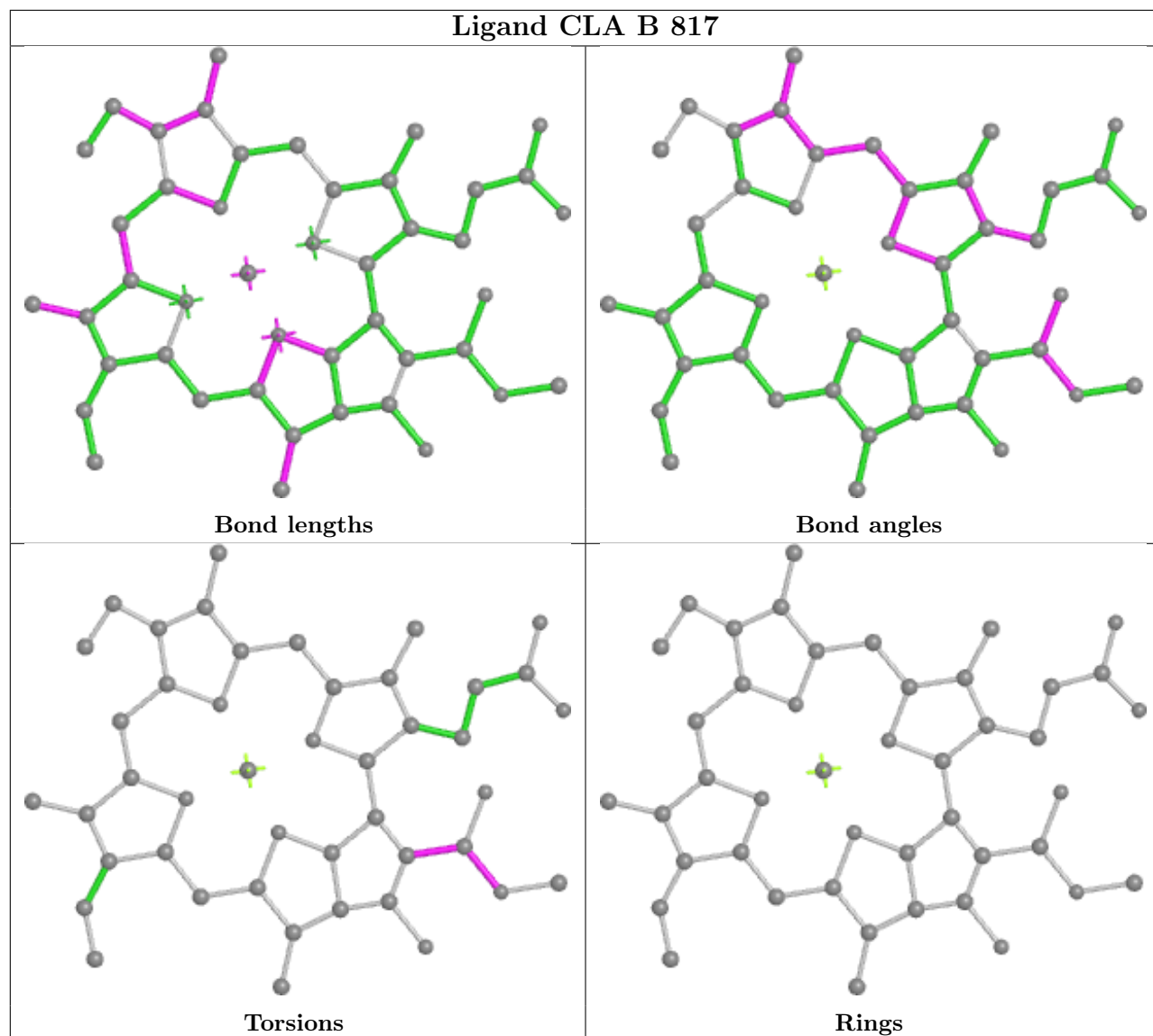


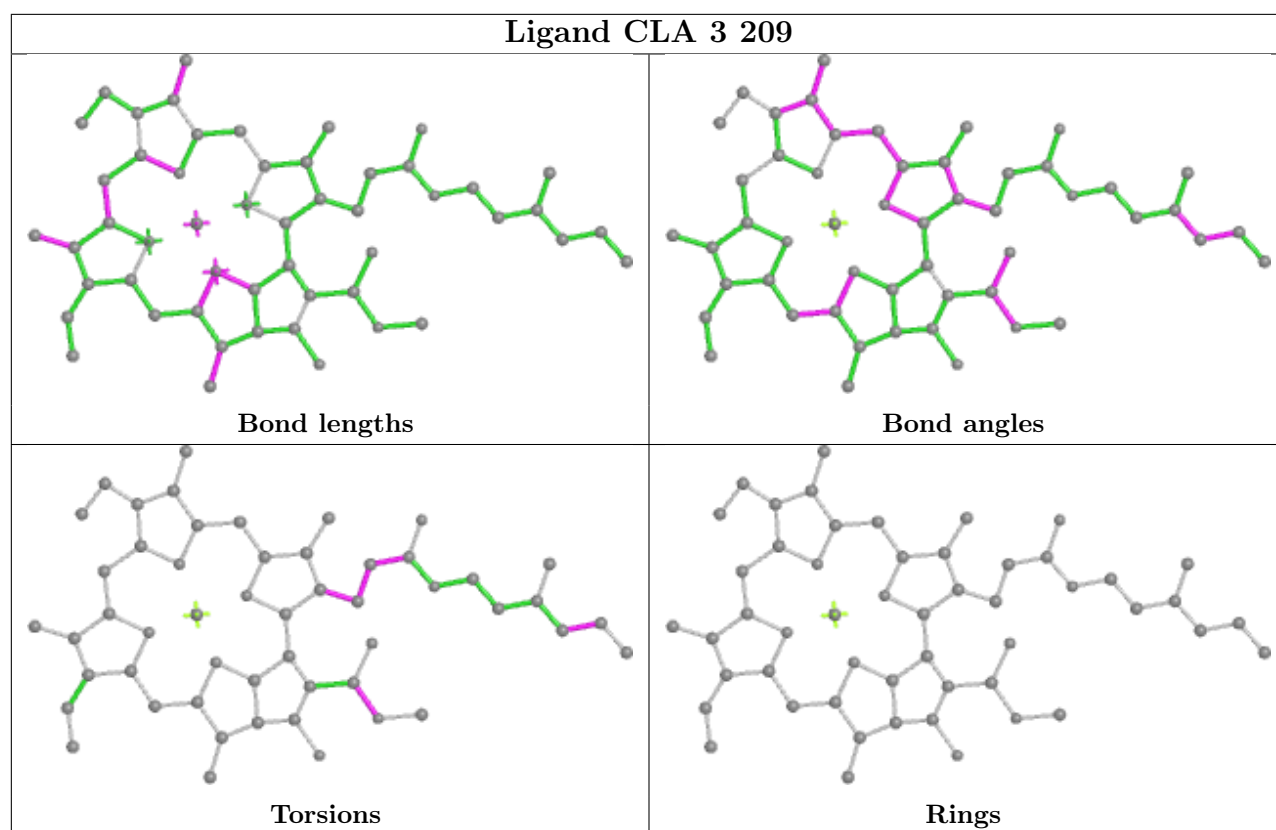


Ligand CLA 1 610

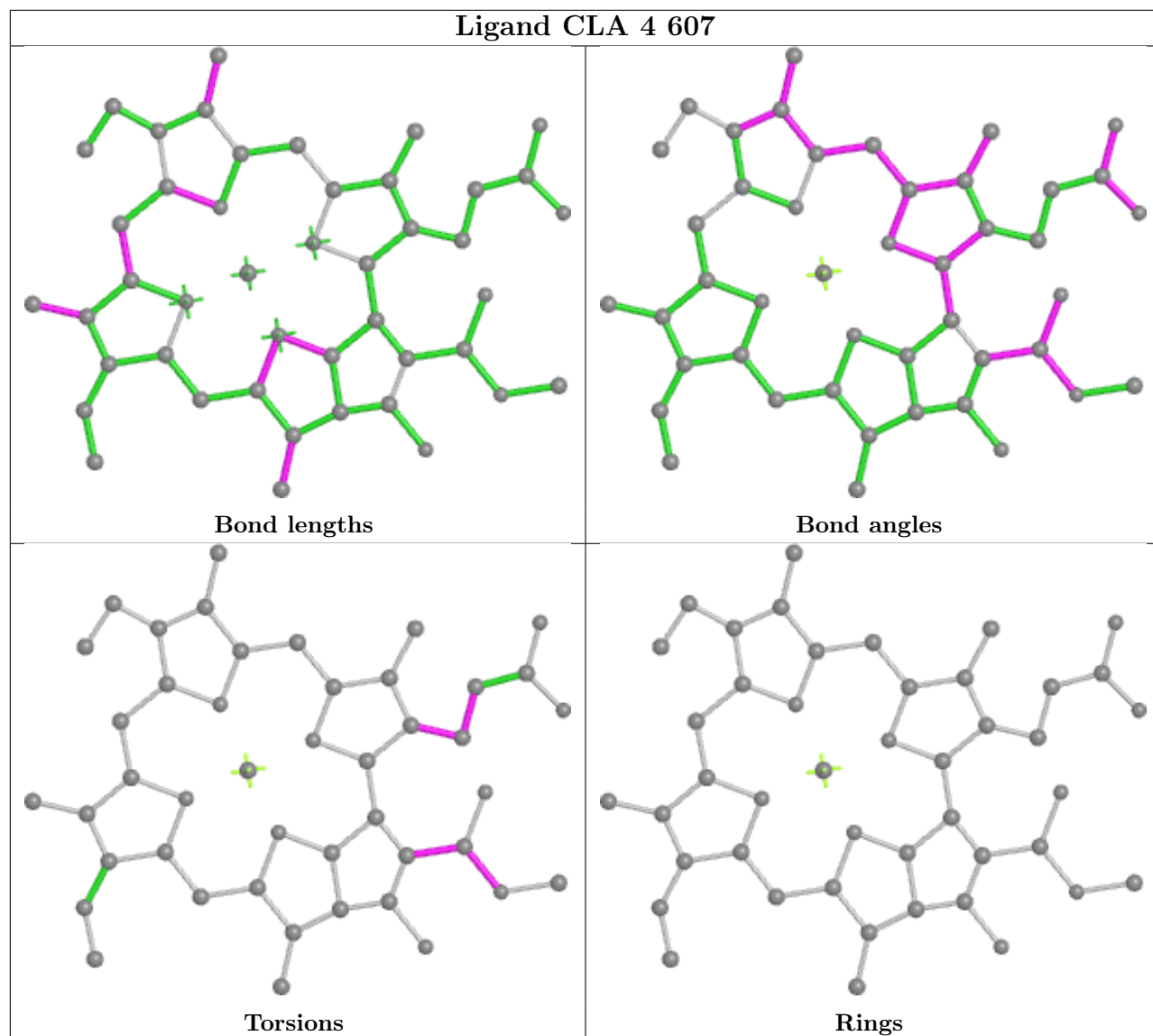


Ligand CLA B 817

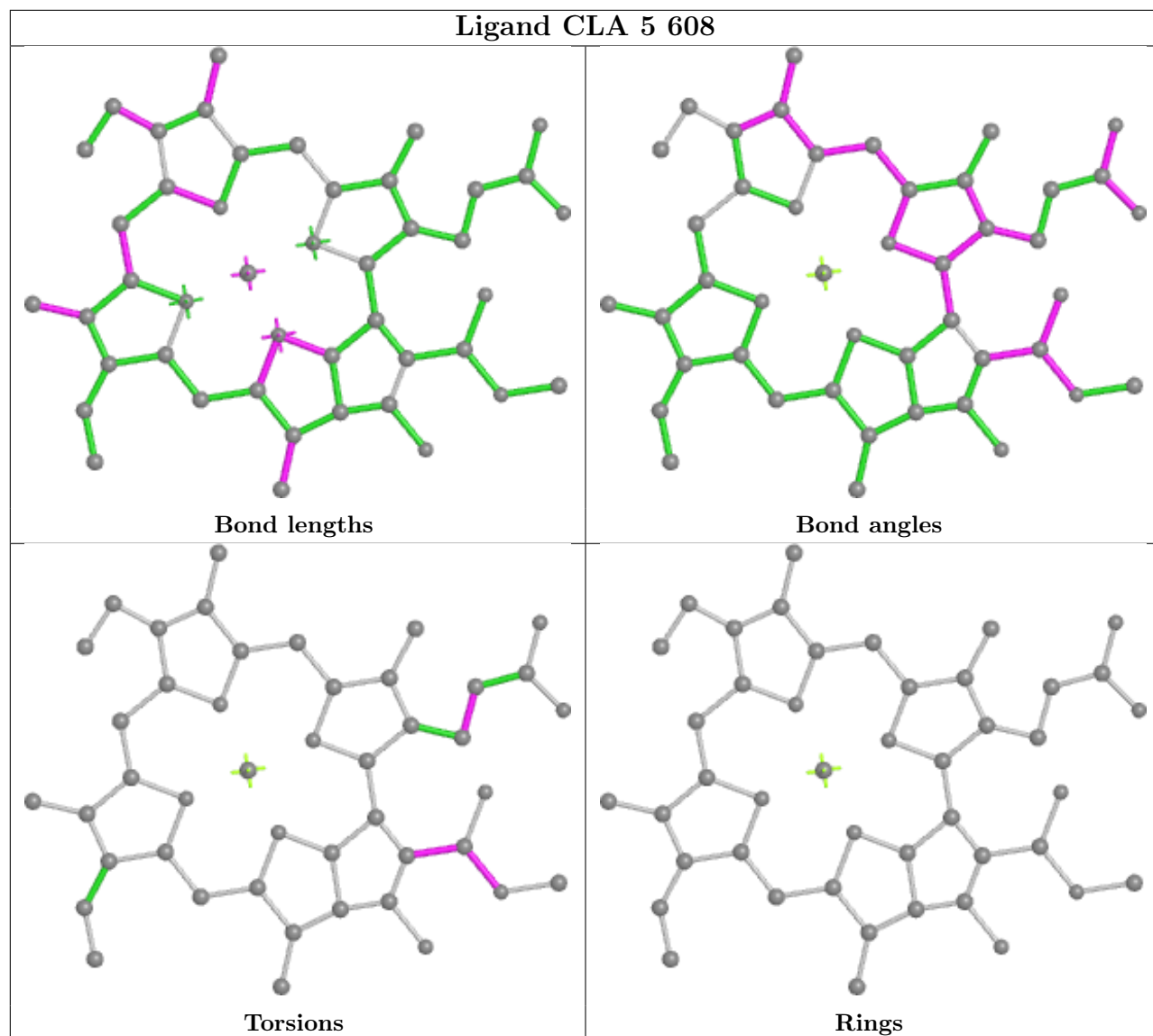


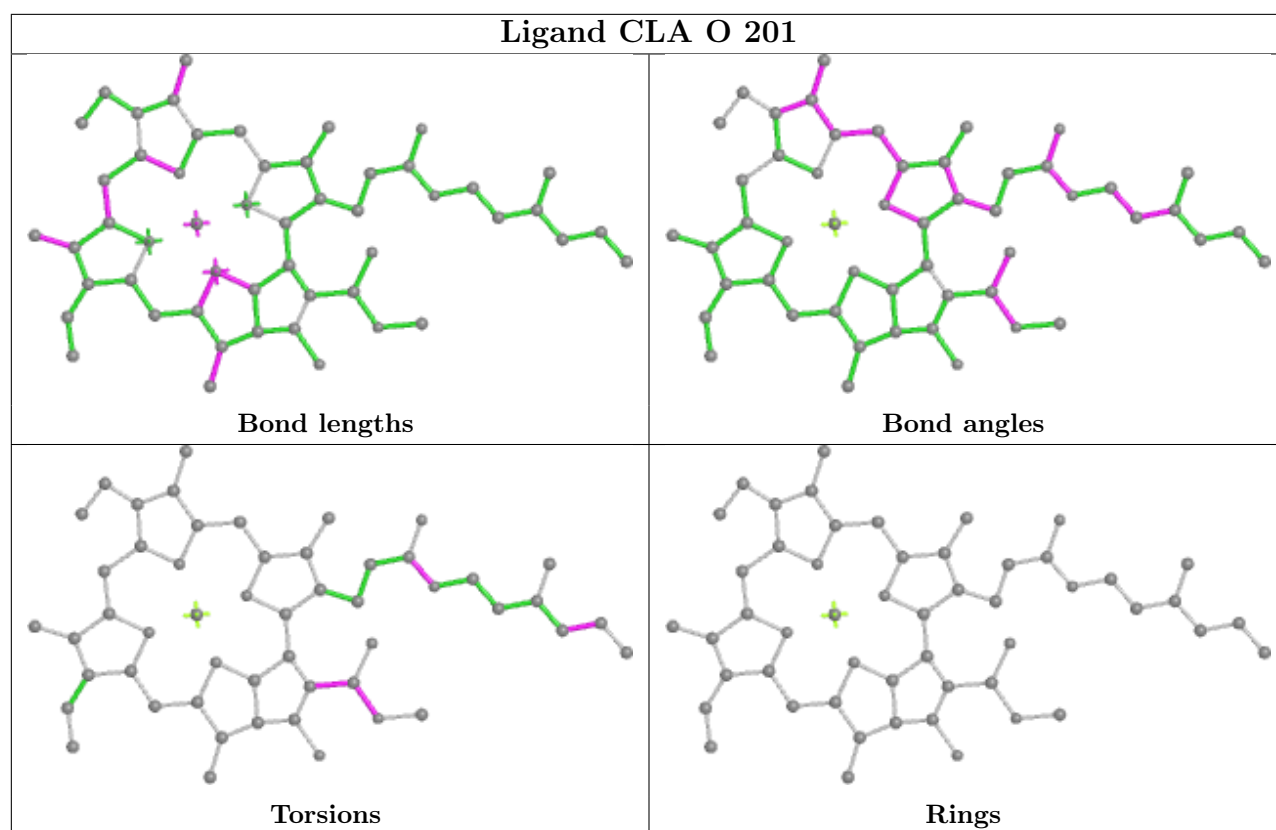


Ligand CLA 4 607

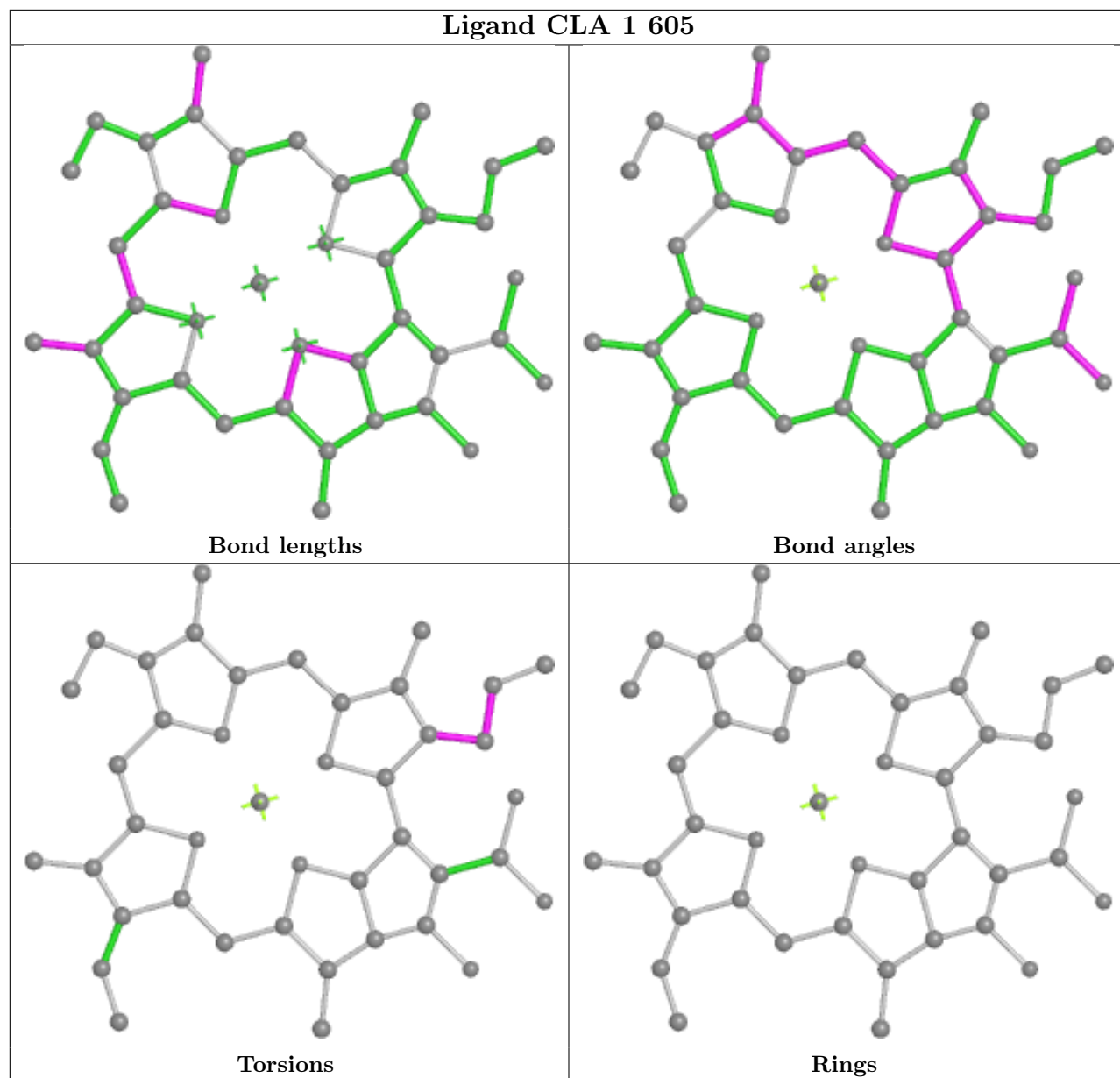


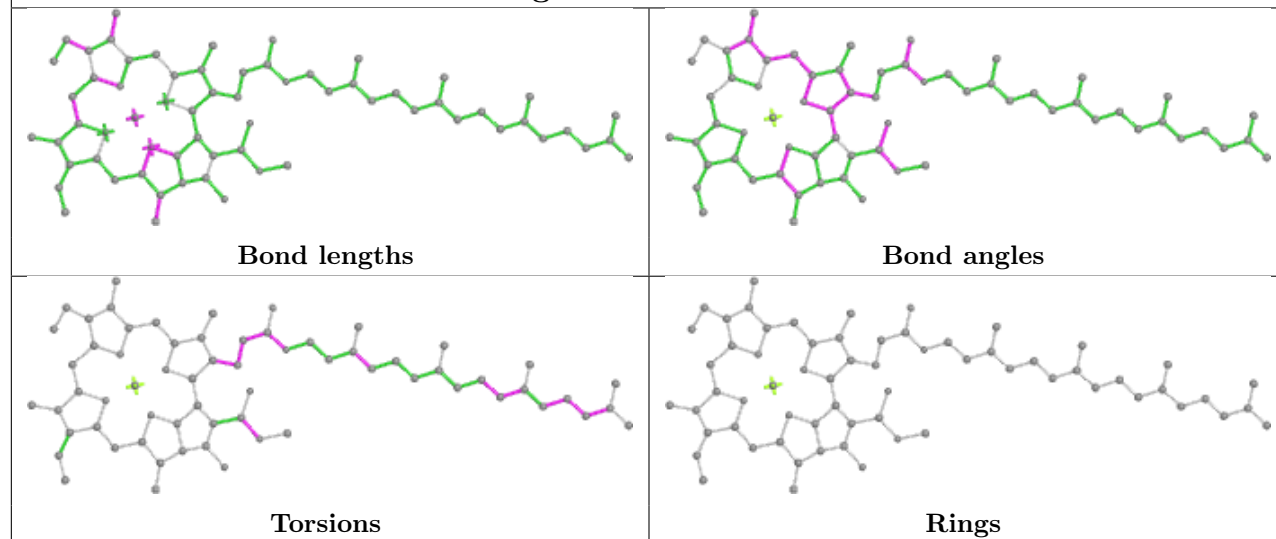
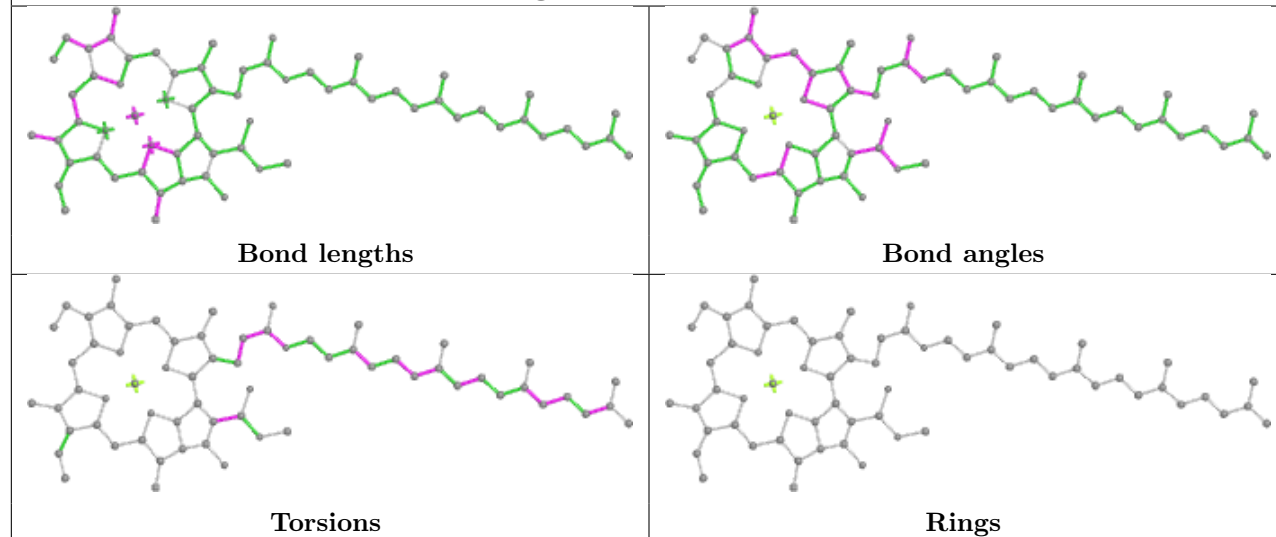
Ligand CLA 5 608



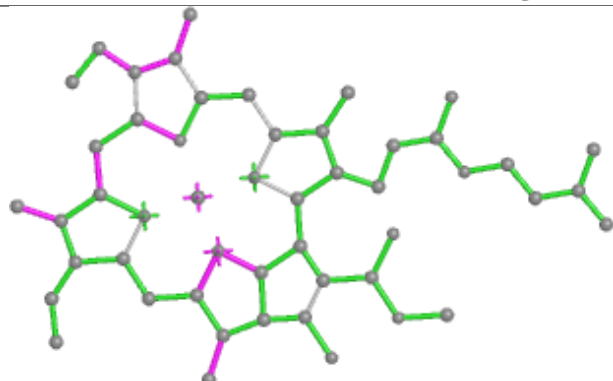


Ligand CLA 1 605

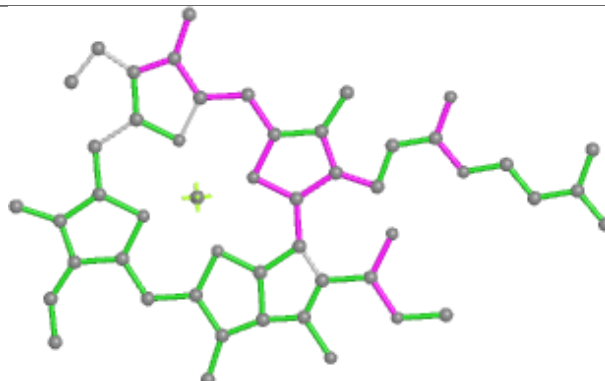


Ligand CLA B 843**Ligand CLA B 810**

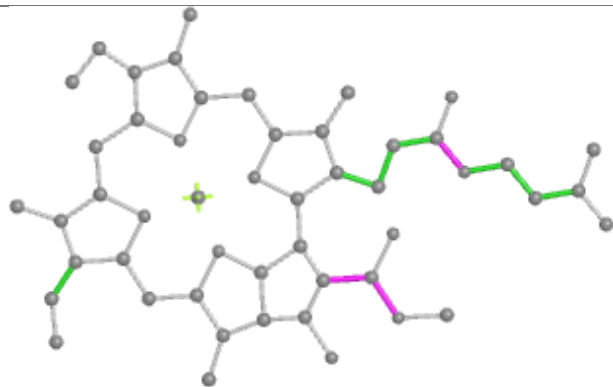
Ligand CLA L 204



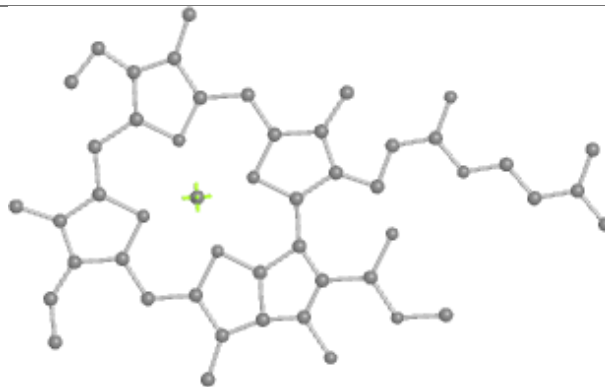
Bond lengths



Bond angles

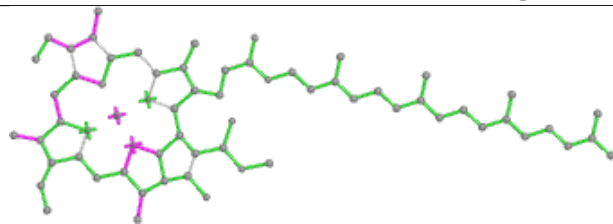


Torsions

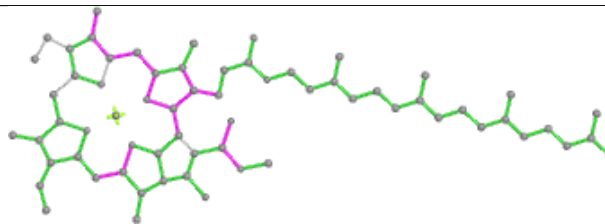


Rings

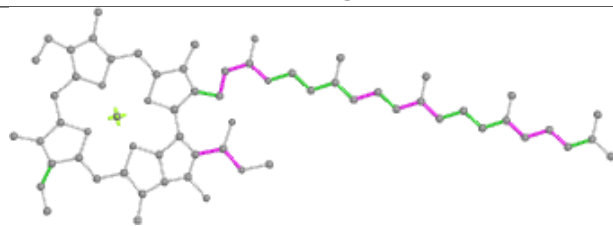
Ligand CLA B 835



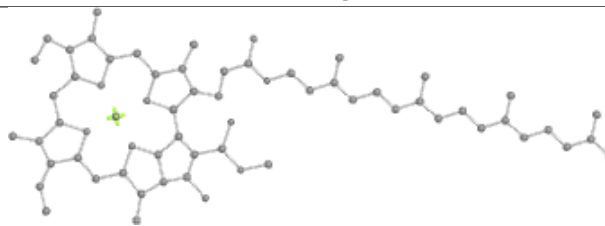
Bond lengths



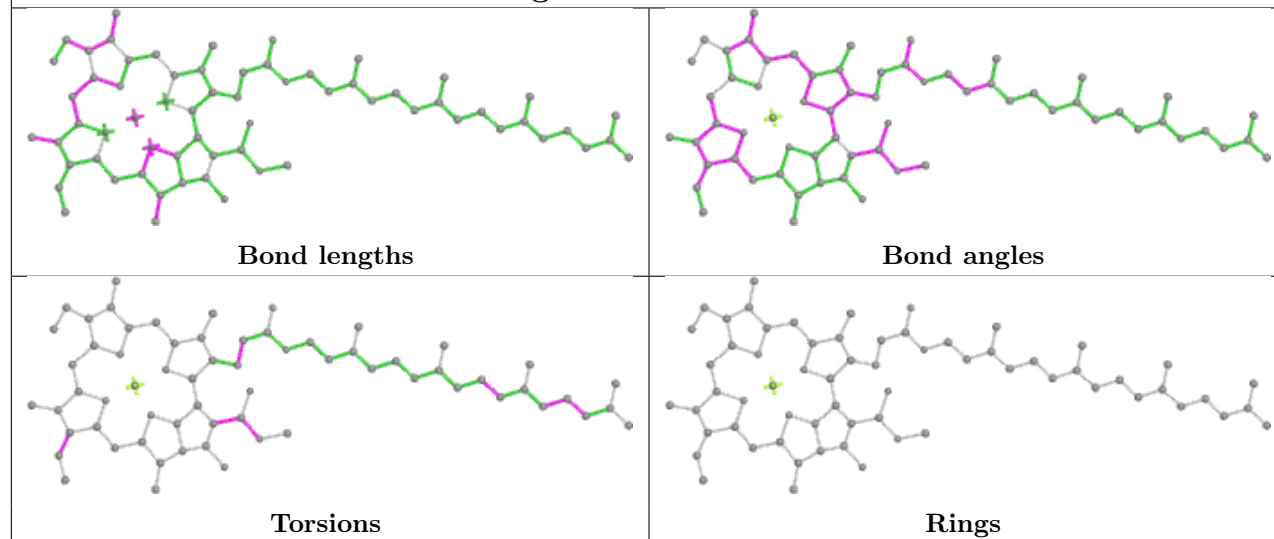
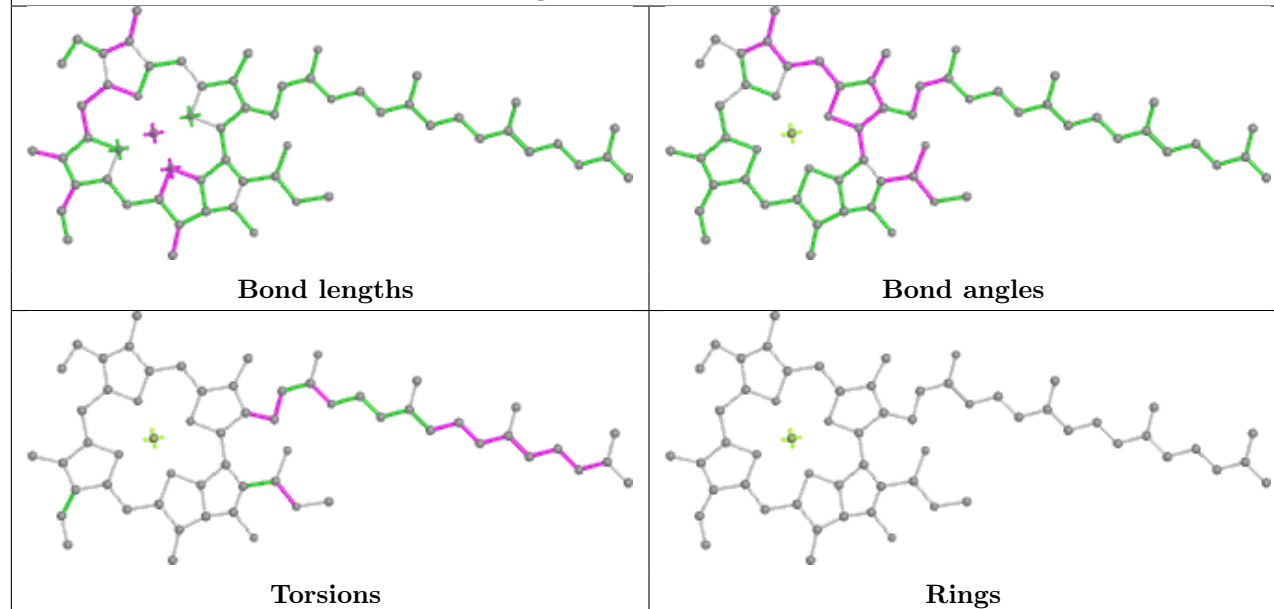
Bond angles



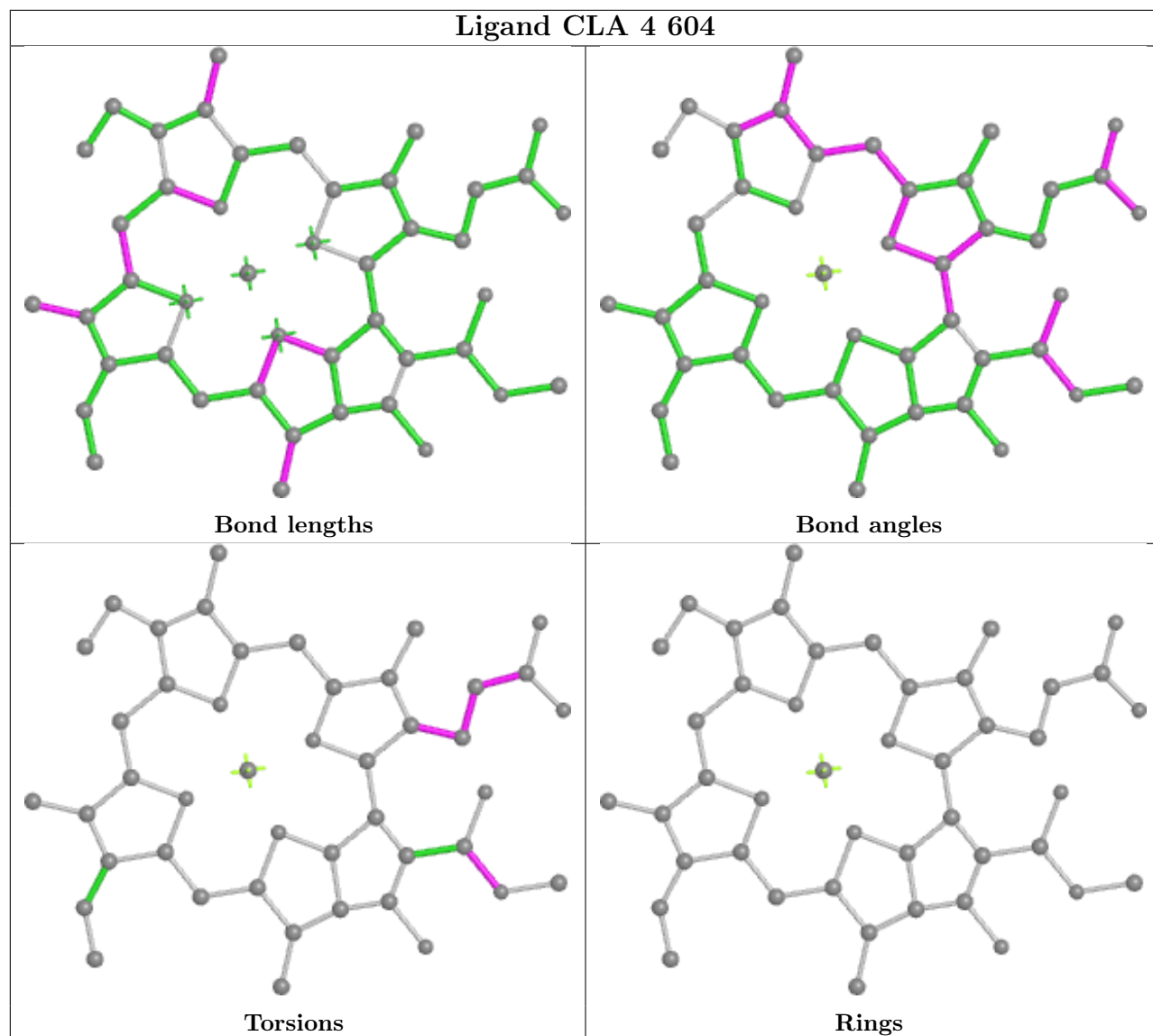
Torsions



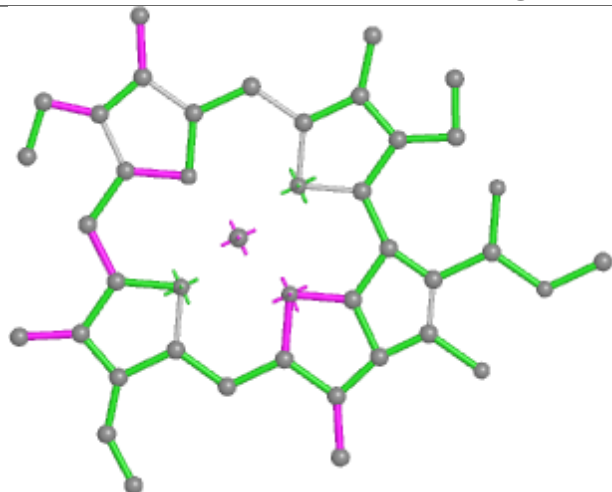
Rings

Ligand CLA A 848**Ligand CLA B 821**

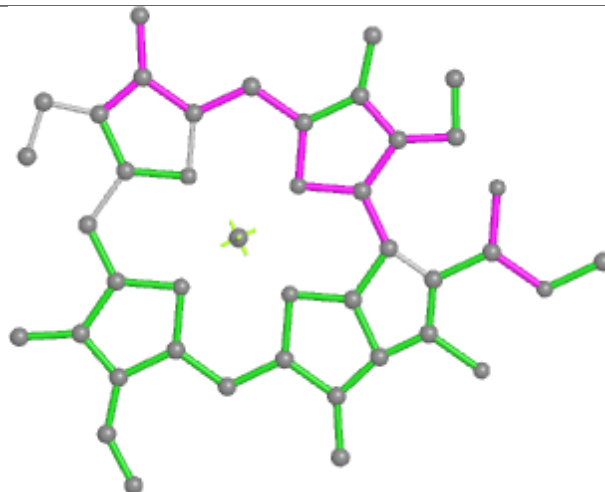
Ligand CLA 4 604



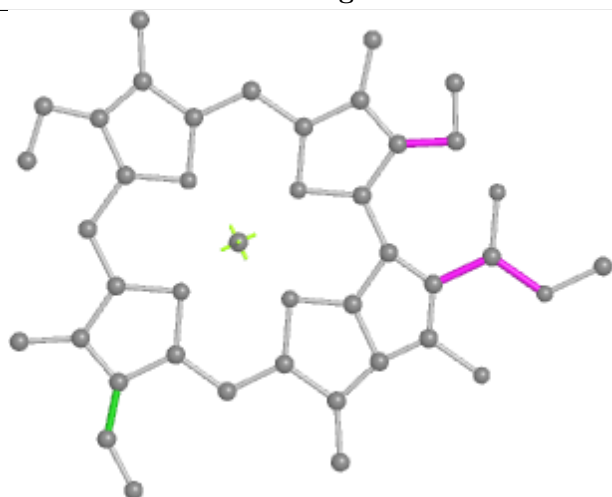
Ligand CLA K 103



Bond lengths



Bond angles

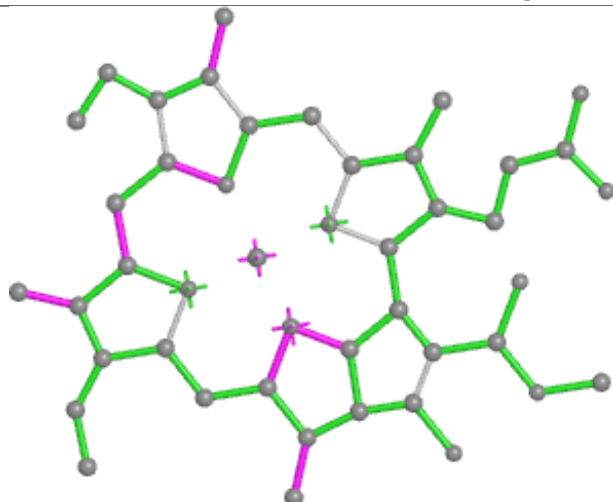


Torsions

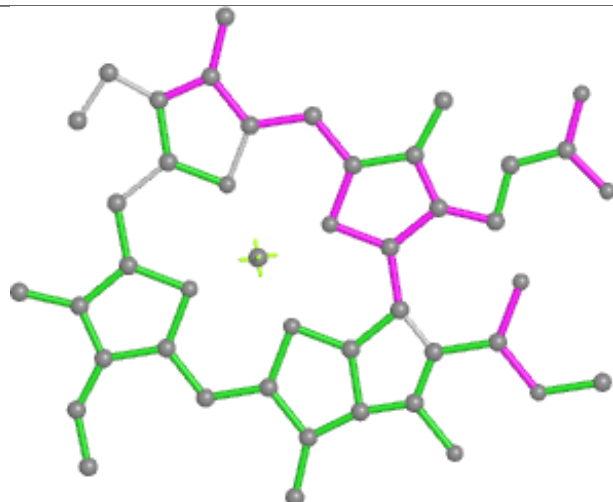


Rings

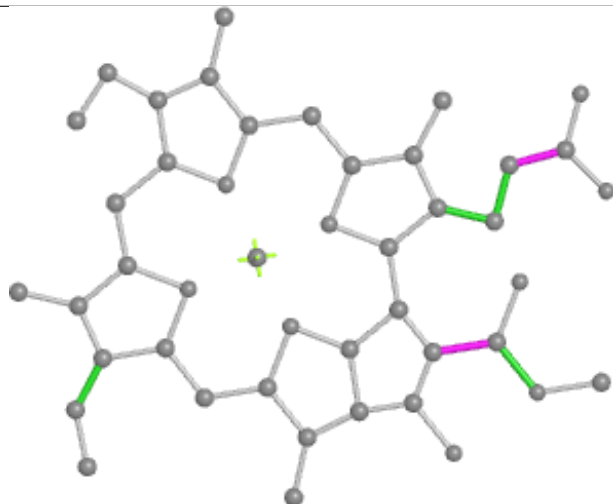
Ligand CLA 3 204



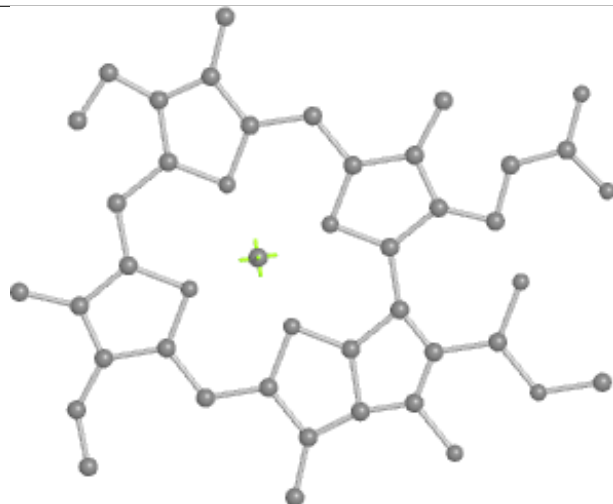
Bond lengths



Bond angles

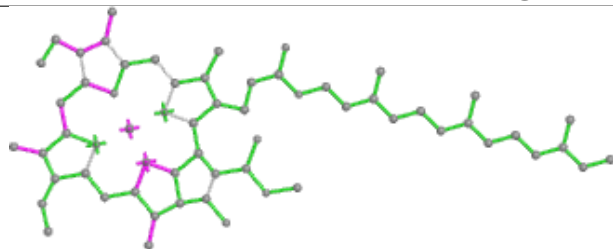


Torsions

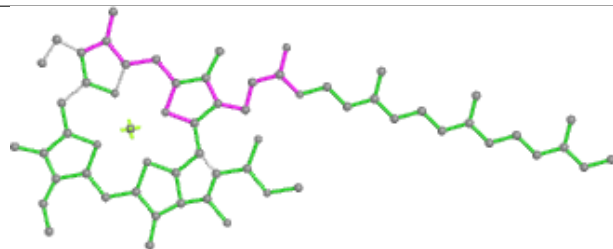


Rings

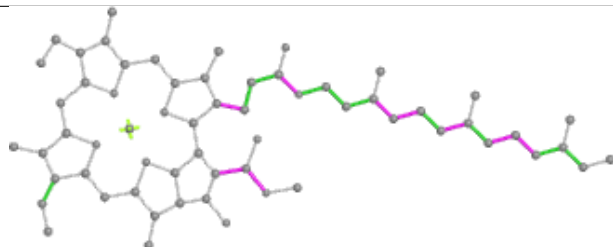
Ligand CLA F 301



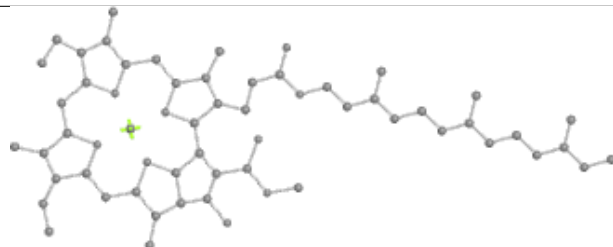
Bond lengths



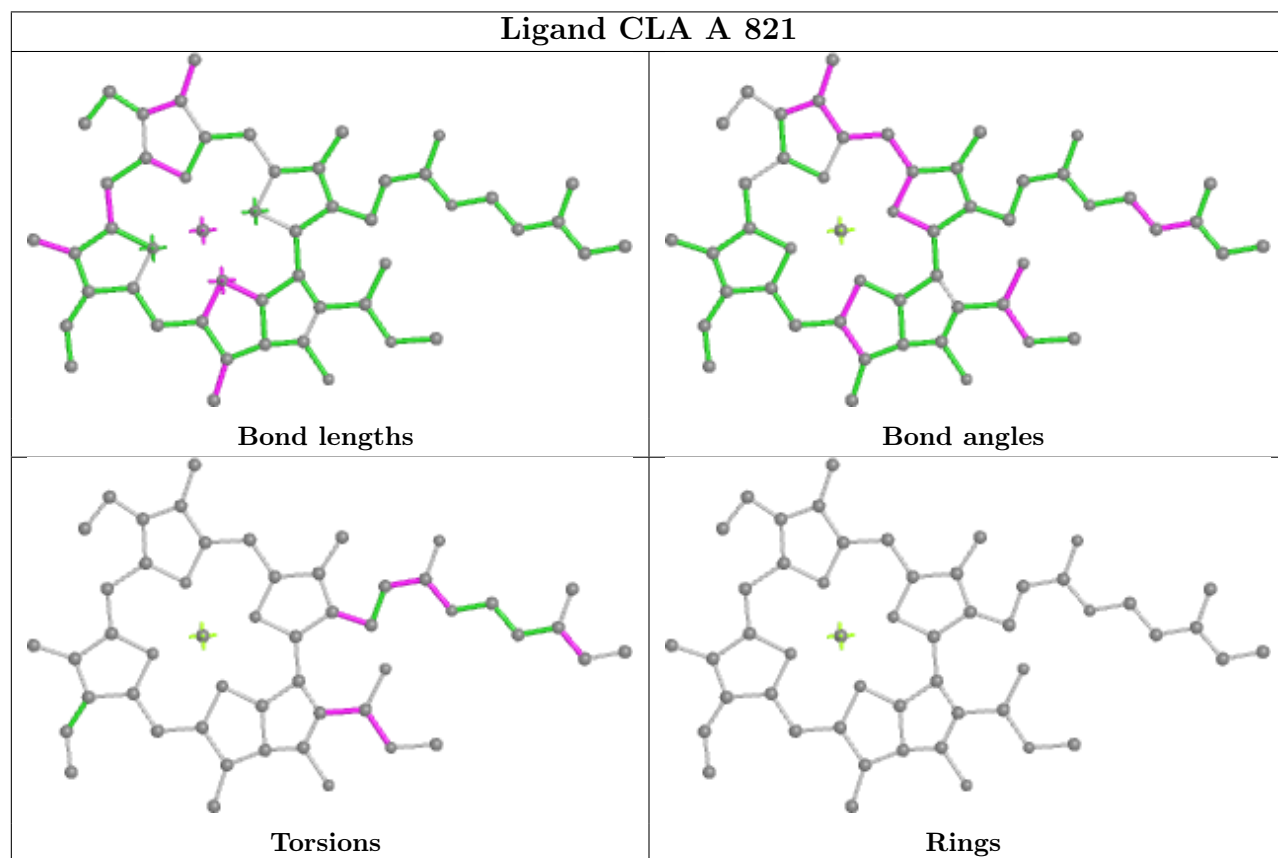
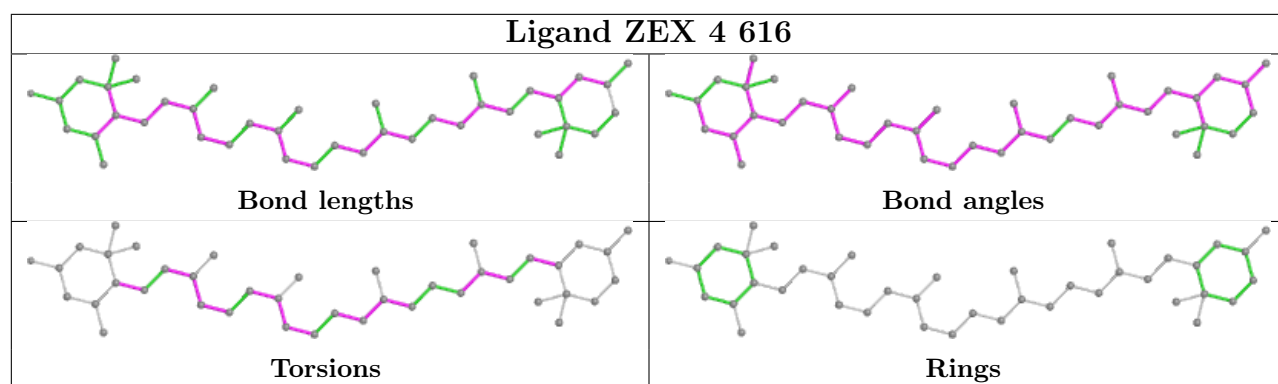
Bond angles



