



wwPDB EM Validation Summary Report ⓘ

Nov 4, 2024 – 07:58 AM JST

PDB ID : 7WFD
EMDB ID : EMD-32462
Title : Left PSI in the cyclic electron transport supercomplex NDH-PSI from Arabidopsis
Authors : Pan, X.; Li, M.
Deposited on : 2021-12-26
Resolution : 3.25 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

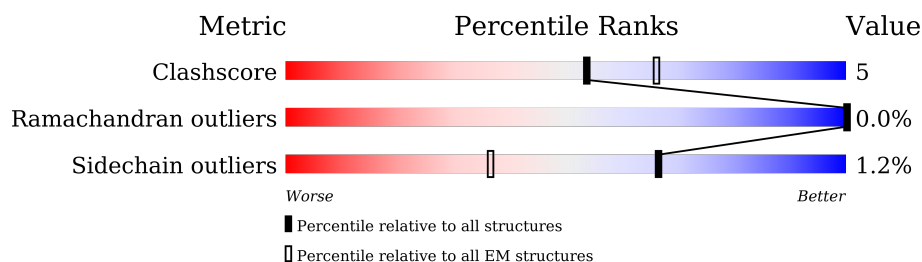
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.25 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	AA	750	 88% 11% .
2	AB	734	 85% 15%
3	AC	81	 78% 21% .
4	AD	204	 60% 9% 31%
5	AE	143	 42% 5% 53%
6	AF	221	 62% 7% 31%
7	AG	160	 55% 6% 39%
8	AH	145	 59% 6% 34%

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Mol	Chain	Length	Quality of chain
9	AI	37	
10	AJ	44	
11	AK	130	
12	AL	219	
13	A1	241	
14	A3	273	
15	A4	251	
16	A6	270	

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
17	CLA	A1	304	X	-	-	-
17	CLA	A1	305	X	-	-	-
17	CLA	A1	306	X	-	-	-
17	CLA	A1	307	X	-	-	-
17	CLA	A1	309	X	-	-	-
17	CLA	A1	310	X	-	-	-
17	CLA	A1	311	X	-	-	-
17	CLA	A1	312	X	-	-	-
17	CLA	A1	313	X	-	-	-
17	CLA	A1	314	X	-	-	-
17	CLA	A1	315	X	-	-	-
17	CLA	A1	316	X	-	-	-
17	CLA	A3	302	X	-	-	-
17	CLA	A3	303	X	-	-	-
17	CLA	A3	304	X	-	-	-
17	CLA	A3	305	X	-	-	-
17	CLA	A3	306	X	-	-	-
17	CLA	A3	308	X	-	-	-
17	CLA	A3	309	X	-	-	-
17	CLA	A3	310	X	-	-	-
17	CLA	A3	311	X	-	-	-
17	CLA	A3	312	X	-	-	-
17	CLA	A3	314	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	A3	315	X	-	-	-
17	CLA	A4	301	X	-	-	-
17	CLA	A4	302	X	-	-	-
17	CLA	A4	303	X	-	-	-
17	CLA	A4	307	X	-	-	-
17	CLA	A4	308	X	-	-	-
17	CLA	A4	309	X	-	-	-
17	CLA	A4	310	X	-	-	-
17	CLA	A4	311	X	-	-	-
17	CLA	A4	312	X	-	-	-
17	CLA	A4	313	X	-	-	-
17	CLA	A6	601	X	-	-	-
17	CLA	A6	602	X	-	-	-
17	CLA	A6	603	X	-	-	-
17	CLA	A6	604	X	-	-	-
17	CLA	A6	608	X	-	-	-
17	CLA	A6	609	X	-	-	-
17	CLA	A6	610	X	-	-	-
17	CLA	A6	611	X	-	-	-
17	CLA	A6	612	X	-	-	-
17	CLA	A6	613	X	-	-	-
17	CLA	AA	801	X	-	-	-
17	CLA	AA	802	X	-	-	-
17	CLA	AA	803	X	-	-	-
17	CLA	AA	805	X	-	-	-
17	CLA	AA	806	X	-	-	-
17	CLA	AA	807	X	-	-	-
17	CLA	AA	808	X	-	-	-
17	CLA	AA	809	X	-	-	-
17	CLA	AA	810	X	-	-	-
17	CLA	AA	811	X	-	-	-
17	CLA	AA	812	X	-	-	-
17	CLA	AA	813	X	-	-	-
17	CLA	AA	814	X	-	-	-
17	CLA	AA	816	X	-	-	-
17	CLA	AA	817	X	-	-	-
17	CLA	AA	819	X	-	-	-
17	CLA	AA	820	X	-	-	-
17	CLA	AA	821	X	-	-	-
17	CLA	AA	822	X	-	-	-
17	CLA	AA	823	X	-	-	-
17	CLA	AA	824	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	AA	825	X	-	-	-
17	CLA	AA	826	X	-	-	-
17	CLA	AA	827	X	-	-	-
17	CLA	AA	828	X	-	-	-
17	CLA	AA	829	X	-	-	-
17	CLA	AA	830	X	-	-	-
17	CLA	AA	831	X	-	-	-
17	CLA	AA	832	X	-	-	-
17	CLA	AA	833	X	-	-	-
17	CLA	AA	835	X	-	-	-
17	CLA	AA	837	X	-	-	-
17	CLA	AA	840	X	-	-	-
17	CLA	AA	842	X	-	-	-
17	CLA	AB	801	X	-	-	-
17	CLA	AB	802	X	-	-	-
17	CLA	AB	803	X	-	-	-
17	CLA	AB	804	X	-	-	-
17	CLA	AB	805	X	-	-	-
17	CLA	AB	806	X	-	-	-
17	CLA	AB	807	X	-	-	-
17	CLA	AB	809	X	-	-	-
17	CLA	AB	810	X	-	-	-
17	CLA	AB	811	X	-	-	-
17	CLA	AB	812	X	-	-	-
17	CLA	AB	813	X	-	-	-
17	CLA	AB	814	X	-	-	-
17	CLA	AB	815	X	-	-	-
17	CLA	AB	816	X	-	-	-
17	CLA	AB	817	X	-	-	-
17	CLA	AB	818	X	-	-	-
17	CLA	AB	819	X	-	-	-
17	CLA	AB	820	X	-	-	-
17	CLA	AB	821	X	-	-	-
17	CLA	AB	822	X	-	-	-
17	CLA	AB	824	X	-	-	-
17	CLA	AB	825	X	-	-	-
17	CLA	AB	826	X	-	-	-
17	CLA	AB	827	X	-	-	-
17	CLA	AB	828	X	-	-	-
17	CLA	AB	829	X	-	-	-
17	CLA	AB	830	X	-	-	-
17	CLA	AB	831	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	AB	833	X	-	-	-
17	CLA	AB	834	X	-	-	-
17	CLA	AB	837	X	-	-	-
17	CLA	AB	839	X	-	-	-
17	CLA	AB	840	X	-	-	-
17	CLA	AB	841	X	-	-	-
17	CLA	AB	842	X	-	-	-
17	CLA	AF	802	X	-	-	-
17	CLA	AF	803	X	-	-	-
17	CLA	AF	804	X	-	-	-
17	CLA	AG	201	X	-	-	-
17	CLA	AG	203	X	-	-	-
17	CLA	AG	204	X	-	-	-
17	CLA	AH	201	X	-	-	-
17	CLA	AJ	102	X	-	-	-
17	CLA	AK	201	X	-	-	-
17	CLA	AK	203	X	-	-	-
17	CLA	AK	204	X	-	-	-
17	CLA	AL	302	X	-	-	-
17	CLA	AL	304	X	-	-	-
26	CHL	A1	303	X	-	-	-
26	CHL	A1	308	X	-	-	-
26	CHL	A3	307	X	-	-	-
26	CHL	A3	320	X	-	-	-
26	CHL	A4	304	X	-	-	-
26	CHL	A4	305	X	-	-	-
26	CHL	A4	306	X	-	-	-
26	CHL	A4	314	X	-	-	-
26	CHL	A6	605	X	-	-	-
26	CHL	A6	606	X	-	-	-
26	CHL	A6	607	X	-	-	-

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 35603 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	742	Total	C	N	O	S	0	0
			5839	3826	992	1003	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	734	Total	C	N	O	S	0	0
			5862	3847	999	1001	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	80	Total	C	N	O	S	0	0
			615	381	107	116	11		

- Molecule 4 is a protein called Photosystem I reaction center subunit II-2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	141	Total	C	N	O	S	0	0
			1112	712	193	203	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	AE	67	Total	C	N	O	0	0
			530	341	94	95		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	153	Total	C	N	O	S	0	0
			1213	792	208	210	3		

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	AG	98	Total	C	N	O	0	0
			767	499	125	143		

- Molecule 8 is a protein called Photosystem I reaction center subunit VI-2, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	AH	95	Total	C	N	O	0	0
			730	476	119	135		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	33	Total	C	N	O	S	0	0
			257	175	41	40	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	42	Total	C	N	O	S	0	0
			338	230	51	56	1		

- Molecule 11 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	65	Total	C	N	O	S	0	0
			451	290	74	84	3		

- Molecule 12 is a protein called Photosystem I reaction center subunit XI, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	157	Total	C	N	O	S	0	0
			1173	775	187	209	2		

- Molecule 13 is a protein called Chlorophyll a-b binding protein 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A1	196	Total	C	N	O	S	0	0
			1511	984	251	271	5		

- Molecule 14 is a protein called Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	A3	219	Total	C	N	O	S	0	0
			1675	1096	272	302	5		

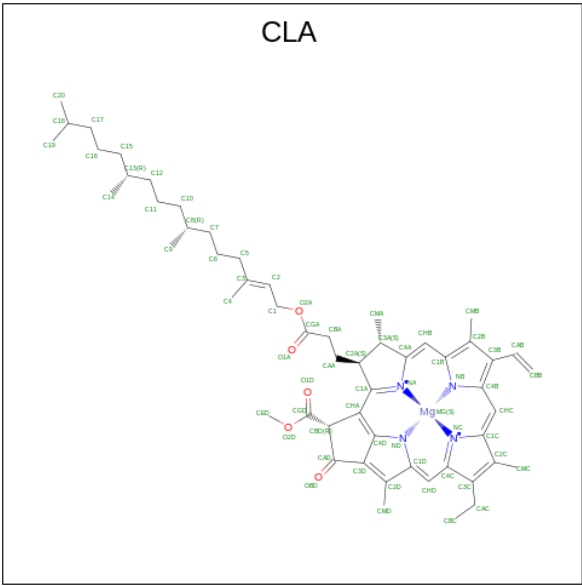
- Molecule 15 is a protein called Chlorophyll a-b binding protein 4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	A4	197	Total	C	N	O	S	0	0
			1562	1022	254	283	3		

- Molecule 16 is a protein called Photosystem I chlorophyll a/b-binding protein 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	A6	212	Total	C	N	O	S	0	0
			1671	1088	272	299	12		

- Molecule 17 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
17	AA	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AA	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AA	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	AA	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AA	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	AA	1	Total 64	C 55	Mg 1	N 4	O 4	0
17	AA	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AA	1	Total 54	C 44	Mg 1	N 4	O 5	0
17	AA	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AA	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	AA	1	Total 41	C 33	Mg 1	N 4	O 3	0
17	AA	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	AA	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	AA	1	Total 59	C 49	Mg 1	N 4	O 5	0
17	AA	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AA	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	AA	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AA	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	AA	1	Total 41	C 33	Mg 1	N 4	O 3	0
17	AA	1	Total 54	C 44	Mg 1	N 4	O 5	0
17	AA	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
17	AA	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
17	AB	1	Total 41	C 33	Mg 1	N 4	O 3	0
17	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AB	1	Total 51	C 42	Mg 1	N 4	O 4	0
17	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AB	1	Total 54	C 44	Mg 1	N 4	O 5	0
17	AB	1	Total 43	C 35	Mg 1	N 4	O 3	0
17	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AB	1	Total 43	C 35	Mg 1	N 4	O 3	0
17	AB	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	AB	1	Total 59	C 49	Mg 1	N 4	O 5	0
17	AB	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	AB	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	AB	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	AB	1	Total 47	C 37	Mg 1	N 4	O 5	0
17	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AB	1	Total 43	C 35	Mg 1	N 4	O 3	0
17	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
17	AB	1	Total 62	C 52	Mg 1	N 4	O 5	0
17	AB	1	Total 62	C 52	Mg 1	N 4	O 5	0
17	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AB	1	Total 56	C 46	Mg 1	N 4	O 5	0
17	AB	1	Total 43	C 35	Mg 1	N 4	O 3	0
17	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AB	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	AB	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	AB	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AB	1	Total 47	C 37	Mg 1	N 4	O 5	0
17	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	AF	1	Total 57	C 47	Mg 1	N 4	O 5	0
17	AF	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	AF	1	Total 41	C 33	Mg 1	N 4	O 3	0
17	AG	1	Total 44	C 34	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
17	AG	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	AG	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	AH	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	AJ	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	AK	1	Total 35	C 29	Mg 1	N 4	O 1	0
17	AK	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	AK	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	AL	1	Total 41	C 33	Mg 1	N 4	O 3	0
17	AL	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	AL	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	A1	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	A1	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	A1	1	Total 49	C 39	Mg 1	N 4	O 5	0
17	A1	1	Total 40	C 32	Mg 1	N 4	O 3	0
17	A1	1	Total 44	C 34	Mg 1	N 4	O 5	0
17	A1	1	Total 40	C 32	Mg 1	N 4	O 3	0
17	A1	1	Total 59	C 49	Mg 1	N 4	O 5	0
17	A1	1	Total 38	C 30	Mg 1	N 4	O 3	0
17	A1	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	A1	1	Total 64	C 54	Mg 1	N 4	O 5	0
17	A1	1	Total 38	C 30	Mg 1	N 4	O 3	0

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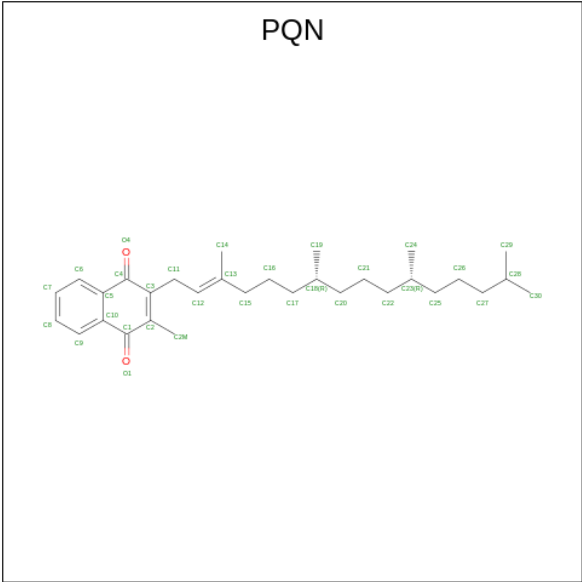
Mol	Chain	Residues	Atoms					AltConf
17	A1	1	Total 43	C 33	Mg 1	N 4	O 5	0
17	A3	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	A3	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	A3	1	Total 42	C 32	Mg 1	N 4	O 5	0
17	A3	1	Total 41	C 33	Mg 1	N 4	O 3	0
17	A3	1	Total 41	C 33	Mg 1	N 4	O 3	0
17	A3	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	A3	1	Total 41	C 33	Mg 1	N 4	O 3	0
17	A3	1	Total 37	C 31	Mg 1	N 4	O 1	0
17	A3	1	Total 43	C 35	Mg 1	N 4	O 3	0
17	A3	1	Total 54	C 44	Mg 1	N 4	O 5	0
17	A3	1	Total 40	C 32	Mg 1	N 4	O 3	0
17	A3	1	Total 36	C 30	Mg 1	N 4	O 1	0
17	A3	1	Total 40	C 32	Mg 1	N 4	O 3	0
17	A4	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	A4	1	Total 44	C 34	Mg 1	N 4	O 5	0
17	A4	1	Total 43	C 33	Mg 1	N 4	O 5	0
17	A4	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	A4	1	Total 54	C 44	Mg 1	N 4	O 5	0
17	A4	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	A4	1	Total 41	C 33	Mg 1	N 4	O 3	0

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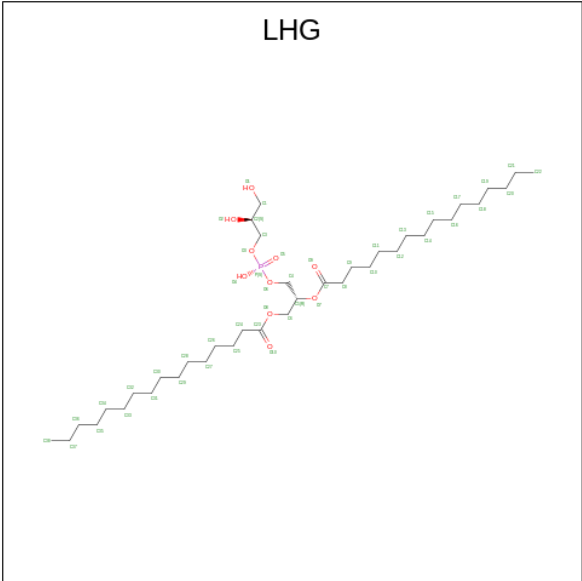
Mol	Chain	Residues	Atoms					AltConf
17	A4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
17	A4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	A4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	A6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	A6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
17	A6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	A6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	A6	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
17	A6	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
17	A6	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
17	A6	1	Total	C	Mg	N	O	0
			43	35	1	4	3	

- Molecule 18 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
18	AA	1	Total	C	O	0
			33	31	2	
18	AB	1	Total	C	O	0
			33	31	2	

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



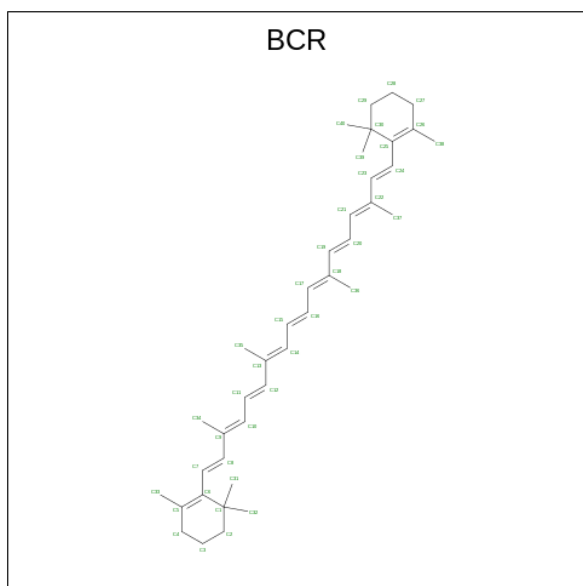
Mol	Chain	Residues	Atoms				AltConf
19	AA	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
19	AJ	1	Total	C	O	P	0
			40	29	10	1	
19	A1	1	Total	C	O	P	0
			38	27	10	1	
19	A1	1	Total	C	O	P	0
			36	25	10	1	
19	A1	1	Total	C	O	P	0
			49	38	10	1	
19	A3	1	Total	C	O	P	0
			36	25	10	1	
19	A3	1	Total	C	O	P	0
			23	12	10	1	
19	A6	1	Total	C	O	P	0
			36	25	10	1	

- Molecule 20 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
20	AA	1	Total	C	0
			40	40	
20	AA	1	Total	C	0
			40	40	
20	AA	1	Total	C	0
			40	40	
20	AA	1	Total	C	0
			40	40	

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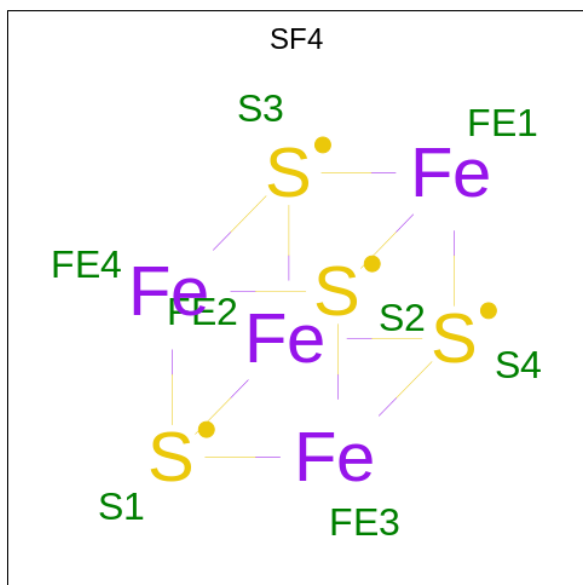
Mol	Chain	Residues	Atoms	AltConf
20	AA	1	Total C 40 40	0
20	AB	1	Total C 40 40	0
20	AB	1	Total C 40 40	0
20	AB	1	Total C 40 40	0
20	AB	1	Total C 40 40	0
20	AB	1	Total C 40 40	0
20	AB	1	Total C 40 40	0
20	AF	1	Total C 40 40	0
20	AF	1	Total C 40 40	0
20	AG	1	Total C 40 40	0
20	AI	1	Total C 40 40	0
20	AI	1	Total C 40 40	0
20	AJ	1	Total C 40 40	0
20	AJ	1	Total C 40 40	0
20	AK	1	Total C 40 40	0
20	AK	1	Total C 40 40	0
20	AL	1	Total C 40 40	0
20	AL	1	Total C 40 40	0
20	A1	1	Total C 40 40	0
20	A3	1	Total C 40 40	0
20	A4	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms		AltConf
20	A6	1	Total	C	0
			40	40	

- Molecule 21 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



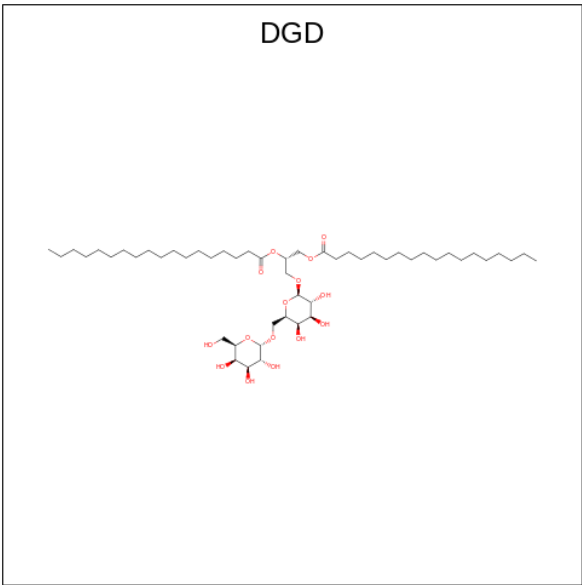
Mol	Chain	Residues	Atoms			AltConf
21	AA	1	Total	Fe	S	0
			8	4	4	
21	AC	1	Total	Fe	S	0
			8	4	4	
21	AC	1	Total	Fe	S	0
			8	4	4	

- Molecule 22 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: $\text{C}_{24}\text{H}_{46}\text{O}_{11}$).



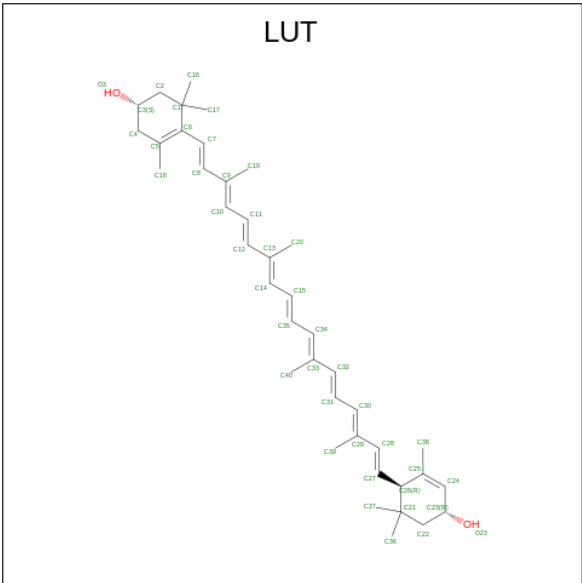
Mol	Chain	Residues	Atoms			AltConf
22	AA	1	Total 35	C 24	O 11	0
22	AB	1	Total 35	C 24	O 11	0
22	AB	1	Total 35	C 24	O 11	0
22	AB	1	Total 35	C 24	O 11	0
22	AL	1	Total 34	C 23	O 11	0

- Molecule 23 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

- Molecule 24 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



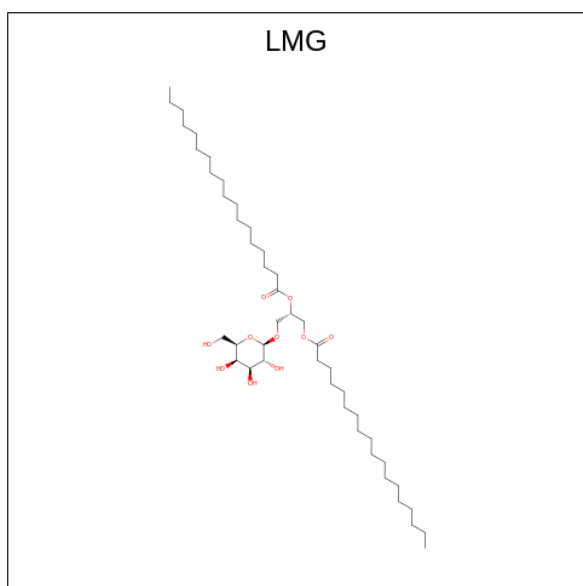
Mol	Chain	Residues	Atoms			AltConf
24	AF	1	Total	C	O	0
			42	40	2	
24	A1	1	Total	C	O	0
			42	40	2	

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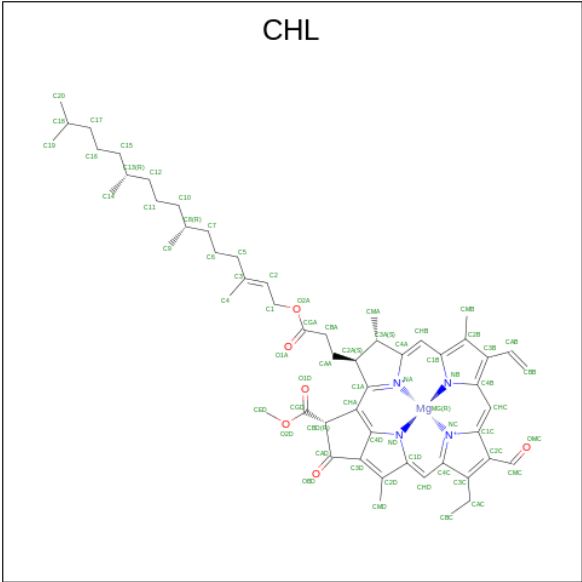
Mol	Chain	Residues	Atoms			AltConf
24	A3	1	Total	C	O	0
			42	40	2	
24	A4	1	Total	C	O	0
			42	40	2	
24	A6	1	Total	C	O	0
			42	40	2	

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



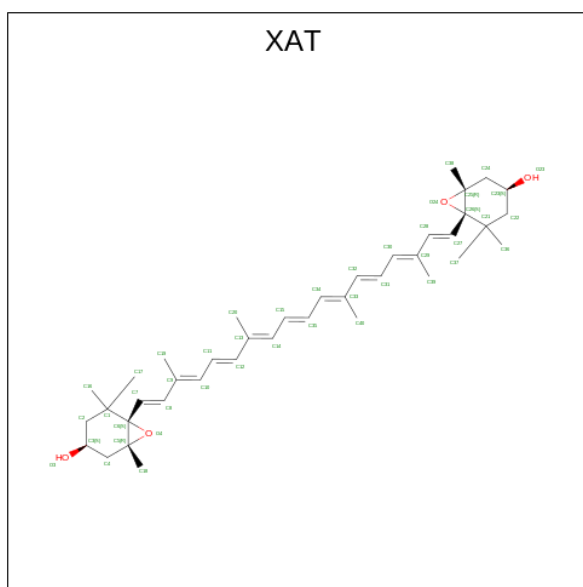
Mol	Chain	Residues	Atoms			AltConf
25	AG	1	Total	C	O	0
			38	28	10	
25	A1	1	Total	C	O	0
			44	34	10	
25	A4	1	Total	C	O	0
			39	29	10	

- Molecule 26 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
26	A1	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
26	A1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
26	A3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	A3	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
26	A4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
26	A4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
26	A4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
26	A4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
26	A6	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
26	A6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
26	A6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

- Molecule 27 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).

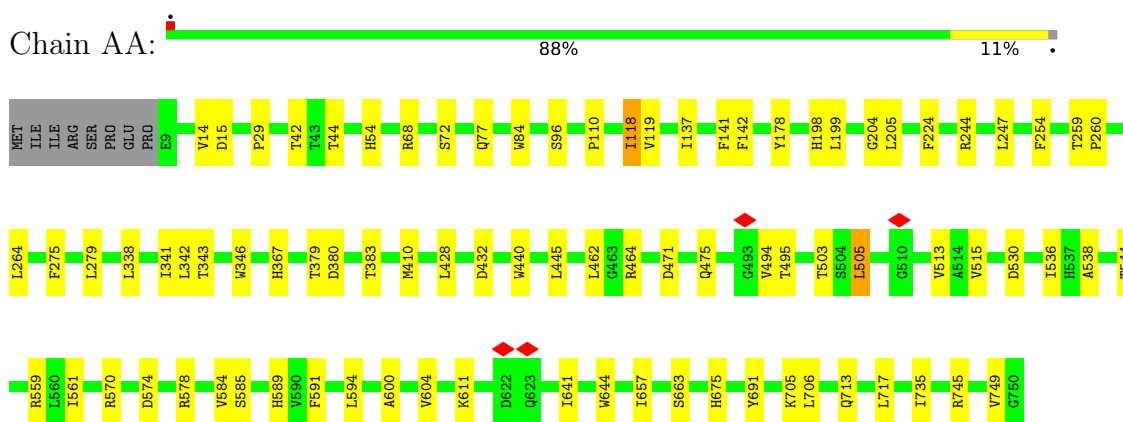


Mol	Chain	Residues	Atoms			AltConf
27	A1	1	Total 44	C 40	O 4	0
27	A3	1	Total 44	C 40	O 4	0
27	A4	1	Total 44	C 40	O 4	0
27	A6	1	Total 44	C 40	O 4	0

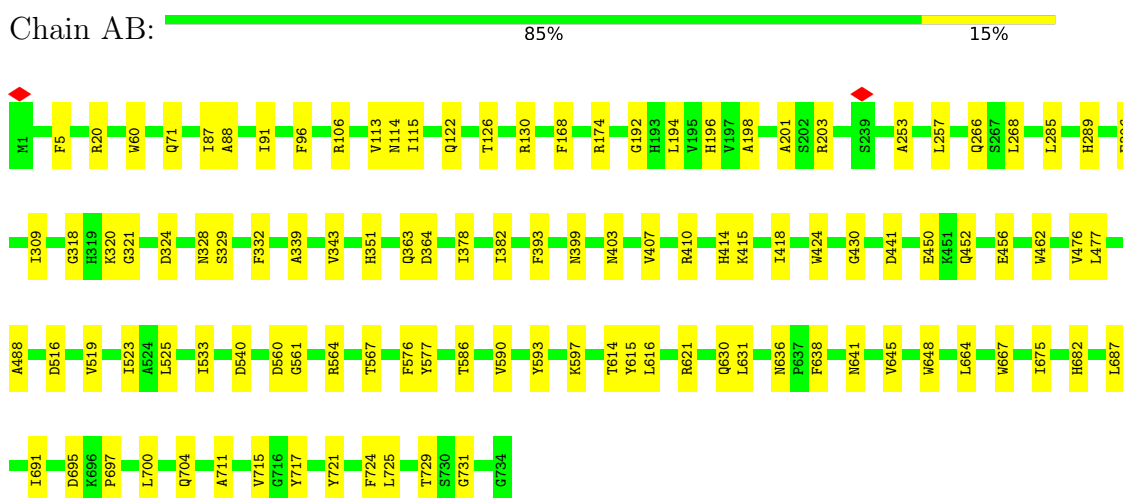
3 Residue-property plots

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

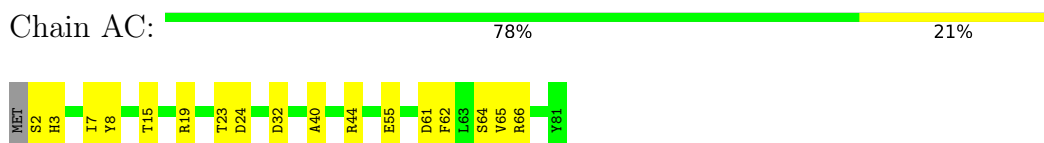
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2




- Molecule 3: Photosystem I iron-sulfur center




-

- Molecule 9: Photosystem I reaction center subunit VIII

Chain AI:  89% 11%



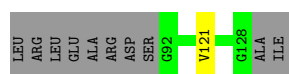
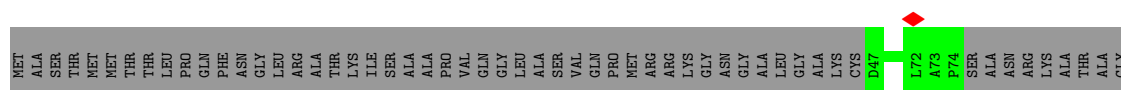
- Molecule 10: Photosystem I reaction center subunit IX

Chain AJ:  84% 11% 5%



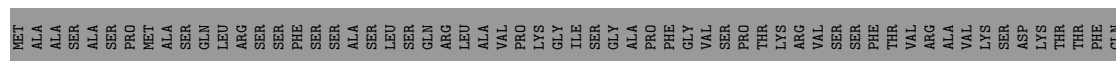
- Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic

Chain AK:  49% 50%



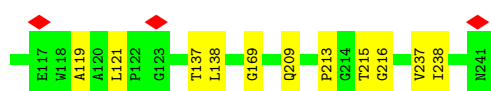
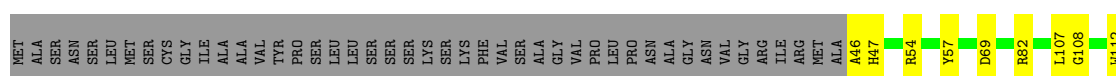
- Molecule 12: Photosystem I reaction center subunit XI, chloroplastic

Chain AL:  64% 7% 28%



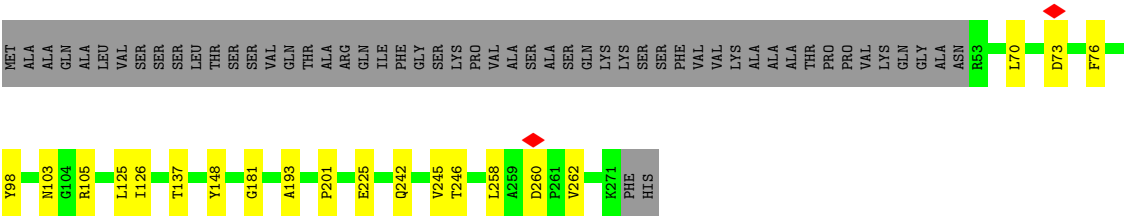
- Molecule 13: Chlorophyll a-b binding protein 6, chloroplastic

Chain A1:  73% 8% 19%

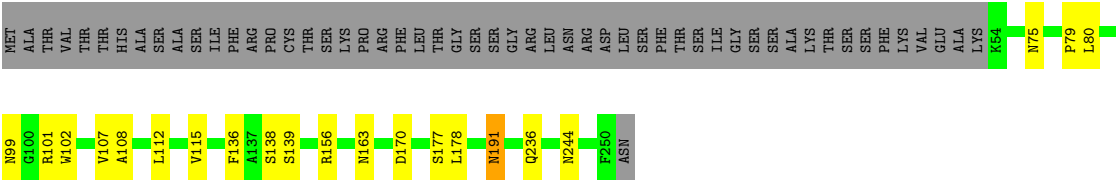


- Molecule 14: Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic

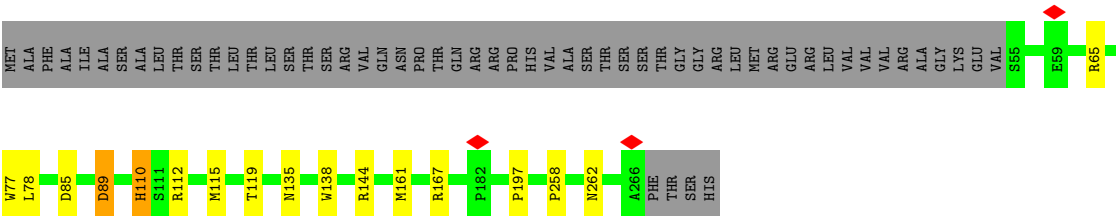
Chain A3:  73% 7% 20%



• Molecule 15: Chlorophyll a-b binding protein 4, chloroplastic



• Molecule 16: Photosystem I chlorophyll a/b-binding protein 6, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	136022	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.0	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.422	Depositor
Minimum map value	-0.153	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	416.0, 416.0, 416.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

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

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	AA	0.38	0/6037	0.53	0/8236
2	AB	0.36	0/6073	0.53	0/8291
3	AC	0.34	0/628	0.59	0/852
4	AD	0.31	0/1140	0.58	0/1542
5	AE	0.32	0/542	0.50	0/736
6	AF	0.31	0/1243	0.53	0/1677
7	AG	0.36	0/787	0.51	0/1067
8	AH	0.32	0/751	0.52	0/1018
9	AI	0.30	0/264	0.45	0/359
10	AJ	0.33	0/348	0.56	0/474
11	AK	0.29	0/456	0.51	0/617
12	AL	0.31	0/1208	0.52	0/1650
13	A1	0.31	0/1562	0.51	0/2131
14	A3	0.31	0/1726	0.51	0/2347
15	A4	0.33	0/1611	0.52	0/2194
16	A6	0.31	0/1732	0.54	0/2363
All	All	0.34	0/26108	0.53	0/35554

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	5839	0	5683	71	0
2	AB	5862	0	5649	92	0
3	AC	615	0	592	14	0
4	AD	1112	0	1122	10	0
5	AE	530	0	536	11	0
6	AF	1213	0	1243	11	0
7	AG	767	0	746	10	0
8	AH	730	0	720	7	0
9	AI	257	0	274	0	0
10	AJ	338	0	351	4	0
11	AK	451	0	462	1	0
12	AL	1173	0	1162	15	0
13	A1	1511	0	1464	13	0
14	A3	1675	0	1647	14	0
15	A4	1562	0	1516	16	0
16	A6	1671	0	1599	16	0
17	A1	575	0	447	6	0
17	A3	575	0	420	3	0
17	A4	480	0	376	5	0
17	A6	485	0	399	4	0
17	AA	2411	0	2371	43	0
17	AB	2452	0	2461	38	0
17	AF	140	0	113	0	0
17	AG	131	0	94	4	0
17	AH	60	0	59	0	0
17	AJ	42	0	31	0	0
17	AK	126	0	88	0	0
17	AL	143	0	119	1	0
18	AA	33	0	46	3	0
18	AB	33	0	46	2	0
19	A1	123	0	162	0	0
19	A3	59	0	58	1	0
19	A6	36	0	42	1	0
19	AA	49	0	74	1	0
19	AJ	40	0	53	0	0
20	A1	40	0	56	3	0
20	A3	40	0	56	3	0
20	A4	40	0	56	0	0
20	A6	40	0	56	3	0
20	AA	200	0	280	6	0
20	AB	240	0	336	10	0
20	AF	80	0	112	6	0
20	AG	40	0	56	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	AI	80	0	112	1	0
20	AJ	80	0	112	2	0
20	AK	80	0	112	1	0
20	AL	80	0	112	1	0
21	AA	8	0	0	0	0
21	AC	16	0	0	2	0
22	AA	35	0	46	0	0
22	AB	105	0	138	0	0
22	AL	34	0	41	1	0
23	AB	66	0	96	0	0
24	A1	42	0	56	0	0
24	A3	42	0	56	0	0
24	A4	42	0	56	2	0
24	A6	42	0	56	1	0
24	AF	42	0	56	2	0
25	A1	44	0	58	1	0
25	A4	39	0	48	4	0
25	AG	38	0	46	0	0
26	A1	92	0	60	3	0
26	A3	97	0	68	4	0
26	A4	169	0	100	3	0
26	A6	135	0	89	3	0
27	A1	44	0	56	1	0
27	A3	44	0	56	3	0
27	A4	44	0	56	2	0
27	A6	44	0	56	4	0
All	All	35603	0	34975	354	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 354 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:87:ILE:HG23	2:AB:113:VAL:CG1	1.58	1.33
2:AB:87:ILE:CG2	2:AB:113:VAL:HG11	1.78	1.14
7:AG:76:LEU:HD13	17:AG:204:CLA:CMB	1.81	1.09
2:AB:106:ARG:CZ	2:AB:115:ILE:HG12	1.83	1.08
2:AB:687:LEU:HD21	12:AL:91:LEU:HD11	1.34	1.06

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	AA	740/750 (99%)	688 (93%)	51 (7%)	1 (0%)	48	77
2	AB	732/734 (100%)	695 (95%)	37 (5%)	0	100	100
3	AC	78/81 (96%)	72 (92%)	6 (8%)	0	100	100
4	AD	139/204 (68%)	126 (91%)	13 (9%)	0	100	100
5	AE	65/143 (46%)	58 (89%)	7 (11%)	0	100	100
6	AF	151/221 (68%)	144 (95%)	7 (5%)	0	100	100
7	AG	96/160 (60%)	88 (92%)	8 (8%)	0	100	100
8	AH	93/145 (64%)	90 (97%)	3 (3%)	0	100	100
9	AI	31/37 (84%)	30 (97%)	1 (3%)	0	100	100
10	AJ	40/44 (91%)	38 (95%)	2 (5%)	0	100	100
11	AK	61/130 (47%)	57 (93%)	4 (7%)	0	100	100
12	AL	155/219 (71%)	145 (94%)	10 (6%)	0	100	100
13	A1	194/241 (80%)	178 (92%)	16 (8%)	0	100	100
14	A3	217/273 (80%)	191 (88%)	26 (12%)	0	100	100
15	A4	195/251 (78%)	185 (95%)	10 (5%)	0	100	100
16	A6	210/270 (78%)	198 (94%)	12 (6%)	0	100	100
All	All	3197/3903 (82%)	2983 (93%)	213 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AA	663	SER

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	AA	600/610 (98%)	594 (99%)	6 (1%)	73	82
2	AB	598/600 (100%)	591 (99%)	7 (1%)	67	79
3	AC	70/71 (99%)	70 (100%)	0	100	100
4	AD	120/170 (71%)	120 (100%)	0	100	100
5	AE	56/114 (49%)	55 (98%)	1 (2%)	54	72
6	AF	125/185 (68%)	124 (99%)	1 (1%)	79	86
7	AG	83/133 (62%)	81 (98%)	2 (2%)	44	66
8	AH	77/113 (68%)	75 (97%)	2 (3%)	41	64
9	AI	29/33 (88%)	29 (100%)	0	100	100
10	AJ	37/39 (95%)	37 (100%)	0	100	100
11	AK	47/95 (50%)	47 (100%)	0	100	100
12	AL	119/174 (68%)	116 (98%)	3 (2%)	42	65
13	A1	151/190 (80%)	149 (99%)	2 (1%)	65	78
14	A3	168/211 (80%)	167 (99%)	1 (1%)	84	89
15	A4	164/210 (78%)	160 (98%)	4 (2%)	44	66
16	A6	177/226 (78%)	175 (99%)	2 (1%)	70	81
All	All	2621/3174 (83%)	2590 (99%)	31 (1%)	66	79

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	AF	145	ARG
15	A4	170	ASP
8	AH	71	TRP
16	A6	89	ASP
14	A3	98	TYR

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

Mol	Chain	Res	Type
15	A4	248	GLN
15	A4	191	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	AL	66	ASN
15	A4	75	ASN
11	AK	54	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

211 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	$\# Z > 2$
26	CHL	A6	607	-	50,58,74	2.26	16 (32%)	58,95,114	2.64	21 (36%)
17	CLA	A6	609	16	55,63,73	1.67	9 (16%)	64,101,113	1.33	10 (15%)
17	CLA	AB	807	2	65,73,73	1.45	10 (15%)	76,113,113	1.35	8 (10%)
17	CLA	A3	305	-	40,49,73	1.90	7 (17%)	45,84,113	1.45	7 (15%)
17	CLA	AB	831	-	43,51,73	1.84	9 (20%)	49,86,113	1.33	8 (16%)
17	CLA	A6	613	-	43,51,73	1.89	6 (13%)	49,86,113	1.47	7 (14%)
17	CLA	AB	839	-	47,55,73	1.74	8 (17%)	54,91,113	1.56	7 (12%)
17	CLA	AB	808	-	51,59,73	1.67	9 (17%)	58,95,113	1.45	7 (12%)
17	CLA	AA	803	-	65,73,73	1.47	10 (15%)	76,113,113	1.36	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A3	311	14	43,51,73	1.82	5 (11%)	49,86,113	1.48	7 (14%)
17	CLA	AA	842	-	65,73,73	1.48	8 (12%)	76,113,113	1.41	11 (14%)
17	CLA	AA	813	-	65,73,73	1.47	9 (13%)	76,113,113	1.38	8 (10%)
17	CLA	AB	823	-	65,73,73	1.50	9 (13%)	76,113,113	1.31	9 (11%)
17	CLA	AA	809	1	50,58,73	1.77	9 (18%)	58,95,113	1.48	11 (18%)
17	CLA	AB	812	-	54,62,73	1.66	8 (14%)	67,100,113	1.52	12 (17%)
17	CLA	A6	604	-	43,51,73	1.83	8 (18%)	48,86,113	1.40	7 (14%)
17	CLA	AA	827	-	65,73,73	1.48	7 (10%)	76,113,113	1.34	8 (10%)
17	CLA	AB	801	-	65,73,73	1.47	9 (13%)	76,113,113	1.59	14 (18%)
17	CLA	A3	310	19	36,45,73	1.97	6 (16%)	43,79,113	1.48	8 (18%)
17	CLA	AA	811	-	65,73,73	1.49	7 (10%)	76,113,113	1.31	8 (10%)
17	CLA	AB	820	-	55,63,73	1.70	8 (14%)	64,101,113	1.28	6 (9%)
17	CLA	AB	815	-	65,73,73	1.46	8 (12%)	76,113,113	1.39	9 (11%)
17	CLA	AA	830	-	65,73,73	1.52	9 (13%)	76,113,113	1.31	8 (10%)
17	CLA	AF	802	-	57,65,73	1.58	11 (19%)	66,103,113	1.43	9 (13%)
17	CLA	AB	802	-	64,72,73	1.60	8 (12%)	79,112,113	1.34	9 (11%)
19	LHG	A1	301	17	37,37,48	1.07	2 (5%)	40,43,54	0.97	3 (7%)
17	CLA	AA	801	-	65,73,73	1.50	7 (10%)	76,113,113	1.27	8 (10%)
17	CLA	AA	840	-	65,73,73	1.51	8 (12%)	76,113,113	1.31	10 (13%)
17	CLA	A4	302	15	44,52,73	1.85	8 (18%)	55,88,113	1.61	9 (16%)
25	LMG	A1	321	-	44,44,55	1.03	2 (4%)	52,52,63	1.19	5 (9%)
17	CLA	A3	314	-	37,44,73	1.97	8 (21%)	42,77,113	1.42	7 (16%)
19	LHG	A1	320	17	48,48,48	0.93	2 (4%)	51,54,54	0.84	2 (3%)
26	CHL	A1	303	13	50,59,74	2.22	15 (30%)	53,96,114	2.68	24 (45%)
17	CLA	AA	806	1	65,73,73	1.49	9 (13%)	76,113,113	1.38	8 (10%)
22	LMU	AB	852	-	36,36,36	1.14	2 (5%)	47,47,47	0.94	1 (2%)
17	CLA	A1	309	-	43,52,73	1.87	6 (13%)	49,88,113	1.42	9 (18%)
17	CLA	AG	204	7	45,53,73	1.84	7 (15%)	52,89,113	1.46	7 (13%)
17	CLA	A4	307	15	45,53,73	1.85	7 (15%)	52,89,113	1.36	7 (13%)
17	CLA	AB	838	-	65,73,73	1.46	7 (10%)	76,113,113	1.34	8 (10%)
17	CLA	AK	203	-	45,53,73	1.82	6 (13%)	52,89,113	1.41	7 (13%)
26	CHL	A3	320	16	51,60,74	2.19	16 (31%)	54,97,114	2.65	20 (37%)
17	CLA	AB	805	-	41,49,73	1.81	6 (14%)	47,84,113	1.55	8 (17%)
17	CLA	AB	828	-	65,73,73	1.46	8 (12%)	76,113,113	1.43	8 (10%)
17	CLA	AB	827	-	62,70,73	1.50	7 (11%)	72,109,113	1.50	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	AA	834	-	65,73,73	1.47	10 (15%)	76,113,113	1.48	14 (18%)
17	CLA	AK	201	11	37,43,73	2.45	10 (27%)	45,75,113	1.48	8 (17%)
20	BCR	A3	318	-	41,41,41	0.98	1 (2%)	56,56,56	2.77	20 (35%)
17	CLA	A3	303	14	55,63,73	1.67	9 (16%)	64,101,113	1.46	9 (14%)
20	BCR	AA	845	-	41,41,41	1.03	2 (4%)	56,56,56	1.91	13 (23%)
17	CLA	AG	203	-	42,50,73	1.85	6 (14%)	48,85,113	1.44	7 (14%)
17	CLA	AB	830	-	56,64,73	1.62	9 (16%)	65,102,113	1.39	7 (10%)
21	SF4	AC	101	3	0,12,12	-	-	-	-	-
18	PQN	AA	843	-	34,34,34	3.42	10 (29%)	42,45,45	1.74	8 (19%)
17	CLA	AA	837	-	51,59,73	1.62	7 (13%)	59,96,113	1.59	9 (15%)
17	CLA	A1	316	13	43,51,73	1.89	7 (16%)	54,87,113	1.63	9 (16%)
17	CLA	AA	805	-	65,73,73	1.48	8 (12%)	76,113,113	1.40	12 (15%)
20	BCR	AB	847	-	41,41,41	0.87	0	56,56,56	2.02	14 (25%)
19	LHG	AA	844	-	48,48,48	0.93	2 (4%)	51,54,54	0.89	2 (3%)
17	CLA	AB	803	-	65,73,73	1.49	8 (12%)	76,113,113	1.23	7 (9%)
20	BCR	AB	848	-	41,41,41	0.89	1 (2%)	56,56,56	1.97	18 (32%)
17	CLA	AA	841	-	65,73,73	1.50	9 (13%)	76,113,113	1.34	8 (10%)
17	CLA	AJ	102	10	42,50,73	1.84	5 (11%)	48,85,113	1.48	7 (14%)
24	LUT	A3	316	-	42,43,43	0.84	0	51,60,60	1.78	14 (27%)
20	BCR	AL	305	-	41,41,41	0.86	0	56,56,56	2.54	18 (32%)
17	CLA	AA	816	-	45,53,73	1.82	9 (20%)	52,89,113	1.58	9 (17%)
17	CLA	AA	817	-	60,68,73	1.55	6 (10%)	70,107,113	1.36	9 (12%)
17	CLA	AB	822	-	47,55,73	1.77	7 (14%)	54,91,113	1.35	7 (12%)
17	CLA	AA	804	-	52,60,73	1.65	8 (15%)	60,97,113	1.54	7 (11%)
19	LHG	A1	302	-	35,35,48	1.10	2 (5%)	38,41,54	1.04	2 (5%)
17	CLA	A4	301	15	60,68,73	1.55	9 (15%)	70,107,113	1.33	10 (14%)
17	CLA	A6	610	19	38,45,73	2.96	10 (26%)	41,76,113	1.56	10 (24%)
20	BCR	AA	846	-	41,41,41	0.82	0	56,56,56	2.12	21 (37%)
21	SF4	AA	850	2,1	0,12,12	-	-	-	-	-
17	CLA	A3	304	-	41,50,73	1.94	7 (17%)	51,86,113	1.50	9 (17%)
17	CLA	AB	829	-	65,73,73	1.50	9 (13%)	76,113,113	1.33	9 (11%)
17	CLA	AF	804	-	41,49,73	1.87	7 (17%)	47,84,113	1.59	8 (17%)
17	CLA	AA	812	-	54,62,73	1.61	9 (16%)	62,99,113	1.51	8 (12%)
17	CLA	AA	822	-	42,50,73	1.86	6 (14%)	48,85,113	1.50	8 (16%)
17	CLA	A3	313	-	39,48,73	1.91	7 (17%)	44,83,113	1.46	8 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	BCR	A6	616	-	41,41,41	0.99	2 (4%)	56,56,56	2.01	16 (28%)
17	CLA	AA	832	-	56,64,73	1.60	6 (10%)	65,102,113	1.36	10 (15%)
17	CLA	AB	809	-	65,73,73	1.52	8 (12%)	76,113,113	1.36	10 (13%)
26	CHL	A4	305	-	41,49,74	2.25	13 (31%)	51,84,114	2.78	20 (39%)
26	CHL	A6	606	-	43,51,74	2.34	16 (37%)	45,86,114	2.83	19 (42%)
17	CLA	AB	816	-	43,51,73	1.80	7 (16%)	49,86,113	1.42	6 (12%)
17	CLA	AB	825	-	65,73,73	1.49	10 (15%)	76,113,113	1.34	9 (11%)
17	CLA	AA	818	-	59,67,73	1.58	9 (15%)	68,105,113	1.33	8 (11%)
17	CLA	A1	310	13	40,48,73	1.92	7 (17%)	50,83,113	1.65	10 (20%)
22	LMU	AA	851	-	36,36,36	1.16	2 (5%)	47,47,47	1.04	2 (4%)
17	CLA	AA	824	-	53,62,73	1.68	8 (15%)	61,100,113	1.50	11 (18%)
17	CLA	A1	304	13	60,68,73	1.52	9 (15%)	69,106,113	1.33	8 (11%)
20	BCR	AJ	103	-	41,41,41	0.74	0	56,56,56	2.38	22 (39%)
20	BCR	AI	101	-	41,41,41	0.92	1 (2%)	56,56,56	2.05	20 (35%)
17	CLA	AA	825	-	65,73,73	1.48	6 (9%)	76,113,113	1.33	6 (7%)
20	BCR	AF	805	-	41,41,41	0.81	0	56,56,56	1.86	14 (25%)
23	DGD	AB	851	-	67,67,67	0.80	2 (2%)	81,81,81	0.99	4 (4%)
17	CLA	AB	818	-	59,67,73	1.58	8 (13%)	68,105,113	1.34	10 (14%)
17	CLA	AL	303	-	60,68,73	1.57	9 (15%)	70,107,113	1.41	10 (14%)
17	CLA	AA	839	-	52,60,73	1.66	8 (15%)	60,97,113	1.37	7 (11%)
17	CLA	A6	603	-	41,50,73	1.90	6 (14%)	46,85,113	1.60	7 (15%)
20	BCR	AA	847	-	41,41,41	1.00	2 (4%)	56,56,56	2.28	24 (42%)
17	CLA	AA	808	1	65,73,73	1.50	7 (10%)	76,113,113	1.34	9 (11%)
17	CLA	AB	821	-	50,58,73	1.70	8 (16%)	58,95,113	1.49	8 (13%)
17	CLA	AA	823	-	41,49,73	1.93	7 (17%)	47,84,113	1.46	8 (17%)
17	CLA	AB	810	2	65,73,73	1.48	11 (16%)	76,113,113	1.38	6 (7%)
20	BCR	AA	849	-	41,41,41	0.91	2 (4%)	56,56,56	2.12	20 (35%)
22	LMU	AB	850	-	36,36,36	1.13	2 (5%)	47,47,47	1.08	4 (8%)
17	CLA	AA	815	-	40,49,73	1.79	5 (12%)	44,83,113	1.62	8 (18%)
17	CLA	A1	312	19	37,46,73	2.01	7 (18%)	46,81,113	1.43	10 (21%)
17	CLA	AA	802	-	65,73,73	1.53	10 (15%)	76,113,113	1.42	6 (7%)
27	XAT	A4	316	-	39,47,47	0.95	2 (5%)	54,74,74	2.29	16 (29%)
17	CLA	A4	308	15	54,62,73	1.67	8 (14%)	62,99,113	1.29	9 (14%)
17	CLA	A4	310	15	40,49,73	1.90	8 (20%)	45,84,113	1.47	7 (15%)
17	CLA	A3	308	14	45,53,73	1.80	8 (17%)	52,89,113	1.43	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A4	311	-	55,64,73	1.64	7 (12%)	63,102,113	1.31	7 (11%)
17	CLA	A3	312	-	53,62,73	1.67	7 (13%)	61,100,113	1.39	8 (13%)
17	CLA	A6	611	16	44,52,73	1.84	7 (15%)	51,88,113	1.37	6 (11%)
24	LUT	A4	315	-	42,43,43	0.95	2 (4%)	51,60,60	1.84	15 (29%)
20	BCR	AG	205	-	41,41,41	0.93	0	56,56,56	2.00	18 (32%)
17	CLA	AB	842	19	65,73,73	1.46	8 (12%)	76,113,113	1.37	10 (13%)
17	CLA	AB	833	-	65,73,73	1.49	9 (13%)	76,113,113	1.18	7 (9%)
17	CLA	A6	608	16	45,53,73	1.80	7 (15%)	52,89,113	1.42	7 (13%)
17	CLA	A1	313	13	45,53,73	1.78	7 (15%)	52,89,113	1.57	7 (13%)
17	CLA	A1	305	-	55,63,73	1.63	7 (12%)	64,101,113	1.60	10 (15%)
21	SF4	AC	102	3	0,12,12	-	-	-	-	-
17	CLA	AB	811	-	65,73,73	1.46	8 (12%)	76,113,113	1.48	10 (13%)
17	CLA	A1	311	13	59,67,73	1.57	7 (11%)	69,106,113	1.27	8 (11%)
22	LMU	AL	301	-	35,35,36	1.23	2 (5%)	46,46,47	1.05	5 (10%)
26	CHL	A1	308	13	40,49,74	2.48	18 (45%)	41,84,114	2.86	17 (41%)
20	BCR	AB	844	-	41,41,41	0.86	0	56,56,56	2.28	23 (41%)
17	CLA	AA	838	-	55,63,73	1.61	9 (16%)	64,101,113	1.29	10 (15%)
17	CLA	AA	828	-	65,73,73	1.45	7 (10%)	76,113,113	1.56	9 (11%)
17	CLA	AB	840	-	65,73,73	1.54	9 (13%)	76,113,113	1.25	7 (9%)
17	CLA	A4	312	-	45,53,73	1.81	7 (15%)	52,89,113	1.40	7 (13%)
19	LHG	A6	617	17	35,35,48	1.05	2 (5%)	38,41,54	0.97	2 (5%)
17	CLA	AK	204	-	46,54,73	1.78	9 (19%)	53,90,113	1.47	7 (13%)
20	BCR	AB	849	-	41,41,41	0.83	0	56,56,56	2.41	24 (42%)
25	LMG	AG	202	-	38,38,55	1.14	3 (7%)	46,46,63	1.07	2 (4%)
22	LMU	AB	853	-	36,36,36	1.13	2 (5%)	47,47,47	1.05	2 (4%)
17	CLA	A4	309	-	42,50,73	1.79	5 (11%)	48,85,113	1.53	7 (14%)
17	CLA	A1	307	-	39,48,73	1.89	9 (23%)	45,82,113	1.74	11 (24%)
17	CLA	AA	807	-	50,58,73	1.69	8 (16%)	58,95,113	1.43	6 (10%)
17	CLA	AA	814	-	45,53,73	1.81	9 (20%)	52,89,113	1.45	8 (15%)
17	CLA	AB	806	-	65,73,73	1.47	6 (9%)	76,113,113	1.36	9 (11%)
17	CLA	A3	306	14	41,49,73	1.90	7 (17%)	51,84,113	1.67	9 (17%)
17	CLA	AB	813	-	43,51,73	1.78	6 (13%)	49,86,113	1.44	8 (16%)
17	CLA	AB	814	-	65,73,73	1.49	10 (15%)	76,113,113	1.30	7 (9%)
17	CLA	A4	303	-	43,51,73	1.86	7 (16%)	54,87,113	1.59	9 (16%)
17	CLA	AG	201	-	43,52,73	1.87	7 (16%)	49,88,113	1.48	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	BCR	AB	846	-	41,41,41	0.86	0	56,56,56	2.07	16 (28%)
17	CLA	AB	826	-	62,70,73	1.52	9 (14%)	72,109,113	1.32	7 (9%)
24	LUT	A1	317	-	42,43,43	0.94	1 (2%)	51,60,60	1.88	13 (25%)
17	CLA	AB	817	-	55,63,73	1.63	8 (14%)	64,101,113	1.34	7 (10%)
24	LUT	A6	614	-	42,43,43	0.90	1 (2%)	51,60,60	1.59	12 (23%)
26	CHL	A4	314	15	40,49,74	2.26	13 (32%)	45,84,114	2.77	17 (37%)
17	CLA	A6	601	15	46,54,73	1.73	8 (17%)	53,90,113	1.46	8 (15%)
20	BCR	AL	306	-	41,41,41	0.94	1 (2%)	56,56,56	2.01	21 (37%)
19	LHG	A3	301	-	35,35,48	1.09	2 (5%)	38,41,54	1.01	2 (5%)
17	CLA	AB	834	-	65,73,73	1.49	9 (13%)	76,113,113	1.23	9 (11%)
17	CLA	AA	820	-	45,53,73	1.78	8 (17%)	52,89,113	1.46	7 (13%)
17	CLA	A1	314	-	63,72,73	1.52	8 (12%)	73,112,113	1.30	9 (12%)
20	BCR	AK	202	-	41,41,41	0.94	2 (4%)	56,56,56	2.19	17 (30%)
17	CLA	A1	306	-	49,57,73	1.71	7 (14%)	55,93,113	1.45	8 (14%)
17	CLA	AA	833	-	65,73,73	1.51	7 (10%)	76,113,113	1.38	9 (11%)
17	CLA	AB	804	-	65,73,73	1.45	10 (15%)	76,113,113	1.69	15 (19%)
19	LHG	AJ	104	-	39,39,48	1.06	2 (5%)	42,45,54	0.92	2 (4%)
18	PQN	AB	843	-	34,34,34	3.39	11 (32%)	42,45,45	1.83	6 (14%)
26	CHL	A4	306	-	46,54,74	2.32	17 (36%)	49,90,114	2.85	21 (42%)
17	CLA	A1	315	-	37,46,73	1.99	7 (18%)	46,81,113	1.69	11 (23%)
17	CLA	AA	829	-	65,73,73	1.46	9 (13%)	76,113,113	1.49	11 (14%)
17	CLA	AB	837	-	50,58,73	1.69	9 (18%)	58,95,113	1.51	8 (13%)
20	BCR	AI	102	-	41,41,41	0.78	0	56,56,56	2.22	22 (39%)
20	BCR	AK	205	-	41,41,41	1.02	3 (7%)	56,56,56	2.06	14 (25%)
17	CLA	AH	201	-	60,68,73	1.60	7 (11%)	70,107,113	1.36	10 (14%)
17	CLA	AA	831	-	47,55,73	1.78	9 (19%)	54,91,113	1.43	7 (12%)
17	CLA	AA	835	-	43,52,73	1.85	8 (18%)	49,88,113	1.47	7 (14%)
17	CLA	A3	302	14	60,68,73	1.57	8 (13%)	70,107,113	1.22	9 (12%)
17	CLA	AA	819	-	65,73,73	1.48	10 (15%)	76,113,113	1.43	9 (11%)
17	CLA	AB	835	-	60,68,73	1.55	8 (13%)	70,107,113	1.37	8 (11%)
17	CLA	AF	803	-	42,50,73	1.88	8 (19%)	48,85,113	1.57	8 (16%)
17	CLA	A3	315	-	39,48,73	1.86	6 (15%)	44,83,113	1.42	7 (15%)
20	BCR	AA	848	-	41,41,41	0.77	1 (2%)	56,56,56	1.97	16 (28%)
20	BCR	AJ	101	-	41,41,41	0.89	1 (2%)	56,56,56	1.98	16 (28%)
20	BCR	A4	317	-	41,41,41	0.82	0	56,56,56	2.37	23 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	AB	819	-	60,68,73	1.53	9 (15%)	70,107,113	1.64	12 (17%)
25	LMG	A4	318	-	39,39,55	1.00	2 (5%)	47,47,63	1.40	7 (14%)
17	CLA	A6	602	16	65,73,73	1.51	9 (13%)	76,113,113	1.29	9 (11%)
20	BCR	AB	845	-	41,41,41	0.85	1 (2%)	56,56,56	1.93	17 (30%)
27	XAT	A3	317	-	39,47,47	0.97	1 (2%)	54,74,74	2.31	19 (35%)
17	CLA	AL	302	12	41,49,73	1.91	7 (17%)	47,84,113	1.46	8 (17%)
27	XAT	A6	615	-	39,47,47	0.98	2 (5%)	54,74,74	2.49	21 (38%)
20	BCR	A1	319	-	41,41,41	0.90	1 (2%)	56,56,56	3.13	20 (35%)
20	BCR	AF	801	-	41,41,41	0.86	1 (2%)	56,56,56	1.56	10 (17%)
17	CLA	A6	612	16	64,72,73	1.53	8 (12%)	74,111,113	1.28	7 (9%)
26	CHL	A6	605	-	42,50,74	2.35	15 (35%)	45,85,114	2.88	20 (44%)
17	CLA	AA	826	-	59,67,73	1.56	9 (15%)	68,105,113	1.28	8 (11%)
17	CLA	A4	313	-	50,58,73	1.72	8 (16%)	58,95,113	1.47	10 (17%)
17	CLA	AA	821	-	65,73,73	1.49	7 (10%)	76,113,113	1.40	9 (11%)
17	CLA	AB	832	-	65,73,73	1.50	10 (15%)	76,113,113	1.30	9 (11%)
26	CHL	A4	304	-	40,49,74	2.45	16 (40%)	42,84,114	2.82	20 (47%)
27	XAT	A1	318	-	39,47,47	0.91	2 (5%)	54,74,74	2.42	24 (44%)
17	CLA	AA	836	1	45,53,73	1.85	7 (15%)	52,89,113	1.47	8 (15%)
17	CLA	A3	309	14	41,49,73	1.88	8 (19%)	47,84,113	1.49	10 (21%)
24	LUT	AF	806	-	42,43,43	1.03	3 (7%)	51,60,60	1.72	12 (23%)
17	CLA	AA	810	-	65,72,73	1.55	9 (13%)	71,111,113	1.29	7 (9%)
19	LHG	A3	319	17	22,22,48	1.44	2 (9%)	25,28,54	1.27	2 (8%)
26	CHL	A3	307	-	45,53,74	2.29	16 (35%)	52,89,114	2.69	21 (40%)
17	CLA	AB	836	-	42,50,73	1.86	7 (16%)	48,85,113	1.52	7 (14%)
17	CLA	AB	841	-	65,73,73	1.54	9 (13%)	76,113,113	1.22	6 (7%)
17	CLA	AB	824	-	43,51,73	1.77	10 (23%)	49,86,113	1.57	8 (16%)
17	CLA	AL	304	-	42,50,73	1.85	8 (19%)	48,85,113	1.57	8 (16%)

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
26	CHL	A6	607	-	3/3/17/26	8/19/117/137	-
17	CLA	A6	609	16	1/1/13/20	4/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	AB	807	2	1/1/15/20	11/37/115/115	-
17	CLA	A3	305	-	1/1/10/20	4/8/86/115	-
17	CLA	AB	831	-	1/1/10/20	3/11/89/115	-
17	CLA	A6	613	-	1/1/10/20	2/11/89/115	-
17	CLA	AB	839	-	1/1/11/20	3/16/94/115	-
17	CLA	AB	808	-	-	5/20/98/115	-
17	CLA	AA	803	-	1/1/15/20	15/37/115/115	-
17	CLA	A3	311	14	1/1/10/20	0/11/89/115	-
17	CLA	AA	842	-	1/1/15/20	18/37/115/115	-
17	CLA	AA	813	-	1/1/15/20	17/37/115/115	-
17	CLA	AB	823	-	-	19/37/115/115	-
17	CLA	AA	809	1	1/1/12/20	5/19/97/115	-
17	CLA	AB	812	-	1/1/13/20	8/25/101/115	-
17	CLA	A6	604	-	1/1/10/20	1/9/88/115	-
17	CLA	AA	827	-	1/1/15/20	18/37/115/115	-
17	CLA	AB	801	-	1/1/15/20	17/37/115/115	-
17	CLA	A3	310	19	1/1/9/20	0/0/78/115	-
17	CLA	AA	811	-	1/1/15/20	11/37/115/115	-
17	CLA	AB	820	-	1/1/13/20	8/25/103/115	-
17	CLA	AB	815	-	1/1/15/20	17/37/115/115	-
17	CLA	AA	830	-	1/1/15/20	14/37/115/115	-
17	CLA	AF	802	-	1/1/13/20	10/28/106/115	-
17	CLA	AB	802	-	1/1/15/20	16/37/113/115	-
19	LHG	A1	301	17	-	11/42/42/53	-
17	CLA	AA	801	-	1/1/15/20	13/37/115/115	-
17	CLA	AA	840	-	1/1/15/20	14/37/115/115	-
17	CLA	A4	302	15	1/1/11/20	5/13/89/115	-
25	LMG	A1	321	-	-	17/39/59/70	0/1/1/1
17	CLA	A3	314	-	1/1/8/20	0/0/74/115	-
26	CHL	A1	303	13	3/3/17/26	4/21/119/137	-
19	LHG	A1	320	17	-	16/53/53/53	-
17	CLA	AA	806	1	1/1/15/20	13/37/115/115	-
22	LMU	AB	852	-	-	9/21/61/61	0/2/2/2
17	CLA	A1	309	-	1/1/11/20	5/11/89/115	-
17	CLA	AG	204	7	1/1/11/20	4/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A4	307	15	1/1/11/20	1/13/91/115	-
17	CLA	AK	203	-	1/1/11/20	5/13/91/115	-
17	CLA	AB	838	-	-	7/37/115/115	-
26	CHL	A3	320	16	3/3/17/26	6/22/120/137	-
17	CLA	AB	805	-	1/1/10/20	2/8/86/115	-
17	CLA	AB	828	-	1/1/15/20	13/37/115/115	-
17	CLA	AB	827	-	1/1/14/20	14/34/112/115	-
17	CLA	AA	834	-	-	15/37/115/115	-
17	CLA	AK	201	11	1/1/8/20	0/2/74/115	-
20	BCR	A3	318	-	-	4/29/63/63	0/2/2/2
17	CLA	A3	303	14	1/1/13/20	8/25/103/115	-
20	BCR	AA	845	-	-	2/29/63/63	0/2/2/2
17	CLA	AG	203	-	1/1/10/20	3/10/88/115	-
17	CLA	AB	830	-	1/1/13/20	10/27/105/115	-
21	SF4	AC	101	3	-	-	0/6/5/5
18	PQN	AA	843	-	-	6/23/43/43	0/2/2/2
17	CLA	AA	837	-	1/1/12/20	6/21/99/115	-
17	CLA	A1	316	13	1/1/11/20	9/11/87/115	-
17	CLA	AA	805	-	1/1/15/20	17/37/115/115	-
20	BCR	AB	847	-	-	0/29/63/63	0/2/2/2
19	LHG	AA	844	-	-	18/53/53/53	-
17	CLA	AB	803	-	1/1/15/20	17/37/115/115	-
20	BCR	AB	848	-	-	2/29/63/63	0/2/2/2
17	CLA	AA	841	-	-	10/37/115/115	-
17	CLA	AJ	102	10	1/1/10/20	3/10/88/115	-
24	LUT	A3	316	-	-	0/29/67/67	0/2/2/2
20	BCR	AL	305	-	-	3/29/63/63	0/2/2/2
17	CLA	AA	816	-	1/1/11/20	6/13/91/115	-
17	CLA	AA	817	-	1/1/14/20	6/31/109/115	-
17	CLA	AB	822	-	1/1/11/20	5/16/94/115	-
17	CLA	AA	804	-	-	7/22/100/115	-
19	LHG	A1	302	-	-	15/40/40/53	-
17	CLA	A4	301	15	1/1/14/20	8/31/109/115	-
17	CLA	A6	610	19	1/1/7/20	5/10/70/115	-
20	BCR	AA	846	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	SF4	AA	850	2,1	-	-	0/6/5/5
17	CLA	A3	304	-	1/1/11/20	0/9/85/115	-
17	CLA	AB	829	-	1/1/15/20	15/37/115/115	-
17	CLA	AF	804	-	1/1/10/20	2/8/86/115	-
17	CLA	AA	812	-	1/1/12/20	9/24/102/115	-
17	CLA	AA	822	-	1/1/10/20	3/10/88/115	-
17	CLA	A3	313	-	-	1/6/84/115	-
20	BCR	A6	616	-	-	2/29/63/63	0/2/2/2
17	CLA	AA	832	-	1/1/13/20	7/27/105/115	-
17	CLA	AB	809	-	1/1/15/20	16/37/115/115	-
26	CHL	A4	305	-	3/3/15/26	0/10/106/137	-
26	CHL	A6	606	-	3/3/15/26	2/12/110/137	-
17	CLA	AB	816	-	1/1/10/20	4/11/89/115	-
17	CLA	AB	825	-	1/1/15/20	14/37/115/115	-
17	CLA	AA	818	-	-	7/30/108/115	-
17	CLA	A1	310	13	1/1/10/20	2/8/84/115	-
22	LMU	AA	851	-	-	10/21/61/61	0/2/2/2
17	CLA	AA	824	-	1/1/13/20	7/23/101/115	-
17	CLA	A1	304	13	1/1/13/20	11/31/109/115	-
20	BCR	AJ	103	-	-	5/29/63/63	0/2/2/2
20	BCR	AI	101	-	-	7/29/63/63	0/2/2/2
17	CLA	AA	825	-	1/1/15/20	10/37/115/115	-
20	BCR	AF	805	-	-	6/29/63/63	0/2/2/2
23	DGD	AB	851	-	-	21/55/95/95	0/2/2/2
17	CLA	AB	818	-	1/1/13/20	10/30/108/115	-
17	CLA	AL	303	-	-	9/31/109/115	-
17	CLA	AA	839	-	-	6/22/100/115	-
17	CLA	A6	603	-	1/1/10/20	2/9/87/115	-
20	BCR	AA	847	-	-	13/29/63/63	0/2/2/2
17	CLA	AA	808	1	1/1/15/20	10/37/115/115	-
17	CLA	AB	821	-	1/1/12/20	7/19/97/115	-
17	CLA	AA	823	-	1/1/10/20	4/8/86/115	-
17	CLA	AB	810	2	1/1/15/20	16/37/115/115	-
20	BCR	AA	849	-	-	8/29/63/63	0/2/2/2
22	LMU	AB	850	-	-	9/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	AA	815	-	-	3/10/88/115	-
17	CLA	A1	312	19	1/1/10/20	0/4/80/115	-
17	CLA	AA	802	-	1/1/15/20	8/37/115/115	-
27	XAT	A4	316	-	-	0/31/93/93	0/4/4/4
17	CLA	A4	308	15	1/1/12/20	4/24/102/115	-
17	CLA	A4	310	15	1/1/10/20	5/8/86/115	-
17	CLA	A3	308	14	1/1/11/20	5/13/91/115	-
17	CLA	A4	311	-	1/1/13/20	7/26/104/115	-
17	CLA	A3	312	-	1/1/13/20	11/23/101/115	-
17	CLA	A6	611	16	1/1/11/20	6/11/89/115	-
24	LUT	A4	315	-	-	1/29/67/67	0/2/2/2
20	BCR	AG	205	-	-	2/29/63/63	0/2/2/2
17	CLA	AB	842	19	1/1/15/20	18/37/115/115	-
17	CLA	AB	833	-	1/1/15/20	10/37/115/115	-
17	CLA	A6	608	16	1/1/11/20	3/13/91/115	-
17	CLA	A1	313	13	1/1/11/20	4/13/91/115	-
17	CLA	A1	305	-	1/1/13/20	7/25/103/115	-
21	SF4	AC	102	3	-	-	0/6/5/5
17	CLA	AB	811	-	1/1/15/20	15/37/115/115	-
17	CLA	A1	311	13	1/1/14/20	3/29/107/115	-
22	LMU	AL	301	-	-	11/20/60/61	0/2/2/2
26	CHL	A1	308	13	3/3/15/26	2/8/106/137	-
20	BCR	AB	844	-	-	5/29/63/63	0/2/2/2
17	CLA	AA	838	-	-	6/25/103/115	-
17	CLA	AA	828	-	1/1/15/20	15/37/115/115	-
17	CLA	AB	840	-	1/1/15/20	7/37/115/115	-
17	CLA	A4	312	-	1/1/11/20	4/13/91/115	-
19	LHG	A6	617	17	-	17/40/40/53	-
17	CLA	AK	204	-	1/1/11/20	7/15/93/115	-
20	BCR	AB	849	-	-	5/29/63/63	0/2/2/2
25	LMG	AG	202	-	-	5/33/53/70	0/1/1/1
22	LMU	AB	853	-	-	13/21/61/61	0/2/2/2
17	CLA	A4	309	-	1/1/10/20	3/10/88/115	-
17	CLA	A1	307	-	1/1/9/20	4/8/82/115	-
17	CLA	AA	807	-	1/1/12/20	4/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	AA	814	-	1/1/11/20	5/13/91/115	-
17	CLA	AB	806	-	1/1/15/20	15/37/115/115	-
17	CLA	A3	306	14	1/1/10/20	0/10/86/115	-
17	CLA	AB	813	-	1/1/10/20	3/11/89/115	-
17	CLA	AB	814	-	1/1/15/20	14/37/115/115	-
17	CLA	A4	303	-	1/1/11/20	4/11/87/115	-
17	CLA	AG	201	-	1/1/11/20	3/11/89/115	-
20	BCR	AB	846	-	-	6/29/63/63	0/2/2/2
17	CLA	AB	826	-	1/1/14/20	6/34/112/115	-
24	LUT	A1	317	-	-	0/29/67/67	0/2/2/2
17	CLA	AB	817	-	1/1/13/20	8/25/103/115	-
26	CHL	A4	314	15	3/3/15/26	0/10/106/137	-
24	LUT	A6	614	-	-	0/29/67/67	0/2/2/2
17	CLA	A6	601	15	1/1/11/20	2/15/93/115	-
20	BCR	AL	306	-	-	5/29/63/63	0/2/2/2
19	LHG	A3	301	-	-	11/40/40/53	-
17	CLA	AB	834	-	1/1/15/20	16/37/115/115	-
17	CLA	AA	820	-	1/1/11/20	3/13/91/115	-
17	CLA	A1	314	-	1/1/15/20	12/35/113/115	-
20	BCR	AK	202	-	-	5/29/63/63	0/2/2/2
17	CLA	A1	306	-	1/1/11/20	9/18/96/115	-
17	CLA	AA	833	-	1/1/15/20	19/37/115/115	-
17	CLA	AB	804	-	1/1/15/20	16/37/115/115	-
19	LHG	AJ	104	-	-	16/44/44/53	-
18	PQN	AB	843	-	-	8/23/43/43	0/2/2/2
26	CHL	A4	306	-	3/3/16/26	2/15/113/137	-
17	CLA	A1	315	-	1/1/10/20	0/4/80/115	-
17	CLA	AA	829	-	1/1/15/20	18/37/115/115	-
17	CLA	AB	837	-	1/1/12/20	7/19/97/115	-
20	BCR	AI	102	-	-	5/29/63/63	0/2/2/2
20	BCR	AK	205	-	-	6/29/63/63	0/2/2/2
17	CLA	AH	201	-	1/1/14/20	10/31/109/115	-
17	CLA	AA	831	-	1/1/11/20	7/16/94/115	-
17	CLA	AA	835	-	1/1/11/20	0/11/89/115	-
17	CLA	A3	302	14	1/1/14/20	6/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	AA	819	-	1/1/15/20	14/37/115/115	-
17	CLA	AF	803	-	1/1/10/20	2/10/88/115	-
17	CLA	A3	315	-	1/1/10/20	0/6/84/115	-
17	CLA	AB	835	-	-	7/31/109/115	-
20	BCR	AA	848	-	-	4/29/63/63	0/2/2/2
20	BCR	AJ	101	-	-	1/29/63/63	0/2/2/2
20	BCR	A4	317	-	-	2/29/63/63	0/2/2/2
17	CLA	AB	819	-	1/1/14/20	14/31/109/115	-
25	LMG	A4	318	-	-	15/34/54/70	0/1/1/1
17	CLA	A6	602	16	1/1/15/20	9/37/115/115	-
20	BCR	AB	845	-	-	6/29/63/63	0/2/2/2
27	XAT	A3	317	-	-	0/31/93/93	0/4/4/4
17	CLA	AL	302	12	1/1/10/20	5/8/86/115	-
27	XAT	A6	615	-	-	0/31/93/93	0/4/4/4
20	BCR	A1	319	-	-	4/29/63/63	0/2/2/2
20	BCR	AF	801	-	-	2/29/63/63	0/2/2/2
17	CLA	A6	612	16	1/1/14/20	7/35/113/115	-
26	CHL	A6	605	-	3/3/15/26	2/10/108/137	-
17	CLA	AA	826	-	1/1/13/20	11/30/108/115	-
17	CLA	A4	313	-	1/1/12/20	9/19/97/115	-
17	CLA	AA	821	-	1/1/15/20	15/37/115/115	-
17	CLA	AB	832	-	-	7/37/115/115	-
26	CHL	A4	304	-	3/3/15/26	1/8/106/137	-
27	XAT	A1	318	-	-	0/31/93/93	0/4/4/4
17	CLA	AA	836	1	-	7/13/91/115	-
17	CLA	A3	309	14	1/1/10/20	3/8/86/115	-
24	LUT	AF	806	-	-	0/29/67/67	0/2/2/2
17	CLA	AA	810	-	1/1/14/20	10/37/111/115	-
19	LHG	A3	319	17	-	14/26/26/53	-
26	CHL	A3	307	-	3/3/16/26	4/13/111/137	-
17	CLA	AB	836	-	-	2/10/88/115	-
17	CLA	AB	841	-	1/1/15/20	7/37/115/115	-
17	CLA	AB	824	-	1/1/10/20	4/11/89/115	-
17	CLA	AL	304	-	1/1/10/20	5/10/88/115	-

The worst 5 of 1393 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A6	610	CLA	C1A-NA	12.69	1.40	1.29
18	AA	843	PQN	C12-C13	9.56	1.55	1.33
18	AB	843	PQN	C12-C13	9.36	1.55	1.33
17	AK	201	CLA	C3B-C4B	8.50	1.49	1.39
17	A6	613	CLA	C4B-NB	7.99	1.42	1.35

The worst 5 of 2111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A1	319	BCR	C40-C30-C25	-13.95	87.67	110.30
20	A3	318	BCR	C40-C30-C25	-10.15	93.83	110.30
20	AL	305	BCR	C7-C8-C9	-9.80	111.42	126.23
20	A1	319	BCR	C39-C30-C25	9.45	125.63	110.30
27	A4	316	XAT	O4-C5-C4	9.12	120.24	113.38

5 of 160 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	AA	801	CLA	ND
17	AA	802	CLA	ND
17	AA	803	CLA	ND
17	AA	805	CLA	ND
17	AA	806	CLA	ND

5 of 1499 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	AA	801	CLA	CBD-CGD-O2D-CED
17	AA	802	CLA	CBD-CGD-O2D-CED
17	AA	804	CLA	C1A-C2A-CAA-CBA
17	AA	804	CLA	C3A-C2A-CAA-CBA
17	AA	805	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

110 monomers are involved in 161 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A6	607	CHL	2	0
17	AB	807	CLA	1	0
17	AB	831	CLA	1	0
17	A6	613	CLA	1	0
17	AB	839	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	AB	808	CLA	1	0
17	AA	803	CLA	1	0
17	AA	827	CLA	1	0
17	AB	801	CLA	2	0
17	AA	811	CLA	3	0
17	AA	830	CLA	1	0
17	AB	802	CLA	4	0
17	AA	801	CLA	12	0
25	A1	321	LMG	1	0
26	A1	303	CHL	2	0
17	AA	806	CLA	1	0
17	AG	204	CLA	3	0
17	A4	307	CLA	1	0
26	A3	320	CHL	2	0
17	AB	805	CLA	1	0
17	AB	828	CLA	1	0
17	AB	827	CLA	4	0
17	AA	834	CLA	2	0
20	A3	318	BCR	3	0
17	AG	203	CLA	1	0
17	AB	830	CLA	1	0
21	AC	101	SF4	1	0
18	AA	843	PQN	3	0
17	A1	316	CLA	1	0
17	AA	805	CLA	2	0
20	AB	847	BCR	3	0
19	AA	844	LHG	1	0
17	AB	803	CLA	4	0
20	AB	848	BCR	2	0
17	AA	841	CLA	2	0
20	AL	305	BCR	1	0
17	AB	822	CLA	1	0
17	A4	301	CLA	1	0
20	AA	846	BCR	1	0
17	A3	304	CLA	1	0
17	A3	313	CLA	1	0
20	A6	616	BCR	3	0
17	AA	832	CLA	1	0
17	AB	809	CLA	1	0
17	AB	825	CLA	1	0
17	AA	818	CLA	1	0
20	AJ	103	BCR	1	0

