



wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 08:54 AM JST

PDB ID : 5ZGH
EMDB ID : EMD-6930
Title : Cryo-EM structure of the red algal PSI-LHCR
Authors : Pi, X.
Deposited on : 2018-03-09
Resolution : 3.82 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

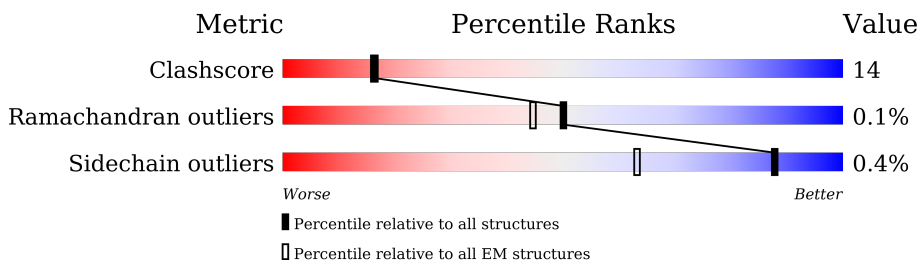
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.82 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	1	175	<div> <div>47%</div> <div>70%</div> <div>27%</div> <div>.</div> </div>
2	2	199	<div> <div>37%</div> <div>63%</div> <div>25%</div> <div>12%</div> </div>
3	3	188	<div> <div>62%</div> <div>61%</div> <div>29%</div> <div>10%</div> </div>
4	A	748	<div> <div>13%</div> <div>69%</div> <div>30%</div> <div>.</div> </div>
5	B	732	<div> <div>17%</div> <div>73%</div> <div>26%</div> </div>
6	C	81	<div> <div>20%</div> <div>73%</div> <div>26%</div> <div>.</div> </div>
7	D	139	<div> <div>40%</div> <div>65%</div> <div>20%</div> <div>14%</div> </div>
8	E	94	<div> <div>26%</div> <div>56%</div> <div>9%</div> <div>35%</div> </div>

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Mol	Chain	Length	Quality of chain
9	F	185	
10	I	32	
11	J	38	
12	K	60	
13	L	140	
14	M	29	
15	O	155	

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	CLA	1	601	X	-	-	-
16	CLA	1	602	X	-	-	-
16	CLA	1	603	X	-	-	-
16	CLA	1	604	X	-	-	-
16	CLA	1	605	X	-	-	-
16	CLA	1	606	X	-	-	-
16	CLA	1	607	X	-	-	-
16	CLA	1	608	X	-	-	-
16	CLA	1	609	X	-	-	-
16	CLA	1	610	X	-	-	-
16	CLA	1	611	X	-	-	-
16	CLA	1	612	X	-	-	-
16	CLA	2	601	X	-	-	-
16	CLA	2	602	X	-	-	-
16	CLA	2	603	X	-	-	-
16	CLA	2	604	X	-	-	-
16	CLA	2	605	X	-	-	-
16	CLA	2	606	X	-	-	-
16	CLA	2	607	X	-	-	-
16	CLA	2	608	X	-	-	-
16	CLA	2	609	X	-	-	-
16	CLA	2	610	X	-	-	-
16	CLA	2	611	X	-	-	-
16	CLA	2	612	X	-	-	-
16	CLA	2	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	3	202	X	-	-	-
16	CLA	3	203	X	-	-	-
16	CLA	3	204	X	-	-	-
16	CLA	3	205	X	-	-	-
16	CLA	3	206	X	-	-	-
16	CLA	3	207	X	-	-	-
16	CLA	3	208	X	-	-	-
16	CLA	3	209	X	-	-	-
16	CLA	3	210	X	-	-	-
16	CLA	3	211	X	-	-	-
16	CLA	3	212	X	-	-	-
16	CLA	3	213	X	-	-	-
16	CLA	A	802	X	-	-	-
16	CLA	A	803	X	-	-	-
16	CLA	A	804	X	-	-	-
16	CLA	A	805	X	-	-	-
16	CLA	A	806	X	-	-	-
16	CLA	A	807	X	-	-	-
16	CLA	A	808	X	-	-	-
16	CLA	A	809	X	-	-	-
16	CLA	A	810	X	-	-	-
16	CLA	A	811	X	-	-	-
16	CLA	A	812	X	-	-	-
16	CLA	A	813	X	-	-	-
16	CLA	A	814	X	-	-	-
16	CLA	A	815	X	-	-	-
16	CLA	A	816	X	-	-	-
16	CLA	A	817	X	-	-	-
16	CLA	A	818	X	-	-	-
16	CLA	A	819	X	-	-	-
16	CLA	A	820	X	-	-	-
16	CLA	A	821	X	-	-	-
16	CLA	A	822	X	-	-	-
16	CLA	A	823	X	-	-	-
16	CLA	A	824	X	-	-	-
16	CLA	A	825	X	-	-	-
16	CLA	A	826	X	-	-	-
16	CLA	A	827	X	-	-	-
16	CLA	A	828	X	-	-	-
16	CLA	A	829	X	-	-	-
16	CLA	A	830	X	-	-	-
16	CLA	A	831	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	A	832	X	-	-	-
16	CLA	A	833	X	-	-	-
16	CLA	A	834	X	-	-	-
16	CLA	A	835	X	-	-	-
16	CLA	A	836	X	-	-	-
16	CLA	A	837	X	-	-	-
16	CLA	A	838	X	-	-	-
16	CLA	A	839	X	-	-	-
16	CLA	A	850	X	-	-	-
16	CLA	A	851	X	-	-	-
16	CLA	A	852	X	-	-	-
16	CLA	B	801	X	-	-	-
16	CLA	B	802	X	-	X	-
16	CLA	B	803	X	-	-	-
16	CLA	B	804	X	-	-	-
16	CLA	B	805	X	-	-	-
16	CLA	B	806	X	-	-	-
16	CLA	B	807	X	-	-	-
16	CLA	B	808	X	-	-	-
16	CLA	B	809	X	-	-	-
16	CLA	B	810	X	-	-	-
16	CLA	B	811	X	-	-	-
16	CLA	B	812	X	-	-	-
16	CLA	B	813	X	-	-	-
16	CLA	B	814	X	-	-	-
16	CLA	B	815	X	-	-	-
16	CLA	B	816	X	-	-	-
16	CLA	B	817	X	-	-	-
16	CLA	B	818	X	-	-	-
16	CLA	B	819	X	-	-	-
16	CLA	B	820	X	-	-	-
16	CLA	B	821	X	-	-	-
16	CLA	B	822	X	-	-	-
16	CLA	B	823	X	-	-	-
16	CLA	B	824	X	-	-	-
16	CLA	B	825	X	-	-	-
16	CLA	B	826	X	-	-	-
16	CLA	B	827	X	-	-	-
16	CLA	B	828	X	-	-	-
16	CLA	B	829	X	-	-	-
16	CLA	B	830	X	-	-	-
16	CLA	B	831	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	B	832	X	-	-	-
16	CLA	B	833	X	-	-	-
16	CLA	B	834	X	-	-	-
16	CLA	B	835	X	-	-	-
16	CLA	B	836	X	-	-	-
16	CLA	B	837	X	-	-	-
16	CLA	B	838	X	-	-	-
16	CLA	B	839	X	-	-	-
16	CLA	B	840	X	-	-	-
16	CLA	B	841	X	-	-	-
16	CLA	B	842	X	-	-	-
16	CLA	F	802	X	-	-	-
16	CLA	F	803	X	-	-	-
16	CLA	J	101	X	-	-	-
16	CLA	K	101	X	-	-	-
16	CLA	K	102	X	-	-	-
16	CLA	L	201	X	-	-	-
16	CLA	L	203	X	-	-	-
16	CLA	L	204	X	-	-	-
16	CLA	L	205	X	-	-	-
16	CLA	O	201	X	-	-	-
16	CLA	O	202	X	-	-	-
16	CLA	O	203	X	-	-	-
16	CLA	O	204	X	-	-	-
17	ZEX	2	614	-	X	-	-
17	ZEX	2	616	-	X	-	-
17	ZEX	3	218	-	X	-	-
19	CL0	A	801	X	-	X	-

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 30757 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 Lhcr1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	169	Total	C	N	O	S	0	0
			1351	887	227	229	8		

- Molecule 2 is a protein called Lhcr2.

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

- Molecule 3 is a protein called Lhcr3.

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

- Molecule 4 is a protein called PsaA.

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

- Molecule 5 is a protein called PsaB.

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

- Molecule 6 is a protein called PsaC.

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

- Molecule 7 is a protein called PsaD.

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

- Molecule 8 is a protein called PsaE.

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

- Molecule 9 is a protein called PsaF.

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

- Molecule 10 is a protein called PsaI.

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

- Molecule 11 is a protein called PsaJ.

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

- Molecule 12 is a protein called PsaK.

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

- Molecule 13 is a protein called PsaL.

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

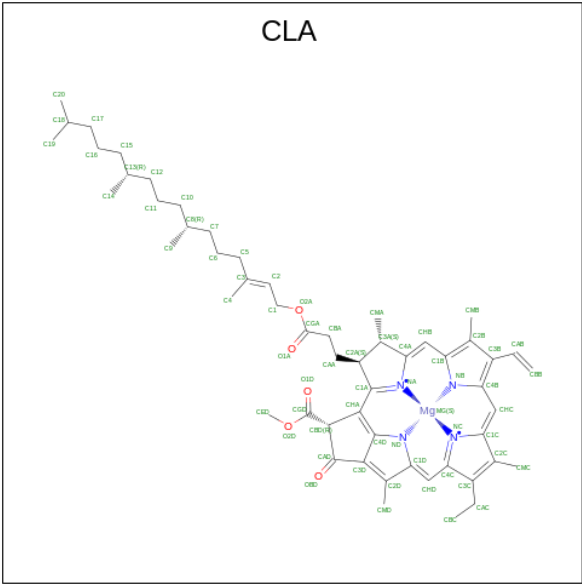
- Molecule 14 is a protein called PsaM.

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

- Molecule 15 is a protein called PsaO.

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

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



Mol	Chain	Residues	Atoms					AltConf
16	1	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
16	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	1	1	Total 41	C 33	Mg 1	N 4	O 3	0
16	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	2	1	Total 42	C 34	Mg 1	N 4	O 3	0
16	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
16	2	1	Total 42	C 34	Mg 1	N 4	O 3	0
16	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	3	1	Total 63	C 53	Mg 1	N 4	O 5	0
16	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	3	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	3	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
16	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
16	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
16	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	3	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	A	1	Total 62	C 52	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
16	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
16	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	A	1	Total 51	C 41	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 43	C 35	Mg 1	N 4	O 3	0
16	A	1	Total 61	C 51	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
16	B	1	Total 55	C 45	Mg 1	N 4	O 5	0

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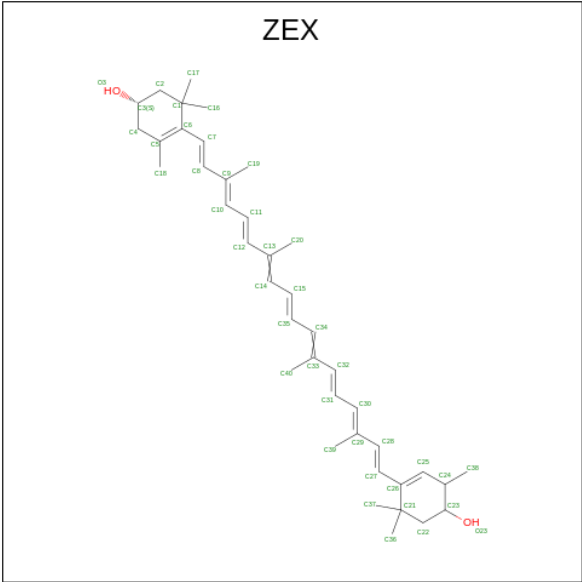
Mol	Chain	Residues	Atoms					AltConf
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
16	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
16	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
16	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	F	1	Total 41	C 33	Mg 1	N 4	O 3	0
16	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
16	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	K	1	Total 42	C 34	Mg 1	N 4	O 3	0
16	L	1	Total 56	C 46	Mg 1	N 4	O 5	0
16	L	1	Total 57	C 47	Mg 1	N 4	O 5	0
16	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	O	1	Total 52	C 42	Mg 1	N 4	O 5	0
16	O	1	Total 41	C 33	Mg 1	N 4	O 3	0
16	O	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	O	1	Total 45	C 35	Mg 1	N 4	O 5	0

- Molecule 17 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).



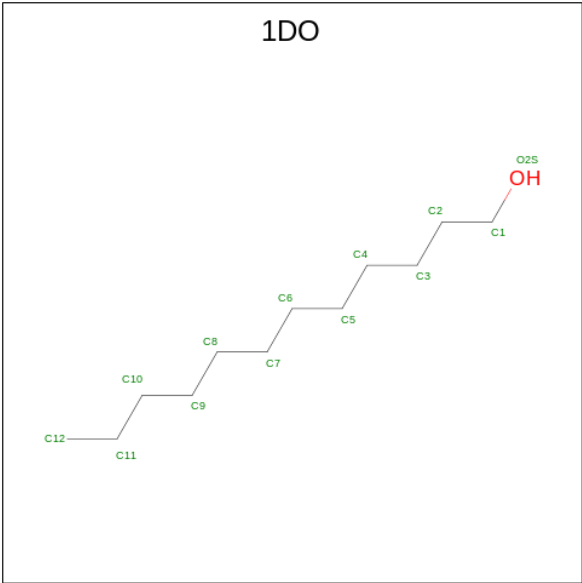
Mol	Chain	Residues	Atoms			AltConf
17	1	1	Total	C	O	0
			42	40	2	
			Total	C	O	
			42	40	2	
			Total	C	O	
17	2	1	Total	C	O	0
			42	40	2	
			Total	C	O	
			42	40	2	
			Total	C	O	
17	3	1	Total	C	O	0
			42	40	2	
			Total	C	O	
			42	40	2	
			Total	C	O	

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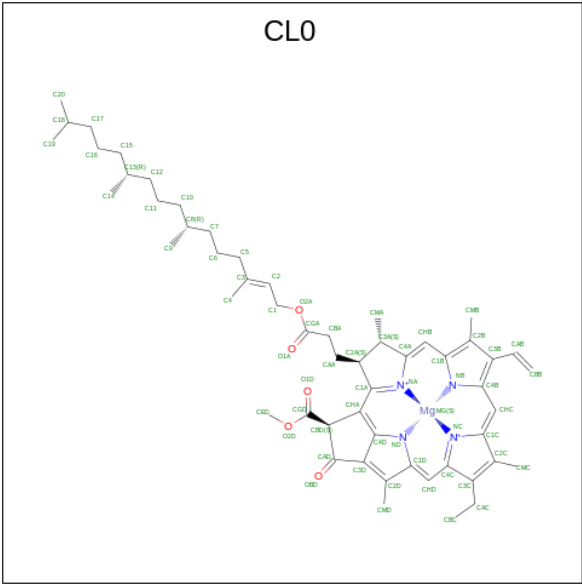
Mol	Chain	Residues	Atoms			AltConf
17	3	1	Total	C	O	0
			42	40	2	

- Molecule 18 is 1-DODECANOL (three-letter code: 1DO) (formula: C₁₂H₂₆O).



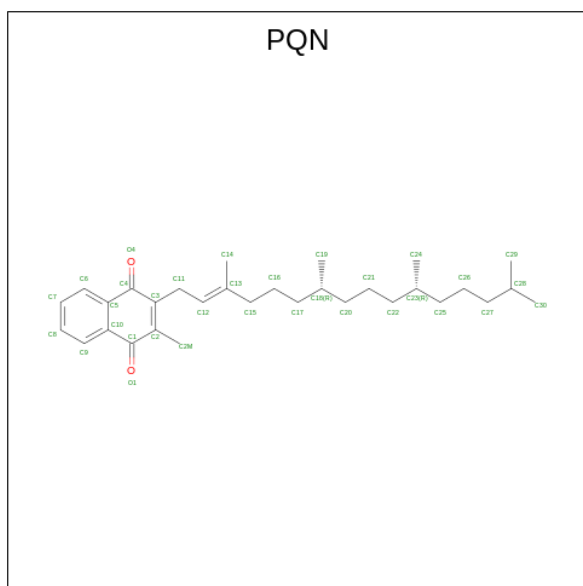
Mol	Chain	Residues	Atoms			AltConf
18	3	1	Total	C	O	0
			13	12	1	

- Molecule 19 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C₅₅H₇₂MgN₄O₅).



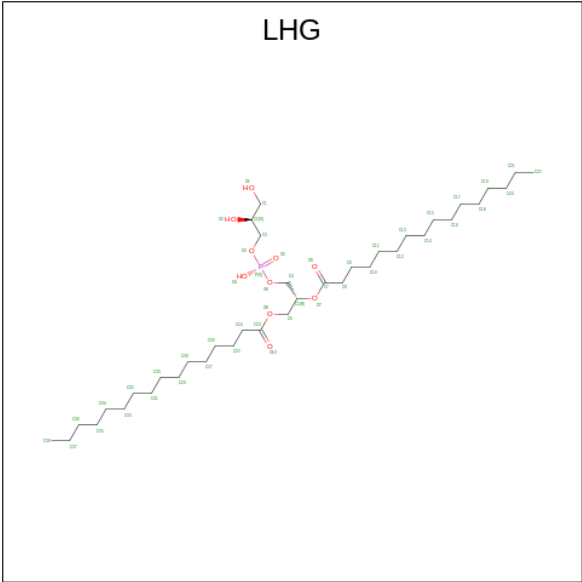
Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 20 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



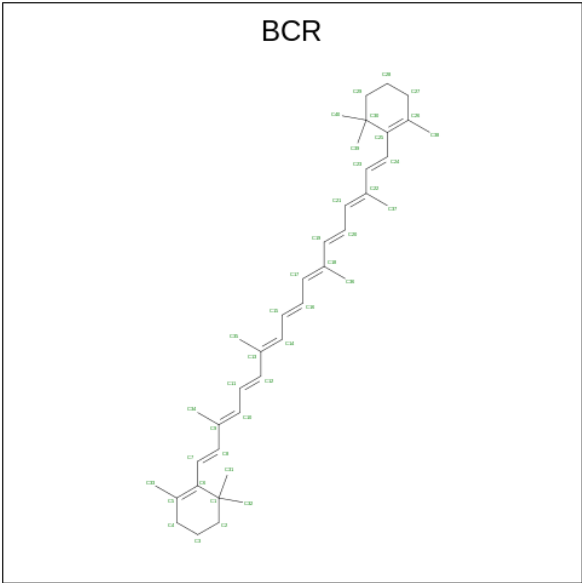
Mol	Chain	Residues	Atoms			AltConf
20	A	1	Total	C	O	0
			33	31	2	
20	B	1	Total	C	O	0
			33	31	2	

- Molecule 21 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



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

- Molecule 22 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



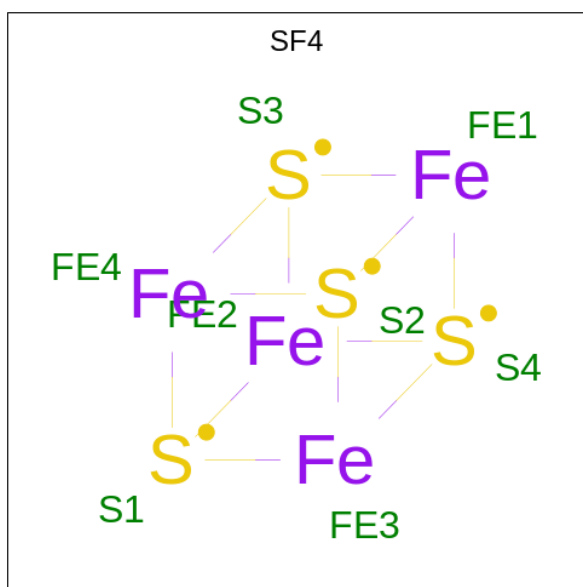
Mol	Chain	Residues	Atoms		AltConf
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	

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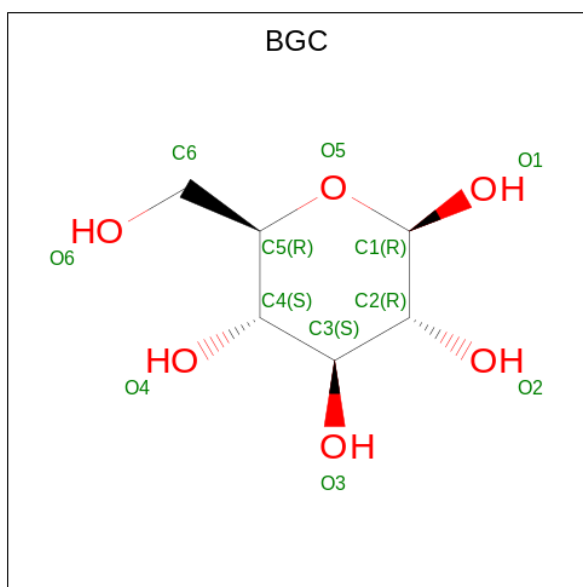
Mol	Chain	Residues	Atoms	AltConf
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	F	1	Total C 40 40	0
22	F	1	Total C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

- Molecule 23 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



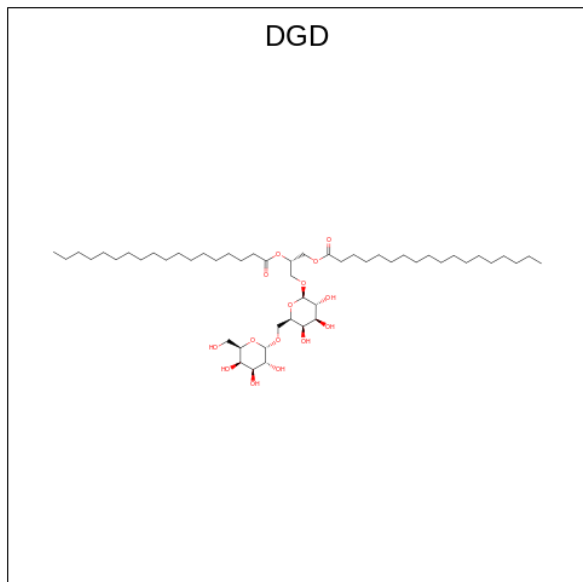
Mol	Chain	Residues	Atoms			AltConf
23	A	1	Total	Fe	S	0
			8	4	4	
23	C	1	Total	Fe	S	0
			8	4	4	
23	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 24 is beta-D-glucopyranose (three-letter code: BGC) (formula: C₆H₁₂O₆).



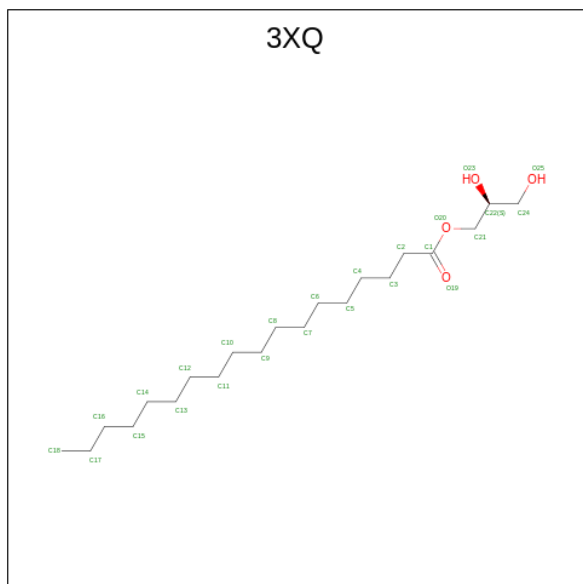
Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total	C	O	0
			11	6	5	

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

- Molecule 26 is (2S)-2,3-dihydroxypropyl octadecanoate (three-letter code: 3XQ) (formula: $C_{21}H_{42}O_4$).

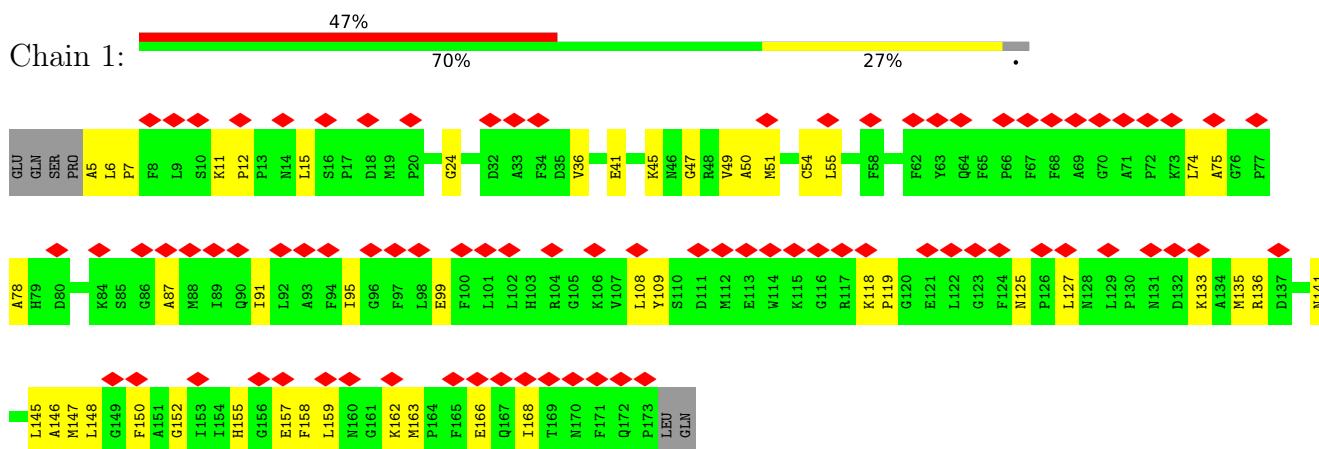


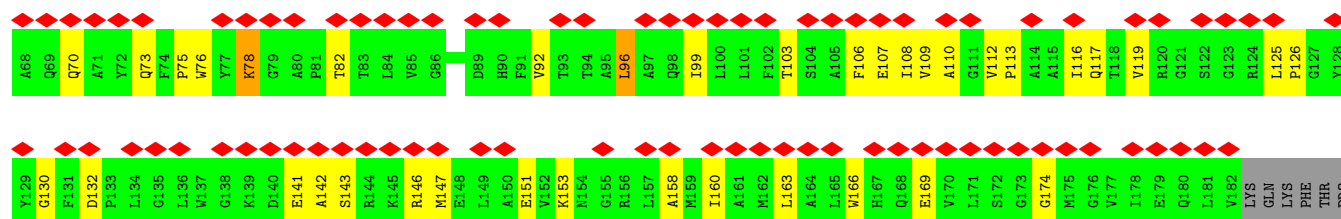
Mol	Chain	Residues	Atoms			AltConf
26	J	1	Total	C	O	0
			25	21	4	

3 Residue-property plots

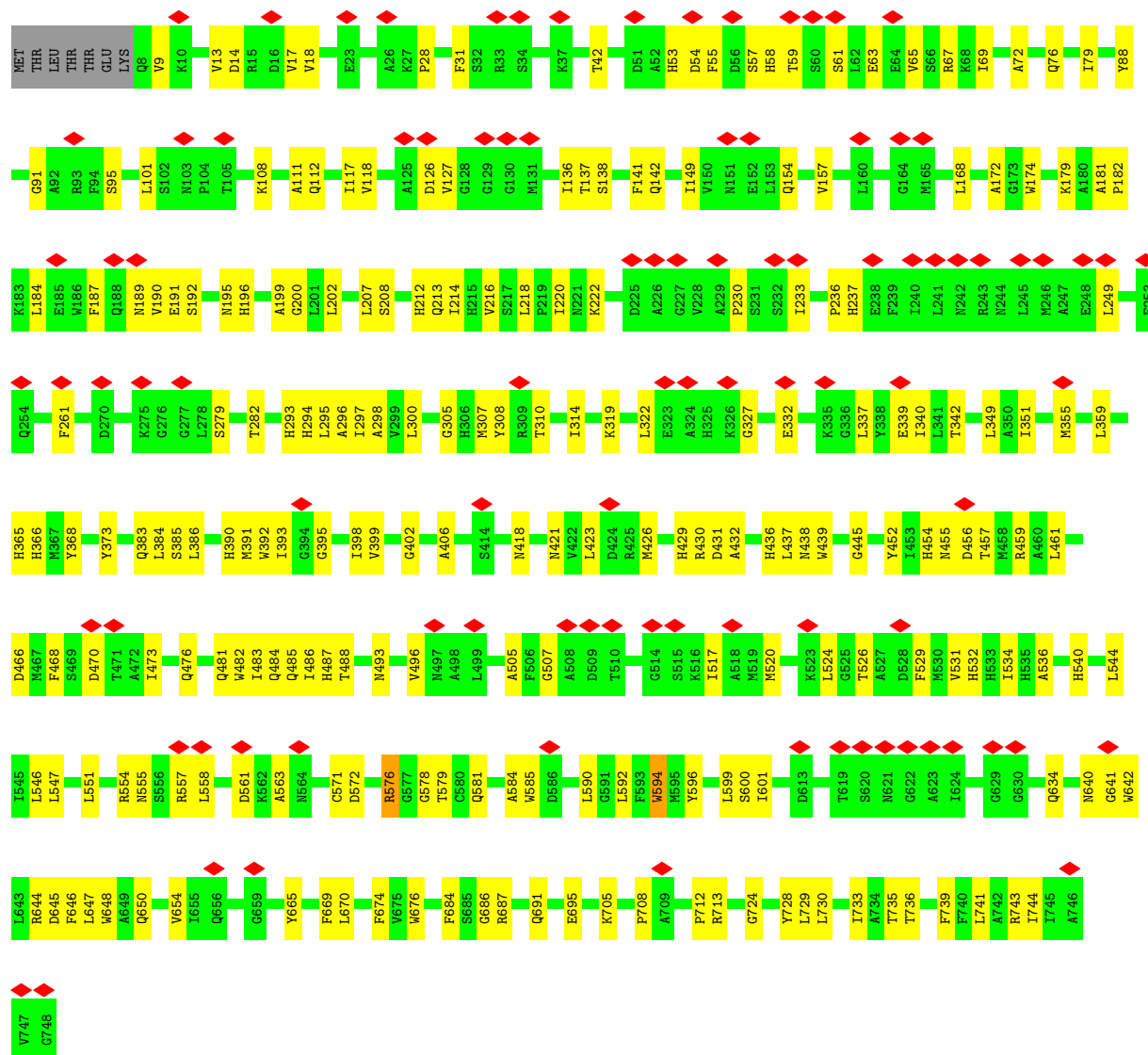
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Lhcr1

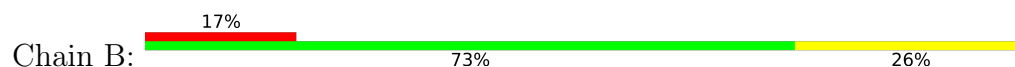


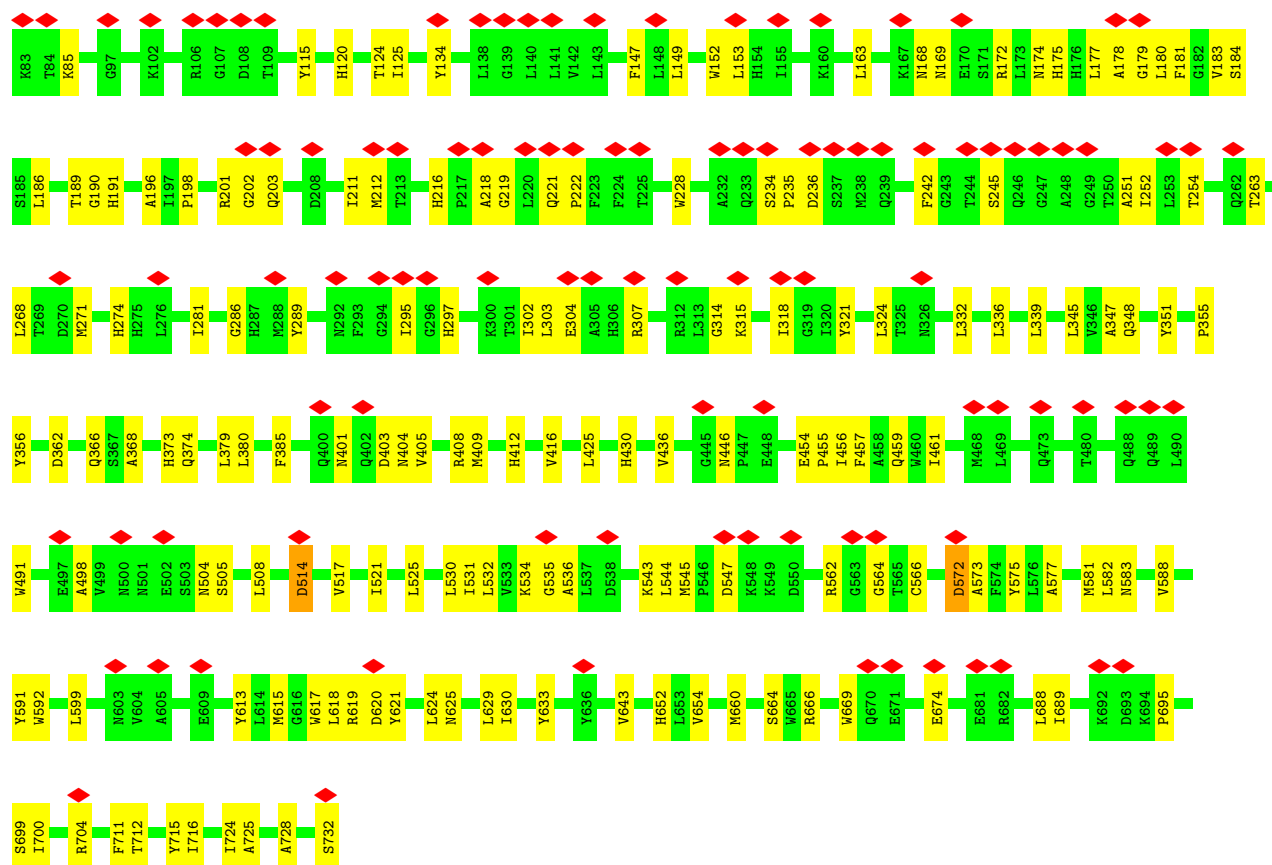


• Molecule 4: PsaA

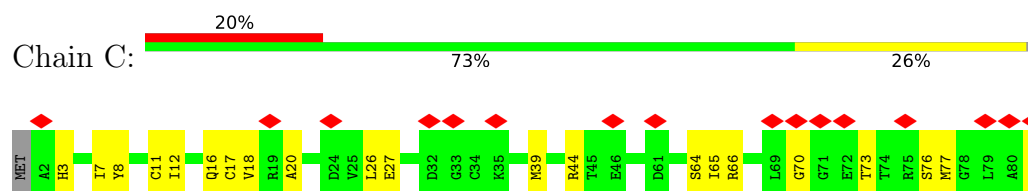


• Molecule 5: PsaB

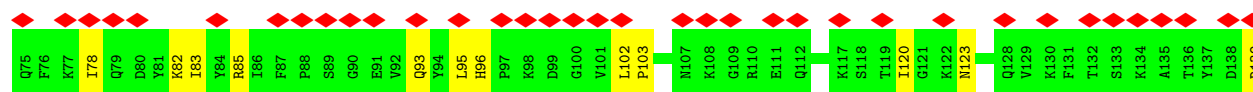
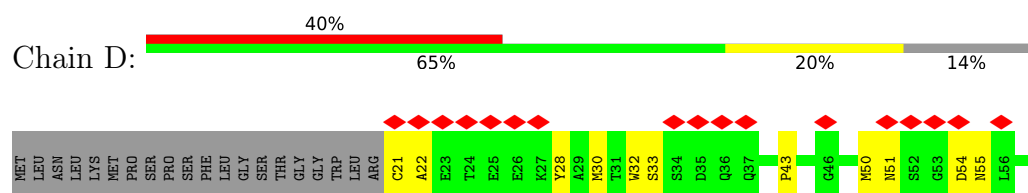




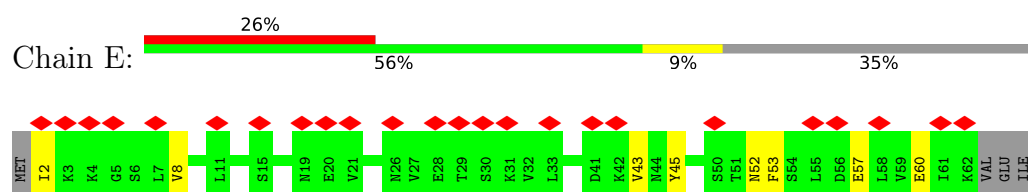
- Molecule 6: PsaC



- Molecule 7: PsaD



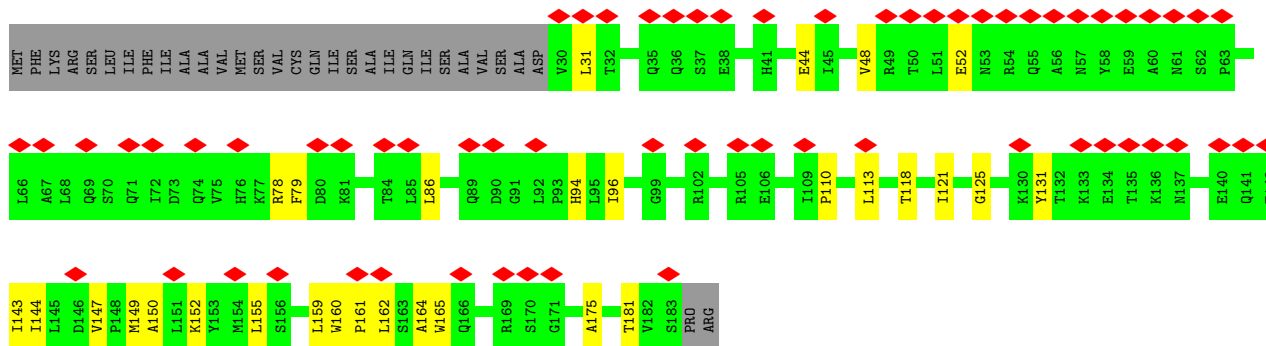
- Molecule 8: PsaE



PRO VAL LYS SER GLU VAL LYS ALA GLU LYS LYS ASN LYS LYS GLY GLY ALA

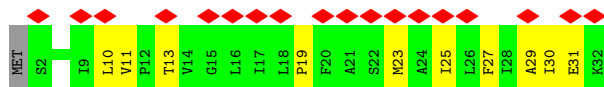
• Molecule 9: PsaF

Chain F: 



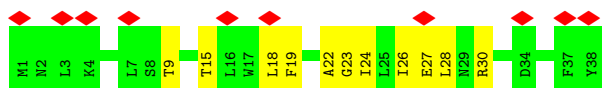
• Molecule 10: PsaI

Chain I: 



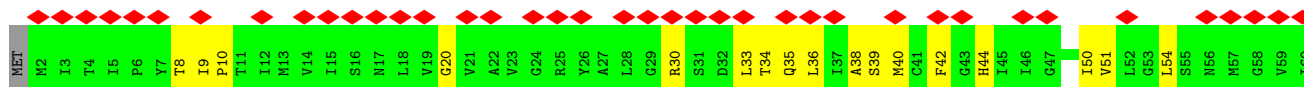
• Molecule 11: PsaJ

Chain J: 



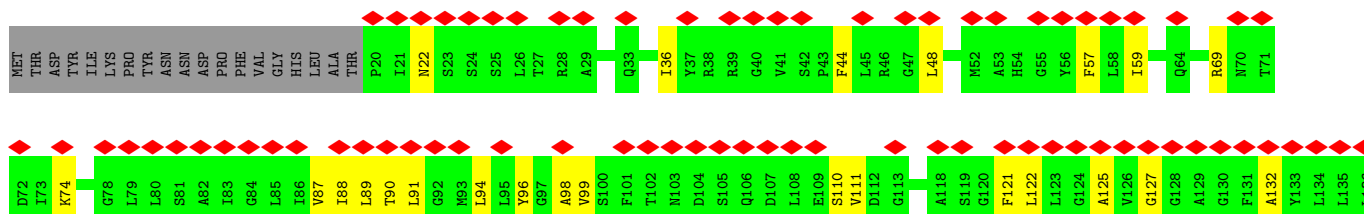
• Molecule 12: PsaK

Chain K: 



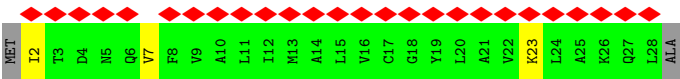
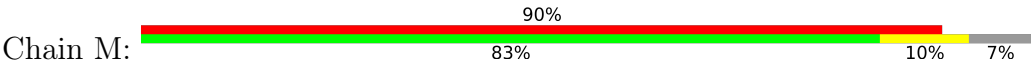
• Molecule 13: PsaL

Chain L: 

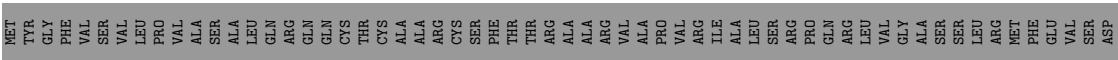
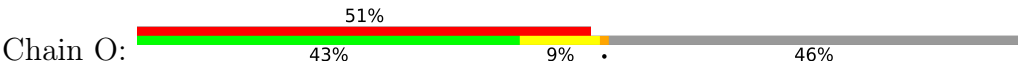




• Molecule 14: PsaM



• Molecule 15: PsaO



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76079	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	0.584	Depositor
Minimum map value	-0.161	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.087	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: BCR, 1DO, DGD, BGC, SF4, CL0, 3XQ, PQN, CLA, LHG, ZEX

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.39	0/1395	0.69	1/1884 (0.1%)
2	2	0.39	0/1407	0.67	0/1898
3	3	0.38	0/1337	0.67	1/1817 (0.1%)
4	A	0.53	1/5985 (0.0%)	0.62	1/8158 (0.0%)
5	B	0.49	0/6028	0.63	3/8236 (0.0%)
6	C	0.46	0/607	0.58	0/822
7	D	0.34	0/969	0.58	0/1307
8	E	0.44	0/502	0.55	0/680
9	F	0.38	0/1296	0.59	0/1760
10	I	0.35	0/235	0.70	0/321
11	J	0.41	0/321	0.63	0/437
12	K	0.32	0/433	0.62	0/588
13	L	0.32	0/919	0.57	0/1247
14	M	0.27	0/205	0.57	0/277
15	O	0.35	0/664	0.67	1/913 (0.1%)
All	All	0.45	1/22303 (0.0%)	0.63	7/30345 (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
2	2	0	1
5	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	594	TRP	CB-CG	-6.00	1.39	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	571	CYS	CA-CB-SG	-6.63	102.06	114.00
5	B	572	ASP	CB-CG-OD1	6.63	124.27	118.30
5	B	514	ASP	CB-CG-OD1	5.68	123.41	118.30
3	3	96	LEU	CA-CB-CG	5.63	128.25	115.30
1	1	159	LEU	CA-CB-CG	5.57	128.12	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	135	PRO	Peptide
5	B	430	HIS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1351	0	1322	34	0
2	2	1371	0	1362	34	0
3	3	1303	0	1305	46	0
4	A	5798	0	5727	196	0
5	B	5819	0	5648	173	0
6	C	597	0	584	19	0
7	D	950	0	944	24	0
8	E	493	0	509	7	0
9	F	1263	0	1236	24	0
10	I	230	0	253	12	0
11	J	312	0	327	13	0
12	K	428	0	464	15	0
13	L	900	0	931	19	0
14	M	204	0	226	3	0
15	O	641	0	650	9	0
16	1	565	0	443	15	0
16	2	600	0	466	19	0
16	3	565	0	440	18	0
16	A	2423	0	2452	140	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	B	2484	0	2521	172	0
16	F	86	0	62	4	0
16	J	42	0	31	2	0
16	K	87	0	64	4	0
16	L	228	0	215	4	0
16	O	188	0	144	3	0
17	1	210	0	280	19	0
17	2	168	0	224	12	0
17	3	252	0	336	25	0
18	3	13	0	25	0	0
19	A	65	0	71	56	0
20	A	33	0	46	2	0
20	B	33	0	46	5	0
21	A	89	0	127	4	0
22	A	240	0	336	16	0
22	B	240	0	336	21	0
22	F	80	0	112	4	0
22	I	40	0	56	2	0
22	J	80	0	112	7	0
22	K	40	0	56	5	0
22	L	120	0	168	11	0
23	A	8	0	0	0	0
23	C	16	0	0	1	0
24	A	11	0	9	0	0
25	B	66	0	96	4	0
26	J	25	0	0	0	0
All	All	30757	0	30762	859	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 14.

The worst 5 of 859 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)
19:A:801:CL0:C19	16:B:802:CLA:HMB3	1.45	1.42
19:A:801:CL0:H66	16:B:802:CLA:CMB	1.58	1.33
4:A:642:TRP:CD1	19:A:801:CL0:H50	1.63	1.32
19:A:801:CL0:C19	16:B:802:CLA:CMB	2.13	1.26
5:B:4:LYS:HB2	5:B:13:ALA:HB1	1.25	1.11

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	167/175 (95%)	129 (77%)	37 (22%)	1 (1%)	22	57
2	2	173/199 (87%)	134 (78%)	39 (22%)	0	100	100
3	3	168/188 (89%)	141 (84%)	27 (16%)	0	100	100
4	A	739/748 (99%)	686 (93%)	52 (7%)	1 (0%)	48	80
5	B	729/732 (100%)	663 (91%)	65 (9%)	1 (0%)	48	80
6	C	78/81 (96%)	67 (86%)	11 (14%)	0	100	100
7	D	117/139 (84%)	103 (88%)	14 (12%)	0	100	100
8	E	59/94 (63%)	53 (90%)	6 (10%)	0	100	100
9	F	152/185 (82%)	136 (90%)	16 (10%)	0	100	100
10	I	29/32 (91%)	28 (97%)	1 (3%)	0	100	100
11	J	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
12	K	57/60 (95%)	49 (86%)	8 (14%)	0	100	100
13	L	117/140 (84%)	107 (92%)	10 (8%)	0	100	100
14	M	25/29 (86%)	23 (92%)	2 (8%)	0	100	100
15	O	81/155 (52%)	67 (83%)	14 (17%)	0	100	100
All	All	2727/2995 (91%)	2421 (89%)	303 (11%)	3 (0%)	50	80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	12	PRO
5	B	7	LYS
4	A	526	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	139/145 (96%)	138 (99%)	1 (1%)	81	86
2	2	142/160 (89%)	141 (99%)	1 (1%)	81	86
3	3	132/148 (89%)	131 (99%)	1 (1%)	79	85
4	A	598/605 (99%)	595 (100%)	3 (0%)	86	90
5	B	598/599 (100%)	596 (100%)	2 (0%)	91	93
6	C	66/67 (98%)	66 (100%)	0	100	100
7	D	101/118 (86%)	101 (100%)	0	100	100
8	E	58/87 (67%)	58 (100%)	0	100	100
9	F	136/162 (84%)	136 (100%)	0	100	100
10	I	26/27 (96%)	26 (100%)	0	100	100
11	J	34/34 (100%)	34 (100%)	0	100	100
12	K	48/49 (98%)	48 (100%)	0	100	100
13	L	94/113 (83%)	93 (99%)	1 (1%)	70	79
14	M	22/23 (96%)	22 (100%)	0	100	100
15	O	64/121 (53%)	63 (98%)	1 (2%)	58	73
All	All	2258/2458 (92%)	2248 (100%)	10 (0%)	88	92

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	B	4	LYS
13	L	22	ASN
15	O	82	ARG
4	A	69	ILE
4	A	438	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
5	B	374	GLN
8	E	52	ASN
13	L	22	ASN
12	K	44	HIS
4	A	320	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

181 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$
22	BCR	A	849	-	41,41,41	1.19	2 (4%)	56,56,56	1.36	8 (14%)
16	CLA	B	818	-	55,63,73	1.53	8 (14%)	64,101,113	1.60	9 (14%)
16	CLA	1	608	-	60,68,73	1.50	9 (15%)	70,107,113	1.57	9 (12%)
16	CLA	B	835	-	65,73,73	1.42	10 (15%)	76,113,113	1.52	9 (11%)
16	CLA	3	205	-	45,53,73	1.76	9 (20%)	52,89,113	1.77	10 (19%)
22	BCR	I	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.34	7 (12%)
22	BCR	B	844	-	41,41,41	1.05	2 (4%)	56,56,56	1.26	8 (14%)
16	CLA	B	840	-	65,73,73	1.45	10 (15%)	76,113,113	1.53	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	ZEX	1	617	-	42,43,43	4.93	19 (45%)	55,60,60	5.31	27 (49%)
16	CLA	B	830	-	65,73,73	1.50	9 (13%)	76,113,113	1.52	10 (13%)
16	CLA	O	201	-	52,60,73	1.62	8 (15%)	60,97,113	1.63	9 (15%)
16	CLA	O	202	-	41,49,73	1.84	6 (14%)	47,84,113	1.79	9 (19%)
23	SF4	C	102	-	0,12,12	-	-	-	-	-
16	CLA	1	609	-	41,49,73	1.76	7 (17%)	47,84,113	1.85	8 (17%)
16	CLA	2	604	-	42,50,73	1.70	10 (23%)	48,85,113	1.81	8 (16%)
16	CLA	A	818	-	65,73,73	1.48	11 (16%)	76,113,113	1.58	11 (14%)
16	CLA	A	819	-	45,53,73	1.73	9 (20%)	52,89,113	1.74	7 (13%)
16	CLA	B	836	-	45,53,73	1.78	10 (22%)	52,89,113	1.67	7 (13%)
16	CLA	1	606	-	45,53,73	1.73	10 (22%)	52,89,113	1.70	11 (21%)
16	CLA	B	811	-	65,73,73	1.45	11 (16%)	76,113,113	1.54	12 (15%)
16	CLA	B	833	-	65,73,73	1.51	9 (13%)	76,113,113	1.46	9 (11%)
16	CLA	2	608	-	50,58,73	1.62	9 (18%)	58,95,113	1.77	11 (18%)
16	CLA	A	814	-	42,50,73	1.73	8 (19%)	48,85,113	2.01	8 (16%)
22	BCR	K	103	-	41,41,41	1.14	2 (4%)	56,56,56	1.31	5 (8%)
16	CLA	3	210	-	41,49,73	1.81	6 (14%)	47,84,113	1.80	8 (17%)
16	CLA	B	832	-	45,53,73	1.74	10 (22%)	52,89,113	1.68	9 (17%)
17	ZEX	1	614	-	42,43,43	5.04	19 (45%)	55,60,60	5.49	29 (52%)
16	CLA	2	602	-	65,73,73	1.48	8 (12%)	76,113,113	1.52	7 (9%)
16	CLA	1	605	-	41,50,73	1.84	5 (12%)	46,85,113	1.72	8 (17%)
16	CLA	A	817	-	65,73,73	1.44	11 (16%)	76,113,113	1.53	11 (14%)
16	CLA	3	206	-	45,53,73	1.84	9 (20%)	52,89,113	1.87	12 (23%)
16	CLA	A	804	-	65,73,73	1.51	11 (16%)	76,113,113	1.67	11 (14%)
16	CLA	B	819	-	59,67,73	1.54	10 (16%)	68,105,113	1.60	10 (14%)
16	CLA	3	203	-	63,71,73	1.47	9 (14%)	73,110,113	1.58	9 (12%)
16	CLA	B	838	-	65,73,73	1.52	10 (15%)	76,113,113	1.51	9 (11%)
16	CLA	O	203	-	50,58,73	1.68	6 (12%)	58,95,113	1.59	9 (15%)
16	CLA	B	827	-	65,73,73	1.43	10 (15%)	76,113,113	1.52	11 (14%)
16	CLA	A	851	-	43,51,73	1.77	9 (20%)	49,86,113	1.81	8 (16%)
16	CLA	L	203	-	57,65,73	1.54	7 (12%)	66,103,113	1.54	8 (12%)
21	LHG	A	842	-	39,39,48	0.75	1 (2%)	42,45,54	1.30	6 (14%)
16	CLA	A	824	-	65,73,73	1.49	10 (15%)	76,113,113	1.55	13 (17%)
16	CLA	A	828	-	65,73,73	1.53	10 (15%)	76,113,113	1.58	13 (17%)
16	CLA	B	812	-	65,73,73	1.46	9 (13%)	76,113,113	1.49	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	1	607	-	45,53,73	1.71	8 (17%)	52,89,113	1.78	9 (17%)
16	CLA	L	205	-	50,58,73	1.64	9 (18%)	58,95,113	1.70	10 (17%)
22	BCR	A	846	-	41,41,41	1.27	2 (4%)	56,56,56	1.33	7 (12%)
16	CLA	B	820	-	60,68,73	1.47	11 (18%)	70,107,113	1.68	11 (15%)
19	CL0	A	801	-	65,73,73	2.87	20 (30%)	76,113,113	3.27	39 (51%)
16	CLA	1	612	-	45,53,73	1.73	7 (15%)	52,89,113	1.67	8 (15%)
16	CLA	B	826	-	65,73,73	1.49	10 (15%)	76,113,113	1.51	10 (13%)
16	CLA	A	823	-	55,63,73	1.55	10 (18%)	64,101,113	1.67	8 (12%)
16	CLA	1	603	-	45,53,73	1.76	10 (22%)	52,89,113	1.61	8 (15%)
16	CLA	1	601	-	48,56,73	1.68	9 (18%)	55,92,113	2.08	12 (21%)
16	CLA	1	610	-	45,53,73	1.76	9 (20%)	52,89,113	1.76	9 (17%)
16	CLA	B	829	-	65,73,73	1.42	10 (15%)	76,113,113	1.48	11 (14%)
26	3XQ	J	104	-	24,24,24	0.58	1 (4%)	25,25,25	1.12	1 (4%)
16	CLA	B	837	-	60,68,73	1.55	11 (18%)	70,107,113	1.63	13 (18%)
16	CLA	A	827	-	65,73,73	1.47	10 (15%)	76,113,113	1.63	11 (14%)
17	ZEX	2	617	-	42,43,43	4.87	19 (45%)	55,60,60	5.24	30 (54%)
22	BCR	B	848	-	41,41,41	1.20	2 (4%)	56,56,56	1.53	10 (17%)
16	CLA	B	823	-	46,54,73	1.70	8 (17%)	53,90,113	1.64	7 (13%)
24	BGC	A	853	18	11,11,12	1.60	3 (27%)	15,15,17	1.00	0
17	ZEX	2	614	-	42,43,43	4.96	19 (45%)	55,60,60	5.27	34 (61%)
16	CLA	A	835	-	51,59,73	1.56	9 (17%)	59,96,113	1.82	11 (18%)
20	PQN	B	843	-	34,34,34	2.79	10 (29%)	42,45,45	2.16	5 (11%)
16	CLA	B	813	-	54,62,73	1.66	7 (12%)	67,100,113	1.59	11 (16%)
16	CLA	A	834	-	45,53,73	1.76	9 (20%)	52,89,113	1.82	9 (17%)
16	CLA	B	807	-	65,73,73	1.43	10 (15%)	76,113,113	1.60	11 (14%)
17	ZEX	1	616	-	42,43,43	5.08	19 (45%)	55,60,60	5.13	28 (50%)
16	CLA	3	212	-	46,54,73	1.70	7 (15%)	53,90,113	1.65	7 (13%)
16	CLA	A	830	-	50,58,73	1.67	10 (20%)	58,95,113	1.52	10 (17%)
16	CLA	F	802	-	45,53,73	1.76	9 (20%)	52,89,113	1.72	11 (21%)
22	BCR	A	847	-	41,41,41	1.31	3 (7%)	56,56,56	1.29	7 (12%)
16	CLA	A	829	-	65,73,73	1.61	13 (20%)	76,113,113	1.84	22 (28%)
16	CLA	2	605	-	45,53,73	1.71	9 (20%)	52,89,113	1.86	9 (17%)
16	CLA	A	837	-	65,73,73	1.39	8 (12%)	76,113,113	1.52	9 (11%)
16	CLA	A	811	-	54,62,73	1.55	9 (16%)	62,99,113	1.56	9 (14%)
16	CLA	B	821	-	65,73,73	1.48	10 (15%)	76,113,113	1.45	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	A	833	-	65,73,73	1.44	9 (13%)	76,113,113	1.57	11 (14%)
16	CLA	B	809	-	65,73,73	1.42	10 (15%)	76,113,113	1.46	10 (13%)
16	CLA	B	808	-	65,73,73	1.48	11 (16%)	76,113,113	1.48	11 (14%)
16	CLA	A	813	-	45,53,73	1.66	8 (17%)	52,89,113	1.81	10 (19%)
16	CLA	B	822	-	45,53,73	1.75	10 (22%)	52,89,113	1.72	8 (15%)
23	SF4	A	848	-	0,12,12	-	-	-	-	-
16	CLA	B	810	-	65,73,73	1.44	10 (15%)	76,113,113	1.67	11 (14%)
22	BCR	J	102	-	41,41,41	1.23	4 (9%)	56,56,56	1.34	7 (12%)
16	CLA	A	852	-	61,69,73	1.45	11 (18%)	71,108,113	1.58	9 (12%)
16	CLA	A	831	-	65,73,73	1.44	10 (15%)	76,113,113	1.55	10 (13%)
21	LHG	A	841	-	48,48,48	0.69	1 (2%)	51,54,54	1.28	6 (11%)
16	CLA	B	831	-	65,73,73	1.51	10 (15%)	76,113,113	1.85	15 (19%)
16	CLA	B	842	-	65,73,73	1.43	7 (10%)	76,113,113	1.41	7 (9%)
23	SF4	C	101	-	0,12,12	-	-	-	-	-
16	CLA	O	204	-	45,53,73	1.76	7 (15%)	52,89,113	1.60	8 (15%)
16	CLA	3	211	-	42,50,73	1.76	6 (14%)	48,85,113	1.75	8 (16%)
16	CLA	A	809	-	55,63,73	1.57	9 (16%)	64,101,113	1.55	8 (12%)
16	CLA	J	101	-	42,50,73	1.75	10 (23%)	48,85,113	1.70	9 (18%)
17	ZEX	3	201	-	42,43,43	5.24	19 (45%)	55,60,60	5.24	28 (50%)
16	CLA	A	810	-	65,73,73	1.44	10 (15%)	76,113,113	1.57	11 (14%)
16	CLA	A	839	-	65,73,73	1.43	11 (16%)	76,113,113	1.61	9 (11%)
16	CLA	2	612	-	45,53,73	1.74	10 (22%)	52,89,113	1.70	8 (15%)
16	CLA	B	824	-	43,51,73	1.76	10 (23%)	49,86,113	1.70	8 (16%)
16	CLA	1	611	-	45,53,73	1.70	8 (17%)	52,89,113	1.73	8 (15%)
16	CLA	B	805	-	65,73,73	1.53	10 (15%)	76,113,113	1.87	14 (18%)
16	CLA	2	603	-	45,53,73	1.73	10 (22%)	52,89,113	1.71	8 (15%)
16	CLA	A	812	-	65,73,73	1.43	10 (15%)	76,113,113	1.54	10 (13%)
16	CLA	2	610	-	42,50,73	1.79	9 (21%)	48,85,113	1.77	8 (16%)
16	CLA	1	604	-	45,53,73	1.64	8 (17%)	52,89,113	1.86	8 (15%)
16	CLA	K	102	-	42,50,73	1.79	9 (21%)	48,85,113	1.75	7 (14%)
17	ZEX	2	616	-	42,43,43	5.14	20 (47%)	55,60,60	5.01	29 (52%)
16	CLA	3	213	-	51,59,73	1.64	7 (13%)	59,96,113	1.60	8 (13%)
16	CLA	L	204	-	65,73,73	1.42	10 (15%)	76,113,113	1.46	8 (10%)
22	BCR	L	207	-	41,41,41	1.09	2 (4%)	56,56,56	1.17	5 (8%)
17	ZEX	3	216	-	42,43,43	5.10	19 (45%)	55,60,60	5.10	30 (54%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	B	803	-	65,73,73	1.42	10 (15%)	76,113,113	1.59	11 (14%)
16	CLA	2	611	-	45,53,73	1.71	9 (20%)	52,89,113	1.85	10 (19%)
16	CLA	B	802	-	65,73,73	1.57	10 (15%)	76,113,113	1.60	17 (22%)
16	CLA	2	606	-	45,53,73	1.72	9 (20%)	52,89,113	1.69	9 (17%)
16	CLA	A	836	-	65,73,73	1.46	10 (15%)	76,113,113	1.58	11 (14%)
25	DGD	B	850	-	67,67,67	0.98	4 (5%)	81,81,81	1.51	13 (16%)
16	CLA	A	805	-	65,73,73	1.45	10 (15%)	76,113,113	1.66	10 (13%)
16	CLA	B	834	-	58,66,73	1.54	11 (18%)	67,104,113	1.59	10 (14%)
17	ZEX	3	217	-	42,43,43	5.10	19 (45%)	55,60,60	4.92	29 (52%)
22	BCR	J	103	-	41,41,41	1.27	3 (7%)	56,56,56	1.29	5 (8%)
17	ZEX	1	613	-	42,43,43	5.00	18 (42%)	55,60,60	5.30	32 (58%)
16	CLA	A	807	4	65,73,73	1.39	10 (15%)	76,113,113	1.53	10 (13%)
16	CLA	K	101	-	45,53,73	1.72	10 (22%)	52,89,113	1.72	7 (13%)
17	ZEX	2	615	-	42,43,43	4.82	18 (42%)	55,60,60	5.28	30 (54%)
17	ZEX	3	218	-	42,43,43	5.46	20 (47%)	55,60,60	4.43	32 (58%)
20	PQN	A	840	-	34,34,34	2.79	10 (29%)	42,45,45	2.16	6 (14%)
22	BCR	F	801	-	41,41,41	1.26	3 (7%)	56,56,56	1.47	8 (14%)
16	CLA	A	820	-	65,73,73	1.49	10 (15%)	76,113,113	1.60	9 (11%)
22	BCR	B	846	-	41,41,41	1.11	2 (4%)	56,56,56	1.31	8 (14%)
16	CLA	A	850	-	65,73,73	1.48	11 (16%)	76,113,113	2.15	17 (22%)
22	BCR	L	202	-	41,41,41	1.24	2 (4%)	56,56,56	1.34	6 (10%)
16	CLA	B	816	-	45,53,73	1.70	9 (20%)	52,89,113	1.69	8 (15%)
22	BCR	B	845	-	41,41,41	1.11	2 (4%)	56,56,56	1.26	6 (10%)
16	CLA	A	821	-	49,57,73	1.62	9 (18%)	55,93,113	1.72	9 (16%)
16	CLA	3	209	-	52,60,73	1.58	6 (11%)	60,97,113	1.70	8 (13%)
16	CLA	A	808	4	65,73,73	1.50	10 (15%)	76,113,113	1.63	12 (15%)
16	CLA	A	822	-	51,59,73	1.67	9 (17%)	59,96,113	1.57	7 (11%)
16	CLA	2	607	-	45,53,73	1.72	10 (22%)	52,89,113	1.61	11 (21%)
22	BCR	A	844	-	41,41,41	1.18	2 (4%)	56,56,56	1.43	9 (16%)
16	CLA	3	207	-	45,53,73	1.73	9 (20%)	52,89,113	1.71	7 (13%)
16	CLA	B	801	-	65,73,73	1.46	12 (18%)	76,113,113	2.01	15 (19%)
16	CLA	F	803	-	41,49,73	1.80	8 (19%)	47,84,113	1.76	7 (14%)
16	CLA	B	815	-	65,73,73	1.42	10 (15%)	76,113,113	1.53	11 (14%)
22	BCR	F	804	-	41,41,41	1.13	2 (4%)	56,56,56	1.41	11 (19%)
16	CLA	B	828	-	65,73,73	1.47	10 (15%)	76,113,113	1.49	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	A	826	-	65,73,73	1.45	10 (15%)	76,113,113	1.56	10 (13%)
16	CLA	2	613	-	45,53,73	1.75	7 (15%)	52,89,113	1.68	7 (13%)
16	CLA	A	816	-	62,70,73	1.47	10 (16%)	72,109,113	1.53	9 (12%)
22	BCR	B	847	-	41,41,41	1.15	2 (4%)	56,56,56	1.32	7 (12%)
22	BCR	A	845	-	41,41,41	1.27	3 (7%)	56,56,56	1.43	8 (14%)
22	BCR	A	843	-	41,41,41	1.15	2 (4%)	56,56,56	1.30	6 (10%)
16	CLA	B	825	-	55,63,73	1.59	10 (18%)	64,101,113	1.53	9 (14%)
16	CLA	B	806	-	45,53,73	1.72	9 (20%)	52,89,113	1.80	8 (15%)
16	CLA	B	817	-	42,50,73	1.77	9 (21%)	48,85,113	1.75	8 (16%)
16	CLA	A	832	-	65,73,73	1.42	11 (16%)	76,113,113	1.64	12 (15%)
16	CLA	B	839	-	47,55,73	1.64	9 (19%)	54,91,113	1.73	9 (16%)
17	ZEX	3	215	-	42,43,43	5.04	19 (45%)	55,60,60	5.26	30 (54%)
17	ZEX	3	214	-	42,43,43	5.09	19 (45%)	55,60,60	5.14	32 (58%)
16	CLA	A	815	-	45,53,73	1.72	9 (20%)	52,89,113	1.84	10 (19%)
17	ZEX	1	615	-	42,43,43	5.00	19 (45%)	55,60,60	5.04	29 (52%)
16	CLA	2	609	-	41,49,73	1.76	6 (14%)	47,84,113	1.87	7 (14%)
16	CLA	3	202	-	45,53,73	1.74	7 (15%)	52,89,113	1.72	10 (19%)
16	CLA	3	204	-	45,53,73	1.73	9 (20%)	52,89,113	1.76	8 (15%)
22	BCR	B	849	-	41,41,41	1.24	3 (7%)	56,56,56	1.51	9 (16%)
16	CLA	B	841	-	65,73,73	1.49	11 (16%)	76,113,113	1.49	7 (9%)
16	CLA	B	804	-	65,73,73	1.51	10 (15%)	76,113,113	1.61	14 (18%)
16	CLA	A	803	-	55,63,73	1.54	10 (18%)	64,101,113	1.77	9 (14%)
16	CLA	1	602	-	59,67,73	1.44	8 (13%)	68,105,113	1.63	7 (10%)
16	CLA	A	825	-	55,63,73	1.57	10 (18%)	64,101,113	1.70	11 (17%)
16	CLA	A	802	-	65,73,73	1.46	9 (13%)	76,113,113	1.65	9 (11%)
16	CLA	A	806	-	65,73,73	1.49	10 (15%)	76,113,113	1.69	15 (19%)
22	BCR	L	206	-	41,41,41	1.13	2 (4%)	56,56,56	1.49	10 (17%)
16	CLA	L	201	-	56,64,73	1.53	10 (17%)	65,102,113	1.52	7 (10%)
16	CLA	B	814	-	55,63,73	1.53	8 (14%)	64,101,113	1.72	7 (10%)
16	CLA	2	601	-	45,53,73	1.75	10 (22%)	52,89,113	1.79	9 (17%)
16	CLA	3	208	-	45,53,73	1.78	8 (17%)	52,89,113	1.64	8 (15%)
18	1DO	3	219	24	12,12,12	0.23	0	11,11,11	0.83	0
16	CLA	A	838	-	65,73,73	1.43	10 (15%)	76,113,113	1.56	9 (11%)

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
22	BCR	A	849	-	-	17/29/63/63	0/2/2/2
16	CLA	B	818	-	1/1/13/20	15/25/103/115	-
16	CLA	1	608	-	1/1/14/20	9/31/109/115	-
16	CLA	B	835	-	1/1/15/20	15/37/115/115	-
16	CLA	3	205	-	1/1/11/20	6/13/91/115	-
22	BCR	I	101	-	-	18/29/63/63	0/2/2/2
22	BCR	B	844	-	-	13/29/63/63	0/2/2/2
16	CLA	B	840	-	1/1/15/20	13/37/115/115	-
17	ZEX	1	617	-	-	17/29/67/67	0/2/2/2
16	CLA	B	830	-	1/1/15/20	15/37/115/115	-
16	CLA	O	201	-	1/1/12/20	8/22/100/115	-
16	CLA	O	202	-	1/1/10/20	3/8/86/115	-
23	SF4	C	102	-	-	-	0/6/5/5
16	CLA	1	609	-	1/1/10/20	0/8/86/115	-
16	CLA	2	604	-	1/1/10/20	4/10/88/115	-
16	CLA	A	818	-	1/1/15/20	15/37/115/115	-
16	CLA	A	819	-	1/1/11/20	9/13/91/115	-
16	CLA	B	836	-	1/1/11/20	9/13/91/115	-
16	CLA	1	606	-	1/1/11/20	6/13/91/115	-
16	CLA	B	811	-	1/1/15/20	13/37/115/115	-
16	CLA	B	833	-	1/1/15/20	21/37/115/115	-
16	CLA	2	608	-	1/1/12/20	8/19/97/115	-
16	CLA	A	814	-	1/1/10/20	5/10/88/115	-
22	BCR	K	103	-	-	18/29/63/63	0/2/2/2
16	CLA	3	210	-	1/1/10/20	4/8/86/115	-
16	CLA	B	832	-	1/1/11/20	4/13/91/115	-
17	ZEX	1	614	-	-	17/29/67/67	0/2/2/2
16	CLA	2	602	-	1/1/15/20	11/37/115/115	-
16	CLA	1	605	-	1/1/10/20	4/9/87/115	-
16	CLA	A	817	-	1/1/15/20	12/37/115/115	-
16	CLA	3	206	-	1/1/11/20	6/13/91/115	-
16	CLA	A	804	-	1/1/15/20	5/37/115/115	-
16	CLA	B	819	-	1/1/13/20	13/30/108/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	3	203	-	1/1/14/20	19/35/113/115	-
16	CLA	B	838	-	1/1/15/20	8/37/115/115	-
16	CLA	O	203	-	1/1/12/20	6/19/97/115	-
16	CLA	B	827	-	1/1/15/20	10/37/115/115	-
16	CLA	A	851	-	1/1/10/20	2/11/89/115	-
16	CLA	L	203	-	1/1/13/20	15/28/106/115	-
21	LHG	A	842	-	-	19/44/44/53	-
16	CLA	A	824	-	1/1/15/20	12/37/115/115	-
16	CLA	A	828	-	1/1/15/20	19/37/115/115	-
16	CLA	B	812	-	1/1/15/20	16/37/115/115	-
16	CLA	1	607	-	1/1/11/20	7/13/91/115	-
16	CLA	L	205	-	1/1/12/20	6/19/97/115	-
22	BCR	A	846	-	-	16/29/63/63	0/2/2/2
16	CLA	B	820	-	1/1/14/20	11/31/109/115	-
19	CL0	A	801	-	3/3/20/25	11/37/135/135	-
16	CLA	1	612	-	1/1/11/20	4/13/91/115	-
16	CLA	B	826	-	1/1/15/20	10/37/115/115	-
16	CLA	A	823	-	1/1/13/20	7/25/103/115	-
16	CLA	1	603	-	1/1/11/20	7/13/91/115	-
16	CLA	1	601	-	1/1/11/20	6/17/95/115	-
16	CLA	1	610	-	1/1/11/20	4/13/91/115	-
16	CLA	B	829	-	1/1/15/20	20/37/115/115	-
26	3XQ	J	104	-	-	14/24/24/24	-
16	CLA	B	837	-	1/1/14/20	16/31/109/115	-
16	CLA	A	827	-	1/1/15/20	12/37/115/115	-
17	ZEX	2	617	-	-	19/29/67/67	0/2/2/2
22	BCR	B	848	-	-	23/29/63/63	0/2/2/2
16	CLA	B	823	-	1/1/11/20	6/15/93/115	-
24	BGC	A	853	18	-	2/2/19/22	0/1/1/1
17	ZEX	2	614	-	-	17/29/67/67	0/2/2/2
16	CLA	A	835	-	1/1/12/20	9/21/99/115	-
20	PQN	B	843	-	-	7/23/43/43	0/2/2/2
16	CLA	B	813	-	1/1/13/20	6/25/101/115	-
16	CLA	A	834	-	1/1/11/20	6/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	B	807	-	1/1/15/20	14/37/115/115	-
17	ZEX	1	616	-	-	18/29/67/67	0/2/2/2
16	CLA	3	212	-	1/1/11/20	8/15/93/115	-
16	CLA	A	830	-	1/1/12/20	4/19/97/115	-
16	CLA	F	802	-	1/1/11/20	4/13/91/115	-
22	BCR	A	847	-	-	18/29/63/63	0/2/2/2
16	CLA	A	829	-	1/1/15/20	10/37/115/115	-
16	CLA	2	605	-	1/1/11/20	5/13/91/115	-
16	CLA	A	837	-	1/1/15/20	13/37/115/115	-
16	CLA	A	811	-	1/1/12/20	6/24/102/115	-
16	CLA	B	821	-	1/1/15/20	13/37/115/115	-
16	CLA	A	833	-	1/1/15/20	9/37/115/115	-
16	CLA	B	809	-	1/1/15/20	15/37/115/115	-
16	CLA	B	808	-	1/1/15/20	16/37/115/115	-
16	CLA	A	813	-	1/1/11/20	8/13/91/115	-
16	CLA	B	822	-	1/1/11/20	5/13/91/115	-
23	SF4	A	848	-	-	-	0/6/5/5
16	CLA	B	810	-	1/1/15/20	8/37/115/115	-
22	BCR	J	102	-	-	16/29/63/63	0/2/2/2
16	CLA	A	852	-	1/1/14/20	13/33/111/115	-
16	CLA	A	831	-	1/1/15/20	18/37/115/115	-
21	LHG	A	841	-	-	27/53/53/53	-
16	CLA	B	831	-	1/1/15/20	14/37/115/115	-
16	CLA	B	842	-	1/1/15/20	12/37/115/115	-
23	SF4	C	101	-	-	-	0/6/5/5
16	CLA	O	204	-	1/1/11/20	4/13/91/115	-
16	CLA	3	211	-	1/1/10/20	0/10/88/115	-
16	CLA	A	809	-	1/1/13/20	6/25/103/115	-
16	CLA	J	101	-	1/1/10/20	7/10/88/115	-
17	ZEX	3	201	-	-	18/29/67/67	0/2/2/2
16	CLA	A	810	-	1/1/15/20	16/37/115/115	-
16	CLA	A	839	-	1/1/15/20	21/37/115/115	-
16	CLA	2	612	-	1/1/11/20	7/13/91/115	-
16	CLA	B	824	-	1/1/10/20	4/11/89/115	-
16	CLA	1	611	-	1/1/11/20	8/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	B	805	-	1/1/15/20	17/37/115/115	-
16	CLA	2	603	-	1/1/11/20	4/13/91/115	-
16	CLA	A	812	-	1/1/15/20	9/37/115/115	-
16	CLA	2	610	-	1/1/10/20	6/10/88/115	-
16	CLA	1	604	-	1/1/11/20	7/13/91/115	-
16	CLA	K	102	-	1/1/10/20	3/10/88/115	-
17	ZEX	2	616	-	-	20/29/67/67	0/2/2/2
16	CLA	3	213	-	1/1/12/20	7/21/99/115	-
16	CLA	L	204	-	1/1/15/20	17/37/115/115	-
22	BCR	L	207	-	-	16/29/63/63	0/2/2/2
17	ZEX	3	216	-	-	15/29/67/67	0/2/2/2
16	CLA	B	803	-	1/1/15/20	16/37/115/115	-
16	CLA	2	611	-	1/1/11/20	6/13/91/115	-
16	CLA	B	802	-	1/1/15/20	11/37/115/115	-
16	CLA	2	606	-	1/1/11/20	5/13/91/115	-
16	CLA	A	836	-	1/1/15/20	15/37/115/115	-
25	DGD	B	850	-	-	31/55/95/95	0/2/2/2
16	CLA	A	805	-	1/1/15/20	18/37/115/115	-
16	CLA	B	834	-	1/1/13/20	8/29/107/115	-
17	ZEX	3	217	-	-	17/29/67/67	0/2/2/2
22	BCR	J	103	-	-	15/29/63/63	0/2/2/2
17	ZEX	1	613	-	-	18/29/67/67	0/2/2/2
16	CLA	A	807	4	1/1/15/20	13/37/115/115	-
16	CLA	K	101	-	1/1/11/20	4/13/91/115	-
17	ZEX	2	615	-	-	20/29/67/67	0/2/2/2
17	ZEX	3	218	-	-	17/29/67/67	0/2/2/2
20	PQN	A	840	-	-	9/23/43/43	0/2/2/2
22	BCR	F	801	-	-	17/29/63/63	0/2/2/2
16	CLA	A	820	-	1/1/15/20	15/37/115/115	-
22	BCR	B	846	-	-	20/29/63/63	0/2/2/2
16	CLA	A	850	-	1/1/15/20	11/37/115/115	-
22	BCR	L	202	-	-	20/29/63/63	0/2/2/2
16	CLA	B	816	-	1/1/11/20	4/13/91/115	-
22	BCR	B	845	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	A	821	-	1/1/11/20	6/18/96/115	-
16	CLA	3	209	-	1/1/12/20	6/22/100/115	-
16	CLA	A	808	4	1/1/15/20	19/37/115/115	-
16	CLA	A	822	-	1/1/12/20	11/21/99/115	-
16	CLA	2	607	-	1/1/11/20	7/13/91/115	-
22	BCR	A	844	-	-	17/29/63/63	0/2/2/2
16	CLA	3	207	-	1/1/11/20	4/13/91/115	-
16	CLA	B	801	-	1/1/15/20	15/37/115/115	-
16	CLA	F	803	-	1/1/10/20	3/8/86/115	-
16	CLA	B	815	-	1/1/15/20	21/37/115/115	-
22	BCR	F	804	-	-	19/29/63/63	0/2/2/2
16	CLA	B	828	-	1/1/15/20	12/37/115/115	-
16	CLA	A	826	-	1/1/15/20	10/37/115/115	-
16	CLA	2	613	-	1/1/11/20	1/13/91/115	-
16	CLA	A	816	-	1/1/14/20	11/34/112/115	-
22	BCR	B	847	-	-	18/29/63/63	0/2/2/2
22	BCR	A	845	-	-	18/29/63/63	0/2/2/2
22	BCR	A	843	-	-	13/29/63/63	0/2/2/2
16	CLA	B	825	-	1/1/13/20	10/25/103/115	-
16	CLA	B	806	-	1/1/11/20	7/13/91/115	-
16	CLA	B	817	-	1/1/10/20	4/10/88/115	-
16	CLA	A	832	-	1/1/15/20	13/37/115/115	-
16	CLA	B	839	-	1/1/11/20	2/16/94/115	-
17	ZEX	3	215	-	-	16/29/67/67	0/2/2/2
17	ZEX	3	214	-	-	15/29/67/67	0/2/2/2
16	CLA	A	815	-	1/1/11/20	6/13/91/115	-
17	ZEX	1	615	-	-	18/29/67/67	0/2/2/2
16	CLA	2	609	-	1/1/10/20	4/8/86/115	-
16	CLA	3	202	-	1/1/11/20	7/13/91/115	-
16	CLA	3	204	-	1/1/11/20	10/13/91/115	-
22	BCR	B	849	-	-	14/29/63/63	0/2/2/2
16	CLA	B	841	-	1/1/15/20	12/37/115/115	-
16	CLA	B	804	-	1/1/15/20	14/37/115/115	-
16	CLA	A	803	-	1/1/13/20	7/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	1	602	-	1/1/13/20	9/30/108/115	-
16	CLA	A	825	-	1/1/13/20	4/25/103/115	-
16	CLA	A	802	-	1/1/15/20	21/37/115/115	-
16	CLA	A	806	-	1/1/15/20	18/37/115/115	-
22	BCR	L	206	-	-	18/29/63/63	0/2/2/2
16	CLA	L	201	-	1/1/13/20	5/27/105/115	-
16	CLA	B	814	-	1/1/13/20	6/25/103/115	-
16	CLA	2	601	-	1/1/11/20	7/13/91/115	-
16	CLA	3	208	-	1/1/11/20	8/13/91/115	-
18	1DO	3	219	24	-	1/10/10/10	-
16	CLA	A	838	-	1/1/15/20	11/37/115/115	-

The worst 5 of 1611 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	218	ZEX	C14-C13	15.79	1.56	1.35
17	1	616	ZEX	C14-C13	14.77	1.55	1.35
17	3	201	ZEX	C14-C13	14.74	1.55	1.35
17	3	217	ZEX	C14-C13	14.51	1.55	1.35
17	2	616	ZEX	C14-C13	14.43	1.54	1.35

The worst 5 of 1960 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	614	ZEX	C31-C30-C29	-16.56	103.68	127.31
19	A	801	CL0	C4A-NA-C1A	14.24	113.11	106.71
17	1	617	ZEX	C31-C30-C29	-13.77	107.66	127.31
17	3	201	ZEX	C31-C30-C29	-13.19	108.48	127.31
17	1	615	ZEX	C18-C5-C6	-13.08	109.84	124.53

5 of 136 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	1	601	CLA	ND
16	1	602	CLA	ND
16	1	603	CLA	ND
16	1	604	CLA	ND
16	1	605	CLA	ND

5 of 1990 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	1	601	CLA	CBD-CGD-O2D-CED
16	1	602	CLA	CBD-CGD-O2D-CED
16	1	603	CLA	CBD-CGD-O2D-CED
16	1	604	CLA	C1A-C2A-CAA-CBA
16	1	604	CLA	CBD-CGD-O2D-CED

There are no ring outliers.