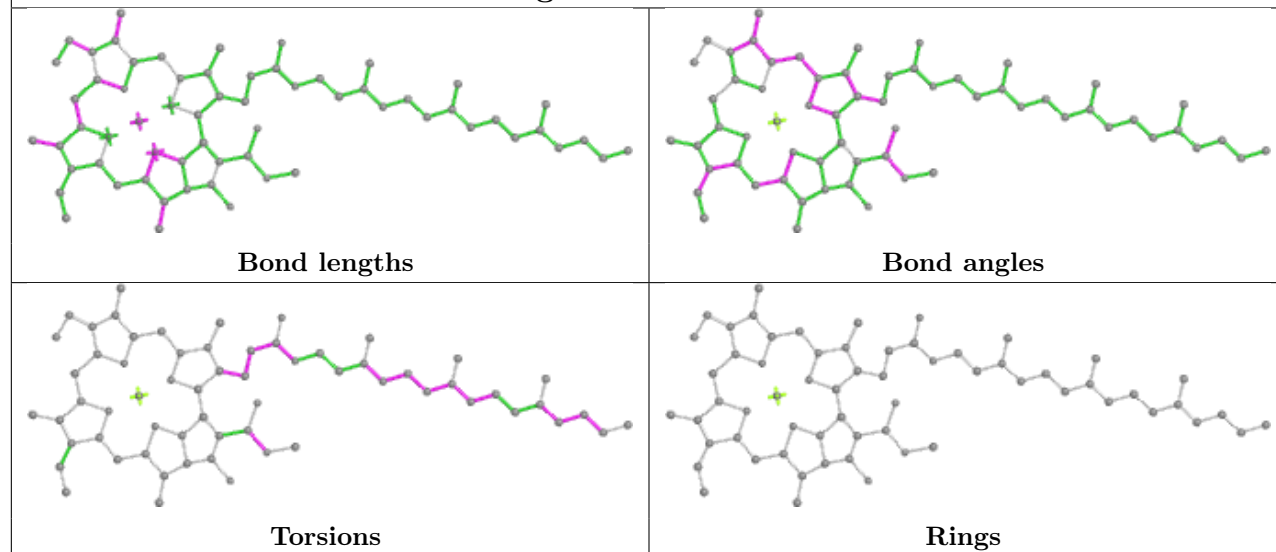
Torsions



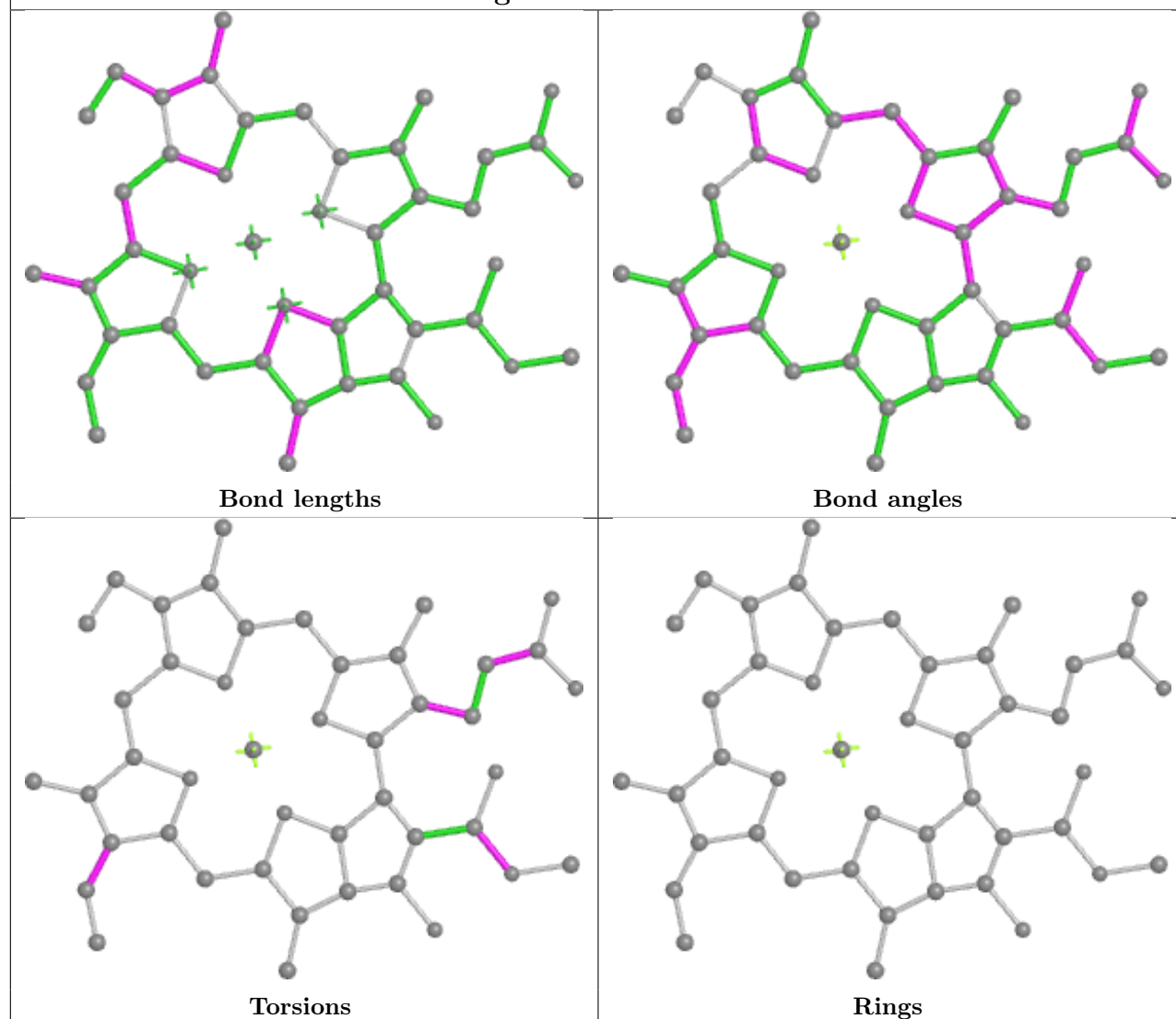
Rings



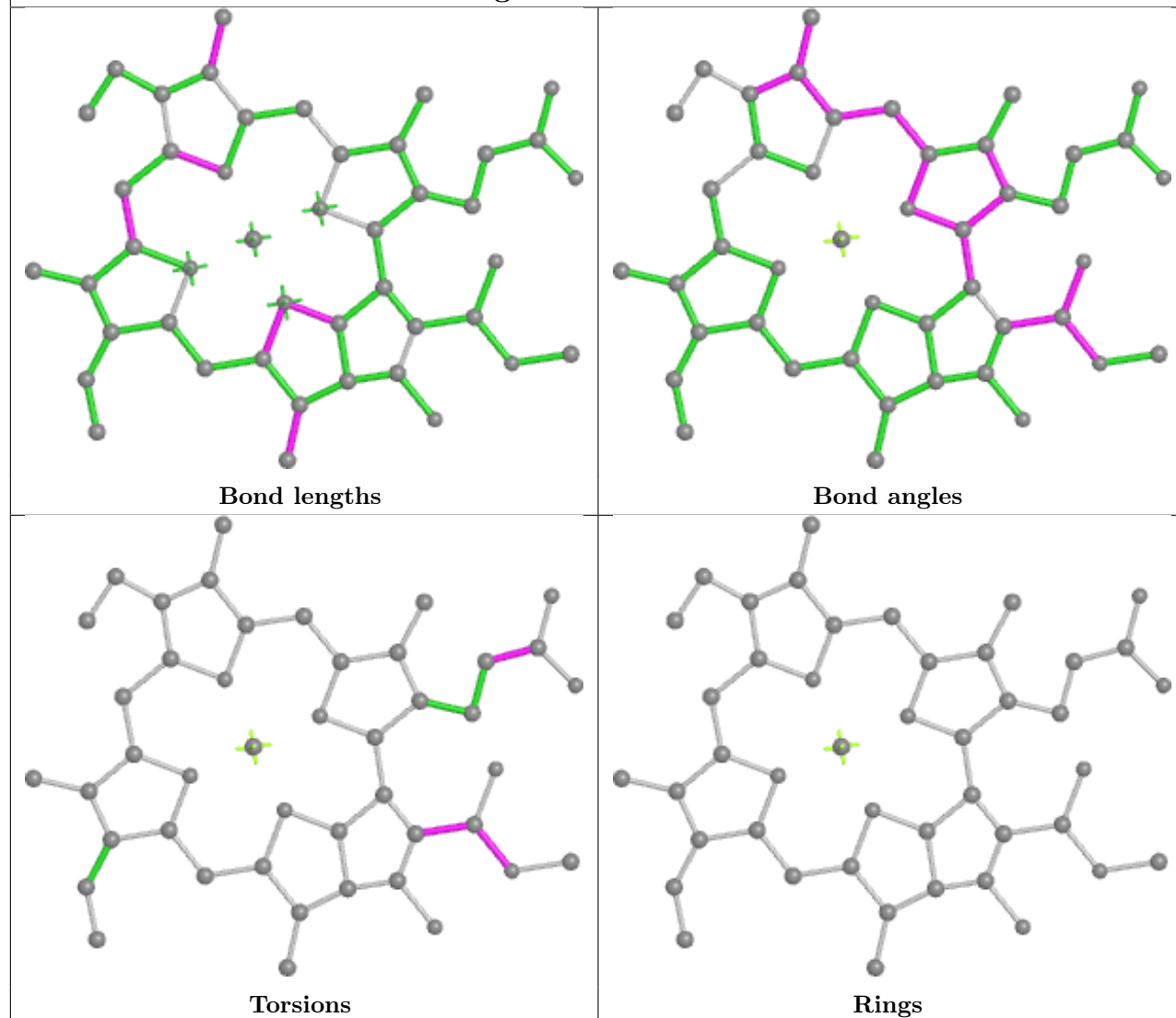
Ligand CLA 3 203



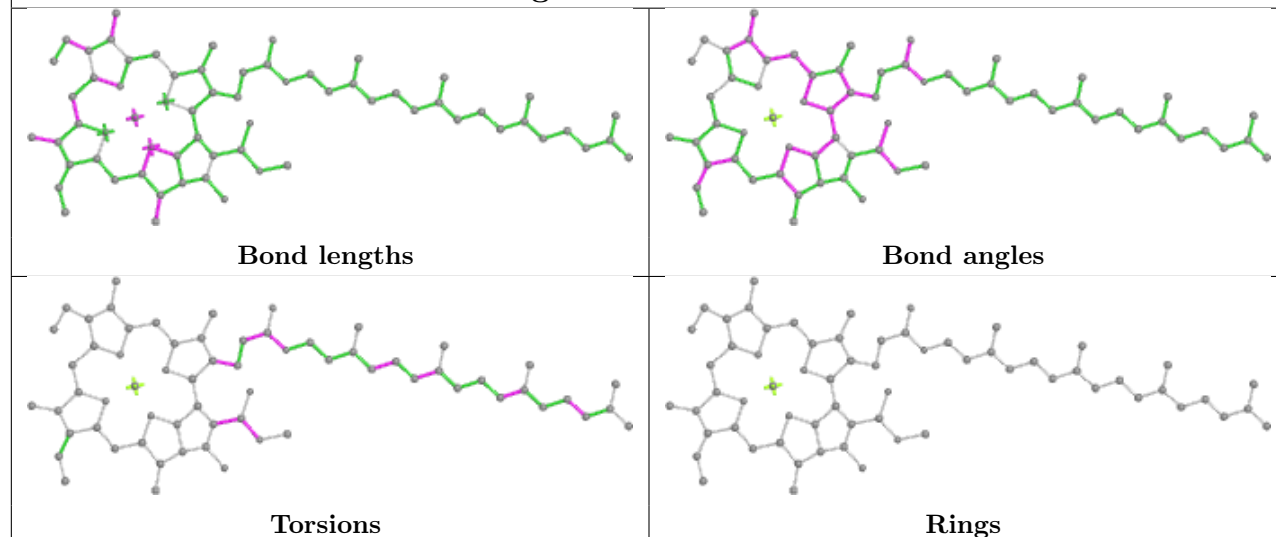
Ligand CLA 5 607

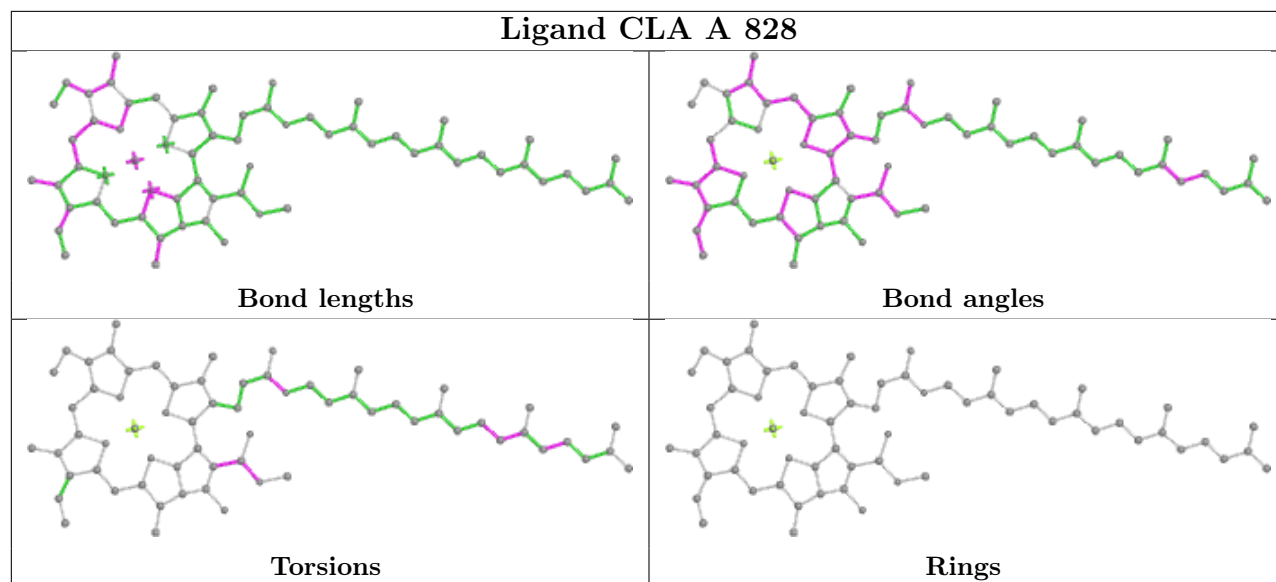
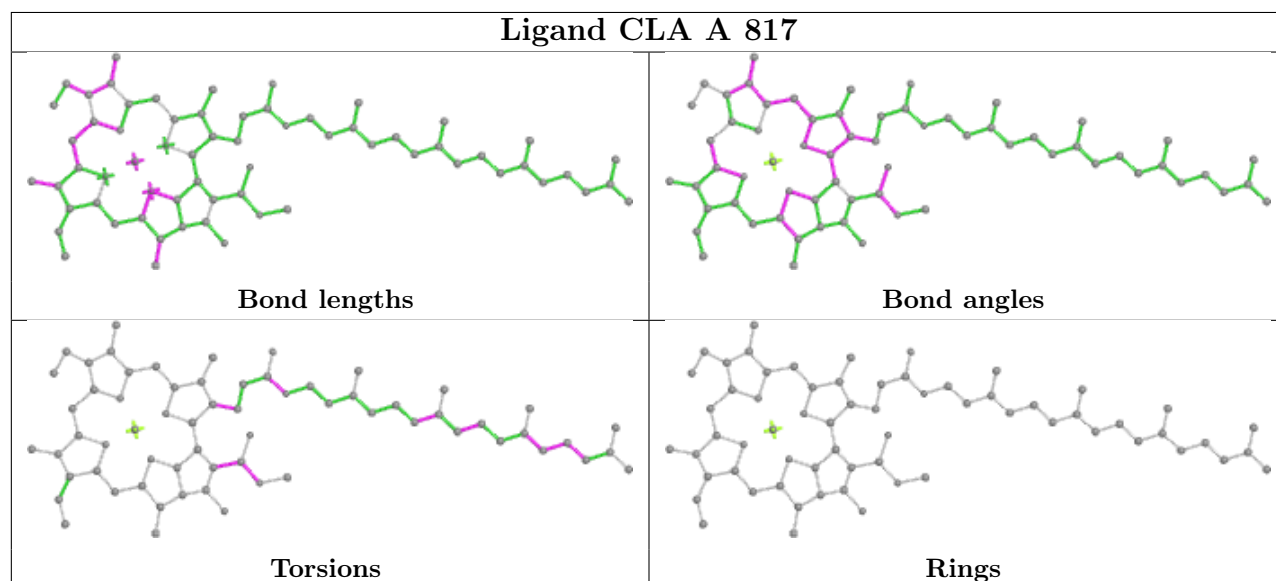
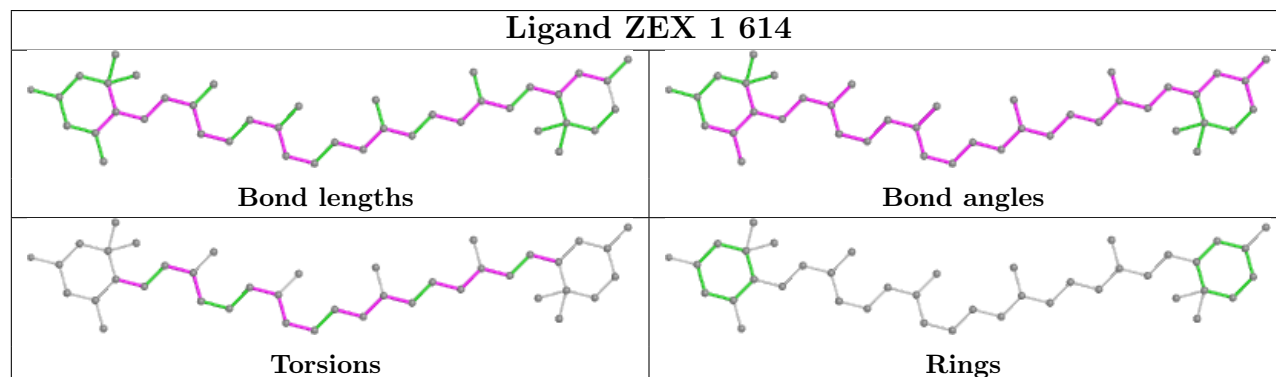


Ligand CLA 5 612

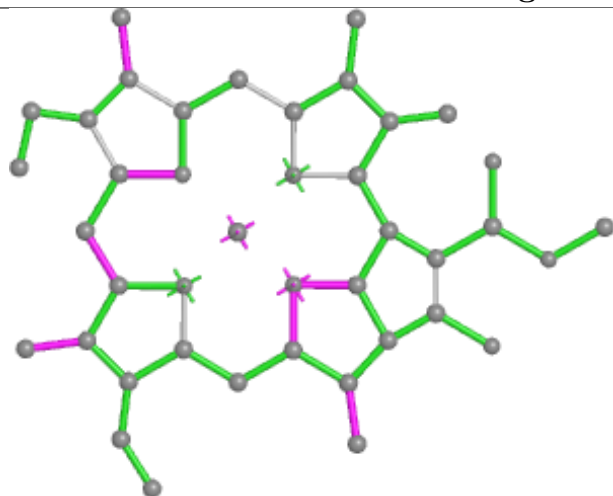


Ligand CLA A 805

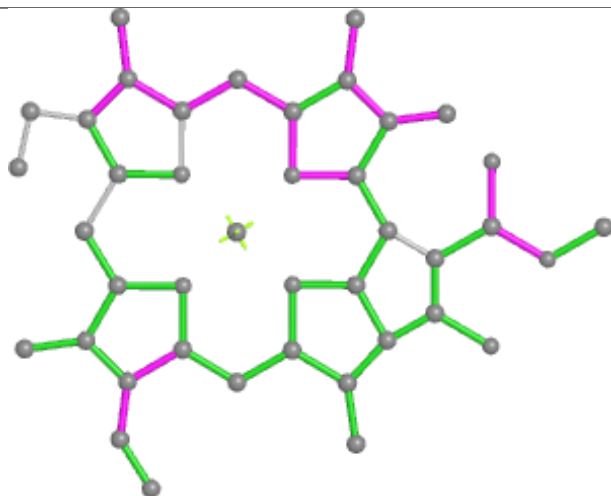


Ligand CLA A 828**Ligand CLA A 817****Ligand ZEX 1 614**

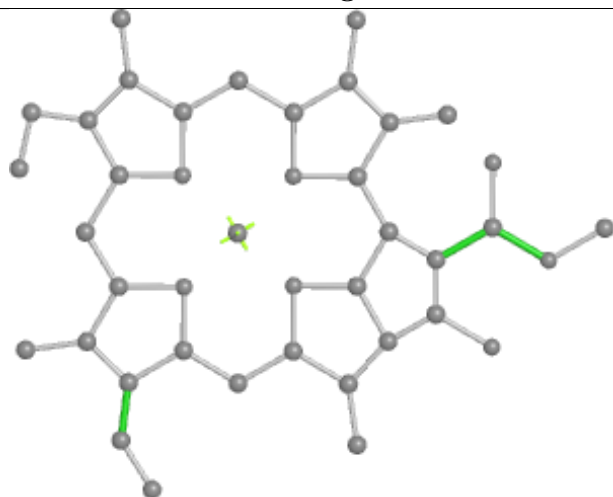
Ligand CLA 1 609



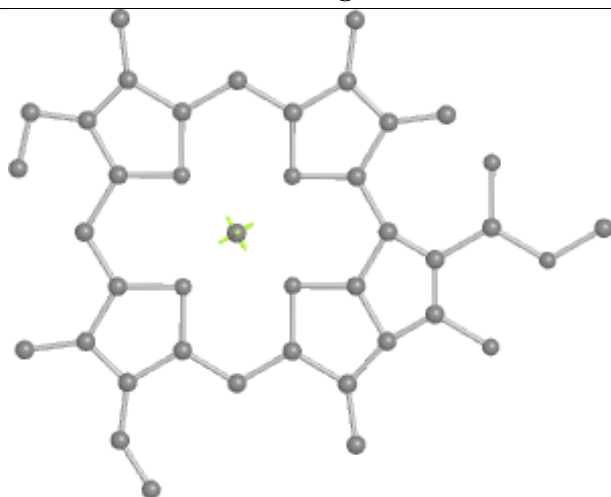
Bond lengths



Bond angles

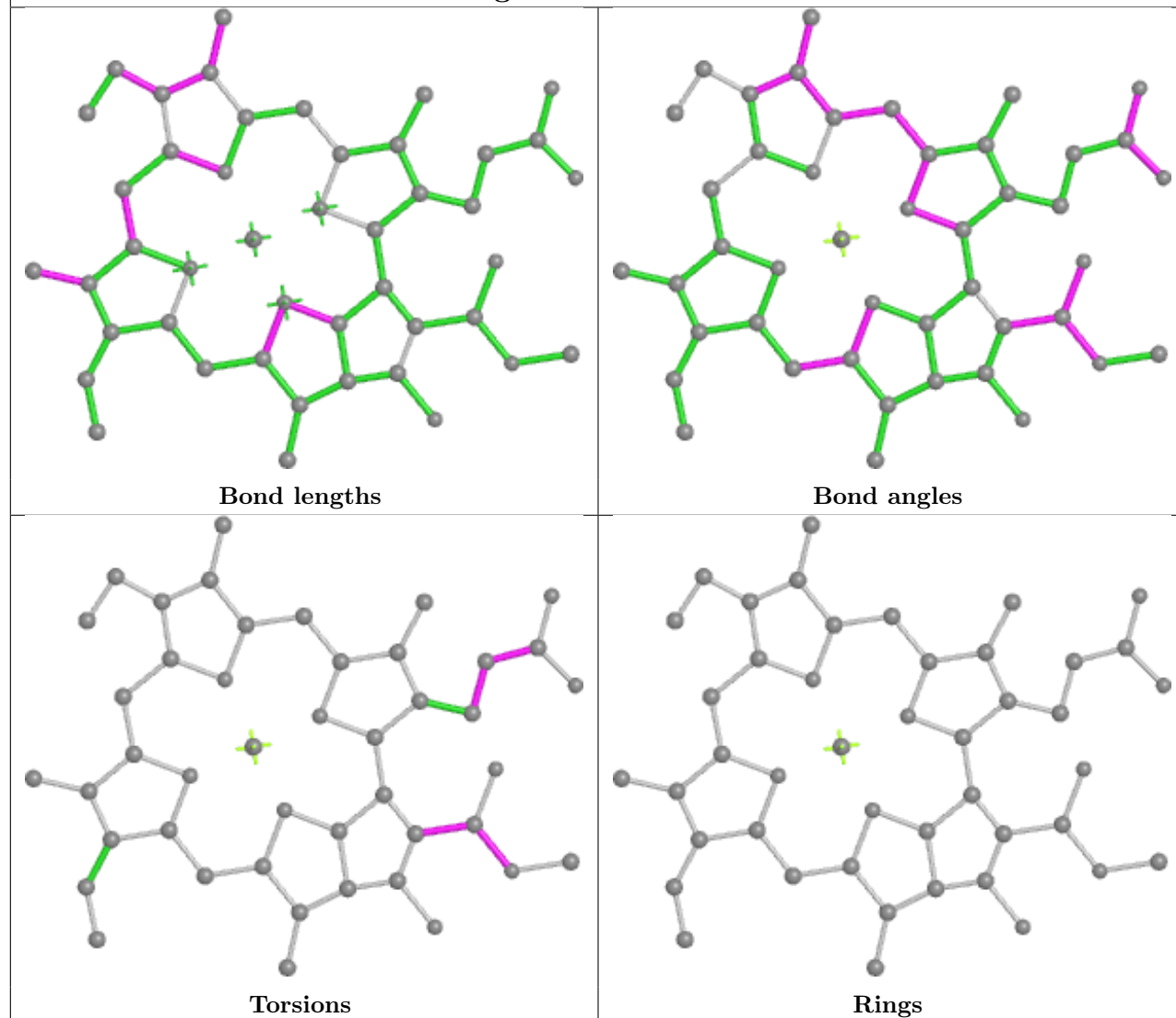


Torsions

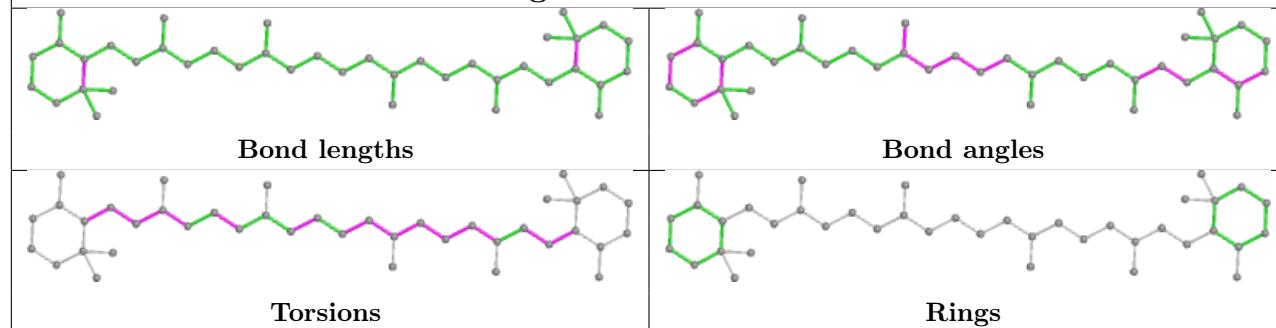


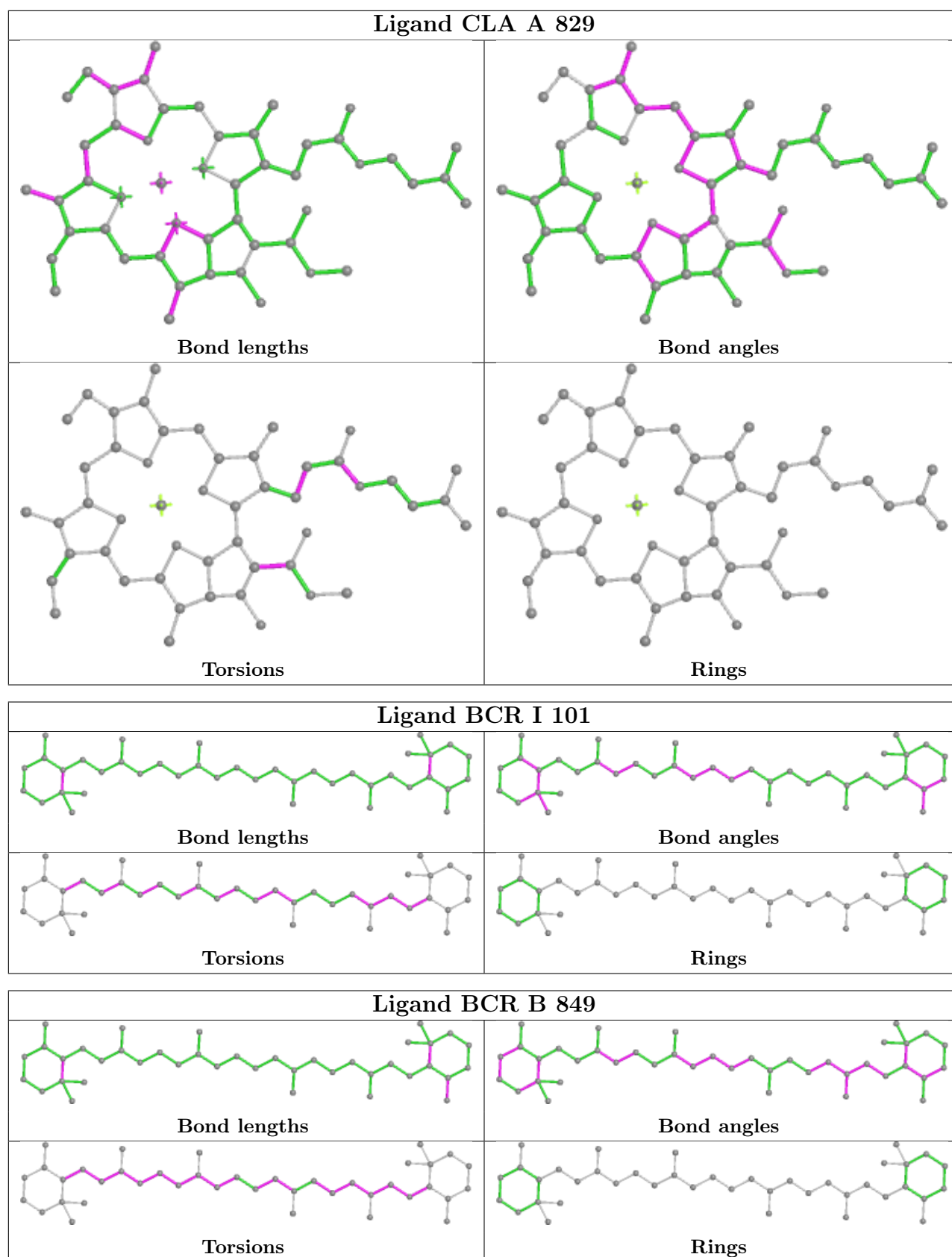
Rings

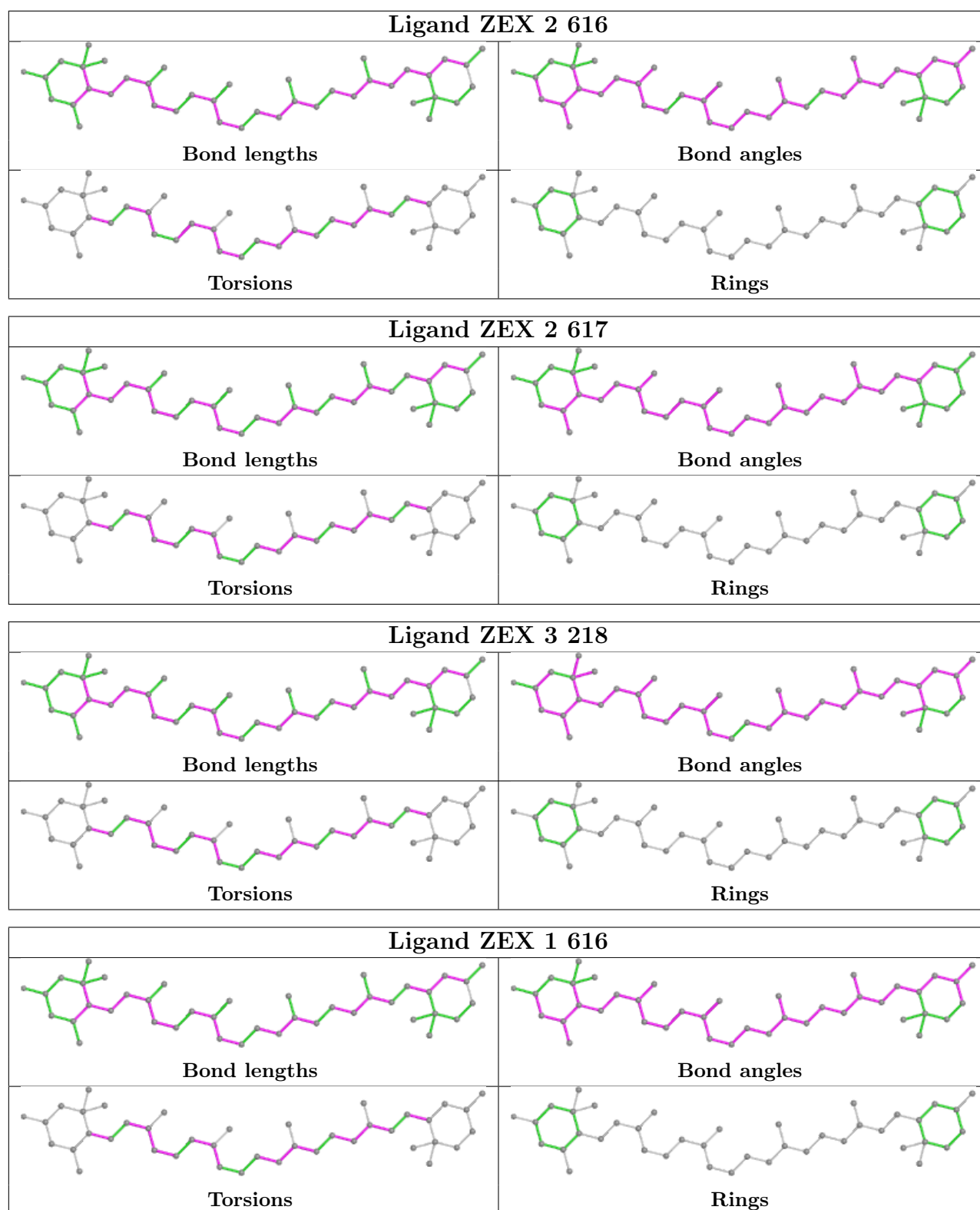
Ligand CLA 2 601

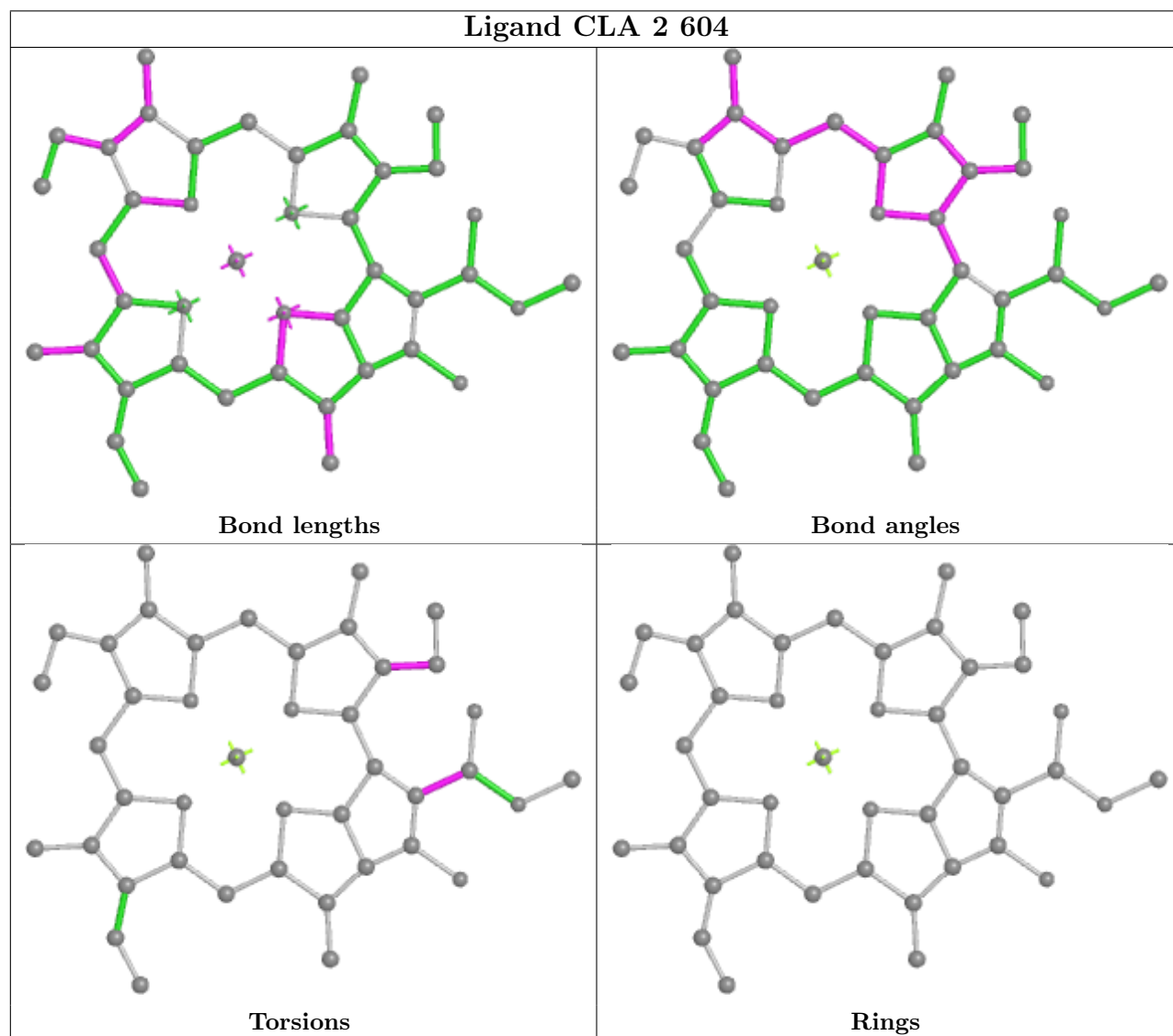
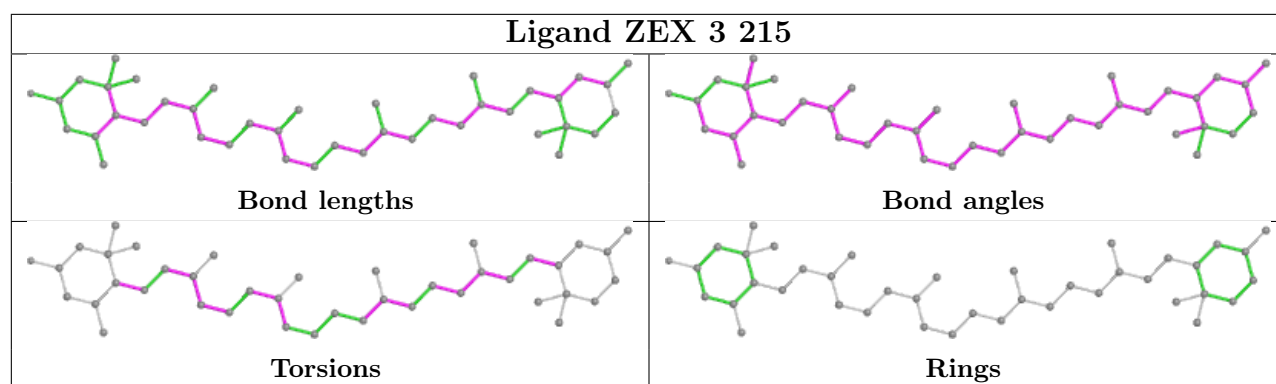


