



## wwPDB EM Validation Summary Report ⓘ

Nov 4, 2024 – 12:44 am GMT

PDB ID : 8BCV  
EMDB ID : EMD-15969  
Title : Photosystem I assembly intermediate of Avena sativa  
Authors : Naschberger, A.; Amunts, A.; Nelson, N.  
Deposited on : 2022-10-17  
Resolution : 2.20 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	:	1.8.4, 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

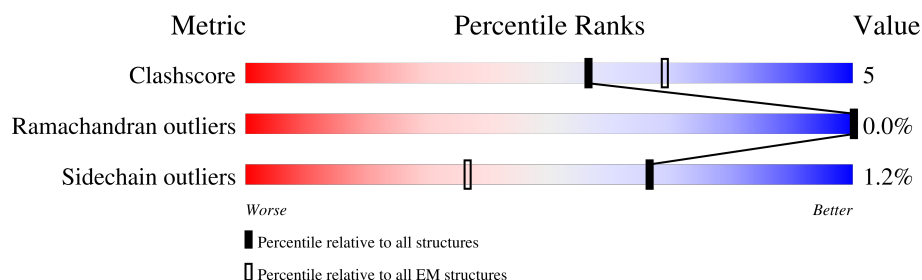
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.20 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	A	750	<div> <div>5%</div> <div>92%</div> <div>6%</div> <div>.</div> </div>
2	B	734	<div> <div>95%</div> <div>.</div> </div>
3	C	81	<div> <div>99%</div> <div>.</div> </div>
4	D	206	<div> <div>65%</div> <div>31%</div> </div>
5	E	143	<div> <div>6%</div> <div>46%</div> <div>53%</div> </div>
6	H	94	<div> <div>61%</div> <div>94%</div> <div>6%</div> </div>
7	I	36	<div> <div>11%</div> <div>81%</div> <div>11%</div> <div>8%</div> </div>
8	L	213	<div> <div>22%</div> <div>69%</div> <div>6%</div> <div>25%</div> </div>

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Mol	Chain	Length	Quality of chain
9	F	178	
10	G	144	
11	J	52	
12	K	130	
13	1	242	
14	2	207	
15	3	269	
16	4	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	CL0	A	801	X	-	-	-
17	CL0	H	202	X	-	-	-
18	CLA	1	303	X	-	-	-
18	CLA	1	304	X	-	-	-
18	CLA	1	305	X	-	-	-
18	CLA	1	306	X	-	-	-
18	CLA	1	308	X	-	-	-
18	CLA	1	309	X	-	-	-
18	CLA	1	310	X	-	-	-
18	CLA	1	311	X	-	-	-
18	CLA	1	312	X	-	-	-
18	CLA	1	313	X	-	-	-
18	CLA	1	314	X	-	-	-
18	CLA	1	315	X	-	-	-
18	CLA	2	601	X	-	-	-
18	CLA	2	602	X	-	-	-
18	CLA	2	603	X	-	-	-
18	CLA	2	604	X	-	-	-
18	CLA	2	608	X	-	-	-
18	CLA	2	609	X	-	-	-
18	CLA	2	610	X	-	-	-
18	CLA	2	611	X	-	-	-
18	CLA	2	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	2	613	X	-	-	-
18	CLA	3	302	X	-	-	-
18	CLA	3	303	X	-	-	-
18	CLA	3	304	X	-	-	-
18	CLA	3	305	X	-	-	-
18	CLA	3	307	X	-	-	-
18	CLA	3	308	X	-	-	-
18	CLA	3	309	X	-	-	-
18	CLA	3	310	X	-	-	-
18	CLA	3	311	X	-	-	-
18	CLA	3	312	X	-	-	-
18	CLA	4	601	X	-	-	-
18	CLA	4	602	X	-	-	-
18	CLA	4	603	X	-	-	-
18	CLA	4	604	X	-	-	-
18	CLA	4	608	X	-	-	-
18	CLA	4	609	X	-	-	-
18	CLA	4	610	X	-	-	-
18	CLA	4	611	X	-	-	-
18	CLA	4	612	X	-	-	-
18	CLA	4	613	X	-	-	-
18	CLA	4	614	X	-	-	-
18	CLA	A	802	X	-	-	-
18	CLA	A	803	X	-	-	-
18	CLA	A	804	X	-	-	-
18	CLA	A	805	X	-	-	-
18	CLA	A	806	X	-	-	-
18	CLA	A	807	X	-	-	-
18	CLA	A	808	X	-	-	-
18	CLA	A	809	X	-	-	-
18	CLA	A	810	X	-	-	-
18	CLA	A	811	X	-	-	-
18	CLA	A	812	X	-	-	-
18	CLA	A	813	X	-	-	-
18	CLA	A	814	X	-	-	-
18	CLA	A	815	X	-	-	-
18	CLA	A	816	X	-	-	-
18	CLA	A	817	X	-	-	-
18	CLA	A	818	X	-	-	-
18	CLA	A	819	X	-	-	-
18	CLA	A	820	X	-	-	-
18	CLA	A	821	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	A	822	X	-	-	-
18	CLA	A	823	X	-	-	-
18	CLA	A	824	X	-	-	-
18	CLA	A	825	X	-	-	-
18	CLA	A	826	X	-	-	-
18	CLA	A	827	X	-	-	-
18	CLA	A	828	X	-	-	-
18	CLA	A	829	X	-	-	-
18	CLA	A	830	X	-	-	-
18	CLA	A	831	X	-	-	-
18	CLA	A	832	X	-	-	-
18	CLA	A	833	X	-	-	-
18	CLA	A	834	X	-	-	-
18	CLA	A	835	X	-	-	-
18	CLA	A	836	X	-	-	-
18	CLA	A	837	X	-	-	-
18	CLA	A	838	X	-	-	-
18	CLA	A	839	X	-	-	-
18	CLA	A	840	X	-	-	-
18	CLA	A	841	X	-	-	-
18	CLA	A	842	X	-	-	-
18	CLA	A	843	X	-	-	-
18	CLA	A	845	X	-	-	-
18	CLA	A	854	X	-	-	-
18	CLA	A	855	X	-	-	-
18	CLA	A	856	X	-	-	-
18	CLA	B	801	X	-	-	-
18	CLA	B	802	X	-	-	-
18	CLA	B	803	X	-	-	-
18	CLA	B	804	X	-	-	-
18	CLA	B	805	X	-	-	-
18	CLA	B	806	X	-	-	-
18	CLA	B	807	X	-	-	-
18	CLA	B	808	X	-	-	-
18	CLA	B	809	X	-	-	-
18	CLA	B	810	X	-	-	-
18	CLA	B	811	X	-	-	-
18	CLA	B	812	X	-	-	-
18	CLA	B	813	X	-	-	-
18	CLA	B	814	X	-	-	-
18	CLA	B	815	X	-	-	-
18	CLA	B	816	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	B	817	X	-	-	-
18	CLA	B	818	X	-	-	-
18	CLA	B	819	X	-	-	-
18	CLA	B	820	X	-	-	-
18	CLA	B	821	X	-	-	-
18	CLA	B	822	X	-	-	-
18	CLA	B	823	X	-	-	-
18	CLA	B	824	X	-	-	-
18	CLA	B	825	X	-	-	-
18	CLA	B	826	X	-	-	-
18	CLA	B	827	X	-	-	-
18	CLA	B	828	X	-	-	-
18	CLA	B	829	X	-	-	-
18	CLA	B	830	X	-	-	-
18	CLA	B	831	X	-	-	-
18	CLA	B	832	X	-	-	-
18	CLA	B	833	X	-	-	-
18	CLA	B	834	X	-	-	-
18	CLA	B	835	X	-	-	-
18	CLA	B	836	X	-	-	-
18	CLA	B	837	X	-	-	-
18	CLA	B	839	X	-	-	-
18	CLA	F	802	X	-	-	-
18	CLA	F	804	X	-	-	-
18	CLA	F	805	X	-	-	-
18	CLA	G	201	X	-	-	-
18	CLA	G	204	X	-	-	-
18	CLA	G	205	X	-	-	-
18	CLA	J	102	X	-	-	-
18	CLA	K	201	X	-	-	-
18	CLA	K	203	X	-	-	-
18	CLA	K	204	X	-	-	-
18	CLA	L	303	X	-	-	-
18	CLA	L	304	X	-	-	-
18	CLA	L	305	X	-	-	-
27	CHL	1	302	X	-	-	-
27	CHL	1	307	X	-	-	-
27	CHL	2	605	X	-	-	-
27	CHL	2	606	X	-	-	-
27	CHL	2	607	X	-	-	-
27	CHL	2	614	X	-	-	-
27	CHL	3	301	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CHL	3	306	X	-	-	-
27	CHL	4	605	X	-	-	-
27	CHL	4	606	X	-	-	-
27	CHL	4	607	X	-	-	-
27	CHL	4	615	X	-	-	-

## 2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 37485 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	742	Total	C	N	O	S	0	0
			5840	3826	992	1003	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5864	3848	996	1007	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			605	372	104	118	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	143	Total	C	N	O	S	0	0
			1124	722	196	203	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	67	Total	C	N	O	0	0
			533	340	94	99		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
6	H	94	Total	C	N	O	0	0
			715	469	114	132		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	33	Total	C	N	O	S	0	0
			258	178	38	41	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	159	Total	C	N	O	S	0	0
			1192	788	189	214	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	158	Total	C	N	O	S	0	0
			1238	804	210	221	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	94	Total	C	N	O	S	0	0
			721	467	121	133			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	43	Total	C	N	O	S	0	0
			342	232	52	57	1		

- Molecule 12 is a protein called Photosystem I reaction center subunit X.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	88	Total	C	N	O	S	0	0
			628	397	107	121	3		

- Molecule 13 is a protein called Chlorophyll a-b binding protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1	196	Total	C	N	O	S	0	0
			1519	990	254	271	4		

- Molecule 14 is a protein called Chlorophyll a-b binding protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	2	207	Total	C	N	O	S	0	0
			1609	1050	263	292	4		

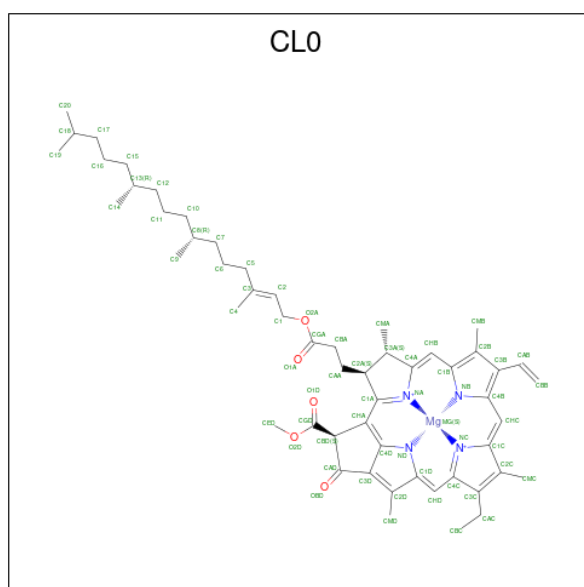
- Molecule 15 is a protein called Chlorophyll a-b binding protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	3	222	Total	C	N	O	S	0	0
			1725	1130	278	309	8		

- Molecule 16 is a protein called Chlorophyll a-b binding protein 4, chloroplastic.

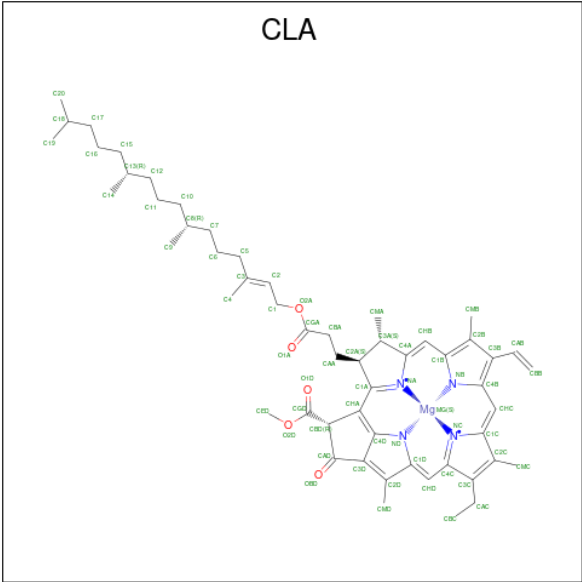
Mol	Chain	Residues	Atoms					AltConf	Trace
16	4	199	Total	C	N	O	S	0	0
			1555	1012	257	282	4		

- Molecule 17 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

- Molecule 18 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
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 56	C 46	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
18	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	B	1	Total 61	C 51	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	F	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	G	1	Total 57	C 47	Mg 1	N 4	O 5	0
18	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
18	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	K	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	1	1	Total 65	C 55	Mg 1	N 4	O 5	0

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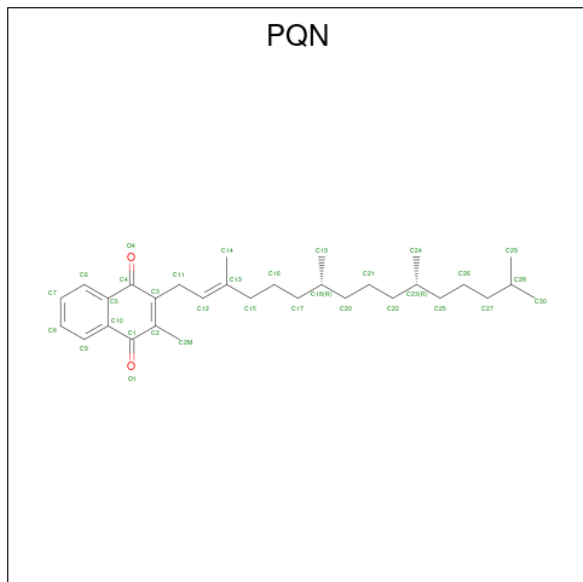
Mol	Chain	Residues	Atoms					AltConf
18	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	1	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	2	1	Total 50	C 40	Mg 1	N 4	O 5	0

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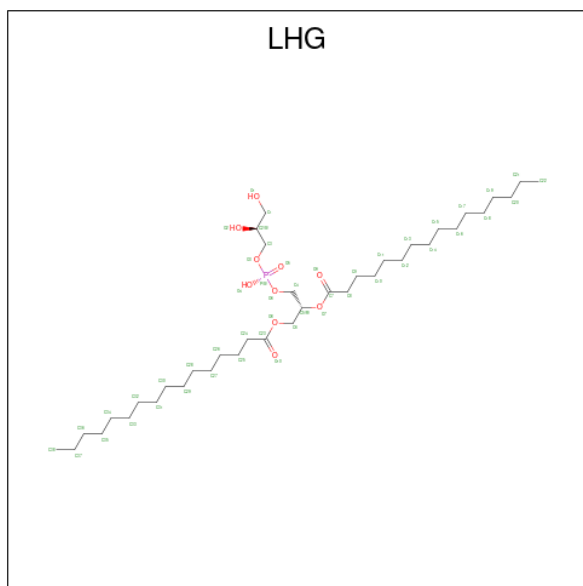
Mol	Chain	Residues	Atoms					AltConf
18	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	3	1	Total 61	C 51	Mg 1	N 4	O 5	0
18	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	4	1	Total 47	C 37	Mg 1	N 4	O 5	0
18	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
18	4	1	Total 50	C 40	Mg 1	N 4	O 5	0

- Molecule 19 is PHYLLOQUINONE (three-letter code: PQN) (formula:  $C_{31}H_{46}O_2$ ) (labeled as "Ligand of Interest" by depositor).



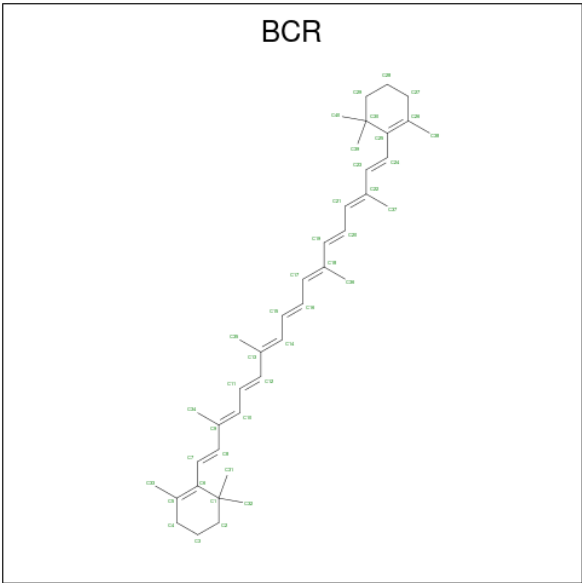
Mol	Chain	Residues	Atoms			AltConf
19	A	1	Total	C	O	0
			33	31	2	
19	B	1	Total	C	O	0
			33	31	2	

- Molecule 20 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



Mol	Chain	Residues	Atoms				AltConf
20	A	1	Total	C	O	P	0
			49	38	10	1	
20	A	1	Total	C	O	P	0
			31	20	10	1	
20	B	1	Total	C	O	P	0
			39	28	10	1	
20	B	1	Total	C	O	P	0
			49	38	10	1	
20	1	1	Total	C	O	P	0
			49	38	10	1	
20	2	1	Total	C	O	P	0
			43	32	10	1	

- Molecule 21 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
21	A	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	

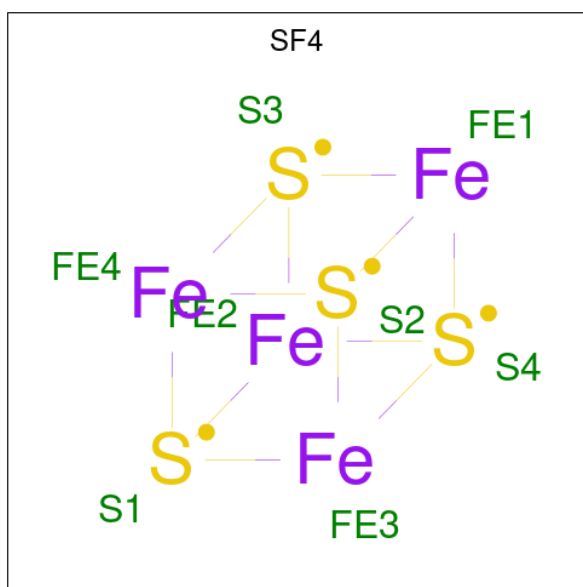
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Mol	Chain	Residues	Atoms	AltConf
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	I	1	Total C 40 40	0
21	L	1	Total C 40 40	0
21	L	1	Total C 40 40	0
21	L	1	Total C 40 40	0
21	F	1	Total C 40 40	0
21	F	1	Total C 40 40	0
21	G	1	Total C 40 40	0
21	G	1	Total C 40 40	0
21	J	1	Total C 40 40	0
21	K	1	Total C 40 40	0
21	K	1	Total C 40 40	0
21	3	1	Total C 40 40	0
21	4	1	Total C 40 40	0

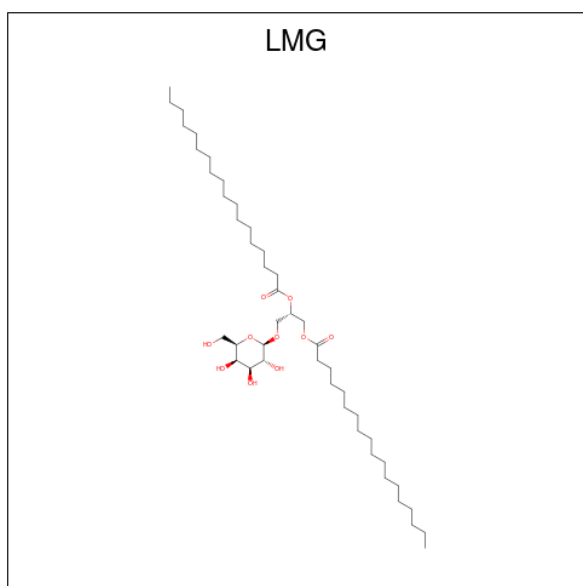
- Molecule 22 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).





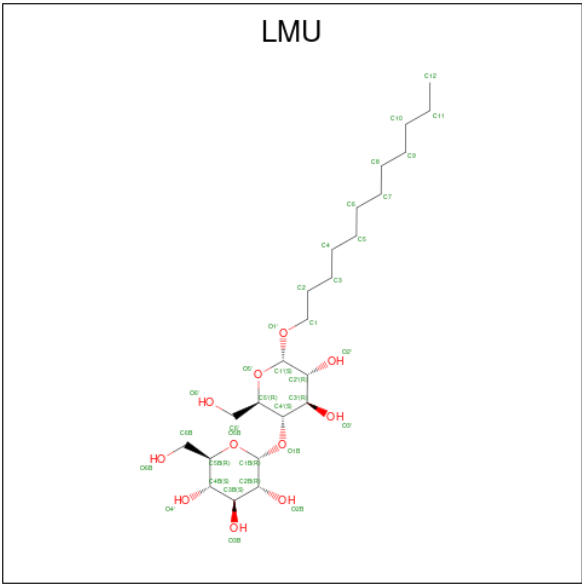
Mol	Chain	Residues	Atoms			AltConf
22	A	1	Total	Fe	S	0
			8	4	4	
22	C	1	Total	Fe	S	0
			8	4	4	
22	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
23	A	1	Total	C	O	0
			43	33	10	
23	F	1	Total	C	O	0
			30	20	10	
23	4	1	Total	C	O	0
			46	36	10	
23	4	1	Total	C	O	0
			45	35	10	

- Molecule 24 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>) (labeled as "Ligand of Interest" by depositor).



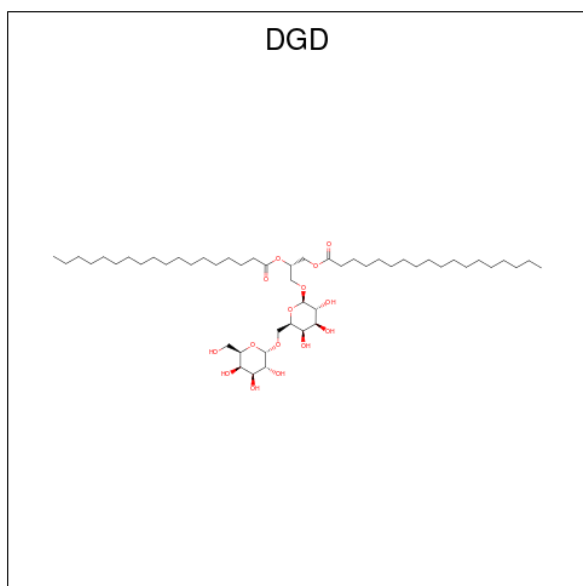
Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total	C	O	0
			24	18	6	
24	A	1	Total	C	O	0
			35	24	11	
24	B	1	Total	C	O	0
			24	18	6	
24	H	1	Total	C	O	0
			24	18	6	
24	L	1	Total	C	O	0
			20	14	6	
24	F	1	Total	C	O	0
			35	24	11	
24	F	1	Total	C	O	0
			35	24	11	

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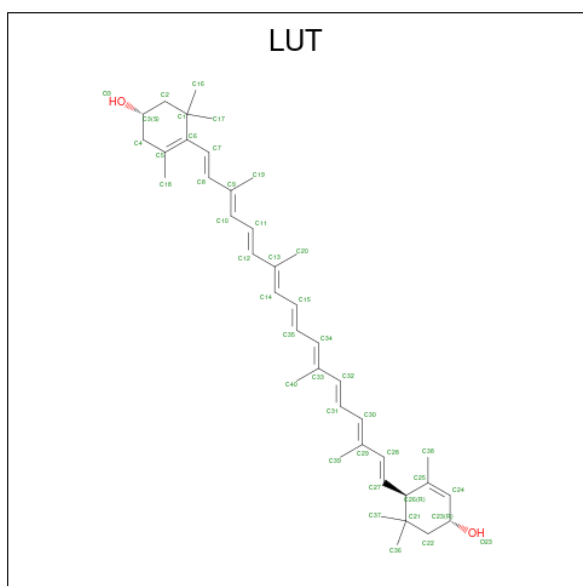
Mol	Chain	Residues	Atoms			AltConf
24	F	1	Total	C	O	0
			35	24	11	
24	F	1	Total	C	O	0
			35	24	11	
24	G	1	Total	C	O	0
			35	24	11	
24	G	1	Total	C	O	0
			35	24	11	
24	1	1	Total	C	O	0
			35	24	11	
24	1	1	Total	C	O	0
			35	24	11	
24	1	1	Total	C	O	0
			24	18	6	
24	2	1	Total	C	O	0
			35	24	11	
24	4	1	Total	C	O	0
			23	17	6	
24	4	1	Total	C	O	0
			35	24	11	
24	4	1	Total	C	O	0
			24	18	6	

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



Mol	Chain	Residues	Atoms			AltConf
25	B	1	Total	C	O	0
			61	46	15	
25	J	1	Total	C	O	0
			58	43	15	
25	4	1	Total	C	O	0
			49	34	15	

- Molecule 26 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula:  $C_{40}H_{56}O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
26	J	1	Total	C	O	0
			42	40	2	
26	1	1	Total	C	O	0
			42	40	2	
26	1	1	Total	C	O	0
			42	40	2	
26	2	1	Total	C	O	0
			42	40	2	
26	3	1	Total	C	O	0
			42	40	2	
26	3	1	Total	C	O	0
			42	40	2	
26	4	1	Total	C	O	0
			42	40	2	

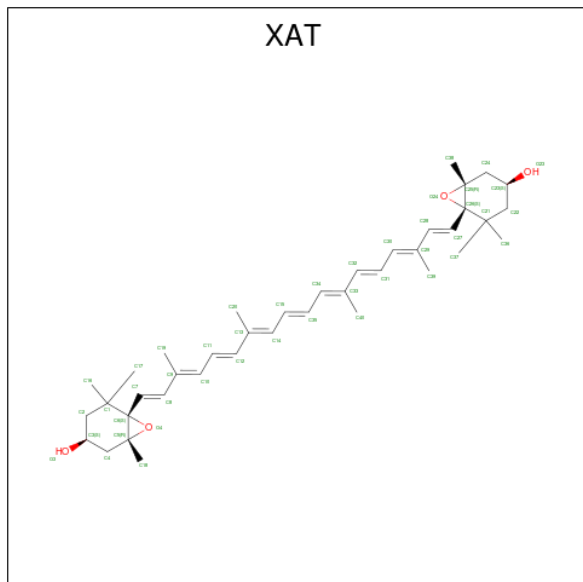
- Molecule 27 is CHLOROPHYLL B (three-letter code: CHL) (formula:  $C_{55}H_{70}MgN_4O_6$ )

# CHL

Mol	Chain	Residues	Atoms					AltConf
27	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
27	1	1	Total 46	C 35	Mg 1	N 4	O 6	0
27	2	1	Total 51	C 40	Mg 1	N 4	O 6	0
27	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
27	2	1	Total 51	C 40	Mg 1	N 4	O 6	0
27	2	1	Total 47	C 36	Mg 1	N 4	O 6	0
27	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
27	3	1	Total 51	C 40	Mg 1	N 4	O 6	0
27	4	1	Total 66	C 55	Mg 1	N 4	O 6	0
27	4	1	Total 46	C 35	Mg 1	N 4	O 6	0
27	4	1	Total 51	C 40	Mg 1	N 4	O 6	0
27	4	1	Total 46	C 35	Mg 1	N 4	O 6	0

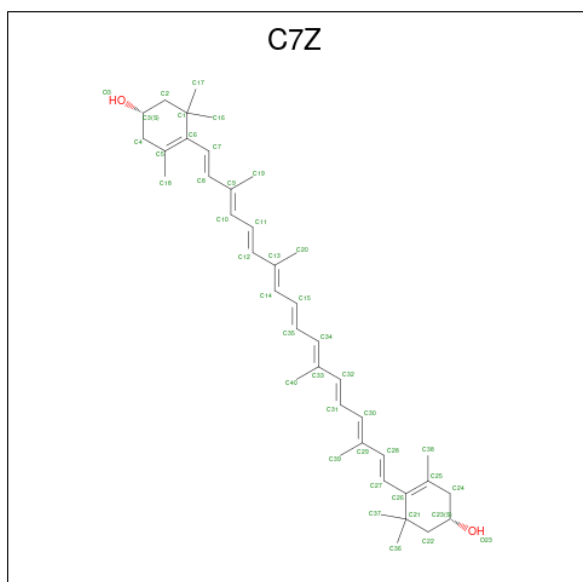
- Molecule 28 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA

,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula:  $C_{40}H_{56}O_4$ ) (labeled as "Ligand of Interest" by depositor).



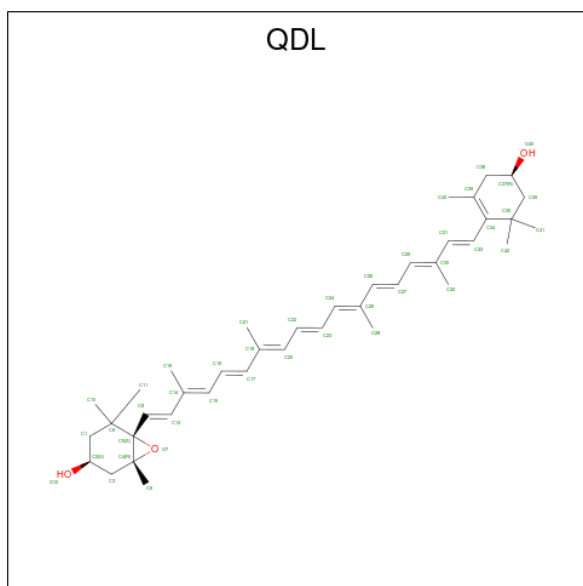
Mol	Chain	Residues	Atoms			AltConf
28	1	1	Total	C	O	0
			44	40	4	
28	2	1	Total	C	O	0
			44	40	4	

- Molecule 29 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (three-letter code: C7Z) (formula:  $C_{40}H_{56}O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
29	1	1	Total	C	O	0
			42	40	2	

- Molecule 30 is Anthraxanthin (three-letter code: QDL) (formula:  $C_{40}H_{56}O_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
30	4	1	Total	C	O	0
			43	40	3	

- Molecule 31 is water.

Mol	Chain	Residues	Atoms		AltConf
31	A	199	Total	O	0
			199	199	
31	B	267	Total	O	0
			267	267	
31	C	75	Total	O	0
			75	75	
31	D	58	Total	O	0
			58	58	
31	E	22	Total	O	0
			22	22	
31	H	7	Total	O	0
			7	7	
31	I	5	Total	O	0
			5	5	

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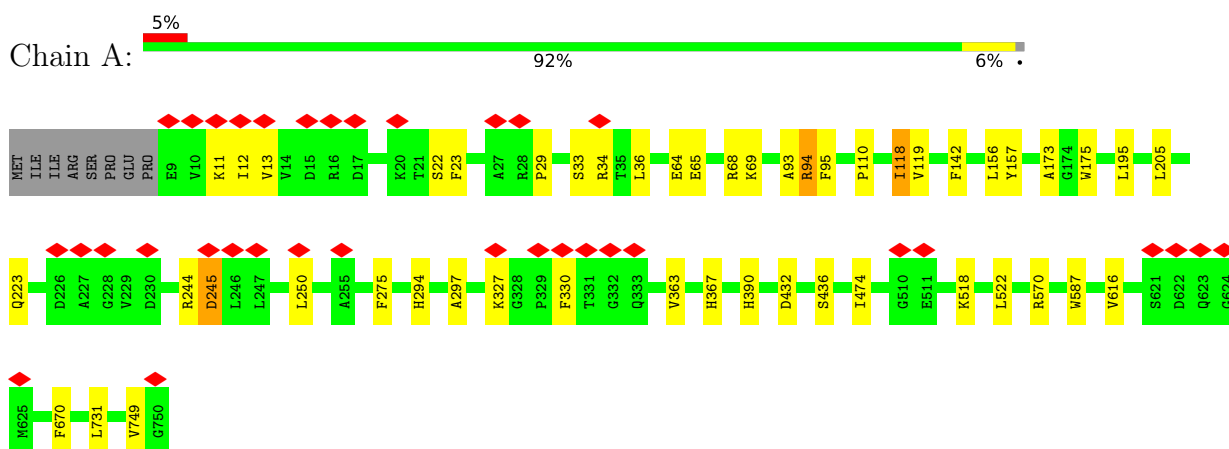
Mol	Chain	Residues	Atoms		AltConf
31	L	12	Total 12	O 12	0
31	F	32	Total 32	O 32	0
31	G	2	Total 2	O 2	0
31	J	8	Total 8	O 8	0
31	K	2	Total 2	O 2	0
31	1	4	Total 4	O 4	0
31	2	4	Total 4	O 4	0
31	3	2	Total 2	O 2	0
31	4	4	Total 4	O 4	0



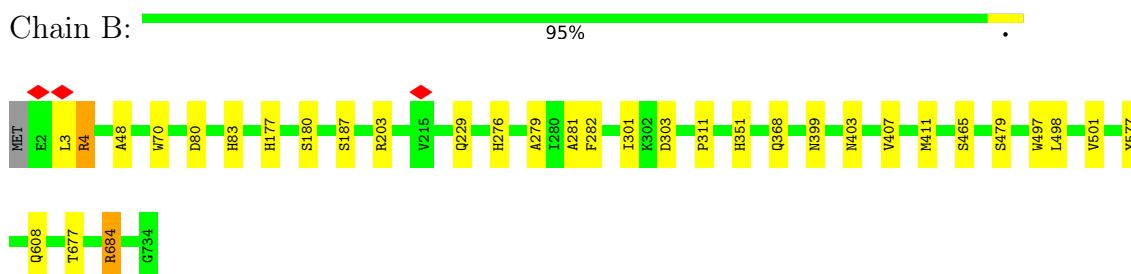
### 3 Residue-property plots

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

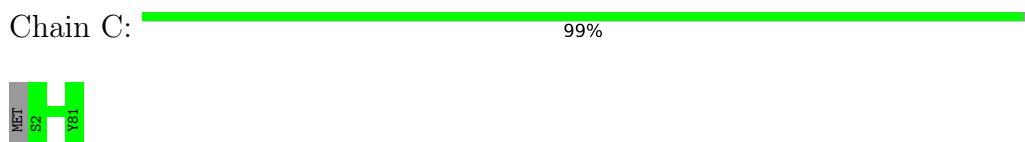
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

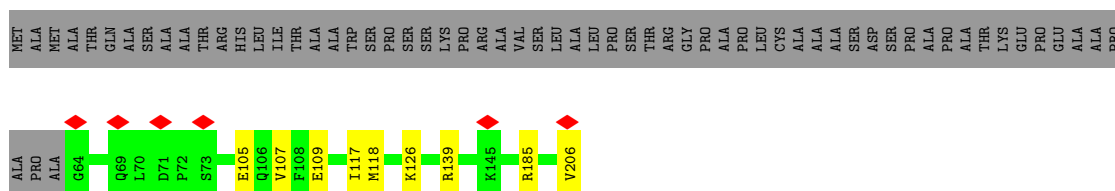


- Molecule 3: Photosystem I iron-sulfur center

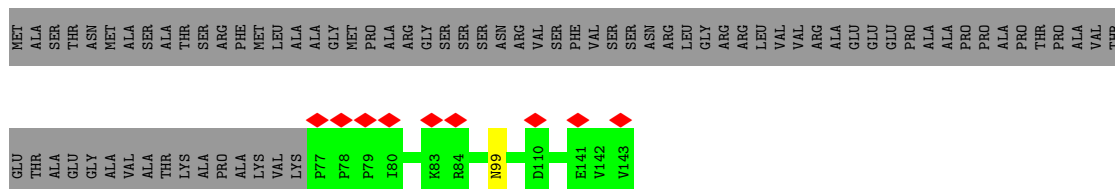


- Molecule 4: Photosystem I reaction center subunit II

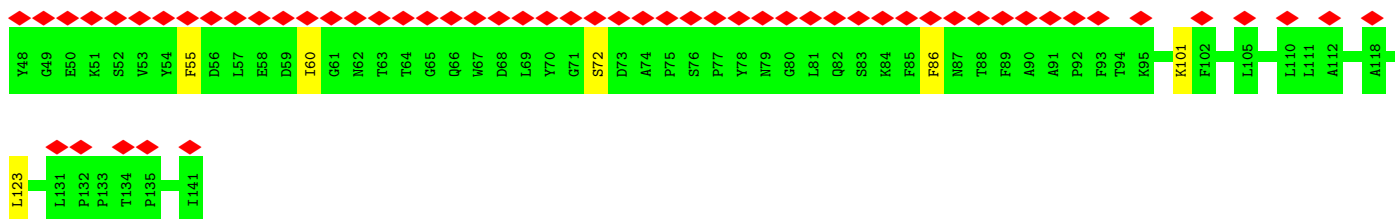




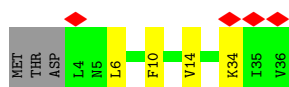
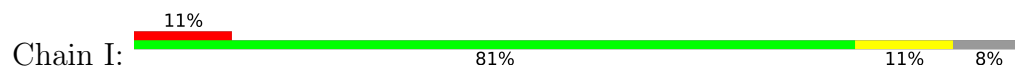
• Molecule 5: Photosystem I reaction center subunit IV



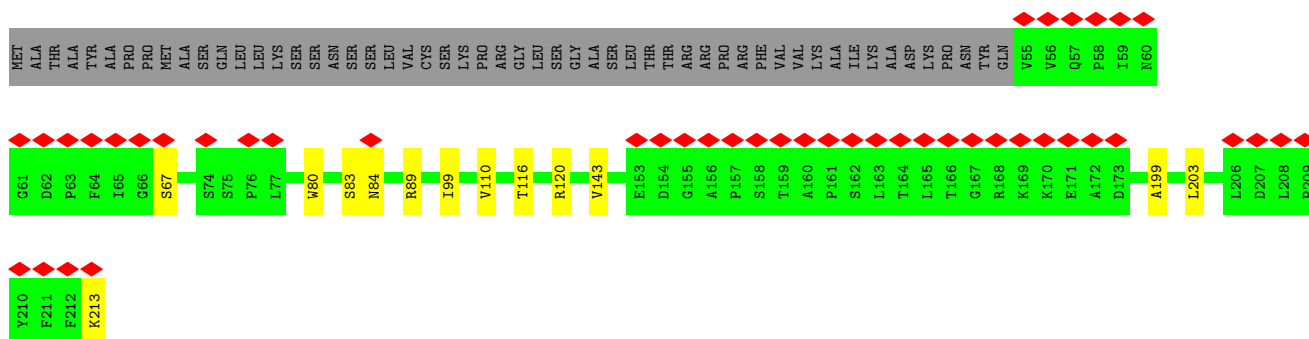
• Molecule 6: Photosystem I reaction center subunit VI




• Molecule 7: Photosystem I reaction center subunit VIII

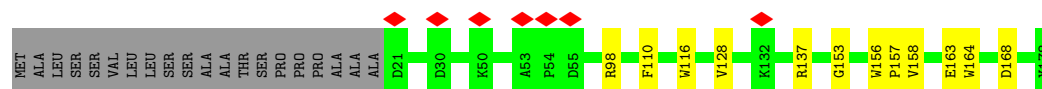


• Molecule 8: Photosystem I reaction center subunit XI



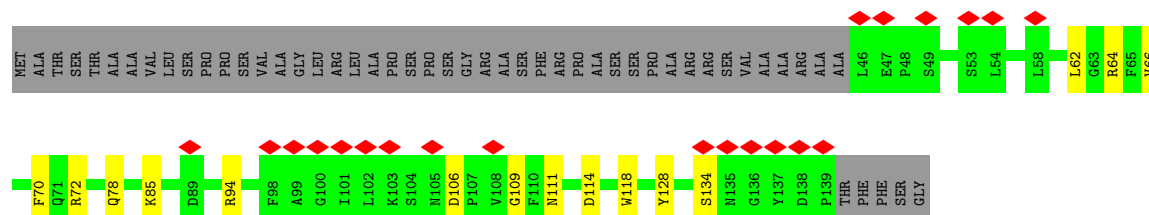
• Molecule 9: Photosystem I reaction center subunit III

Chain F: 



• Molecule 10: Photosystem I reaction center subunit V

Chain G: 



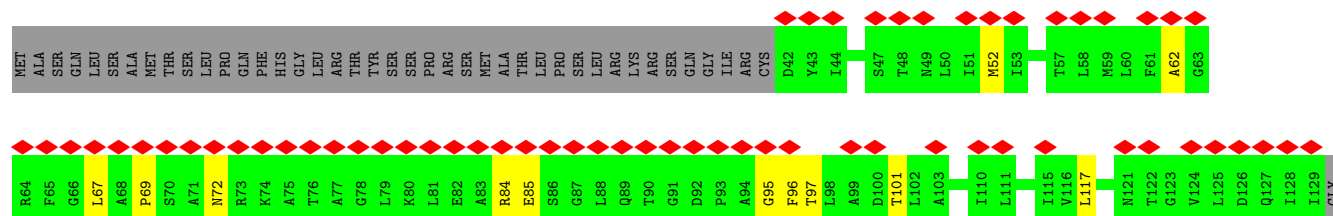
• Molecule 11: Photosystem I reaction center subunit IX

Chain J: 



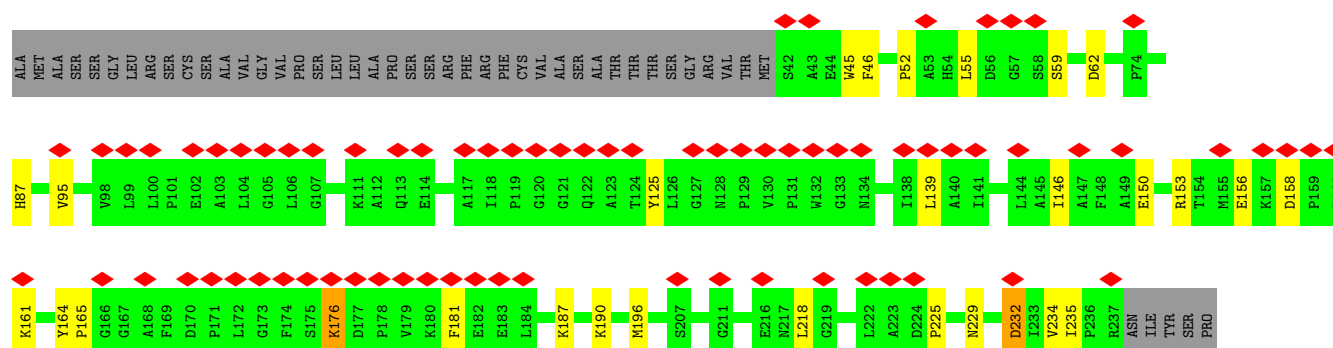
• Molecule 12: Photosystem I reaction center subunit X

Chain K: 

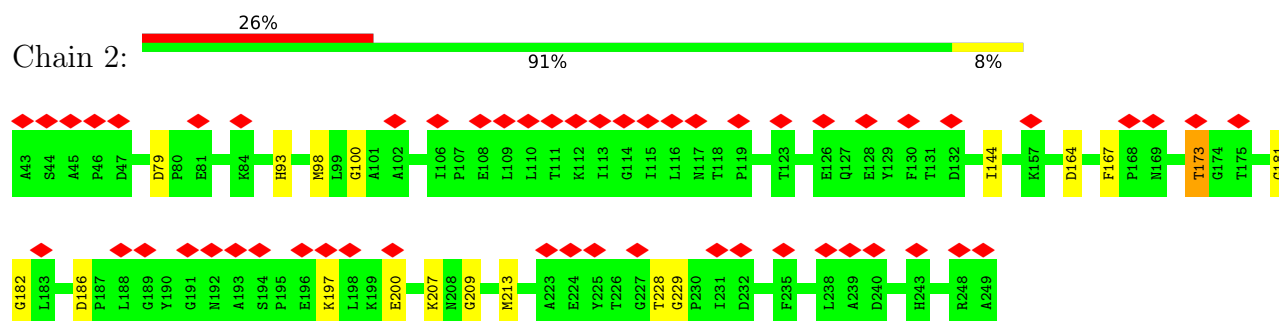


• Molecule 13: Chlorophyll a-b binding protein 1, chloroplastic

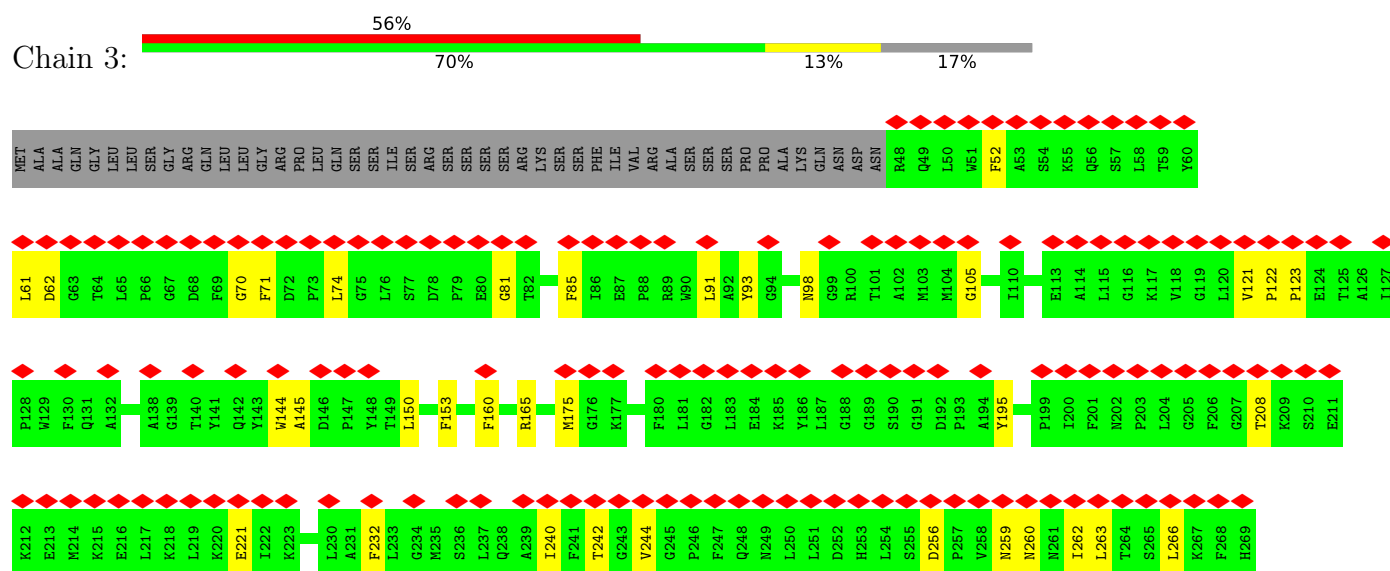
Chain 1: 



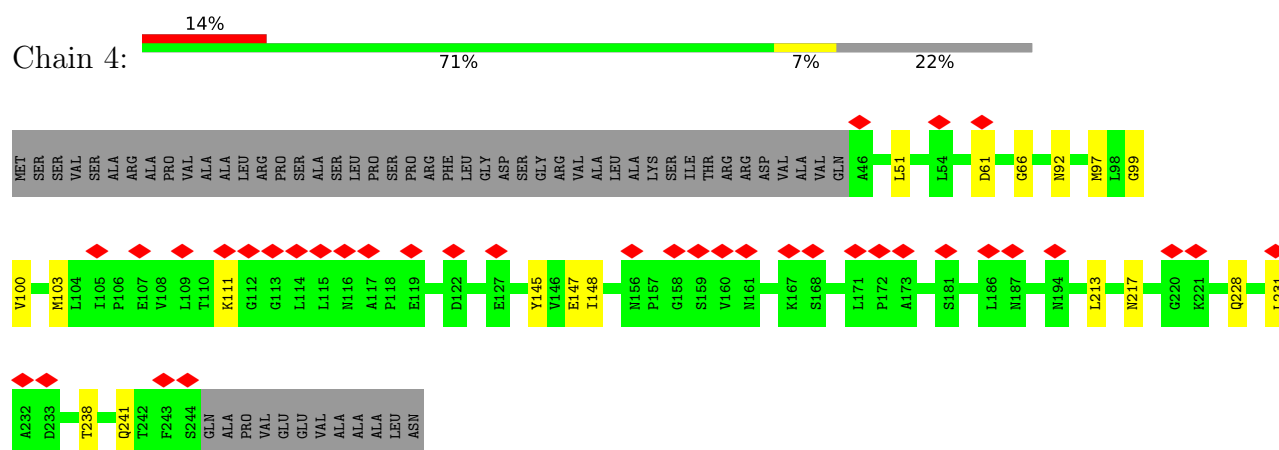
- Molecule 14: Chlorophyll a-b binding protein 2, chloroplastic



- Molecule 15: Chlorophyll a-b binding protein 3, chloroplastic



- Molecule 16: Chlorophyll a-b binding protein 4, chloroplastic



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	96997	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 ( $e^-/\text{\AA}^2$ )	51.346	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.434	Depositor
Minimum map value	-0.157	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	425.0, 425.0, 425.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CHL, C7Z, LMU, CLA, DGD, QDL, LHG, CL0, PQN, LMG, XAT, SF4, BCR, LUT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.27	0/6038	0.48	0/8237
2	B	0.27	0/6075	0.47	0/8297
3	C	0.23	0/616	0.55	0/834
4	D	0.25	0/1153	0.51	0/1557
5	E	0.25	0/546	0.51	0/743
6	H	0.25	0/737	0.44	0/1002
7	I	0.26	0/264	0.44	0/359
8	L	0.26	0/1227	0.46	0/1678
9	F	0.27	0/1269	0.47	0/1716
10	G	0.25	0/738	0.44	0/1004
11	J	0.26	0/352	0.46	0/479
12	K	0.24	0/633	0.46	0/855
13	1	0.26	0/1569	0.43	0/2137
14	2	0.24	0/1666	0.43	0/2282
15	3	0.26	0/1780	0.43	0/2414
16	4	0.27	0/1604	0.44	0/2187
All	All	0.26	0/26267	0.46	0/35781

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5840	0	5691	39	0
2	B	5864	0	5642	26	0
3	C	605	0	587	0	0
4	D	1124	0	1128	5	0
5	E	533	0	538	0	0
6	H	715	0	715	5	0
7	I	258	0	285	3	0
8	L	1192	0	1196	10	0
9	F	1238	0	1257	8	0
10	G	721	0	713	13	0
11	J	342	0	351	4	0
12	K	628	0	653	7	0
13	1	1519	0	1485	25	0
14	2	1609	0	1554	12	0
15	3	1725	0	1689	27	0
16	4	1555	0	1502	13	0
17	A	65	0	72	0	0
17	H	55	0	49	2	0
18	1	630	0	561	27	0
18	2	565	0	544	8	0
18	3	511	0	432	16	0
18	4	598	0	546	17	0
18	A	2670	0	2645	58	0
18	B	2297	0	2368	36	0
18	F	180	0	183	6	0
18	G	148	0	119	9	0
18	J	45	0	33	0	0
18	K	150	0	125	1	0
18	L	150	0	125	2	0
19	A	33	0	46	0	0
19	B	33	0	46	0	0
20	1	49	0	74	6	0
20	2	43	0	56	2	0
20	A	80	0	106	4	0
20	B	88	0	125	2	0
21	3	40	0	56	4	0
21	4	40	0	56	4	0
21	A	200	0	280	11	0
21	B	200	0	280	5	0
21	F	80	0	111	2	0
21	G	80	0	112	5	0
21	I	40	0	56	0	0
21	J	40	0	56	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	K	80	0	112	2	0
21	L	120	0	168	3	0
22	A	8	0	0	0	0
22	C	16	0	0	0	0
23	4	91	0	128	5	0
23	A	43	0	59	4	0
23	F	30	0	30	2	0
24	1	94	0	127	4	0
24	2	35	0	46	1	0
24	4	82	0	111	2	0
24	A	59	0	81	1	0
24	B	24	0	35	1	0
24	F	140	0	184	5	0
24	G	70	0	92	4	0
24	H	24	0	35	1	0
24	L	20	0	24	2	0
25	4	49	0	56	1	0
25	B	61	0	83	0	0
25	J	58	0	77	3	0
26	1	84	0	112	6	0
26	2	42	0	56	1	0
26	3	84	0	112	4	0
26	4	42	0	56	5	0
26	J	42	0	56	3	0
27	1	112	0	101	6	0
27	2	195	0	136	1	0
27	3	117	0	107	5	0
27	4	209	0	169	4	0
28	1	44	0	56	2	0
28	2	44	0	56	1	0
29	1	42	0	0	0	0
30	4	43	0	0	0	0
31	1	4	0	0	0	0
31	2	4	0	0	0	0
31	3	2	0	0	0	0
31	4	4	0	0	0	0
31	A	199	0	0	2	0
31	B	267	0	0	3	0
31	C	75	0	0	0	0
31	D	58	0	0	0	0
31	E	22	0	0	0	0
31	F	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	G	2	0	0	1	0
31	H	7	0	0	0	0
31	I	5	0	0	0	0
31	J	8	0	0	0	0
31	K	2	0	0	0	0
31	L	12	0	0	0	0
All	All	37485	0	36713	345	0

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

The worst 5 of 345 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)
18:4:609:CLA:HAB	26:4:616:LUT:H12	1.60	0.81
13:1:146:ILE:HG22	18:1:309:CLA:HAB	1.66	0.77
13:1:95:VAL:HG11	26:1:316:LUT:H32	1.65	0.76
13:1:87:HIS:HD2	28:1:317:XAT:H35	1.49	0.75
18:A:823:CLA:HAB	18:A:845:CLA:HBB1	1.72	0.72

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	740/750 (99%)	717 (97%)	22 (3%)	1 (0%)	48	57
2	B	731/734 (100%)	715 (98%)	16 (2%)	0	100	100
3	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
4	D	141/206 (68%)	136 (96%)	5 (4%)	0	100	100
5	E	65/143 (46%)	65 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	H	92/94 (98%)	92 (100%)	0	0	100	100
7	I	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
8	L	155/213 (73%)	152 (98%)	3 (2%)	0	100	100
9	F	156/178 (88%)	153 (98%)	3 (2%)	0	100	100
10	G	92/144 (64%)	86 (94%)	6 (6%)	0	100	100
11	J	41/52 (79%)	41 (100%)	0	0	100	100
12	K	84/130 (65%)	82 (98%)	2 (2%)	0	100	100
13	1	193/242 (80%)	186 (96%)	7 (4%)	0	100	100
14	2	205/207 (99%)	201 (98%)	4 (2%)	0	100	100
15	3	220/269 (82%)	205 (93%)	15 (7%)	0	100	100
16	4	197/256 (77%)	189 (96%)	8 (4%)	0	100	100
All	All	3221/3735 (86%)	3126 (97%)	94 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	600/608 (99%)	593 (99%)	7 (1%)	67	80
2	B	598/599 (100%)	594 (99%)	4 (1%)	81	90
3	C	70/71 (99%)	70 (100%)	0	100	100
4	D	120/163 (74%)	120 (100%)	0	100	100
5	E	59/115 (51%)	58 (98%)	1 (2%)	56	71
6	H	76/76 (100%)	75 (99%)	1 (1%)	65	78
7	I	30/33 (91%)	30 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	L	123/168 (73%)	122 (99%)	1 (1%)	79	88
9	F	128/142 (90%)	126 (98%)	2 (2%)	58	73
10	G	77/112 (69%)	77 (100%)	0	100	100
11	J	37/44 (84%)	36 (97%)	1 (3%)	40	53
12	K	66/102 (65%)	64 (97%)	2 (3%)	36	48
13	1	155/192 (81%)	151 (97%)	4 (3%)	41	54
14	2	165/165 (100%)	164 (99%)	1 (1%)	84	91
15	3	176/216 (82%)	170 (97%)	6 (3%)	32	42
16	4	160/203 (79%)	159 (99%)	1 (1%)	84	91
All	All	2640/3009 (88%)	2609 (99%)	31 (1%)	66	80

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

Mol	Chain	Res	Type
9	F	128	VAL
15	3	160	PHE
12	K	52	MET
15	3	208	THR
15	3	93	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
6	H	66	GLN
8	L	84	ASN
16	4	92	ASN
15	3	260	ASN
2	B	220	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

224 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
18	CLA	B	803	-	45,53,73	1.26	3 (6%)	52,89,113	0.97	2 (3%)
18	CLA	B	808	2	65,73,73	1.03	3 (4%)	76,113,113	0.85	2 (2%)
18	CLA	L	304	-	60,68,73	1.03	4 (6%)	70,107,113	0.94	3 (4%)
18	CLA	1	310	13	55,63,73	1.14	3 (5%)	64,101,113	1.00	2 (3%)
18	CLA	1	305	31	50,58,73	1.19	3 (6%)	58,95,113	0.98	2 (3%)
18	CLA	B	837	-	65,73,73	0.98	3 (4%)	76,113,113	0.85	2 (2%)
18	CLA	L	303	8	45,53,73	1.26	3 (6%)	52,89,113	1.05	2 (3%)
21	BCR	3	313	-	41,41,41	0.14	0	56,56,56	0.40	0
21	BCR	G	206	-	41,41,41	0.14	0	56,56,56	0.37	0
20	LHG	A	847	18	30,30,48	0.29	0	33,36,54	0.33	0
18	CLA	A	816	-	60,68,73	1.05	3 (5%)	70,107,113	0.91	2 (2%)
18	CLA	A	821	-	45,53,73	1.23	3 (6%)	52,89,113	0.99	2 (3%)
18	CLA	B	828	-	45,53,73	1.24	3 (6%)	52,89,113	1.02	2 (3%)
18	CLA	B	802	-	65,73,73	1.01	3 (4%)	76,113,113	0.80	2 (2%)
18	CLA	A	831	-	65,73,73	1.06	3 (4%)	76,113,113	0.82	2 (2%)
18	CLA	A	833	-	55,63,73	1.11	3 (5%)	64,101,113	0.93	2 (3%)
18	CLA	2	608	14	45,53,73	1.23	3 (6%)	52,89,113	1.01	2 (3%)
26	LUT	3	315	-	42,43,43	0.19	0	51,60,60	0.32	0
21	BCR	I	101	-	41,41,41	0.15	0	56,56,56	0.40	0
18	CLA	1	304	-	60,68,73	1.08	3 (5%)	70,107,113	0.91	2 (2%)
18	CLA	2	601	14	65,73,73	1.04	3 (4%)	76,113,113	0.86	2 (2%)
27	CHL	4	615	16	46,54,74	2.41	8 (17%)	49,90,114	1.43	8 (16%)
21	BCR	A	850	-	41,41,41	0.13	0	56,56,56	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	BCR	4	618	-	41,41,41	0.17	0	56,56,56	0.45	0
18	CLA	A	824	-	45,53,73	1.22	3 (6%)	52,89,113	1.04	2 (3%)
18	CLA	A	820	-	65,73,73	1.07	3 (4%)	76,113,113	0.85	2 (2%)
18	CLA	B	822	31	65,73,73	1.06	3 (4%)	76,113,113	0.85	2 (2%)
22	SF4	C	101	3	0,12,12	-	-	-	-	-
18	CLA	A	841	-	65,73,73	0.99	3 (4%)	76,113,113	0.84	2 (2%)
18	CLA	B	827	-	65,73,73	1.02	3 (4%)	76,113,113	0.86	2 (2%)
18	CLA	A	840	-	55,63,73	1.13	3 (5%)	64,101,113	0.98	2 (3%)
29	C7Z	1	322	-	43,43,43	0.11	0	58,60,60	0.34	0
24	LMU	1	320	-	36,36,36	0.11	0	47,47,47	0.17	0
18	CLA	3	312	-	45,53,73	1.25	3 (6%)	52,89,113	1.02	2 (3%)
19	PQN	B	838	-	34,34,34	0.32	0	42,45,45	0.34	0
18	CLA	1	306	-	45,53,73	1.26	3 (6%)	52,89,113	1.05	2 (3%)
24	LMU	2	618	-	36,36,36	0.10	0	47,47,47	0.15	0
21	BCR	B	841	-	41,41,41	0.15	0	56,56,56	0.34	0
18	CLA	B	821	-	45,53,73	1.28	3 (6%)	52,89,113	1.01	2 (3%)
18	CLA	3	310	15	55,63,73	1.12	3 (5%)	64,101,113	0.92	2 (3%)
18	CLA	4	610	-	45,53,73	1.25	3 (6%)	52,89,113	1.00	2 (3%)
18	CLA	B	814	-	45,53,73	1.21	3 (6%)	52,89,113	1.02	2 (3%)
18	CLA	3	303	-	45,53,73	1.26	3 (6%)	52,89,113	1.02	2 (3%)
18	CLA	2	610	20	60,68,73	1.09	3 (5%)	70,107,113	0.88	2 (2%)
18	CLA	1	313	13	65,73,73	1.03	3 (4%)	76,113,113	0.92	2 (2%)
26	LUT	1	318	-	42,43,43	0.22	0	51,60,60	0.32	0
18	CLA	A	830	-	65,73,73	1.05	3 (4%)	76,113,113	0.85	2 (2%)
18	CLA	B	816	-	65,73,73	1.02	3 (4%)	76,113,113	0.87	2 (2%)
18	CLA	A	807	1	65,73,73	1.05	3 (4%)	76,113,113	0.82	2 (2%)
18	CLA	A	842	-	65,73,73	1.00	3 (4%)	76,113,113	0.96	3 (3%)
17	CL0	A	801	-	65,73,73	2.03	8 (12%)	76,113,113	1.10	5 (6%)
18	CLA	A	832	-	45,53,73	1.22	3 (6%)	52,89,113	1.03	2 (3%)
18	CLA	3	304	31	45,53,73	1.25	3 (6%)	52,89,113	1.04	2 (3%)
23	LMG	A	857	-	43,43,55	0.19	0	51,51,63	0.17	0
18	CLA	B	806	-	60,68,73	1.04	3 (5%)	70,107,113	0.89	2 (2%)
18	CLA	A	803	31	65,73,73	1.03	3 (4%)	76,113,113	0.88	2 (2%)
24	LMU	G	203	-	36,36,36	0.09	0	47,47,47	0.28	0
26	LUT	3	314	-	42,43,43	0.19	0	51,60,60	0.50	0
26	LUT	2	615	-	42,43,43	0.26	0	51,60,60	0.35	0
18	CLA	A	854	31	65,73,73	1.02	3 (4%)	76,113,113	0.86	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	LMU	F	807	-	36,36,36	0.12	0	47,47,47	0.27	0
24	LMU	F	809	-	36,36,36	0.12	0	47,47,47	0.35	0
27	CHL	4	607	-	51,59,74	2.30	9 (17%)	55,96,114	1.47	9 (16%)
18	CLA	4	604	31	45,53,73	1.25	3 (6%)	52,89,113	1.04	2 (3%)
27	CHL	2	607	-	51,59,74	2.29	9 (17%)	55,96,114	1.38	9 (16%)
25	DGD	4	622	-	50,50,67	0.18	0	64,64,81	0.38	0
18	CLA	A	843	31	65,73,73	1.01	3 (4%)	76,113,113	0.90	3 (3%)
18	CLA	A	822	31	65,73,73	1.02	3 (4%)	76,113,113	0.88	2 (2%)
27	CHL	4	605	31	66,74,74	2.00	8 (12%)	73,114,114	1.21	9 (12%)
23	LMG	4	619	-	46,46,55	0.19	0	54,54,63	0.14	0
18	CLA	A	856	-	45,53,73	1.24	3 (6%)	52,89,113	1.02	2 (3%)
18	CLA	1	312	13	45,53,73	1.26	3 (6%)	52,89,113	1.03	2 (3%)
18	CLA	B	825	-	65,73,73	1.07	3 (4%)	76,113,113	0.91	3 (3%)
24	LMU	4	624	-	24,24,36	0.13	0	29,29,47	0.26	0
18	CLA	B	815	-	60,68,73	1.08	3 (5%)	70,107,113	0.91	2 (2%)
18	CLA	K	201	12	45,53,73	1.25	3 (6%)	52,89,113	1.04	2 (3%)
26	LUT	J	101	-	42,43,43	0.19	0	51,60,60	0.43	0
18	CLA	B	811	-	52,60,73	1.19	3 (5%)	60,97,113	0.95	2 (3%)
27	CHL	4	606	31	46,54,74	2.41	10 (21%)	49,90,114	1.39	7 (14%)
27	CHL	2	606	31	46,54,74	2.42	9 (19%)	49,90,114	1.40	8 (16%)
18	CLA	A	845	20	45,53,73	1.27	3 (6%)	52,89,113	1.03	2 (3%)
21	BCR	A	851	-	41,41,41	0.17	0	56,56,56	0.33	0
24	LMU	F	803	-	36,36,36	0.12	0	47,47,47	0.41	0
22	SF4	C	102	3	0,12,12	-	-	-	-	-
18	CLA	A	810	1	50,58,73	1.17	3 (6%)	58,95,113	1.01	2 (3%)
18	CLA	A	814	-	65,73,73	1.04	3 (4%)	76,113,113	0.85	2 (2%)
18	CLA	1	303	13	65,73,73	1.03	3 (4%)	76,113,113	0.86	2 (2%)
27	CHL	3	306	31	51,59,74	2.28	8 (15%)	55,96,114	1.37	8 (14%)
18	CLA	B	804	-	65,73,73	0.98	3 (4%)	76,113,113	0.87	2 (2%)
18	CLA	4	608	16	65,73,73	1.06	3 (4%)	76,113,113	0.93	3 (3%)
24	LMU	1	321	-	24,24,36	0.13	0	29,29,47	0.24	0
20	LHG	B	847	-	48,48,48	0.23	0	51,54,54	0.25	0
18	CLA	K	204	-	45,53,73	1.28	3 (6%)	52,89,113	1.04	2 (3%)
18	CLA	A	804	-	65,73,73	1.03	3 (4%)	76,113,113	0.89	2 (2%)
18	CLA	3	308	15	55,63,73	1.13	3 (5%)	64,101,113	0.94	2 (3%)
21	BCR	K	205	-	41,41,41	0.15	0	56,56,56	0.28	0
28	XAT	1	317	-	39,47,47	0.12	0	54,74,74	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	CLA	A	818	-	60,68,73	1.09	3 (5%)	70,107,113	0.97	3 (4%)
18	CLA	B	820	-	65,73,73	1.01	3 (4%)	76,113,113	0.88	2 (2%)
18	CLA	1	315	13	45,53,73	1.25	3 (6%)	52,89,113	1.00	2 (3%)
20	LHG	1	319	-	48,48,48	0.22	0	51,54,54	0.27	0
18	CLA	B	801	-	65,73,73	1.06	3 (4%)	76,113,113	0.82	2 (2%)
18	CLA	3	302	15	55,63,73	1.16	3 (5%)	64,101,113	0.92	2 (3%)
23	LMG	4	620	-	45,45,55	0.20	0	53,53,63	0.22	0
18	CLA	3	305	15	61,69,73	1.08	3 (4%)	71,108,113	0.88	2 (2%)
18	CLA	B	833	-	61,69,73	1.06	3 (4%)	71,108,113	0.92	2 (2%)
18	CLA	3	309	15	45,53,73	1.26	3 (6%)	52,89,113	1.04	2 (3%)
18	CLA	4	613	-	46,54,73	1.23	3 (6%)	53,90,113	1.01	2 (3%)
18	CLA	A	812	18	65,73,73	1.01	4 (6%)	76,113,113	0.87	2 (2%)
18	CLA	4	602	16	60,68,73	1.09	3 (5%)	70,107,113	0.89	2 (2%)
18	CLA	A	835	-	65,73,73	1.02	3 (4%)	76,113,113	0.88	2 (2%)
26	LUT	1	316	-	42,43,43	0.20	0	51,60,60	0.33	0
18	CLA	J	102	11	45,53,73	1.24	3 (6%)	52,89,113	1.01	2 (3%)
18	CLA	2	602	14	65,73,73	1.05	3 (4%)	76,113,113	0.84	2 (2%)
18	CLA	A	827	31	55,63,73	1.07	4 (7%)	64,101,113	0.94	2 (3%)
24	LMU	H	201	-	24,24,36	0.12	0	29,29,47	0.25	0
18	CLA	A	834	-	65,73,73	1.03	3 (4%)	76,113,113	0.89	2 (2%)
25	DGD	J	104	-	59,59,67	0.16	0	73,73,81	0.16	0
20	LHG	B	846	18	38,38,48	0.26	0	41,44,54	0.30	0
18	CLA	B	826	-	65,73,73	1.06	3 (4%)	76,113,113	0.84	2 (2%)
18	CLA	A	809	1	65,73,73	1.03	3 (4%)	76,113,113	1.02	4 (5%)
18	CLA	A	823	-	52,60,73	1.15	3 (5%)	60,97,113	0.98	2 (3%)
18	CLA	F	804	31	65,73,73	1.04	3 (4%)	76,113,113	0.86	2 (2%)
18	CLA	B	807	-	65,73,73	1.05	3 (4%)	76,113,113	0.83	2 (2%)
18	CLA	4	601	16	50,58,73	1.19	3 (6%)	58,95,113	0.98	2 (3%)
18	CLA	A	819	-	56,64,73	1.10	3 (5%)	65,102,113	0.92	2 (3%)
18	CLA	B	830	-	65,73,73	1.02	3 (4%)	76,113,113	0.84	2 (2%)
18	CLA	K	203	31	60,68,73	1.08	3 (5%)	70,107,113	0.90	2 (2%)
19	PQN	A	844	-	34,34,34	0.35	0	42,45,45	0.34	0
21	BCR	L	302	-	41,41,41	0.15	0	56,56,56	0.33	0
18	CLA	B	813	-	65,73,73	1.02	3 (4%)	76,113,113	0.87	2 (2%)
18	CLA	3	307	15	60,68,73	1.09	3 (5%)	70,107,113	0.90	2 (2%)
27	CHL	3	301	15	66,74,74	2.02	8 (12%)	73,114,114	1.16	7 (9%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	BCR	A	852	-	41,41,41	0.22	0	56,56,56	0.42	0
18	CLA	4	603	16	65,73,73	1.05	3 (4%)	76,113,113	0.86	2 (2%)
23	LMG	F	810	-	30,30,55	0.21	0	38,38,63	0.19	0
24	LMU	G	207	-	36,36,36	0.12	0	47,47,47	0.25	0
18	CLA	2	603	-	65,73,73	1.05	3 (4%)	76,113,113	0.85	2 (2%)
27	CHL	1	302	13	66,74,74	1.99	9 (13%)	73,114,114	1.20	8 (10%)
18	CLA	1	309	13	65,73,73	1.05	3 (4%)	76,113,113	0.80	2 (2%)
18	CLA	B	824	-	65,73,73	1.04	3 (4%)	76,113,113	0.85	2 (2%)
21	BCR	G	202	-	41,41,41	0.16	0	56,56,56	0.36	0
18	CLA	A	828	-	65,73,73	1.04	3 (4%)	76,113,113	0.86	2 (2%)
24	LMU	A	859	-	36,36,36	0.11	0	47,47,47	0.21	0
18	CLA	B	835	-	50,58,73	1.16	3 (6%)	58,95,113	0.97	2 (3%)
18	CLA	A	815	-	54,62,73	1.10	3 (5%)	62,99,113	0.96	2 (3%)
18	CLA	B	831	-	65,73,73	1.01	3 (4%)	76,113,113	0.88	2 (2%)
25	DGD	B	845	-	62,62,67	0.17	0	76,76,81	0.29	0
18	CLA	A	806	-	65,73,73	0.99	3 (4%)	76,113,113	0.86	2 (2%)
18	CLA	A	826	31	65,73,73	1.00	3 (4%)	76,113,113	0.87	2 (2%)
21	BCR	F	801	-	41,41,41	0.33	0	56,56,56	0.47	0
18	CLA	A	802	-	65,73,73	0.94	3 (4%)	76,113,113	0.81	2 (2%)
18	CLA	A	855	31	65,73,73	1.01	3 (4%)	76,113,113	0.86	2 (2%)
18	CLA	3	311	-	45,53,73	1.28	3 (6%)	52,89,113	1.02	2 (3%)
18	CLA	4	611	16	47,55,73	1.23	3 (6%)	54,91,113	1.02	2 (3%)
27	CHL	2	614	14	47,55,74	2.40	8 (17%)	50,91,114	1.41	8 (16%)
18	CLA	2	611	14	45,53,73	1.25	3 (6%)	52,89,113	1.03	2 (3%)
18	CLA	A	805	18	50,58,73	1.16	3 (6%)	58,95,113	0.98	2 (3%)
18	CLA	G	205	10	46,54,73	1.24	3 (6%)	53,90,113	1.02	2 (3%)
27	CHL	1	307	13	46,54,74	2.48	9 (19%)	49,90,114	1.46	8 (16%)
18	CLA	B	809	-	65,73,73	1.02	3 (4%)	76,113,113	0.84	2 (2%)
18	CLA	A	808	-	47,55,73	1.19	3 (6%)	54,91,113	1.00	2 (3%)
21	BCR	K	202	-	41,41,41	0.25	0	56,56,56	0.50	0
24	LMU	B	848	-	24,24,36	0.14	0	29,29,47	0.22	0
27	CHL	2	605	31	51,59,74	2.30	8 (15%)	55,96,114	1.39	9 (16%)
18	CLA	L	305	31	45,53,73	1.27	3 (6%)	52,89,113	1.03	2 (3%)
21	BCR	B	842	-	41,41,41	0.17	0	56,56,56	0.46	0
18	CLA	B	805	2	65,73,73	1.08	3 (4%)	76,113,113	0.80	2 (2%)
18	CLA	A	837	1	45,53,73	1.21	3 (6%)	52,89,113	1.06	3 (5%)
17	CL0	H	202	6	55,63,73	2.24	8 (14%)	64,101,113	1.31	8 (12%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	LHG	A	846	-	48,48,48	0.25	0	51,54,54	0.28	0
24	LMU	A	858	-	24,24,36	0.11	0	29,29,47	0.26	0
21	BCR	B	843	-	41,41,41	0.16	0	56,56,56	0.34	0
18	CLA	B	812	-	65,73,73	1.02	3 (4%)	76,113,113	0.87	2 (2%)
18	CLA	B	810	-	56,64,73	1.10	3 (5%)	65,102,113	0.93	2 (3%)
18	CLA	A	836	-	65,73,73	1.02	3 (4%)	76,113,113	0.86	2 (2%)
18	CLA	B	819	-	58,66,73	1.06	3 (5%)	67,104,113	0.98	3 (4%)
21	BCR	L	306	-	41,41,41	0.23	0	56,56,56	0.50	0
18	CLA	2	609	14	60,68,73	1.07	3 (5%)	70,107,113	0.88	2 (2%)
21	BCR	A	849	-	41,41,41	0.16	0	56,56,56	0.30	0
30	QDL	4	617	-	41,45,45	0.14	0	56,67,67	0.75	2 (3%)
18	CLA	B	839	20	65,73,73	1.04	3 (4%)	76,113,113	0.86	2 (2%)
21	BCR	B	844	-	41,41,41	0.16	0	56,56,56	0.30	0
18	CLA	A	817	31	45,53,73	1.23	3 (6%)	52,89,113	1.03	2 (3%)
18	CLA	F	805	9	50,58,73	1.15	3 (6%)	58,95,113	0.94	2 (3%)
18	CLA	B	829	-	65,73,73	1.03	3 (4%)	76,113,113	0.86	2 (2%)
21	BCR	F	806	-	41,41,41	0.24	0	56,56,56	0.39	0
18	CLA	A	829	-	65,73,73	1.04	3 (4%)	76,113,113	0.87	2 (2%)
18	CLA	G	201	-	57,65,73	1.12	3 (5%)	66,103,113	0.90	2 (3%)
18	CLA	2	612	14	65,73,73	1.04	3 (4%)	76,113,113	0.84	2 (2%)
18	CLA	B	818	-	60,68,73	1.09	3 (5%)	70,107,113	0.86	2 (2%)
21	BCR	J	103	-	41,41,41	0.26	0	56,56,56	0.43	0
18	CLA	4	614	-	50,58,73	1.17	3 (6%)	58,95,113	0.95	2 (3%)
18	CLA	1	314	-	45,53,73	1.26	3 (6%)	52,89,113	1.02	2 (3%)
24	LMU	L	301	-	20,20,36	0.14	0	25,25,47	0.32	0
18	CLA	1	308	31	45,53,73	1.27	3 (6%)	52,89,113	1.04	2 (3%)
18	CLA	B	836	31	65,73,73	0.99	3 (4%)	76,113,113	0.87	2 (2%)
18	CLA	2	604	-	45,53,73	1.25	3 (6%)	52,89,113	1.03	2 (3%)
21	BCR	L	307	-	41,41,41	0.13	0	56,56,56	0.31	0
28	XAT	2	616	-	39,47,47	0.10	0	54,74,74	0.48	0
21	BCR	B	840	-	41,41,41	0.26	0	56,56,56	0.43	0
24	LMU	4	621	-	23,23,36	0.14	0	28,28,47	0.26	0
18	CLA	4	609	16	60,68,73	1.08	3 (5%)	70,107,113	0.86	2 (2%)
18	CLA	4	612	16	65,73,73	1.03	3 (4%)	76,113,113	0.85	2 (2%)
18	CLA	B	817	31	55,63,73	1.08	3 (5%)	64,101,113	0.95	2 (3%)
18	CLA	A	813	-	45,53,73	1.25	3 (6%)	52,89,113	1.02	2 (3%)
18	CLA	A	839	-	65,73,73	1.02	3 (4%)	76,113,113	0.87	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	CLA	B	834	-	65,73,73	0.98	3 (4%)	76,113,113	0.92	3 (3%)
18	CLA	G	204	-	45,53,73	1.26	3 (6%)	52,89,113	1.05	2 (3%)
24	LMU	4	623	-	36,36,36	0.11	0	47,47,47	0.41	0
18	CLA	1	311	-	45,53,73	1.22	3 (6%)	52,89,113	1.02	2 (3%)
22	SF4	A	853	2,1	0,12,12	-	-	-	-	-
20	LHG	2	617	18	42,42,48	0.24	0	45,48,54	0.28	0
18	CLA	A	825	-	60,68,73	1.10	3 (5%)	70,107,113	0.86	2 (2%)
21	BCR	A	848	-	41,41,41	0.14	0	56,56,56	0.27	0
18	CLA	2	613	-	50,58,73	1.18	3 (6%)	58,95,113	0.99	2 (3%)
24	LMU	1	301	-	36,36,36	0.12	0	47,47,47	0.39	0
18	CLA	A	811	-	45,53,73	1.21	3 (6%)	52,89,113	1.06	2 (3%)
26	LUT	4	616	-	42,43,43	0.22	0	51,60,60	0.34	0
18	CLA	B	832	31	45,53,73	1.25	3 (6%)	52,89,113	1.04	2 (3%)
18	CLA	F	802	-	65,73,73	1.03	3 (4%)	76,113,113	0.97	3 (3%)
18	CLA	B	823	31	65,73,73	1.00	3 (4%)	76,113,113	0.86	2 (2%)
24	LMU	F	808	-	36,36,36	0.11	0	47,47,47	0.20	0
18	CLA	A	838	-	51,59,73	1.16	3 (5%)	59,96,113	0.99	2 (3%)

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
18	CLA	B	803	-	1/1/11/20	0/13/91/115	-
18	CLA	B	808	2	1/1/15/20	4/37/115/115	-
18	CLA	L	304	-	1/1/14/20	3/31/109/115	-
18	CLA	1	310	13	1/1/13/20	3/25/103/115	-
18	CLA	1	305	31	1/1/12/20	2/19/97/115	-
18	CLA	B	837	-	1/1/15/20	3/37/115/115	-
18	CLA	L	303	8	1/1/11/20	4/13/91/115	-
21	BCR	3	313	-	-	4/29/63/63	0/2/2/2
21	BCR	G	206	-	-	4/29/63/63	0/2/2/2
20	LHG	A	847	18	-	12/35/35/53	-
18	CLA	A	816	-	1/1/14/20	3/31/109/115	-
18	CLA	A	821	-	1/1/11/20	3/13/91/115	-
18	CLA	B	828	-	1/1/11/20	0/13/91/115	-
18	CLA	B	802	-	1/1/15/20	1/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	831	-	1/1/15/20	3/37/115/115	-
18	CLA	A	833	-	1/1/13/20	1/25/103/115	-
18	CLA	2	608	14	1/1/11/20	0/13/91/115	-
26	LUT	3	315	-	-	0/29/67/67	0/2/2/2
21	BCR	I	101	-	-	0/29/63/63	0/2/2/2
18	CLA	1	304	-	1/1/14/20	3/31/109/115	-
18	CLA	2	601	14	1/1/15/20	5/37/115/115	-
27	CHL	4	615	16	3/3/16/26	2/15/113/137	-
21	BCR	A	850	-	-	2/29/63/63	0/2/2/2
21	BCR	4	618	-	-	2/29/63/63	0/2/2/2
18	CLA	A	824	-	1/1/11/20	3/13/91/115	-
18	CLA	A	820	-	1/1/15/20	7/37/115/115	-
18	CLA	B	822	31	1/1/15/20	5/37/115/115	-
22	SF4	C	101	3	-	-	0/6/5/5
18	CLA	A	841	-	1/1/15/20	3/37/115/115	-
18	CLA	B	827	-	1/1/15/20	5/37/115/115	-
18	CLA	A	840	-	1/1/13/20	2/25/103/115	-
29	C7Z	1	322	-	-	4/29/67/67	0/2/2/2
24	LMU	1	320	-	-	3/21/61/61	0/2/2/2
18	CLA	3	312	-	1/1/11/20	0/13/91/115	-
19	PQN	B	838	-	-	3/23/43/43	0/2/2/2
18	CLA	1	306	-	1/1/11/20	0/13/91/115	-
24	LMU	2	618	-	-	2/21/61/61	0/2/2/2
21	BCR	B	841	-	-	4/29/63/63	0/2/2/2
18	CLA	B	821	-	1/1/11/20	4/13/91/115	-
18	CLA	3	310	15	1/1/13/20	5/25/103/115	-
18	CLA	4	610	-	1/1/11/20	4/13/91/115	-
18	CLA	B	814	-	1/1/11/20	2/13/91/115	-
18	CLA	3	303	-	1/1/11/20	2/13/91/115	-
18	CLA	2	610	20	1/1/14/20	1/31/109/115	-
18	CLA	1	313	13	1/1/15/20	8/37/115/115	-
26	LUT	1	318	-	-	1/29/67/67	0/2/2/2
18	CLA	A	830	-	1/1/15/20	2/37/115/115	-
18	CLA	B	816	-	1/1/15/20	2/37/115/115	-
18	CLA	A	807	1	1/1/15/20	9/37/115/115	-
18	CLA	A	842	-	1/1/15/20	6/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CL0	A	801	-	3/3/20/25	1/37/135/135	-
18	CLA	A	832	-	1/1/11/20	1/13/91/115	-
18	CLA	3	304	31	1/1/11/20	3/13/91/115	-
23	LMG	A	857	-	-	4/38/58/70	0/1/1/1
18	CLA	B	806	-	1/1/14/20	3/31/109/115	-
18	CLA	A	803	31	1/1/15/20	2/37/115/115	-
24	LMU	G	203	-	-	3/21/61/61	0/2/2/2
26	LUT	3	314	-	-	0/29/67/67	0/2/2/2
26	LUT	2	615	-	-	2/29/67/67	0/2/2/2
18	CLA	A	854	31	1/1/15/20	4/37/115/115	-
24	LMU	F	807	-	-	4/21/61/61	0/2/2/2
24	LMU	F	809	-	-	1/21/61/61	0/2/2/2
27	CHL	4	607	-	3/3/17/26	1/21/119/137	-
18	CLA	4	604	31	1/1/11/20	5/13/91/115	-
27	CHL	2	607	-	3/3/17/26	6/21/119/137	-
25	DGD	4	622	-	-	5/38/78/95	0/2/2/2
18	CLA	A	843	31	1/1/15/20	5/37/115/115	-
18	CLA	A	822	31	1/1/15/20	5/37/115/115	-
27	CHL	4	605	31	3/3/20/26	5/39/137/137	-
23	LMG	4	619	-	-	1/41/61/70	0/1/1/1
18	CLA	A	856	-	1/1/11/20	3/13/91/115	-
18	CLA	1	312	13	1/1/11/20	5/13/91/115	-
18	CLA	B	825	-	1/1/15/20	5/37/115/115	-
27	CHL	4	606	31	3/3/16/26	0/15/113/137	-
18	CLA	B	815	-	1/1/14/20	4/31/109/115	-
18	CLA	K	201	12	1/1/11/20	4/13/91/115	-
24	LMU	4	624	-	-	1/15/35/61	0/1/1/2
18	CLA	B	811	-	1/1/12/20	1/22/100/115	-
26	LUT	J	101	-	-	4/29/67/67	0/2/2/2
27	CHL	2	606	31	3/3/16/26	3/15/113/137	-
18	CLA	A	845	20	1/1/11/20	3/13/91/115	-
21	BCR	A	851	-	-	2/29/63/63	0/2/2/2
24	LMU	F	803	-	-	3/21/61/61	0/2/2/2
22	SF4	C	102	3	-	-	0/6/5/5
18	CLA	A	810	1	1/1/12/20	2/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	814	-	1/1/15/20	5/37/115/115	-
18	CLA	1	303	13	1/1/15/20	2/37/115/115	-
27	CHL	3	306	31	3/3/17/26	4/21/119/137	-
18	CLA	B	804	-	1/1/15/20	8/37/115/115	-
18	CLA	4	608	16	1/1/15/20	10/37/115/115	-
24	LMU	1	321	-	-	0/15/35/61	0/1/1/2
20	LHG	B	847	-	-	14/53/53/53	-
18	CLA	K	204	-	1/1/11/20	4/13/91/115	-
18	CLA	A	804	-	1/1/15/20	5/37/115/115	-
18	CLA	3	308	15	1/1/13/20	5/25/103/115	-
21	BCR	K	205	-	-	2/29/63/63	0/2/2/2
28	XAT	1	317	-	-	0/31/93/93	0/4/4/4
18	CLA	A	818	-	1/1/14/20	3/31/109/115	-
18	CLA	B	820	-	1/1/15/20	4/37/115/115	-
18	CLA	1	315	13	1/1/11/20	1/13/91/115	-
20	LHG	1	319	-	-	9/53/53/53	-
18	CLA	B	801	-	1/1/15/20	3/37/115/115	-
18	CLA	3	302	15	1/1/13/20	0/25/103/115	-
23	LMG	4	620	-	-	5/40/60/70	0/1/1/1
18	CLA	3	305	15	1/1/14/20	5/33/111/115	-
18	CLA	B	833	-	1/1/14/20	3/33/111/115	-
18	CLA	3	309	15	1/1/11/20	4/13/91/115	-
18	CLA	4	613	-	1/1/11/20	0/15/93/115	-
18	CLA	A	812	18	1/1/15/20	5/37/115/115	-
18	CLA	4	602	16	1/1/14/20	2/31/109/115	-
18	CLA	A	835	-	1/1/15/20	4/37/115/115	-
26	LUT	1	316	-	-	0/29/67/67	0/2/2/2
18	CLA	J	102	11	1/1/11/20	1/13/91/115	-
18	CLA	2	602	14	1/1/15/20	1/37/115/115	-
18	CLA	A	827	31	1/1/13/20	5/25/103/115	-
24	LMU	H	201	-	-	3/15/35/61	0/1/1/2
18	CLA	A	834	-	1/1/15/20	3/37/115/115	-
25	DGD	J	104	-	-	5/47/87/95	0/2/2/2
20	LHG	B	846	18	-	8/43/43/53	-
18	CLA	B	826	-	1/1/15/20	1/37/115/115	-
18	CLA	A	809	1	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	823	-	1/1/12/20	3/22/100/115	-
18	CLA	F	804	31	1/1/15/20	7/37/115/115	-
18	CLA	B	807	-	1/1/15/20	8/37/115/115	-
18	CLA	4	601	16	1/1/12/20	4/19/97/115	-
18	CLA	A	819	-	1/1/13/20	4/27/105/115	-
18	CLA	B	830	-	1/1/15/20	3/37/115/115	-
18	CLA	K	203	31	1/1/14/20	5/31/109/115	-
27	CHL	3	301	15	3/3/20/26	7/39/137/137	-
19	PQN	A	844	-	-	0/23/43/43	0/2/2/2
18	CLA	B	813	-	1/1/15/20	4/37/115/115	-
18	CLA	3	307	15	1/1/14/20	6/31/109/115	-
21	BCR	L	302	-	-	4/29/63/63	0/2/2/2
21	BCR	A	852	-	-	4/29/63/63	0/2/2/2
18	CLA	4	603	16	1/1/15/20	3/37/115/115	-
27	CHL	1	302	13	3/3/20/26	5/39/137/137	-
23	LMG	F	810	-	-	2/25/45/70	0/1/1/1
18	CLA	2	603	-	1/1/15/20	5/37/115/115	-
24	LMU	G	207	-	-	2/21/61/61	0/2/2/2
18	CLA	1	309	13	1/1/15/20	5/37/115/115	-
18	CLA	B	824	-	1/1/15/20	2/37/115/115	-
21	BCR	G	202	-	-	0/29/63/63	0/2/2/2
18	CLA	A	828	-	1/1/15/20	2/37/115/115	-
24	LMU	A	859	-	-	3/21/61/61	0/2/2/2
18	CLA	B	835	-	1/1/12/20	0/19/97/115	-
18	CLA	A	815	-	1/1/12/20	2/24/102/115	-
18	CLA	B	831	-	1/1/15/20	5/37/115/115	-
25	DGD	B	845	-	-	10/50/90/95	0/2/2/2
18	CLA	A	806	-	1/1/15/20	3/37/115/115	-
18	CLA	A	826	31	1/1/15/20	7/37/115/115	-
21	BCR	F	801	-	-	0/29/63/63	0/2/2/2
18	CLA	A	802	-	1/1/15/20	1/37/115/115	-
18	CLA	A	855	31	1/1/15/20	3/37/115/115	-
18	CLA	3	311	-	1/1/11/20	4/13/91/115	-
18	CLA	4	611	16	1/1/11/20	4/16/94/115	-
27	CHL	2	614	14	3/3/16/26	0/17/115/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	2	611	14	1/1/11/20	4/13/91/115	-
18	CLA	A	805	18	1/1/12/20	2/19/97/115	-
18	CLA	G	205	10	1/1/11/20	3/15/93/115	-
27	CHL	1	307	13	3/3/16/26	4/15/113/137	-
18	CLA	B	809	-	1/1/15/20	3/37/115/115	-
18	CLA	A	808	-	1/1/11/20	0/16/94/115	-
21	BCR	K	202	-	-	0/29/63/63	0/2/2/2
24	LMU	B	848	-	-	1/15/35/61	0/1/1/2
27	CHL	2	605	31	3/3/17/26	2/21/119/137	-
18	CLA	L	305	31	1/1/11/20	1/13/91/115	-
21	BCR	B	842	-	-	2/29/63/63	0/2/2/2
18	CLA	B	805	2	1/1/15/20	4/37/115/115	-
18	CLA	A	837	1	1/1/11/20	2/13/91/115	-
17	CL0	H	202	6	3/3/18/25	7/25/123/135	-
20	LHG	A	846	-	-	6/53/53/53	-
24	LMU	A	858	-	-	2/15/35/61	0/1/1/2
21	BCR	B	843	-	-	2/29/63/63	0/2/2/2
18	CLA	B	812	-	1/1/15/20	3/37/115/115	-
18	CLA	B	810	-	1/1/13/20	2/27/105/115	-
18	CLA	A	836	-	1/1/15/20	1/37/115/115	-
18	CLA	B	819	-	1/1/13/20	5/29/107/115	-
21	BCR	L	306	-	-	2/29/63/63	0/2/2/2
18	CLA	2	609	14	1/1/14/20	6/31/109/115	-
21	BCR	A	849	-	-	2/29/63/63	0/2/2/2
30	QDL	4	617	-	-	0/30/80/80	0/3/3/3
18	CLA	B	839	20	1/1/15/20	8/37/115/115	-
21	BCR	B	844	-	-	2/29/63/63	0/2/2/2
18	CLA	A	817	31	1/1/11/20	3/13/91/115	-
18	CLA	F	805	9	1/1/12/20	4/19/97/115	-
18	CLA	B	829	-	1/1/15/20	4/37/115/115	-
21	BCR	F	806	-	-	2/29/63/63	0/2/2/2
18	CLA	A	829	-	1/1/15/20	5/37/115/115	-
18	CLA	G	201	-	1/1/13/20	6/28/106/115	-
18	CLA	2	612	14	1/1/15/20	5/37/115/115	-
18	CLA	B	818	-	1/1/14/20	4/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	BCR	J	103	-	-	2/29/63/63	0/2/2/2
18	CLA	4	614	-	1/1/12/20	2/19/97/115	-
18	CLA	1	314	-	1/1/11/20	4/13/91/115	-
24	LMU	L	301	-	-	0/11/31/61	0/1/1/2
18	CLA	1	308	31	1/1/11/20	4/13/91/115	-
18	CLA	B	836	31	1/1/15/20	3/37/115/115	-
18	CLA	2	604	-	1/1/11/20	0/13/91/115	-
21	BCR	L	307	-	-	2/29/63/63	0/2/2/2
28	XAT	2	616	-	-	0/31/93/93	0/4/4/4
21	BCR	B	840	-	-	2/29/63/63	0/2/2/2
24	LMU	4	621	-	-	2/14/34/61	0/1/1/2
18	CLA	4	609	16	1/1/14/20	4/31/109/115	-
18	CLA	4	612	16	1/1/15/20	5/37/115/115	-
18	CLA	B	817	31	1/1/13/20	0/25/103/115	-
18	CLA	A	813	-	1/1/11/20	3/13/91/115	-
18	CLA	A	839	-	1/1/15/20	4/37/115/115	-
18	CLA	B	834	-	1/1/15/20	0/37/115/115	-
18	CLA	G	204	-	1/1/11/20	3/13/91/115	-
24	LMU	4	623	-	-	4/21/61/61	0/2/2/2
18	CLA	1	311	-	1/1/11/20	3/13/91/115	-
22	SF4	A	853	2,1	-	-	0/6/5/5
20	LHG	2	617	18	-	15/47/47/53	-
18	CLA	A	825	-	1/1/14/20	5/31/109/115	-
21	BCR	A	848	-	-	2/29/63/63	0/2/2/2
18	CLA	2	613	-	1/1/12/20	1/19/97/115	-
24	LMU	1	301	-	-	2/21/61/61	0/2/2/2
18	CLA	A	811	-	1/1/11/20	2/13/91/115	-
26	LUT	4	616	-	-	2/29/67/67	0/2/2/2
18	CLA	B	832	31	1/1/11/20	0/13/91/115	-
18	CLA	F	802	-	1/1/15/20	0/37/115/115	-
18	CLA	B	823	31	1/1/15/20	2/37/115/115	-
24	LMU	F	808	-	-	4/21/61/61	0/2/2/2
18	CLA	A	838	-	1/1/12/20	1/21/99/115	-

The worst 5 of 542 bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	2	614	CHL	C4B-NB	12.24	1.46	1.35
27	1	307	CHL	C4B-NB	12.13	1.46	1.35
27	2	606	CHL	C4B-NB	12.05	1.46	1.35
27	4	615	CHL	C4B-NB	12.04	1.46	1.35
27	3	306	CHL	C4B-NB	12.03	1.45	1.35

The worst 5 of 405 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	603	CLA	C1D-ND-C4D	-4.45	103.18	106.33
18	B	833	CLA	C1D-ND-C4D	-4.39	103.22	106.33
27	4	607	CHL	CHD-C1D-ND	-4.39	120.42	124.45
17	H	202	CL0	CHD-C1D-ND	-4.37	120.44	124.45
18	A	842	CLA	C1D-ND-C4D	-4.34	103.25	106.33

5 of 182 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	A	801	CL0	NA
17	A	801	CL0	NC
17	A	801	CL0	ND
17	H	202	CL0	NA
17	H	202	CL0	NC

5 of 713 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	H	202	CL0	C2-C3-C5-C6
17	H	202	CL0	C4-C3-C5-C6
18	A	804	CLA	C1A-C2A-CAA-CBA
18	A	809	CLA	O2A-C1-C2-C3
18	A	812	CLA	C4-C3-C5-C6

There are no ring outliers.

157 monomers are involved in 254 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	1	310	CLA	7	0
18	L	303	CLA	2	0
21	3	313	BCR	4	0
21	G	206	BCR	3	0
20	A	847	LHG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	816	CLA	1	0
18	B	828	CLA	1	0
18	A	831	CLA	1	0
18	A	833	CLA	2	0
18	2	608	CLA	2	0
26	3	315	LUT	3	0
18	2	601	CLA	2	0
21	A	850	BCR	2	0
21	4	618	BCR	4	0
18	A	824	CLA	1	0
18	A	820	CLA	3	0
18	B	822	CLA	4	0
18	A	841	CLA	1	0
18	A	840	CLA	2	0
24	1	320	LMU	1	0
18	3	312	CLA	1	0
18	1	306	CLA	2	0
24	2	618	LMU	1	0
18	3	303	CLA	2	0
18	2	610	CLA	2	0
18	1	313	CLA	4	0
26	1	318	LUT	1	0
18	A	830	CLA	1	0
18	3	304	CLA	2	0
23	A	857	LMG	4	0
18	B	806	CLA	1	0
18	A	803	CLA	1	0
24	G	203	LMU	2	0
26	3	314	LUT	1	0
26	2	615	LUT	1	0
18	A	854	CLA	2	0
24	F	807	LMU	2	0
24	F	809	LMU	2	0
27	4	607	CHL	1	0
25	4	622	DGD	1	0
18	A	843	CLA	4	0
18	A	822	CLA	3	0
27	4	605	CHL	2	0
23	4	619	LMG	2	0
18	A	856	CLA	1	0
18	1	312	CLA	3	0
18	B	825	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	4	624	LMU	1	0
18	B	815	CLA	2	0
18	K	201	CLA	1	0
26	J	101	LUT	3	0
18	B	811	CLA	1	0
27	4	606	CHL	2	0
27	2	606	CHL	1	0
18	A	845	CLA	1	0
21	A	851	BCR	2	0
24	F	803	LMU	1	0
18	A	810	CLA	1	0
18	1	303	CLA	3	0
18	B	804	CLA	1	0
18	4	608	CLA	4	0
24	1	321	LMU	1	0
20	B	847	LHG	1	0
18	A	804	CLA	1	0
18	3	308	CLA	3	0
28	1	317	XAT	2	0
18	A	818	CLA	3	0
18	B	820	CLA	6	0
18	1	315	CLA	1	0
20	1	319	LHG	6	0
18	3	302	CLA	3	0
23	4	620	LMG	3	0
18	3	305	CLA	1	0
18	B	833	CLA	1	0
18	4	613	CLA	1	0
18	A	812	CLA	2	0
18	4	602	CLA	1	0
26	1	316	LUT	5	0
18	2	602	CLA	1	0
18	A	827	CLA	2	0
24	H	201	LMU	1	0
25	J	104	DGD	3	0
20	B	846	LHG	1	0
18	A	823	CLA	2	0
18	F	804	CLA	4	0
18	B	807	CLA	2	0
18	4	601	CLA	1	0
18	A	819	CLA	2	0
18	B	830	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	3	307	CLA	5	0
27	3	301	CHL	5	0
21	A	852	BCR	1	0
18	4	603	CLA	2	0
23	F	810	LMG	2	0
24	G	207	LMU	2	0
27	1	302	CHL	4	0
18	1	309	CLA	5	0
18	B	824	CLA	3	0
21	G	202	BCR	2	0
18	A	828	CLA	2	0
24	A	859	LMU	1	0
18	B	835	CLA	1	0
18	A	815	CLA	2	0
18	A	806	CLA	1	0
18	A	826	CLA	4	0
18	A	855	CLA	5	0
18	3	311	CLA	1	0
18	4	611	CLA	2	0
18	G	205	CLA	3	0
27	1	307	CHL	2	0
21	K	202	BCR	2	0
24	B	848	LMU	1	0
18	B	805	CLA	1	0
17	H	202	CL0	2	0
20	A	846	LHG	3	0
21	B	843	BCR	1	0
18	B	812	CLA	2	0
18	B	810	CLA	2	0
18	A	836	CLA	1	0
18	B	819	CLA	2	0
21	L	306	BCR	2	0
18	2	609	CLA	1	0
21	A	849	BCR	2	0
18	B	839	CLA	1	0
21	B	844	BCR	3	0
18	A	817	CLA	3	0
18	B	829	CLA	3	0
21	F	806	BCR	2	0
18	A	829	CLA	4	0
18	G	201	CLA	5	0
18	B	818	CLA	1	0

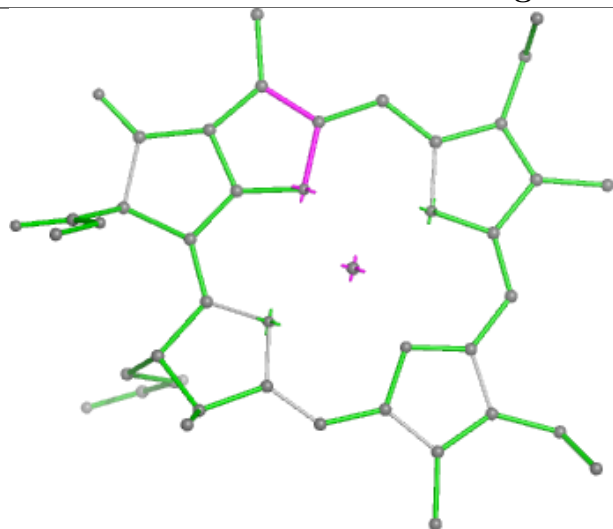
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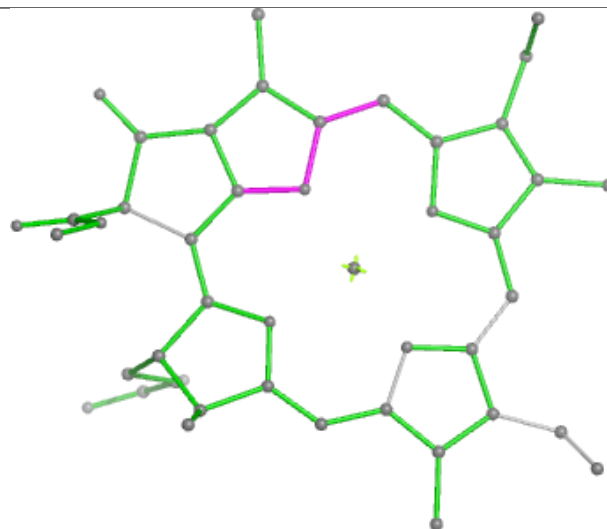
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	J	103	BCR	1	0
18	4	614	CLA	1	0
24	L	301	LMU	2	0
18	1	308	CLA	2	0
18	B	836	CLA	1	0
21	L	307	BCR	1	0
28	2	616	XAT	1	0
21	B	840	BCR	1	0
18	4	609	CLA	5	0
18	4	612	CLA	2	0
18	B	817	CLA	2	0
18	A	813	CLA	1	0
18	A	839	CLA	1	0
18	B	834	CLA	2	0
18	G	204	CLA	1	0
24	4	623	LMU	2	0
18	1	311	CLA	1	0
20	2	617	LHG	2	0
18	A	825	CLA	2	0
21	A	848	BCR	4	0
24	1	301	LMU	2	0
18	A	811	CLA	3	0
26	4	616	LUT	5	0
18	F	802	CLA	2	0
18	B	823	CLA	1	0
18	A	838	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.

