



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 03:33 PM UTC

PDB ID : 8XLS / pdb_00008xls
EMDB ID : EMD-38457
Title : PSI-FCPI of the diatom *Thalassiosira pseudonana* CCMP1335
Authors : Kato, K.; Nakajima, Y.; Shen, J.R.; Nagao, R.
Deposited on : 2023-12-26
Resolution : 2.30 Å(reported)
Based on initial model : .

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

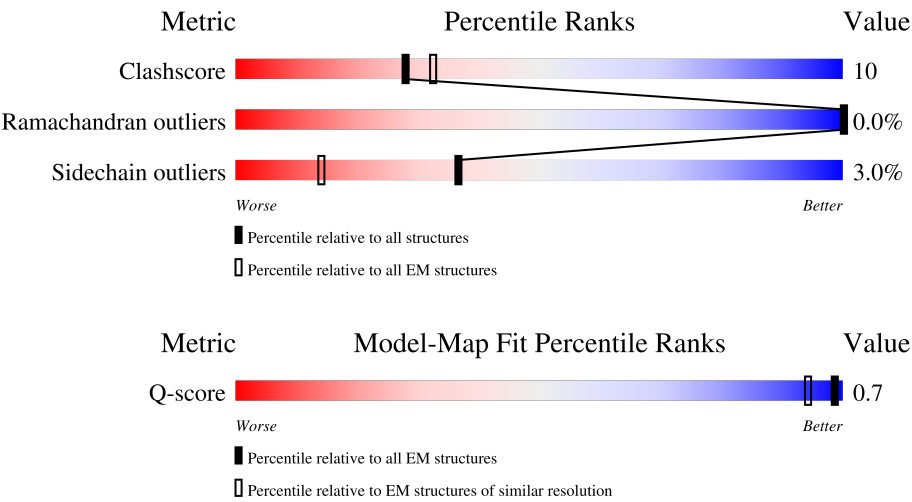
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.30 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.



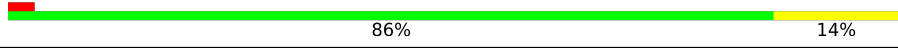
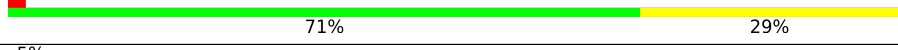
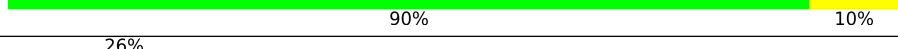
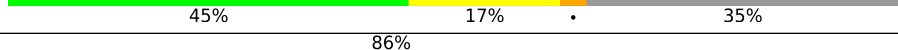
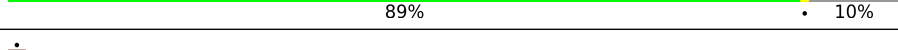
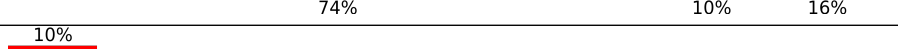
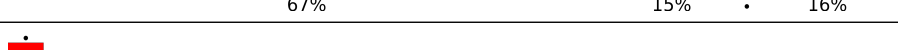
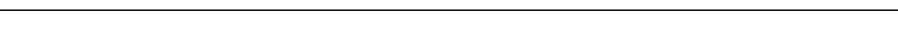
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4254 (1.80 - 2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	752	
2	B	733	
3	C	81	
4	D	139	

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Mol	Chain	Length	Quality of chain
5	E	65	
6	F	185	
7	I	36	
8	J	41	
9	L	148	
10	M	30	
11	W	188	
12	u	84	
13	1	221	
14	2	198	
15	3	196	
16	4	201	
17	5	194	

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
18	CL0	A	801	X	-	-	-
19	CLA	1	301	X	-	-	-
19	CLA	1	303	X	-	-	-
19	CLA	1	304	X	-	-	-
19	CLA	1	306	X	-	-	-
19	CLA	1	307	X	-	-	-
19	CLA	1	308	X	-	-	-
19	CLA	1	309	X	-	-	-
19	CLA	1	310	X	-	-	-
19	CLA	2	205	X	-	-	-
19	CLA	2	206	X	-	-	-
19	CLA	2	207	X	-	-	-
19	CLA	2	208	X	-	-	-
19	CLA	2	209	X	-	-	-
19	CLA	2	210	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	2	212	X	-	-	-
19	CLA	2	213	X	-	-	-
19	CLA	2	214	X	-	-	-
19	CLA	2	215	X	-	-	-
19	CLA	3	202	X	-	-	-
19	CLA	3	203	X	-	-	-
19	CLA	3	204	X	-	-	-
19	CLA	3	206	X	-	-	-
19	CLA	3	207	X	-	-	-
19	CLA	3	209	X	-	-	-
19	CLA	3	210	X	-	-	-
19	CLA	4	301	X	-	-	-
19	CLA	4	303	X	-	-	-
19	CLA	4	304	X	-	-	-
19	CLA	4	305	X	-	-	-
19	CLA	4	306	X	-	-	-
19	CLA	4	311	X	-	-	-
19	CLA	4	312	X	-	-	-
19	CLA	4	313	X	-	-	-
19	CLA	5	207	X	-	-	-
19	CLA	5	208	X	-	-	-
19	CLA	5	209	X	-	-	-
19	CLA	5	210	X	-	-	-
19	CLA	5	211	X	-	-	-
19	CLA	5	212	X	-	-	-
19	CLA	5	213	X	-	-	-
19	CLA	5	214	X	-	-	-
19	CLA	A	802	X	-	-	-
19	CLA	A	803	X	-	-	-
19	CLA	A	804	X	-	-	-
19	CLA	A	805	X	-	-	-
19	CLA	A	806	X	-	-	-
19	CLA	A	807	X	-	-	-
19	CLA	A	808	X	-	-	-
19	CLA	A	809	X	-	-	-
19	CLA	A	810	X	-	-	-
19	CLA	A	811	X	-	-	-
19	CLA	A	812	X	-	-	-
19	CLA	A	813	X	-	-	-
19	CLA	A	814	X	-	-	-
19	CLA	A	815	X	-	-	-
19	CLA	A	816	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	818	X	-	-	-
19	CLA	A	819	X	-	-	-
19	CLA	A	820	X	-	-	-
19	CLA	A	822	X	-	-	-
19	CLA	A	824	X	-	-	-
19	CLA	A	825	X	-	-	-
19	CLA	A	826	X	-	-	-
19	CLA	A	827	X	-	-	-
19	CLA	A	828	X	-	-	-
19	CLA	A	829	X	-	-	-
19	CLA	A	830	X	-	-	-
19	CLA	A	831	X	-	-	-
19	CLA	A	832	X	-	-	-
19	CLA	A	833	X	-	-	-
19	CLA	A	834	X	-	-	-
19	CLA	A	835	X	-	-	-
19	CLA	A	836	X	-	-	-
19	CLA	A	837	X	-	-	-
19	CLA	A	838	X	-	-	-
19	CLA	A	839	X	-	-	-
19	CLA	A	840	X	-	-	-
19	CLA	A	841	X	-	-	-
19	CLA	A	842	X	-	-	-
19	CLA	A	843	X	-	-	-
19	CLA	A	844	X	-	-	-
19	CLA	A	878	X	-	-	-
19	CLA	A	880	X	-	-	-
19	CLA	B	802	X	-	-	-
19	CLA	B	803	X	-	-	-
19	CLA	B	804	X	-	-	-
19	CLA	B	805	X	-	-	-
19	CLA	B	806	X	-	-	-
19	CLA	B	807	X	-	-	-
19	CLA	B	808	X	-	-	-
19	CLA	B	809	X	-	-	-
19	CLA	B	810	X	-	-	-
19	CLA	B	811	X	-	-	-
19	CLA	B	812	X	-	-	-
19	CLA	B	813	X	-	-	-
19	CLA	B	814	X	-	-	-
19	CLA	B	815	X	-	-	-
19	CLA	B	816	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	817	X	-	-	-
19	CLA	B	818	X	-	-	-
19	CLA	B	819	X	-	-	-
19	CLA	B	821	X	-	-	-
19	CLA	B	822	X	-	-	-
19	CLA	B	823	X	-	-	-
19	CLA	B	824	X	-	-	-
19	CLA	B	825	X	-	-	-
19	CLA	B	826	X	-	-	-
19	CLA	B	827	X	-	-	-
19	CLA	B	829	X	-	-	-
19	CLA	B	830	X	-	-	-
19	CLA	B	831	X	-	-	-
19	CLA	B	832	X	-	-	-
19	CLA	B	833	X	-	-	-
19	CLA	B	834	X	-	-	-
19	CLA	B	835	X	-	-	-
19	CLA	B	836	X	-	-	-
19	CLA	B	837	X	-	-	-
19	CLA	B	838	X	-	-	-
19	CLA	B	846	X	-	-	-
19	CLA	F	203	X	-	-	-
19	CLA	F	204	X	-	-	-
19	CLA	J	103	X	-	-	-
19	CLA	L	204	X	-	-	-
19	CLA	L	206	X	-	-	-
19	CLA	u	201	X	-	-	-
19	CLA	u	202	X	-	-	-
27	5X6	J	105	-	X	-	-

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 37637 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	741	Total	C	N	O	S	2	0
			5858	3828	994	1007	29		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	731	Total	C	N	O	S	2	0
			5835	3833	985	998	19		

- 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	1	0
			607	373	105	119	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	132	Total	C	N	O	S	1	0
			1050	671	181	195	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	61	Total	C	N	O	0	0
			494	312	88	94		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	161	Total	C	N	O	S	0	0
			1253	801	215	234	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	36	Total	C	N	O	S	0	0
			276	191	37	46	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	41	Total	C	N	O	S	0	0
			342	233	49	57	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	146	Total	C	N	O	S	1	0
			1106	728	182	194	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	30	Total	C	N	O	S	0	0
			228	152	35	39	2		

- Molecule 11 is a protein called Photosystem I reaction center subunit Psa29.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	W	122	Total	C	N	O	S	0	0
			912	576	144	188	4		

- Molecule 12 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	u	76	Total	C	N	O	0	0
			380	228	76	76		

- Molecule 13 is a protein called Fucoxanthin chlorophyll a/c-binding protein RedCAP.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1	185	Total	C	N	O	S	0	0
			1413	902	235	262	14		

- Molecule 14 is a protein called Fucoxanthin chl a/c light-harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	2	167	Total	C	N	O	S	0	0
			1288	825	213	240	10		

- Molecule 15 is a protein called Pt17531-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	3	164	Total	C	N	O	S	0	0
			1273	821	208	234	10		

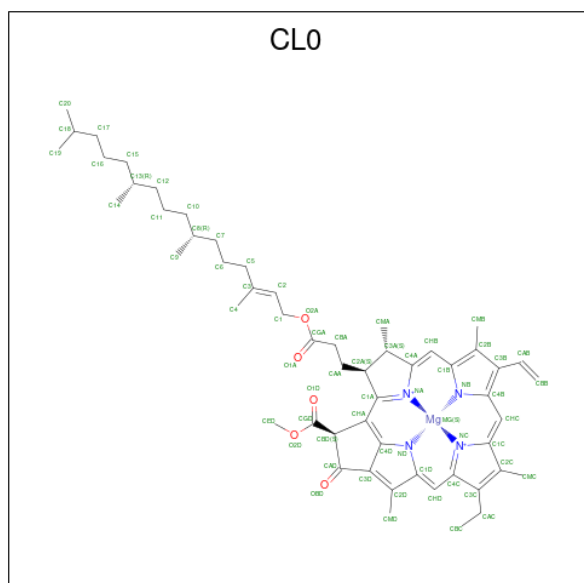
- Molecule 16 is a protein called Fucoxanthin chl a/c light-harvesting protein, major type.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	4	167	Total	C	N	O	S	0	0
			1289	834	210	237	8		

- Molecule 17 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq8.

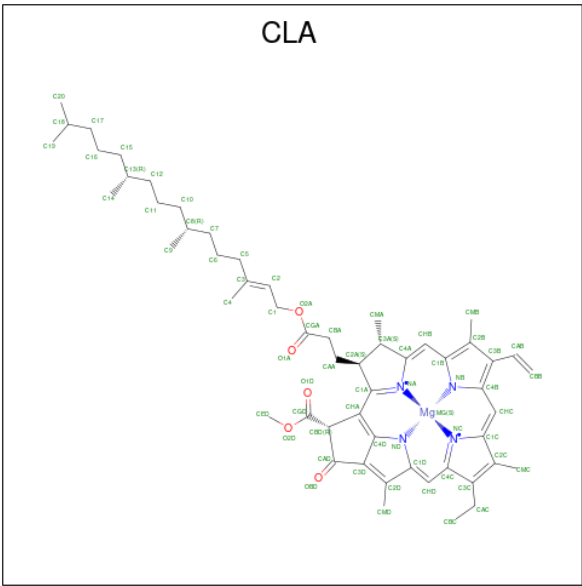
Mol	Chain	Residues	Atoms					AltConf	Trace
17	5	165	Total	C	N	O	S	0	0
			1285	833	204	240	8		

- Molecule 18 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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

- Molecule 19 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
19	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	F	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	u	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	u	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	1	1	Total 51	C 41	Mg 1	N 4	O 5	0
19	1	1	Total 55	C 45	Mg 1	N 4	O 5	0

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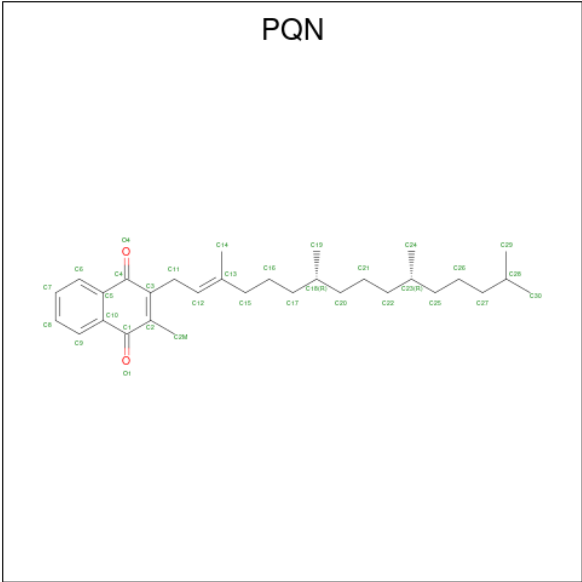
Mol	Chain	Residues	Atoms					AltConf
19	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	2	1	Total 52	C 42	Mg 1	N 4	O 5	0
19	2	1	Total 58	C 48	Mg 1	N 4	O 5	0
19	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	2	1	Total 42	C 34	Mg 1	N 4	O 3	0
19	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	3	1	Total 61	C 51	Mg 1	N 4	O 5	0
19	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	3	1	Total 51	C 41	Mg 1	N 4	O 5	0
19	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	4	1	Total 65	C 55	Mg 1	N 4	O 5	0

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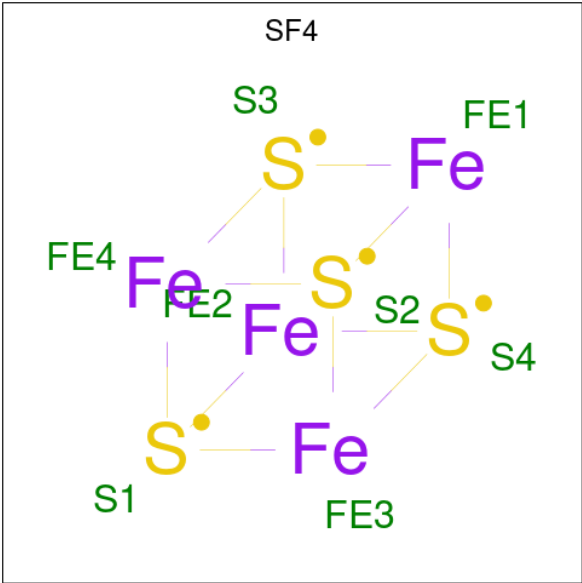
Mol	Chain	Residues	Atoms					AltConf
19	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

- Molecule 20 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



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

- Molecule 21 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



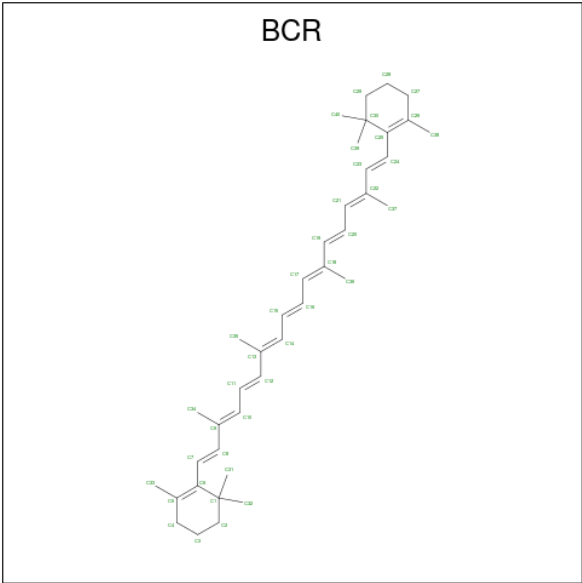
Mol	Chain	Residues	Atoms			AltConf
21	A	1	Total	Fe	S	0
			8	4	4	
21	C	1	Total	Fe	S	0
			8	4	4	

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

- Molecule 22 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



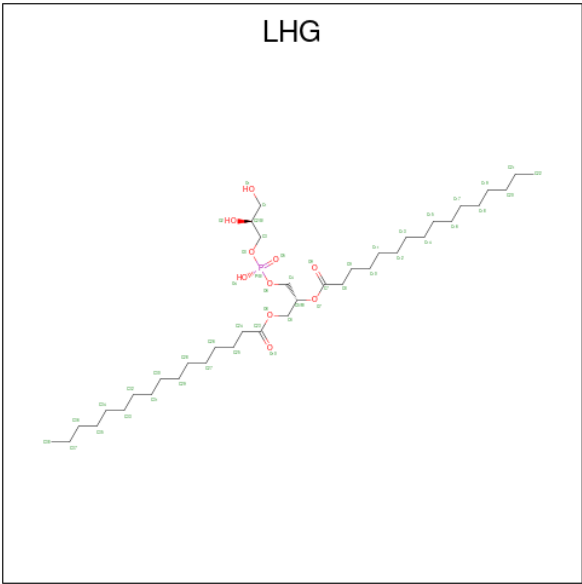
Mol	Chain	Residues	Atoms		AltConf
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms		AltConf
22	F	1	Total	C	0
			40	40	
22	F	1	Total	C	0
			40	40	
22	I	1	Total	C	0
			40	40	
22	I	1	Total	C	0
			40	40	
22	J	1	Total	C	0
			40	40	
22	L	1	Total	C	0
			40	40	
22	L	1	Total	C	0
			40	40	
22	M	1	Total	C	0
			40	40	
22	1	1	Total	C	0
			40	40	
22	1	1	Total	C	0
			40	40	

- Molecule 23 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



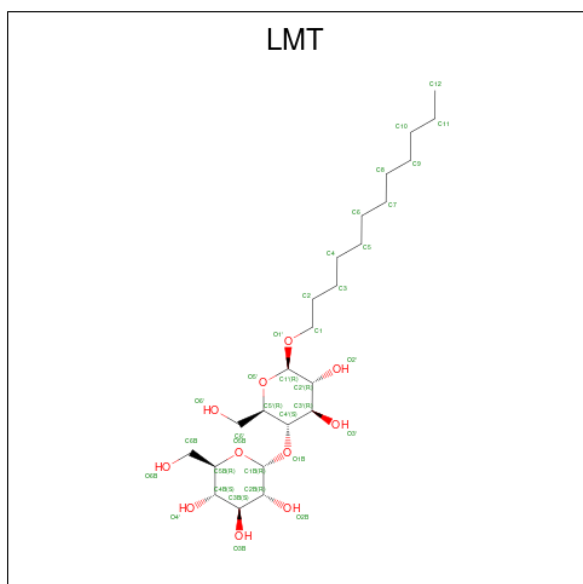
Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total	C	O	P	0
			47	36	10	1	

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Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total	C	O	P	0
			49	38	10	1	
23	B	1	Total	C	O	P	0
			35	24	10	1	
23	M	1	Total	C	O	P	0
			41	30	10	1	
23	1	1	Total	C	O	P	0
			41	30	10	1	
23	3	1	Total	C	O	P	0
			34	23	10	1	
23	4	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 24 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).

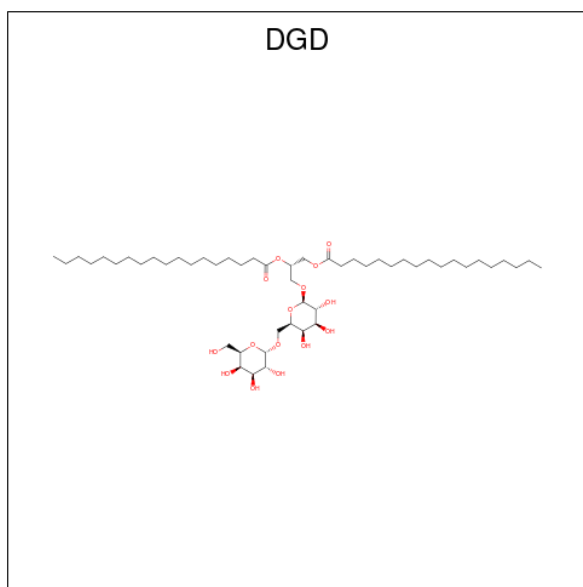


Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total	C	O	0
			35	24	11	
24	1	1	Total	C	O	0
			35	24	11	
24	2	1	Total	C	O	0
			35	24	11	
24	3	1	Total	C	O	0
			35	24	11	

- Molecule 25 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

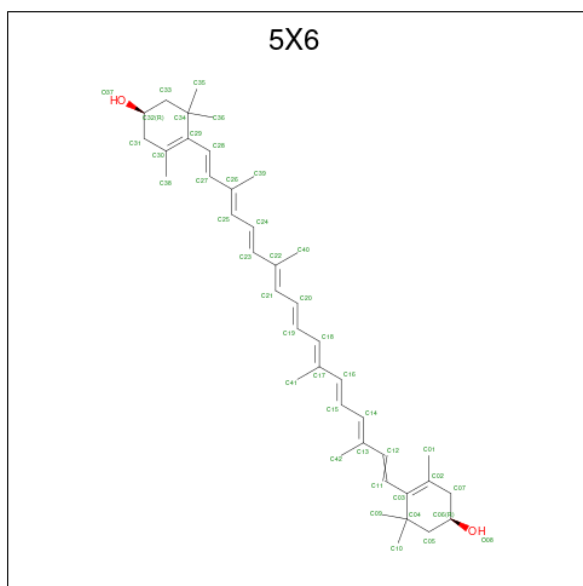
Mol	Chain	Residues	Atoms	AltConf
25	A	25	Total C 230 230	0
25	B	8	Total C 73 73	0
25	F	3	Total C 38 38	0
25	J	4	Total C 39 39	0
25	L	5	Total C 72 72	0
25	M	3	Total C 28 28	0
25	1	4	Total C 38 38	0
25	2	12	Total C 86 86	0
25	3	12	Total C 124 124	0
25	4	3	Total C 21 21	0
25	5	10	Total C 111 111	0

- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



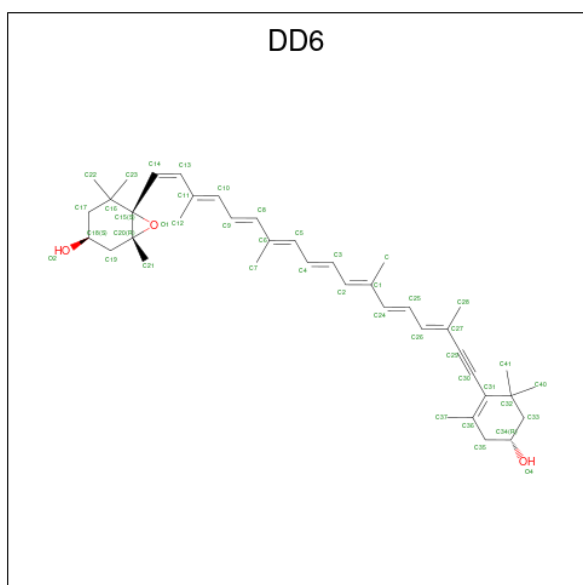
Mol	Chain	Residues	Atoms			AltConf
26	B	1	Total	C	O	0
			66	51	15	

- Molecule 27 is Zeaxanthin (CCD ID: 5X6) (formula: $C_{40}H_{56}O_2$).



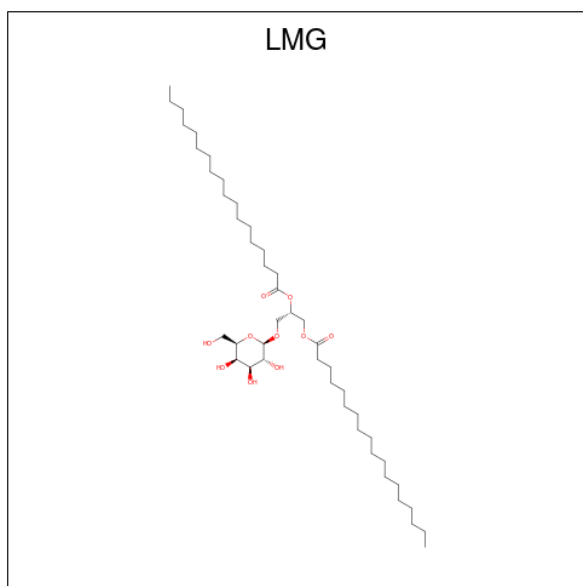
Mol	Chain	Residues	Atoms			AltConf
27	J	1	Total	C	O	0
			42	40	2	

- Molecule 28 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula: $C_{40}H_{54}O_3$).



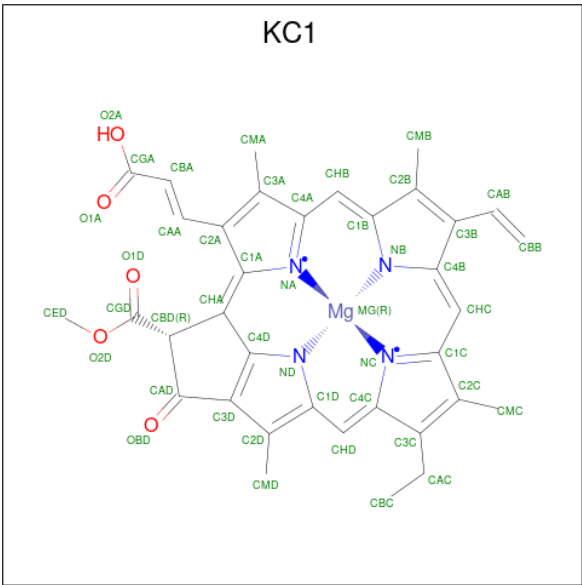
Mol	Chain	Residues	Atoms			AltConf
28	L	1	Total	C	O	0
			43	40	3	
28	1	1	Total	C	O	0
			43	40	3	
28	1	1	Total	C	O	0
			43	40	3	
28	1	1	Total	C	O	0
			43	40	3	
28	2	1	Total	C	O	0
			43	40	3	
28	3	1	Total	C	O	0
			43	40	3	
28	5	1	Total	C	O	0
			43	40	3	

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



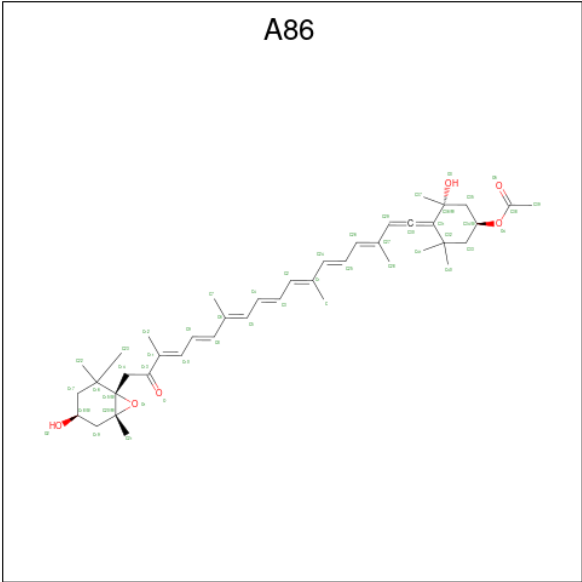
Mol	Chain	Residues	Atoms			AltConf
29	1	1	Total	C	O	0
			49	39	10	

- Molecule 30 is Chlorophyll c1 (CCD ID: KC1) (formula: $C_{35}H_{30}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
30	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 31 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'-yl acetate (CCD ID: A86) (formula: C₄₂H₅₈O₆).



Mol	Chain	Residues	Atoms			AltConf
31	1	1	Total	C	O	0
			48	42	6	
31	1	1	Total	C	O	0
			48	42	6	
31	2	1	Total	C	O	0
			48	42	6	
31	2	1	Total	C	O	0
			48	42	6	
31	2	1	Total	C	O	0
			48	42	6	
31	3	1	Total	C	O	0
			48	42	6	
31	3	1	Total	C	O	0
			48	42	6	
31	3	1	Total	C	O	0
			48	42	6	
31	4	1	Total	C	O	0
			48	42	6	
31	4	1	Total	C	O	0
			48	42	6	
31	4	1	Total	C	O	0
			48	42	6	
31	5	1	Total	C	O	0
			48	42	6	
31	5	1	Total	C	O	0
			48	42	6	
31	5	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
31	5	1	Total	C	O	0
			48	42	6	

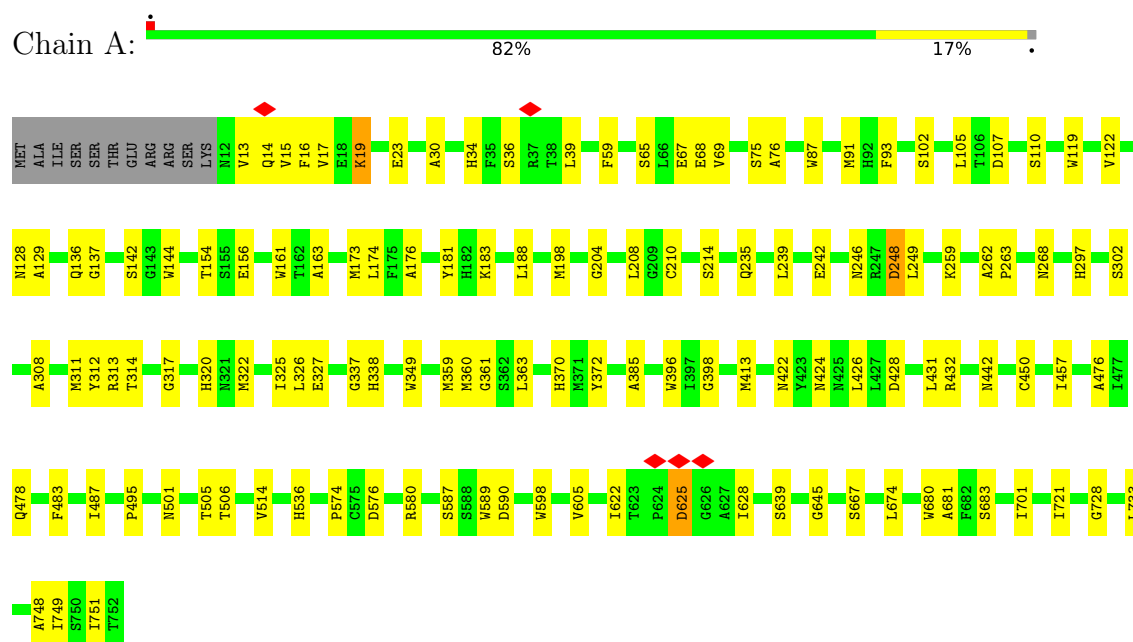
- Molecule 32 is water.

Mol	Chain	Residues	Atoms		AltConf
32	A	240	Total	O	0
			240	240	
32	B	300	Total	O	0
			300	300	
32	C	50	Total	O	0
			50	50	
32	D	56	Total	O	0
			56	56	
32	E	24	Total	O	0
			24	24	
32	F	46	Total	O	0
			46	46	
32	I	6	Total	O	0
			6	6	
32	J	7	Total	O	0
			7	7	
32	L	30	Total	O	0
			30	30	
32	M	7	Total	O	0
			7	7	
32	W	20	Total	O	0
			20	20	
32	u	3	Total	O	0
			3	3	
32	1	49	Total	O	0
			49	49	
32	2	22	Total	O	0
			22	22	
32	3	34	Total	O	0
			34	34	
32	4	11	Total	O	0
			11	11	
32	5	17	Total	O	0
			17	17	

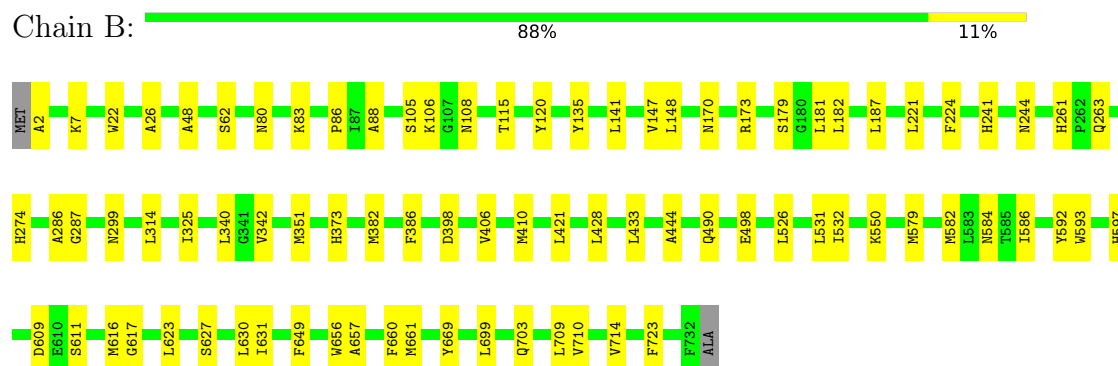
3 Residue-property plots [i](#)

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

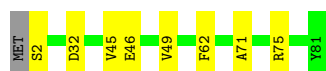


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



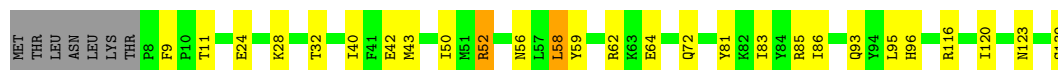
- Molecule 3: Photosystem I iron-sulfur center





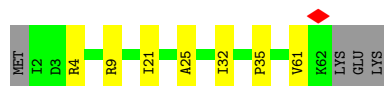
- Molecule 4: Photosystem I reaction center subunit II

Chain D: 76% 18% 5%



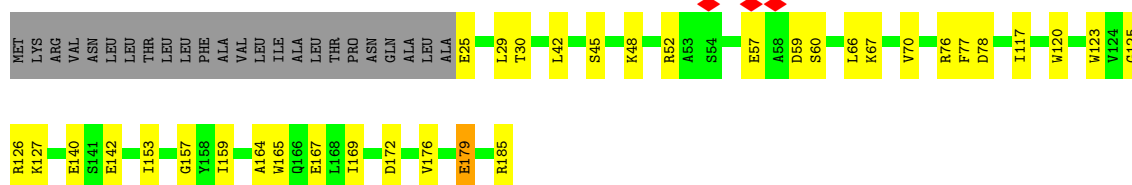
- Molecule 5: Photosystem I reaction center subunit IV

Chain E: 83% 11% 6%



- Molecule 6: Photosystem I reaction center subunit III

Chain F: 68% 18% 13%



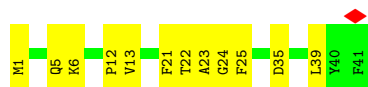
- Molecule 7: Photosystem I reaction center subunit VIII

Chain I: 86% 14%



- Molecule 8: Photosystem I reaction center subunit IX

Chain J: 71% 29%



- Molecule 9: Photosystem I reaction center subunit XI

Chain L: 5% 84% 13% ..

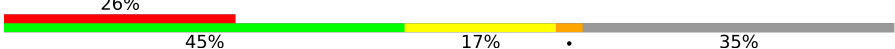


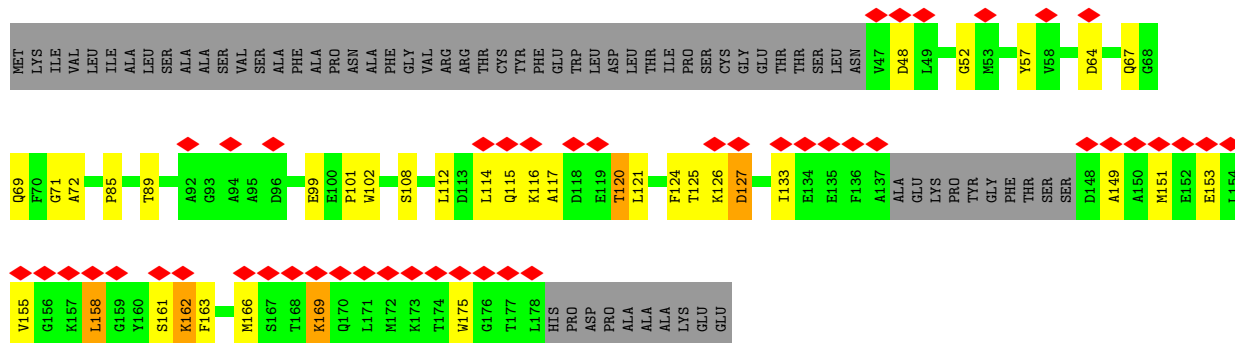
- Molecule 10: Photosystem I reaction center subunit XII

Chain M:  90% 10%



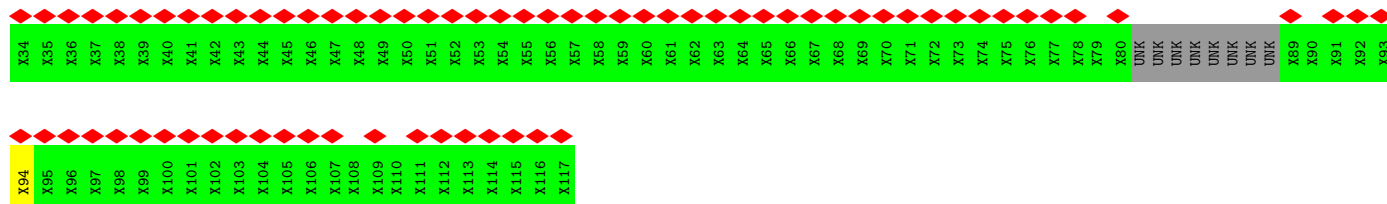
- Molecule 11: Photosystem I reaction center subunit Psa29

Chain W:  26% 45% 17% . 35%



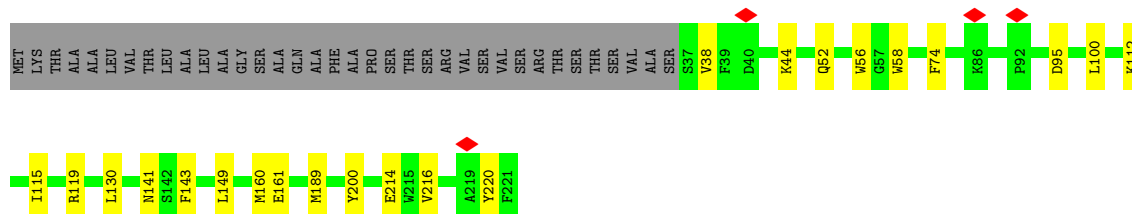
- Molecule 12: Unknown protein

Chain u:  86% 89% . 10%



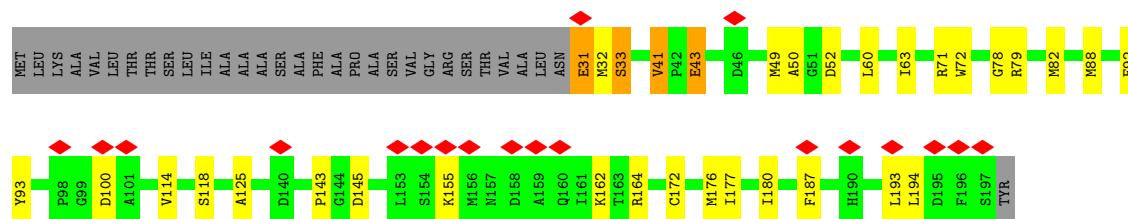
- Molecule 13: Fucoxanthin chlorophyll a/c-binding protein RedCAP

Chain 1:  74% 10% 16%



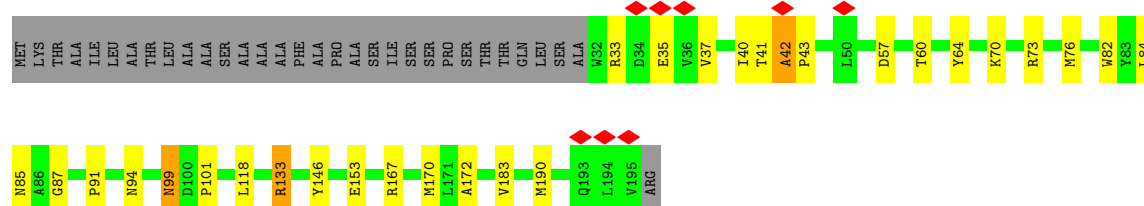
- Molecule 14: Fucoxanthin chl a/c light-harvesting protein

Chain 2:  10% 67% 15% . 16%



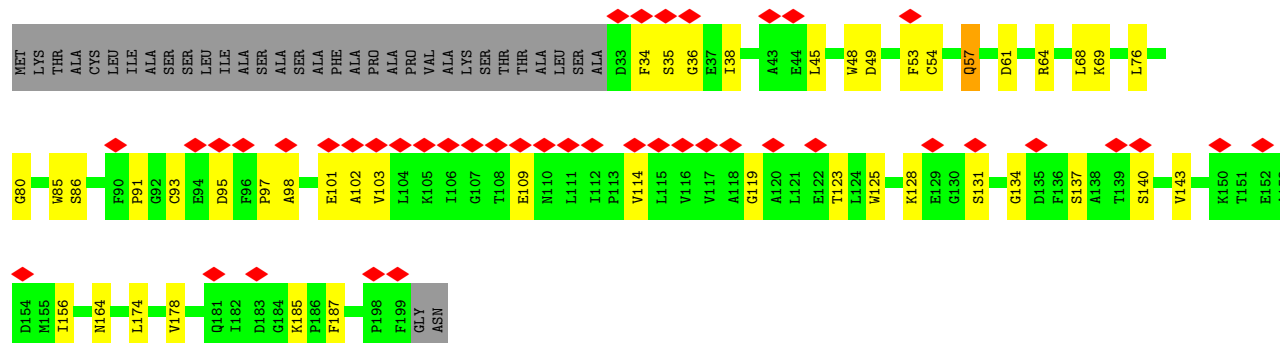
- Molecule 15: Pt17531-like protein

Chain 3: 68% 14% 16%



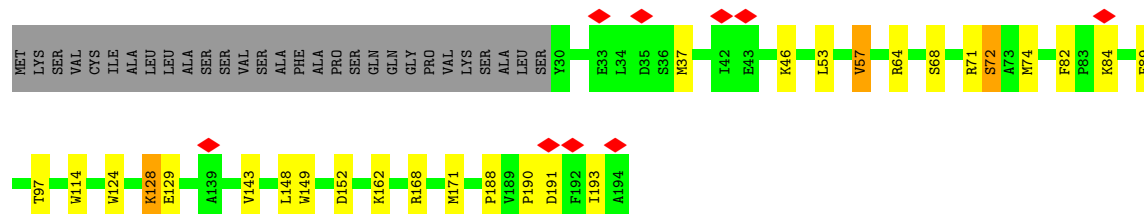
- Molecule 16: Fucoxanthin chl a/c light-harvesting protein, major type

Chain 4: 21% 62% 21% 17%



- Molecule 17: Fucoxanthin chlorophyll a/c-binding protein Lhcq8

Chain 5: 5% 71% 13% 15%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	75667	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	60000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.097	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	191.008, 191.008, 191.008	wwPDB
Map dimensions	254, 254, 254	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.752, 0.752, 0.752	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMG, LMT, UNL, DGD, DD6, LHG, 5X6, BCR, SF4, A86, PQN, CLA, KC1, CL0

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	0.22	0/6056	0.41	0/8245
2	B	0.22	0/6045	0.42	0/8252
3	C	0.22	0/617	0.45	0/838
4	D	0.20	0/1077	0.41	0/1455
5	E	0.19	0/502	0.35	0/680
6	F	0.19	0/1282	0.35	0/1741
7	I	0.22	0/284	0.39	0/388
8	J	0.23	0/353	0.43	0/479
9	L	0.22	0/1134	0.42	0/1537
10	M	0.19	0/230	0.37	0/312
11	W	0.21	0/930	0.42	0/1255
13	1	0.19	0/1450	0.34	0/1974
14	2	0.18	0/1321	0.39	0/1791
15	3	0.21	0/1306	0.42	0/1774
16	4	0.20	0/1326	0.43	0/1795
17	5	0.20	0/1324	0.40	0/1804
All	All	0.21	0/25237	0.40	0/34320

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

Mol	Chain	#Chirality outliers	#Planarity outliers
15	3	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	3	42	ALA	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5858	0	5684	89	0
2	B	5835	0	5649	77	0
3	C	607	0	586	7	0
4	D	1050	0	1039	19	0
5	E	494	0	488	4	0
6	F	1253	0	1252	21	0
7	I	276	0	287	6	0
8	J	342	0	340	10	0
9	L	1106	0	1128	16	0
10	M	228	0	249	3	0
11	W	912	0	863	24	0
12	u	380	0	81	1	0
13	1	1413	0	1365	10	0
14	2	1288	0	1253	23	0
15	3	1273	0	1231	19	0
16	4	1289	0	1235	33	0
17	5	1285	0	1239	19	0
18	A	65	0	72	5	0
19	1	476	0	483	24	0
19	2	542	0	503	33	0
19	3	407	0	400	25	0
19	4	585	0	517	31	0
19	5	541	0	498	17	0
19	A	2707	0	2766	144	0
19	B	2409	0	2542	123	0
19	F	100	0	82	3	0
19	J	45	0	33	3	0
19	L	170	0	164	9	0
19	u	100	0	80	5	0
20	A	33	0	46	1	0
20	B	33	0	46	2	0
21	A	8	0	0	0	0
21	C	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	1	80	0	112	7	0
22	A	200	0	280	10	0
22	B	200	0	280	16	0
22	F	80	0	112	6	0
22	I	80	0	112	8	0
22	J	40	0	56	3	0
22	L	80	0	112	5	0
22	M	40	0	56	3	0
23	1	41	0	52	5	0
23	3	34	0	38	2	0
23	4	49	0	73	6	0
23	A	96	0	141	10	0
23	B	35	0	40	2	0
23	M	41	0	55	3	0
24	1	35	0	43	4	0
24	2	35	0	43	1	0
24	3	35	0	46	1	0
24	A	35	0	45	0	0
25	1	38	0	0	1	0
25	2	86	0	0	0	0
25	3	124	0	0	0	0
25	4	21	0	0	0	0
25	5	111	0	0	0	0
25	A	230	0	0	0	0
25	B	73	0	0	0	0
25	F	38	0	0	0	0
25	J	39	0	0	0	0
25	L	72	0	0	0	0
25	M	28	0	0	0	0
26	B	66	0	96	9	0
27	J	42	0	0	0	0
28	1	129	0	0	0	0
28	2	43	0	0	0	0
28	3	43	0	0	0	0
28	5	43	0	0	0	0
28	L	43	0	0	0	0
29	1	49	0	71	0	0
30	1	45	0	0	0	0
30	2	45	0	0	0	0
30	3	135	0	0	1	0
30	4	90	0	0	0	0
31	1	96	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	2	144	0	0	1	0
31	3	144	0	0	1	0
31	4	144	0	0	5	0
31	5	192	0	0	3	0
32	1	49	0	0	0	0
32	2	22	0	0	1	0
32	3	34	0	0	2	0
32	4	11	0	0	1	0
32	5	17	0	0	0	0
32	A	240	0	0	0	0
32	B	300	0	0	11	0
32	C	50	0	0	1	0
32	D	56	0	0	0	0
32	E	24	0	0	0	0
32	F	46	0	0	2	0
32	I	6	0	0	0	0
32	J	7	0	0	0	0
32	L	30	0	0	0	0
32	M	7	0	0	0	0
32	W	20	0	0	1	0
32	u	3	0	0	0	0
All	All	37637	0	34064	678	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 10.