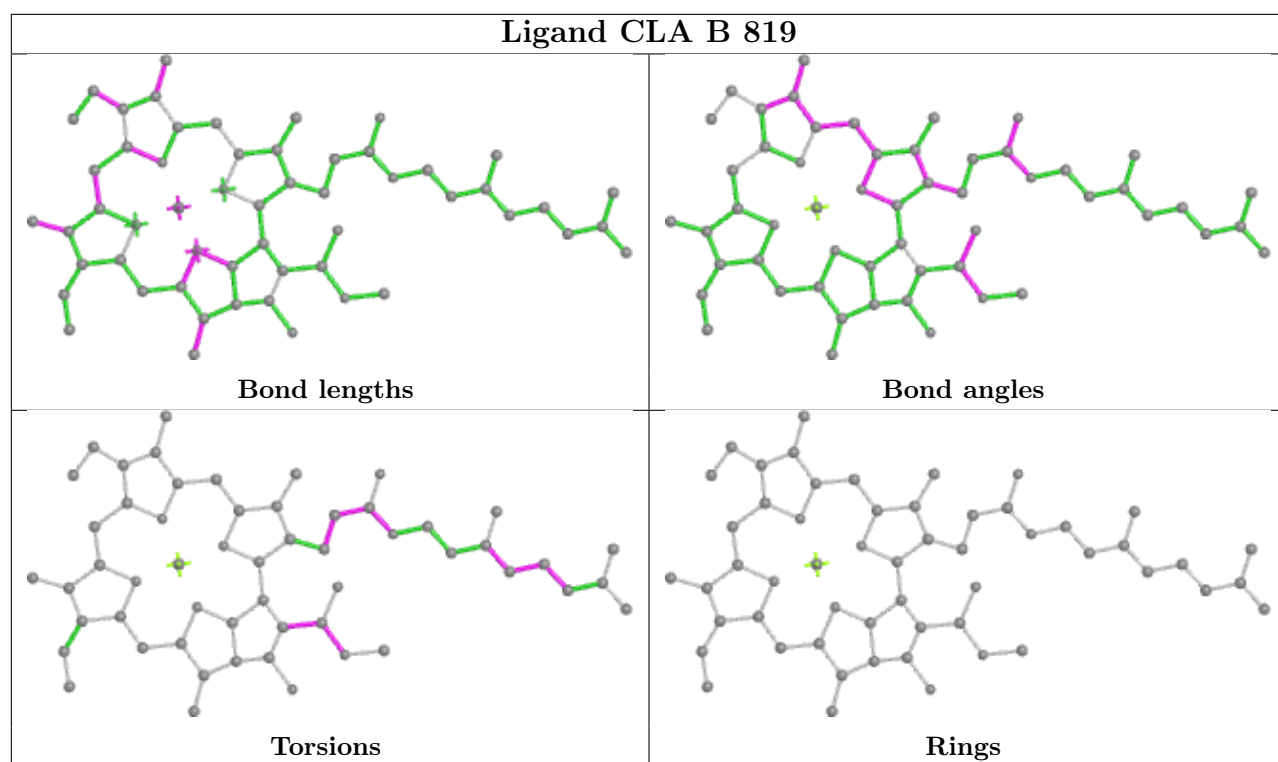
Ligand BCR K 104



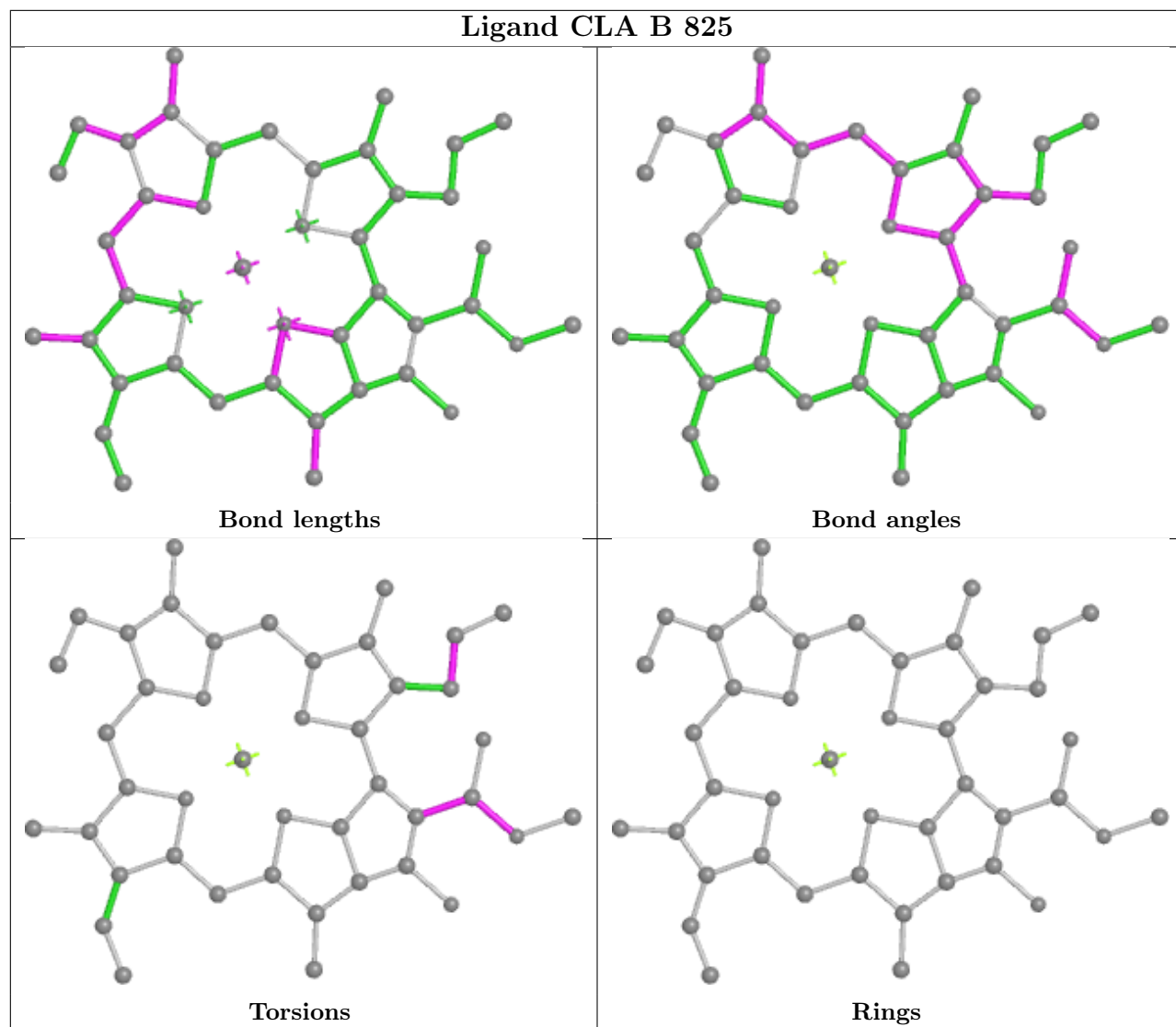




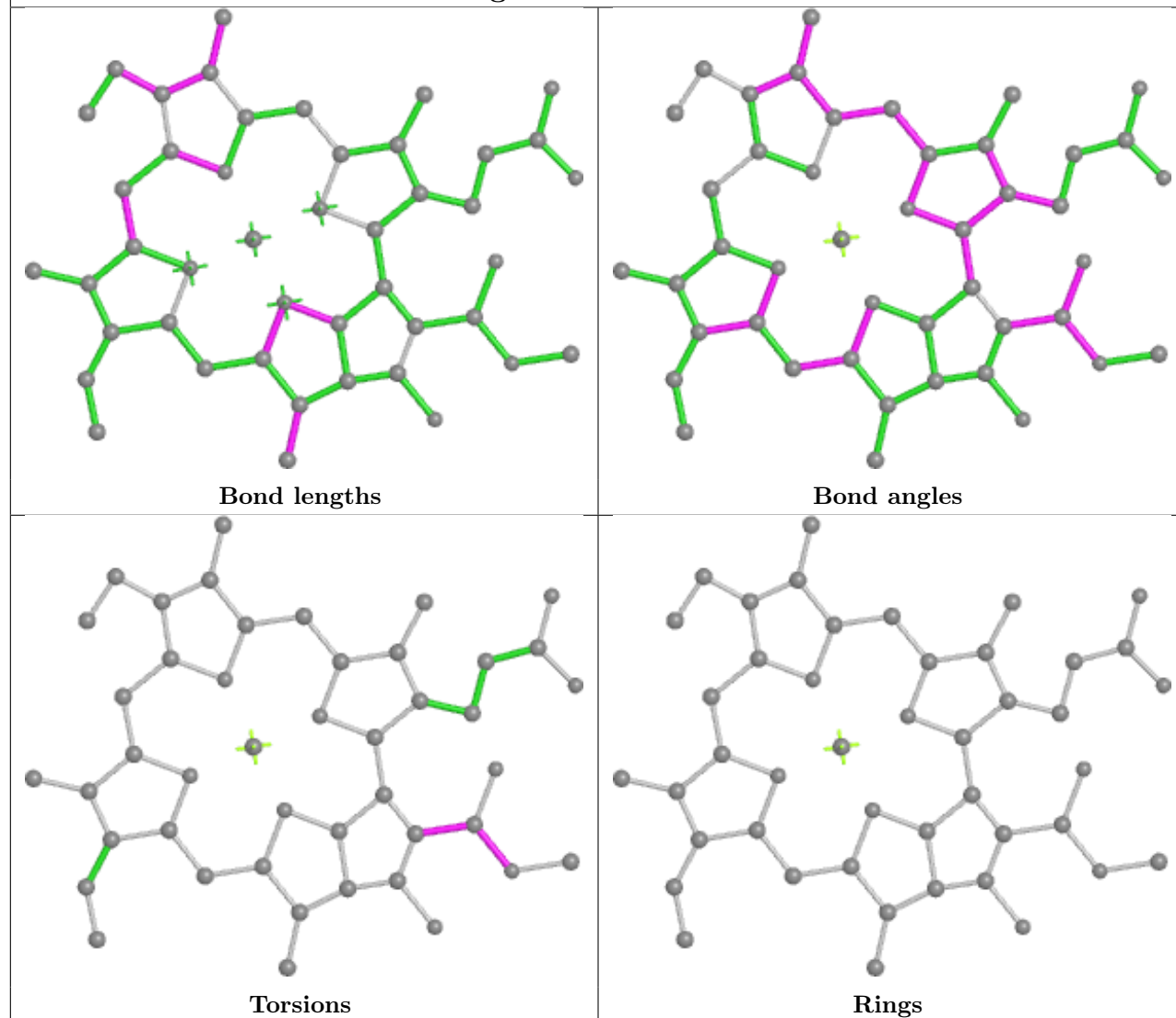




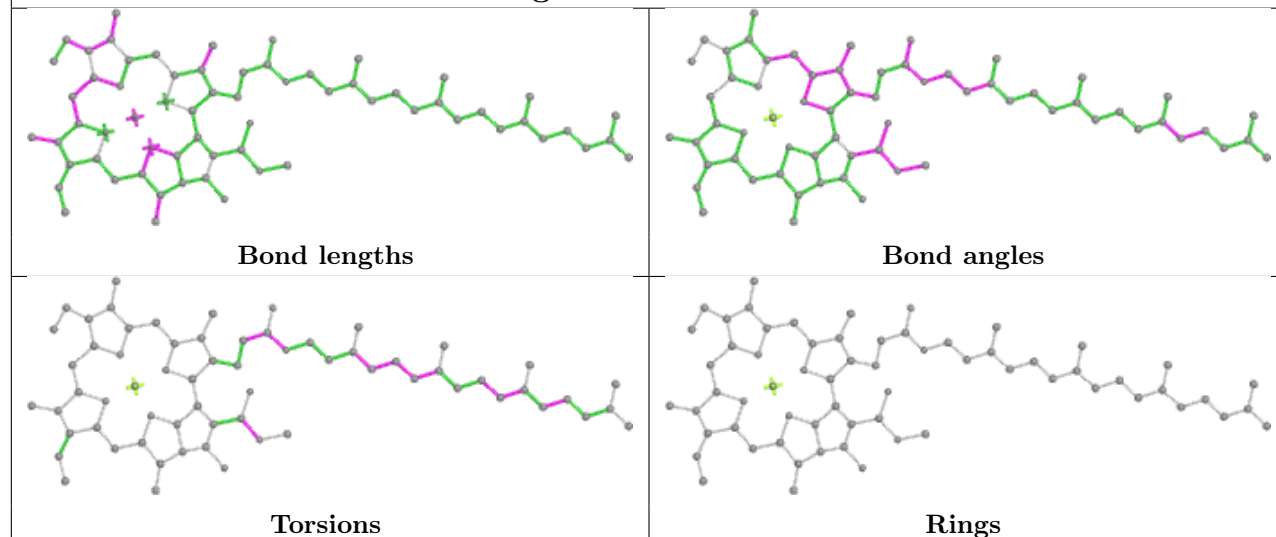
Ligand CLA B 825

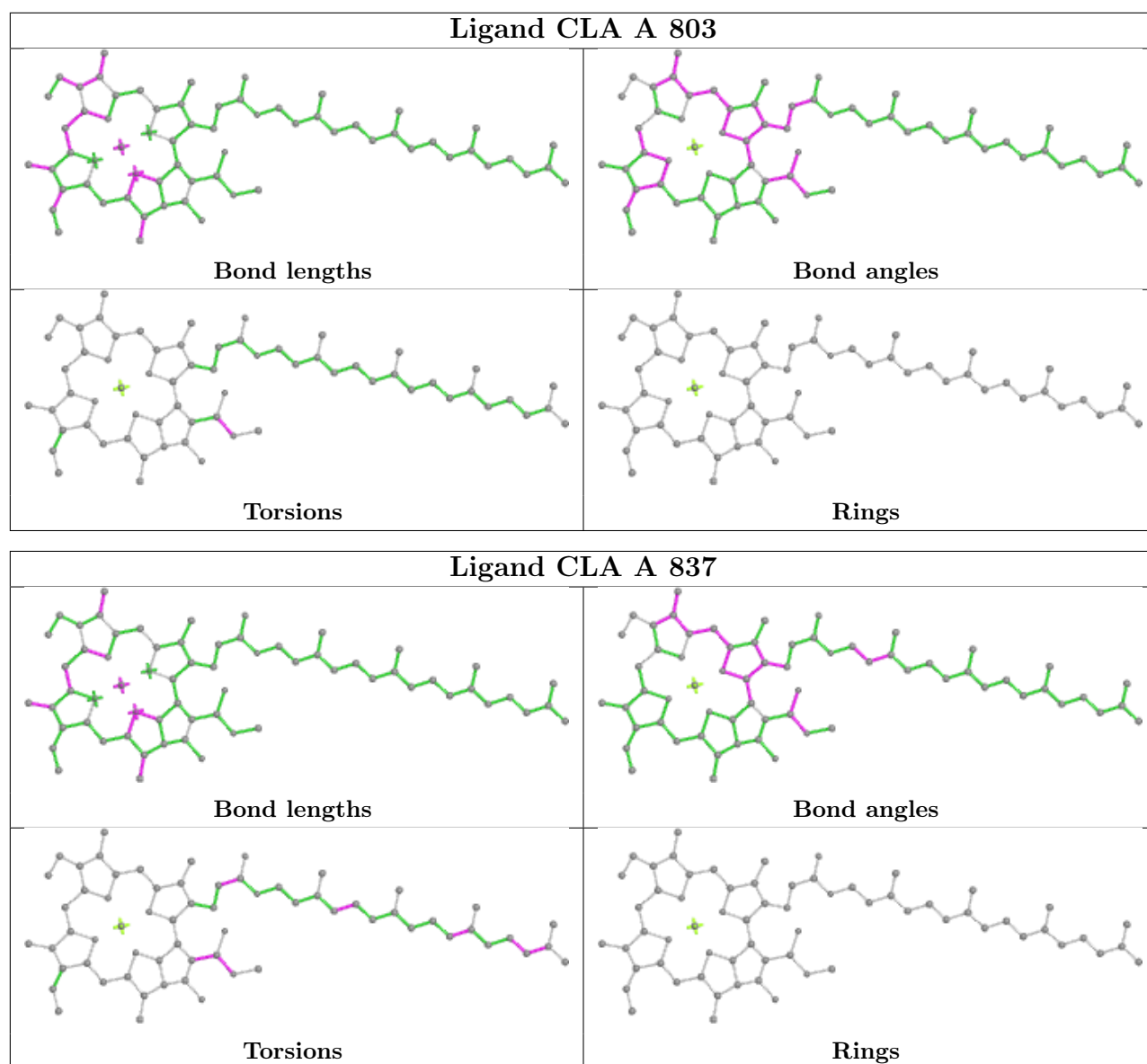


Ligand CLA A 814

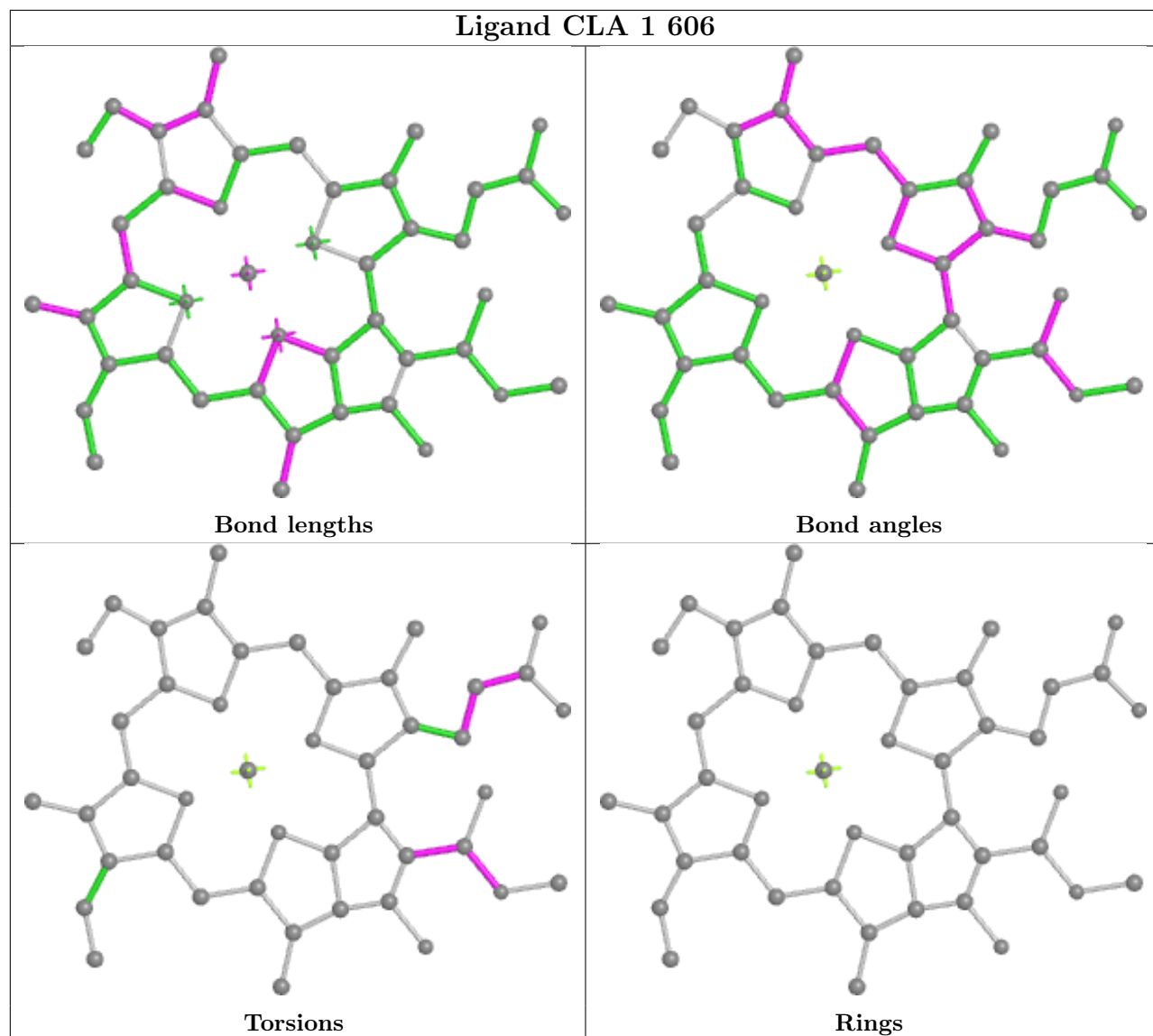


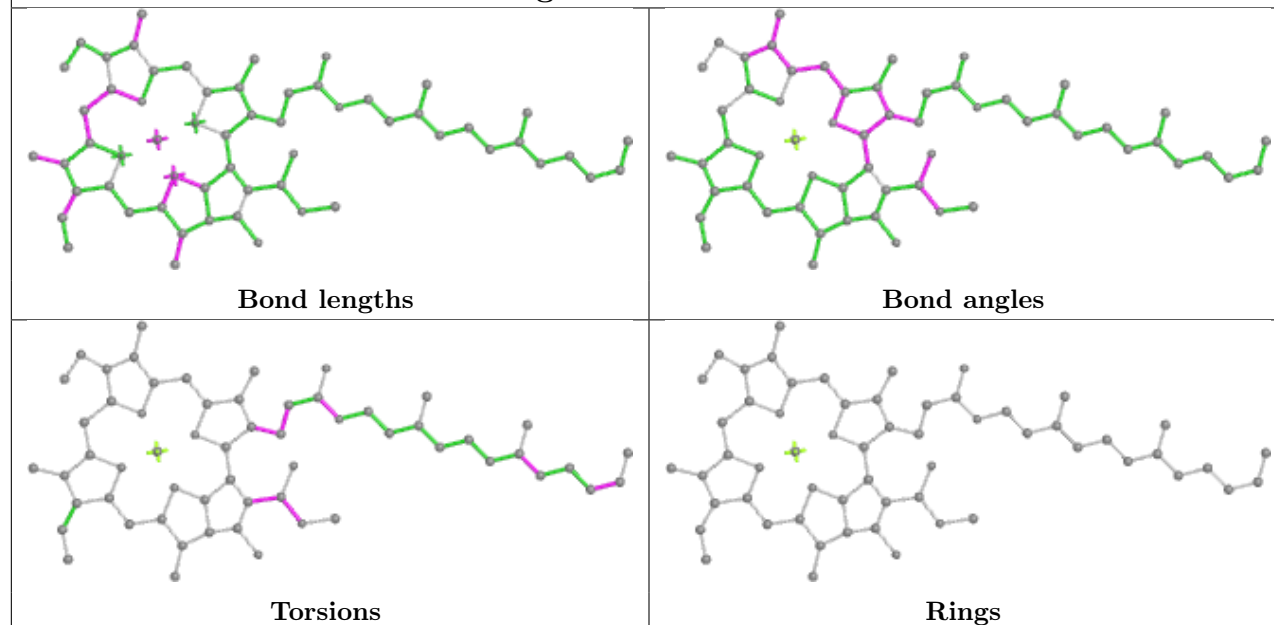
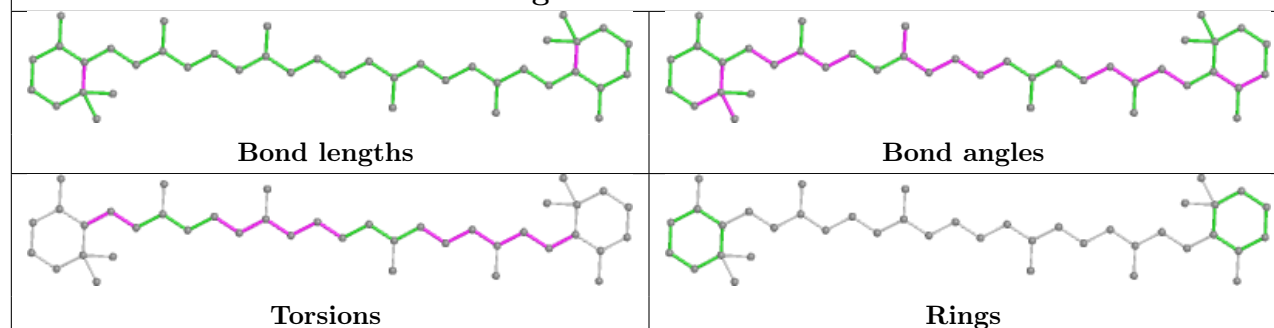
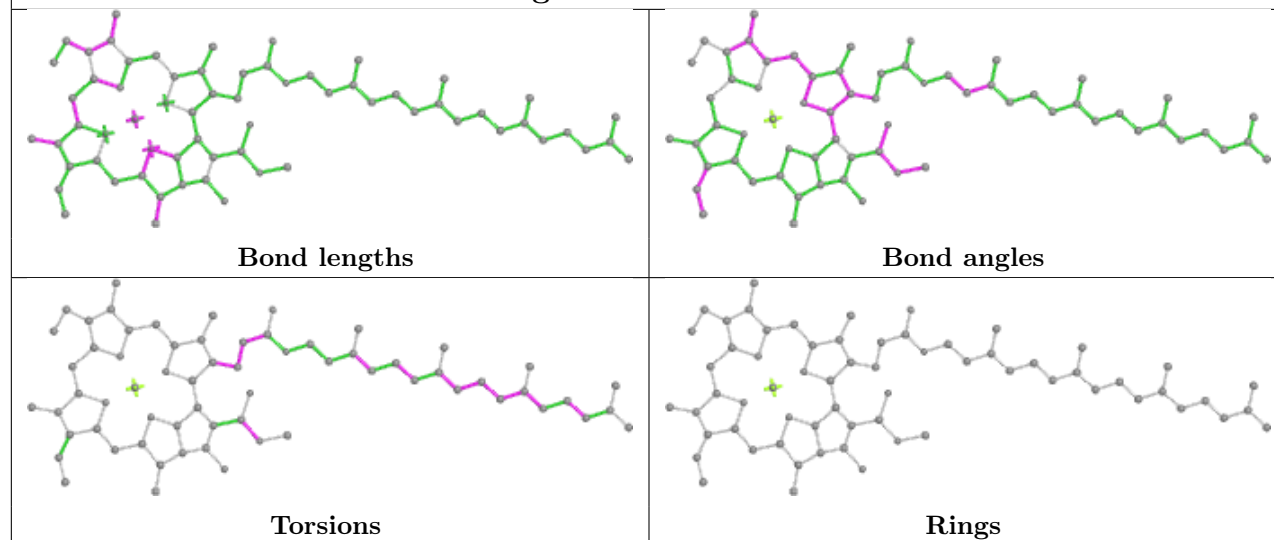
Ligand CLA B 806

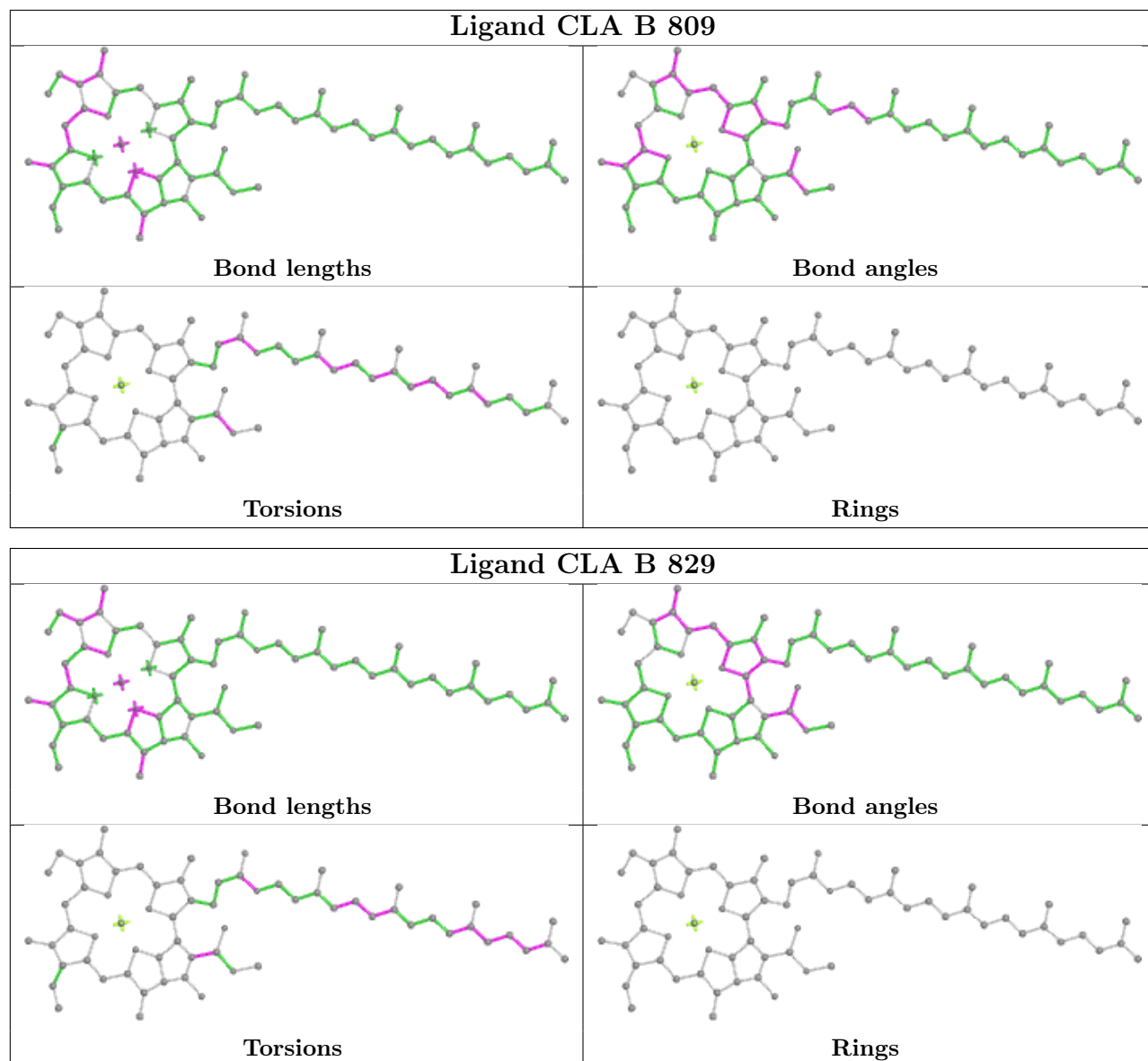




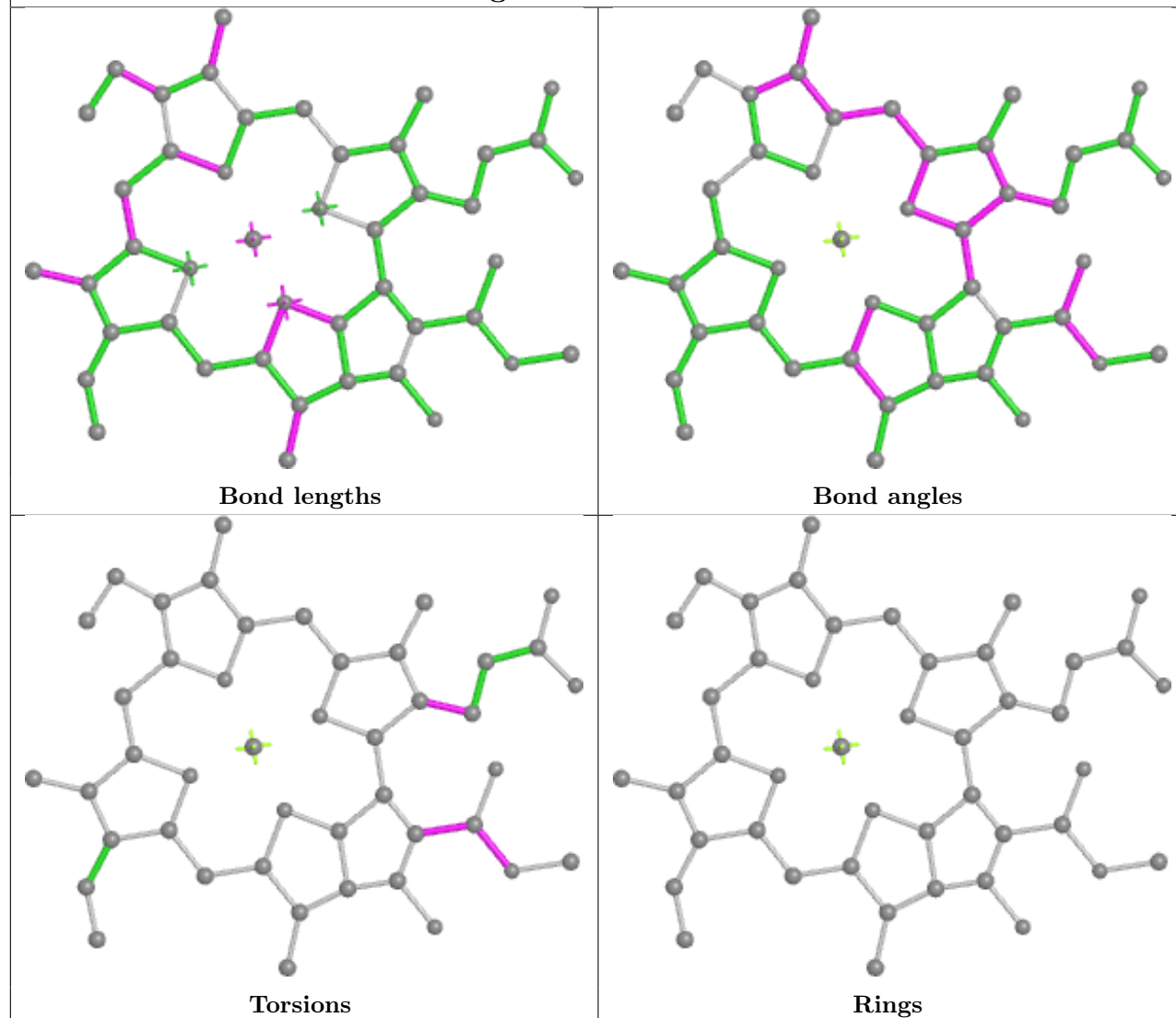
Ligand CLA 1 606



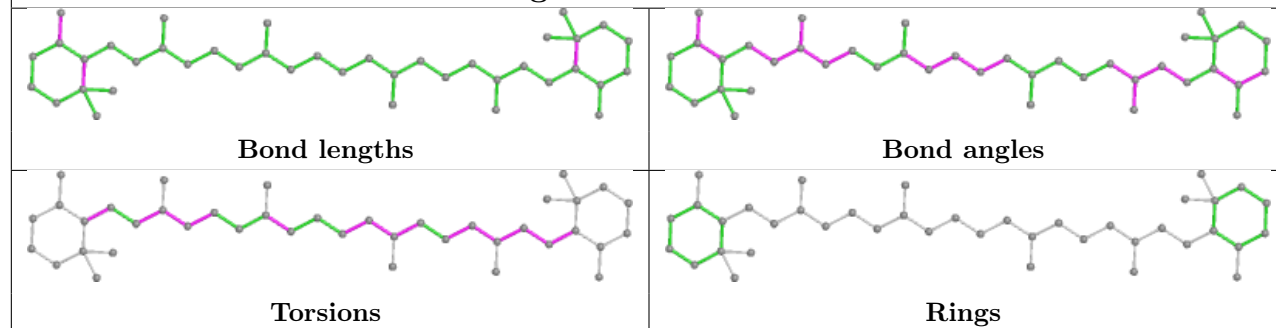
Ligand CLA 1 602**Ligand BCR F 304****Ligand CLA B 816**

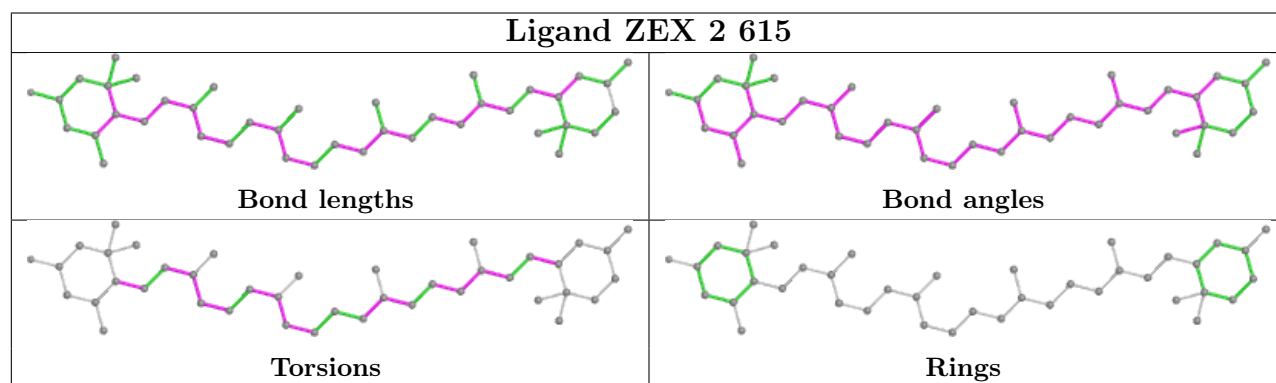
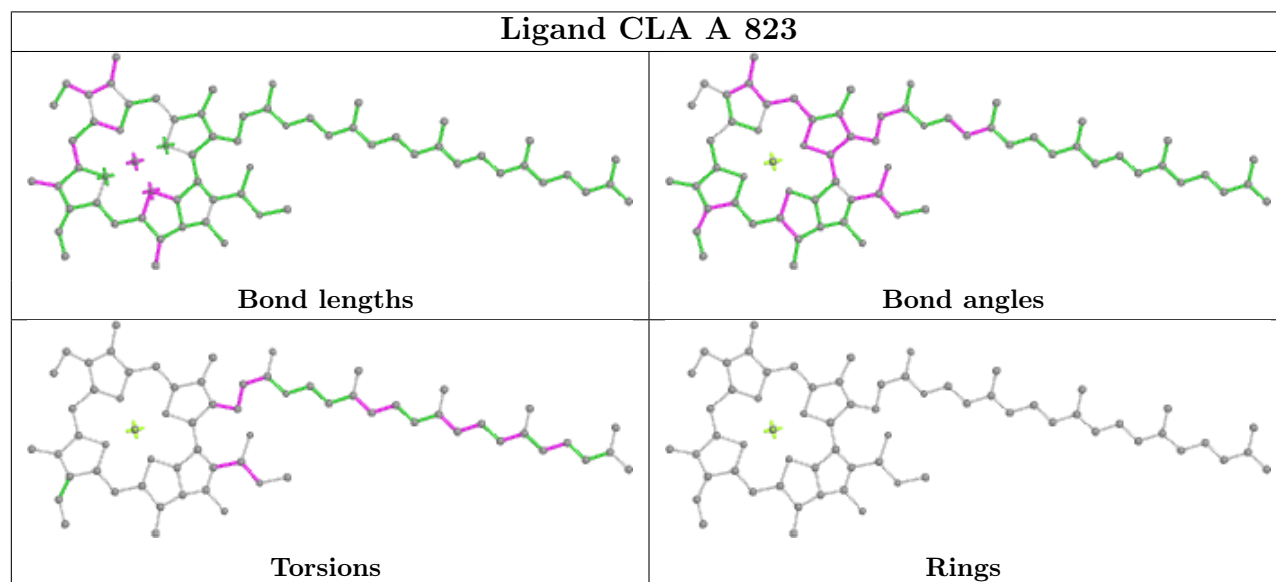
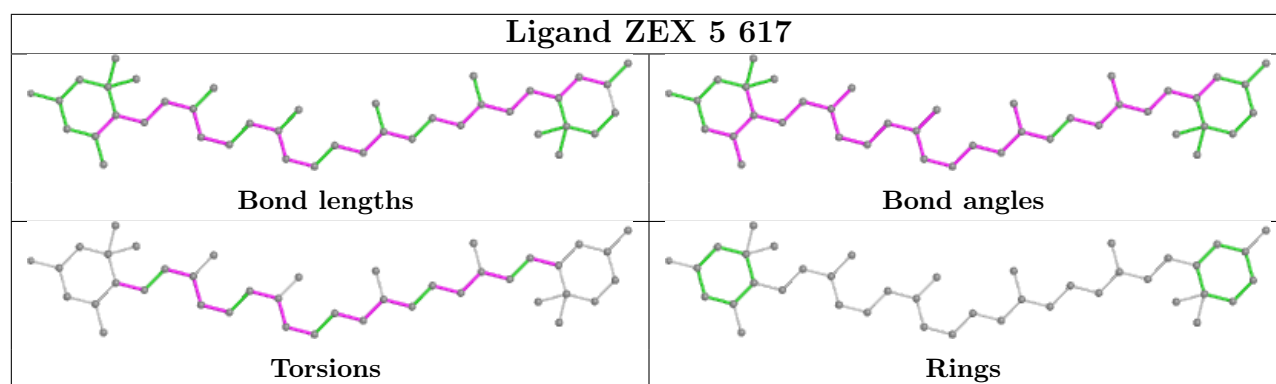


Ligand CLA A 812

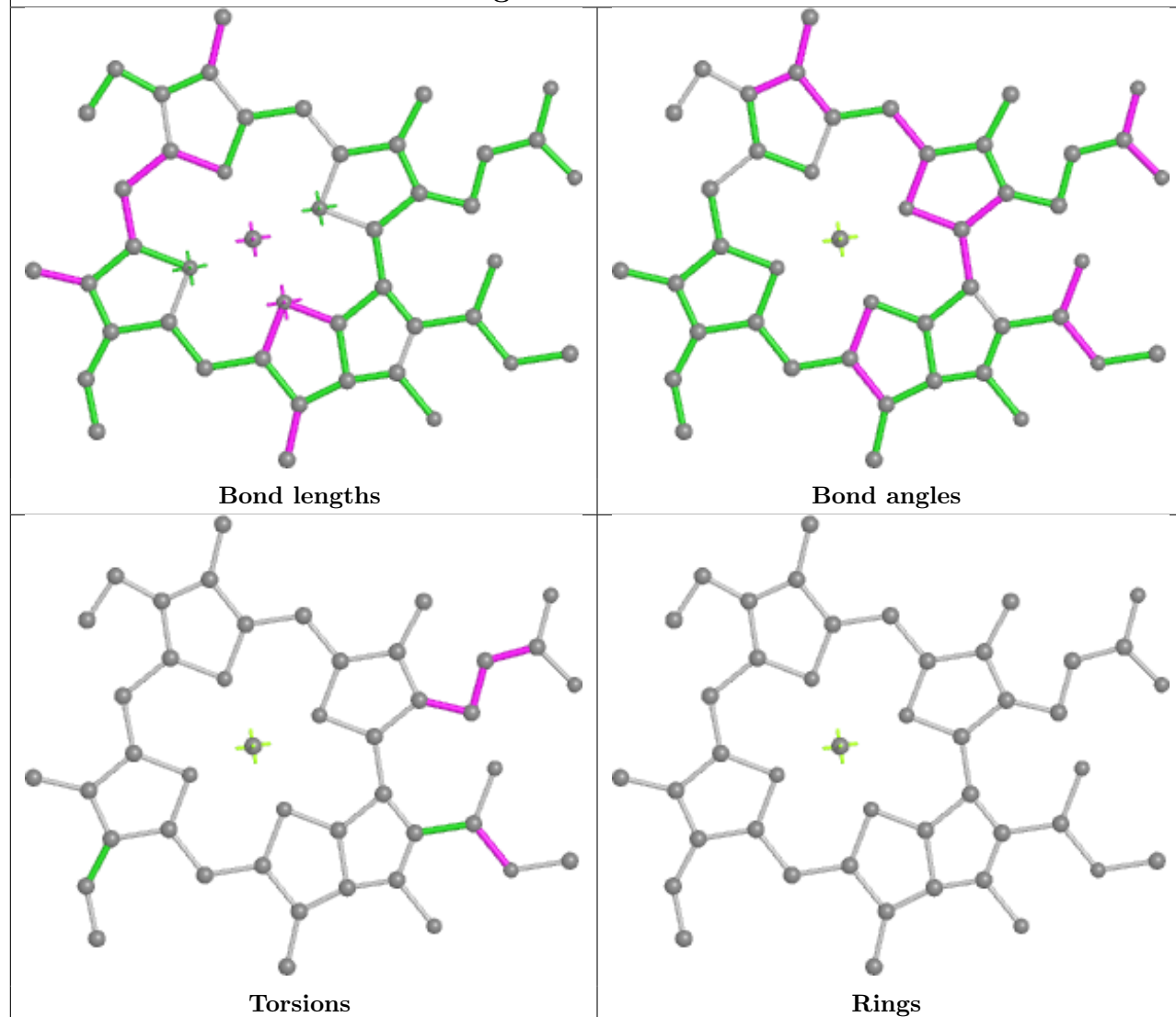


Ligand BCR A 845

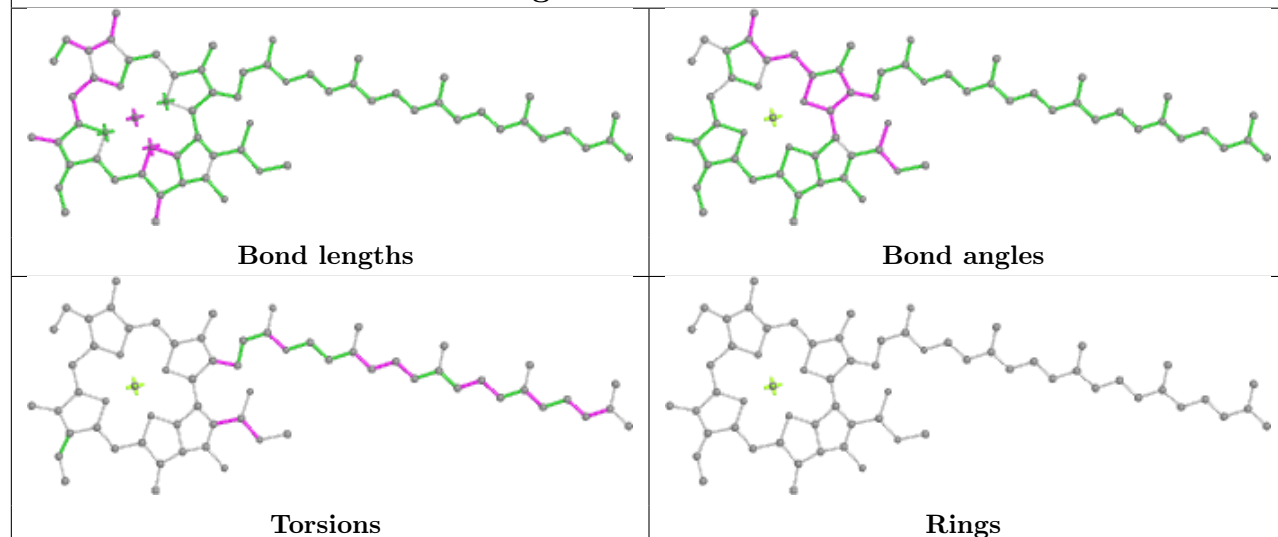




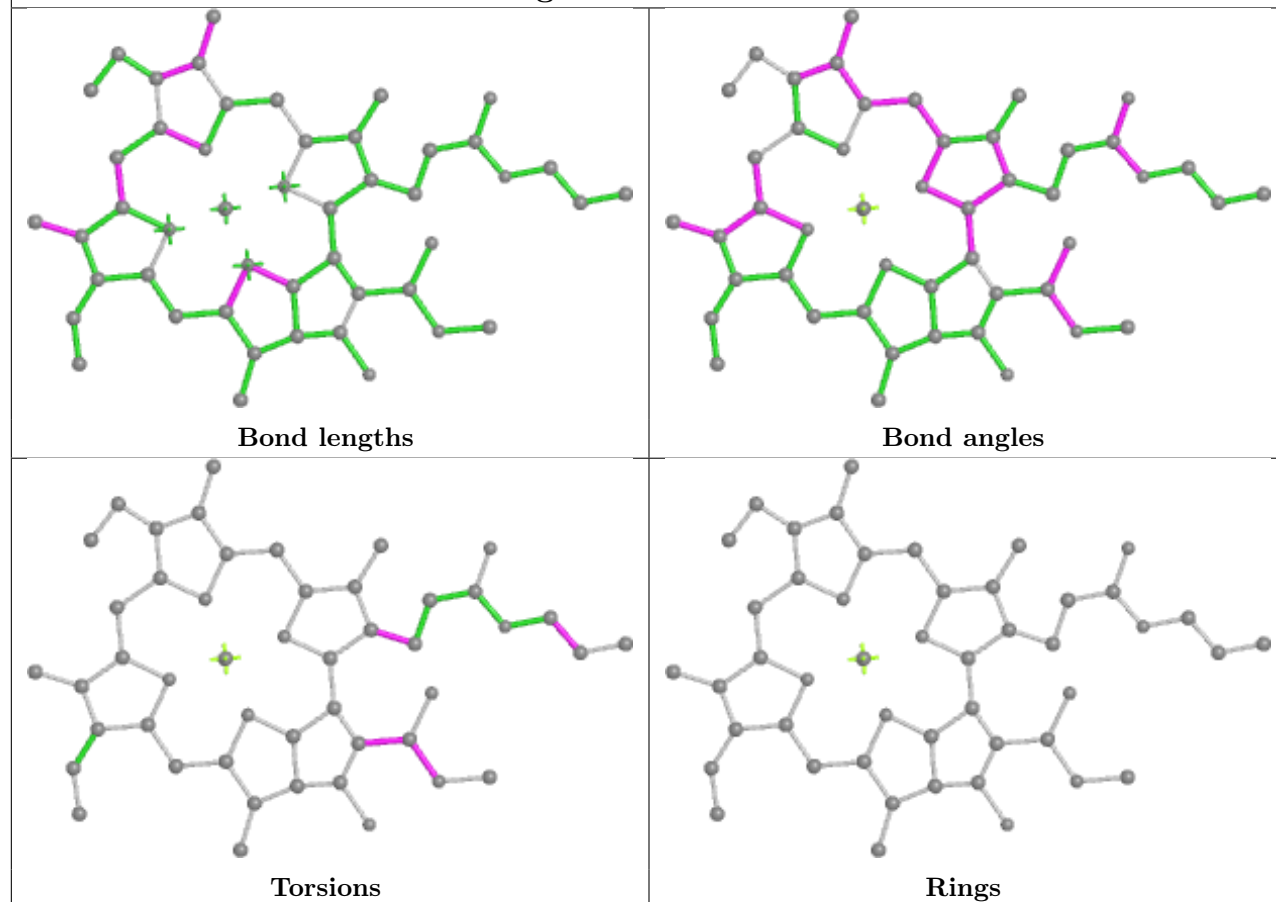
Ligand CLA 1 612



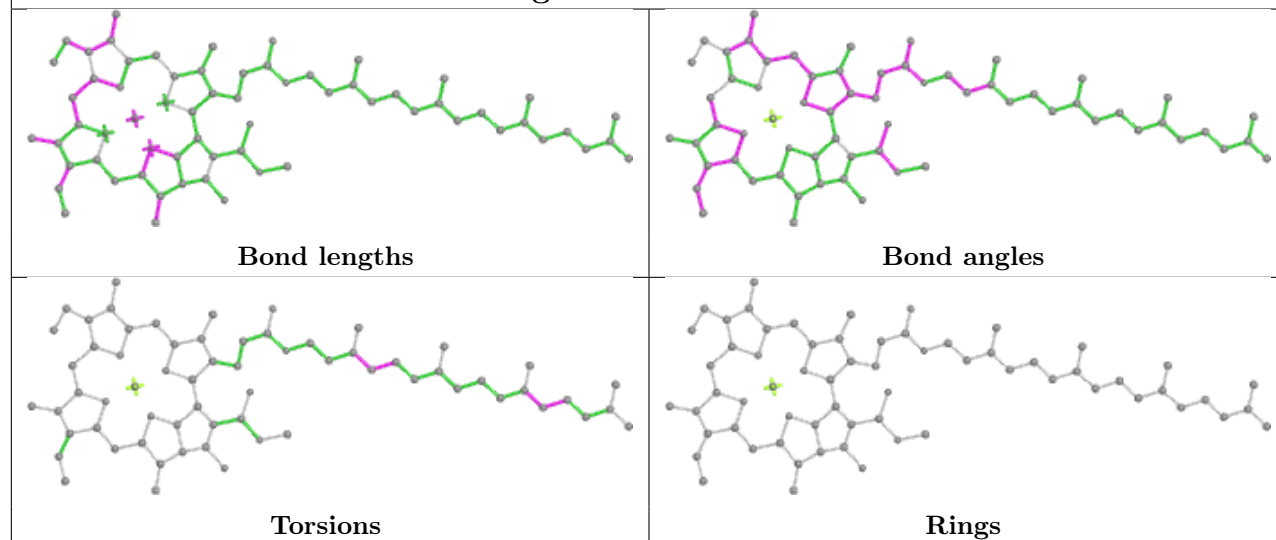
Ligand CLA B 822

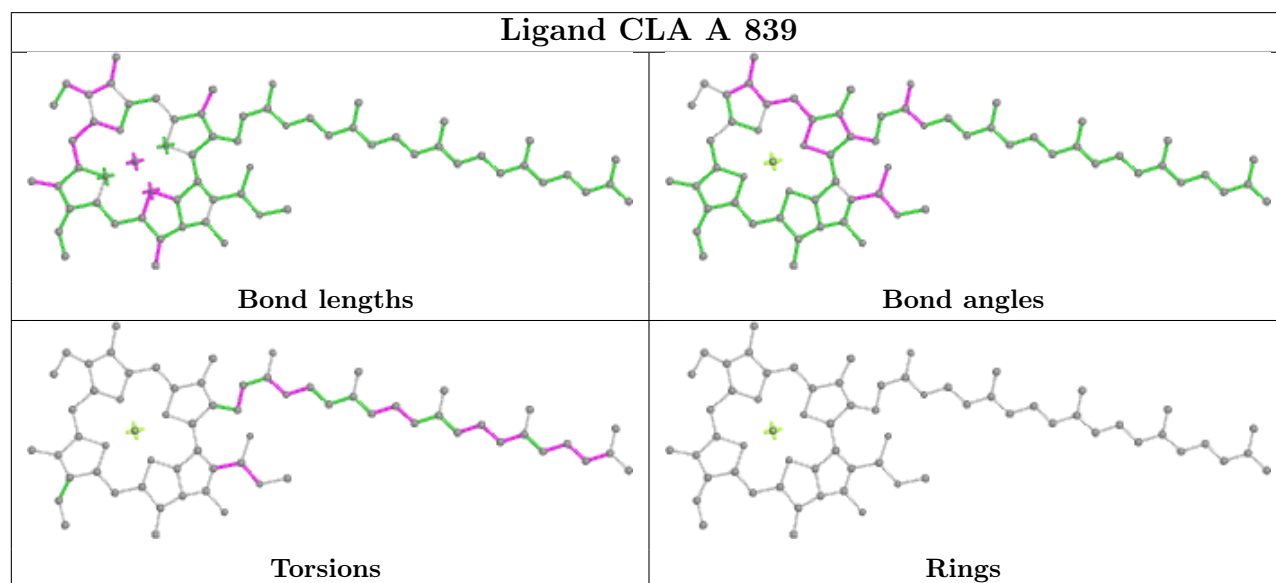
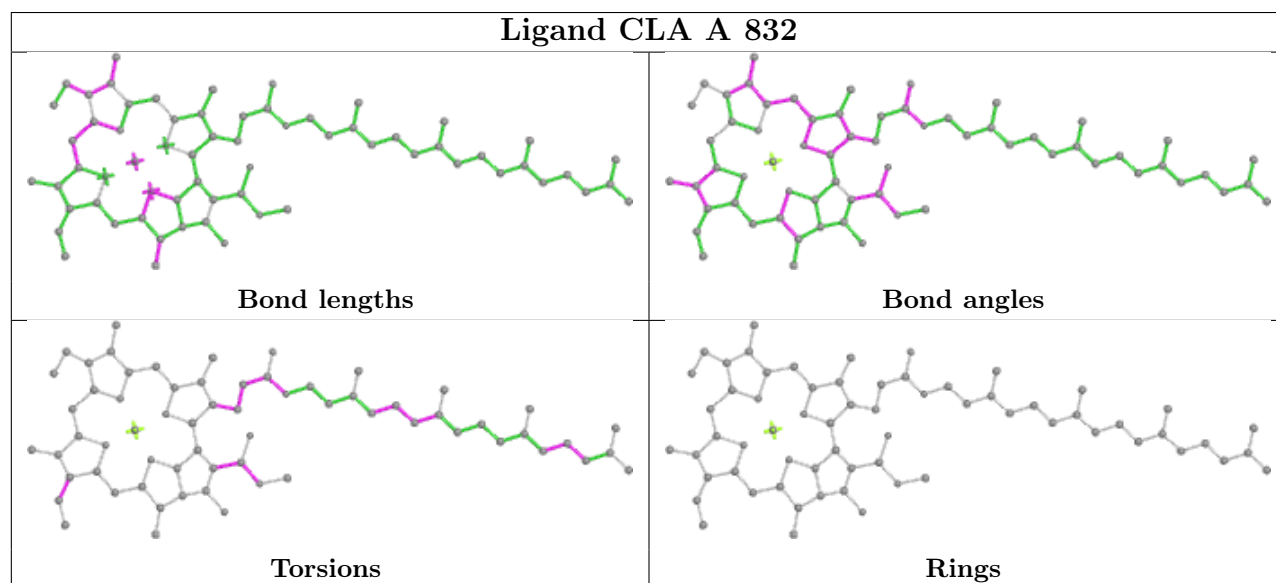
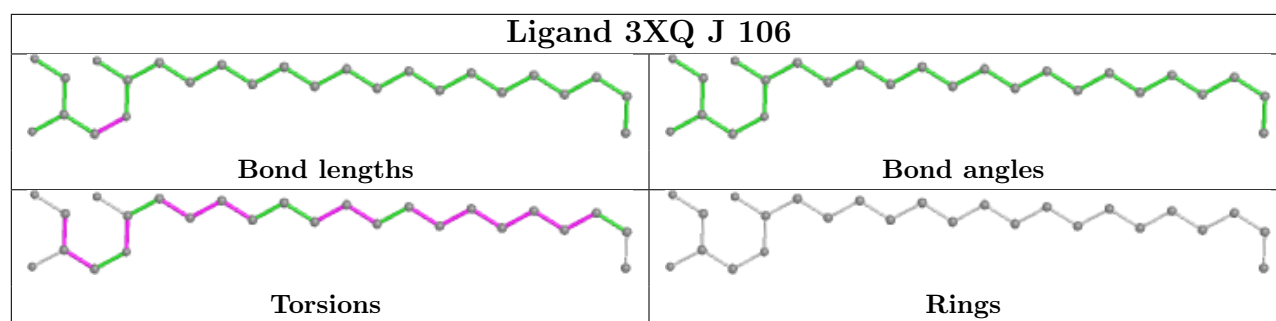


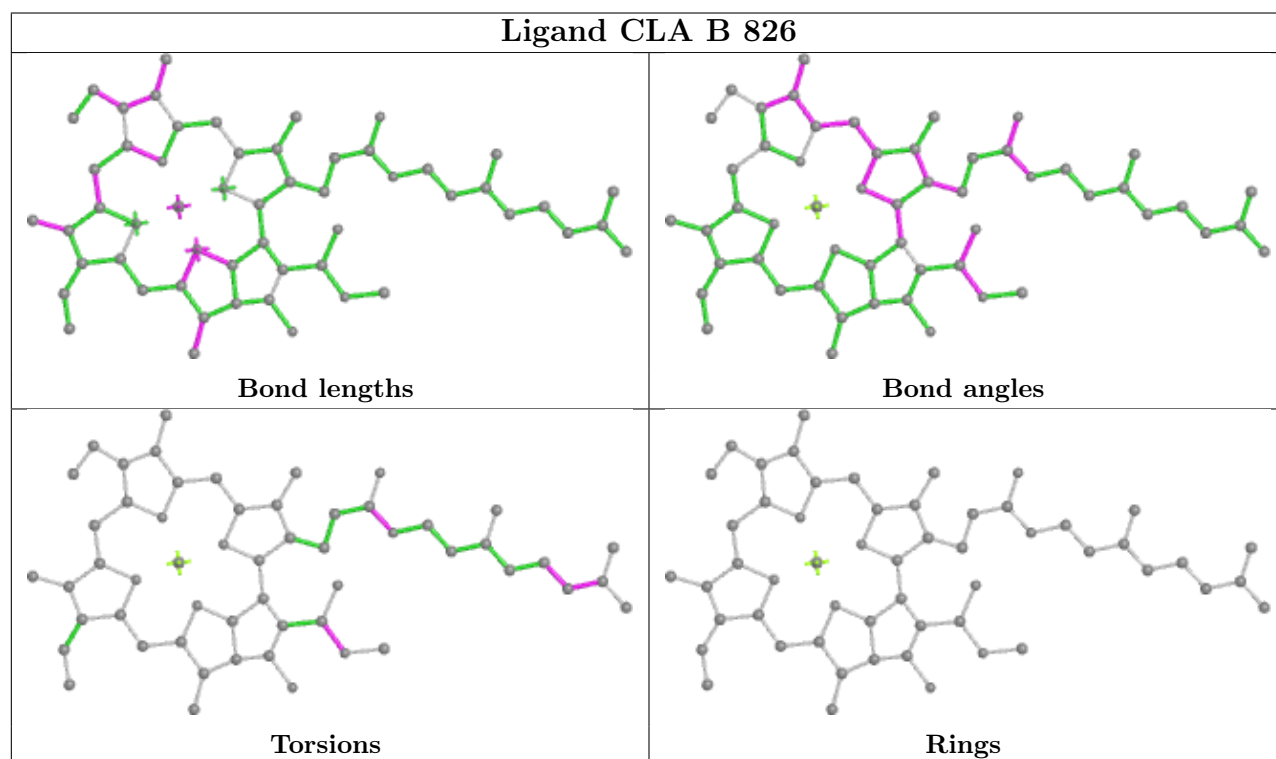
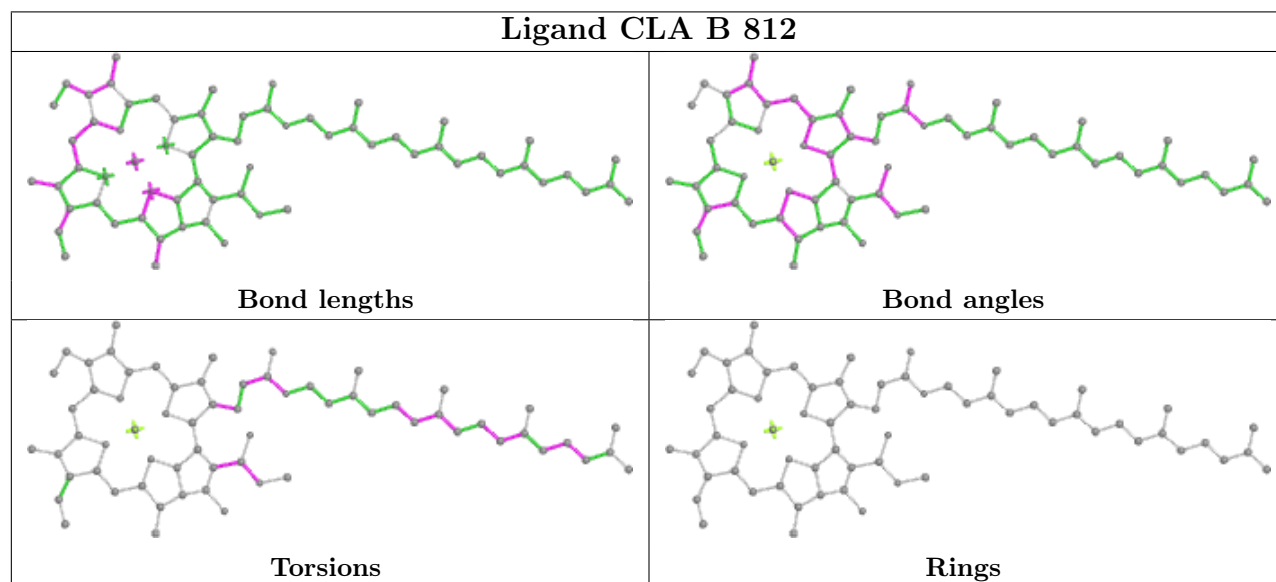
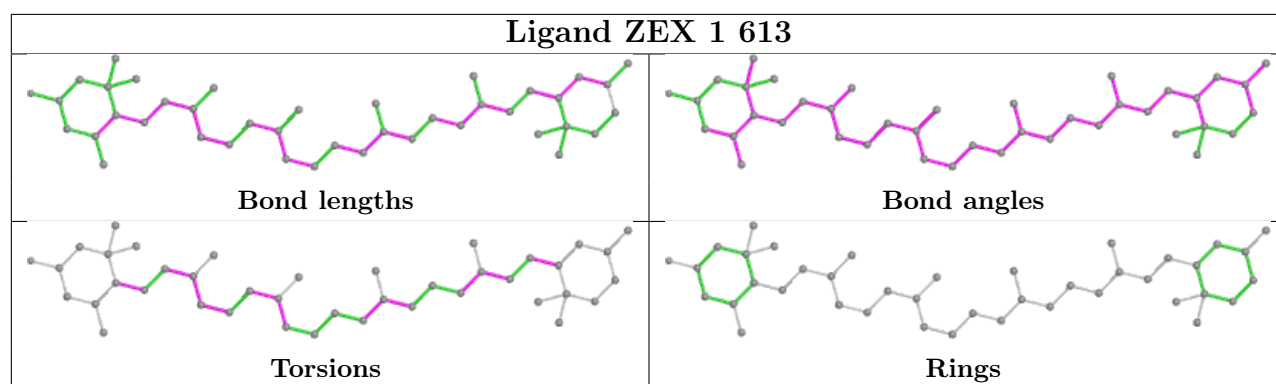
Ligand CLA 4 601

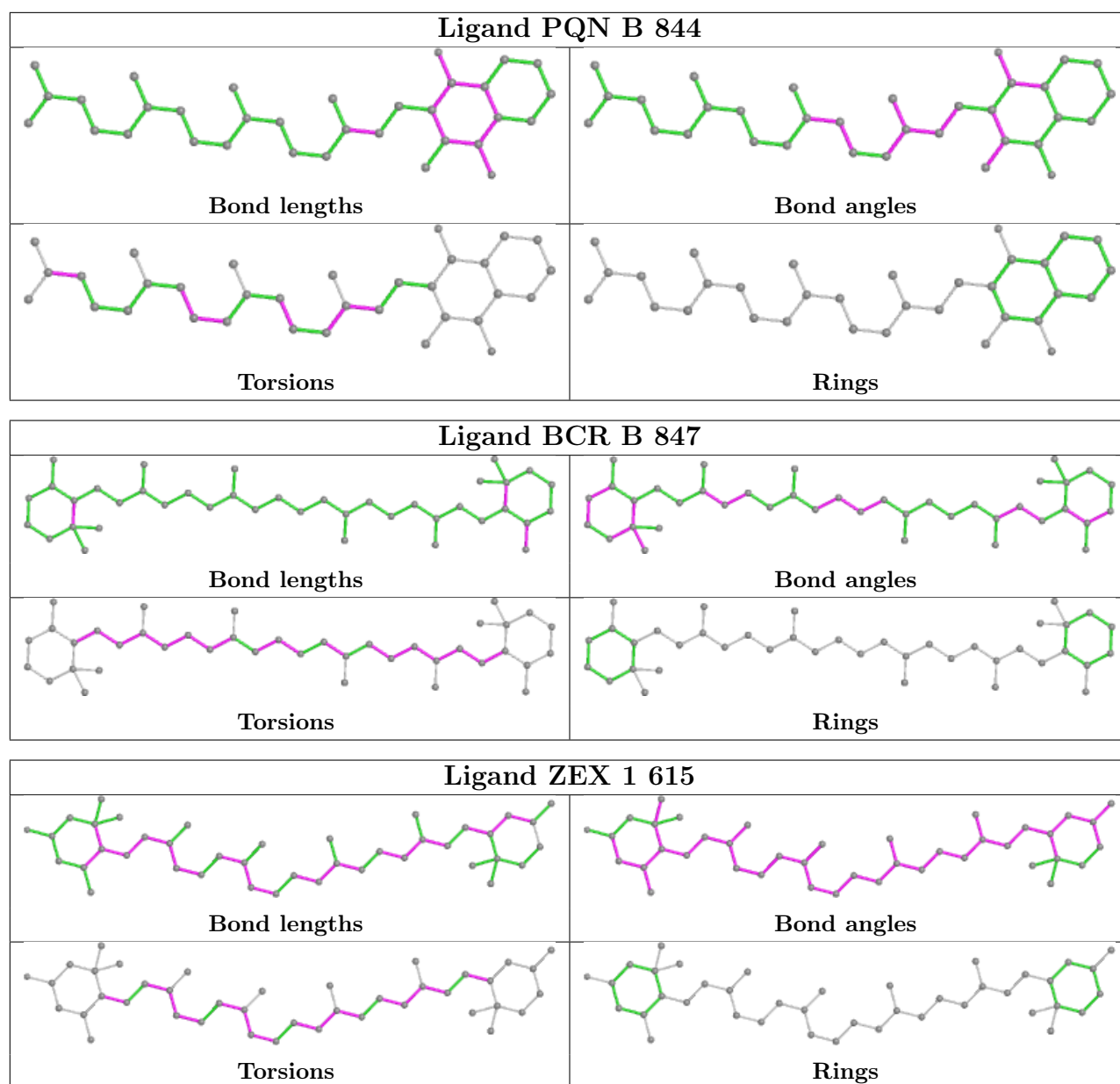


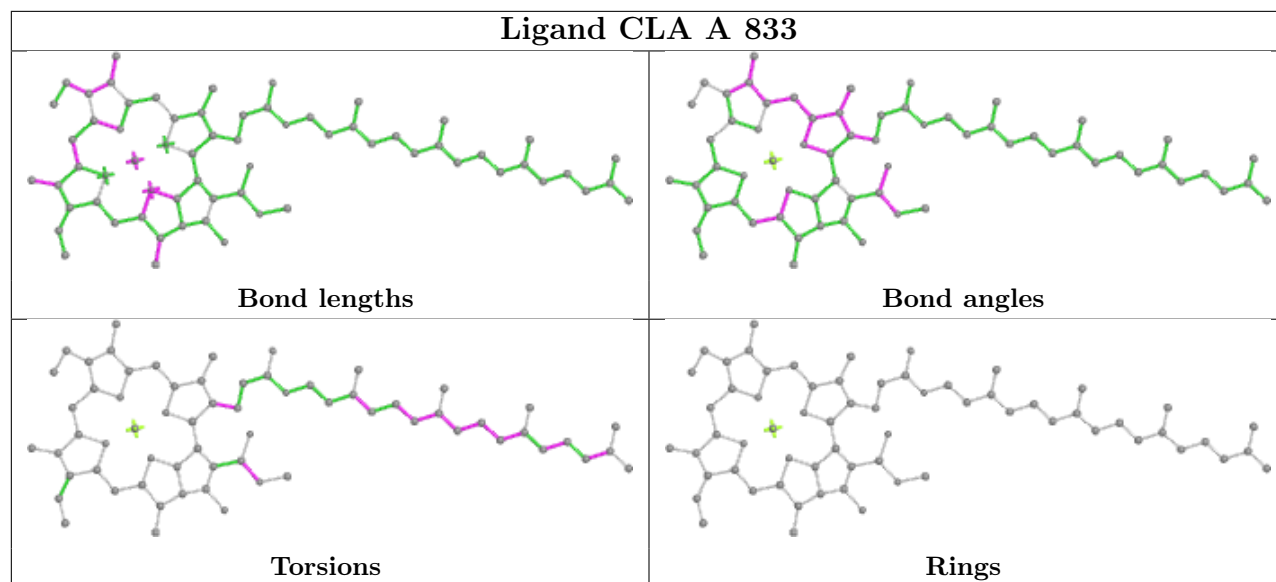
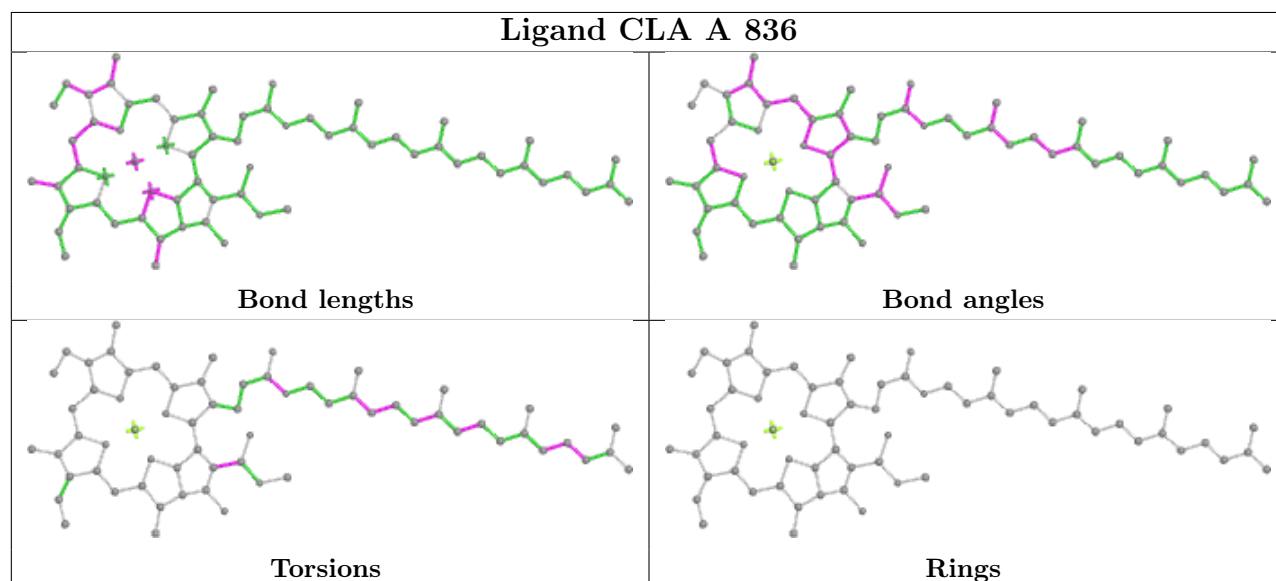
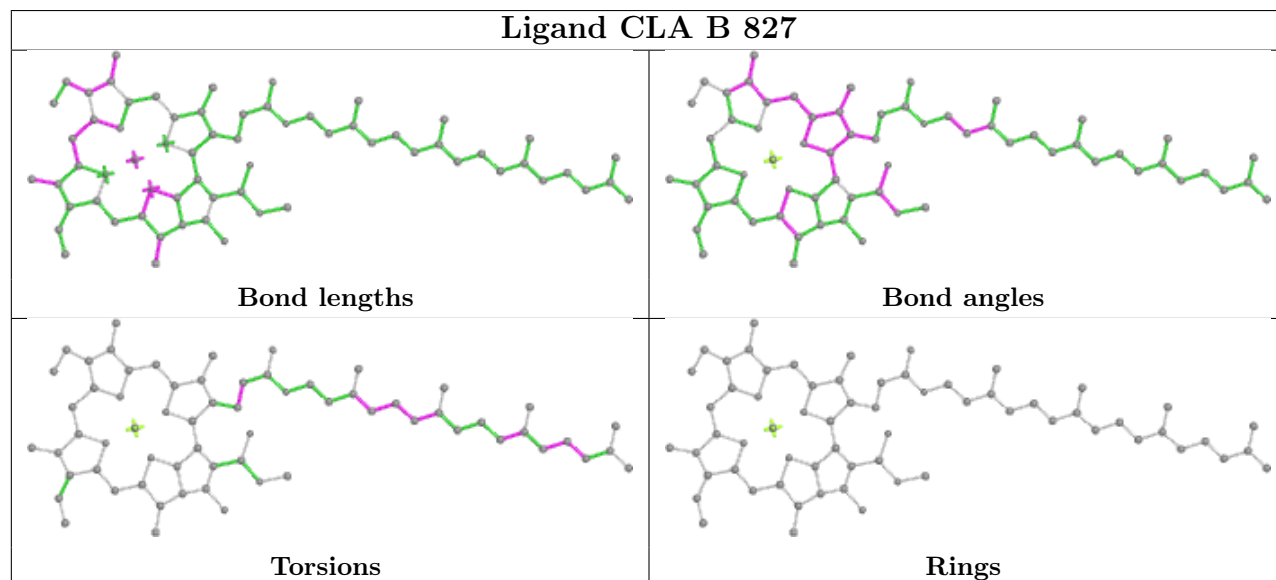
Ligand CLA B 811