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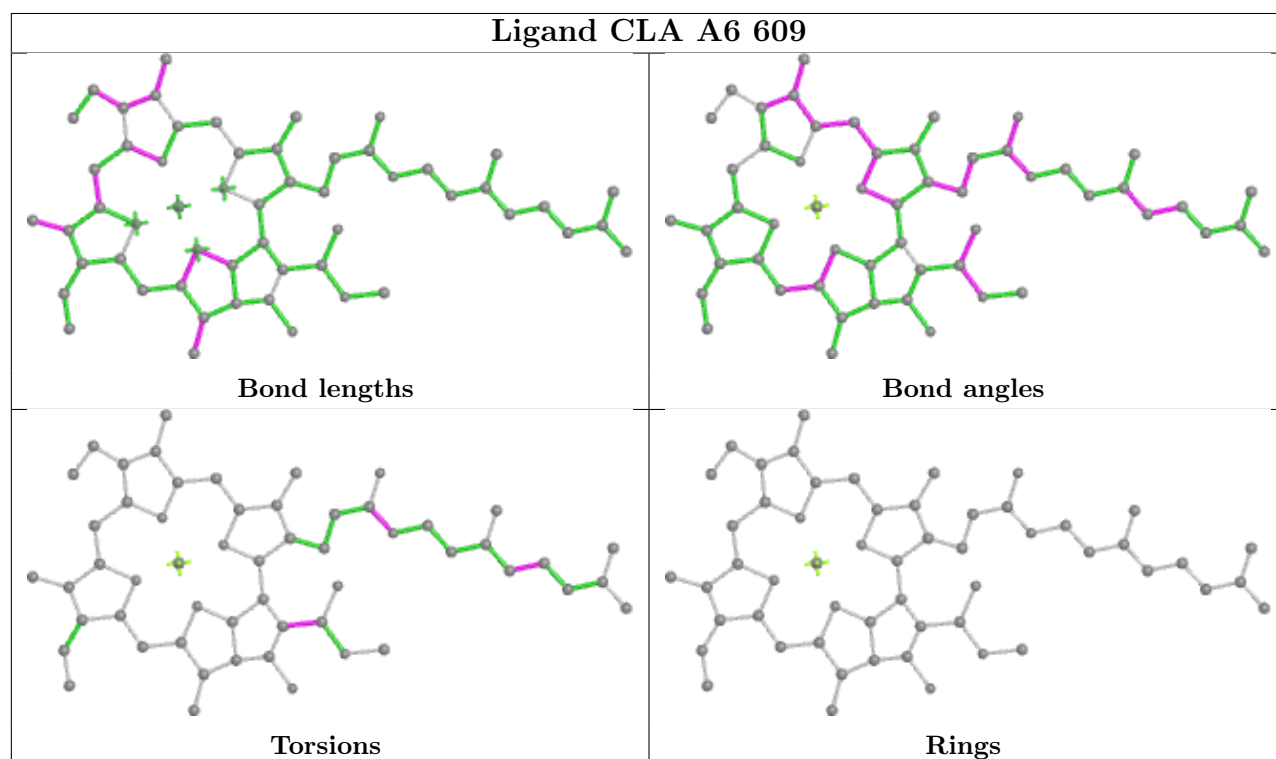
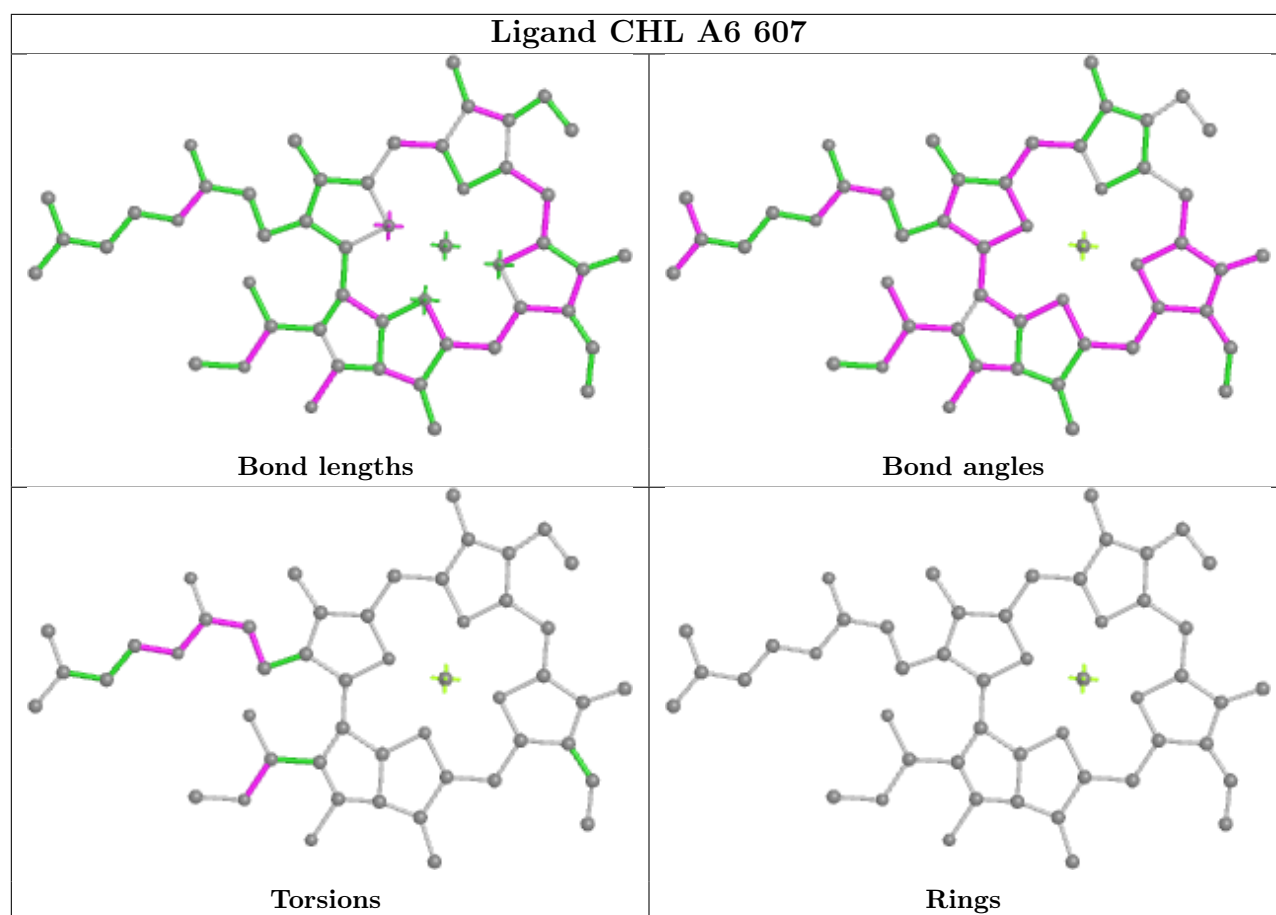
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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20	AF	805	BCR	2	0
17	AB	818	CLA	3	0
17	AL	303	CLA	1	0
17	A6	603	CLA	2	0
20	AA	847	BCR	1	0
17	AB	810	CLA	2	0
20	AA	849	BCR	2	0
17	AA	815	CLA	1	0
17	AA	802	CLA	1	0
27	A4	316	XAT	2	0
17	A4	308	CLA	1	0
17	A3	308	CLA	1	0
24	A4	315	LUT	2	0
20	AG	205	BCR	2	0
17	AB	842	CLA	1	0
17	AB	833	CLA	2	0
17	A1	305	CLA	1	0
21	AC	102	SF4	1	0
17	A1	311	CLA	2	0
22	AL	301	LMU	1	0
26	A1	308	CHL	1	0
20	AB	844	BCR	2	0
17	AA	838	CLA	3	0
17	AA	828	CLA	2	0
17	AB	840	CLA	1	0
19	A6	617	LHG	1	0
20	AB	849	BCR	1	0
17	A4	309	CLA	1	0
17	AB	814	CLA	1	0
20	AB	846	BCR	1	0
24	A6	614	LUT	1	0
17	A6	601	CLA	1	0
19	A3	301	LHG	1	0
17	AB	834	CLA	3	0
17	AA	820	CLA	1	0
17	A1	306	CLA	2	0
17	AA	833	CLA	1	0
18	AB	843	PQN	2	0
26	A4	306	CHL	2	0
20	AI	102	BCR	1	0
20	AK	205	BCR	1	0

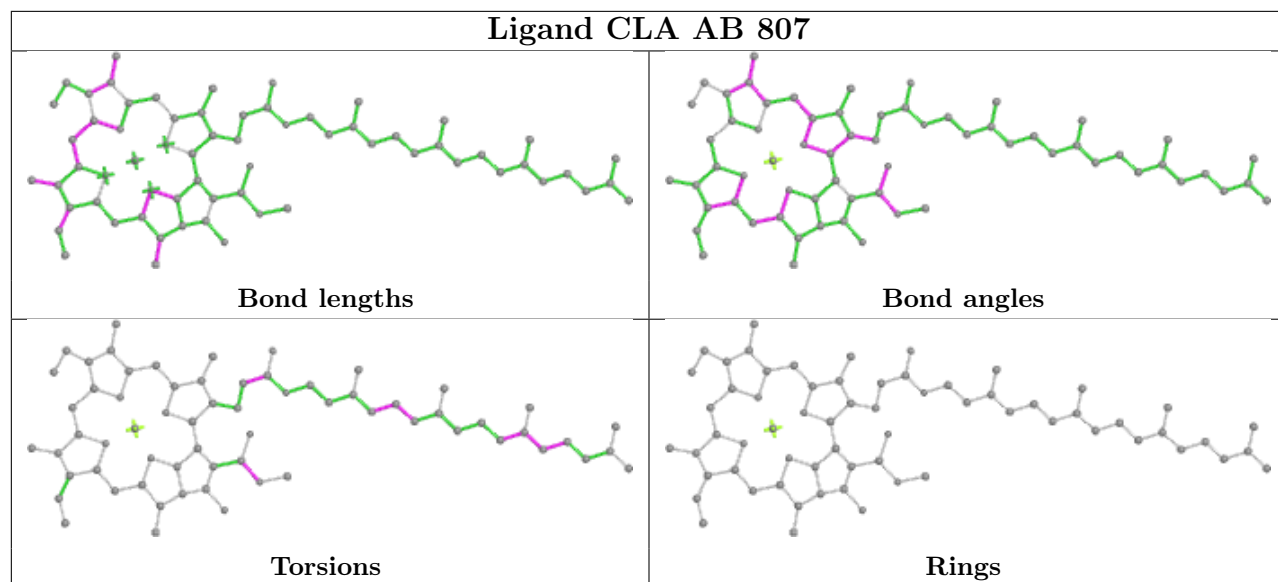
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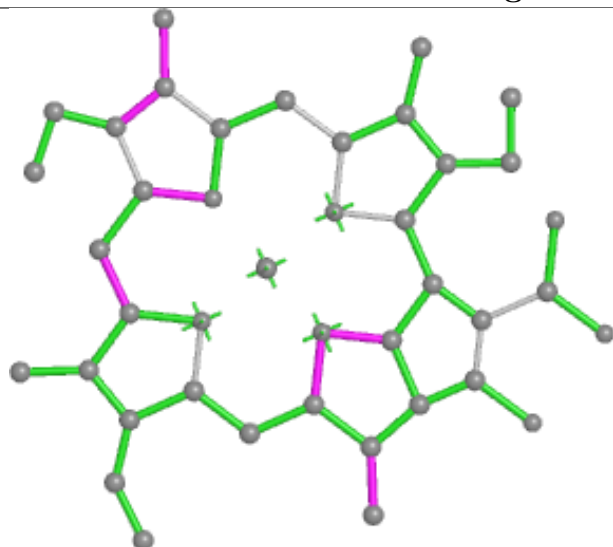
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	AA	835	CLA	1	0
20	AA	848	BCR	2	0
20	AJ	101	BCR	1	0
25	A4	318	LMG	4	0
20	AB	845	BCR	1	0
27	A3	317	XAT	3	0
27	A6	615	XAT	4	0
20	A1	319	BCR	3	0
20	AF	801	BCR	4	0
17	A6	612	CLA	1	0
26	A6	605	CHL	1	0
17	AA	826	CLA	2	0
17	A4	313	CLA	1	0
26	A4	304	CHL	1	0
27	A1	318	XAT	1	0
24	AF	806	LUT	2	0
17	AA	810	CLA	1	0
26	A3	307	CHL	2	0
17	AB	836	CLA	1	0
17	AB	841	CLA	1	0
17	AB	824	CLA	2	0

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

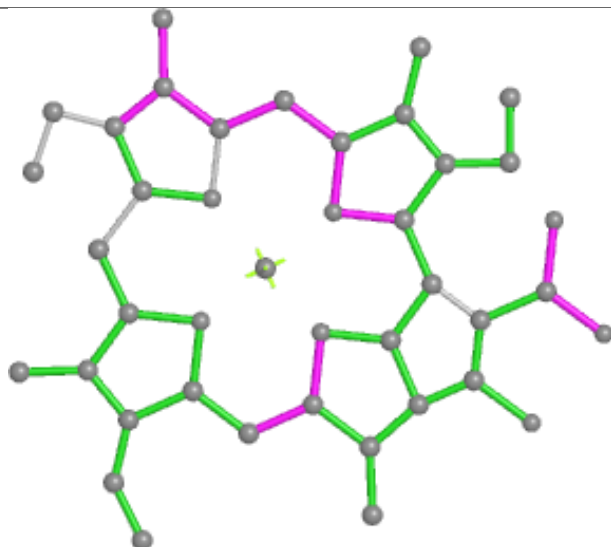




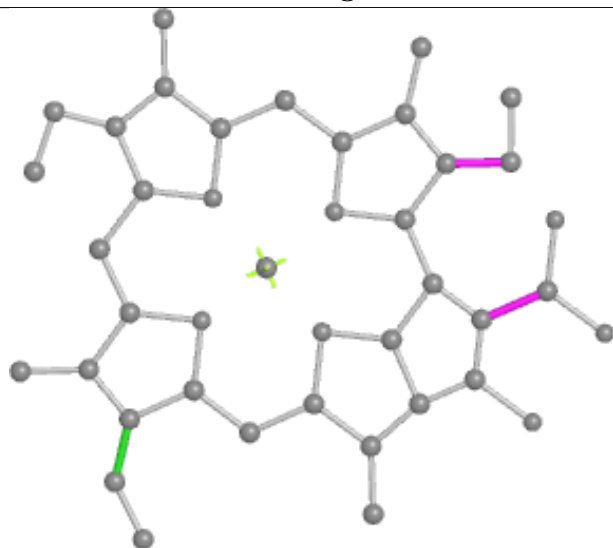
Ligand CLA A3 305



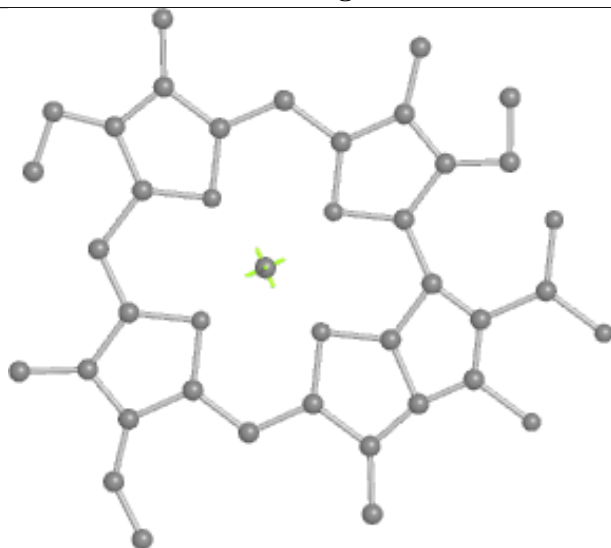
Bond lengths



Bond angles

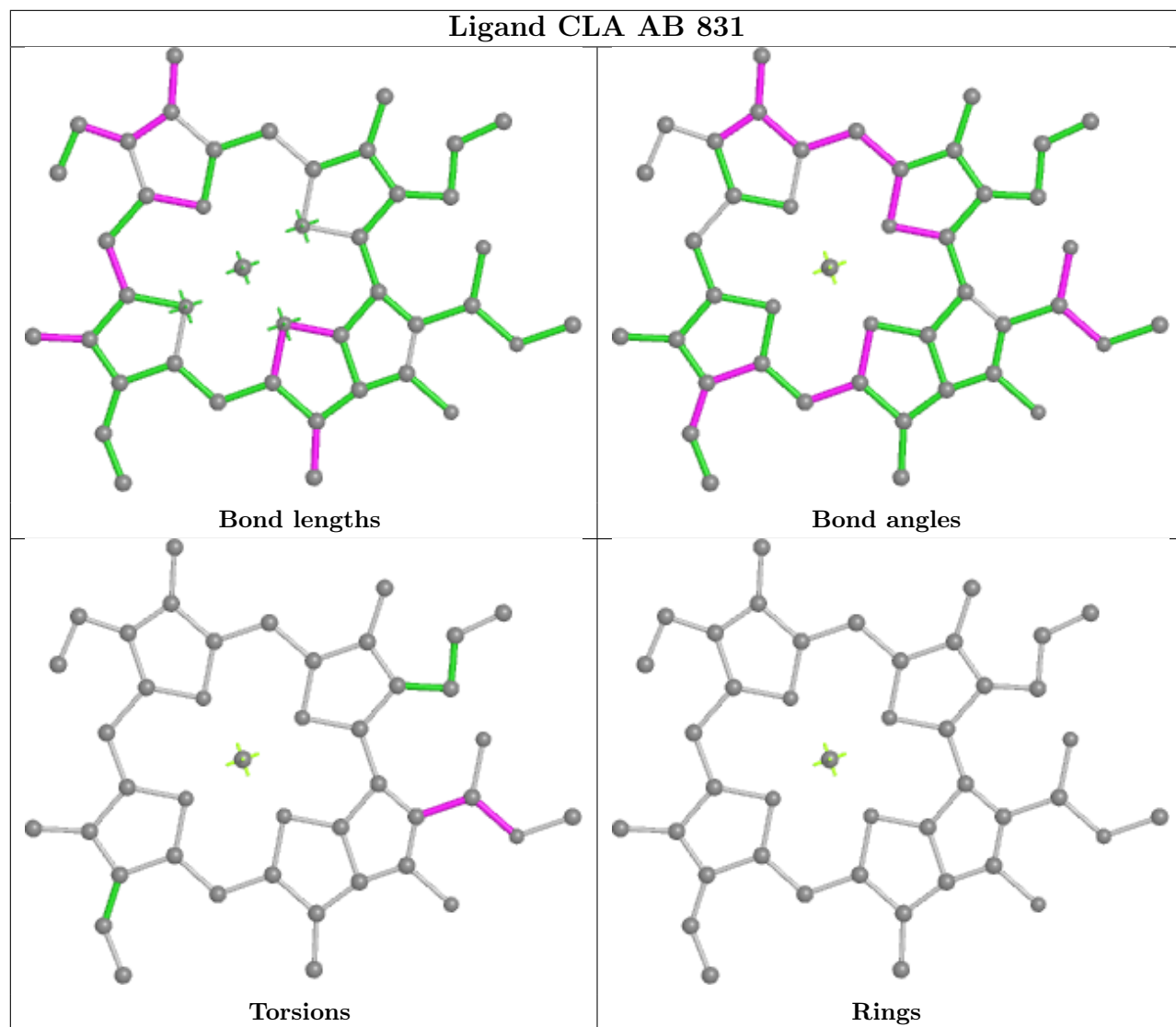


Torsions

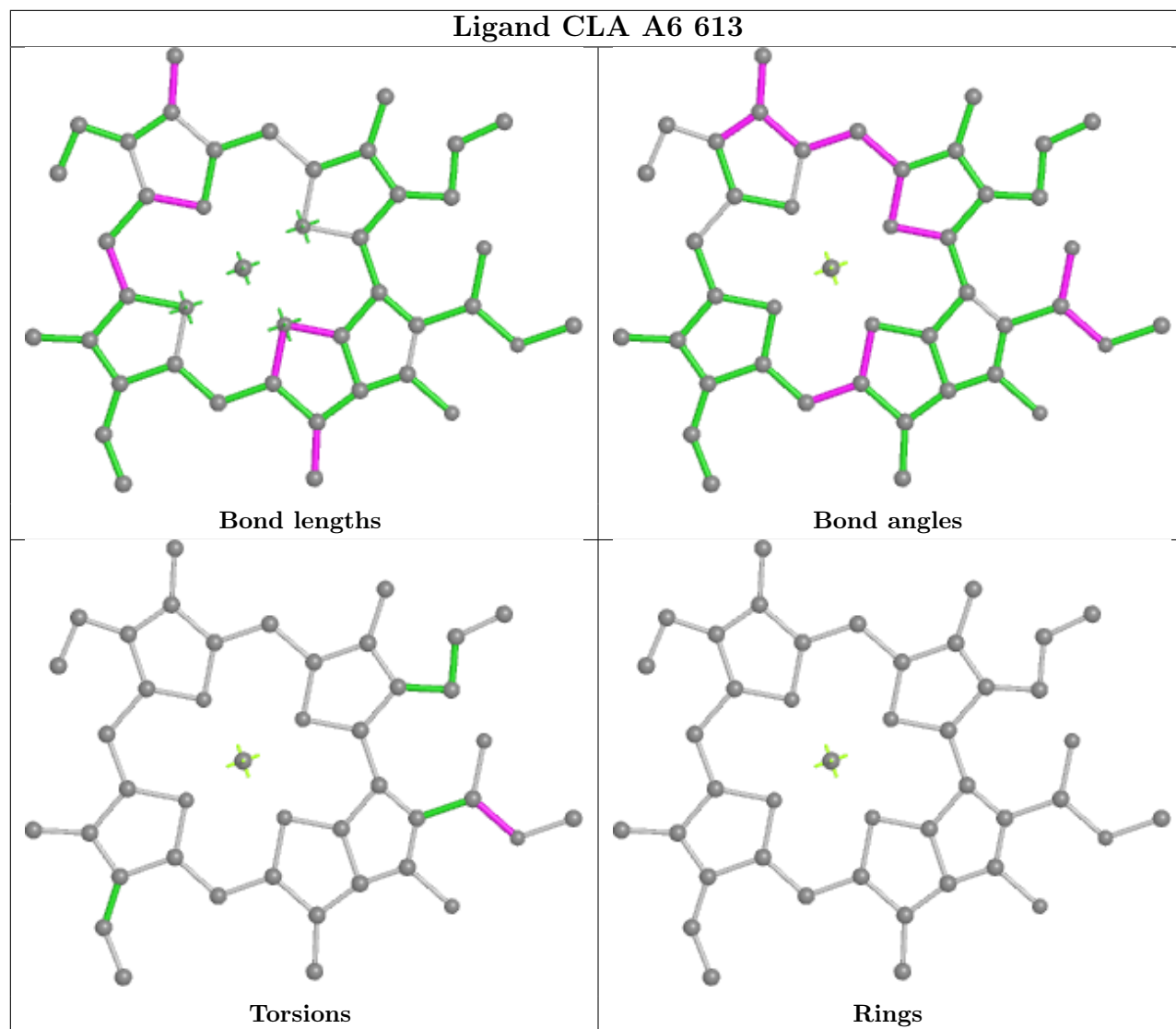


Rings

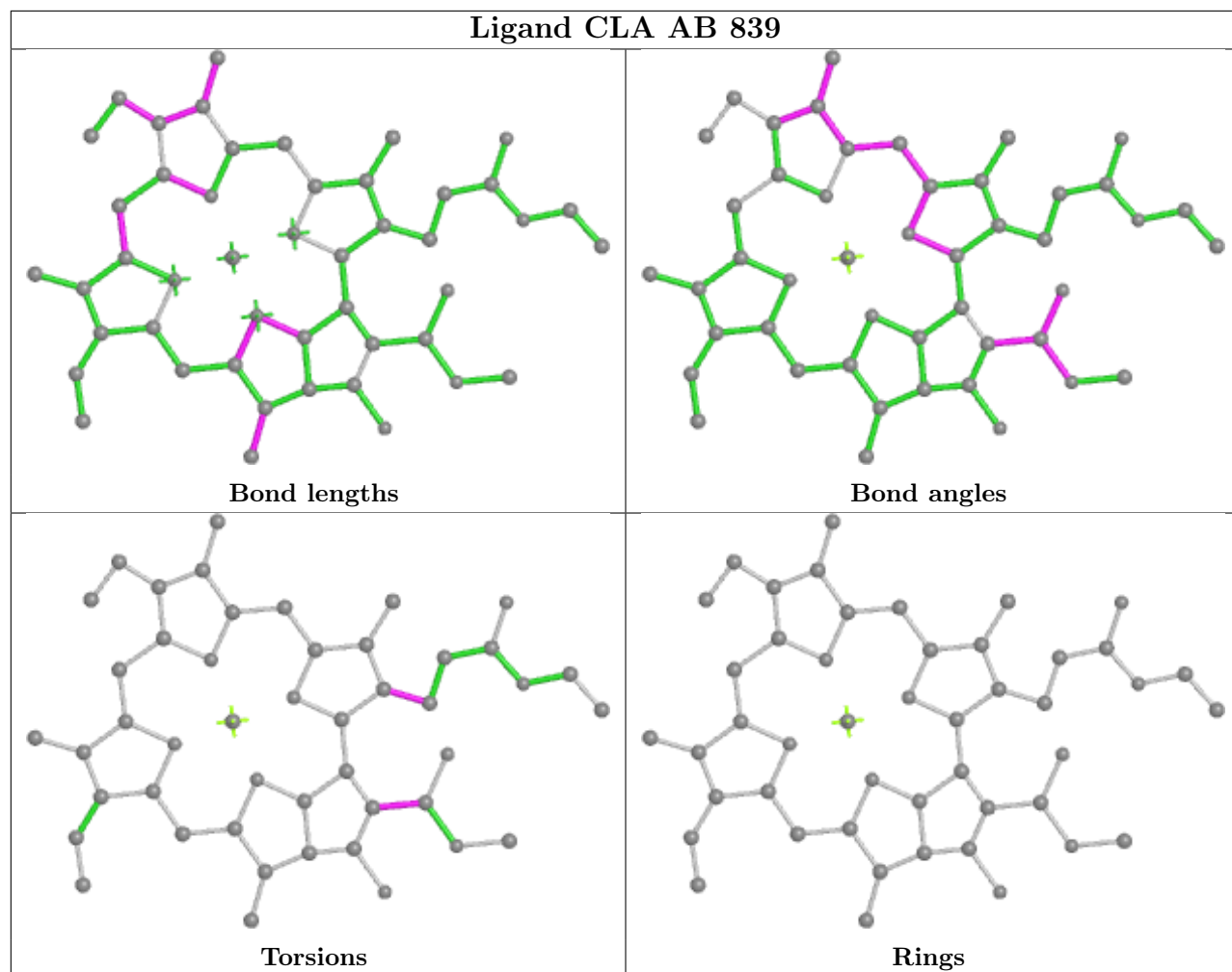
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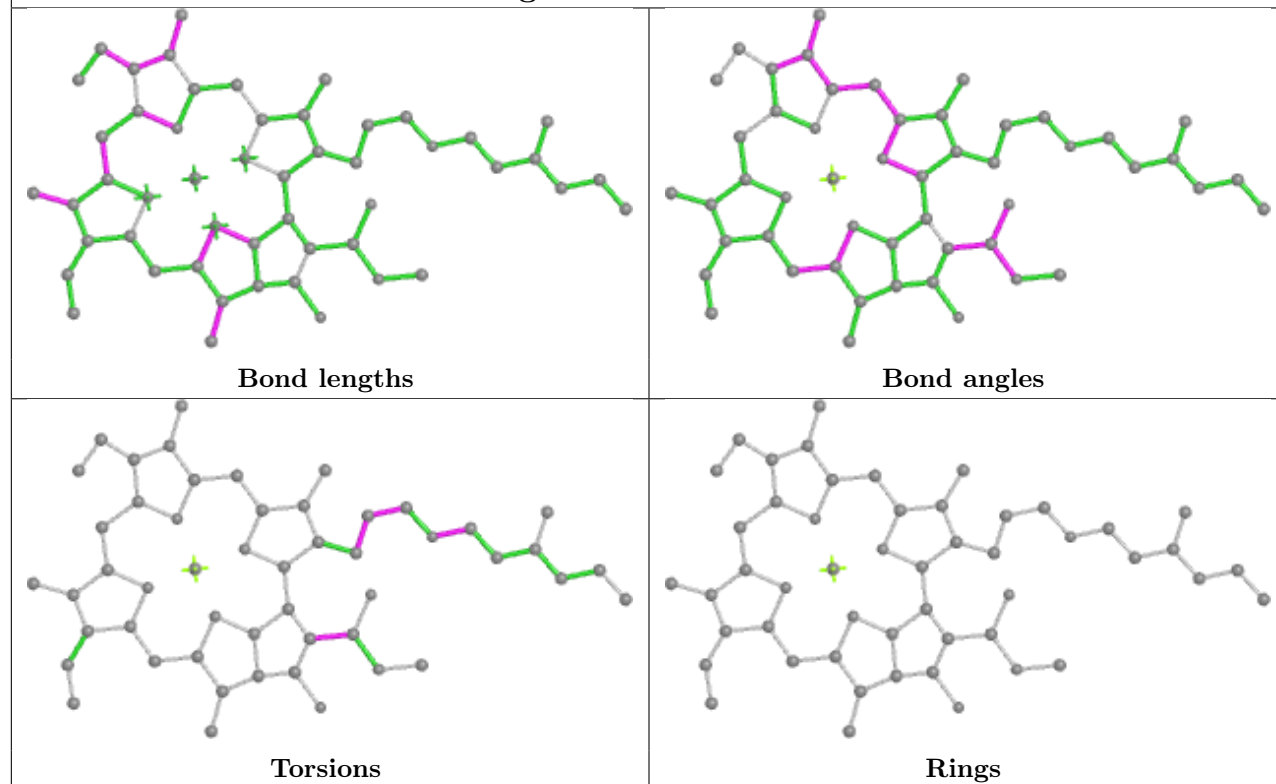
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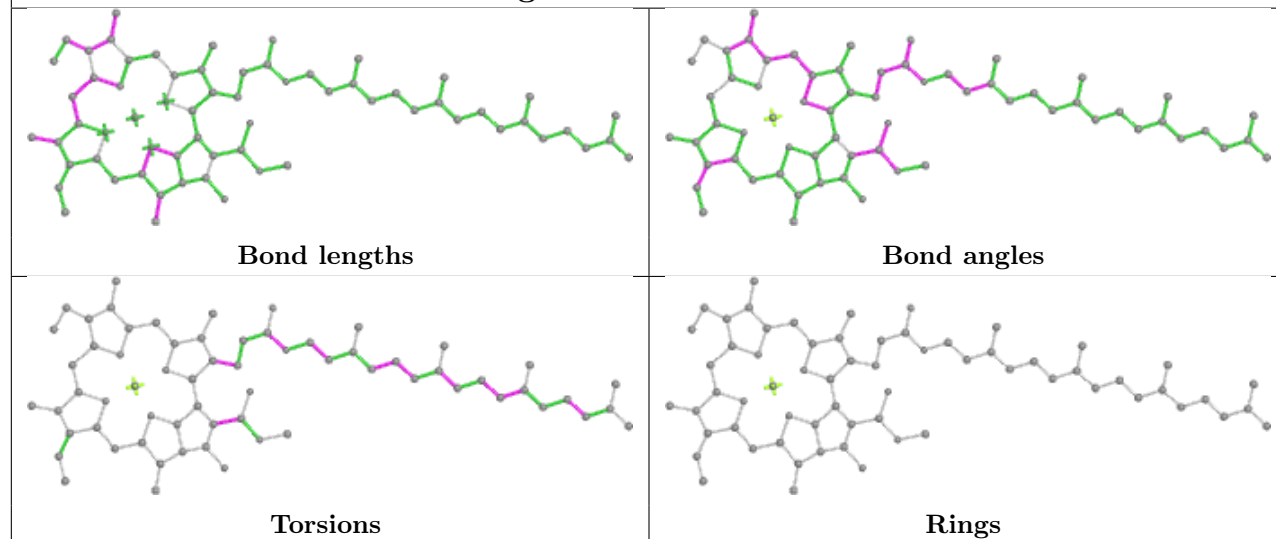
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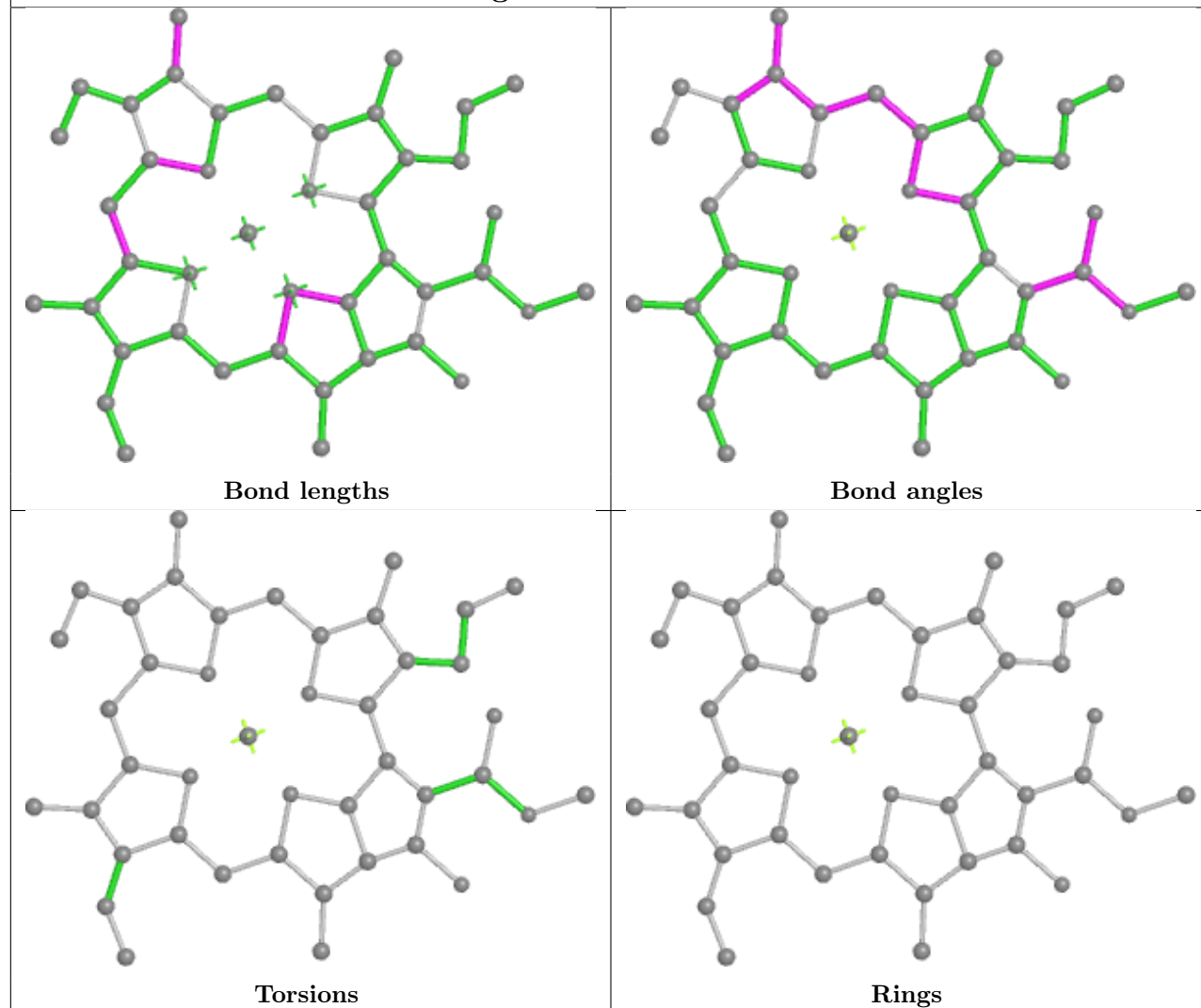
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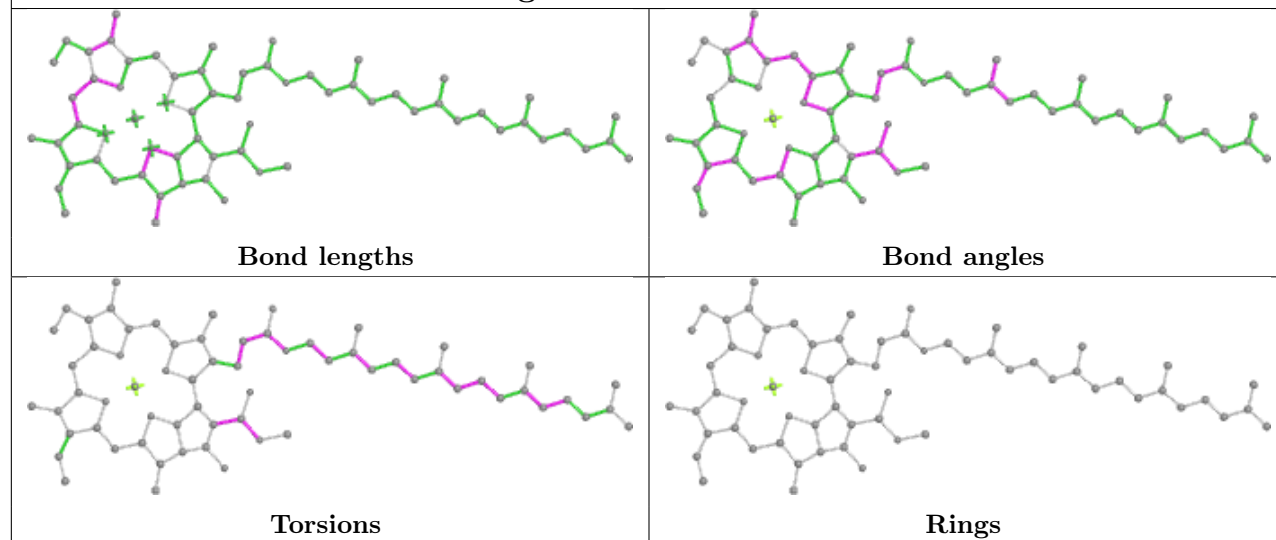
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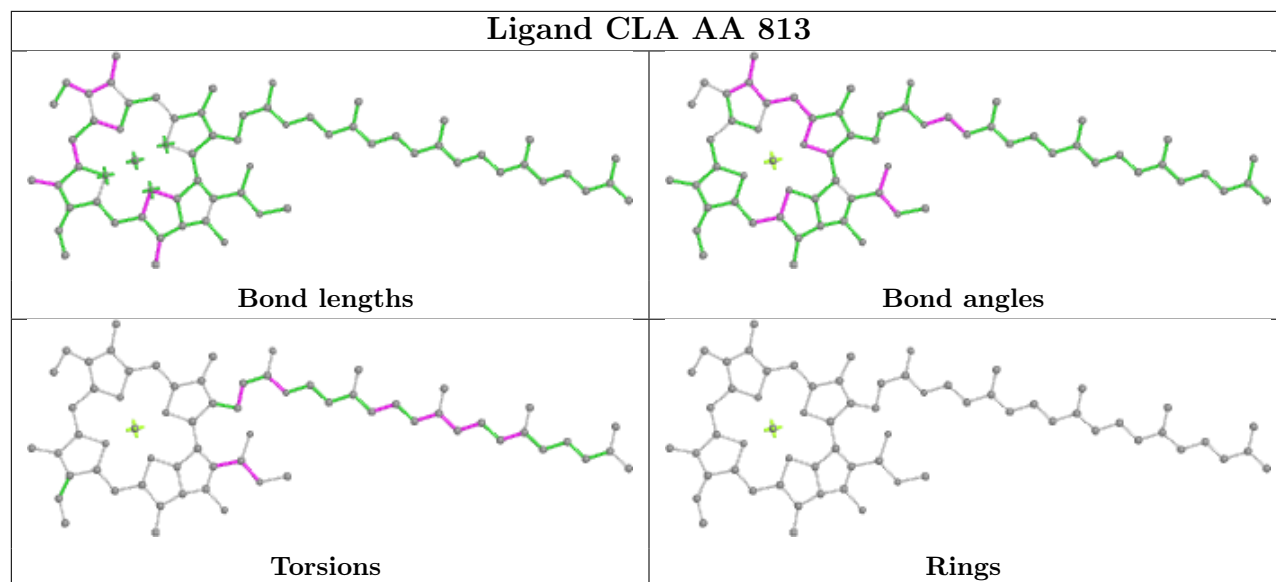
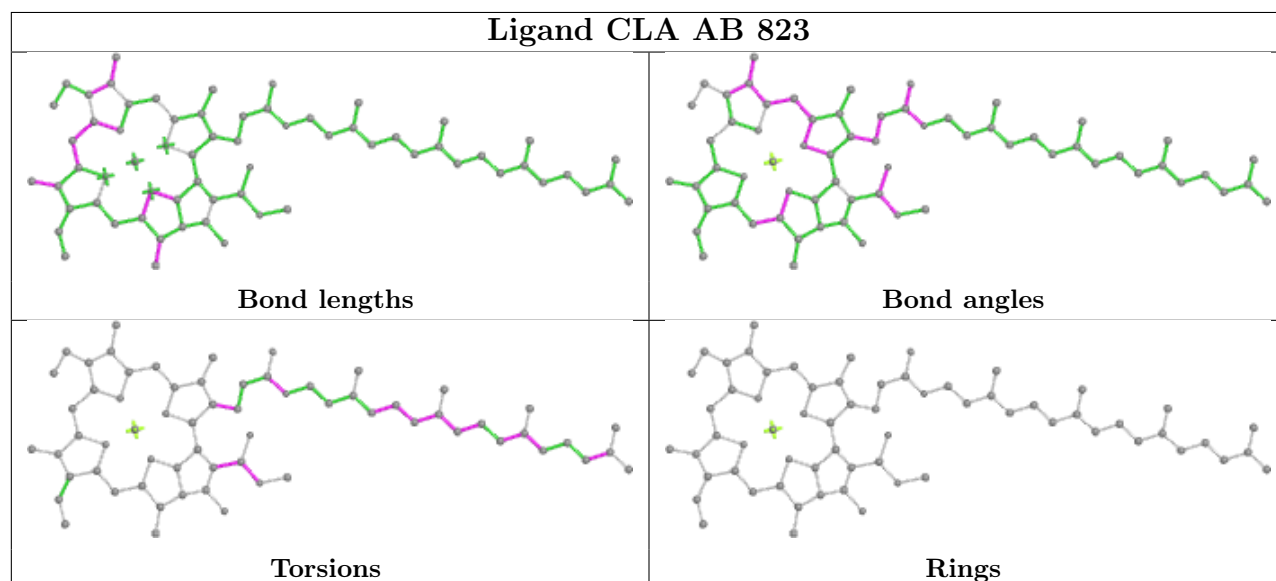


Ligand CLA A3 311

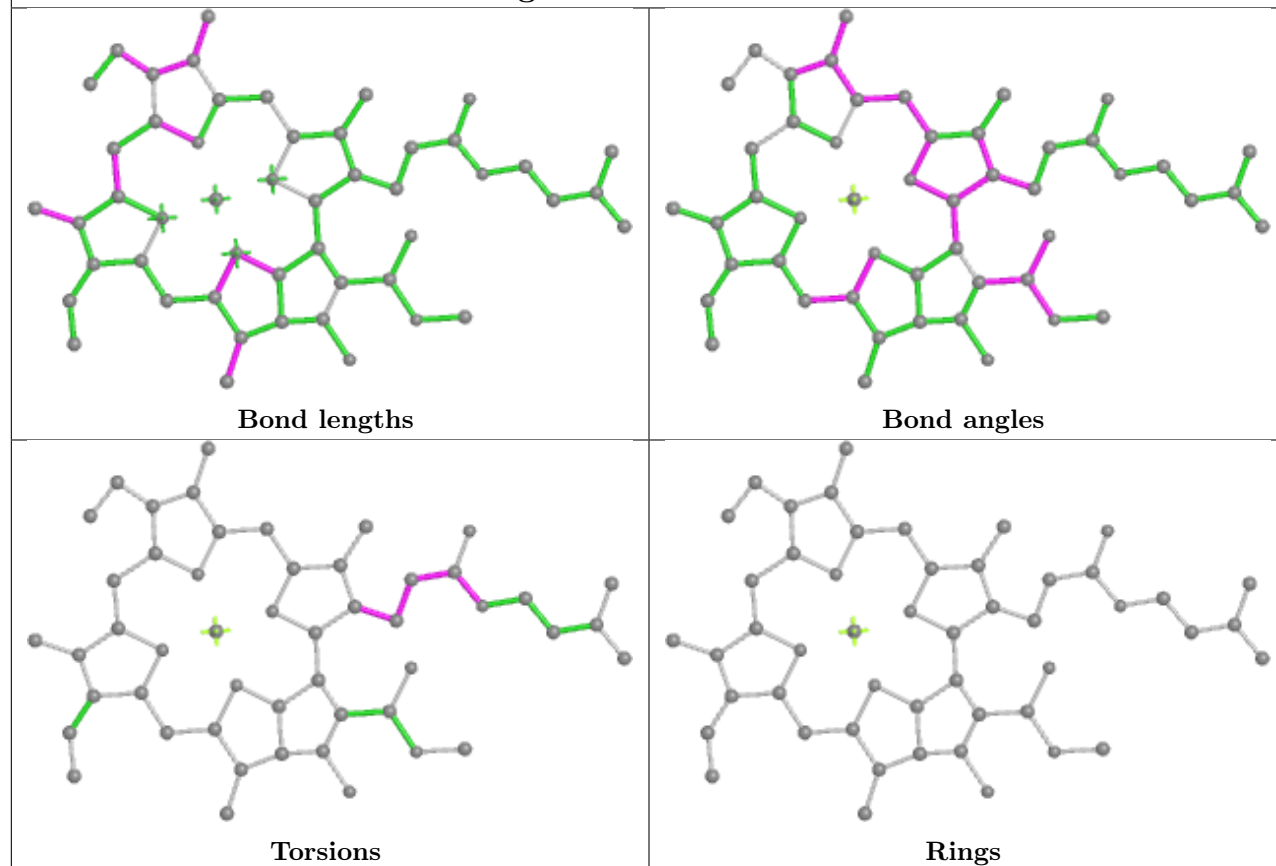


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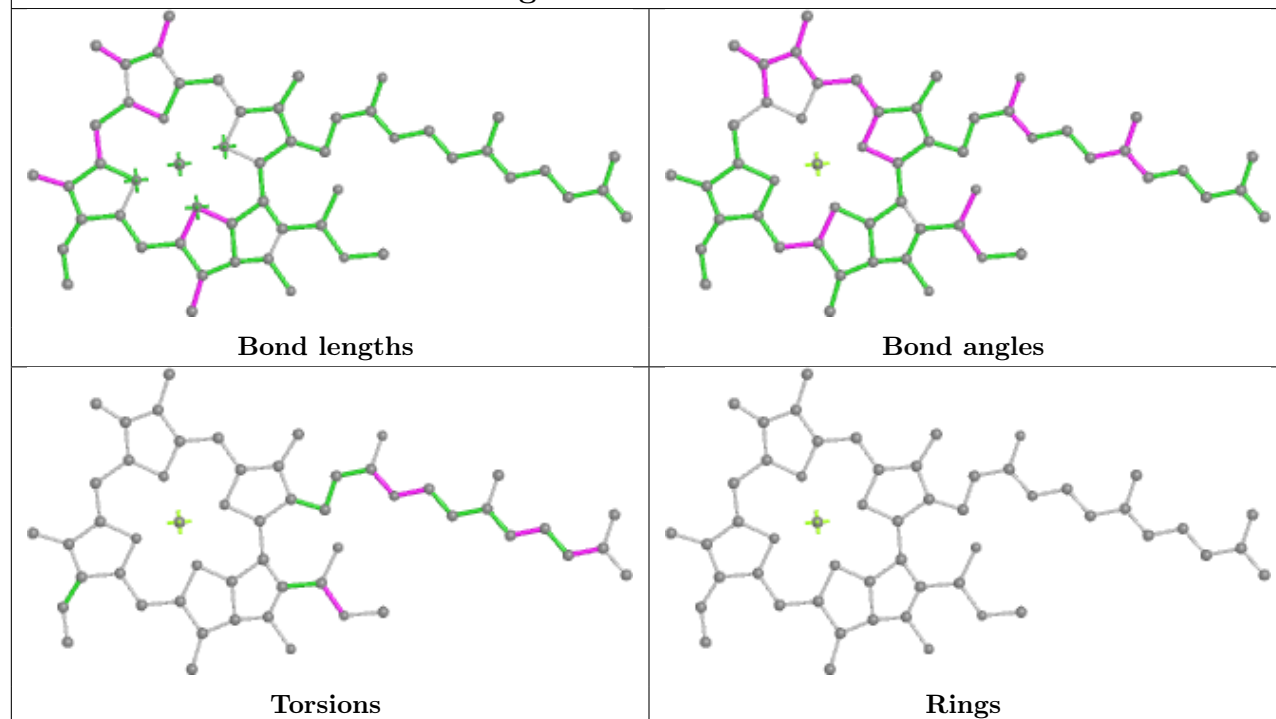


Ligand CLA AA 813**Ligand CLA AB 823**

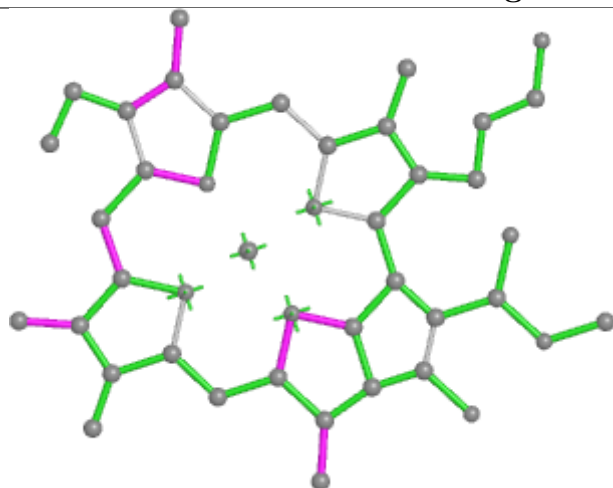
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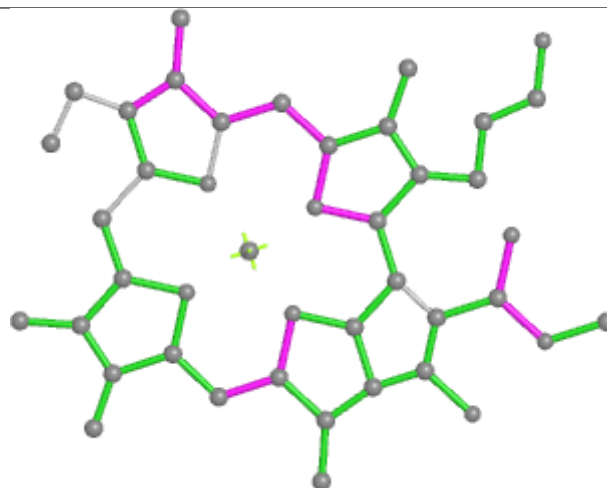
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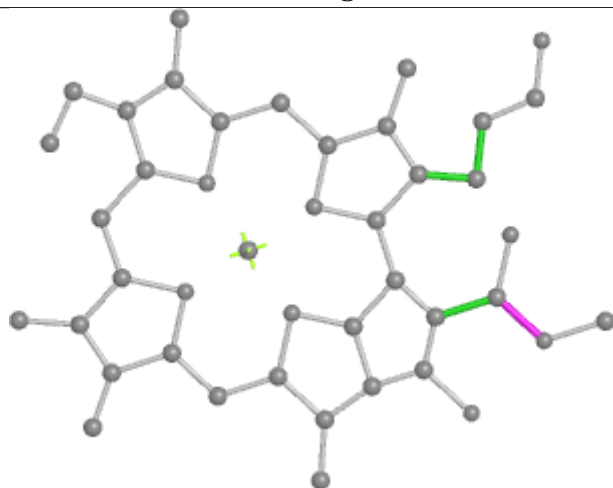
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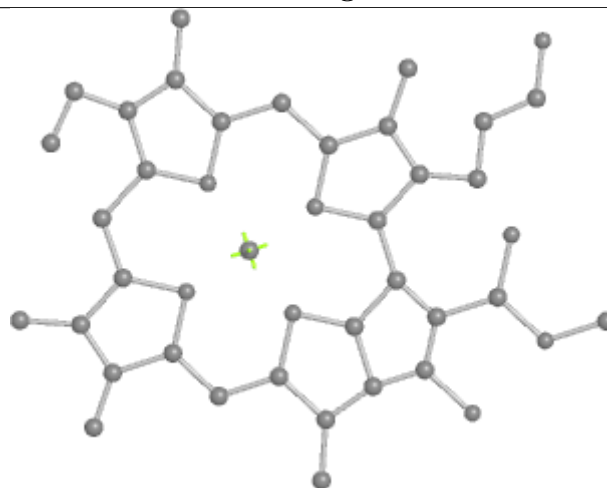
Bond lengths



Bond angles

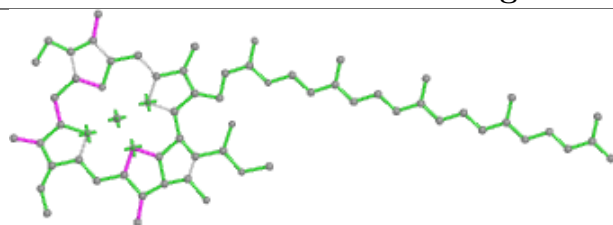


Torsions

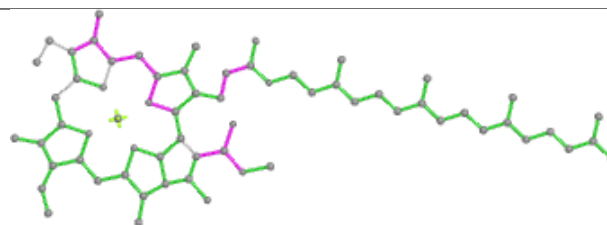


Rings

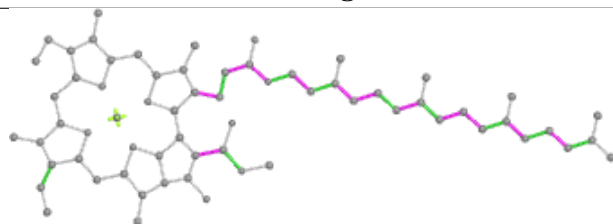
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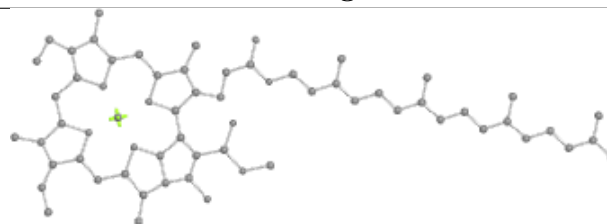
Bond lengths



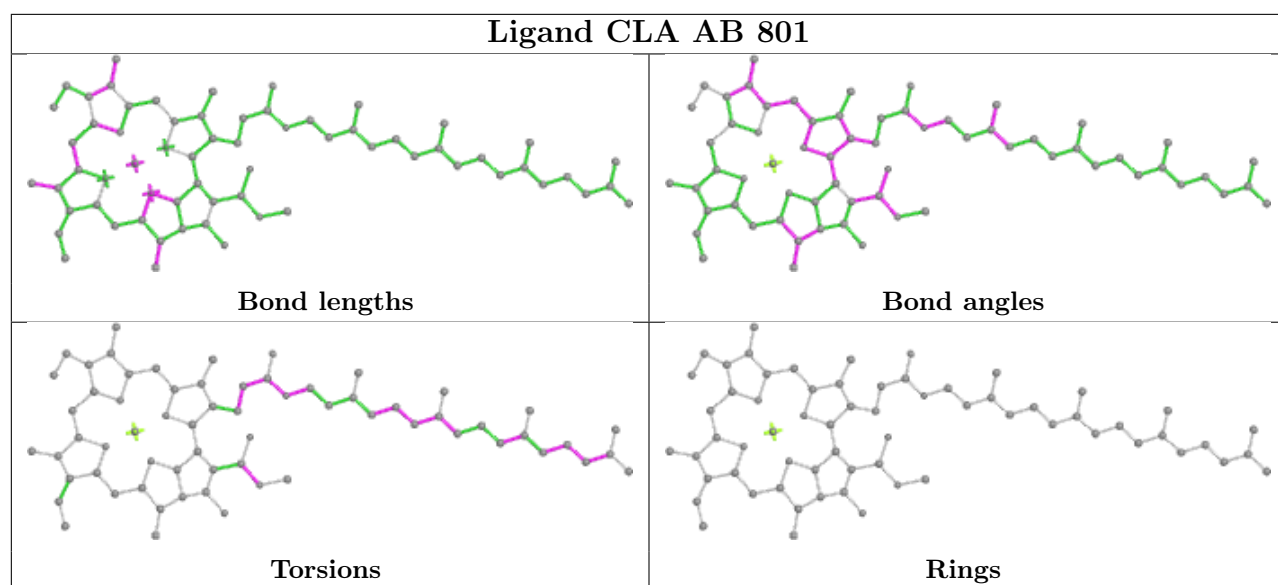
Bond angles

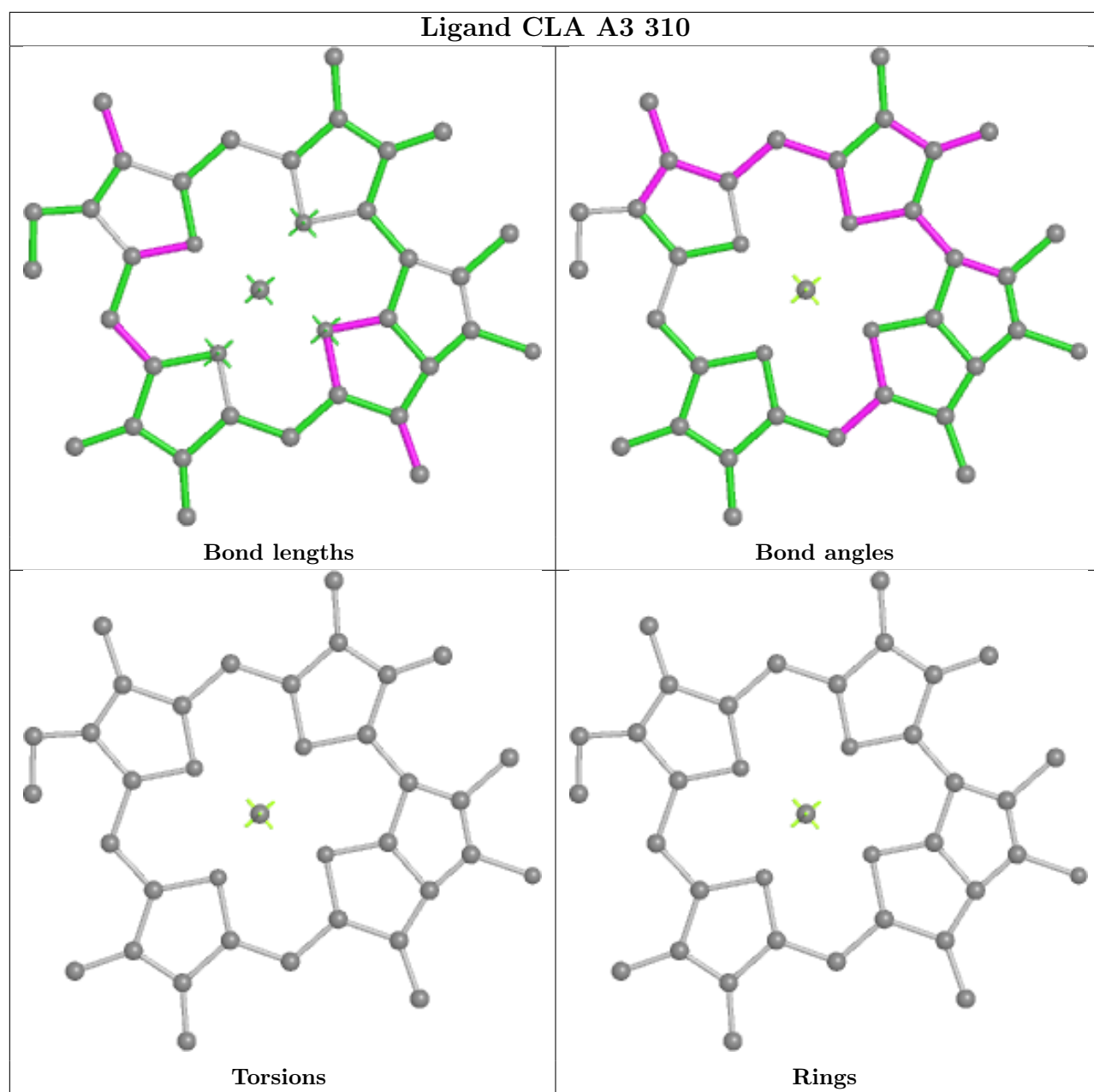


Torsions

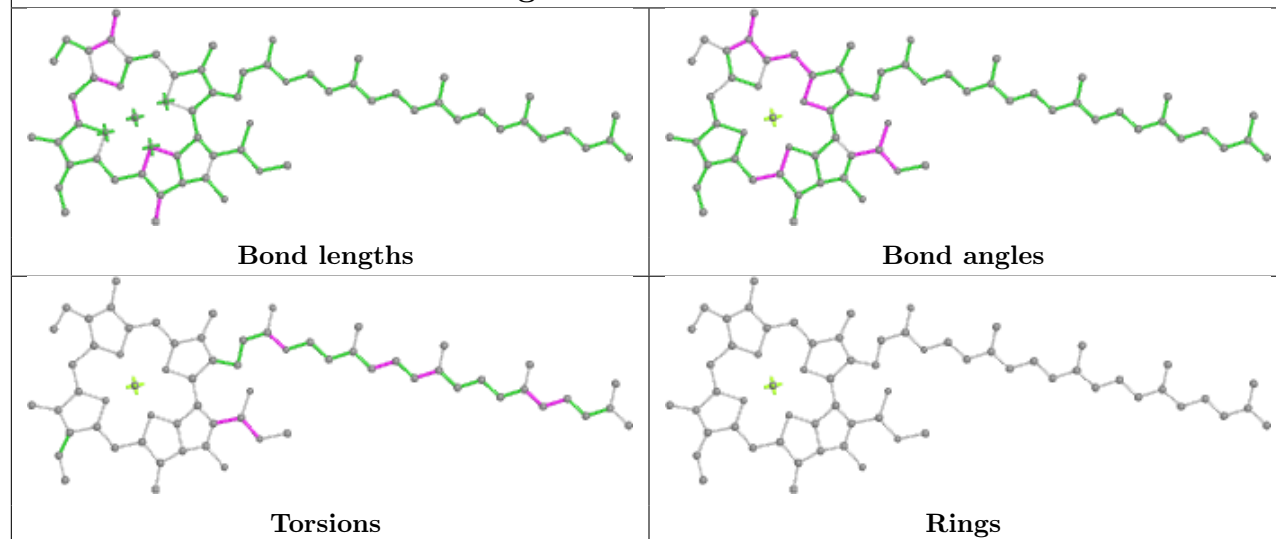


Rings

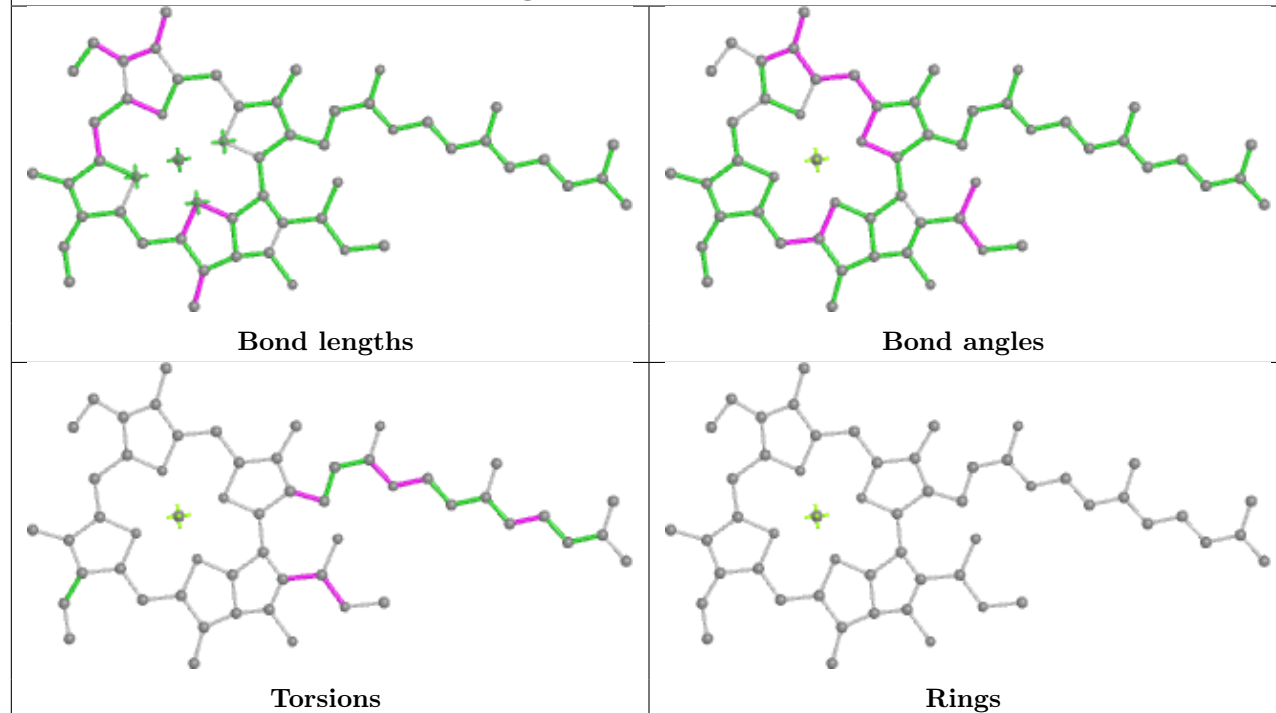


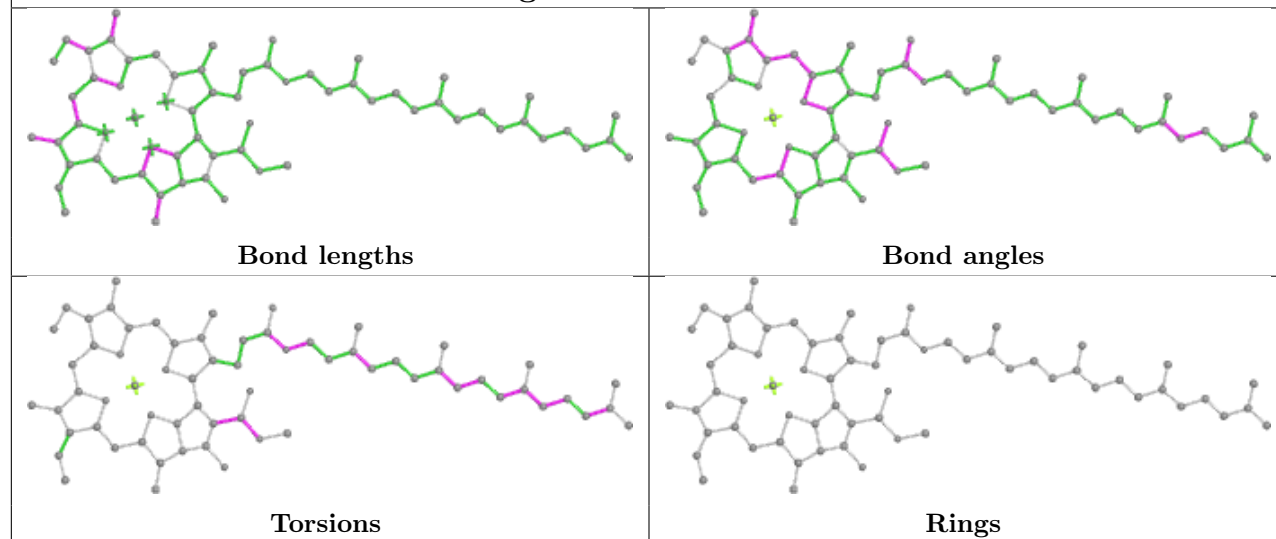
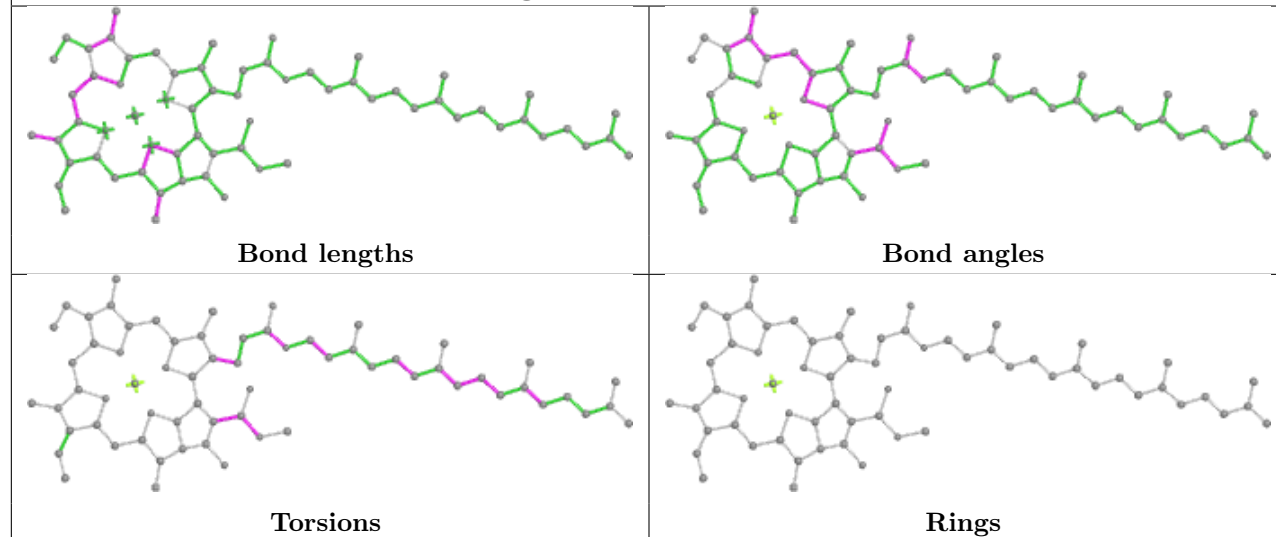


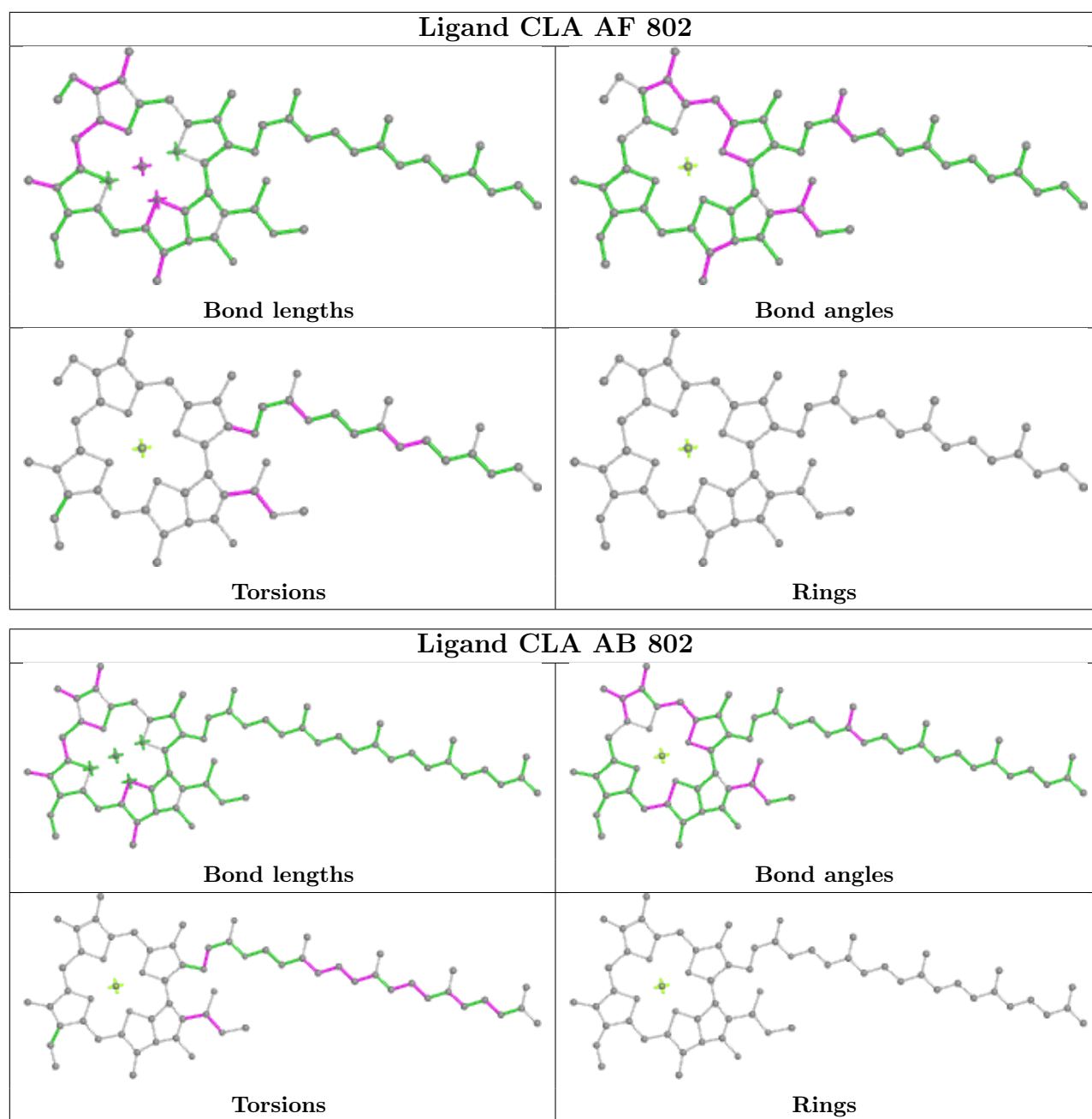
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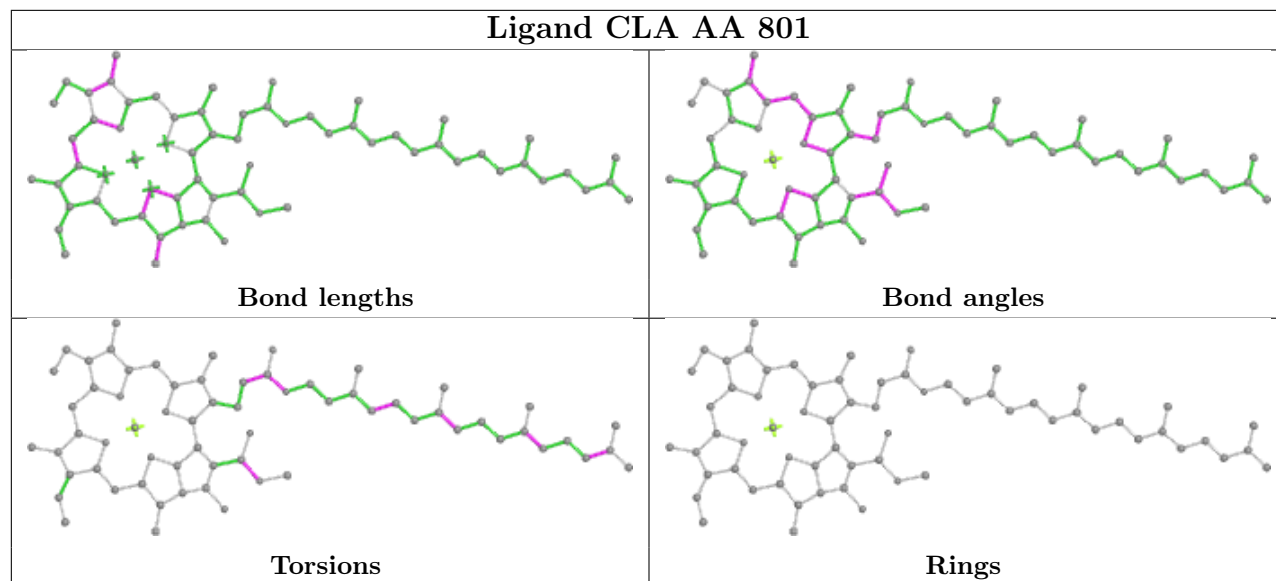
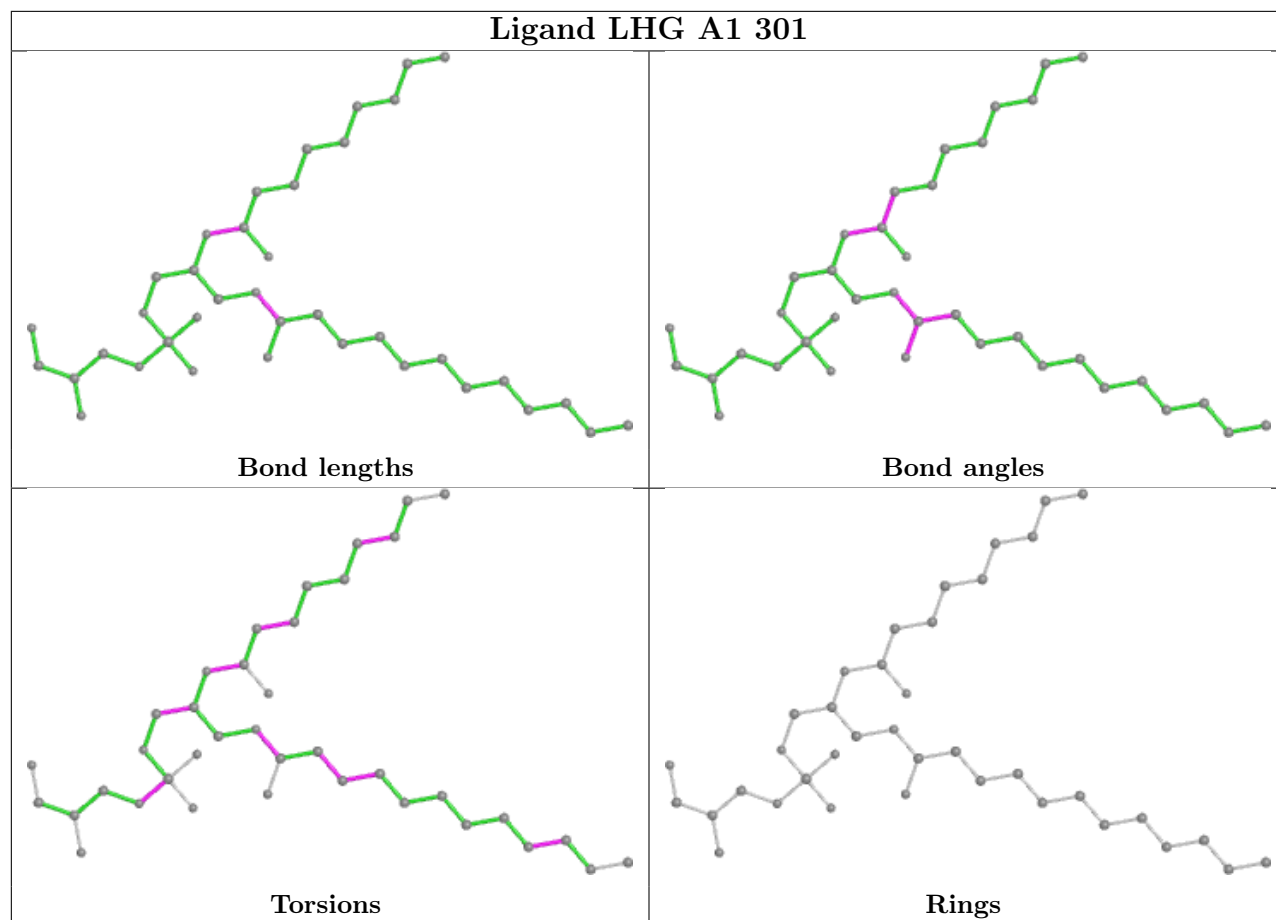


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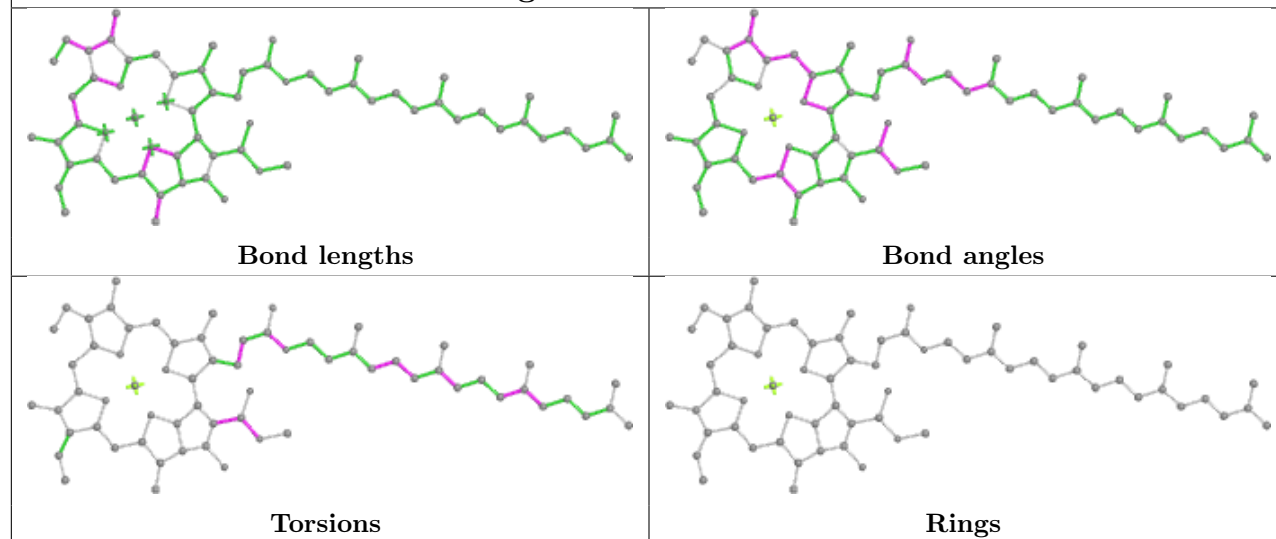