The worst 5 of 678 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)
4:D:42:GLU:H	4:D:72:GLN:HE22	1.17	0.93
19:2:206:CLA:HHC	19:2:206:CLA:HBB1	1.56	0.88
1:A:87:TRP:HA	19:A:808:CLA:HBB2	1.56	0.84
1:A:313:ARG:NH1	1:A:317:GLY:O	2.11	0.81
19:A:804:CLA:HHC	19:A:804:CLA:HBB1	1.61	0.80

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	741/752 (98%)	728 (98%)	13 (2%)	0	100	100
2	B	731/733 (100%)	716 (98%)	15 (2%)	0	100	100
3	C	79/81 (98%)	78 (99%)	1 (1%)	0	100	100
4	D	131/139 (94%)	127 (97%)	4 (3%)	0	100	100
5	E	59/65 (91%)	58 (98%)	1 (2%)	0	100	100
6	F	159/185 (86%)	156 (98%)	3 (2%)	0	100	100
7	I	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
8	J	39/41 (95%)	39 (100%)	0	0	100	100
9	L	145/148 (98%)	144 (99%)	1 (1%)	0	100	100
10	M	28/30 (93%)	28 (100%)	0	0	100	100
11	W	118/188 (63%)	114 (97%)	4 (3%)	0	100	100
13	1	183/221 (83%)	180 (98%)	3 (2%)	0	100	100
14	2	165/198 (83%)	159 (96%)	6 (4%)	0	100	100
15	3	162/196 (83%)	158 (98%)	3 (2%)	1 (1%)	21	27
16	4	165/201 (82%)	158 (96%)	7 (4%)	0	100	100
17	5	163/194 (84%)	161 (99%)	2 (1%)	0	100	100
All	All	3102/3408 (91%)	3037 (98%)	64 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	3	43	PRO

5.3.2 Protein sidechains

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	603/611 (99%)	586 (97%)	17 (3%)	38	56
2	B	599/598 (100%)	597 (100%)	2 (0%)	86	93
3	C	70/70 (100%)	70 (100%)	0	100	100
4	D	112/118 (95%)	108 (96%)	4 (4%)	31	47
5	E	54/58 (93%)	54 (100%)	0	100	100
6	F	133/153 (87%)	127 (96%)	6 (4%)	24	37
7	I	30/30 (100%)	30 (100%)	0	100	100
8	J	37/37 (100%)	37 (100%)	0	100	100
9	L	114/115 (99%)	111 (97%)	3 (3%)	40	59
10	M	23/23 (100%)	23 (100%)	0	100	100
11	W	91/144 (63%)	81 (89%)	10 (11%)	6	7
13	1	144/171 (84%)	136 (94%)	8 (6%)	19	28
14	2	135/157 (86%)	127 (94%)	8 (6%)	18	26
15	3	129/151 (85%)	120 (93%)	9 (7%)	14	19
16	4	129/152 (85%)	125 (97%)	4 (3%)	35	52
17	5	133/156 (85%)	126 (95%)	7 (5%)	20	30
All	All	2536/2744 (92%)	2458 (97%)	78 (3%)	37	52

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	2	155	LYS
17	5	37	MET
15	3	35	GLU
15	3	183	VAL
17	5	128	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
15	3	71	ASN
17	5	180	ASN

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Mol	Chain	Res	Type
15	3	85	ASN
15	3	179	GLN
2	B	703	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 296 ligands modelled in this entry, 89 are unknown - leaving 207 for Mogul analysis.

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	$\# Z > 2$
24	LMT	1	323	-	36,36,36	1.25	6 (16%)	47,47,47	1.11	3 (6%)
30	KC1	4	307	16	49,53,53	3.03	24 (48%)	61,89,89	3.93	35 (57%)
23	LHG	M	103	-	40,40,48	0.69	1 (2%)	43,46,54	1.32	6 (13%)
19	CLA	1	309	32	69,73,73	2.03	19 (27%)	82,113,113	2.68	34 (41%)
19	CLA	B	809	2	69,73,73	1.95	17 (24%)	82,113,113	2.54	32 (39%)
22	BCR	M	102	-	41,41,41	1.18	2 (4%)	56,56,56	1.19	4 (7%)
22	BCR	A	849	-	41,41,41	1.14	2 (4%)	56,56,56	1.18	5 (8%)
19	CLA	A	837	1	49,53,73	2.41	20 (40%)	58,89,113	3.03	28 (48%)
24	LMT	A	854	-	36,36,36	1.11	3 (8%)	47,47,47	1.17	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A	833	-	69,73,73	2.01	19 (27%)	82,113,113	2.59	32 (39%)
22	BCR	A	850	-	41,41,41	1.17	3 (7%)	56,56,56	1.25	6 (10%)
19	CLA	B	802	-	69,73,73	1.96	19 (27%)	82,113,113	2.66	32 (39%)
19	CLA	L	204	32	49,53,73	2.38	20 (40%)	58,89,113	3.00	27 (46%)
19	CLA	u	202	-	49,53,73	2.41	20 (40%)	58,89,113	3.06	27 (46%)
31	A86	2	219	-	47,50,50	4.23	23 (48%)	51,76,76	6.15	18 (35%)
19	CLA	A	818	-	58,62,73	2.16	20 (34%)	68,99,113	2.87	29 (42%)
19	CLA	L	206	9	64,68,73	2.09	20 (31%)	76,107,113	2.77	31 (40%)
19	CLA	2	207	-	69,73,73	2.01	20 (28%)	82,113,113	2.69	33 (40%)
22	BCR	B	844	-	41,41,41	1.12	3 (7%)	56,56,56	1.12	4 (7%)
30	KC1	1	305	-	49,53,53	3.05	25 (51%)	61,89,89	3.90	36 (59%)
19	CLA	A	809	1	69,73,73	2.00	19 (27%)	82,113,113	2.62	31 (37%)
19	CLA	B	816	-	59,63,73	2.16	19 (32%)	70,101,113	2.88	30 (42%)
30	KC1	3	205	15	49,53,53	3.10	24 (48%)	61,89,89	3.73	34 (55%)
19	CLA	1	303	13	69,73,73	2.02	19 (27%)	82,113,113	2.60	31 (37%)
30	KC1	3	211	15	49,53,53	3.06	24 (48%)	61,89,89	3.87	37 (60%)
23	LHG	1	318	-	40,40,48	0.63	0	43,46,54	1.32	4 (9%)
19	CLA	B	803	-	69,73,73	1.95	20 (28%)	82,113,113	2.58	30 (36%)
19	CLA	5	208	17	64,68,73	2.08	20 (31%)	76,107,113	2.71	30 (39%)
22	BCR	A	847	-	41,41,41	1.14	3 (7%)	56,56,56	1.23	5 (8%)
19	CLA	4	313	16	59,63,73	2.20	20 (33%)	70,101,113	2.87	31 (44%)
20	PQN	B	839	-	34,34,34	0.42	0	43,45,45	0.69	1 (2%)
30	KC1	2	211	-	49,53,53	3.06	25 (51%)	61,89,89	3.94	37 (60%)
19	CLA	A	830	-	69,73,73	1.98	20 (28%)	82,113,113	2.60	30 (36%)
19	CLA	4	303	-	59,63,73	2.21	20 (33%)	70,101,113	2.95	30 (42%)
19	CLA	B	808	-	69,73,73	1.95	18 (26%)	82,113,113	2.66	32 (39%)
19	CLA	5	209	32	69,73,73	2.04	18 (26%)	82,113,113	2.63	31 (37%)
28	DD6	1	313	-	40,45,45	5.44	23 (57%)	51,67,67	6.10	24 (47%)
19	CLA	A	815	-	54,58,73	2.29	20 (37%)	64,95,113	2.89	31 (48%)
19	CLA	A	819	-	58,62,73	2.20	21 (36%)	68,99,113	2.87	29 (42%)
19	CLA	A	827	32	69,73,73	1.98	21 (30%)	82,113,113	2.65	32 (39%)
19	CLA	4	311	32	54,58,73	2.33	20 (37%)	64,95,113	2.92	31 (48%)
19	CLA	B	806	-	69,73,73	1.99	20 (28%)	82,113,113	2.59	30 (36%)
19	CLA	2	205	14	69,73,73	2.01	19 (27%)	82,113,113	2.59	32 (39%)
21	SF4	C	101	3	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	5	214	17	49,53,73	2.42	20 (40%)	58,89,113	3.06	25 (43%)
19	CLA	B	829	-	69,73,73	1.98	19 (27%)	82,113,113	2.61	27 (32%)
19	CLA	5	216	17	46,50,73	2.40	19 (41%)	53,85,113	3.20	27 (50%)
19	CLA	B	812	-	69,73,73	2.02	21 (30%)	82,113,113	2.62	30 (36%)
19	CLA	A	820	-	69,73,73	2.02	20 (28%)	82,113,113	2.63	32 (39%)
30	KC1	3	208	32	49,53,53	3.07	26 (53%)	61,89,89	3.85	36 (59%)
22	BCR	B	841	-	41,41,41	1.16	2 (4%)	56,56,56	1.19	5 (8%)
19	CLA	3	204	32	65,69,73	2.09	20 (30%)	77,108,113	2.80	31 (40%)
19	CLA	B	820	-	49,53,73	2.40	20 (40%)	58,89,113	3.08	27 (46%)
19	CLA	2	213	14	49,53,73	2.40	21 (42%)	58,89,113	3.03	28 (48%)
18	CL0	A	801	-	58,73,73	3.05	17 (29%)	60,113,113	2.63	20 (33%)
19	CLA	A	841	-	69,73,73	1.99	19 (27%)	82,113,113	2.62	34 (41%)
19	CLA	B	826	-	69,73,73	2.01	19 (27%)	82,113,113	3.86	32 (39%)
19	CLA	A	831	-	69,73,73	1.98	19 (27%)	82,113,113	2.64	31 (37%)
22	BCR	1	311	-	41,41,41	1.16	3 (7%)	56,56,56	1.24	5 (8%)
19	CLA	2	214	14	49,53,73	2.44	21 (42%)	58,89,113	3.09	28 (48%)
28	DD6	2	217	-	40,45,45	5.45	24 (60%)	51,67,67	5.69	25 (49%)
19	CLA	4	305	16	69,73,73	2.04	20 (28%)	82,113,113	2.54	31 (37%)
19	CLA	A	835	-	69,73,73	1.99	21 (30%)	82,113,113	2.66	29 (35%)
24	LMT	2	220	-	36,36,36	1.16	6 (16%)	47,47,47	0.95	2 (4%)
19	CLA	3	206	15	69,73,73	2.00	20 (28%)	82,113,113	2.62	28 (34%)
19	CLA	A	821	-	58,62,73	2.15	19 (32%)	68,99,113	2.90	31 (45%)
22	BCR	L	202	-	41,41,41	1.10	2 (4%)	56,56,56	1.11	3 (5%)
19	CLA	F	203	-	59,63,73	2.16	19 (32%)	70,101,113	2.81	28 (40%)
19	CLA	A	878	32	69,73,73	1.96	19 (27%)	82,113,113	2.64	31 (37%)
19	CLA	A	843	32	69,73,73	1.97	20 (28%)	82,113,113	2.57	31 (37%)
19	CLA	2	208	14	56,60,73	2.25	20 (35%)	65,97,113	3.02	29 (44%)
31	A86	1	317	-	47,50,50	4.23	23 (48%)	51,76,76	6.39	20 (39%)
20	PQN	A	845	-	34,34,34	0.37	0	43,45,45	0.73	1 (2%)
19	CLA	1	307	13	59,63,73	2.19	20 (33%)	70,101,113	4.71	31 (44%)
19	CLA	A	842	-	69,73,73	1.98	20 (28%)	82,113,113	2.62	31 (37%)
19	CLA	4	309	-	49,53,73	2.44	20 (40%)	58,89,113	3.05	26 (44%)
19	CLA	B	804	-	69,73,73	1.98	19 (27%)	82,113,113	2.71	32 (39%)
19	CLA	B	828	-	49,53,73	2.38	20 (40%)	58,89,113	2.99	30 (51%)
19	CLA	2	209	14	62,66,73	2.12	20 (32%)	73,104,113	2.71	32 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	LHG	3	215	-	33,33,48	0.77	1 (3%)	36,39,54	1.30	4 (11%)
19	CLA	A	823	-	53,57,73	2.30	20 (37%)	61,93,113	2.97	28 (45%)
19	CLA	A	834	-	69,73,73	1.98	20 (28%)	82,113,113	2.62	30 (36%)
19	CLA	1	304	13	69,73,73	1.99	19 (27%)	82,113,113	2.68	32 (39%)
26	DGD	B	847	-	67,67,67	0.96	2 (2%)	81,81,81	1.35	10 (12%)
19	CLA	2	212	-	49,53,73	2.38	19 (38%)	58,89,113	3.12	29 (50%)
19	CLA	A	828	-	69,73,73	1.95	19 (27%)	82,113,113	2.65	30 (36%)
19	CLA	4	310	16	49,53,73	2.44	20 (40%)	58,89,113	3.12	26 (44%)
19	CLA	5	212	17	60,64,73	2.17	20 (33%)	71,102,113	4.64	35 (49%)
19	CLA	A	817	32	53,57,73	2.30	19 (35%)	61,93,113	2.99	28 (45%)
19	CLA	2	210	14	64,68,73	2.08	20 (31%)	76,107,113	2.68	29 (38%)
28	DD6	1	312	-	40,45,45	5.49	24 (60%)	51,67,67	5.84	24 (47%)
19	CLA	3	203	15	59,63,73	2.17	19 (32%)	70,101,113	2.84	29 (41%)
19	CLA	A	808	-	69,73,73	1.99	18 (26%)	82,113,113	2.65	29 (35%)
19	CLA	A	832	-	64,68,73	2.06	20 (31%)	76,107,113	2.75	32 (42%)
19	CLA	B	818	-	69,73,73	2.00	19 (27%)	82,113,113	2.63	30 (36%)
19	CLA	B	834	-	69,73,73	2.01	20 (28%)	82,113,113	2.61	31 (37%)
22	BCR	B	840	-	41,41,41	1.16	3 (7%)	56,56,56	1.15	5 (8%)
31	A86	3	214	-	47,50,50	4.20	23 (48%)	51,76,76	5.93	20 (39%)
19	CLA	B	831	32	69,73,73	2.01	20 (28%)	82,113,113	2.65	36 (43%)
22	BCR	J	104	-	41,41,41	1.18	3 (7%)	56,56,56	1.17	3 (5%)
31	A86	2	218	-	47,50,50	4.22	23 (48%)	51,76,76	5.94	21 (41%)
19	CLA	B	830	-	62,66,73	2.11	19 (30%)	73,104,113	2.86	32 (43%)
19	CLA	A	804	-	69,73,73	1.98	21 (30%)	82,113,113	2.66	34 (41%)
31	A86	1	316	-	47,50,50	4.32	24 (51%)	51,76,76	6.30	15 (29%)
23	LHG	B	842	19	34,34,48	0.83	1 (2%)	37,40,54	1.24	4 (10%)
31	A86	2	216	-	47,50,50	4.28	24 (51%)	51,76,76	5.81	18 (35%)
19	CLA	A	814	-	64,68,73	2.07	19 (29%)	76,107,113	2.74	33 (43%)
19	CLA	A	805	19	60,64,73	2.13	19 (31%)	71,102,113	2.81	32 (45%)
22	BCR	A	851	-	41,41,41	1.09	3 (7%)	56,56,56	1.30	8 (14%)
19	CLA	B	825	-	69,73,73	2.00	20 (28%)	82,113,113	2.59	33 (40%)
19	CLA	3	209	15	55,59,73	2.26	20 (36%)	64,96,113	3.02	31 (48%)
19	CLA	1	308	13	49,53,73	2.42	19 (38%)	58,89,113	3.05	26 (44%)
22	BCR	F	201	-	41,41,41	1.09	2 (4%)	56,56,56	1.12	4 (7%)
31	A86	4	315	-	47,50,50	4.12	23 (48%)	51,76,76	6.21	19 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	817	-	63,67,73	2.11	21 (33%)	74,105,113	2.80	30 (40%)
19	CLA	A	802	32	69,73,73	2.00	20 (28%)	82,113,113	2.65	30 (36%)
19	CLA	B	814	-	69,73,73	1.99	21 (30%)	82,113,113	2.65	30 (36%)
21	SF4	A	846	1,2	0,12,12	-	-	-	-	-
28	DD6	L	209	-	40,45,45	5.48	24 (60%)	51,67,67	5.89	26 (50%)
19	CLA	5	215	17	49,53,73	2.42	20 (40%)	58,89,113	3.06	27 (46%)
19	CLA	L	203	-	69,73,73	1.98	20 (28%)	82,113,113	2.69	30 (36%)
31	A86	5	217	-	47,50,50	4.22	23 (48%)	51,76,76	6.03	20 (39%)
21	SF4	C	102	3	0,12,12	-	-	-	-	-
19	CLA	B	846	-	69,73,73	1.99	19 (27%)	82,113,113	2.65	28 (34%)
28	DD6	1	315	-	40,45,45	5.47	24 (60%)	51,67,67	5.83	27 (52%)
19	CLA	A	880	32	69,73,73	1.96	20 (28%)	82,113,113	2.61	32 (39%)
22	BCR	L	205	-	41,41,41	1.14	3 (7%)	56,56,56	1.19	4 (7%)
19	CLA	1	306	-	55,59,73	2.26	21 (38%)	64,96,113	3.13	37 (57%)
19	CLA	B	822	32	58,62,73	2.18	20 (34%)	68,99,113	2.80	29 (42%)
19	CLA	B	823	32	60,64,73	2.10	21 (35%)	71,102,113	2.90	32 (45%)
22	BCR	B	843	-	41,41,41	1.13	3 (7%)	56,56,56	1.26	6 (10%)
19	CLA	B	827	-	69,73,73	1.95	19 (27%)	82,113,113	2.68	31 (37%)
31	A86	5	221	-	47,50,50	4.15	25 (53%)	51,76,76	6.47	18 (35%)
19	CLA	A	825	-	63,67,73	2.11	20 (31%)	74,105,113	2.72	32 (43%)
19	CLA	3	210	32	49,53,73	2.42	21 (42%)	58,89,113	3.11	27 (46%)
19	CLA	B	811	-	69,73,73	2.00	20 (28%)	82,113,113	2.67	33 (40%)
23	LHG	A	852	-	46,46,48	0.70	1 (2%)	49,52,54	1.26	5 (10%)
19	CLA	B	810	-	69,73,73	1.99	20 (28%)	82,113,113	4.40	34 (41%)
19	CLA	5	207	17	64,68,73	2.12	20 (31%)	76,107,113	2.76	32 (42%)
19	CLA	3	202	15	69,73,73	2.01	18 (26%)	82,113,113	2.65	32 (39%)
19	CLA	B	821	-	69,73,73	1.98	21 (30%)	82,113,113	2.60	33 (40%)
19	CLA	B	805	-	69,73,73	2.02	20 (28%)	82,113,113	2.66	29 (35%)
22	BCR	I	102	-	41,41,41	1.06	2 (4%)	56,56,56	1.23	7 (12%)
22	BCR	1	314	-	41,41,41	1.11	2 (4%)	56,56,56	1.25	5 (8%)
19	CLA	A	810	1	69,73,73	2.00	20 (28%)	82,113,113	2.60	31 (37%)
19	CLA	1	310	13	69,73,73	2.05	19 (27%)	82,113,113	2.63	32 (39%)
19	CLA	A	822	32	69,73,73	2.05	19 (27%)	82,113,113	2.54	30 (36%)
31	A86	5	219	-	47,50,50	4.23	23 (48%)	51,76,76	6.09	18 (35%)
19	CLA	B	845	-	69,73,73	2.00	21 (30%)	82,113,113	2.66	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	u	201	-	59,63,73	2.16	20 (33%)	70,101,113	2.86	30 (42%)
31	A86	3	212	-	47,50,50	4.19	22 (46%)	51,76,76	5.96	22 (43%)
19	CLA	A	816	-	54,58,73	2.30	19 (35%)	64,95,113	2.97	33 (51%)
19	CLA	B	838	23	69,73,73	1.99	20 (28%)	82,113,113	2.63	31 (37%)
19	CLA	4	304	16	54,58,73	2.29	19 (35%)	64,95,113	3.09	33 (51%)
19	CLA	5	213	17	49,53,73	2.43	20 (40%)	58,89,113	3.08	27 (46%)
28	DD6	3	213	-	40,45,45	5.41	24 (60%)	51,67,67	5.89	25 (49%)
19	CLA	A	803	-	69,73,73	2.00	20 (28%)	82,113,113	2.48	30 (36%)
22	BCR	I	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.19	4 (7%)
19	CLA	B	833	-	64,68,73	2.06	20 (31%)	76,107,113	2.71	27 (35%)
19	CLA	B	835	-	51,55,73	2.30	19 (37%)	60,91,113	3.01	28 (46%)
29	LMG	1	302	-	49,49,55	0.79	0	57,57,63	1.30	6 (10%)
19	CLA	B	819	32	69,73,73	2.01	20 (28%)	82,113,113	2.59	34 (41%)
19	CLA	F	204	6	49,53,73	2.42	20 (40%)	58,89,113	3.02	27 (46%)
19	CLA	1	301	32	69,73,73	2.01	20 (28%)	82,113,113	2.67	31 (37%)
19	CLA	A	826	32	69,73,73	1.96	19 (27%)	82,113,113	2.69	29 (35%)
19	CLA	A	844	23	69,73,73	1.98	21 (30%)	82,113,113	2.68	31 (37%)
19	CLA	3	207	15	69,73,73	2.03	20 (28%)	82,113,113	2.61	29 (35%)
19	CLA	B	837	-	69,73,73	1.97	20 (28%)	82,113,113	2.66	32 (39%)
22	BCR	A	848	-	41,41,41	1.14	2 (4%)	56,56,56	1.28	5 (8%)
19	CLA	B	836	32	69,73,73	2.03	20 (28%)	82,113,113	2.54	30 (36%)
31	A86	5	220	-	47,50,50	4.40	25 (53%)	51,76,76	6.71	18 (35%)
19	CLA	A	807	1	69,73,73	2.02	20 (28%)	82,113,113	2.70	32 (39%)
22	BCR	B	852	-	41,41,41	1.11	3 (7%)	56,56,56	1.23	5 (8%)
19	CLA	A	829	-	69,73,73	2.01	21 (30%)	82,113,113	2.66	32 (39%)
19	CLA	A	840	-	51,55,73	2.32	20 (39%)	60,91,113	3.01	27 (45%)
19	CLA	5	211	17	62,66,73	2.10	21 (33%)	73,104,113	2.79	29 (39%)
19	CLA	J	103	8	49,53,73	2.38	20 (40%)	58,89,113	3.02	27 (46%)
31	A86	4	316	-	47,50,50	4.33	26 (55%)	51,76,76	6.16	16 (31%)
30	KC1	4	302	-	49,53,53	3.02	21 (42%)	61,89,89	3.99	37 (60%)
19	CLA	B	824	-	69,73,73	1.96	20 (28%)	82,113,113	2.72	31 (37%)
19	CLA	2	215	-	46,50,73	2.41	19 (41%)	53,85,113	3.14	29 (54%)
19	CLA	5	210	17	69,73,73	2.00	20 (28%)	82,113,113	2.67	31 (37%)
31	A86	4	314	-	47,50,50	4.23	24 (51%)	51,76,76	6.35	18 (35%)
19	CLA	A	811	-	58,62,73	2.21	20 (34%)	68,99,113	2.86	30 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	5X6	J	105	-	43,43,43	4.36	23 (53%)	56,60,60	4.85	31 (55%)
19	CLA	A	824	-	55,59,73	2.25	20 (36%)	64,96,113	2.93	28 (43%)
31	A86	3	228	-	47,50,50	4.31	24 (51%)	51,76,76	6.02	15 (29%)
19	CLA	A	839	-	69,73,73	2.00	20 (28%)	82,113,113	2.64	31 (37%)
22	BCR	F	205	-	41,41,41	1.17	3 (7%)	56,56,56	1.25	5 (8%)
19	CLA	B	813	-	69,73,73	2.01	20 (28%)	82,113,113	2.61	30 (36%)
19	CLA	4	308	-	49,53,73	2.42	20 (40%)	58,89,113	3.13	26 (44%)
19	CLA	4	301	16	69,73,73	2.04	21 (30%)	82,113,113	2.64	30 (36%)
19	CLA	A	836	-	58,62,73	2.17	19 (32%)	68,99,113	2.80	34 (50%)
19	CLA	A	838	-	55,59,73	2.22	21 (38%)	64,96,113	2.96	30 (46%)
24	LMT	3	216	-	36,36,36	1.15	6 (16%)	47,47,47	1.08	3 (6%)
19	CLA	A	812	19	69,73,73	2.00	20 (28%)	82,113,113	2.68	31 (37%)
19	CLA	4	306	23	62,66,73	2.13	20 (32%)	73,104,113	2.82	28 (38%)
19	CLA	B	815	-	49,53,73	2.35	21 (42%)	58,89,113	3.10	27 (46%)
19	CLA	B	832	32	69,73,73	2.03	20 (28%)	82,113,113	2.61	29 (35%)
19	CLA	4	312	16	56,60,73	2.24	20 (35%)	65,97,113	2.95	30 (46%)
19	CLA	A	806	-	69,73,73	2.01	20 (28%)	82,113,113	2.72	30 (36%)
23	LHG	4	317	19	48,48,48	0.67	2 (4%)	51,54,54	1.26	6 (11%)
19	CLA	B	807	-	69,73,73	1.97	19 (27%)	82,113,113	2.67	32 (39%)
19	CLA	2	206	-	69,73,73	2.00	21 (30%)	82,113,113	2.70	31 (37%)
28	DD6	5	218	-	40,45,45	5.51	23 (57%)	51,67,67	5.47	27 (52%)
23	LHG	A	853	19	48,48,48	0.62	1 (2%)	51,54,54	1.28	5 (9%)
19	CLA	A	813	-	59,63,73	2.19	21 (35%)	70,101,113	2.83	30 (42%)

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
24	LMT	1	323	-	-	12/21/61/61	0/2/2/2
30	KC1	4	307	16	-	5/15/71/71	-
23	LHG	M	103	-	-	22/45/45/53	-
19	CLA	1	309	32	1/1/15/20	12/39/115/115	-
19	CLA	B	809	2	1/1/15/20	7/39/115/115	-
22	BCR	M	102	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	A	849	-	-	5/29/63/63	0/2/2/2
19	CLA	A	837	1	1/1/11/20	3/15/91/115	-
24	LMT	A	854	-	-	8/21/61/61	0/2/2/2
19	CLA	A	833	-	1/1/15/20	11/39/115/115	-
22	BCR	A	850	-	-	7/29/63/63	0/2/2/2
19	CLA	B	802	-	1/1/15/20	13/39/115/115	-
19	CLA	L	204	32	1/1/11/20	5/15/91/115	-
19	CLA	u	202	-	1/1/11/20	2/15/91/115	-
31	A86	2	219	-	-	6/34/90/90	0/3/3/3
19	CLA	A	818	-	1/1/12/20	6/26/102/115	-
19	CLA	L	206	9	1/1/14/20	5/33/109/115	-
19	CLA	2	207	-	1/1/15/20	8/39/115/115	-
22	BCR	B	844	-	-	3/29/63/63	0/2/2/2
30	KC1	1	305	-	-	5/15/71/71	-
19	CLA	A	809	1	1/1/15/20	9/39/115/115	-
19	CLA	B	816	-	1/1/13/20	13/27/103/115	-
30	KC1	3	205	15	-	6/15/71/71	-
19	CLA	1	303	13	1/1/15/20	14/39/115/115	-
30	KC1	3	211	15	-	4/15/71/71	-
23	LHG	1	318	-	-	28/45/45/53	-
19	CLA	B	803	-	1/1/15/20	7/39/115/115	-
19	CLA	5	208	17	1/1/14/20	12/33/109/115	-
22	BCR	A	847	-	-	6/29/63/63	0/2/2/2
19	CLA	4	313	16	1/1/13/20	4/27/103/115	-
20	PQN	B	839	-	-	9/23/43/43	0/2/2/2
30	KC1	2	211	-	-	8/15/71/71	-
19	CLA	A	830	-	1/1/15/20	8/39/115/115	-
19	CLA	4	303	-	1/1/13/20	7/27/103/115	-
19	CLA	B	808	-	1/1/15/20	7/39/115/115	-
19	CLA	5	209	32	1/1/15/20	20/39/115/115	-
28	DD6	1	313	-	-	16/26/80/80	0/3/3/3
19	CLA	A	815	-	1/1/12/20	5/21/97/115	-
19	CLA	A	819	-	1/1/12/20	9/26/102/115	-
19	CLA	A	827	32	1/1/15/20	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	4	311	32	1/1/12/20	4/21/97/115	-
19	CLA	B	806	-	1/1/15/20	10/39/115/115	-
19	CLA	2	205	14	1/1/15/20	13/39/115/115	-
21	SF4	C	101	3	-	-	0/6/5/5
19	CLA	5	214	17	1/1/11/20	3/15/91/115	-
19	CLA	B	829	-	1/1/15/20	11/39/115/115	-
19	CLA	5	216	17	-	0/12/88/115	-
19	CLA	B	812	-	1/1/15/20	6/39/115/115	-
19	CLA	A	820	-	1/1/15/20	12/39/115/115	-
30	KC1	3	208	32	-	3/15/71/71	-
22	BCR	B	841	-	-	2/29/63/63	0/2/2/2
19	CLA	3	204	32	1/1/14/20	10/35/111/115	-
19	CLA	B	820	-	-	2/15/91/115	-
19	CLA	2	213	14	1/1/11/20	8/15/91/115	-
18	CL0	A	801	-	3/3/20/25	10/37/135/135	-
19	CLA	A	841	-	1/1/15/20	5/39/115/115	-
19	CLA	B	826	-	1/1/15/20	9/39/115/115	-
19	CLA	A	831	-	1/1/15/20	9/39/115/115	-
22	BCR	1	311	-	-	7/29/63/63	0/2/2/2
19	CLA	2	214	14	1/1/11/20	2/15/91/115	-
28	DD6	2	217	-	-	10/26/80/80	0/3/3/3
19	CLA	4	305	16	1/1/15/20	12/39/115/115	-
19	CLA	A	835	-	1/1/15/20	11/39/115/115	-
24	LMT	2	220	-	-	9/21/61/61	0/2/2/2
19	CLA	3	206	15	1/1/15/20	19/39/115/115	-
19	CLA	A	821	-	-	9/26/102/115	-
22	BCR	L	202	-	-	8/29/63/63	0/2/2/2
19	CLA	F	203	-	1/1/13/20	10/27/103/115	-
19	CLA	A	878	32	1/1/15/20	7/39/115/115	-
19	CLA	A	843	32	1/1/15/20	9/39/115/115	-
19	CLA	2	208	14	1/1/12/20	11/24/100/115	-
31	A86	1	317	-	-	9/34/90/90	0/3/3/3
20	PQN	A	845	-	-	6/23/43/43	0/2/2/2
19	CLA	1	307	13	1/1/13/20	7/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	842	-	1/1/15/20	12/39/115/115	-
19	CLA	4	309	-	-	2/15/91/115	-
19	CLA	B	804	-	1/1/15/20	14/39/115/115	-
19	CLA	B	828	-	-	2/15/91/115	-
19	CLA	2	209	14	1/1/13/20	9/31/107/115	-
23	LHG	3	215	-	-	16/38/38/53	-
19	CLA	A	823	-	-	2/20/96/115	-
19	CLA	A	834	-	1/1/15/20	10/39/115/115	-
19	CLA	1	304	13	1/1/15/20	10/39/115/115	-
26	DGD	B	847	-	-	24/55/95/95	0/2/2/2
19	CLA	2	212	-	1/1/11/20	4/15/91/115	-
19	CLA	A	828	-	1/1/15/20	11/39/115/115	-
19	CLA	5	212	17	1/1/13/20	10/29/105/115	-
19	CLA	4	310	16	-	5/15/91/115	-
19	CLA	A	817	32	-	9/20/96/115	-
19	CLA	2	210	14	1/1/14/20	10/33/109/115	-
28	DD6	1	312	-	-	11/26/80/80	0/3/3/3
19	CLA	3	203	15	1/1/13/20	8/27/103/115	-
19	CLA	A	808	-	1/1/15/20	7/39/115/115	-
19	CLA	A	832	-	1/1/14/20	10/33/109/115	-
19	CLA	B	818	-	1/1/15/20	7/39/115/115	-
19	CLA	B	834	-	1/1/15/20	8/39/115/115	-
22	BCR	B	840	-	-	8/29/63/63	0/2/2/2
31	A86	3	214	-	-	3/34/90/90	0/3/3/3
19	CLA	B	831	32	1/1/15/20	7/39/115/115	-
22	BCR	J	104	-	-	9/29/63/63	0/2/2/2
31	A86	2	218	-	-	2/34/90/90	0/3/3/3
19	CLA	B	830	-	1/1/13/20	8/31/107/115	-
19	CLA	A	804	-	1/1/15/20	12/39/115/115	-
31	A86	1	316	-	-	5/34/90/90	0/3/3/3
23	LHG	B	842	19	-	20/39/39/53	-
31	A86	2	216	-	-	6/34/90/90	0/3/3/3
19	CLA	A	814	-	1/1/14/20	8/33/109/115	-
19	CLA	A	805	19	1/1/13/20	9/29/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	A	851	-	-	7/29/63/63	0/2/2/2
19	CLA	B	825	-	1/1/15/20	8/39/115/115	-
19	CLA	3	209	15	1/1/12/20	7/23/99/115	-
19	CLA	1	308	13	1/1/11/20	4/15/91/115	-
22	BCR	F	201	-	-	8/29/63/63	0/2/2/2
31	A86	4	315	-	-	6/34/90/90	0/3/3/3
19	CLA	B	817	-	1/1/13/20	4/32/108/115	-
19	CLA	A	802	32	1/1/15/20	4/39/115/115	-
19	CLA	B	814	-	1/1/15/20	11/39/115/115	-
28	DD6	L	209	-	-	9/26/80/80	0/3/3/3
31	A86	5	217	-	-	6/34/90/90	0/3/3/3
19	CLA	5	215	17	-	3/15/91/115	-
19	CLA	L	203	-	-	4/39/115/115	-
21	SF4	A	846	1,2	-	-	0/6/5/5
21	SF4	C	102	3	-	-	0/6/5/5
19	CLA	B	846	-	1/1/15/20	11/39/115/115	-
28	DD6	1	315	-	-	11/26/80/80	0/3/3/3
19	CLA	A	880	32	1/1/15/20	3/39/115/115	-
22	BCR	L	205	-	-	5/29/63/63	0/2/2/2
19	CLA	1	306	-	1/1/12/20	9/23/99/115	-
19	CLA	B	822	32	1/1/12/20	7/26/102/115	-
19	CLA	B	823	32	1/1/13/20	4/29/105/115	-
22	BCR	B	843	-	-	5/29/63/63	0/2/2/2
19	CLA	B	827	-	1/1/15/20	13/39/115/115	-
31	A86	5	221	-	-	7/34/90/90	0/3/3/3
19	CLA	A	825	-	1/1/13/20	11/32/108/115	-
19	CLA	3	210	32	1/1/11/20	6/15/91/115	-
19	CLA	B	811	-	1/1/15/20	9/39/115/115	-
23	LHG	A	852	-	-	25/51/51/53	-
19	CLA	B	810	-	1/1/15/20	13/39/115/115	-
19	CLA	5	207	17	1/1/14/20	14/33/109/115	-
19	CLA	3	202	15	1/1/15/20	9/39/115/115	-
19	CLA	B	821	-	1/1/15/20	19/39/115/115	-
19	CLA	B	805	-	1/1/15/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	I	102	-	-	6/29/63/63	0/2/2/2
22	BCR	1	314	-	-	13/29/63/63	0/2/2/2
19	CLA	A	810	1	1/1/15/20	8/39/115/115	-
19	CLA	1	310	13	1/1/15/20	14/39/115/115	-
19	CLA	A	822	32	1/1/15/20	9/39/115/115	-
31	A86	5	219	-	-	3/34/90/90	0/3/3/3
19	CLA	u	201	-	1/1/13/20	15/27/103/115	-
19	CLA	B	845	-	-	9/39/115/115	-
31	A86	3	212	-	-	5/34/90/90	0/3/3/3
19	CLA	A	816	-	1/1/12/20	3/21/97/115	-
19	CLA	B	838	23	1/1/15/20	13/39/115/115	-
19	CLA	4	304	16	1/1/12/20	3/21/97/115	-
19	CLA	5	213	17	1/1/11/20	4/15/91/115	-
28	DD6	3	213	-	-	9/26/80/80	0/3/3/3
19	CLA	A	803	-	1/1/15/20	9/39/115/115	-
22	BCR	I	101	-	-	2/29/63/63	0/2/2/2
19	CLA	B	835	-	1/1/11/20	2/18/94/115	-
19	CLA	B	833	-	1/1/14/20	6/33/109/115	-
29	LMG	1	302	-	-	23/44/64/70	0/1/1/1
19	CLA	B	819	32	1/1/15/20	9/39/115/115	-
19	CLA	F	204	6	1/1/11/20	9/15/91/115	-
19	CLA	1	301	32	1/1/15/20	7/39/115/115	-
19	CLA	A	826	32	1/1/15/20	14/39/115/115	-
19	CLA	A	844	23	1/1/15/20	8/39/115/115	-
19	CLA	3	207	15	1/1/15/20	18/39/115/115	-
19	CLA	B	837	-	1/1/15/20	15/39/115/115	-
22	BCR	A	848	-	-	11/29/63/63	0/2/2/2
19	CLA	B	836	32	1/1/15/20	5/39/115/115	-
31	A86	5	220	-	-	14/34/90/90	0/3/3/3
19	CLA	A	807	1	1/1/15/20	14/39/115/115	-
22	BCR	B	852	-	-	10/29/63/63	0/2/2/2
19	CLA	A	829	-	1/1/15/20	8/39/115/115	-
19	CLA	A	840	-	1/1/11/20	2/18/94/115	-
19	CLA	5	211	17	1/1/13/20	9/31/107/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	J	103	8	1/1/11/20	2/15/91/115	-
31	A86	4	316	-	-	8/34/90/90	0/3/3/3
30	KC1	4	302	-	-	6/15/71/71	-
19	CLA	B	824	-	1/1/15/20	5/39/115/115	-
19	CLA	2	215	-	1/1/10/20	0/12/88/115	-
19	CLA	5	210	17	1/1/15/20	12/39/115/115	-
31	A86	4	314	-	-	6/34/90/90	0/3/3/3
19	CLA	A	811	-	1/1/12/20	9/26/102/115	-
27	5X6	J	105	-	-	20/29/67/67	0/2/2/2
19	CLA	A	824	-	1/1/12/20	5/23/99/115	-
31	A86	3	228	-	-	9/34/90/90	0/3/3/3
19	CLA	A	839	-	1/1/15/20	8/39/115/115	-
22	BCR	F	205	-	-	3/29/63/63	0/2/2/2
19	CLA	B	813	-	1/1/15/20	20/39/115/115	-
19	CLA	4	308	-	-	4/15/91/115	-
19	CLA	4	301	16	1/1/15/20	15/39/115/115	-
19	CLA	A	836	-	1/1/12/20	5/26/102/115	-
19	CLA	A	838	-	1/1/12/20	2/23/99/115	-
24	LMT	3	216	-	-	8/21/61/61	0/2/2/2
19	CLA	A	812	19	1/1/15/20	13/39/115/115	-
19	CLA	4	306	23	1/1/13/20	11/31/107/115	-
19	CLA	B	815	-	1/1/11/20	4/15/91/115	-
19	CLA	B	832	32	1/1/15/20	12/39/115/115	-
19	CLA	4	312	16	1/1/12/20	5/24/100/115	-
19	CLA	A	806	-	1/1/15/20	14/39/115/115	-
23	LHG	4	317	19	-	33/53/53/53	-
19	CLA	B	807	-	1/1/15/20	12/39/115/115	-
19	CLA	2	206	-	1/1/15/20	10/39/115/115	-
28	DD6	5	218	-	-	9/26/80/80	0/3/3/3
23	LHG	A	853	19	-	26/53/53/53	-
19	CLA	A	813	-	1/1/13/20	7/27/103/115	-

The worst 5 of 3545 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	2	216	A86	C14-C13	15.80	1.68	1.51
31	1	316	A86	C14-C13	15.28	1.68	1.51
31	1	317	A86	C14-C13	15.21	1.68	1.51
31	5	217	A86	C14-C13	15.19	1.68	1.51
31	3	212	A86	C14-C13	15.18	1.68	1.51

The worst 5 of 5100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	5	220	A86	O1-C20-C19	41.65	152.53	113.49
31	5	221	A86	O1-C20-C19	40.82	151.75	113.49
31	1	317	A86	O1-C20-C19	39.92	150.91	113.49
31	4	314	A86	O1-C20-C19	39.85	150.84	113.49
31	1	316	A86	O1-C20-C19	39.81	150.80	113.49

5 of 129 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	A	801	CL0	ND
18	A	801	CL0	NA
18	A	801	CL0	NC
19	A	802	CLA	ND
19	A	803	CLA	ND

5 of 1796 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	804	CLA	CHA-CBD-CGD-O1D
19	A	804	CLA	CHA-CBD-CGD-O2D
19	A	805	CLA	C3A-C2A-CAA-CBA
19	A	806	CLA	C1A-C2A-CAA-CBA
19	A	806	CLA	C3A-C2A-CAA-CBA

There are no ring outliers.