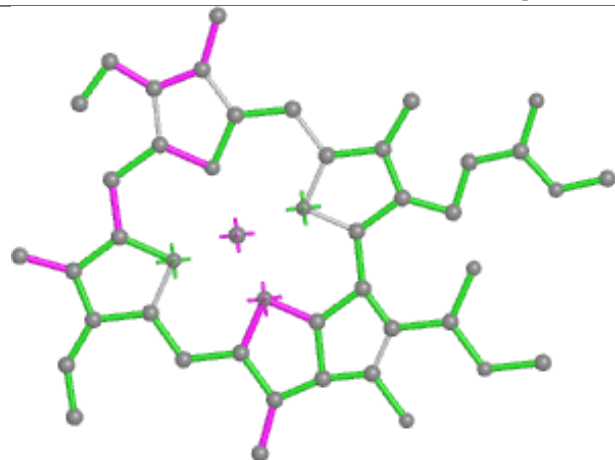




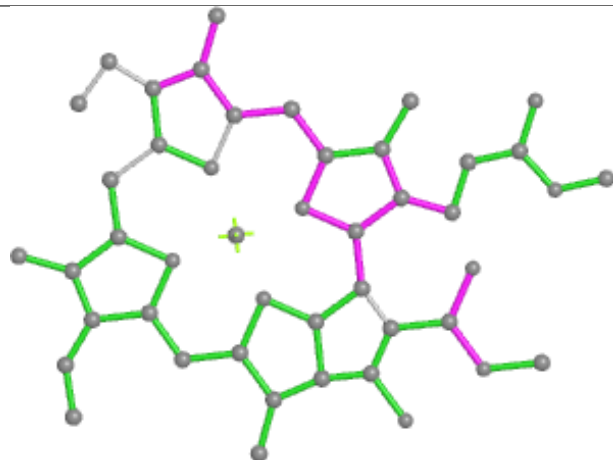


Ligand CLA A 833**Ligand CLA A 836****Ligand CLA B 827**

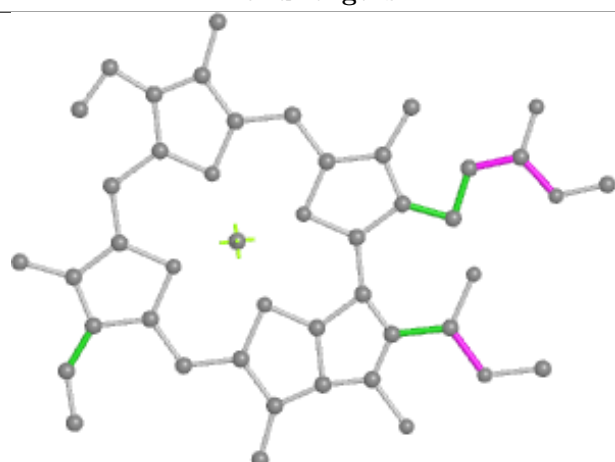
Ligand CLA B 824



Bond lengths



Bond angles

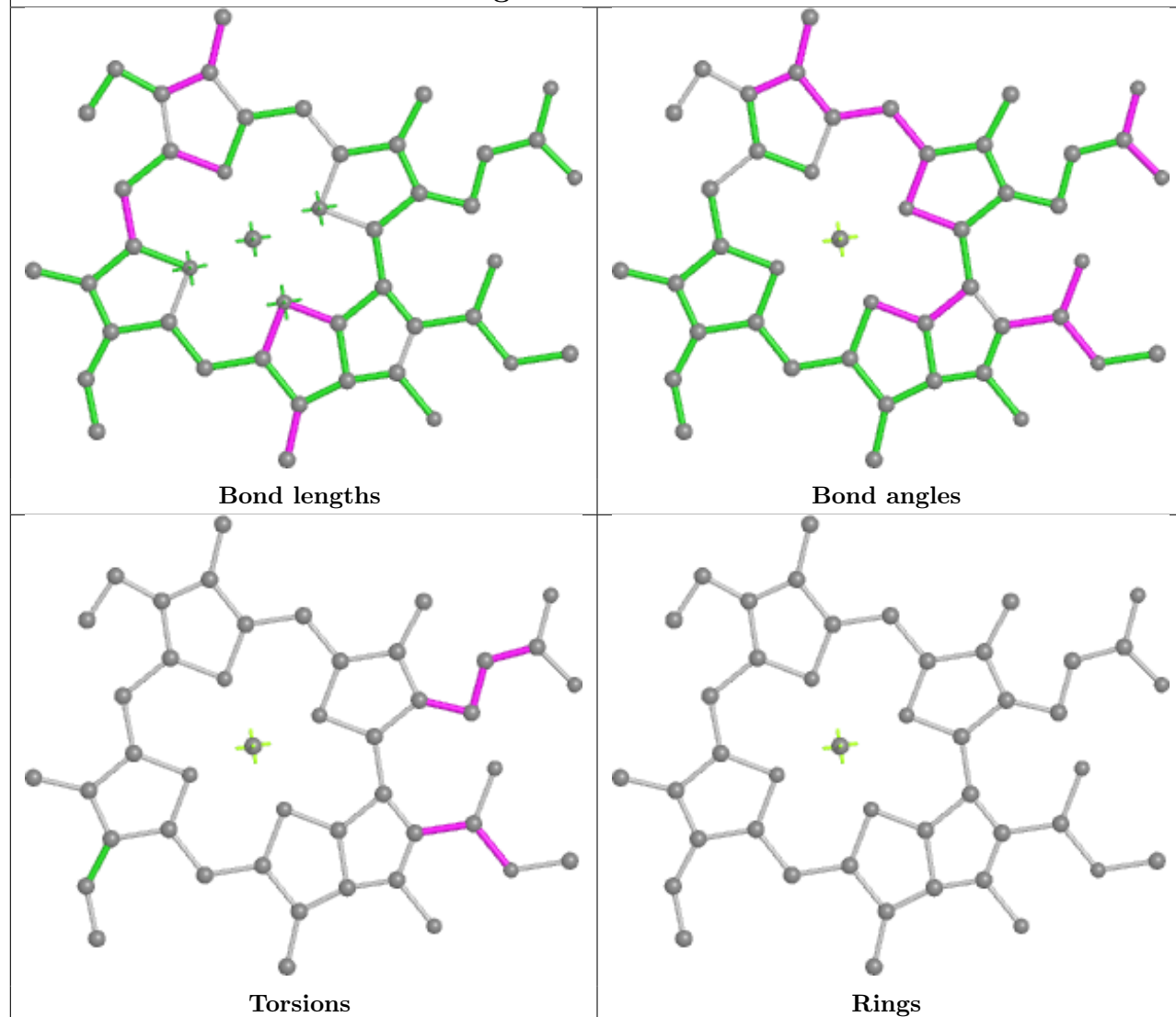


Torsions

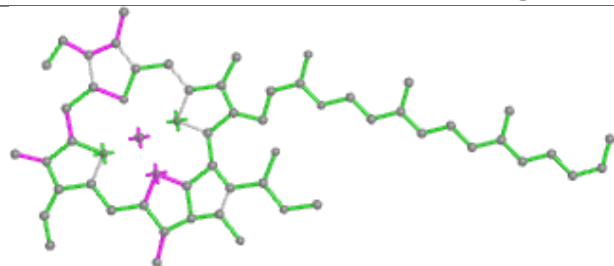


Rings

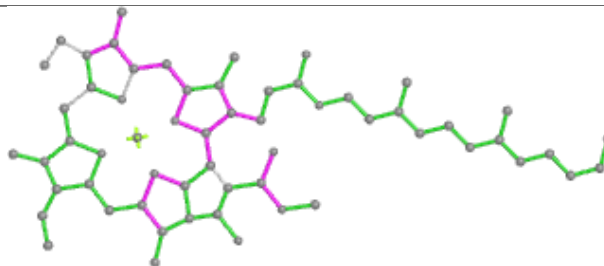
Ligand CLA 4 611



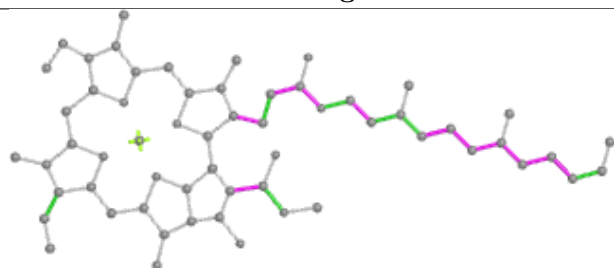
Ligand CLA B 820



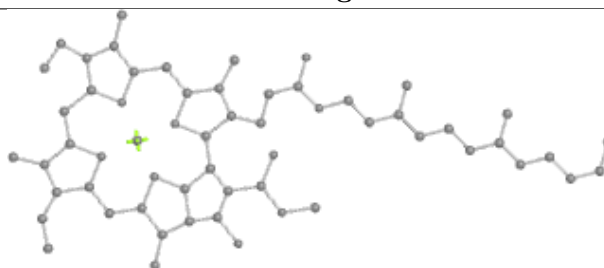
Bond lengths



Bond angles

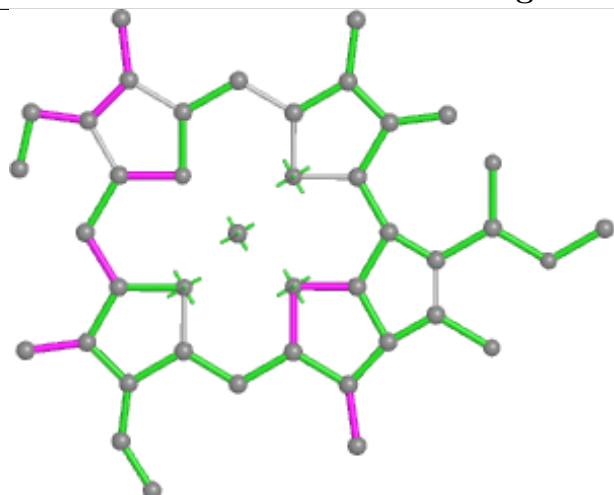


Torsions

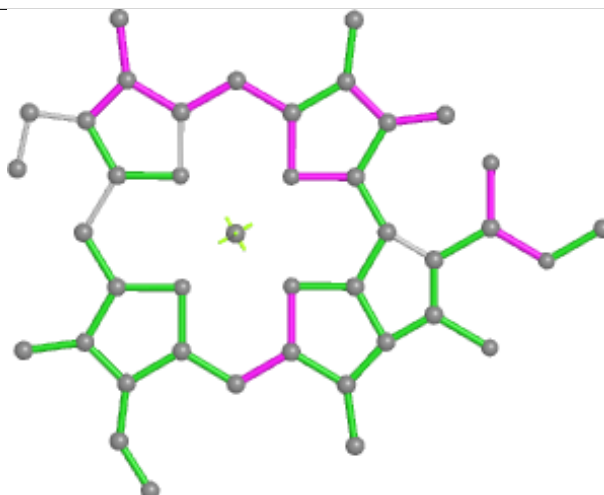


Rings

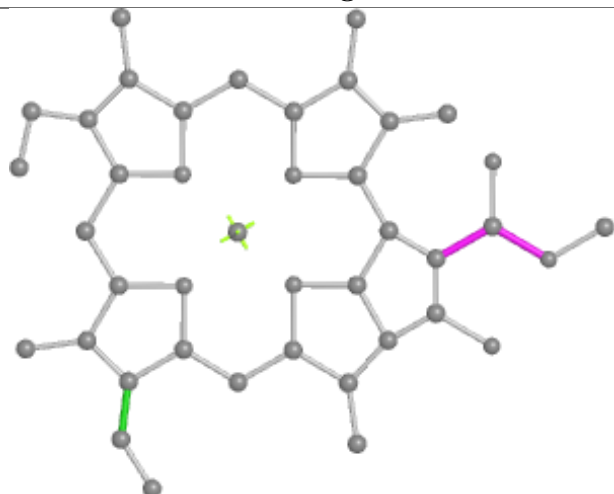
Ligand CLA F 303



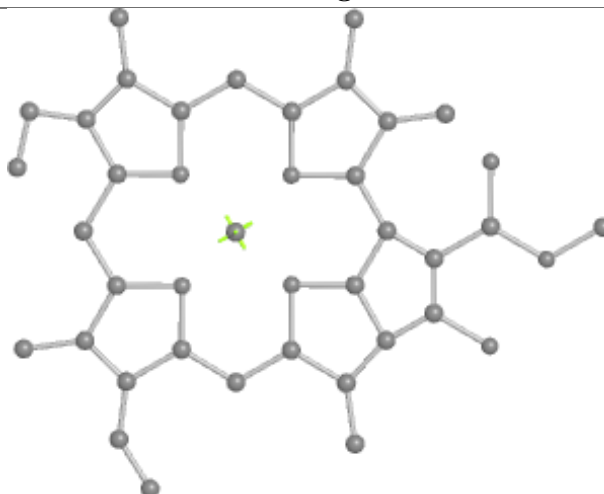
Bond lengths



Bond angles

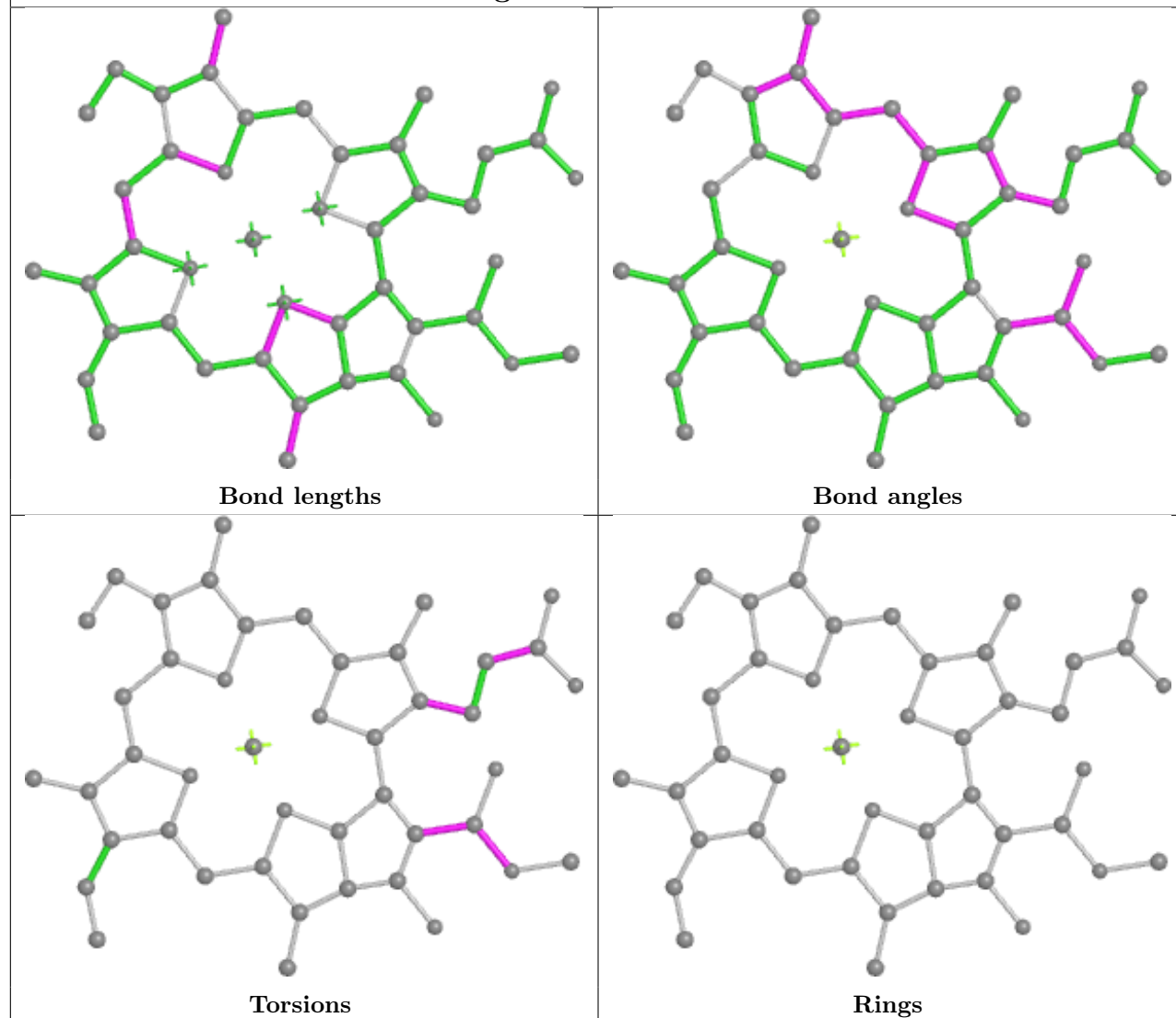


Torsions

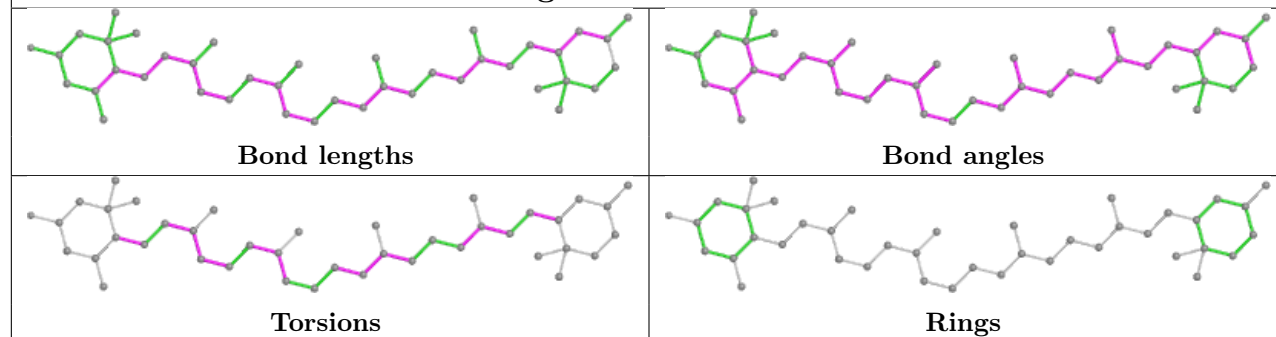


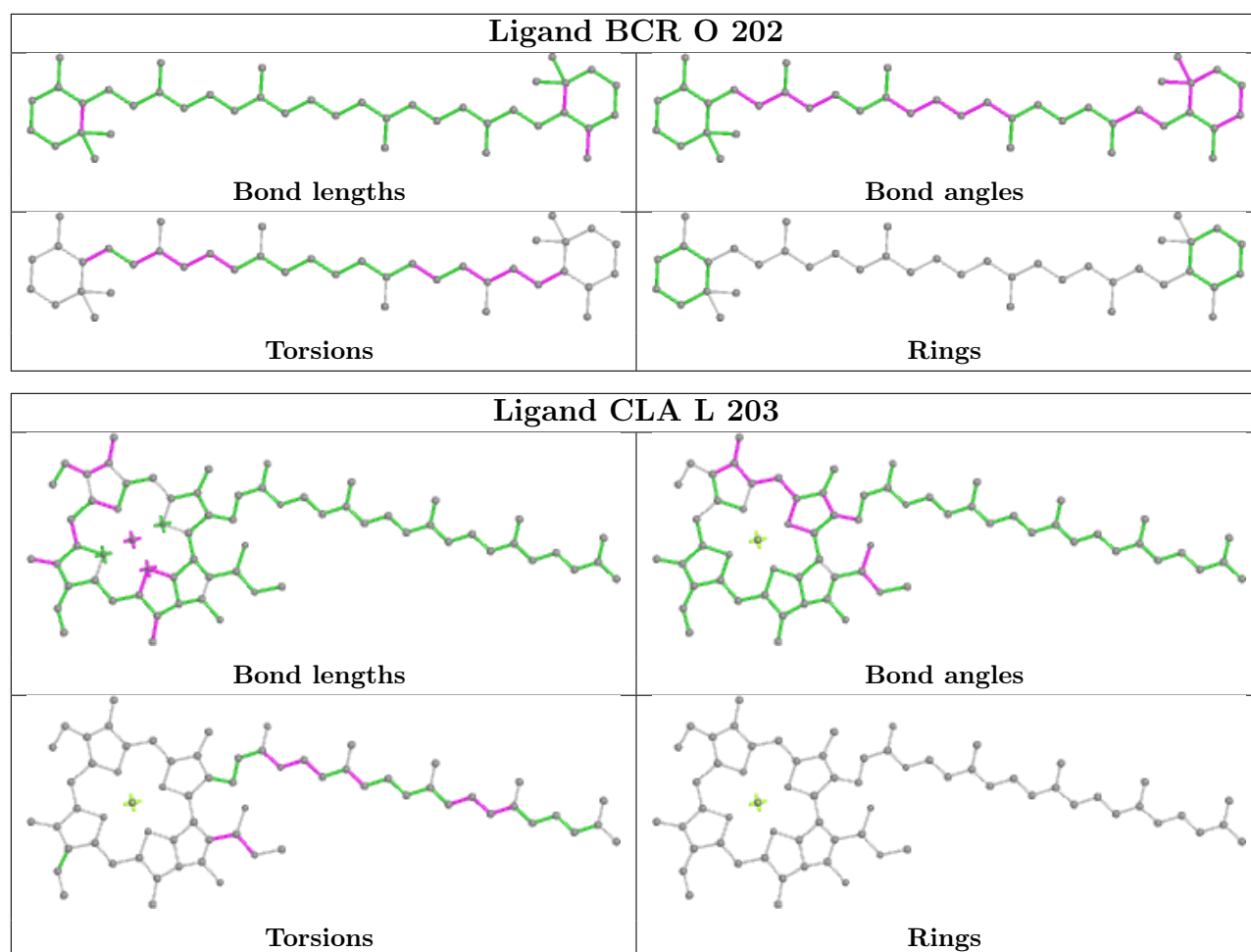
Rings

Ligand CLA 5 605

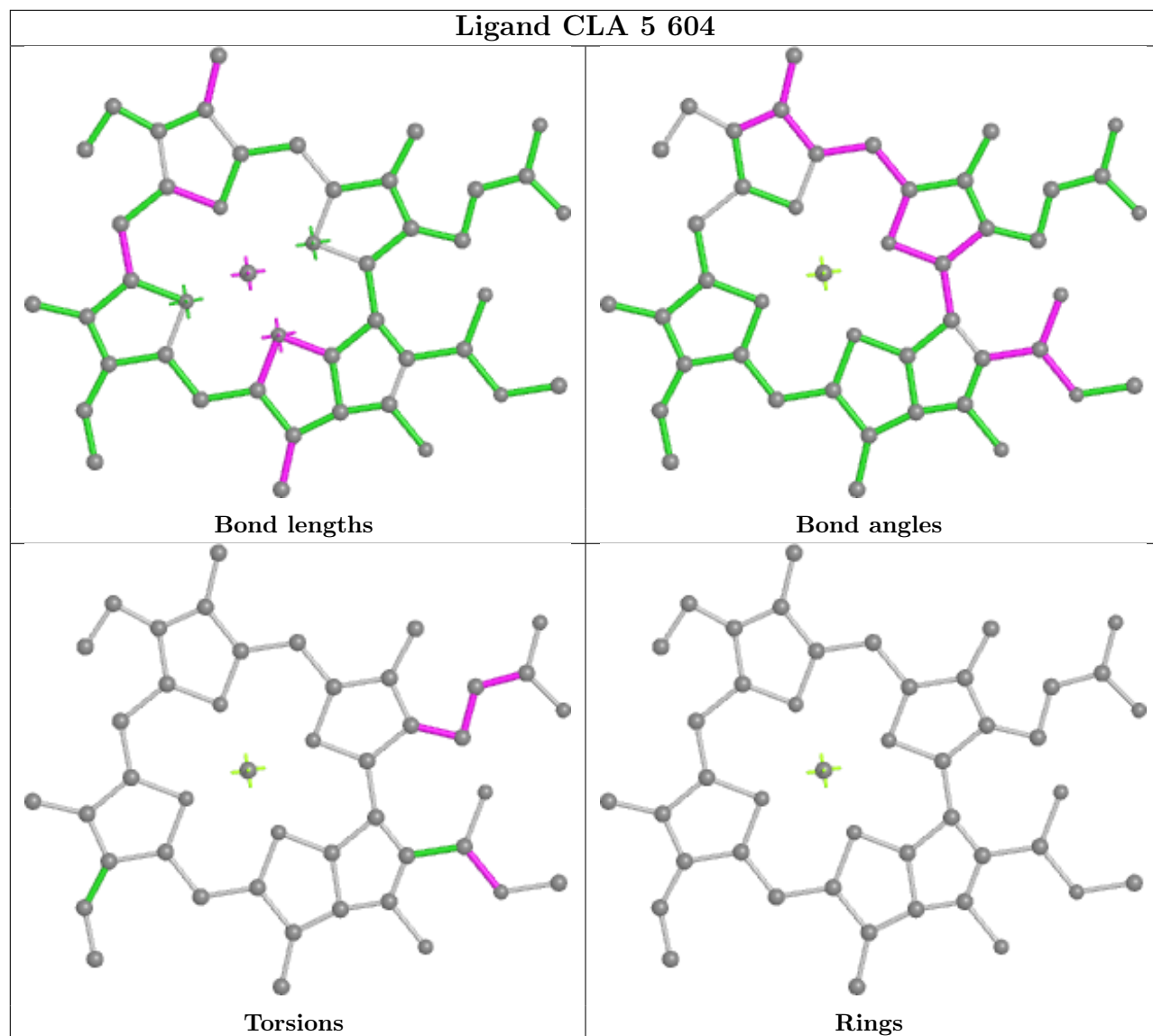


Ligand ZEX 1 617

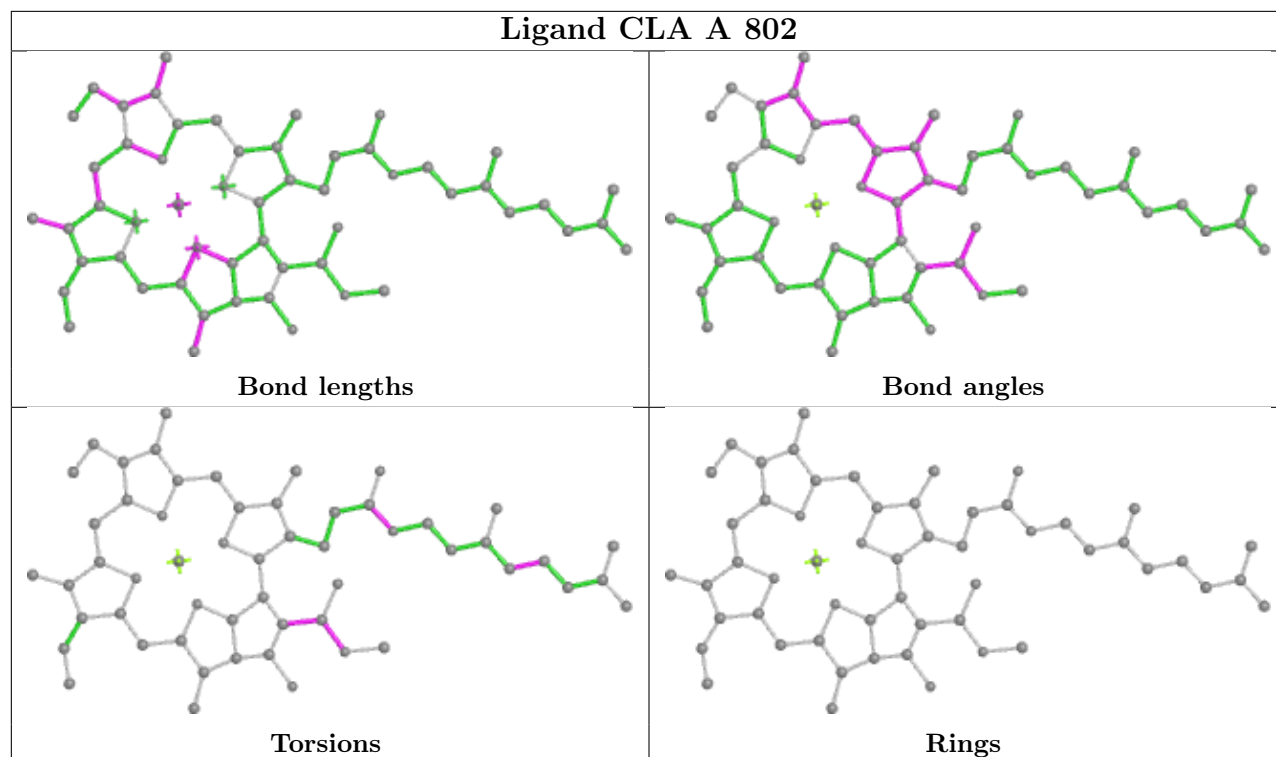




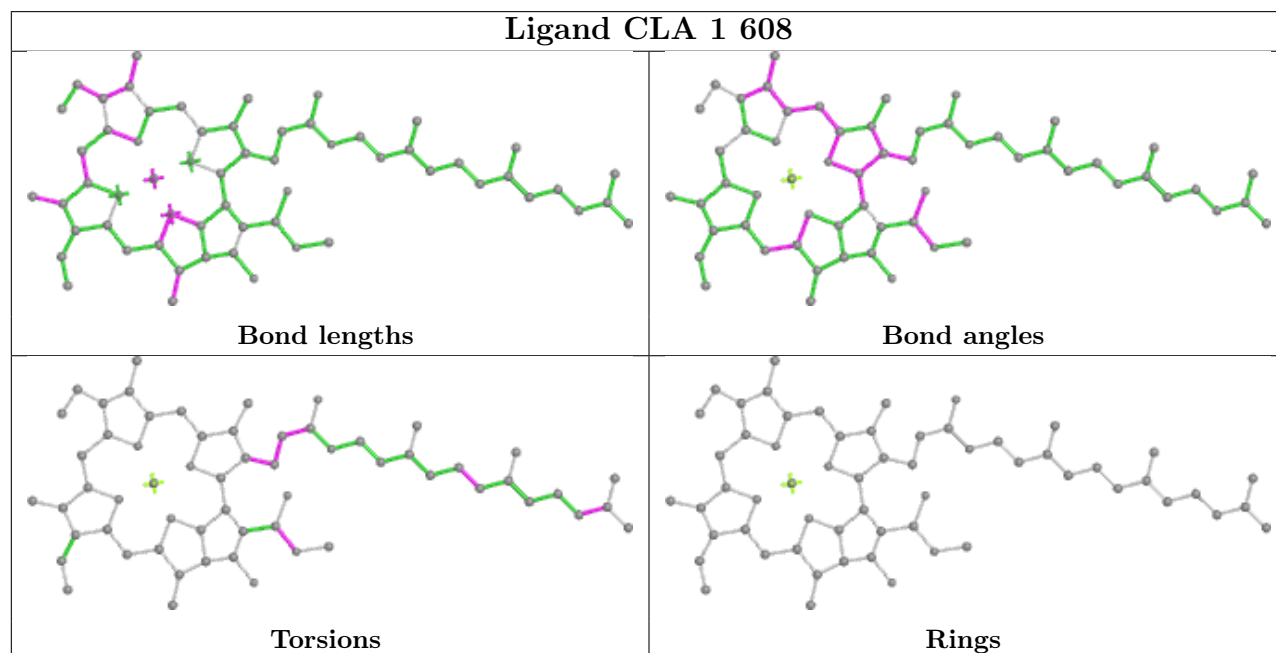
Ligand CLA 5 604



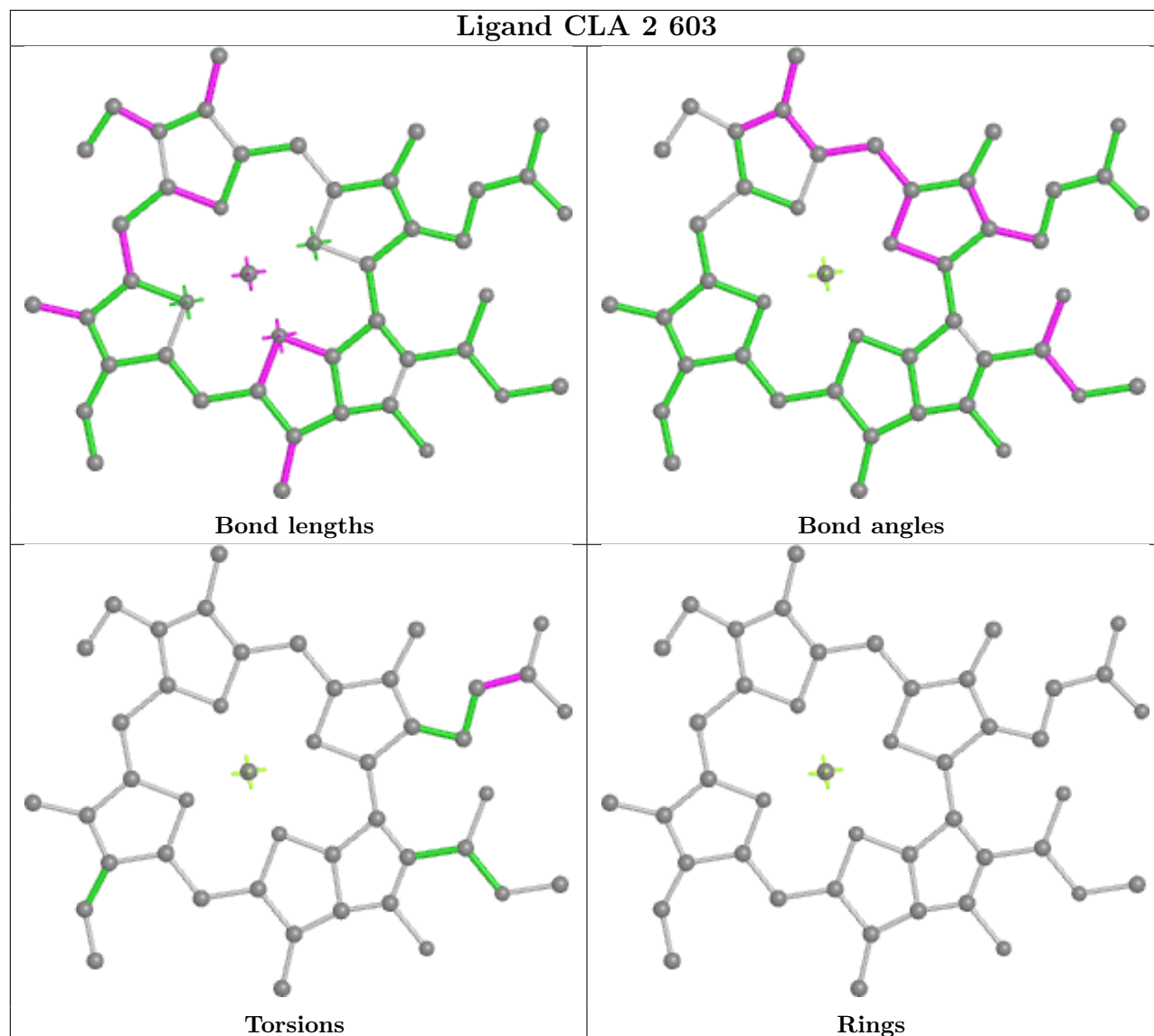
Ligand CLA A 802



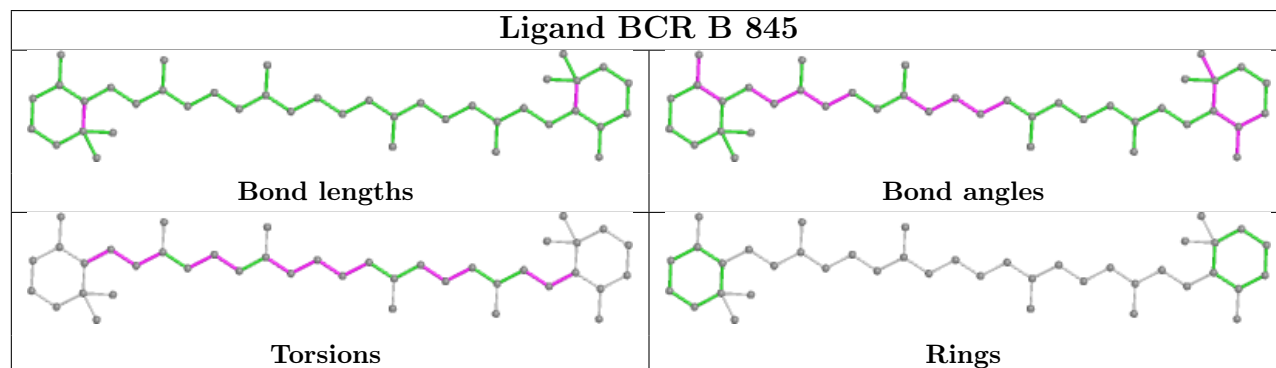
Ligand CLA 1 608

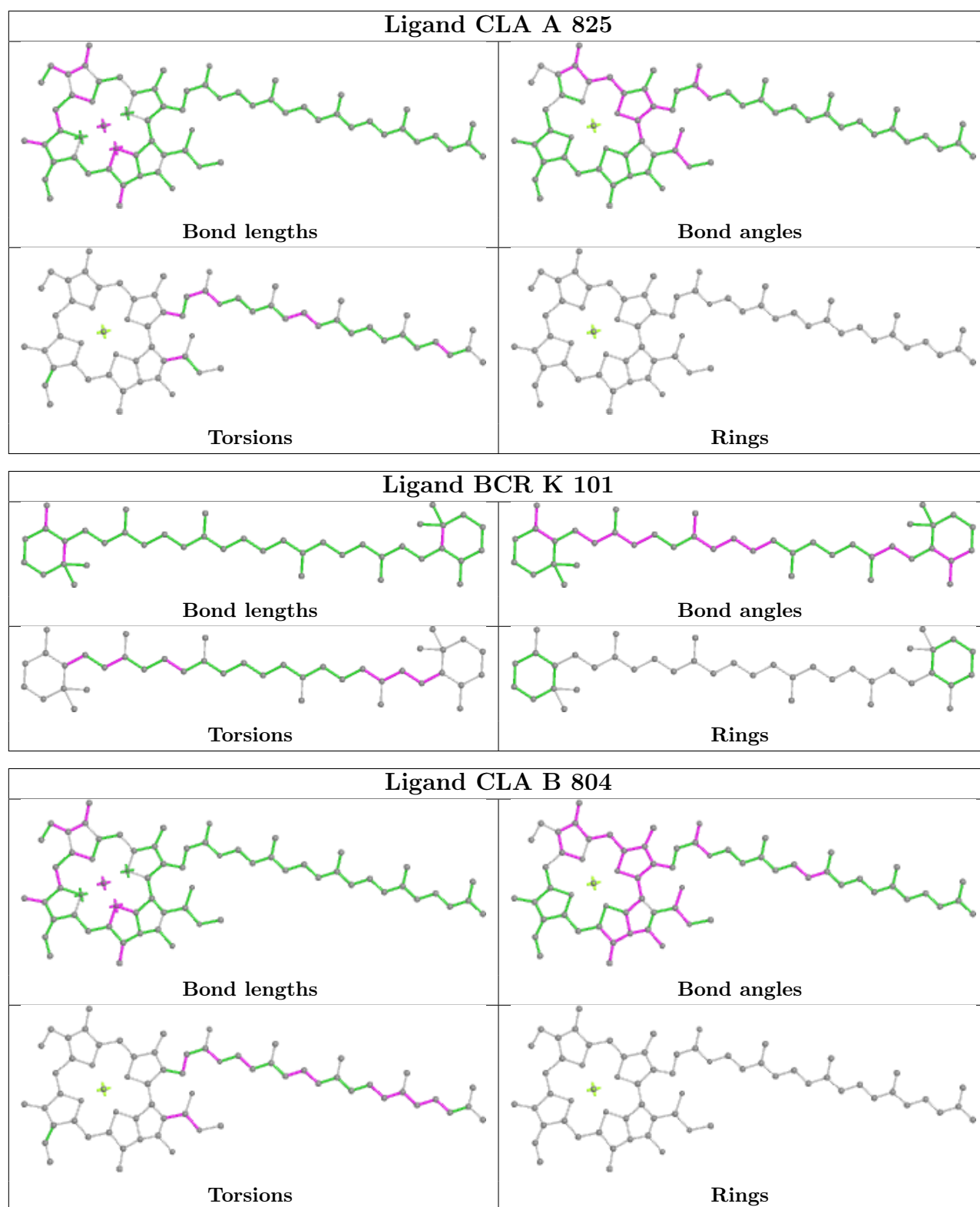


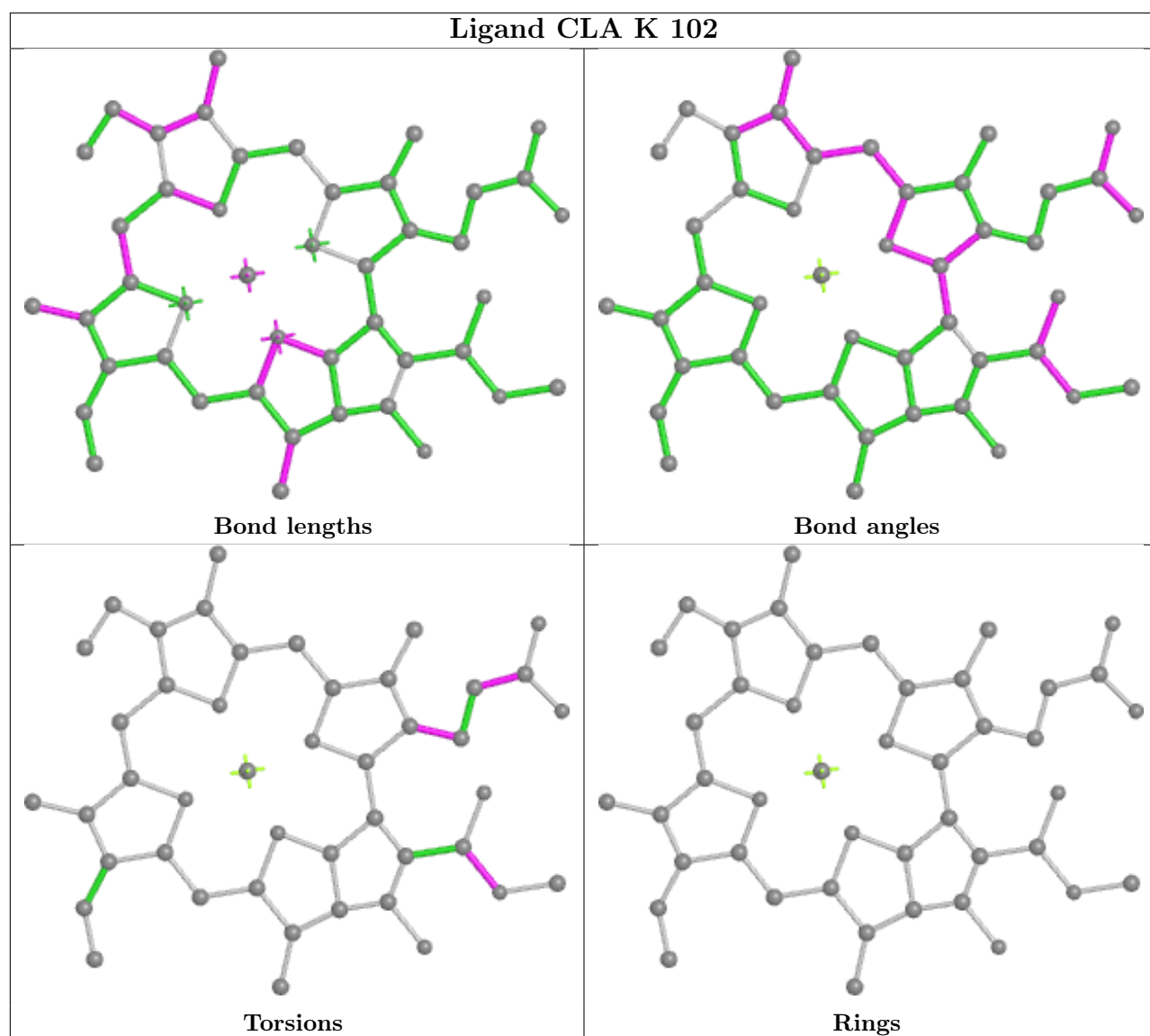
Ligand CLA 2 603



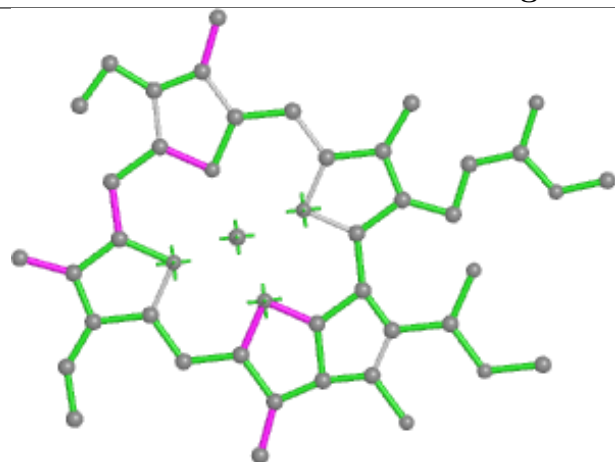
Ligand BCR B 845



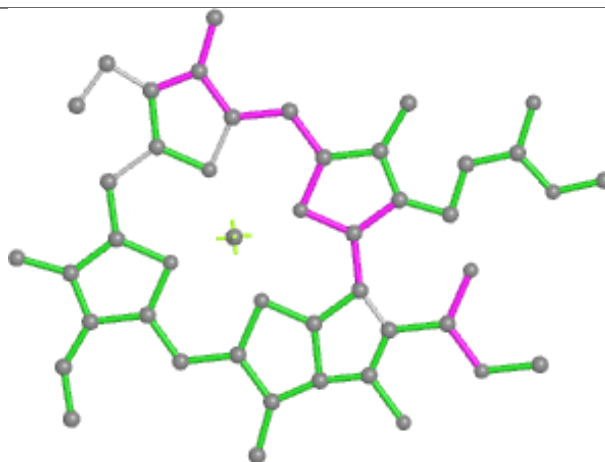




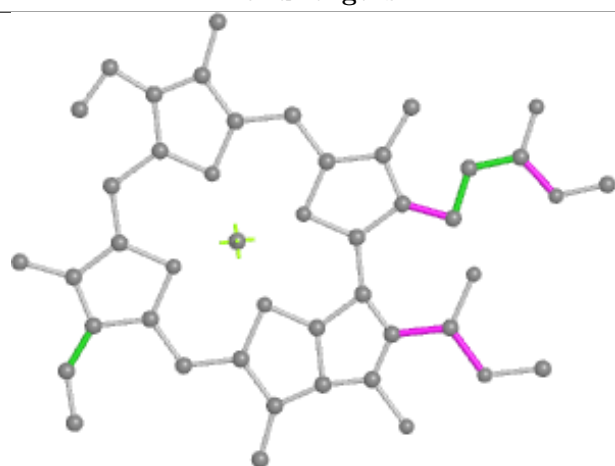
Ligand CLA 3 212



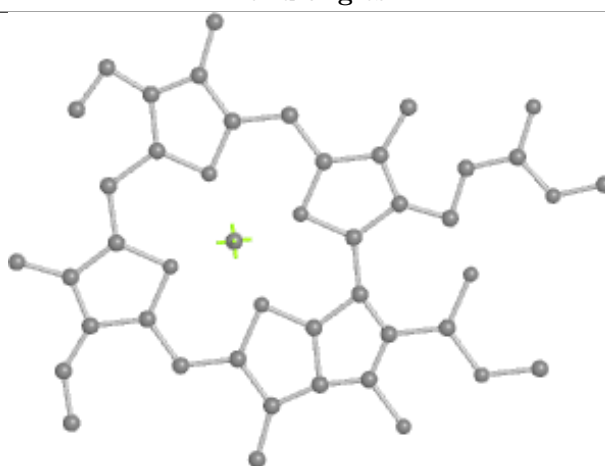
Bond lengths



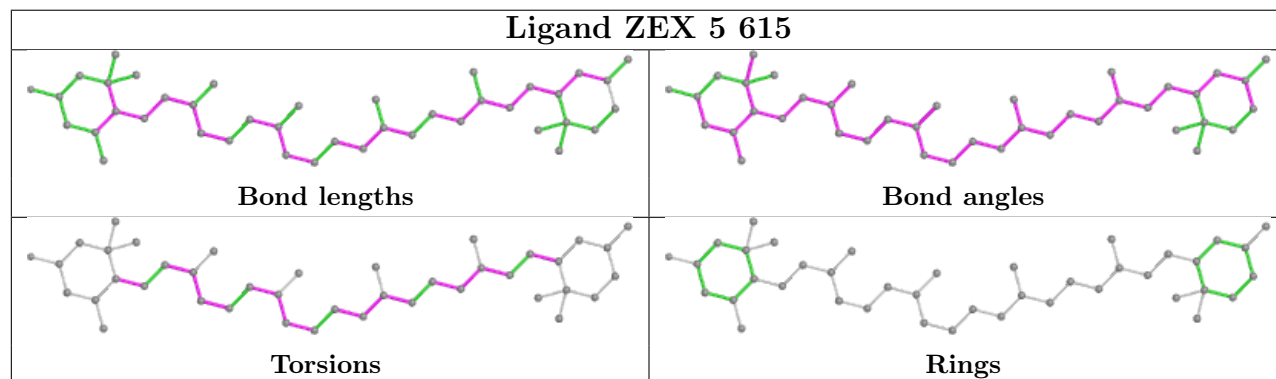
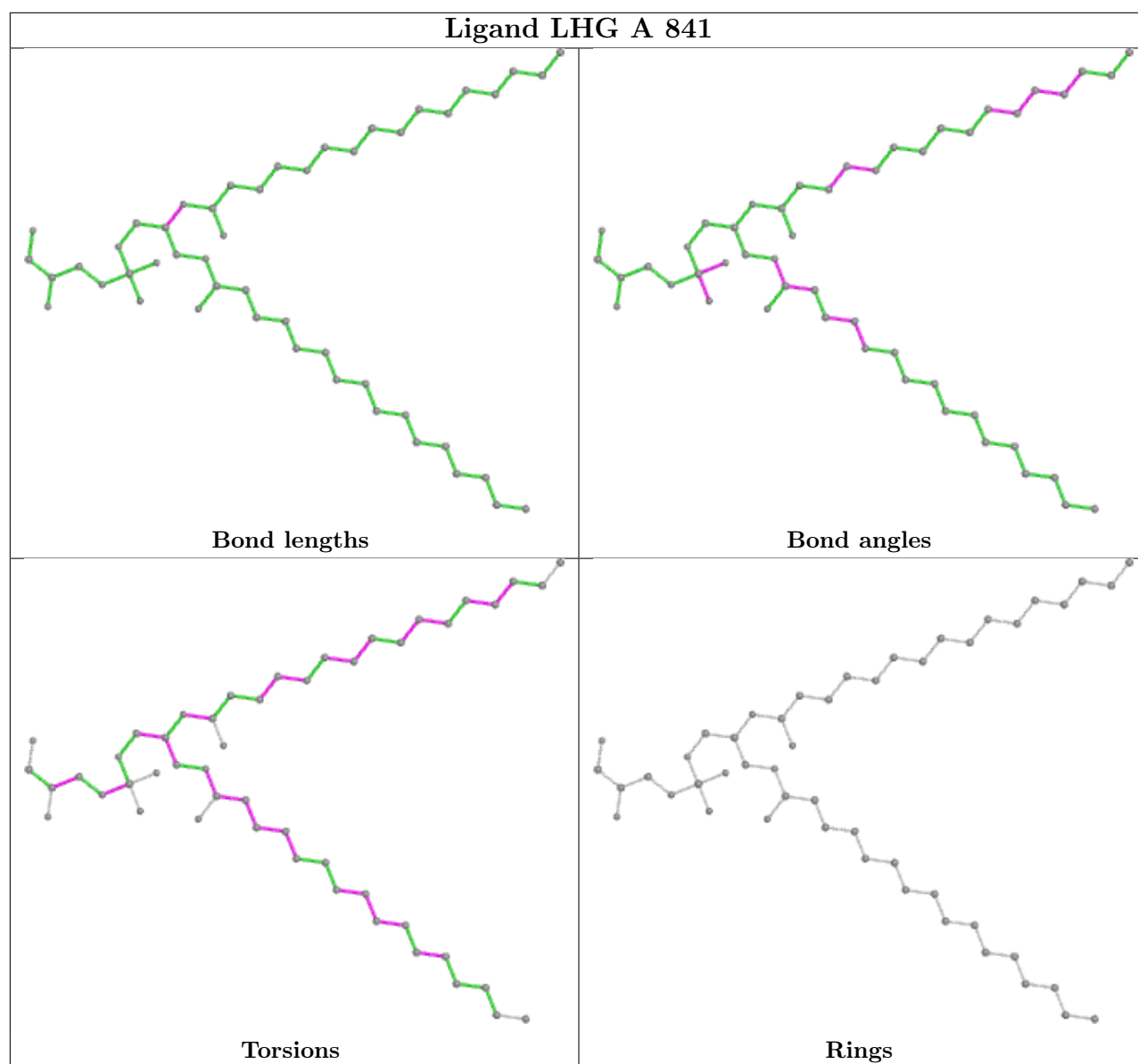
Bond angles