Ligand CLA AB 815**Ligand CLA AA 830**

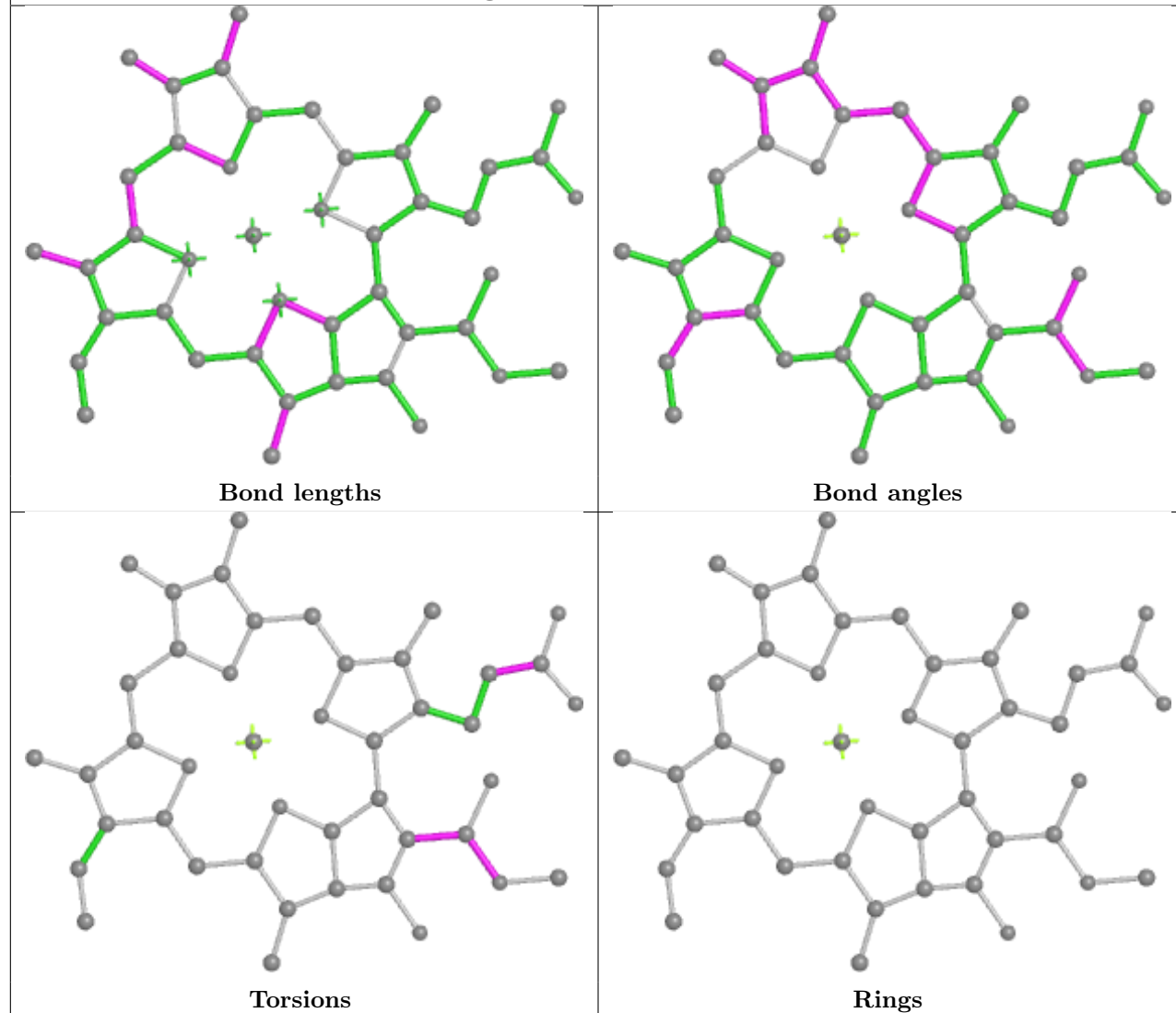


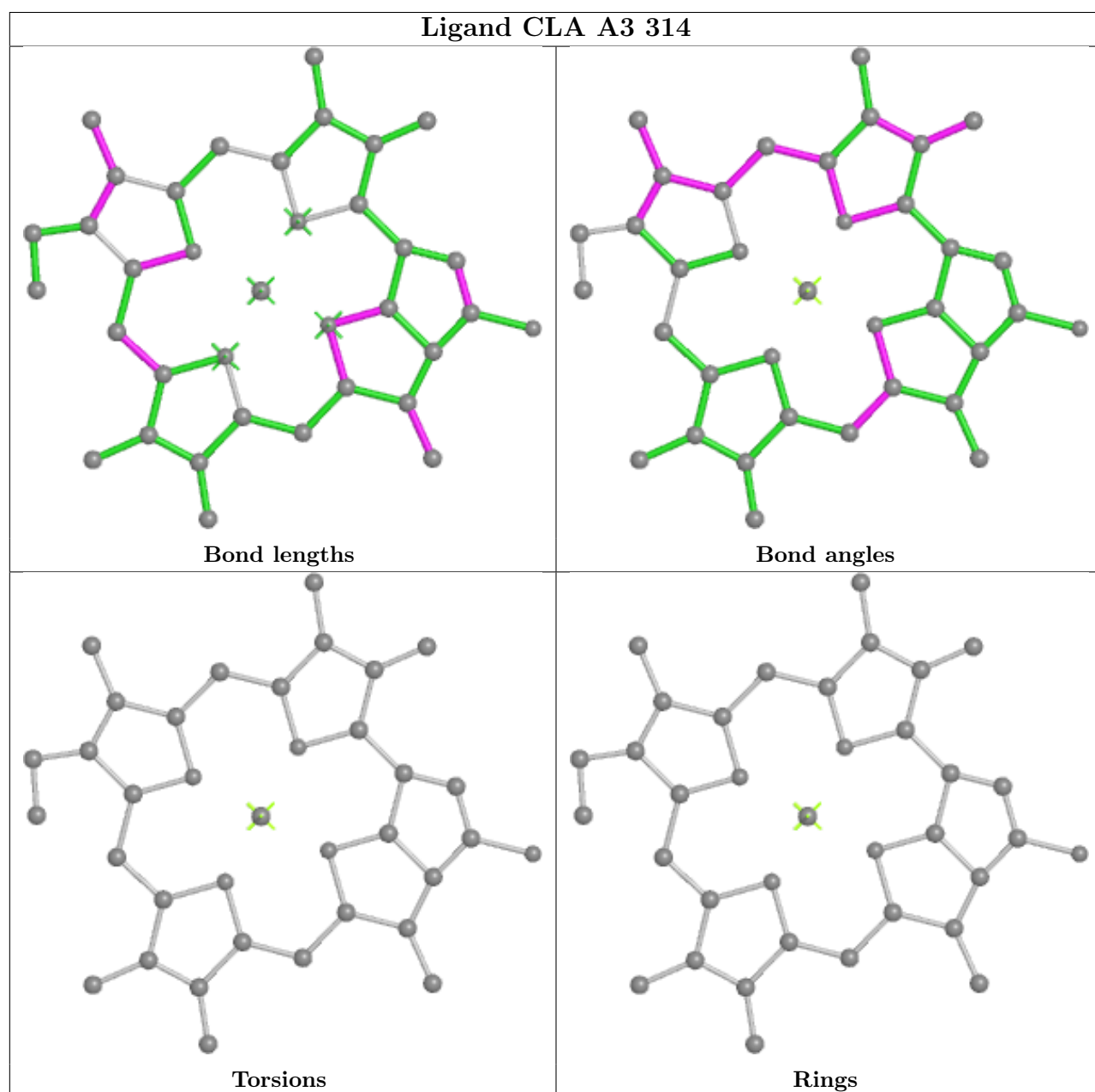
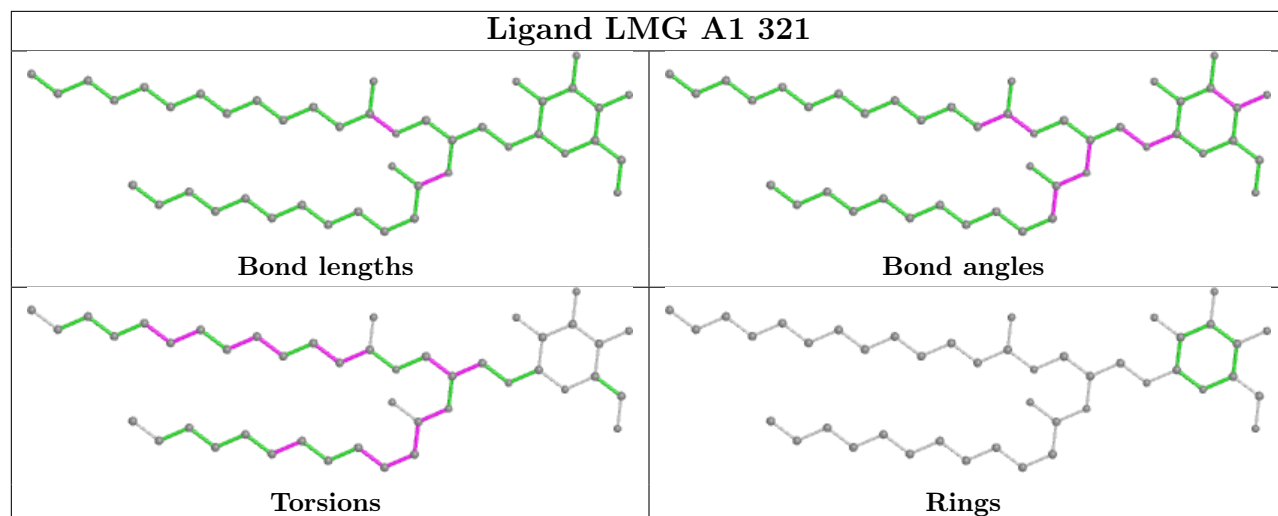


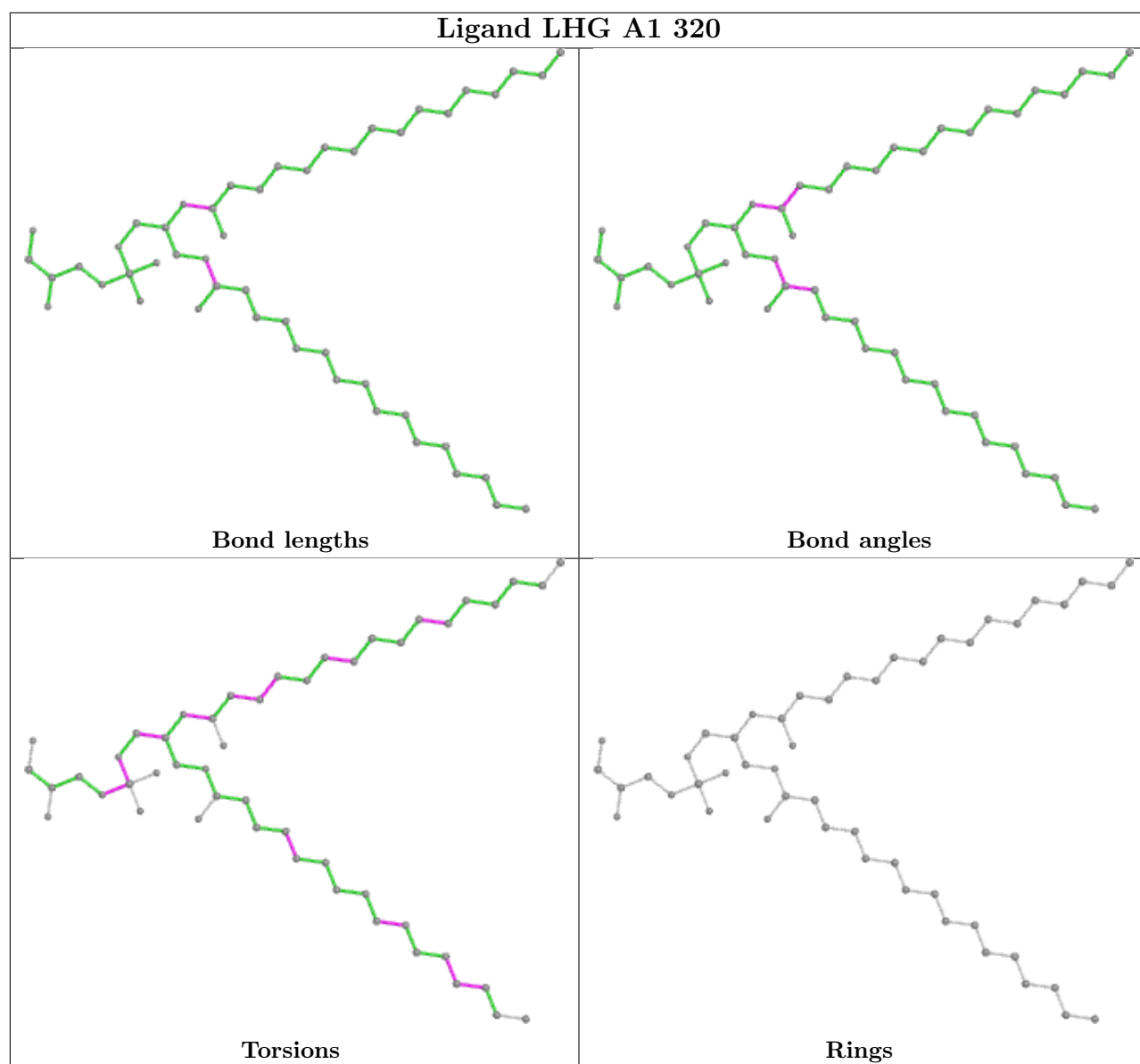
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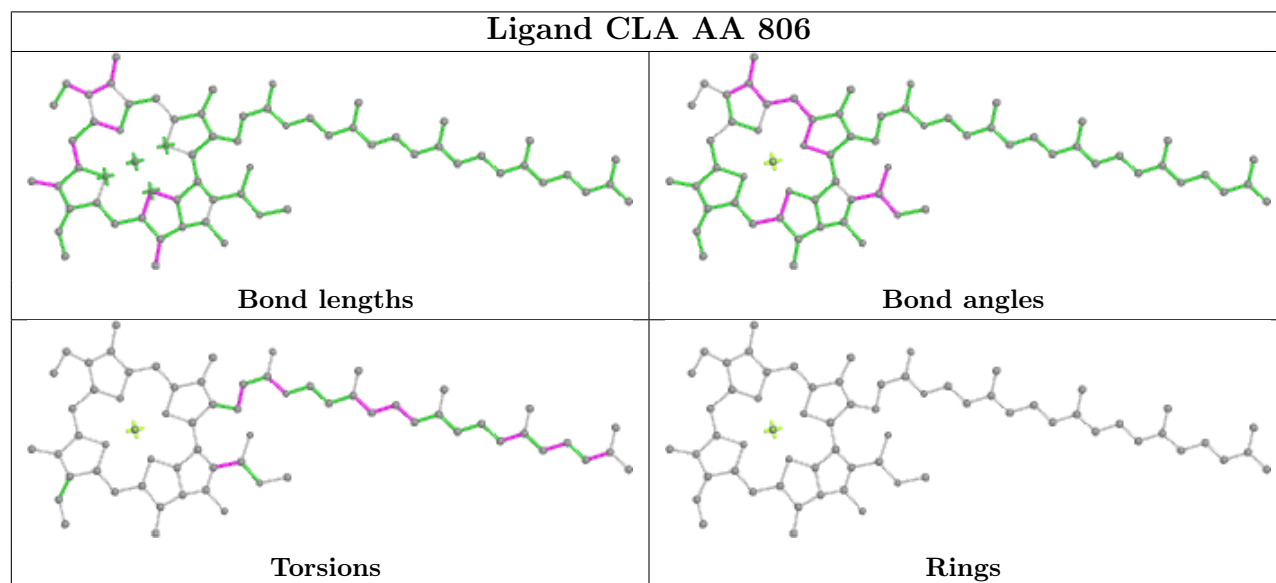
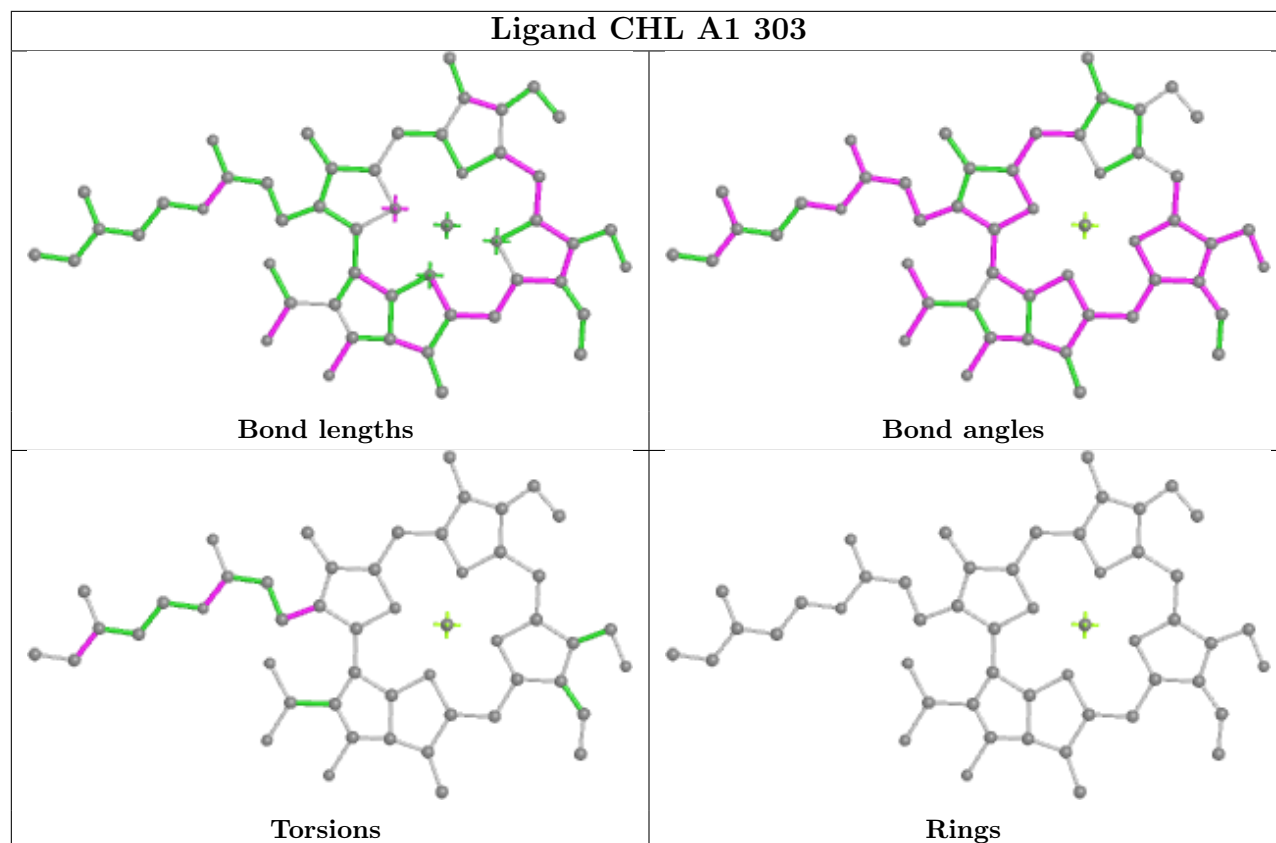


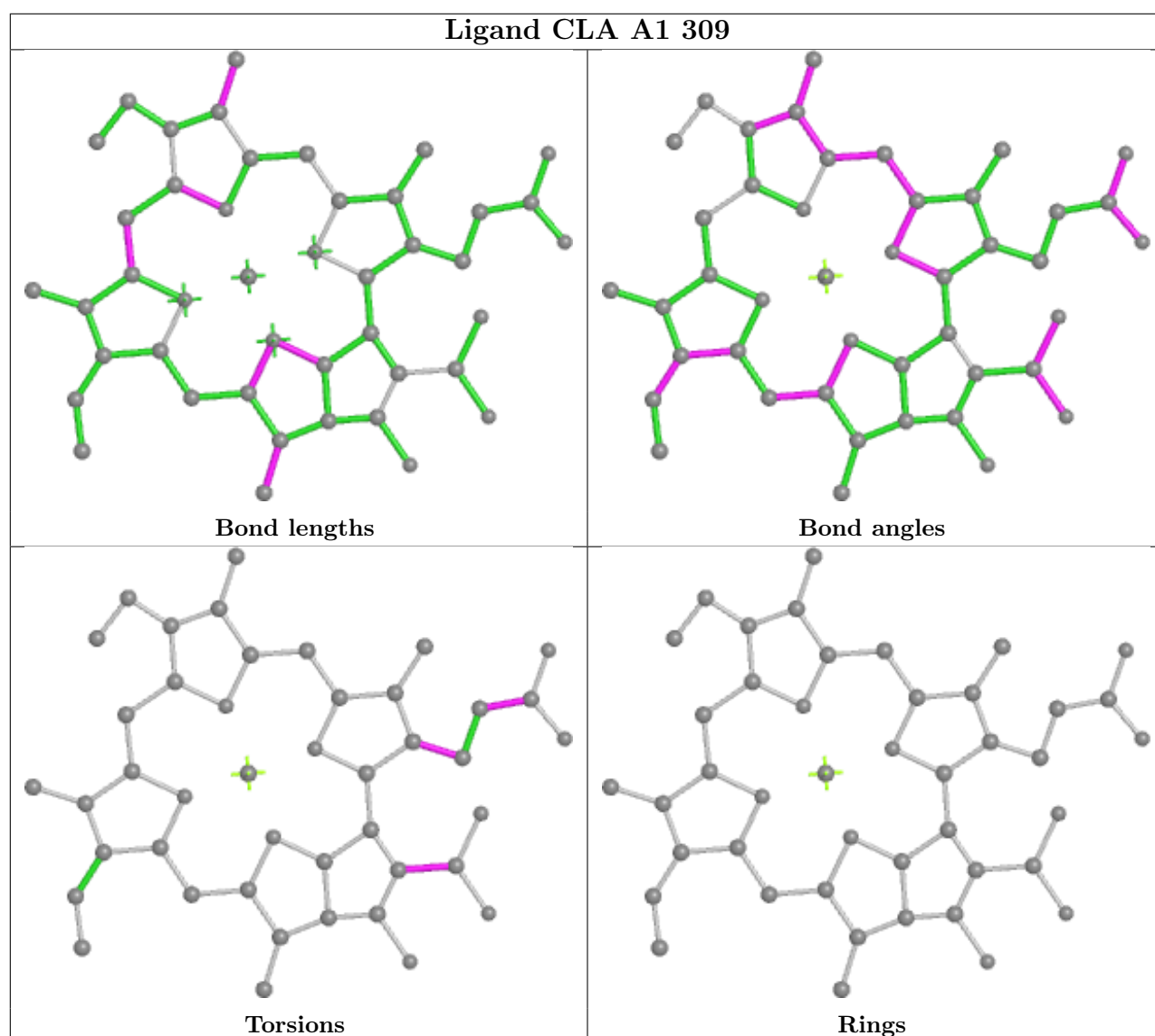
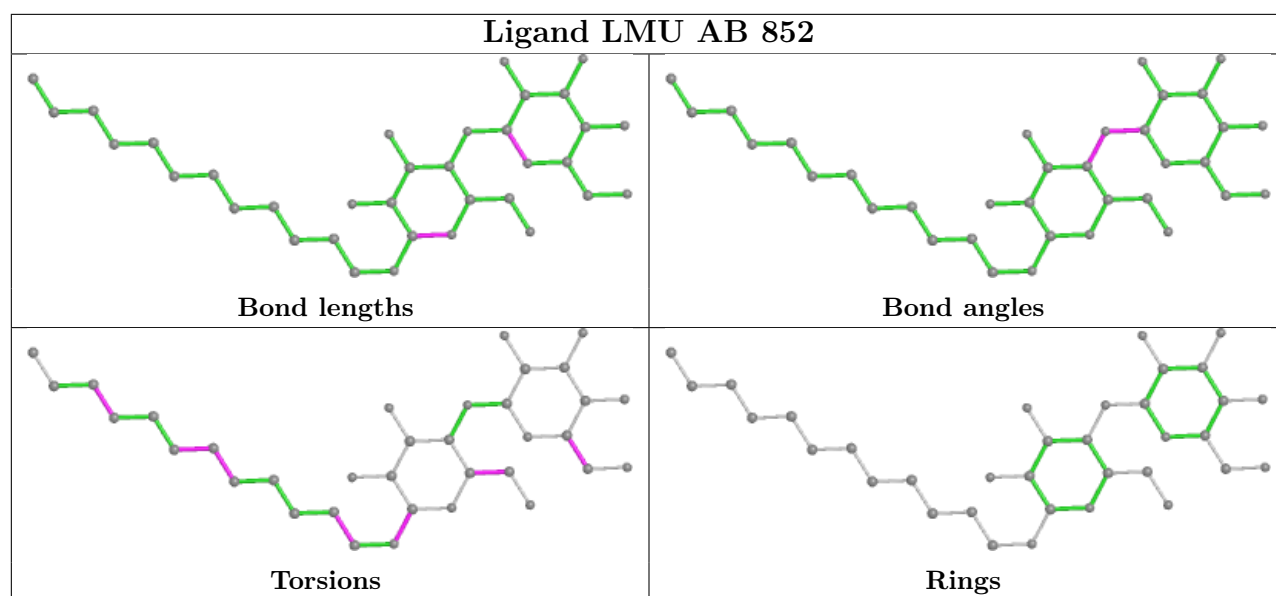
Ligand CLA A4 302



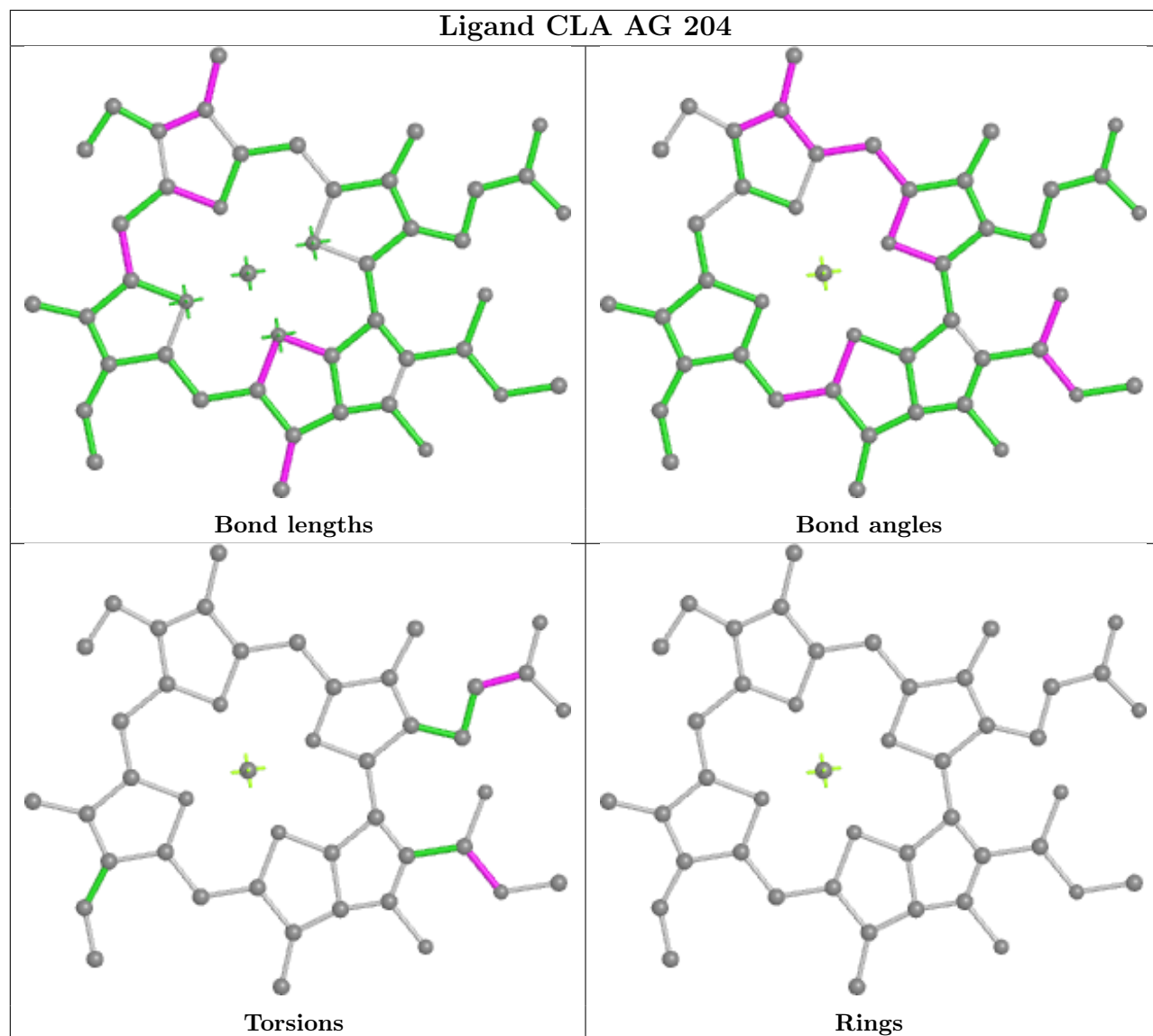




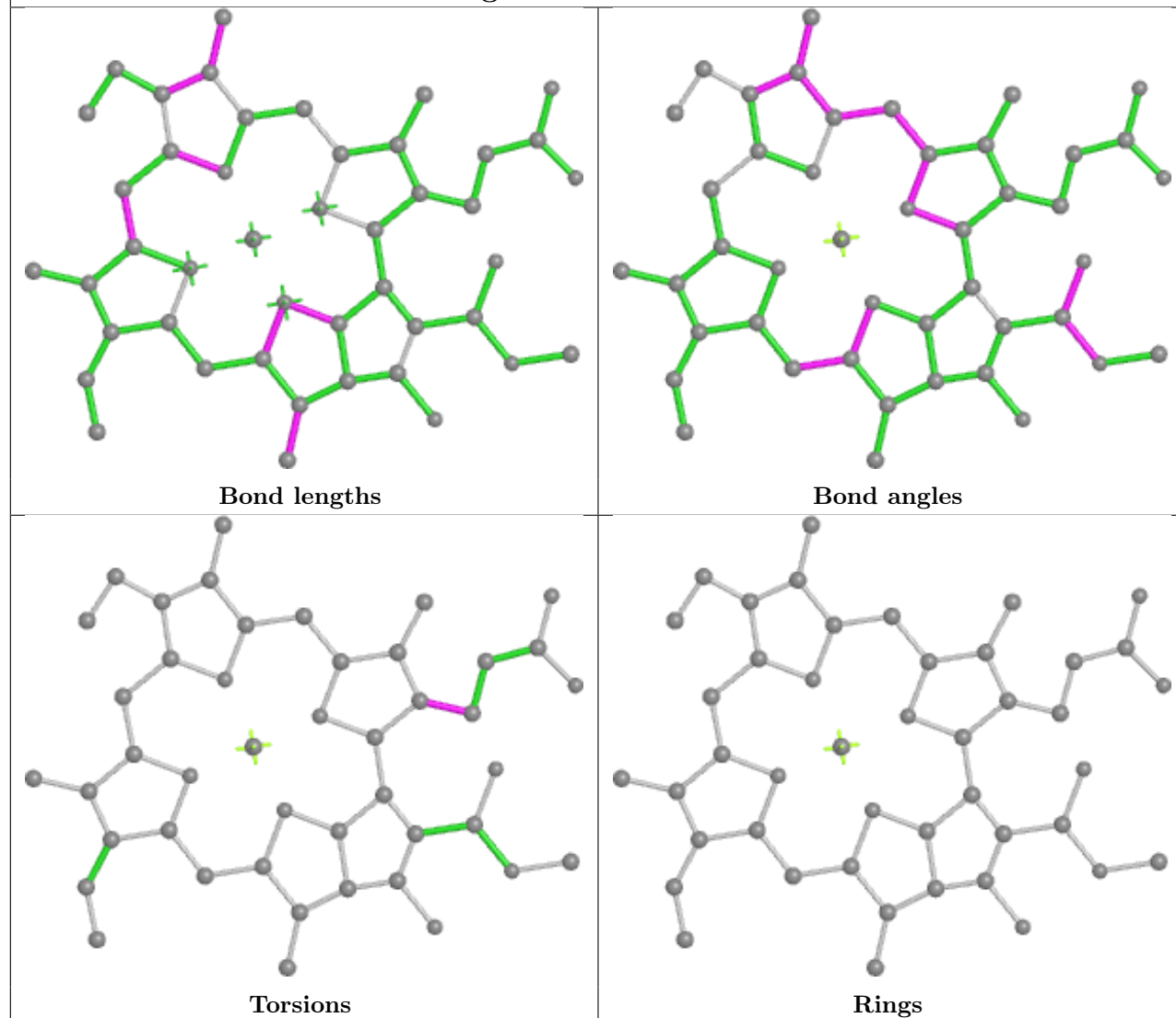




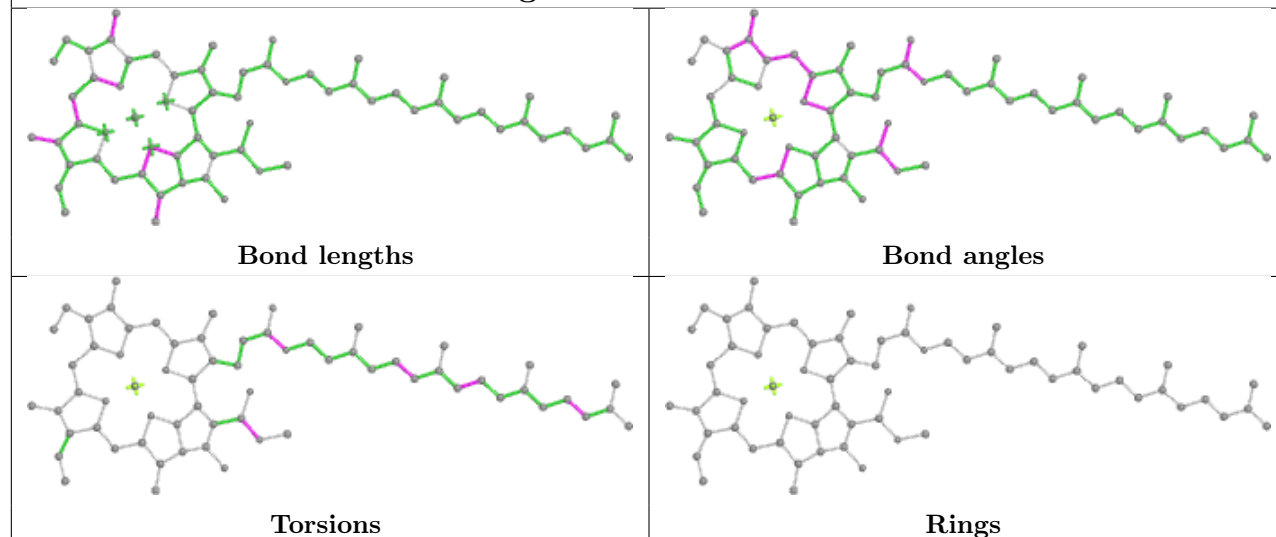
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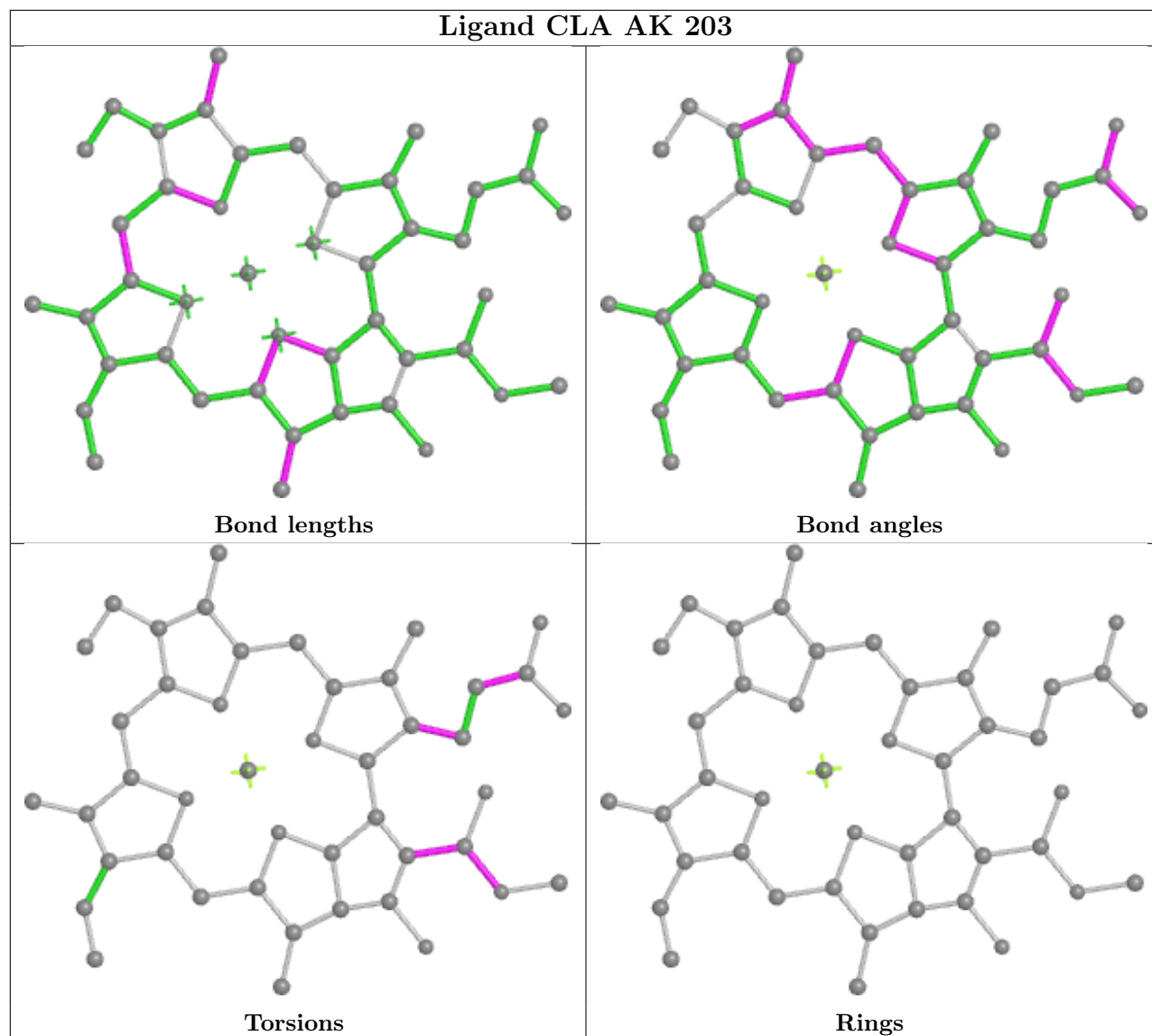
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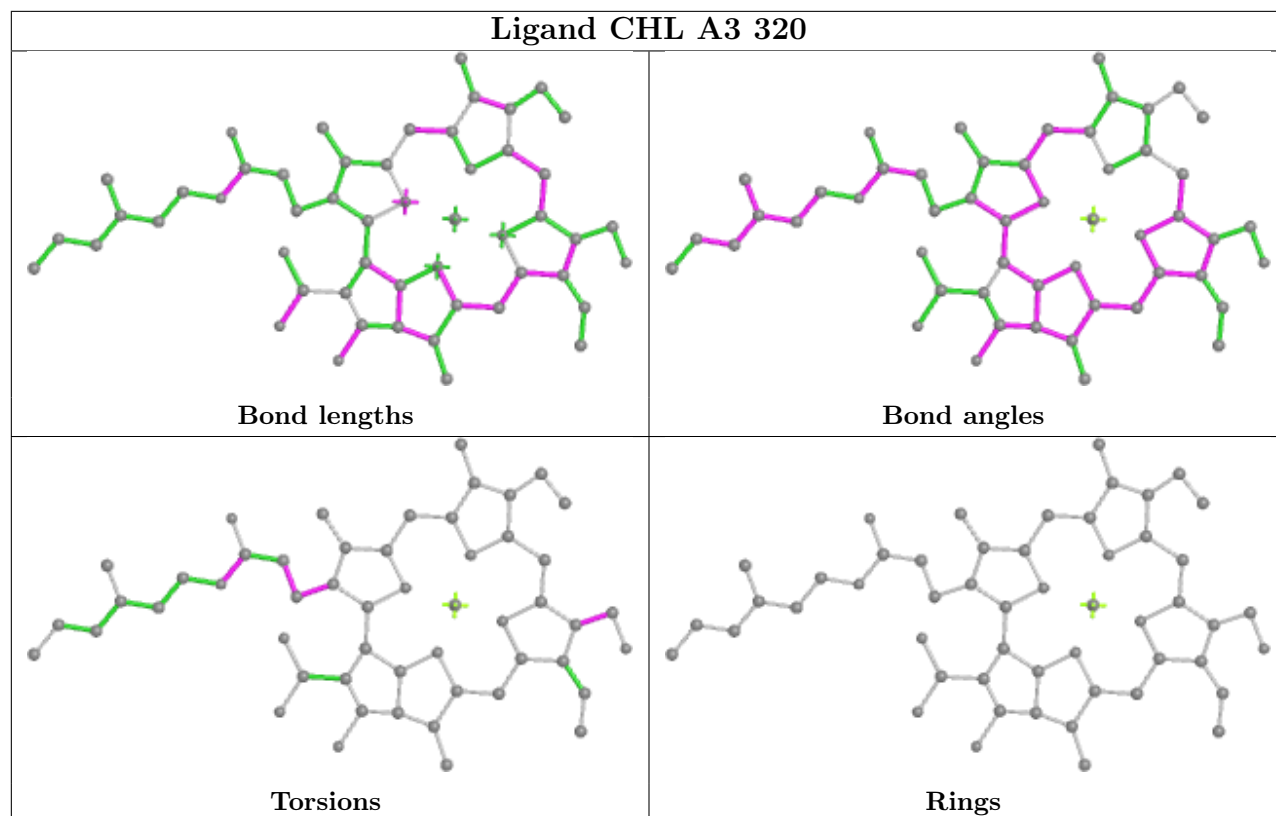


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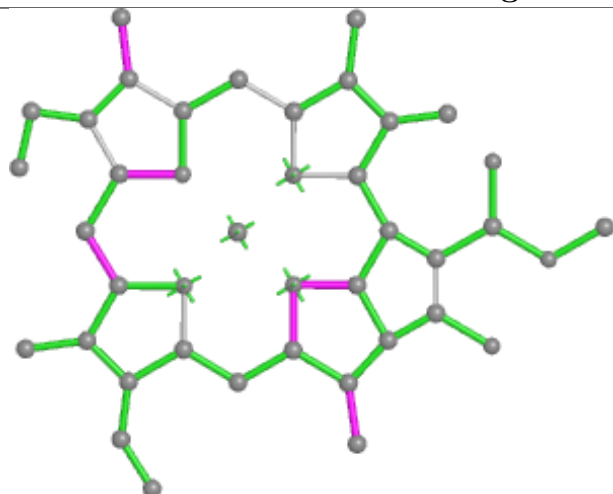


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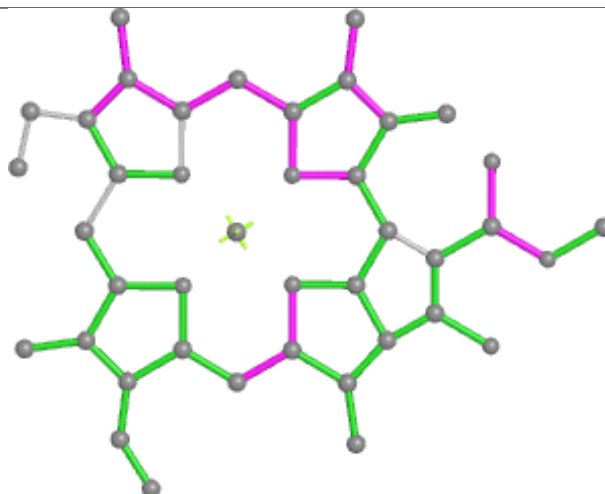




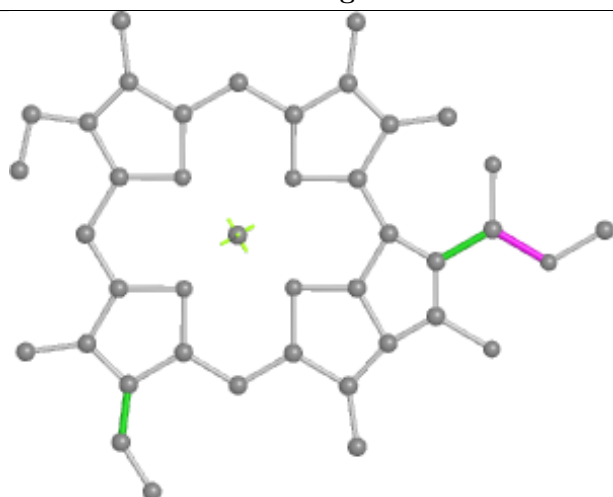
Ligand CLA AB 805



Bond lengths



Bond angles

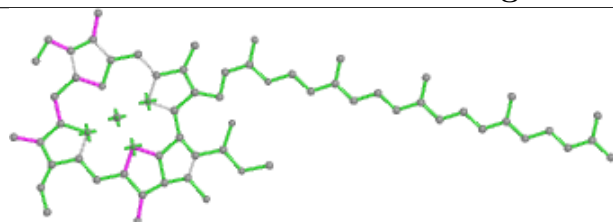


Torsions

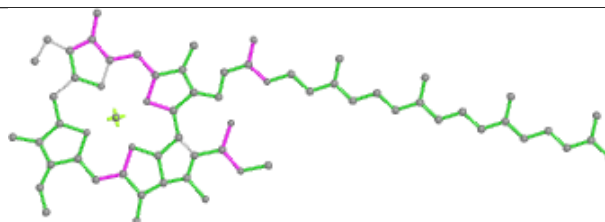


Rings

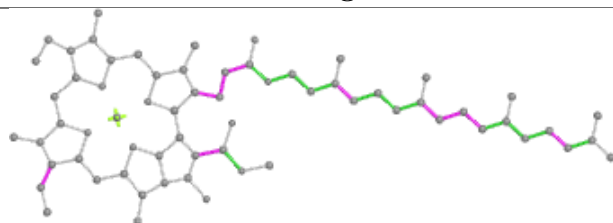
Ligand CLA AB 828



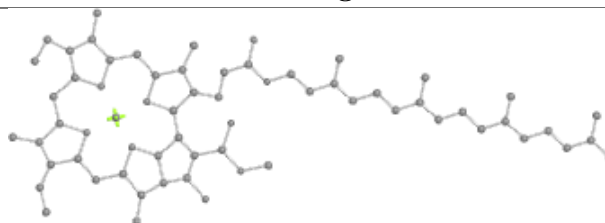
Bond lengths



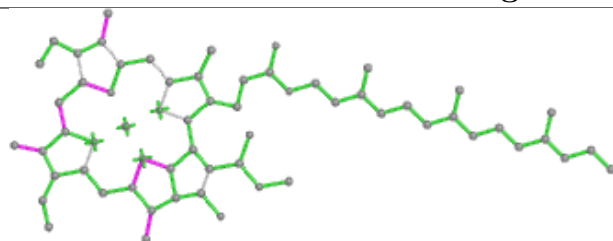
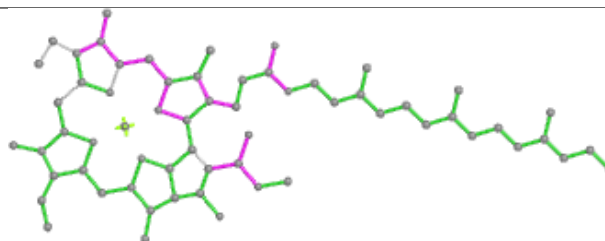
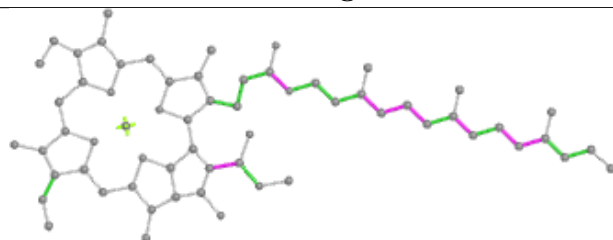
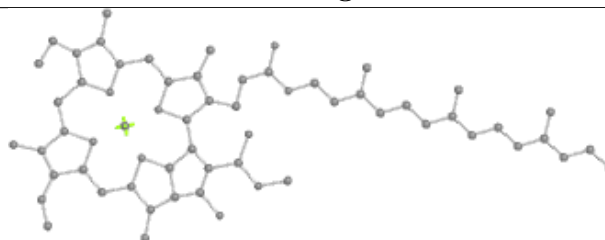
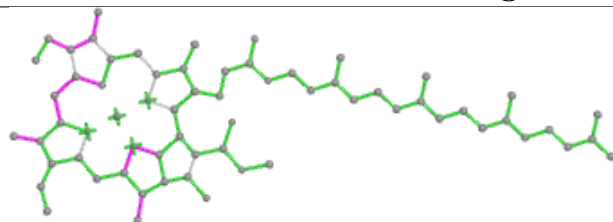
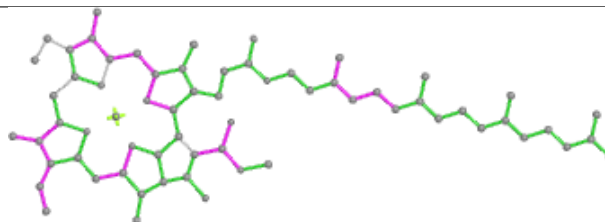
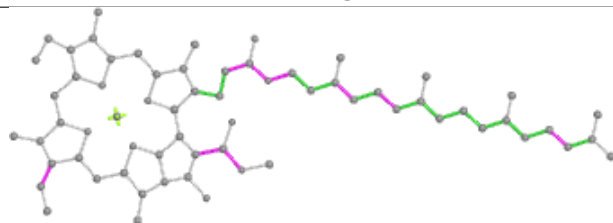
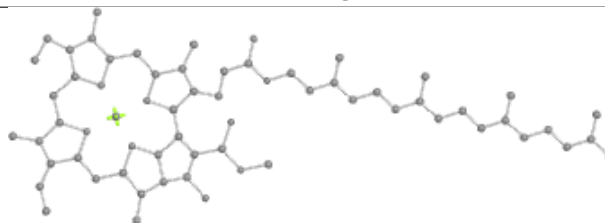
Bond angles



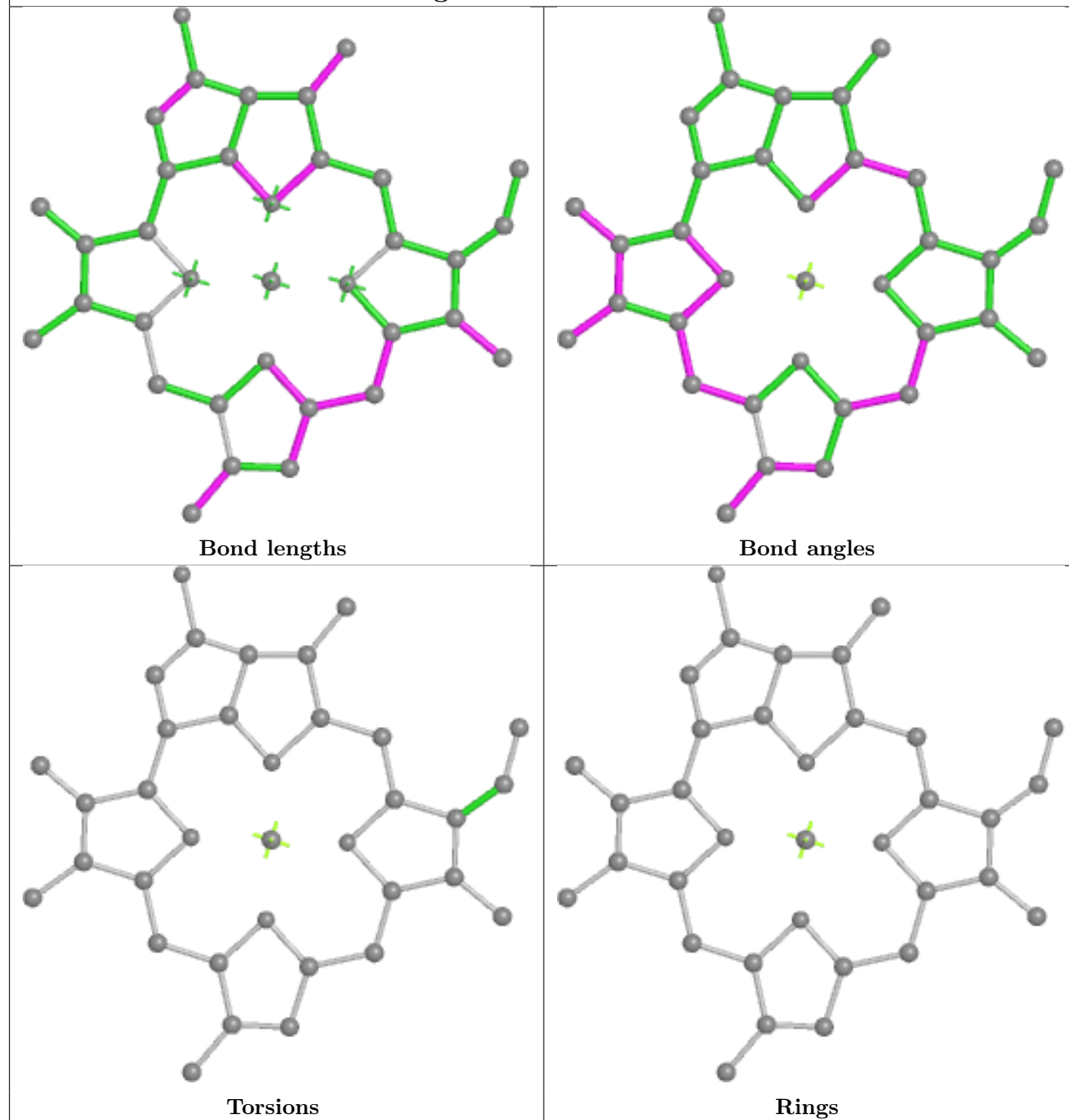
Torsions



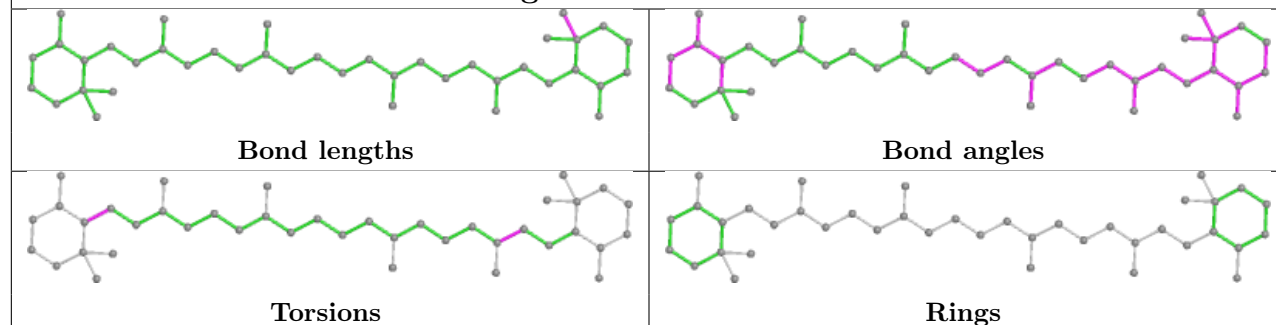
Rings

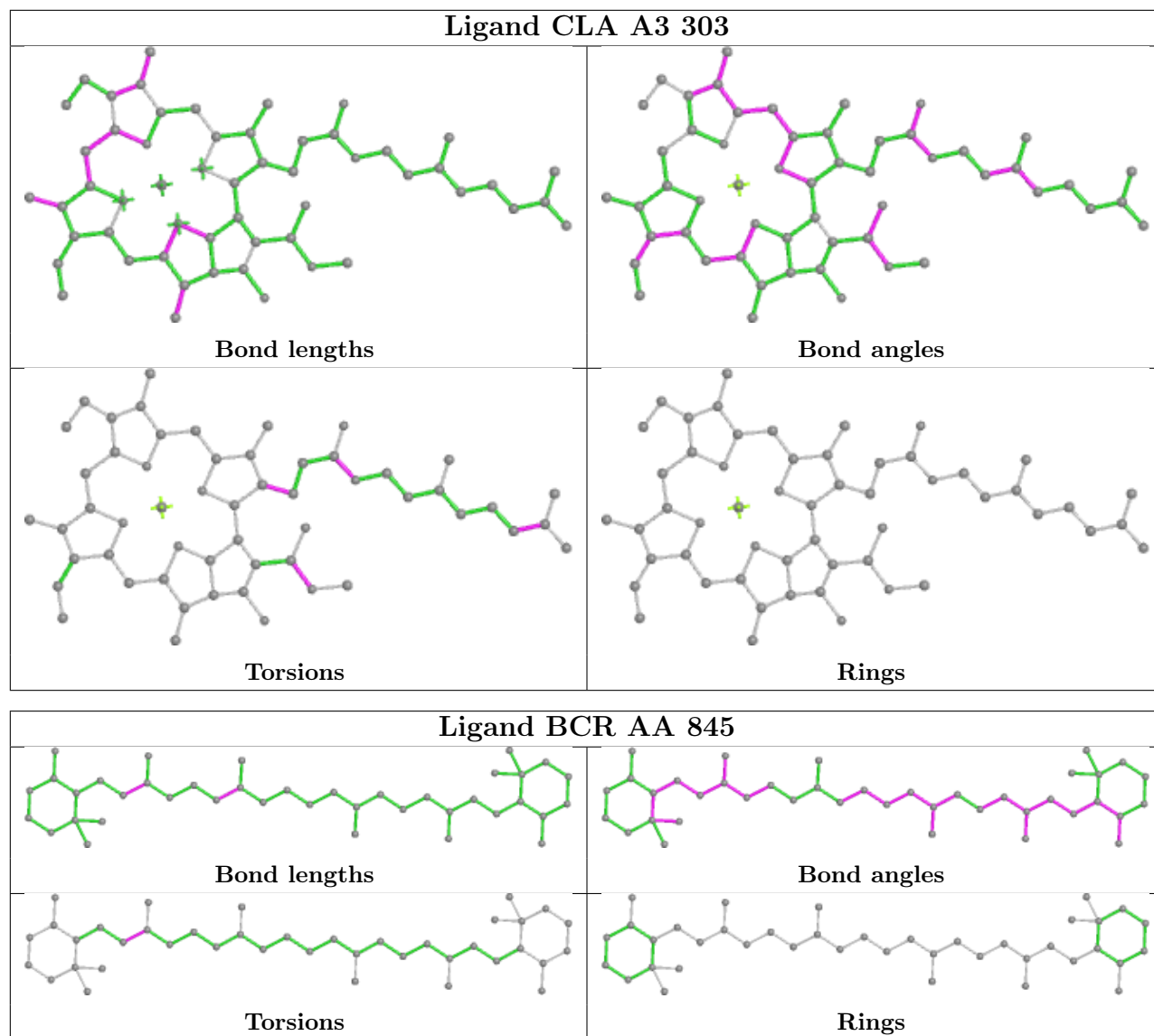
Ligand CLA AB 827**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA AA 834****Bond lengths****Bond angles****Torsions****Rings**

Ligand CLA AK 201

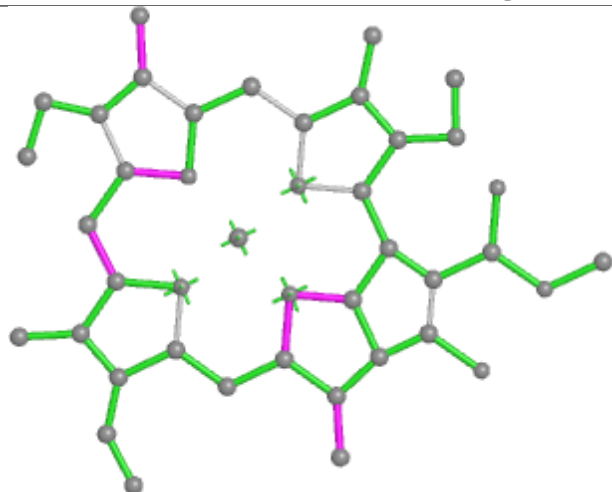


Ligand BCR A3 318

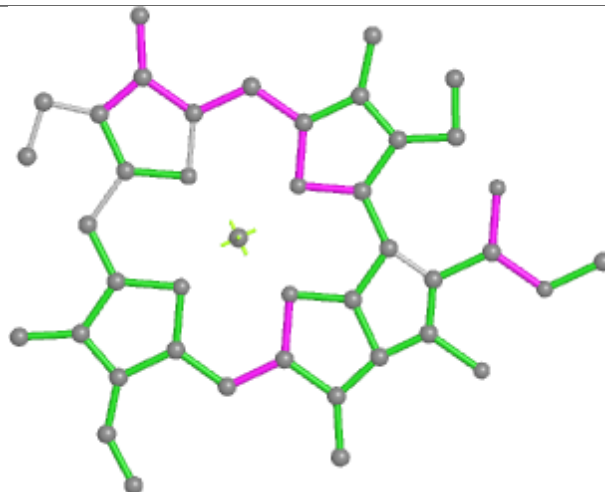




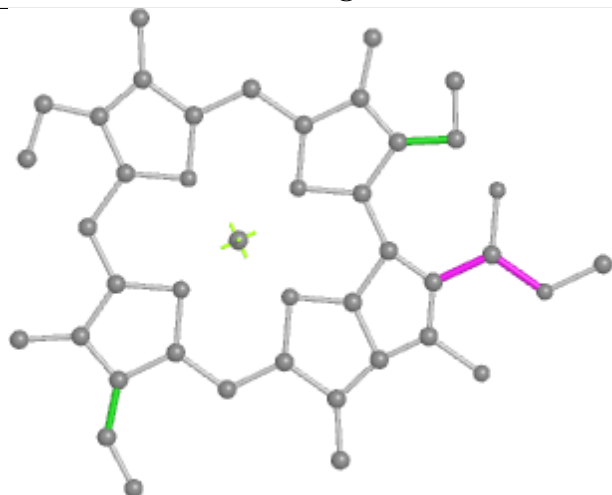
Ligand CLA AG 203



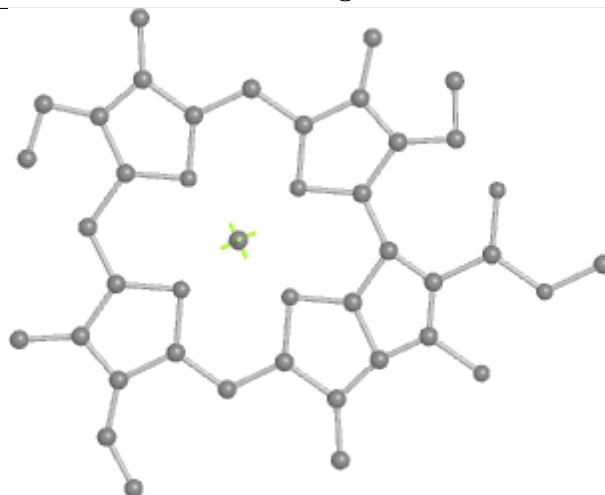
Bond lengths



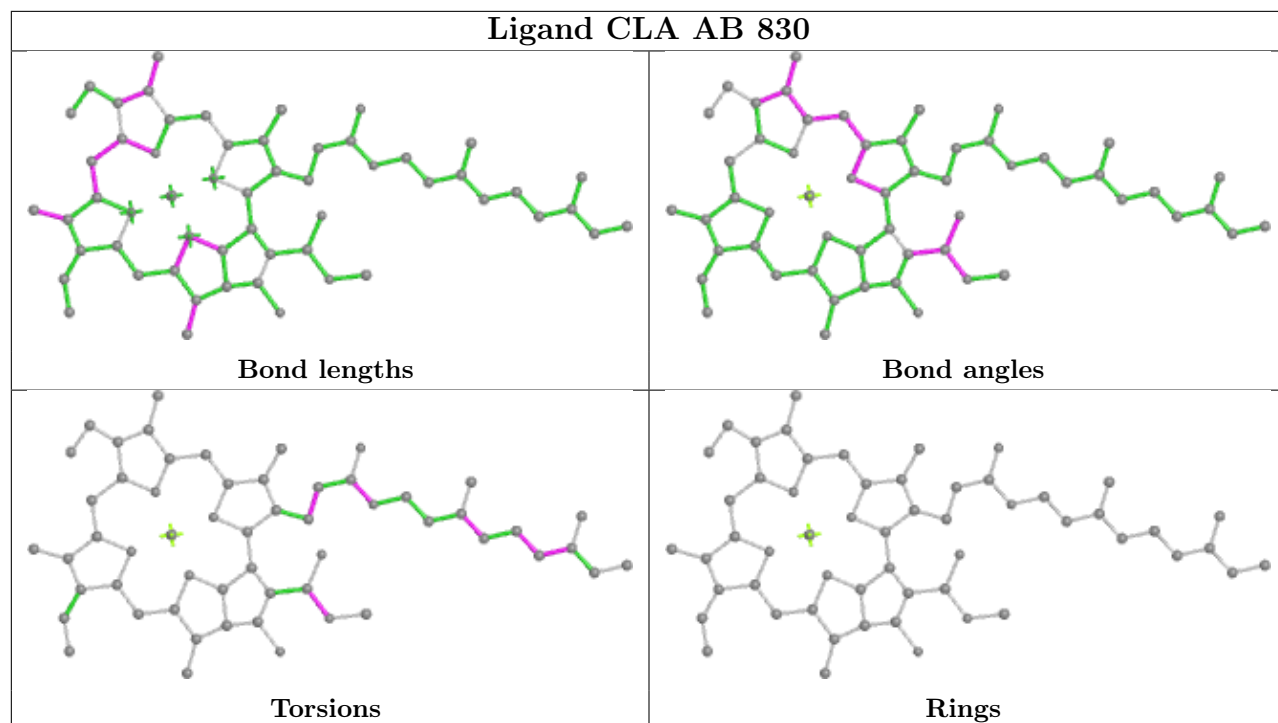
Bond angles

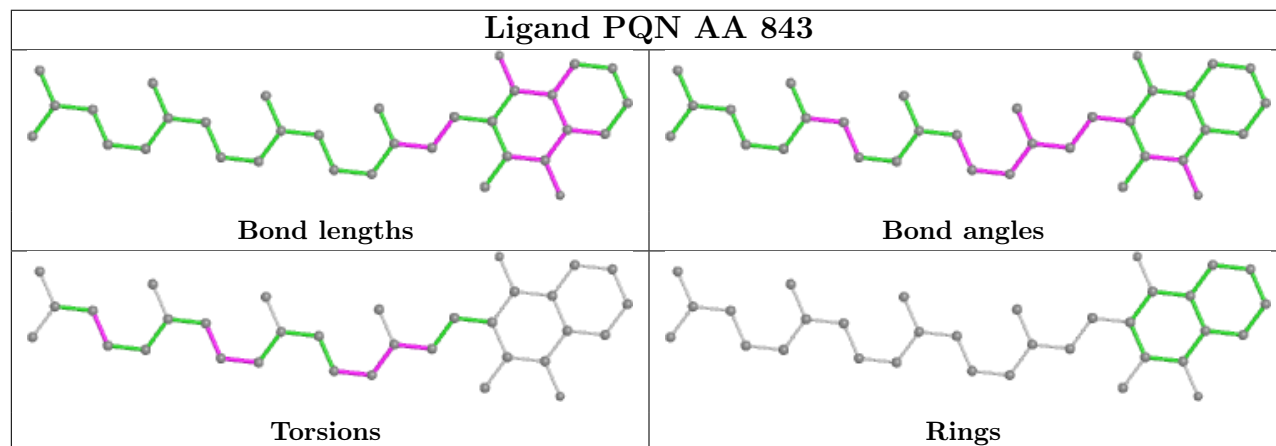
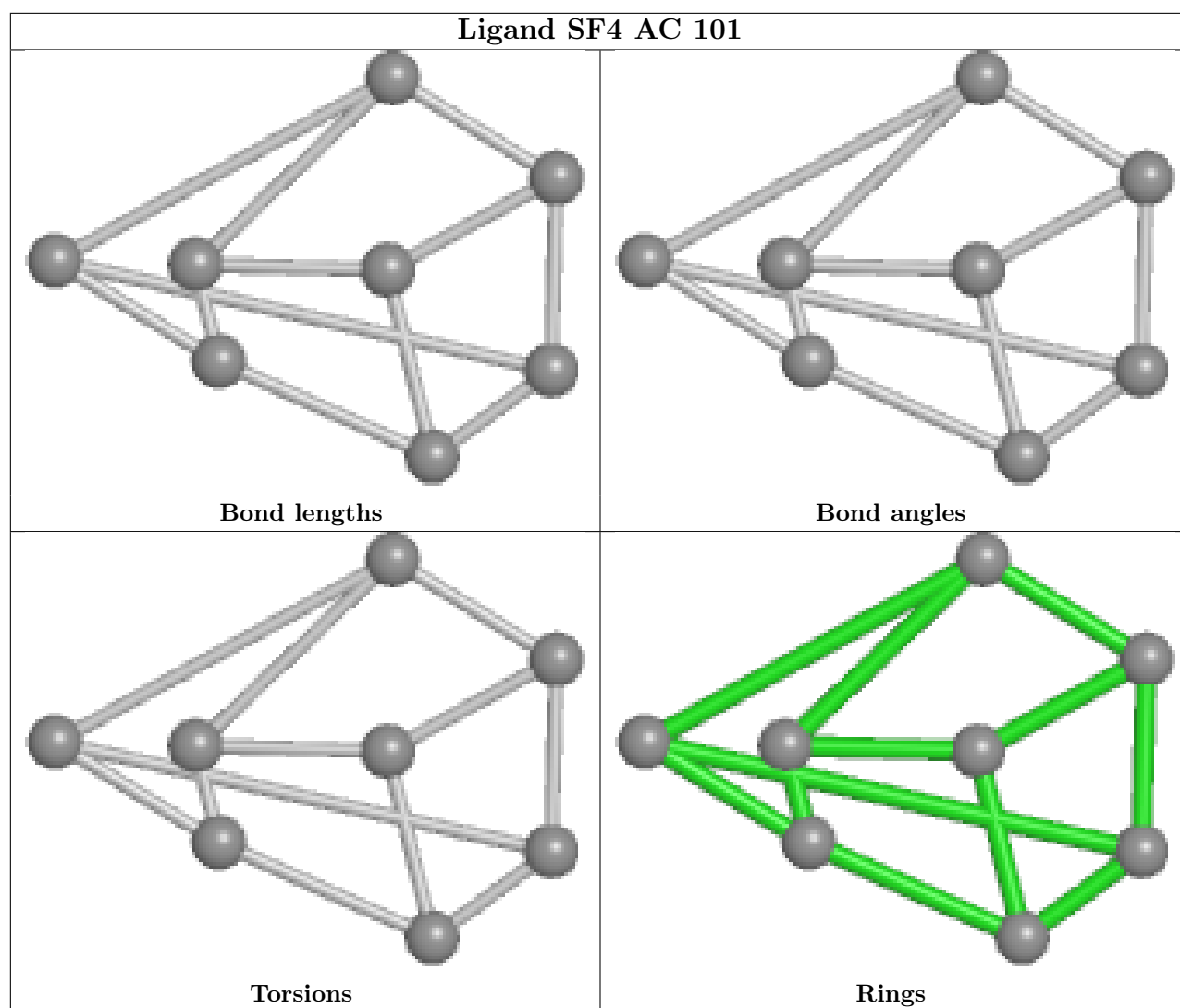


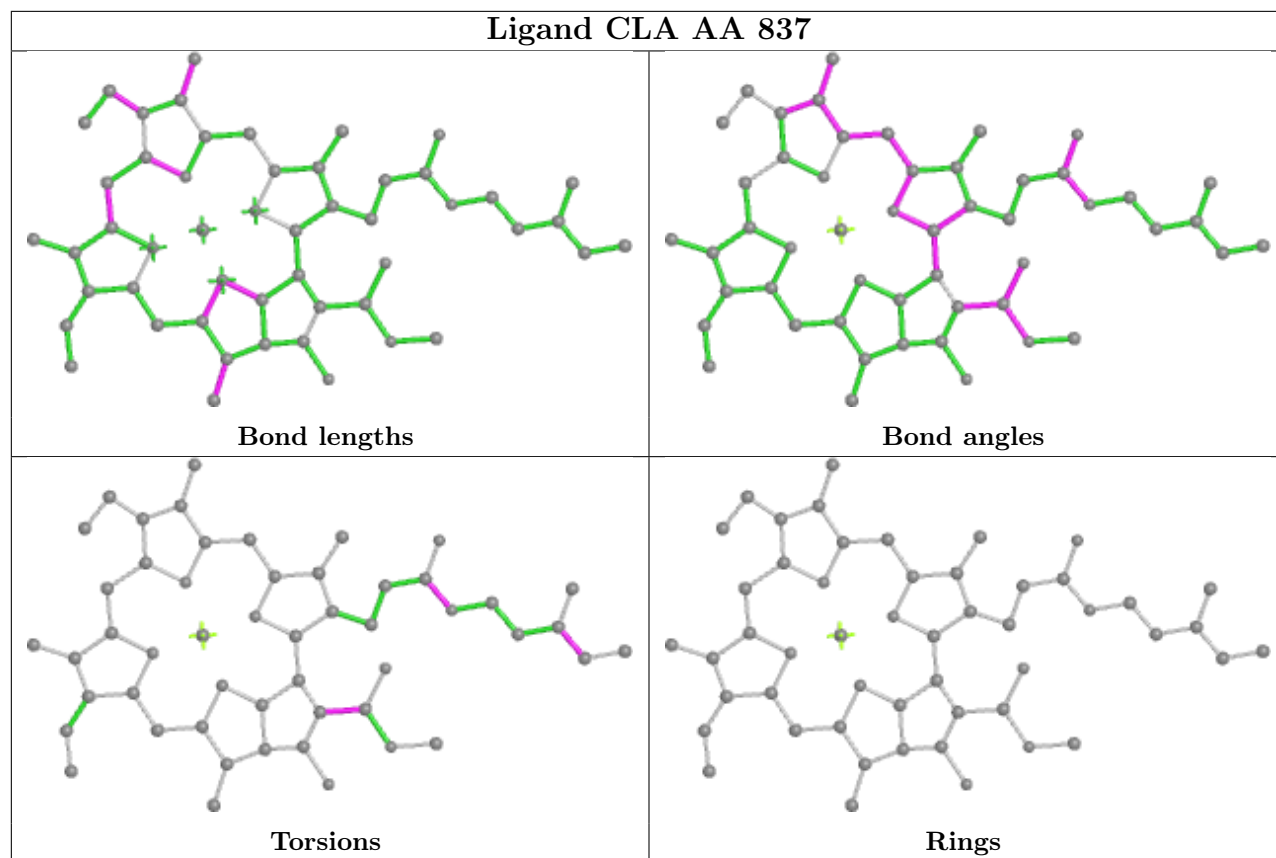
Torsions



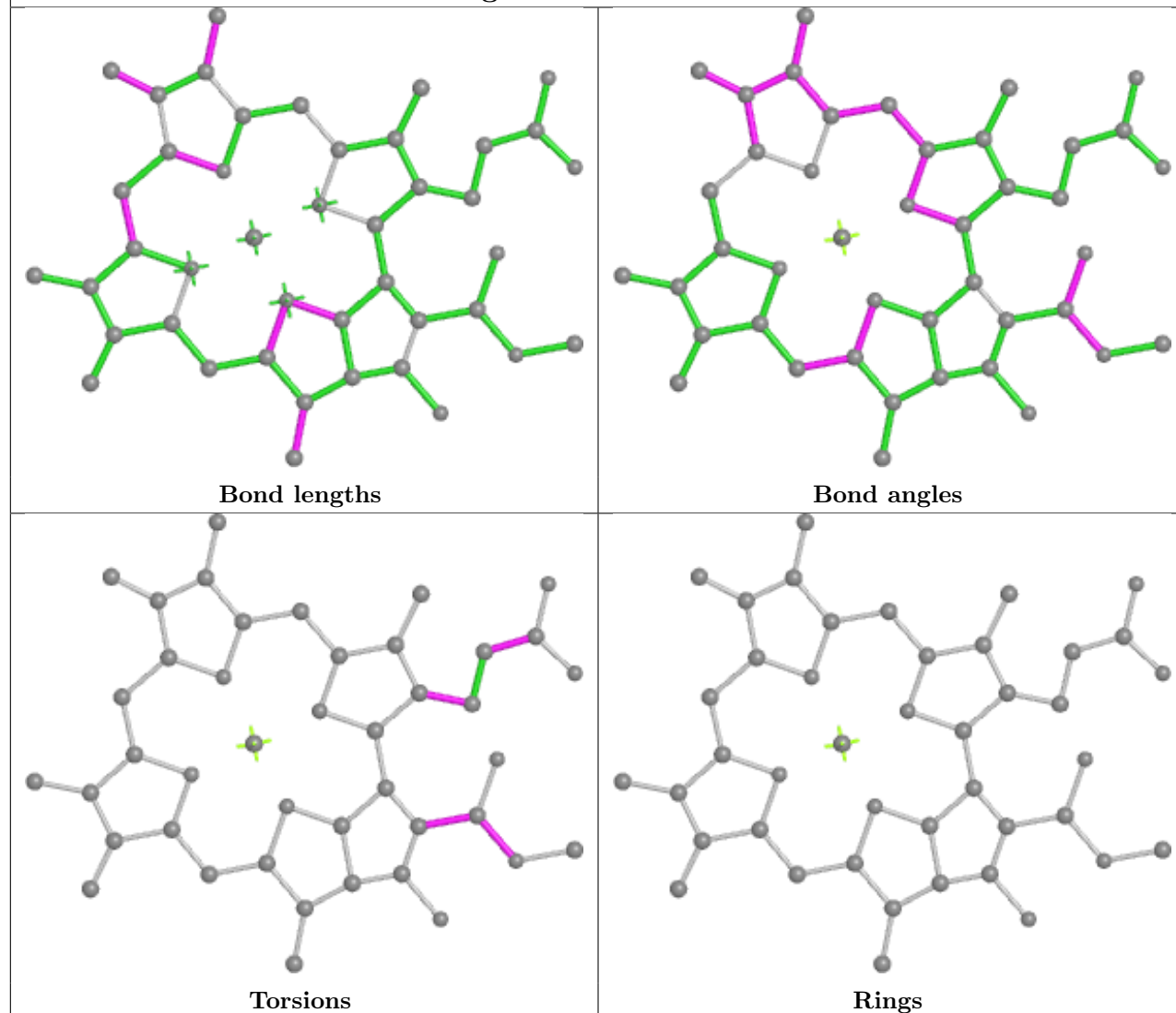
Rings



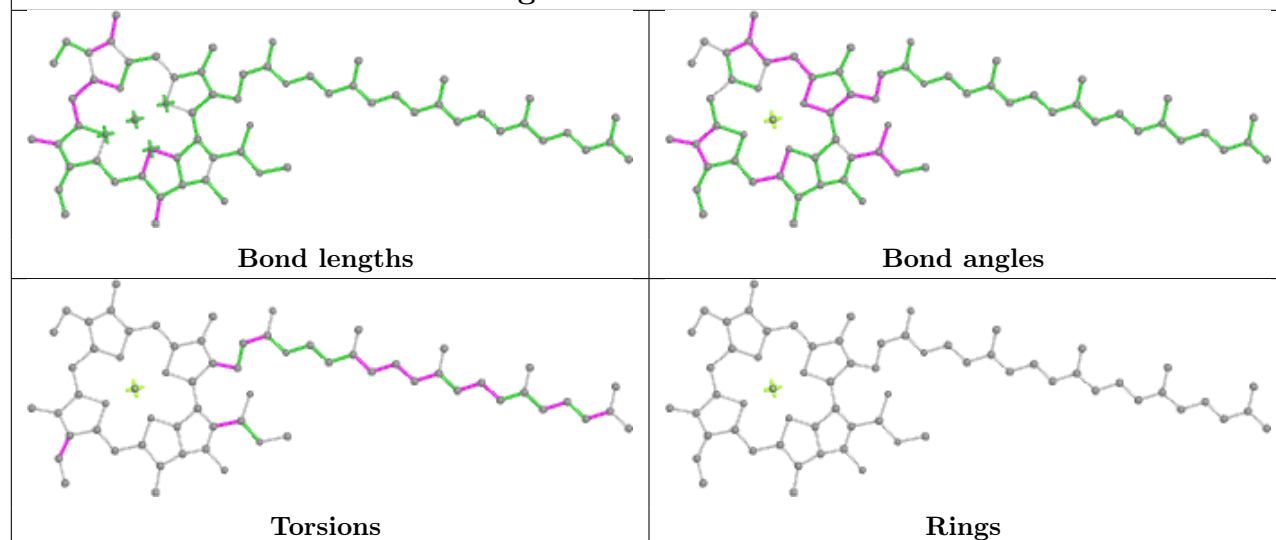


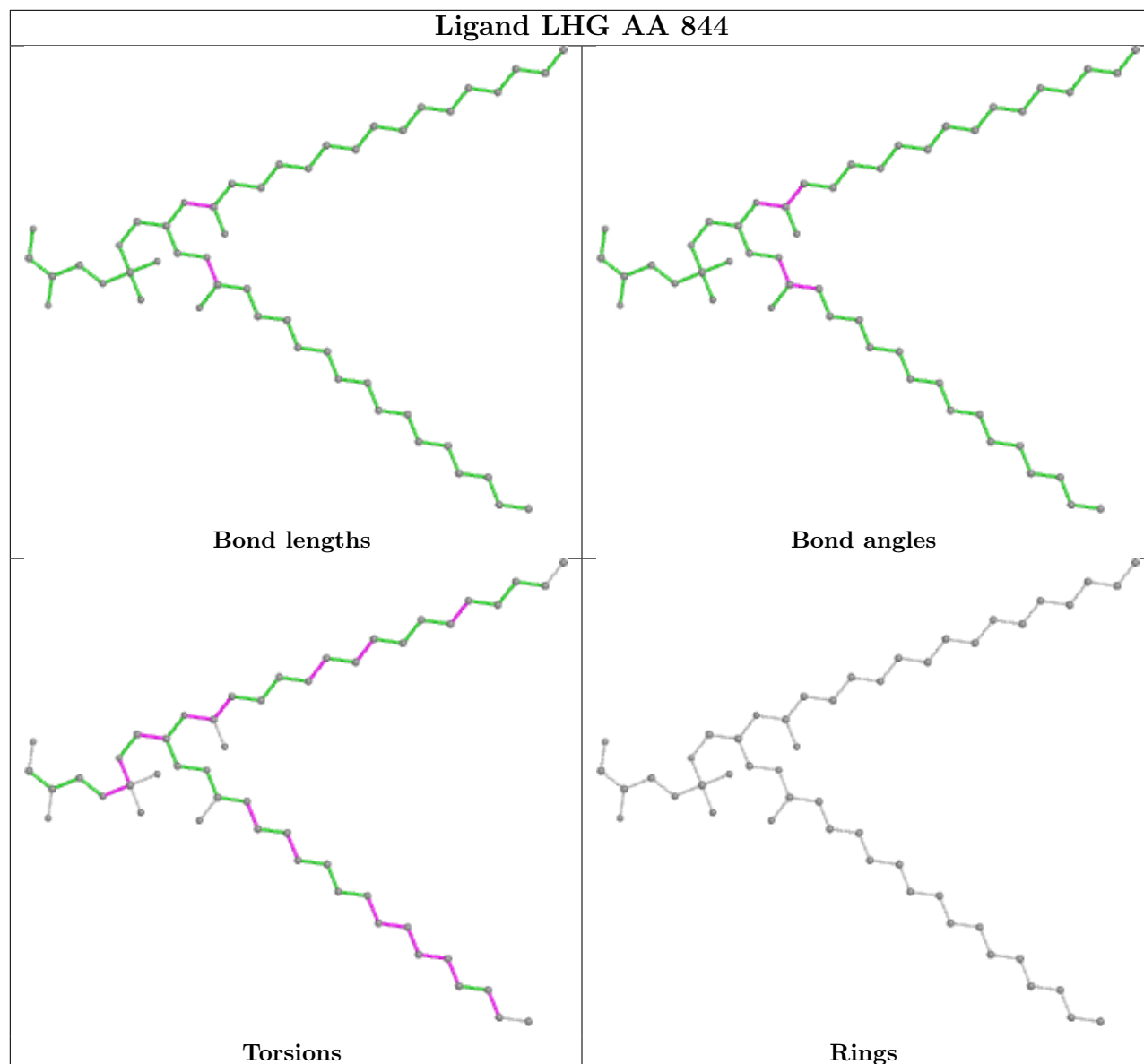
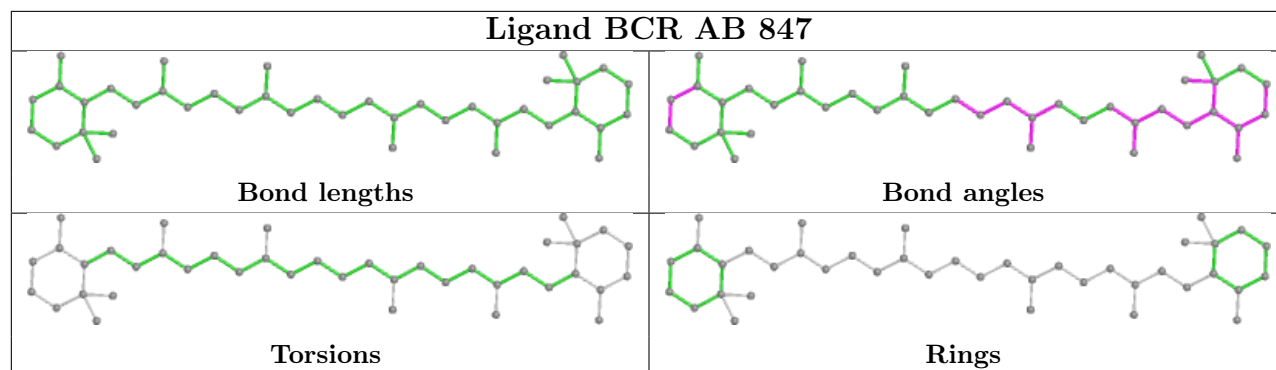