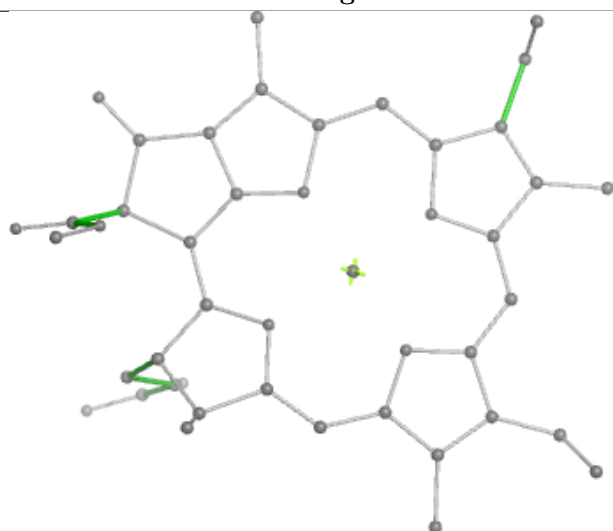
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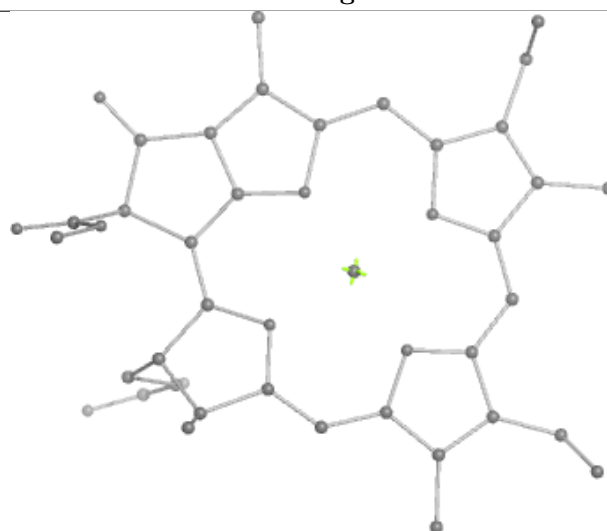
Bond lengths



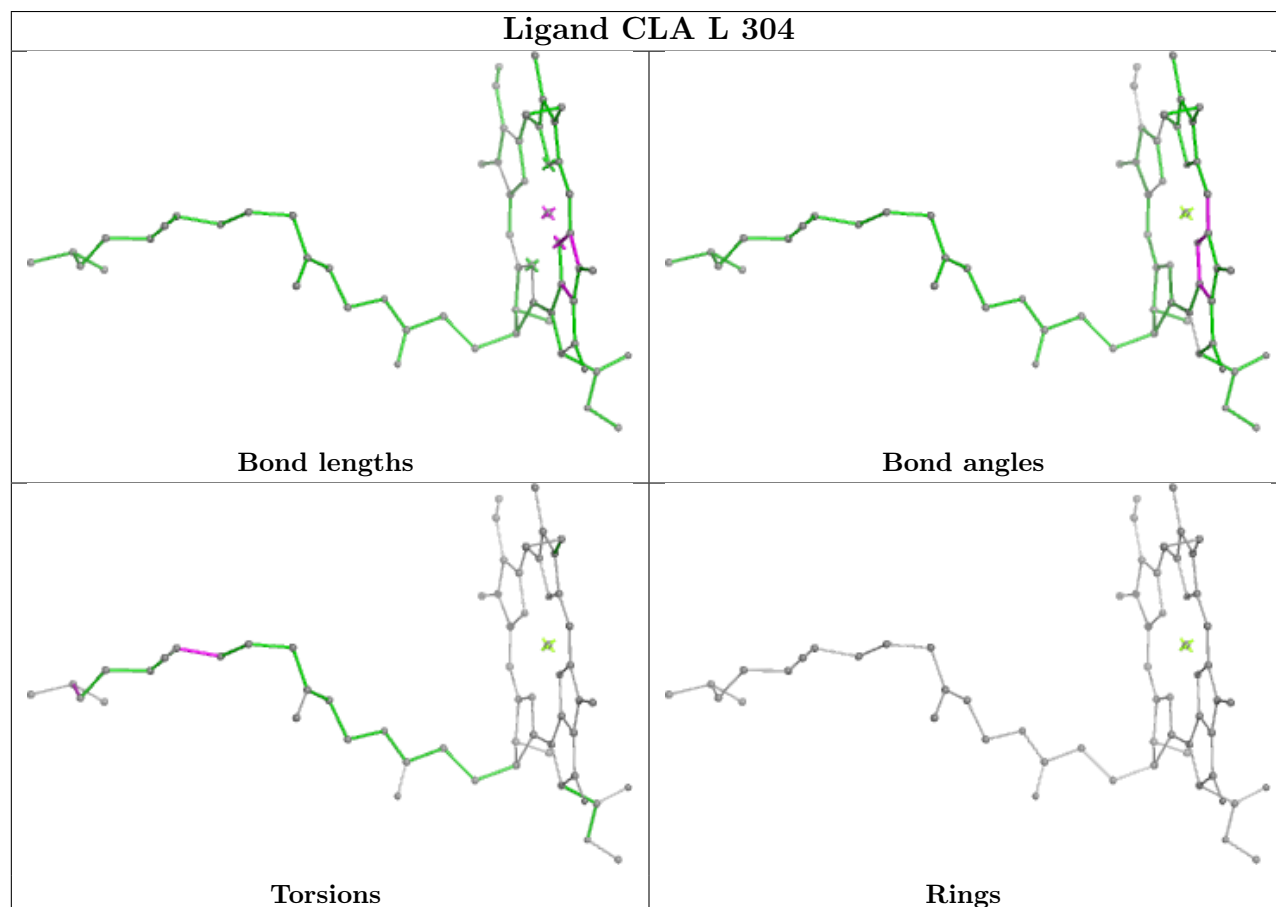
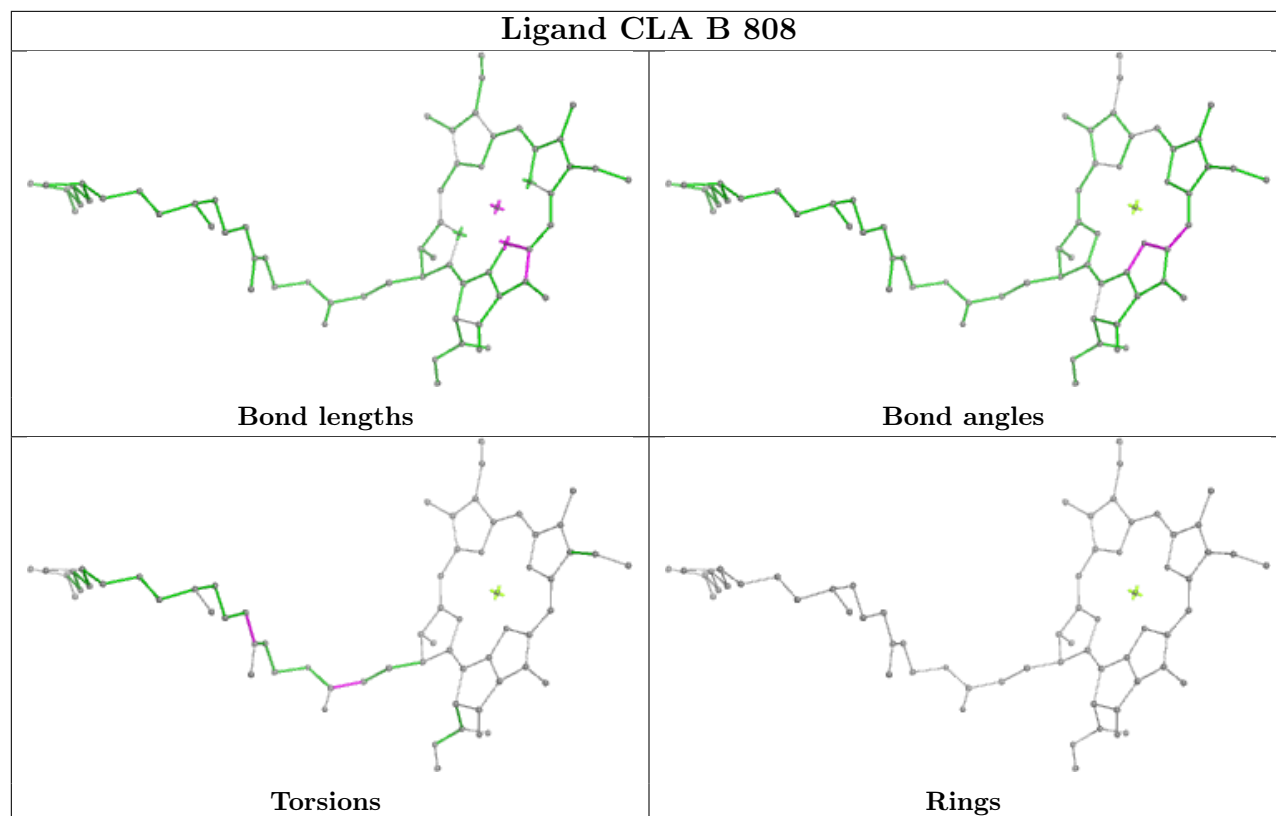
Bond angles



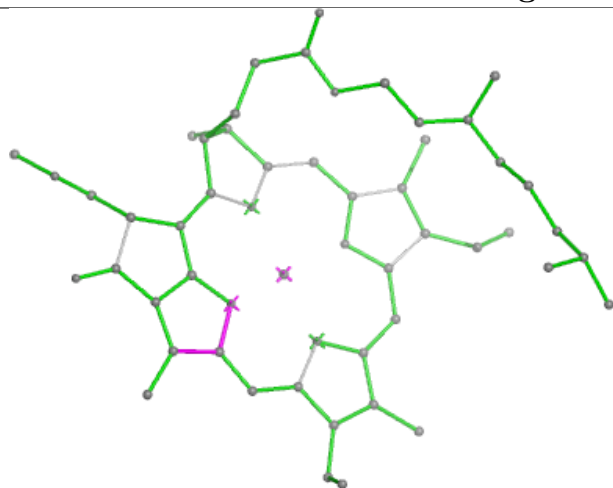
Torsions



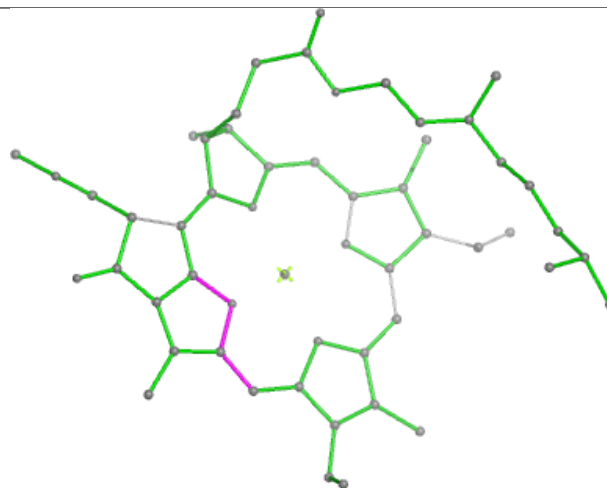
Rings



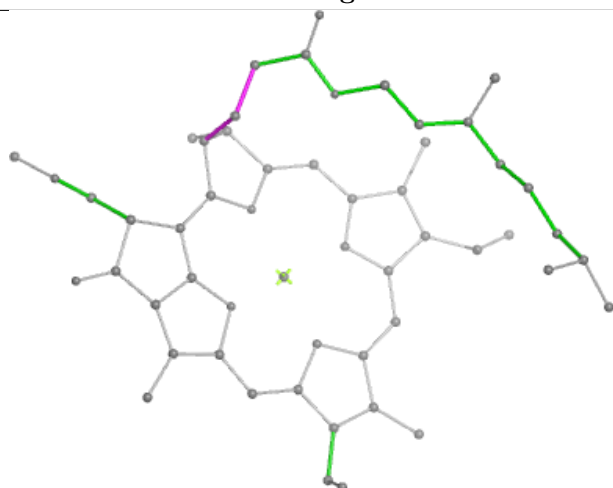
## Ligand CLA 1 310



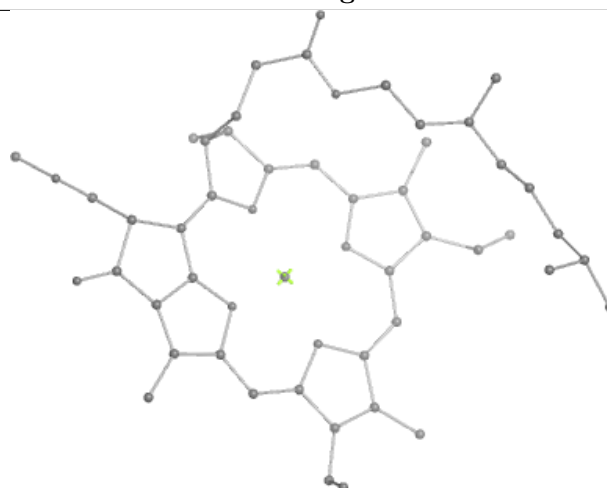
Bond lengths



Bond angles



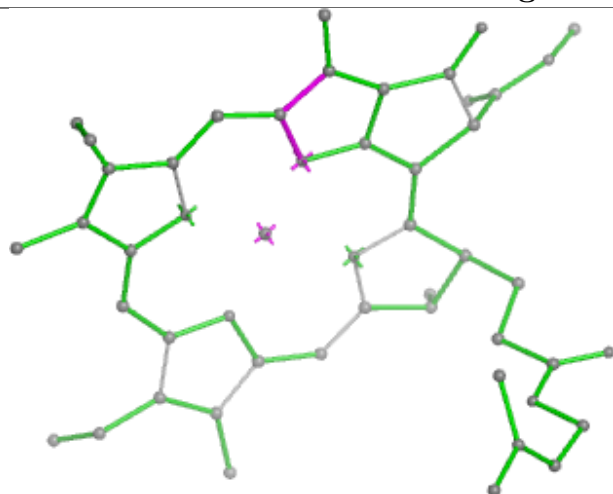
Torsions



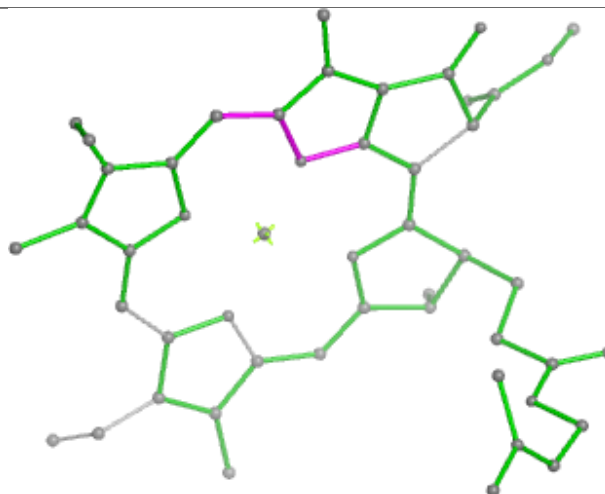
Rings



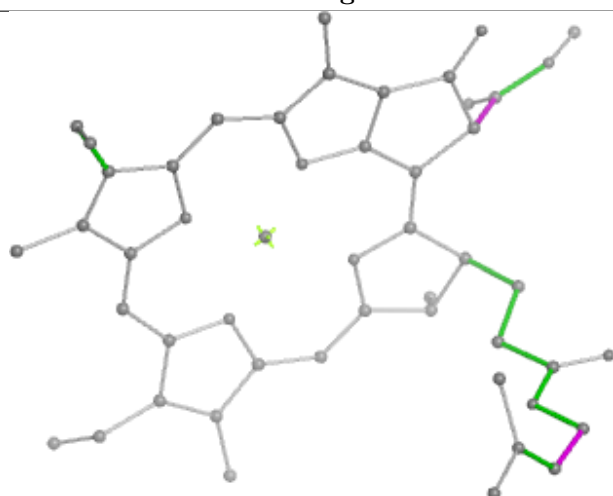
## Ligand CLA 1 305



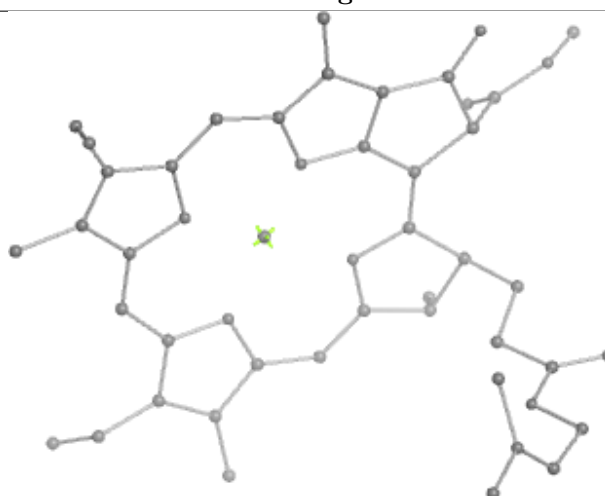
Bond lengths



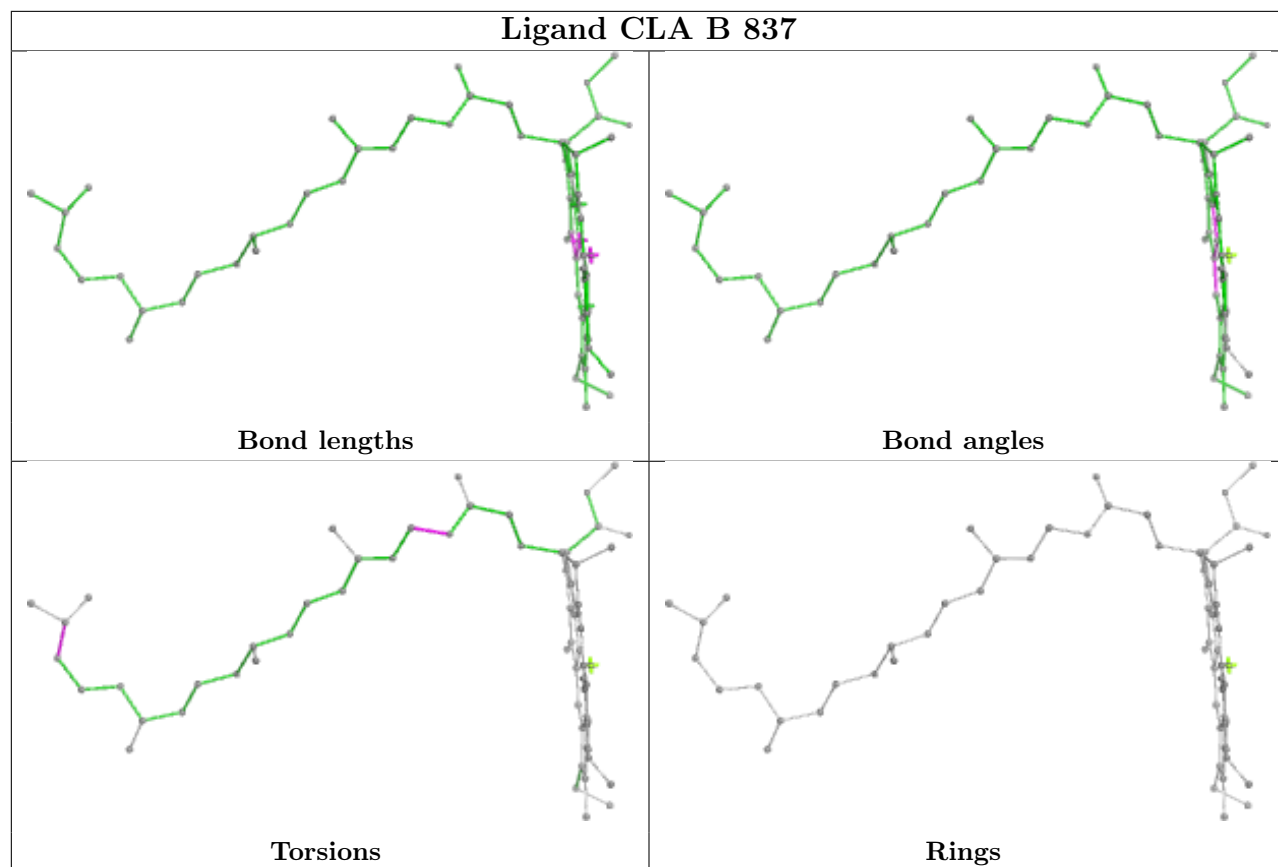
Bond angles



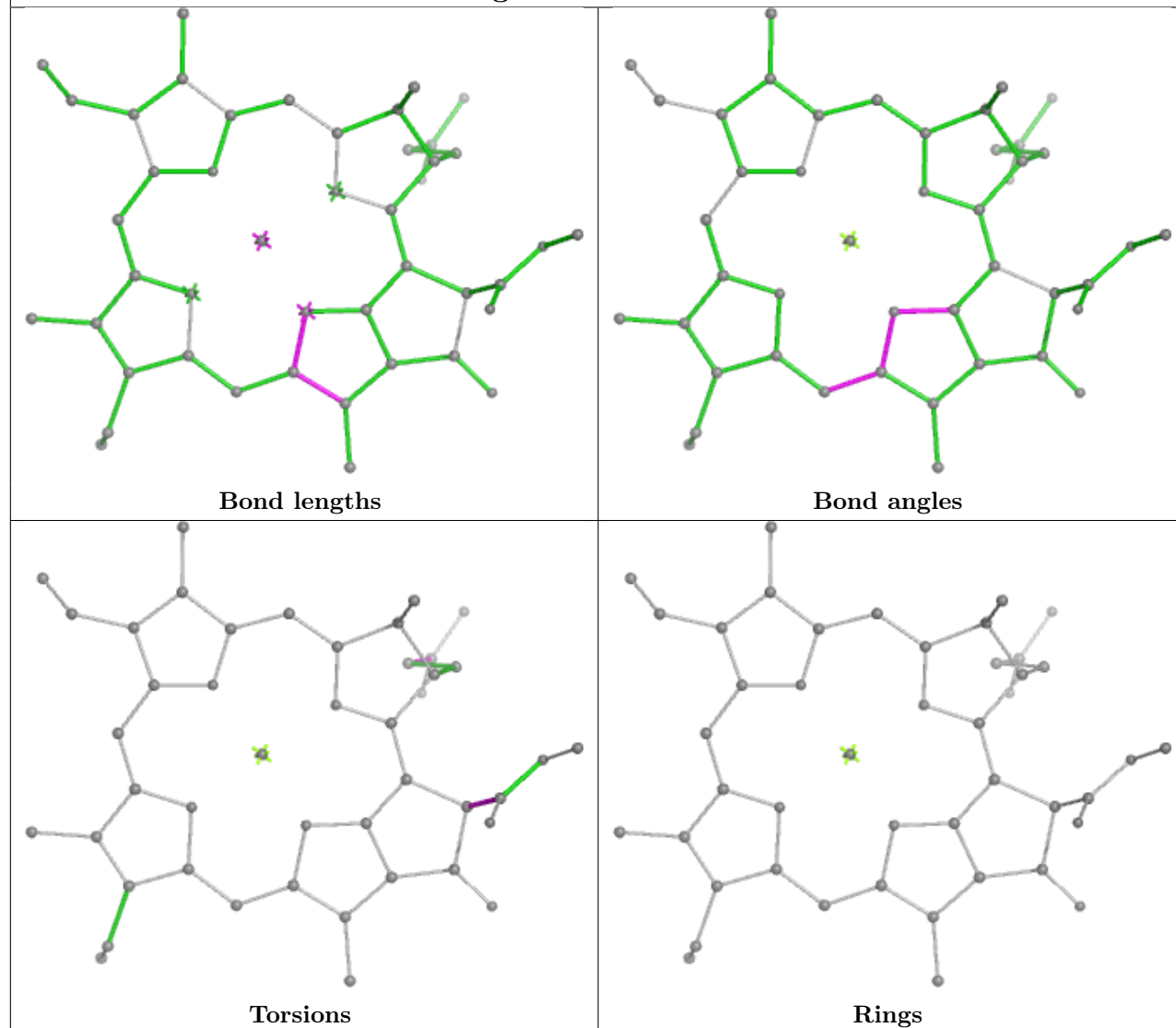
Torsions



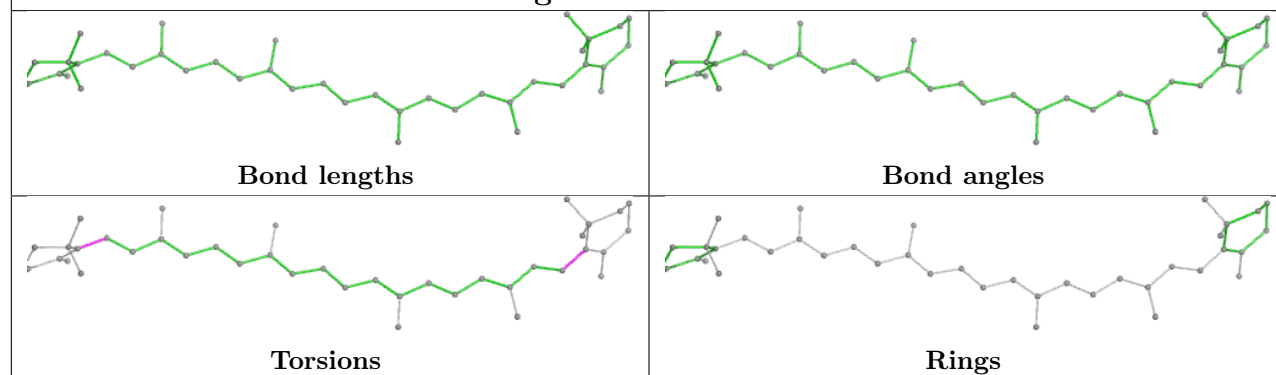
Rings

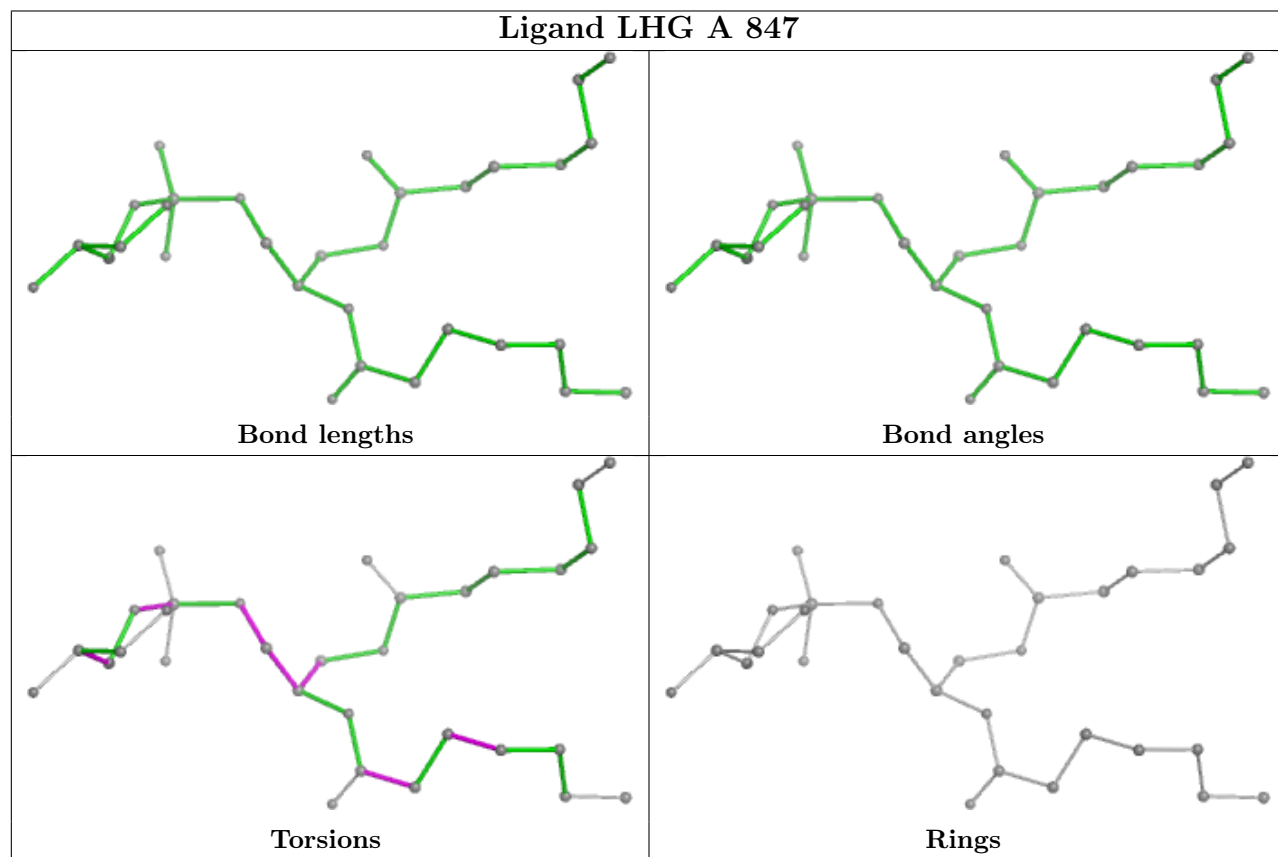
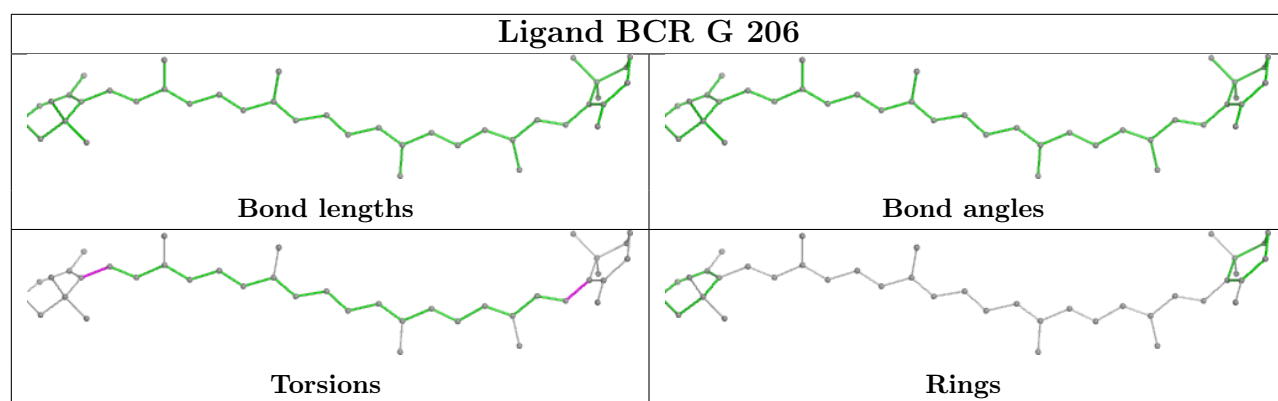


## Ligand CLA L 303

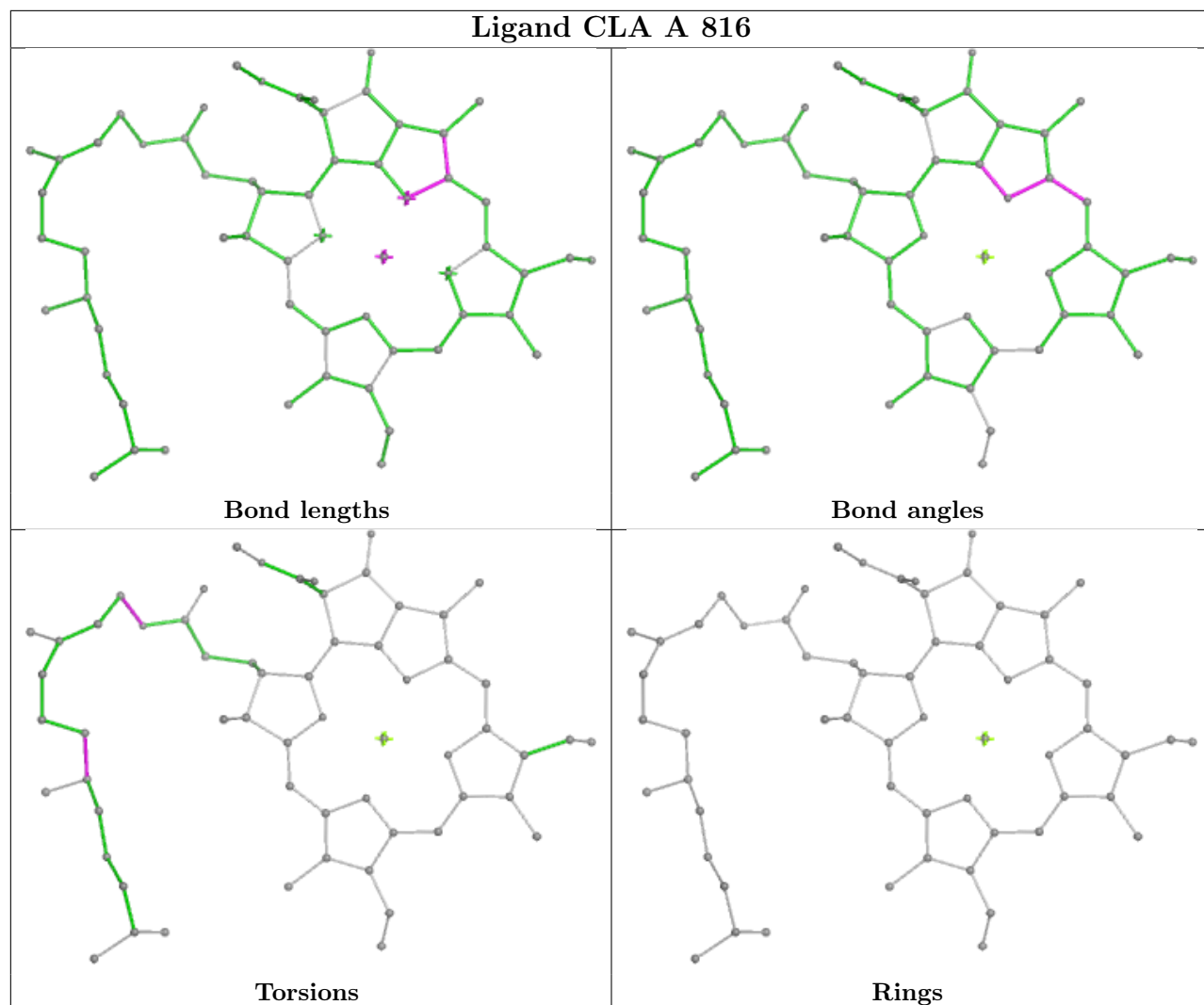


## Ligand BCR 3 313

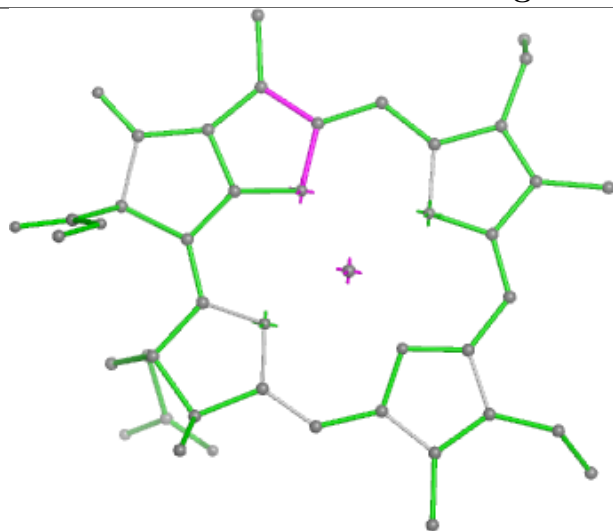




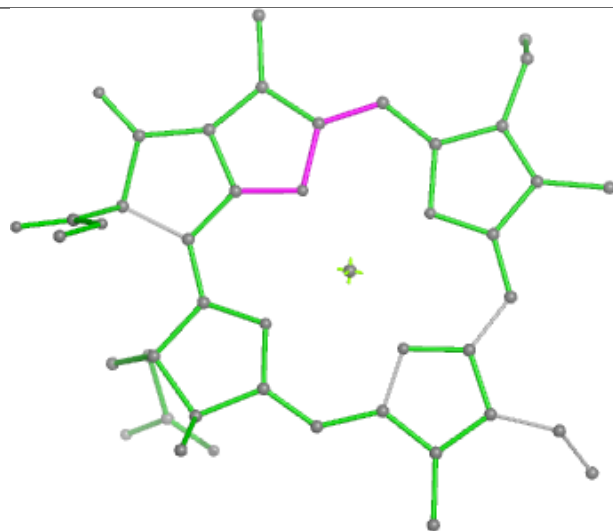
## Ligand CLA A 816



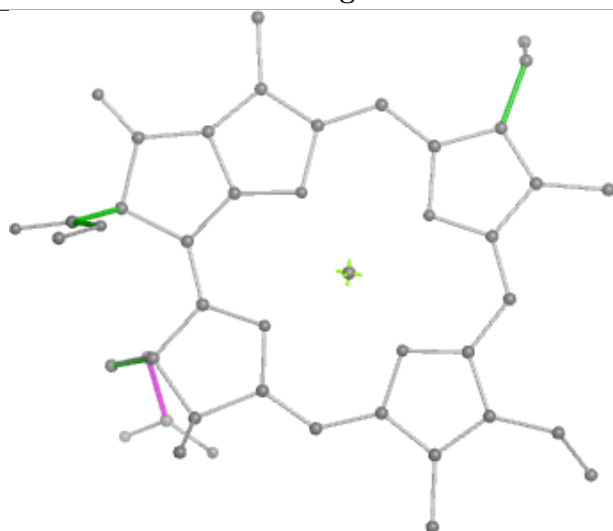
## Ligand CLA A 821



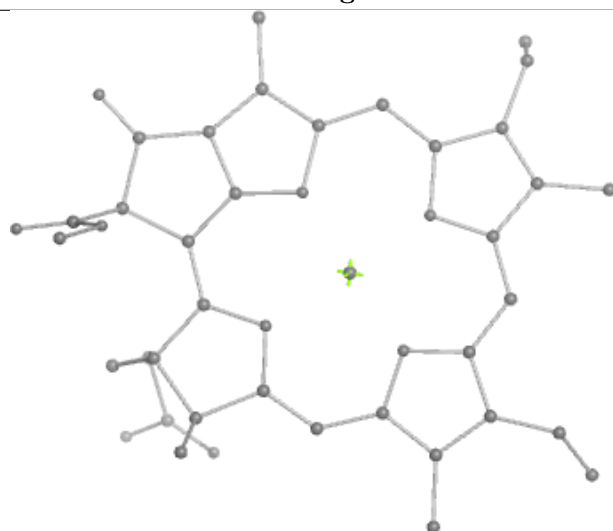
Bond lengths



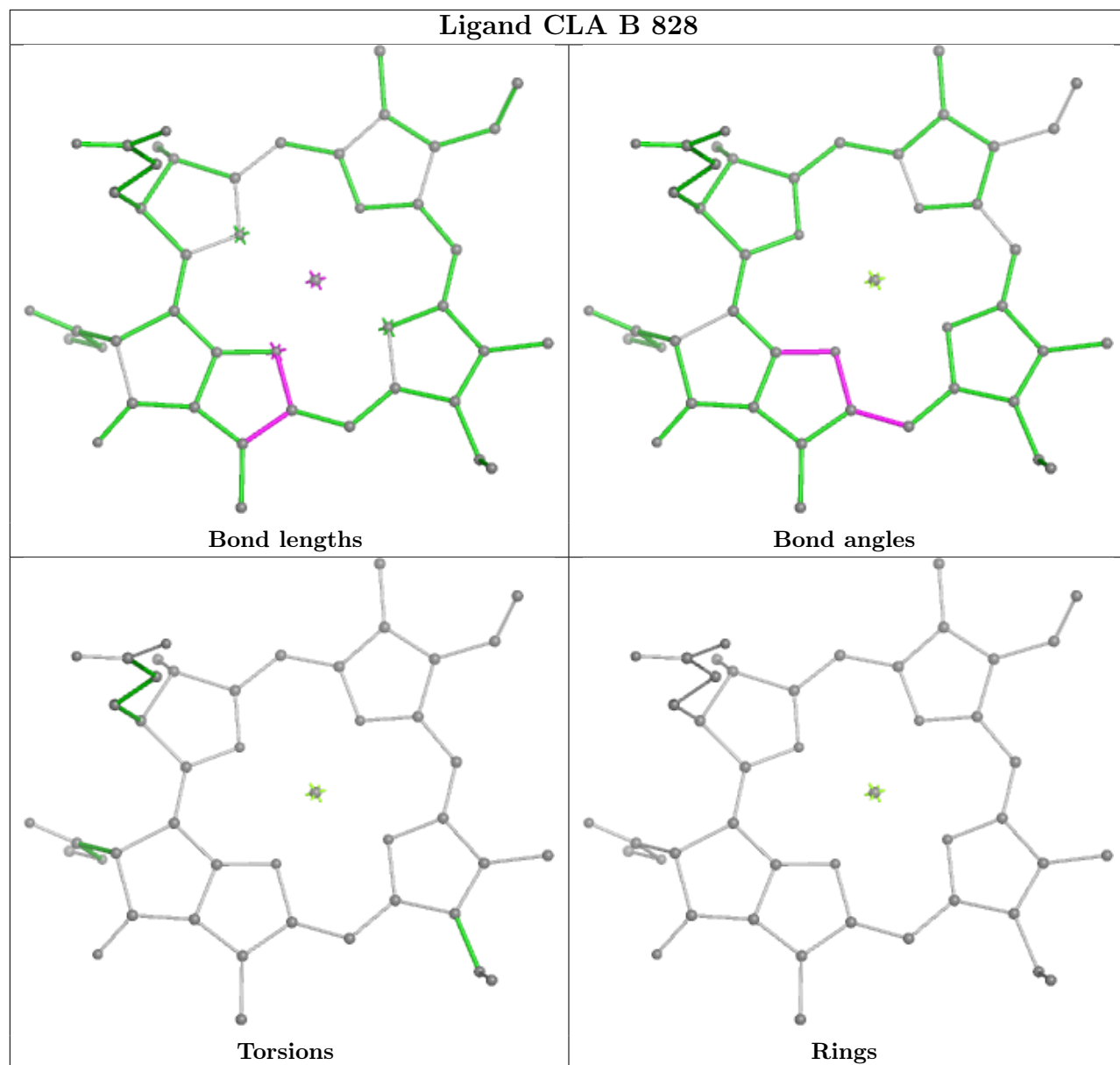
Bond angles

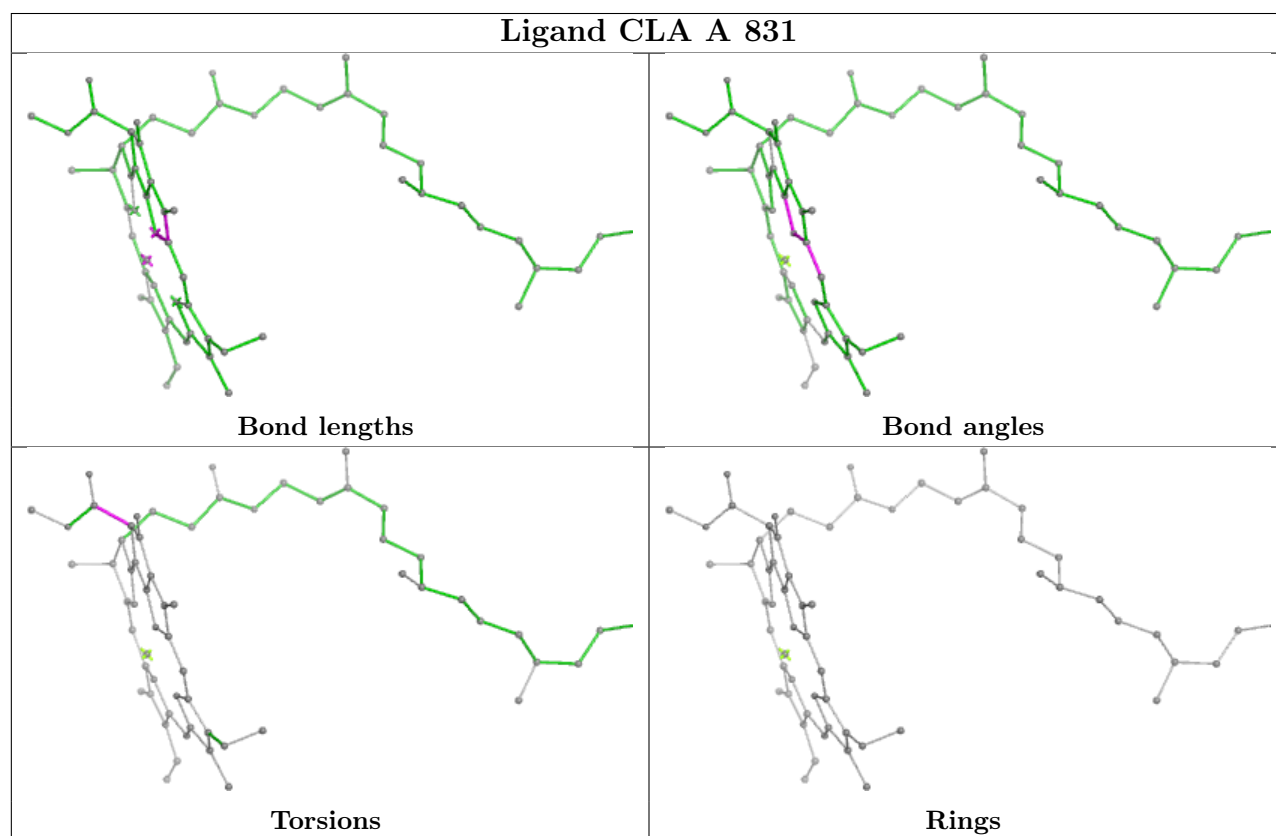
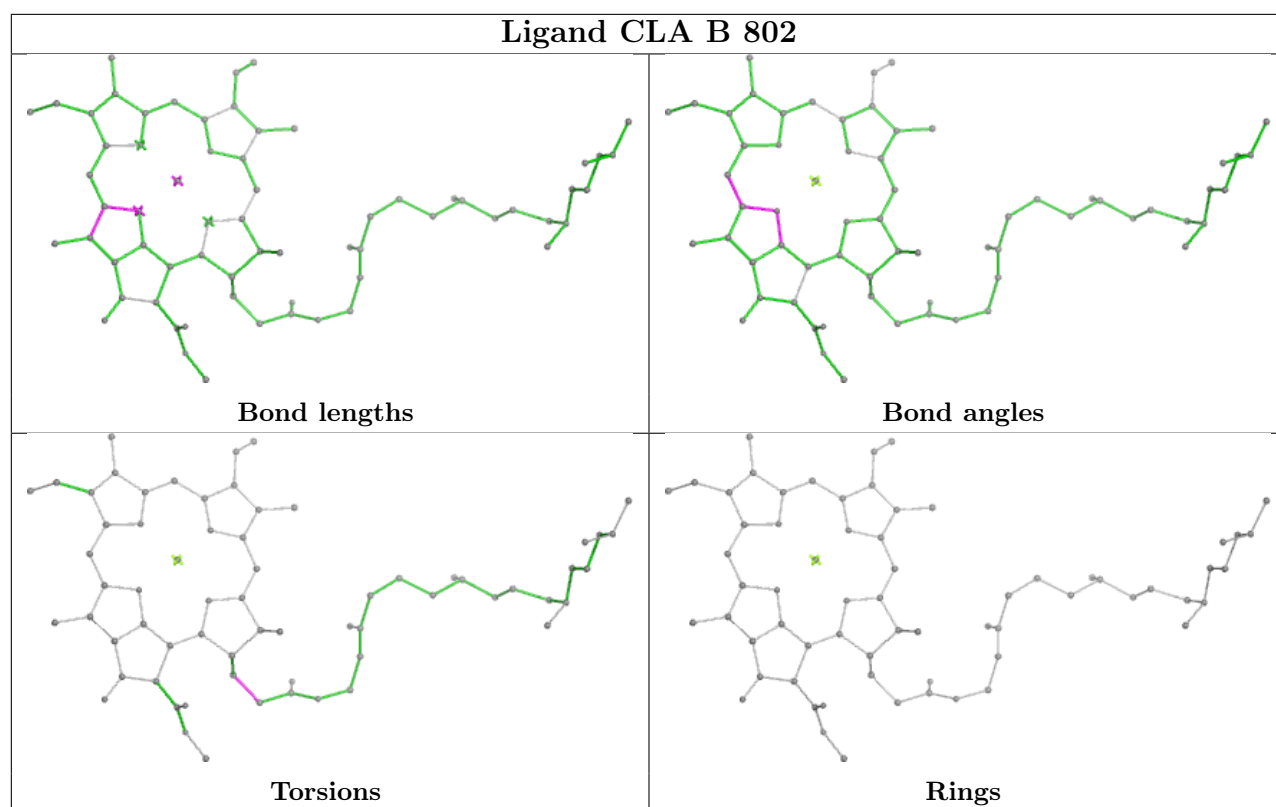


Torsions

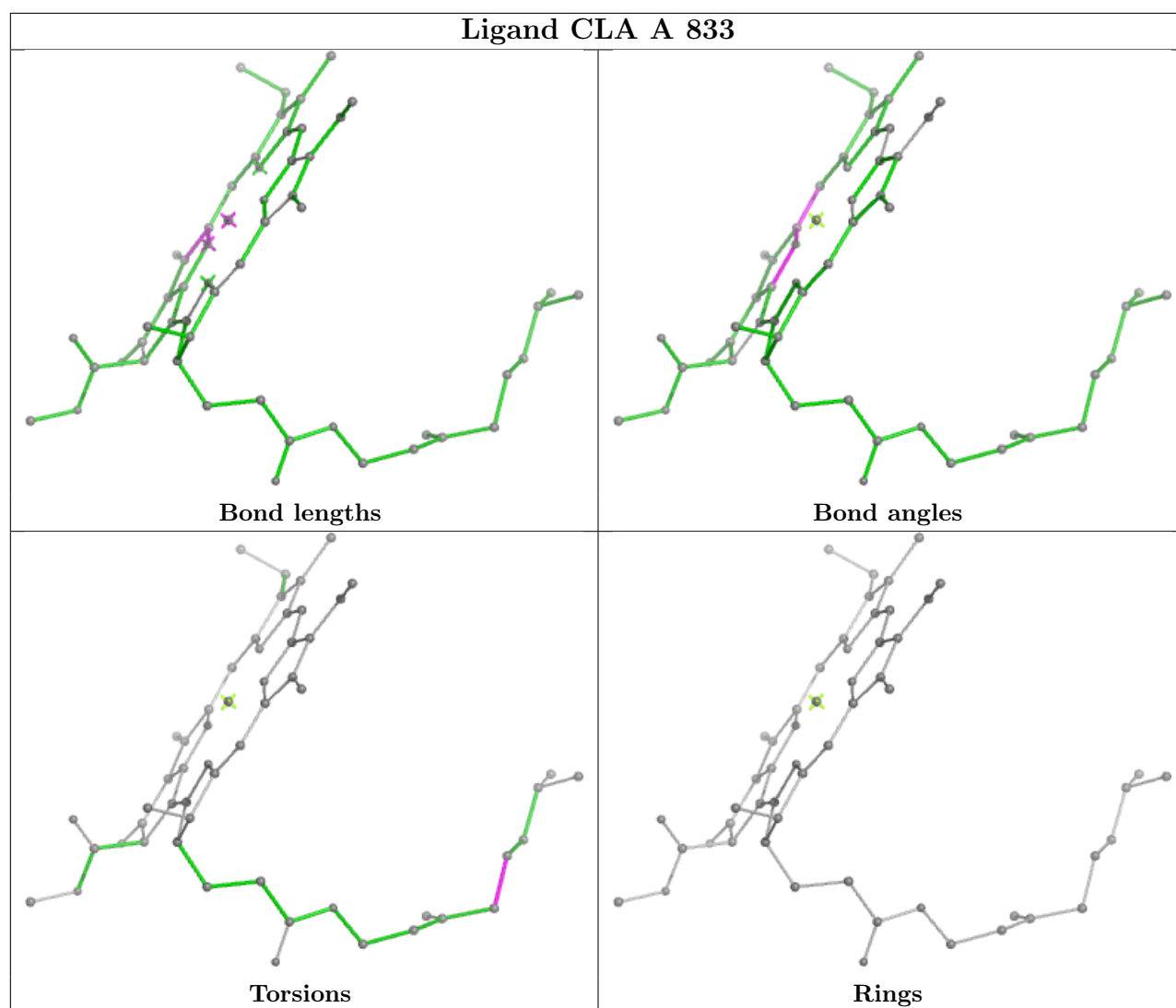


Rings

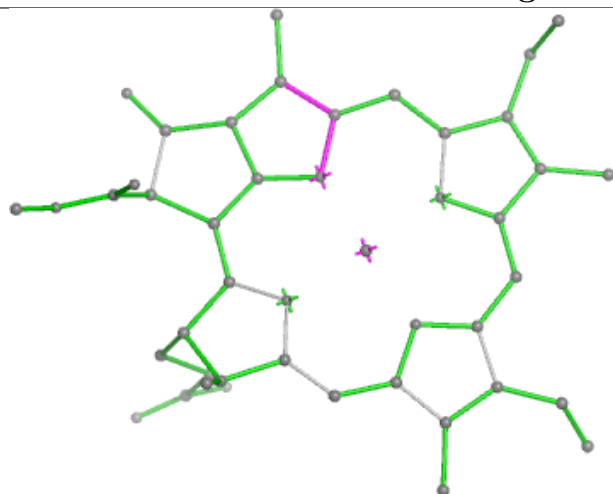




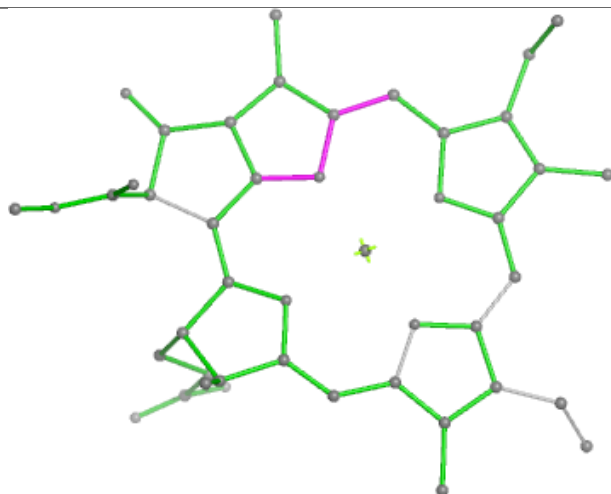




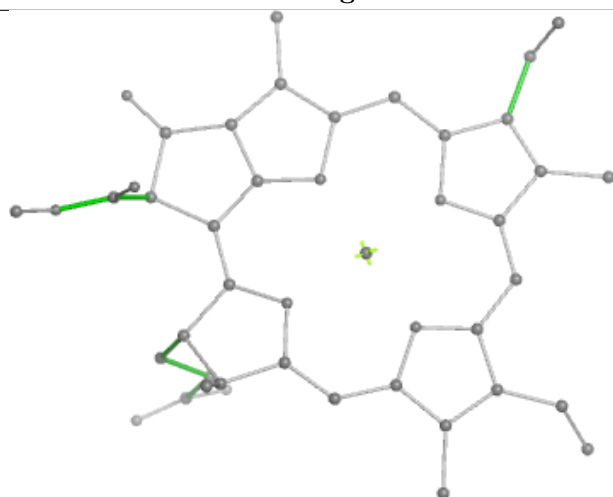
## Ligand CLA 2 608



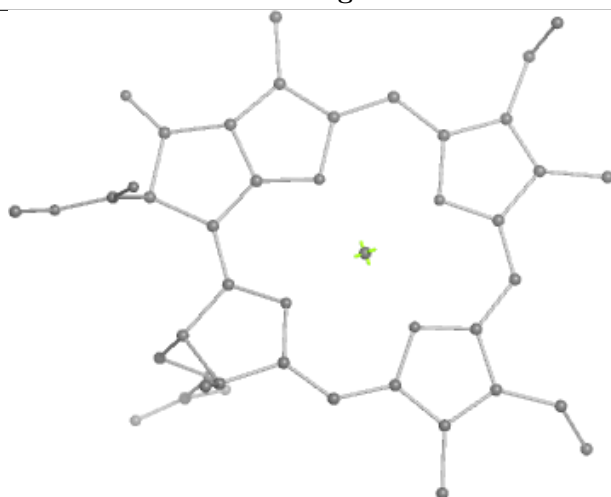
Bond lengths



Bond angles



Torsions



Rings

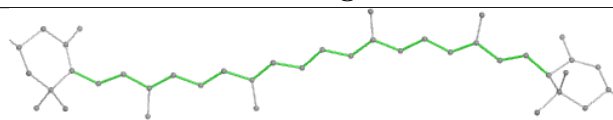
## Ligand LUT 3 315



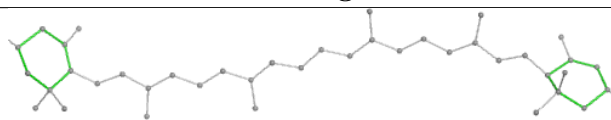
Bond lengths



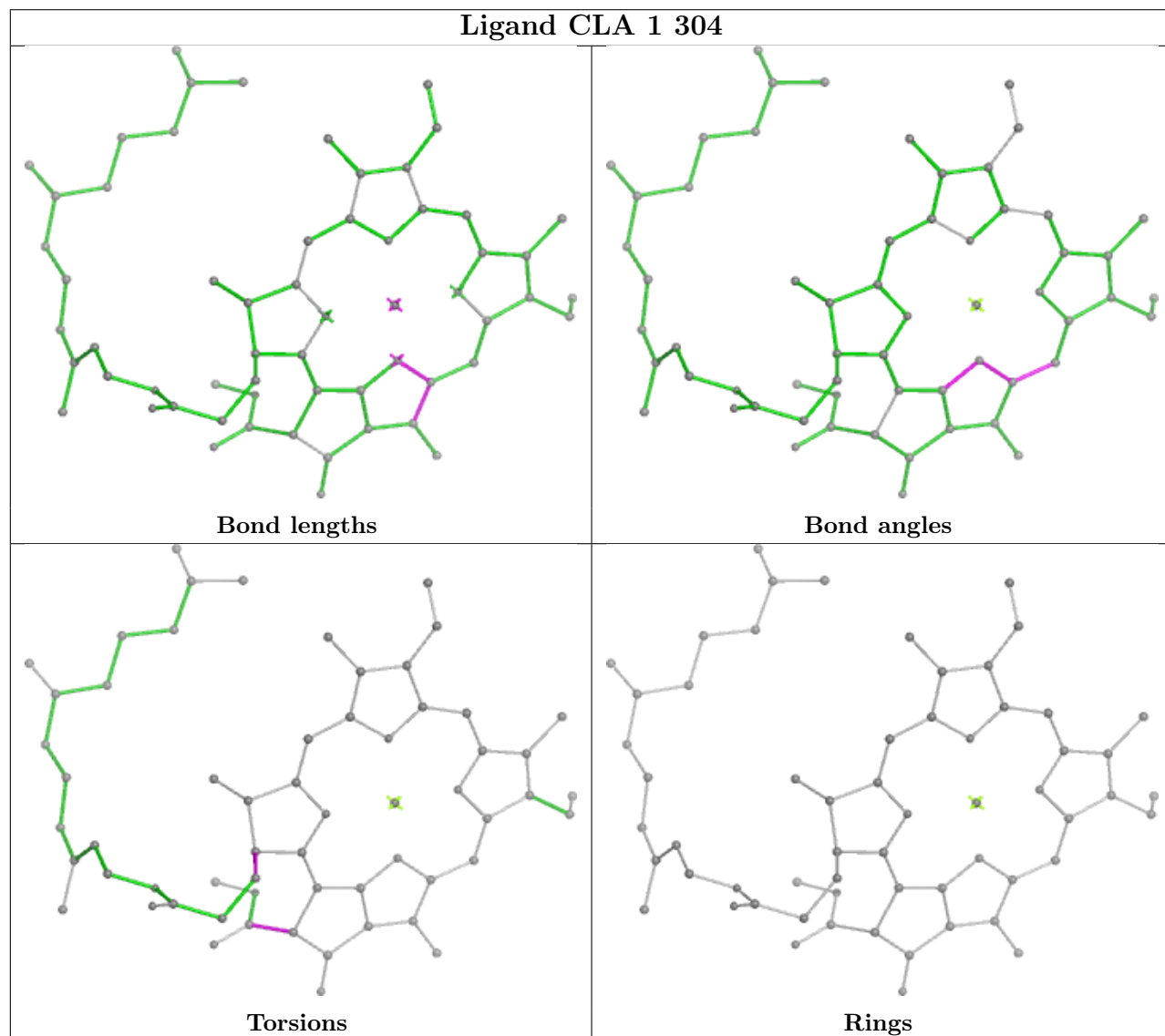
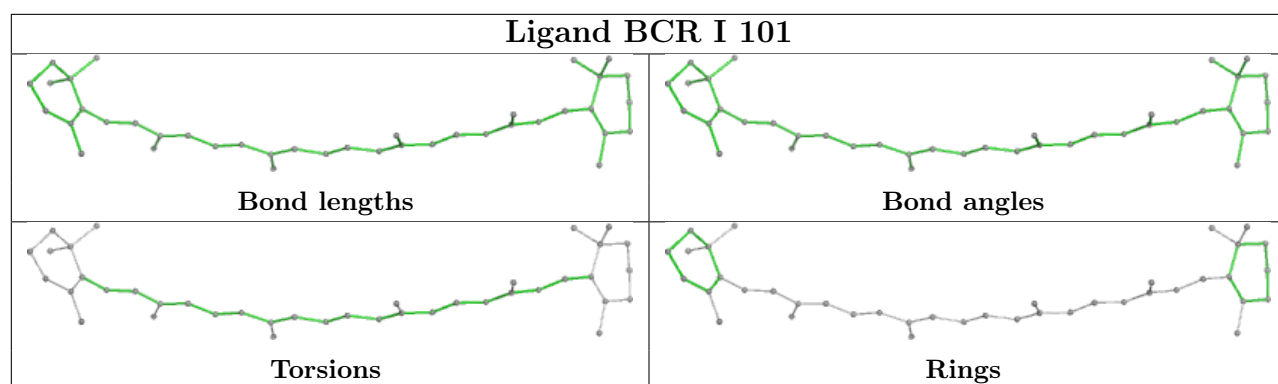
Bond angles

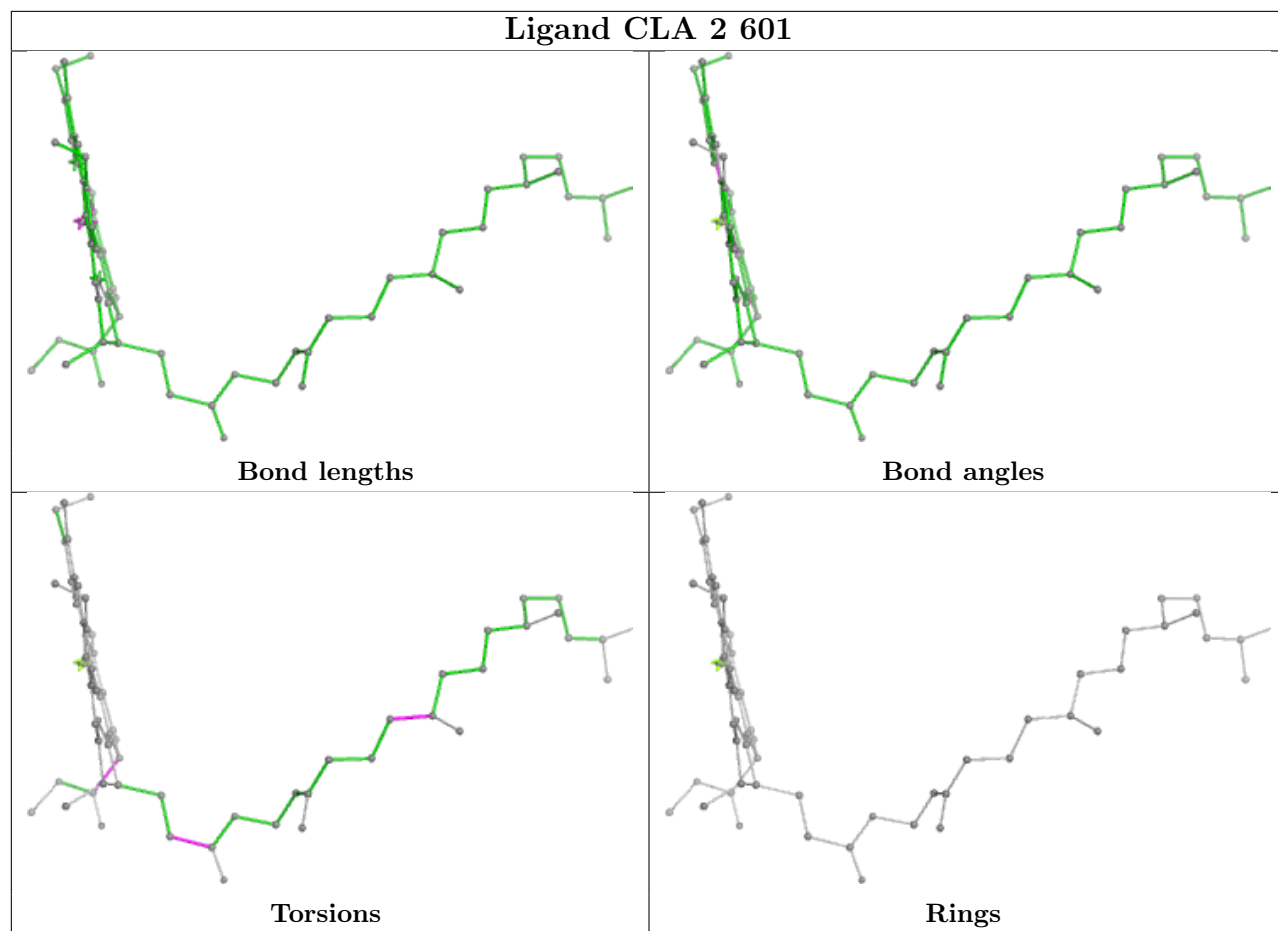


Torsions

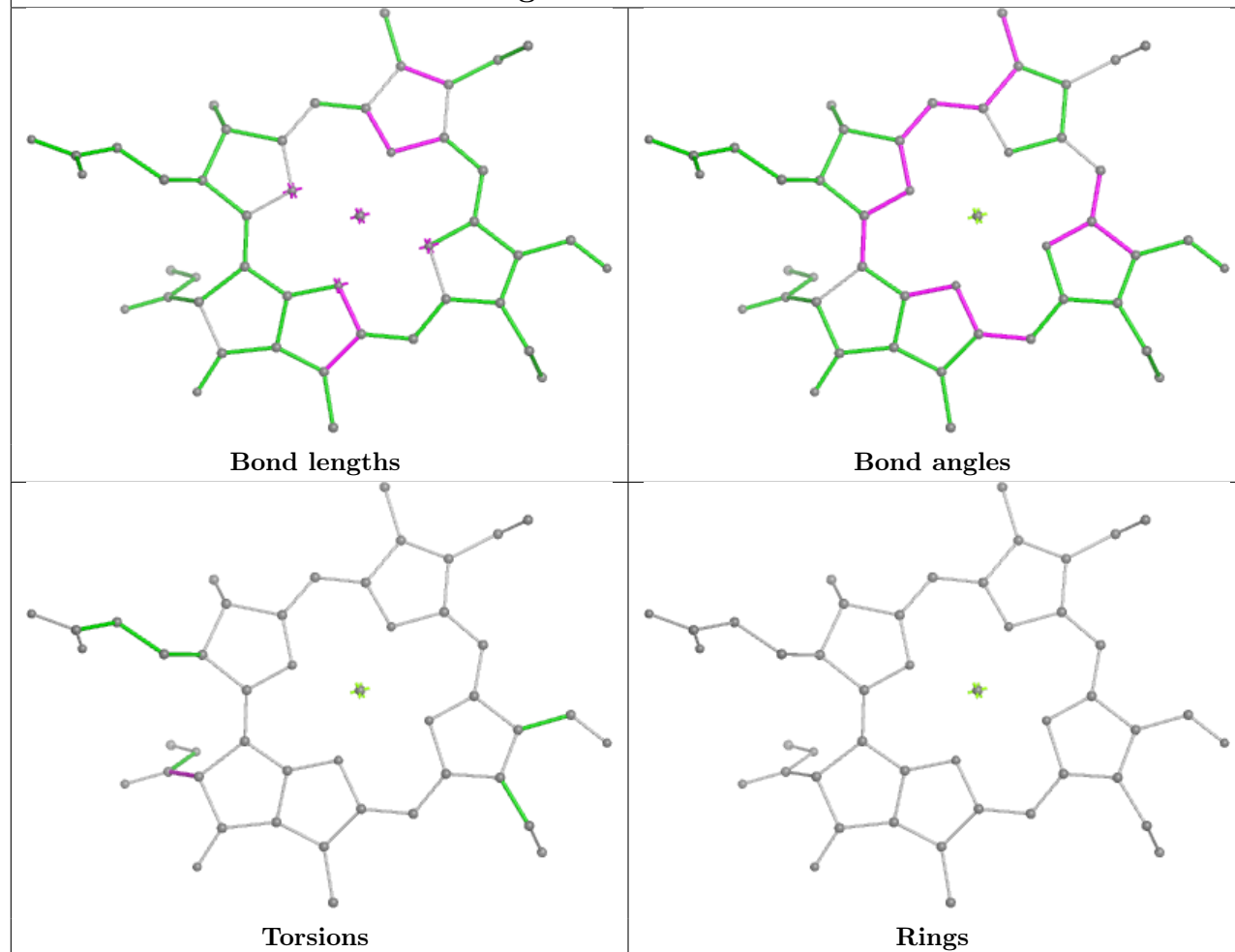


Rings

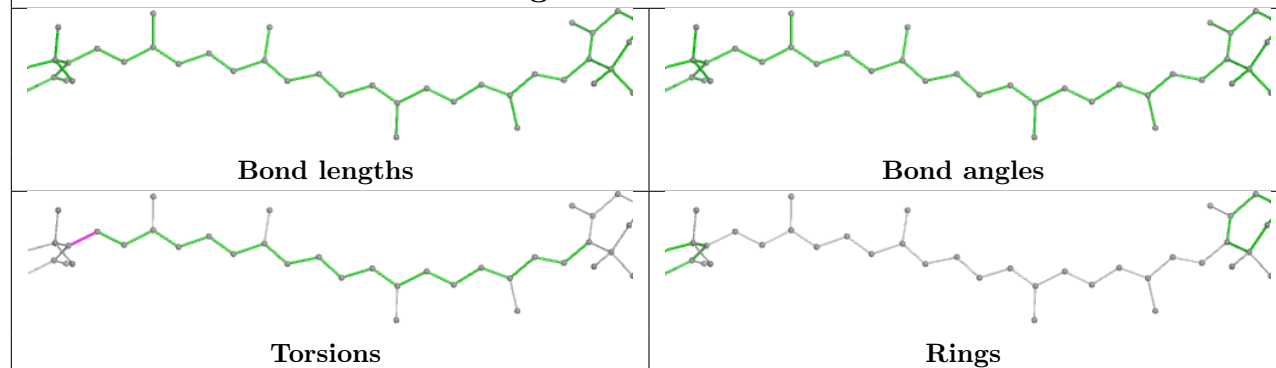


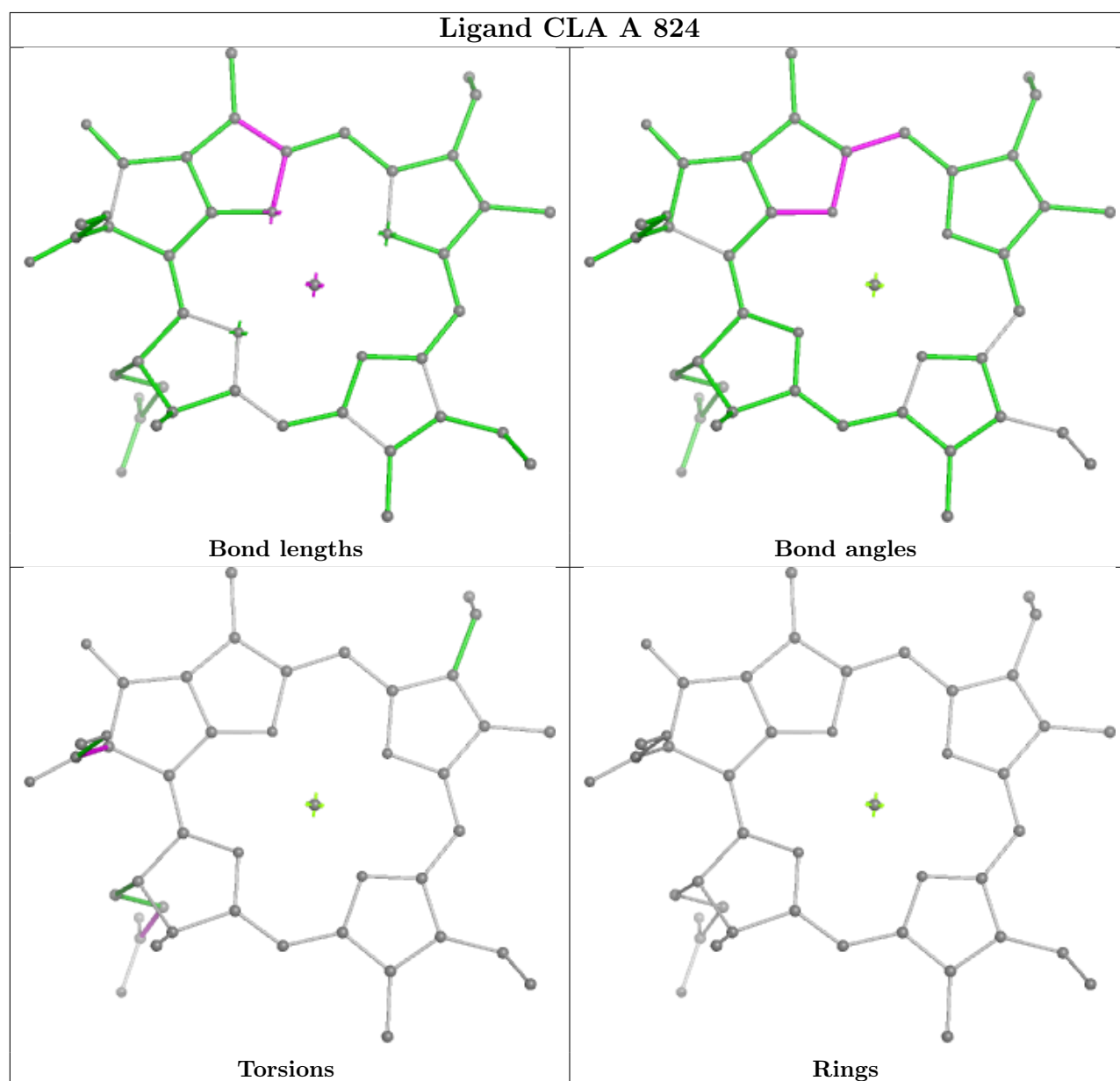
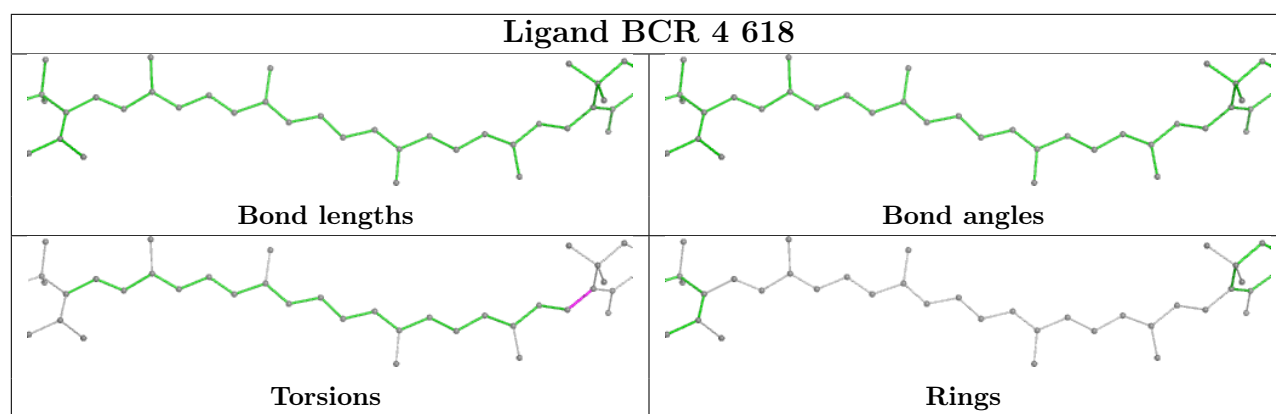


## Ligand CHL 4 615

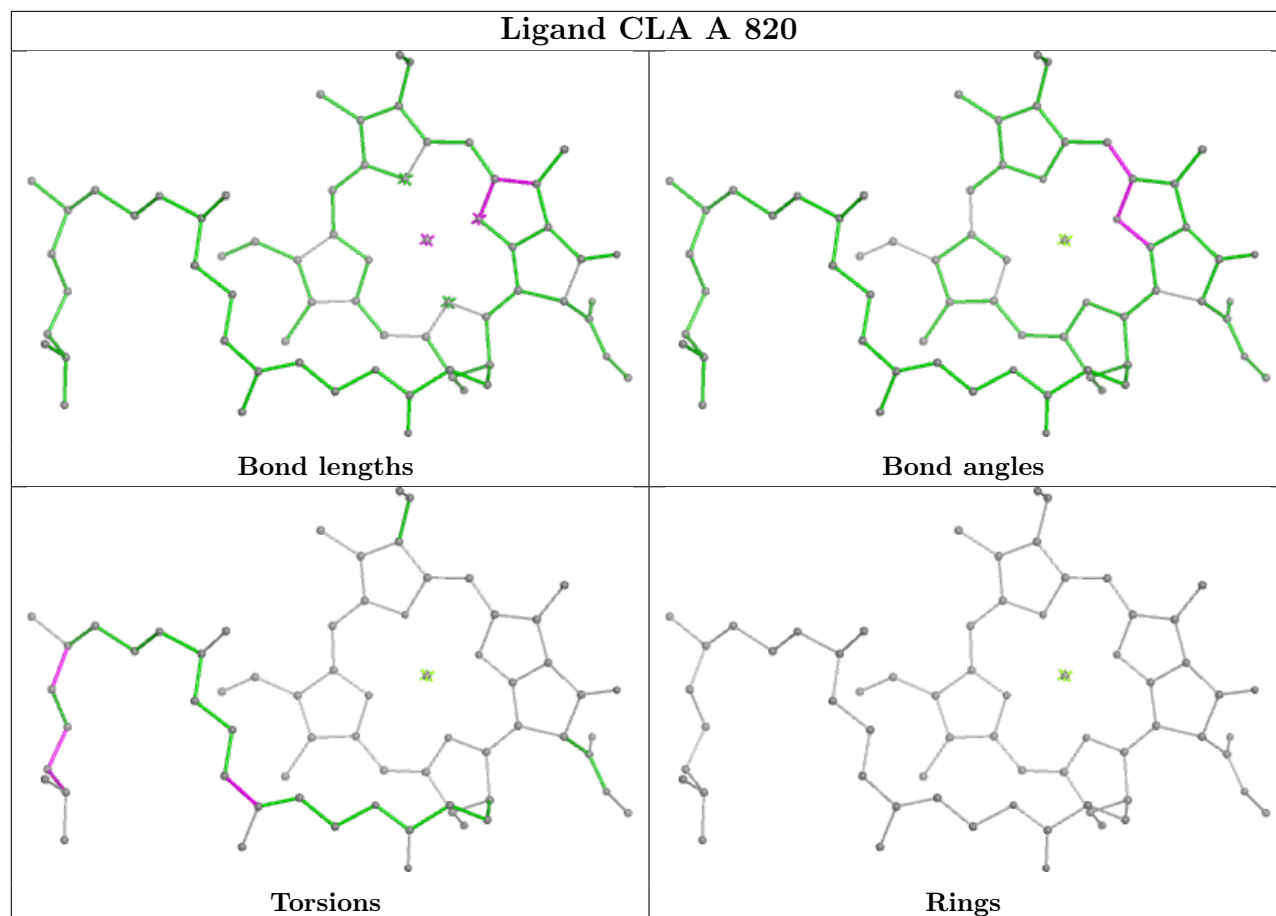


## Ligand BCR A 850

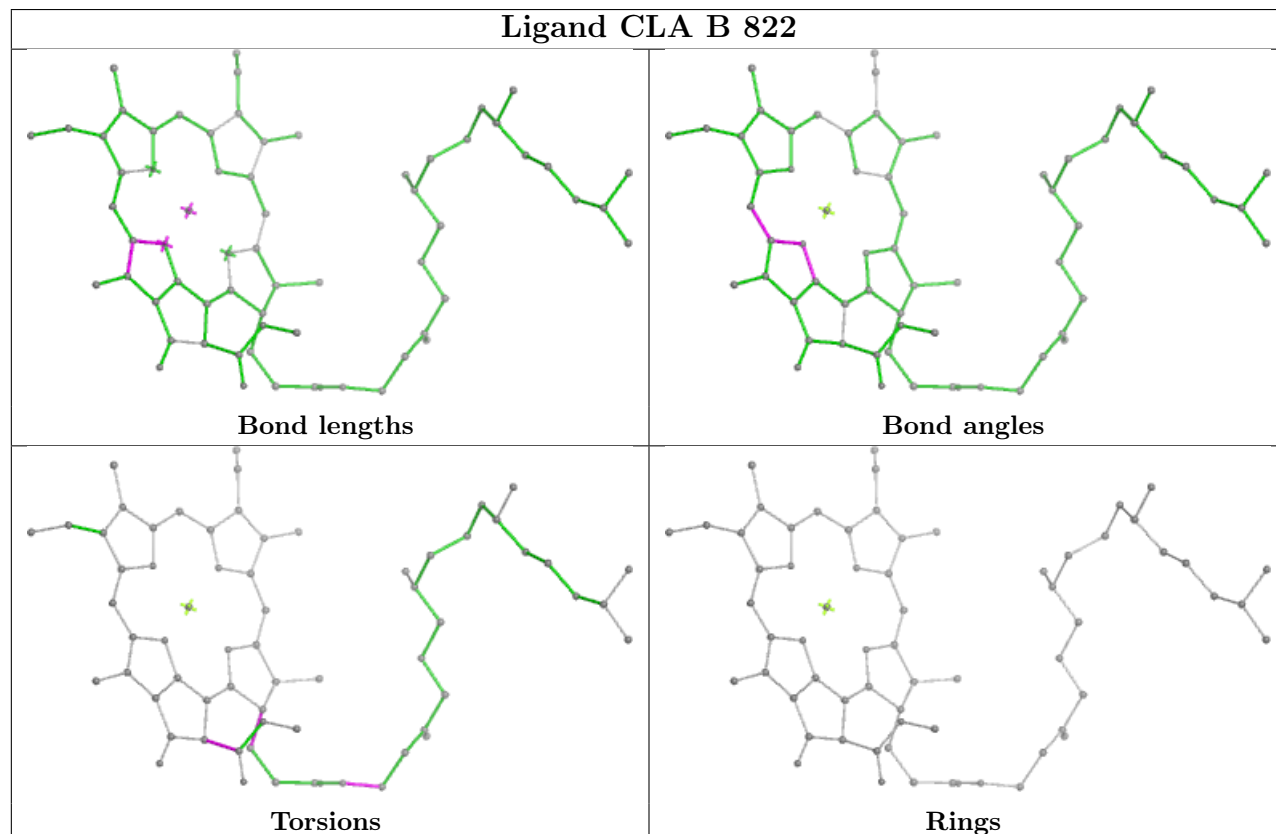


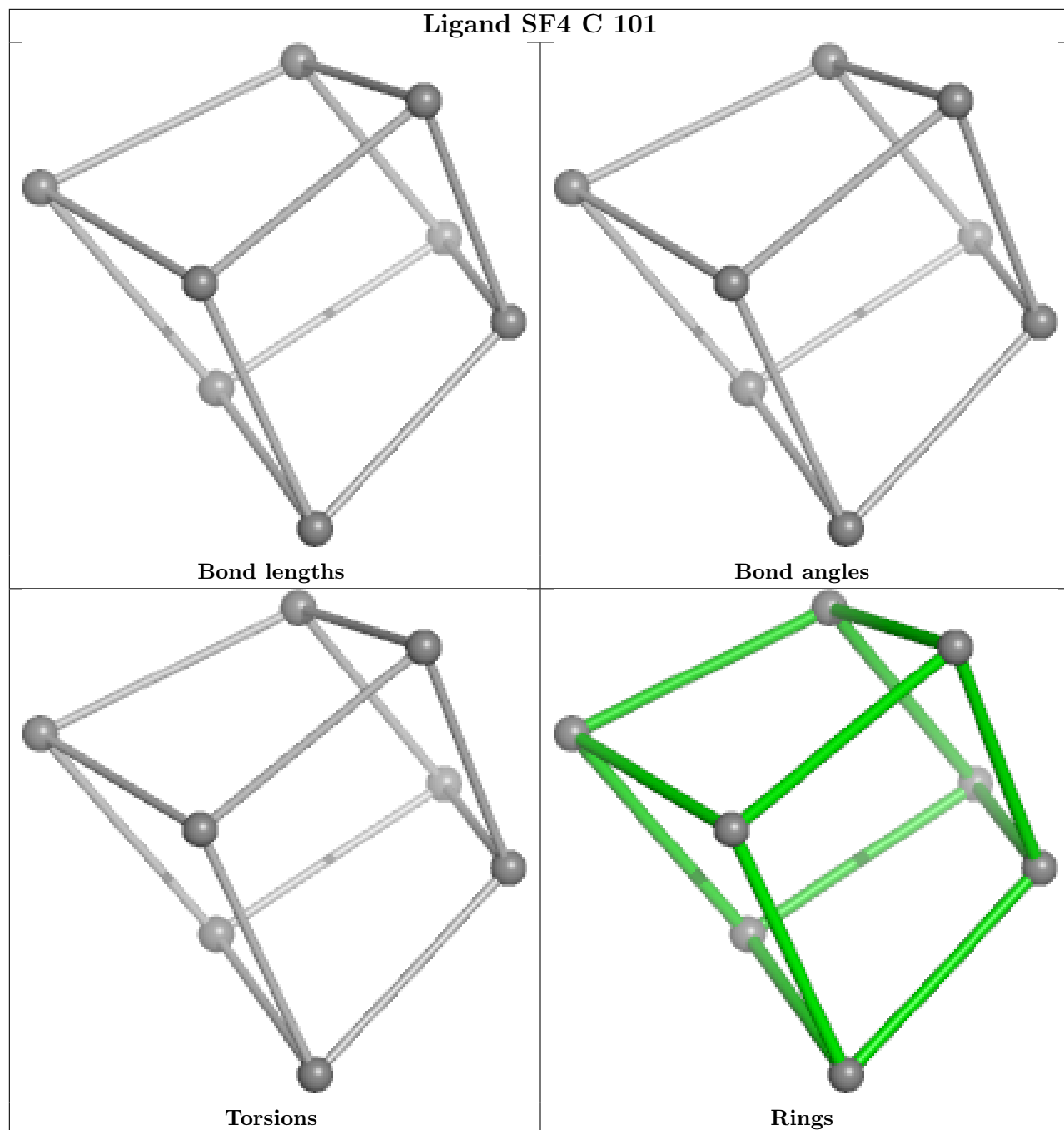


## Ligand CLA A 820



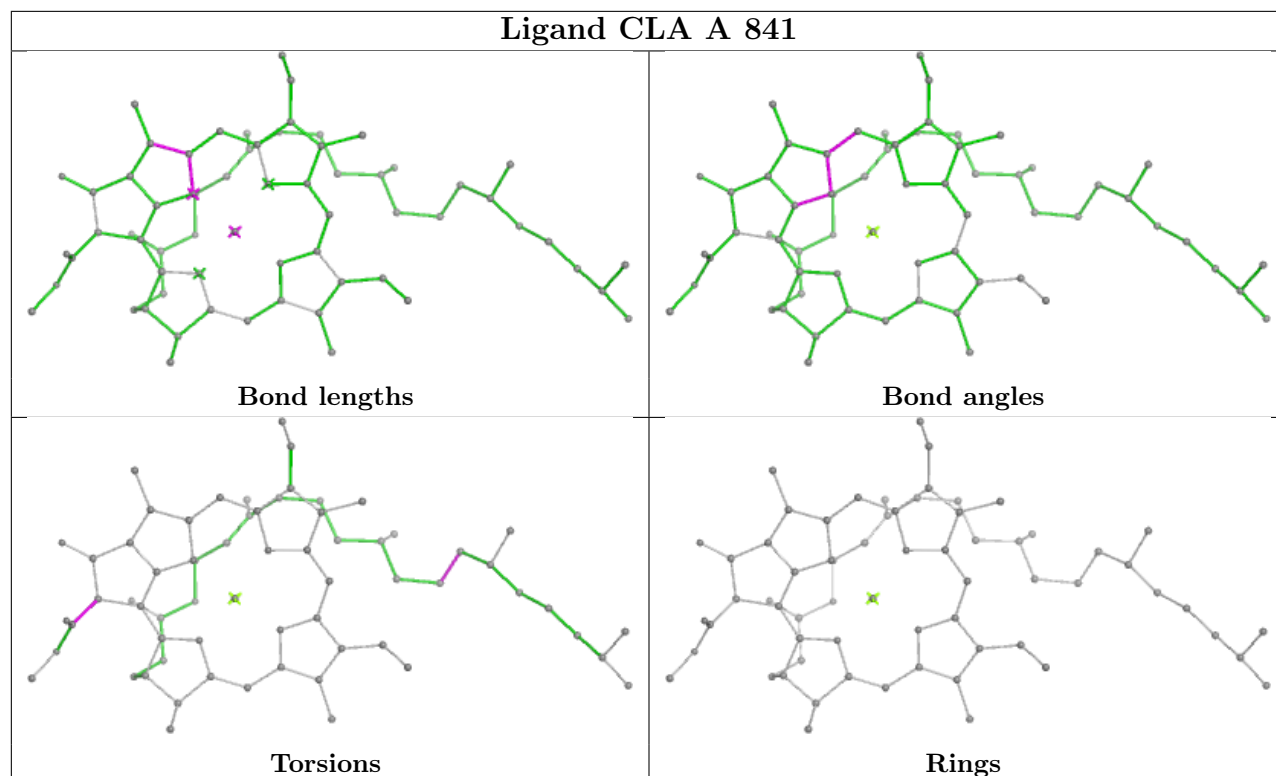
## Ligand CLA B 822



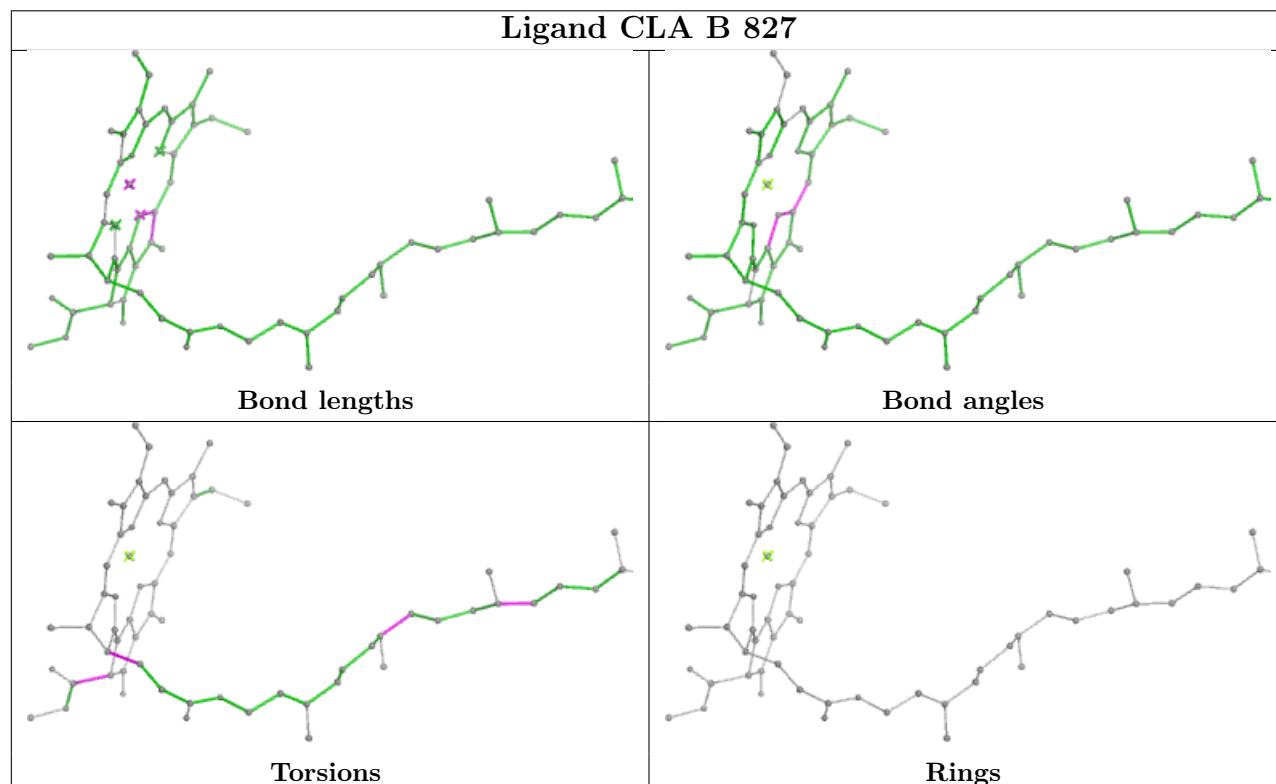


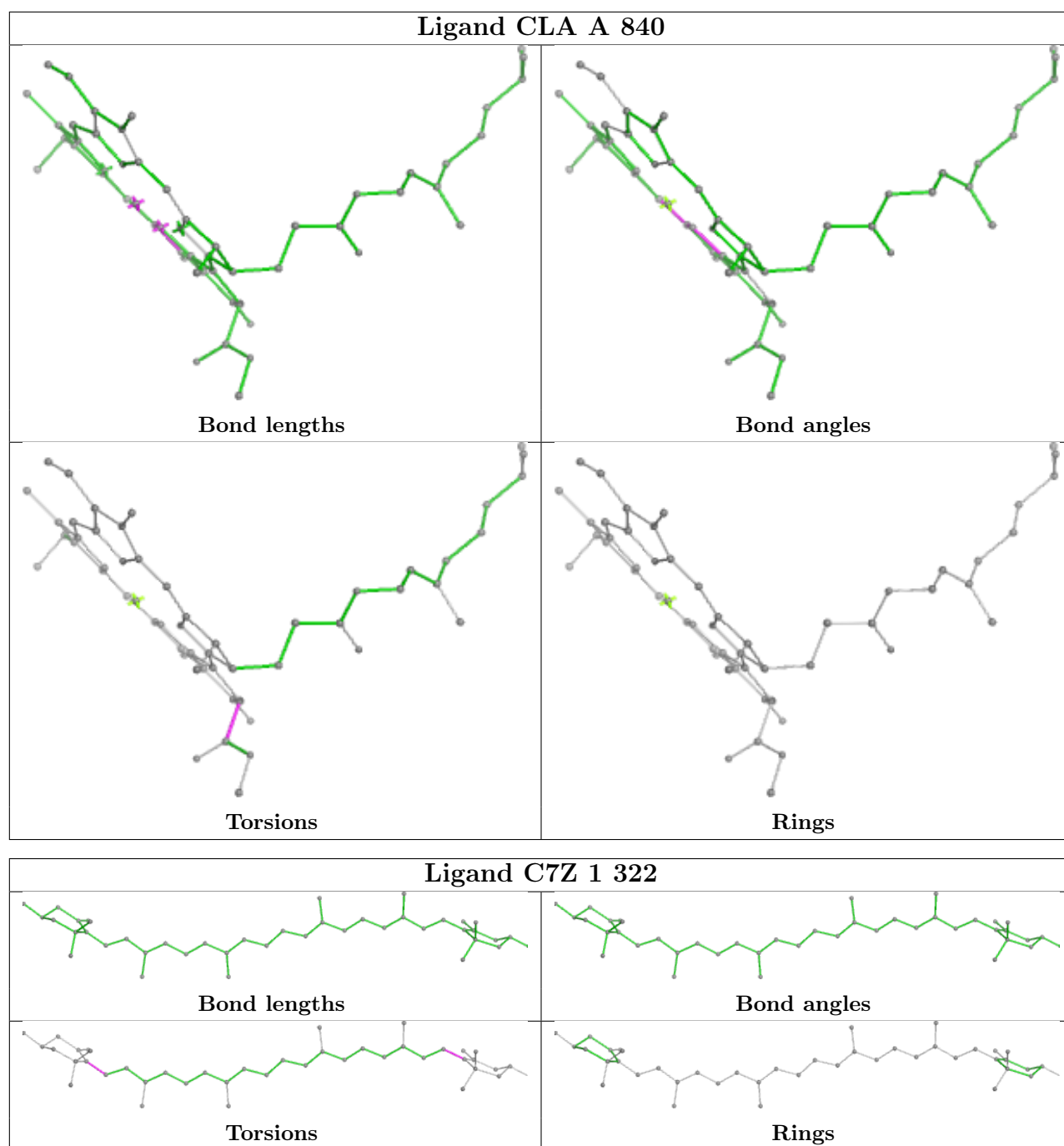


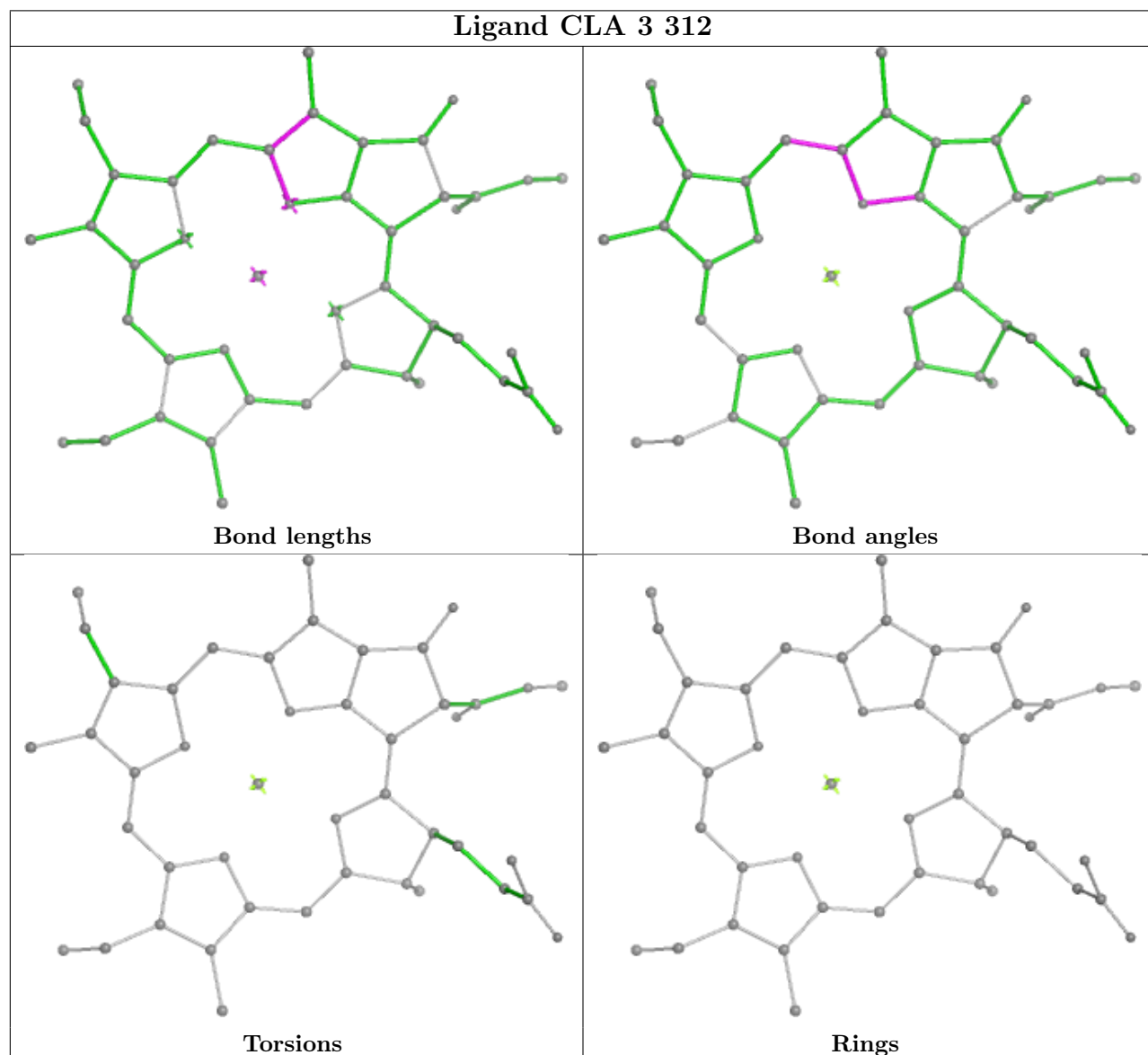
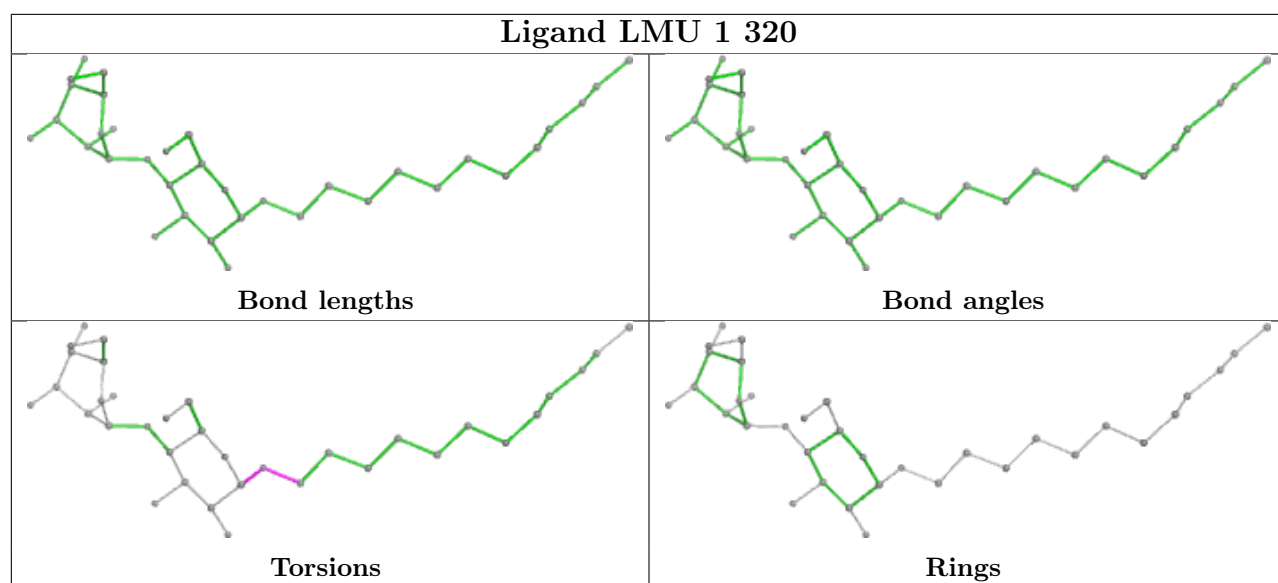
## Ligand CLA A 841