158 monomers are involved in 473 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	849	BCR	1	0
16	B	818	CLA	2	0
16	B	835	CLA	6	0
16	3	205	CLA	2	0
22	I	101	BCR	2	0
22	B	844	BCR	1	0
16	B	840	CLA	7	0
17	1	617	ZEX	2	0
16	B	830	CLA	4	0
16	O	201	CLA	1	0
23	C	102	SF4	1	0
16	1	609	CLA	2	0
16	2	604	CLA	1	0
16	A	818	CLA	8	0
16	A	819	CLA	3	0
16	B	836	CLA	2	0
16	1	606	CLA	1	0
16	B	811	CLA	8	0
16	B	833	CLA	9	0
16	2	608	CLA	1	0
16	A	814	CLA	1	0
22	K	103	BCR	5	0
16	3	210	CLA	1	0
16	B	832	CLA	6	0
17	1	614	ZEX	6	0
16	2	602	CLA	4	0
16	1	605	CLA	2	0
16	A	817	CLA	5	0
16	3	206	CLA	5	0
16	A	804	CLA	7	0
16	B	819	CLA	1	0
16	3	203	CLA	5	0
16	B	838	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	O	203	CLA	1	0
16	B	827	CLA	6	0
16	A	851	CLA	2	0
21	A	842	LHG	2	0
16	A	824	CLA	4	0
16	A	828	CLA	3	0
16	B	812	CLA	3	0
16	1	607	CLA	3	0
16	L	205	CLA	1	0
22	A	846	BCR	4	0
16	B	820	CLA	3	0
19	A	801	CL0	56	0
16	1	612	CLA	1	0
16	B	826	CLA	4	0
16	A	823	CLA	2	0
16	1	603	CLA	2	0
16	1	610	CLA	1	0
16	B	829	CLA	10	0
16	B	837	CLA	3	0
16	A	827	CLA	10	0
17	2	617	ZEX	4	0
22	B	848	BCR	5	0
16	B	823	CLA	2	0
17	2	614	ZEX	3	0
16	A	835	CLA	1	0
20	B	843	PQN	5	0
16	A	834	CLA	6	0
16	B	807	CLA	10	0
17	1	616	ZEX	2	0
16	3	212	CLA	1	0
16	A	830	CLA	1	0
16	F	802	CLA	3	0
22	A	847	BCR	4	0
16	A	829	CLA	7	0
16	2	605	CLA	1	0
16	A	837	CLA	2	0
16	B	821	CLA	3	0
16	A	833	CLA	5	0
16	B	809	CLA	3	0
16	B	808	CLA	5	0
16	B	810	CLA	5	0
22	J	102	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	852	CLA	3	0
16	A	831	CLA	9	0
21	A	841	LHG	2	0
16	B	831	CLA	5	0
16	B	842	CLA	4	0
16	O	204	CLA	1	0
16	A	809	CLA	3	0
16	J	101	CLA	2	0
17	3	201	ZEX	7	0
16	A	810	CLA	5	0
16	A	839	CLA	3	0
16	B	824	CLA	3	0
16	1	611	CLA	1	0
16	B	805	CLA	6	0
16	2	603	CLA	1	0
16	A	812	CLA	6	0
16	2	610	CLA	1	0
16	1	604	CLA	2	0
16	K	102	CLA	3	0
17	2	616	ZEX	1	0
16	L	204	CLA	2	0
22	L	207	BCR	1	0
17	3	216	ZEX	3	0
16	B	803	CLA	6	0
16	2	611	CLA	2	0
16	B	802	CLA	22	0
16	2	606	CLA	1	0
16	A	836	CLA	9	0
25	B	850	DGD	4	0
16	A	805	CLA	5	0
16	B	834	CLA	3	0
17	3	217	ZEX	2	0
22	J	103	BCR	5	0
17	1	613	ZEX	7	0
16	A	807	CLA	5	0
16	K	101	CLA	1	0
17	2	615	ZEX	4	0
17	3	218	ZEX	6	0
20	A	840	PQN	2	0
22	F	801	BCR	4	0
16	A	820	CLA	3	0
22	B	846	BCR	4	0

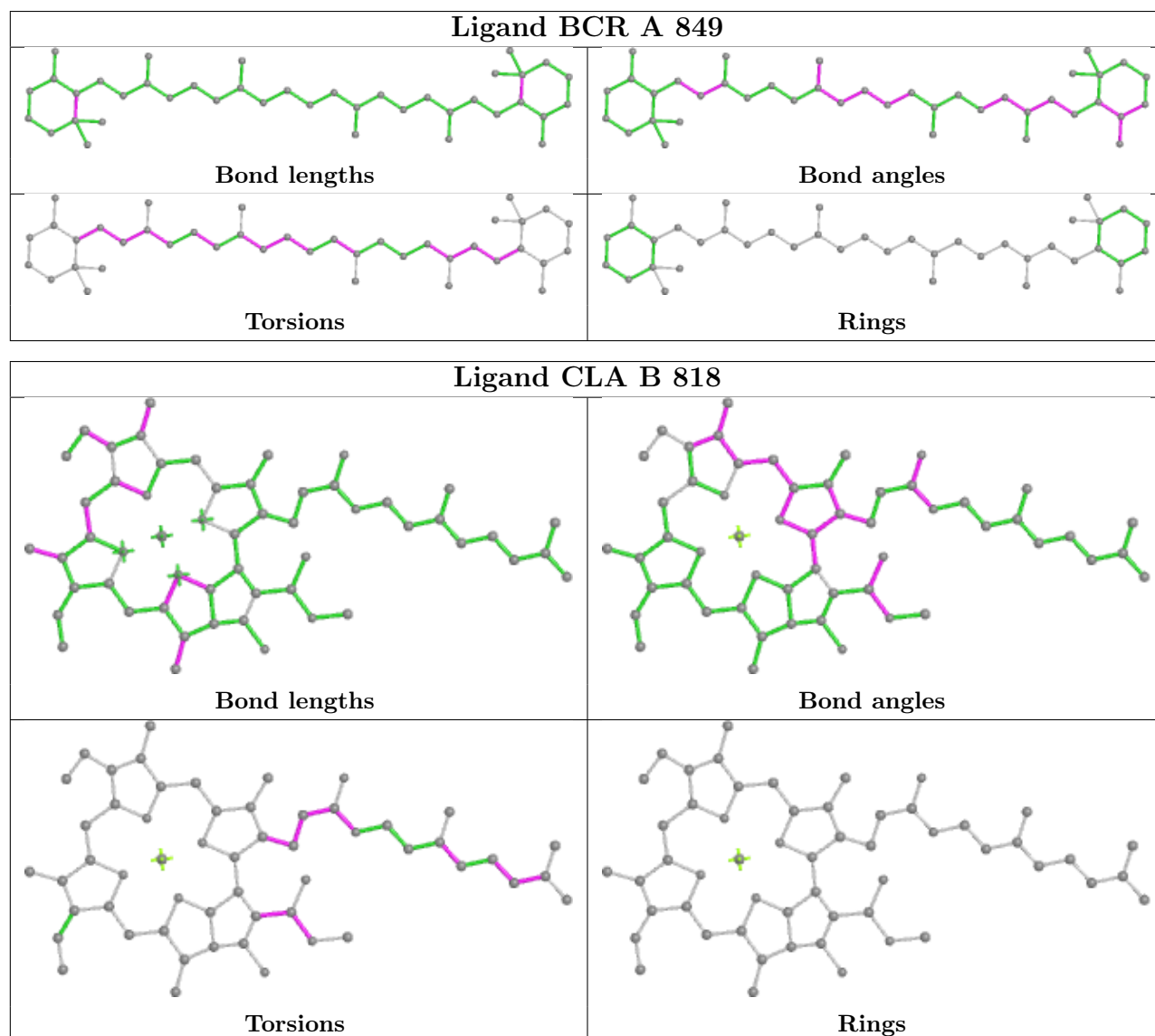
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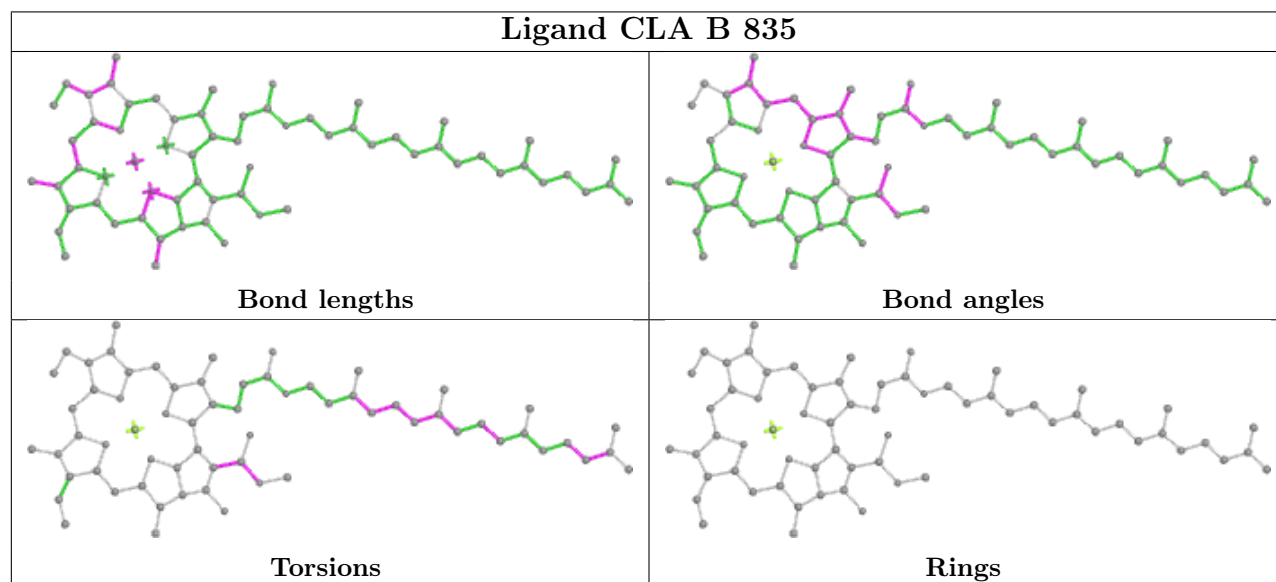
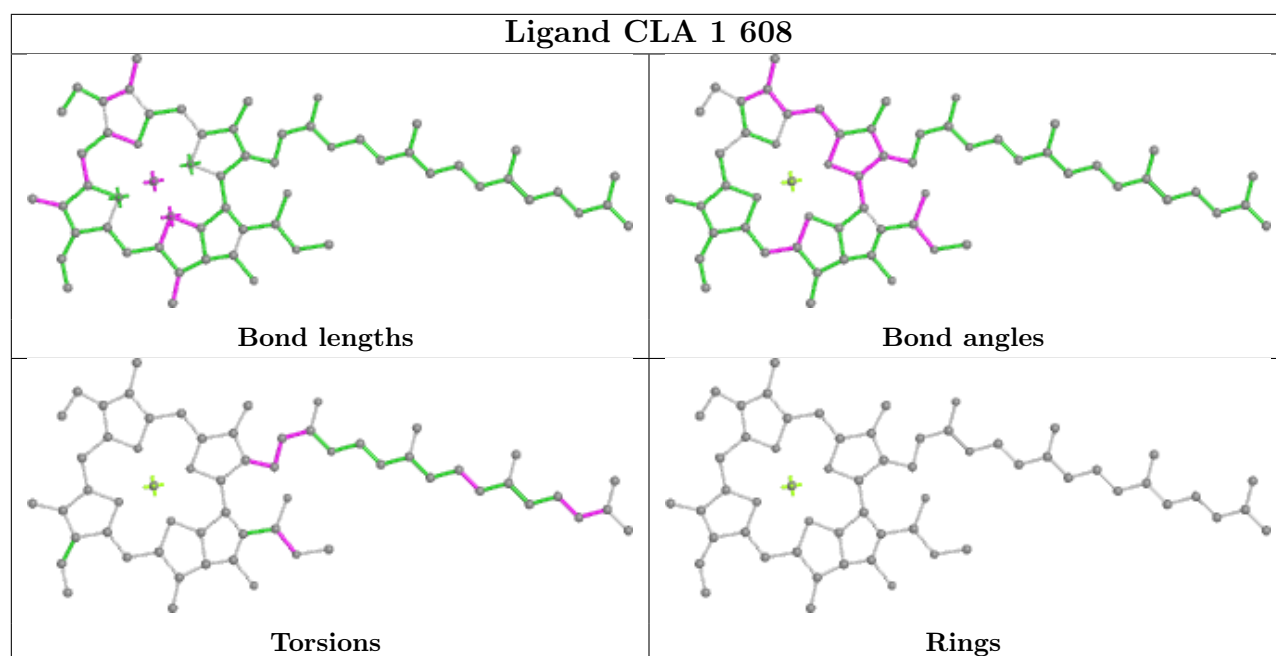
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	850	CLA	6	0
22	L	202	BCR	1	0
16	B	816	CLA	2	0
22	B	845	BCR	4	0
16	A	821	CLA	1	0
16	3	209	CLA	2	0
16	A	808	CLA	5	0
16	A	822	CLA	1	0
16	2	607	CLA	4	0
16	3	207	CLA	1	0
16	B	801	CLA	6	0
16	F	803	CLA	1	0
16	B	815	CLA	9	0
16	B	828	CLA	6	0
16	A	826	CLA	7	0
16	A	816	CLA	4	0
22	B	847	BCR	5	0
22	A	845	BCR	4	0
22	A	843	BCR	3	0
16	B	825	CLA	6	0
16	B	817	CLA	2	0
16	A	832	CLA	3	0
16	B	839	CLA	6	0
17	3	215	ZEX	5	0
17	3	214	ZEX	4	0
16	A	815	CLA	2	0
17	1	615	ZEX	2	0
16	3	204	CLA	1	0
22	B	849	BCR	3	0
16	B	841	CLA	9	0
16	B	804	CLA	10	0
16	A	803	CLA	2	0
16	1	602	CLA	1	0
16	A	825	CLA	4	0
16	A	802	CLA	9	0
16	A	806	CLA	2	0
22	L	206	BCR	9	0
16	L	201	CLA	1	0
16	2	601	CLA	4	0
16	3	208	CLA	1	0
16	A	838	CLA	4	0

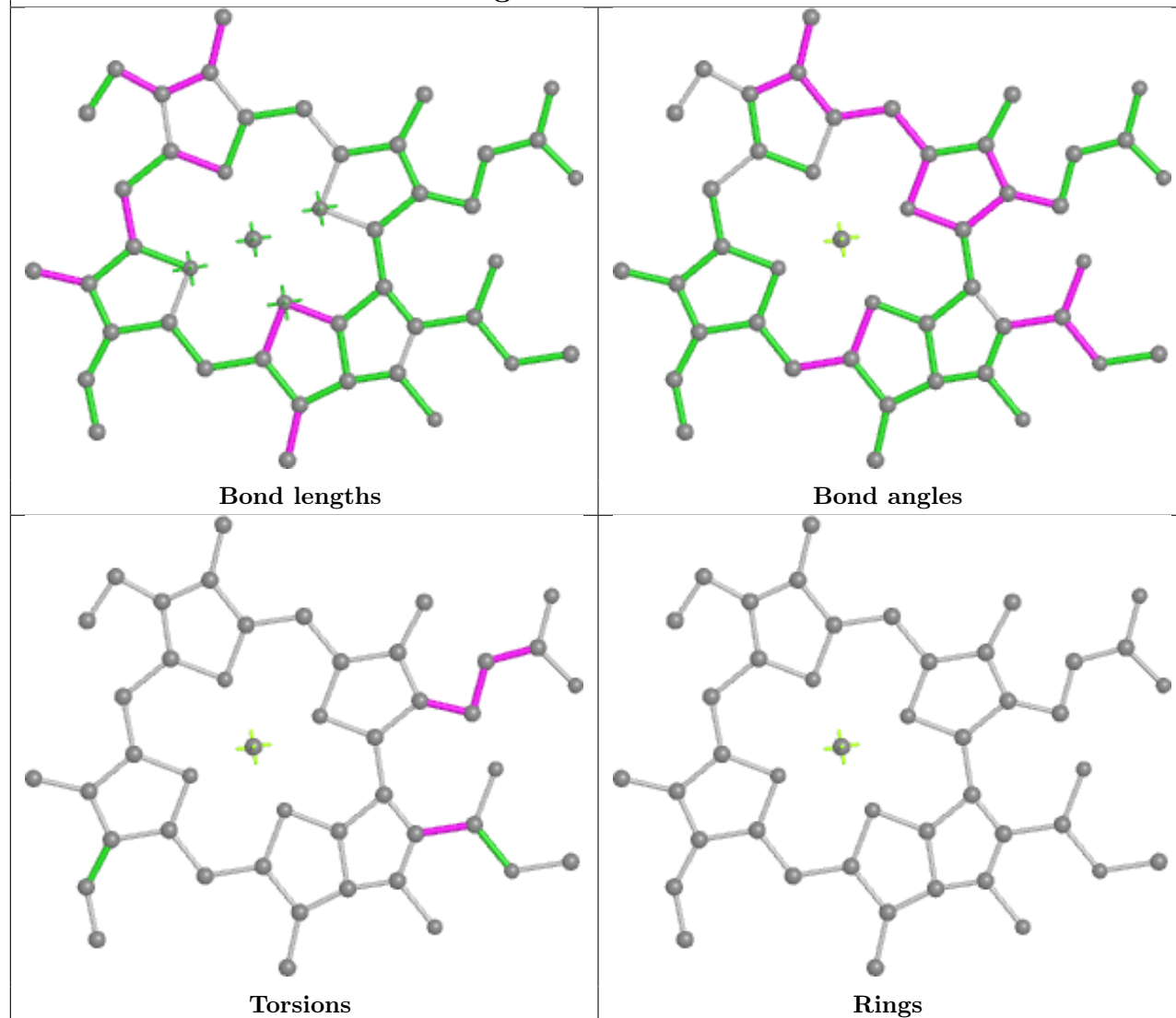
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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

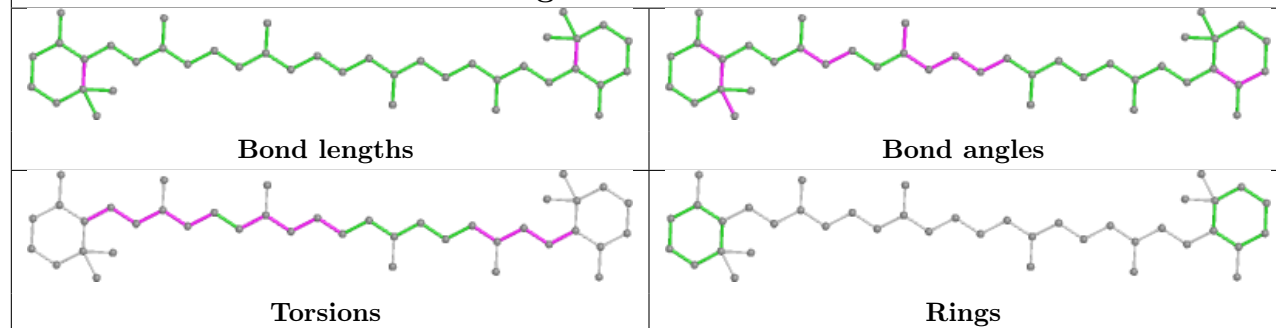


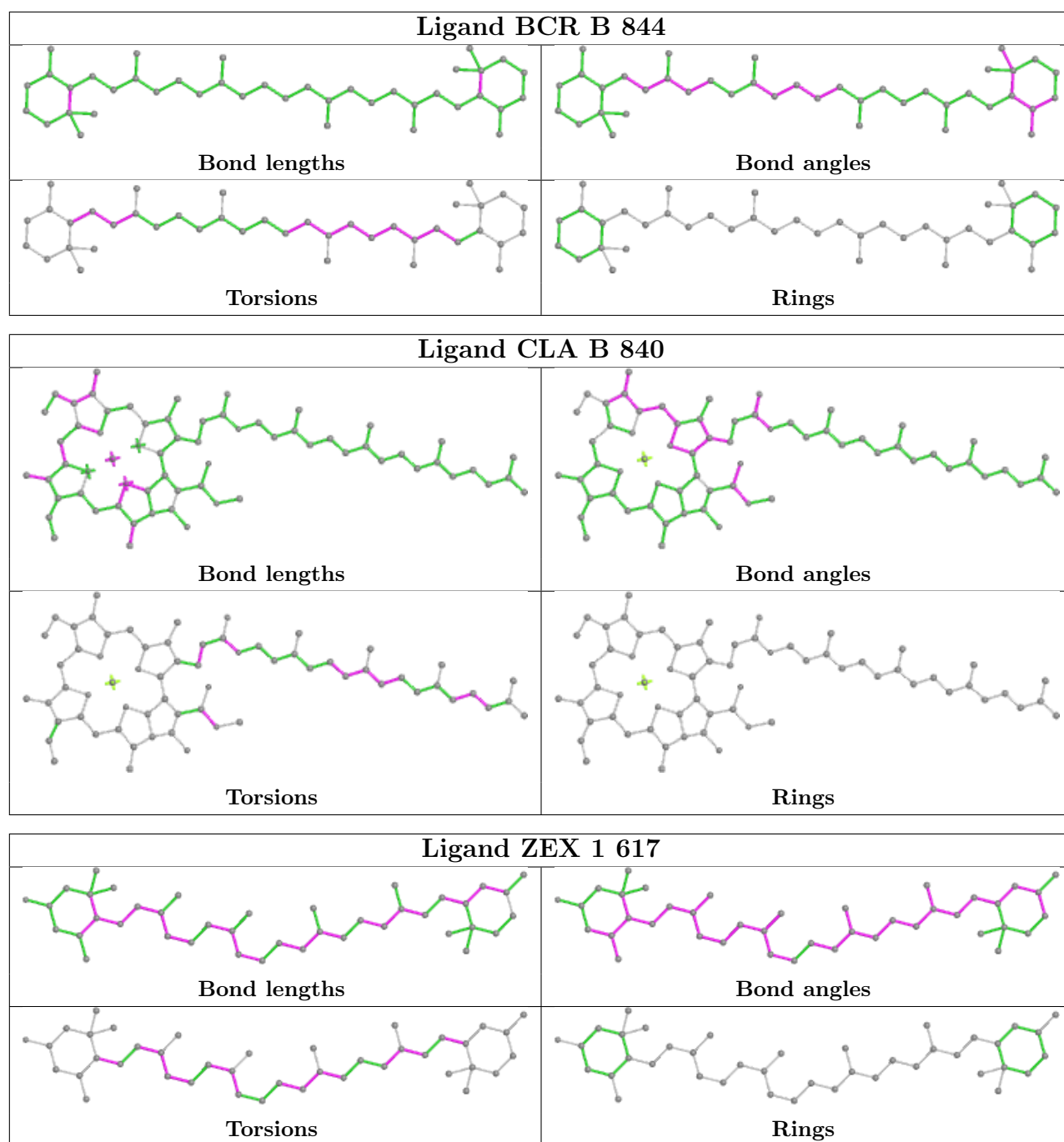


Ligand CLA 3 205

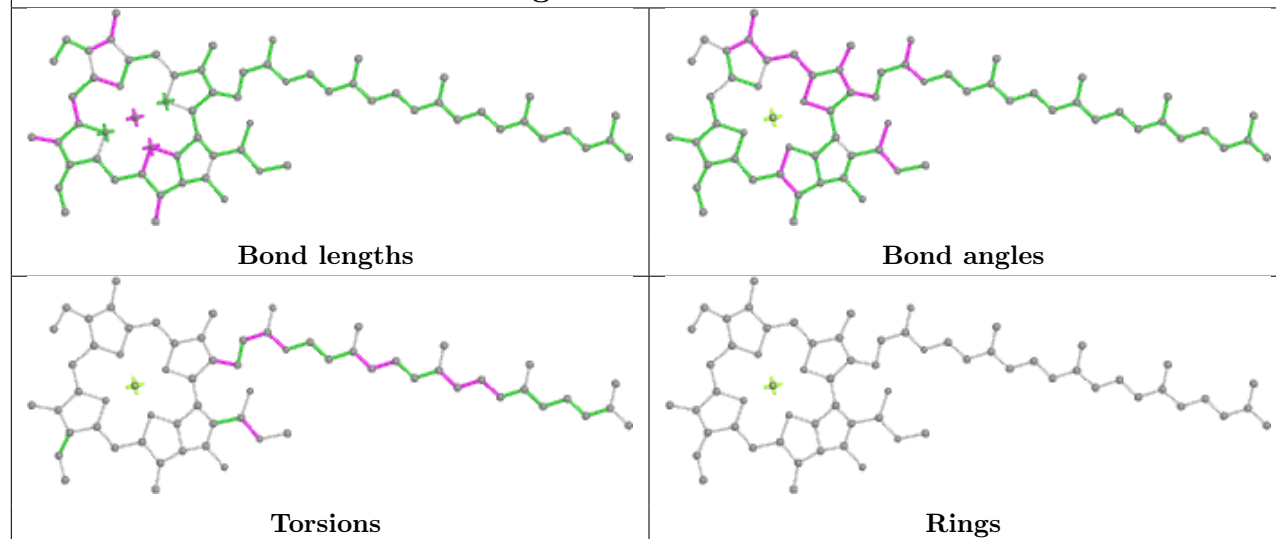


Ligand BCR I 101

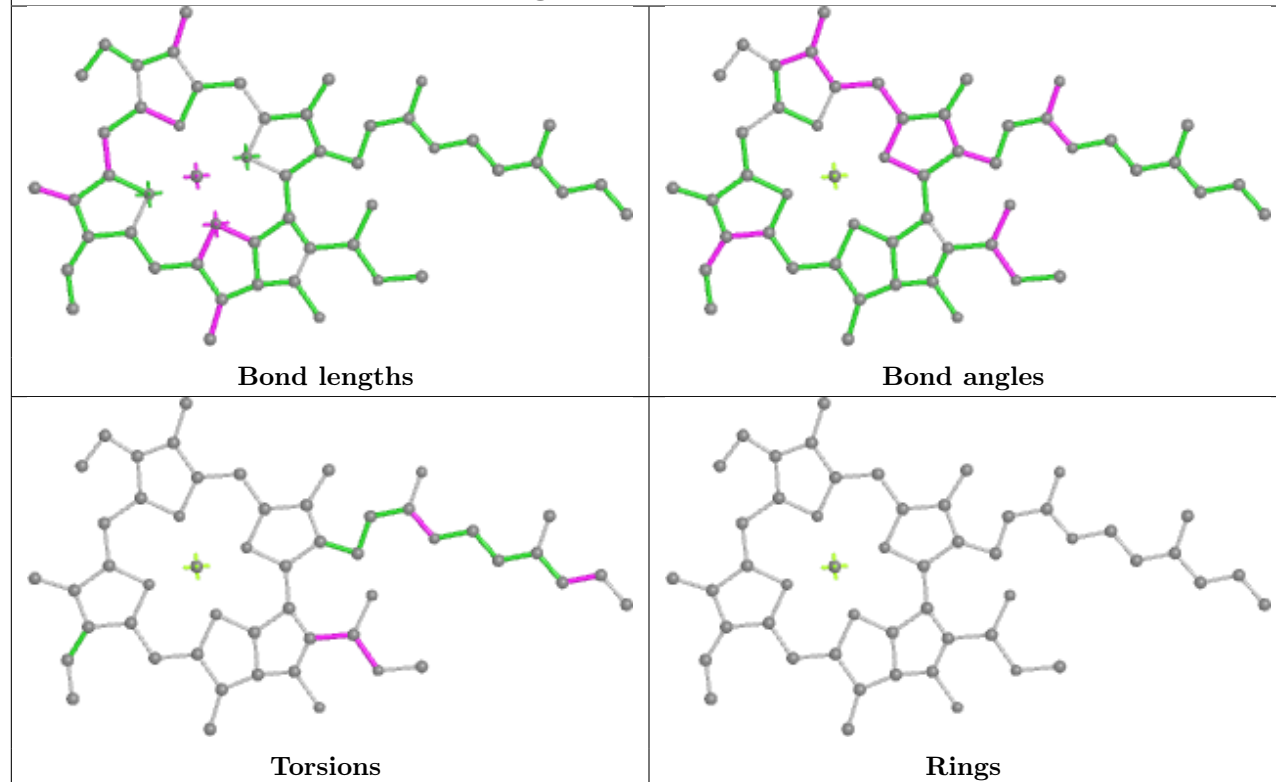


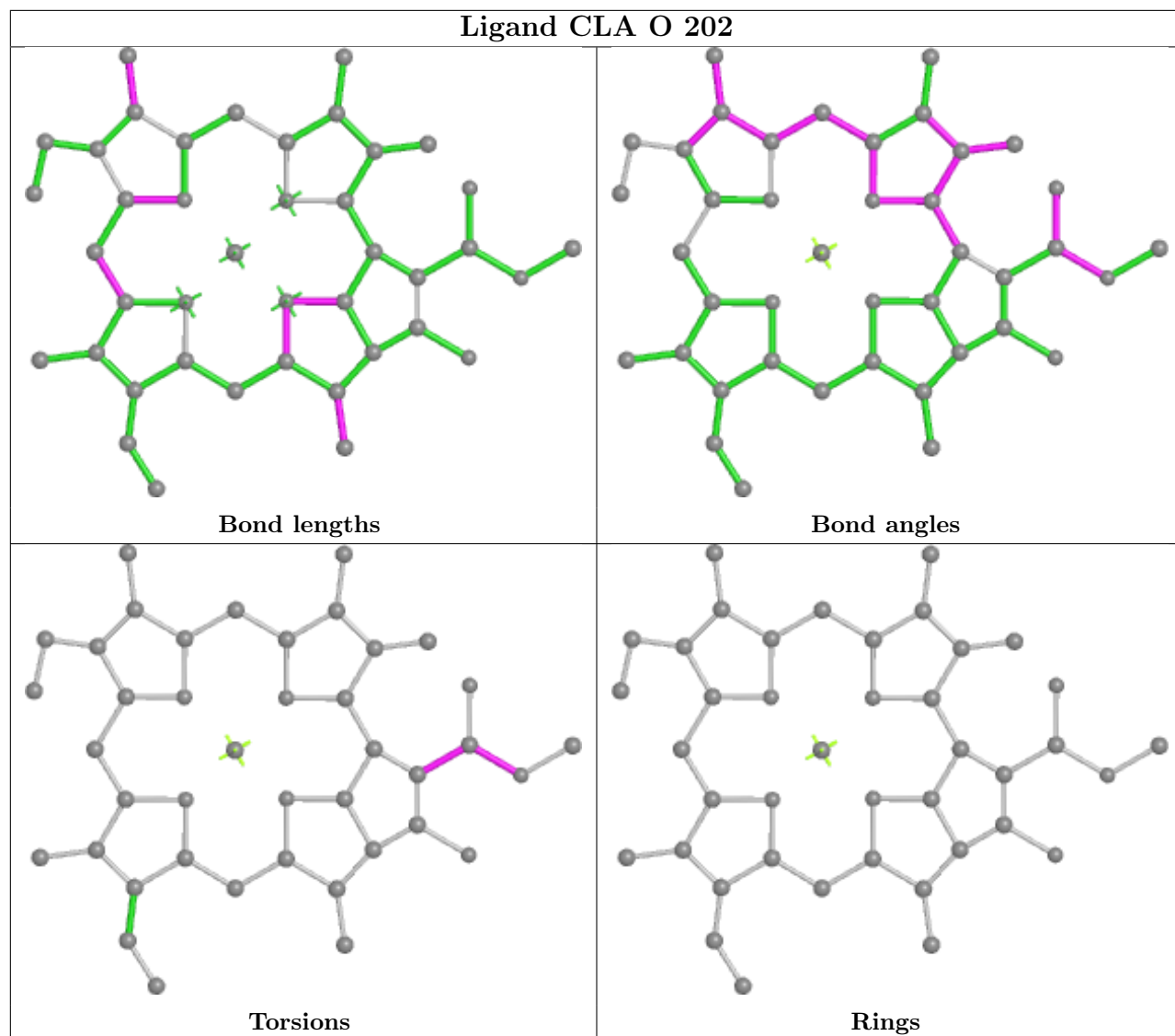


Ligand CLA B 830

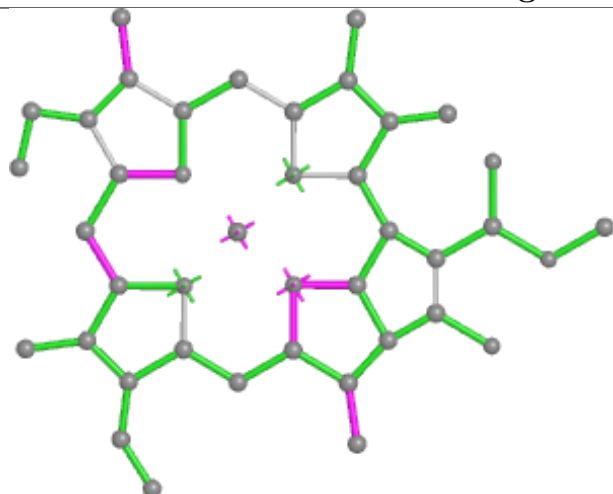


Ligand CLA O 201

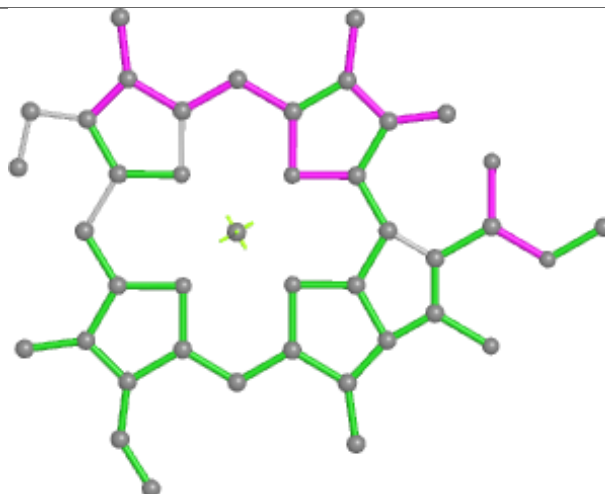




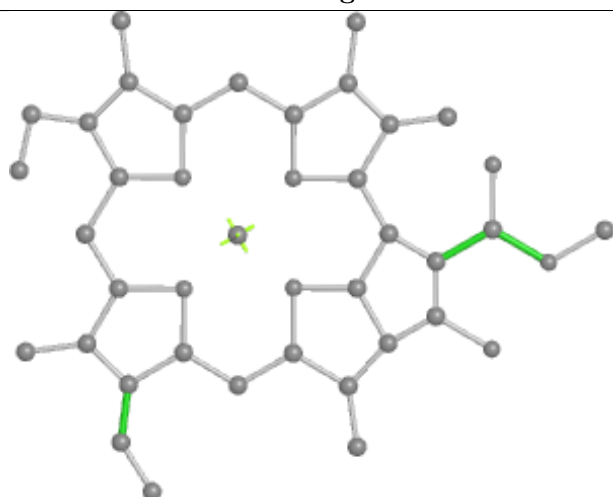
Ligand CLA 1 609



Bond lengths



Bond angles

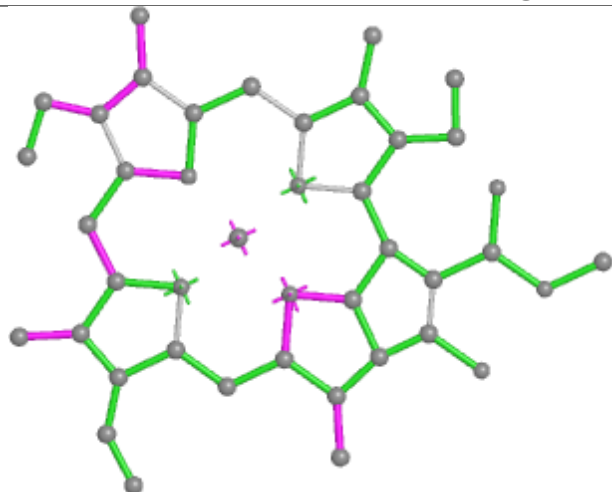


Torsions

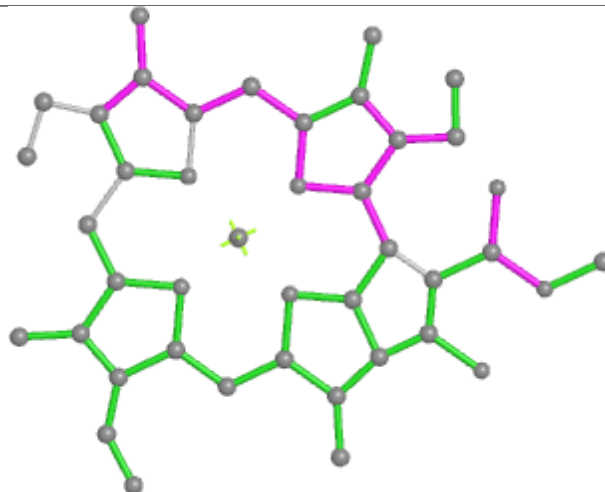


Rings

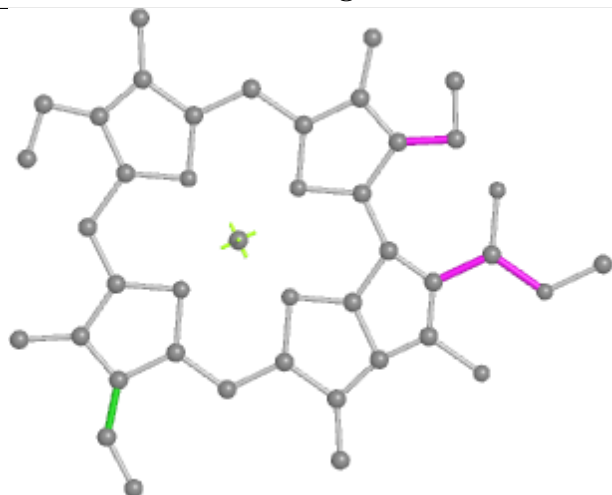
Ligand CLA 2 604



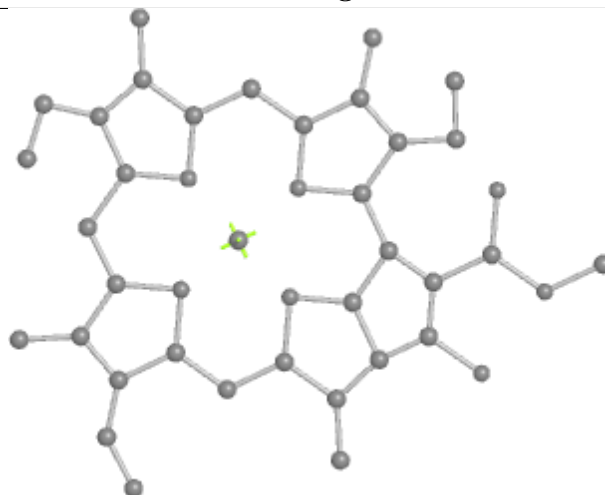
Bond lengths



Bond angles

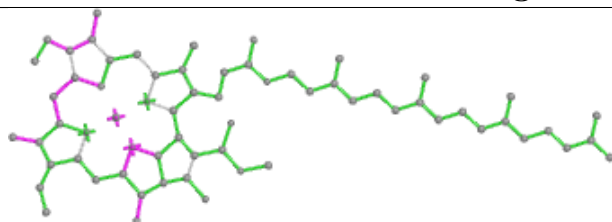


Torsions

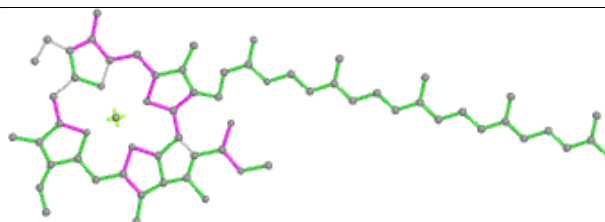


Rings

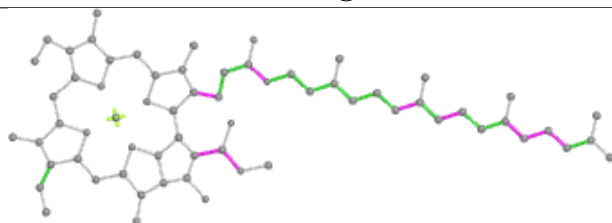
Ligand CLA A 818



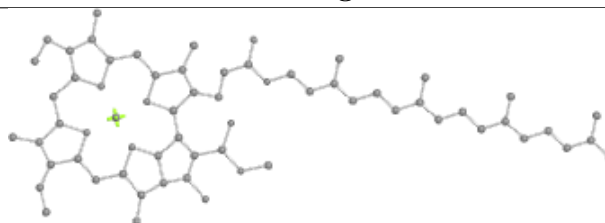
Bond lengths



Bond angles

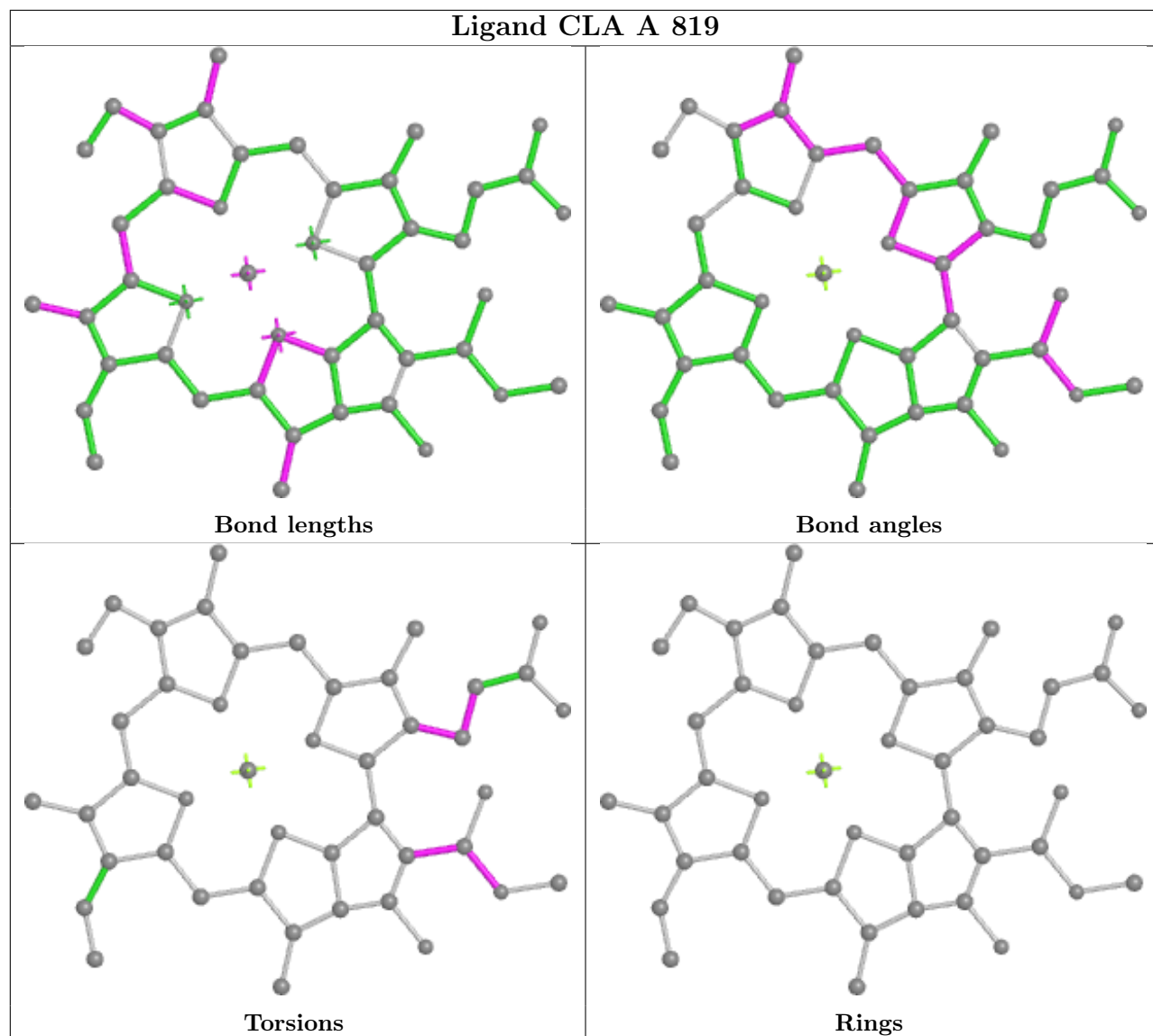


Torsions

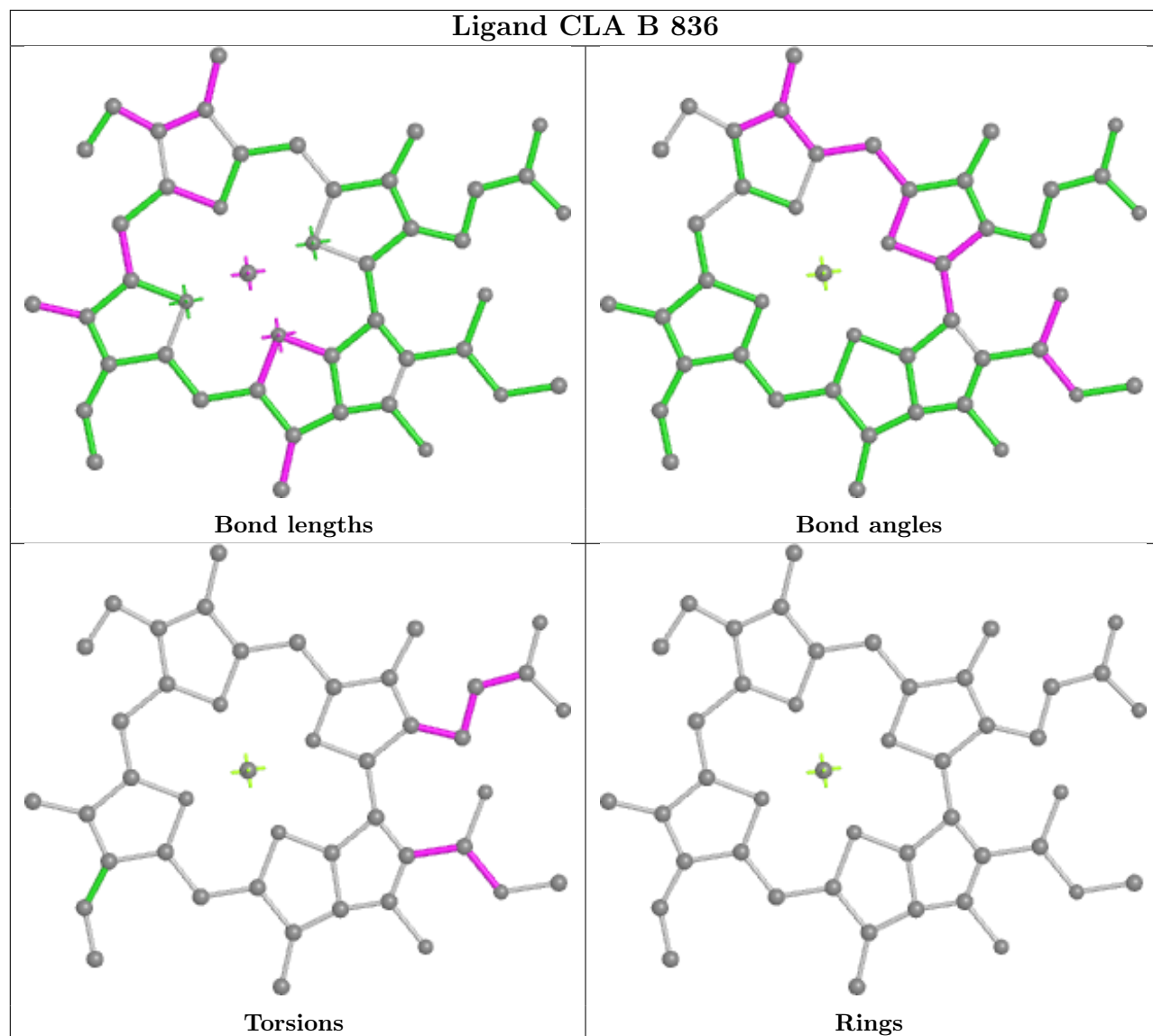


Rings

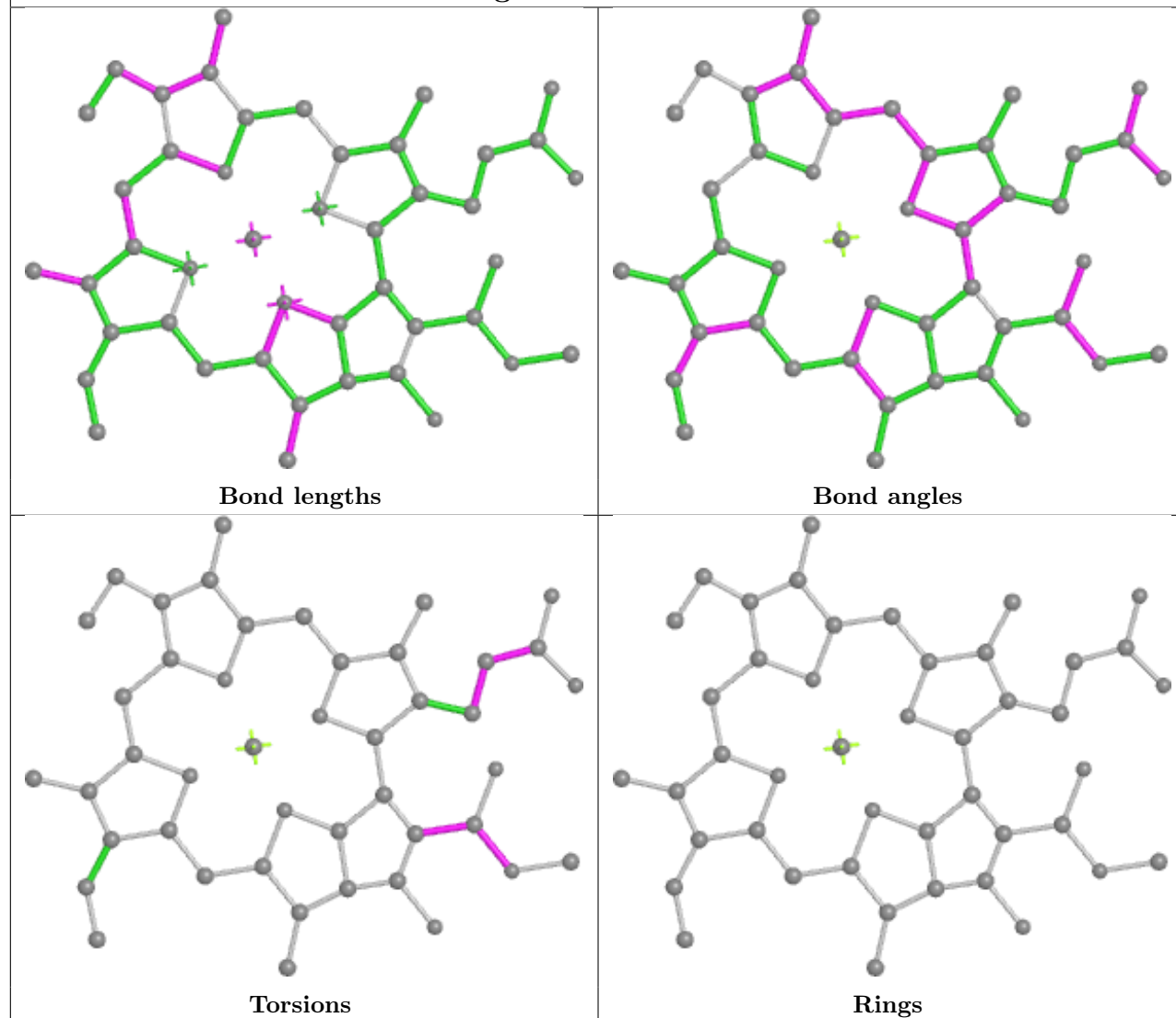
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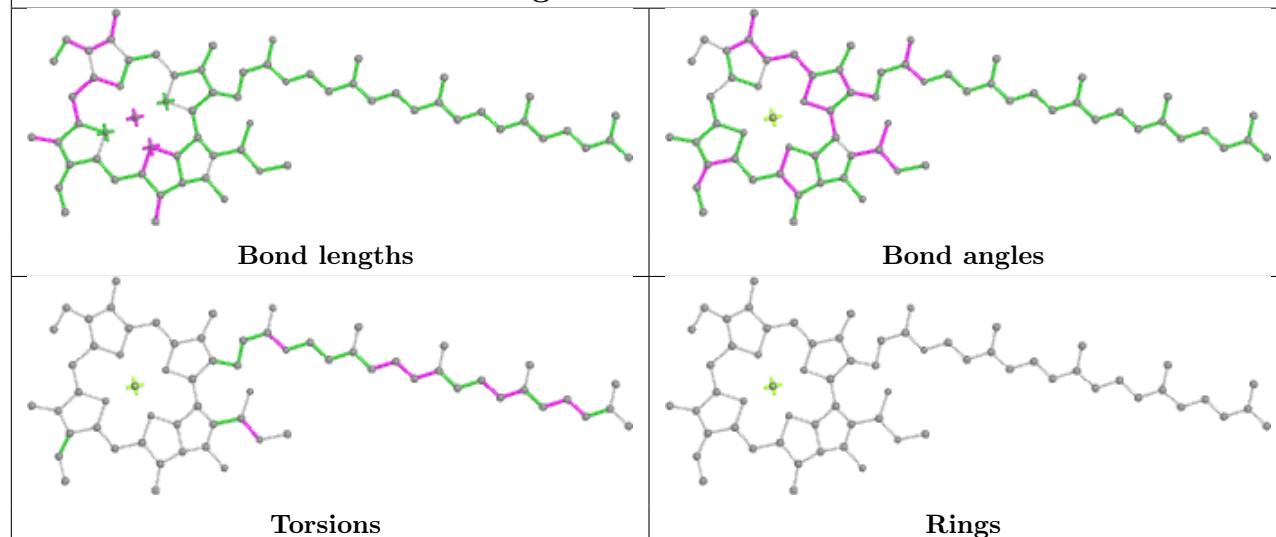
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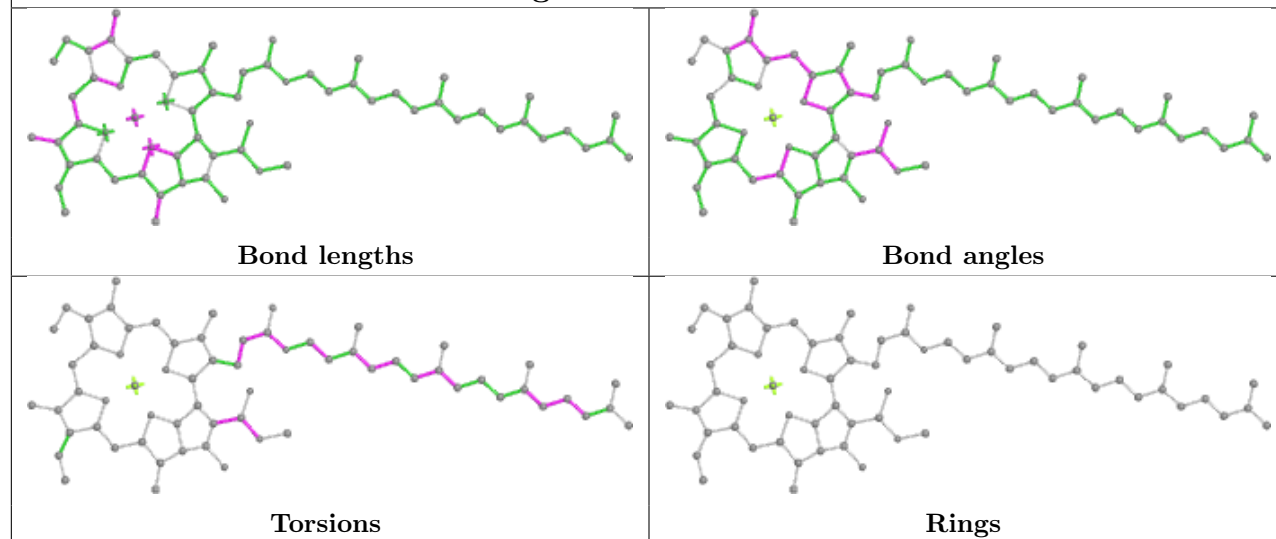
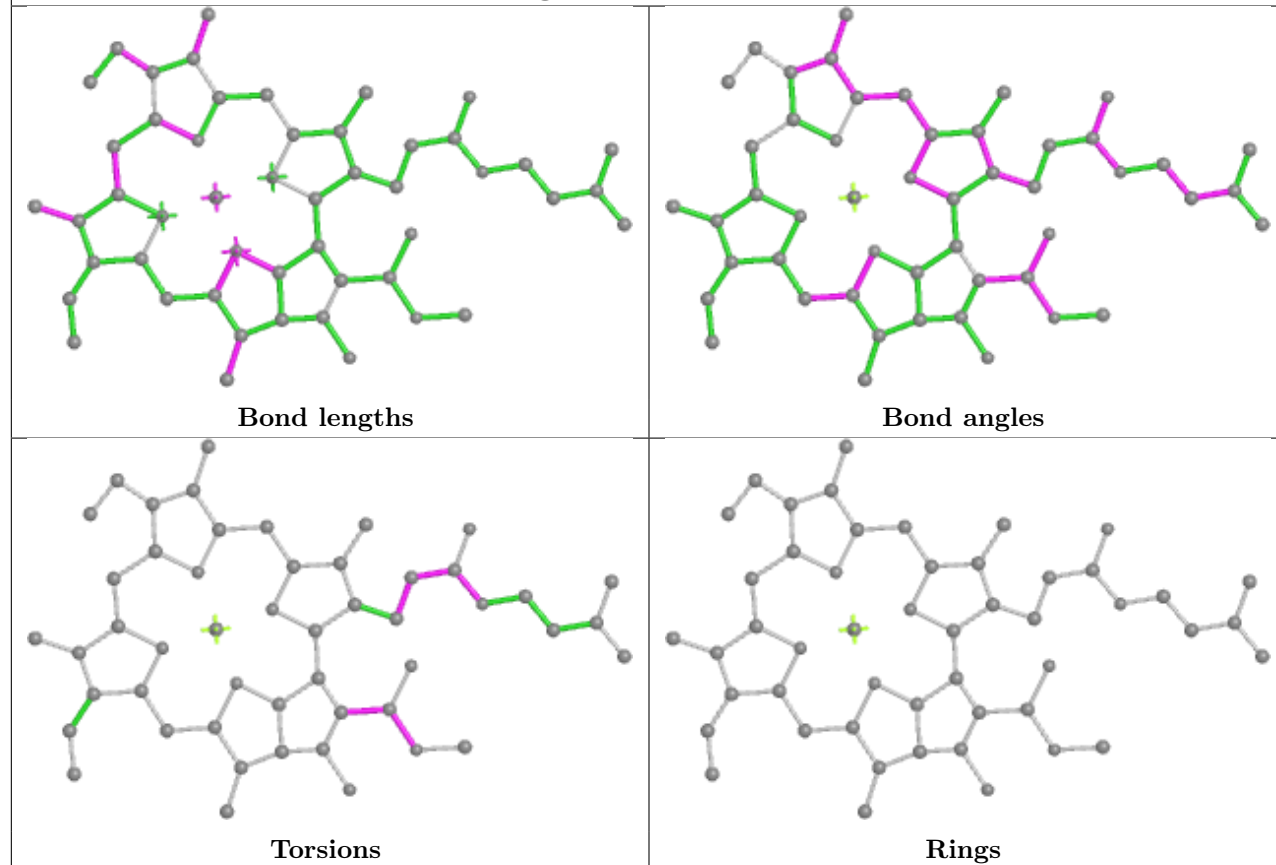