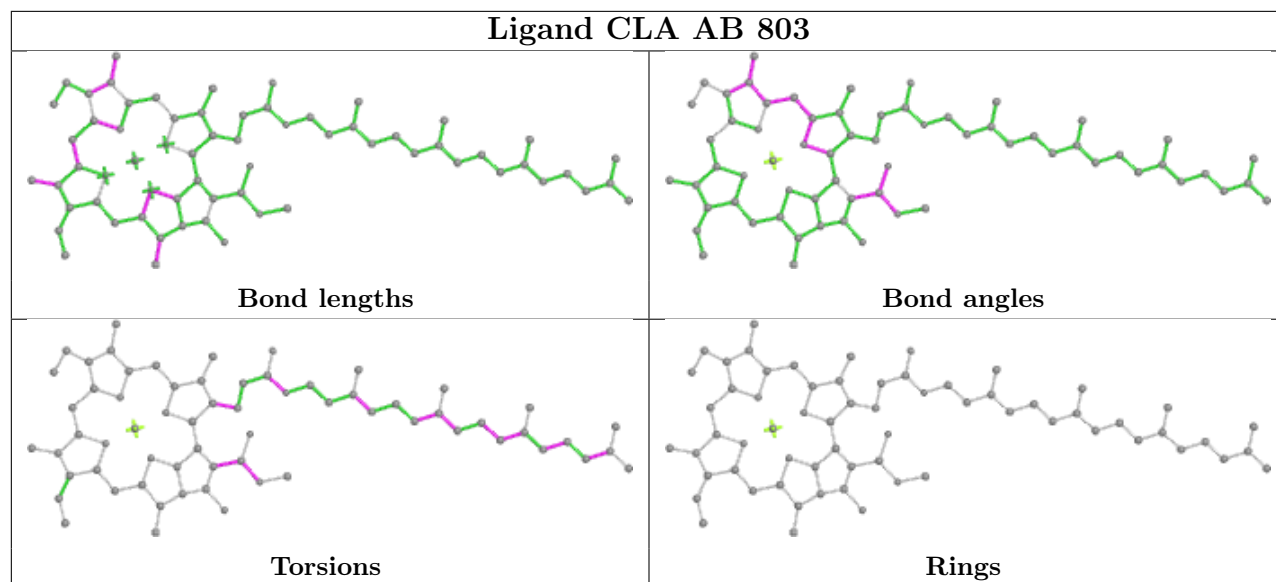
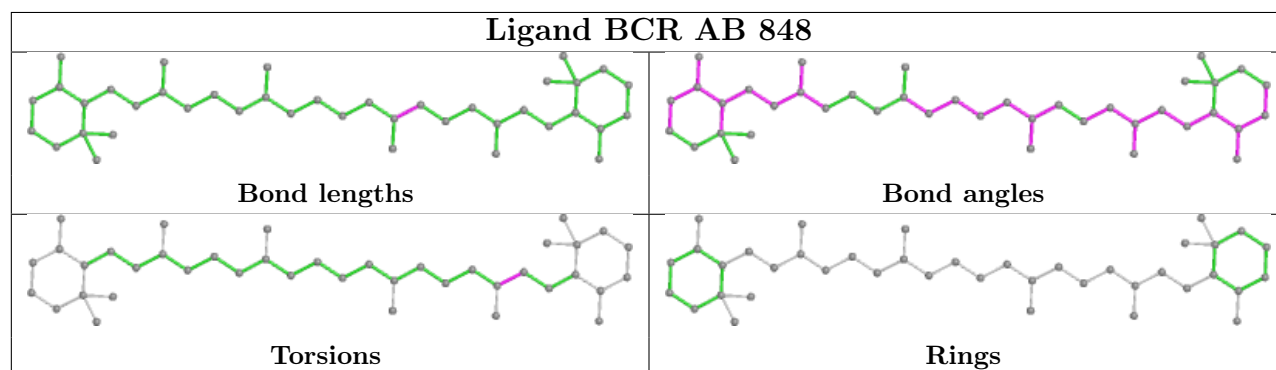
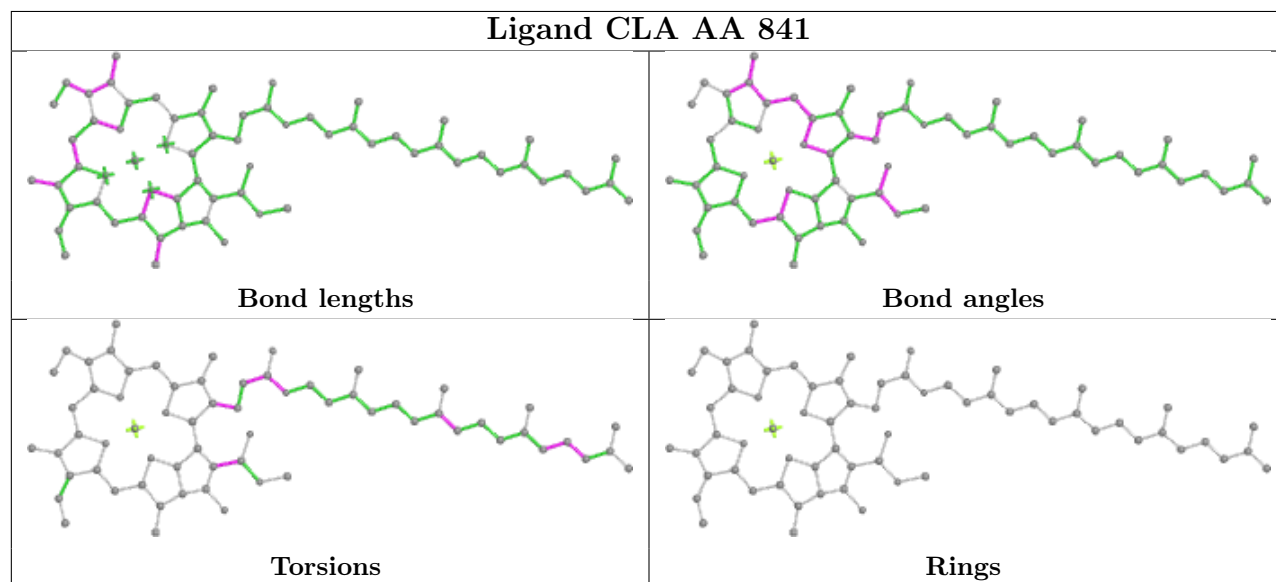
Ligand CLA A1 316



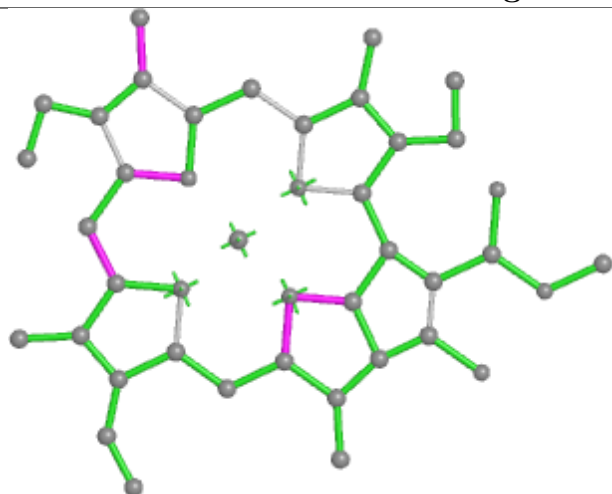
Ligand CLA AA 805



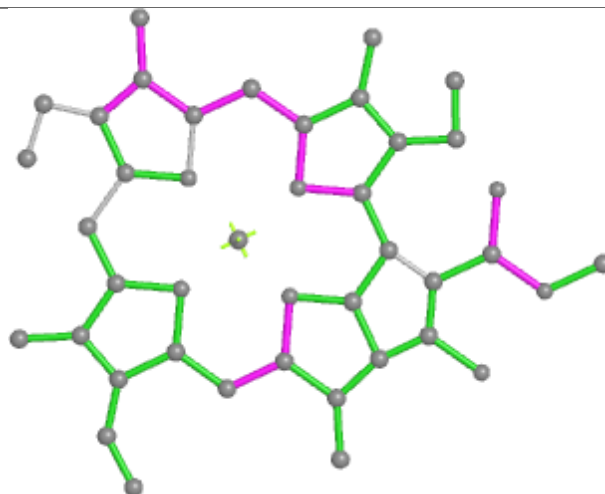


Ligand CLA AB 803**Ligand BCR AB 848****Ligand CLA AA 841**

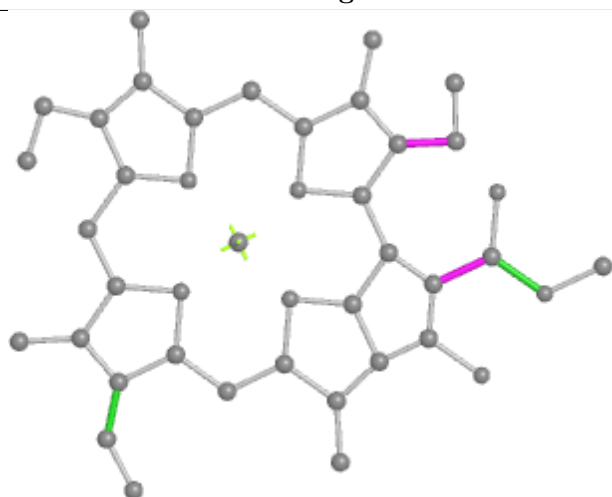
Ligand CLA AJ 102



Bond lengths



Bond angles

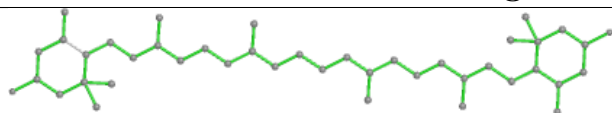


Torsions

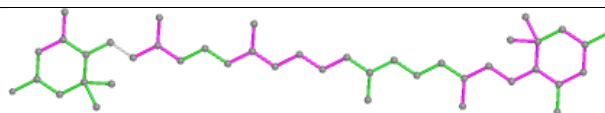


Rings

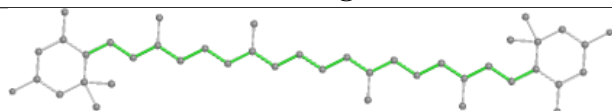
Ligand LUT A3 316



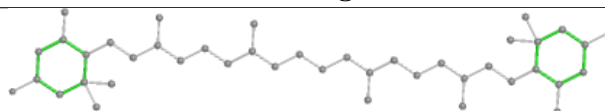
Bond lengths



Bond angles

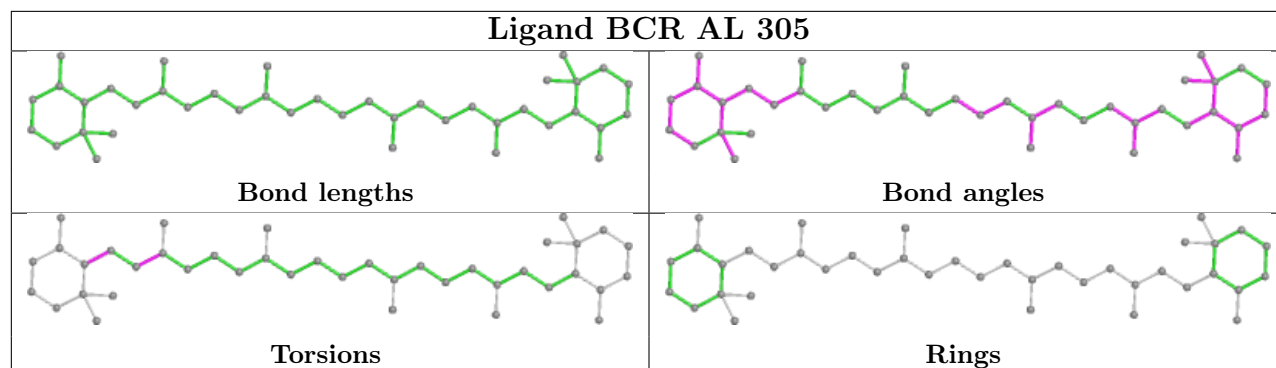


Torsions

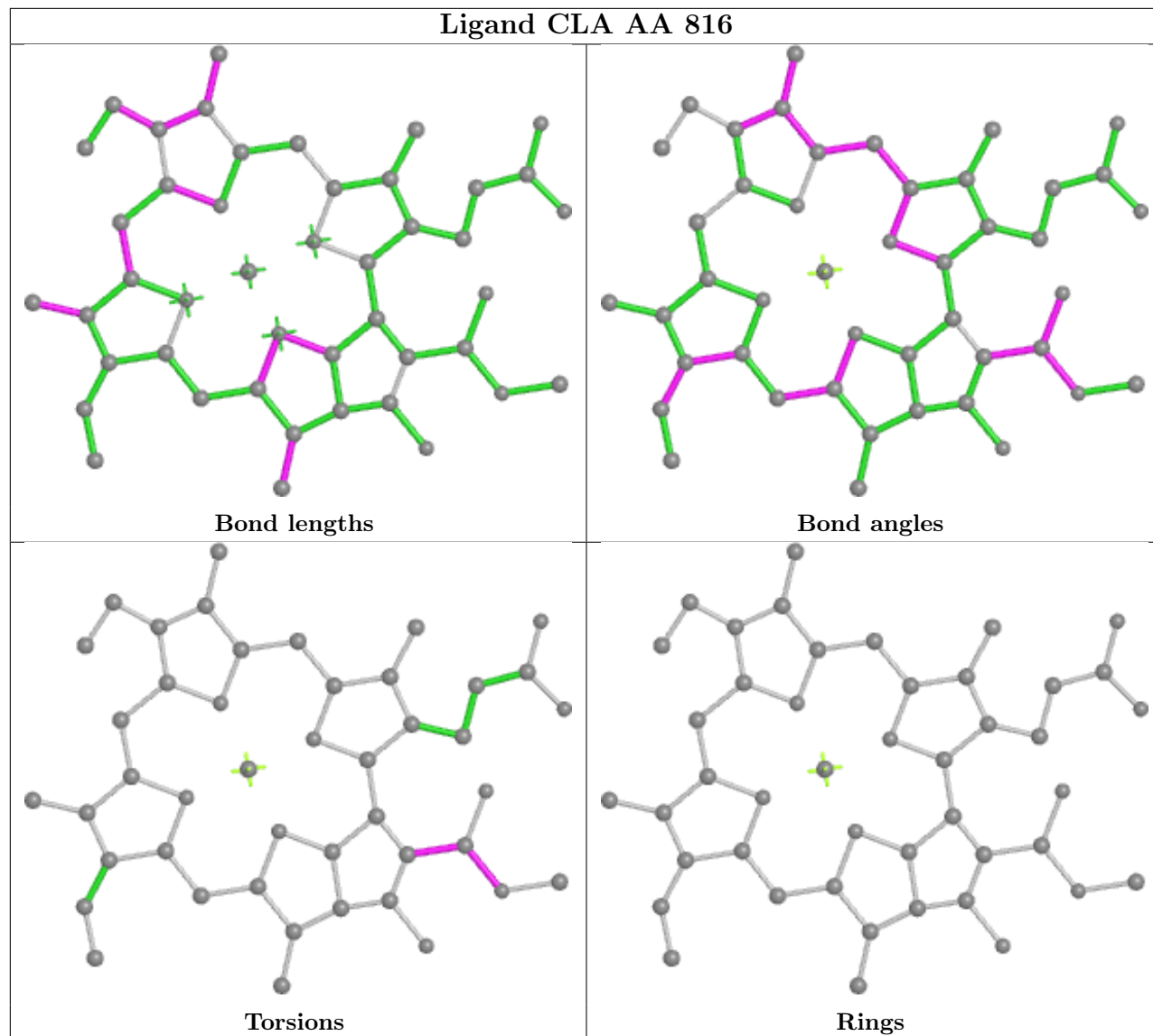


Rings

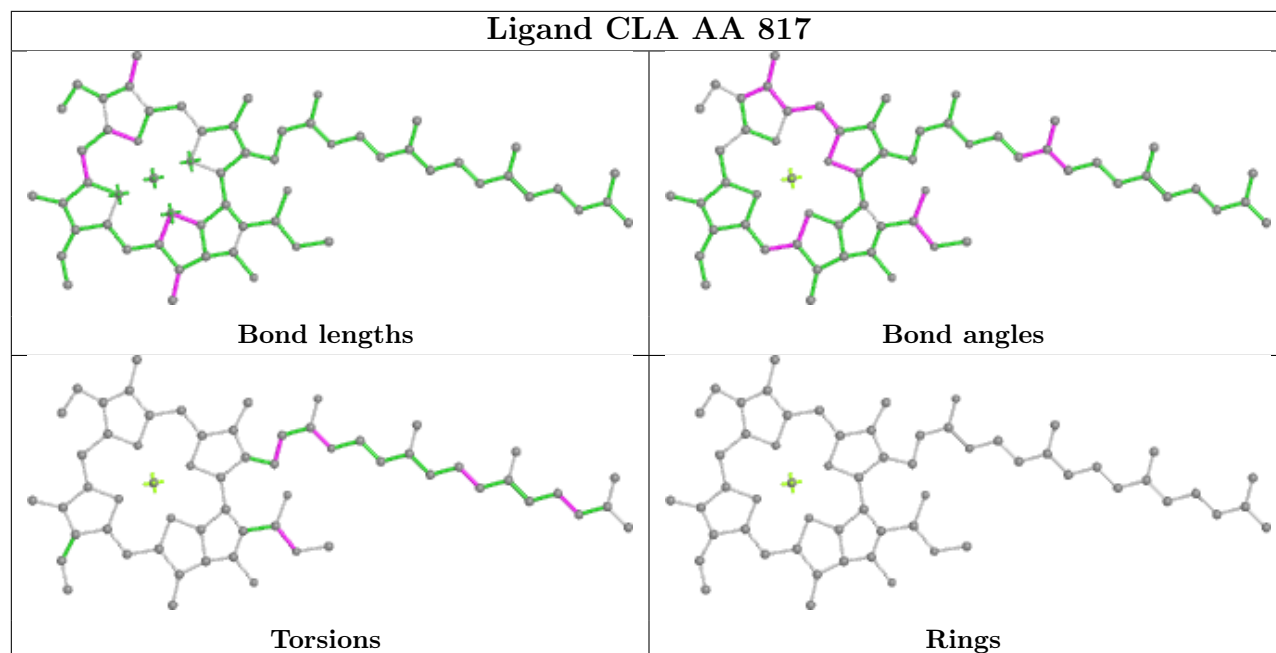
Ligand BCR AL 305



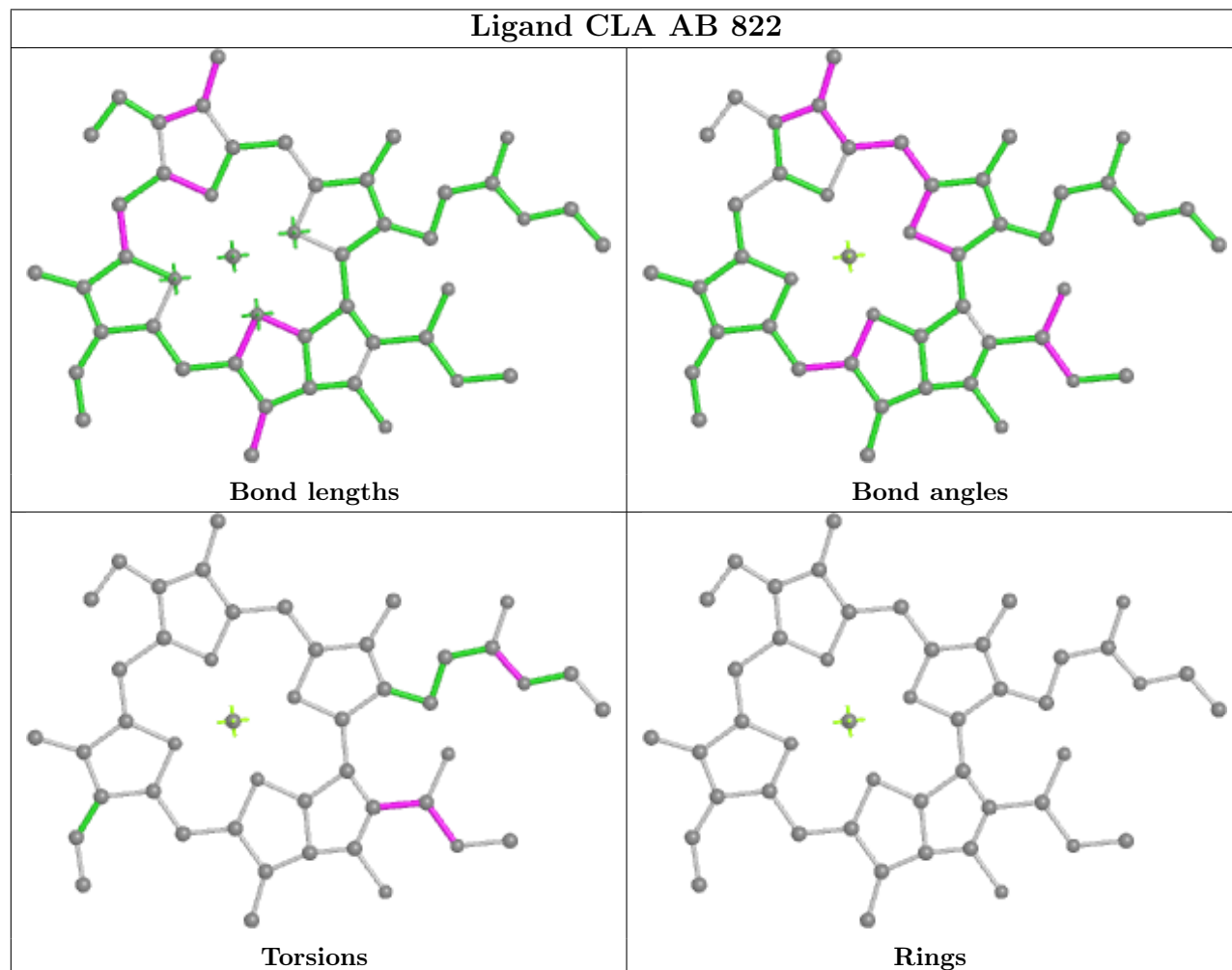
Ligand CLA AA 816

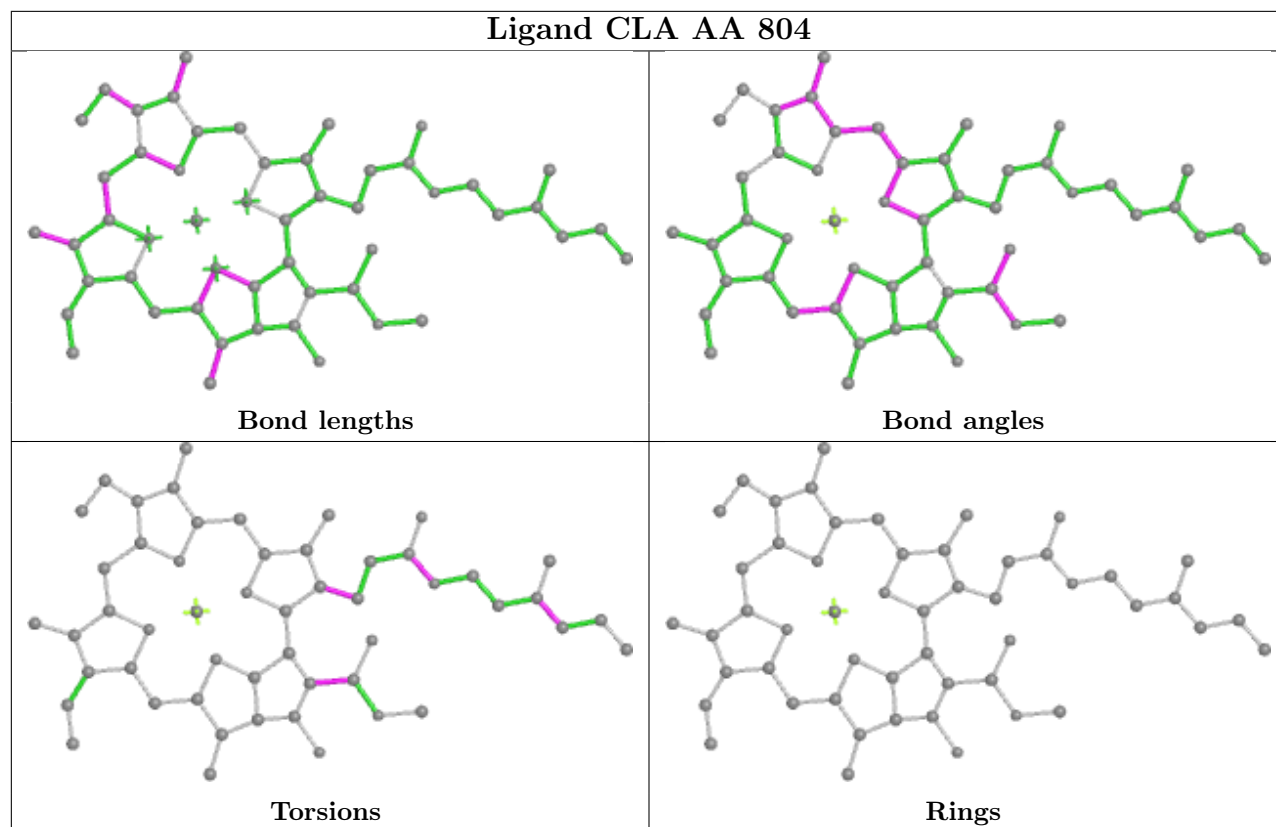


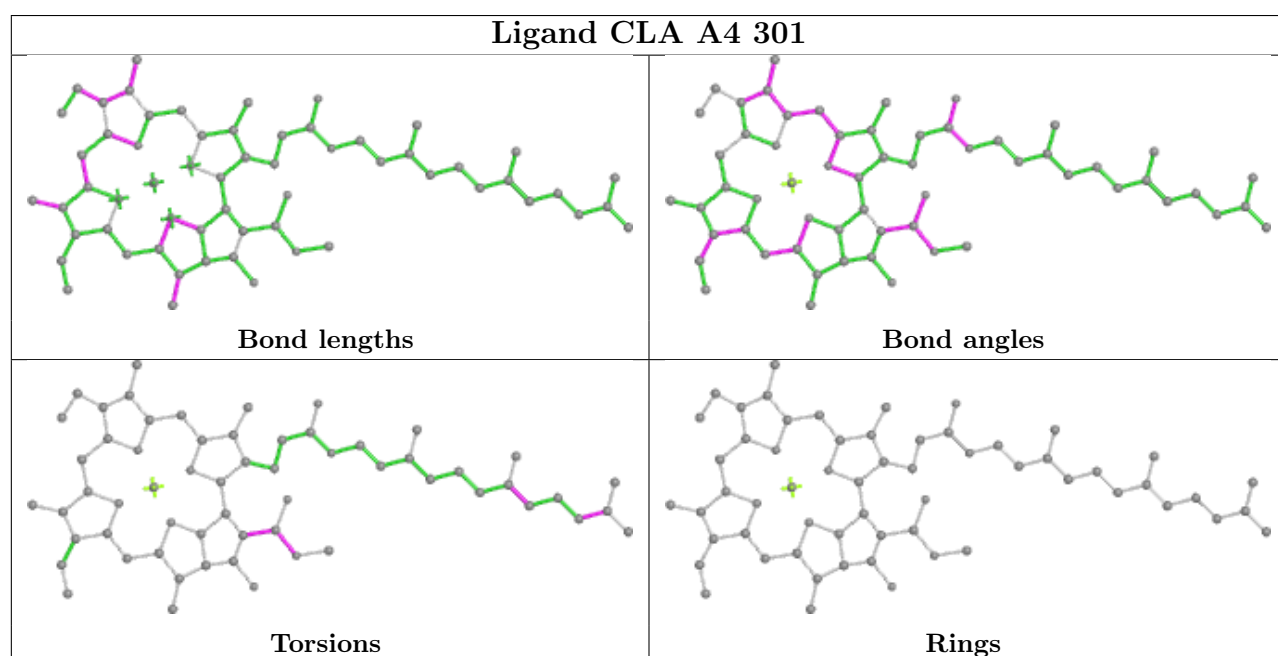
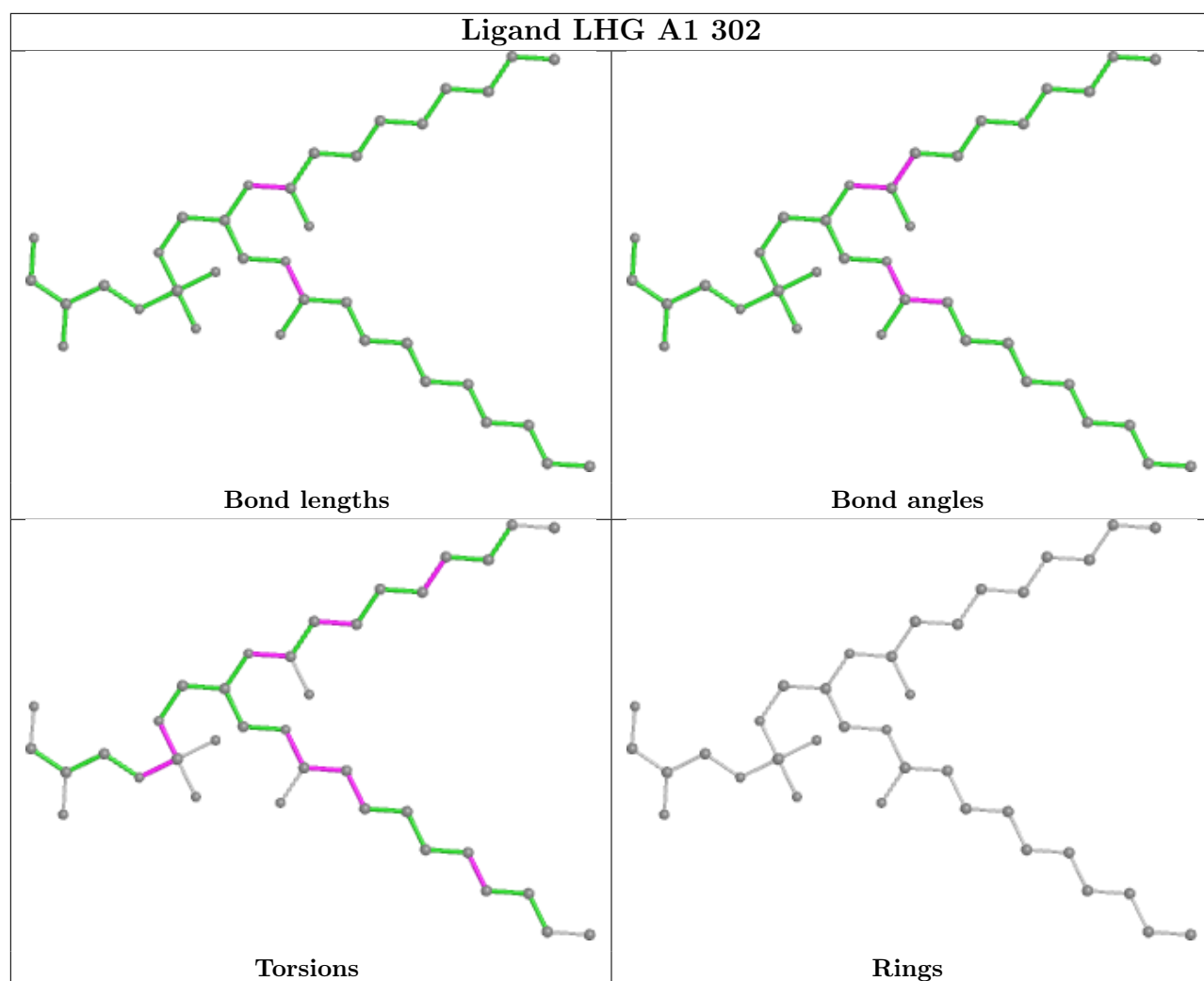
Ligand CLA AA 817



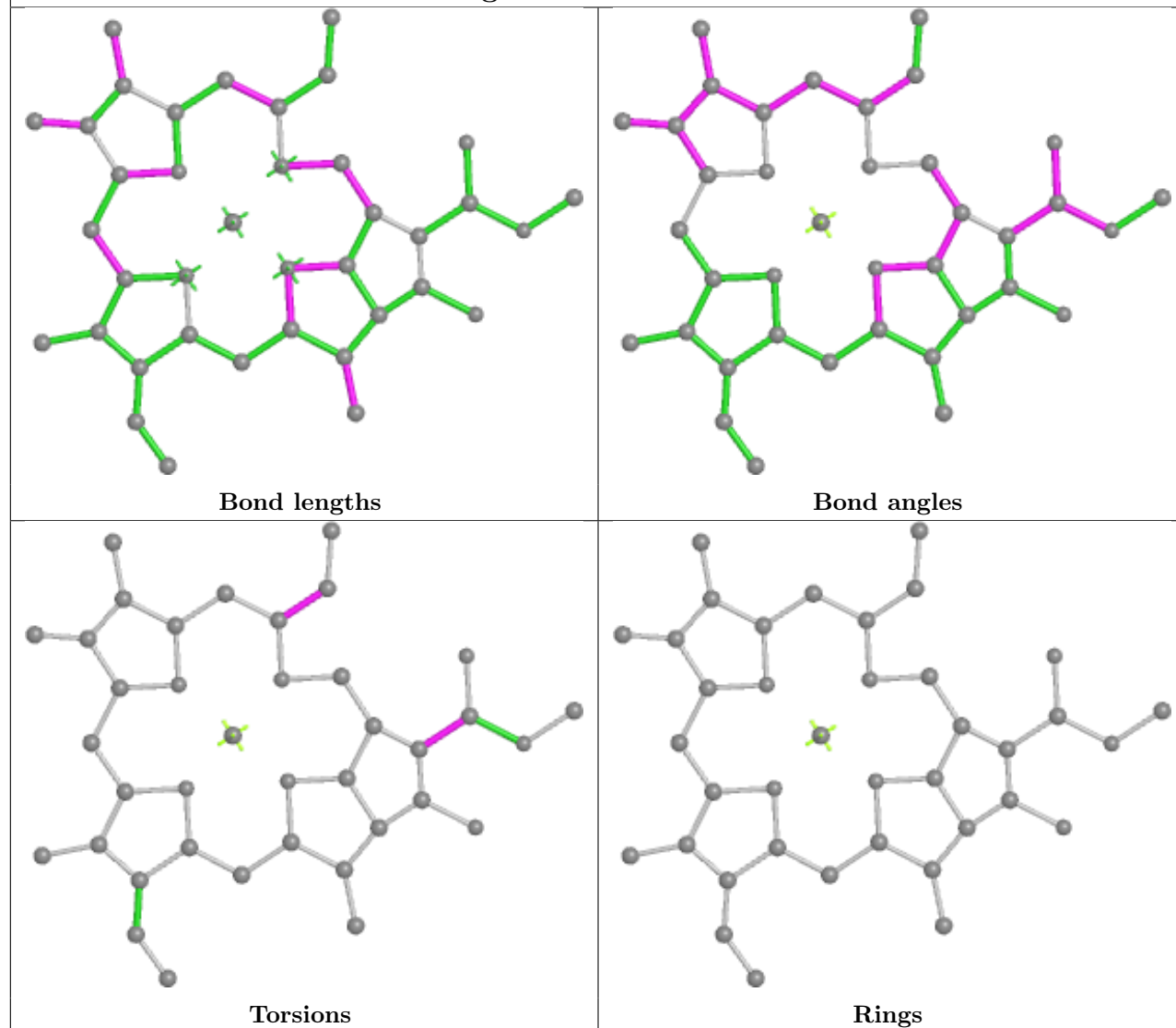
Ligand CLA AB 822



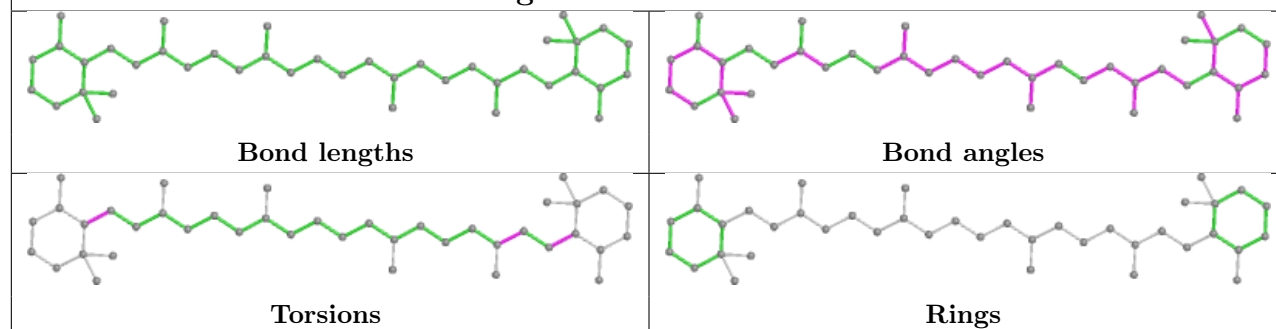


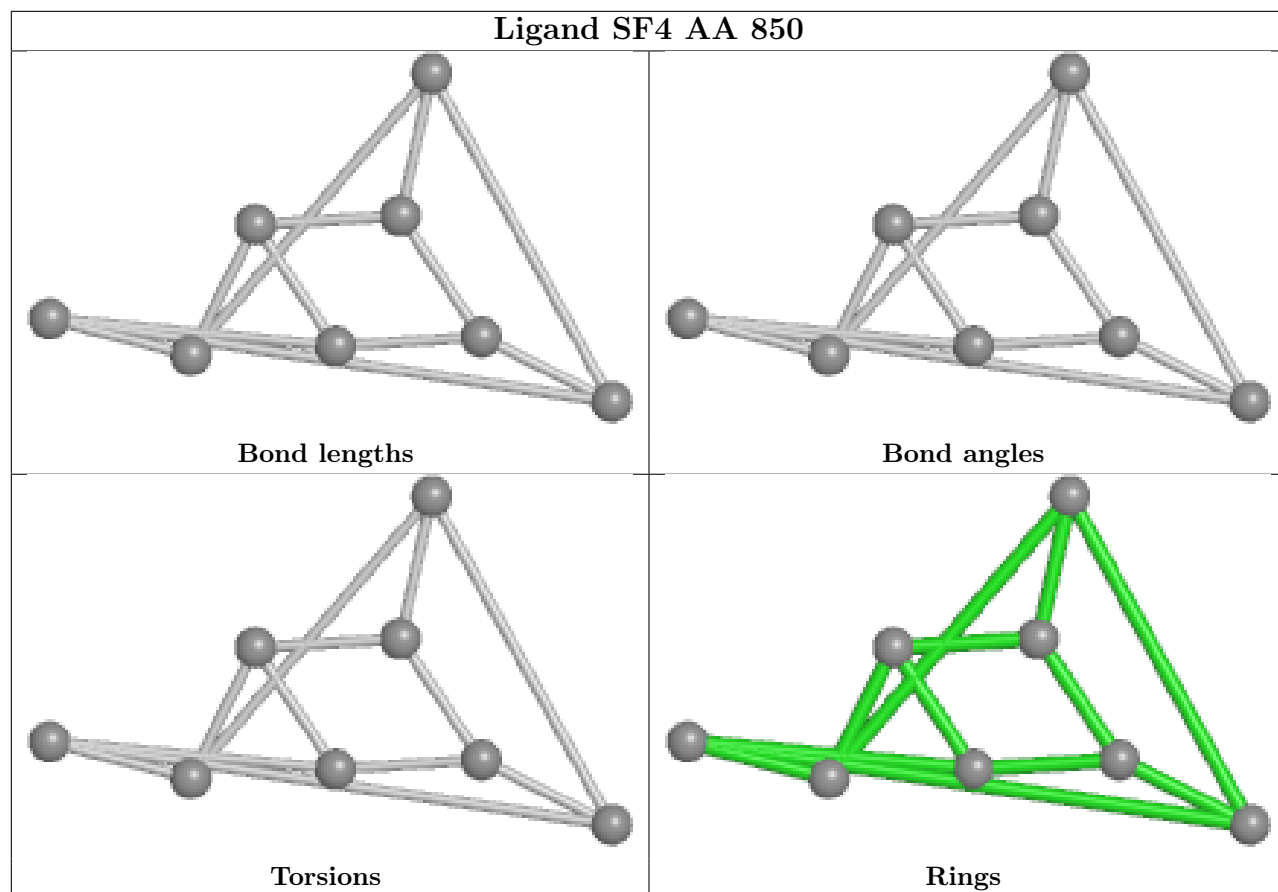


Ligand CLA A6 610

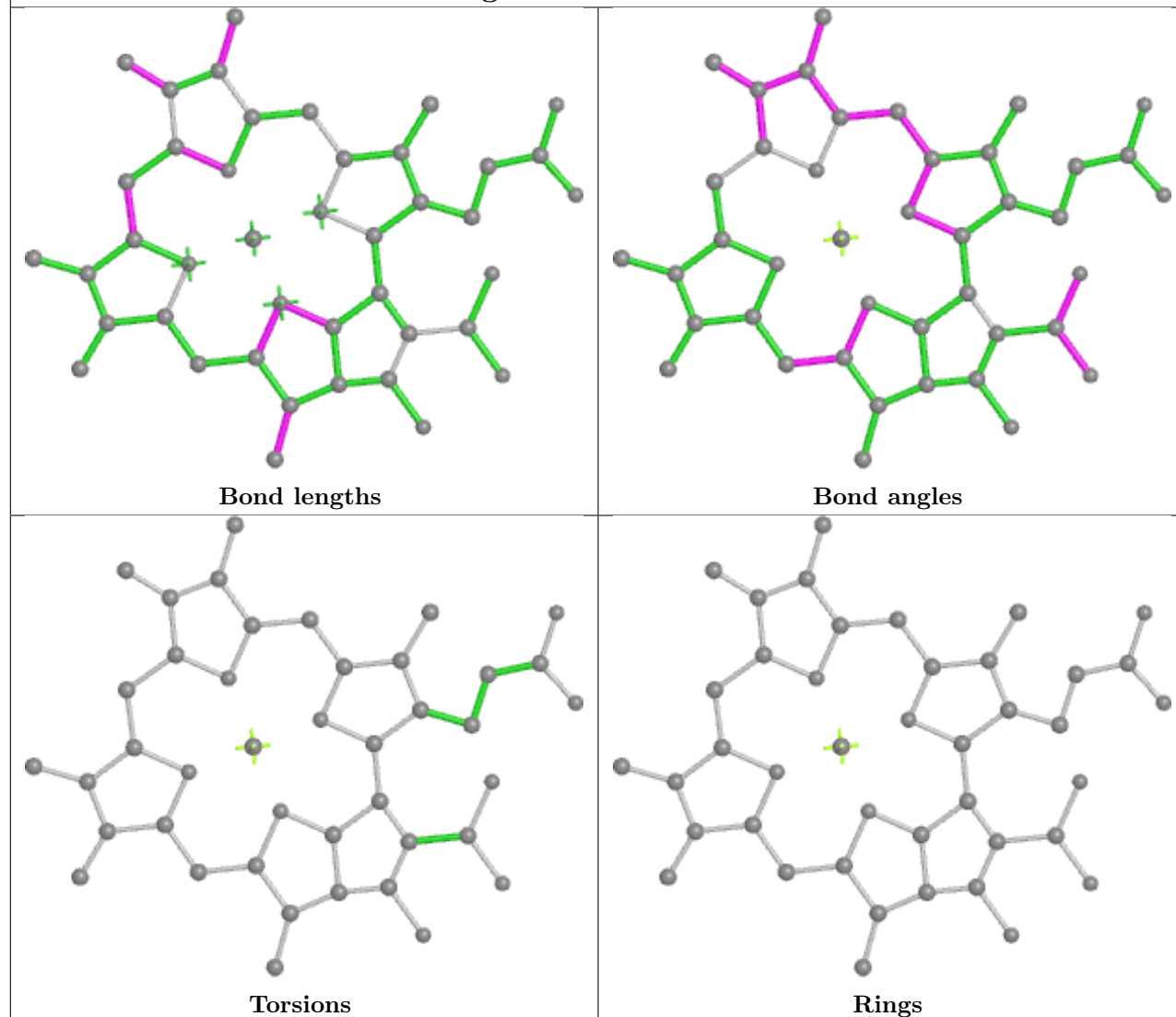


Ligand BCR AA 846

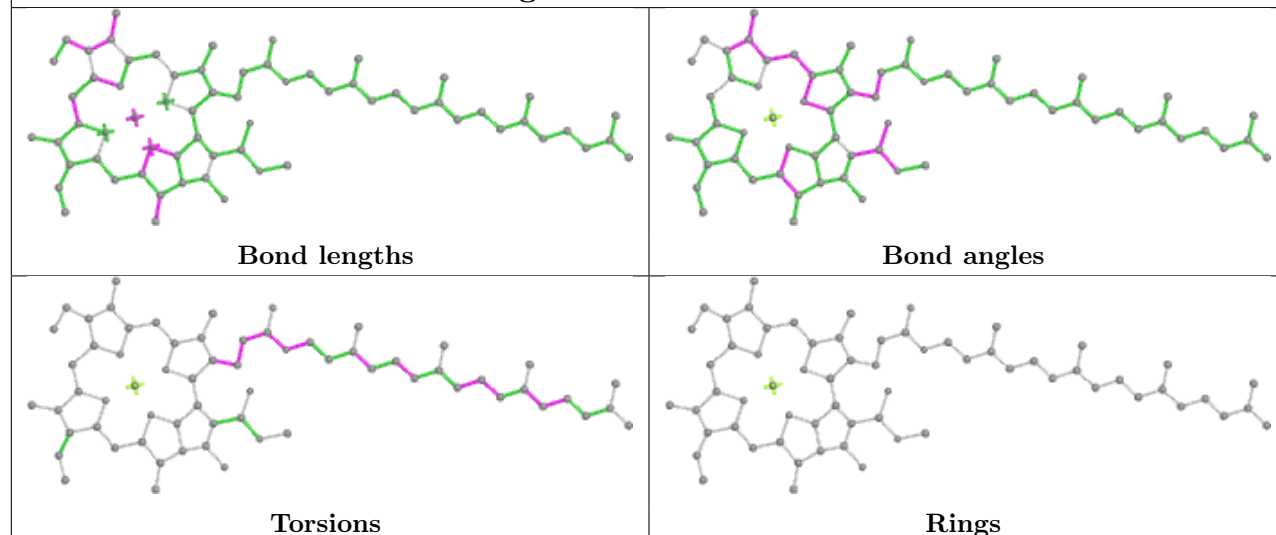




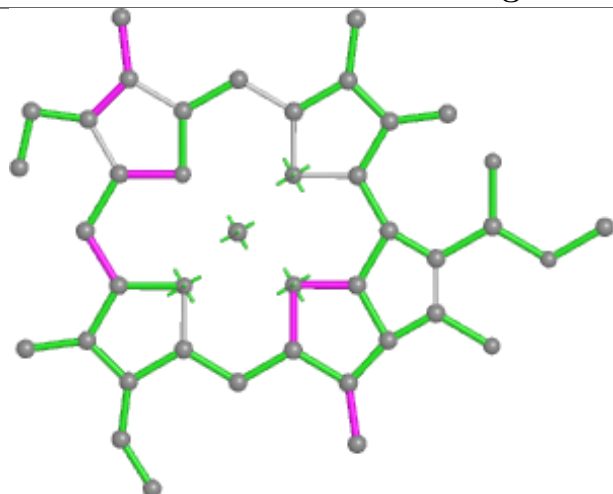
Ligand CLA A3 304



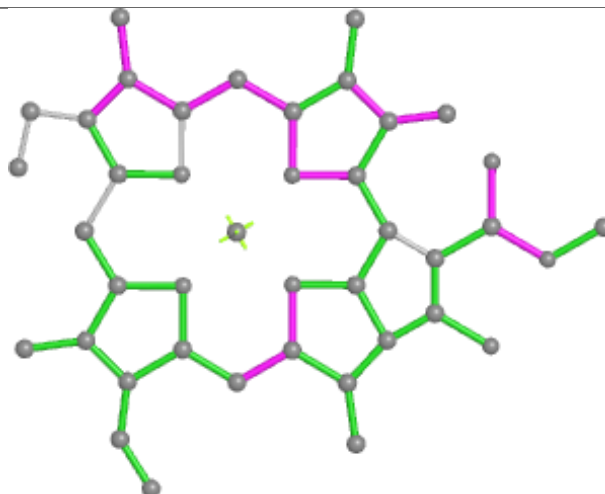
Ligand CLA AB 829



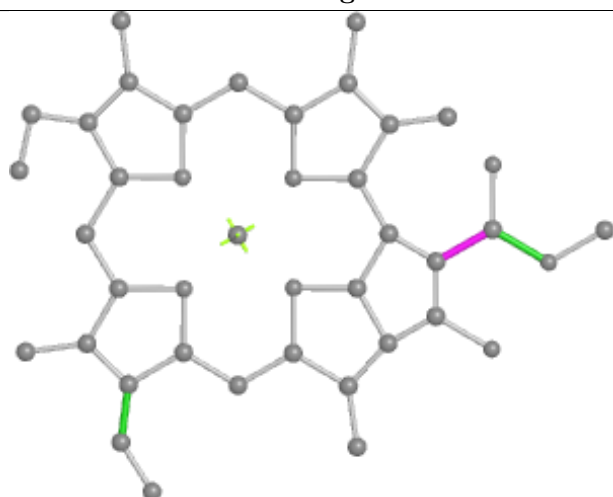
Ligand CLA AF 804



Bond lengths



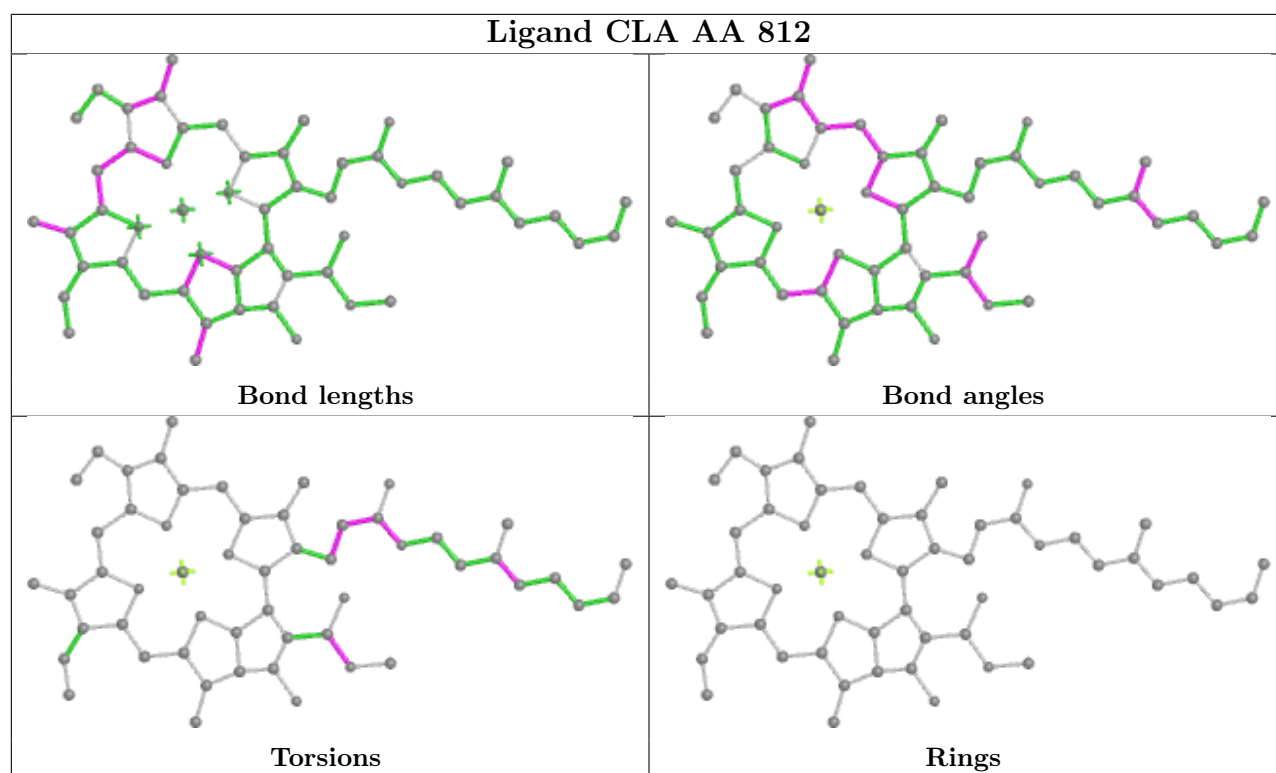
Bond angles



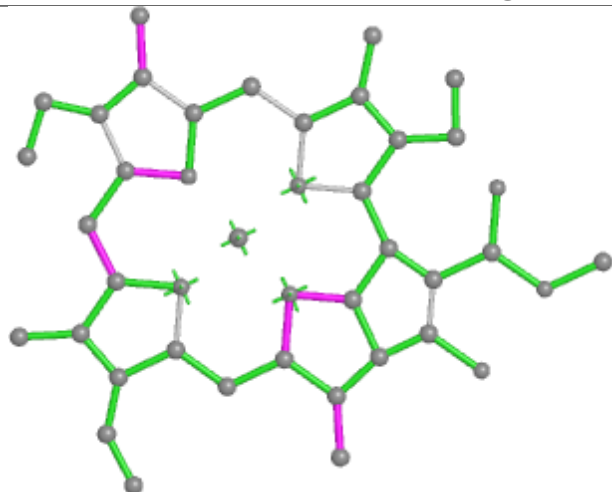
Torsions



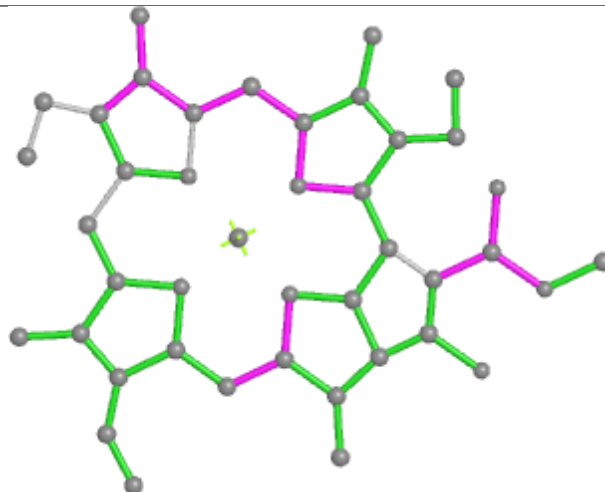
Rings



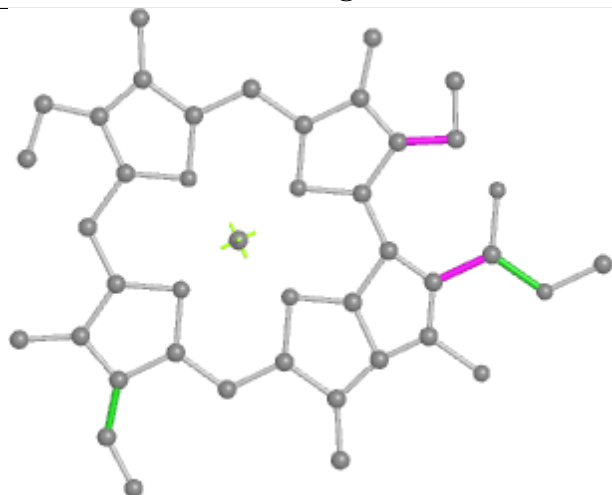
Ligand CLA AA 822



Bond lengths



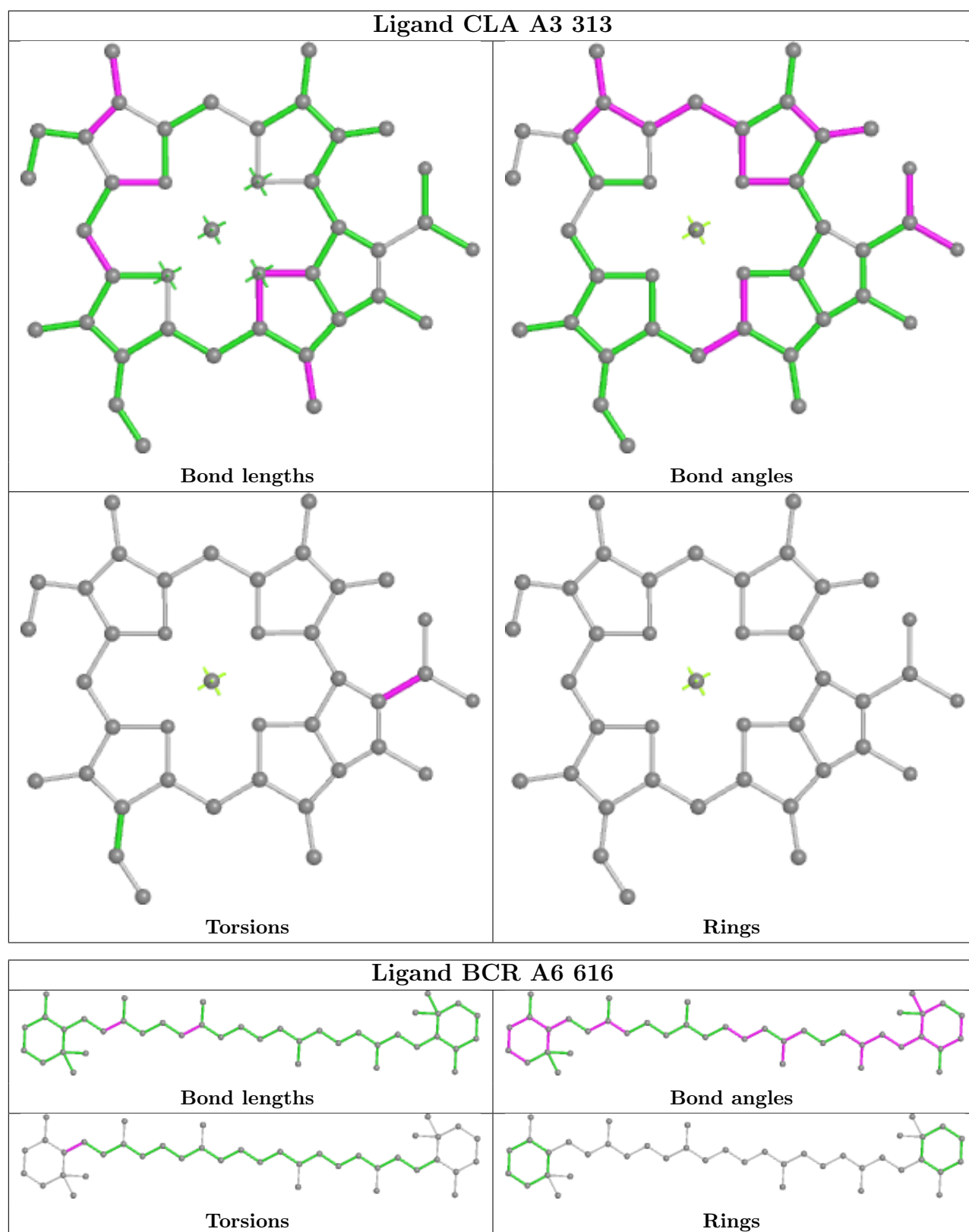
Bond angles



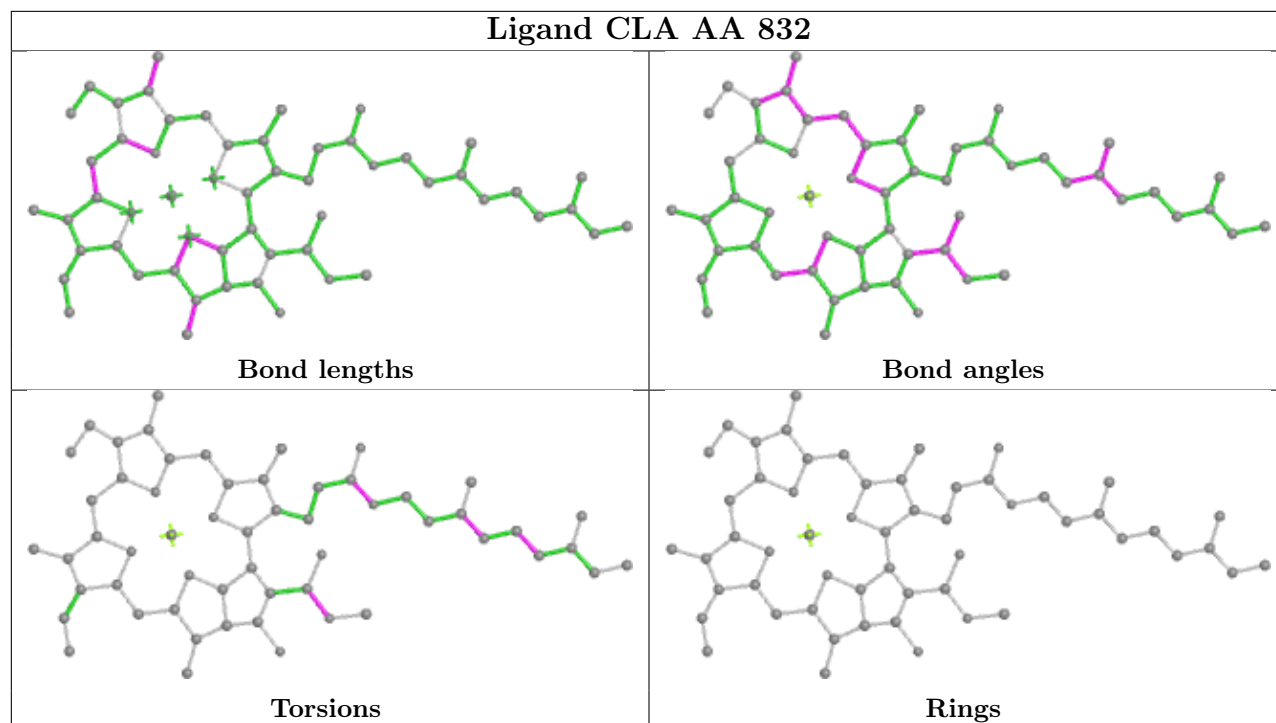
Torsions



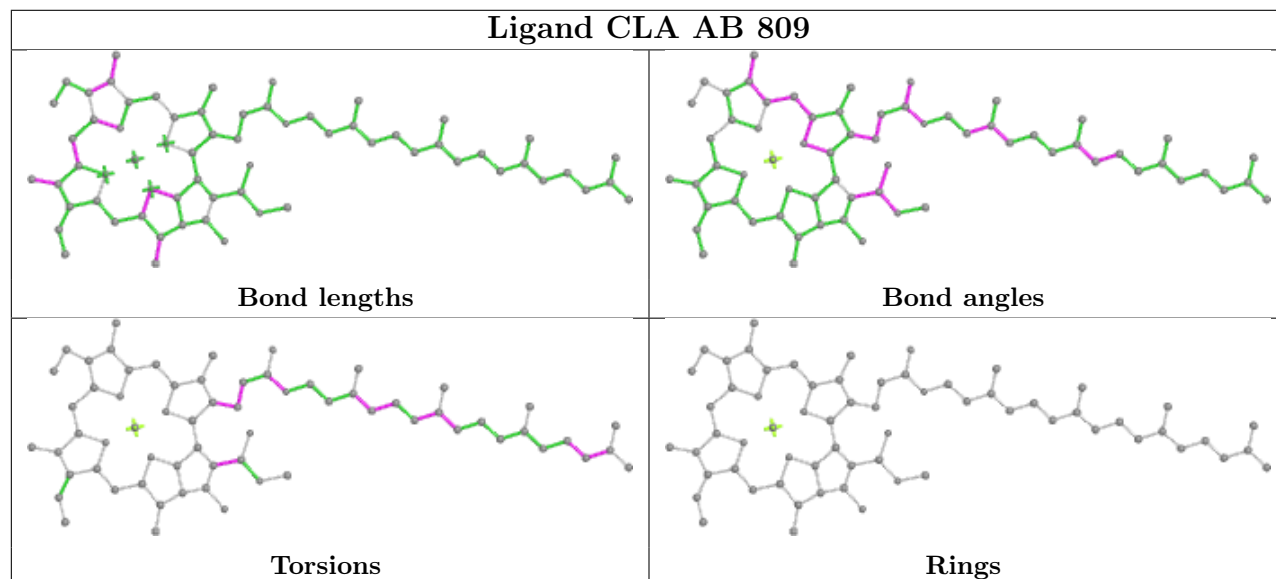
Rings



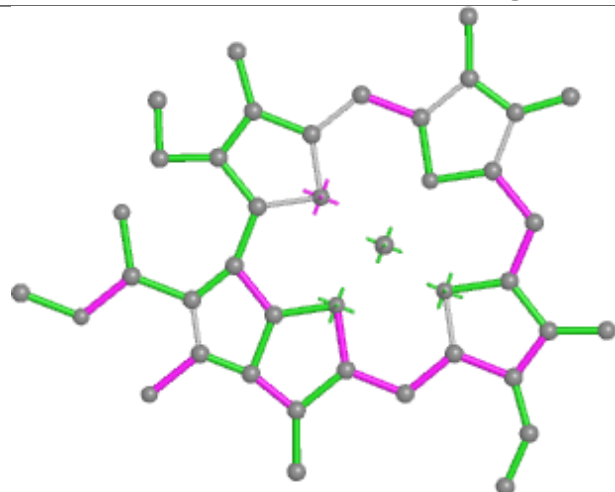
Ligand CLA AA 832



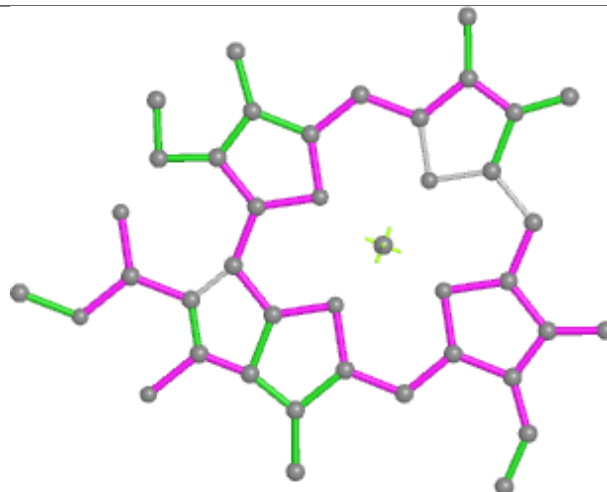
Ligand CLA AB 809



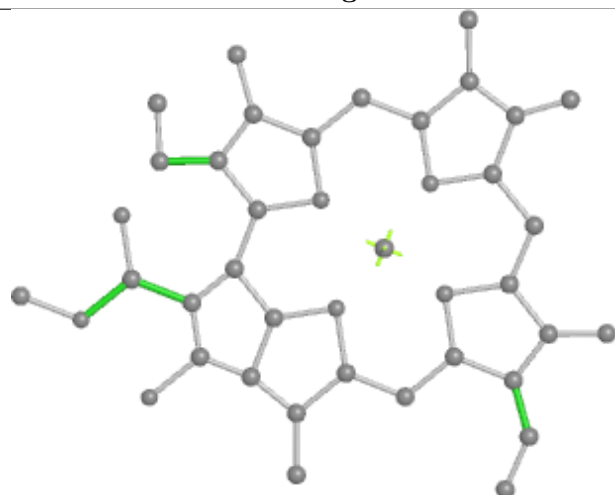
Ligand CHL A4 305



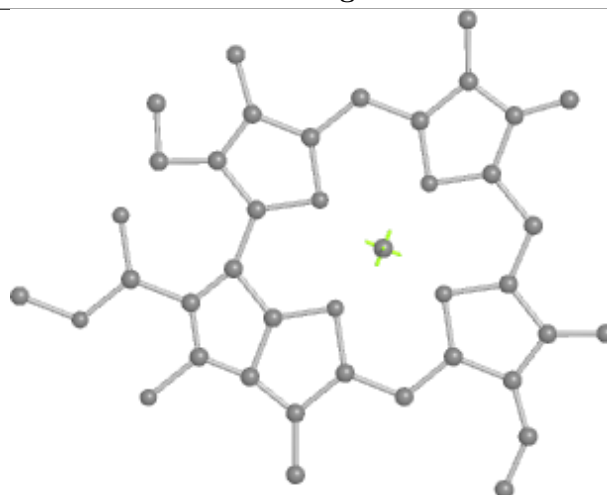
Bond lengths



Bond angles

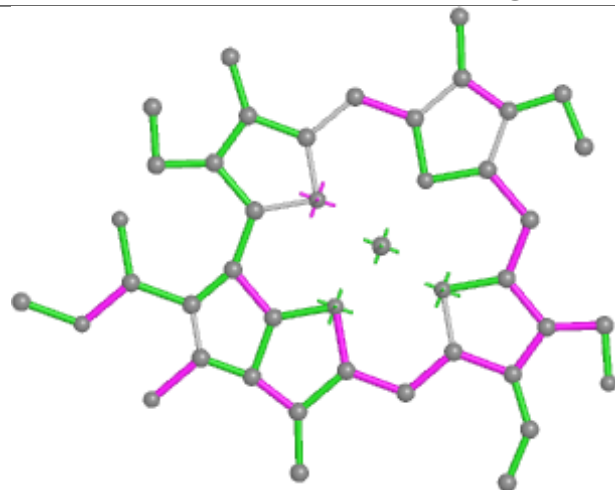


Torsions

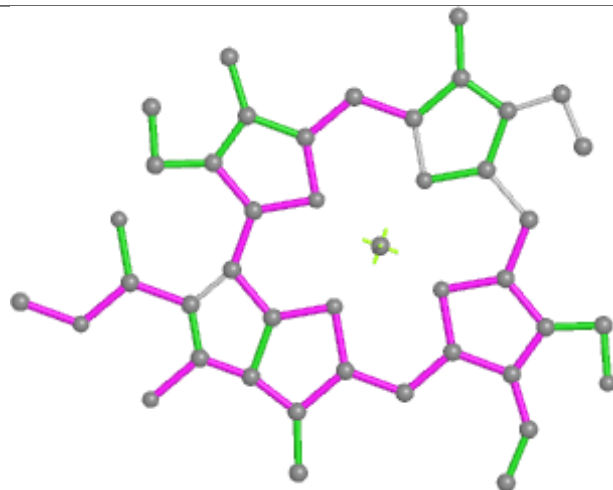


Rings

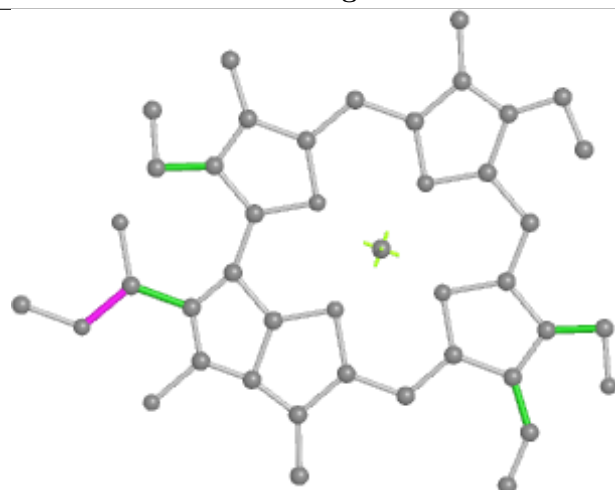
Ligand CHL A6 606



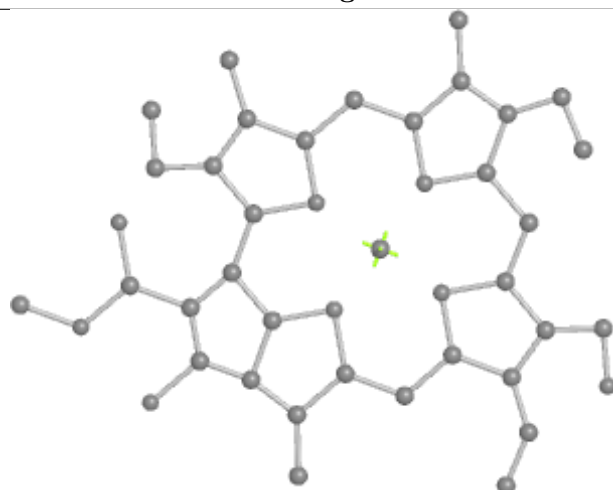
Bond lengths



Bond angles

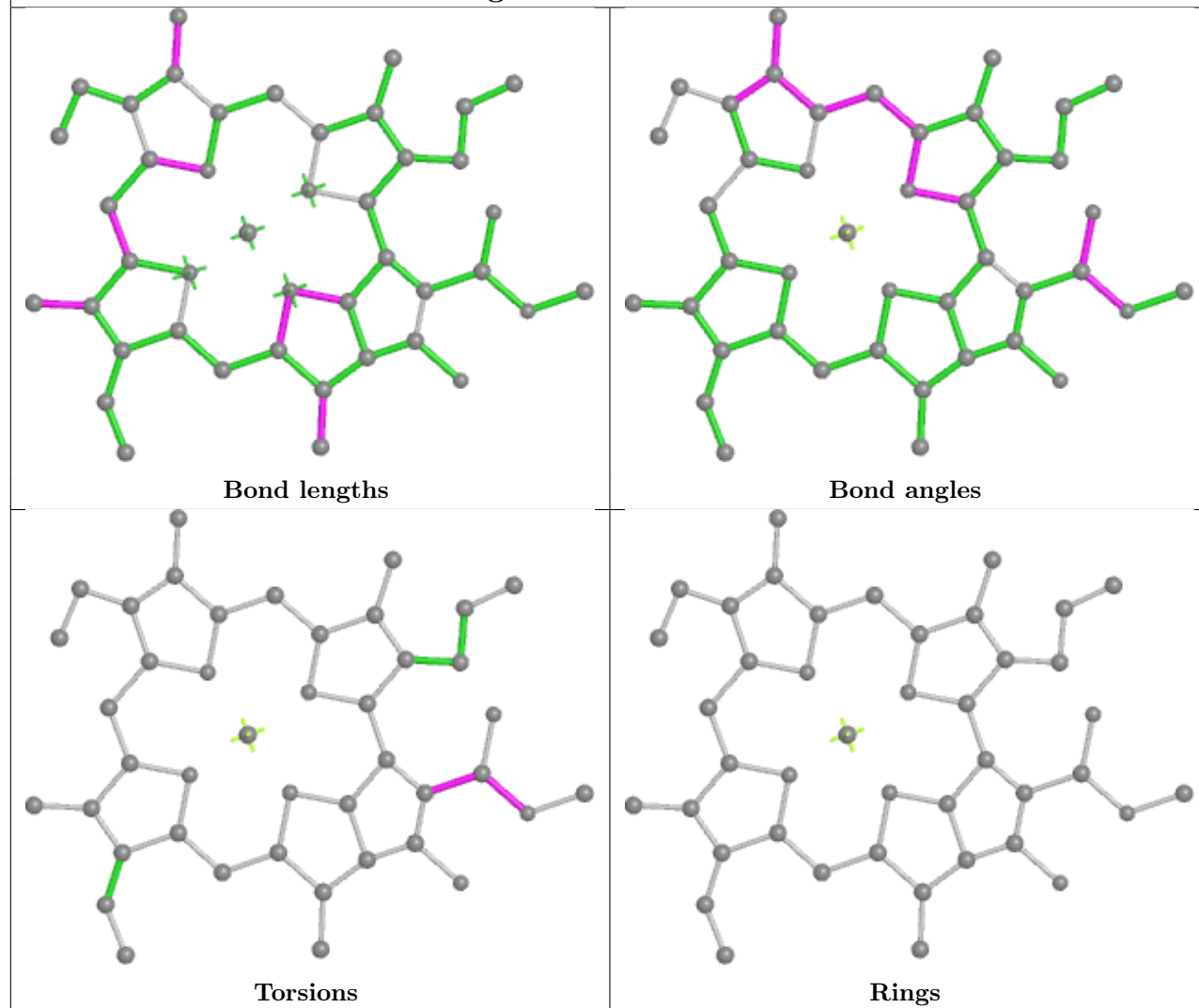


Torsions

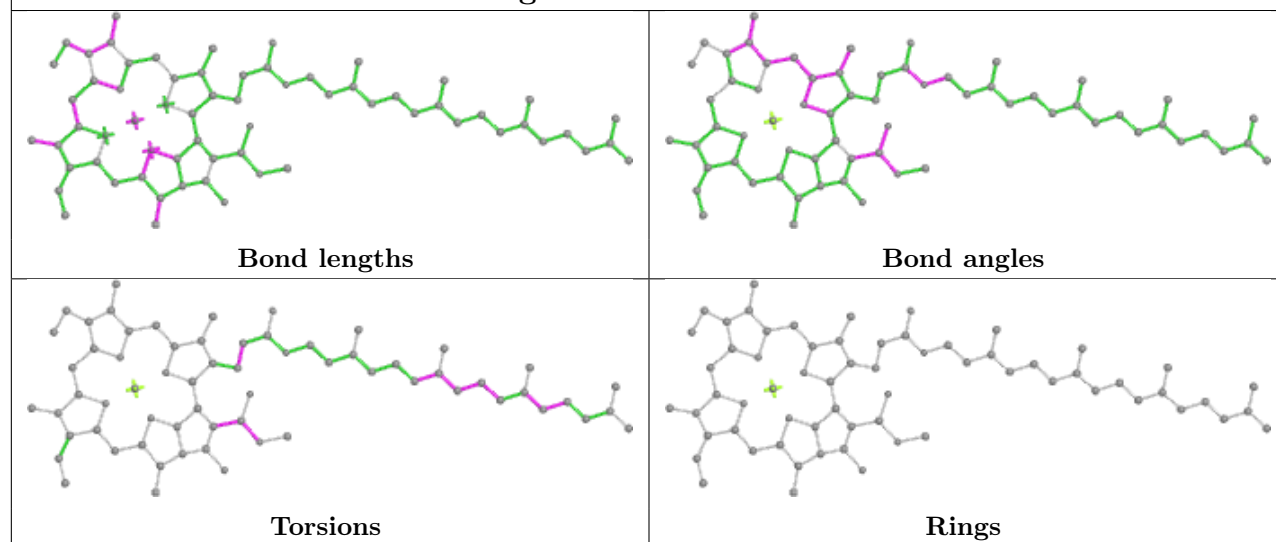


Rings

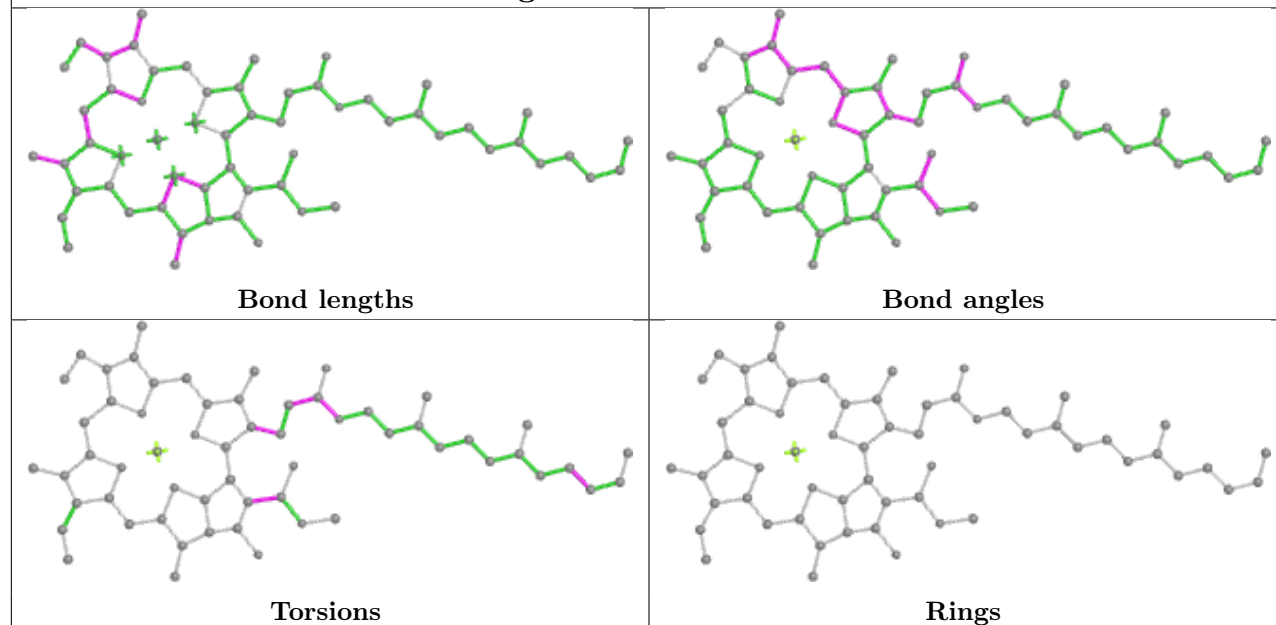
Ligand CLA AB 816



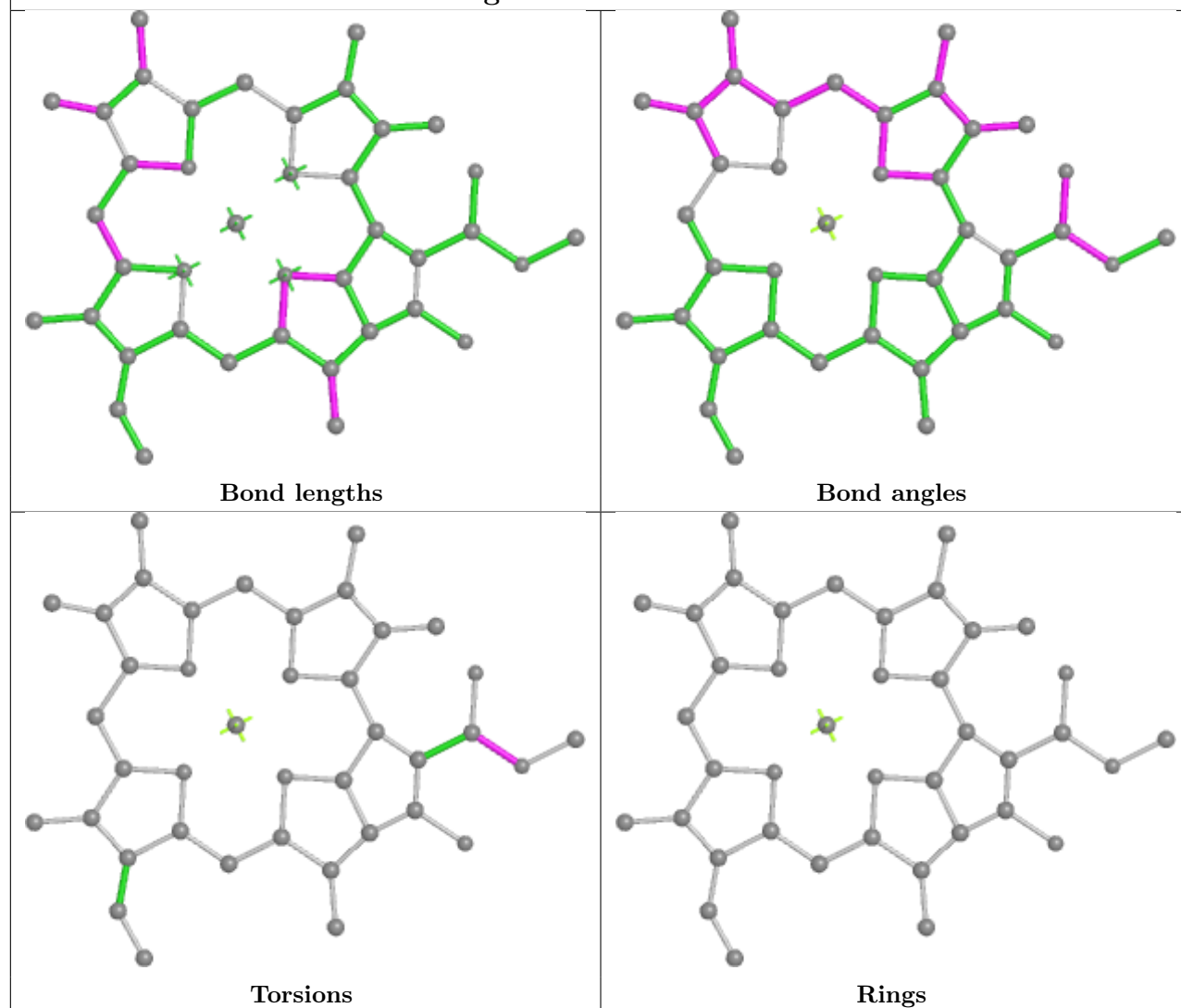
Ligand CLA AB 825

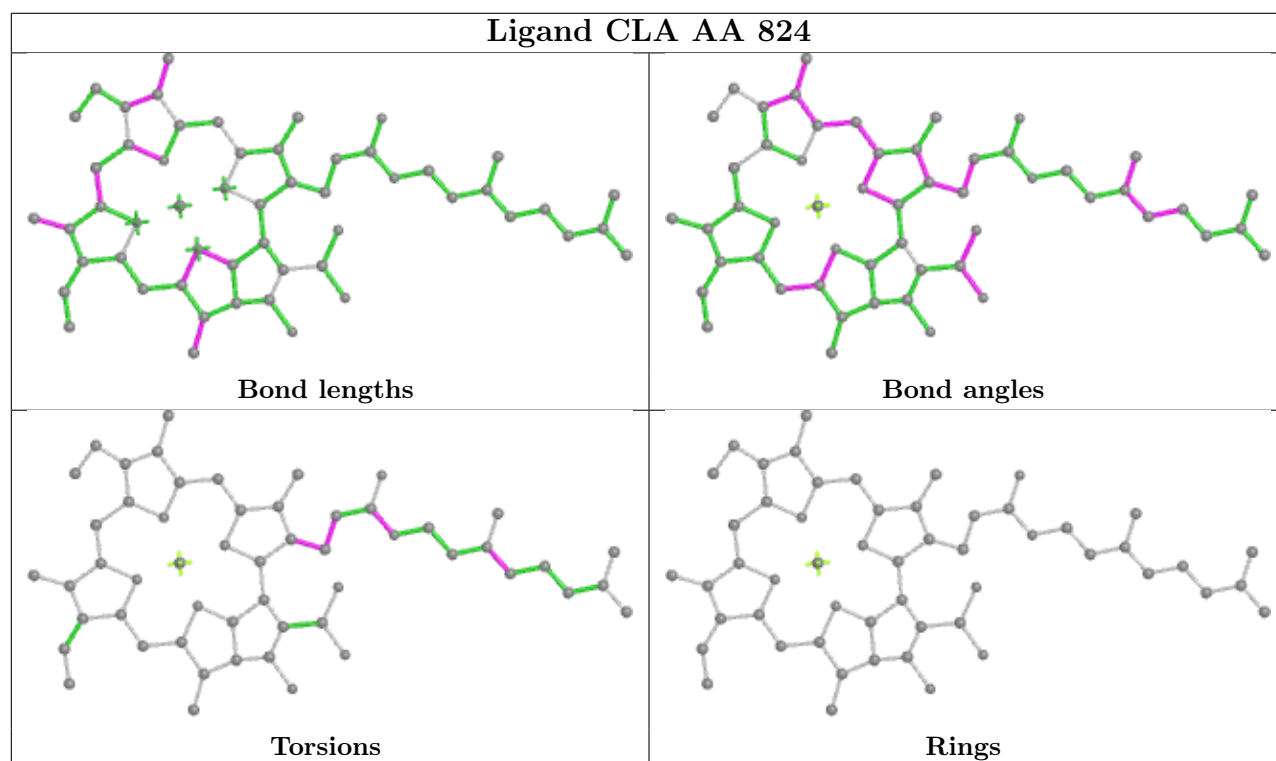
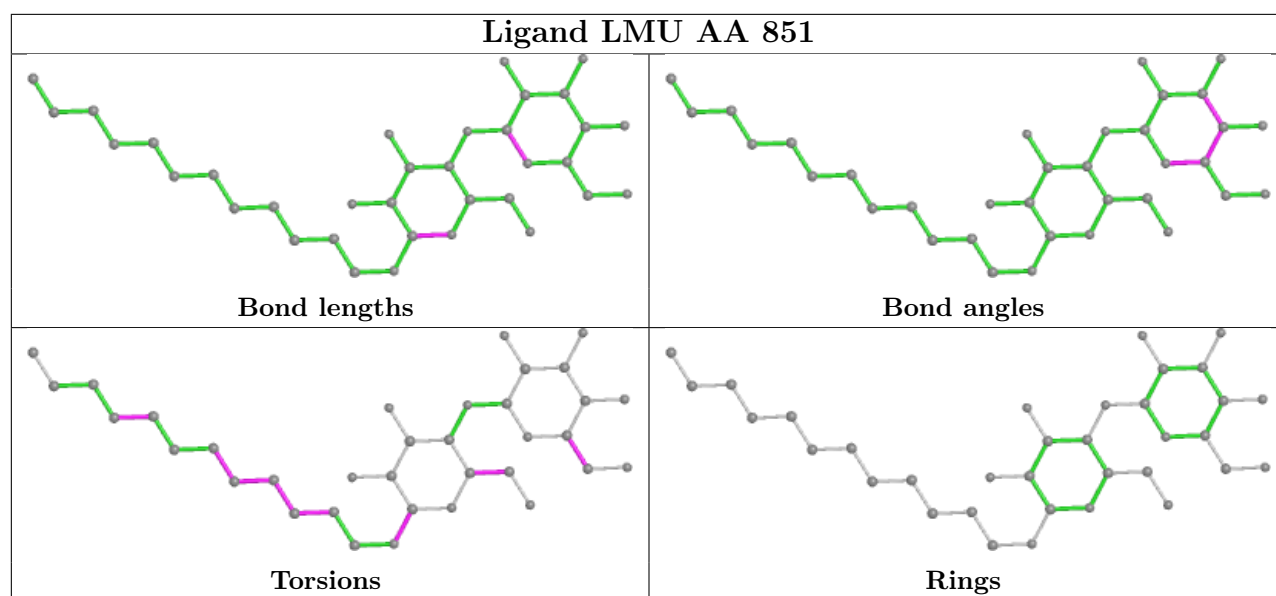