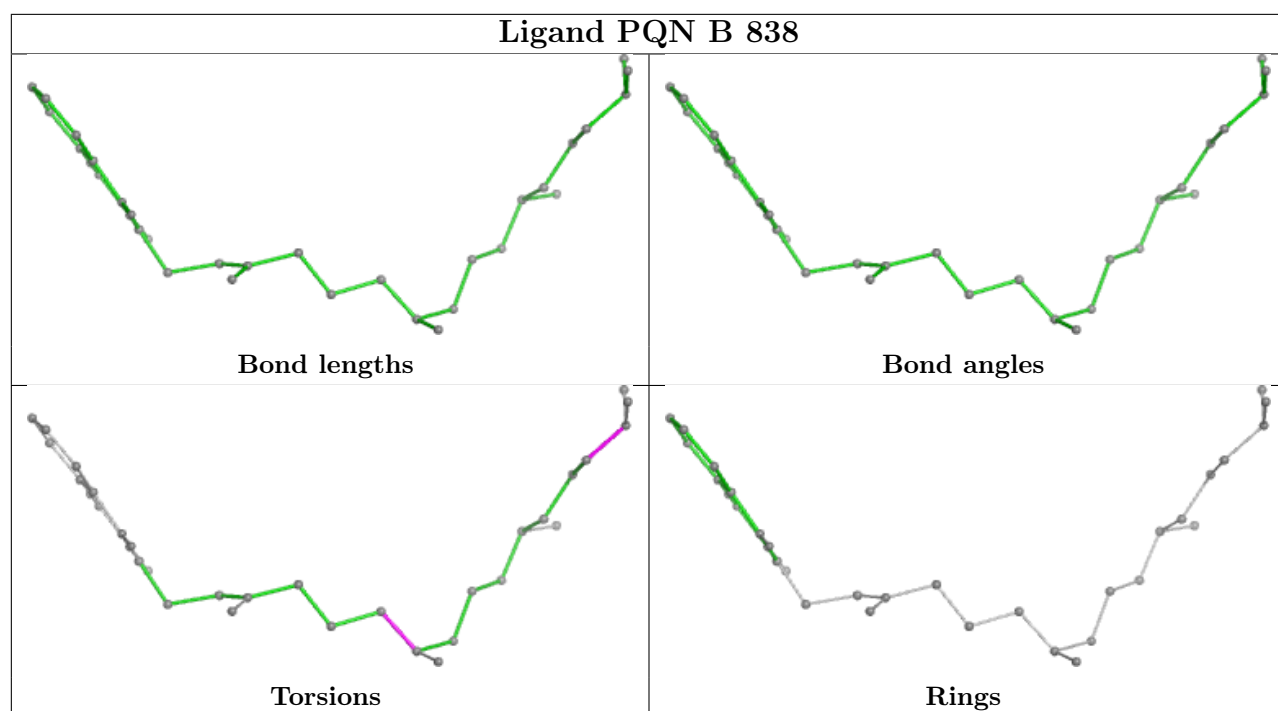


## Ligand CLA B 827

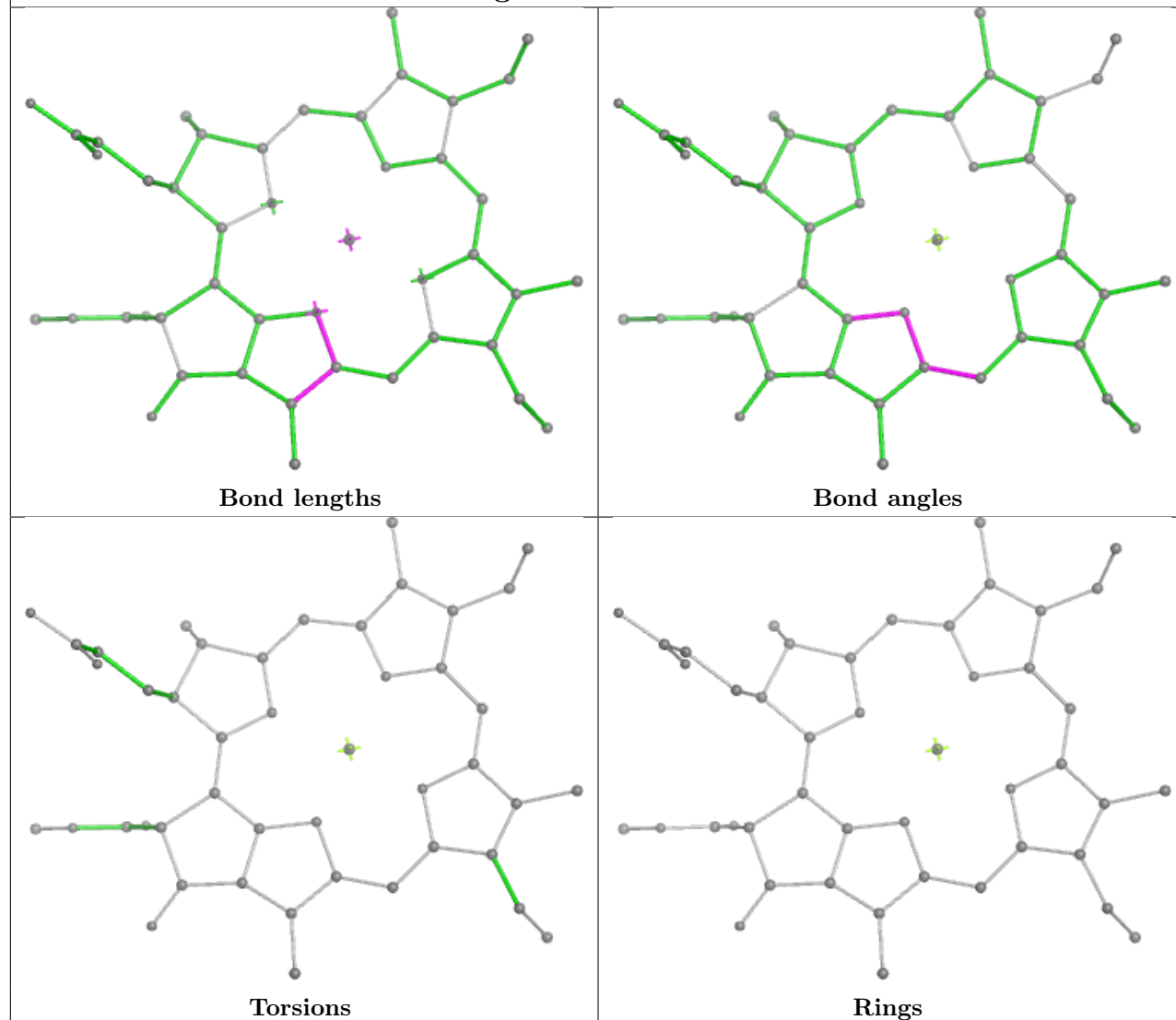




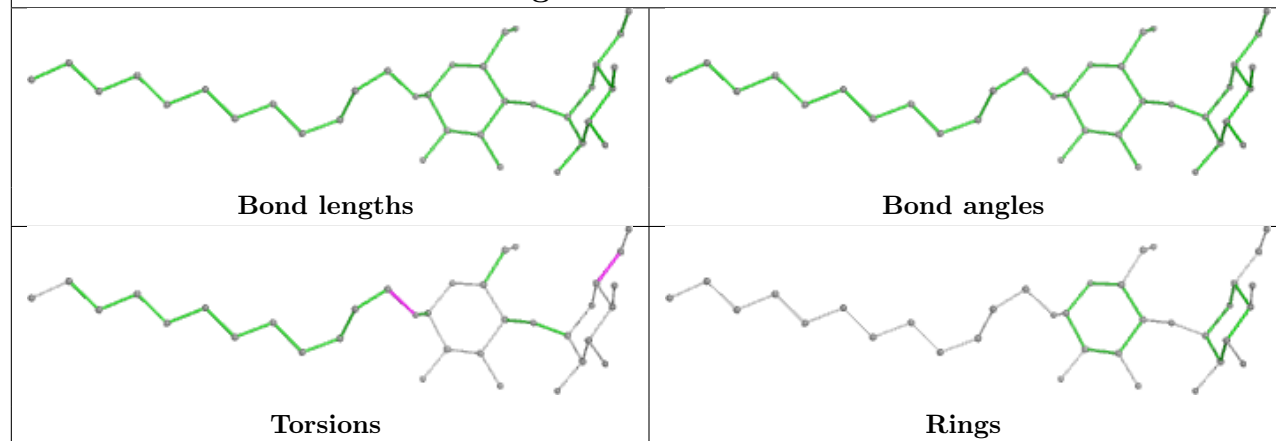


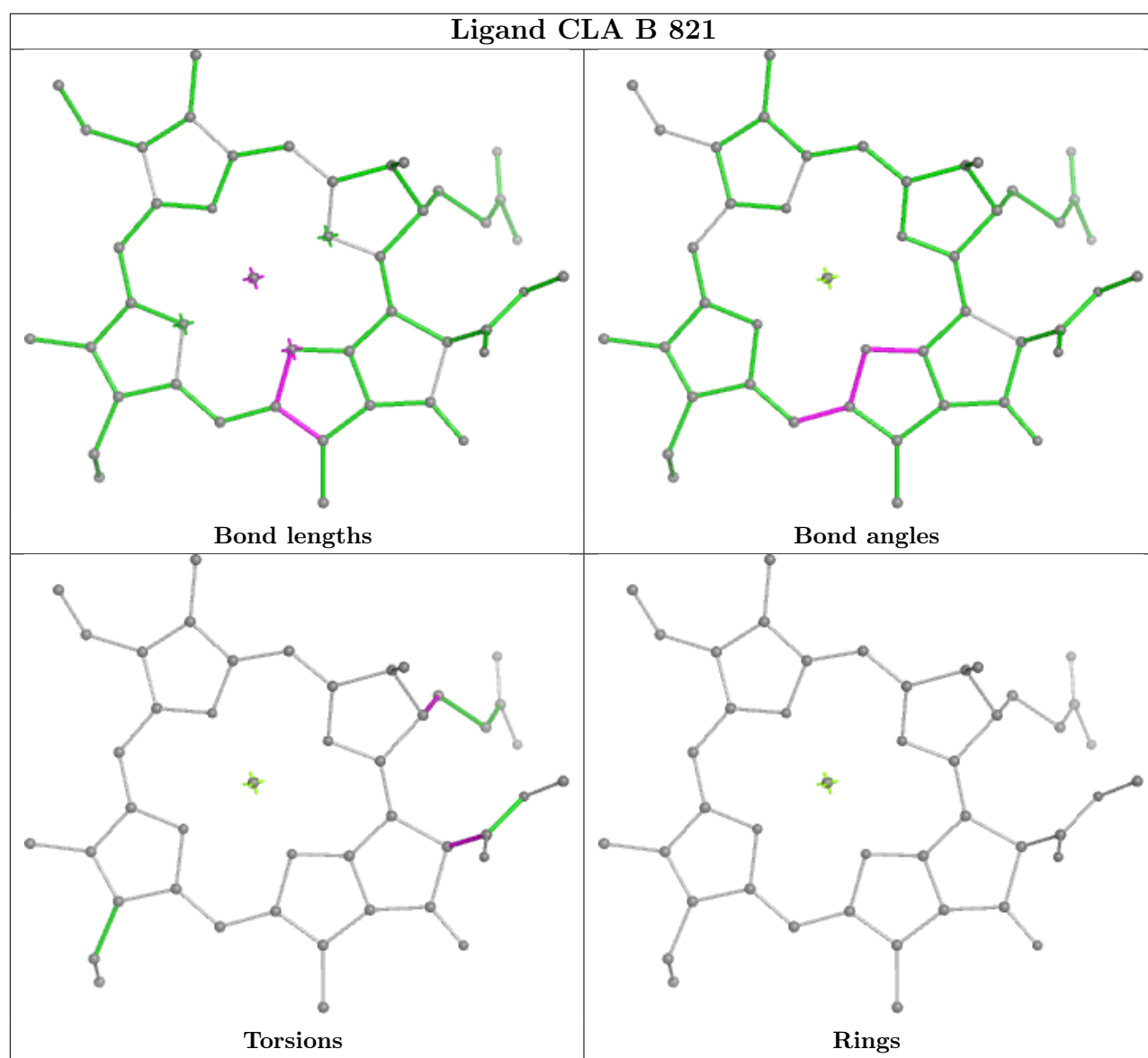
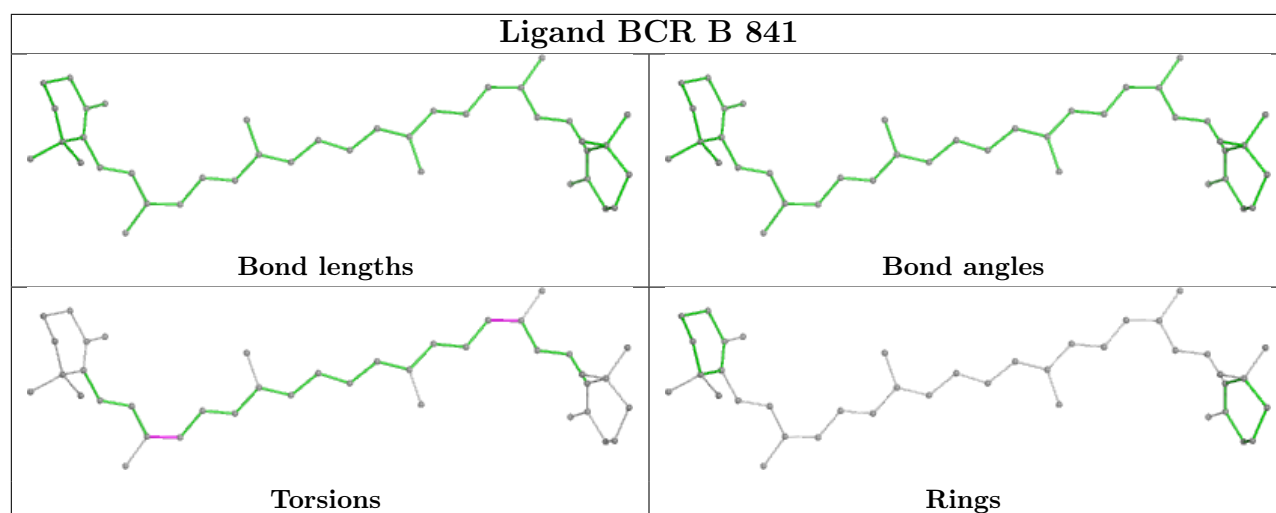


## Ligand CLA 1 306

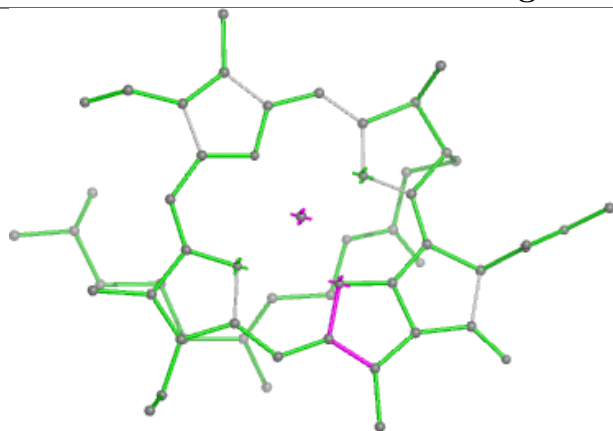


## Ligand LMU 2 618

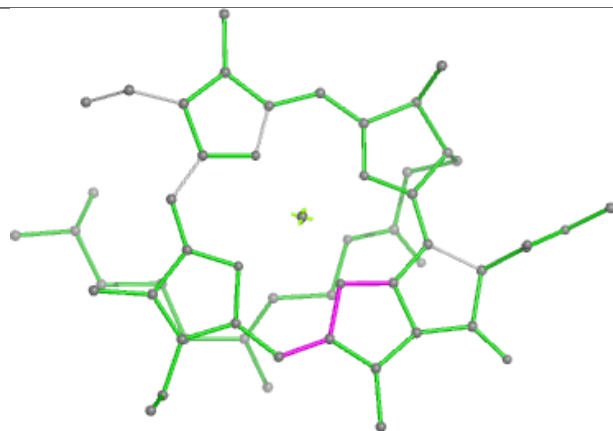




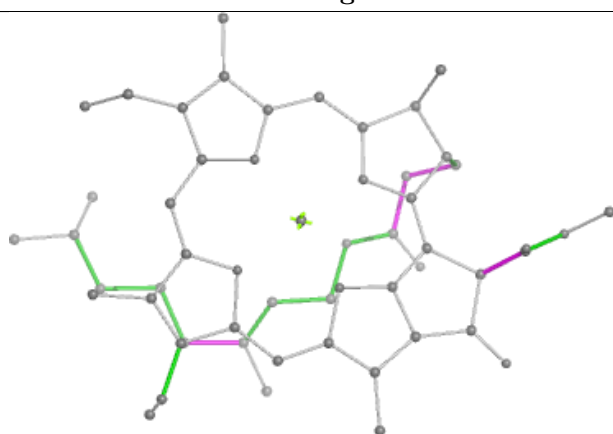
## Ligand CLA 3 310



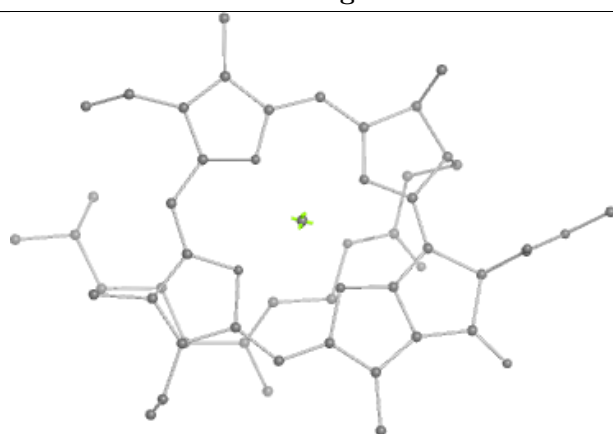
Bond lengths



Bond angles

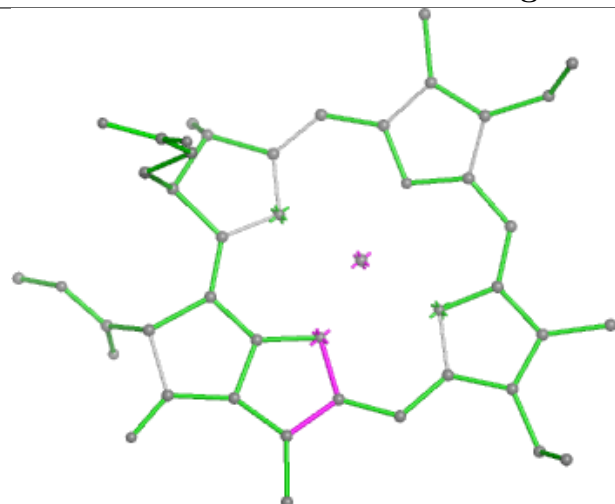


Torsions

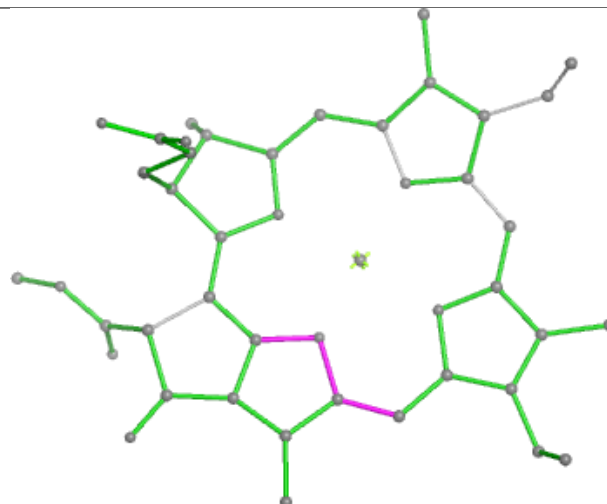


Rings

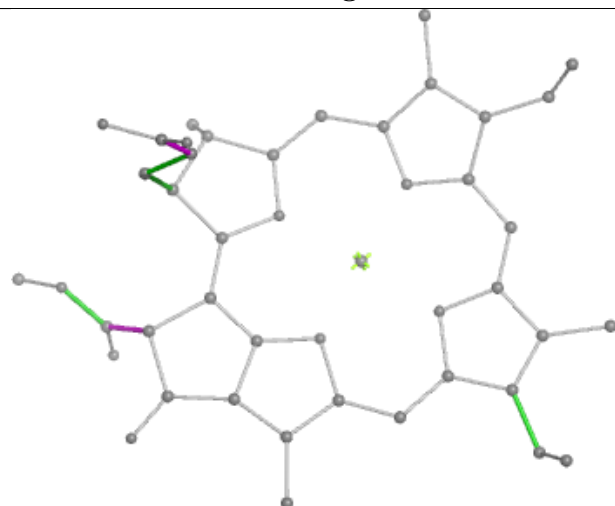
## Ligand CLA 4 610



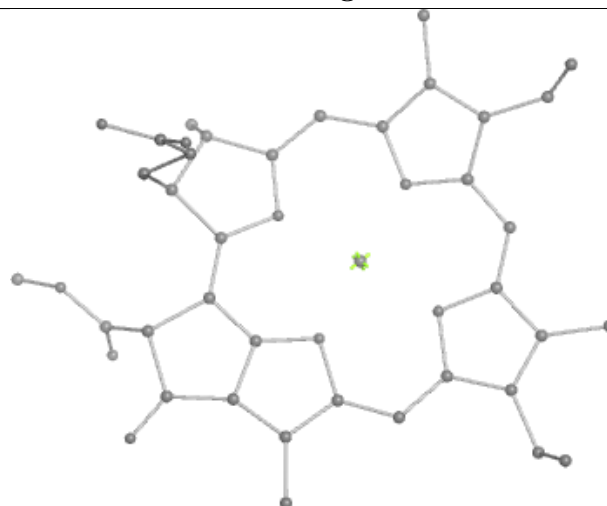
Bond lengths



Bond angles



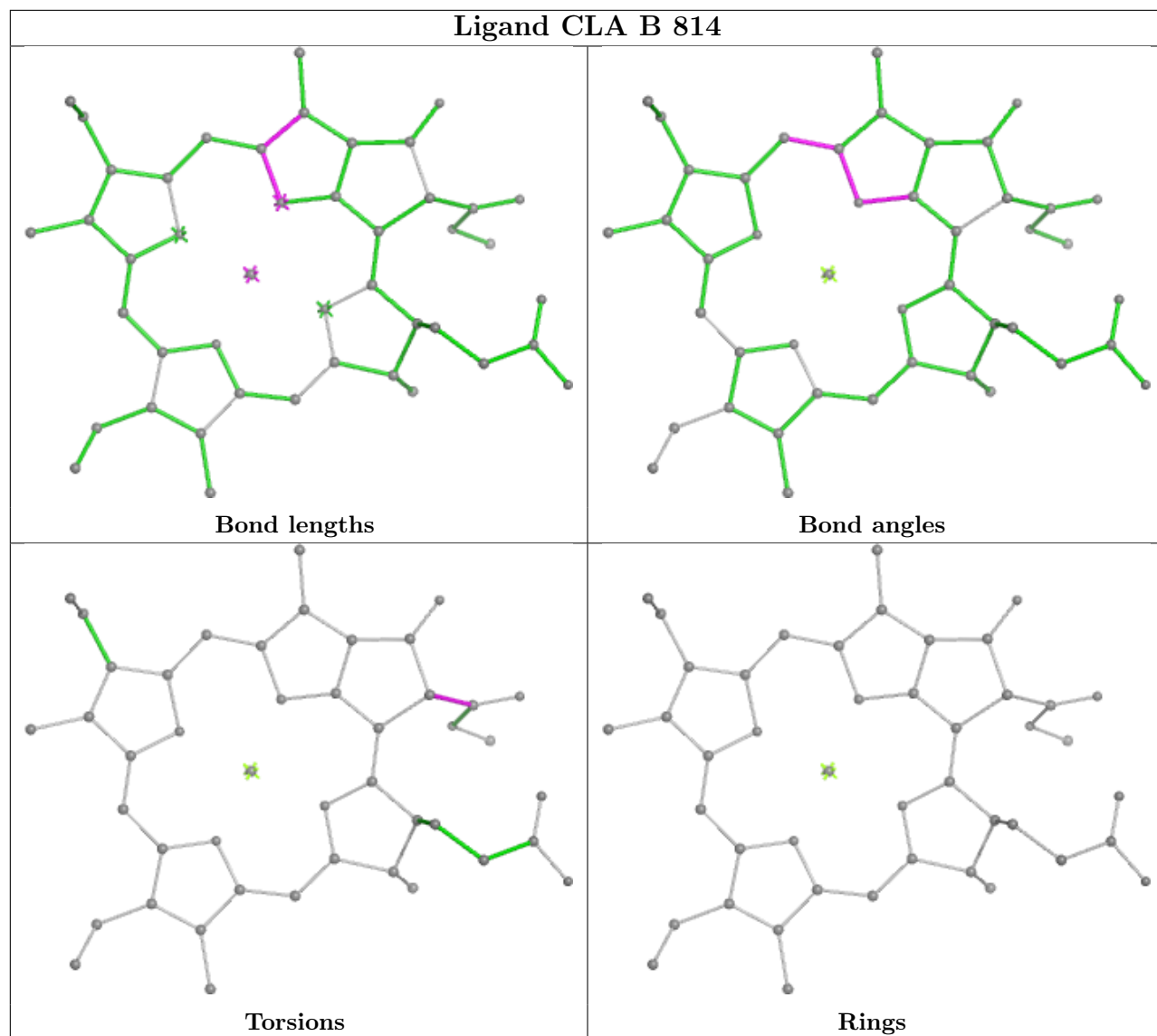
Torsions



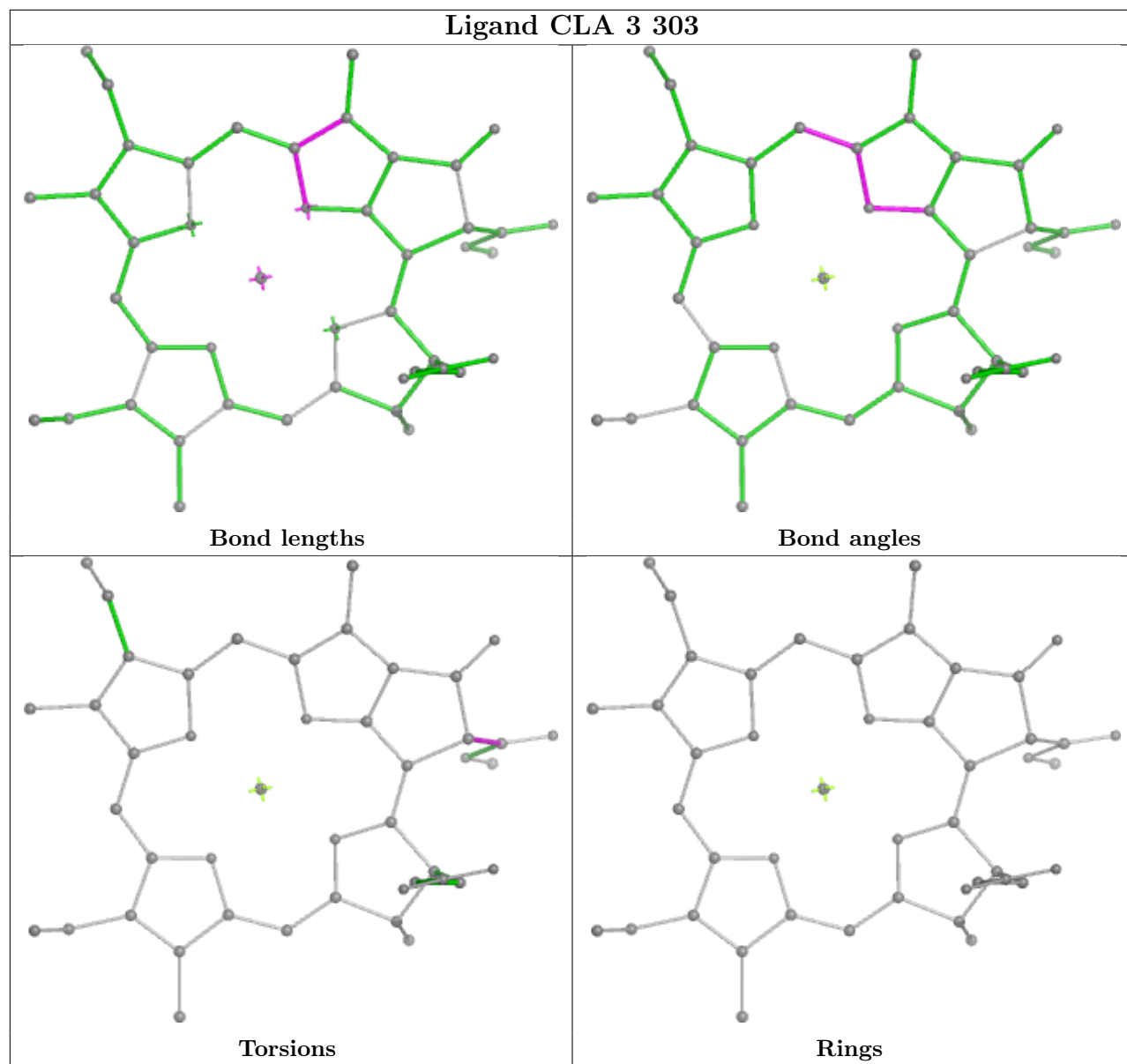
Rings

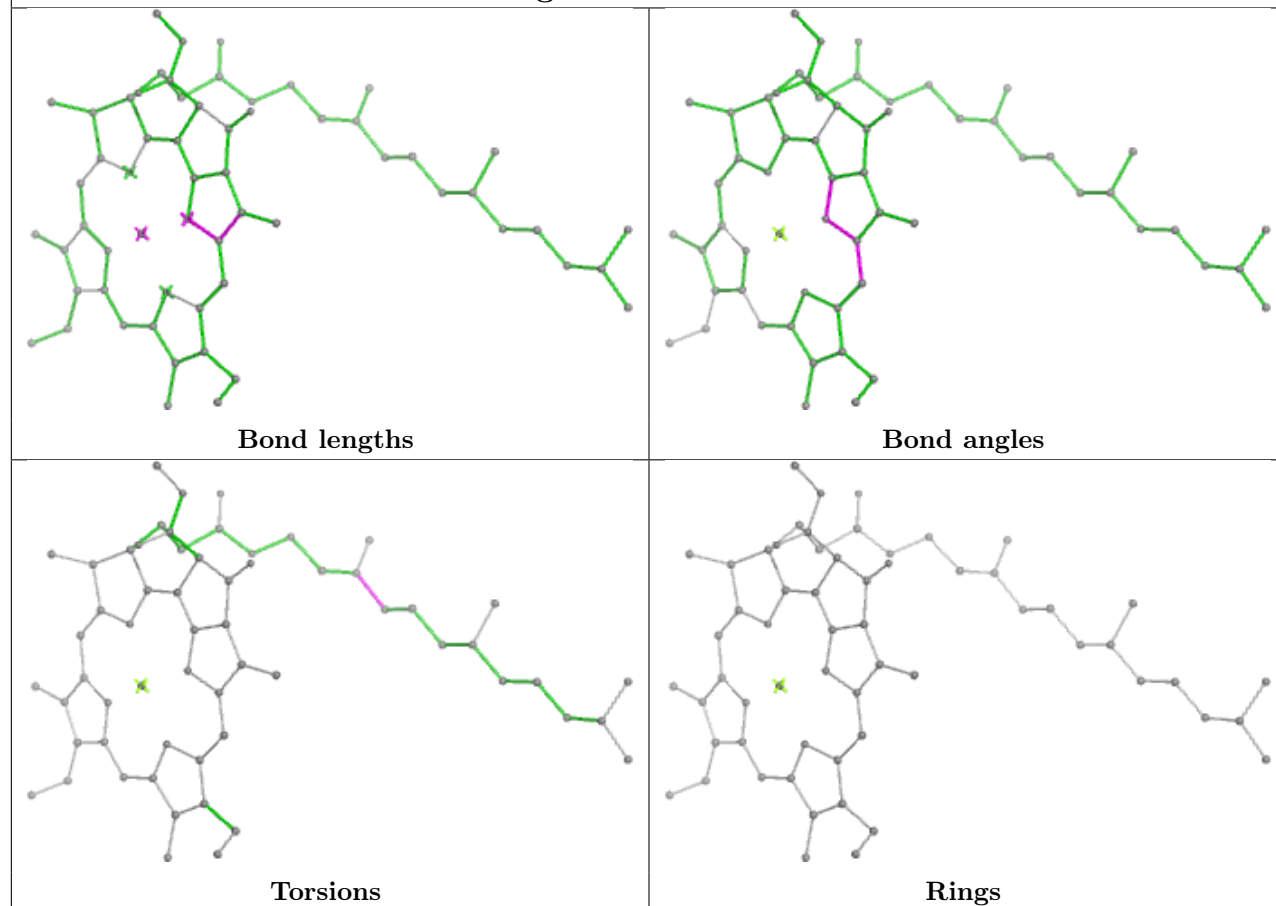
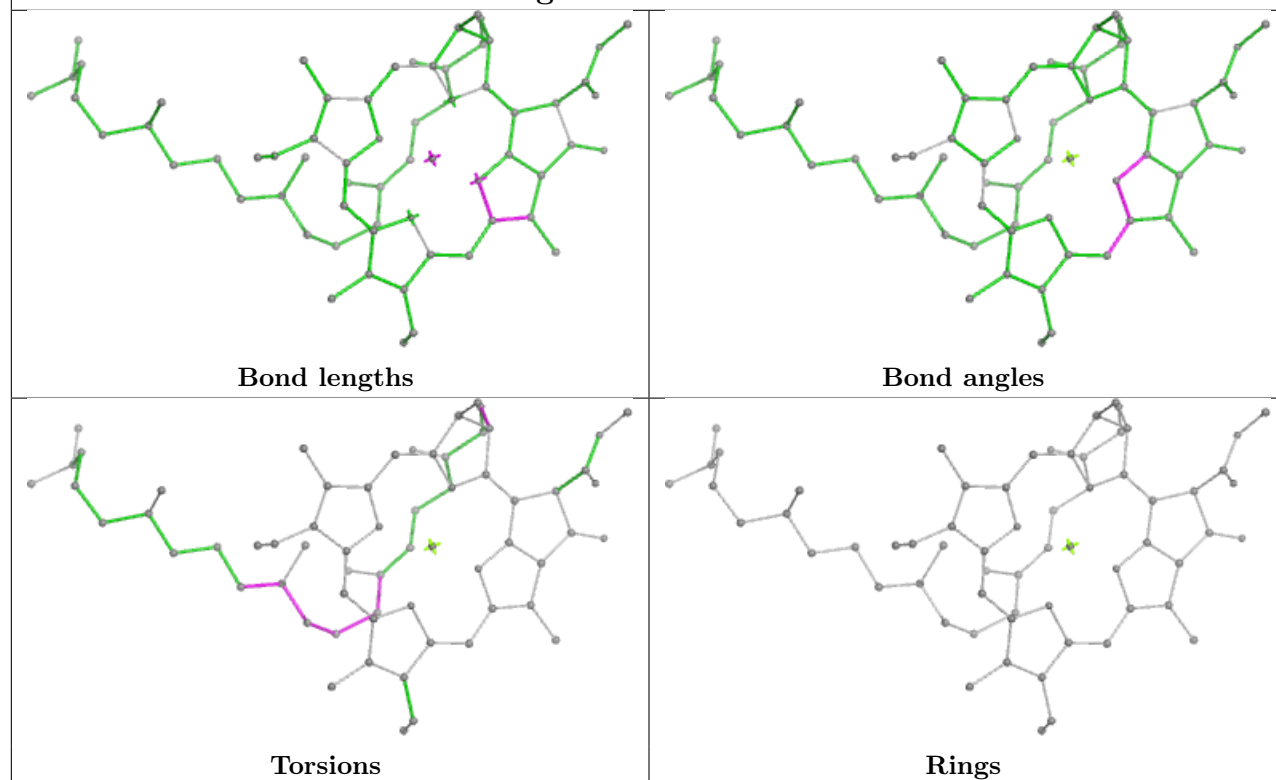


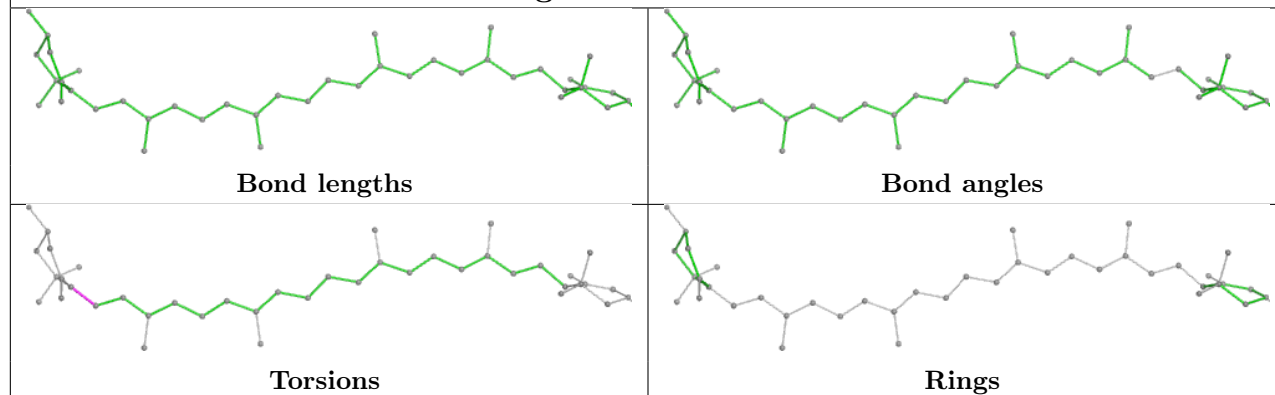
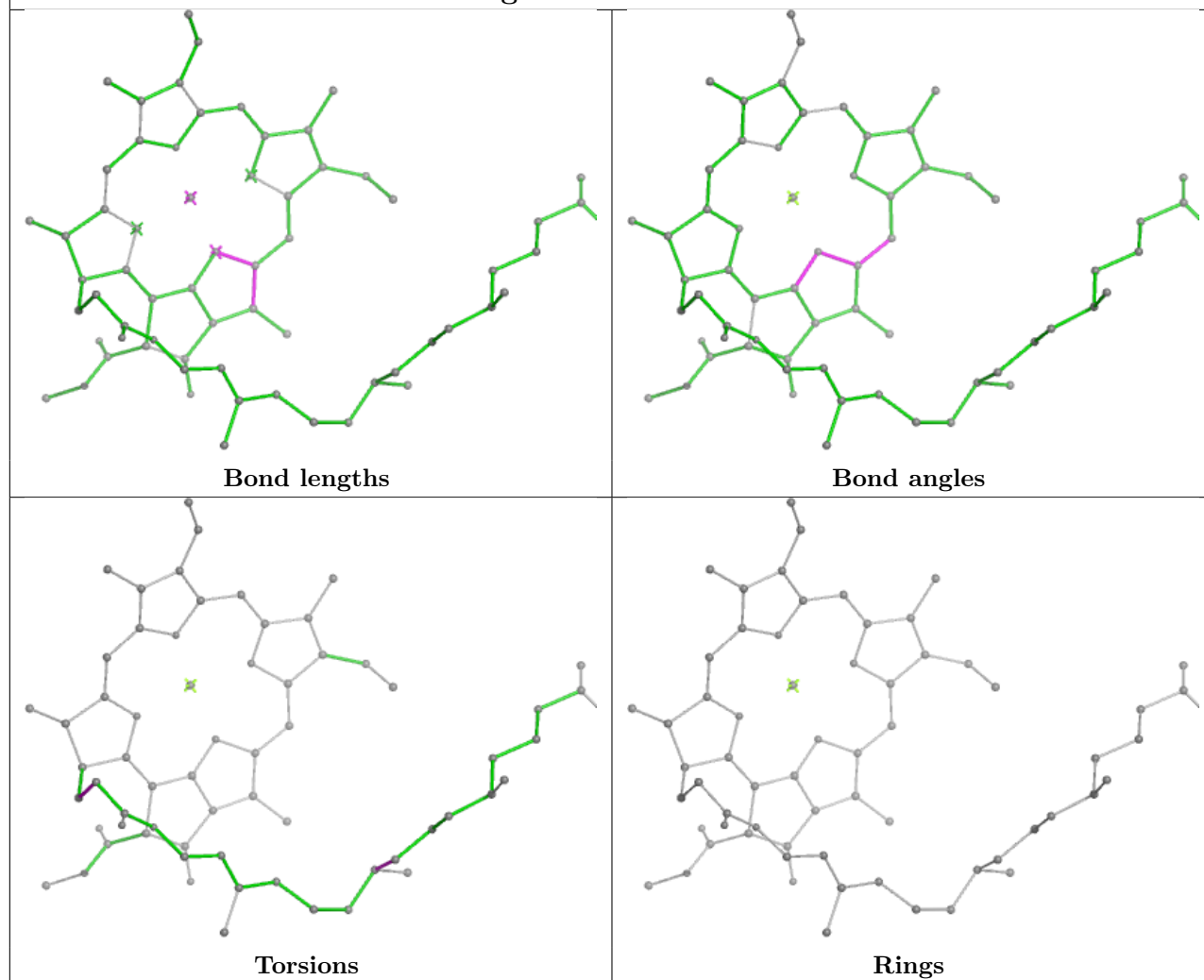
## Ligand CLA B 814

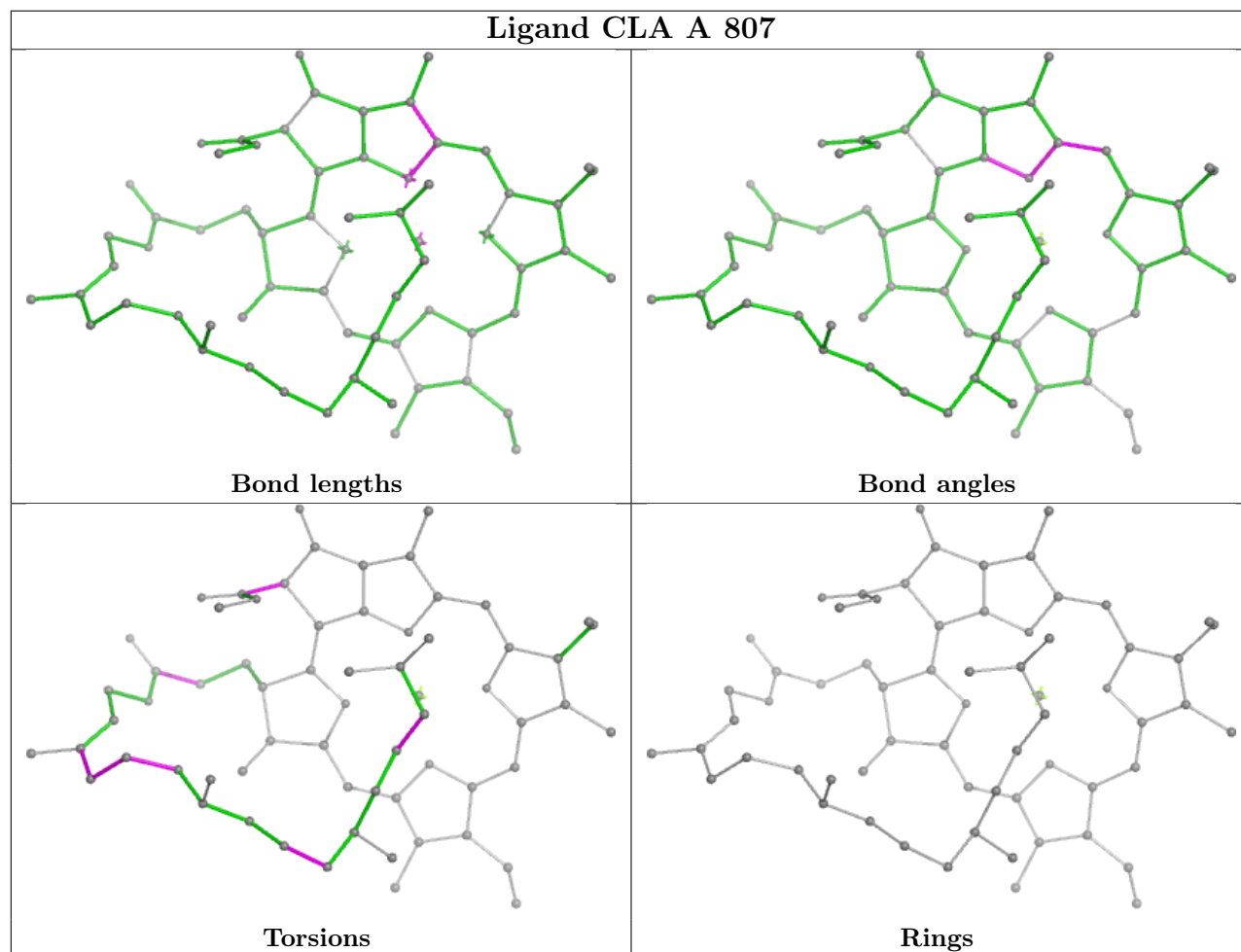
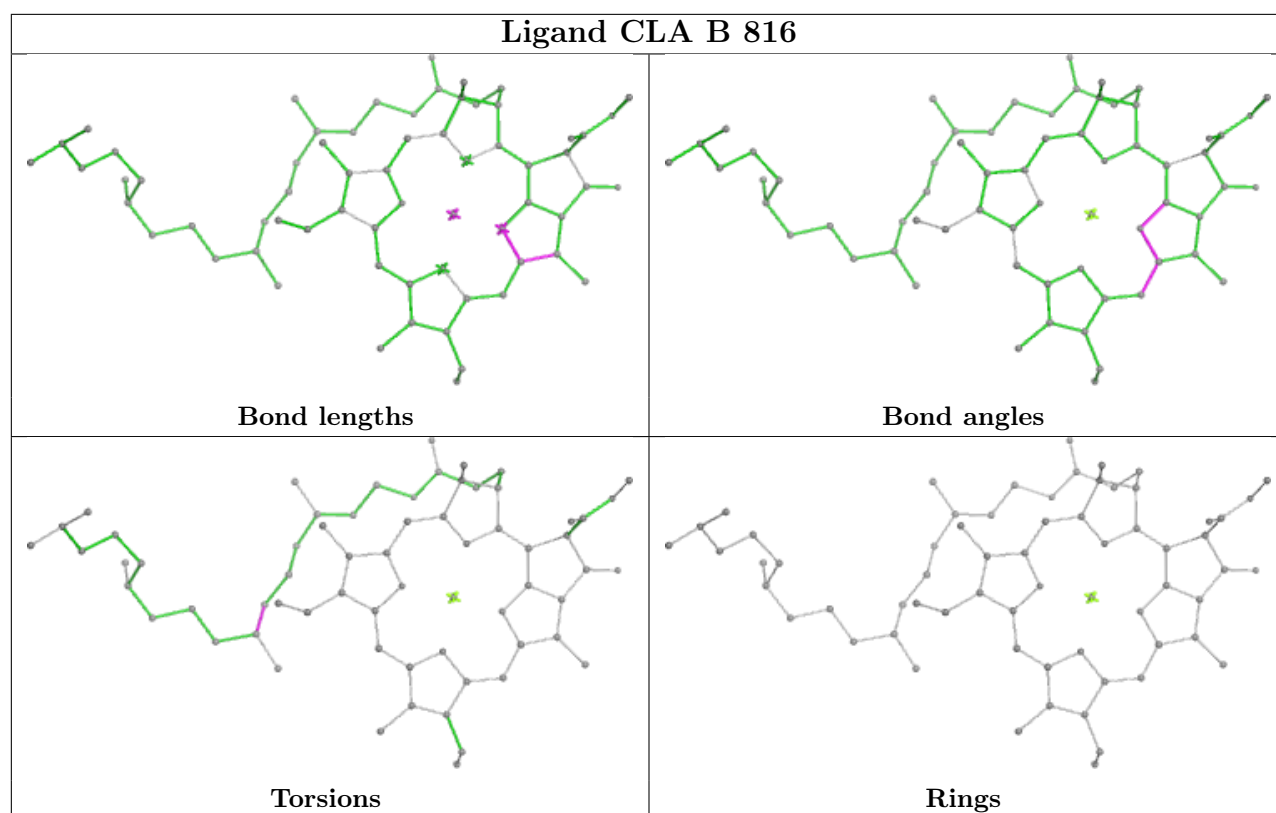


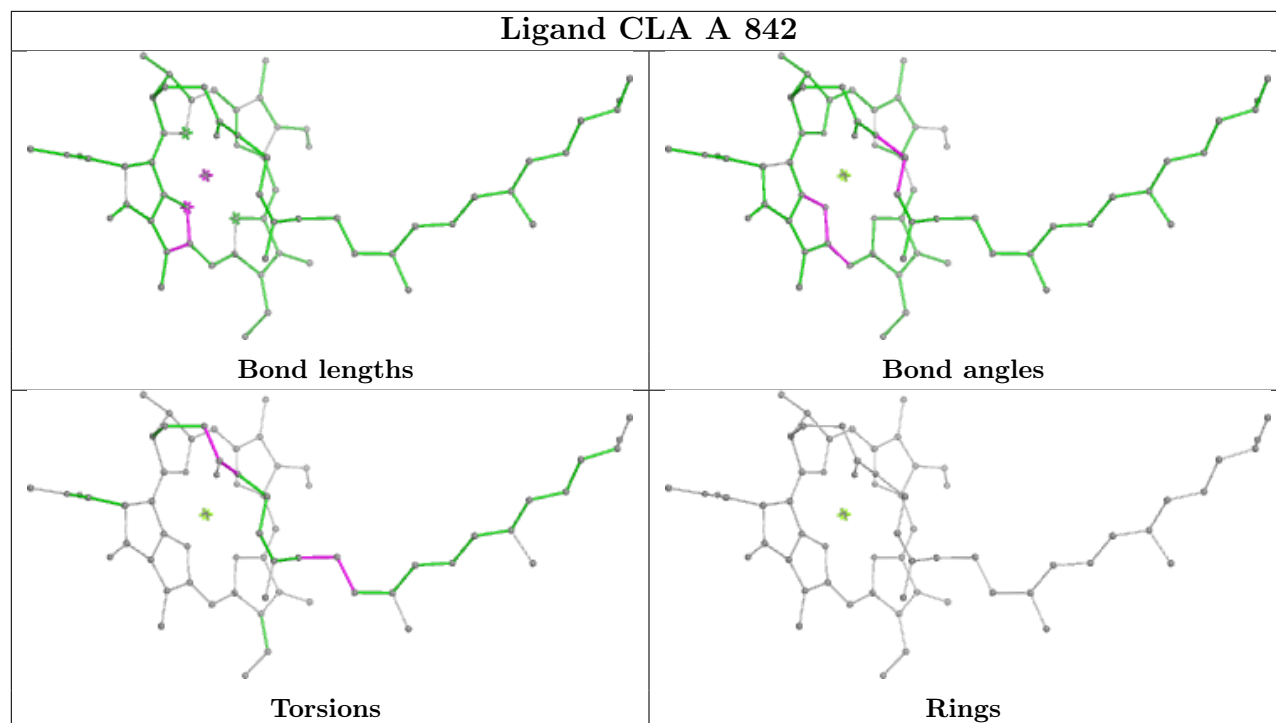
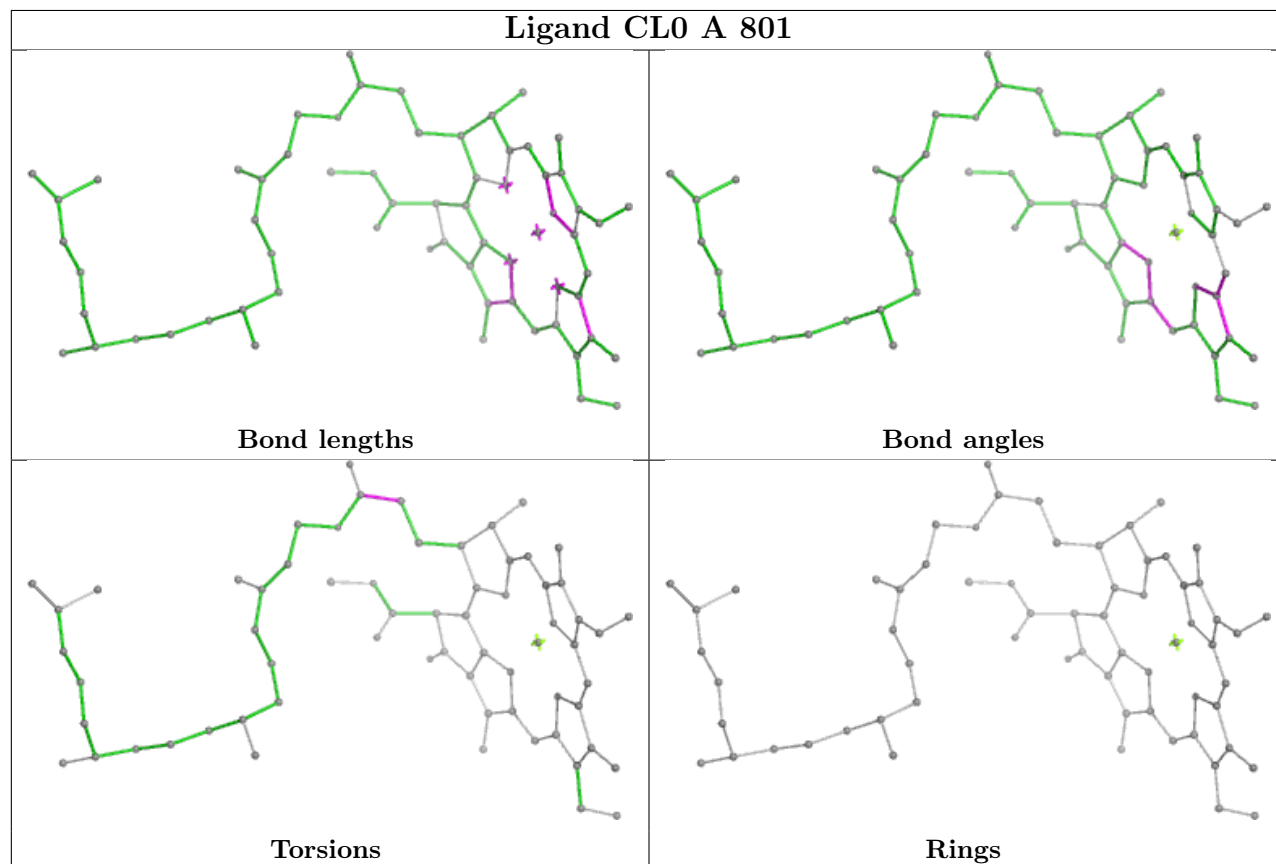
## Ligand CLA 3 303



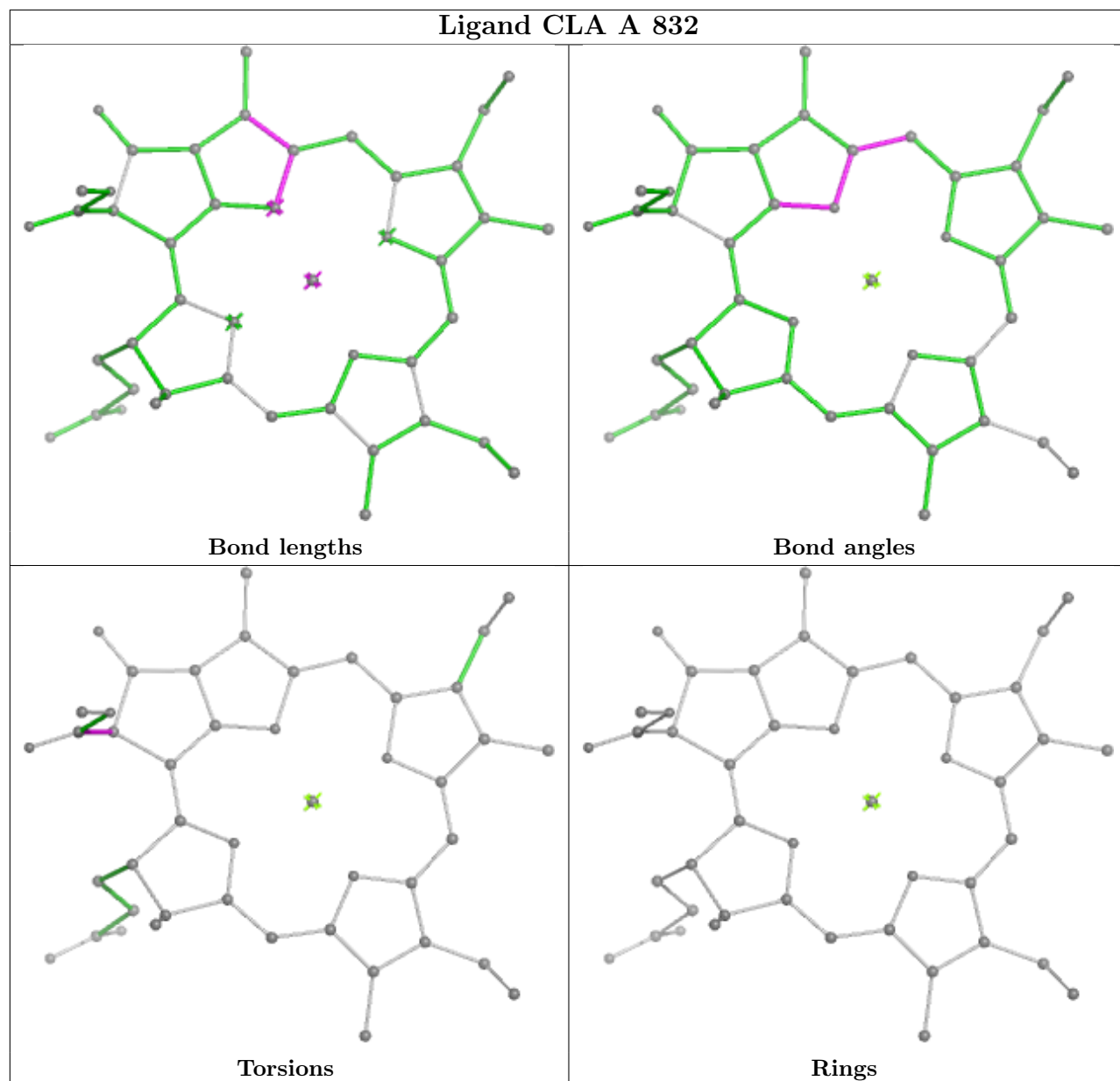
**Ligand CLA 2 610****Ligand CLA 1 313**

**Ligand LUT 1 318****Ligand CLA A 830**

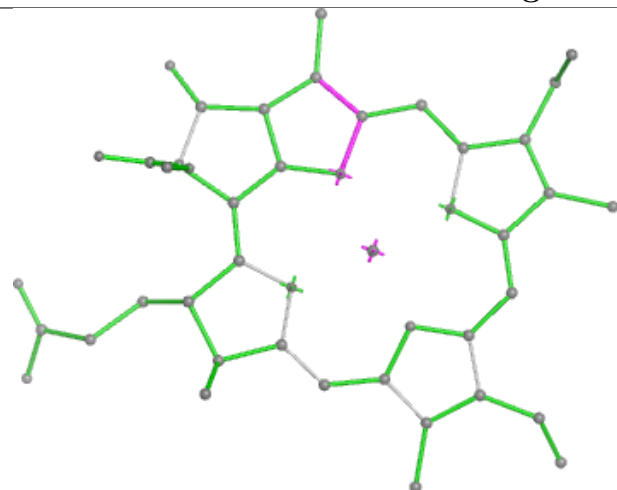


**Ligand CLA A 842****Ligand CL0 A 801**

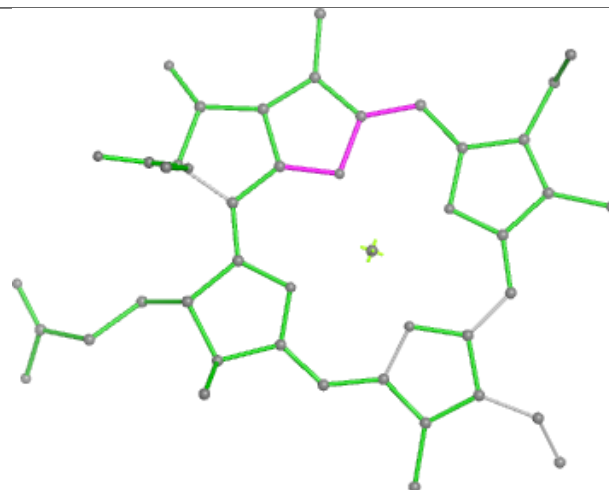
## Ligand CLA A 832



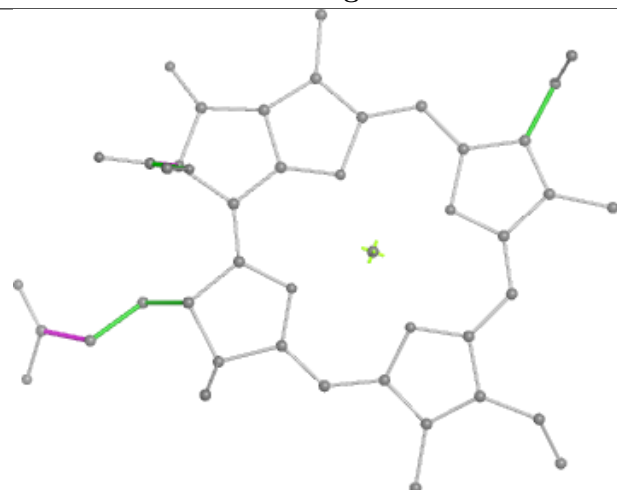
## Ligand CLA 3 304



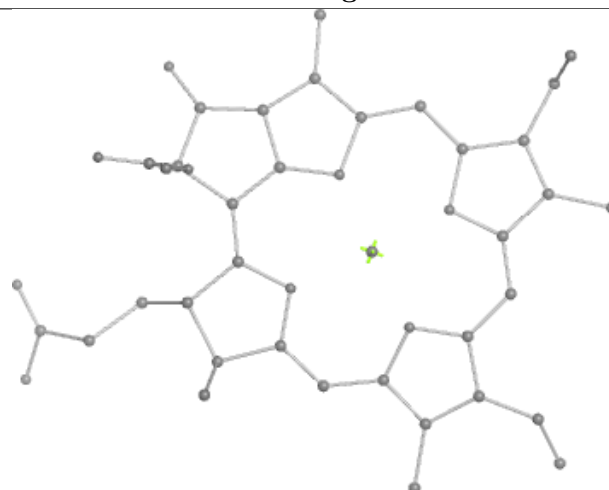
Bond lengths



Bond angles

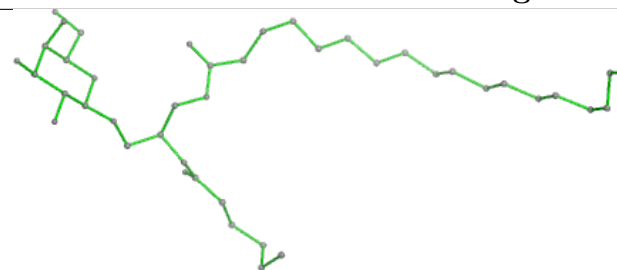


Torsions

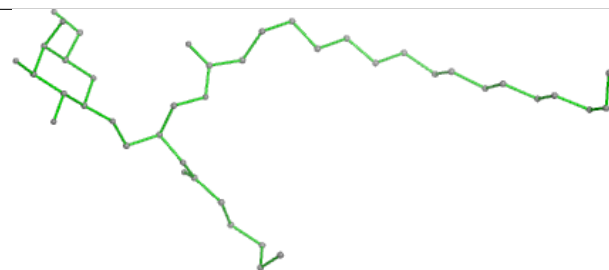


Rings

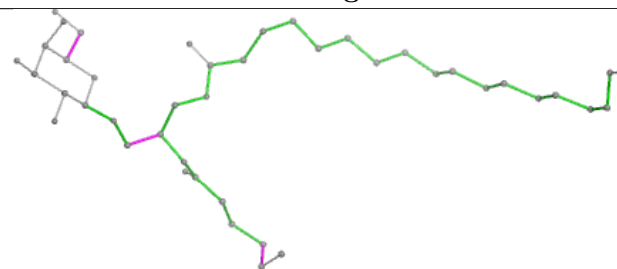
## Ligand LMG A 857



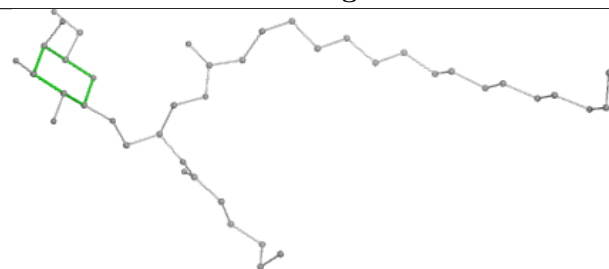
Bond lengths



Bond angles



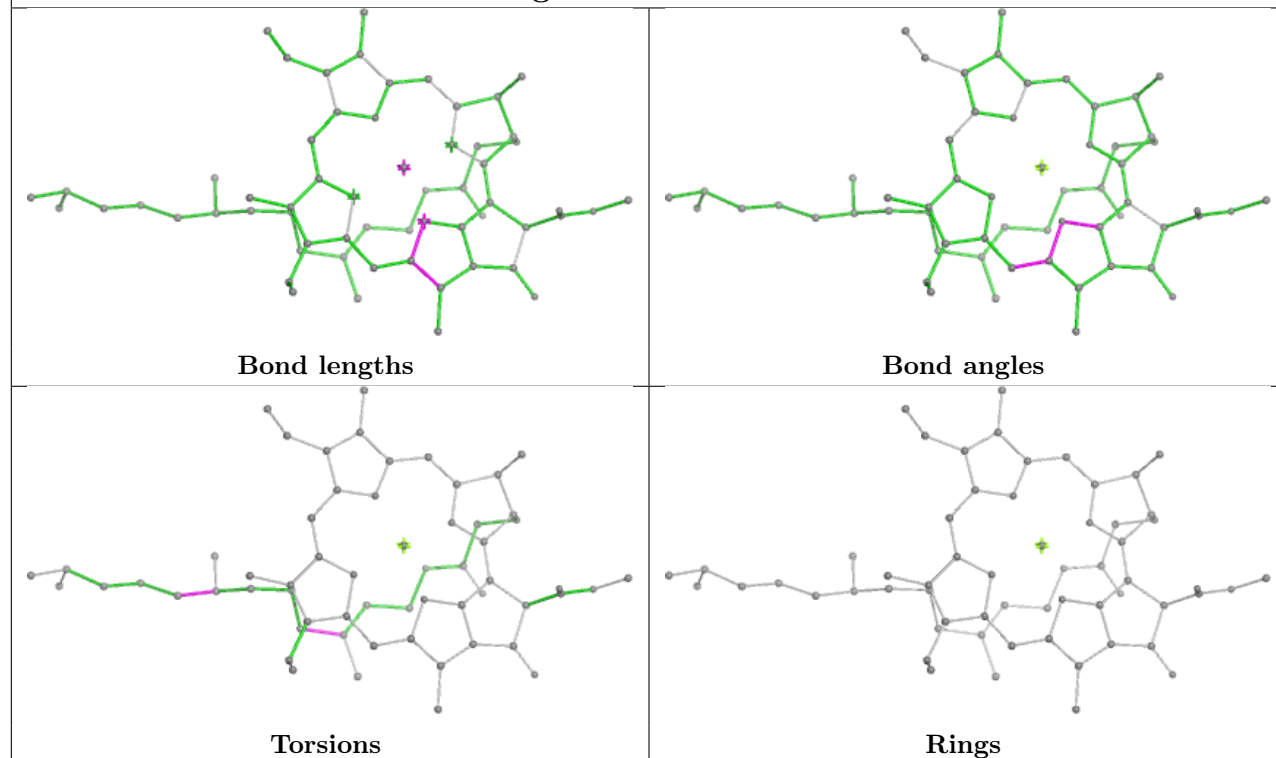
Torsions



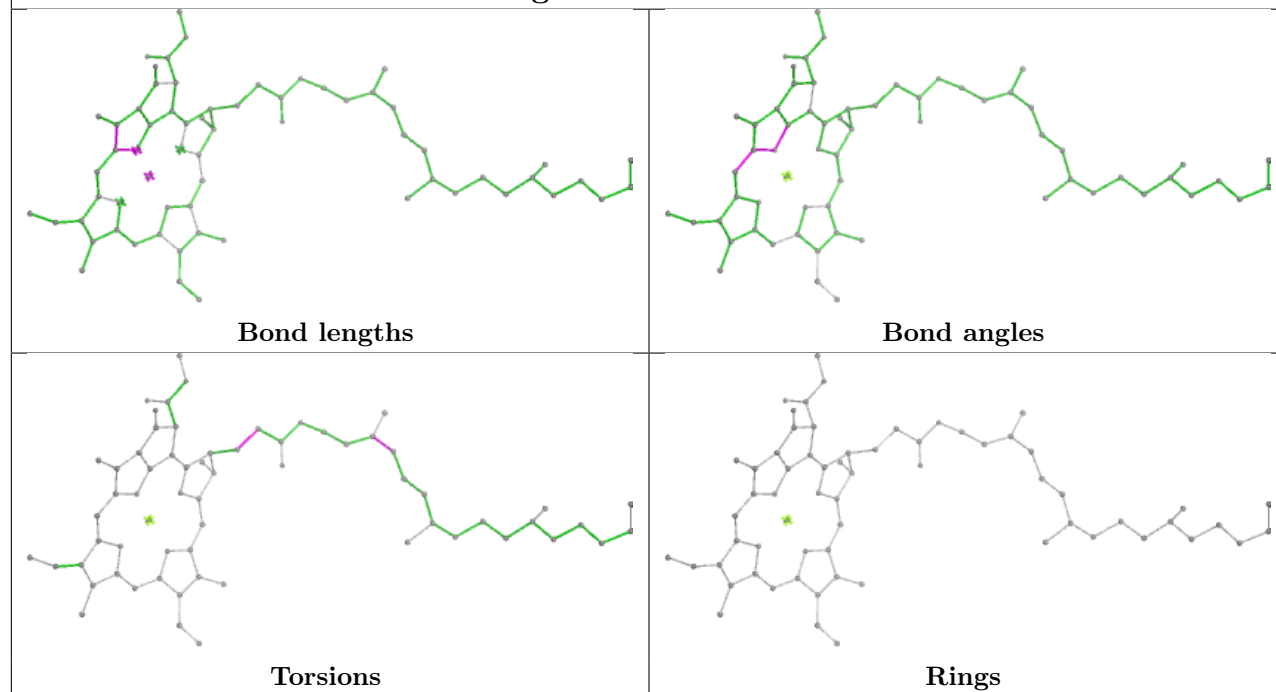
Rings

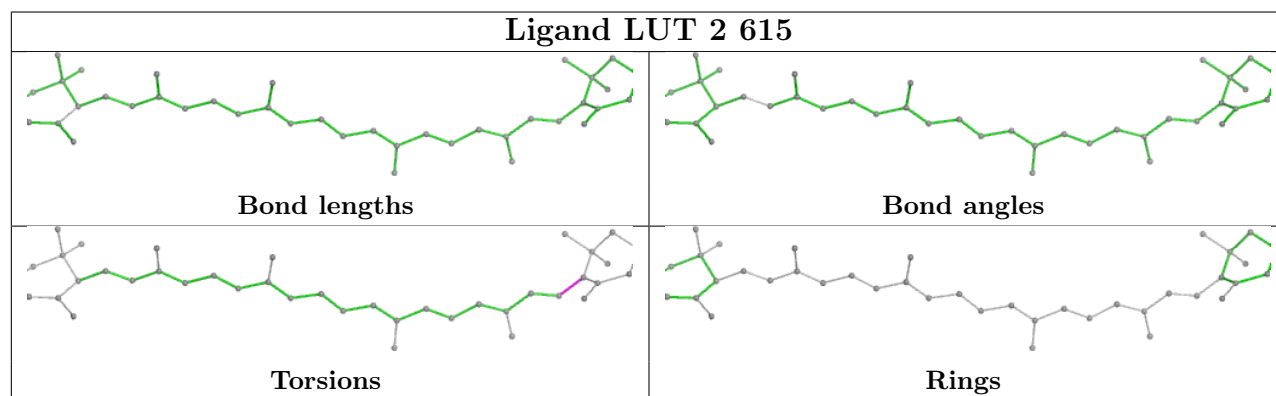
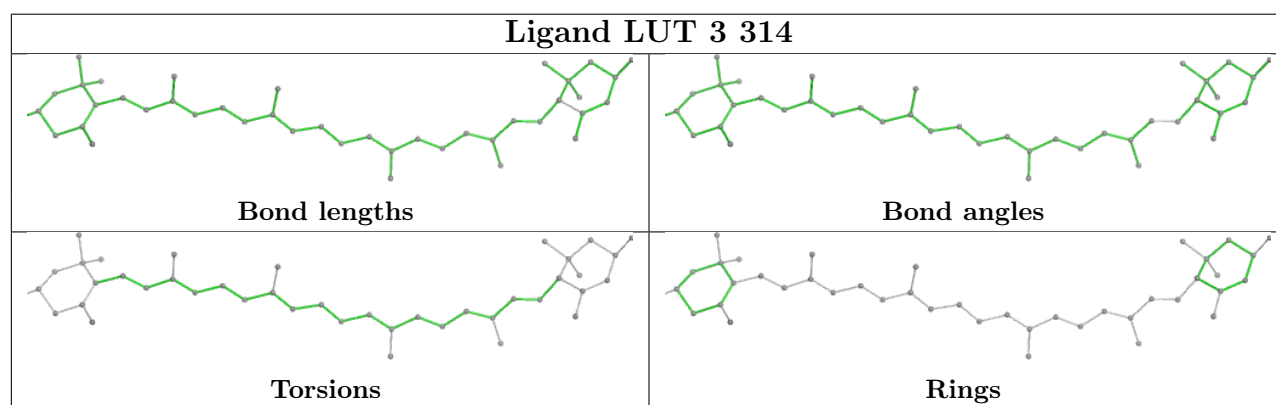
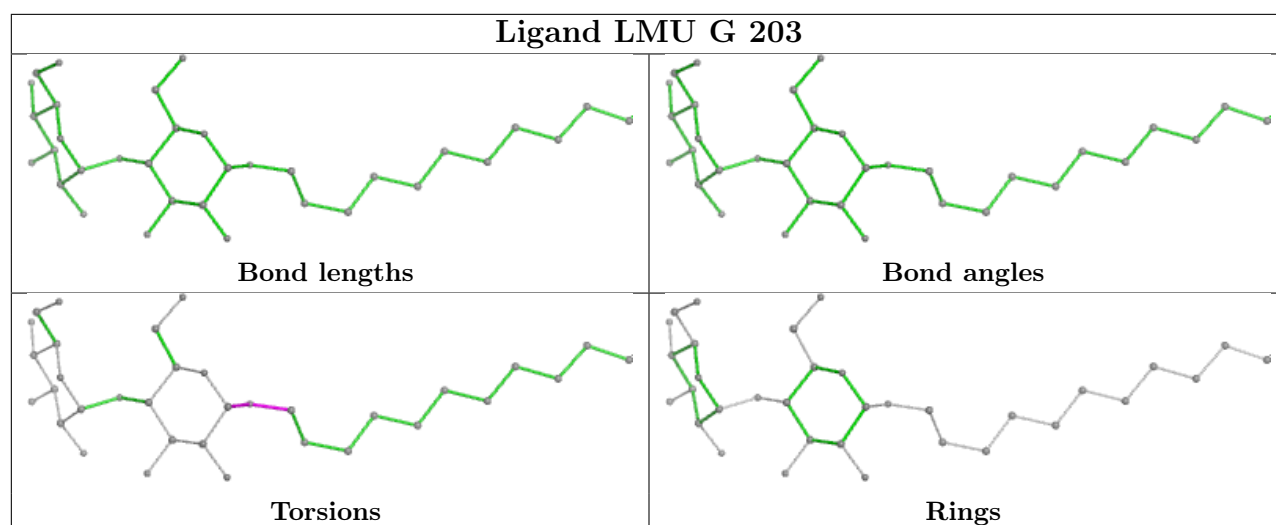


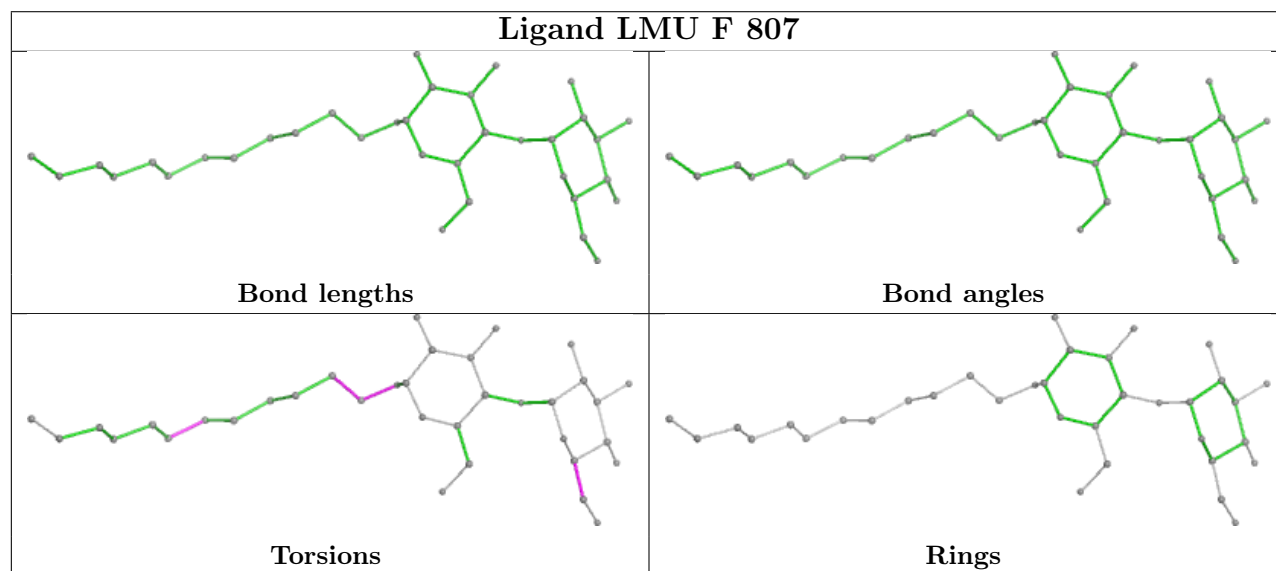
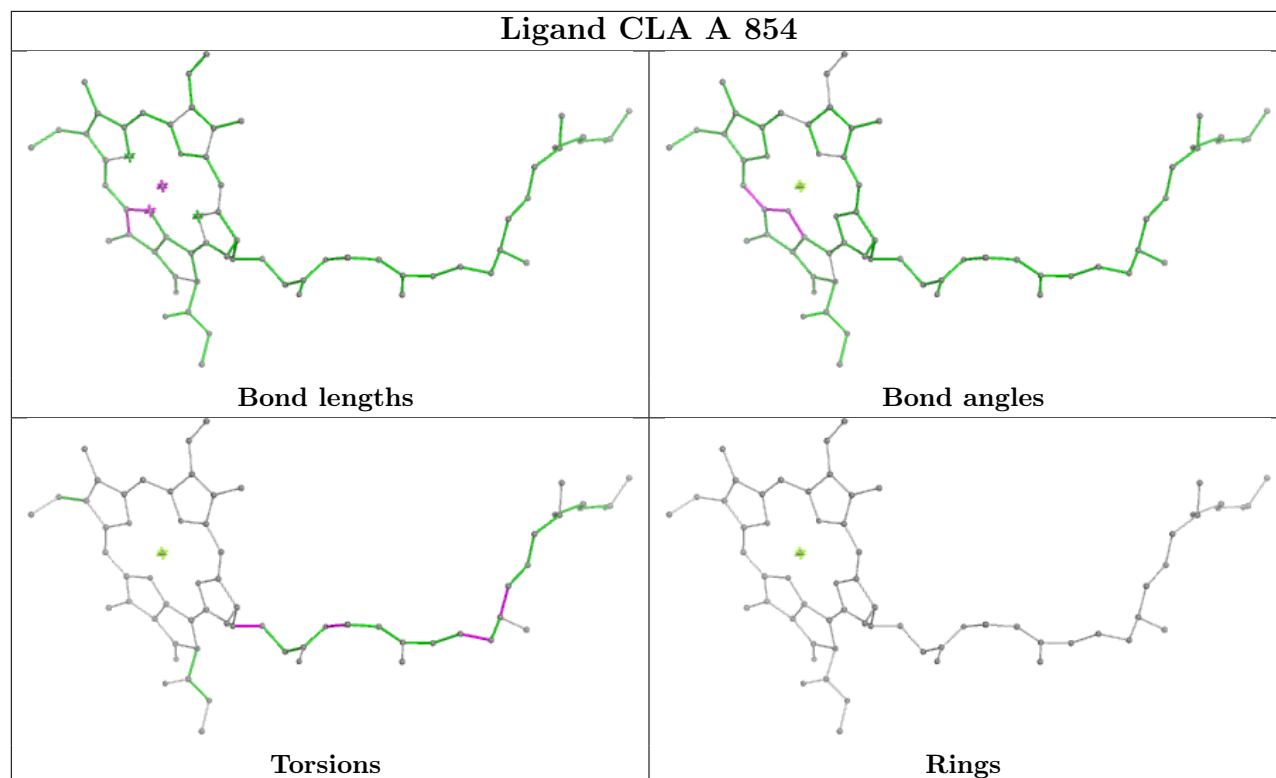
## Ligand CLA B 806

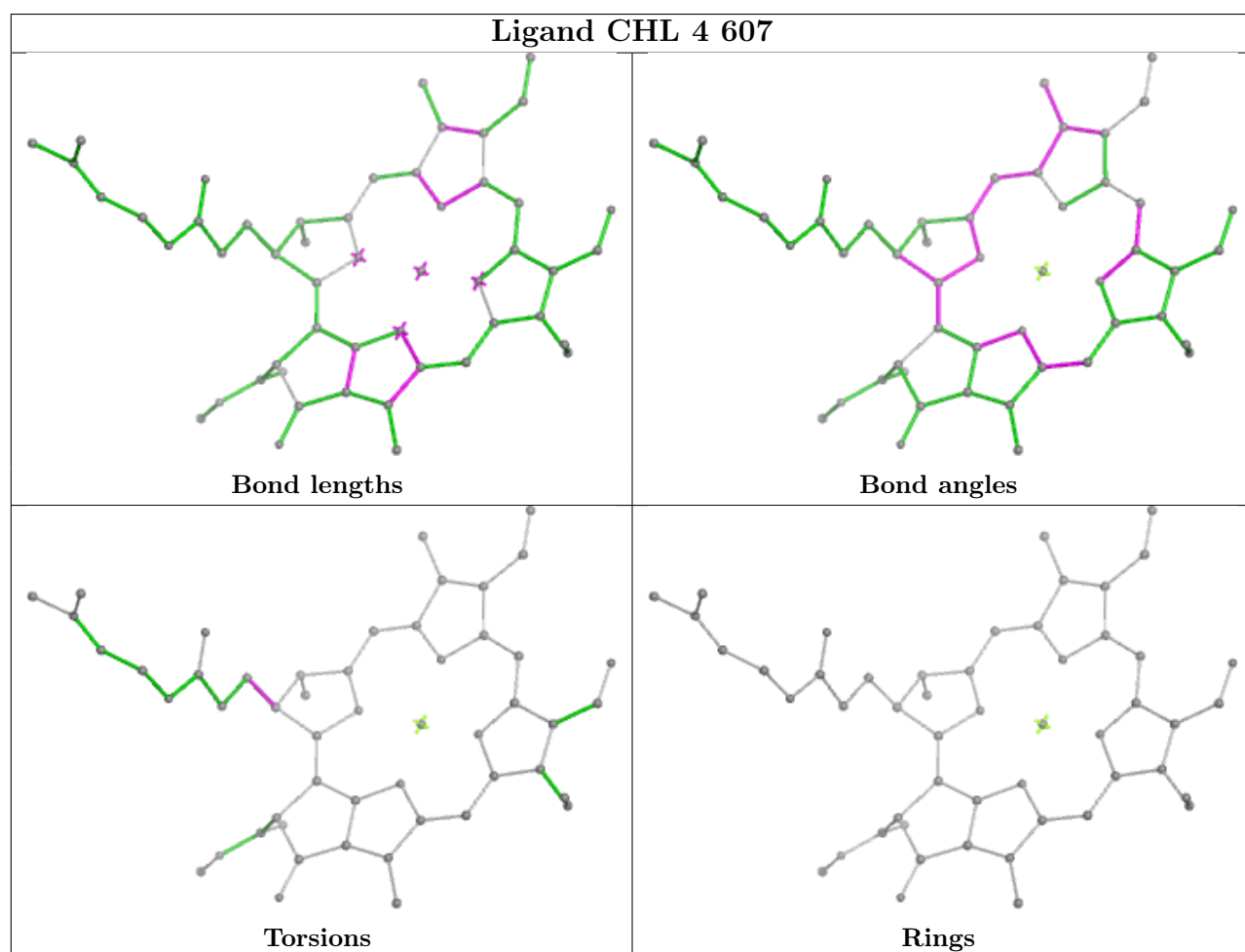
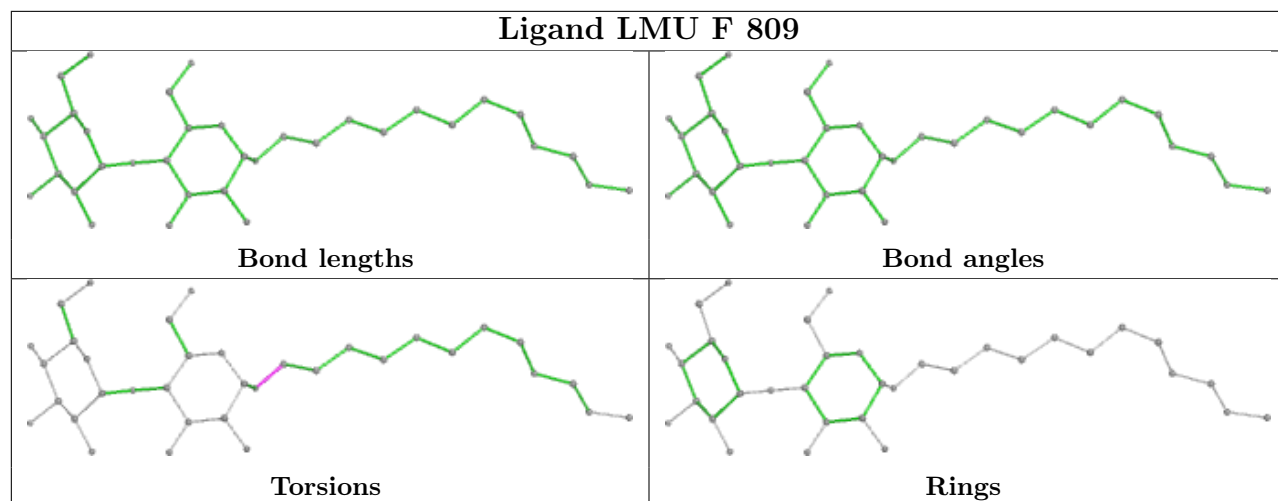


## Ligand CLA A 803

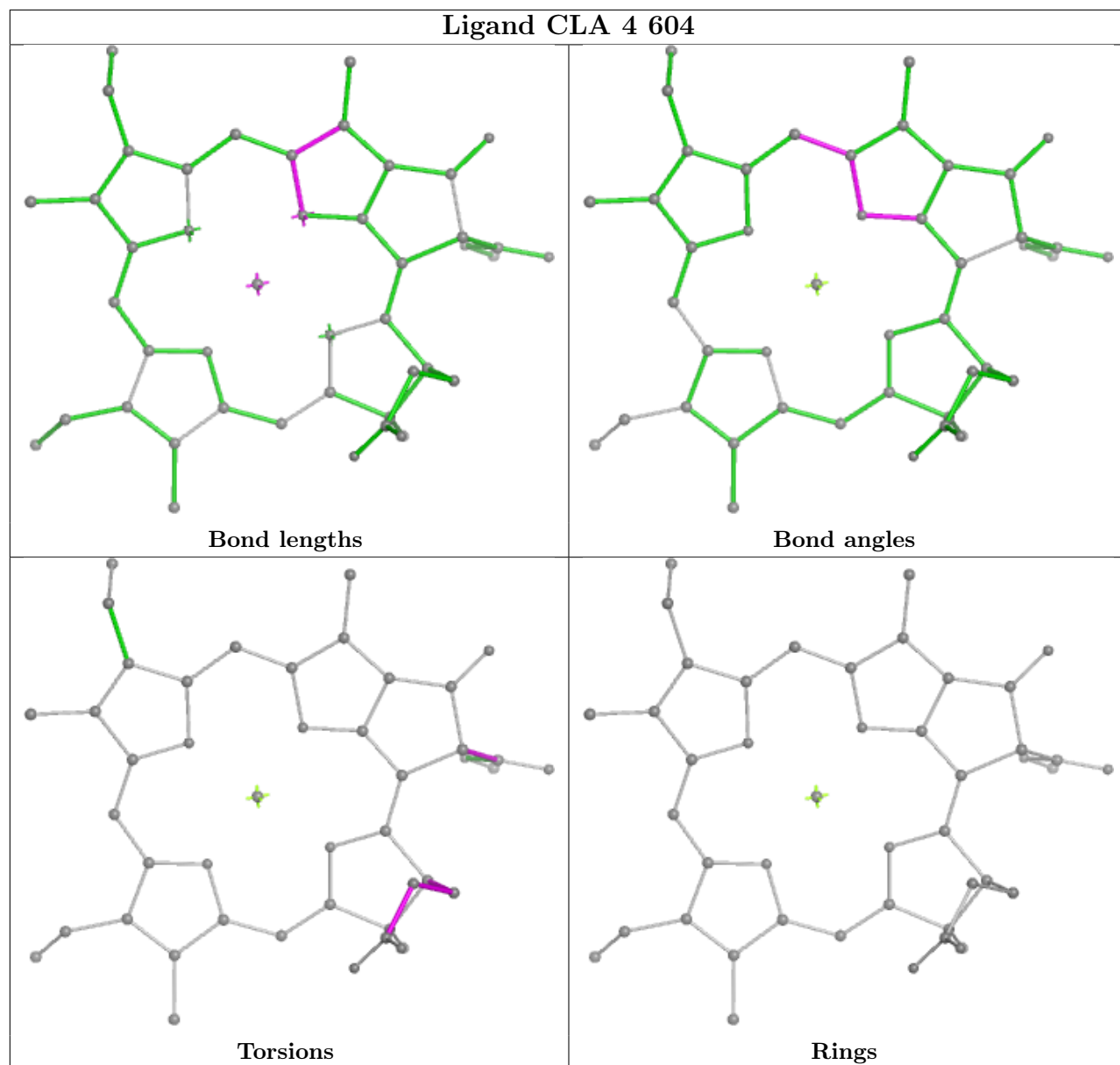




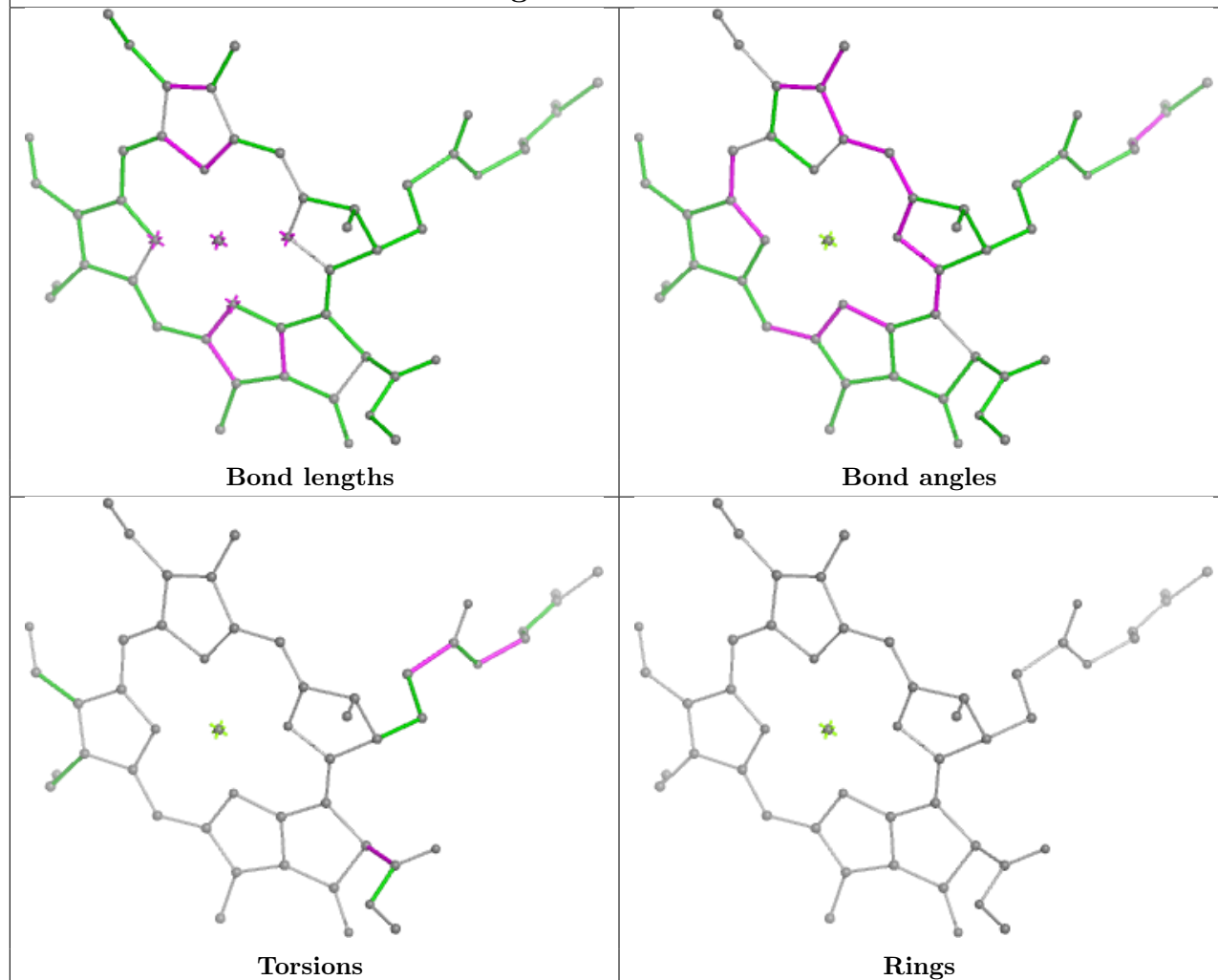




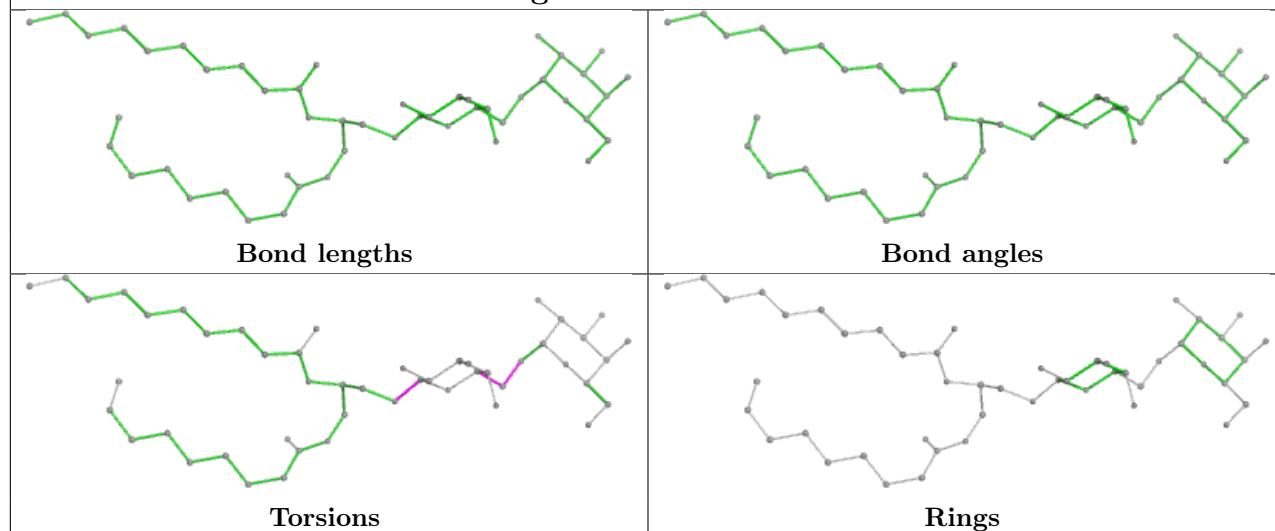
## Ligand CLA 4 604

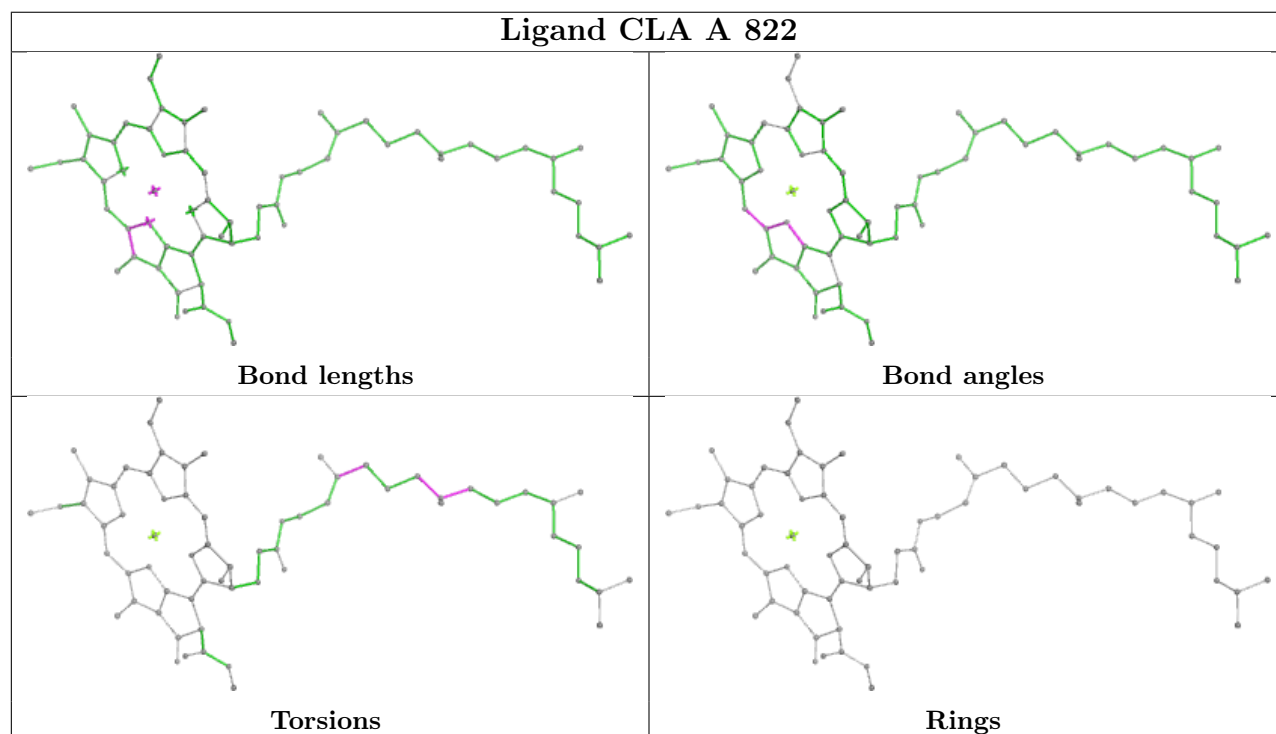
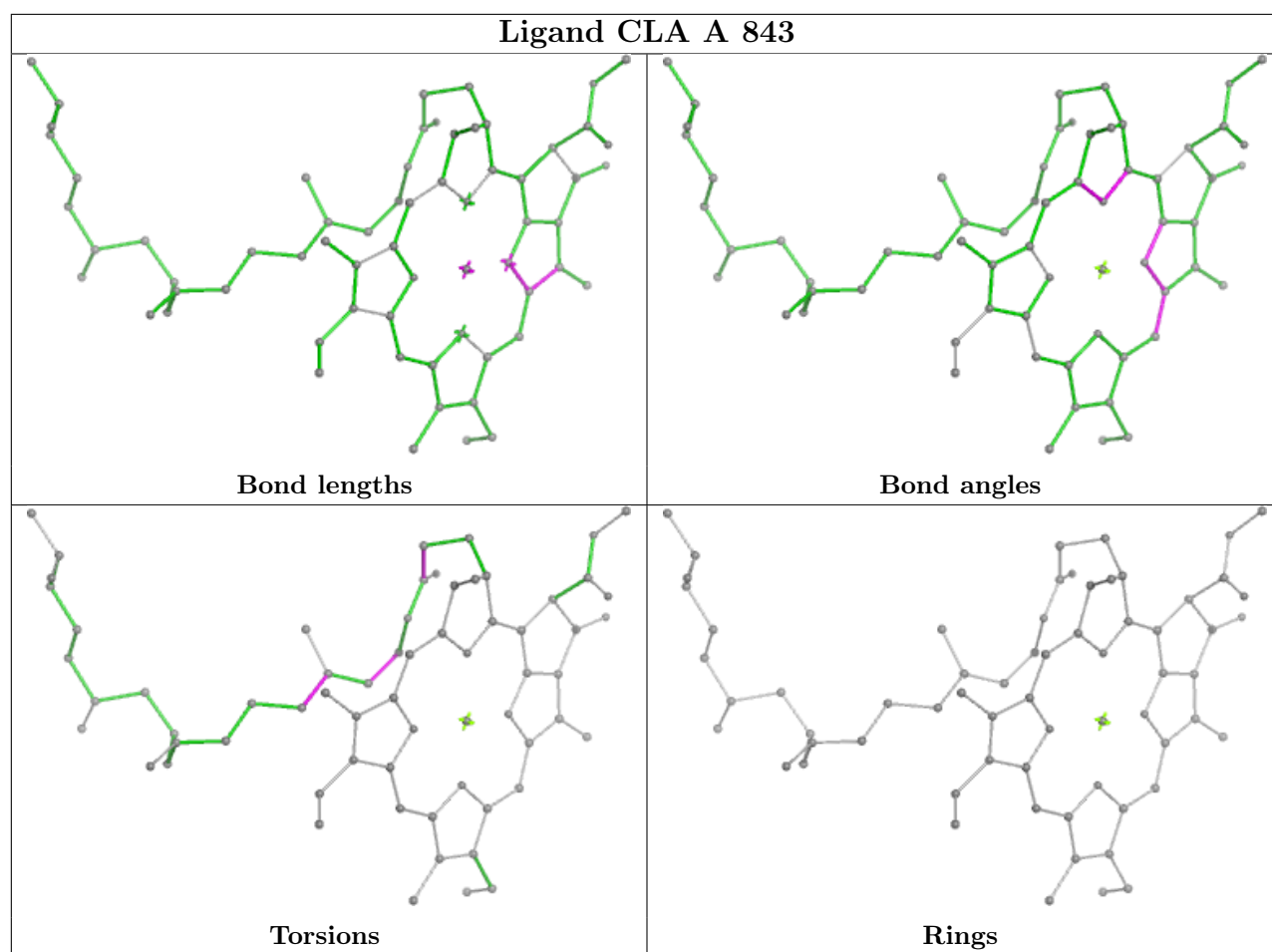


