



## wwPDB EM Validation Summary Report ⓘ

Oct 15, 2024 – 06:53 AM JST

PDB ID : 7WFE  
EMDB ID : EMD-32463  
Title : Right PSI in the cyclic electron transfer supercomplex NDH-PSI from Arabidopsis  
Authors : Pan, X.W.; 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis	:	0.0.1.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

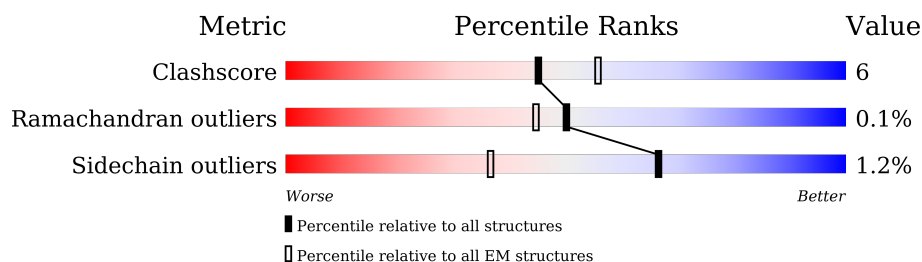
# 1 Overall quality at a glance

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

Mol	Chain	Length	Quality of chain
1	BA	750	
2	BB	734	
3	BC	81	
4	BD	204	
5	BE	143	
6	BF	221	
7	BG	160	
8	BH	145	

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Mol	Chain	Length	Quality of chain
9	BI	37	
10	BJ	44	
11	BK	130	
12	BL	219	
13	B1	241	
14	B2	257	
15	B3	273	
16	B5	256	

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	B1	304	X	-	-	-
17	CLA	B1	305	X	-	-	-
17	CLA	B1	306	X	-	-	-
17	CLA	B1	307	X	-	-	-
17	CLA	B1	310	X	-	-	-
17	CLA	B1	311	X	-	-	-
17	CLA	B1	312	X	-	-	-
17	CLA	B1	313	X	-	-	-
17	CLA	B1	314	X	-	-	-
17	CLA	B1	315	X	-	-	-
17	CLA	B2	301	X	-	-	-
17	CLA	B2	302	X	-	-	-
17	CLA	B2	303	X	-	-	-
17	CLA	B2	307	X	-	-	-
17	CLA	B2	308	X	-	-	-
17	CLA	B2	309	X	-	-	-
17	CLA	B2	310	X	-	-	-
17	CLA	B2	311	X	-	-	-
17	CLA	B2	312	X	-	-	-
17	CLA	B3	602	X	-	-	-
17	CLA	B3	603	X	-	-	-
17	CLA	B3	604	X	-	-	-
17	CLA	B3	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	B3	606	X	-	-	-
17	CLA	B3	608	X	-	-	-
17	CLA	B3	609	X	-	-	-
17	CLA	B3	610	X	-	-	-
17	CLA	B3	611	X	-	-	-
17	CLA	B3	612	X	-	-	-
17	CLA	B3	613	X	-	-	-
17	CLA	B3	614	X	-	-	-
17	CLA	B3	615	X	-	-	-
17	CLA	B5	601	X	-	-	-
17	CLA	B5	603	X	-	-	-
17	CLA	B5	604	X	-	-	-
17	CLA	B5	608	X	-	-	-
17	CLA	B5	609	X	-	-	-
17	CLA	B5	611	X	-	-	-
17	CLA	B5	612	X	-	-	-
17	CLA	B5	613	X	-	-	-
17	CLA	BA	801	X	-	-	-
17	CLA	BA	802	X	-	-	-
17	CLA	BA	803	X	-	-	-
17	CLA	BA	805	X	-	-	-
17	CLA	BA	806	X	-	-	-
17	CLA	BA	807	X	-	-	-
17	CLA	BA	808	X	-	-	-
17	CLA	BA	810	X	-	-	-
17	CLA	BA	811	X	-	-	-
17	CLA	BA	812	X	-	-	-
17	CLA	BA	813	X	-	-	-
17	CLA	BA	814	X	-	-	-
17	CLA	BA	816	X	-	-	-
17	CLA	BA	819	X	-	-	-
17	CLA	BA	820	X	-	-	-
17	CLA	BA	822	X	-	-	-
17	CLA	BA	823	X	-	-	-
17	CLA	BA	824	X	-	-	-
17	CLA	BA	825	X	-	-	-
17	CLA	BA	827	X	-	-	-
17	CLA	BA	828	X	-	-	-
17	CLA	BA	829	X	-	-	-
17	CLA	BA	830	X	-	-	-
17	CLA	BA	831	X	-	-	-
17	CLA	BA	833	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	BA	835	X	-	-	-
17	CLA	BA	837	X	-	-	-
17	CLA	BA	838	X	-	-	-
17	CLA	BA	840	X	-	-	-
17	CLA	BA	841	X	-	-	-
17	CLA	BA	842	X	-	-	-
17	CLA	BA	844	X	-	-	-
17	CLA	BB	801	X	-	-	-
17	CLA	BB	802	X	-	-	-
17	CLA	BB	804	X	-	-	-
17	CLA	BB	805	X	-	-	-
17	CLA	BB	806	X	-	-	-
17	CLA	BB	807	X	-	-	-
17	CLA	BB	808	X	-	-	-
17	CLA	BB	810	X	-	-	-
17	CLA	BB	811	X	-	-	-
17	CLA	BB	812	X	-	-	-
17	CLA	BB	813	X	-	-	-
17	CLA	BB	814	X	-	-	-
17	CLA	BB	815	X	-	-	-
17	CLA	BB	816	X	-	-	-
17	CLA	BB	817	X	-	-	-
17	CLA	BB	818	X	-	-	-
17	CLA	BB	819	X	-	-	-
17	CLA	BB	820	X	-	-	-
17	CLA	BB	821	X	-	-	-
17	CLA	BB	822	X	-	-	-
17	CLA	BB	823	X	-	-	-
17	CLA	BB	825	X	-	-	-
17	CLA	BB	826	X	-	-	-
17	CLA	BB	828	X	-	-	-
17	CLA	BB	829	X	-	-	-
17	CLA	BB	830	X	-	-	-
17	CLA	BB	831	X	-	-	-
17	CLA	BB	832	X	-	-	-
17	CLA	BB	835	X	-	-	-
17	CLA	BB	837	X	-	-	-
17	CLA	BB	838	X	-	-	-
17	CLA	BB	841	X	-	-	-
17	CLA	BB	842	X	-	-	-
17	CLA	BB	843	X	-	-	-
17	CLA	BF	301	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	BF	302	X	-	-	-
17	CLA	BF	303	X	-	-	-
17	CLA	BG	201	X	-	-	-
17	CLA	BG	202	X	-	-	-
17	CLA	BH	201	X	-	-	-
17	CLA	BJ	102	X	-	-	-
17	CLA	BK	201	X	-	-	-
17	CLA	BK	202	X	-	-	-
17	CLA	BK	203	X	-	-	-
17	CLA	BL	304	X	-	-	-
25	CHL	B1	303	X	-	-	-
25	CHL	B1	308	X	-	-	-
25	CHL	B2	304	X	-	-	-
25	CHL	B2	305	X	-	-	-
25	CHL	B2	306	X	-	-	-
25	CHL	B2	313	X	-	-	-
25	CHL	B3	601	X	-	-	-
25	CHL	B3	607	X	-	-	-
25	CHL	B5	605	X	-	-	-
25	CHL	B5	606	X	-	-	-
25	CHL	B5	607	X	-	-	-

## 2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 35123 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	BA	742	Total	C	N	O	S	0	0
			5841	3828	992	1003	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BB	733	Total	C	N	O	S	0	0
			5854	3842	998	1000	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	BC	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	BD	143	Total	C	N	O	S	0	0
			1127	723	195	205	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	BE	69	Total	C	N	O	0	0
			546	352	97	97		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BF	154	Total	C	N	O	S	0	0
			1220	797	209	211	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	BG	94	Total	C	N	O	0	0
			733	474	121	138		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	BH	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	BI	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	BJ	43	Total	C	N	O	S	0	0
			344	233	52	58	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BK	64	Total	C	N	O	S	0	0
			445	285	73	84	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BL	159	Total	C	N	O	S	0	0
			1184	781	190	211	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	B1	172	Total	C	N	O	S	0	0
			1339	873	221	240	5		

- Molecule 14 is a protein called Photosystem I chlorophyll a/b-binding protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	B2	208	Total	C	N	O	S	0	0
			1607	1051	261	291	4		

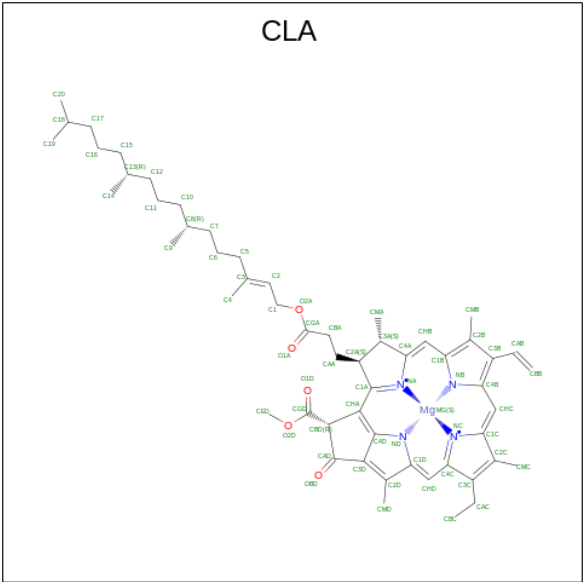
- Molecule 15 is a protein called Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	B3	221	Total	C	N	O	S	0	0
			1696	1111	276	304	5		

- Molecule 16 is a protein called Photosystem I chlorophyll a/b-binding protein 5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	B5	206	Total	C	N	O	S	0	0
			1603	1047	263	287	6		

- 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	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
17	BA	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	BA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	BA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	BA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
17	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	BA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	BA	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	BA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	BA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	BA	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
17	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	BA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	BA	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	BA	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	BA	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
17	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	BA	1	Total 53	C 43	Mg 1	N 4	O 5	0
17	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	BA	1	Total 47	C 37	Mg 1	N 4	O 5	0
17	BA	1	Total 56	C 46	Mg 1	N 4	O 5	0
17	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	BA	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	BA	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	BA	1	Total 51	C 41	Mg 1	N 4	O 5	0
17	BA	1	Total 54	C 45	Mg 1	N 4	O 4	0
17	BA	1	Total 51	C 41	Mg 1	N 4	O 5	0
17	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	BA	1	Total 42	C 33	Mg 1	N 4	O 4	0
17	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
17	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	BB	1	Total 41	C 33	Mg 1	N 4	O 3	0
17	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	BB	1	Total 52	C 42	Mg 1	N 4	O 5	0
17	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	BB	1	Total 54	C 44	Mg 1	N 4	O 5	0
17	BB	1	Total 43	C 35	Mg 1	N 4	O 3	0
17	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	BB	1	Total 64	C 54	Mg 1	N 4	O 5	0
17	BB	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	BB	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	BB	1	Total 59	C 49	Mg 1	N 4	O 5	0
17	BB	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	BB	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	BB	1	Total 41	C 33	Mg 1	N 4	O 3	0
17	BB	1	Total 47	C 37	Mg 1	N 4	O 5	0
17	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
17	BB	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	BB	1	Total 62	C 52	Mg 1	N 4	O 5	0
17	BB	1	Total 62	C 52	Mg 1	N 4	O 5	0
17	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	BB	1	Total 56	C 46	Mg 1	N 4	O 5	0
17	BB	1	Total 43	C 35	Mg 1	N 4	O 3	0
17	BB	1	Total 43	C 35	Mg 1	N 4	O 3	0
17	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	BB	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	BB	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	BB	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	BB	1	Total 47	C 37	Mg 1	N 4	O 5	0
17	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	BF	1	Total 55	C 46	Mg 1	N 4	O 4	0
17	BF	1	Total 42	C 34	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
17	BF	1	Total 41	C 33	Mg 1	N 4	O 3	0
17	BG	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	BG	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	BH	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	BJ	1	Total 42	C 34	Mg 1	N 4	O 3	0
17	BK	1	Total 36	C 30	Mg 1	N 4	O 1	0
17	BK	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	BK	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	BL	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	BL	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	BL	1	Total 43	C 35	Mg 1	N 4	O 3	0
17	B1	1	Total 61	C 51	Mg 1	N 4	O 5	0
17	B1	1	Total 54	C 45	Mg 1	N 4	O 4	0
17	B1	1	Total 41	C 33	Mg 1	N 4	O 3	0
17	B1	1	Total 40	C 32	Mg 1	N 4	O 3	0
17	B1	1	Total 44	C 34	Mg 1	N 4	O 5	0
17	B1	1	Total 39	C 31	Mg 1	N 4	O 3	0
17	B1	1	Total 59	C 49	Mg 1	N 4	O 5	0
17	B1	1	Total 38	C 30	Mg 1	N 4	O 3	0
17	B1	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	B1	1	Total 60	C 50	Mg 1	N 4	O 5	0

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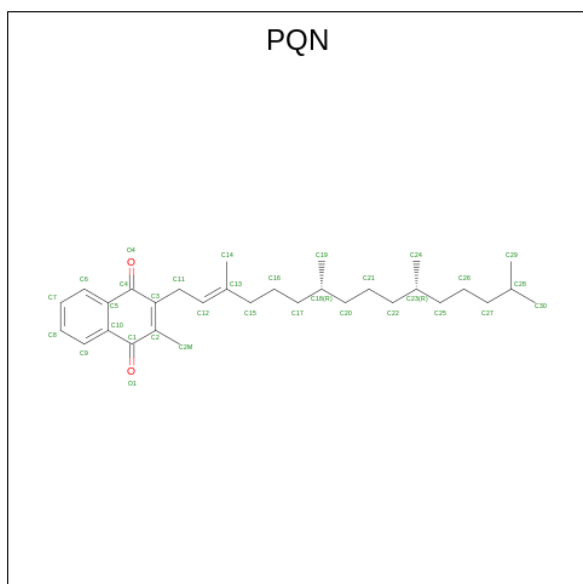
Mol	Chain	Residues	Atoms					AltConf
17	B1	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
17	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
17	B2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
17	B2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	B2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	B2	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
17	B2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
17	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B2	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	B3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	B3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	B3	1	Total	C	Mg	N	O	0
			42	32	1	4	5	
17	B3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	B3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	B3	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	B3	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
17	B3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	

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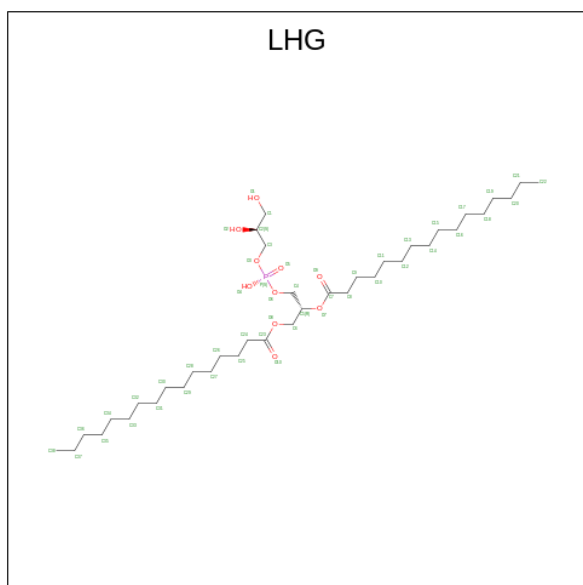
Mol	Chain	Residues	Atoms					AltConf
17	B3	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
17	B3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	B5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	B5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	B5	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
17	B5	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
17	B5	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
17	B5	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
17	B5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B5	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
17	B5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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



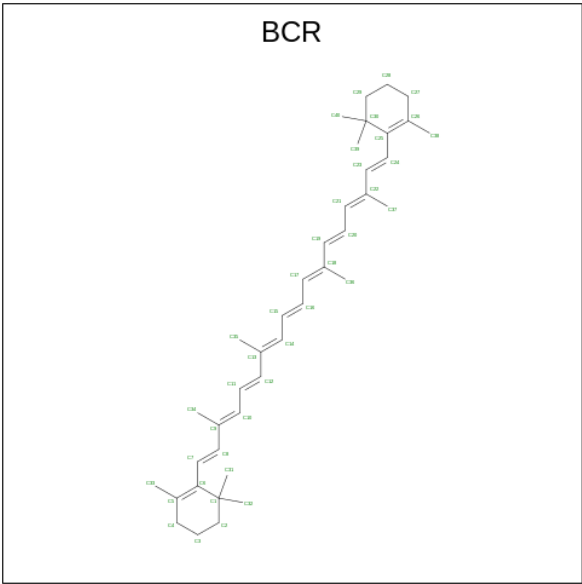
Mol	Chain	Residues	Atoms			AltConf
18	BA	1	Total	C	O	0
			33	31	2	
18	BB	1	Total	C	O	0
			33	31	2	

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



Mol	Chain	Residues	Atoms				AltConf
19	BA	1	Total	C	O	P	0
			49	38	10	1	
19	BA	1	Total	C	O	P	0
			27	16	10	1	
19	BF	1	Total	C	O	P	0
			45	34	10	1	
19	B1	1	Total	C	O	P	0
			38	27	10	1	
19	B1	1	Total	C	O	P	0
			36	25	10	1	
19	B1	1	Total	C	O	P	0
			42	31	10	1	
19	B2	1	Total	C	O	P	0
			35	24	10	1	
19	B3	1	Total	C	O	P	0
			23	12	10	1	
19	B5	1	Total	C	O	P	0
			30	19	10	1	

- Molecule 20 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>) (labeled as "Ligand of Interest" by depositor).



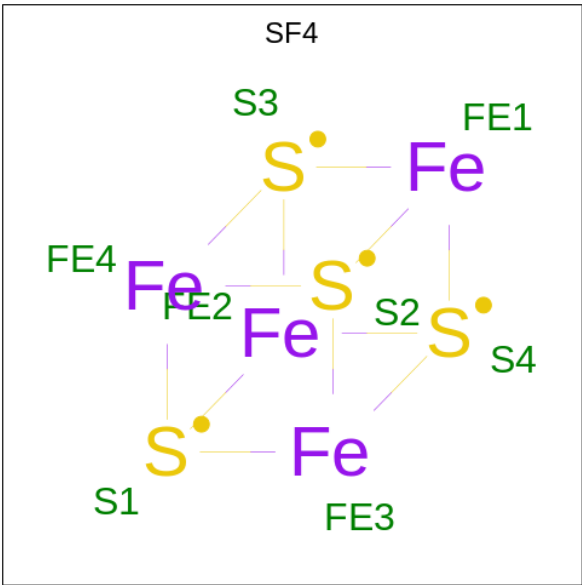
Mol	Chain	Residues	Atoms	AltConf
20	BA	1	Total C 40 40	0
20	BA	1	Total C 40 40	0
20	BA	1	Total C 40 40	0
20	BA	1	Total C 40 40	0
20	BA	1	Total C 40 40	0
20	BA	1	Total C 40 40	0
20	BA	1	Total C 40 40	0
20	BB	1	Total C 40 40	0
20	BB	1	Total C 40 40	0
20	BB	1	Total C 40 40	0
20	BB	1	Total C 40 40	0
20	BB	1	Total C 40 40	0

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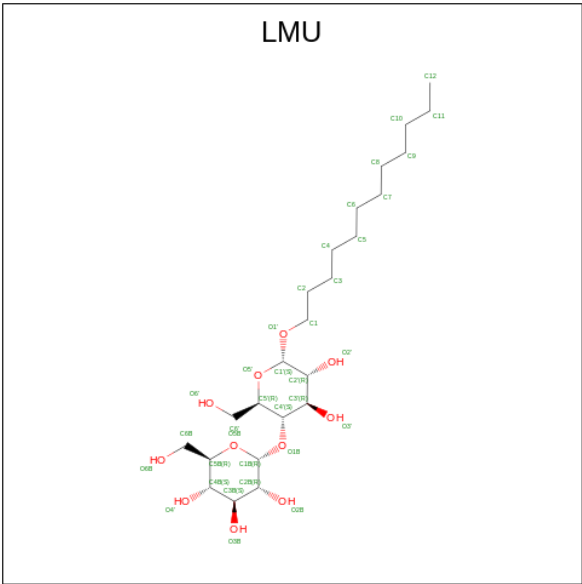
Mol	Chain	Residues	Atoms	AltConf
20	BB	1	Total C 40 40	0
20	BF	1	Total C 40 40	0
20	BG	1	Total C 40 40	0
20	BH	1	Total C 40 40	0
20	BI	1	Total C 40 40	0
20	BJ	1	Total C 40 40	0
20	BJ	1	Total C 40 40	0
20	BK	1	Total C 40 40	0
20	BL	1	Total C 40 40	0
20	BL	1	Total C 40 40	0
20	B2	1	Total C 40 40	0
20	B3	1	Total C 40 40	0
20	B5	1	Total C 40 40	0

- Molecule 21 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
21	BA	1	Total	Fe	S	0
			8	4	4	
21	BC	1	Total	Fe	S	0
			8	4	4	
21	BC	1	Total	Fe	S	0
			8	4	4	

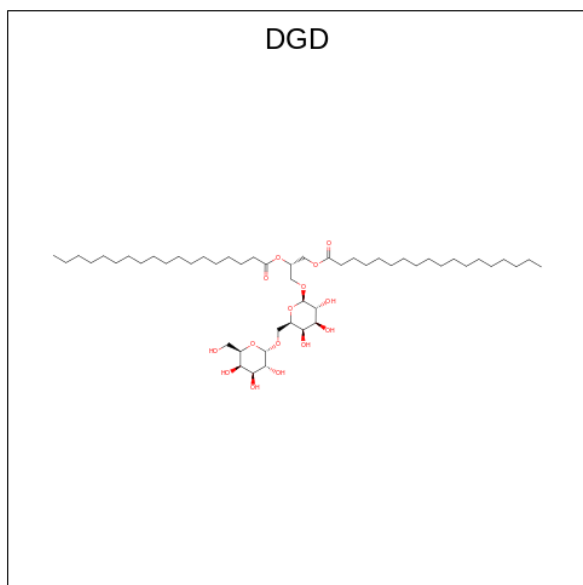
- Molecule 22 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula:  $C_{24}H_{46}O_{11}$ ).





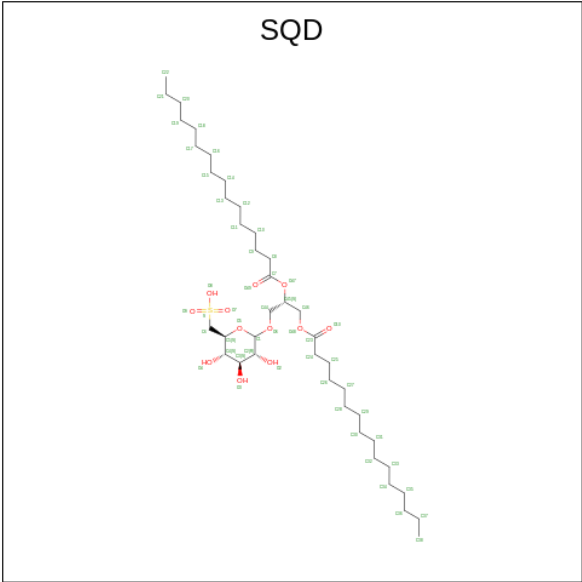
Mol	Chain	Residues	Atoms			AltConf
22	BA	1	Total	C	O	0
			34	23	11	
22	BA	1	Total	C	O	0
			33	22	11	
22	BB	1	Total	C	O	0
			35	24	11	

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



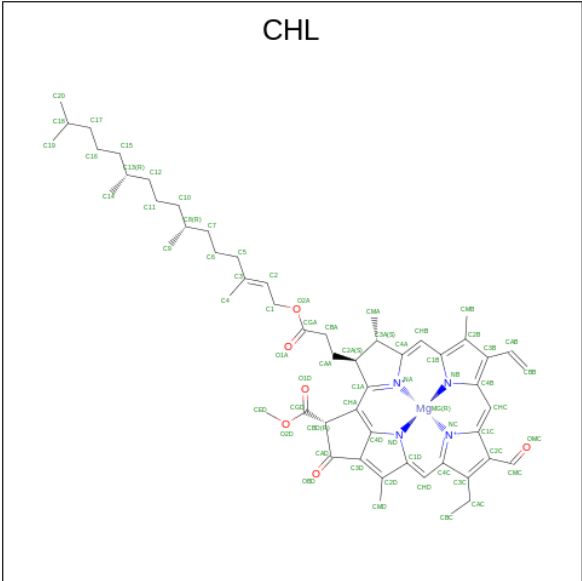
Mol	Chain	Residues	Atoms			AltConf
23	BB	1	Total	C	O	0
			66	51	15	

- Molecule 24 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



Mol	Chain	Residues	Atoms				AltConf
24	BJ	1	Total	C	O	S	0
			47	34	12	1	

- Molecule 25 is CHLOROPHYLL B (three-letter code: CHL) (formula: C<sub>55</sub>H<sub>70</sub>MgN<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



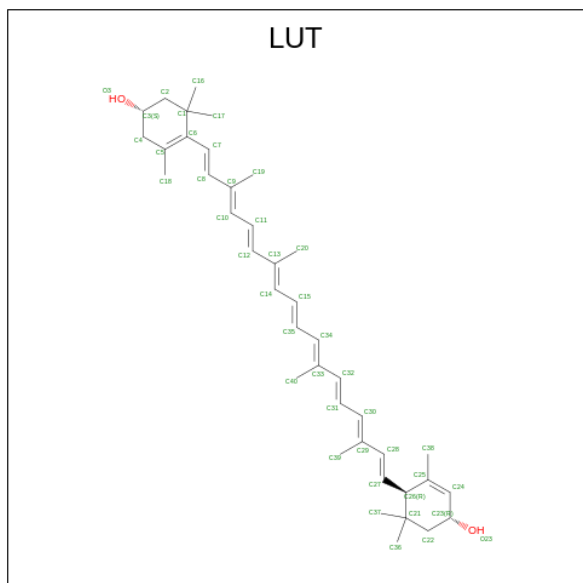
Mol	Chain	Residues	Atoms					AltConf
25	B1	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
25	B1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
25	B2	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
25	B2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
25	B2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	B2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
25	B3	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
25	B3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	B5	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
25	B5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
25	B5	1	Total	C	Mg	N	O	0
			45	34	1	4	6	

- Molecule 26 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



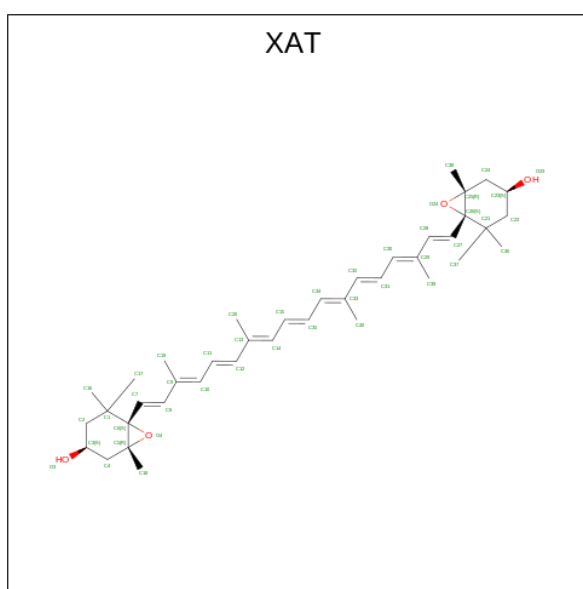
Mol	Chain	Residues	Atoms			AltConf
26	B1	1	Total	C	O	0
			42	40	2	

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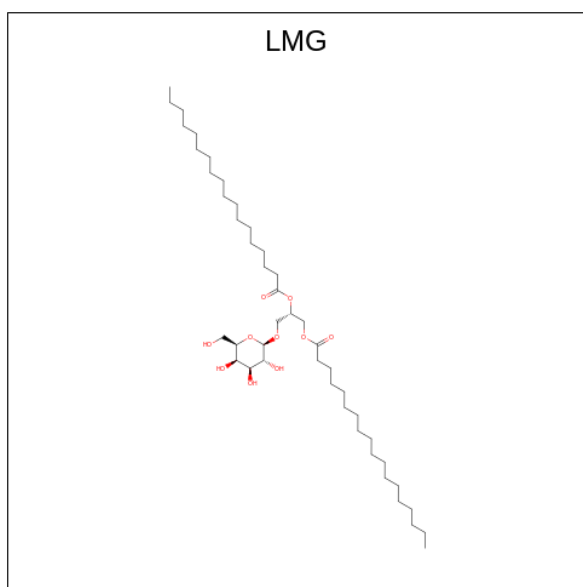
Mol	Chain	Residues	Atoms			AltConf
26	B2	1	Total	C	O	0
			42	40	2	
26	B3	1	Total	C	O	0
			42	40	2	
26	B5	1	Total	C	O	0
			42	40	2	

- 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: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
27	B1	1	Total	C	O	0
			44	40	4	
27	B2	1	Total	C	O	0
			44	40	4	
27	B3	1	Total	C	O	0
			44	40	4	
27	B5	1	Total	C	O	0
			44	40	4	

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).

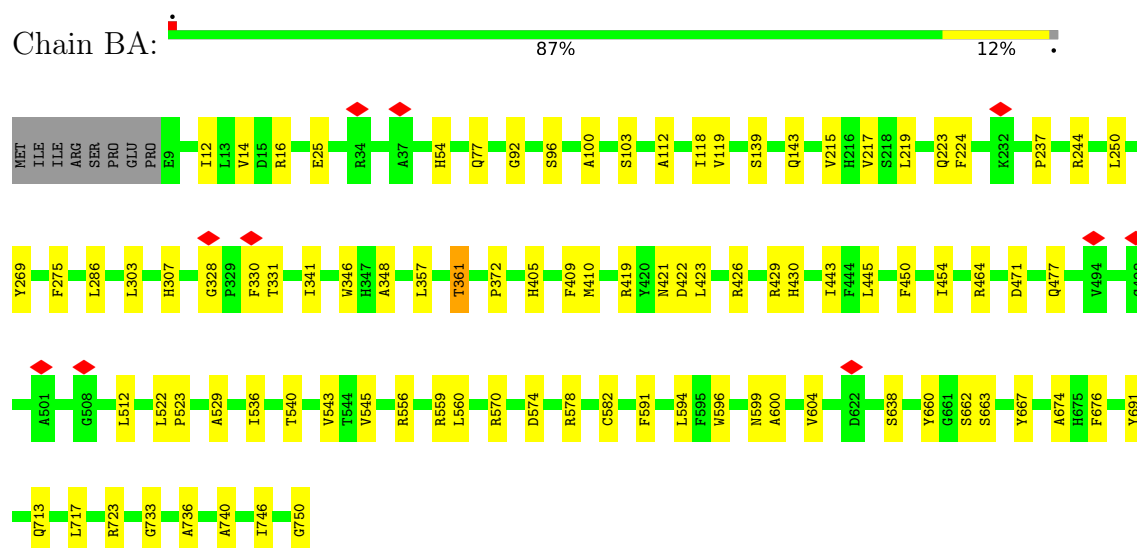


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
28	B5	1	33	23	10	0

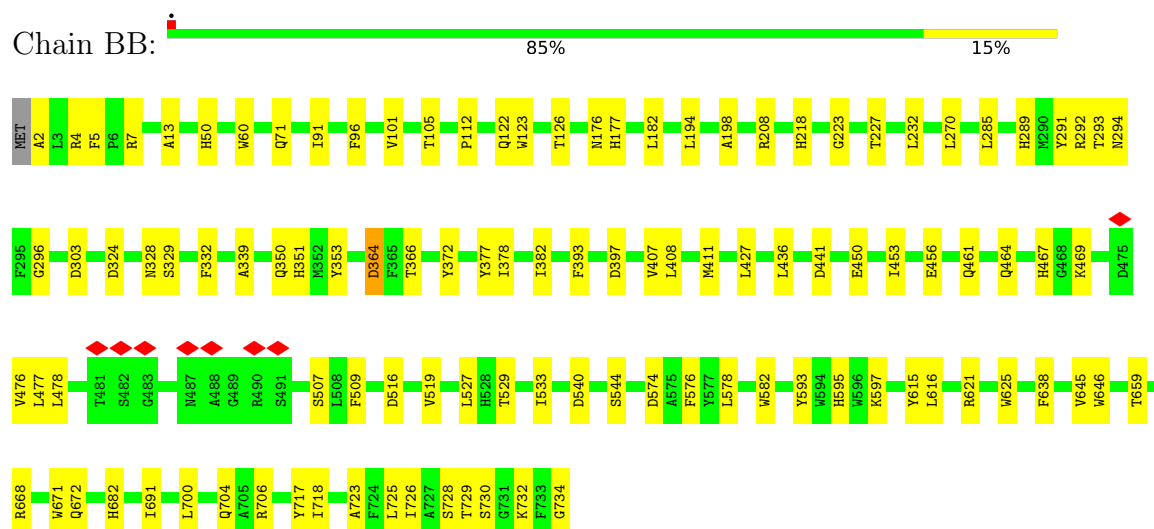
### 3 Residue-property plots

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



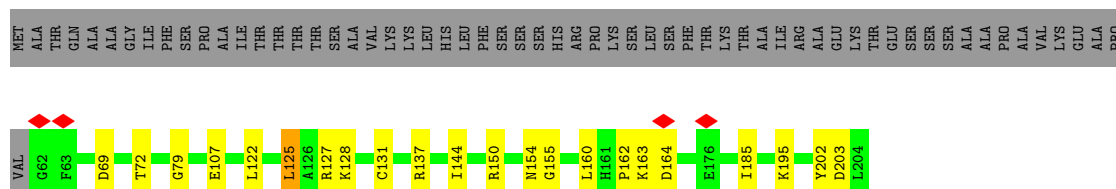
- Molecule 3: Photosystem I iron-sulfur center

Chain BC:  81% 17%



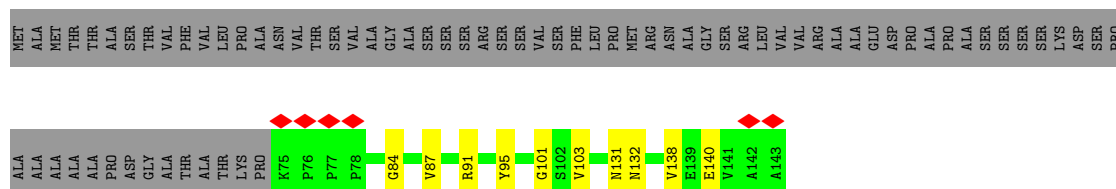
- Molecule 4: Photosystem I reaction center subunit II-2, chloroplastic

Chain BD:  59% 10% 30%



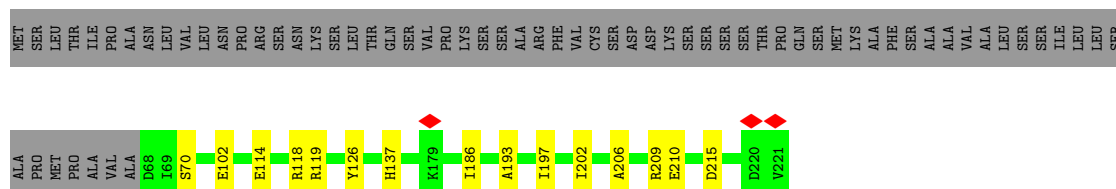
- Molecule 5: Photosystem I reaction center subunit IV A, chloroplastic

Chain BE:  41% 7% 52%



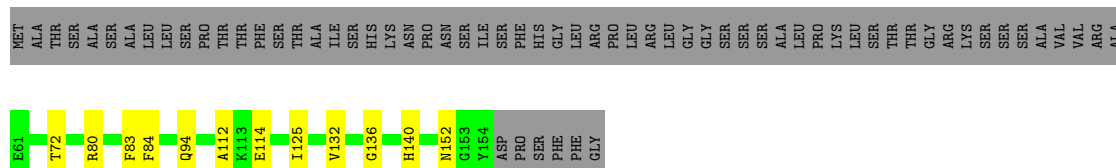
- Molecule 6: Photosystem I reaction center subunit III, chloroplastic

Chain BF:  63% 7% 30%



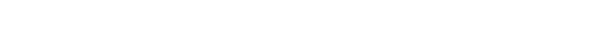
- Molecule 7: Photosystem I reaction center subunit V, chloroplastic

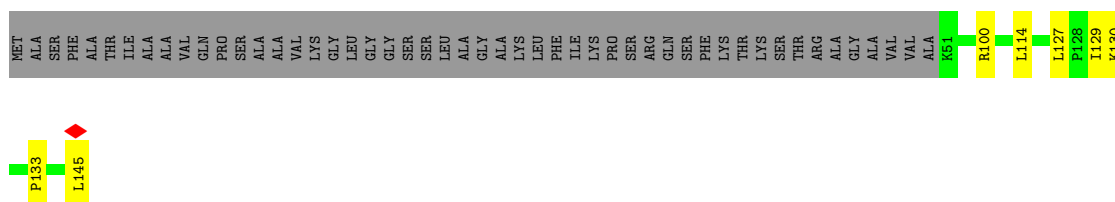
Chain BG:  51% 8% 41%



- Molecule 8: Photosystem I reaction center subunit VI-2, chloroplastic

Chain BH:  61% 5% 34%





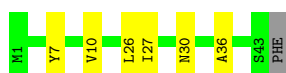
- Molecule 9: Photosystem I reaction center subunit VIII

Chain BI: 84% 5% 11%



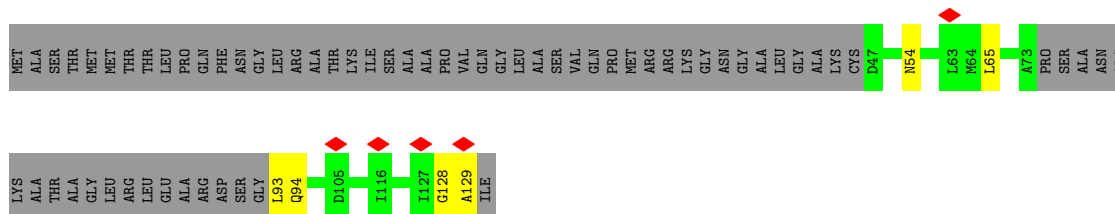
- Molecule 10: Photosystem I reaction center subunit IX

Chain BJ: 84% 14% .



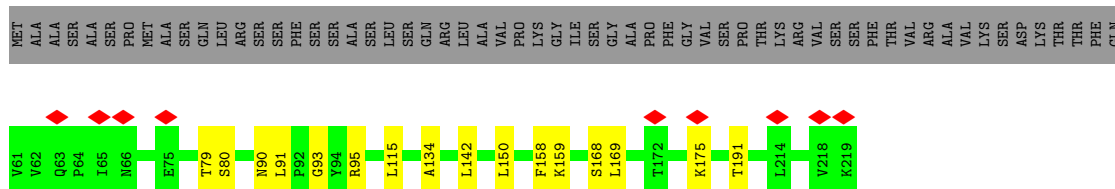
- Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic

Chain BK: 45% 5% 51%



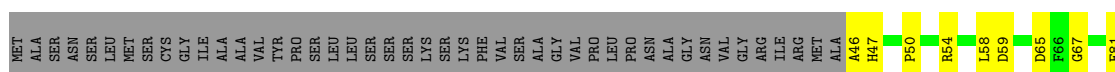
- Molecule 12: Photosystem I reaction center subunit XI, chloroplastic

Chain BL: 65% 7% 27%

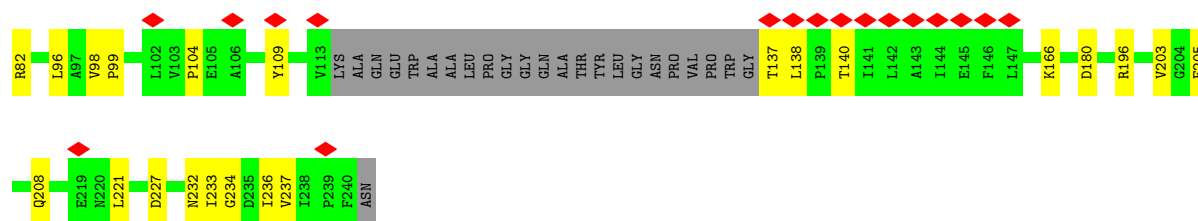


- Molecule 13: Chlorophyll a-b binding protein 6, chloroplastic

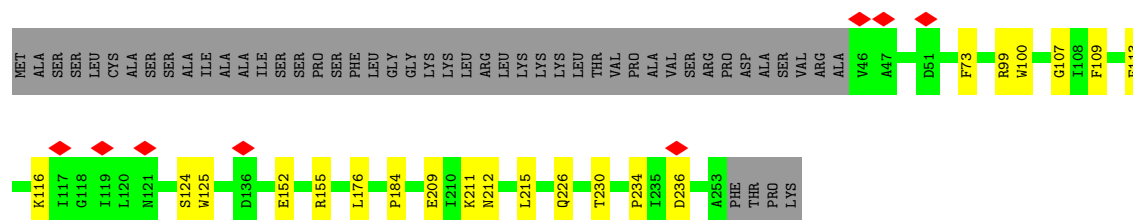
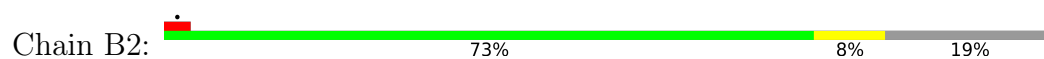
Chain B1: 7% 59% 13% 29%



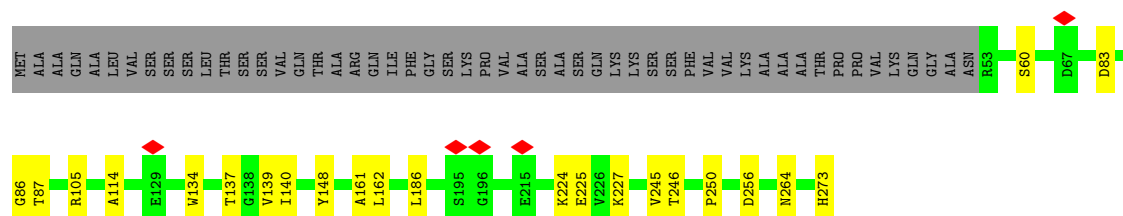
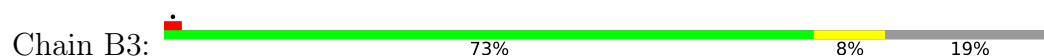




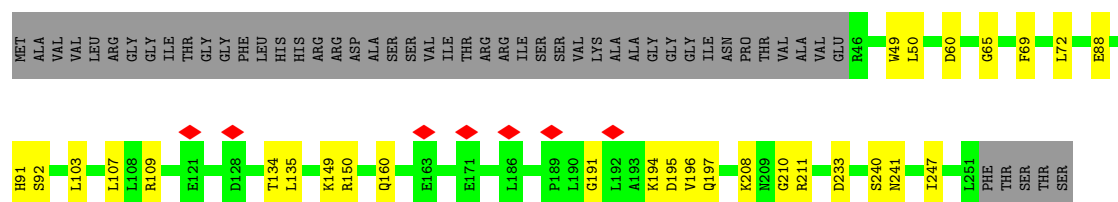
- Molecule 14: Photosystem I chlorophyll a/b-binding protein 2, chloroplastic



- Molecule 15: Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic



- Molecule 16: Photosystem I chlorophyll a/b-binding protein 5, 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	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.354	Depositor
Minimum map value	-0.132	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	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: SQD, SF4, LMU, LHG, CLA, CHL, DGD, LMG, BCR, XAT, LUT, PQN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	BA	0.36	0/6039	0.54	0/8239
2	BB	0.37	0/6065	0.54	1/8281 (0.0%)
3	BC	0.34	0/628	0.56	0/852
4	BD	0.35	0/1156	0.61	0/1563
5	BE	0.30	0/559	0.50	0/760
6	BF	0.31	0/1250	0.55	0/1687
7	BG	0.29	0/750	0.47	0/1016
8	BH	0.29	0/751	0.50	0/1018
9	BI	0.31	0/264	0.49	0/359
10	BJ	0.33	0/354	0.67	0/482
11	BK	0.30	0/449	0.57	0/607
12	BL	0.31	0/1218	0.52	0/1663
13	B1	0.30	0/1381	0.51	0/1879
14	B2	0.29	0/1663	0.53	0/2277
15	B3	0.30	0/1749	0.51	0/2378
16	B5	0.30	0/1650	0.54	0/2244
All	All	0.34	0/25926	0.54	1/35305 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BB	427	LEU	CA-CB-CG	5.01	126.82	115.30

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	BA	5841	0	5690	93	0
2	BB	5854	0	5637	93	0
3	BC	615	0	593	19	0
4	BD	1127	0	1134	13	0
5	BE	546	0	555	13	0
6	BF	1220	0	1252	12	0
7	BG	733	0	718	11	0
8	BH	730	0	720	12	0
9	BI	257	0	274	1	0
10	BJ	344	0	356	5	0
11	BK	445	0	453	5	0
12	BL	1184	0	1179	13	0
13	B1	1339	0	1316	30	0
14	B2	1607	0	1555	14	0
15	B3	1696	0	1663	18	0
16	B5	1603	0	1585	19	0
17	B1	519	0	402	3	0
17	B2	442	0	366	5	0
17	B3	578	0	422	1	0
17	B5	476	0	368	6	0
17	BA	2446	0	2387	46	0
17	BB	2423	0	2407	57	0
17	BF	138	0	110	3	0
17	BG	87	0	64	3	0
17	BH	60	0	59	0	0
17	BJ	42	0	31	0	0
17	BK	127	0	88	1	0
17	BL	148	0	125	1	0
18	BA	33	0	46	3	0
18	BB	33	0	46	3	0
19	B1	116	0	145	0	0
19	B2	35	0	40	1	0
19	B3	23	0	16	1	0
19	B5	30	0	30	0	0
19	BA	76	0	98	2	0
19	BF	45	0	63	1	0
20	B2	40	0	56	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	B3	40	0	56	5	0
20	B5	40	0	56	0	0
20	BA	280	0	392	15	0
20	BB	240	0	336	14	0
20	BF	40	0	56	1	0
20	BG	40	0	56	3	0
20	BH	40	0	55	1	0
20	BI	40	0	56	1	0
20	BJ	80	0	112	4	0
20	BK	40	0	56	2	0
20	BL	80	0	112	4	0
21	BA	8	0	0	1	0
21	BC	16	0	0	0	0
22	BA	67	0	80	0	0
22	BB	35	0	46	0	0
23	BB	66	0	96	1	0
24	BJ	47	0	61	3	0
25	B1	91	0	58	1	0
25	B2	174	0	113	4	0
25	B3	98	0	71	5	0
25	B5	126	0	67	1	0
26	B1	42	0	56	2	0
26	B2	42	0	56	1	0
26	B3	42	0	56	2	0
26	B5	42	0	56	1	0
27	B1	44	0	56	7	0
27	B2	44	0	56	3	0
27	B3	44	0	56	1	0
27	B5	44	0	56	1	0
28	B5	33	0	36	0	0
All	All	35123	0	34468	422	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 6.

The worst 5 of 422 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)
13:B1:203:VAL:HG21	27:B1:317:XAT:C40	1.73	1.19
8:BH:127:LEU:HD13	8:BH:129:ILE:HG22	1.28	1.13
13:B1:203:VAL:CG2	27:B1:317:XAT:C40	2.27	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BL:169:LEU:HD21	12:BL:175:LYS:HD2	1.32	1.09
13:B1:58:LEU:HD11	13:B1:67:GLY:HA2	1.16	1.07

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	BA	740/750 (99%)	692 (94%)	48 (6%)	0	100	100
2	BB	731/734 (100%)	695 (95%)	36 (5%)	0	100	100
3	BC	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
4	BD	141/204 (69%)	121 (86%)	18 (13%)	2 (1%)	9	34
5	BE	67/143 (47%)	61 (91%)	6 (9%)	0	100	100
6	BF	152/221 (69%)	149 (98%)	3 (2%)	0	100	100
7	BG	92/160 (58%)	85 (92%)	7 (8%)	0	100	100
8	BH	93/145 (64%)	86 (92%)	7 (8%)	0	100	100
9	BI	31/37 (84%)	30 (97%)	1 (3%)	0	100	100
10	BJ	41/44 (93%)	38 (93%)	3 (7%)	0	100	100
11	BK	60/130 (46%)	54 (90%)	6 (10%)	0	100	100
12	BL	157/219 (72%)	149 (95%)	8 (5%)	0	100	100
13	B1	168/241 (70%)	160 (95%)	8 (5%)	0	100	100
14	B2	206/257 (80%)	191 (93%)	15 (7%)	0	100	100
15	B3	219/273 (80%)	206 (94%)	13 (6%)	0	100	100
16	B5	204/256 (80%)	188 (92%)	15 (7%)	1 (0%)	25	56
All	All	3180/3895 (82%)	2978 (94%)	199 (6%)	3 (0%)	50	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	BD	164	ASP
16	B5	49	TRP
4	BD	162	PRO

### 5.3.2 Protein sidechains [i](#)

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	BA	601/610 (98%)	595 (99%)	6 (1%)	73	82
2	BB	597/600 (100%)	588 (98%)	9 (2%)	60	75
3	BC	70/71 (99%)	70 (100%)	0	100	100
4	BD	121/170 (71%)	117 (97%)	4 (3%)	33	58
5	BE	58/114 (51%)	58 (100%)	0	100	100
6	BF	126/185 (68%)	126 (100%)	0	100	100
7	BG	79/133 (59%)	77 (98%)	2 (2%)	42	65
8	BH	77/113 (68%)	77 (100%)	0	100	100
9	BI	29/33 (88%)	29 (100%)	0	100	100
10	BJ	38/39 (97%)	38 (100%)	0	100	100
11	BK	46/95 (48%)	45 (98%)	1 (2%)	47	68
12	BL	120/174 (69%)	118 (98%)	2 (2%)	56	73
13	B1	138/190 (73%)	134 (97%)	4 (3%)	37	61
14	B2	165/205 (80%)	165 (100%)	0	100	100
15	B3	170/211 (81%)	170 (100%)	0	100	100
16	B5	167/205 (82%)	164 (98%)	3 (2%)	54	72
All	All	2602/3148 (83%)	2571 (99%)	31 (1%)	66	79

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

Mol	Chain	Res	Type
2	BB	638	PHE

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Mol	Chain	Res	Type
13	B1	180	ASP
4	BD	202	TYR
16	B5	91	HIS
13	B1	47	HIS

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

Mol	Chain	Res	Type
13	B1	208	GLN
15	B3	242	GLN
16	B5	241	ASN
15	B3	253	ASN
4	BD	200	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

205 ligands are modelled in this entry.

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



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	CLA	BA	832	-	56,64,73	1.59	8 (14%)	65,102,113	1.31	8 (12%)
17	CLA	B1	310	13	38,47,73	1.99	7 (18%)	47,82,113	1.54	10 (21%)
19	LHG	B2	317	17	34,34,48	1.04	2 (5%)	37,40,54	0.96	2 (5%)
17	CLA	B5	610	19	42,50,73	1.86	7 (16%)	48,85,113	1.47	7 (14%)
17	CLA	B1	313	13	45,53,73	1.78	7 (15%)	52,89,113	1.51	6 (11%)
17	CLA	BB	837	-	42,50,73	1.86	5 (11%)	48,85,113	1.45	7 (14%)
17	CLA	B3	602	15	60,68,73	1.58	9 (15%)	70,107,113	1.22	8 (11%)
17	CLA	BB	813	-	54,62,73	1.66	8 (14%)	67,100,113	1.50	11 (16%)
17	CLA	BB	831	-	56,64,73	1.63	9 (16%)	65,102,113	1.38	6 (9%)
25	CHL	B2	306	-	46,54,74	2.33	17 (36%)	49,90,114	2.82	20 (40%)
17	CLA	BB	820	-	60,68,73	1.51	7 (11%)	70,107,113	1.62	11 (15%)
17	CLA	BF	301	-	55,63,73	1.58	7 (12%)	62,100,113	1.37	7 (11%)
17	CLA	BB	842	-	65,73,73	1.50	9 (13%)	76,113,113	1.30	7 (9%)
17	CLA	BB	814	-	43,51,73	1.78	6 (13%)	49,86,113	1.48	8 (16%)
21	SF4	BA	852	2,1	0,12,12	-	-	-	-	-
17	CLA	BF	303	-	41,49,73	1.86	6 (14%)	47,84,113	1.47	8 (17%)
17	CLA	BJ	102	10	42,50,73	1.84	5 (11%)	48,85,113	1.48	7 (14%)
17	CLA	B3	606	-	41,49,73	1.89	7 (17%)	51,84,113	1.73	11 (21%)
17	CLA	BA	805	-	65,73,73	1.48	8 (12%)	76,113,113	1.36	9 (11%)
17	CLA	BB	823	-	47,55,73	1.72	6 (12%)	54,91,113	1.32	8 (14%)
17	CLA	BA	838	-	55,62,73	1.69	8 (14%)	59,99,113	1.45	11 (18%)
17	CLA	BB	815	-	65,73,73	1.47	9 (13%)	76,113,113	1.49	11 (14%)
17	CLA	BB	830	-	65,73,73	1.50	9 (13%)	76,113,113	1.26	8 (10%)
17	CLA	B1	311	13	59,67,73	1.59	6 (10%)	69,106,113	1.22	8 (11%)
17	CLA	B3	603	15	55,63,73	1.61	7 (12%)	64,101,113	1.34	8 (12%)
17	CLA	BA	817	-	60,68,73	1.52	6 (10%)	70,107,113	1.37	11 (15%)
26	LUT	B5	614	-	42,43,43	0.83	1 (2%)	51,60,60	1.85	15 (29%)
25	CHL	B2	304	-	42,50,74	2.37	16 (38%)	45,85,114	2.84	18 (40%)
20	BCR	BK	204	-	41,41,41	0.88	1 (2%)	56,56,56	2.14	21 (37%)
17	CLA	BB	822	-	41,49,73	1.83	8 (19%)	47,84,113	1.56	7 (14%)
17	CLA	BA	831	-	47,55,73	1.79	8 (17%)	54,91,113	1.49	10 (18%)
17	CLA	B1	306	-	41,49,73	1.86	5 (12%)	47,84,113	1.45	7 (14%)
17	CLA	B2	307	14	45,53,73	1.80	7 (15%)	52,89,113	1.39	8 (15%)
17	CLA	BB	826	-	65,73,73	1.51	10 (15%)	76,113,113	1.30	7 (9%)
17	CLA	BB	828	-	62,70,73	1.51	7 (11%)	72,109,113	1.48	11 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	CLA	BB	838	-	50,58,73	1.67	7 (14%)	58,95,113	1.50	9 (15%)
26	LUT	B2	314	-	42,43,43	0.81	0	51,60,60	1.98	15 (29%)
17	CLA	B3	609	15	41,49,73	1.85	8 (19%)	47,84,113	1.45	7 (14%)
20	BCR	BL	305	-	41,41,41	0.78	0	56,56,56	2.22	20 (35%)
18	PQN	BA	843	-	34,34,34	3.47	12 (35%)	42,45,45	1.62	5 (11%)
17	CLA	BB	843	19	65,73,73	1.52	9 (13%)	76,113,113	1.27	7 (9%)
24	SQD	BJ	104	-	46,47,54	1.28	5 (10%)	55,58,65	4.16	12 (21%)
17	CLA	BA	842	-	65,73,73	1.50	7 (10%)	76,113,113	1.31	7 (9%)
20	BCR	BA	855	-	41,41,41	0.77	0	56,56,56	2.19	24 (42%)
21	SF4	BC	101	3	0,12,12	-	-	-	-	-
17	CLA	BA	808	1	65,73,73	1.49	8 (12%)	76,113,113	1.23	8 (10%)
17	CLA	BA	815	-	42,50,73	1.79	8 (19%)	48,85,113	1.51	6 (12%)
17	CLA	BK	202	-	45,53,73	1.81	6 (13%)	52,89,113	1.47	7 (13%)
17	CLA	BA	822	-	42,50,73	1.83	6 (14%)	48,85,113	1.56	7 (14%)
17	CLA	B2	310	14	44,52,73	1.85	7 (15%)	51,88,113	1.42	7 (13%)
27	XAT	B1	317	-	39,47,47	0.93	2 (5%)	54,74,74	2.43	18 (33%)
17	CLA	B3	612	-	53,62,73	1.69	7 (13%)	61,100,113	1.25	6 (9%)
20	BCR	BB	845	-	41,41,41	0.93	1 (2%)	56,56,56	2.19	18 (32%)
17	CLA	BA	828	-	65,73,73	1.45	7 (10%)	76,113,113	1.45	11 (14%)
17	CLA	BB	807	-	65,73,73	1.49	7 (10%)	76,113,113	1.33	10 (13%)
19	LHG	BF	305	-	44,44,48	0.97	2 (4%)	47,50,54	1.09	3 (6%)
20	BCR	BB	846	-	41,41,41	0.85	1 (2%)	56,56,56	2.14	19 (33%)
17	CLA	BB	808	2	65,73,73	1.47	9 (13%)	76,113,113	1.33	7 (9%)
17	CLA	BB	817	-	41,50,73	1.80	7 (17%)	46,85,113	1.48	7 (15%)
17	CLA	B2	303	-	43,51,73	1.84	6 (13%)	48,86,113	1.43	7 (14%)
19	LHG	B1	318	17	41,41,48	1.01	2 (4%)	44,47,54	0.95	2 (4%)
21	SF4	BC	102	3	0,12,12	-	-	-	-	-
26	LUT	B3	616	-	42,43,43	0.97	1 (2%)	51,60,60	2.10	17 (33%)
17	CLA	BA	827	-	65,73,73	1.47	6 (9%)	76,113,113	1.23	7 (9%)
17	CLA	BG	201	-	42,50,73	1.85	7 (16%)	48,85,113	1.28	7 (14%)
25	CHL	B1	303	13	49,58,74	2.23	17 (34%)	52,95,114	2.63	22 (42%)
17	CLA	B5	608	16	44,52,73	1.86	9 (20%)	51,88,113	1.44	7 (13%)
17	CLA	BA	814	-	45,53,73	1.81	9 (20%)	52,89,113	1.51	8 (15%)
17	CLA	B3	613	-	39,48,73	1.93	6 (15%)	44,83,113	1.40	7 (15%)
17	CLA	BB	829	-	65,73,73	1.46	9 (13%)	76,113,113	1.32	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	CLA	BB	819	-	59,67,73	1.57	9 (15%)	68,105,113	1.40	9 (13%)
17	CLA	BL	304	-	43,51,73	1.78	6 (13%)	49,86,113	1.47	7 (14%)
25	CHL	B3	607	-	45,53,74	2.28	16 (35%)	52,89,114	2.69	20 (38%)
17	CLA	BA	836	1	45,53,73	1.81	6 (13%)	52,89,113	1.53	8 (15%)
27	XAT	B3	617	-	39,47,47	0.97	1 (2%)	54,74,74	2.48	21 (38%)
17	CLA	B3	610	19	39,48,73	1.93	5 (12%)	44,83,113	1.40	7 (15%)
19	LHG	BA	845	-	48,48,48	0.88	2 (4%)	51,54,54	0.97	3 (5%)
17	CLA	B5	601	16	46,54,73	1.75	8 (17%)	53,90,113	1.37	7 (13%)
17	CLA	BB	804	-	65,73,73	1.49	9 (13%)	76,113,113	1.27	8 (10%)
17	CLA	B5	612	16	57,65,73	1.62	8 (14%)	66,103,113	1.28	7 (10%)
25	CHL	B1	308	-	40,49,74	2.55	18 (45%)	41,84,114	2.79	17 (41%)
20	BCR	BA	851	-	41,41,41	0.87	1 (2%)	56,56,56	1.99	20 (35%)
17	CLA	BA	807	-	50,58,73	1.70	7 (14%)	58,95,113	1.34	7 (12%)
17	CLA	BA	813	-	65,73,73	1.46	7 (10%)	76,113,113	1.33	8 (10%)
17	CLA	B3	614	-	37,44,73	1.95	9 (24%)	42,77,113	1.35	7 (16%)
17	CLA	BA	809	1	50,58,73	1.73	8 (16%)	58,95,113	1.44	10 (17%)
20	BCR	B2	316	-	41,41,41	0.89	1 (2%)	56,56,56	2.47	23 (41%)
20	BCR	BF	304	-	41,41,41	0.87	1 (2%)	56,56,56	1.94	19 (33%)
17	CLA	BL	302	12	45,53,73	1.85	8 (17%)	52,89,113	1.60	11 (21%)
17	CLA	B5	611	16	40,49,73	1.87	8 (20%)	45,84,113	1.47	7 (15%)
19	LHG	B3	619	17	22,22,48	1.49	2 (9%)	25,28,54	1.38	2 (8%)
17	CLA	B2	301	14	65,73,73	1.51	9 (13%)	76,113,113	1.26	10 (13%)
25	CHL	B2	313	14	43,51,74	2.35	15 (34%)	45,86,114	2.87	19 (42%)
17	CLA	BA	834	-	65,73,73	1.49	9 (13%)	76,113,113	1.47	10 (13%)
17	CLA	BA	829	-	65,73,73	1.49	9 (13%)	76,113,113	1.31	9 (11%)
20	BCR	BA	847	-	41,41,41	0.99	1 (2%)	56,56,56	1.63	11 (19%)
19	LHG	B1	302	-	35,35,48	1.09	2 (5%)	38,41,54	0.99	2 (5%)
20	BCR	BI	101	-	41,41,41	0.92	2 (4%)	56,56,56	2.15	21 (37%)
17	CLA	BA	825	-	65,73,73	1.47	7 (10%)	76,113,113	1.31	6 (7%)
17	CLA	B5	613	-	45,53,73	1.80	7 (15%)	52,89,113	1.37	7 (13%)
25	CHL	B2	305	-	43,51,74	2.40	16 (37%)	45,86,114	2.78	17 (37%)
20	BCR	B5	616	-	41,41,41	0.79	0	56,56,56	2.31	23 (41%)
27	XAT	B2	315	-	39,47,47	1.01	1 (2%)	54,74,74	2.30	20 (37%)
20	BCR	BH	202	-	41,41,41	0.88	1 (2%)	56,56,56	11.27	26 (46%)
17	CLA	BA	837	-	51,59,73	1.63	8 (15%)	59,96,113	1.47	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	CLA	B5	604	-	43,51,73	1.91	7 (16%)	54,87,113	1.53	10 (18%)
20	BCR	BA	850	-	41,41,41	0.78	0	56,56,56	2.09	11 (19%)
17	CLA	BB	827	-	62,70,73	1.52	8 (12%)	72,109,113	1.27	8 (11%)
17	CLA	BA	835	-	45,53,73	1.81	7 (15%)	52,89,113	1.43	6 (11%)
17	CLA	BB	811	2	65,73,73	1.48	10 (15%)	76,113,113	1.37	9 (11%)
17	CLA	BA	824	-	55,63,73	1.63	9 (16%)	64,101,113	1.39	8 (12%)
17	CLA	B1	309	-	43,52,73	1.85	7 (16%)	49,88,113	1.44	7 (14%)
17	CLA	B3	611	15	43,51,73	1.82	5 (11%)	49,86,113	1.44	8 (16%)
17	CLA	BB	818	-	55,63,73	1.61	8 (14%)	64,101,113	1.33	8 (12%)
17	CLA	BB	821	-	55,63,73	1.64	8 (14%)	64,101,113	1.14	5 (7%)
17	CLA	B1	305	-	54,62,73	1.64	8 (14%)	62,99,113	1.53	10 (16%)
17	CLA	B3	615	-	39,48,73	1.87	6 (15%)	44,83,113	1.46	7 (15%)
25	CHL	B5	605	-	40,49,74	2.42	17 (42%)	42,84,114	2.80	18 (42%)
17	CLA	BA	826	-	53,61,73	1.62	7 (13%)	61,98,113	1.40	10 (16%)
17	CLA	BA	819	-	65,73,73	1.48	9 (13%)	76,113,113	1.34	9 (11%)
17	CLA	B5	602	16	60,68,73	1.62	9 (15%)	70,107,113	1.29	6 (8%)
27	XAT	B5	615	-	39,47,47	0.99	2 (5%)	54,74,74	2.41	18 (33%)
17	CLA	BB	825	-	45,53,73	1.79	8 (17%)	52,89,113	1.37	6 (11%)
17	CLA	BA	802	-	65,73,73	1.54	9 (13%)	76,113,113	1.38	6 (7%)
17	CLA	BA	811	-	65,73,73	1.50	8 (12%)	76,113,113	1.28	8 (10%)
17	CLA	BB	834	-	65,73,73	1.51	10 (15%)	76,113,113	1.31	8 (10%)
20	BCR	BJ	103	-	41,41,41	0.75	0	56,56,56	2.37	21 (37%)
17	CLA	BA	804	-	52,60,73	1.66	7 (13%)	60,97,113	1.56	11 (18%)
17	CLA	BA	801	-	65,73,73	1.50	7 (10%)	76,113,113	1.20	6 (7%)
28	LMG	B5	617	-	33,33,55	1.18	2 (6%)	41,41,63	1.20	4 (9%)
20	BCR	BB	847	-	41,41,41	0.87	1 (2%)	56,56,56	1.93	11 (19%)
17	CLA	BA	840	-	65,73,73	1.44	8 (12%)	76,113,113	1.33	8 (10%)
17	CLA	BA	818	-	56,64,73	1.64	8 (14%)	65,102,113	1.32	8 (12%)
17	CLA	BB	810	-	65,73,73	1.50	8 (12%)	76,113,113	1.33	12 (15%)
17	CLA	BB	833	-	43,51,73	1.80	7 (16%)	49,86,113	1.65	8 (16%)
17	CLA	BF	302	-	42,50,73	1.85	8 (19%)	48,85,113	1.57	8 (16%)
17	CLA	B2	311	14	65,73,73	1.52	7 (10%)	76,113,113	1.29	8 (10%)
23	DGD	BB	850	-	67,67,67	0.81	2 (2%)	81,81,81	0.98	4 (4%)
17	CLA	BB	839	-	65,73,73	1.49	8 (12%)	76,113,113	1.28	6 (7%)
17	CLA	BK	201	11	37,44,73	2.00	7 (18%)	46,77,113	1.73	9 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	CLA	BB	802	-	65,73,73	1.55	9 (13%)	76,113,113	1.42	8 (10%)
18	PQN	BB	844	-	34,34,34	3.42	10 (29%)	42,45,45	1.66	8 (19%)
22	LMU	BB	851	-	36,36,36	1.10	2 (5%)	47,47,47	0.89	0
20	BCR	BA	856	-	41,41,41	0.93	1 (2%)	56,56,56	2.15	17 (30%)
17	CLA	BB	801	-	65,73,73	1.47	9 (13%)	76,113,113	1.47	13 (17%)
17	CLA	BB	809	-	52,60,73	1.69	8 (15%)	60,97,113	1.33	7 (11%)
20	BCR	BA	848	-	41,41,41	0.80	0	56,56,56	2.03	17 (30%)
17	CLA	B3	608	15	45,53,73	1.79	6 (13%)	52,89,113	1.50	8 (15%)
20	BCR	BL	301	-	41,41,41	0.87	1 (2%)	56,56,56	2.36	14 (25%)
19	LHG	B5	618	17	29,29,48	1.17	2 (6%)	32,35,54	1.20	3 (9%)
17	CLA	BB	816	-	64,72,73	1.51	9 (14%)	75,112,113	1.35	8 (10%)
17	CLA	BA	841	-	65,73,73	1.47	8 (12%)	76,113,113	1.55	11 (14%)
17	CLA	BA	833	-	65,73,73	1.51	7 (10%)	76,113,113	1.30	8 (10%)
17	CLA	BA	810	-	65,73,73	1.50	9 (13%)	76,113,113	1.22	7 (9%)
17	CLA	BB	805	-	65,73,73	1.43	10 (15%)	76,113,113	1.56	12 (15%)
17	CLA	B2	308	14	55,63,73	1.66	8 (14%)	64,101,113	1.34	10 (15%)
20	BCR	BA	849	-	41,41,41	0.84	0	56,56,56	2.01	18 (32%)
17	CLA	BH	201	-	60,68,73	1.60	7 (11%)	70,107,113	1.29	8 (11%)
17	CLA	BA	803	-	65,73,73	1.41	7 (10%)	76,113,113	1.37	10 (13%)
22	LMU	BA	854	-	34,34,36	1.18	2 (5%)	45,45,47	0.91	2 (4%)
17	CLA	B1	314	-	60,68,73	1.60	7 (11%)	70,107,113	1.24	10 (14%)
26	LUT	B1	316	-	42,43,43	1.60	8 (19%)	51,60,60	1.51	10 (19%)
17	CLA	BA	820	-	45,53,73	1.73	7 (15%)	52,89,113	1.50	6 (11%)
17	CLA	BB	824	-	65,73,73	1.48	8 (12%)	76,113,113	1.34	10 (13%)
17	CLA	BG	202	7	45,53,73	1.81	6 (13%)	52,89,113	1.56	7 (13%)
20	BCR	BG	203	-	41,41,41	0.91	2 (4%)	56,56,56	6.99	26 (46%)
17	CLA	B5	609	16	54,62,73	1.67	9 (16%)	62,99,113	1.26	8 (12%)
20	BCR	BB	803	-	41,41,41	0.85	0	56,56,56	1.99	19 (33%)
17	CLA	BA	816	-	45,53,73	1.81	7 (15%)	52,89,113	1.45	8 (15%)
17	CLA	BA	823	-	41,49,73	1.86	6 (14%)	47,84,113	1.49	9 (19%)
17	CLA	BB	841	-	65,73,73	1.48	9 (13%)	76,113,113	1.30	7 (9%)
17	CLA	BA	839	-	51,59,73	1.69	8 (15%)	59,96,113	1.41	8 (13%)
17	CLA	BL	303	-	60,68,73	1.58	8 (13%)	70,107,113	1.37	10 (14%)
20	BCR	BJ	101	-	41,41,41	0.89	0	56,56,56	1.70	14 (25%)
17	CLA	BB	806	-	41,49,73	1.80	7 (17%)	47,84,113	1.58	9 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	BCR	BB	849	-	41,41,41	0.90	1 (2%)	56,56,56	1.86	16 (28%)
17	CLA	B1	307	-	39,48,73	1.94	5 (12%)	45,82,113	1.55	7 (15%)
19	LHG	BA	846	17	26,26,48	1.06	2 (7%)	29,32,54	1.00	1 (3%)
17	CLA	B3	605	-	40,49,73	1.91	7 (17%)	45,84,113	1.44	7 (15%)
25	CHL	B5	606	-	40,48,74	2.31	13 (32%)	50,83,114	2.83	21 (42%)
25	CHL	B3	601	14	53,61,74	2.21	16 (30%)	57,98,114	2.76	25 (43%)
17	CLA	BB	840	-	47,55,73	1.71	7 (14%)	54,91,113	1.43	8 (14%)
17	CLA	BA	821	-	65,73,73	1.50	9 (13%)	76,113,113	1.39	10 (13%)
17	CLA	B1	315	-	37,46,73	2.00	7 (18%)	46,81,113	1.61	9 (19%)
20	BCR	B3	618	-	41,41,41	0.84	0	56,56,56	3.61	28 (50%)
17	CLA	BK	203	-	46,54,73	1.73	6 (13%)	53,90,113	1.54	6 (11%)
17	CLA	BB	832	-	43,51,73	1.83	8 (18%)	49,86,113	1.30	6 (12%)
17	CLA	BA	806	1	65,73,73	1.50	8 (12%)	76,113,113	1.33	7 (9%)
17	CLA	B3	604	-	41,50,73	1.94	7 (17%)	51,86,113	1.55	9 (17%)
19	LHG	B1	301	17	37,37,48	1.08	2 (5%)	40,43,54	1.01	3 (7%)
17	CLA	BA	844	19	41,49,73	1.90	5 (12%)	47,84,113	1.43	8 (17%)
17	CLA	BA	830	-	65,73,73	1.53	9 (13%)	76,113,113	1.23	8 (10%)
17	CLA	BB	836	-	60,68,73	1.56	8 (13%)	70,107,113	1.38	7 (10%)
17	CLA	B1	304	13	61,69,73	1.52	7 (11%)	71,108,113	1.39	8 (11%)
25	CHL	B5	607	-	45,53,74	2.37	17 (37%)	49,89,114	2.81	19 (38%)
17	CLA	BB	835	-	65,73,73	1.53	9 (13%)	76,113,113	1.14	5 (6%)
17	CLA	B1	312	19	37,46,73	1.97	7 (18%)	46,81,113	1.60	9 (19%)
20	BCR	BB	848	-	41,41,41	0.81	0	56,56,56	2.15	19 (33%)
17	CLA	BA	812	-	54,62,73	1.59	9 (16%)	62,99,113	1.46	8 (12%)
17	CLA	B5	603	-	44,52,73	1.87	7 (15%)	55,88,113	1.58	8 (14%)
17	CLA	B2	309	19	38,45,73	2.95	10 (26%)	41,76,113	1.64	10 (24%)
22	LMU	BA	853	-	35,35,36	1.15	2 (5%)	46,46,47	0.93	0
17	CLA	B2	302	-	43,52,73	1.85	7 (16%)	49,88,113	1.58	8 (16%)
17	CLA	B2	312	-	43,51,73	1.81	6 (13%)	49,86,113	1.44	8 (16%)
17	CLA	BB	812	-	65,73,73	1.47	7 (10%)	76,113,113	1.37	10 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	BA	832	-	-	7/27/105/115	-
17	CLA	B1	310	13	1/1/10/20	3/6/82/115	-
19	LHG	B2	317	17	-	22/39/39/53	-
17	CLA	B5	610	19	-	4/10/88/115	-
17	CLA	B1	313	13	1/1/11/20	5/13/91/115	-
17	CLA	BB	837	-	1/1/10/20	4/10/88/115	-
17	CLA	B3	602	15	1/1/14/20	5/31/109/115	-
17	CLA	BB	813	-	1/1/13/20	4/25/101/115	-
17	CLA	BB	831	-	1/1/13/20	8/27/105/115	-
25	CHL	B2	306	-	3/3/16/26	4/15/113/137	-
17	CLA	BB	820	-	1/1/14/20	12/31/109/115	-
17	CLA	BF	301	-	1/1/12/20	8/24/102/115	-
17	CLA	BB	842	-	1/1/15/20	9/37/115/115	-
17	CLA	BB	814	-	1/1/10/20	1/11/89/115	-
21	SF4	BA	852	2,1	-	-	0/6/5/5
17	CLA	BF	303	-	1/1/10/20	2/8/86/115	-
17	CLA	BJ	102	10	1/1/10/20	4/10/88/115	-
17	CLA	B3	606	-	1/1/10/20	2/10/86/115	-
17	CLA	BA	805	-	1/1/15/20	22/37/115/115	-
17	CLA	BB	823	-	1/1/11/20	4/16/94/115	-
17	CLA	BA	838	-	1/1/12/20	11/25/99/115	-
17	CLA	BB	815	-	1/1/15/20	20/37/115/115	-
17	CLA	BB	830	-	1/1/15/20	11/37/115/115	-
17	CLA	B1	311	13	1/1/14/20	3/29/107/115	-
17	CLA	B3	603	15	1/1/13/20	6/25/103/115	-
17	CLA	BA	817	-	-	9/31/109/115	-
26	LUT	B5	614	-	-	1/29/67/67	0/2/2/2
25	CHL	B2	304	-	3/3/15/26	3/10/108/137	-
20	BCR	BK	204	-	-	1/29/63/63	0/2/2/2
17	CLA	BB	822	-	1/1/10/20	2/8/86/115	-
17	CLA	BA	831	-	1/1/11/20	7/16/94/115	-
17	CLA	B1	306	-	1/1/10/20	3/8/86/115	-
17	CLA	B2	307	14	1/1/11/20	3/13/91/115	-
17	CLA	BB	826	-	1/1/15/20	10/37/115/115	-
17	CLA	BB	828	-	1/1/14/20	9/34/112/115	-
17	CLA	BB	838	-	1/1/12/20	5/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LUT	B2	314	-	-	0/29/67/67	0/2/2/2
17	CLA	B3	609	15	1/1/10/20	3/8/86/115	-
20	BCR	BL	305	-	-	2/29/63/63	0/2/2/2
18	PQN	BA	843	-	-	8/23/43/43	0/2/2/2
17	CLA	BB	843	19	1/1/15/20	11/37/115/115	-
24	SQD	BJ	104	-	-	21/42/62/69	0/1/1/1
17	CLA	BA	842	-	1/1/15/20	13/37/115/115	-
20	BCR	BA	855	-	-	4/29/63/63	0/2/2/2
21	SF4	BC	101	3	-	-	0/6/5/5
17	CLA	BA	808	1	1/1/15/20	10/37/115/115	-
17	CLA	BA	815	-	-	4/10/88/115	-
17	CLA	BK	202	-	1/1/11/20	6/13/91/115	-
17	CLA	BA	822	-	1/1/10/20	8/10/88/115	-
17	CLA	B2	310	14	1/1/11/20	7/11/89/115	-
27	XAT	B1	317	-	-	0/31/93/93	0/4/4/4
17	CLA	B3	612	-	1/1/13/20	7/23/101/115	-
20	BCR	BB	845	-	-	4/29/63/63	0/2/2/2
17	CLA	BA	828	-	1/1/15/20	14/37/115/115	-
17	CLA	BB	807	-	1/1/15/20	13/37/115/115	-
19	LHG	BF	305	-	-	18/49/49/53	-
20	BCR	BB	846	-	-	6/29/63/63	0/2/2/2
17	CLA	BB	808	2	1/1/15/20	10/37/115/115	-
17	CLA	BB	817	-	1/1/10/20	4/9/87/115	-
17	CLA	B2	303	-	1/1/10/20	4/9/88/115	-
19	LHG	B1	318	17	-	12/46/46/53	-
21	SF4	BC	102	3	-	-	0/6/5/5
26	LUT	B3	616	-	-	4/29/67/67	0/2/2/2
17	CLA	BA	827	-	1/1/15/20	14/37/115/115	-
17	CLA	BG	201	-	1/1/10/20	7/10/88/115	-
25	CHL	B1	303	13	3/3/17/26	3/19/117/137	-
17	CLA	B5	608	16	1/1/11/20	4/11/89/115	-
17	CLA	BA	814	-	1/1/11/20	6/13/91/115	-
17	CLA	B3	613	-	1/1/10/20	0/6/84/115	-
17	CLA	BB	829	-	1/1/15/20	17/37/115/115	-
17	CLA	BB	819	-	1/1/13/20	12/30/108/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	BL	304	-	1/1/10/20	5/11/89/115	-
25	CHL	B3	607	-	3/3/16/26	5/13/111/137	-
17	CLA	BA	836	1	-	6/13/91/115	-
27	XAT	B3	617	-	-	0/31/93/93	0/4/4/4
17	CLA	B3	610	19	1/1/10/20	0/6/84/115	-
19	LHG	BA	845	-	-	29/53/53/53	-
17	CLA	B5	601	16	1/1/11/20	8/15/93/115	-
17	CLA	BB	804	-	1/1/15/20	15/37/115/115	-
17	CLA	B5	612	16	1/1/13/20	8/28/106/115	-
25	CHL	B1	308	-	3/3/15/26	0/8/106/137	-
20	BCR	BA	851	-	-	8/29/63/63	0/2/2/2
17	CLA	BA	807	-	1/1/12/20	4/19/97/115	-
17	CLA	BA	813	-	1/1/15/20	17/37/115/115	-
17	CLA	B3	614	-	1/1/8/20	0/0/74/115	-
17	CLA	BA	809	1	-	9/19/97/115	-
20	BCR	B2	316	-	-	0/29/63/63	0/2/2/2
20	BCR	BF	304	-	-	7/29/63/63	0/2/2/2
17	CLA	BL	302	12	-	4/13/91/115	-
17	CLA	B5	611	16	1/1/10/20	4/8/86/115	-
19	LHG	B3	619	17	-	11/26/26/53	-
17	CLA	B2	301	14	1/1/15/20	9/37/115/115	-
25	CHL	B2	313	14	3/3/15/26	0/12/110/137	-
17	CLA	BA	834	-	-	11/37/115/115	-
17	CLA	BA	829	-	1/1/15/20	11/37/115/115	-
20	BCR	BA	847	-	-	5/29/63/63	0/2/2/2
19	LHG	B1	302	-	-	14/40/40/53	-
20	BCR	BI	101	-	-	6/29/63/63	0/2/2/2
17	CLA	BA	825	-	1/1/15/20	15/37/115/115	-
17	CLA	B5	613	-	1/1/11/20	5/13/91/115	-
25	CHL	B2	305	-	3/3/15/26	2/12/110/137	-
20	BCR	B5	616	-	-	2/29/63/63	0/2/2/2
27	XAT	B2	315	-	-	0/31/93/93	0/4/4/4
20	BCR	BH	202	-	-	15/29/63/63	0/2/2/2
17	CLA	BA	837	-	1/1/12/20	3/21/99/115	-
17	CLA	B5	604	-	1/1/11/20	3/11/87/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	BCR	BA	850	-	-	3/29/63/63	0/2/2/2
17	CLA	BB	827	-	-	8/34/112/115	-
17	CLA	BA	835	-	1/1/11/20	6/13/91/115	-
17	CLA	BB	811	2	1/1/15/20	15/37/115/115	-
17	CLA	BA	824	-	1/1/13/20	8/25/103/115	-
17	CLA	B1	309	-	-	2/11/89/115	-
17	CLA	B3	611	15	1/1/10/20	2/11/89/115	-
17	CLA	BB	818	-	1/1/13/20	8/25/103/115	-
17	CLA	BB	821	-	1/1/13/20	6/25/103/115	-
17	CLA	B1	305	-	1/1/12/20	6/23/101/115	-
17	CLA	B3	615	-	1/1/10/20	0/6/84/115	-
25	CHL	B5	605	-	3/3/15/26	2/8/106/137	-
17	CLA	BA	826	-	-	6/23/101/115	-
17	CLA	BA	819	-	1/1/15/20	13/37/115/115	-
17	CLA	B5	602	16	-	9/31/109/115	-
27	XAT	B5	615	-	-	0/31/93/93	0/4/4/4
17	CLA	BB	825	-	1/1/11/20	6/13/91/115	-
17	CLA	BA	802	-	1/1/15/20	4/37/115/115	-
17	CLA	BA	811	-	1/1/15/20	14/37/115/115	-
17	CLA	BB	834	-	-	9/37/115/115	-
20	BCR	BJ	103	-	-	5/29/63/63	0/2/2/2
17	CLA	BA	804	-	-	5/22/100/115	-
17	CLA	BA	801	-	1/1/15/20	9/37/115/115	-
28	LMG	B5	617	-	-	14/28/48/70	0/1/1/1
20	BCR	BB	847	-	-	6/29/63/63	0/2/2/2
17	CLA	BA	840	-	1/1/15/20	13/37/115/115	-
17	CLA	BA	818	-	-	6/27/105/115	-
17	CLA	BB	810	-	1/1/15/20	15/37/115/115	-
17	CLA	BB	833	-	-	4/11/89/115	-
17	CLA	BF	302	-	1/1/10/20	3/10/88/115	-
17	CLA	B2	311	14	1/1/15/20	13/37/115/115	-
23	DGD	BB	850	-	-	13/55/95/95	0/2/2/2
17	CLA	BB	839	-	-	8/37/115/115	-
17	CLA	BK	201	11	1/1/8/20	0/2/74/115	-
17	CLA	BB	802	-	1/1/15/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	PQN	BB	844	-	-	9/23/43/43	0/2/2/2
22	LMU	BB	851	-	-	10/21/61/61	0/2/2/2
20	BCR	BA	856	-	-	5/29/63/63	0/2/2/2
17	CLA	BB	801	-	1/1/15/20	17/37/115/115	-
17	CLA	BB	809	-	-	5/22/100/115	-
20	BCR	BA	848	-	-	4/29/63/63	0/2/2/2
17	CLA	B3	608	15	1/1/11/20	3/13/91/115	-
20	BCR	BL	301	-	-	6/29/63/63	0/2/2/2
19	LHG	B5	618	17	-	13/34/34/53	-
17	CLA	BB	816	-	1/1/15/20	15/35/113/115	-
17	CLA	BA	841	-	1/1/15/20	15/37/115/115	-
17	CLA	BA	833	-	1/1/15/20	15/37/115/115	-
17	CLA	BA	810	-	1/1/15/20	12/37/115/115	-
17	CLA	BB	805	-	1/1/15/20	14/37/115/115	-
17	CLA	B2	308	14	1/1/13/20	6/25/103/115	-
20	BCR	BA	849	-	-	4/29/63/63	0/2/2/2
17	CLA	BH	201	-	1/1/14/20	11/31/109/115	-
17	CLA	BA	803	-	1/1/15/20	18/37/115/115	-
22	LMU	BA	854	-	-	8/19/59/61	0/2/2/2
17	CLA	B1	314	-	1/1/14/20	9/31/109/115	-
26	LUT	B1	316	-	-	14/29/67/67	0/2/2/2
17	CLA	BA	820	-	1/1/11/20	4/13/91/115	-
17	CLA	BB	824	-	-	18/37/115/115	-
17	CLA	BG	202	7	1/1/11/20	6/13/91/115	-
20	BCR	BG	203	-	-	6/29/63/63	0/2/2/2
17	CLA	B5	609	16	1/1/12/20	3/24/102/115	-
20	BCR	BB	803	-	-	4/29/63/63	0/2/2/2
17	CLA	BA	816	-	1/1/11/20	2/13/91/115	-
17	CLA	BA	823	-	1/1/10/20	4/8/86/115	-
17	CLA	BB	841	-	1/1/15/20	7/37/115/115	-
17	CLA	BA	839	-	-	6/21/99/115	-
17	CLA	BL	303	-	-	7/31/109/115	-
20	BCR	BJ	101	-	-	0/29/63/63	0/2/2/2
17	CLA	BB	806	-	1/1/10/20	2/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	BCR	BB	849	-	-	2/29/63/63	0/2/2/2
17	CLA	B1	307	-	1/1/9/20	4/8/82/115	-
19	LHG	BA	846	17	-	7/30/30/53	-
17	CLA	B3	605	-	1/1/10/20	4/8/86/115	-
25	CHL	B5	606	-	3/3/15/26	2/8/104/137	-
25	CHL	B3	601	14	3/3/17/26	11/24/122/137	-
17	CLA	BB	840	-	-	4/16/94/115	-
17	CLA	BA	821	-	-	12/37/115/115	-
17	CLA	B1	315	-	1/1/10/20	0/4/80/115	-
20	BCR	B3	618	-	-	6/29/63/63	0/2/2/2
17	CLA	BK	203	-	1/1/11/20	5/15/93/115	-
17	CLA	BB	832	-	1/1/10/20	4/11/89/115	-
17	CLA	BA	806	1	1/1/15/20	18/37/115/115	-
17	CLA	B3	604	-	1/1/11/20	2/9/85/115	-
19	LHG	B1	301	17	-	7/42/42/53	-
17	CLA	BA	844	19	1/1/10/20	4/8/86/115	-
17	CLA	BA	830	-	1/1/15/20	13/37/115/115	-
17	CLA	B1	304	13	1/1/14/20	7/33/111/115	-
17	CLA	BB	836	-	-	11/31/109/115	-
25	CHL	B5	607	-	3/3/16/26	5/13/111/137	-
17	CLA	BB	835	-	1/1/15/20	16/37/115/115	-
17	CLA	B1	312	19	1/1/10/20	0/4/80/115	-
20	BCR	BB	848	-	-	2/29/63/63	0/2/2/2
17	CLA	BA	812	-	1/1/12/20	5/24/102/115	-
17	CLA	B5	603	-	1/1/11/20	4/13/89/115	-
17	CLA	B2	309	19	1/1/7/20	1/10/70/115	-
22	LMU	BA	853	-	-	9/20/60/61	0/2/2/2
17	CLA	B2	302	-	1/1/11/20	4/11/89/115	-
17	CLA	B2	312	-	1/1/10/20	1/11/89/115	-
17	CLA	BB	812	-	1/1/15/20	13/37/115/115	-