176 monomers are involved in 465 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	1	323	LMT	4	0
23	M	103	LHG	3	0
19	1	309	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	809	CLA	1	0
22	M	102	BCR	3	0
22	A	849	BCR	1	0
19	A	837	CLA	2	0
19	A	833	CLA	5	0
22	A	850	BCR	1	0
19	B	802	CLA	2	0
19	L	204	CLA	2	0
19	u	202	CLA	1	0
19	A	818	CLA	4	0
19	L	206	CLA	5	0
19	2	207	CLA	4	0
22	B	844	BCR	6	0
19	A	809	CLA	3	0
19	B	816	CLA	3	0
19	1	303	CLA	3	0
30	3	211	KC1	1	0
23	1	318	LHG	5	0
19	B	803	CLA	8	0
19	5	208	CLA	2	0
22	A	847	BCR	3	0
19	4	313	CLA	1	0
20	B	839	PQN	2	0
19	A	830	CLA	1	0
19	4	303	CLA	5	0
19	B	808	CLA	7	0
19	5	209	CLA	3	0
19	A	815	CLA	1	0
19	A	819	CLA	4	0
19	A	827	CLA	2	0
19	4	311	CLA	2	0
19	B	806	CLA	2	0
19	2	205	CLA	10	0
19	5	214	CLA	2	0
19	B	829	CLA	5	0
19	B	812	CLA	5	0
19	A	820	CLA	5	0
22	B	841	BCR	2	0
19	3	204	CLA	4	0
19	B	820	CLA	1	0
19	2	213	CLA	3	0
18	A	801	CL0	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	841	CLA	8	0
19	B	826	CLA	3	0
19	A	831	CLA	2	0
22	1	311	BCR	4	0
19	2	214	CLA	1	0
19	4	305	CLA	1	0
19	A	835	CLA	2	0
24	2	220	LMT	1	0
19	3	206	CLA	12	0
19	A	821	CLA	7	0
22	L	202	BCR	1	0
19	F	203	CLA	2	0
19	A	878	CLA	9	0
19	A	843	CLA	3	0
19	2	208	CLA	2	0
31	1	317	A86	1	0
20	A	845	PQN	1	0
19	1	307	CLA	2	0
19	A	842	CLA	2	0
19	4	309	CLA	3	0
19	B	804	CLA	8	0
19	B	828	CLA	2	0
23	3	215	LHG	2	0
19	A	823	CLA	2	0
19	A	834	CLA	7	0
19	1	304	CLA	1	0
26	B	847	DGD	9	0
19	2	212	CLA	1	0
19	A	828	CLA	5	0
19	4	310	CLA	3	0
19	5	212	CLA	4	0
19	A	817	CLA	5	0
19	2	210	CLA	6	0
19	3	203	CLA	3	0
19	A	808	CLA	3	0
19	A	832	CLA	1	0
19	B	818	CLA	2	0
19	B	834	CLA	1	0
22	B	840	BCR	4	0
19	B	831	CLA	2	0
22	J	104	BCR	3	0
19	B	830	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	804	CLA	7	0
31	1	316	A86	1	0
23	B	842	LHG	2	0
31	2	216	A86	1	0
19	A	814	CLA	5	0
19	A	805	CLA	2	0
22	A	851	BCR	4	0
19	B	825	CLA	3	0
19	3	209	CLA	2	0
19	1	308	CLA	3	0
22	F	201	BCR	4	0
31	4	315	A86	2	0
19	B	817	CLA	2	0
19	A	802	CLA	5	0
19	B	814	CLA	2	0
19	L	203	CLA	2	0
31	5	217	A86	1	0
19	B	846	CLA	1	0
19	A	880	CLA	5	0
22	L	205	BCR	4	0
19	1	306	CLA	5	0
19	B	822	CLA	3	0
19	B	823	CLA	2	0
22	B	843	BCR	3	0
19	A	825	CLA	1	0
19	3	210	CLA	2	0
19	B	811	CLA	6	0
23	A	852	LHG	3	0
19	B	810	CLA	3	0
19	5	207	CLA	1	0
19	3	202	CLA	2	0
19	B	821	CLA	4	0
19	B	805	CLA	3	0
22	I	102	BCR	7	0
22	1	314	BCR	3	0
19	A	810	CLA	4	0
19	1	310	CLA	6	0
19	A	822	CLA	5	0
31	5	219	A86	1	0
19	B	845	CLA	5	0
19	u	201	CLA	4	0
19	A	816	CLA	1	0

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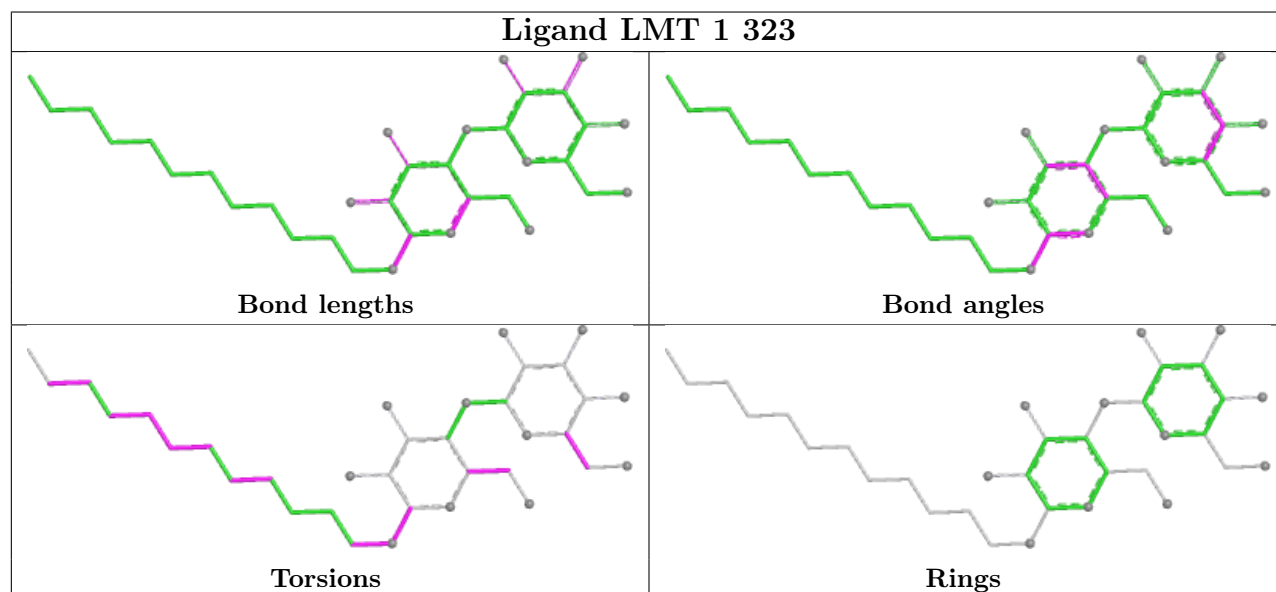
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	838	CLA	6	0
19	4	304	CLA	1	0
19	A	803	CLA	5	0
22	I	101	BCR	1	0
19	B	833	CLA	4	0
19	B	835	CLA	2	0
19	B	819	CLA	4	0
19	F	204	CLA	1	0
19	1	301	CLA	1	0
19	A	826	CLA	8	0
19	A	844	CLA	4	0
19	3	207	CLA	2	0
19	B	837	CLA	6	0
22	A	848	BCR	2	0
19	B	836	CLA	3	0
31	5	220	A86	1	0
19	A	807	CLA	3	0
22	B	852	BCR	1	0
19	A	829	CLA	3	0
19	A	840	CLA	2	0
19	5	211	CLA	1	0
19	J	103	CLA	3	0
31	4	316	A86	3	0
19	B	824	CLA	1	0
19	2	215	CLA	2	0
19	5	210	CLA	5	0
19	A	811	CLA	2	0
19	A	824	CLA	3	0
31	3	228	A86	1	0
19	A	839	CLA	4	0
22	F	205	BCR	2	0
19	B	813	CLA	5	0
19	4	308	CLA	4	0
19	4	301	CLA	7	0
19	A	836	CLA	5	0
24	3	216	LMT	1	0
19	A	812	CLA	1	0
19	4	306	CLA	3	0
19	B	815	CLA	4	0
19	B	832	CLA	4	0
19	4	312	CLA	1	0
19	A	806	CLA	7	0

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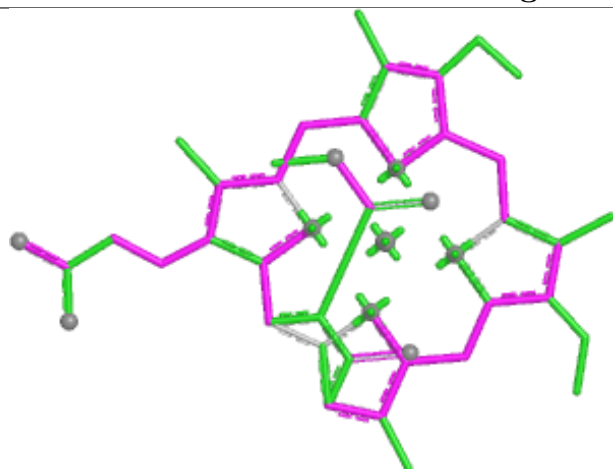
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	4	317	LHG	6	0
19	B	807	CLA	6	0
19	2	206	CLA	8	0
23	A	853	LHG	7	0
19	A	813	CLA	2	0

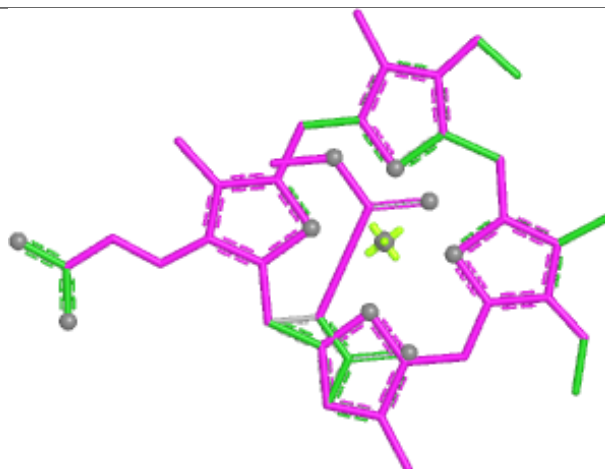
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



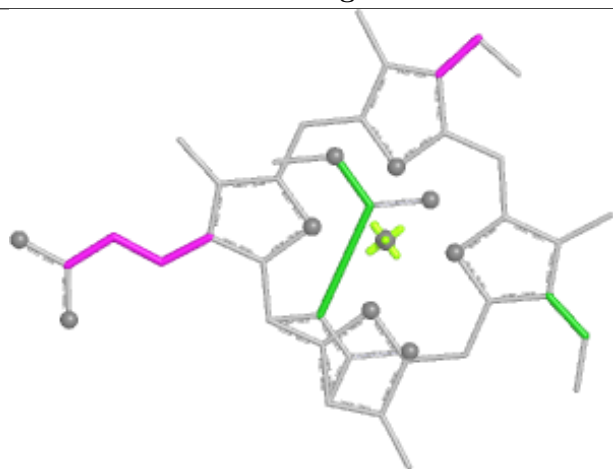
Ligand KC1 4 307



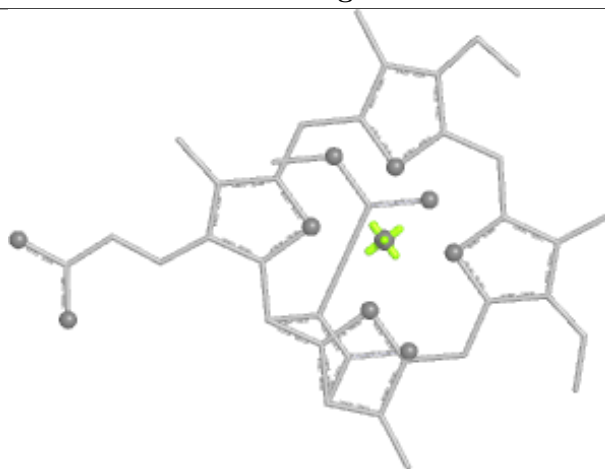
Bond lengths



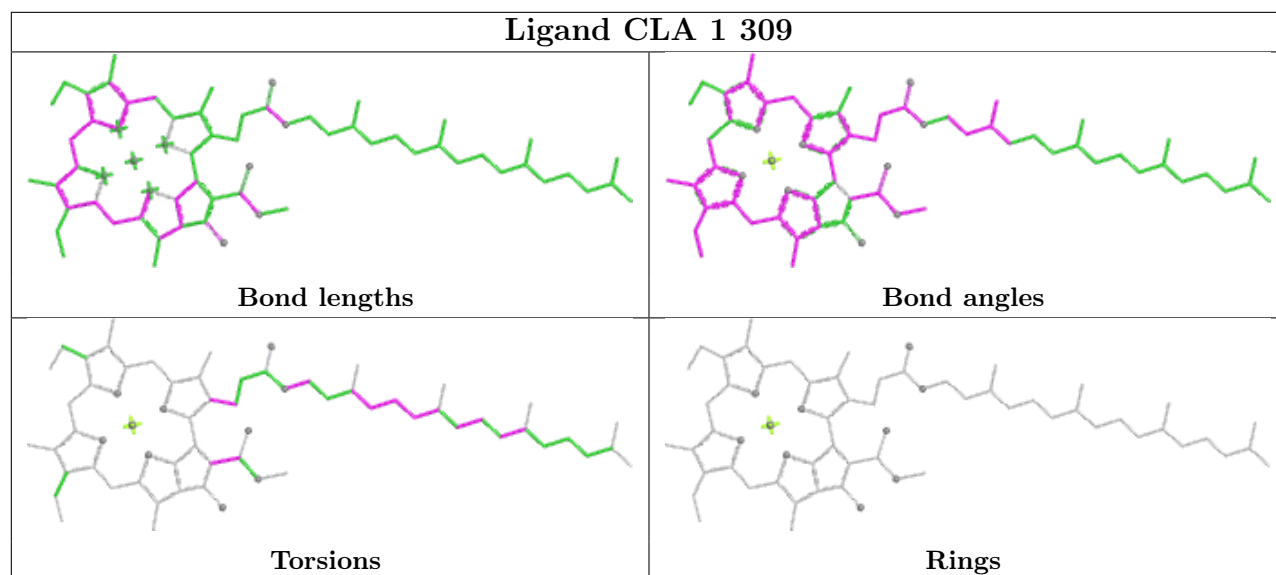
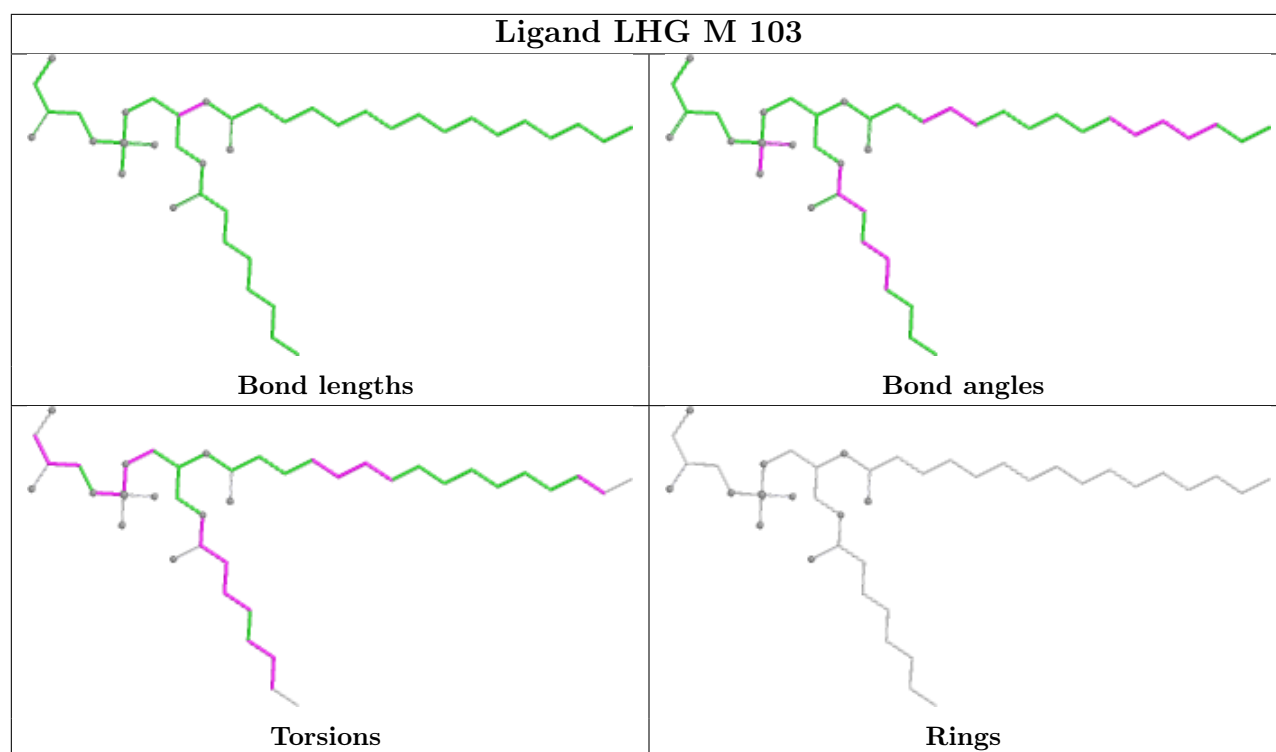
Bond angles

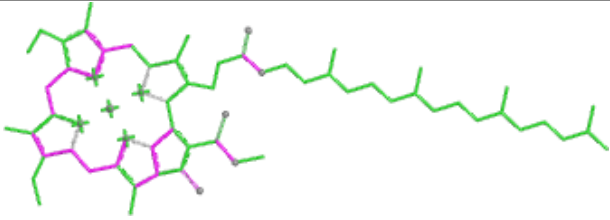
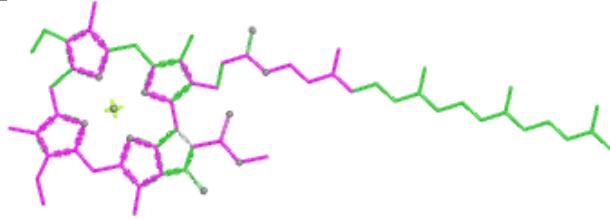
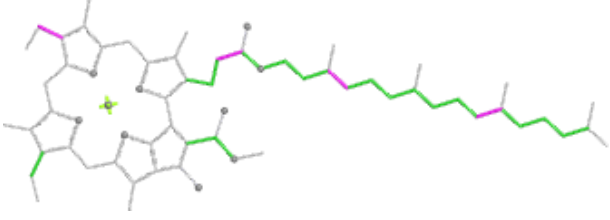
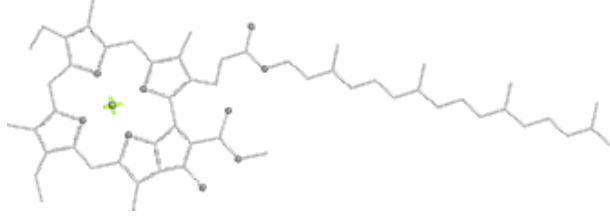
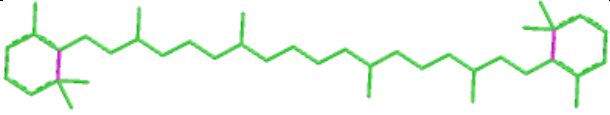
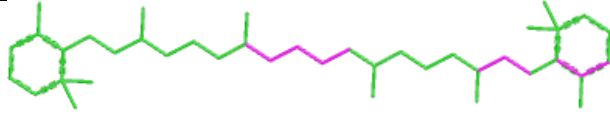
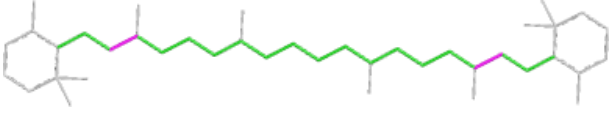
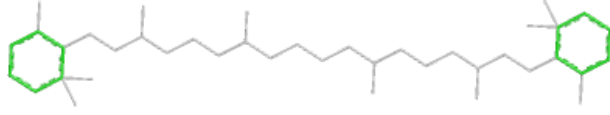
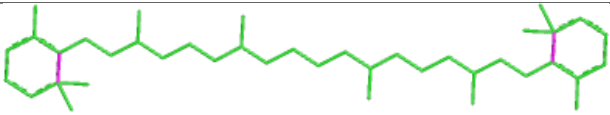
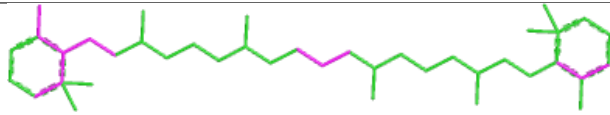
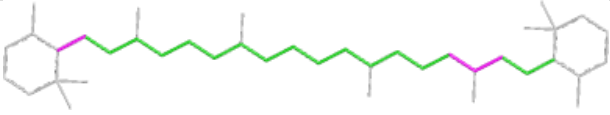
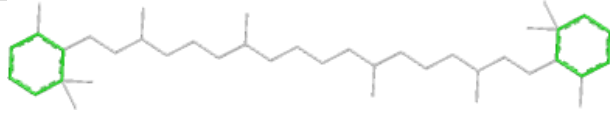


Torsions

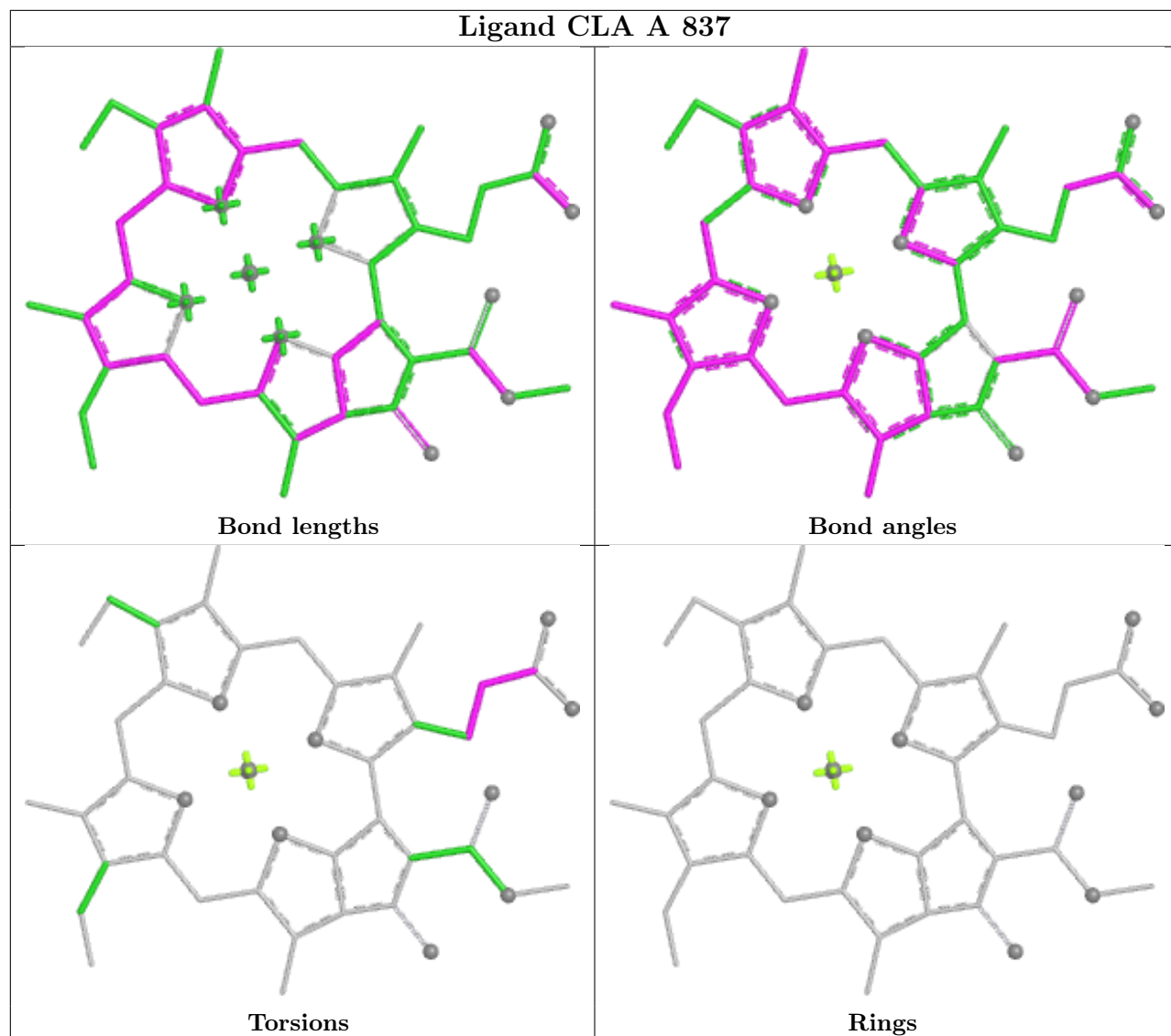


Rings

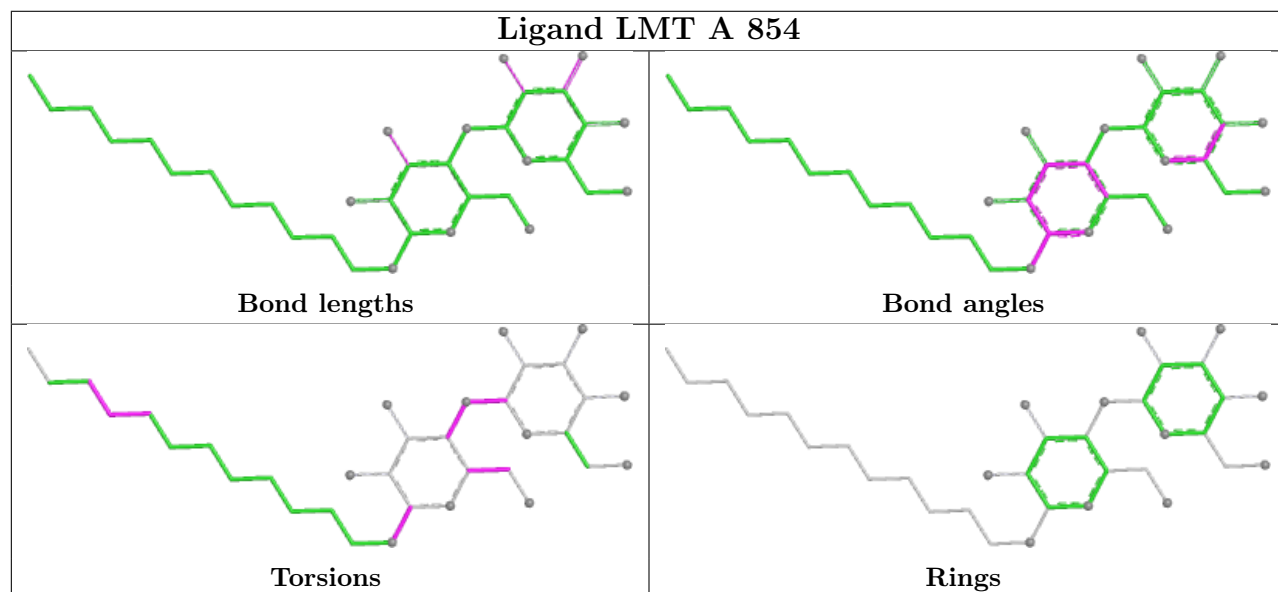


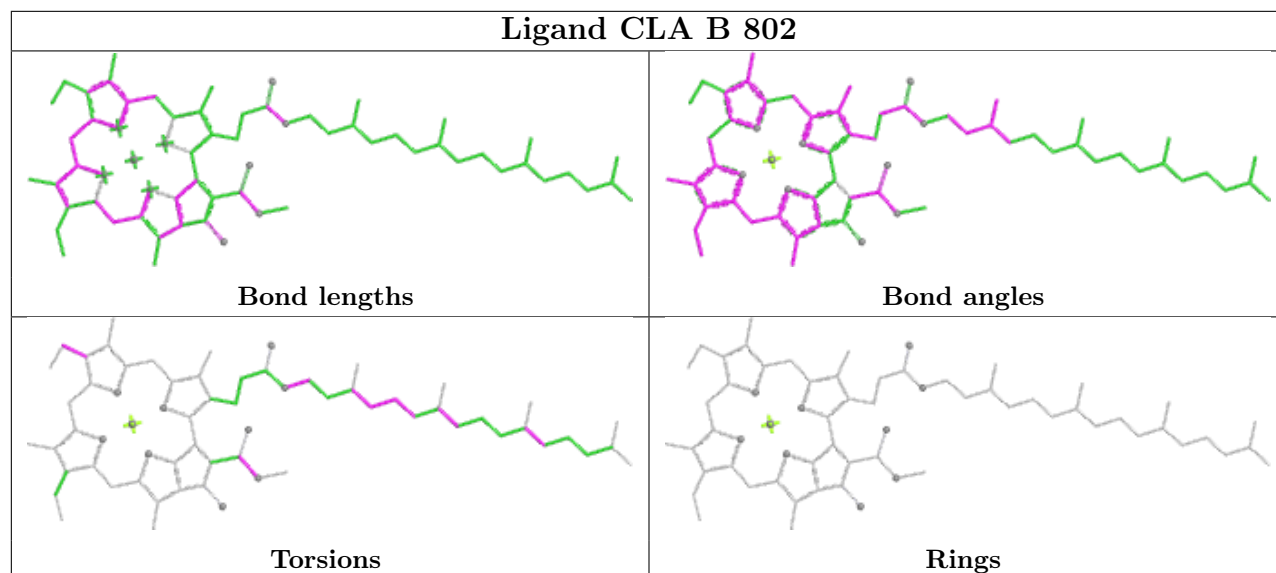
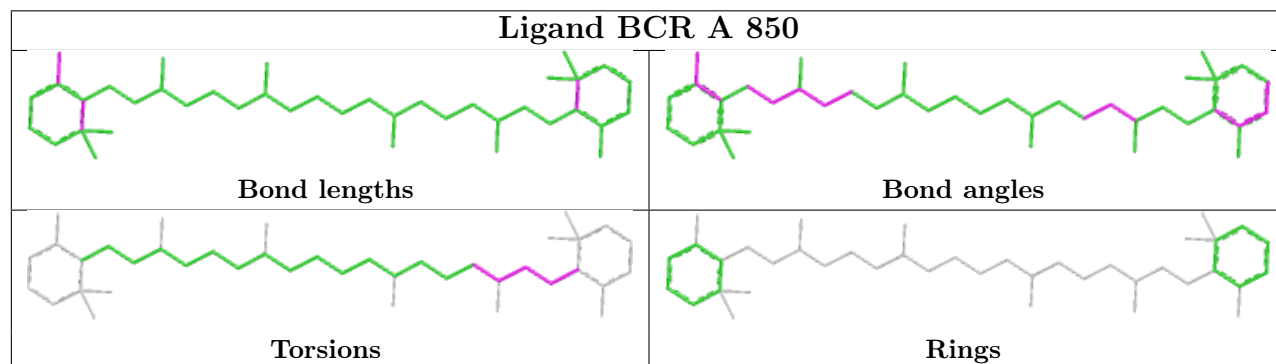
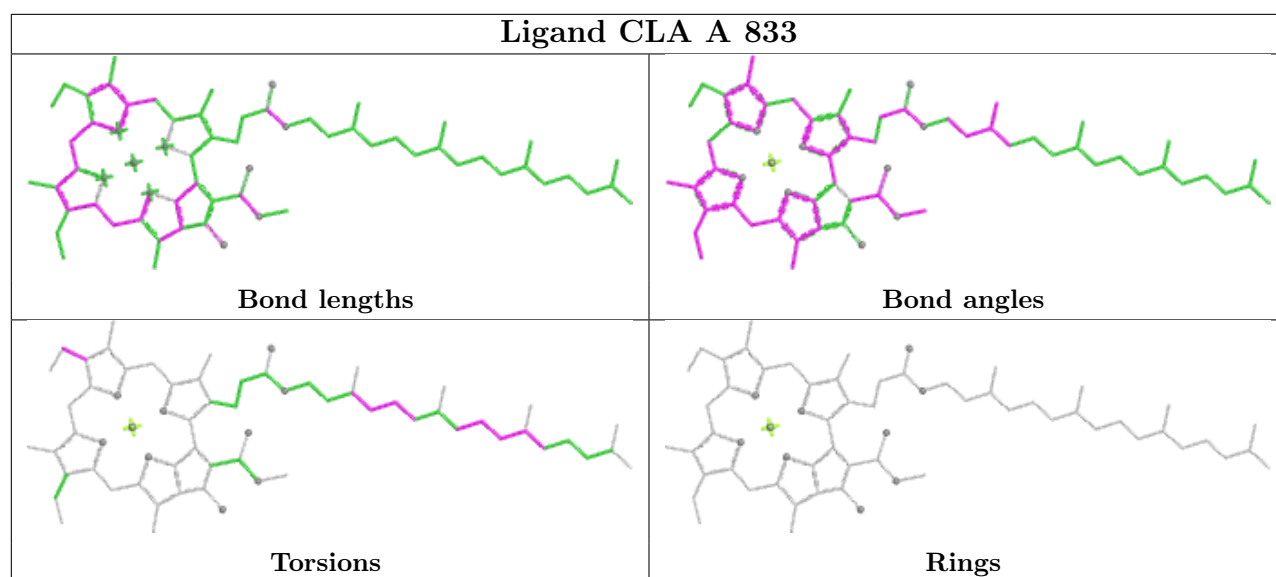
Ligand CLA B 809	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR M 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR A 849	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 837

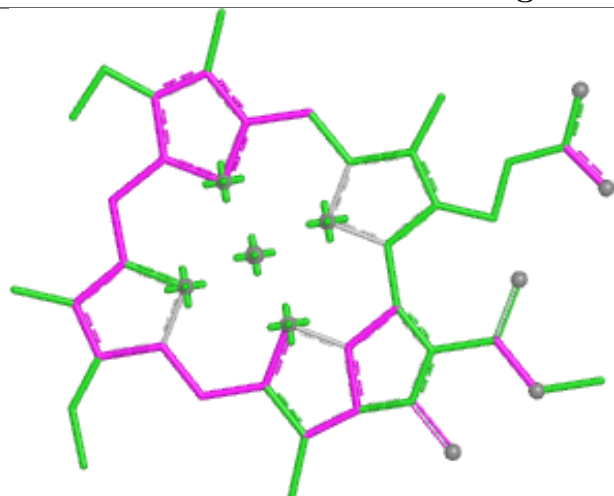


Ligand LMT A 854

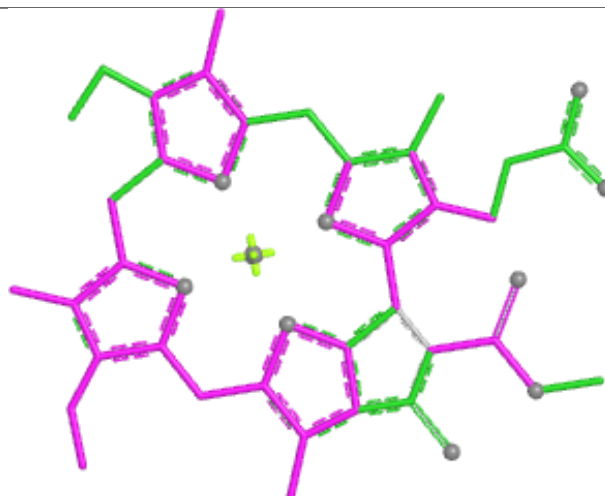




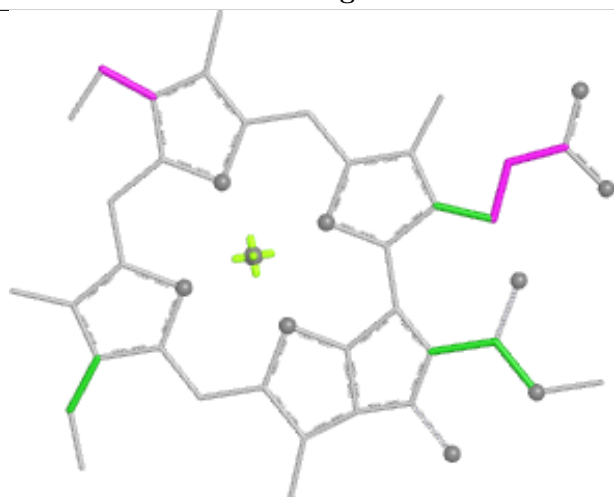
Ligand CLA L 204



Bond lengths



Bond angles

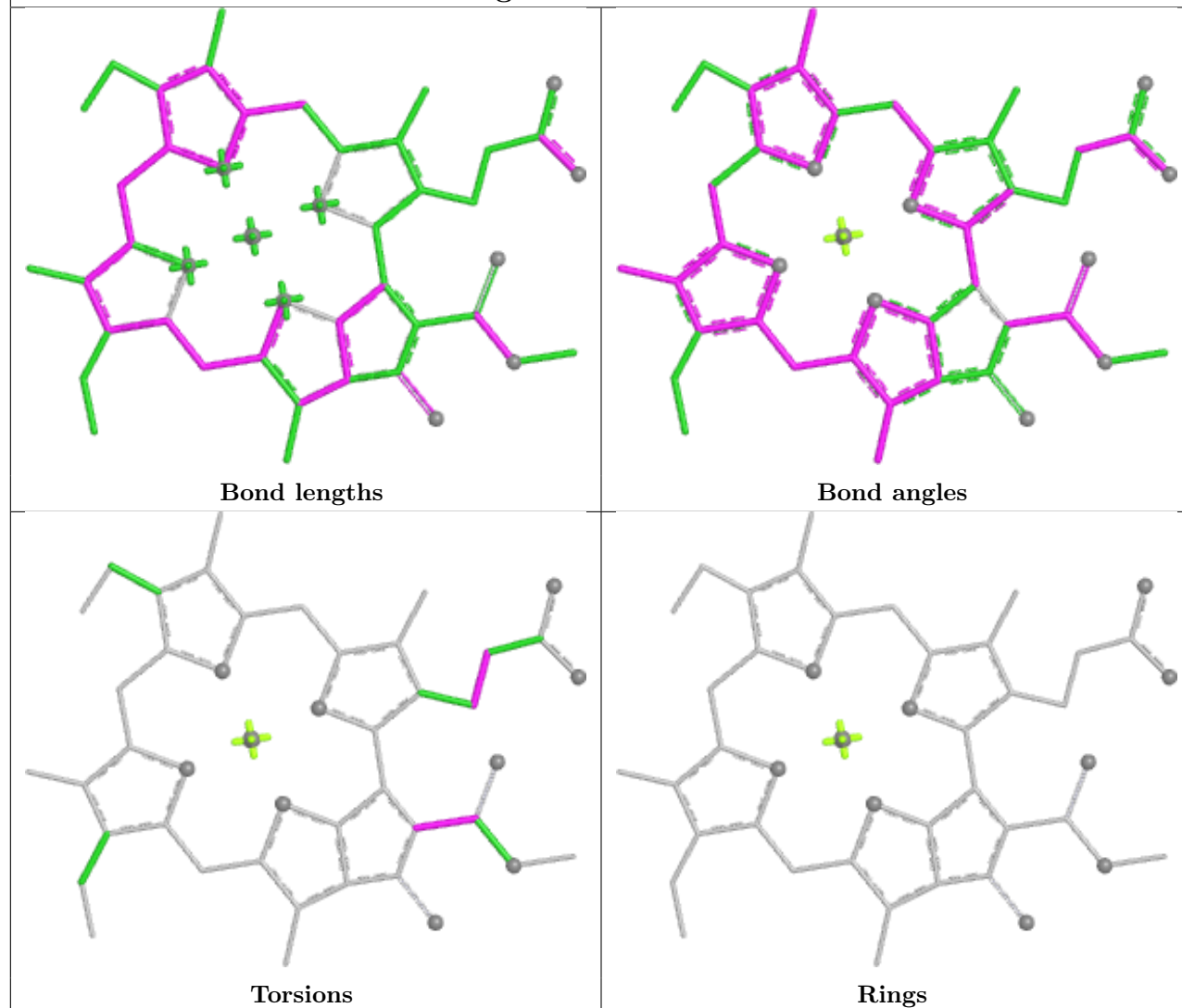


Torsions

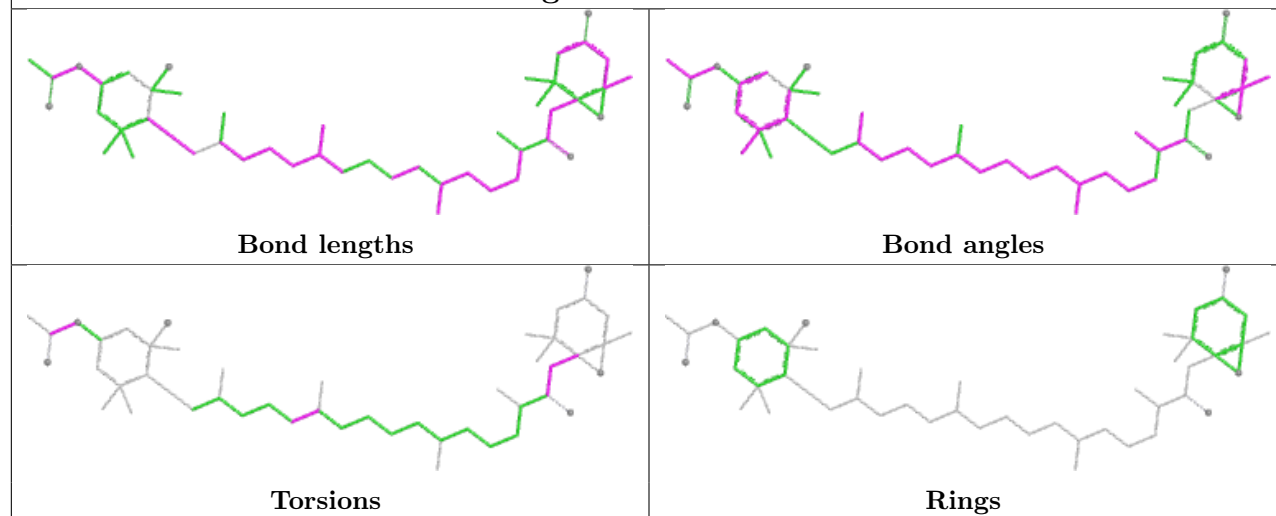


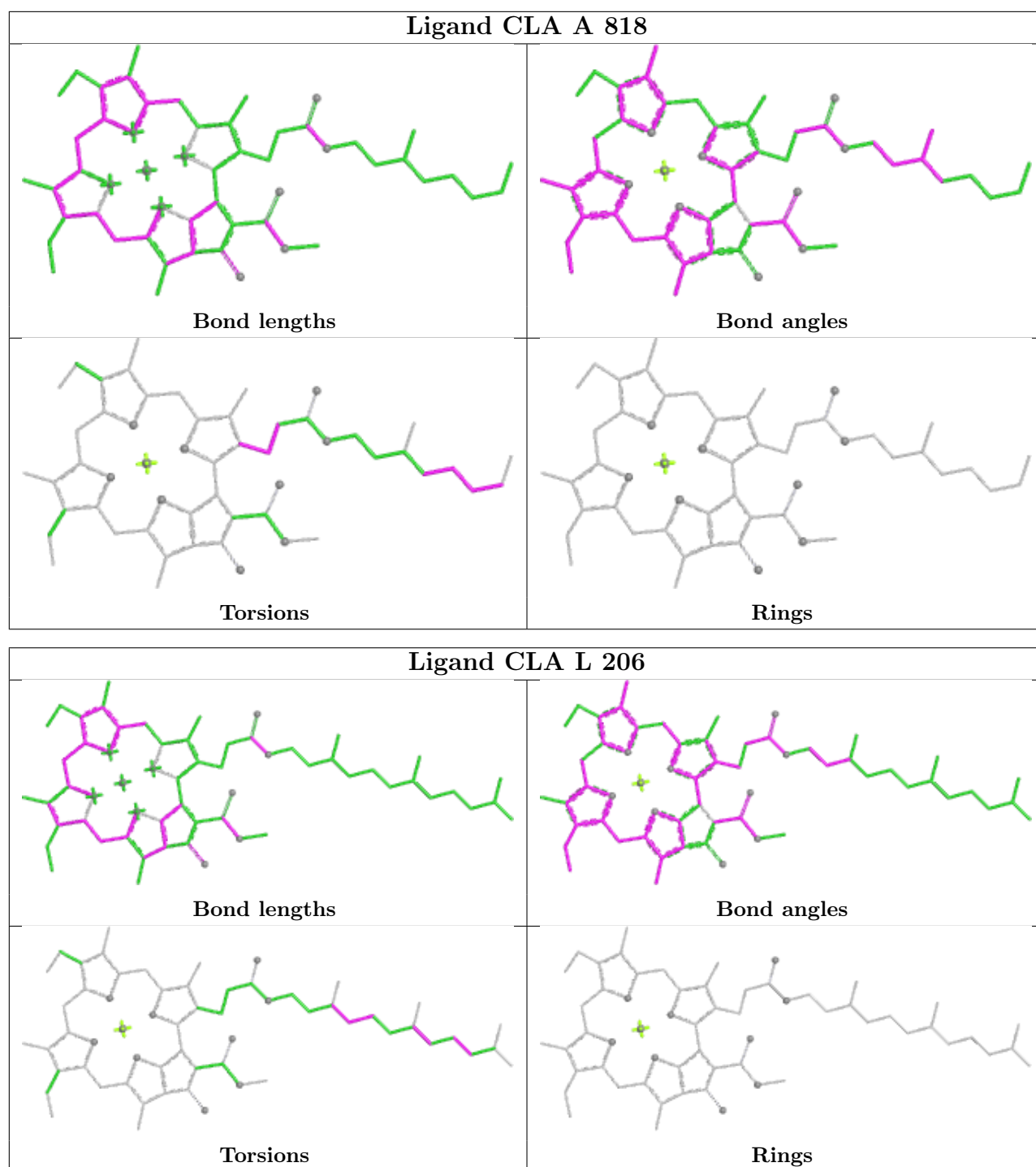
Rings

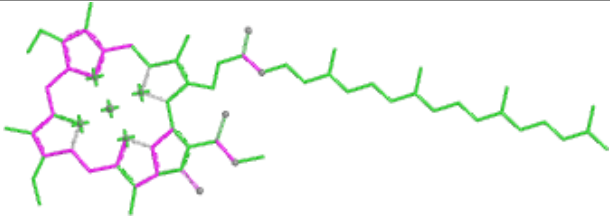
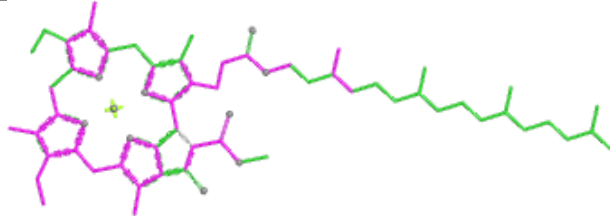
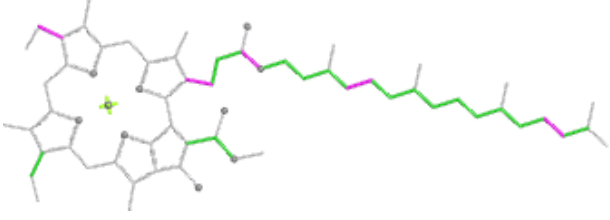
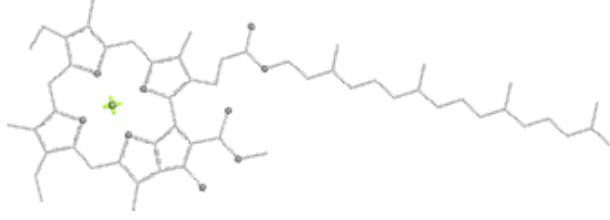
Ligand CLA u 202