Ligand CLA 1 606

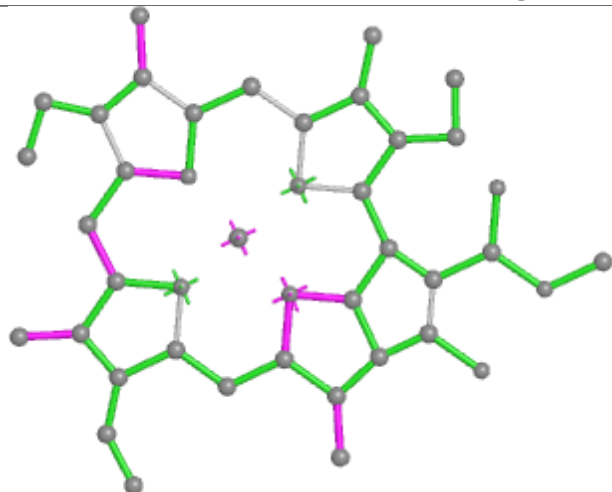


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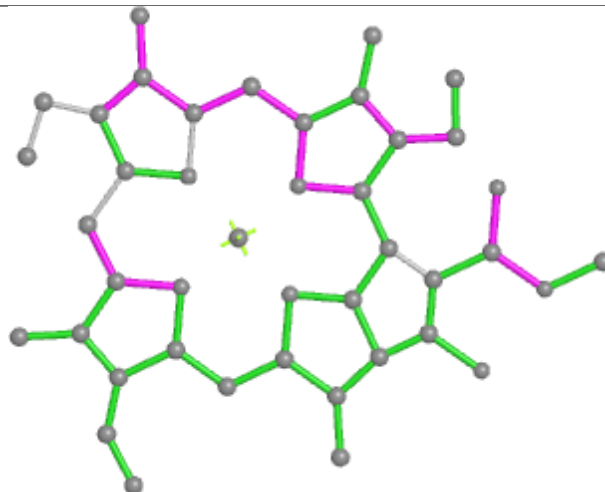


Ligand CLA B 833**Ligand CLA 2 608**

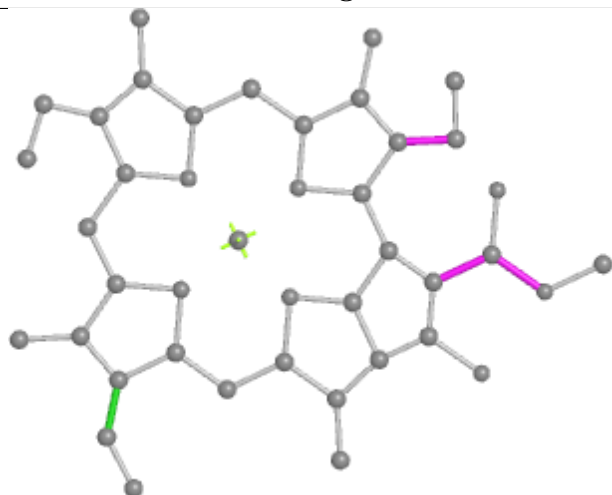
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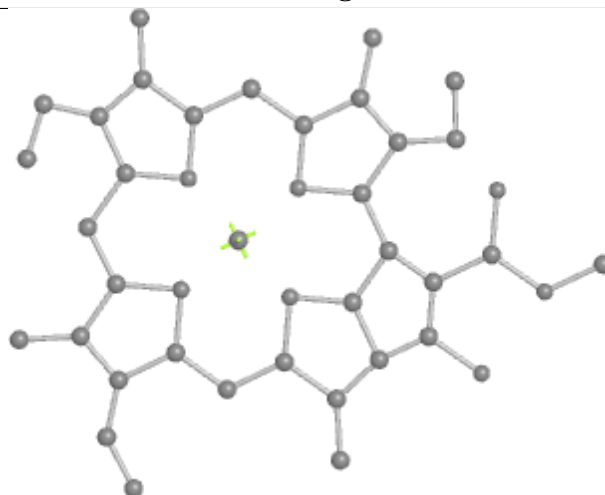
Bond lengths



Bond angles

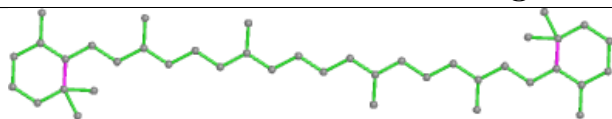


Torsions

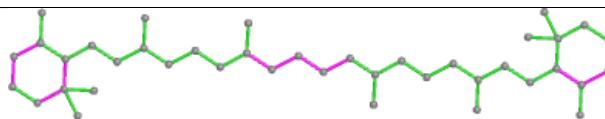


Rings

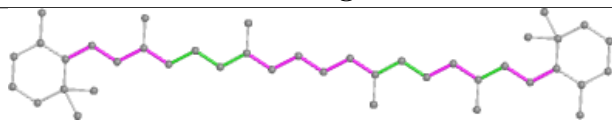
Ligand BCR K 103



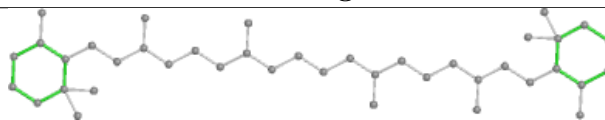
Bond lengths



Bond angles

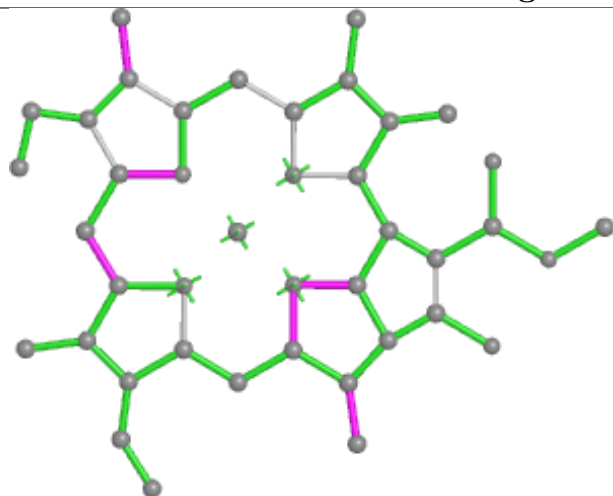


Torsions

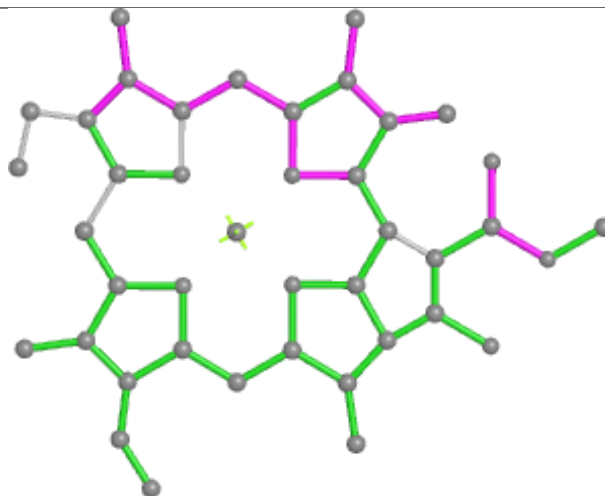


Rings

Ligand CLA 3 210



Bond lengths



Bond angles

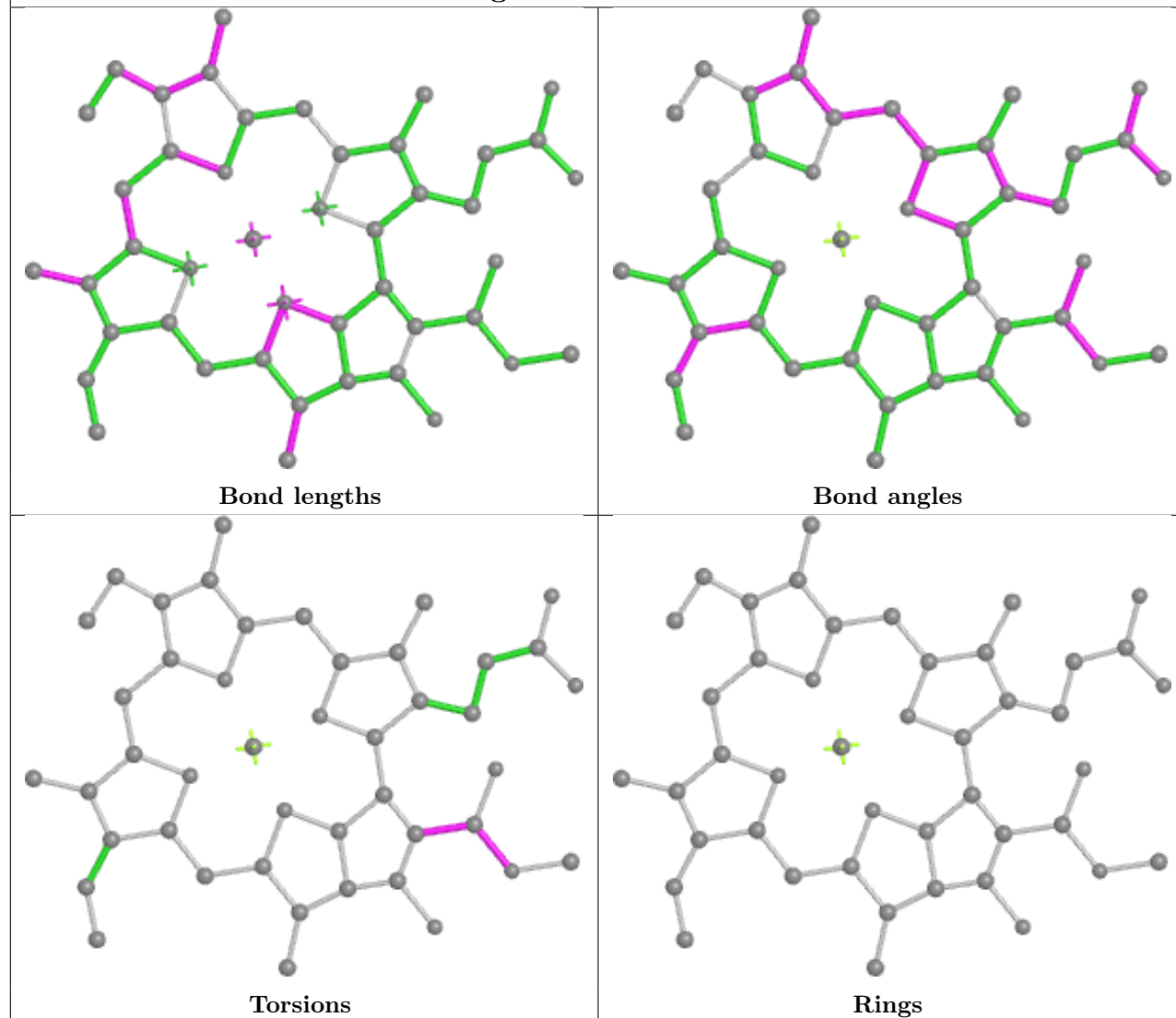


Torsions

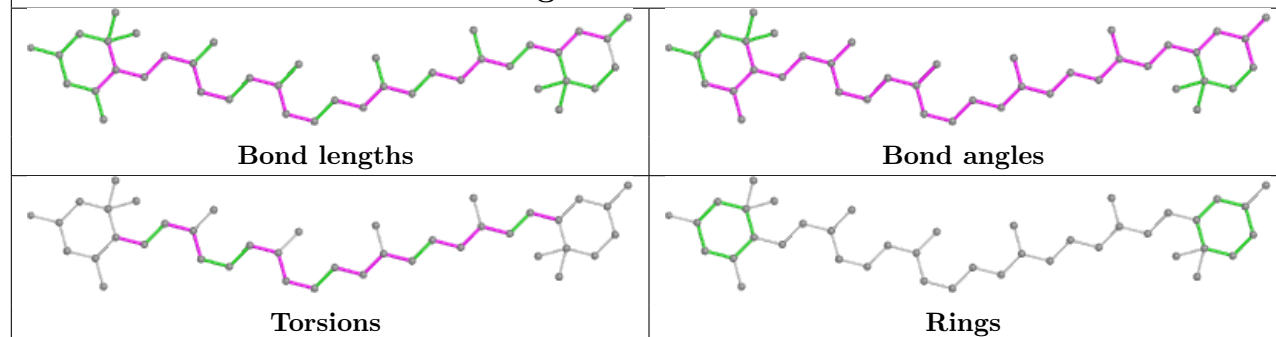


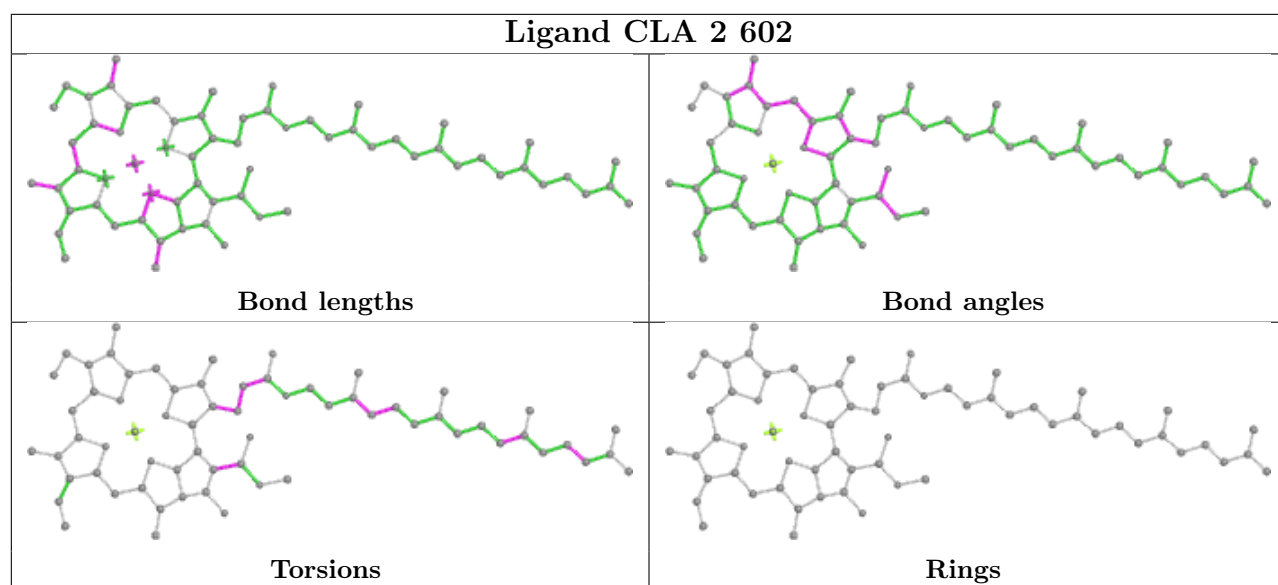
Rings

Ligand CLA B 832

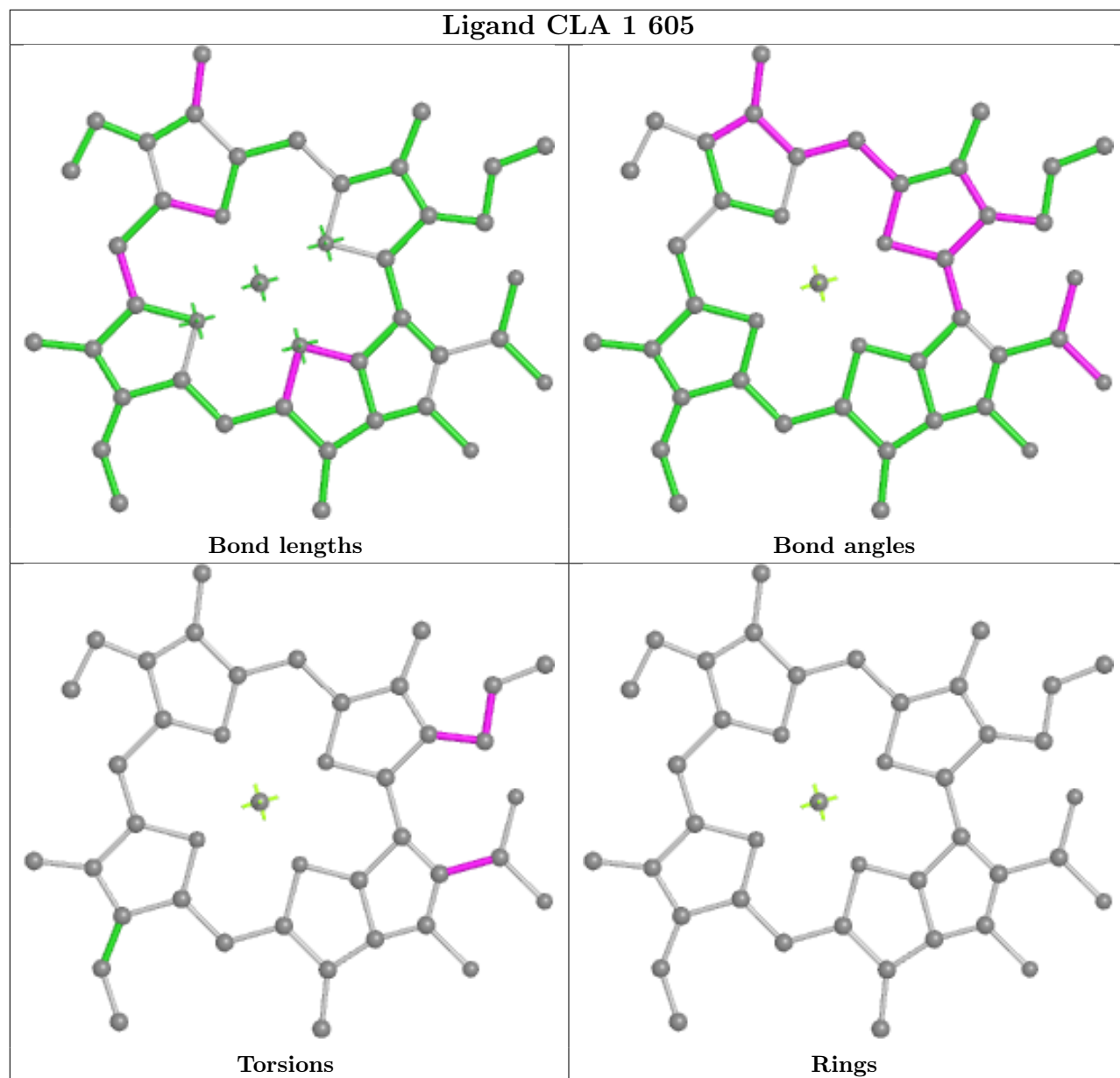


Ligand ZEX 1 614

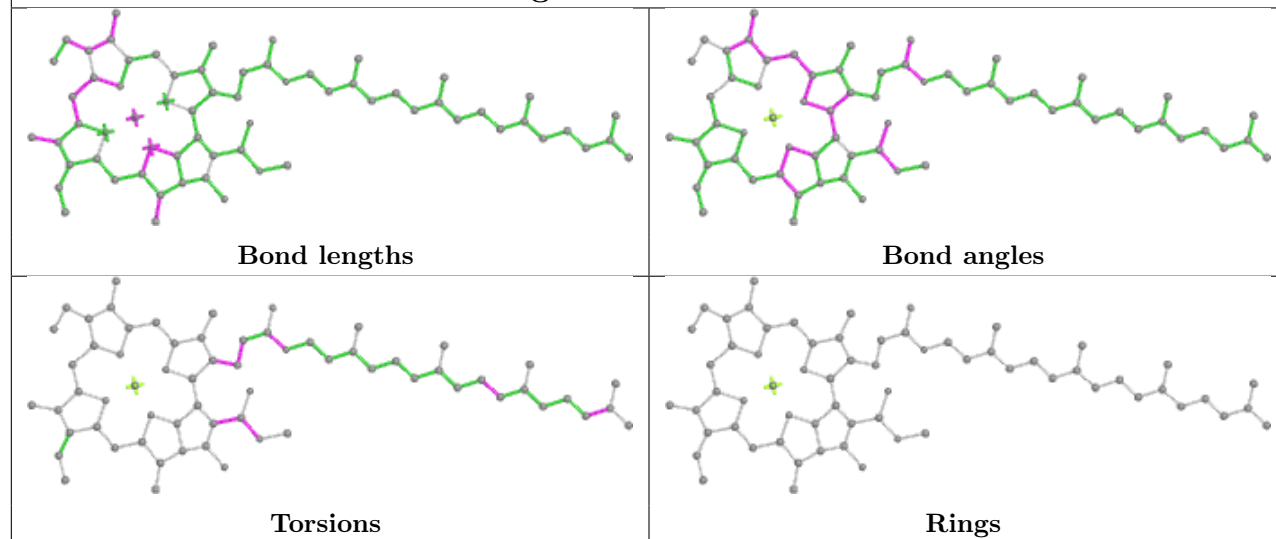




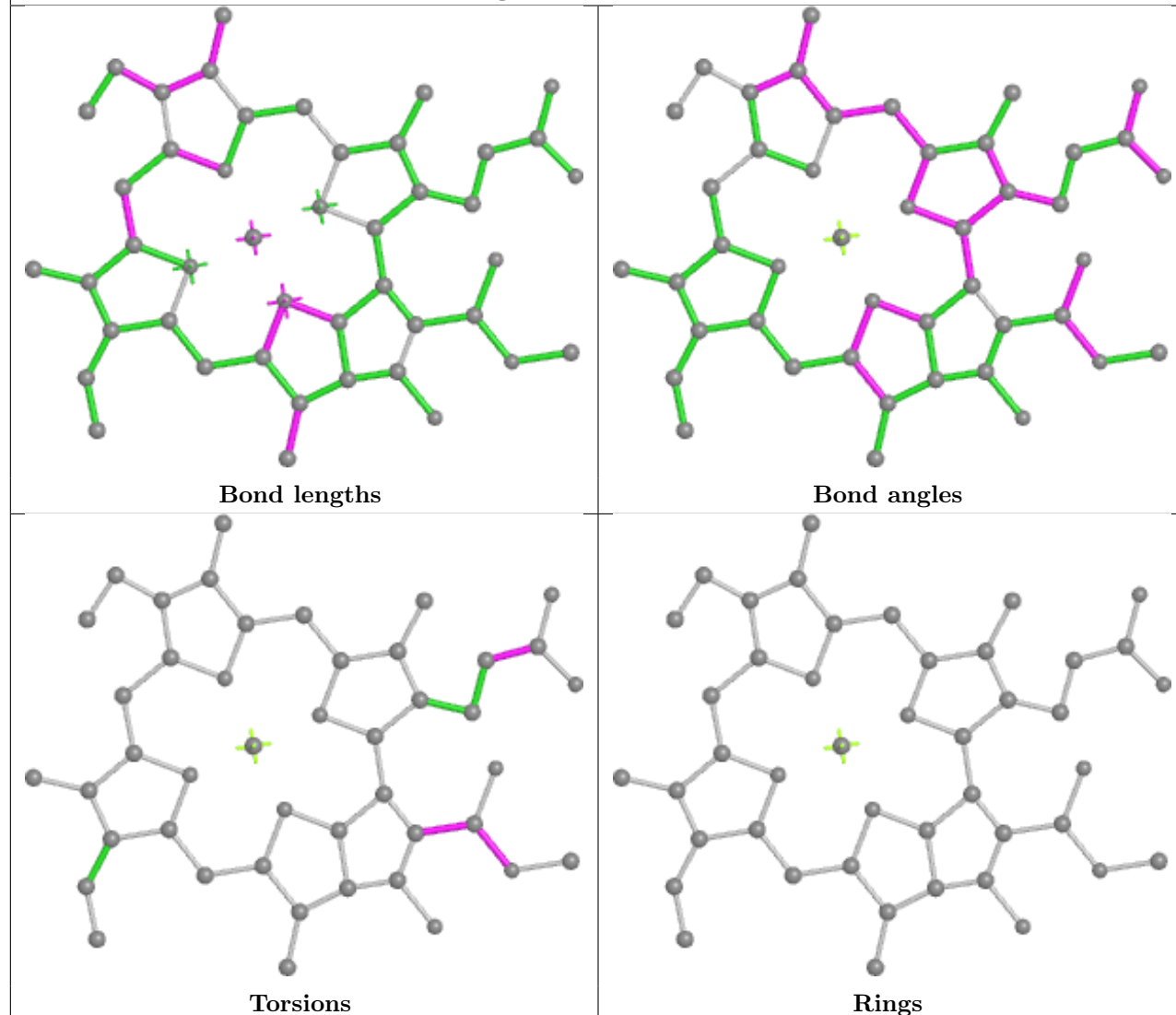
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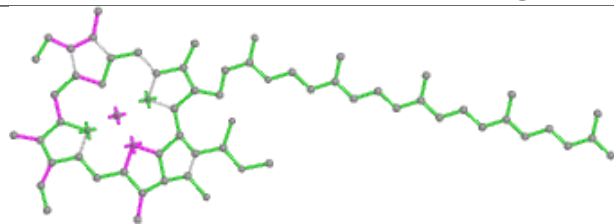
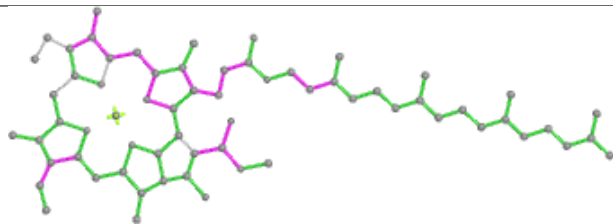
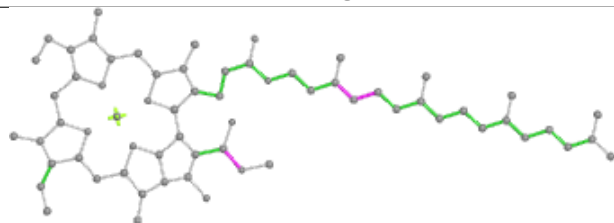
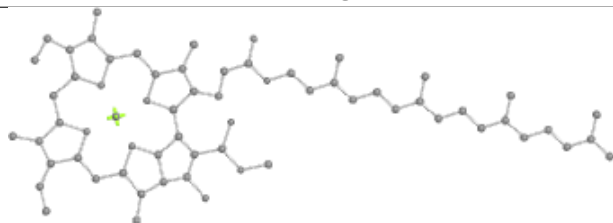
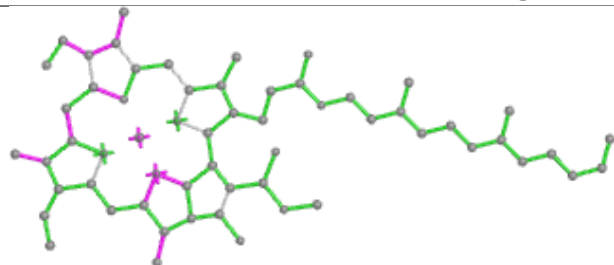
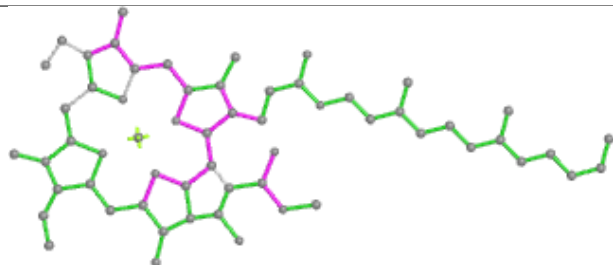
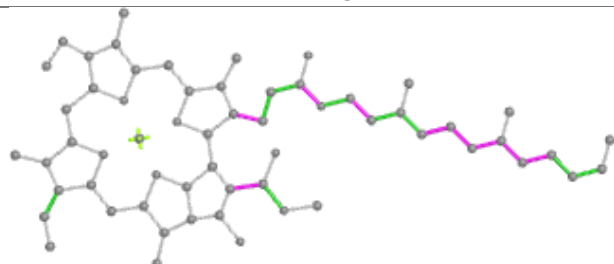
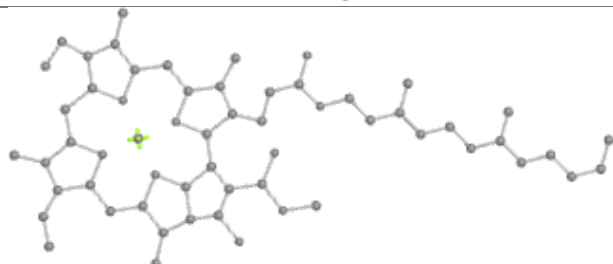


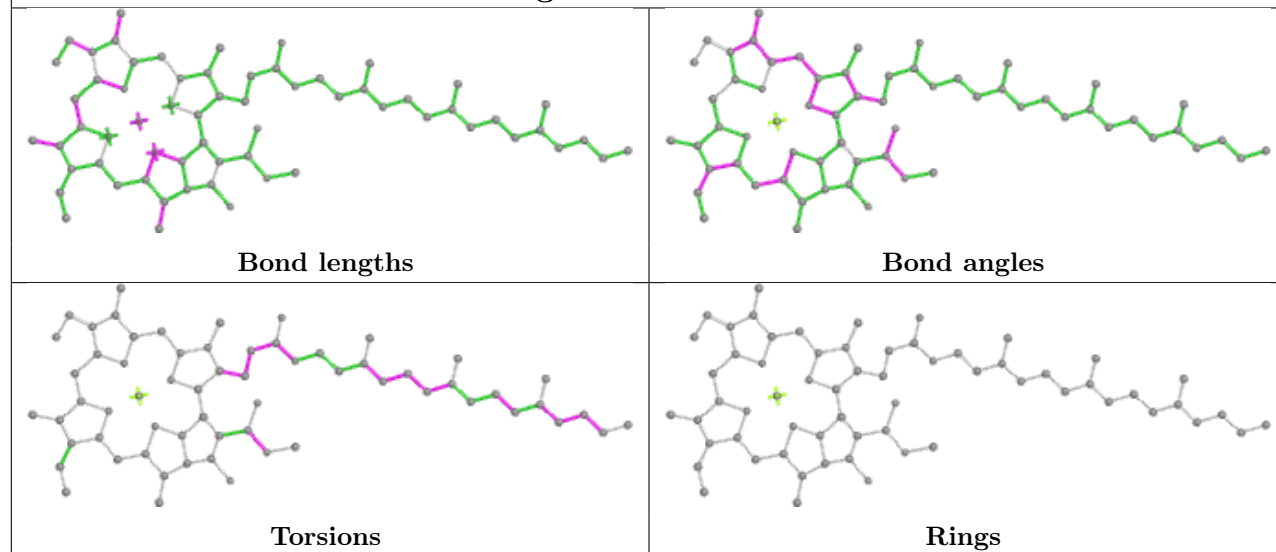
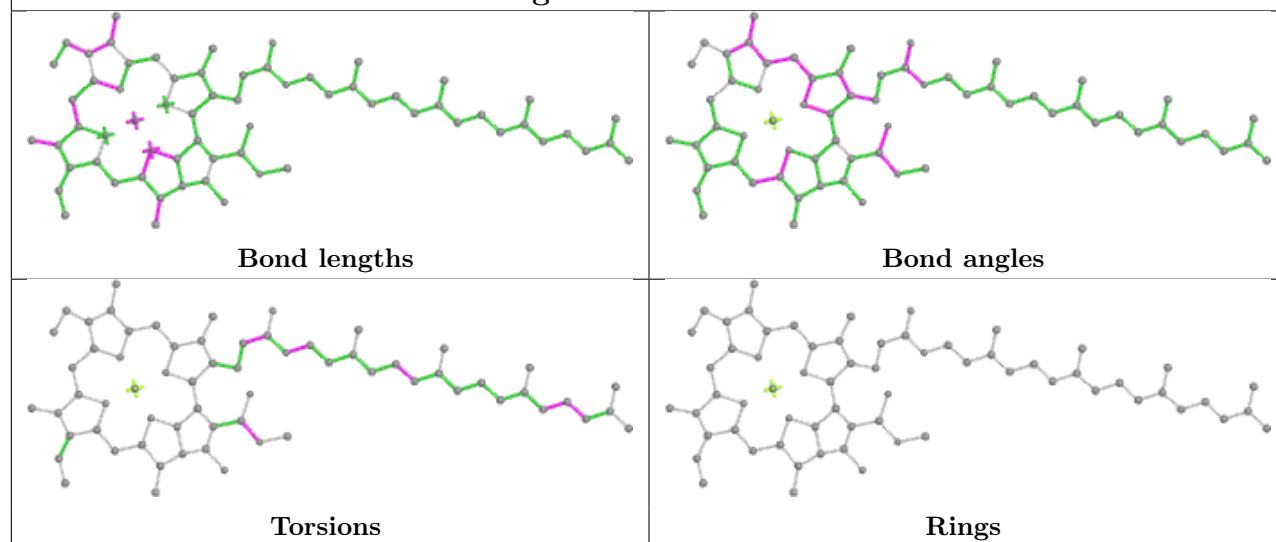
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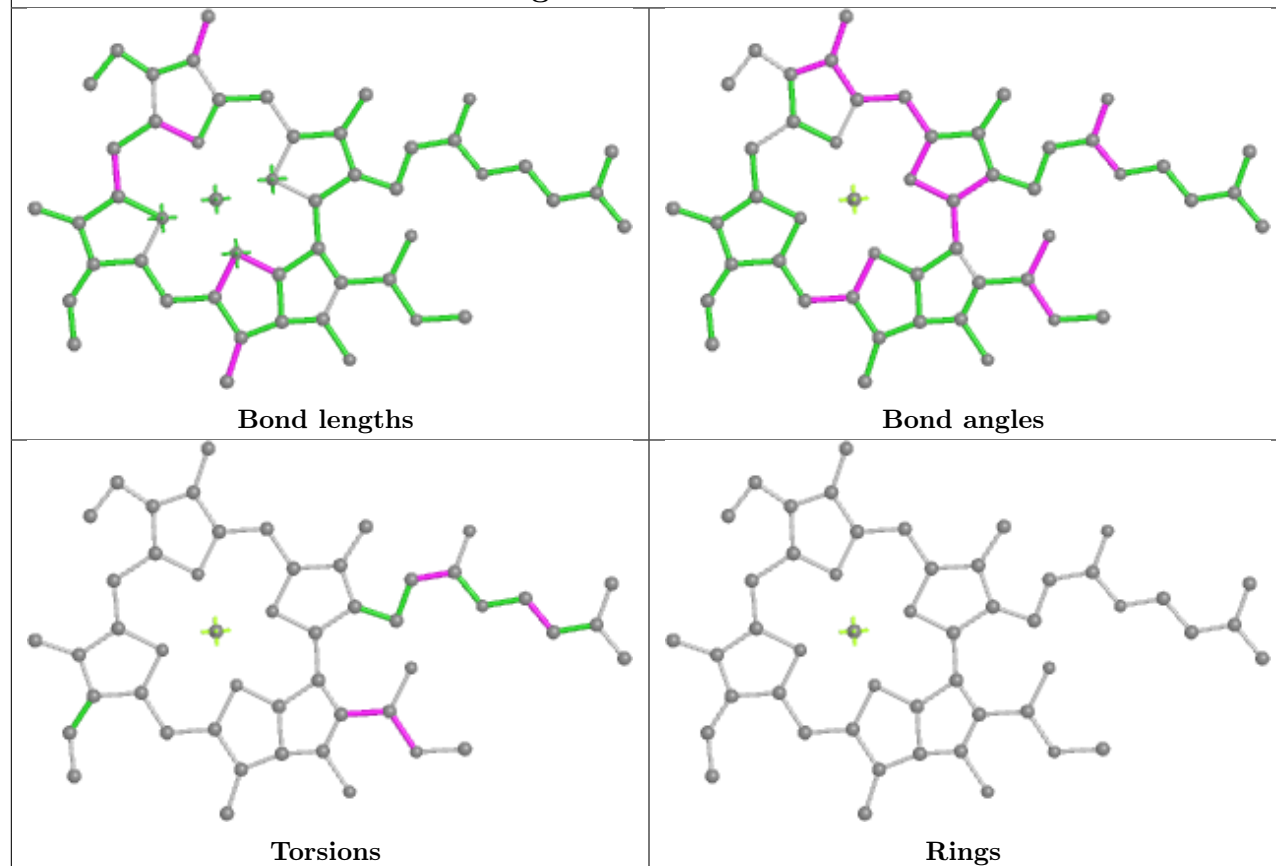
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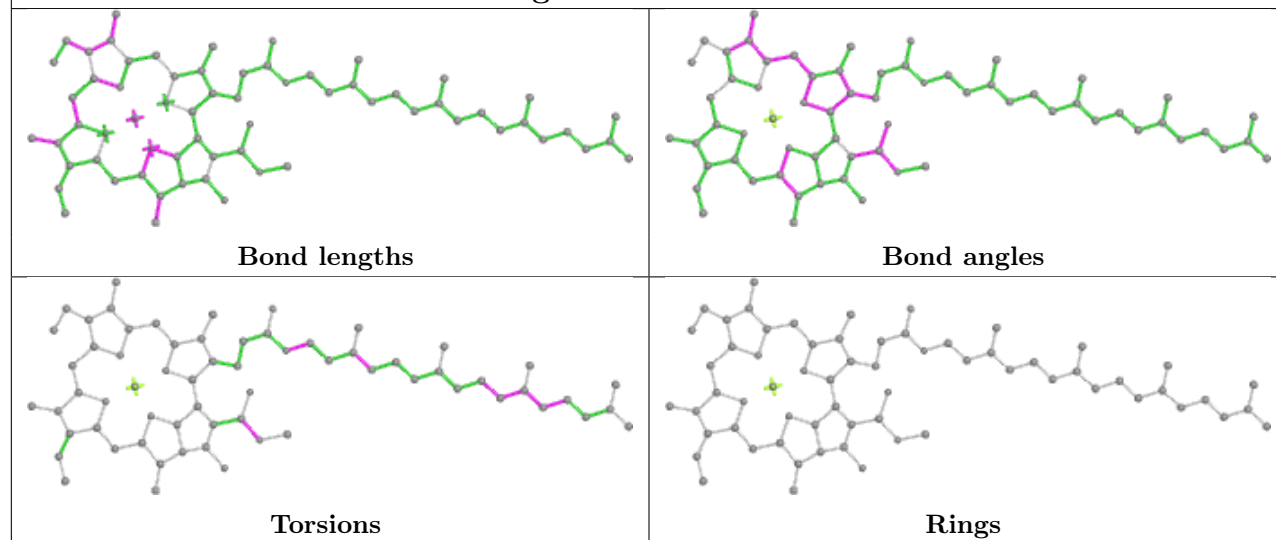
Ligand CLA A 804**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 819****Bond lengths****Bond angles****Torsions****Rings**

Ligand CLA 3 203**Ligand CLA B 838**

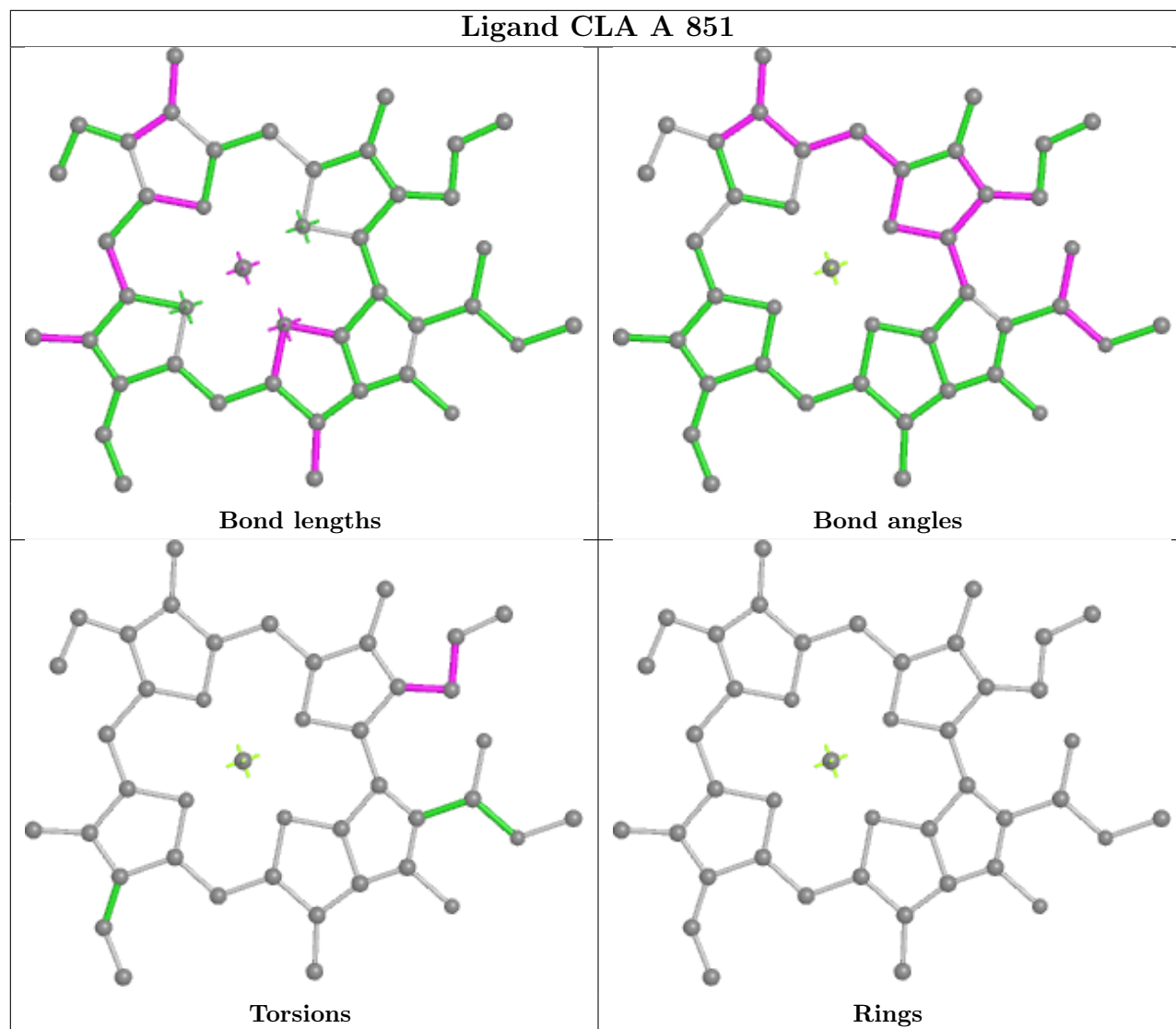
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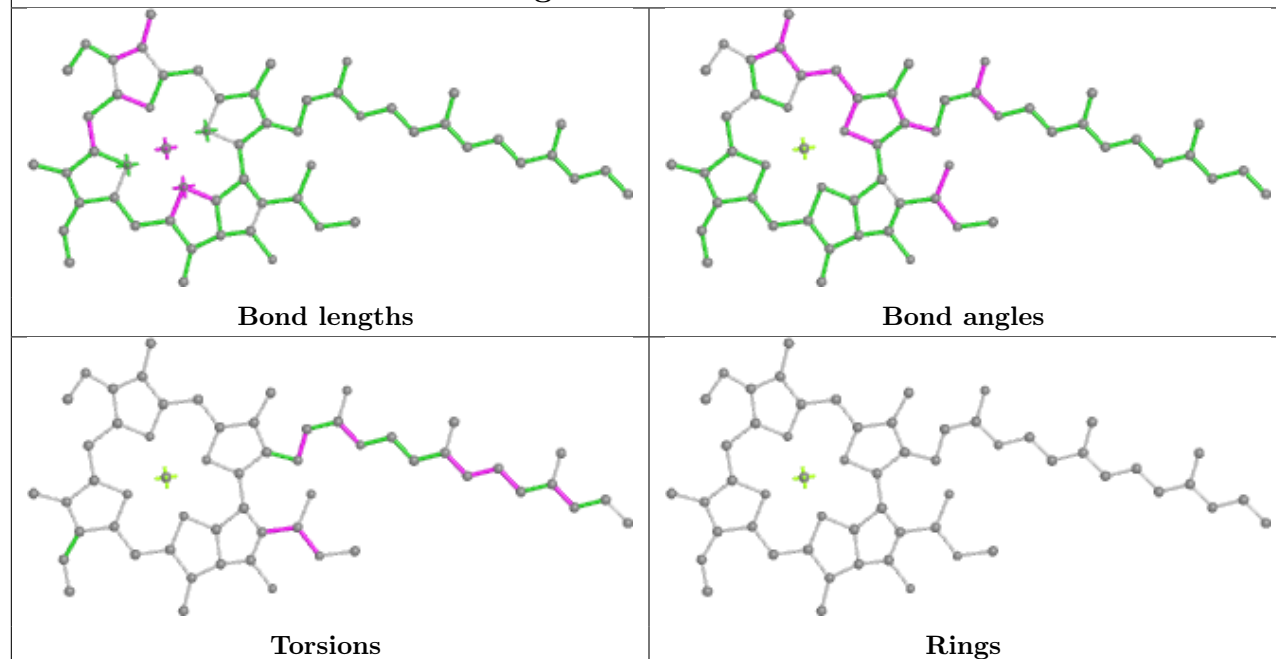
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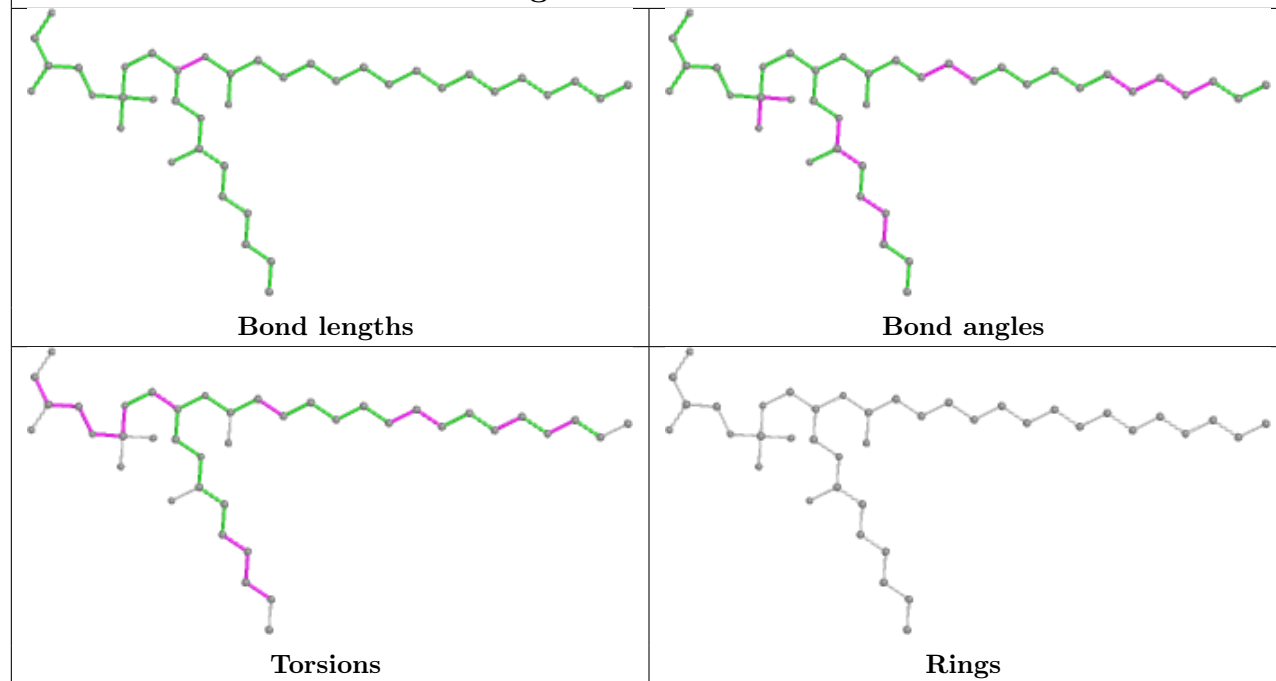
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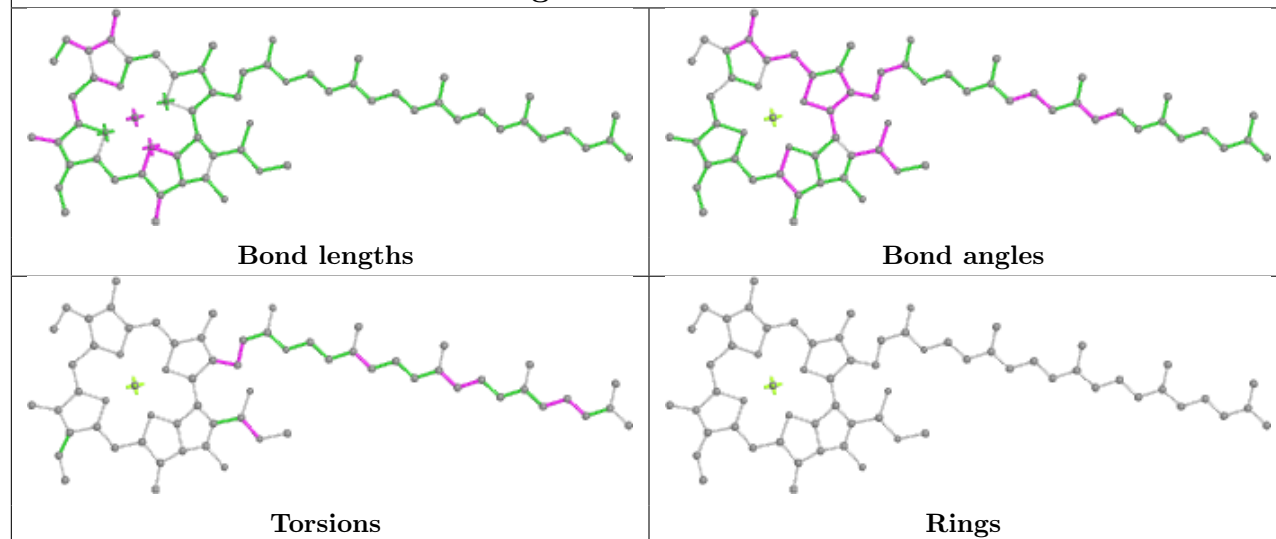
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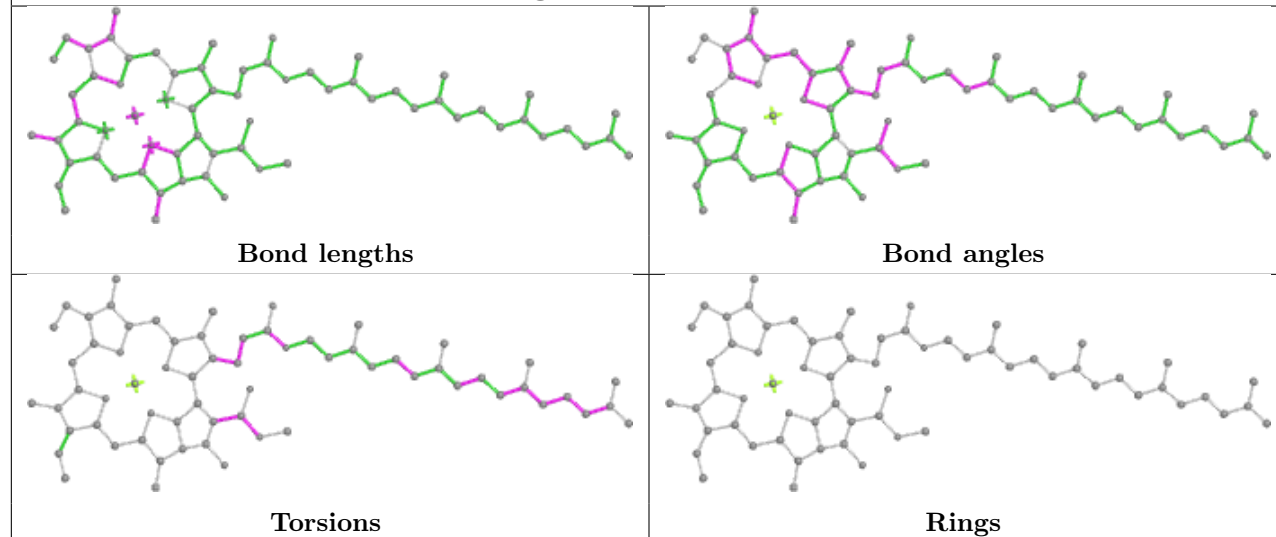
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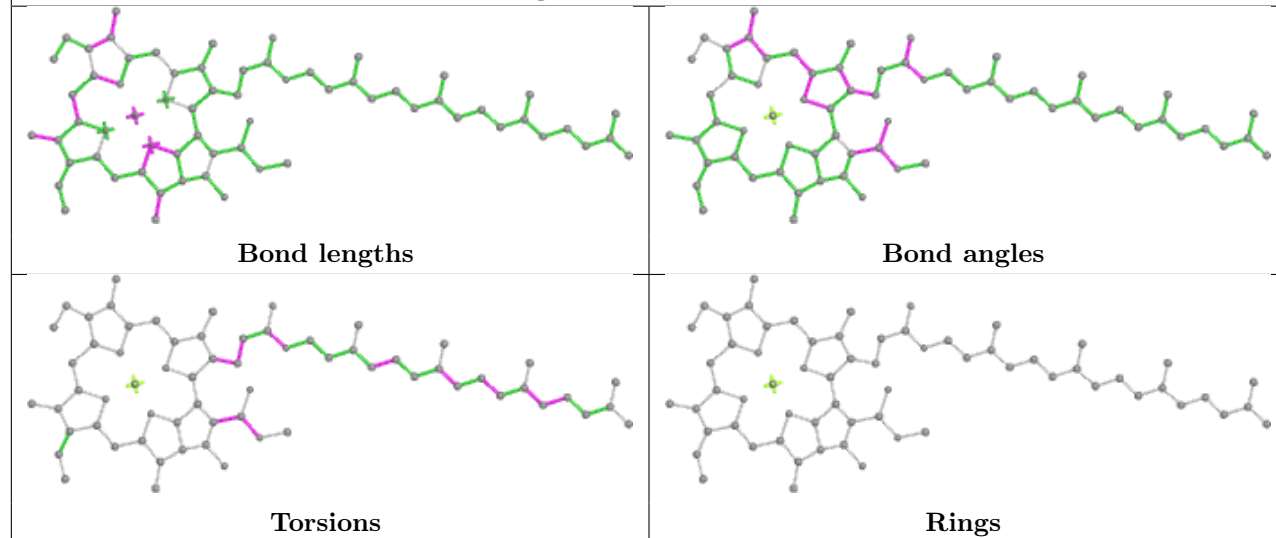
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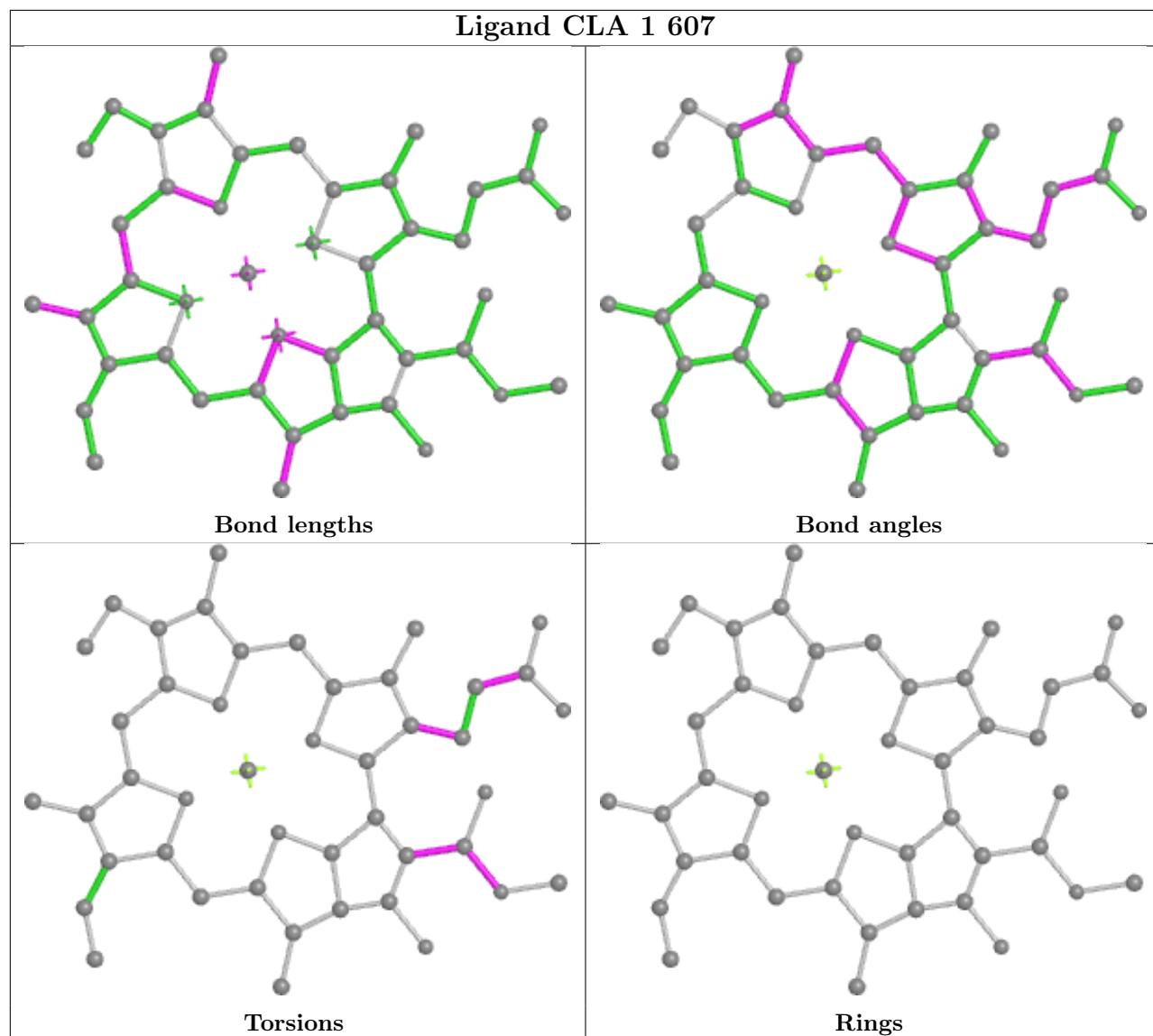
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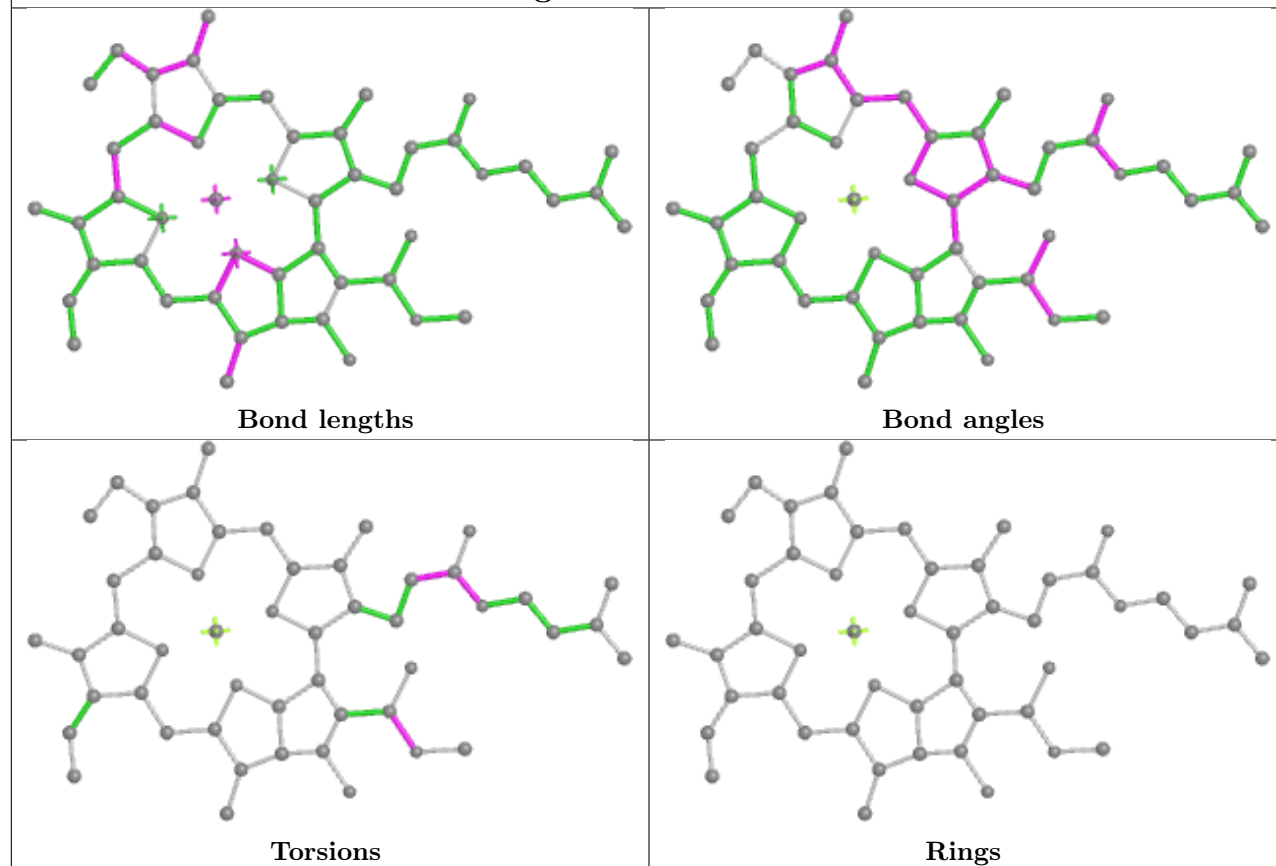
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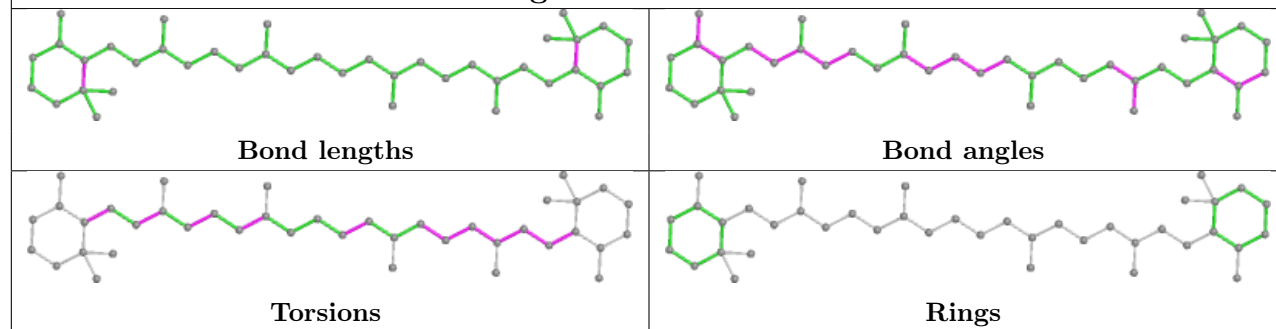
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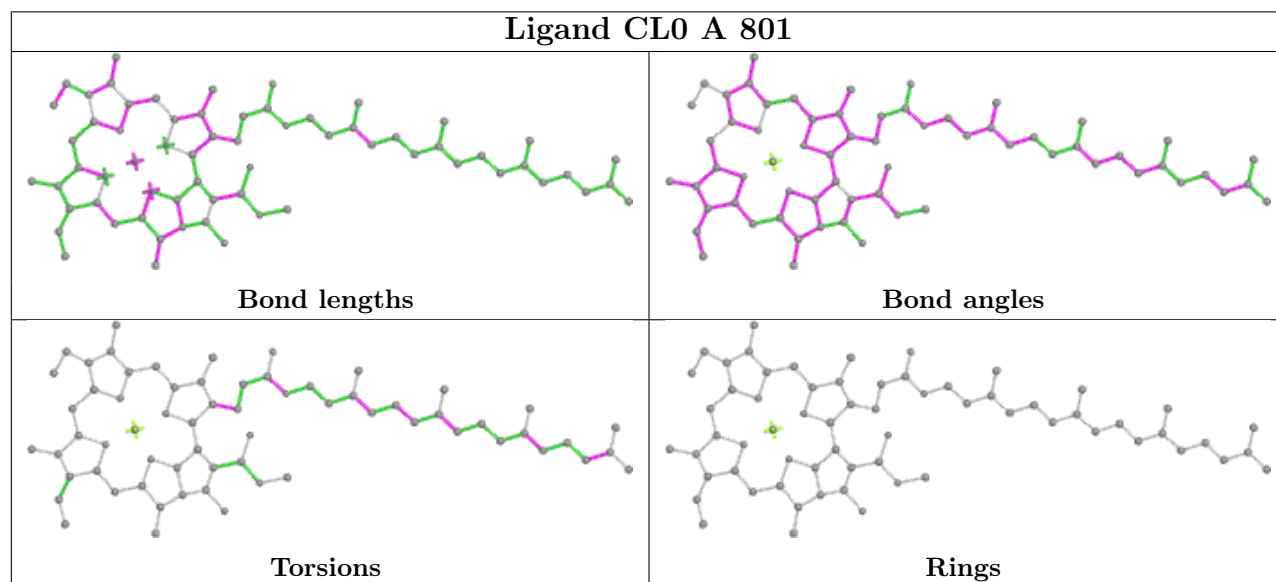
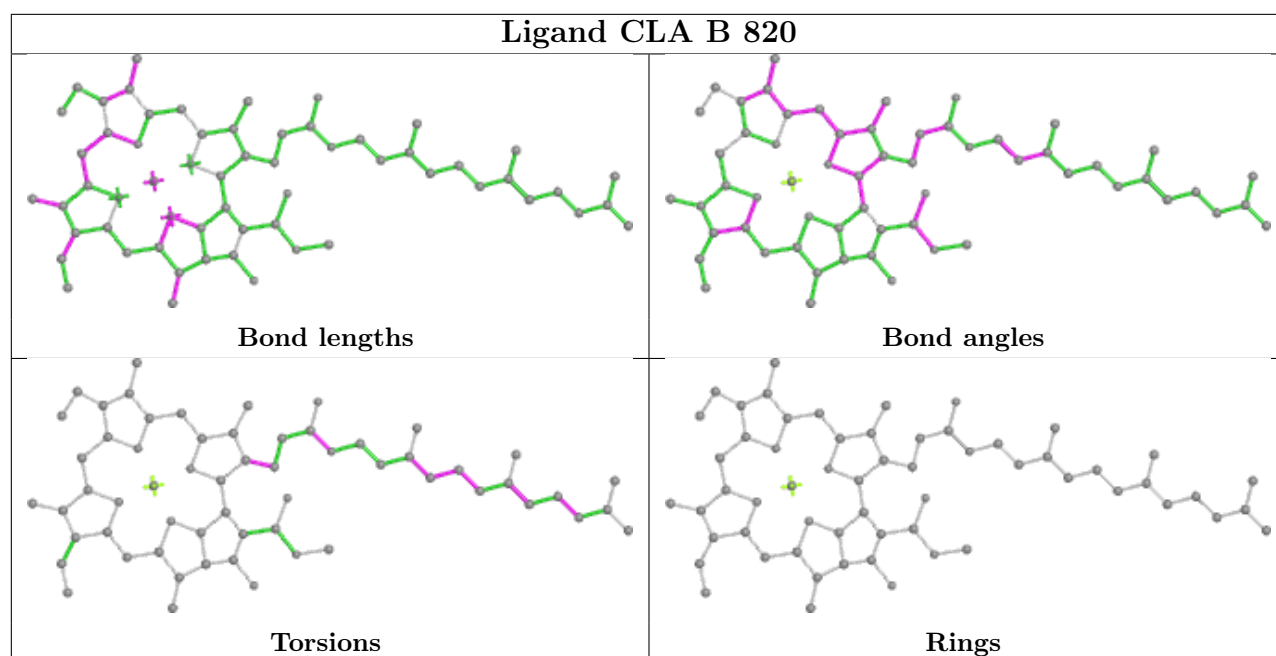


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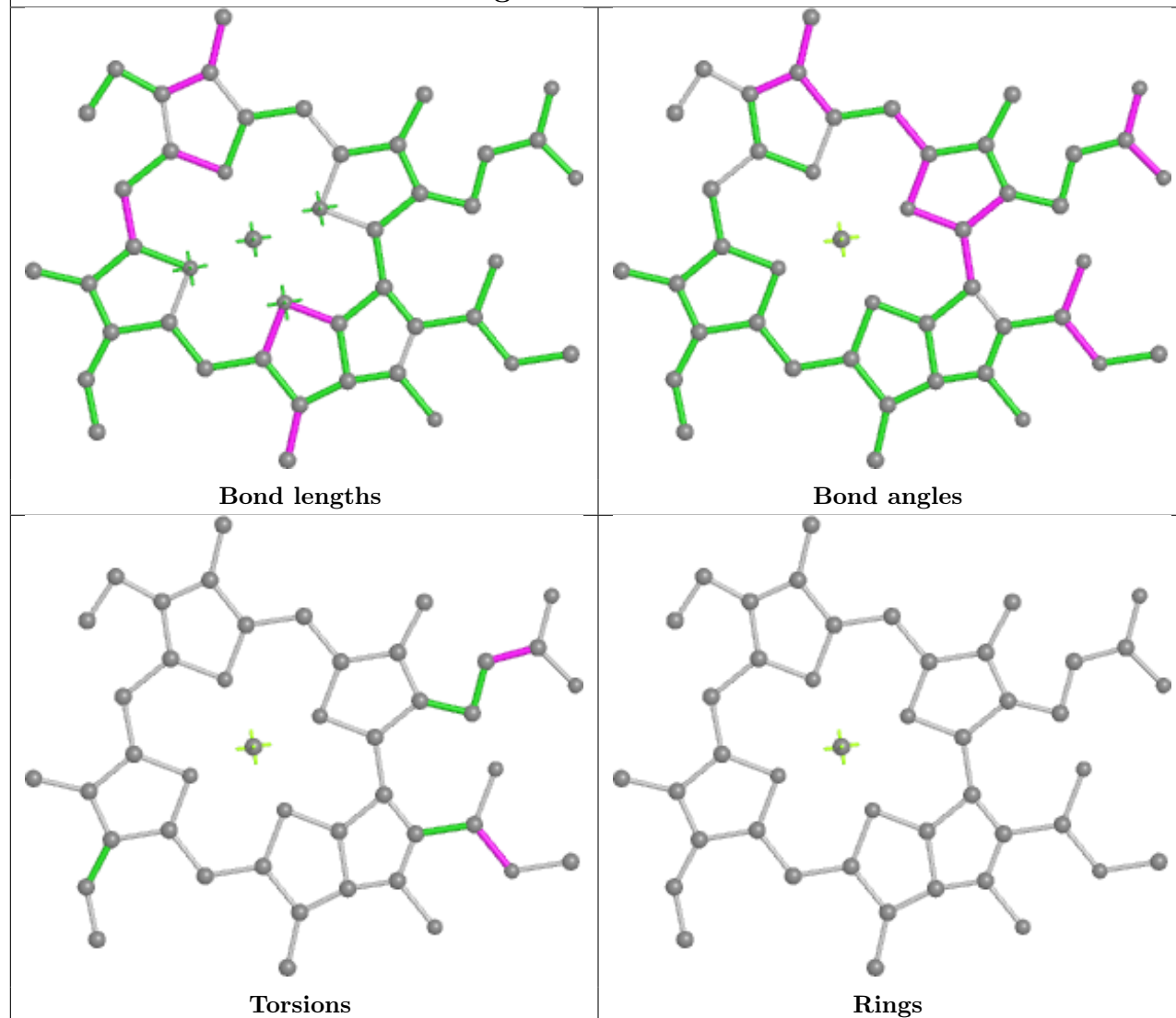