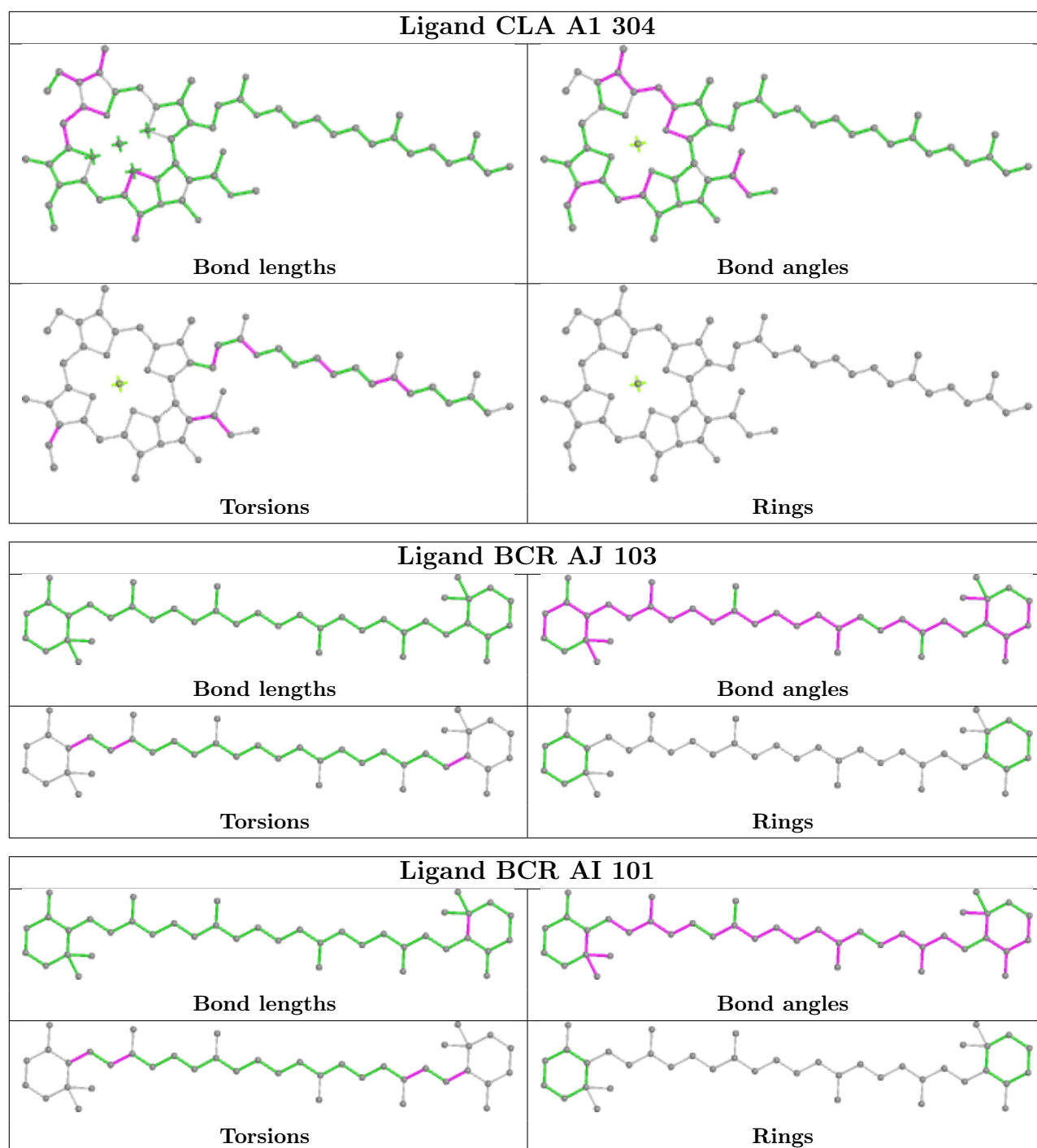
Ligand CLA AA 818



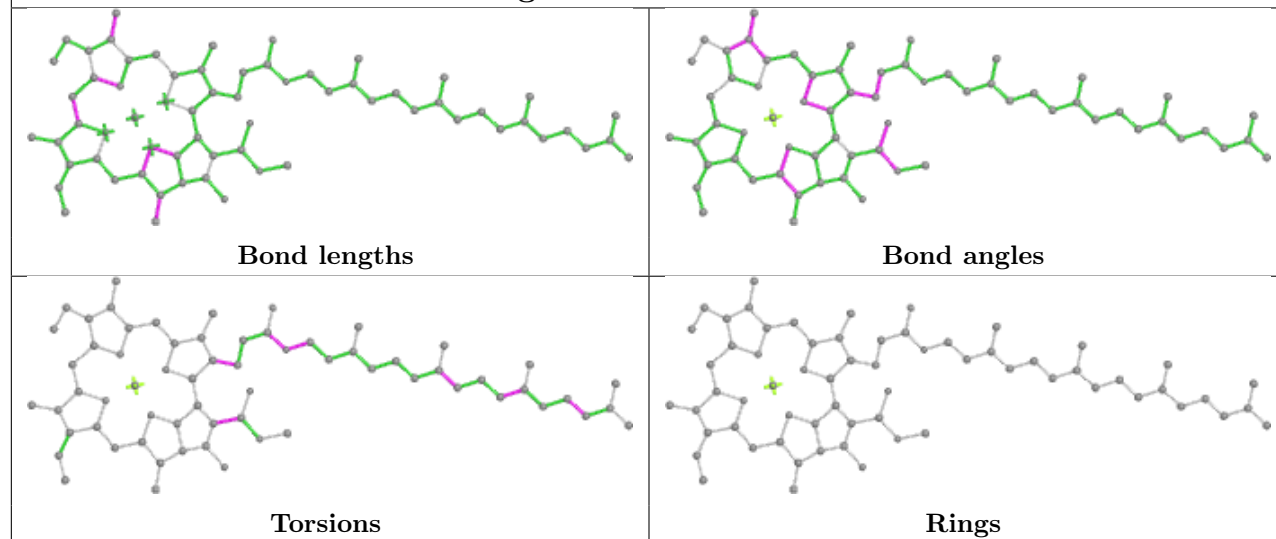
Ligand CLA A1 310



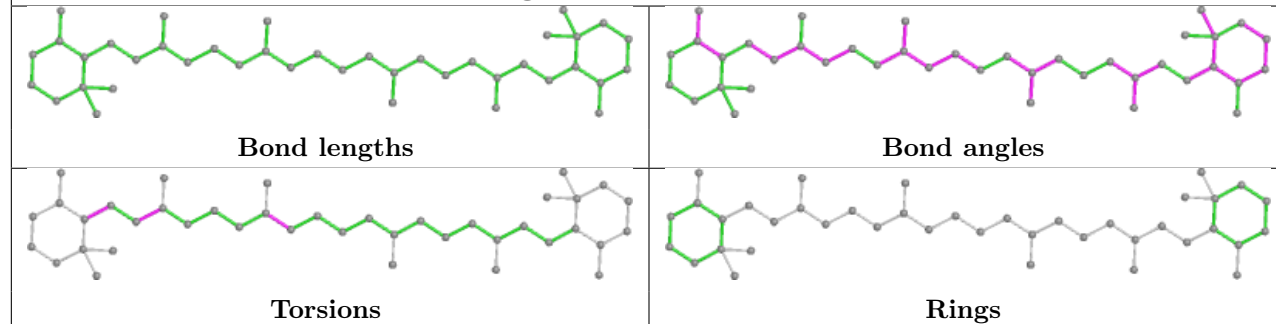




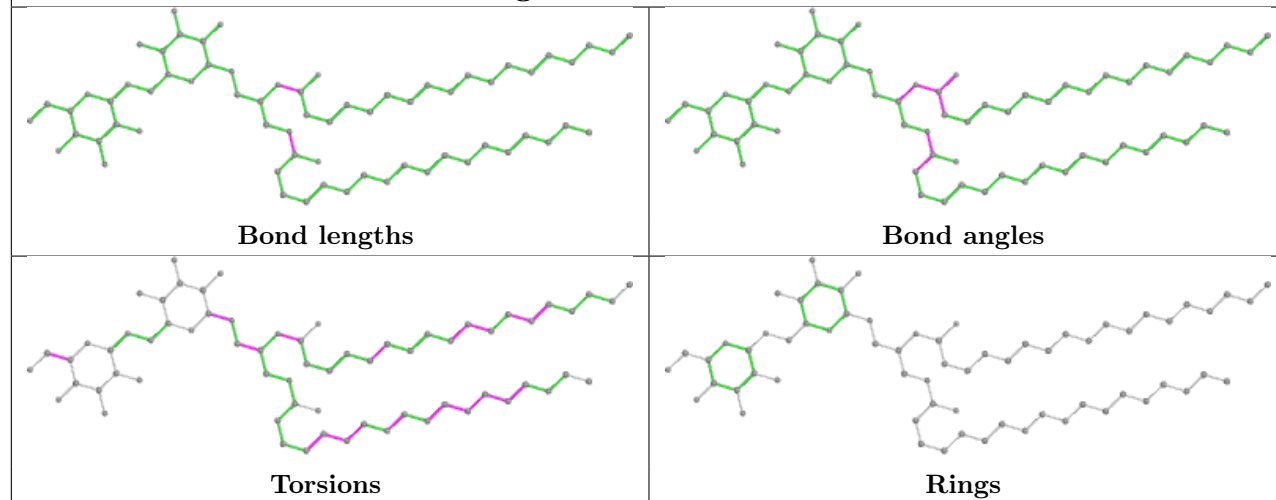
Ligand CLA AA 825



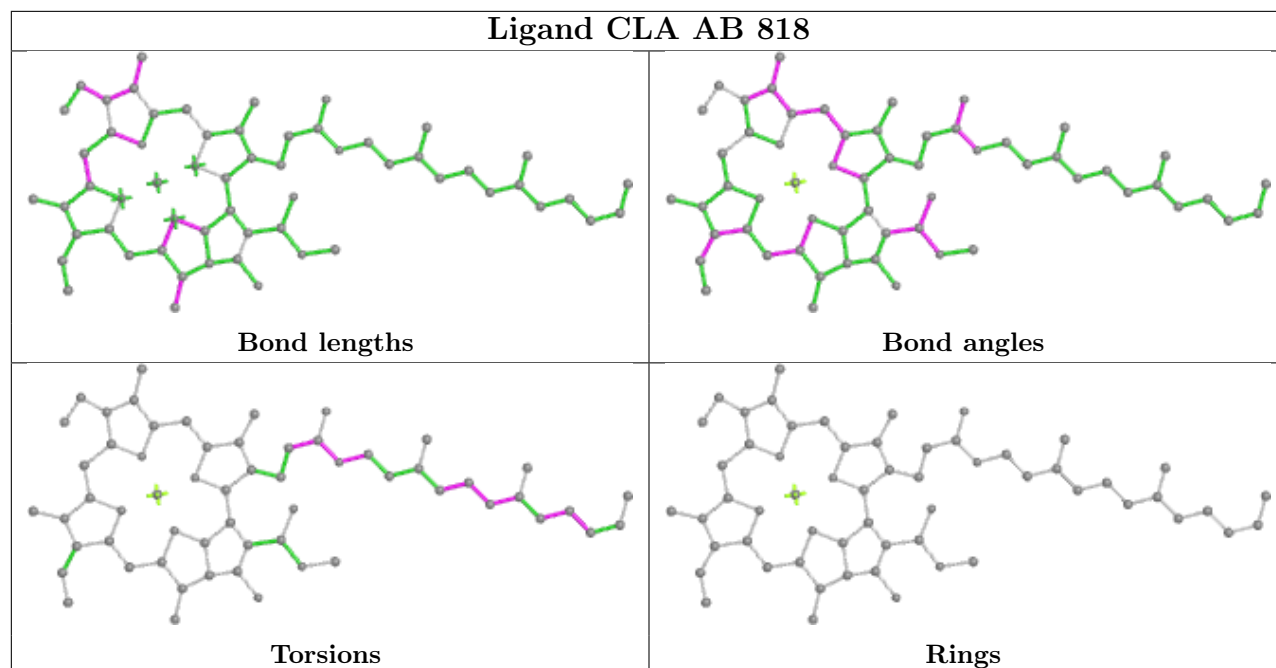
Ligand BCR AF 805



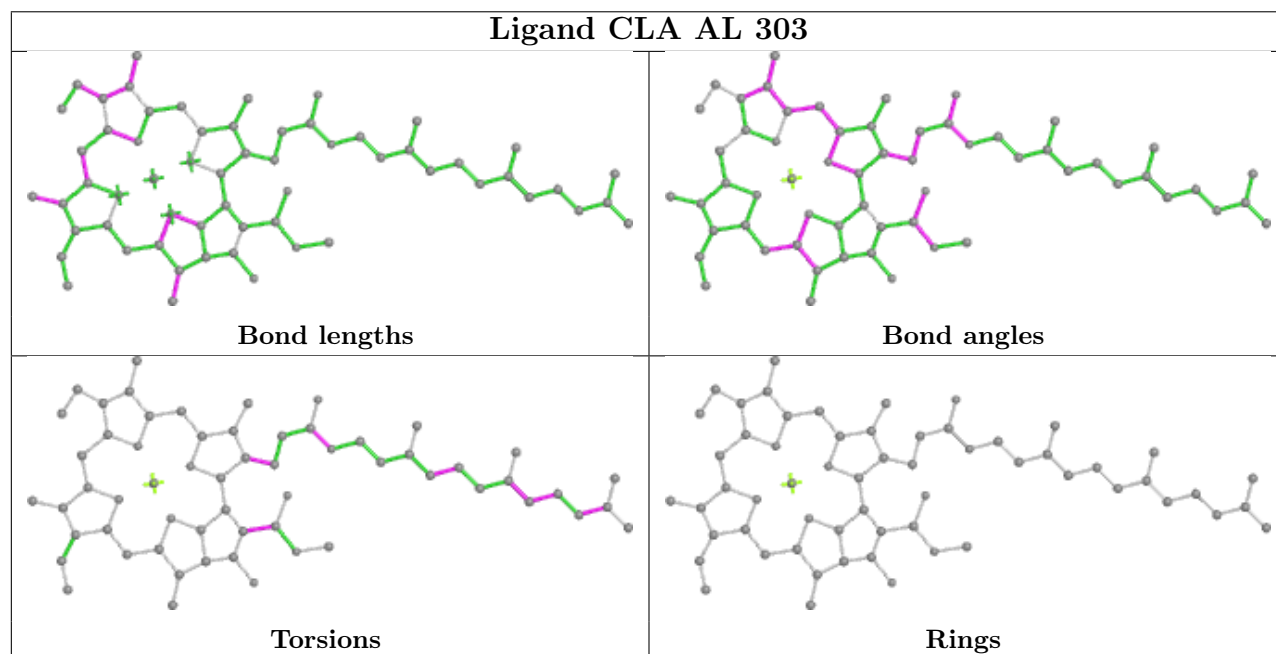
Ligand DGD AB 851

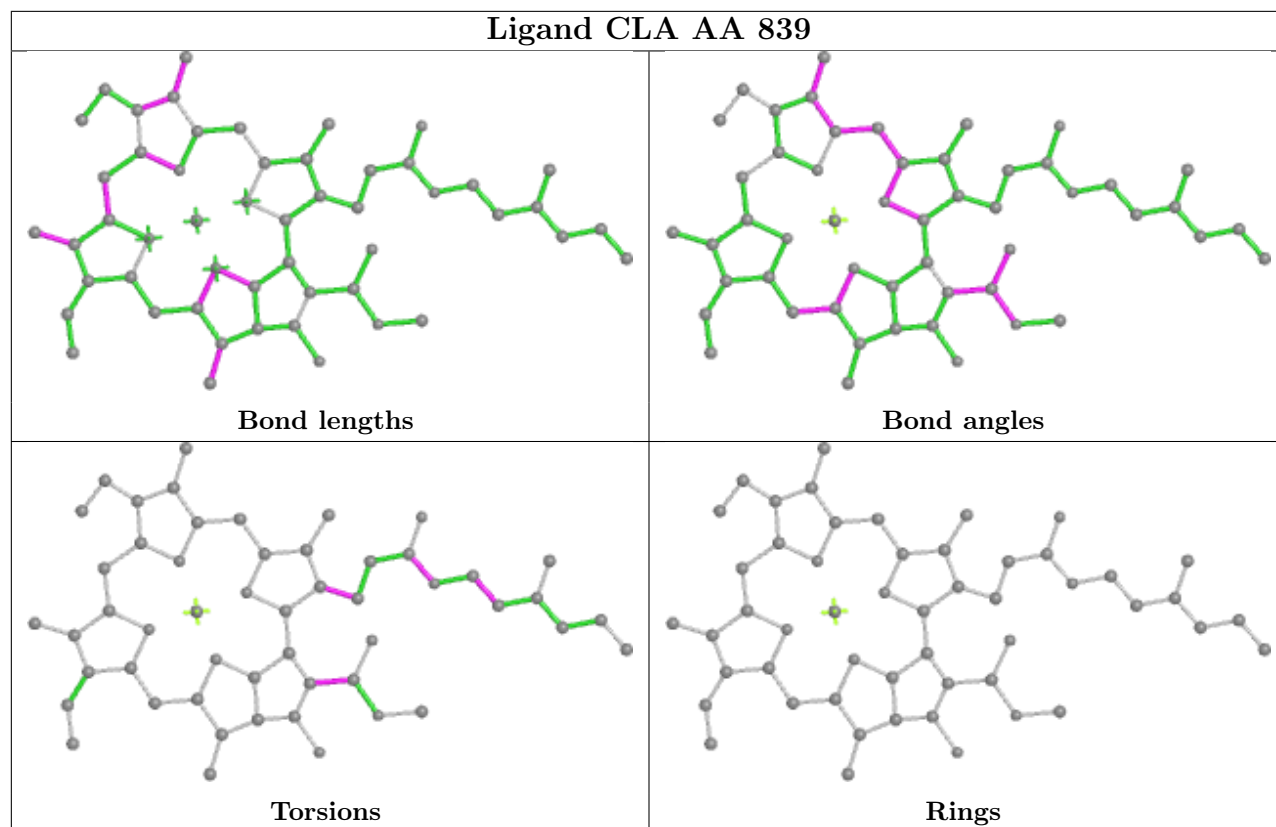


Ligand CLA AB 818

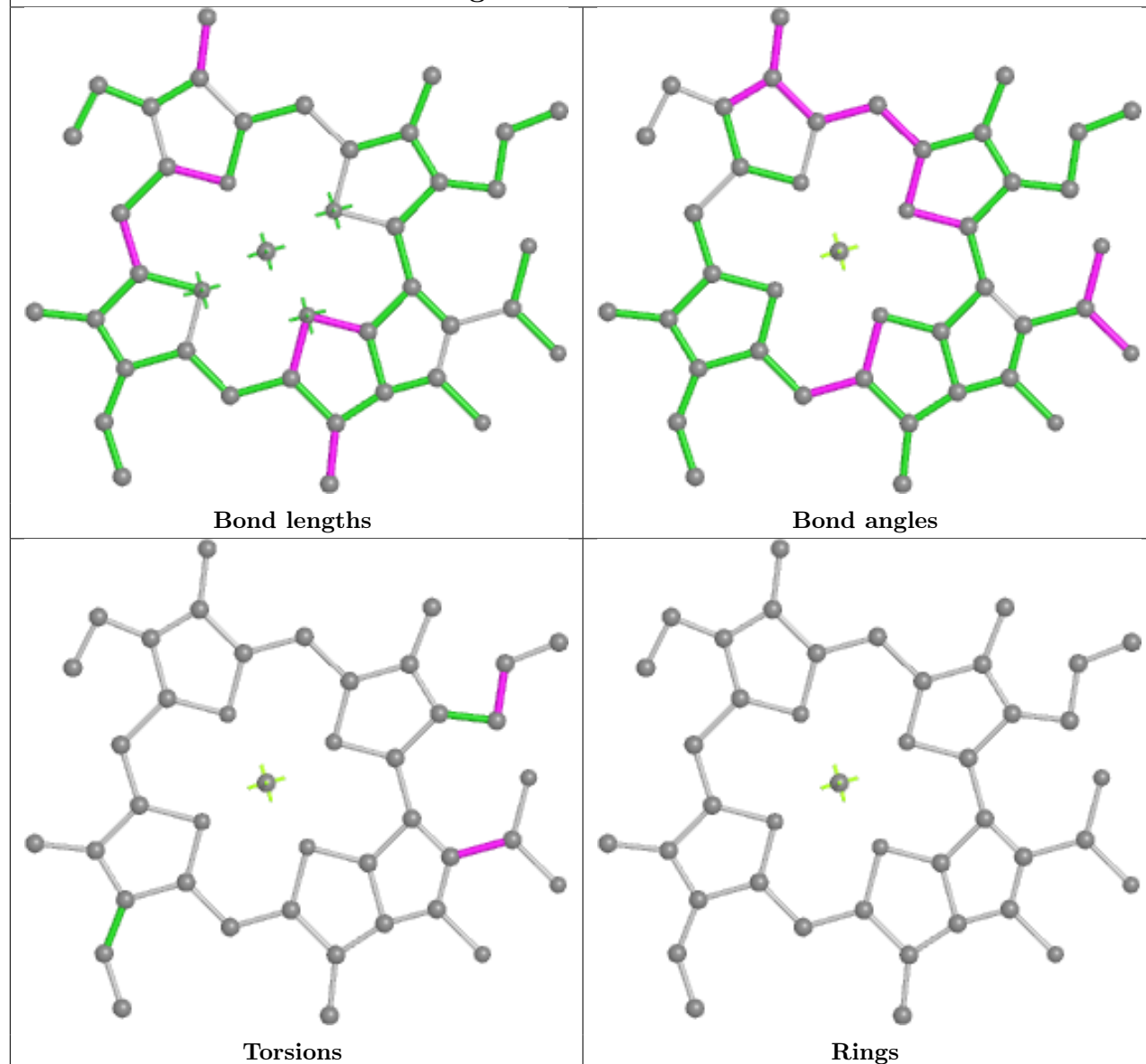


Ligand CLA AL 303

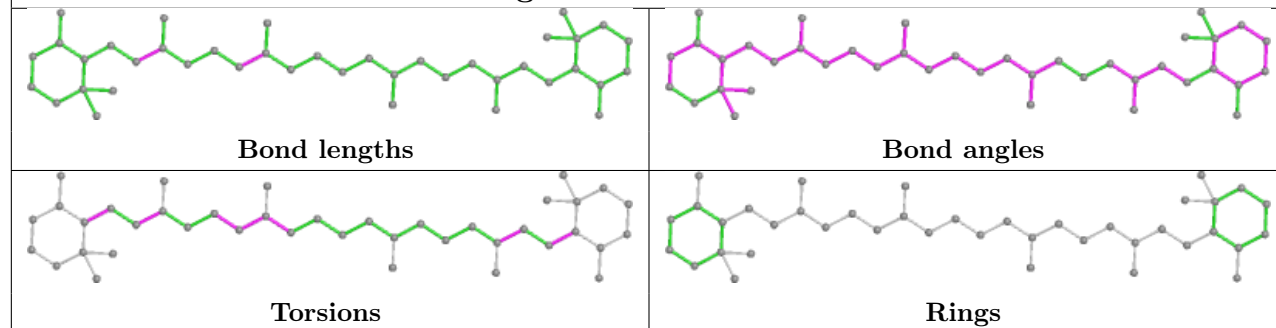




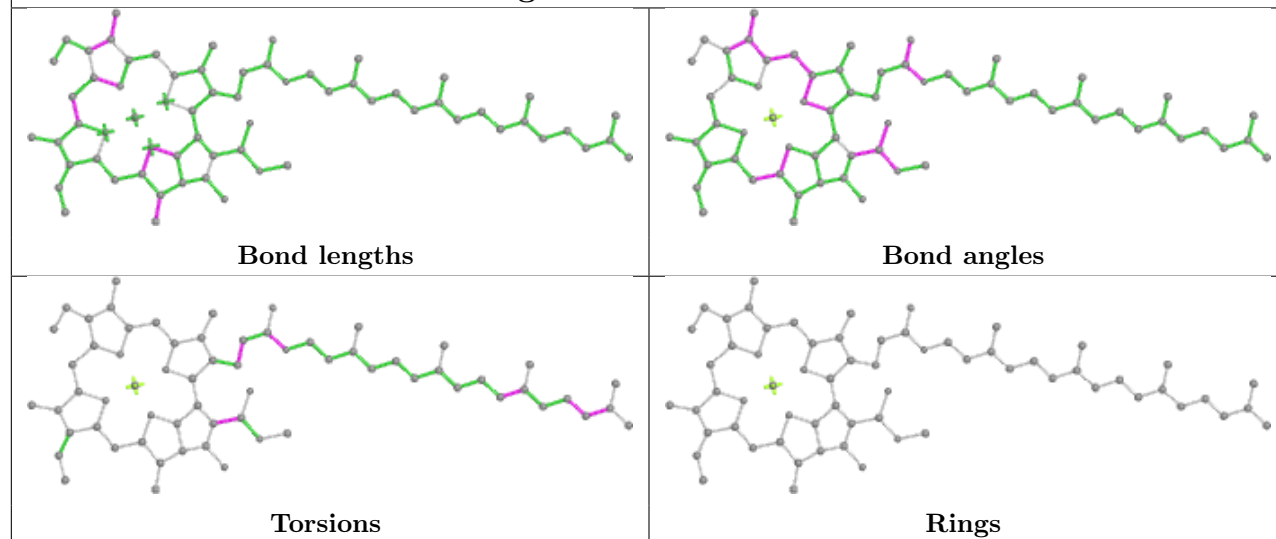
Ligand CLA A6 603



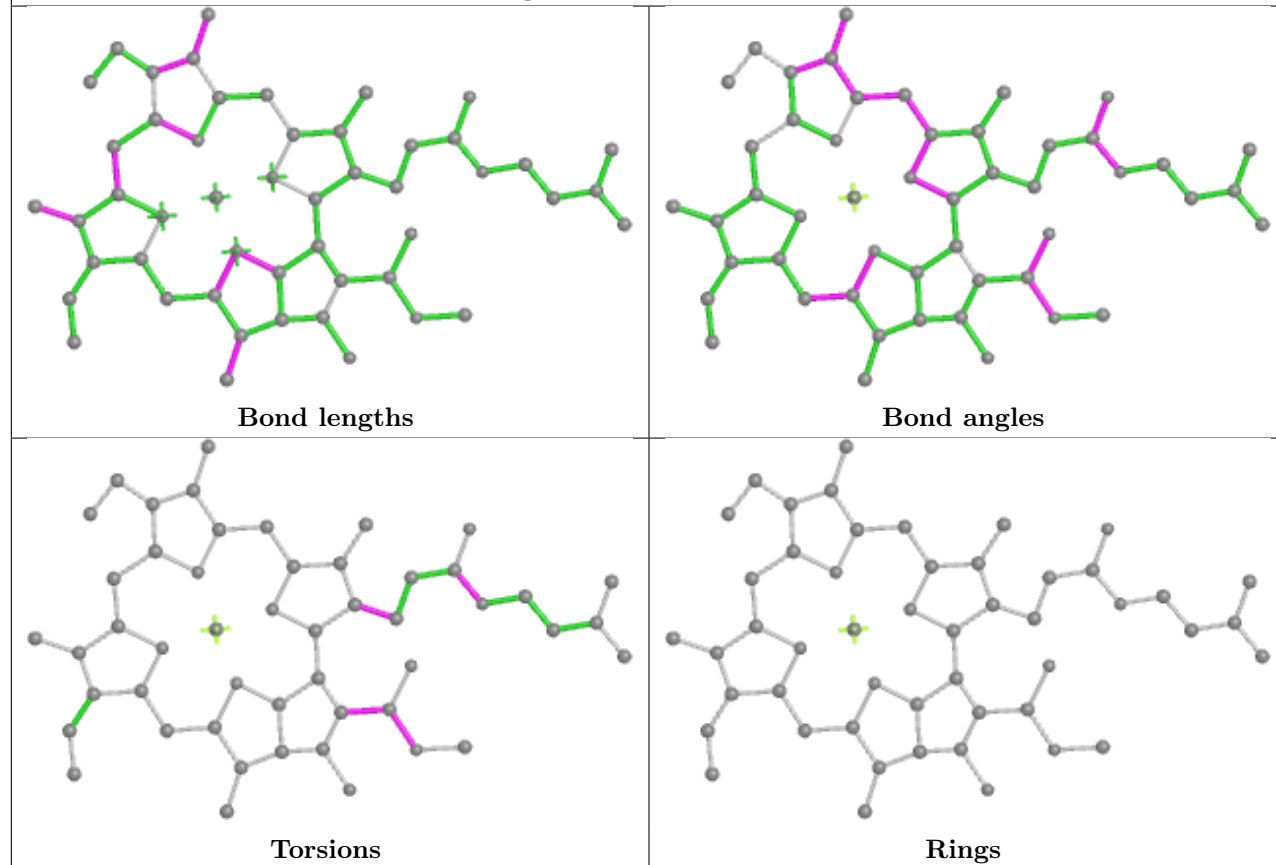
Ligand BCR AA 847



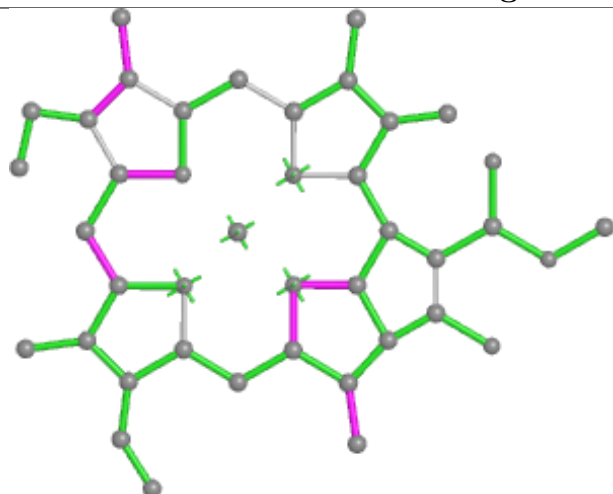
Ligand CLA AA 808



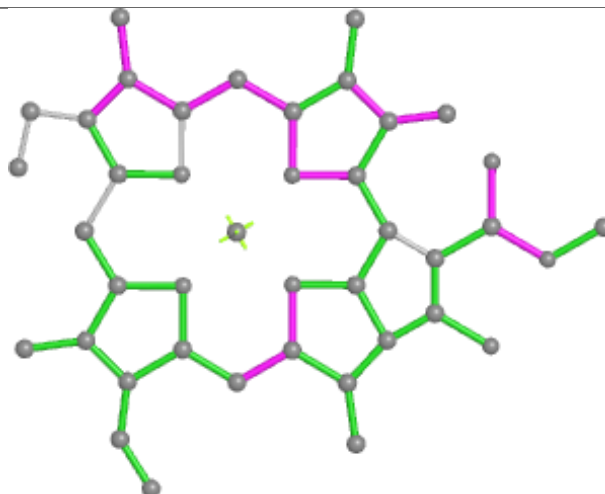
Ligand CLA AB 821



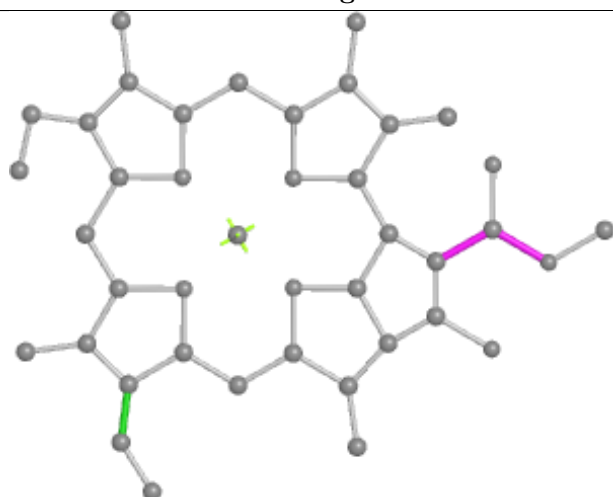
Ligand CLA AA 823



Bond lengths



Bond angles

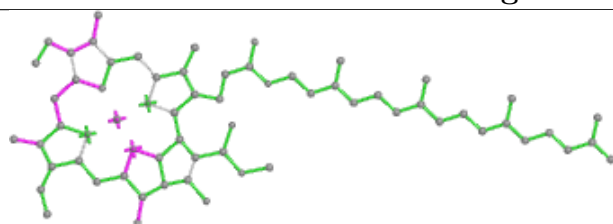


Torsions

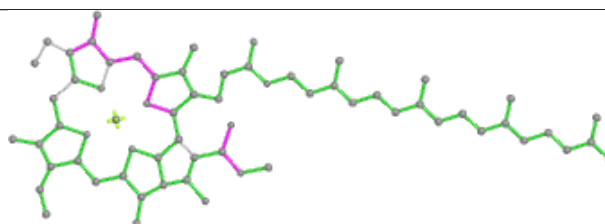


Rings

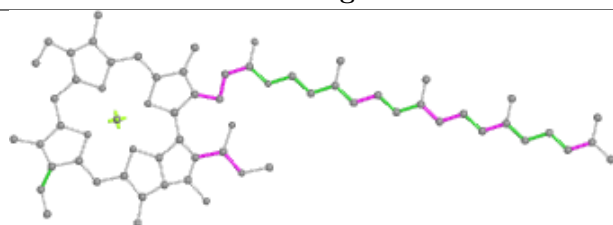
Ligand CLA AB 810



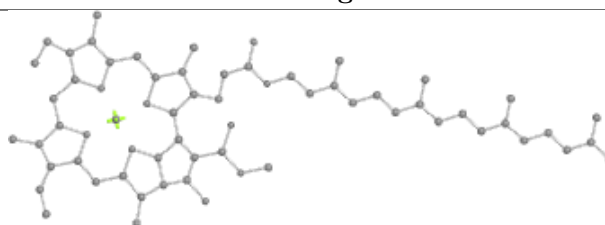
Bond lengths



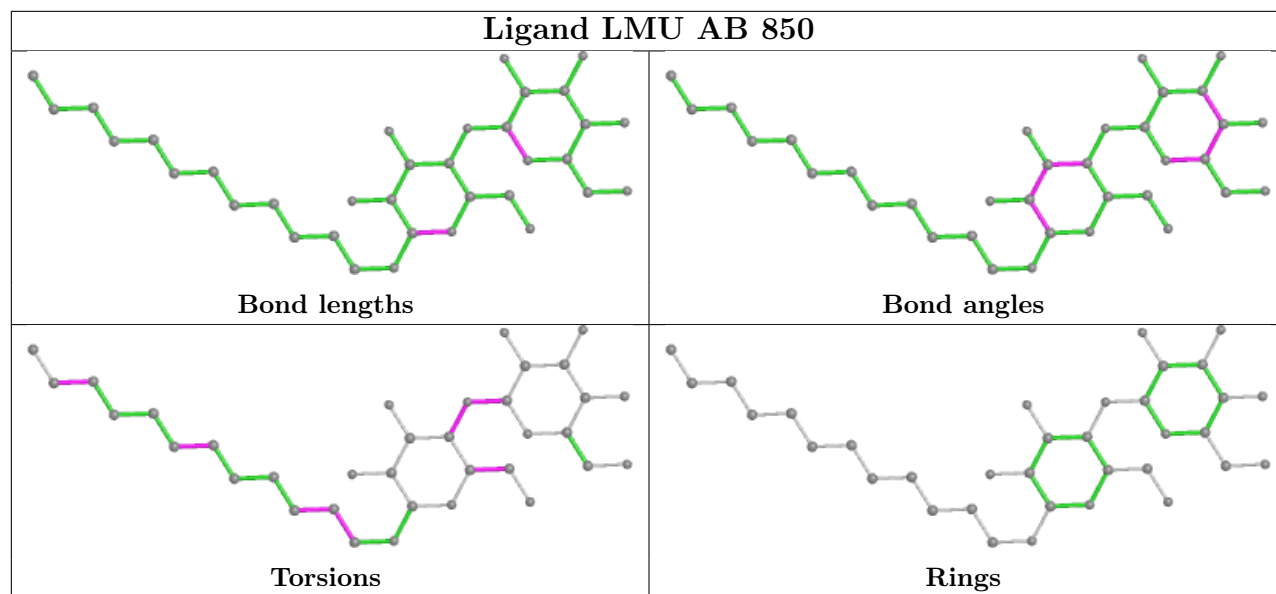
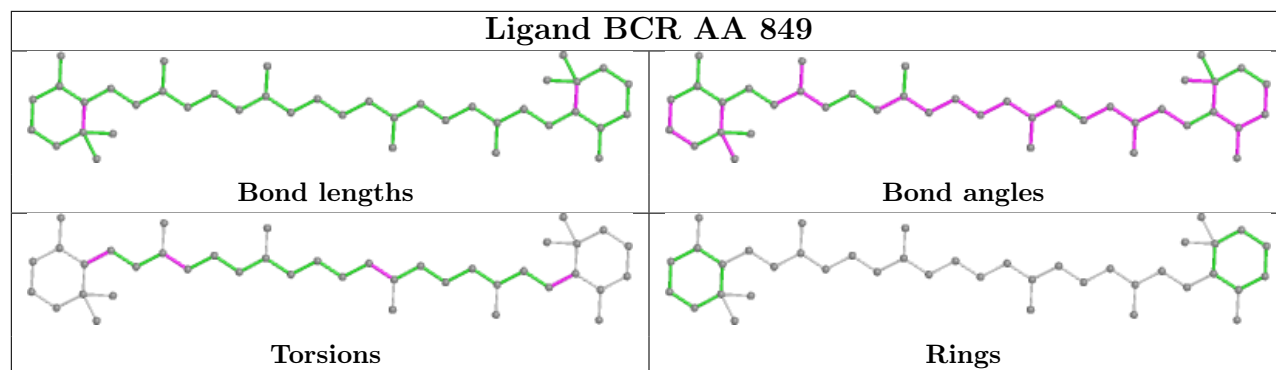
Bond angles



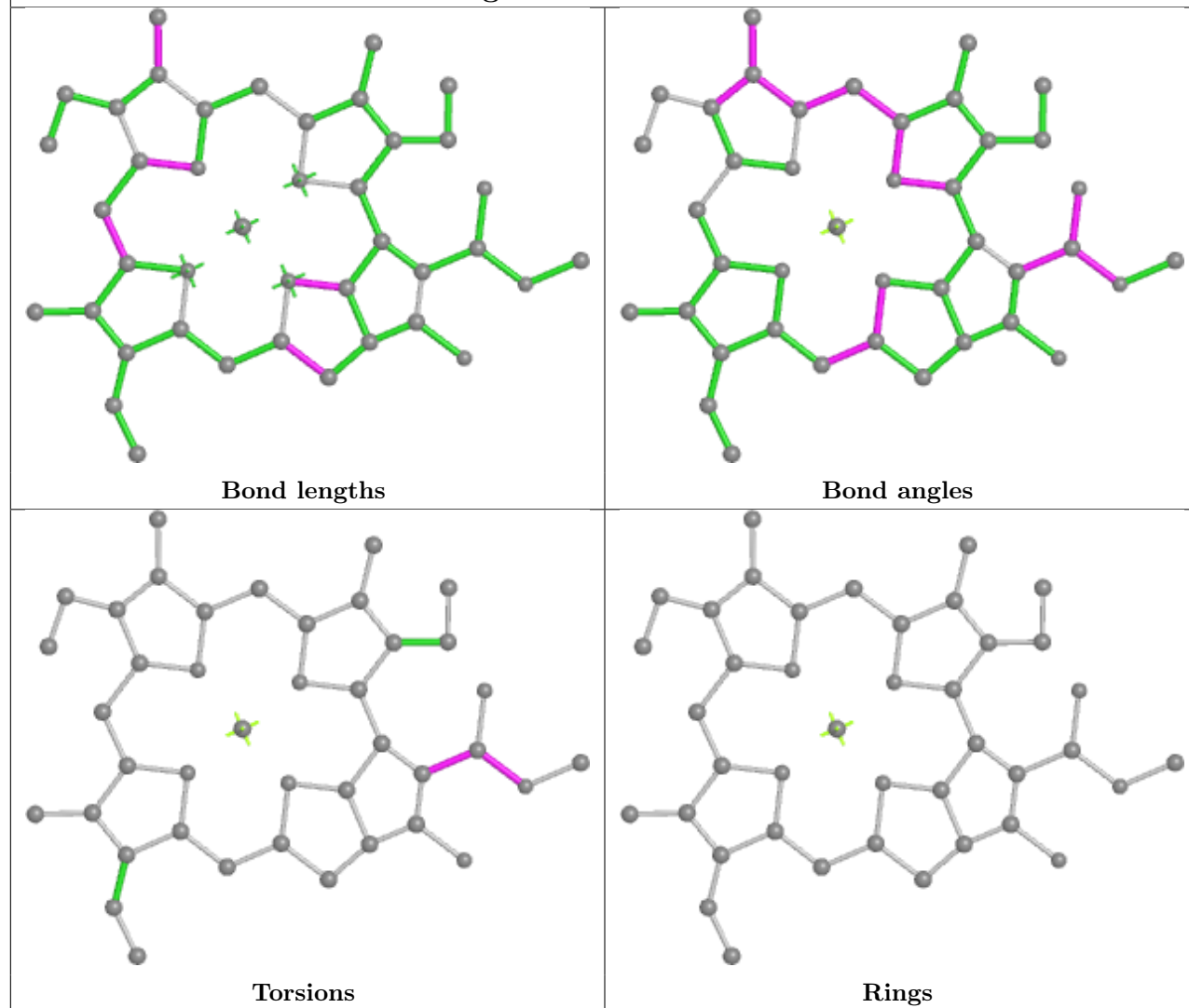
Torsions



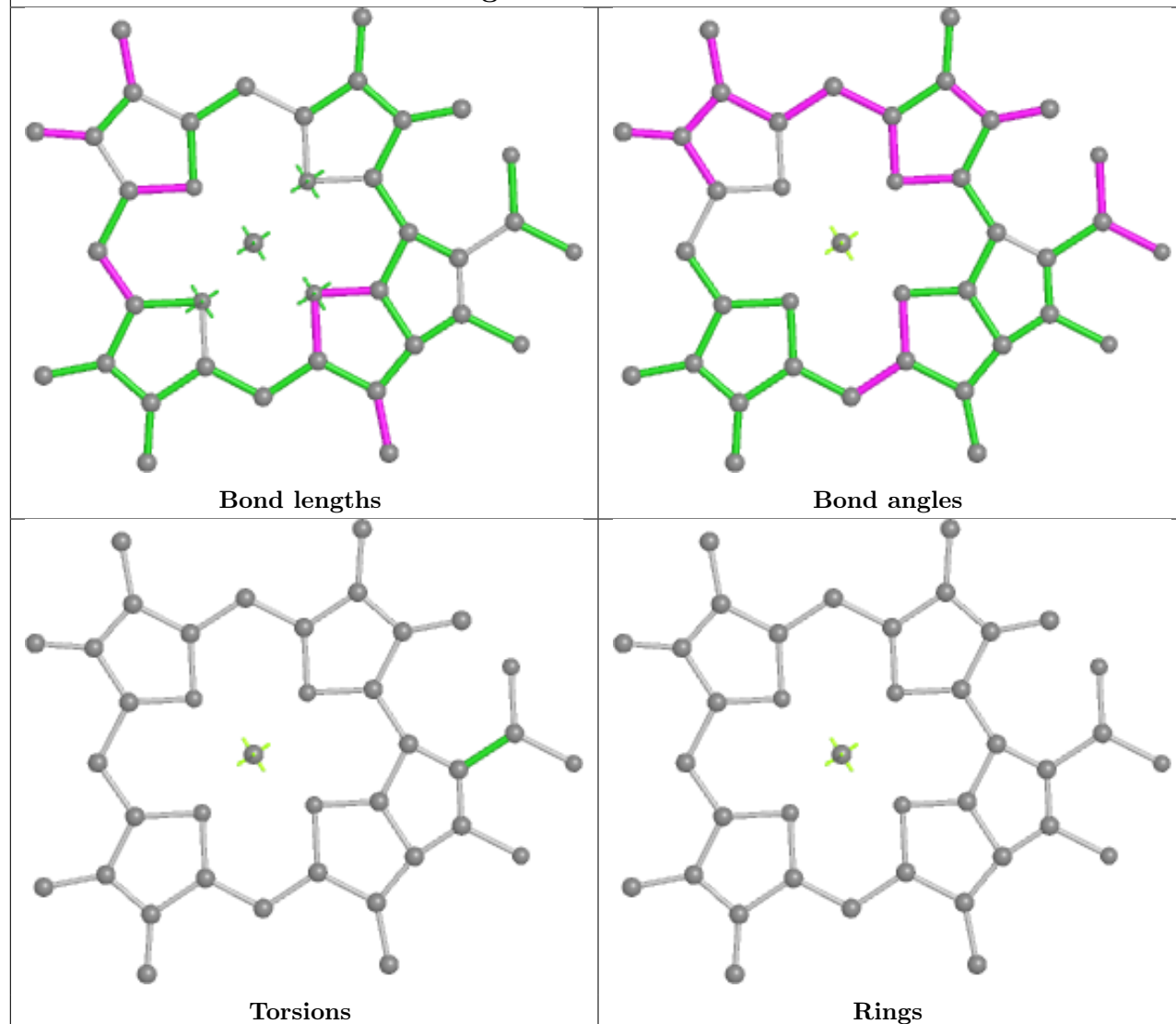
Rings



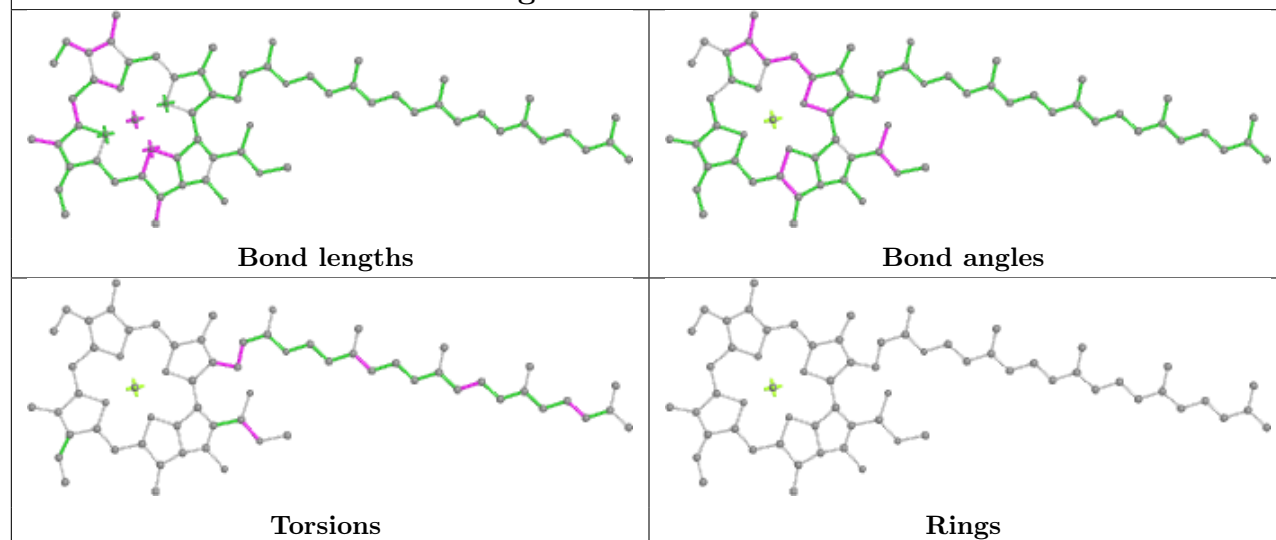
Ligand CLA AA 815

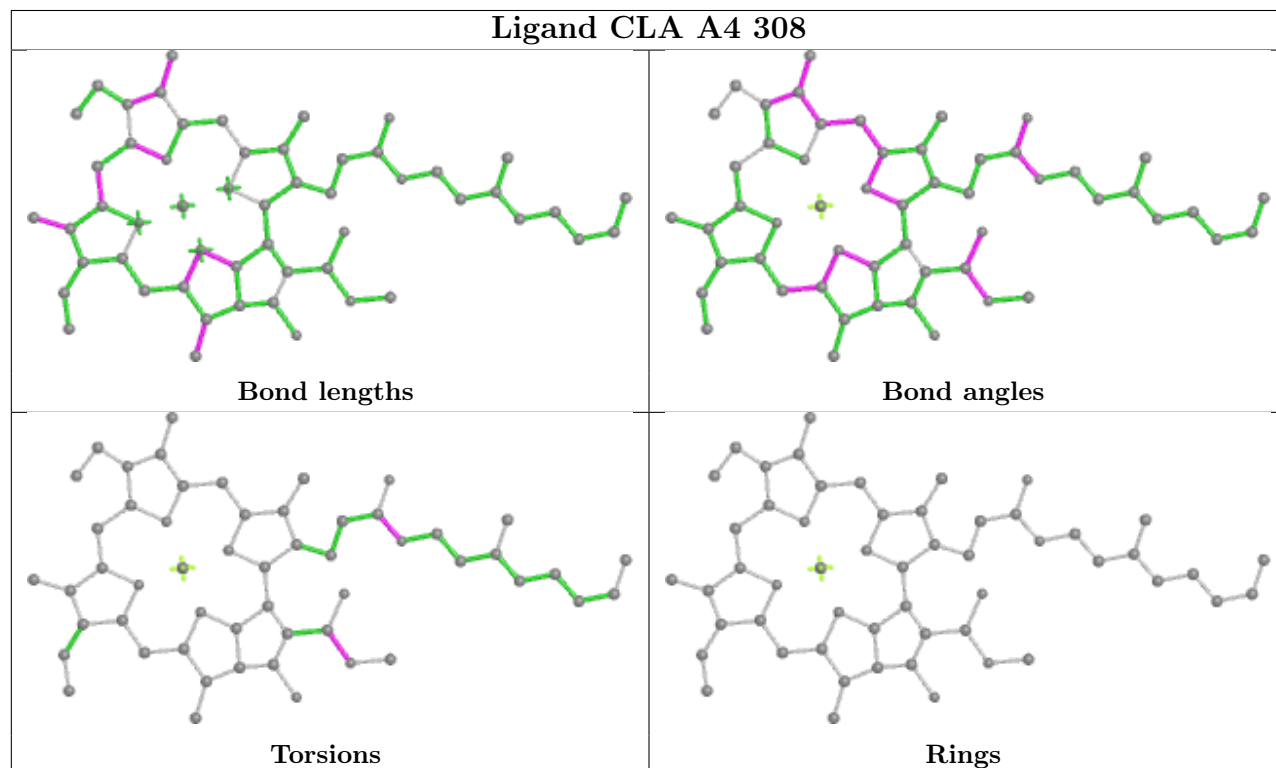
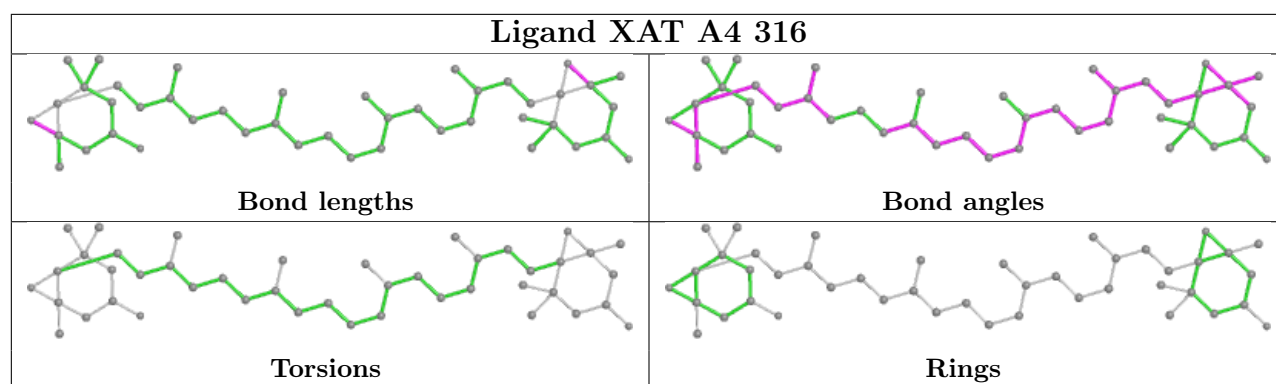


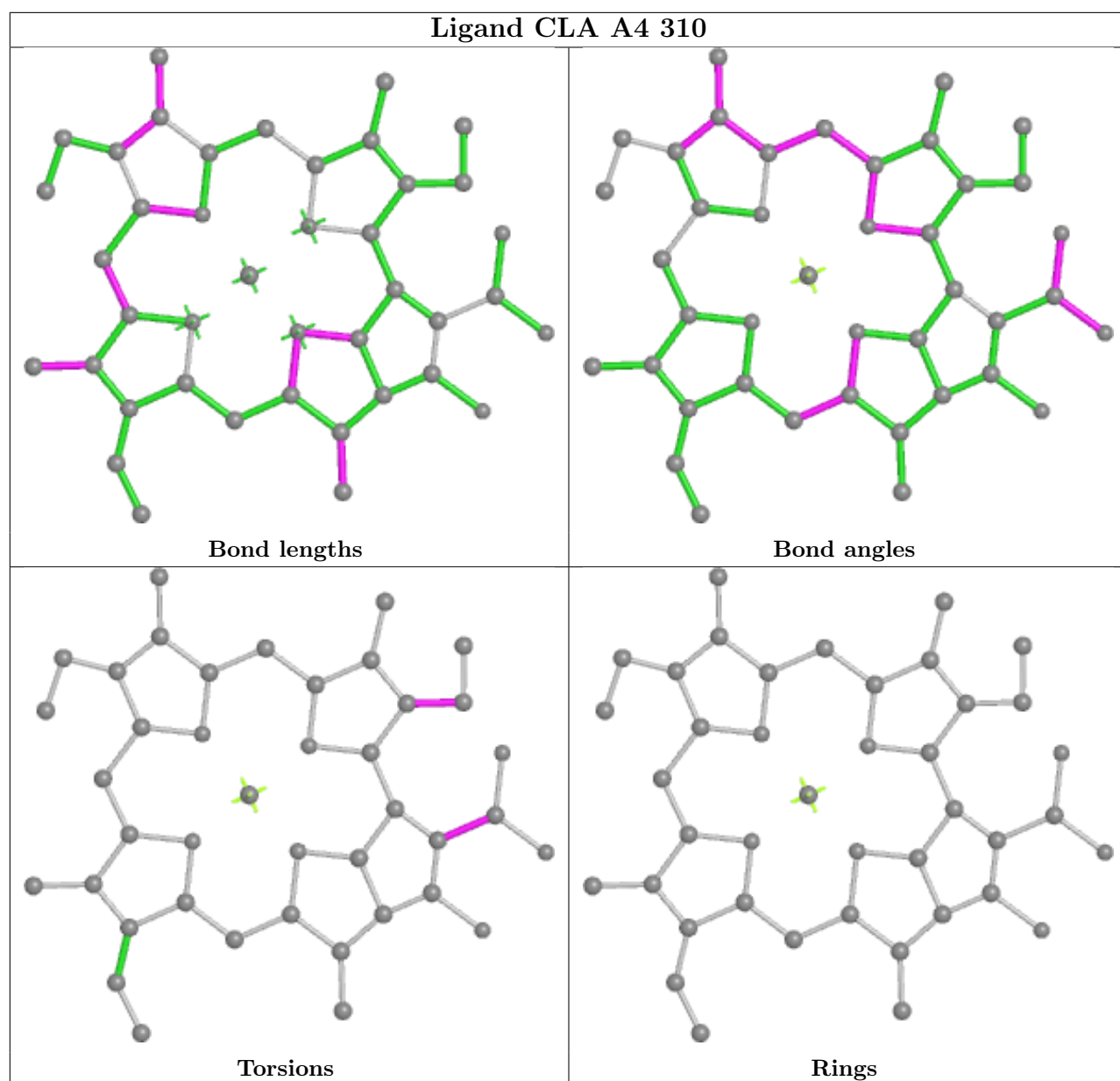
Ligand CLA A1 312



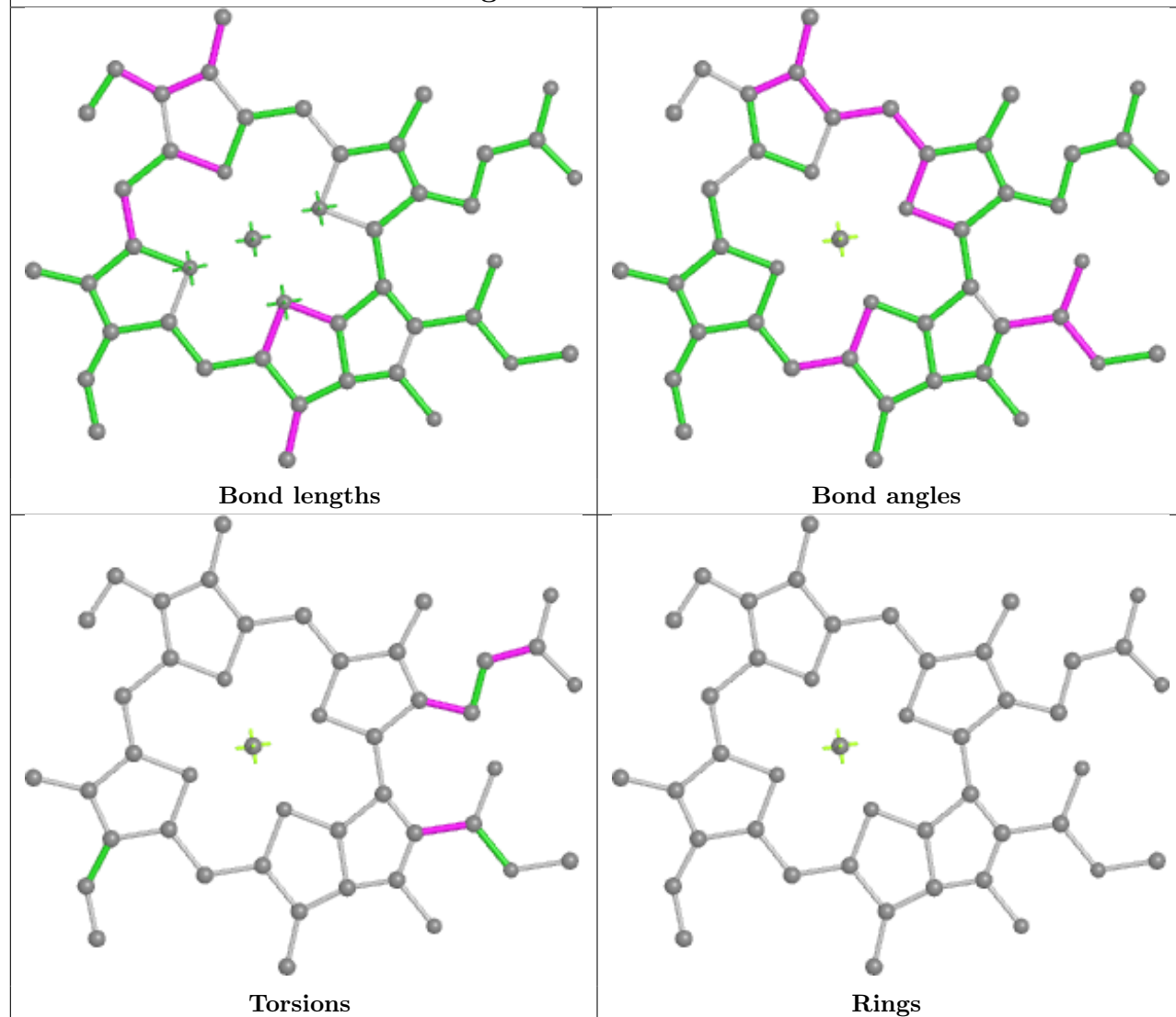
Ligand CLA AA 802



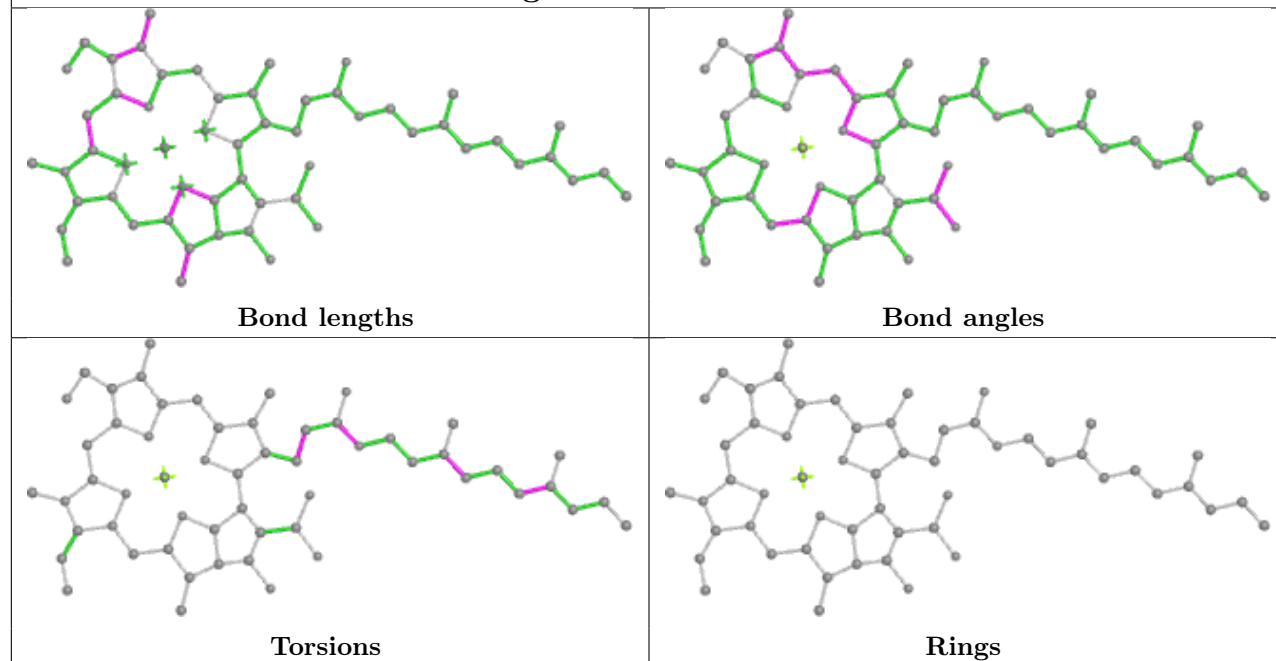




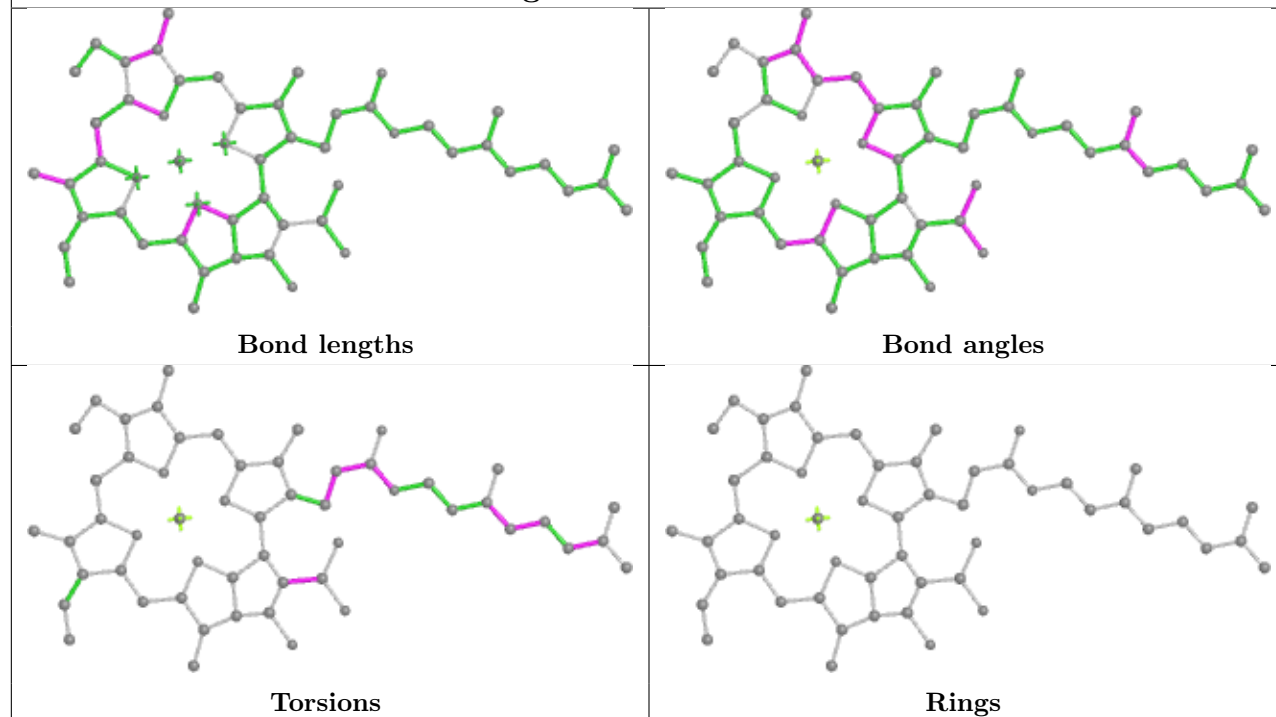
Ligand CLA A3 308



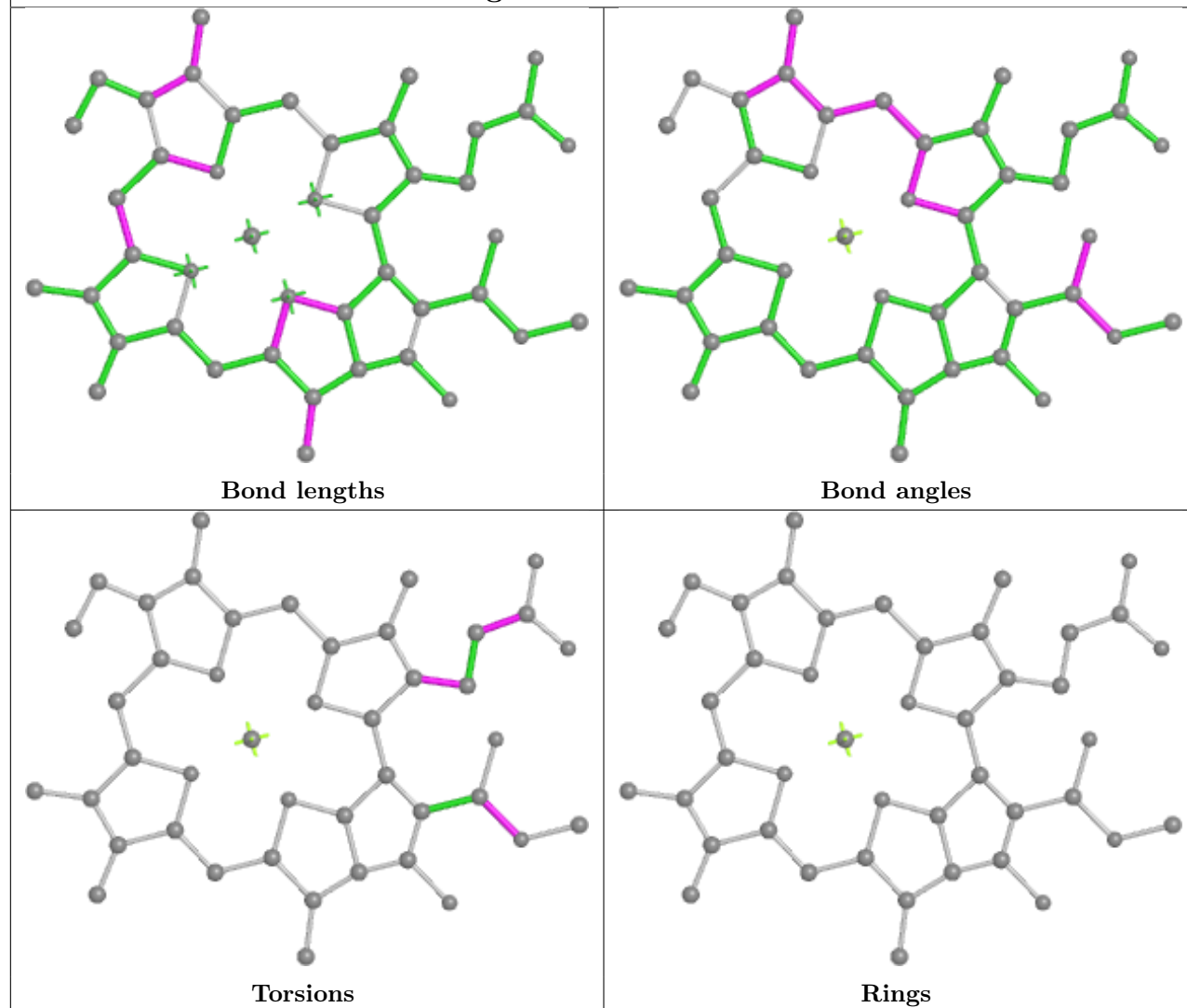
Ligand CLA A4 311



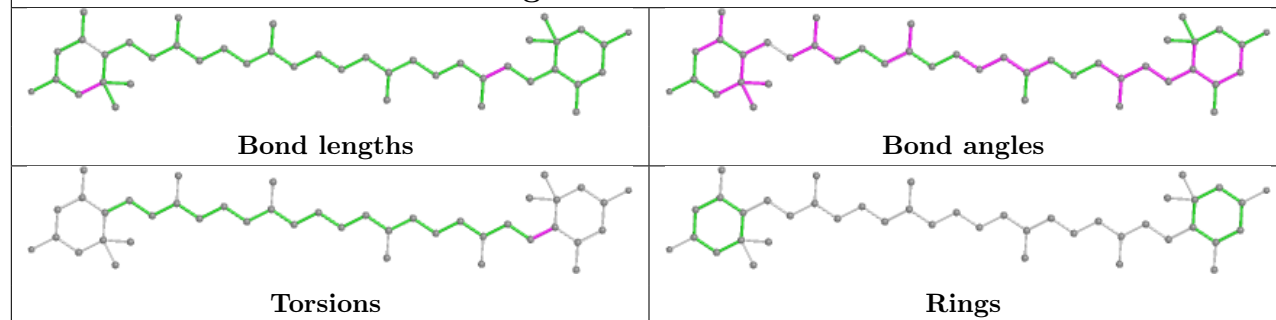
Ligand CLA A3 312

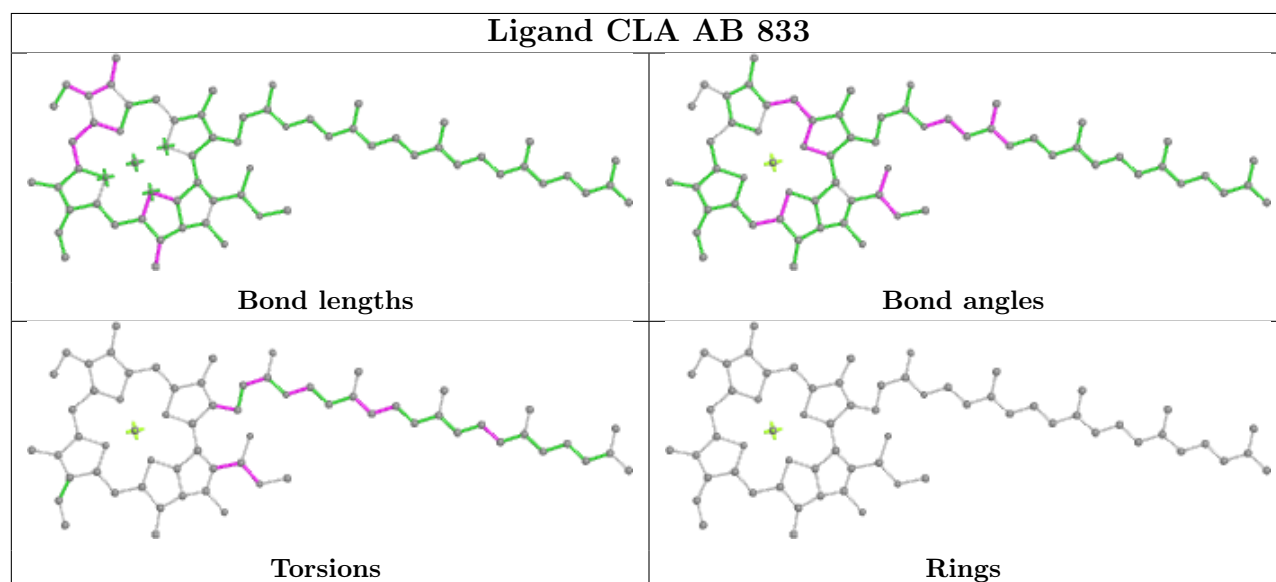
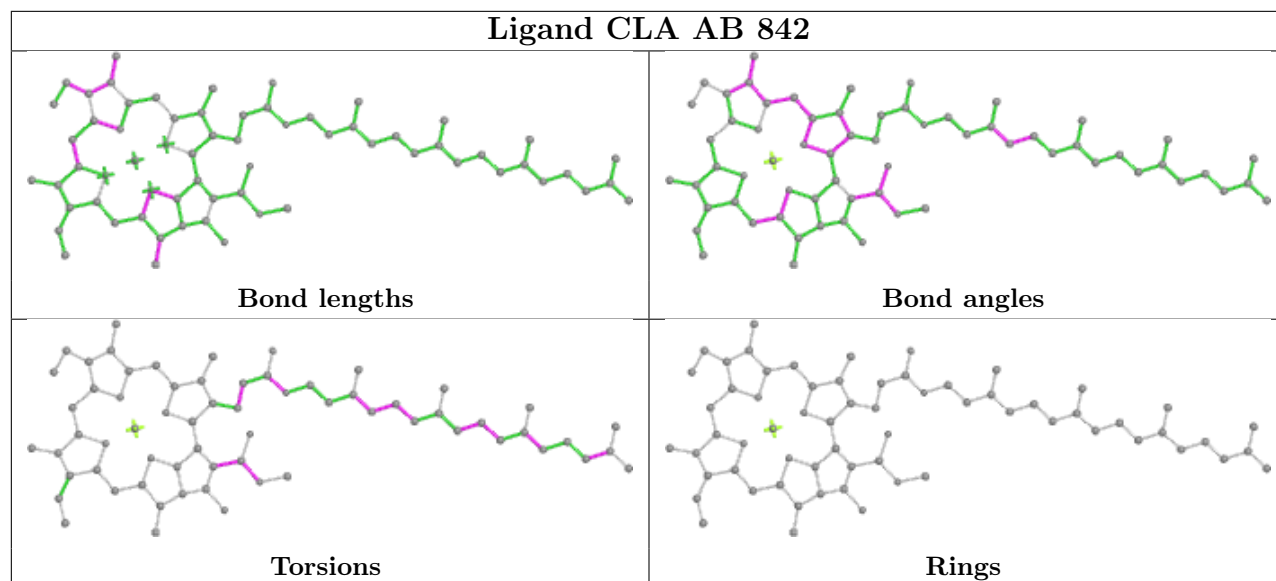
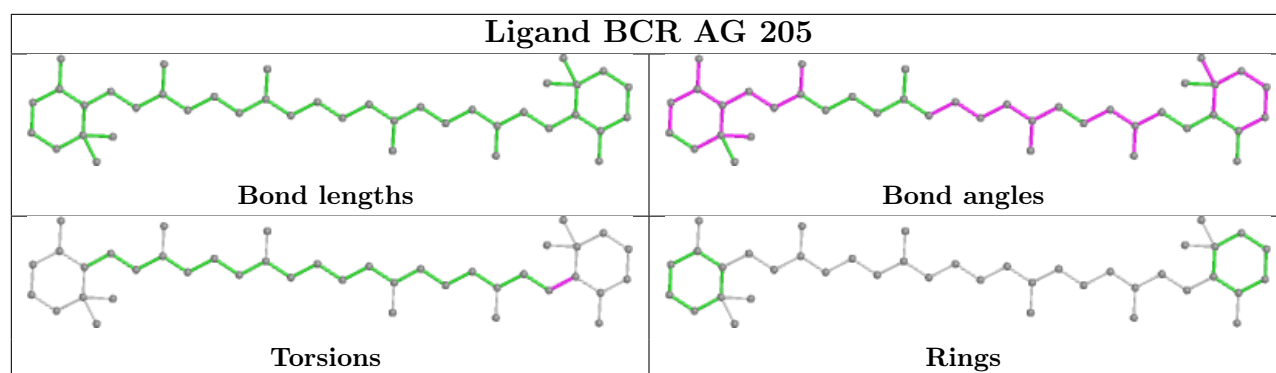