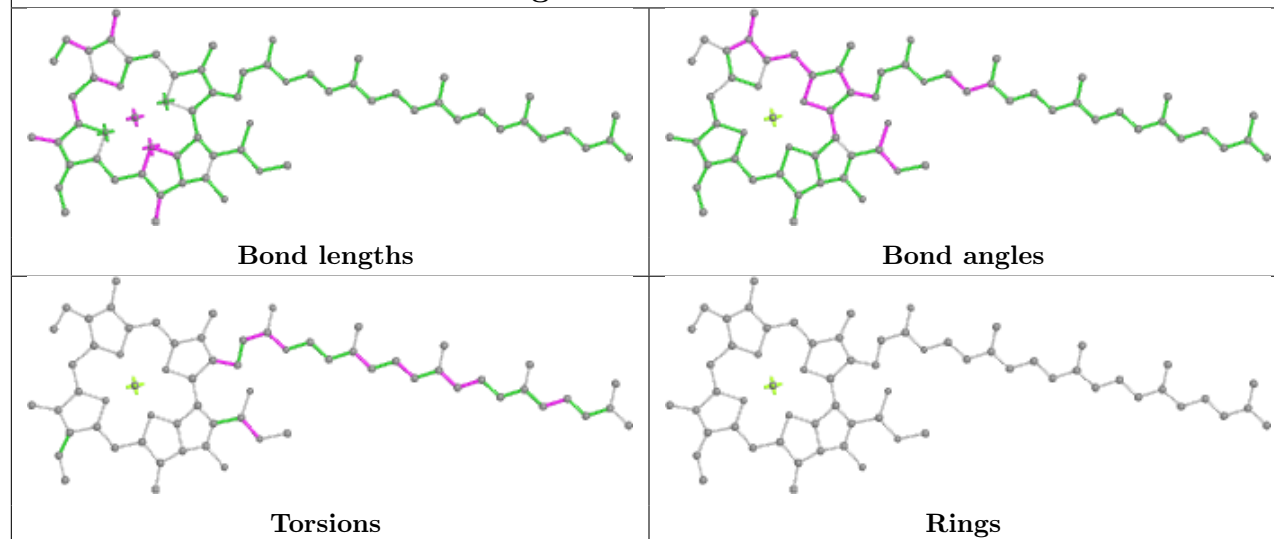
Torsions



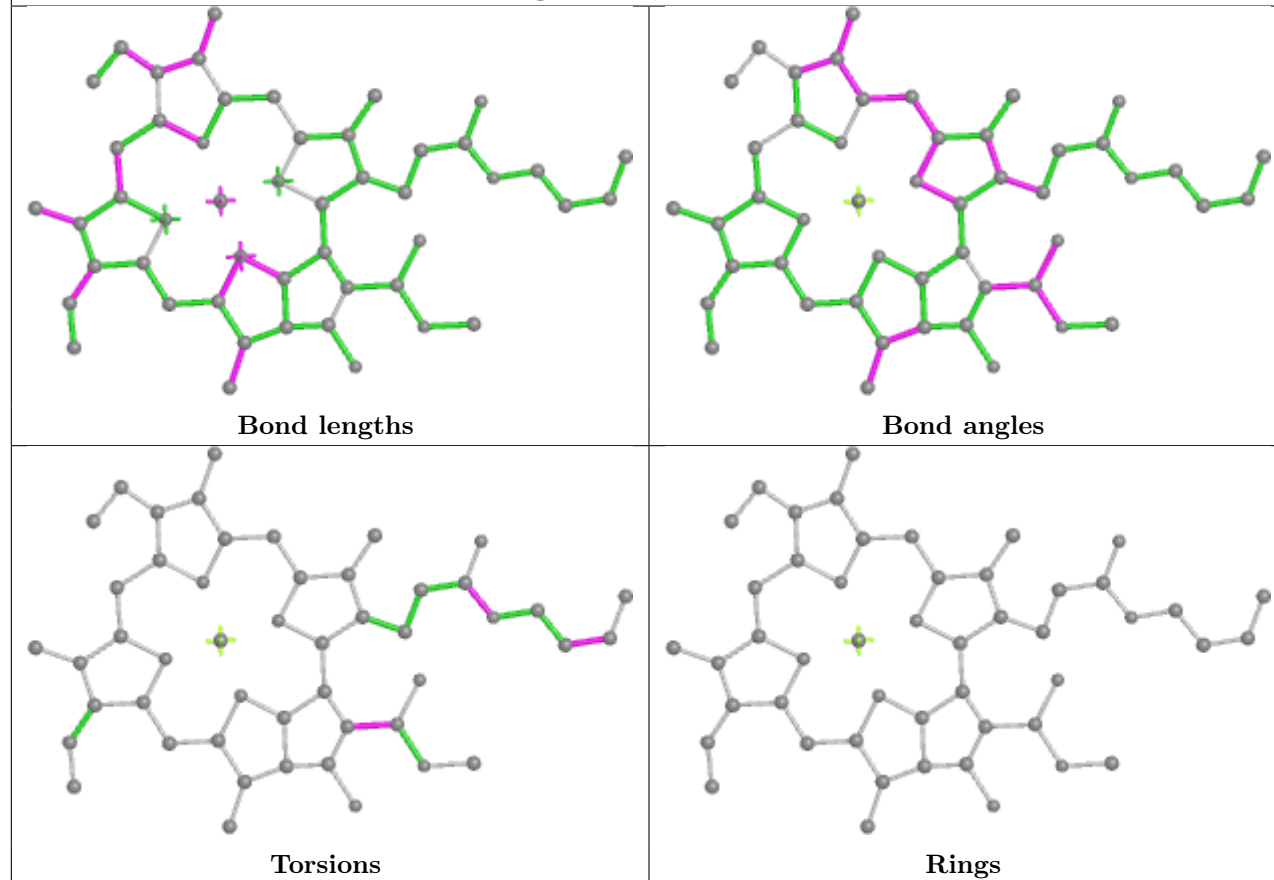
Rings



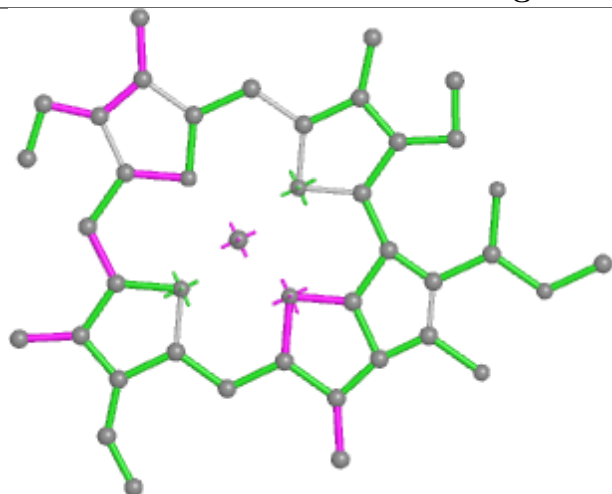
Ligand CLA A 804



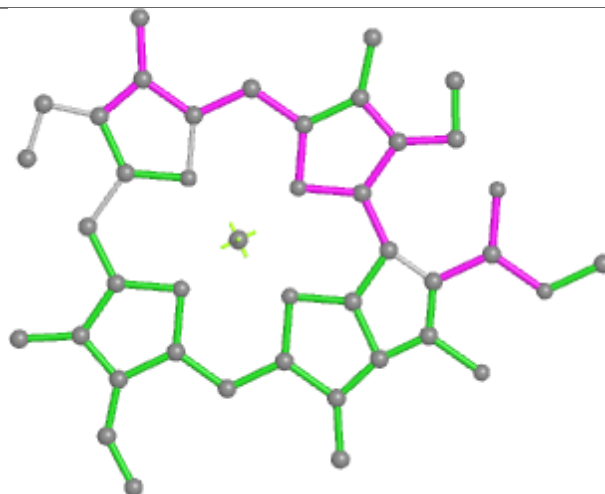
Ligand CLA A 820



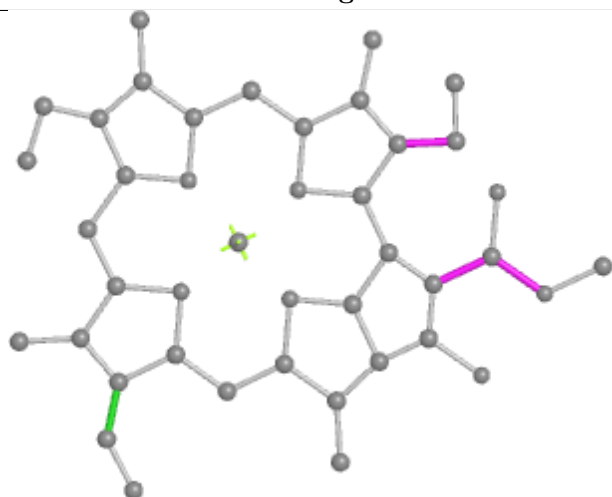
Ligand CLA B 818



Bond lengths



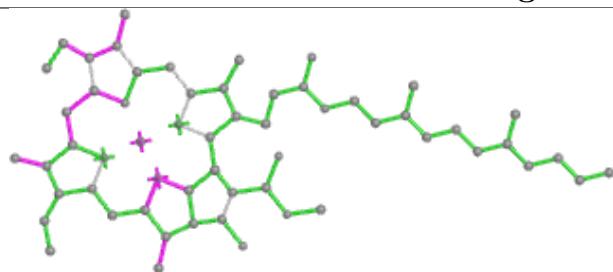
Bond angles



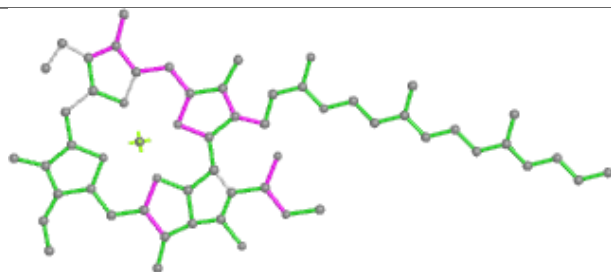
Torsions



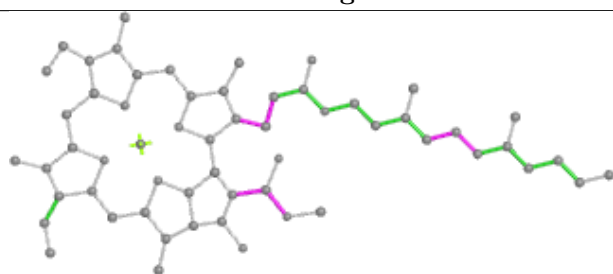
Rings

Ligand CLA J 102

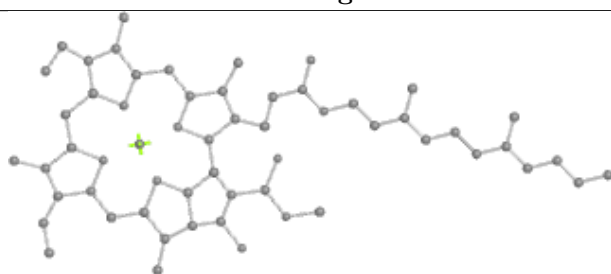
Bond lengths



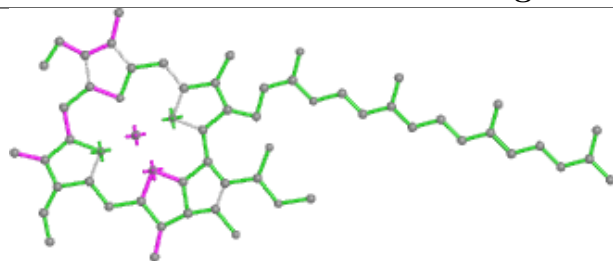
Bond angles



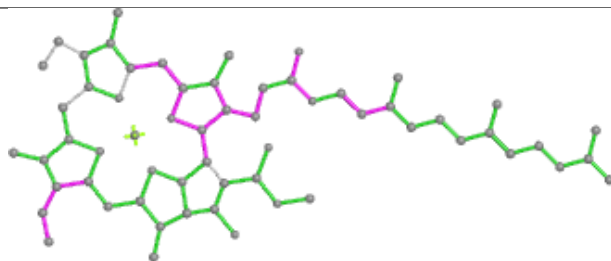
Torsions



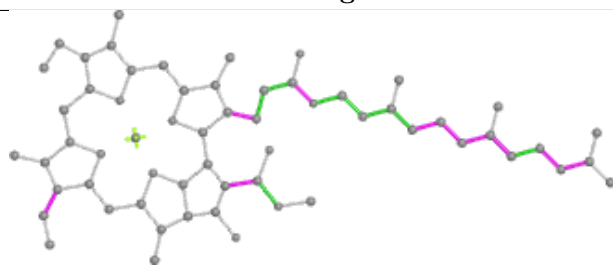
Rings

Ligand CLA B 838

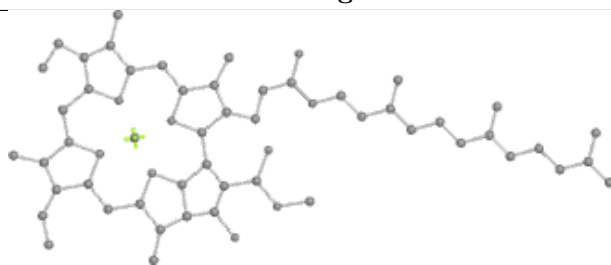
Bond lengths



Bond angles

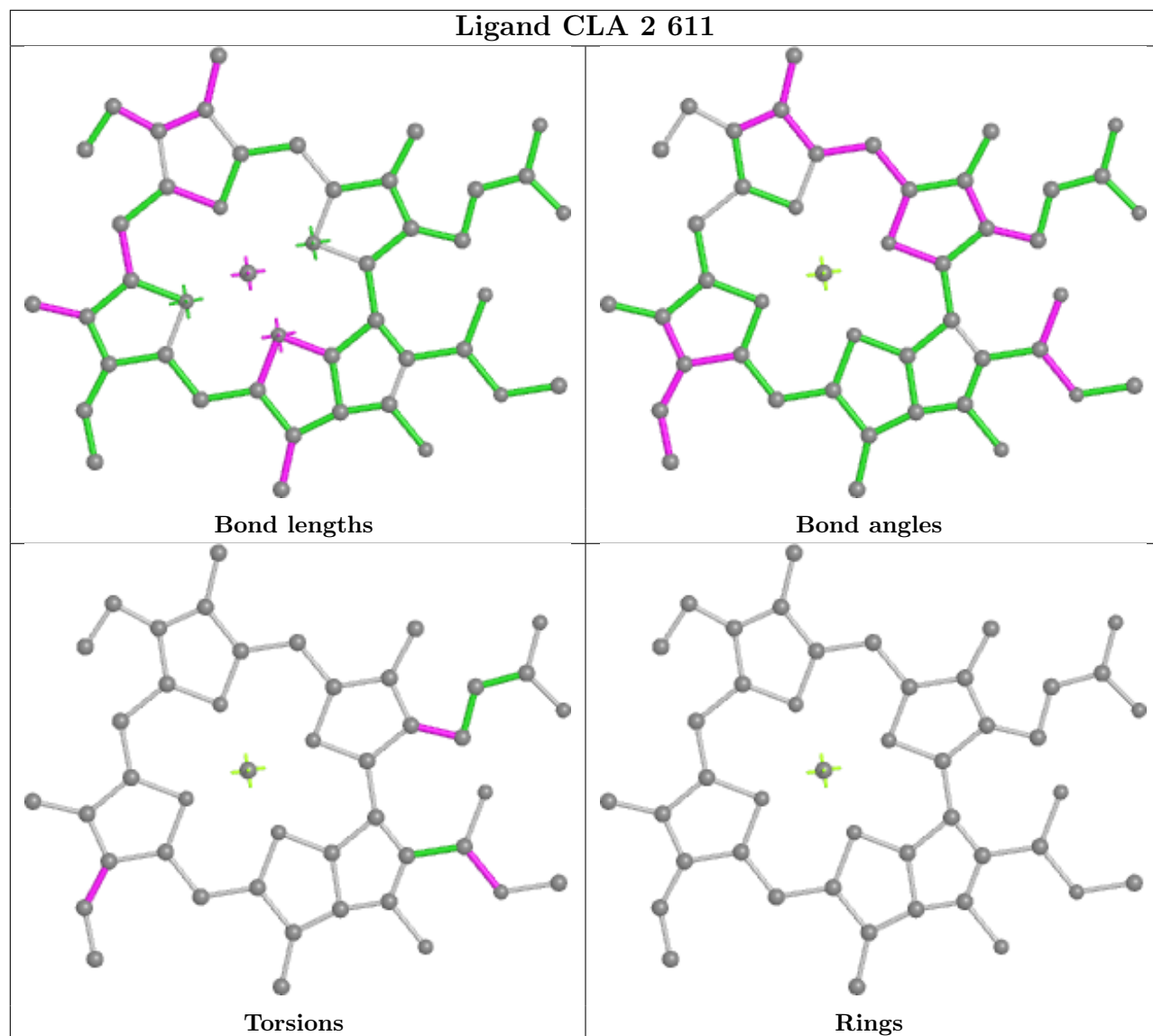


Torsions

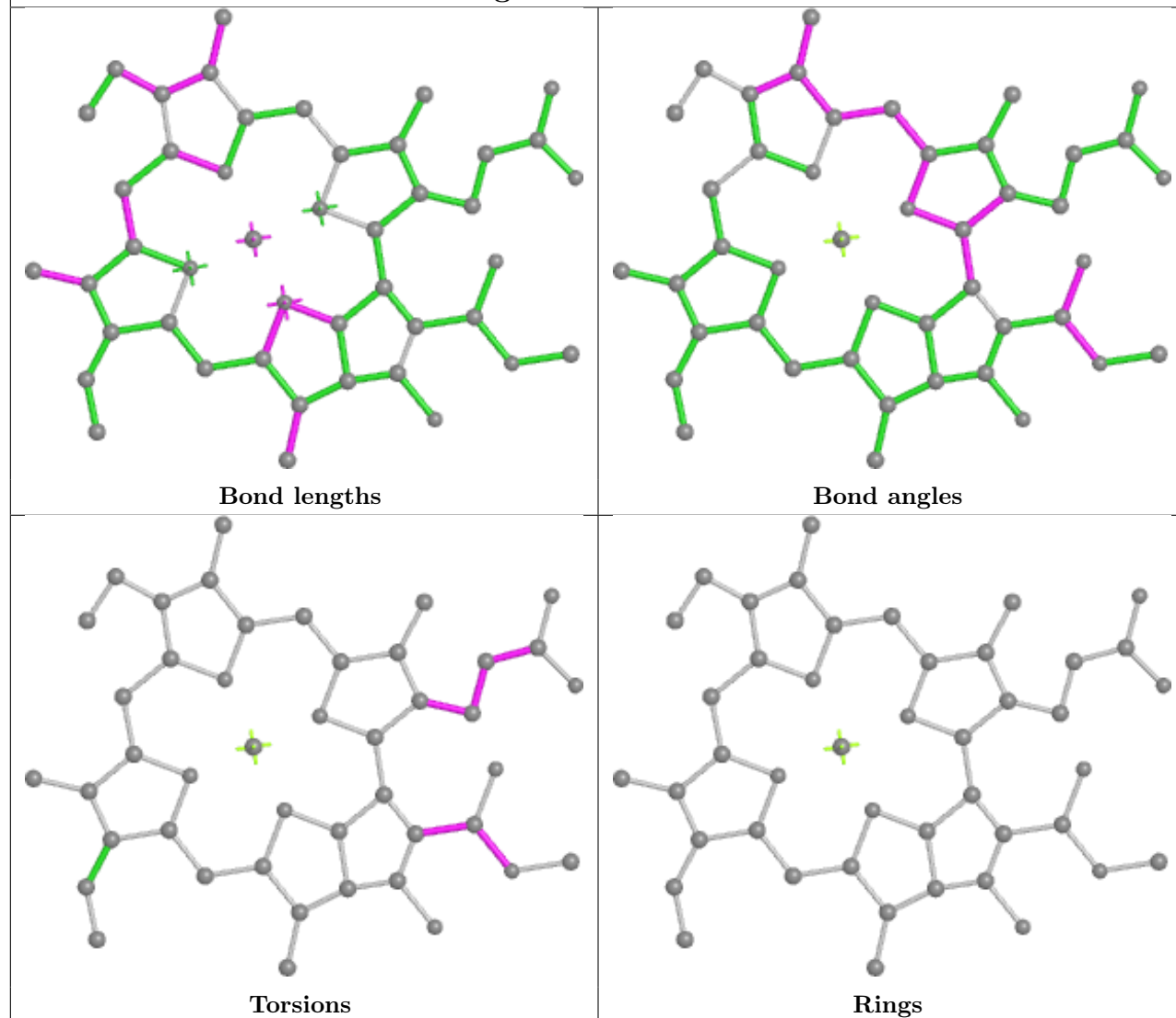


Rings

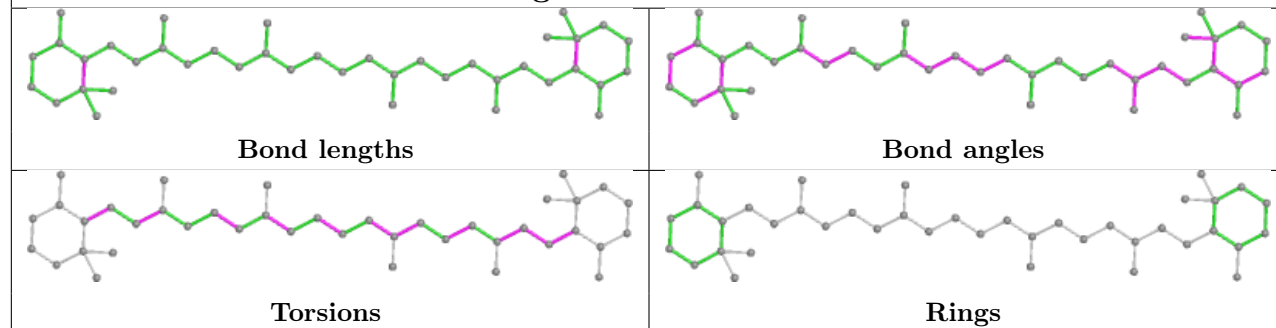
Ligand CLA 2 611



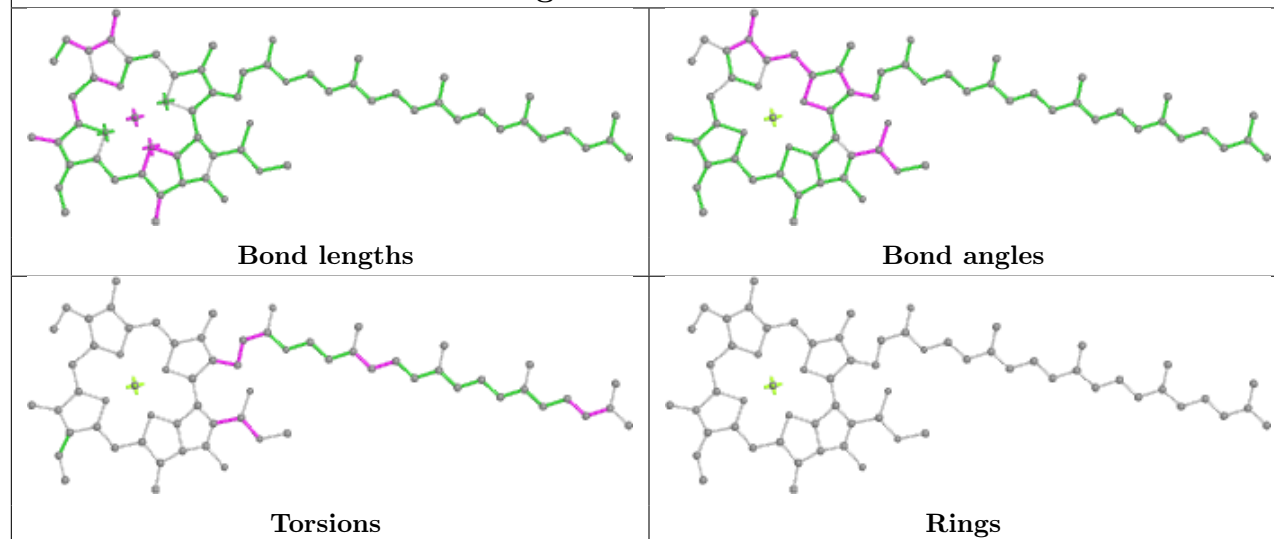
Ligand CLA 3 208



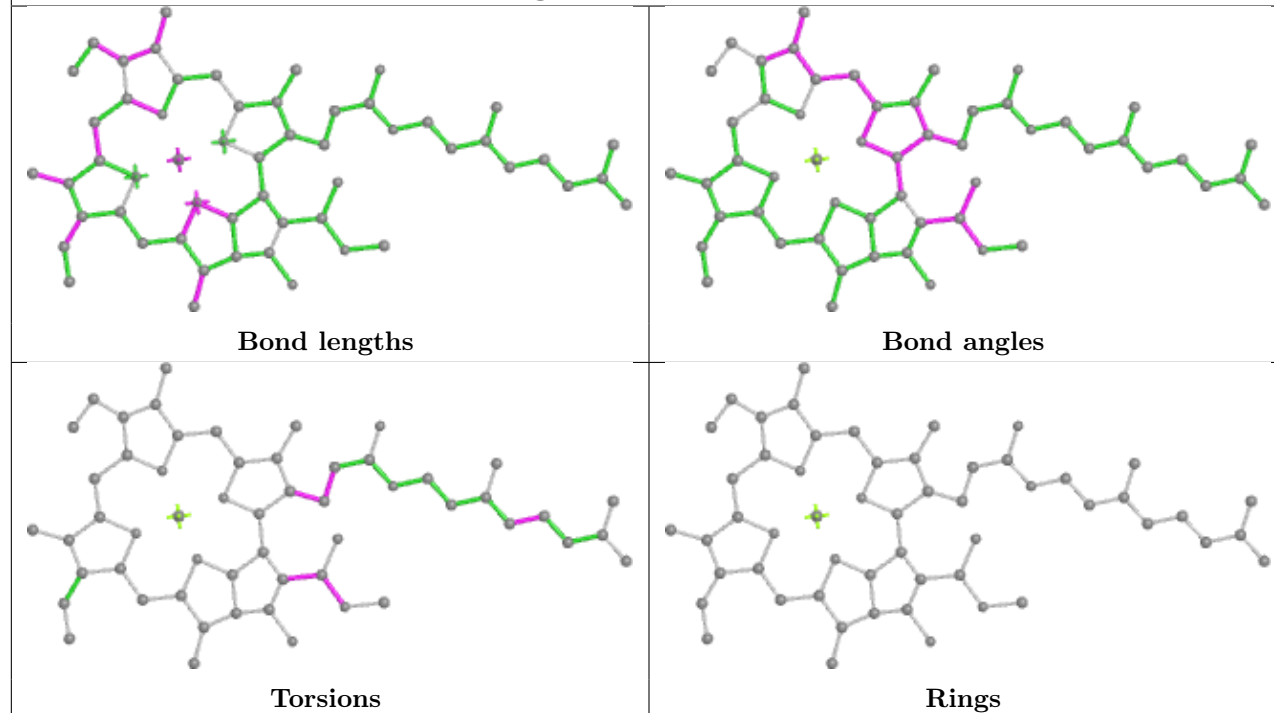
Ligand BCR L 205



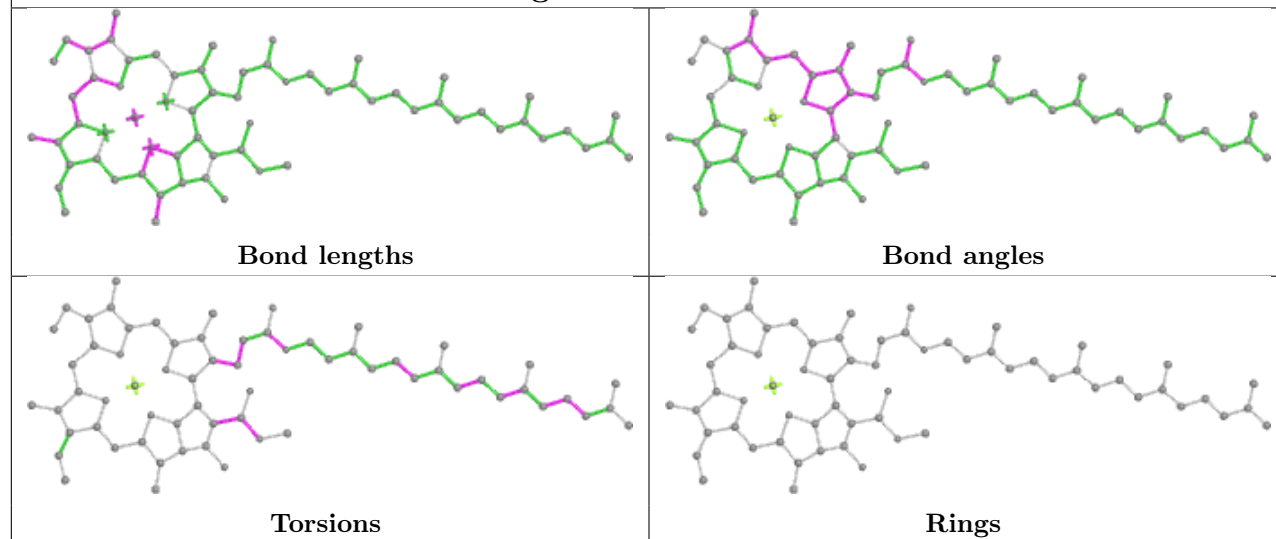
Ligand CLA 2 602



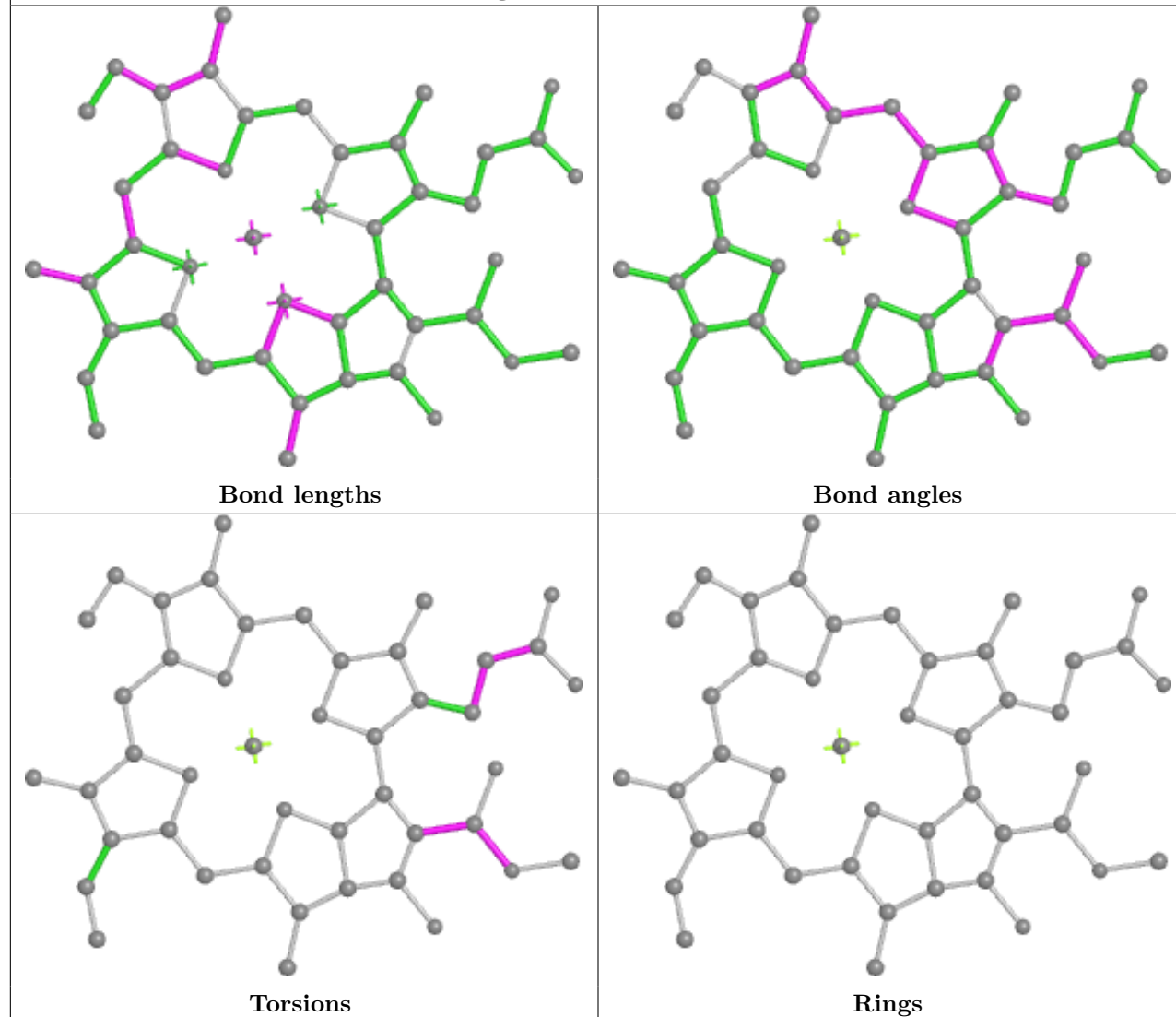
Ligand CLA A 822



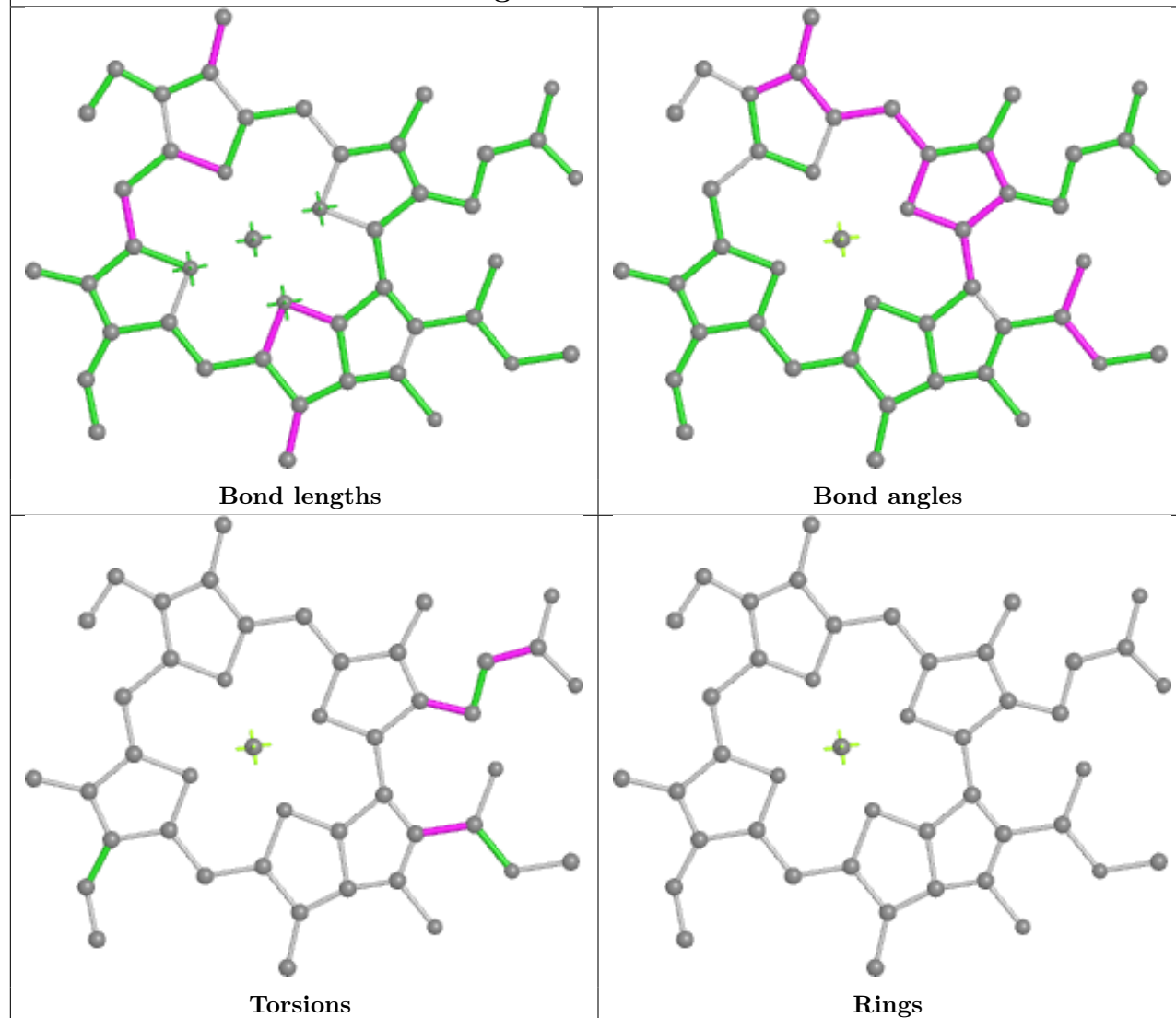
Ligand CLA A 811



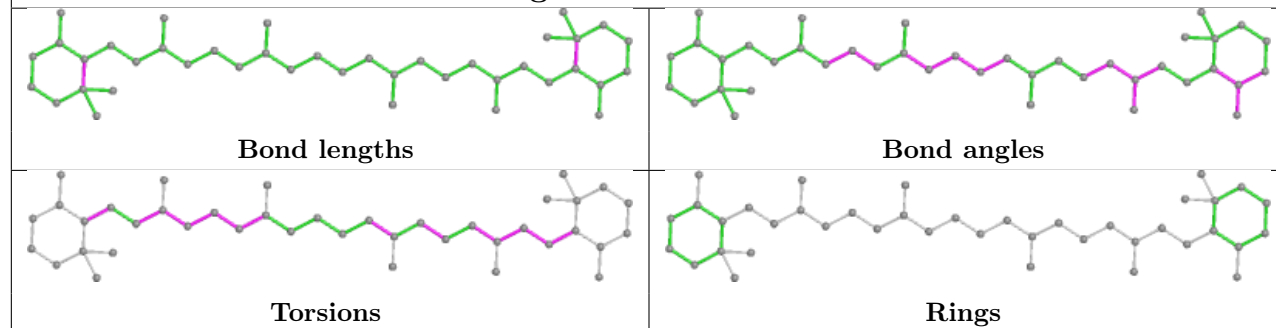
Ligand CLA 3 205

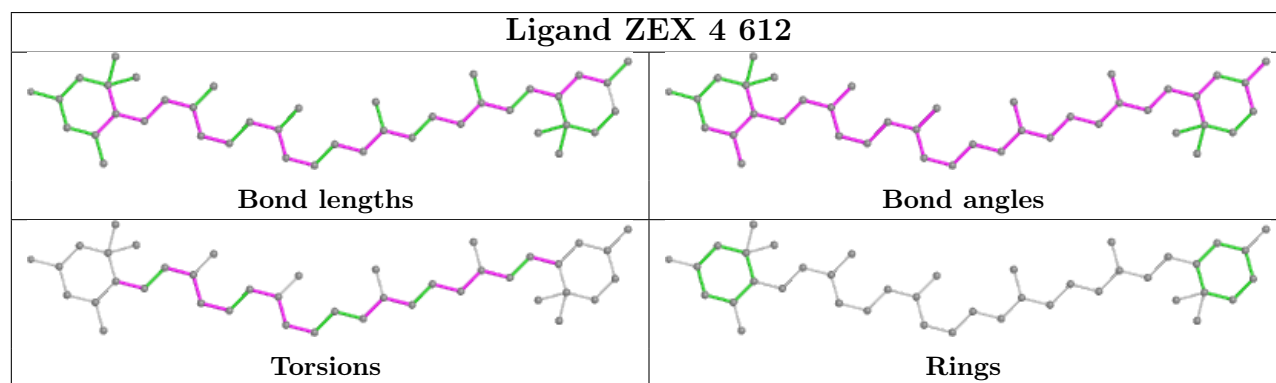
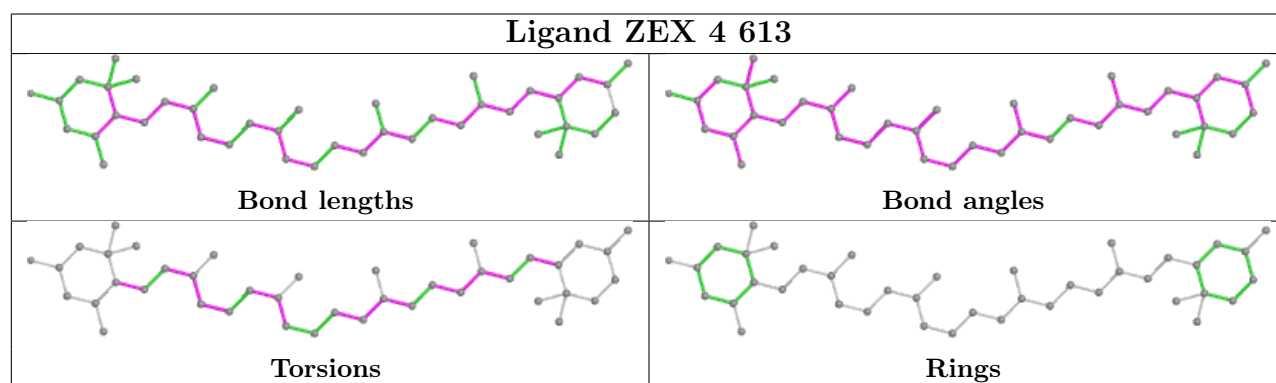
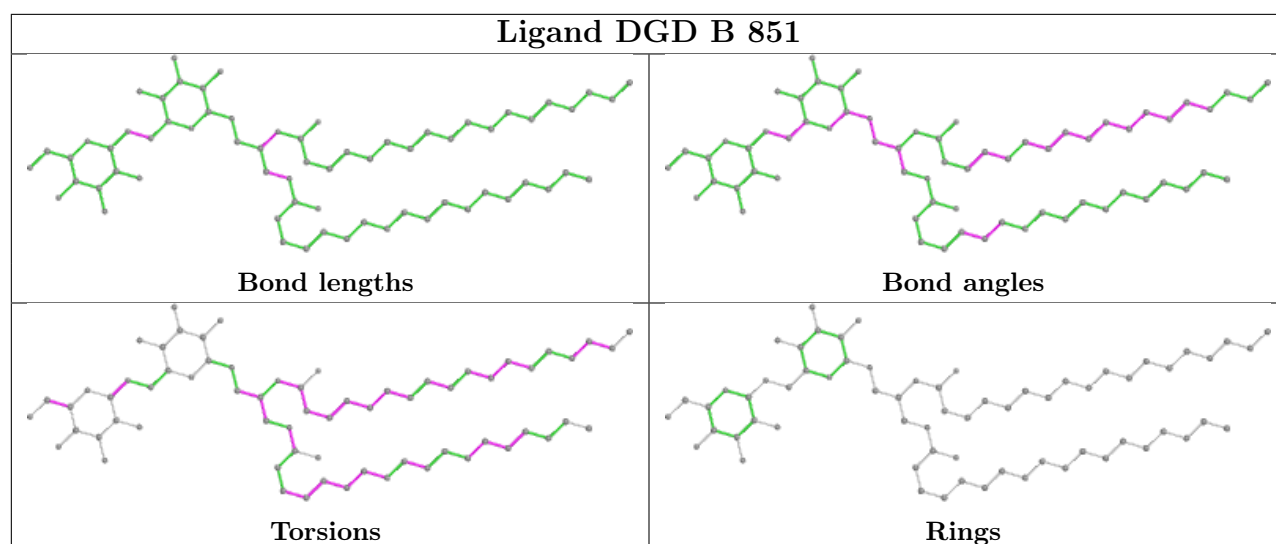