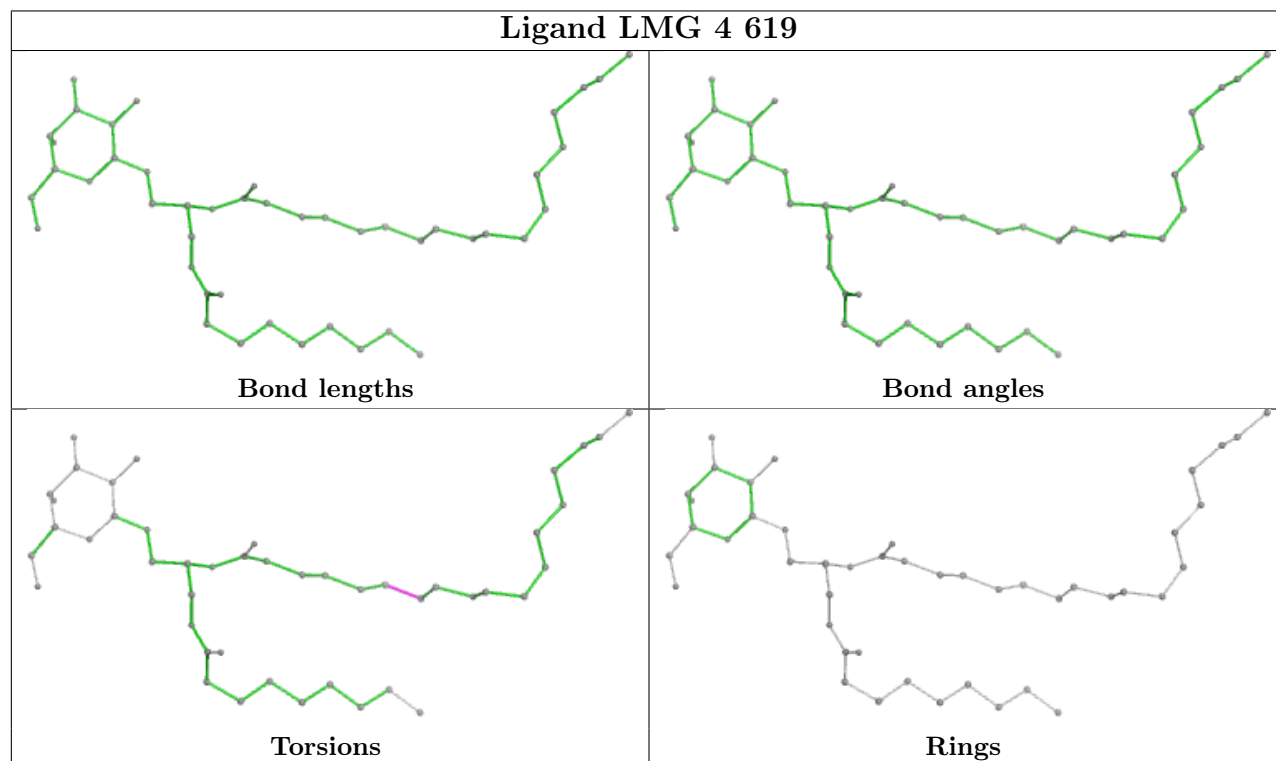
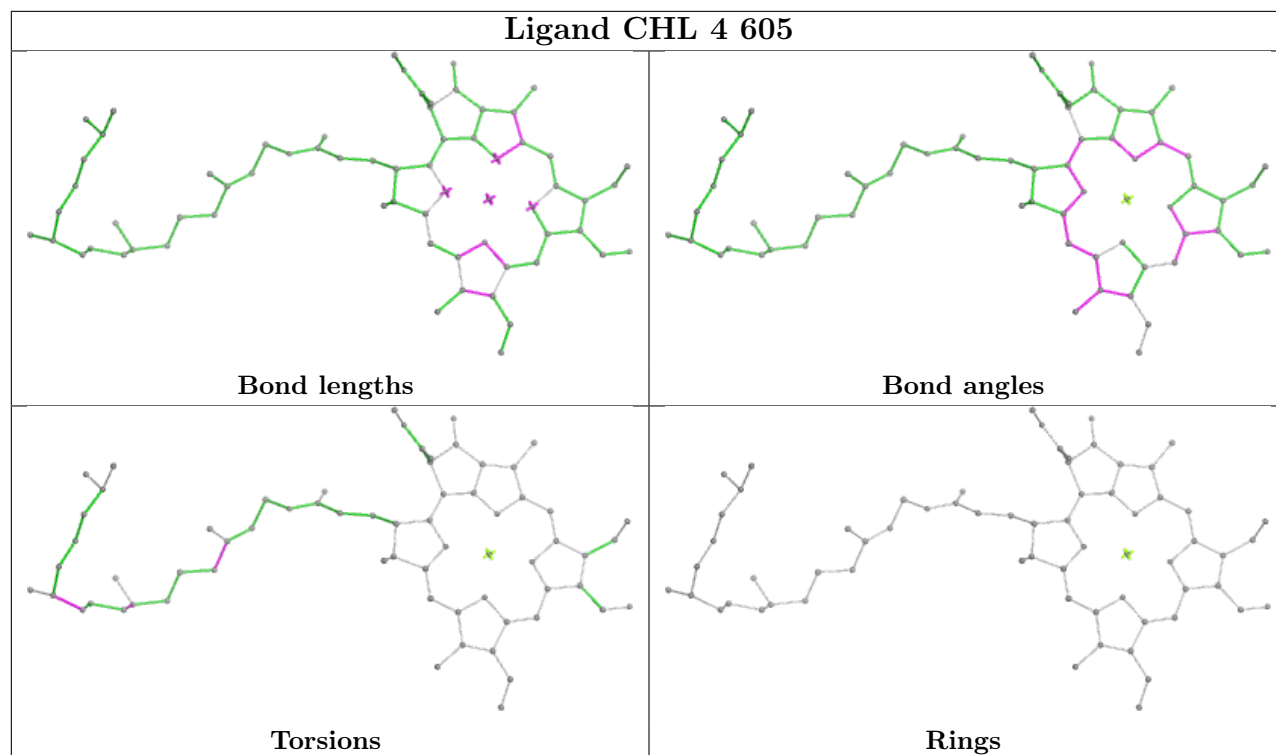
## Ligand CHL 2 607



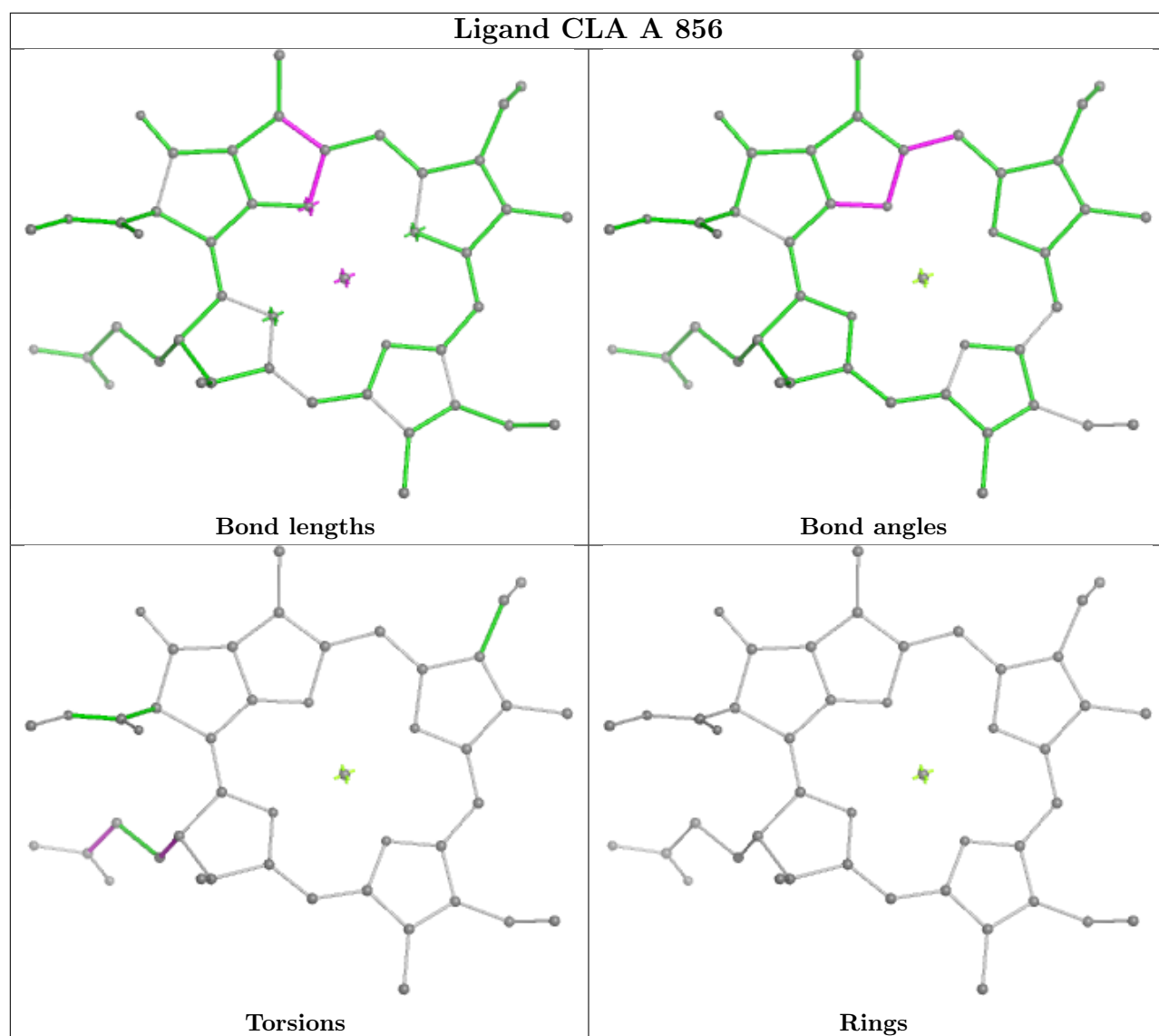
## Ligand DGD 4 622



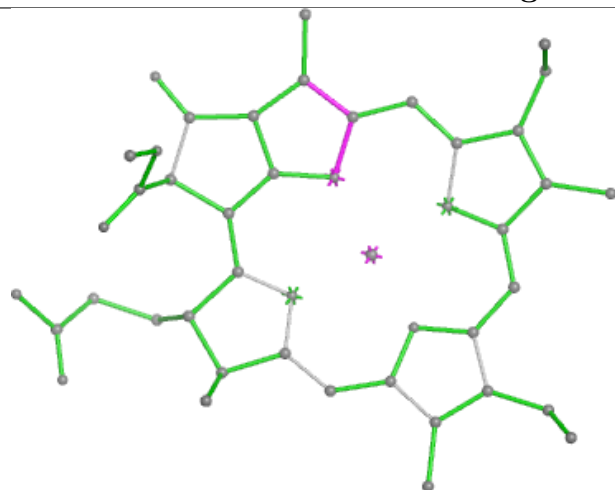




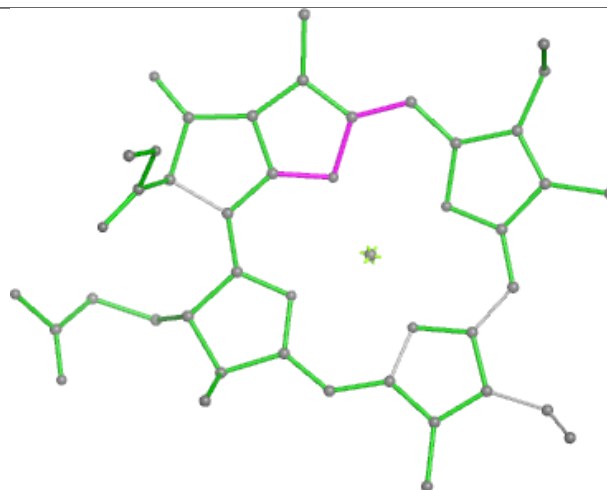




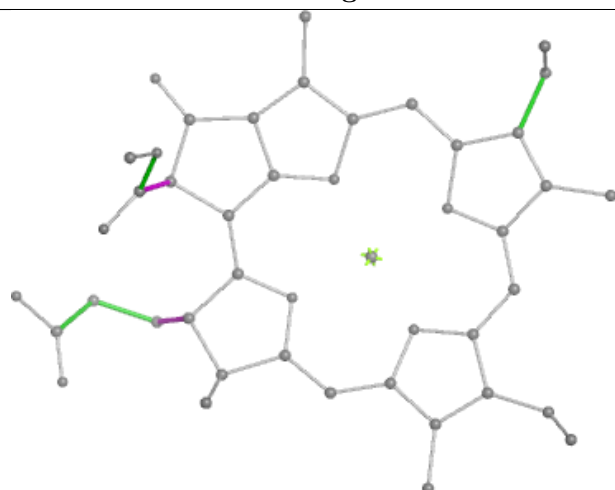
## Ligand CLA 1 312



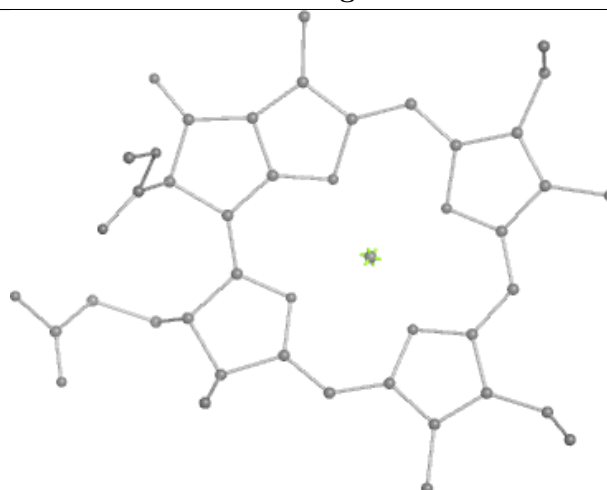
Bond lengths



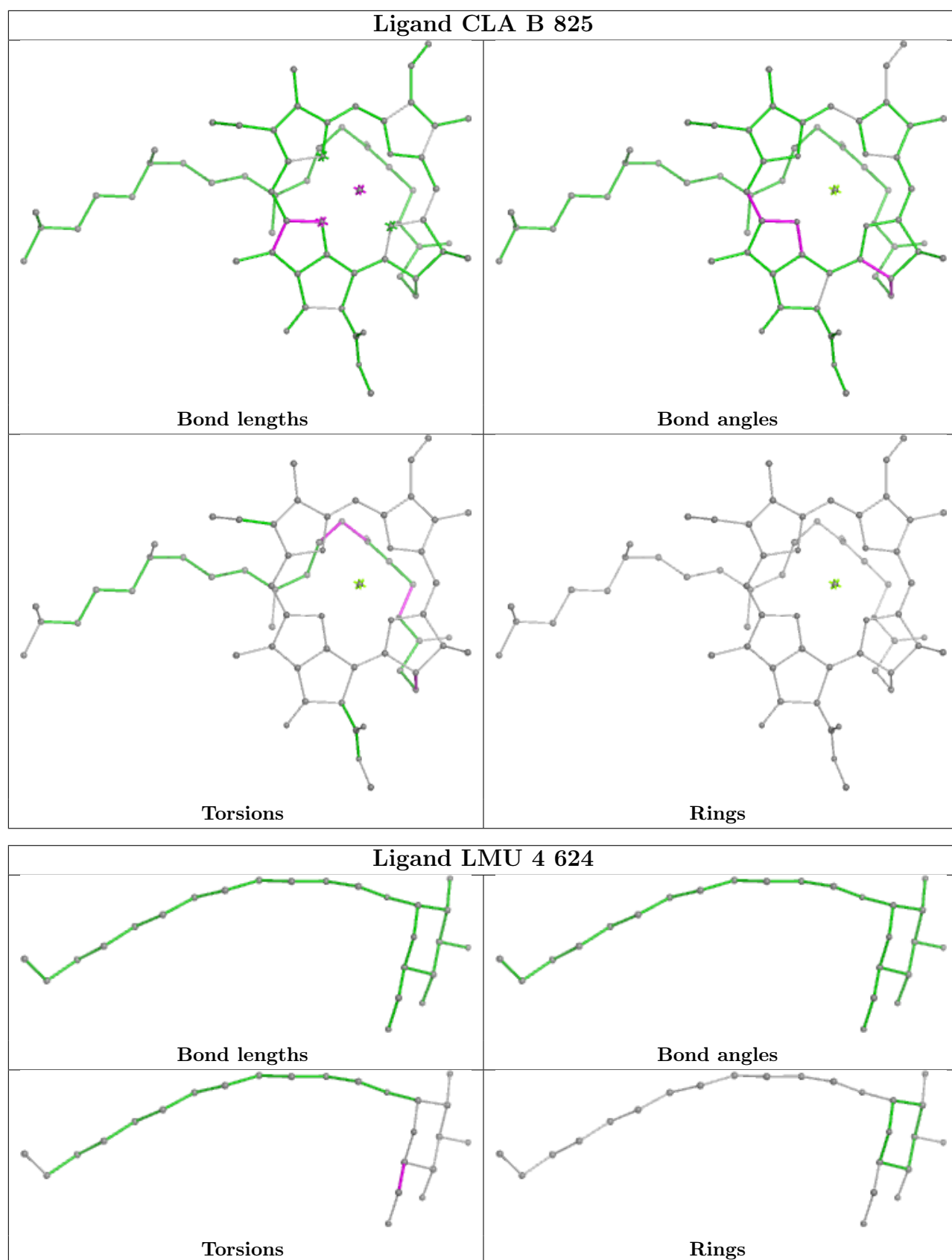
Bond angles

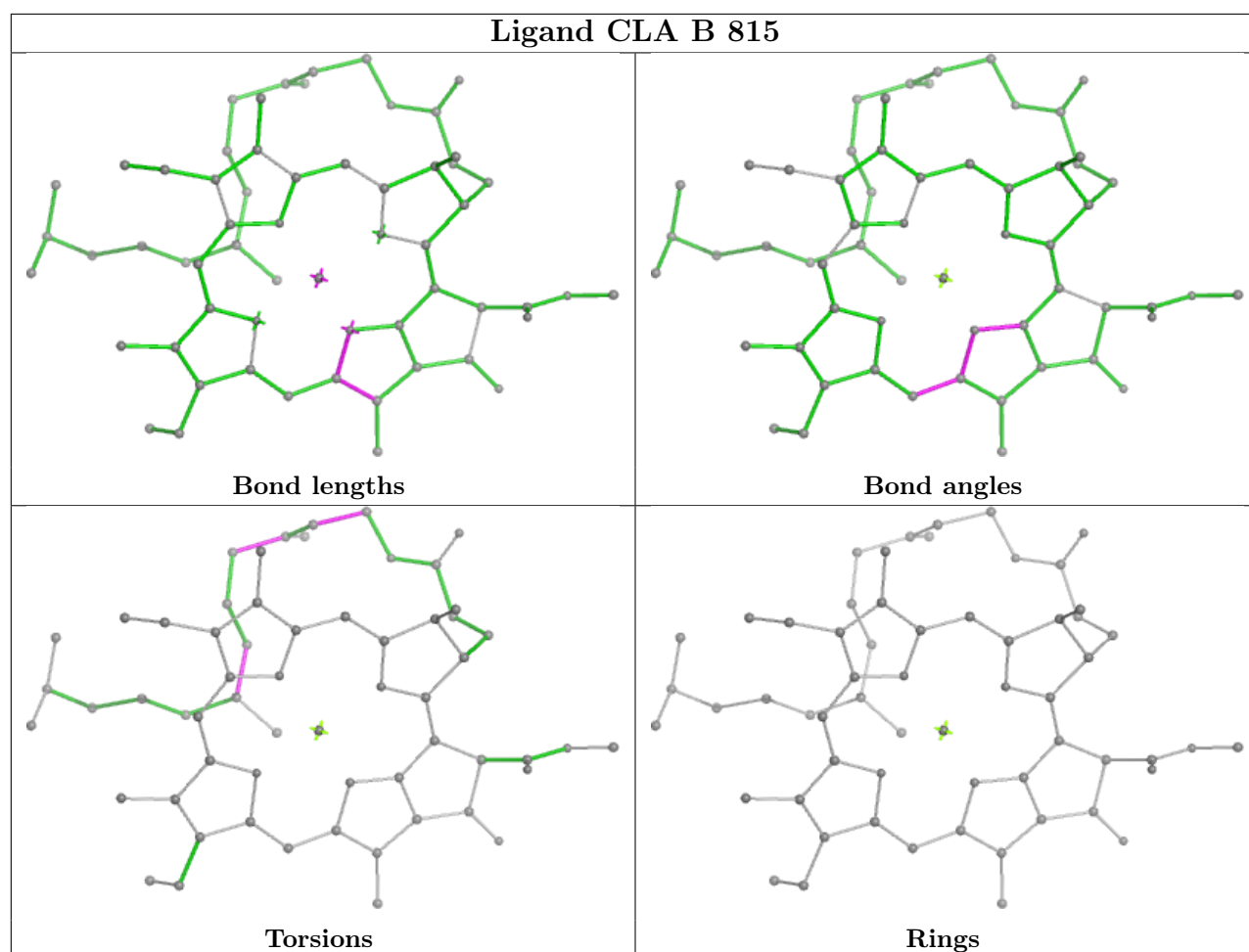


Torsions

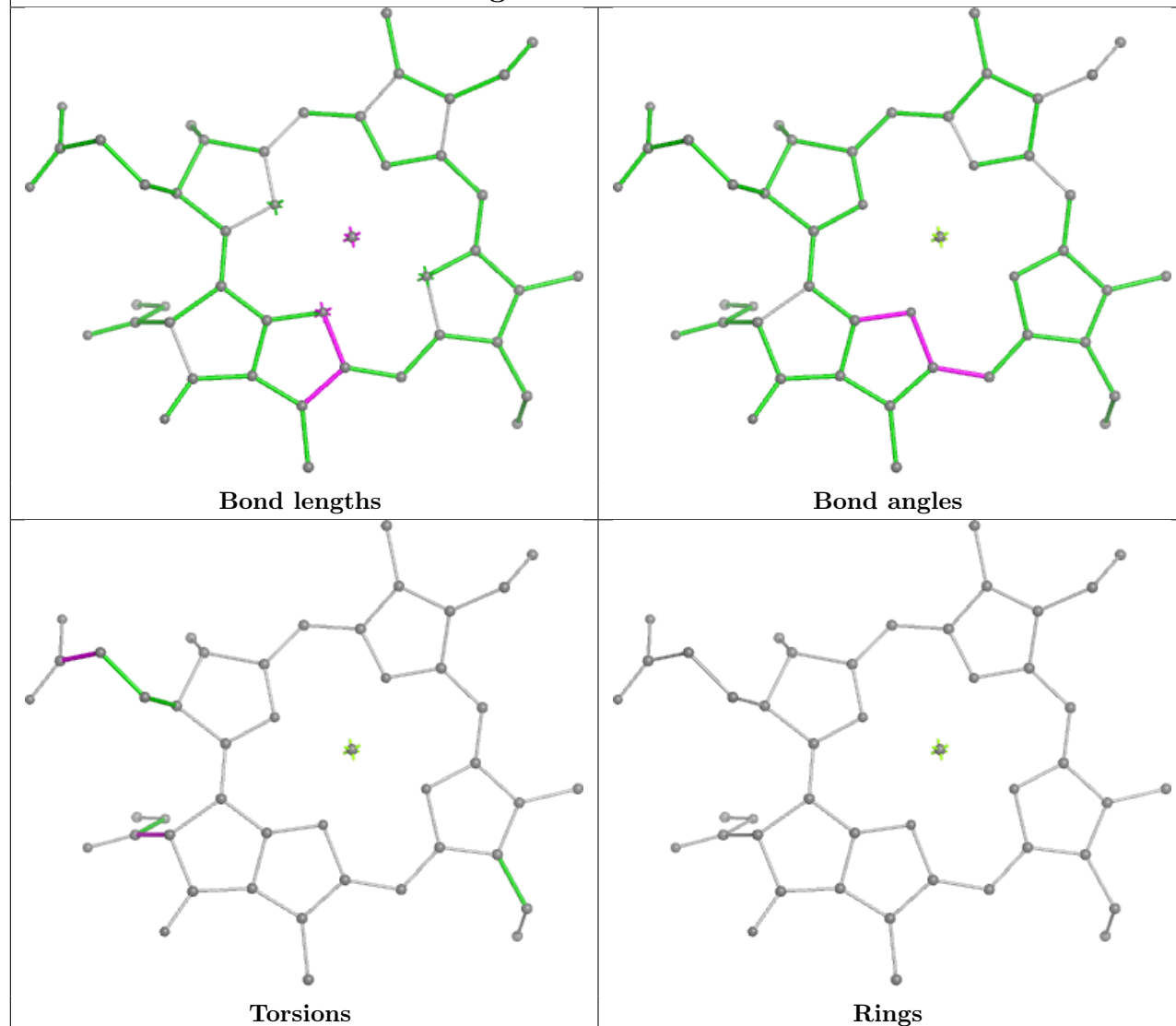


Rings

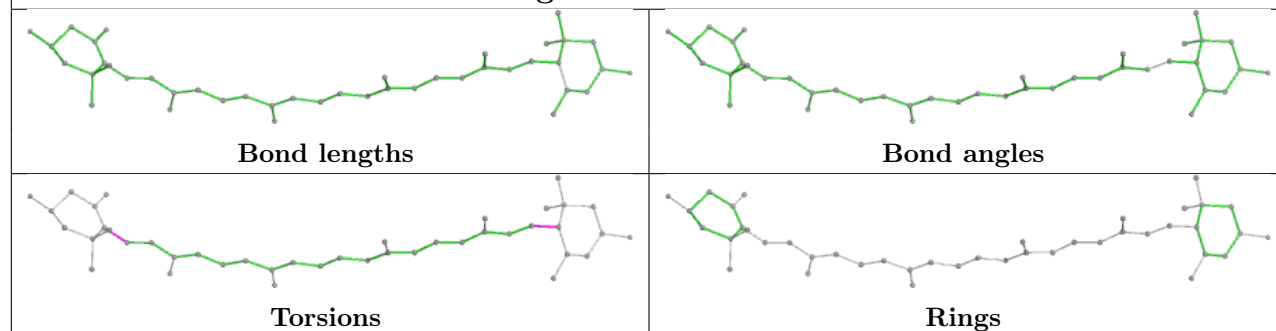




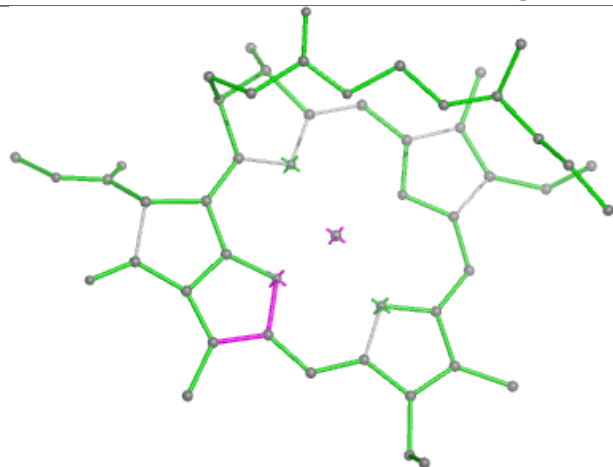
## Ligand CLA K 201



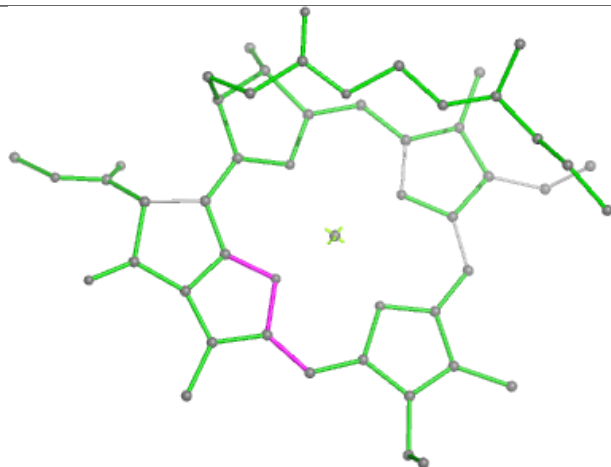
## Ligand LUT J 101



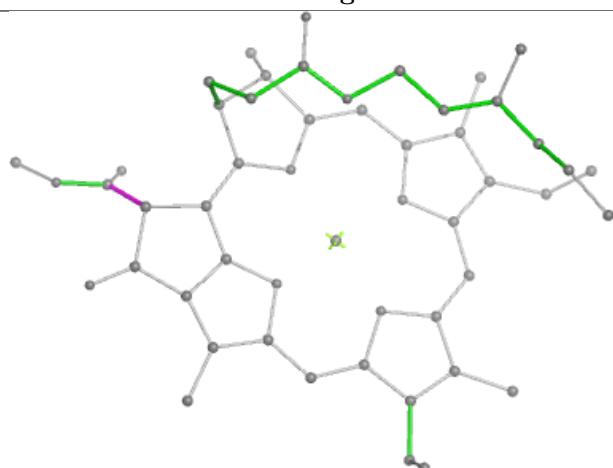
## Ligand CLA B 811



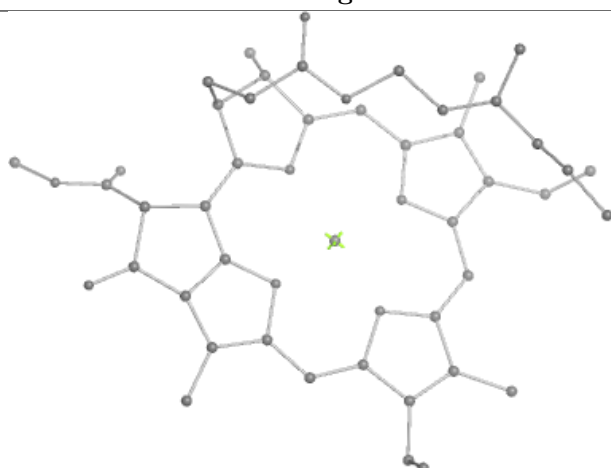
Bond lengths



Bond angles

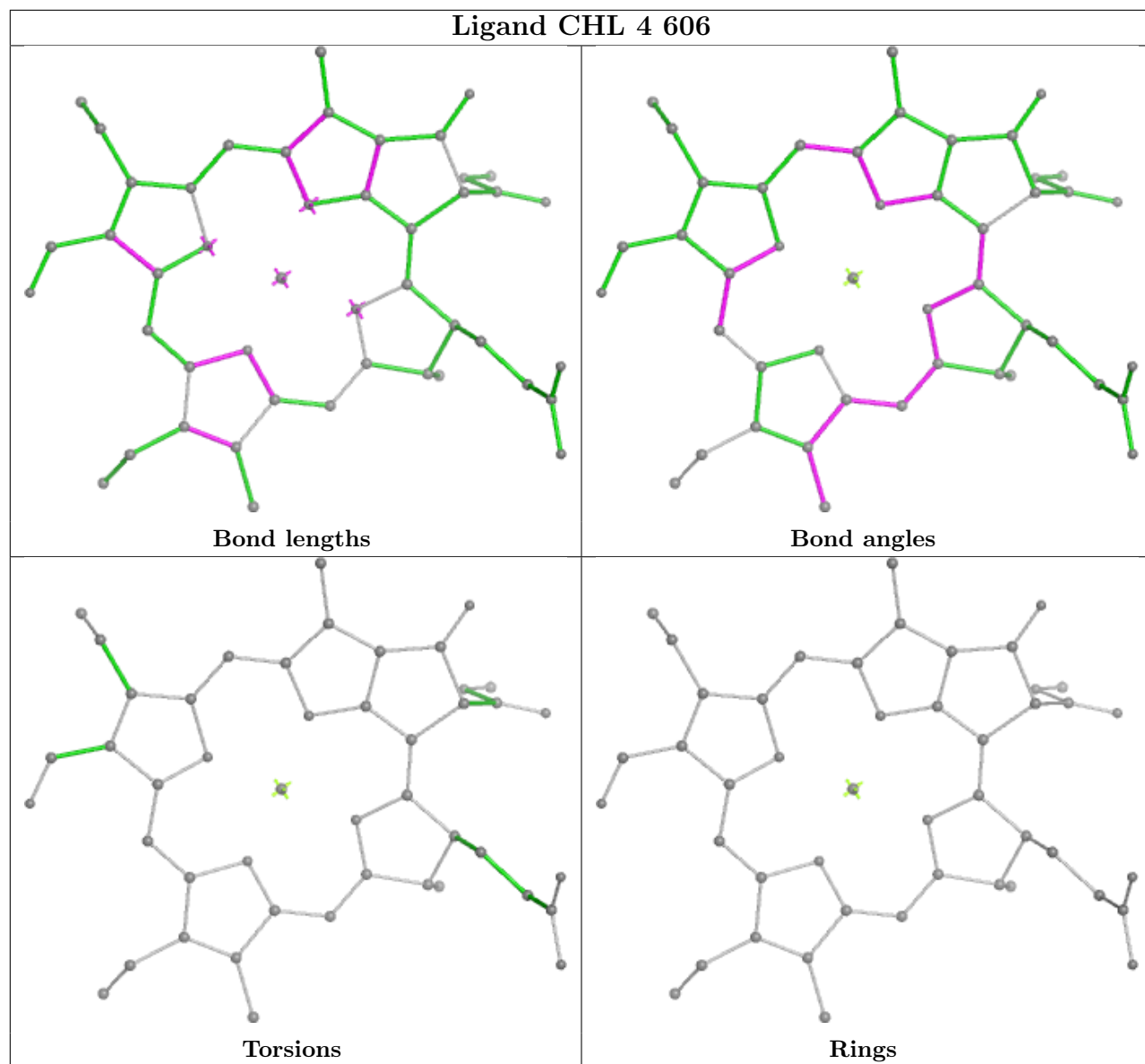


Torsions

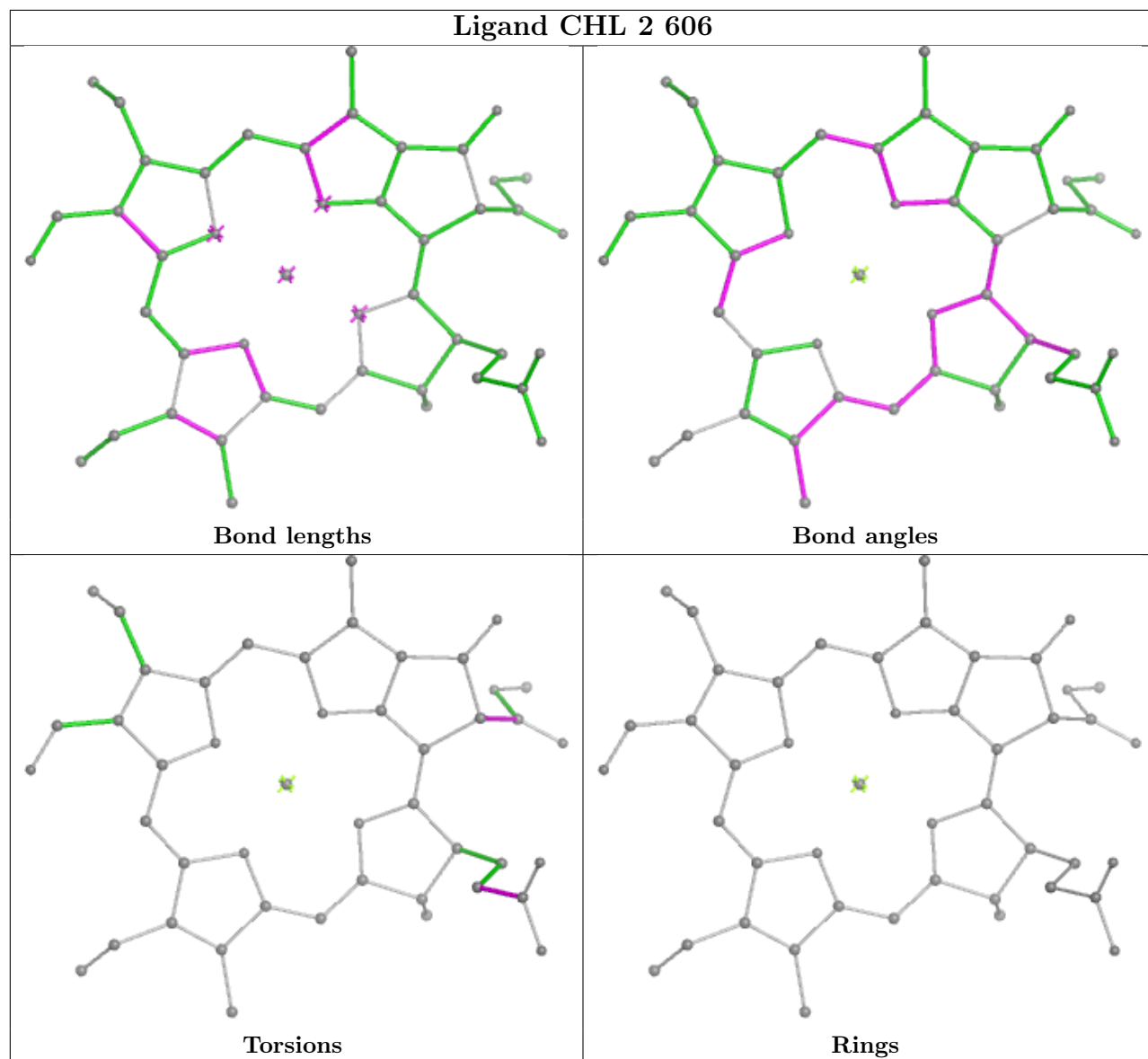


Rings

## Ligand CHL 4 606

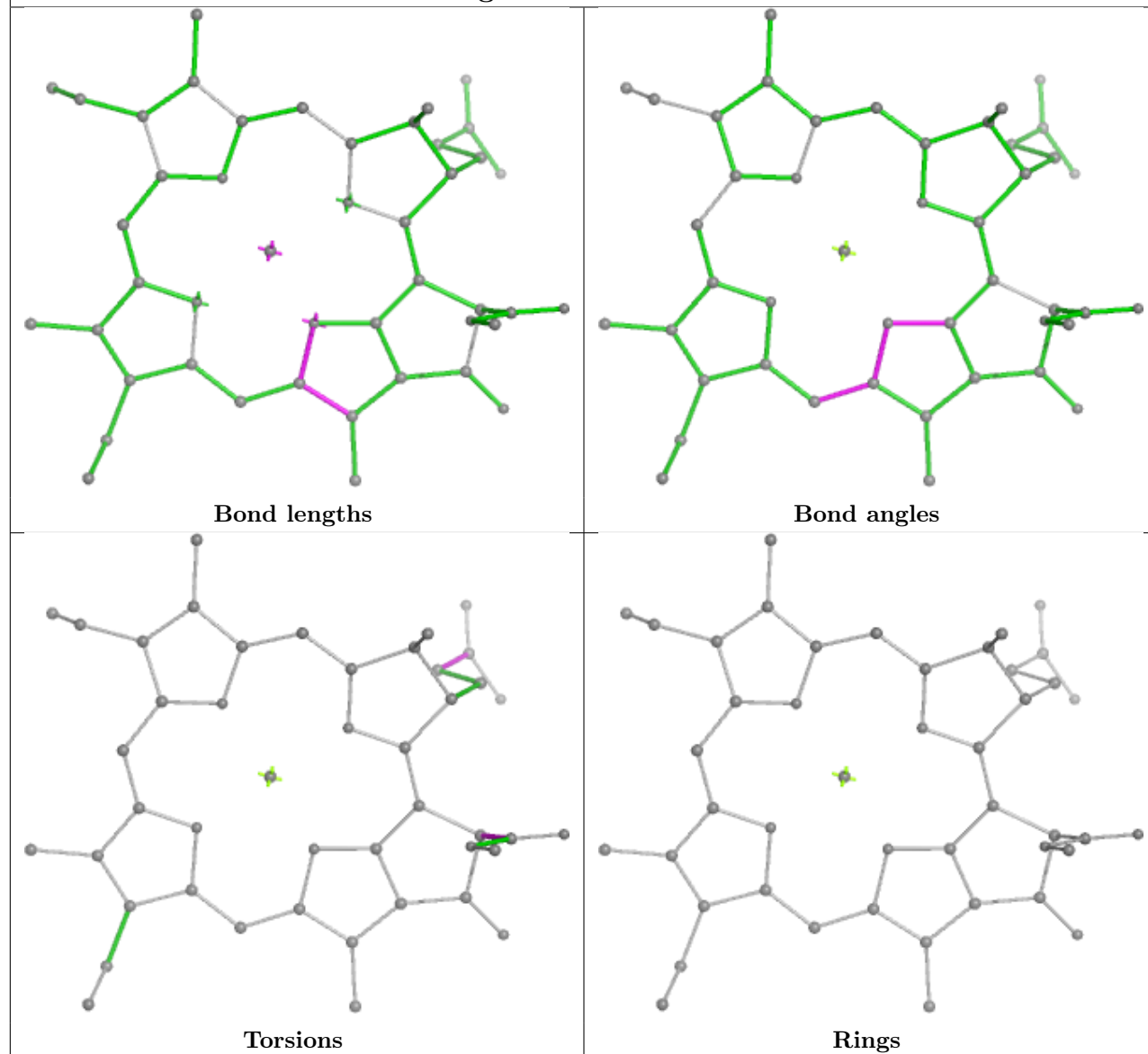


## Ligand CHL 2 606

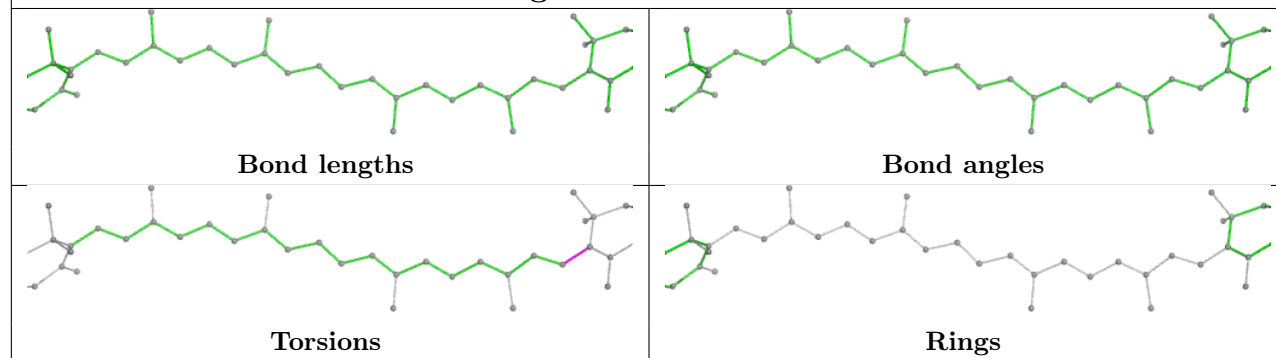


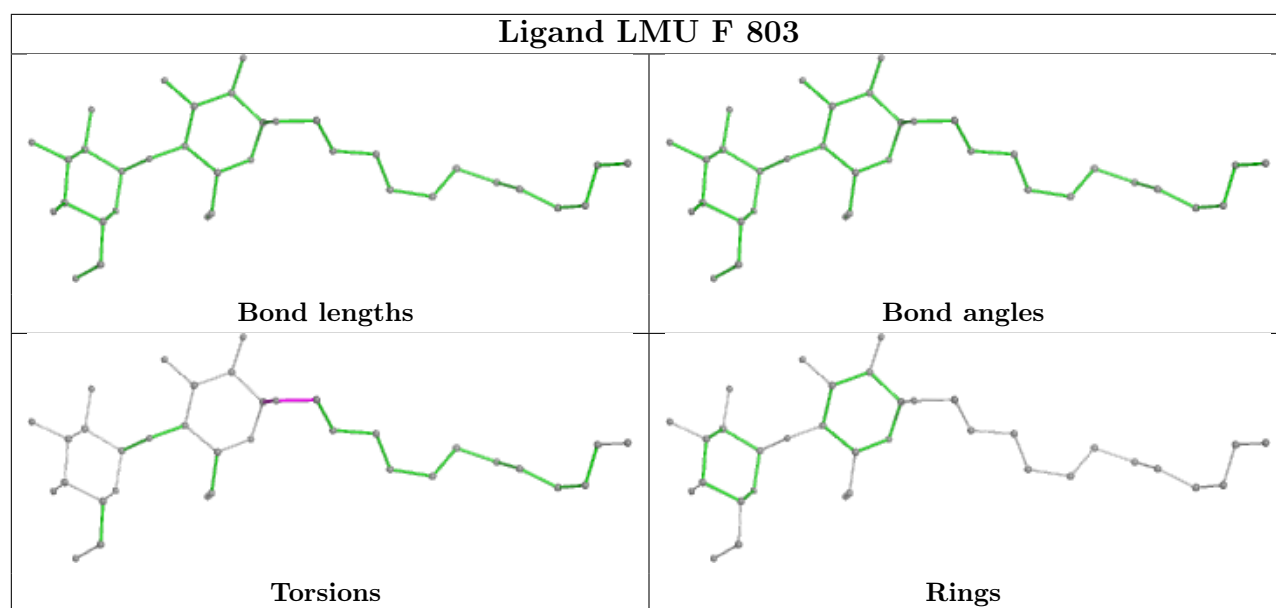


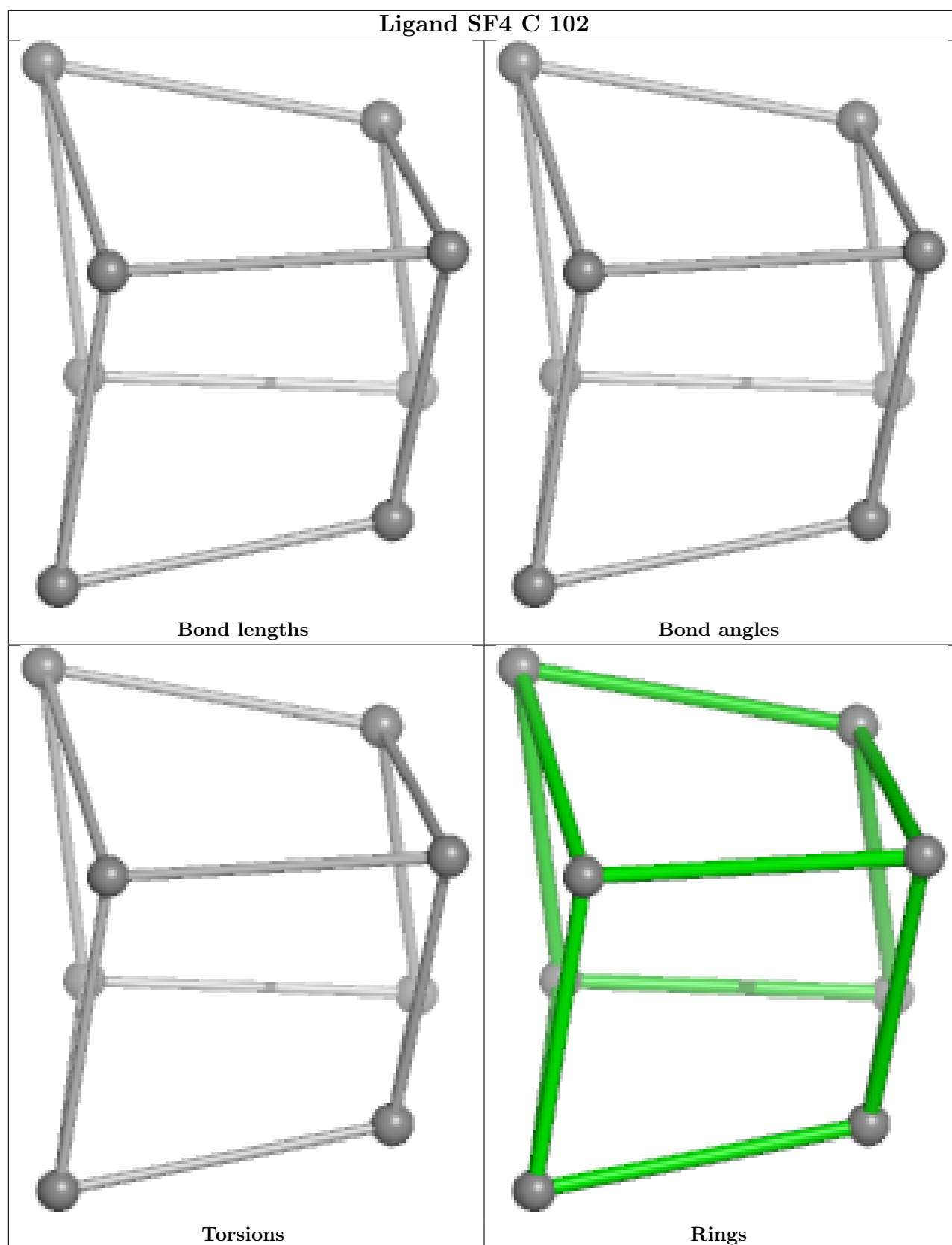
## Ligand CLA A 845

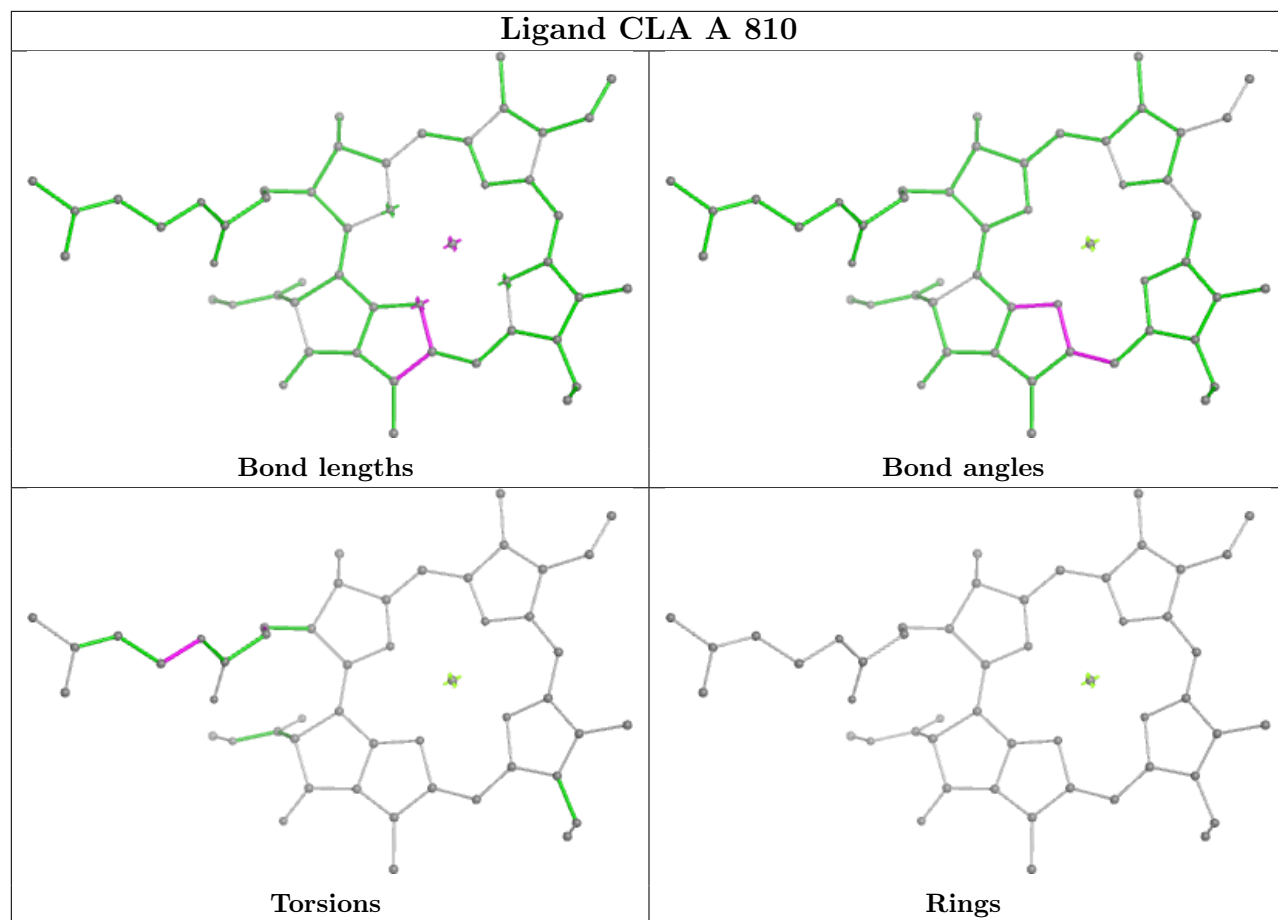


## Ligand BCR A 851

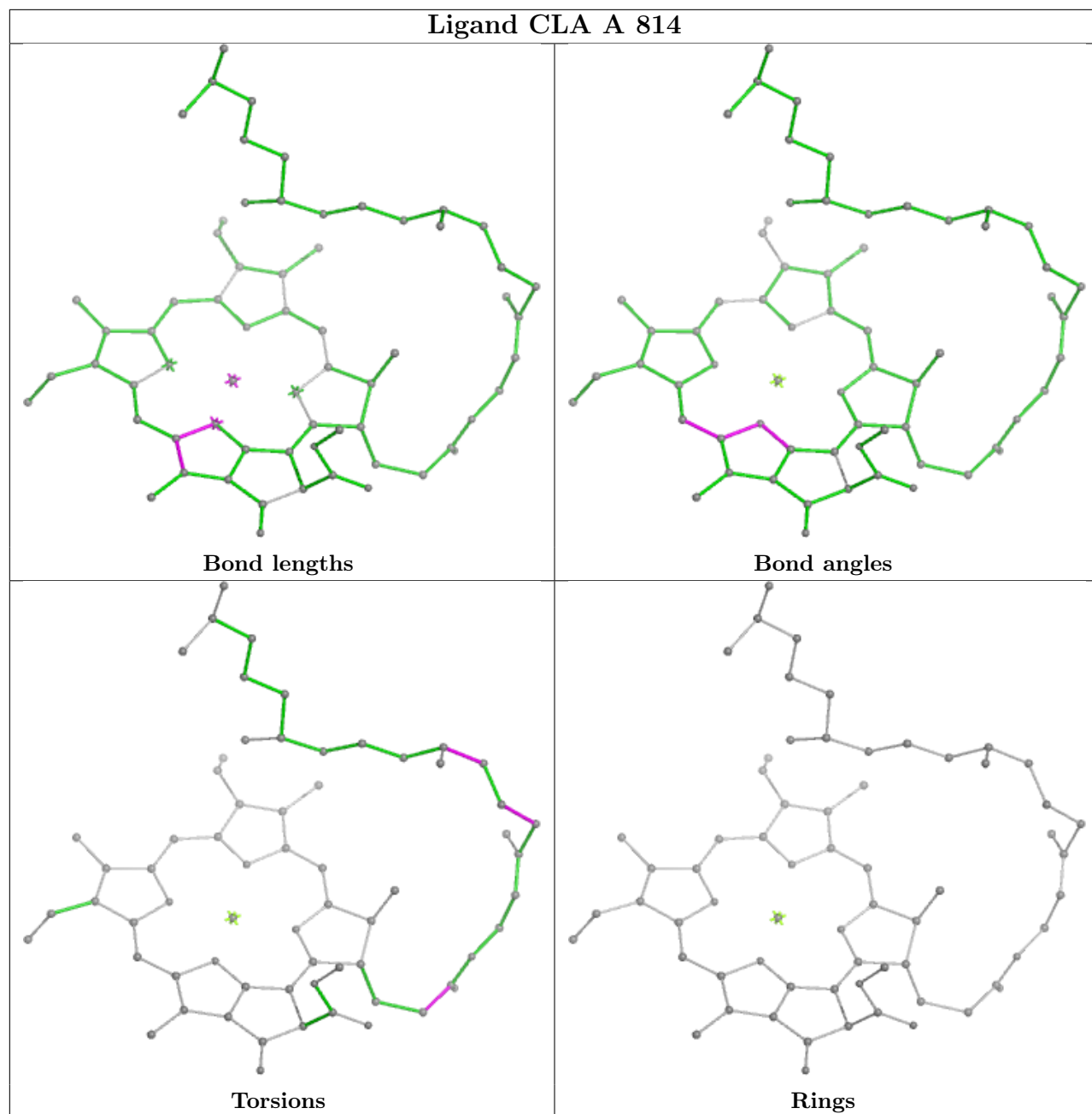




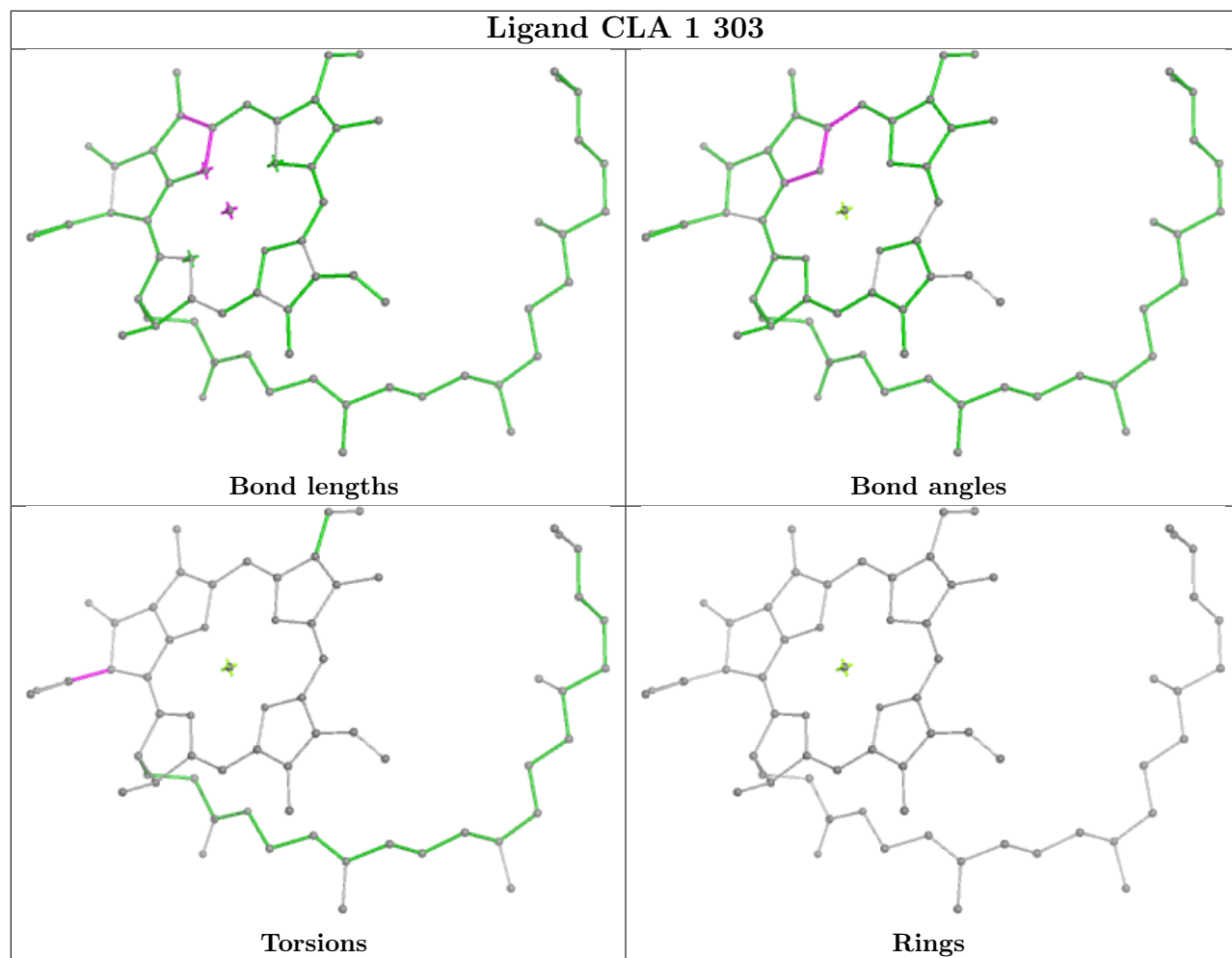




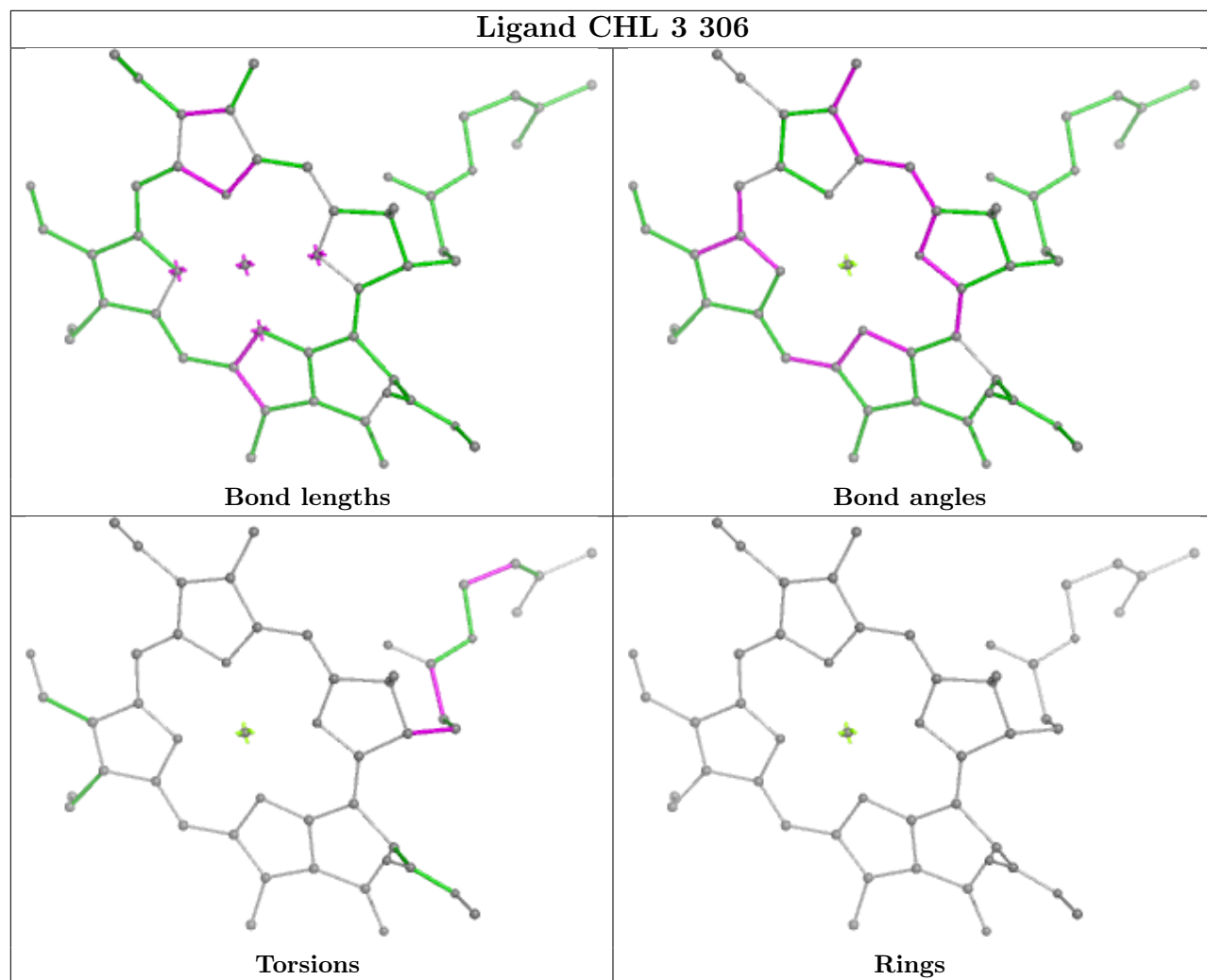
## Ligand CLA A 814



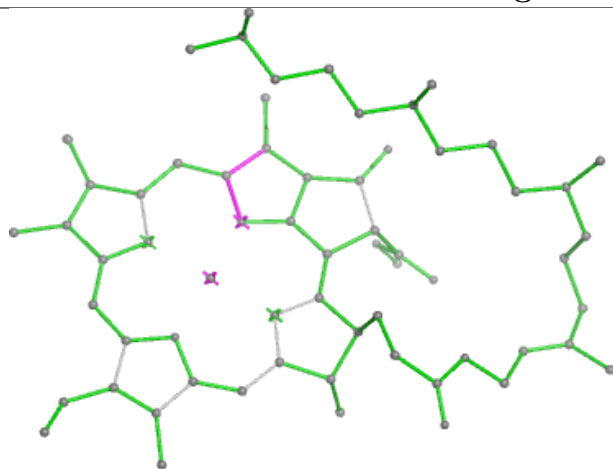
## Ligand CLA 1 303



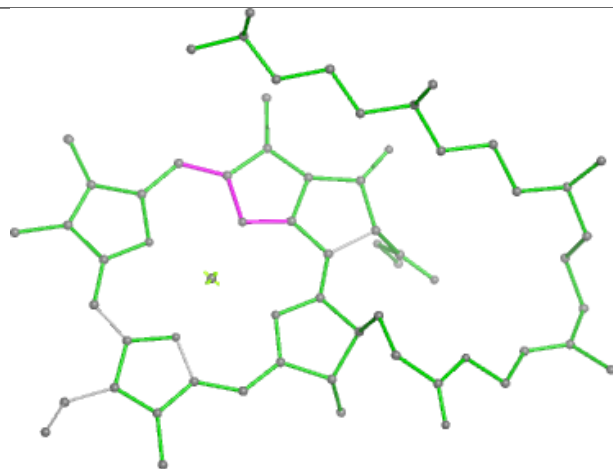
## Ligand CHL 3 306



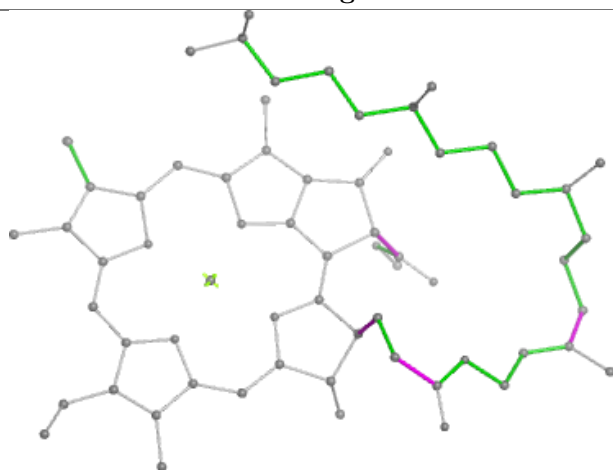
## Ligand CLA B 804



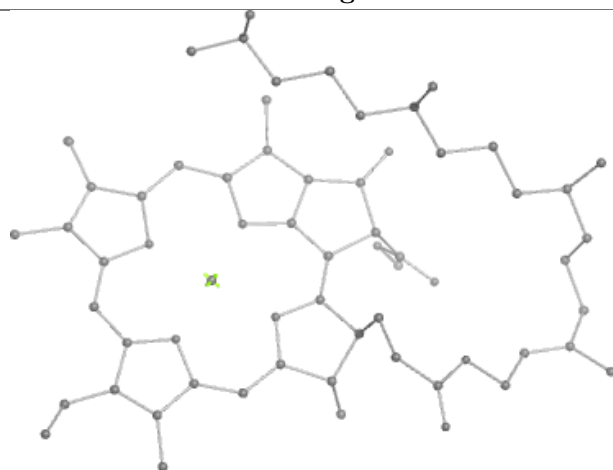
Bond lengths



Bond angles



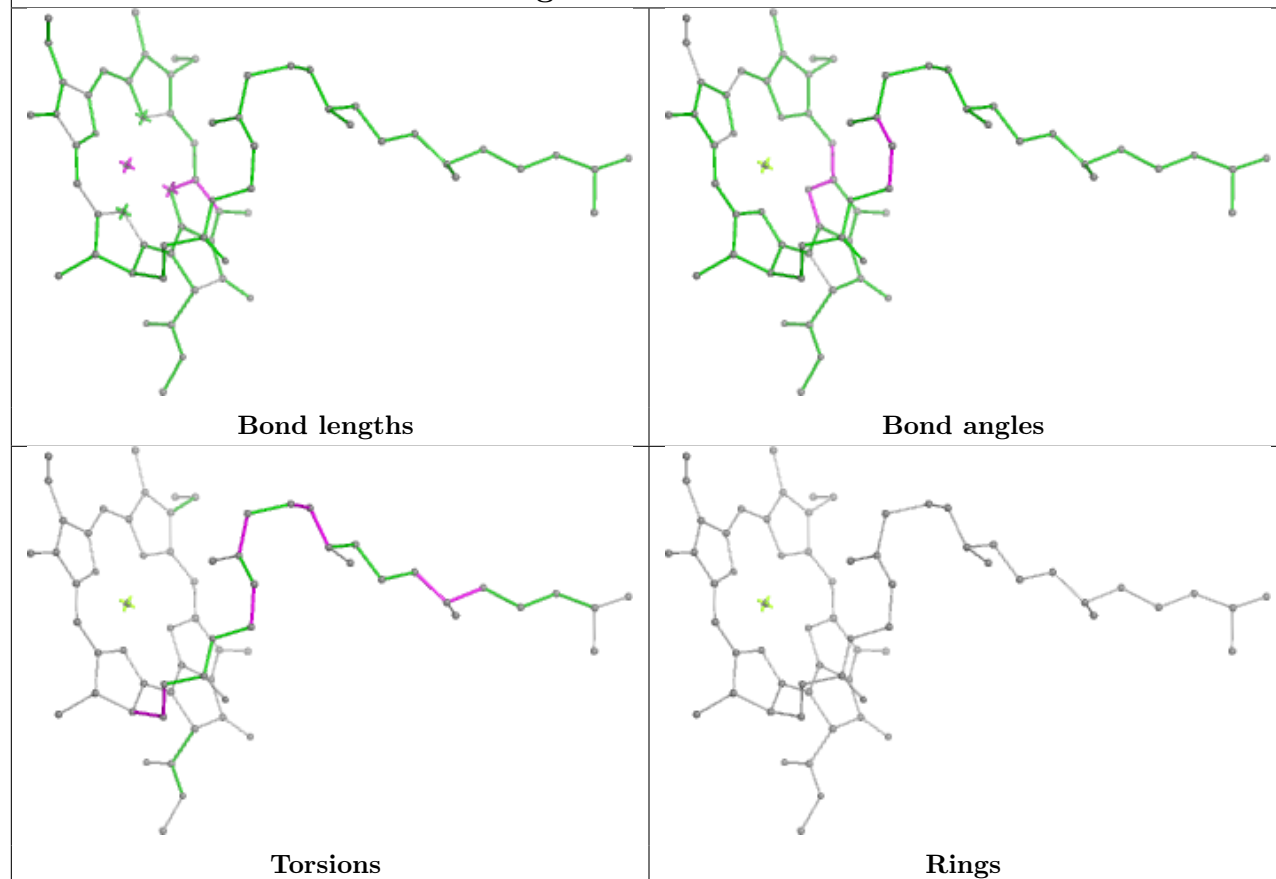
Torsions



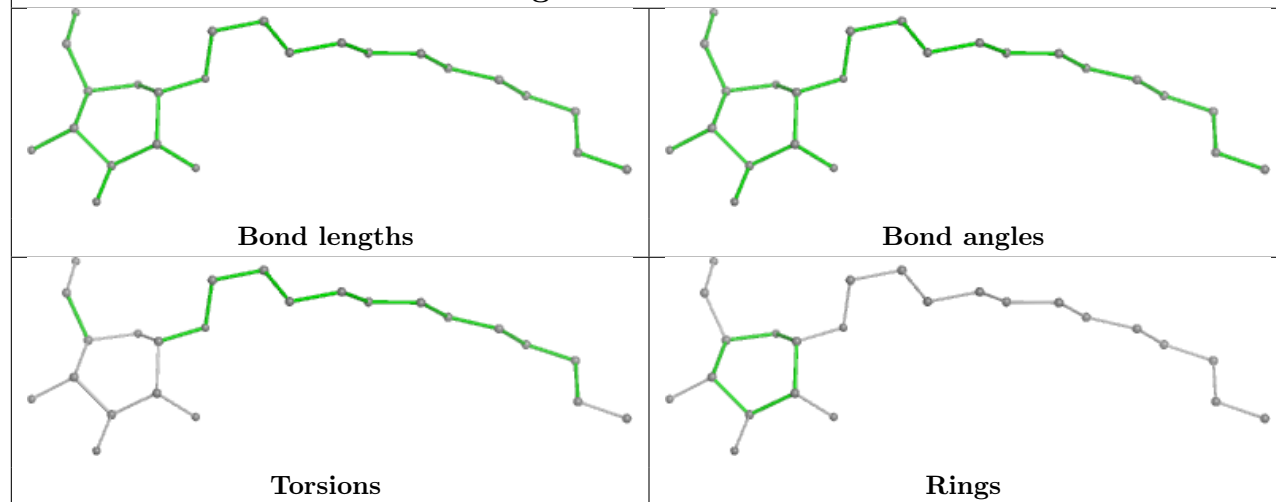
Rings

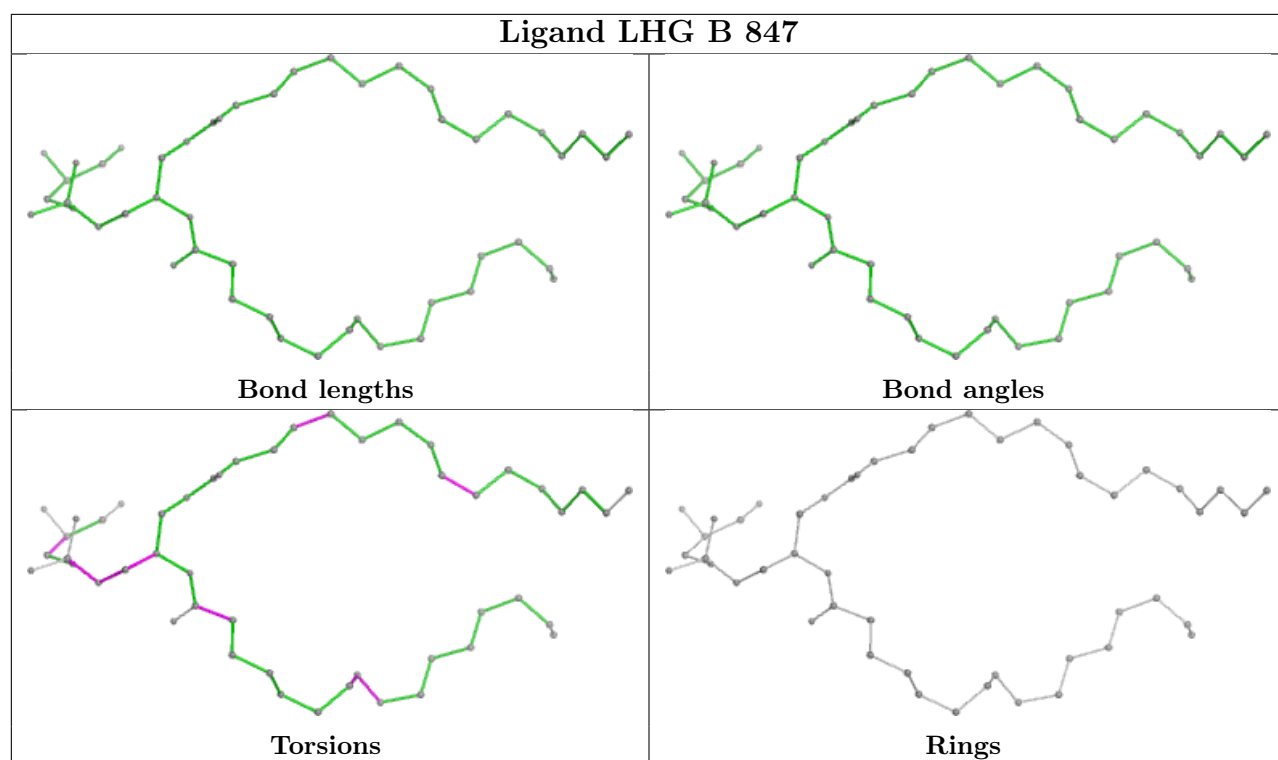


## Ligand CLA 4 608

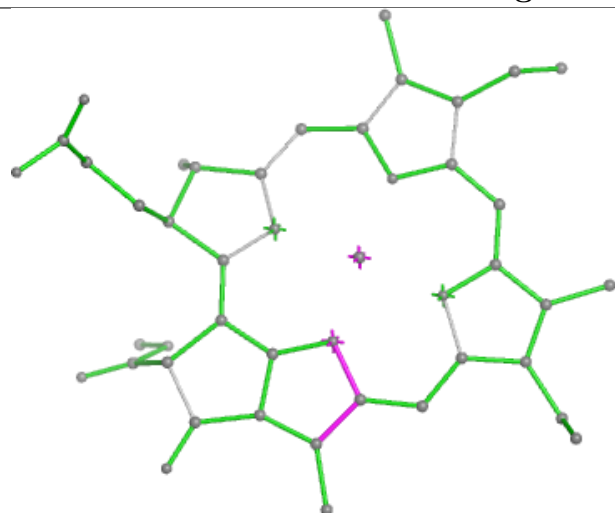


## Ligand LMU 1 321

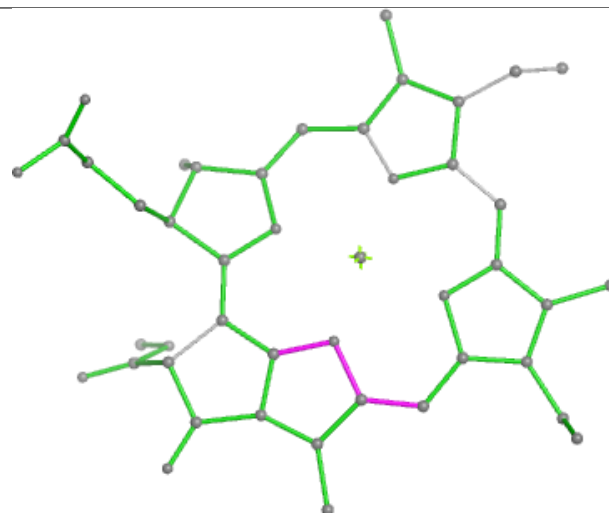




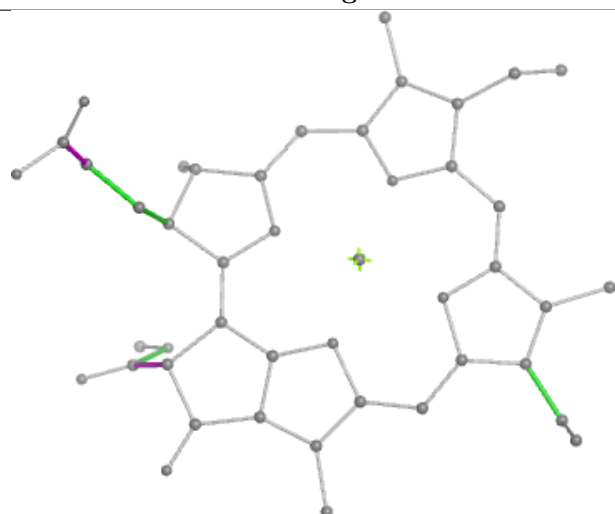
## Ligand CLA K 204



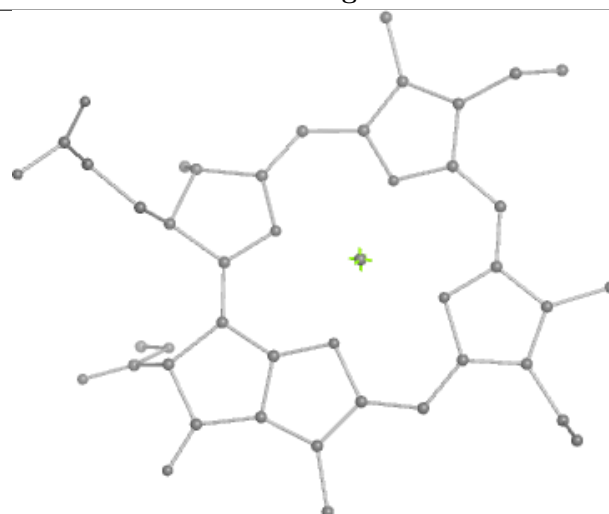
Bond lengths



Bond angles

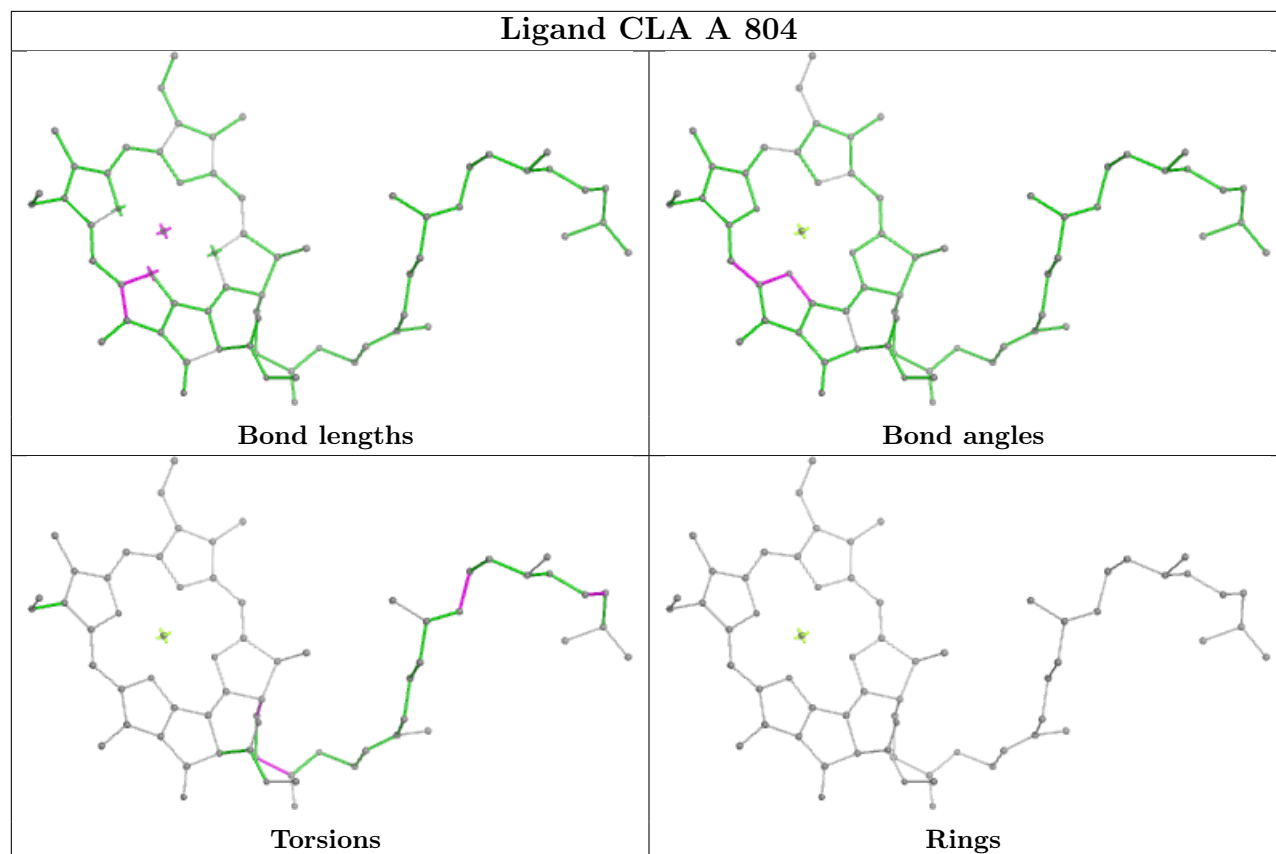


Torsions

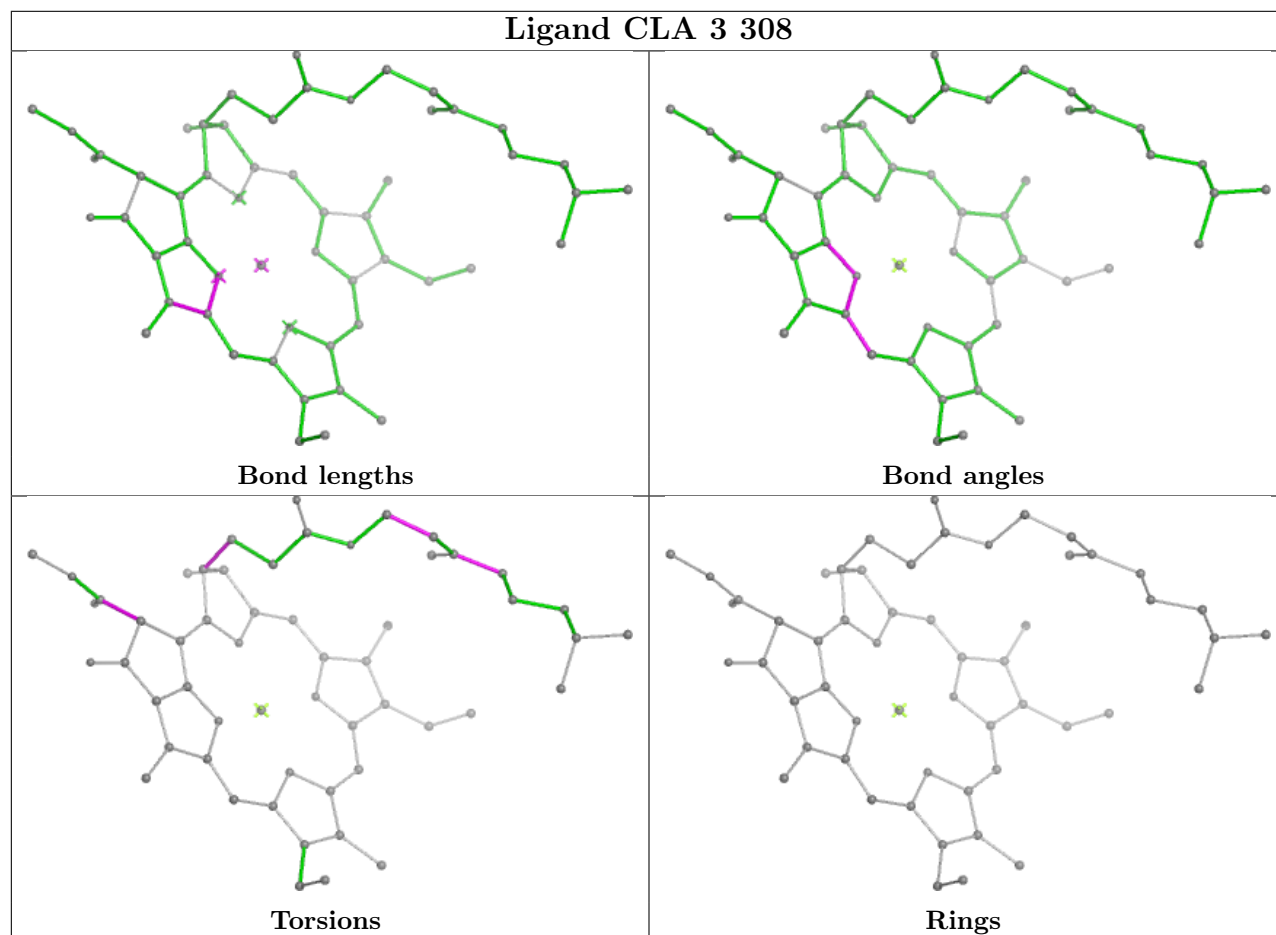


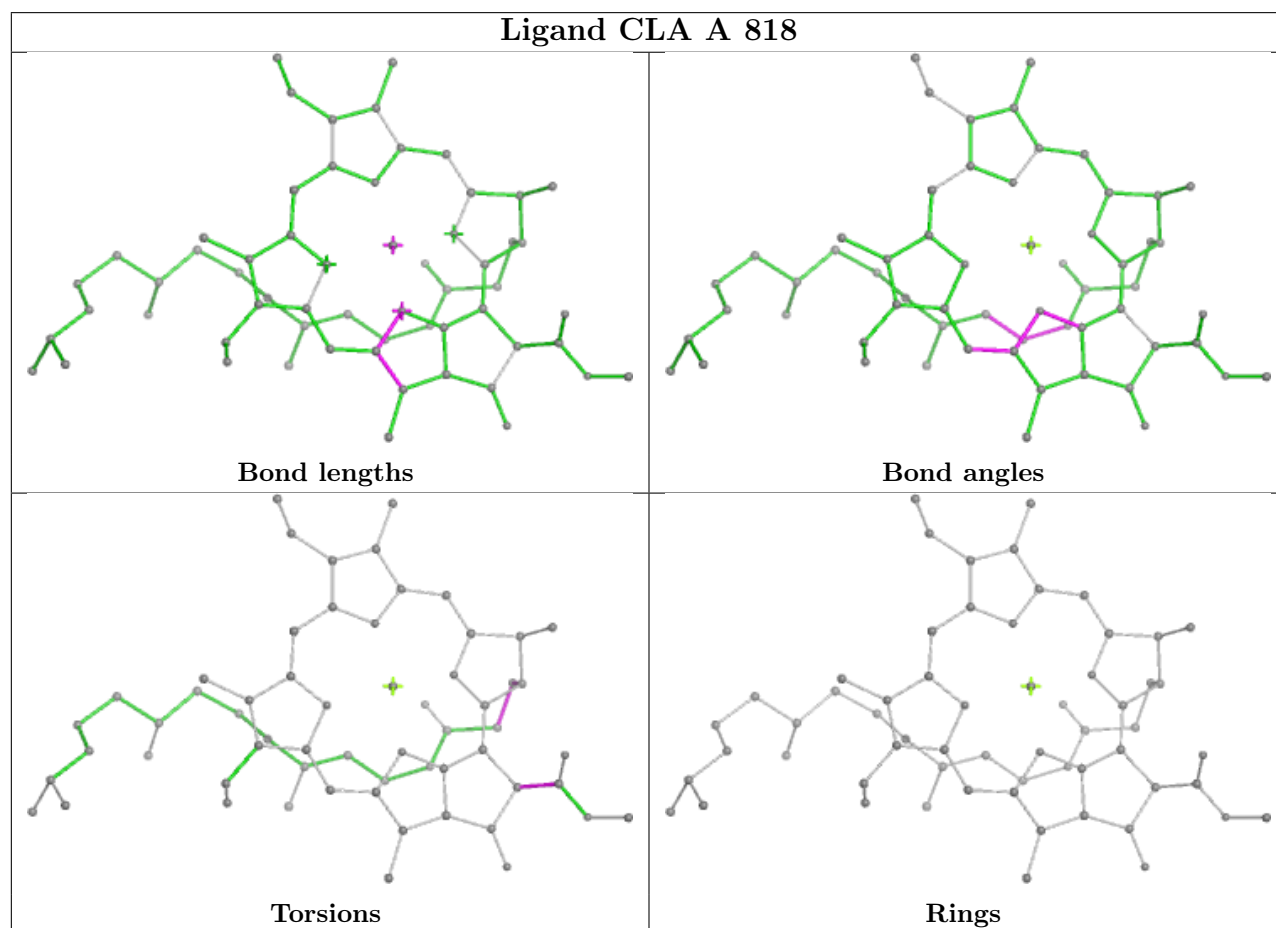
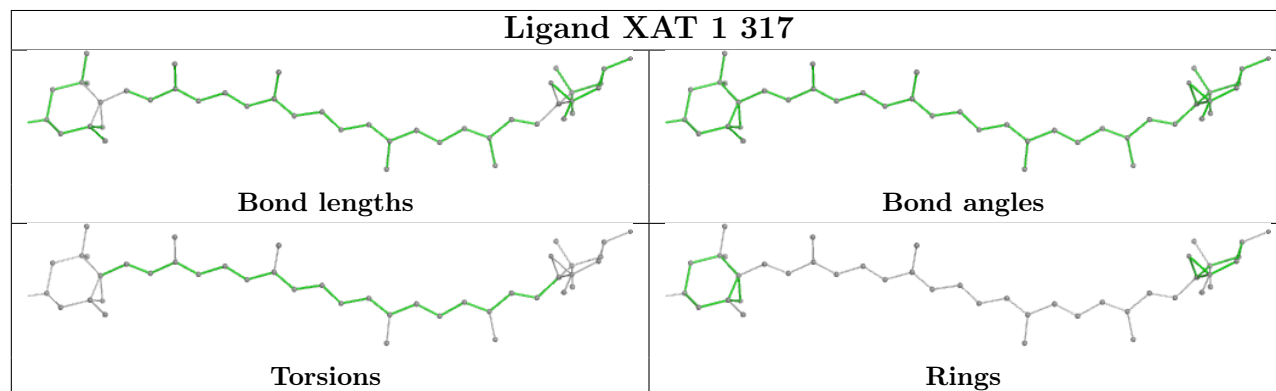
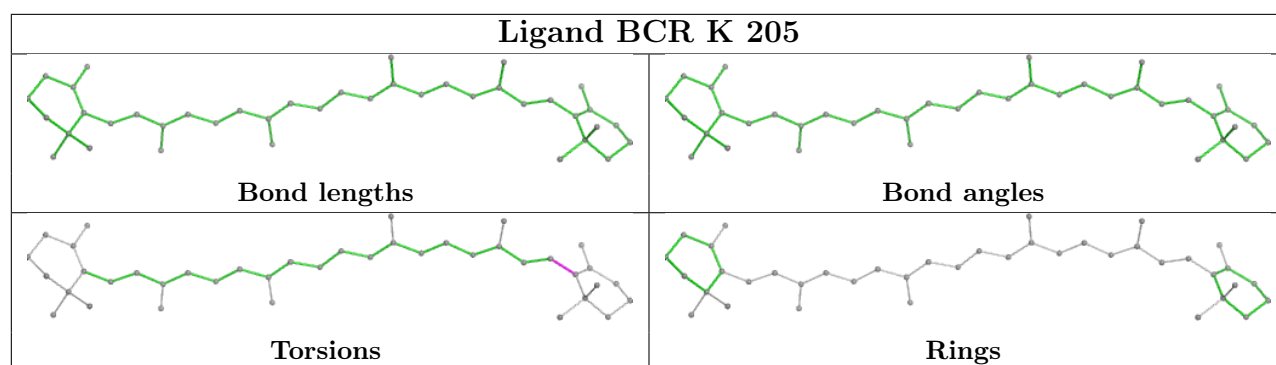
Rings