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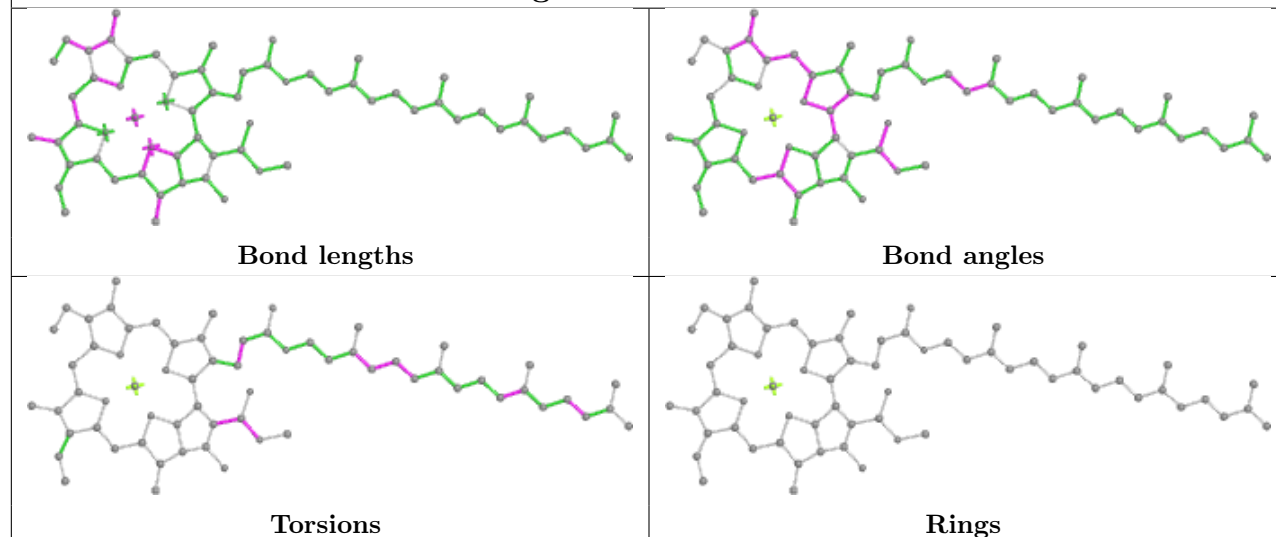


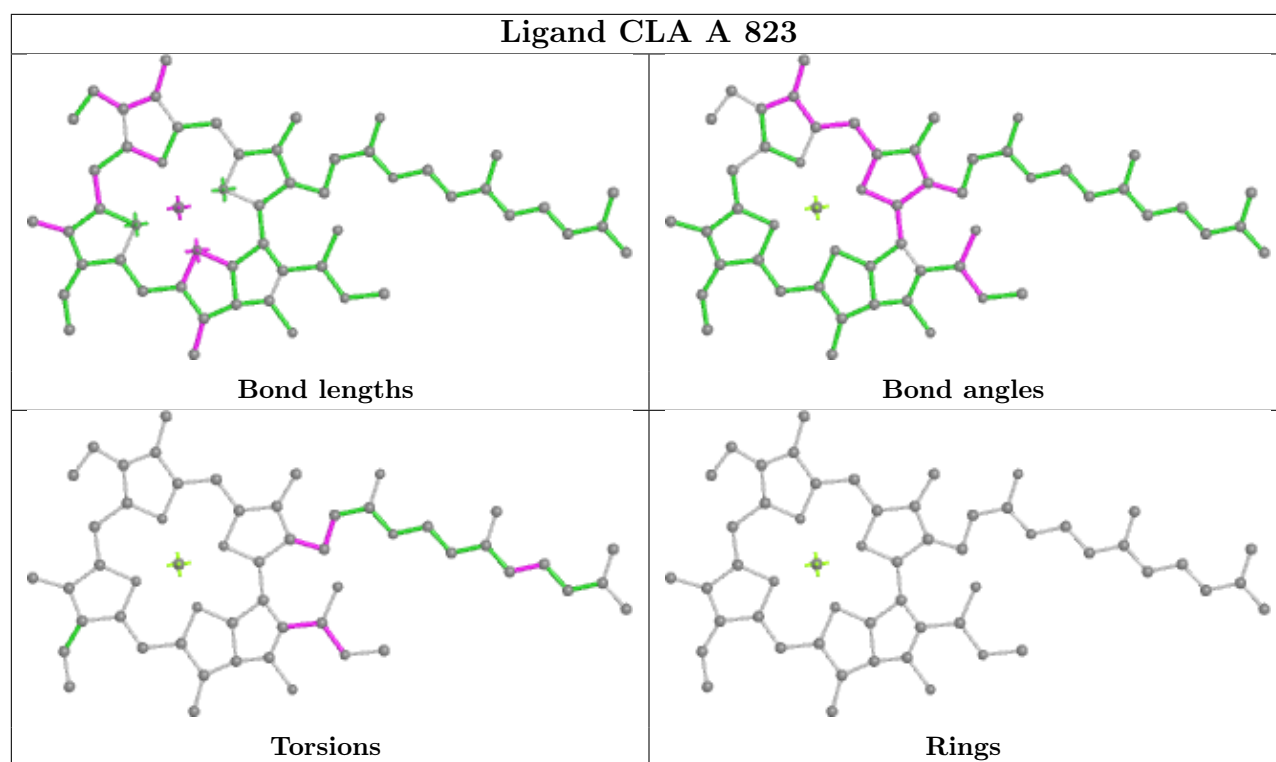


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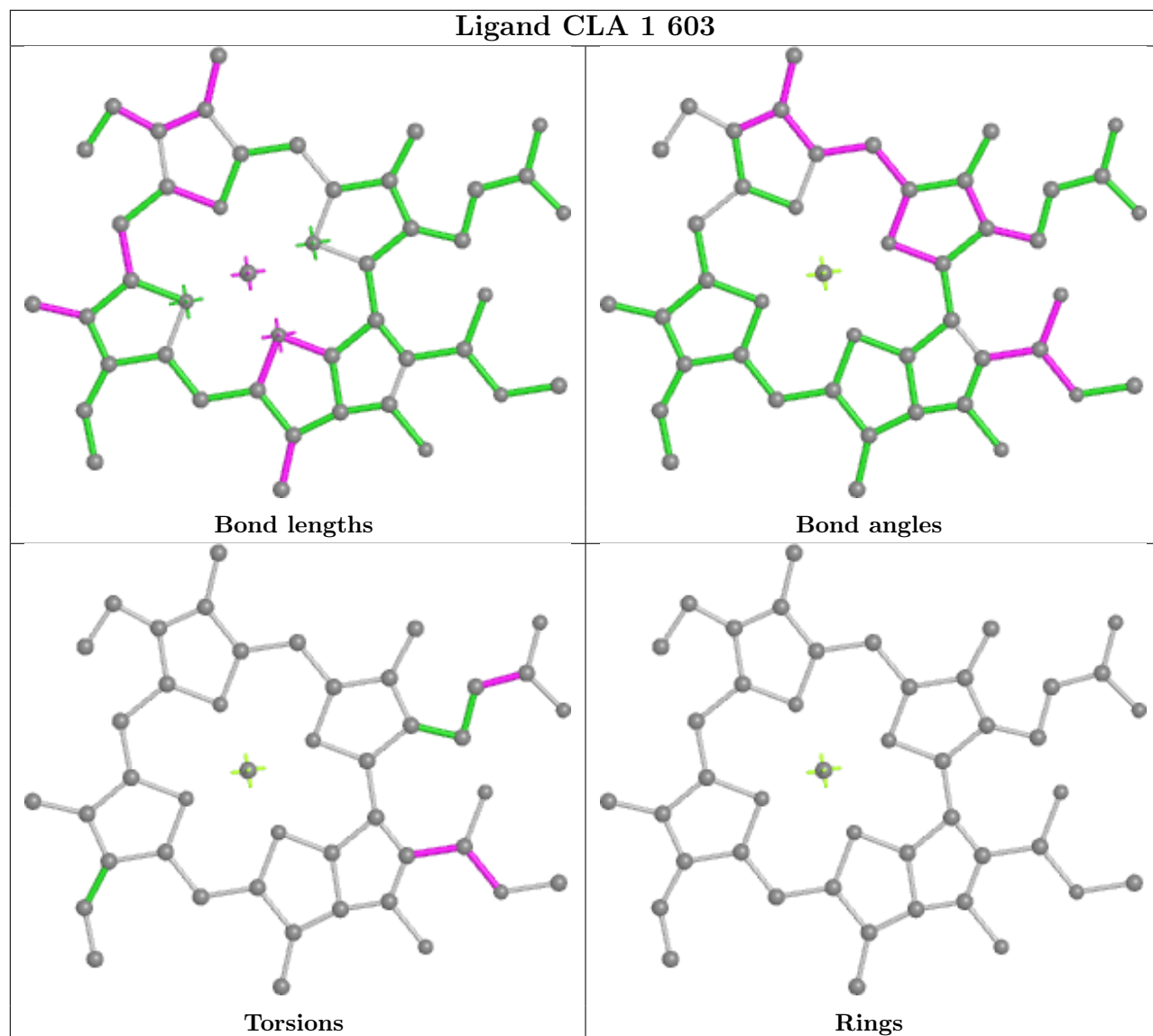


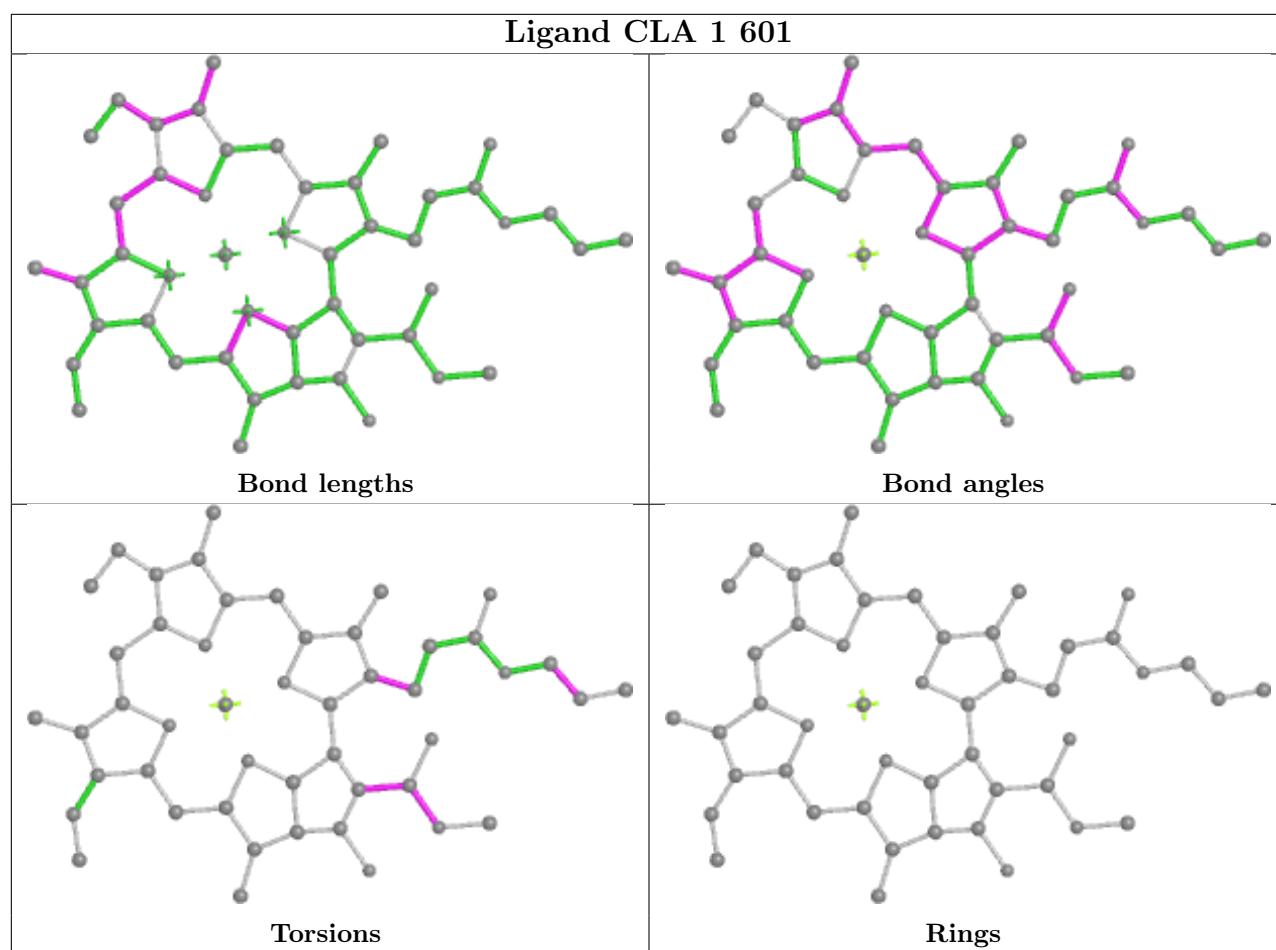
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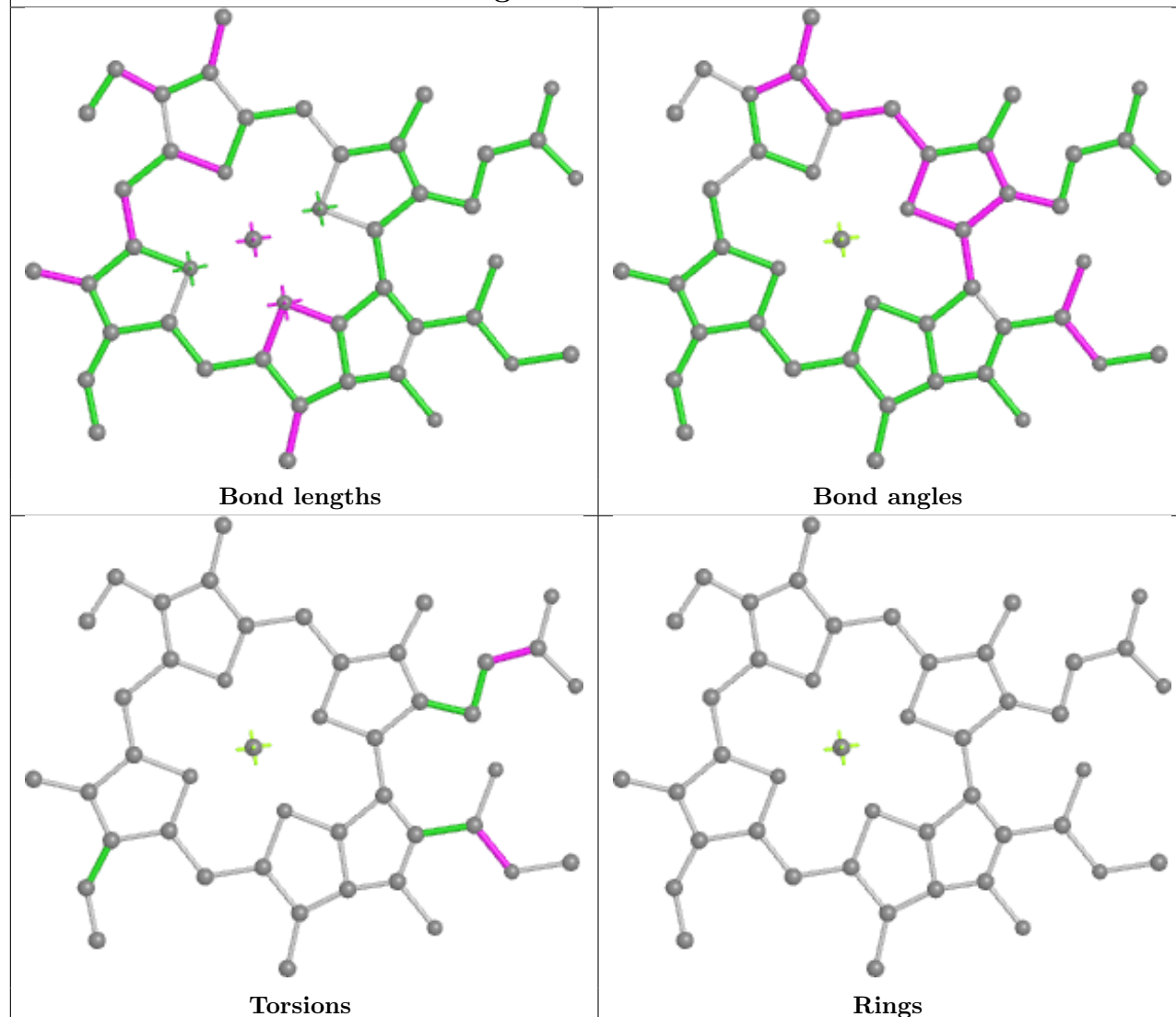


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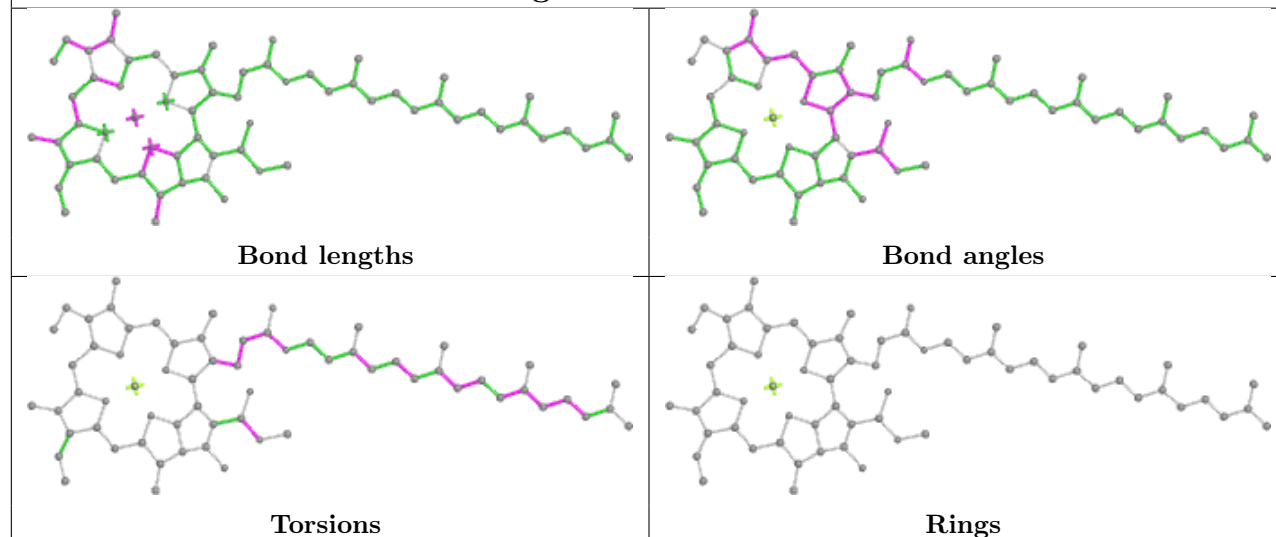


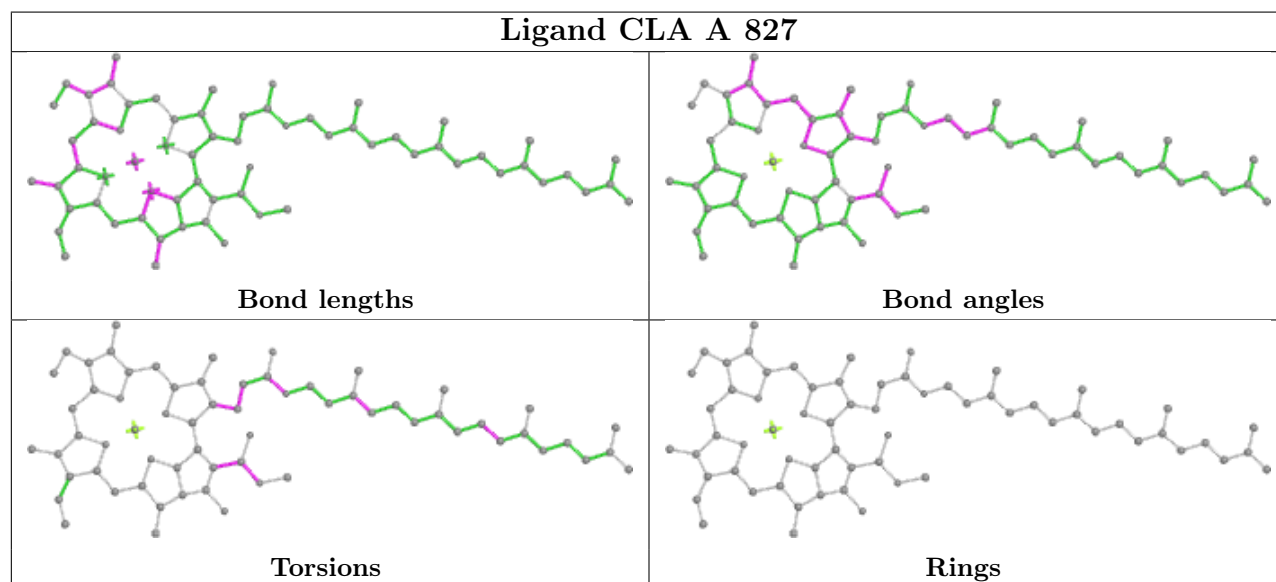
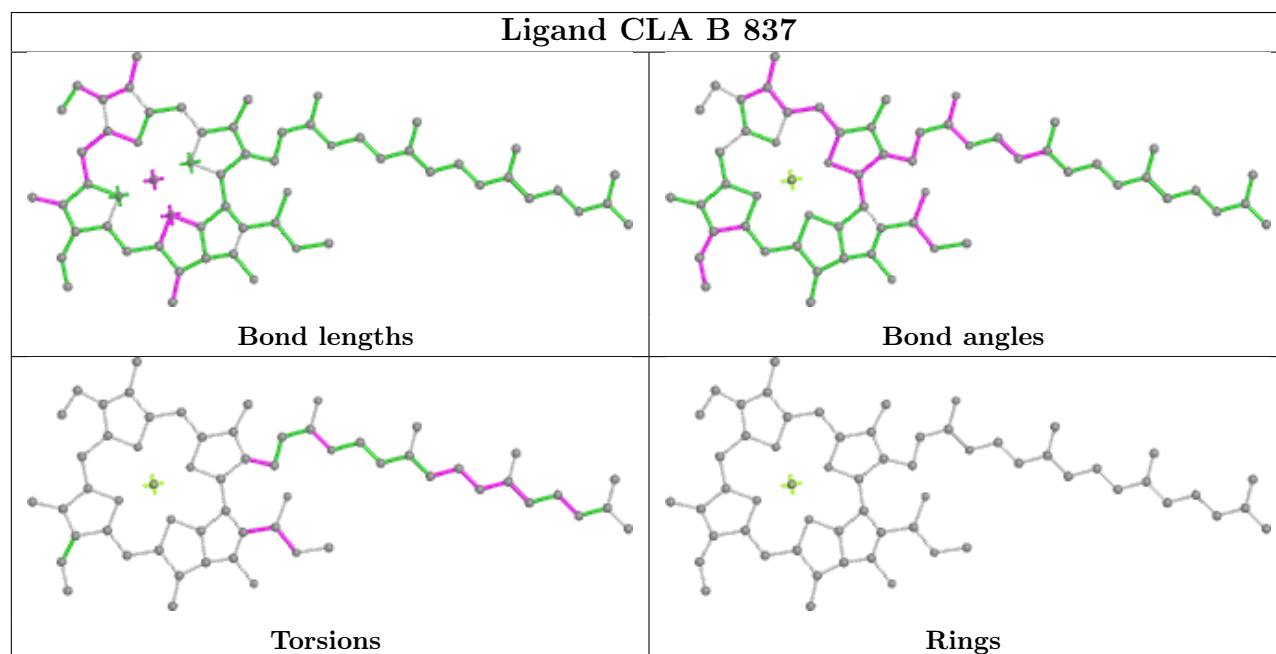
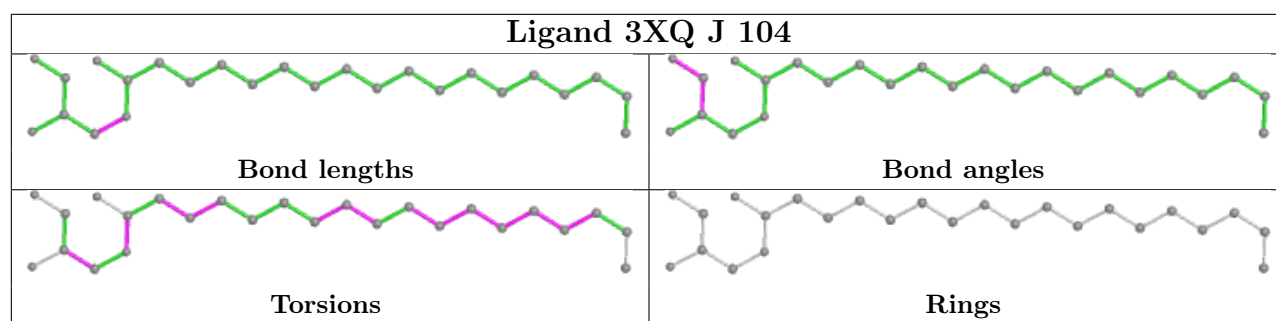


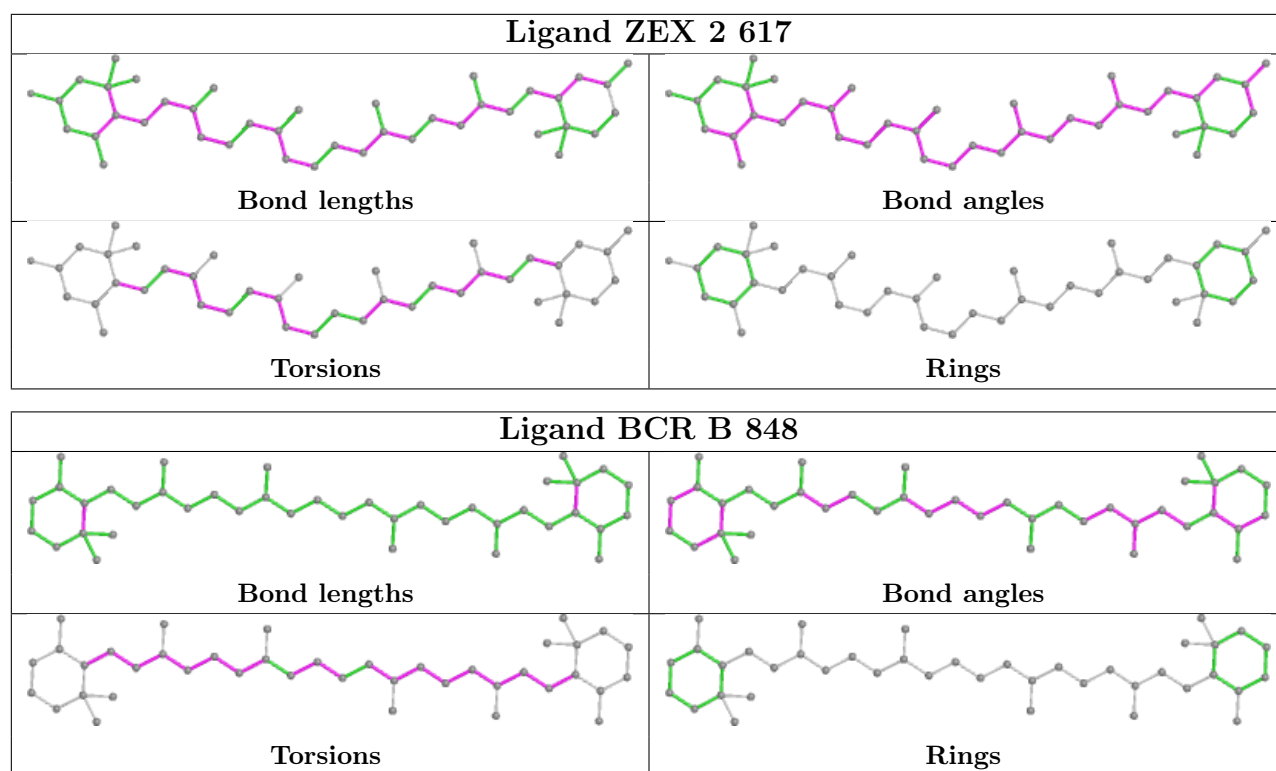
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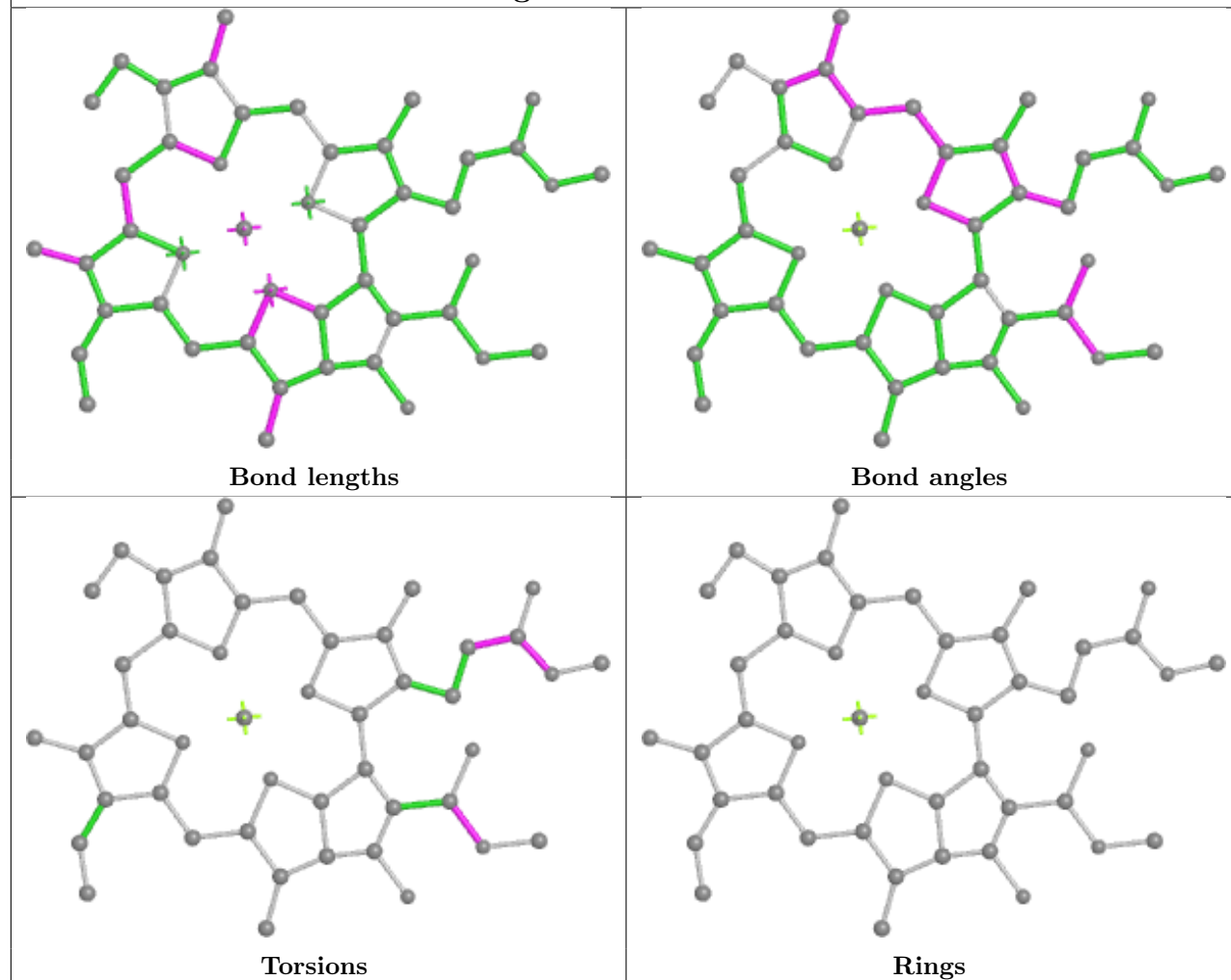
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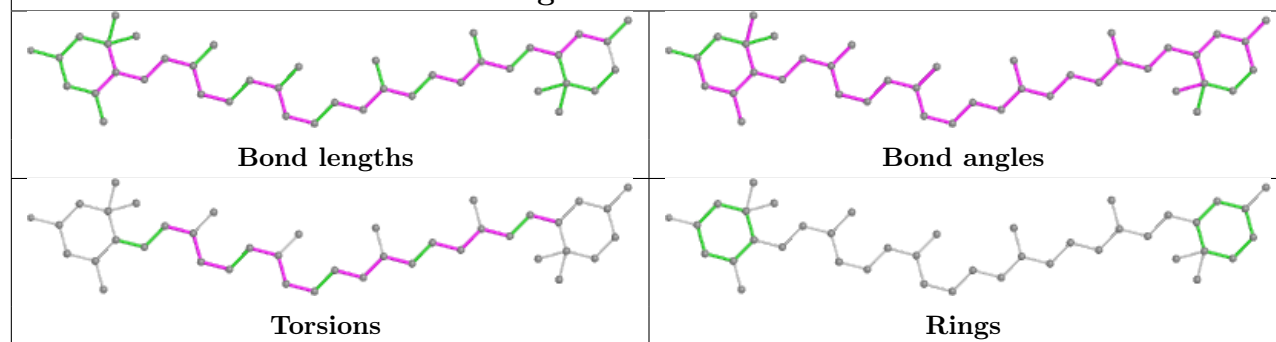


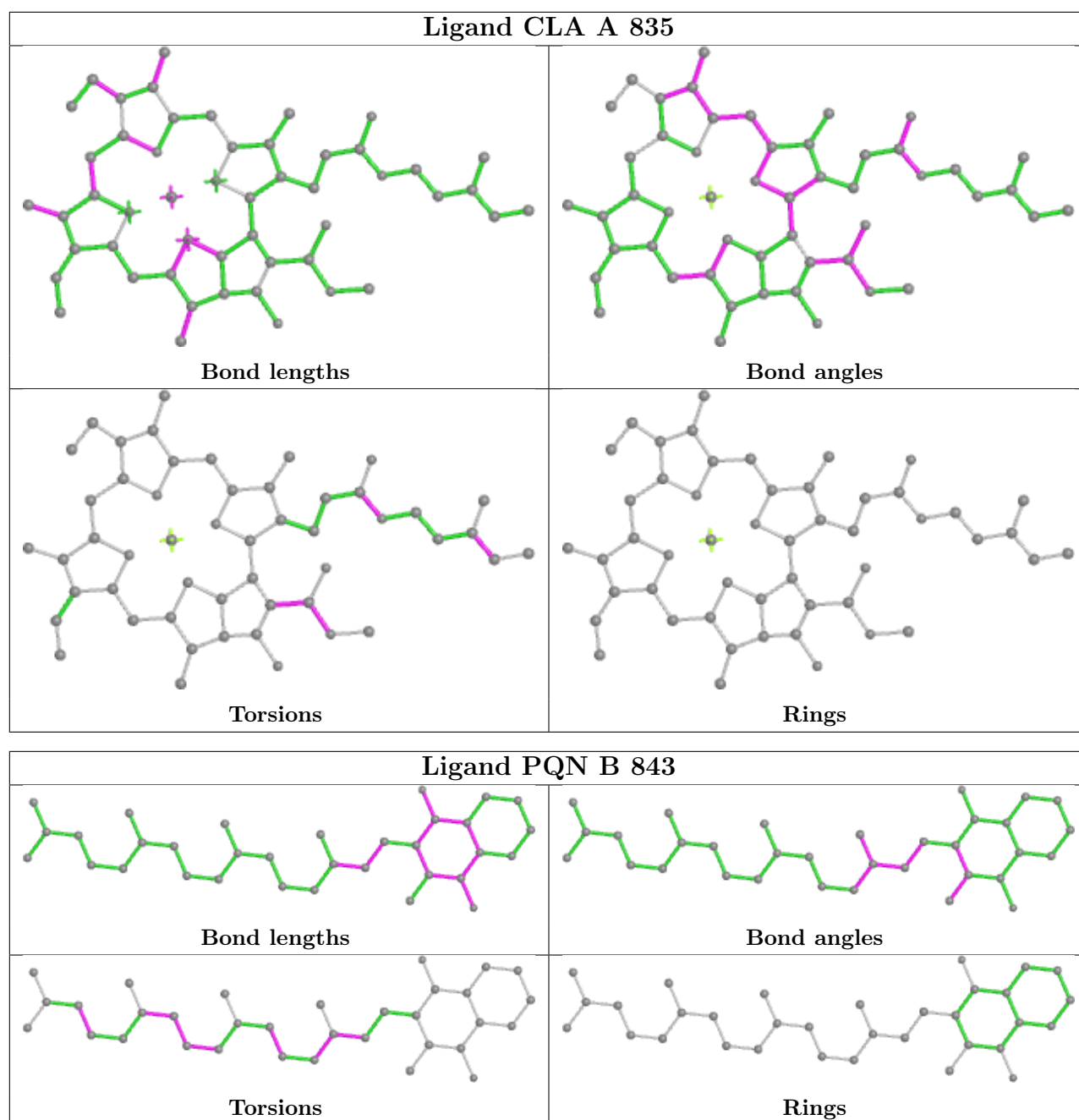


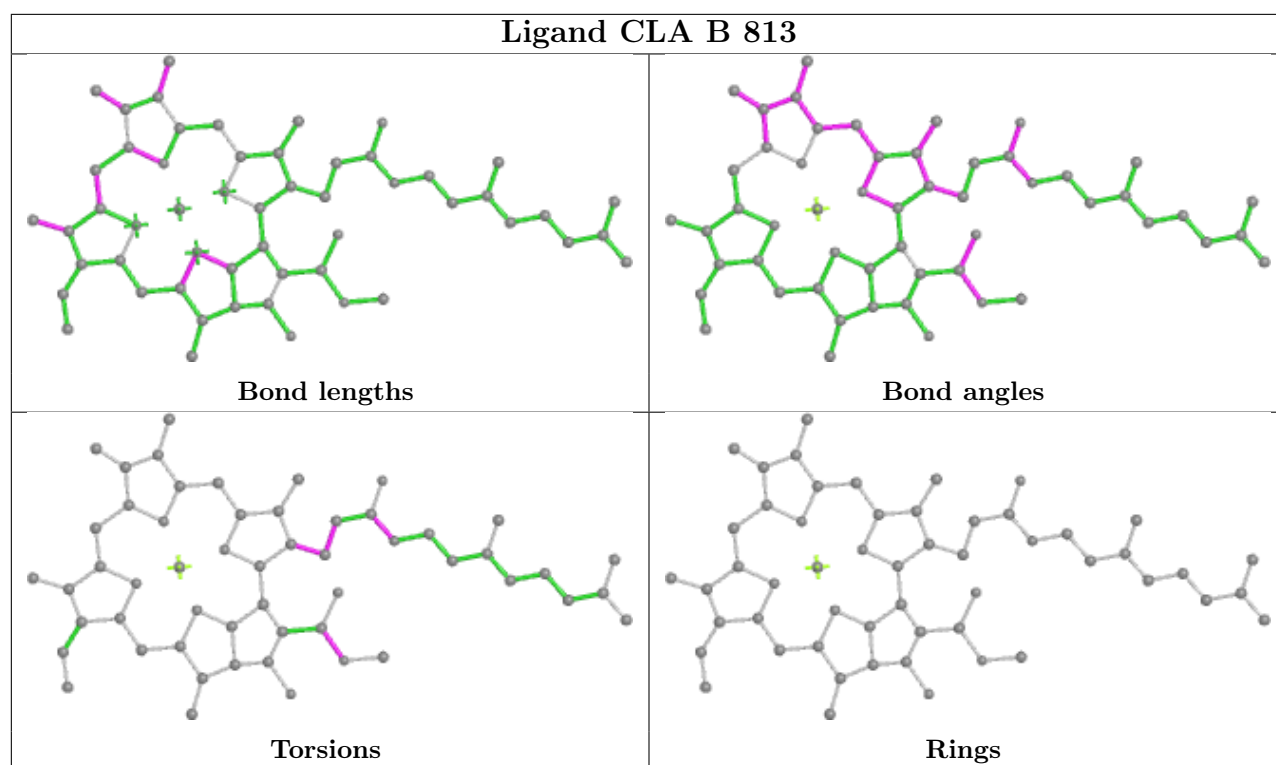
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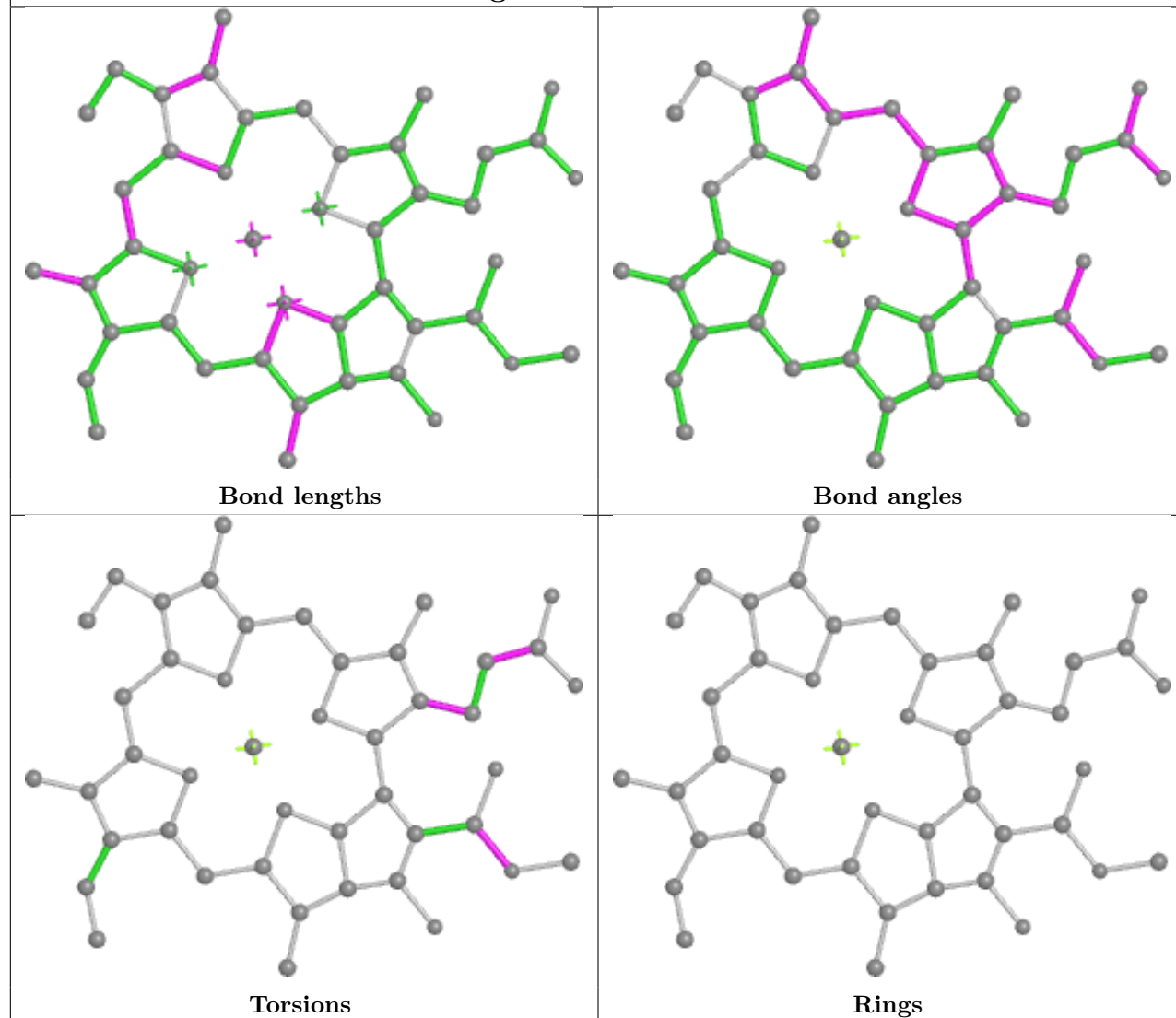
Ligand ZEX 2 614



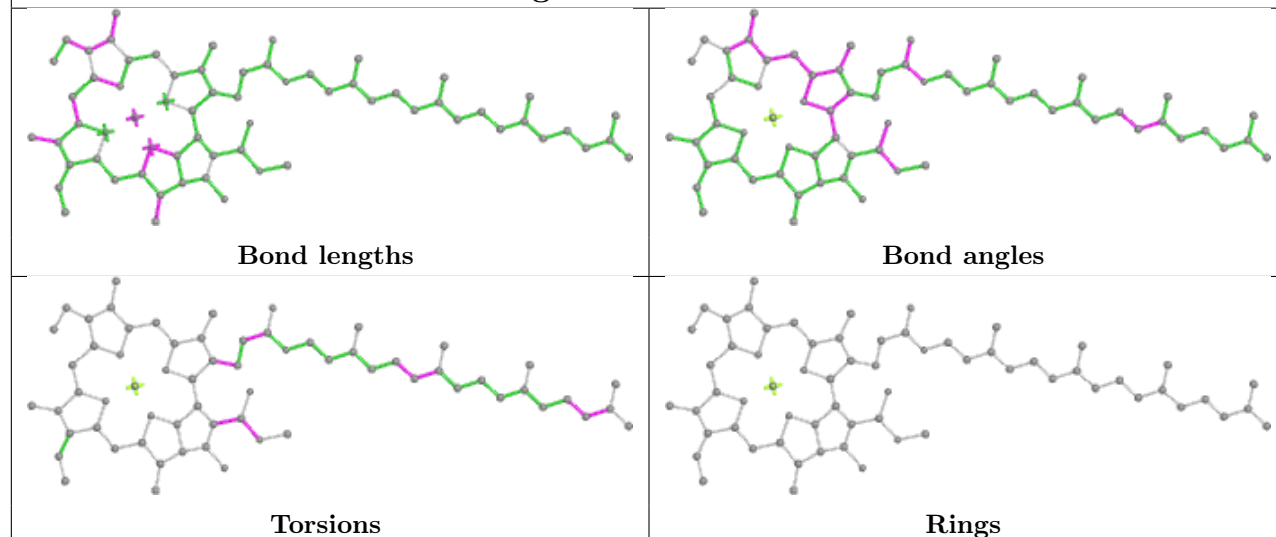


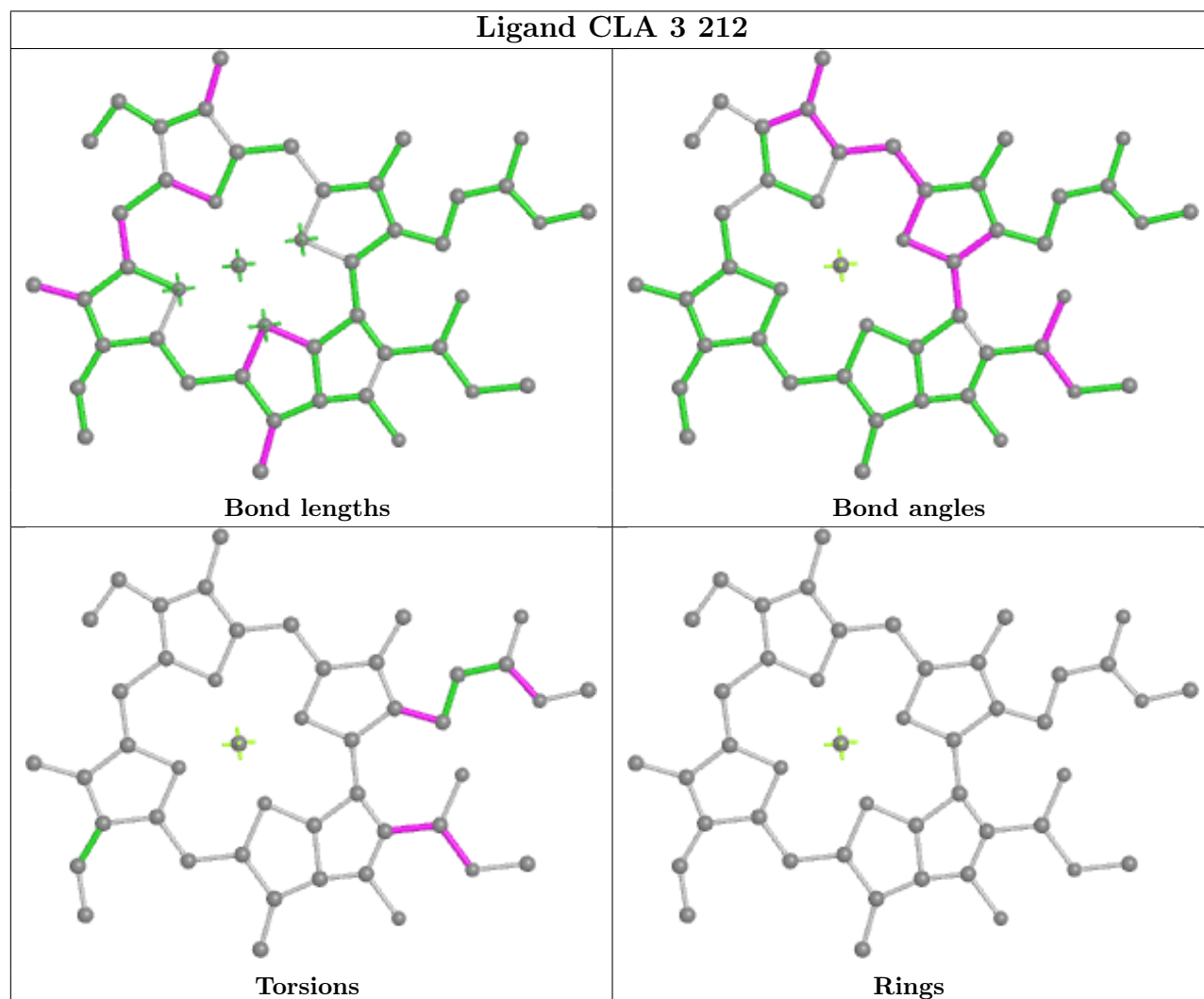
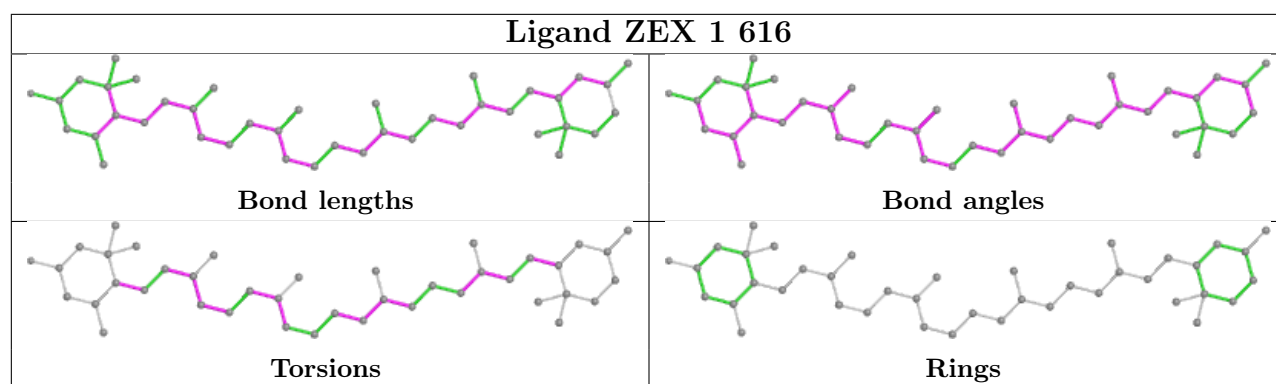


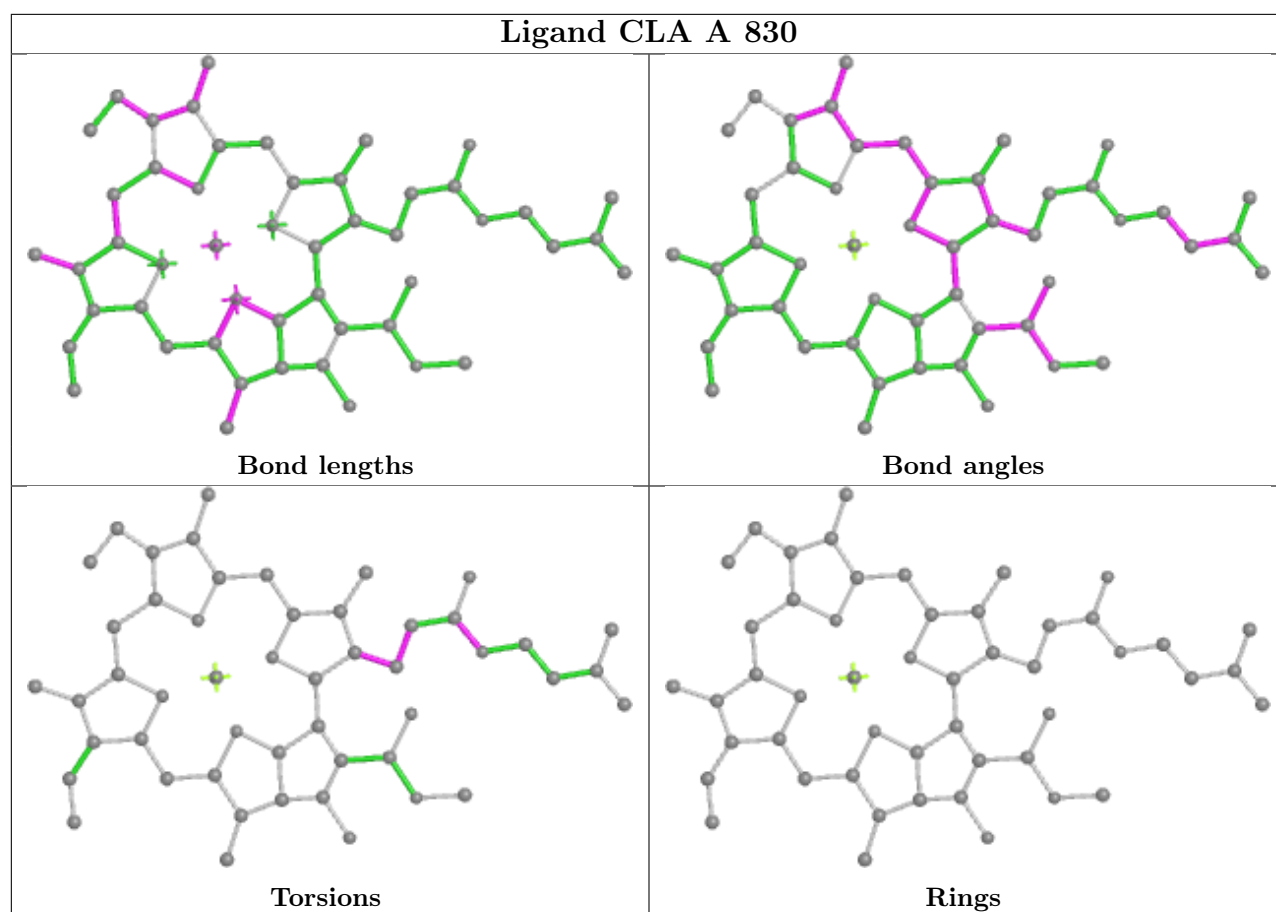
Ligand CLA A 834



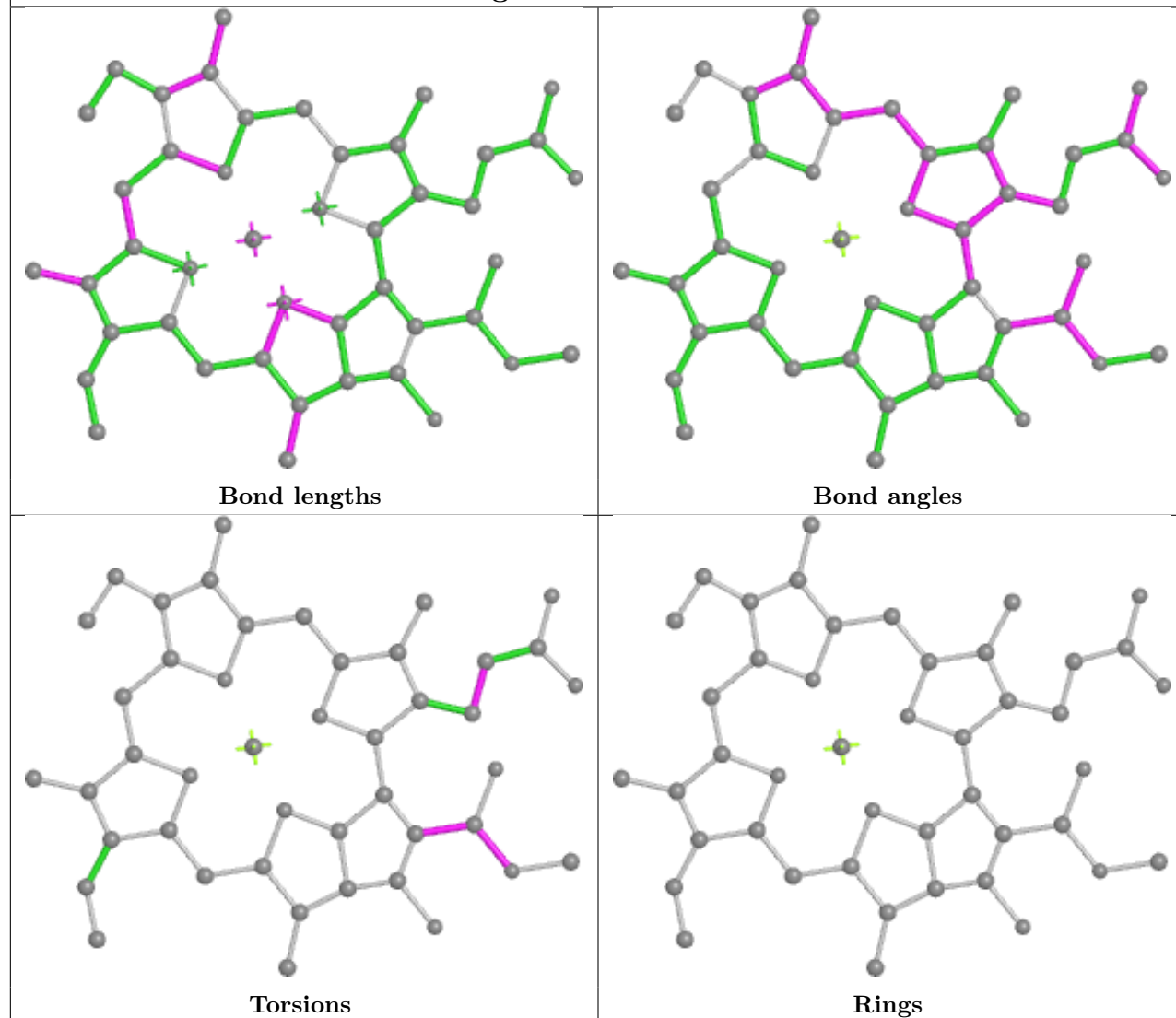
Ligand CLA B 807



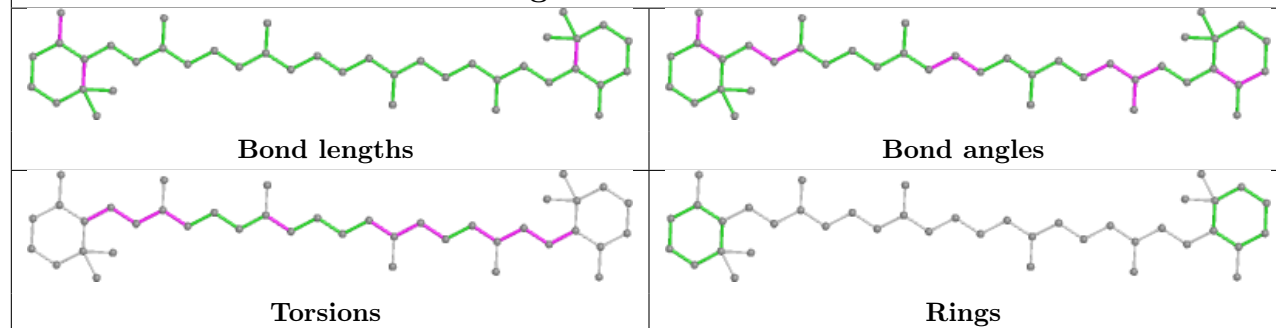




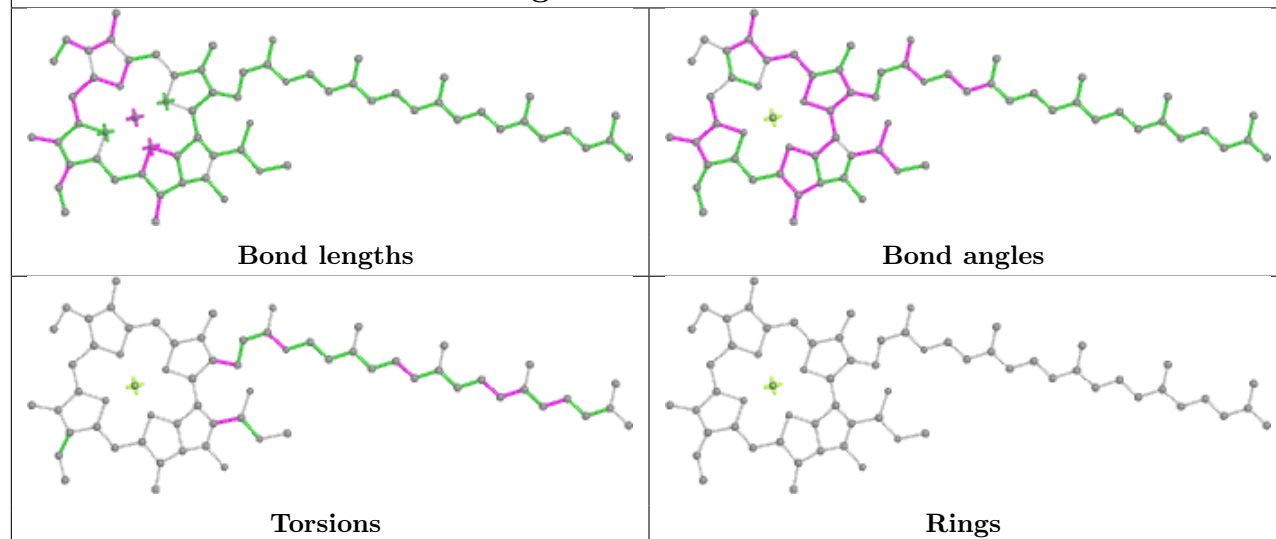
Ligand CLA F 802



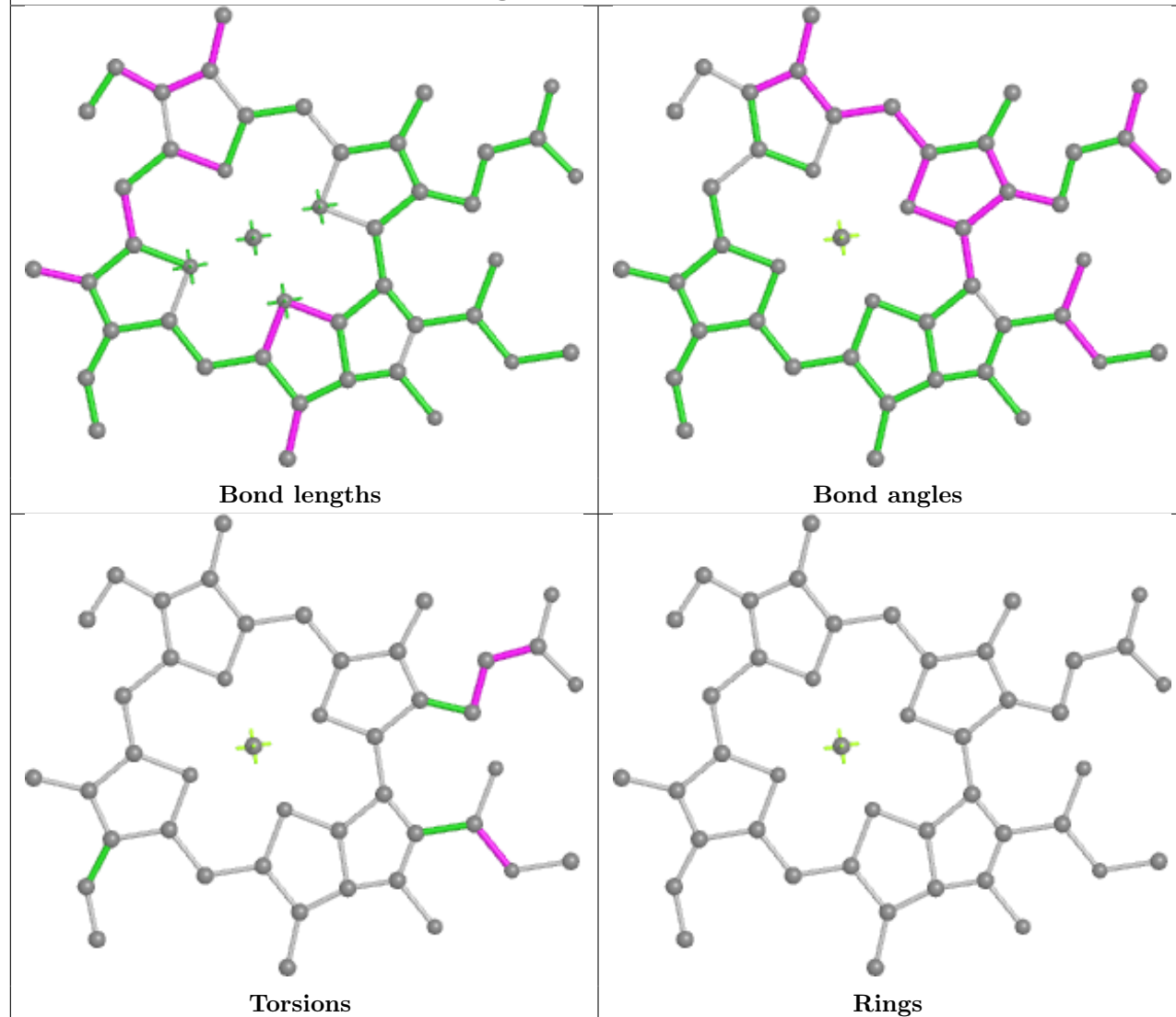
Ligand BCR A 847



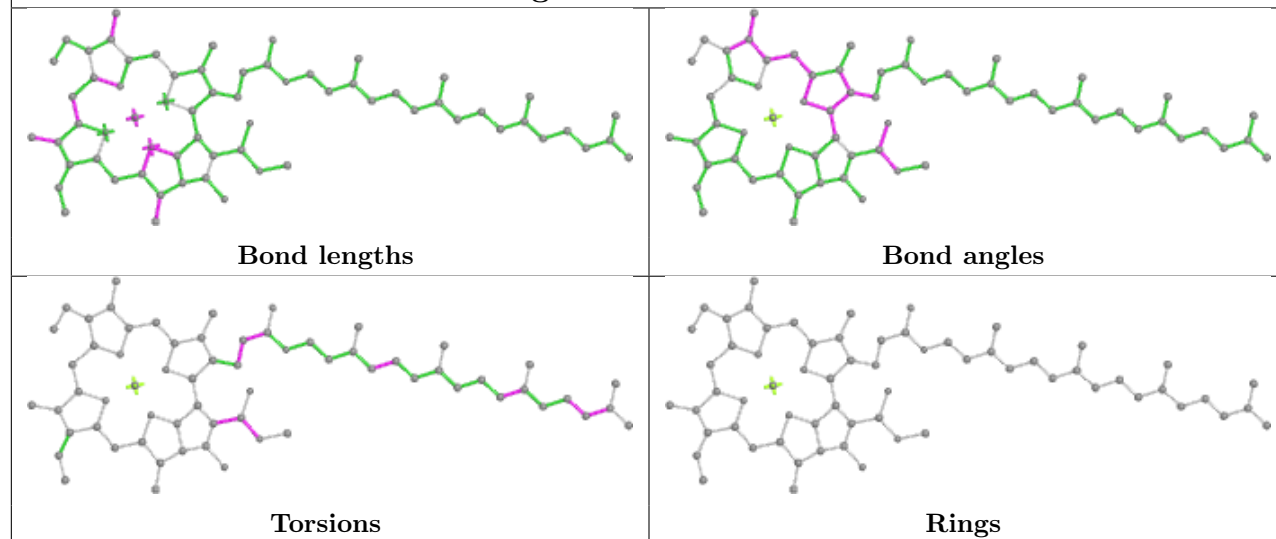
Ligand CLA A 829



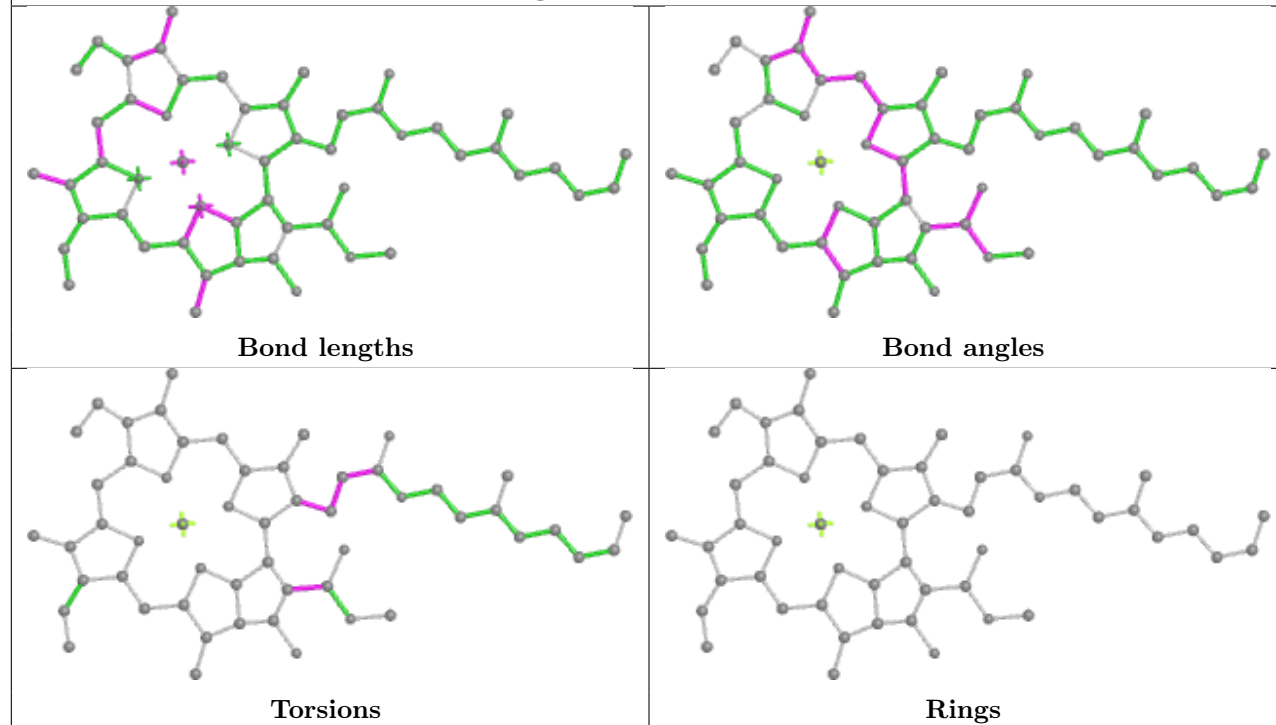
Ligand CLA 2 605

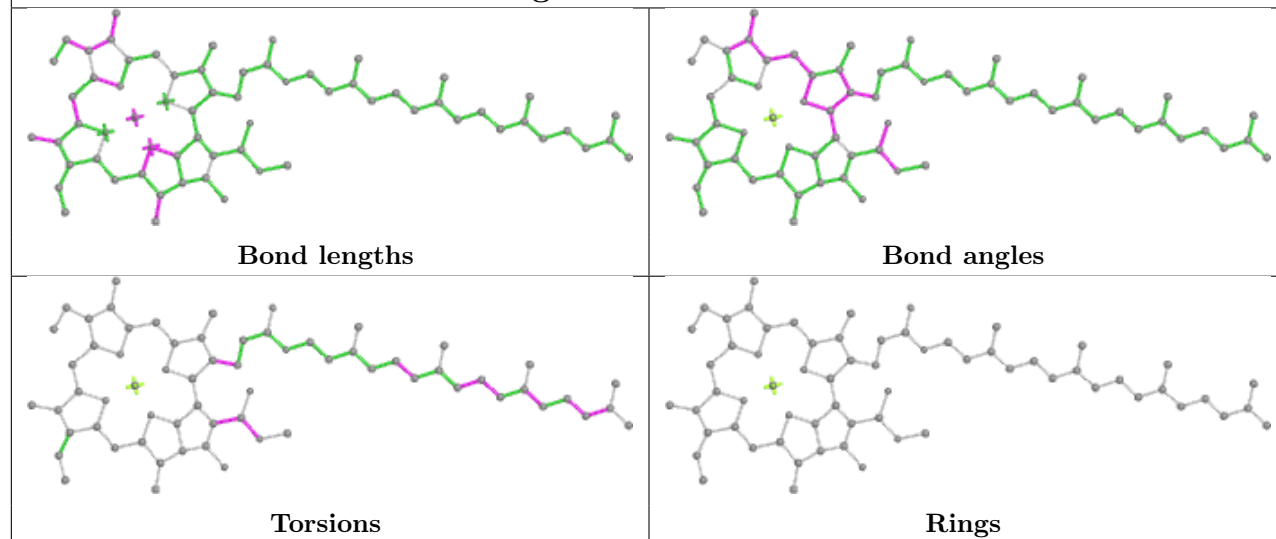
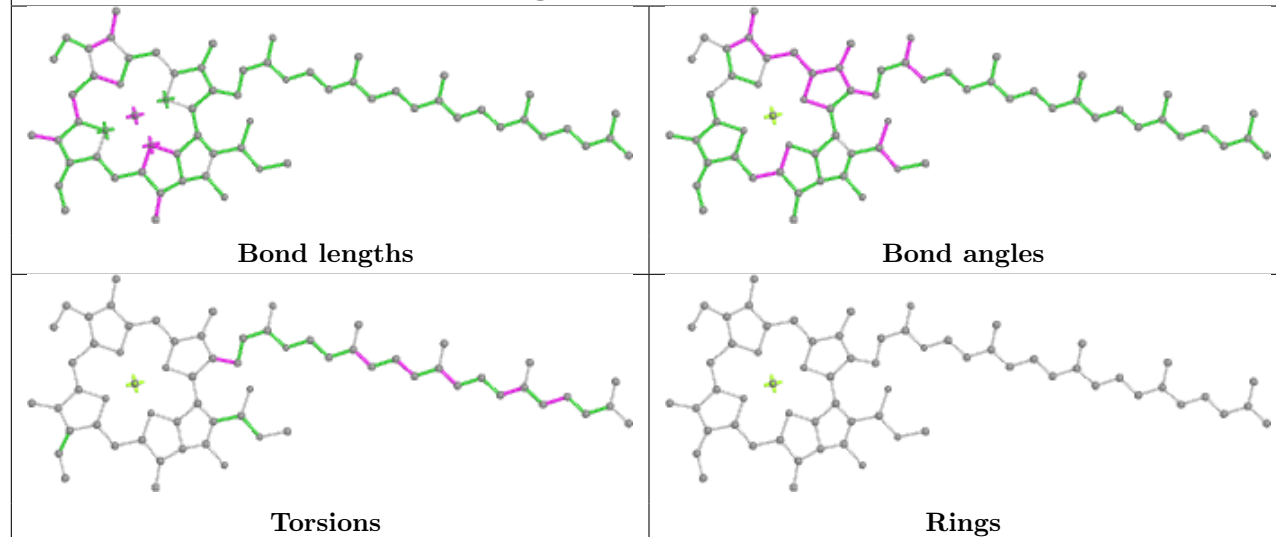
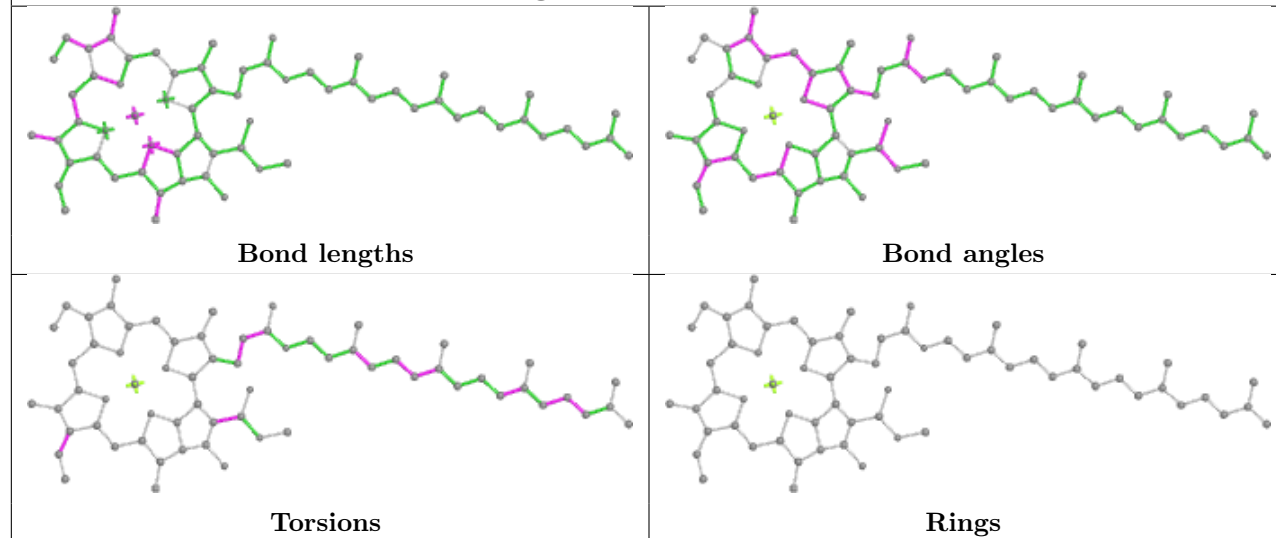