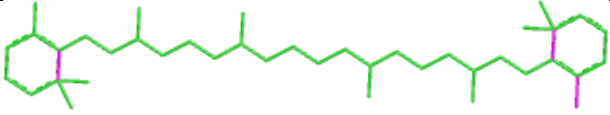
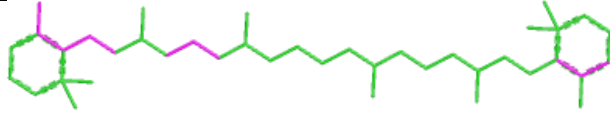
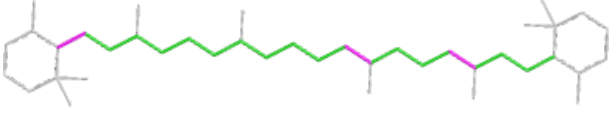
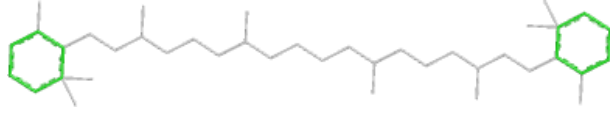


Ligand A86 2 219

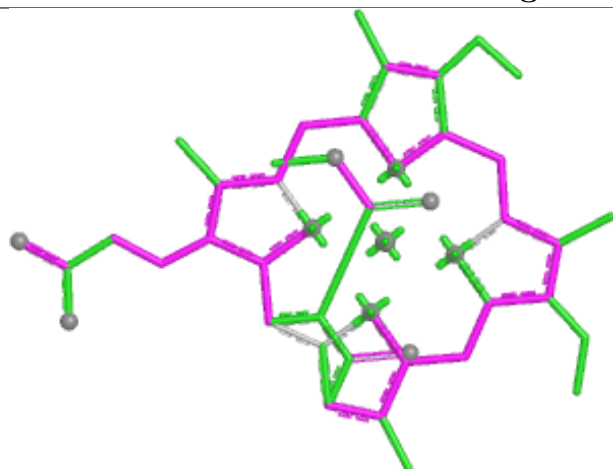




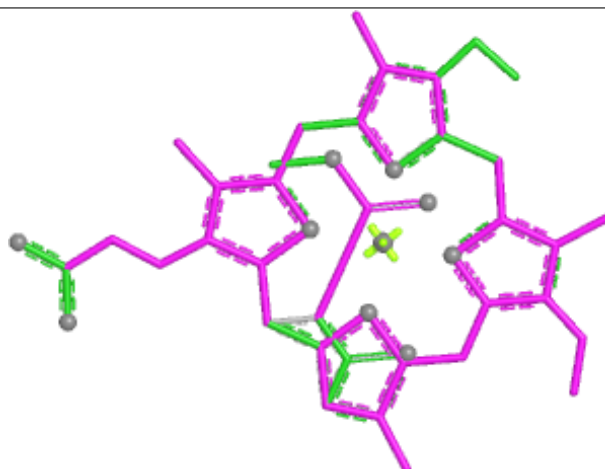
Ligand CLA 2 207			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

Ligand BCR B 844			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

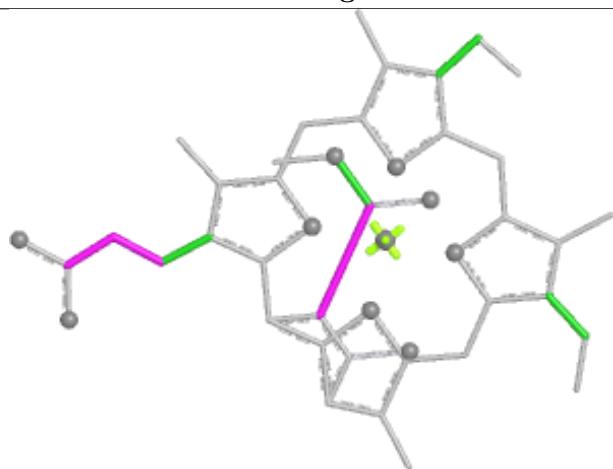
Ligand KC1 1 305



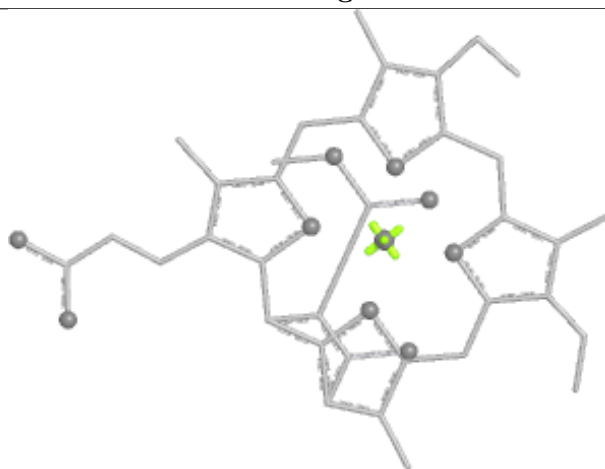
Bond lengths



Bond angles

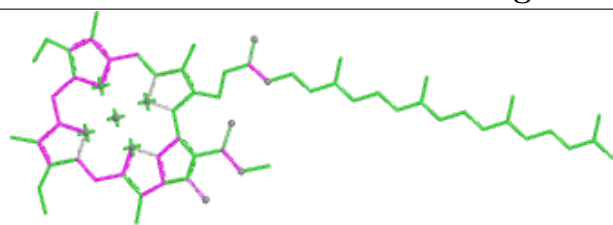


Torsions

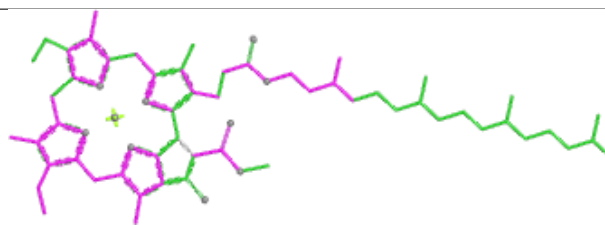


Rings

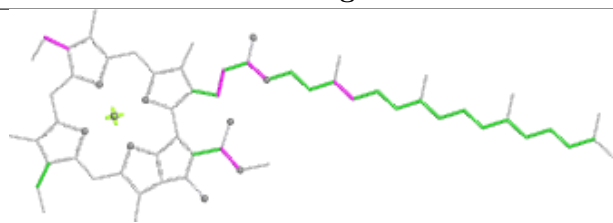
Ligand CLA A 809



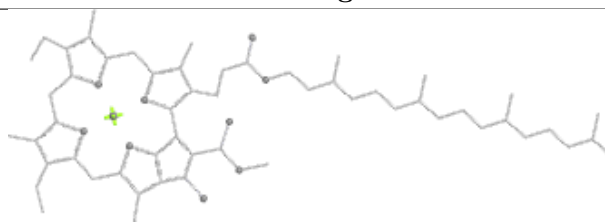
Bond lengths



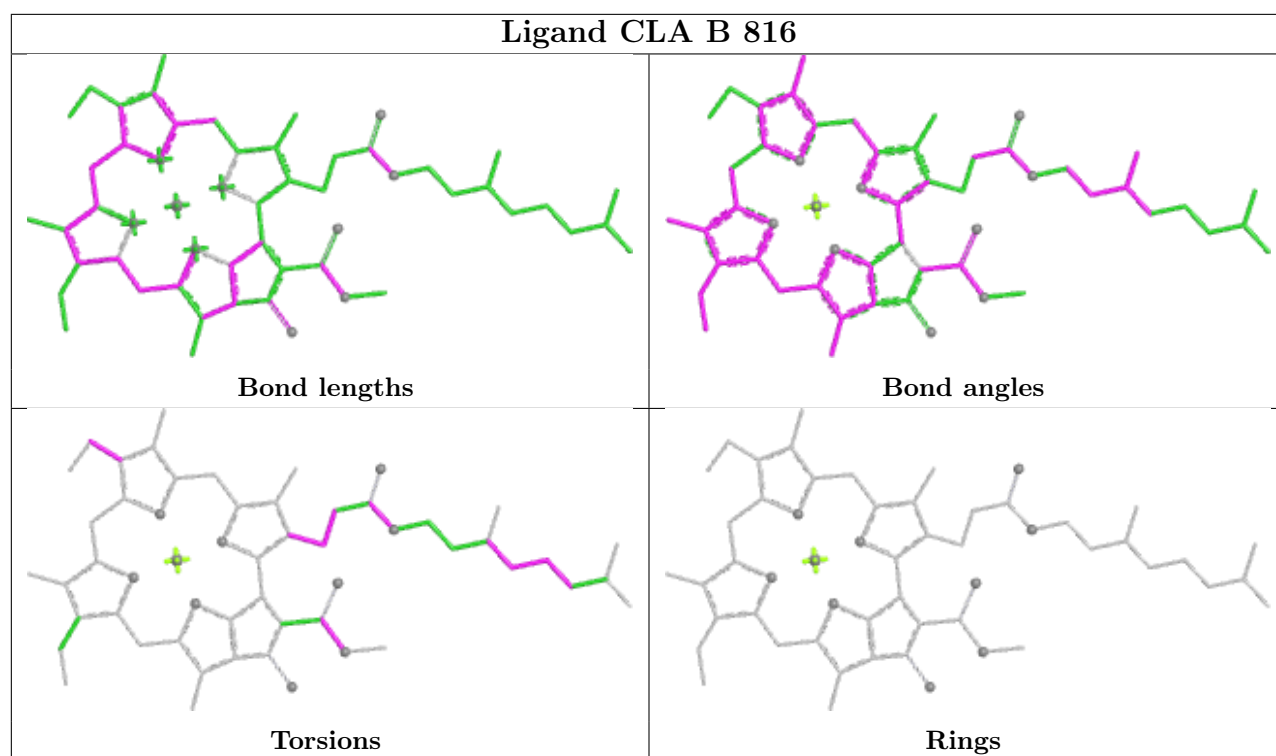
Bond angles



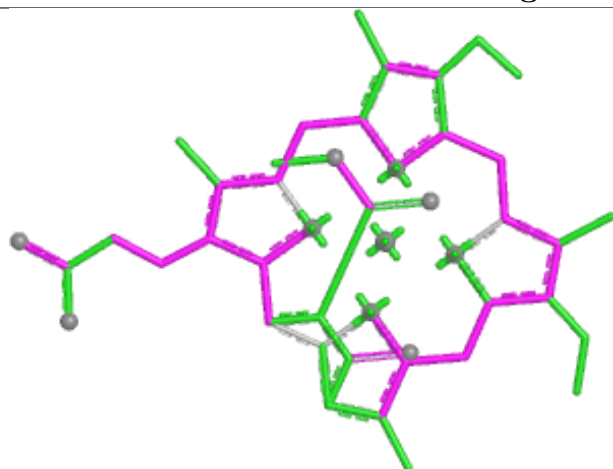
Torsions



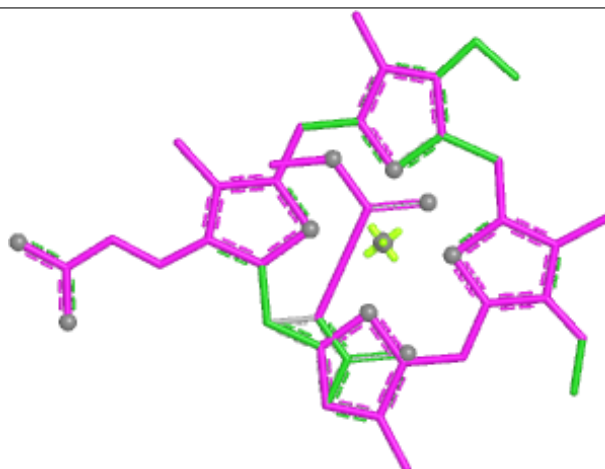
Rings



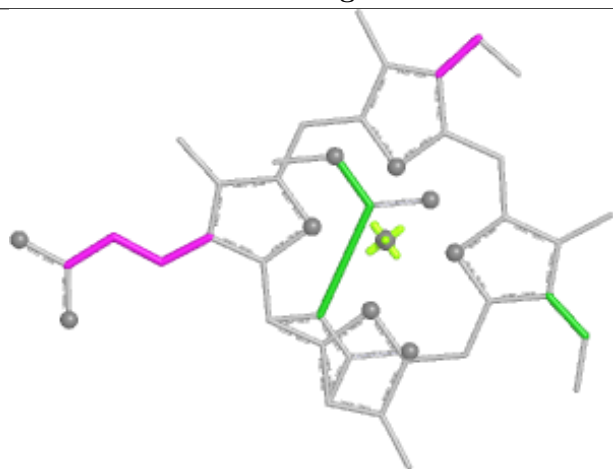
Ligand KC1 3 205



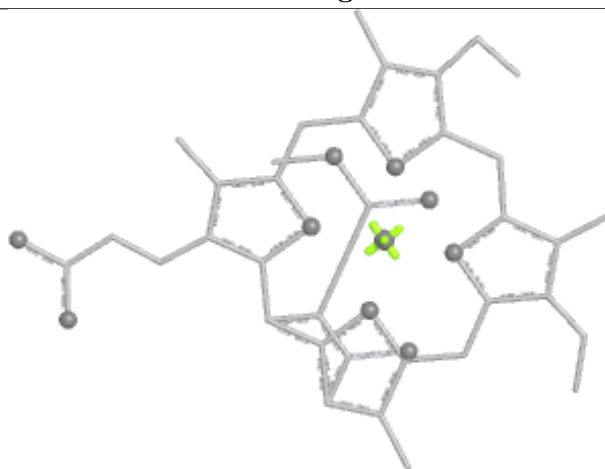
Bond lengths



Bond angles

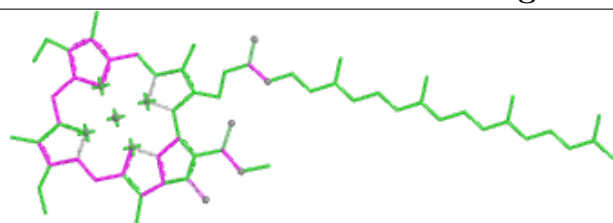


Torsions

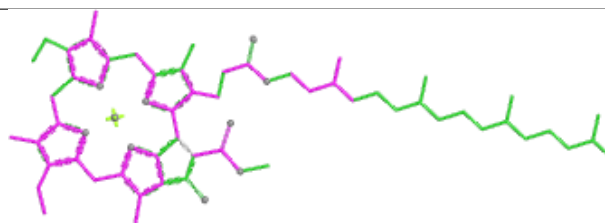


Rings

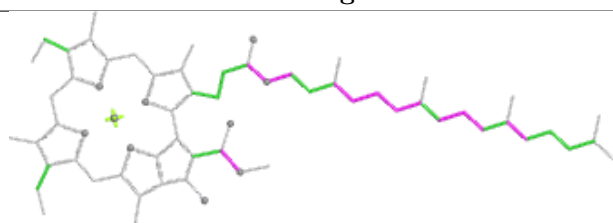
Ligand CLA 1 303



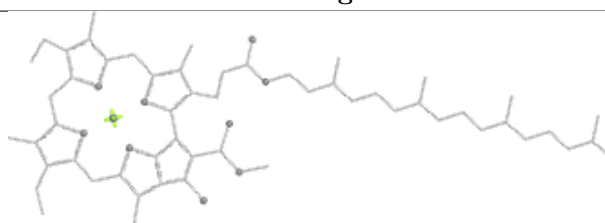
Bond lengths



Bond angles

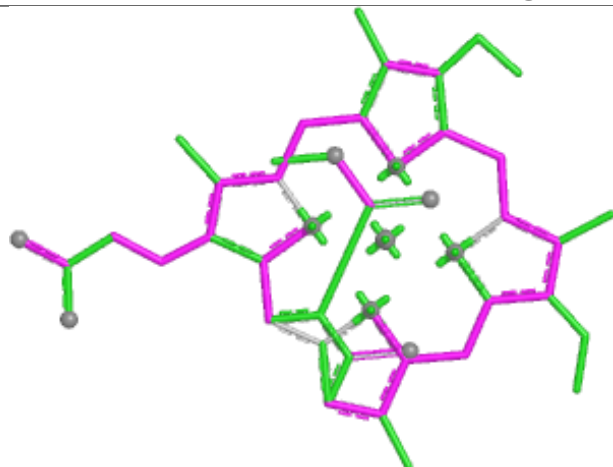


Torsions

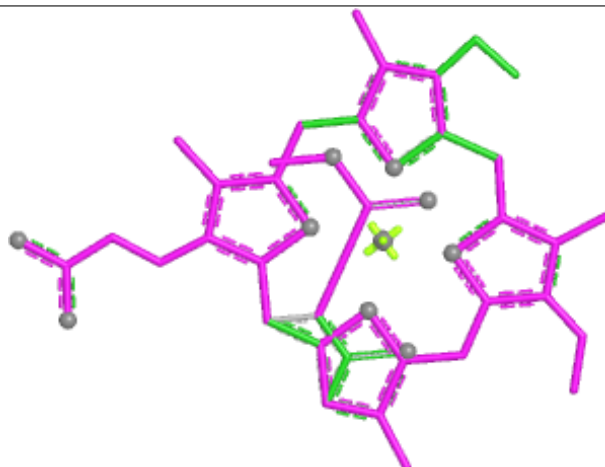


Rings

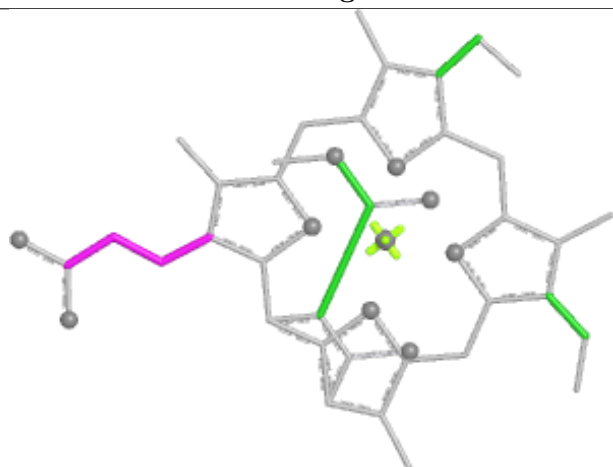
Ligand KC1 3 211



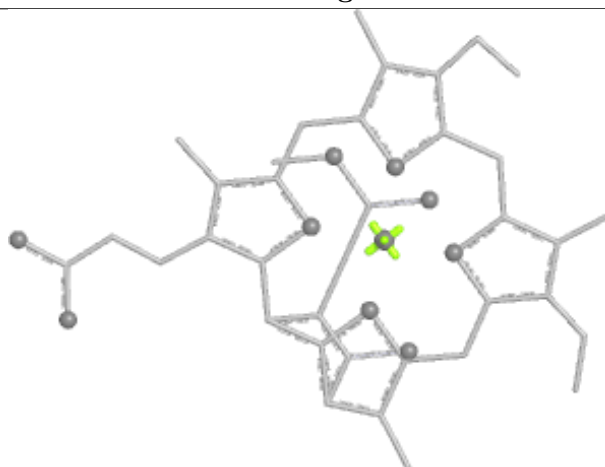
Bond lengths



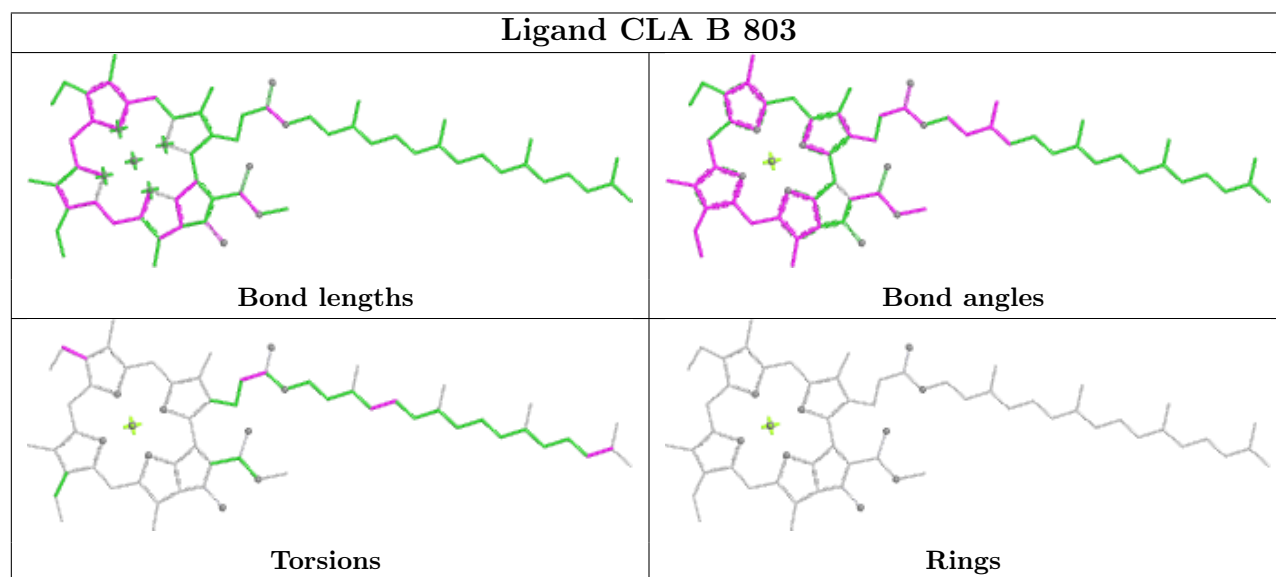
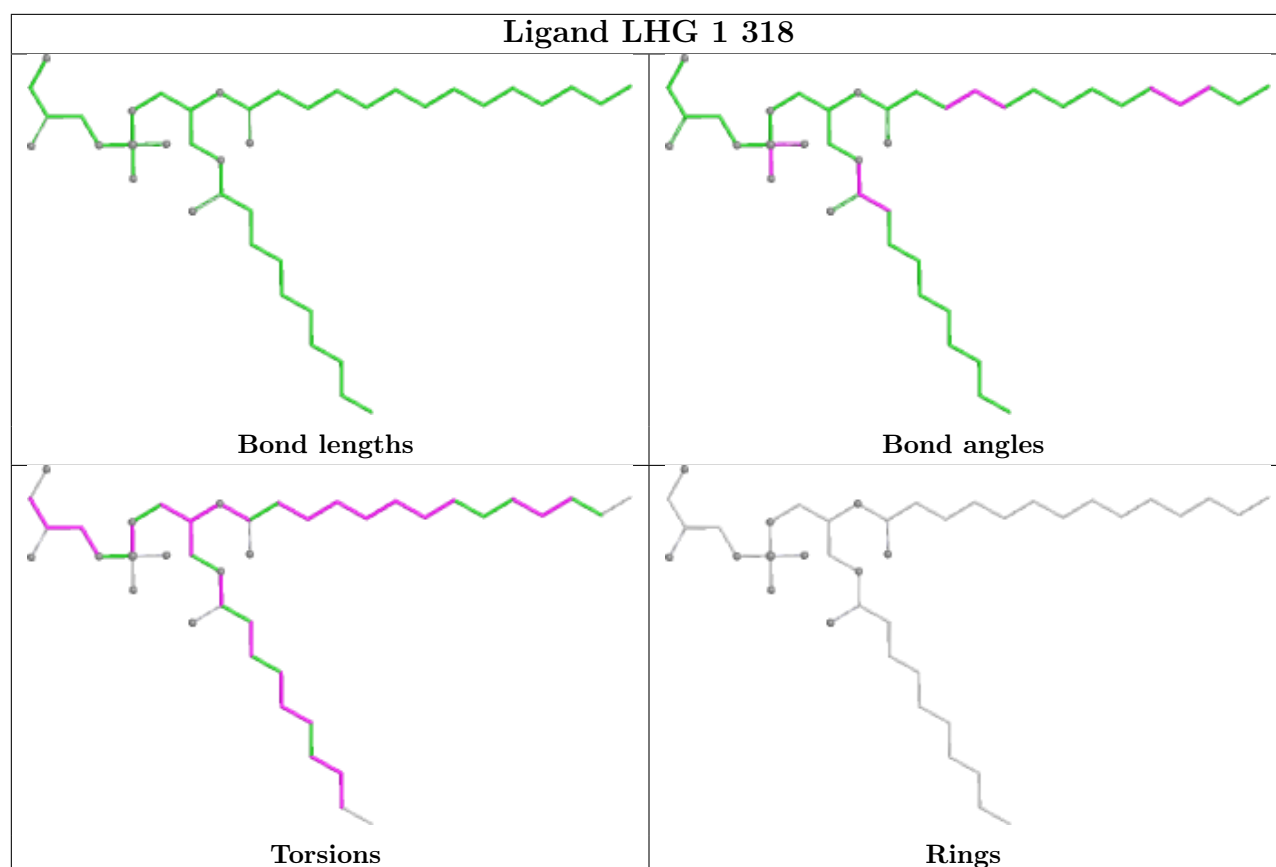
Bond angles

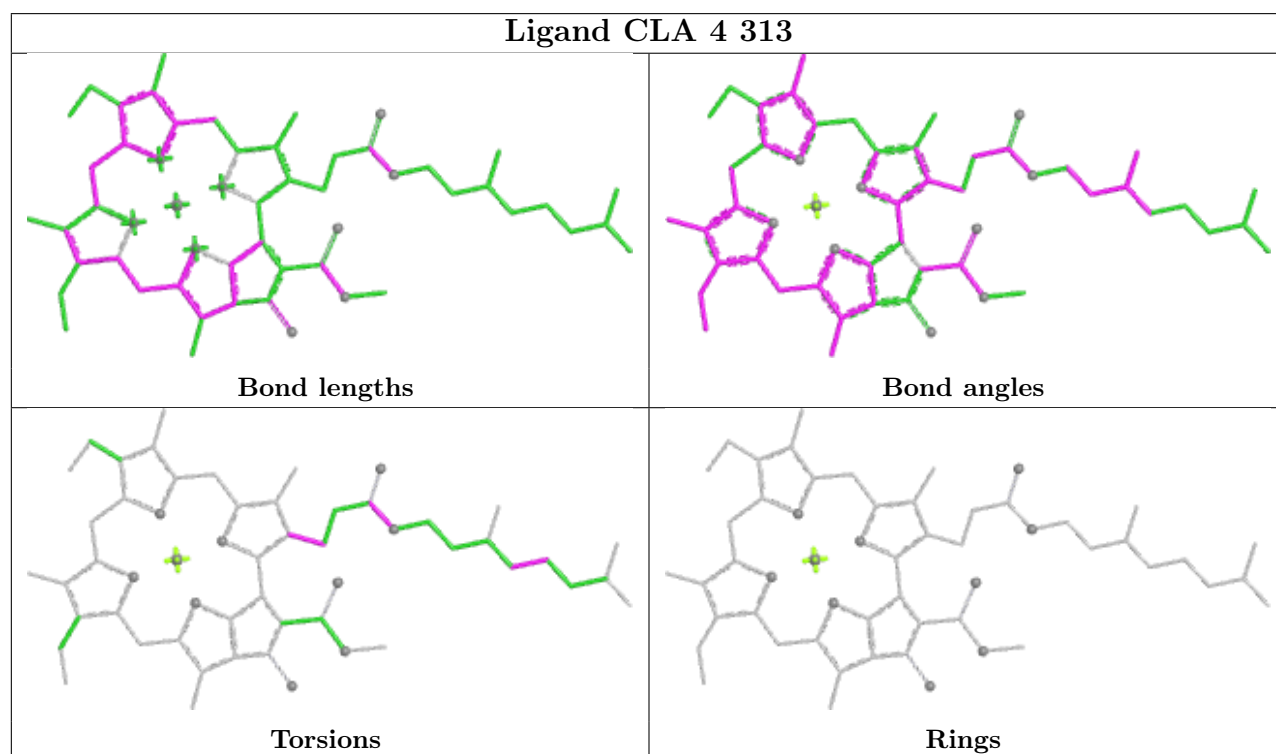
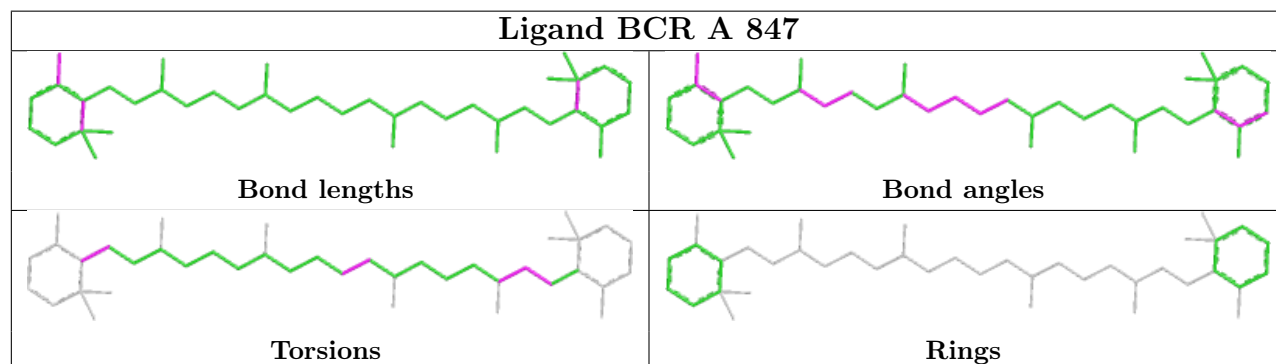
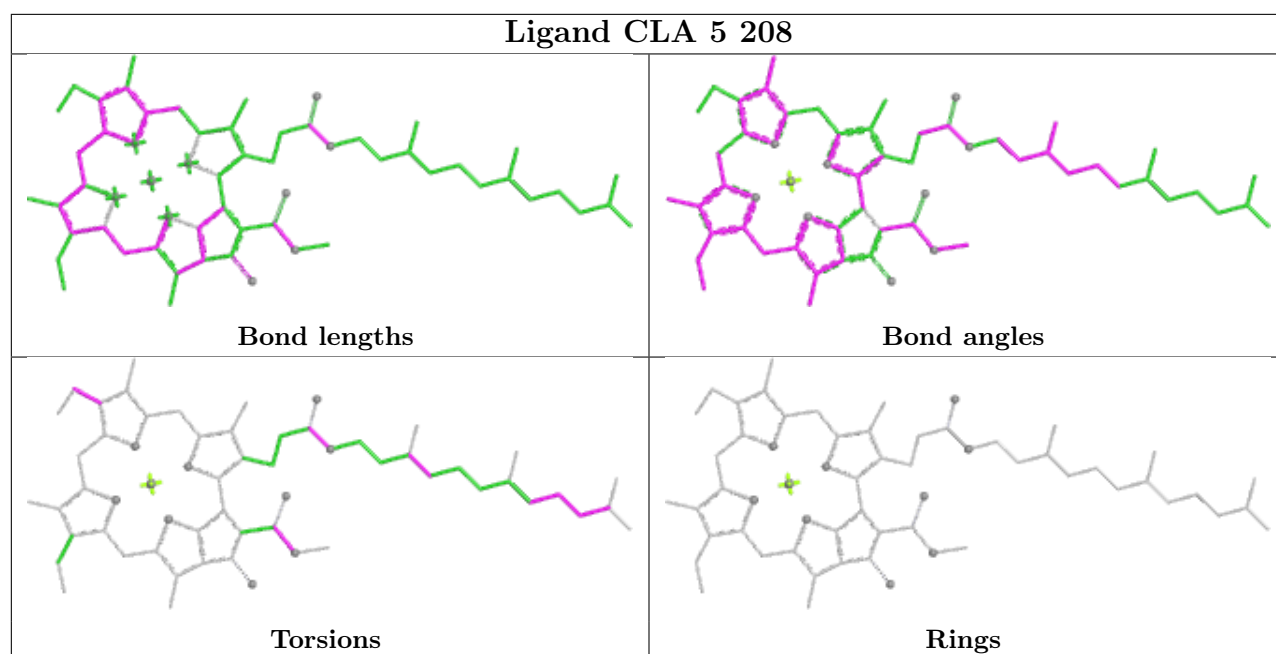


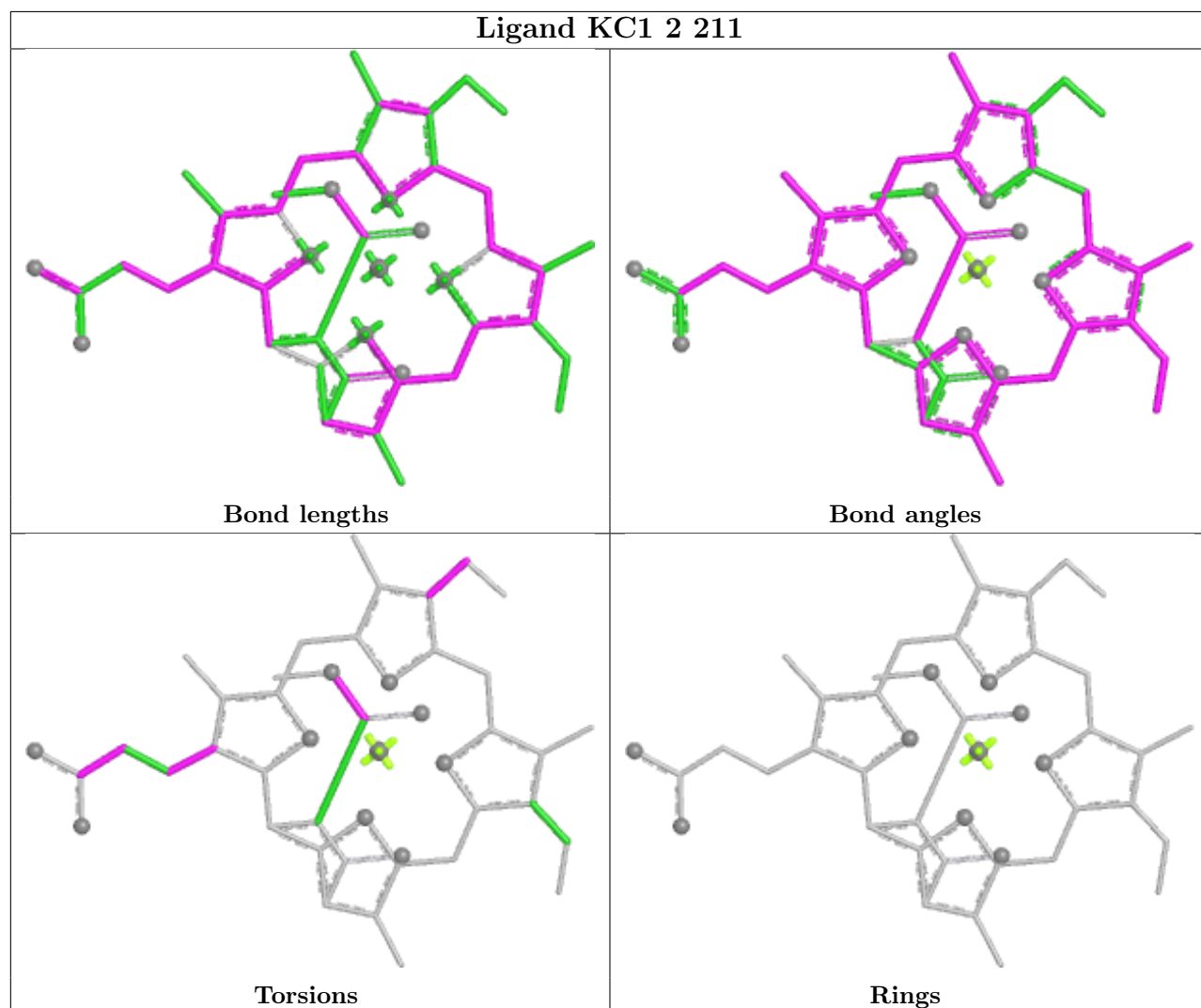
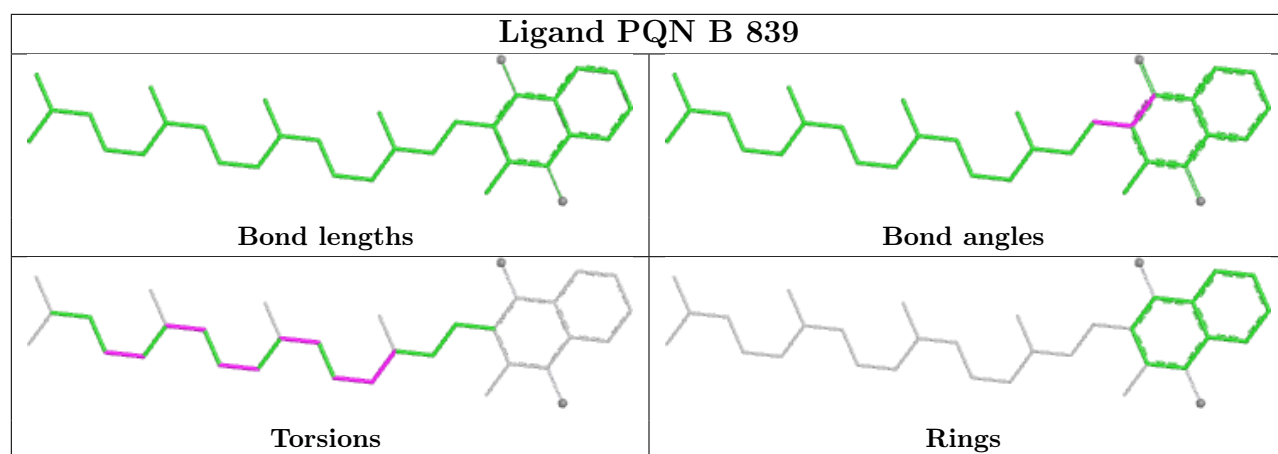
Torsions

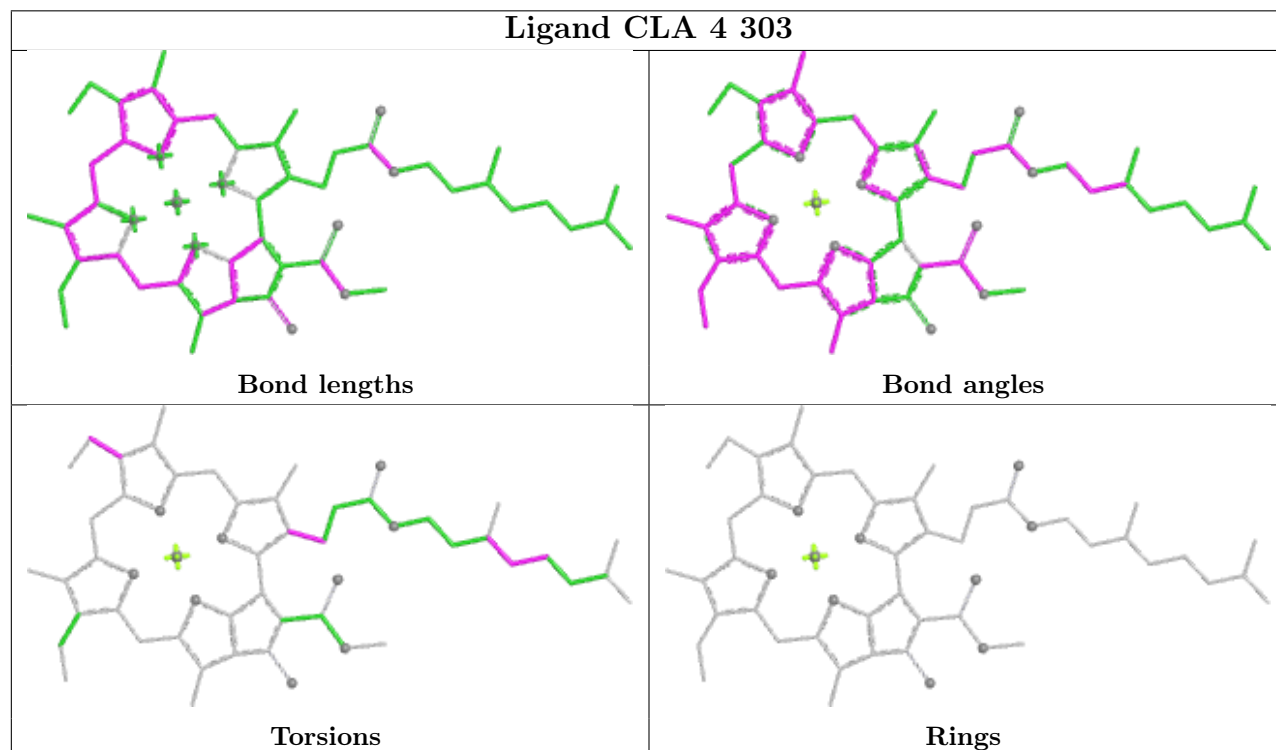
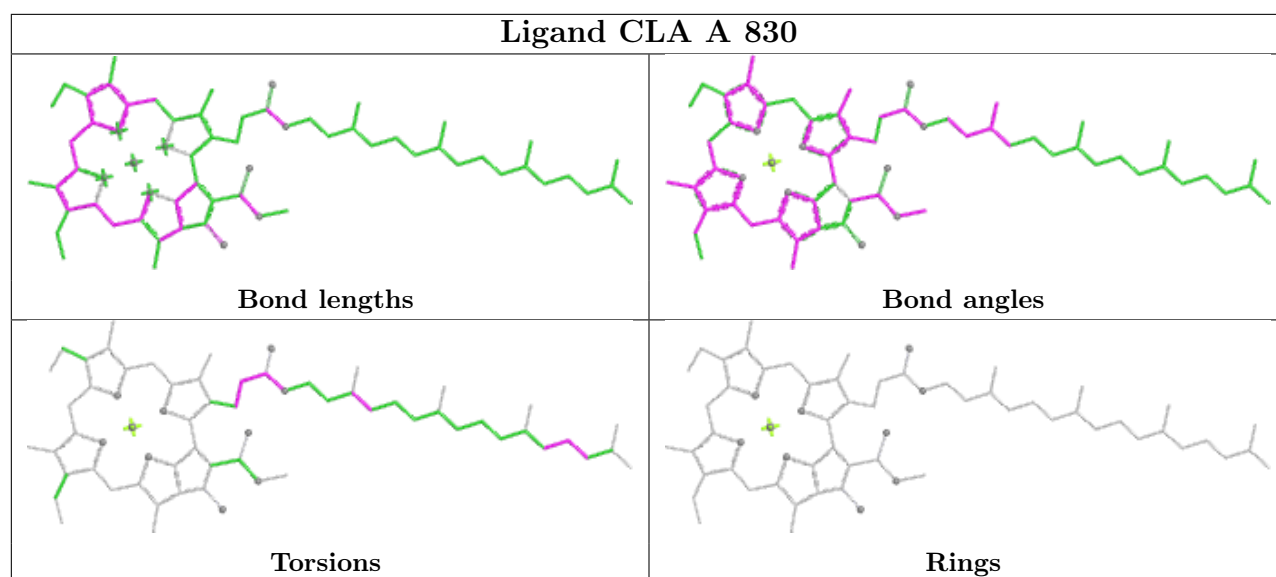