The worst 5 of 1330 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B2	309	CLA	C1A-NA	12.72	1.40	1.29
18	BB	844	PQN	C12-C13	9.75	1.56	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	BA	843	PQN	C12-C13	9.52	1.55	1.33
17	BA	844	CLA	C4B-NB	8.02	1.42	1.35
17	B3	612	CLA	C4B-NB	7.87	1.42	1.35

The worst 5 of 2027 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	BH	202	BCR	C37-C22-C21	-32.50	77.40	122.92
20	BH	202	BCR	C35-C13-C14	-31.52	78.78	122.92
20	BH	202	BCR	C34-C9-C10	-29.92	81.01	122.92
20	BG	203	BCR	C35-C13-C14	-29.72	81.29	122.92
20	BH	202	BCR	C37-C22-C23	-27.87	74.16	118.08

5 of 150 chirality outliers are listed below:

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

5 of 1453 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	BA	801	CLA	CBD-CGD-O2D-CED
17	BA	802	CLA	CBD-CGD-O2D-CED
17	BA	804	CLA	C1A-C2A-CAA-CBA
17	BA	804	CLA	C3A-C2A-CAA-CBA
17	BA	809	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

119 monomers are involved in 185 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	BA	832	CLA	3	0
19	B2	317	LHG	1	0
17	B5	610	CLA	1	0
25	B2	306	CHL	4	0
17	BB	820	CLA	1	0
17	BF	301	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	BA	852	SF4	1	0
17	BA	805	CLA	3	0
17	BB	823	CLA	2	0
17	BA	838	CLA	1	0
17	BB	815	CLA	8	0
17	BB	830	CLA	1	0
26	B5	614	LUT	1	0
20	BK	204	BCR	2	0
17	BB	826	CLA	1	0
17	BB	828	CLA	3	0
17	BB	838	CLA	1	0
26	B2	314	LUT	1	0
20	BL	305	BCR	2	0
18	BA	843	PQN	3	0
17	BB	843	CLA	1	0
24	BJ	104	SQD	3	0
17	BA	842	CLA	1	0
20	BA	855	BCR	3	0
17	BA	808	CLA	4	0
27	B1	317	XAT	7	0
20	BB	845	BCR	2	0
17	BA	828	CLA	1	0
17	BB	807	CLA	1	0
19	BF	305	LHG	1	0
20	BB	846	BCR	1	0
17	BB	808	CLA	1	0
26	B3	616	LUT	2	0
17	BA	827	CLA	1	0
17	BG	201	CLA	2	0
25	B1	303	CHL	1	0
17	B5	608	CLA	1	0
17	BB	829	CLA	1	0
17	BB	819	CLA	1	0
25	B3	607	CHL	2	0
27	B3	617	XAT	1	0
19	BA	845	LHG	1	0
17	BB	804	CLA	4	0
17	B5	612	CLA	2	0
20	BA	851	BCR	7	0
20	B2	316	BCR	2	0
20	BF	304	BCR	1	0
17	B5	611	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B3	619	LHG	1	0
17	B2	301	CLA	2	0
17	BA	834	CLA	1	0
17	BA	829	CLA	2	0
20	BA	847	BCR	1	0
20	BI	101	BCR	1	0
27	B2	315	XAT	3	0
20	BH	202	BCR	1	0
17	BB	827	CLA	1	0
17	BB	811	CLA	3	0
17	B3	611	CLA	1	0
17	BB	818	CLA	1	0
17	BB	821	CLA	1	0
17	B1	305	CLA	1	0
25	B5	605	CHL	1	0
17	BA	819	CLA	1	0
17	B5	602	CLA	1	0
27	B5	615	XAT	1	0
17	BB	825	CLA	1	0
17	BA	802	CLA	3	0
17	BA	811	CLA	2	0
17	BB	834	CLA	3	0
20	BJ	103	BCR	2	0
17	BA	804	CLA	1	0
17	BA	801	CLA	16	0
20	BB	847	BCR	1	0
17	BA	840	CLA	2	0
17	BB	810	CLA	2	0
17	BF	302	CLA	2	0
17	B2	311	CLA	1	0
23	BB	850	DGD	1	0
17	BB	802	CLA	7	0
18	BB	844	PQN	3	0
20	BA	856	BCR	1	0
17	BB	801	CLA	4	0
17	BB	809	CLA	1	0
20	BA	848	BCR	1	0
20	BL	301	BCR	2	0
17	BB	816	CLA	1	0
17	BA	841	CLA	1	0
17	BA	810	CLA	1	0
17	BB	805	CLA	2	0

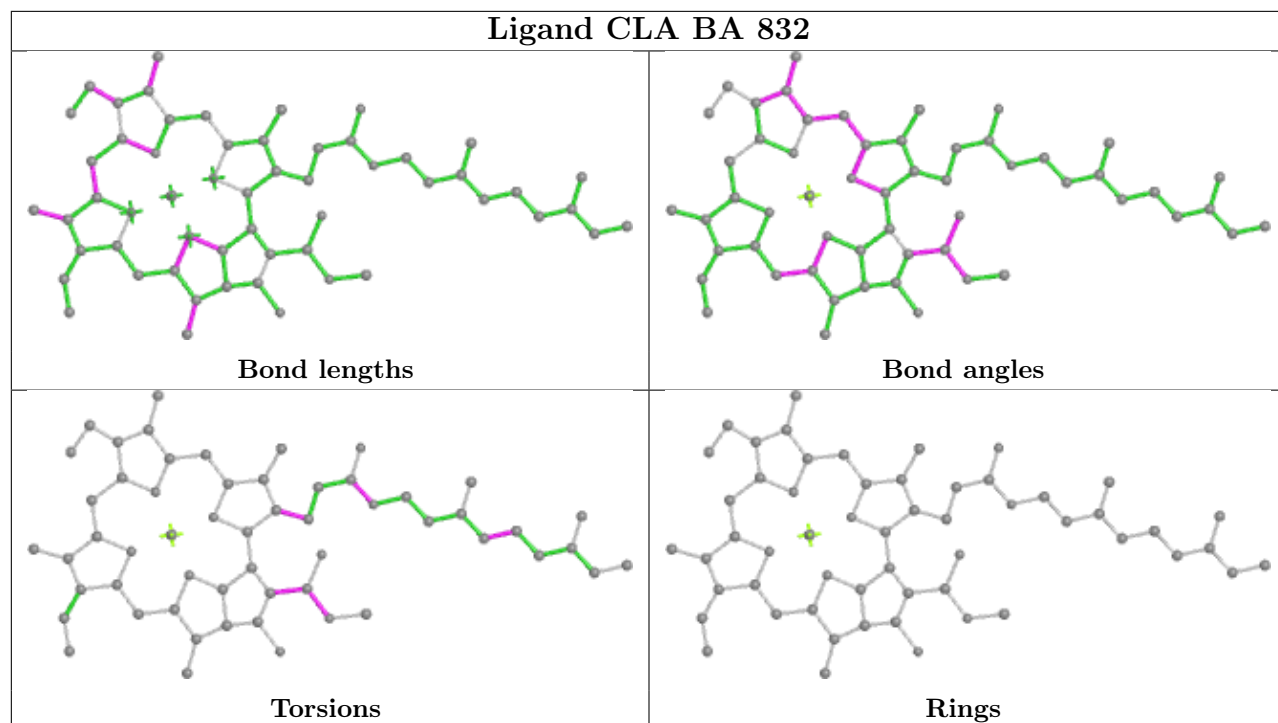
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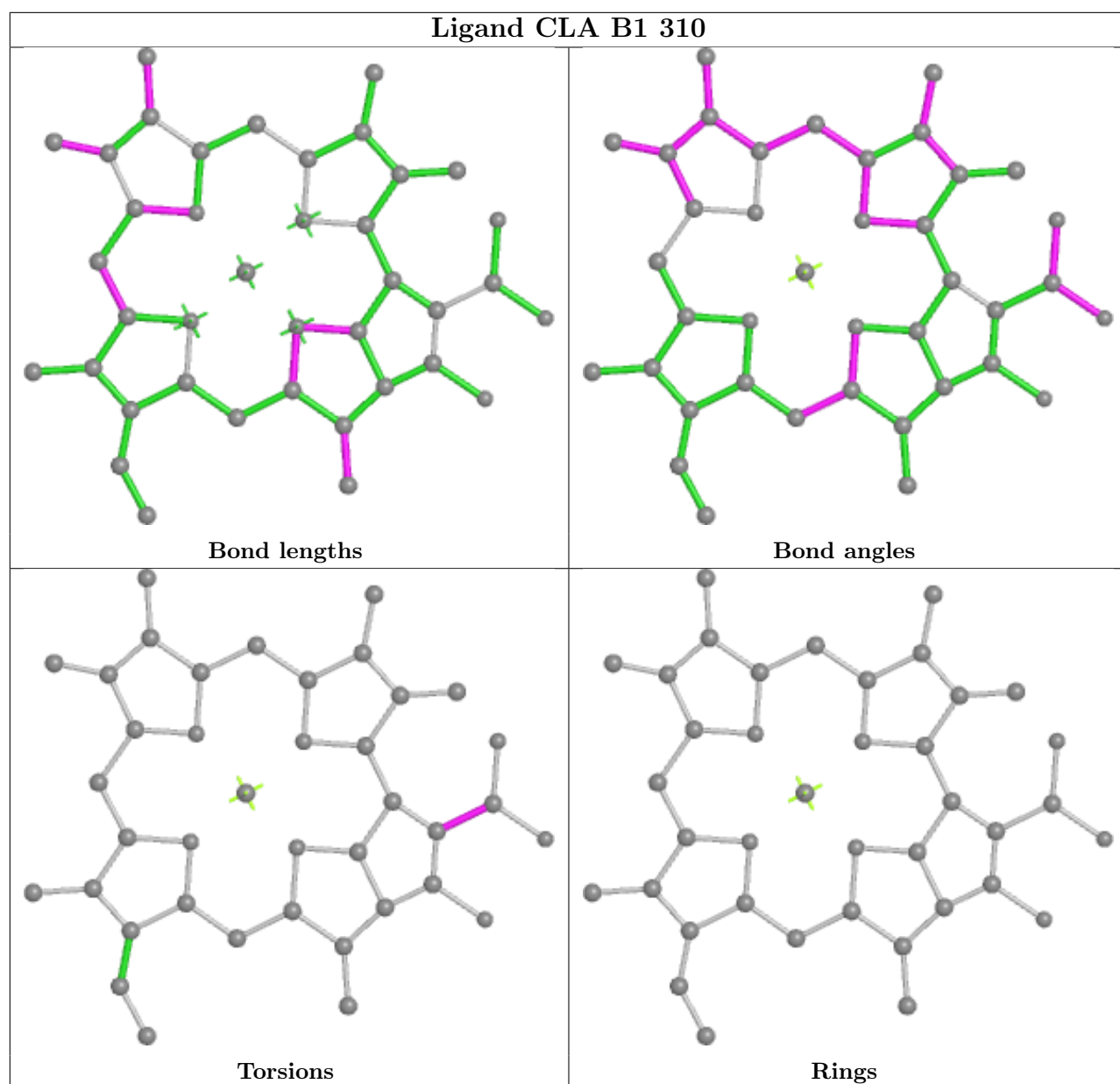
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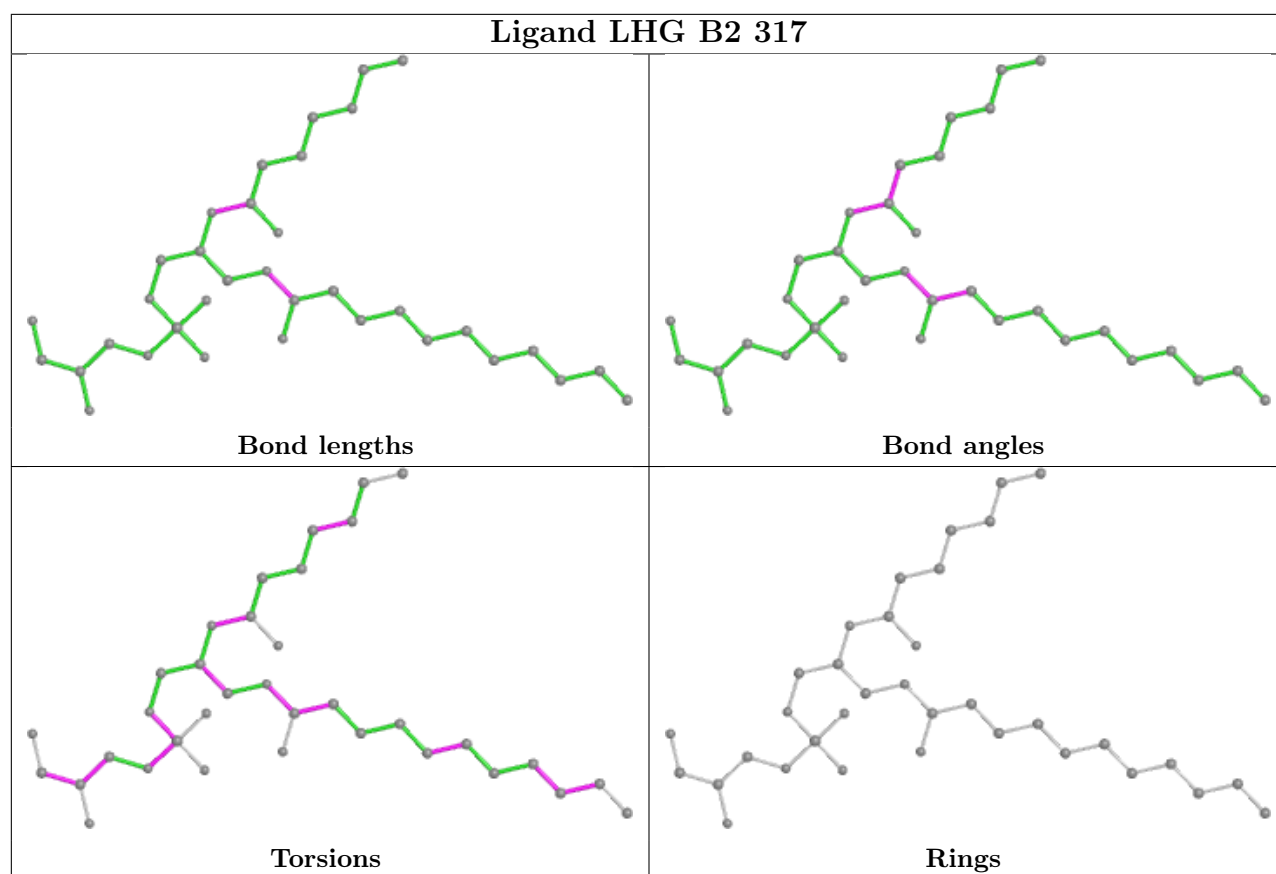
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	BA	849	BCR	2	0
17	BA	803	CLA	2	0
17	B1	314	CLA	1	0
26	B1	316	LUT	2	0
17	BB	824	CLA	1	0
17	BG	202	CLA	1	0
20	BG	203	BCR	3	0
20	BB	803	BCR	5	0
17	BB	841	CLA	1	0
17	BA	839	CLA	1	0
17	BL	303	CLA	1	0
20	BJ	101	BCR	2	0
17	BB	806	CLA	1	0
20	BB	849	BCR	3	0
19	BA	846	LHG	1	0
25	B3	601	CHL	3	0
17	BB	840	CLA	2	0
20	B3	618	BCR	5	0
17	BK	203	CLA	1	0
17	BA	806	CLA	1	0
17	BA	830	CLA	3	0
17	B1	304	CLA	1	0
17	BB	835	CLA	1	0
20	BB	848	BCR	2	0
17	BA	812	CLA	1	0
17	B2	309	CLA	1	0
17	B2	302	CLA	1	0
17	B2	312	CLA	1	0
17	BB	812	CLA	3	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.

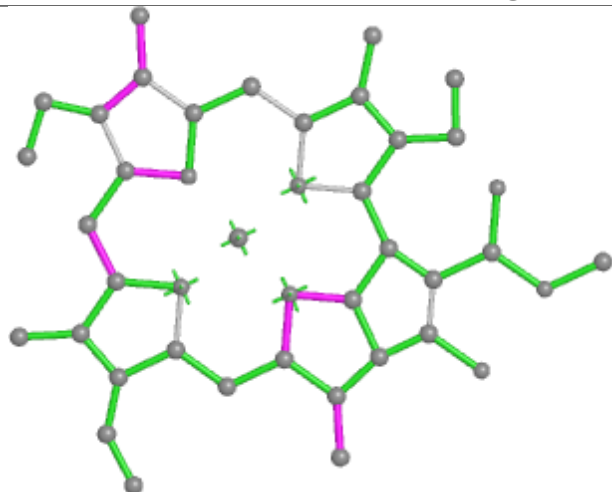




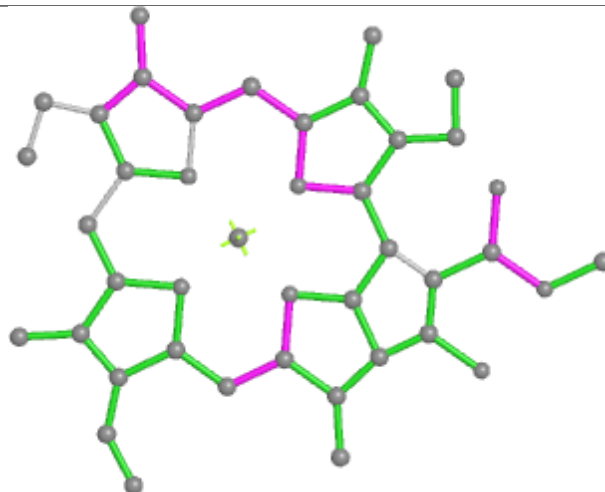




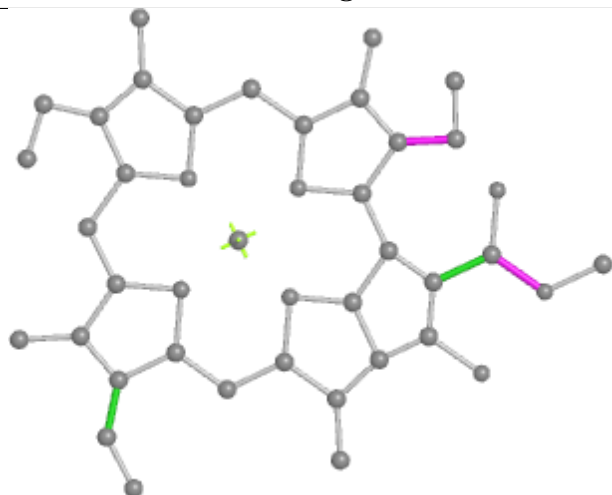
## Ligand CLA B5 610



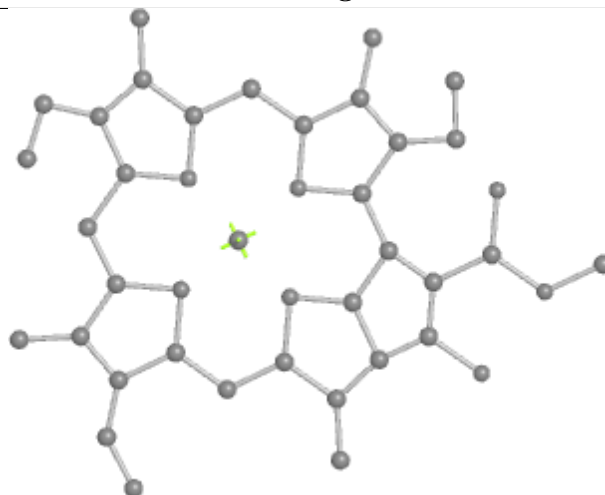
Bond lengths



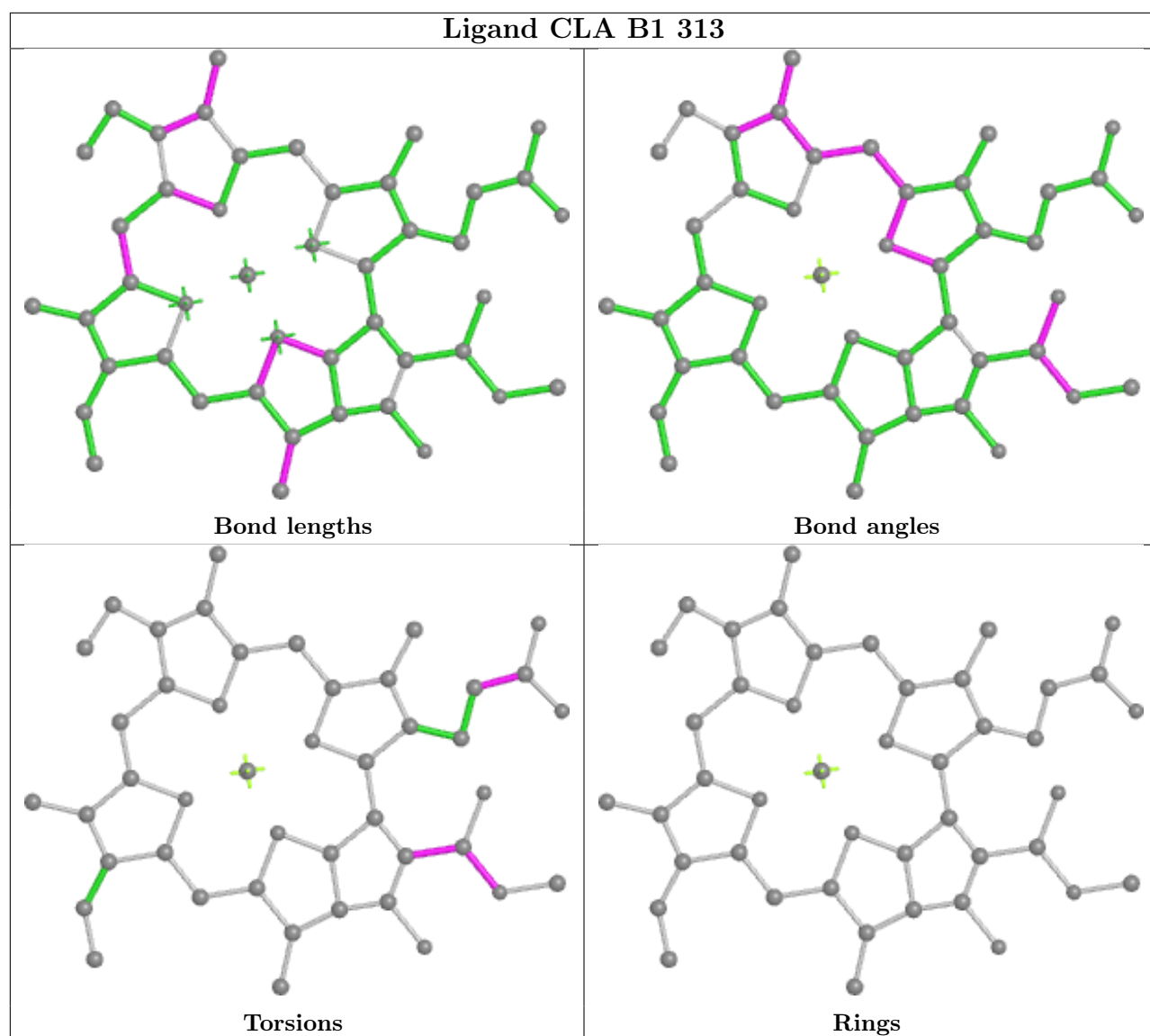
Bond angles



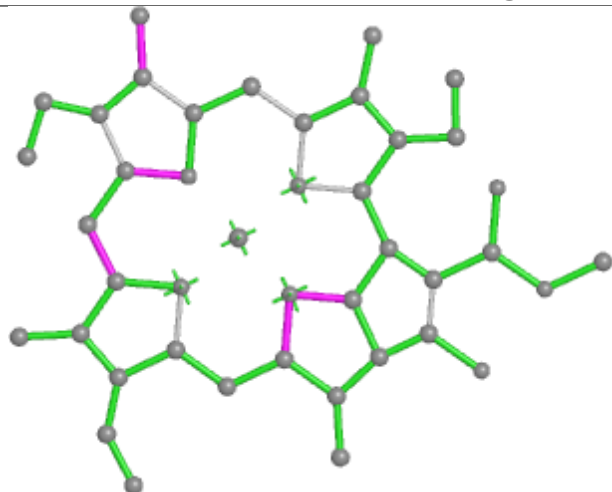
Torsions



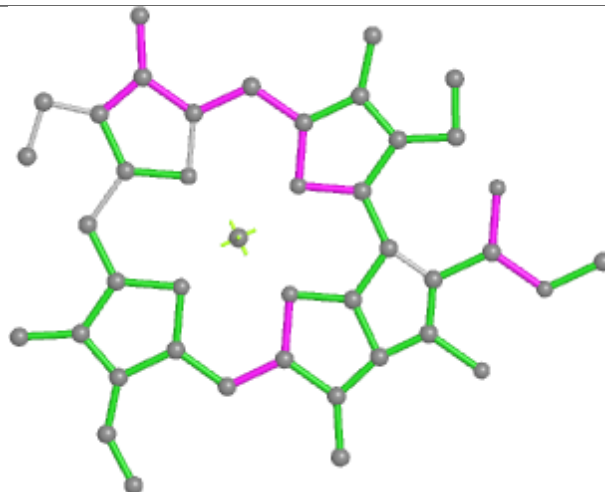
Rings



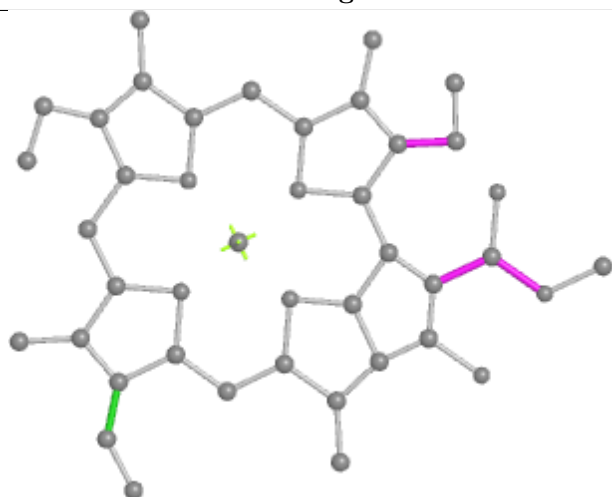
## Ligand CLA BB 837



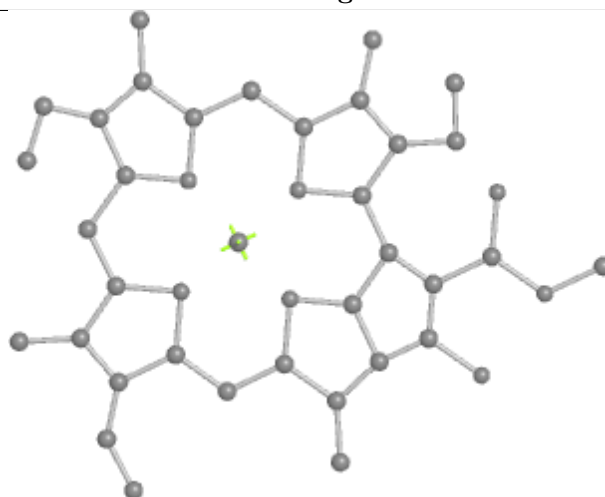
Bond lengths



Bond angles

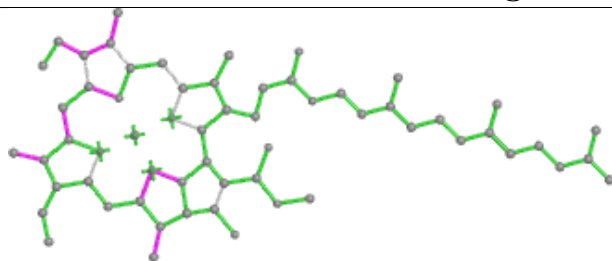


Torsions

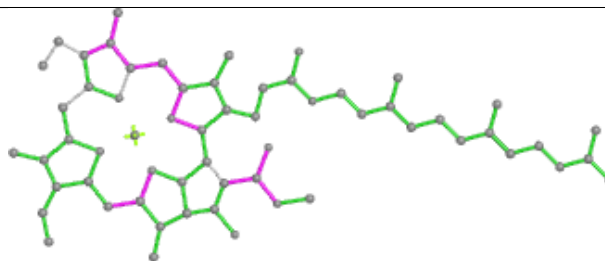


Rings

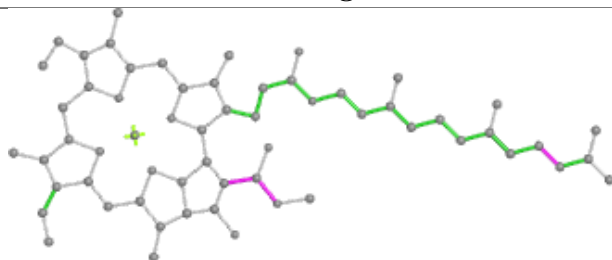
## Ligand CLA B3 602



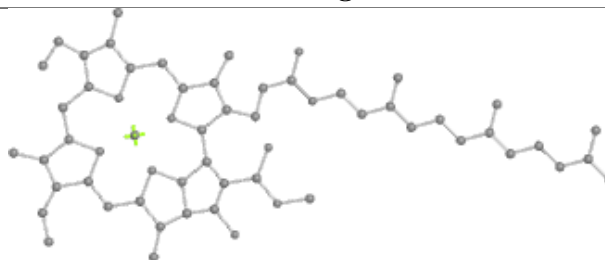
Bond lengths



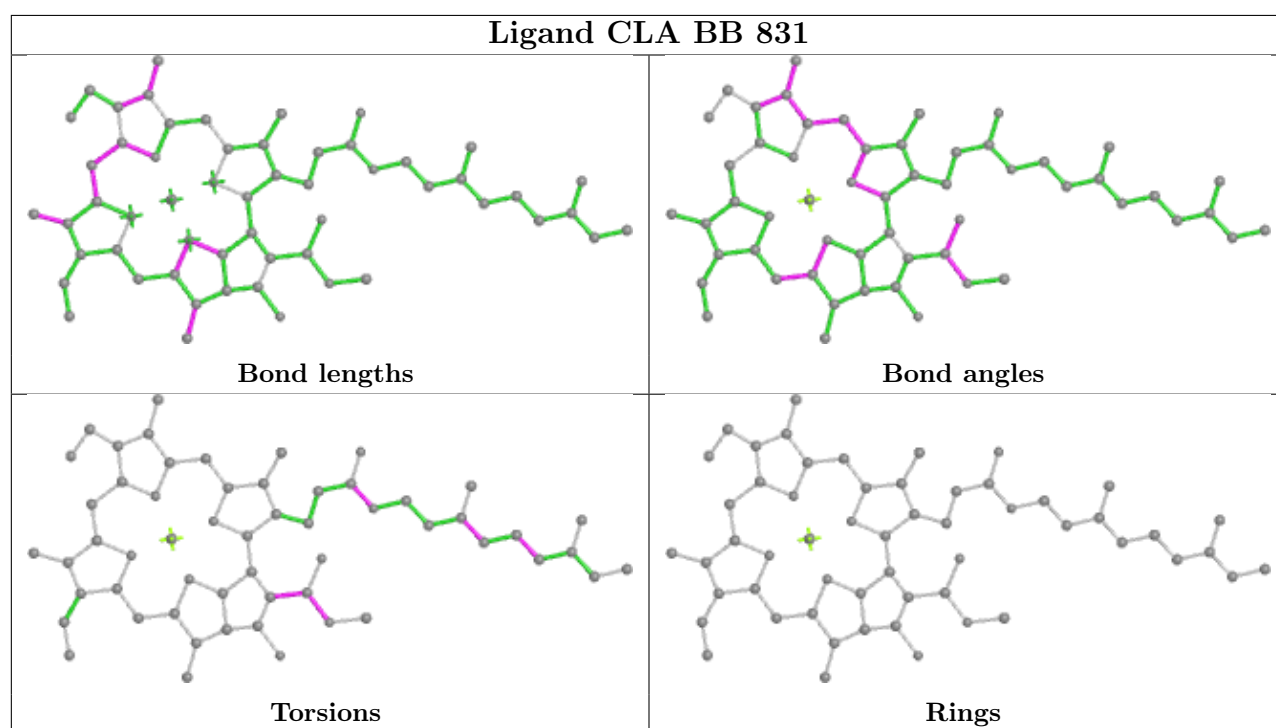
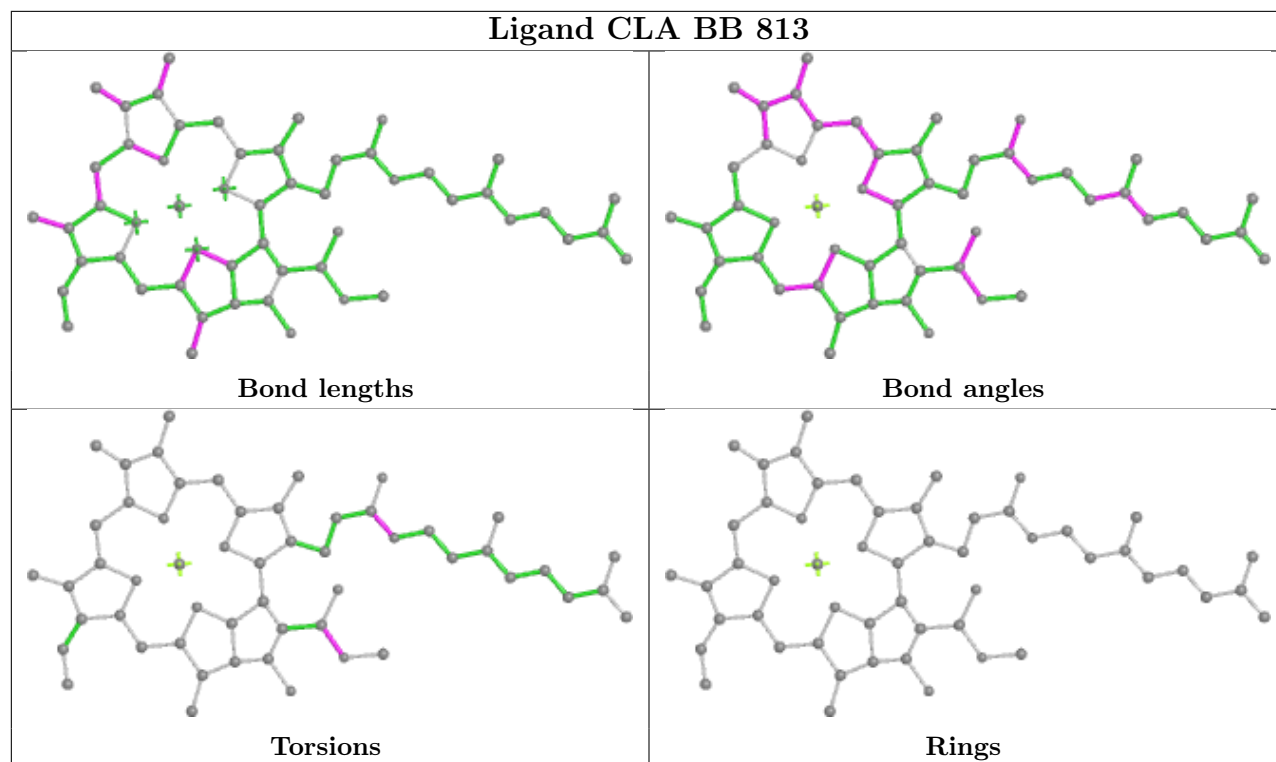
Bond angles



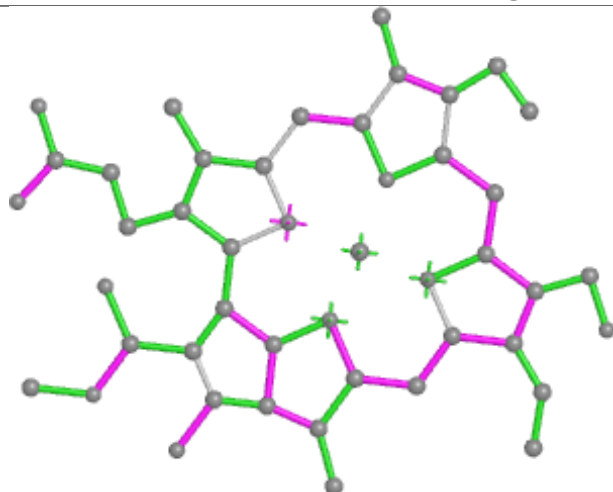
Torsions



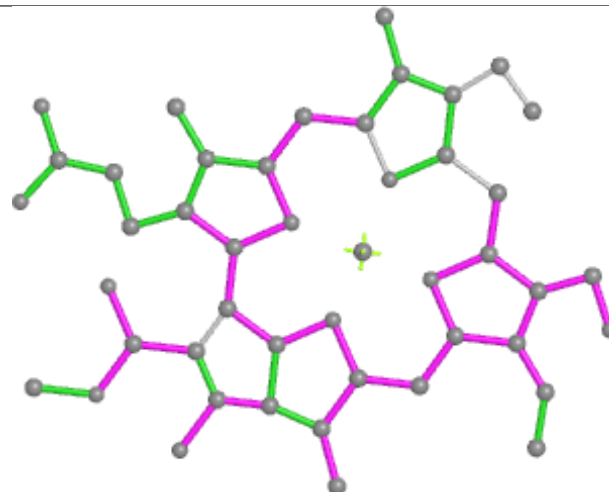
Rings



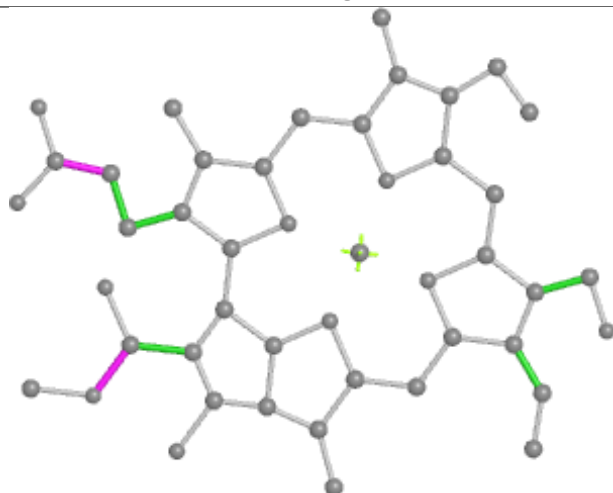
## Ligand CHL B2 306



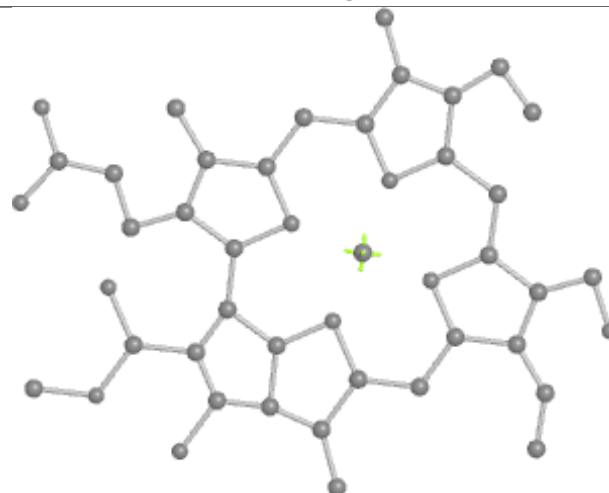
Bond lengths



Bond angles

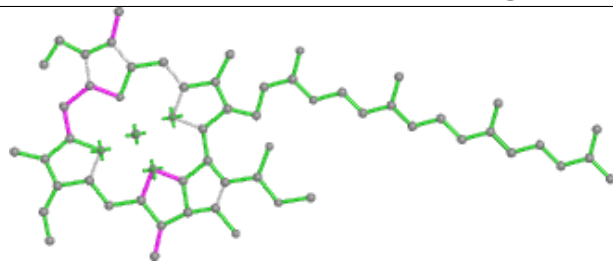


Torsions

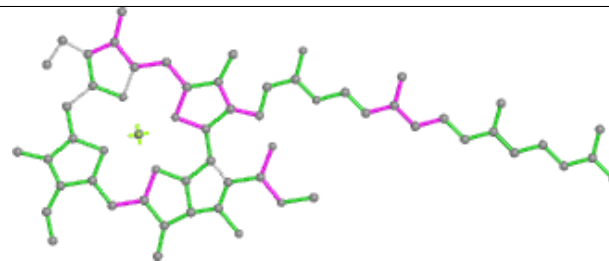


Rings

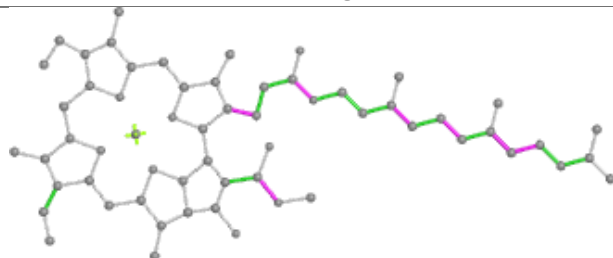
## Ligand CLA BB 820



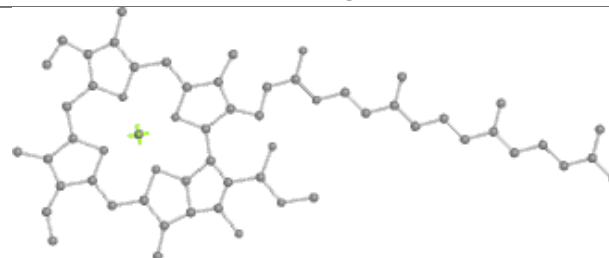
Bond lengths



Bond angles

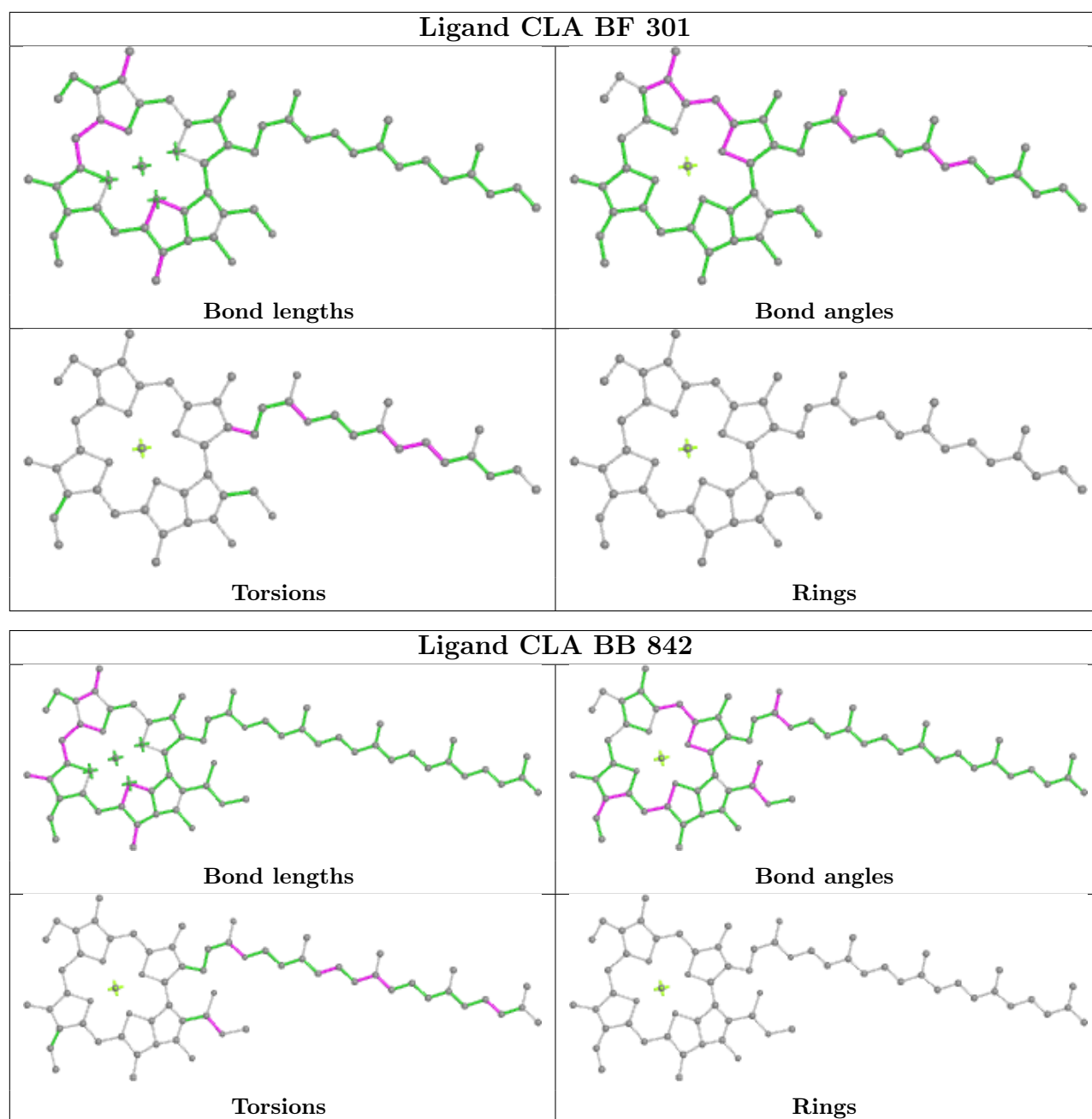


Torsions

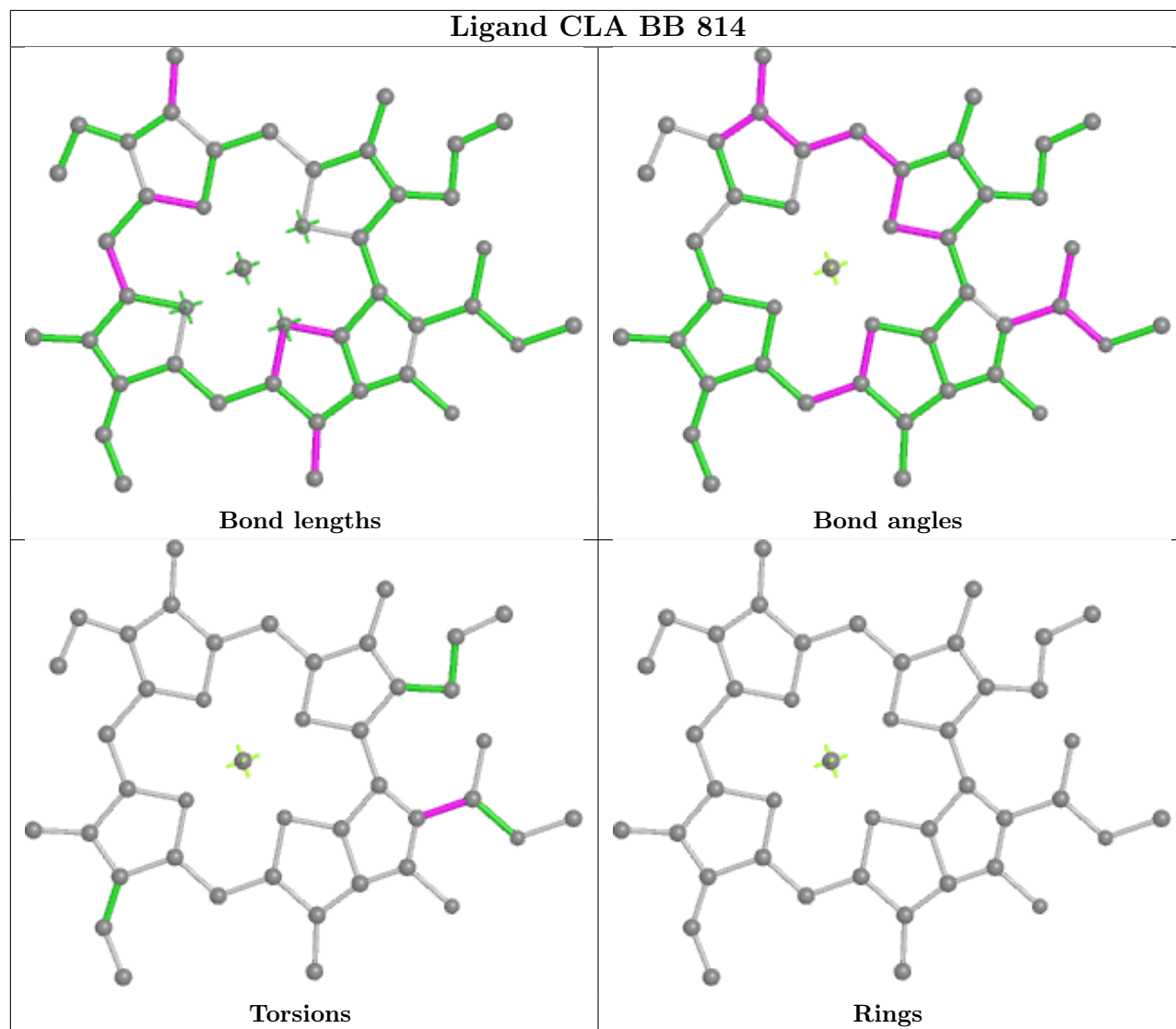


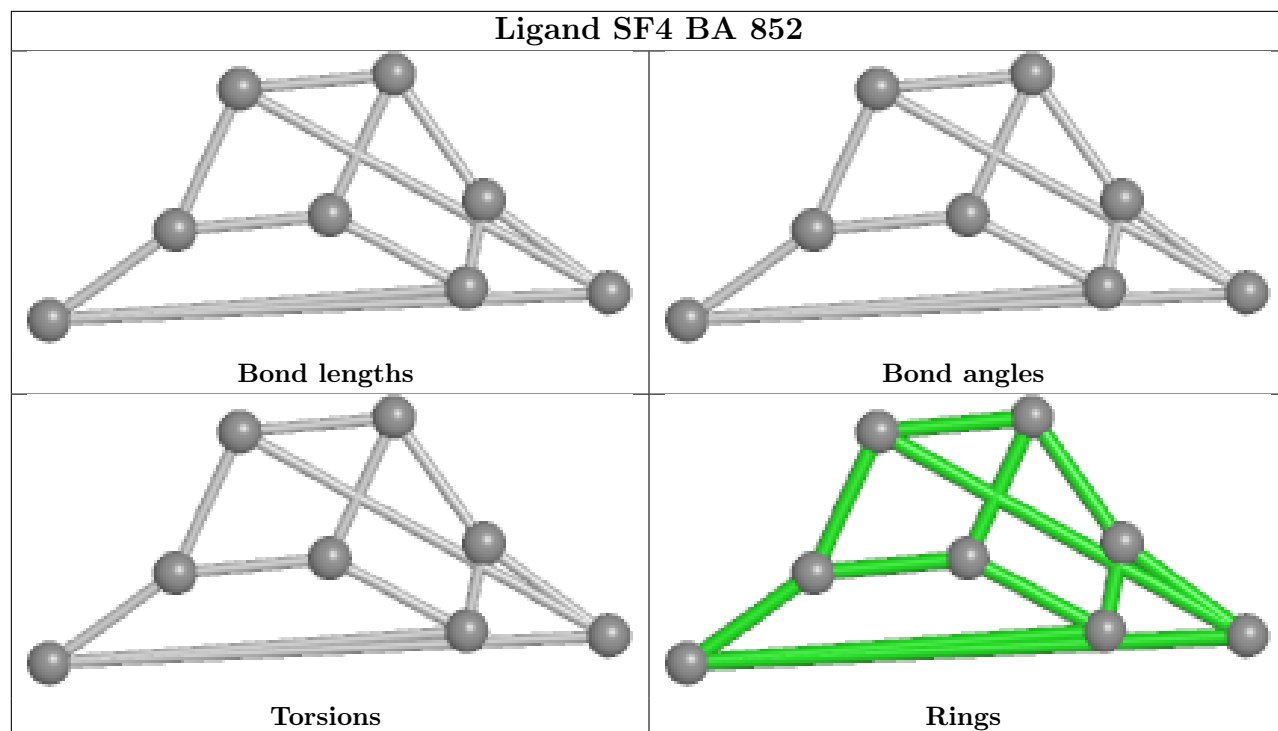
Rings

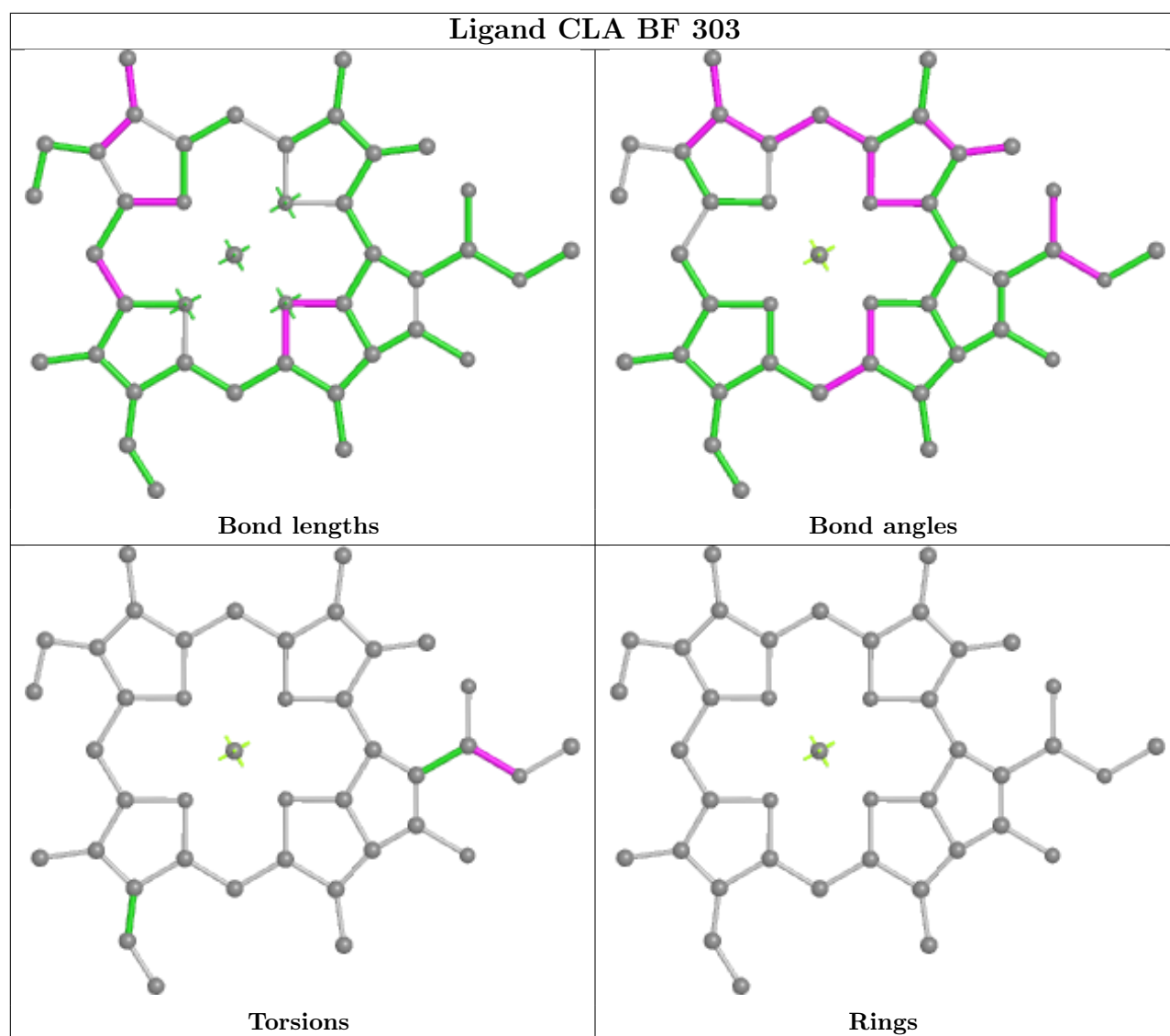




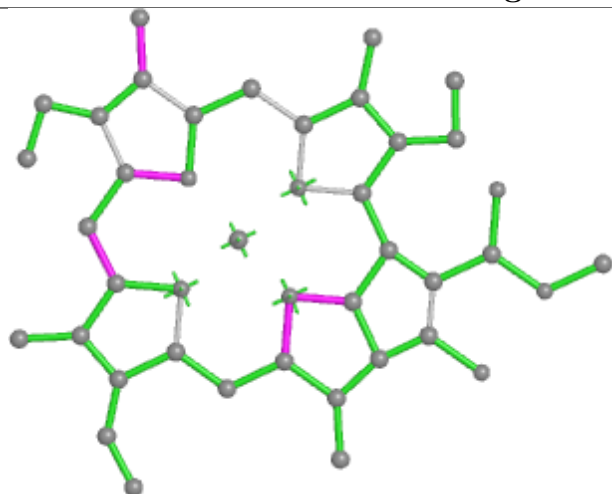
## Ligand CLA BB 814



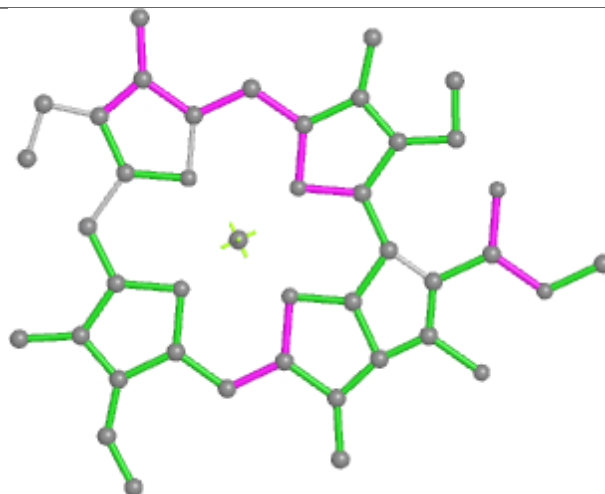




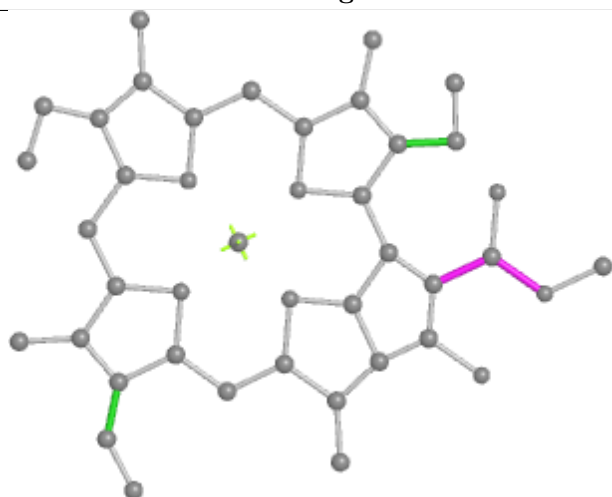
## Ligand CLA BJ 102



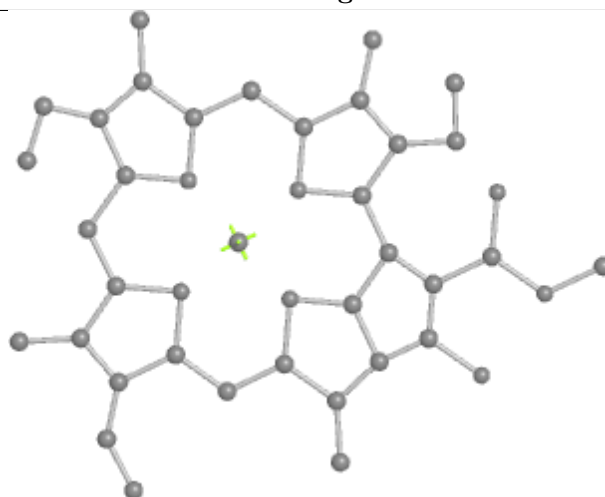
Bond lengths



Bond angles

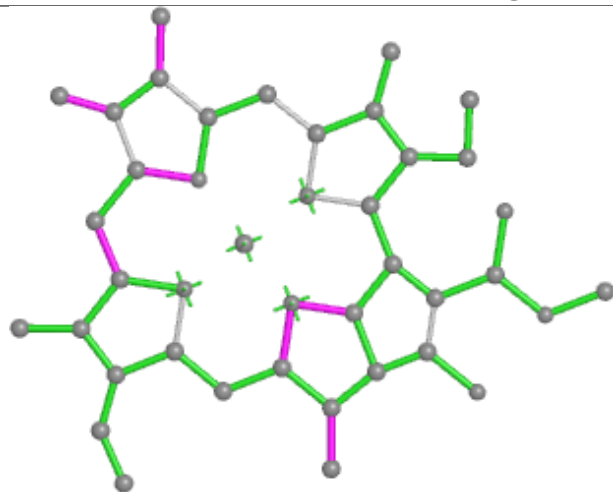


Torsions

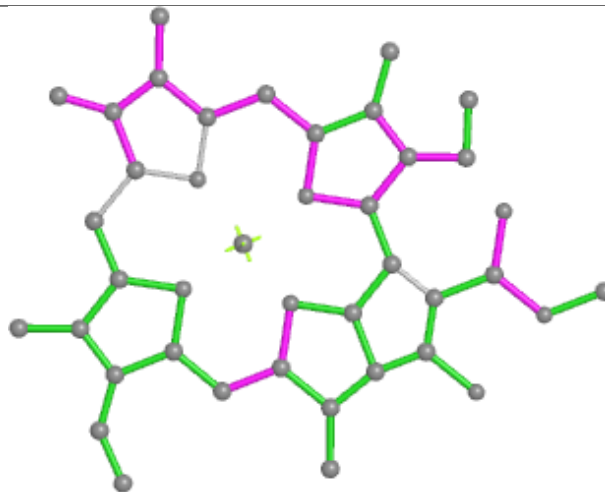


Rings

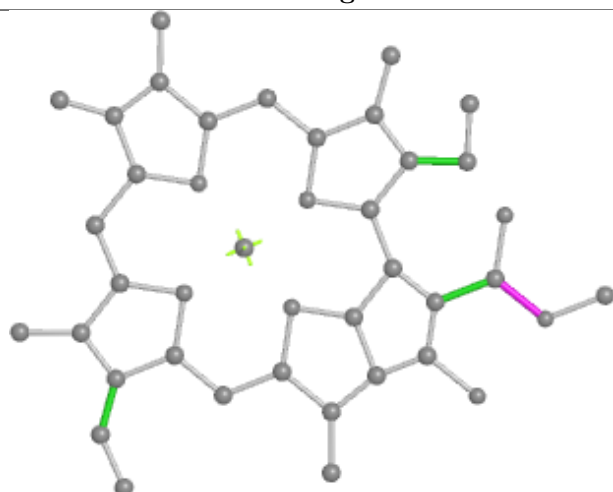
## Ligand CLA B3 606



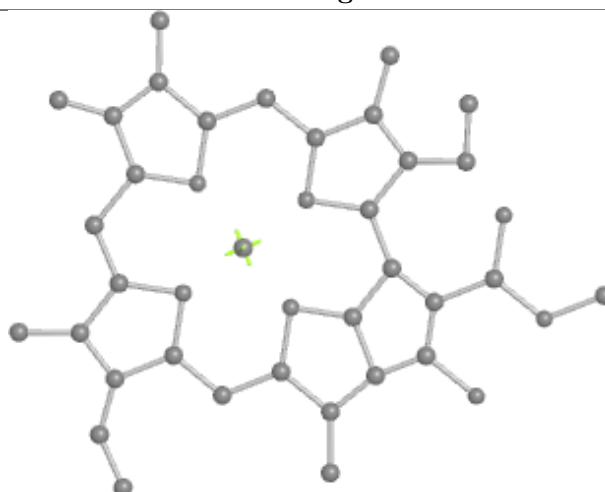
Bond lengths



Bond angles

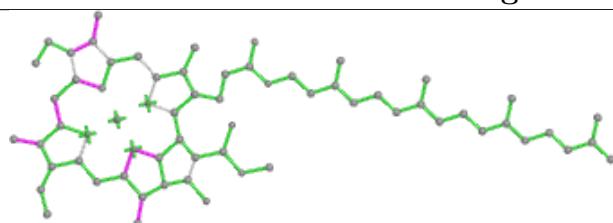


Torsions

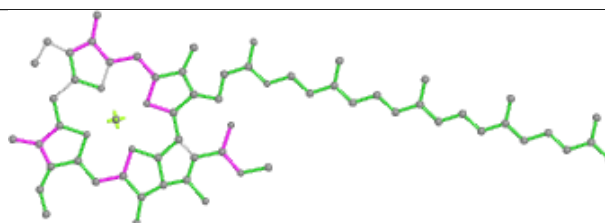


Rings

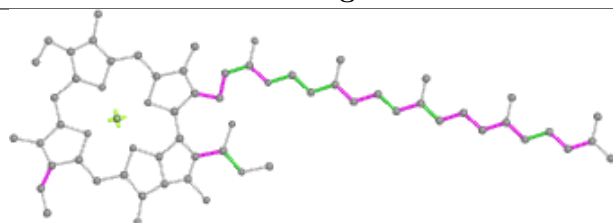
## Ligand CLA BA 805



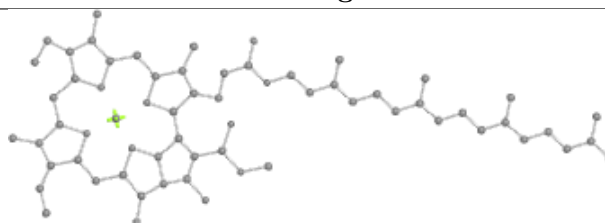
Bond lengths



Bond angles

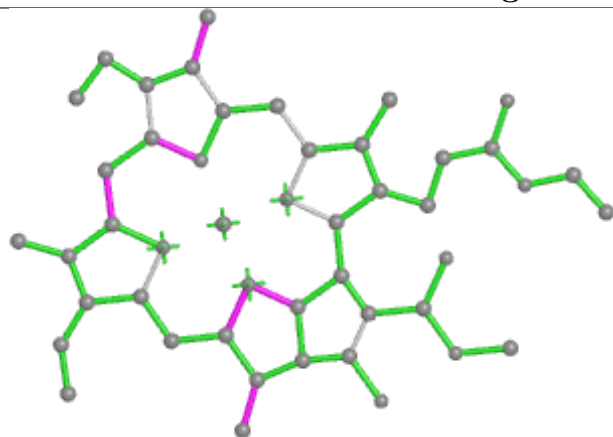


Torsions

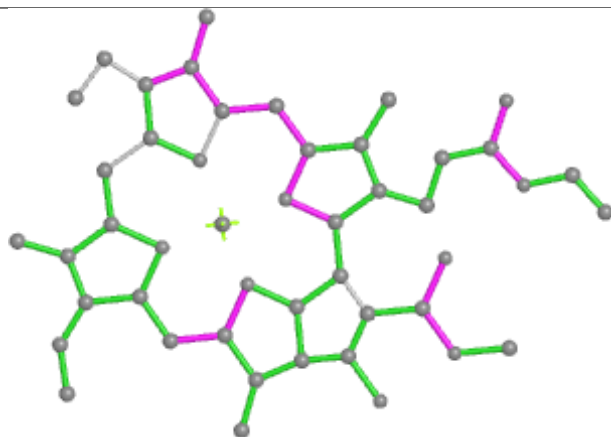


Rings

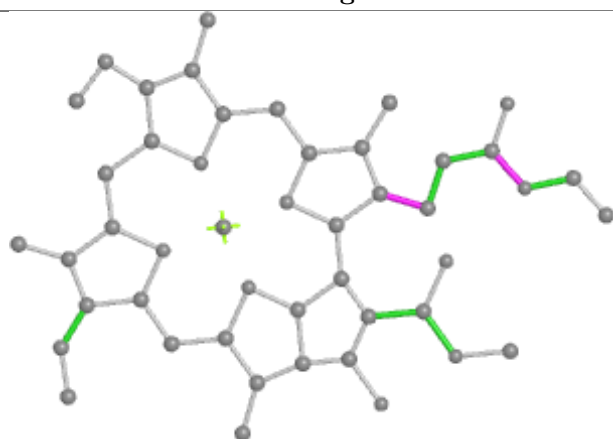
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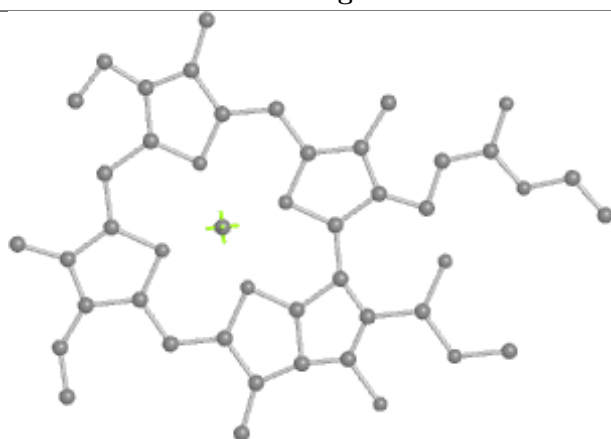
Bond lengths



Bond angles

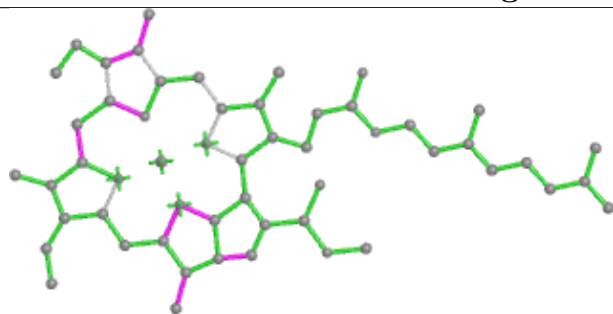


Torsions

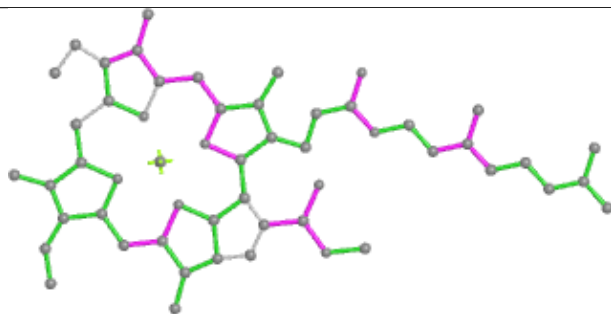


Rings

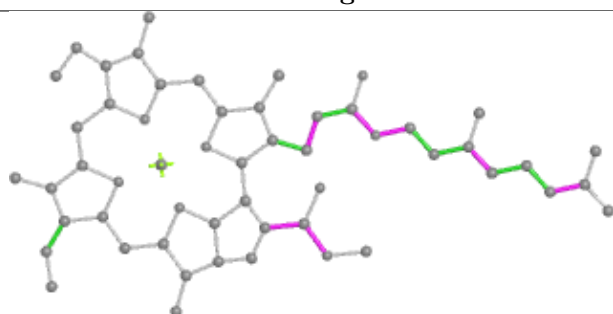
## Ligand CLA BA 838



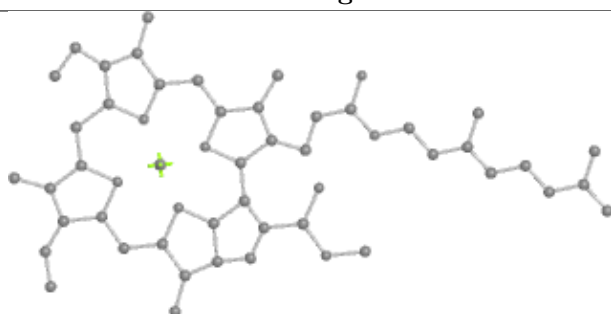
Bond lengths



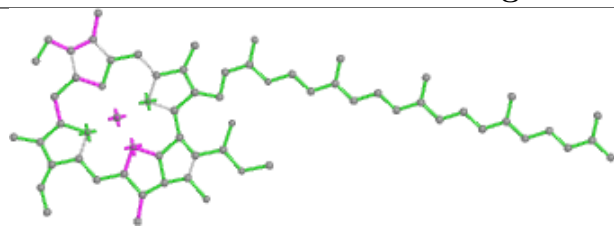
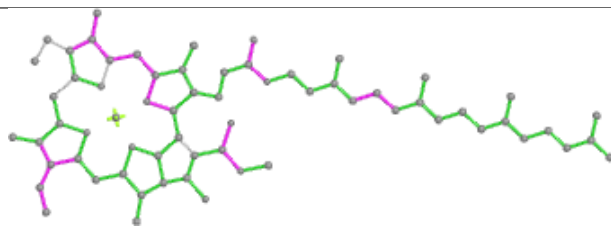
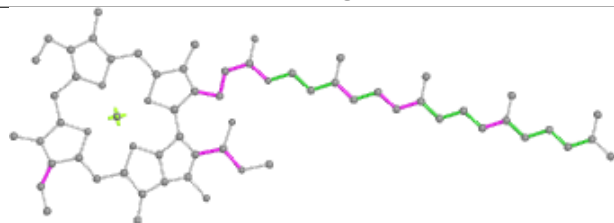
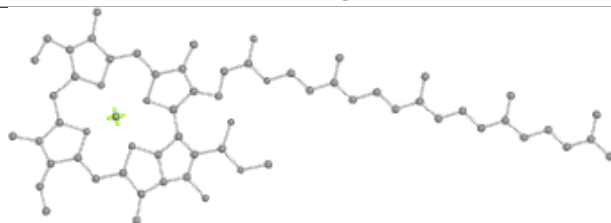
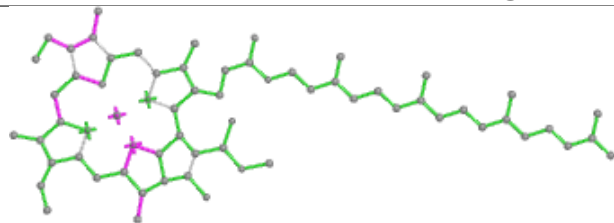
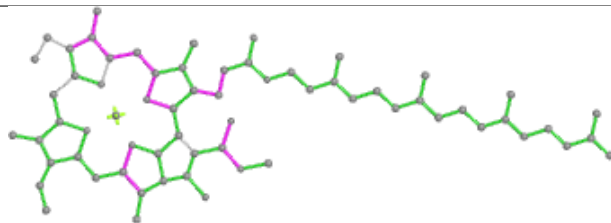
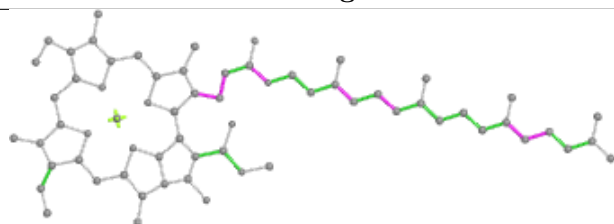
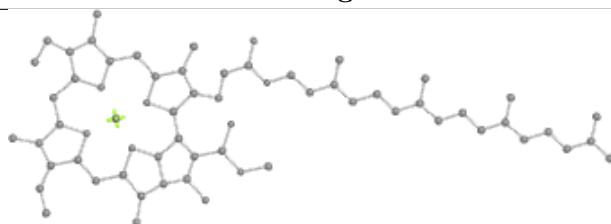
Bond angles



Torsions

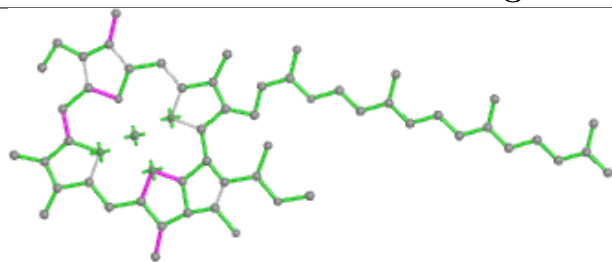


Rings

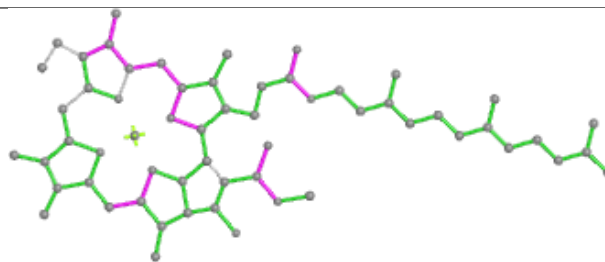
**Ligand CLA BB 815****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA BB 830****Bond lengths****Bond angles****Torsions****Rings**



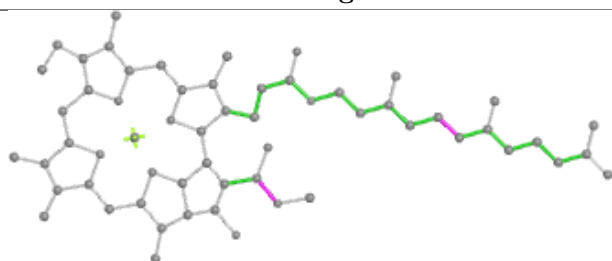
## Ligand CLA B1 311



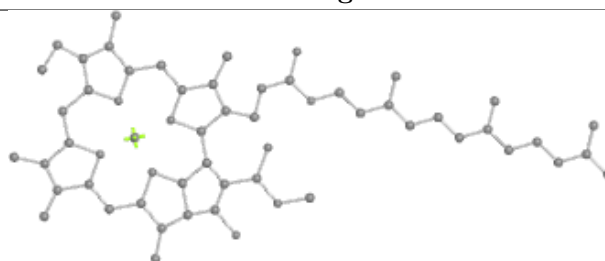
Bond lengths



Bond angles

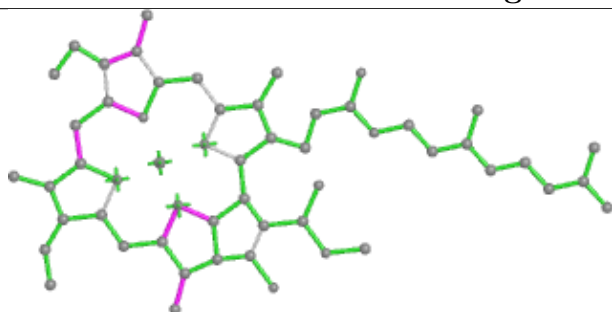


Torsions

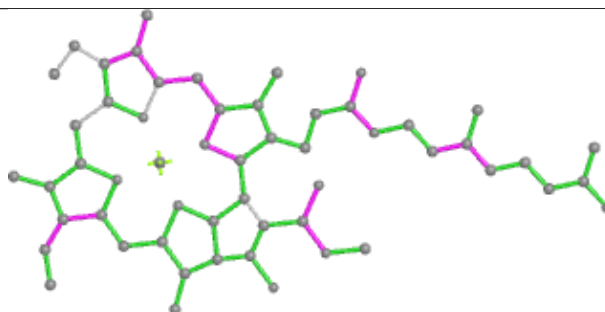


Rings

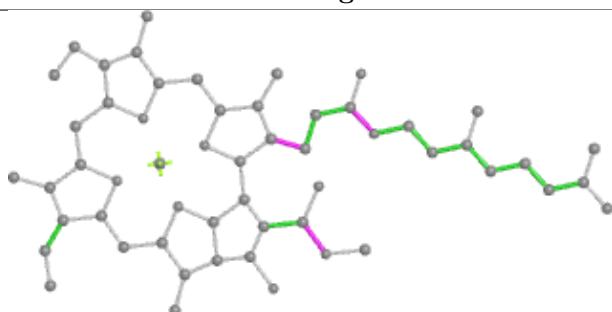
## Ligand CLA B3 603



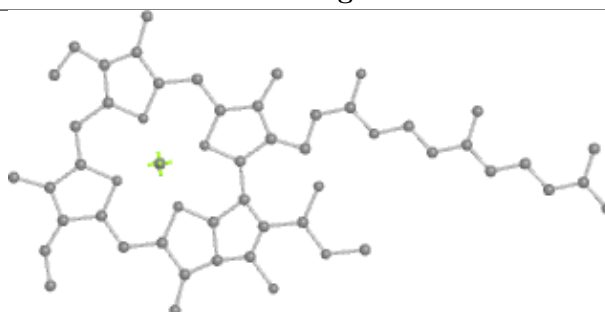
Bond lengths



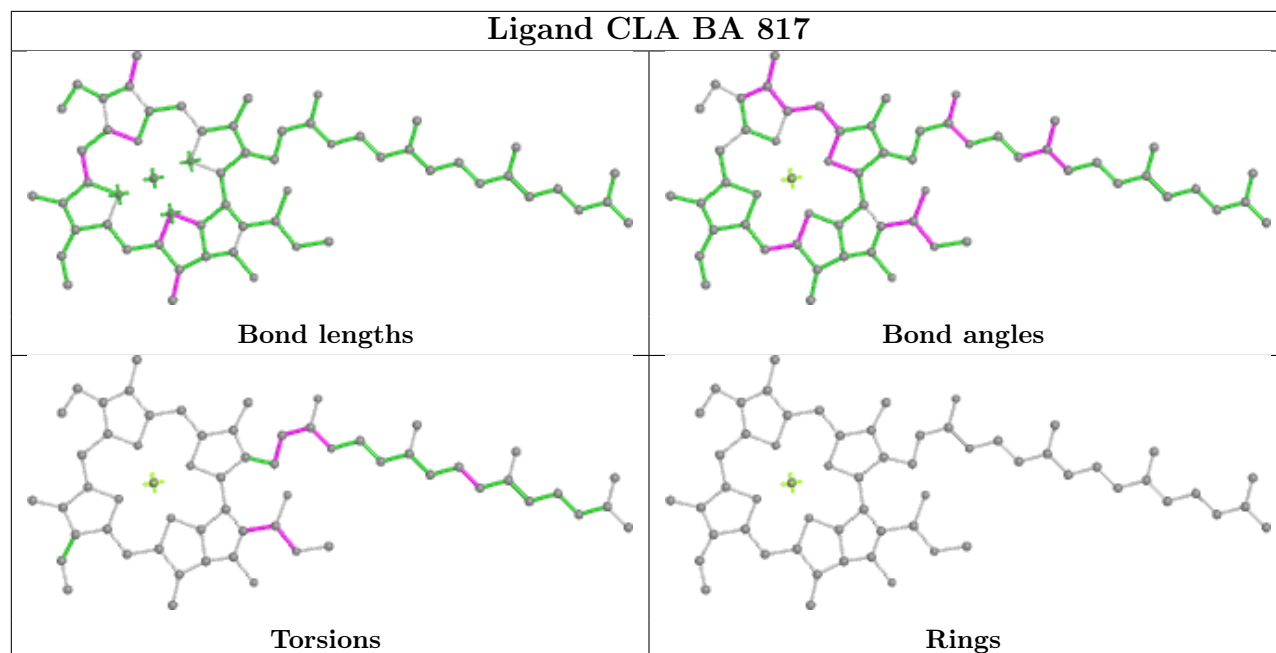
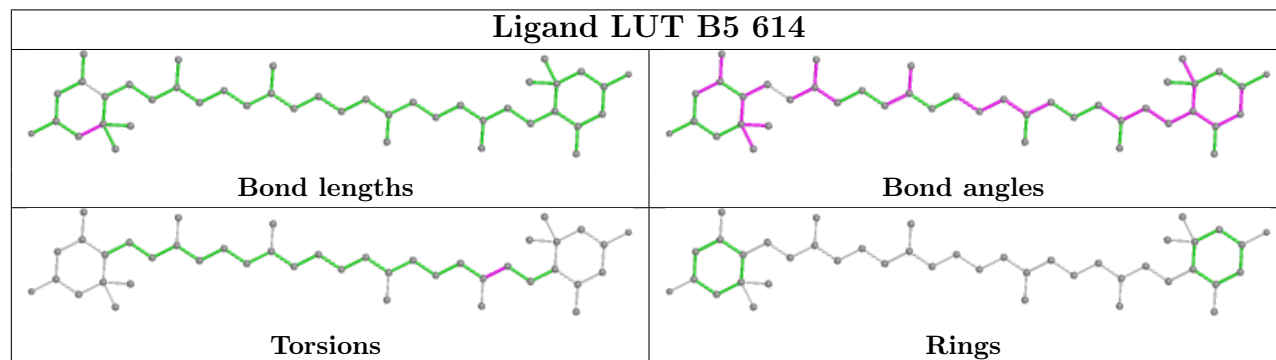
Bond angles