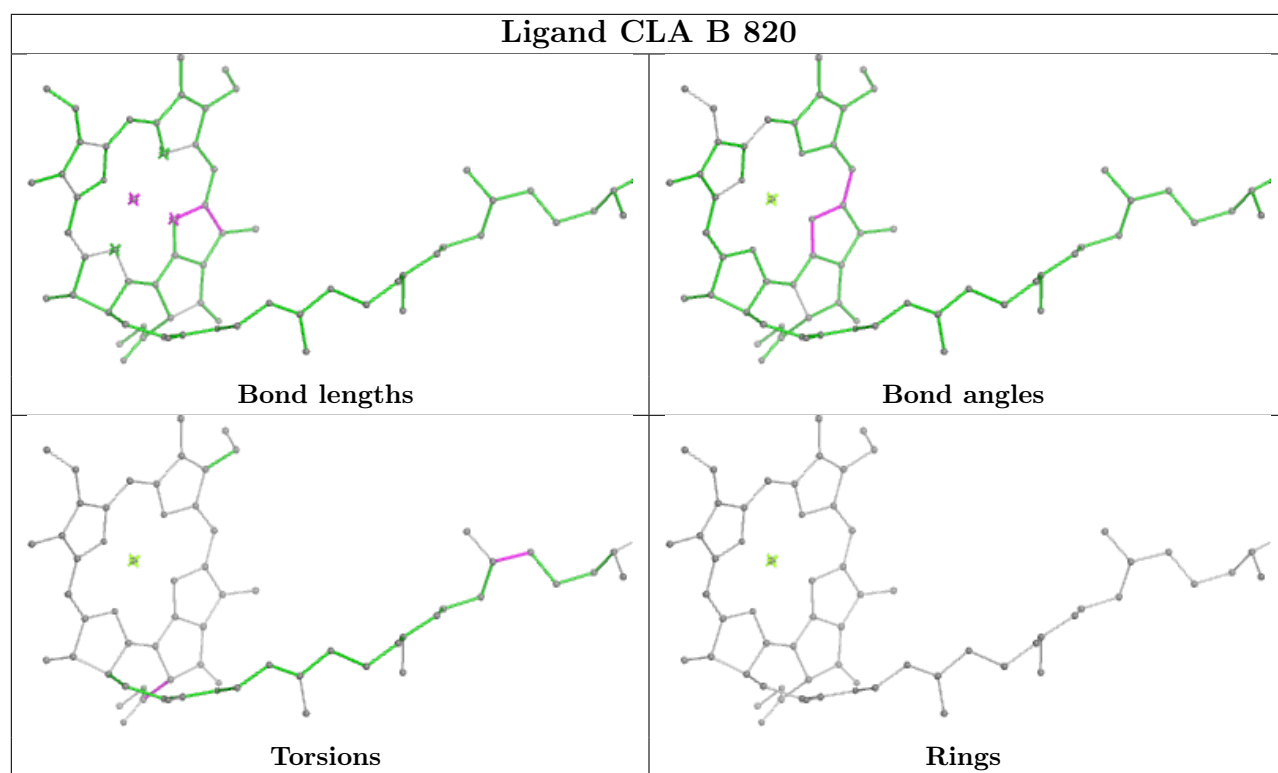
## Ligand CLA A 804



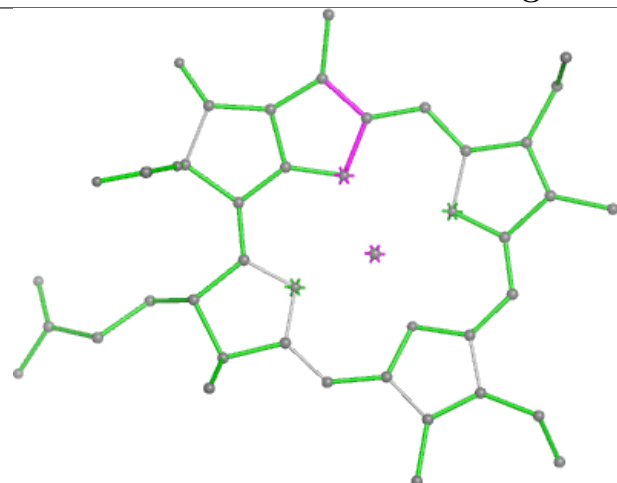
## Ligand CLA 3 308



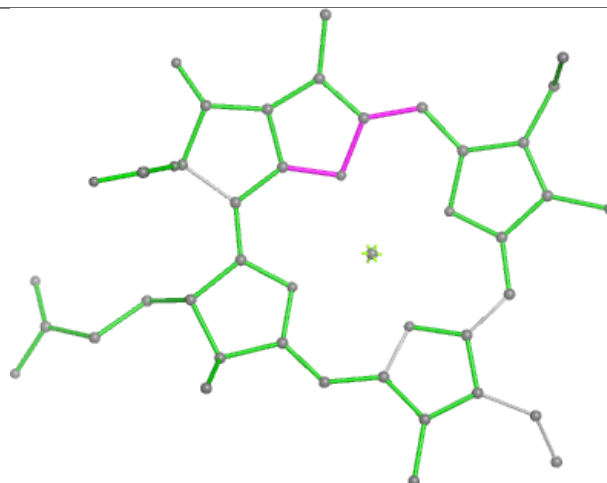




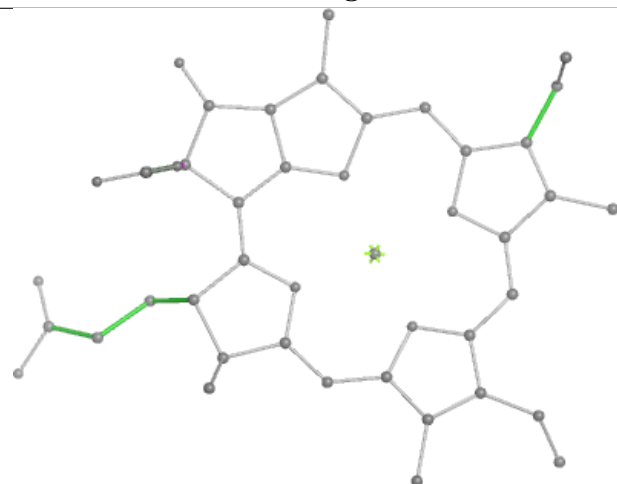
## Ligand CLA 1 315



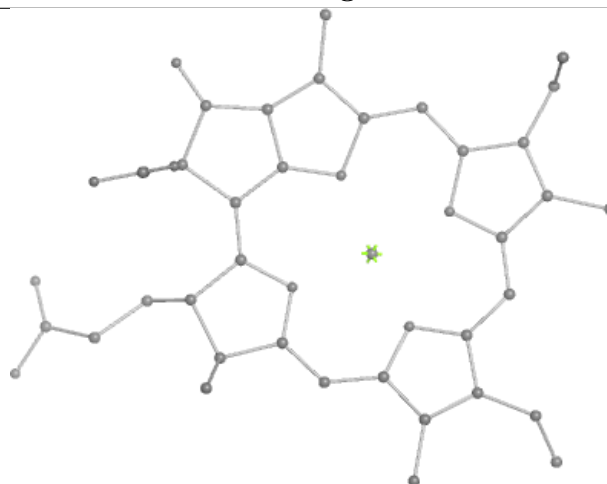
Bond lengths



Bond angles

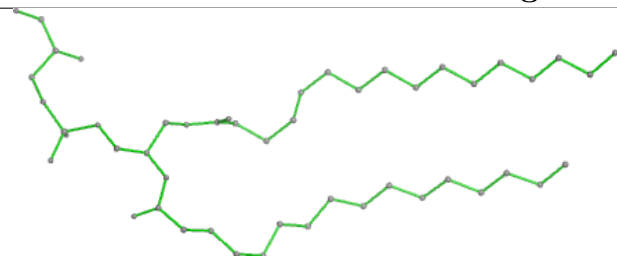


Torsions

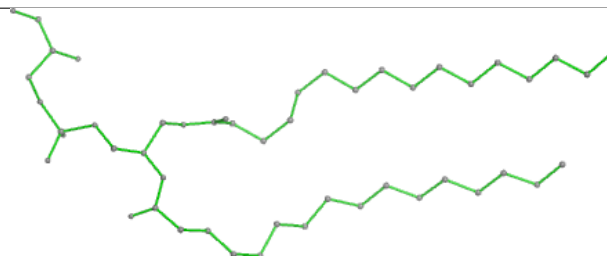


Rings

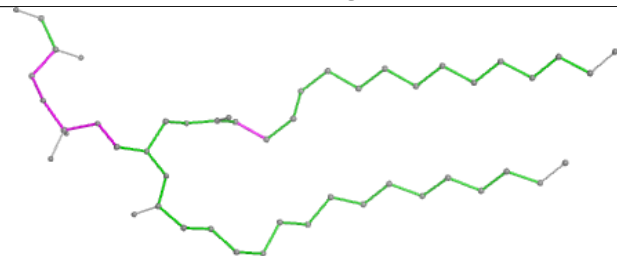
## Ligand LHG 1 319



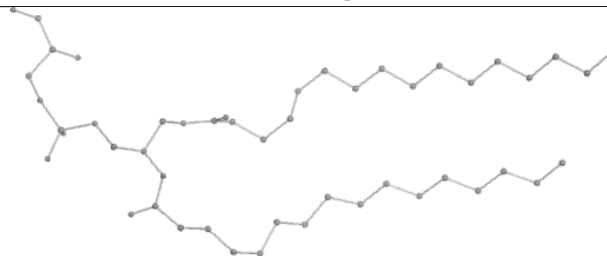
Bond lengths



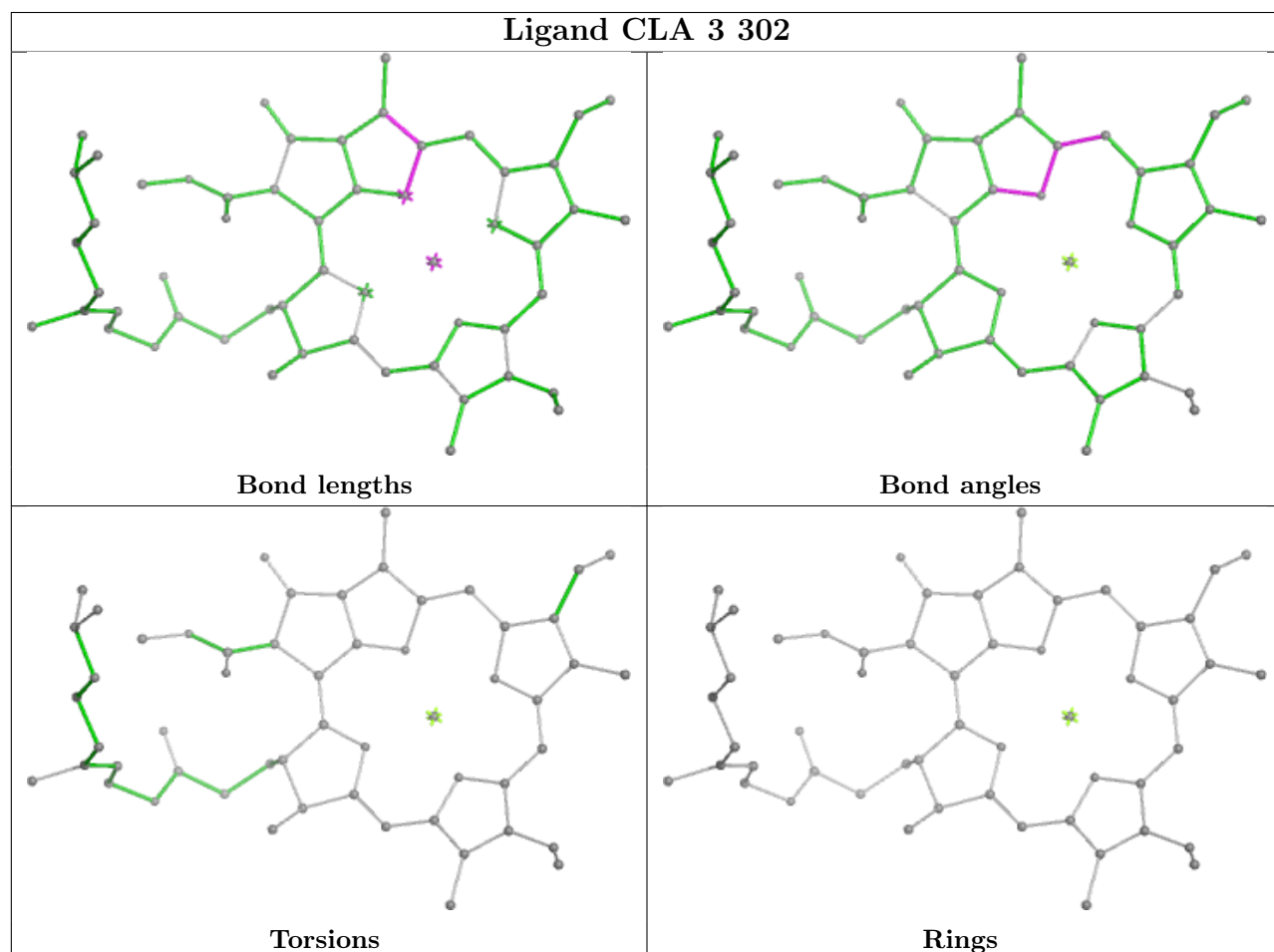
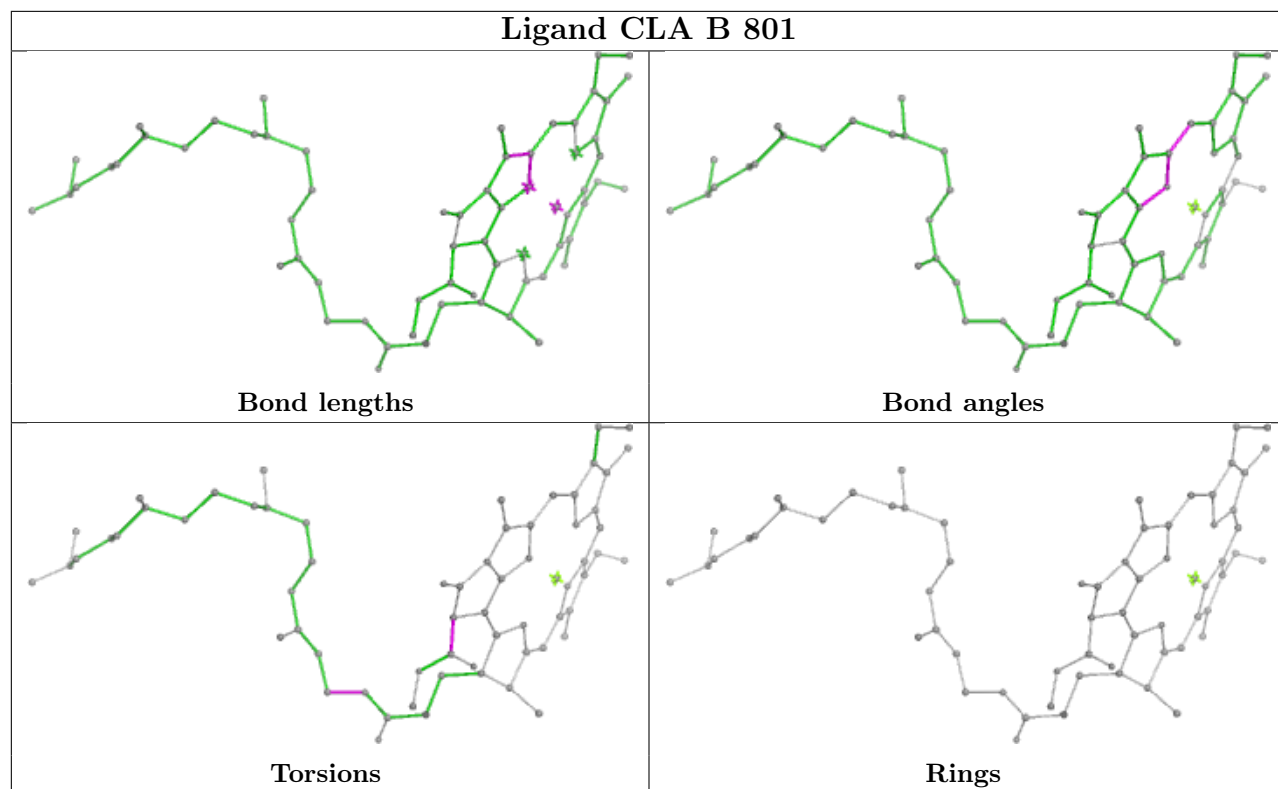
Bond angles



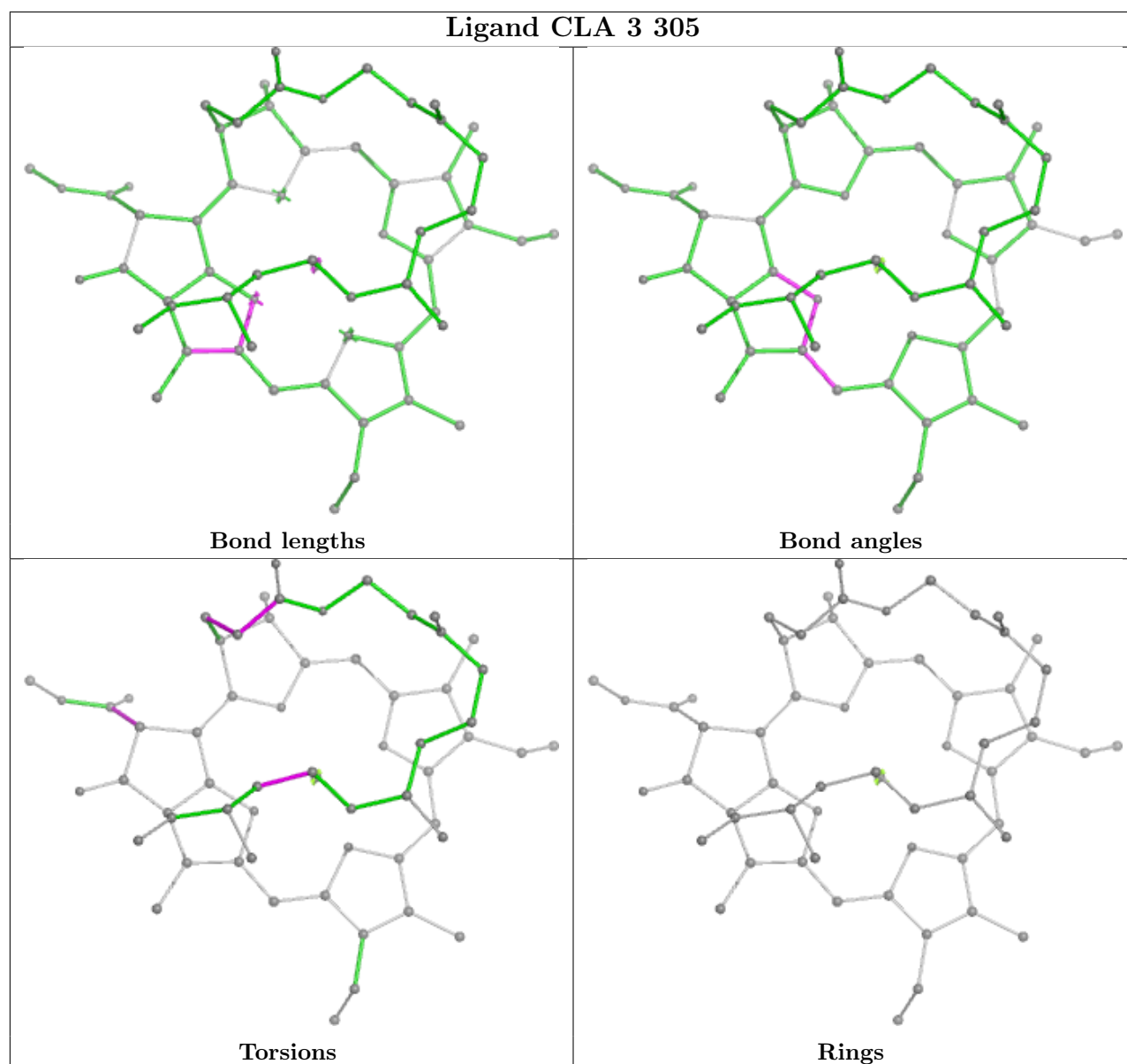
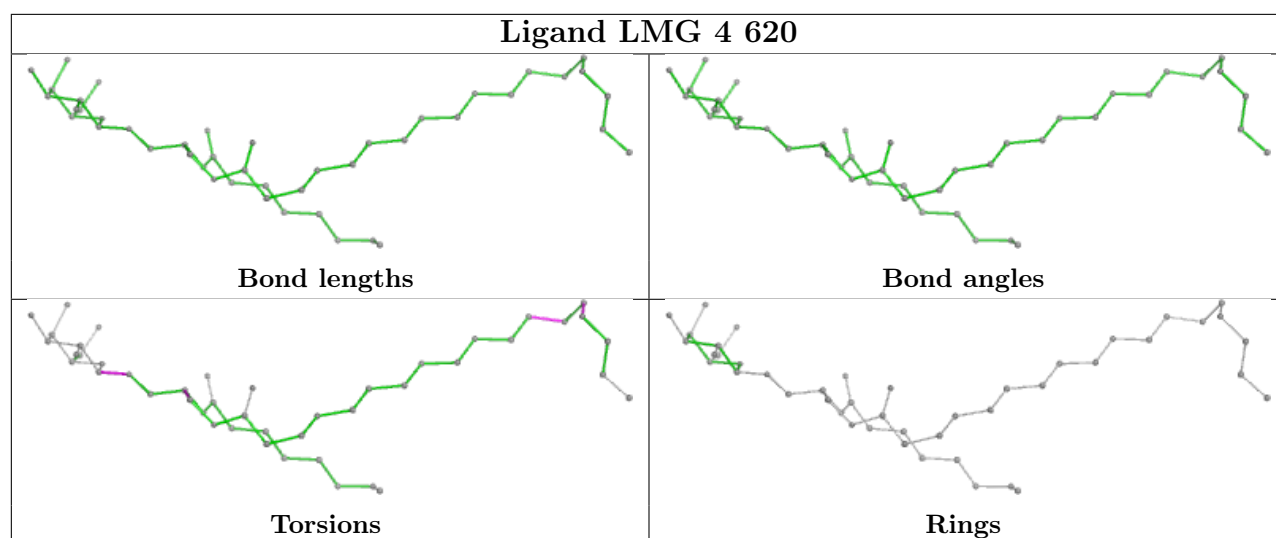
Torsions

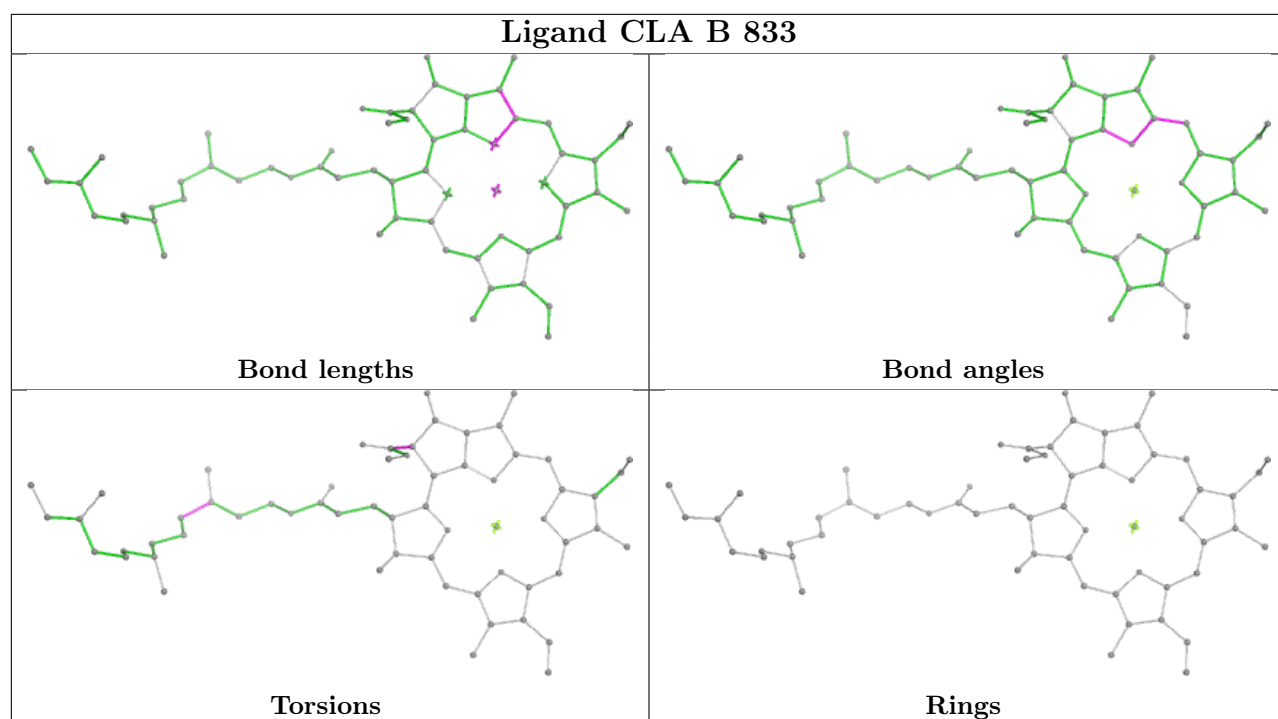


Rings

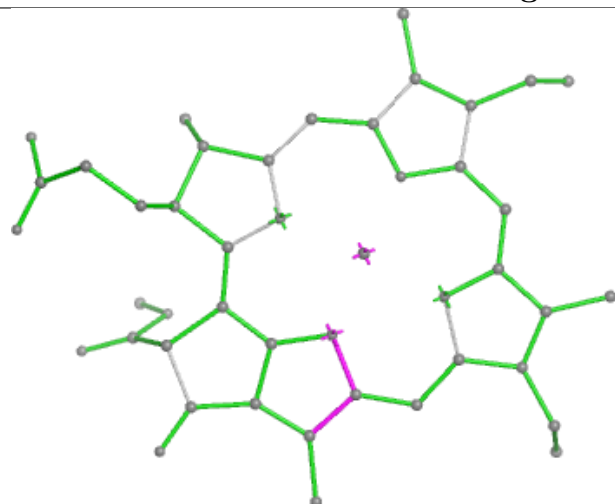




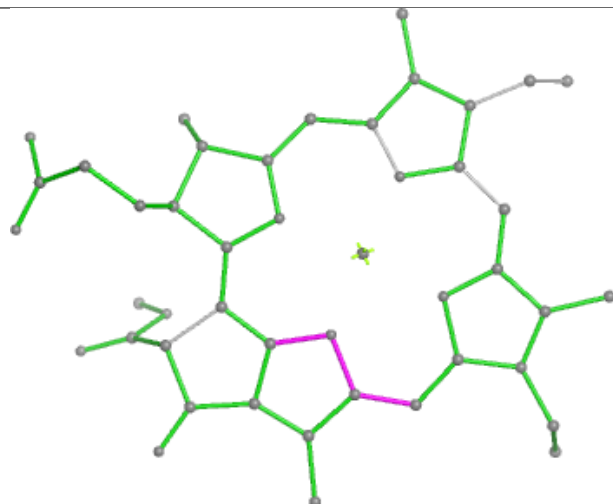




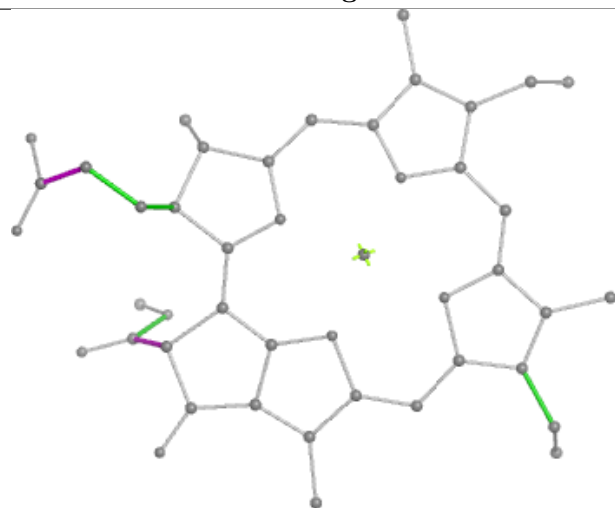
## Ligand CLA 3 309



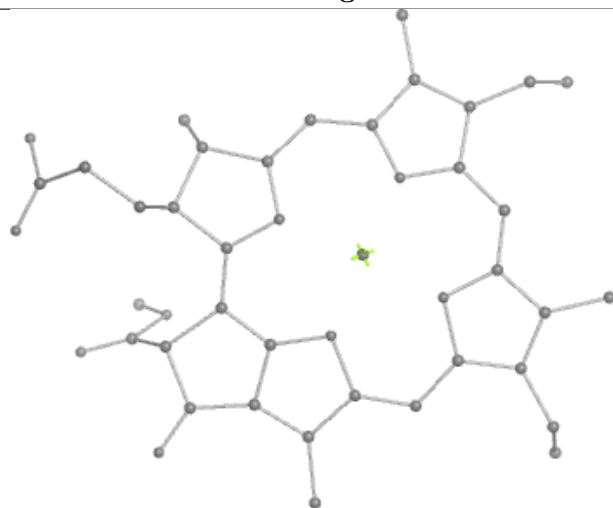
Bond lengths



Bond angles

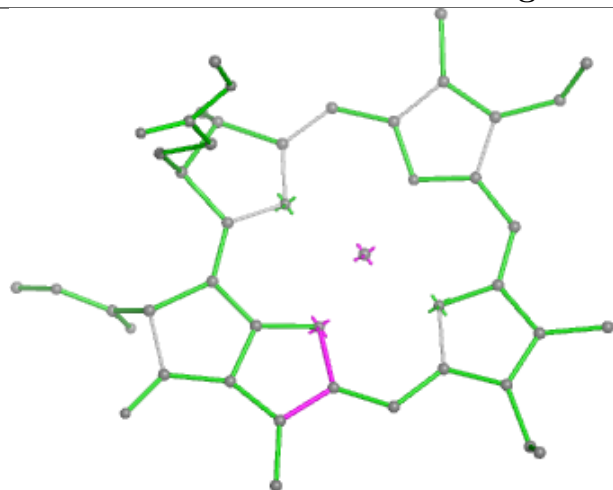


Torsions

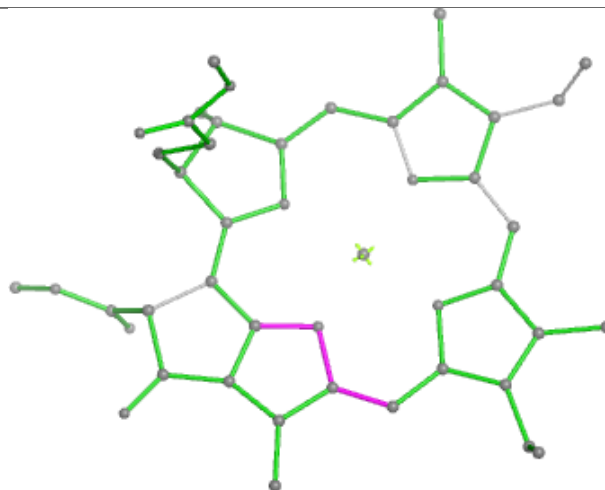


Rings

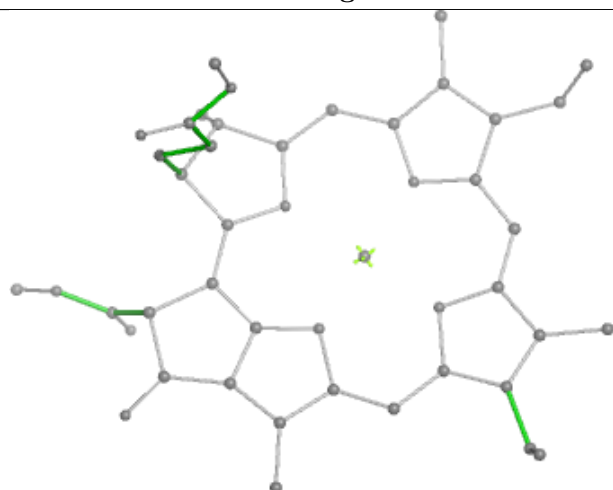
## Ligand CLA 4 613



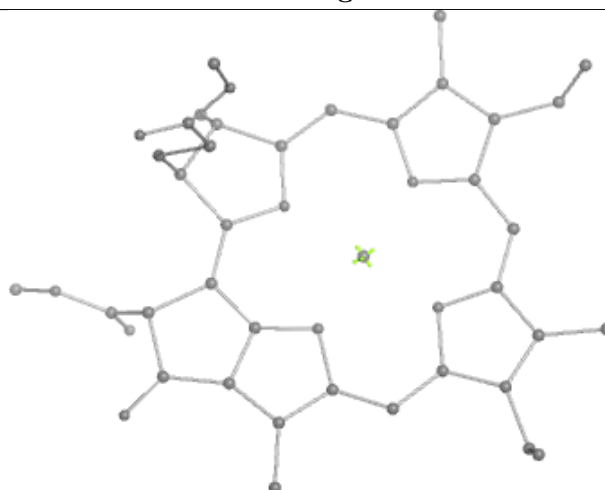
Bond lengths



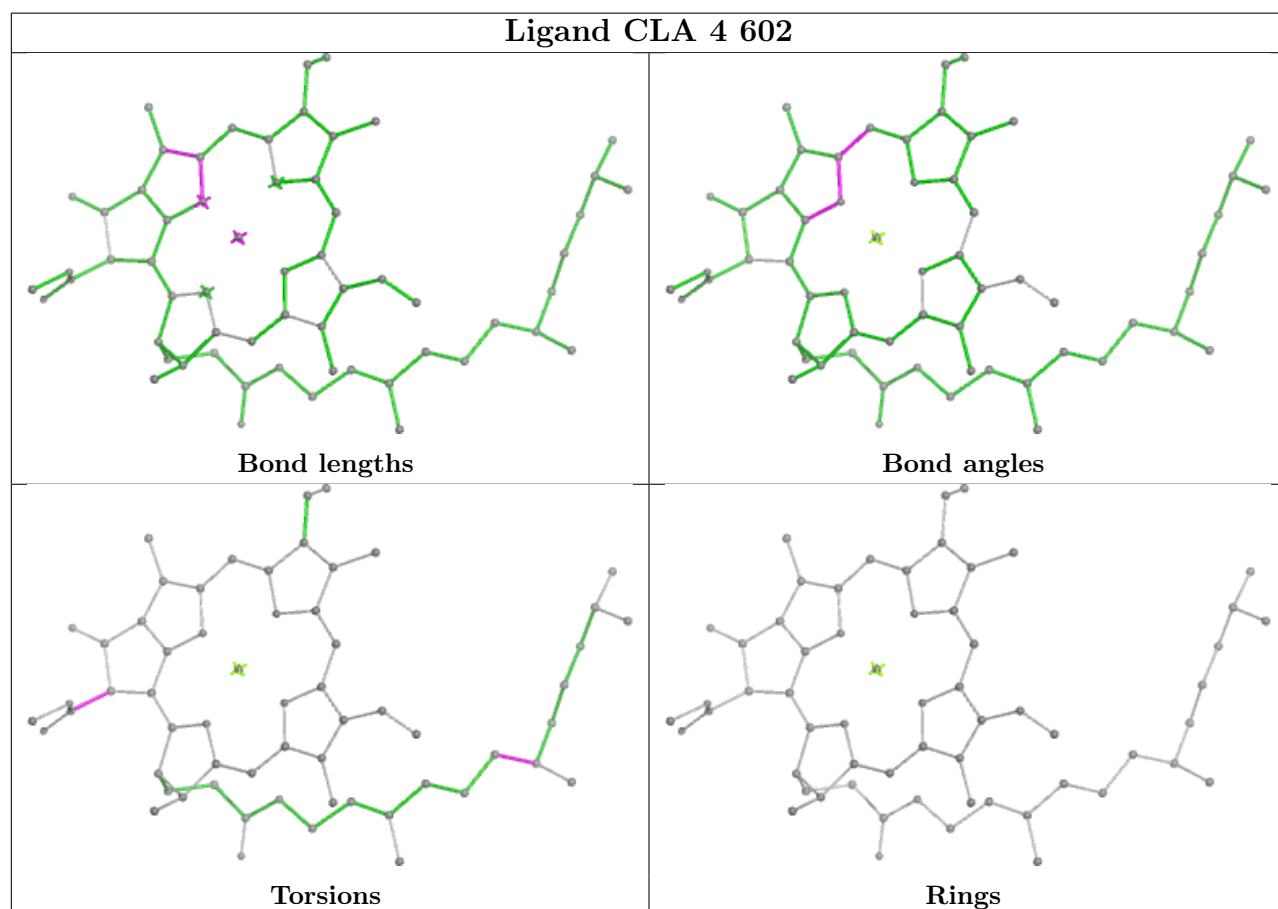
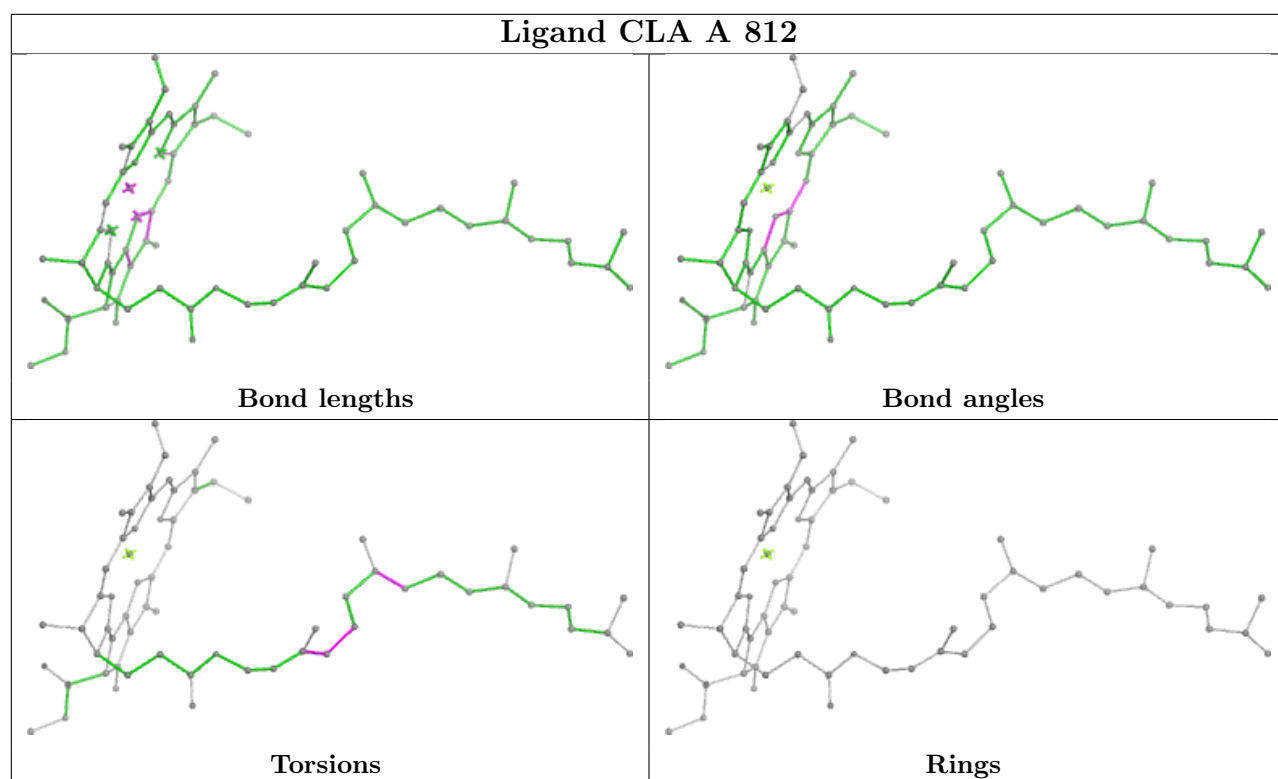
Bond angles

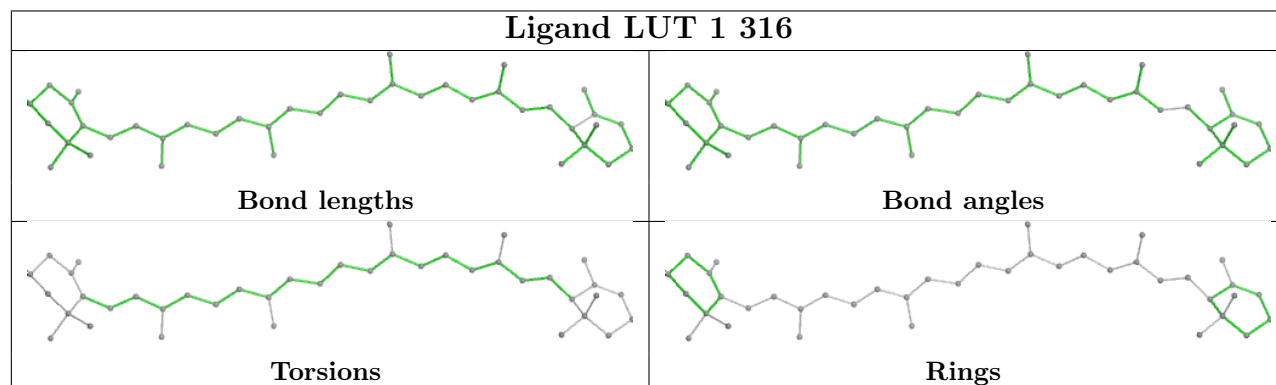
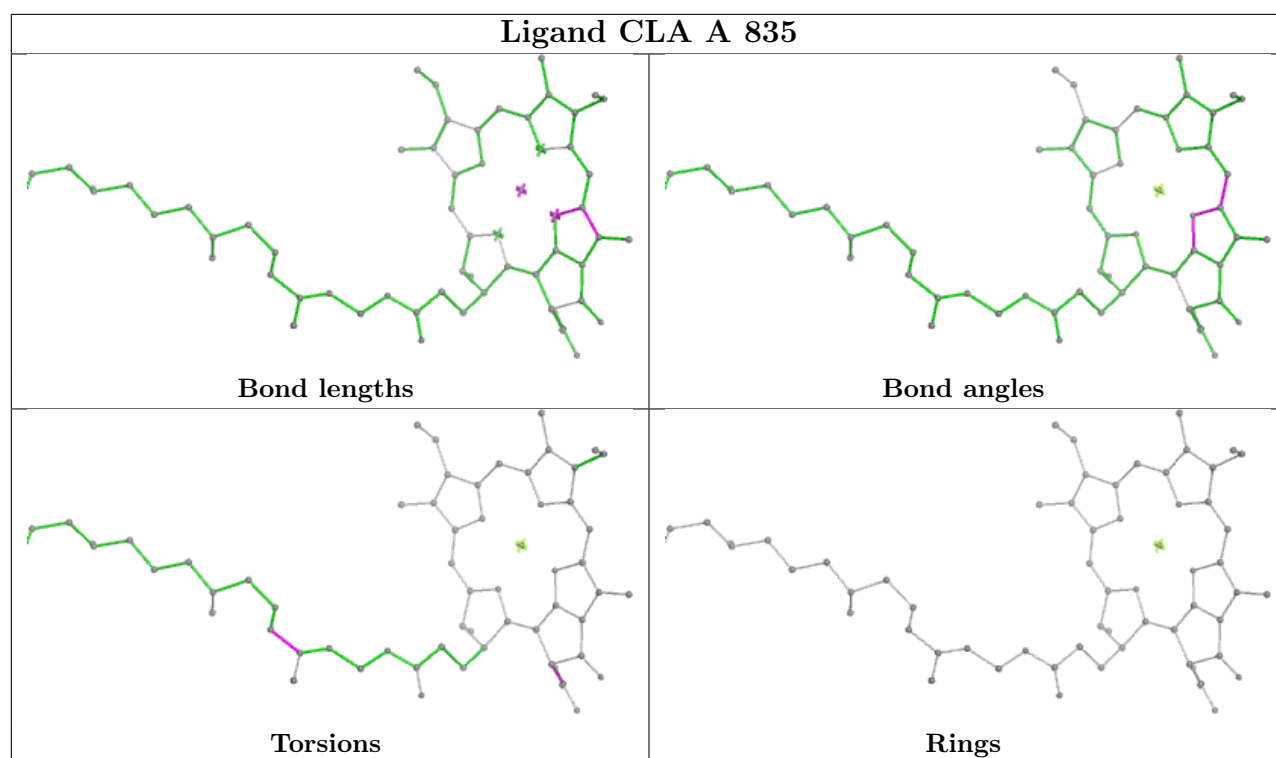


Torsions

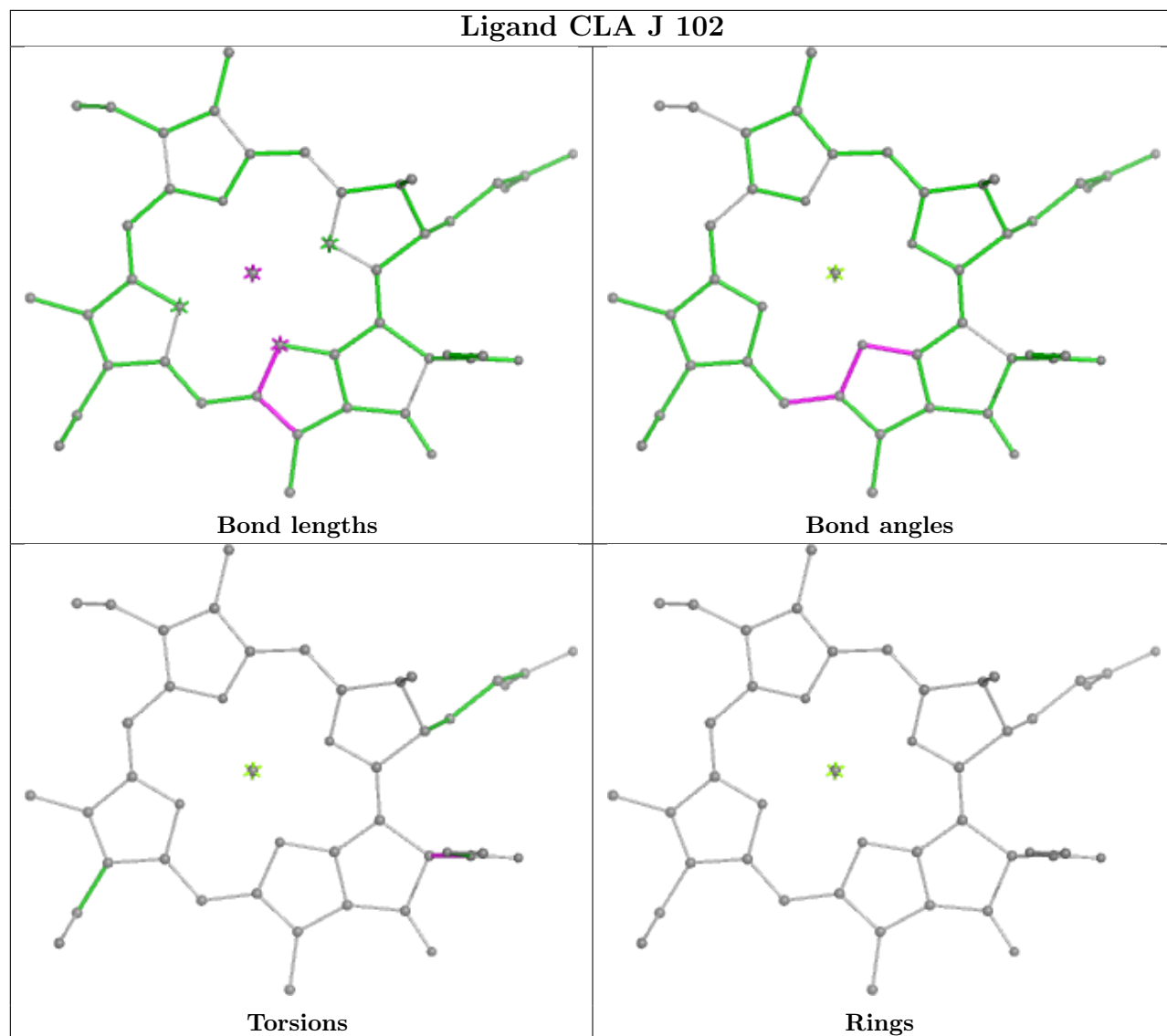


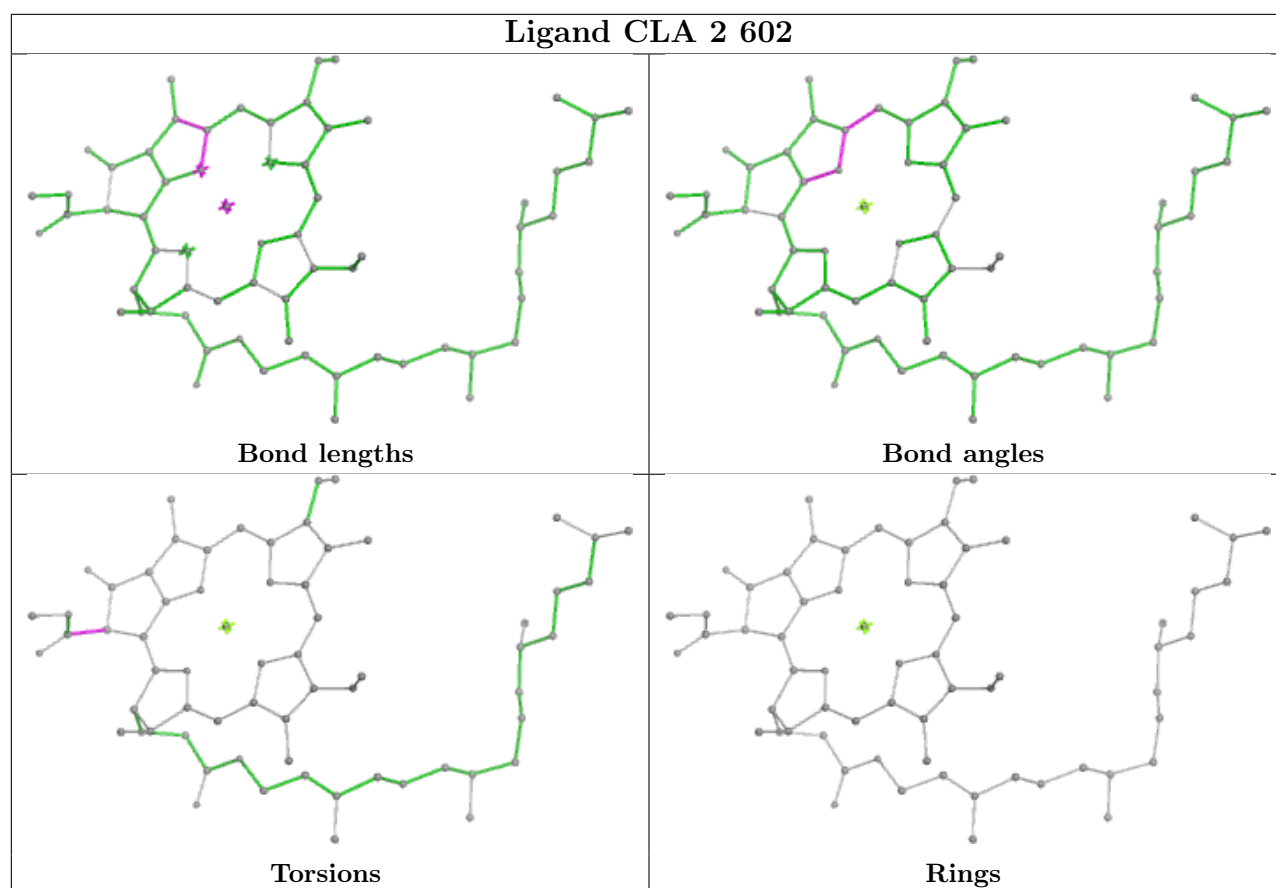
Rings





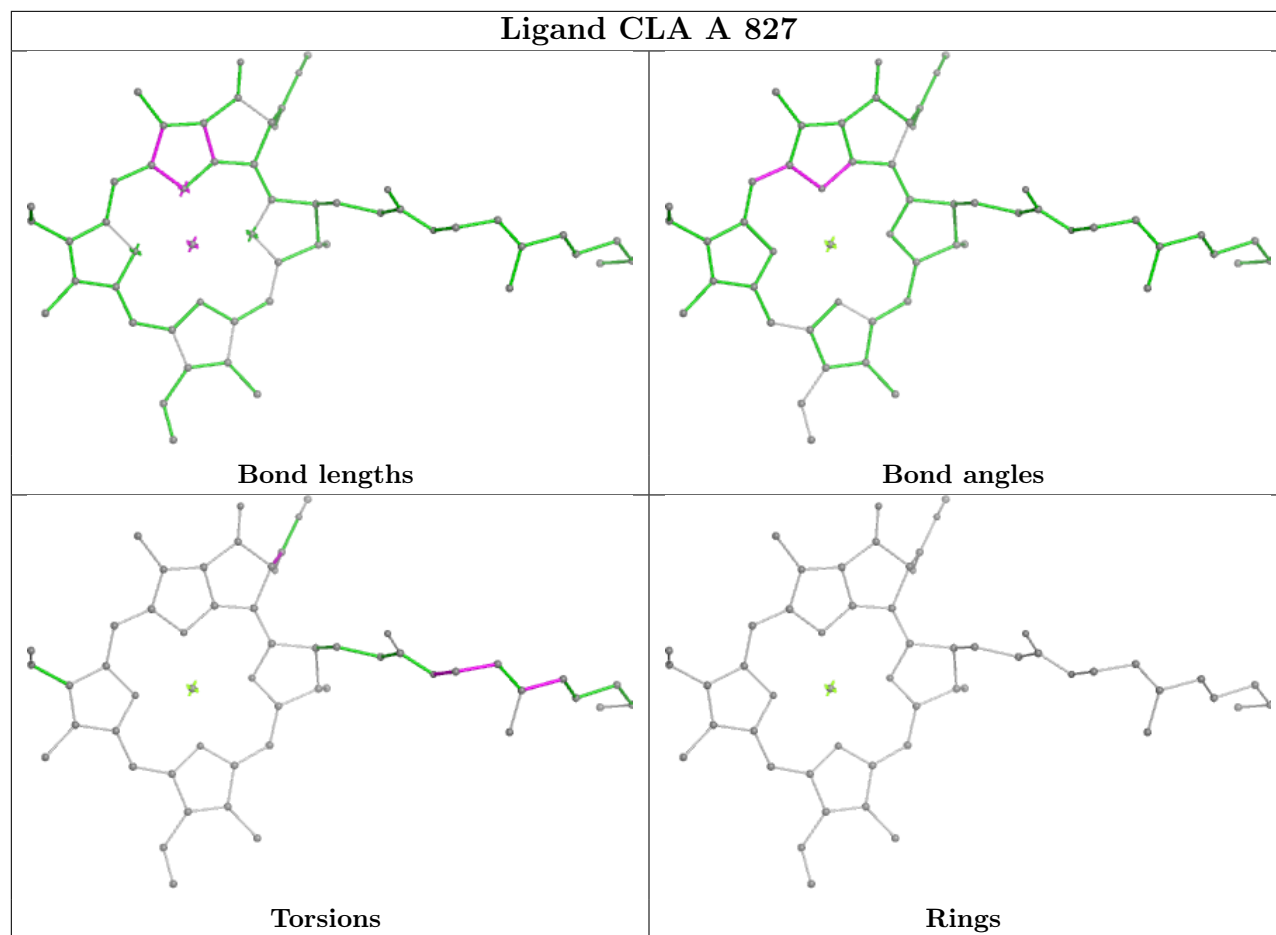
## Ligand CLA J 102



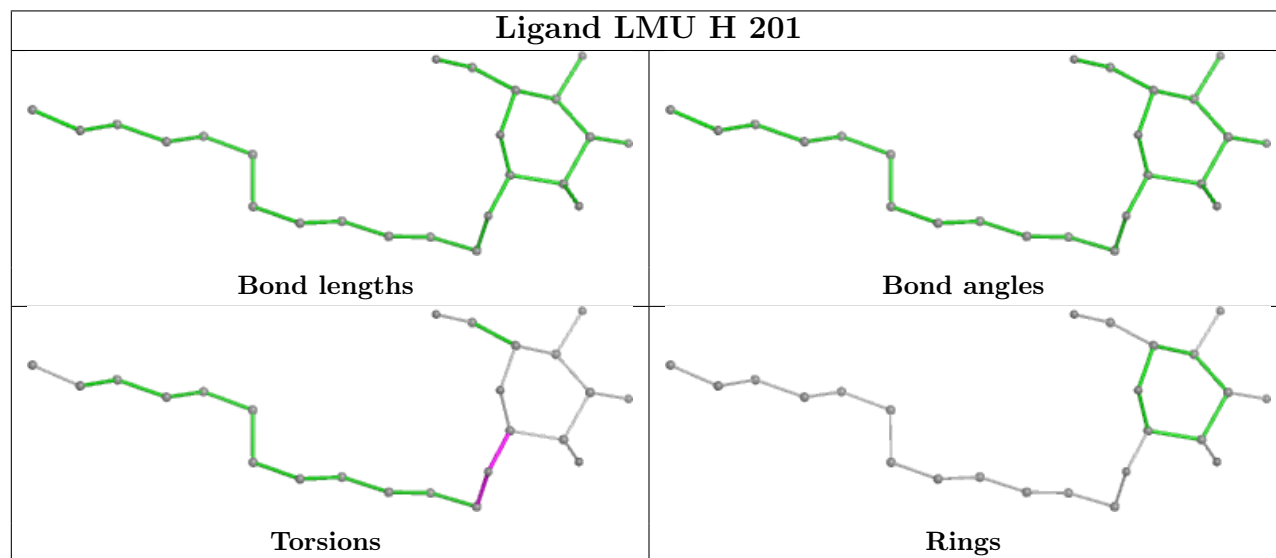


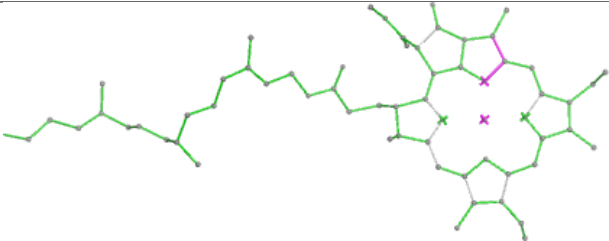
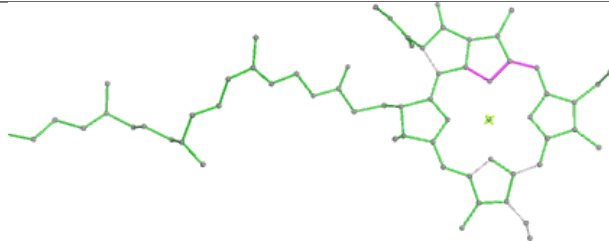
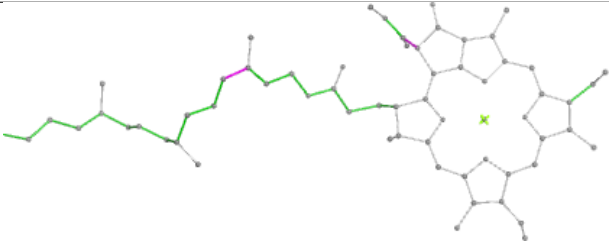
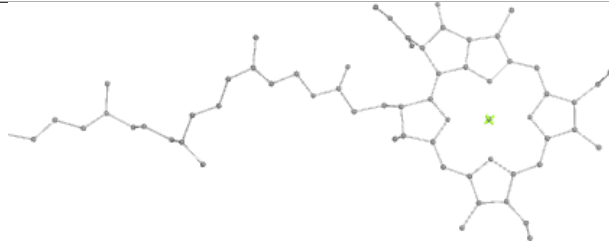


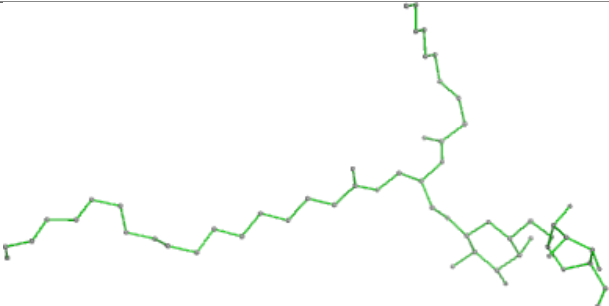
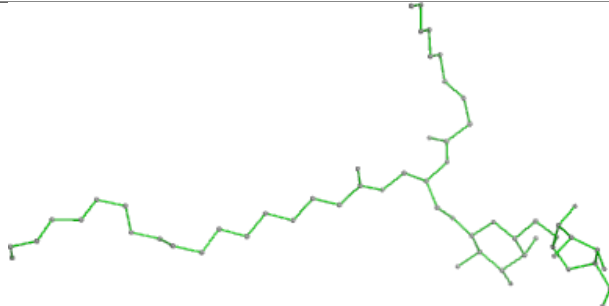
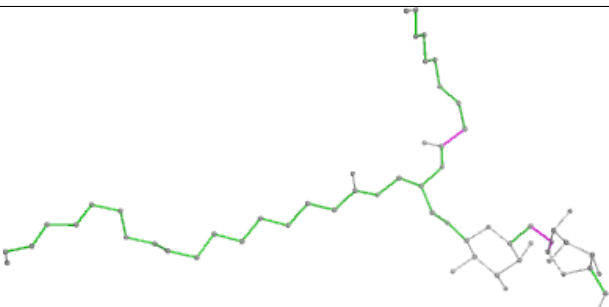
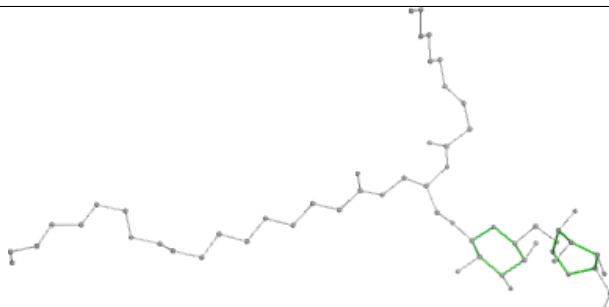
## Ligand CLA A 827

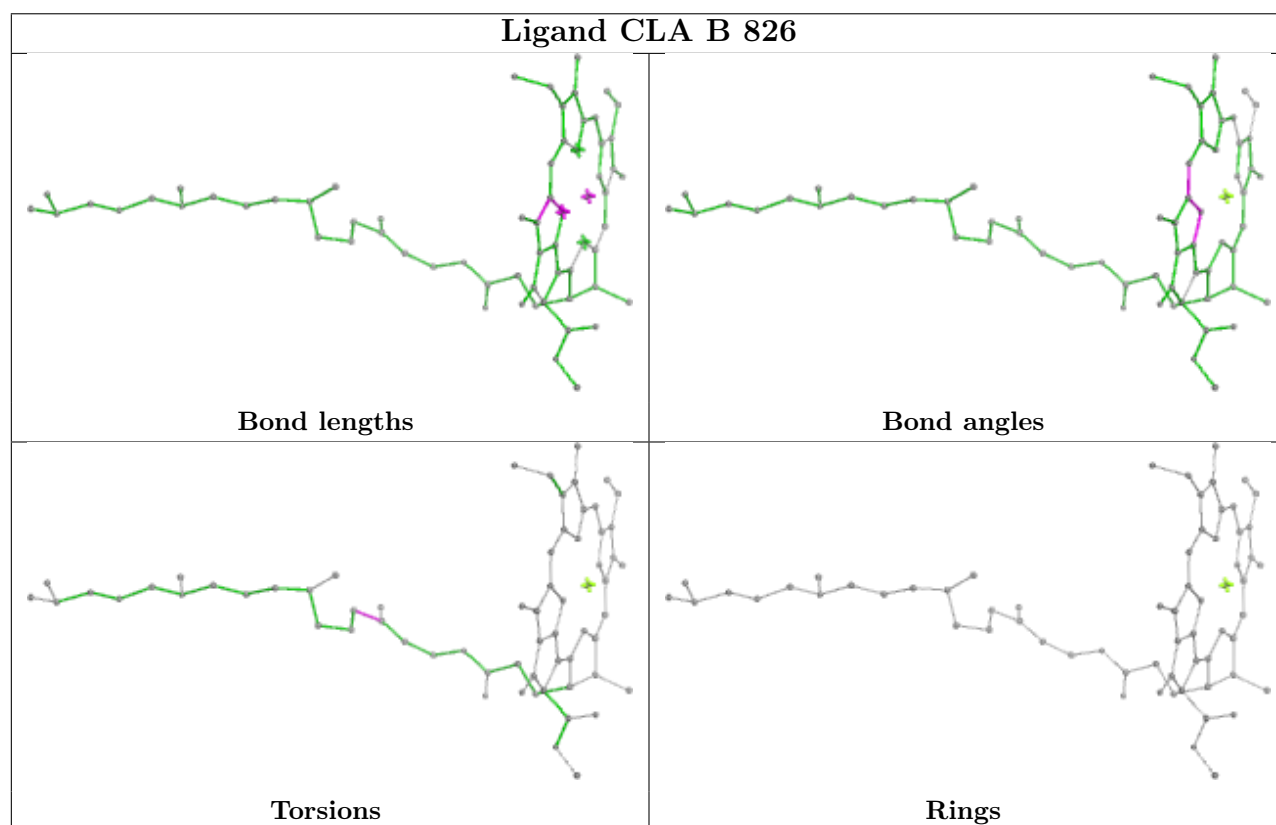
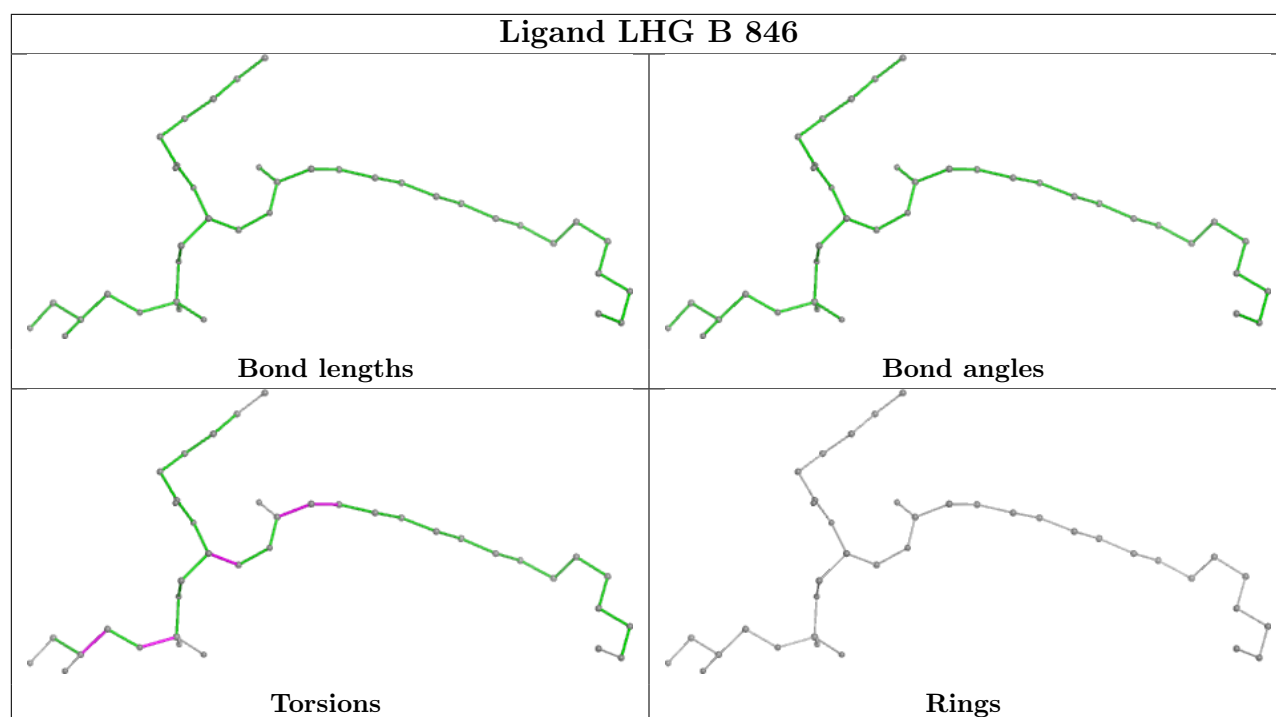


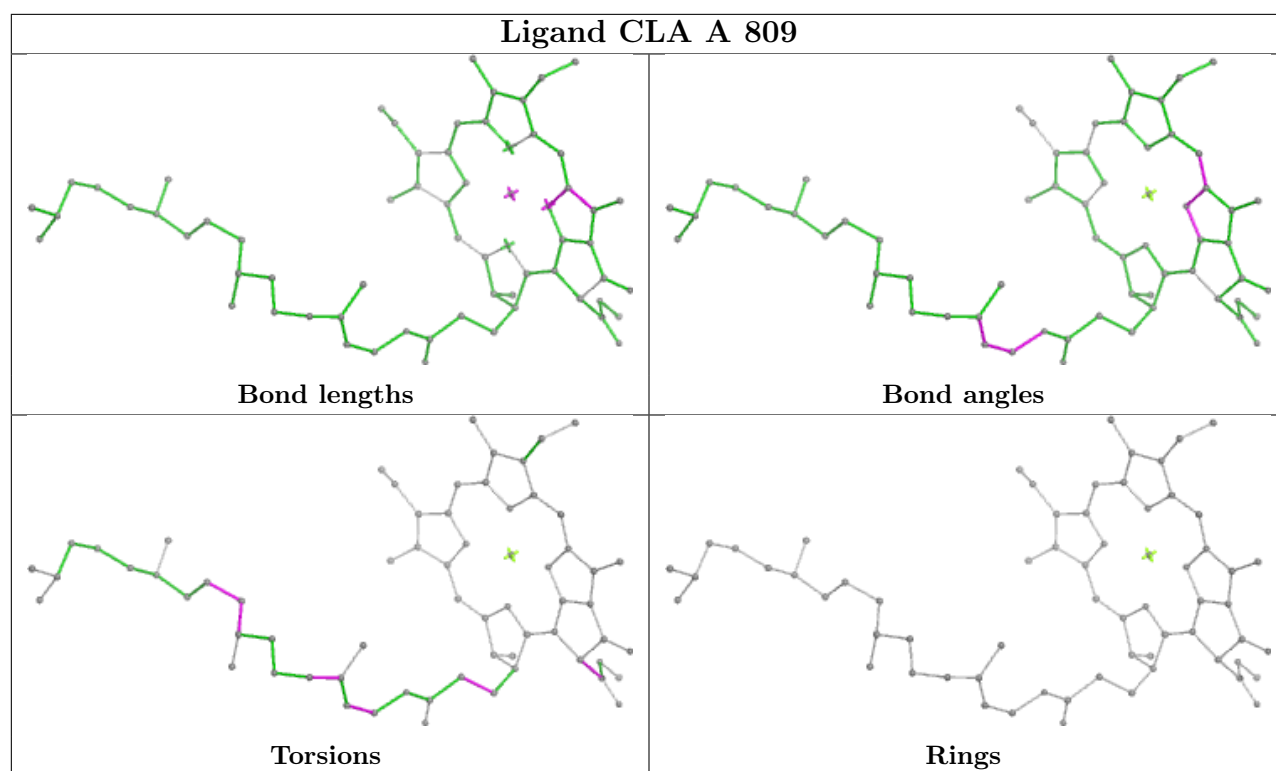
## Ligand LMU H 201



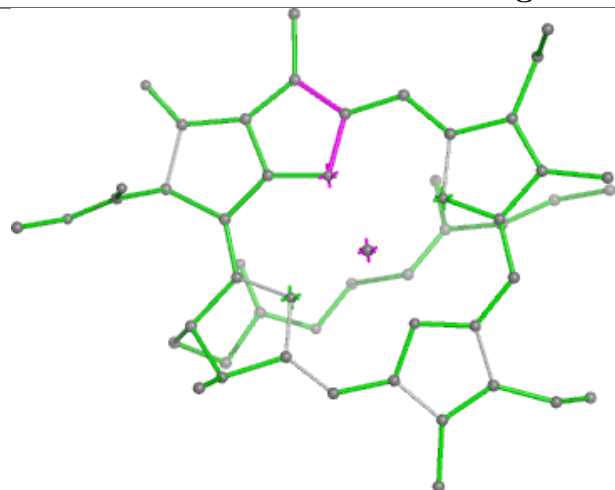
Ligand CLA A 834	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGD J 104	
	
Bond lengths	Bond angles
	
Torsions	Rings

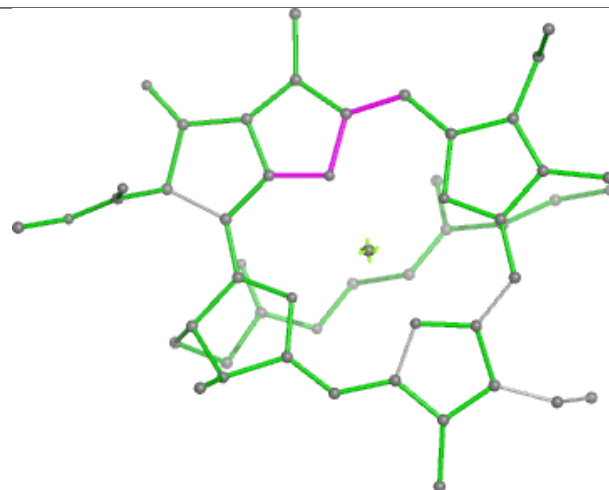




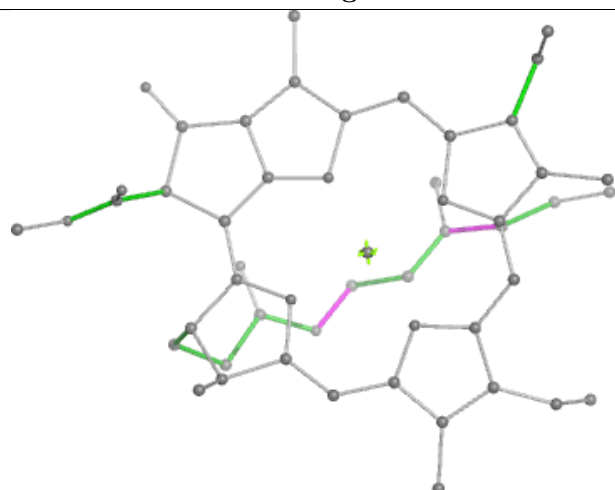
## Ligand CLA A 823



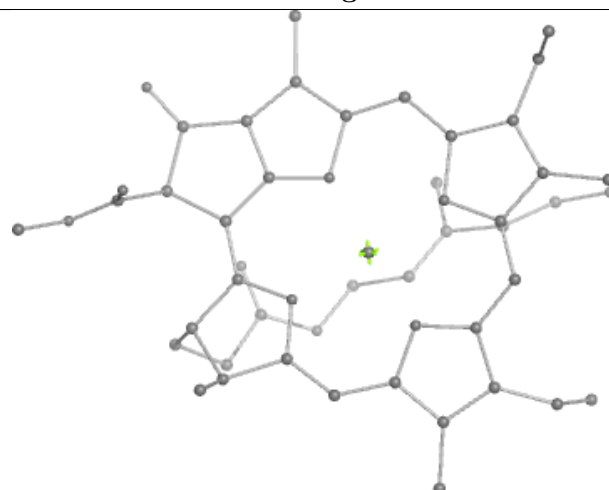
Bond lengths



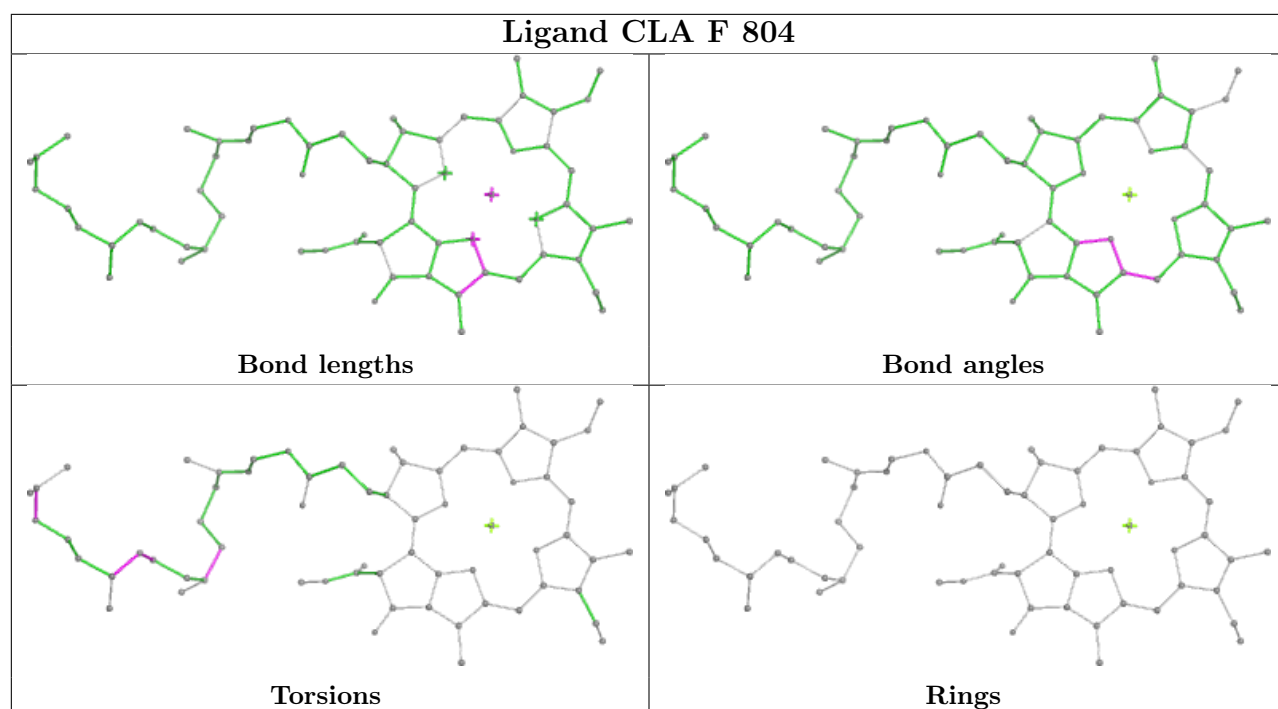
Bond angles



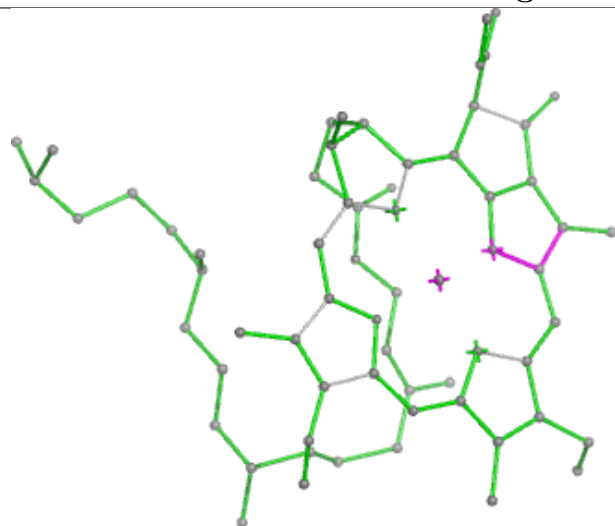
Torsions



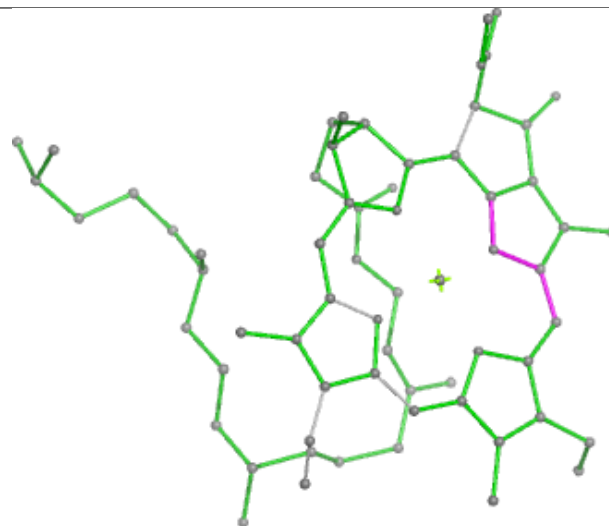
Rings



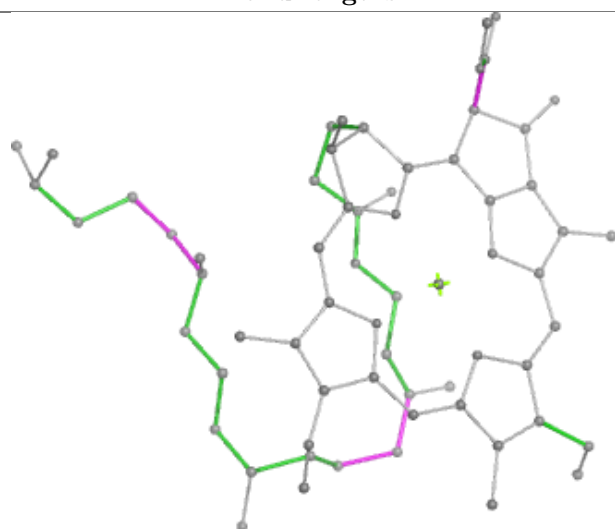
## Ligand CLA B 807



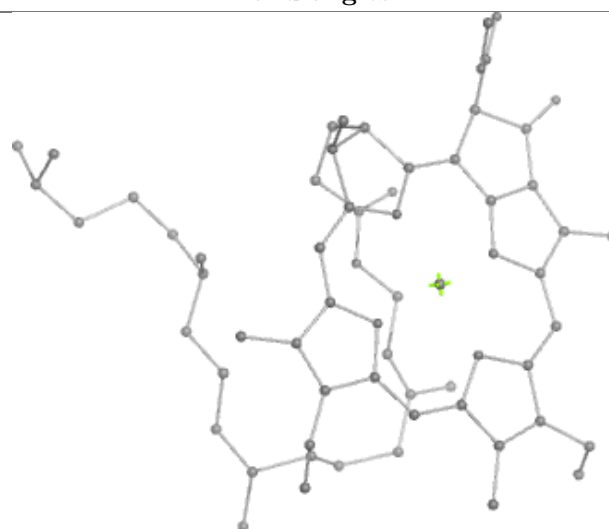
Bond lengths



Bond angles

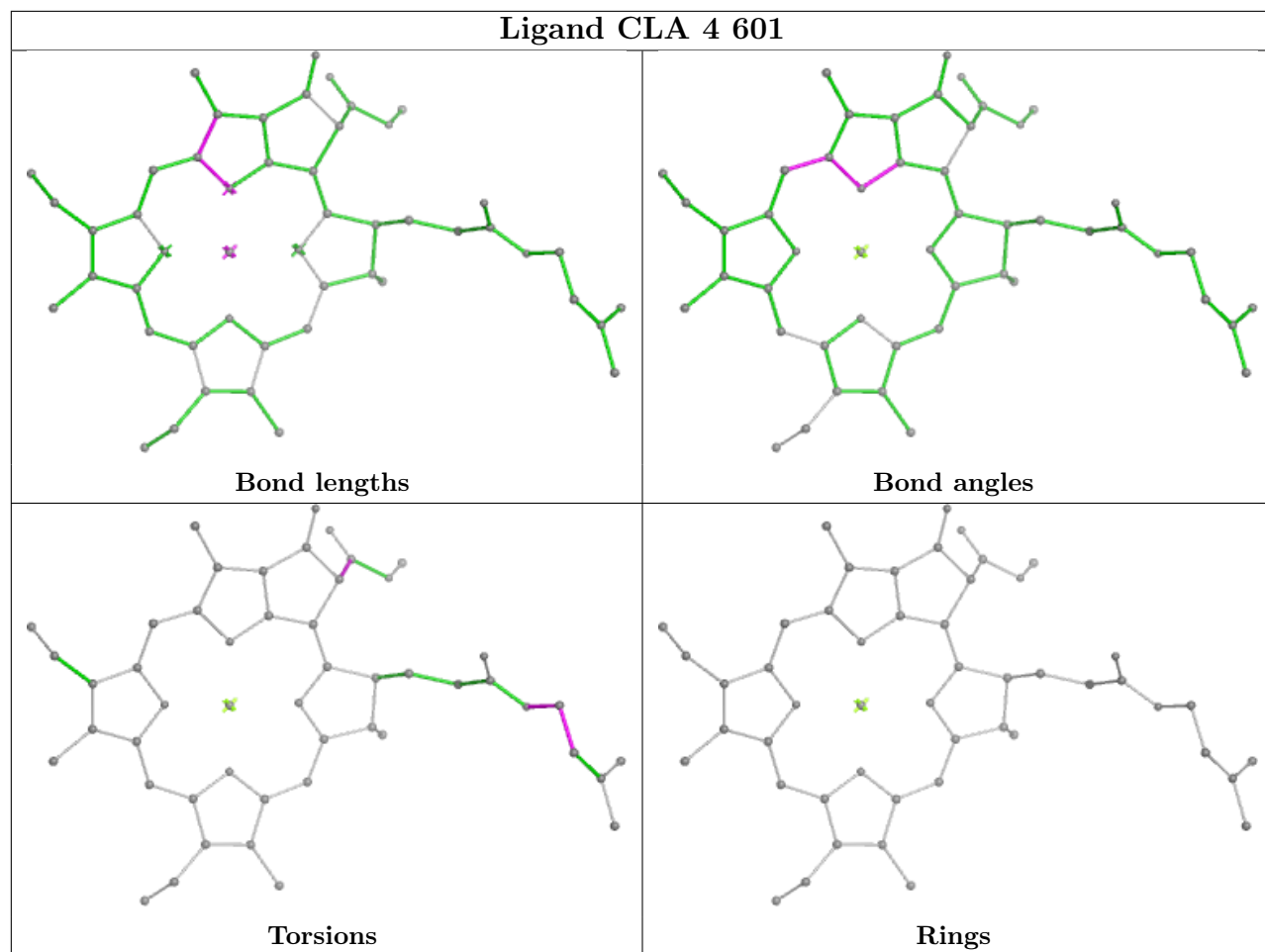


Torsions



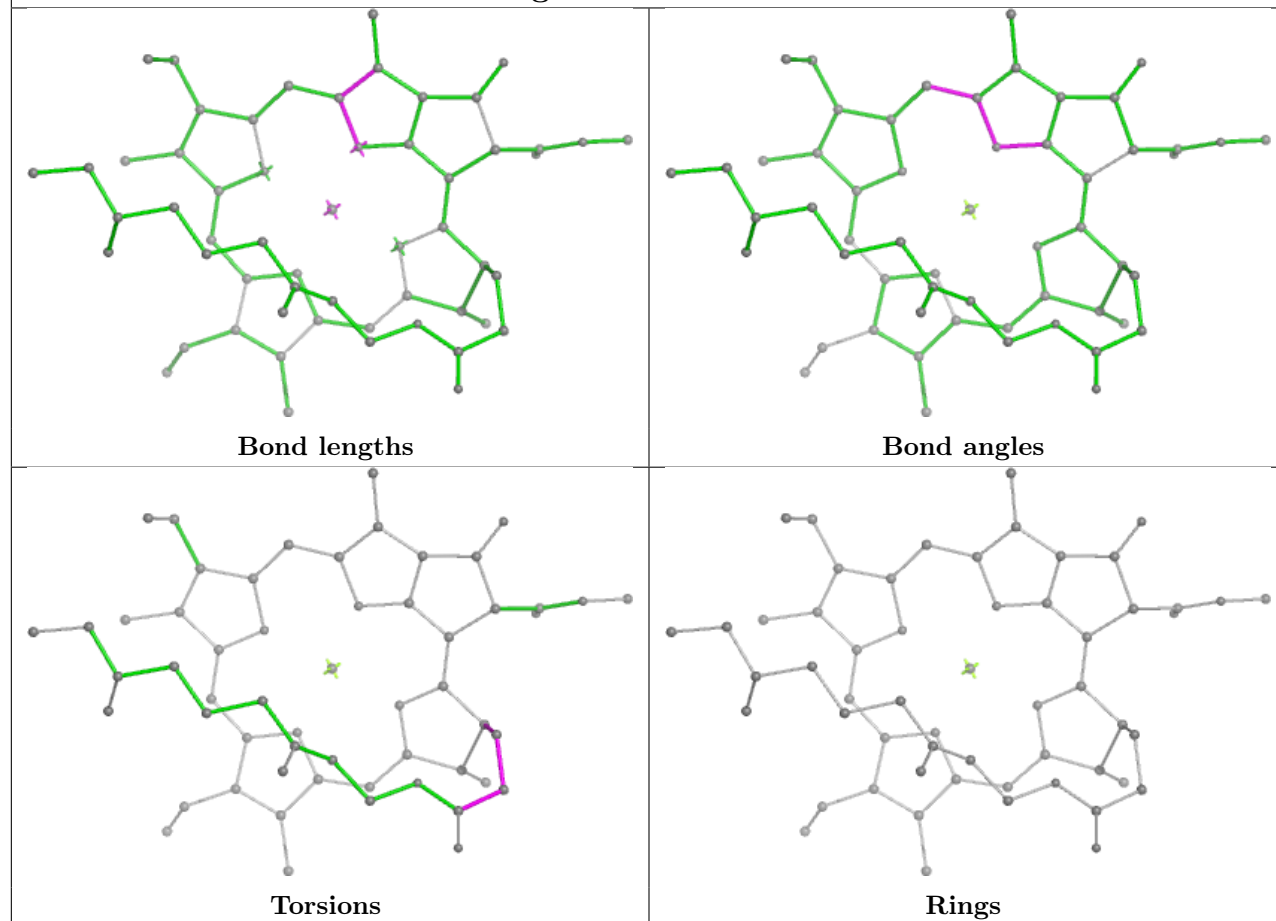
Rings

## Ligand CLA 4 601

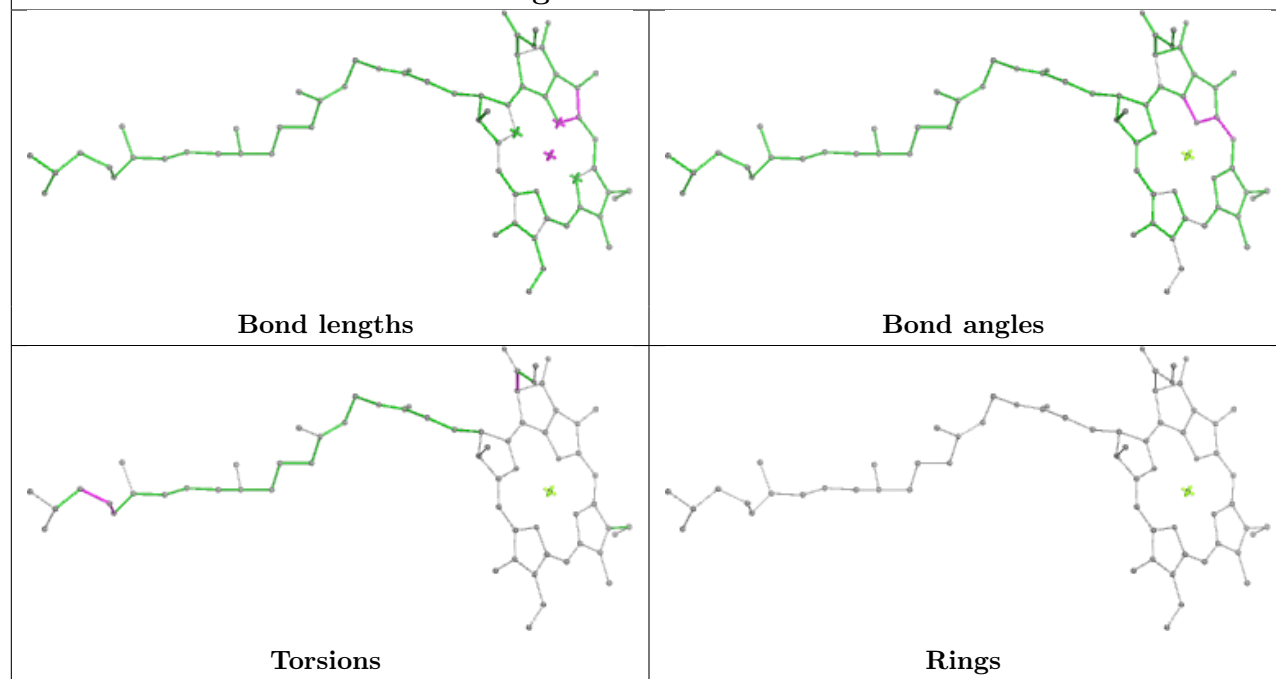


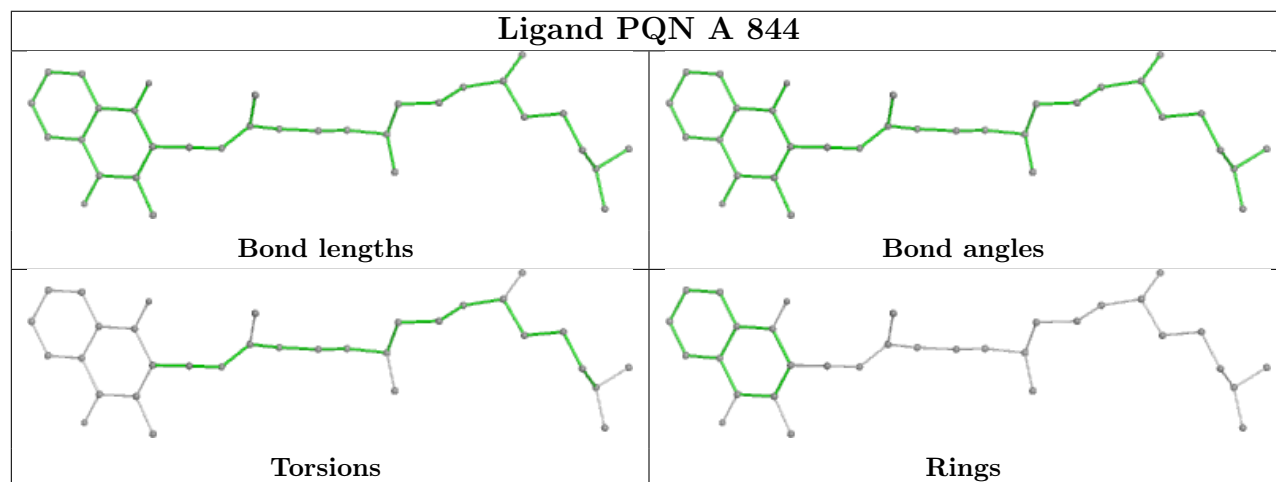
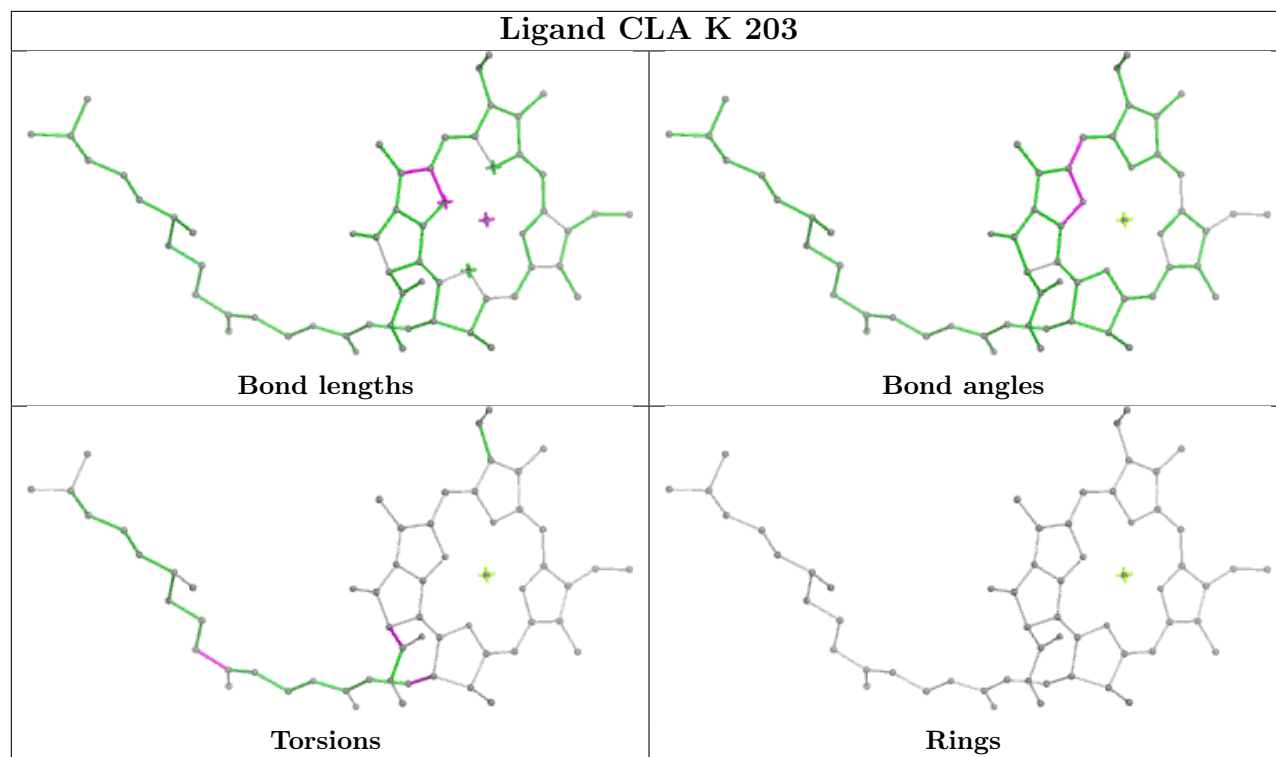


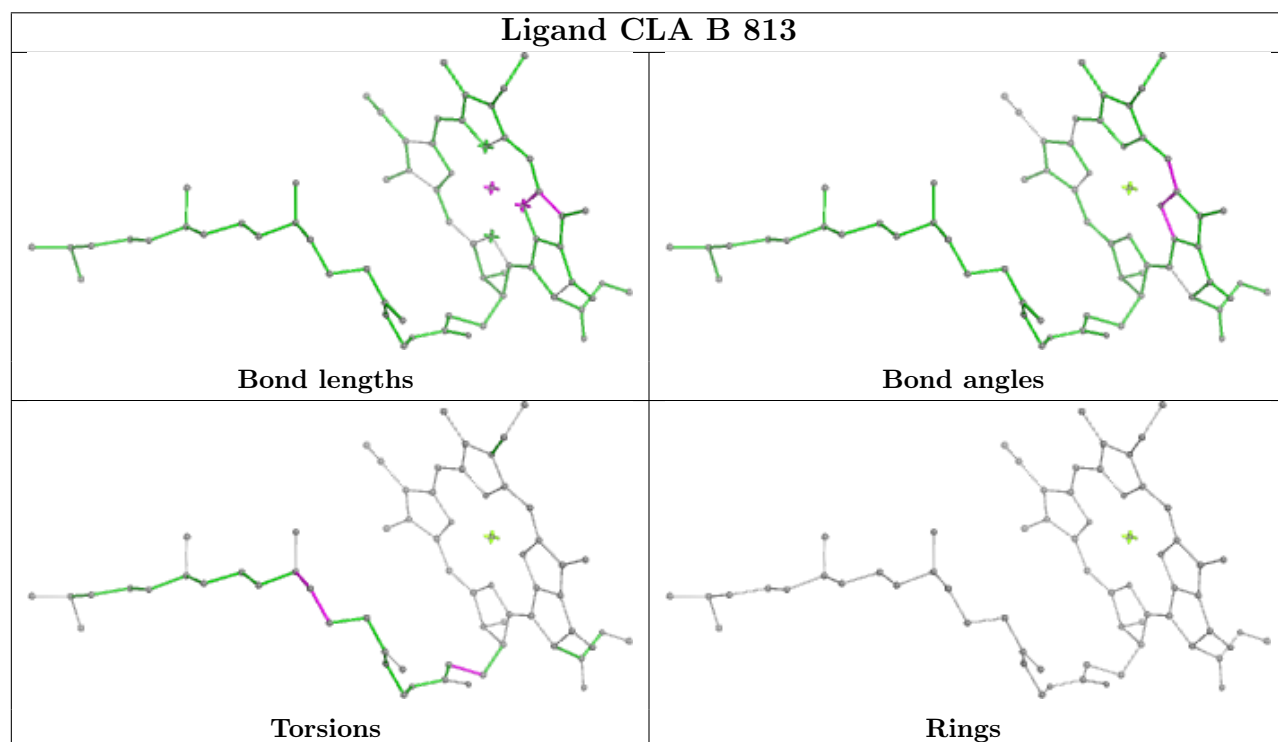
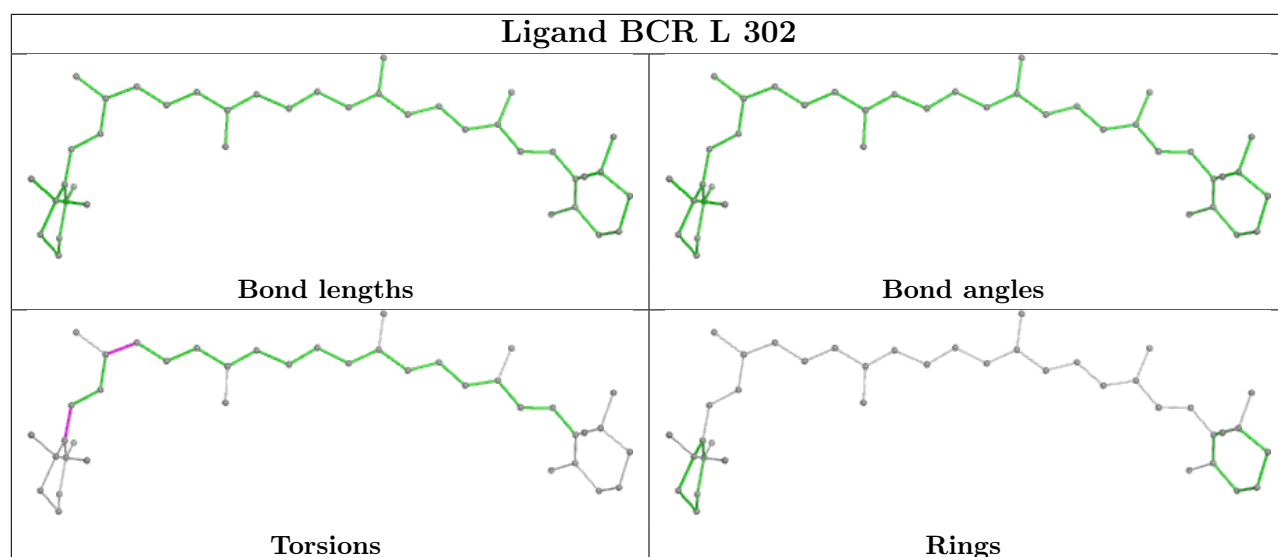
## Ligand CLA A 819



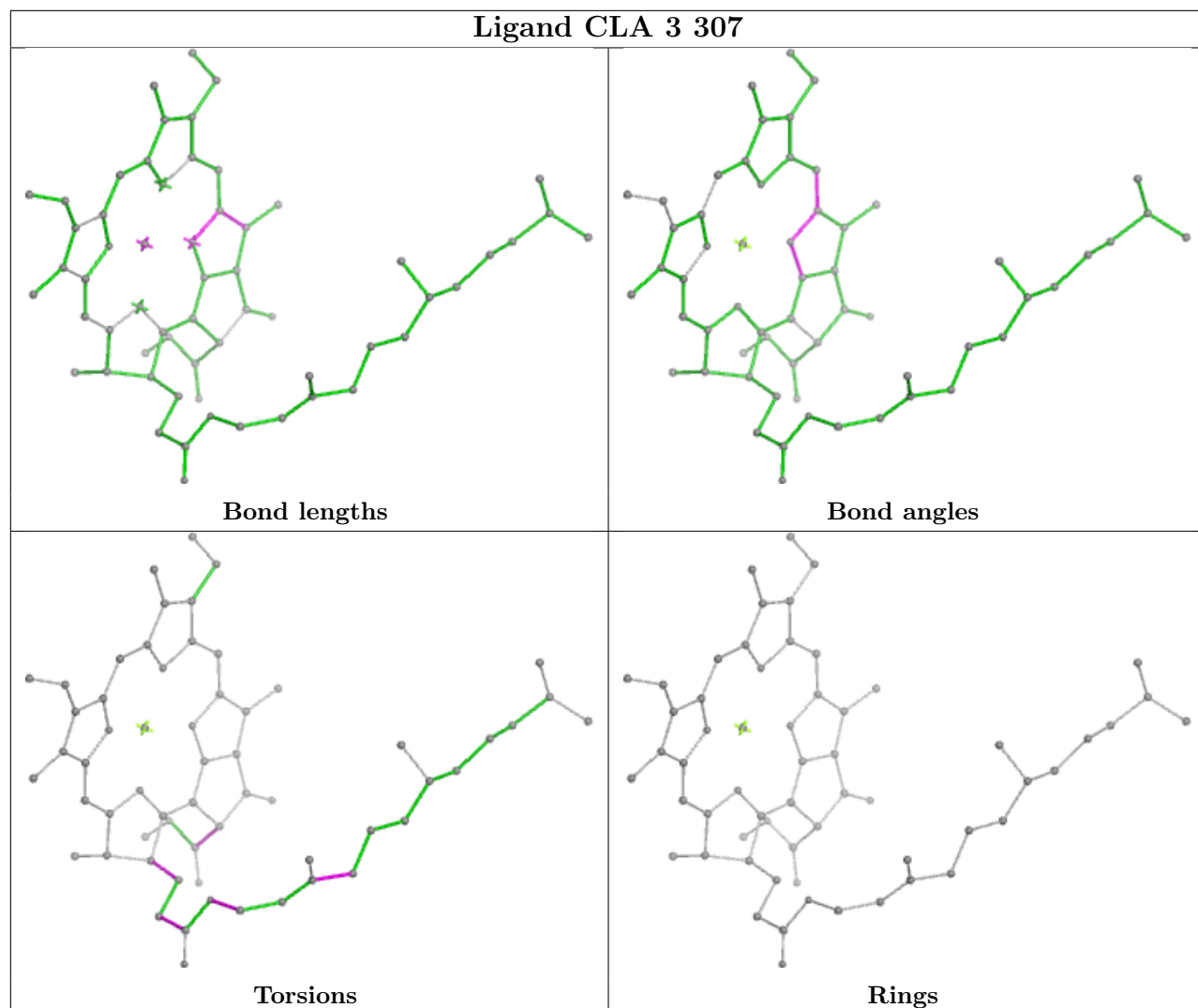
## Ligand CLA B 830

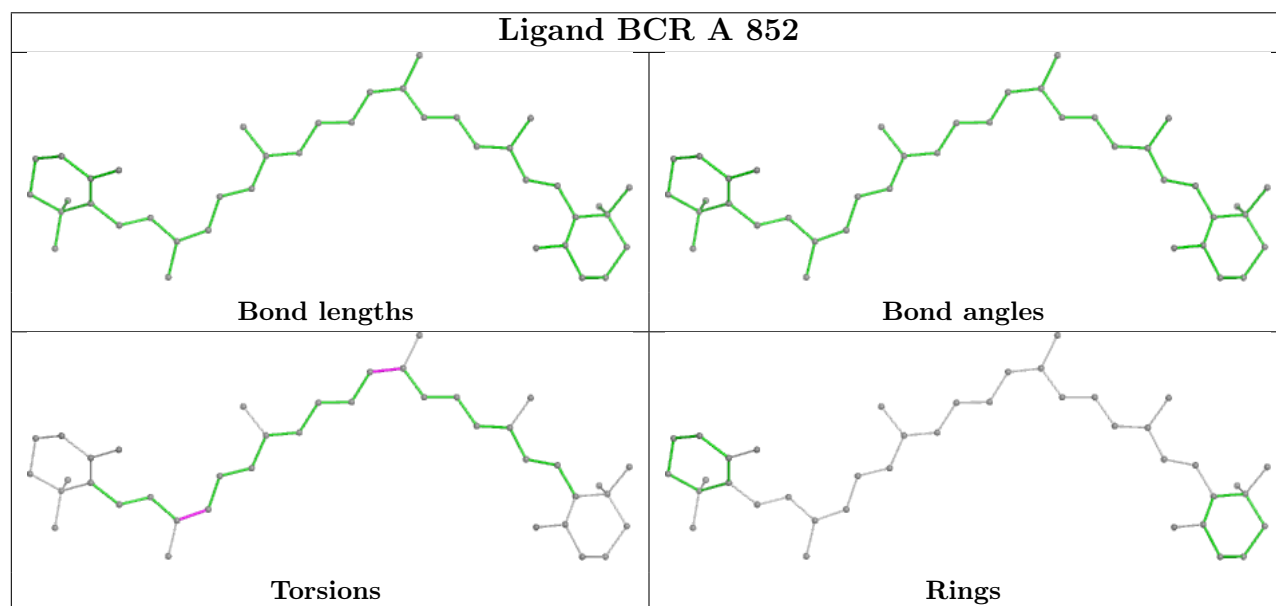
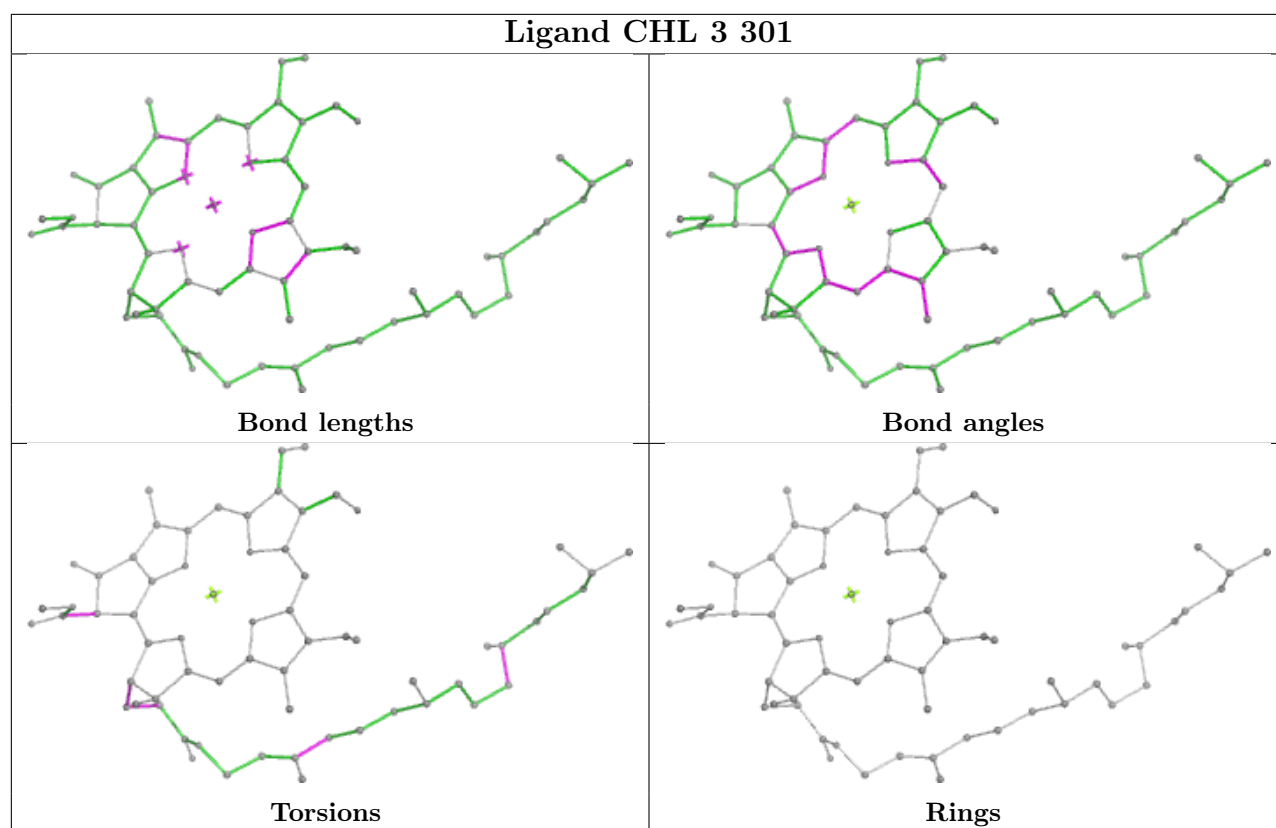