Ligand CLA A 837

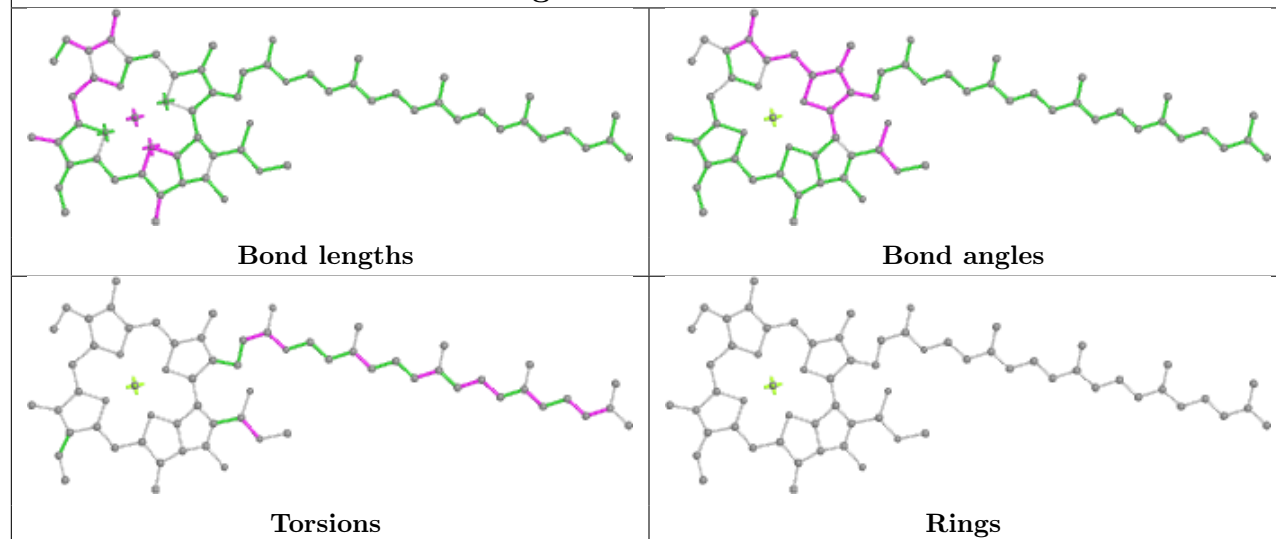


Ligand CLA A 811

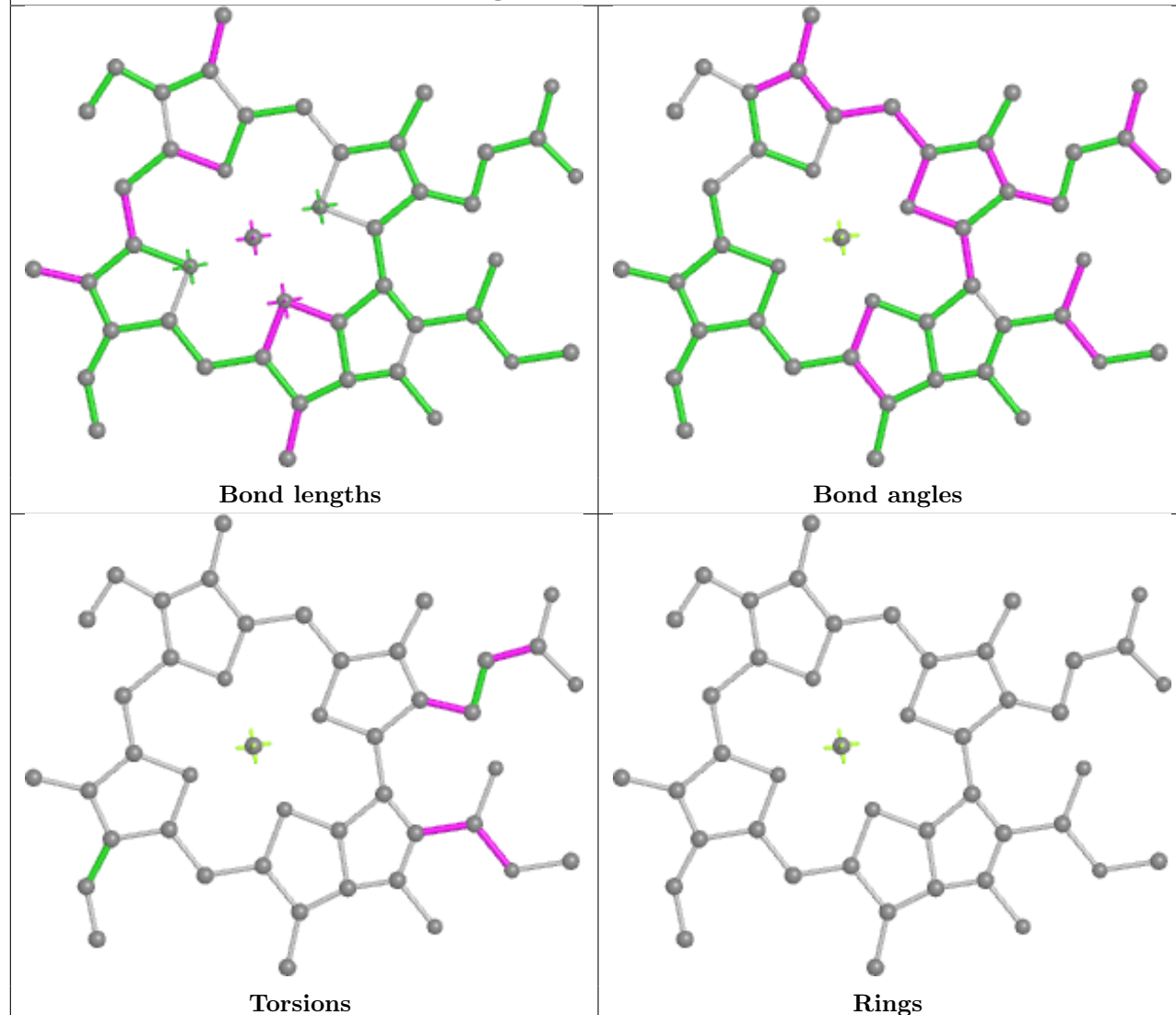


Ligand CLA B 821**Ligand CLA A 833****Ligand CLA B 809**

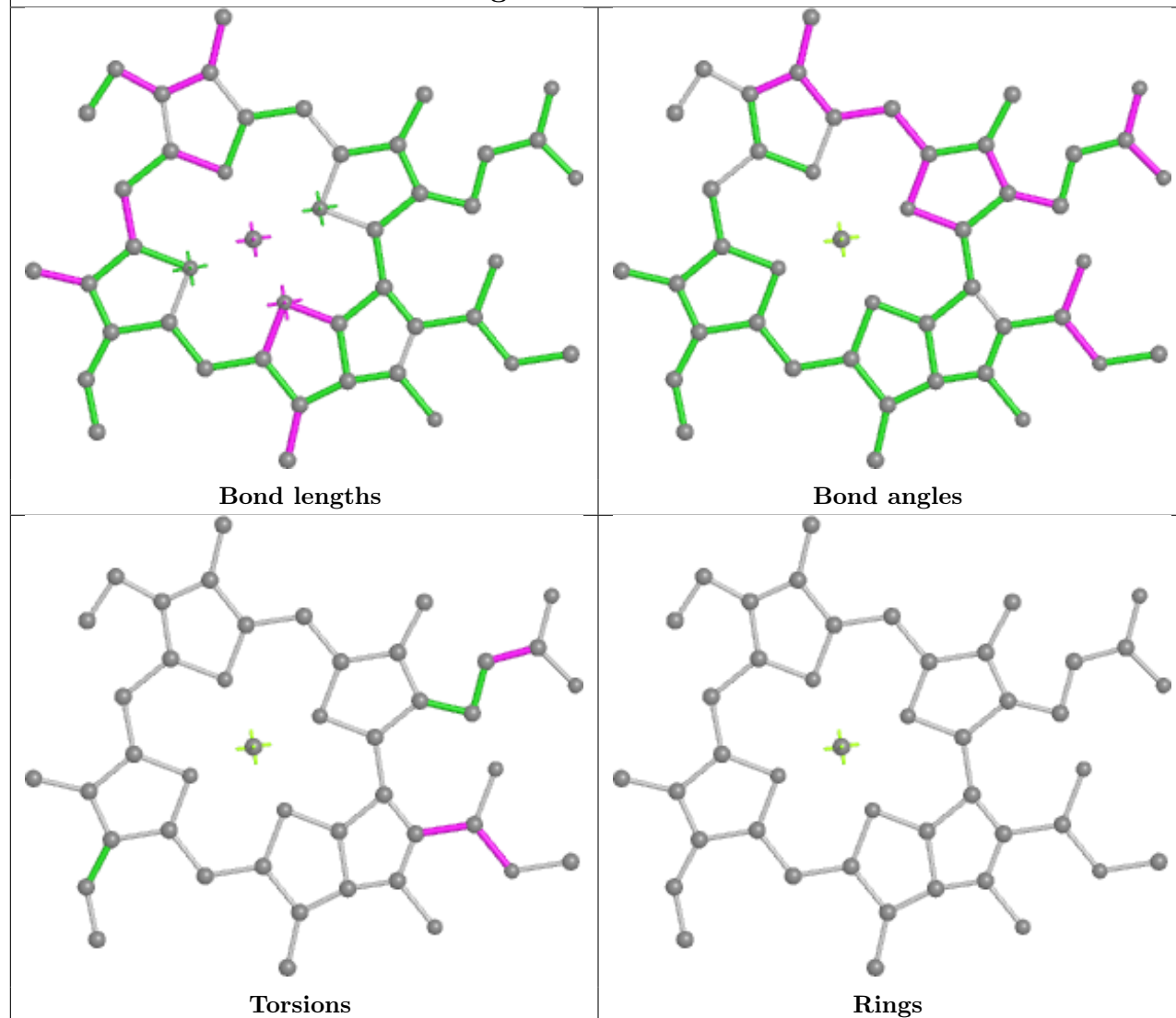
Ligand CLA B 808



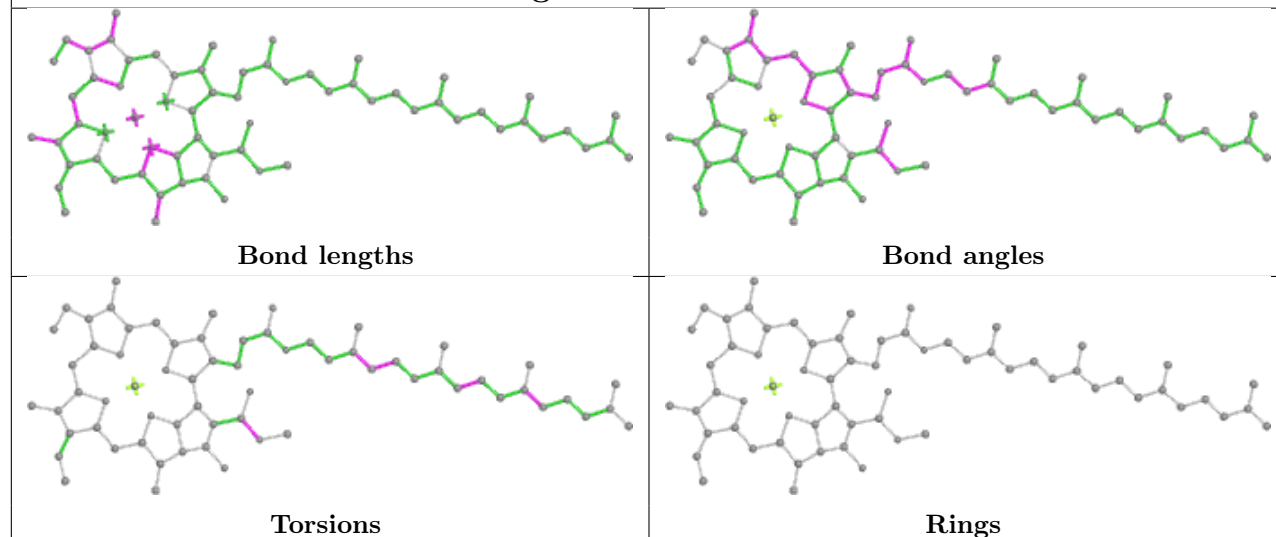
Ligand CLA A 813

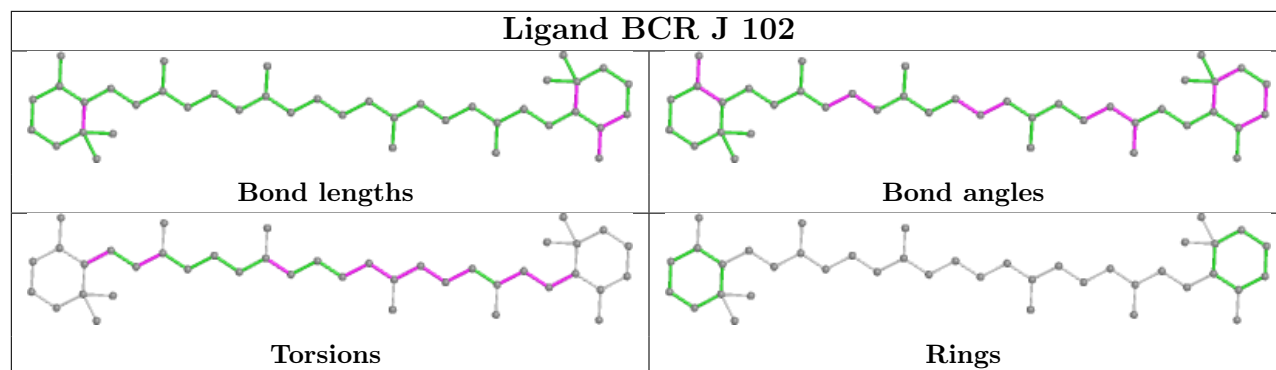
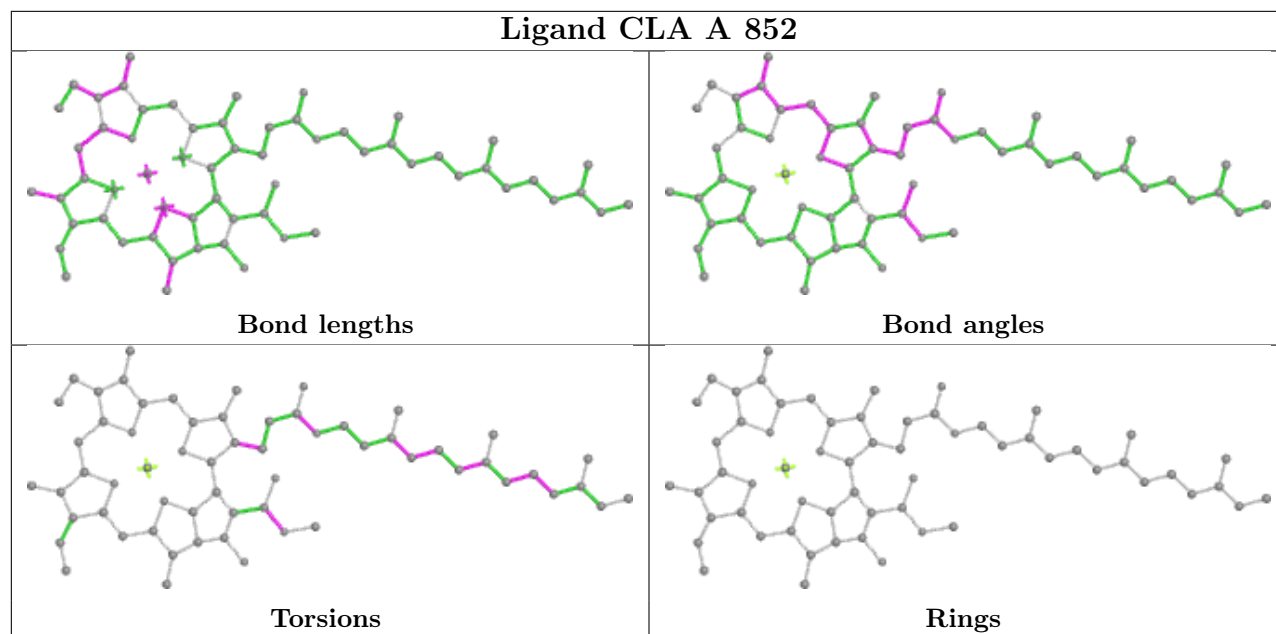
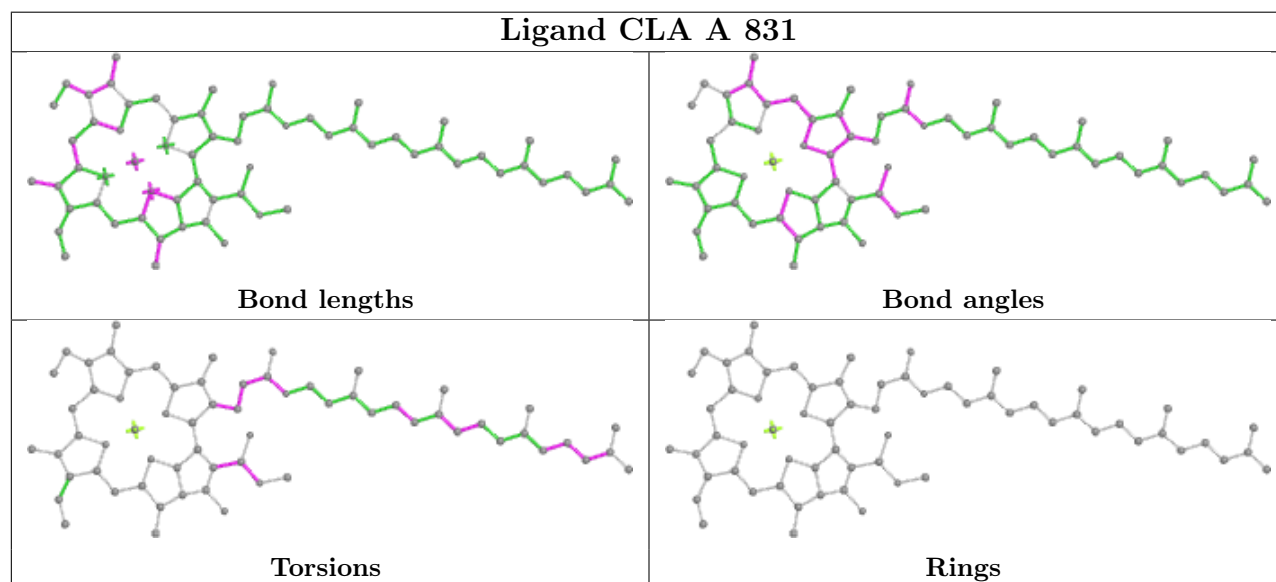


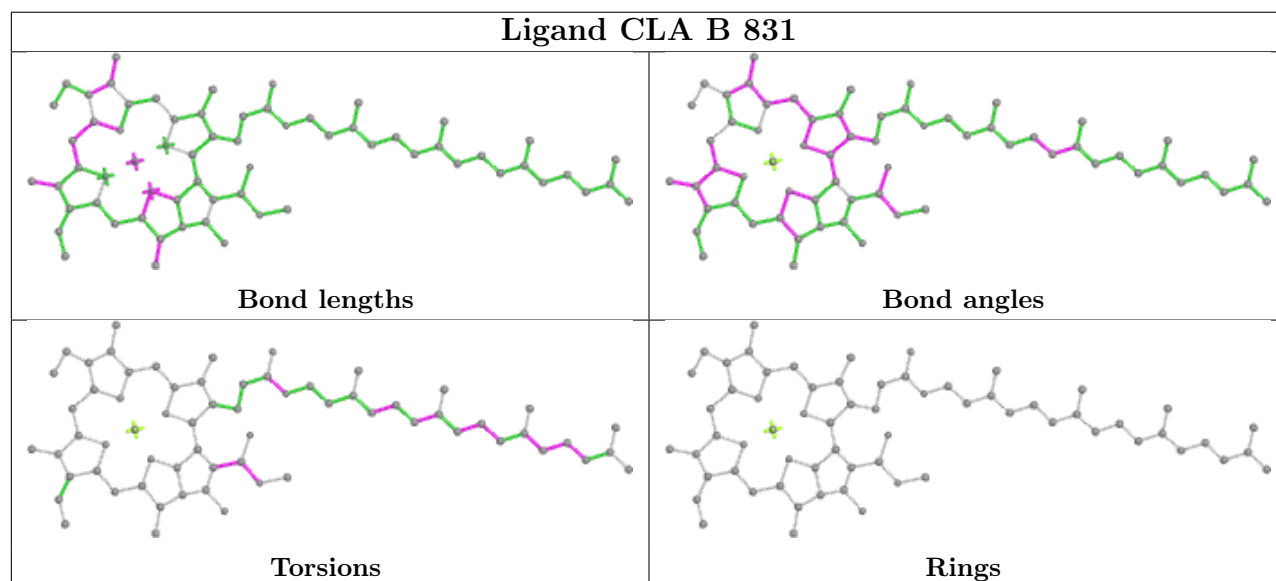
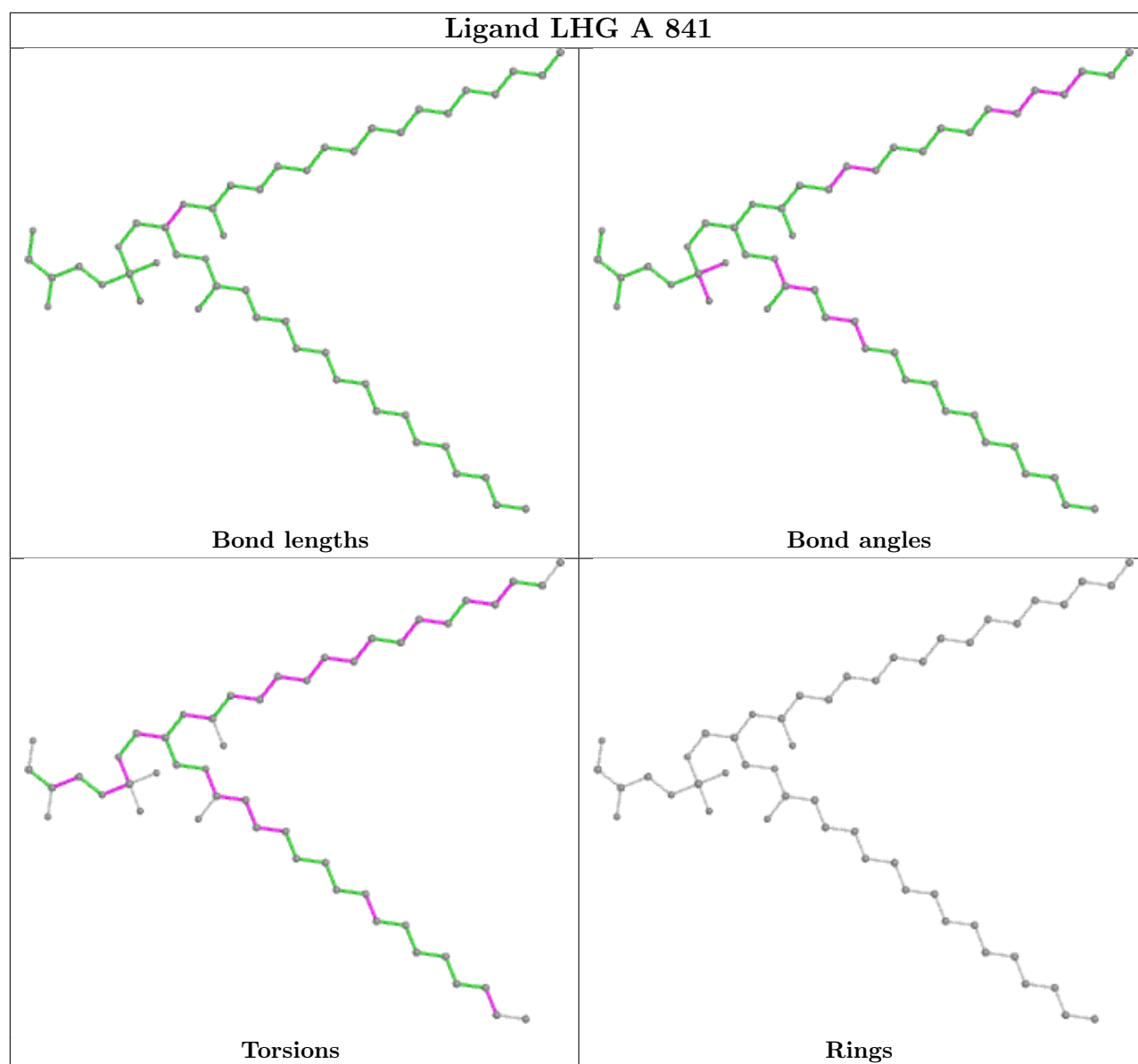
Ligand CLA B 822



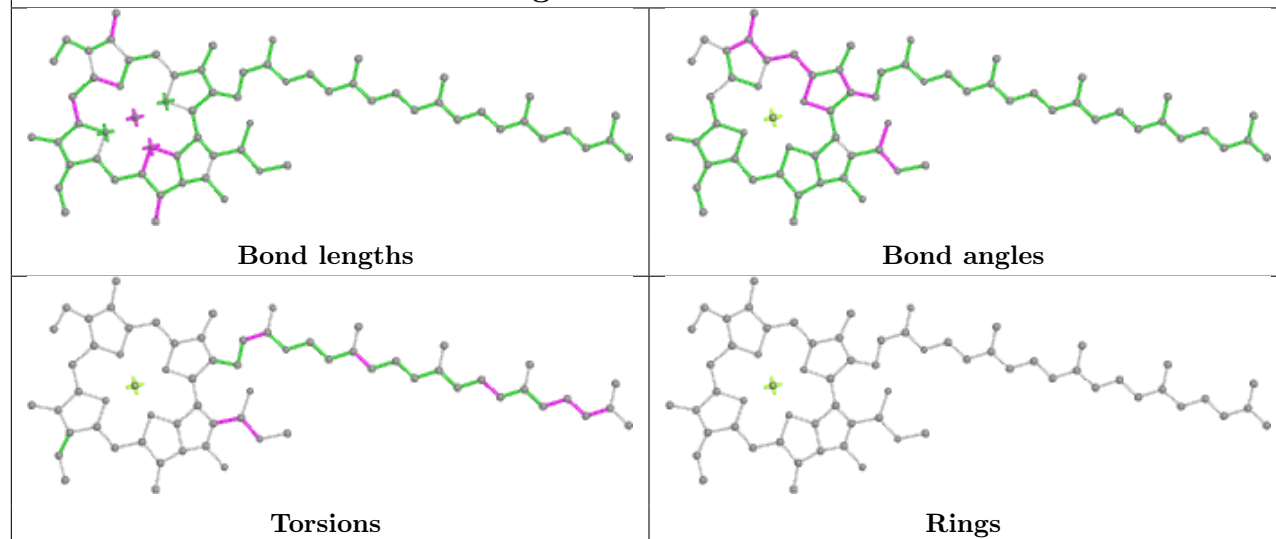
Ligand CLA B 810



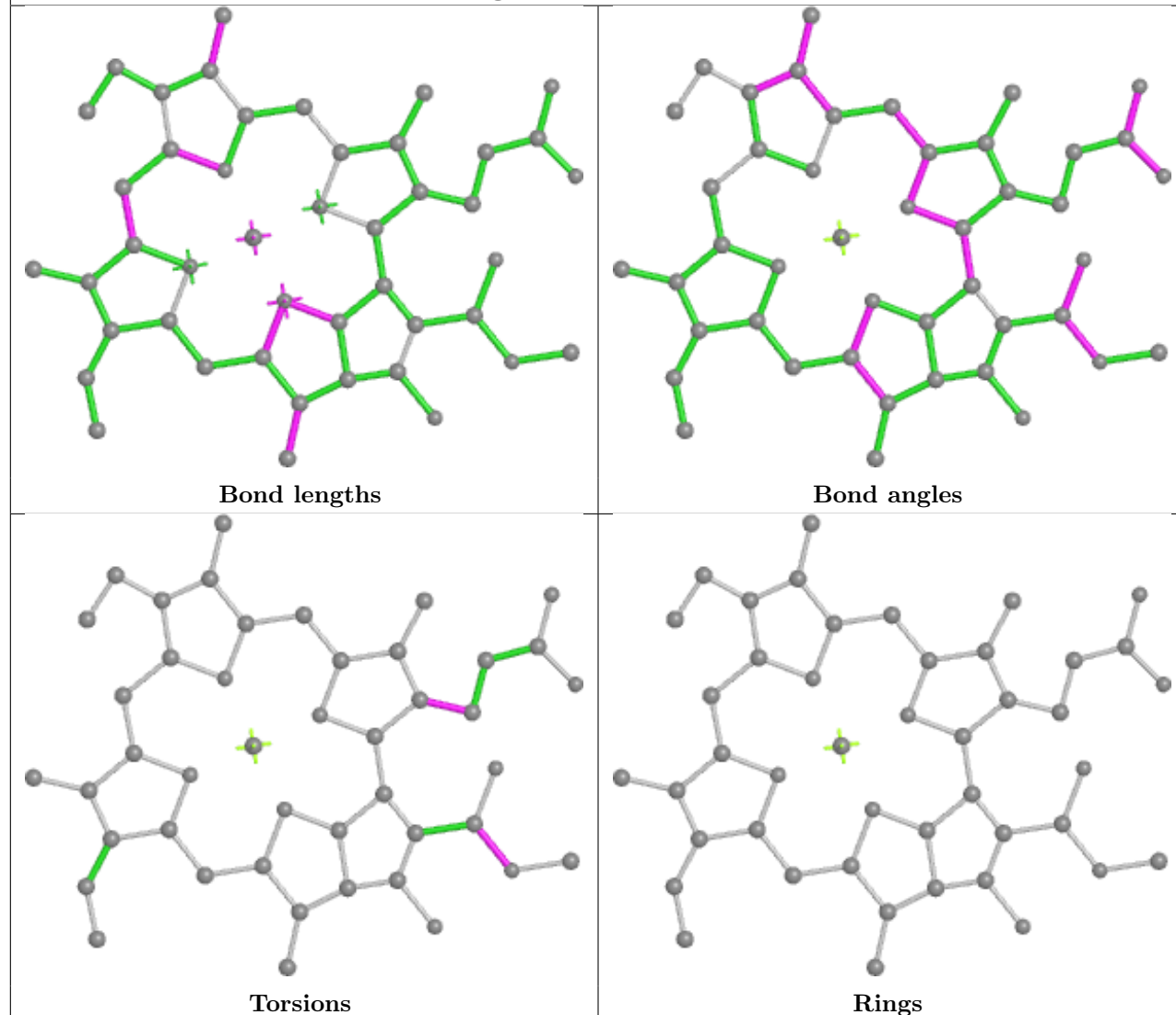
Ligand BCR J 102**Ligand CLA A 852****Ligand CLA A 831**



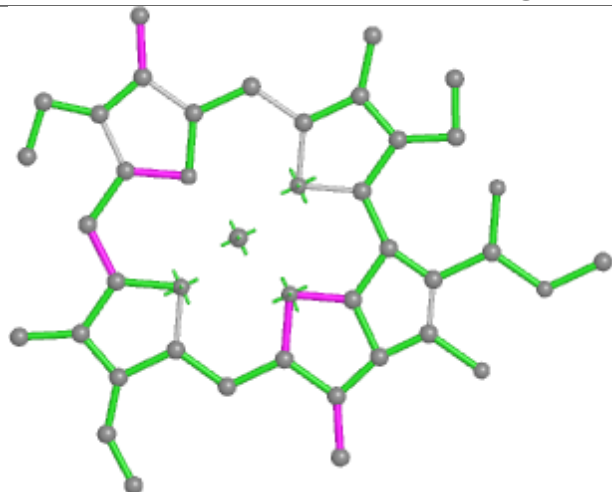
Ligand CLA B 842



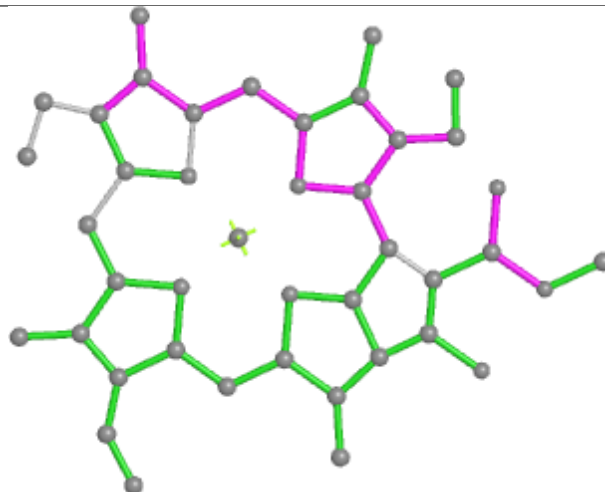
Ligand CLA O 204



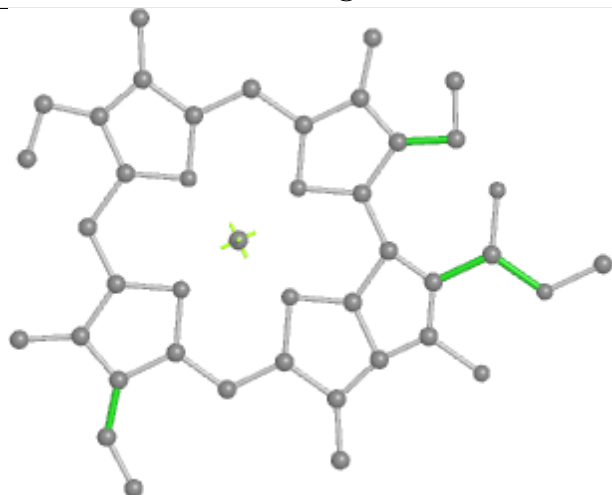
Ligand CLA 3 211



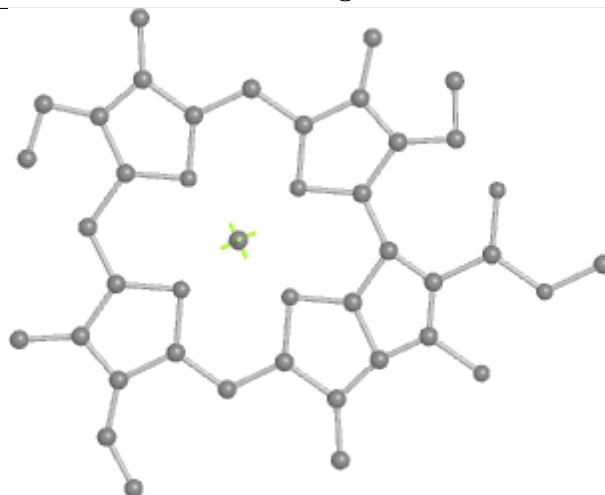
Bond lengths



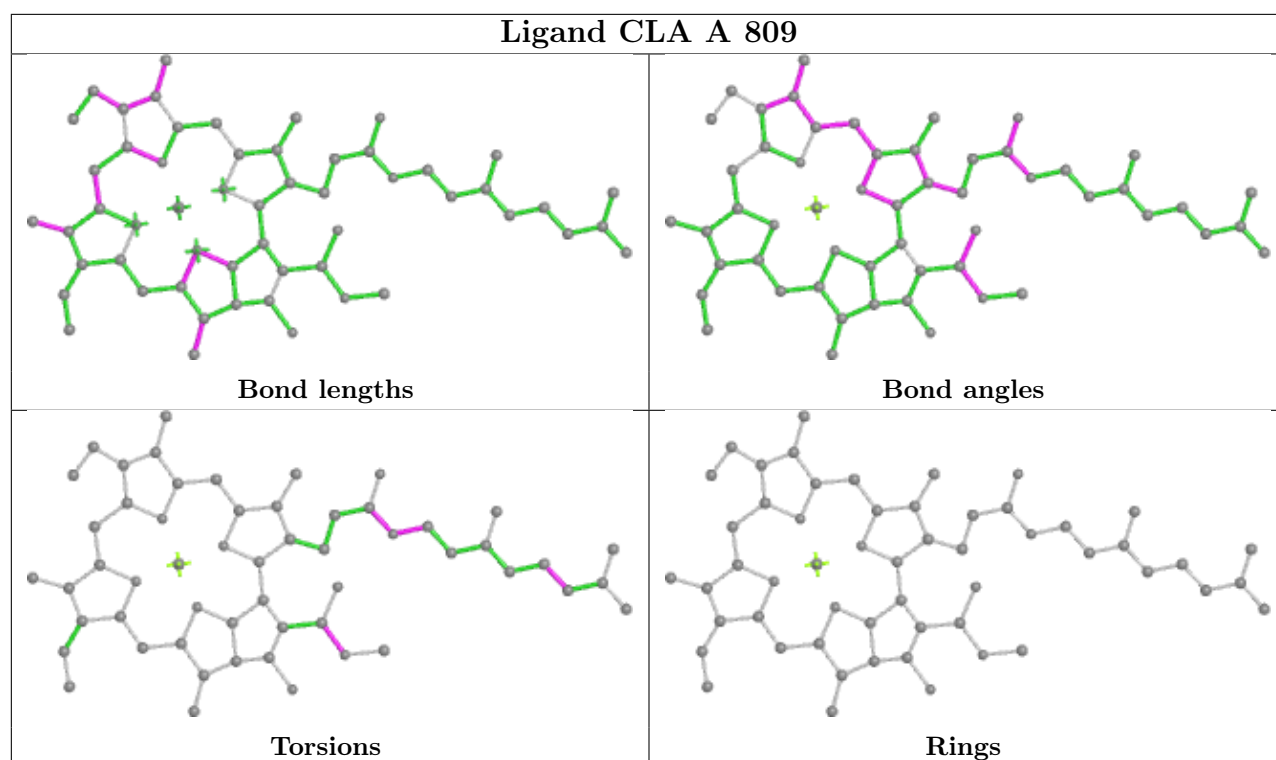
Bond angles



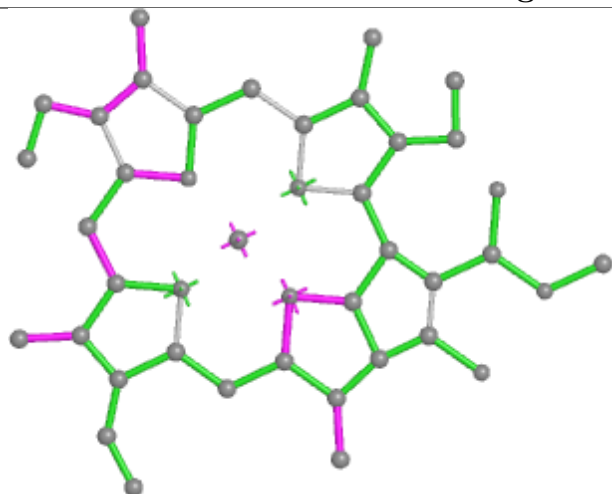
Torsions



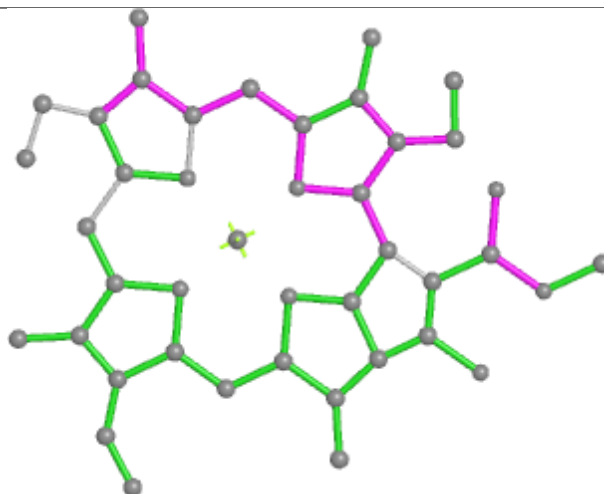
Rings



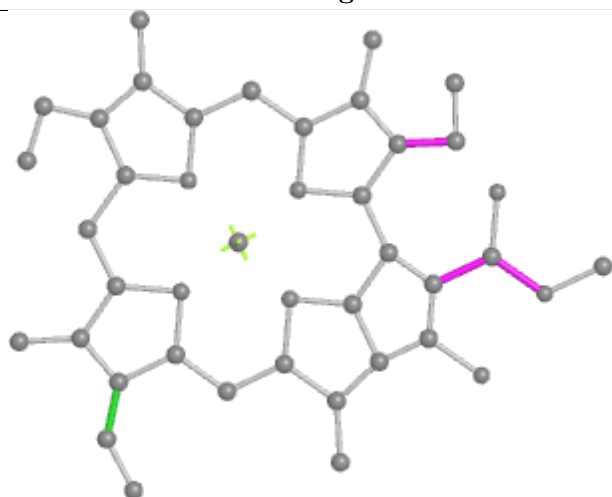
Ligand CLA J 101



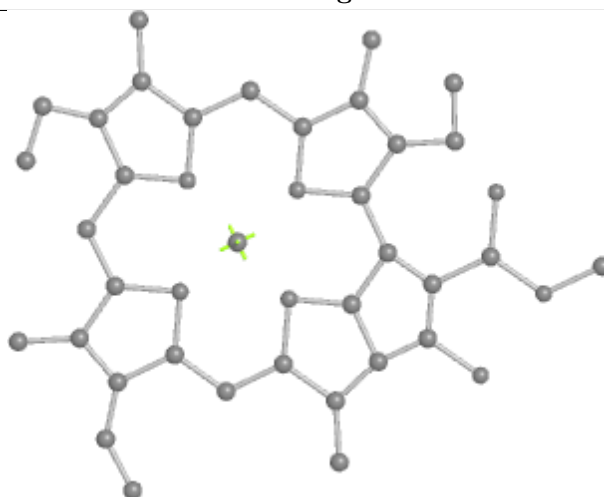
Bond lengths



Bond angles

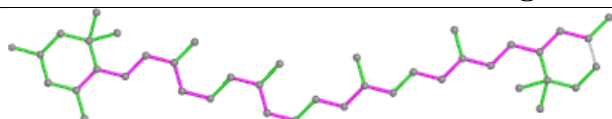


Torsions

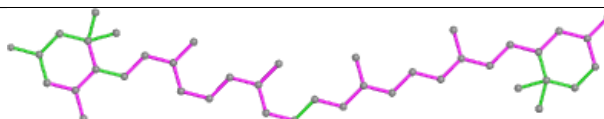


Rings

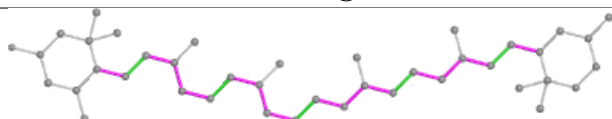
Ligand ZEX 3 201



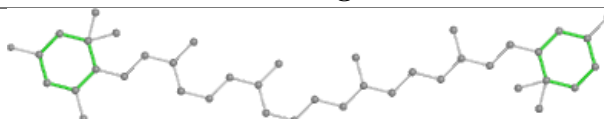
Bond lengths



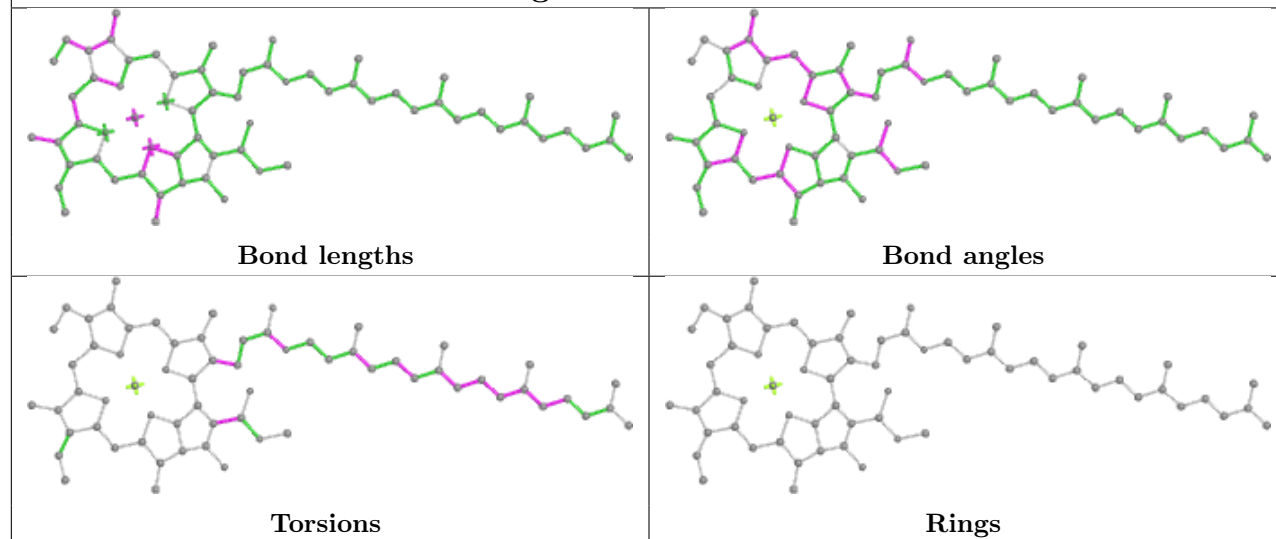
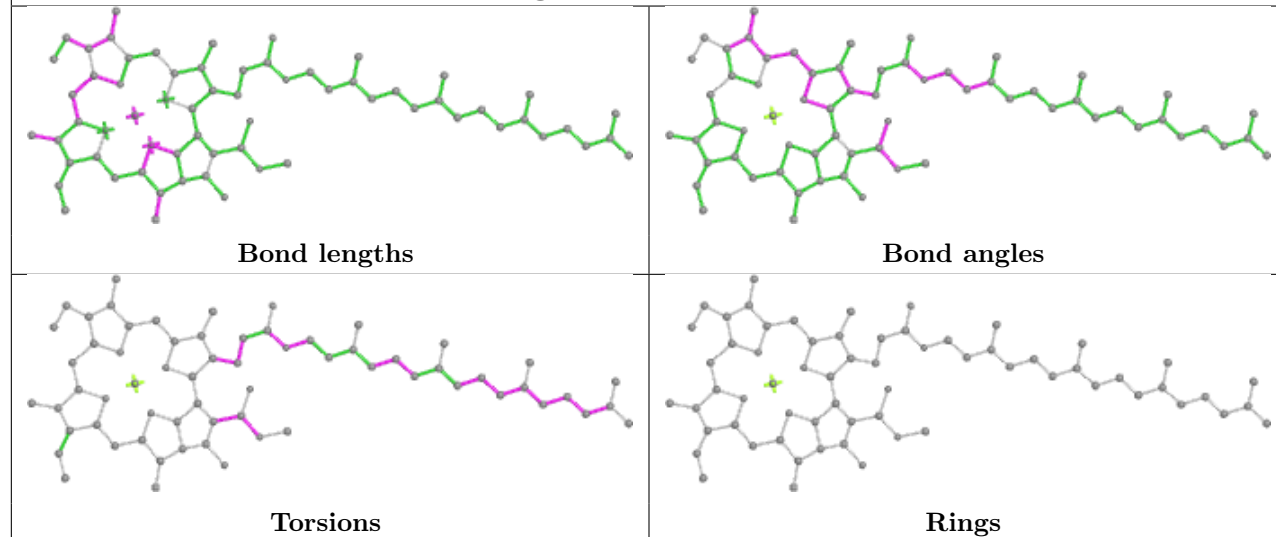
Bond angles