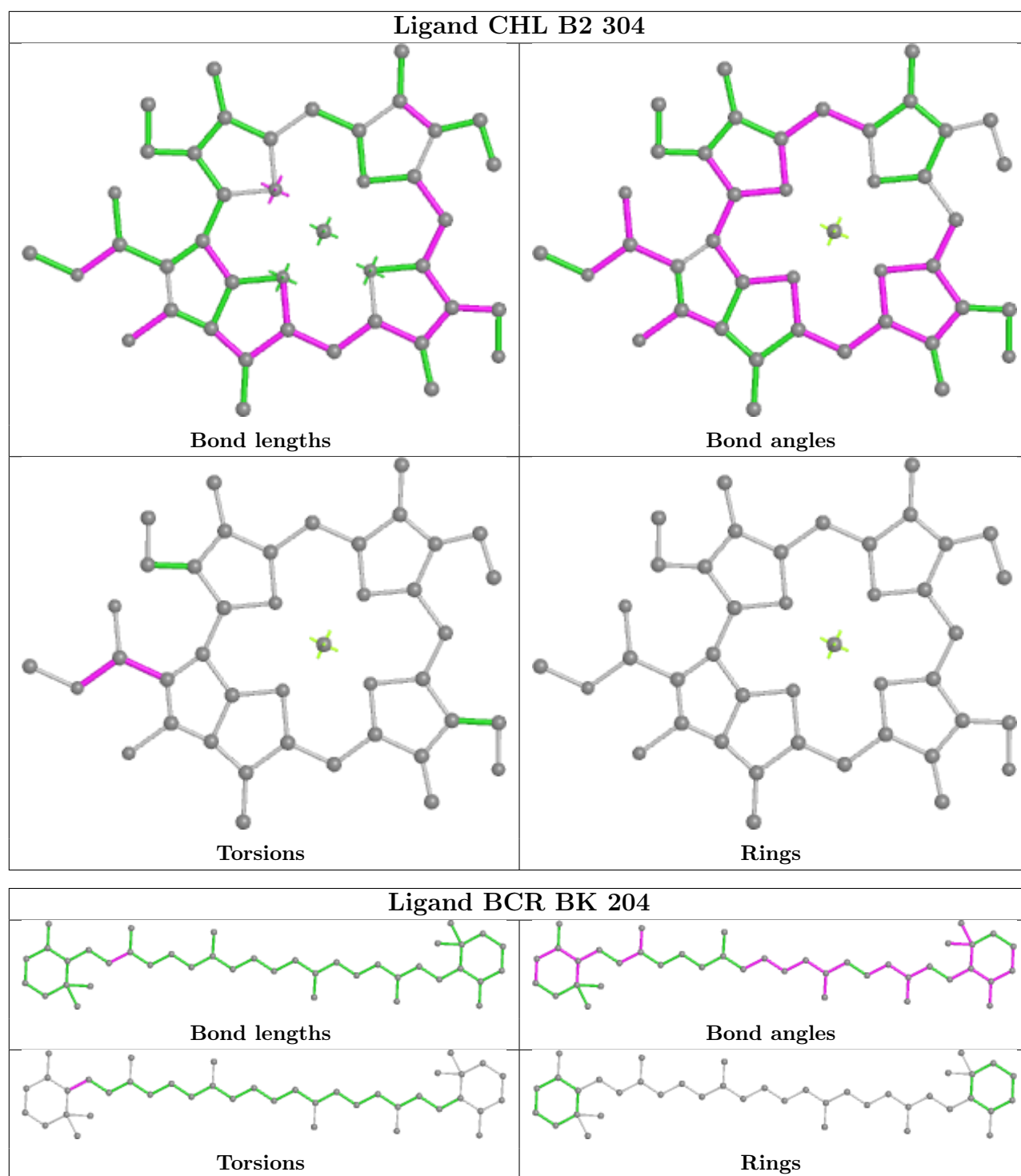


Torsions

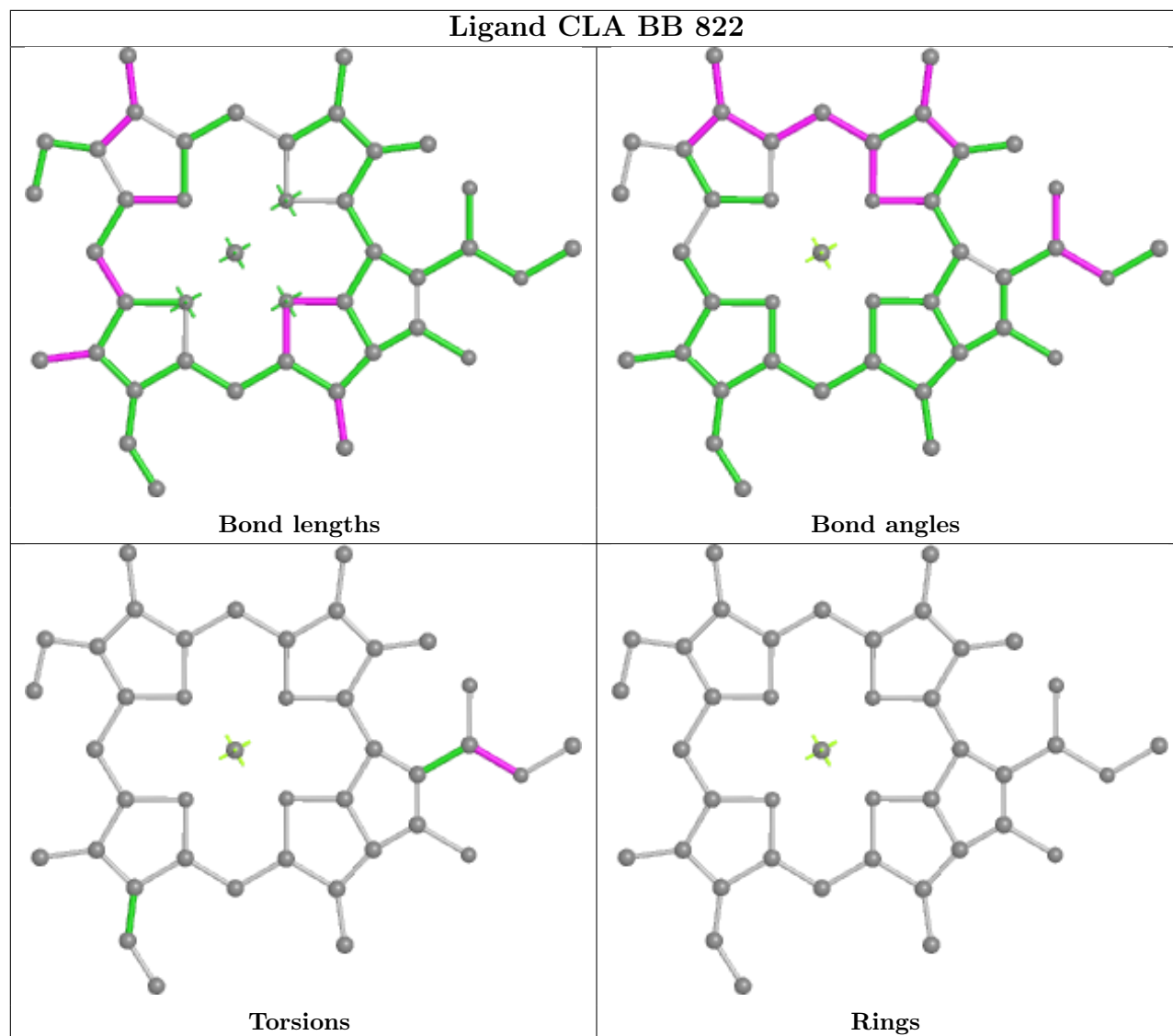


Rings

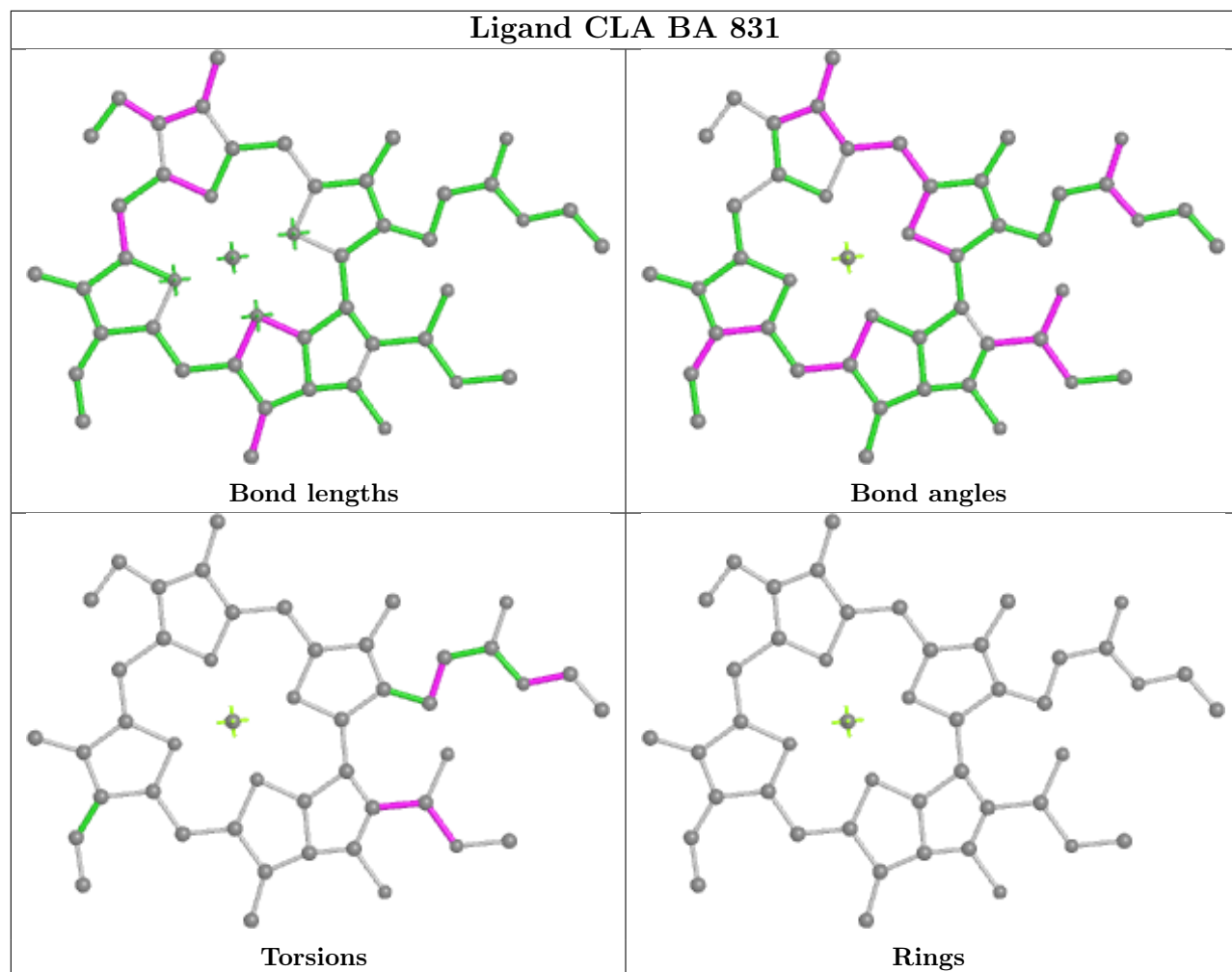
**Ligand CLA BA 817****Ligand LUT B5 614**



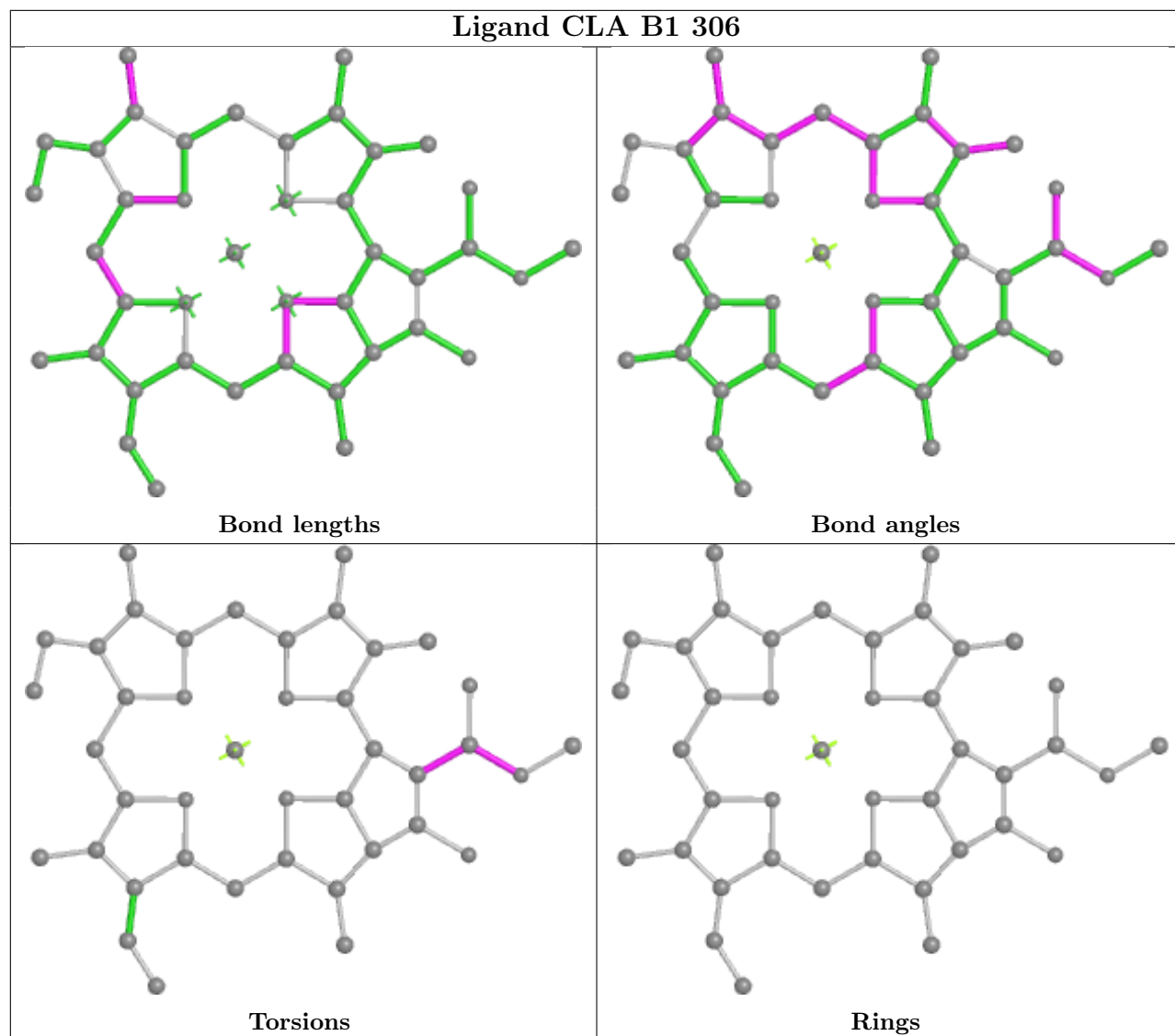
## Ligand CLA BB 822



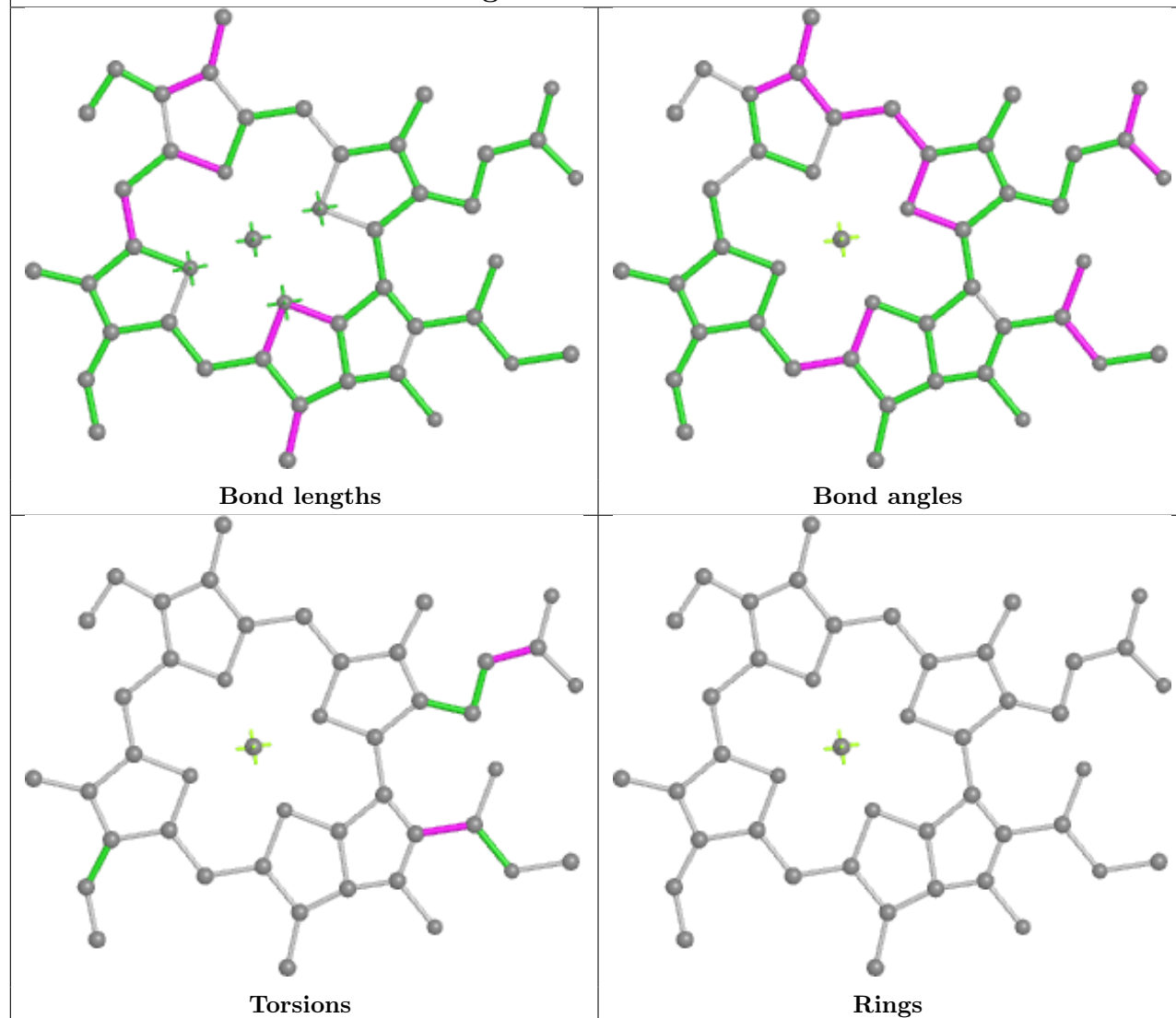
## Ligand CLA BA 831



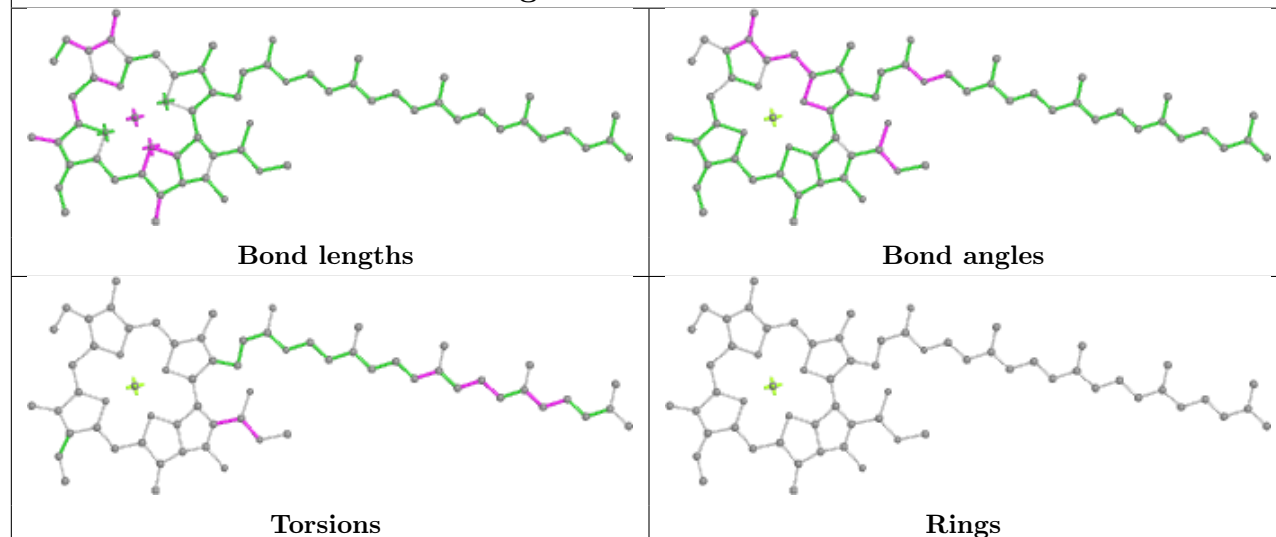
## Ligand CLA B1 306



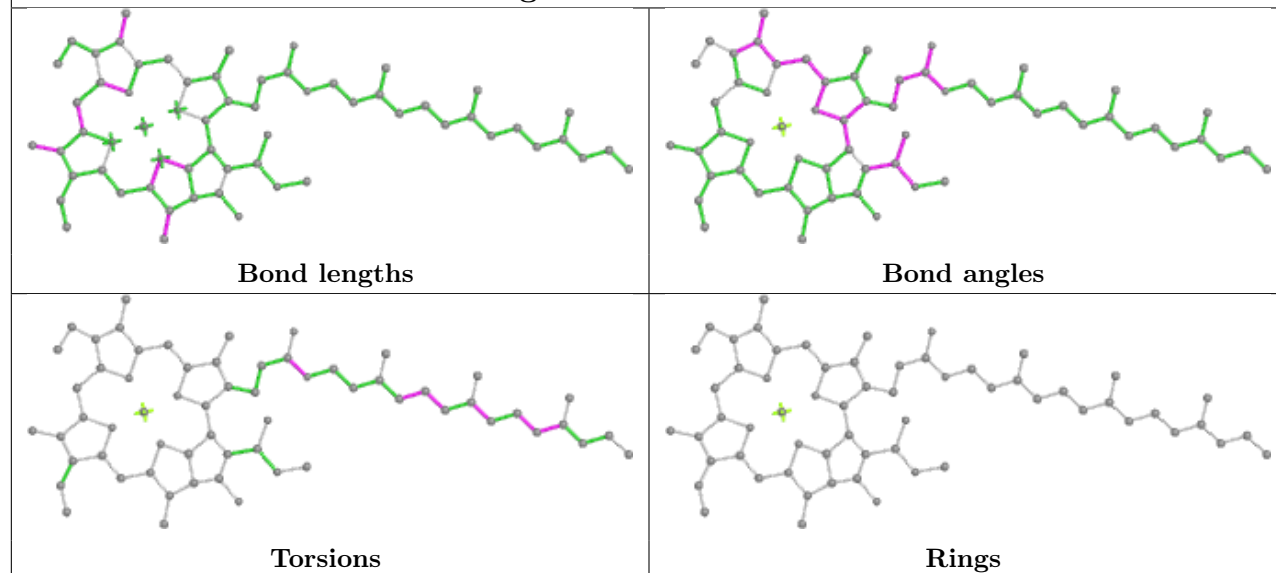
## Ligand CLA B2 307



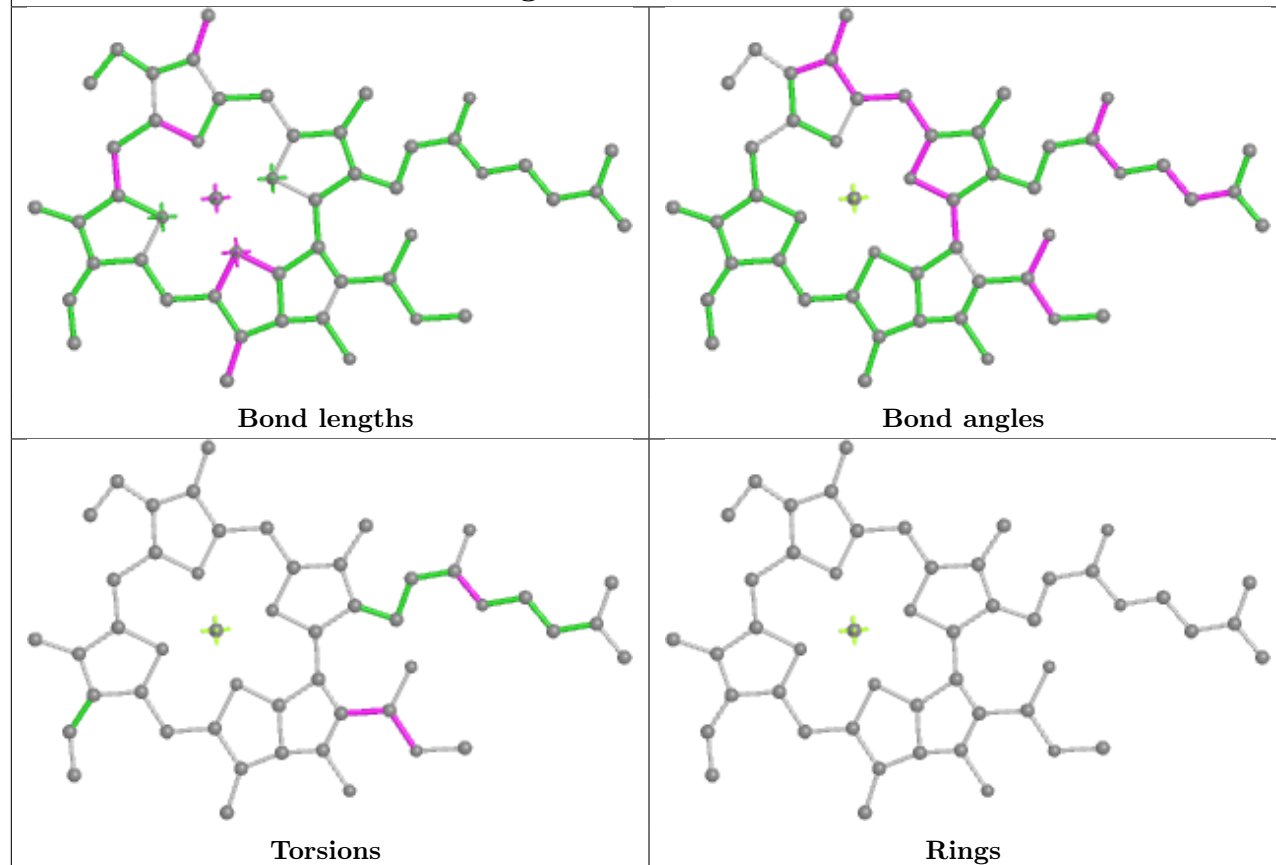
## Ligand CLA BB 826



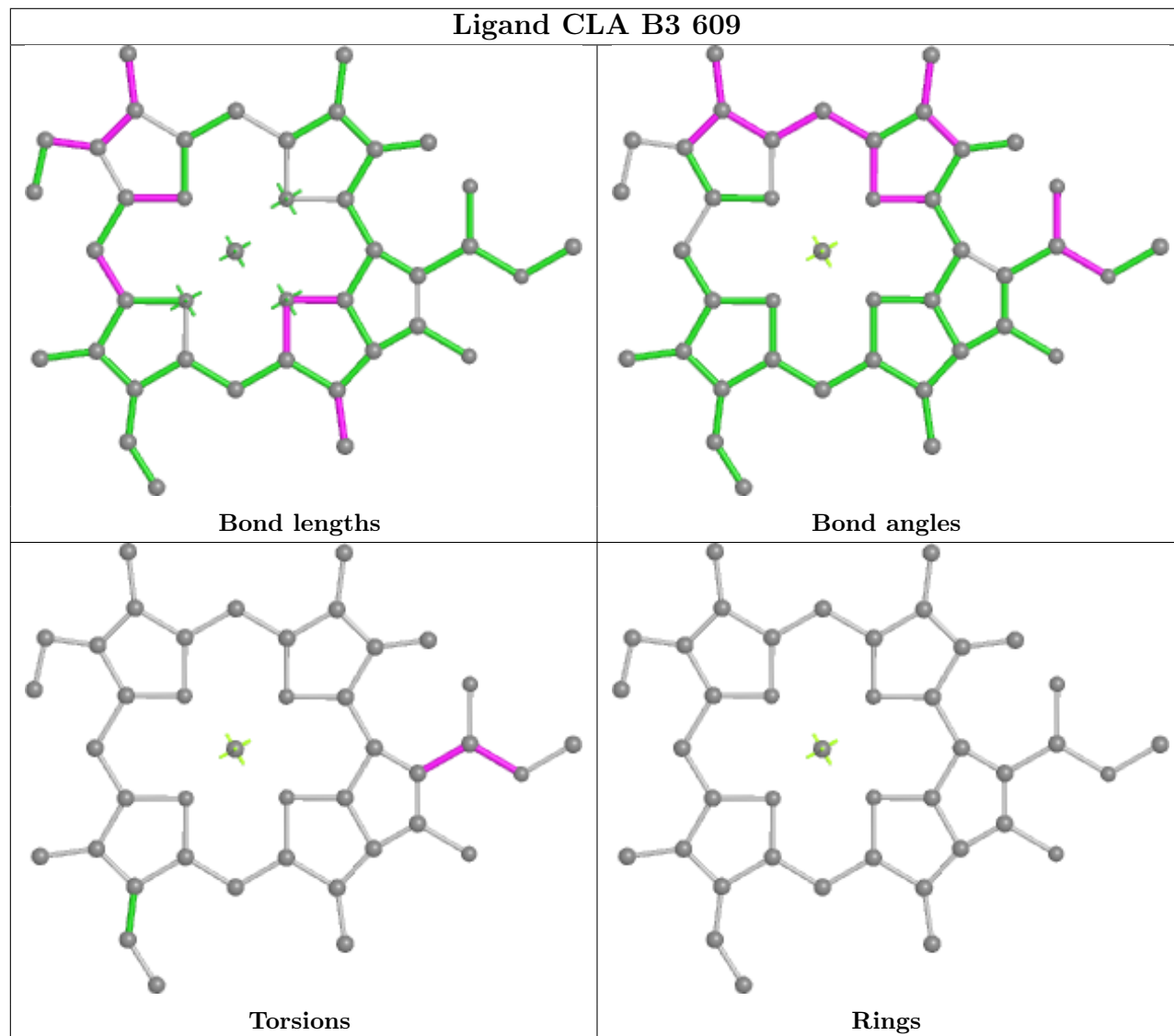
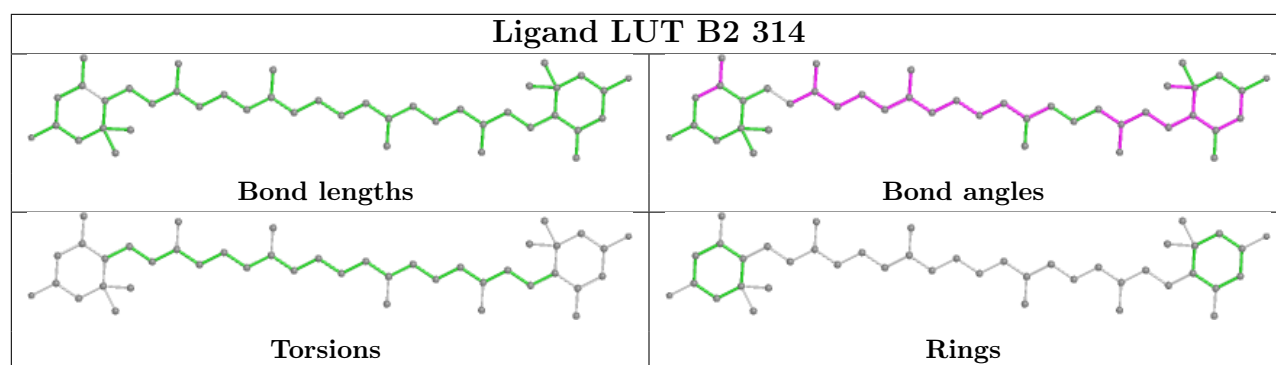
## Ligand CLA BB 828

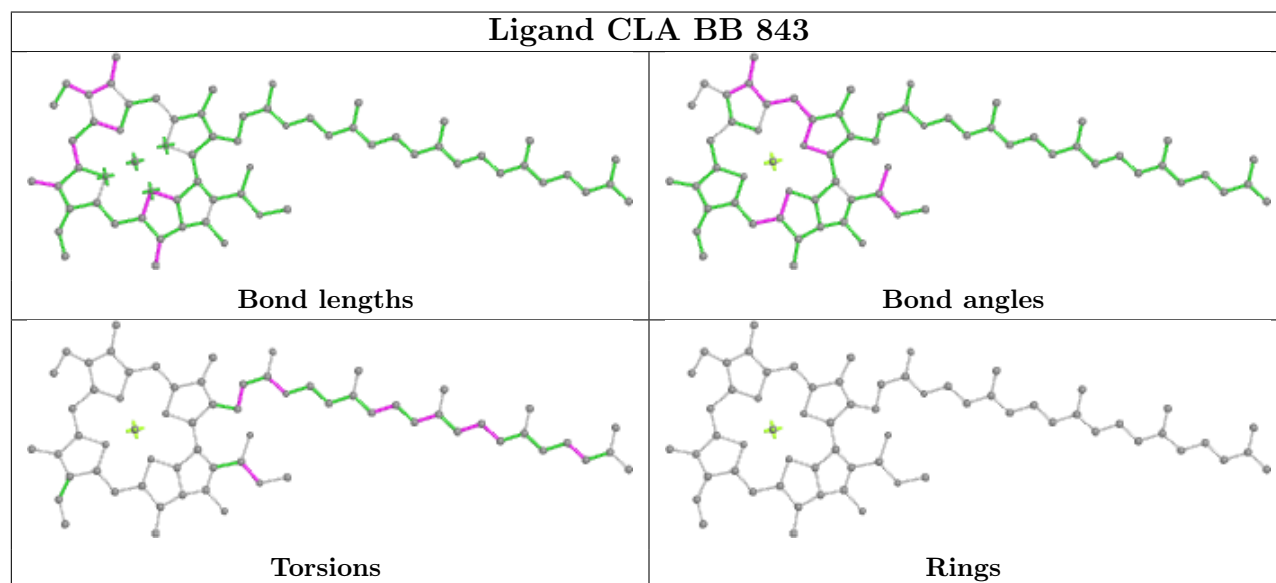
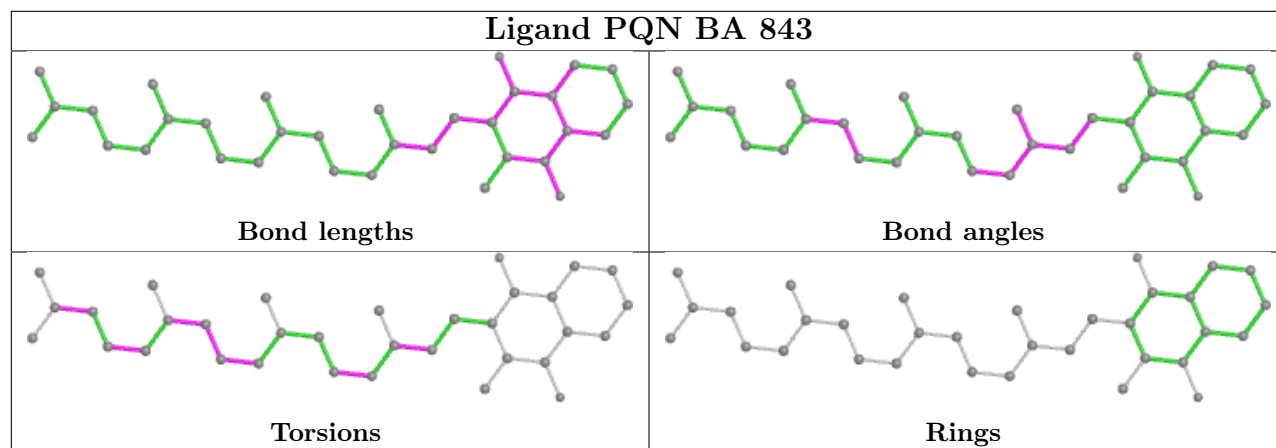
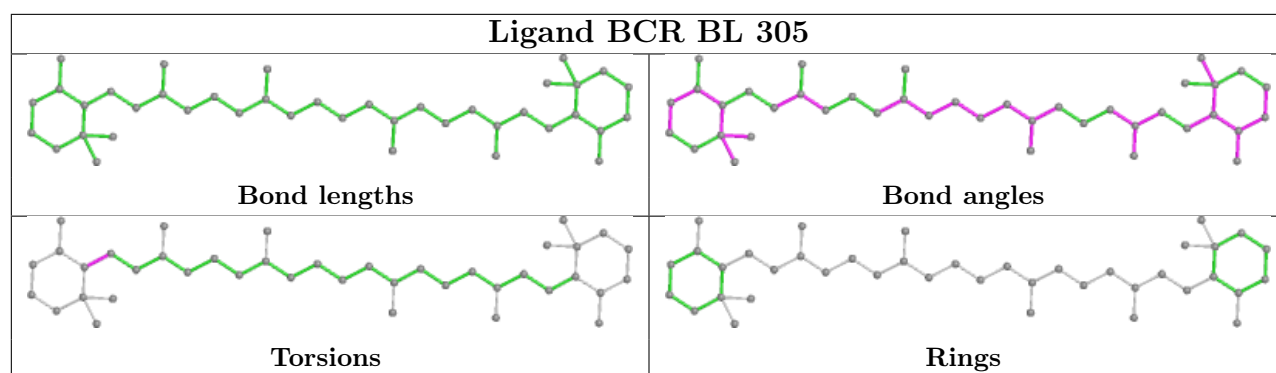


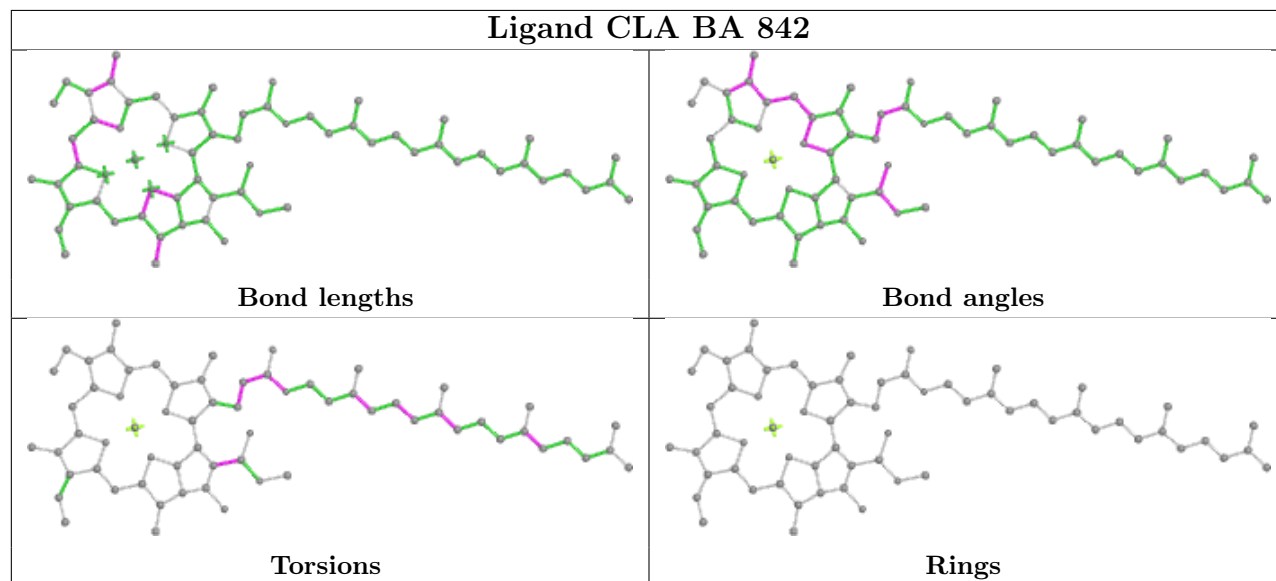
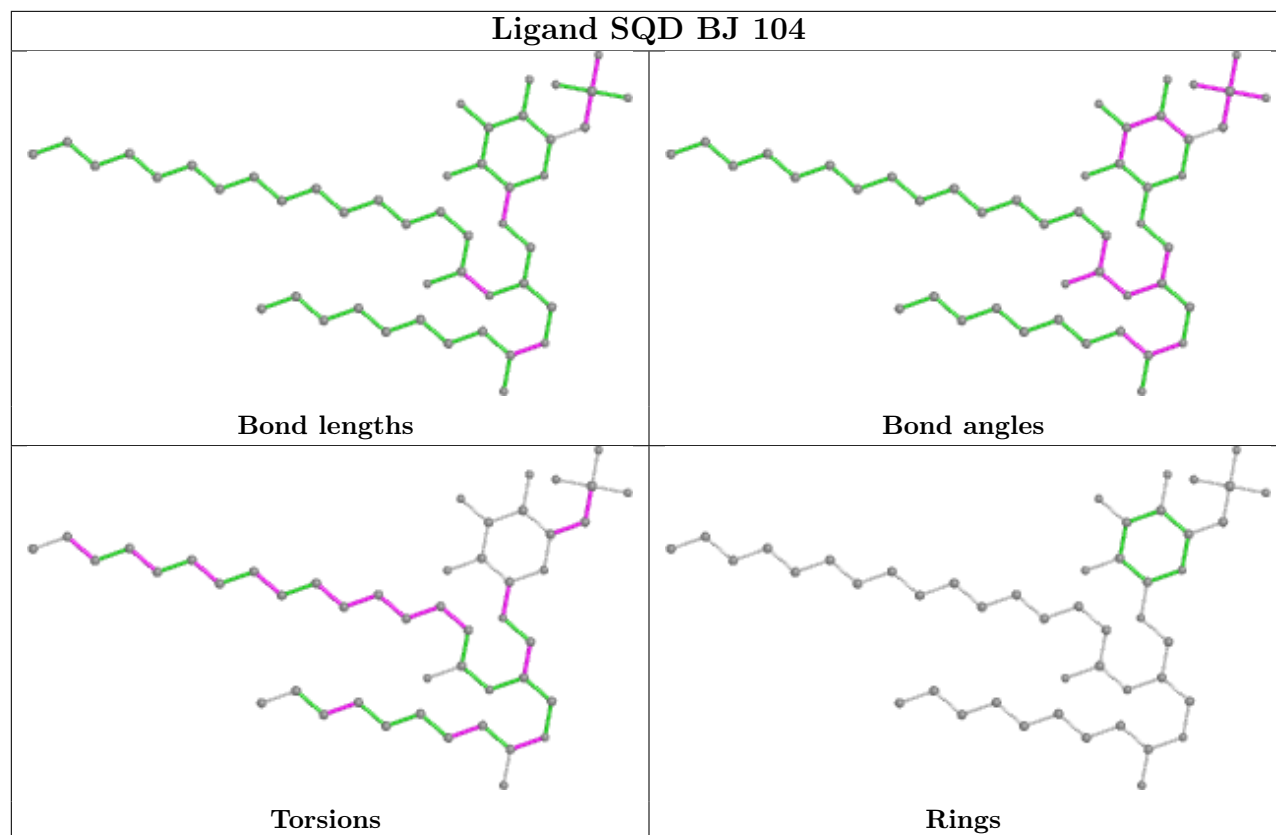
## Ligand CLA BB 838

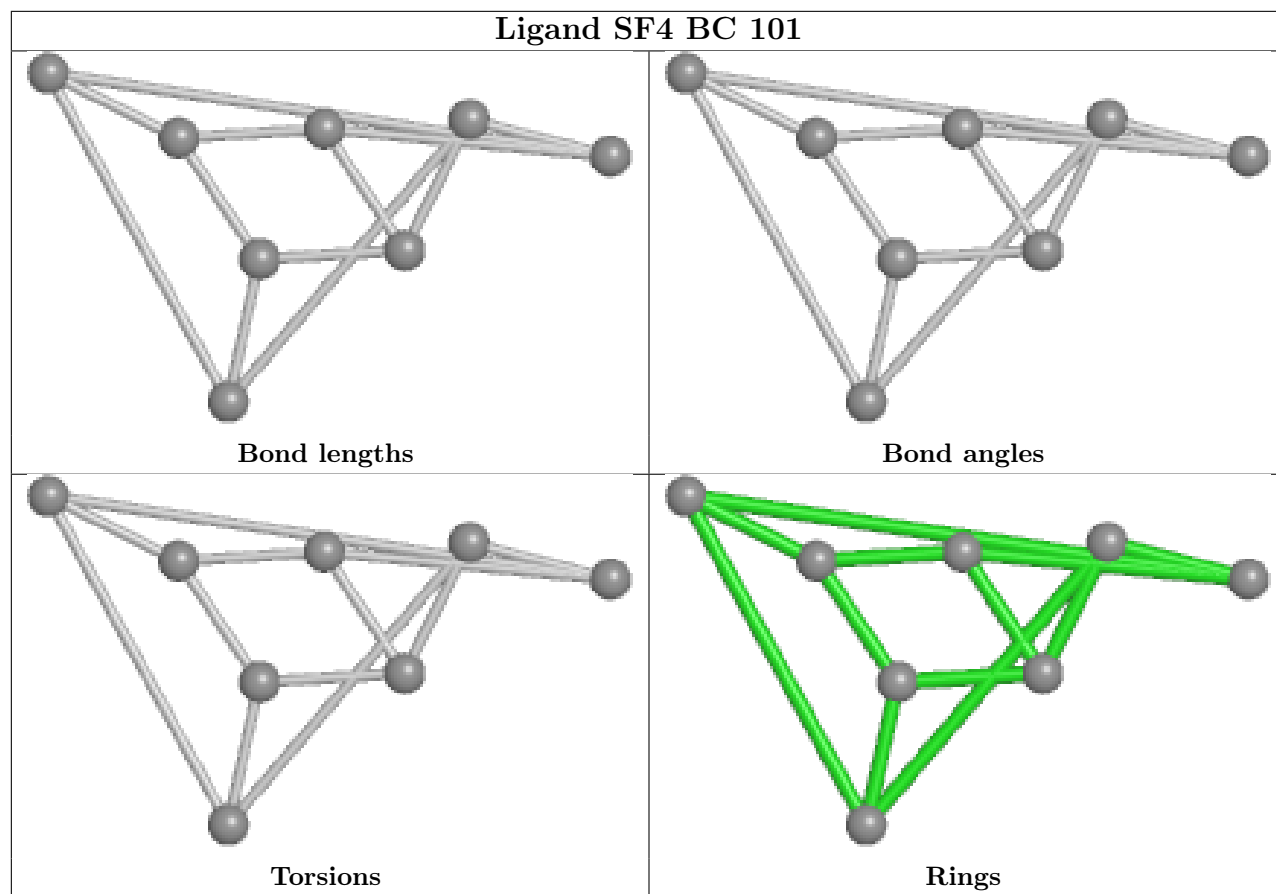
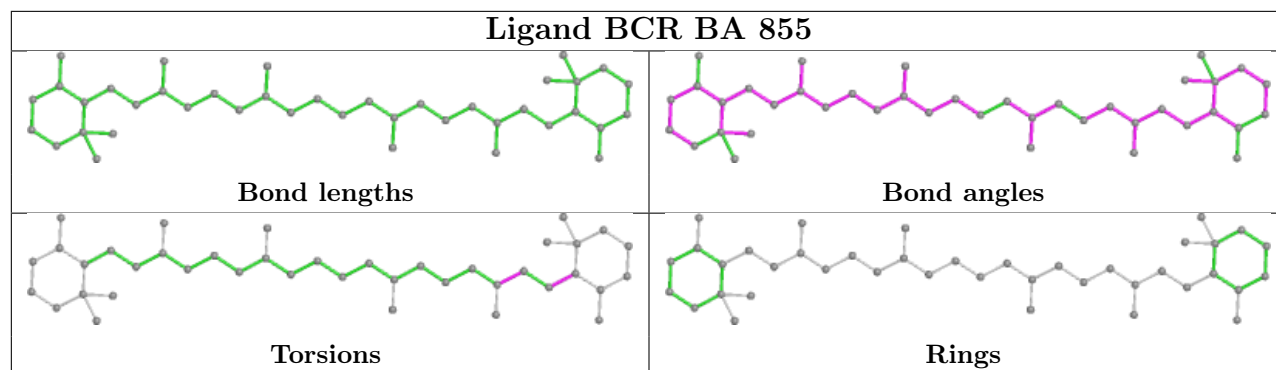




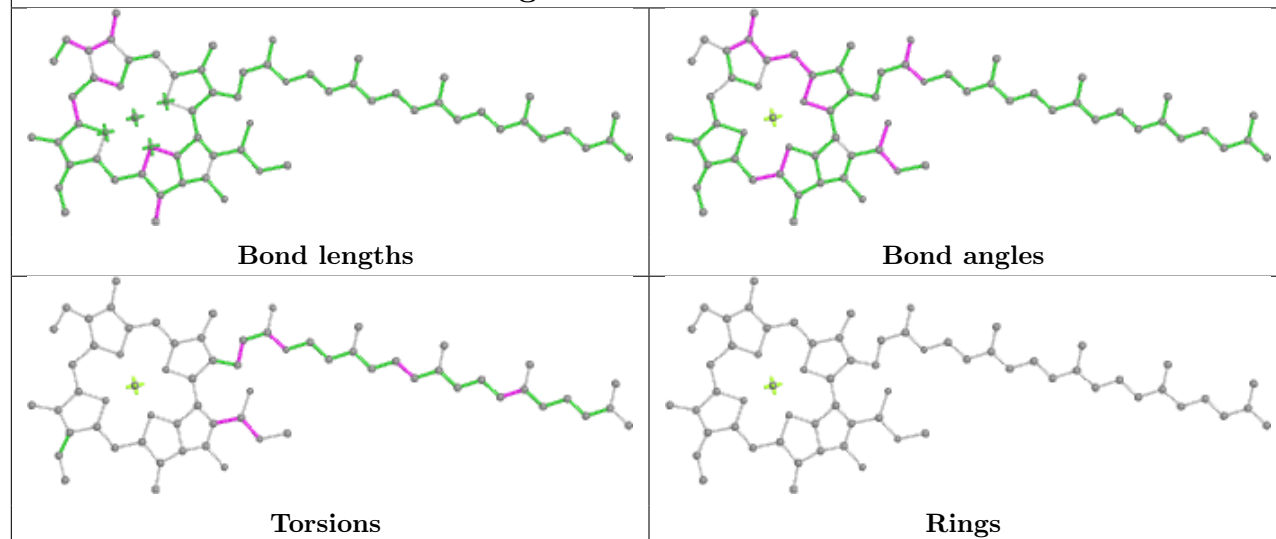




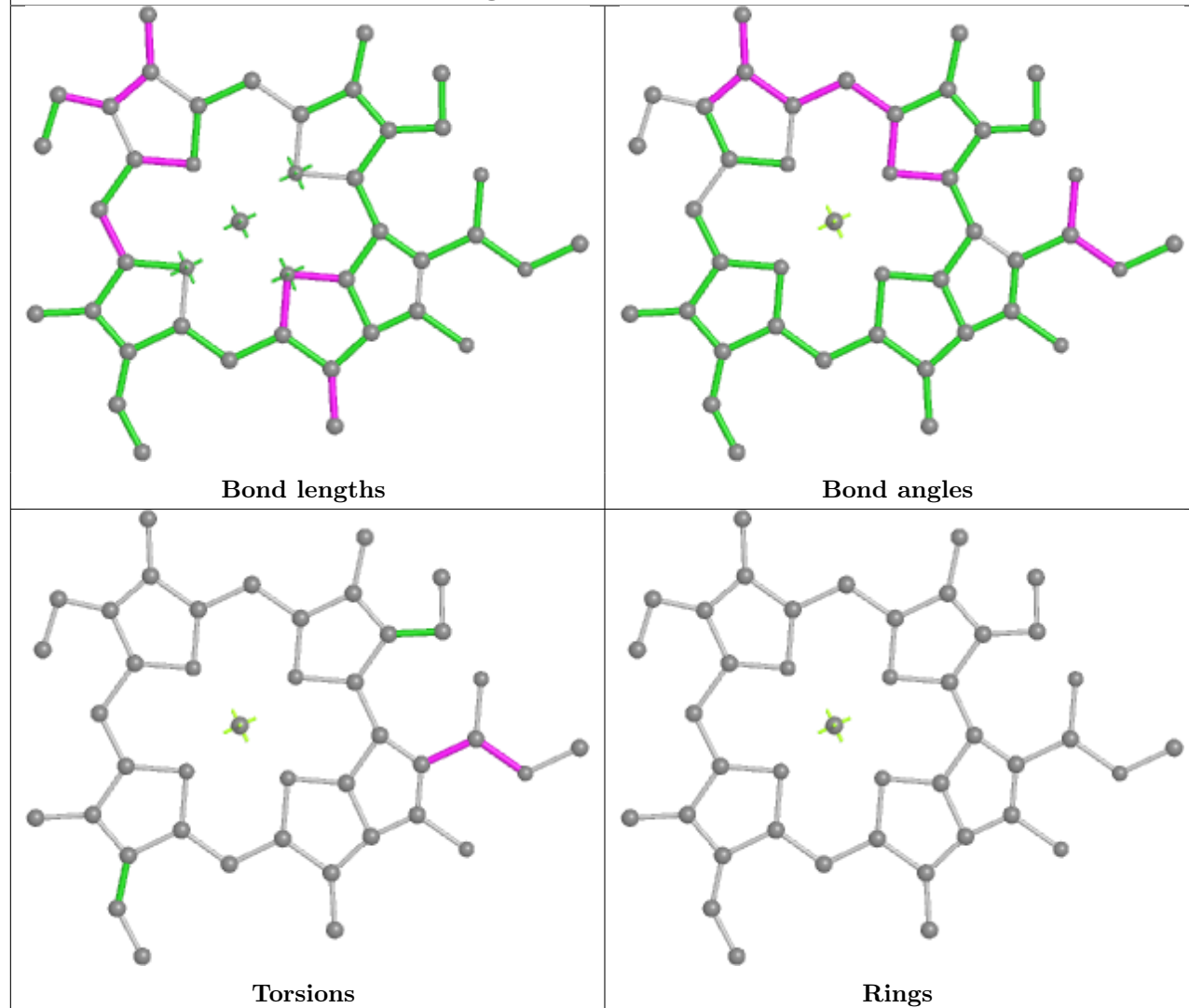




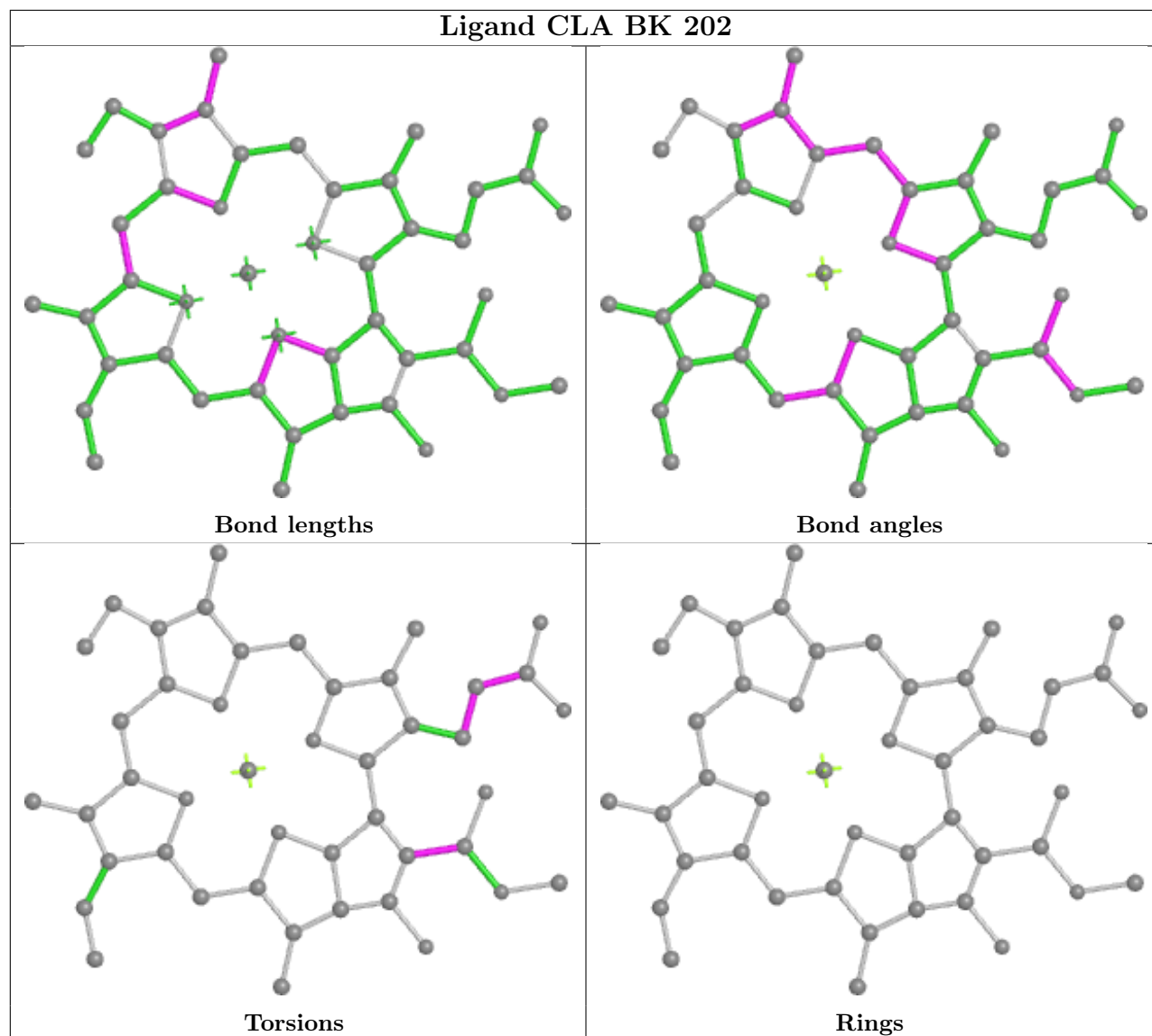
## Ligand CLA BA 808



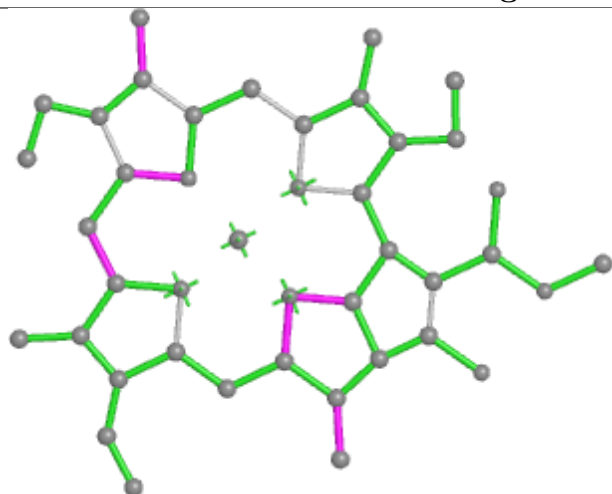
## Ligand CLA BA 815



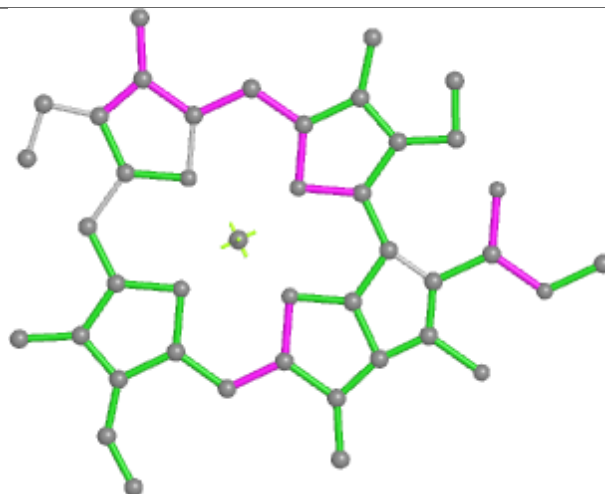
## Ligand CLA BK 202



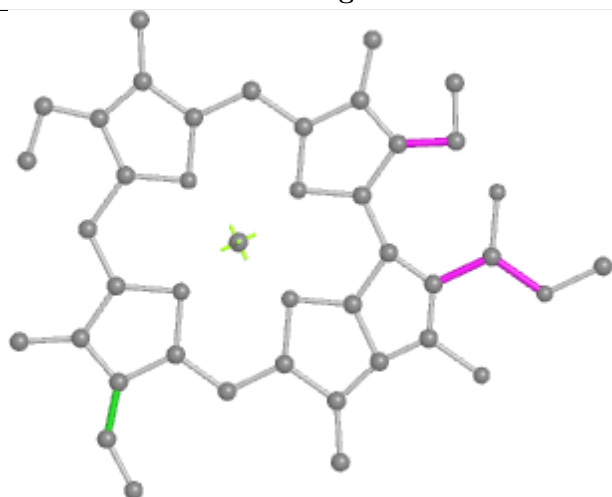
## Ligand CLA BA 822



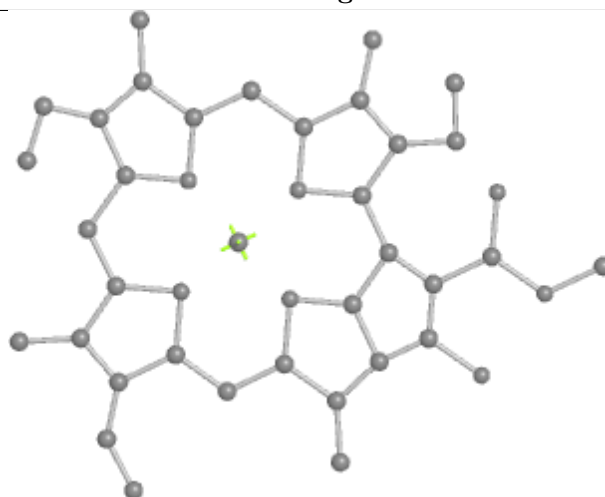
Bond lengths



Bond angles

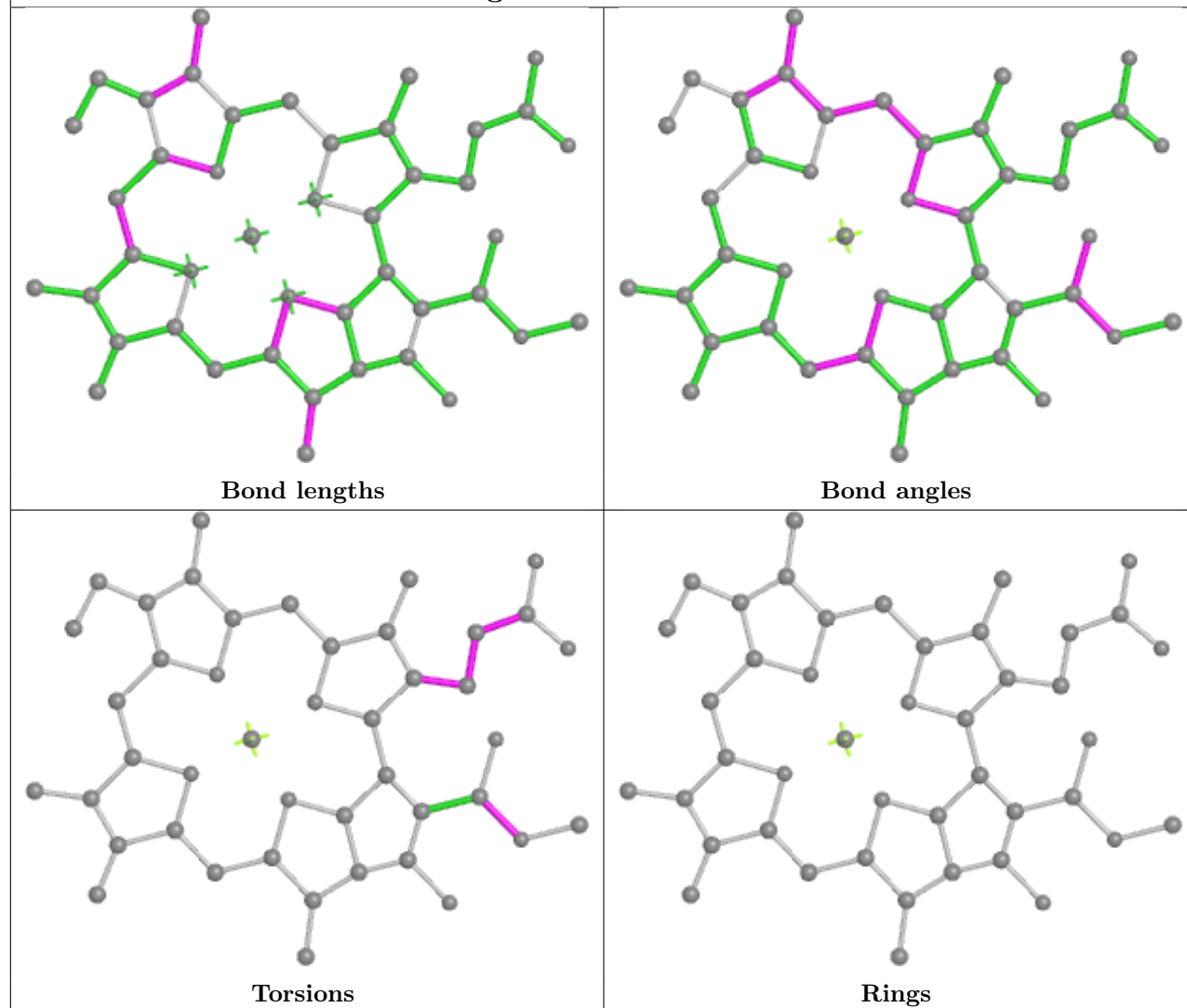


Torsions

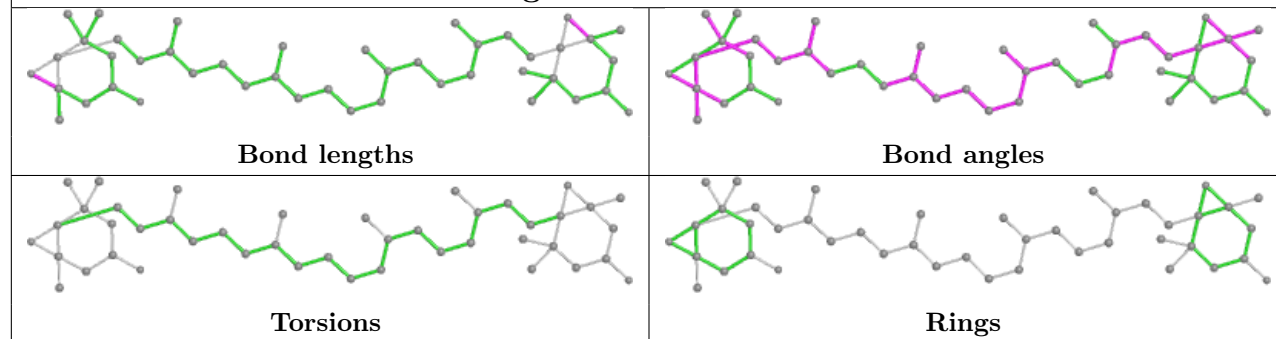


Rings

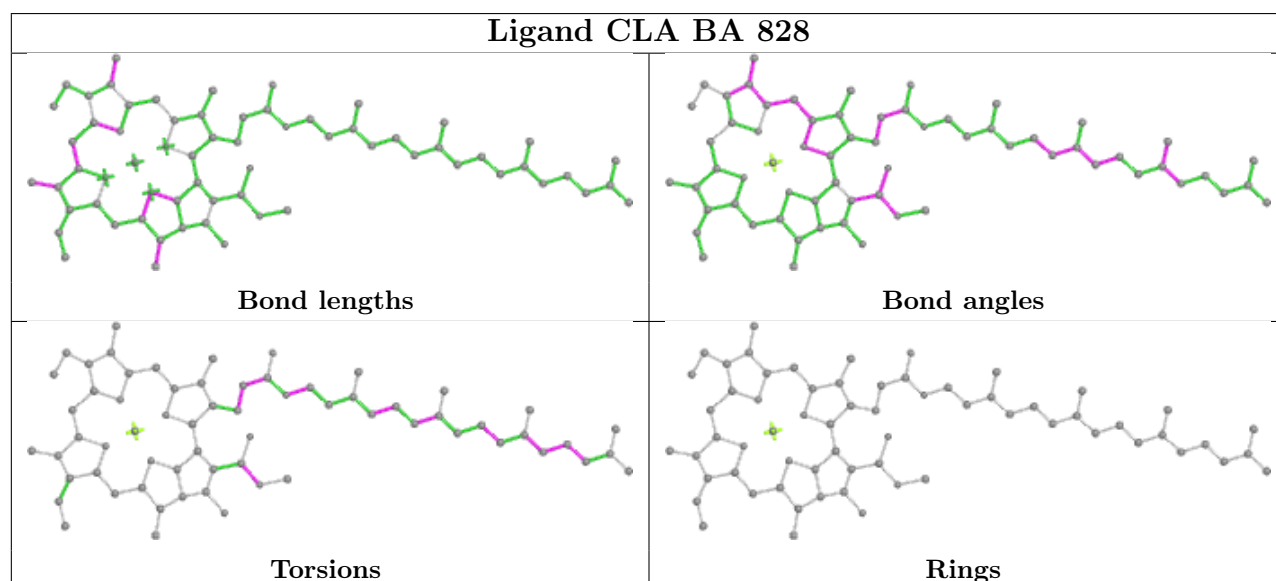
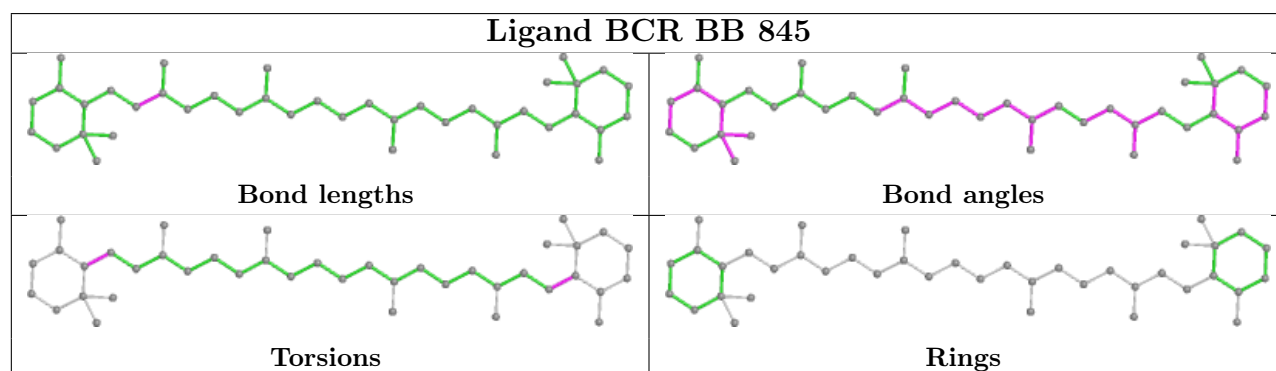
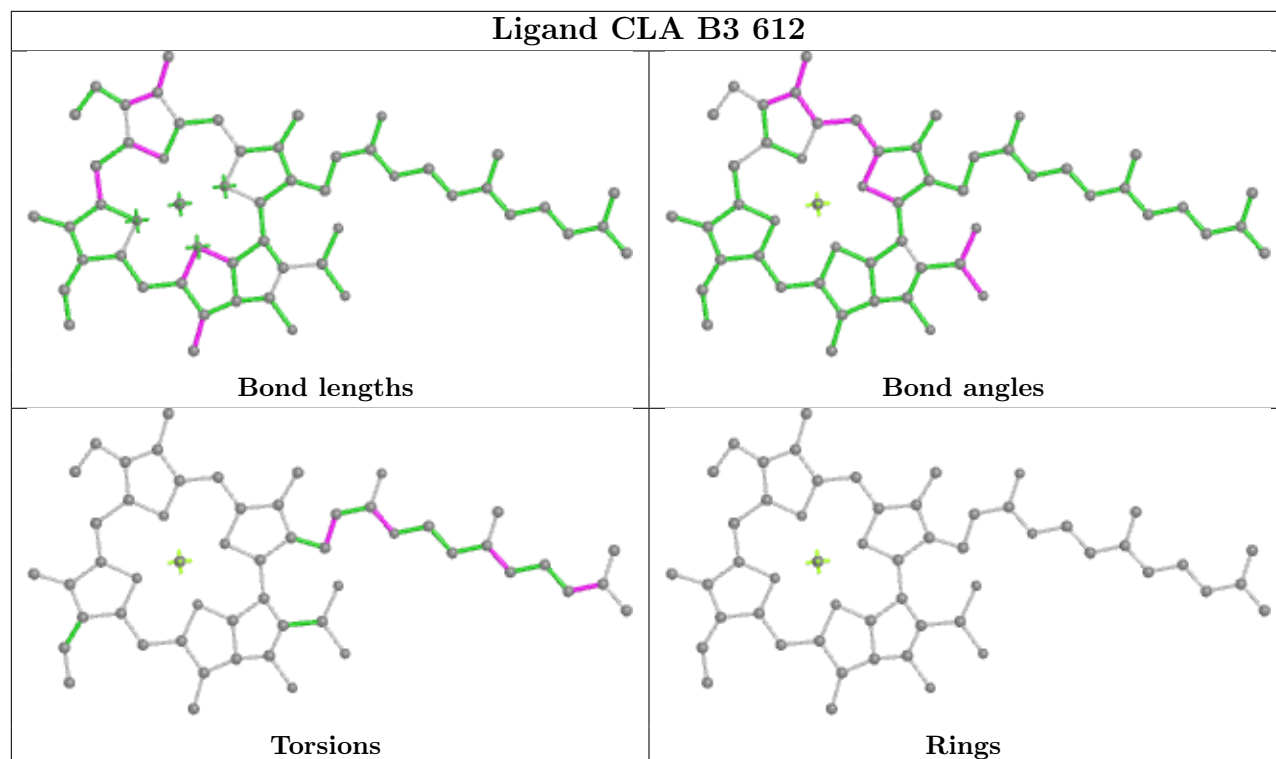
## Ligand CLA B2 310

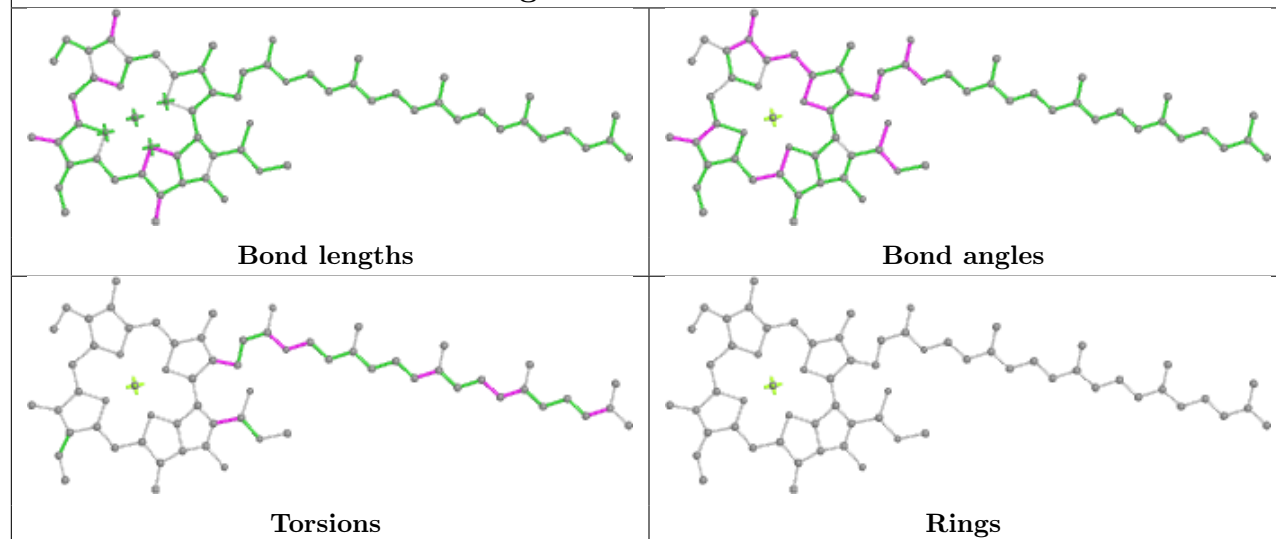
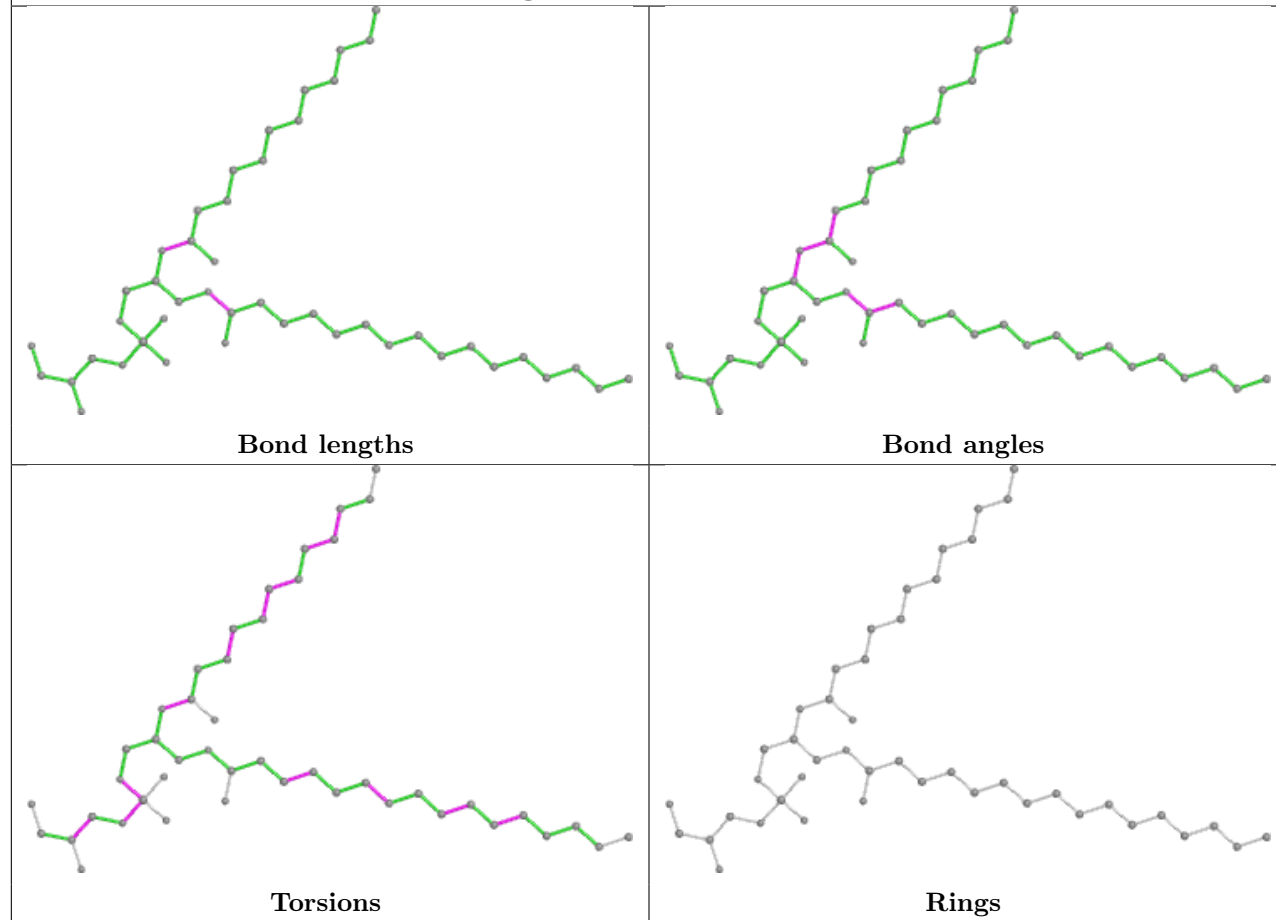


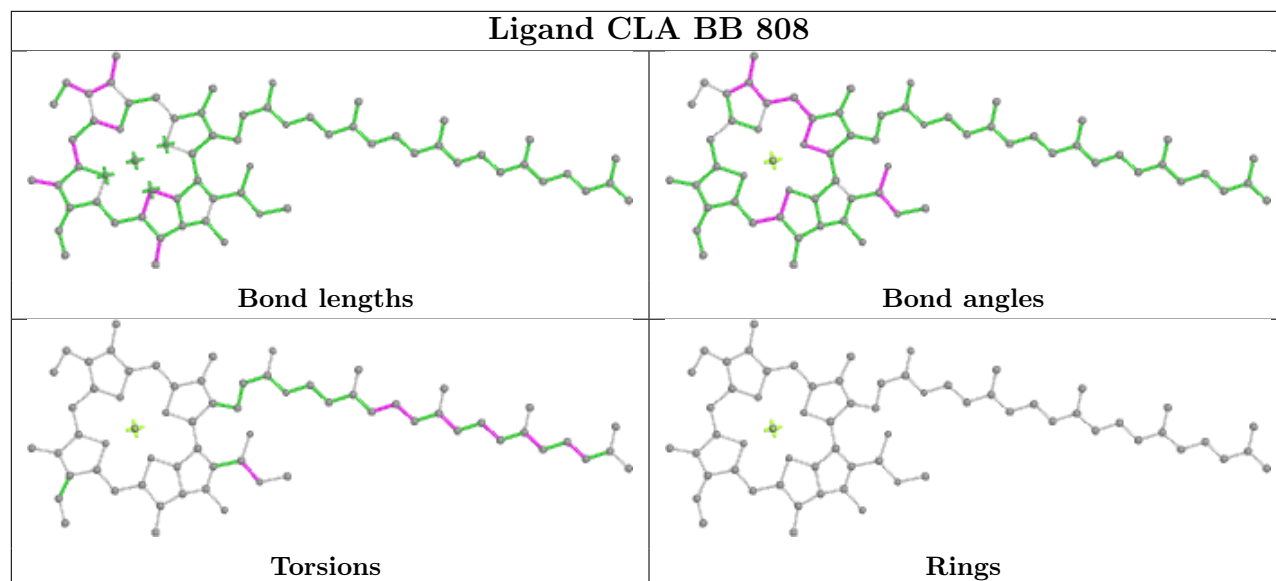
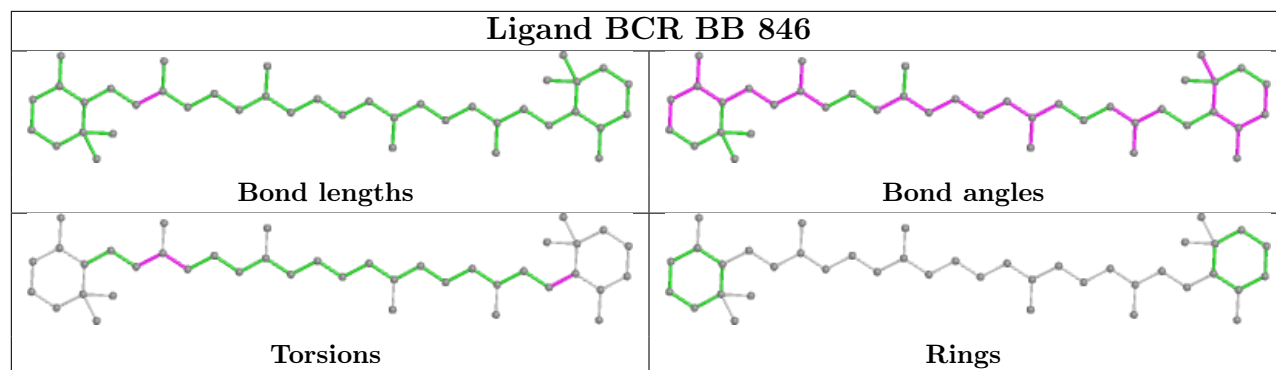
## Ligand XAT B1 317