Ligand CLA A6 611

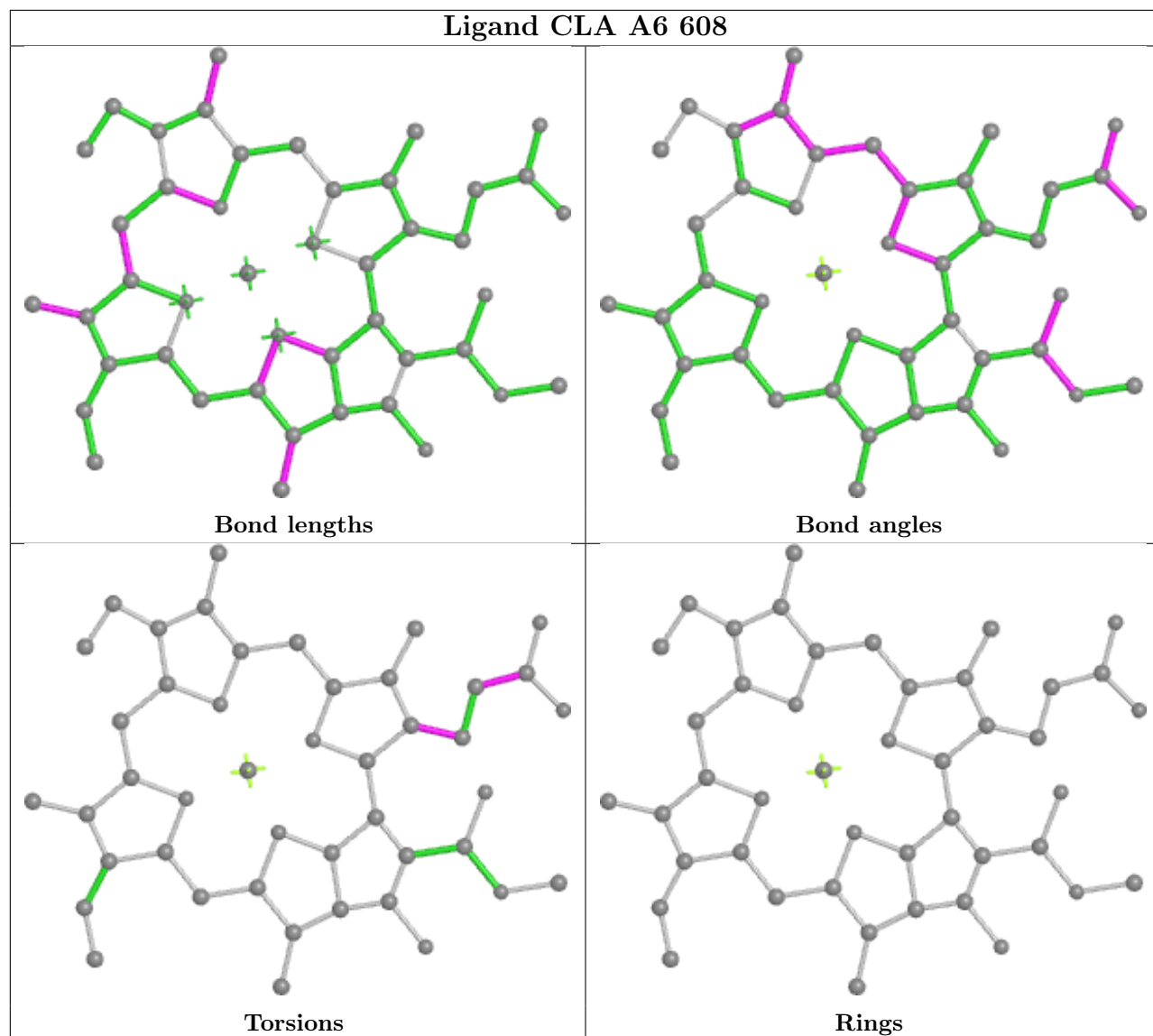


Ligand LUT A4 315

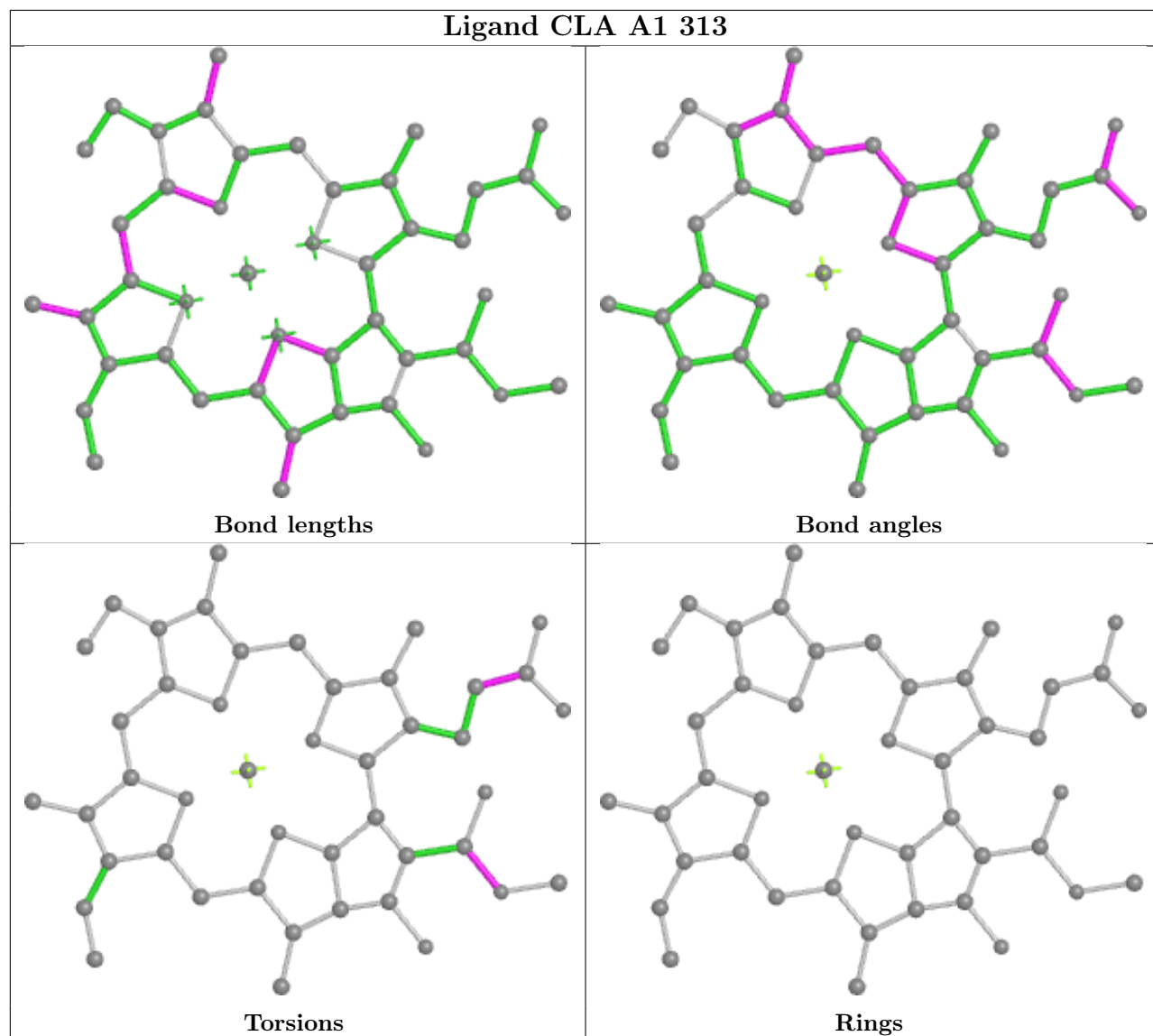




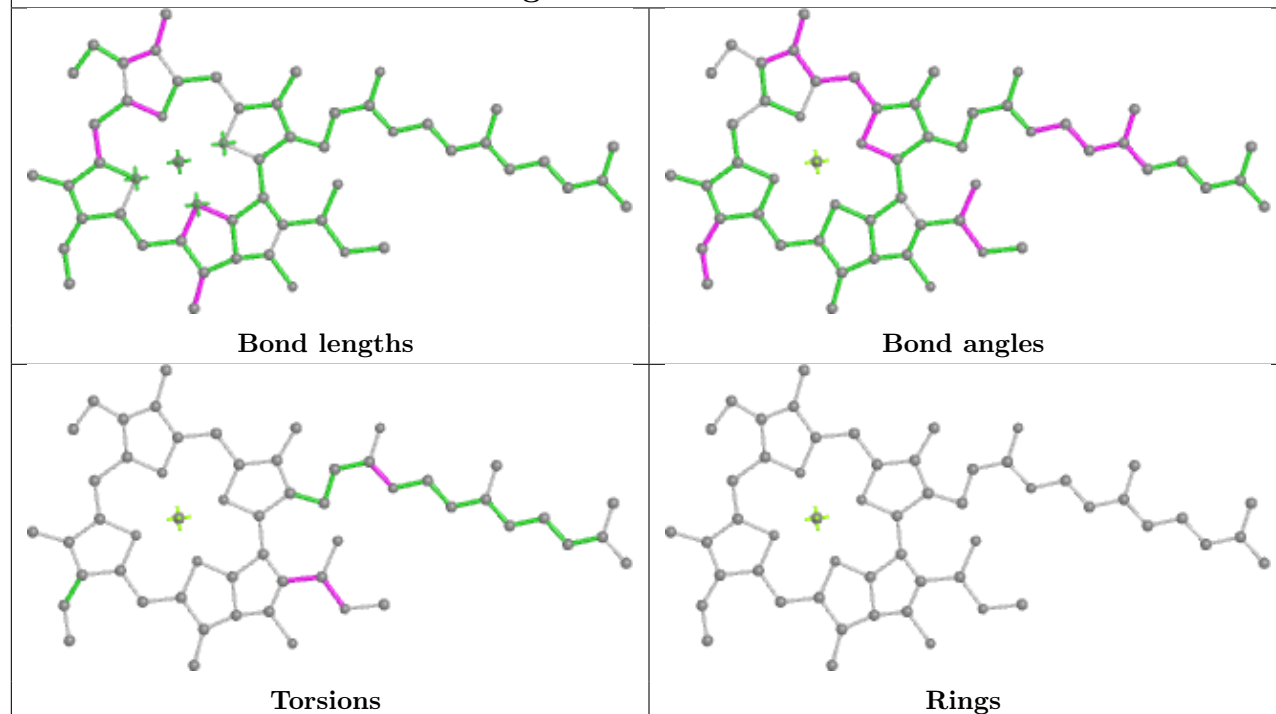
Ligand CLA A6 608



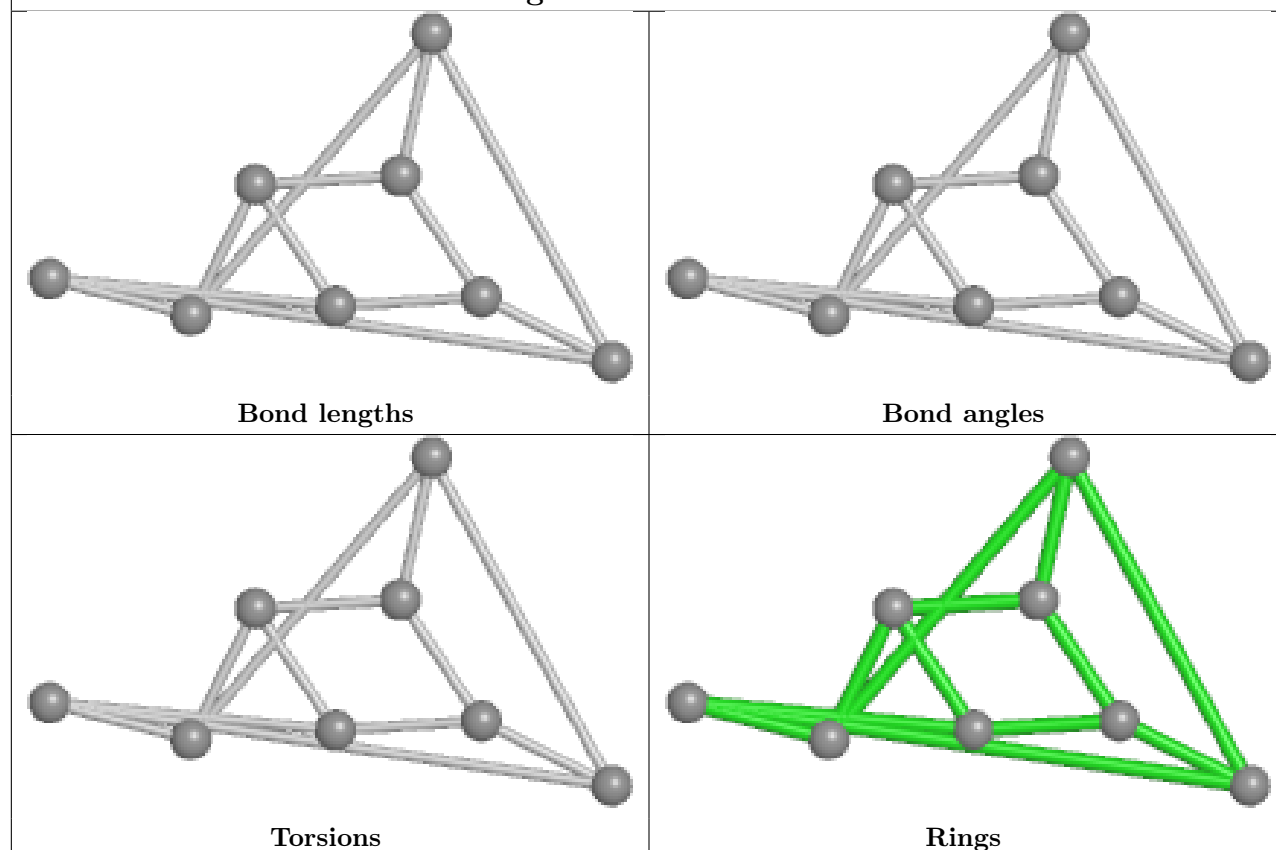
Ligand CLA A1 313



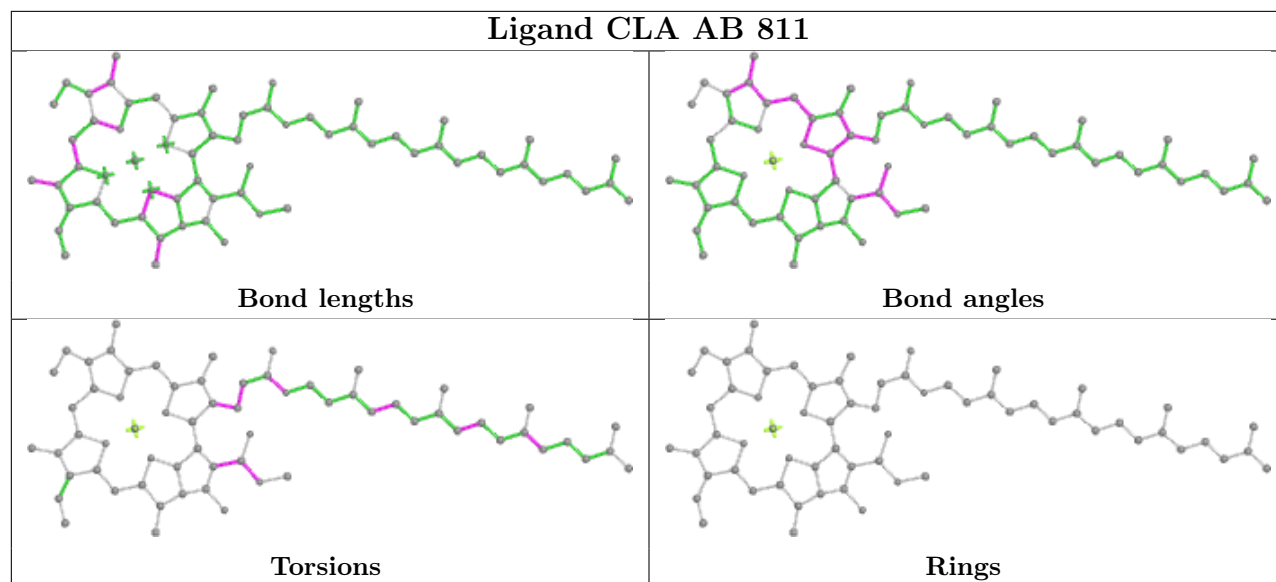
Ligand CLA A1 305



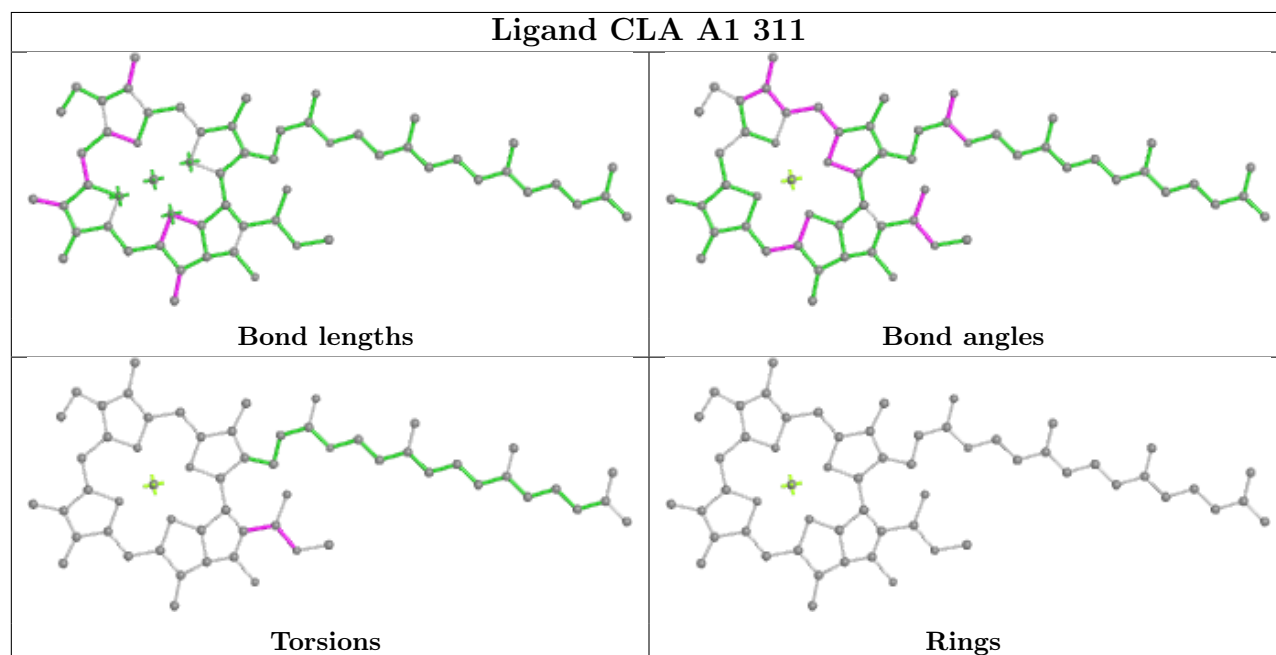
Ligand SF4 AC 102

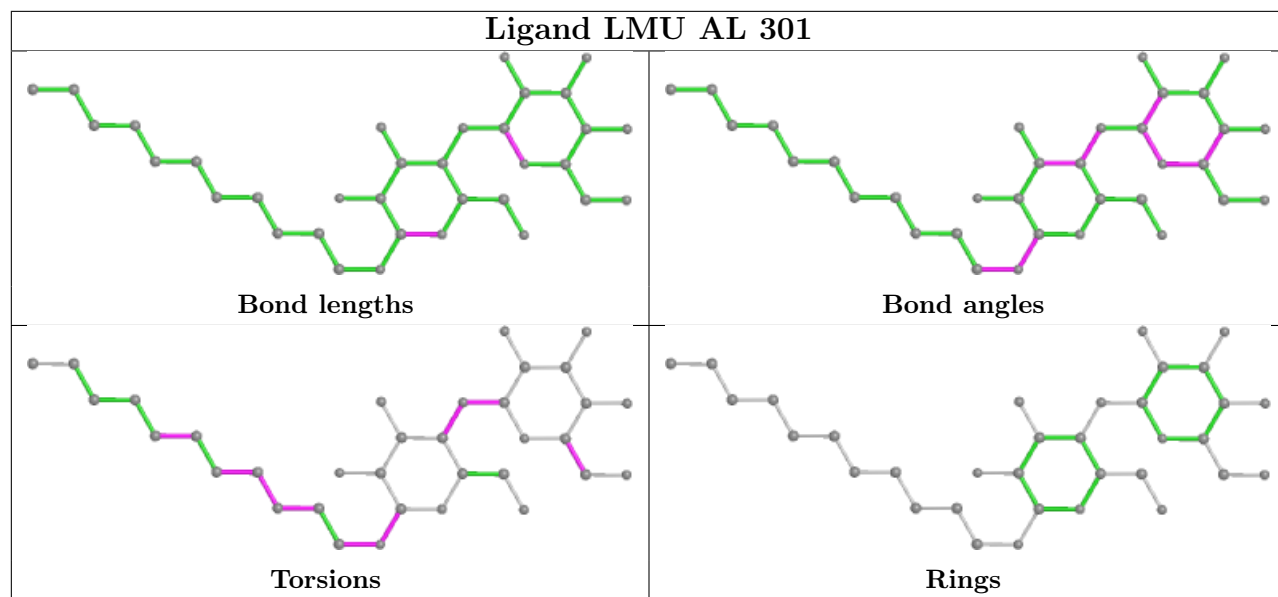


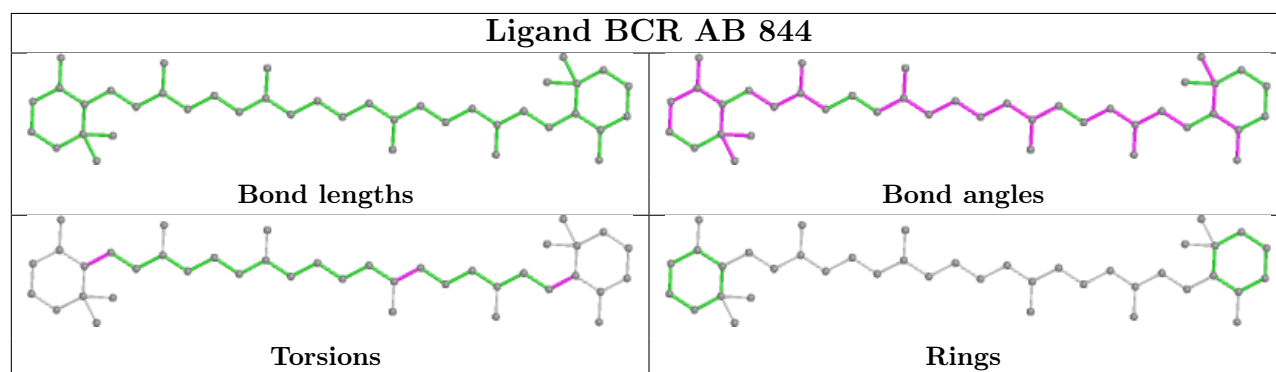
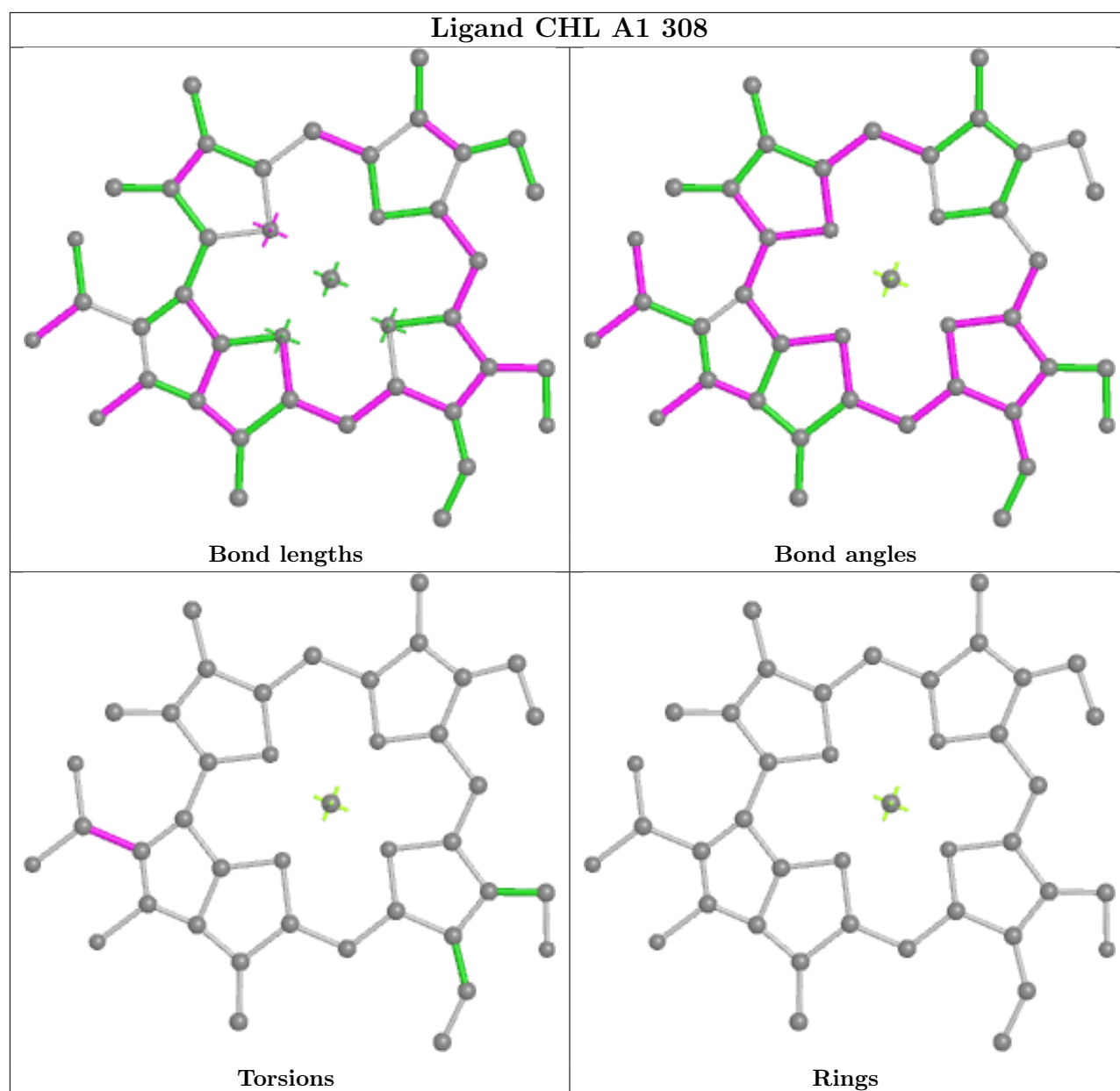
Ligand CLA AB 811



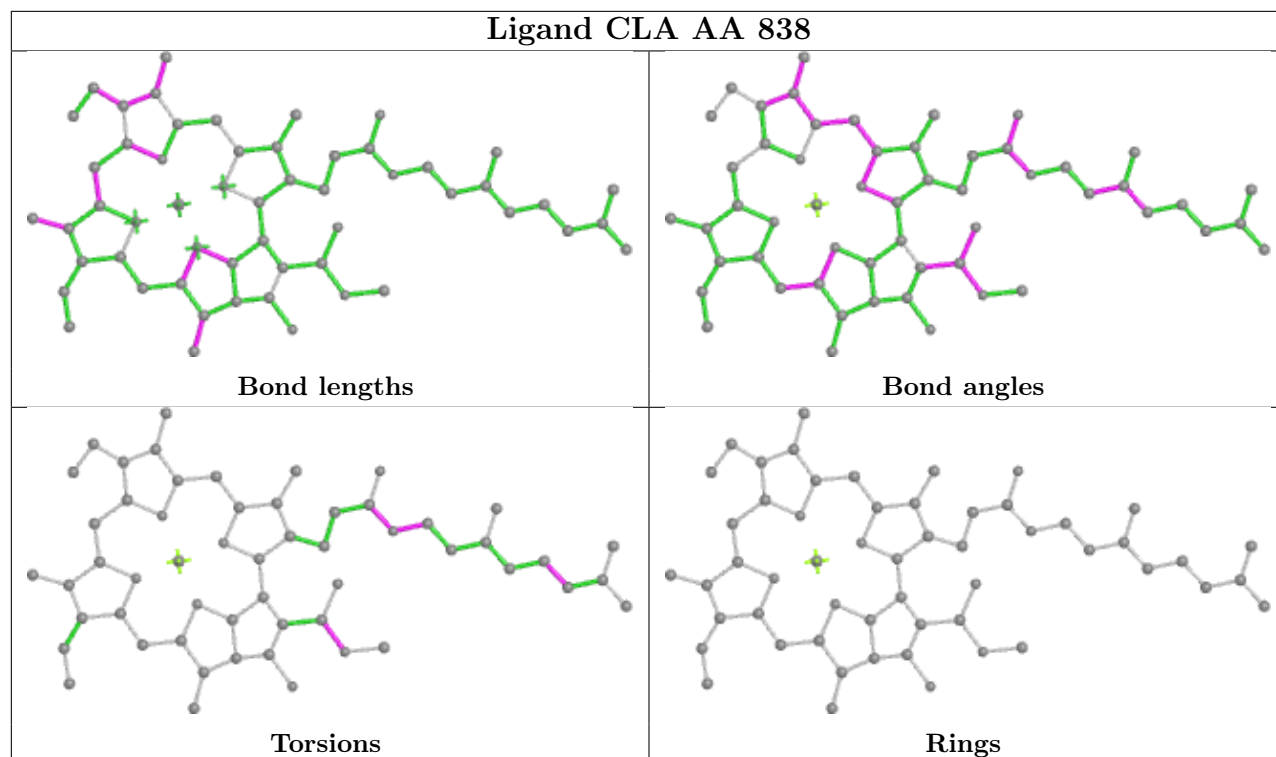
Ligand CLA A1 311



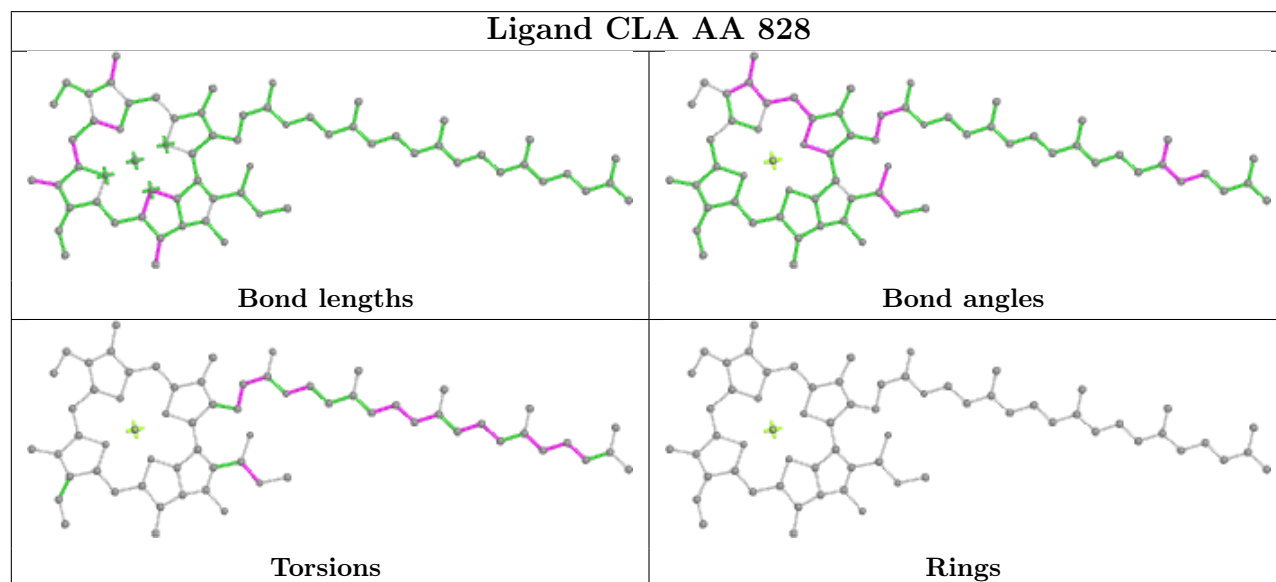




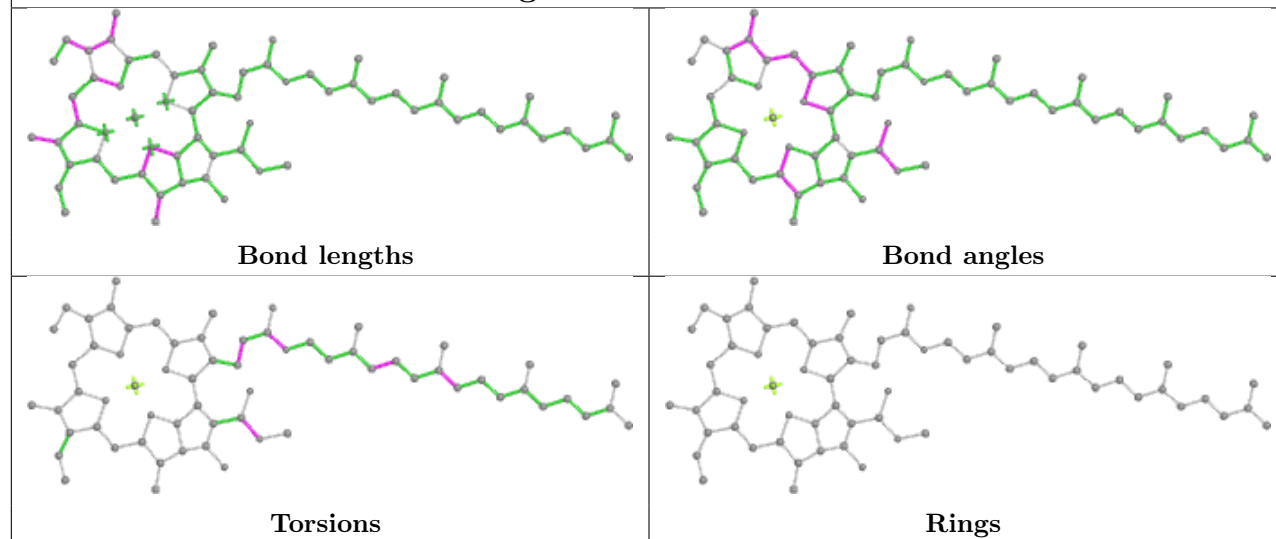
Ligand CLA AA 838



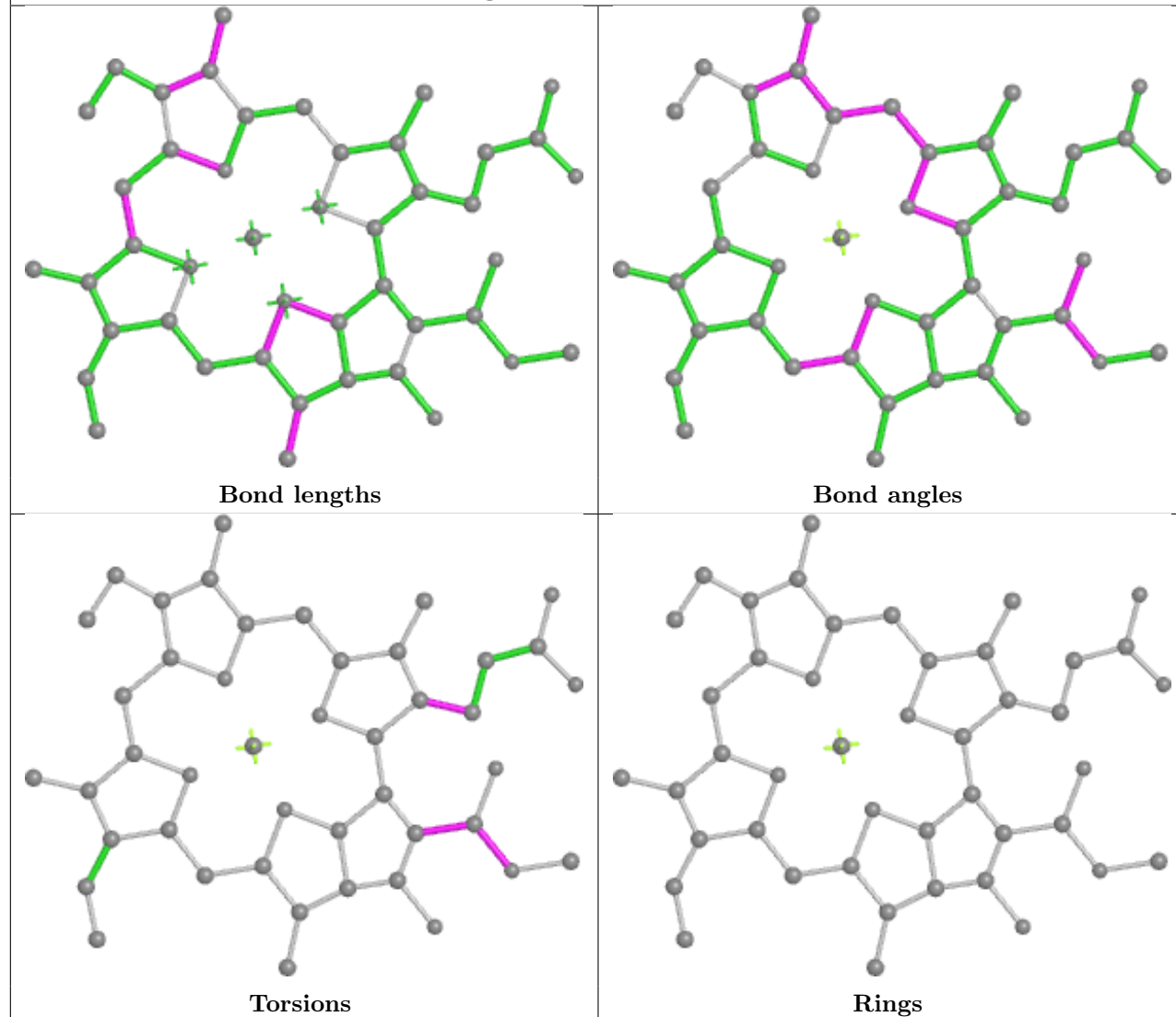
Ligand CLA AA 828

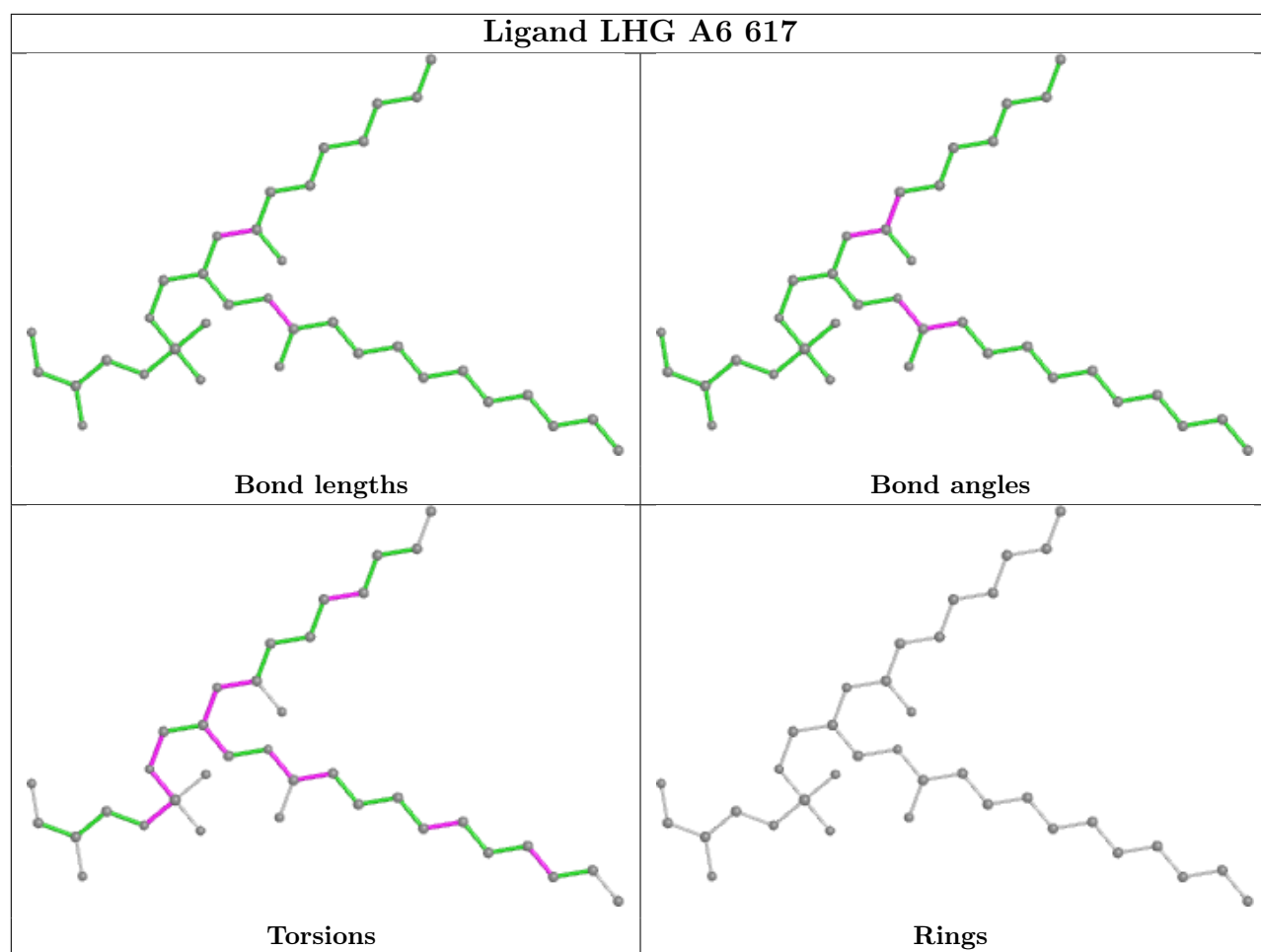


Ligand CLA AB 840

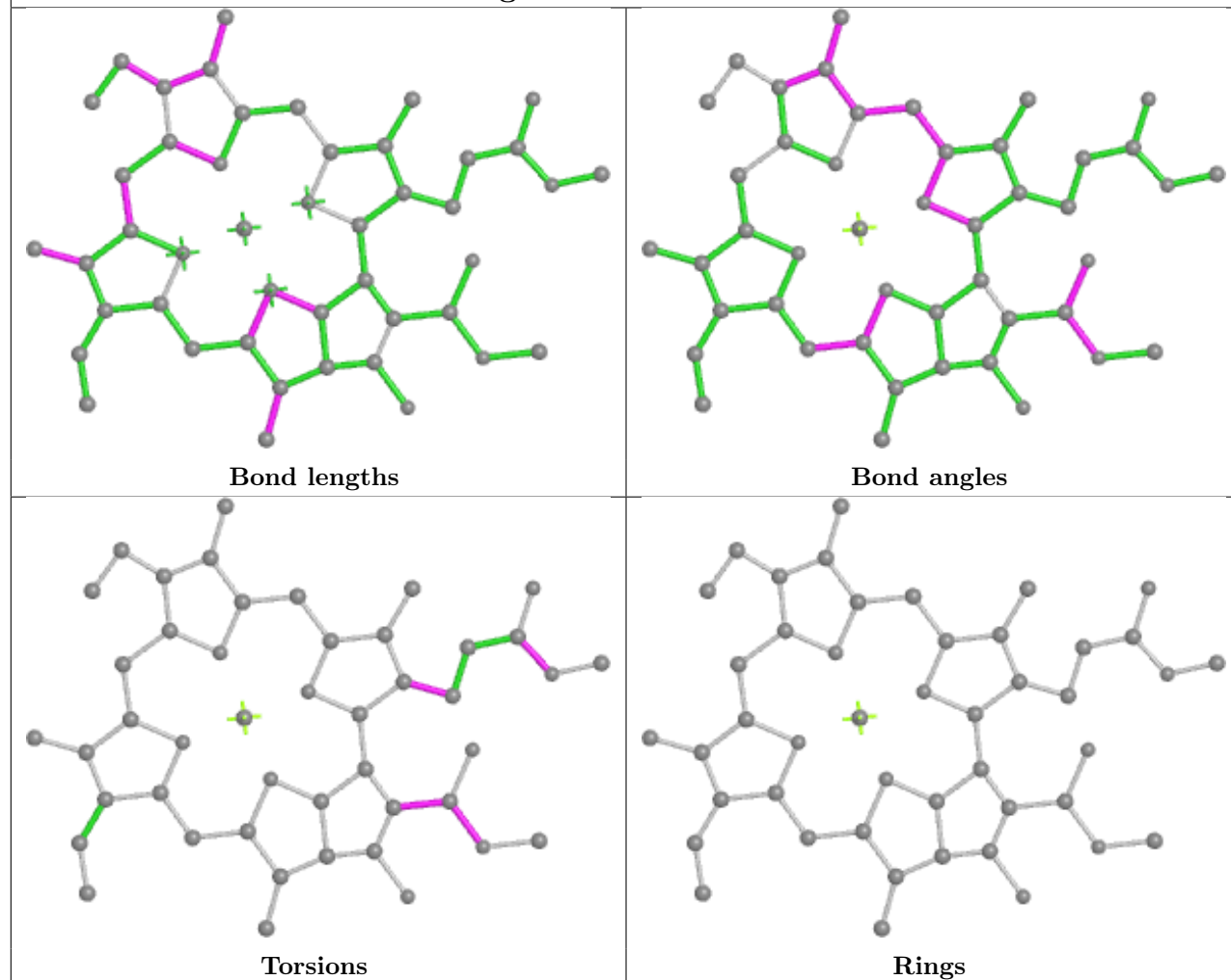


Ligand CLA A4 312

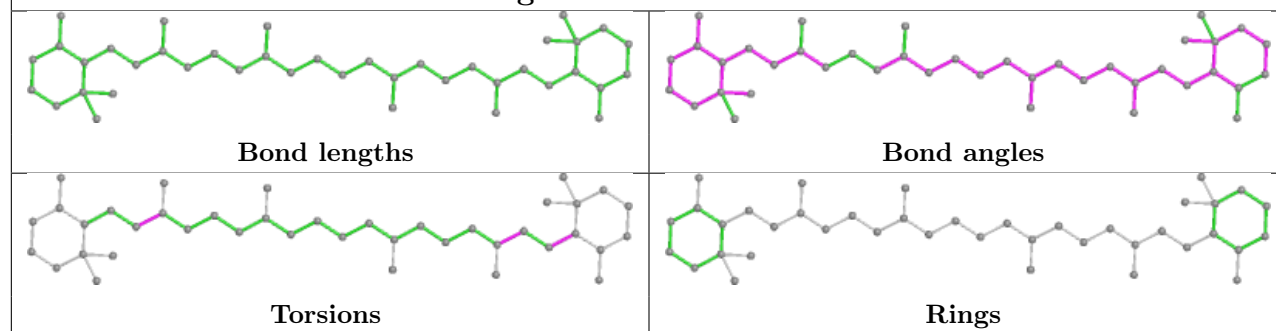


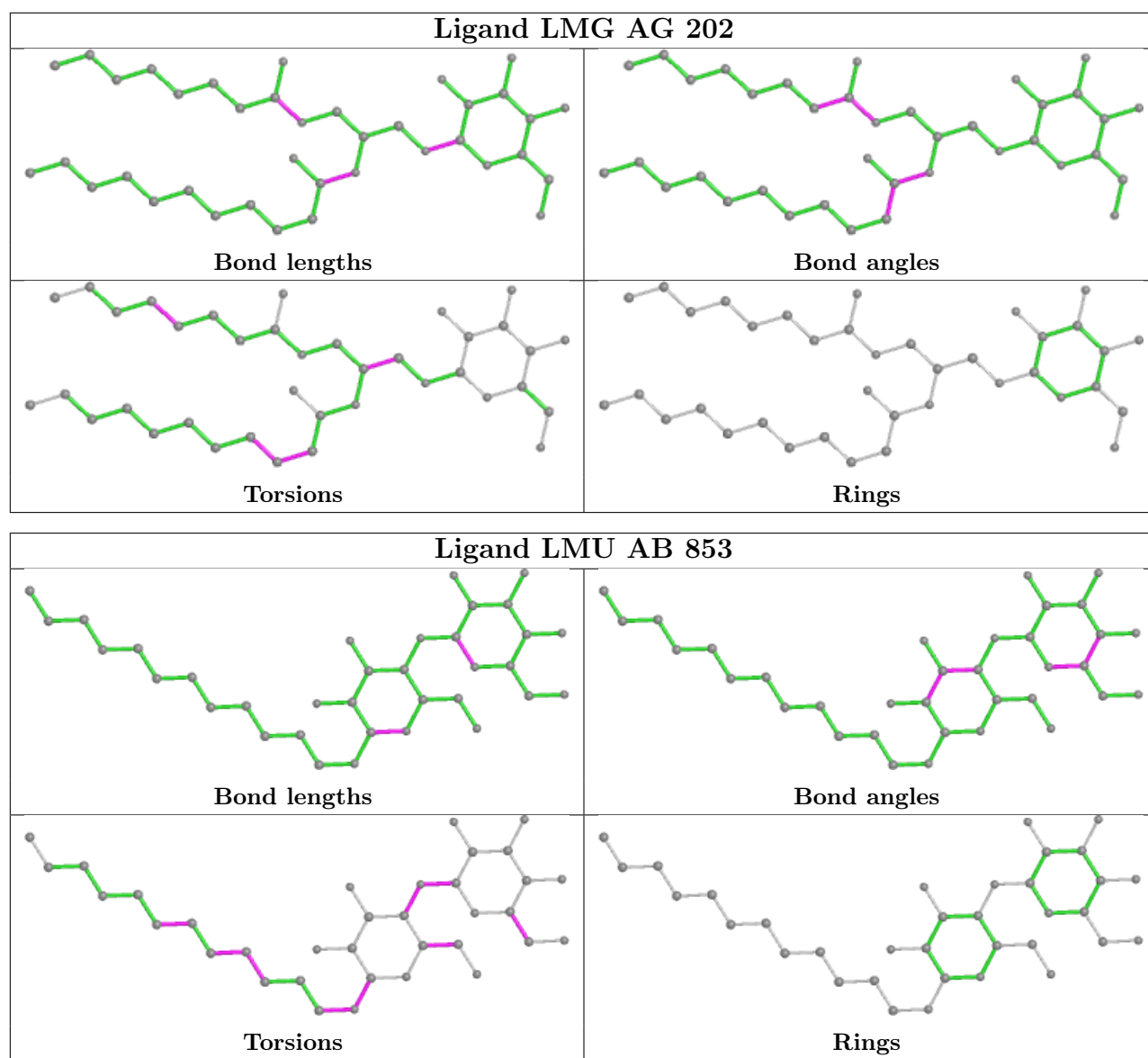


Ligand CLA AK 204

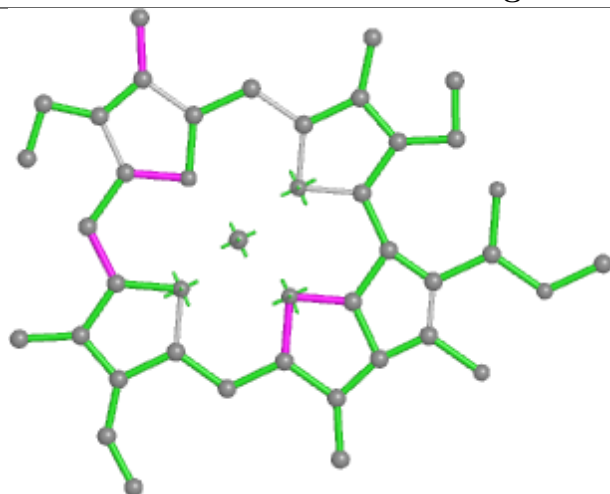


Ligand BCR AB 849

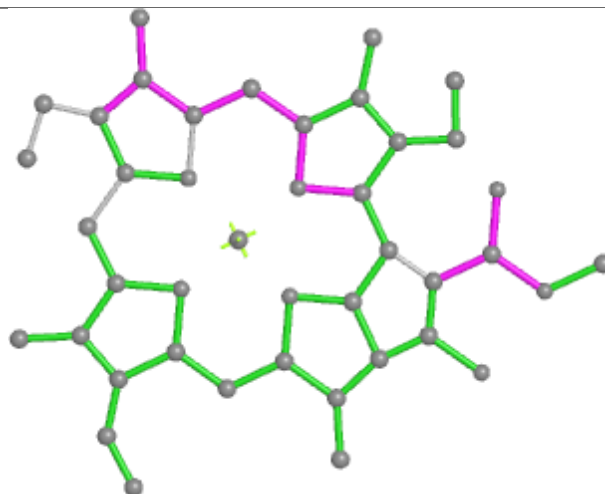




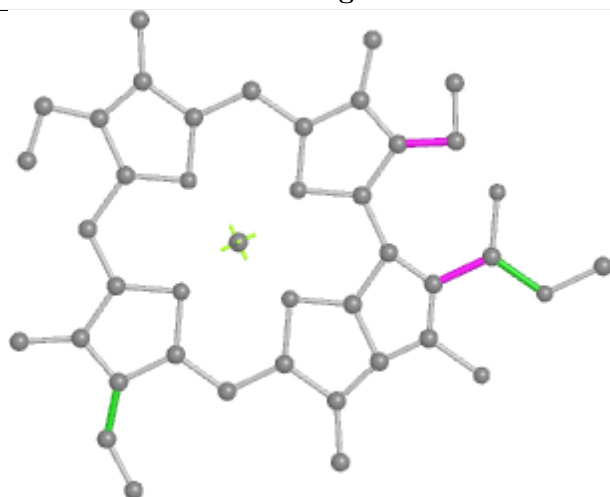
Ligand CLA A4 309



Bond lengths



Bond angles

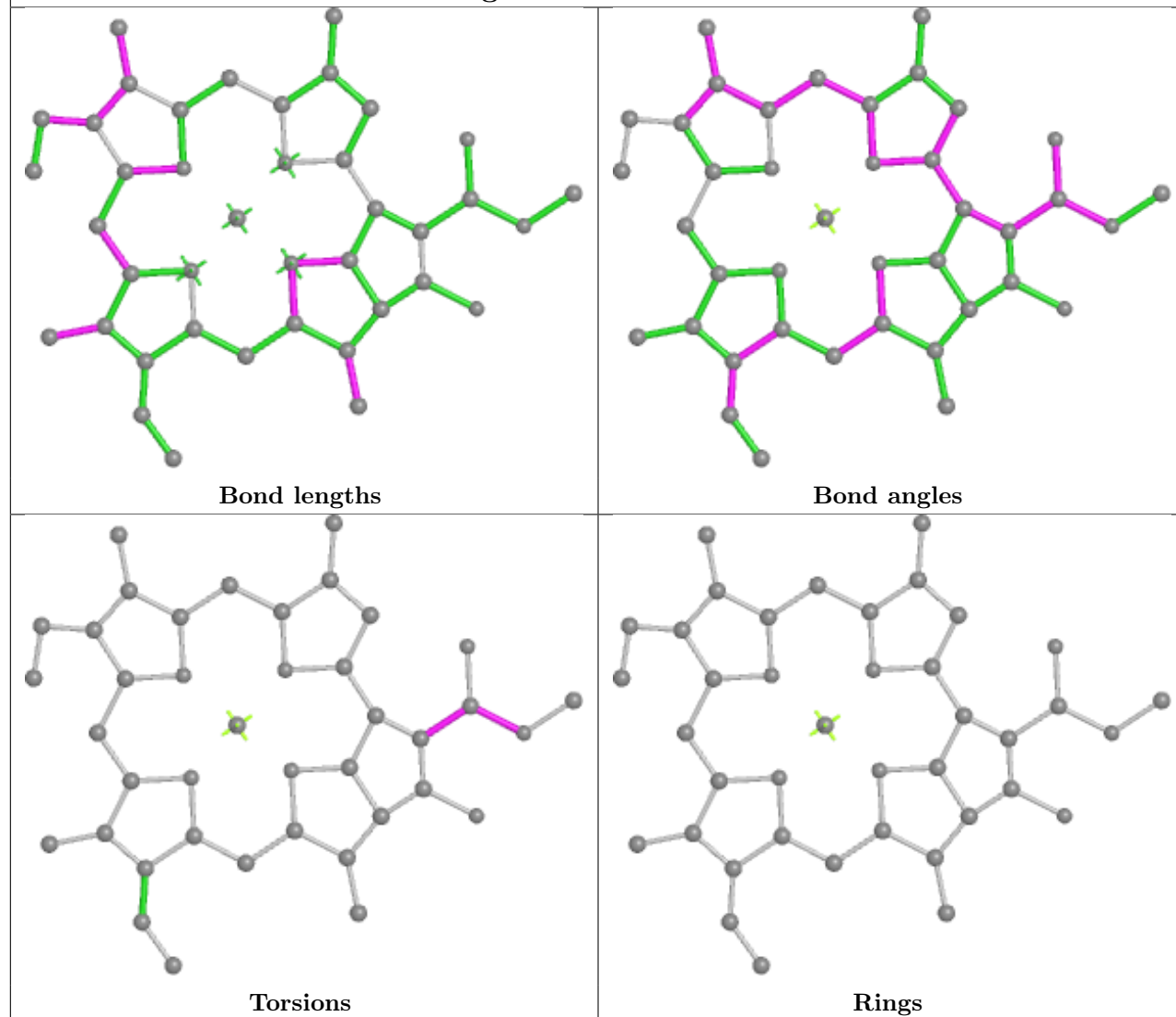


Torsions

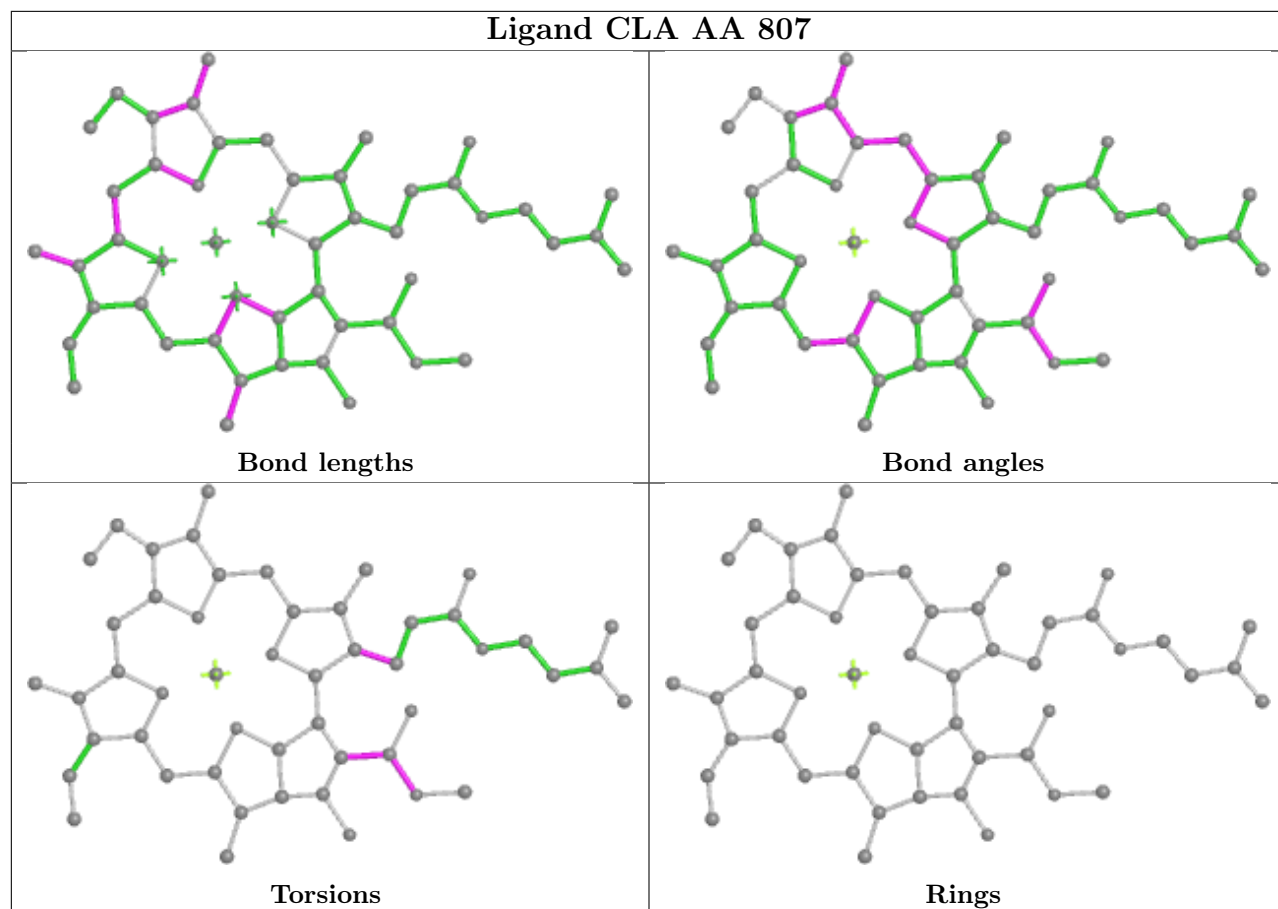


Rings

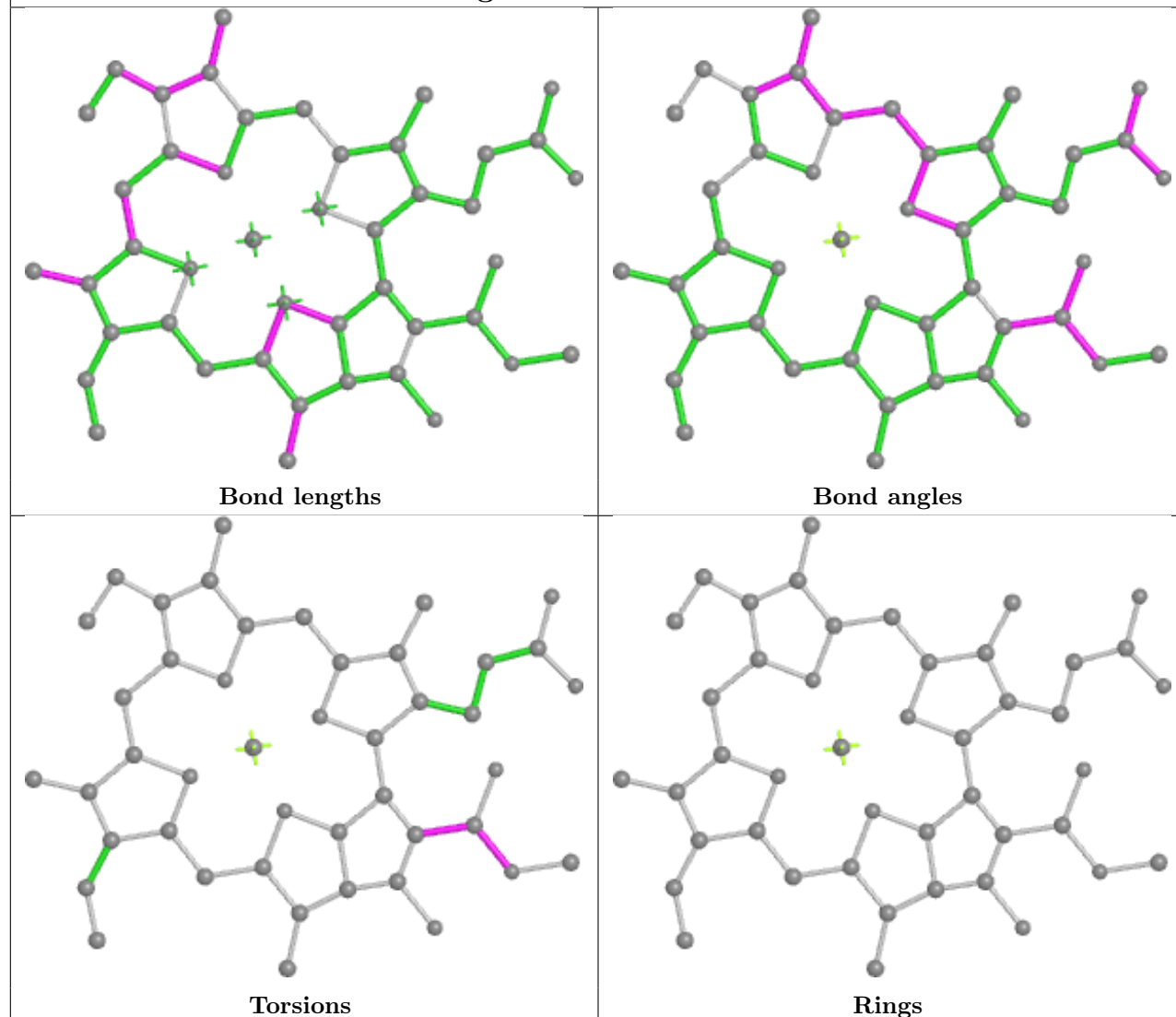
Ligand CLA A1 307



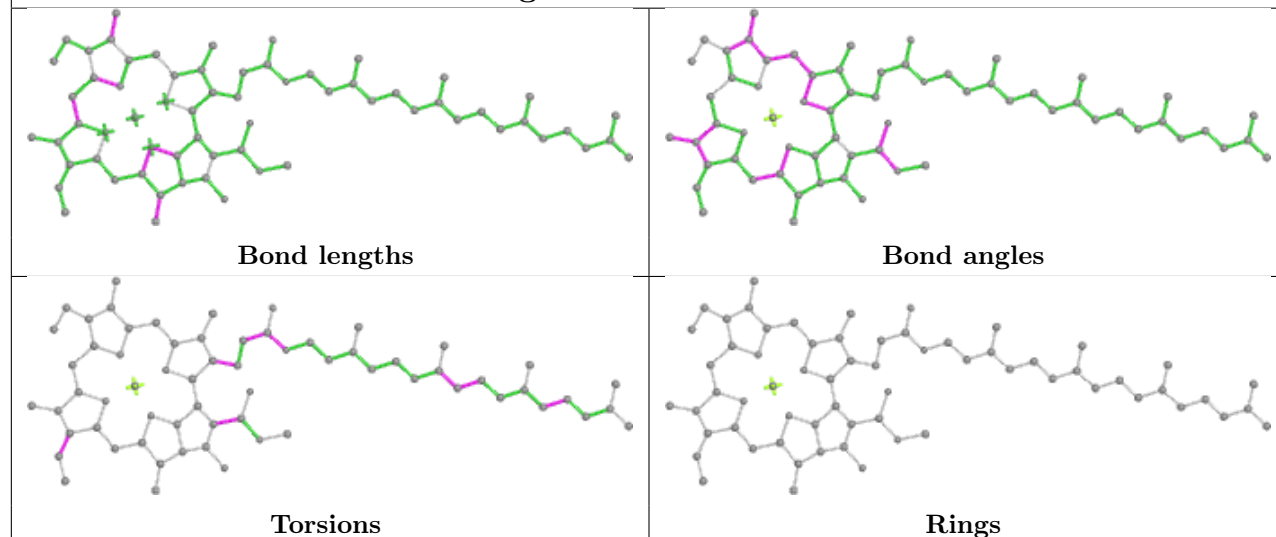
Ligand CLA AA 807



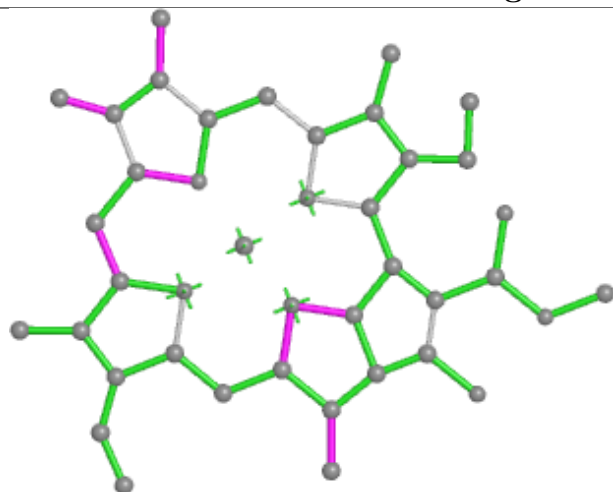
Ligand CLA AA 814



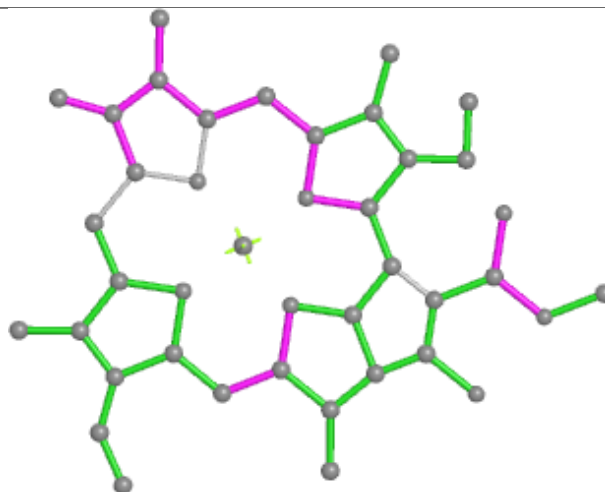
Ligand CLA AB 806



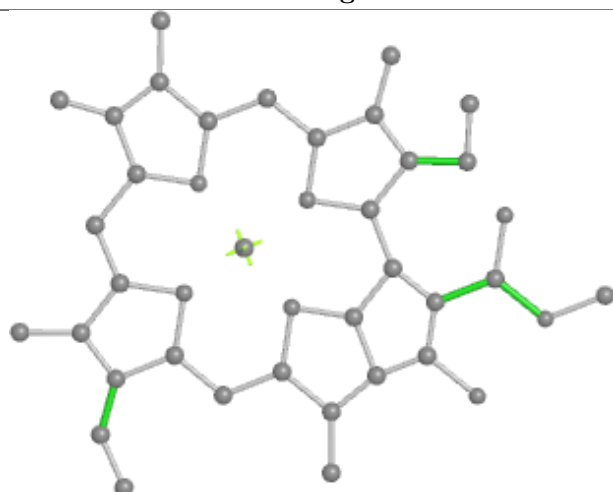
Ligand CLA A3 306



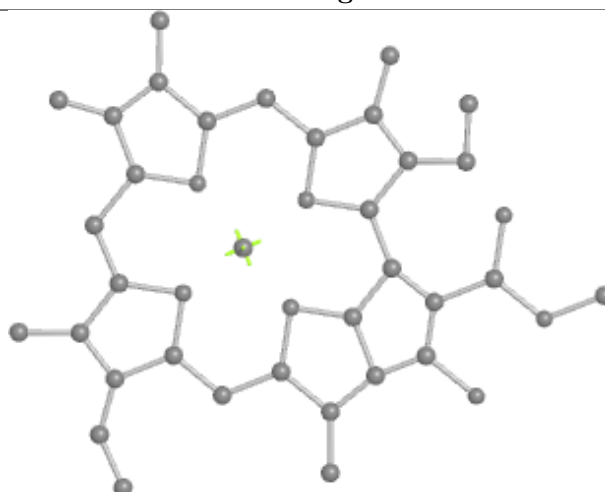
Bond lengths



Bond angles

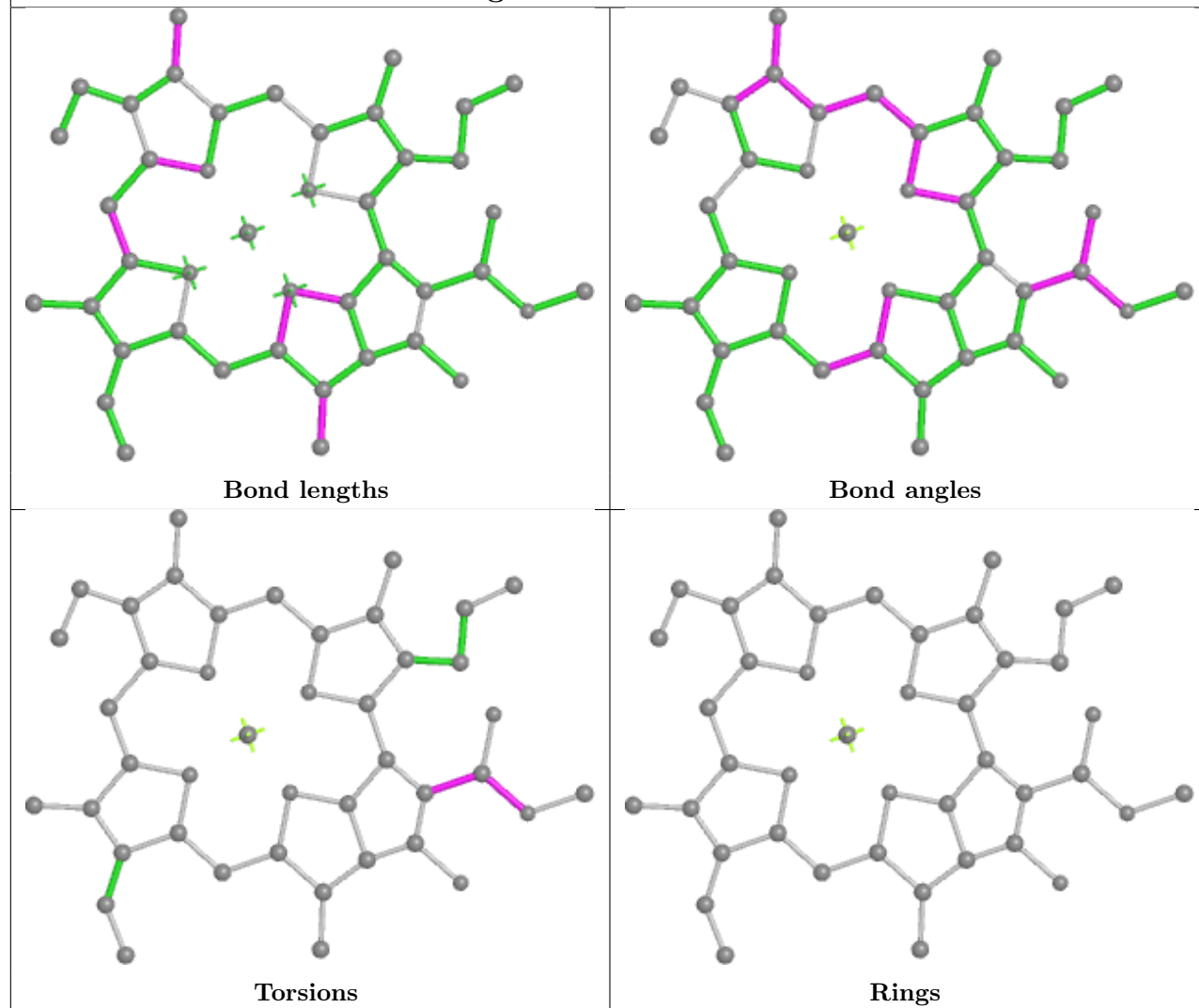


Torsions

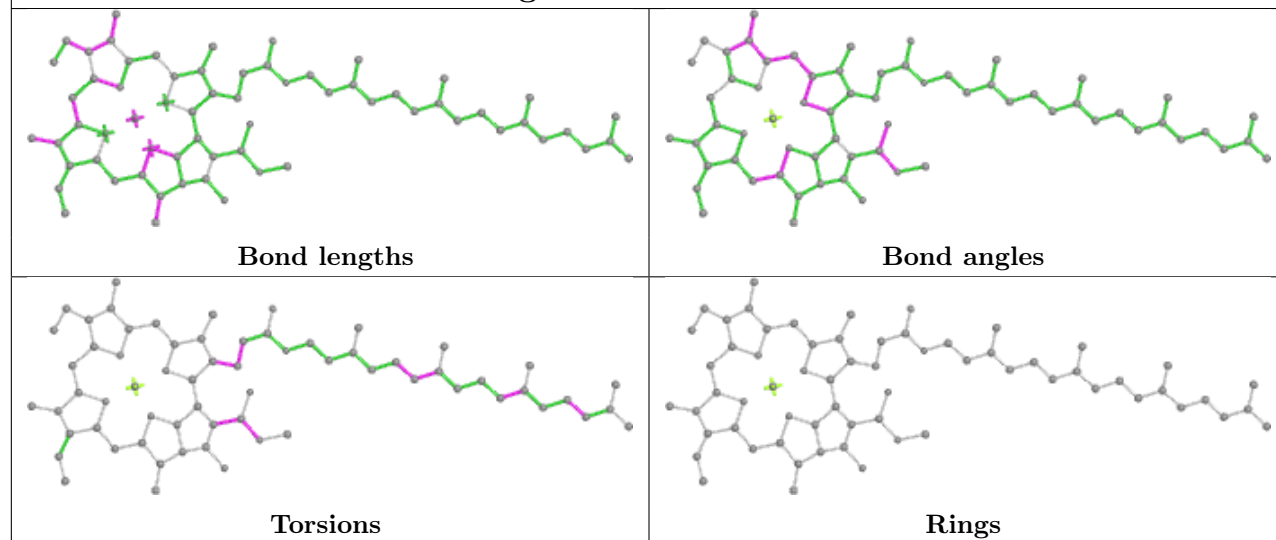


Rings

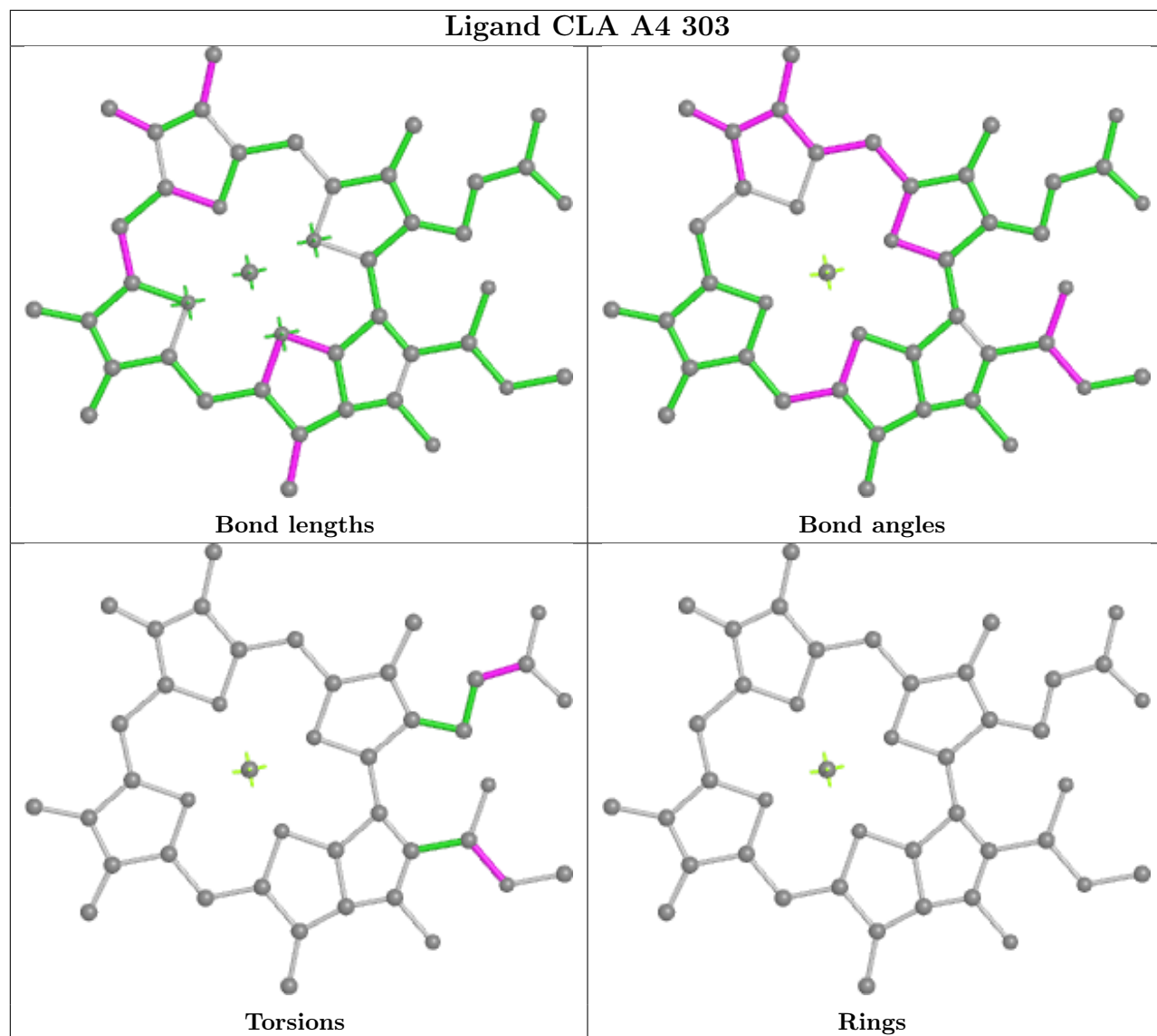
Ligand CLA AB 813



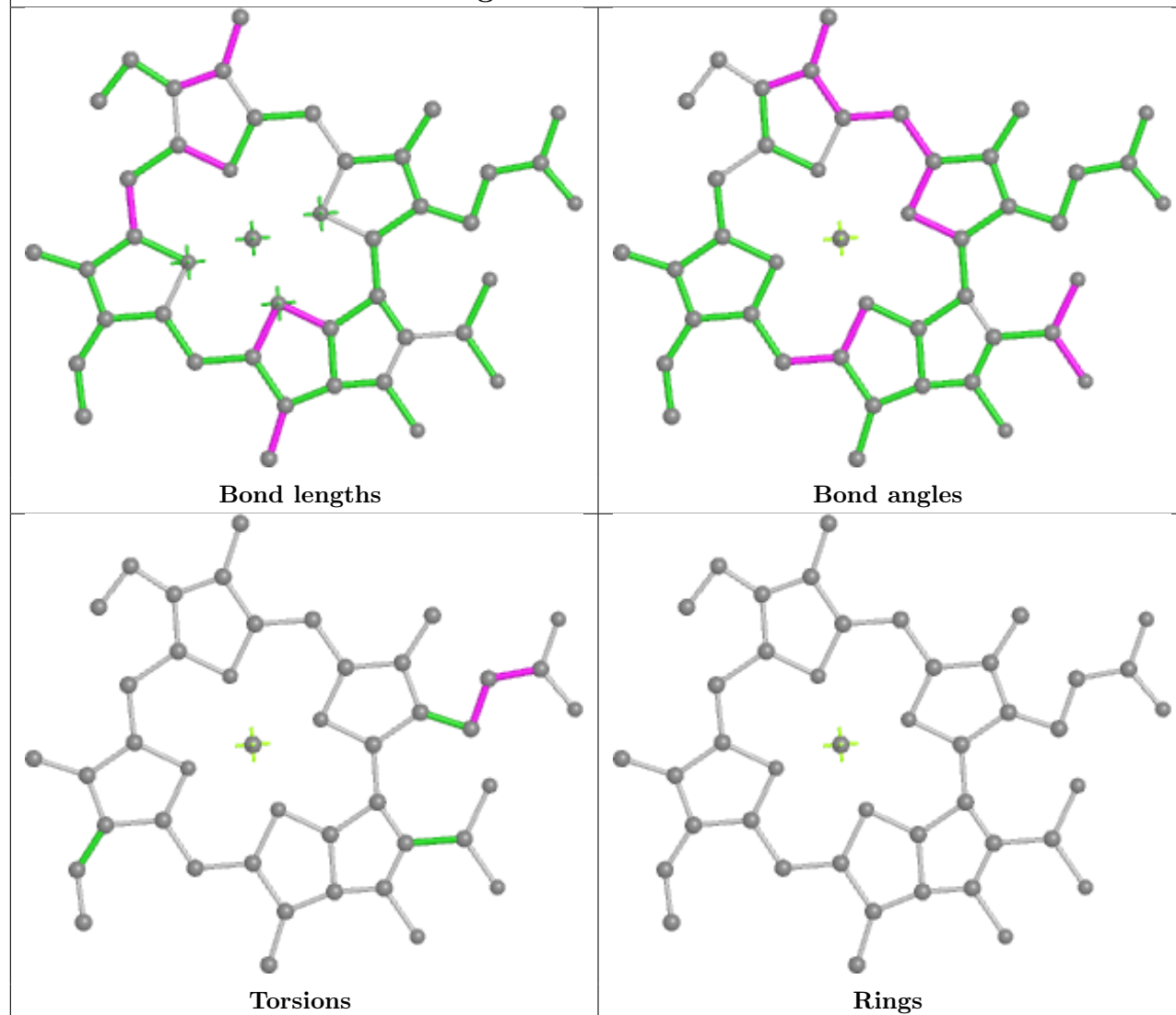
Ligand CLA AB 814



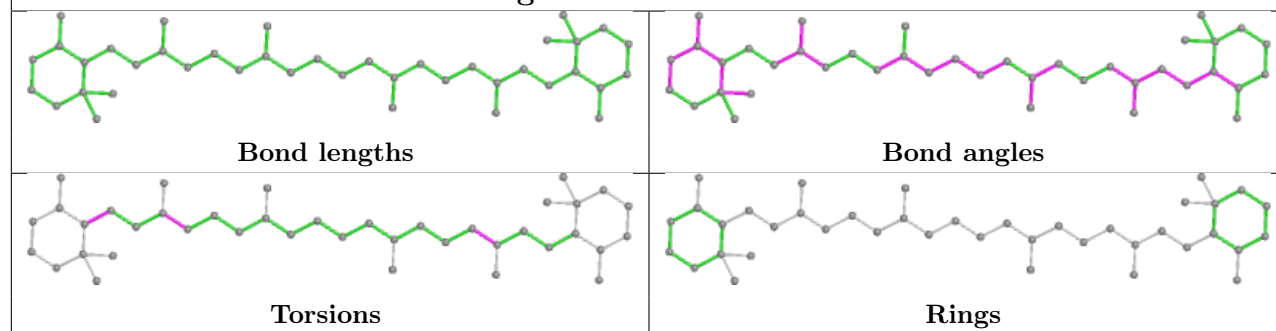
Ligand CLA A4 303



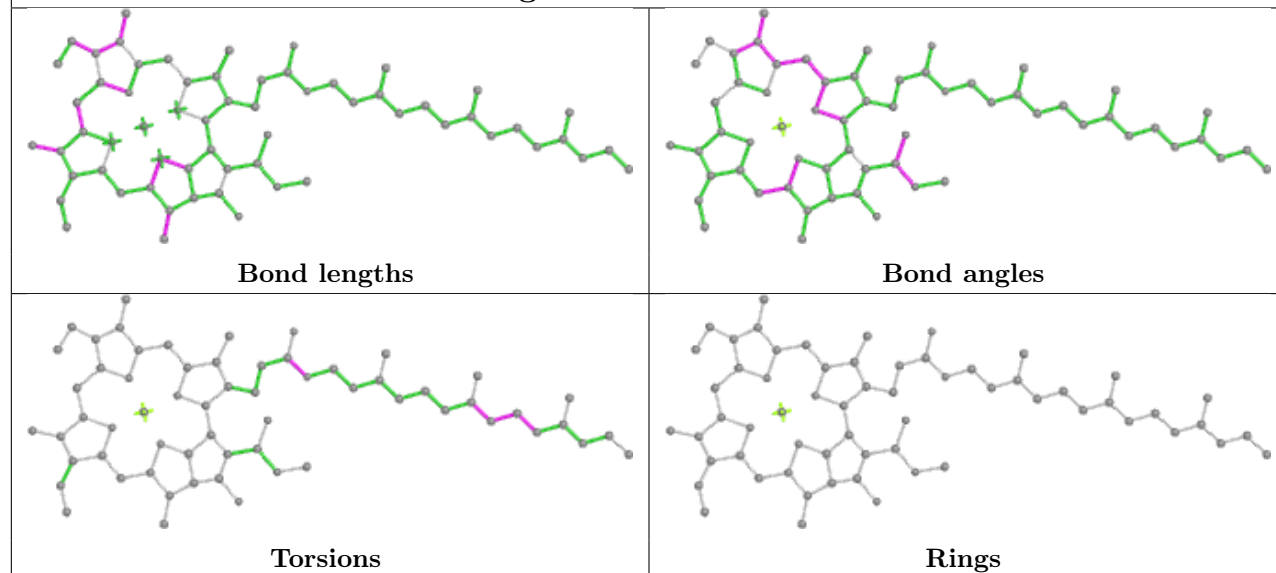
Ligand CLA AG 201



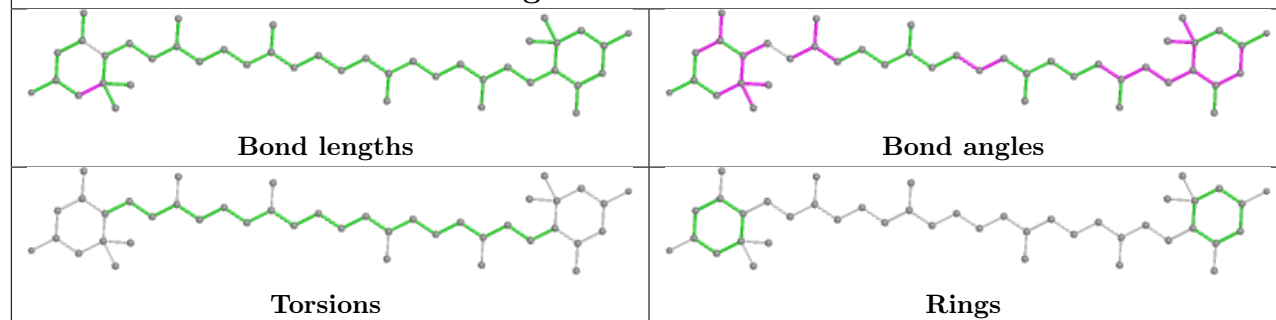
Ligand BCR AB 846



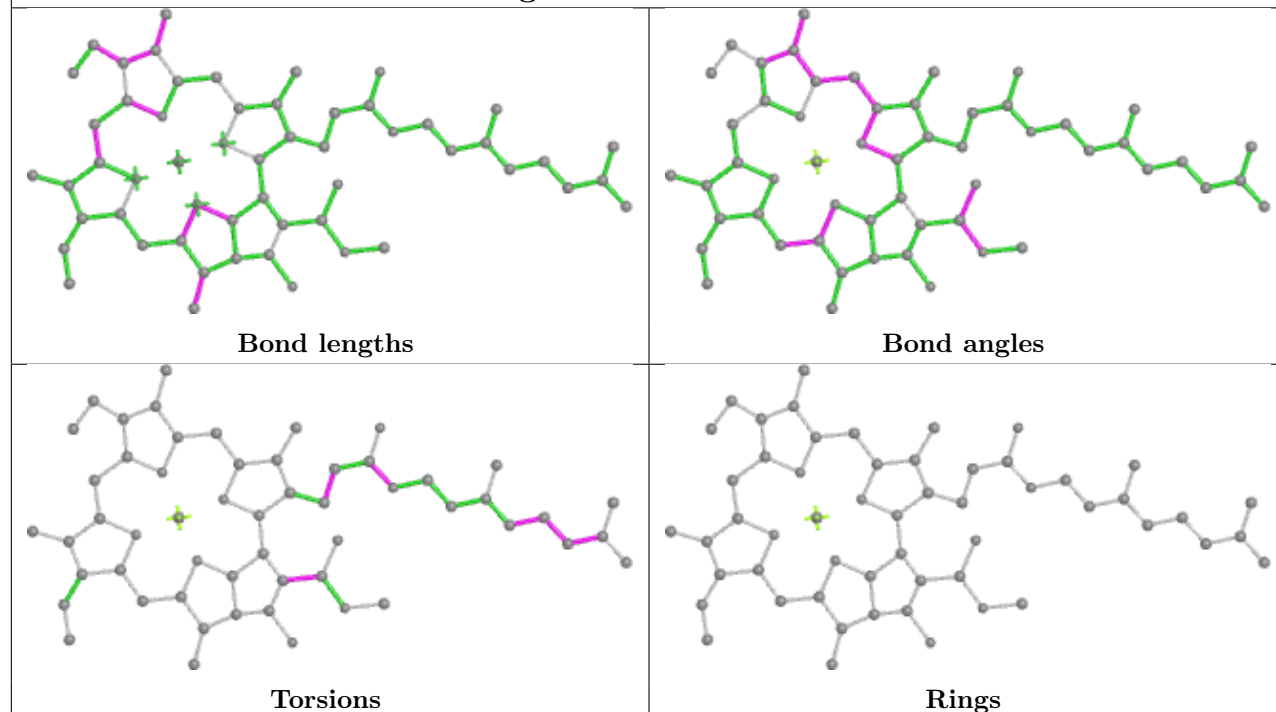
Ligand CLA AB 826

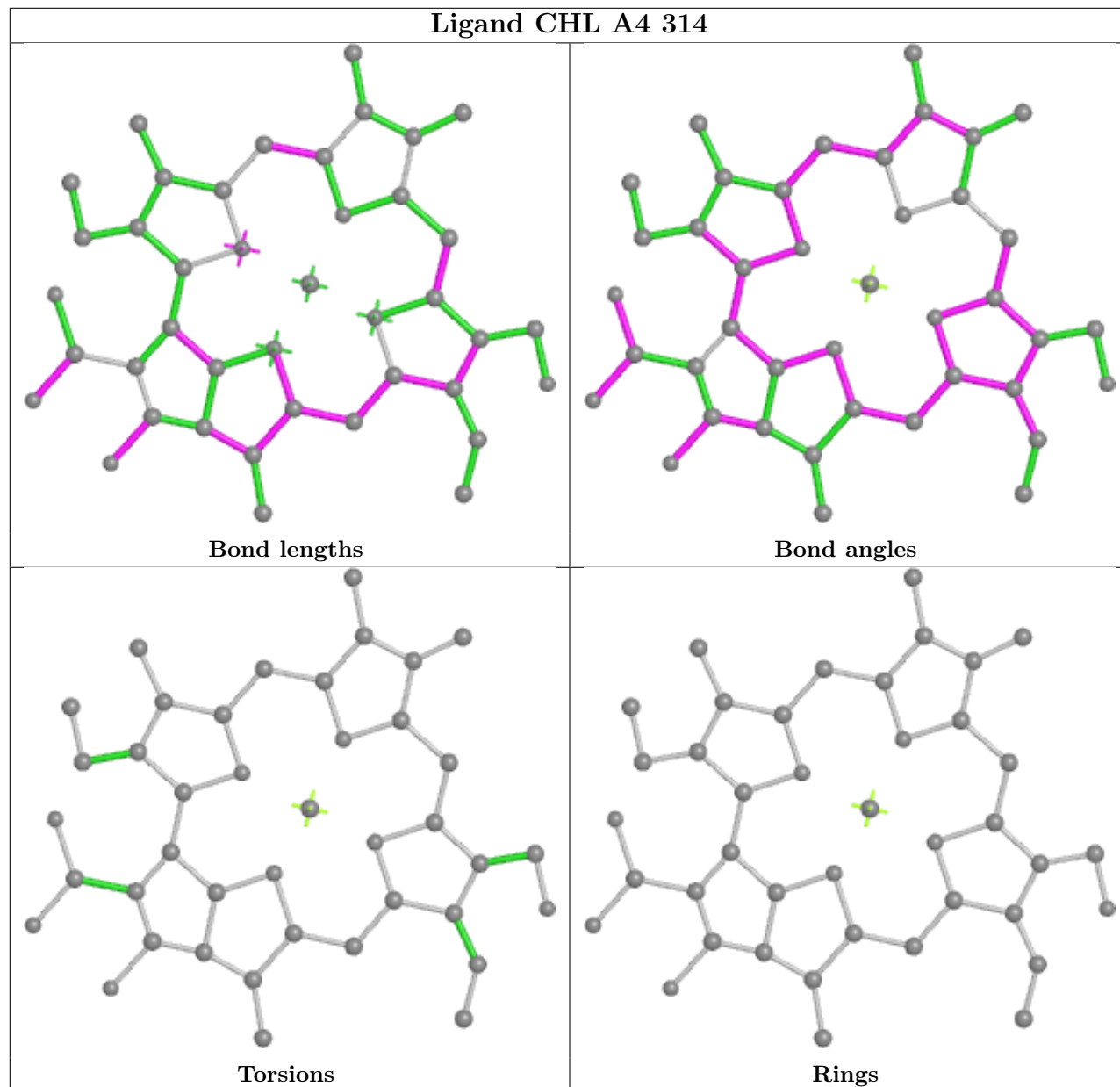
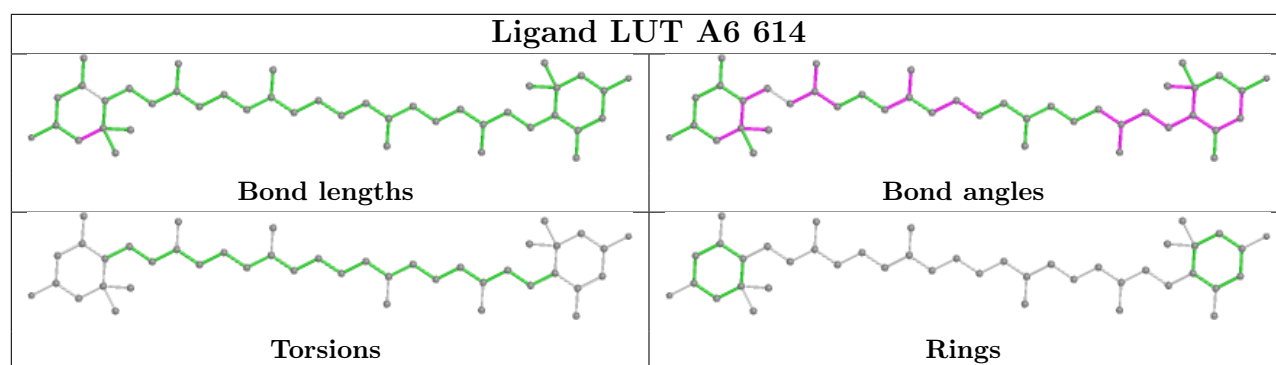