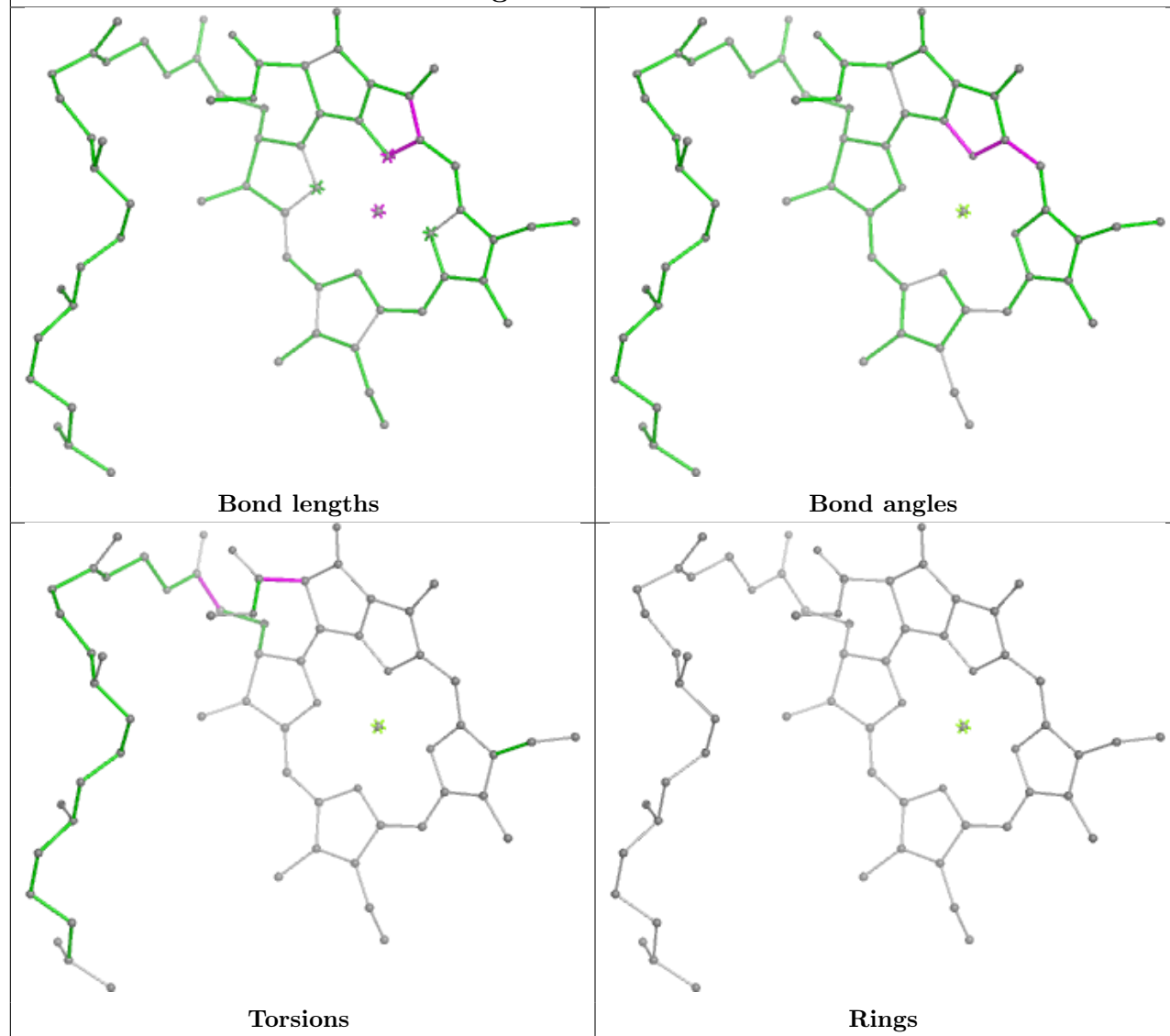


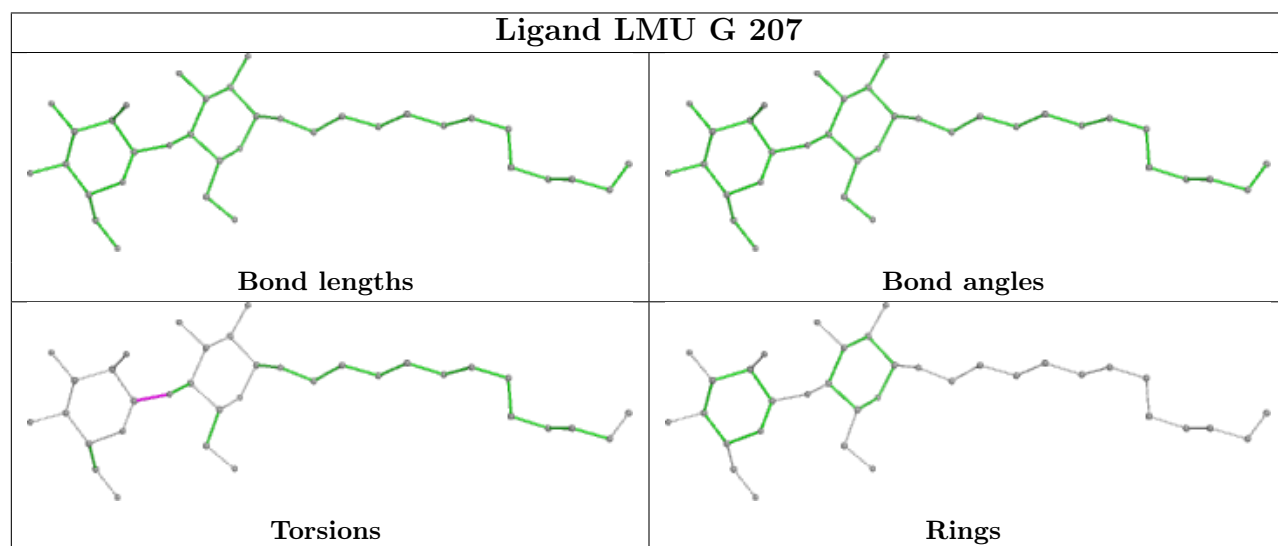
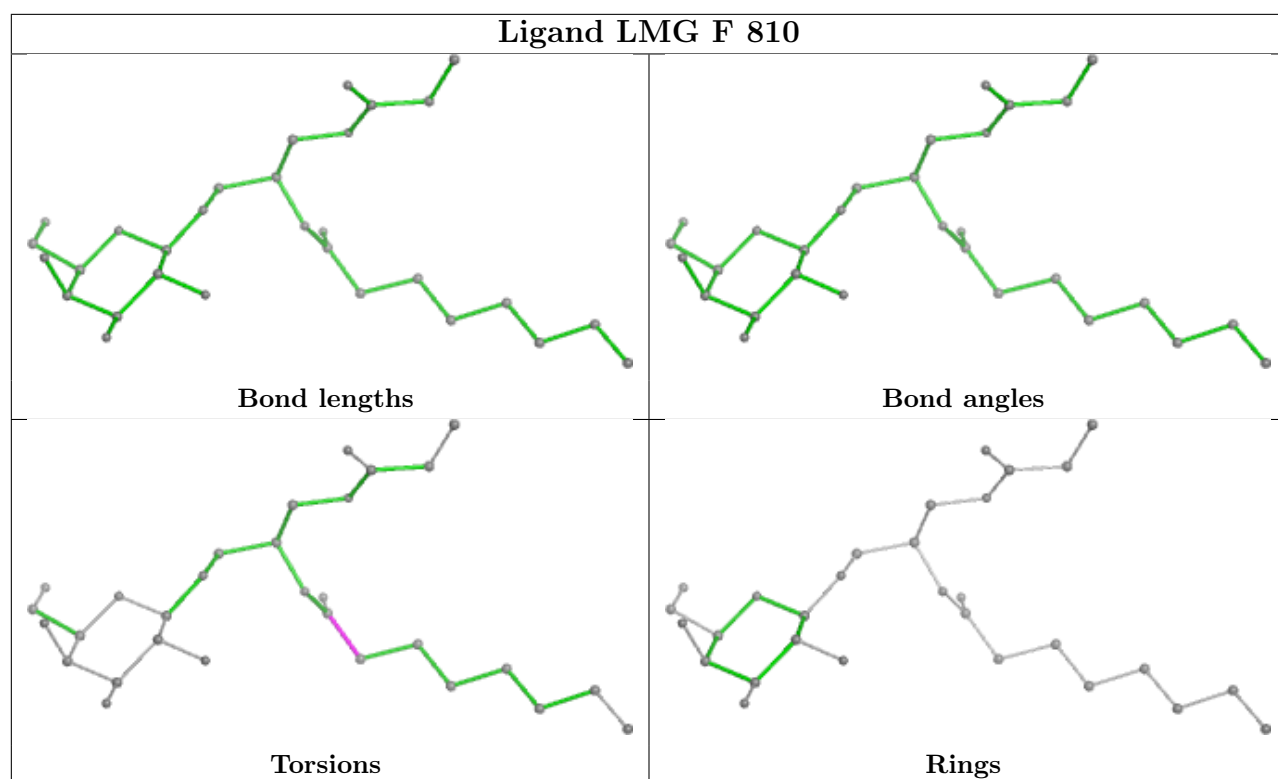
## Ligand CLA 3 307

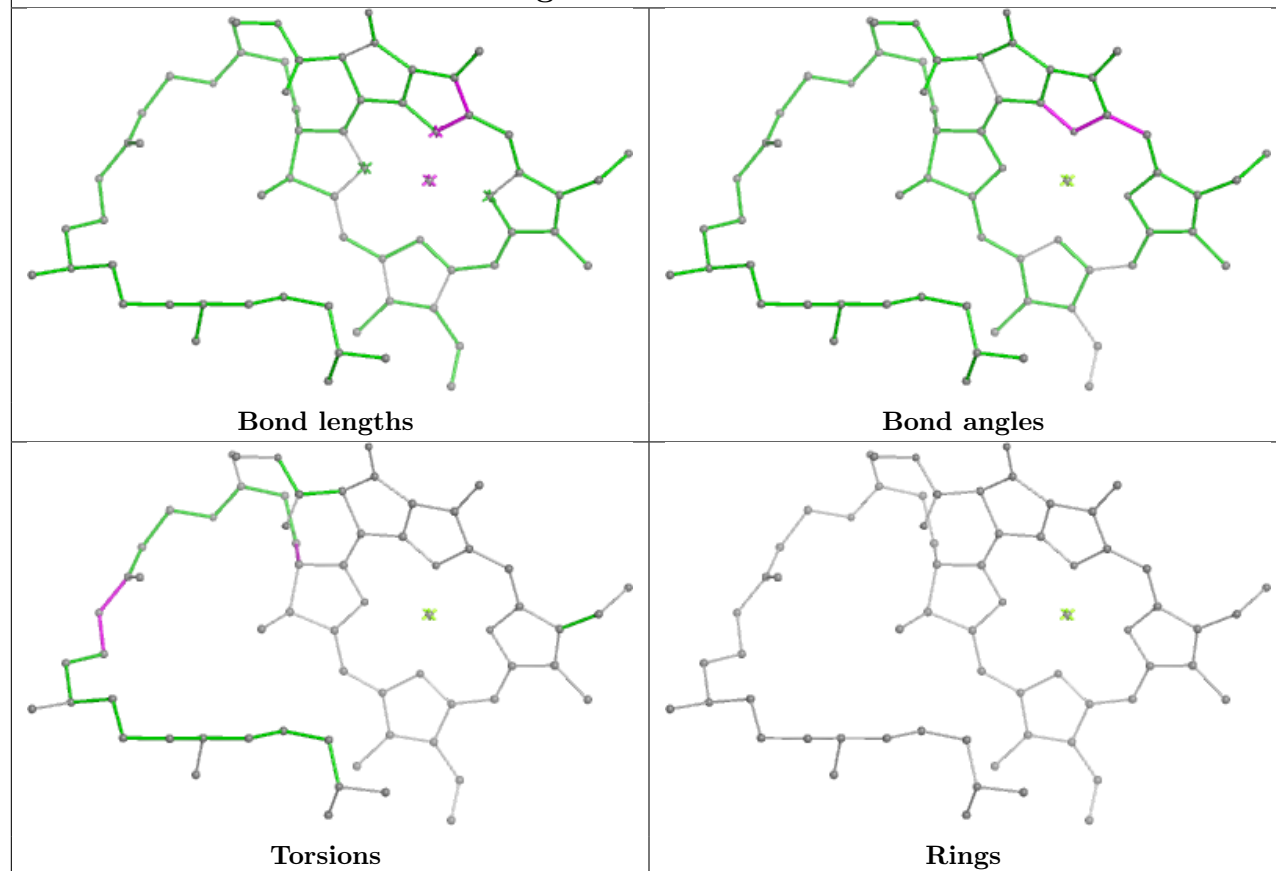
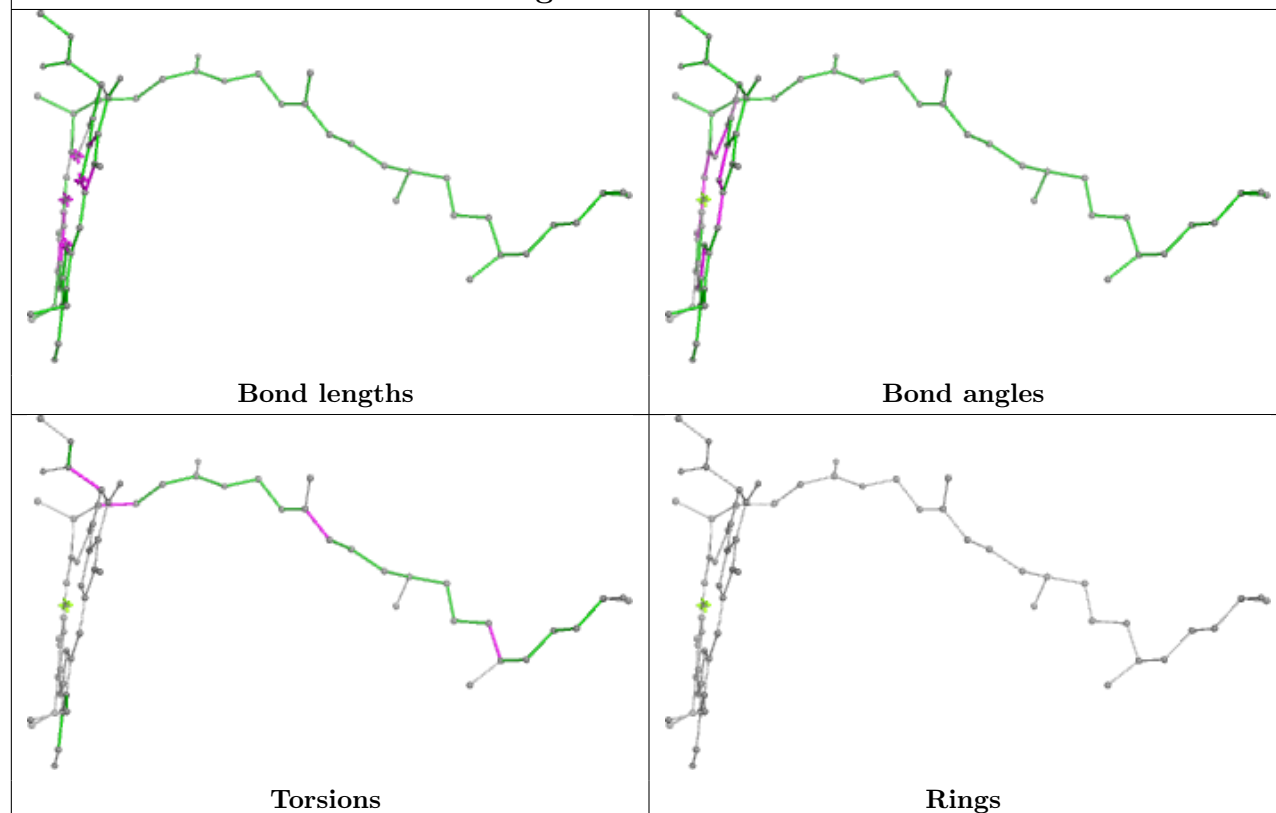




## Ligand CLA 4 603

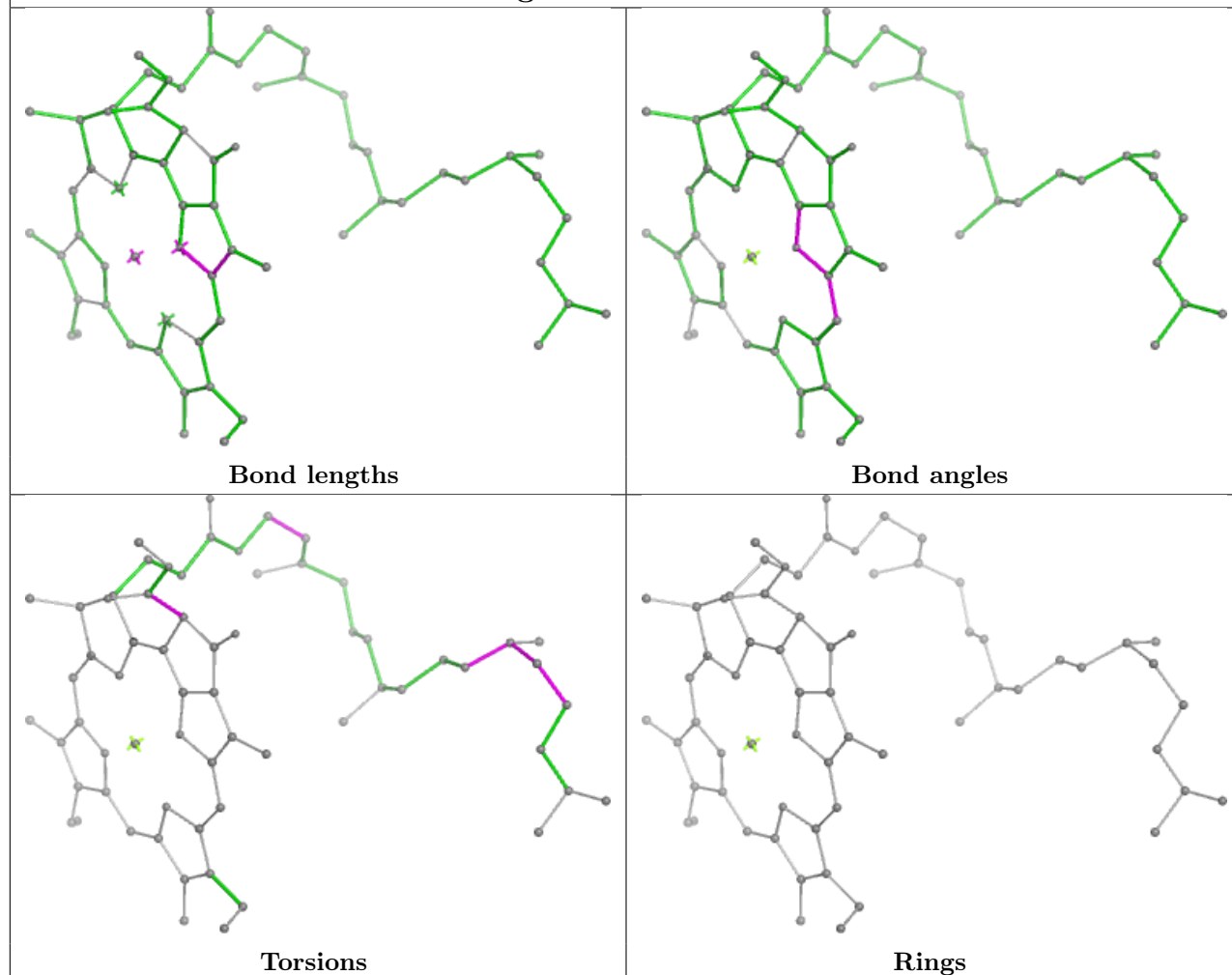




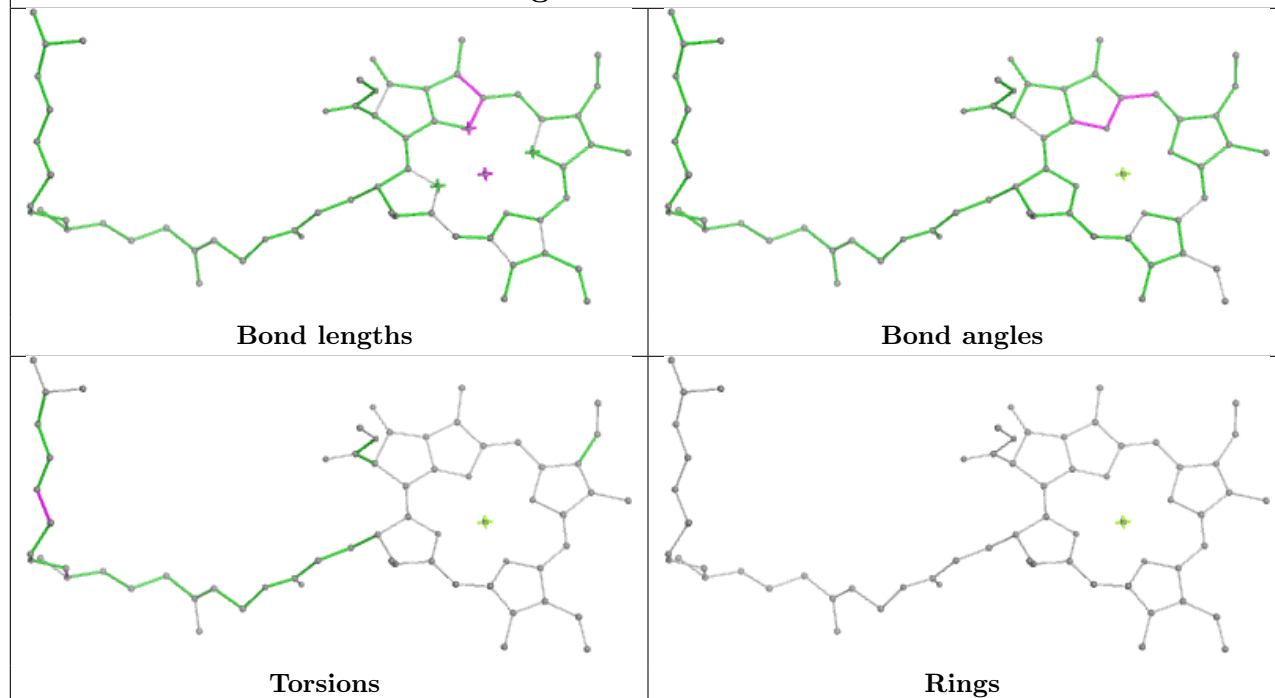
**Ligand CLA 2 603****Ligand CHL 1 302**

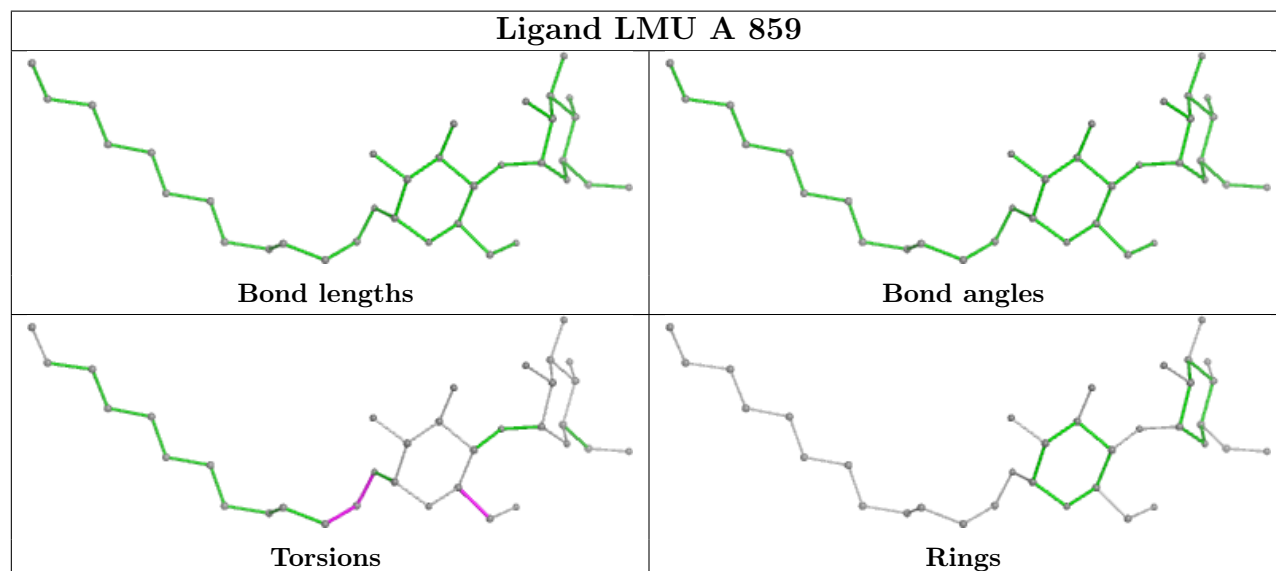
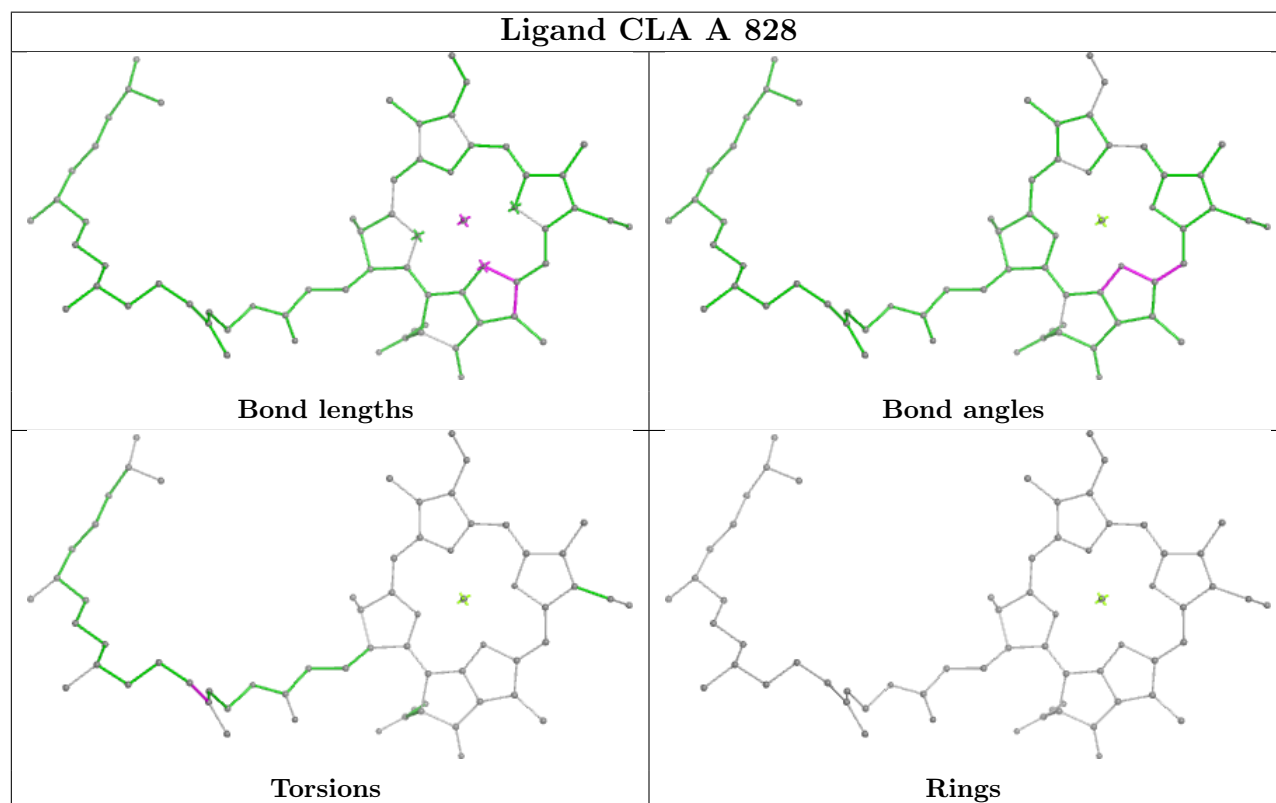
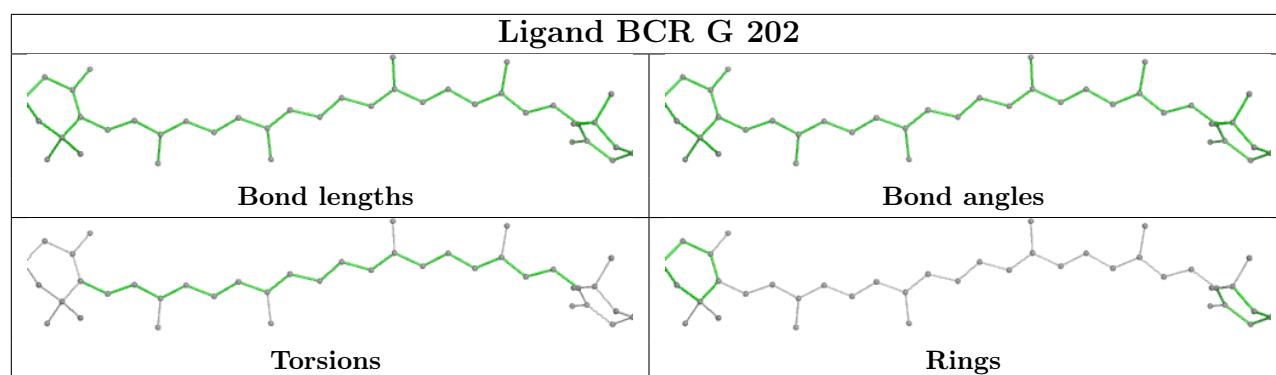


## Ligand CLA 1 309

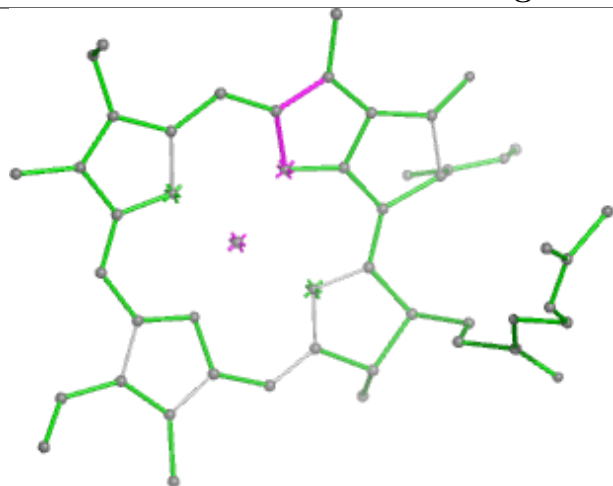


## Ligand CLA B 824

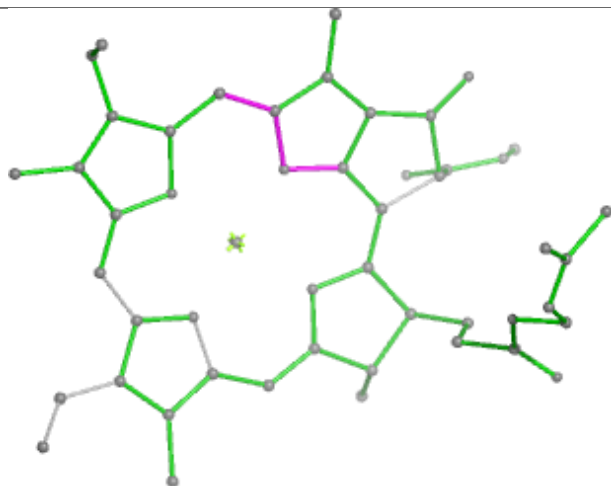




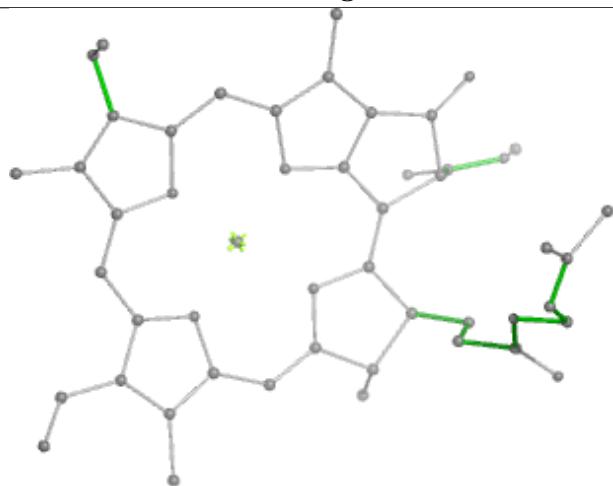
## Ligand CLA B 835



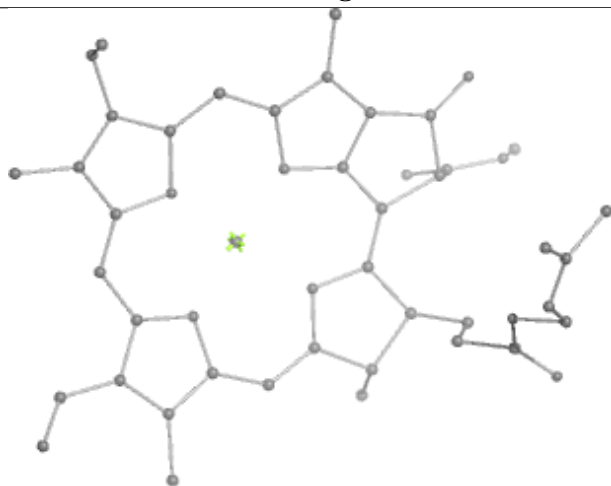
Bond lengths



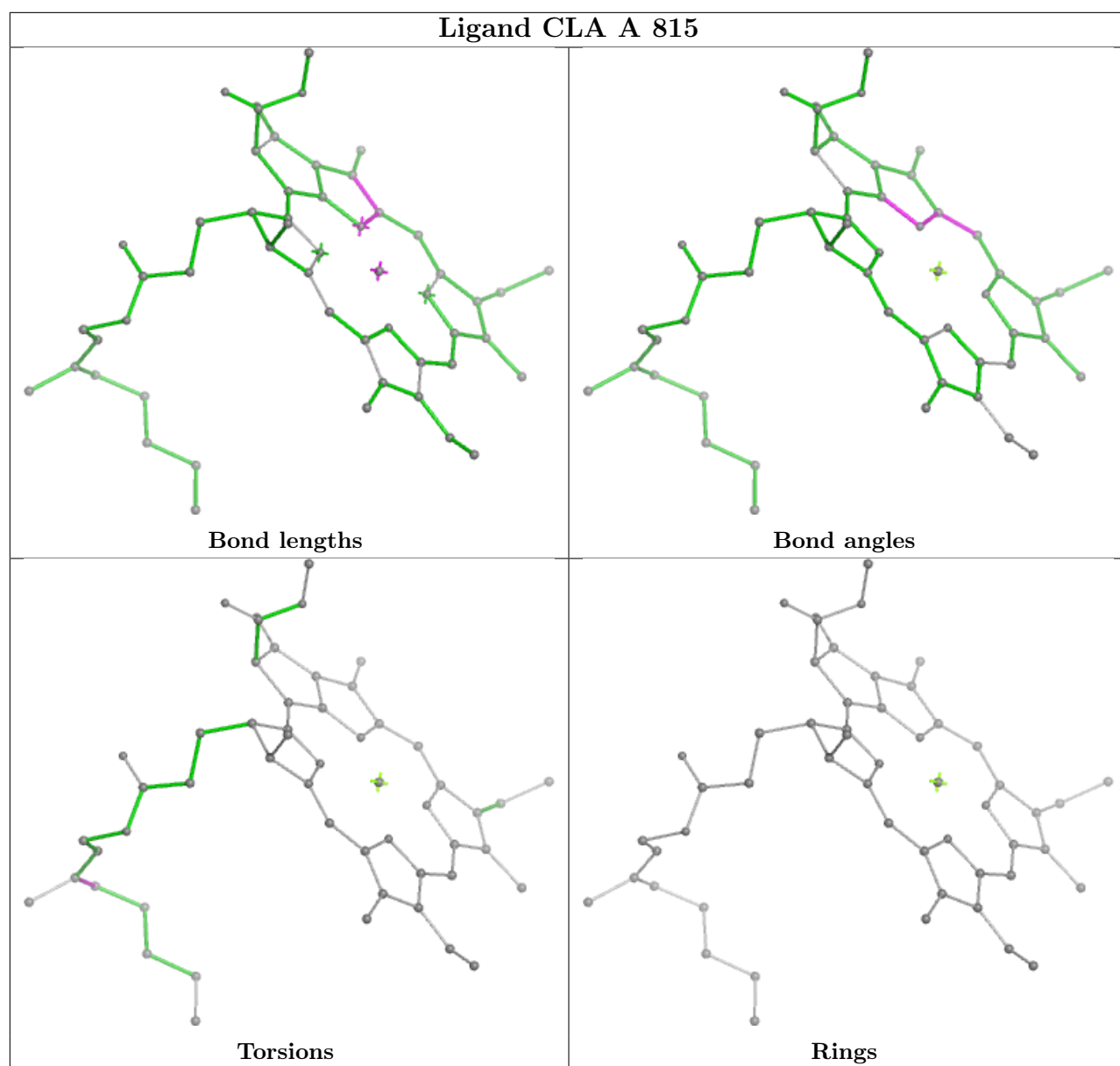
Bond angles

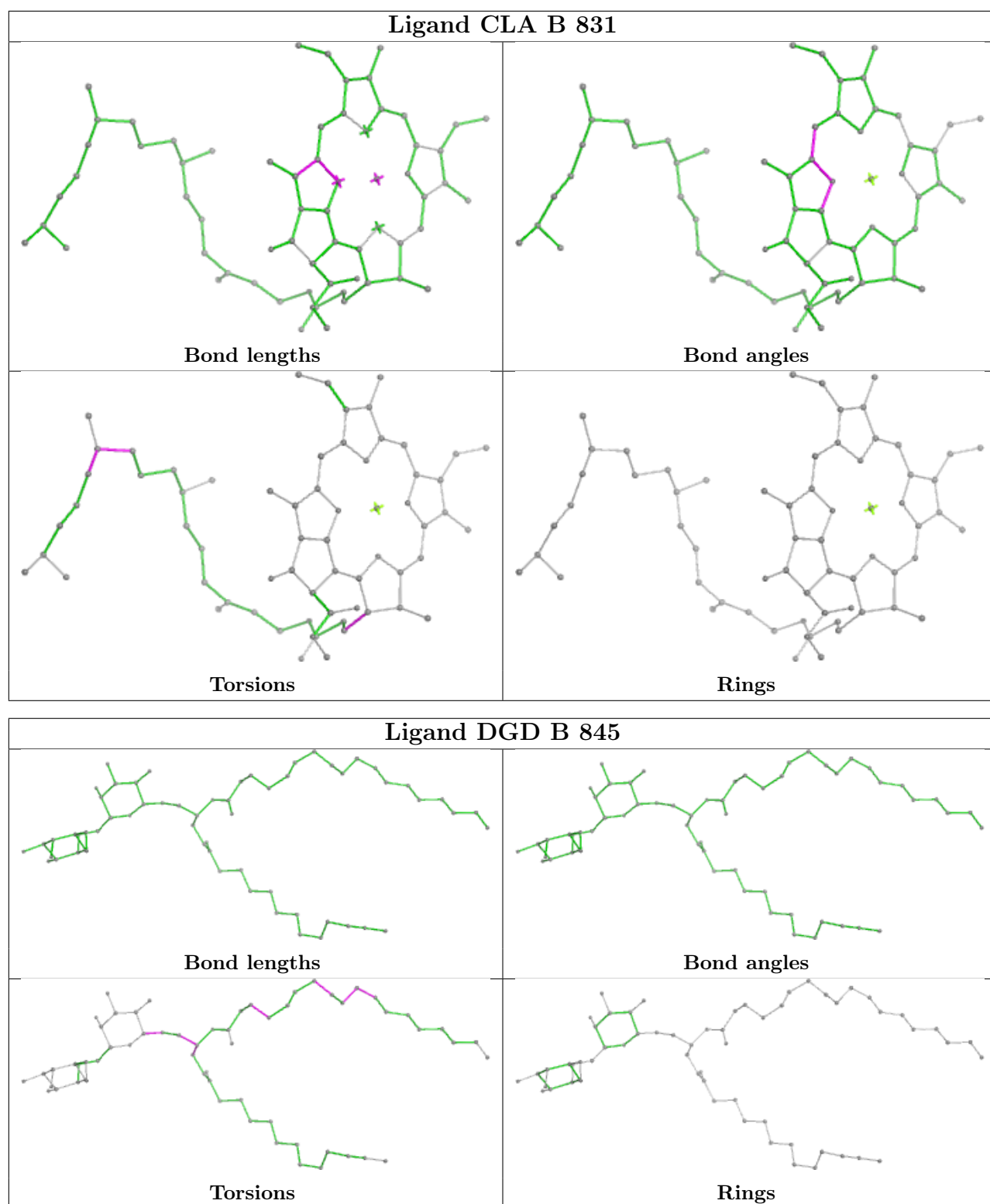


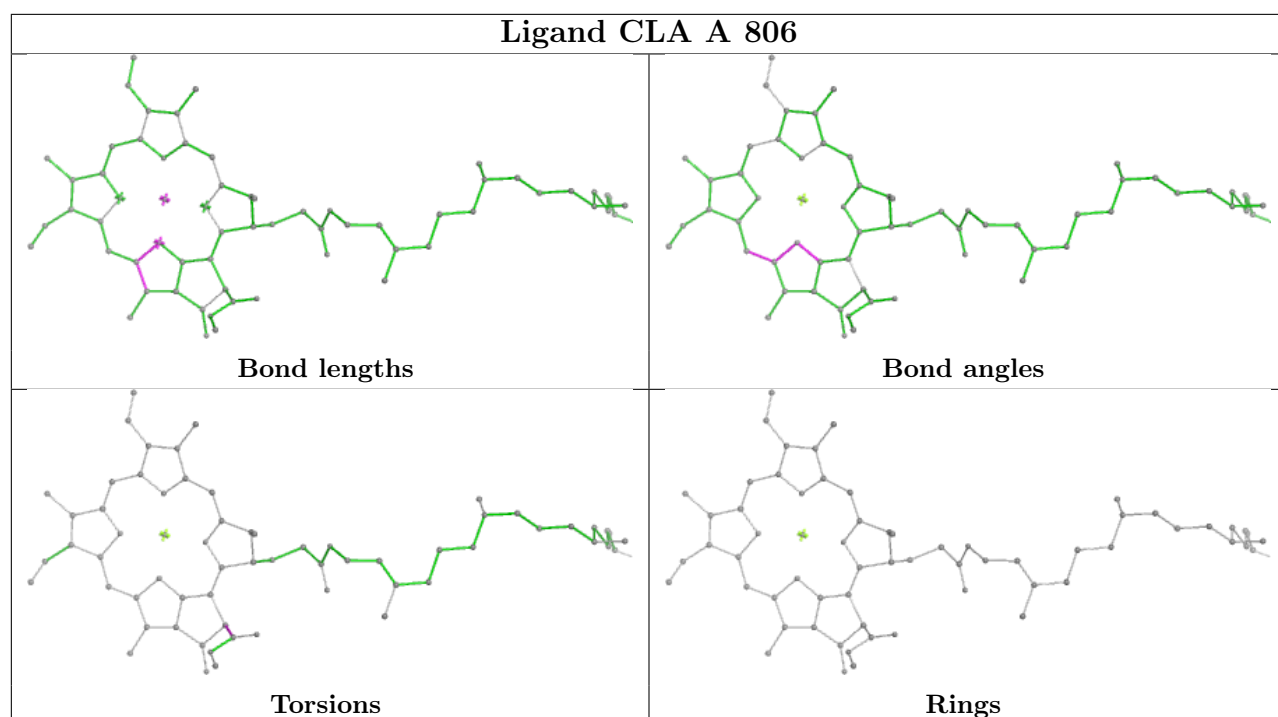
Torsions

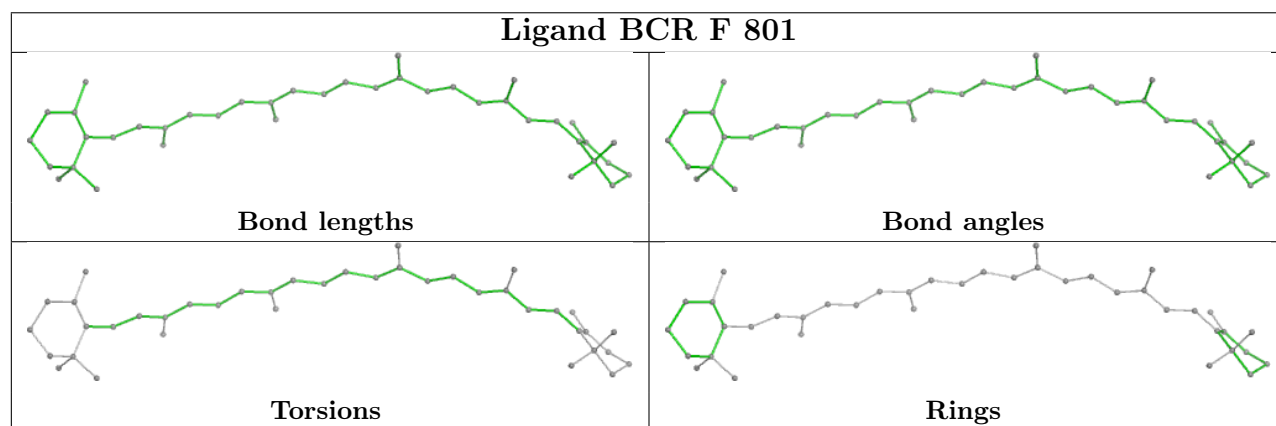
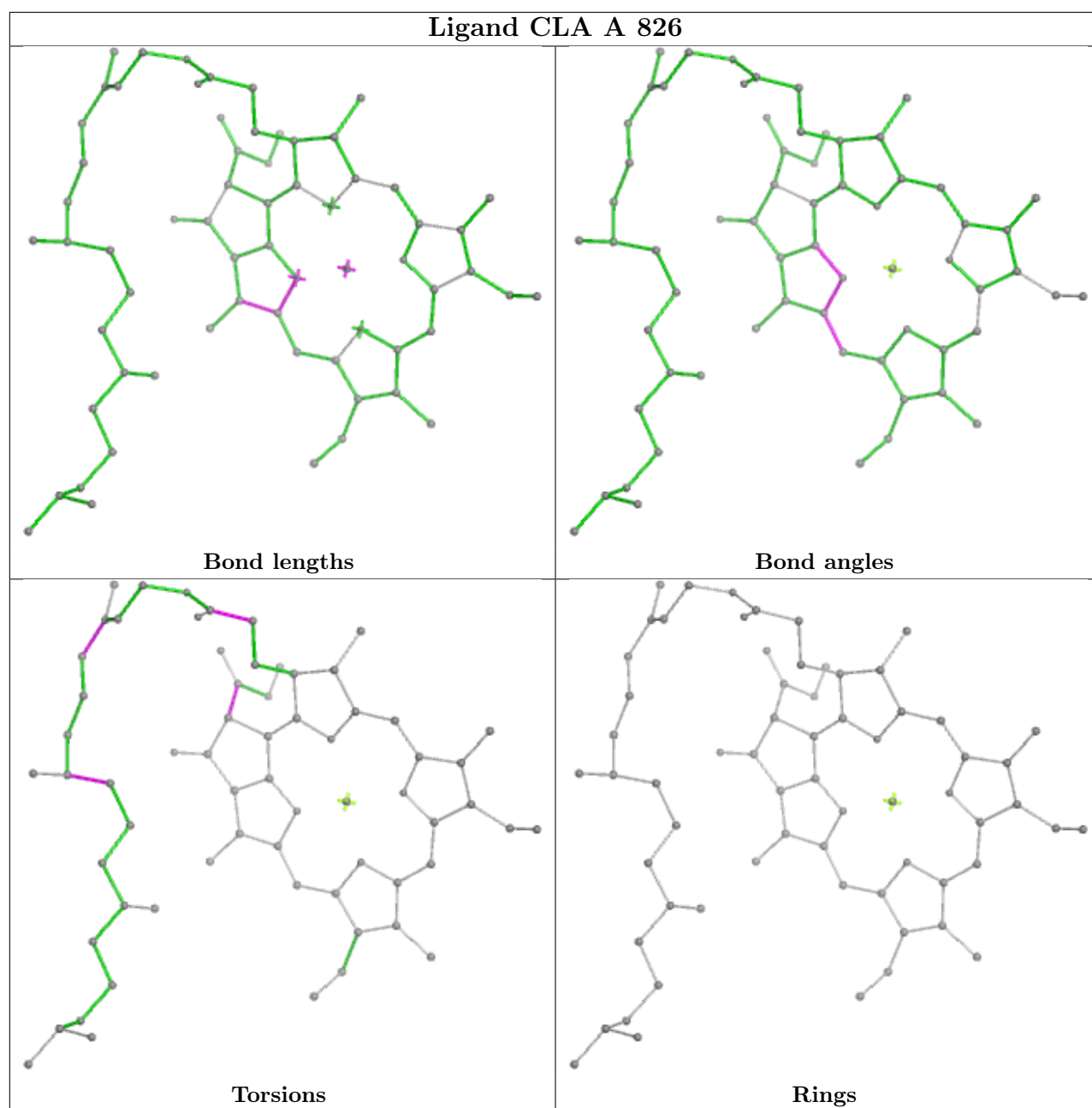


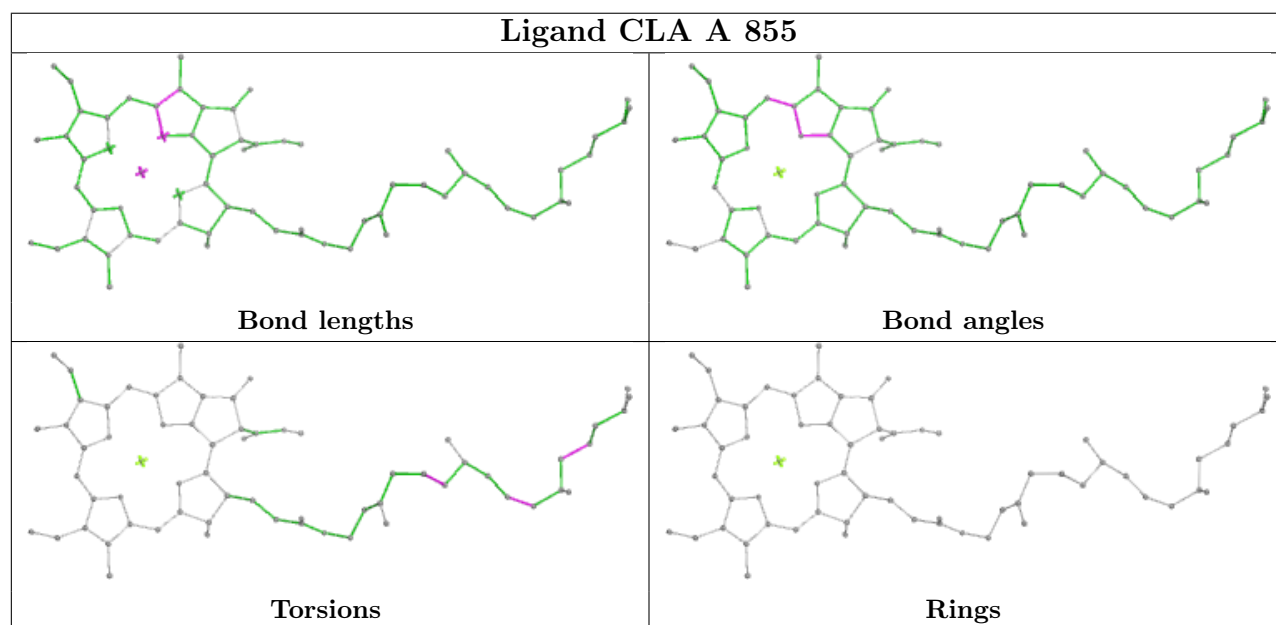
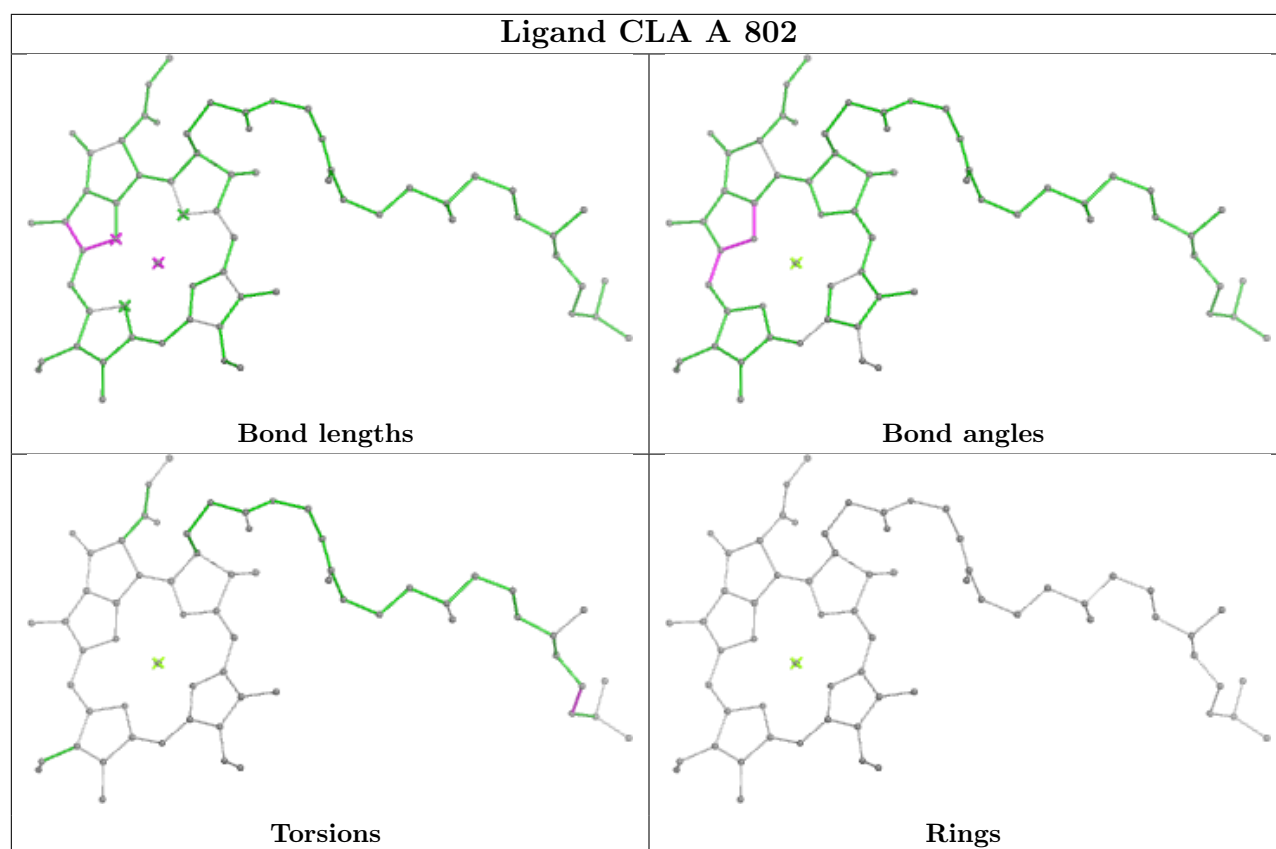
Rings





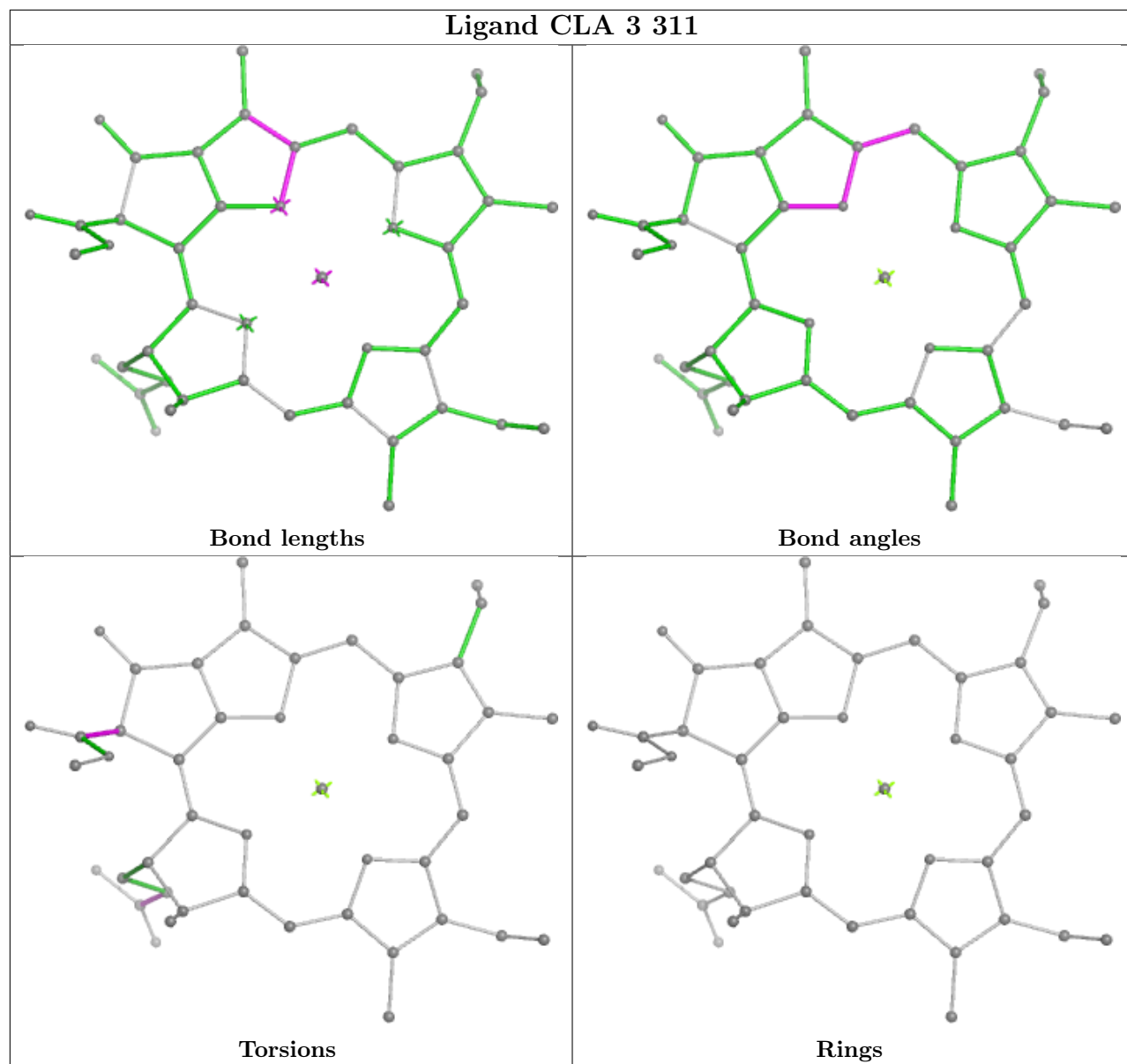




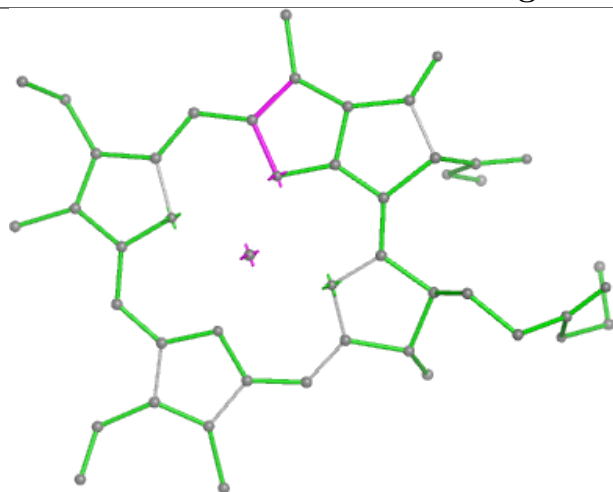




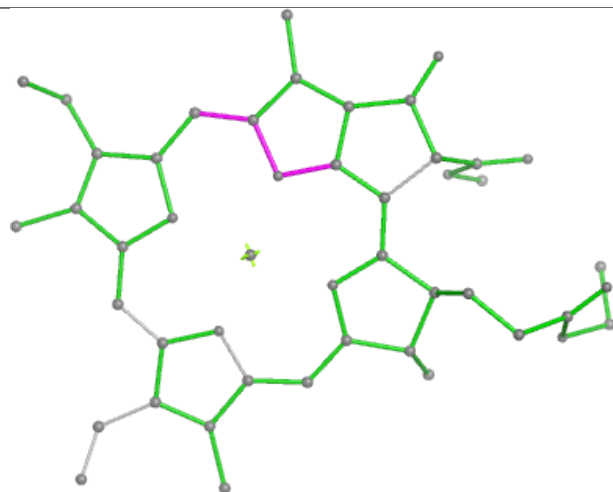
## Ligand CLA 3 311



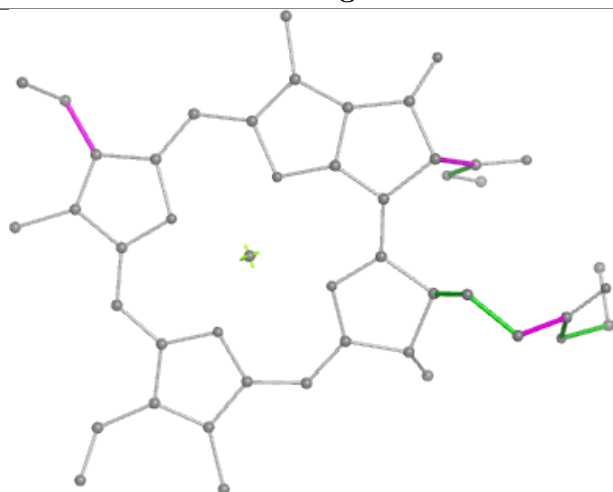
## Ligand CLA 4 611



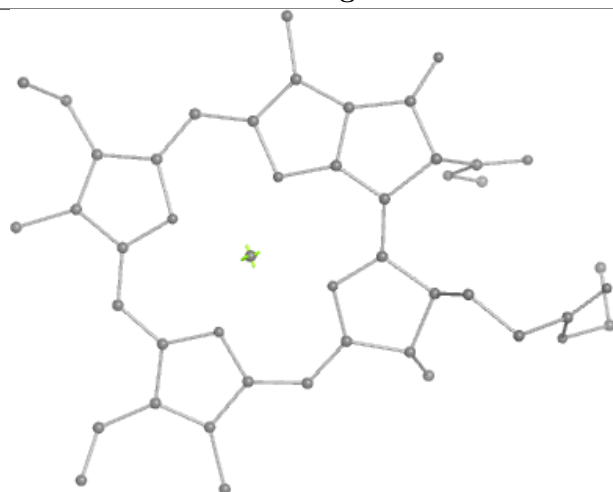
Bond lengths



Bond angles

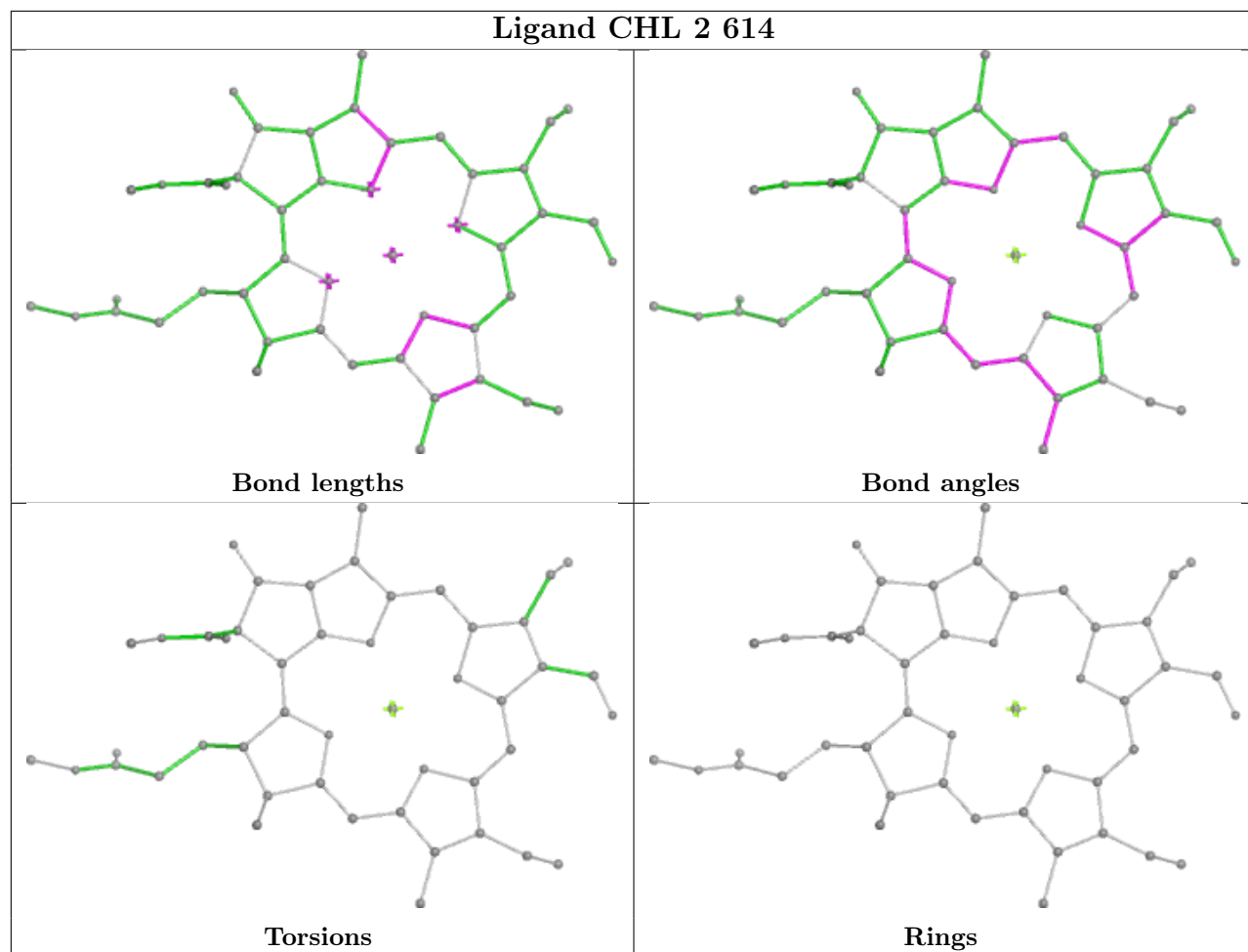


Torsions

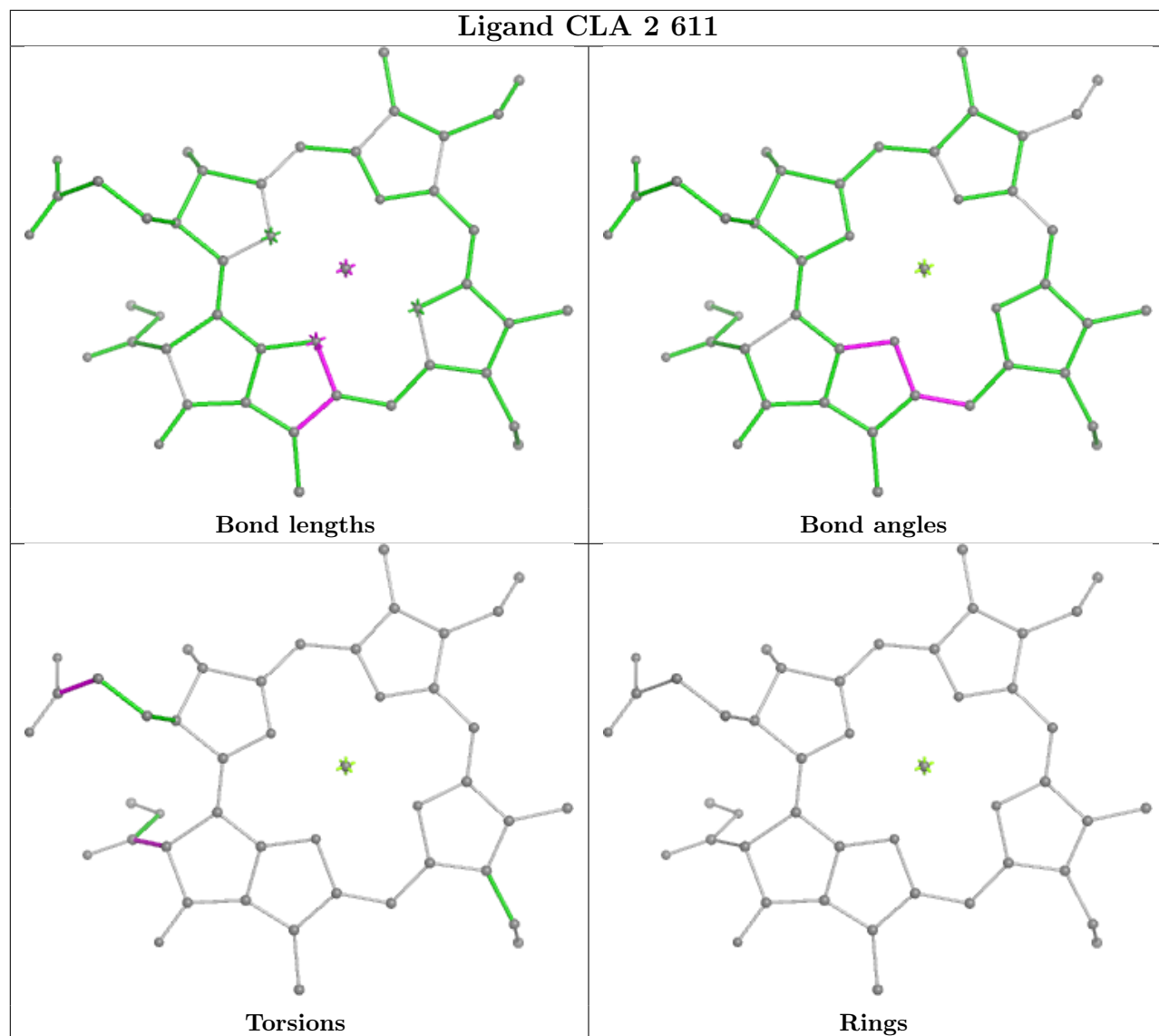


Rings

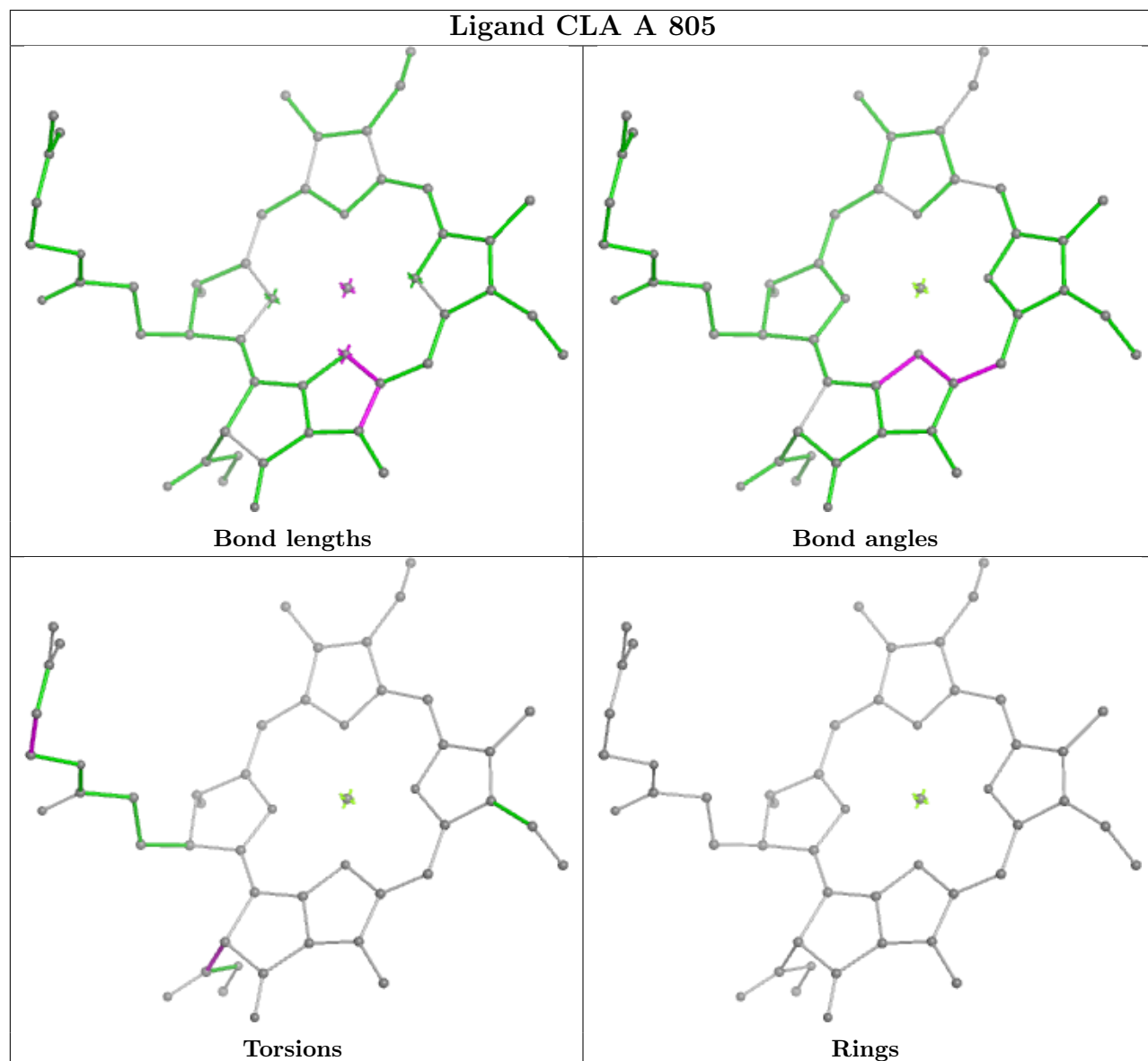
## Ligand CHL 2 614

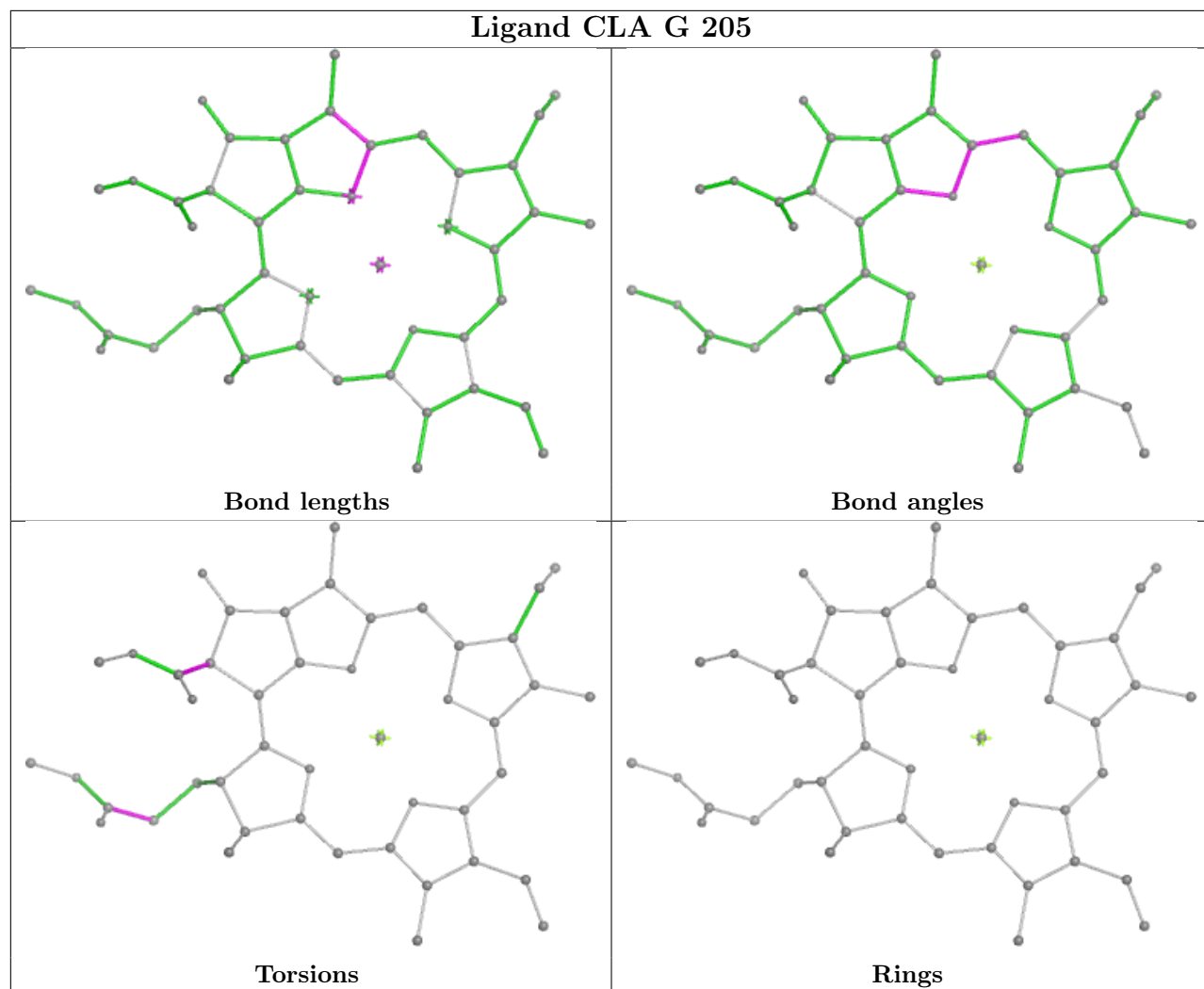


## Ligand CLA 2 611

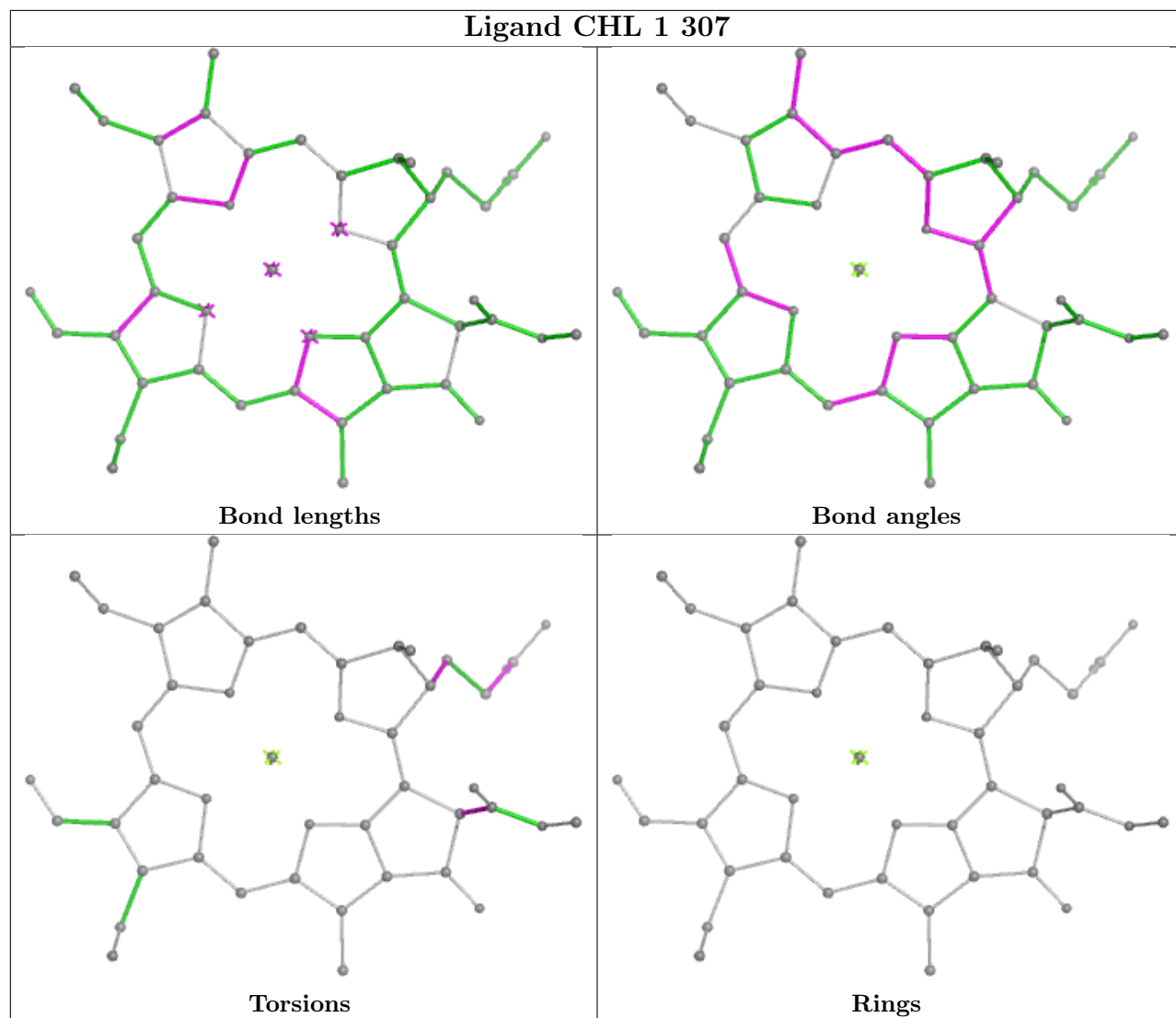


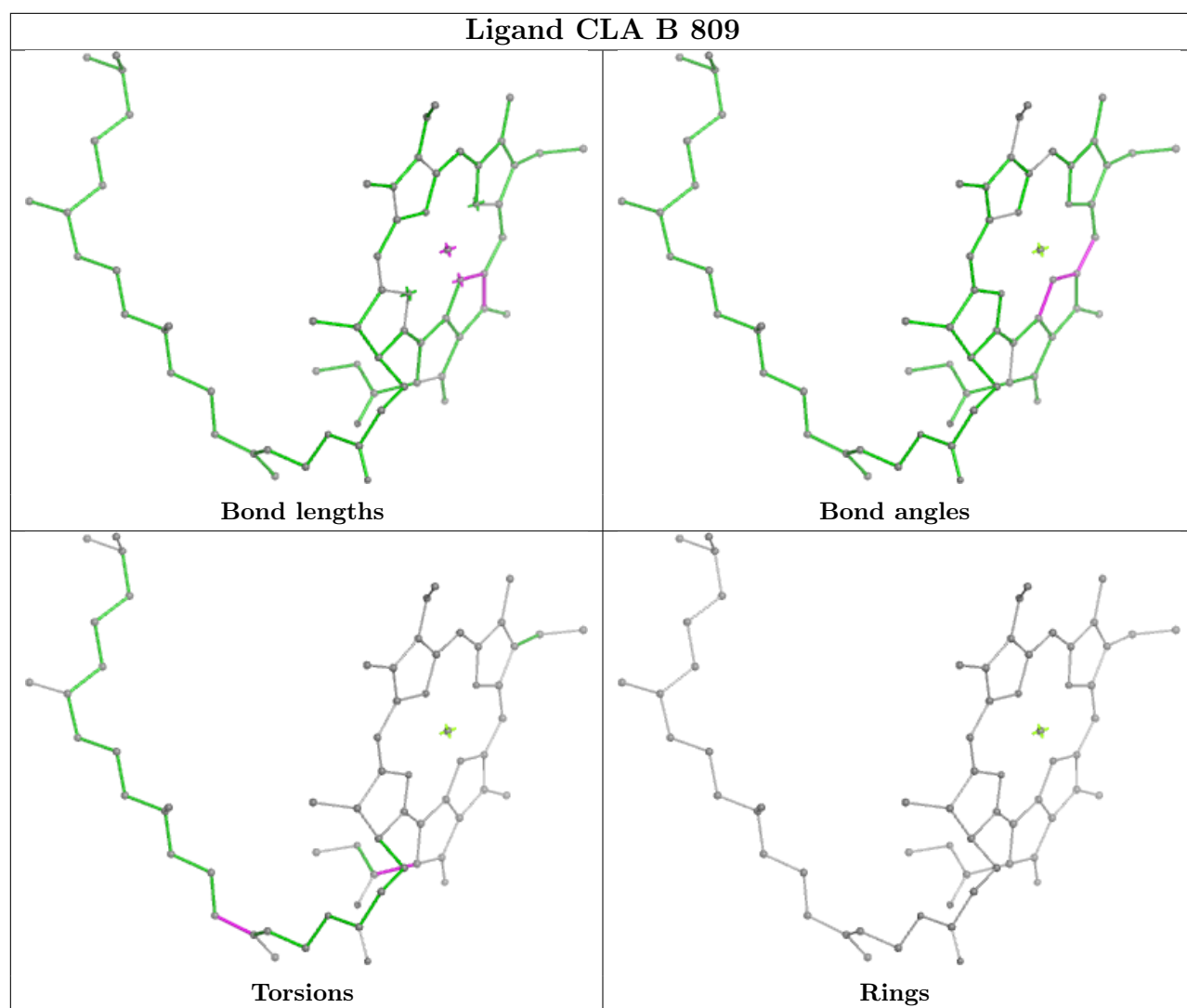
## Ligand CLA A 805





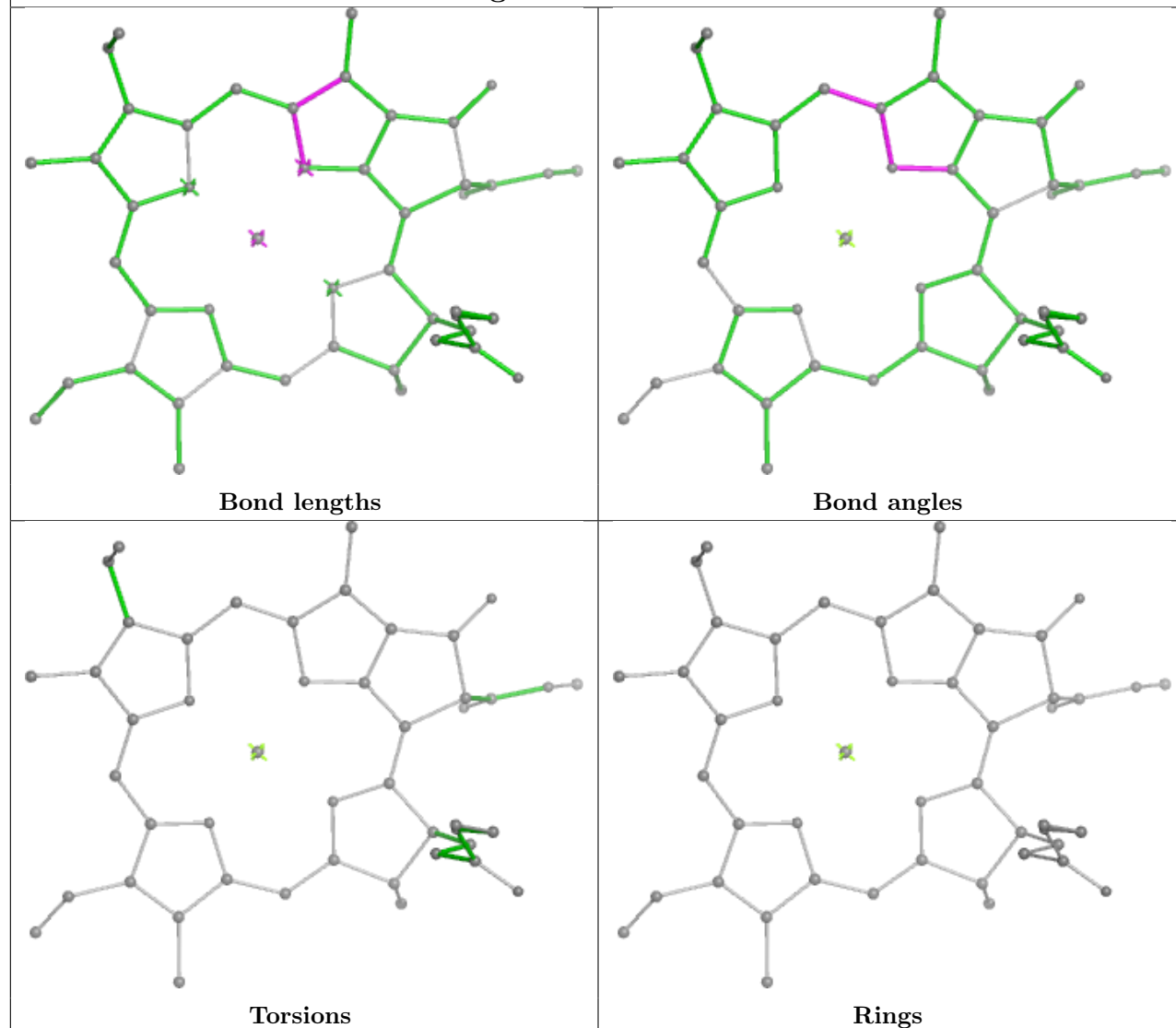
## Ligand CHL 1 307



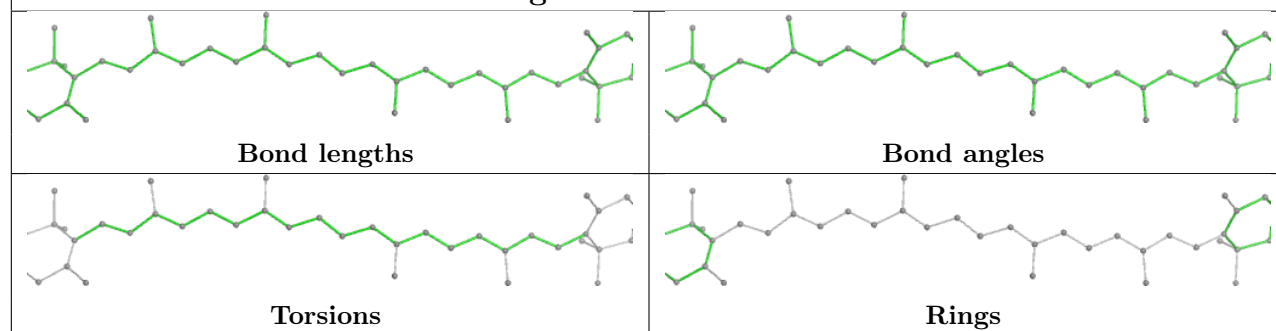


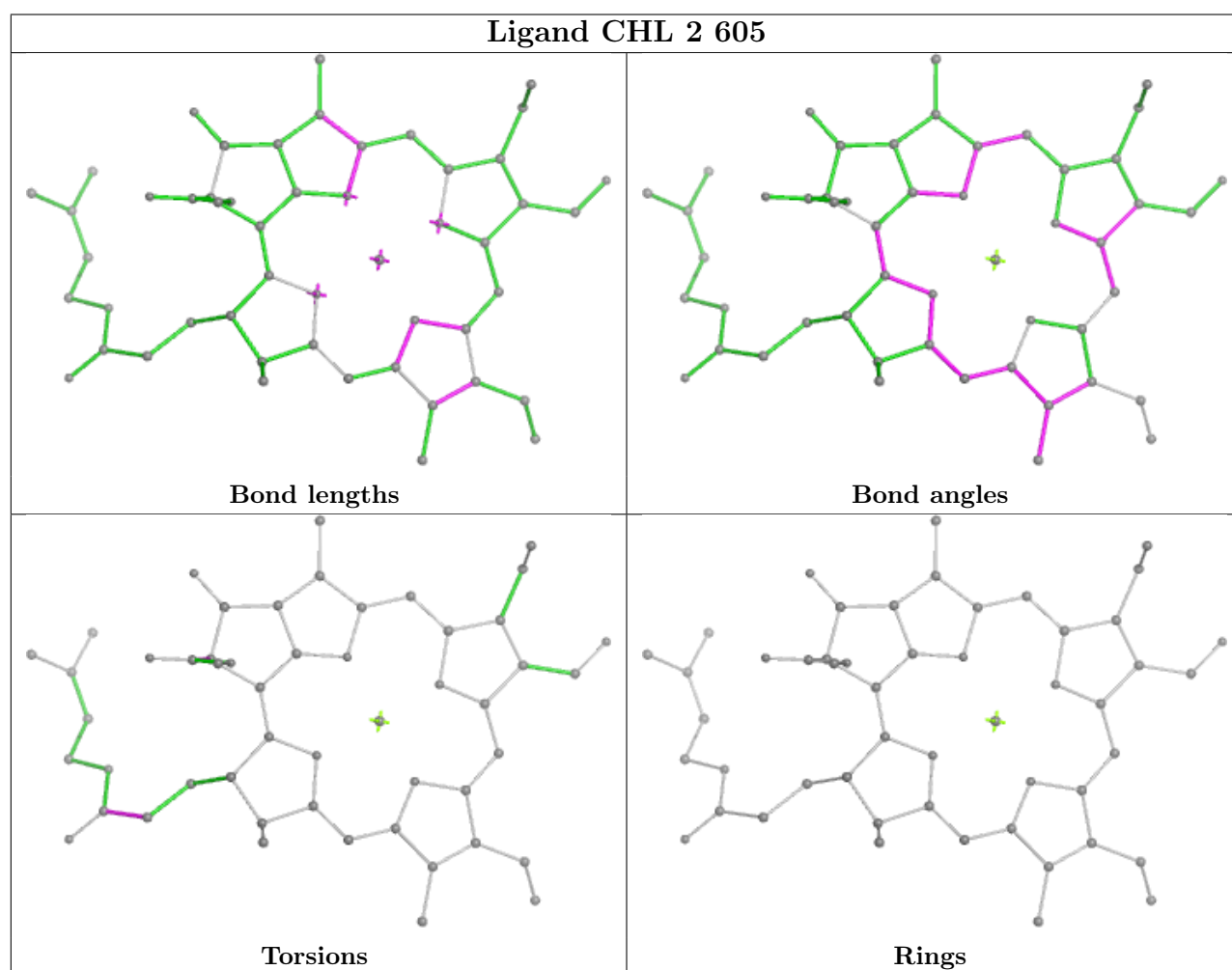
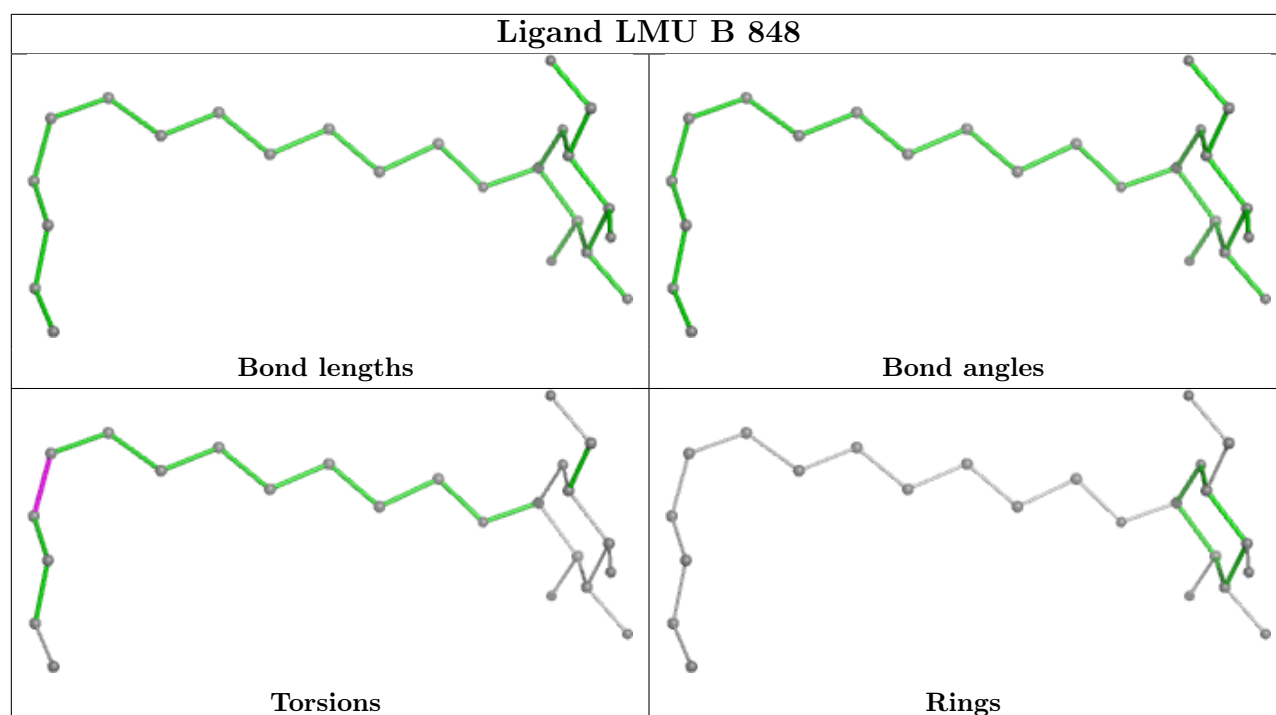