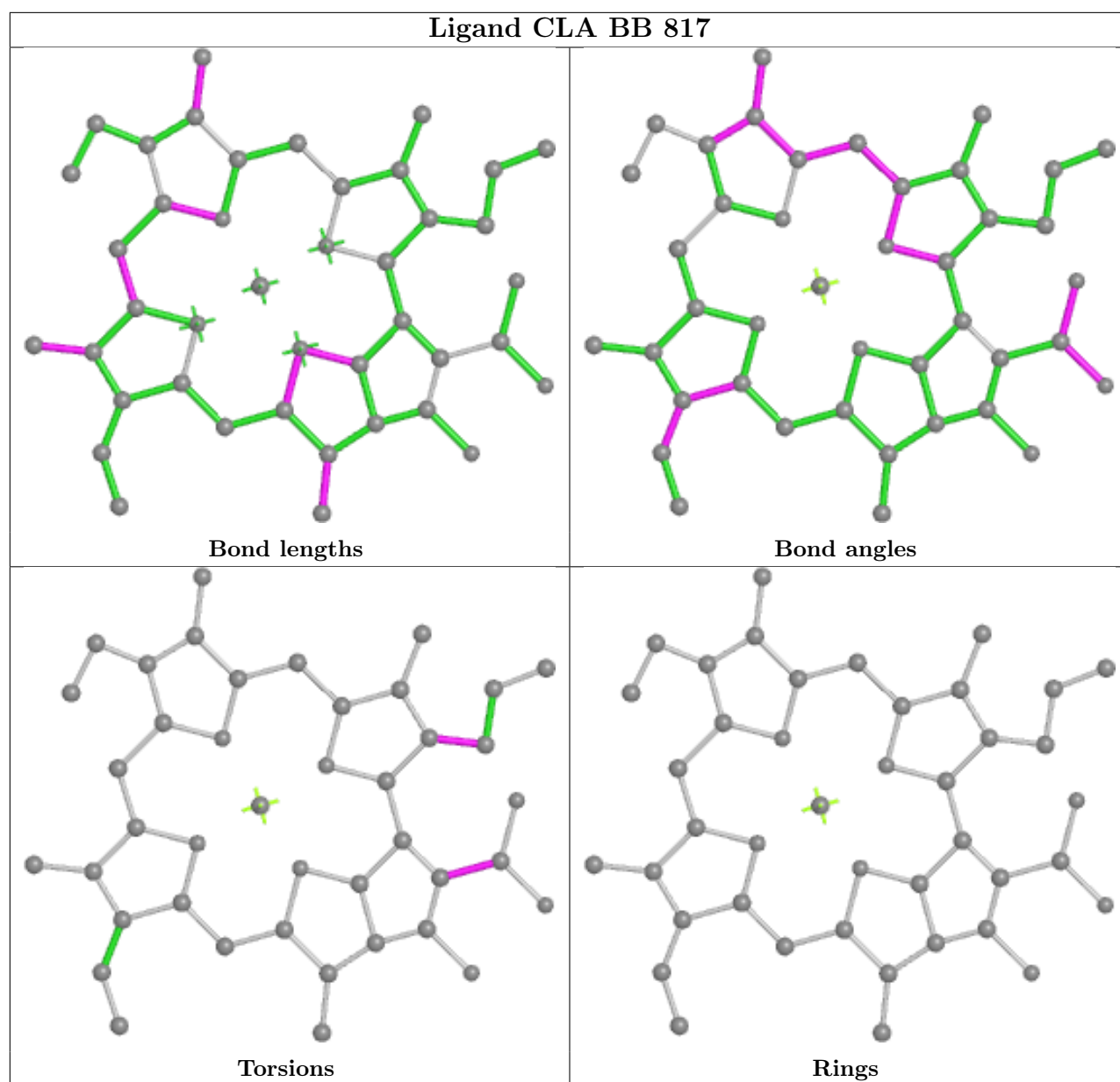


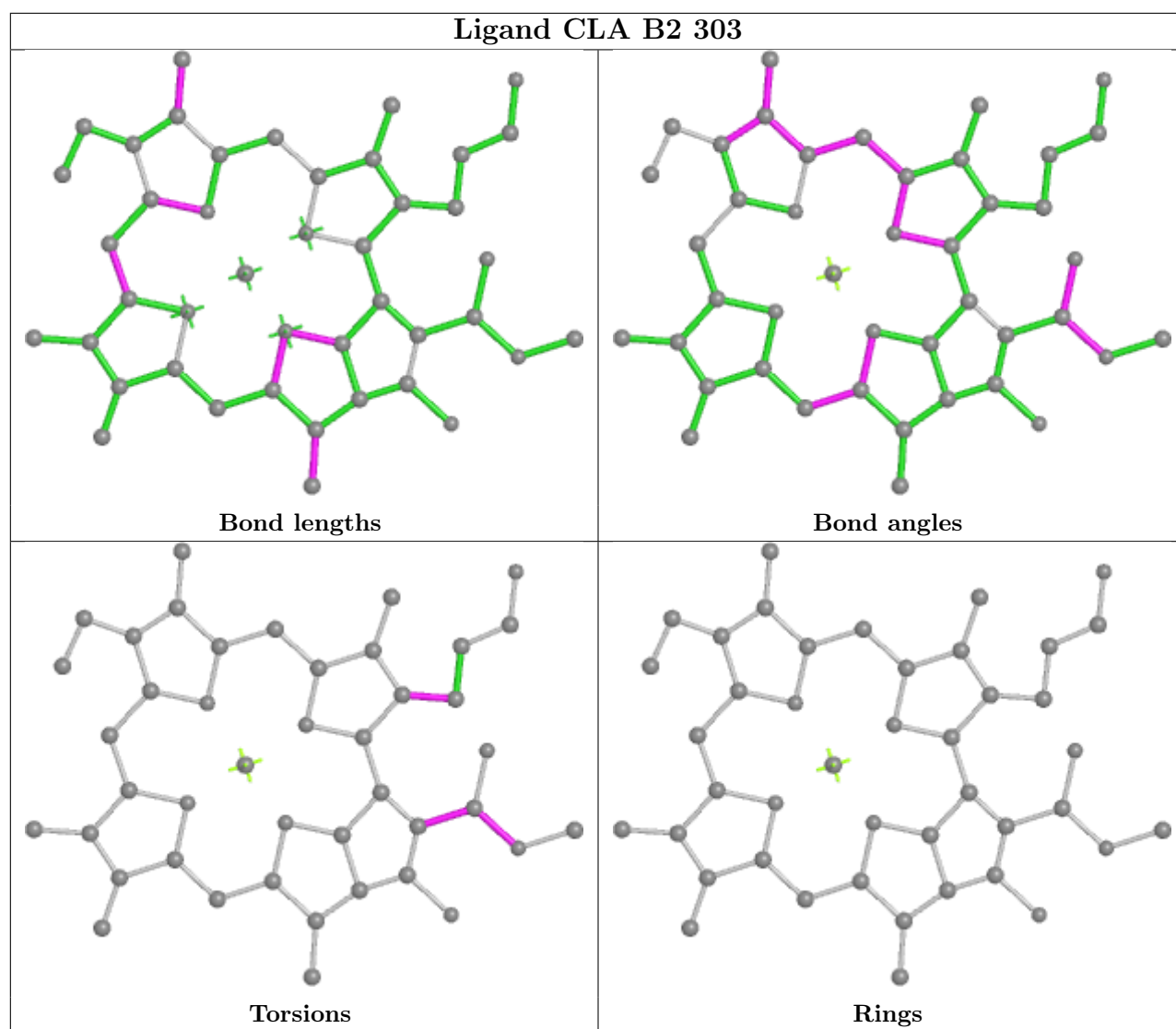


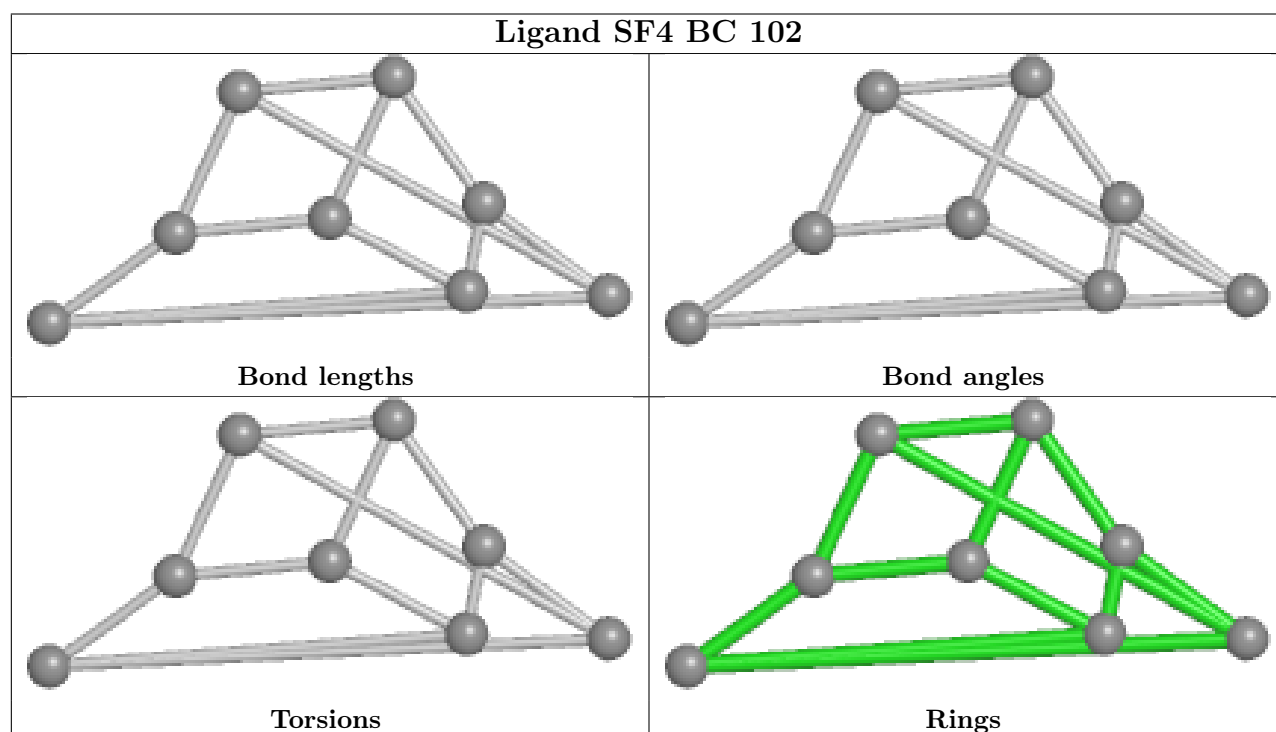
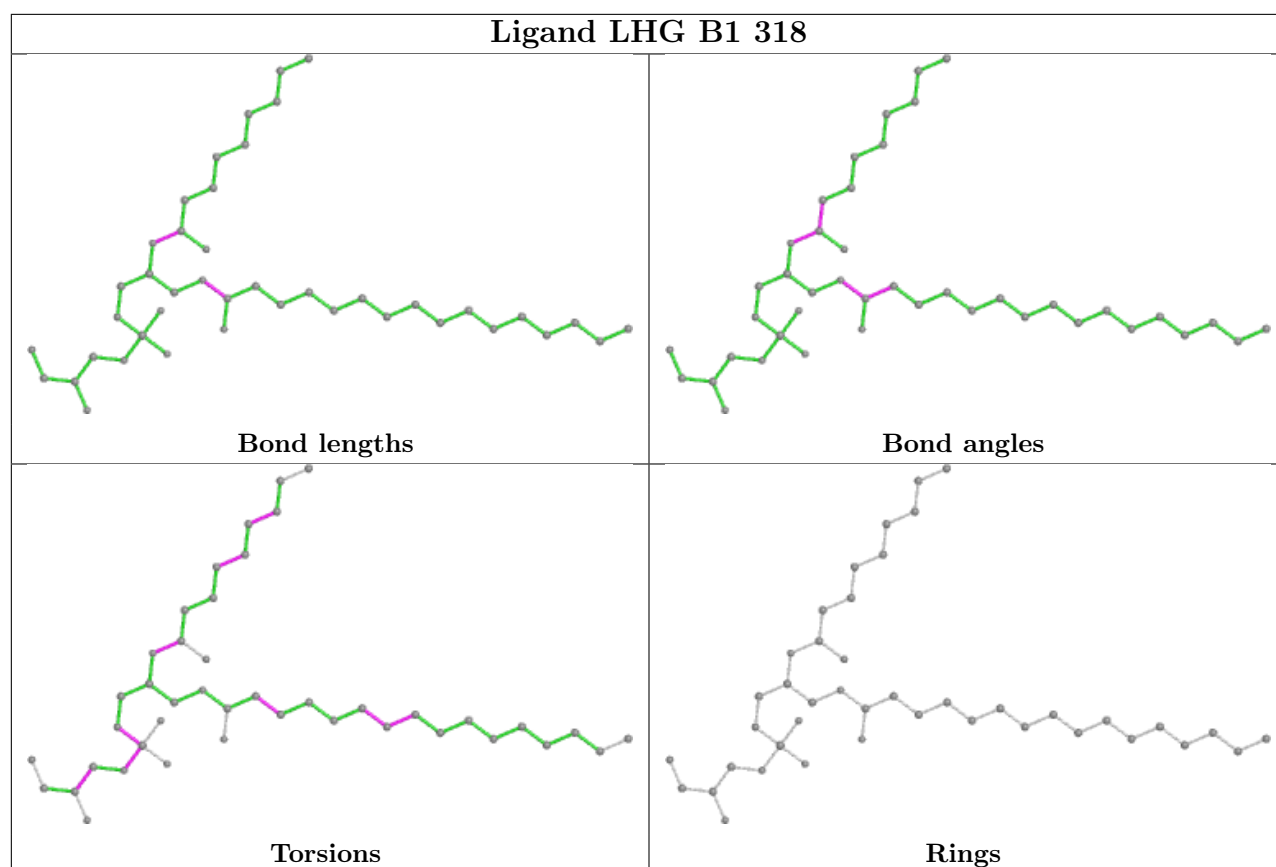


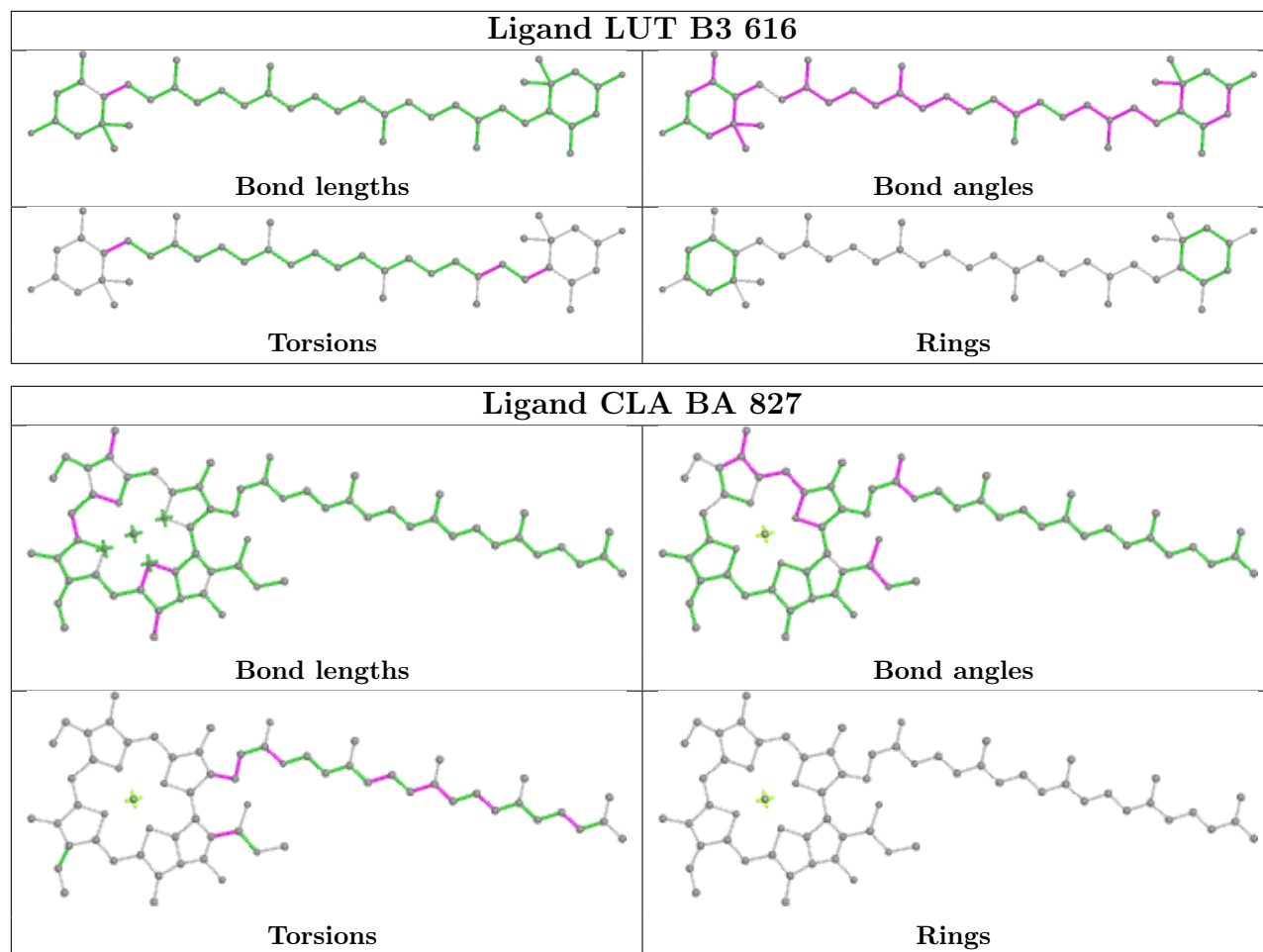
**Ligand CLA BB 807****Ligand LHG BF 305**



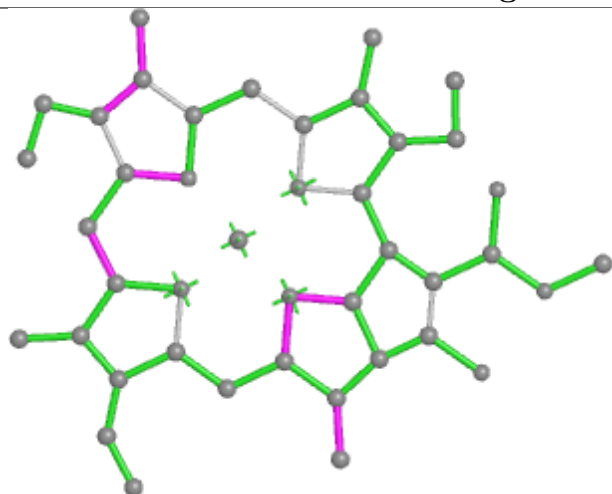




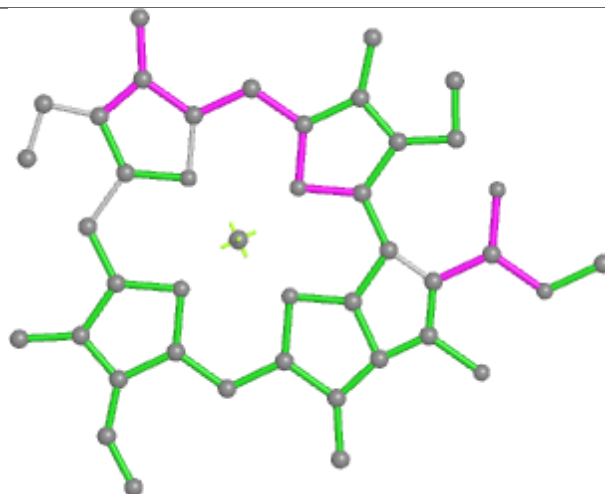




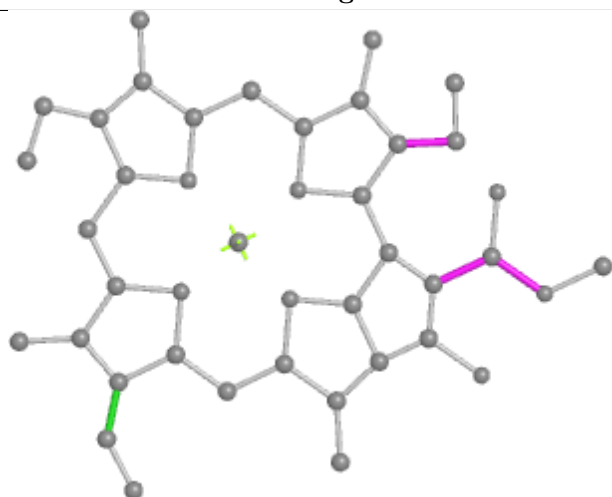
## Ligand CLA BG 201



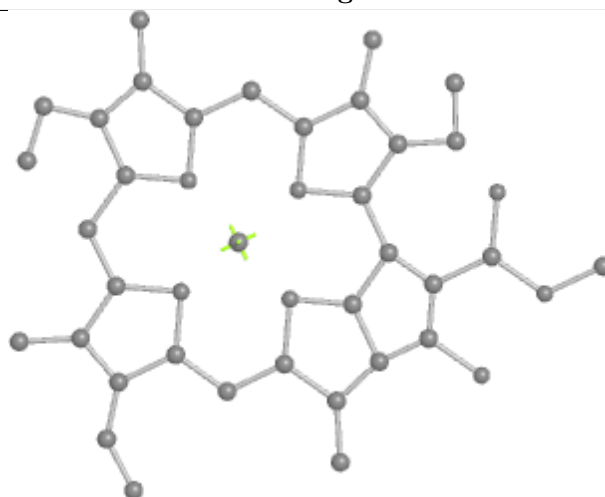
Bond lengths



Bond angles

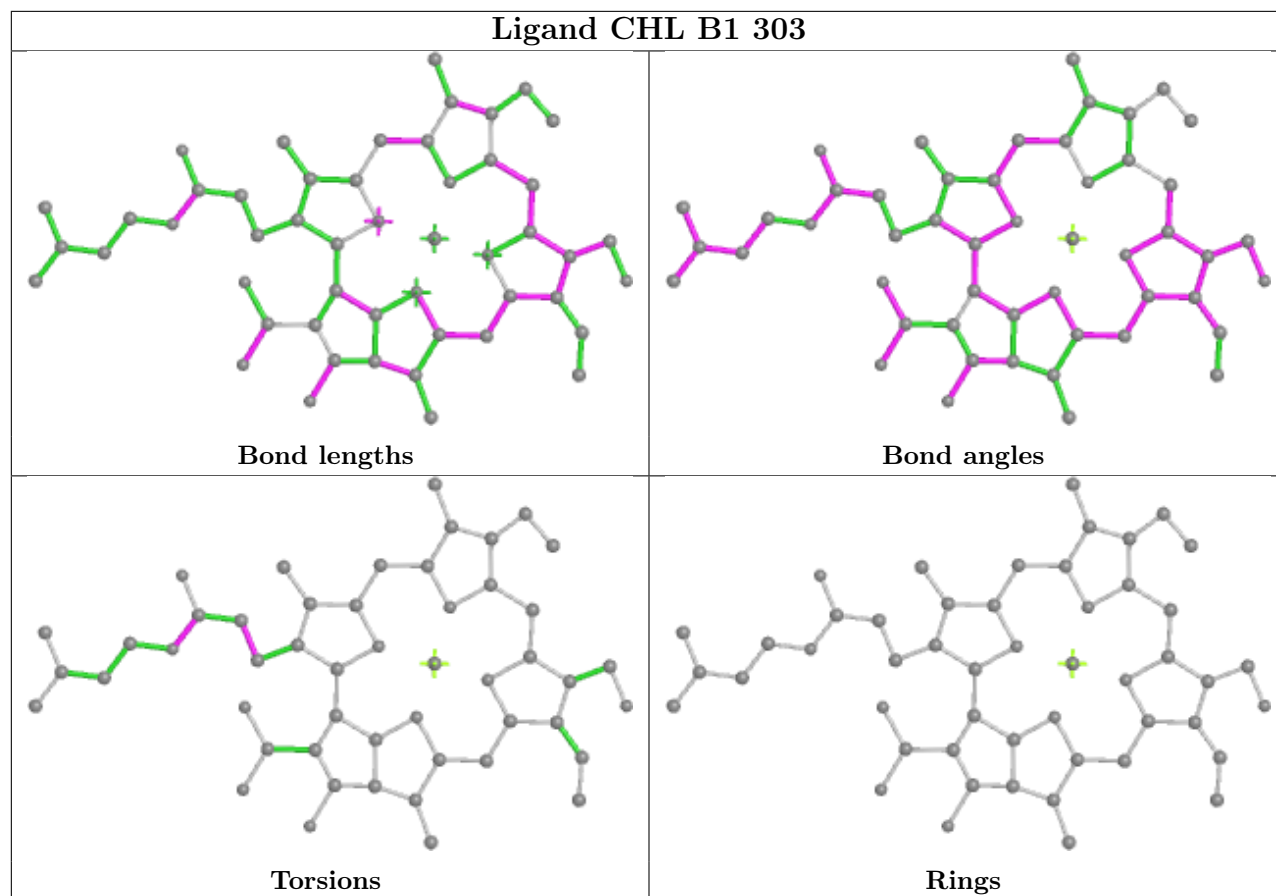


Torsions

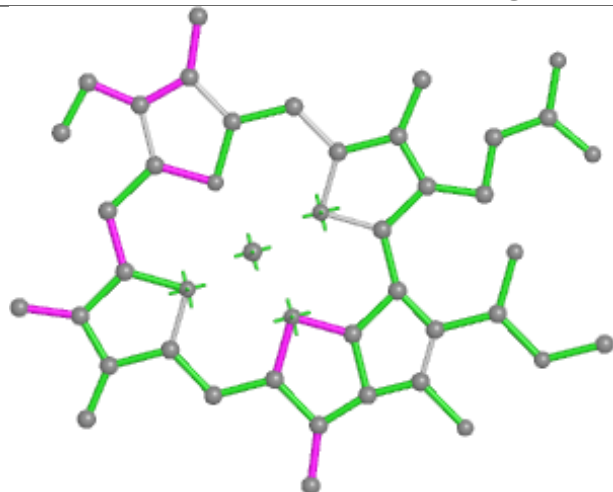


Rings

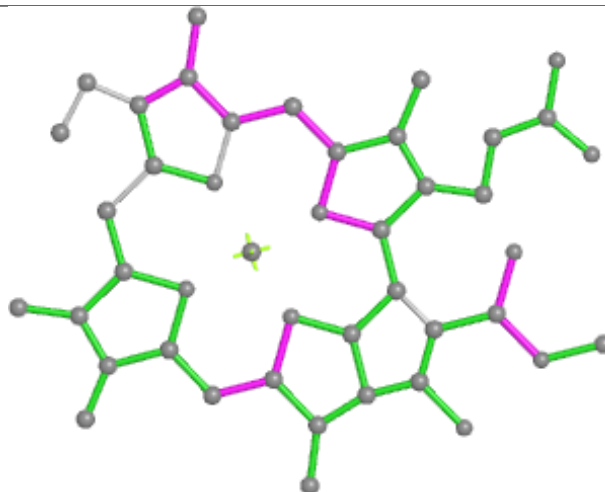




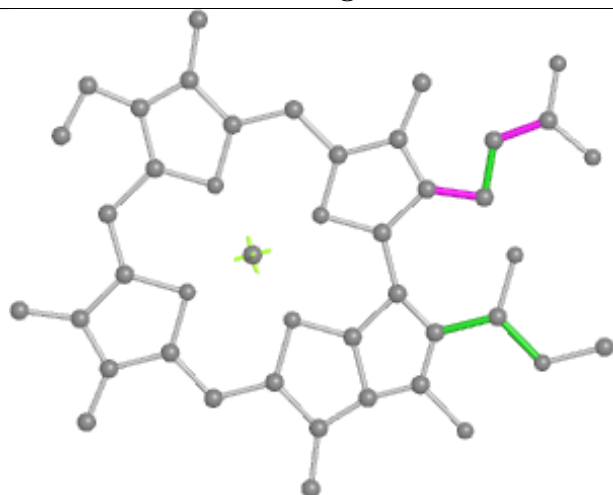
## Ligand CLA B5 608



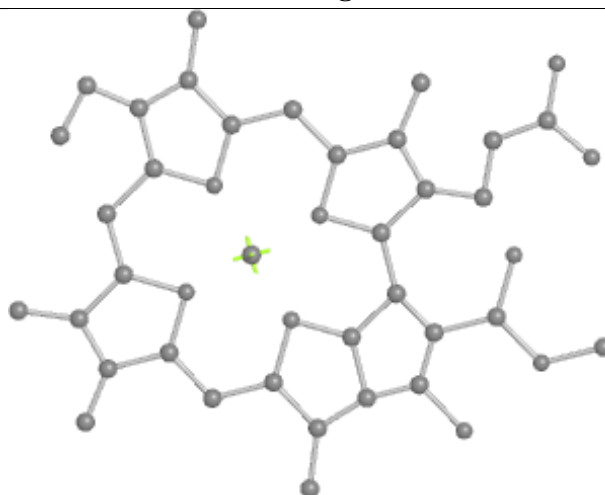
Bond lengths



Bond angles

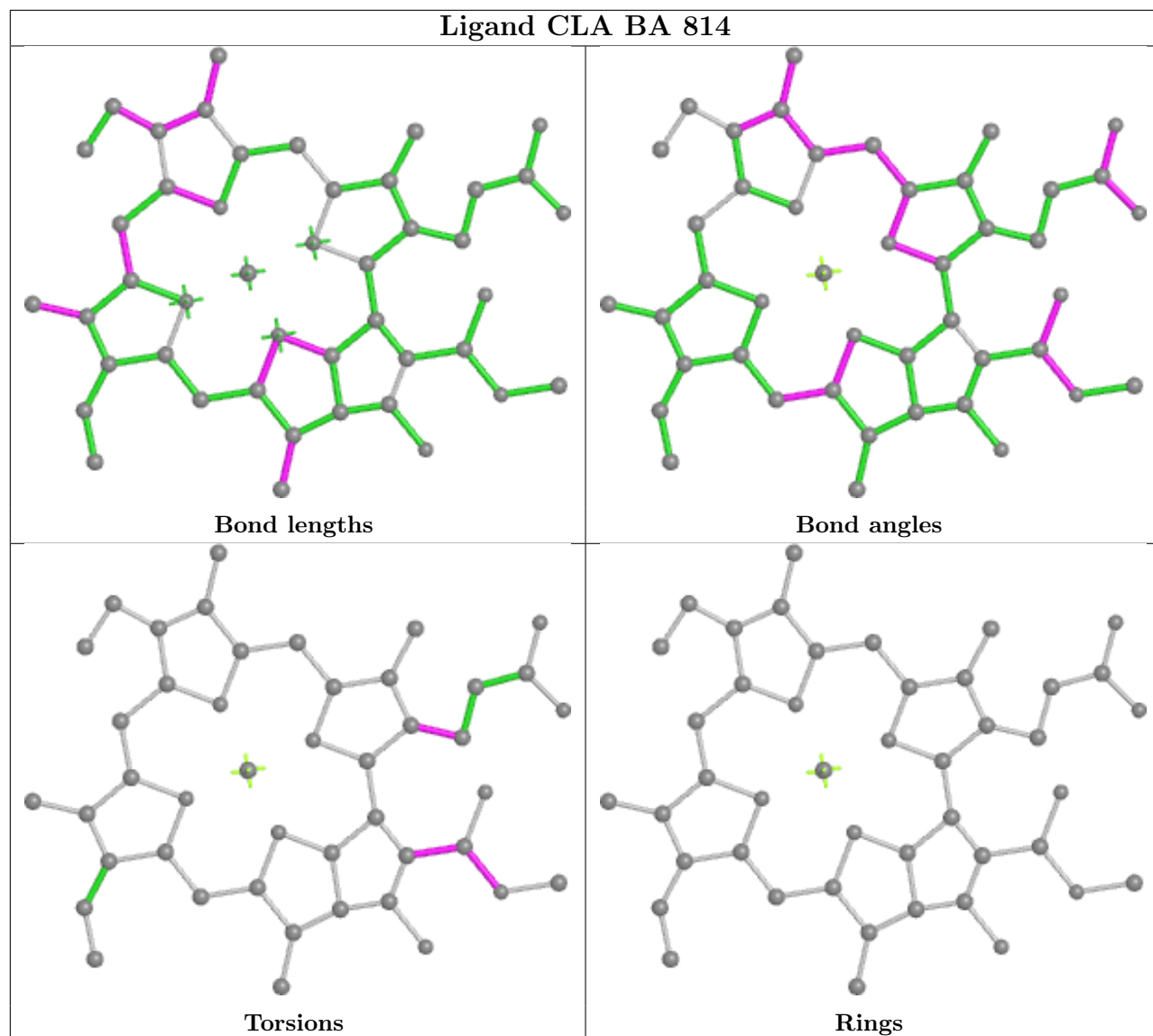


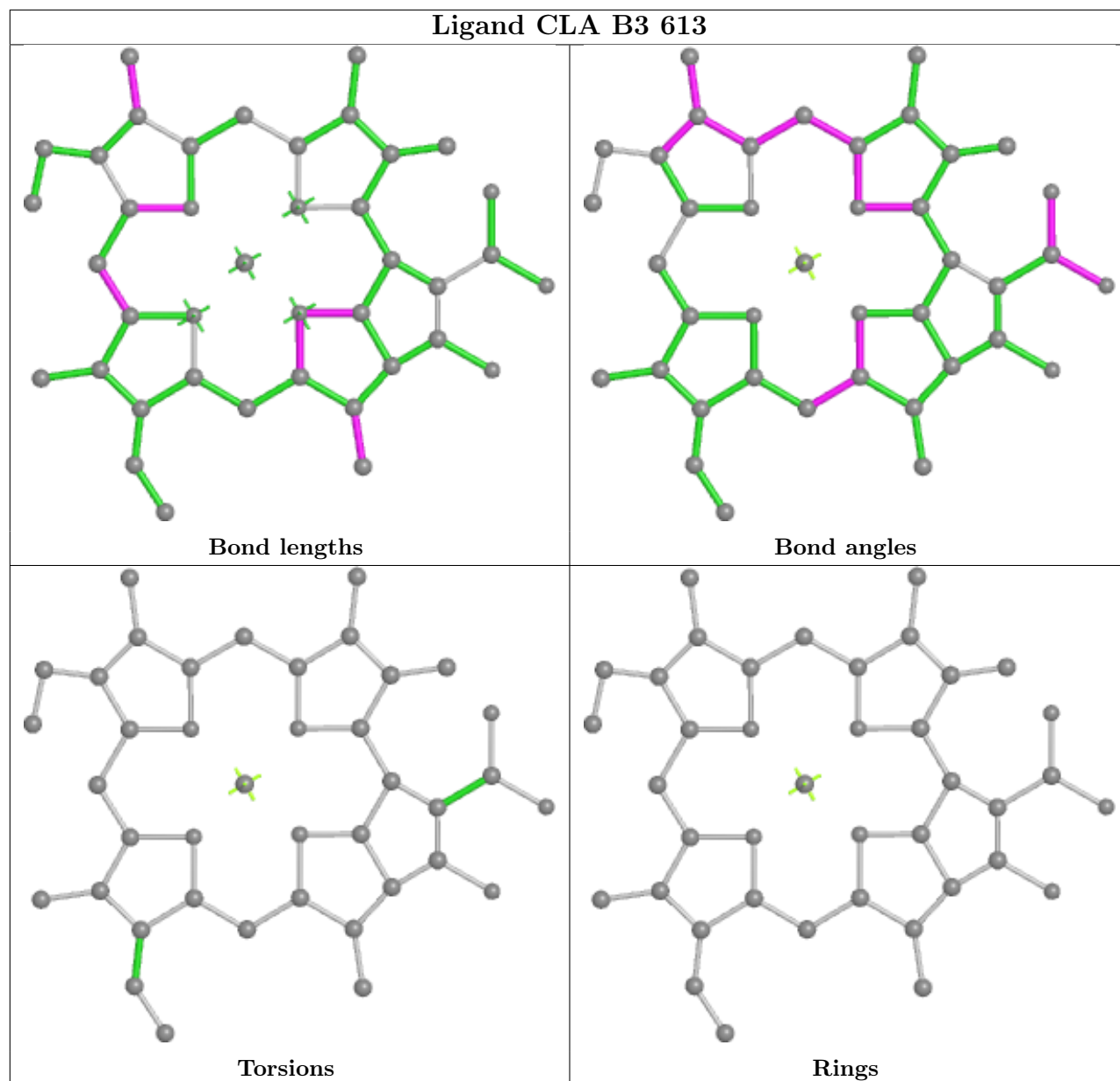
Torsions

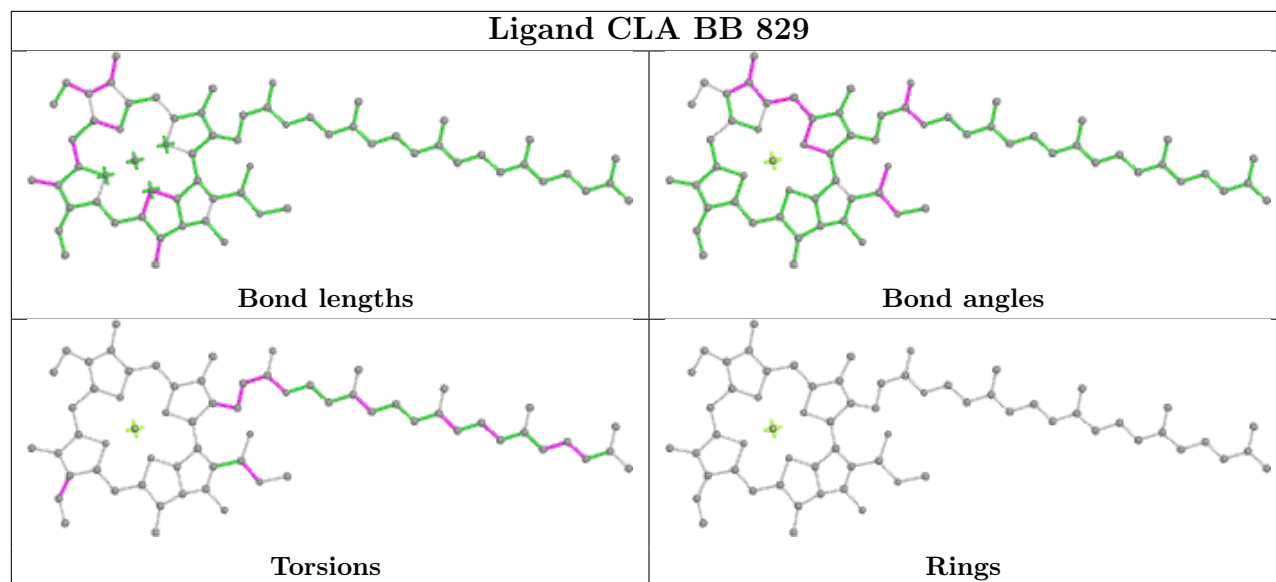
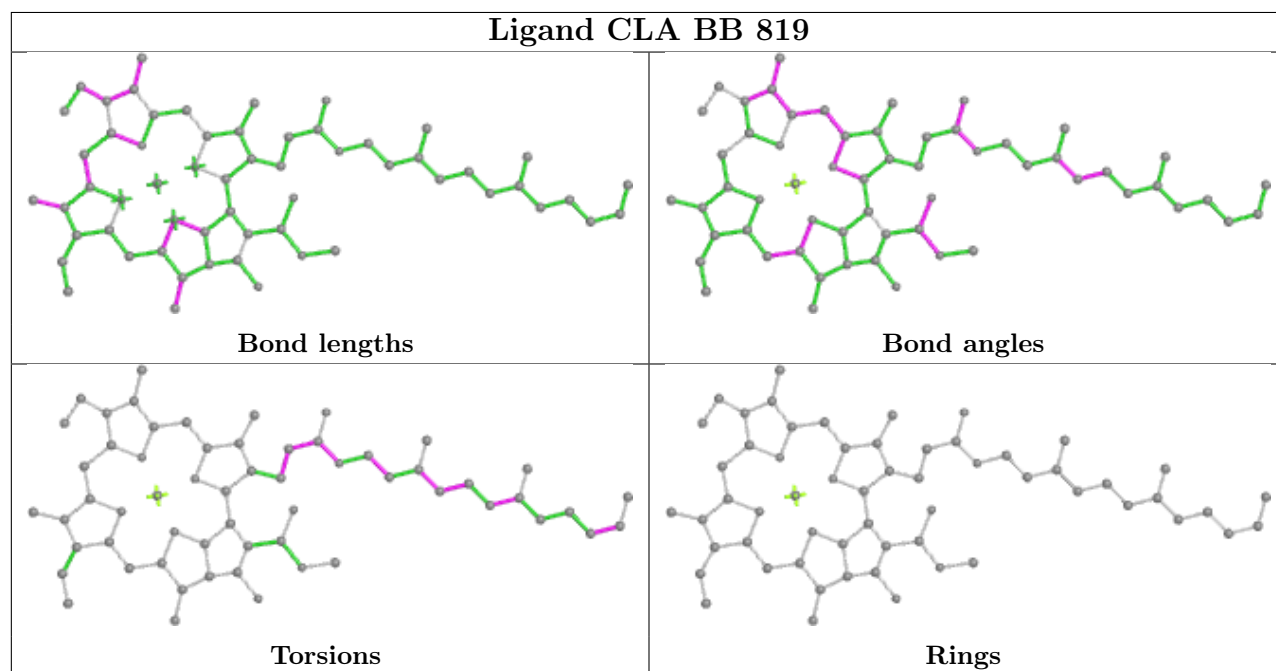


Rings

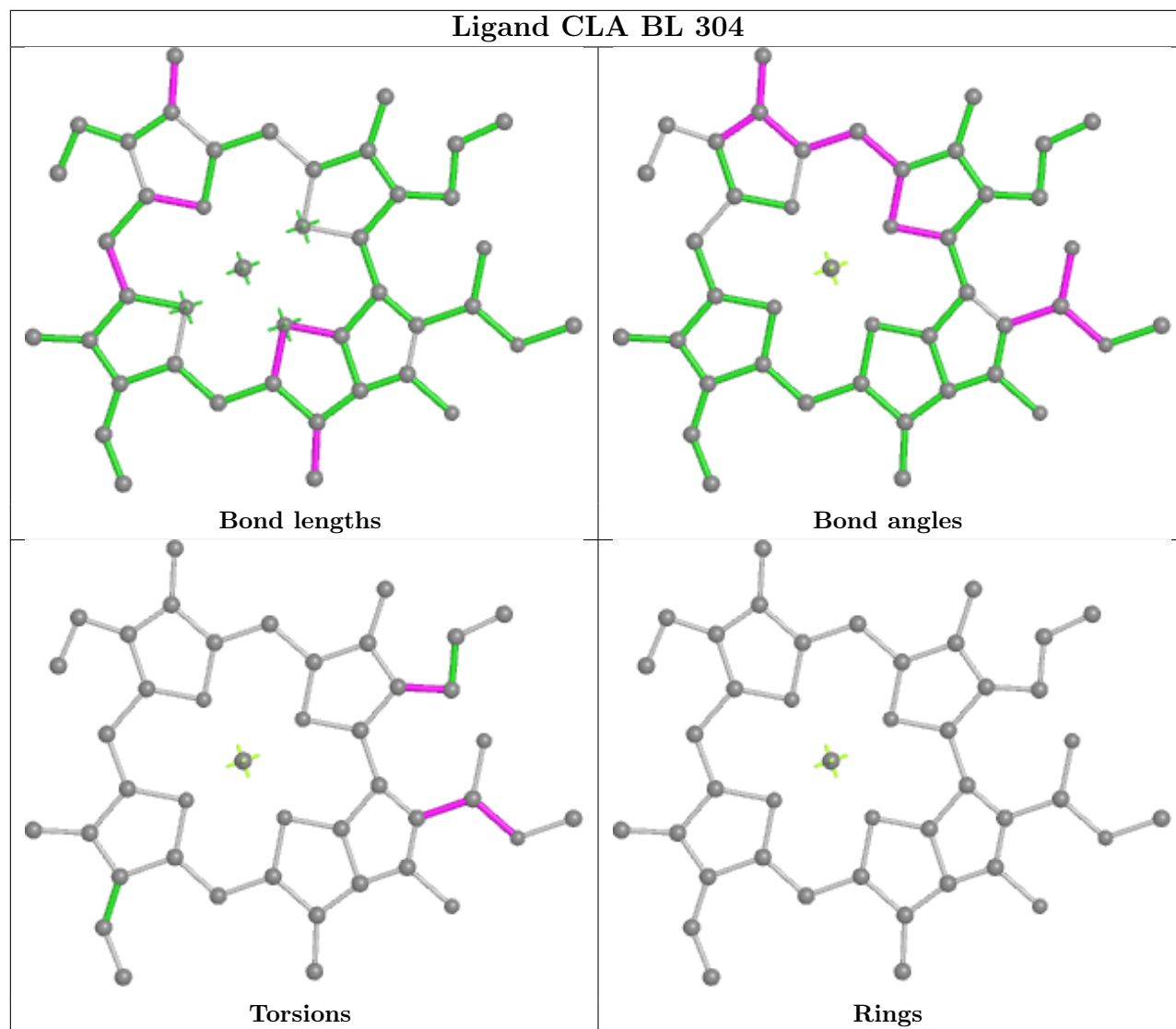
## Ligand CLA BA 814

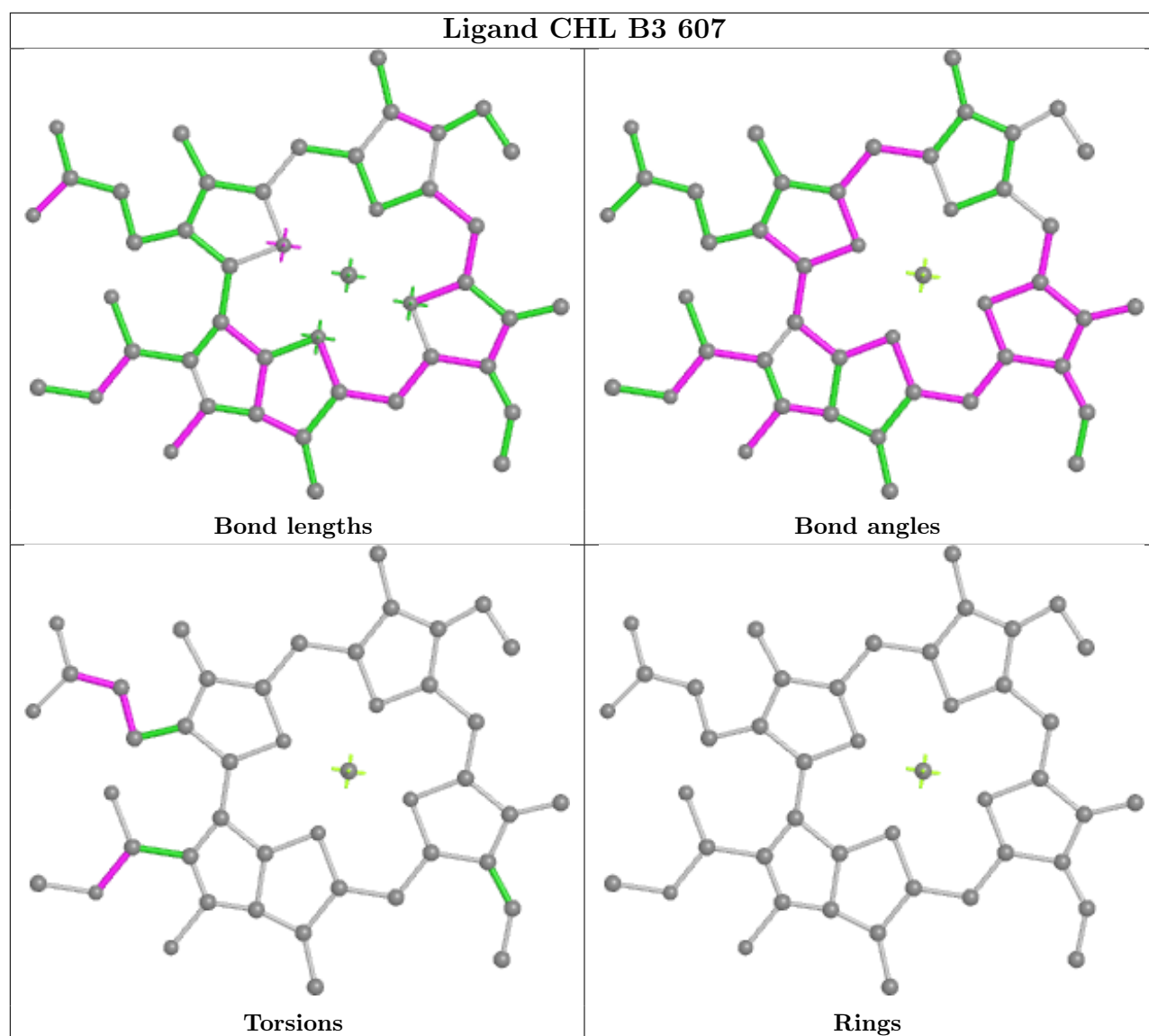




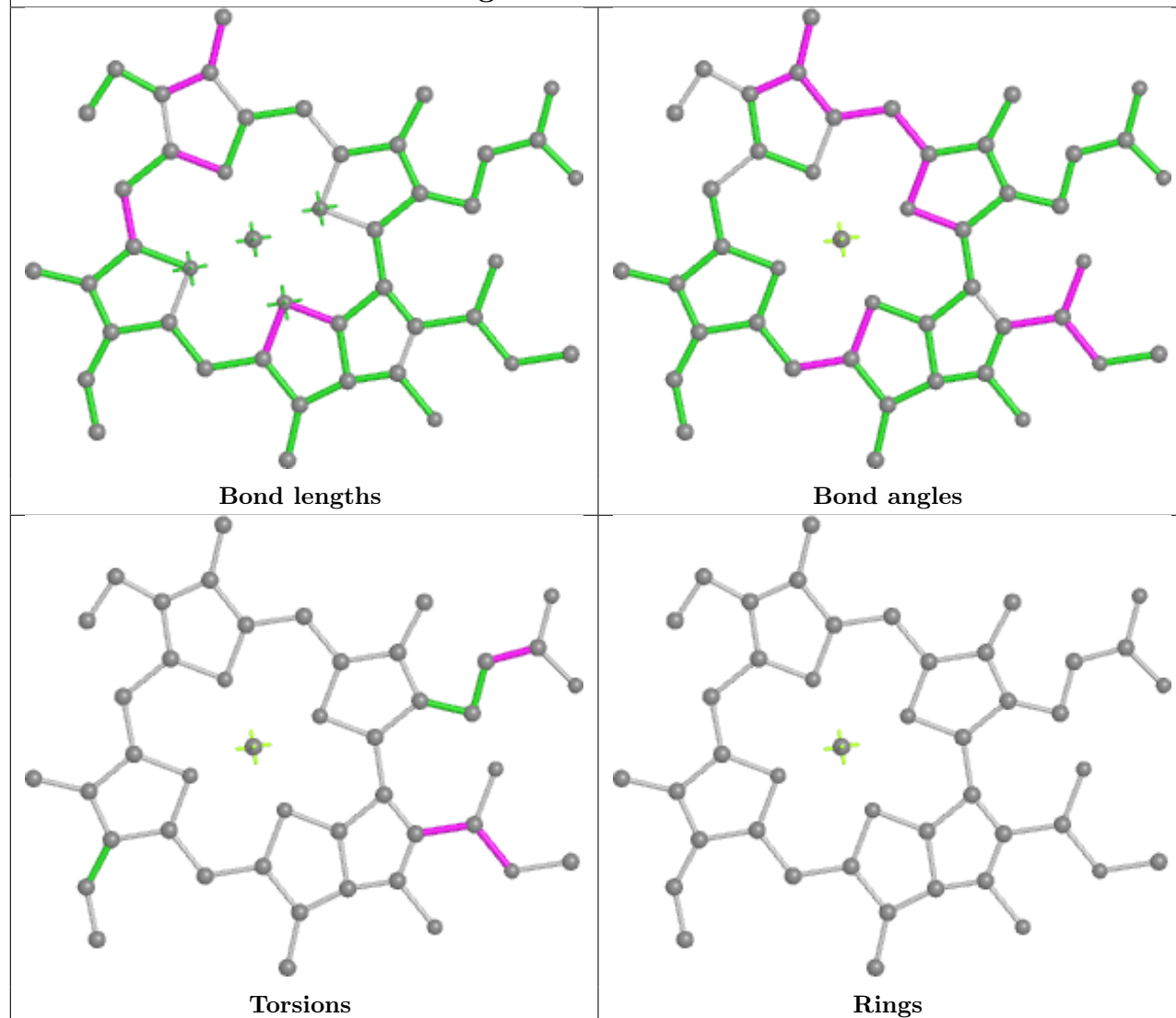
**Ligand CLA BB 829****Ligand CLA BB 819**

## Ligand CLA BL 304

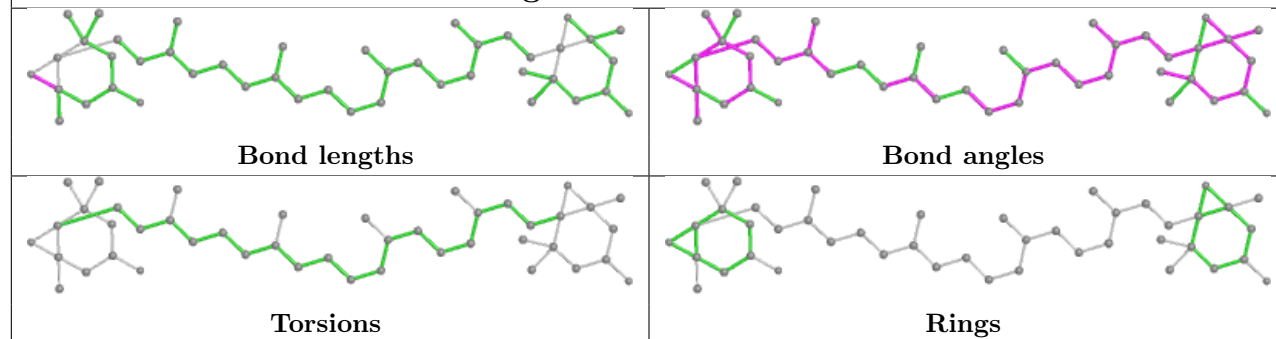




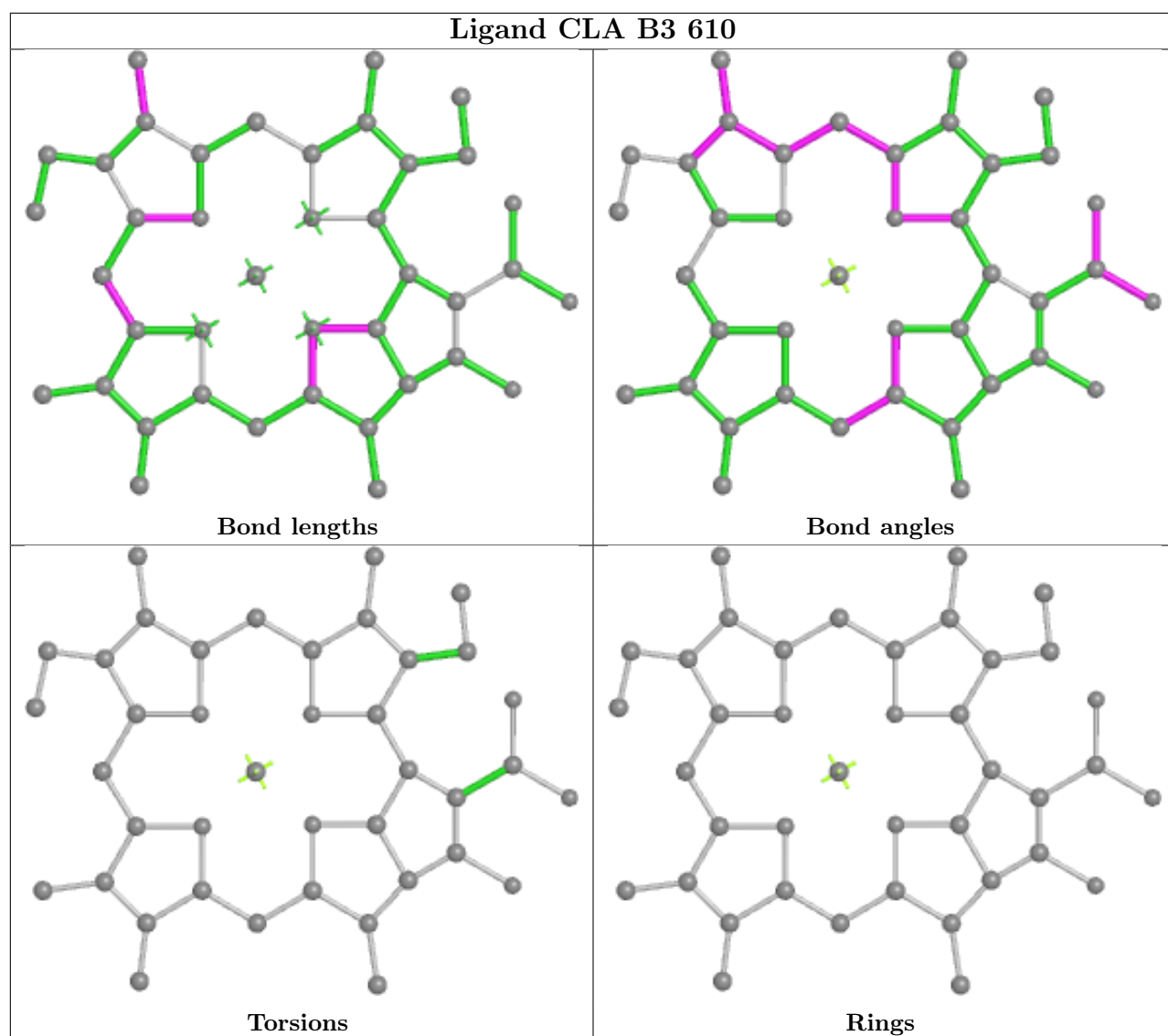
## Ligand CLA BA 836

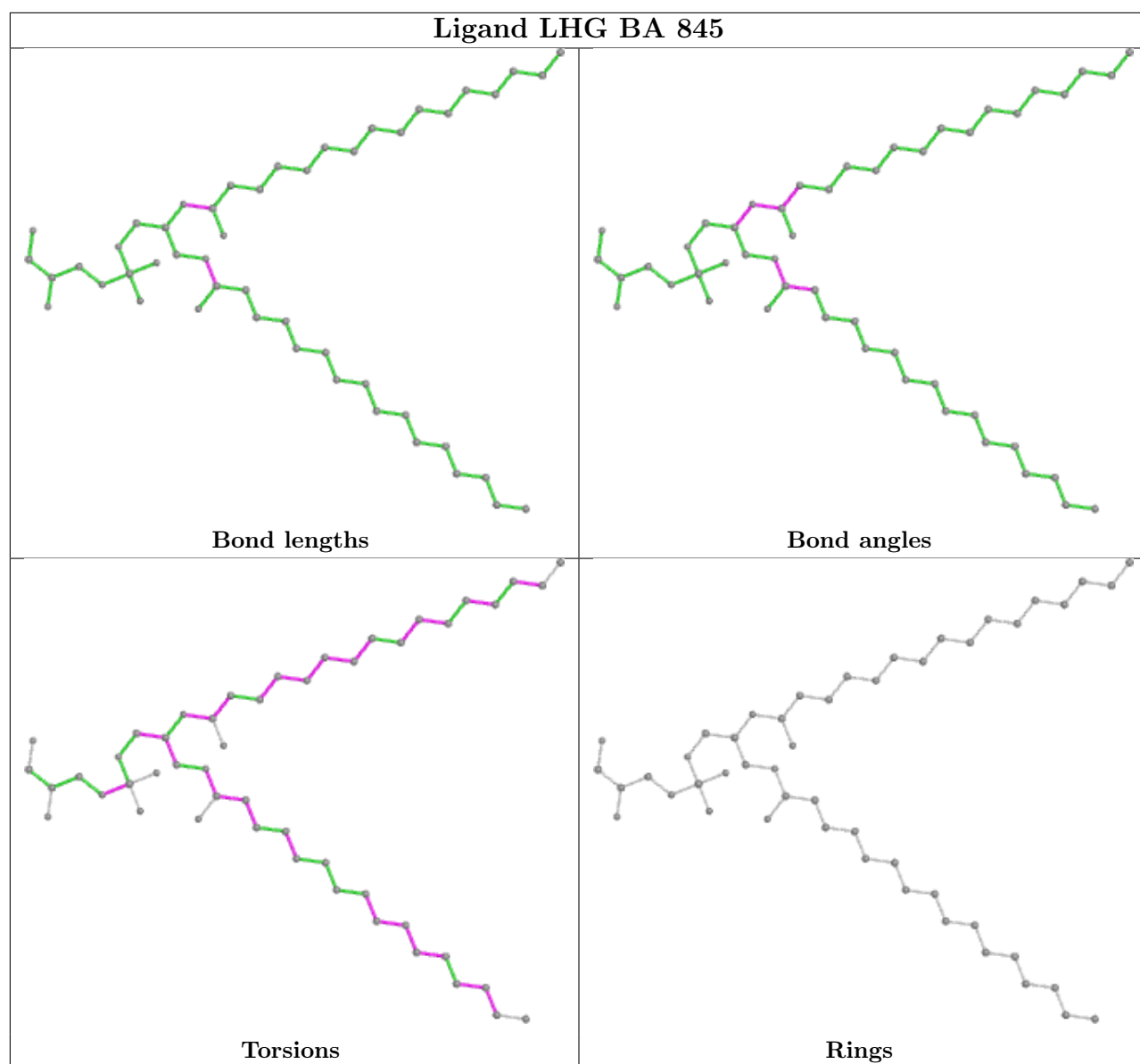


## Ligand XAT B3 617

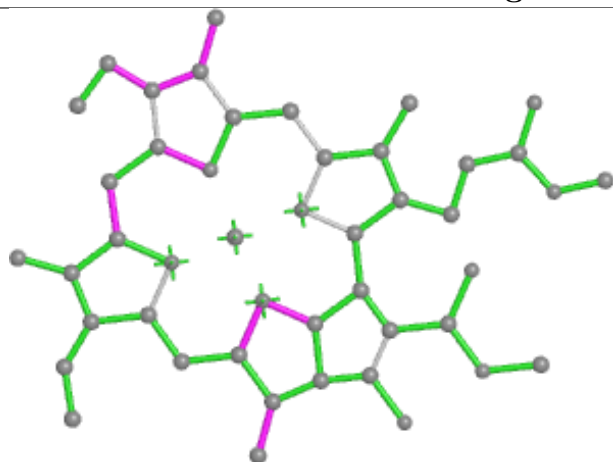




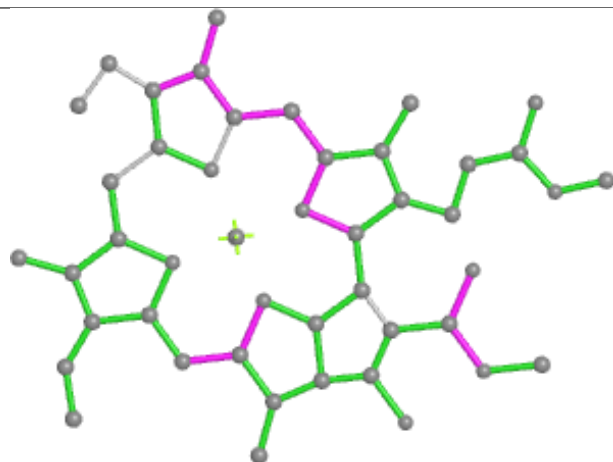




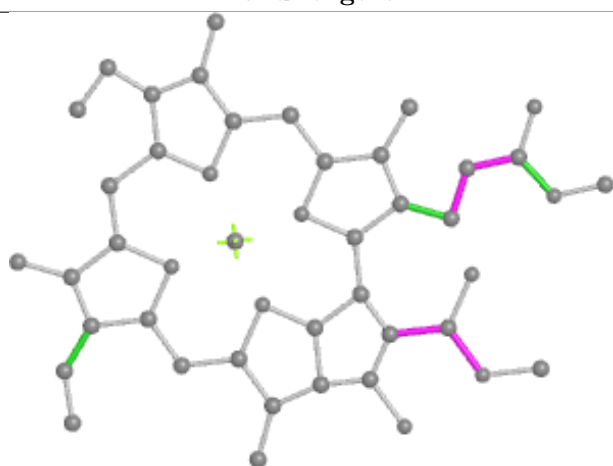
## Ligand CLA B5 601



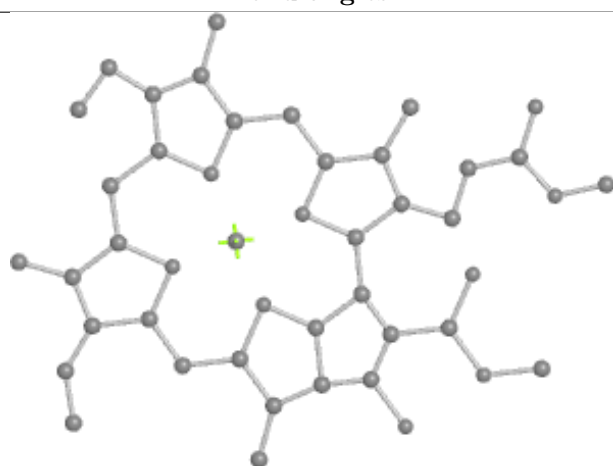
Bond lengths



Bond angles

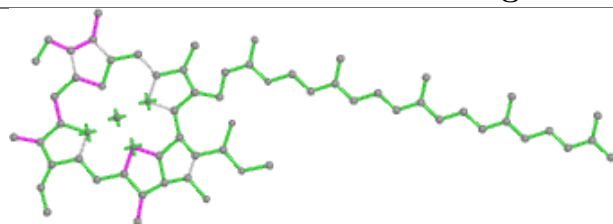


Torsions

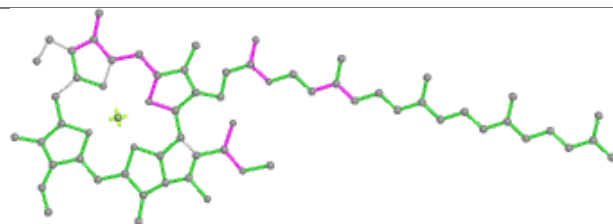


Rings

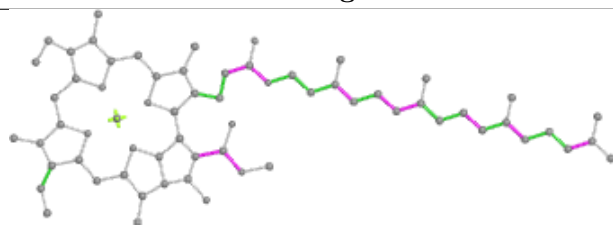
## Ligand CLA BB 804



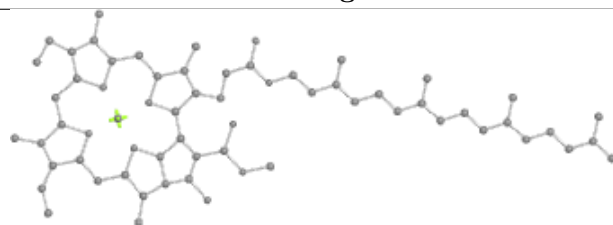
Bond lengths



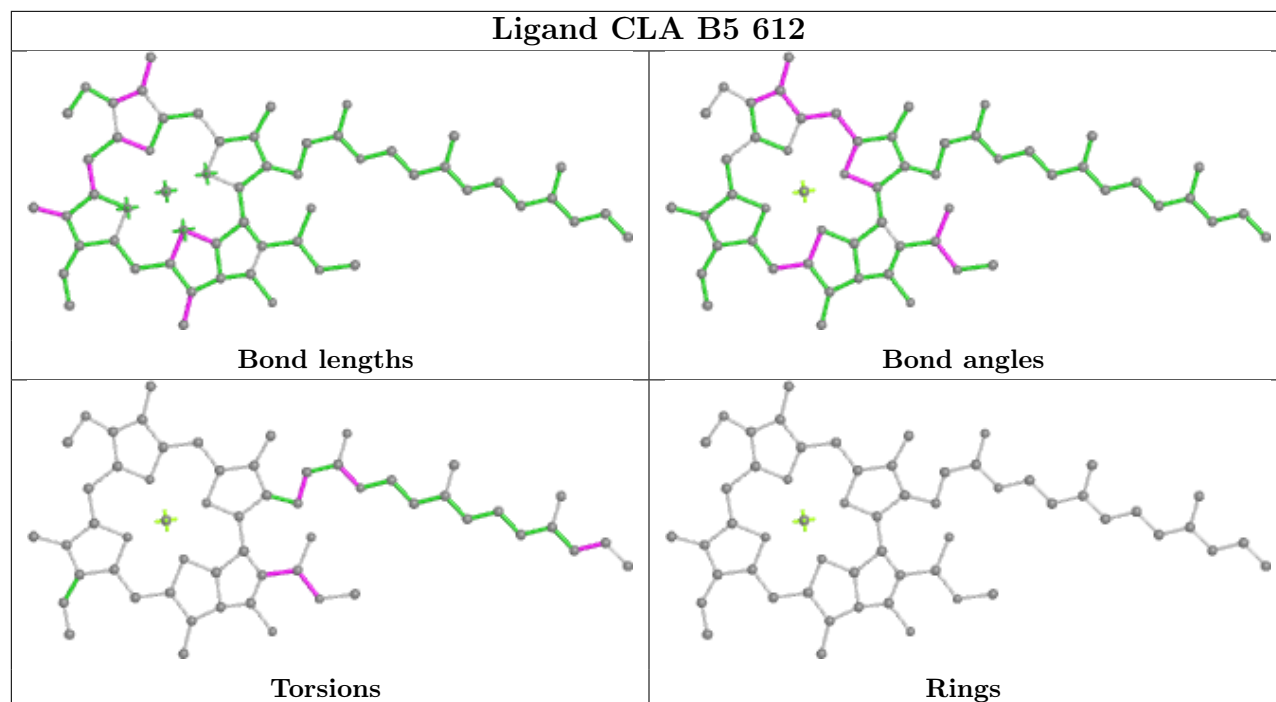
Bond angles

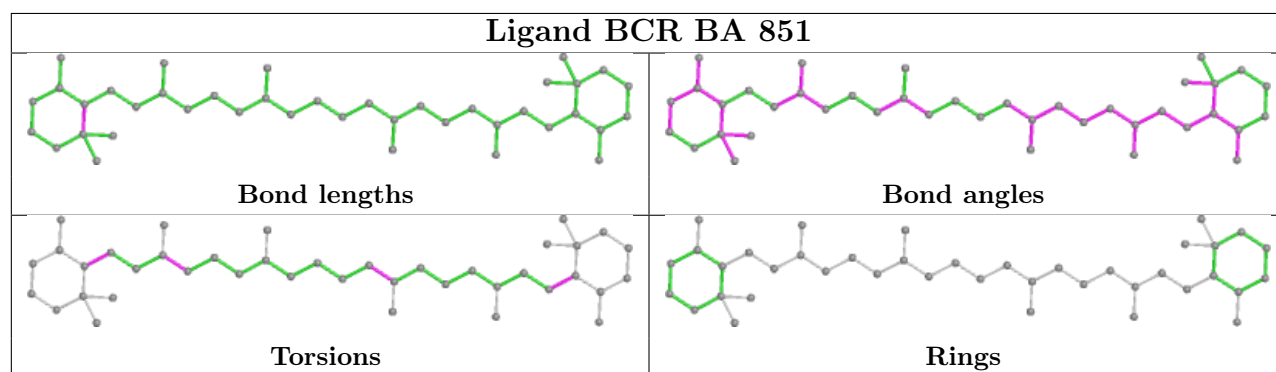
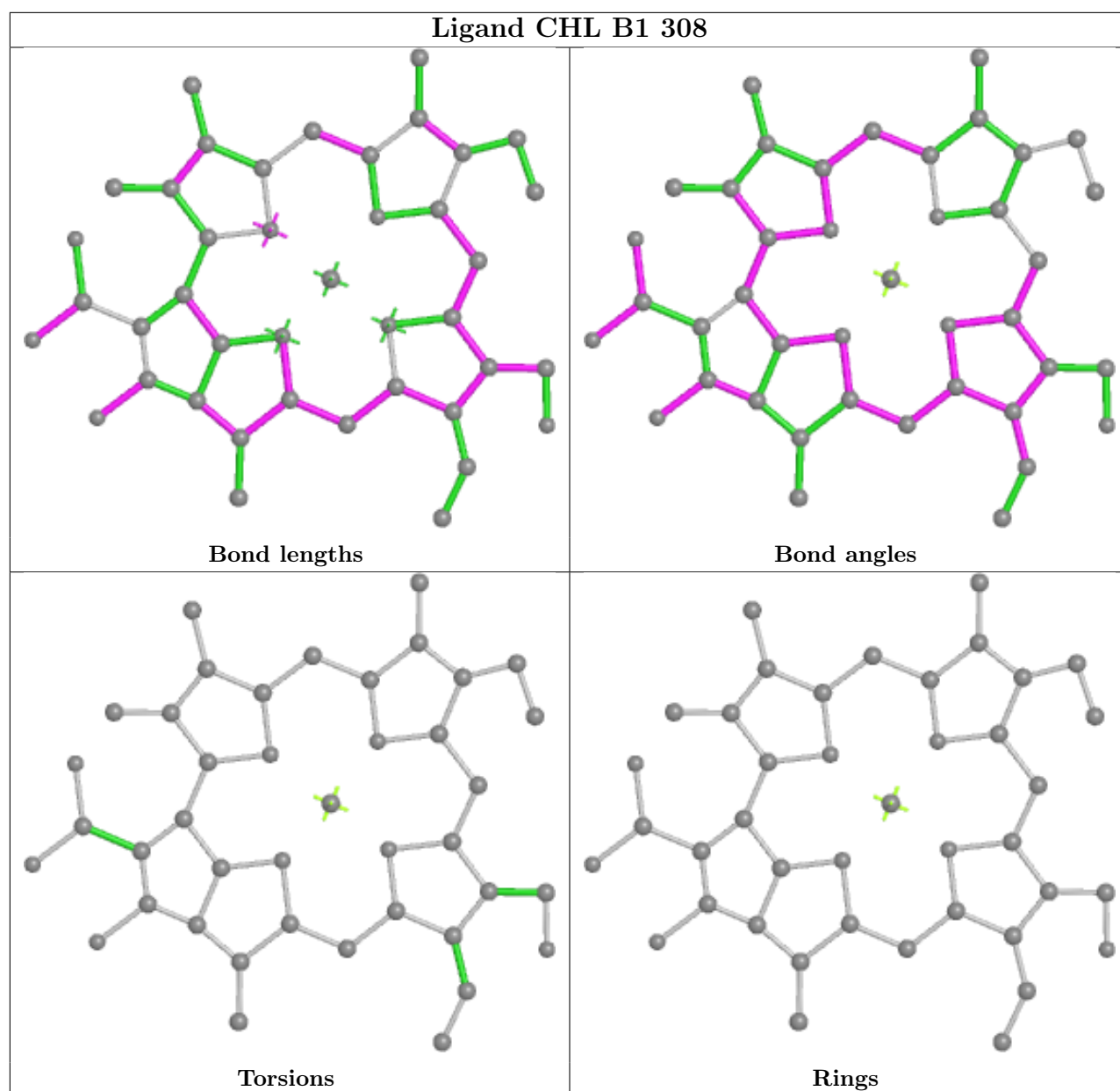