Ligand LUT A1 317

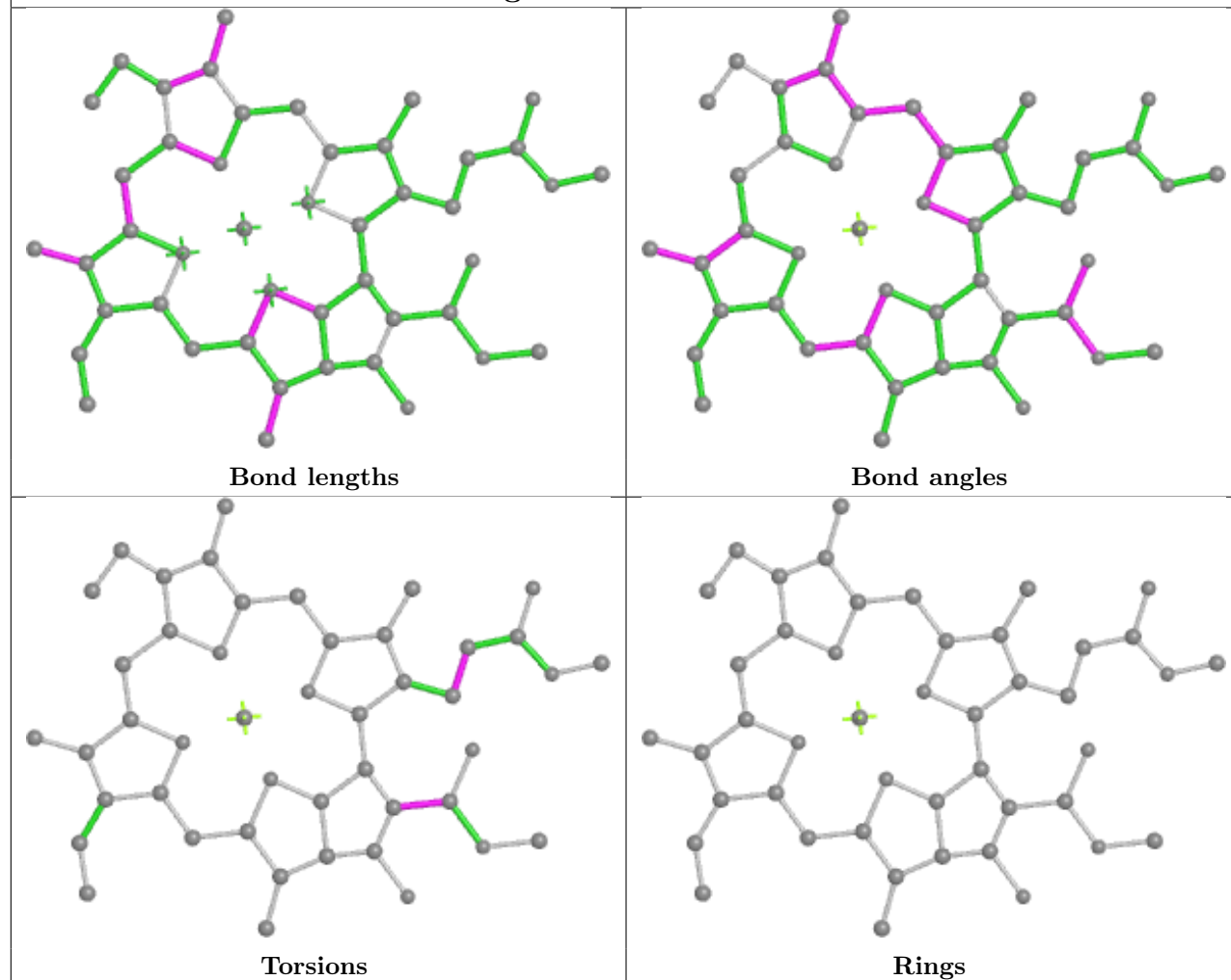


Ligand CLA AB 817

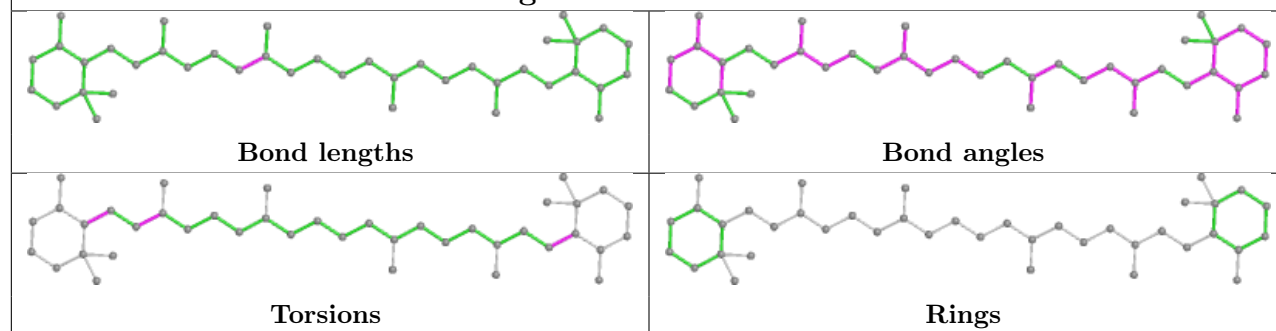




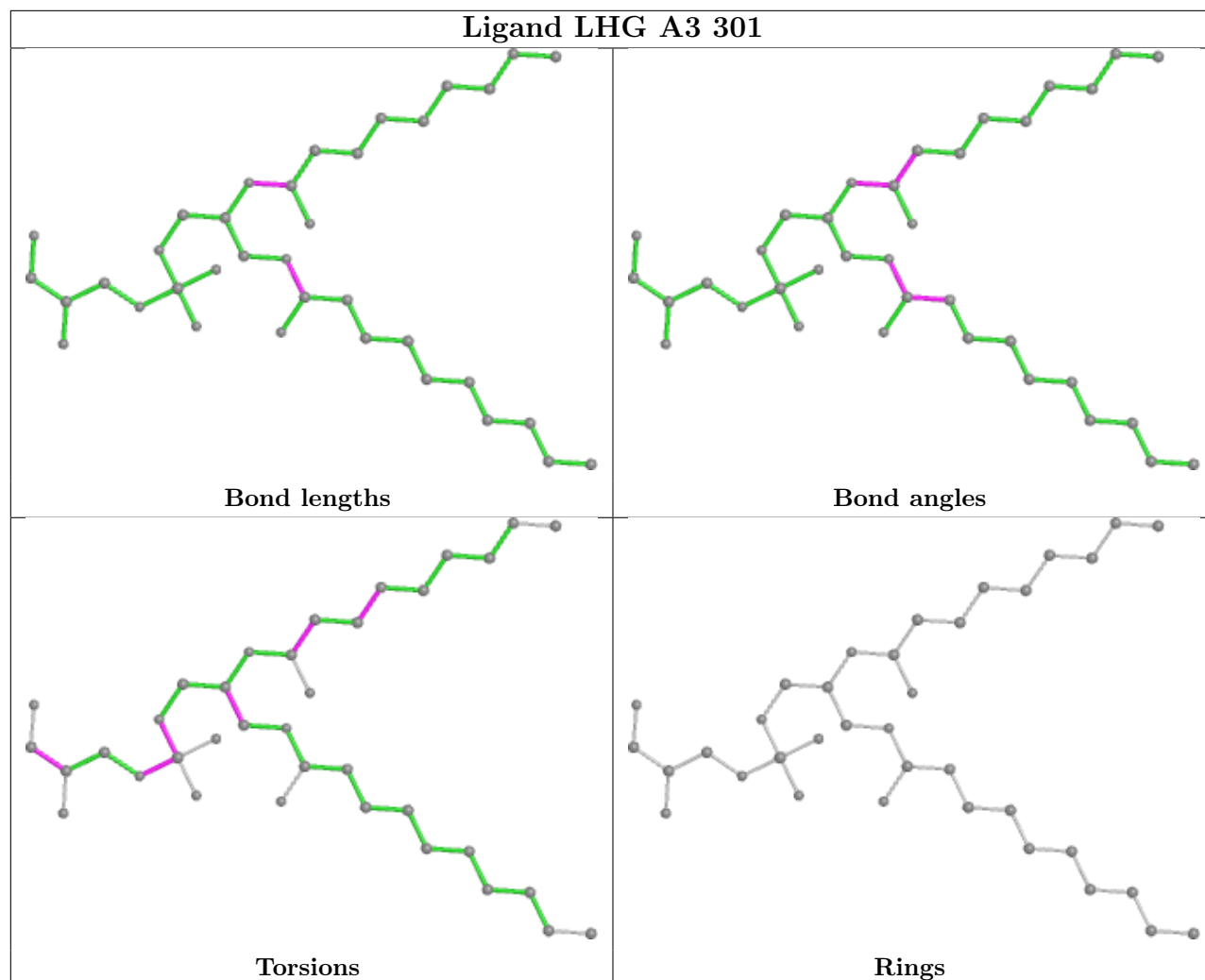
Ligand CLA A6 601



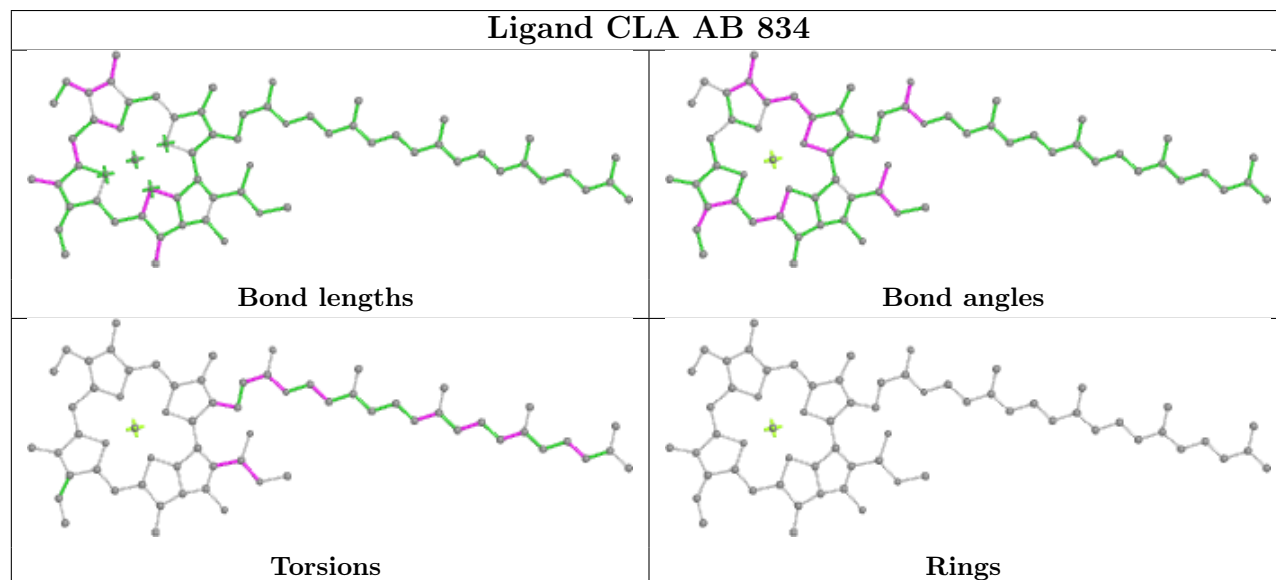
Ligand BCR AL 306



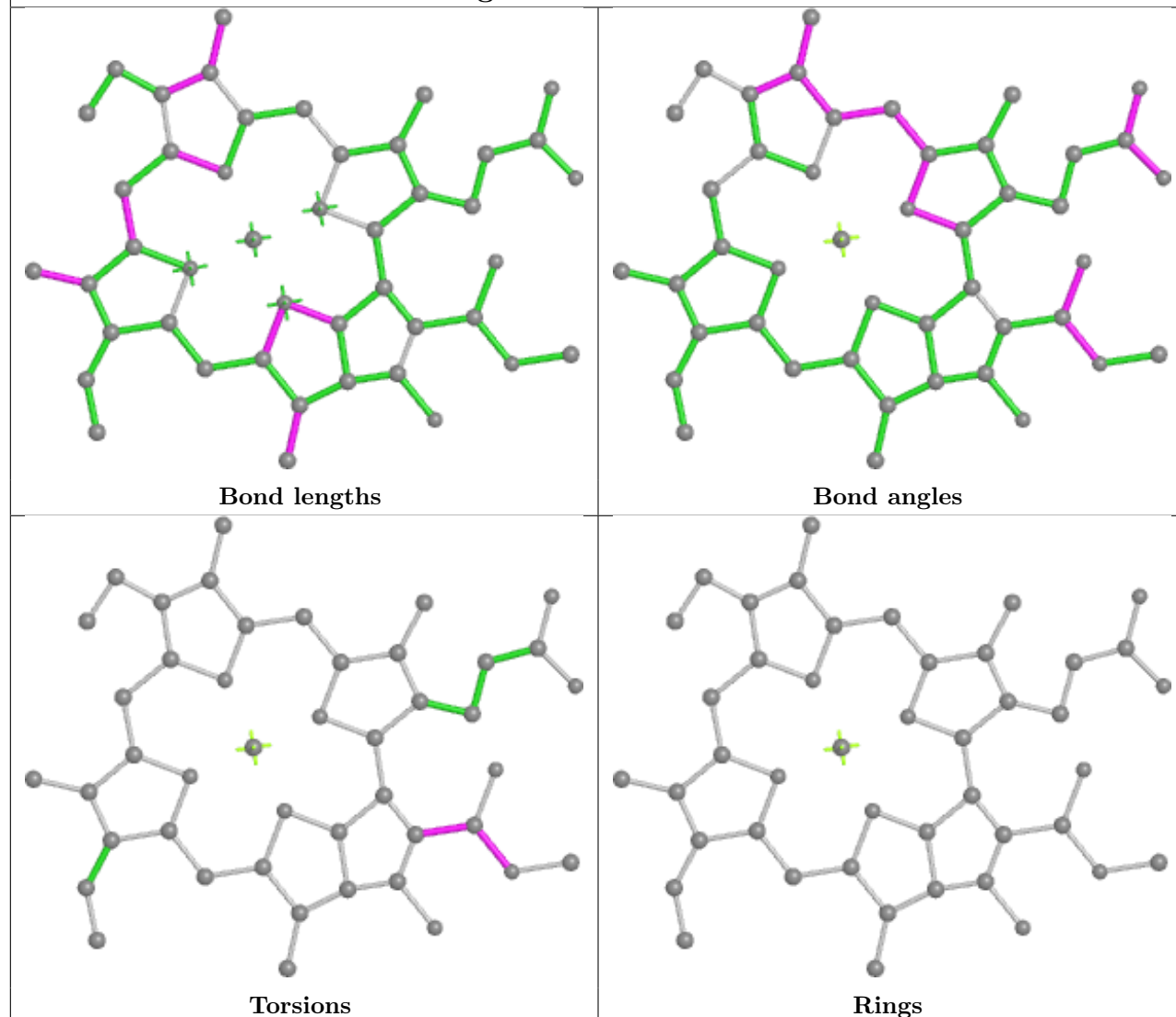
Ligand LHG A3 301



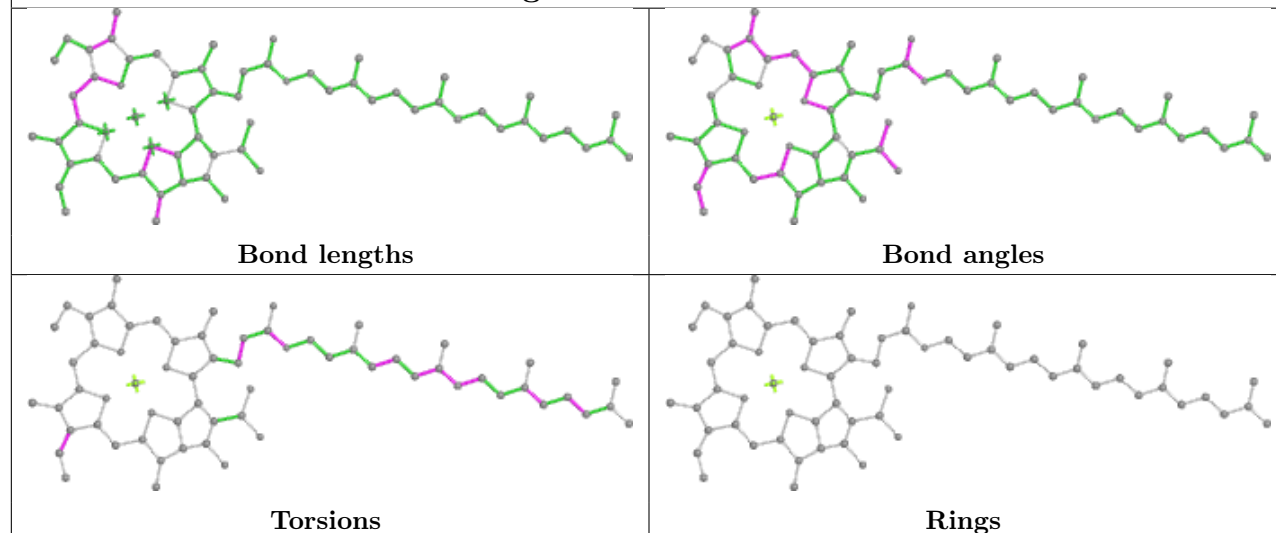
Ligand CLA AB 834

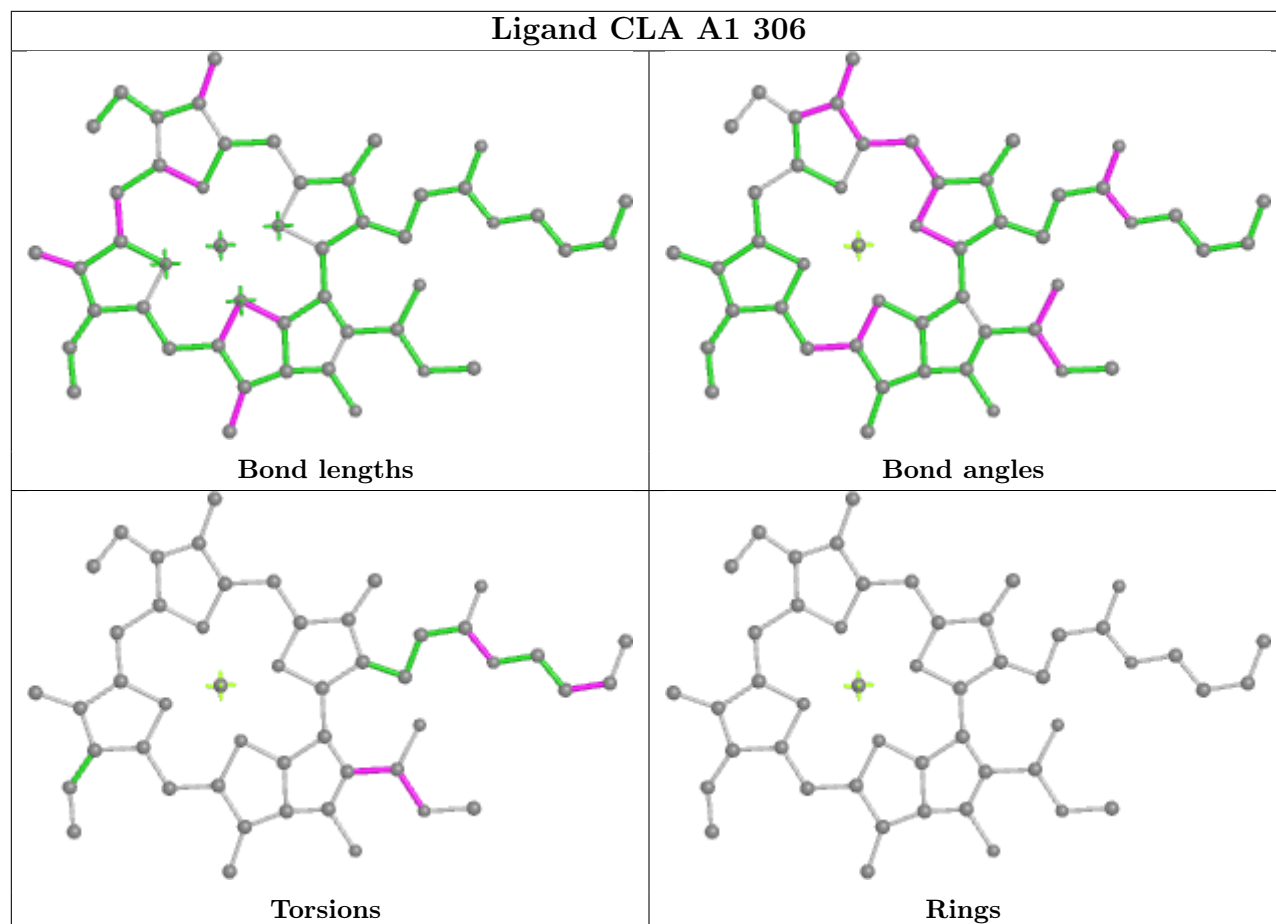
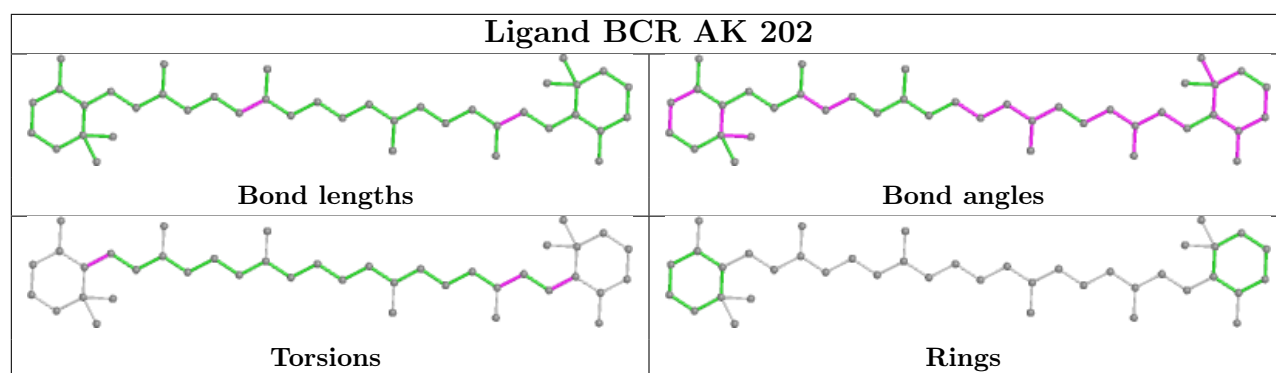


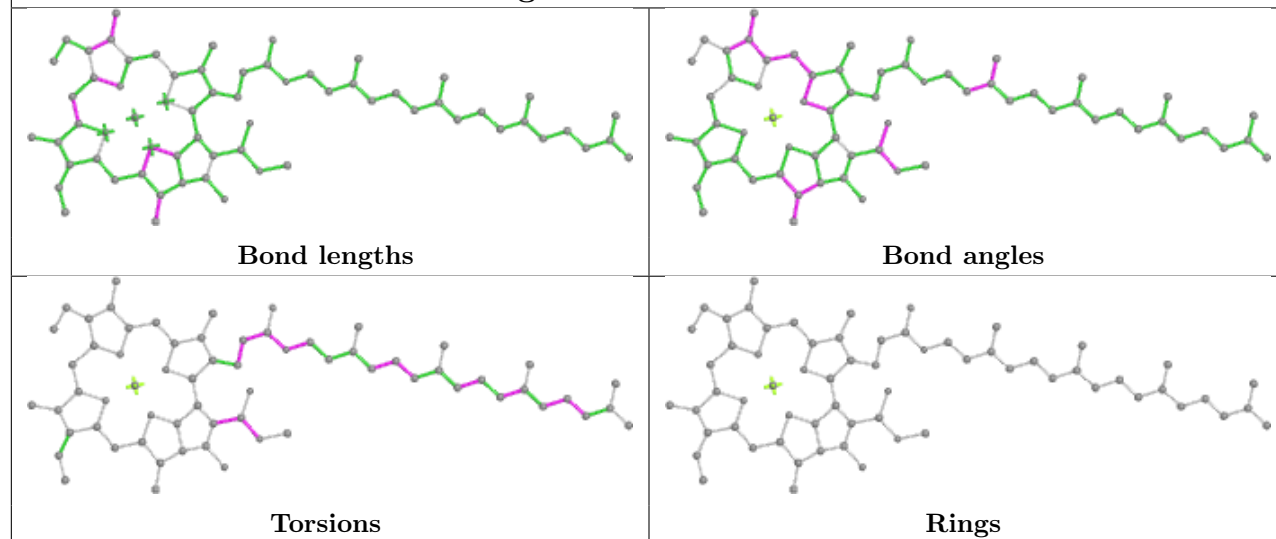
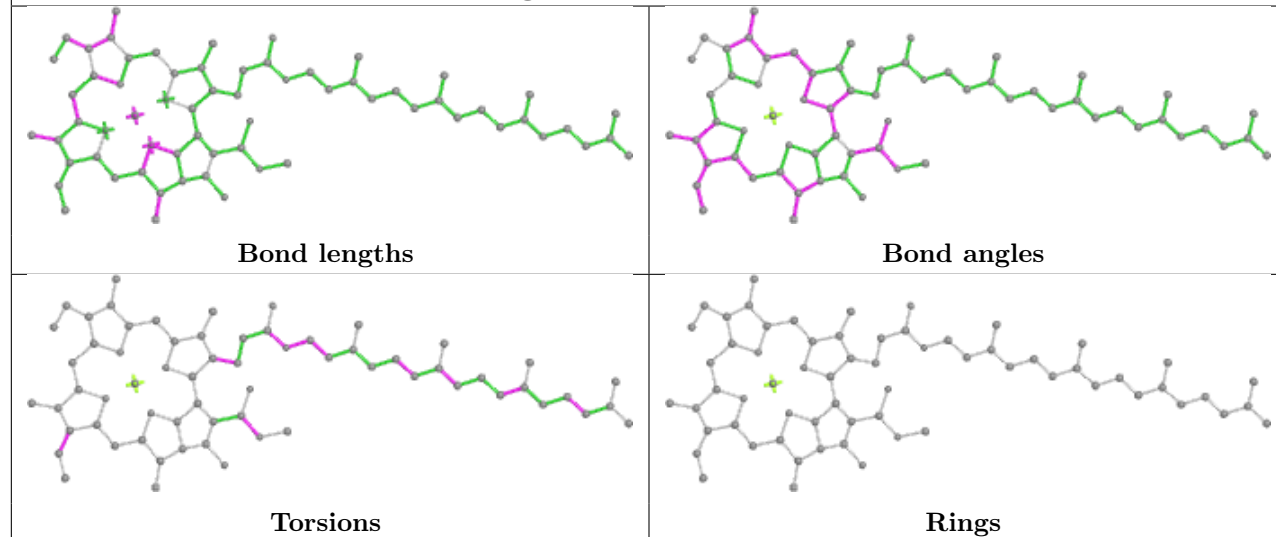
Ligand CLA AA 820



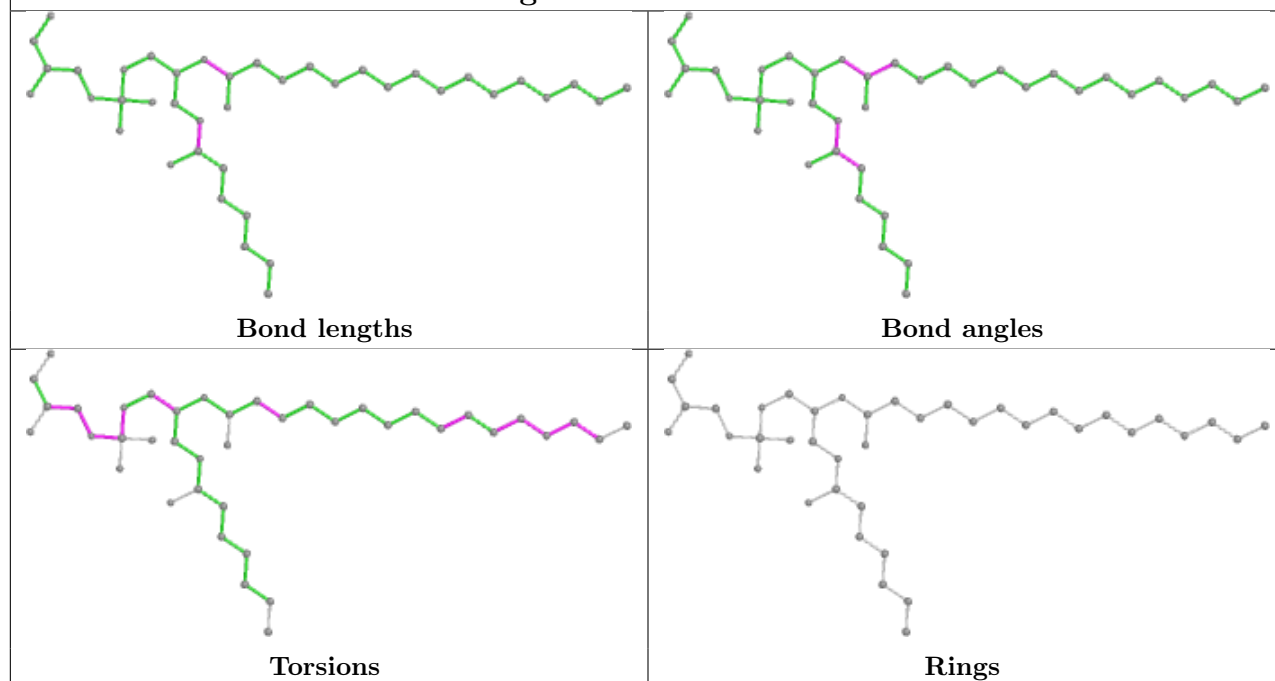
Ligand CLA A1 314



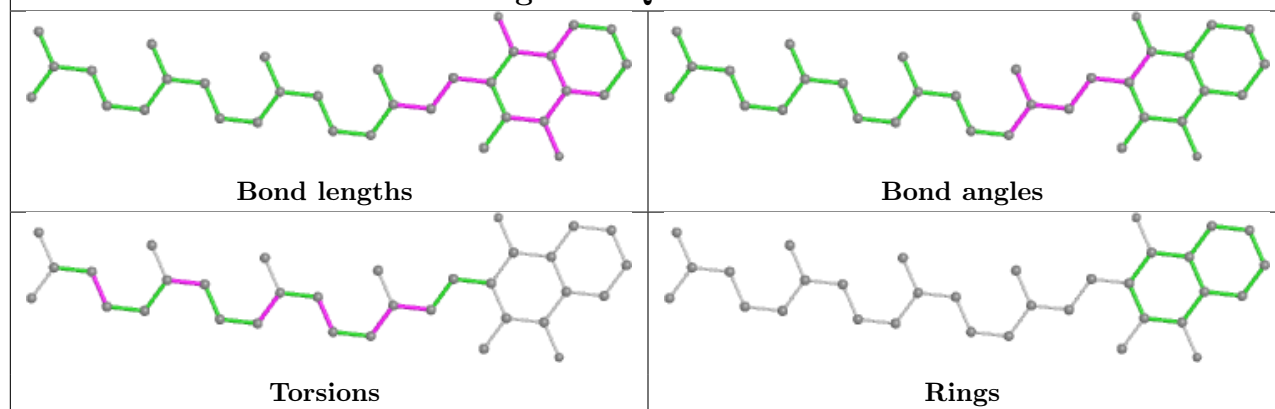


Ligand CLA AA 833**Ligand CLA AB 804**

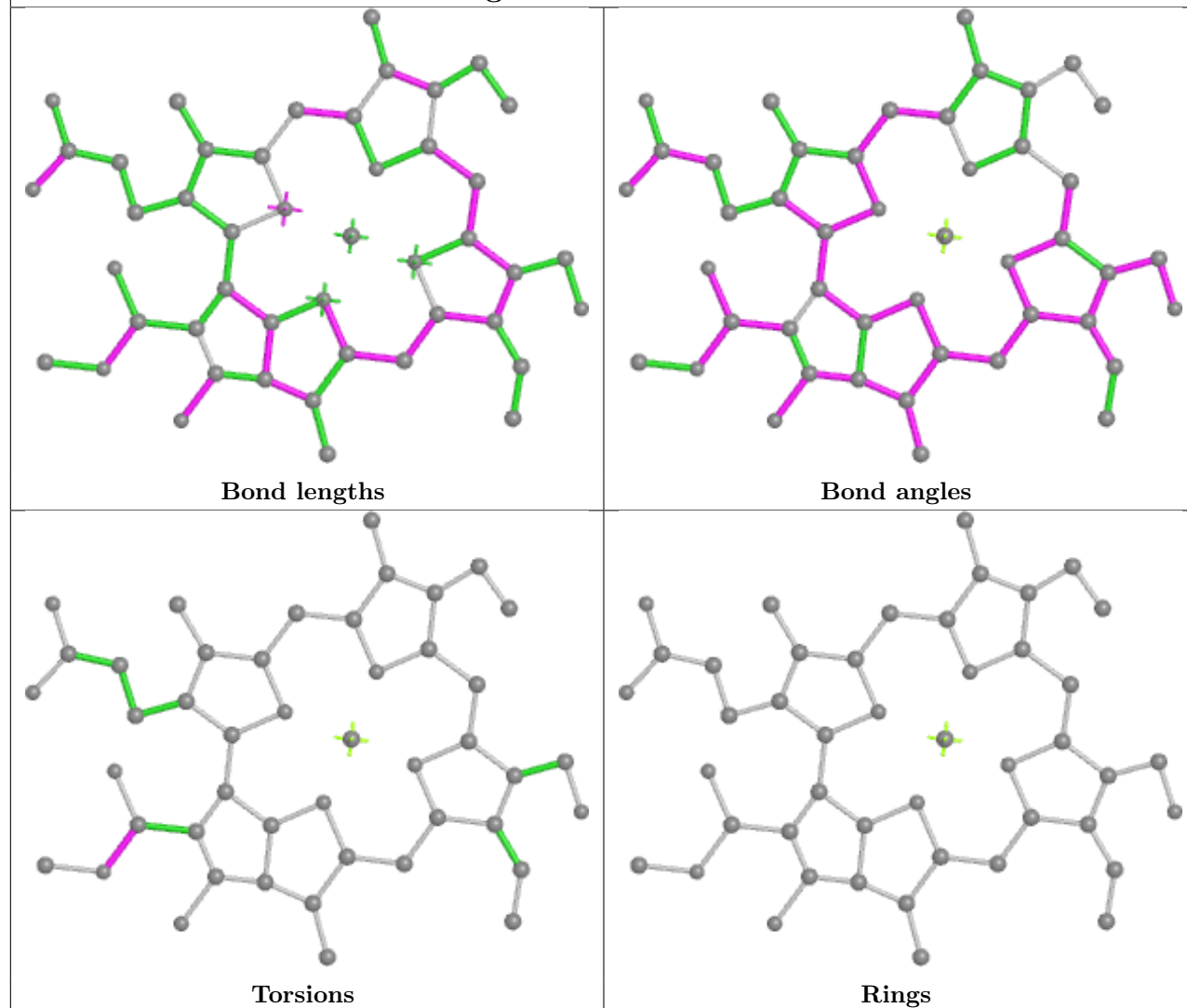
Ligand LHG AJ 104



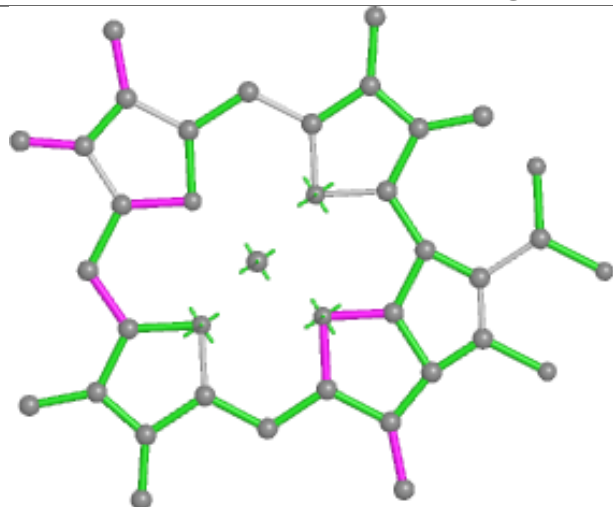
Ligand PQN AB 843



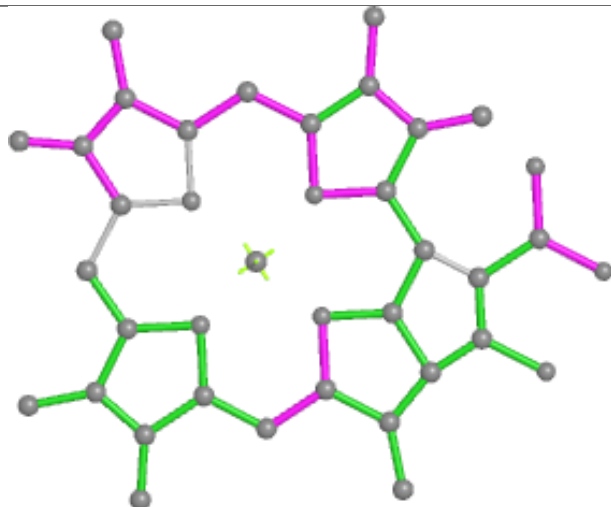
Ligand CHL A4 306



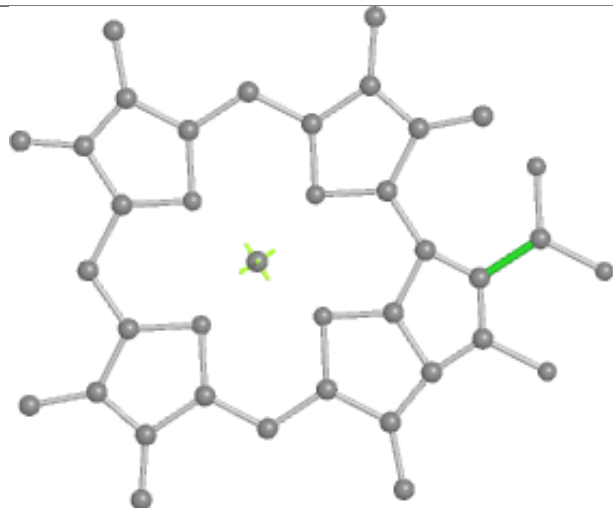
Ligand CLA A1 315



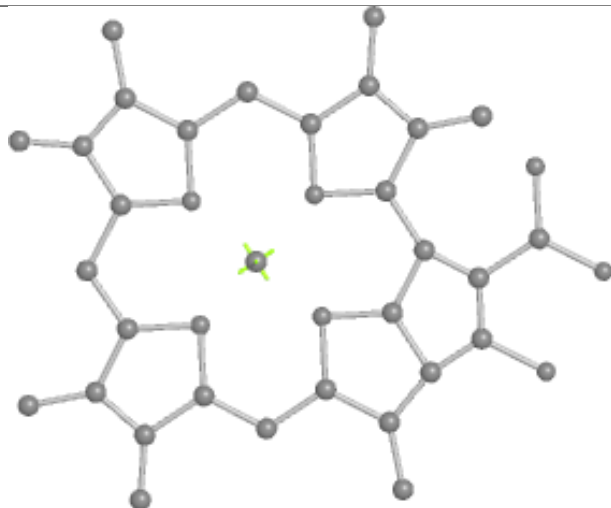
Bond lengths



Bond angles

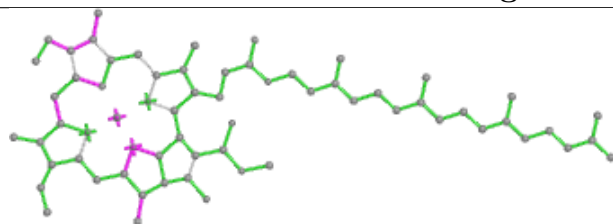


Torsions

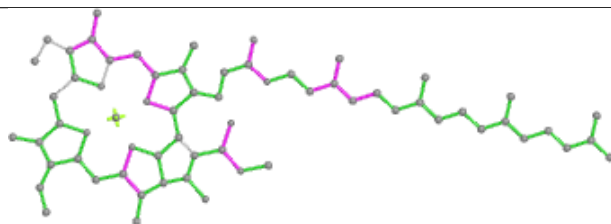


Rings

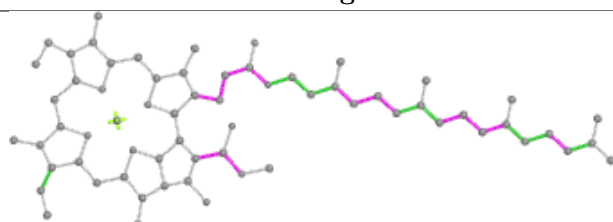
Ligand CLA AA 829



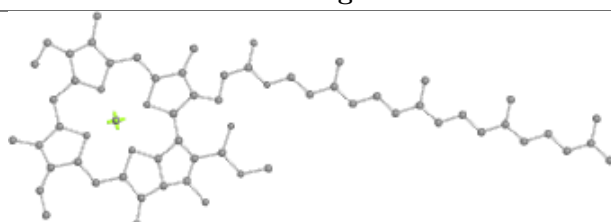
Bond lengths



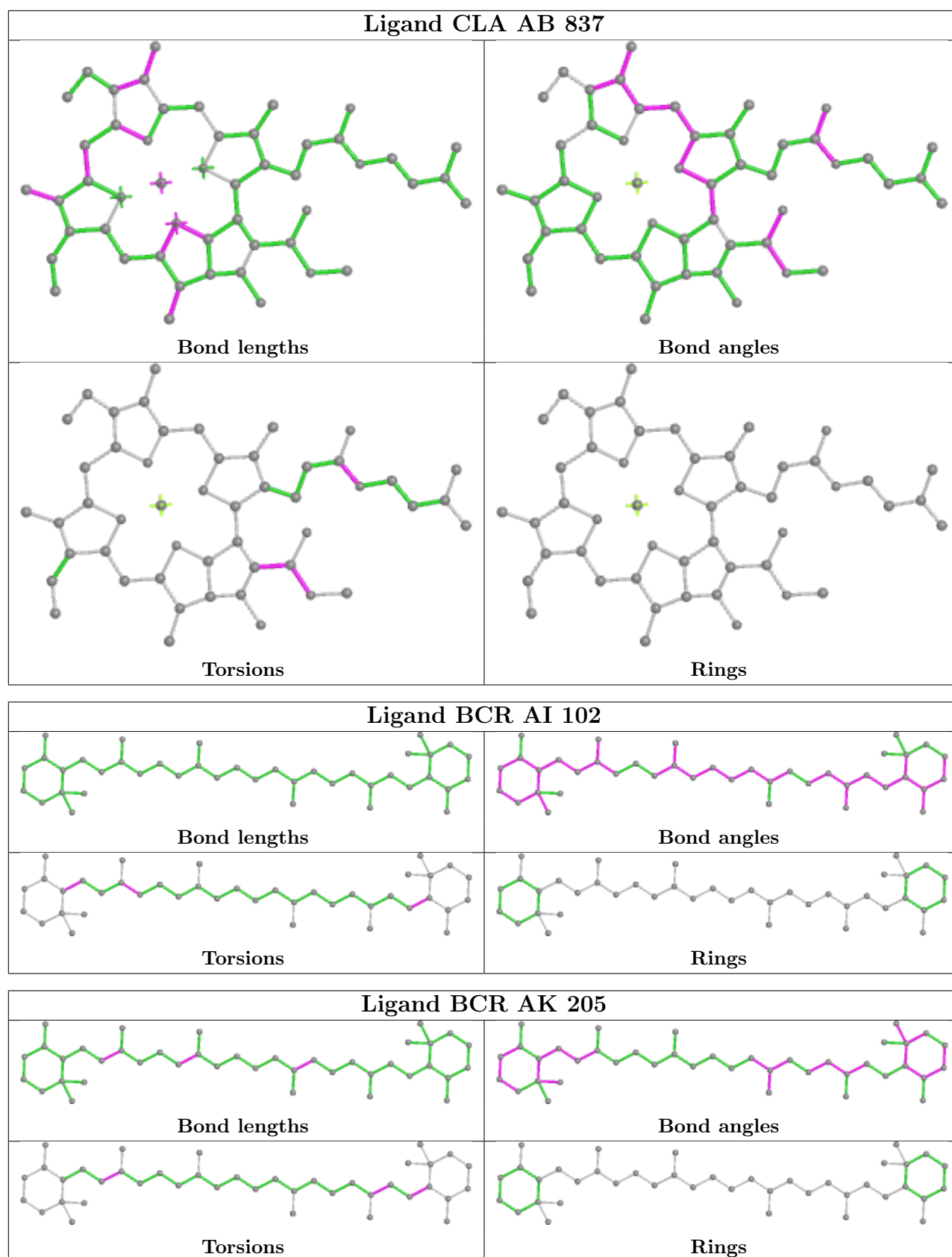
Bond angles



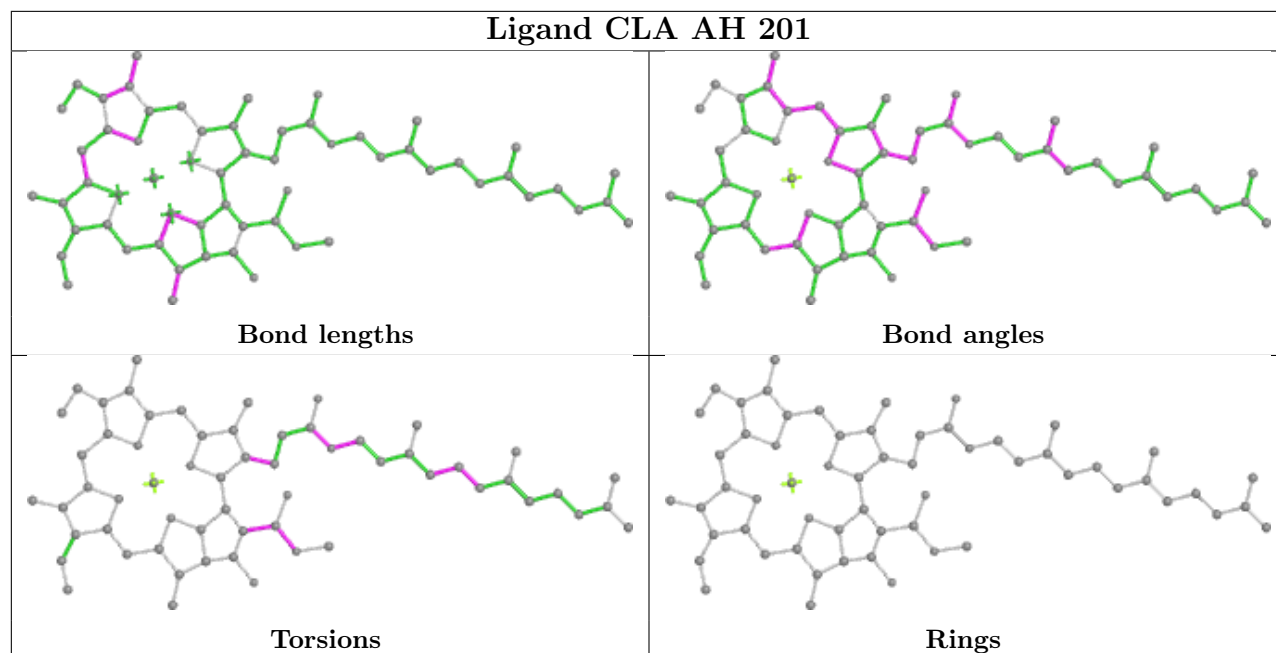
Torsions



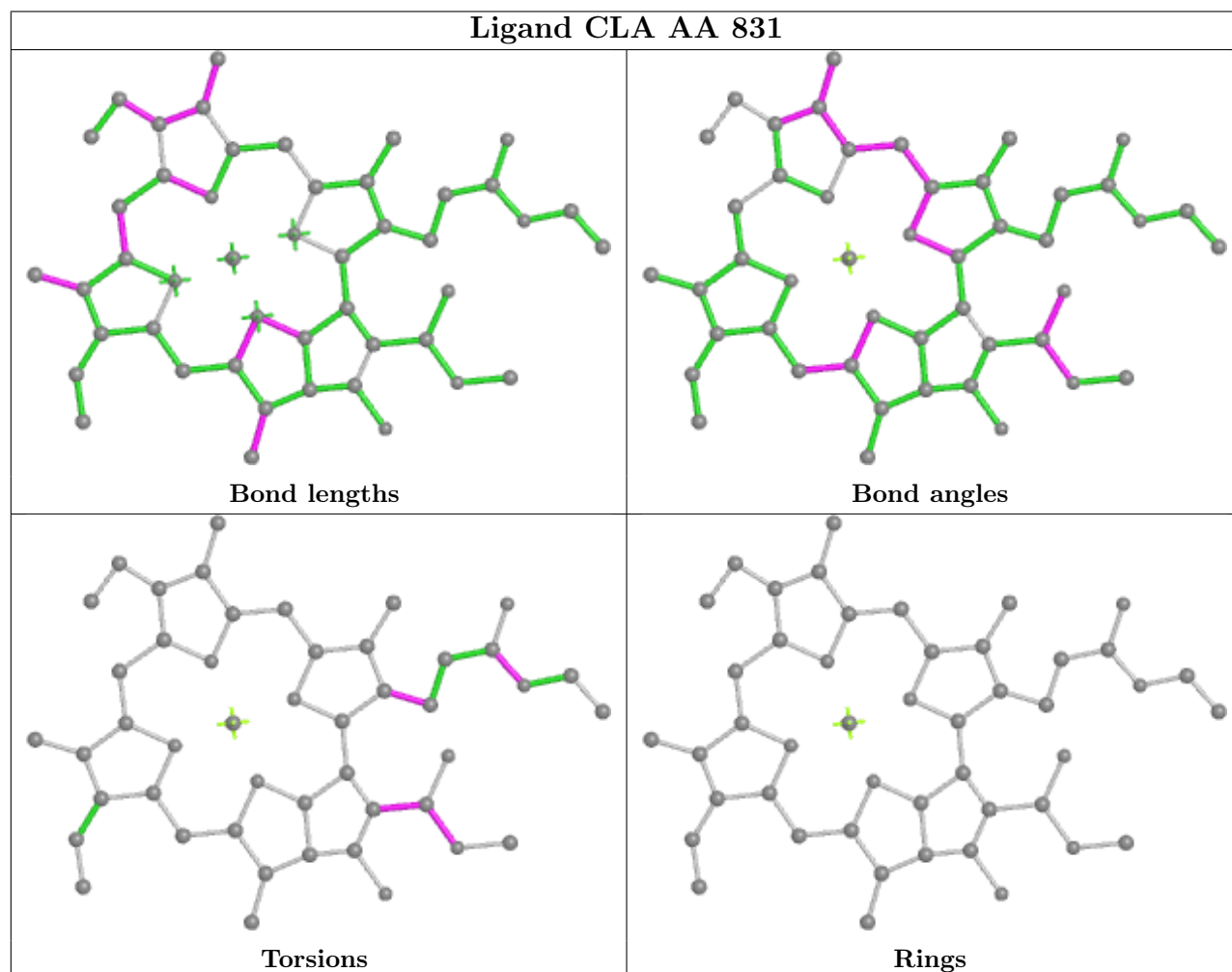
Rings



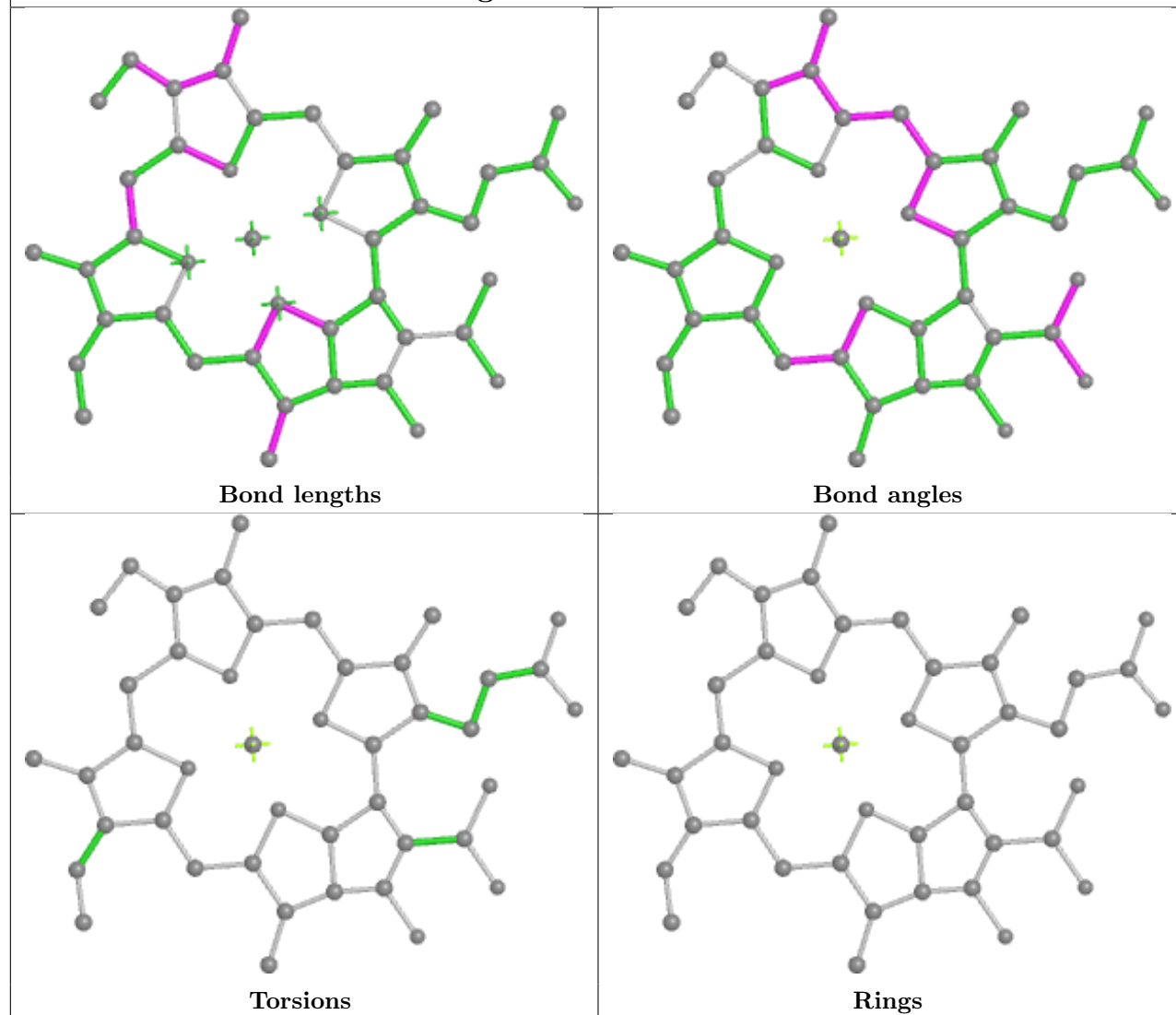
Ligand CLA AH 201



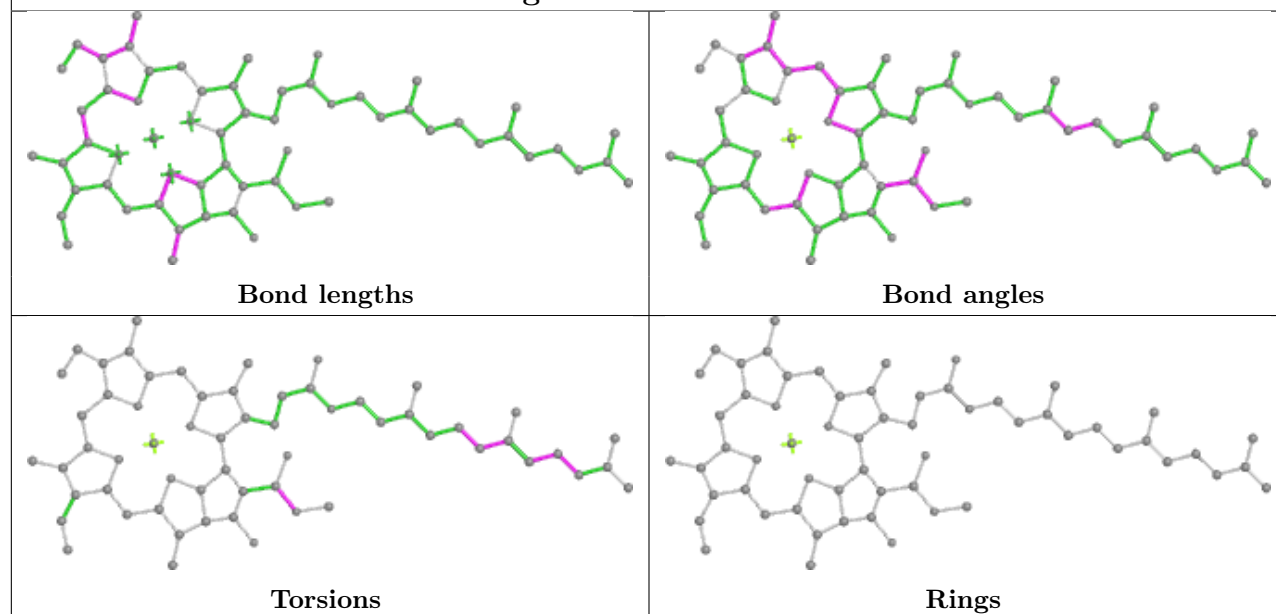
Ligand CLA AA 831

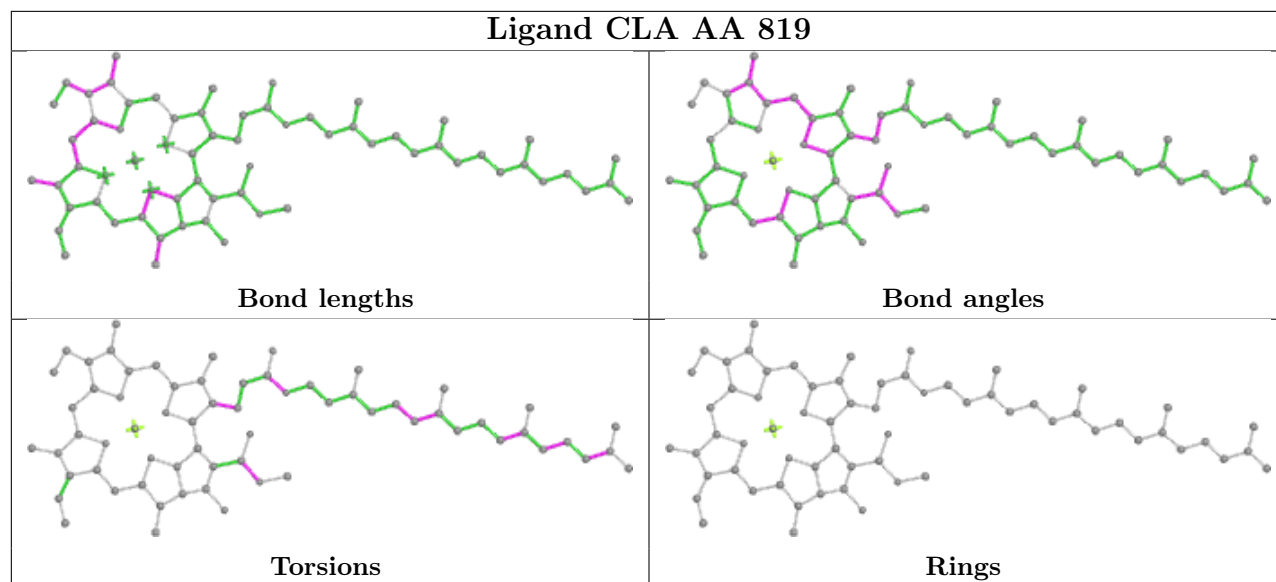
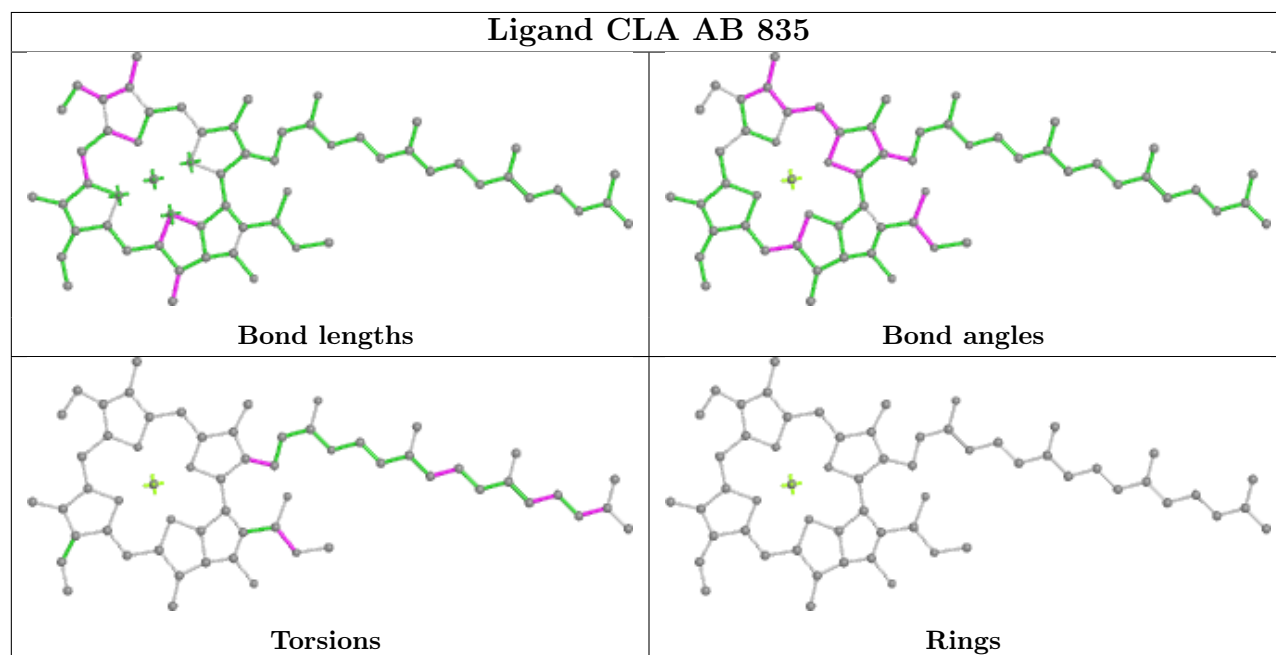