Ligand CLA 4 610

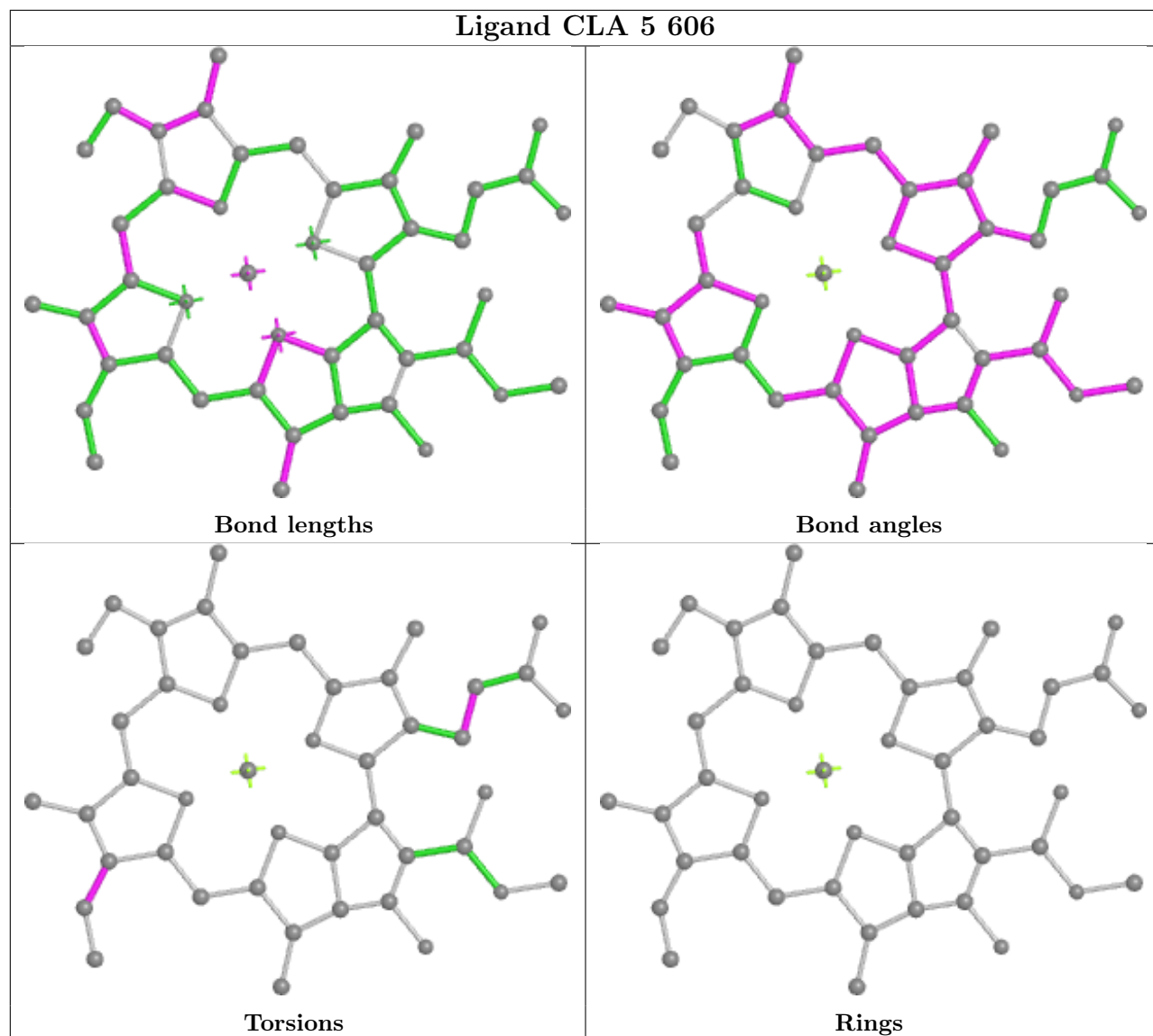


Ligand BCR A 846

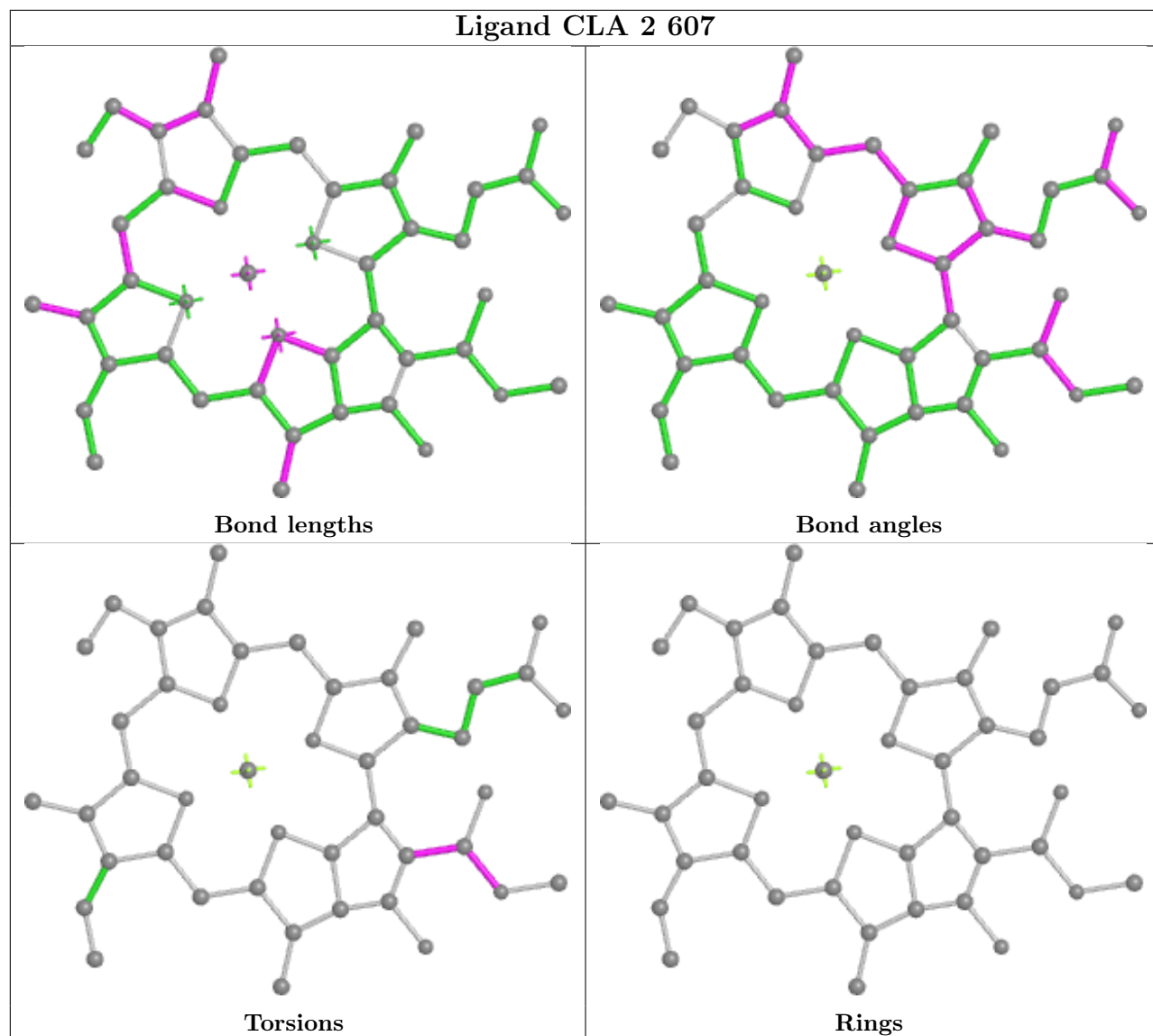




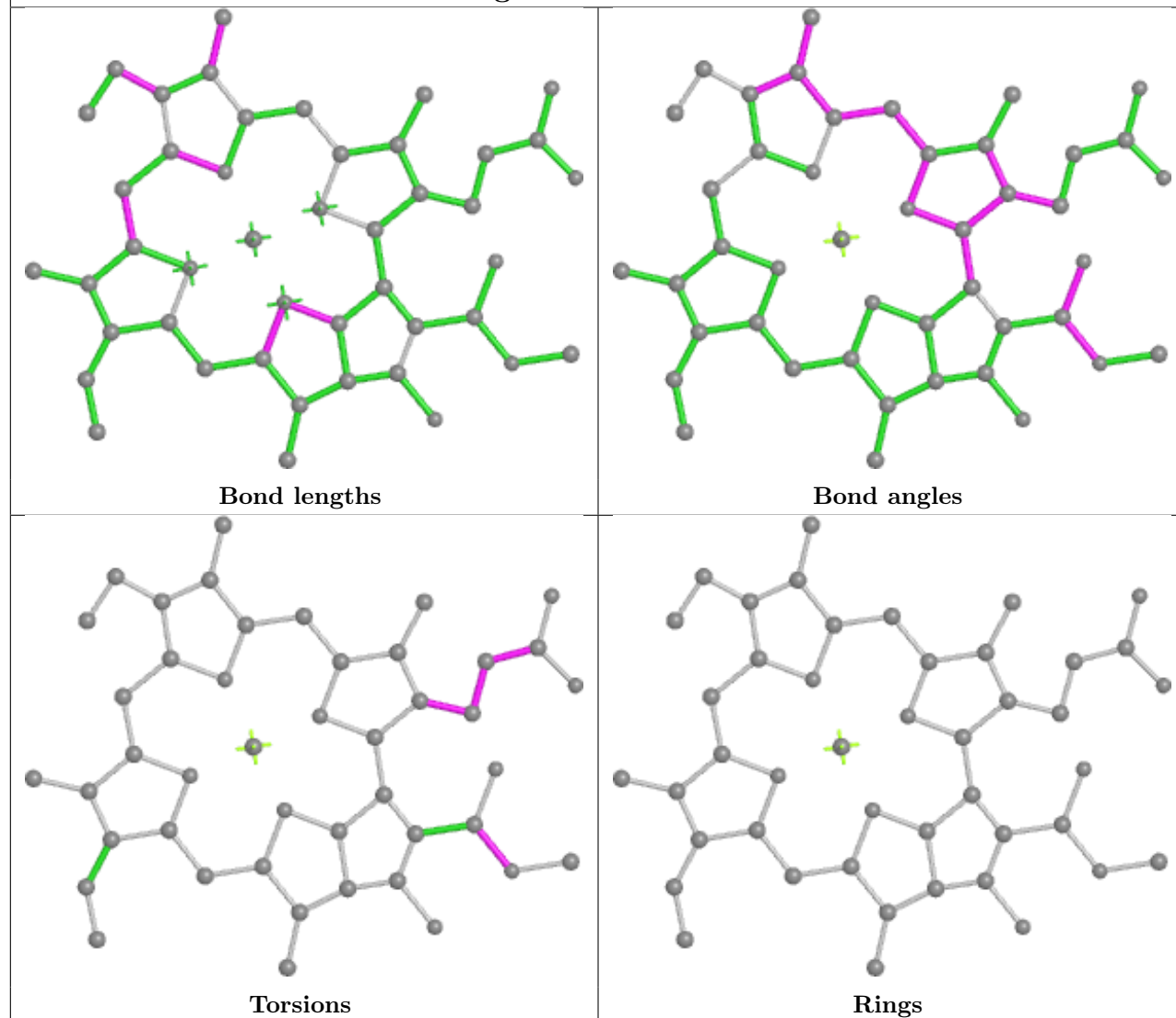
Ligand CLA 5 606



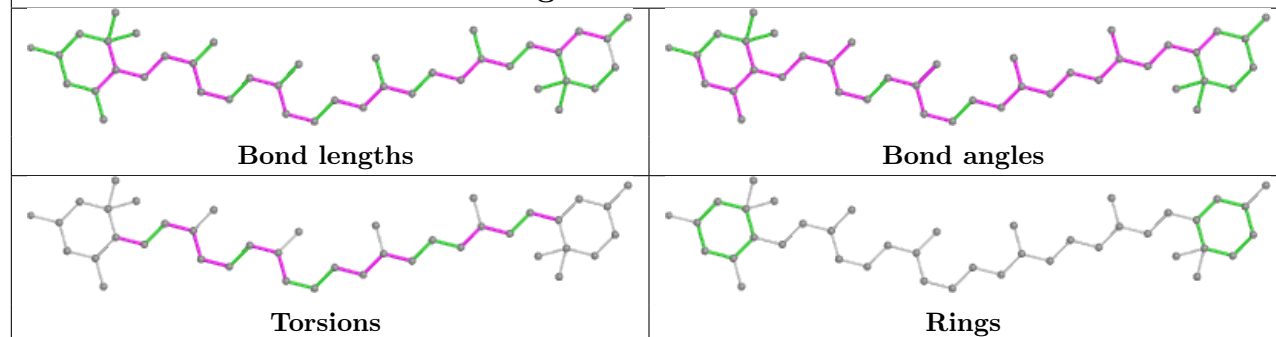
Ligand CLA 2 607



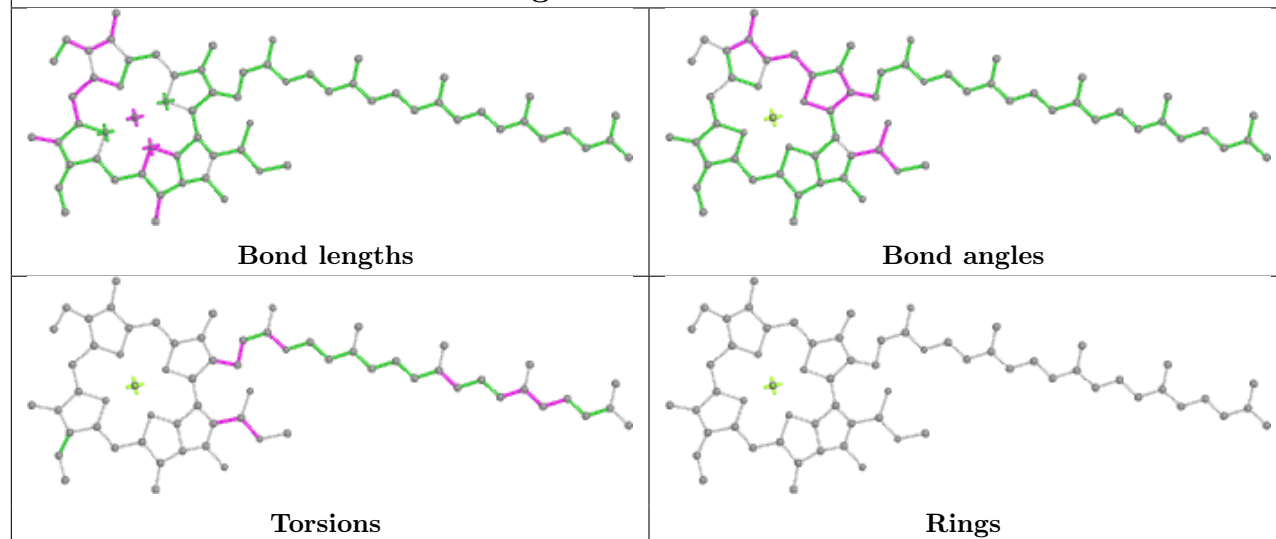
Ligand CLA 5 601



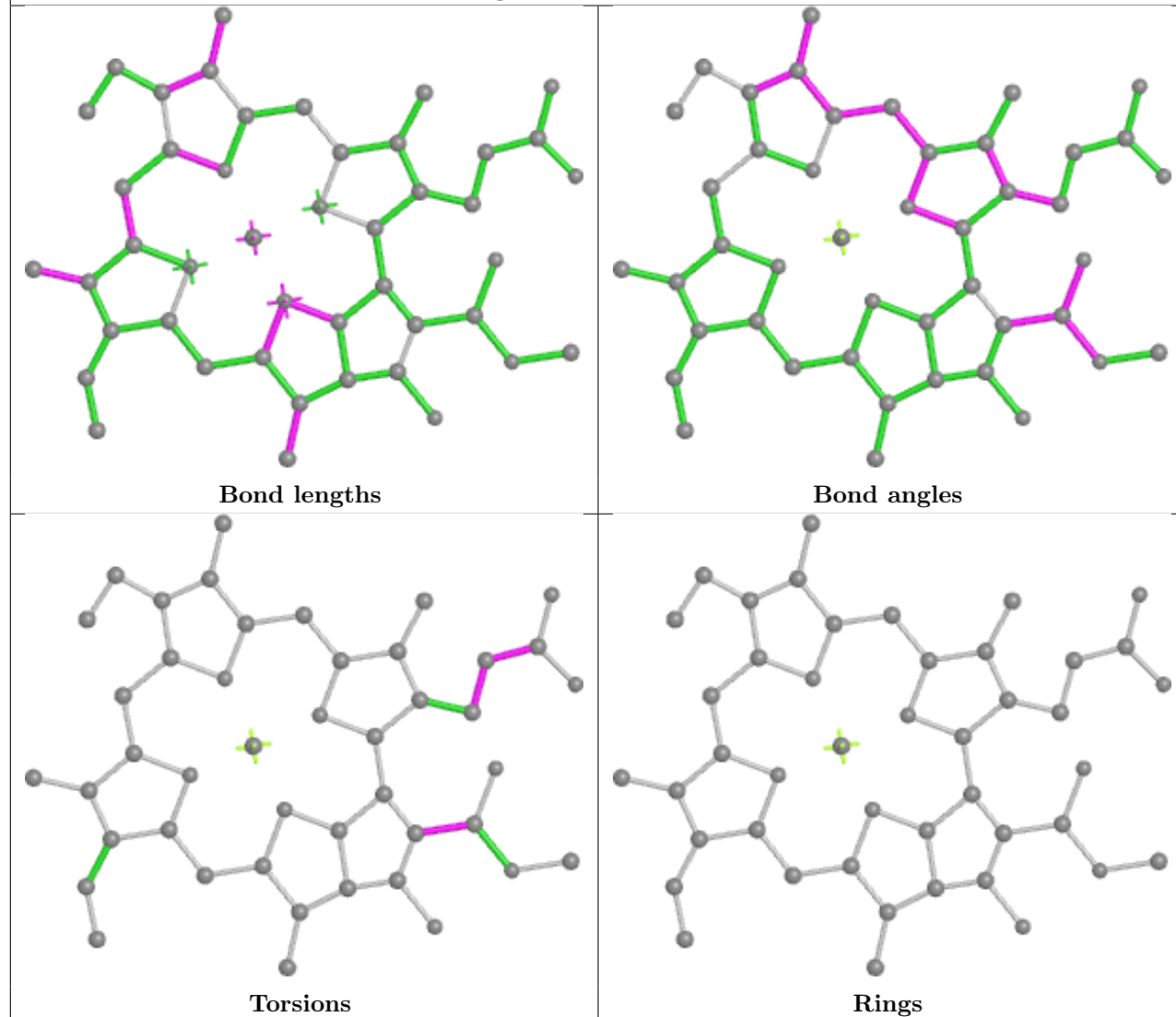
Ligand ZEX 4 615

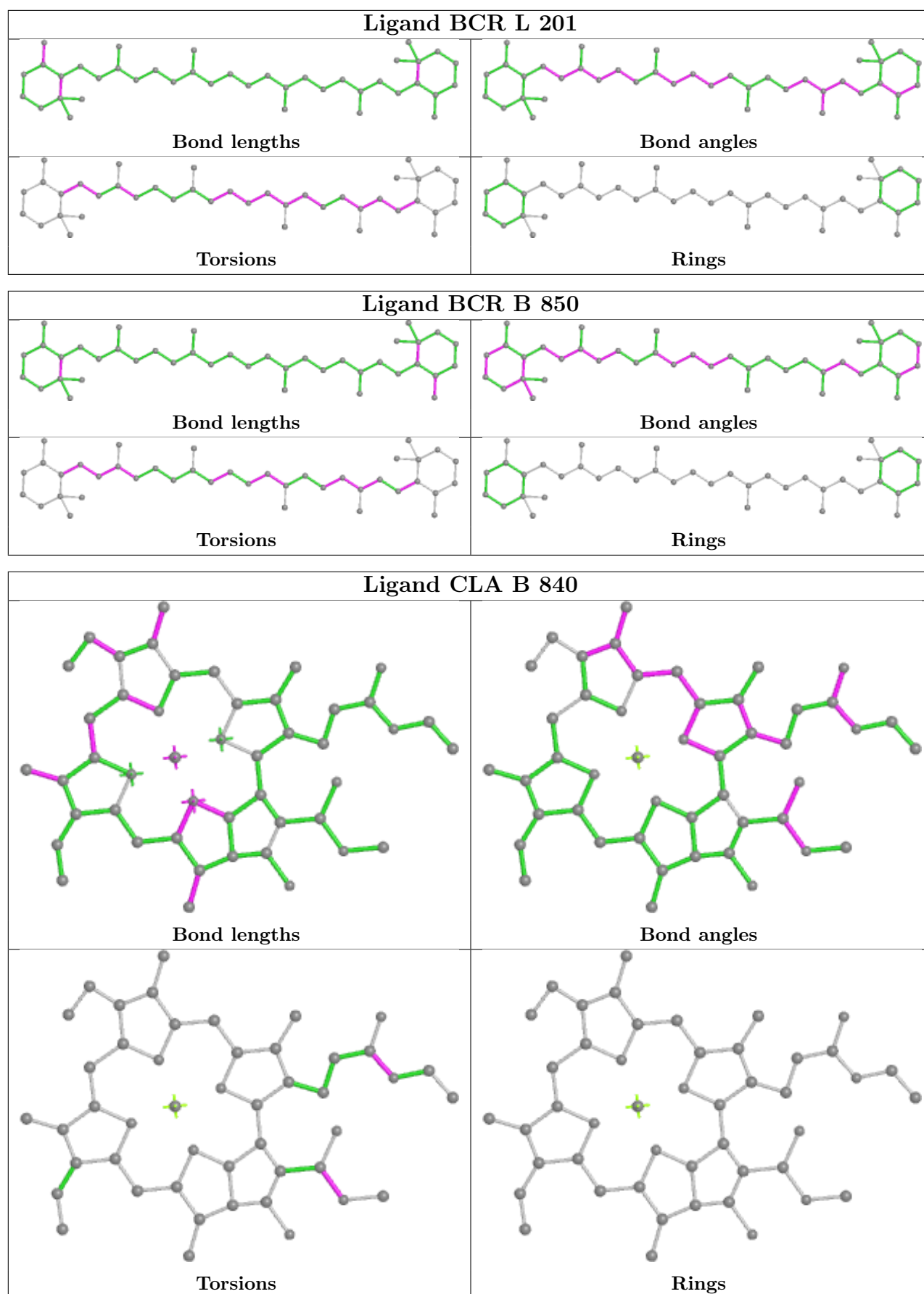


Ligand CLA A 806

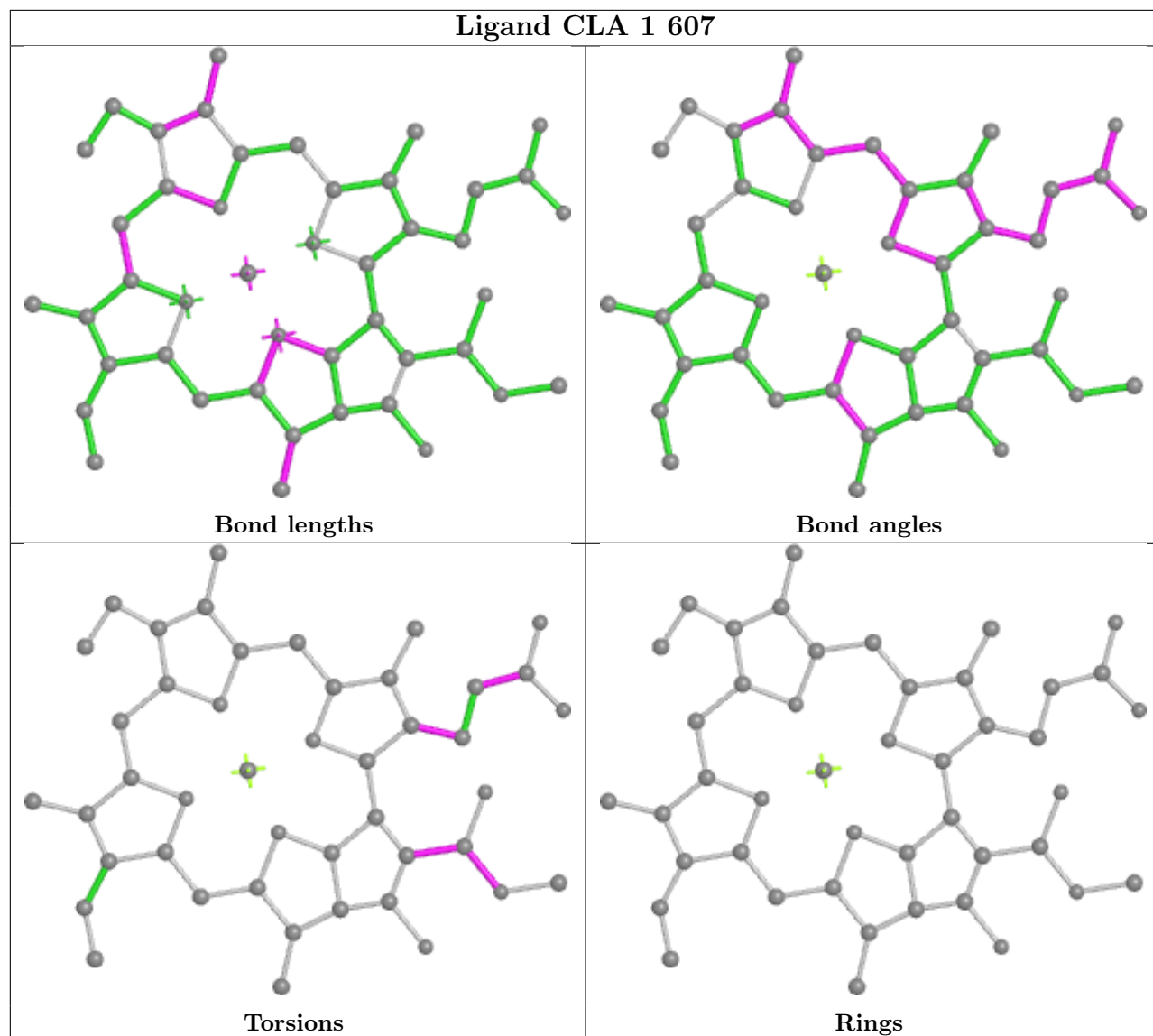


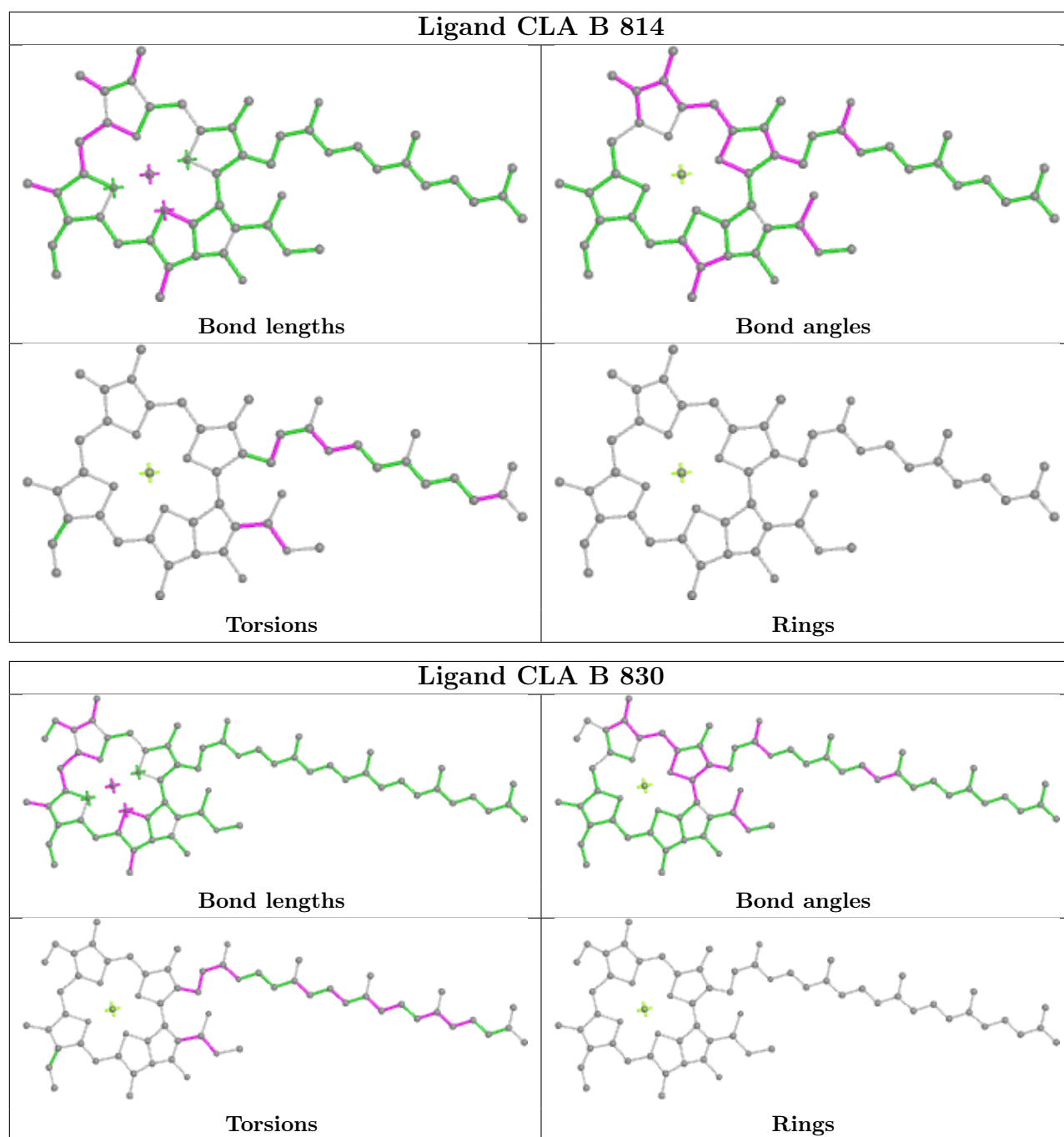
Ligand CLA F 302



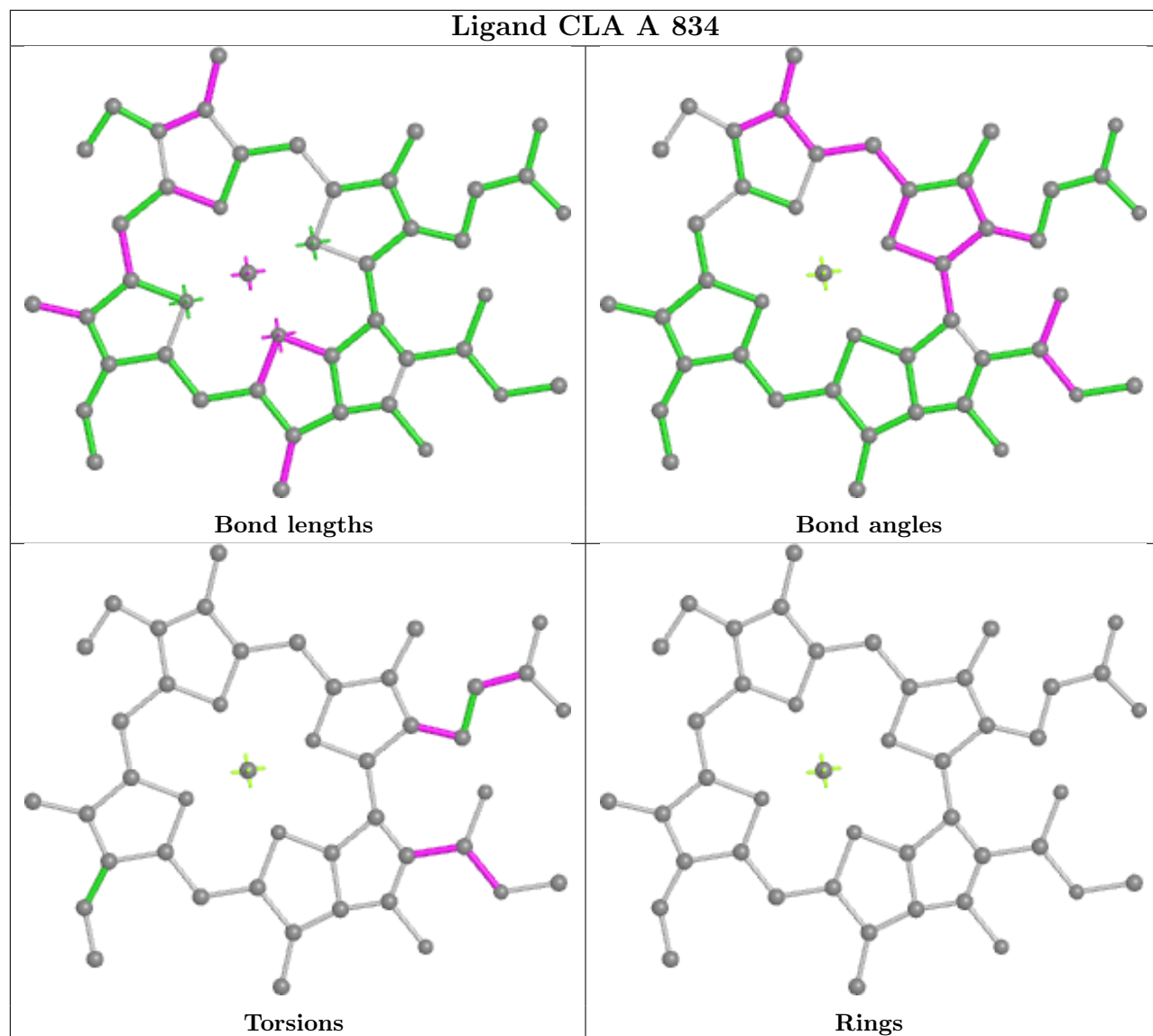


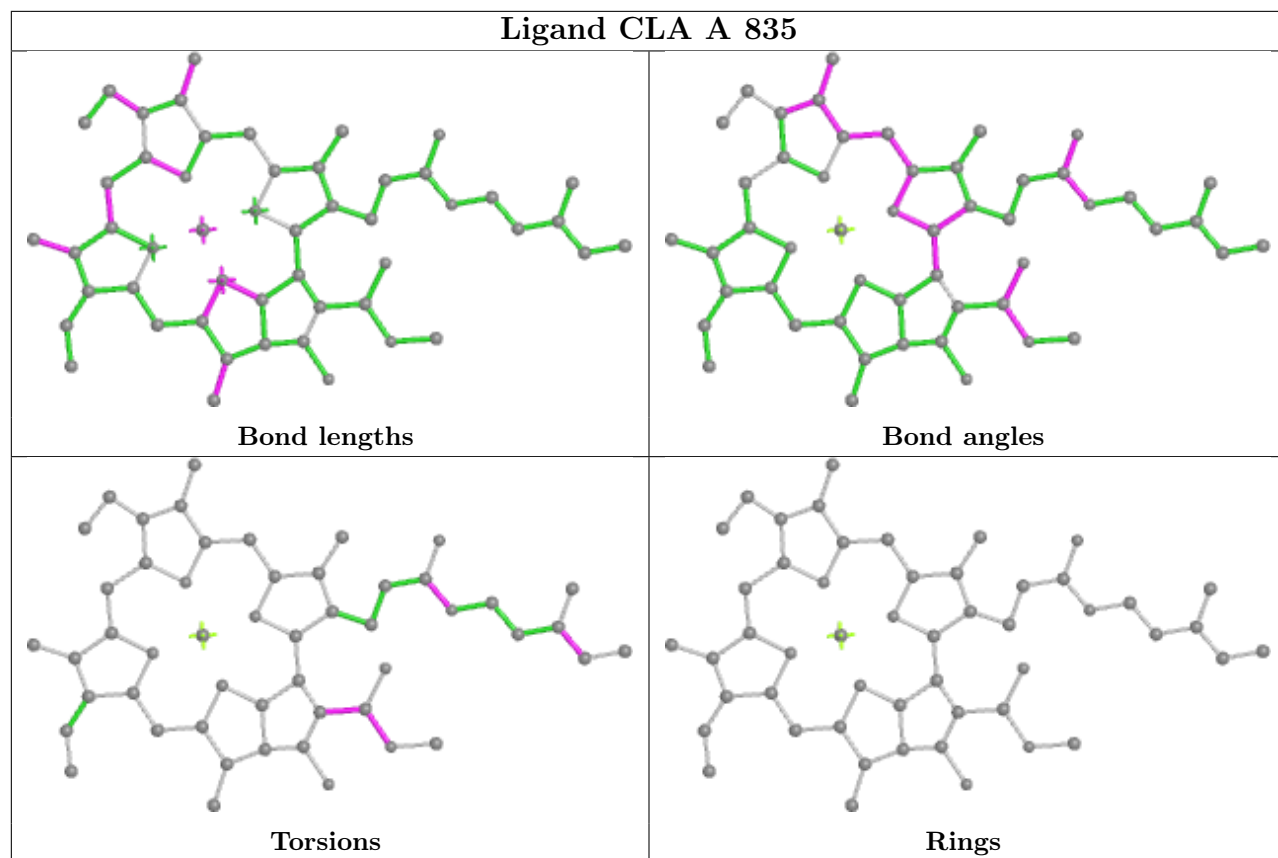
Ligand CLA 1 607



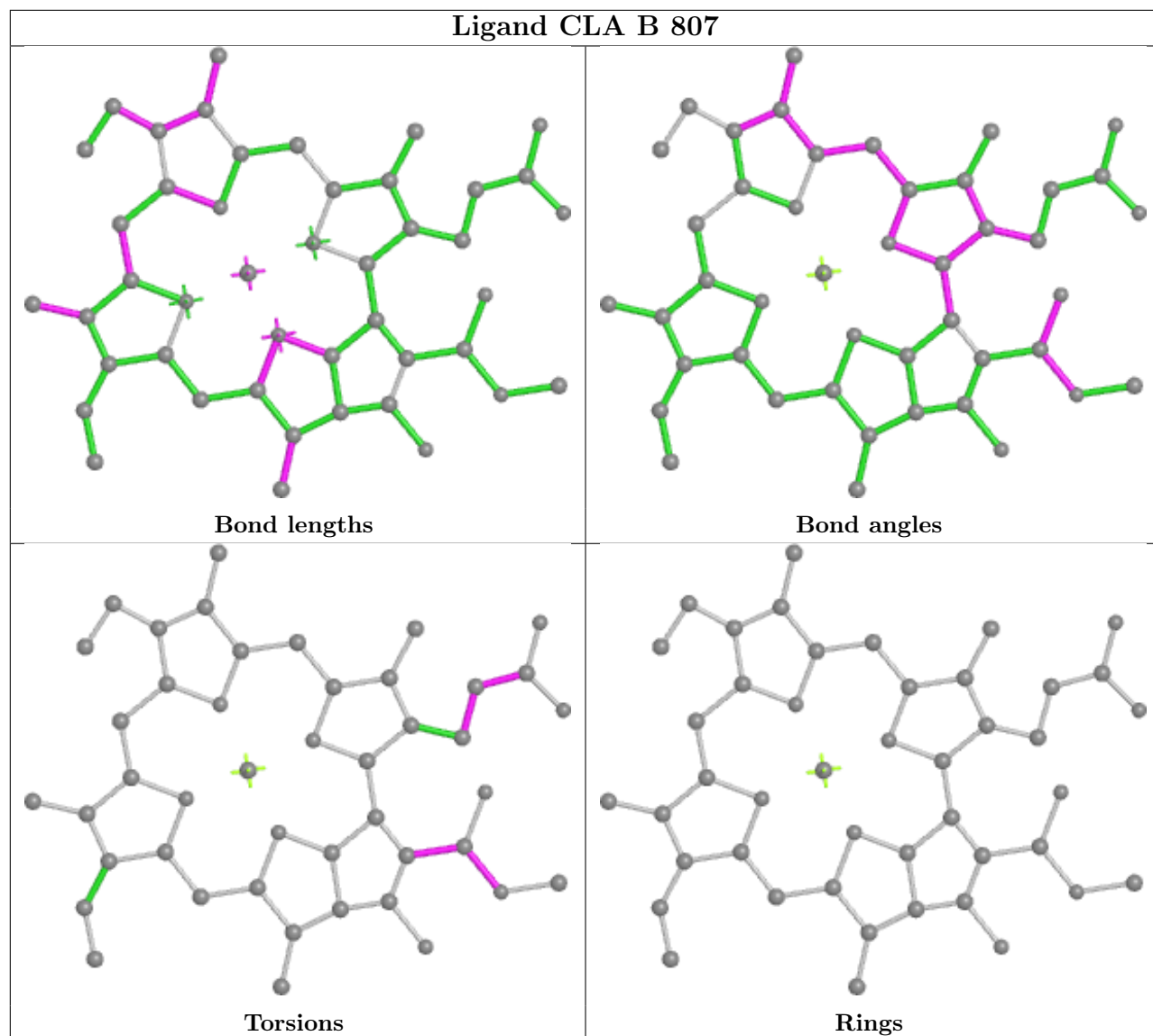


Ligand CLA A 834

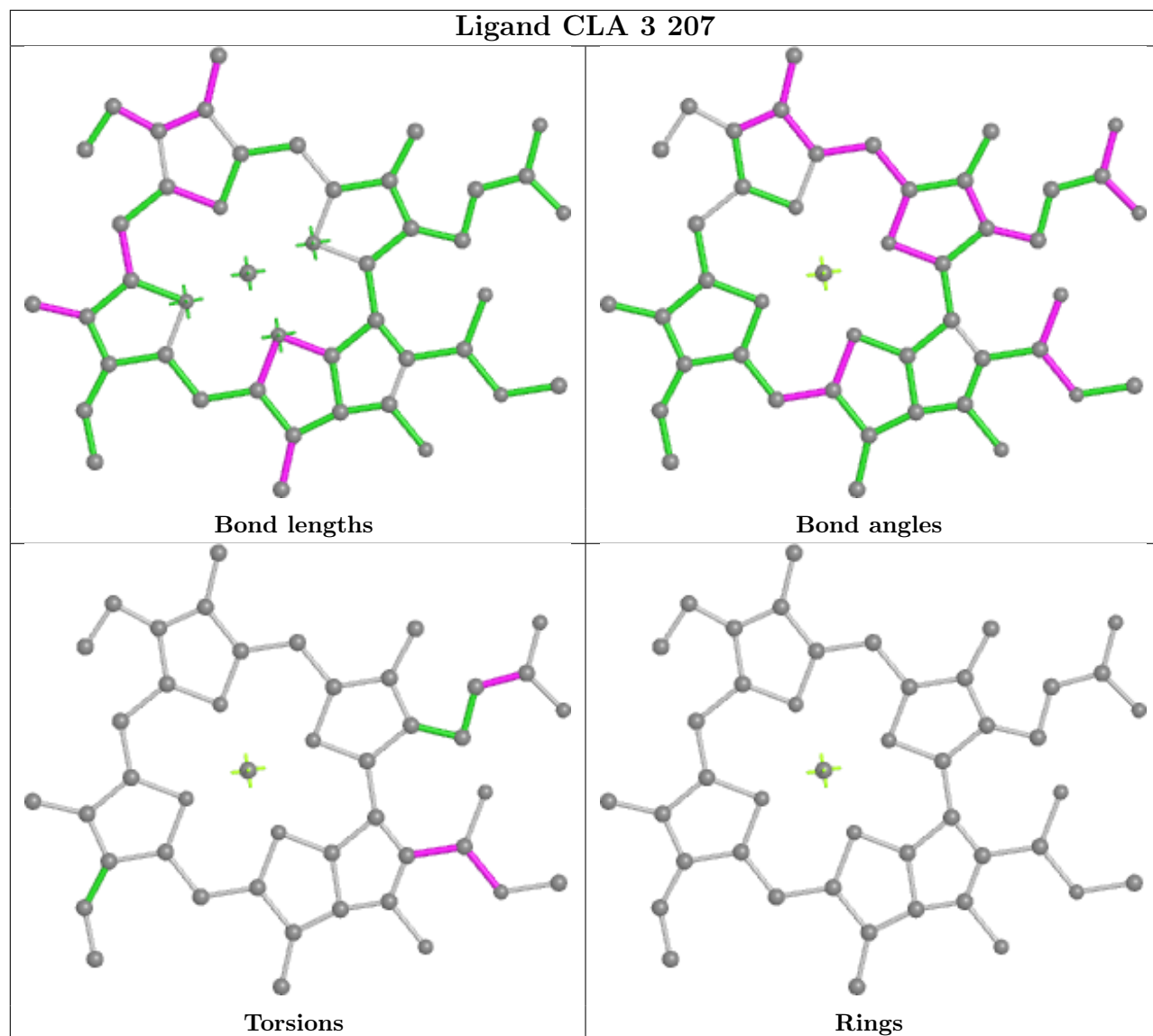




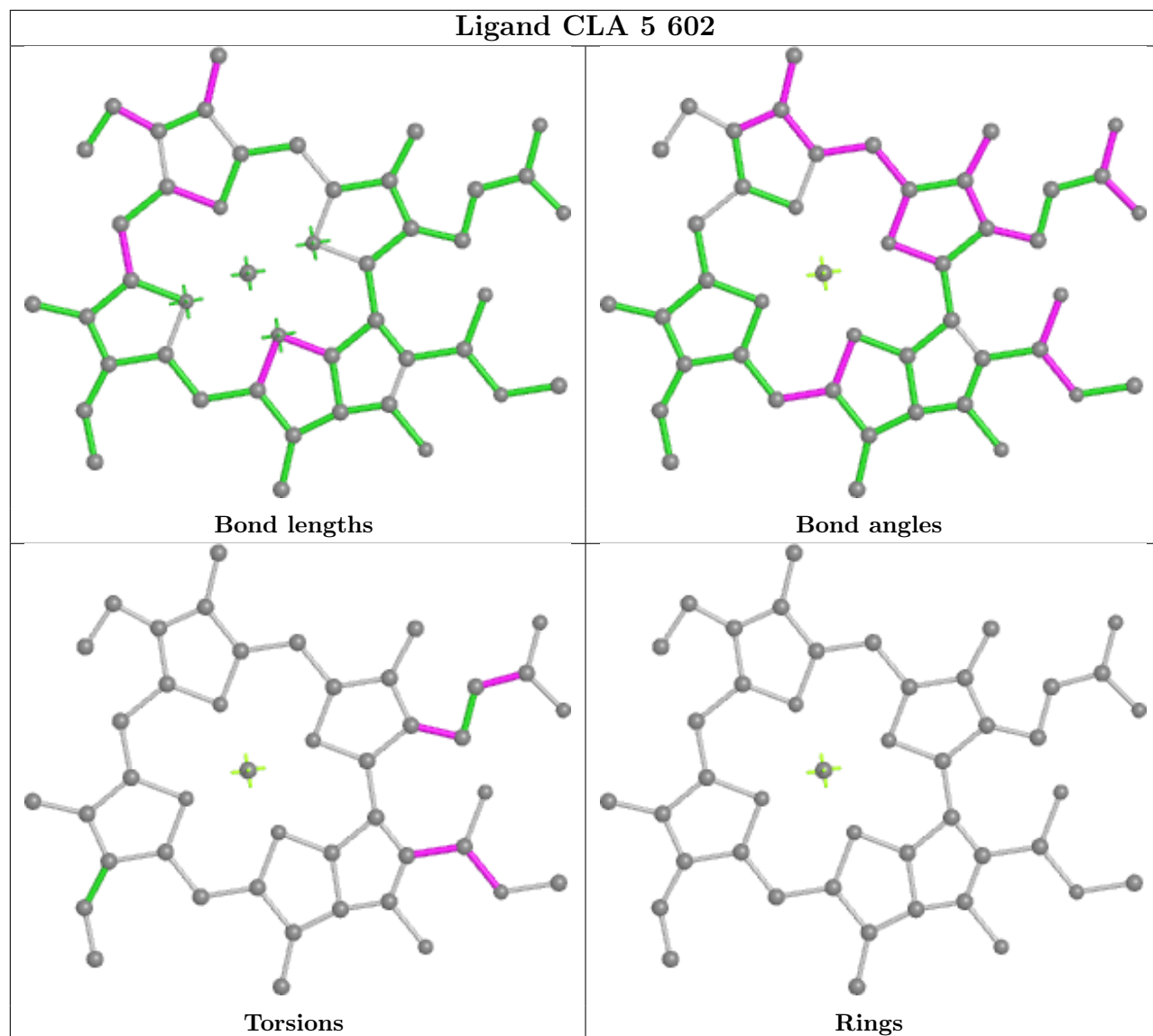
Ligand CLA B 807



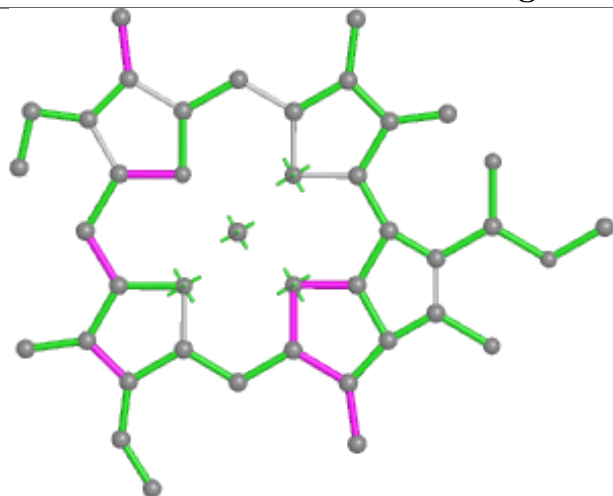
Ligand CLA 3 207



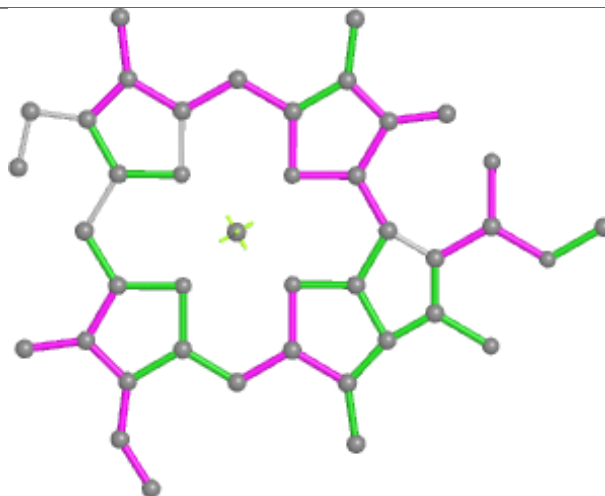
Ligand CLA 5 602



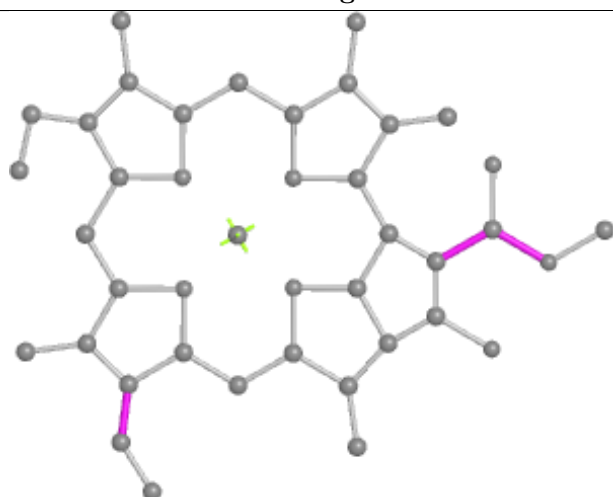
Ligand CLA 5 609



Bond lengths



Bond angles

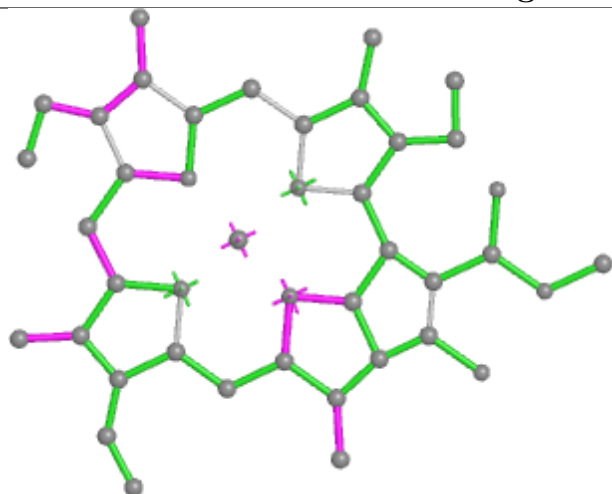


Torsions

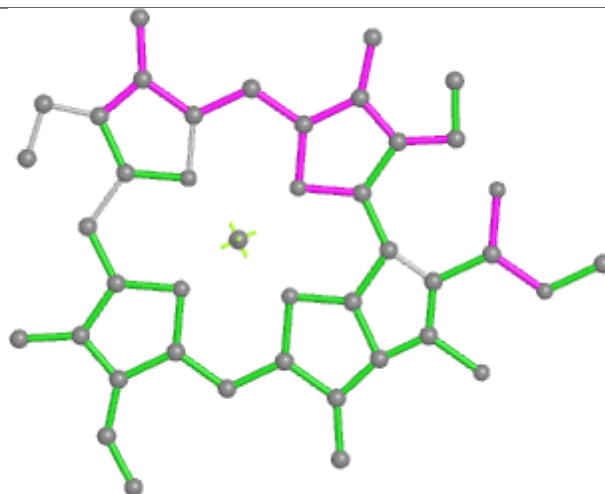


Rings

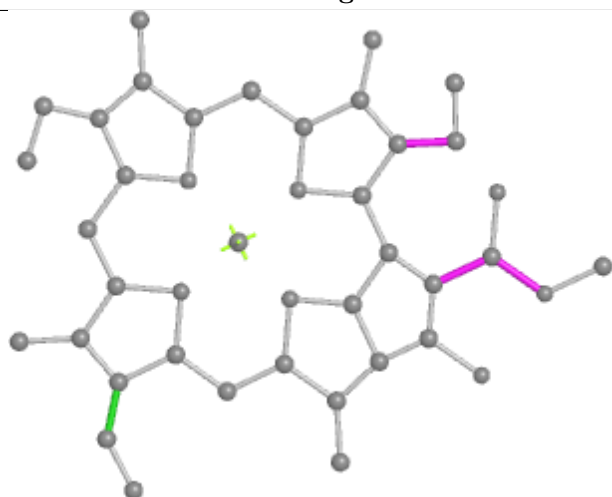
Ligand CLA 2 610



Bond lengths



Bond angles

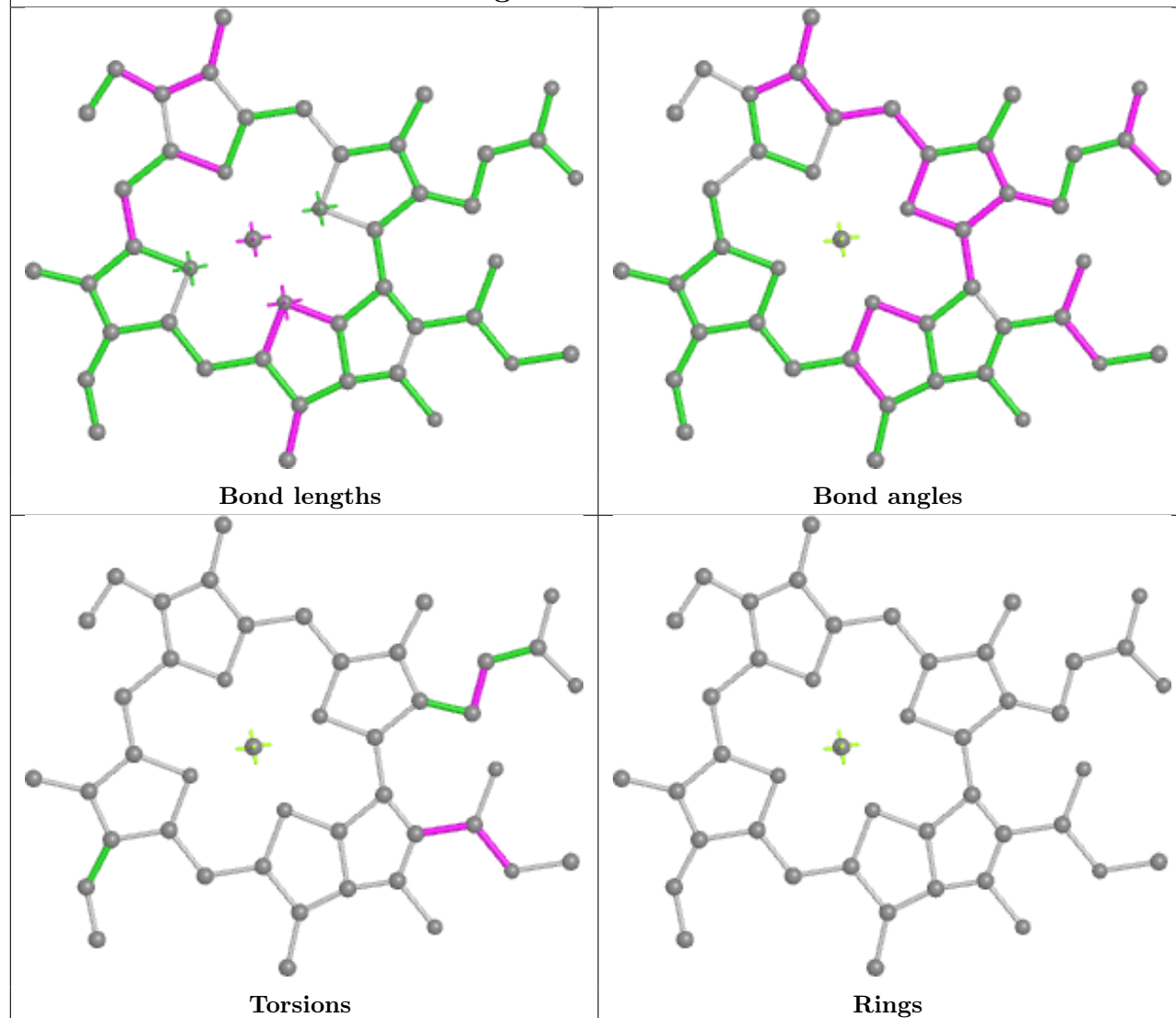


Torsions

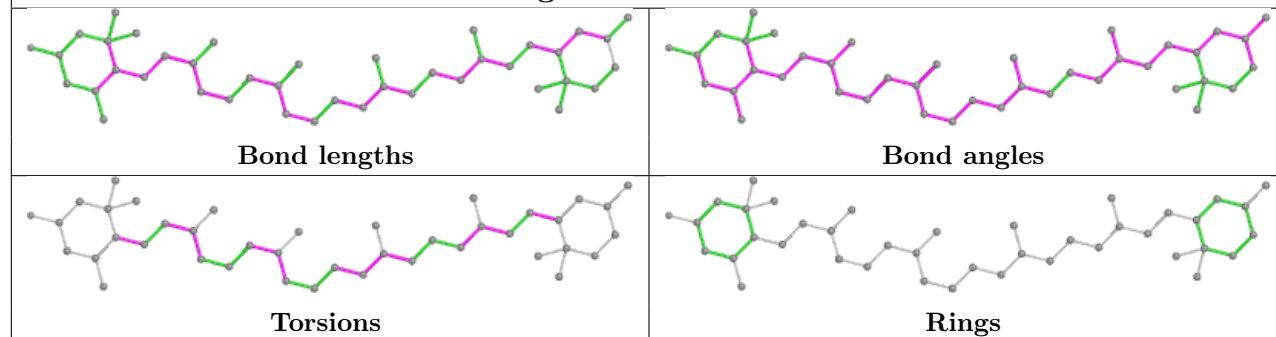


Rings

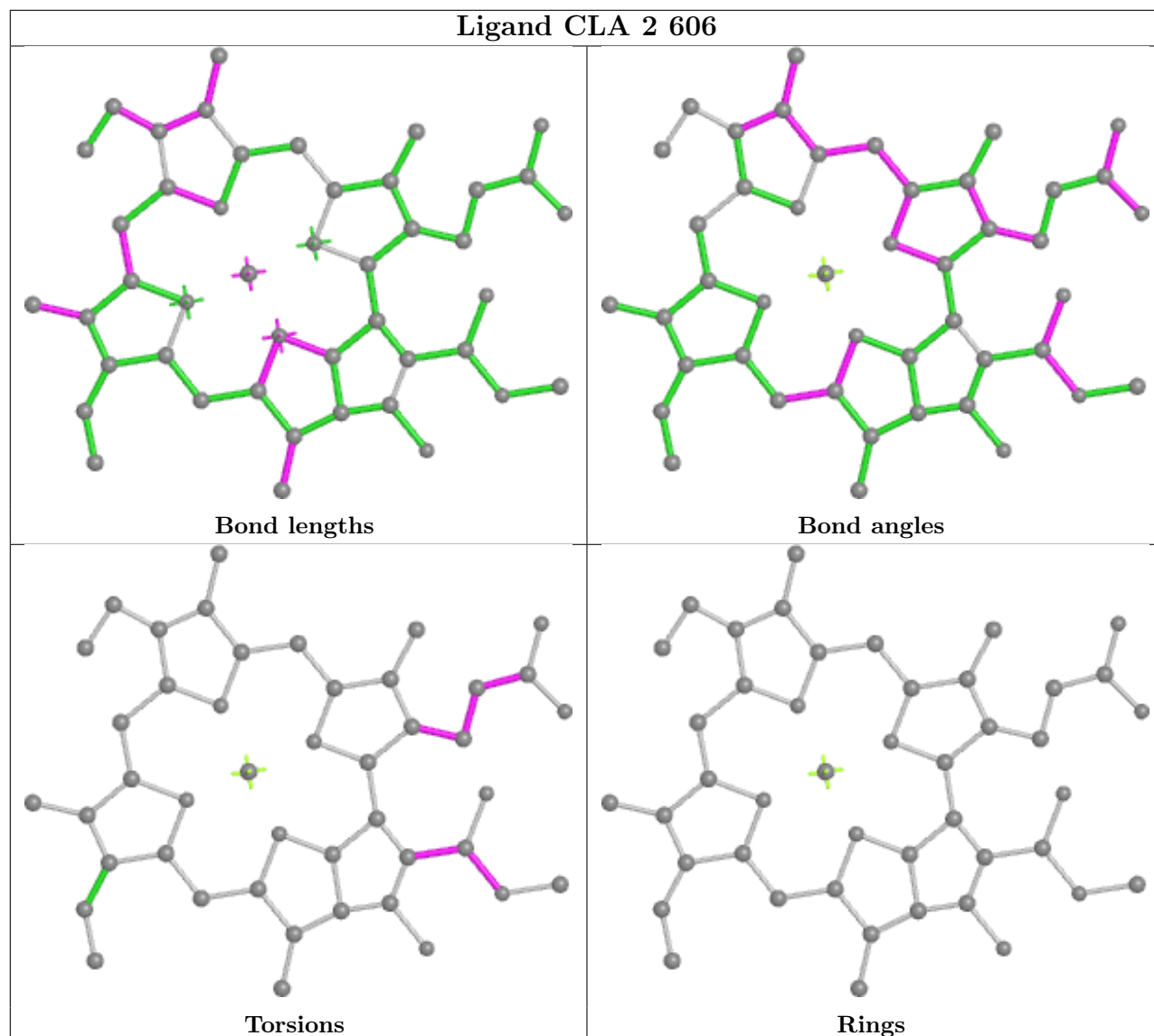
Ligand CLA 3 206



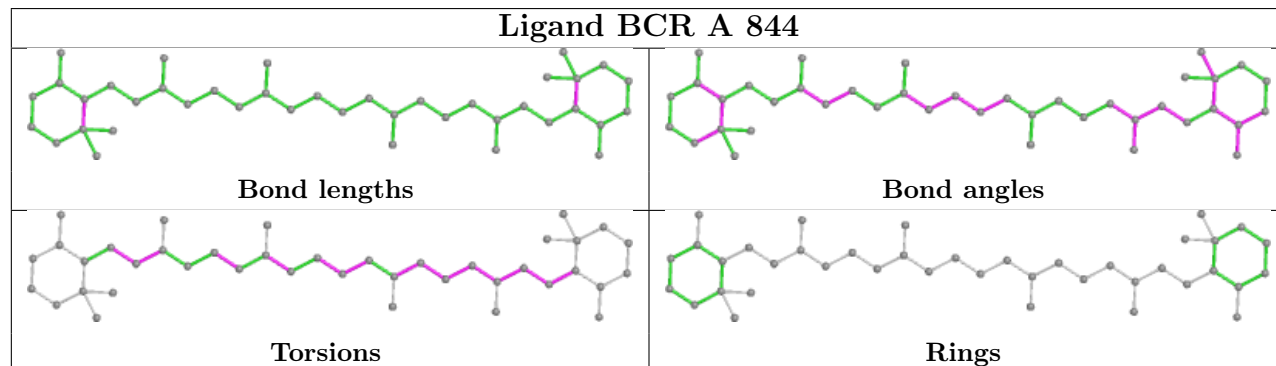
Ligand ZEX 3 214



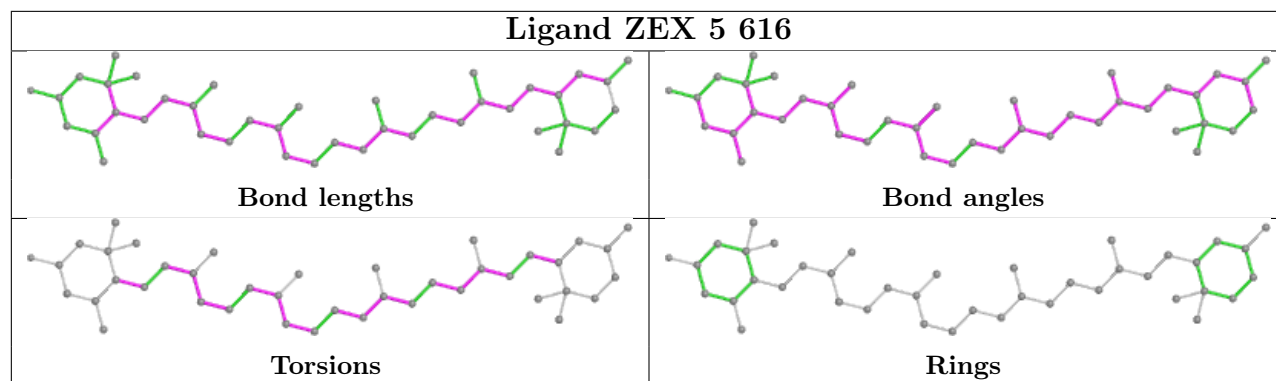
Ligand CLA 2 606



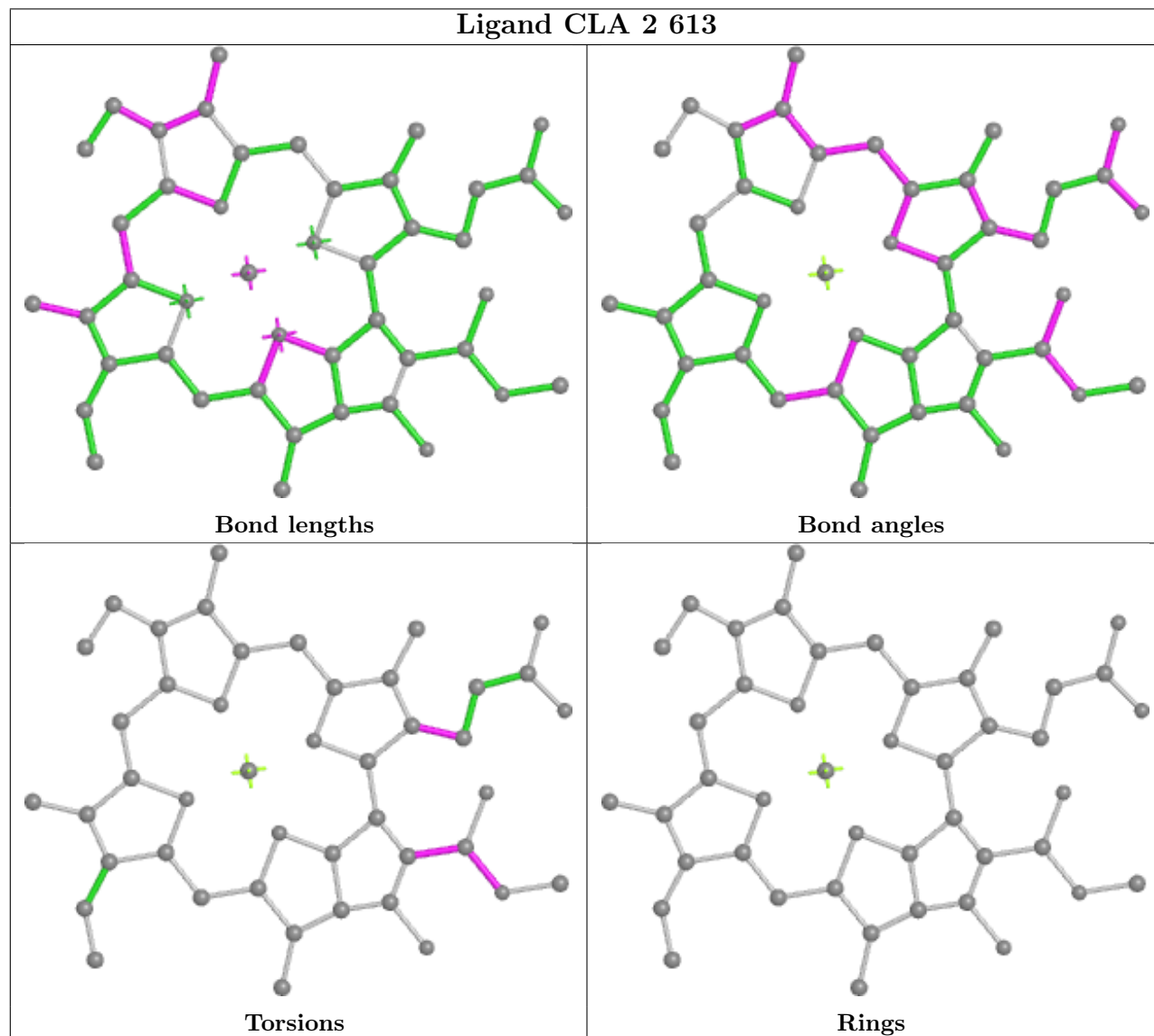
Ligand BCR A 844