Torsions

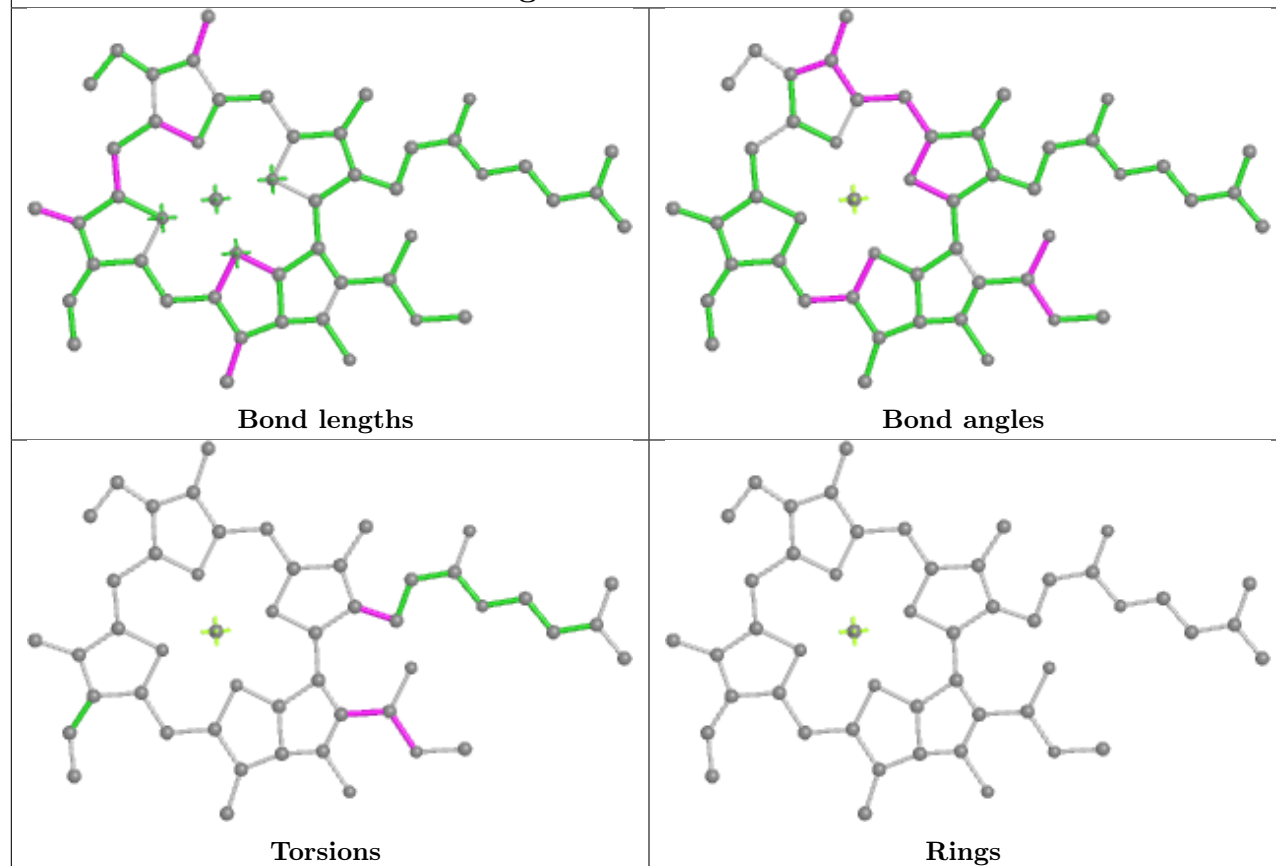


Rings

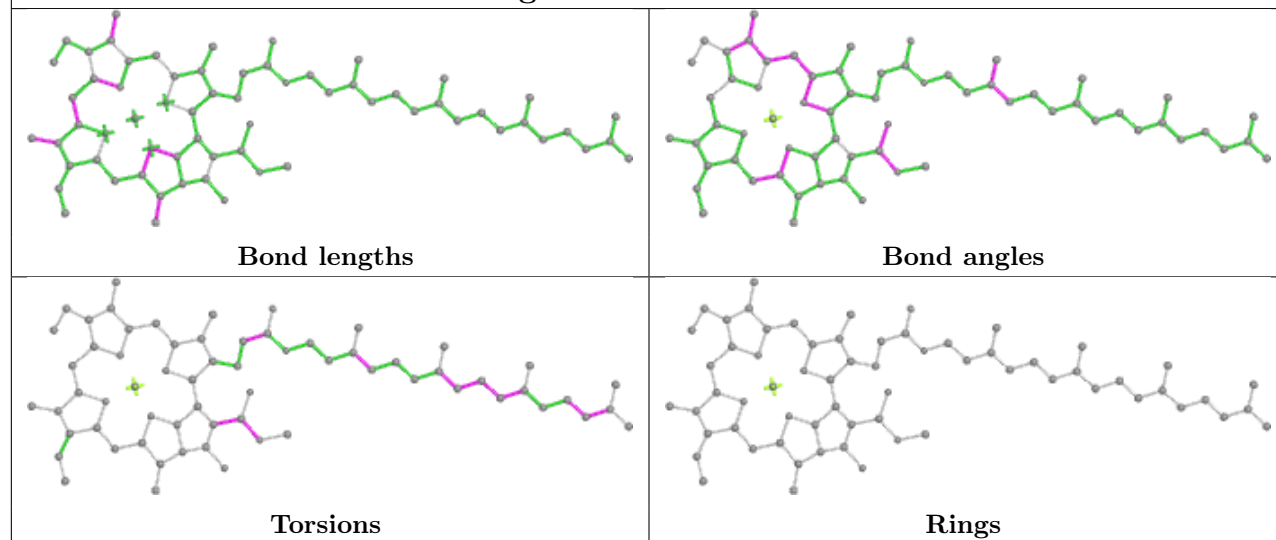




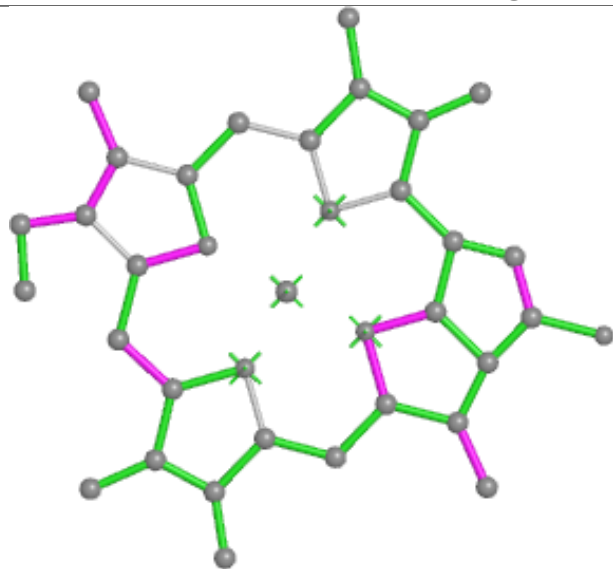
## Ligand CLA BA 807



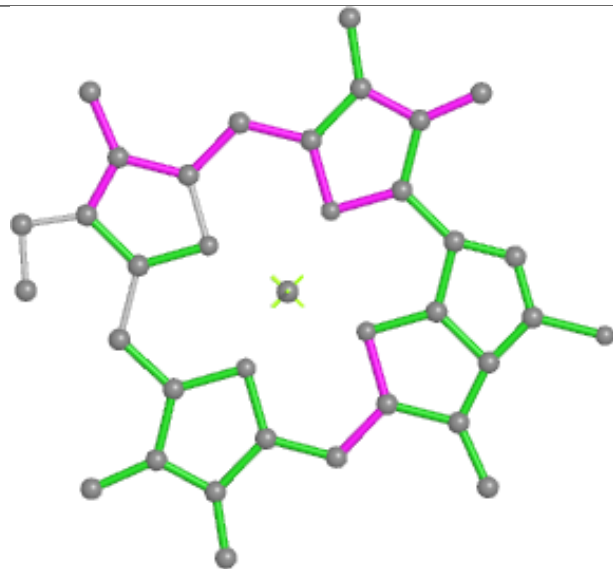
## Ligand CLA BA 813



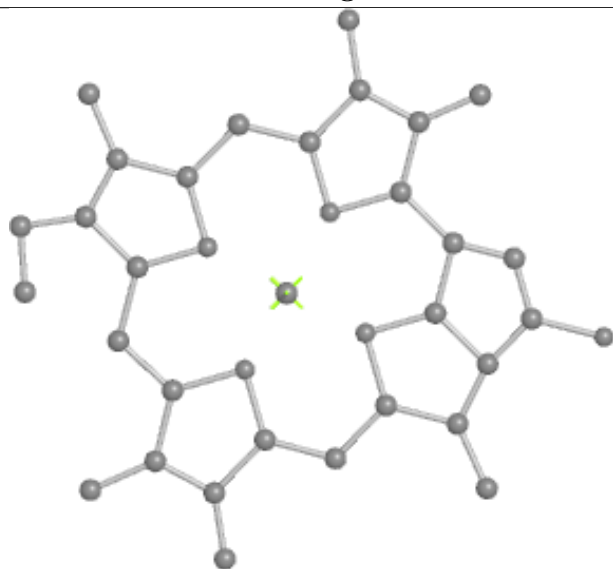
## Ligand CLA B3 614



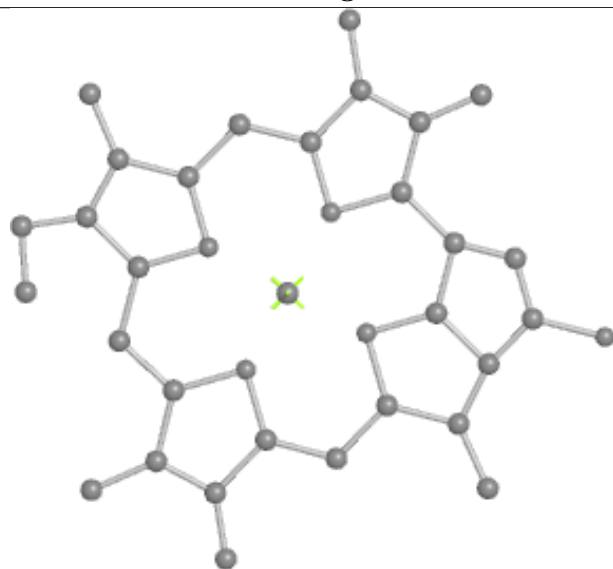
Bond lengths



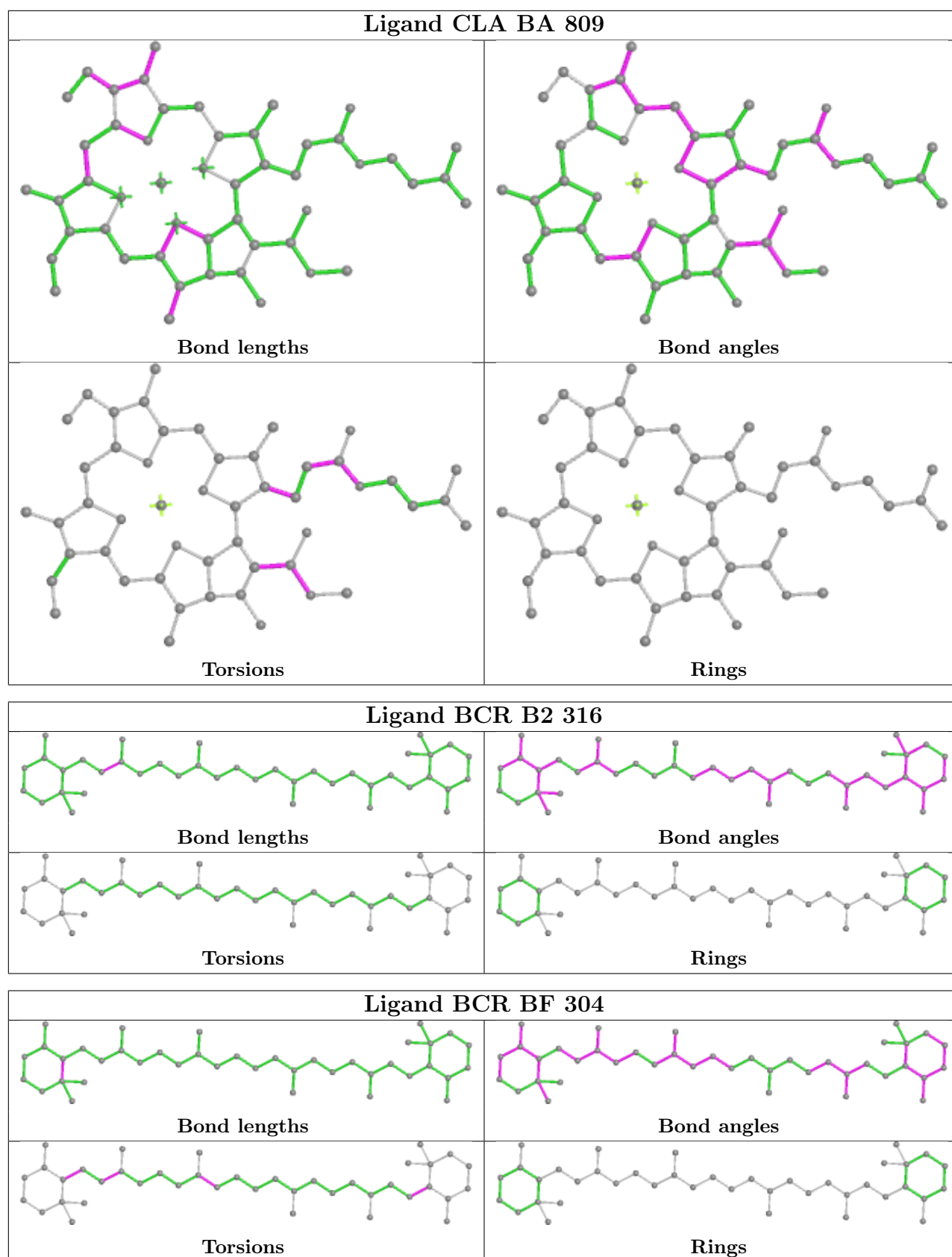
Bond angles



Torsions

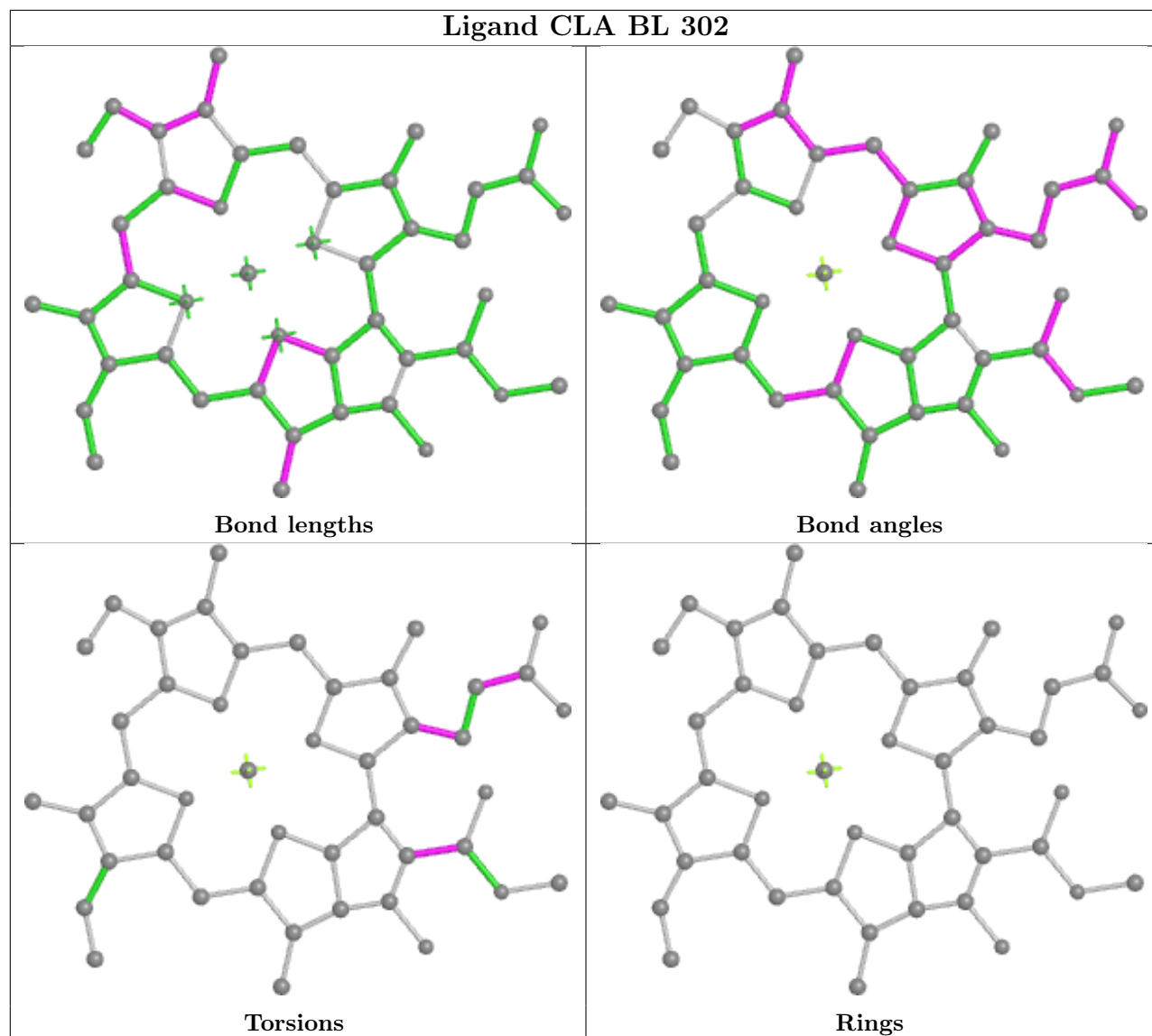


Rings

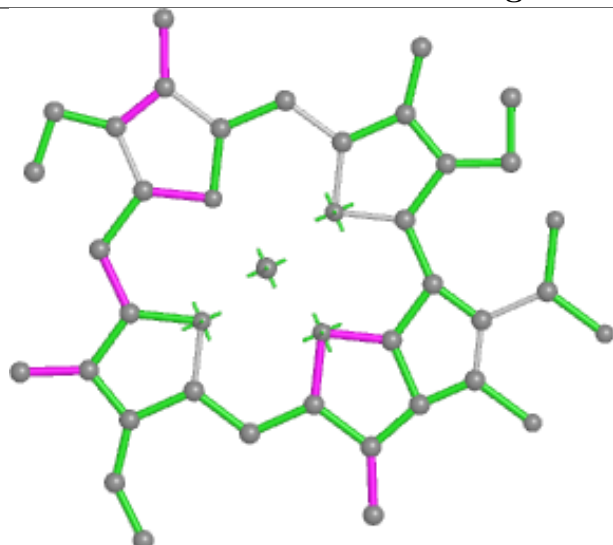




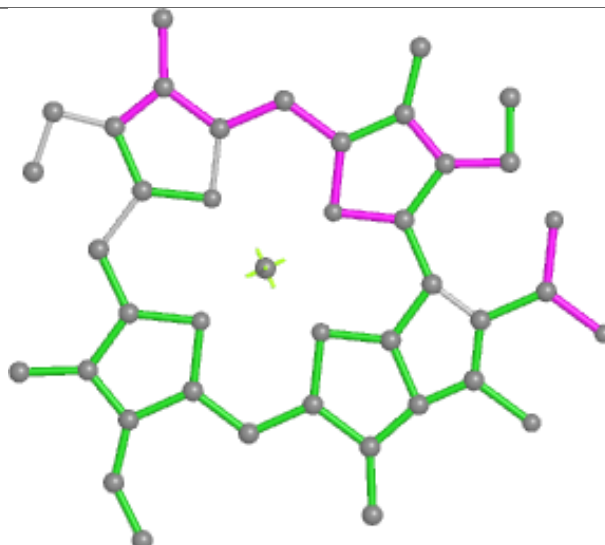
## Ligand CLA BL 302



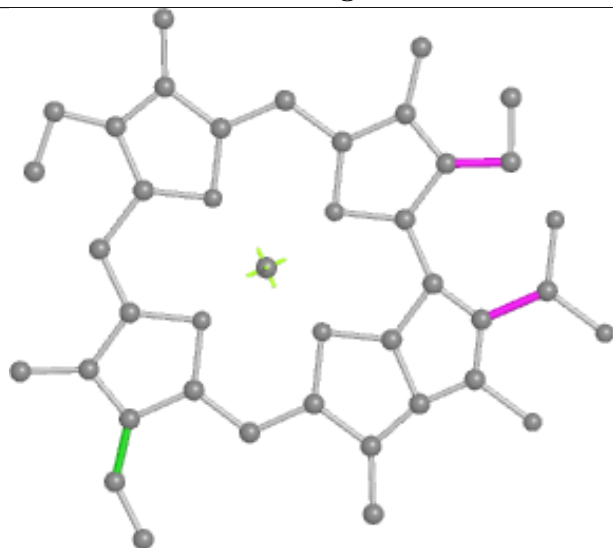
## Ligand CLA B5 611



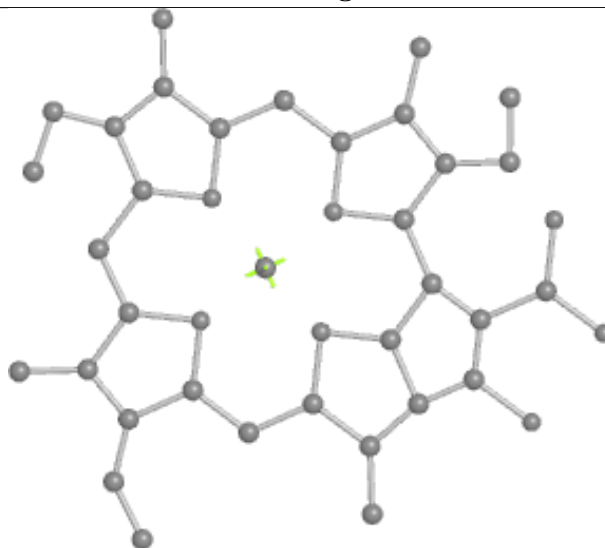
Bond lengths



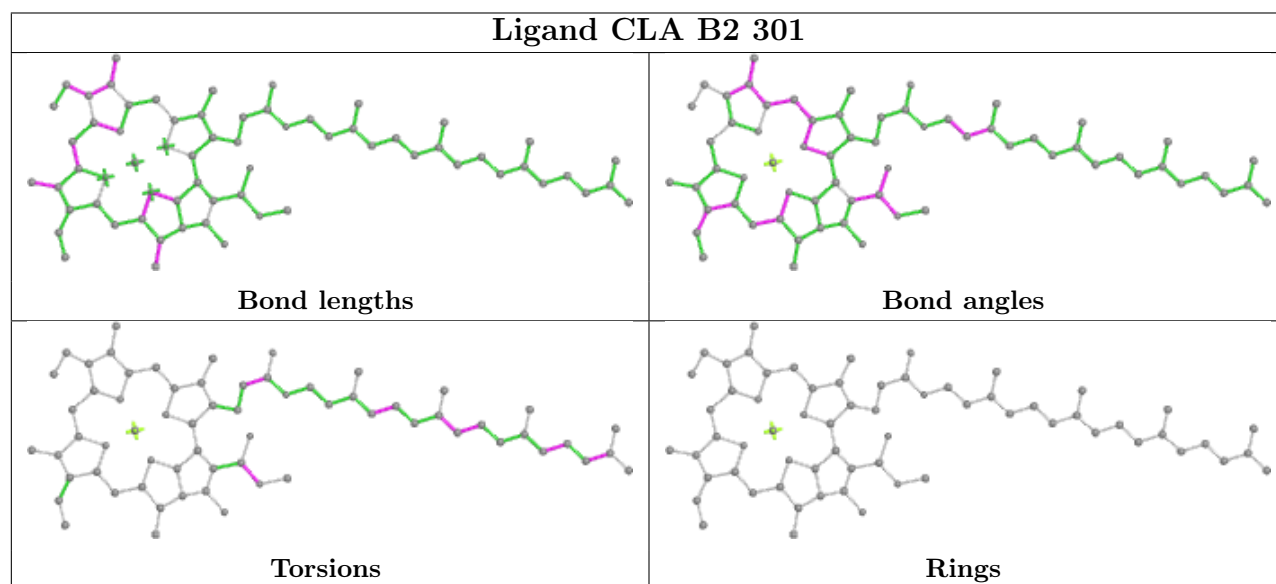
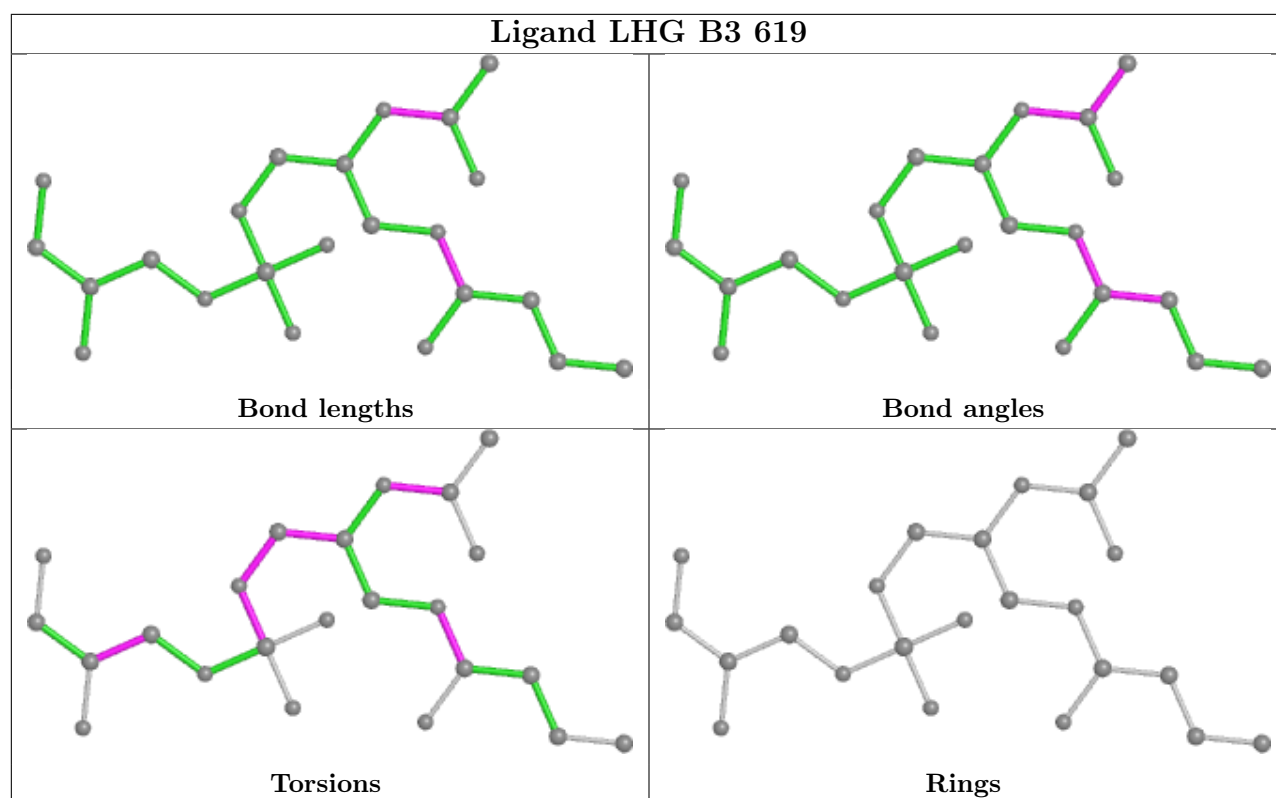
Bond angles



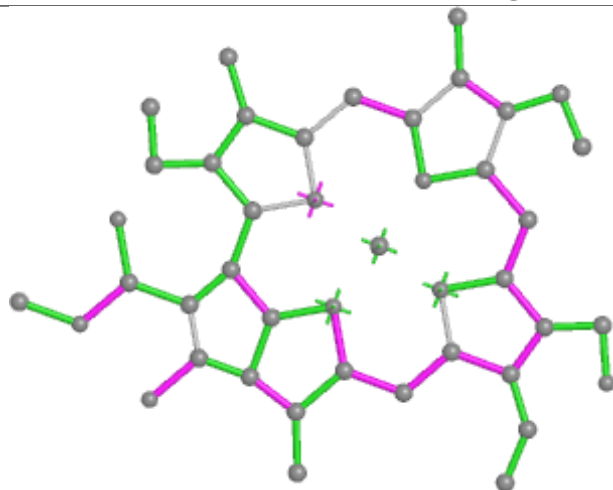
Torsions



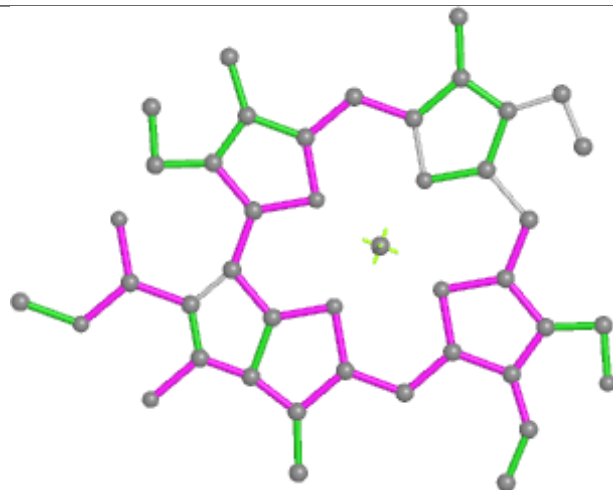
Rings



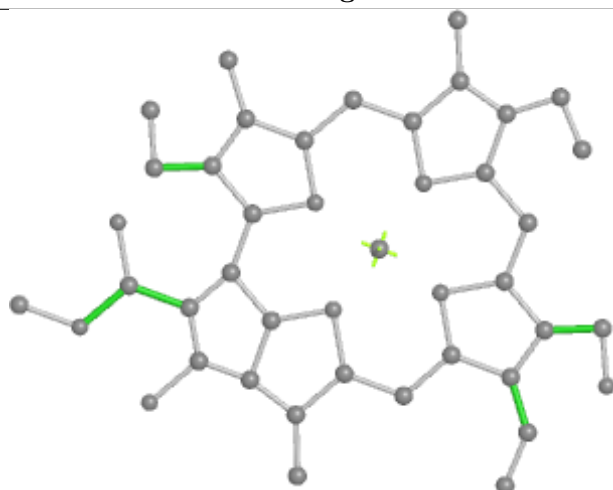
## Ligand CHL B2 313



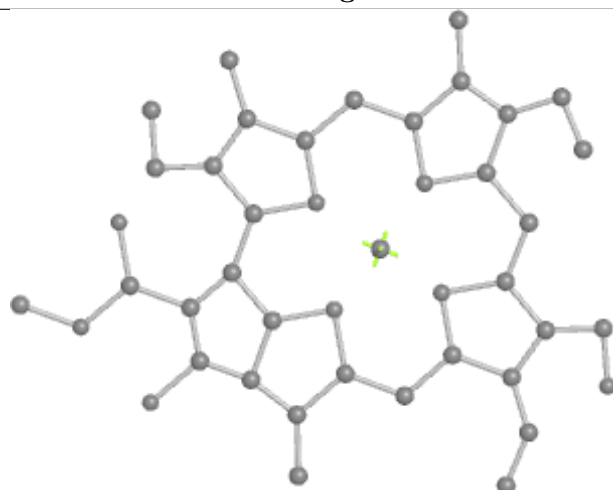
Bond lengths



Bond angles

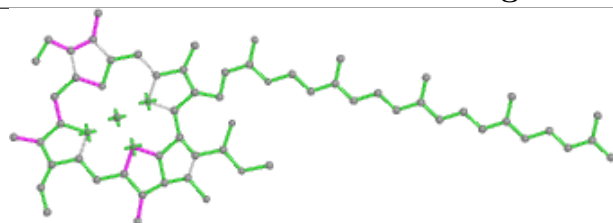


Torsions

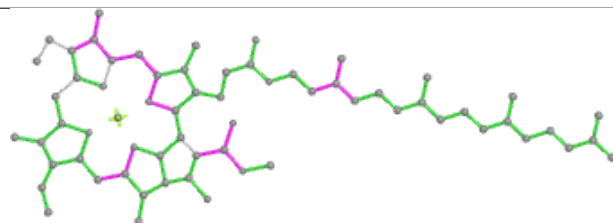


Rings

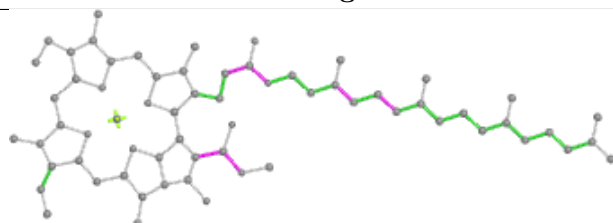
## Ligand CLA BA 834



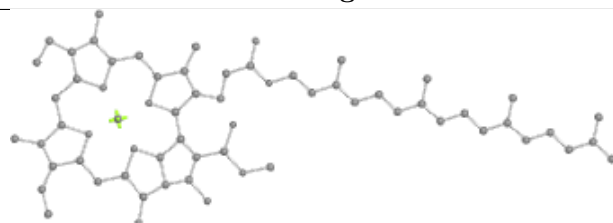
Bond lengths



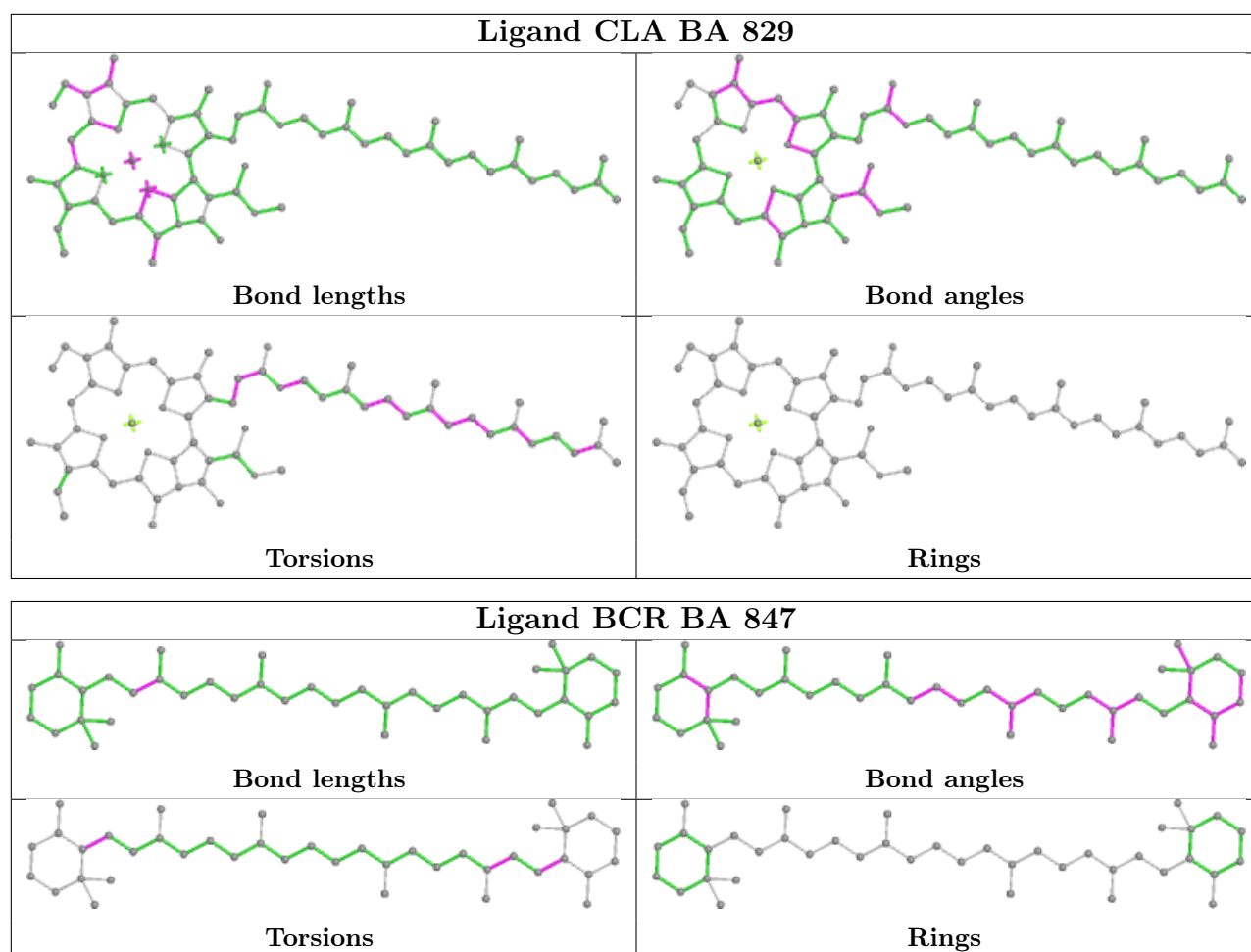
Bond angles

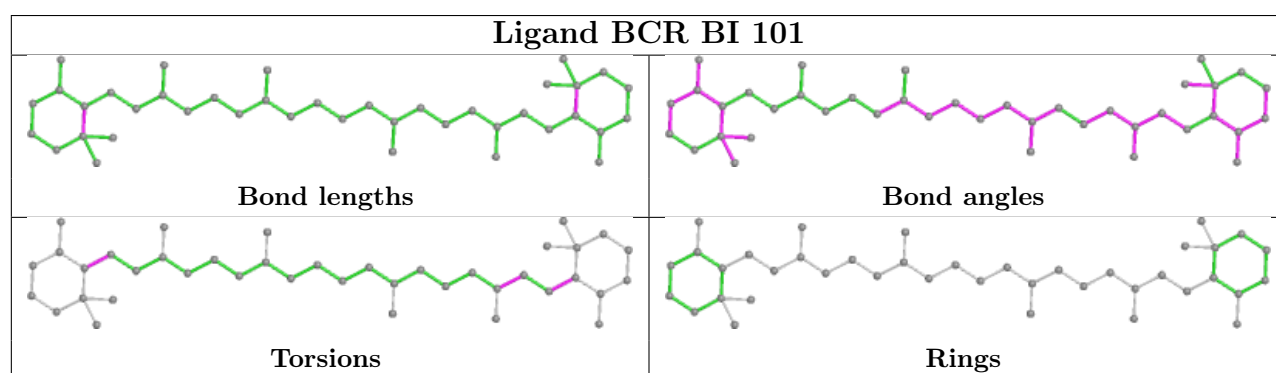
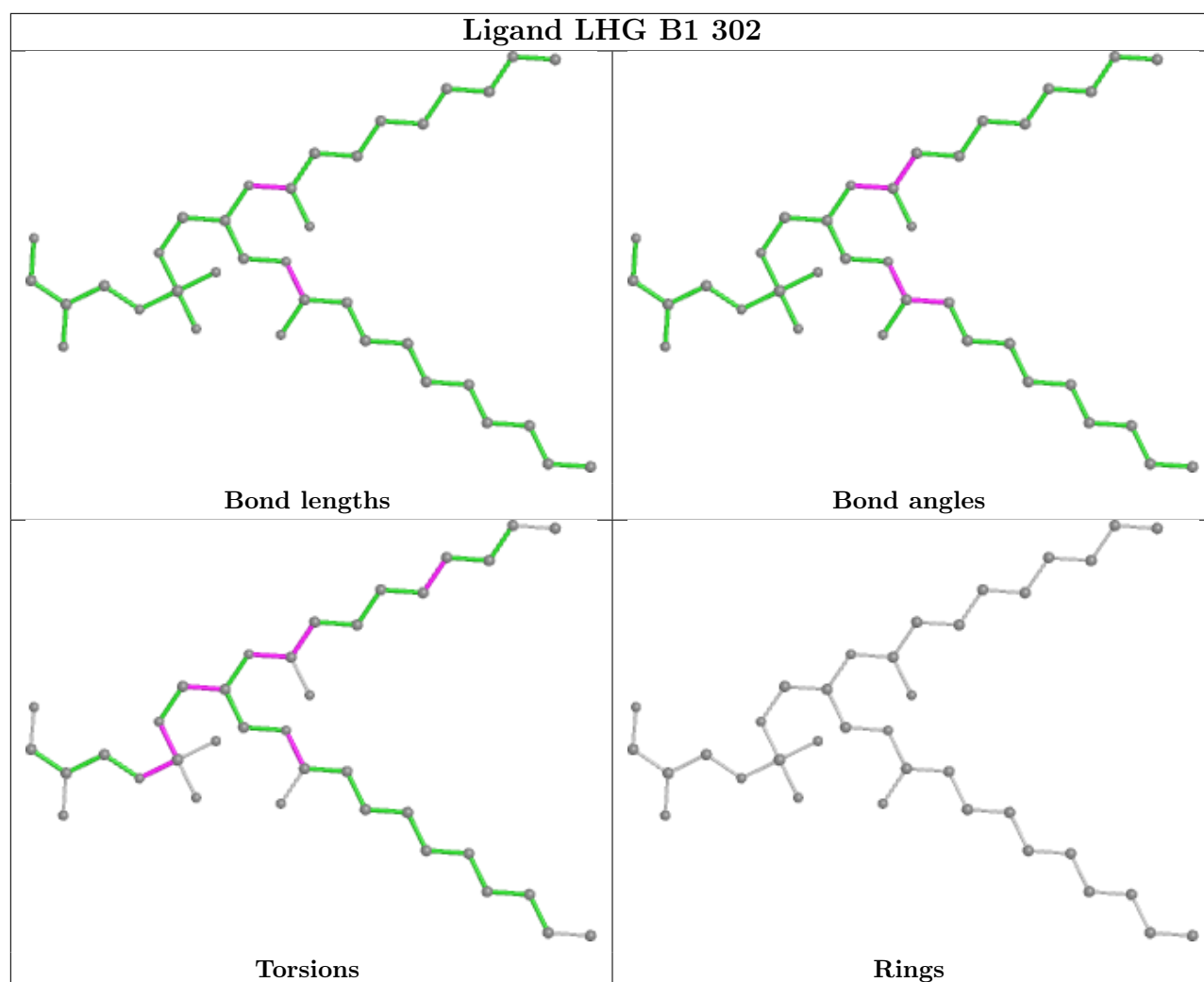


Torsions

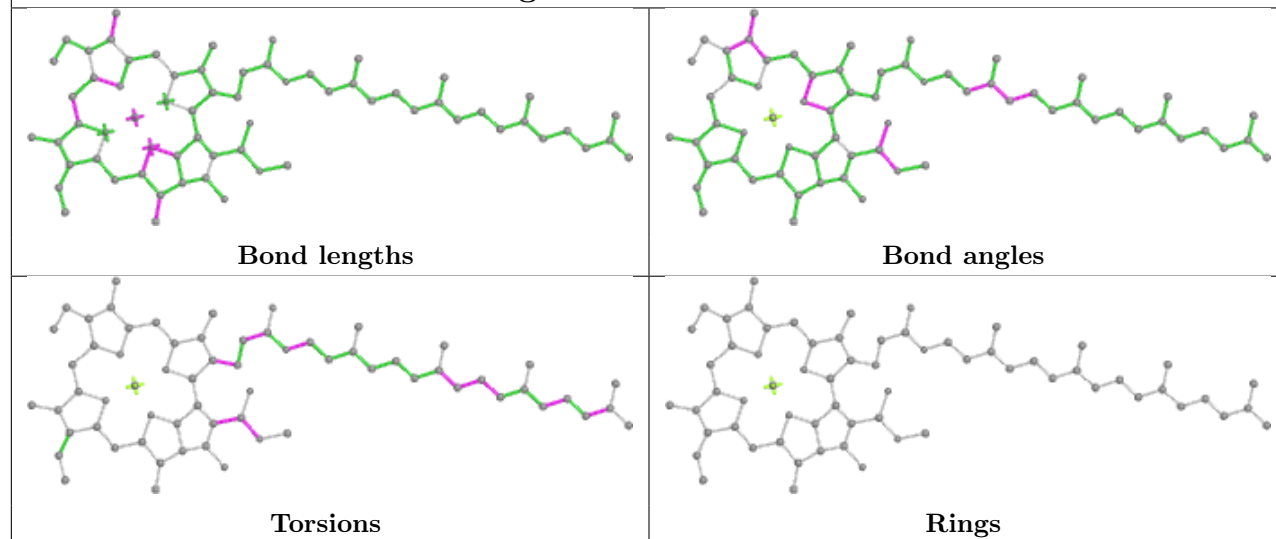


Rings

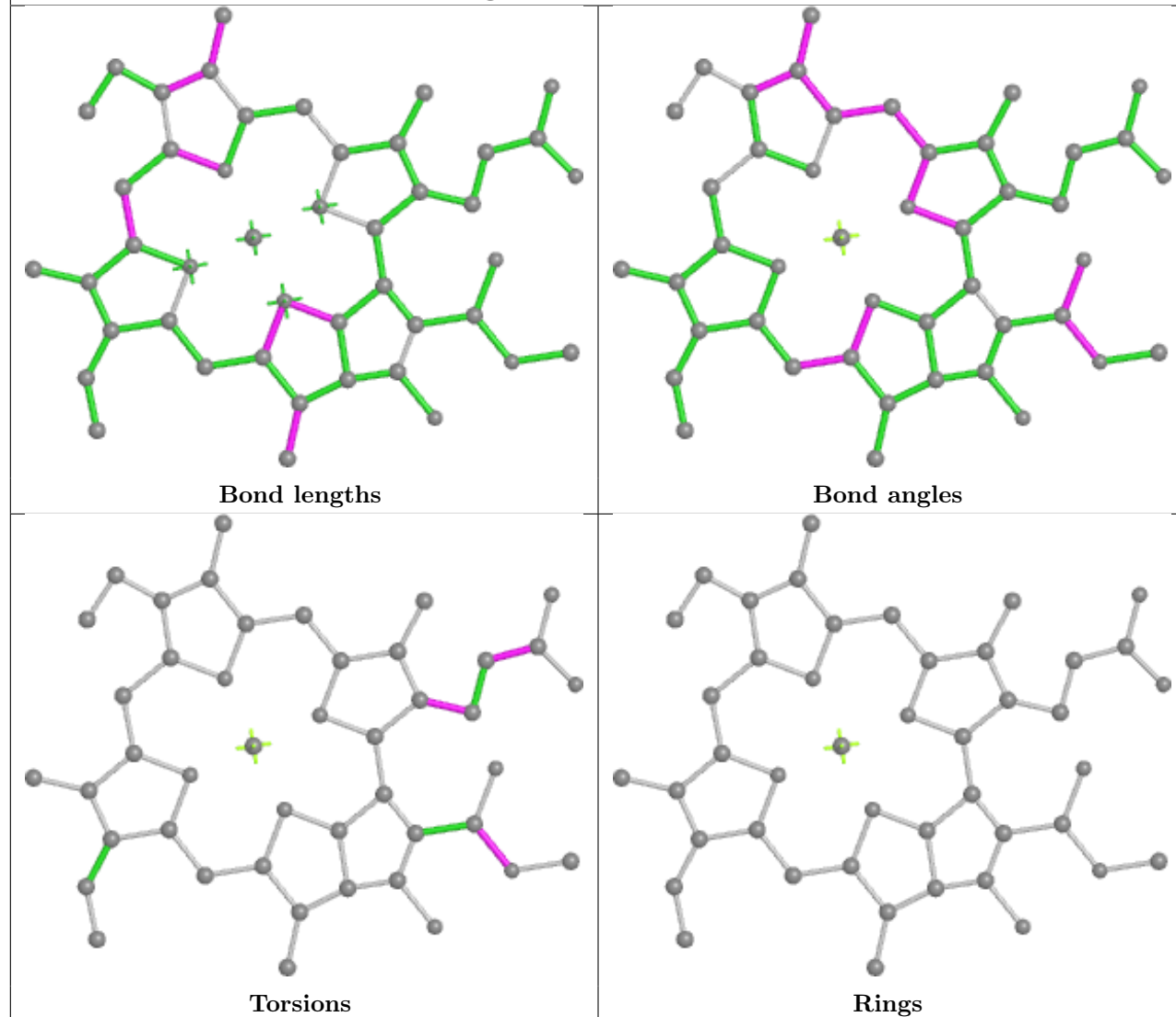




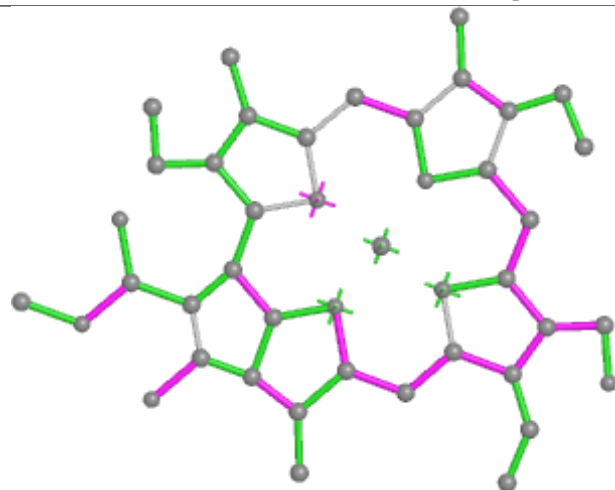
## Ligand CLA BA 825



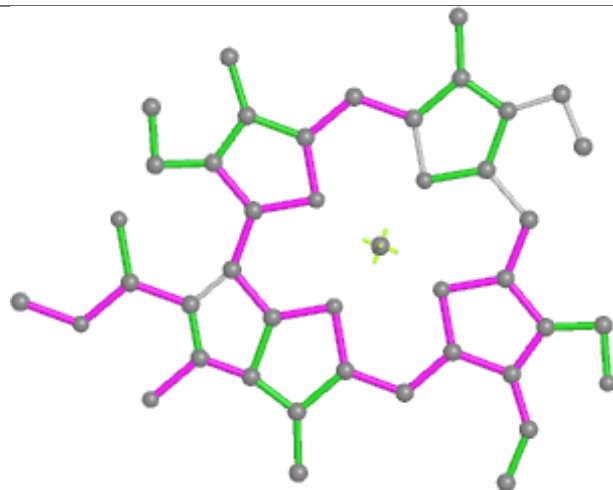
## Ligand CLA B5 613



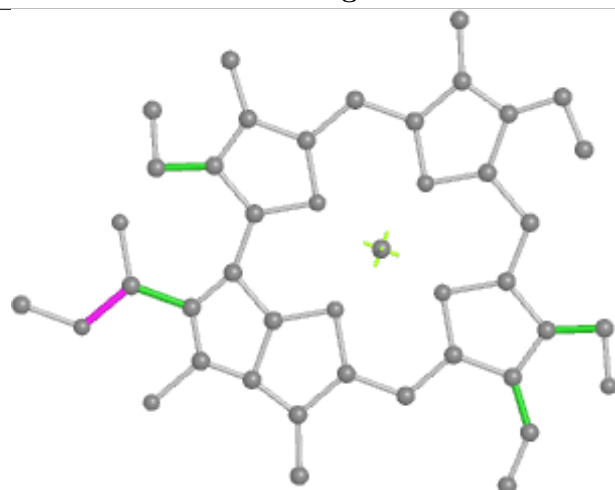
## Ligand CHL B2 305



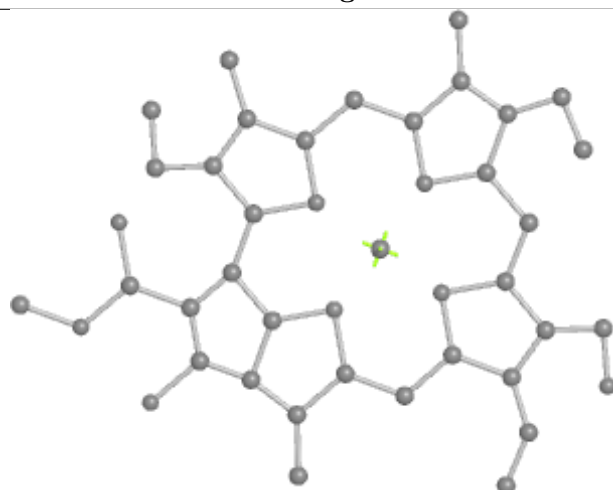
Bond lengths



Bond angles

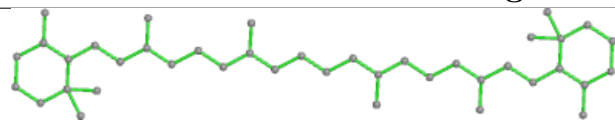


Torsions

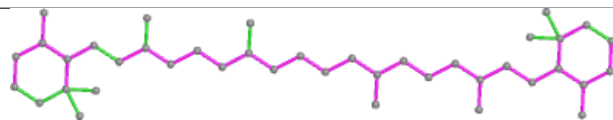


Rings

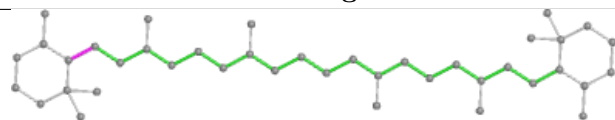
## Ligand BCR B5 616



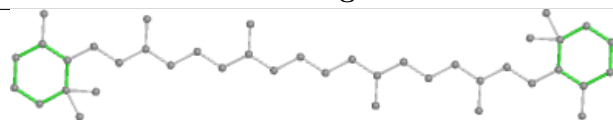
Bond lengths



Bond angles

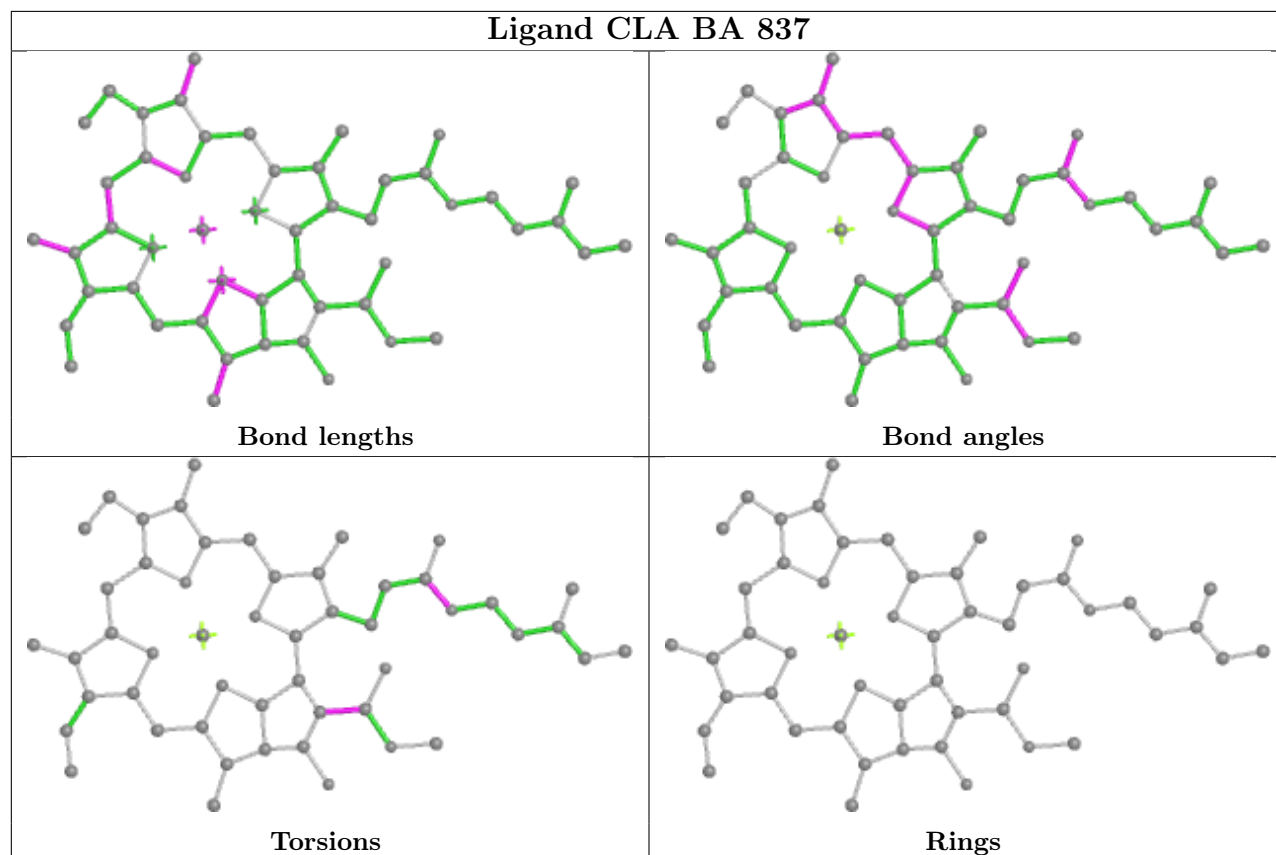
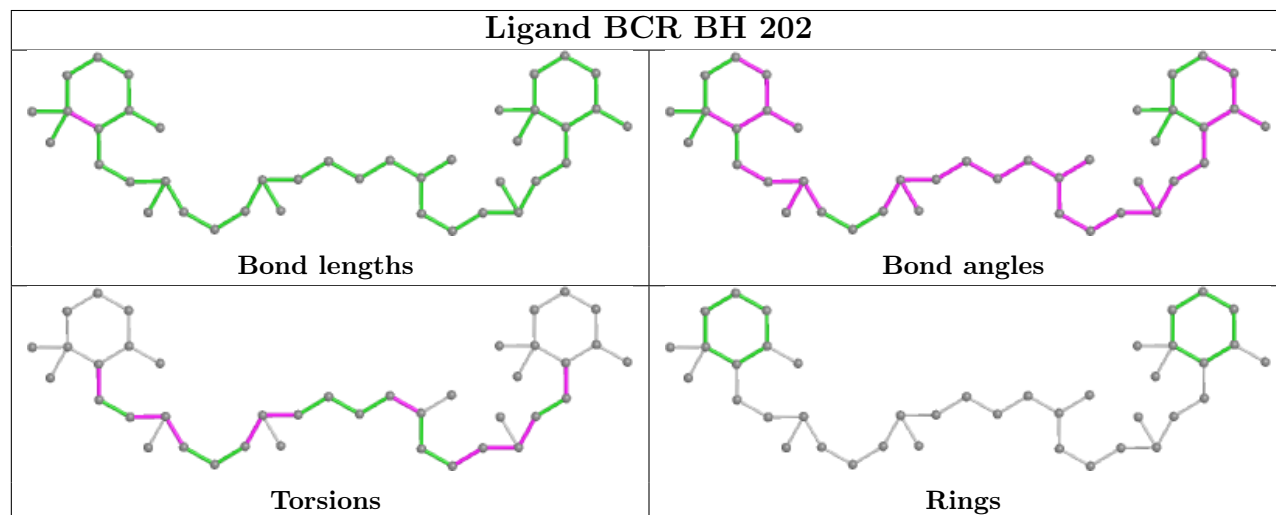
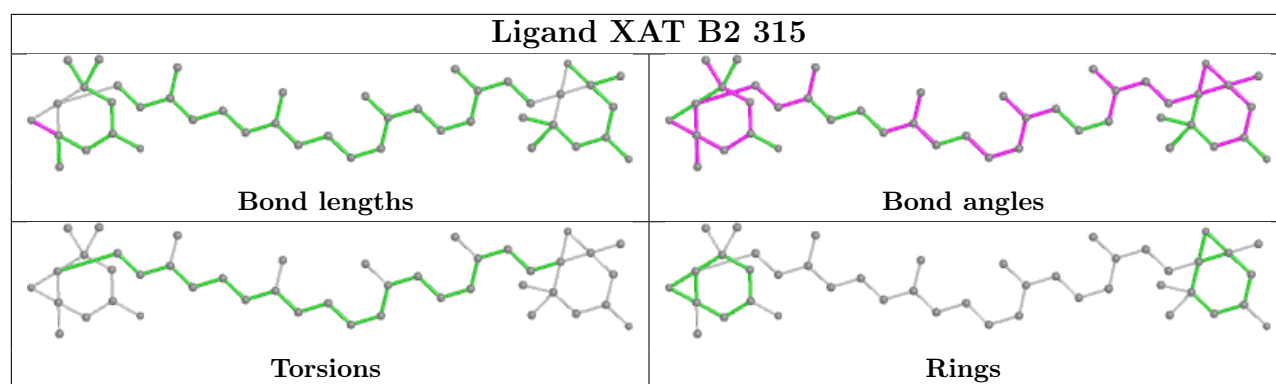