## Ligand CLA A 808

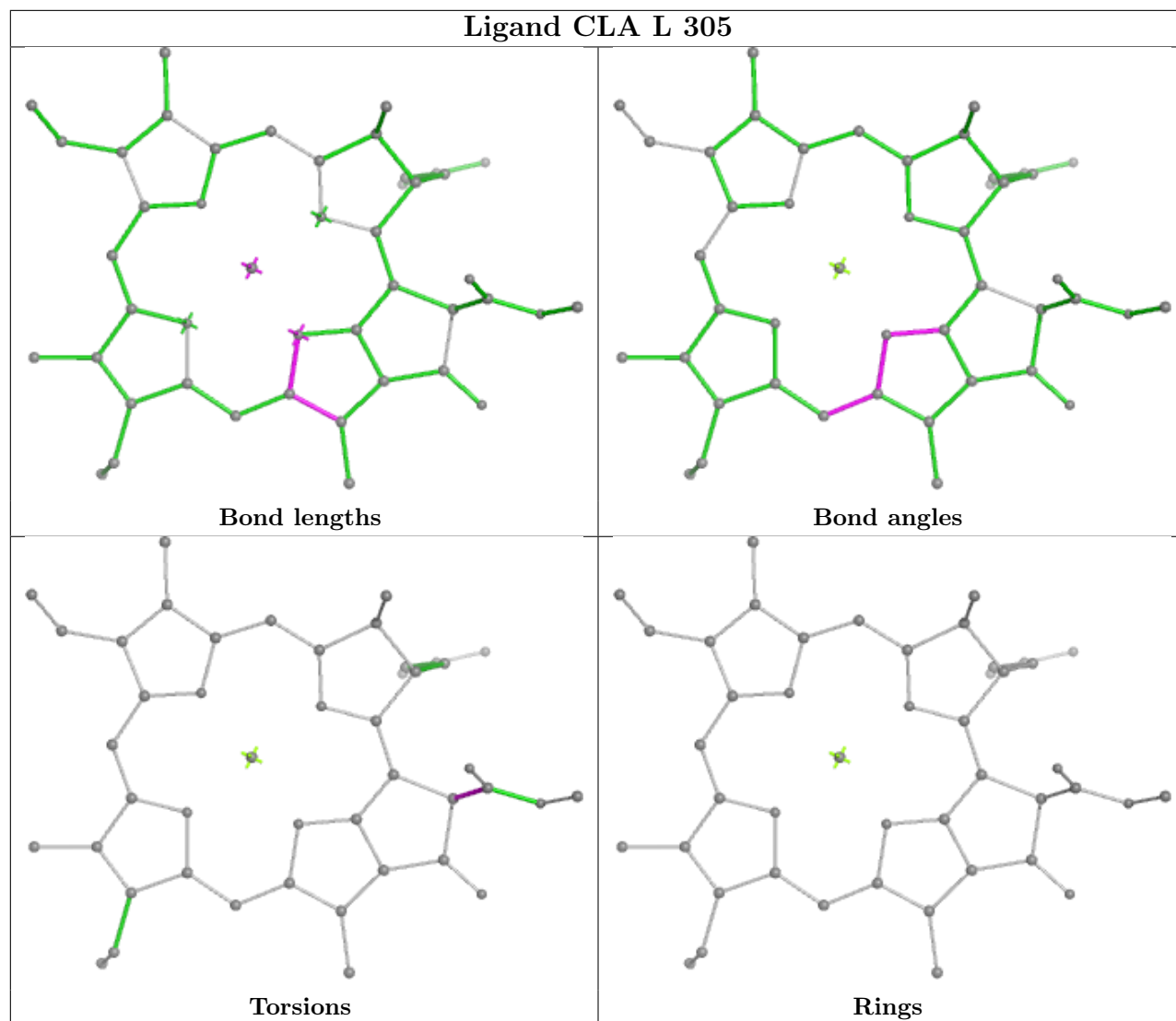


## Ligand BCR K 202

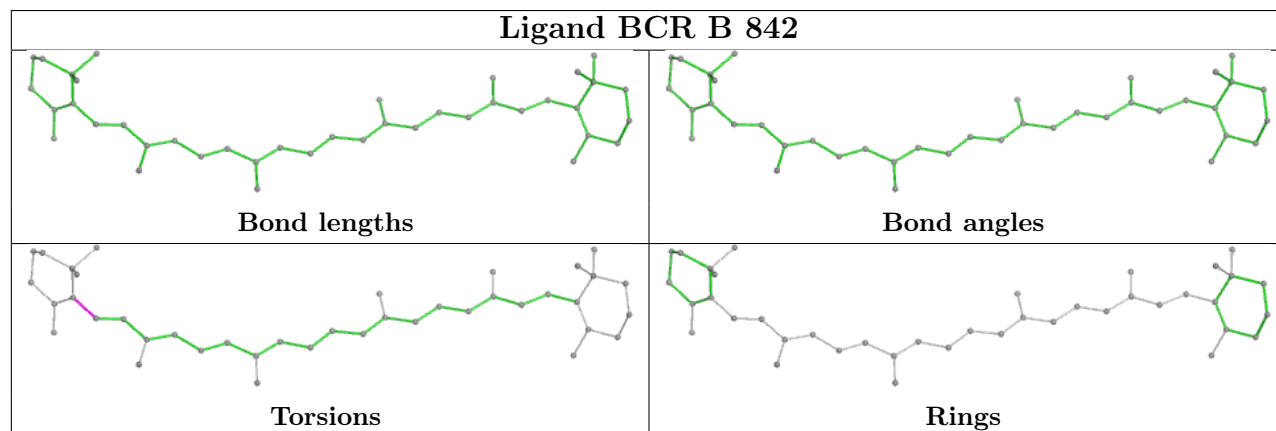




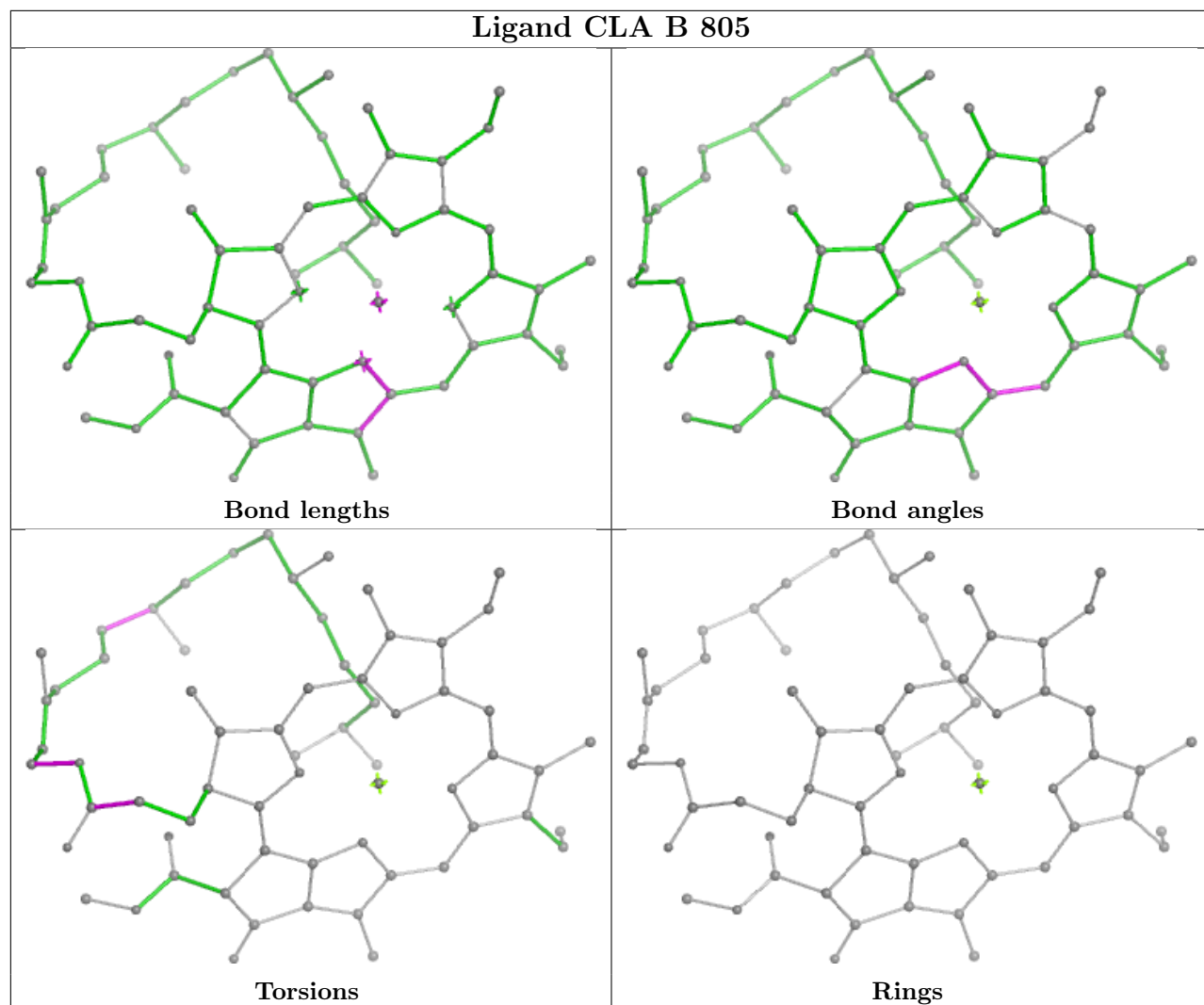
## Ligand CLA L 305



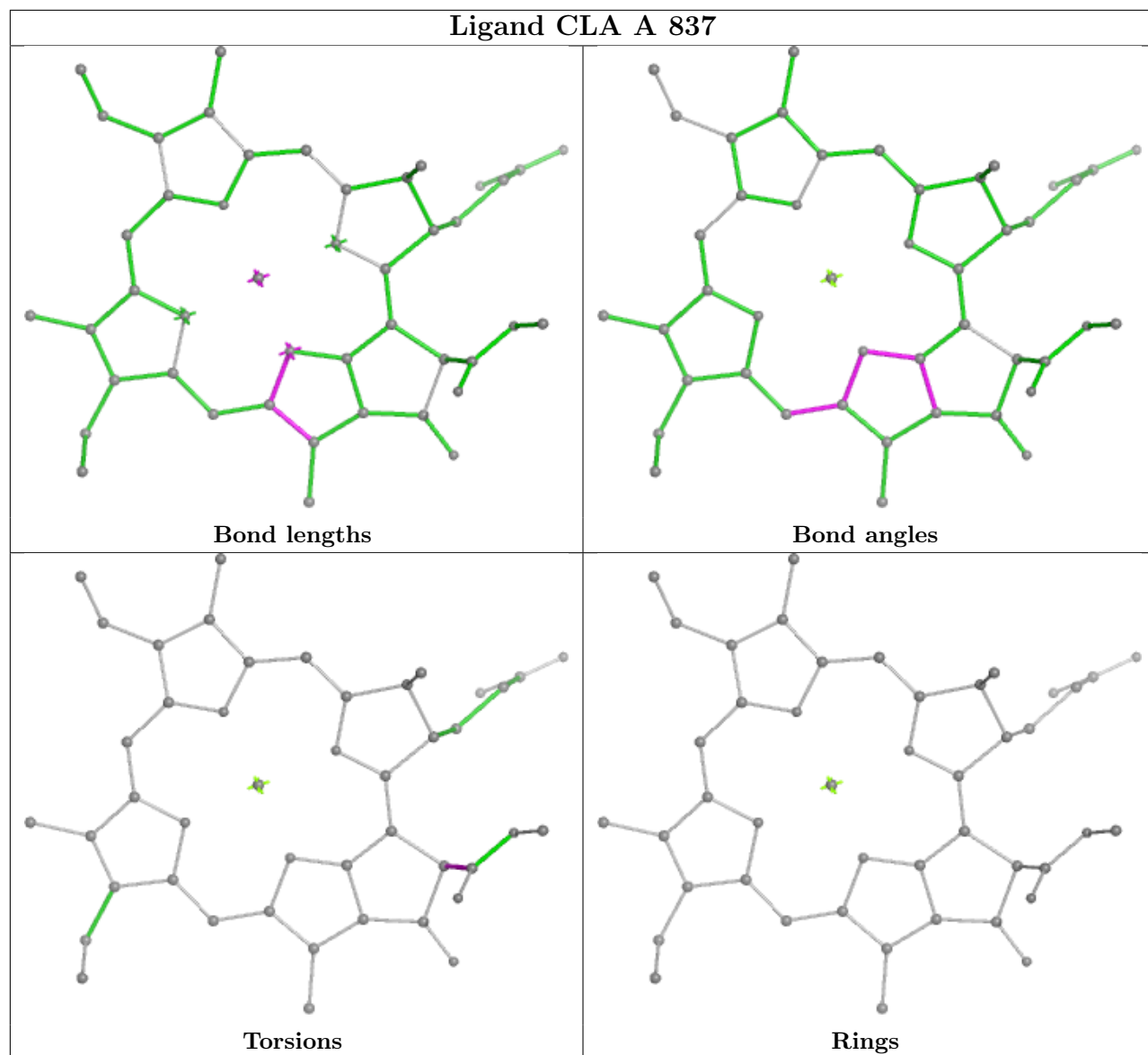
## Ligand BCR B 842

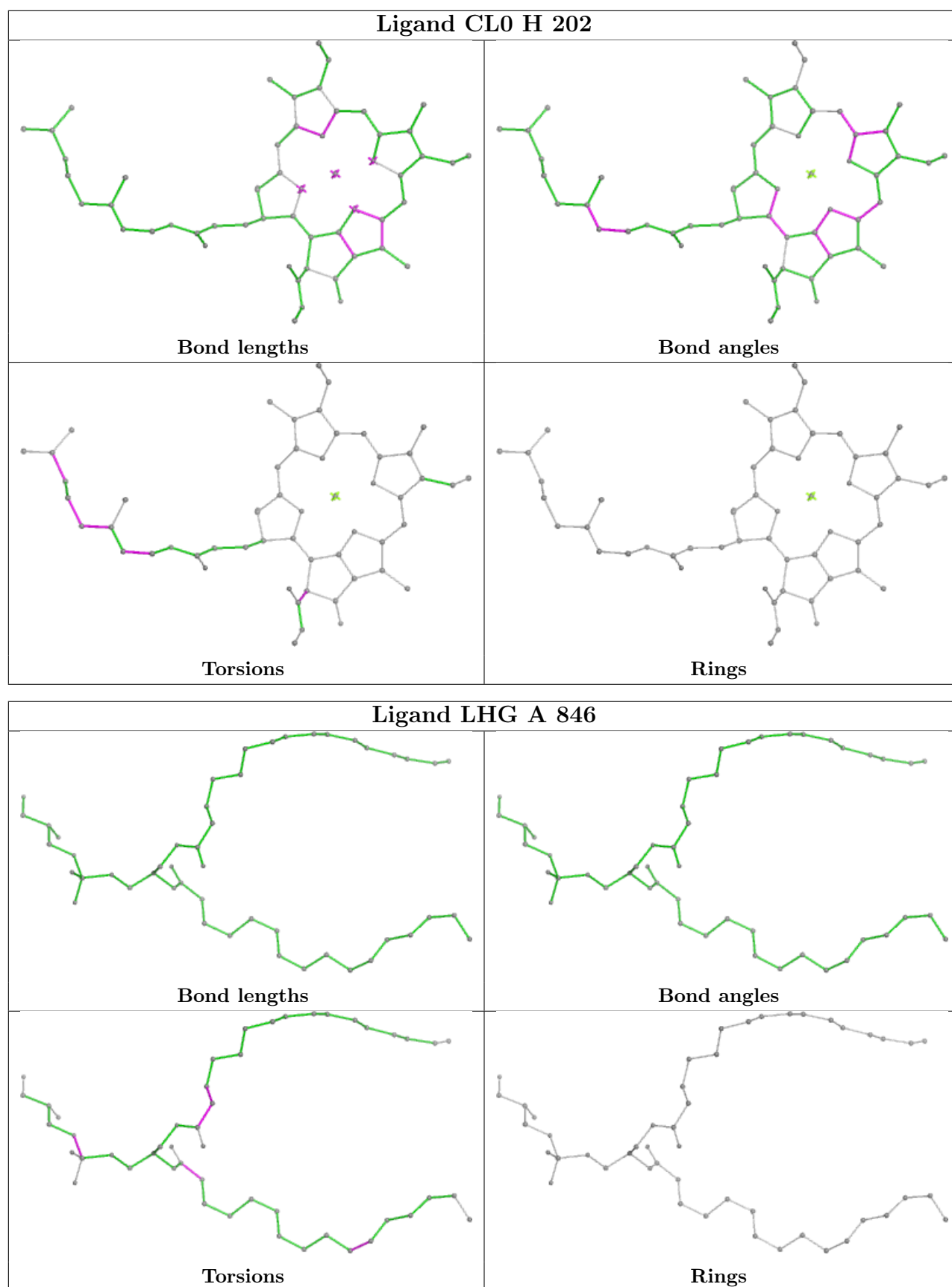


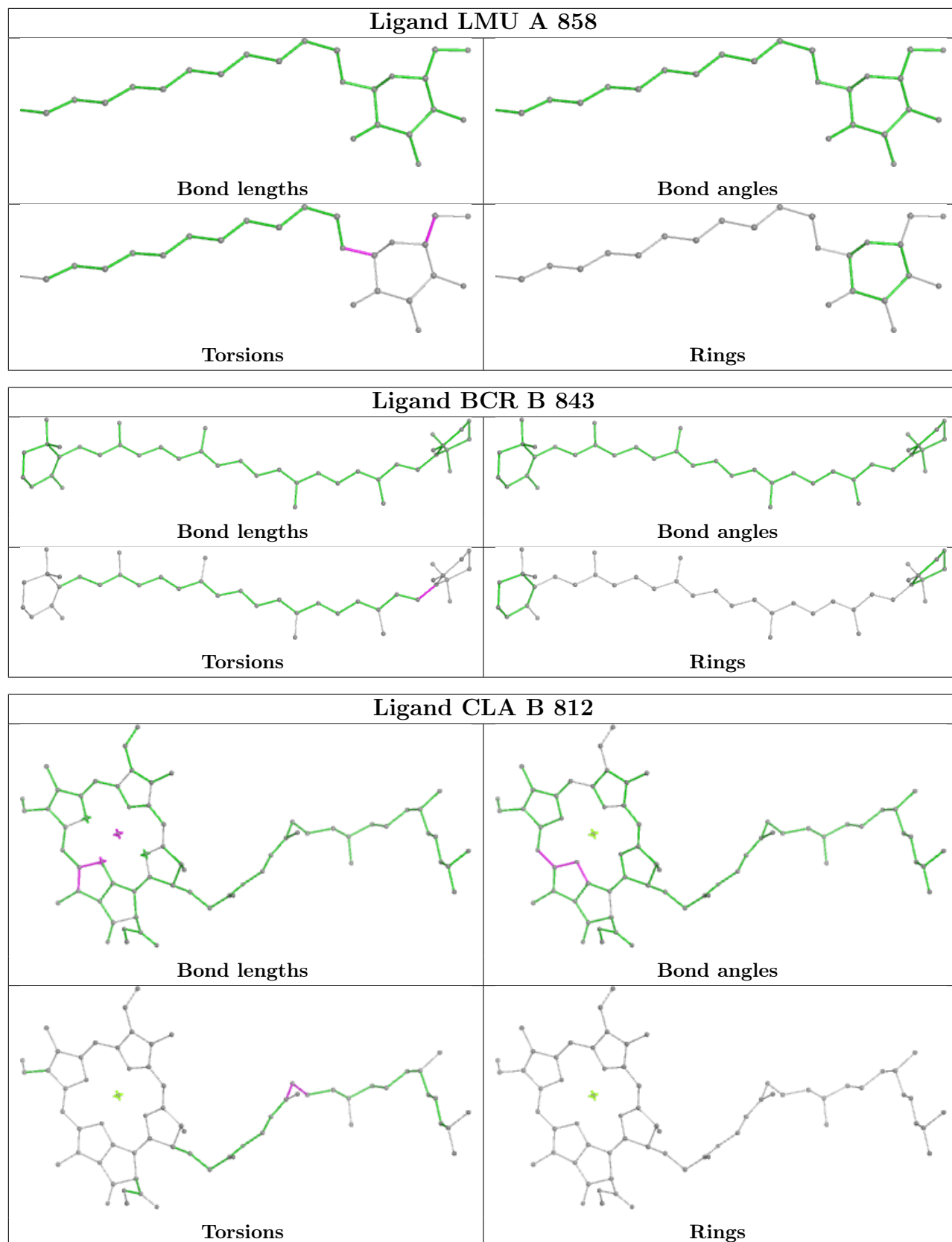
## Ligand CLA B 805

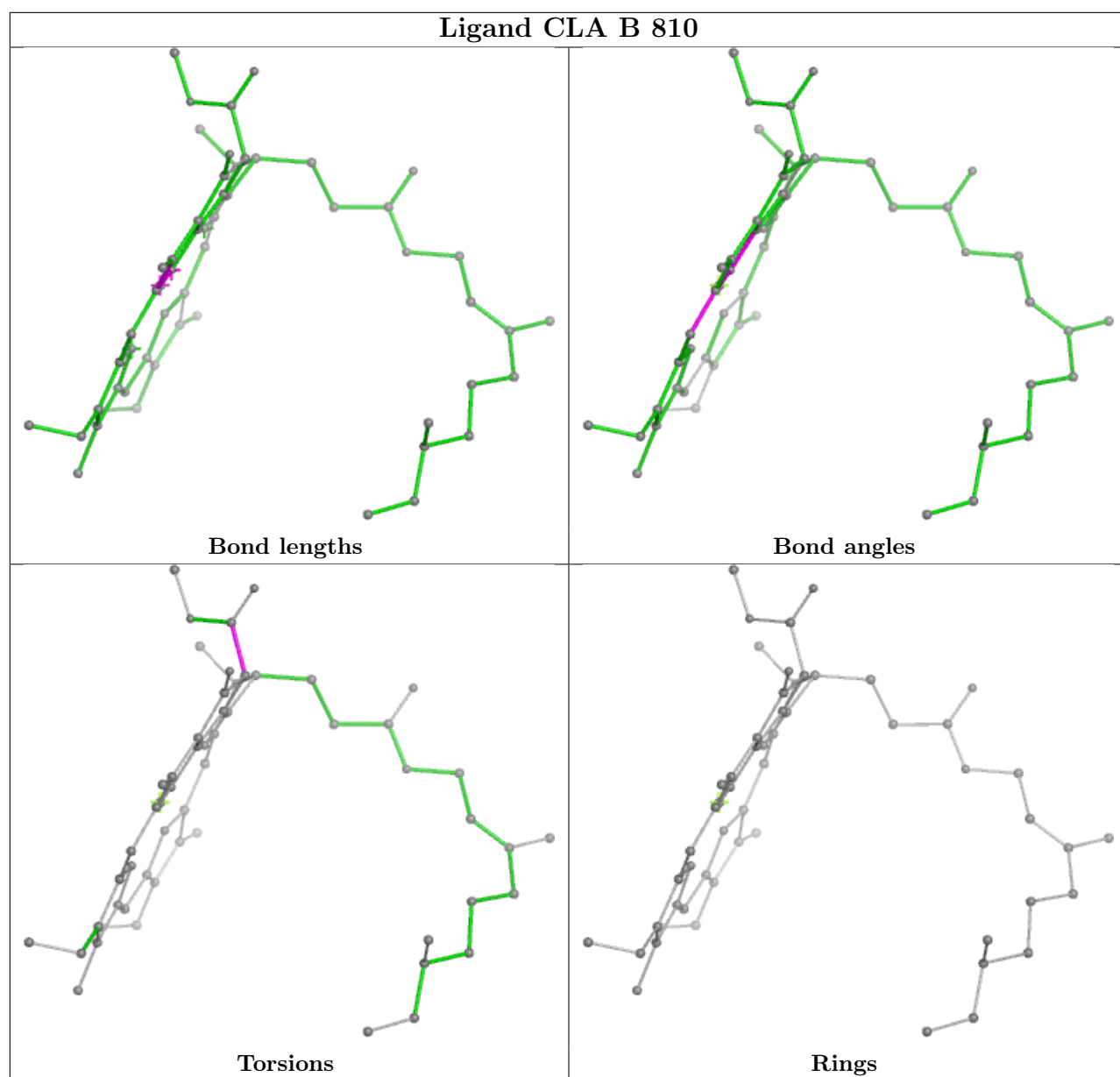


## Ligand CLA A 837

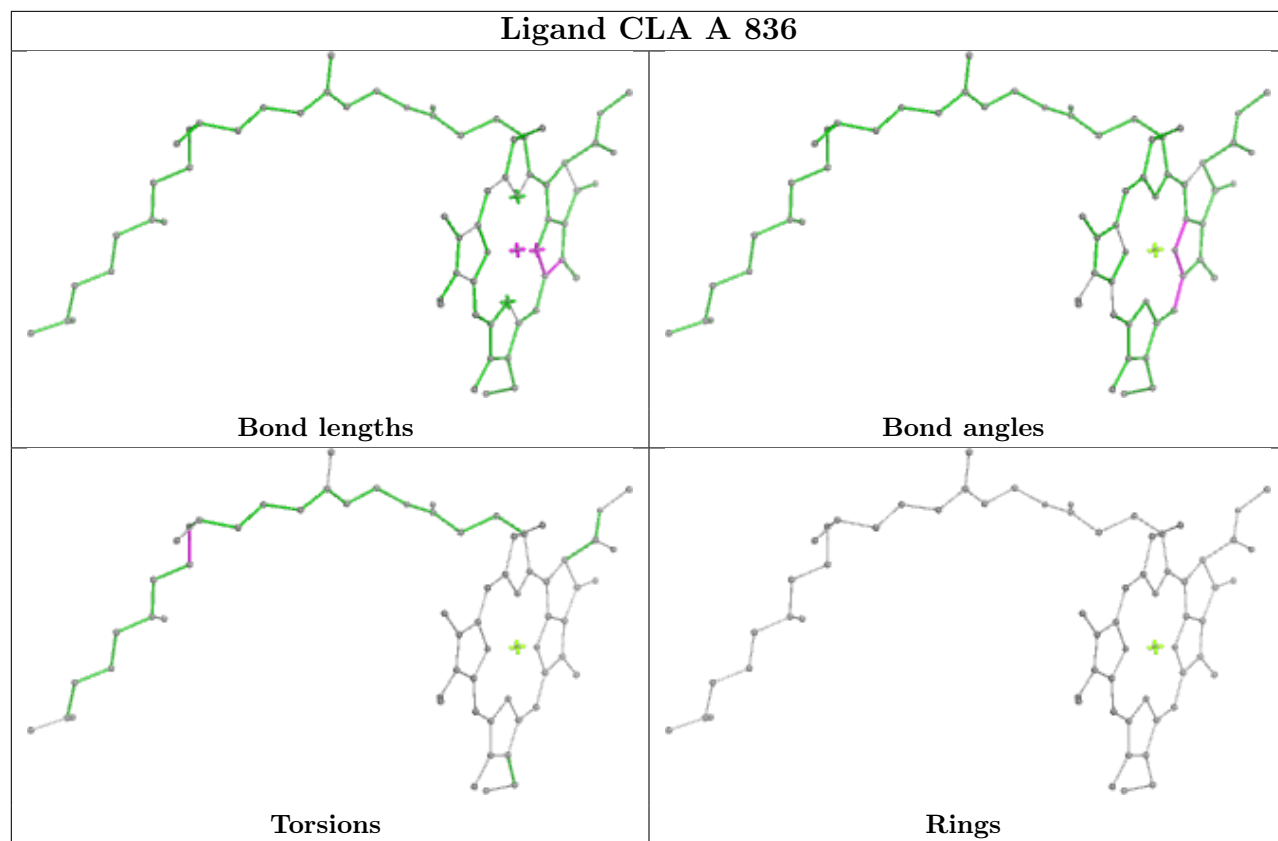


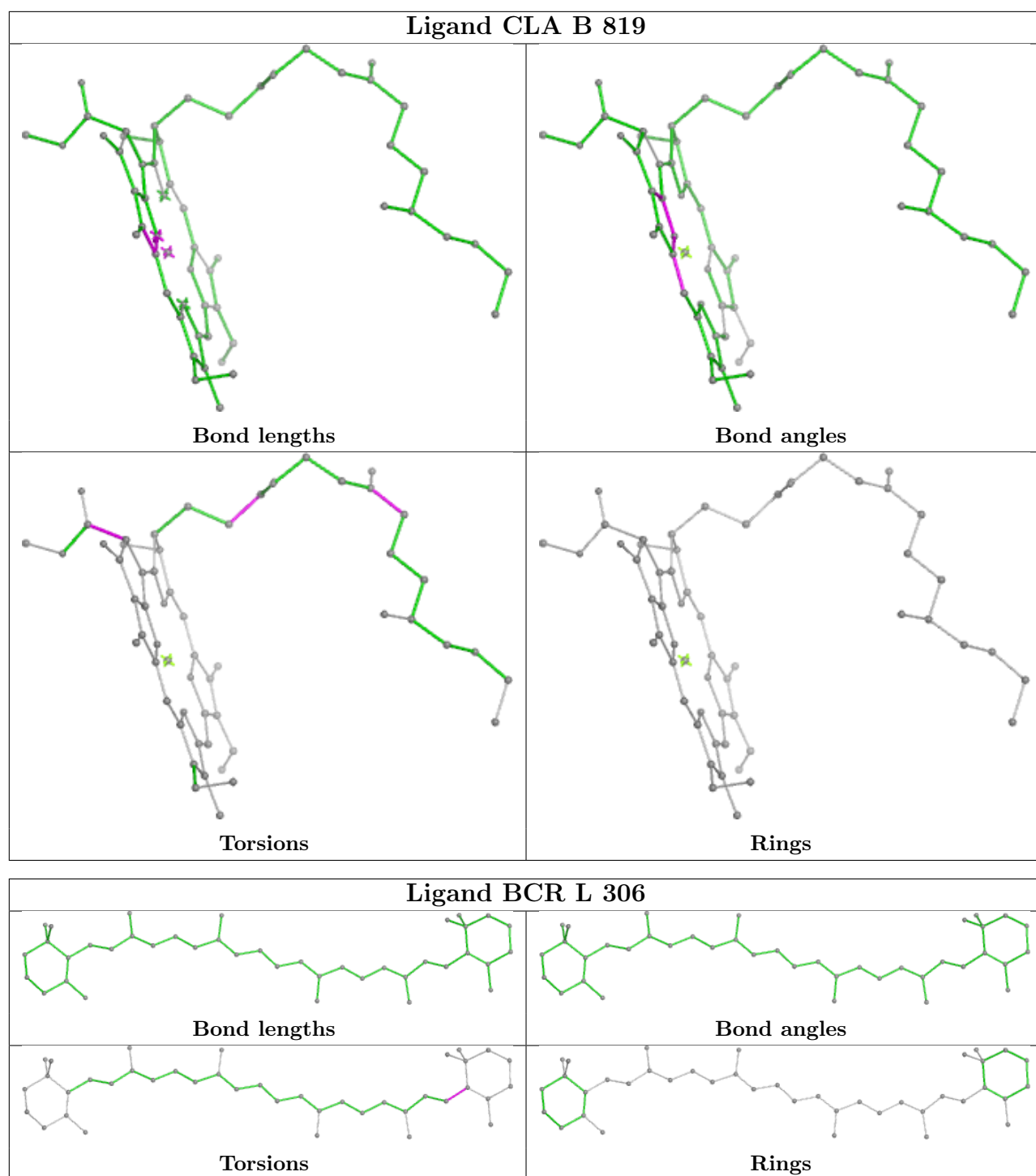




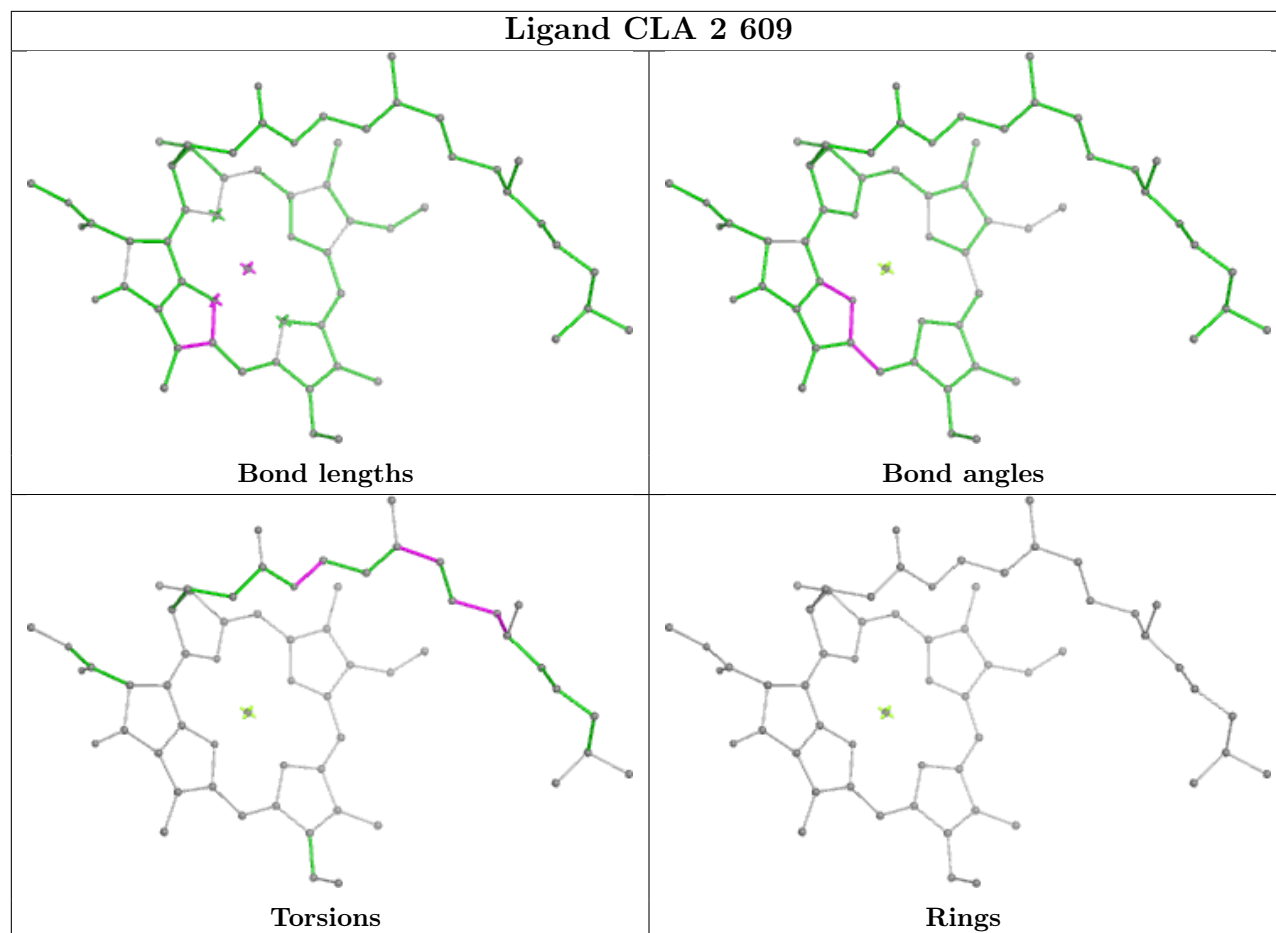




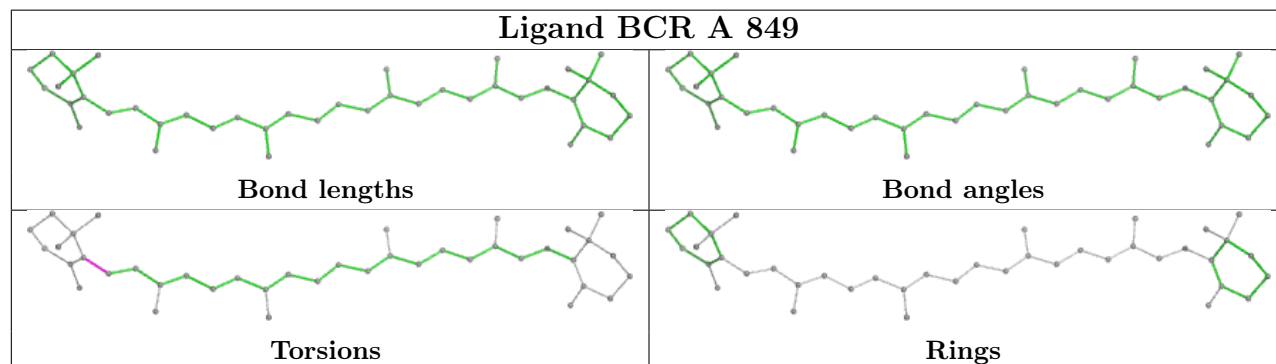




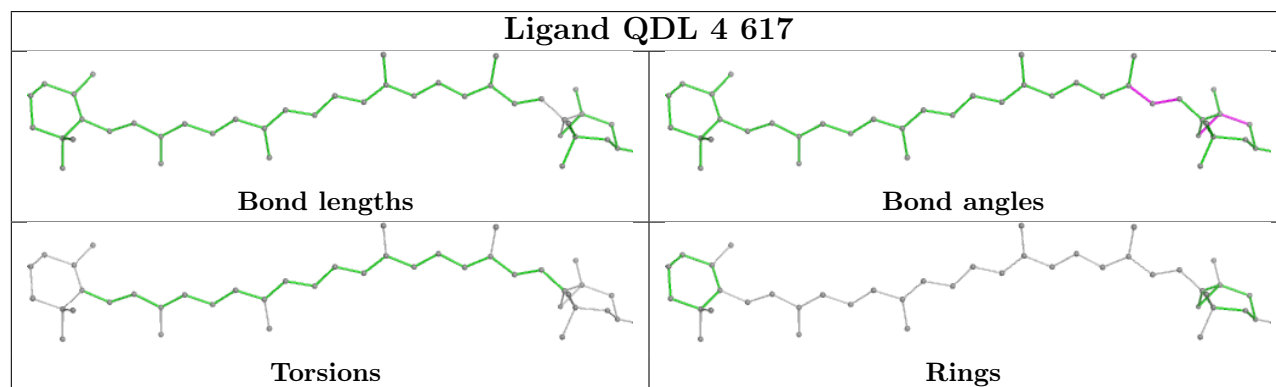
## Ligand CLA 2 609

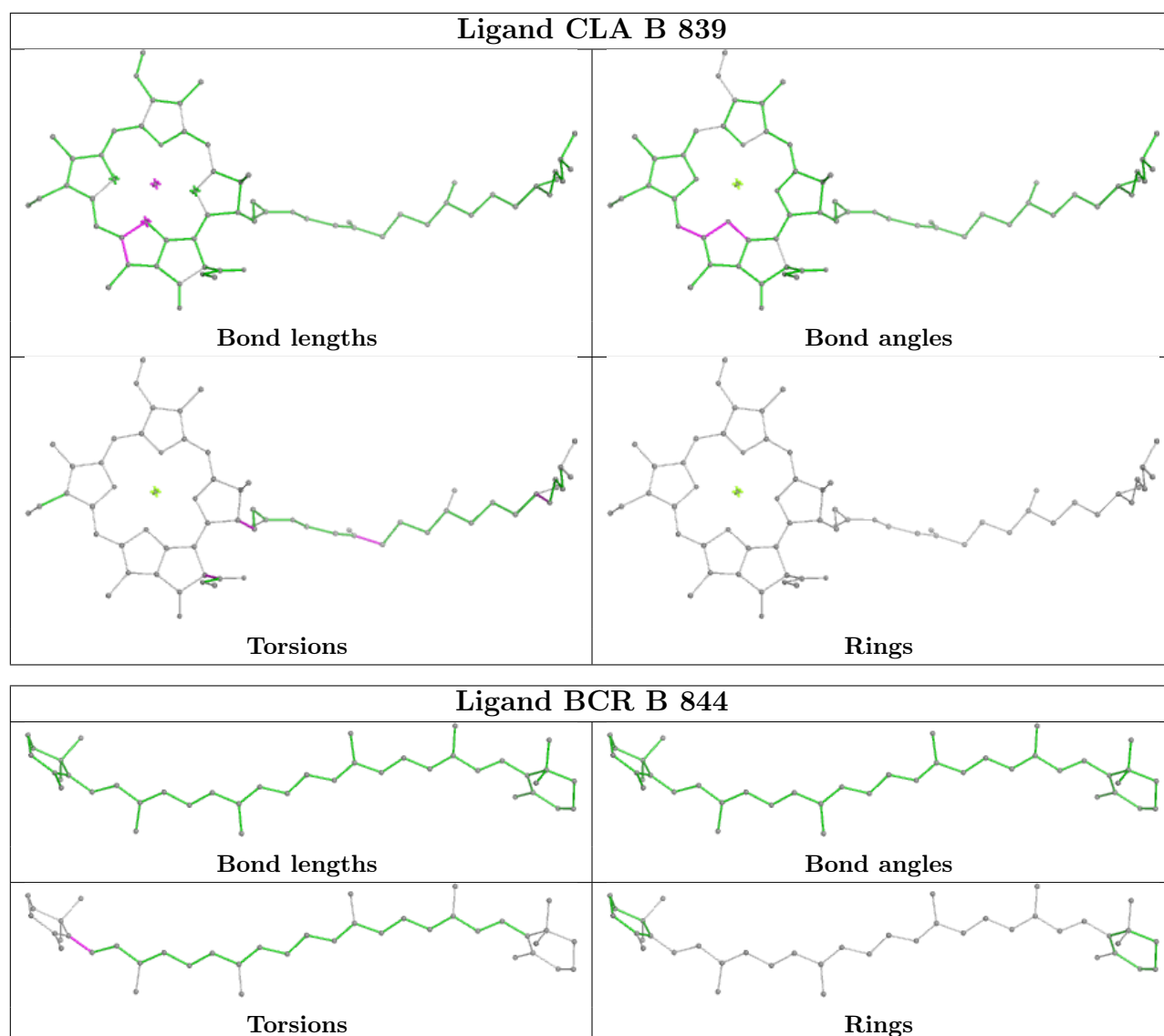


## Ligand BCR A 849

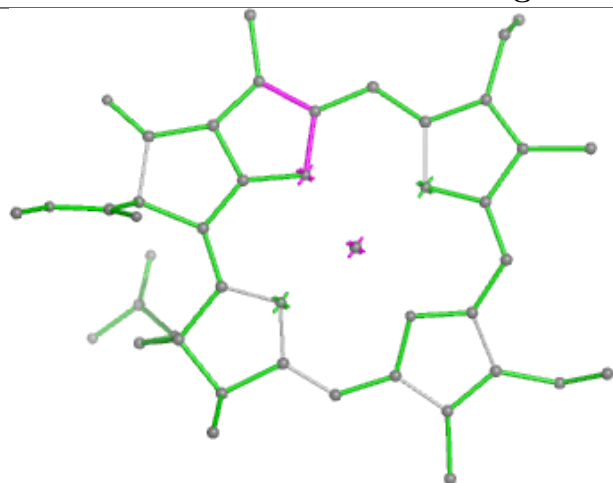


## Ligand QDL 4 617

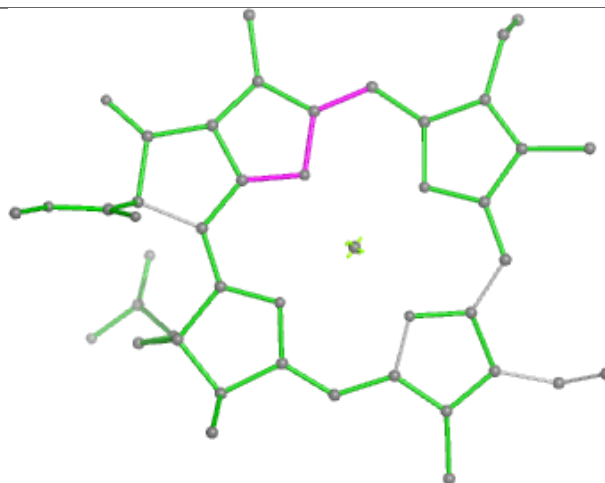




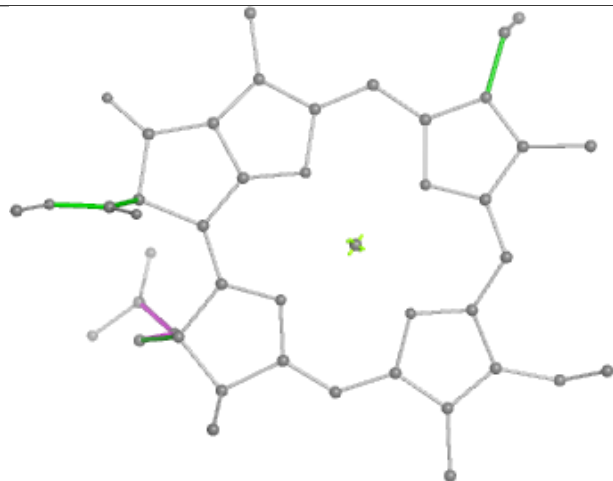
## Ligand CLA A 817



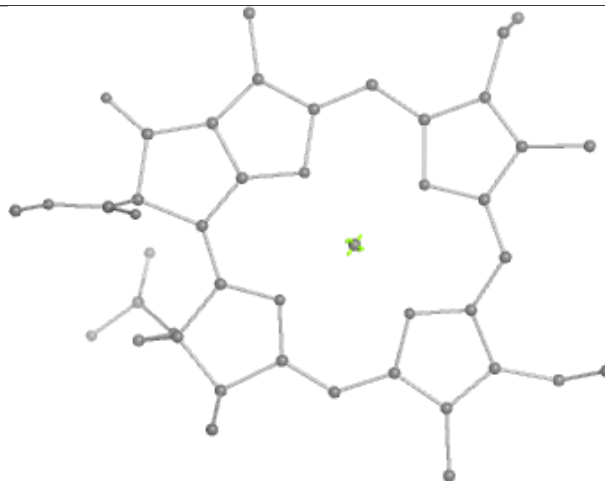
Bond lengths



Bond angles

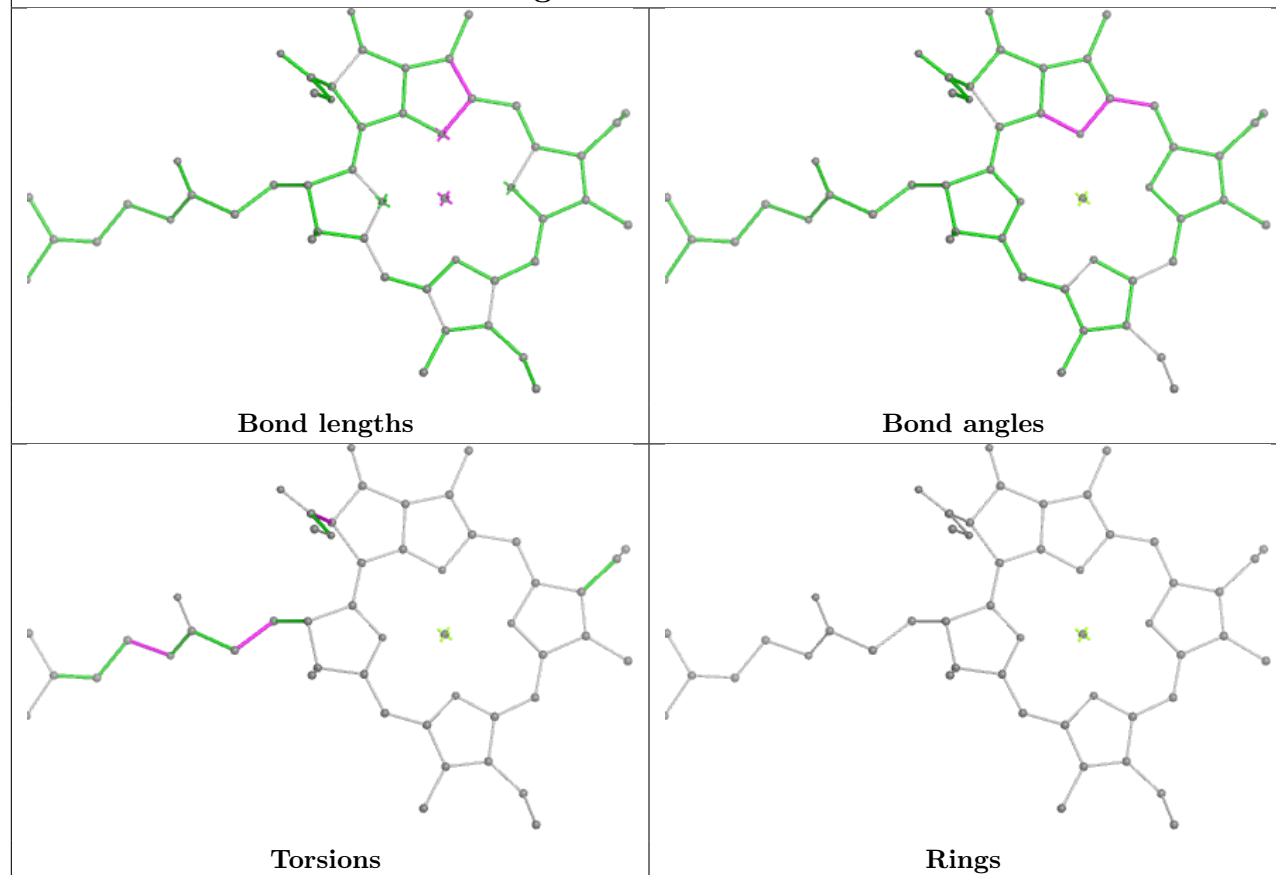


Torsions

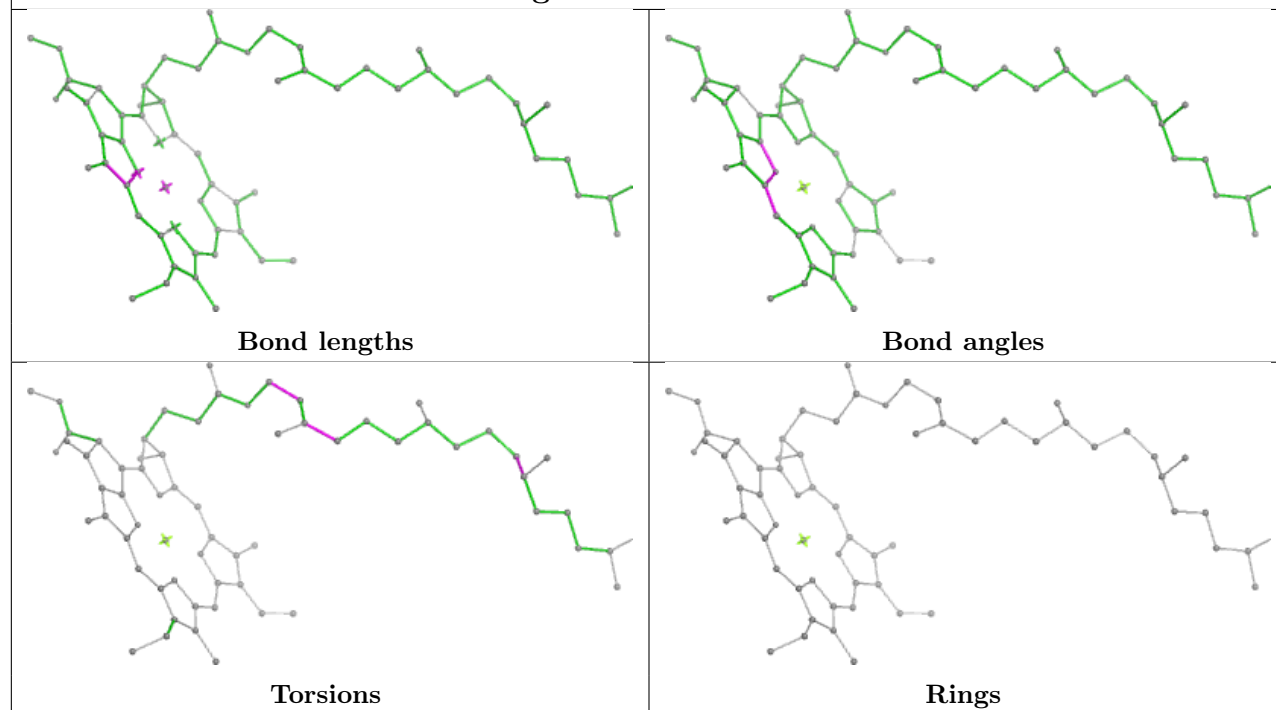


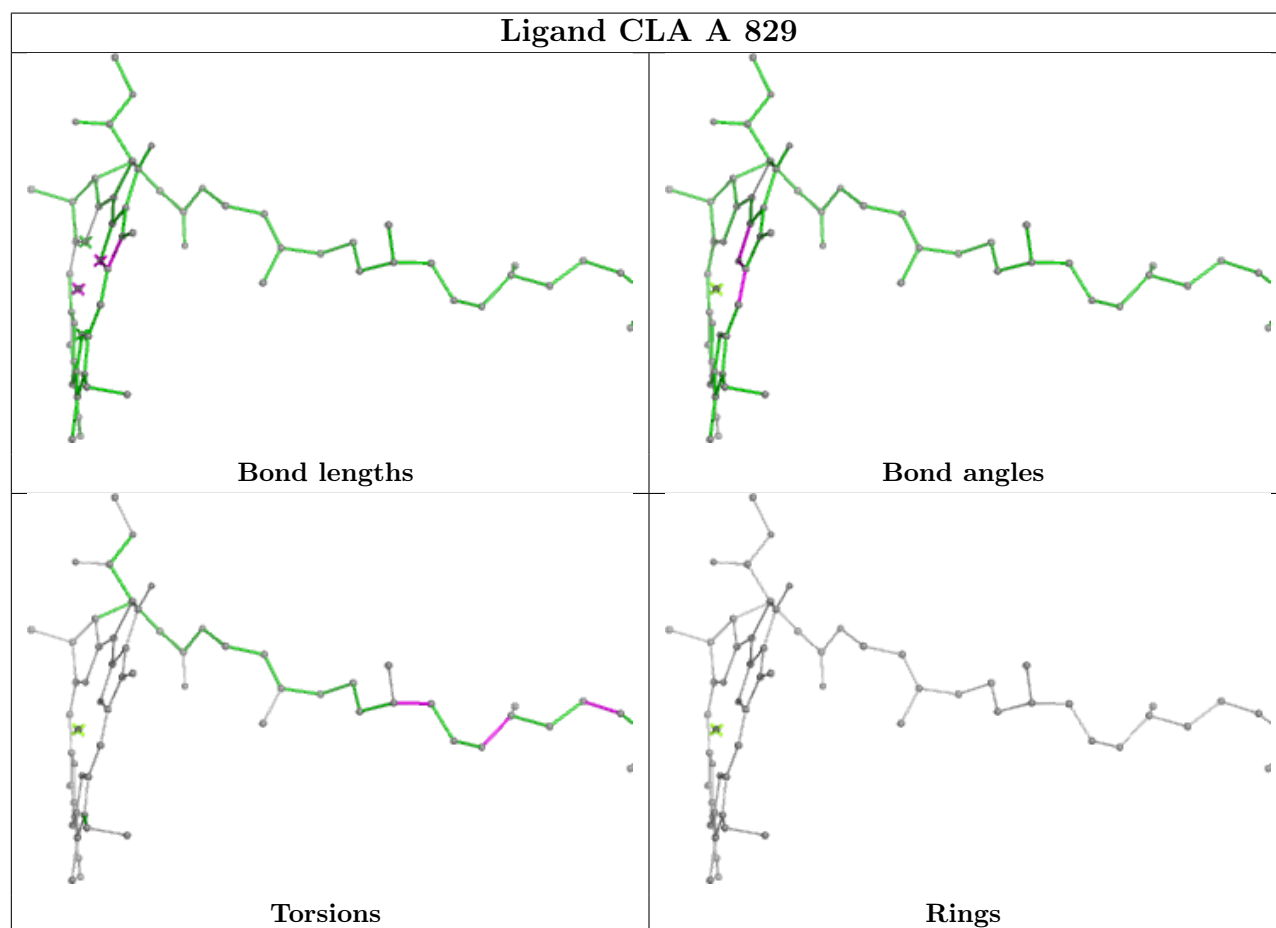
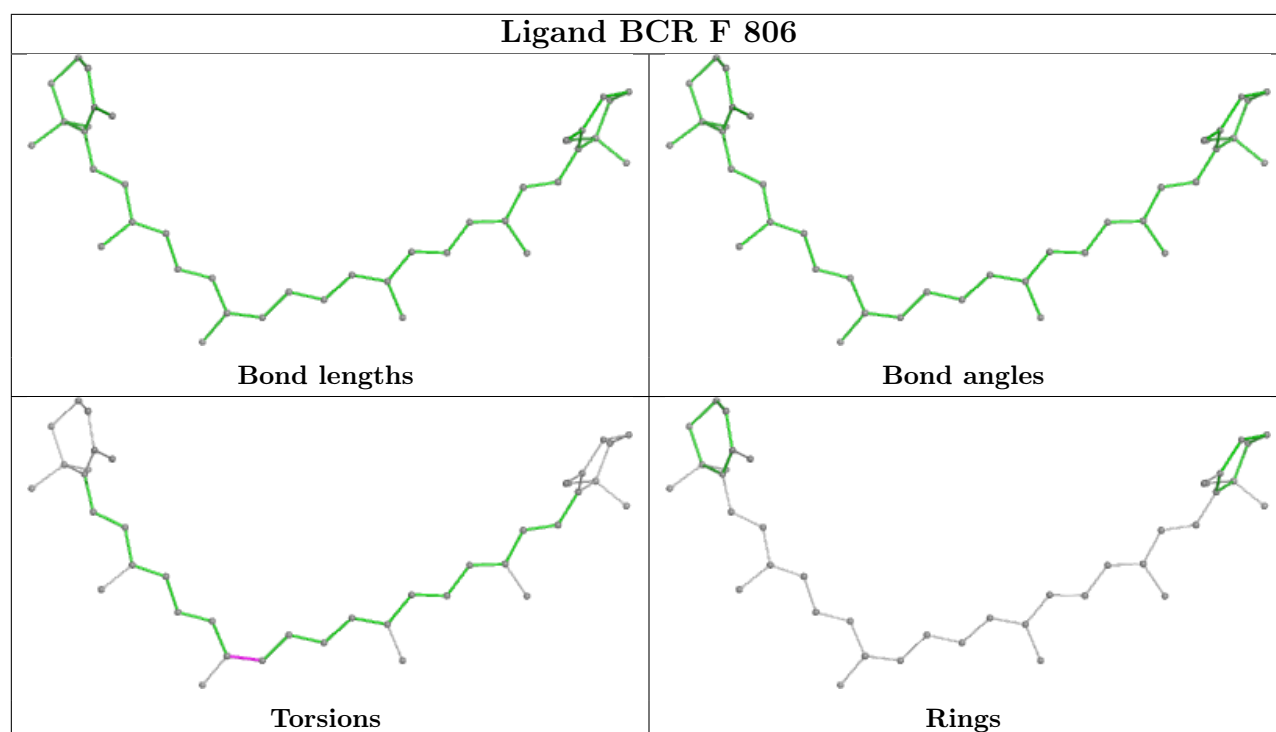
Rings

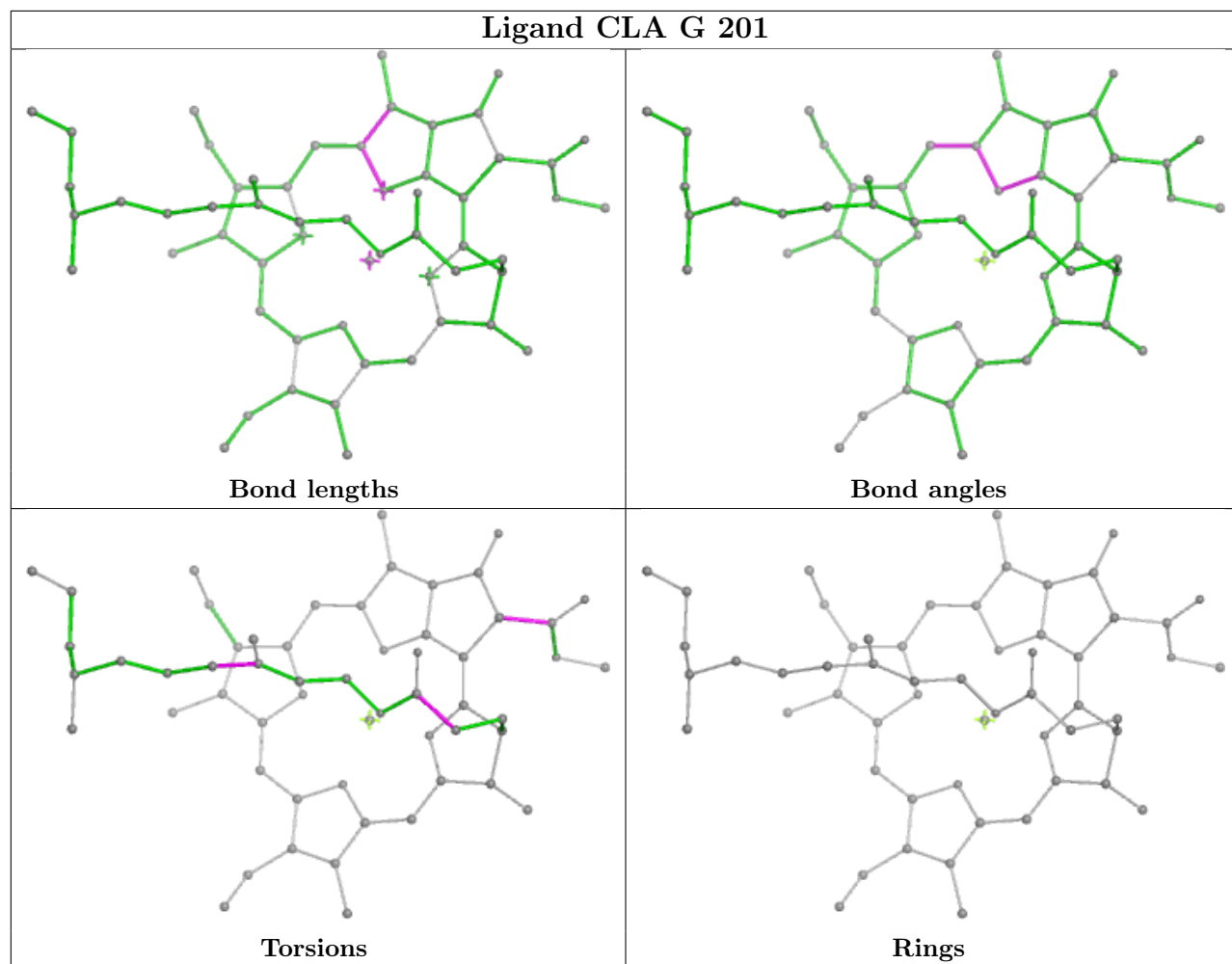
## Ligand CLA F 805



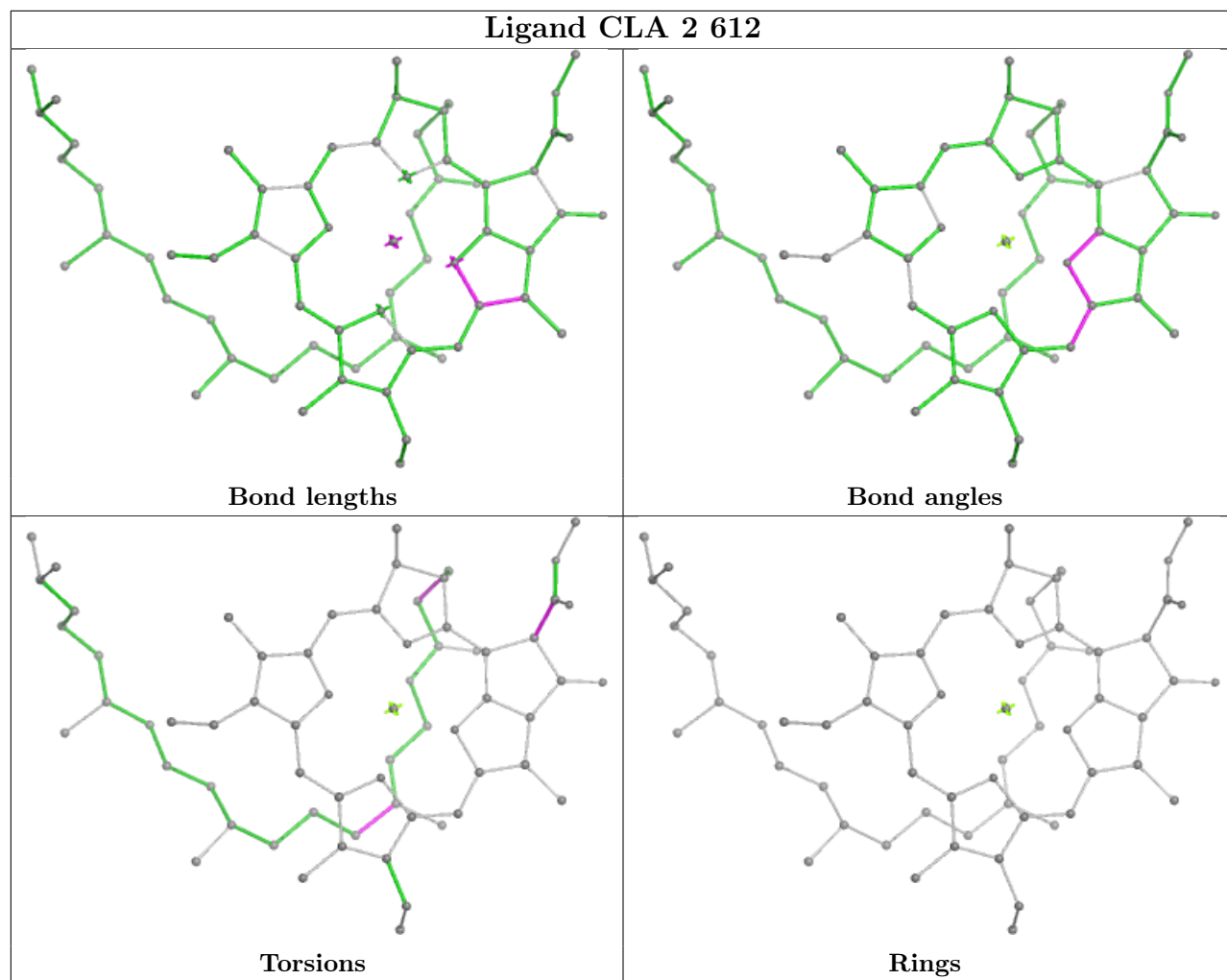
## Ligand CLA B 829

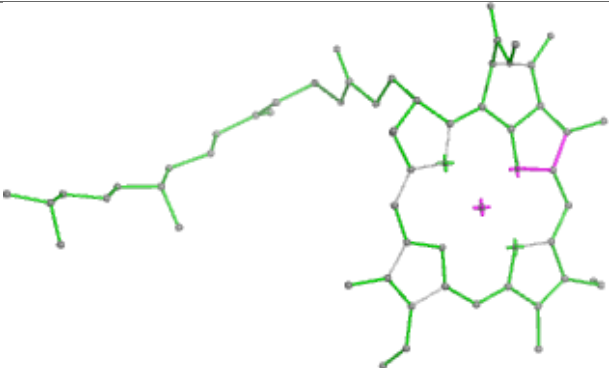
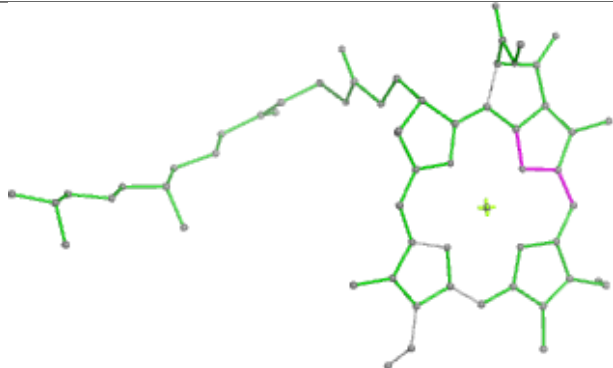
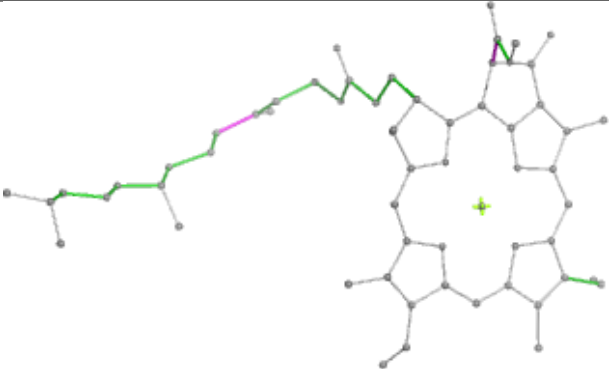
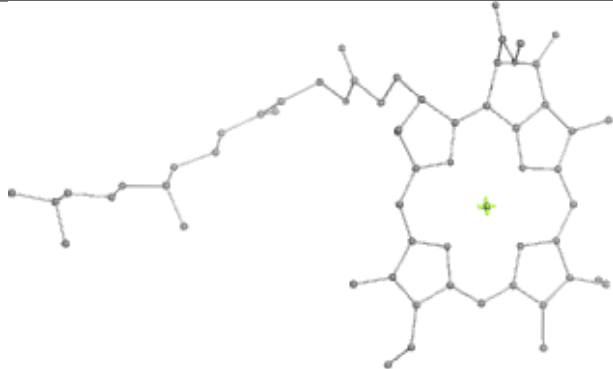




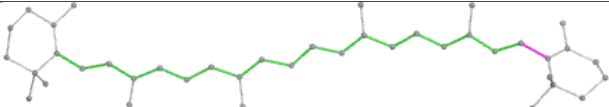
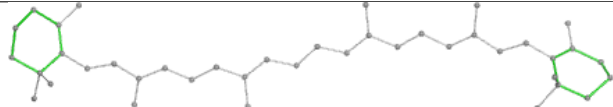




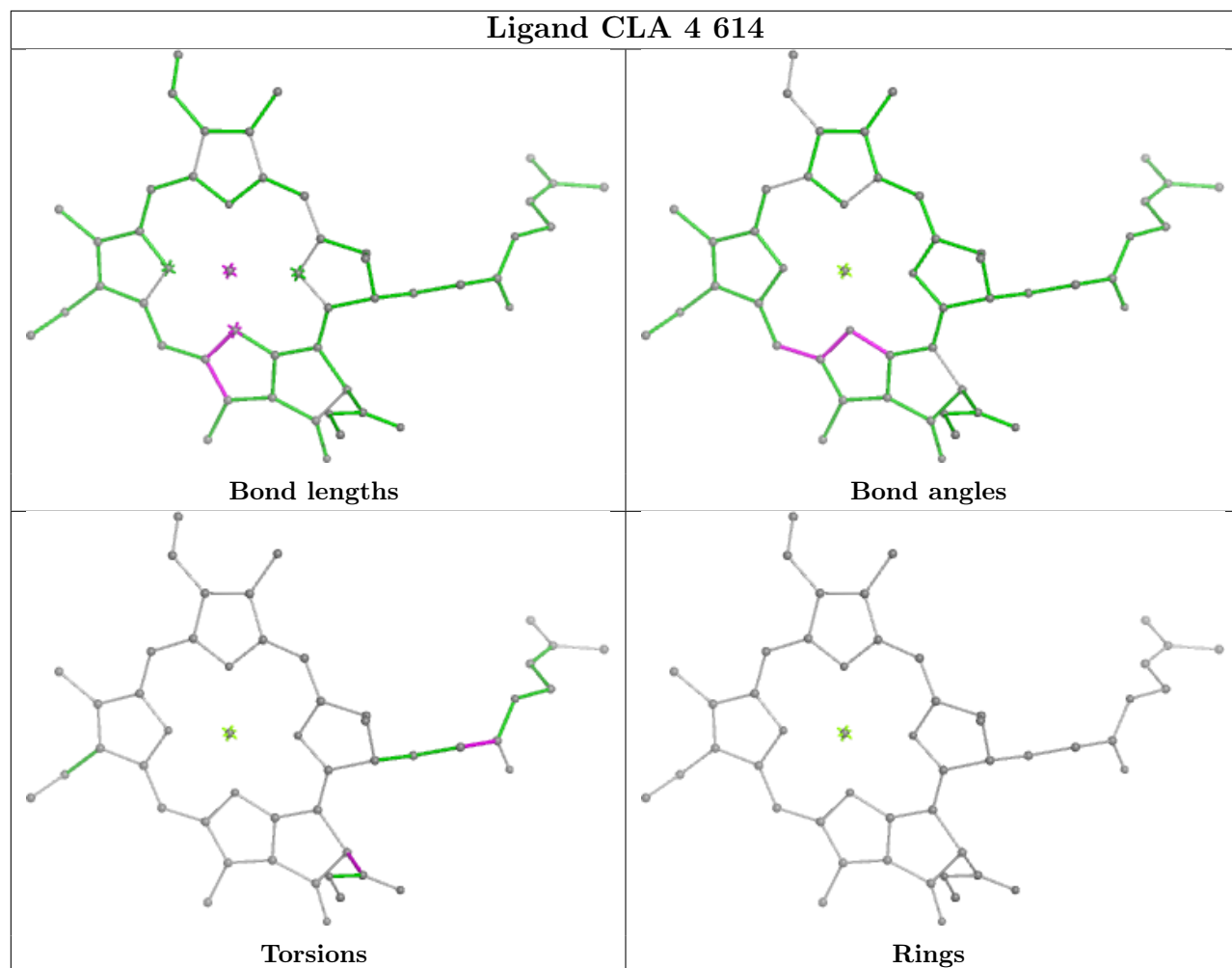




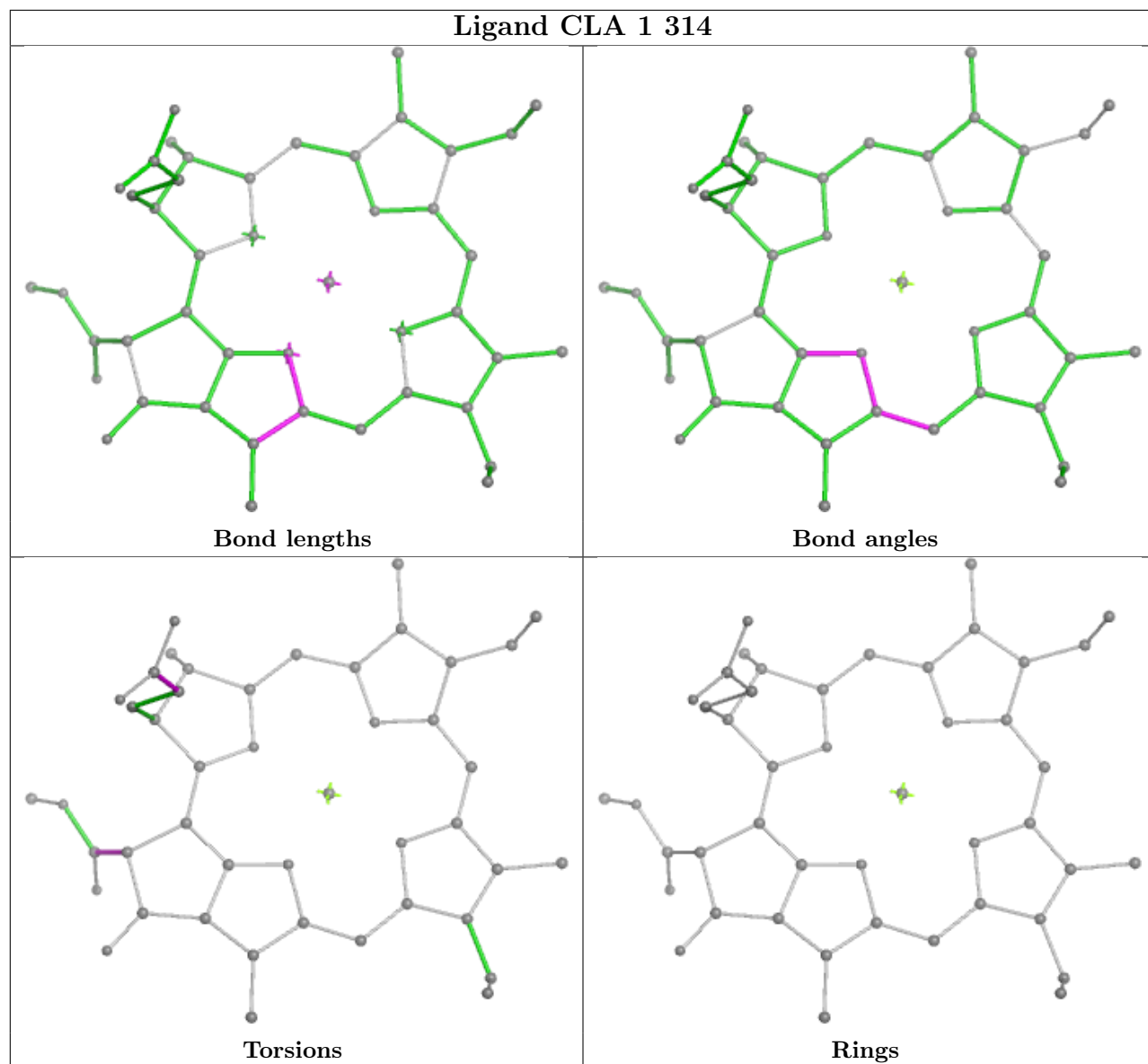
Ligand CLA B 818	
	
Bond lengths	Bond angles
	
Torsions	Rings

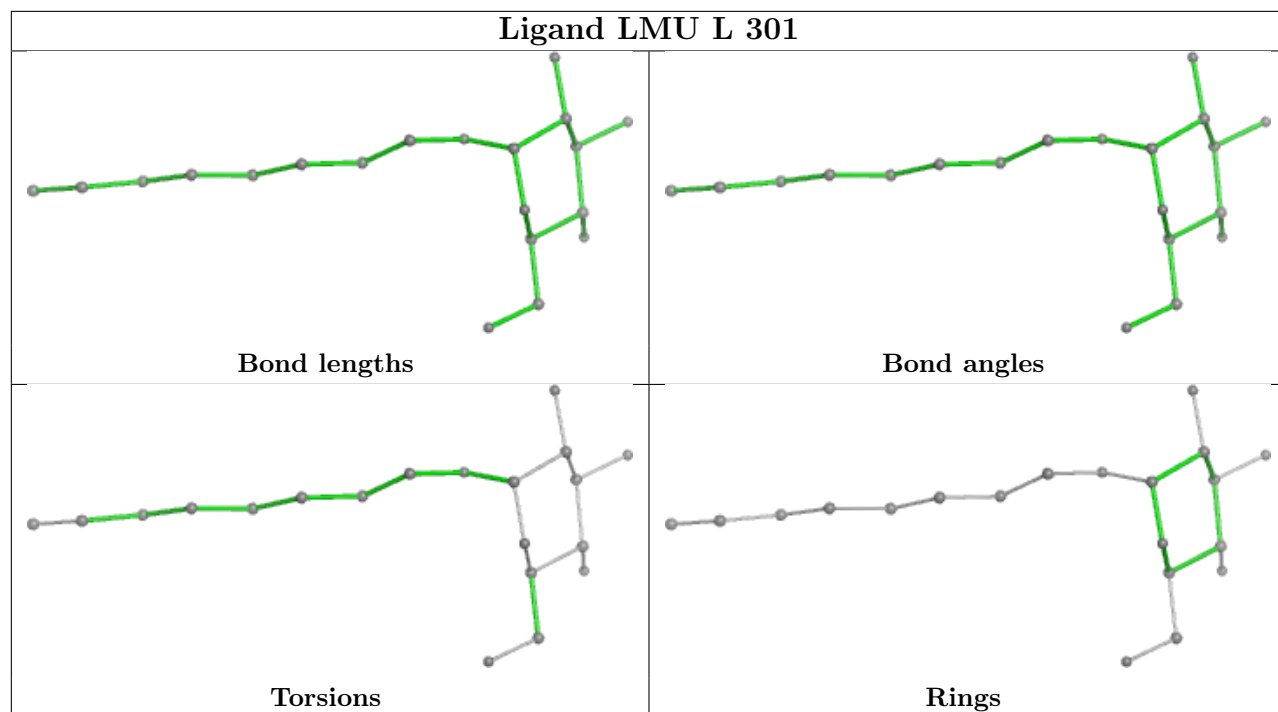
Ligand BCR J 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

## Ligand CLA 4 614

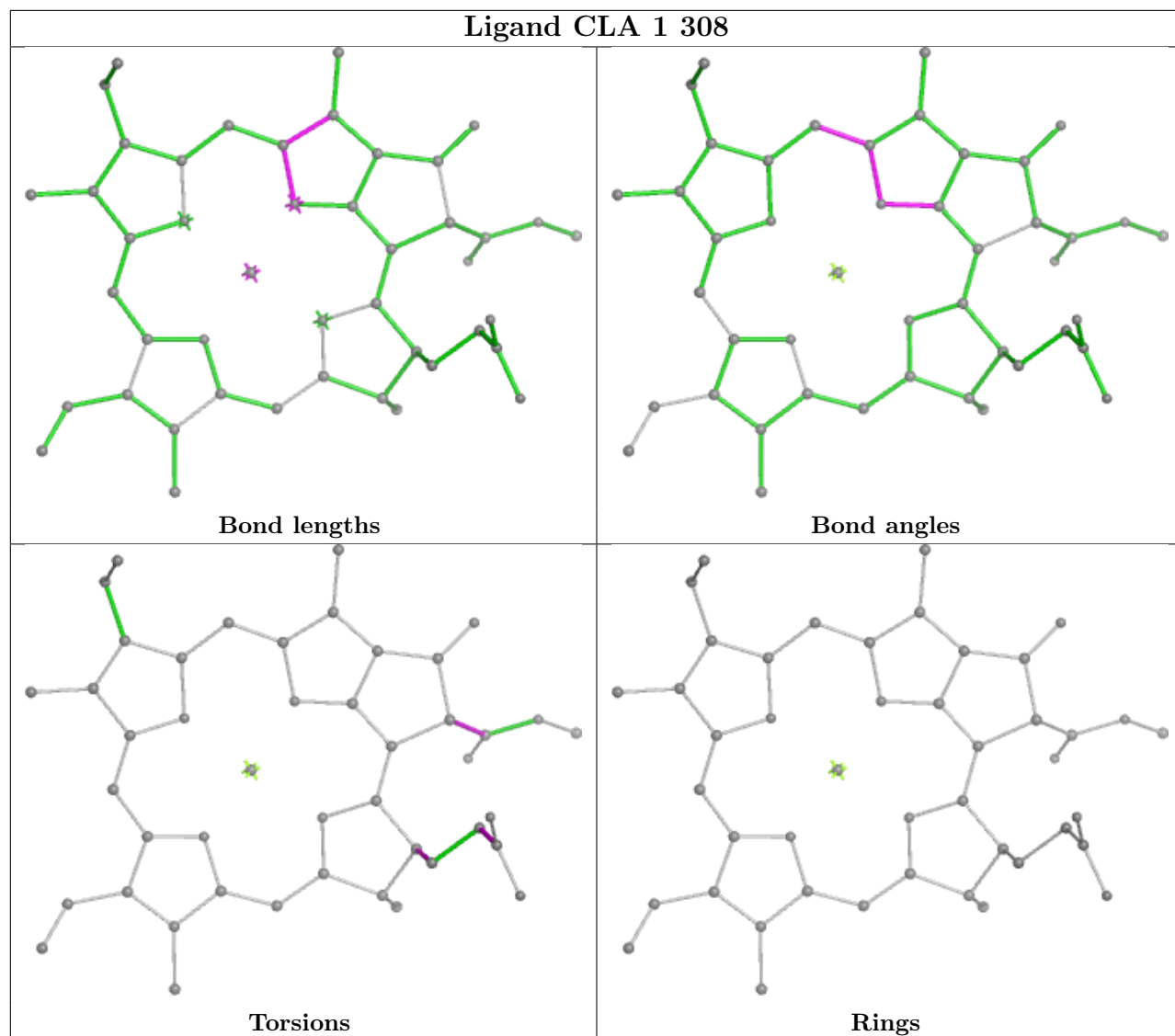


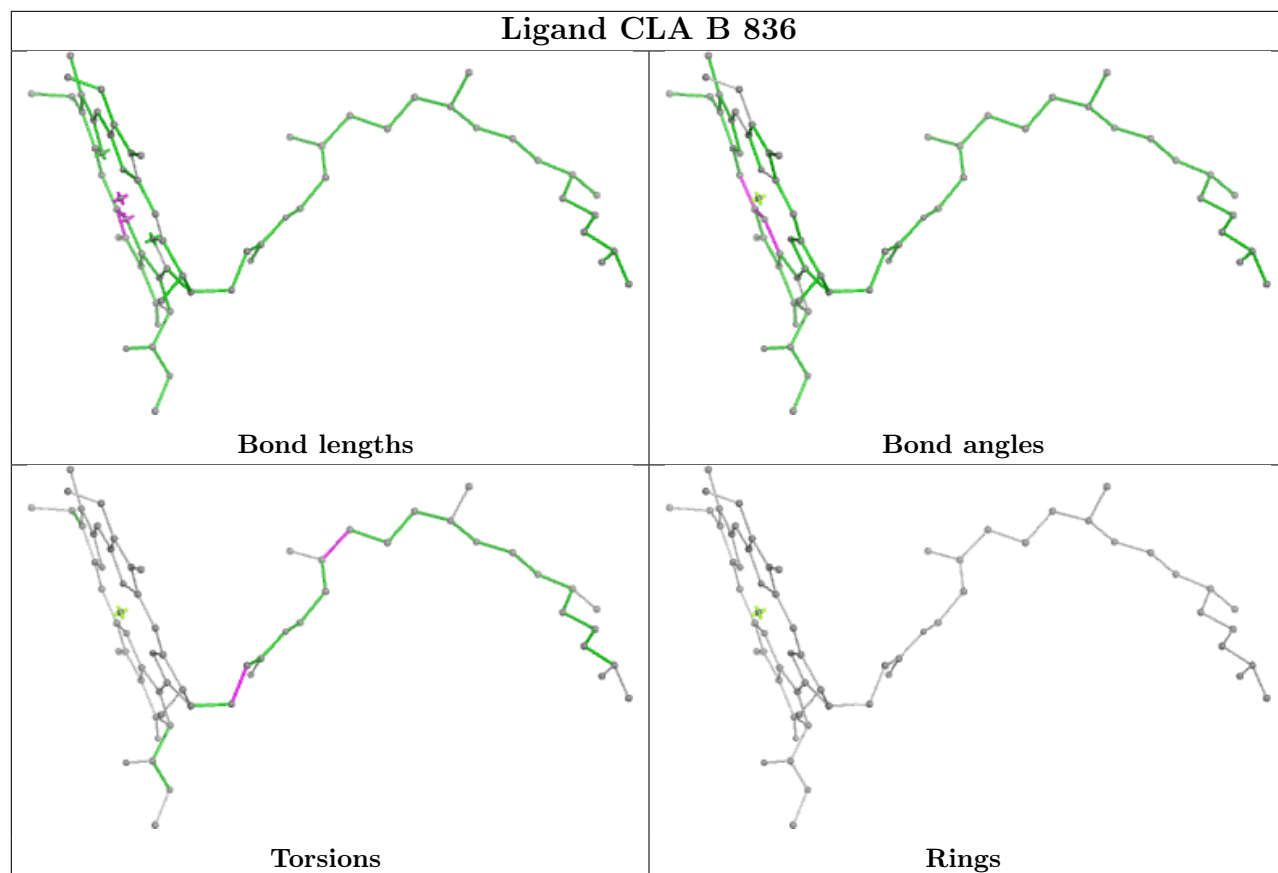
## Ligand CLA 1 314



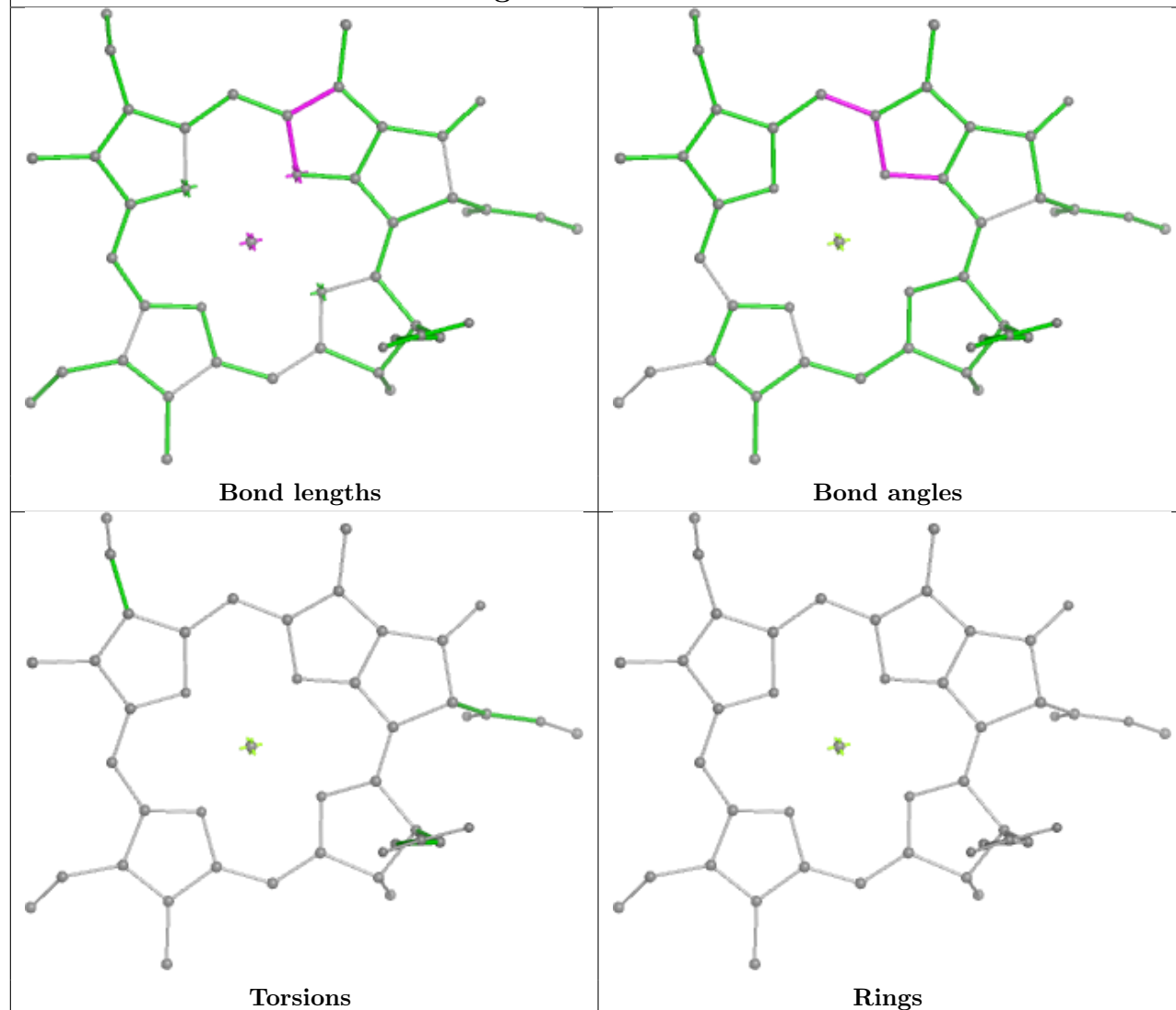


## Ligand CLA 1 308

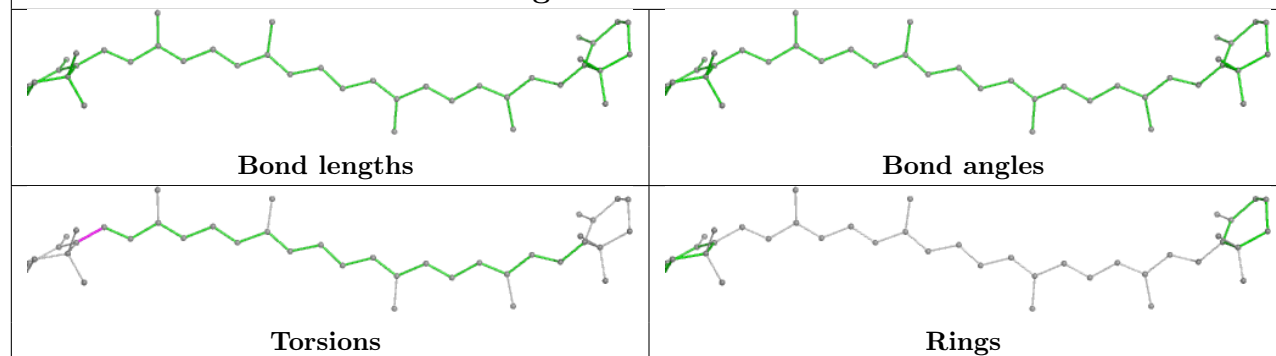








## Ligand CLA 2 604

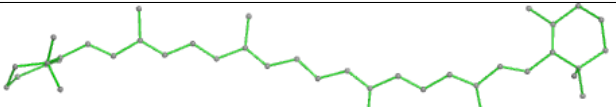
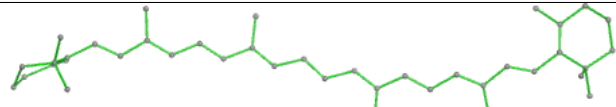
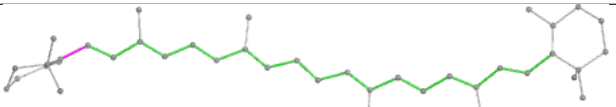
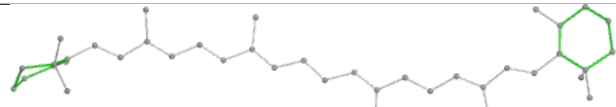


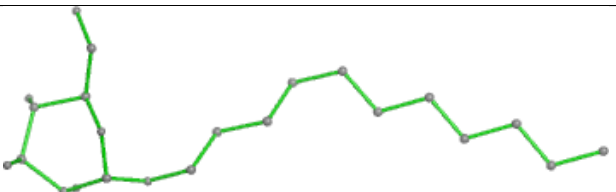
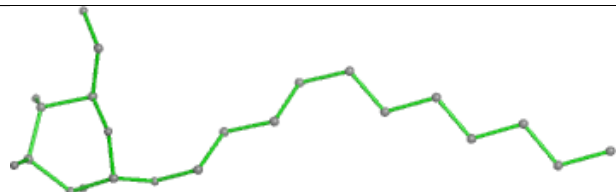


## Ligand BCR L 307

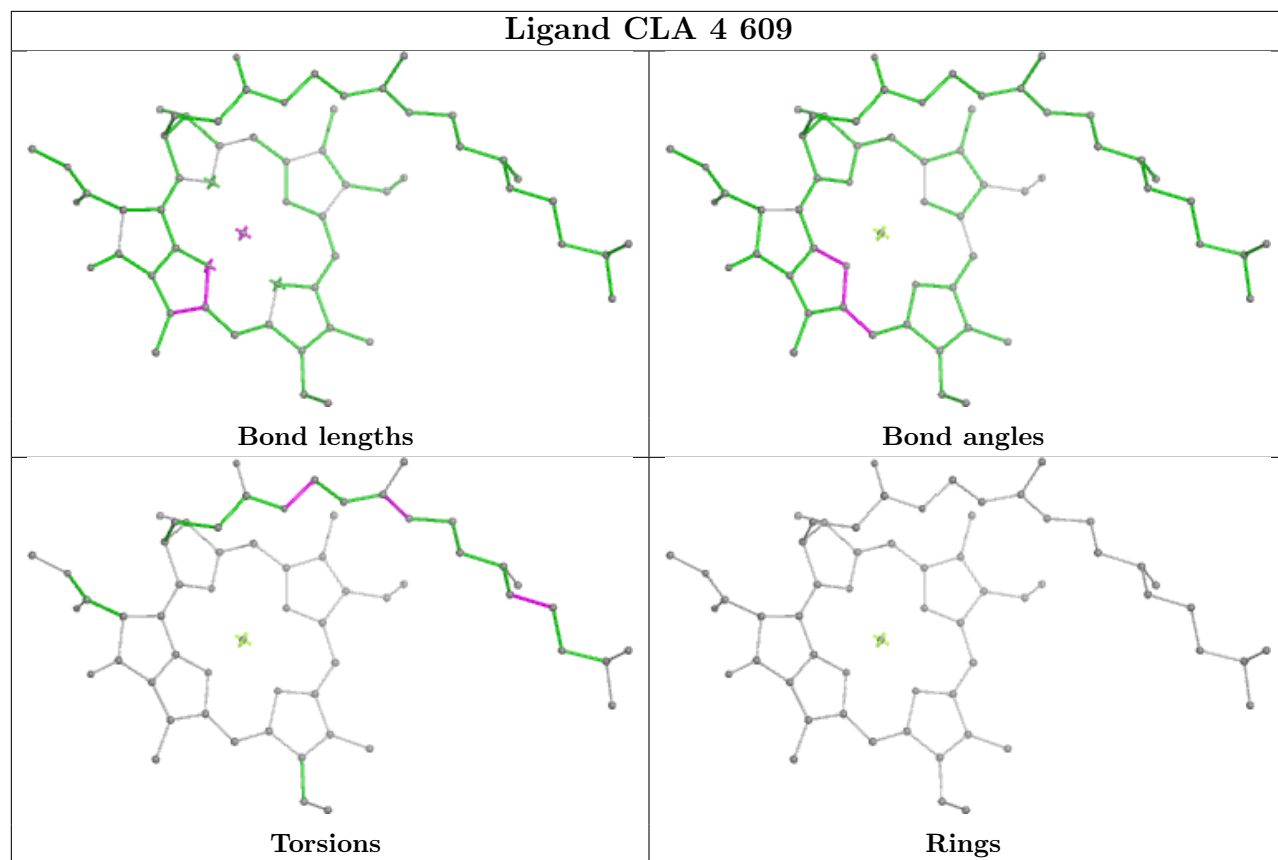


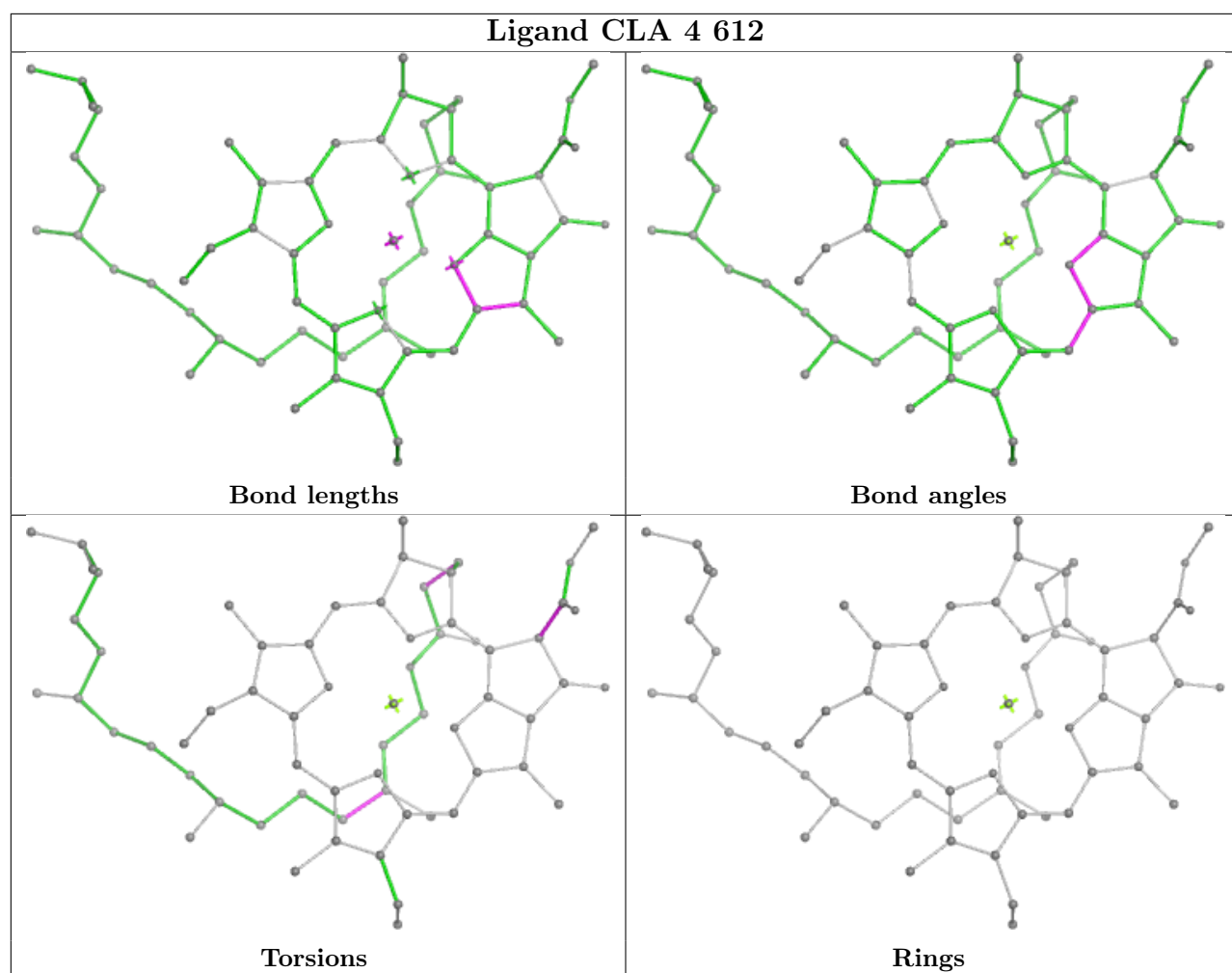


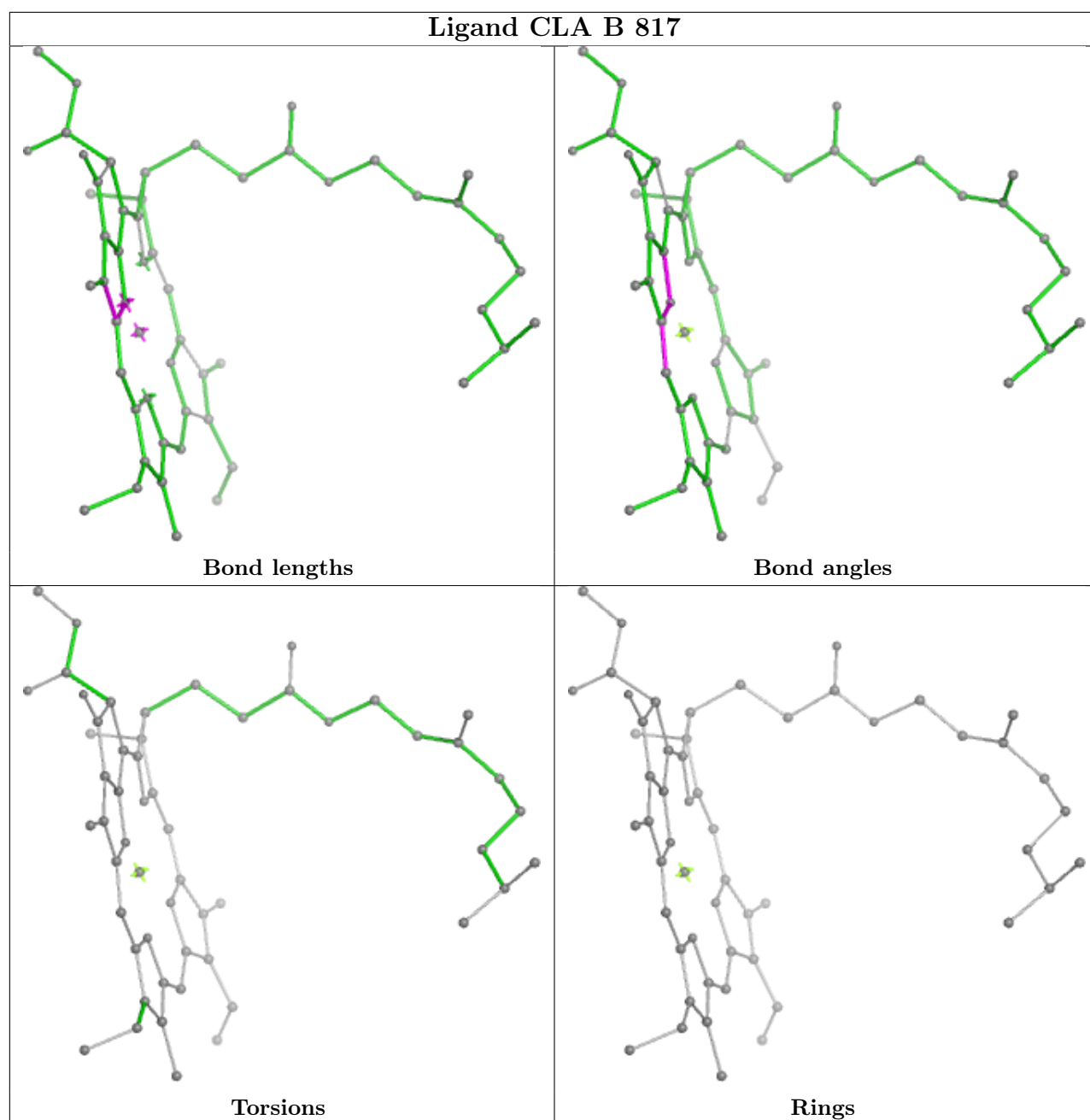
Ligand XAT 2 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 840	
	