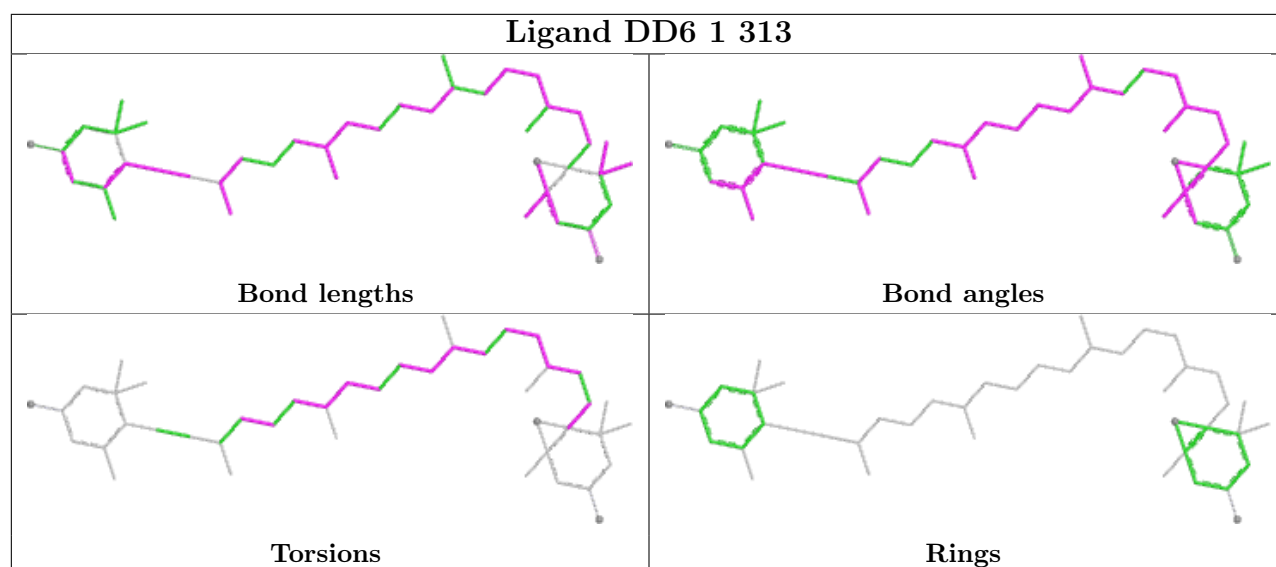
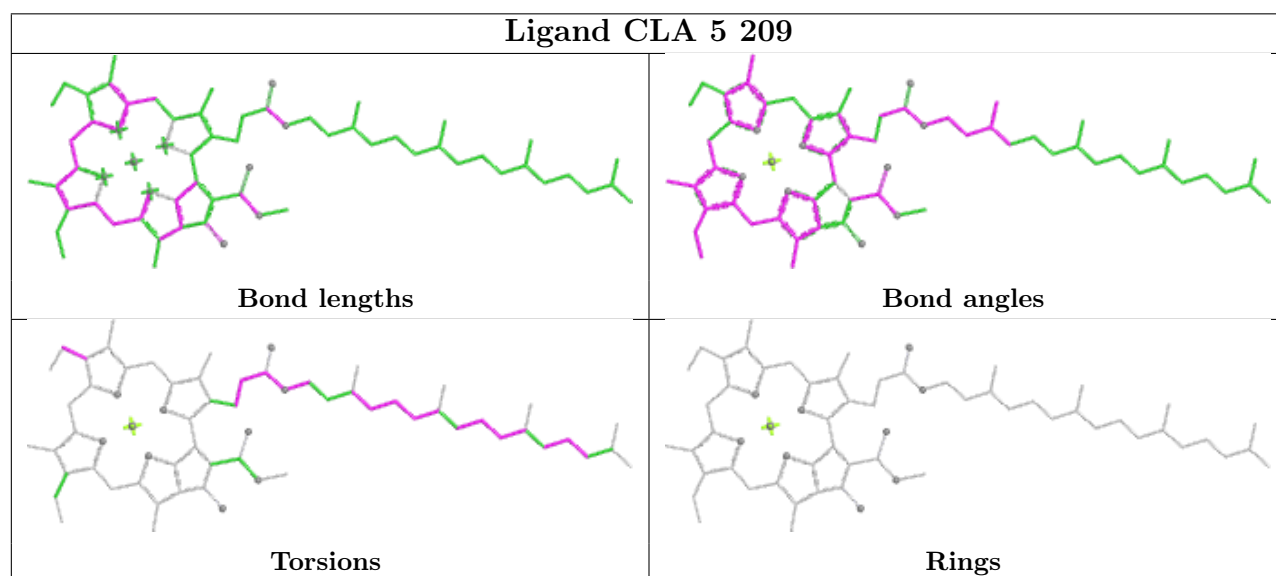
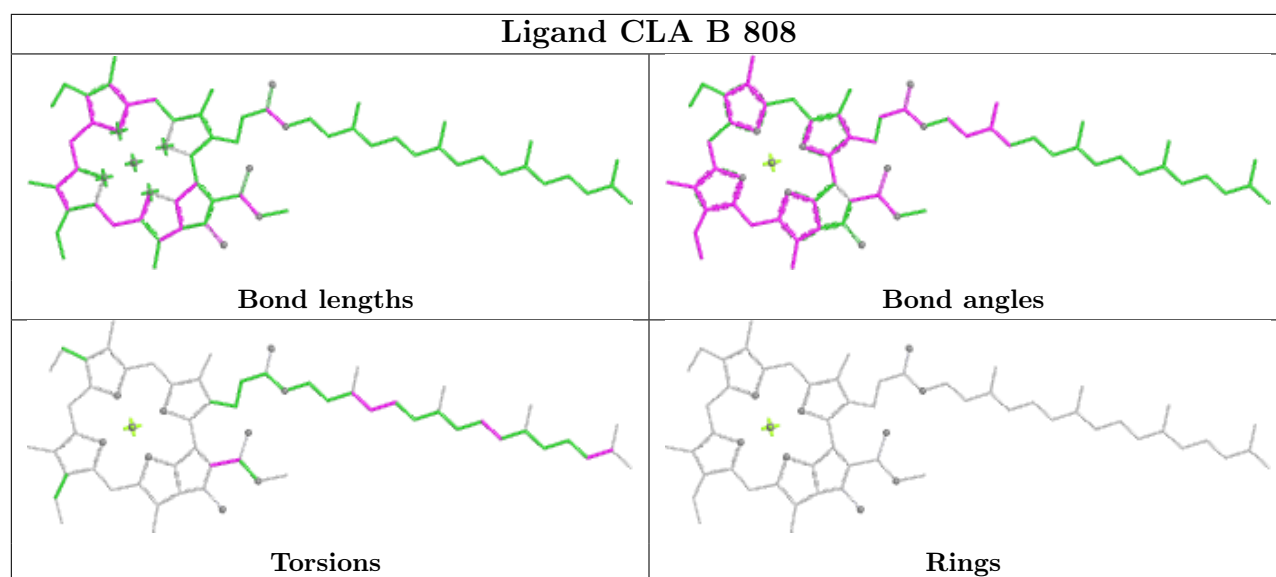
Rings



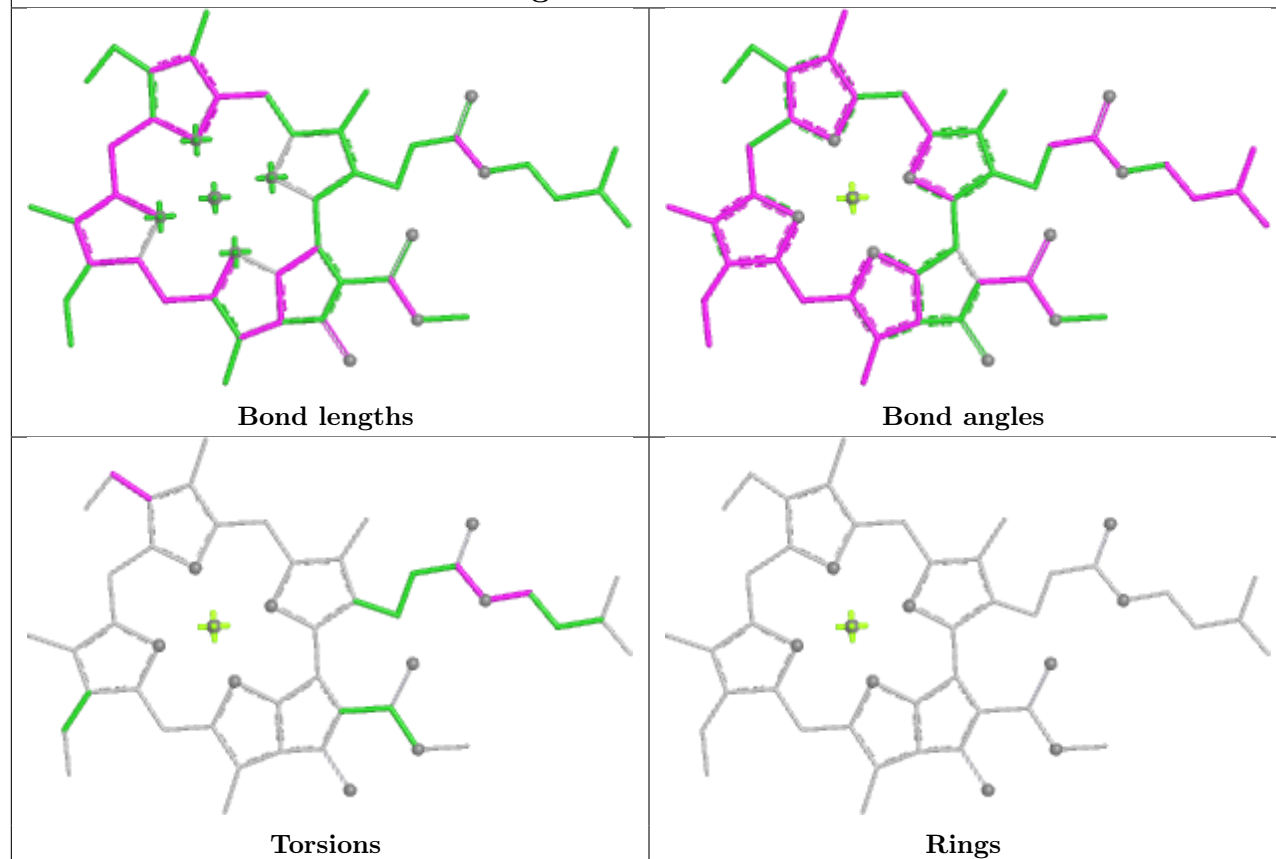




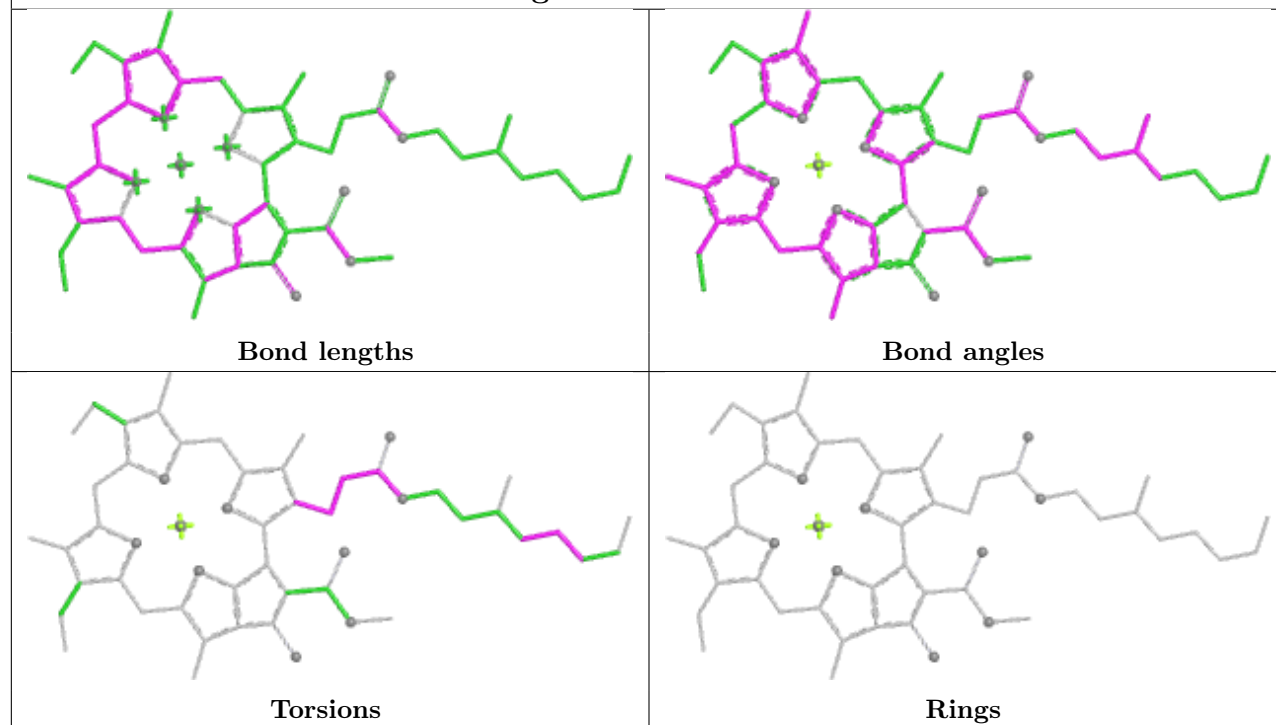




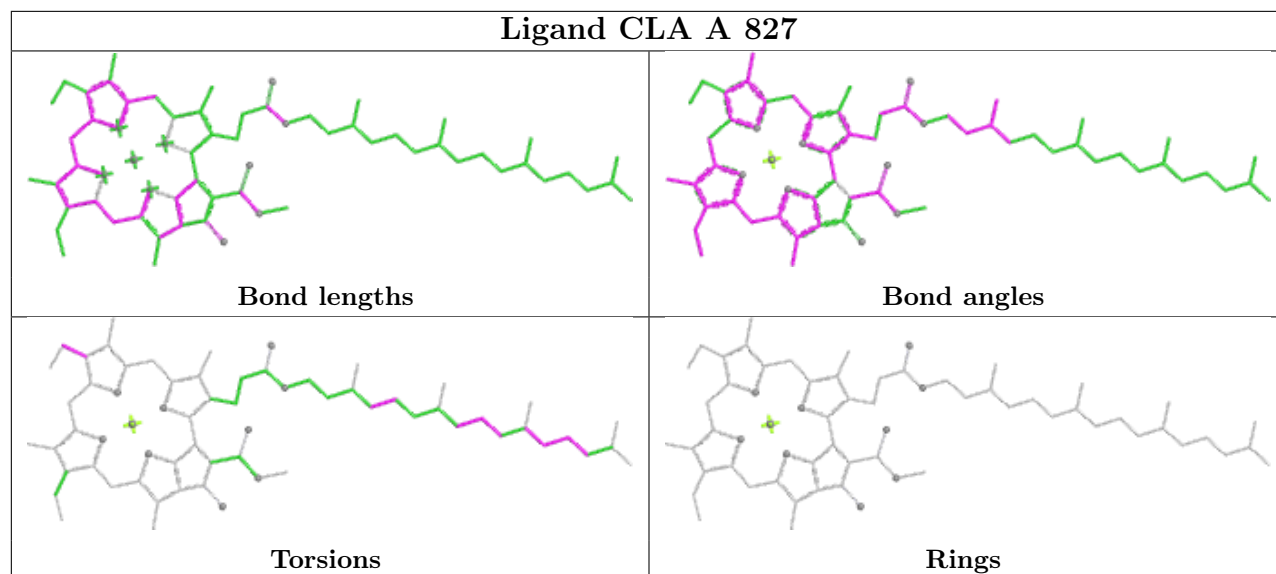
Ligand CLA A 815



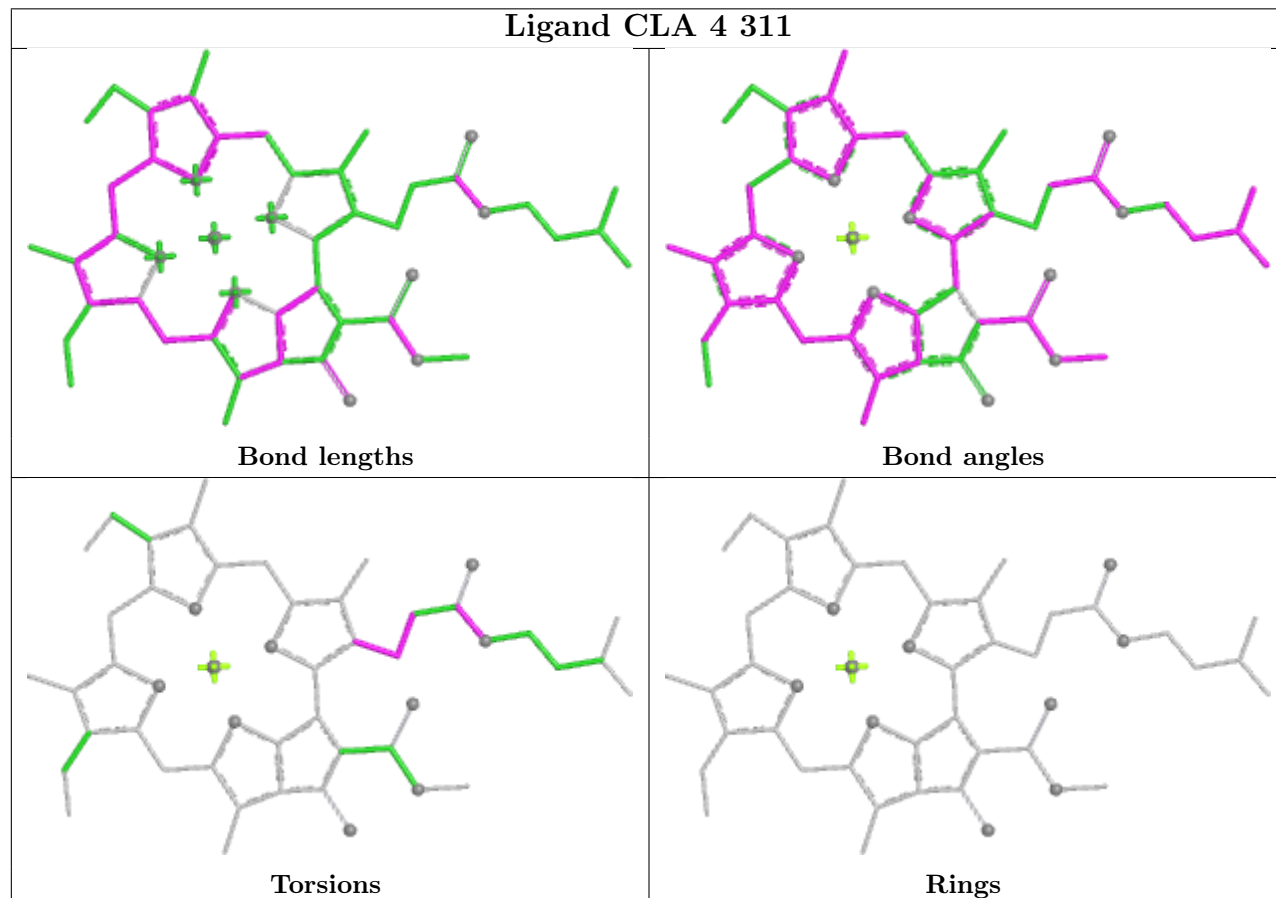
Ligand CLA A 819

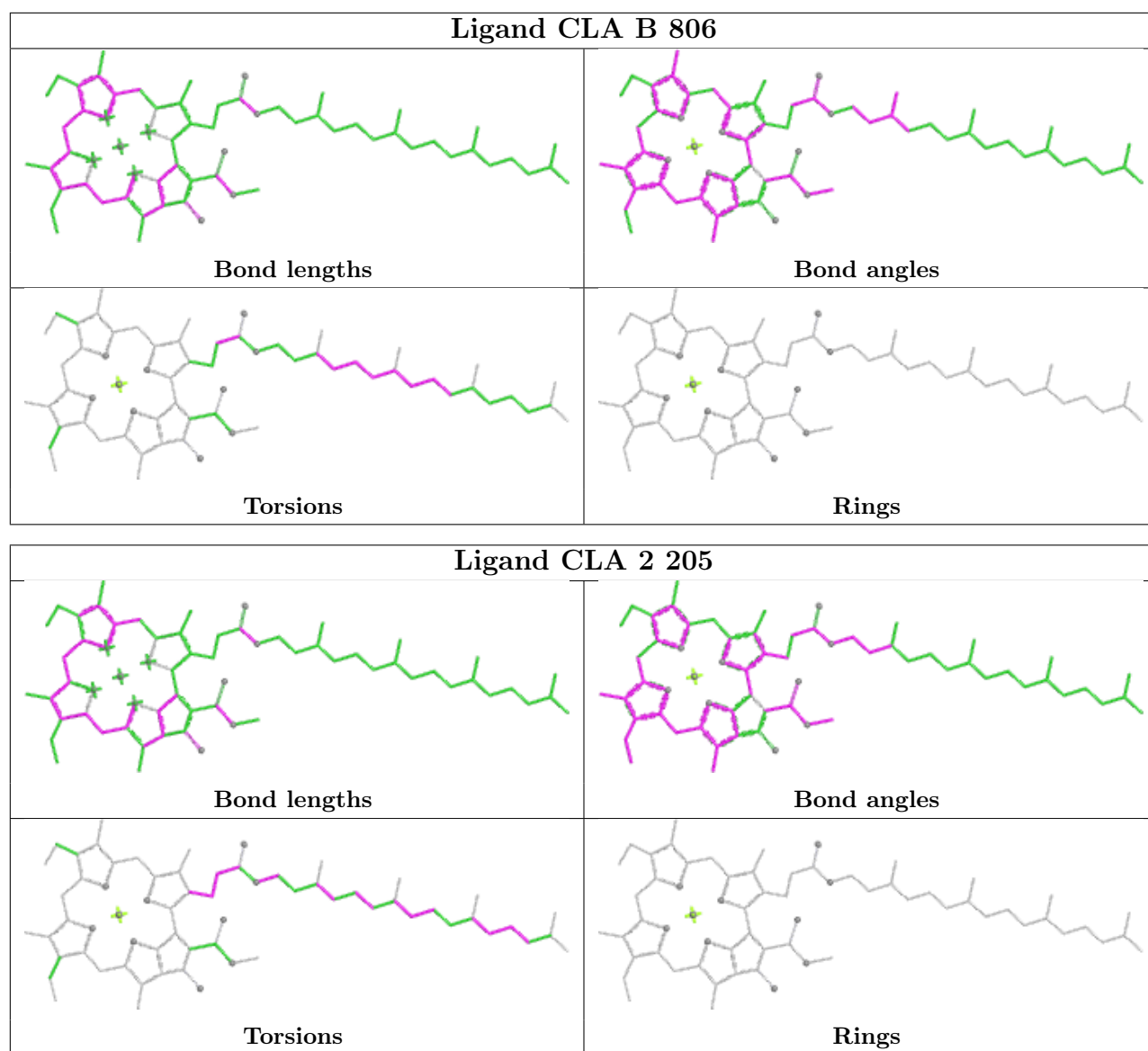


Ligand CLA A 827

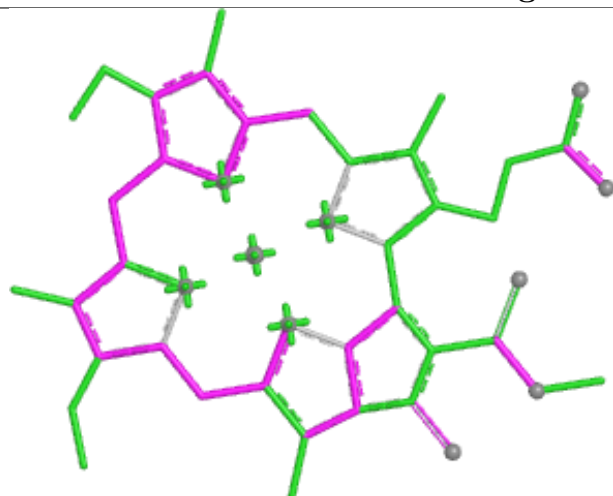


Ligand CLA 4 311

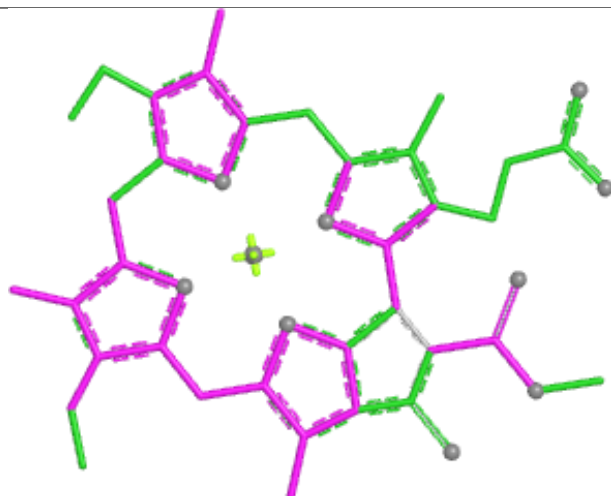




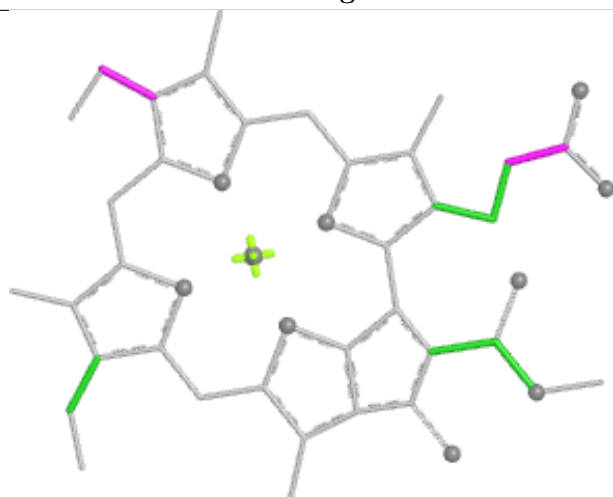
Ligand CLA 5 214



Bond lengths



Bond angles

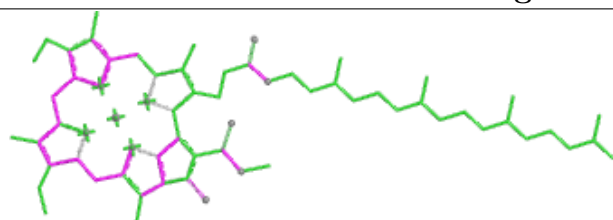


Torsions

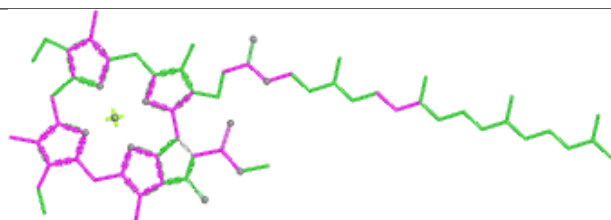


Rings

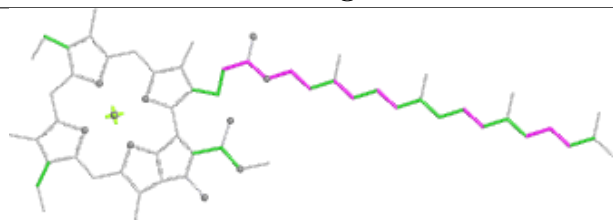
Ligand CLA B 829



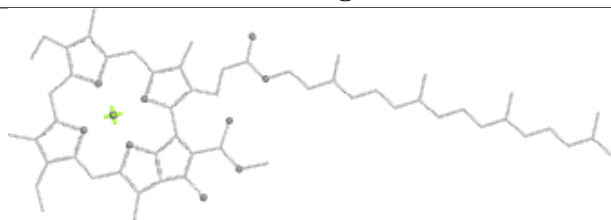
Bond lengths



Bond angles

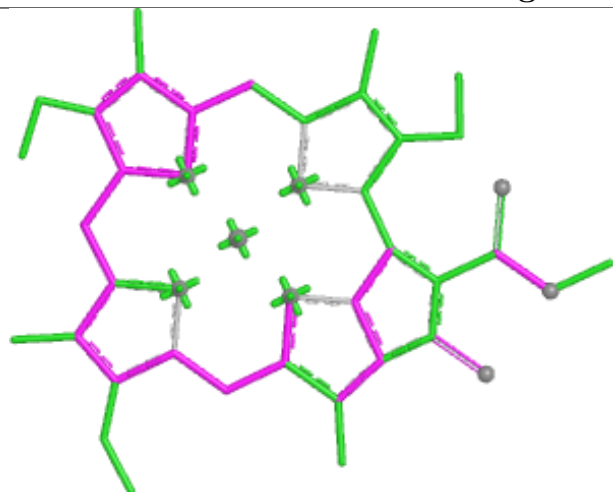


Torsions

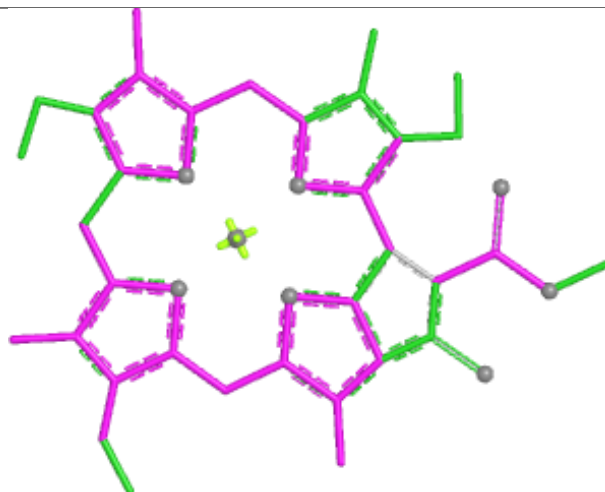


Rings

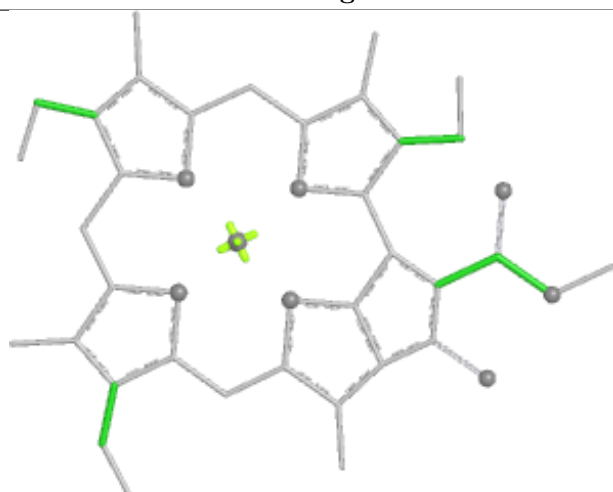
Ligand CLA 5 216



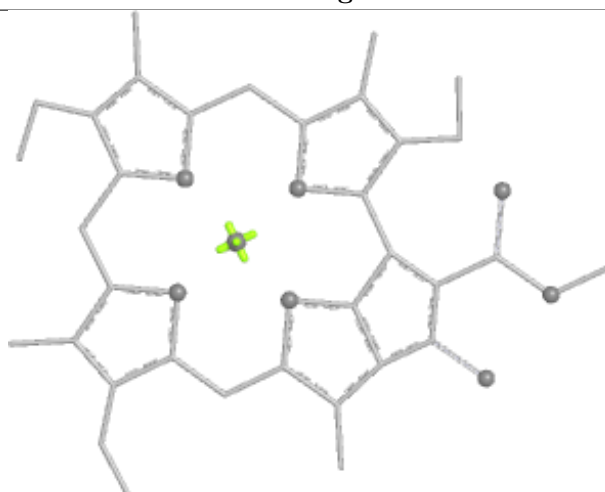
Bond lengths



Bond angles

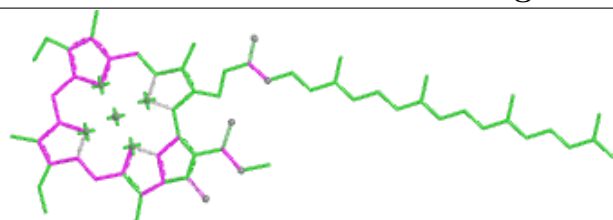


Torsions

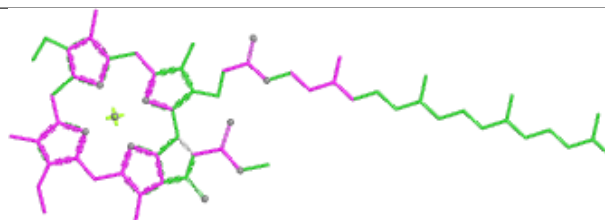


Rings

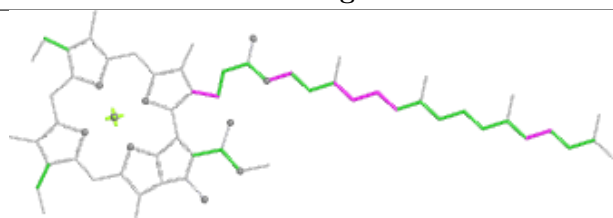
Ligand CLA B 812



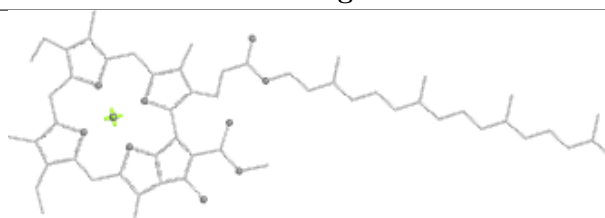
Bond lengths



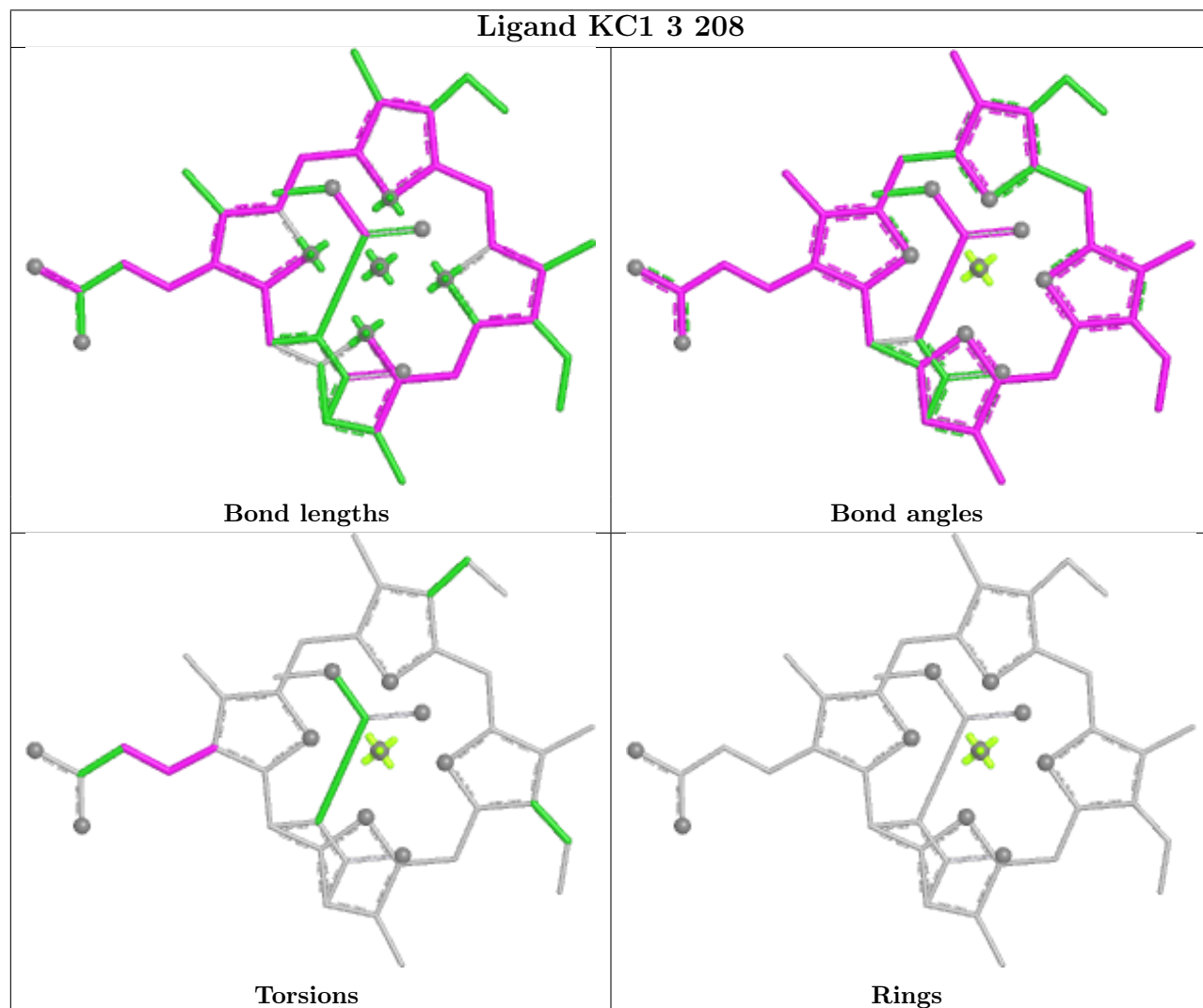
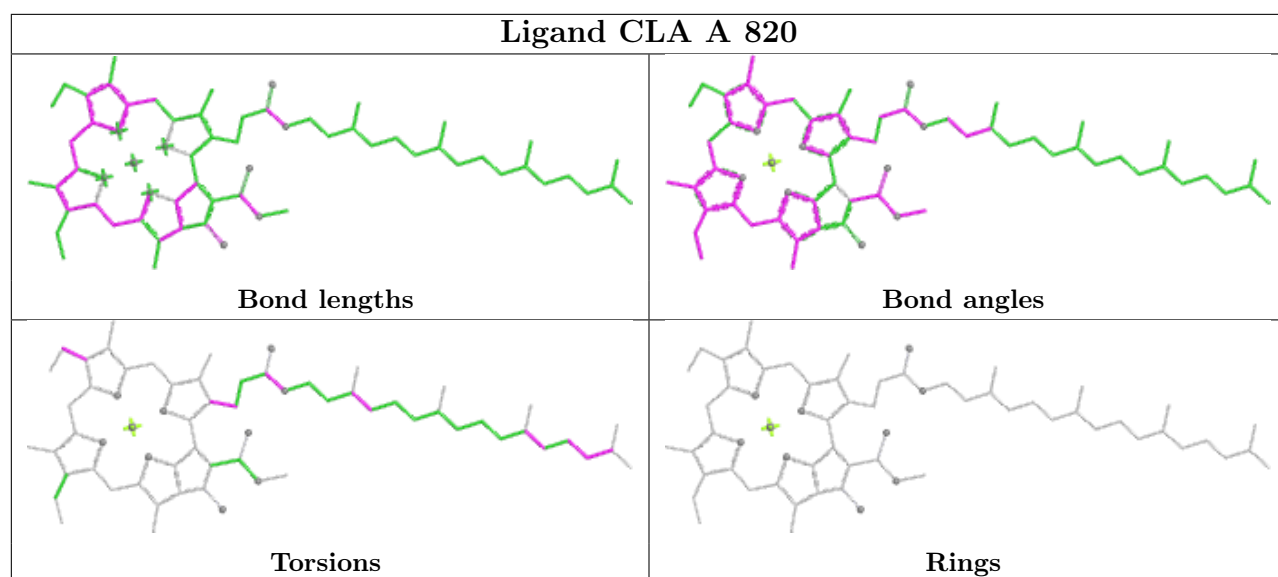
Bond angles