Torsions

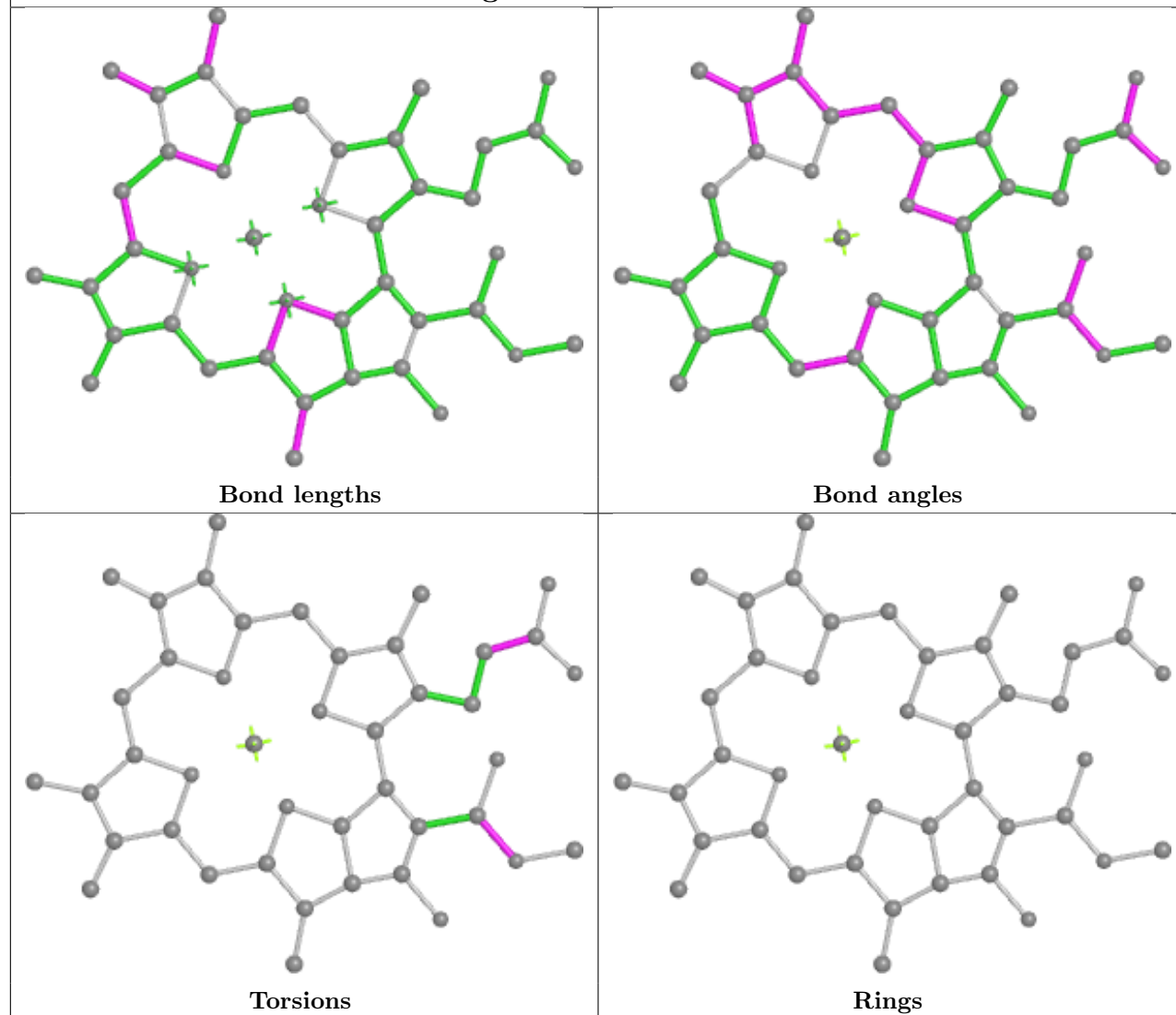


Rings

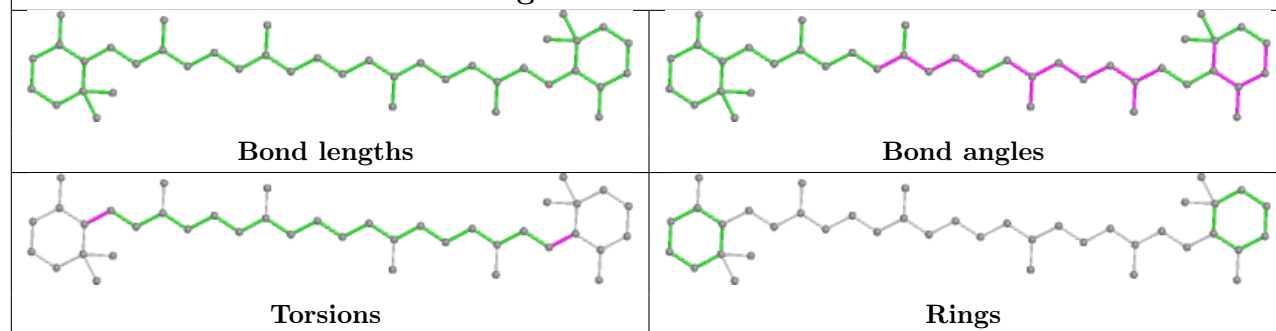




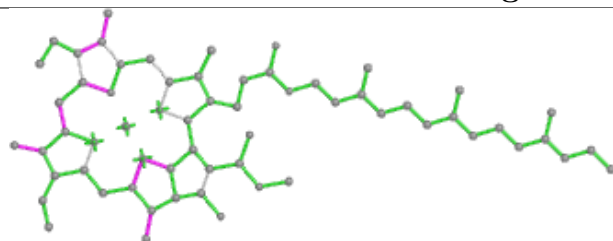
## Ligand CLA B5 604



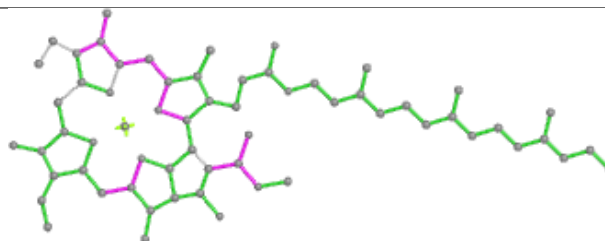
## Ligand BCR BA 850



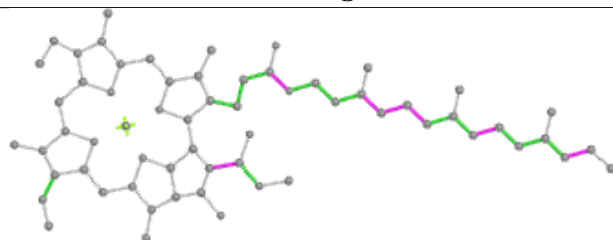
## Ligand CLA BB 827



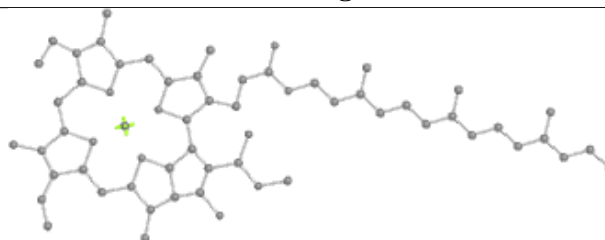
Bond lengths



Bond angles

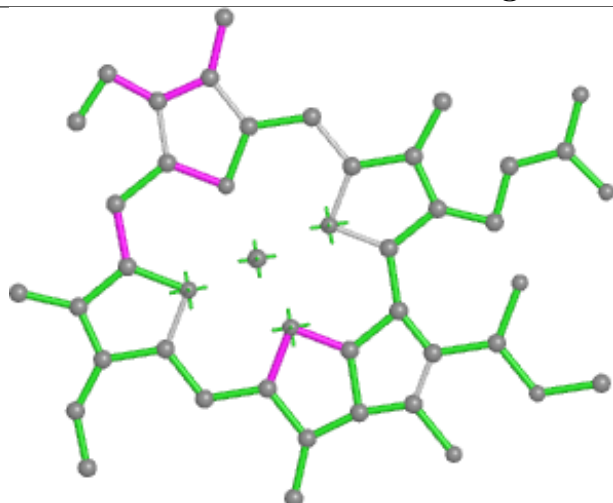


Torsions

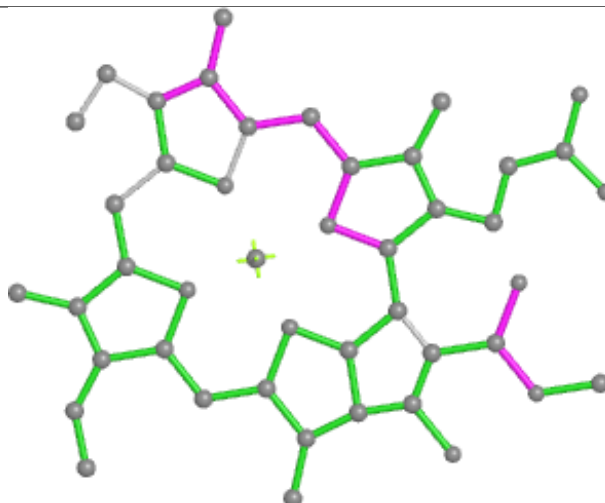


Rings

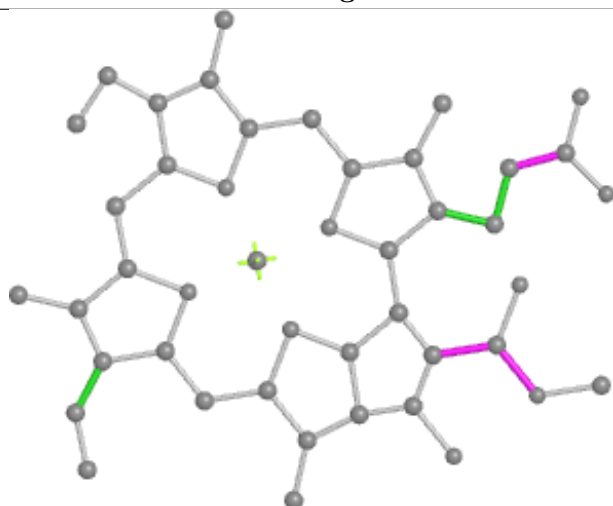
## Ligand CLA BA 835



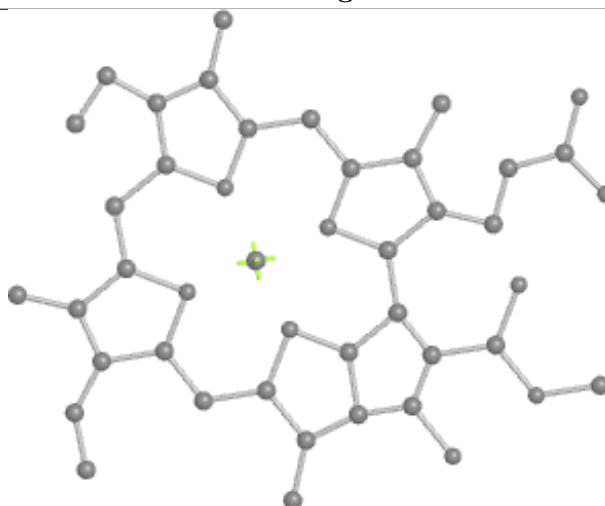
Bond lengths



Bond angles

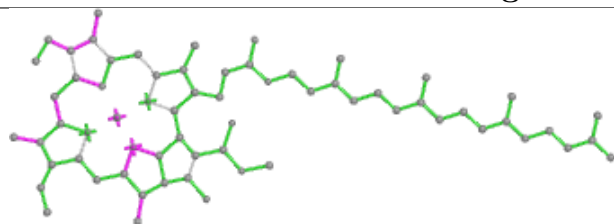


Torsions

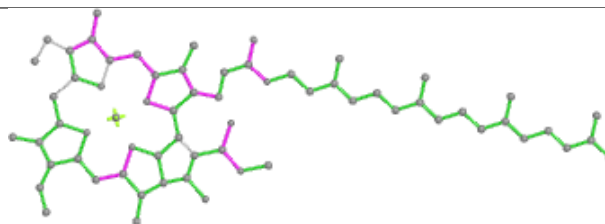


Rings

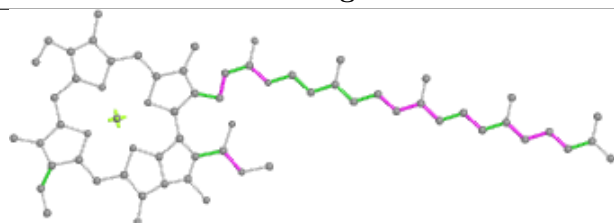
## Ligand CLA BB 811



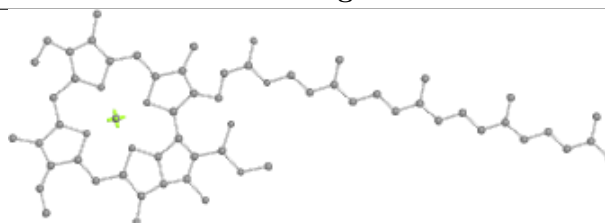
Bond lengths



Bond angles

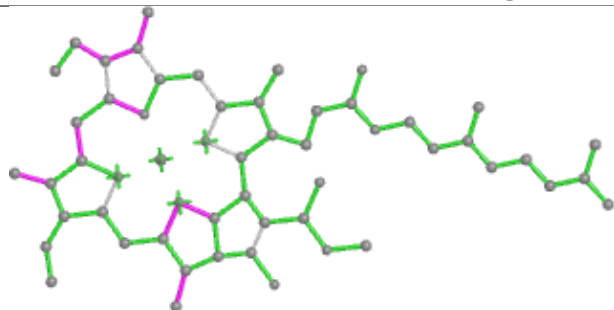


Torsions

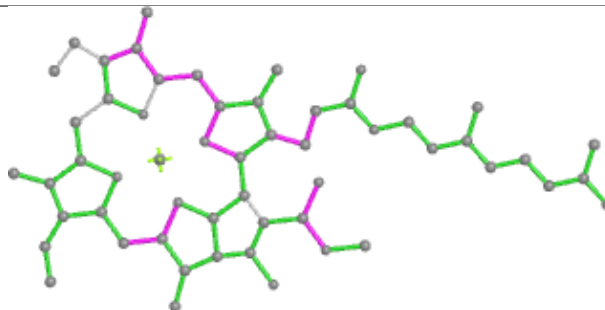


Rings

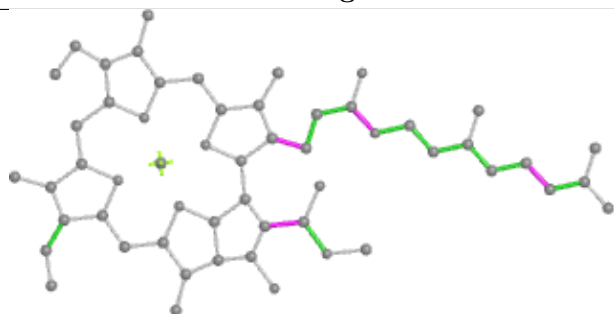
## Ligand CLA BA 824



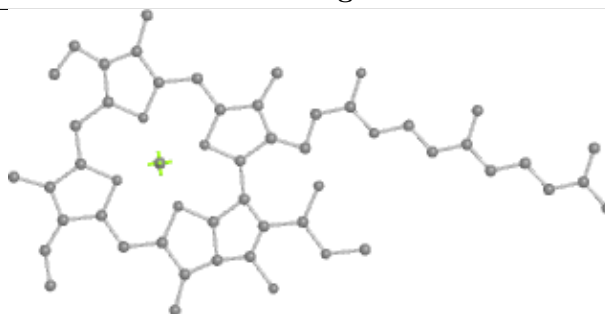
Bond lengths



Bond angles

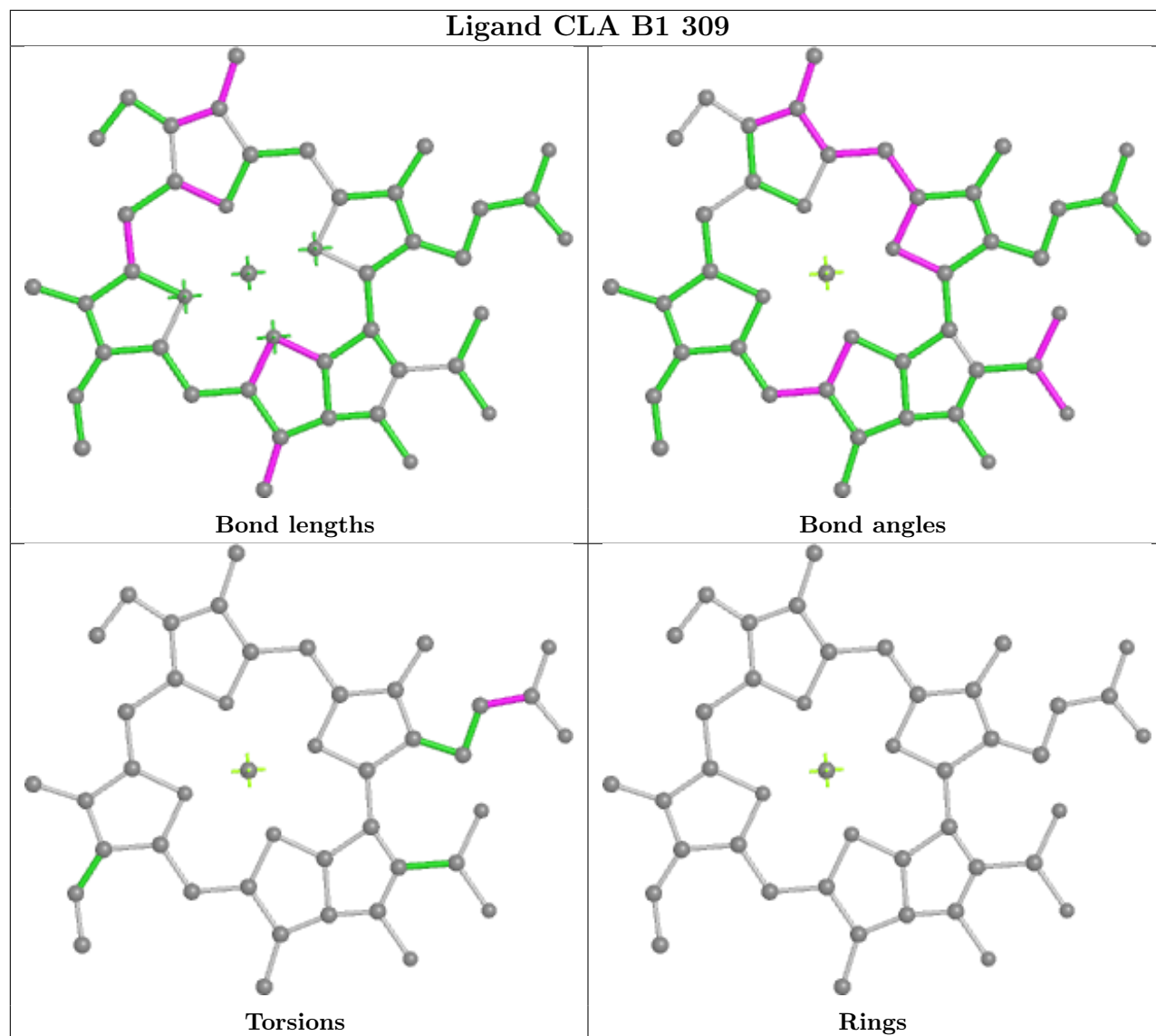


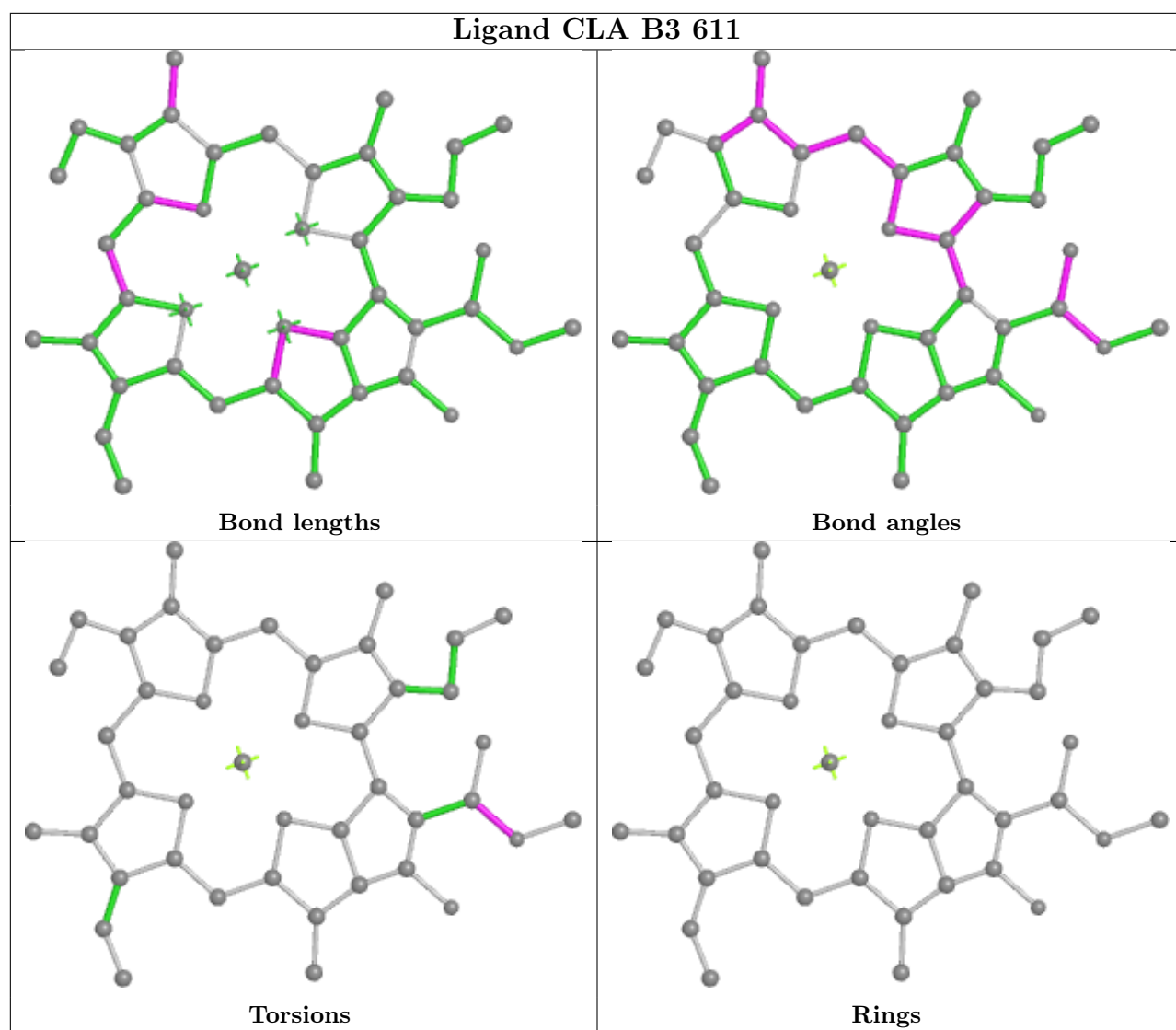
Torsions



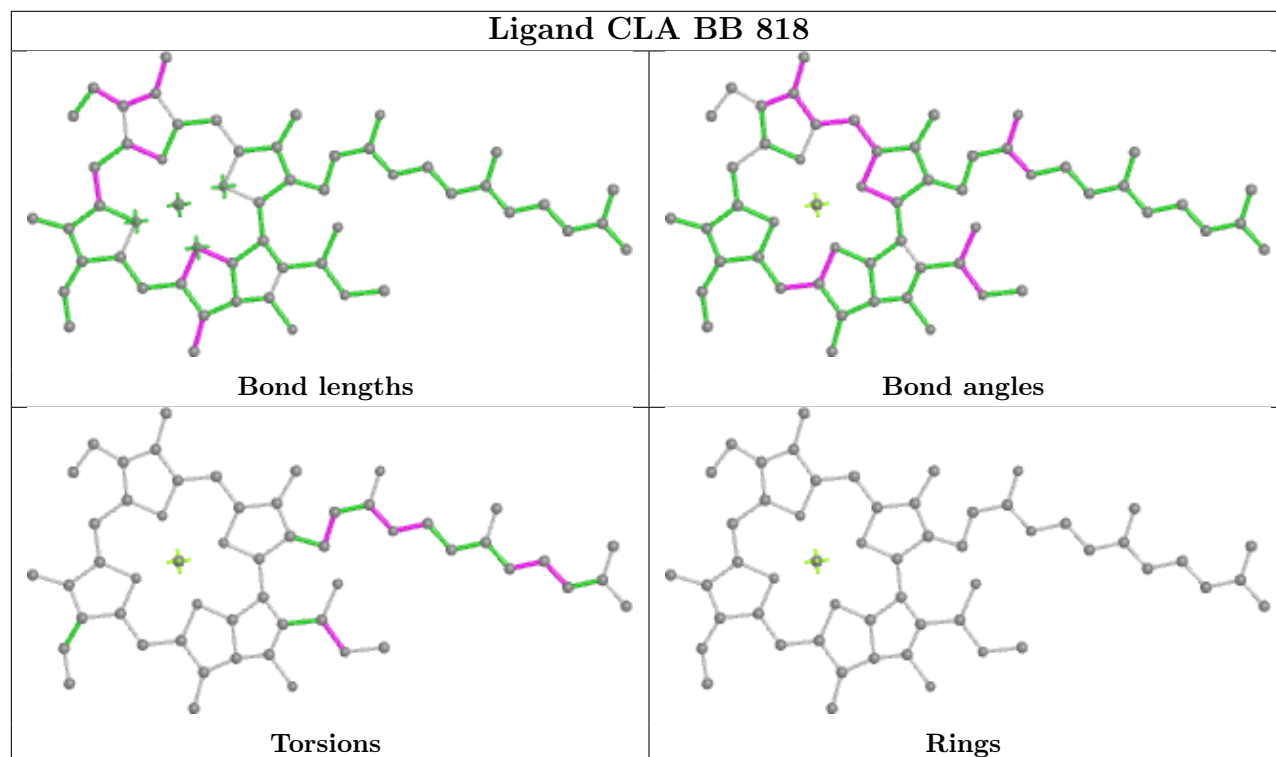
Rings

## Ligand CLA B1 309

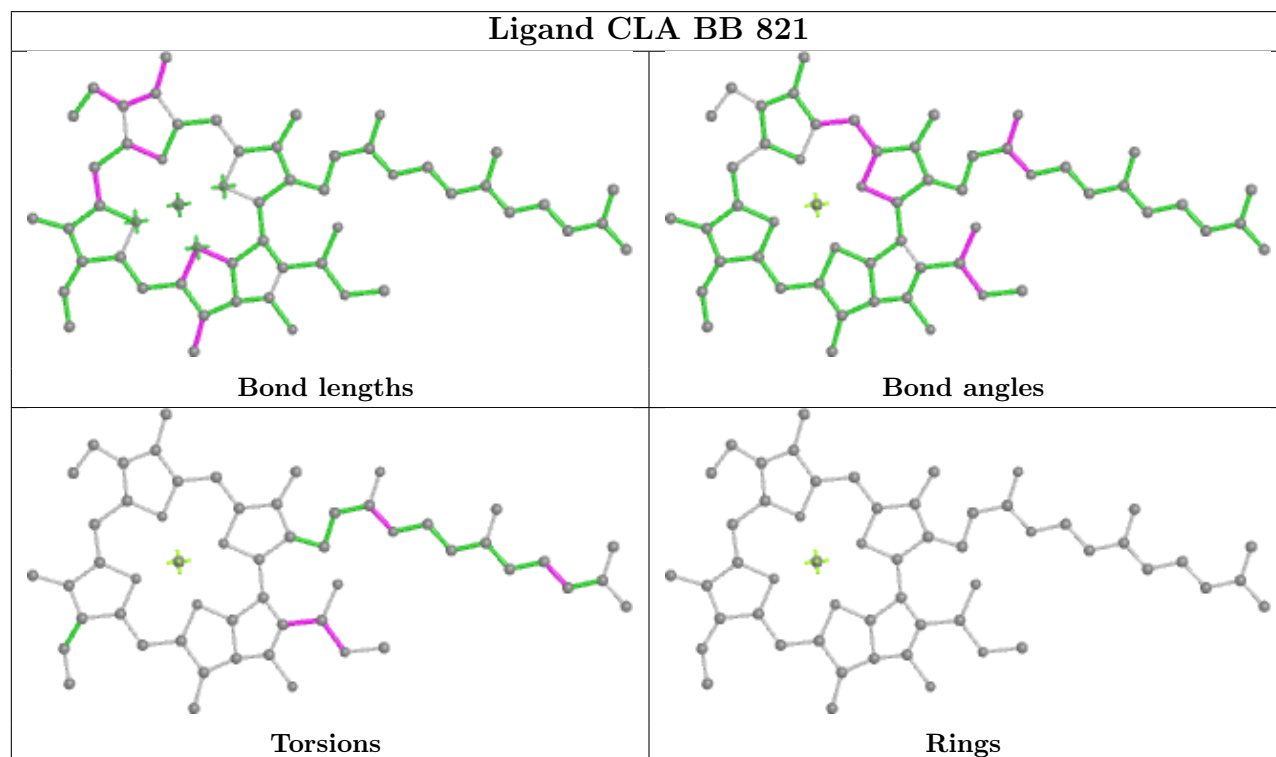


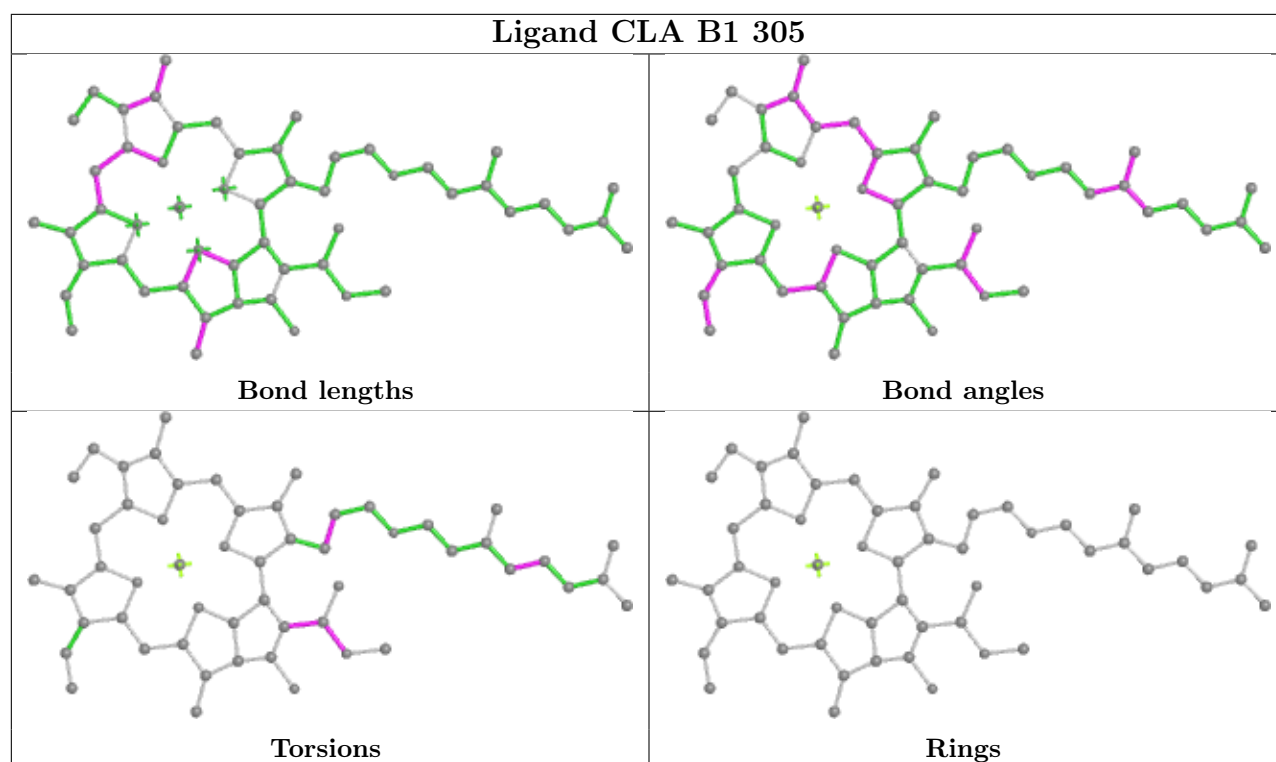


## Ligand CLA BB 818

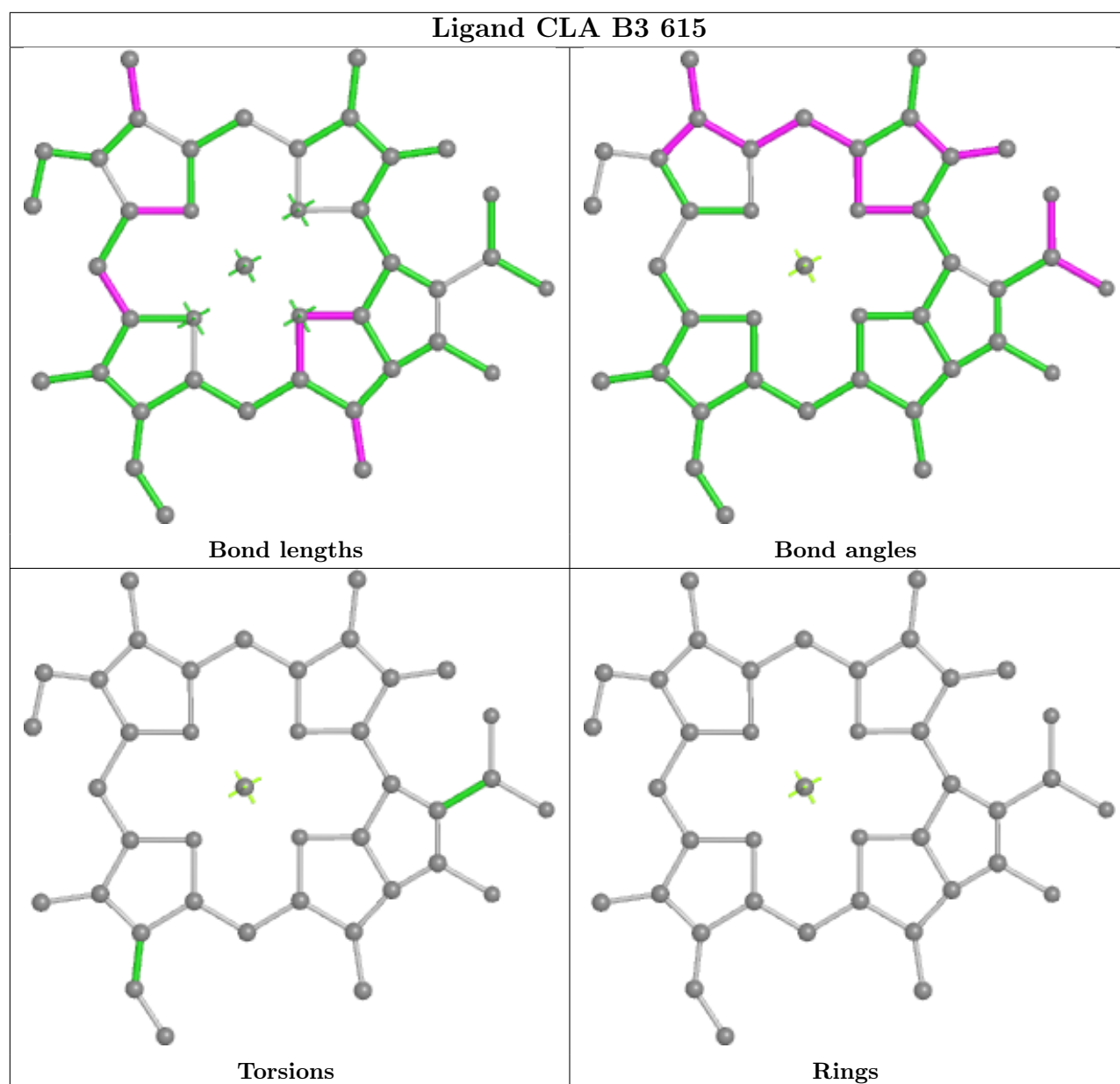


## Ligand CLA BB 821

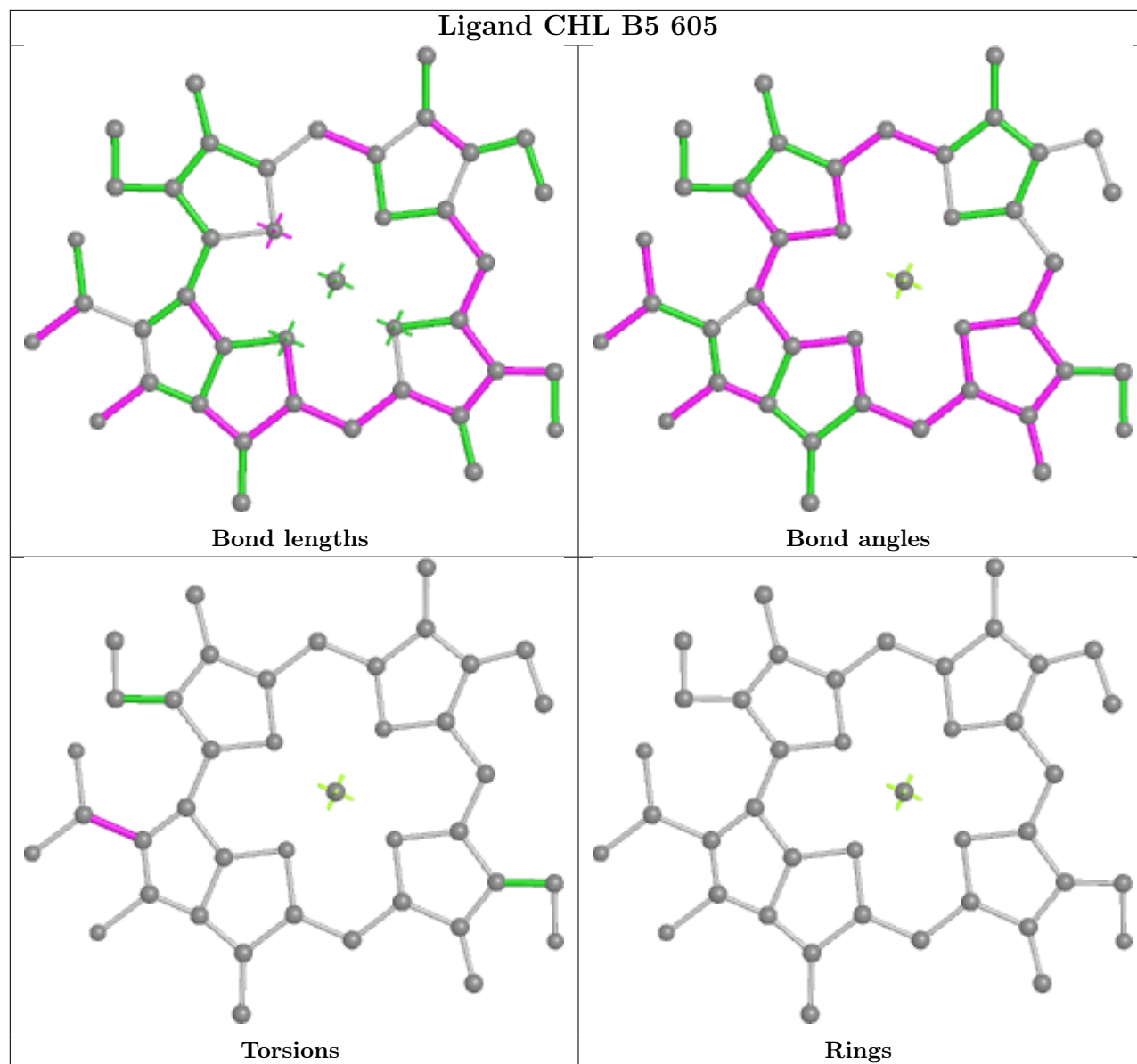




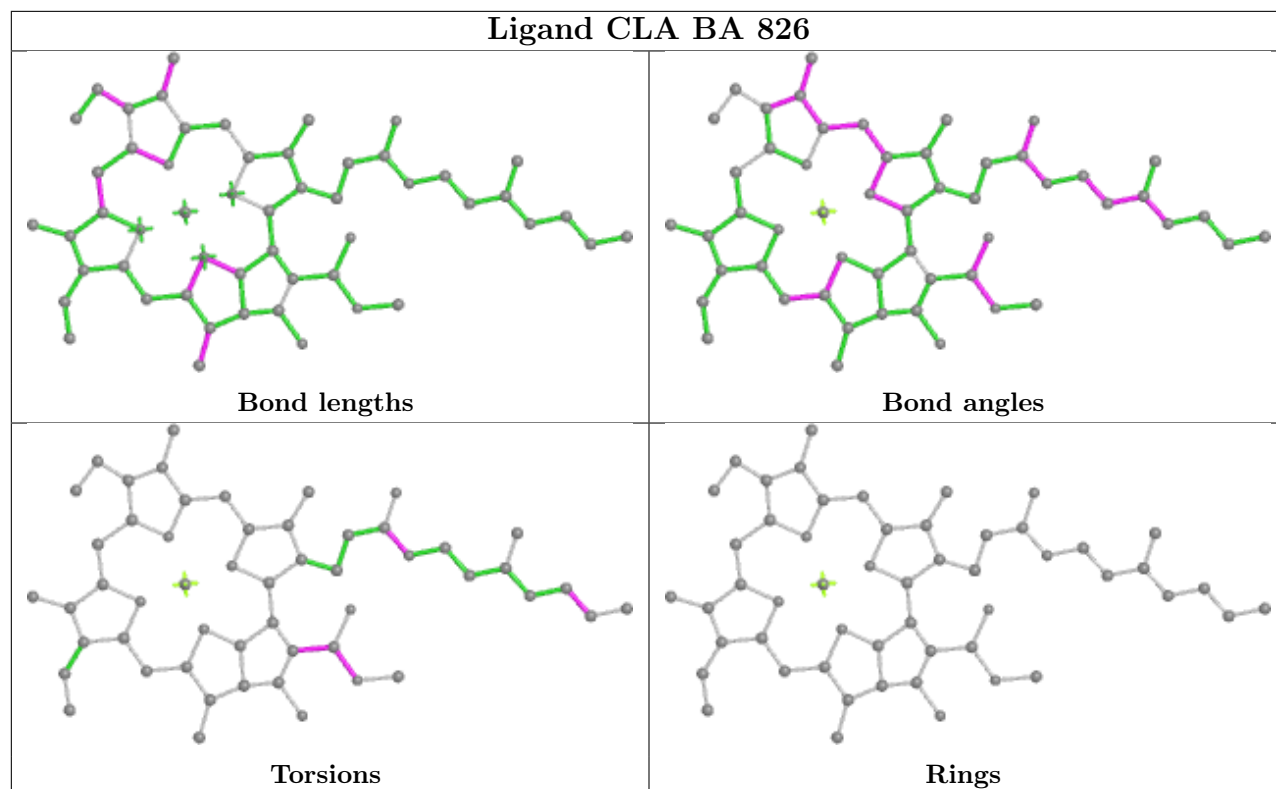




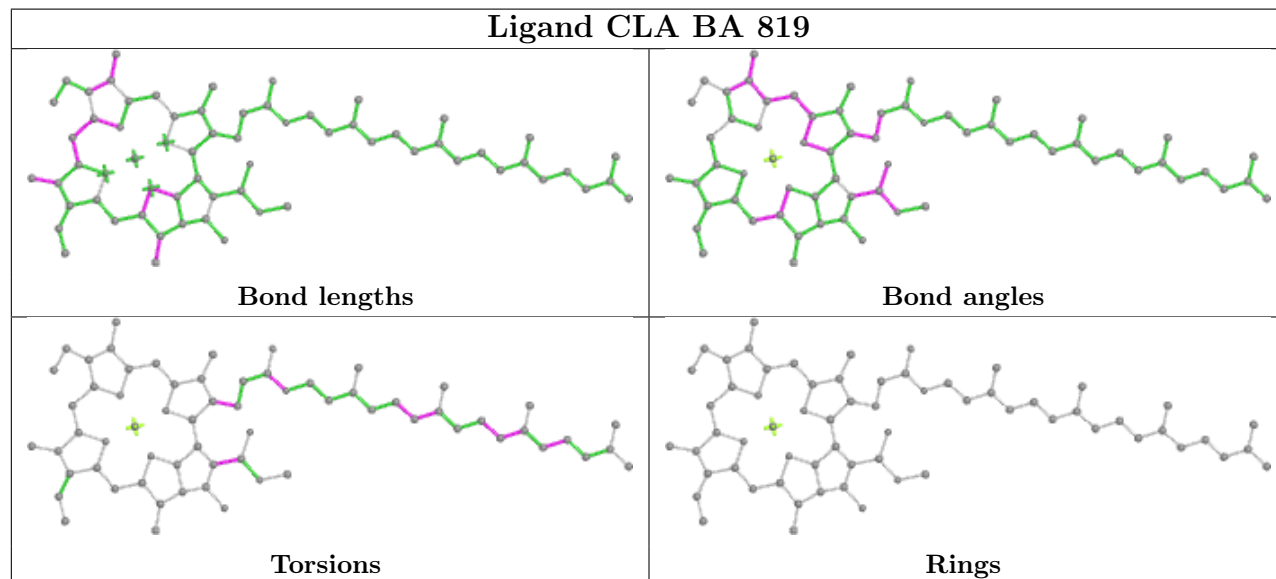
## Ligand CHL B5 605

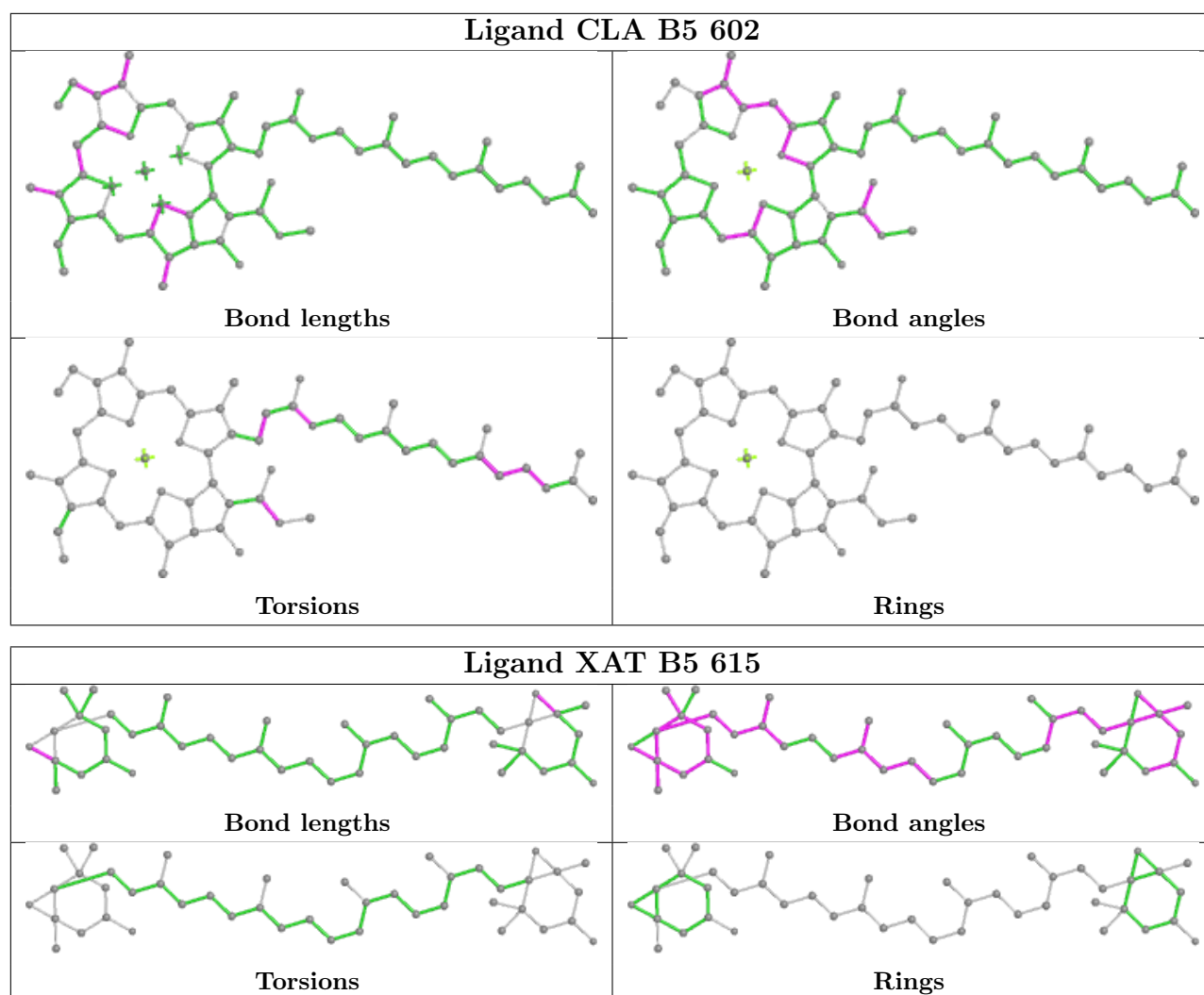


## Ligand CLA BA 826

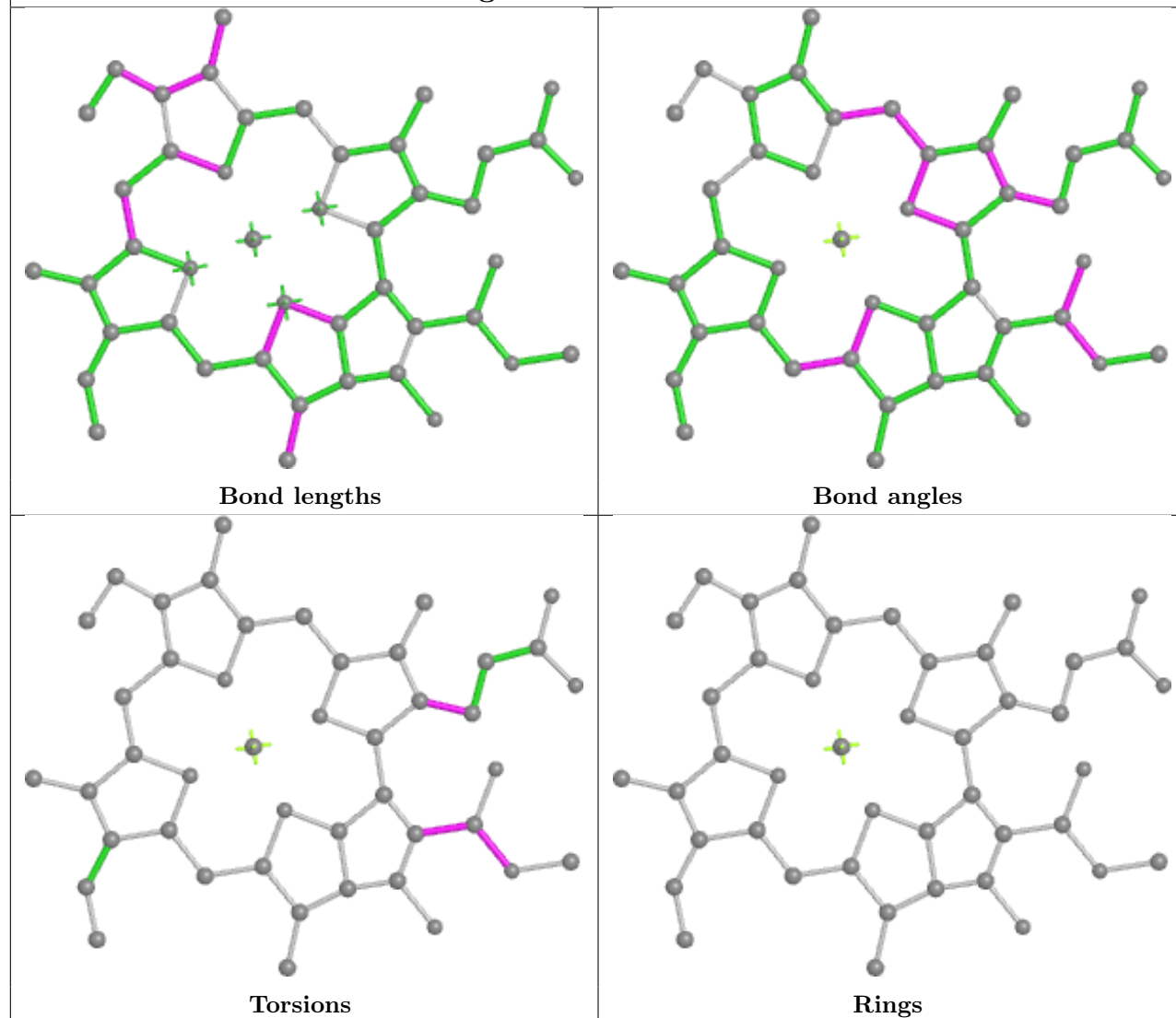


## Ligand CLA BA 819

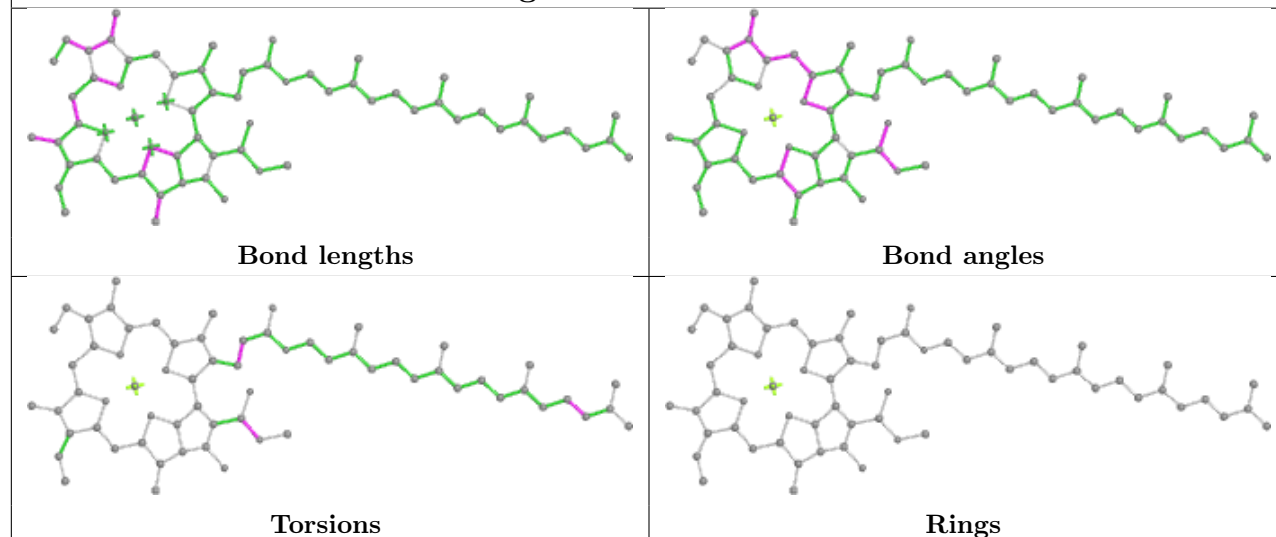


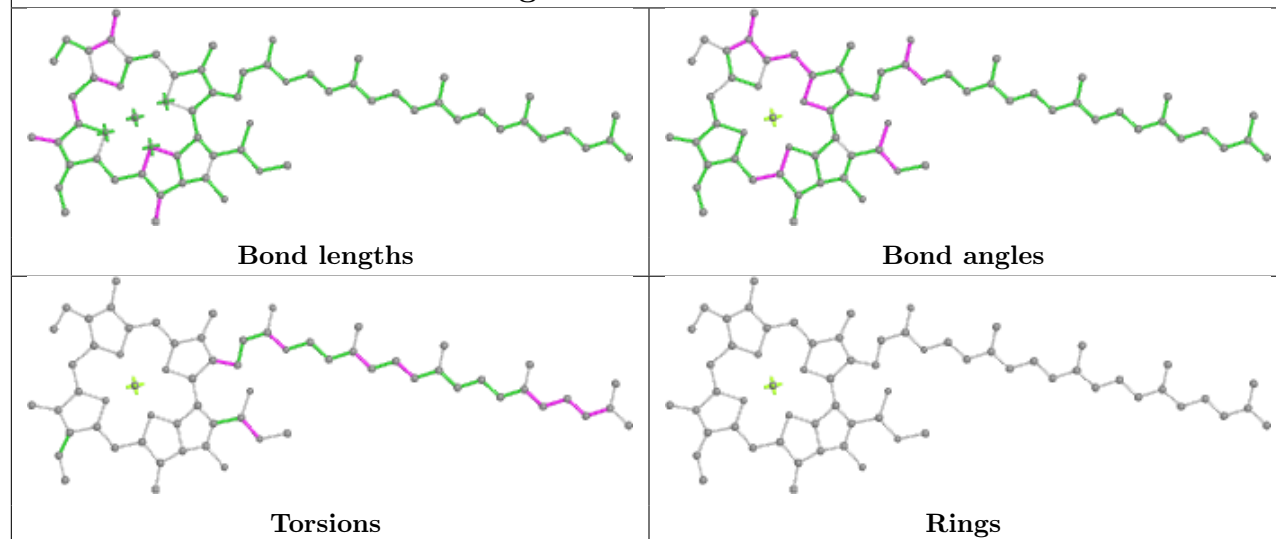
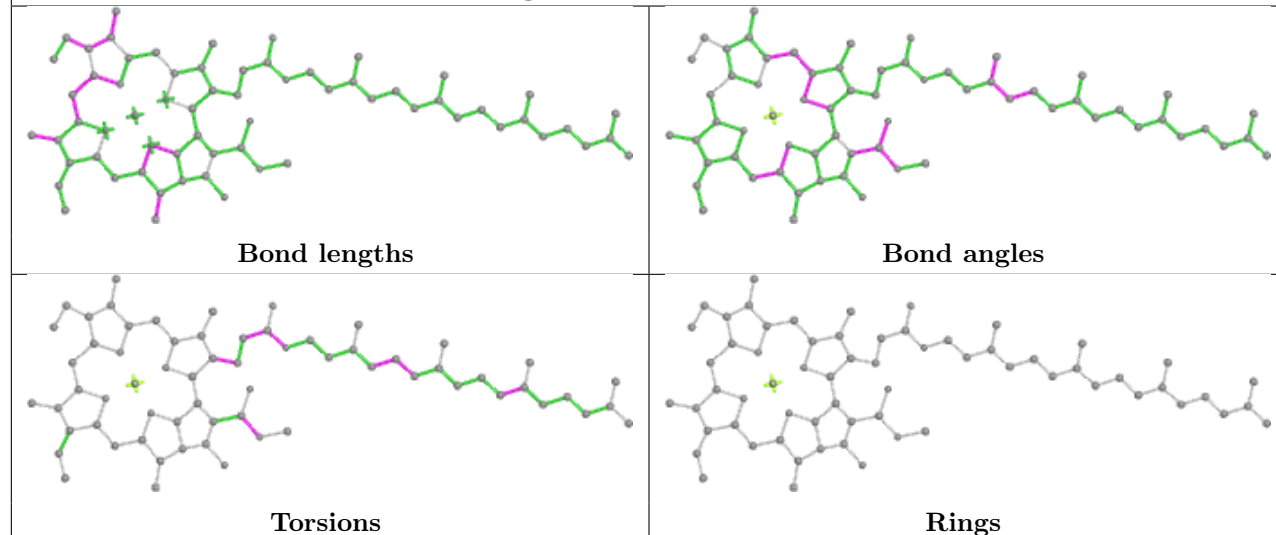
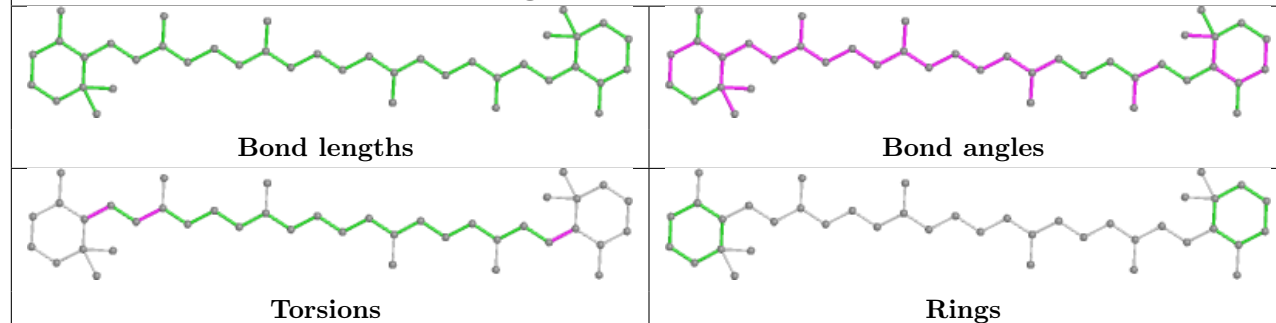


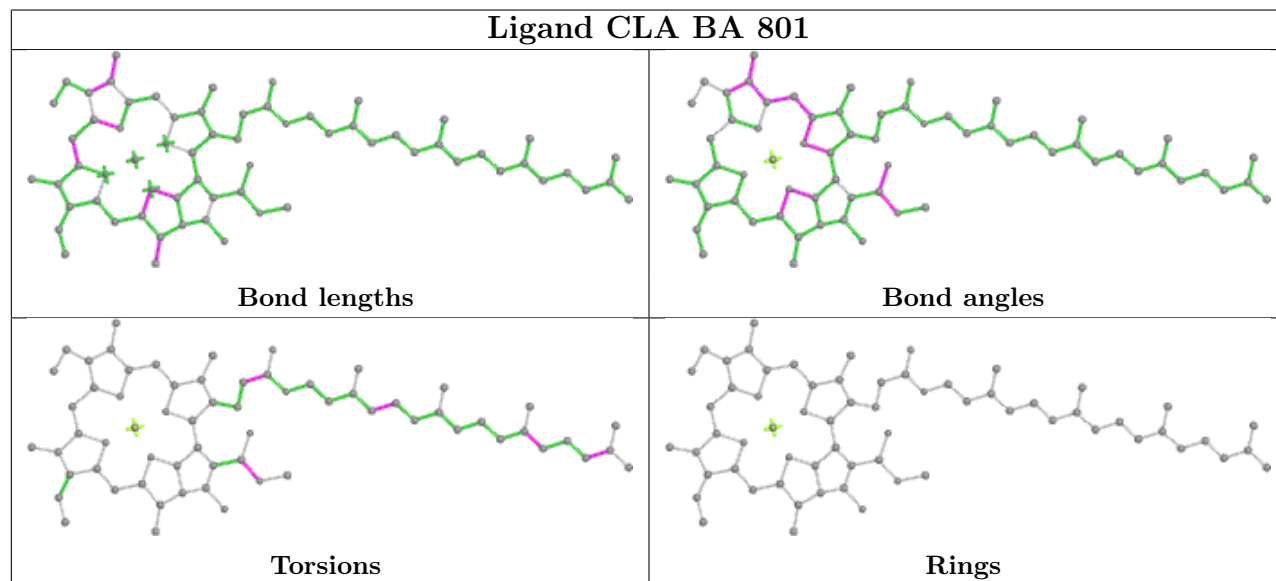
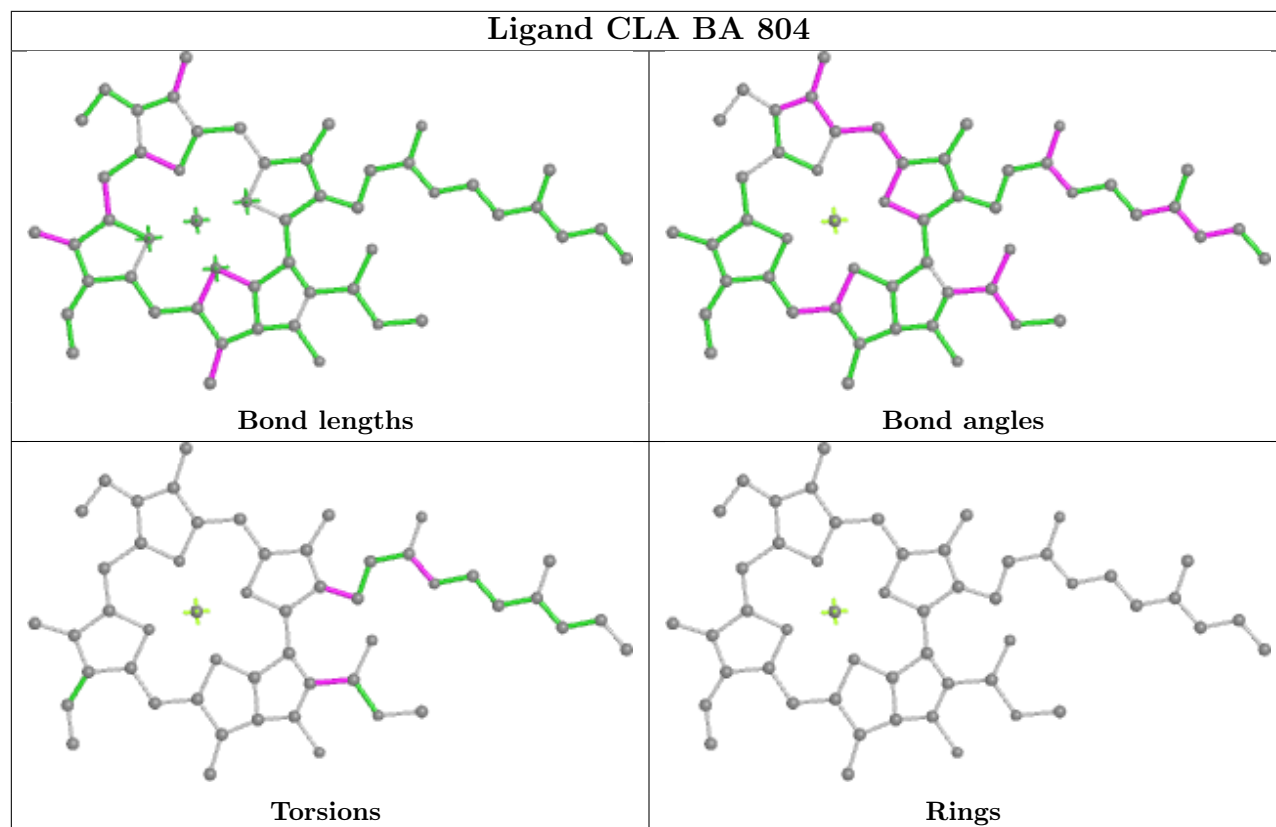
## Ligand CLA BB 825

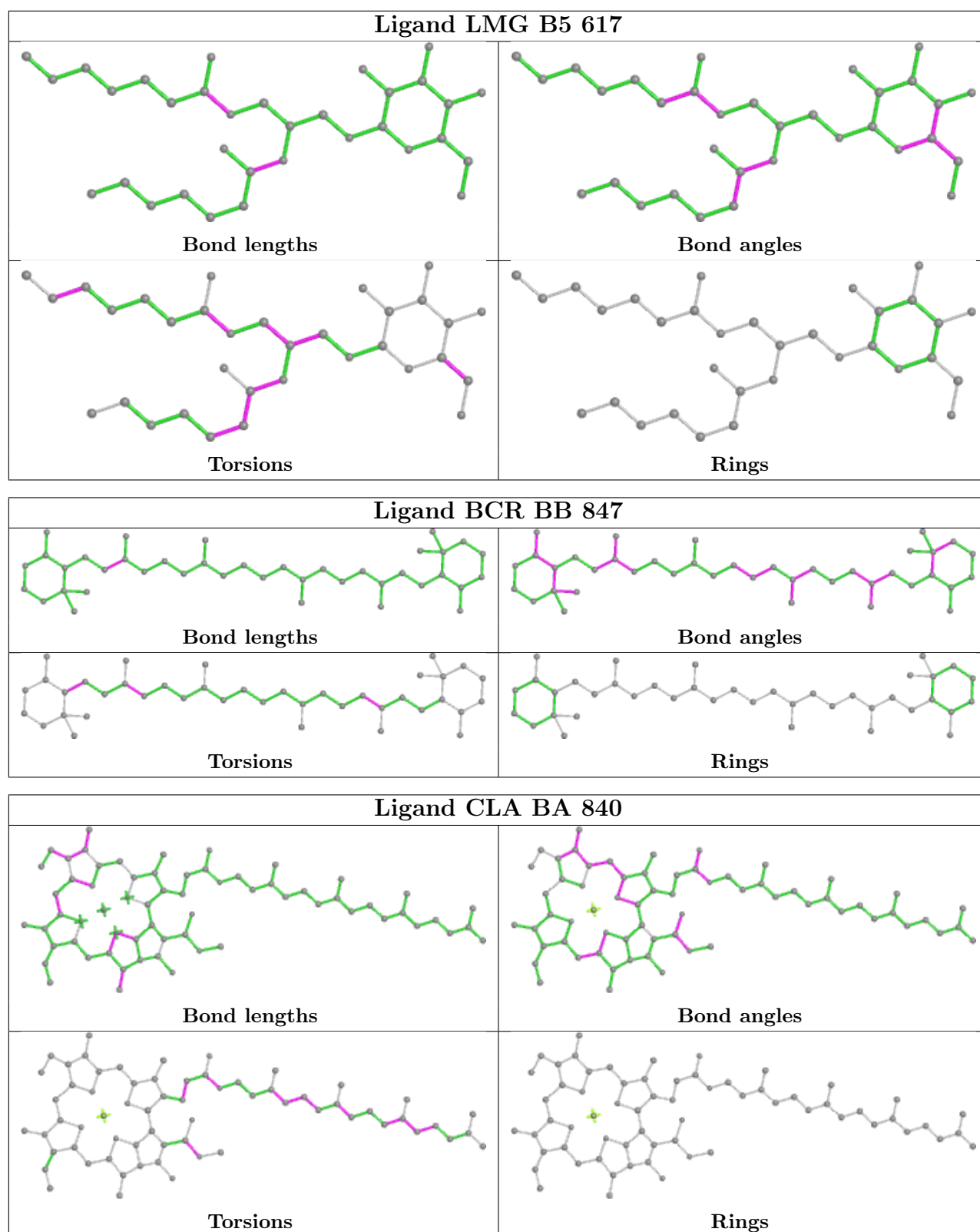


## Ligand CLA BA 802



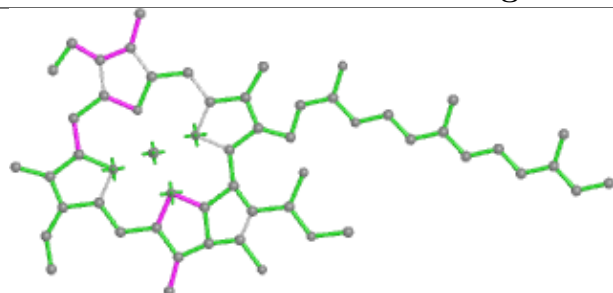
**Ligand CLA BA 811****Ligand CLA BB 834****Ligand BCR BJ 103**



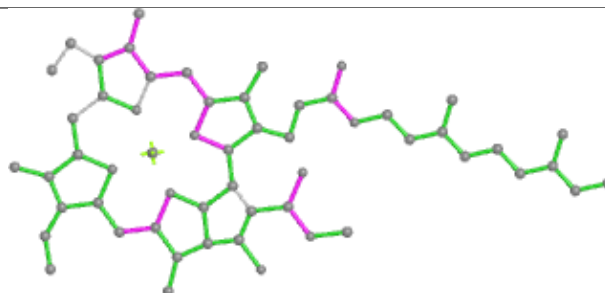




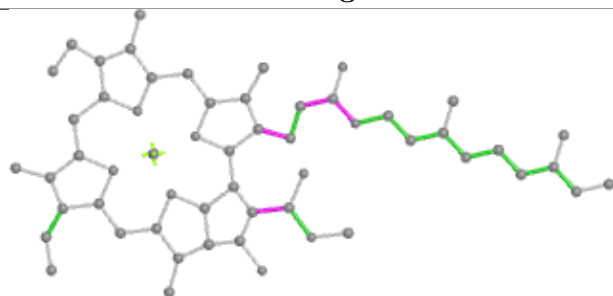
## Ligand CLA BA 818



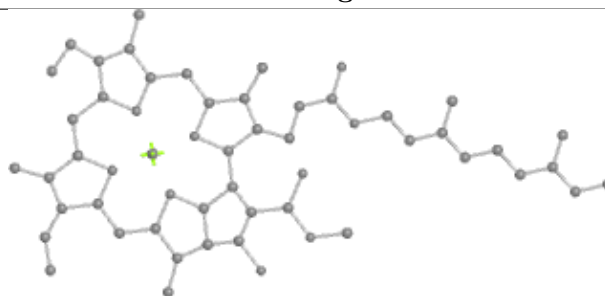
Bond lengths



Bond angles

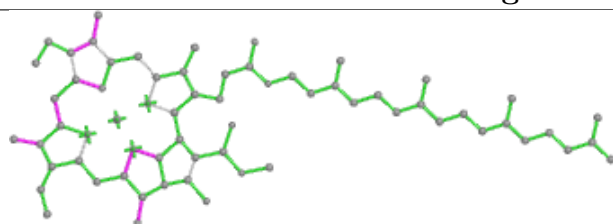


Torsions

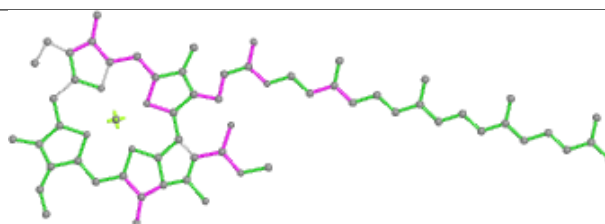


Rings

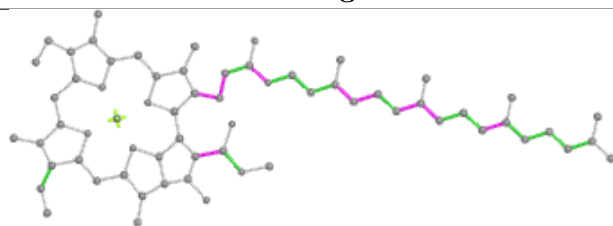
## Ligand CLA BB 810



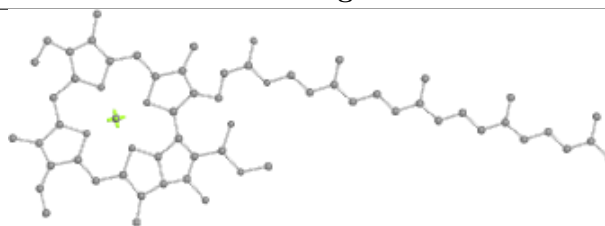
Bond lengths



Bond angles

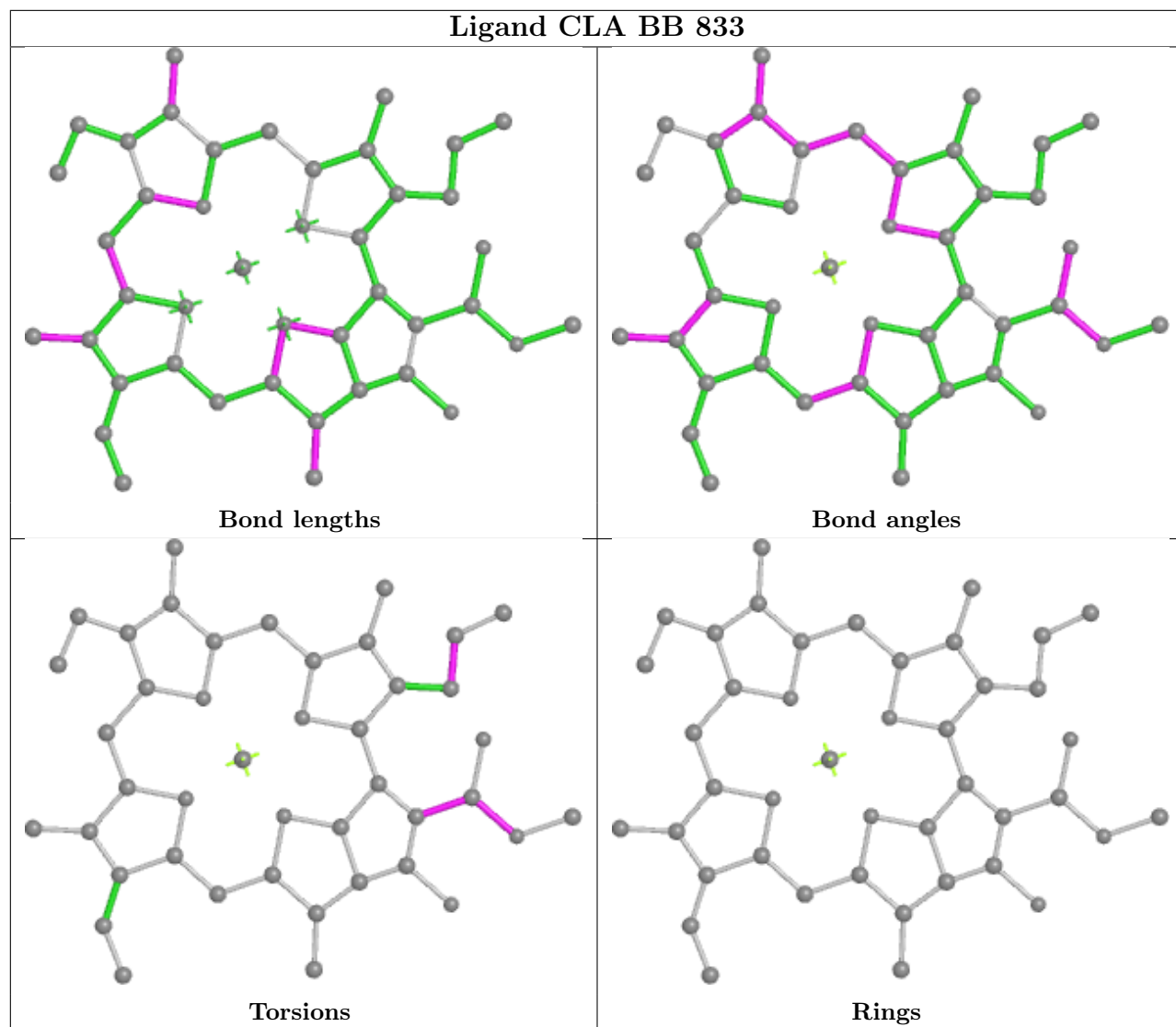


Torsions

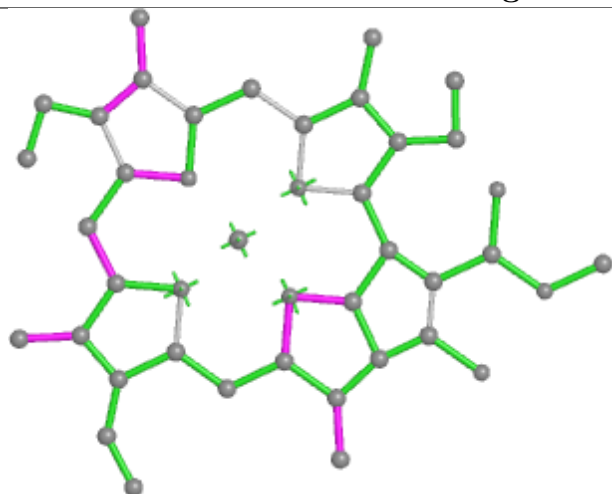


Rings

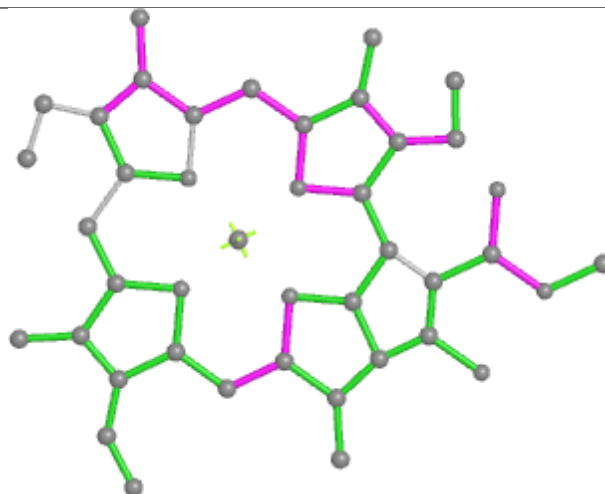
## Ligand CLA BB 833



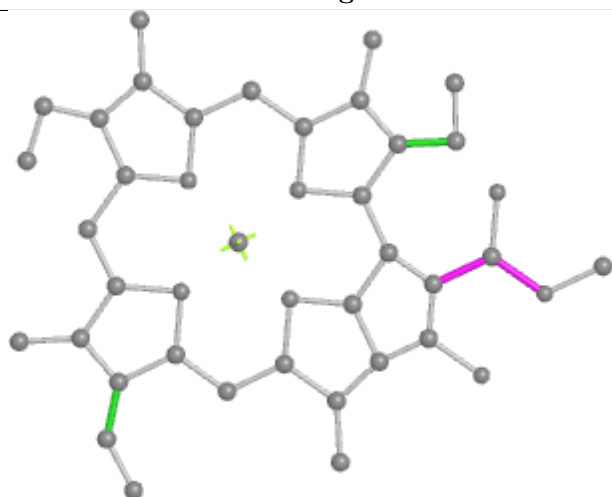
## Ligand CLA BF 302



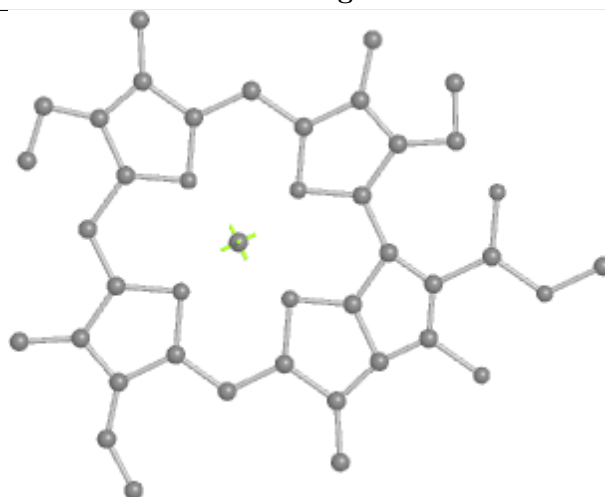
Bond lengths



Bond angles

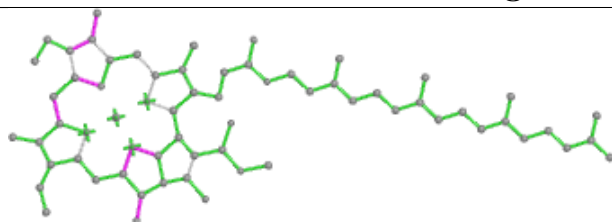


Torsions

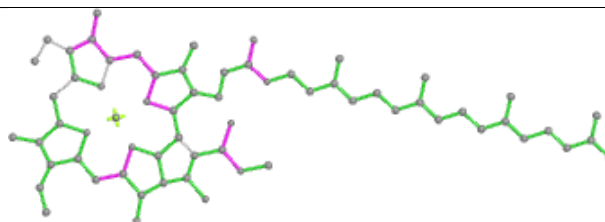


Rings

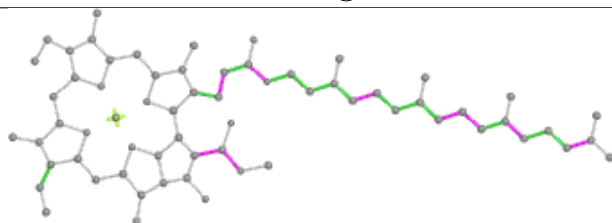
## Ligand CLA B2 311



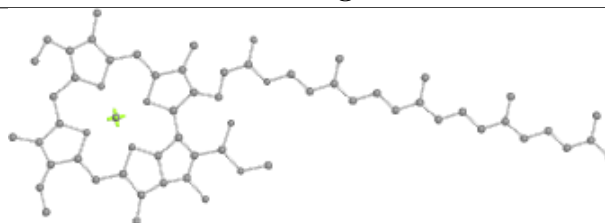
Bond lengths



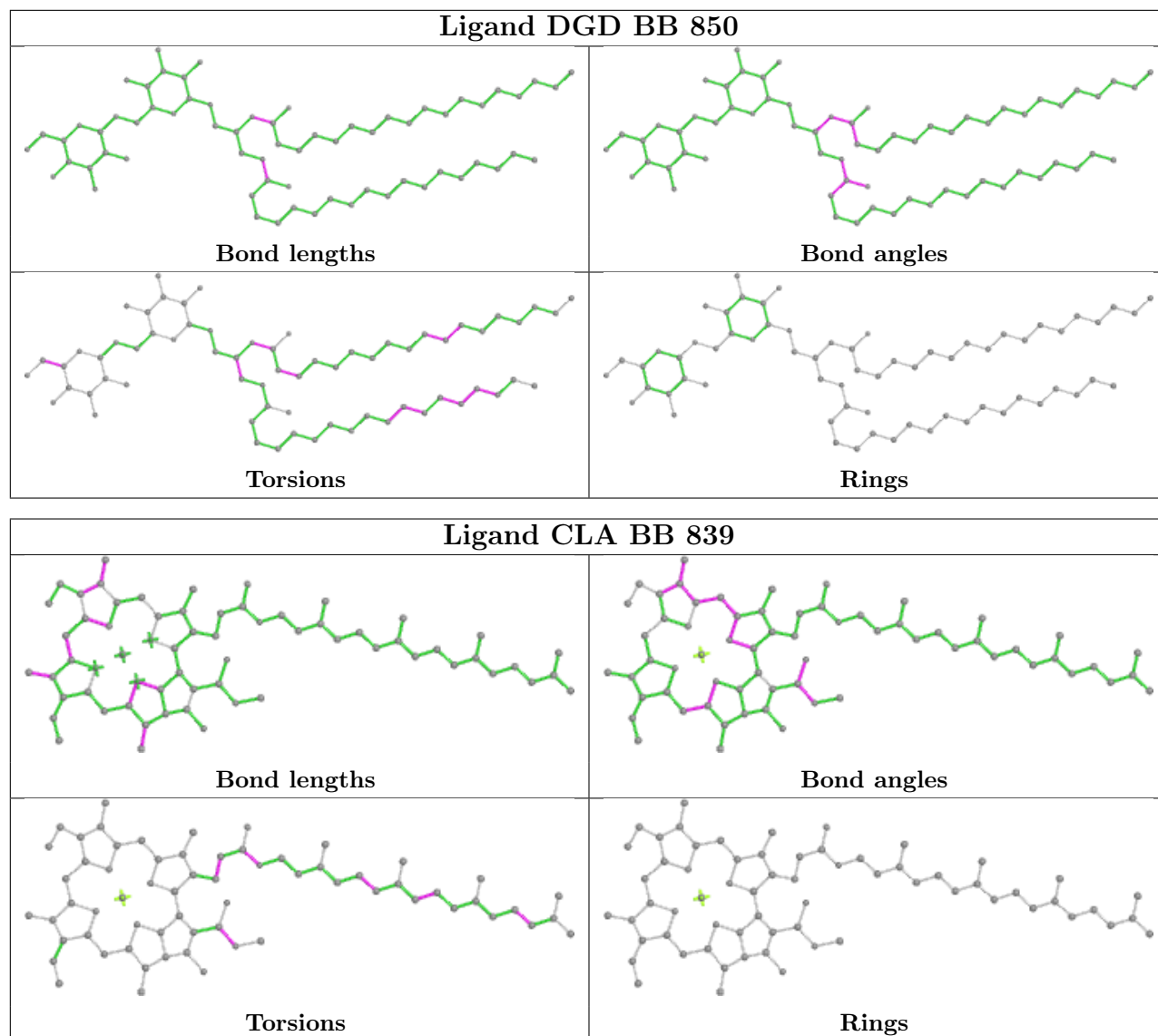
Bond angles



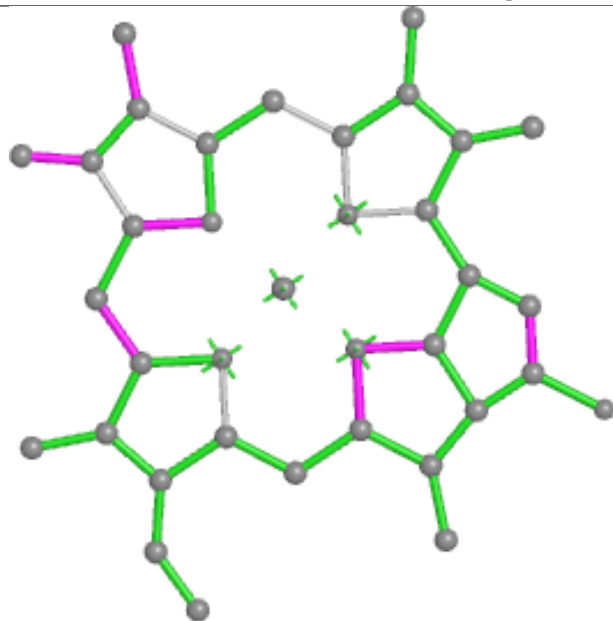
Torsions



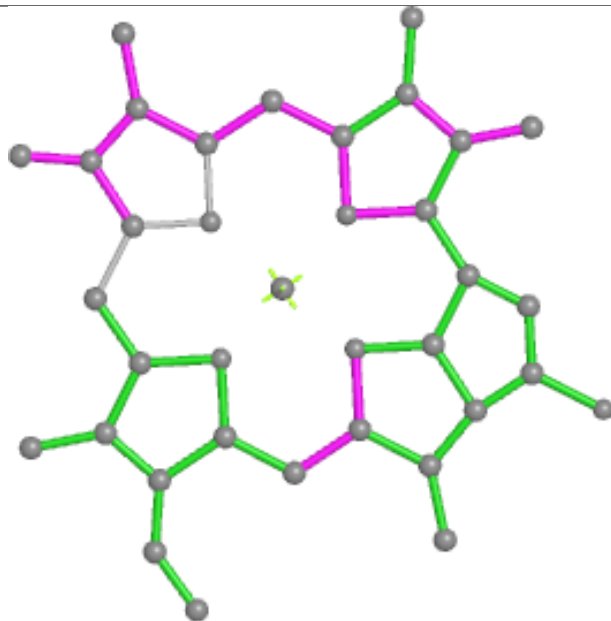
Rings



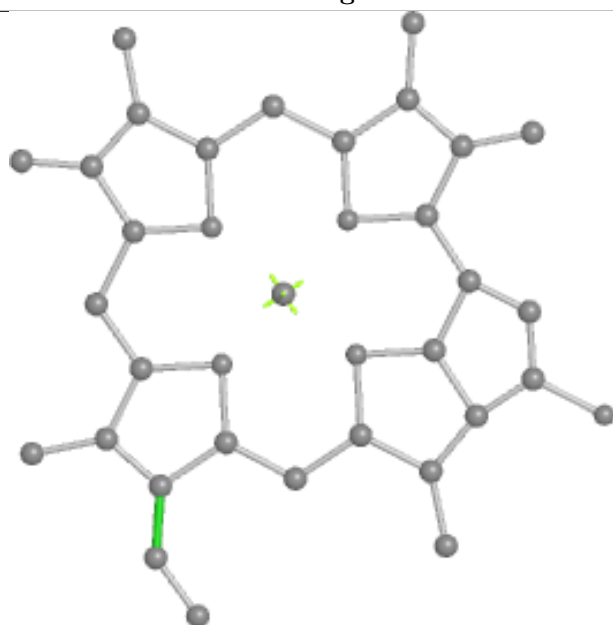
## Ligand CLA BK 201



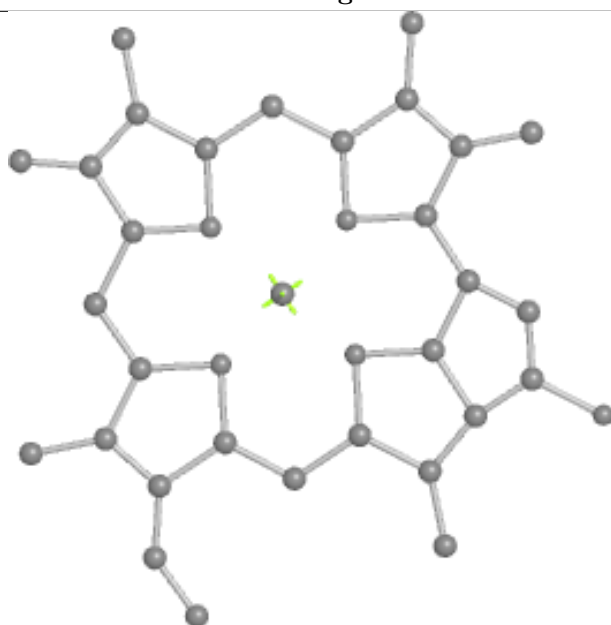
Bond lengths



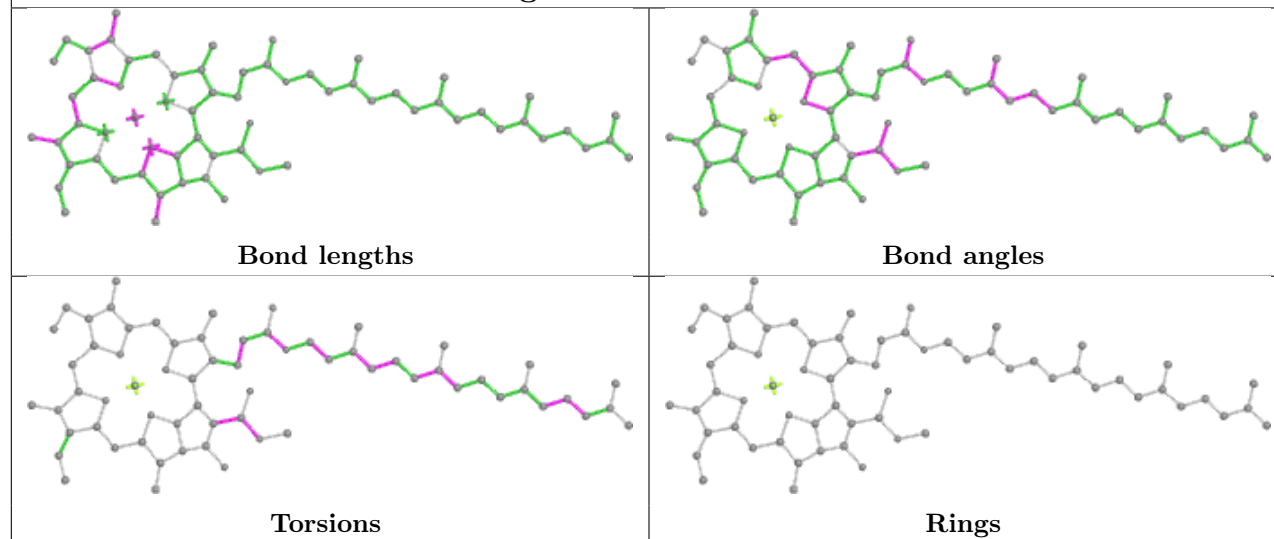
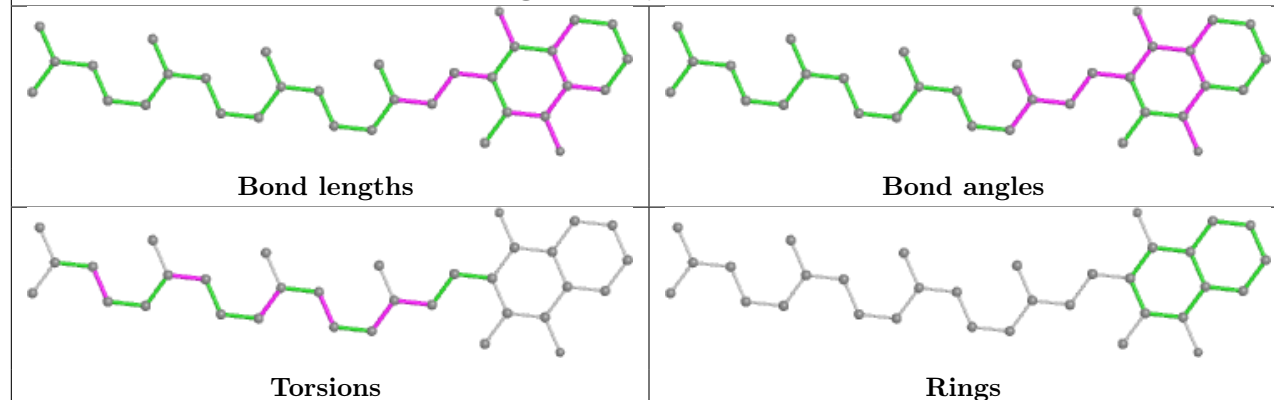
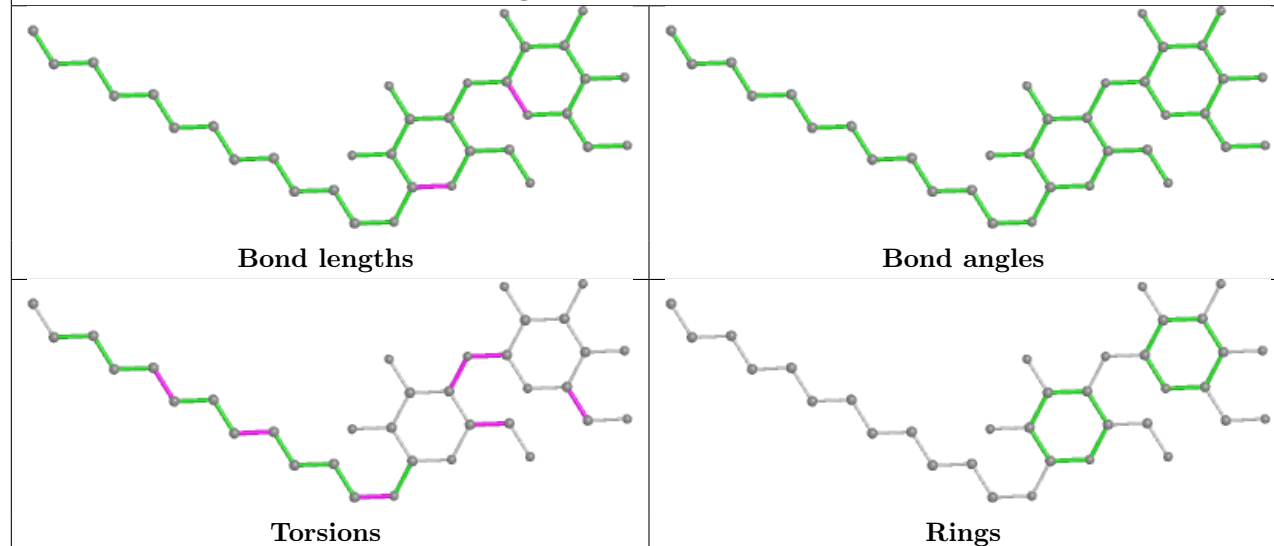
Bond angles



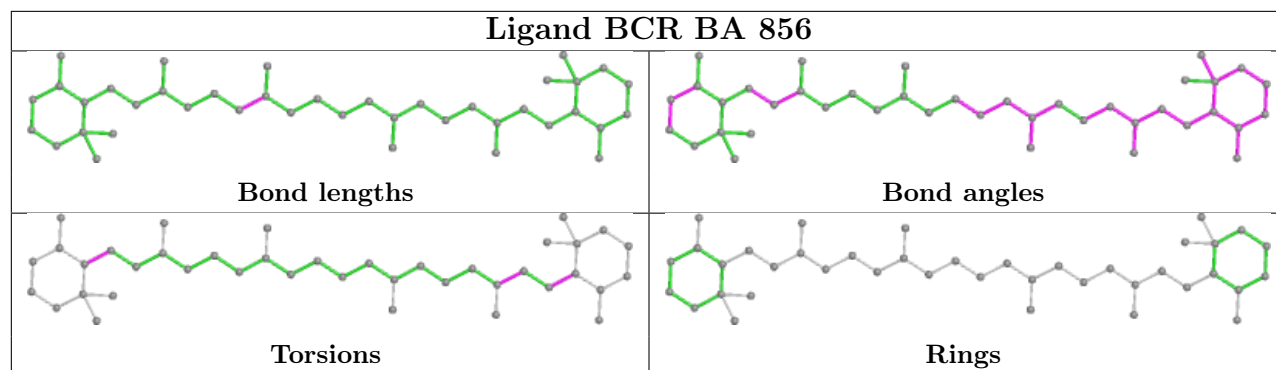
Torsions



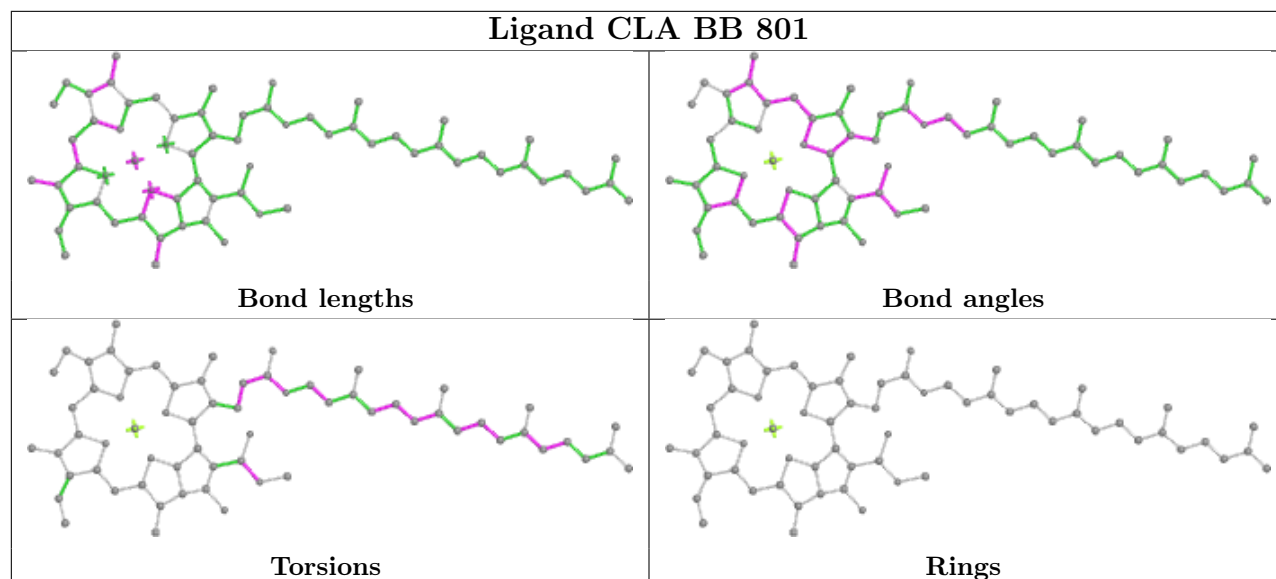
Rings

**Ligand CLA BB 802****Ligand PQN BB 844****Ligand LMU BB 851**

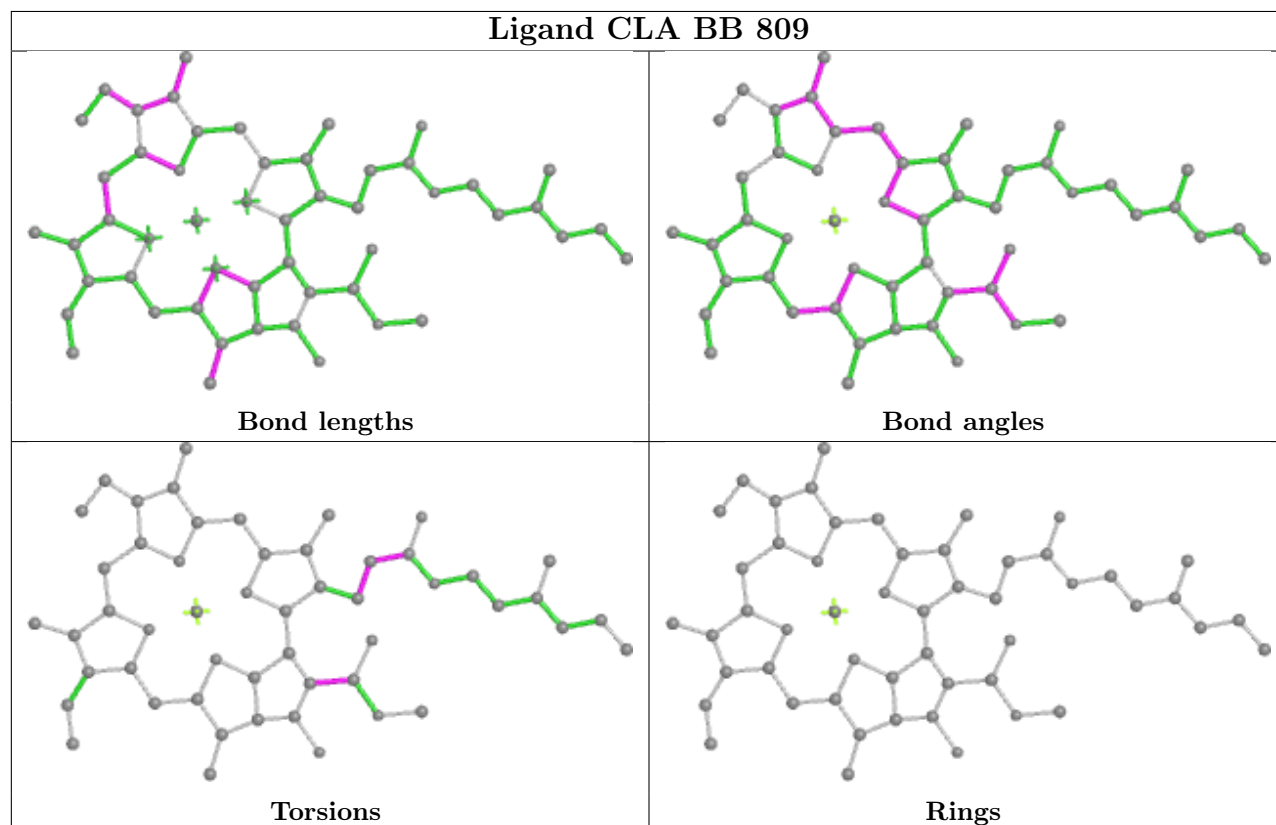
## Ligand BCR BA 856

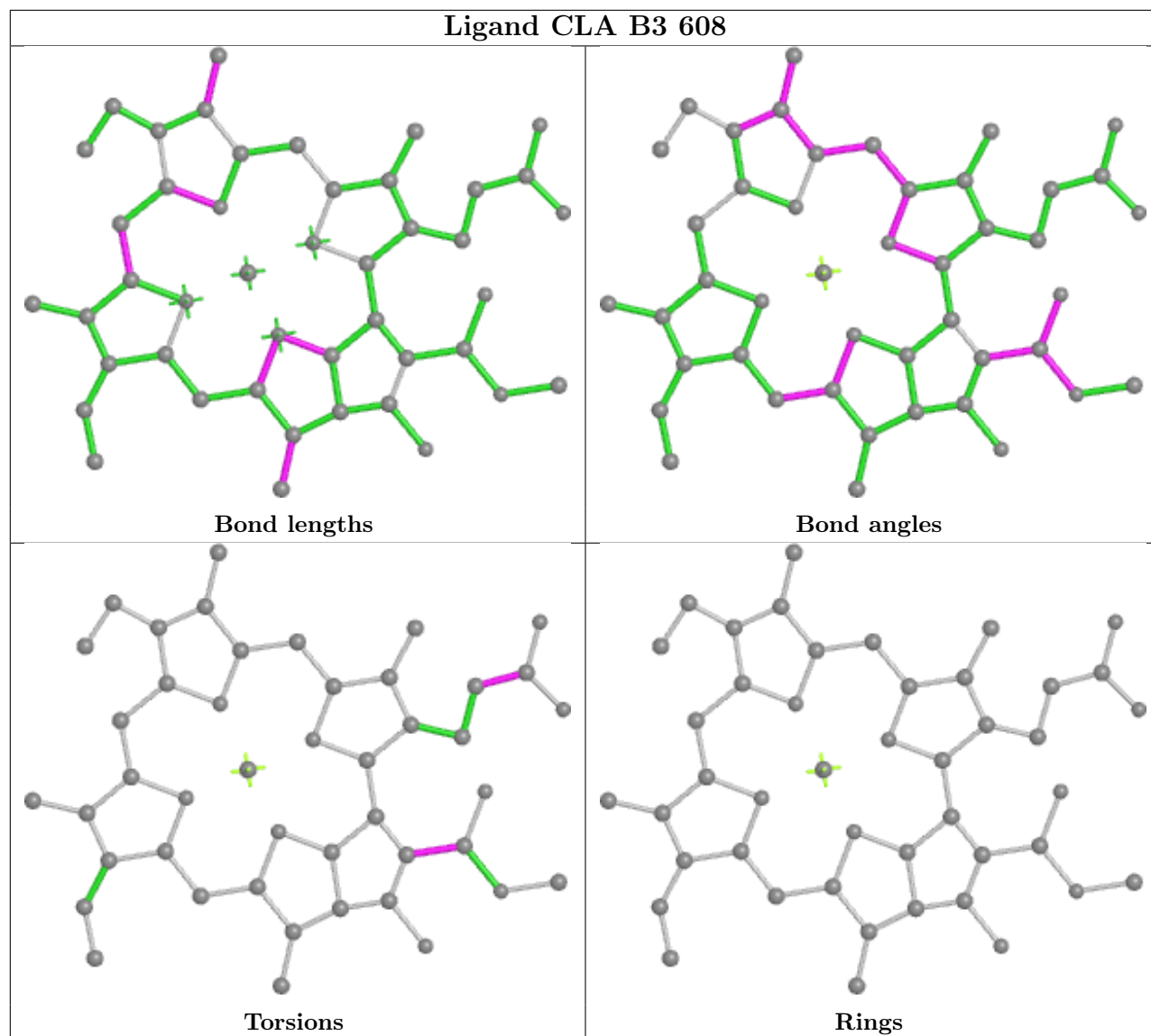
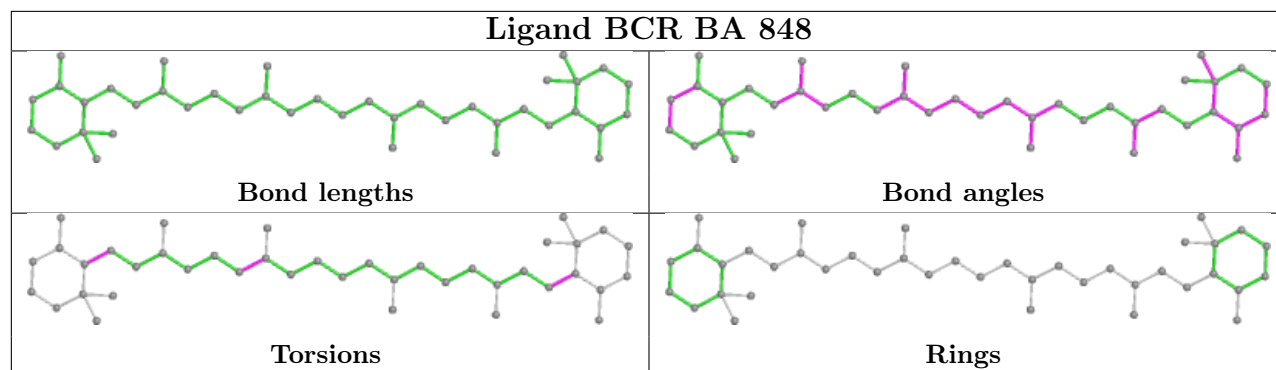


## Ligand CLA BB 801

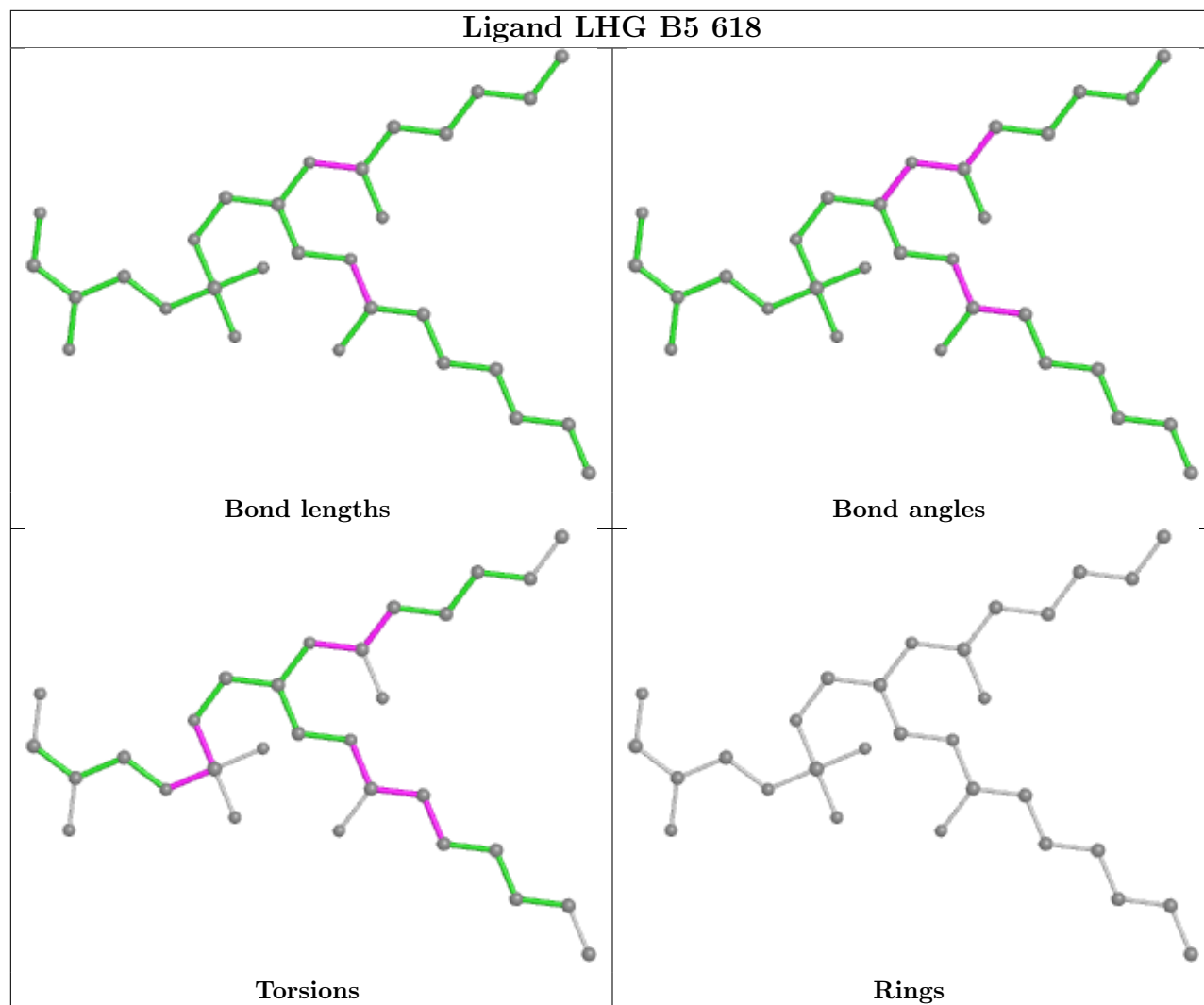
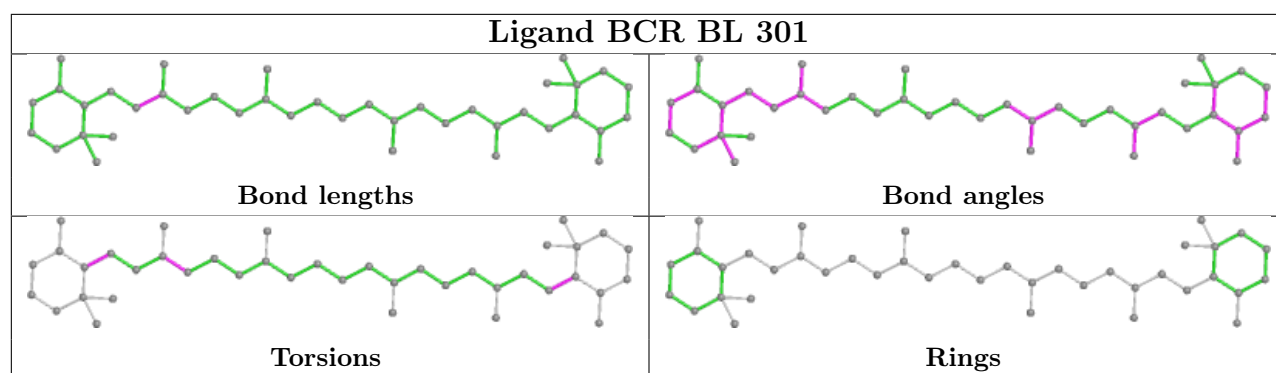


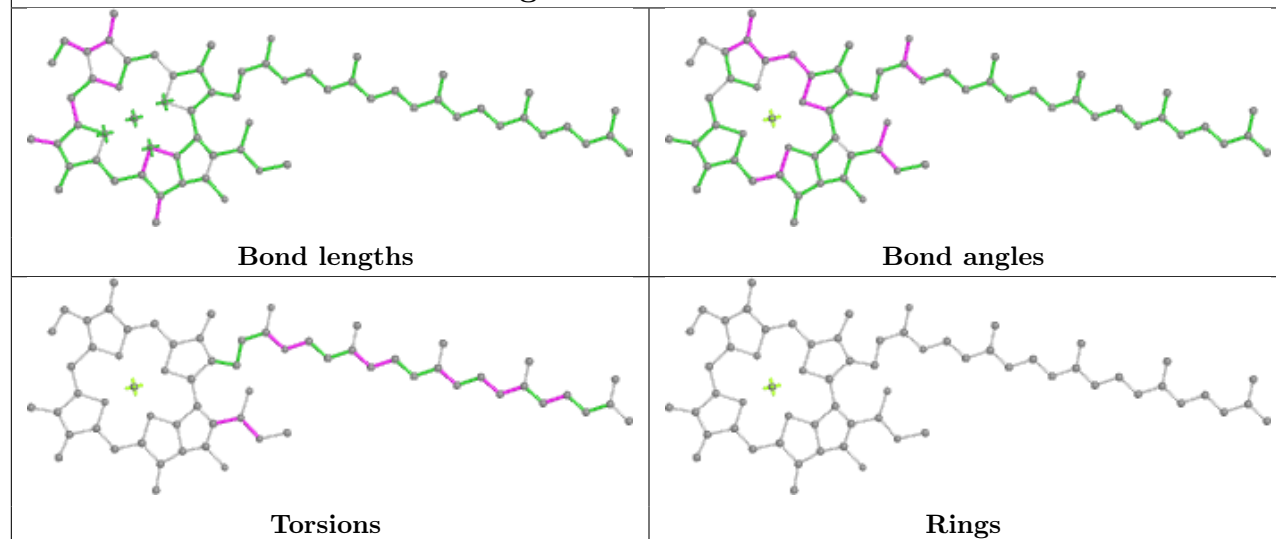
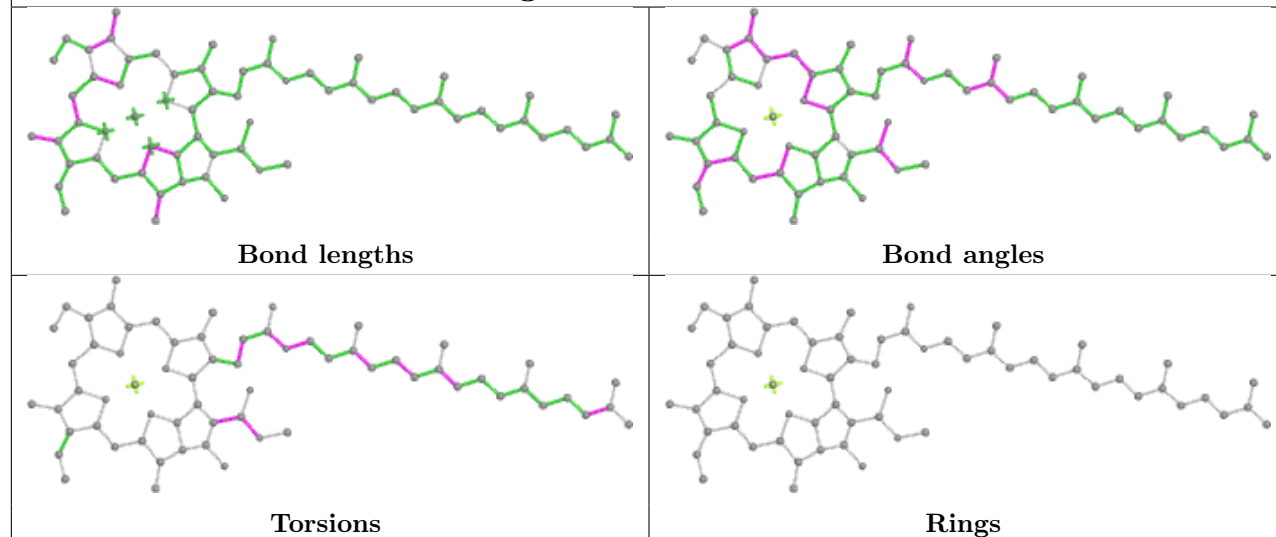
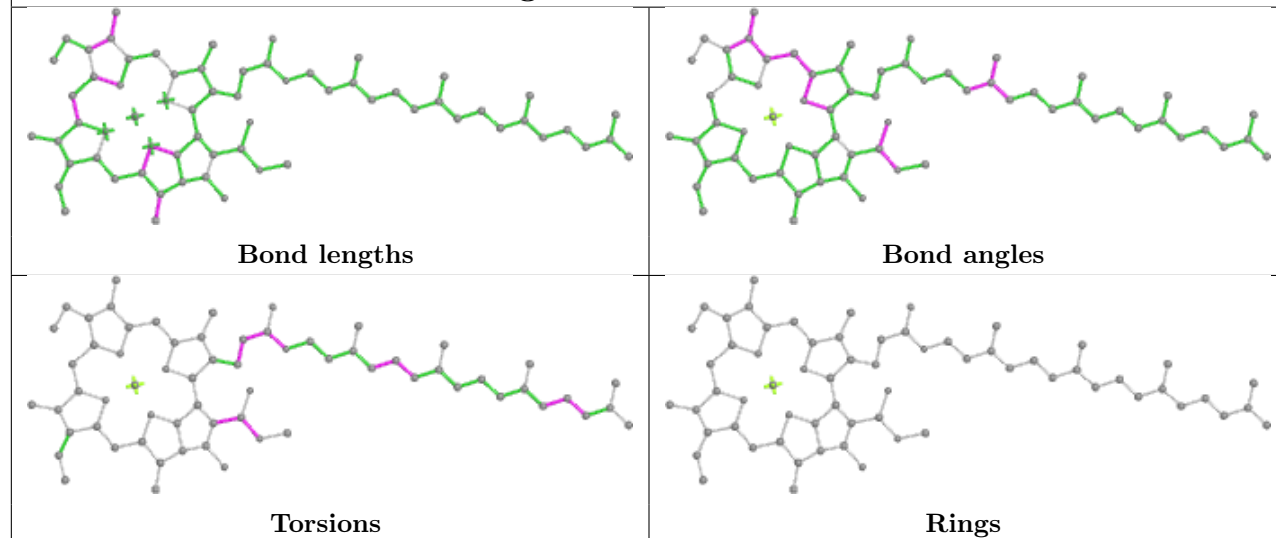
## Ligand CLA BB 809