Ligand CLA AA 835

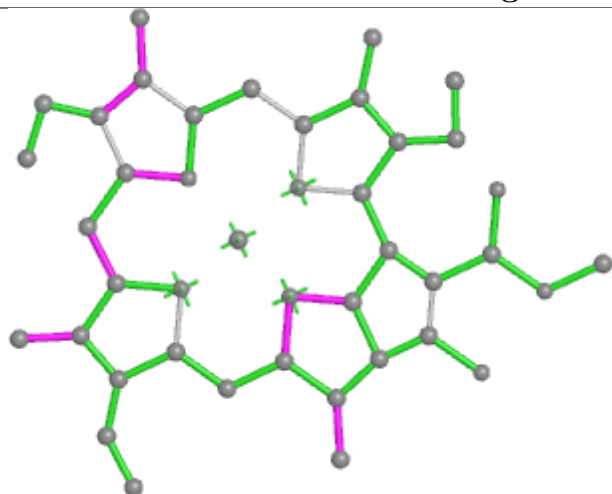


Ligand CLA A3 302

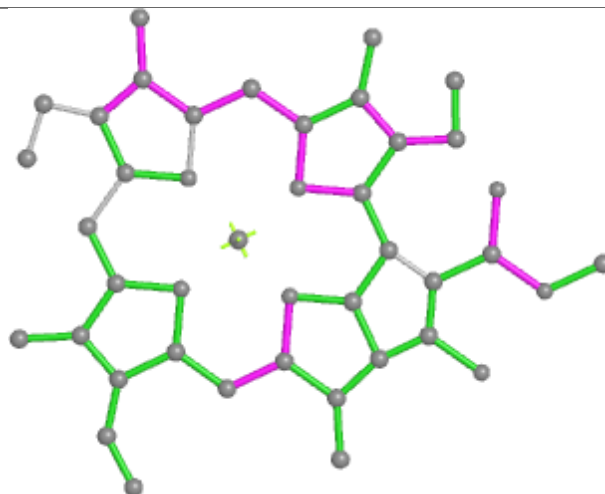


Ligand CLA AA 819**Ligand CLA AB 835**

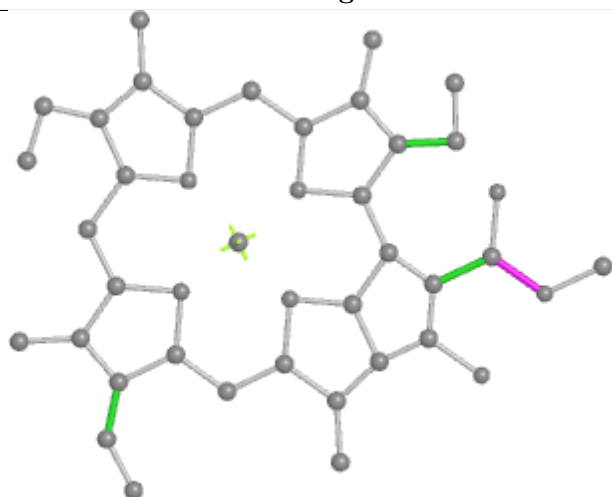
Ligand CLA AF 803



Bond lengths



Bond angles

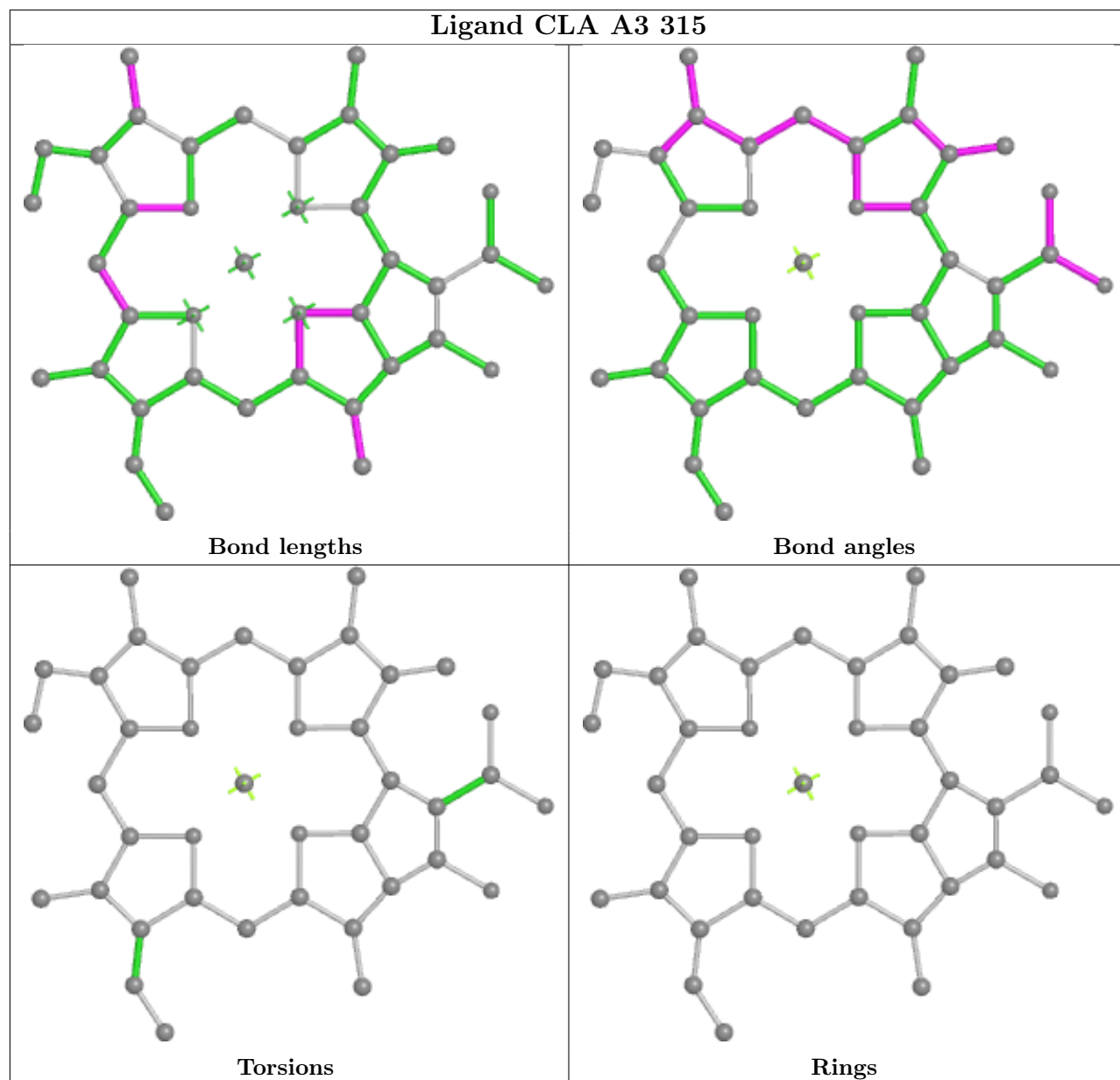


Torsions

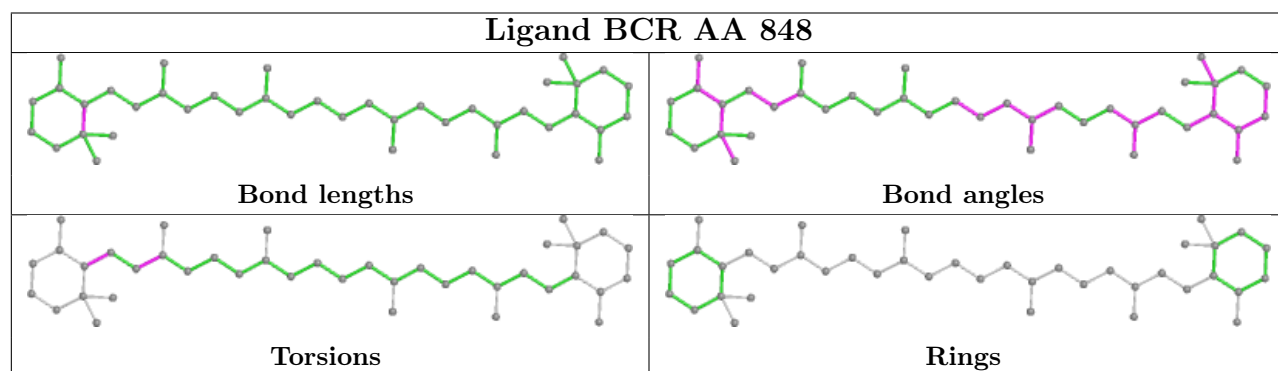


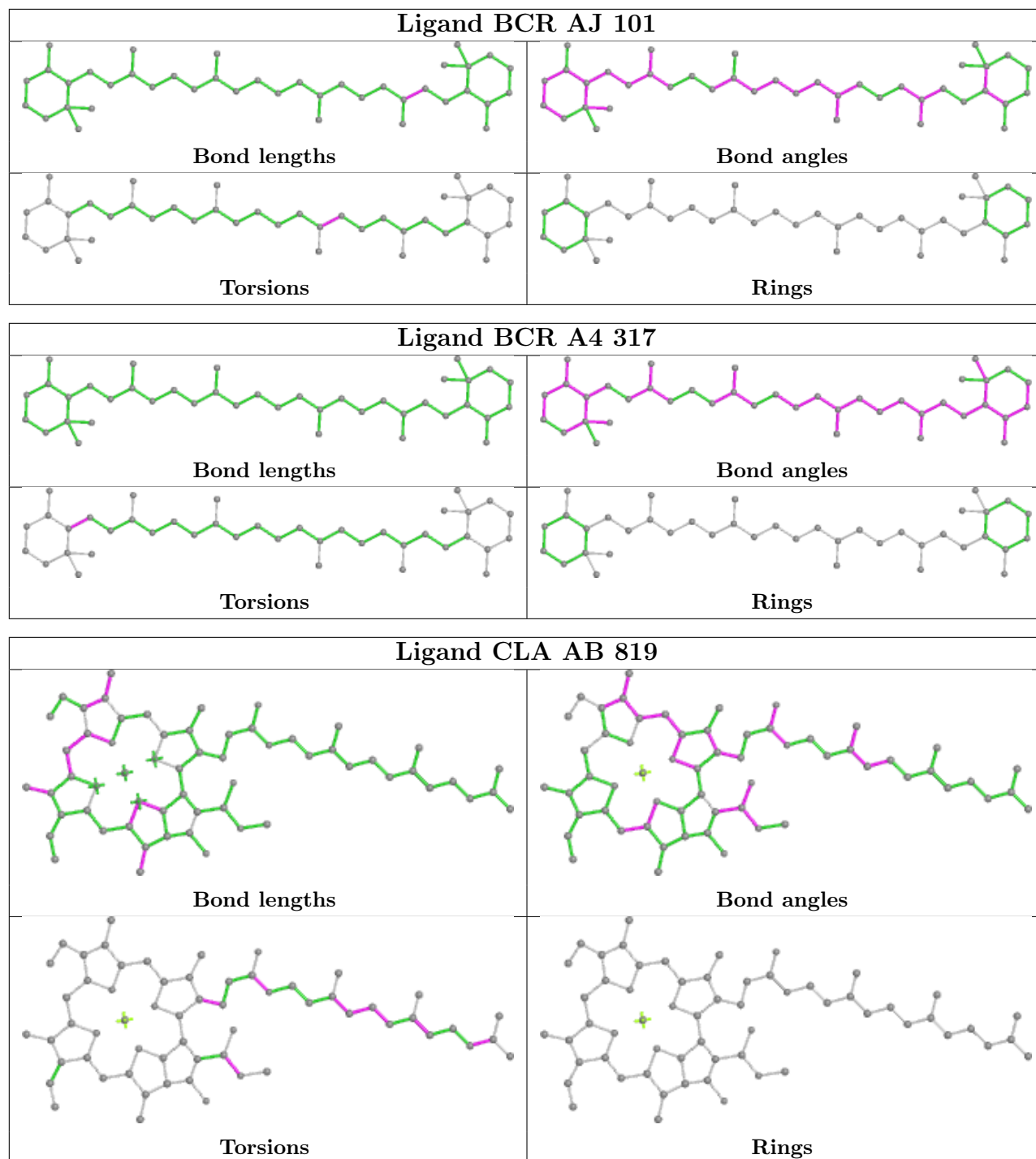
Rings

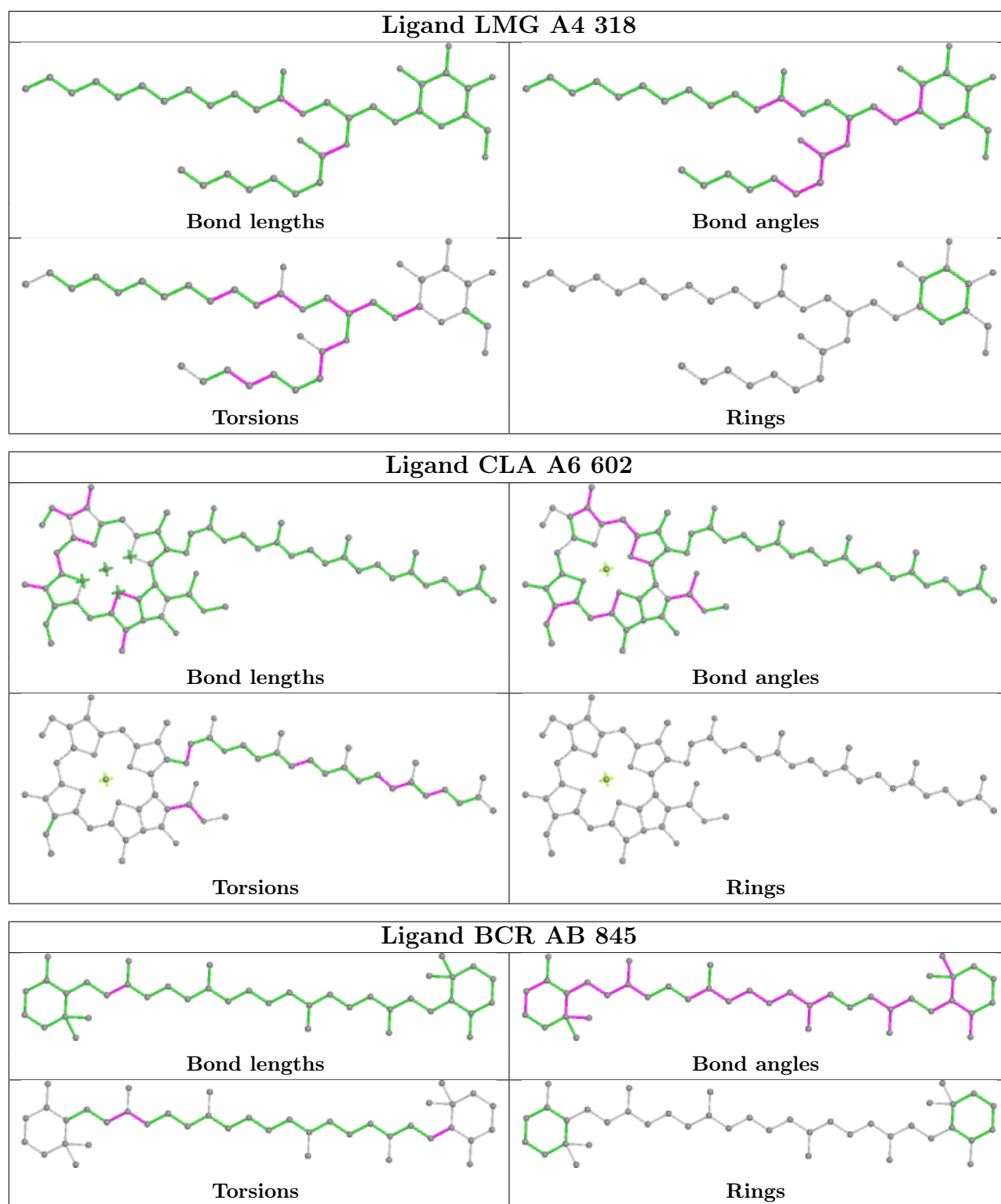
Ligand CLA A3 315



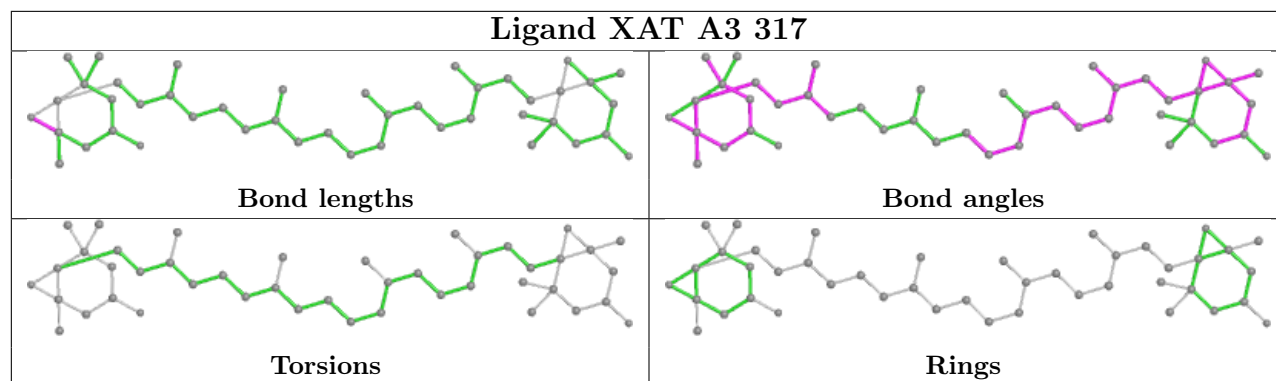
Ligand BCR AA 848



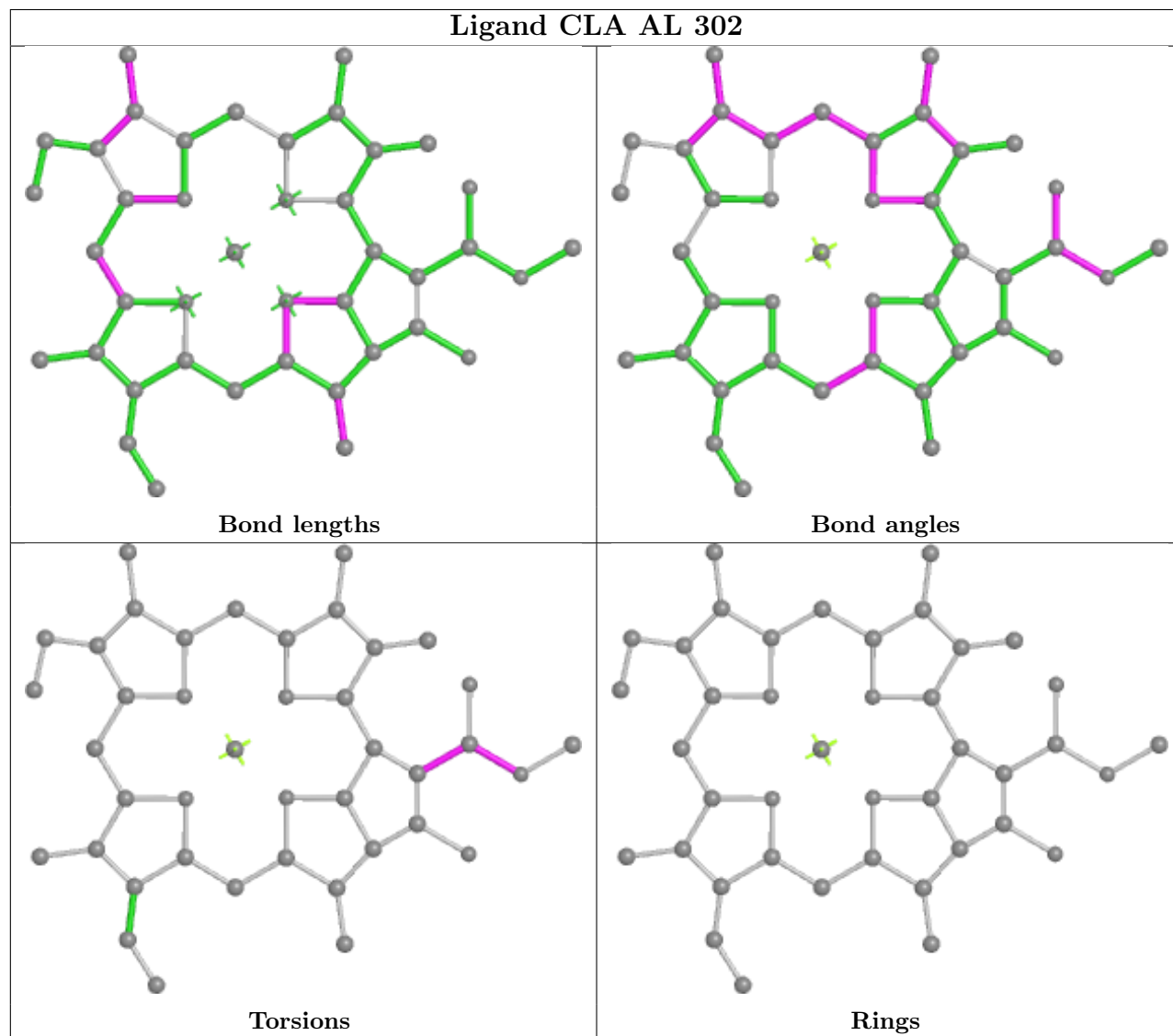


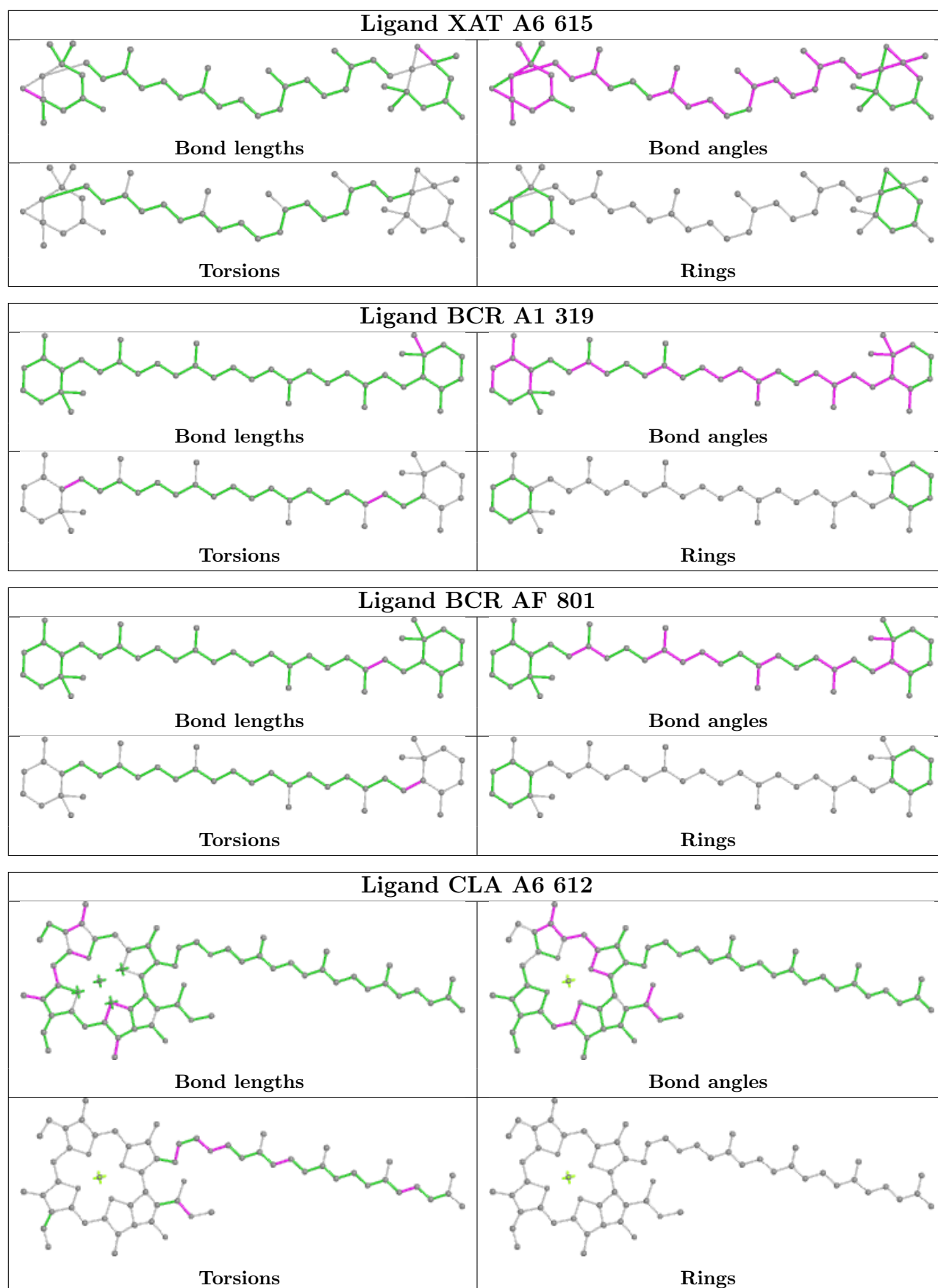


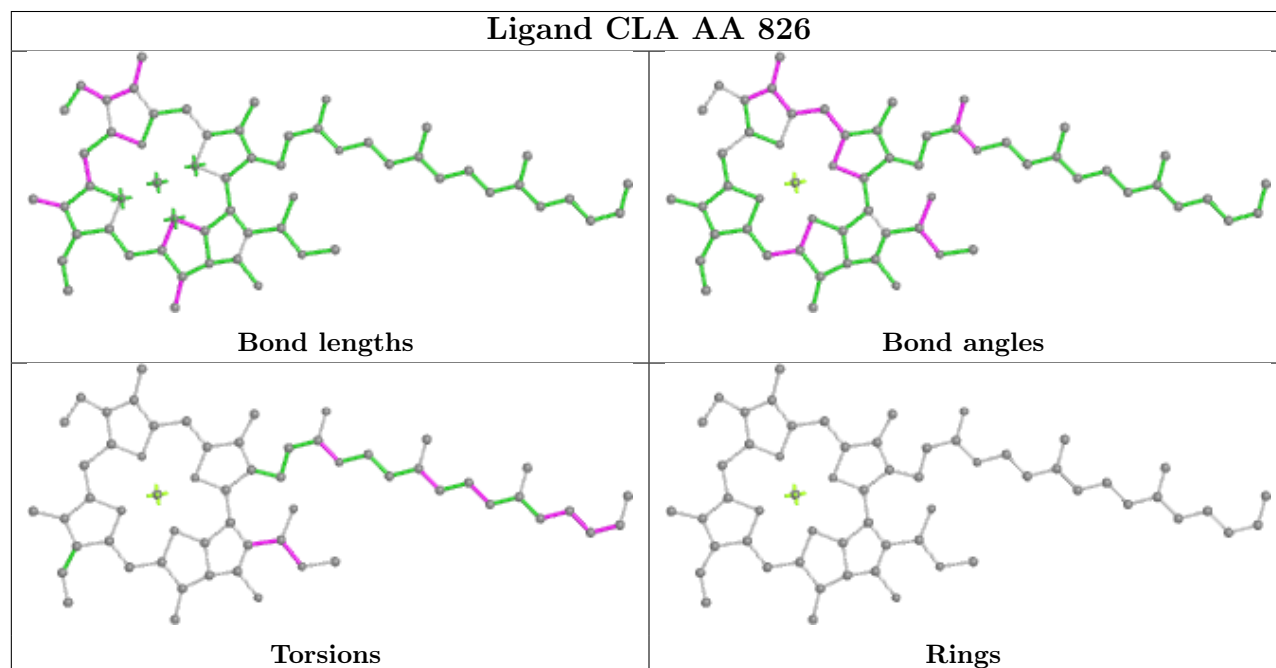
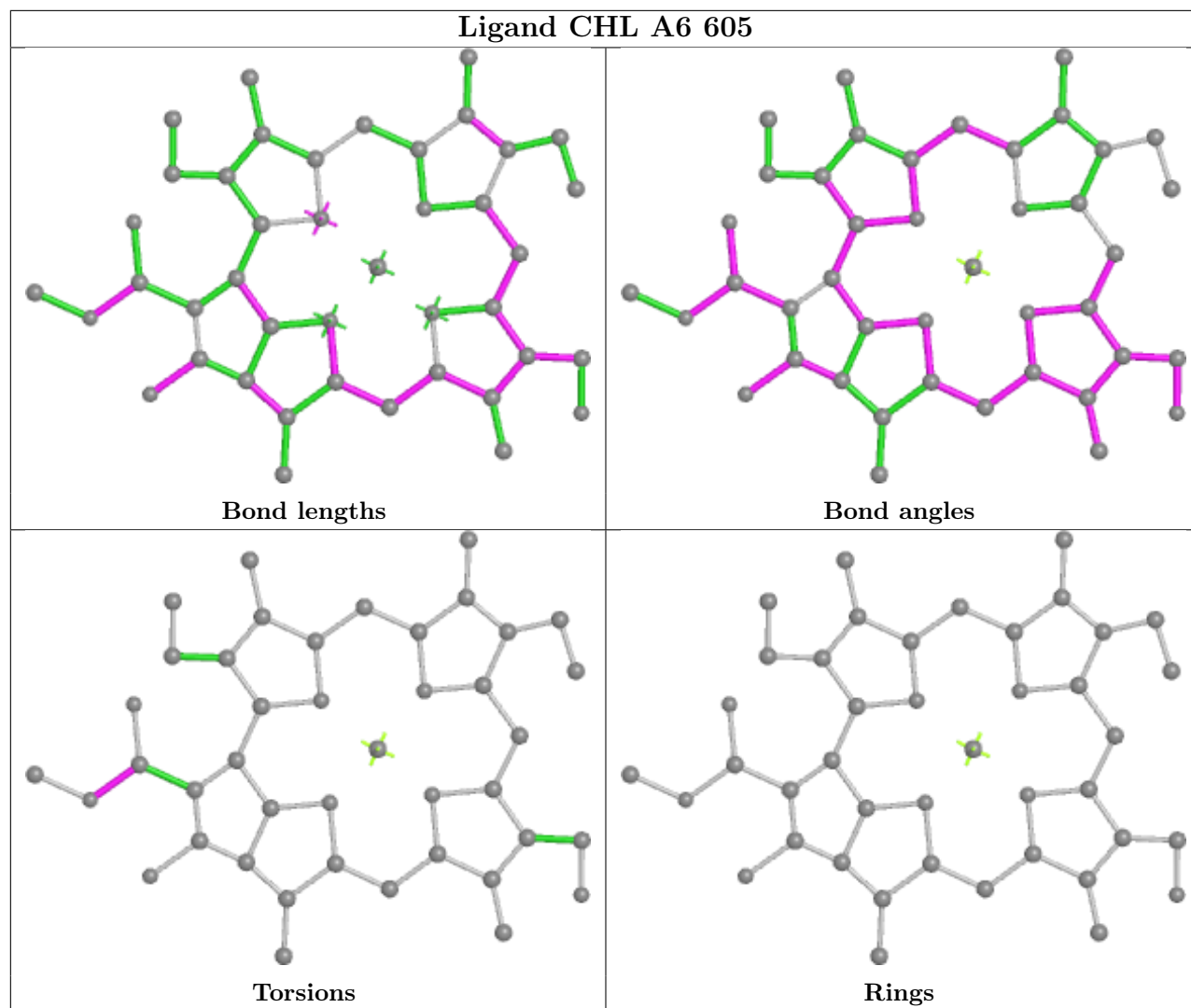
Ligand XAT A3 317



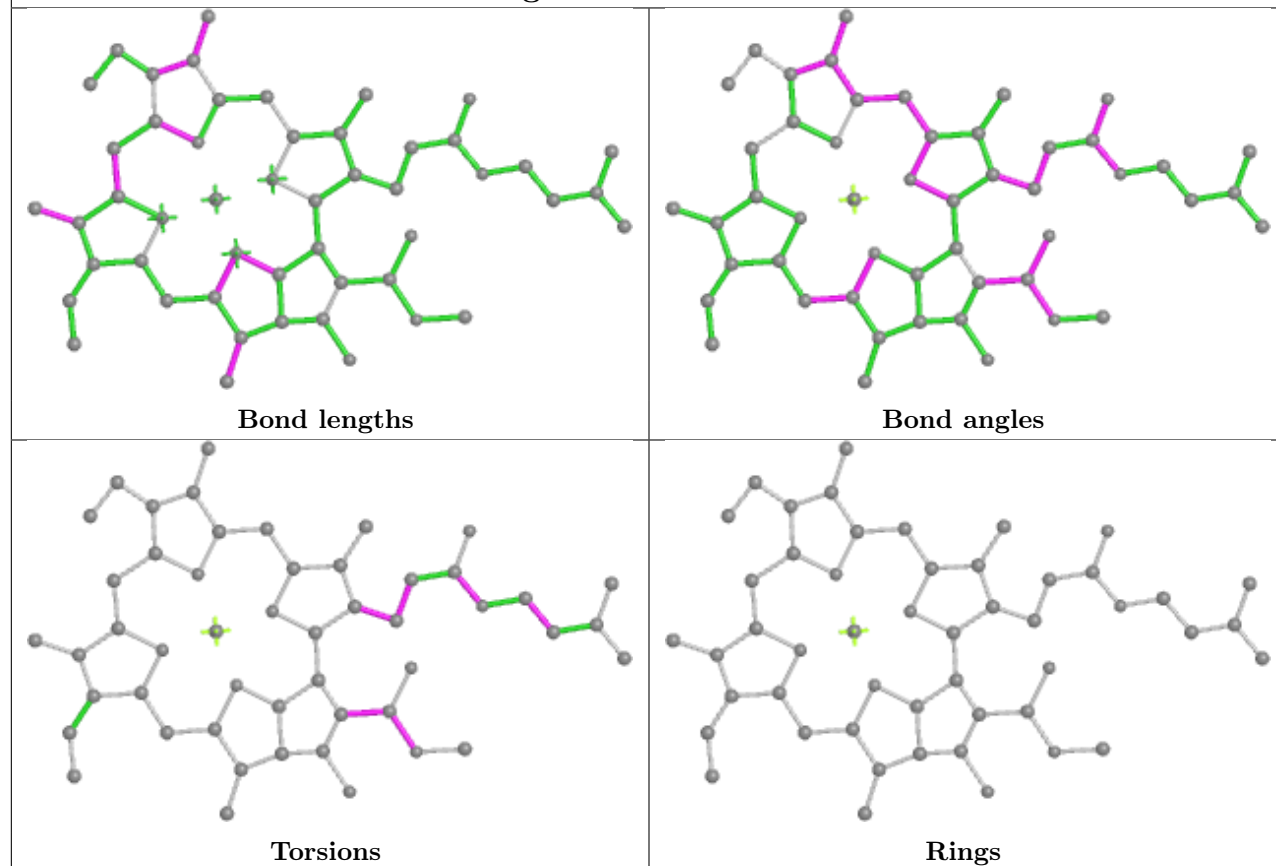
Ligand CLA AL 302



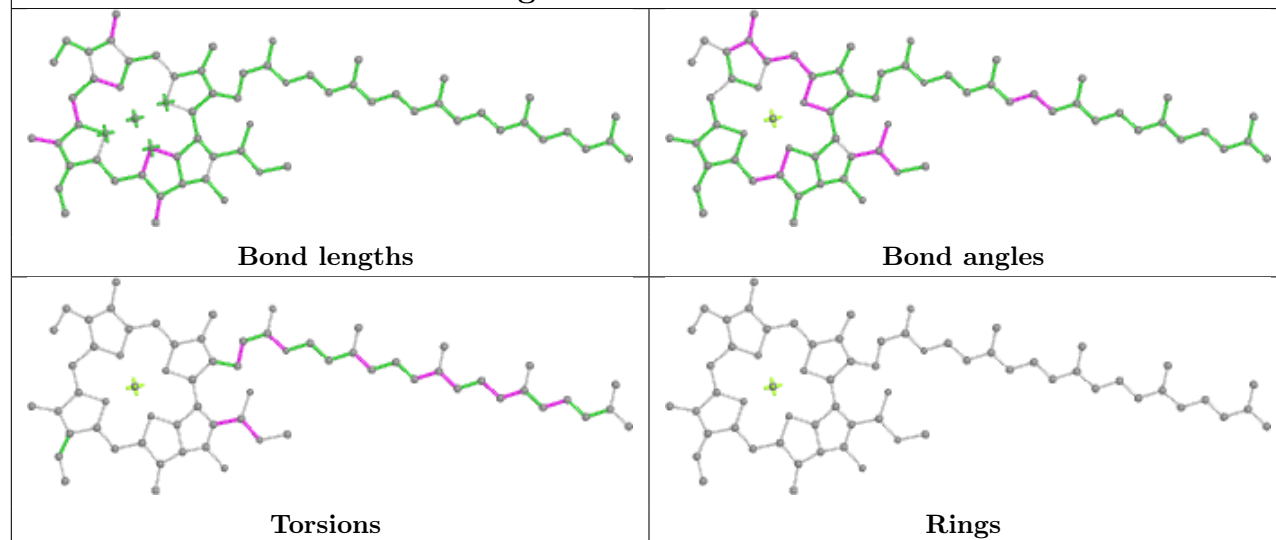




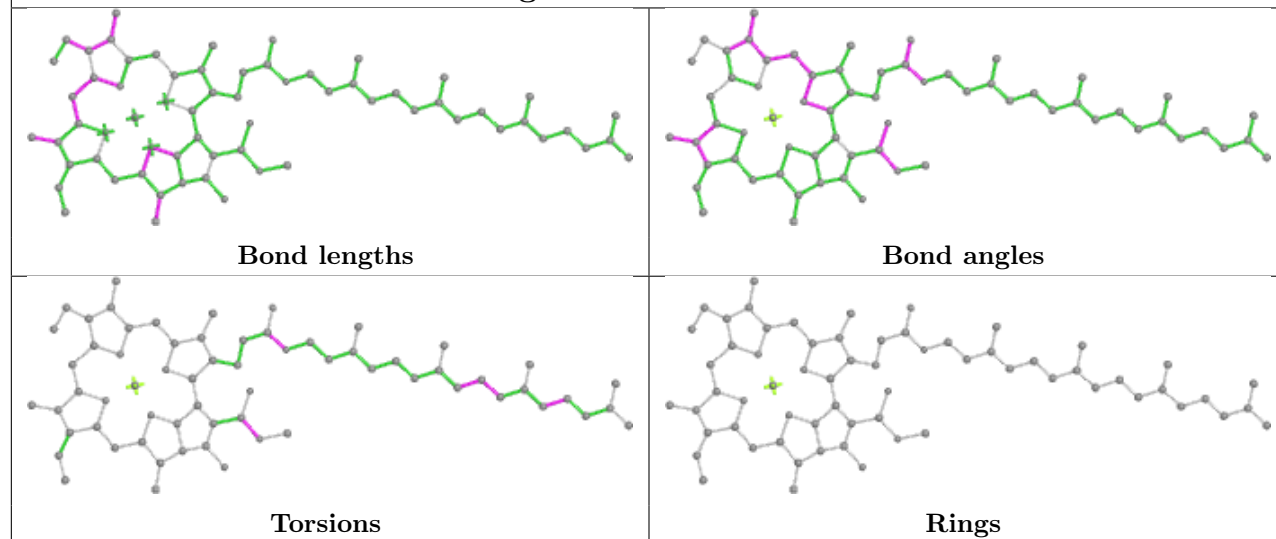
Ligand CLA A4 313



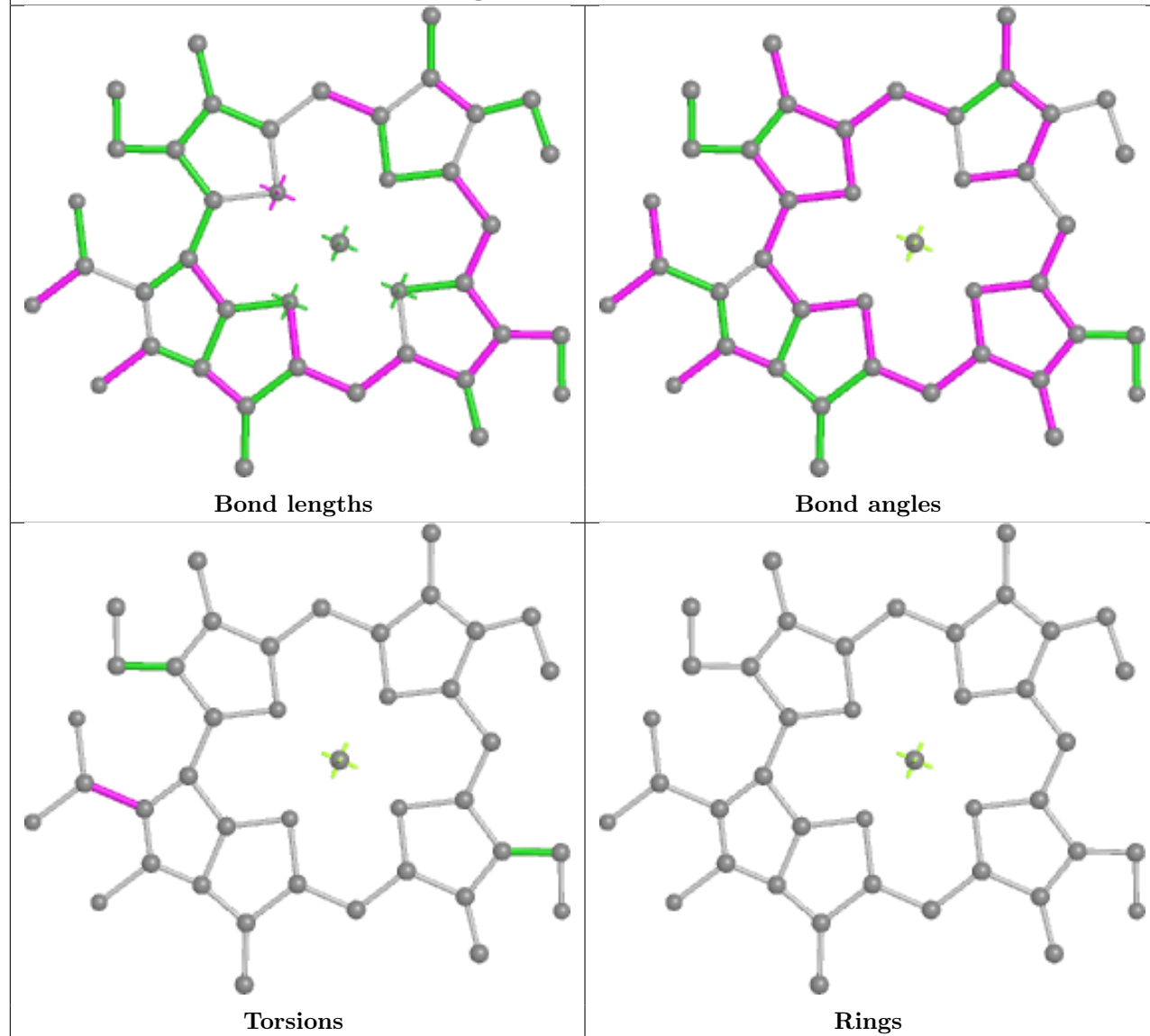
Ligand CLA AA 821



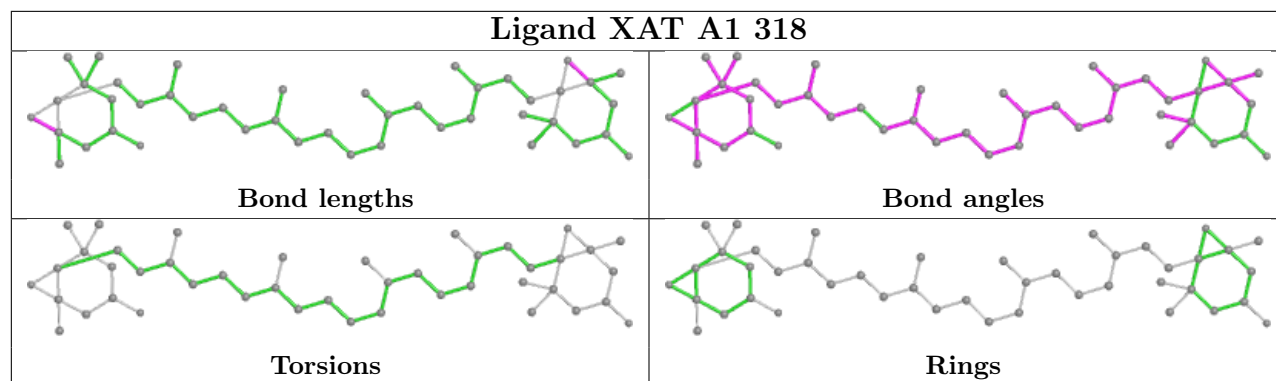
Ligand CLA AB 832



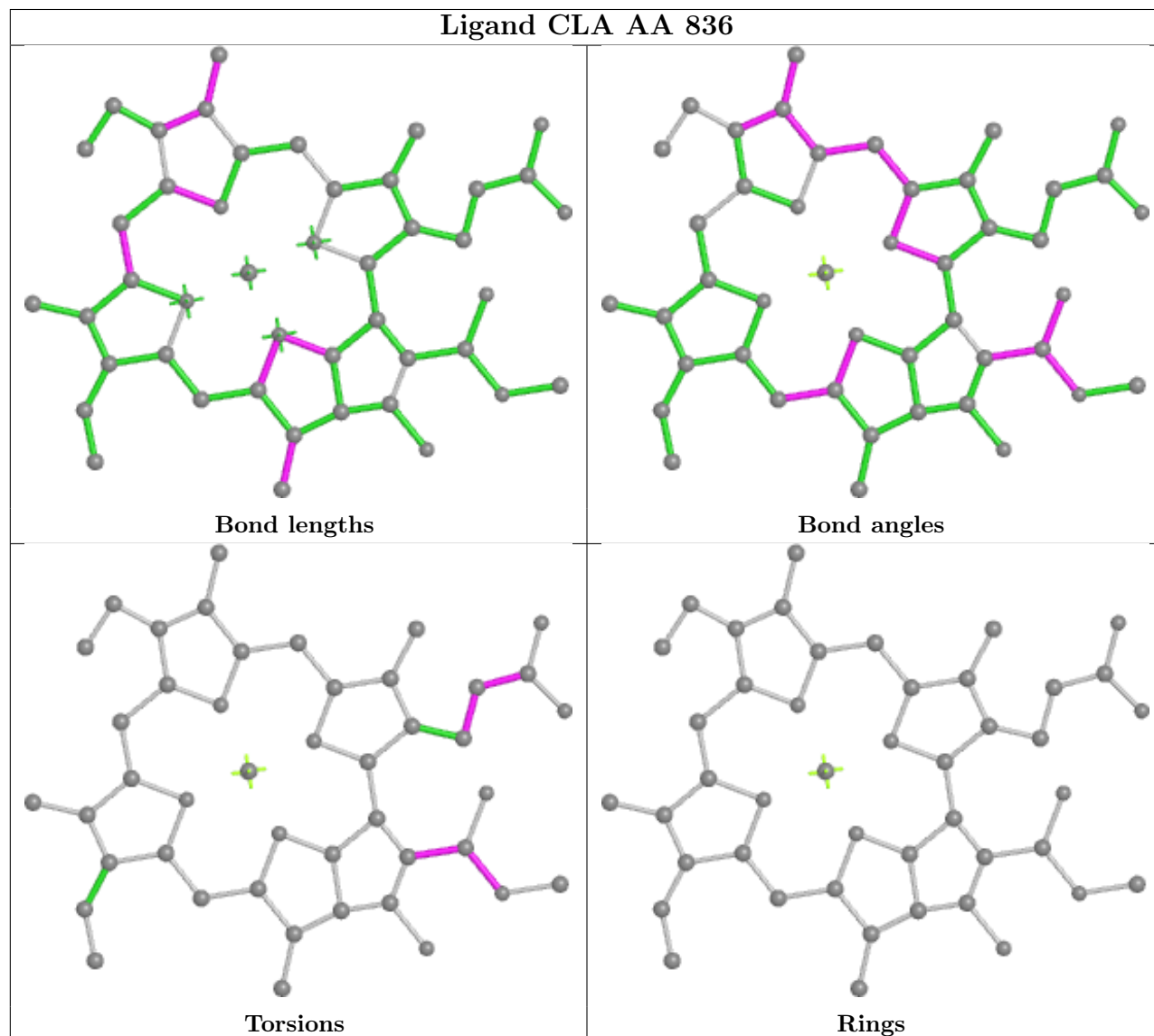
Ligand CHL A4 304



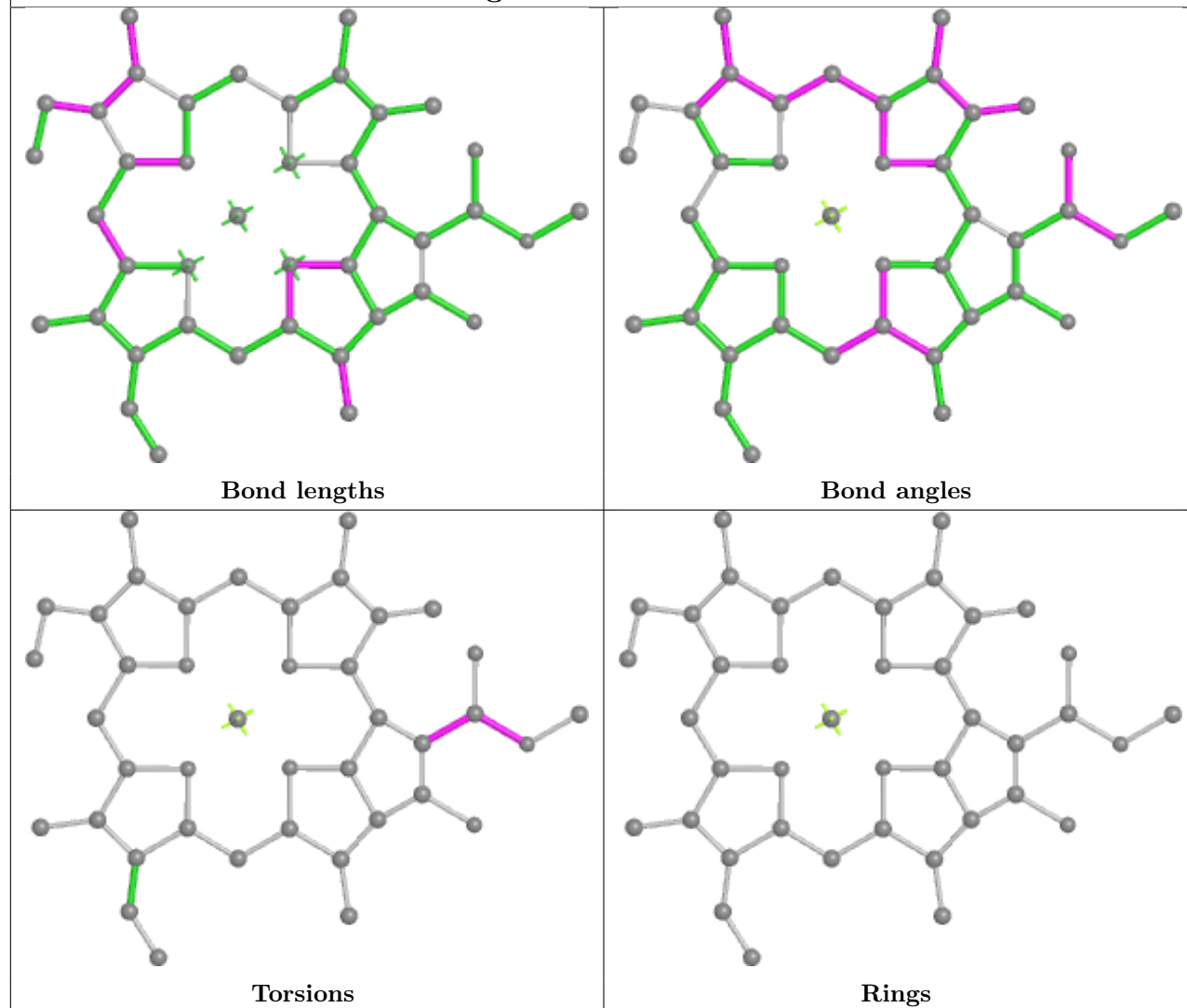
Ligand XAT A1 318



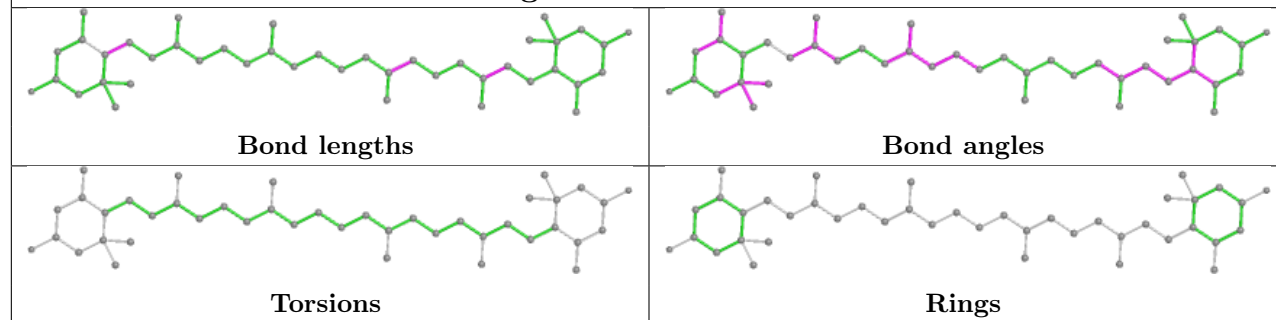
Ligand CLA AA 836



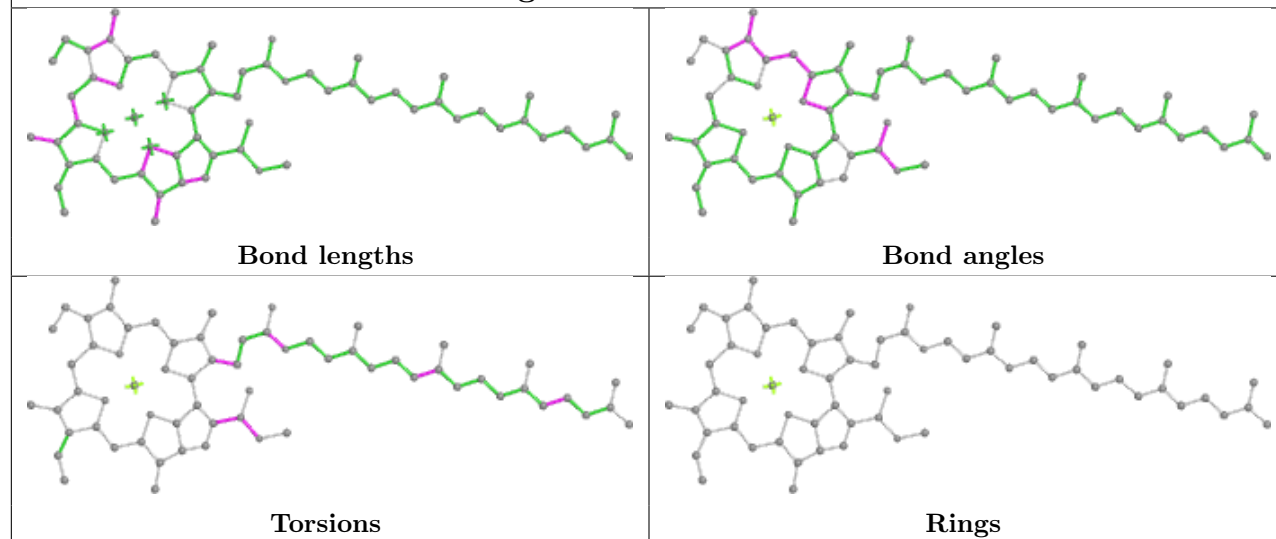
Ligand CLA A3 309



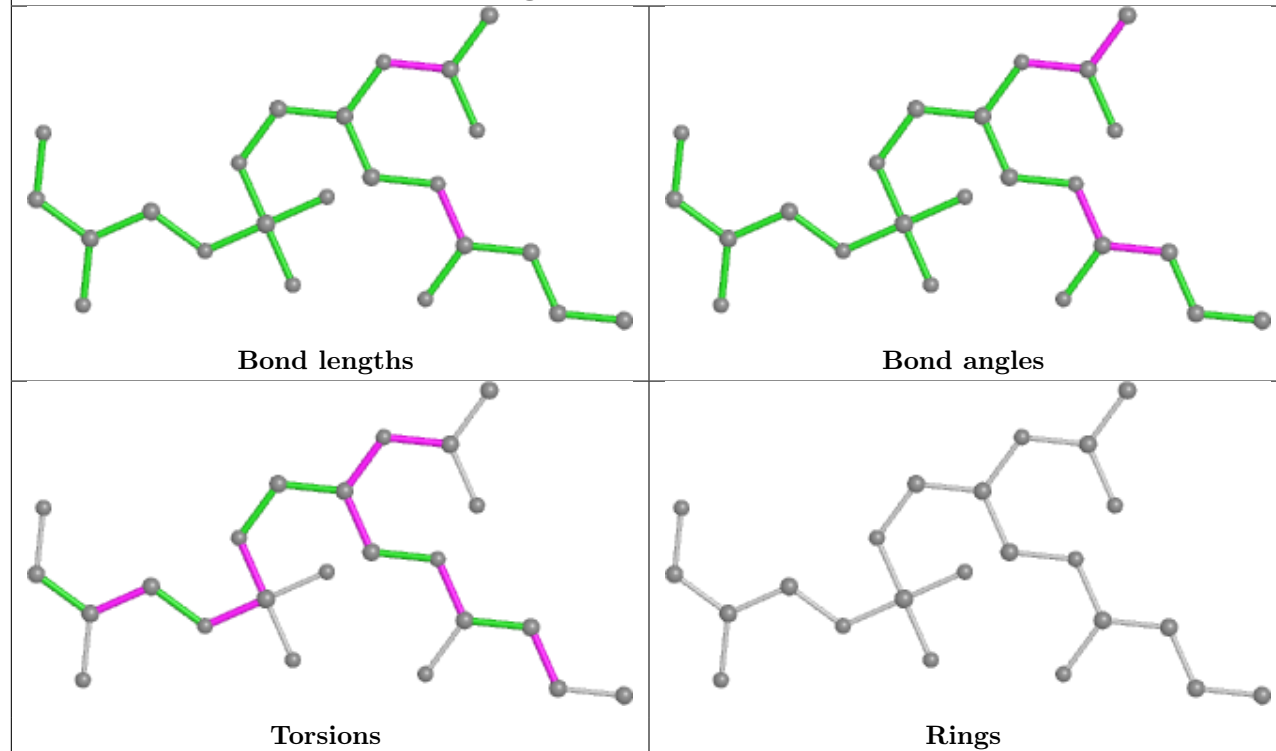
Ligand LUT AF 806

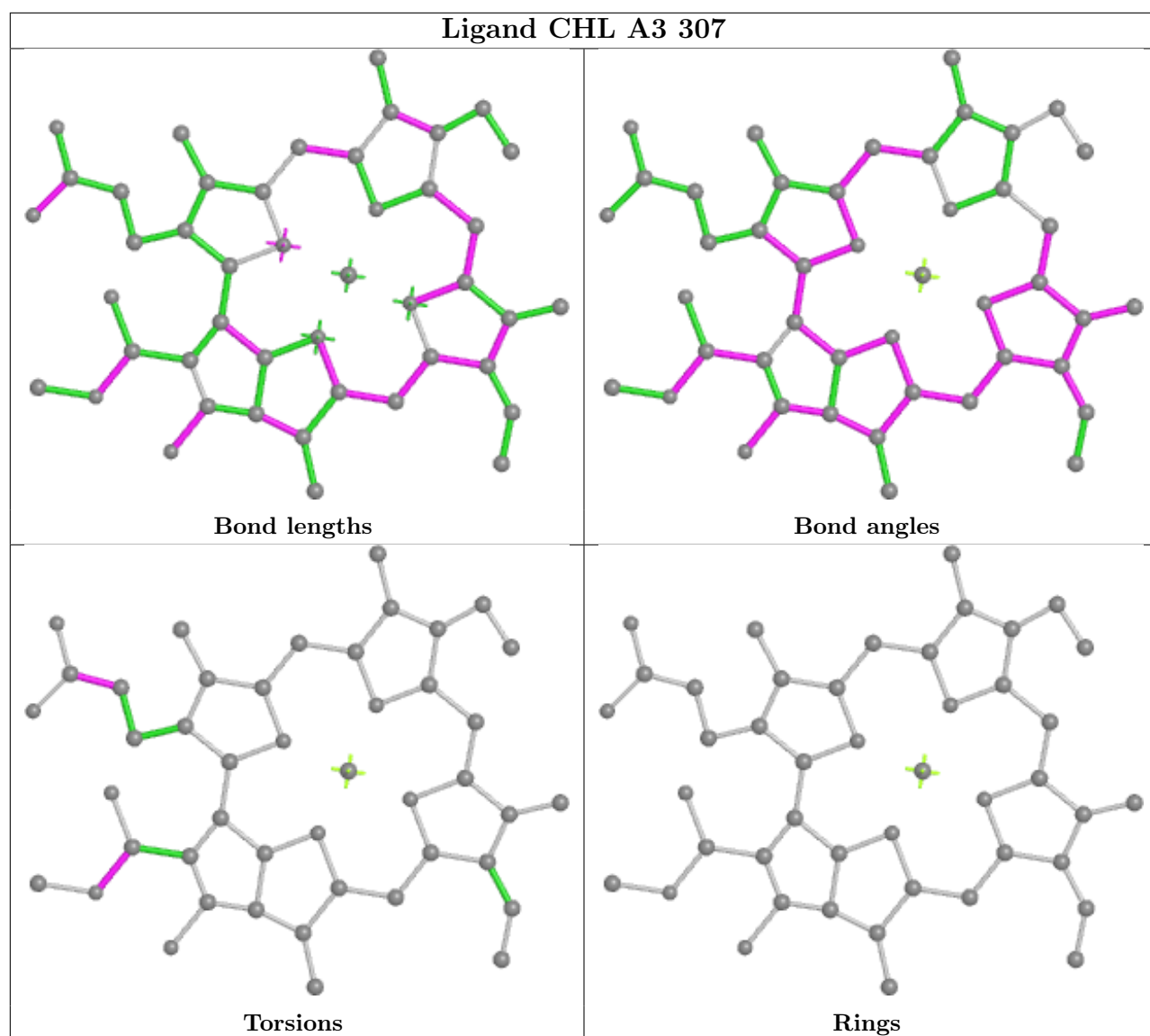


Ligand CLA AA 810

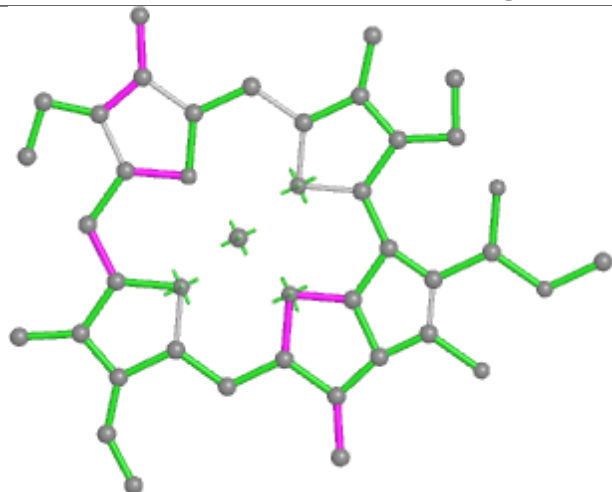


Ligand LHG A3 319

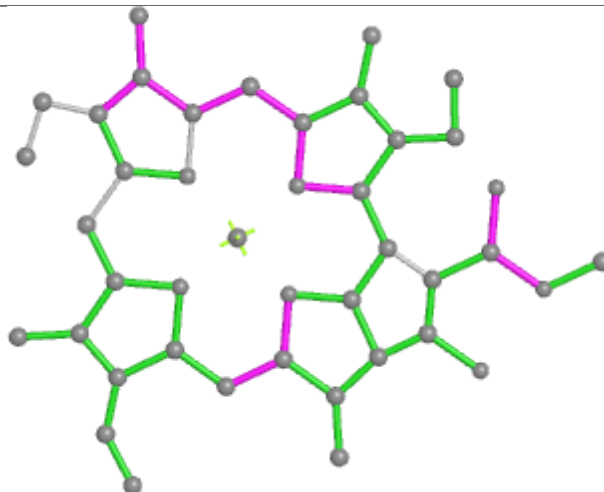




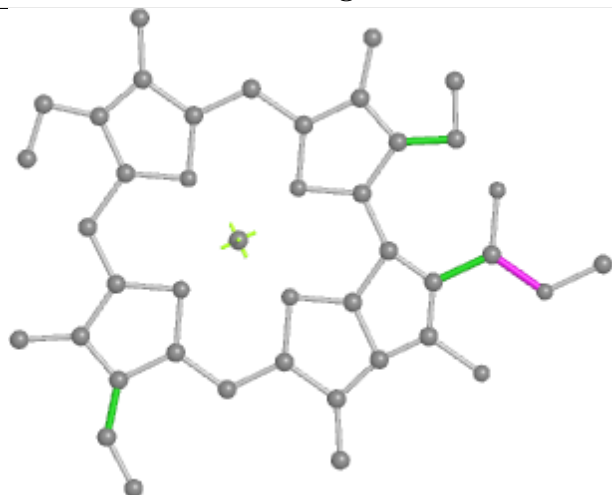
Ligand CLA AB 836



Bond lengths



Bond angles

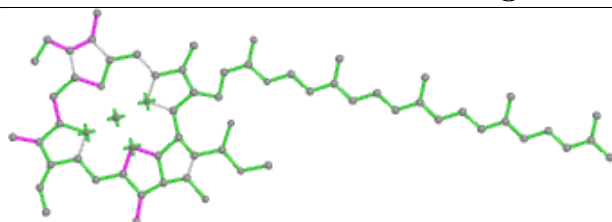


Torsions

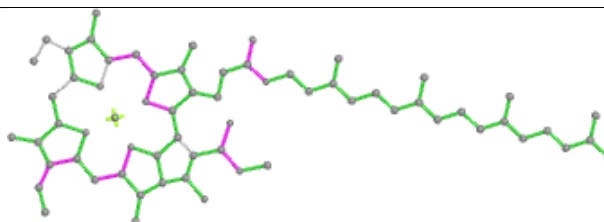


Rings

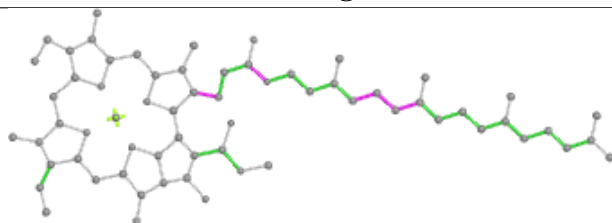
Ligand CLA AB 841



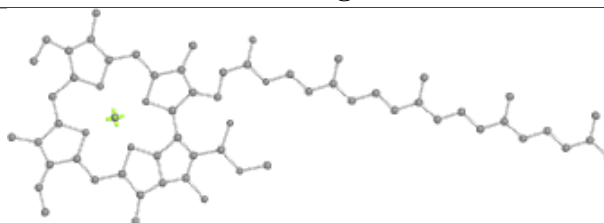
Bond lengths



Bond angles

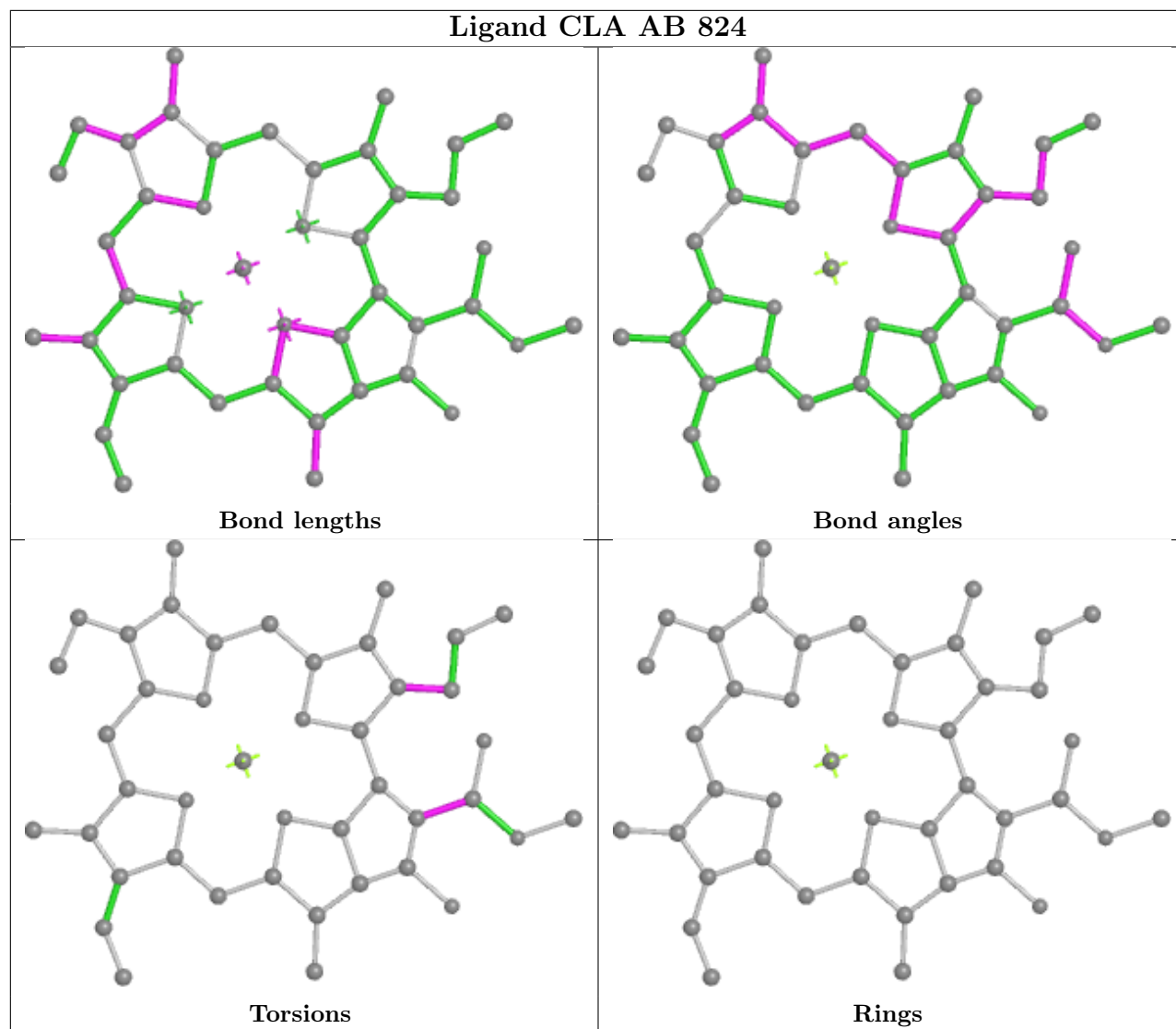


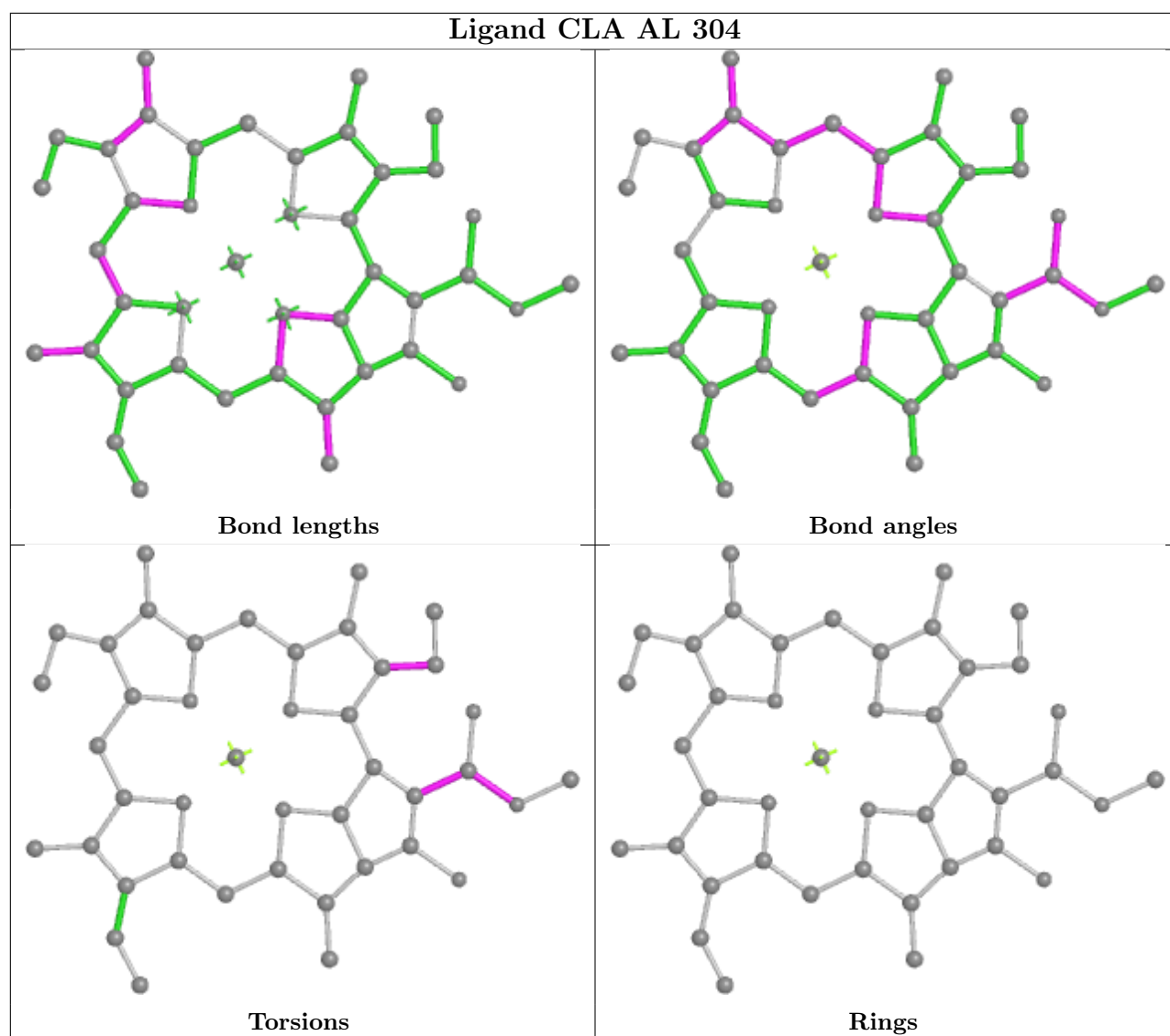
Torsions



Rings

Ligand CLA AB 824





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.

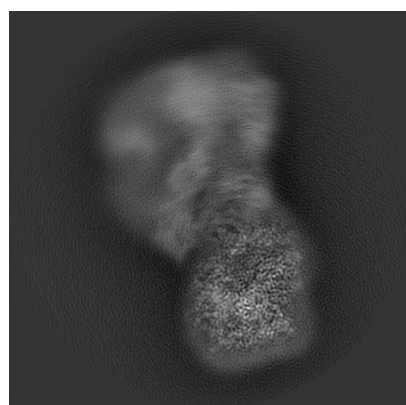
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32462. These allow visual inspection of the internal detail of the map and identification of artifacts.

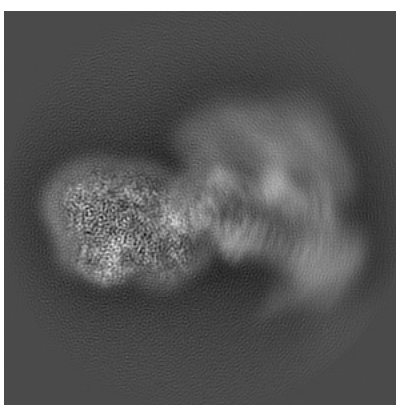
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

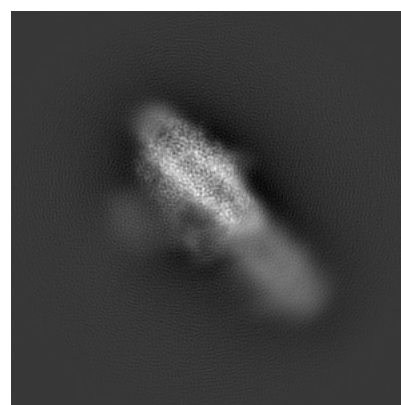
6.1.1 Primary map



X



Y

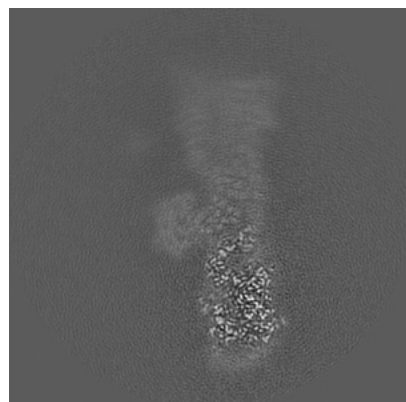


Z

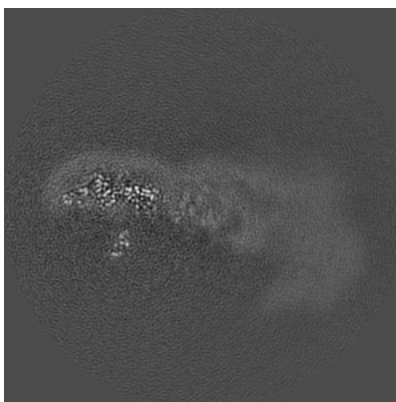
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

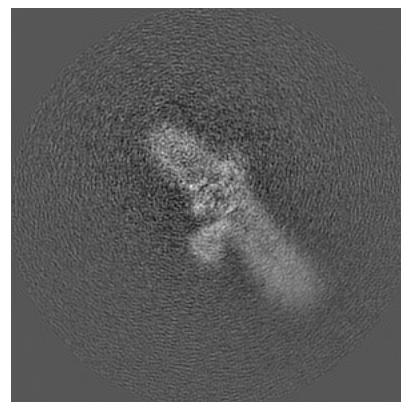
6.2.1 Primary map



X Index: 200



Y Index: 200

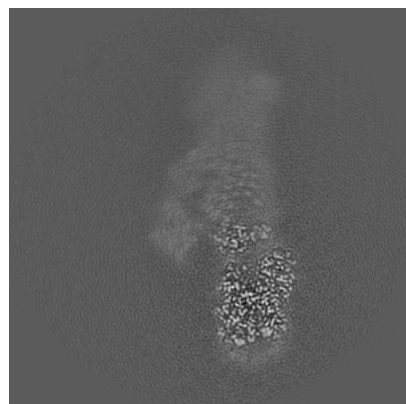


Z Index: 200

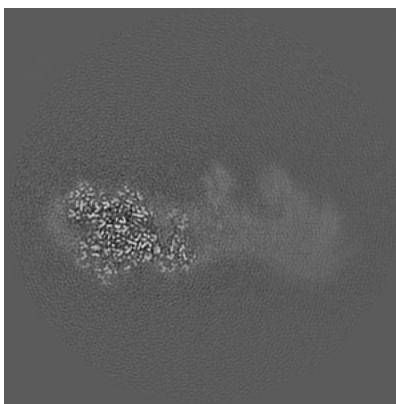
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

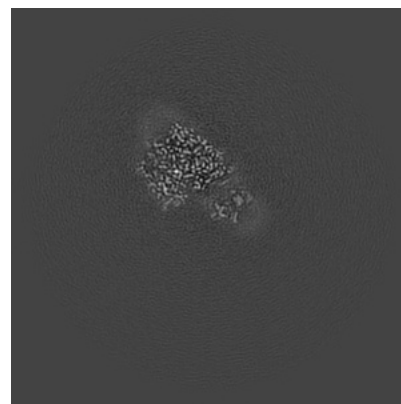
6.3.1 Primary map



X Index: 185



Y Index: 251

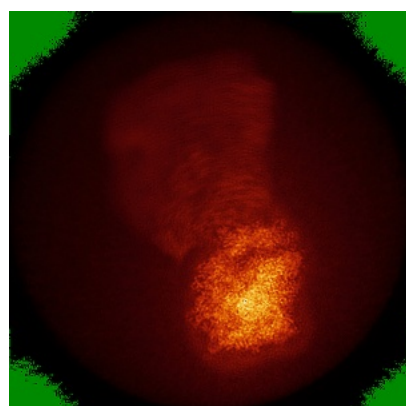


Z Index: 109

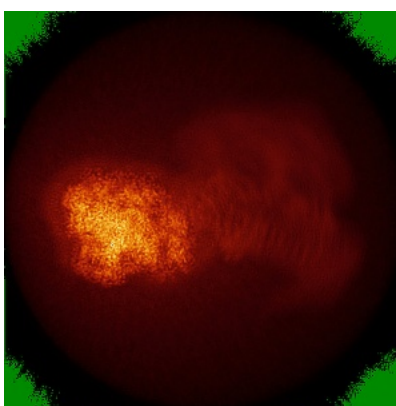
The images above show the largest variance slices of the map in three orthogonal directions.

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

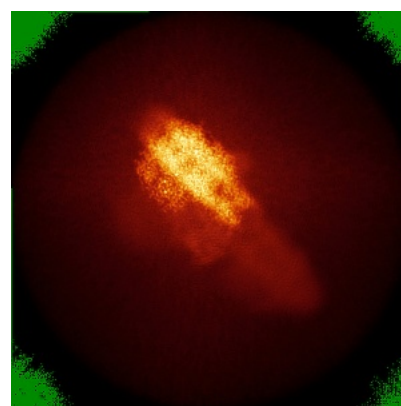
6.4.1 Primary map



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

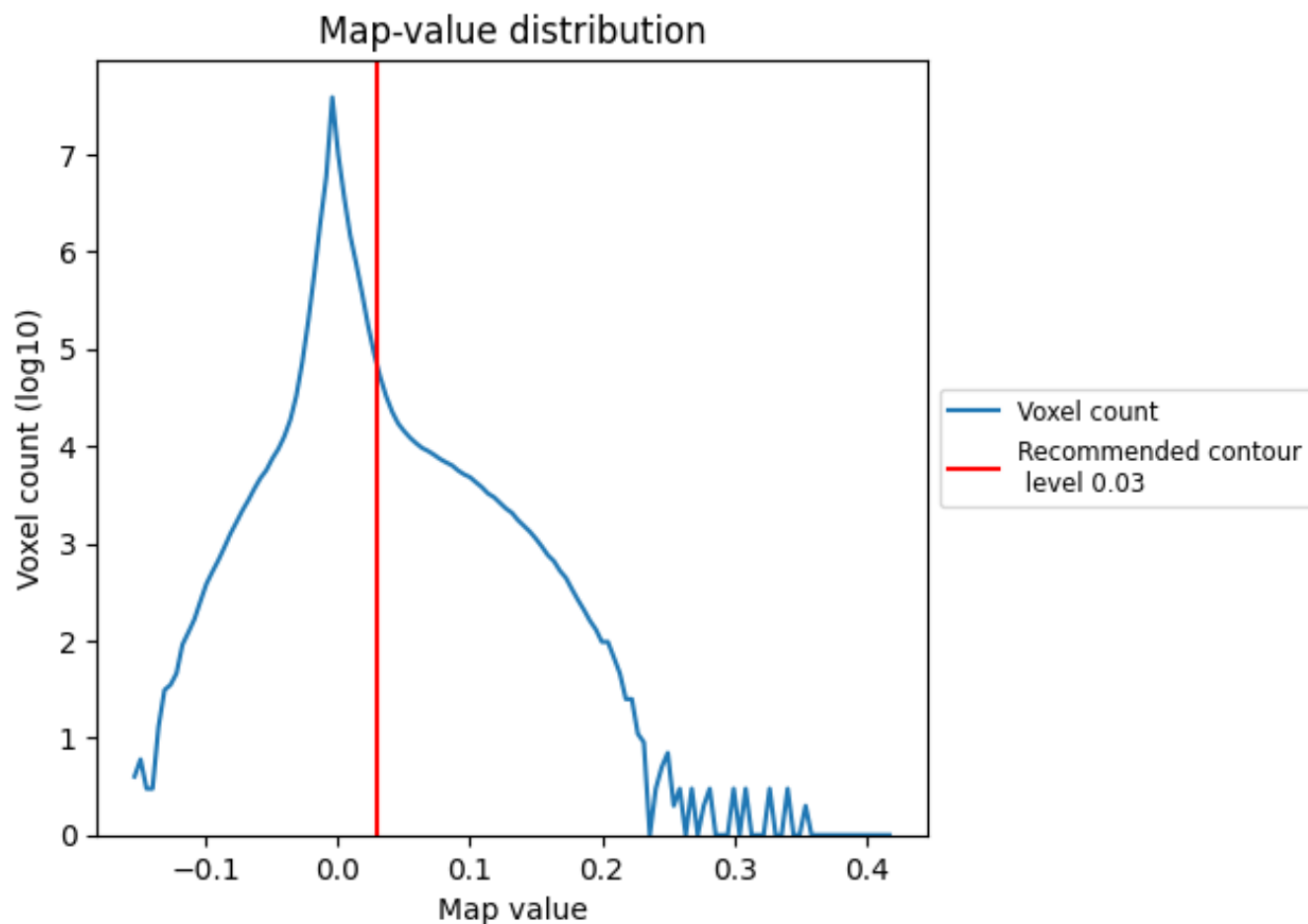
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

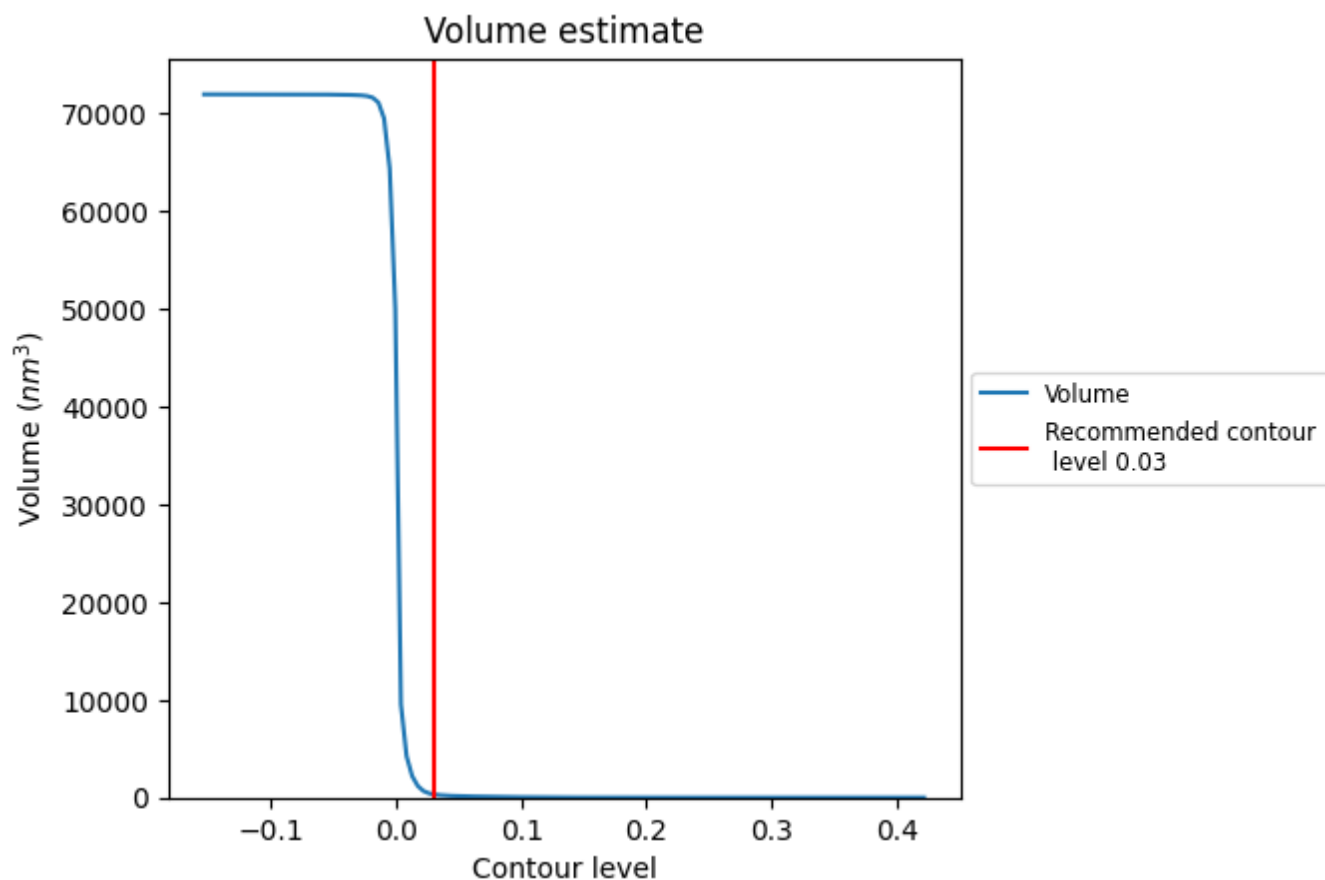
This section contains the results of statistical analysis of the map.

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.

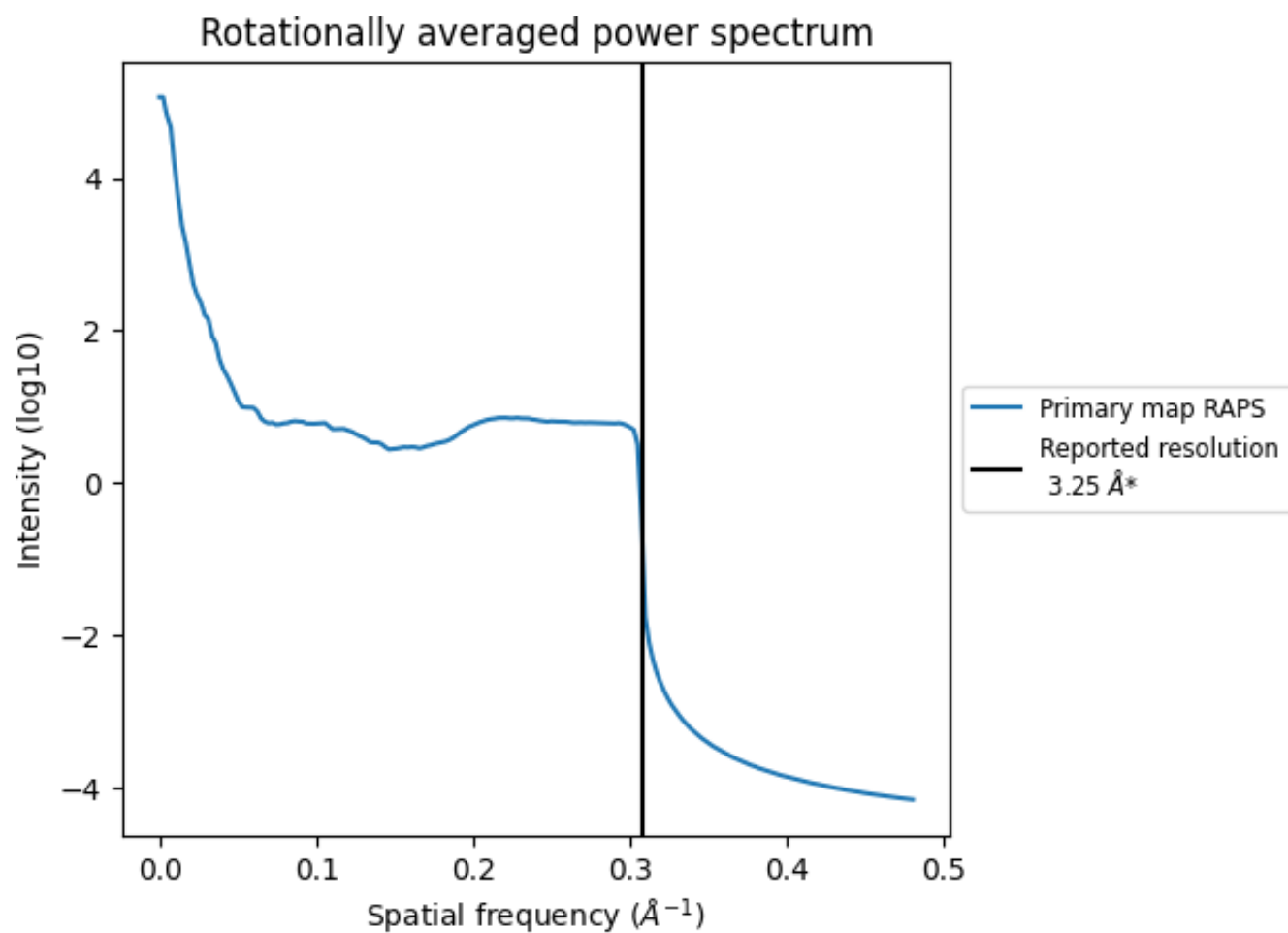
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 338 nm^3 ; this corresponds to an approximate mass of 305 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 0.308 Å⁻¹

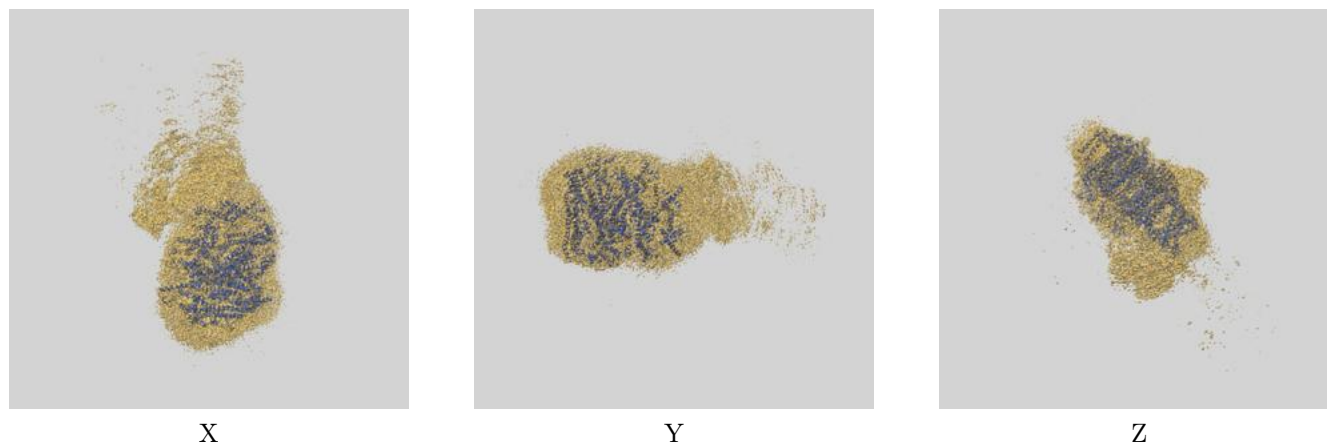
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

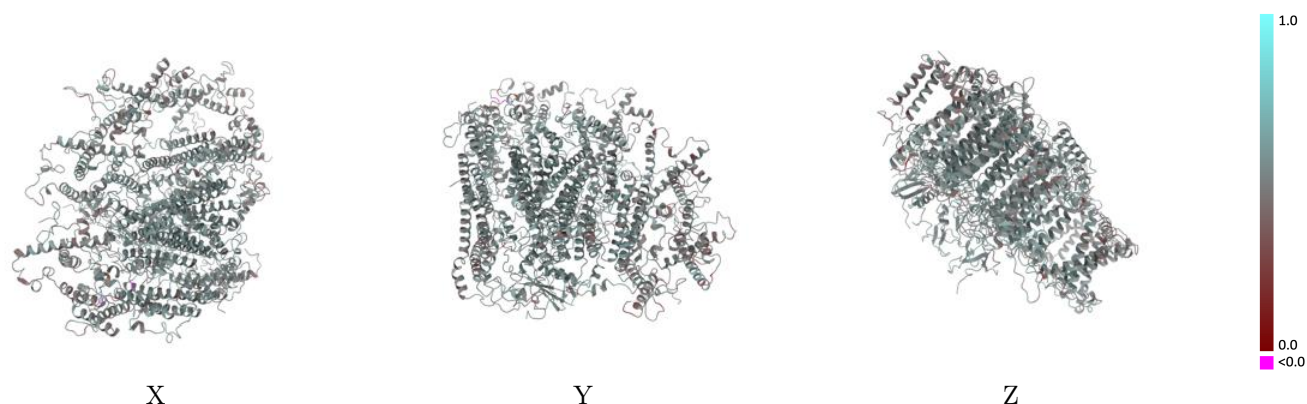
This section contains information regarding the fit between EMDB map EMD-32462 and PDB model 7WFD. Per-residue inclusion information can be found in [section 3](#) on [page 26](#).

9.1 Map-model overlay [i](#)



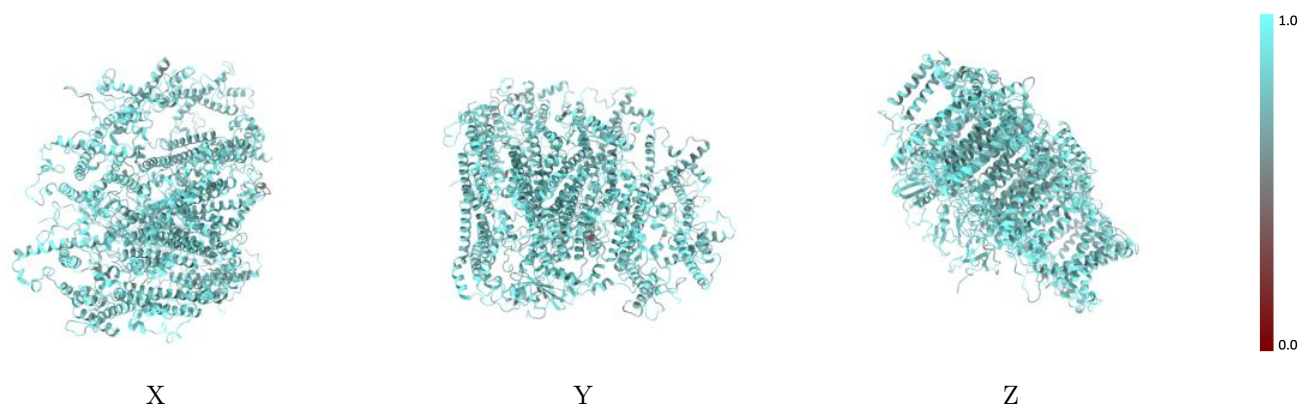
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



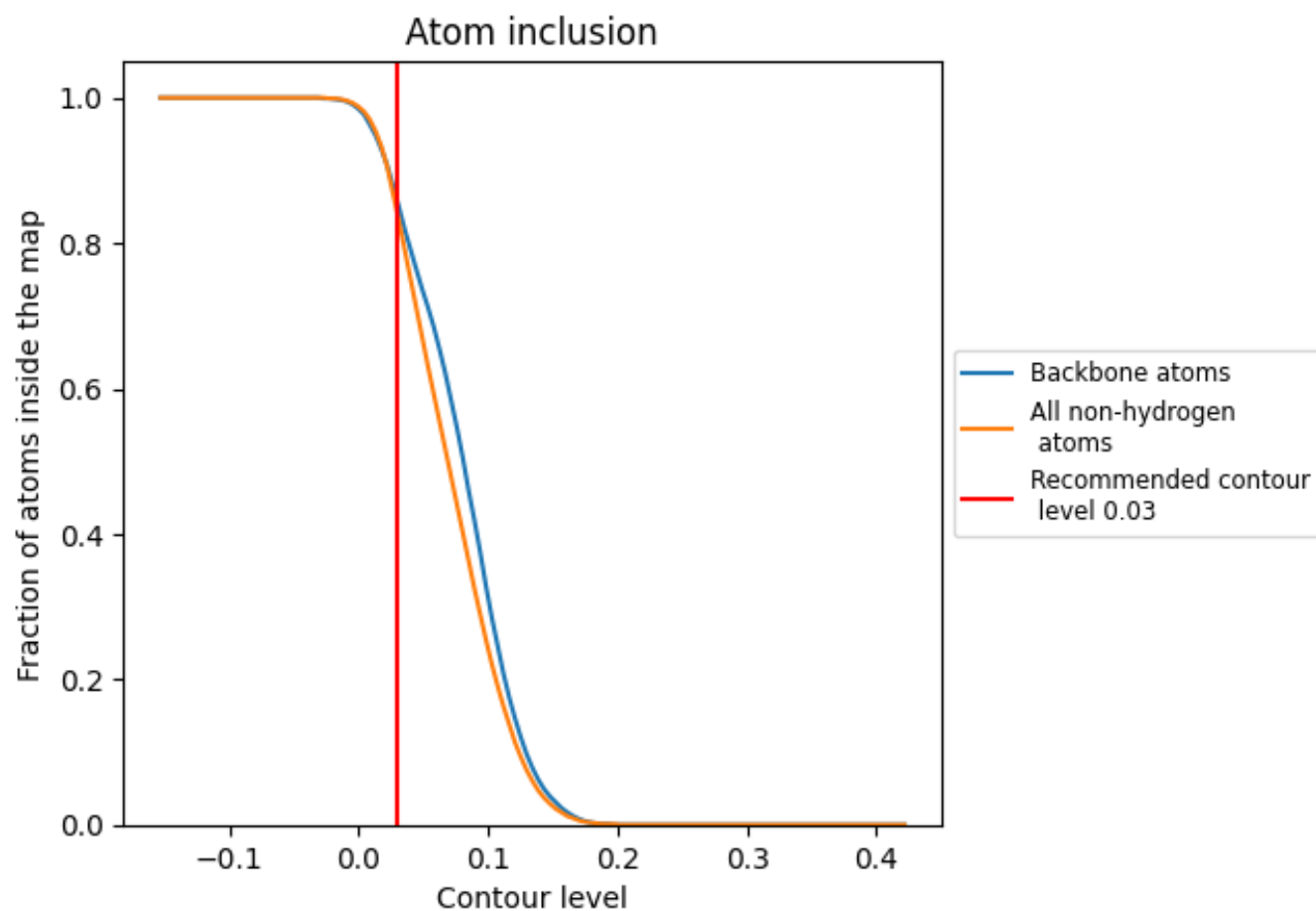
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 84% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8400	<div><div></div></div> 0.5260
A1	<div><div></div></div> 0.8080	<div><div></div></div> 0.4950
A3	<div><div></div></div> 0.8200	<div><div></div></div> 0.4920
A4	<div><div></div></div> 0.8260	<div><div></div></div> 0.5120
A6	<div><div></div></div> 0.7940	<div><div></div></div> 0.5080
AA	<div><div></div></div> 0.8520	<div><div></div></div> 0.5410
AB	<div><div></div></div> 0.8730	<div><div></div></div> 0.5510
AC	<div><div></div></div> 0.9040	<div><div></div></div> 0.5380
AD	<div><div></div></div> 0.8780	<div><div></div></div> 0.5350
AE	<div><div></div></div> 0.8330	<div><div></div></div> 0.5360
AF	<div><div></div></div> 0.8530	<div><div></div></div> 0.5450
AG	<div><div></div></div> 0.8030	<div><div></div></div> 0.4910
AH	<div><div></div></div> 0.8220	<div><div></div></div> 0.4920
AI	<div><div></div></div> 0.8040	<div><div></div></div> 0.5050
AJ	<div><div></div></div> 0.7780	<div><div></div></div> 0.5130
AK	<div><div></div></div> 0.7230	<div><div></div></div> 0.4550
AL	<div><div></div></div> 0.8090	<div><div></div></div> 0.5000

1.0

0.0

<0.0