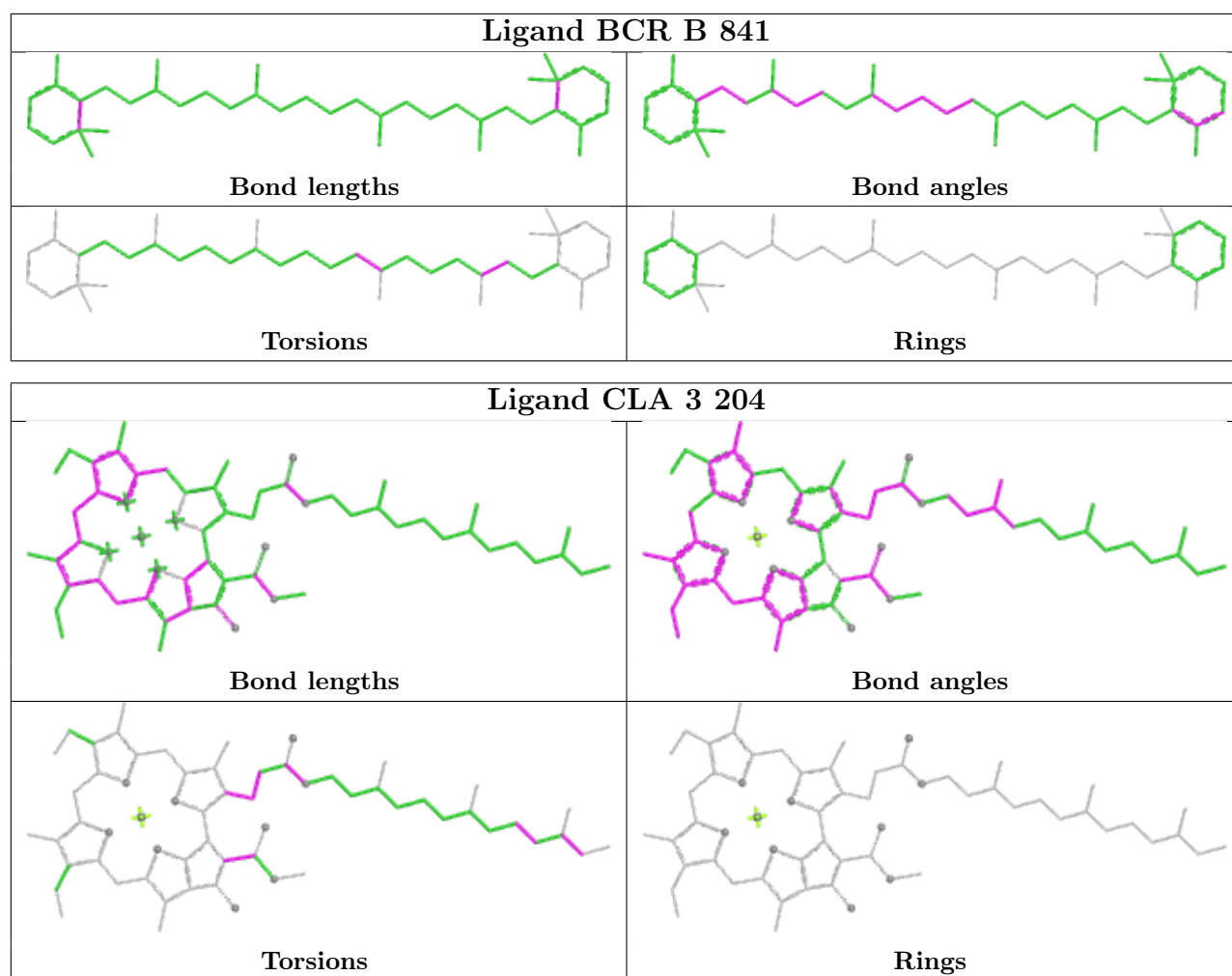


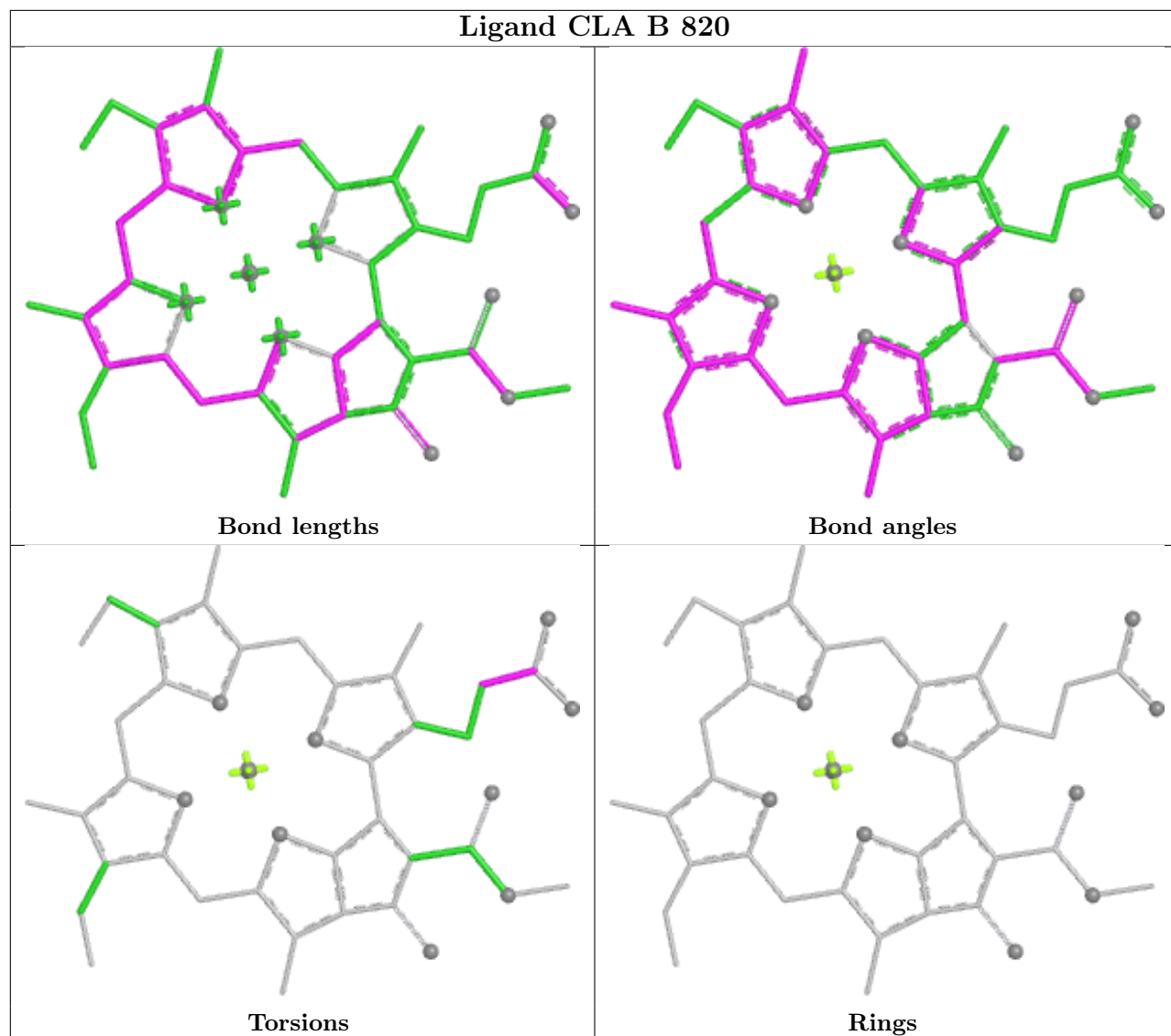
Torsions



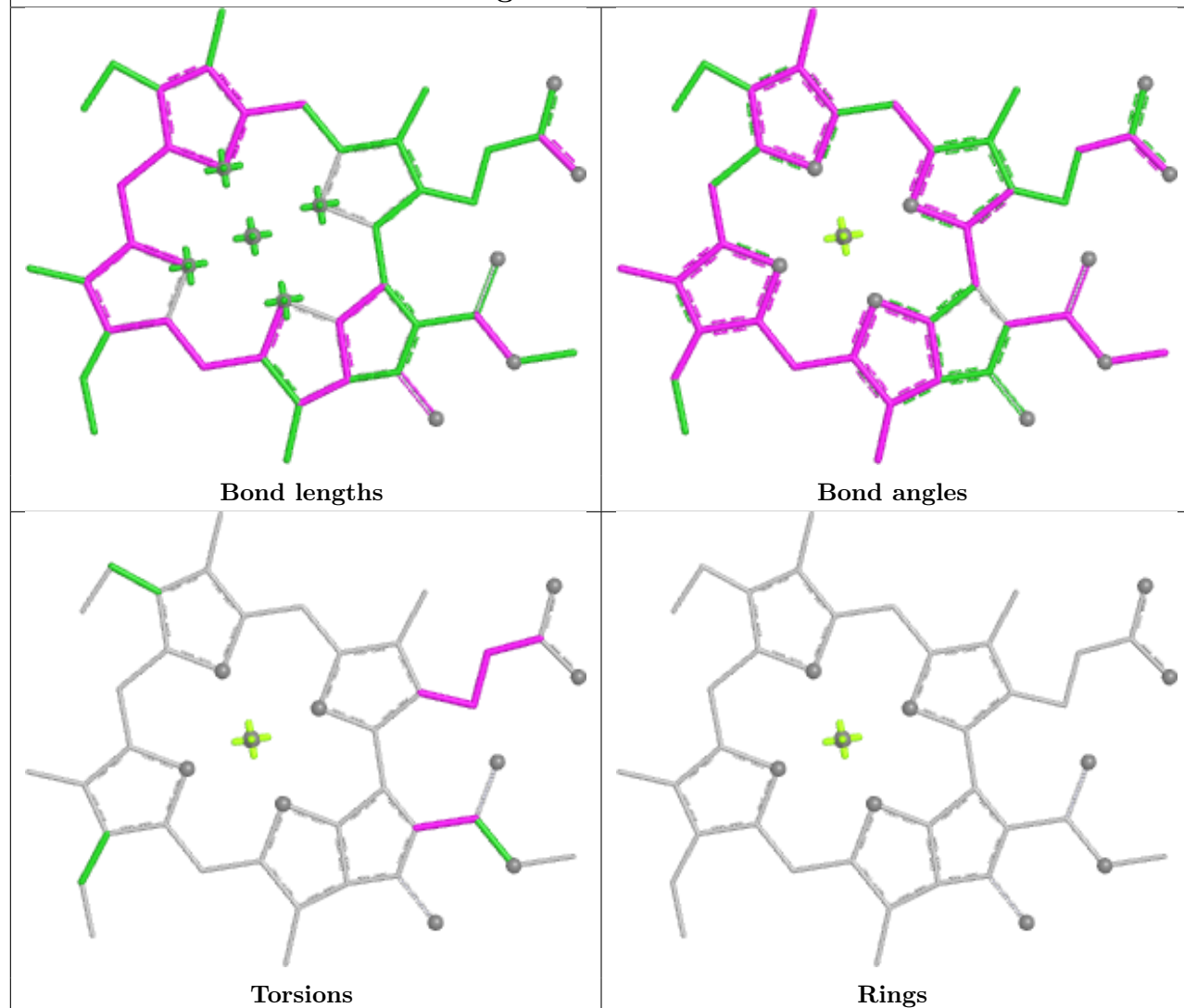
Rings



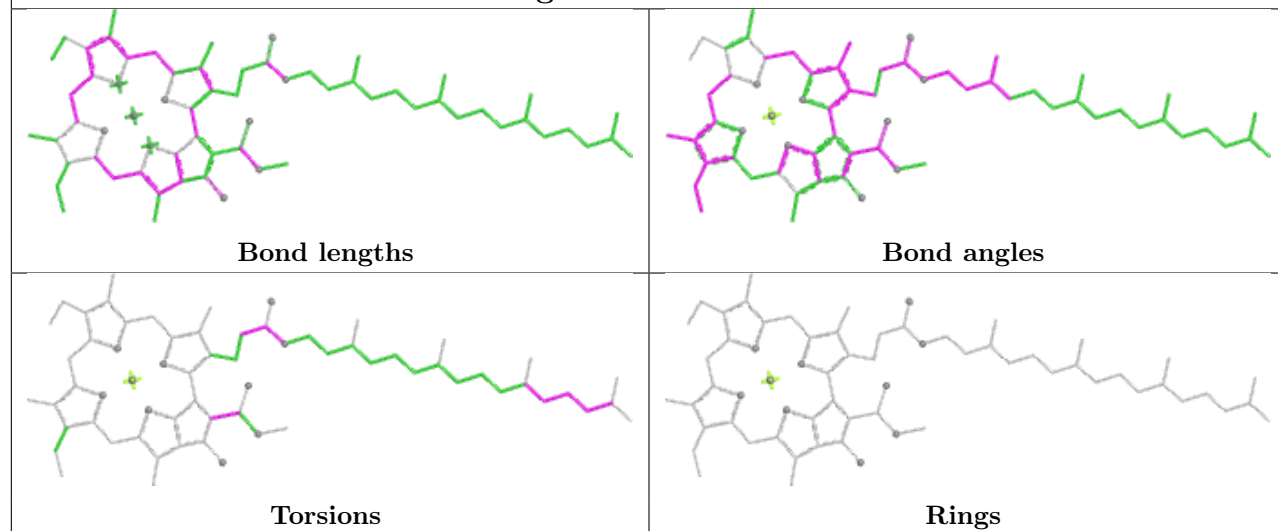


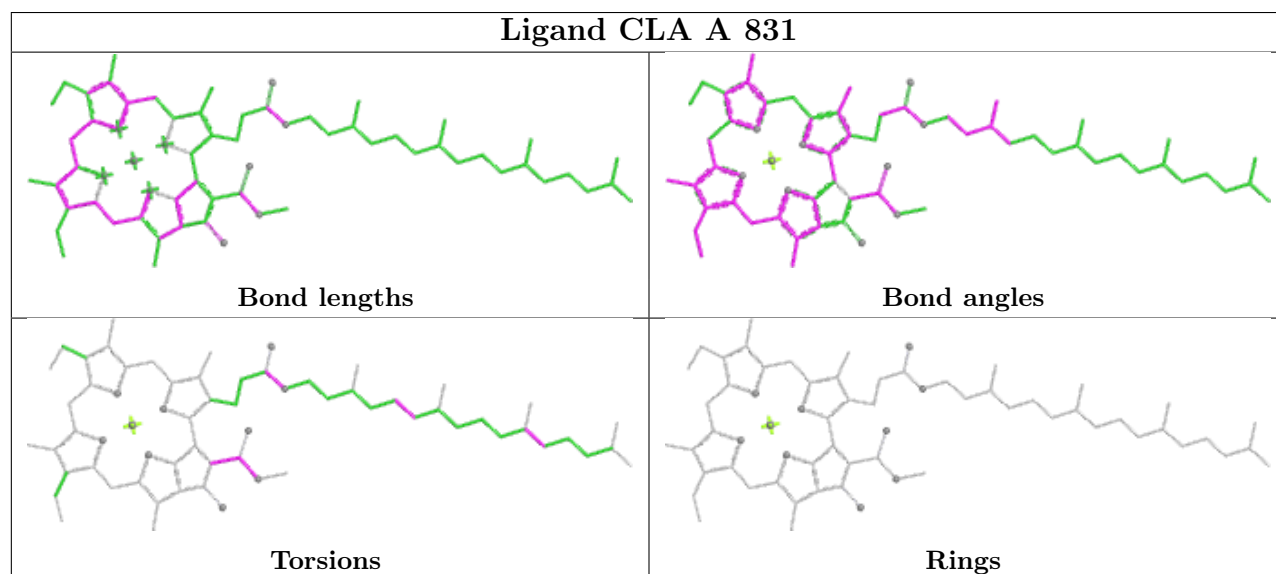
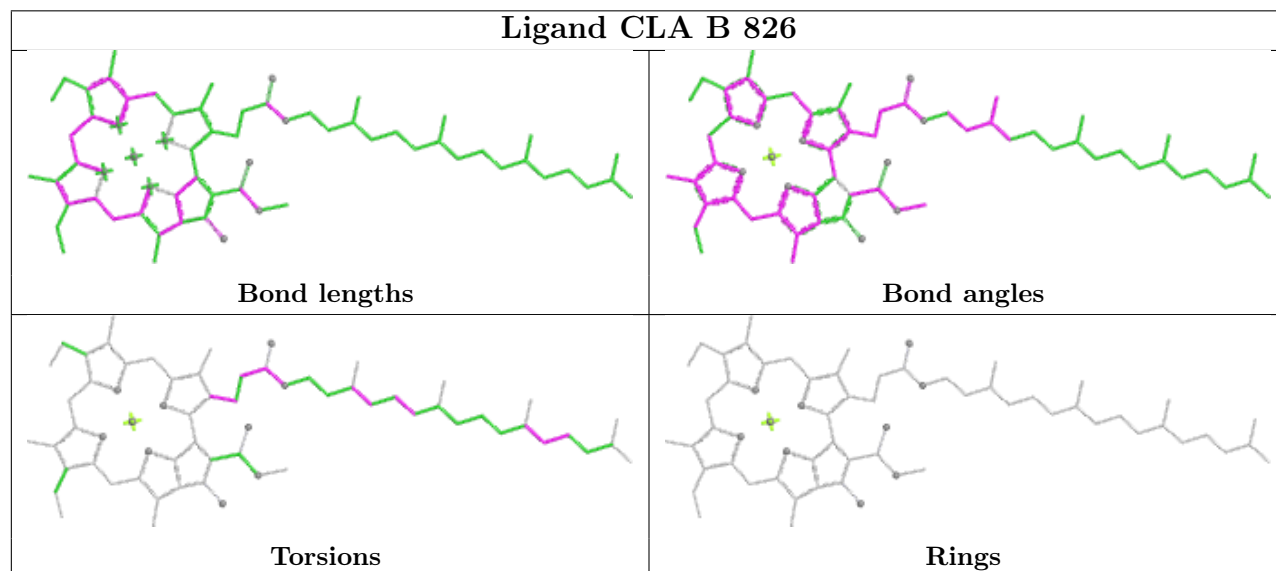
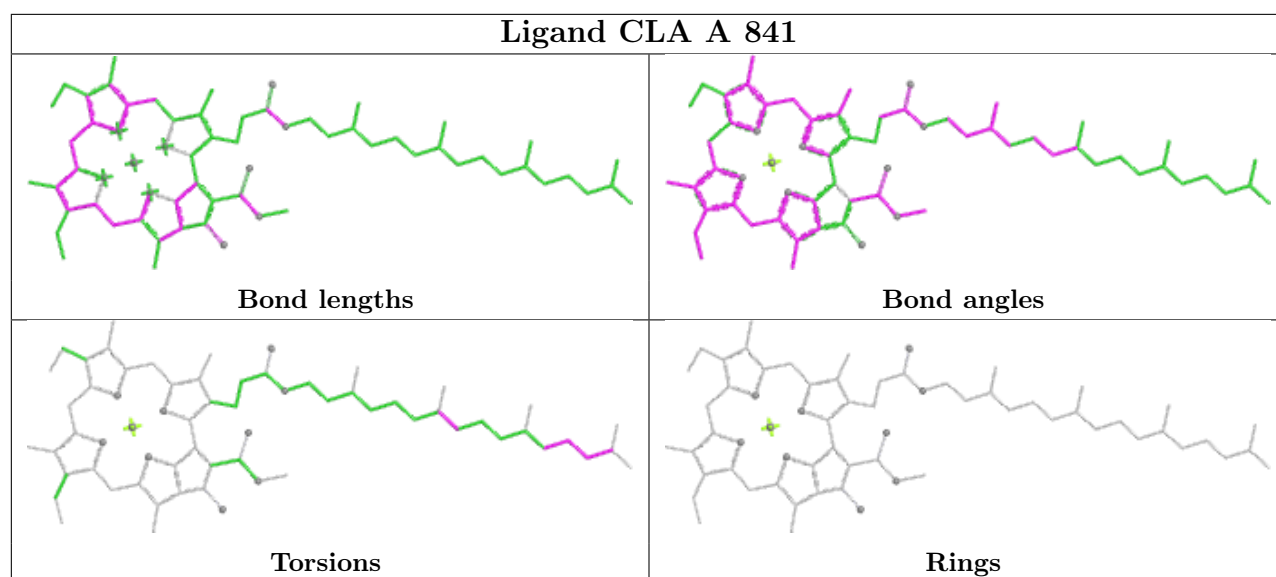


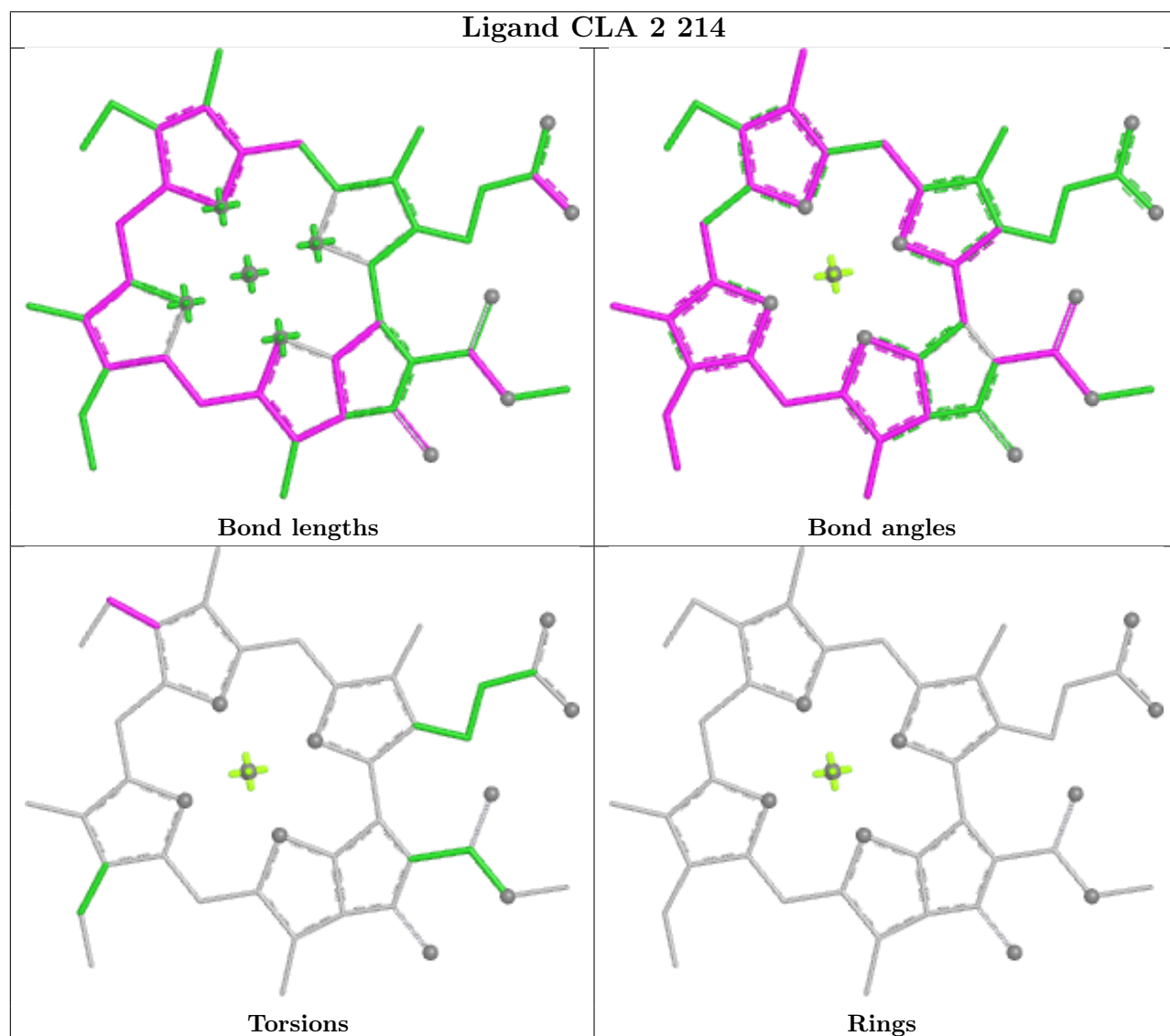
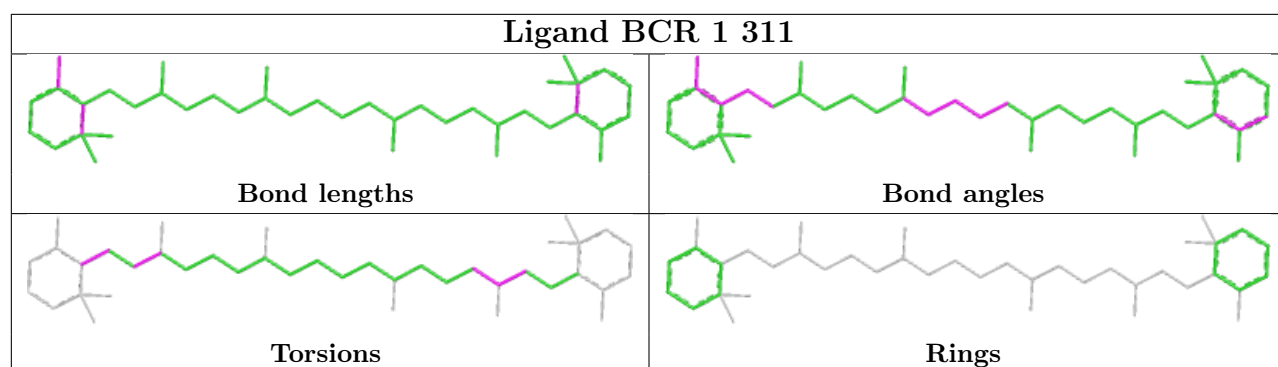
Ligand CLA 2 213



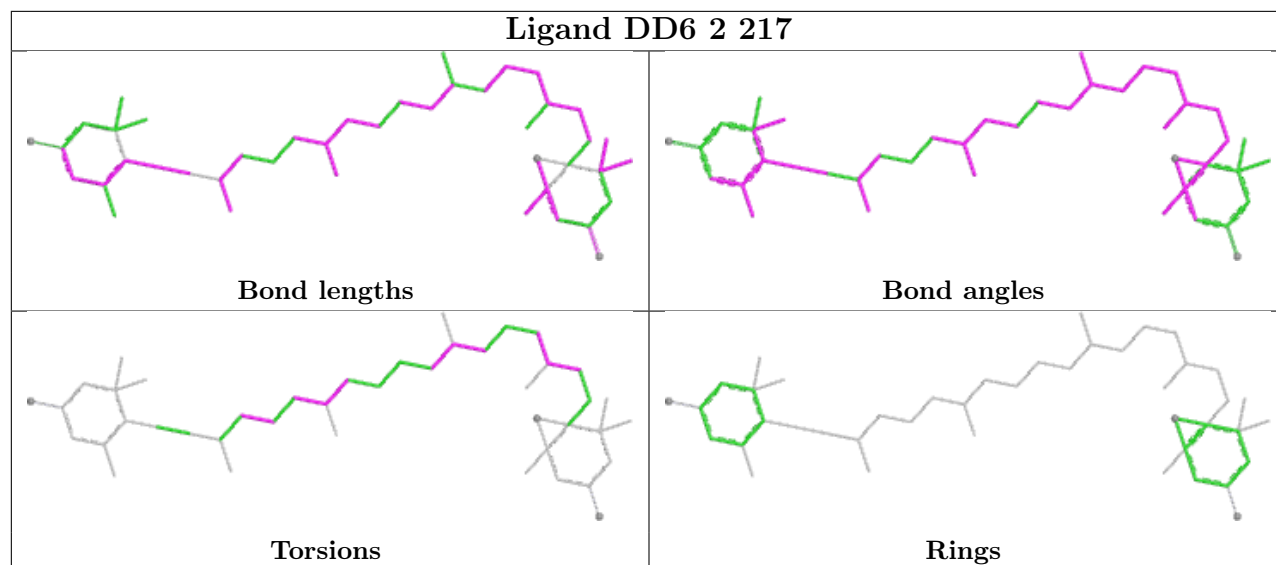
Ligand CL0 A 801



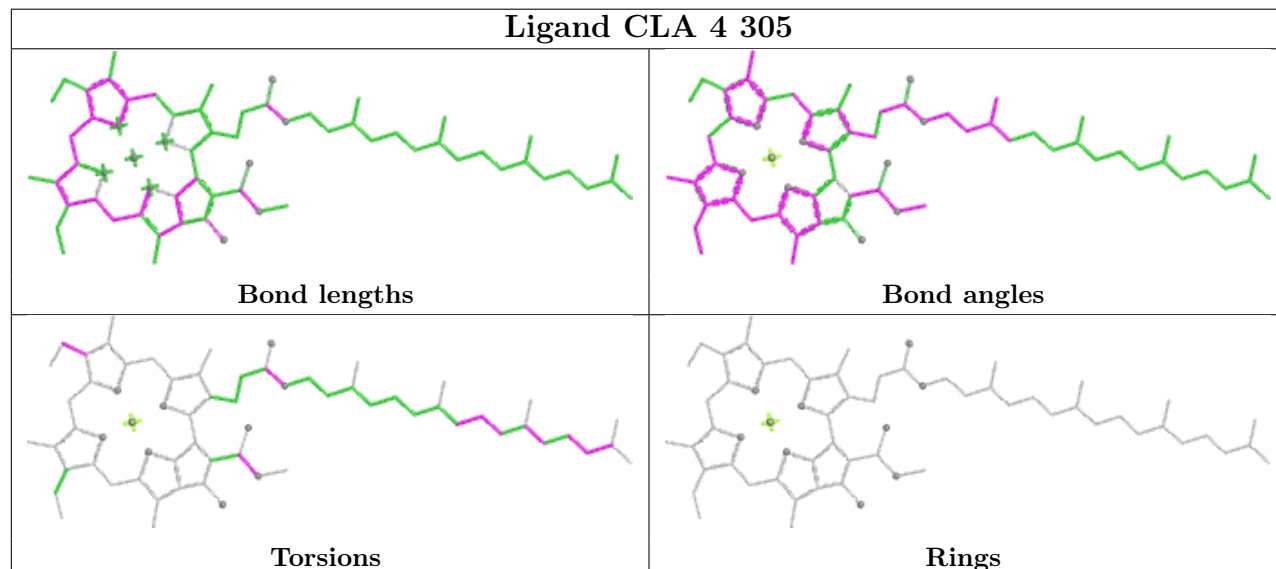




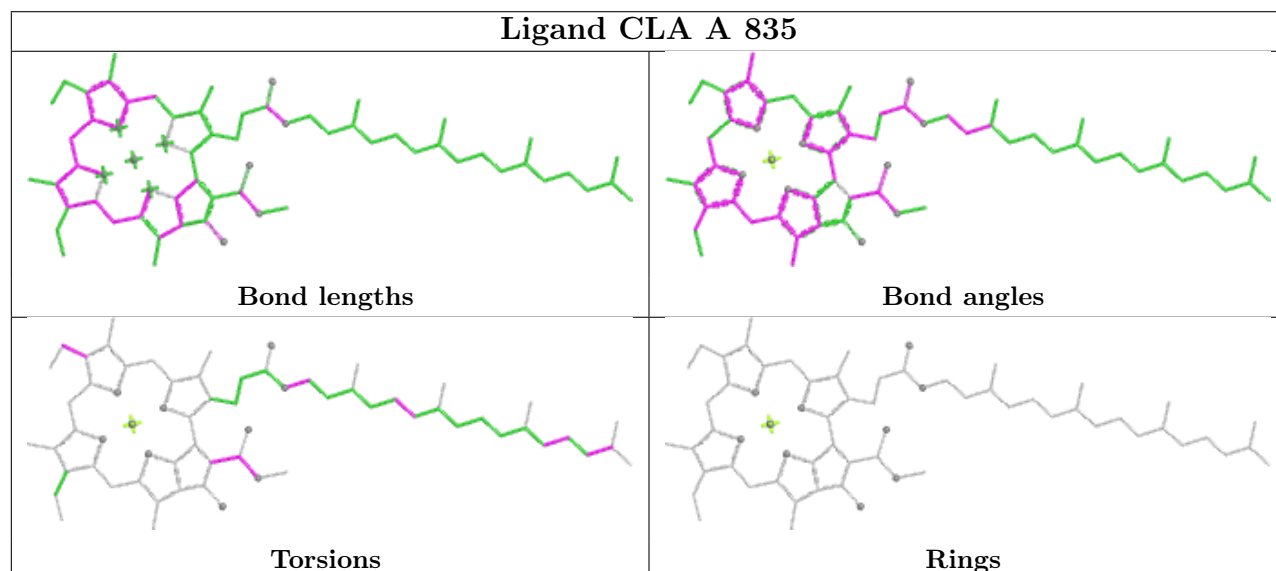
Ligand DD6 2 217

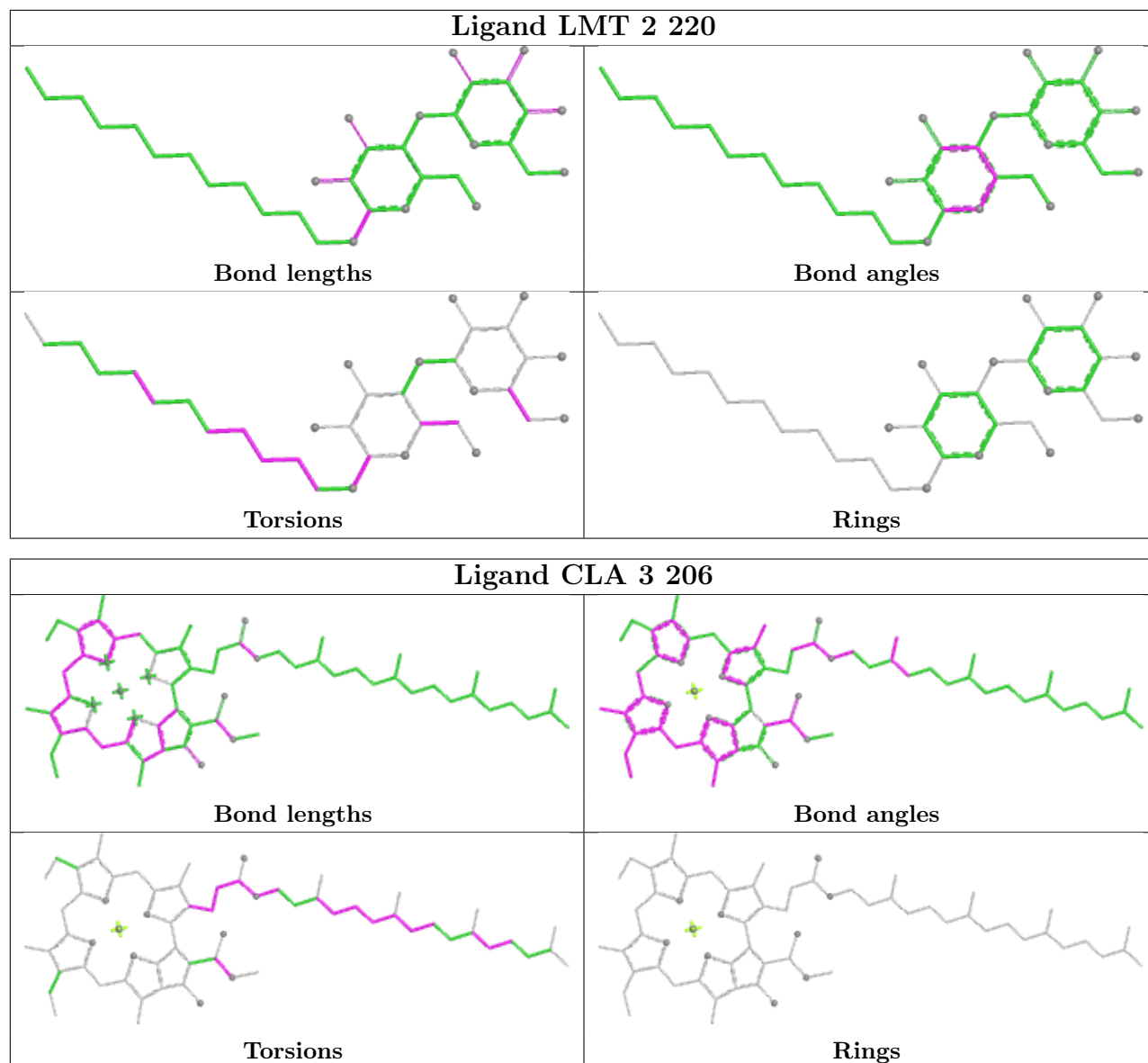


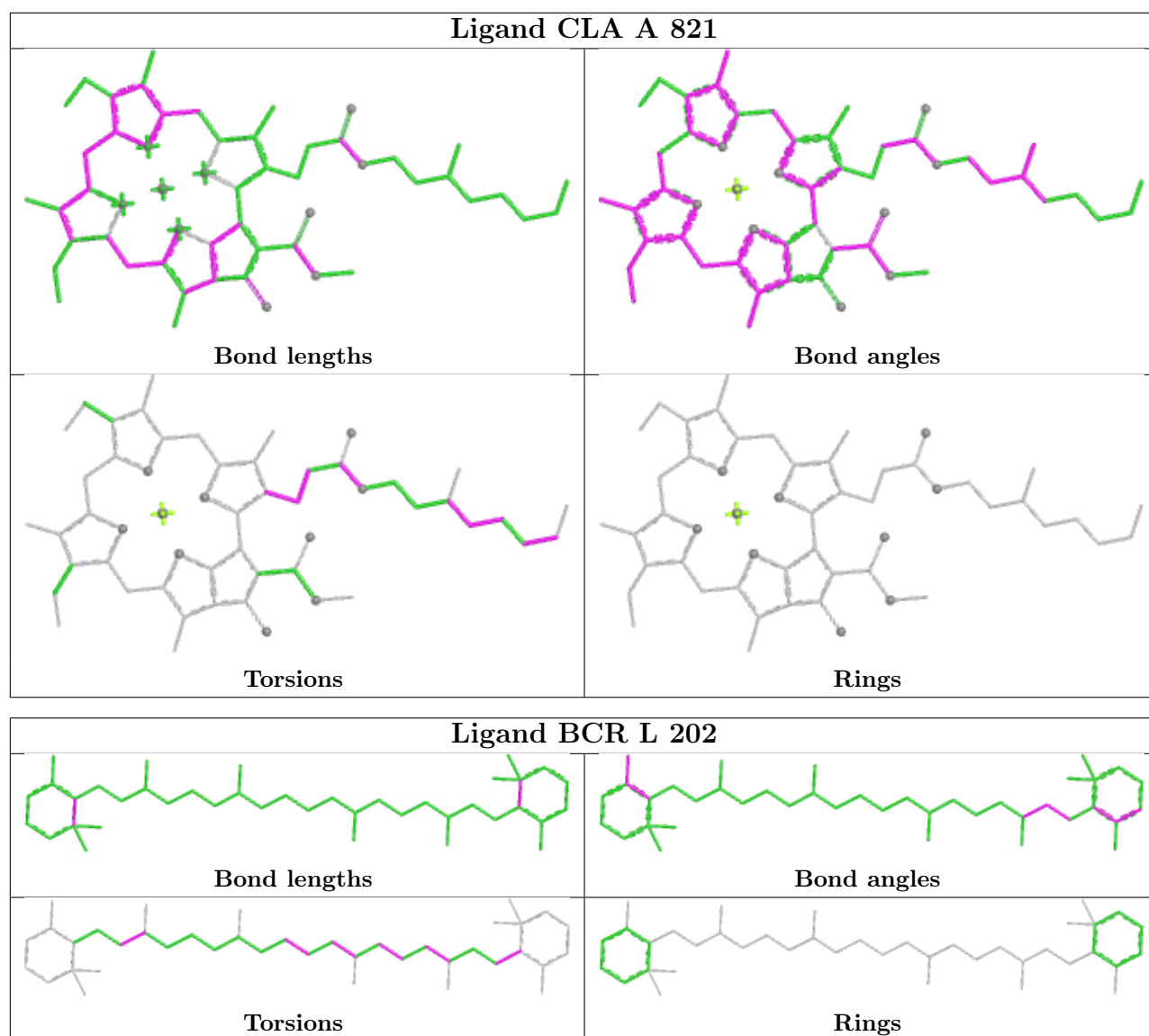
Ligand CLA 4 305

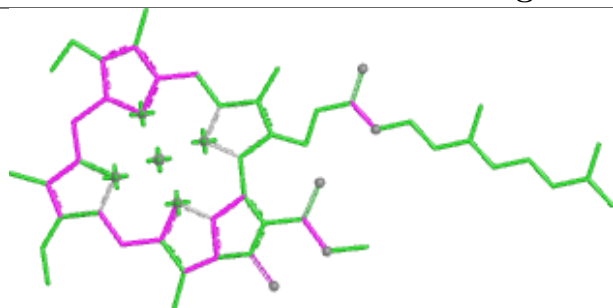


Ligand CLA A 835

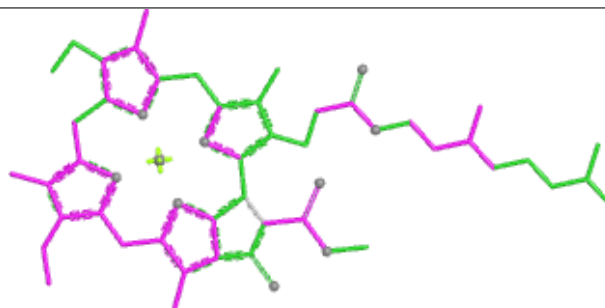




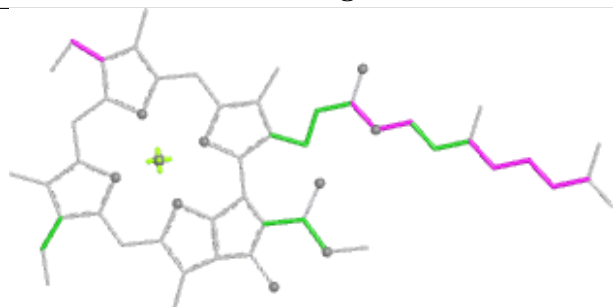


Ligand CLA F 203

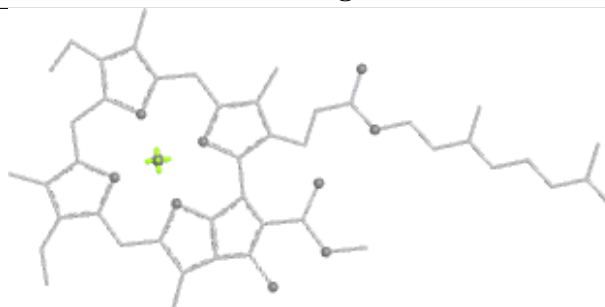
Bond lengths



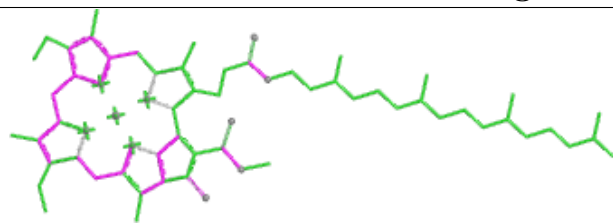
Bond angles



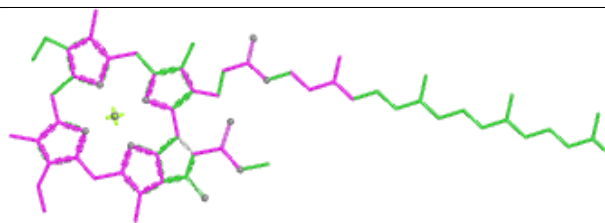
Torsions



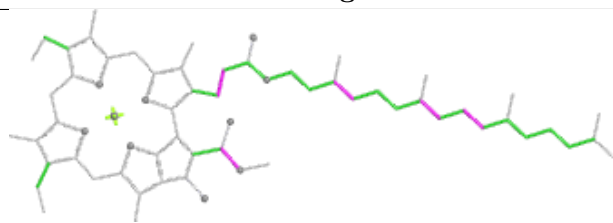
Rings

Ligand CLA A 878

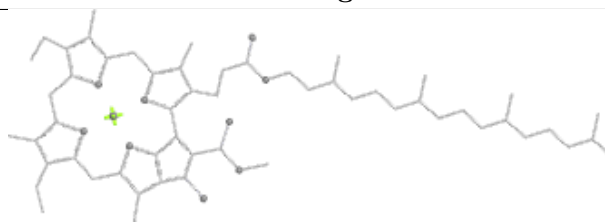
Bond lengths



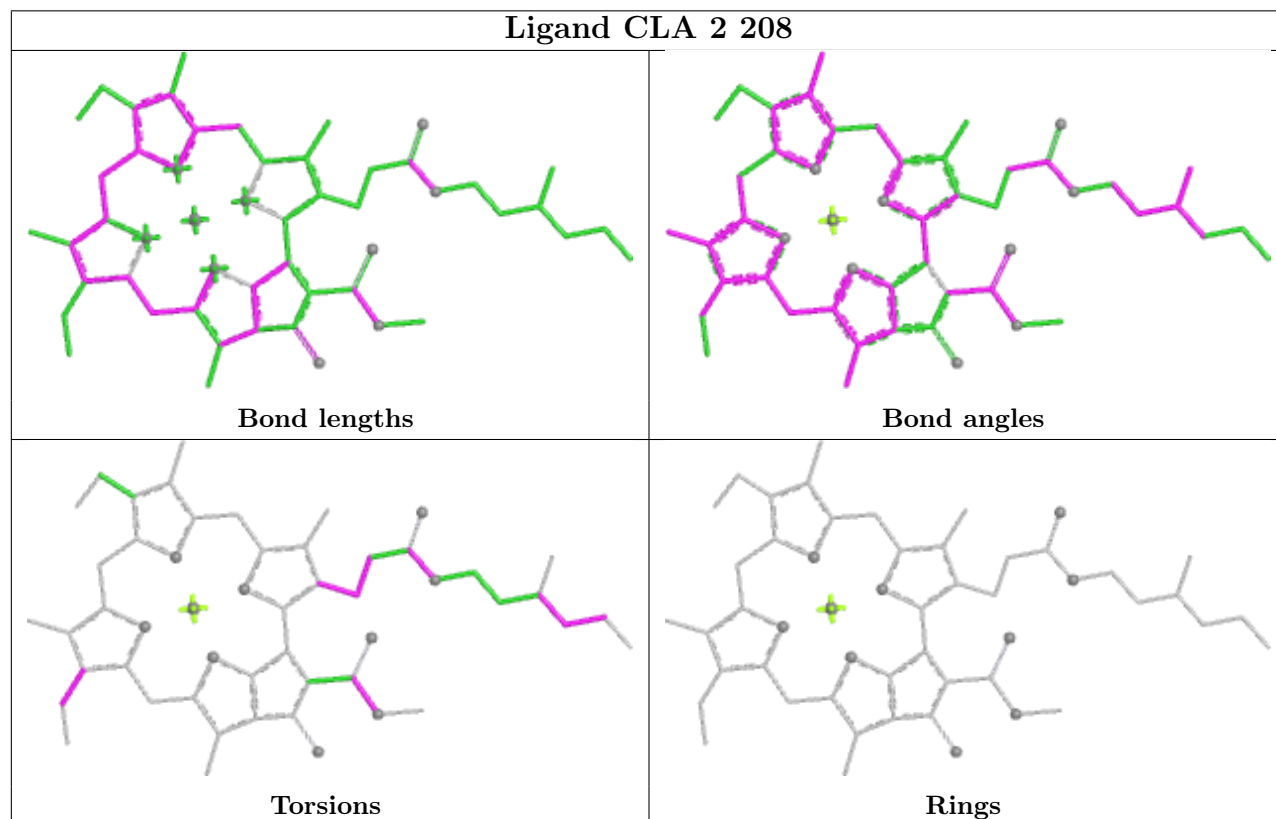
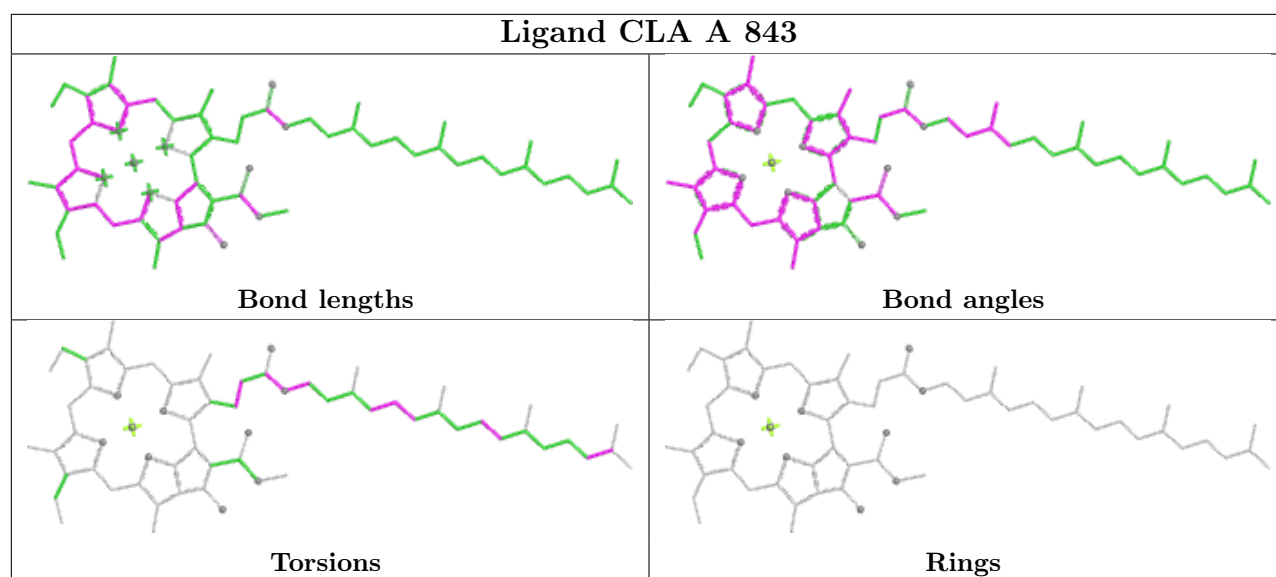
Bond angles