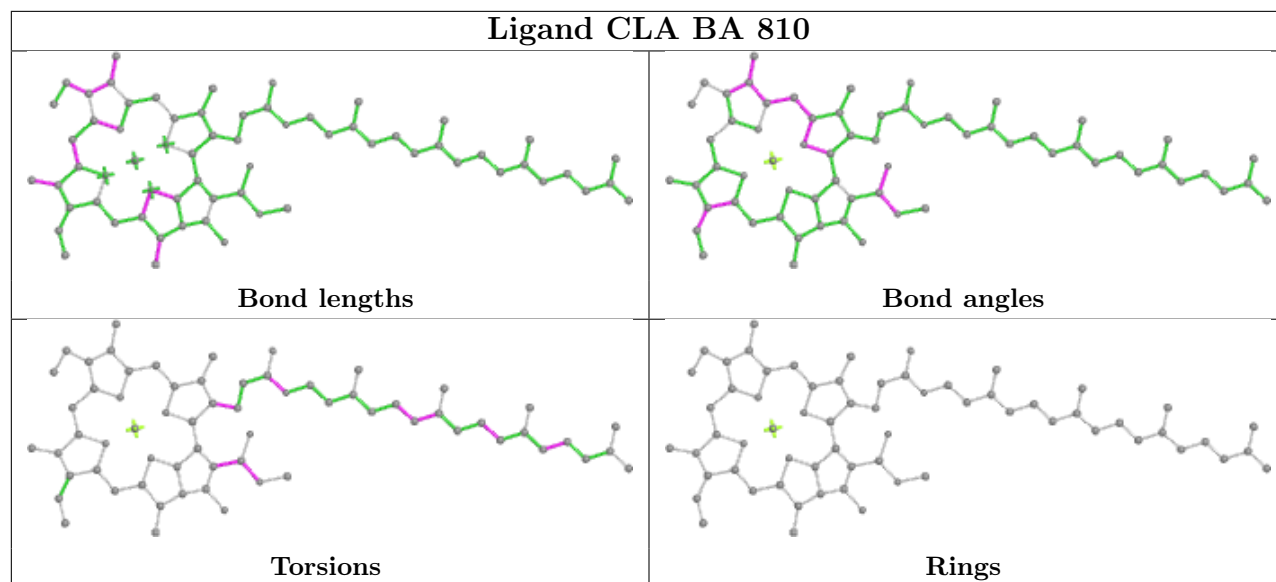
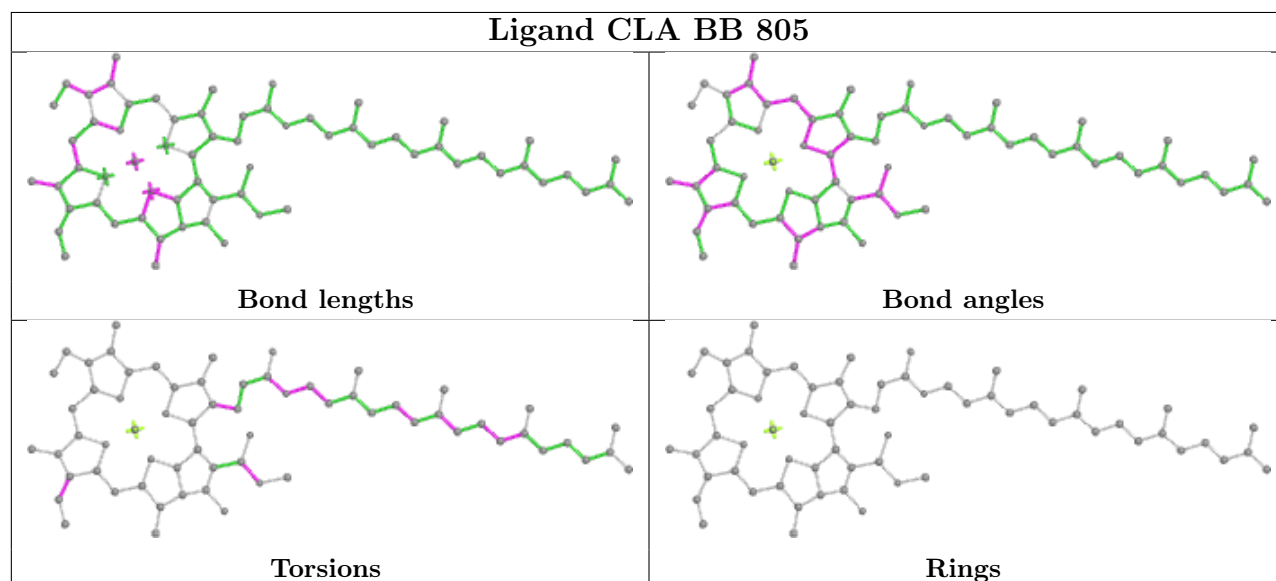


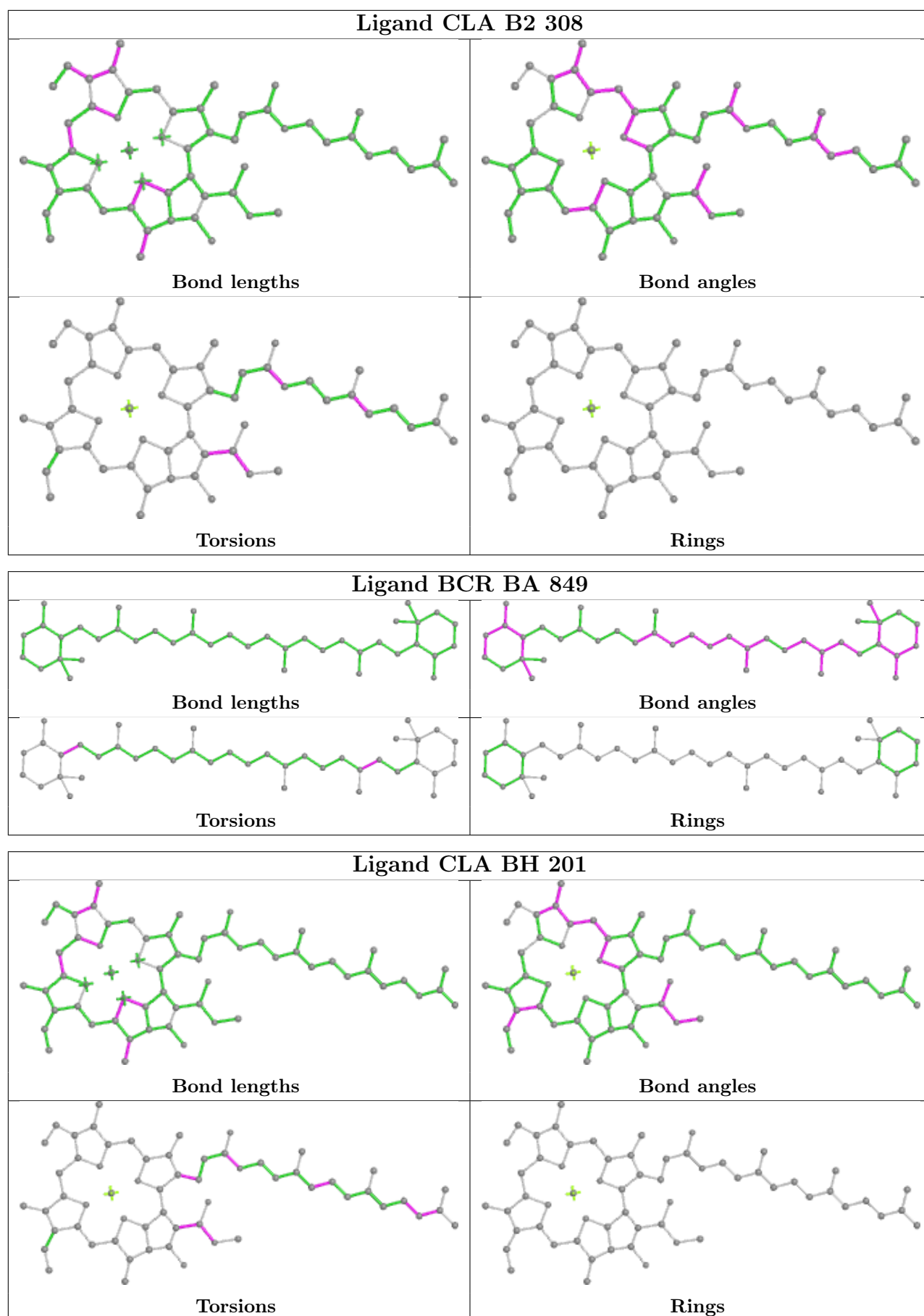


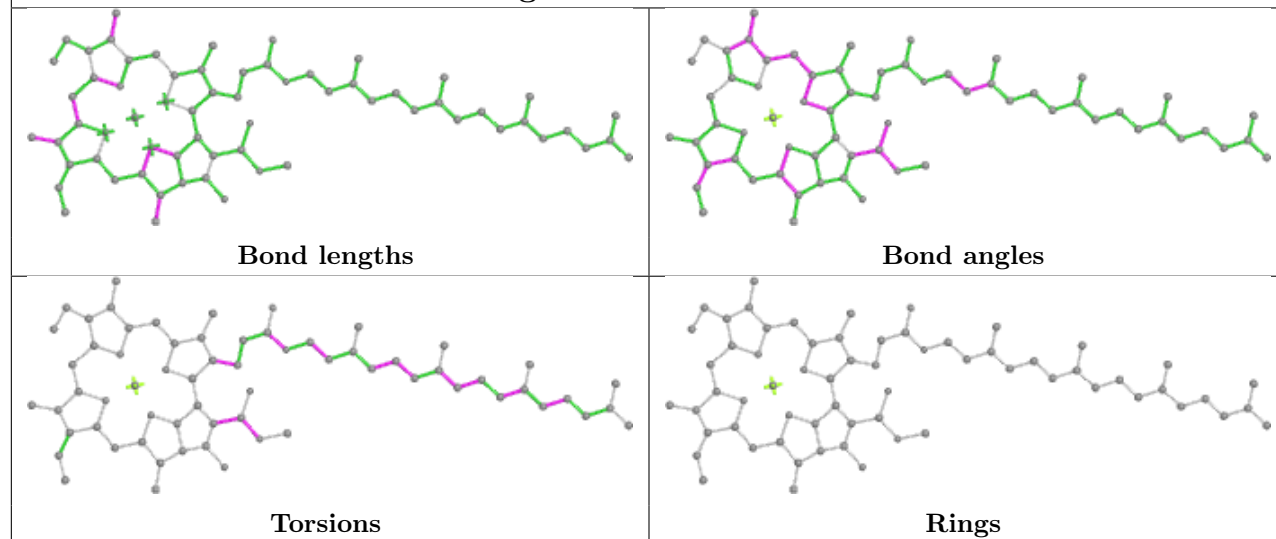
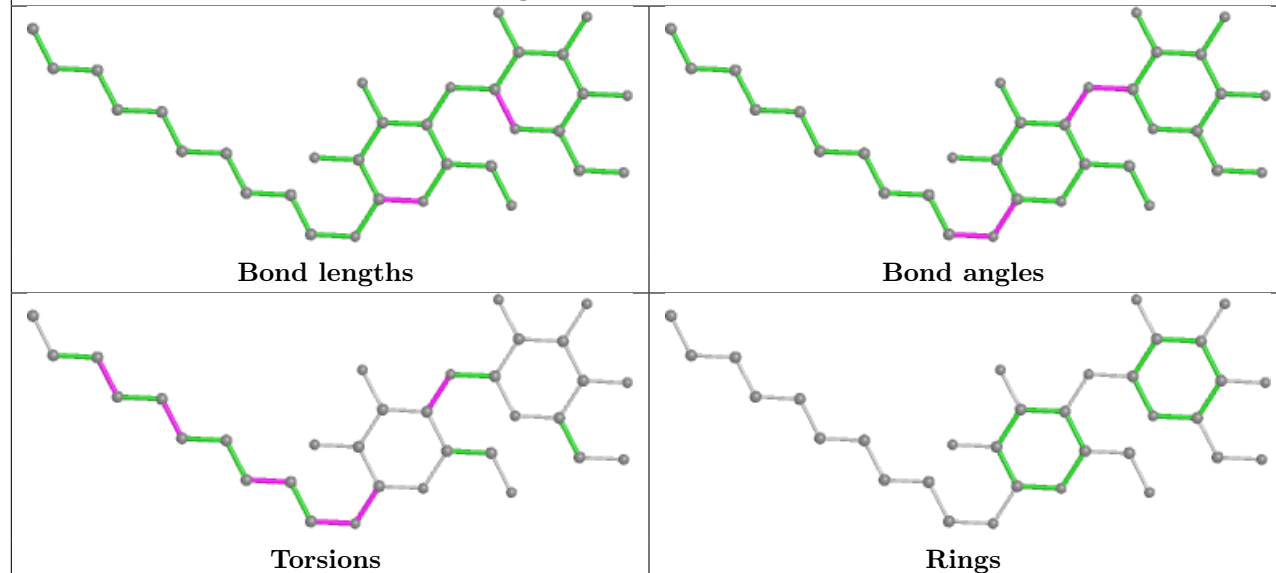


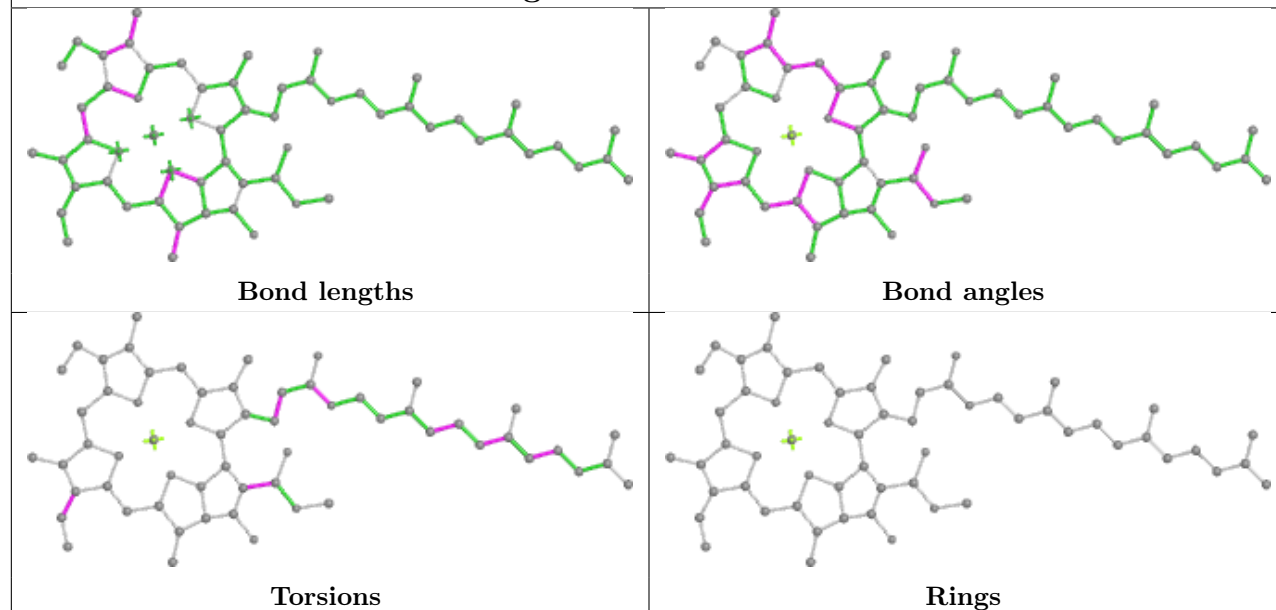
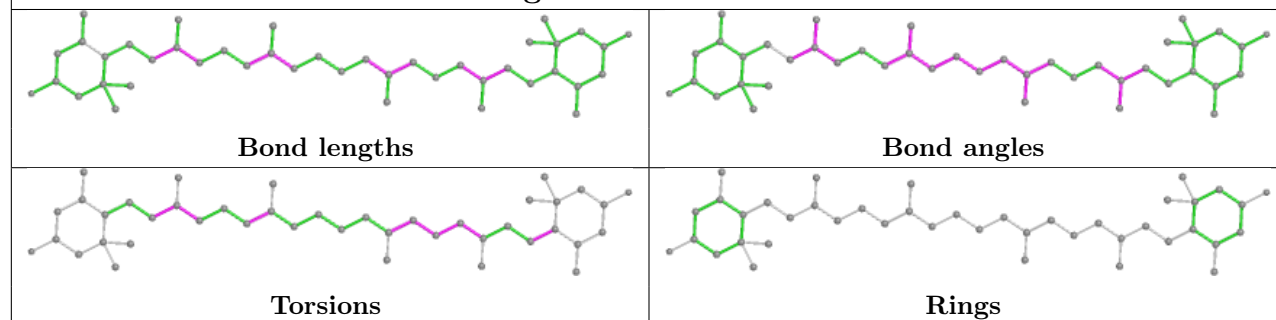


**Ligand CLA BB 816****Ligand CLA BA 841****Ligand CLA BA 833**

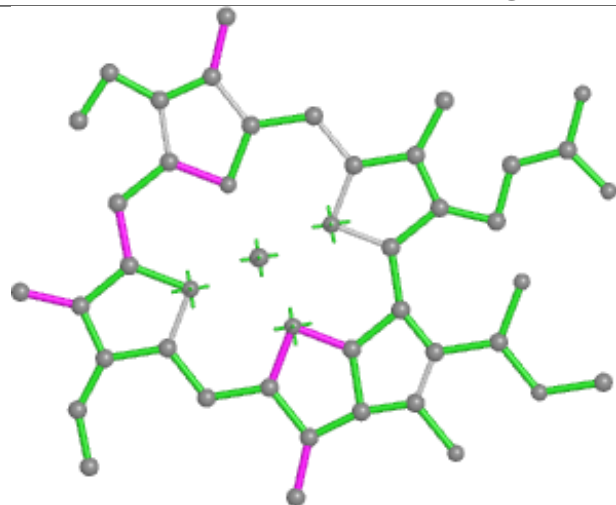
**Ligand CLA BA 810****Ligand CLA BB 805**



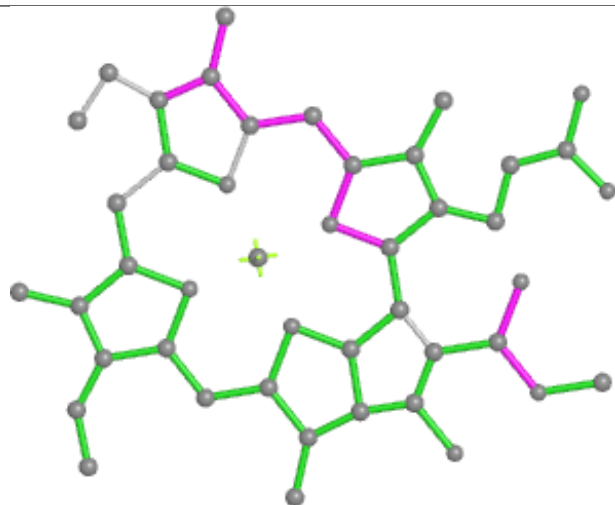
**Ligand CLA BA 803****Ligand LMU BA 854**

**Ligand CLA B1 314****Ligand LUT B1 316**

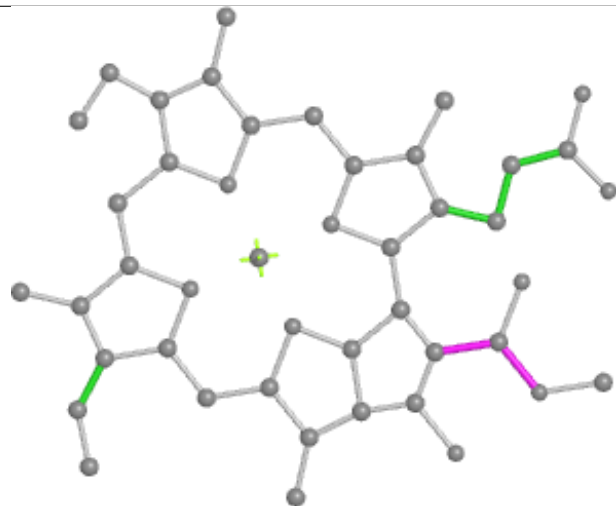
## Ligand CLA BA 820



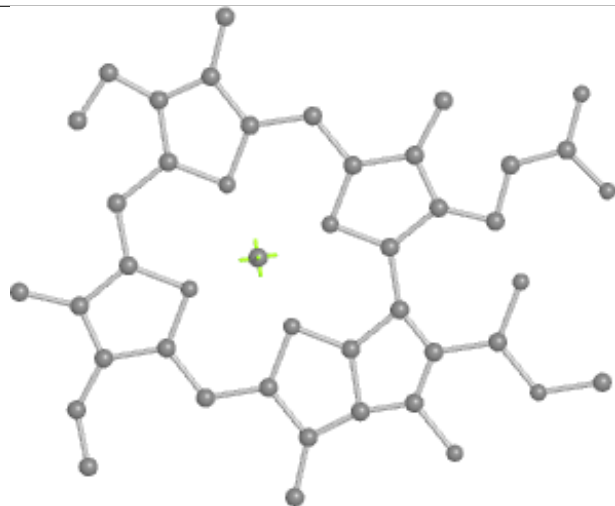
Bond lengths



Bond angles

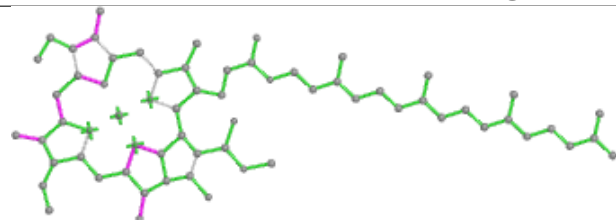


Torsions

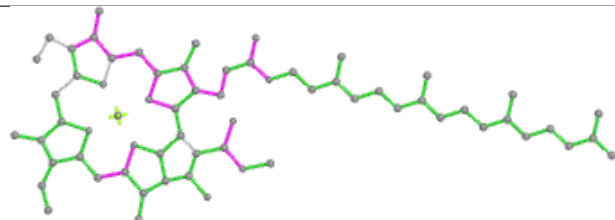


Rings

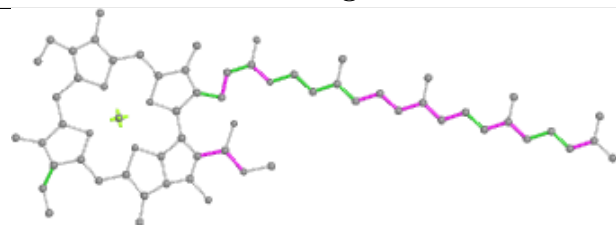
## Ligand CLA BB 824



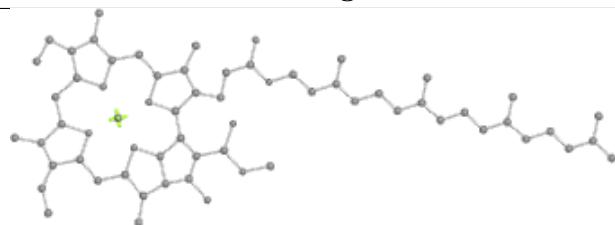
Bond lengths



Bond angles

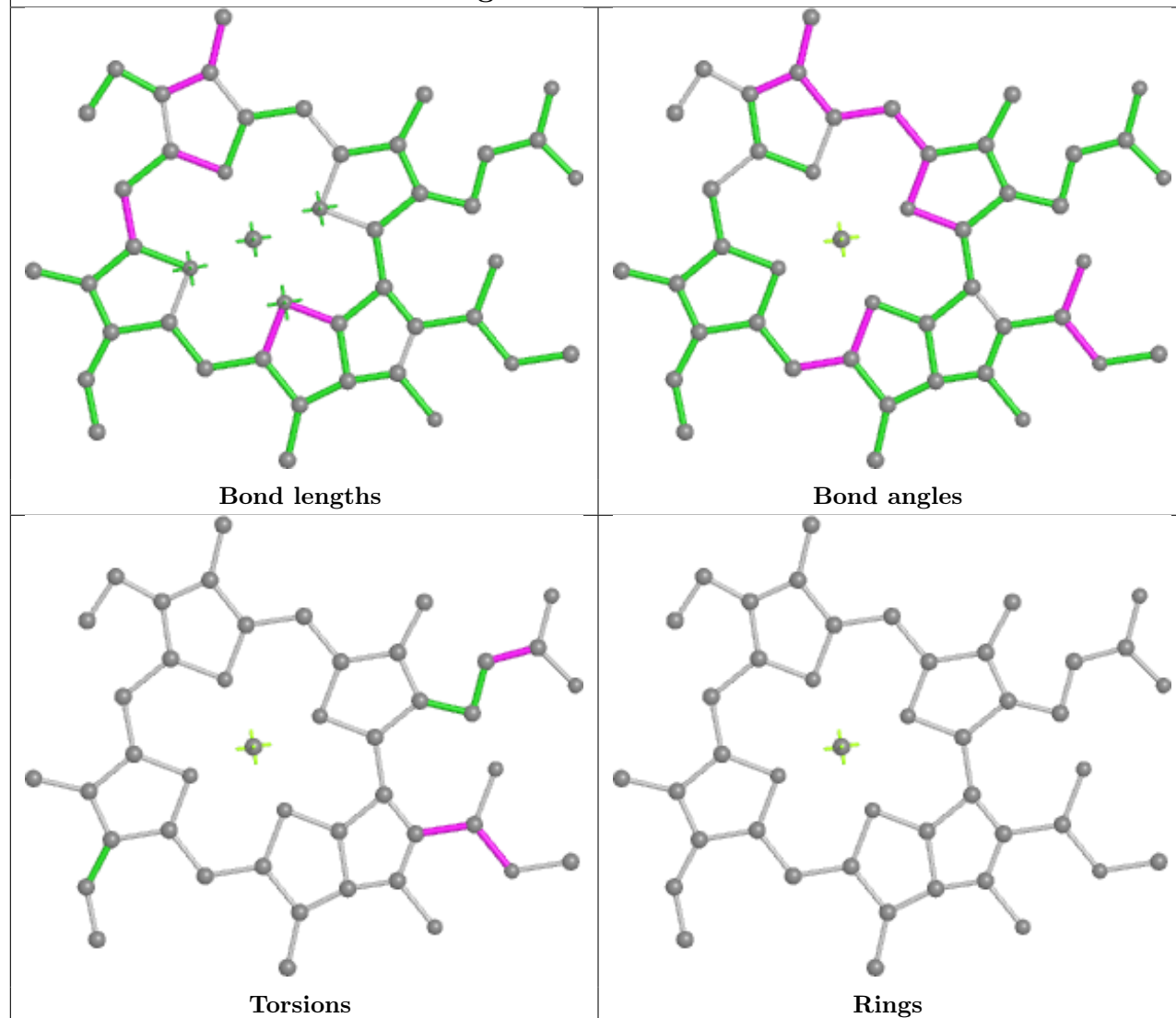


Torsions

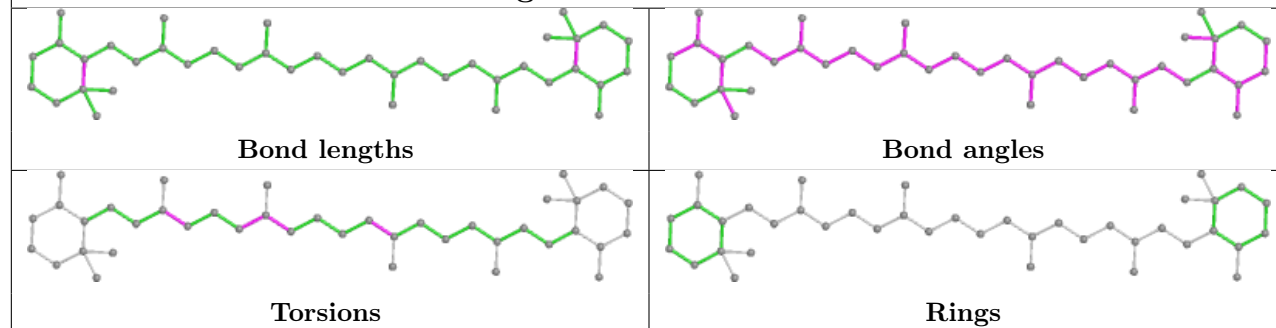


Rings

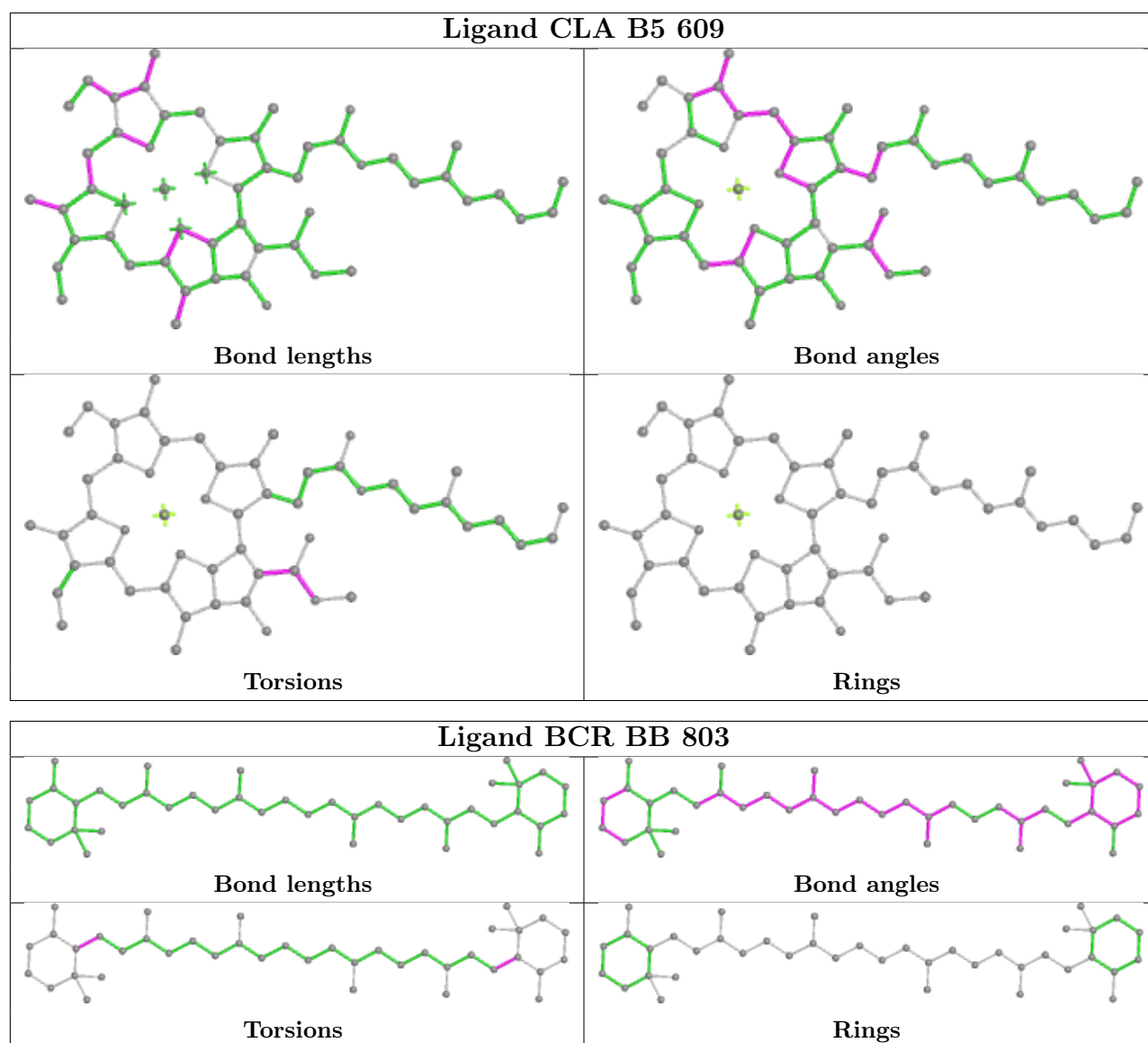
## Ligand CLA BG 202



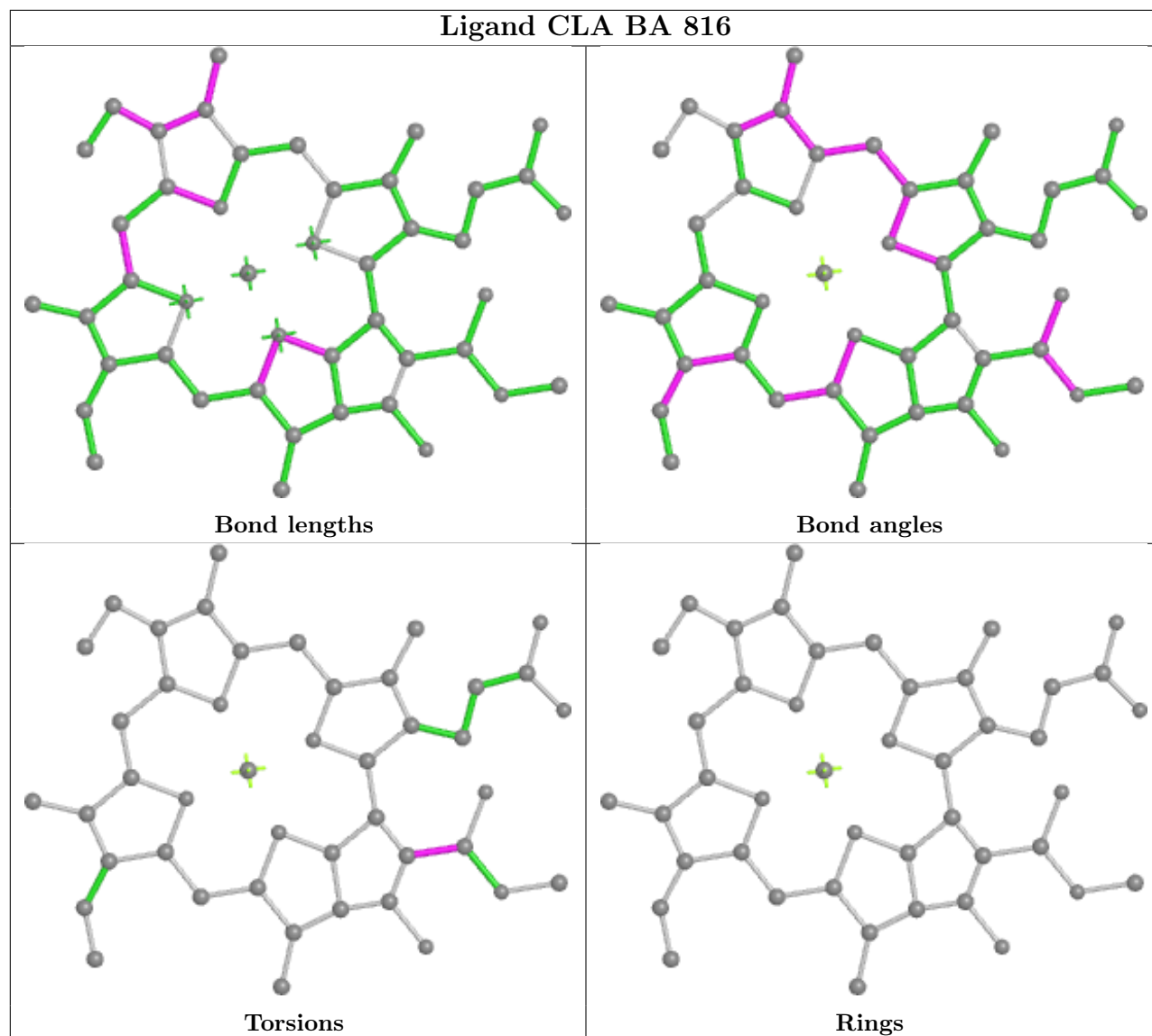
## Ligand BCR BG 203



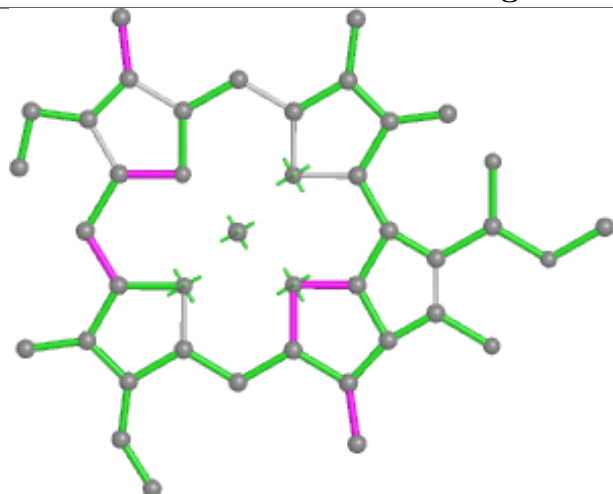




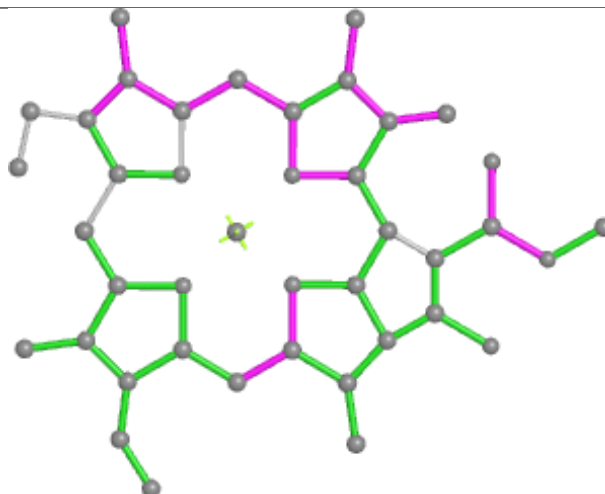
## Ligand CLA BA 816



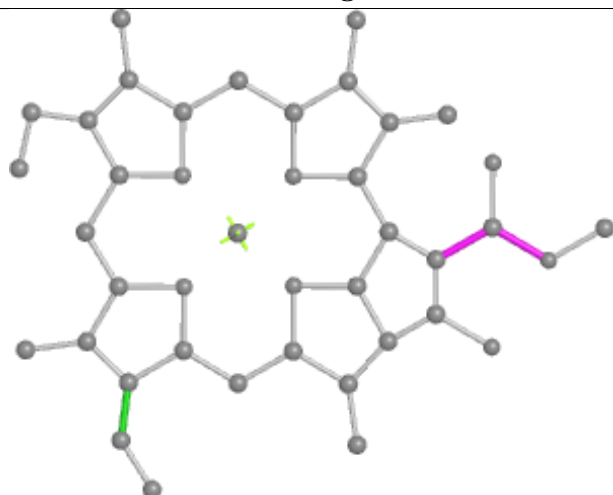
## Ligand CLA BA 823



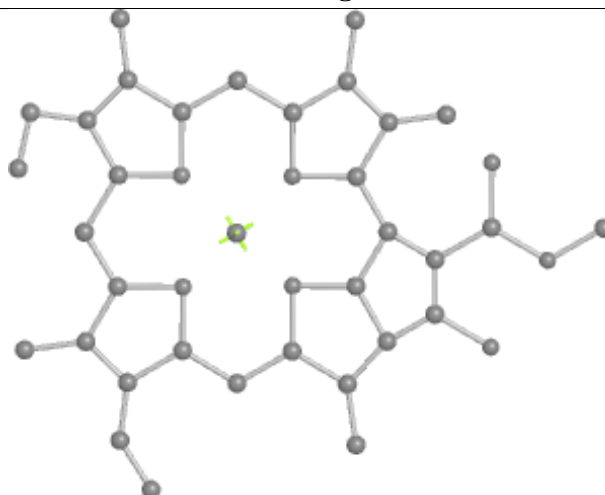
Bond lengths



Bond angles

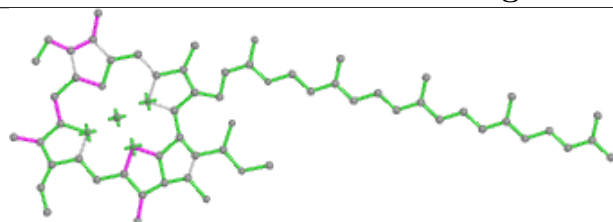


Torsions

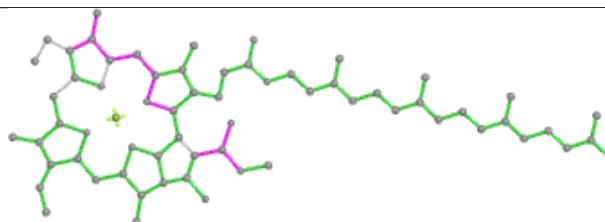


Rings

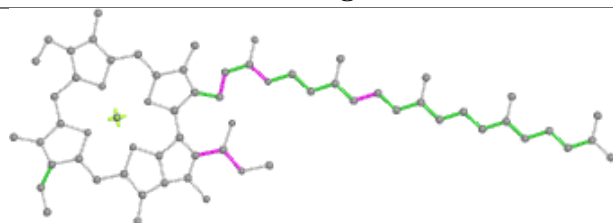
## Ligand CLA BB 841



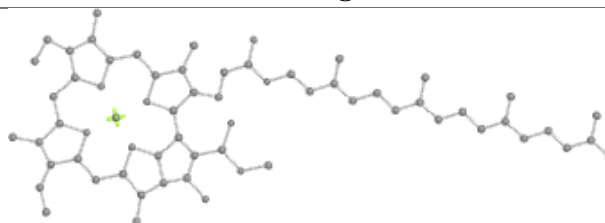
Bond lengths



Bond angles

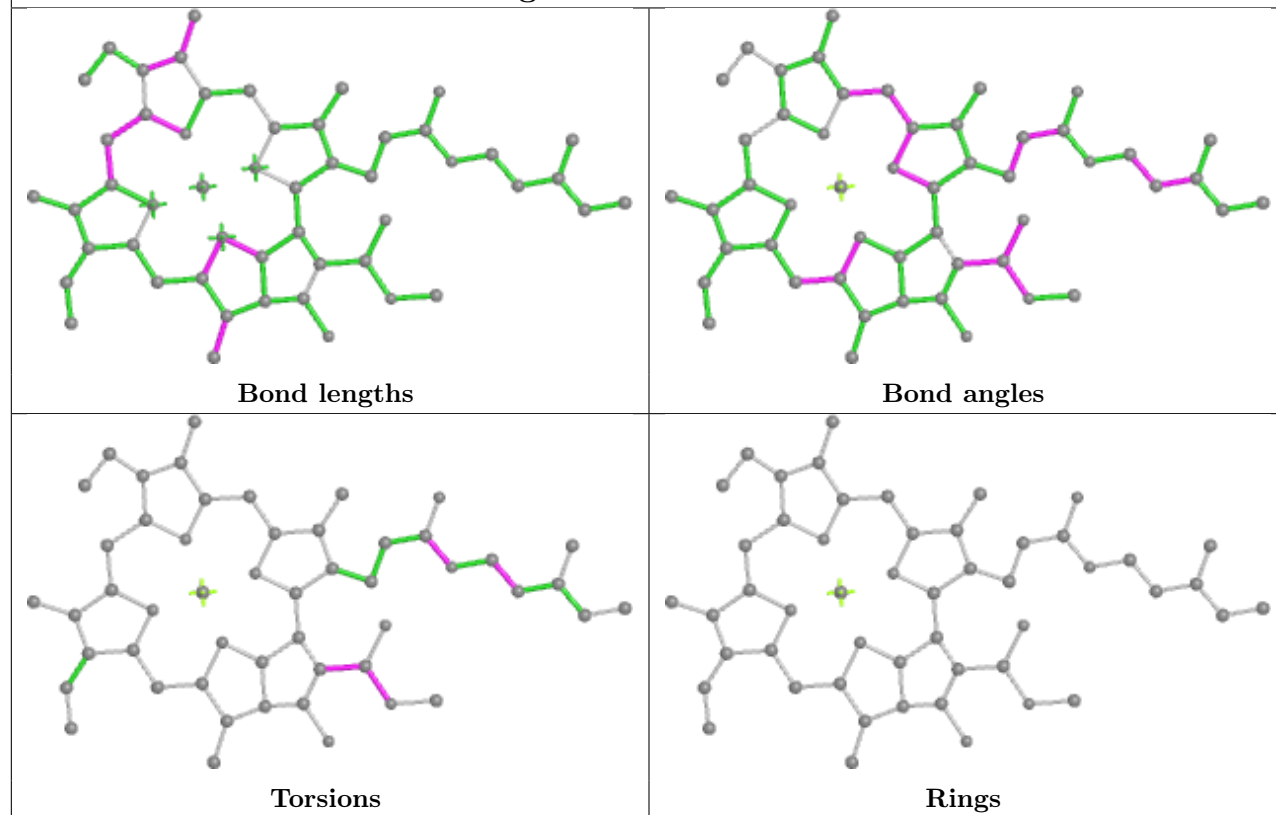


Torsions

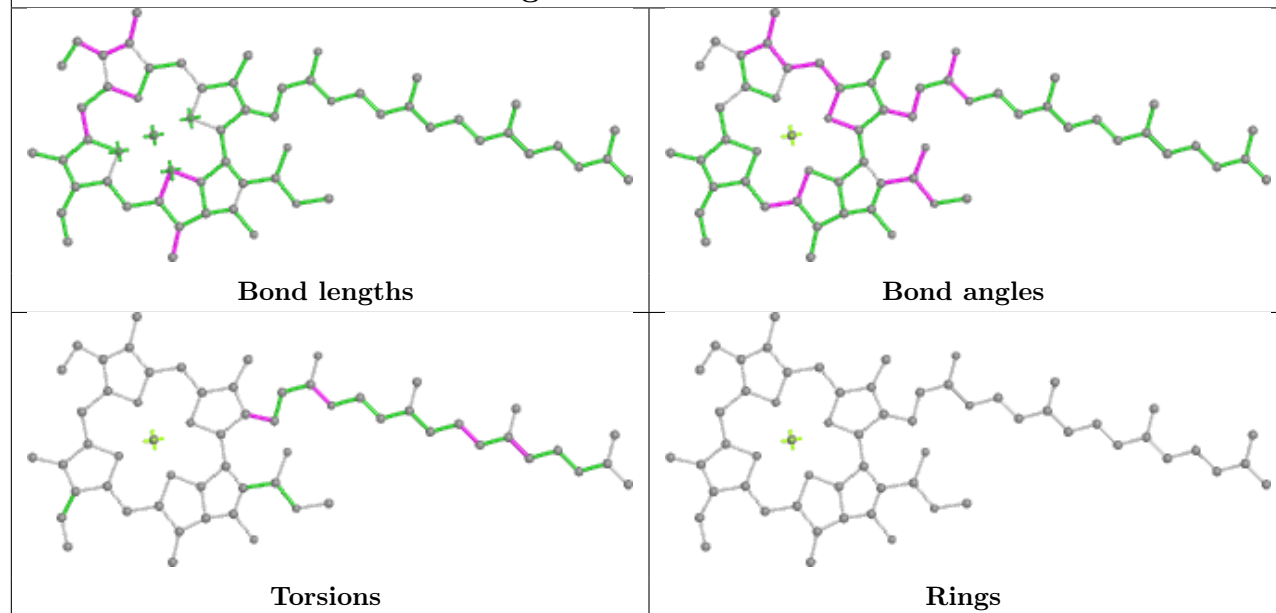


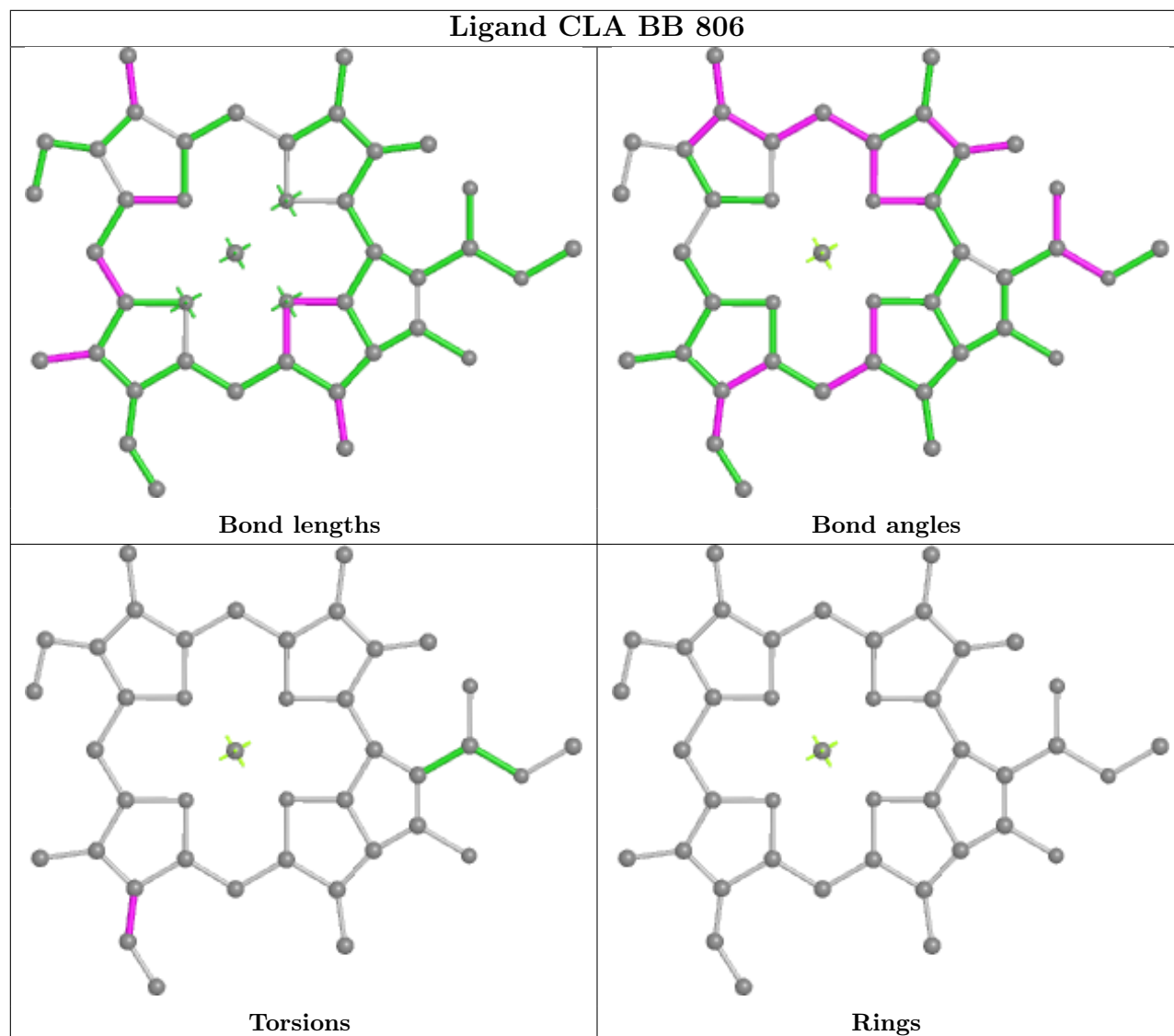
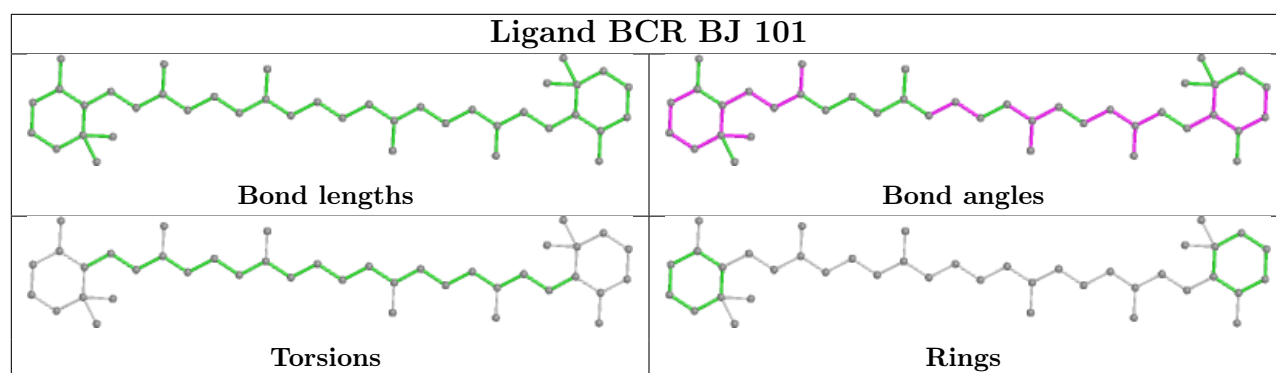
Rings

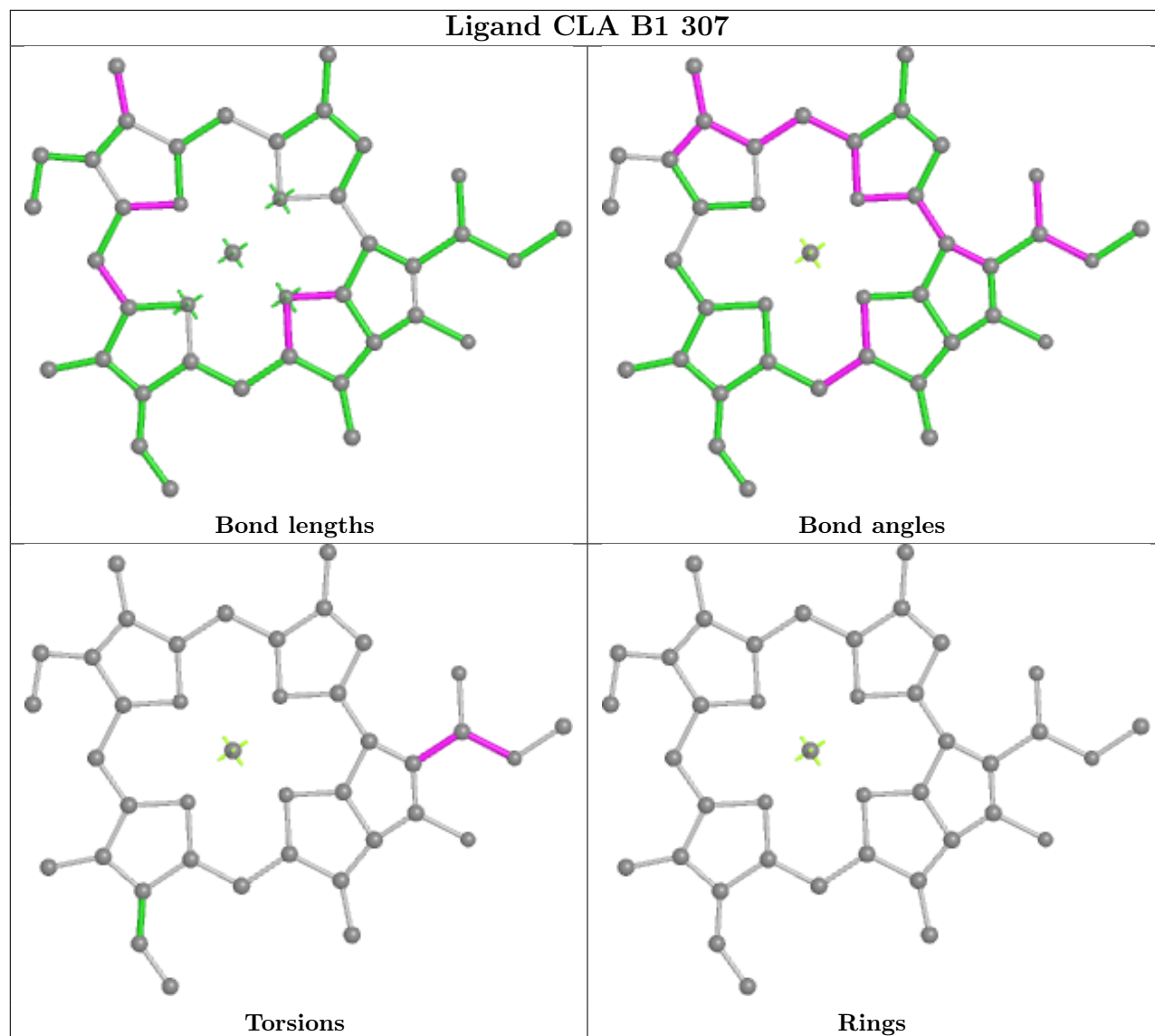
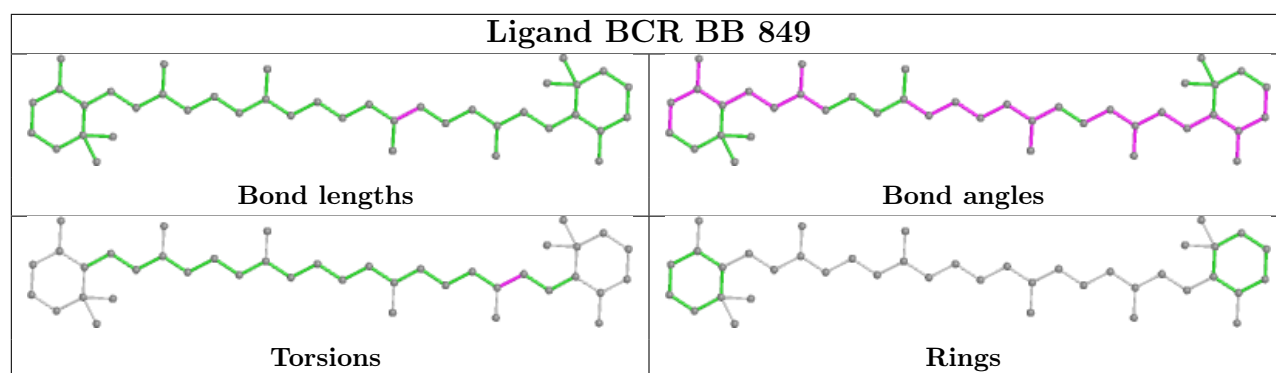
## Ligand CLA BA 839