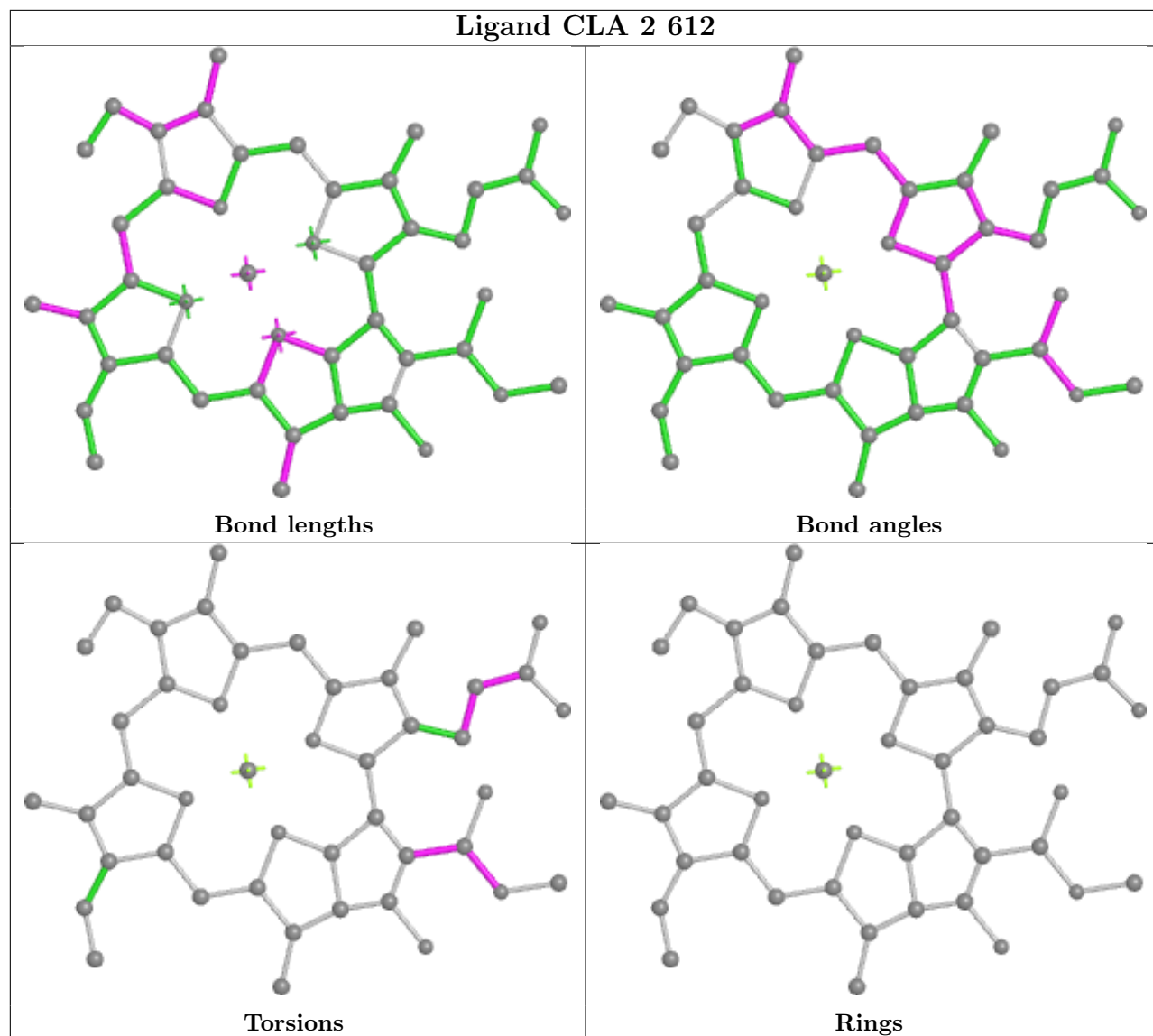
Torsions



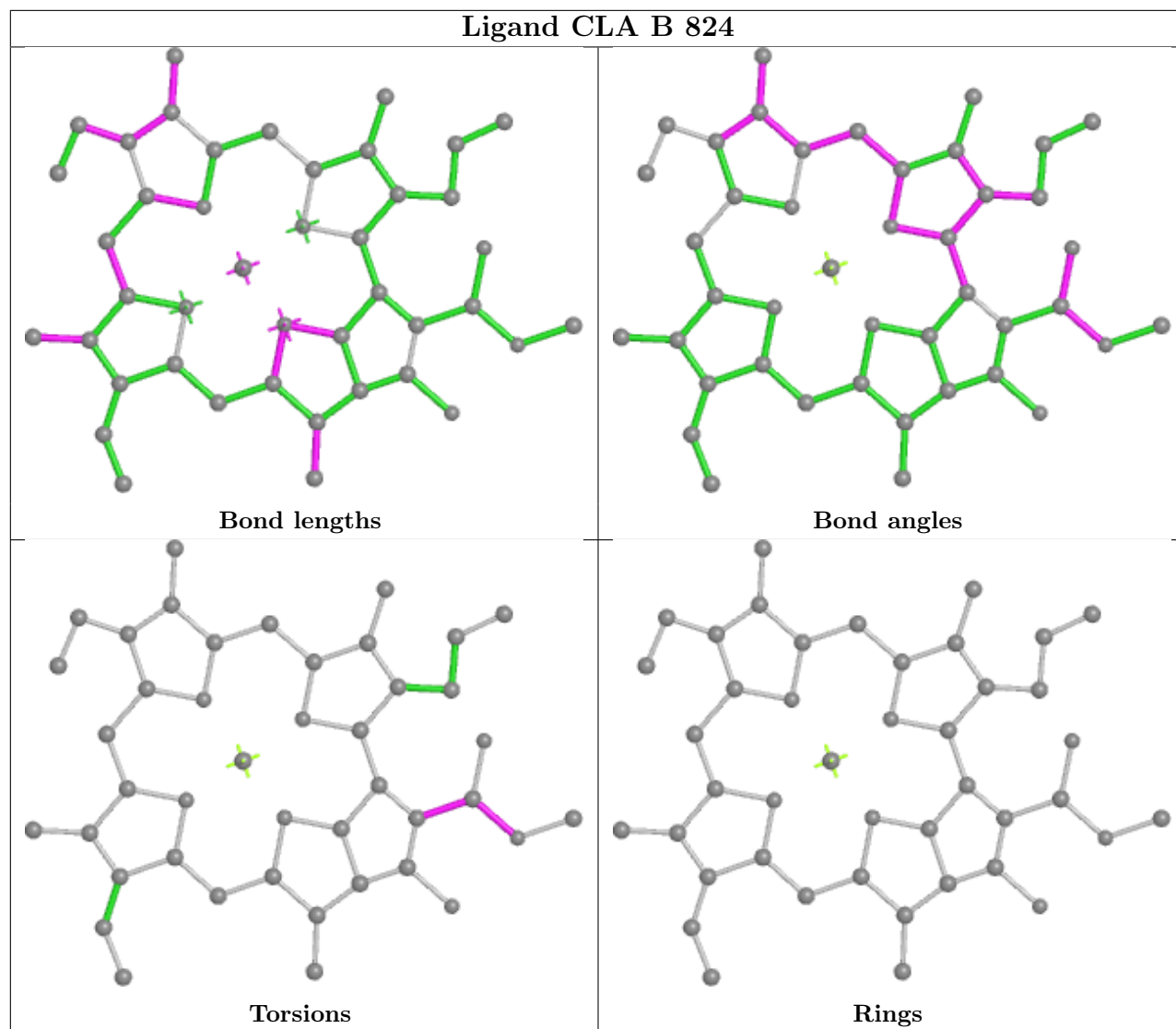
Rings

Ligand CLA A 810**Ligand CLA A 839**

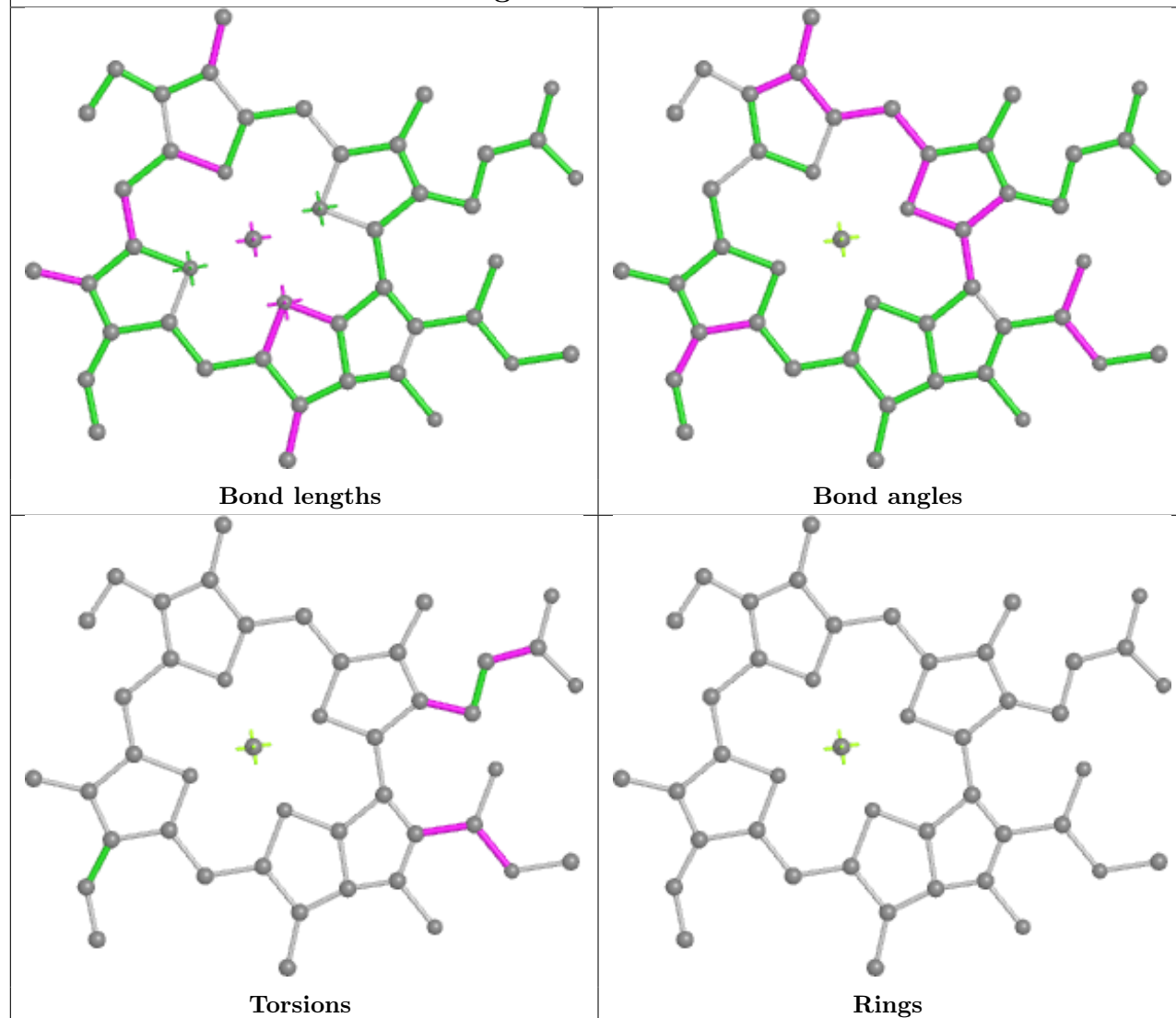
Ligand CLA 2 612



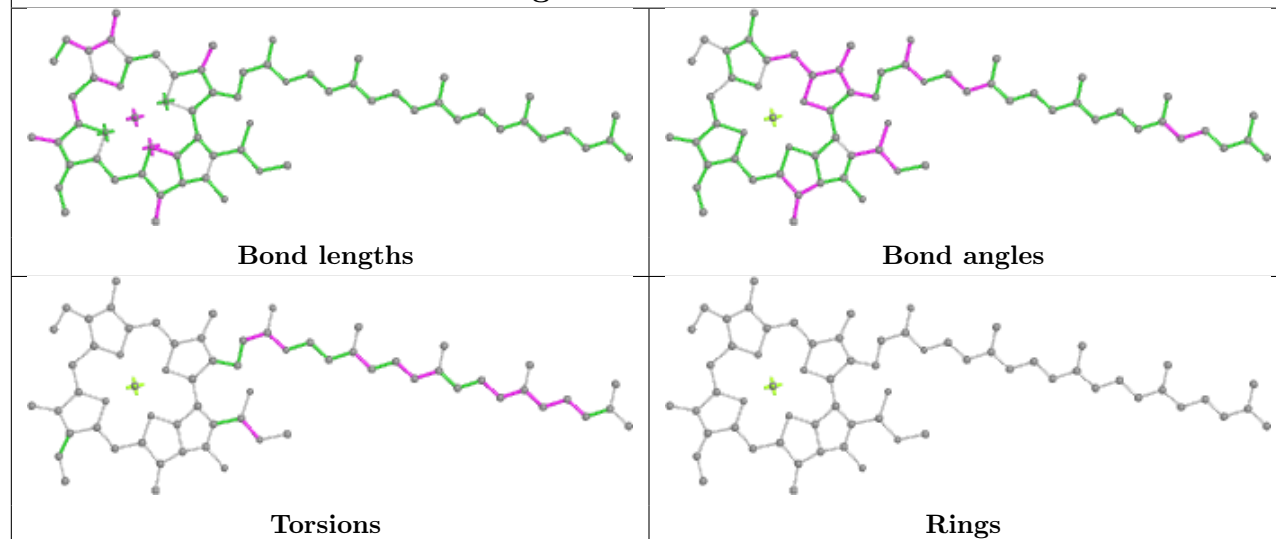
Ligand CLA B 824



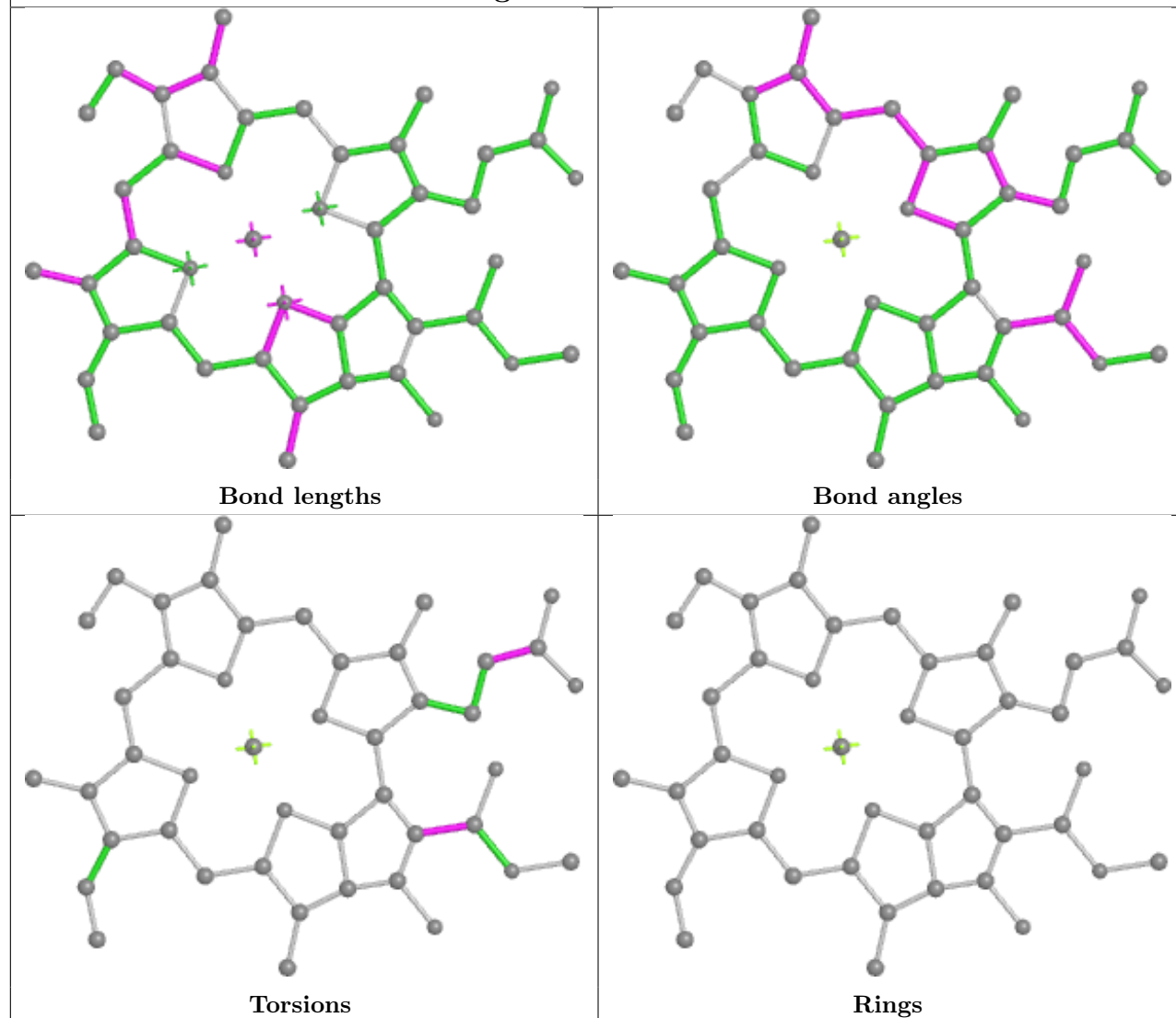
Ligand CLA 1 611



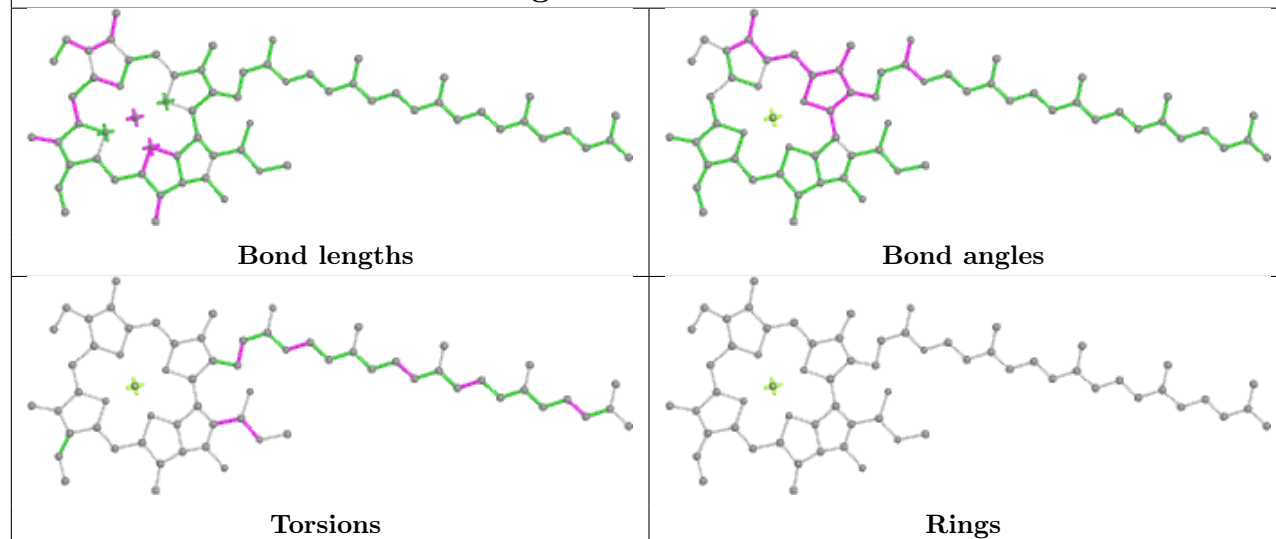
Ligand CLA B 805



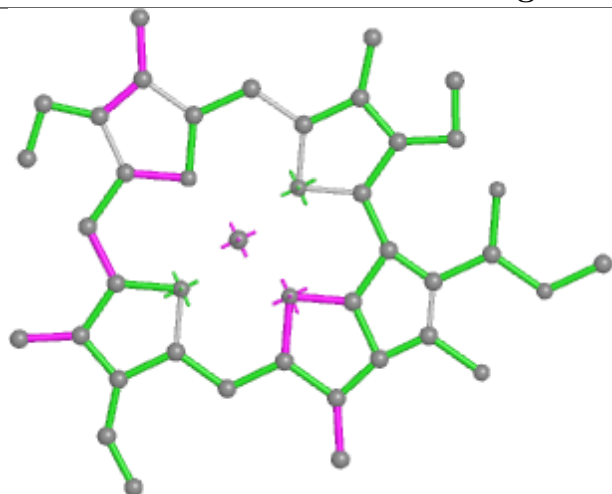
Ligand CLA 2 603



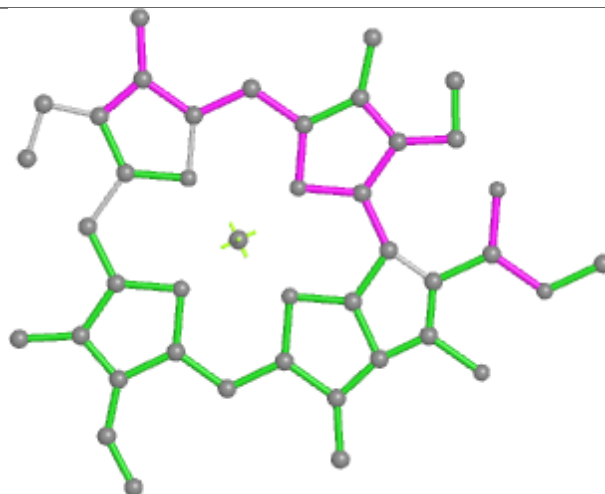
Ligand CLA A 812



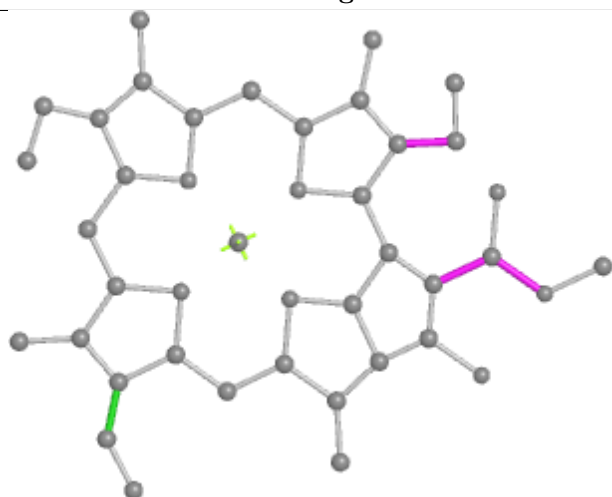
Ligand CLA 2 610



Bond lengths



Bond angles

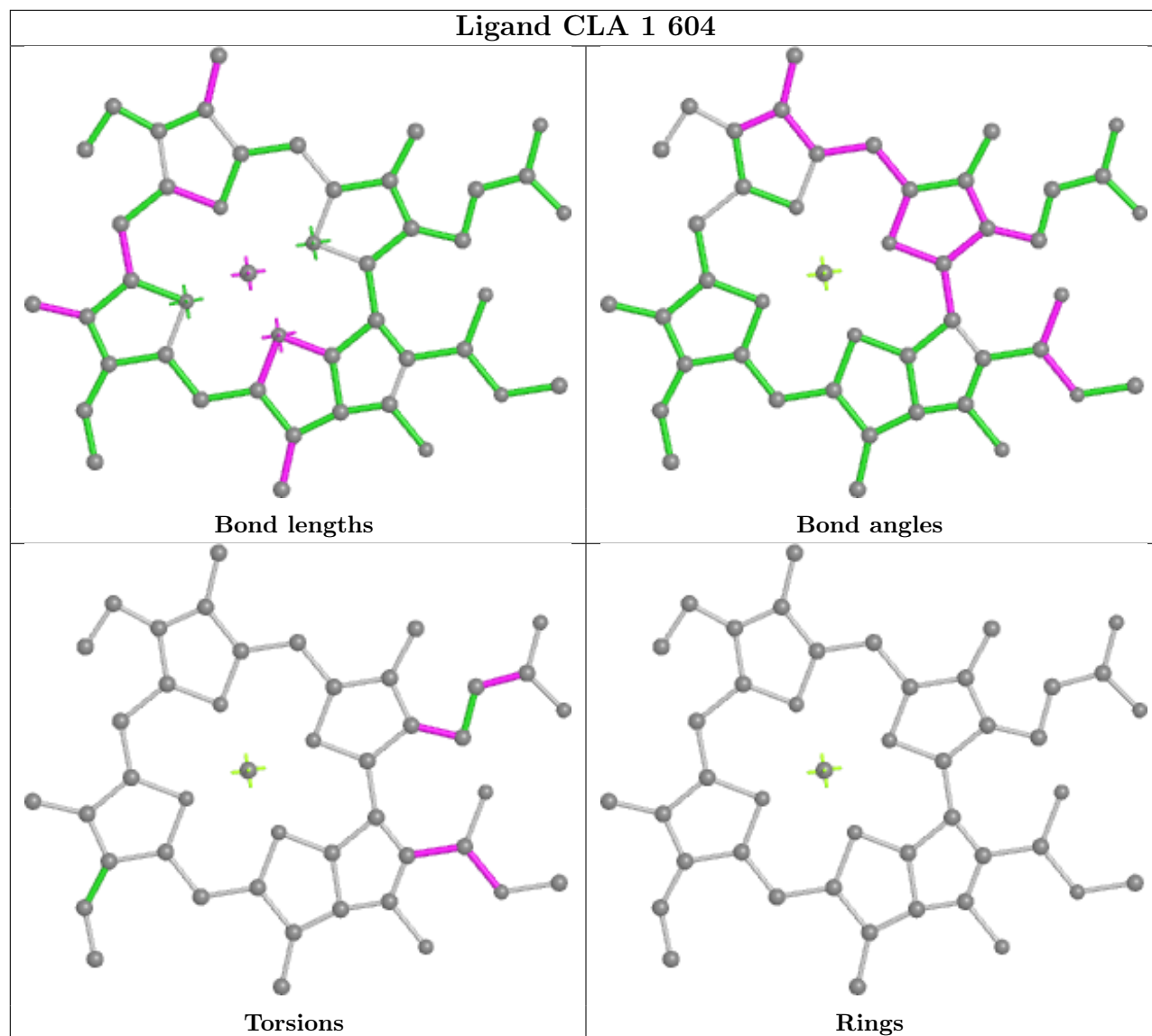


Torsions

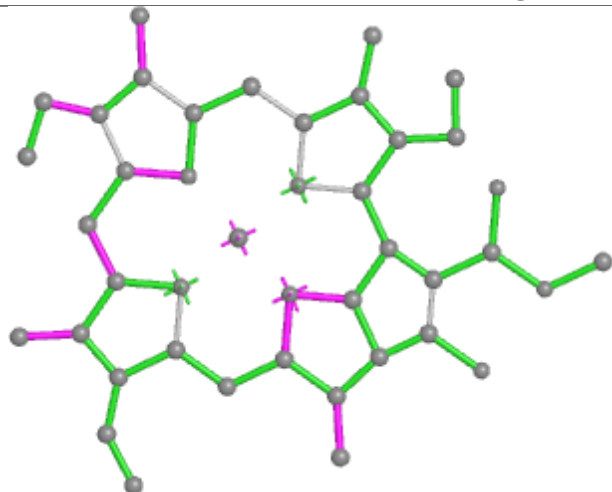


Rings

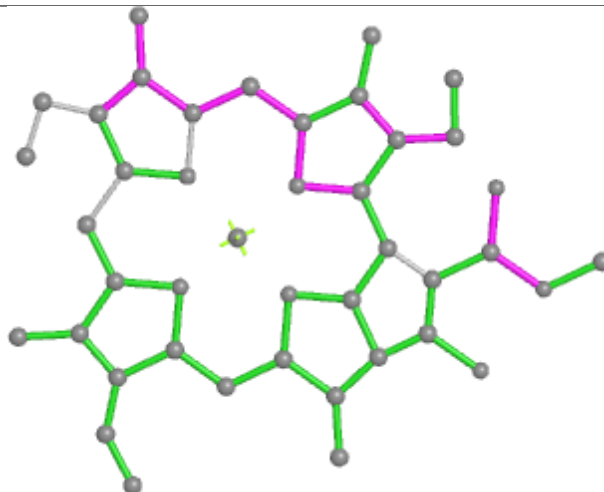
Ligand CLA 1 604



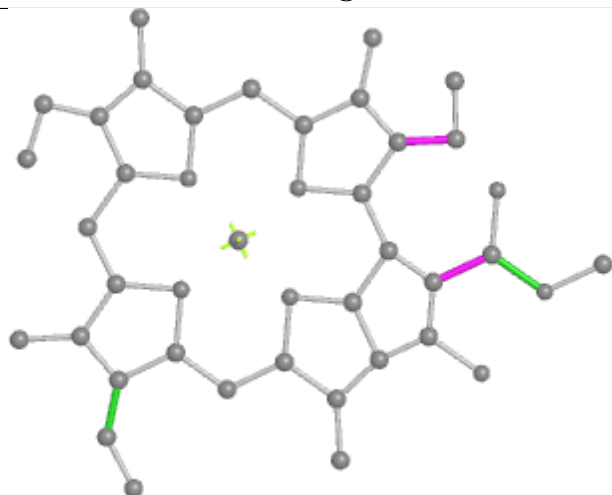
Ligand CLA K 102



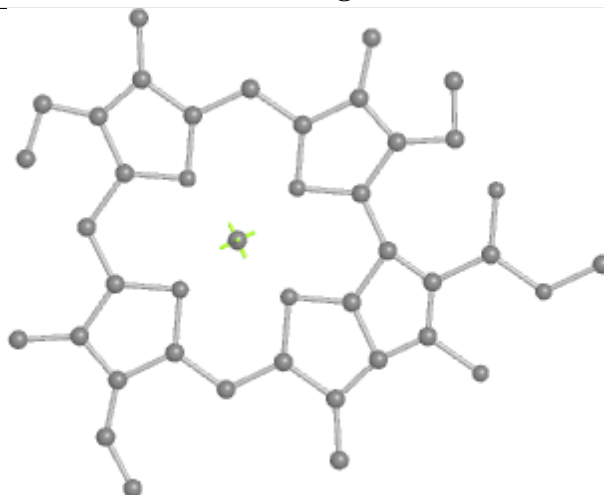
Bond lengths



Bond angles

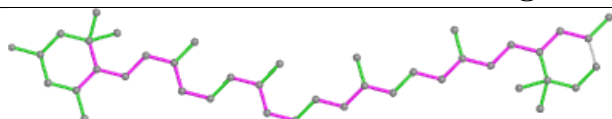


Torsions

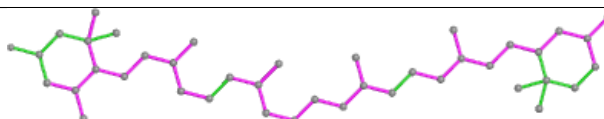


Rings

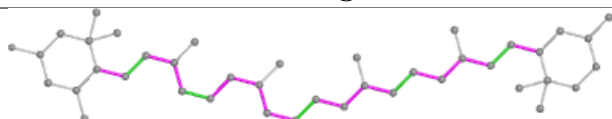
Ligand ZEX 2 616



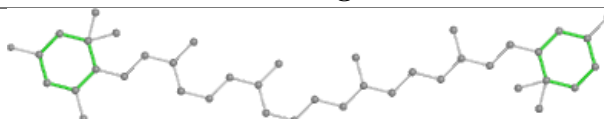
Bond lengths



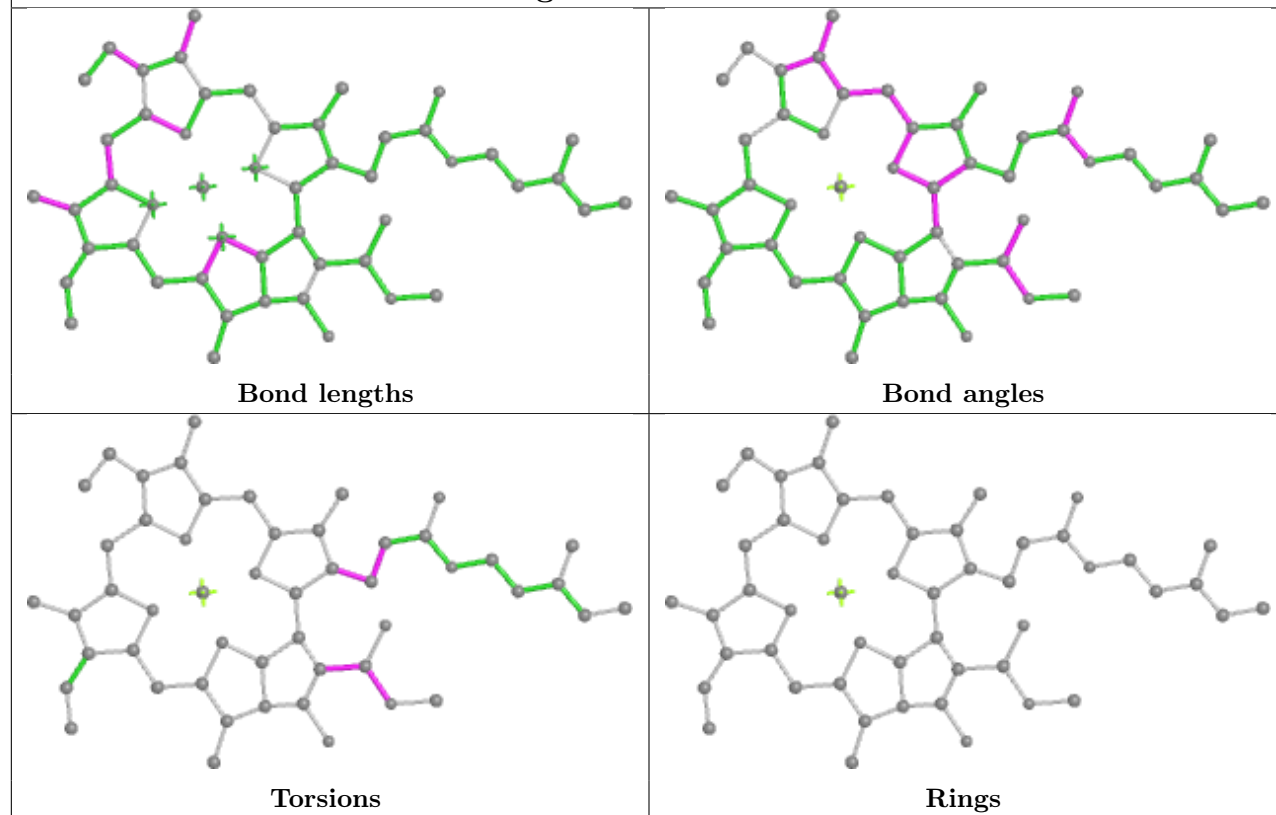
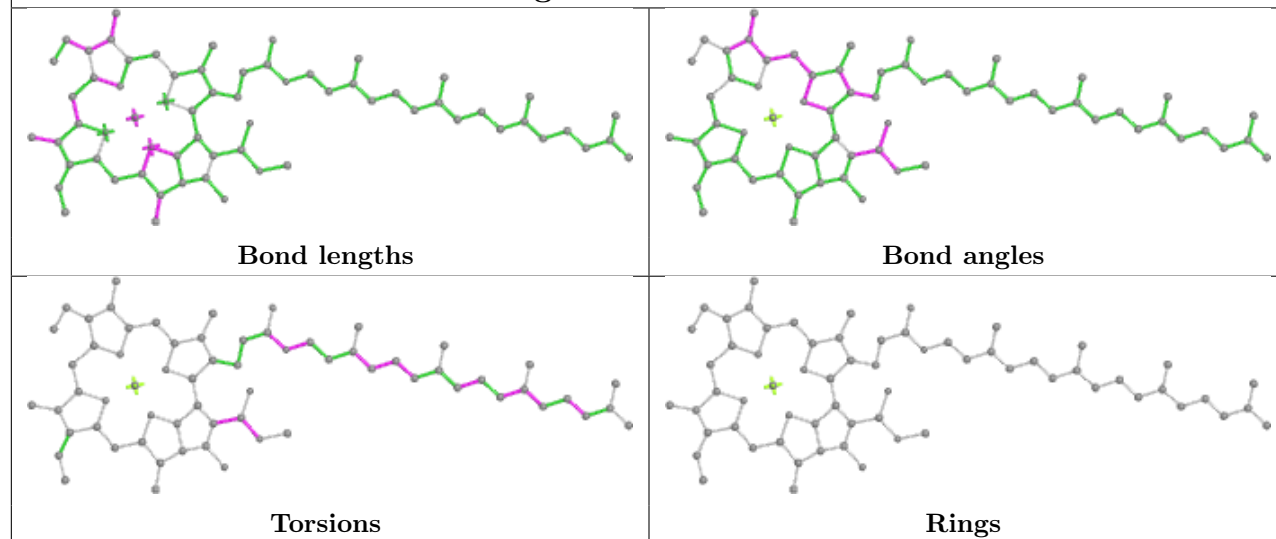
Bond angles

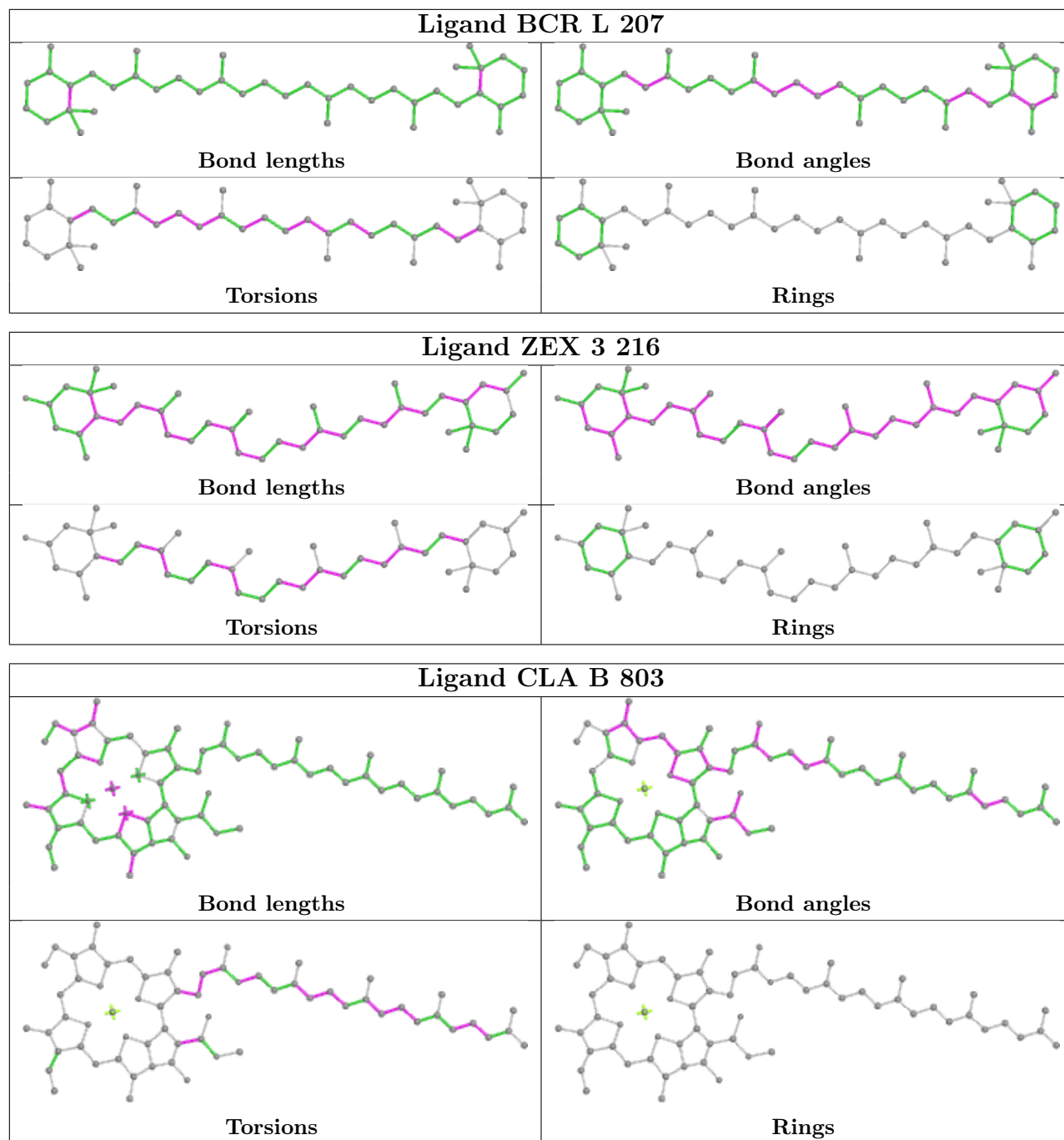


Torsions

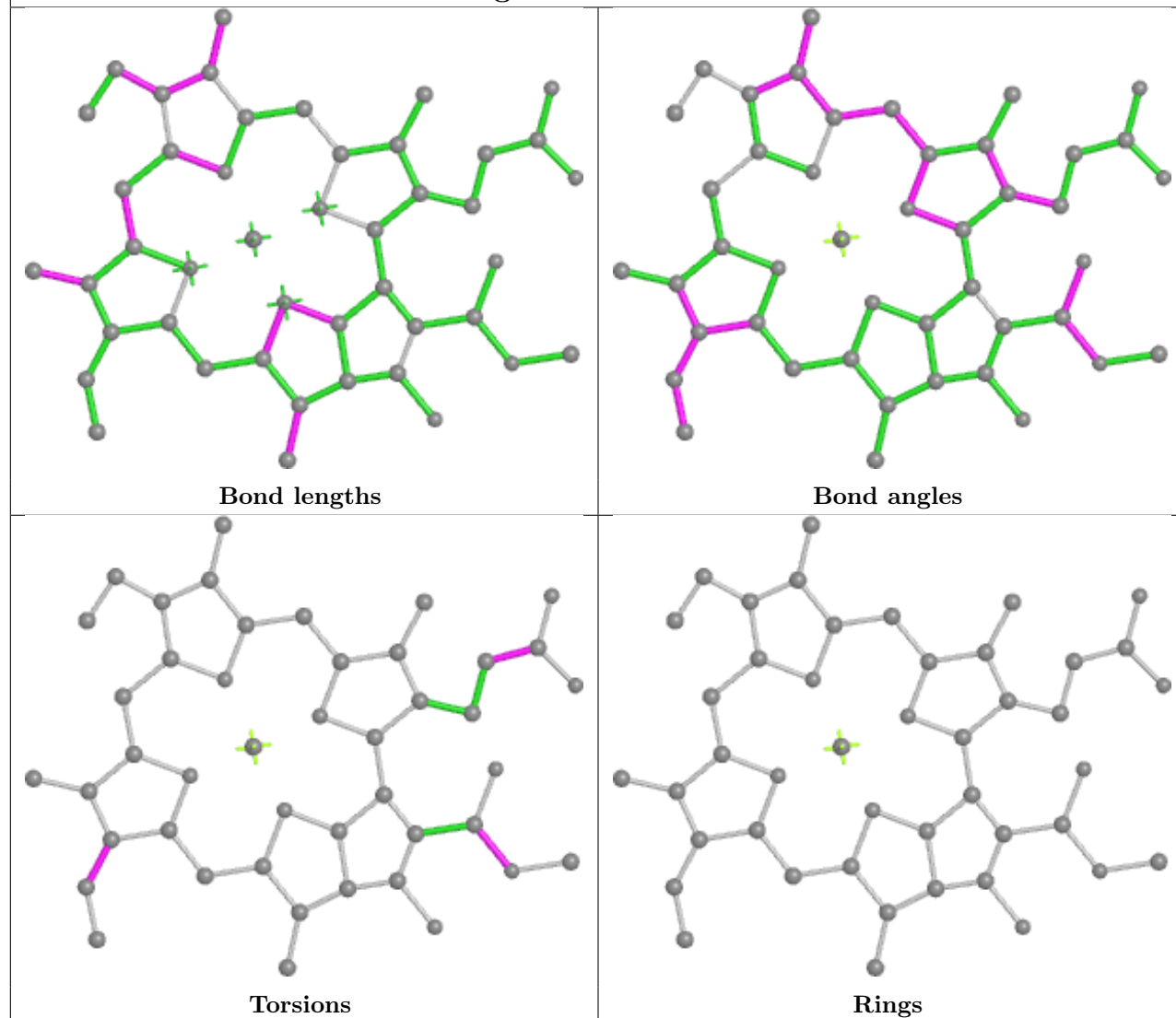


Rings

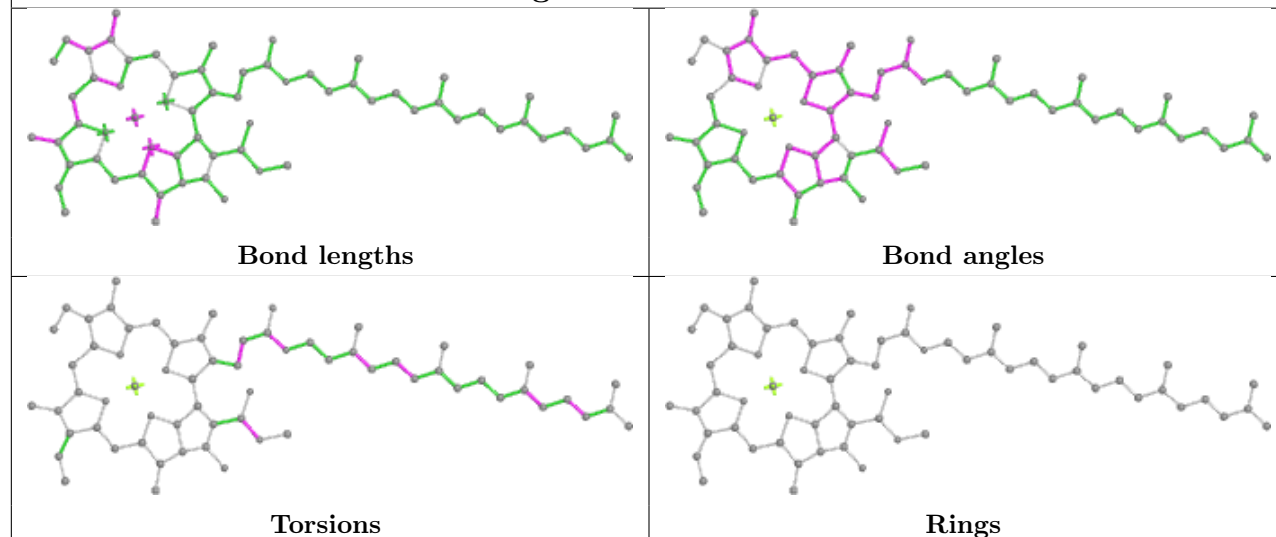
Ligand CLA 3 213**Ligand CLA L 204**



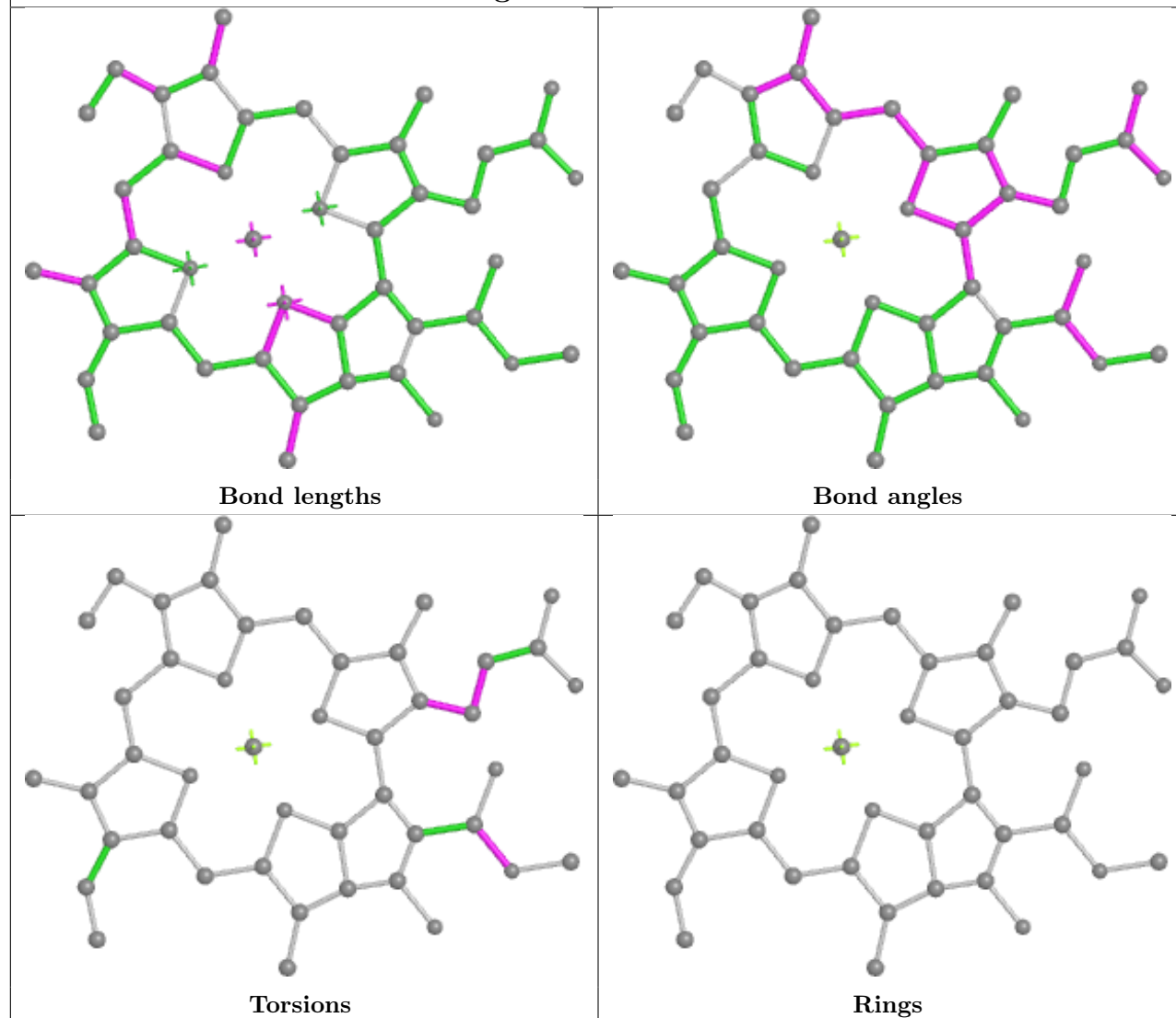
Ligand CLA 2 611



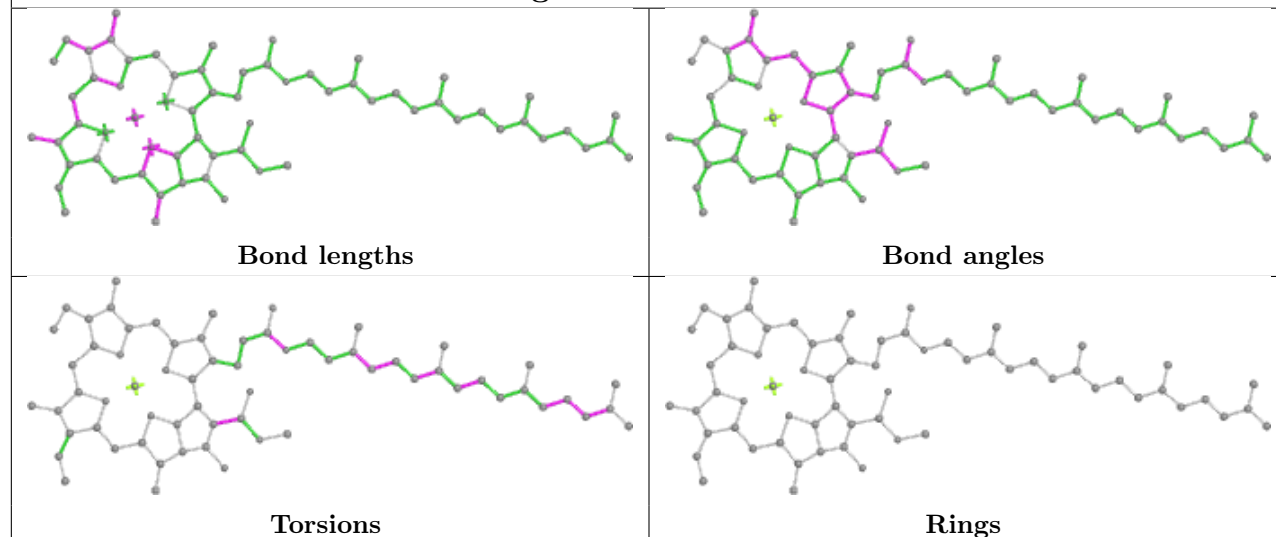
Ligand CLA B 802

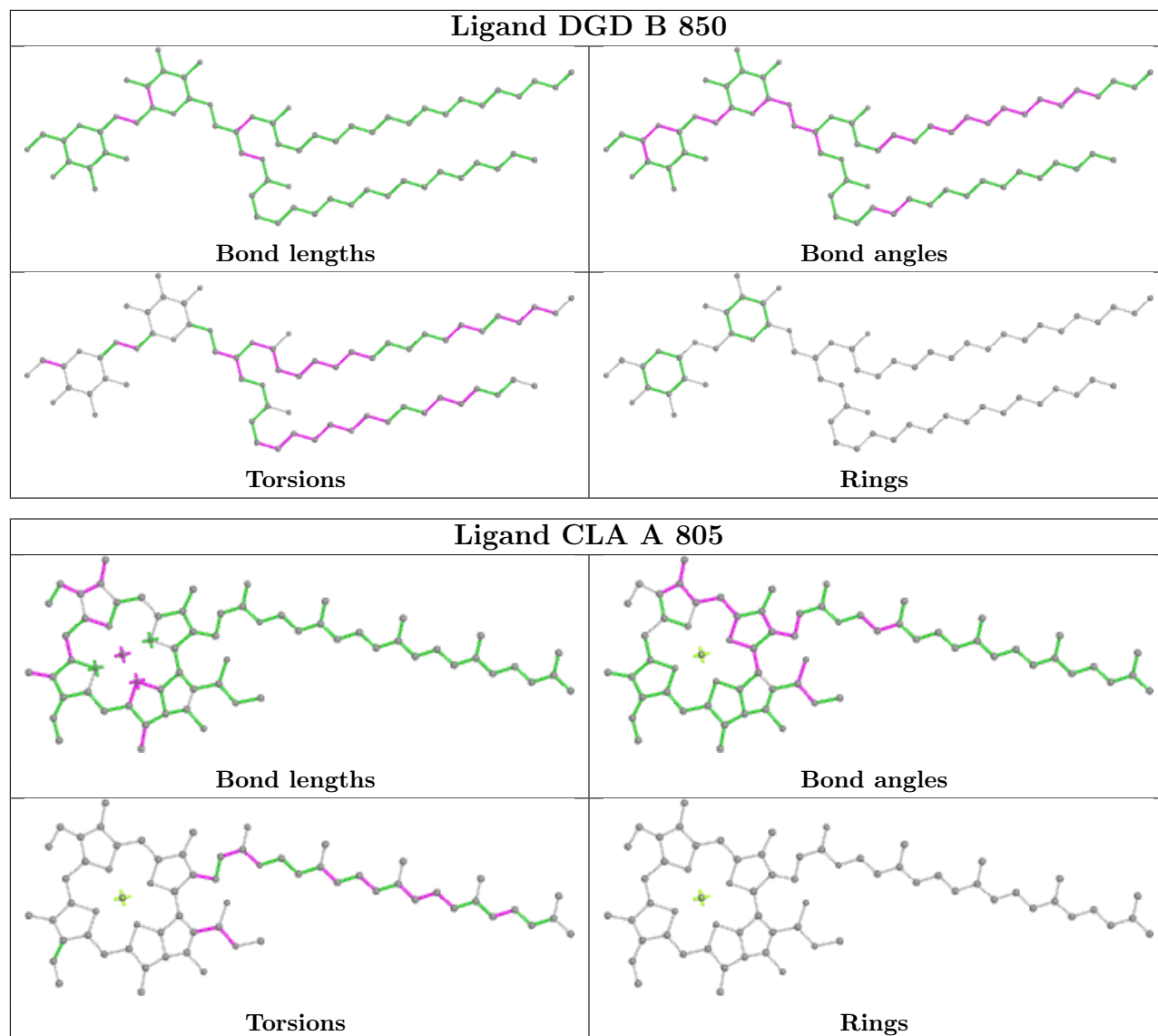


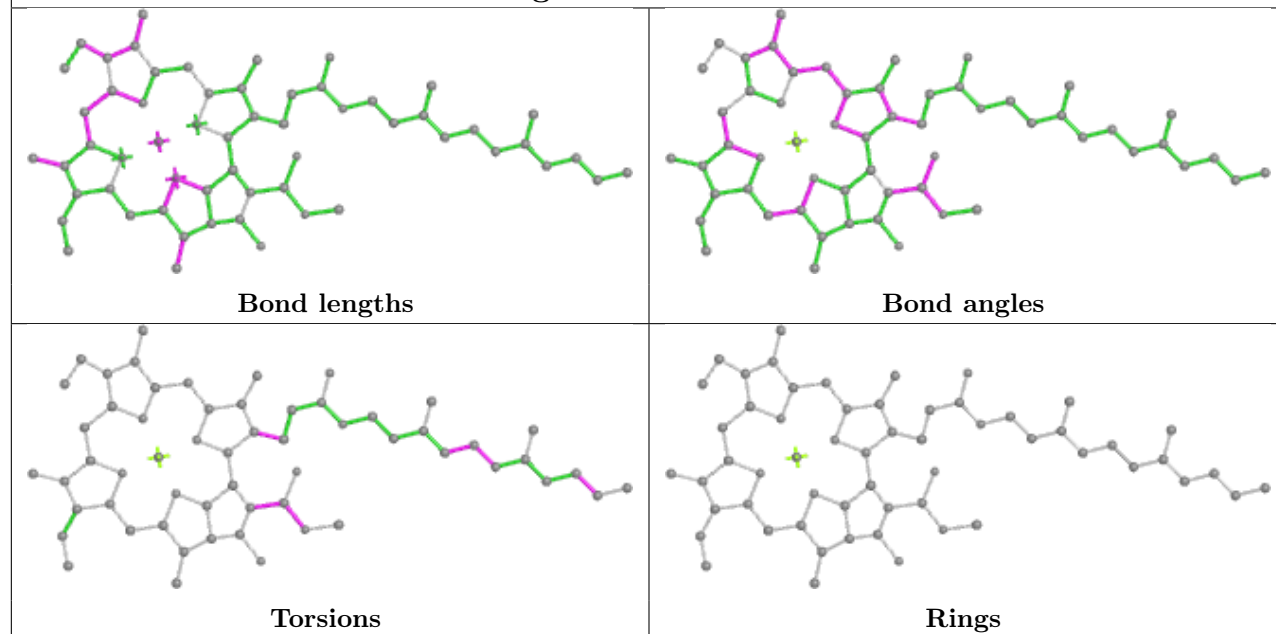
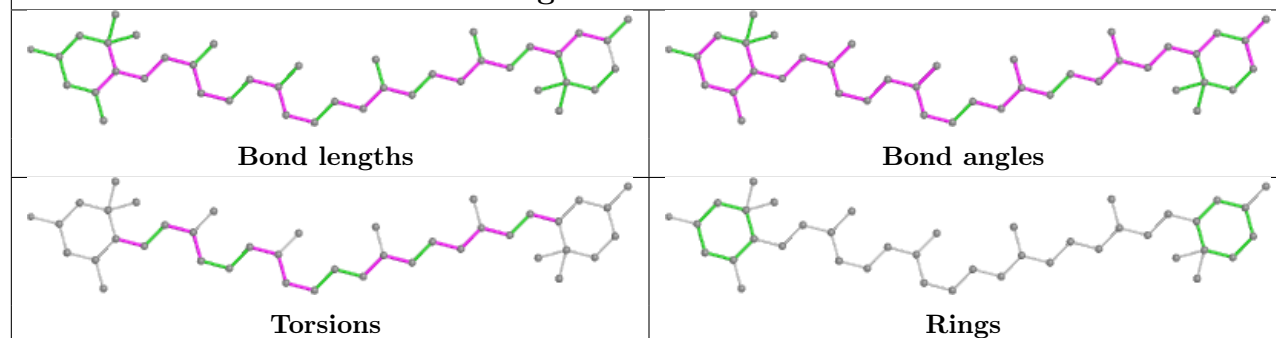
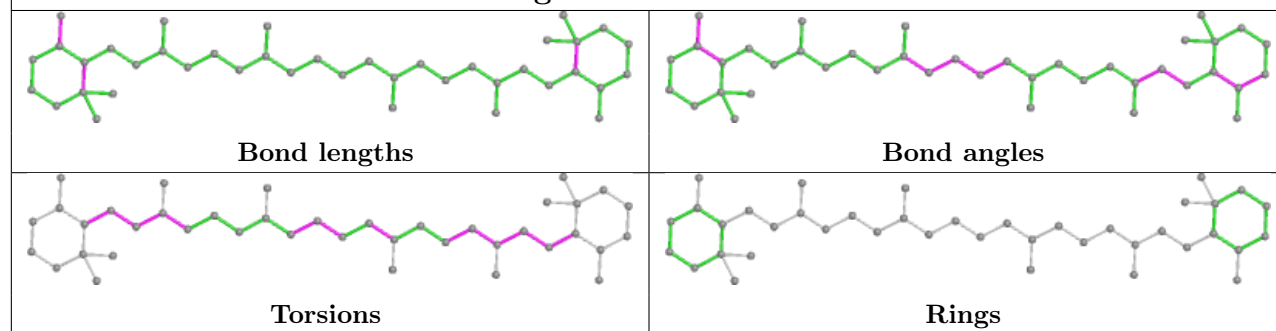
Ligand CLA 2 606

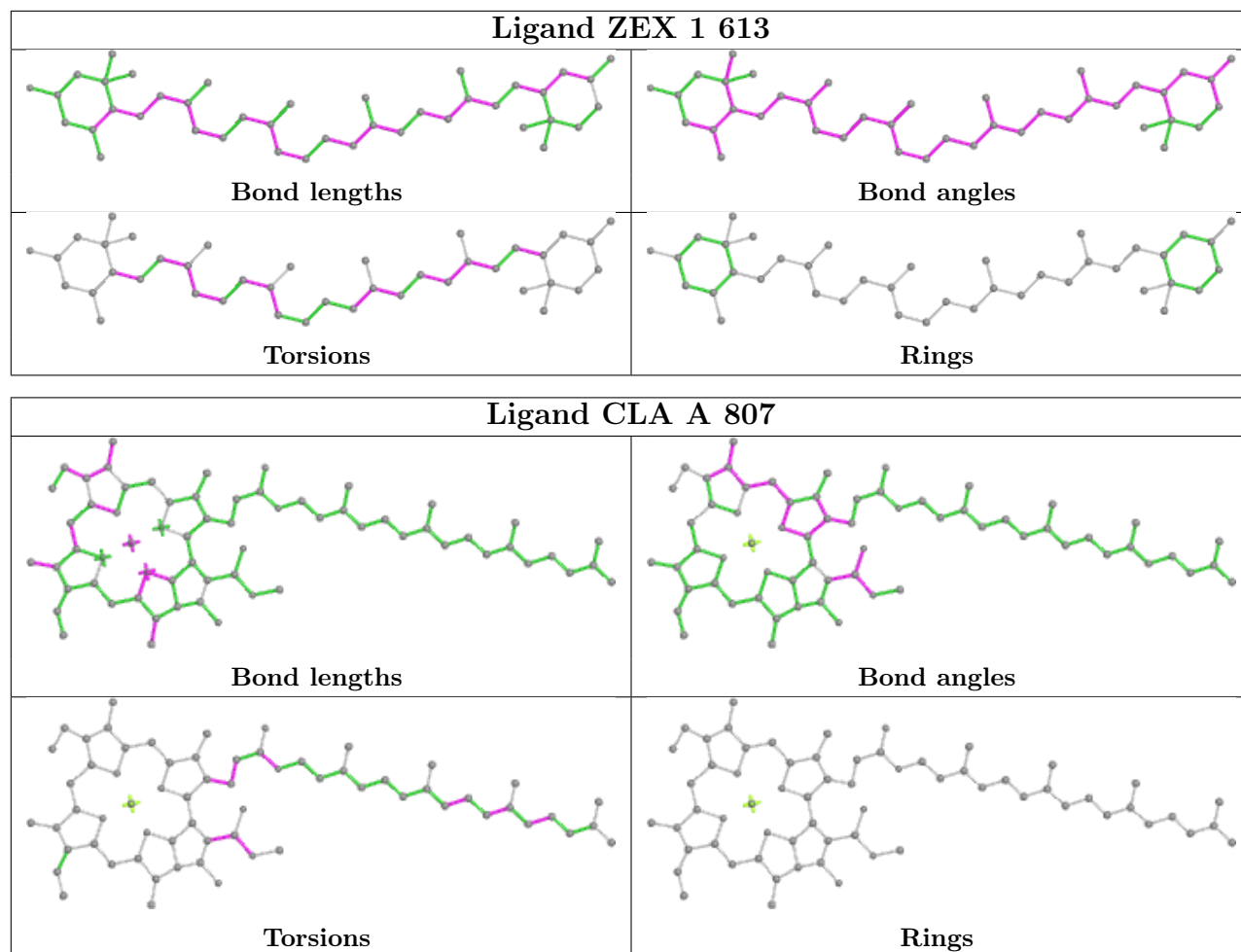


Ligand CLA A 836

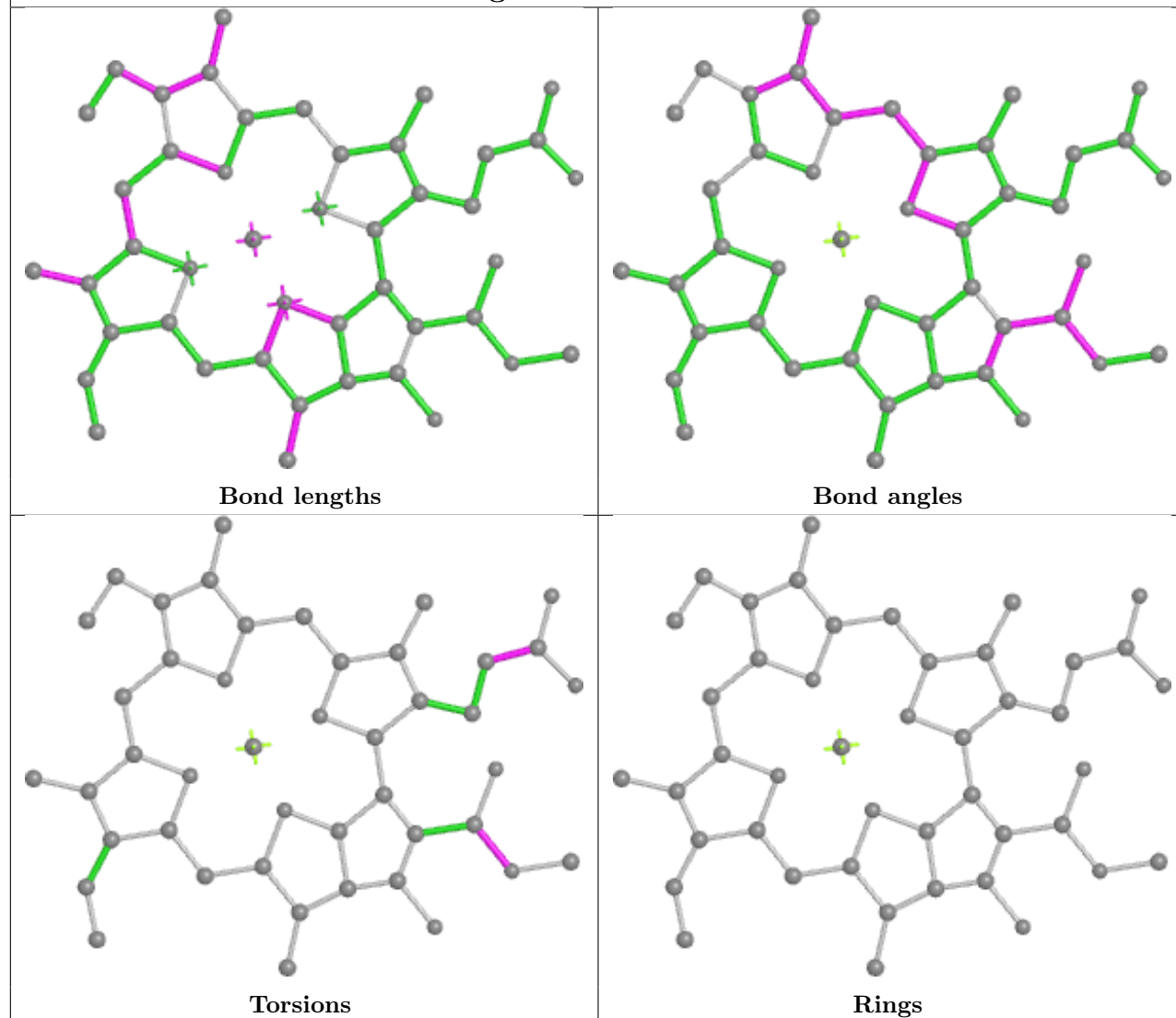




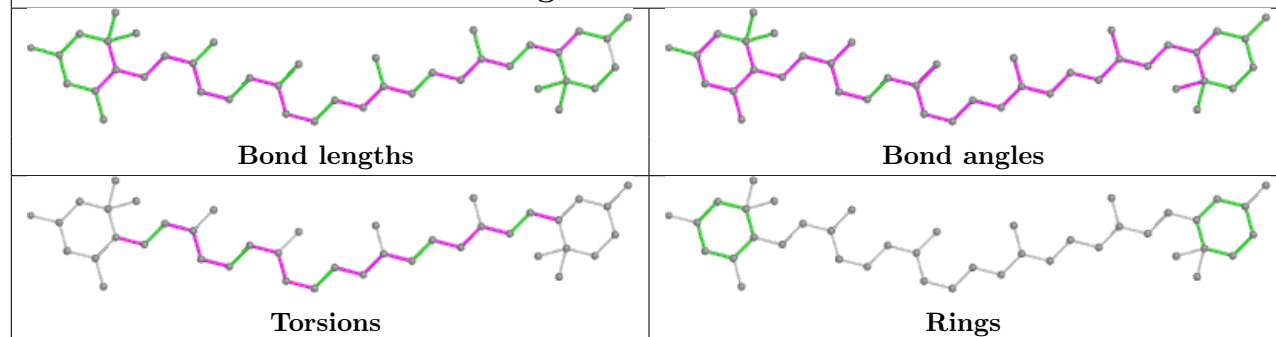
Ligand CLA B 834**Ligand ZEX 3 217****Ligand BCR J 103**

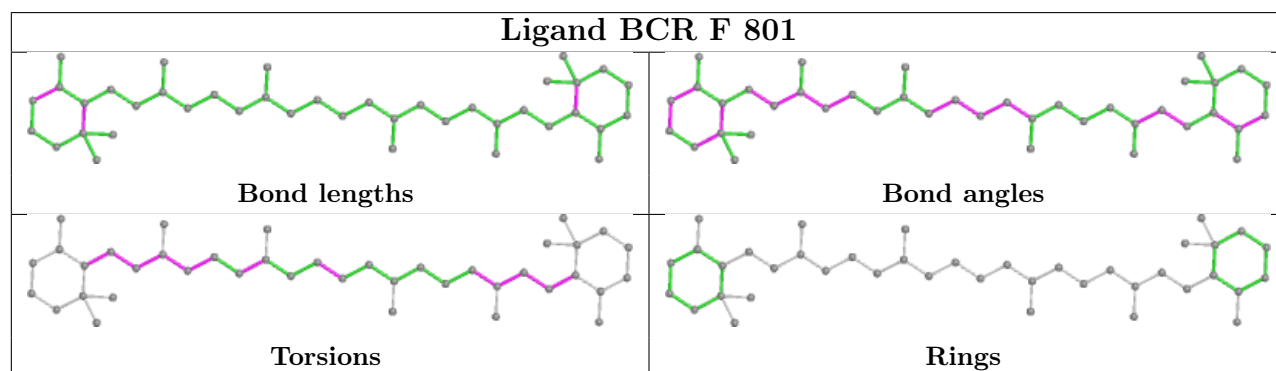
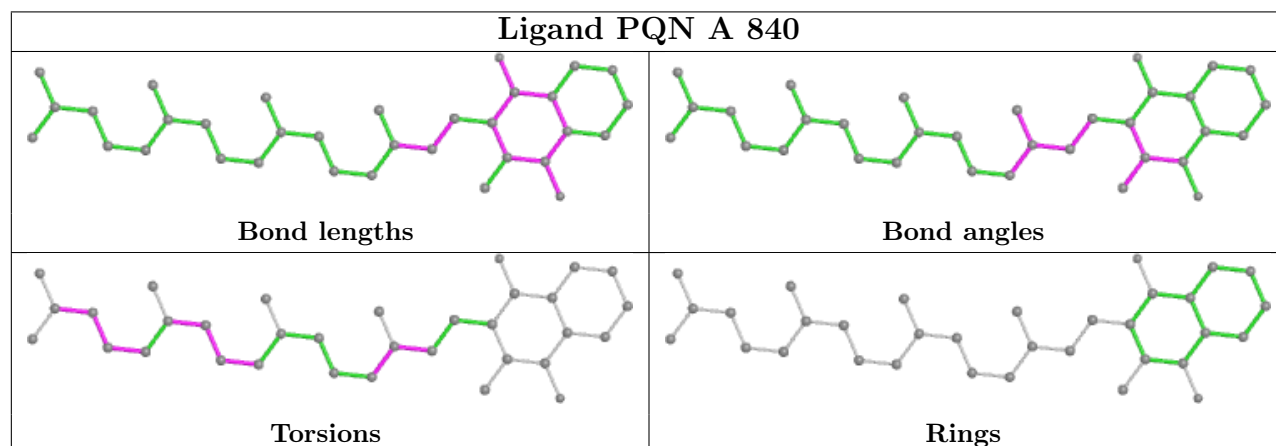
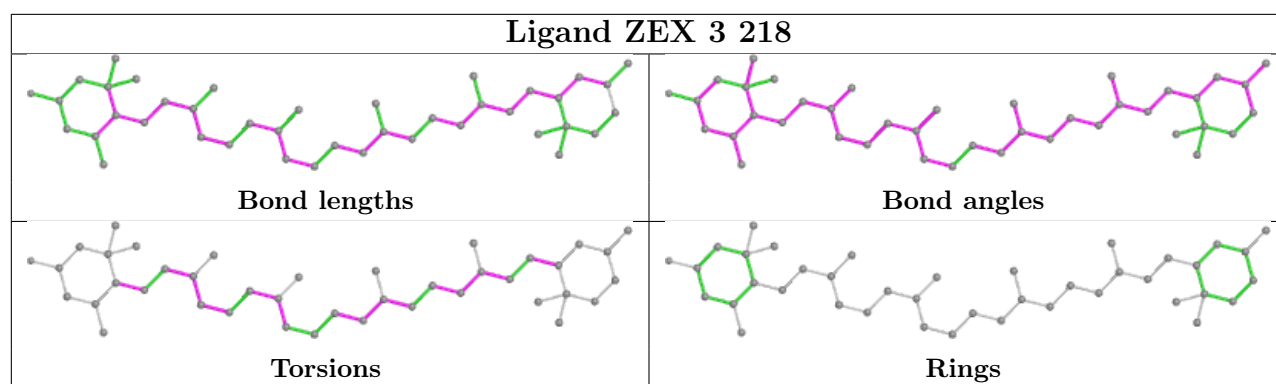


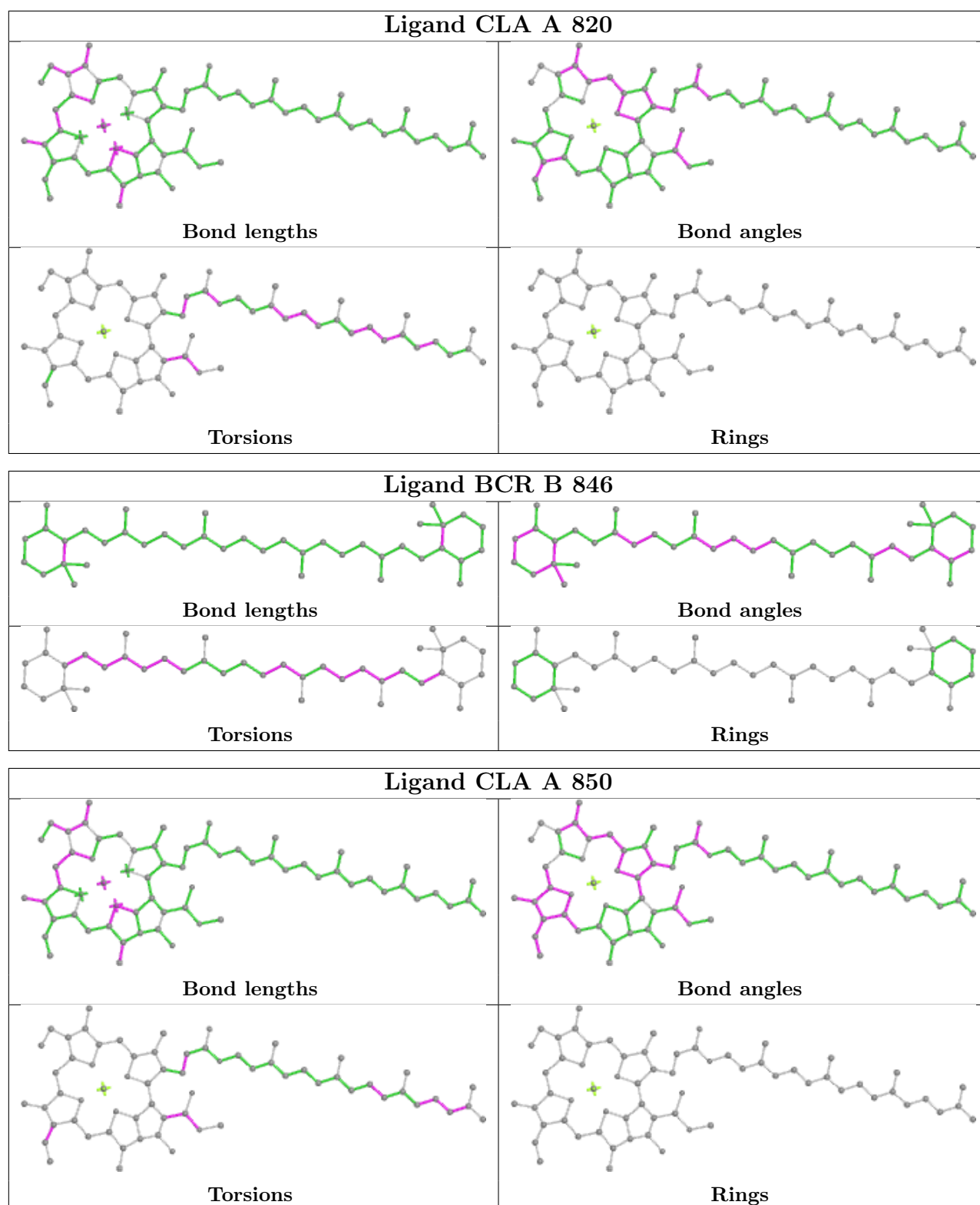
Ligand CLA K 101

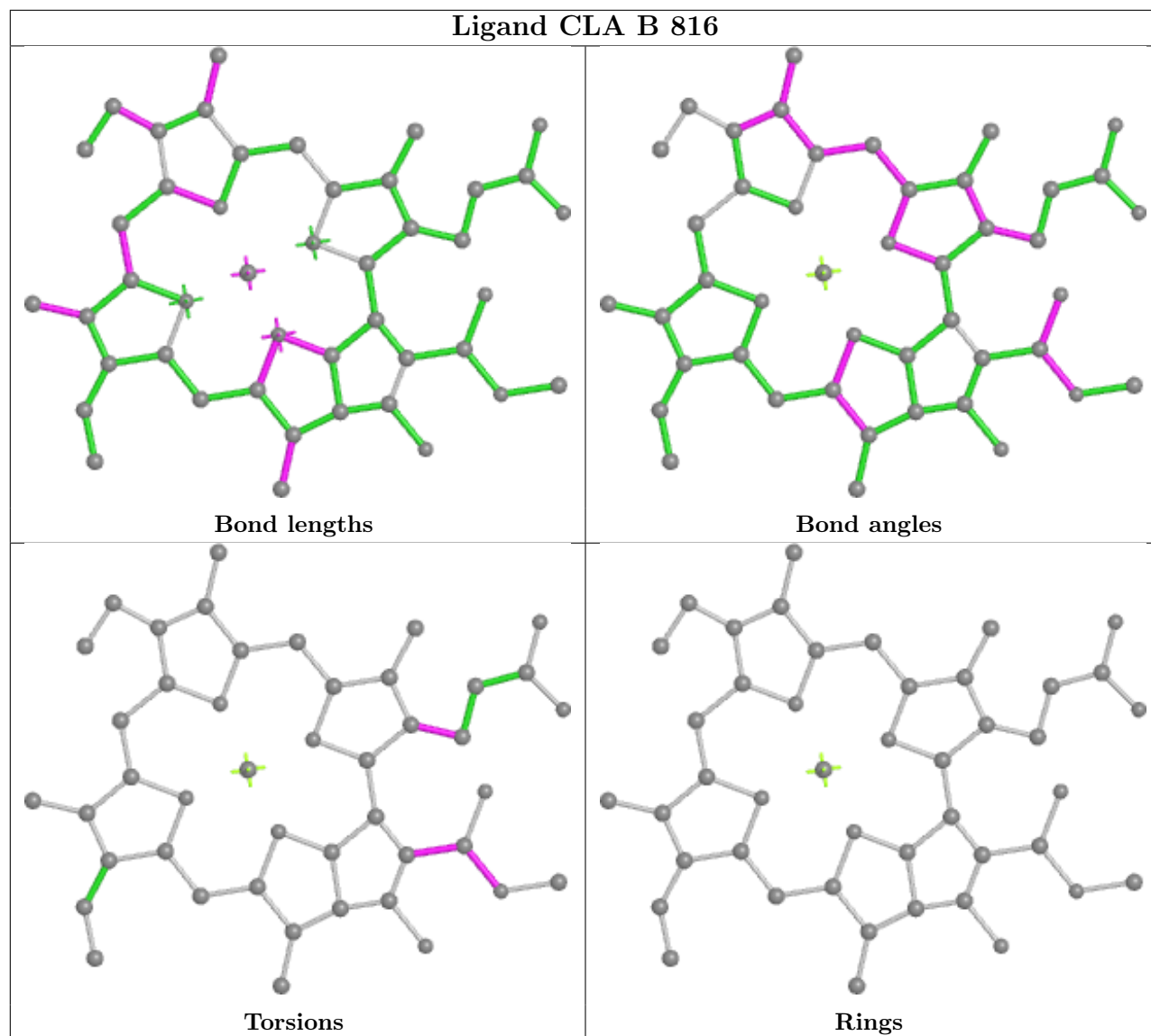
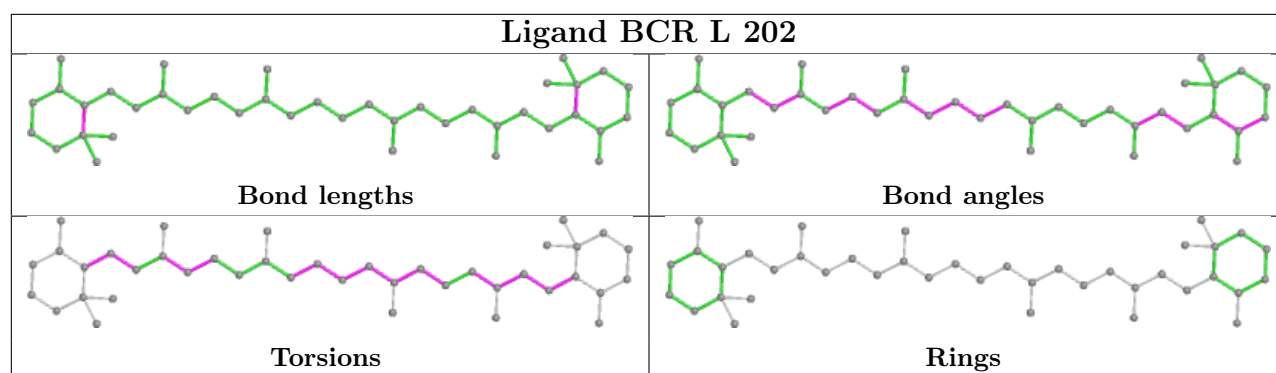


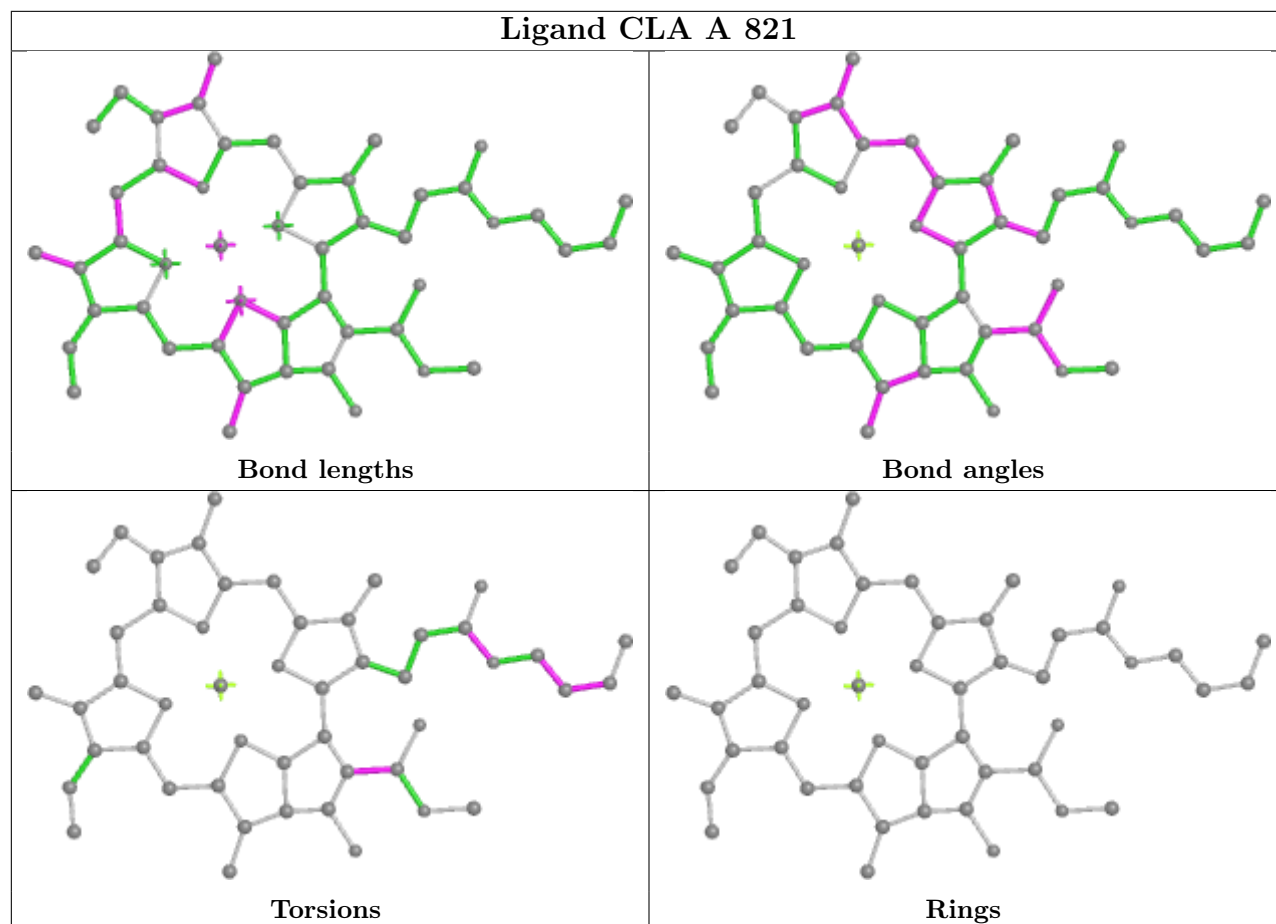
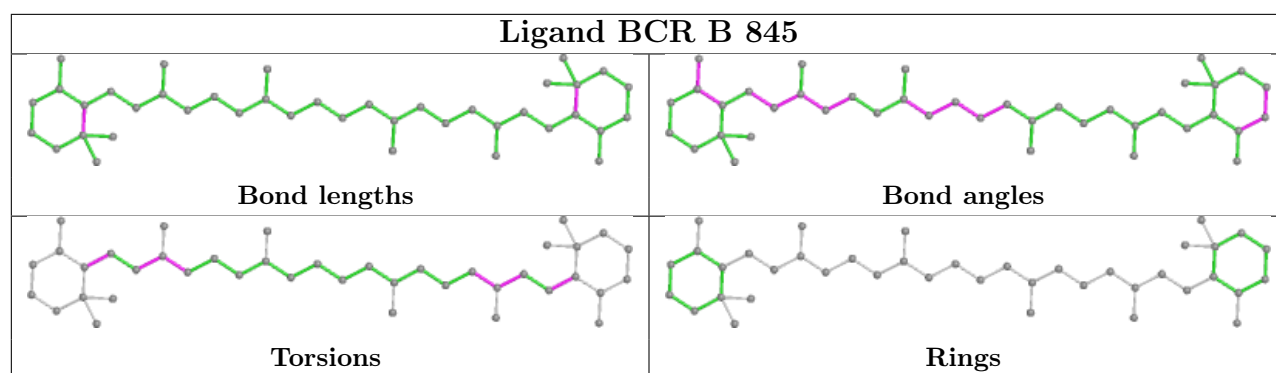
Ligand ZEX 2 615