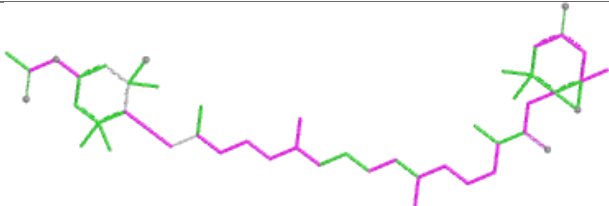
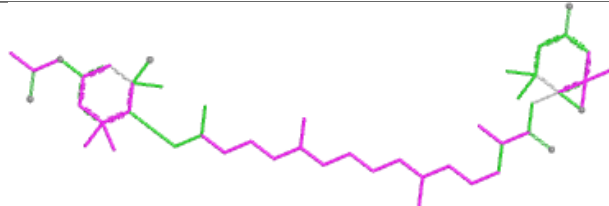
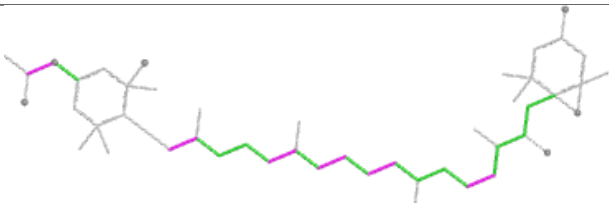
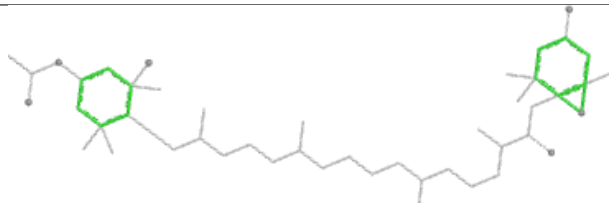


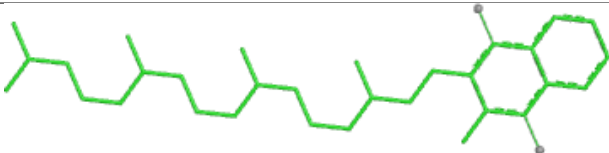
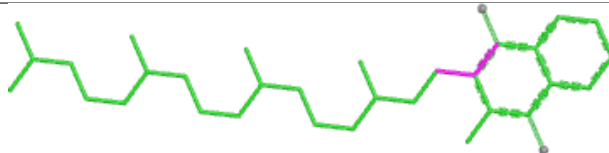
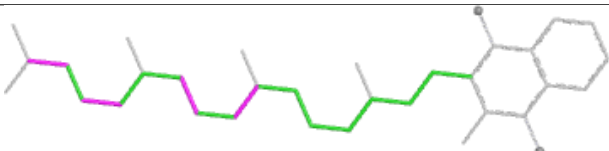
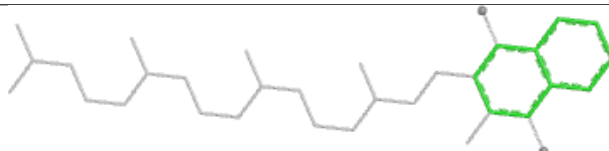
Torsions

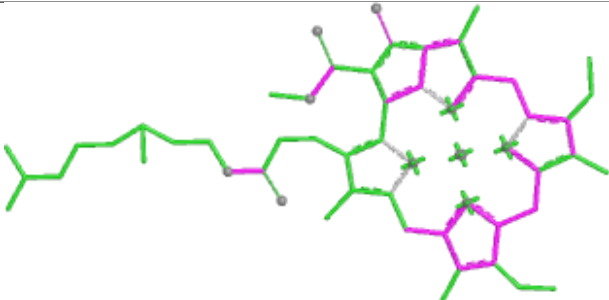
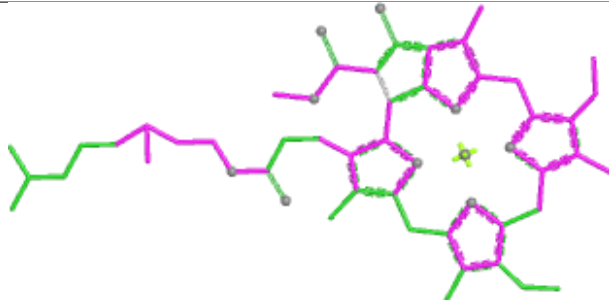
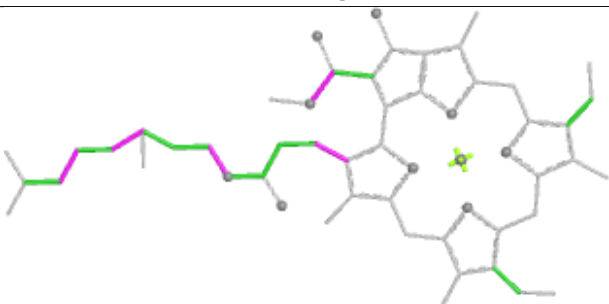
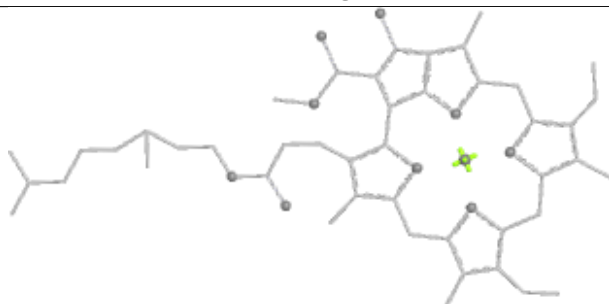


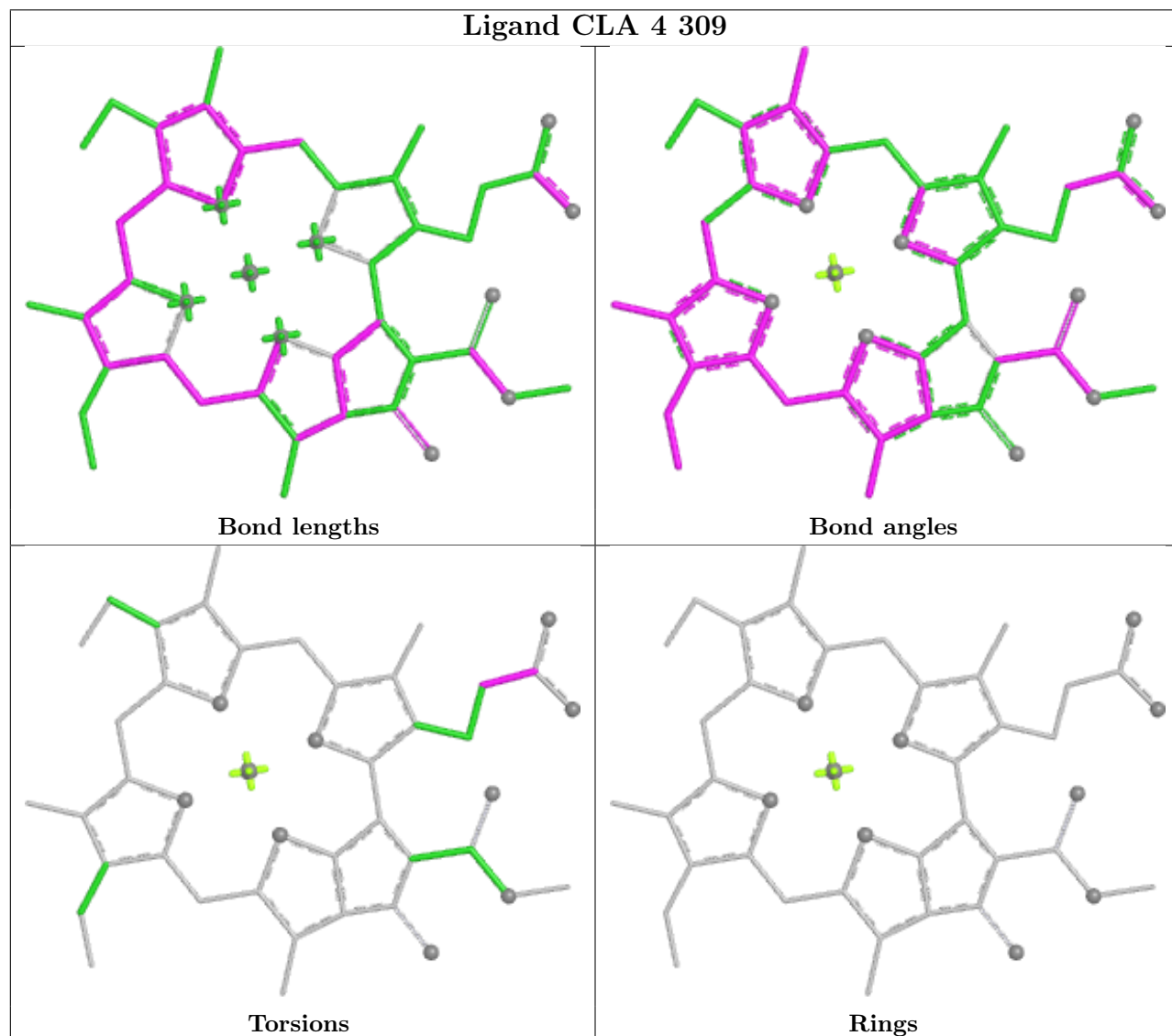
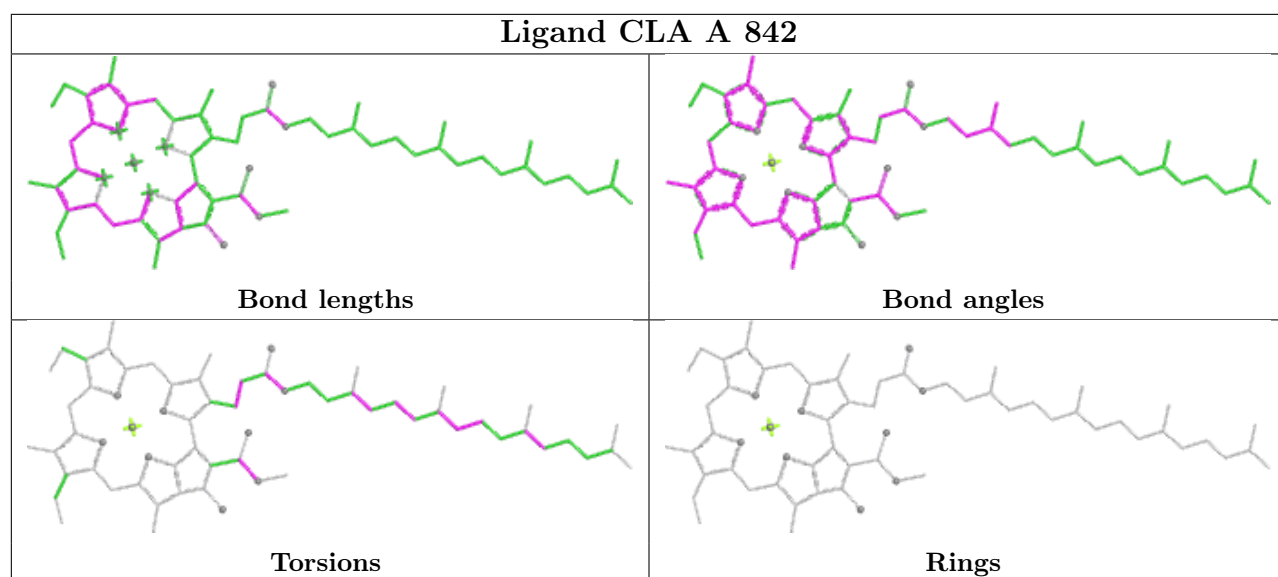
Rings

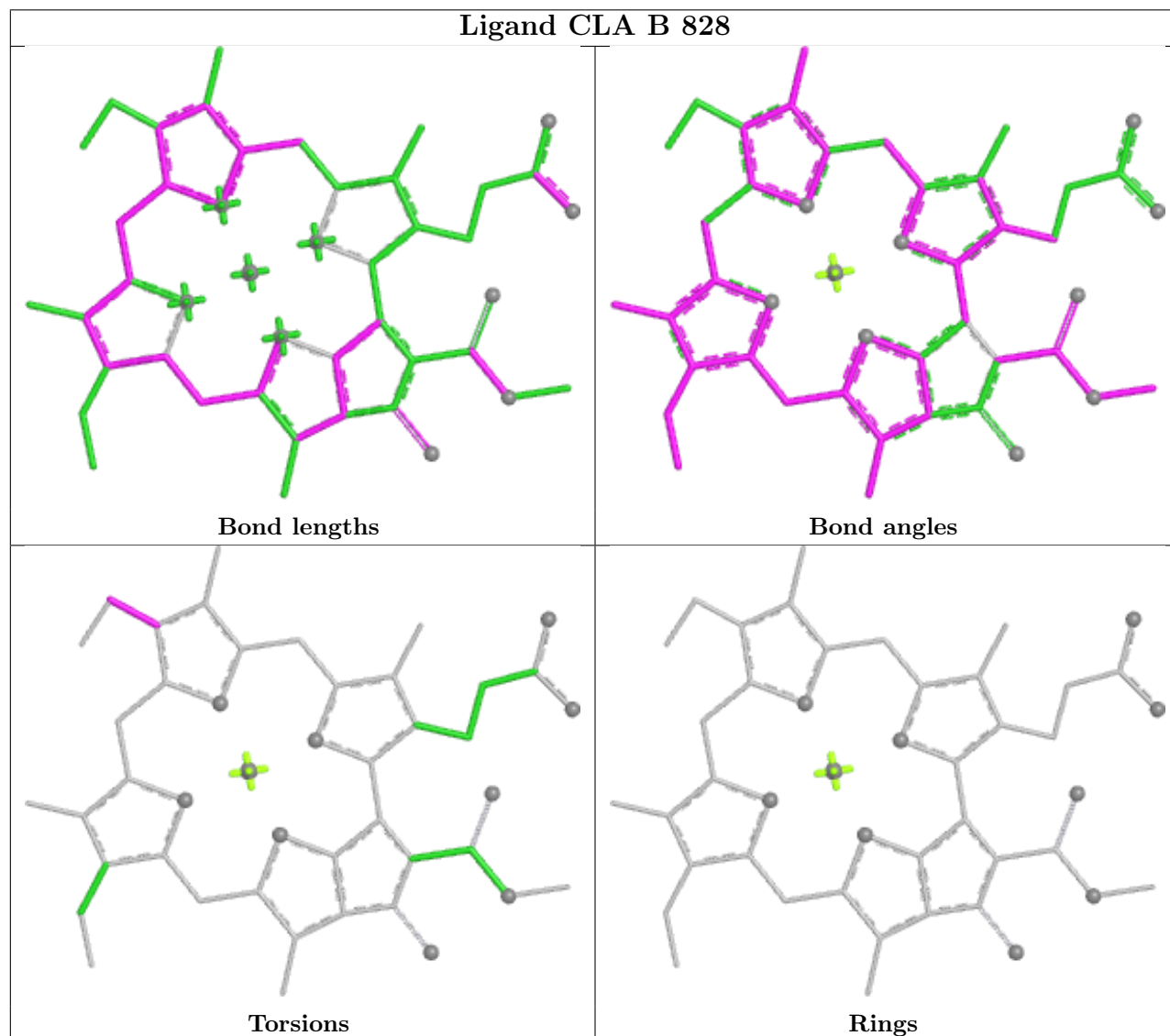
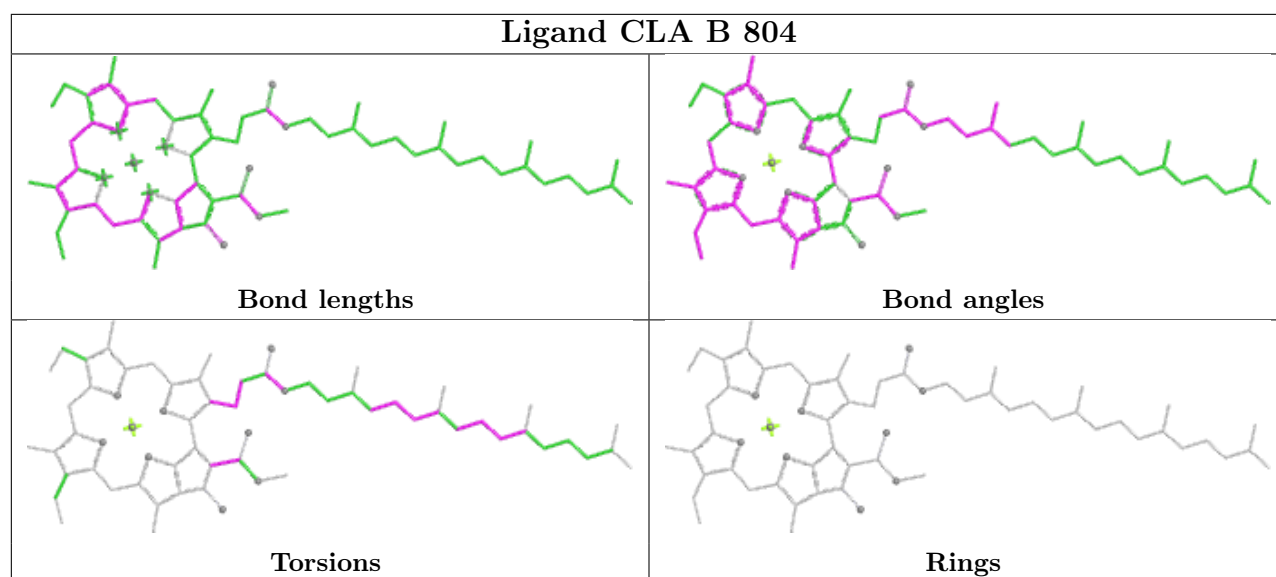


Ligand A86 1 317	
	
Bond lengths	Bond angles
	
Torsions	Rings

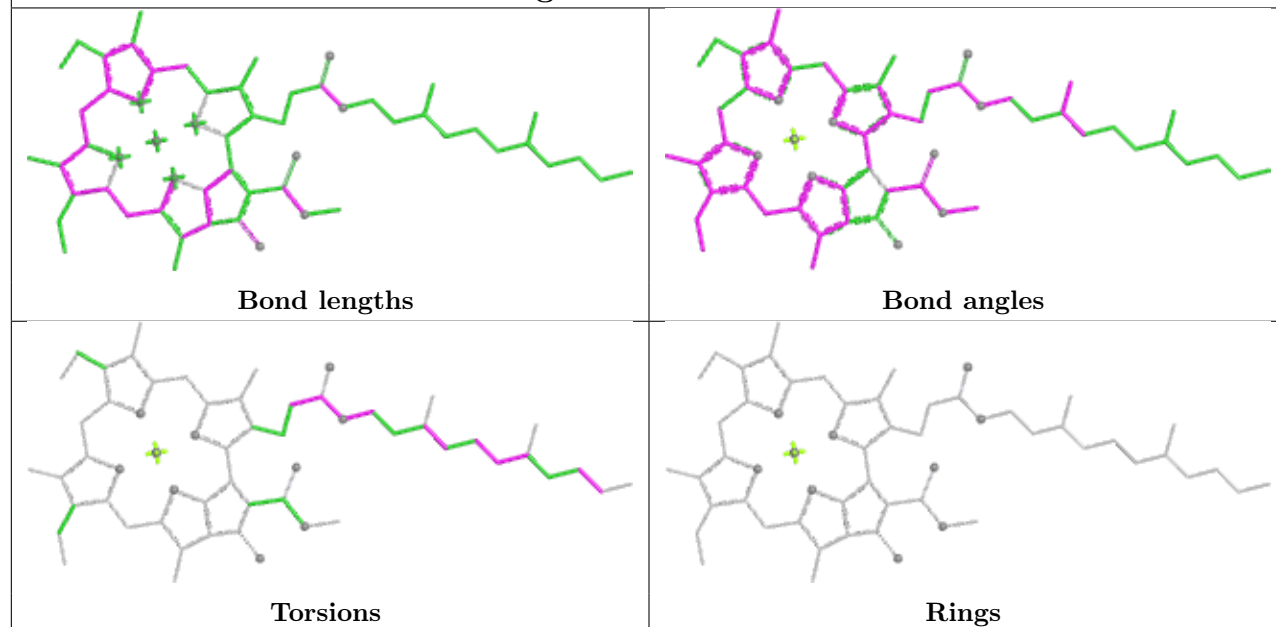
Ligand PQN A 845	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 1 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

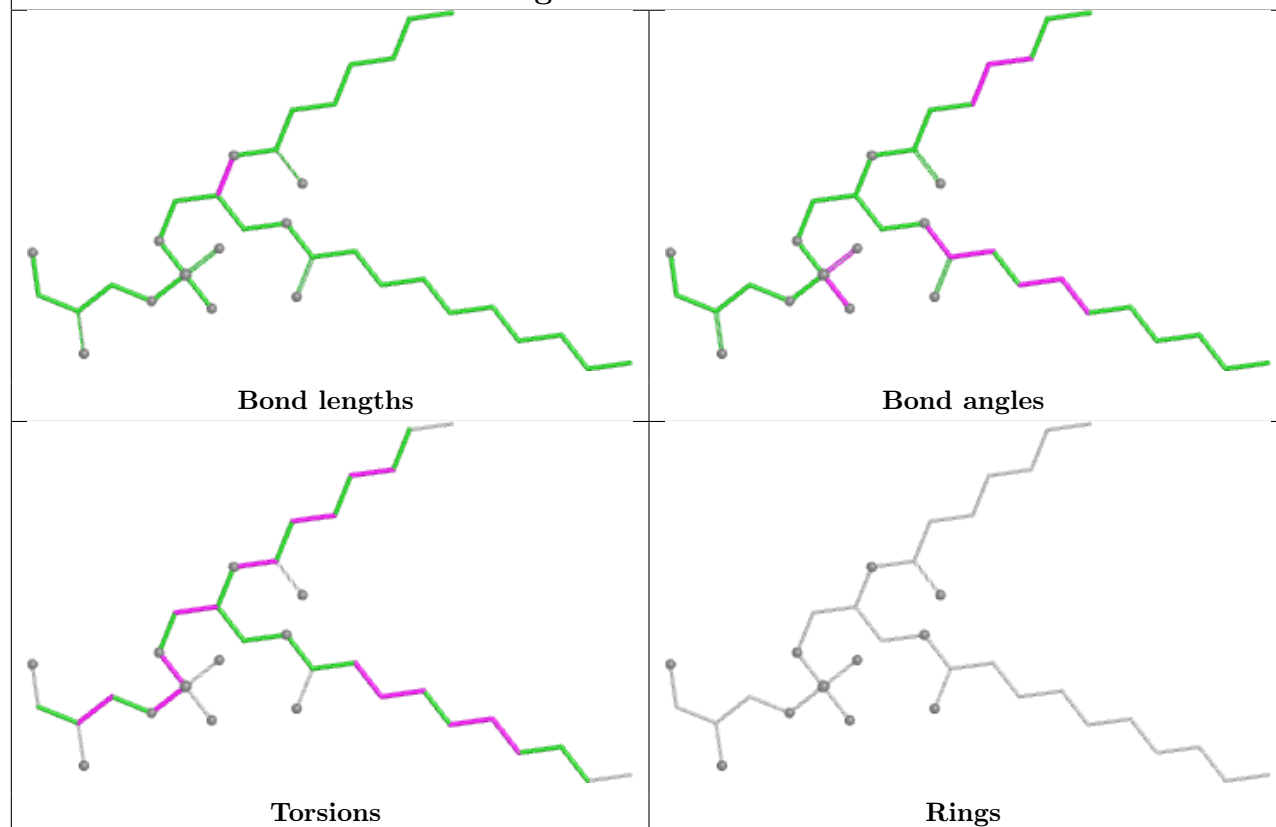




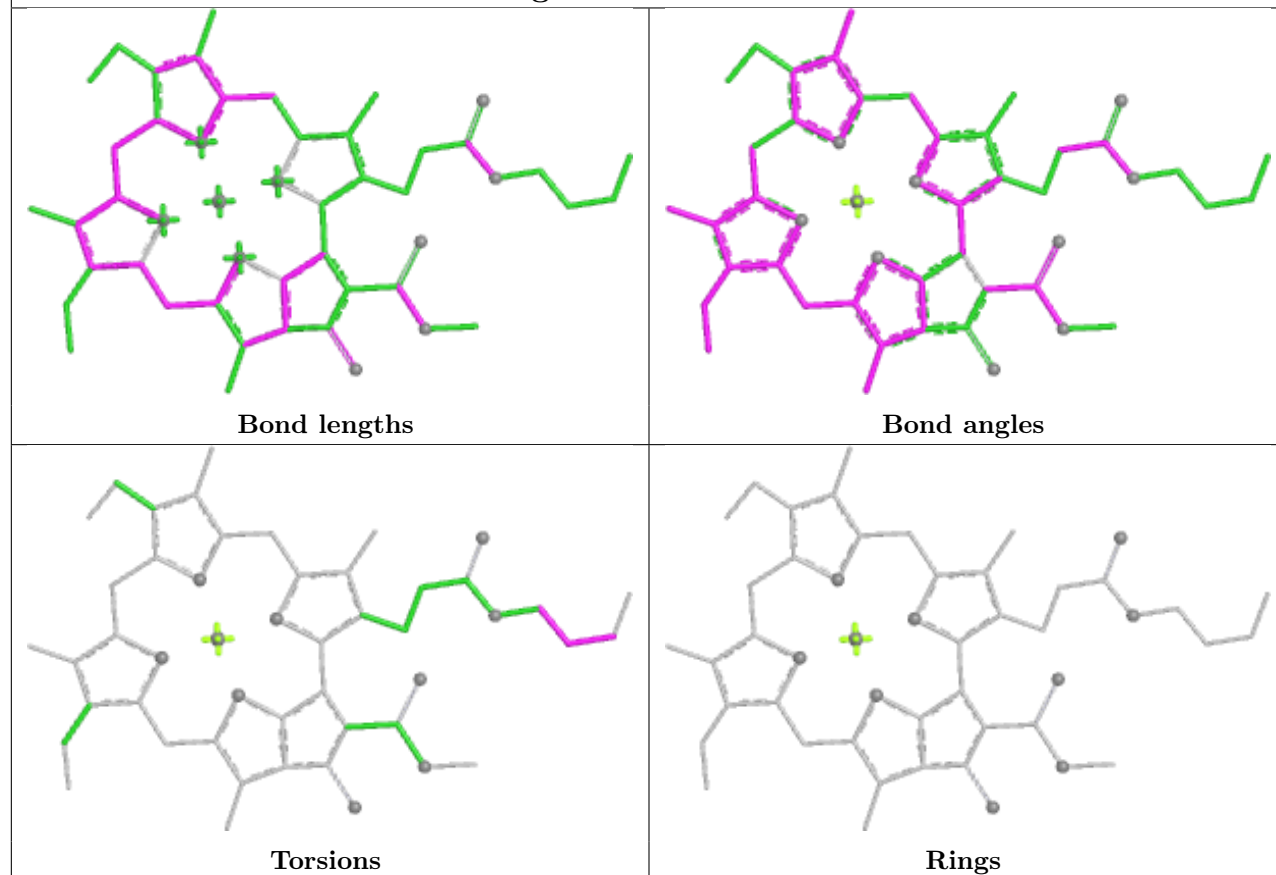
Ligand CLA 2 209



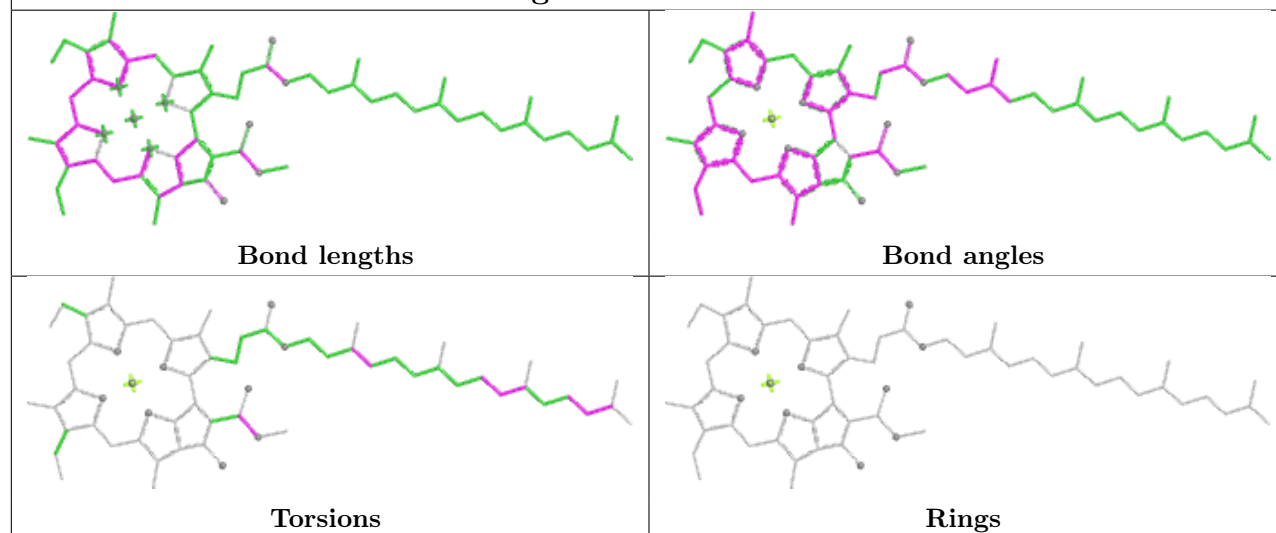
Ligand LHG 3 215

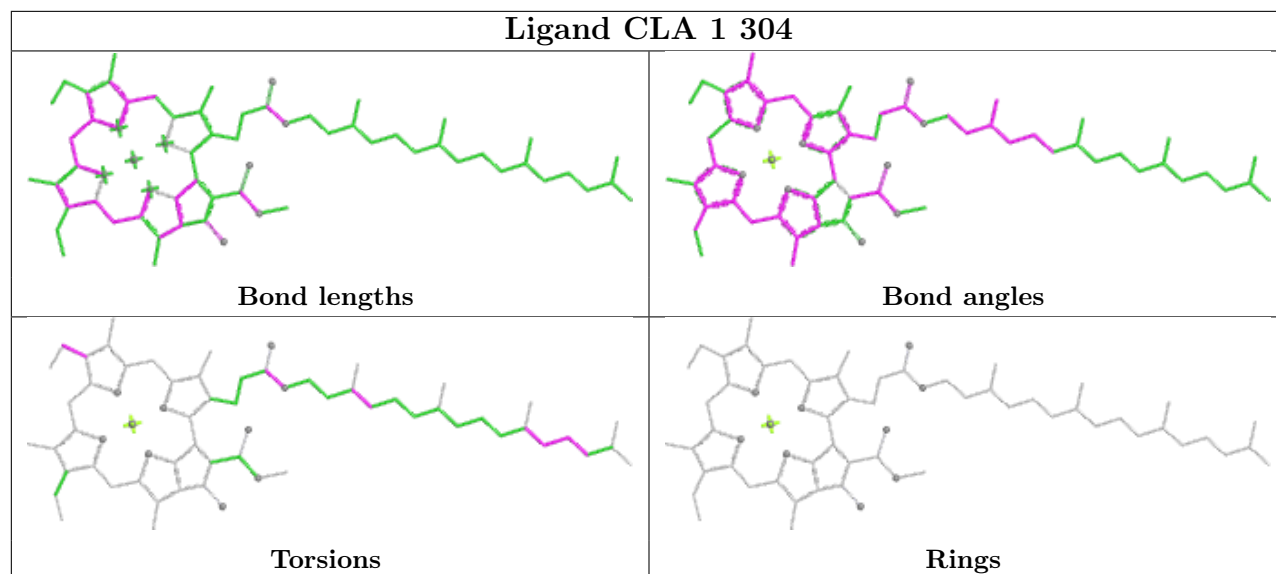
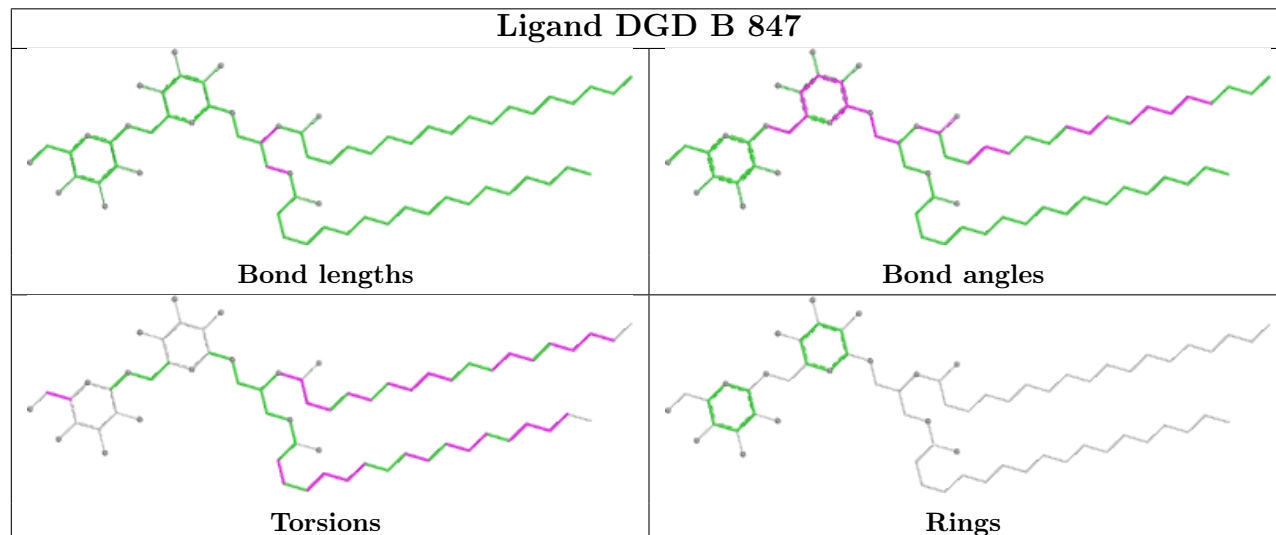