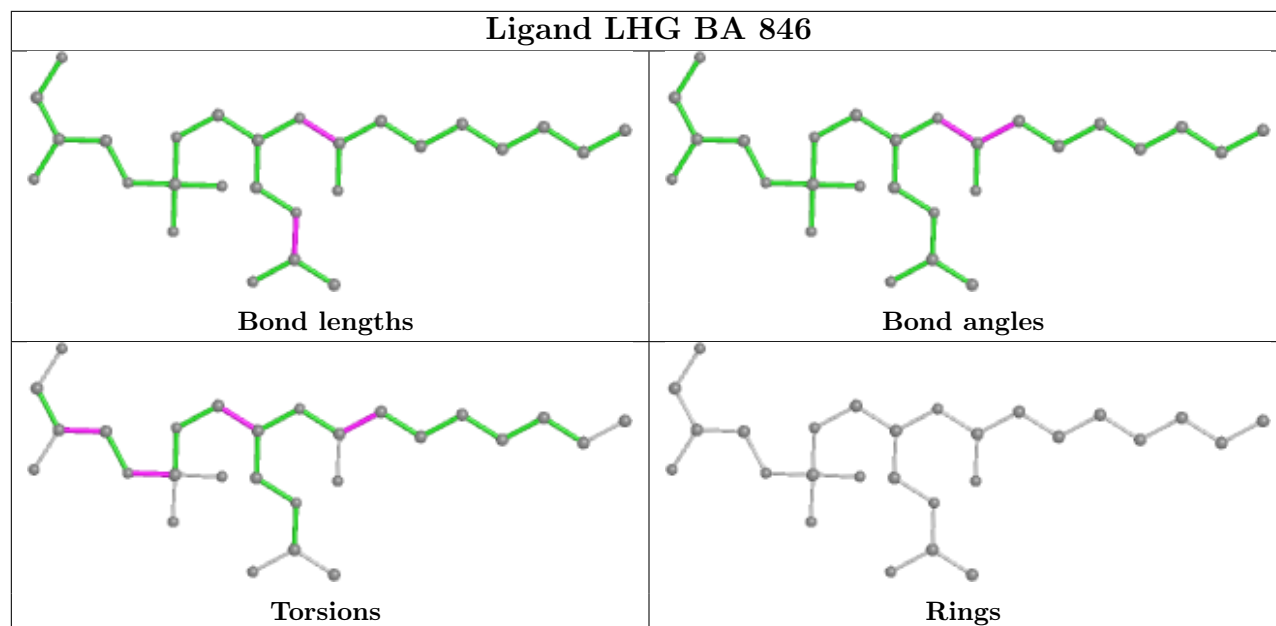


## Ligand CLA BL 303

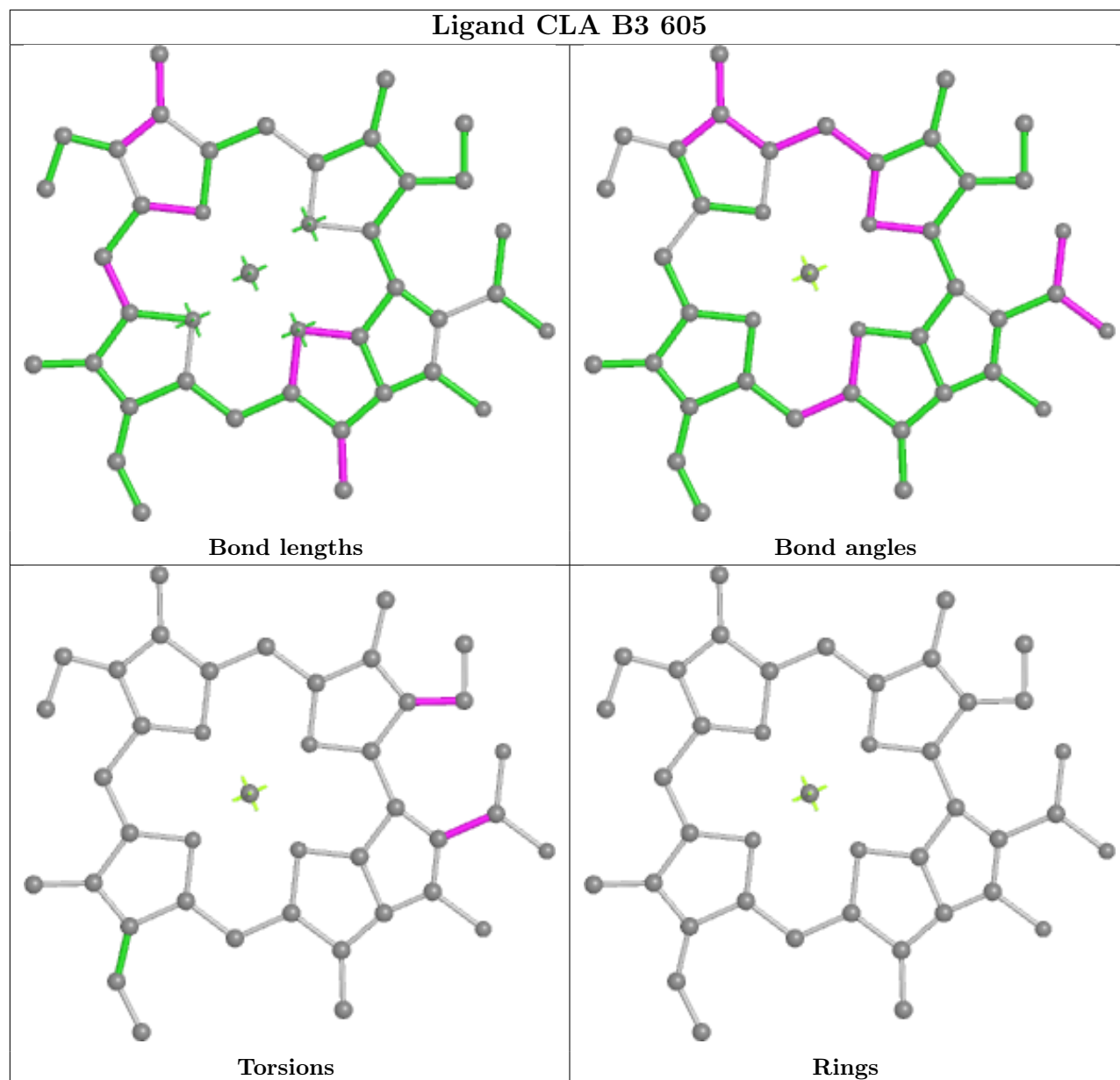






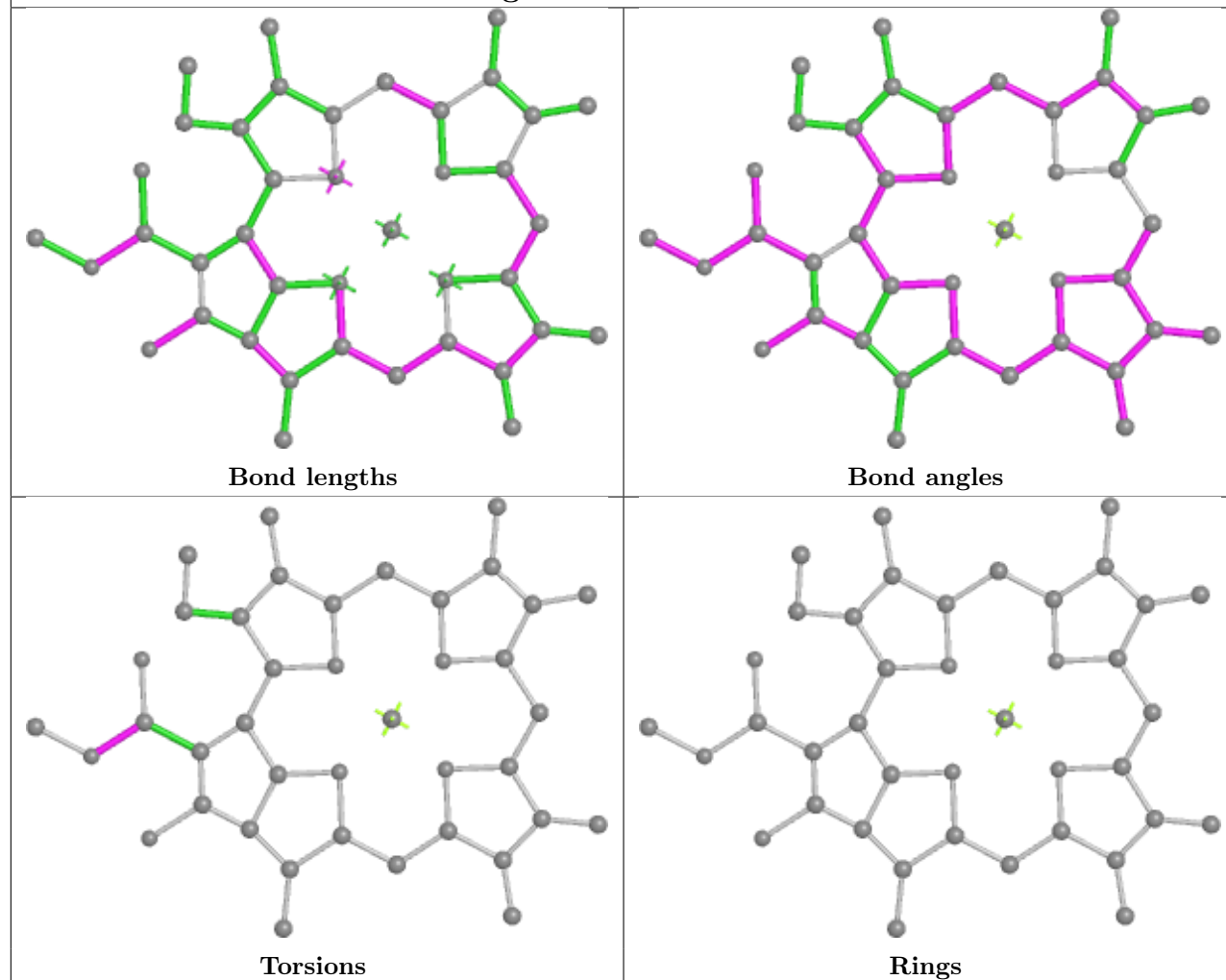


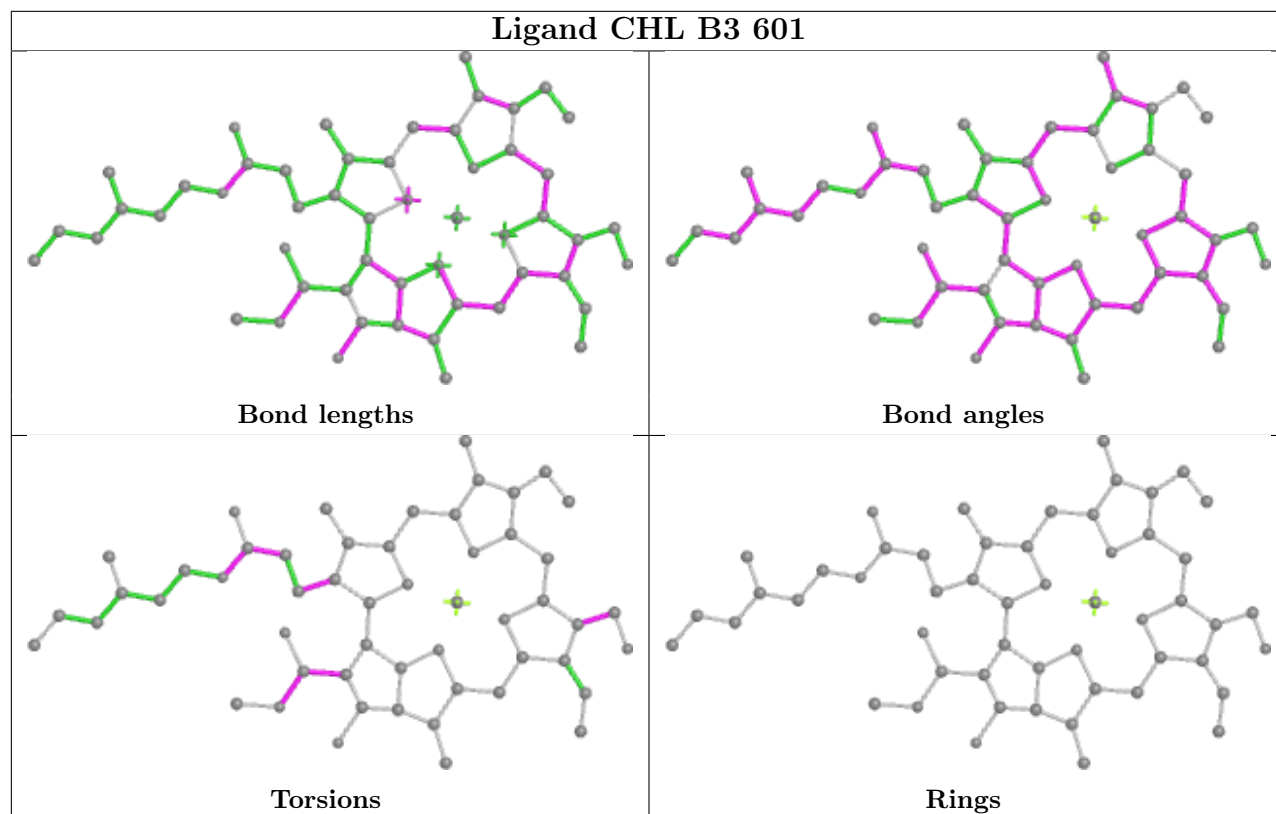
## Ligand CLA B3 605



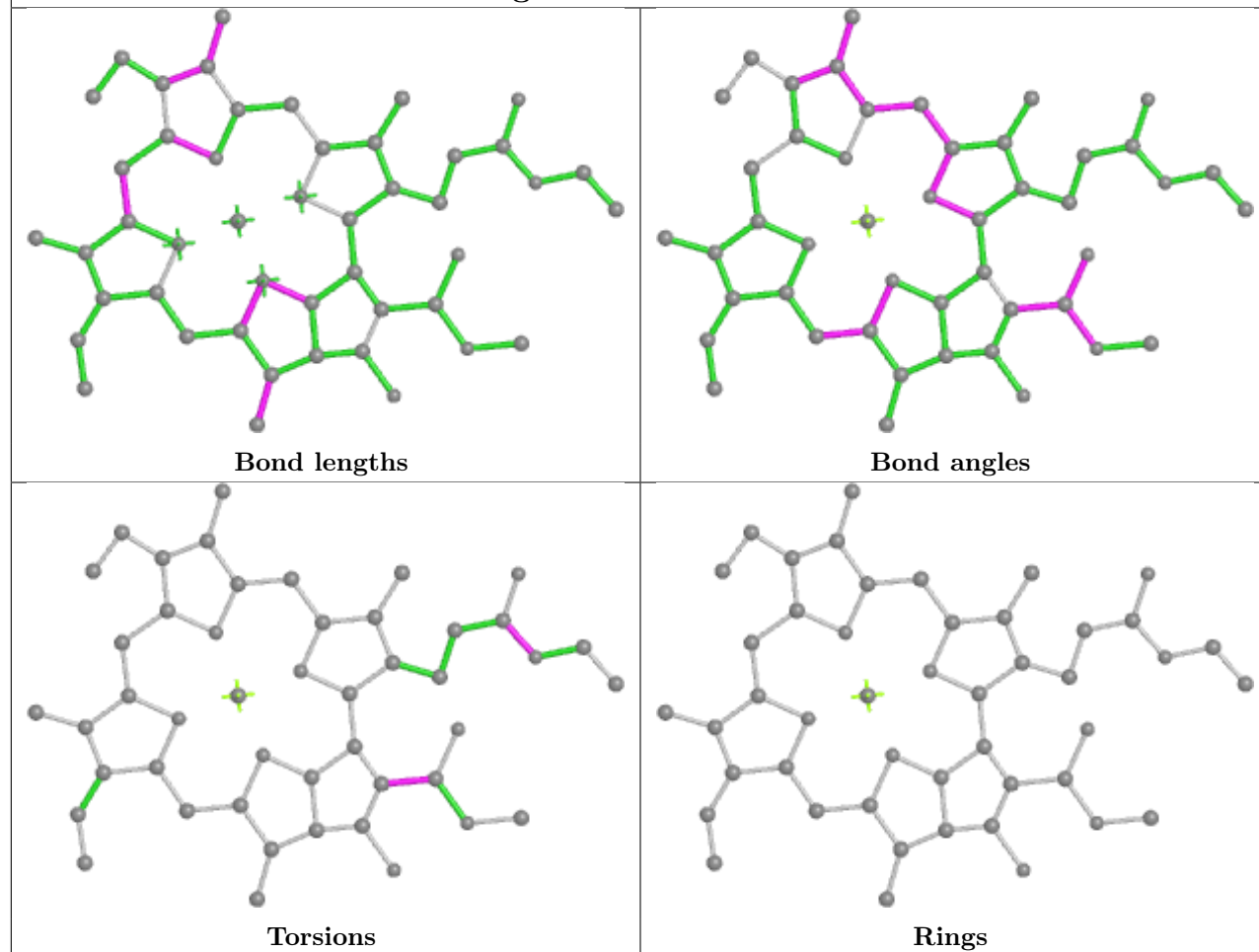


## Ligand CHL B5 606

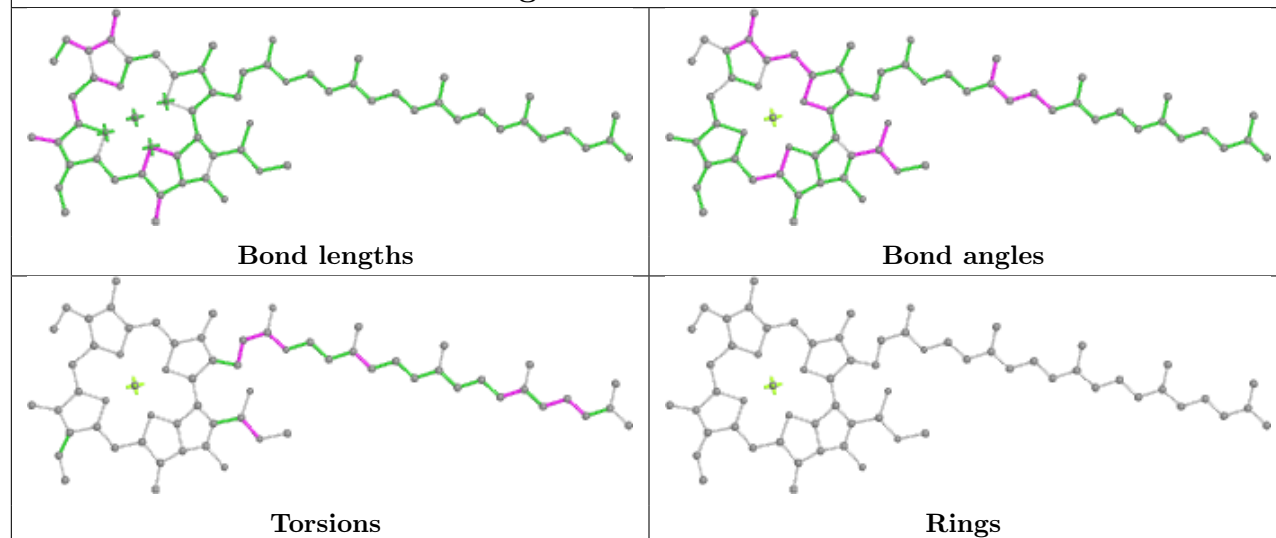




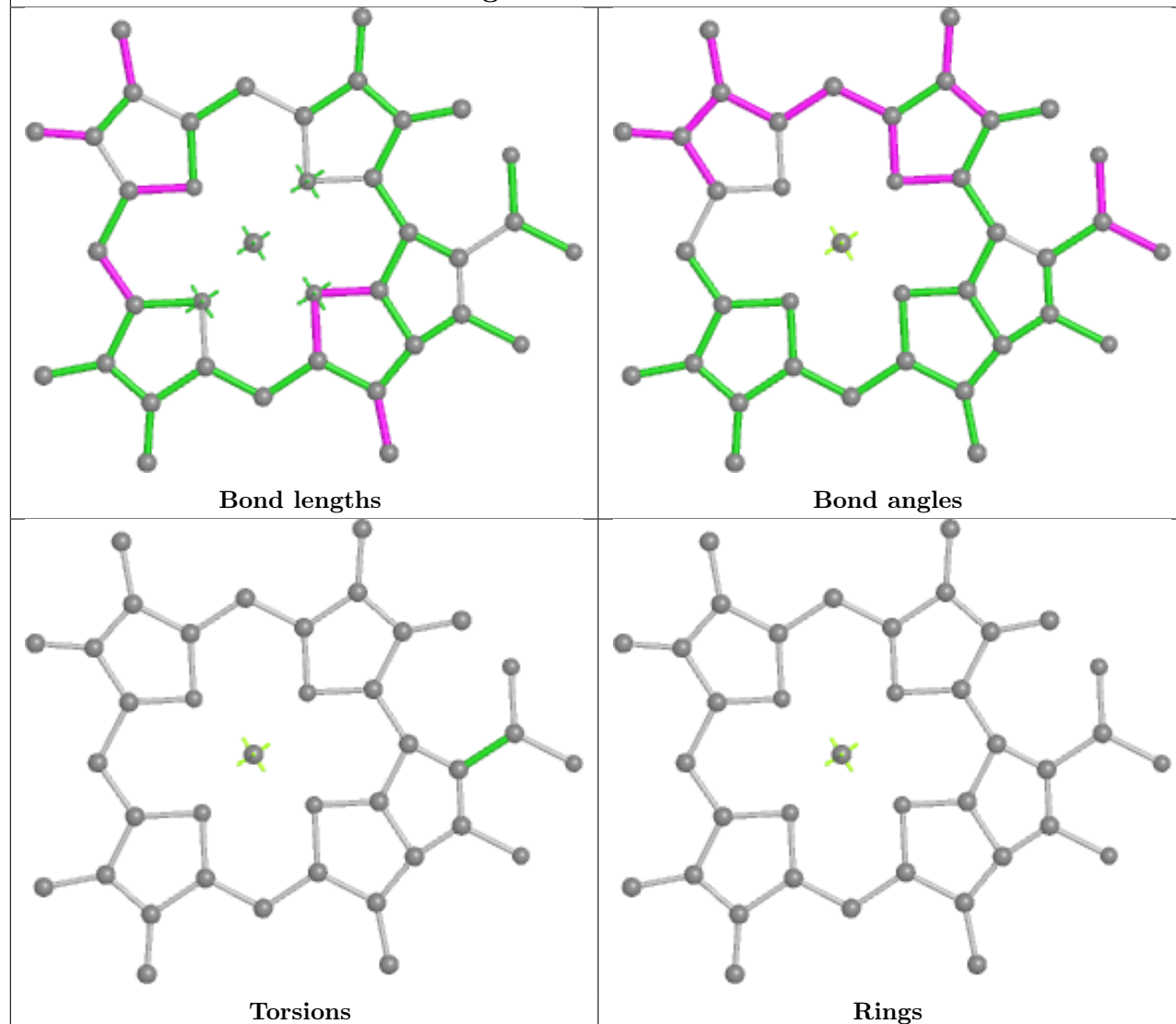
## Ligand CLA BB 840



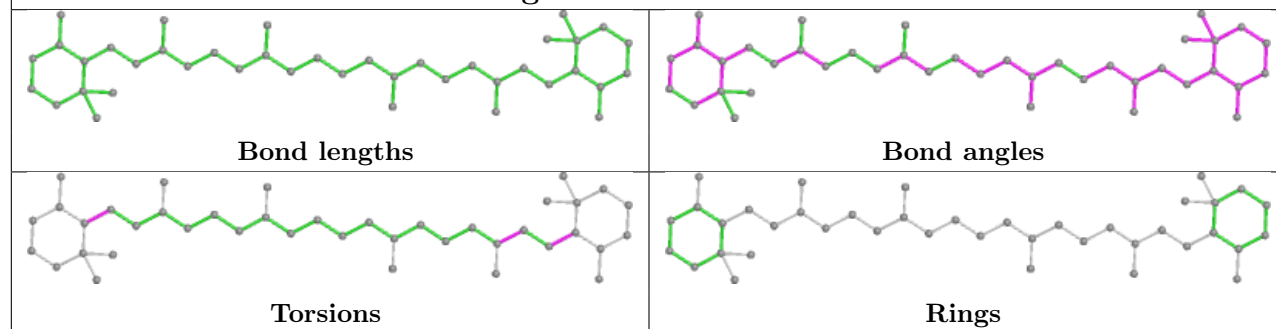
## Ligand CLA BA 821



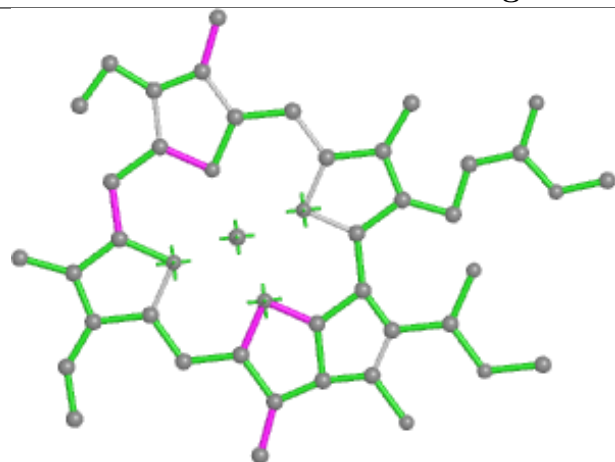
## Ligand CLA B1 315



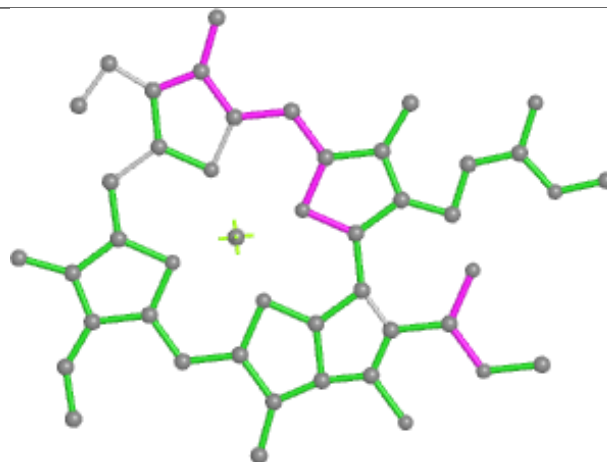
## Ligand BCR B3 618



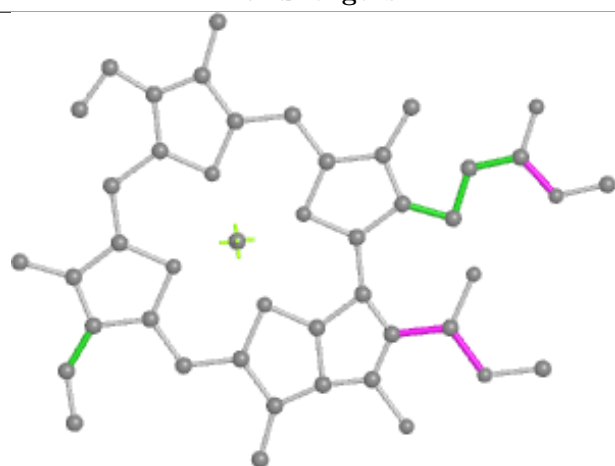
## Ligand CLA BK 203



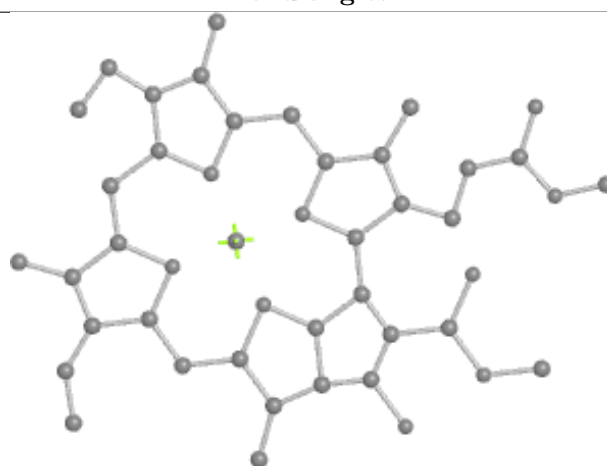
Bond lengths



Bond angles

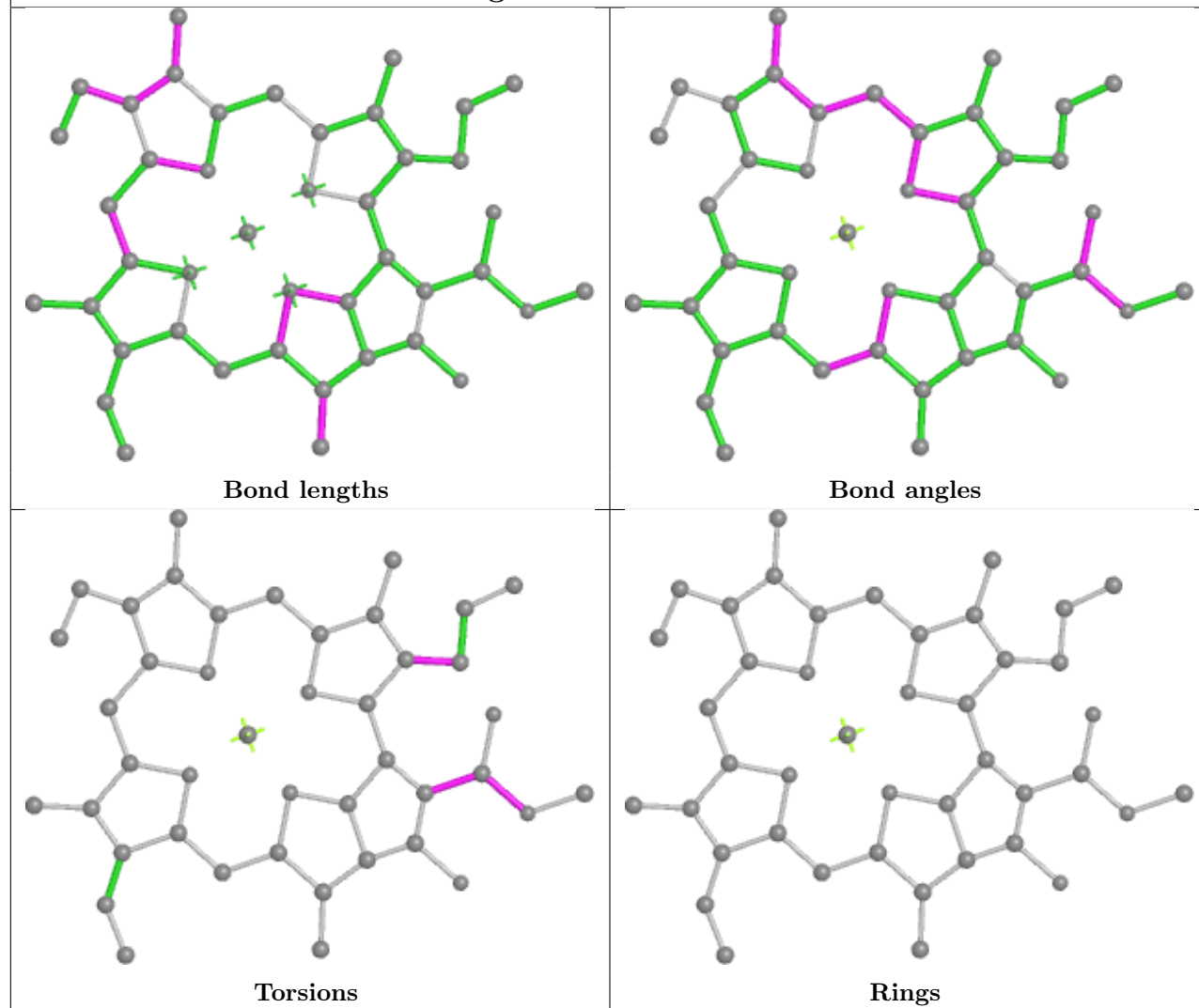


Torsions

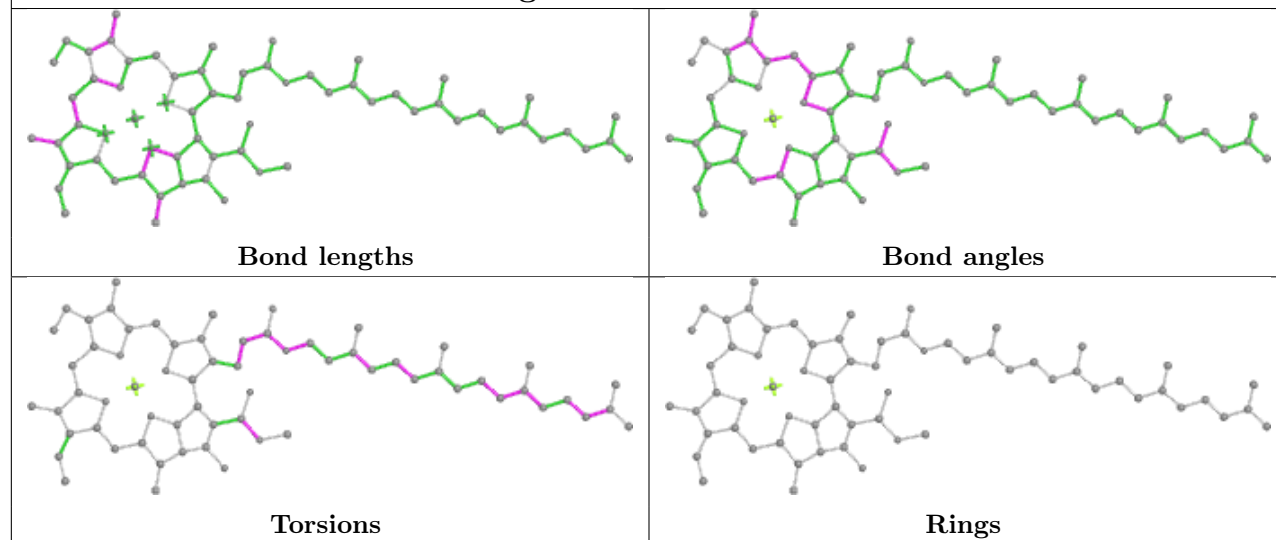


Rings

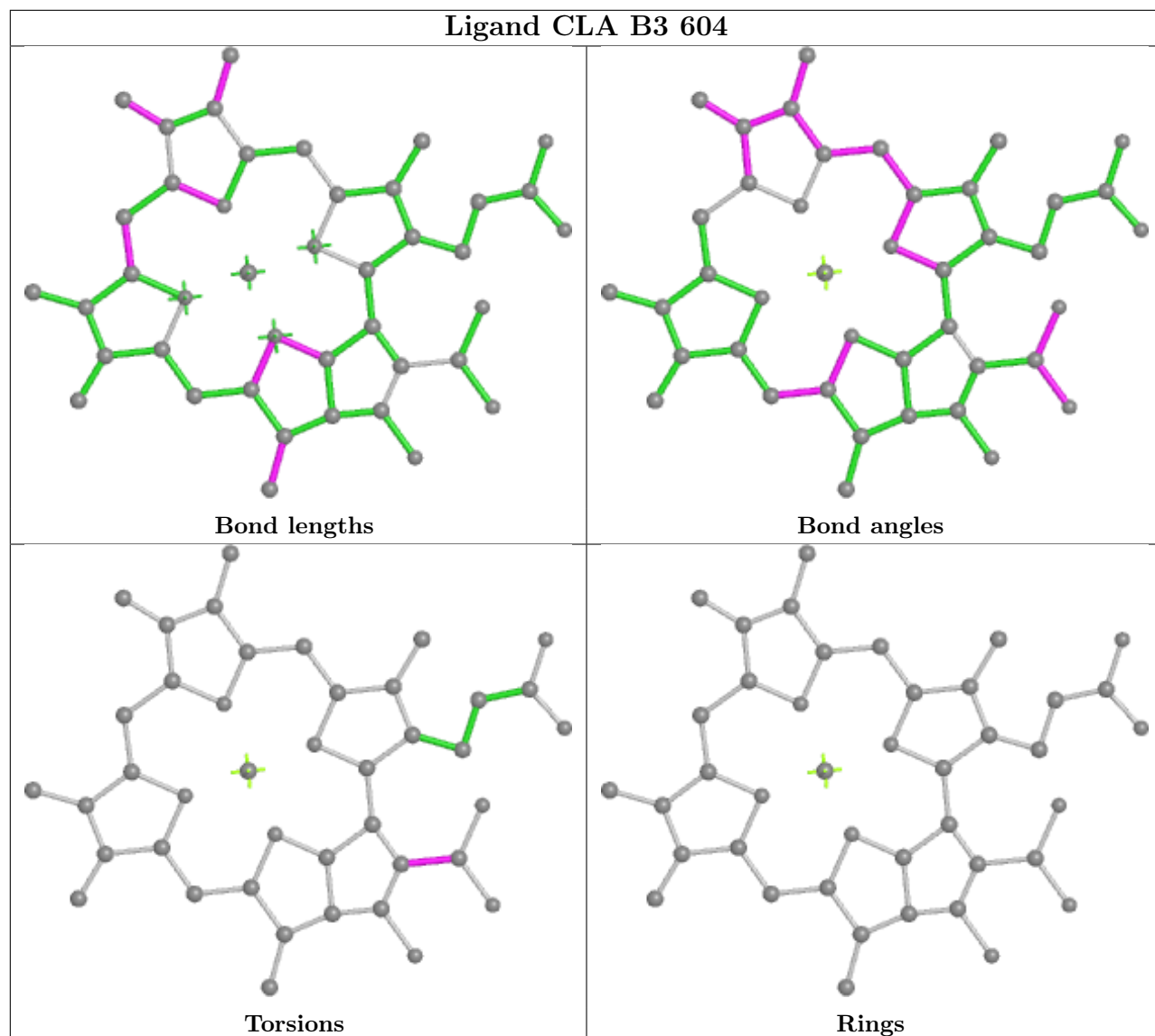
## Ligand CLA BB 832

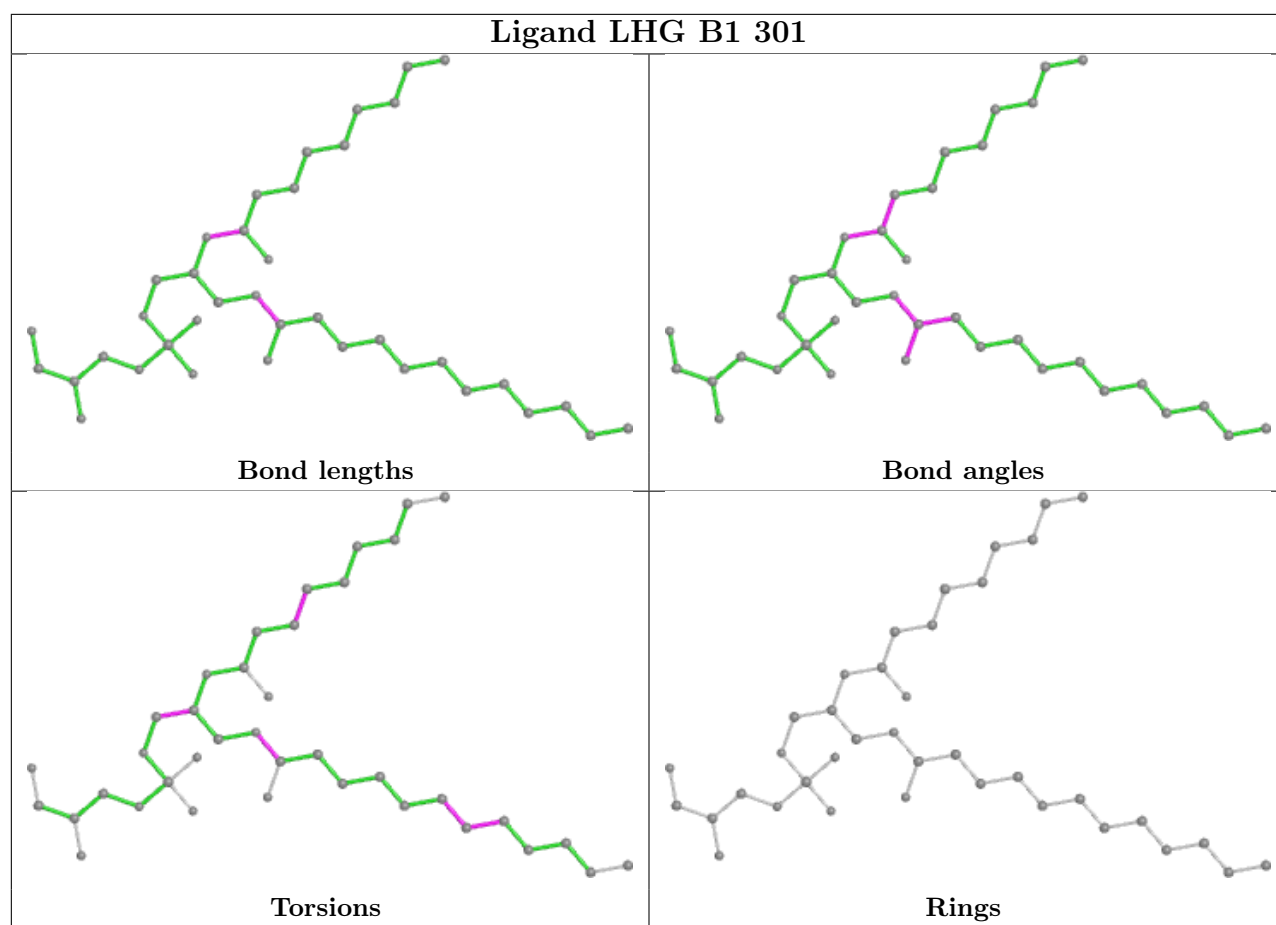


## Ligand CLA BA 806



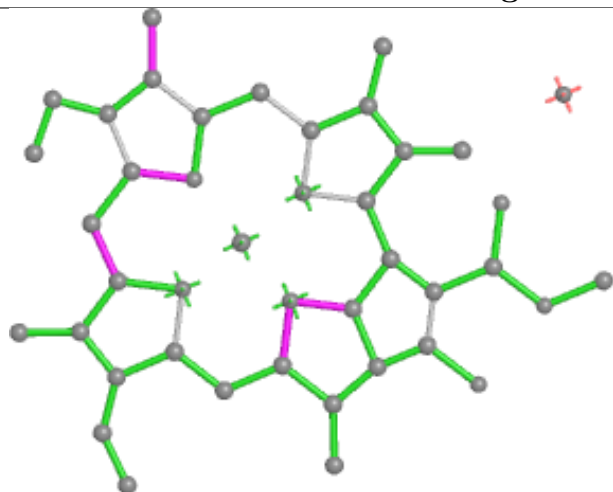
## Ligand CLA B3 604



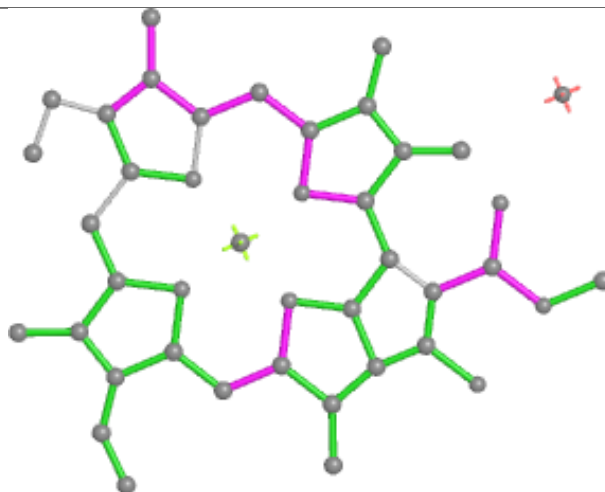




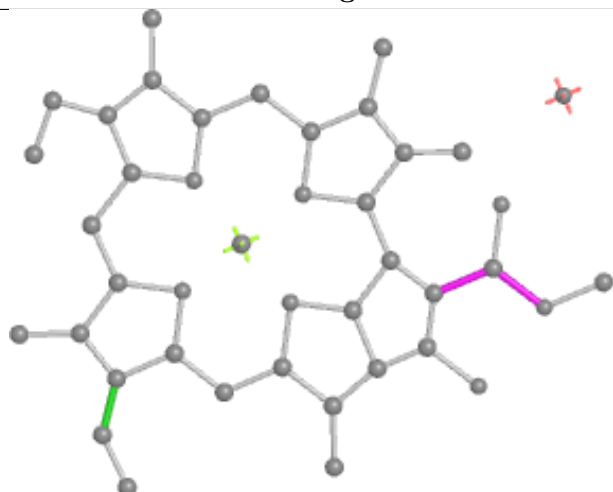
## Ligand CLA BA 844



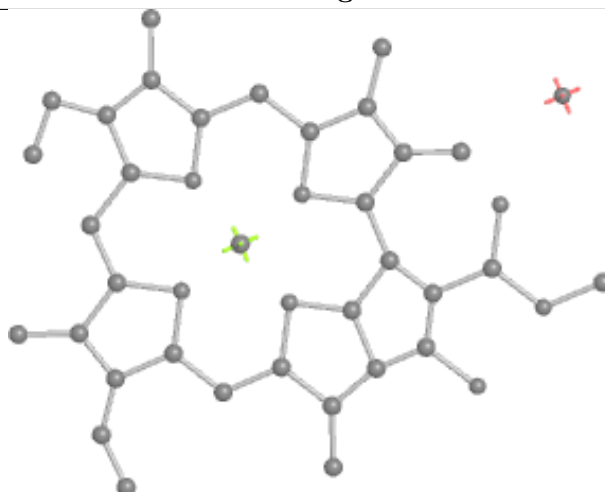
Bond lengths



Bond angles

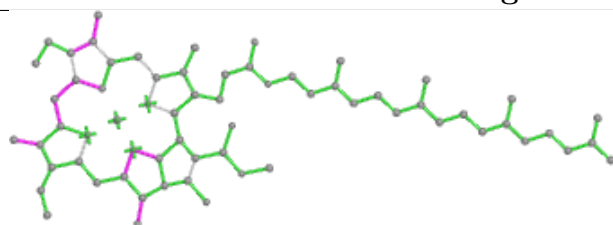


Torsions

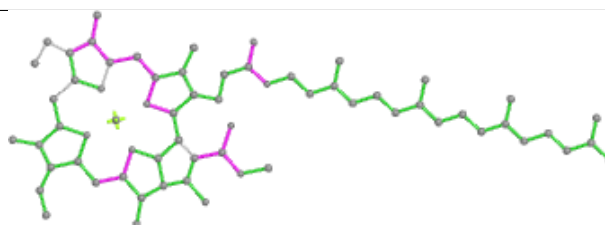


Rings

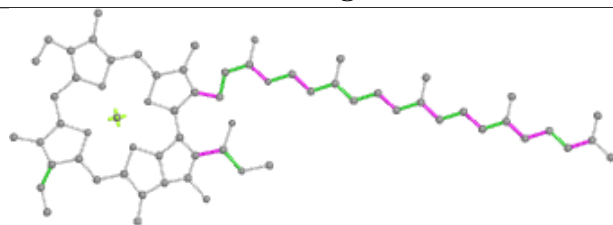
## Ligand CLA BA 830



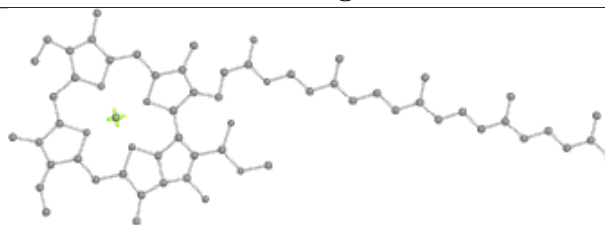
Bond lengths



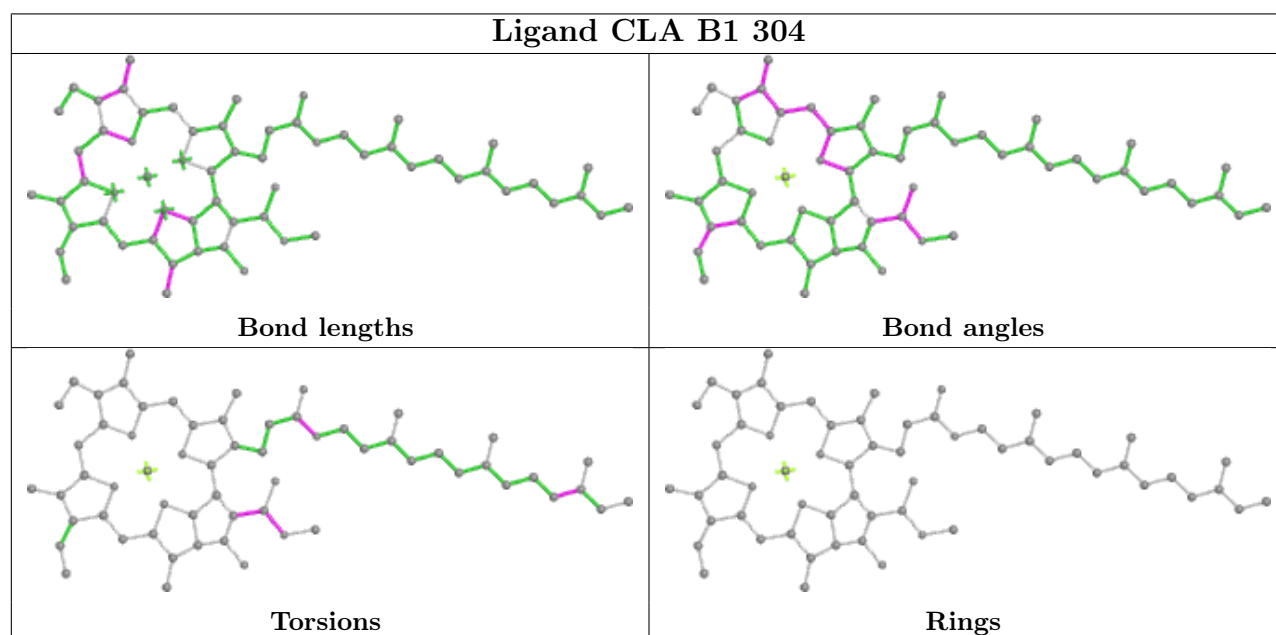
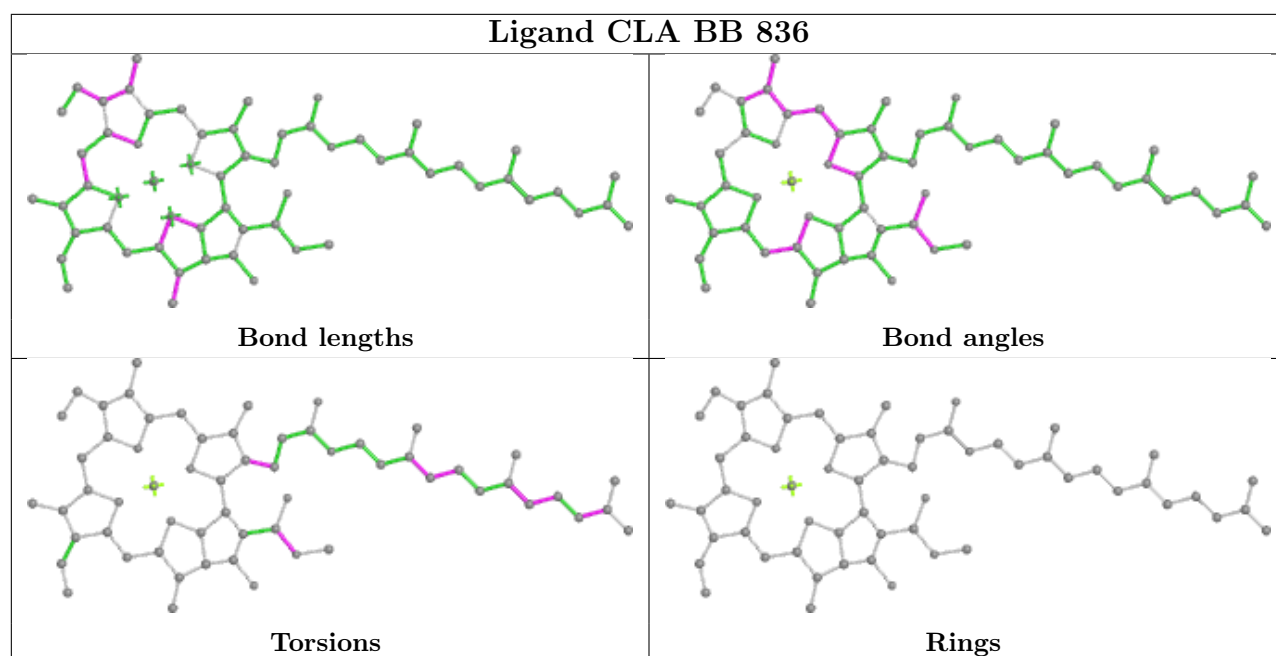
Bond angles



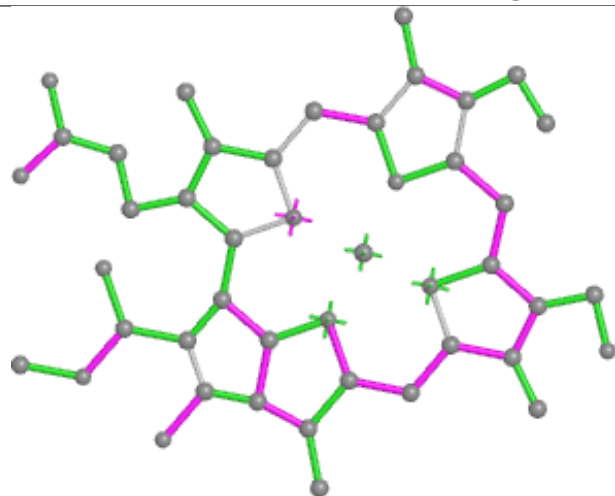
Torsions



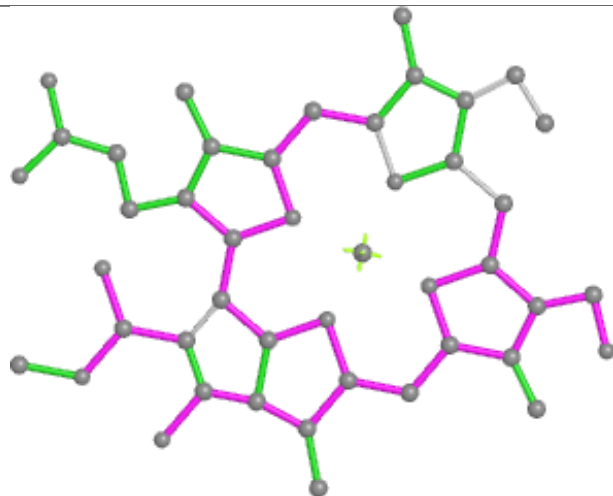
Rings



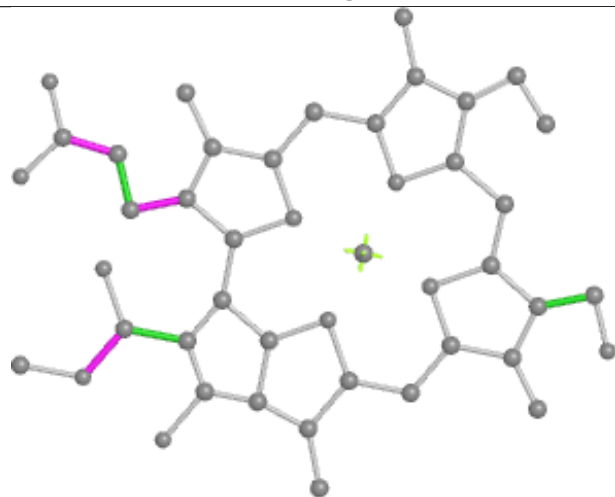
## Ligand CHL B5 607



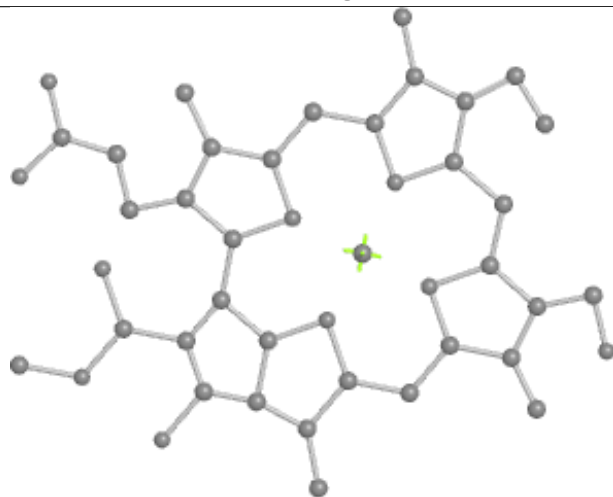
Bond lengths



Bond angles

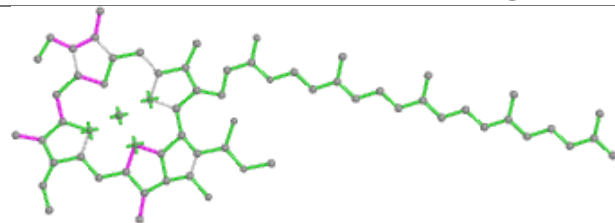


Torsions

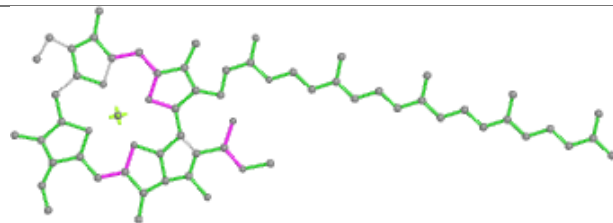


Rings

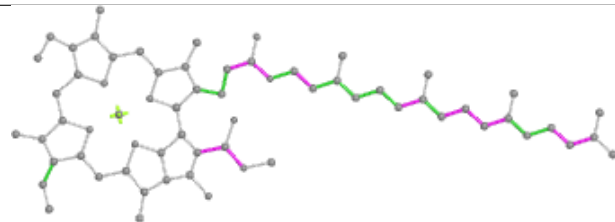
## Ligand CLA BB 835



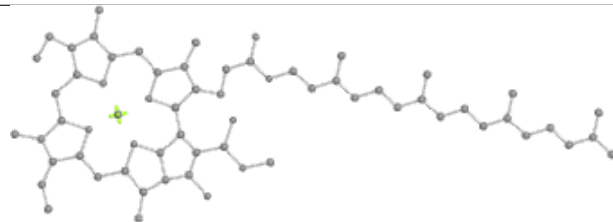
Bond lengths



Bond angles

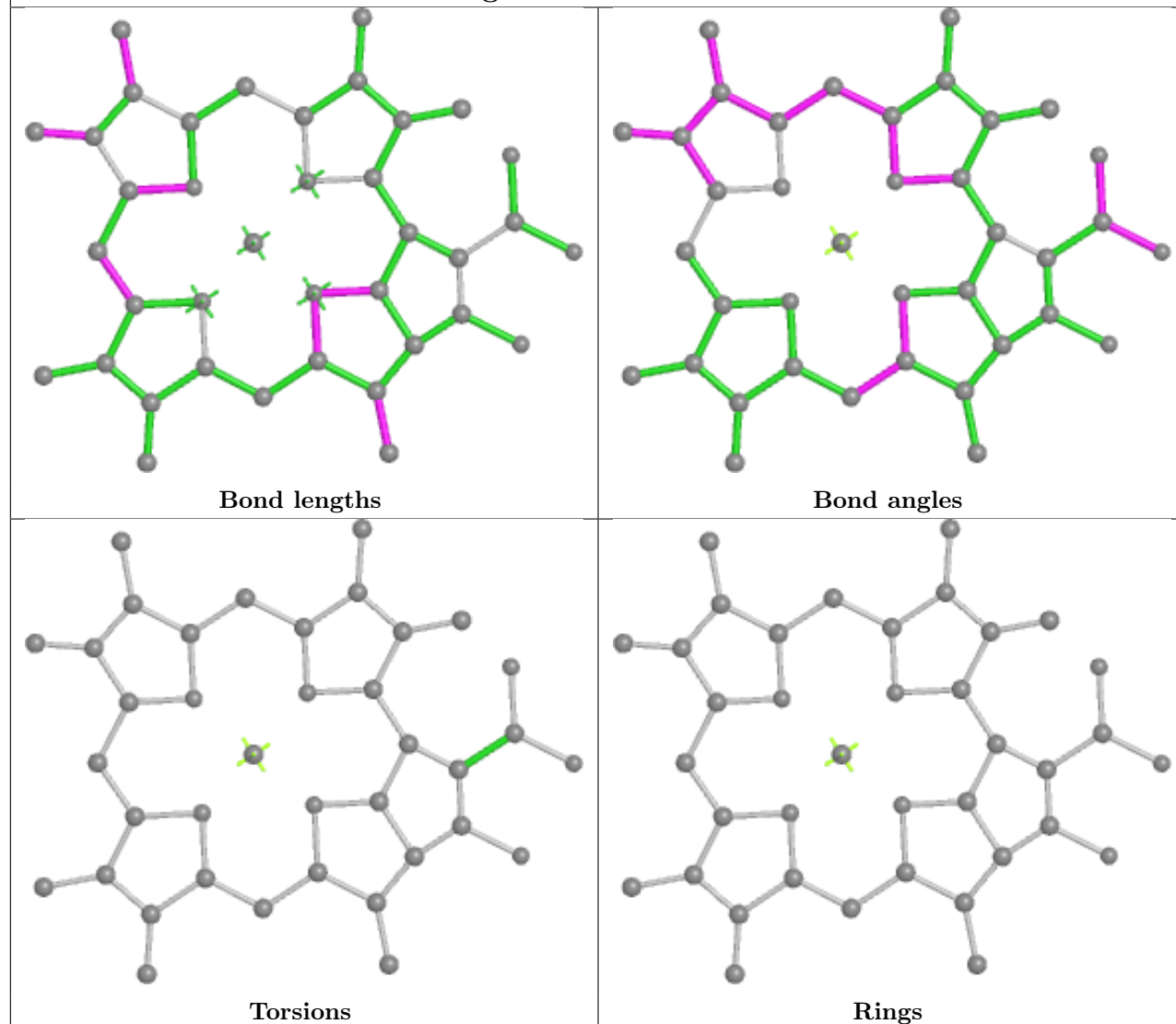


Torsions

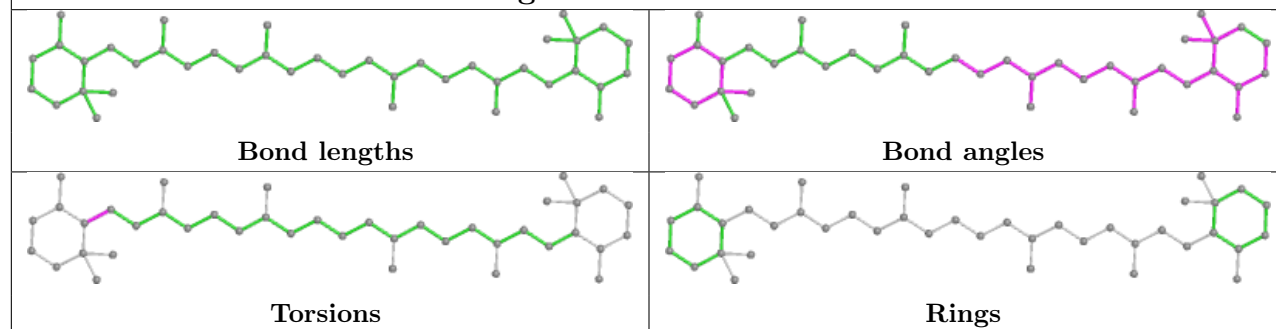


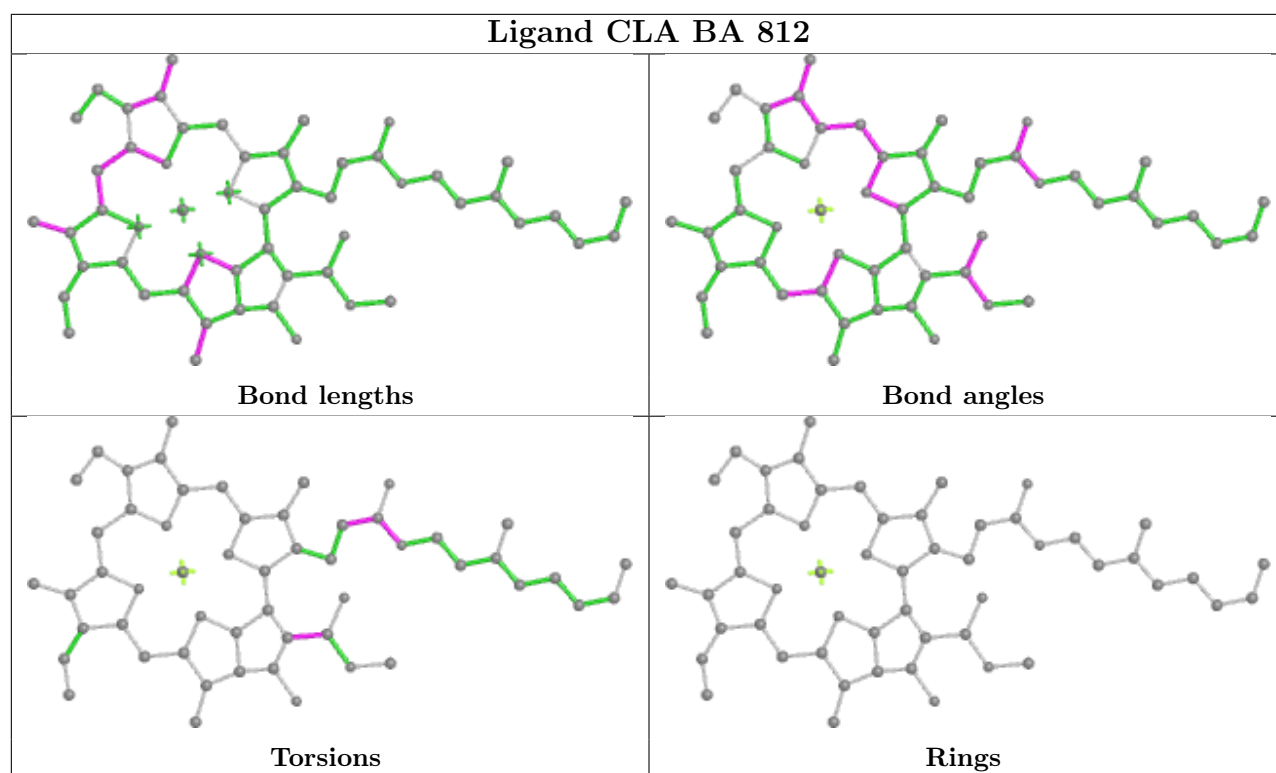
Rings

## Ligand CLA B1 312

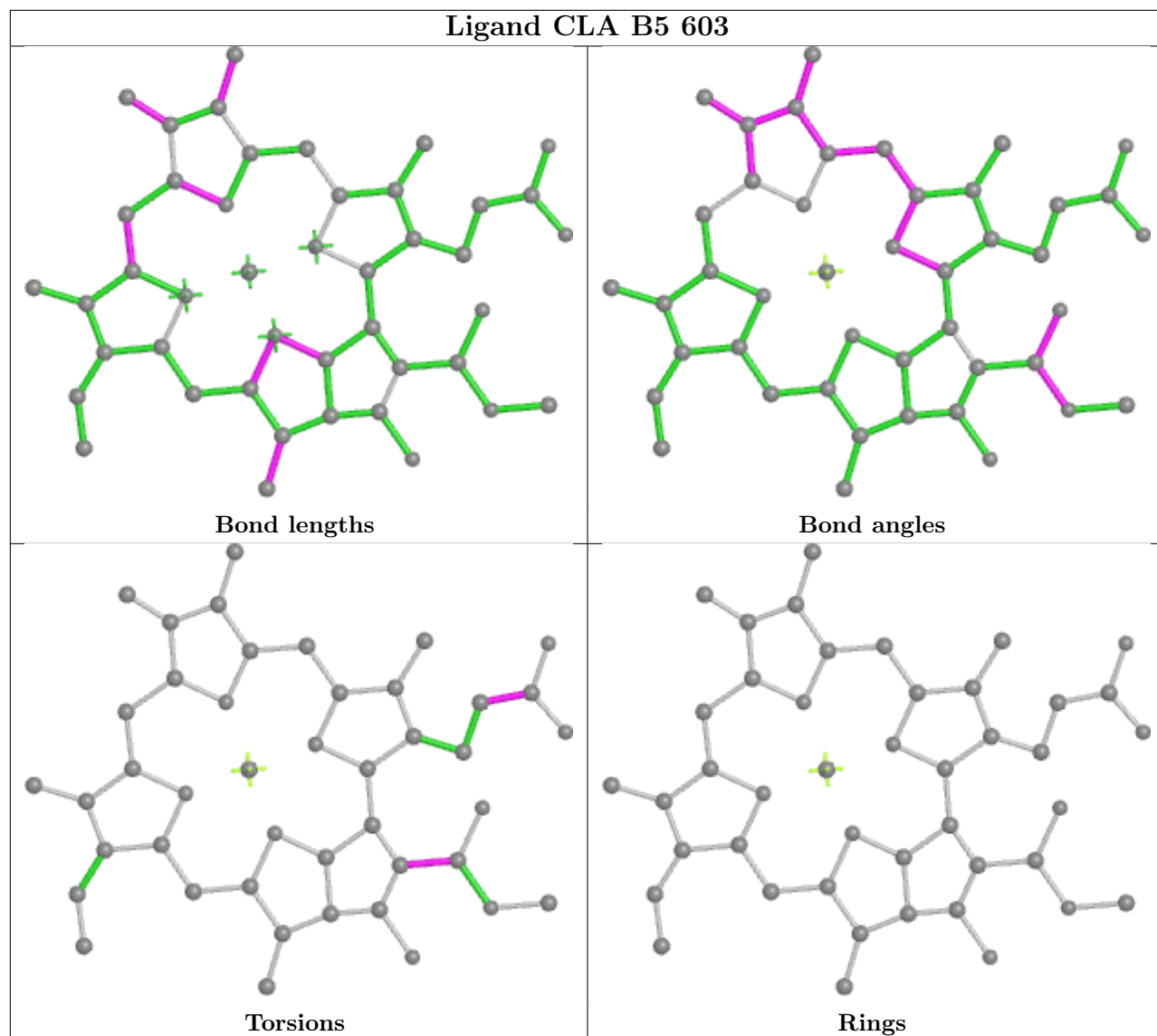


## Ligand BCR BB 848

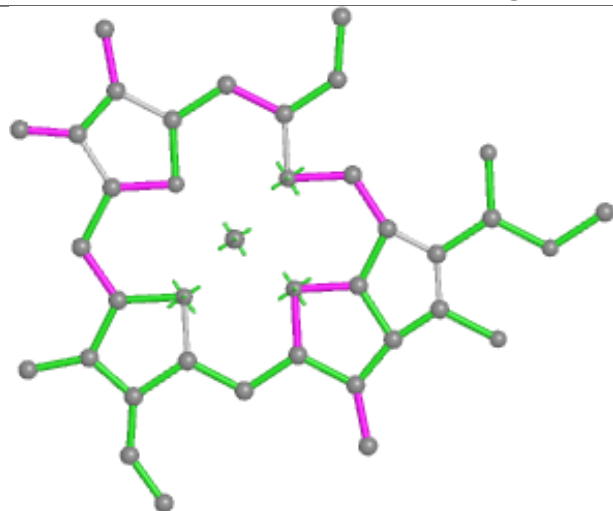




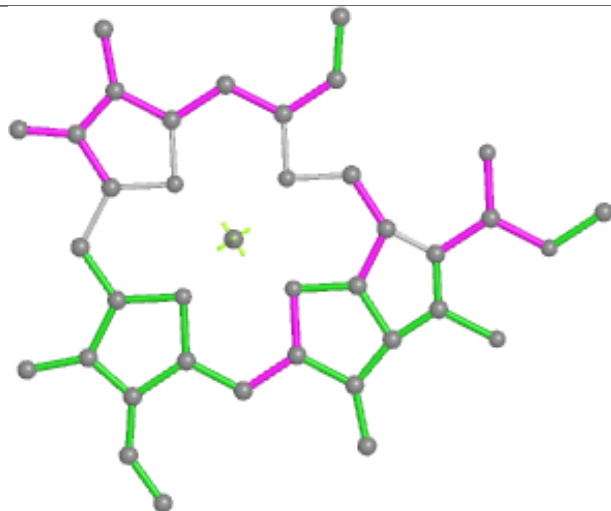
## Ligand CLA B5 603



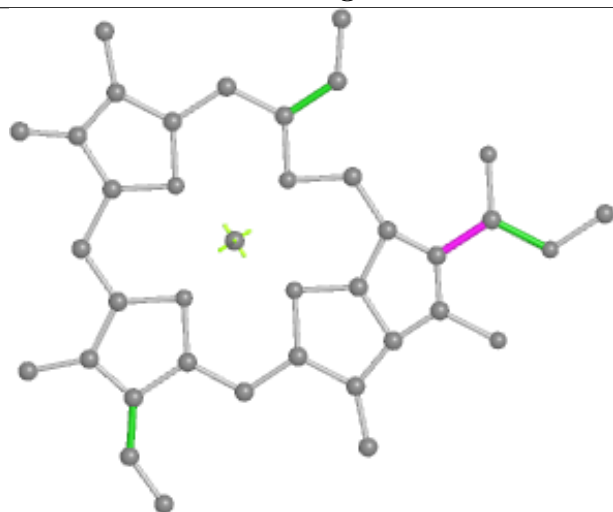
## Ligand CLA B2 309



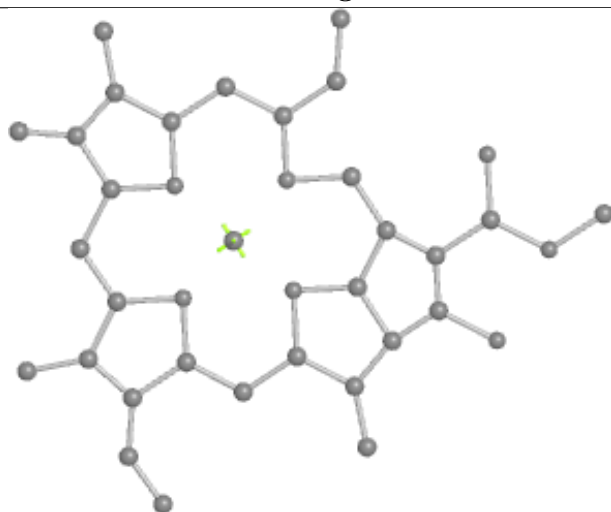
Bond lengths



Bond angles

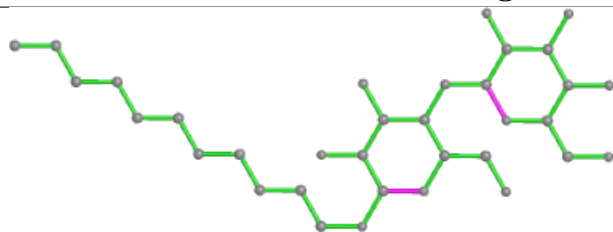


Torsions

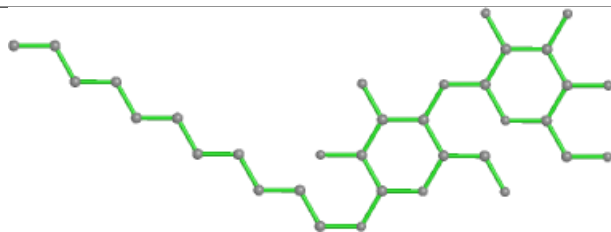


Rings

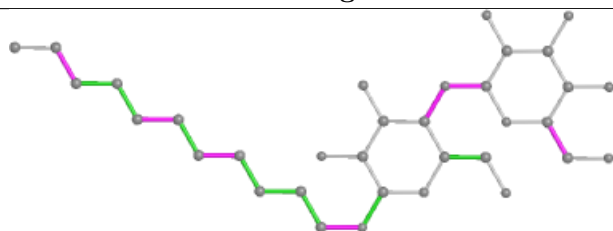
## Ligand LMU BA 853



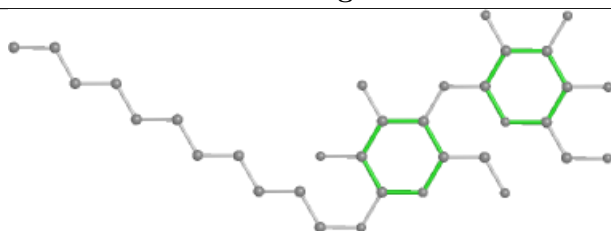
Bond lengths



Bond angles

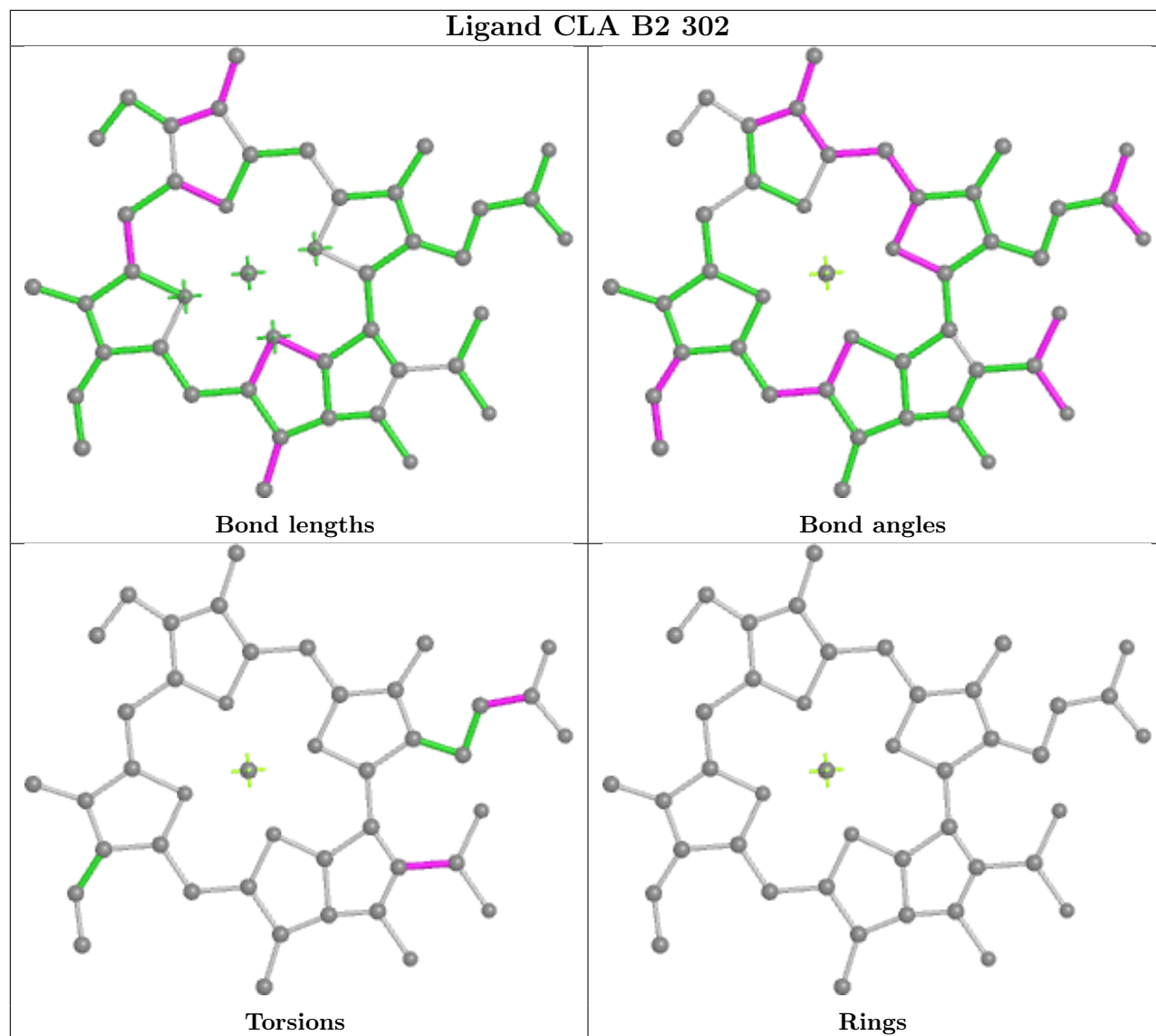


Torsions

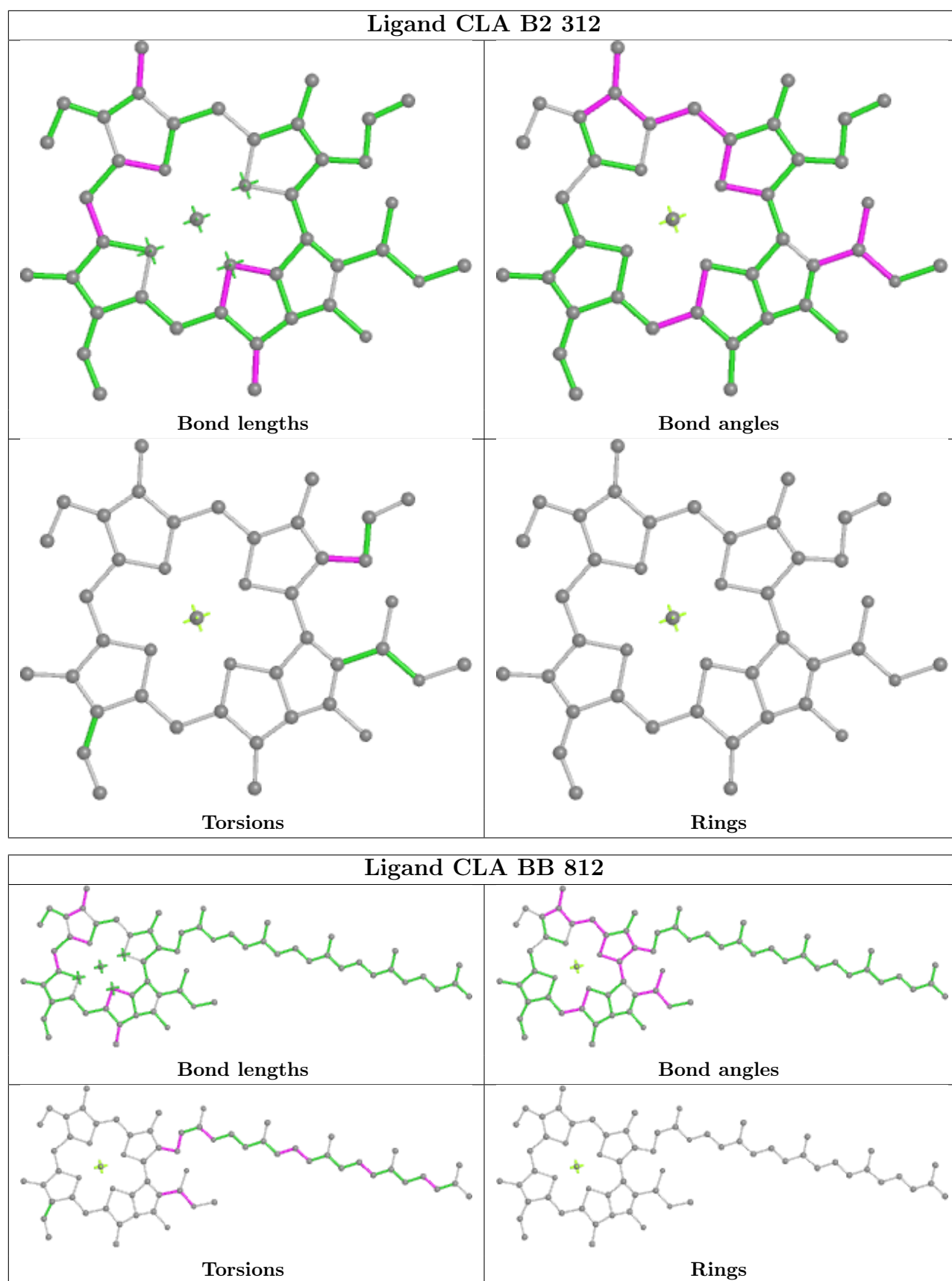


Rings

## Ligand CLA B2 302







## 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.

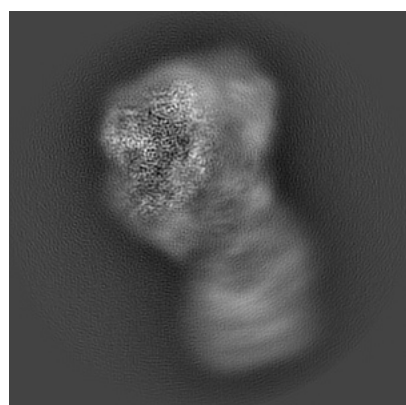
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32463. These allow visual inspection of the internal detail of the map and identification of artifacts.

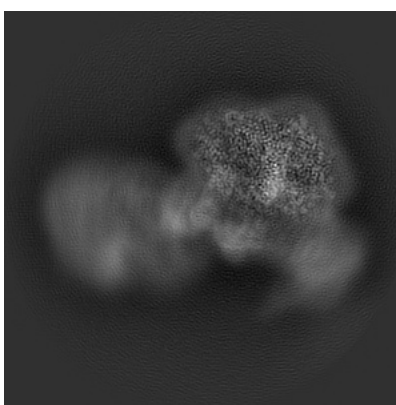
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

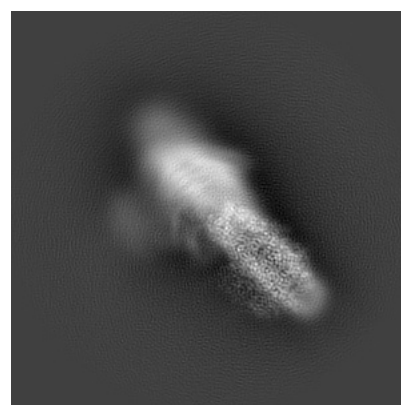
#### 6.1.1 Primary map



X



Y

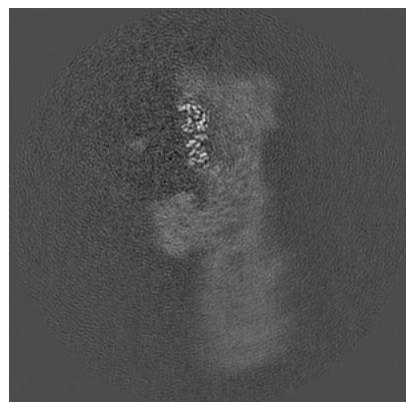


Z

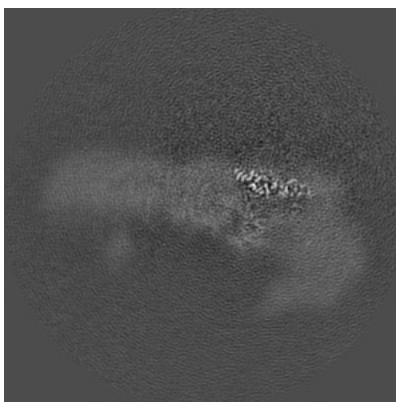
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

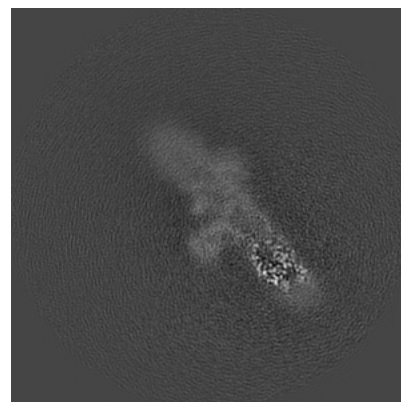
#### 6.2.1 Primary map



X Index: 200



Y Index: 200

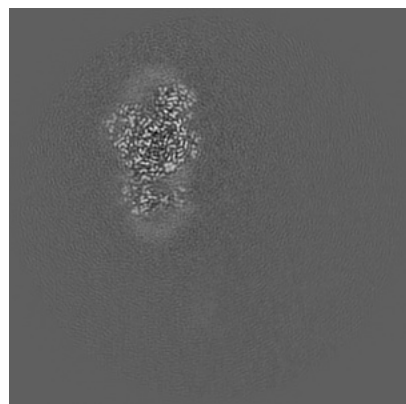


Z Index: 200

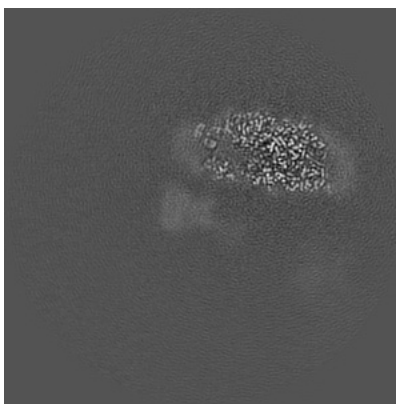
The images above show central slices of the map in three orthogonal directions.

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

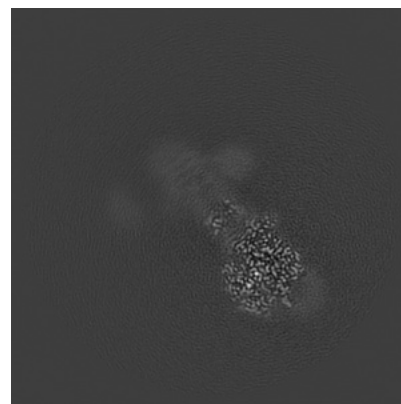
### 6.3.1 Primary map



X Index: 262



Y Index: 156

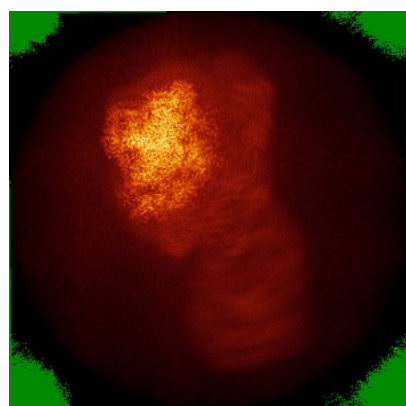


Z Index: 272

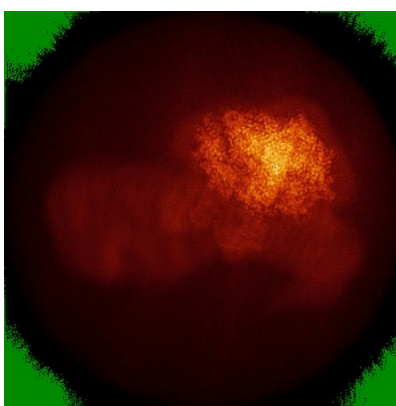
The images above show the largest variance slices of the map in three orthogonal directions.

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

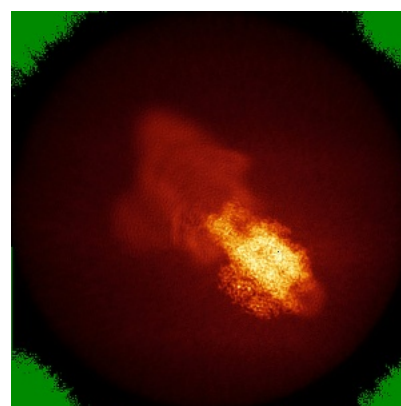
### 6.4.1 Primary map



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



X



Y



Z

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.

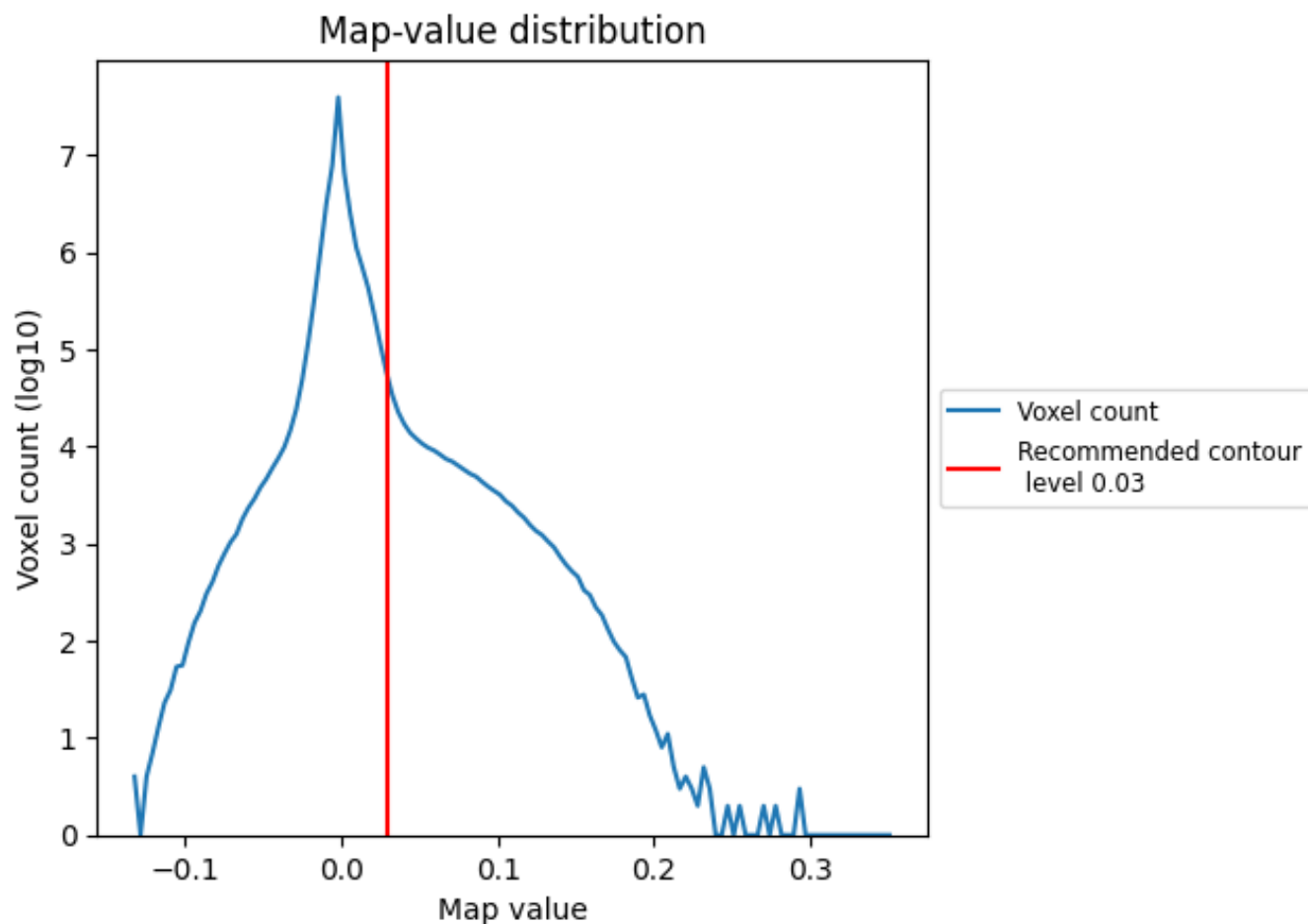
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

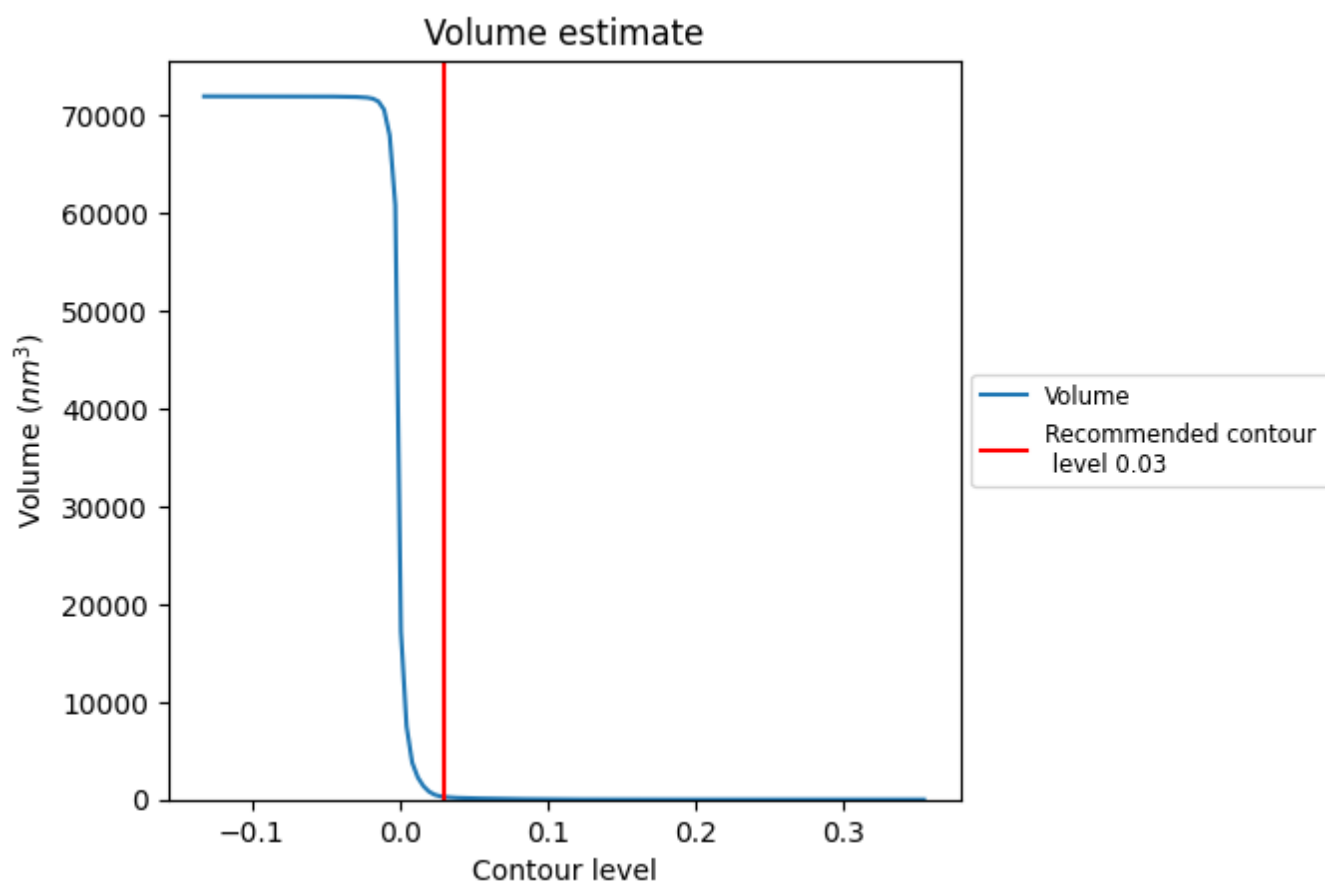
This section contains the results of statistical analysis of the map.

### 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.

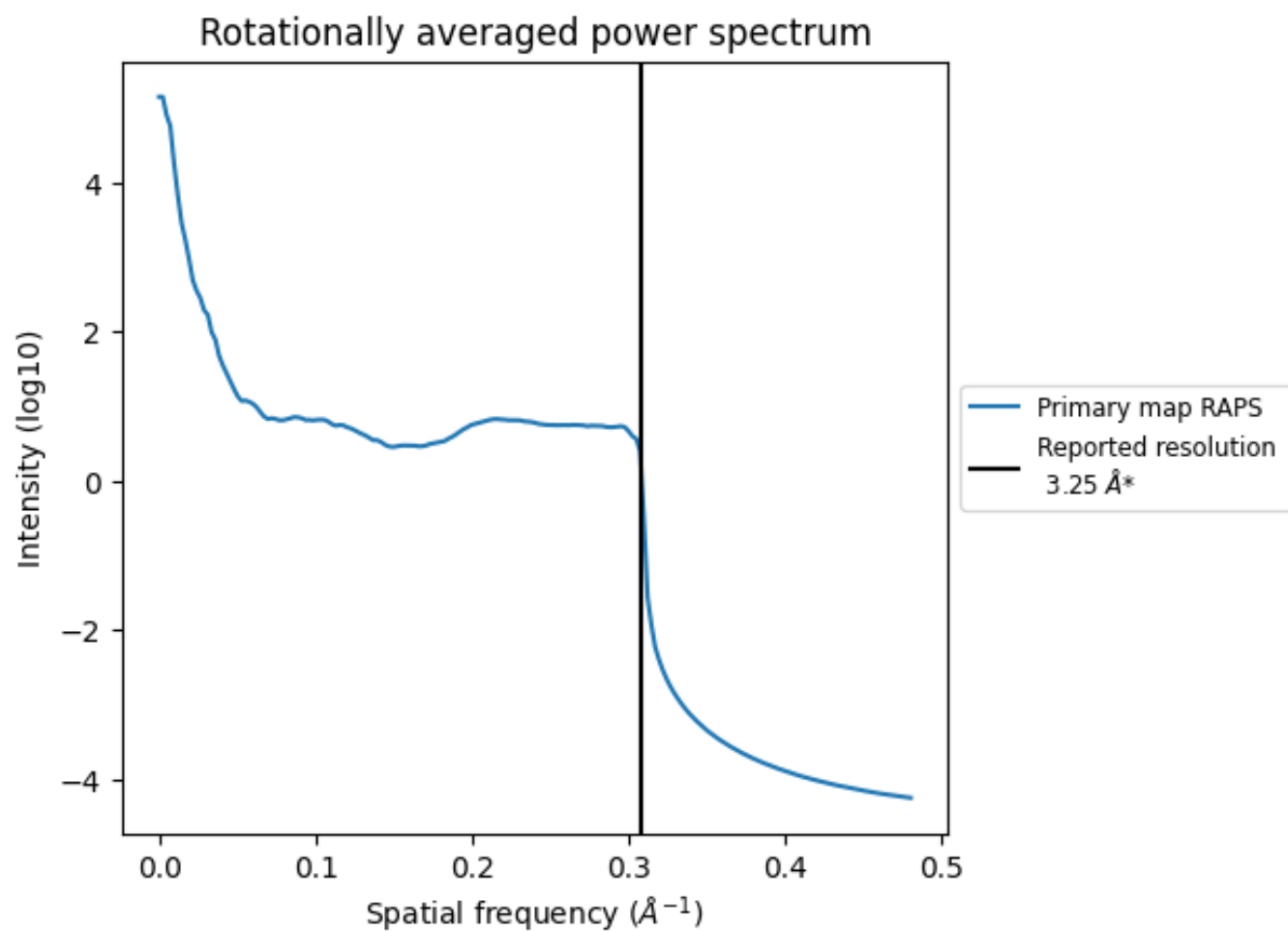
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 281 nm<sup>3</sup>; this corresponds to an approximate mass of 254 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<sup>-1</sup>



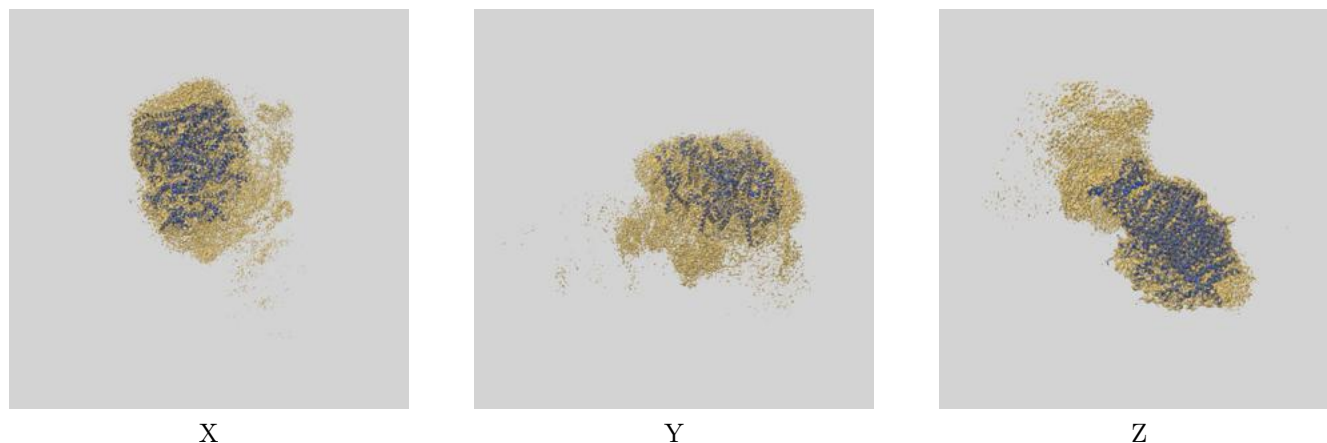
## 8 Fourier-Shell correlation

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

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

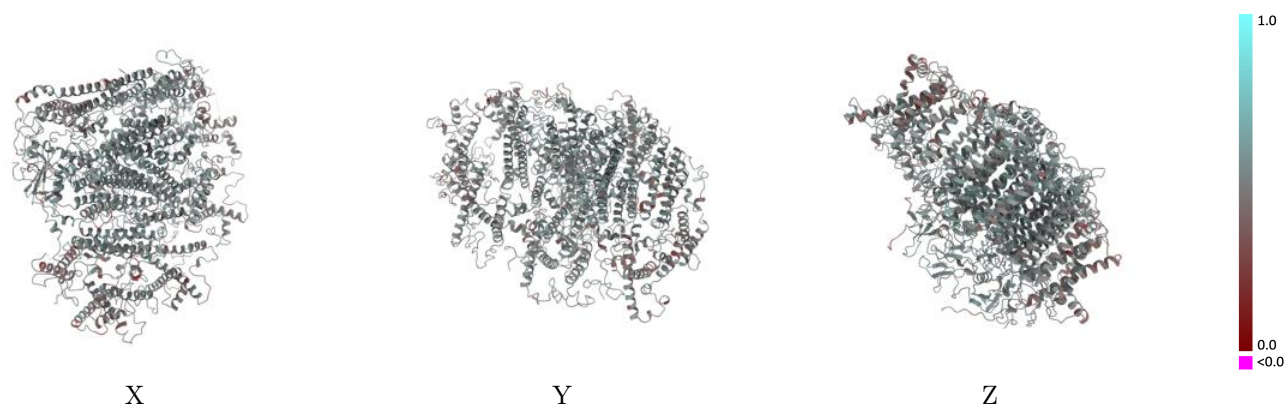
This section contains information regarding the fit between EMDB map EMD-32463 and PDB model 7WFE. Per-residue inclusion information can be found in section [3](#) on page [26](#).

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



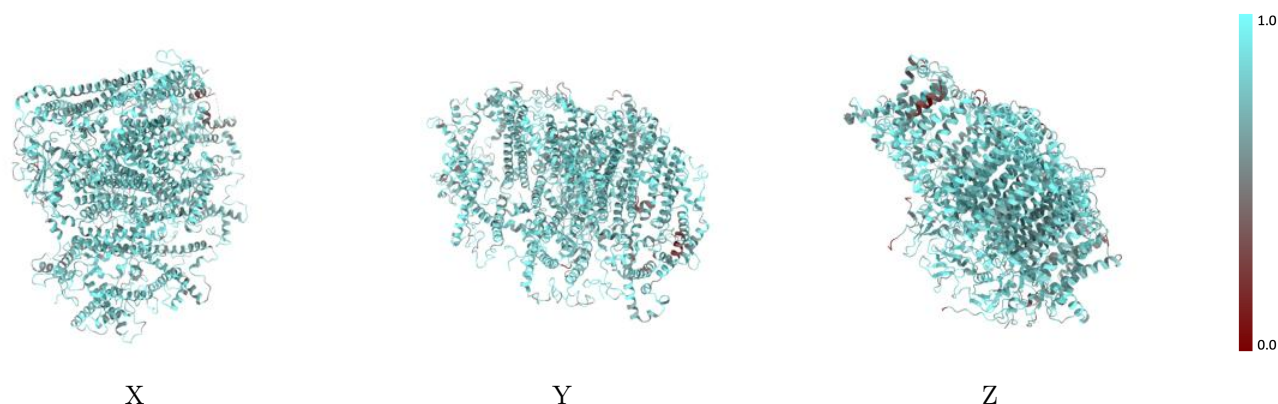
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



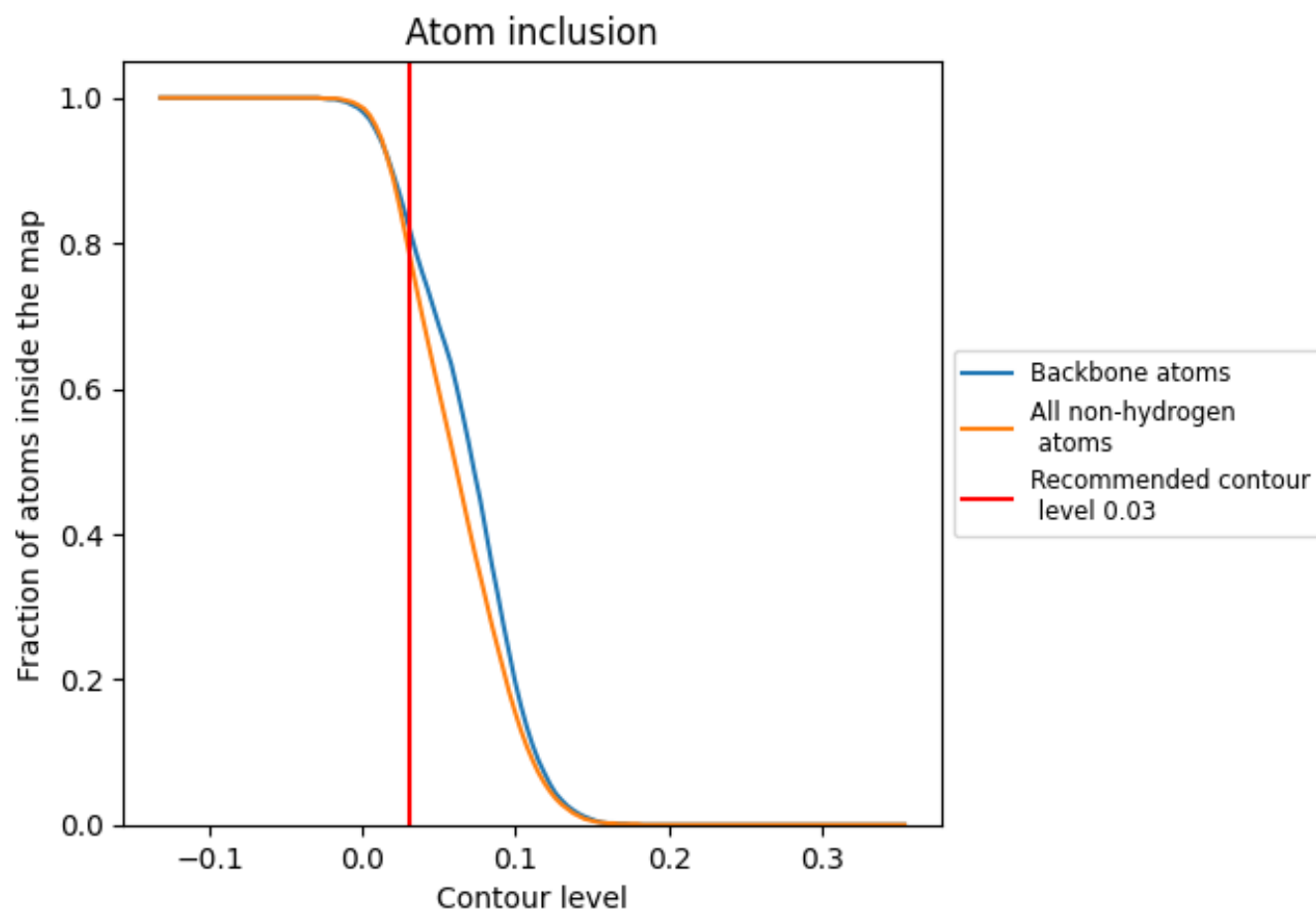
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 79% 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> 0.7910	<div><div></div></div> 0.5080
B1	<div><div></div></div> 0.6860	<div><div></div></div> 0.4640
B2	<div><div></div></div> 0.7580	<div><div></div></div> 0.4820
B3	<div><div></div></div> 0.7750	<div><div></div></div> 0.4780
B5	<div><div></div></div> 0.7860	<div><div></div></div> 0.4970
BA	<div><div></div></div> 0.8120	<div><div></div></div> 0.5280
BB	<div><div></div></div> 0.8310	<div><div></div></div> 0.5360
BC	<div><div></div></div> 0.8780	<div><div></div></div> 0.5280
BD	<div><div></div></div> 0.8200	<div><div></div></div> 0.5150
BE	<div><div></div></div> 0.7550	<div><div></div></div> 0.5090
BF	<div><div></div></div> 0.8060	<div><div></div></div> 0.5190
BG	<div><div></div></div> 0.7550	<div><div></div></div> 0.4740
BH	<div><div></div></div> 0.7260	<div><div></div></div> 0.4620
BI	<div><div></div></div> 0.7840	<div><div></div></div> 0.4960
BJ	<div><div></div></div> 0.7770	<div><div></div></div> 0.4920
BK	<div><div></div></div> 0.6550	<div><div></div></div> 0.4290
BL	<div><div></div></div> 0.7410	<div><div></div></div> 0.4690

1.0

0.0

<0.0