Bond lengths	Bond angles
	
Torsions	Rings

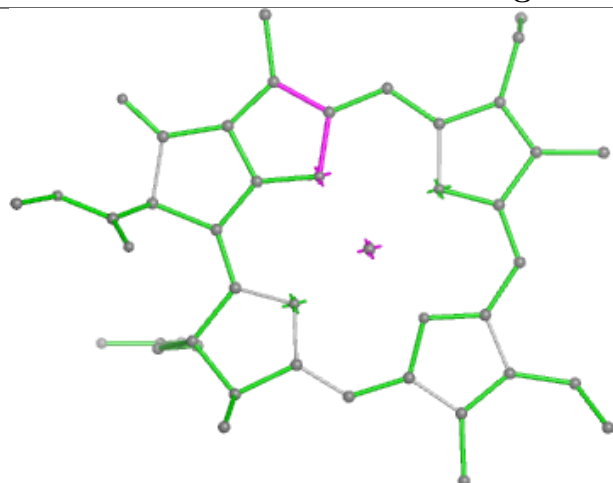
Ligand LMU 4 621	
	
Bond lengths	Bond angles
	
Torsions	Rings



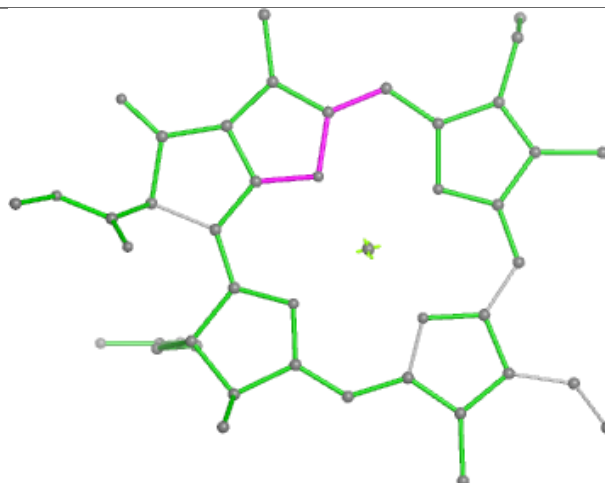




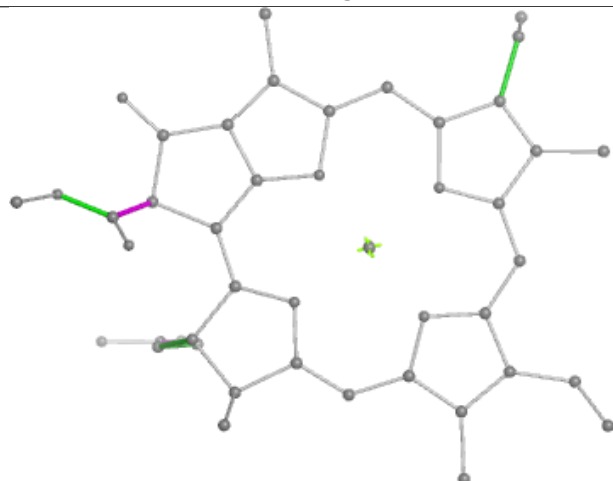
## Ligand CLA A 813



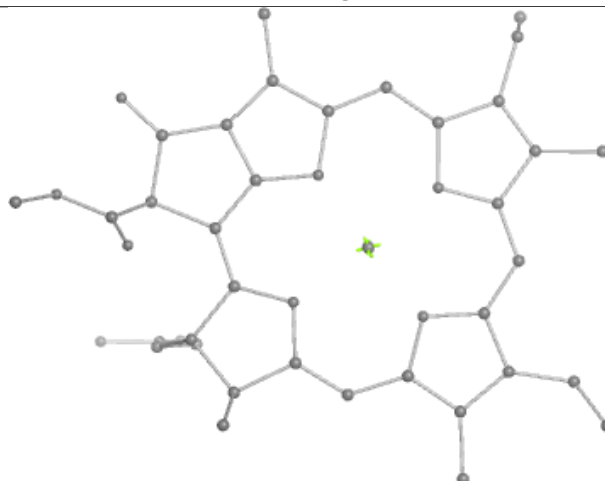
Bond lengths



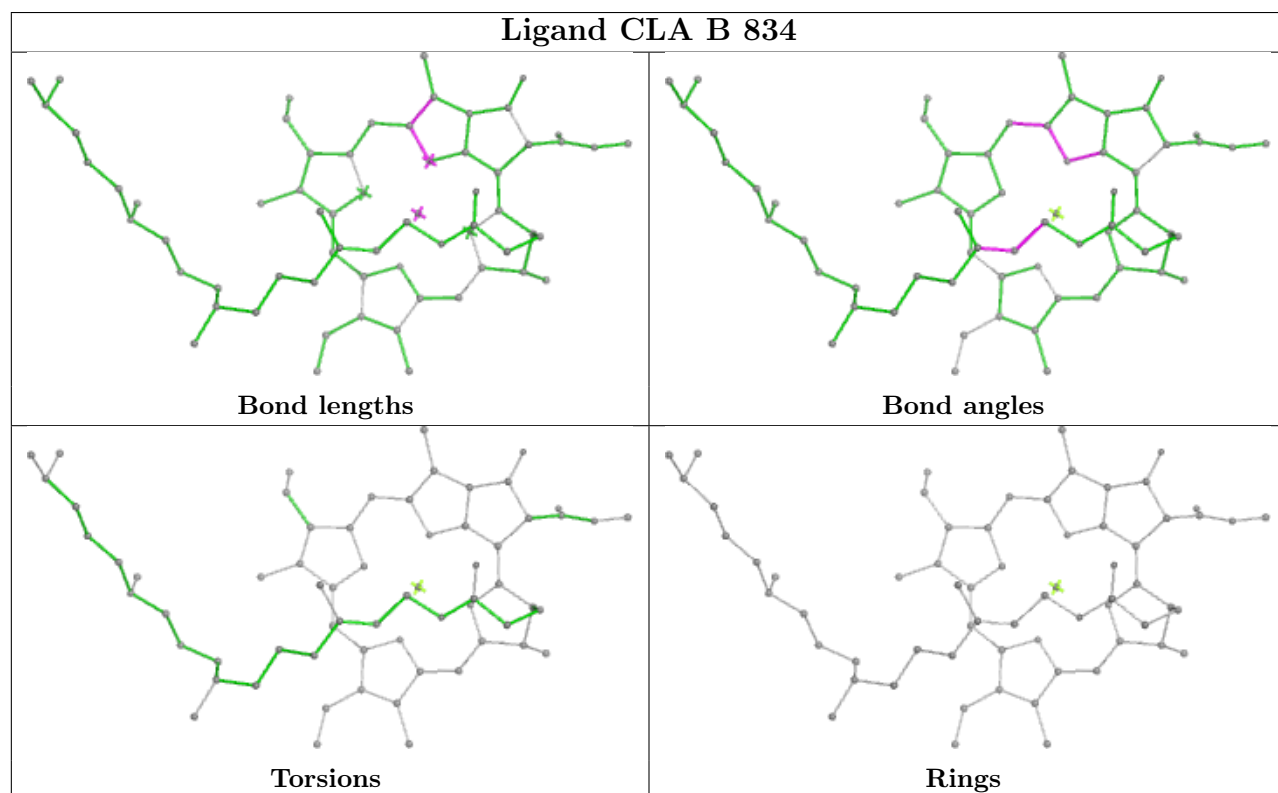
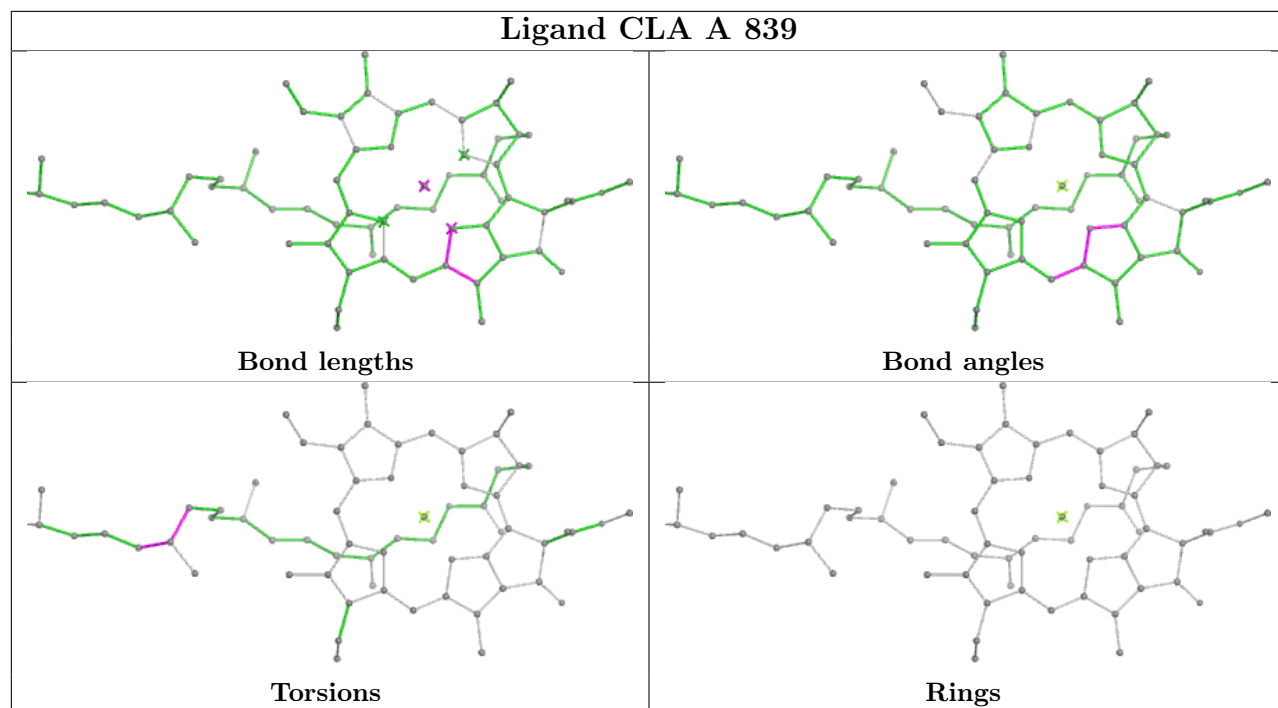
Bond angles



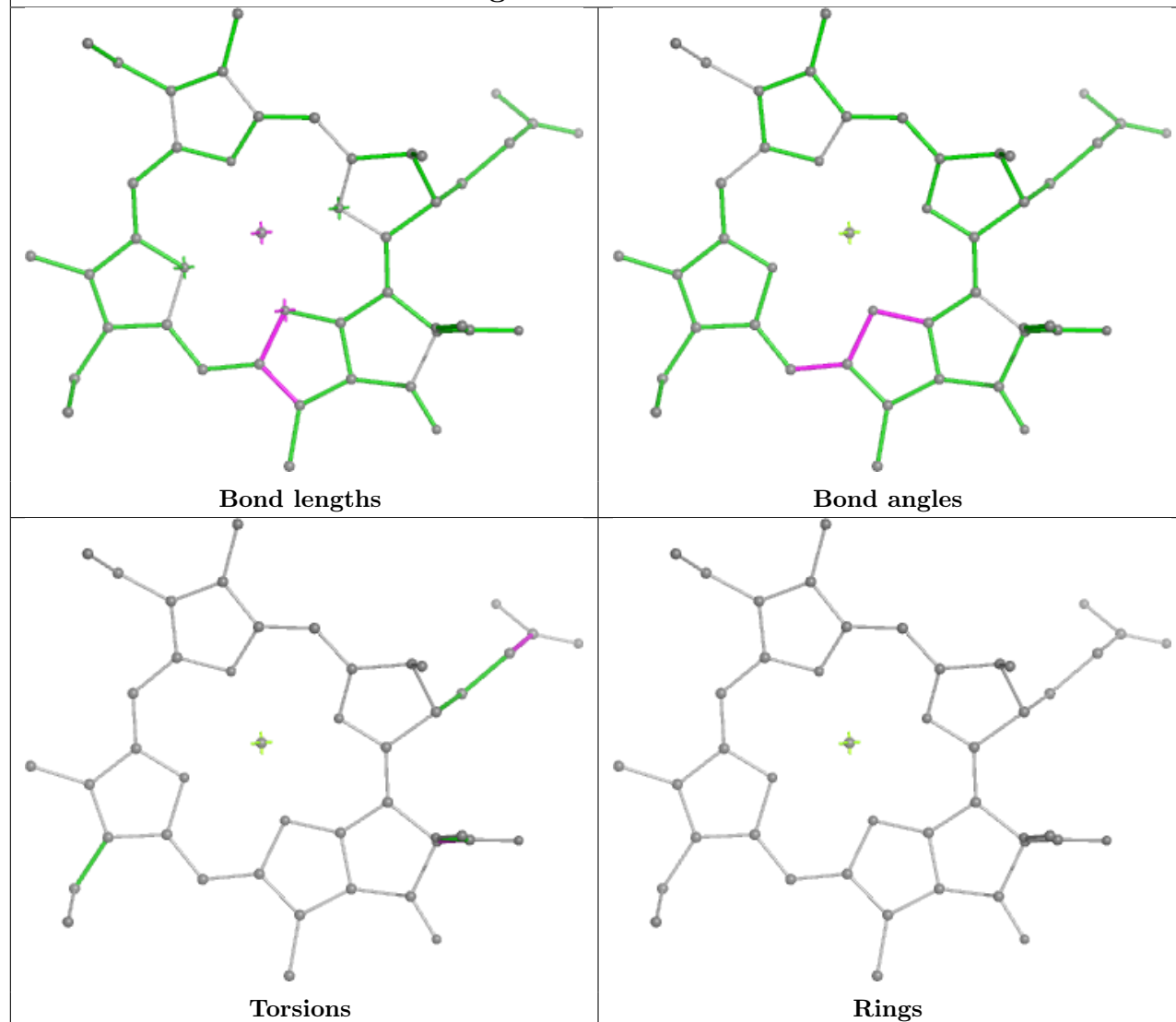
Torsions



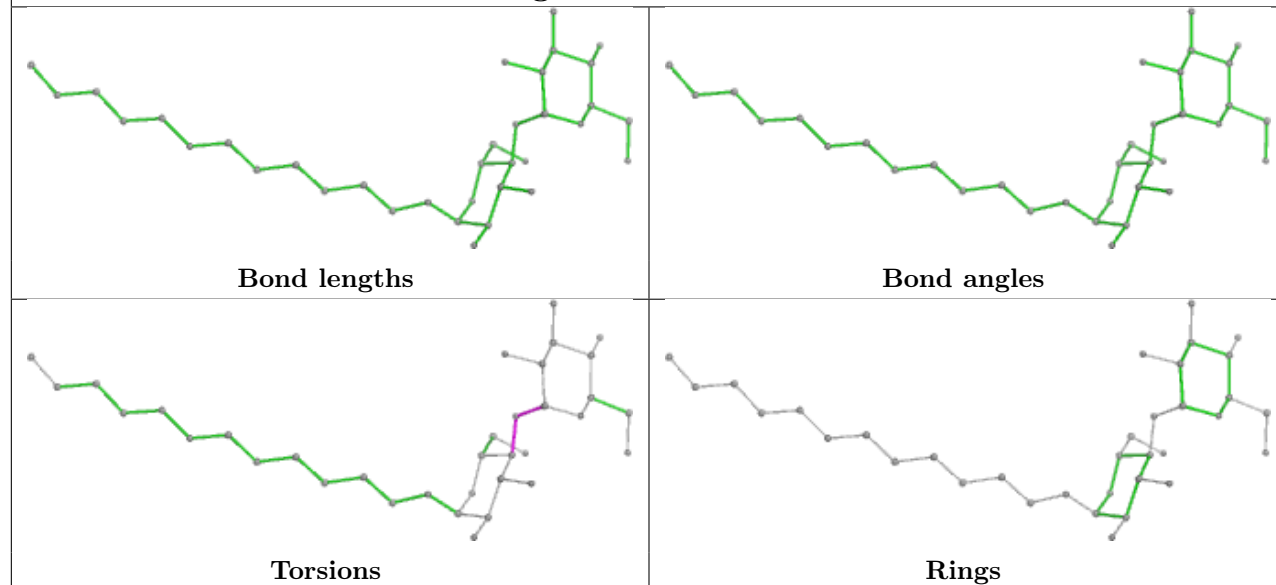
Rings



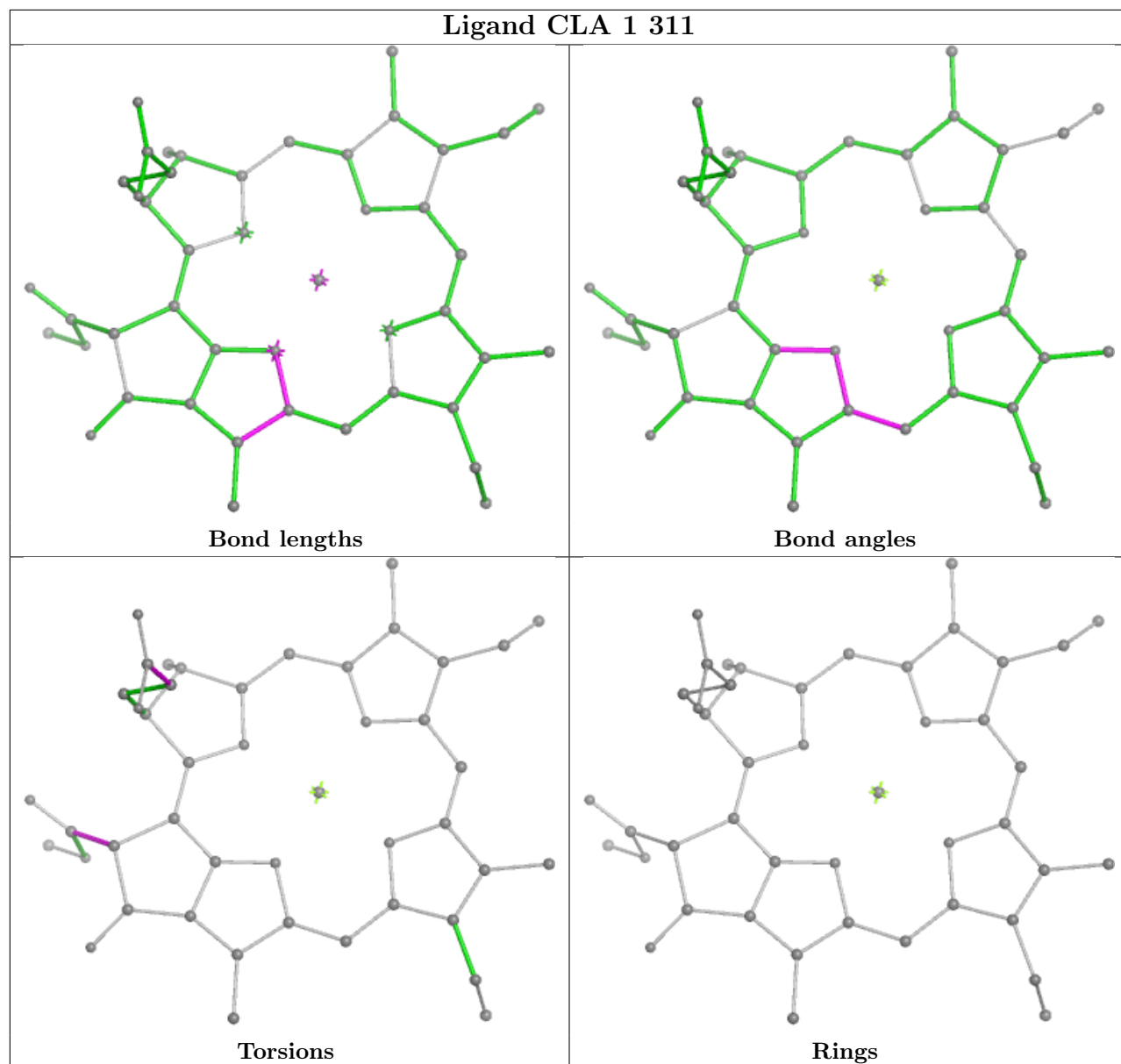
## Ligand CLA G 204



## Ligand LMU 4 623

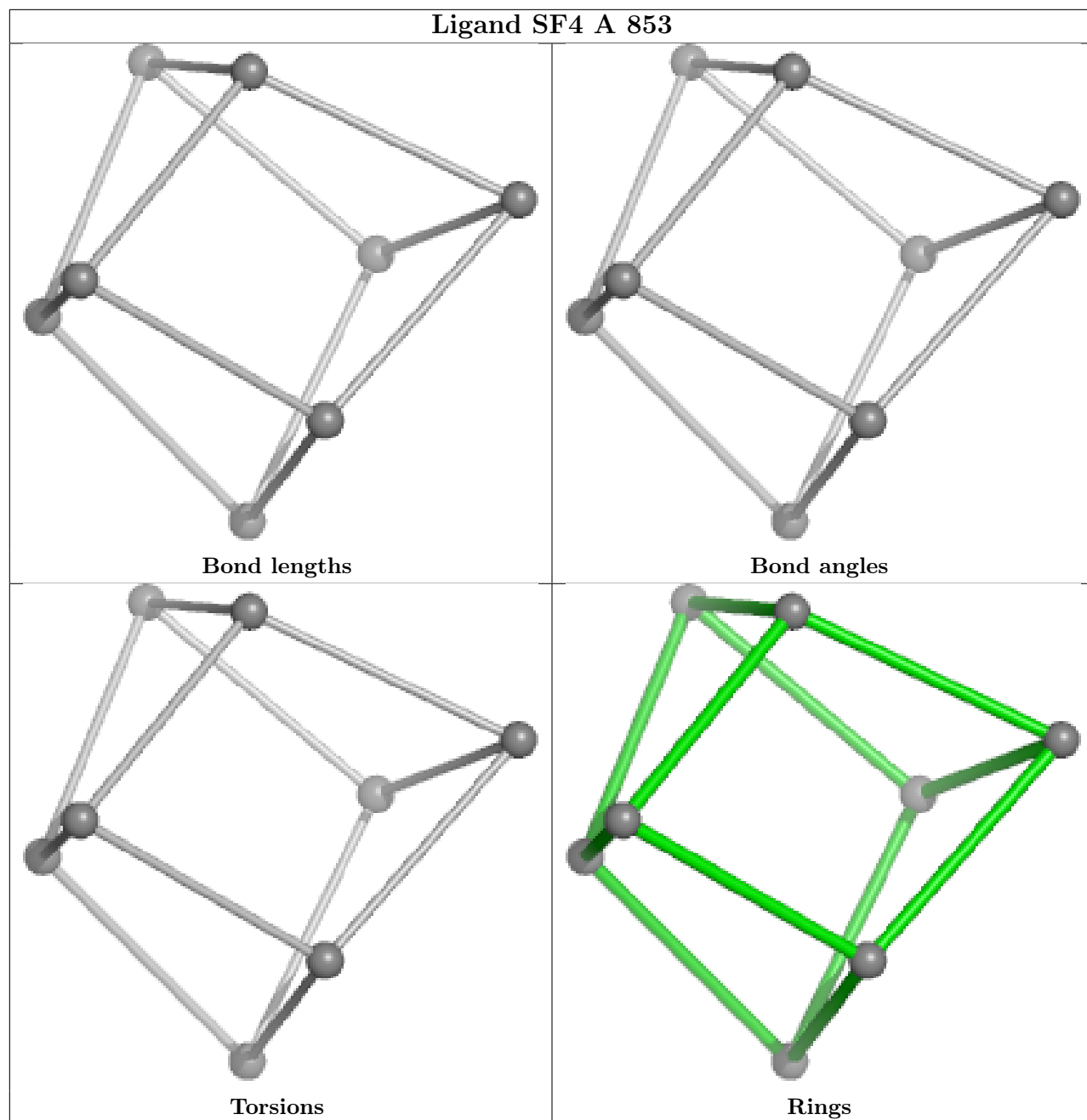


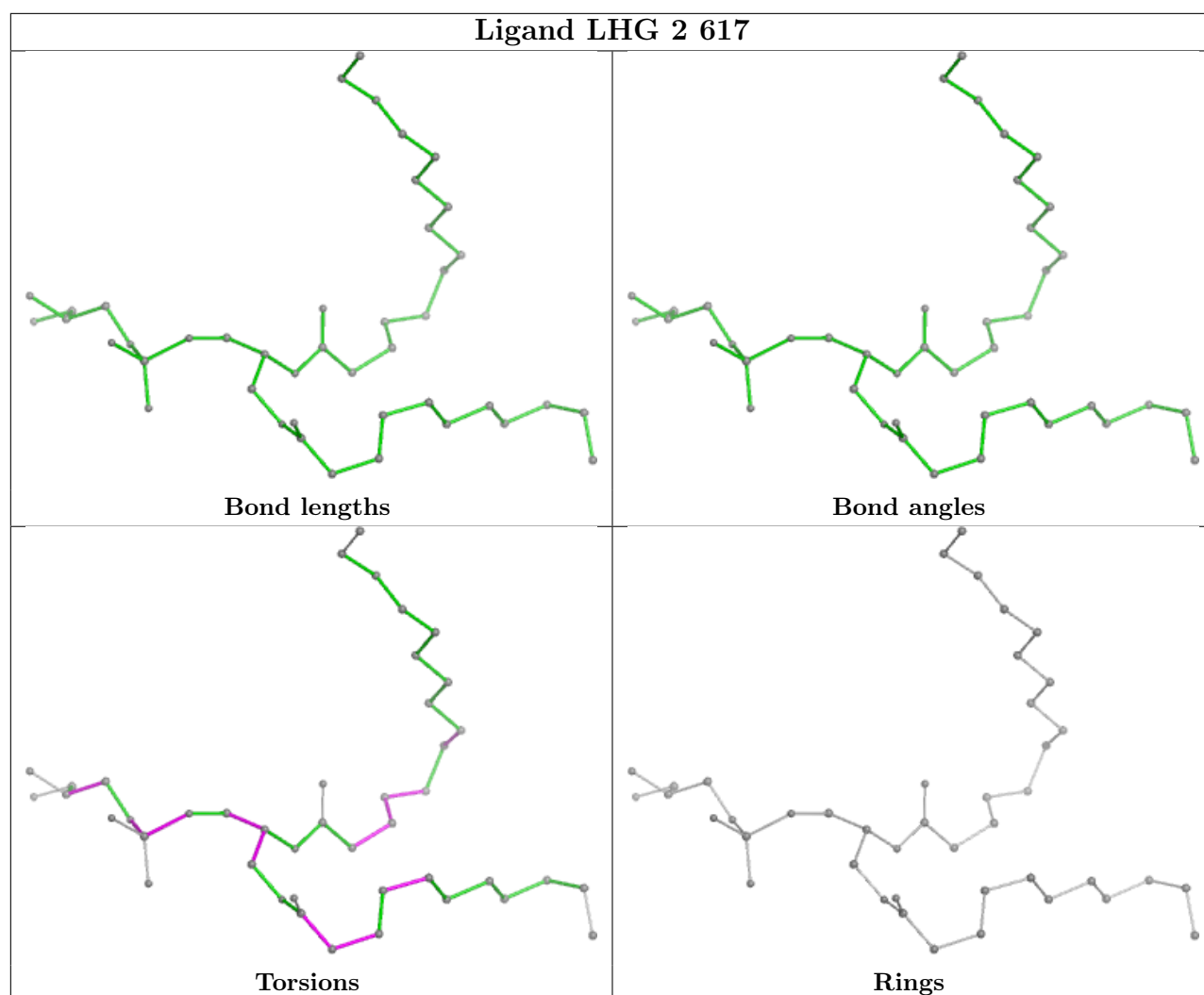
## Ligand CLA 1 311

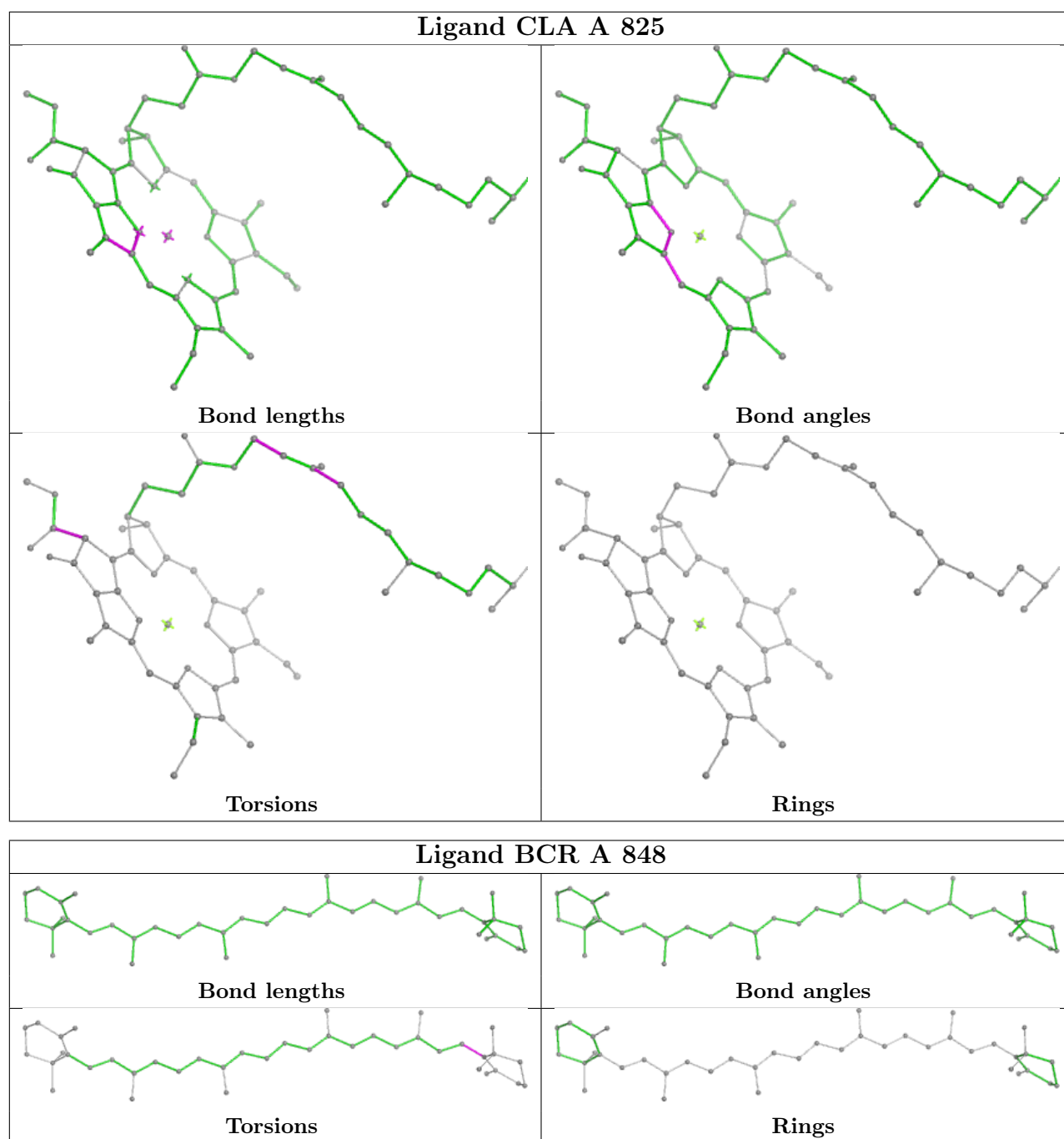




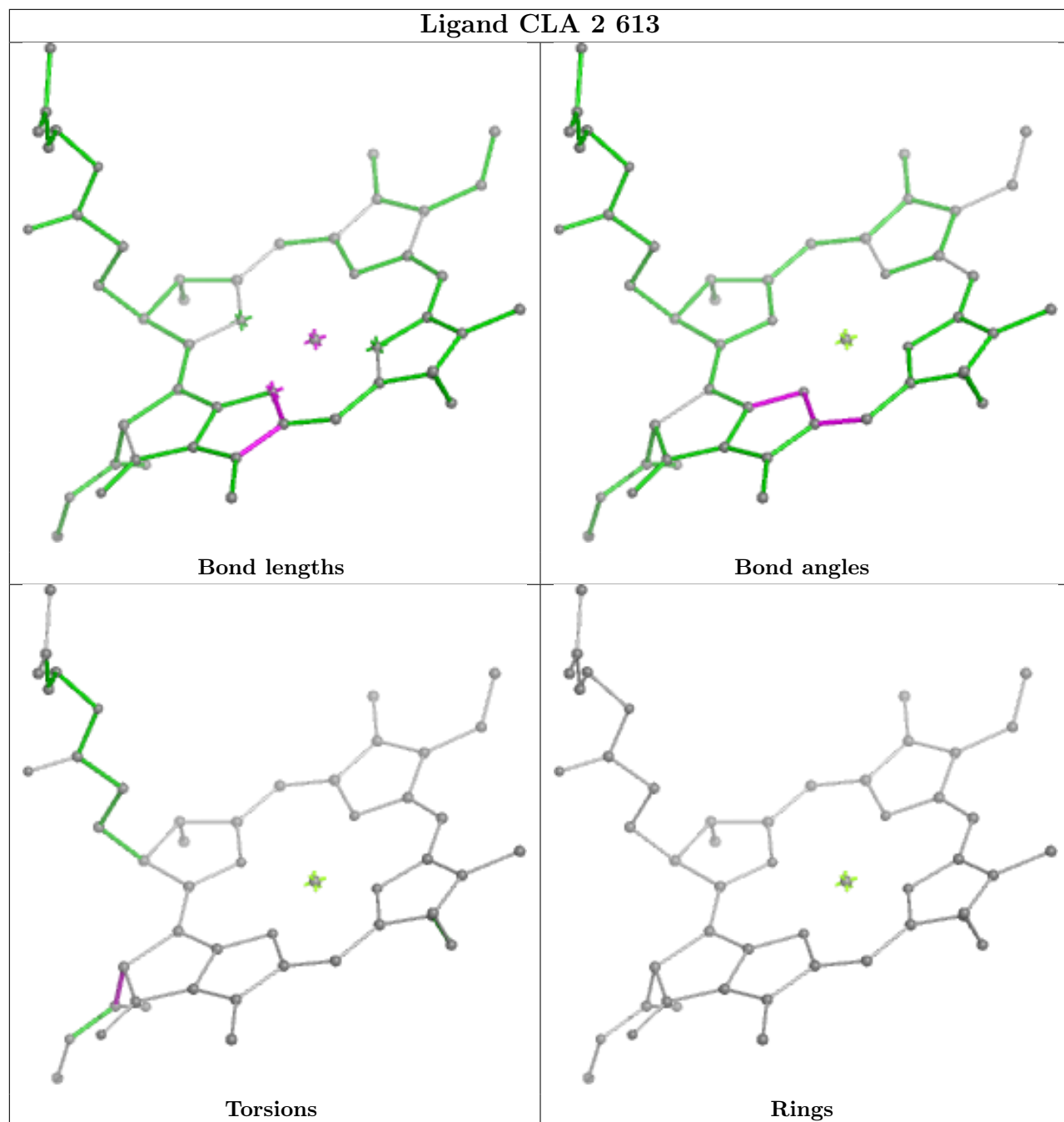
## Ligand SF4 A 853

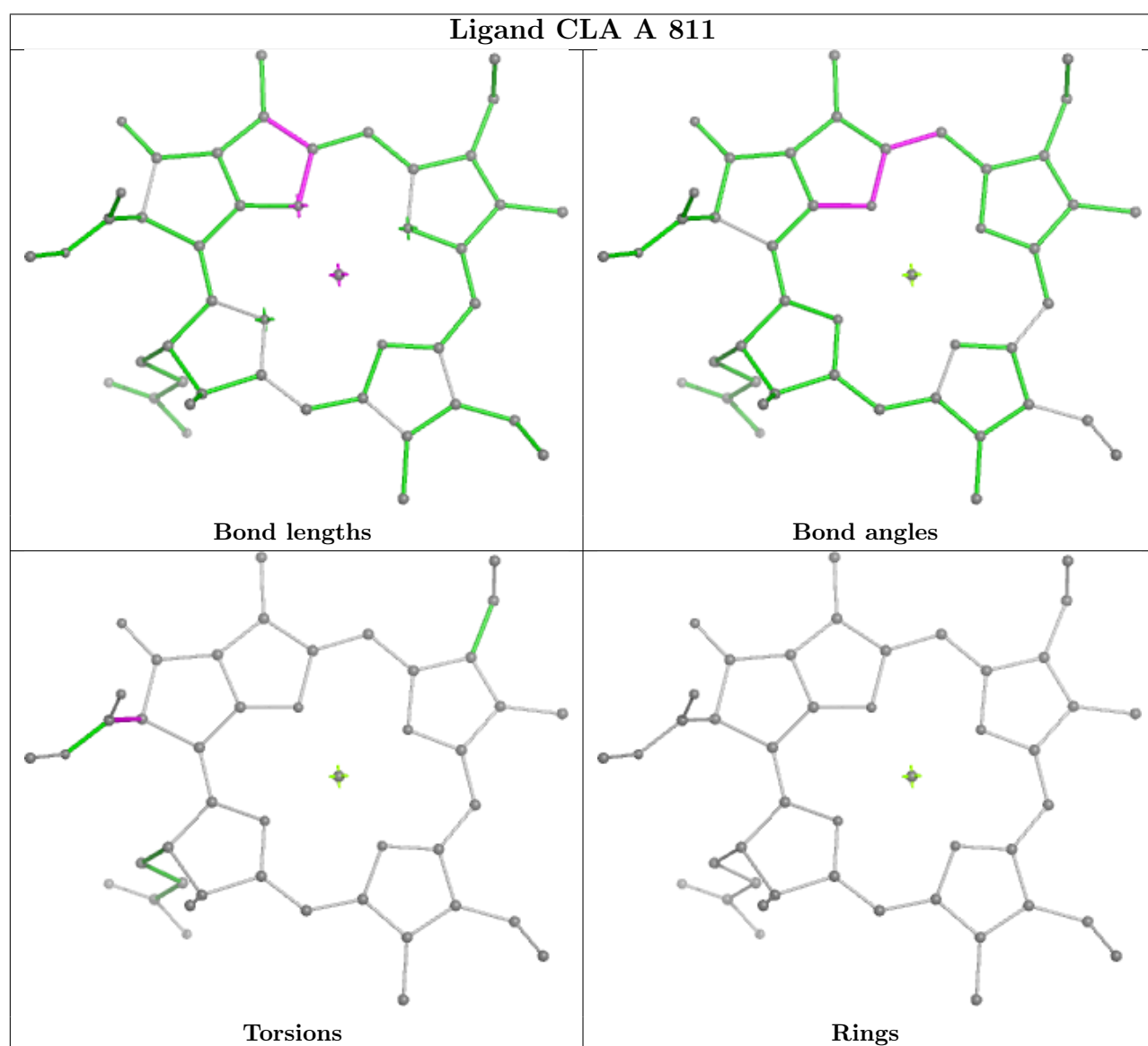
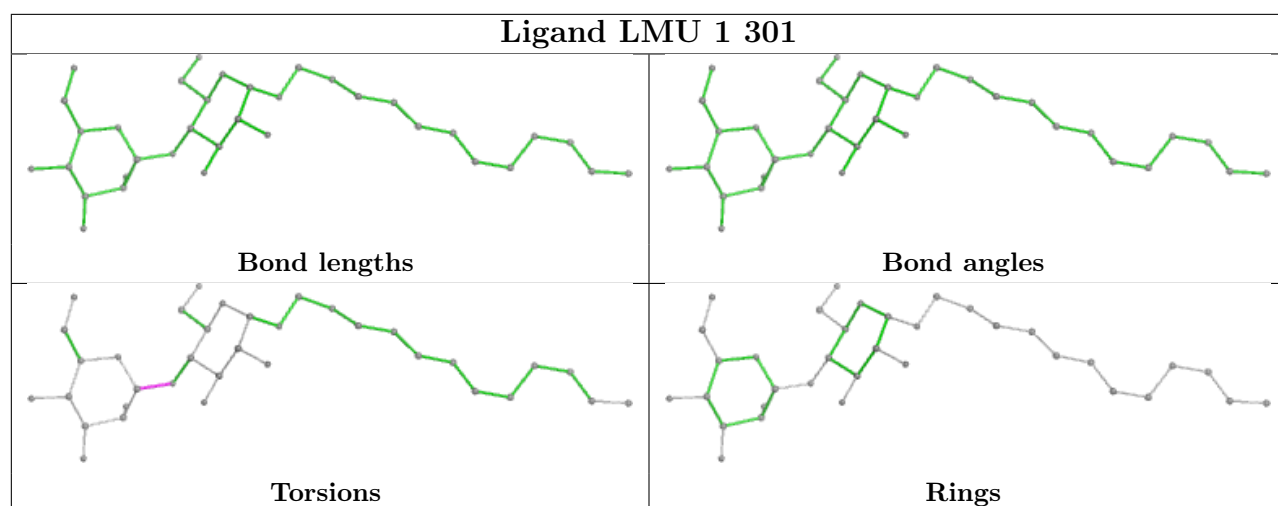


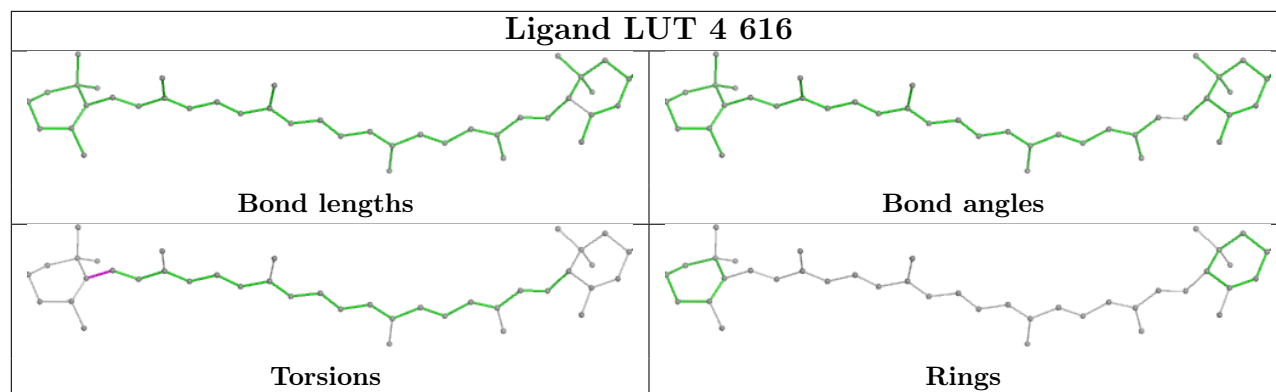
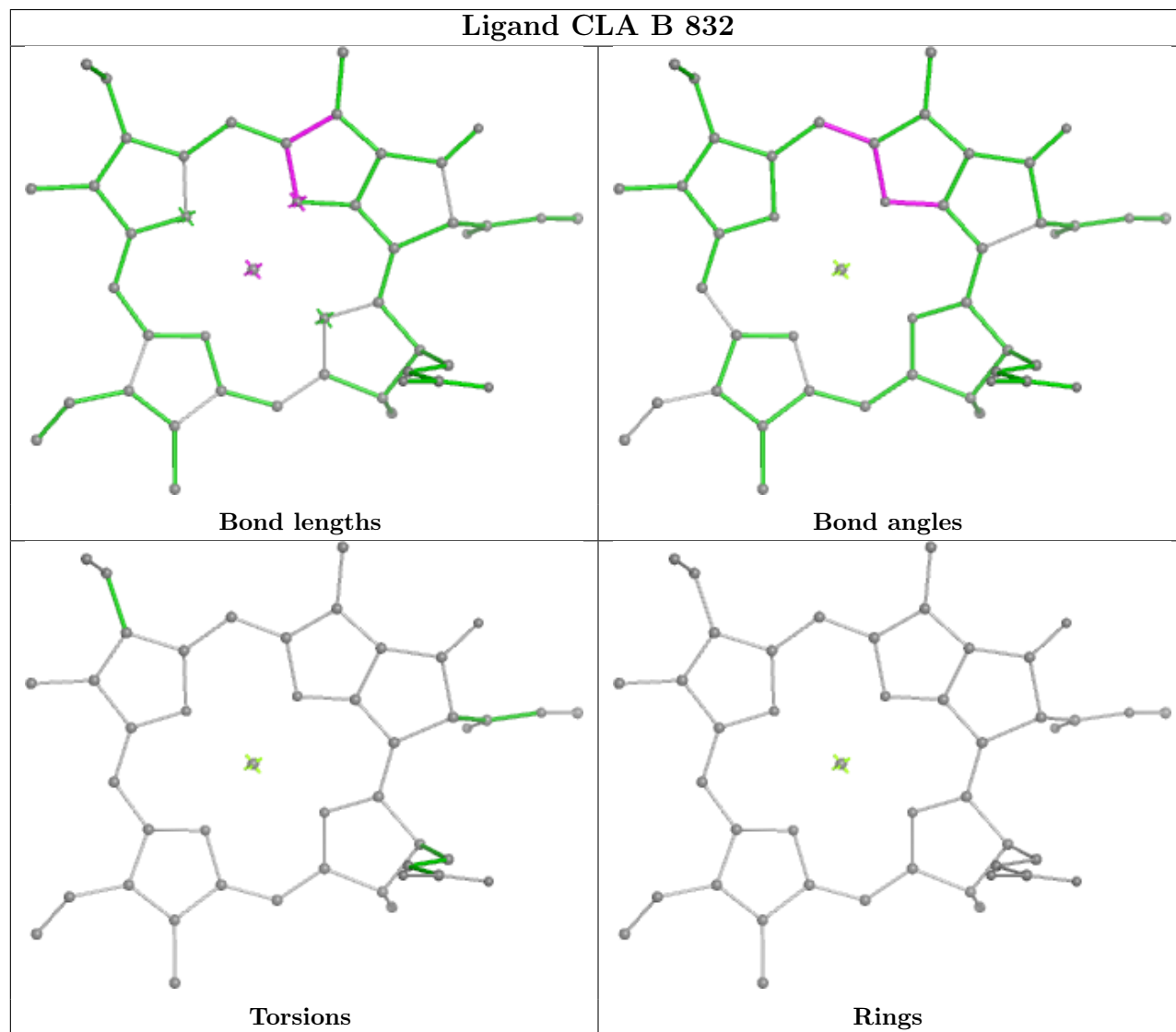


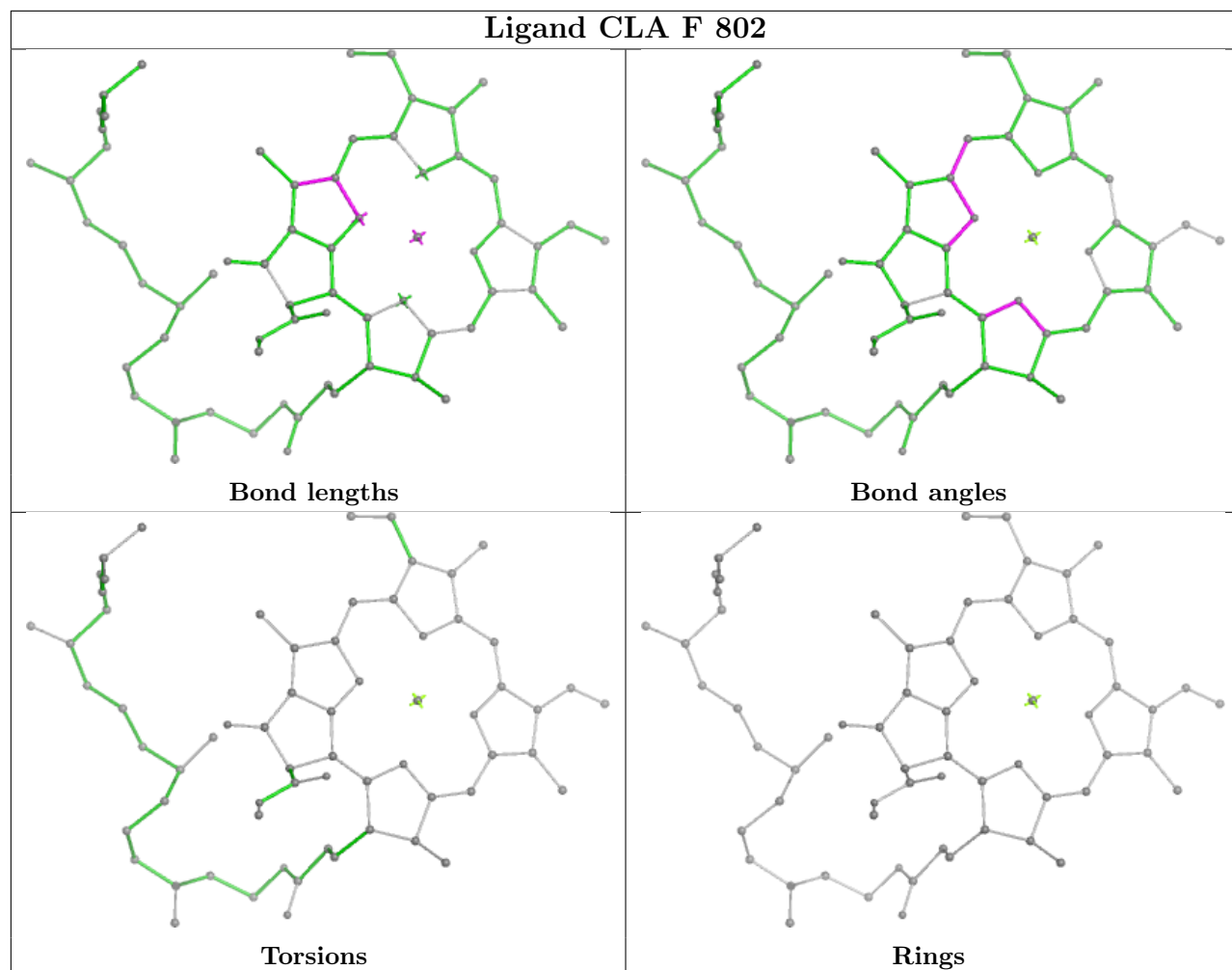


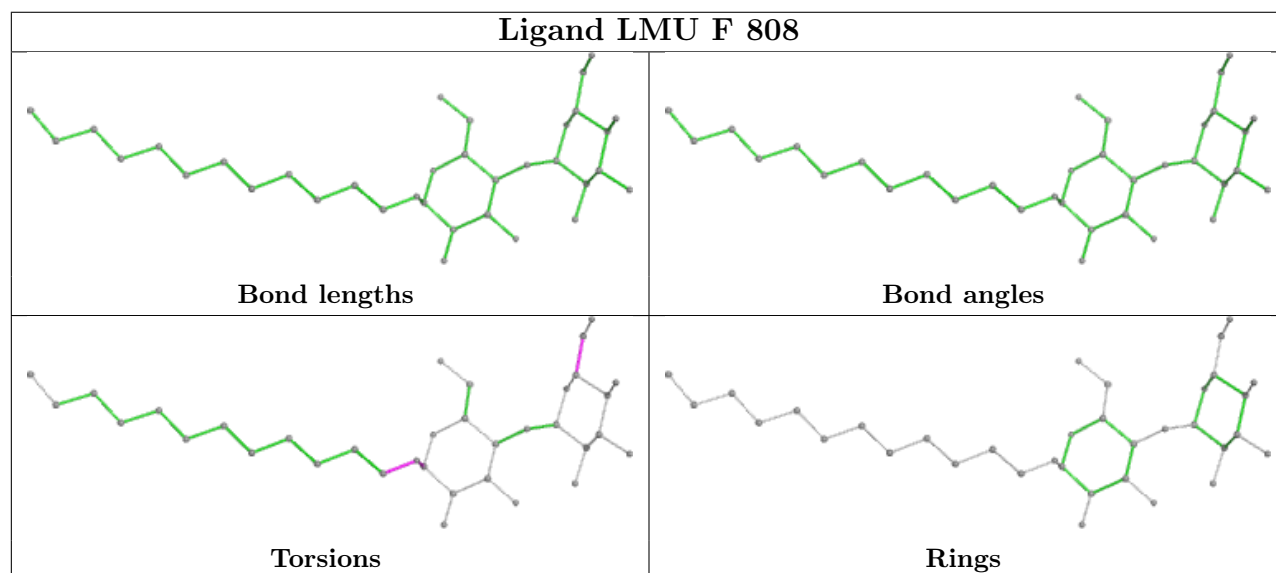
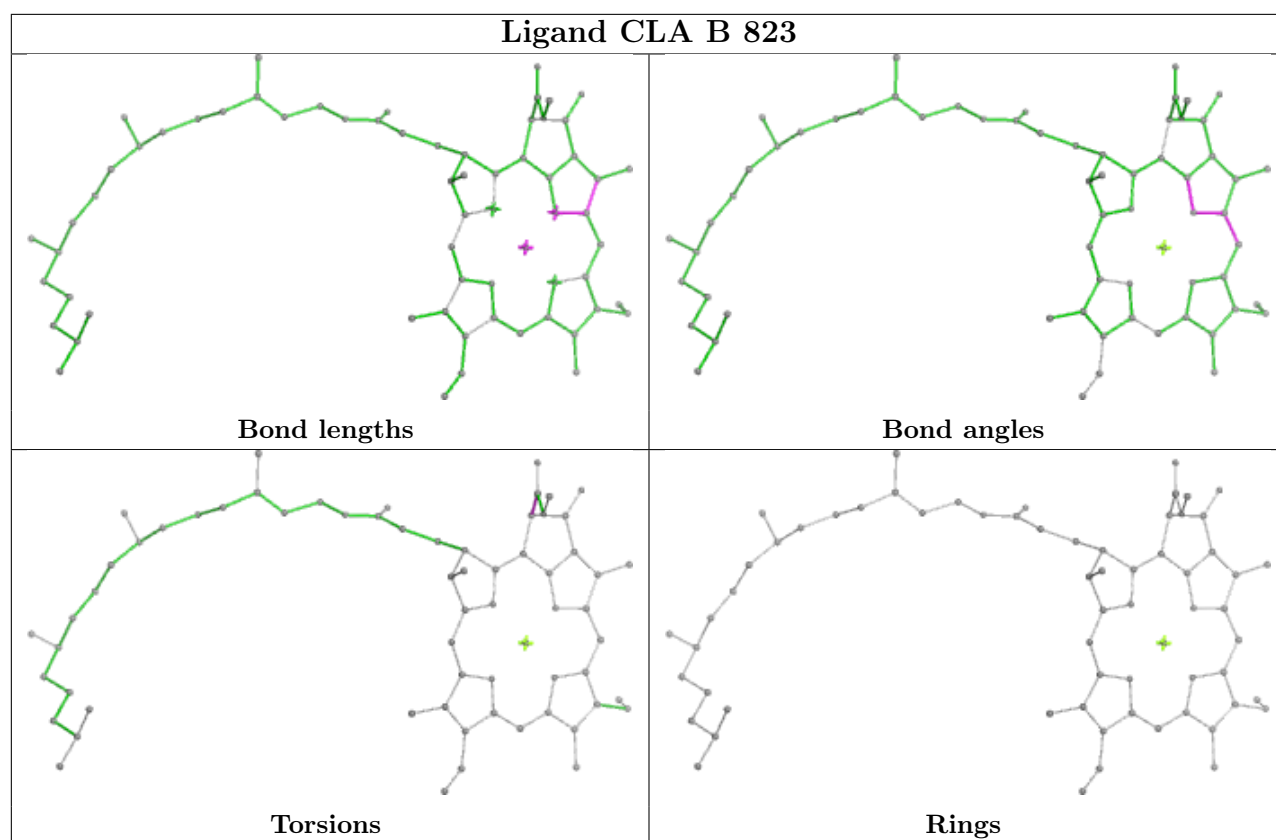
## Ligand CLA 2 613



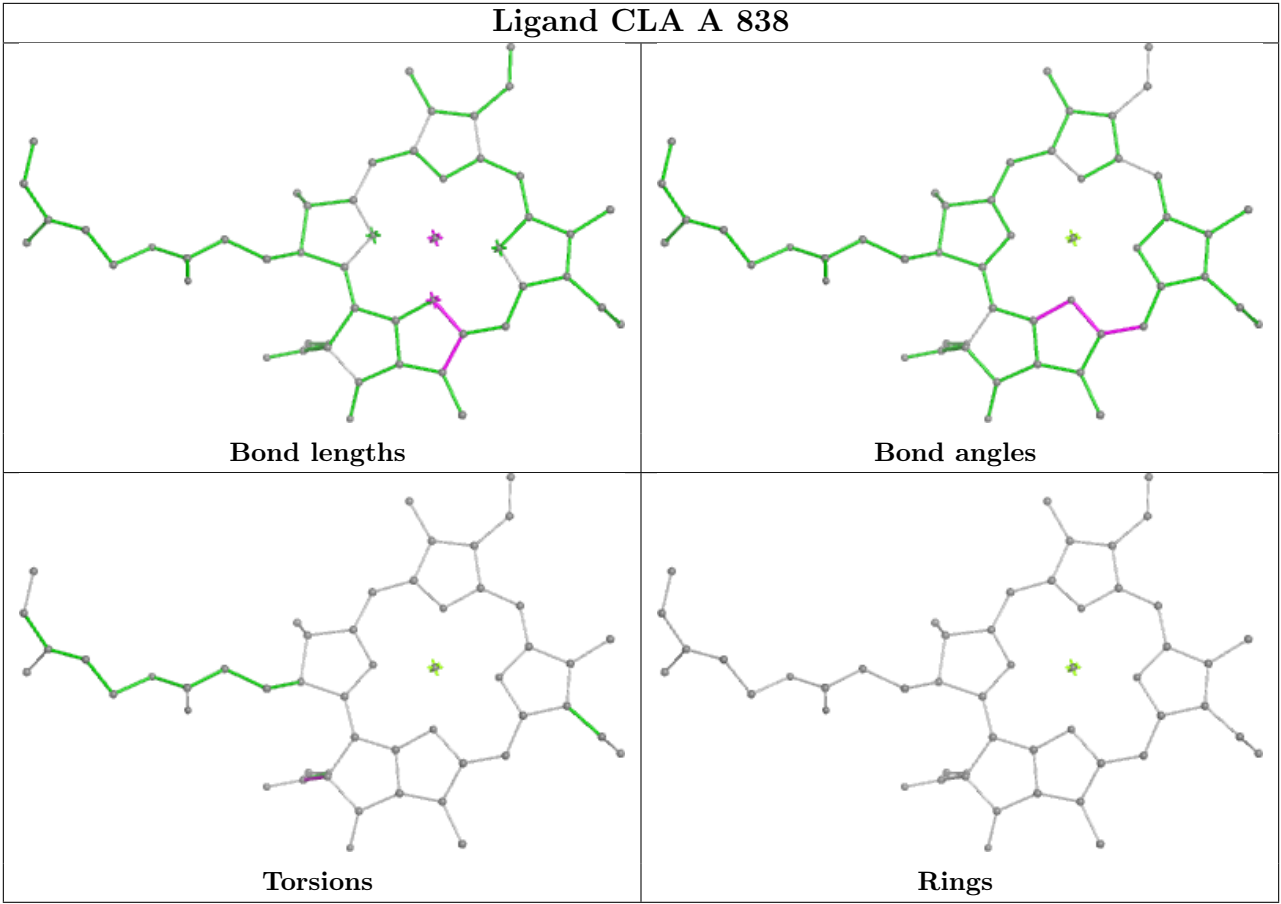


**Ligand LUT 4 616****Ligand CLA B 832**









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	L	1
12	K	1
13	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	209:PRO	C	210:TYR	N	3.43
1	K	123:GLY	C	124:VAL	N	3.22
1	1	236:PRO	C	237:ARG	N	3.17

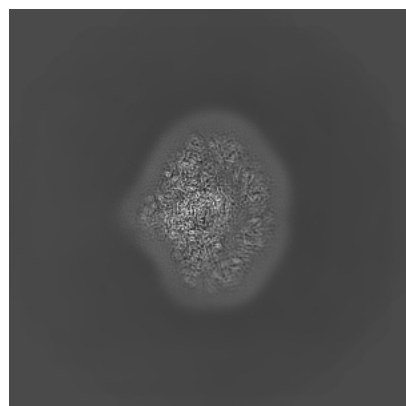
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15969. These allow visual inspection of the internal detail of the map and identification of artifacts.

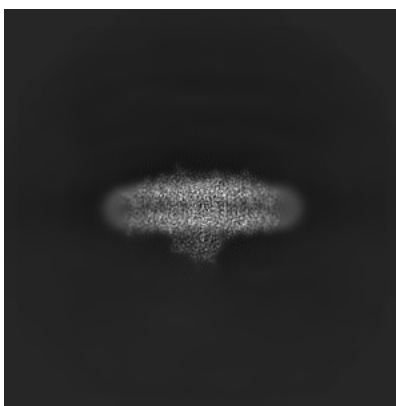
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

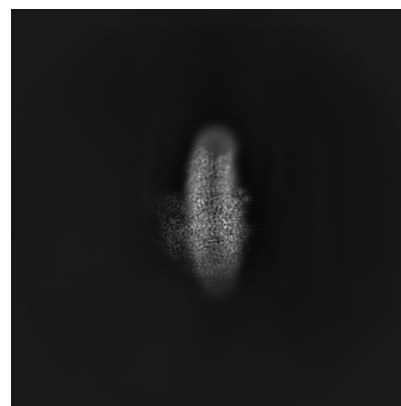
#### 6.1.1 Primary map



X

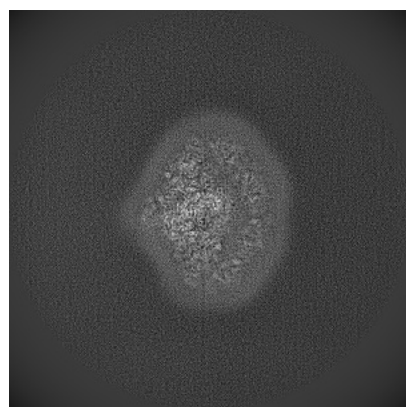


Y

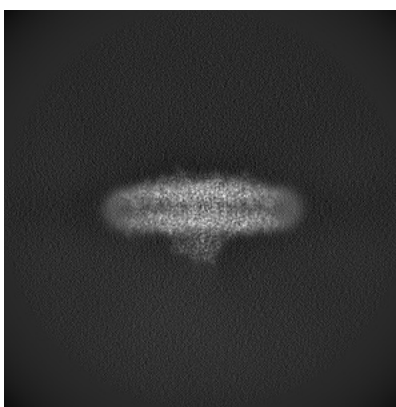


Z

#### 6.1.2 Raw map



X



Y

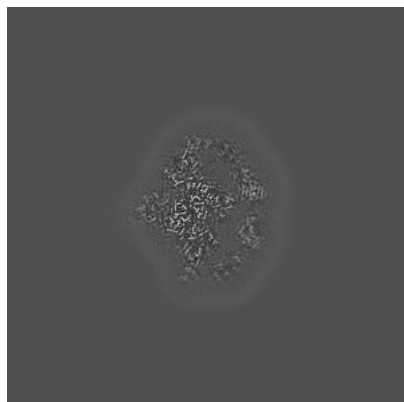


Z

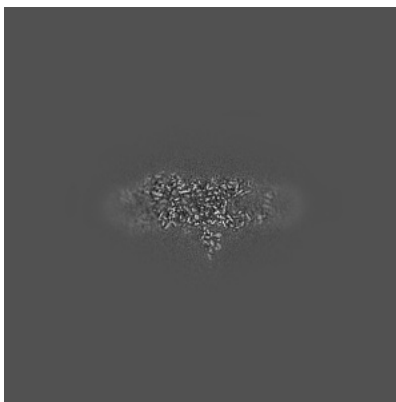
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

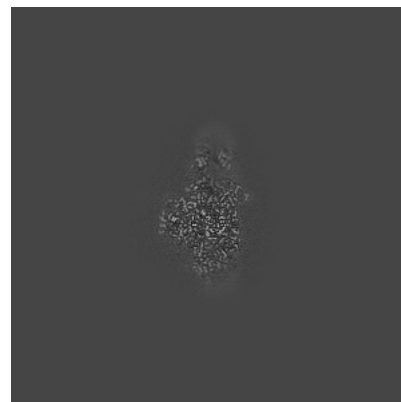
### 6.2.1 Primary map



X Index: 250

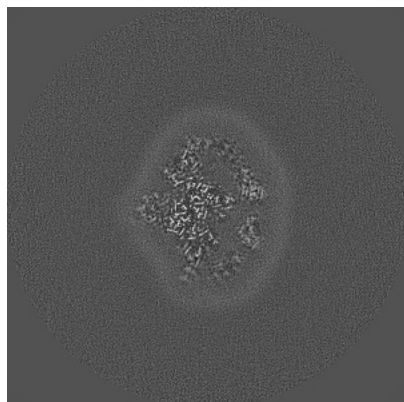


Y Index: 250

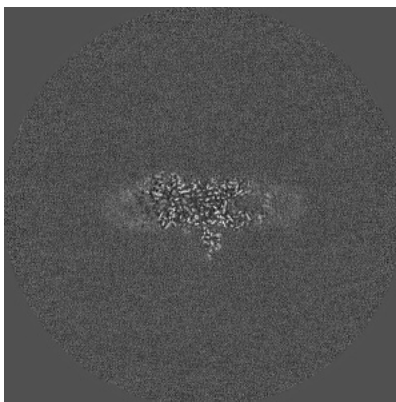


Z Index: 250

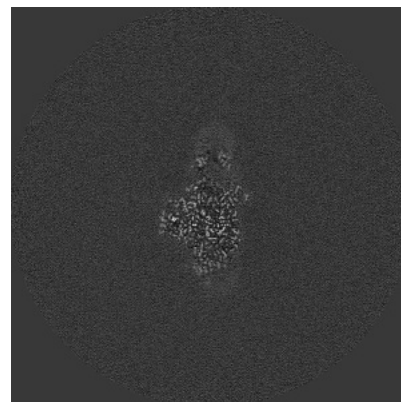
### 6.2.2 Raw map



X Index: 250



Y Index: 250

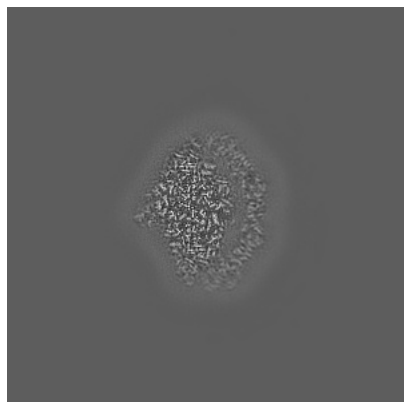


Z Index: 250

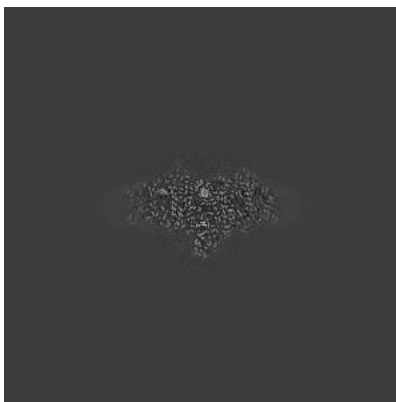
The images above show central slices of the map in three orthogonal directions.

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

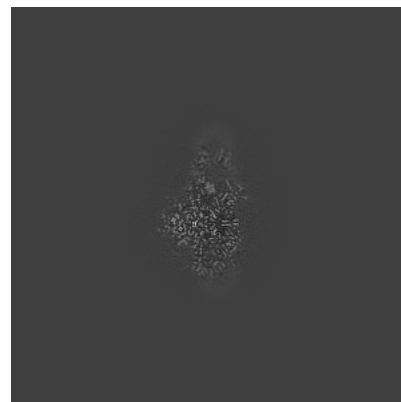
### 6.3.1 Primary map



X Index: 267

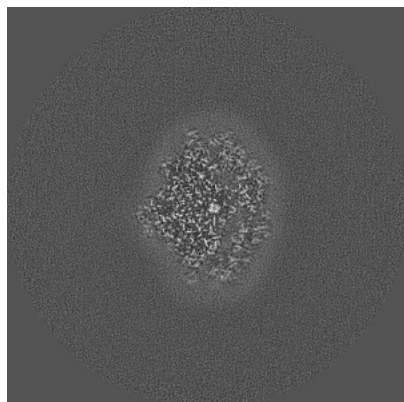


Y Index: 227

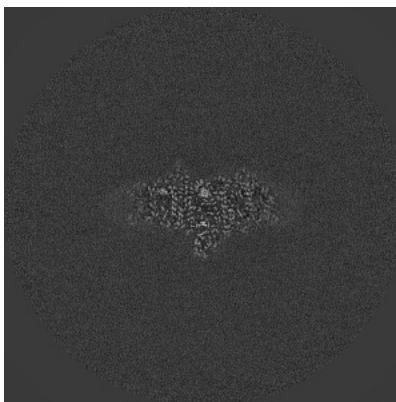


Z Index: 248

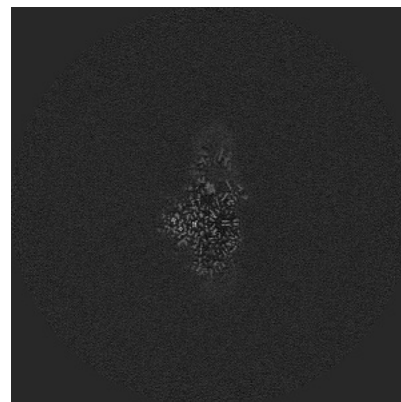
### 6.3.2 Raw map



X Index: 235



Y Index: 227

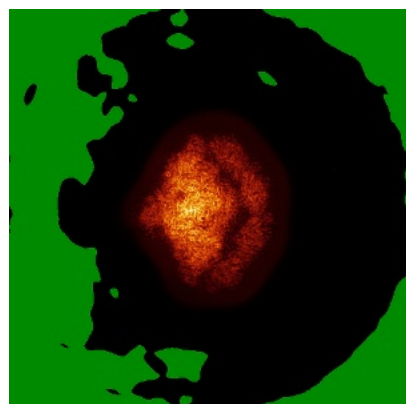


Z Index: 248

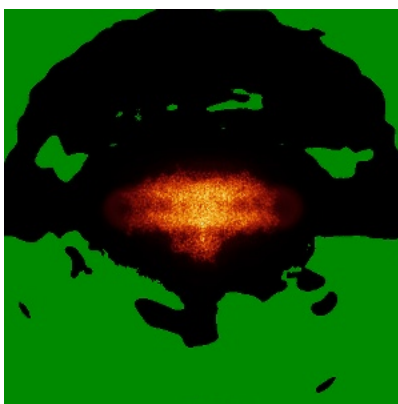
The images above show the largest variance slices of the map in three orthogonal directions.

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

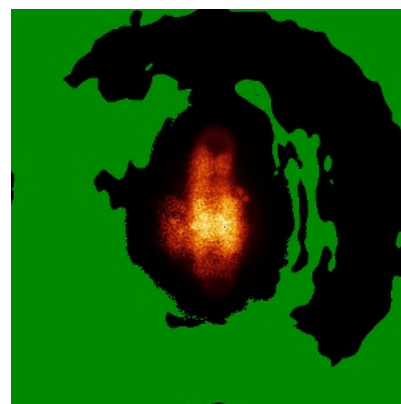
### 6.4.1 Primary map



X

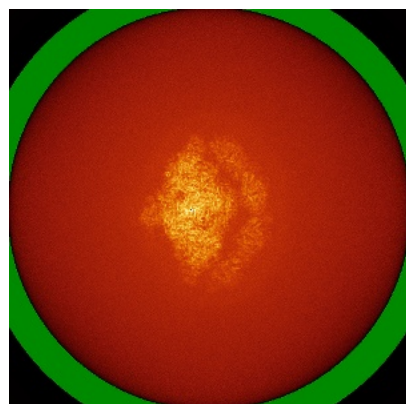


Y

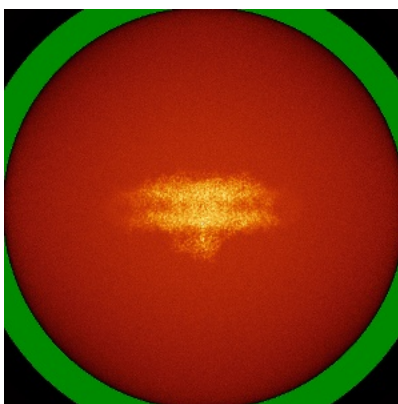


Z

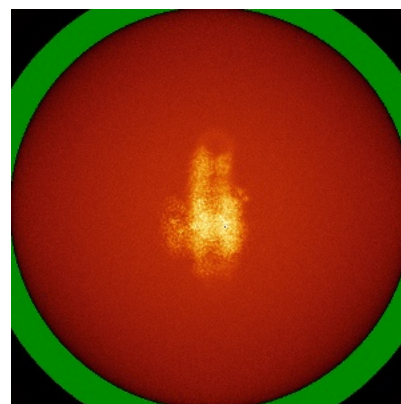
### 6.4.2 Raw map



X



Y

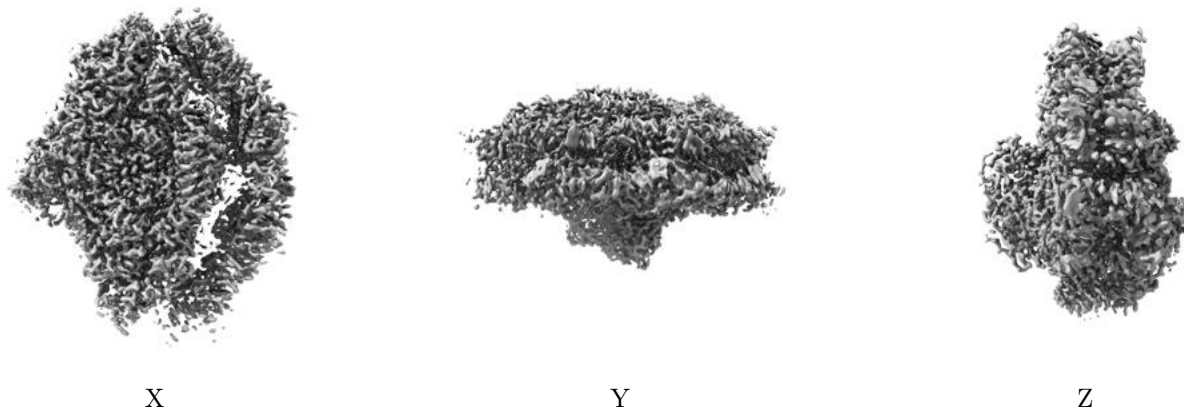


Z

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

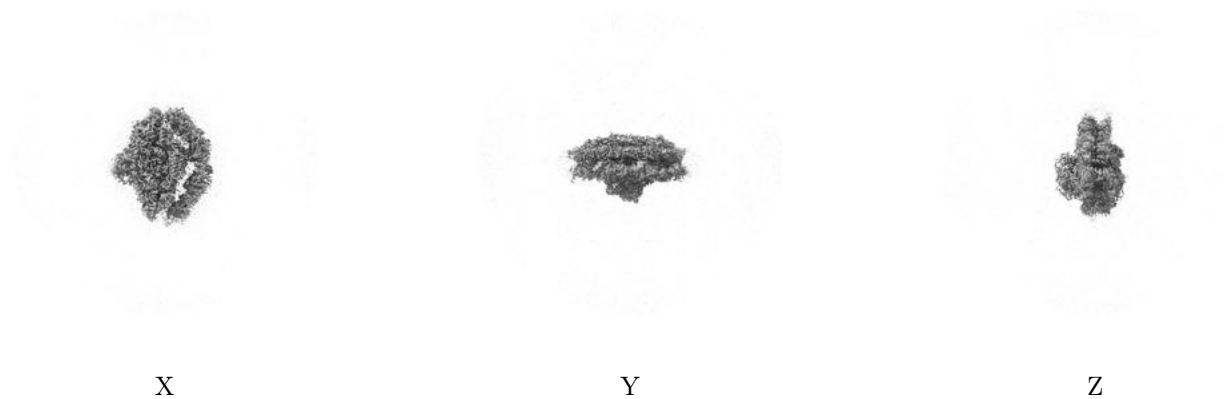
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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



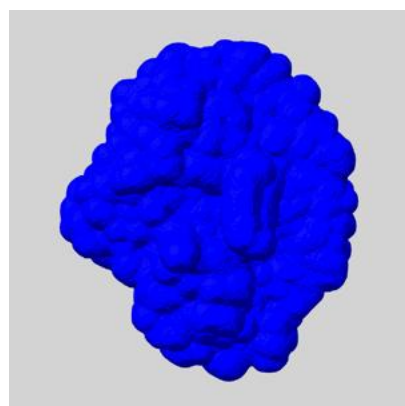
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

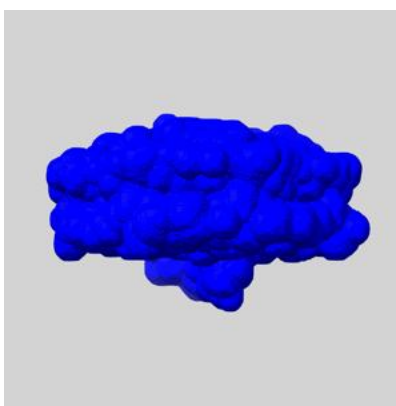
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

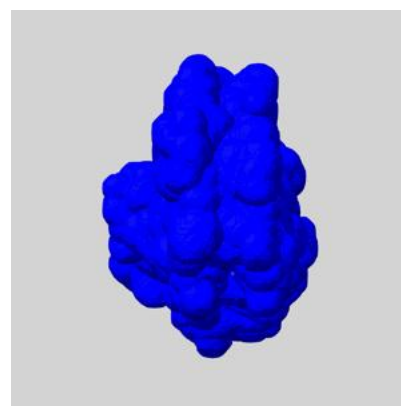
### 6.6.1 emd\_15969\_msk\_1.map [i](#)



X



Y

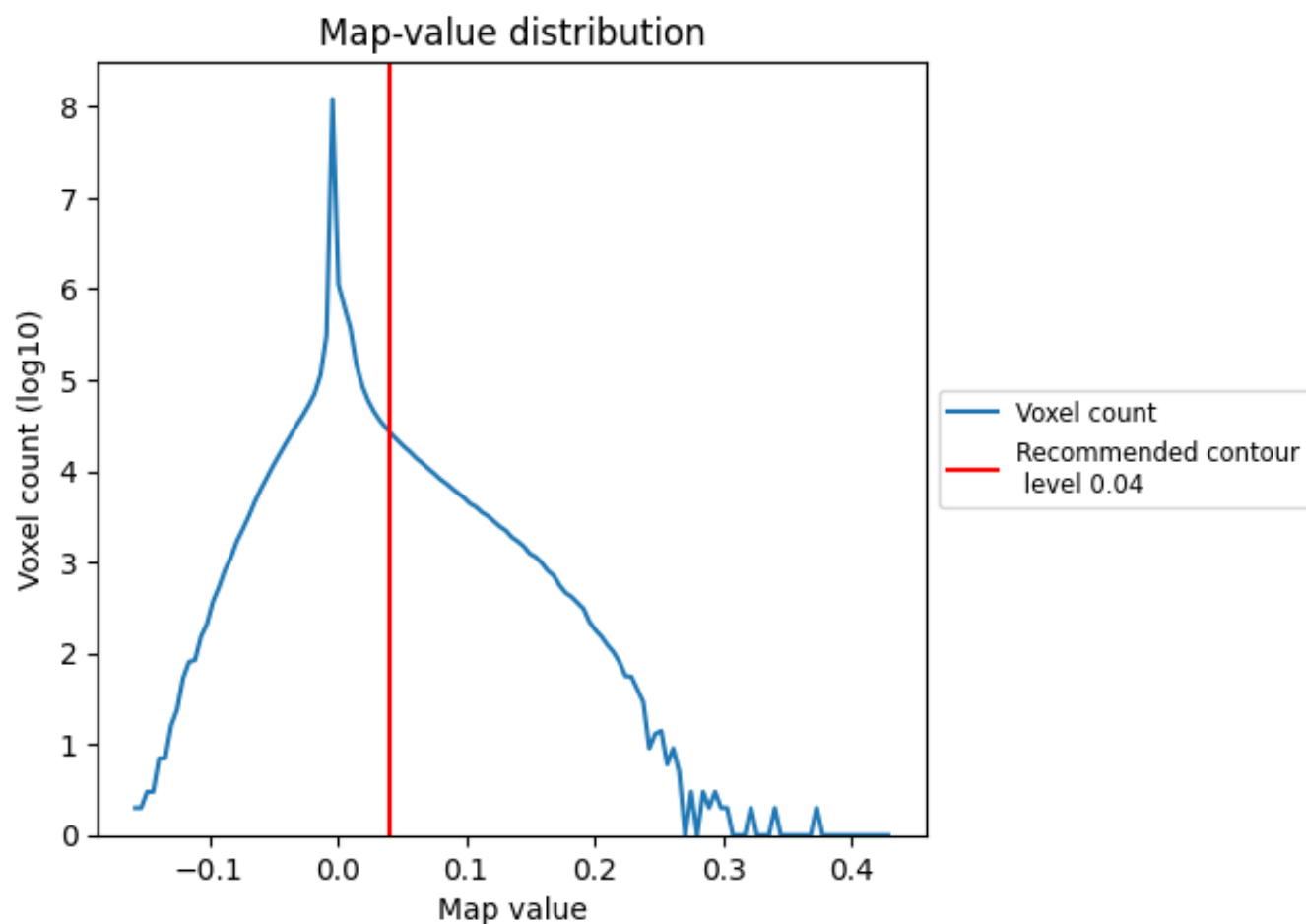


Z

## 7 Map analysis [i](#)

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

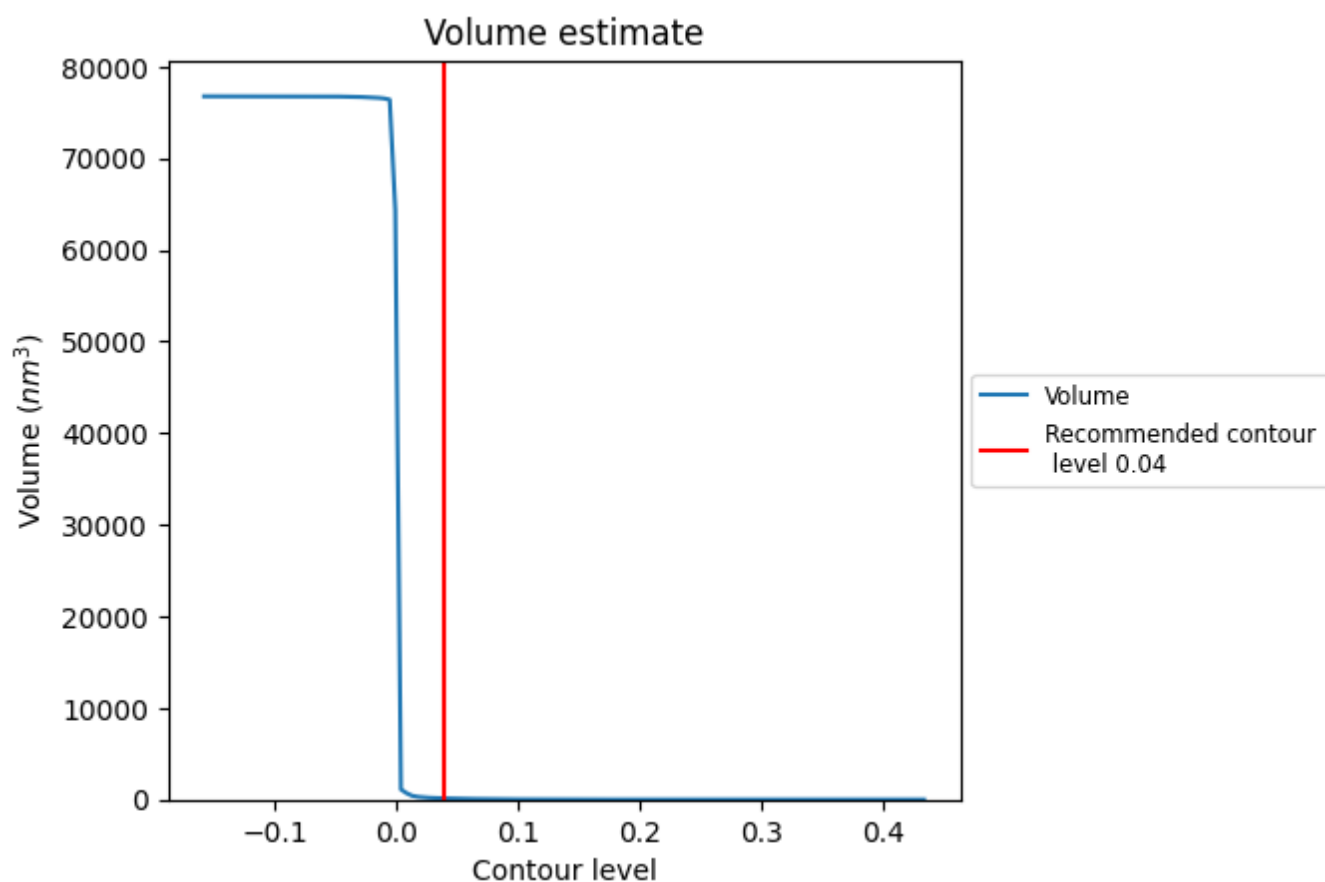
### 7.1 Map-value distribution [i](#)



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.



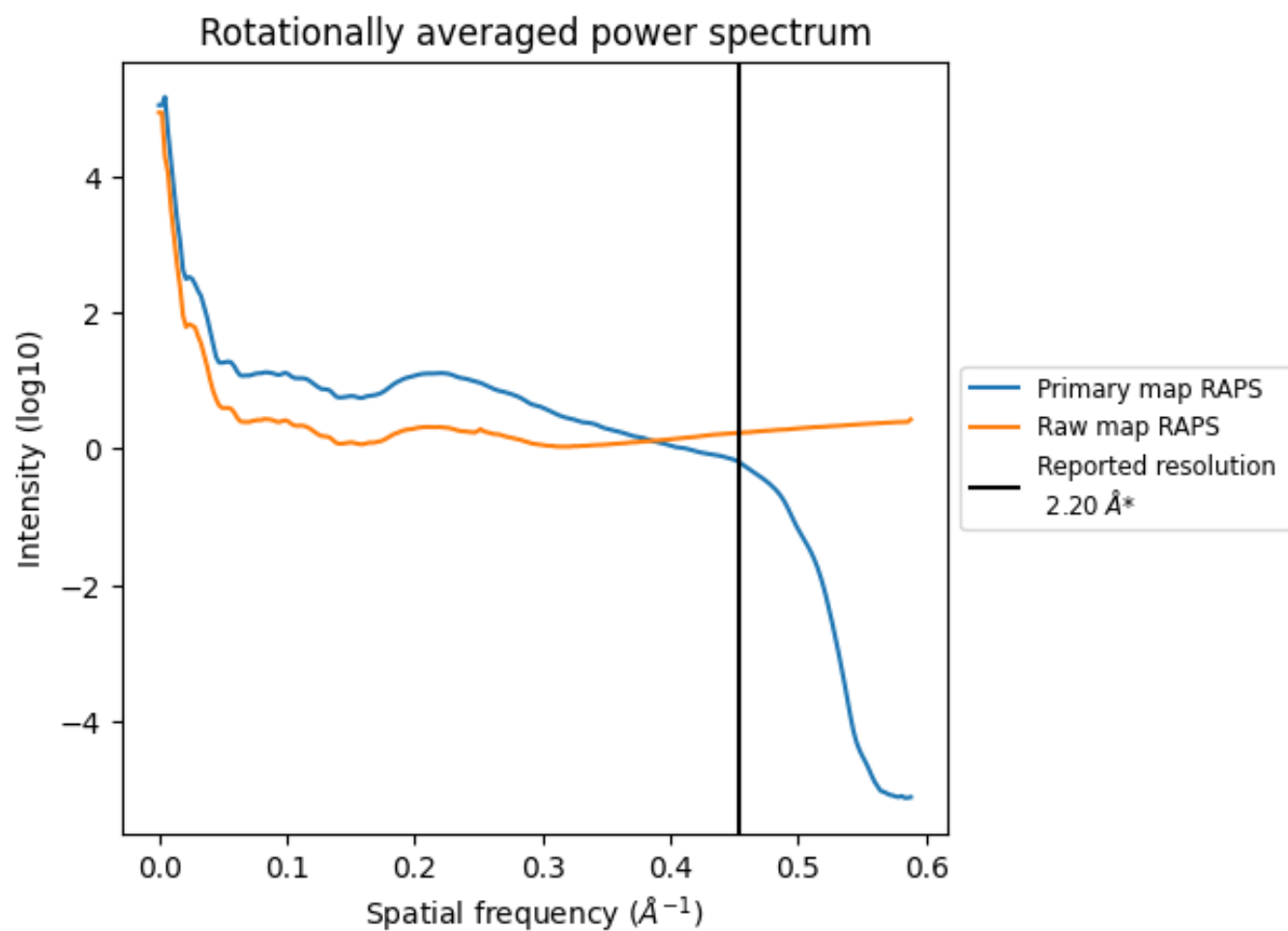
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 130  $\text{nm}^3$ ; this corresponds to an approximate mass of 118 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 ⓘ

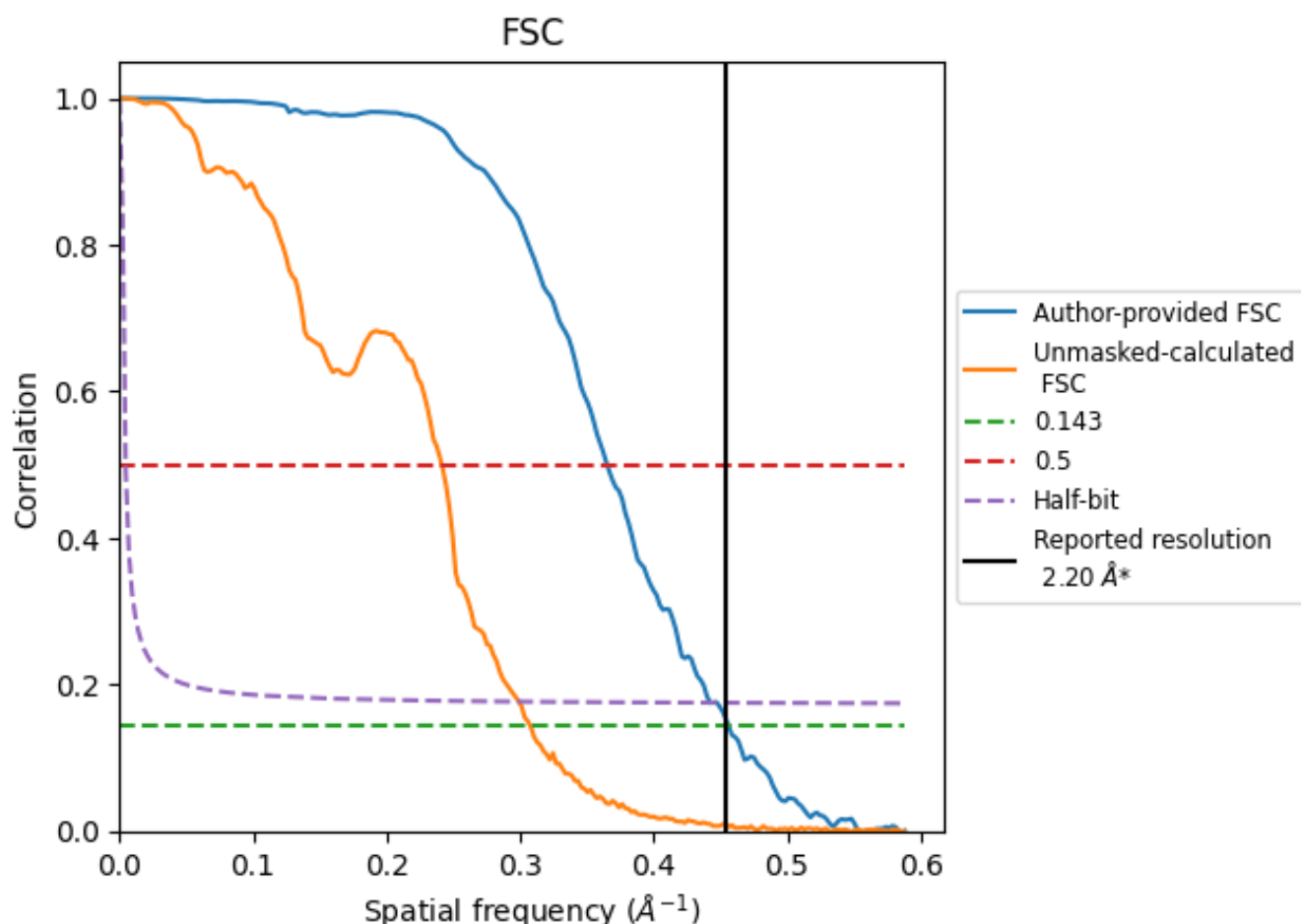


\*Reported resolution corresponds to spatial frequency of 0.455  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.455 Å<sup>-1</sup>

## 8.2 Resolution estimates

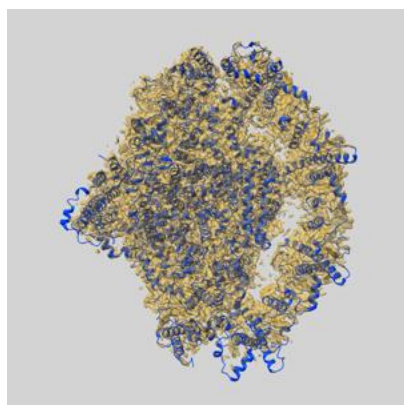
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.19	2.74	2.26
Unmasked-calculated*	3.25	4.14	3.34

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.25 differs from the reported value 2.2 by more than 10 %

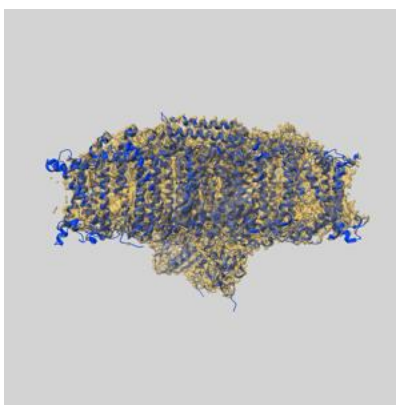
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15969 and PDB model 8BCV. Per-residue inclusion information can be found in section 3 on page 29.

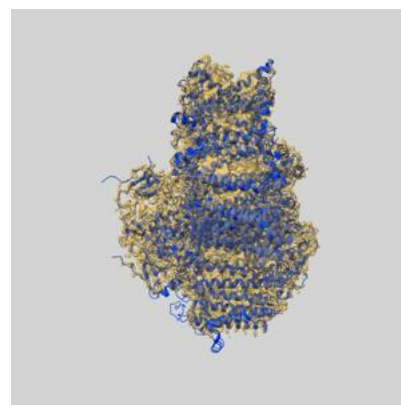
### 9.1 Map-model overlay [i](#)



X



Y



Z

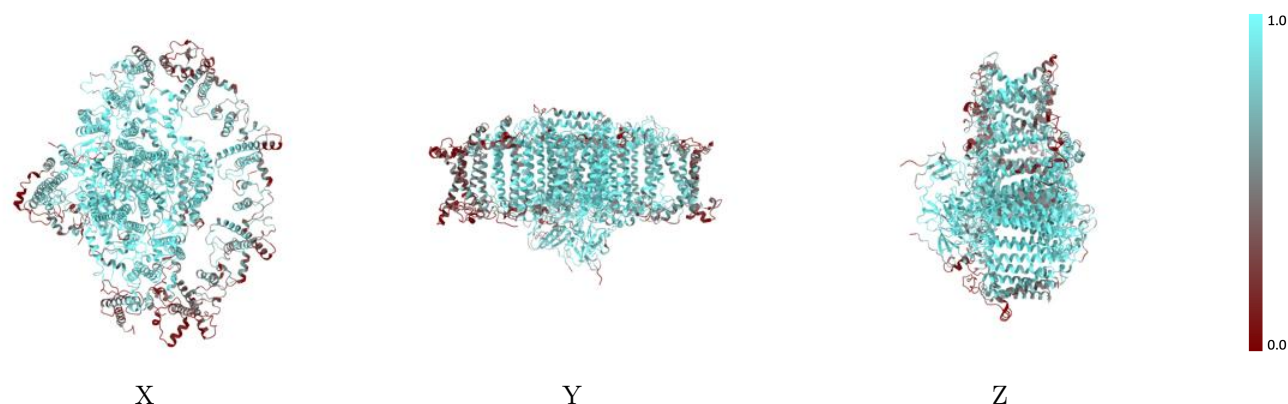
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



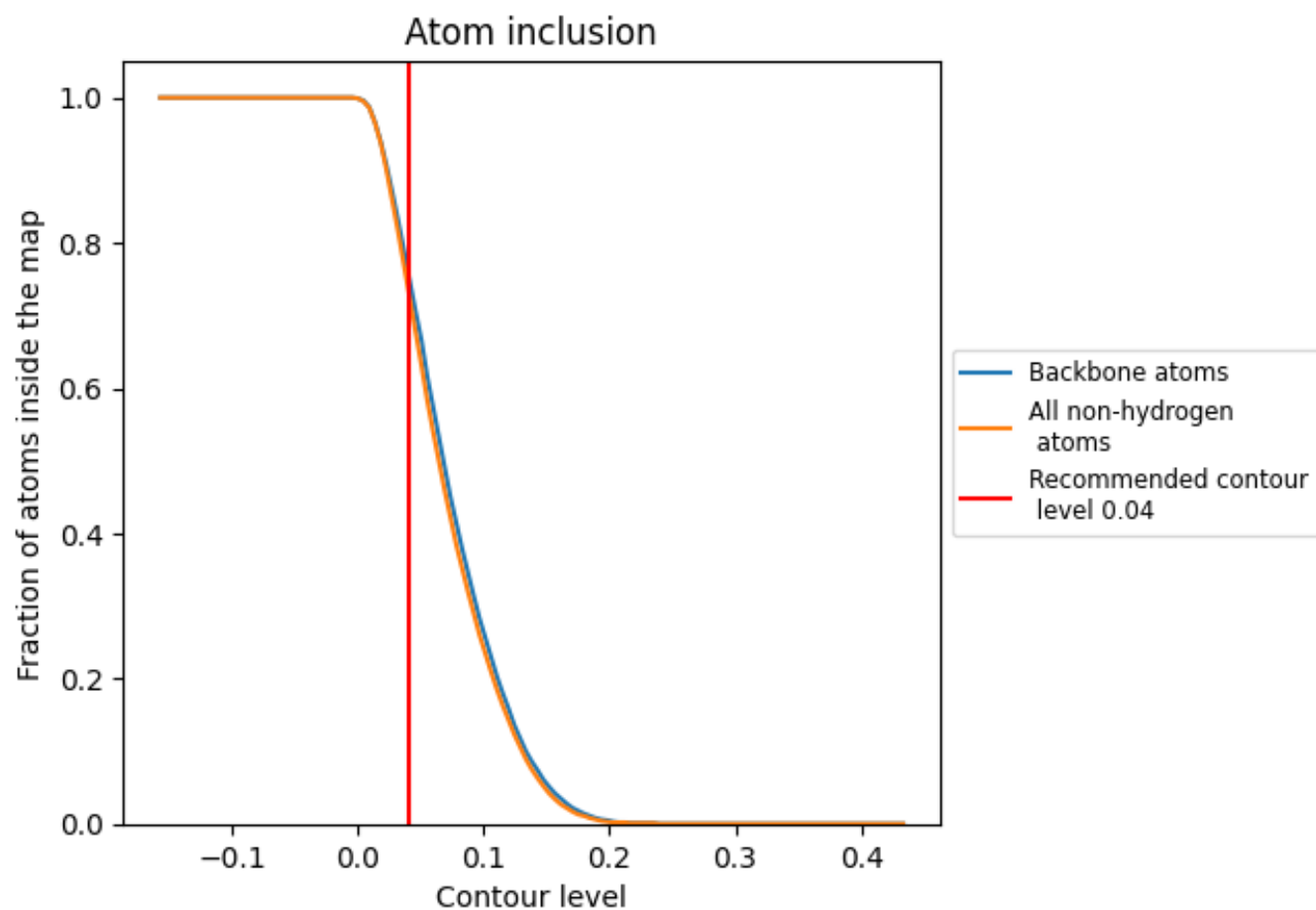
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 73% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7340	<div></div> 0.6450
1	<div></div> 0.5320	<div></div> 0.5570
2	<div></div> 0.5720	<div></div> 0.5760
3	<div></div> 0.3100	<div></div> 0.5110
4	<div></div> 0.6350	<div></div> 0.5870
A	<div></div> 0.8860	<div></div> 0.7030
B	<div></div> 0.9140	<div></div> 0.7110
C	<div></div> 0.9770	<div></div> 0.7440
D	<div></div> 0.8570	<div></div> 0.6840
E	<div></div> 0.7640	<div></div> 0.6740
F	<div></div> 0.7910	<div></div> 0.6720
G	<div></div> 0.6000	<div></div> 0.5730
H	<div></div> 0.2460	<div></div> 0.5230
I	<div></div> 0.7910	<div></div> 0.6630
J	<div></div> 0.7580	<div></div> 0.6520
K	<div></div> 0.2930	<div></div> 0.4840
L	<div></div> 0.5770	<div></div> 0.5950