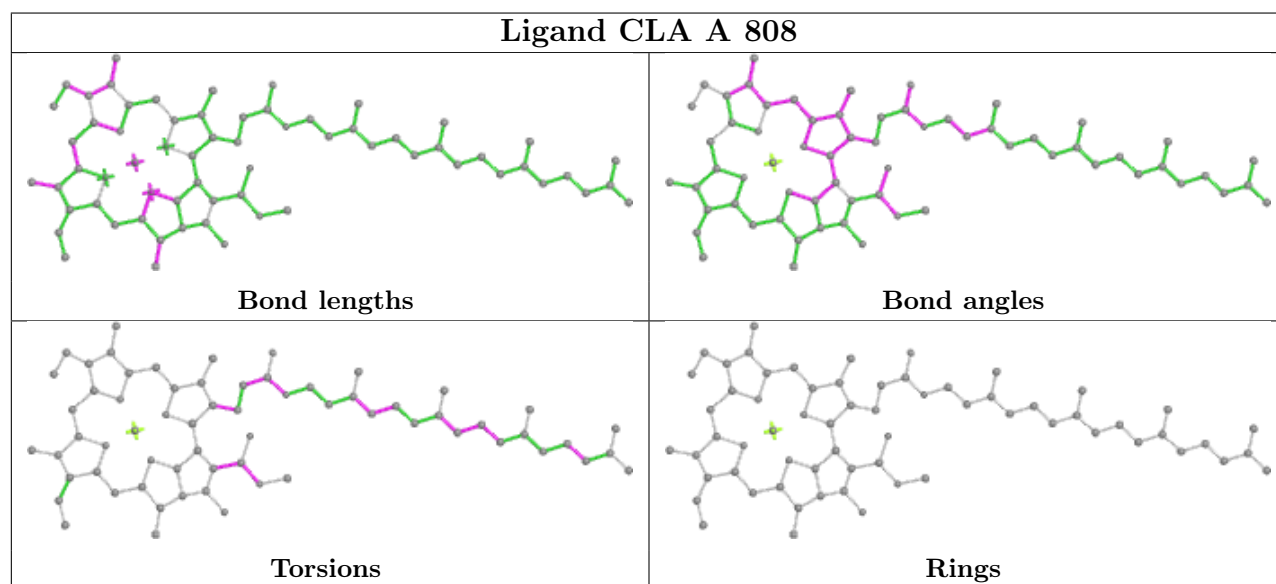
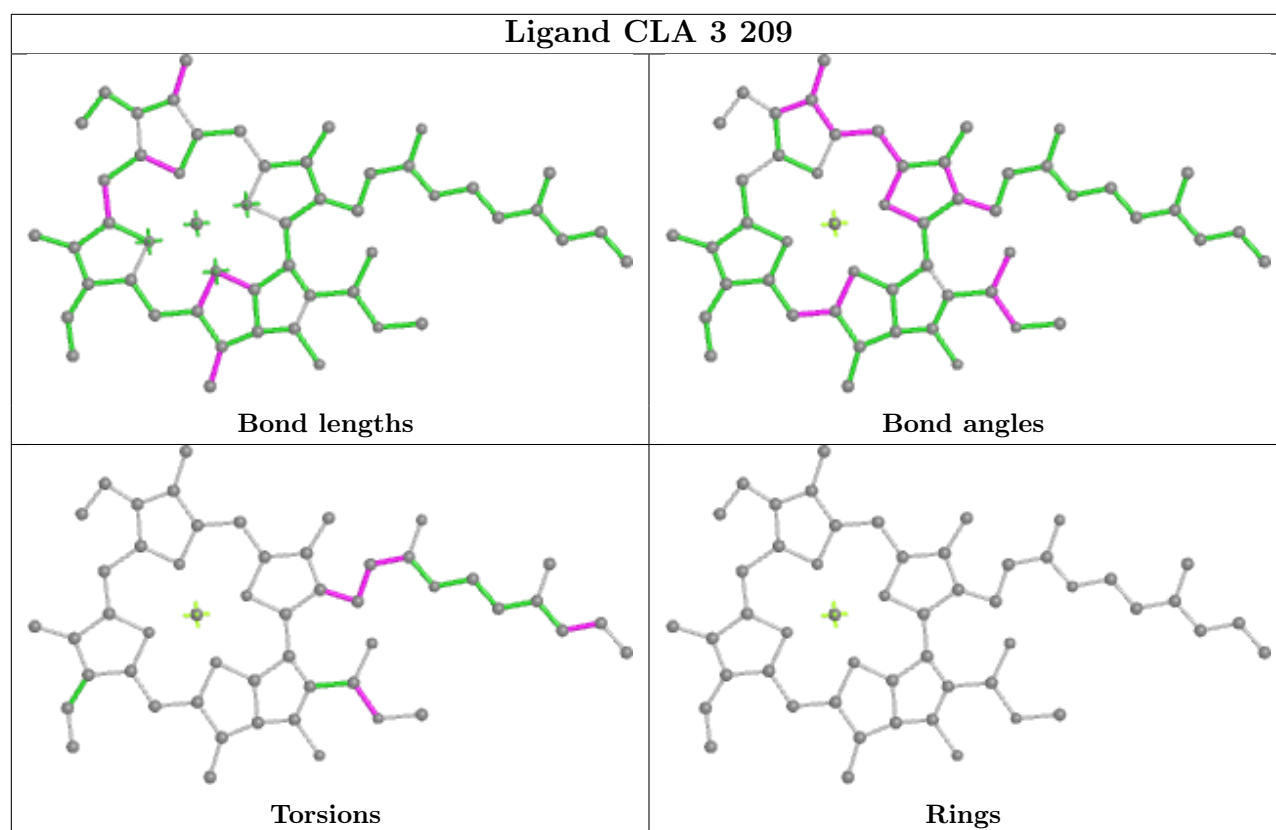


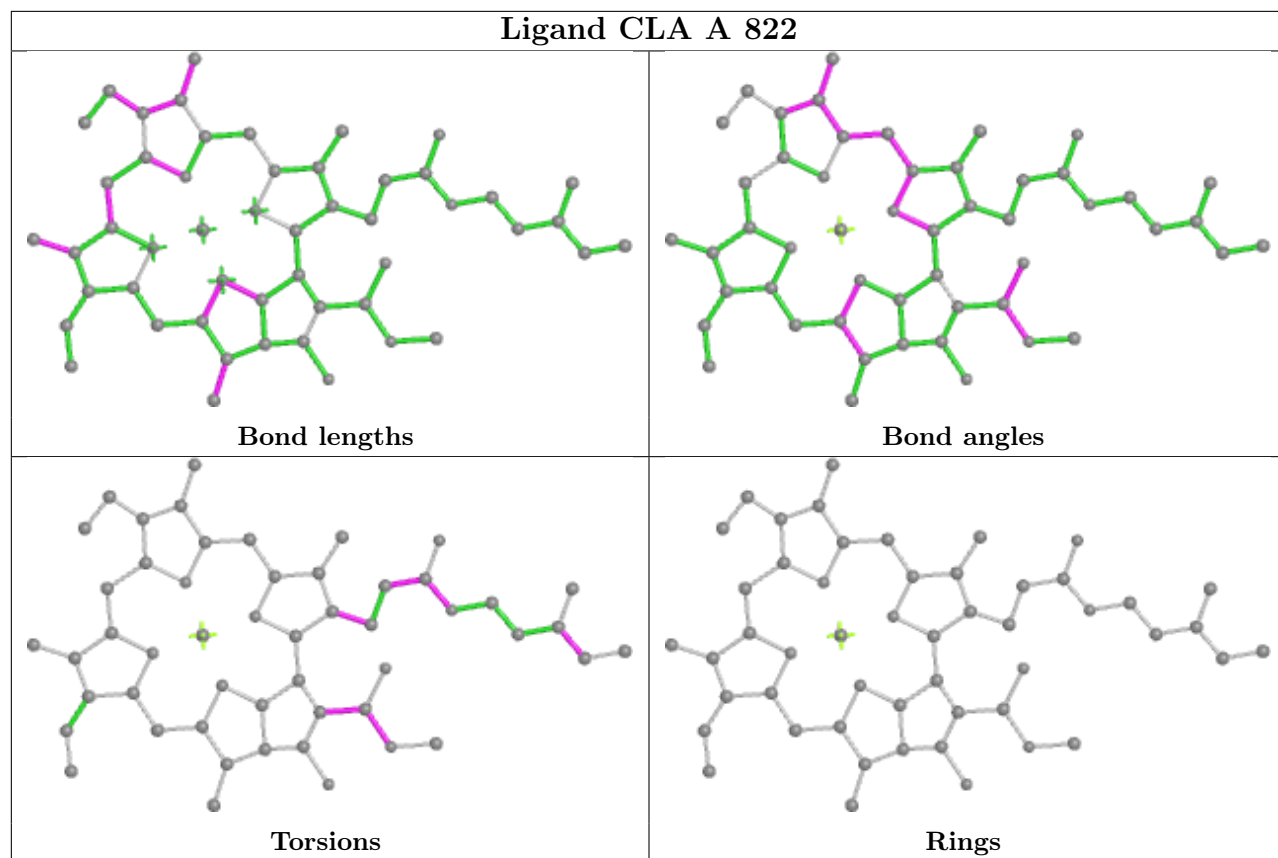




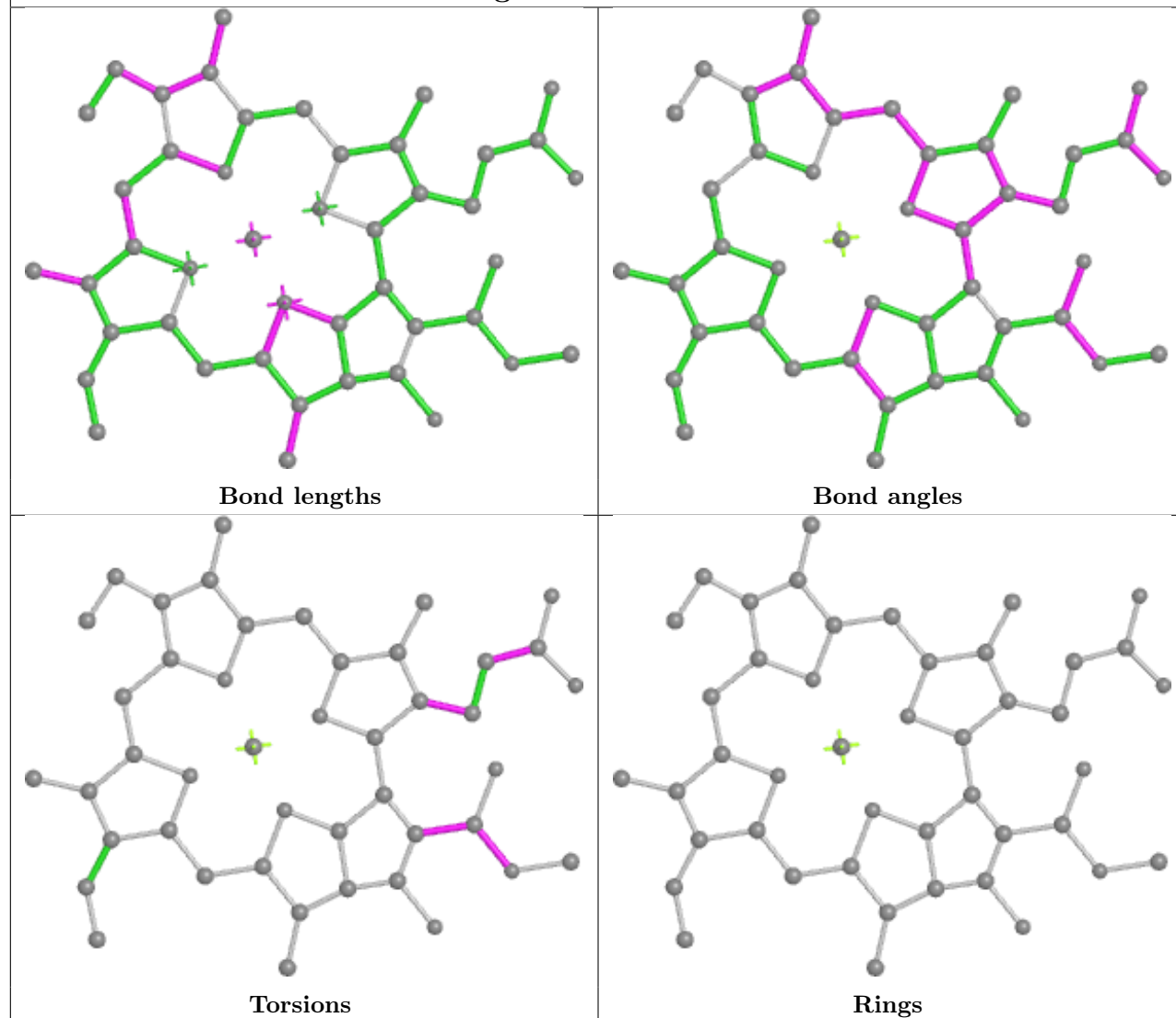




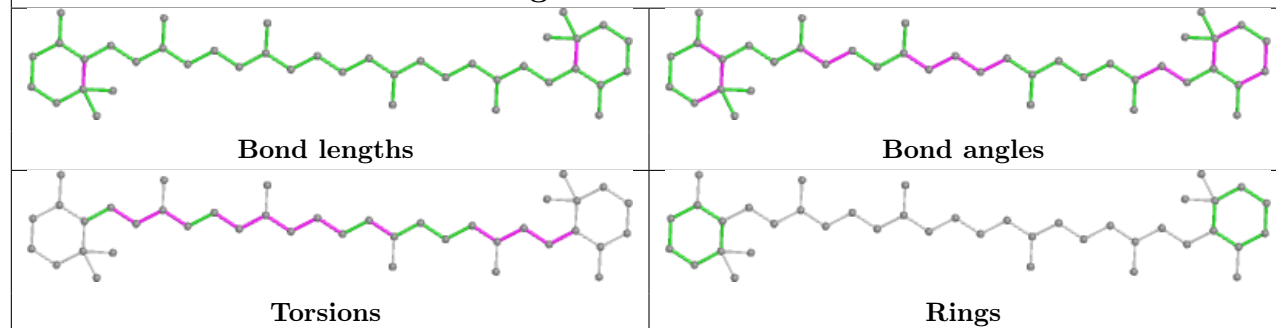




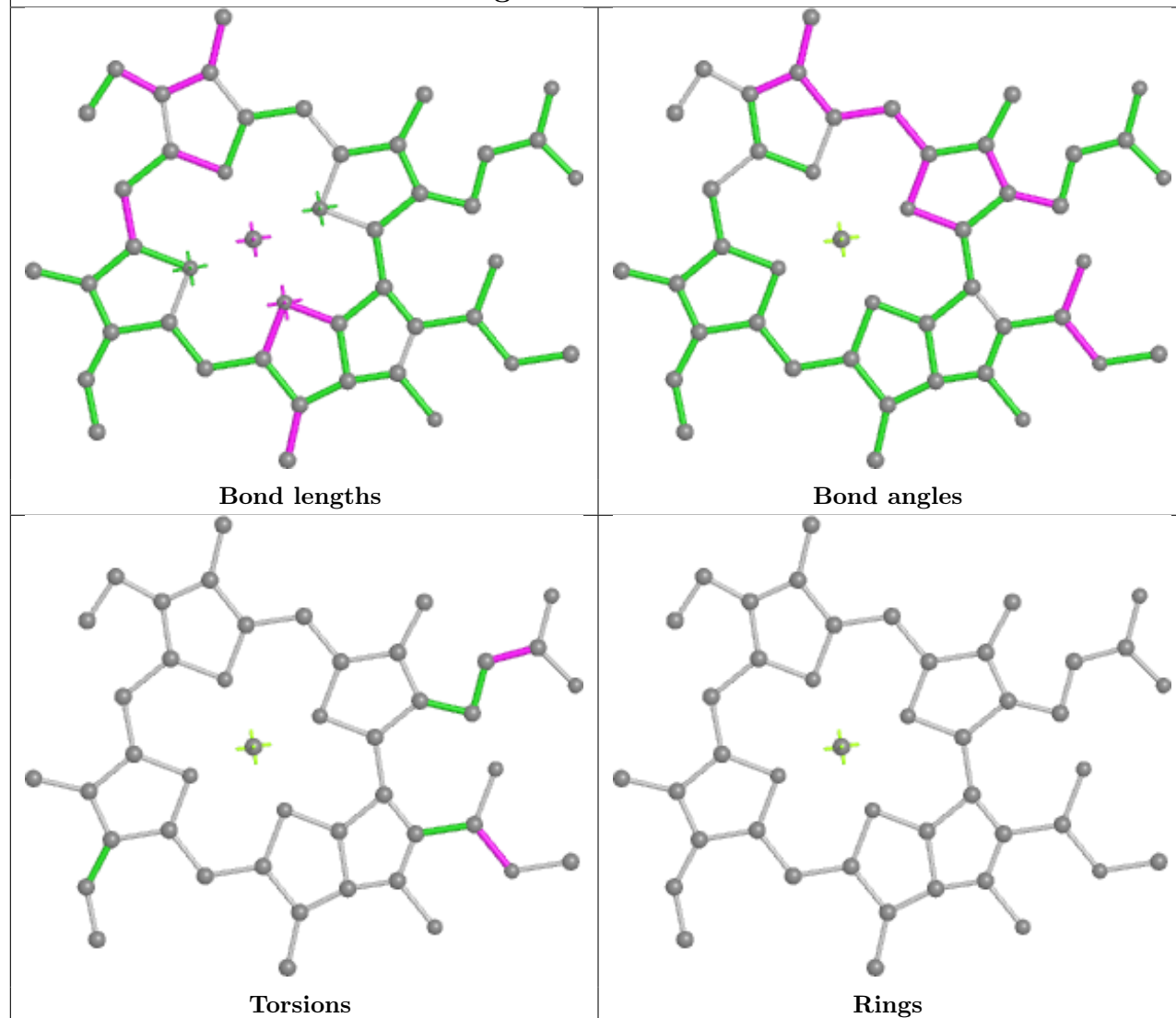
Ligand CLA 2 607



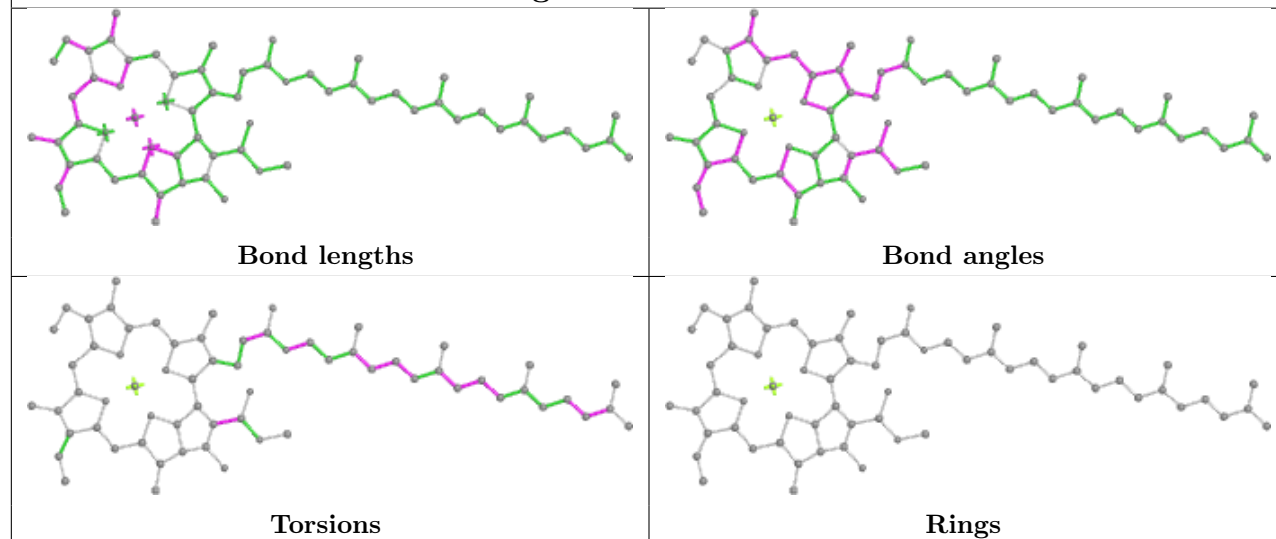
Ligand BCR A 844



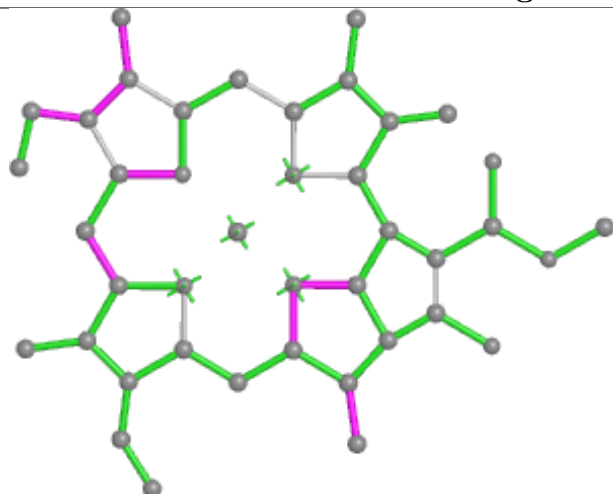
Ligand CLA 3 207



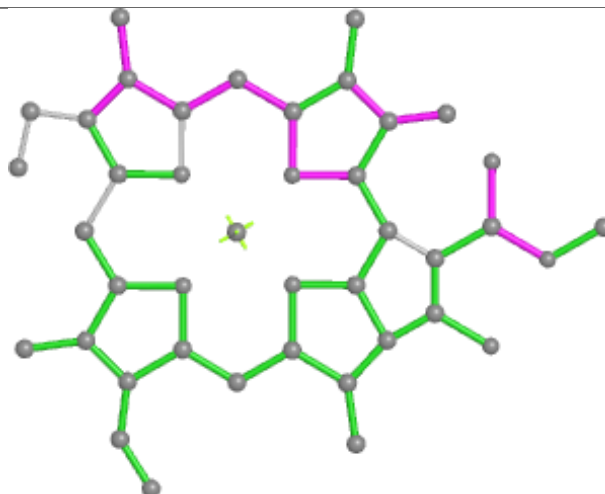
Ligand CLA B 801



Ligand CLA F 803



Bond lengths



Bond angles

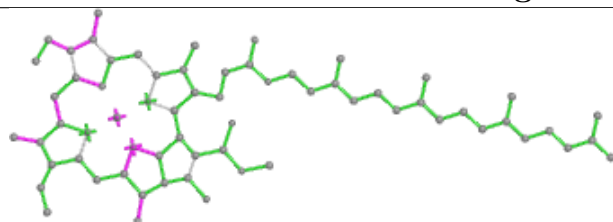


Torsions

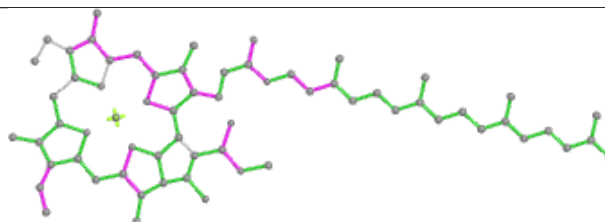


Rings

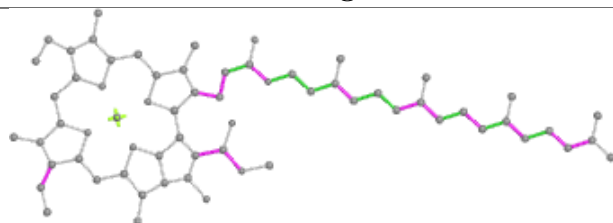
Ligand CLA B 815



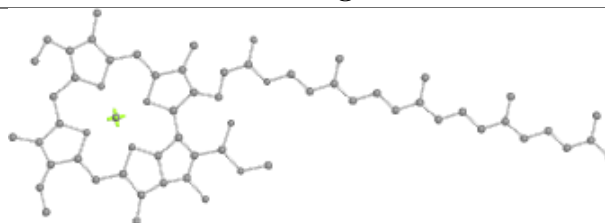
Bond lengths



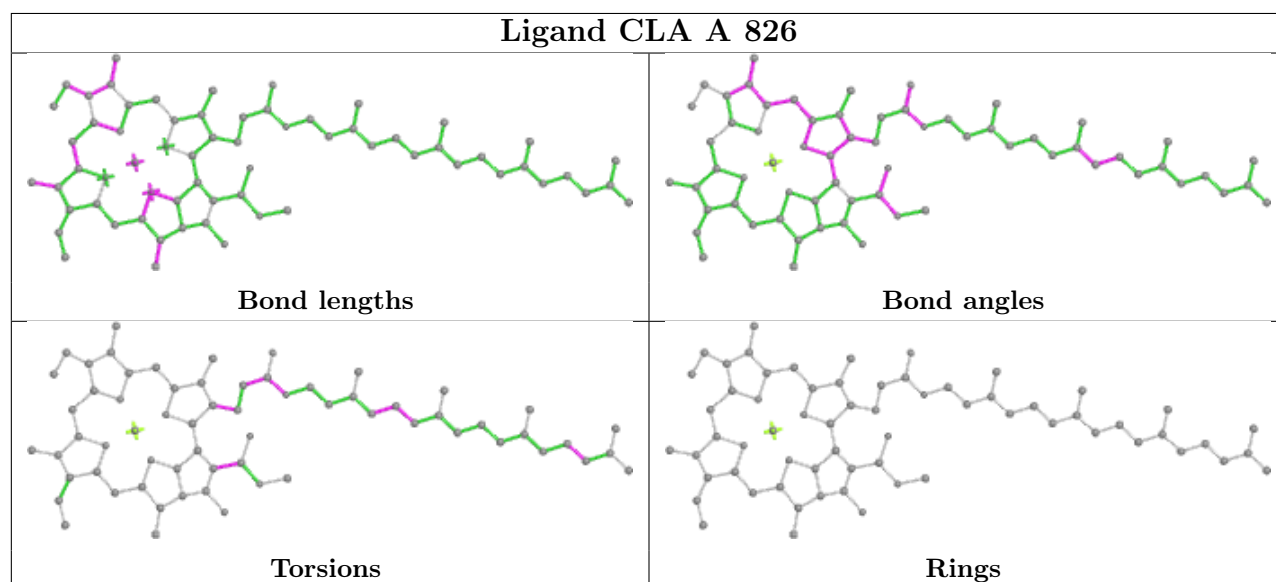
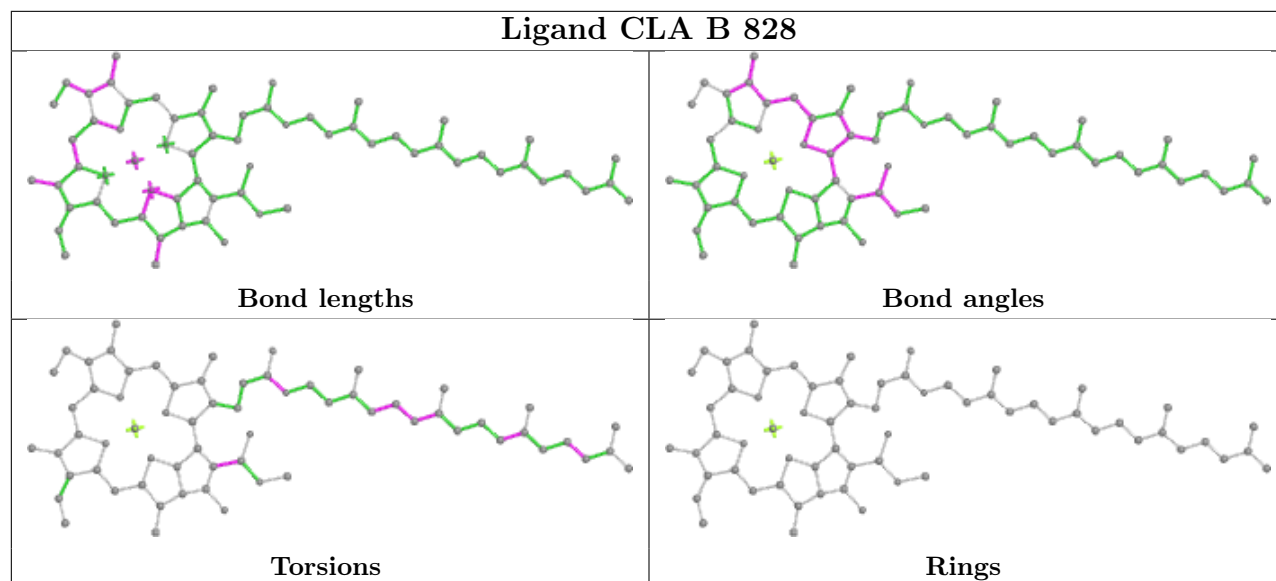
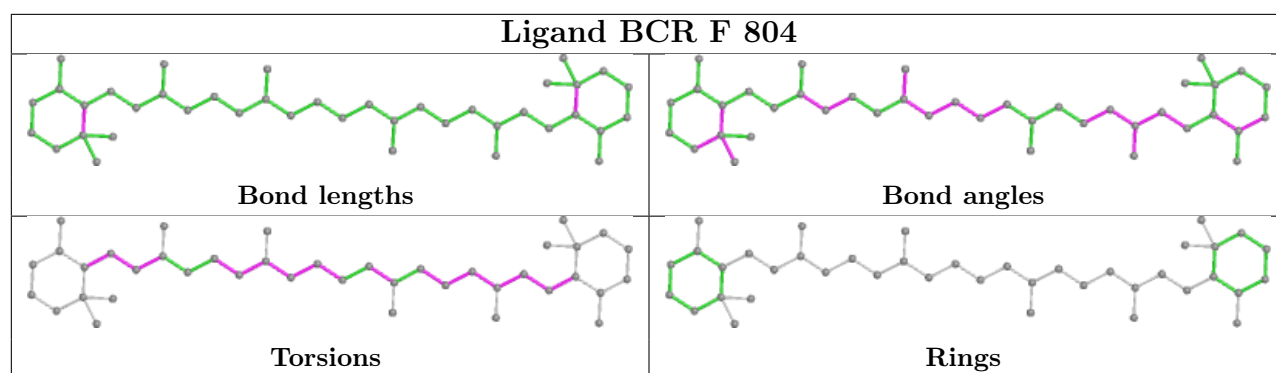
Bond angles