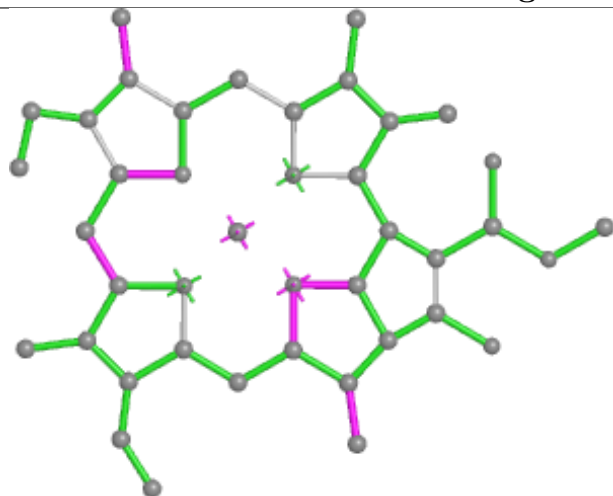
Ligand ZEX 5 616



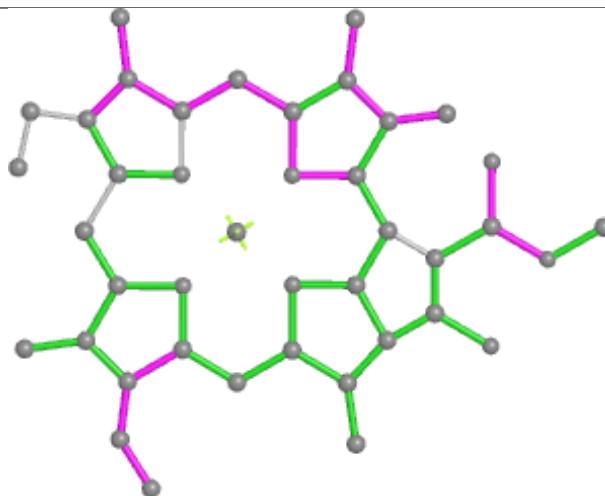
Ligand CLA 2 613



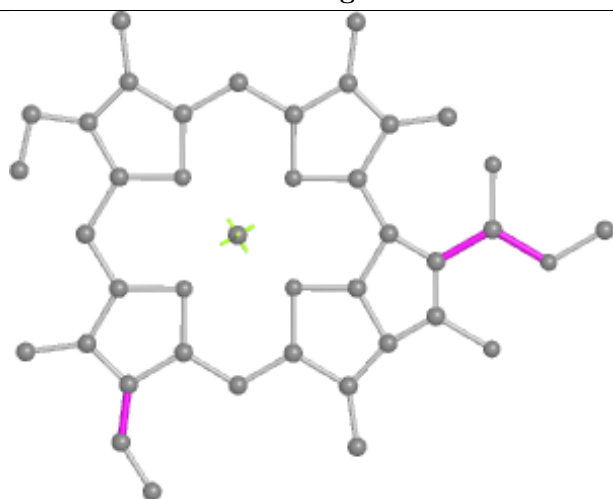
Ligand CLA 3 210



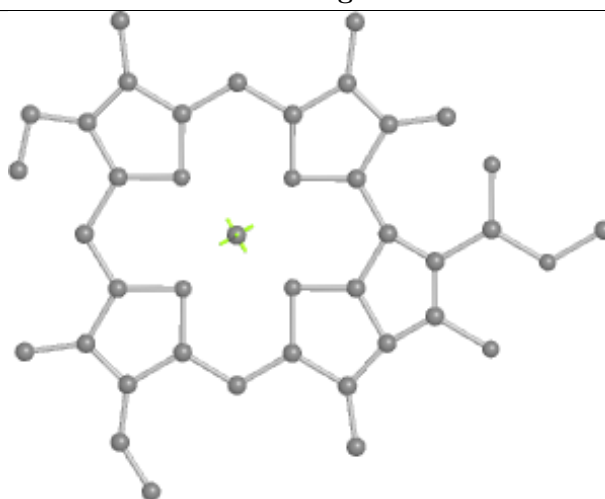
Bond lengths



Bond angles

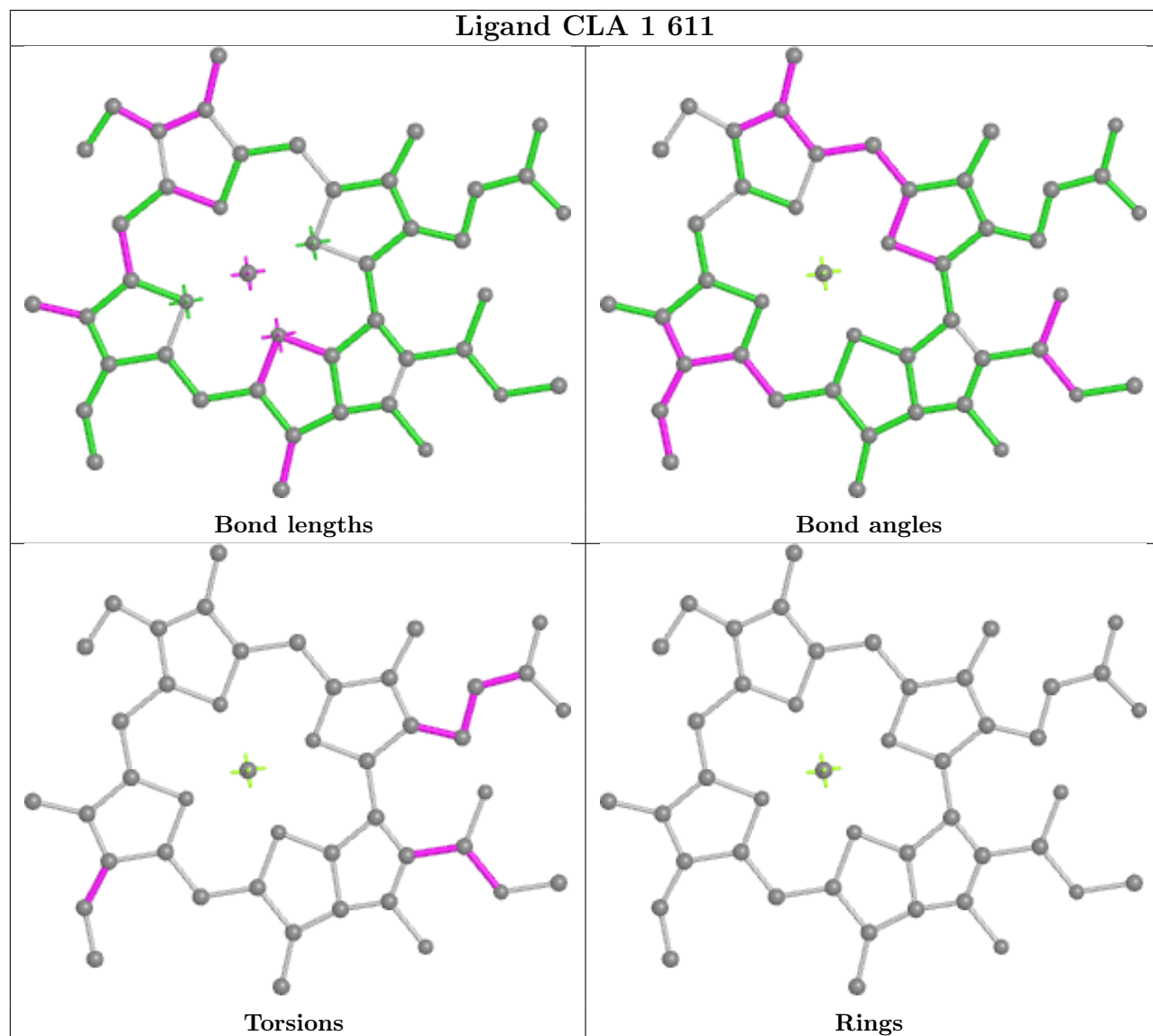


Torsions

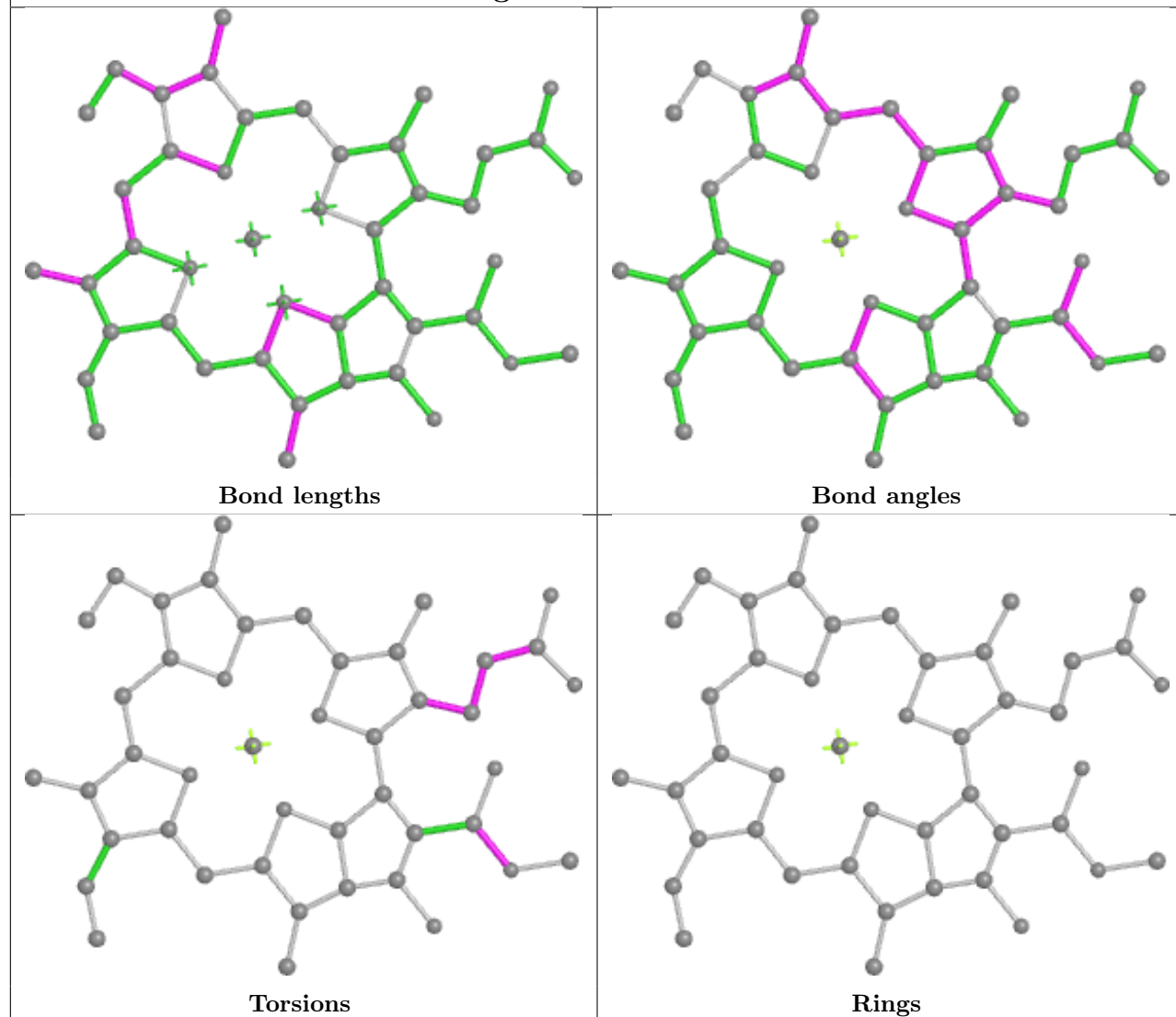


Rings

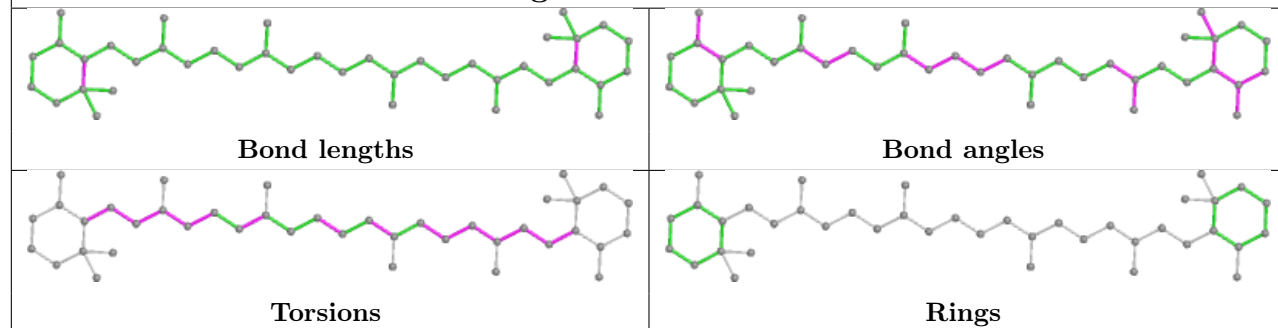
Ligand CLA 1 611

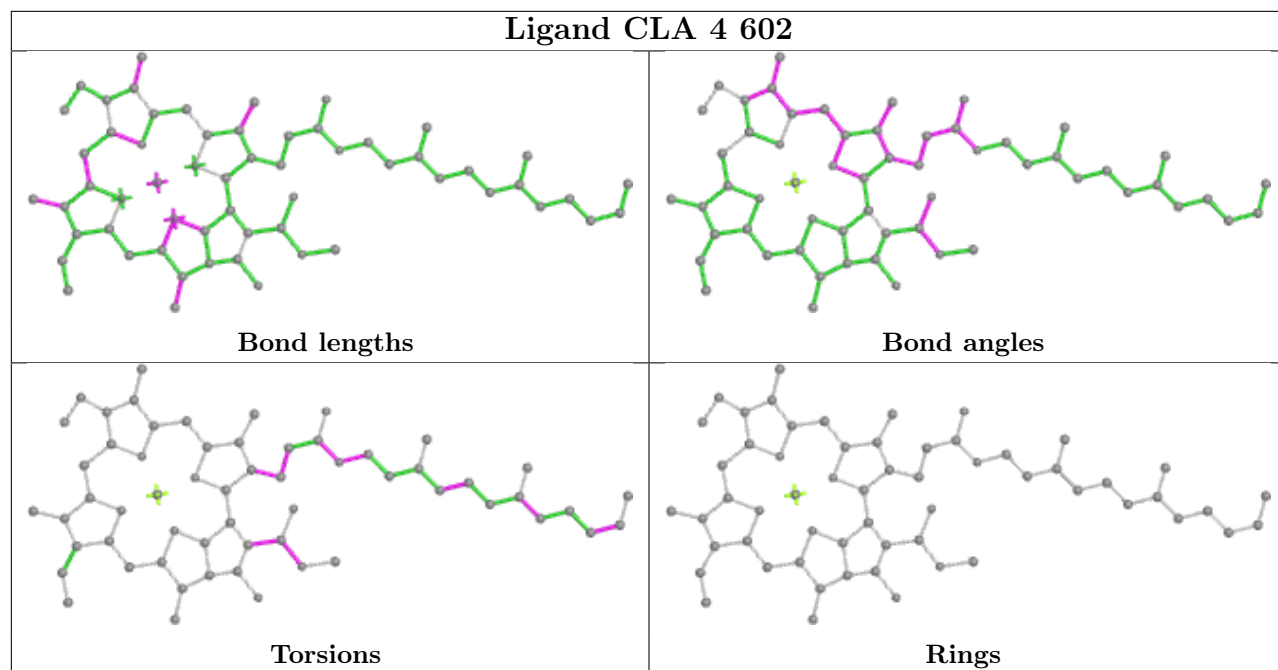


Ligand CLA 4 608

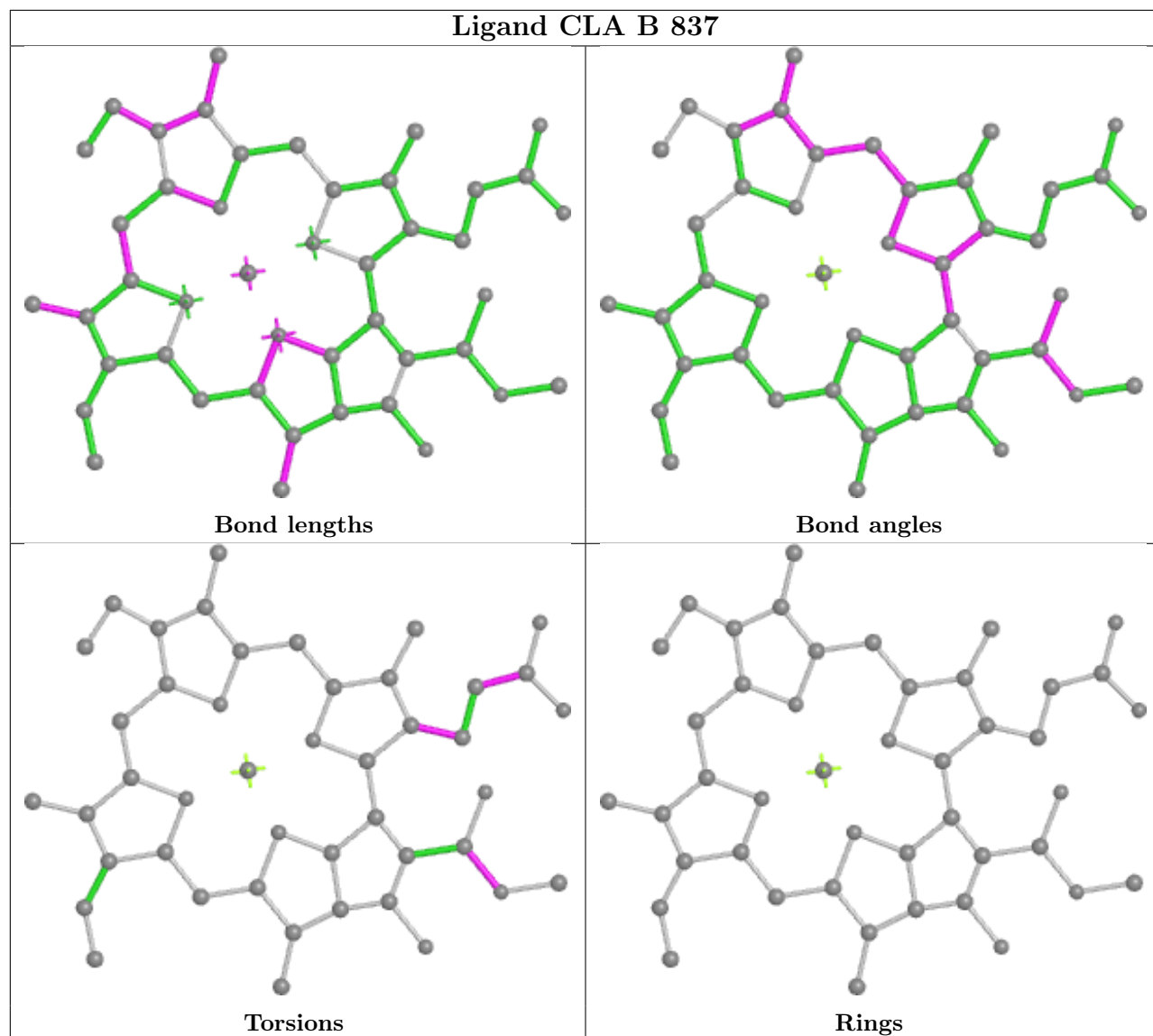


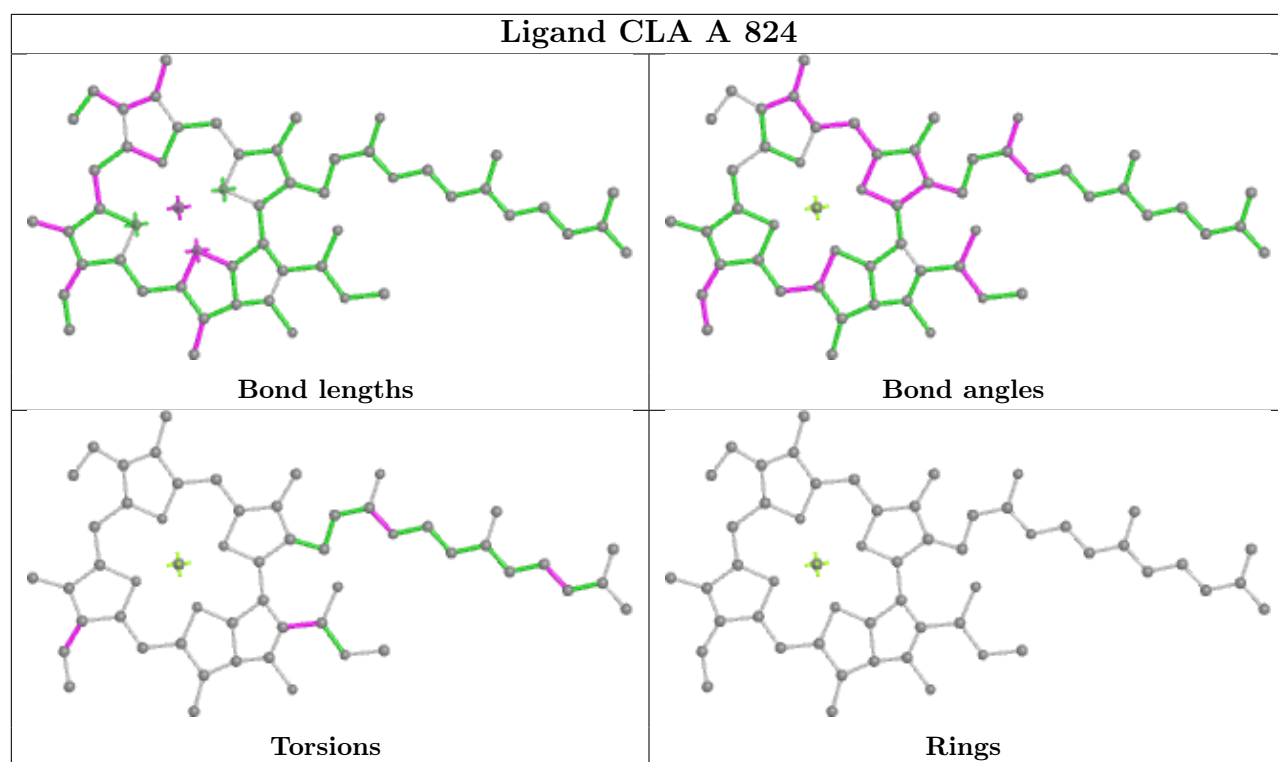
Ligand BCR B 848



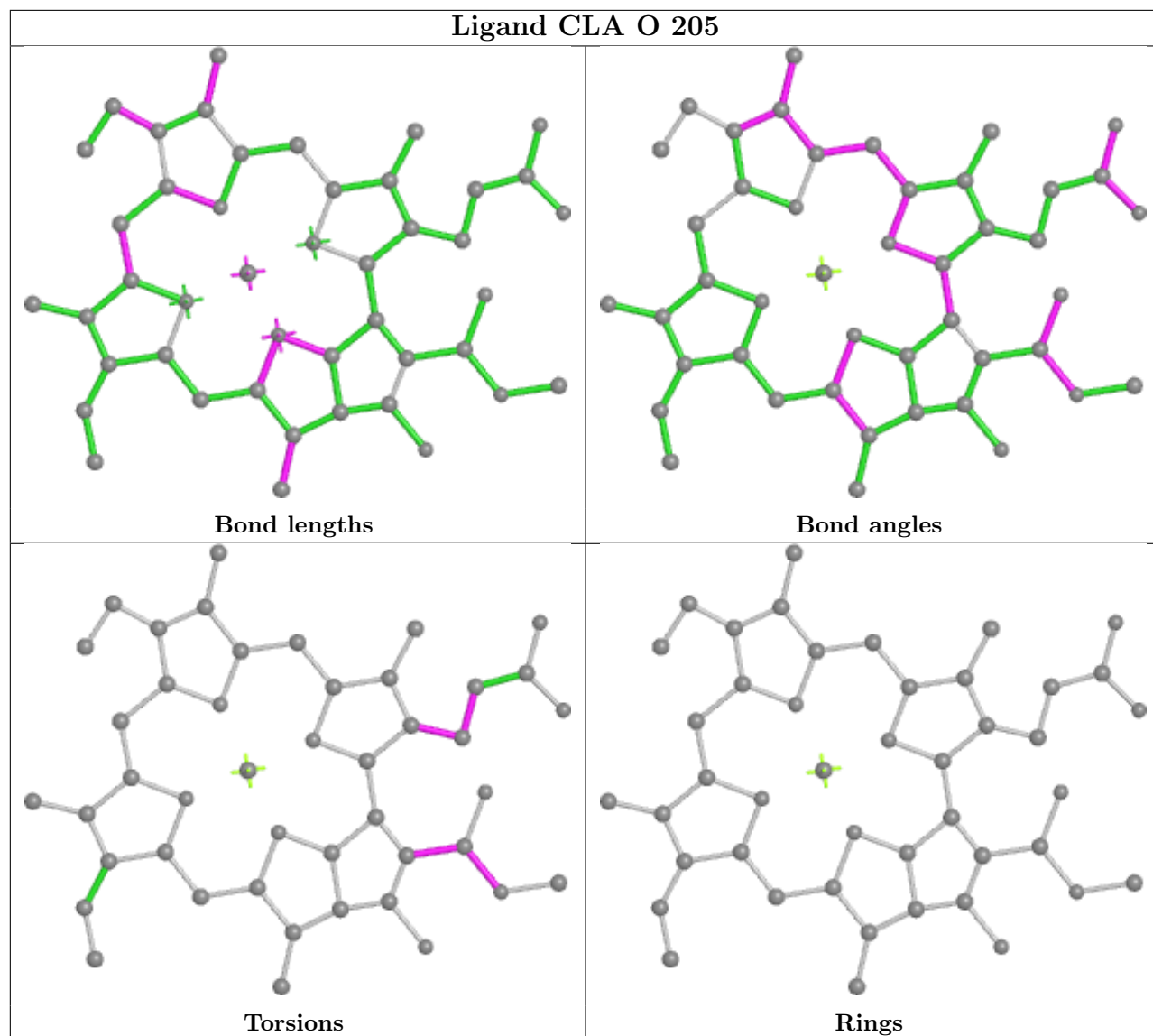


Ligand CLA B 837

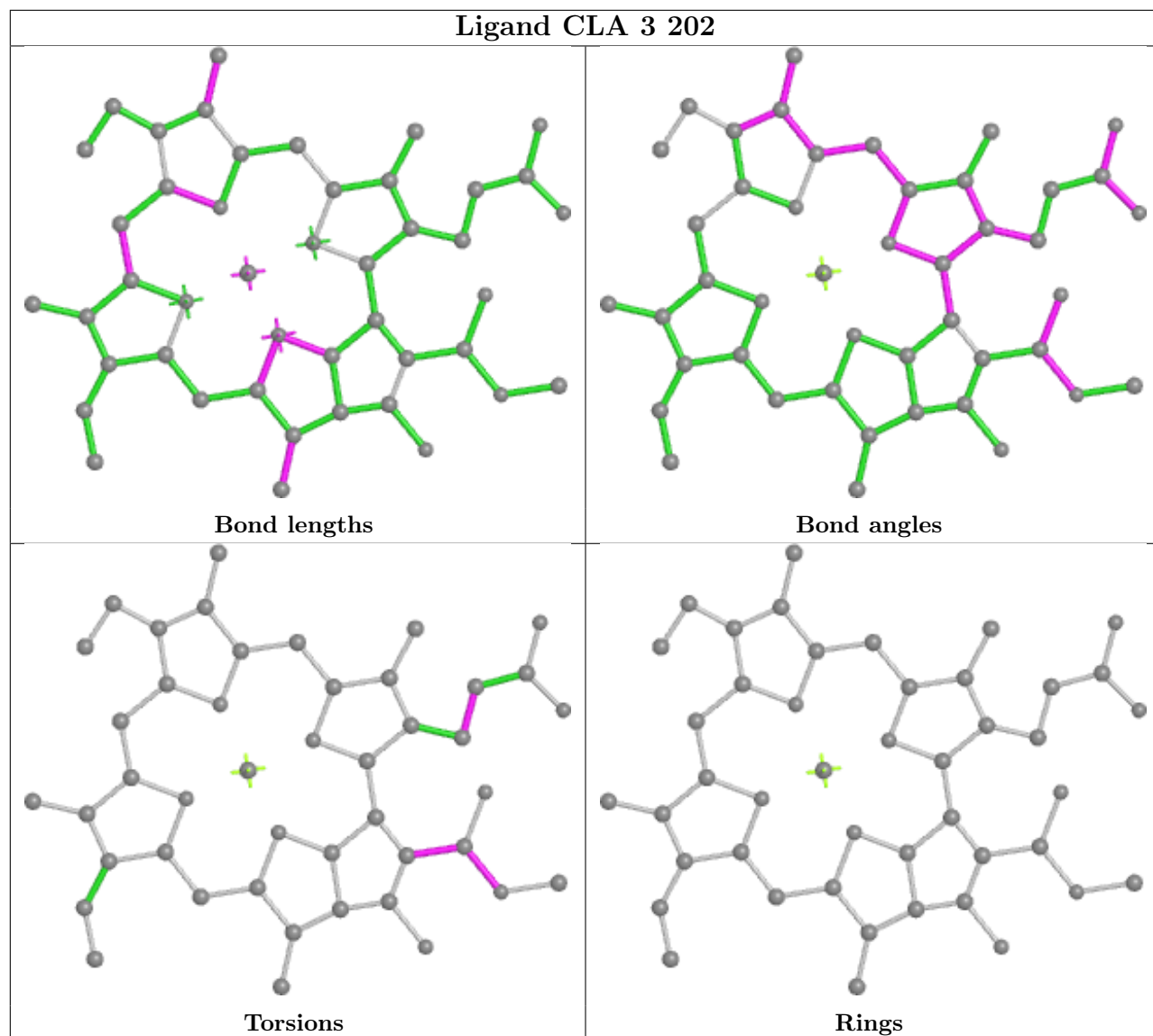




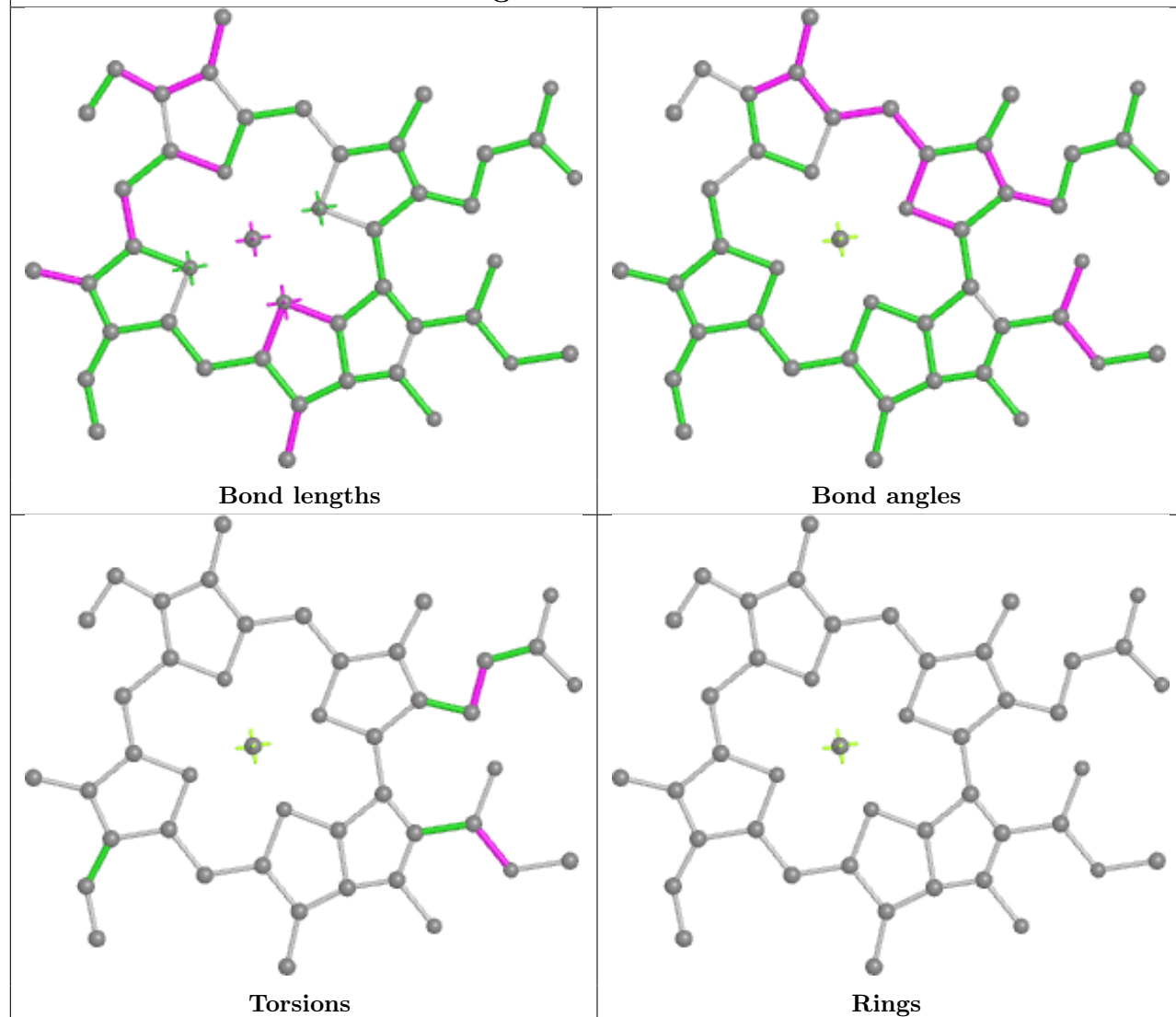
Ligand CLA O 205



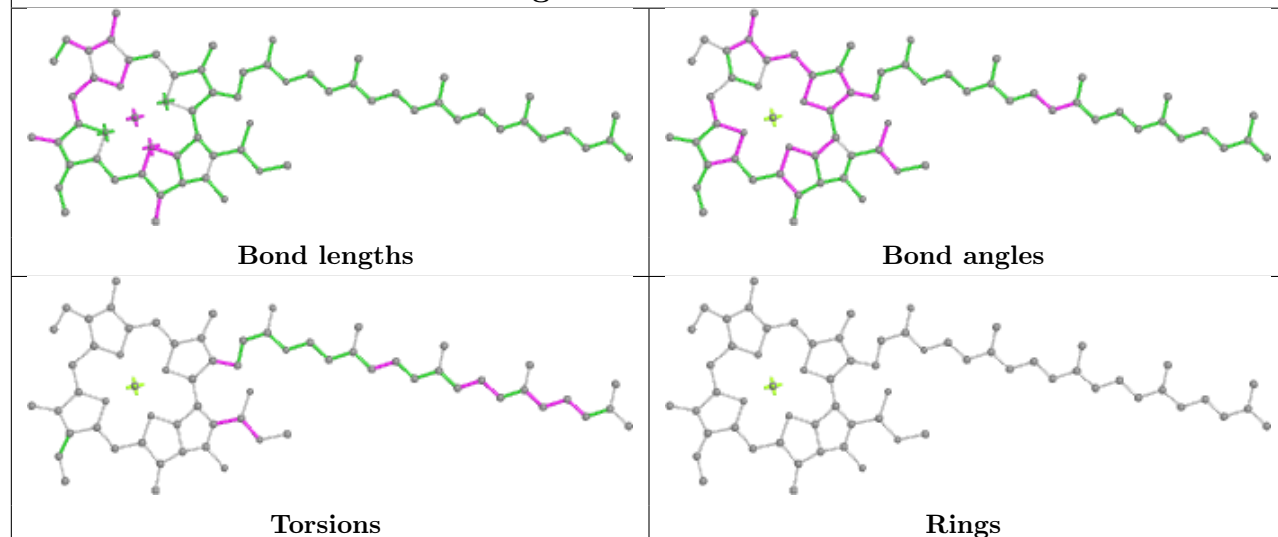
Ligand CLA 3 202



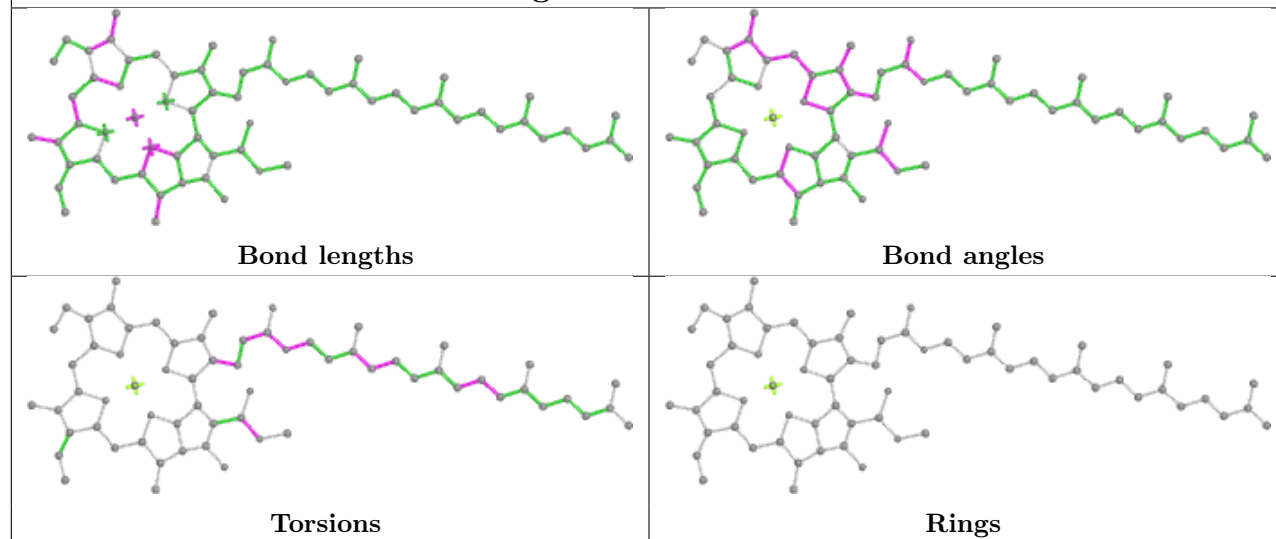
Ligand CLA 2 612



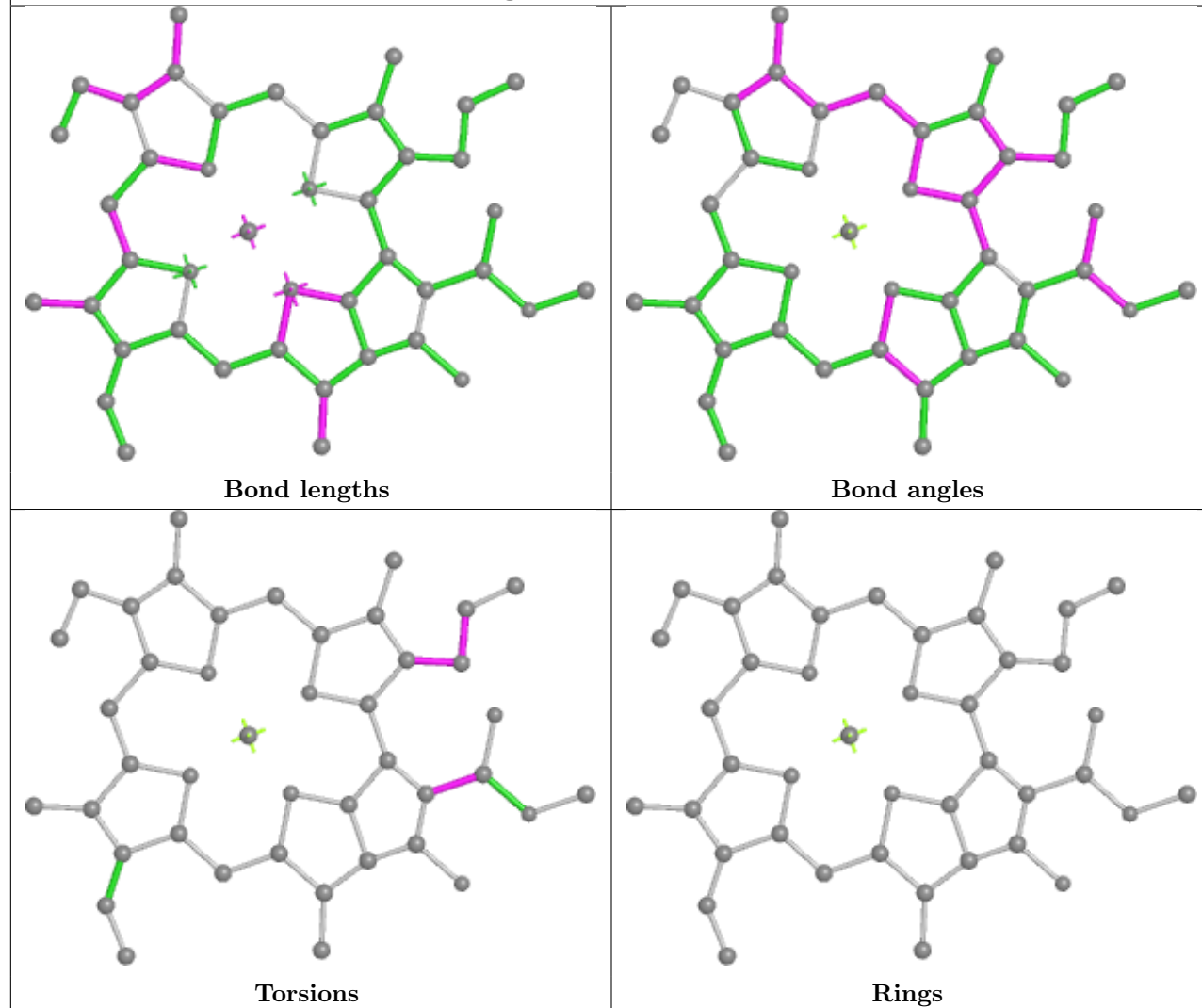
Ligand CLA B 832



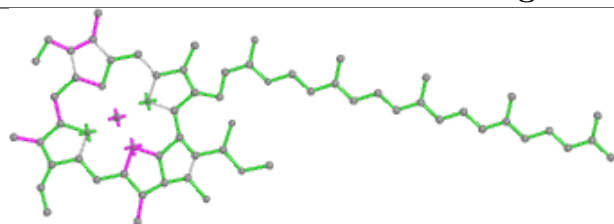
Ligand CLA B 831



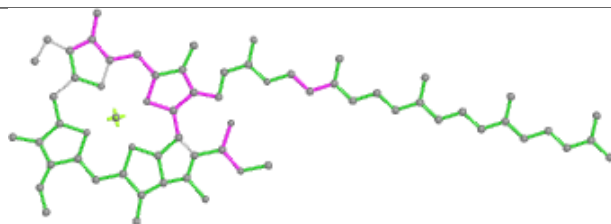
Ligand CLA B 834



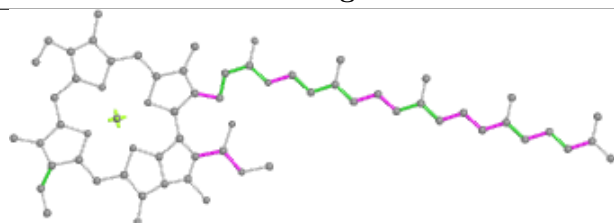
Ligand CLA J 101



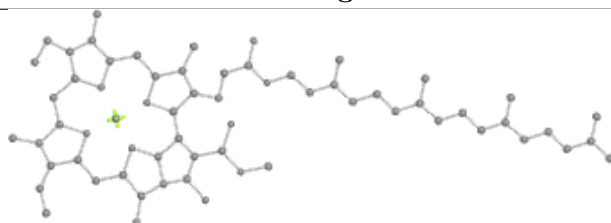
Bond lengths



Bond angles

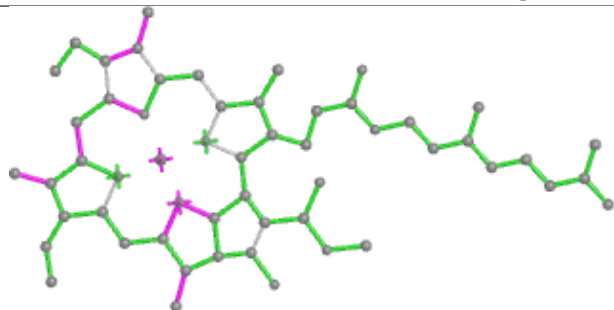


Torsions

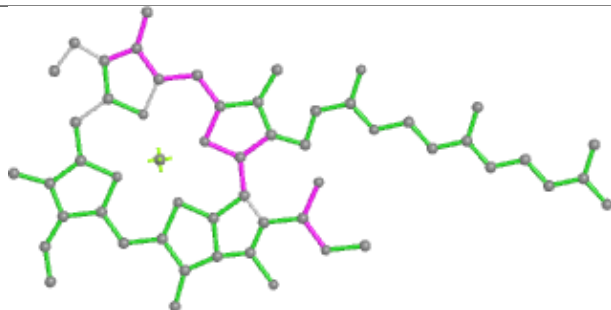


Rings

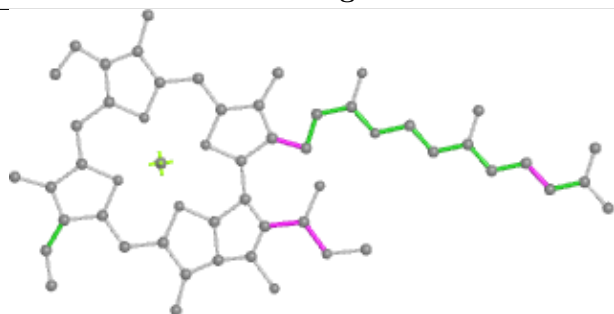
Ligand CLA B 815



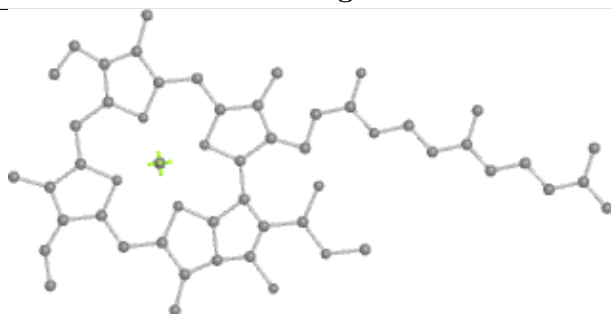
Bond lengths



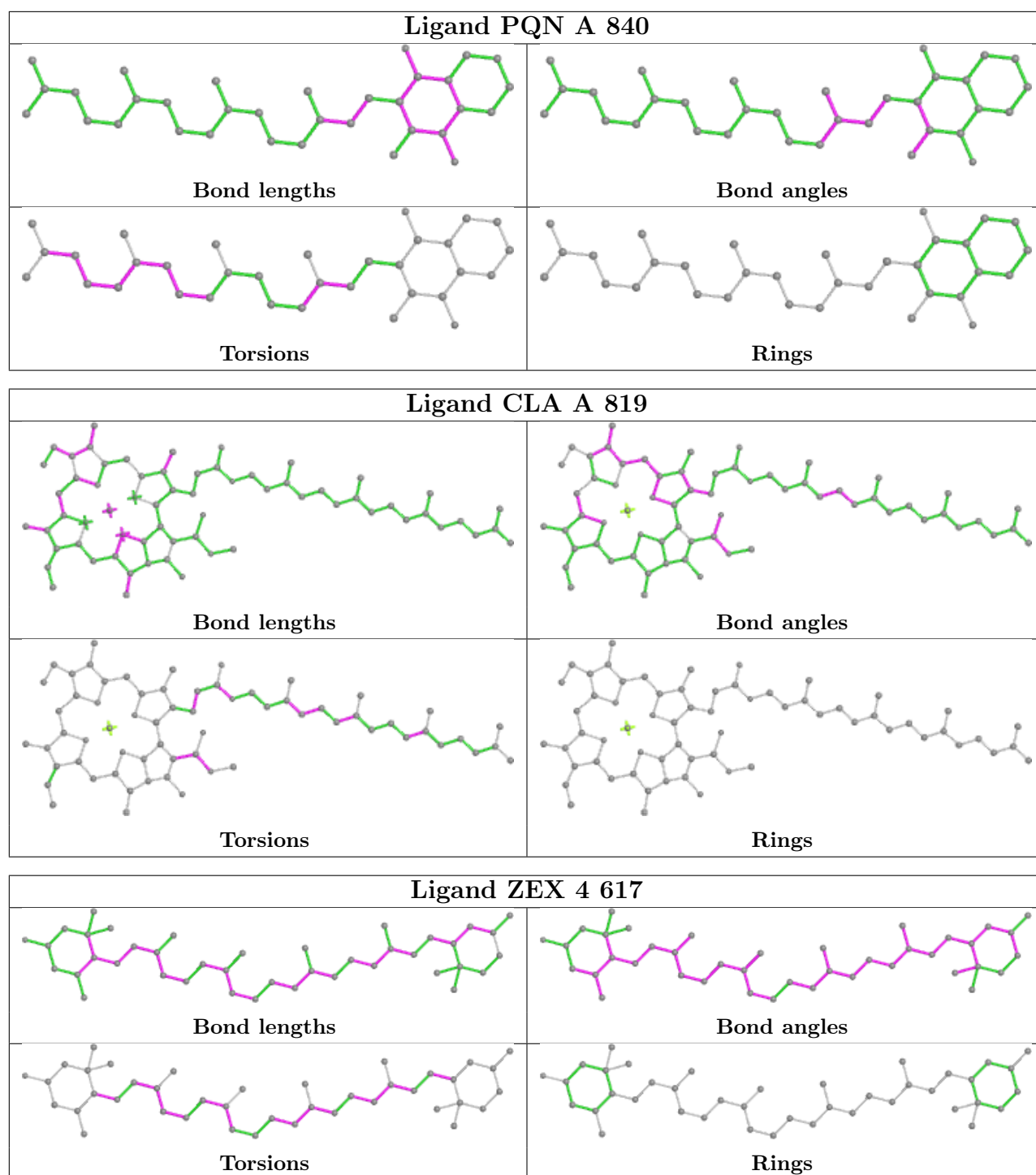
Bond angles

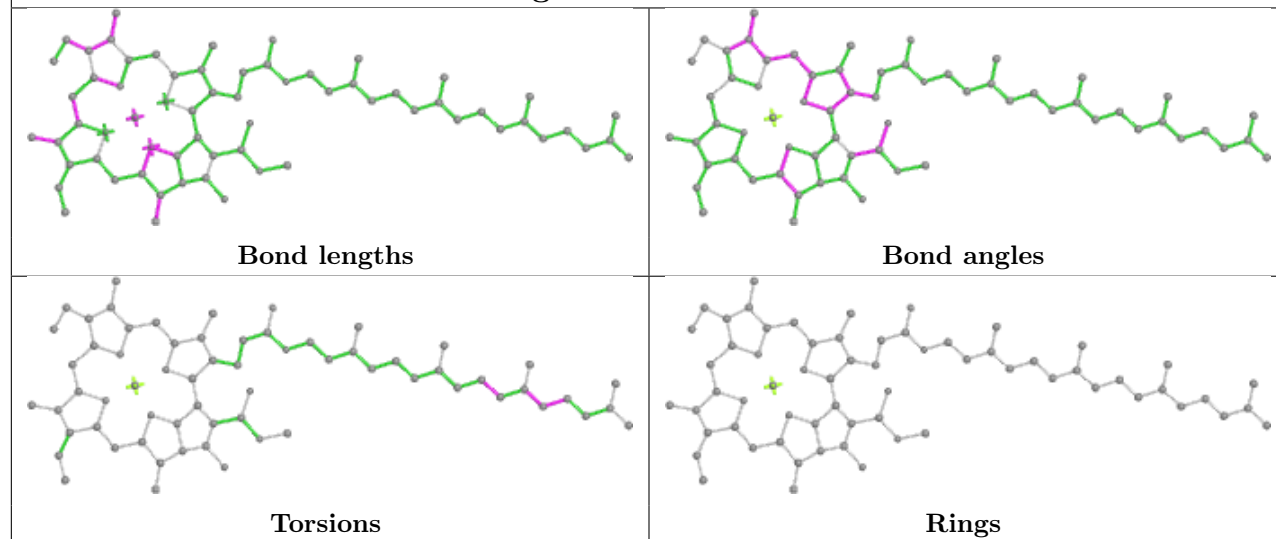
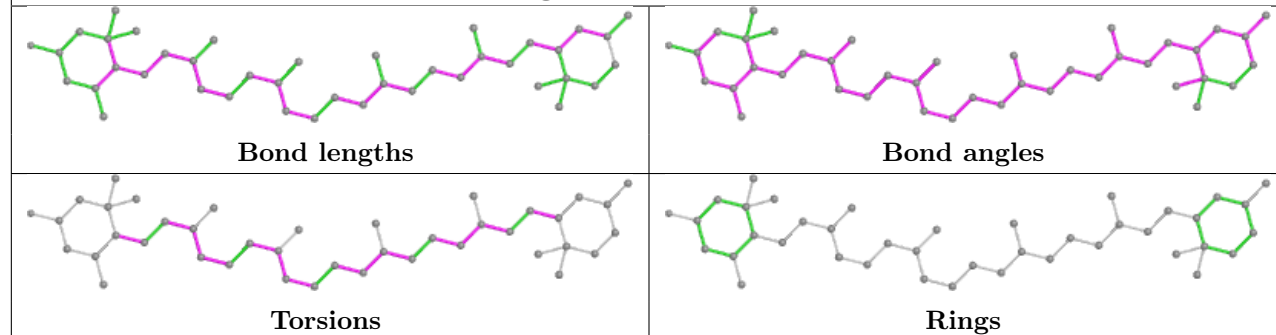
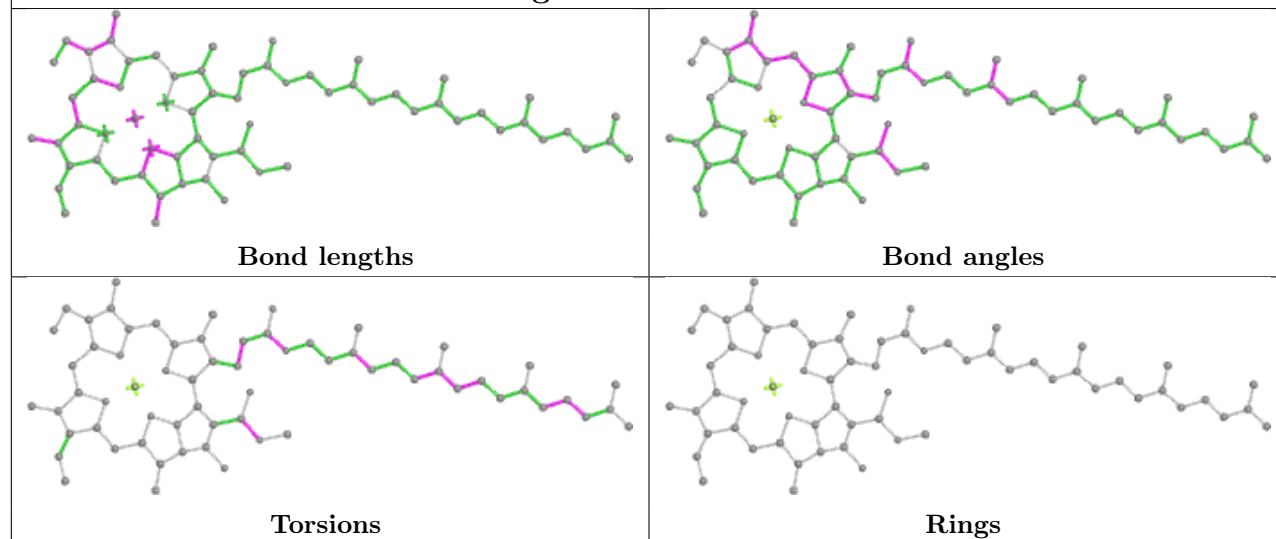


Torsions

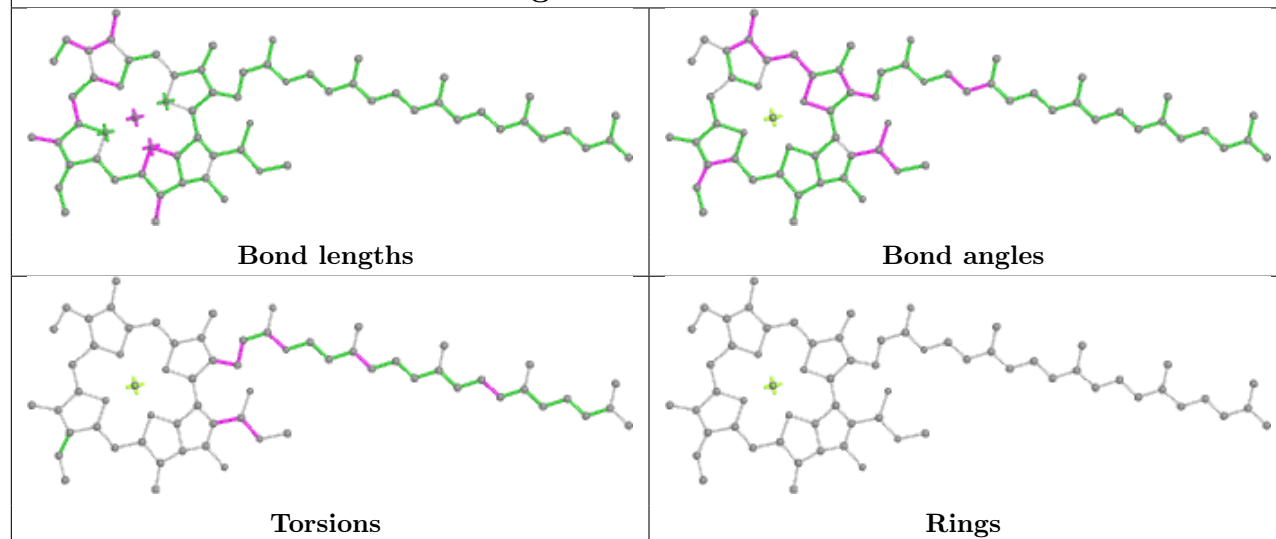


Rings

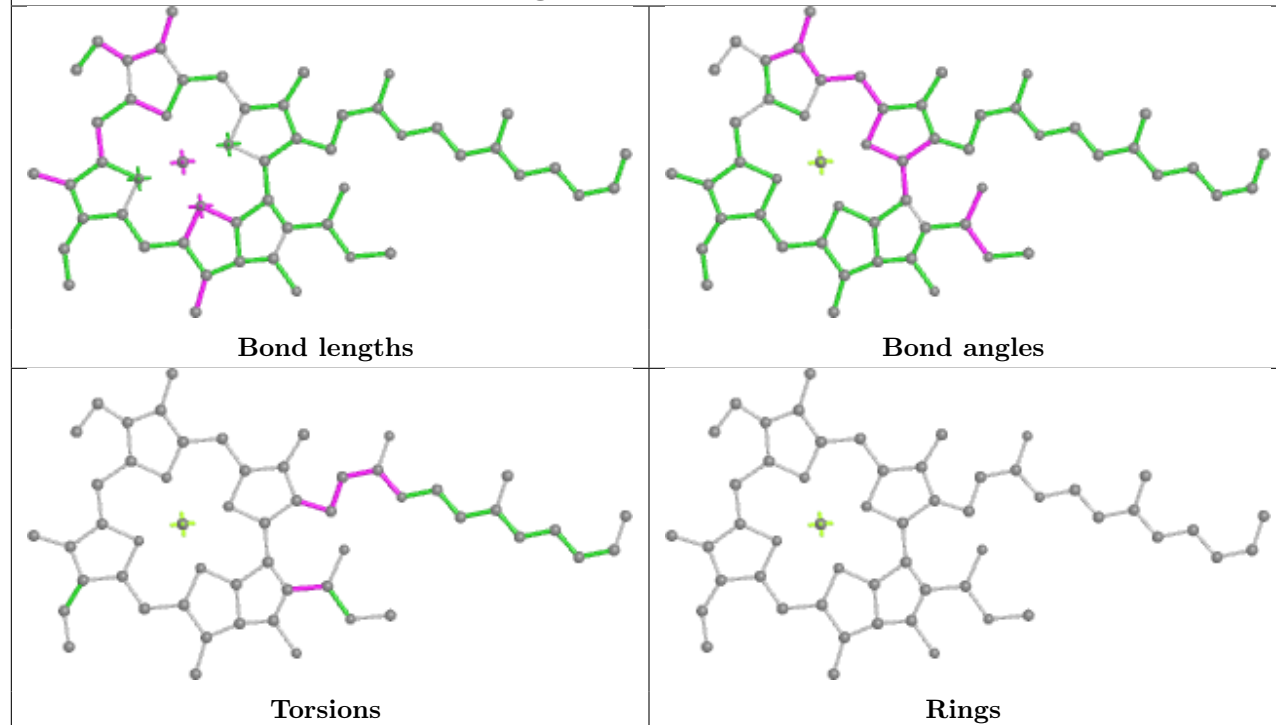


Ligand CLA B 828**Ligand ZEX 2 614****Ligand CLA B 841**

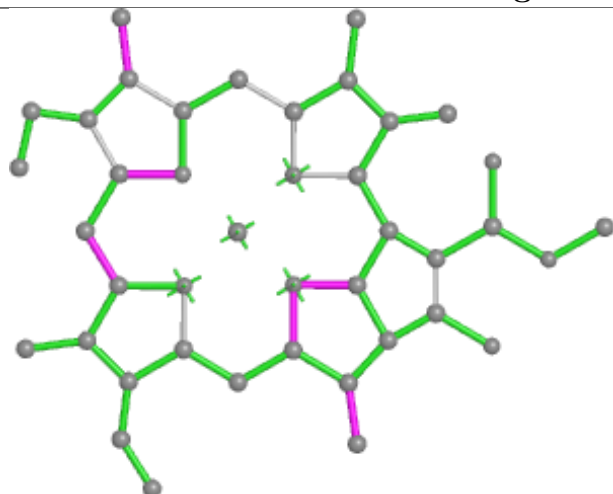
Ligand CLA A 826



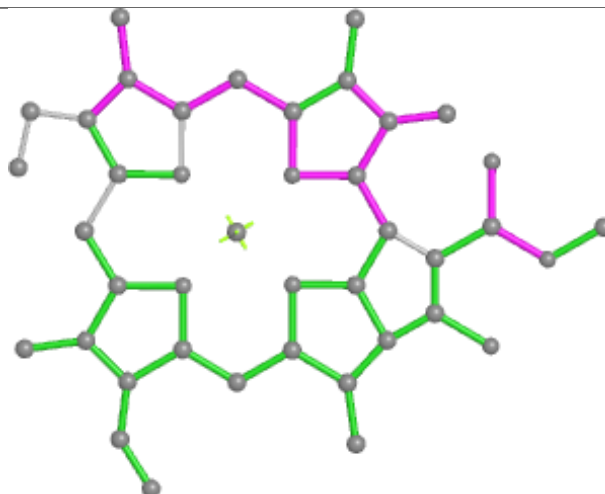
Ligand CLA A 810



Ligand CLA O 203



Bond lengths



Bond angles

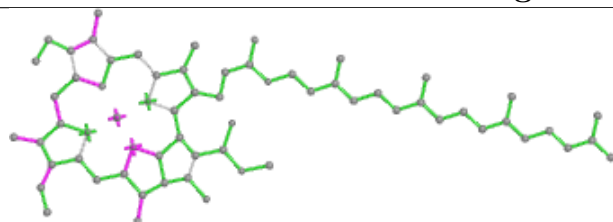


Torsions

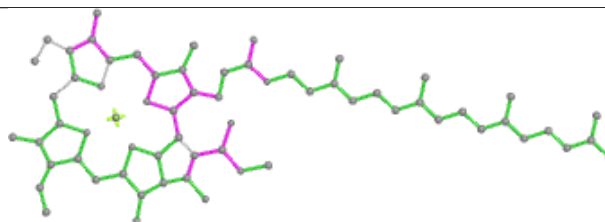


Rings

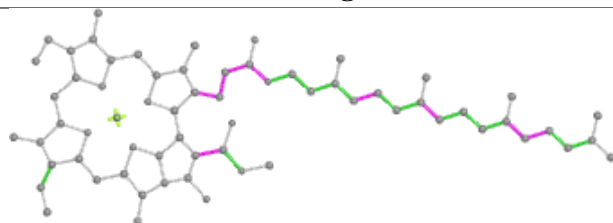
Ligand CLA B 813



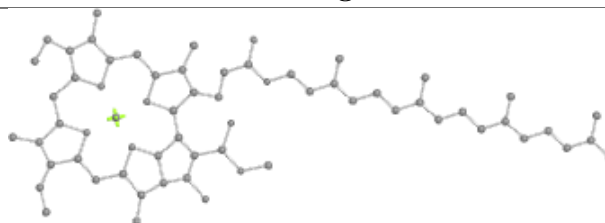
Bond lengths



Bond angles

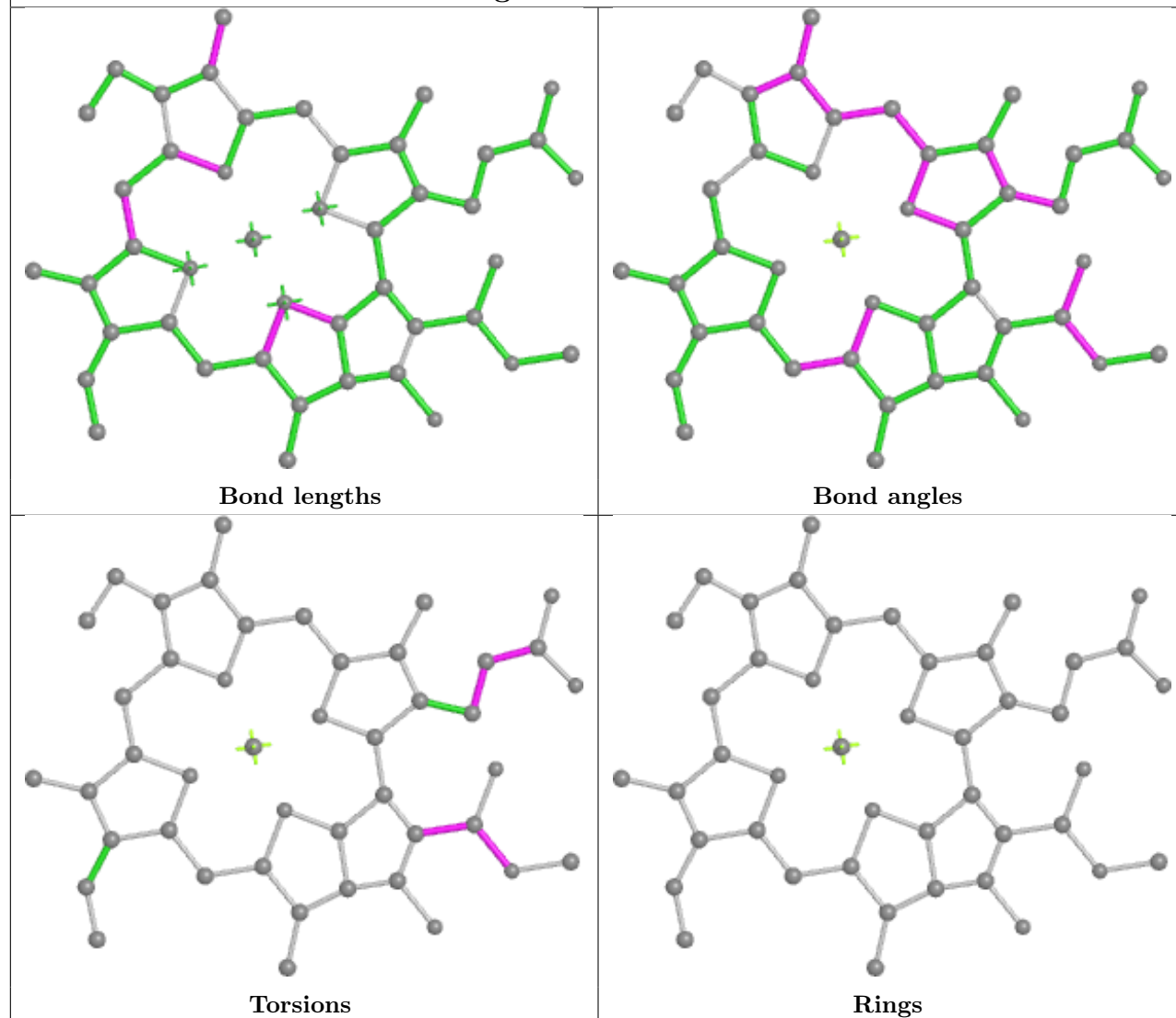


Torsions

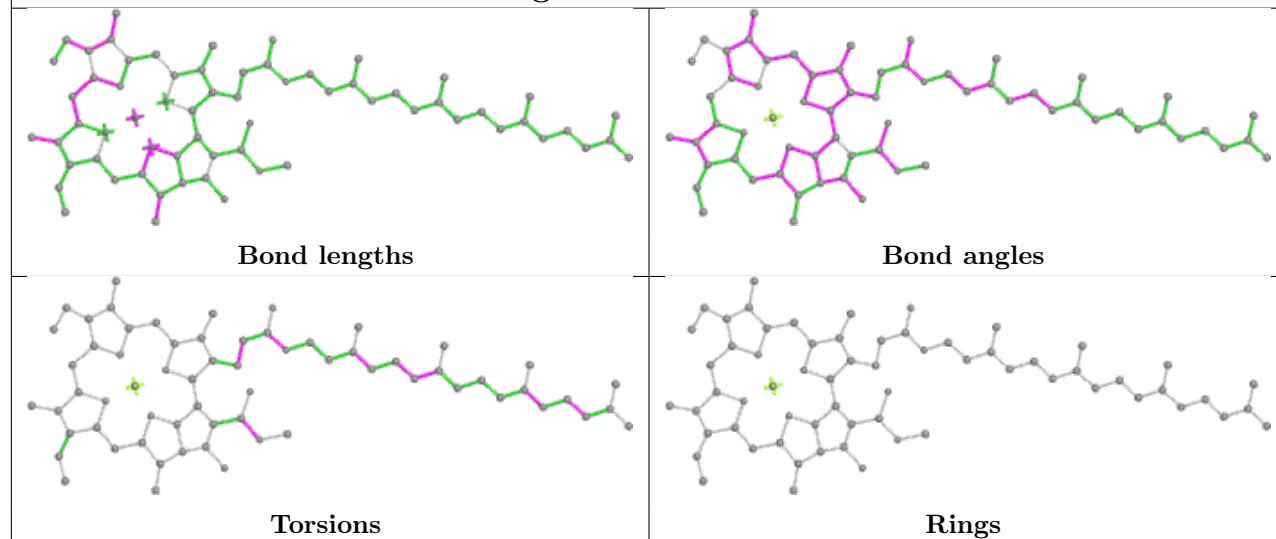


Rings

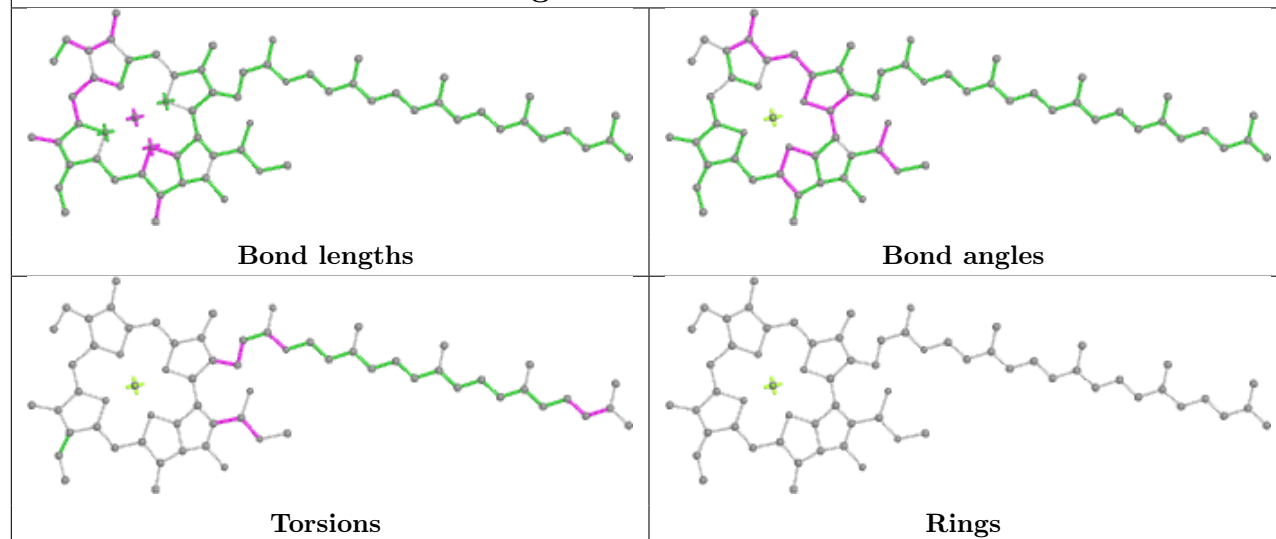
Ligand CLA 5 611



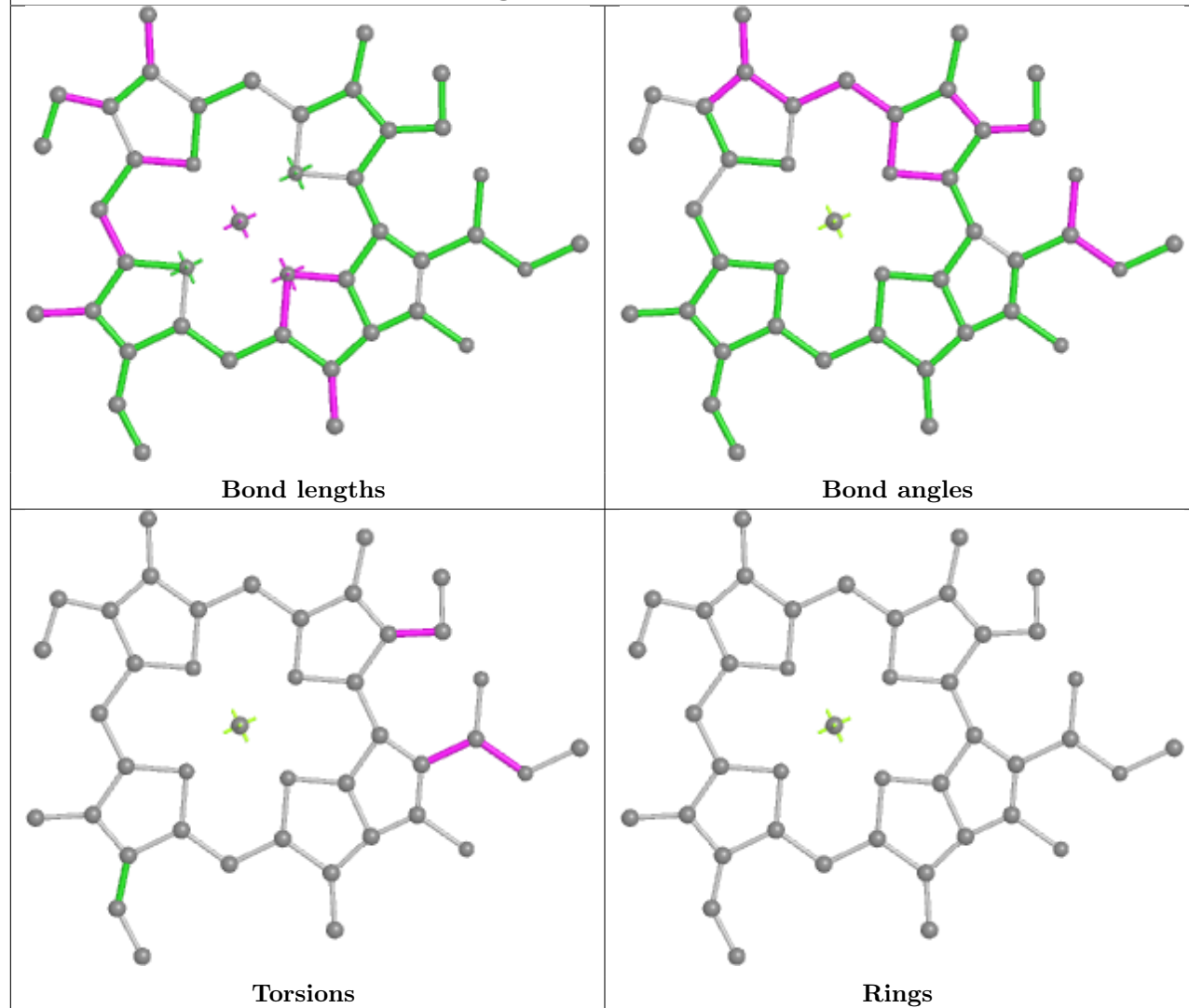
Ligand CLA B 802



Ligand CLA A 816



Ligand CLA A 813



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.

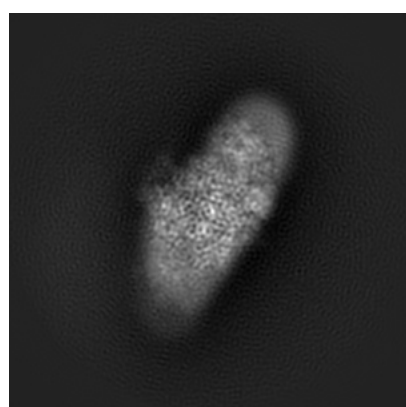
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6929. These allow visual inspection of the internal detail of the map and identification of artifacts.

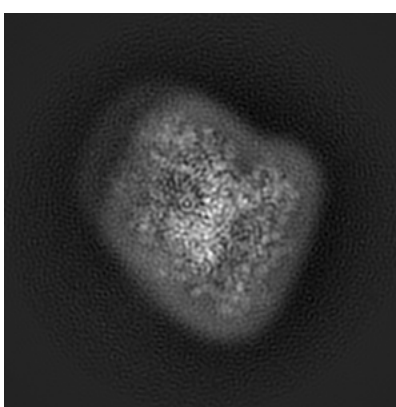
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

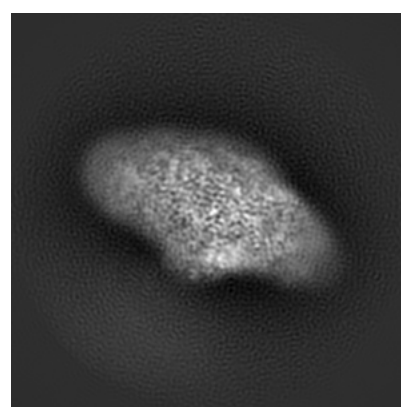
6.1.1 Primary map



X



Y

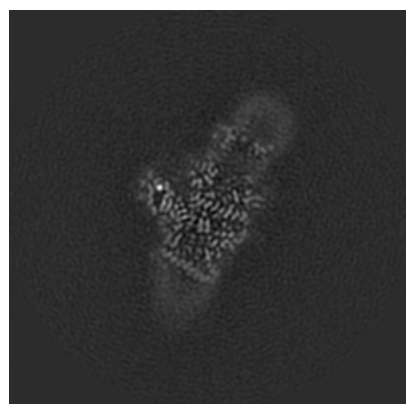


Z

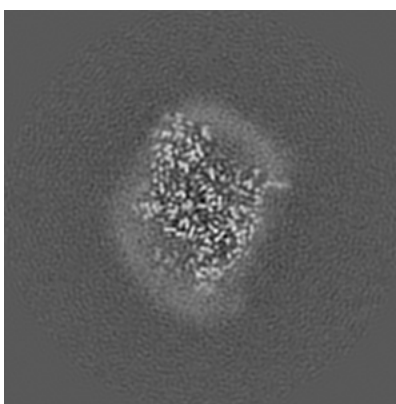
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

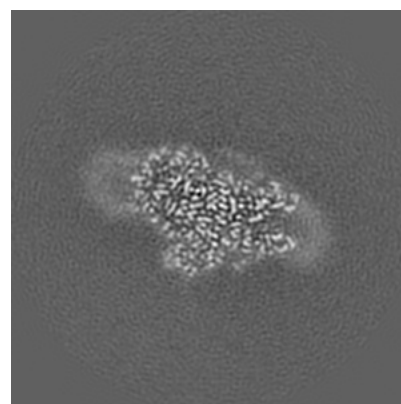
6.2.1 Primary map



X Index: 140



Y Index: 140

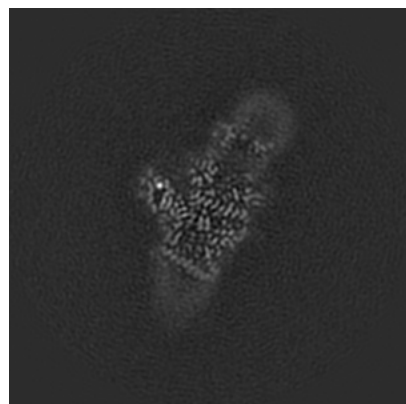


Z Index: 140

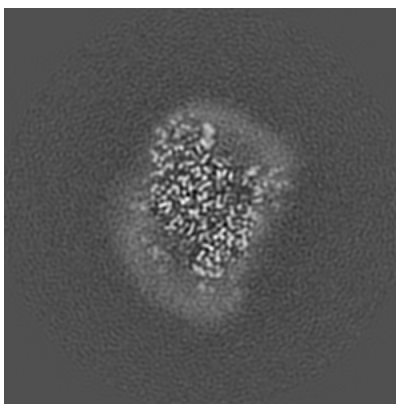
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

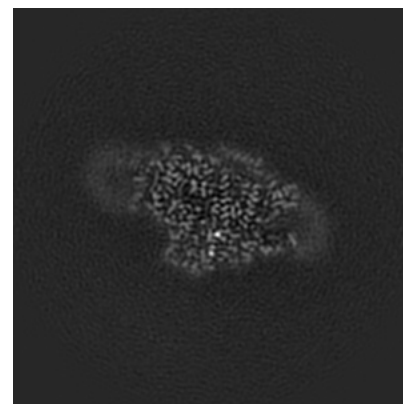
6.3.1 Primary map



X Index: 140



Y Index: 142

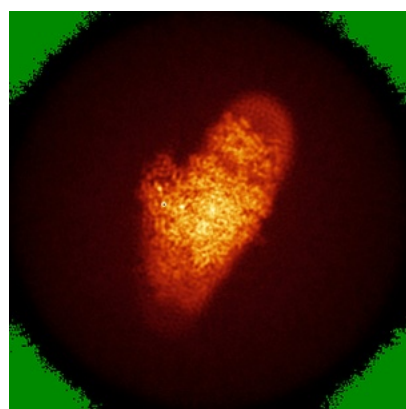


Z Index: 143

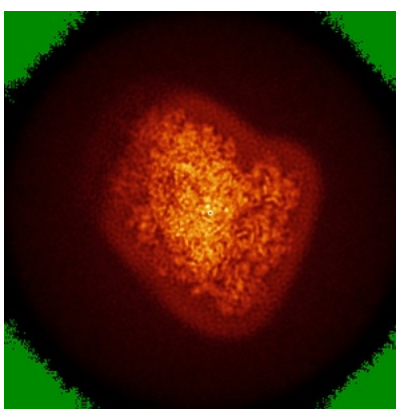
The images above show the largest variance slices of the map in three orthogonal directions.

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

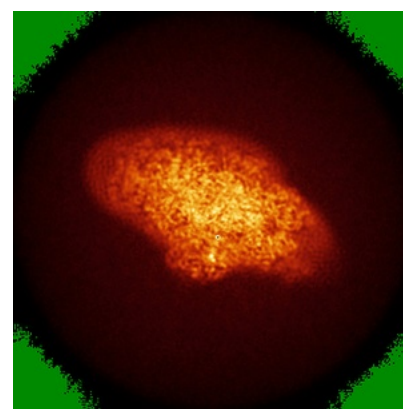
6.4.1 Primary map



X



Y

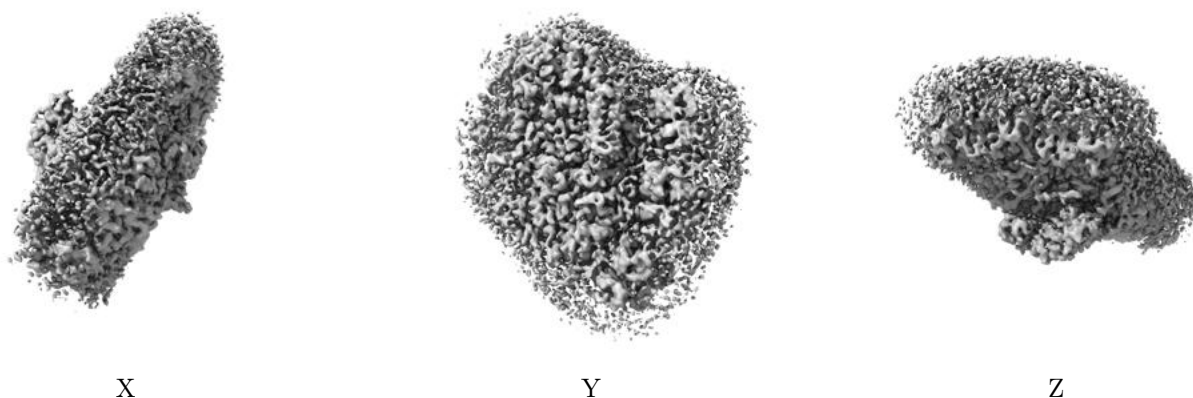


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0562. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

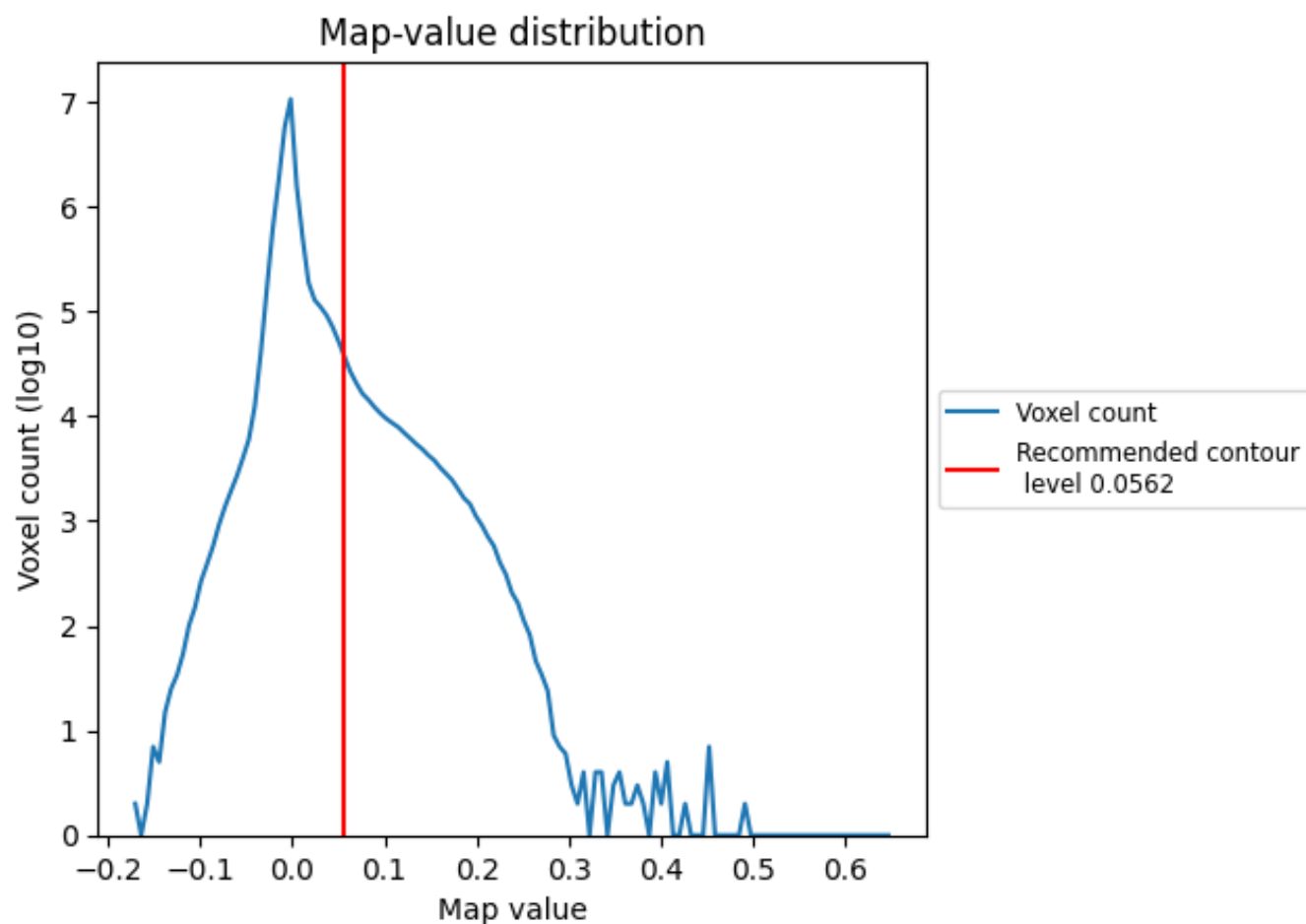
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

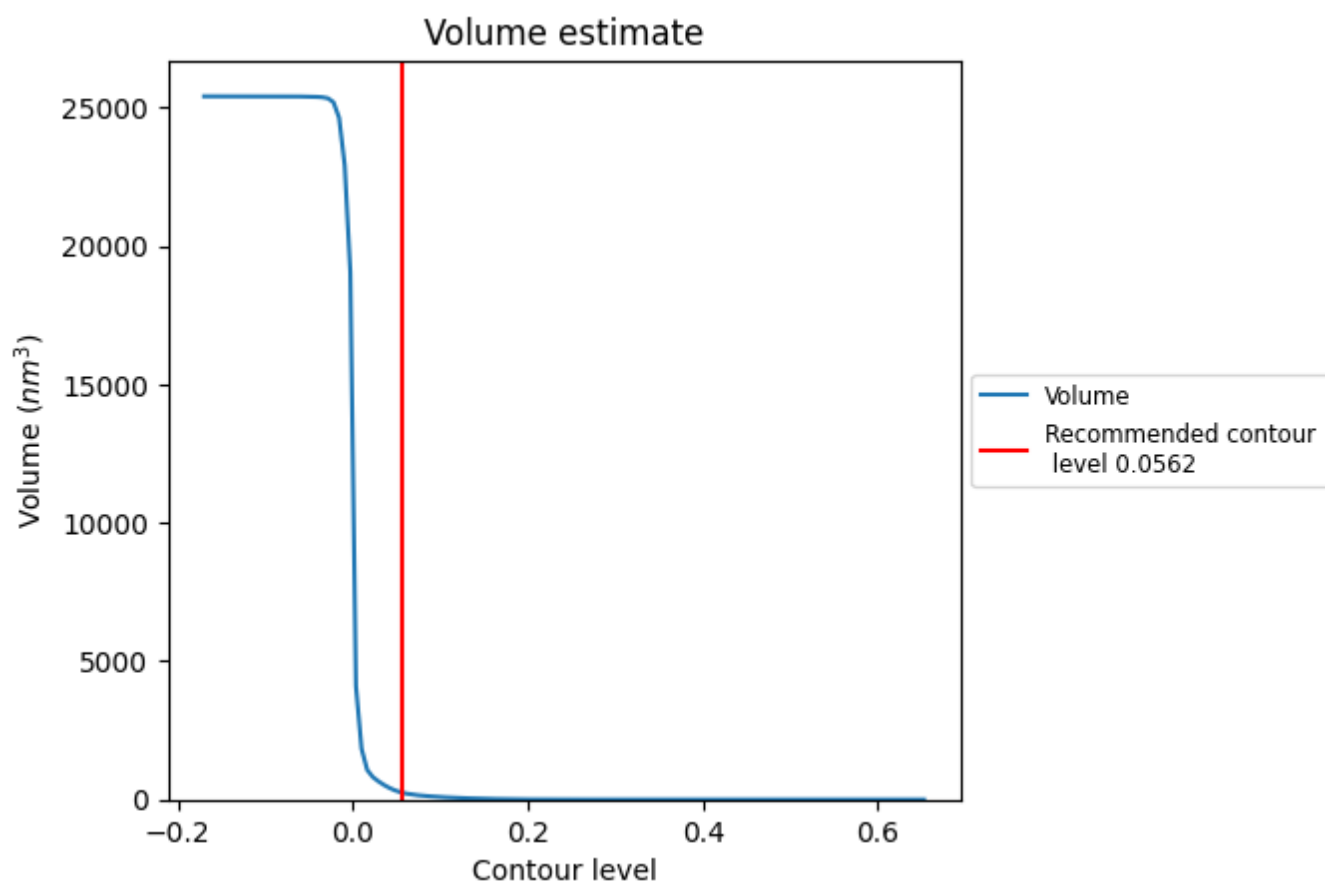
This section contains the results of statistical analysis of the map.

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.

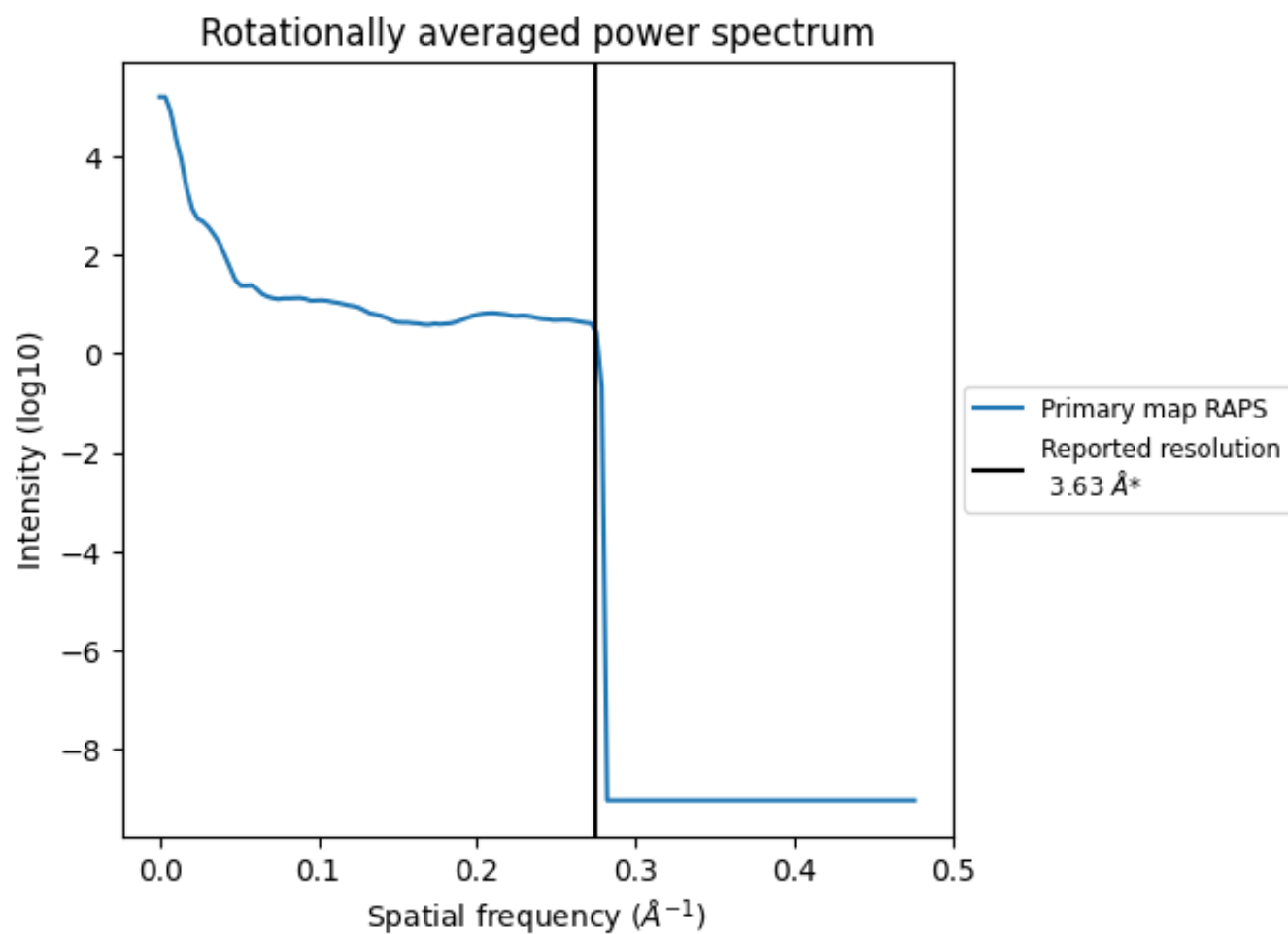
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 253 nm^3 ; this corresponds to an approximate mass of 228 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 0.275 Å⁻¹

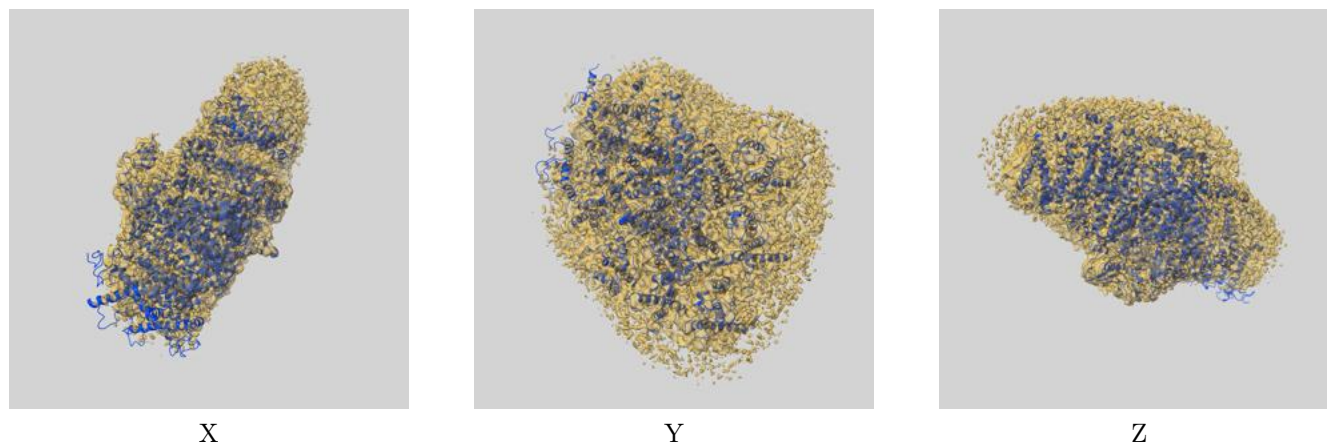
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

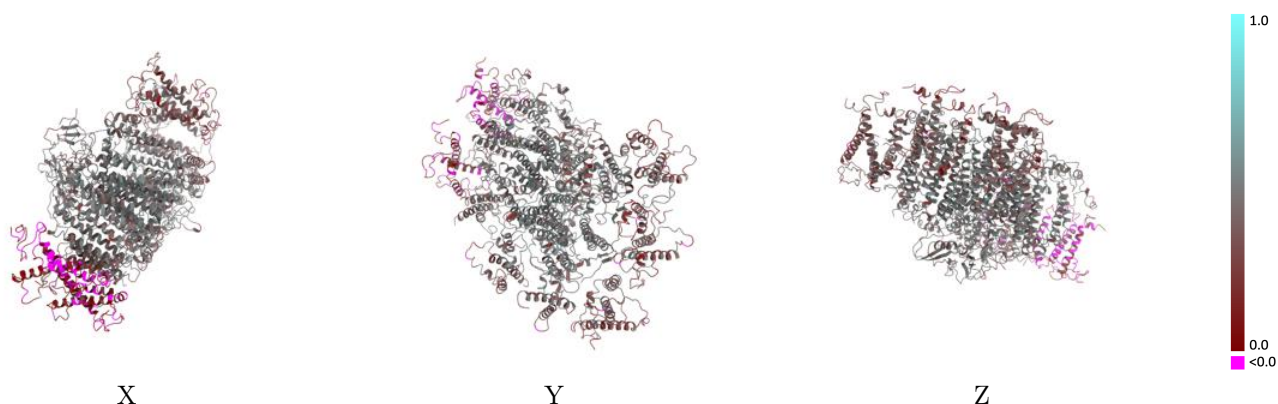
This section contains information regarding the fit between EMDB map EMD-6929 and PDB model 5ZGB. Per-residue inclusion information can be found in section 3 on page 27.

9.1 Map-model overlay [i](#)



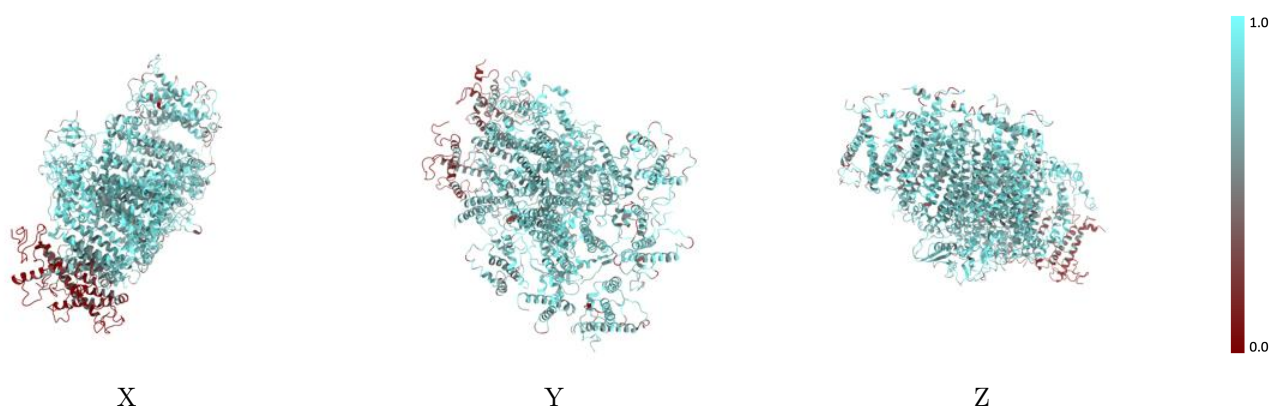
The images above show the 3D surface view of the map at the recommended contour level 0.0562 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



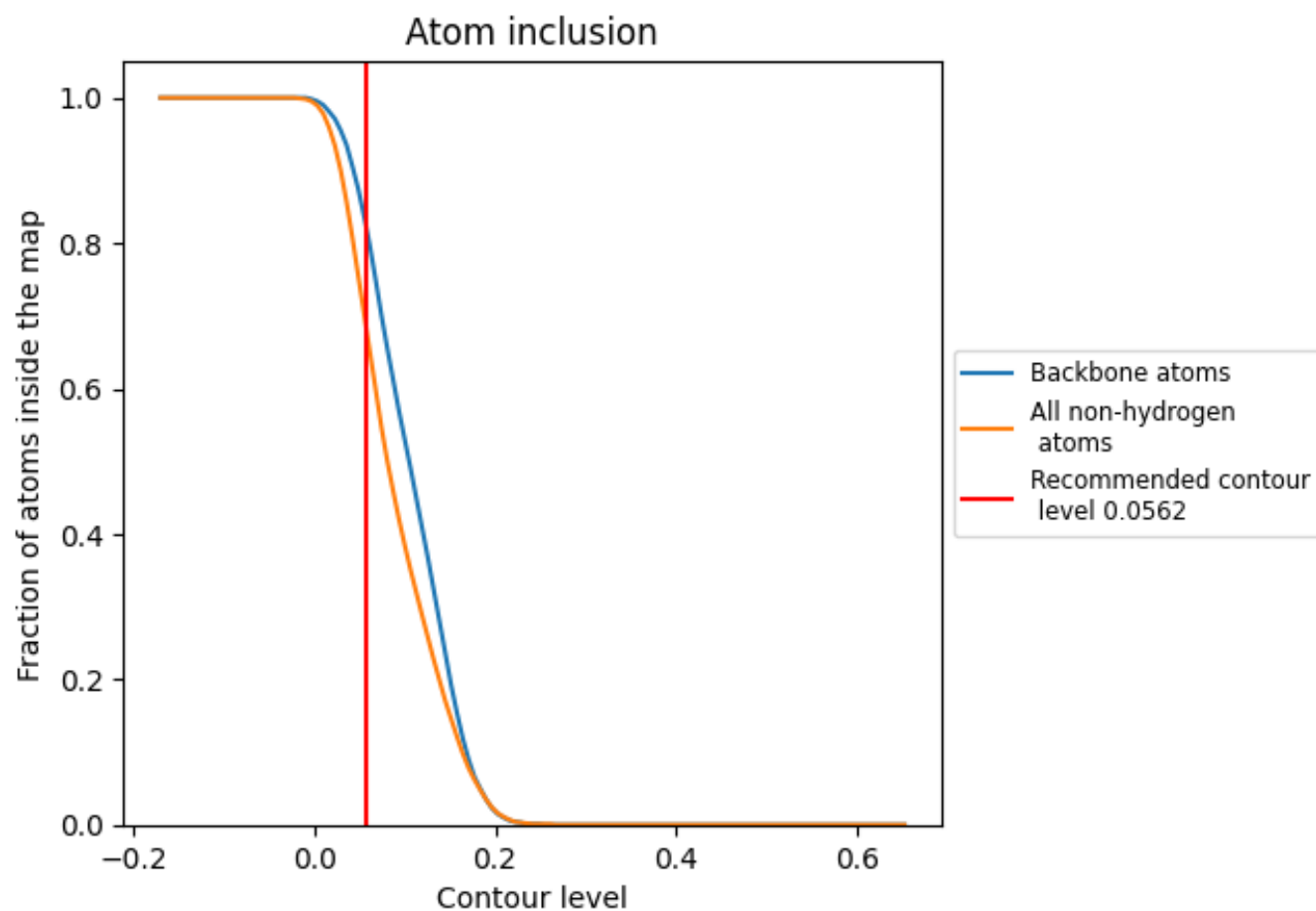
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0562).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 69% 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 (0.0562) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6920	<div></div> 0.3990
1	<div></div> 0.7130	<div></div> 0.3420
2	<div></div> 0.7000	<div></div> 0.3450
3	<div></div> 0.6950	<div></div> 0.3520
4	<div></div> 0.2510	<div></div> 0.1760
5	<div></div> 0.2330	<div></div> 0.0920
A	<div></div> 0.7890	<div></div> 0.4840
B	<div></div> 0.7740	<div></div> 0.4690
C	<div></div> 0.8660	<div></div> 0.4550
D	<div></div> 0.7660	<div></div> 0.4340
E	<div></div> 0.7590	<div></div> 0.4220
F	<div></div> 0.7560	<div></div> 0.4220
I	<div></div> 0.6880	<div></div> 0.4310
J	<div></div> 0.7200	<div></div> 0.4820
K	<div></div> 0.6950	<div></div> 0.3850
L	<div></div> 0.7080	<div></div> 0.4100
M	<div></div> 0.6450	<div></div> 0.3860
O	<div></div> 0.6730	<div></div> 0.3670

1.0

0.0

<0.0