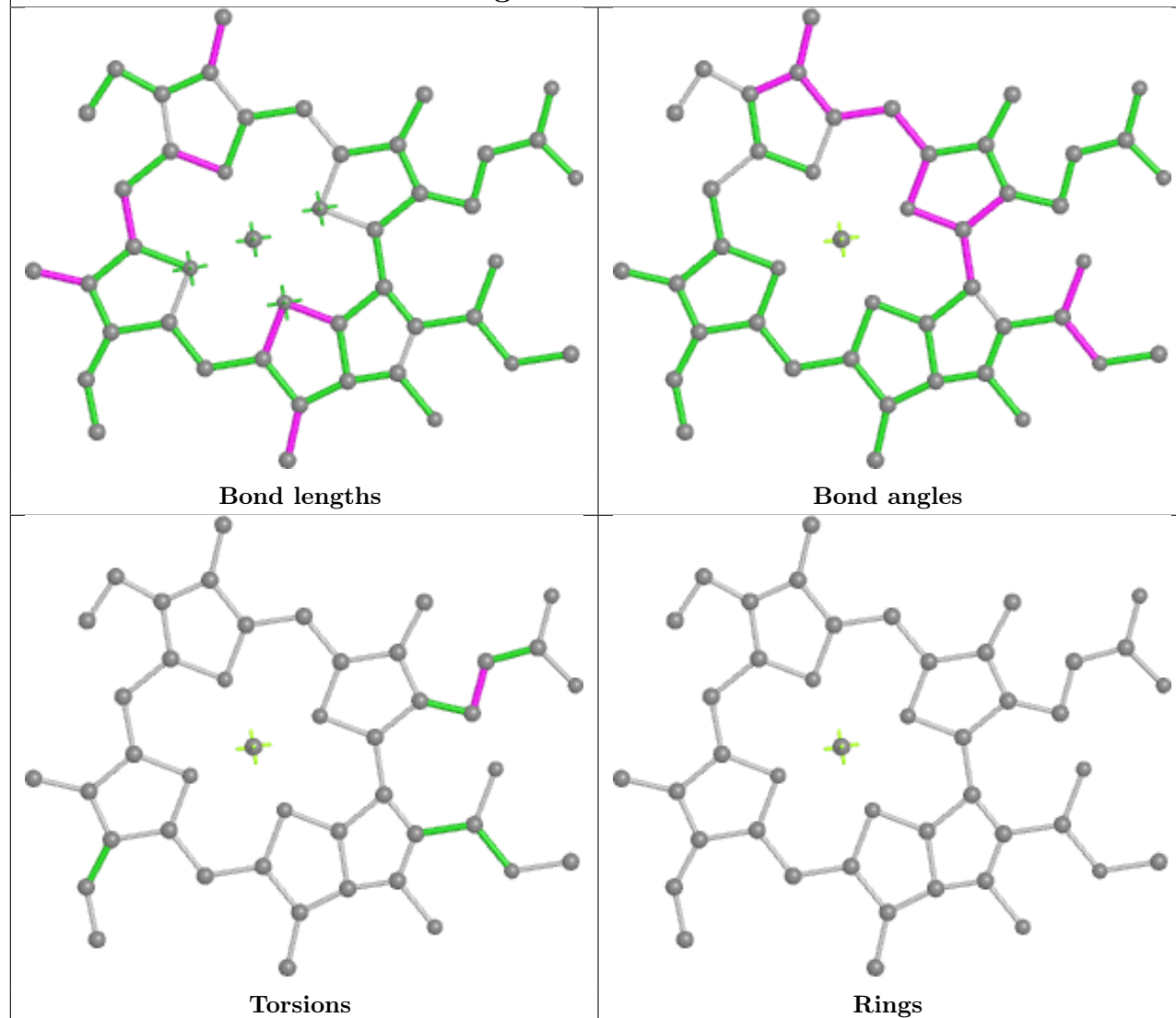
Torsions



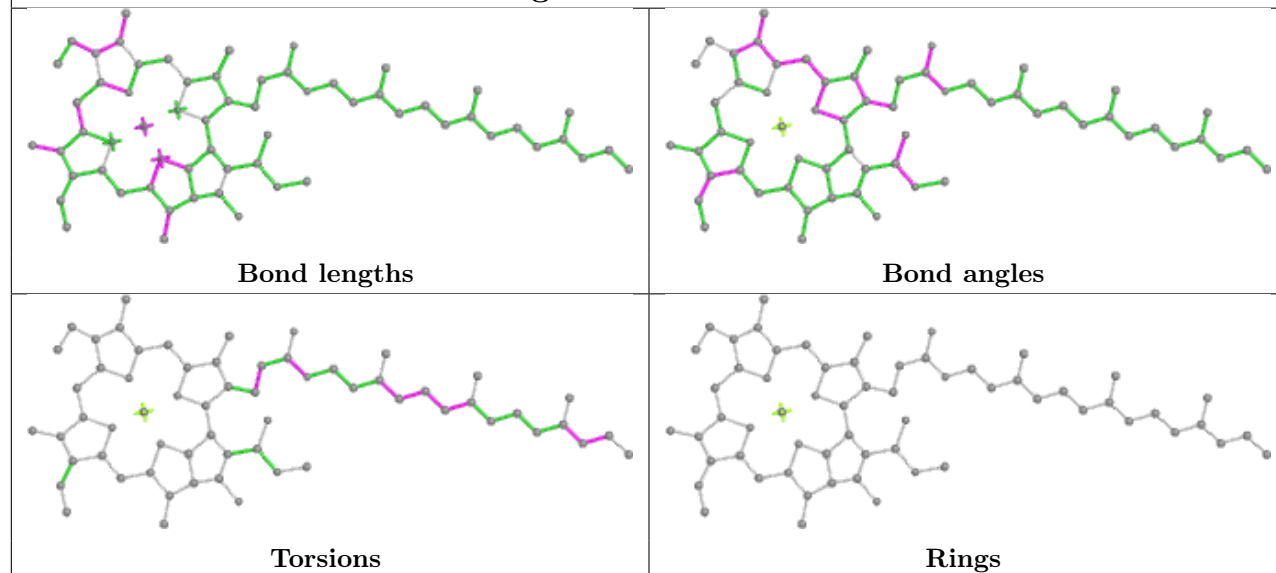
Rings

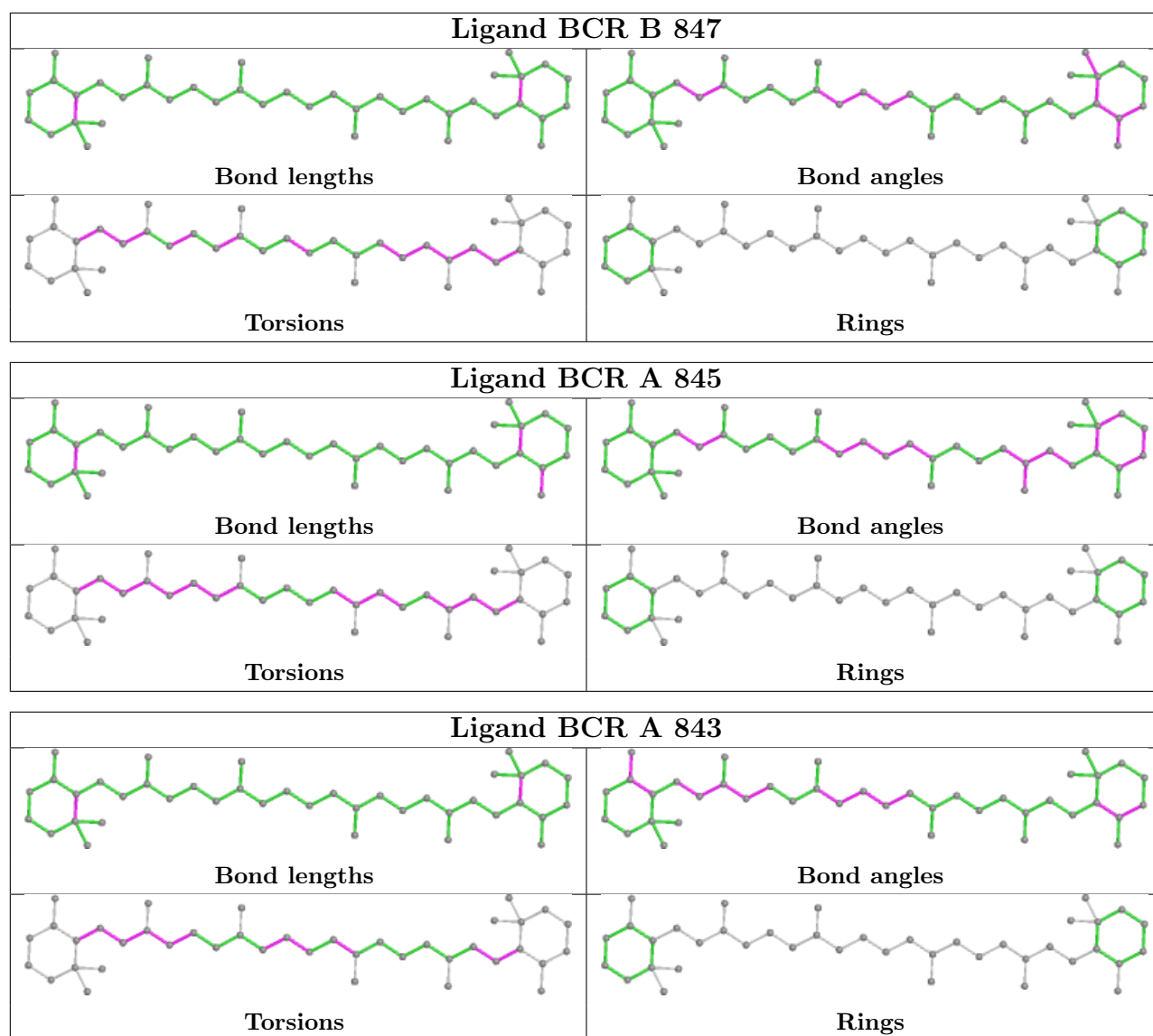


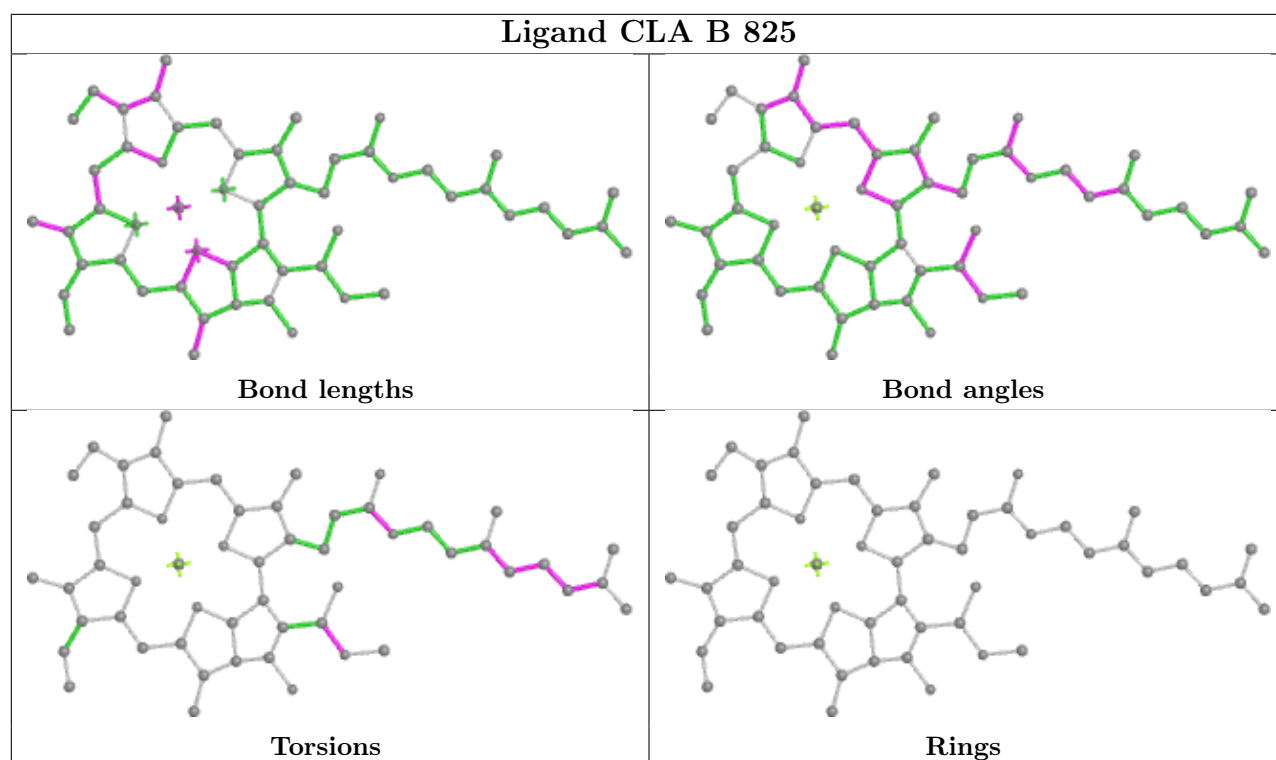
Ligand CLA 2 613



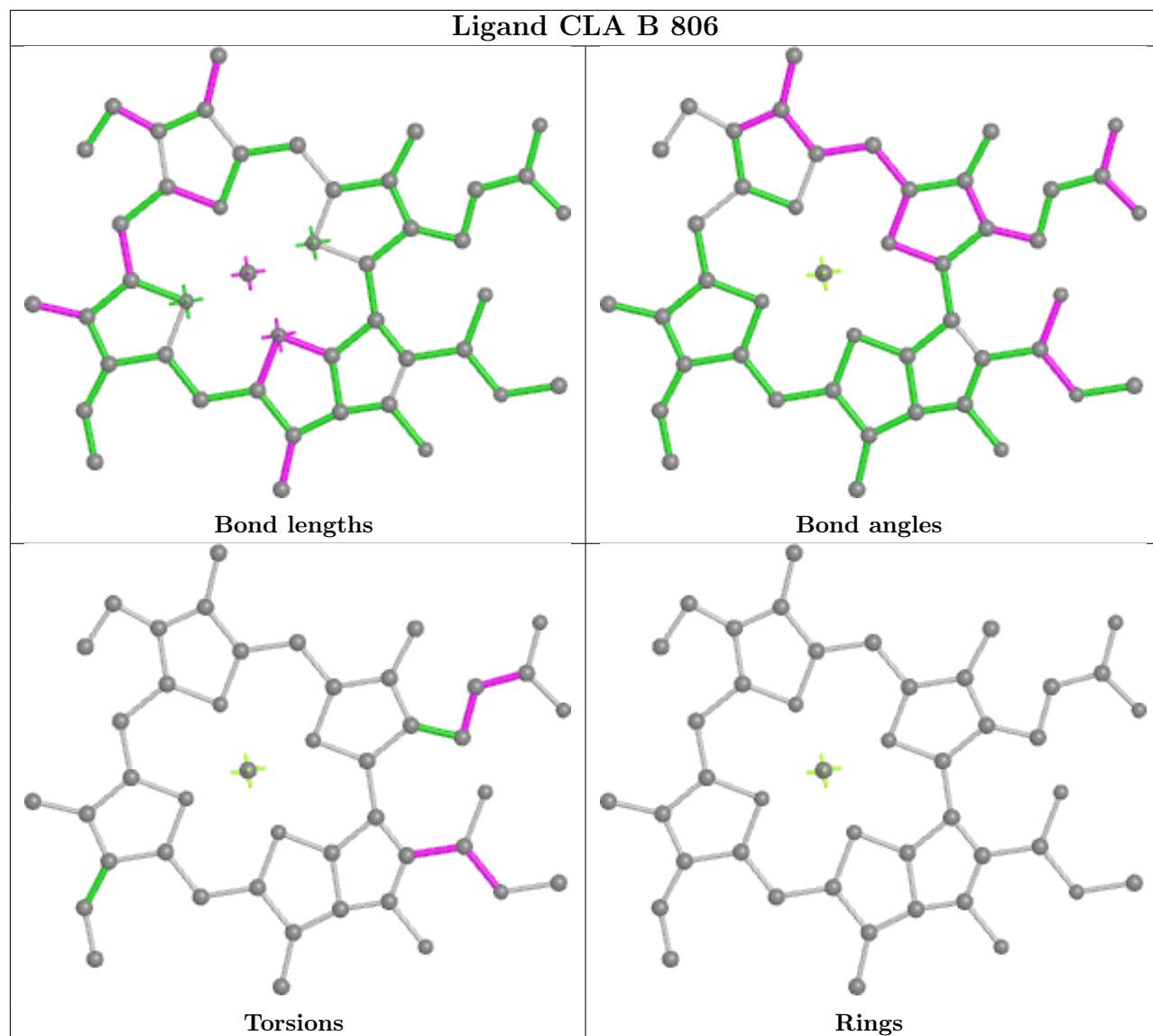
Ligand CLA A 816



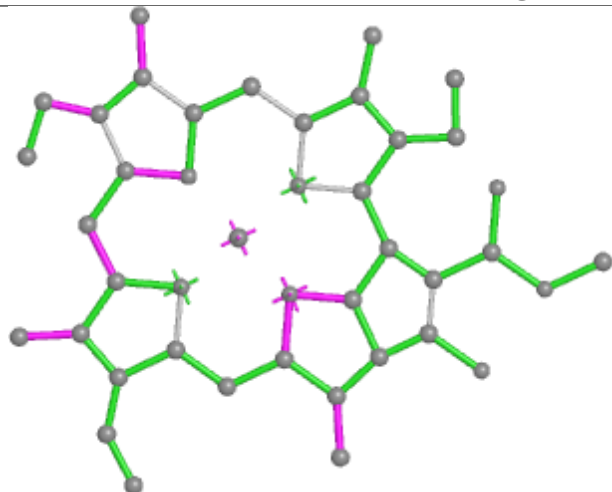




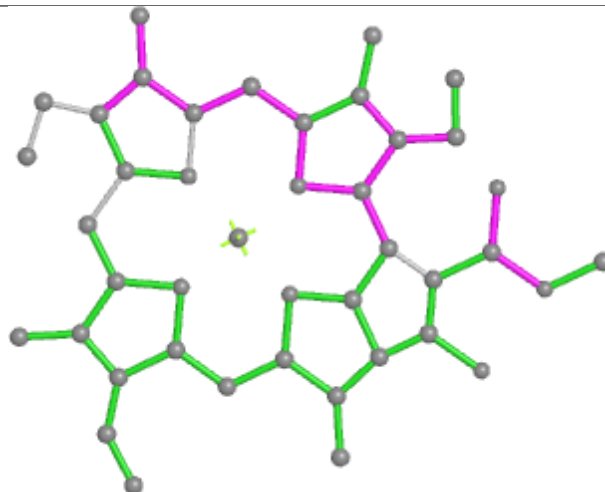
Ligand CLA B 806



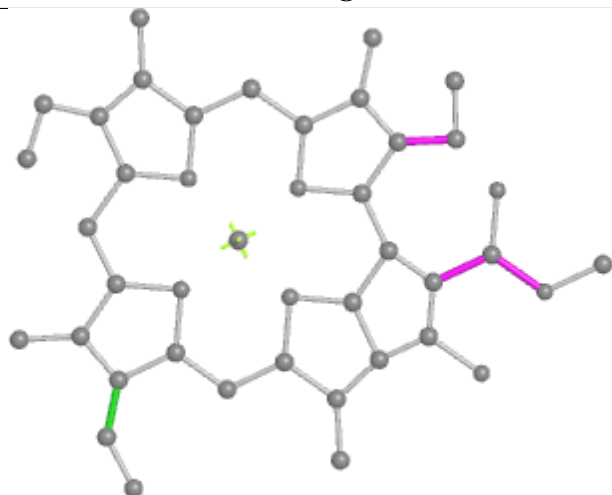
Ligand CLA B 817



Bond lengths



Bond angles

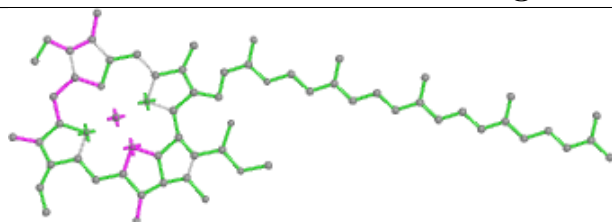


Torsions

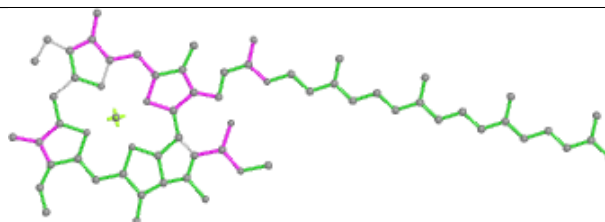


Rings

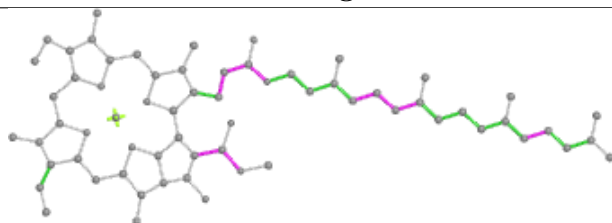
Ligand CLA A 832



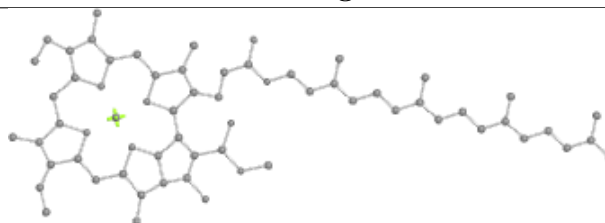
Bond lengths



Bond angles

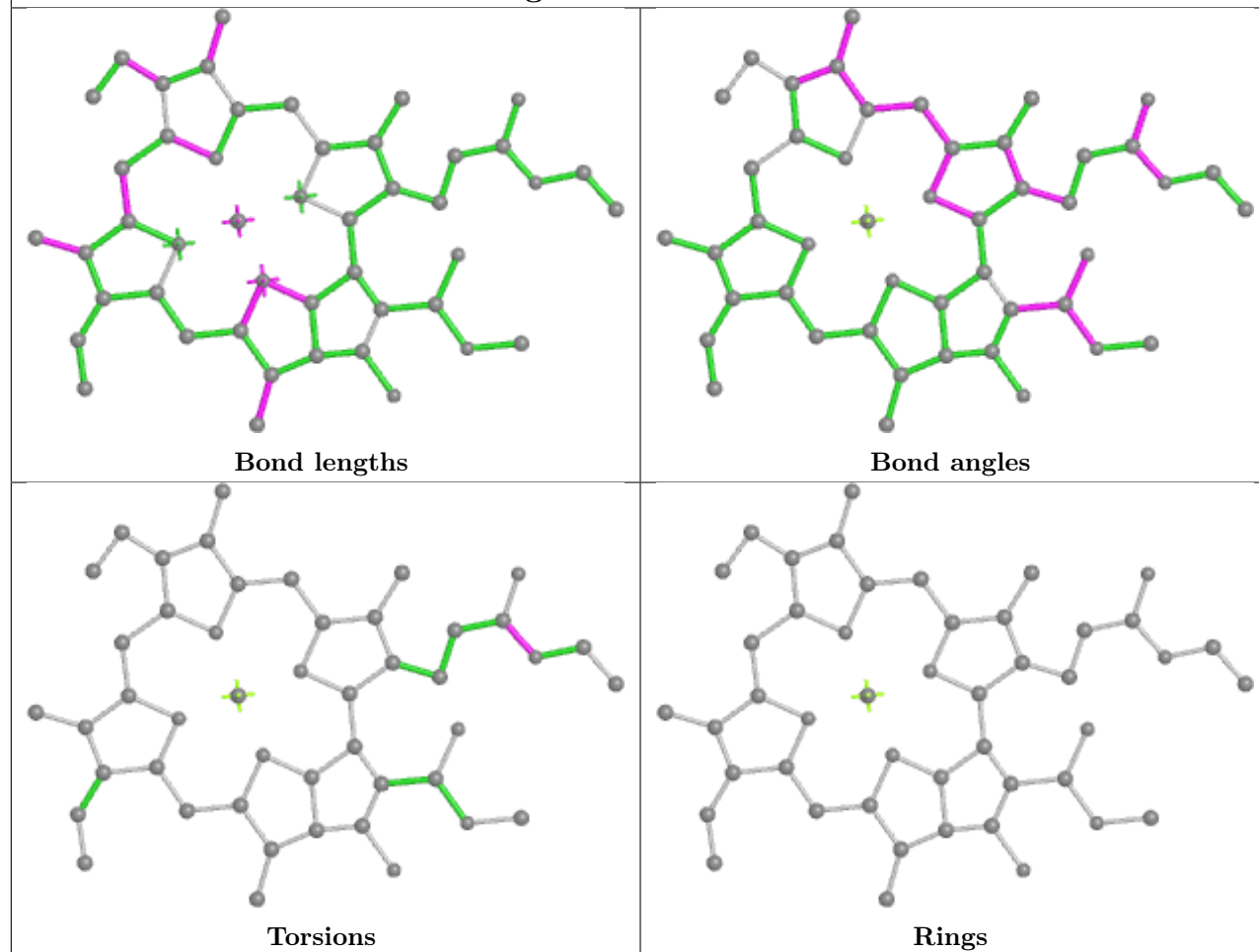


Torsions

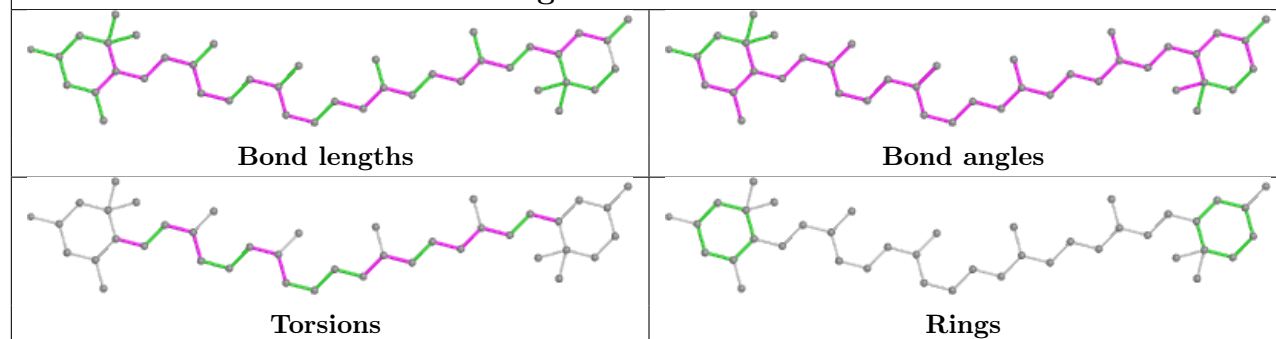


Rings

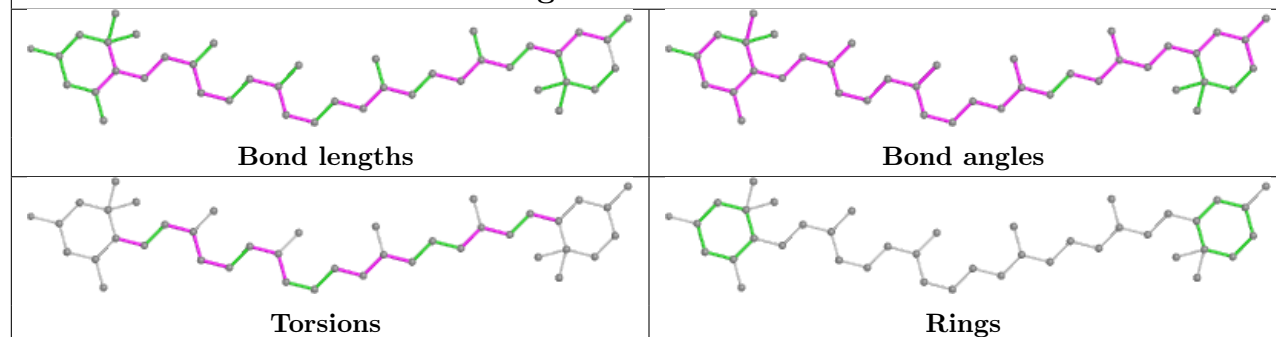
Ligand CLA B 839



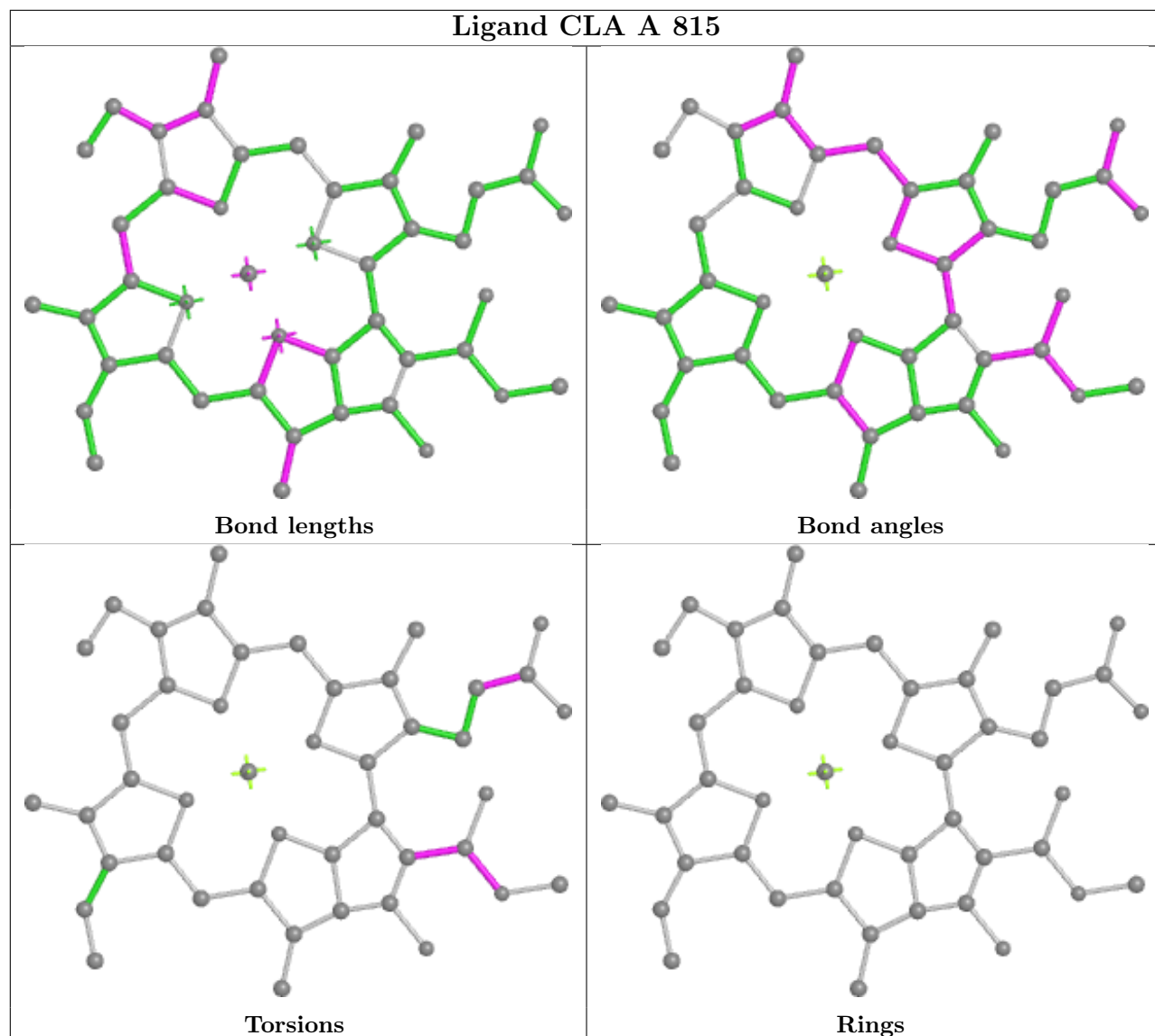
Ligand ZEX 3 215



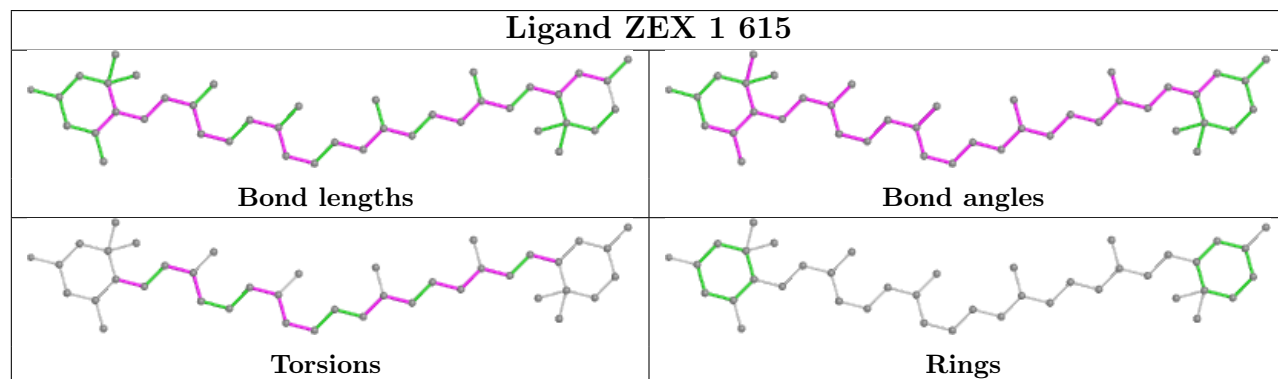
Ligand ZEX 3 214



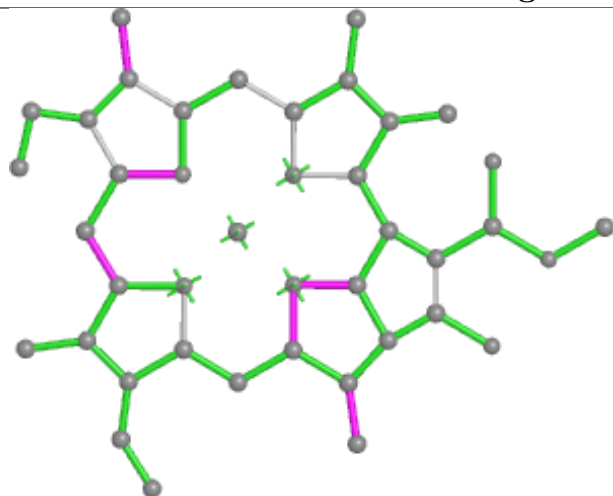
Ligand CLA A 815



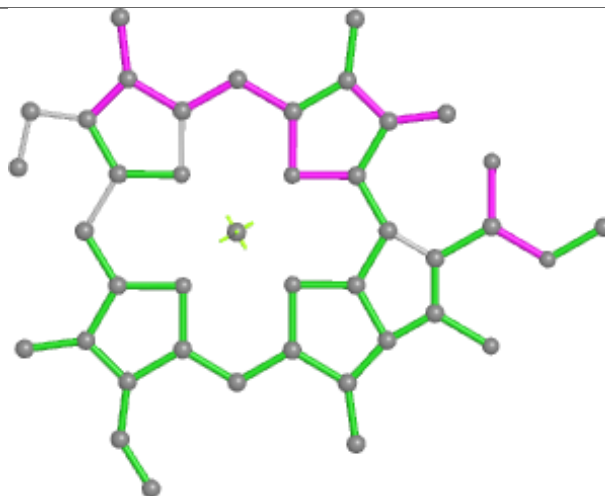
Ligand ZEX 1 615



Ligand CLA 2 609



Bond lengths



Bond angles

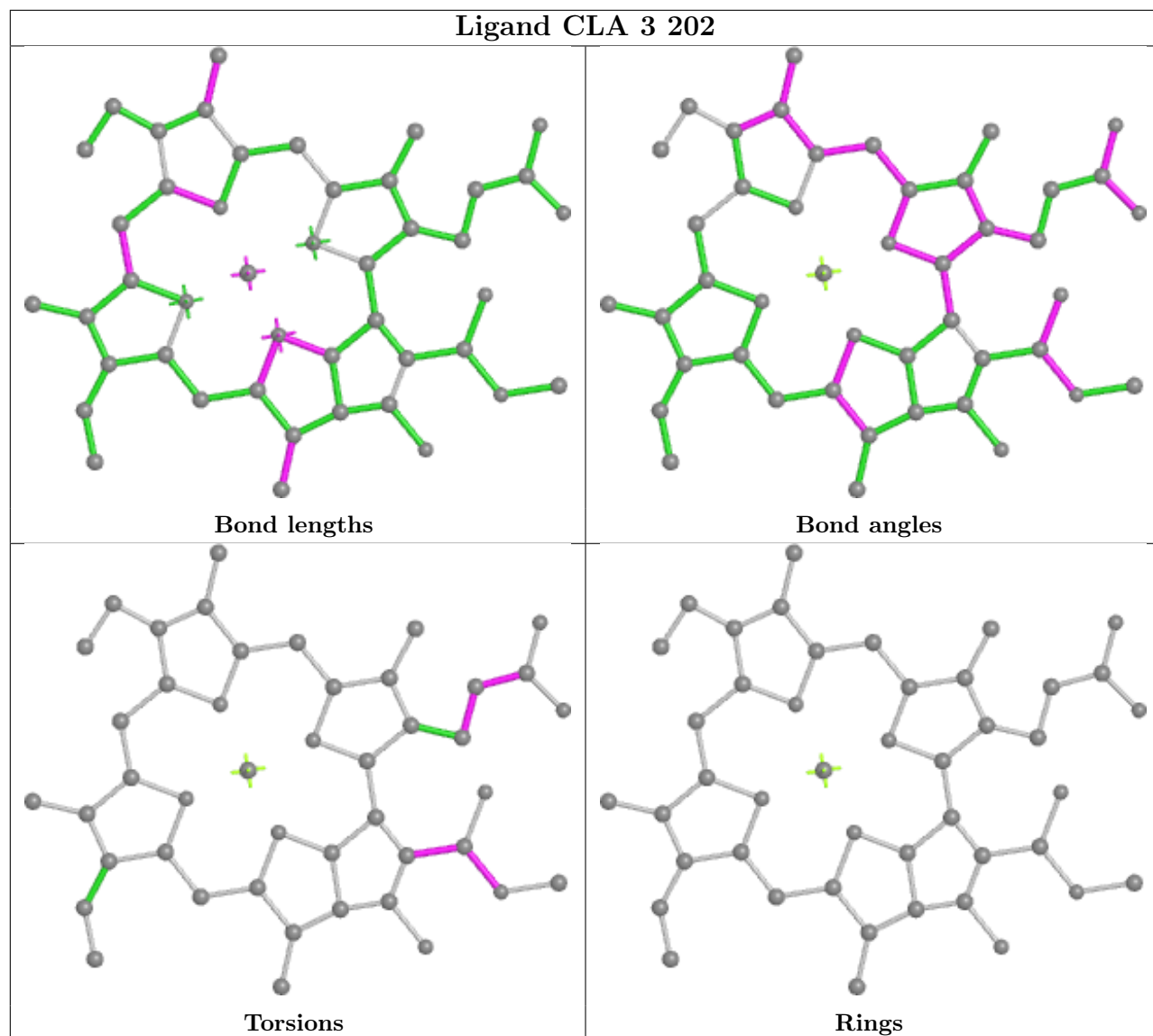


Torsions

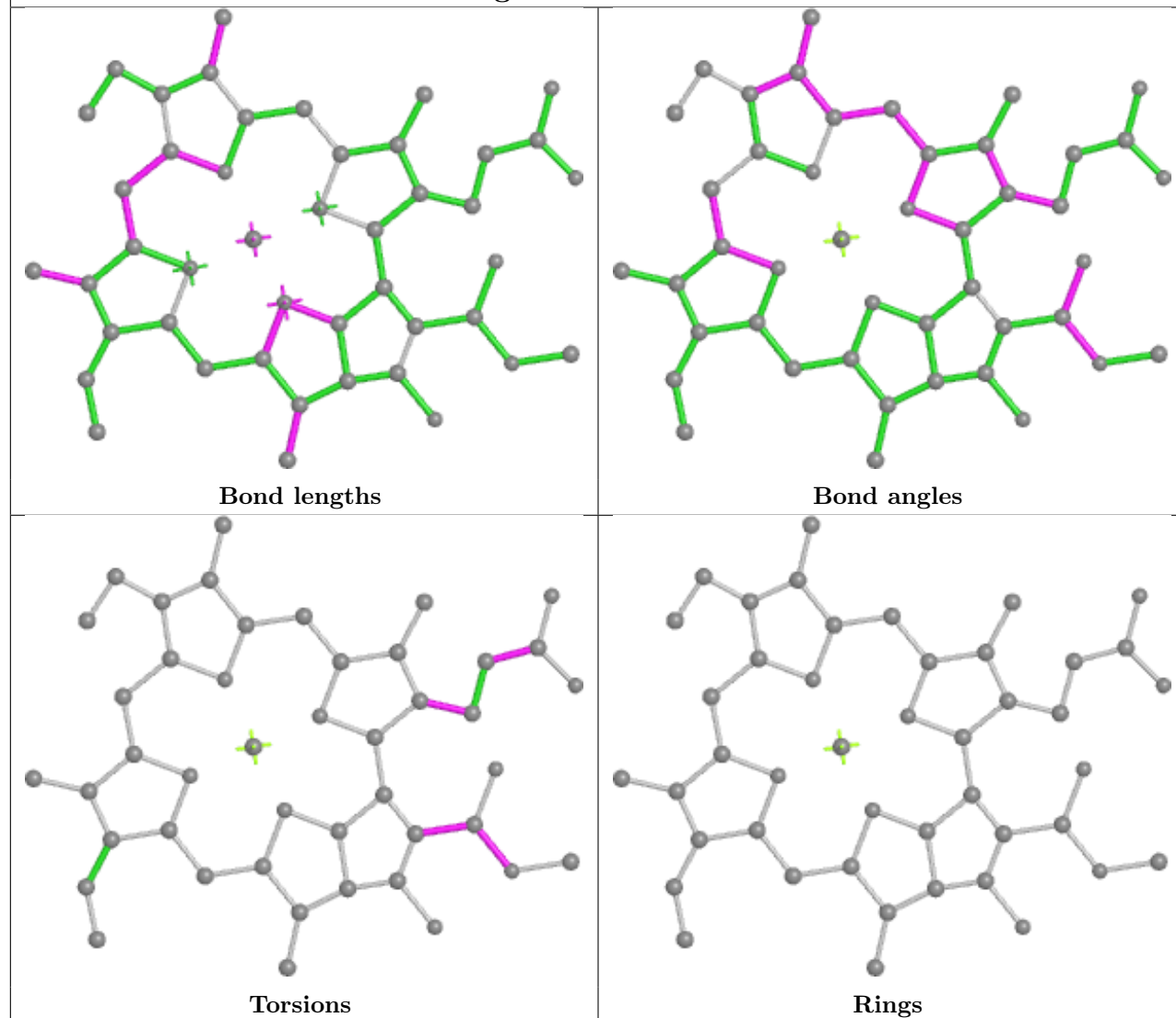


Rings

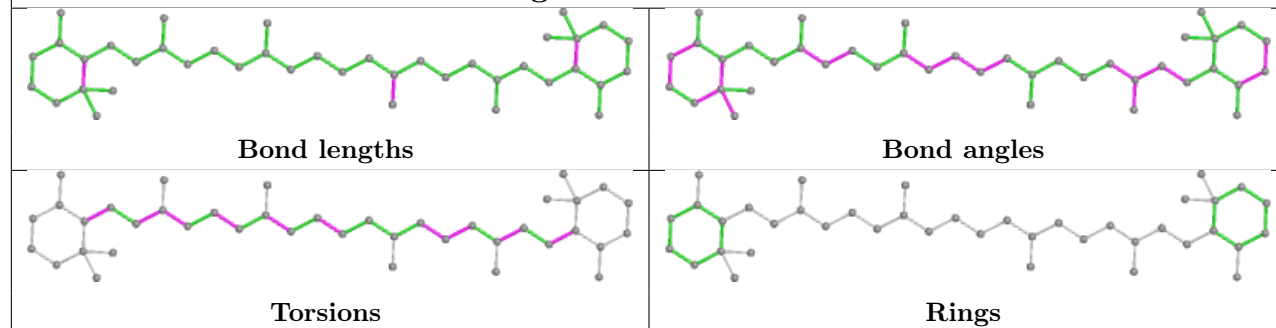
Ligand CLA 3 202



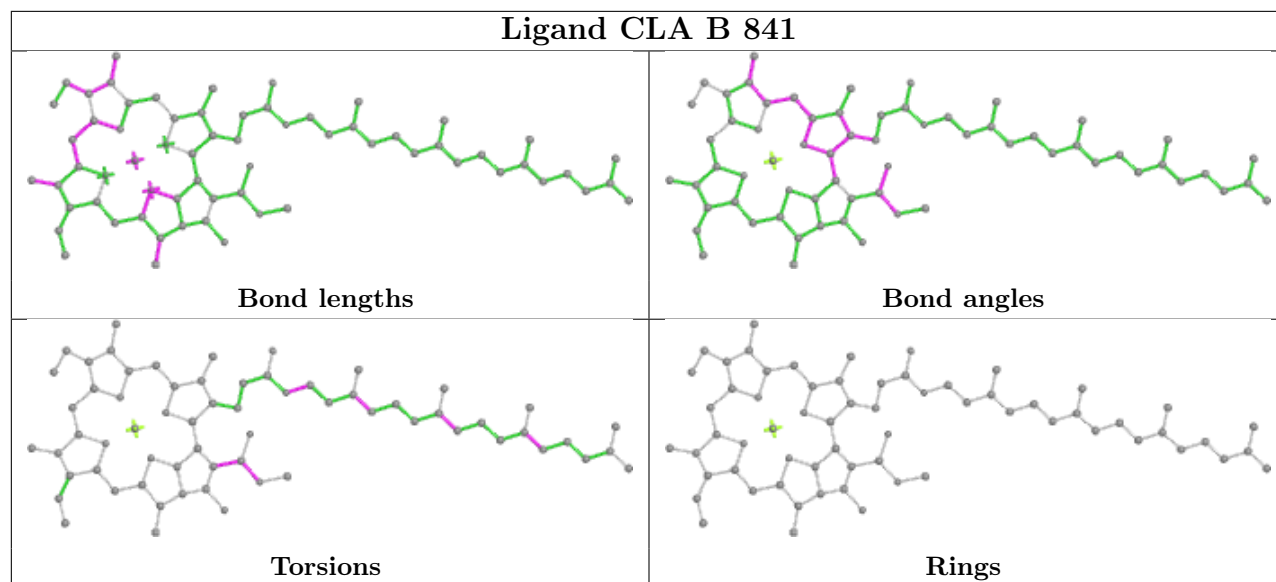
Ligand CLA 3 204



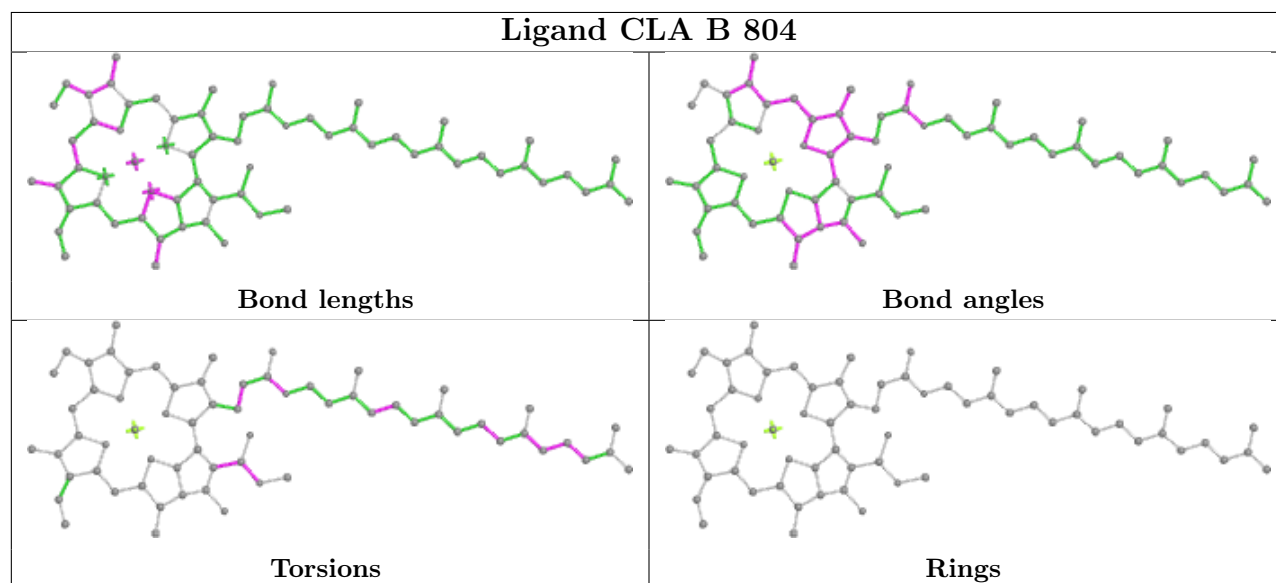
Ligand BCR B 849



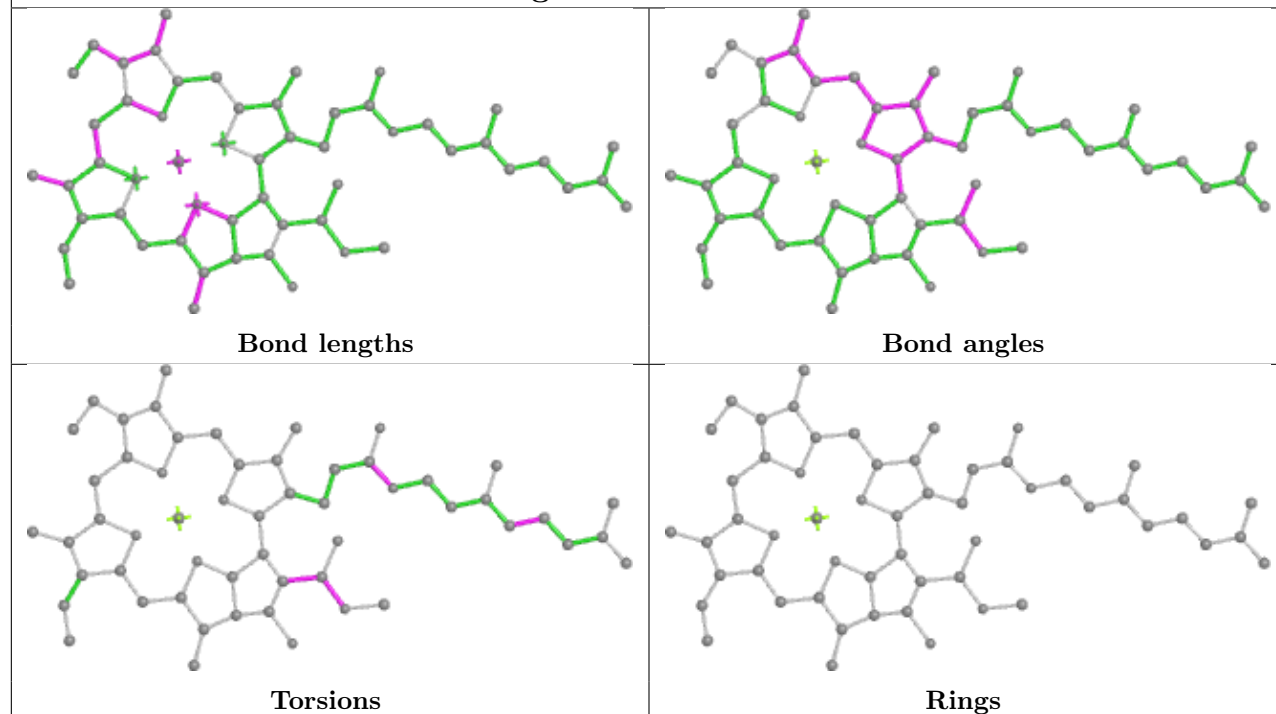
Ligand CLA B 841



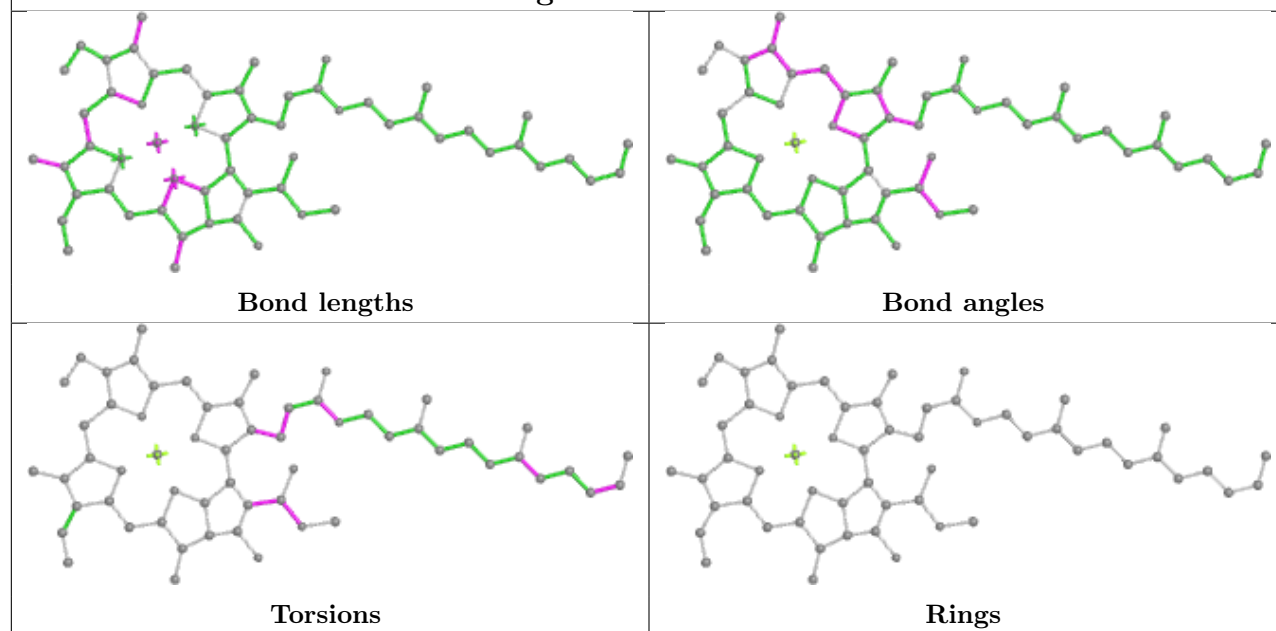
Ligand CLA B 804

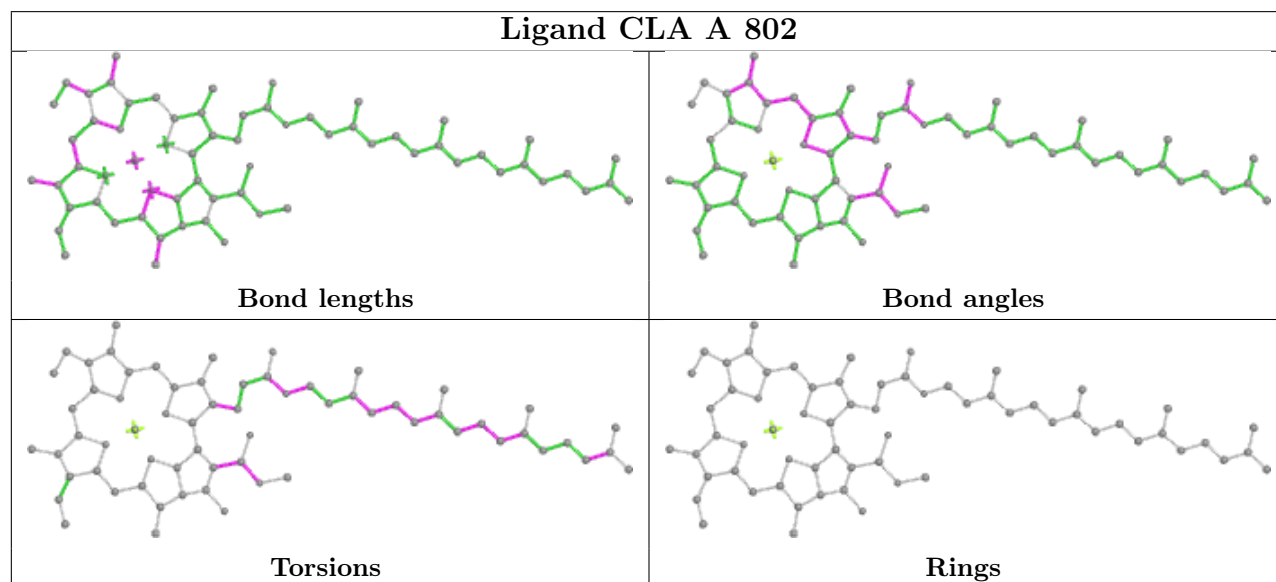
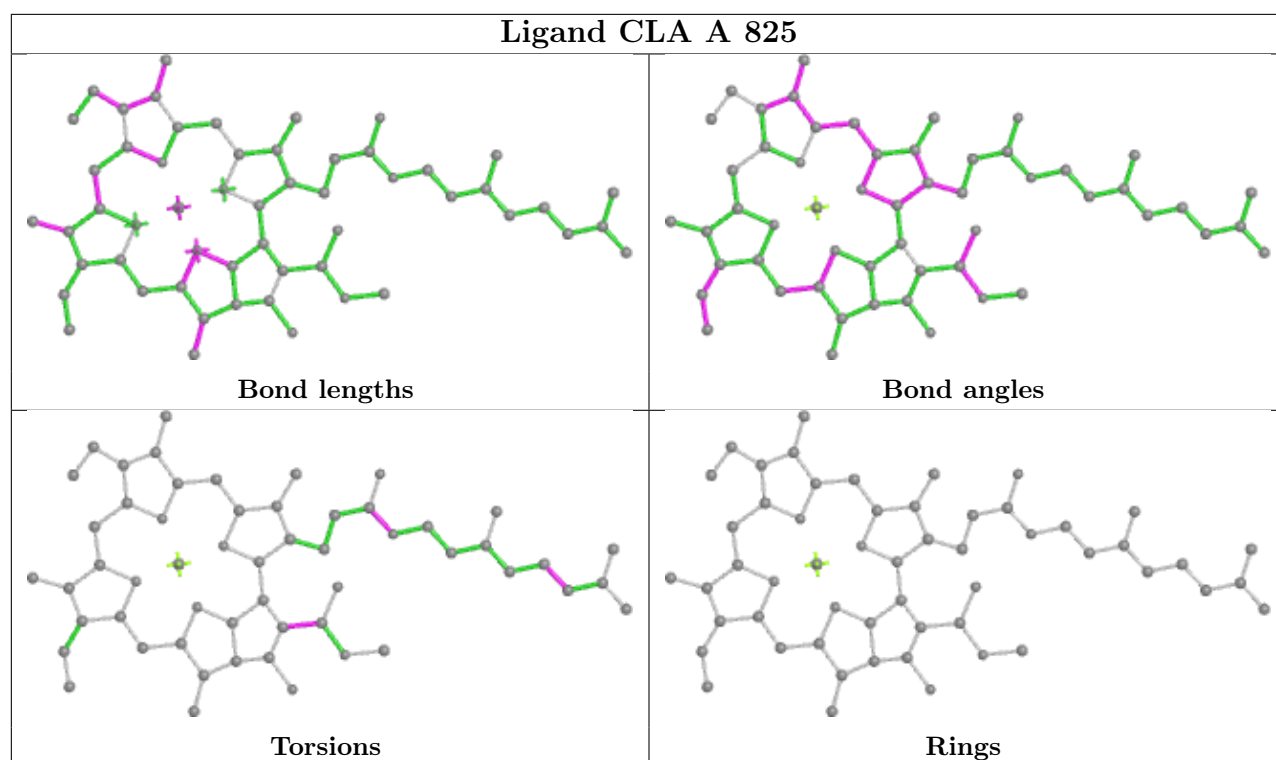


Ligand CLA A 803

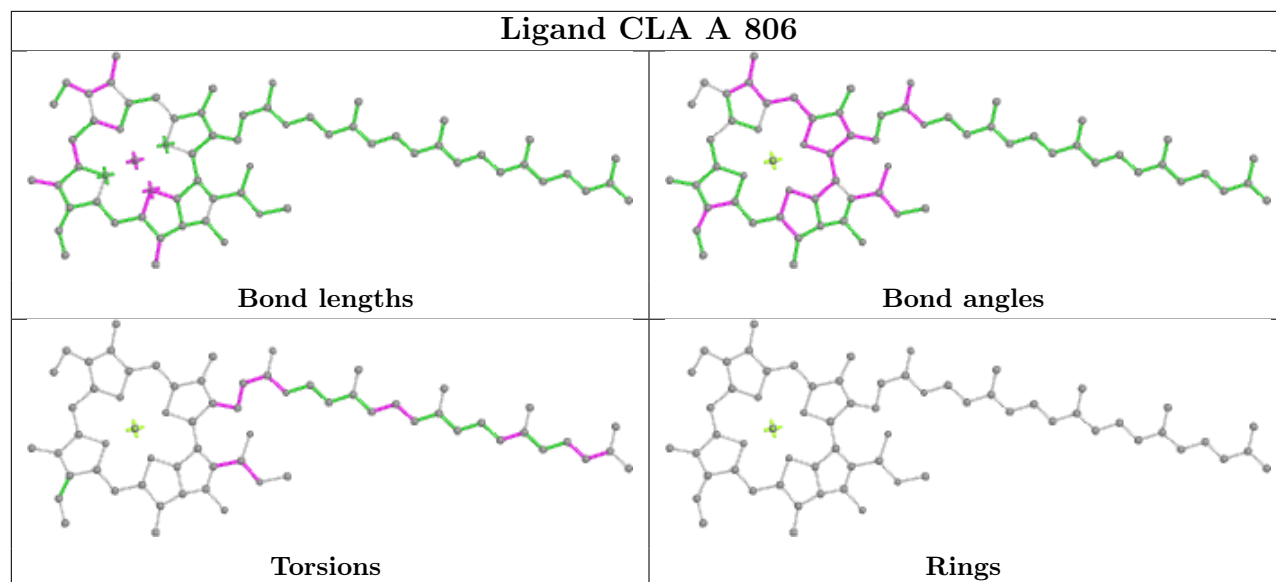


Ligand CLA 1 602

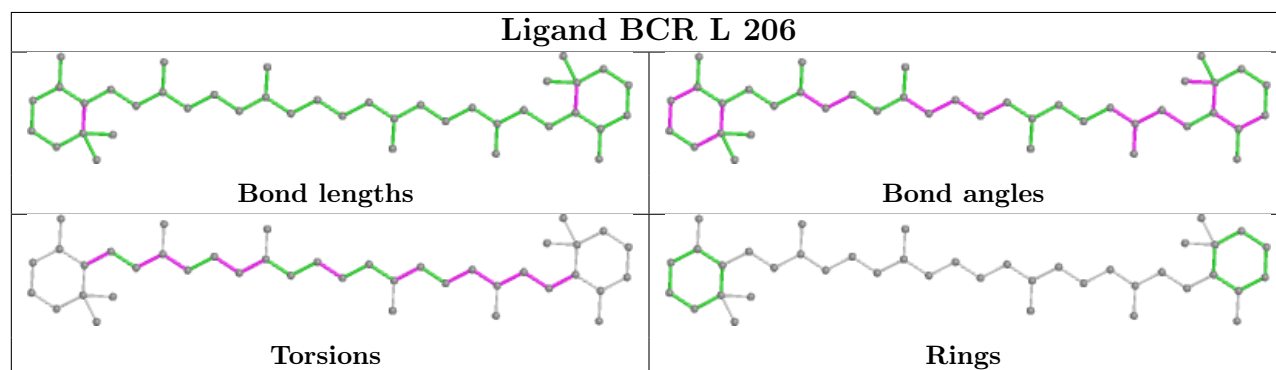




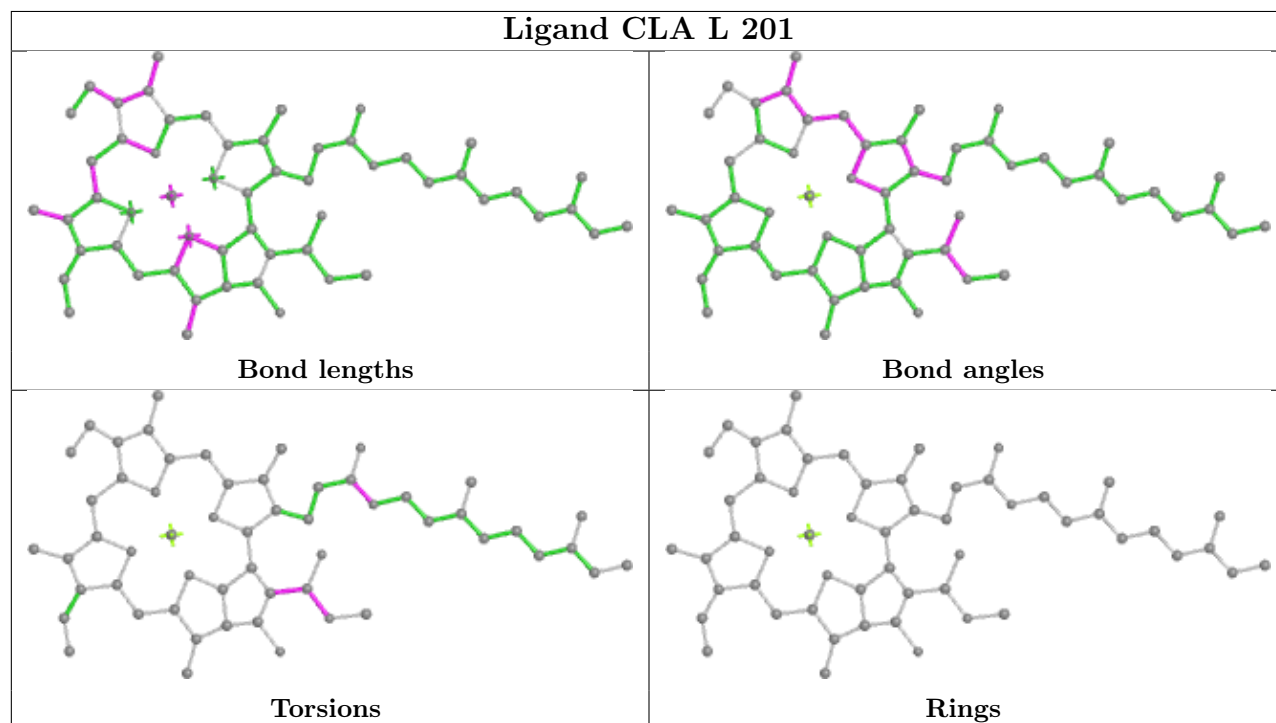
Ligand CLA A 806

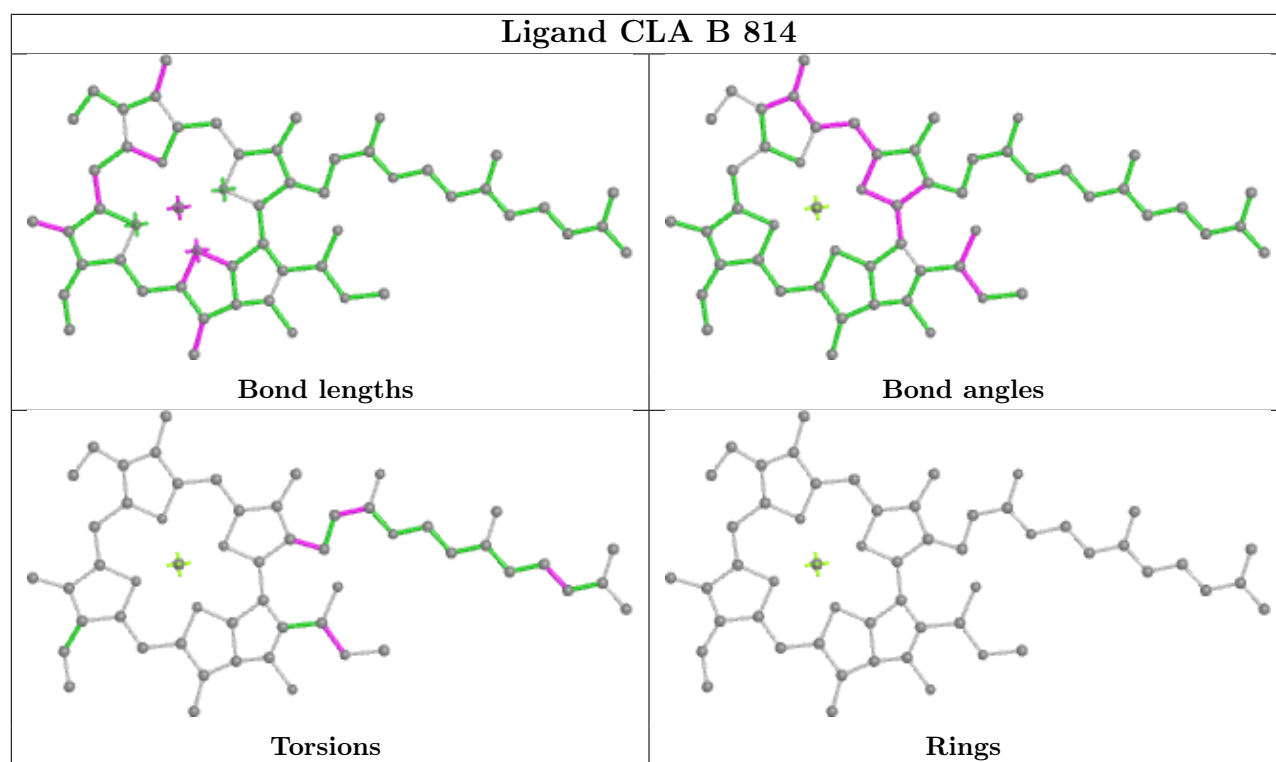


Ligand BCR L 206

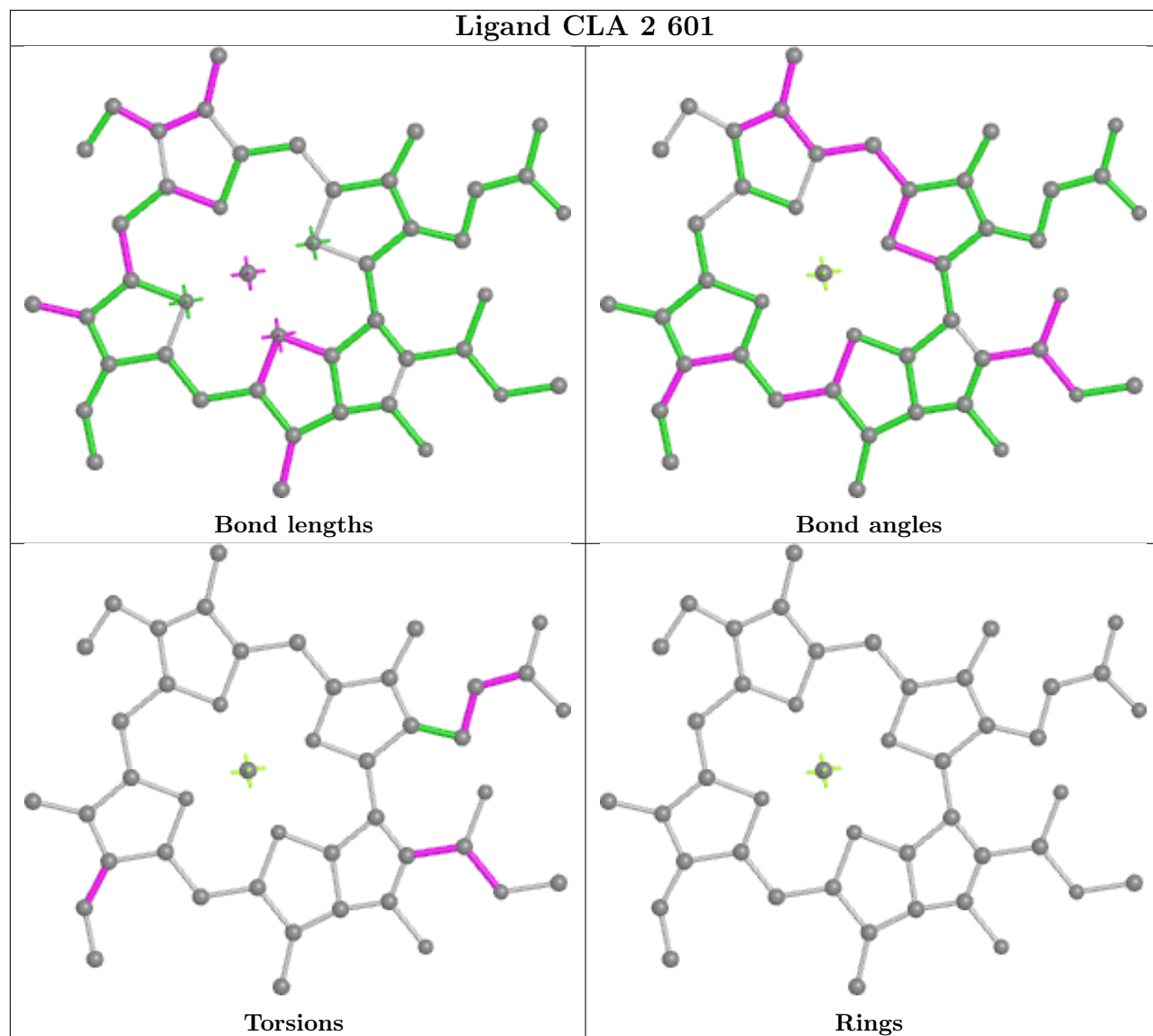


Ligand CLA L 201

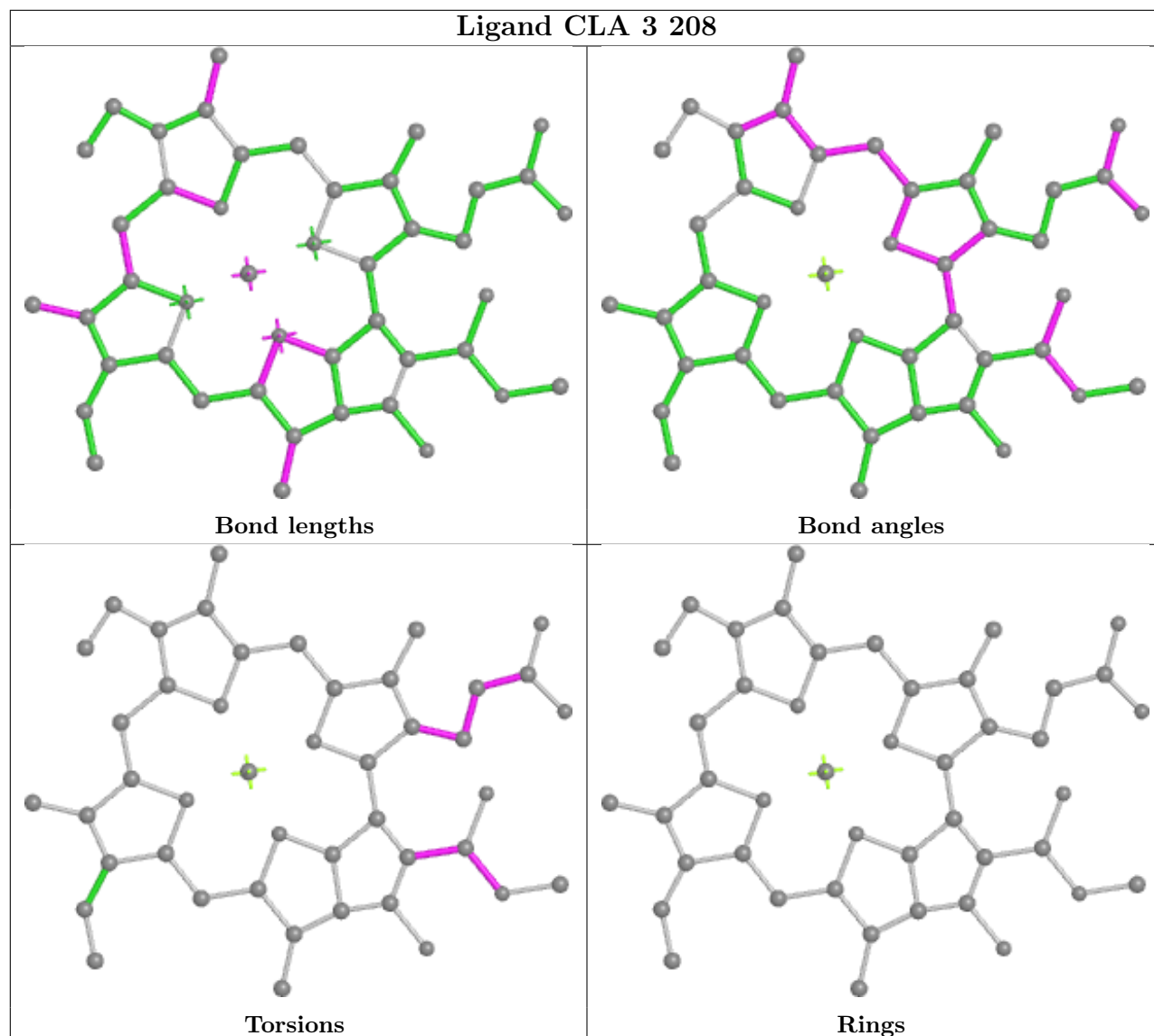




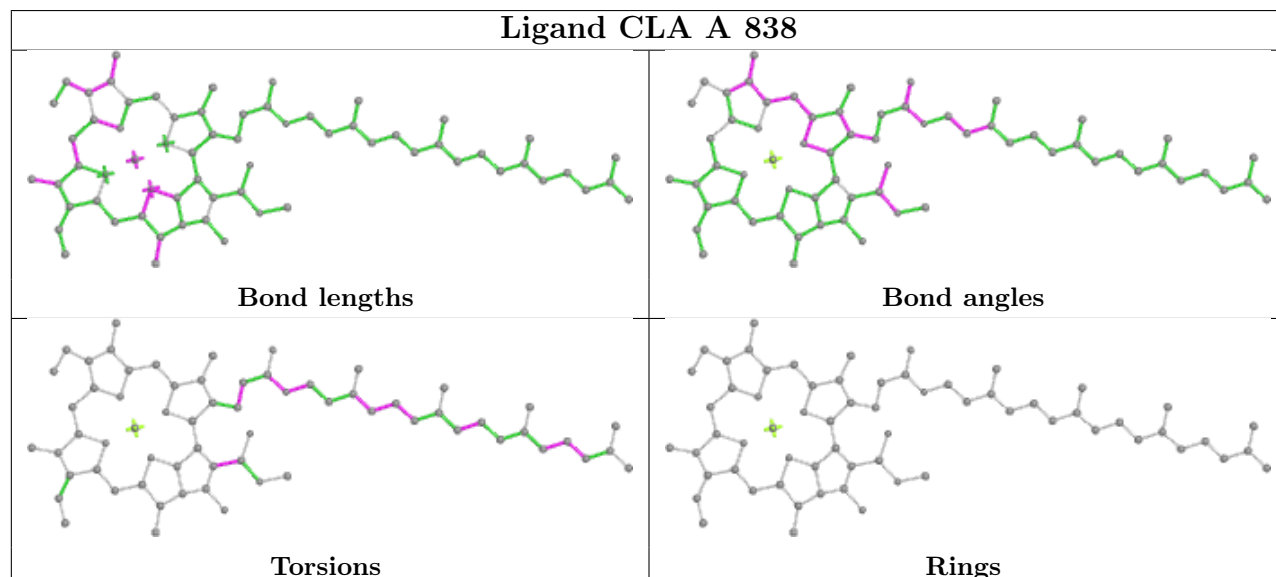
Ligand CLA 2 601



Ligand CLA 3 208



Ligand CLA A 838



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.

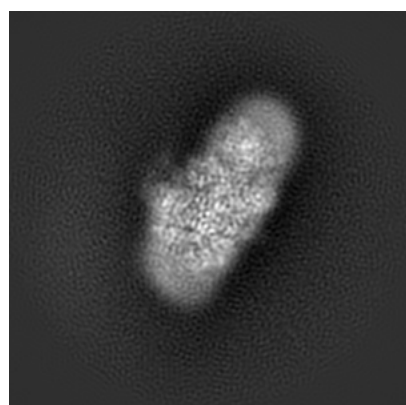
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6930. These allow visual inspection of the internal detail of the map and identification of artifacts.

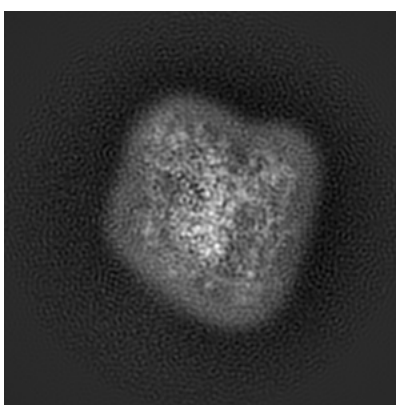
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

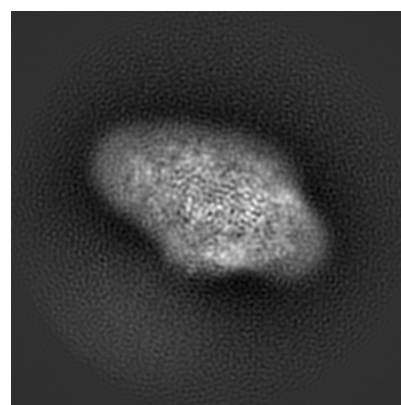
6.1.1 Primary map



X



Y

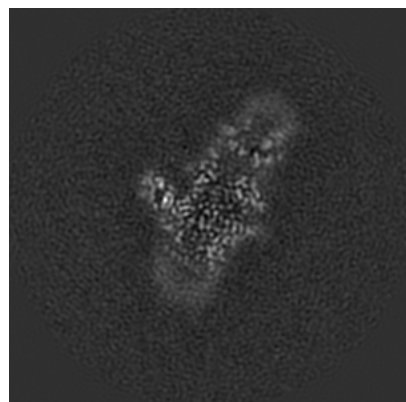


Z

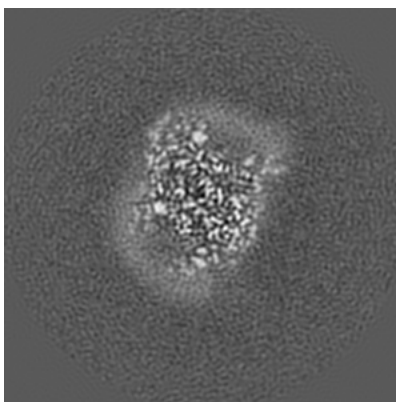
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

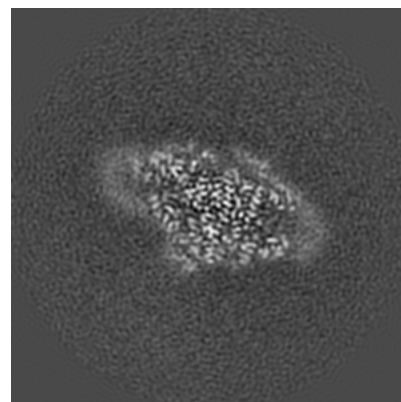
6.2.1 Primary map



X Index: 140



Y Index: 140

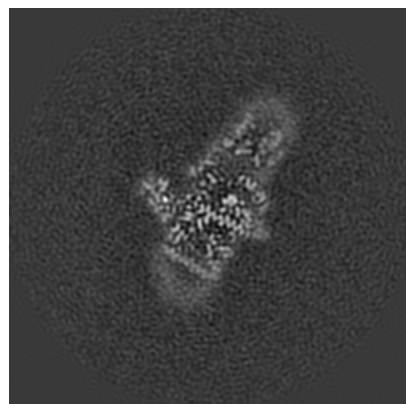


Z Index: 140

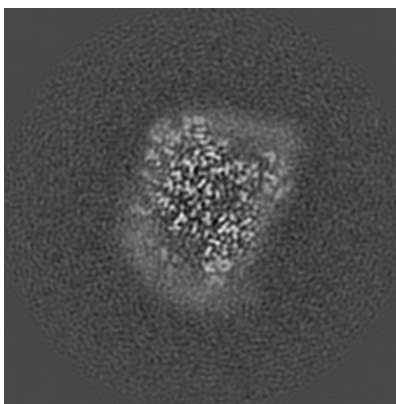
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

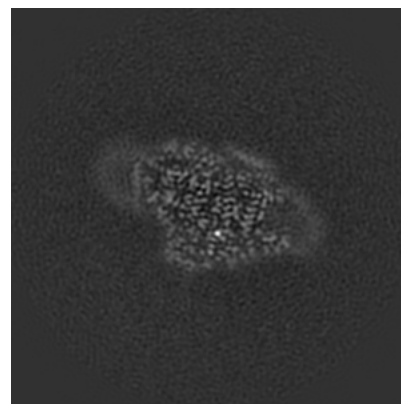
6.3.1 Primary map



X Index: 137



Y Index: 145

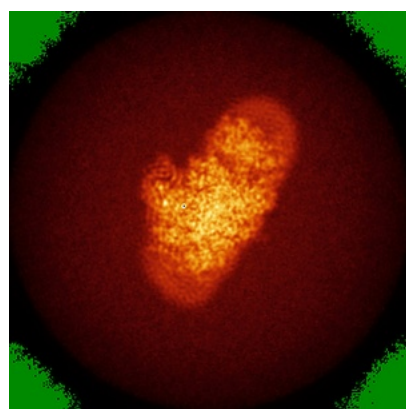


Z Index: 143

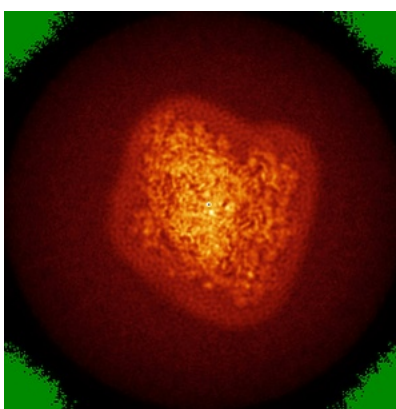
The images above show the largest variance slices of the map in three orthogonal directions.

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

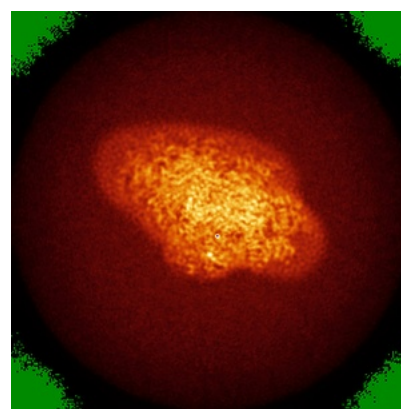
6.4.1 Primary map



X



Y

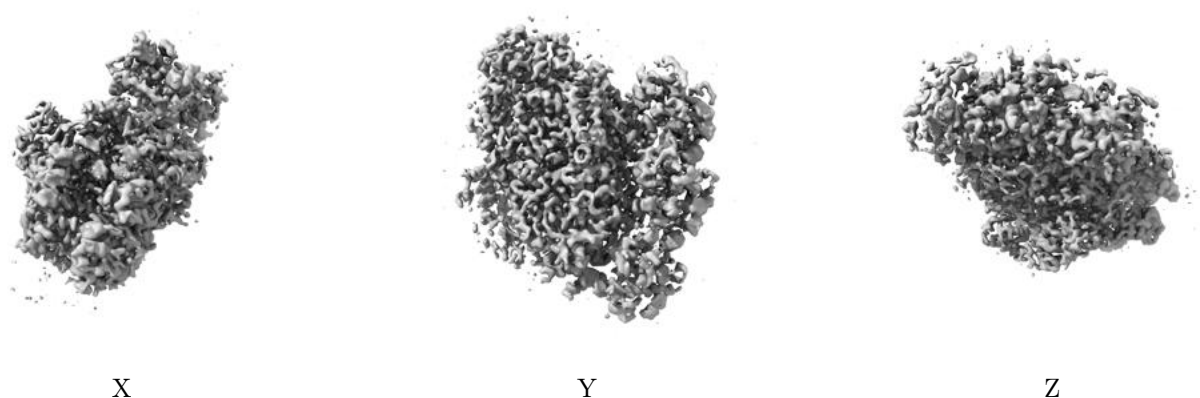


Z

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

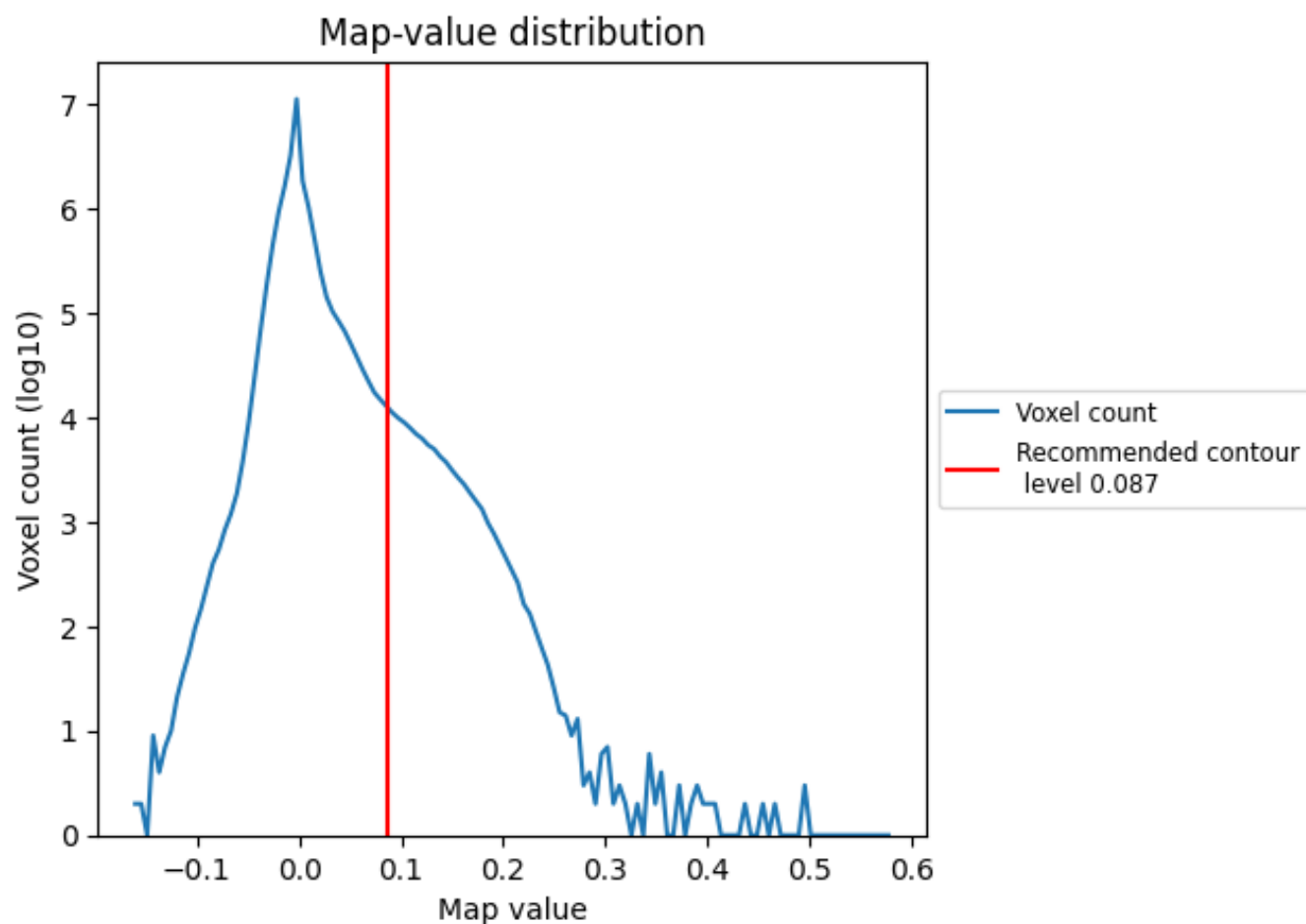
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

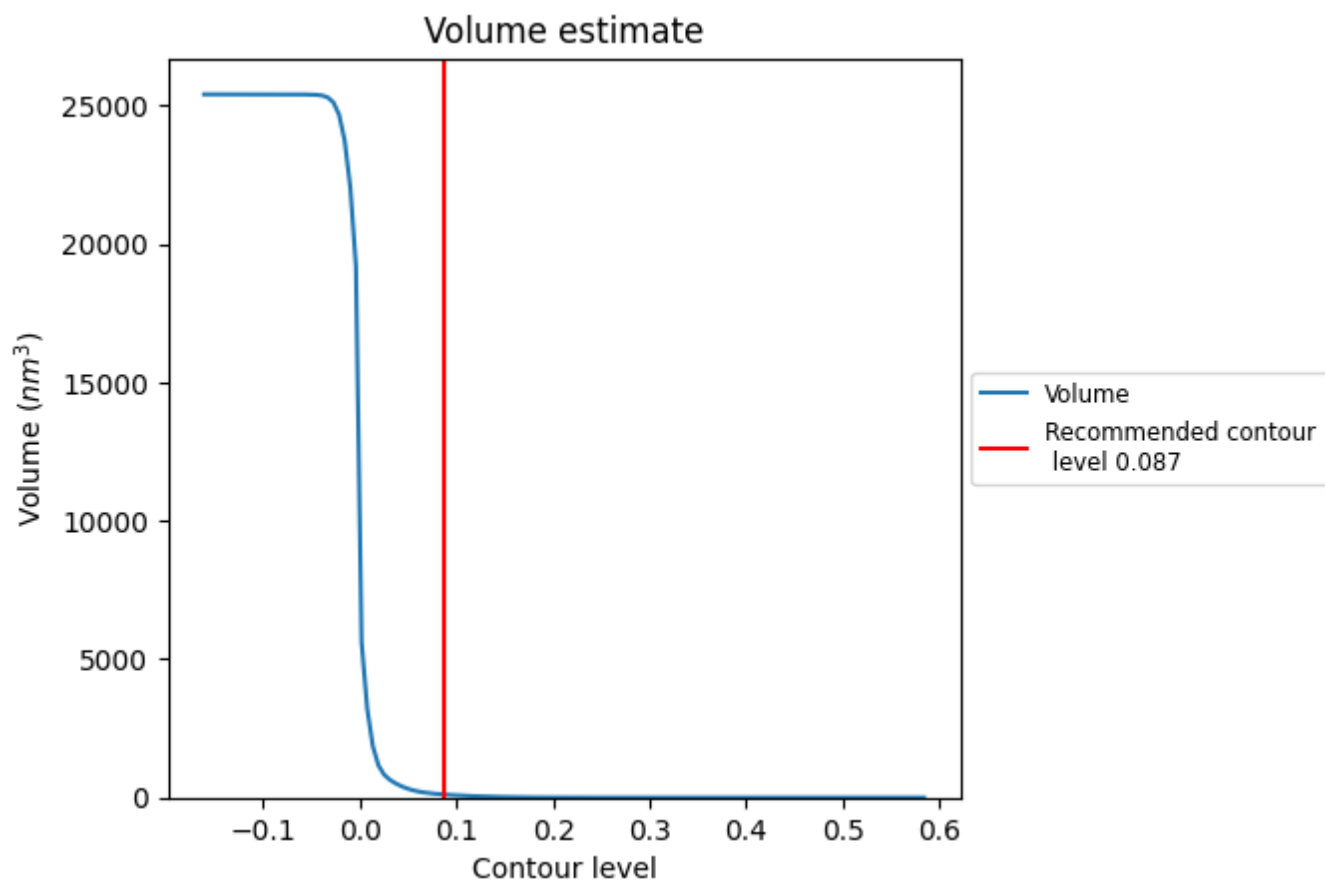
This section contains the results of statistical analysis of the map.

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.

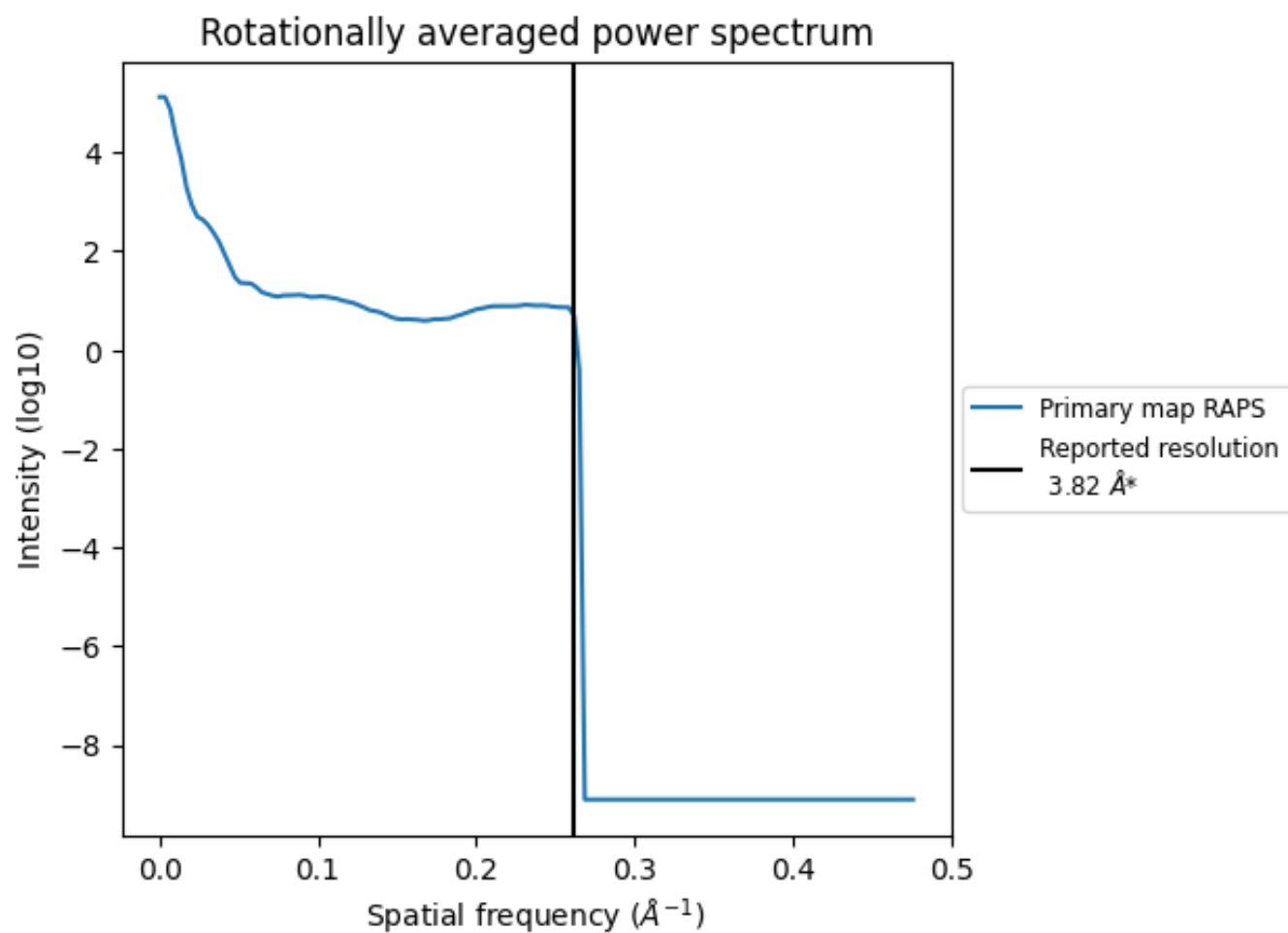
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 111 nm³; this corresponds to an approximate mass of 100 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 0.262 Å⁻¹

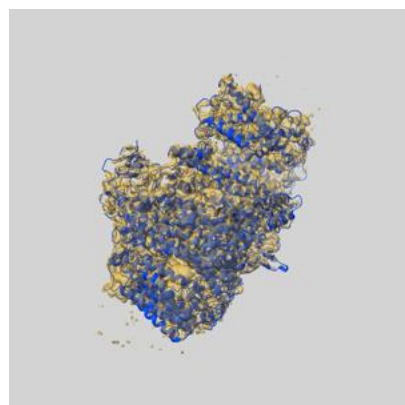
8 Fourier-Shell correlation

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

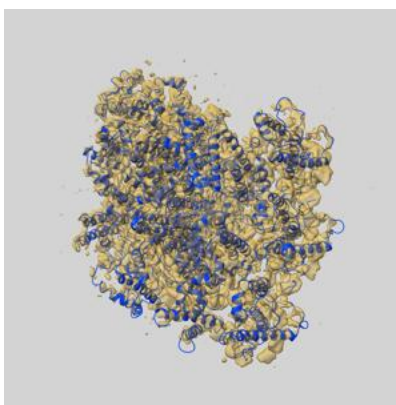
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6930 and PDB model 5ZGH. Per-residue inclusion information can be found in section 3 on page 23.

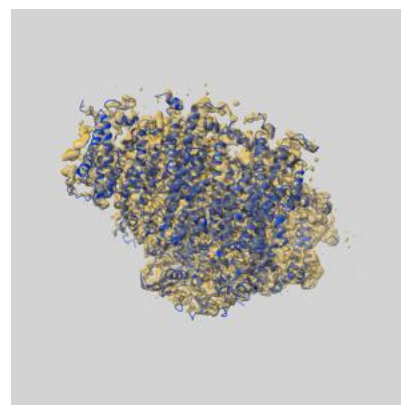
9.1 Map-model overlay [i](#)



X



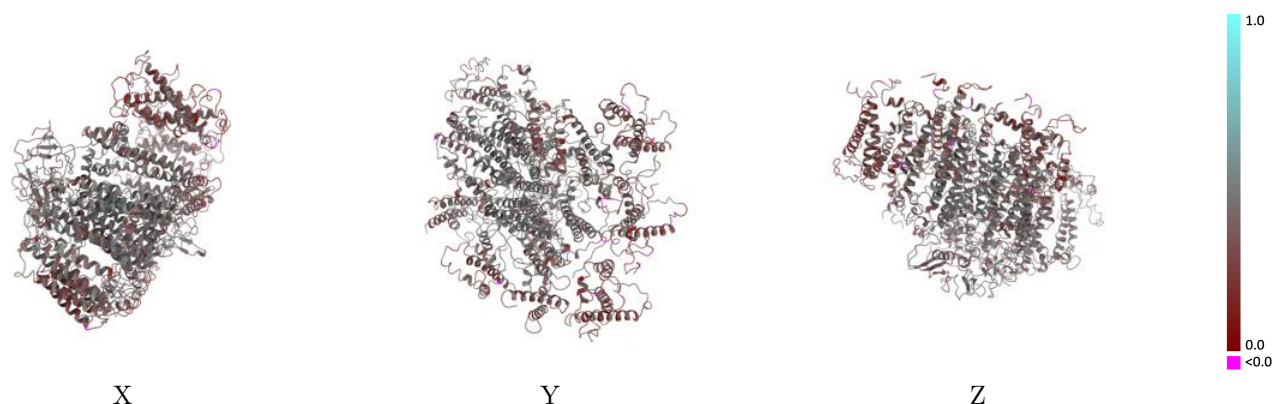
Y



Z

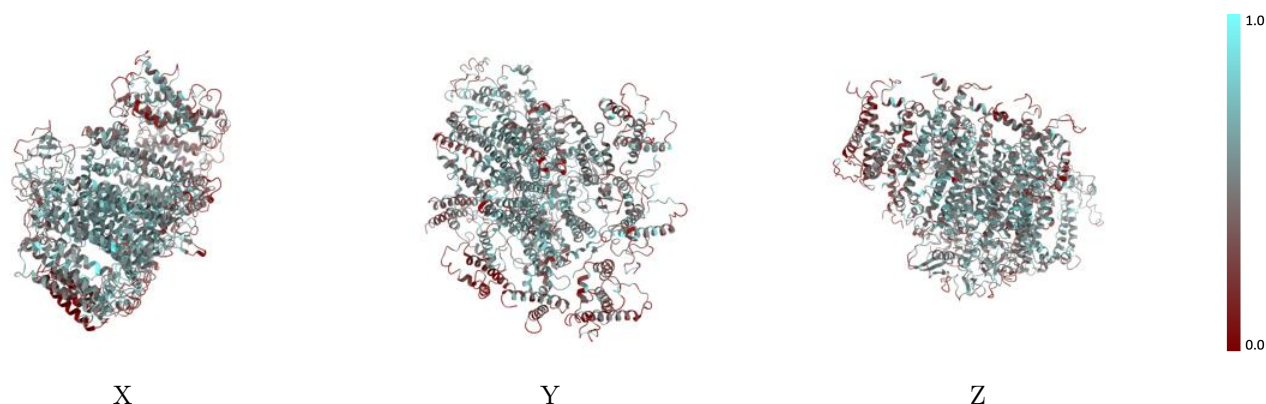
The images above show the 3D surface view of the map at the recommended contour level 0.087 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



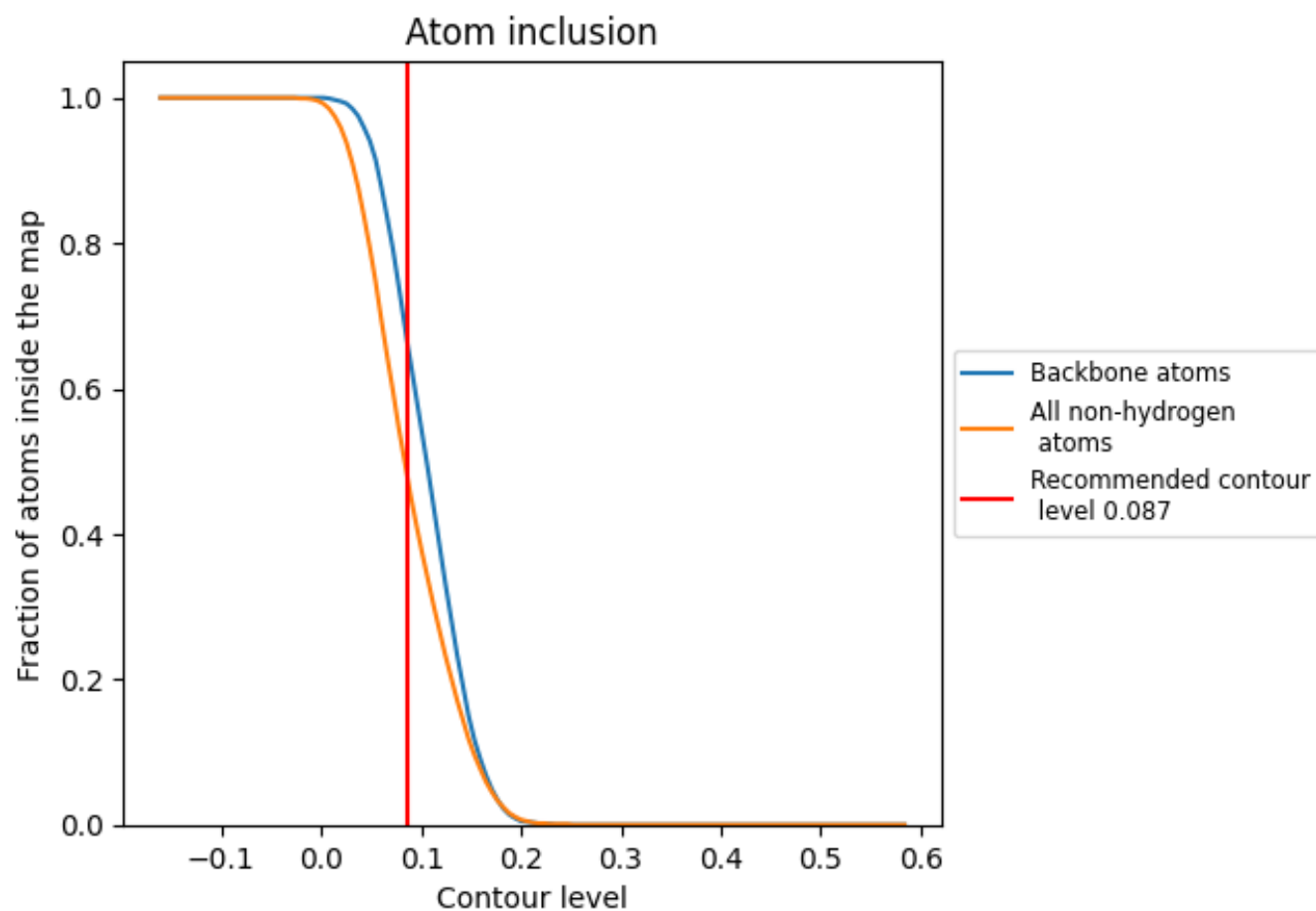
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.087).

9.4 Atom inclusion ⓘ



At the recommended contour level, 66% of all backbone atoms, 47% 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 (0.087) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4720	<div></div> 0.4070
1	<div></div> 0.3970	<div></div> 0.3350
2	<div></div> 0.4380	<div></div> 0.3490
3	<div></div> 0.3080	<div></div> 0.3220
A	<div></div> 0.5530	<div></div> 0.4540
B	<div></div> 0.5330	<div></div> 0.4330
C	<div></div> 0.5690	<div></div> 0.4290
D	<div></div> 0.4150	<div></div> 0.3880
E	<div></div> 0.4450	<div></div> 0.3930
F	<div></div> 0.4480	<div></div> 0.3970
I	<div></div> 0.3420	<div></div> 0.3860
J	<div></div> 0.4420	<div></div> 0.4570
K	<div></div> 0.3350	<div></div> 0.3470
L	<div></div> 0.3460	<div></div> 0.3750
M	<div></div> 0.0440	<div></div> 0.2930
O	<div></div> 0.1860	<div></div> 0.3230