Ligand CLA A 823

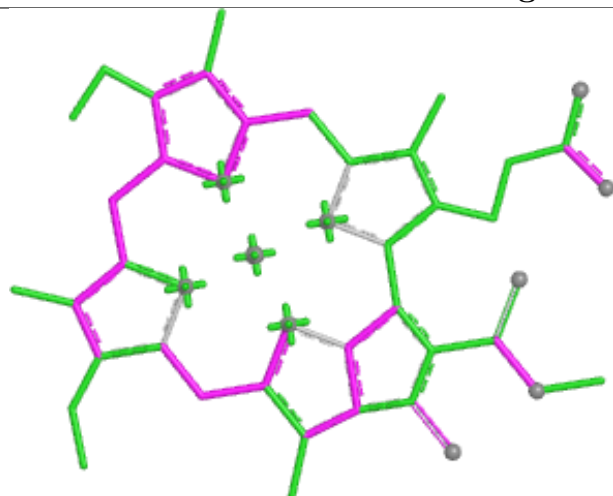


Ligand CLA A 834

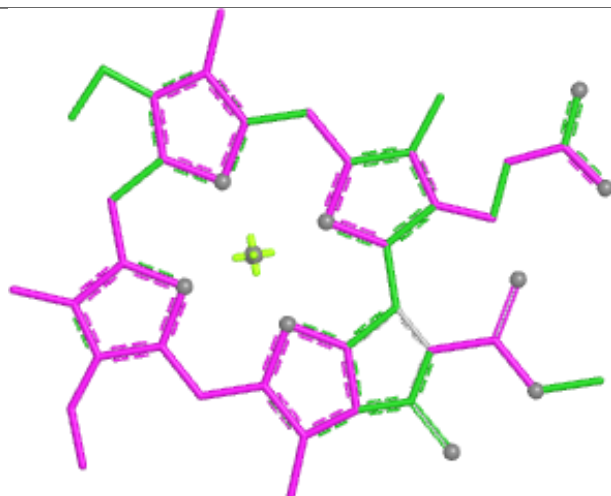


Ligand CLA 1 304**Ligand DGD B 847**

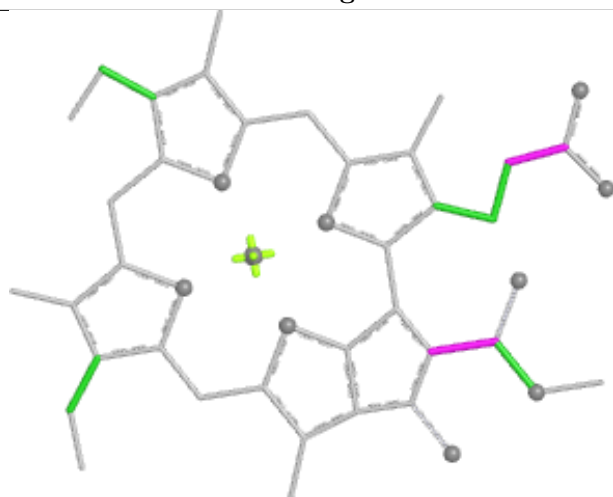
Ligand CLA 2 212



Bond lengths



Bond angles

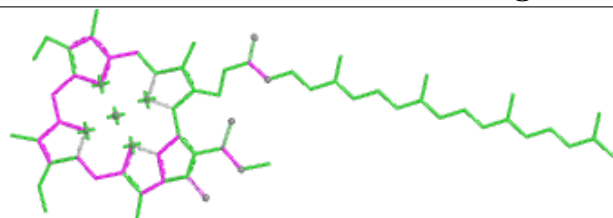


Torsions

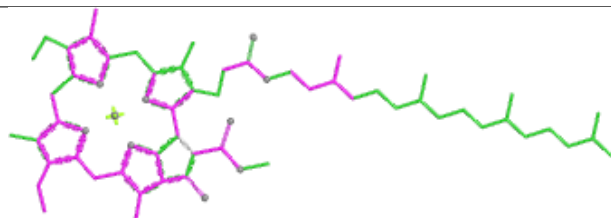


Rings

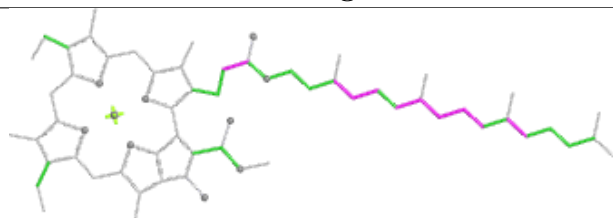
Ligand CLA A 828



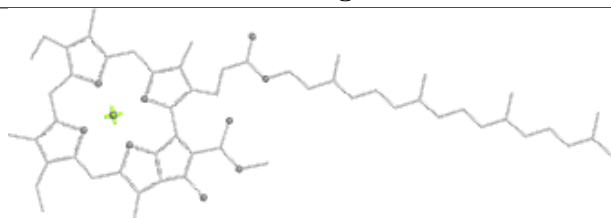
Bond lengths



Bond angles

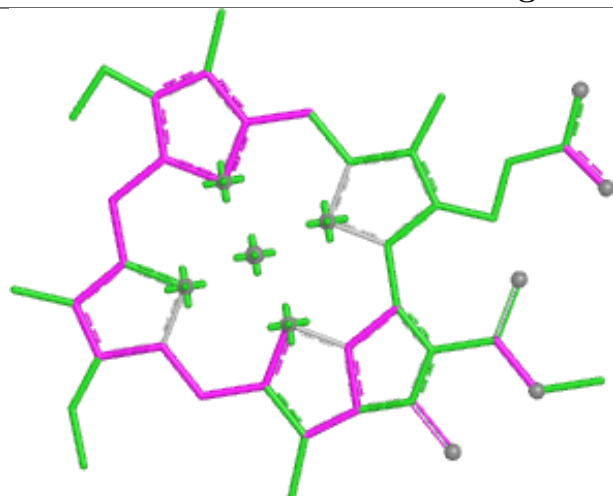


Torsions

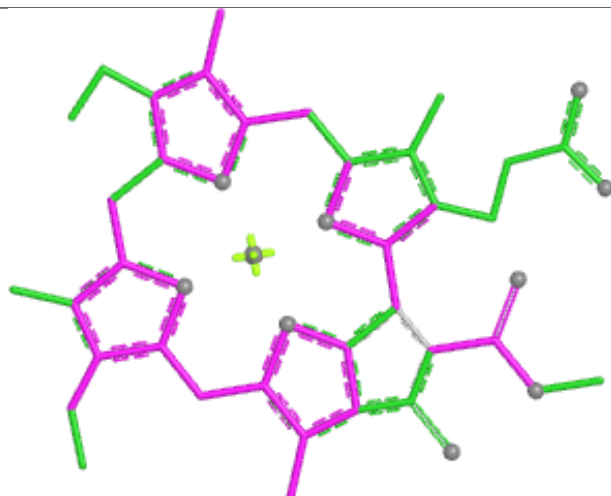


Rings

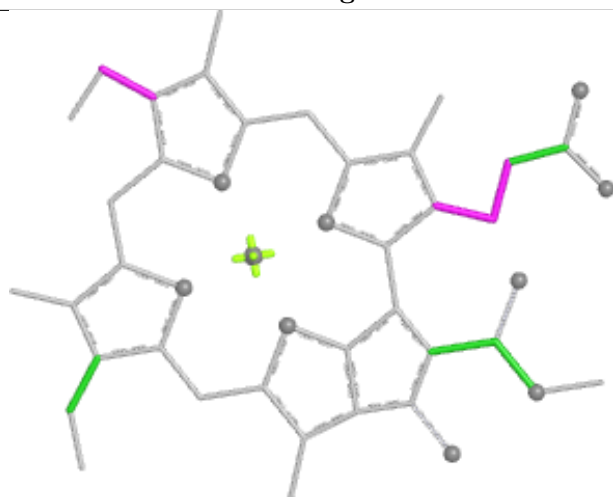
Ligand CLA 4 310



Bond lengths



Bond angles

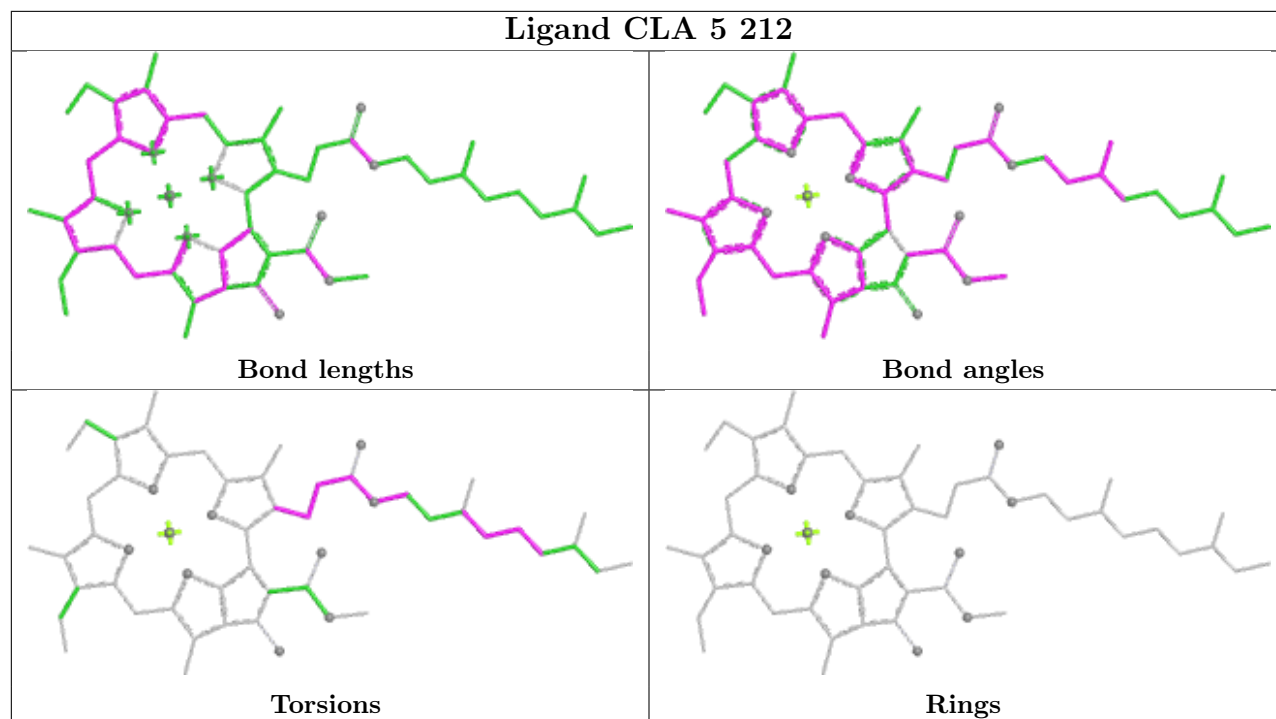


Torsions

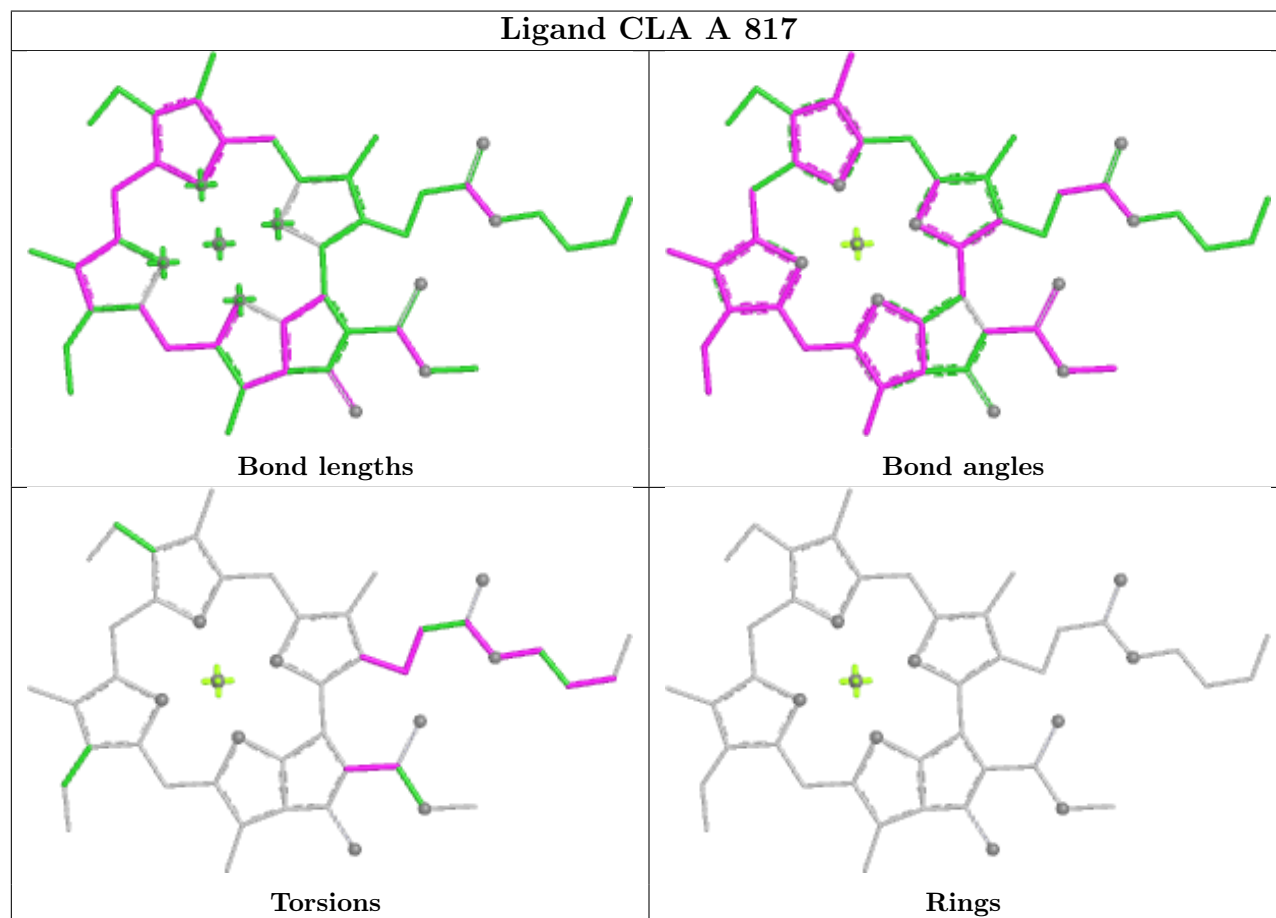


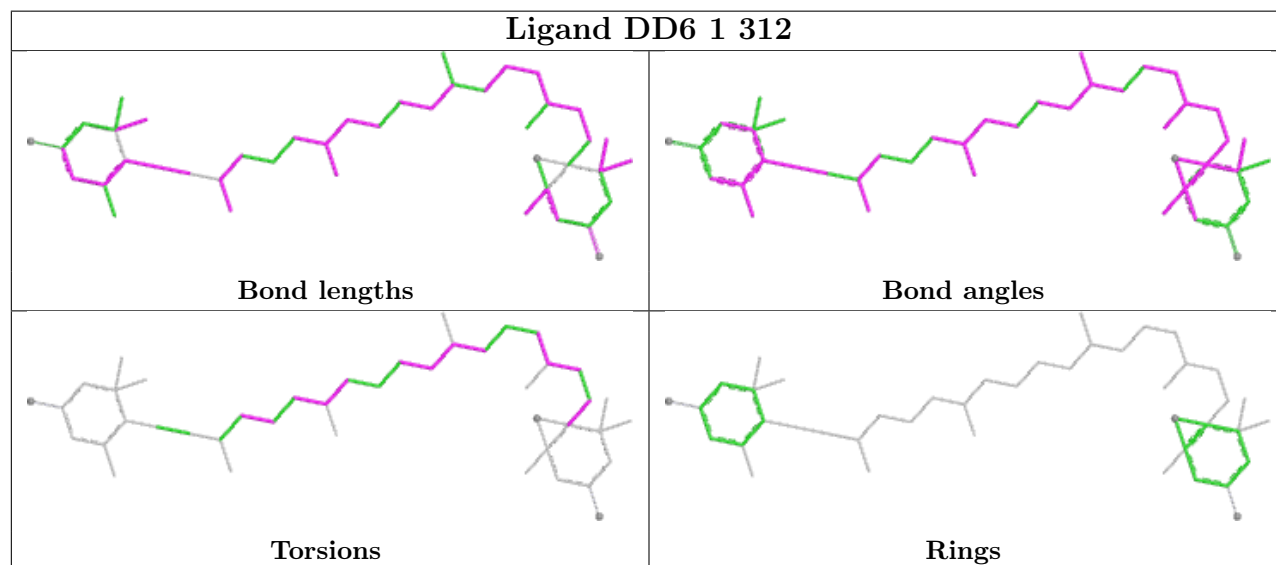
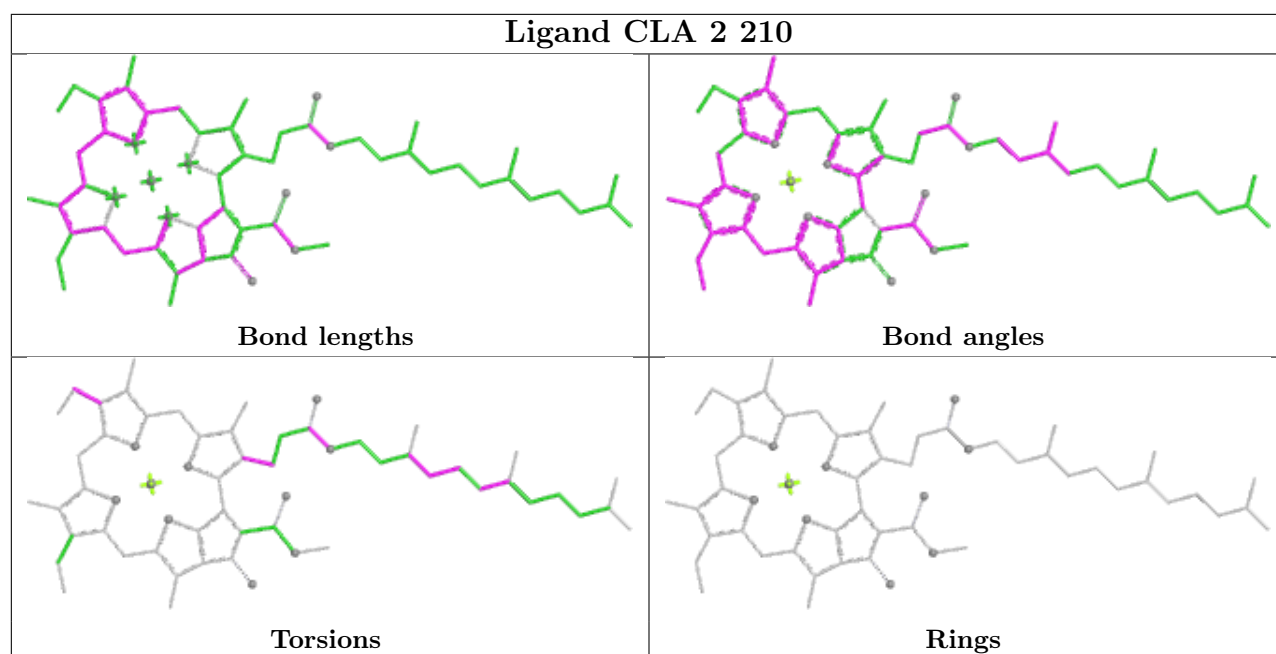
Rings

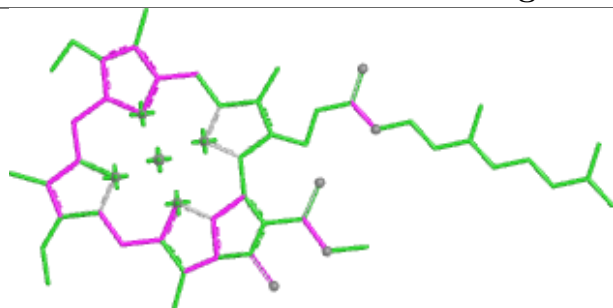
Ligand CLA 5 212



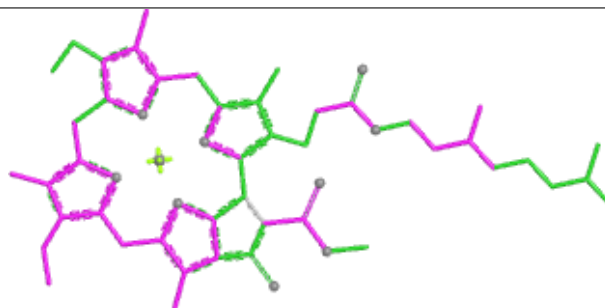
Ligand CLA A 817



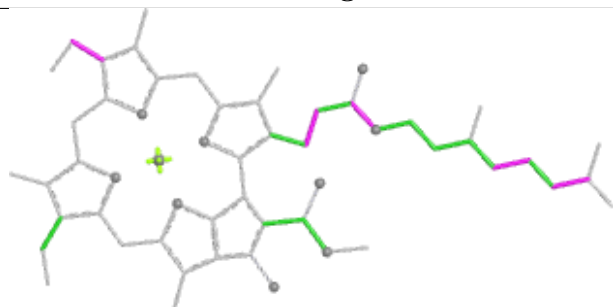


Ligand CLA 3 203

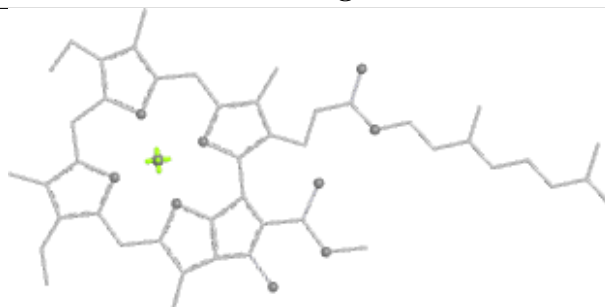
Bond lengths



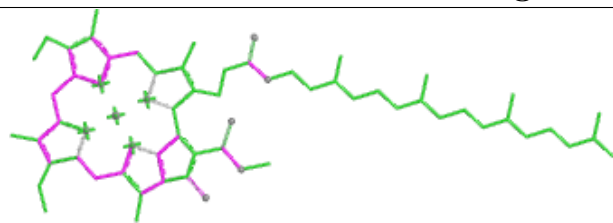
Bond angles



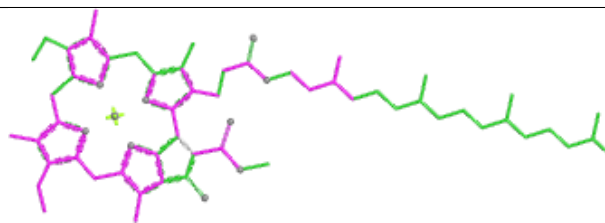
Torsions



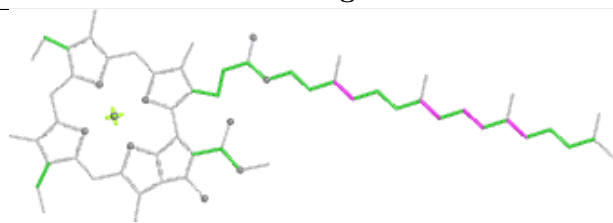
Rings

Ligand CLA A 808

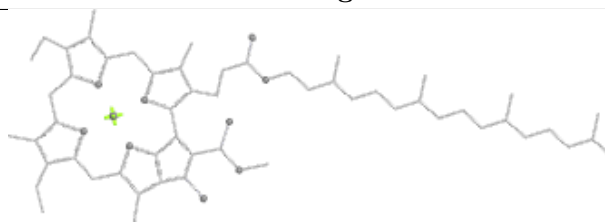
Bond lengths



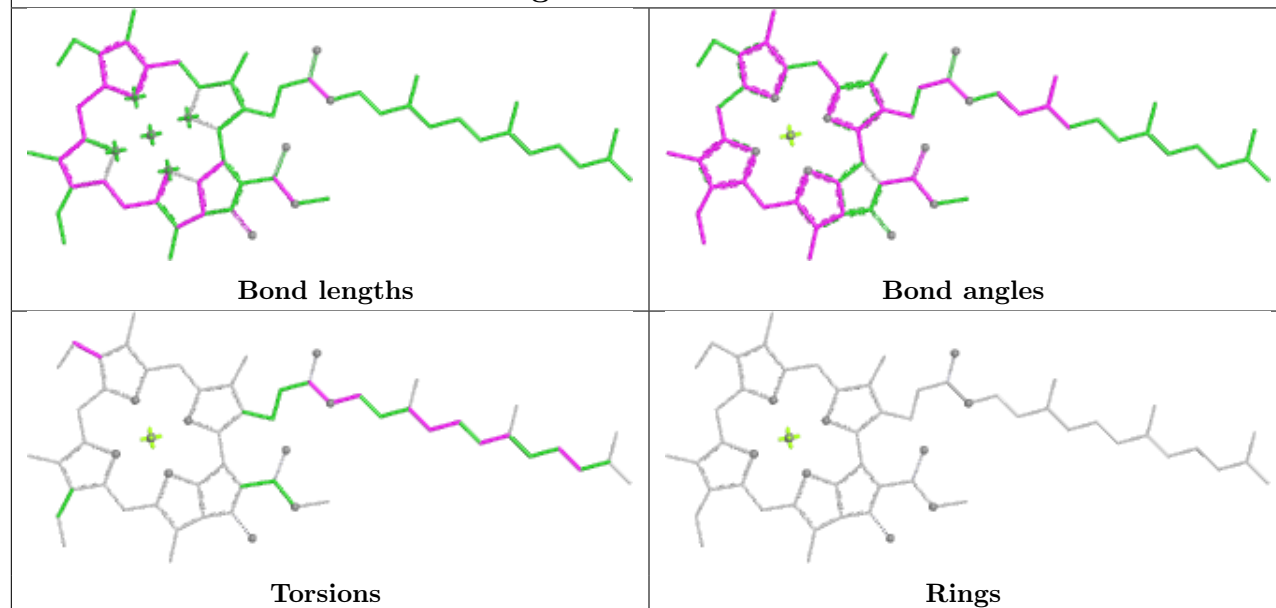
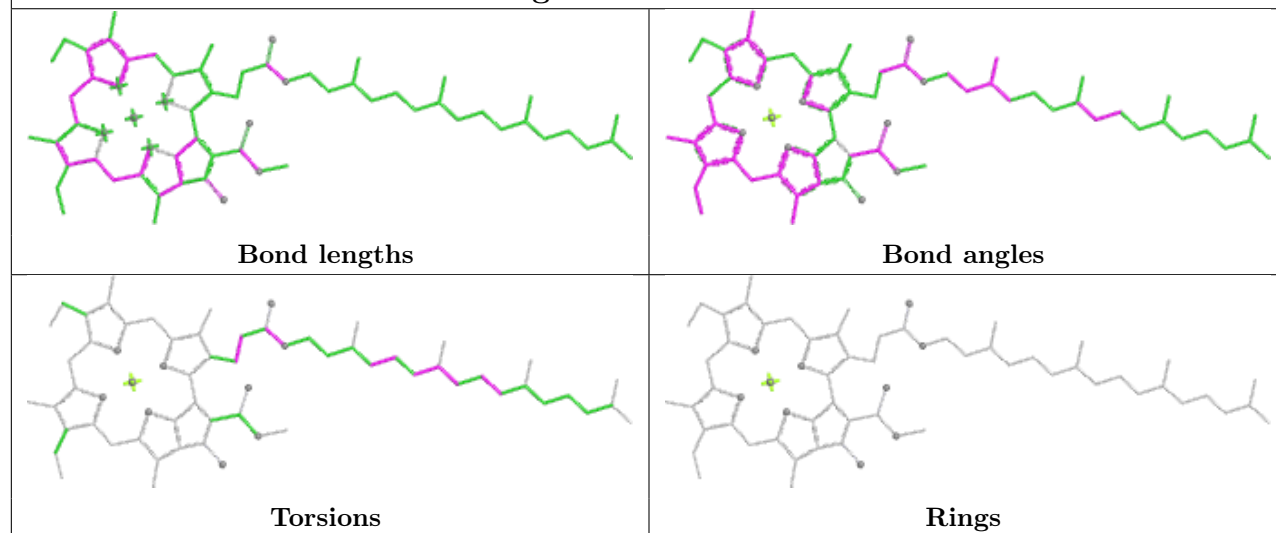
Bond angles

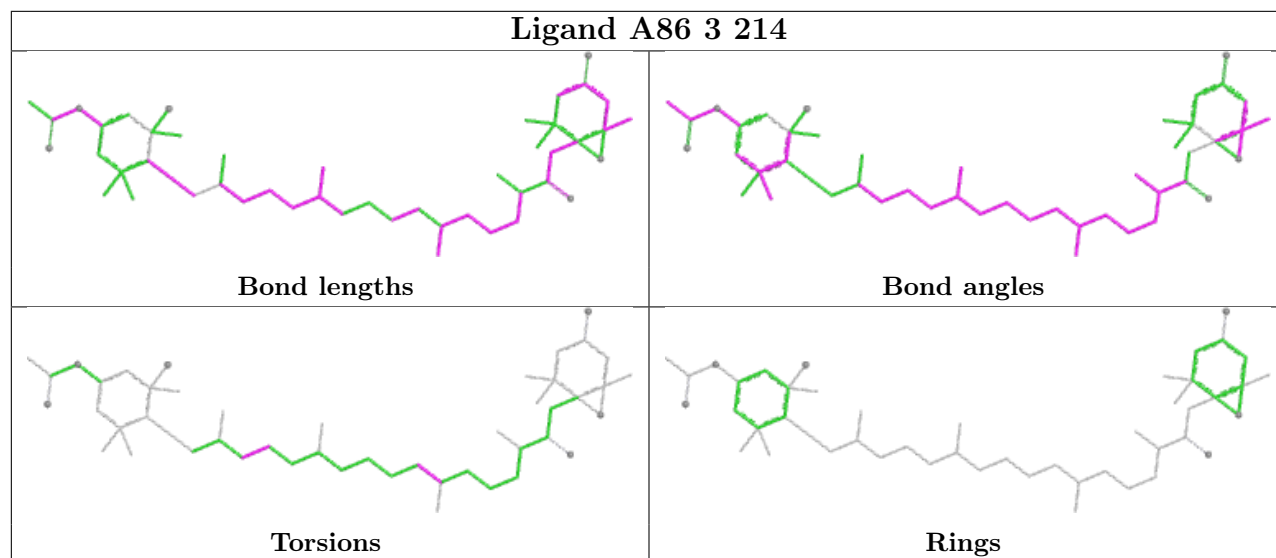
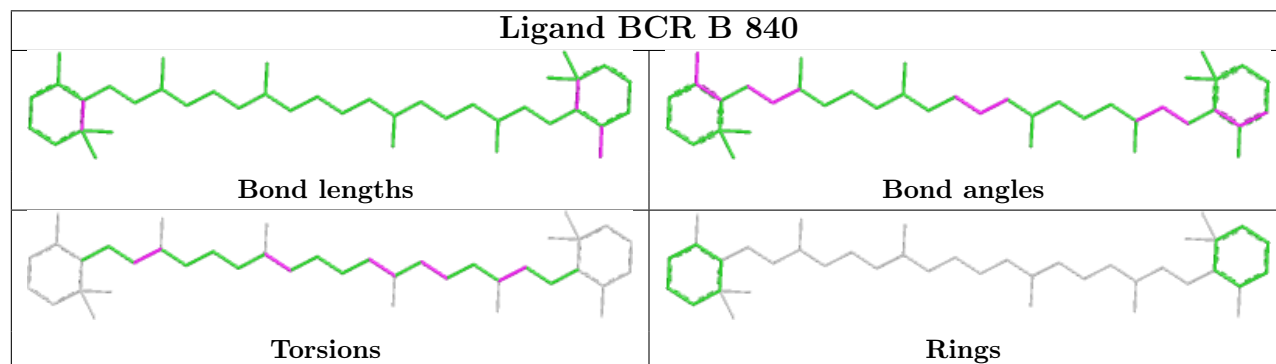
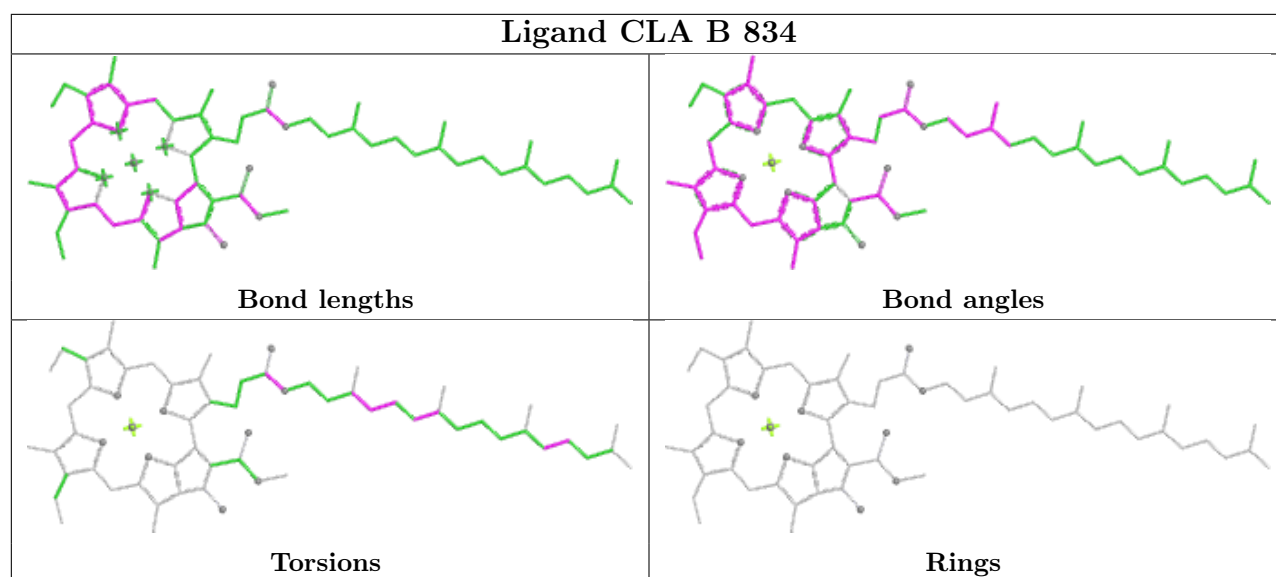


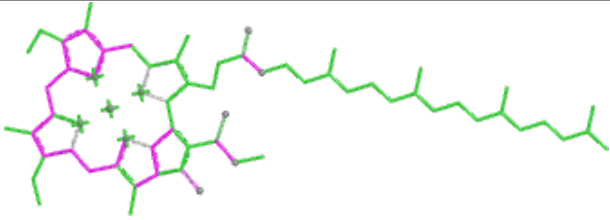
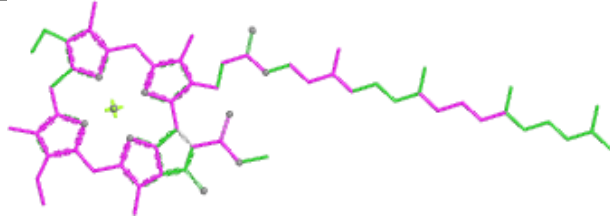
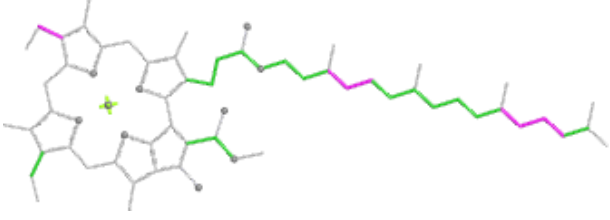
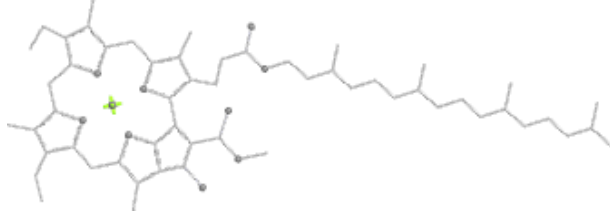
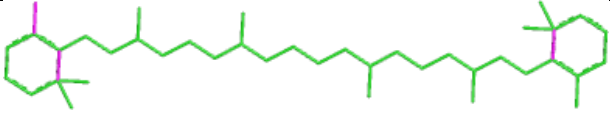
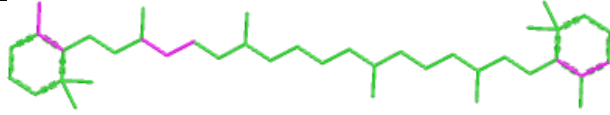
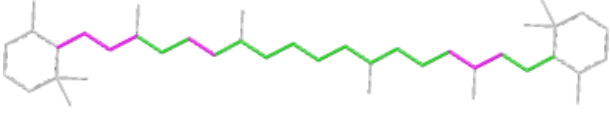
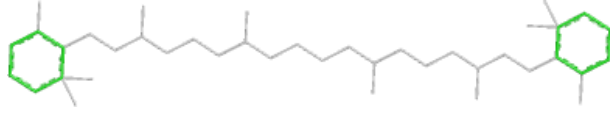
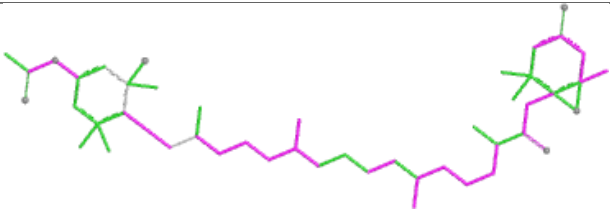
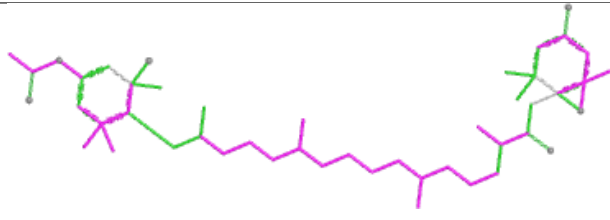
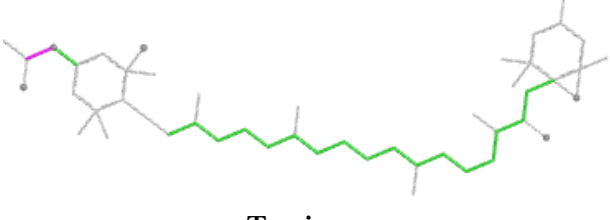
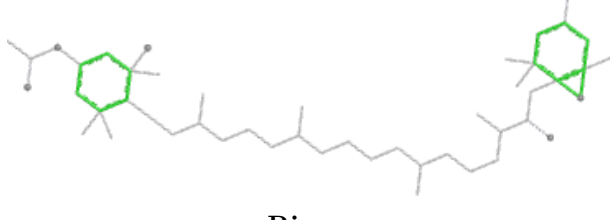
Torsions

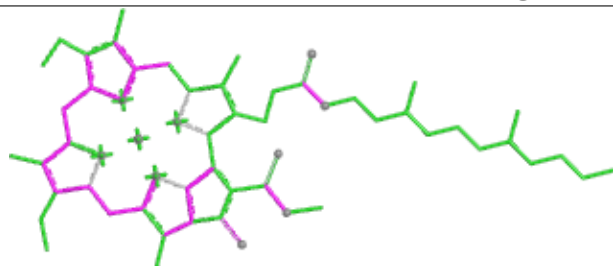
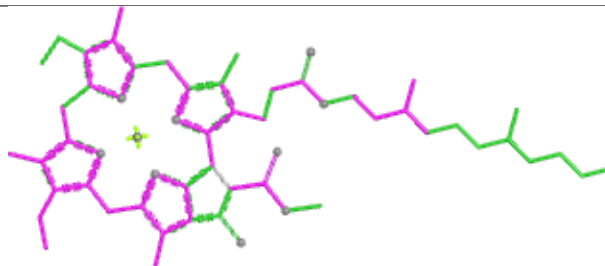
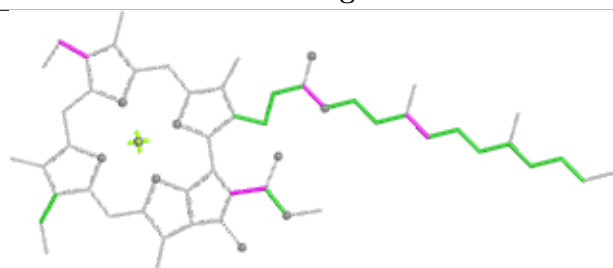
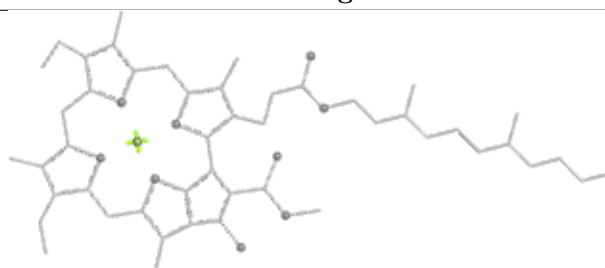
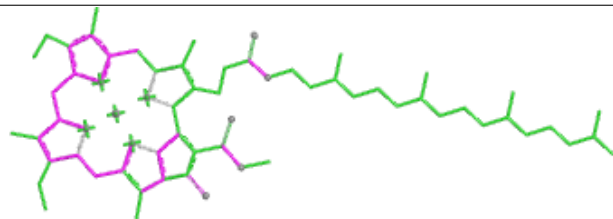
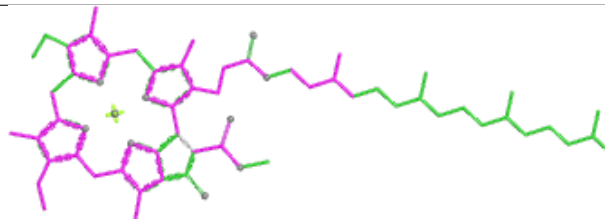
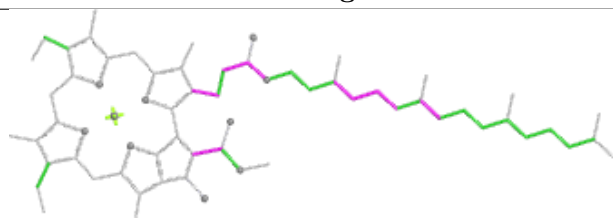
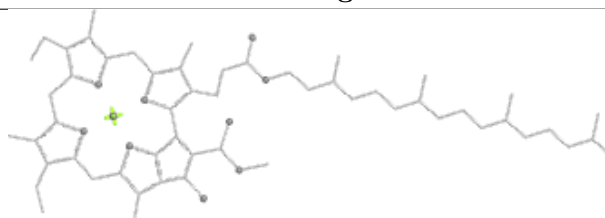


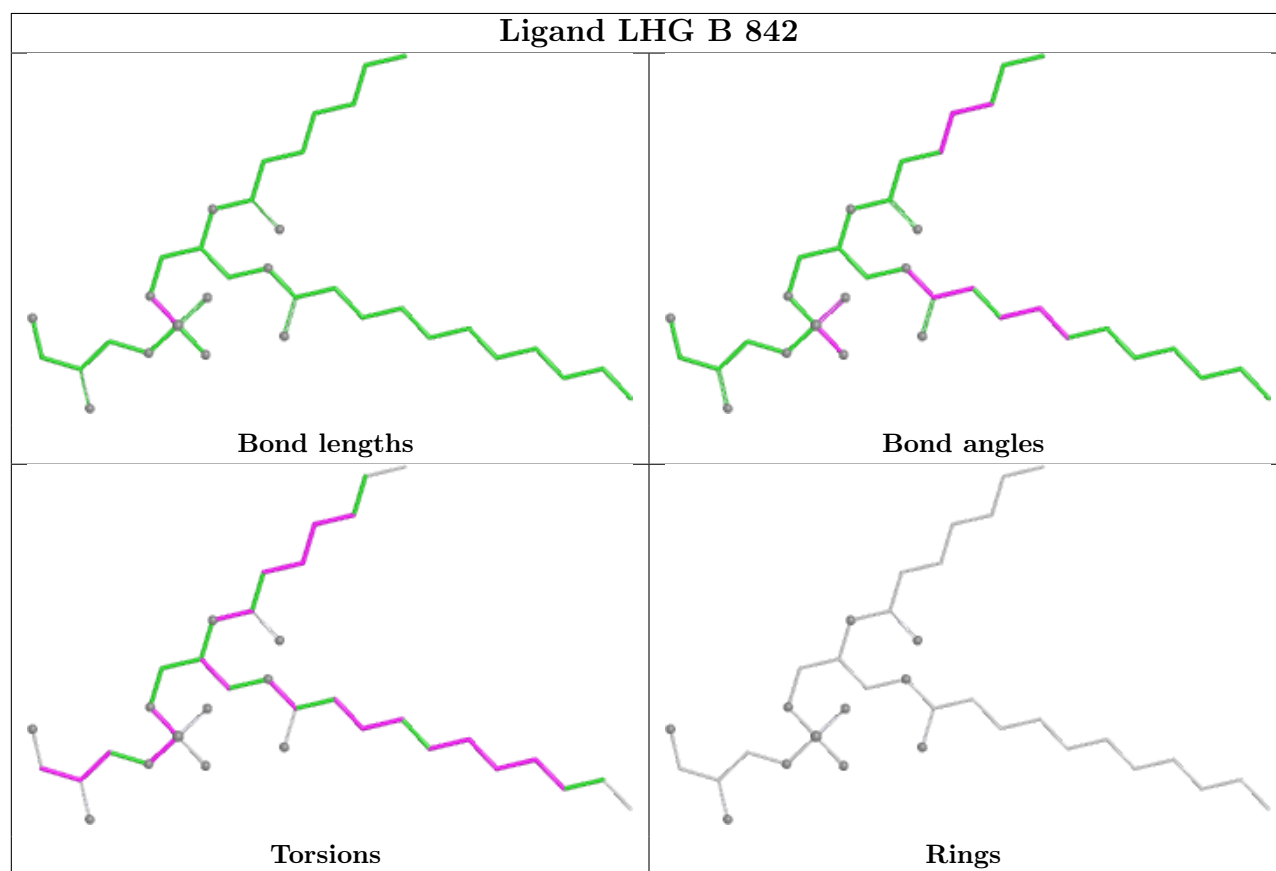
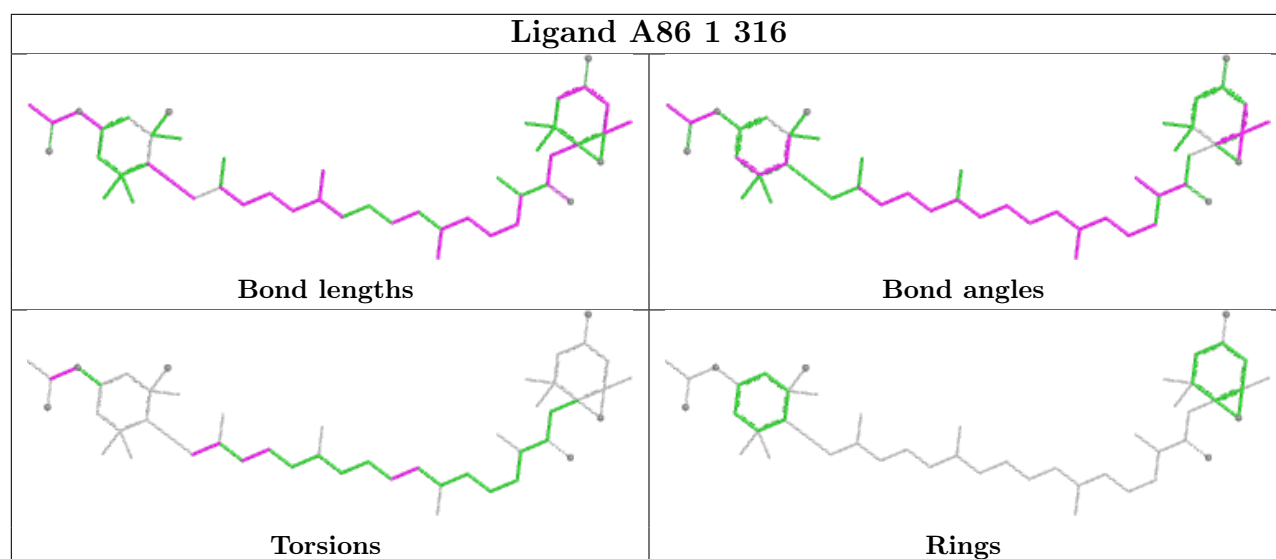
Rings

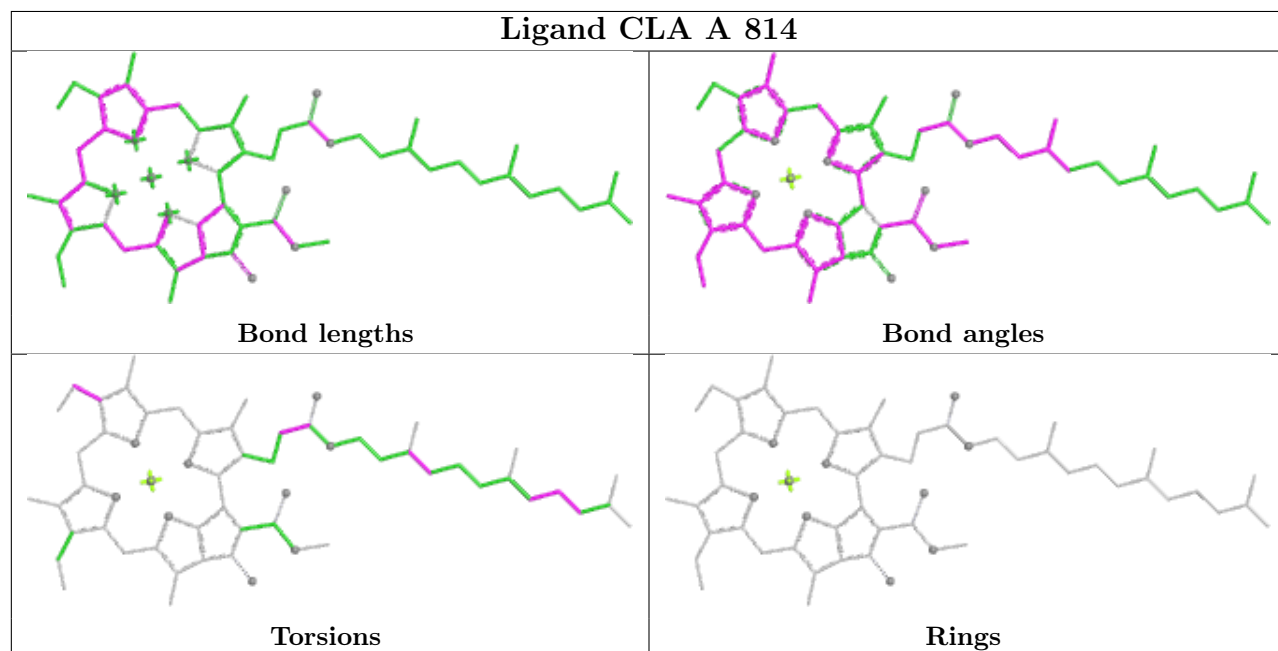
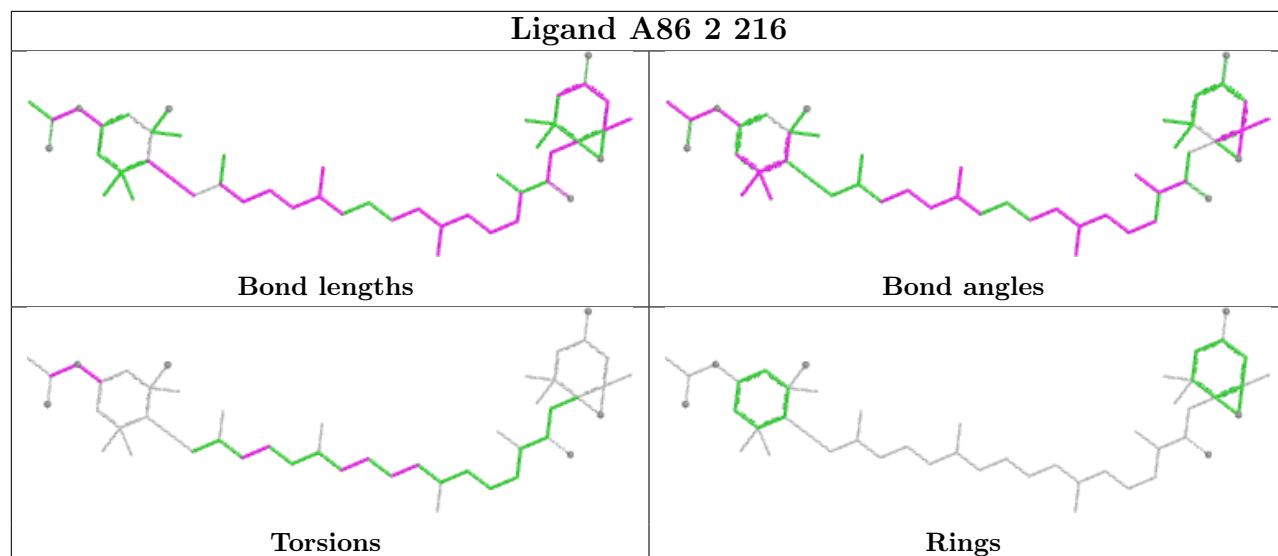
Ligand CLA A 832**Ligand CLA B 818**

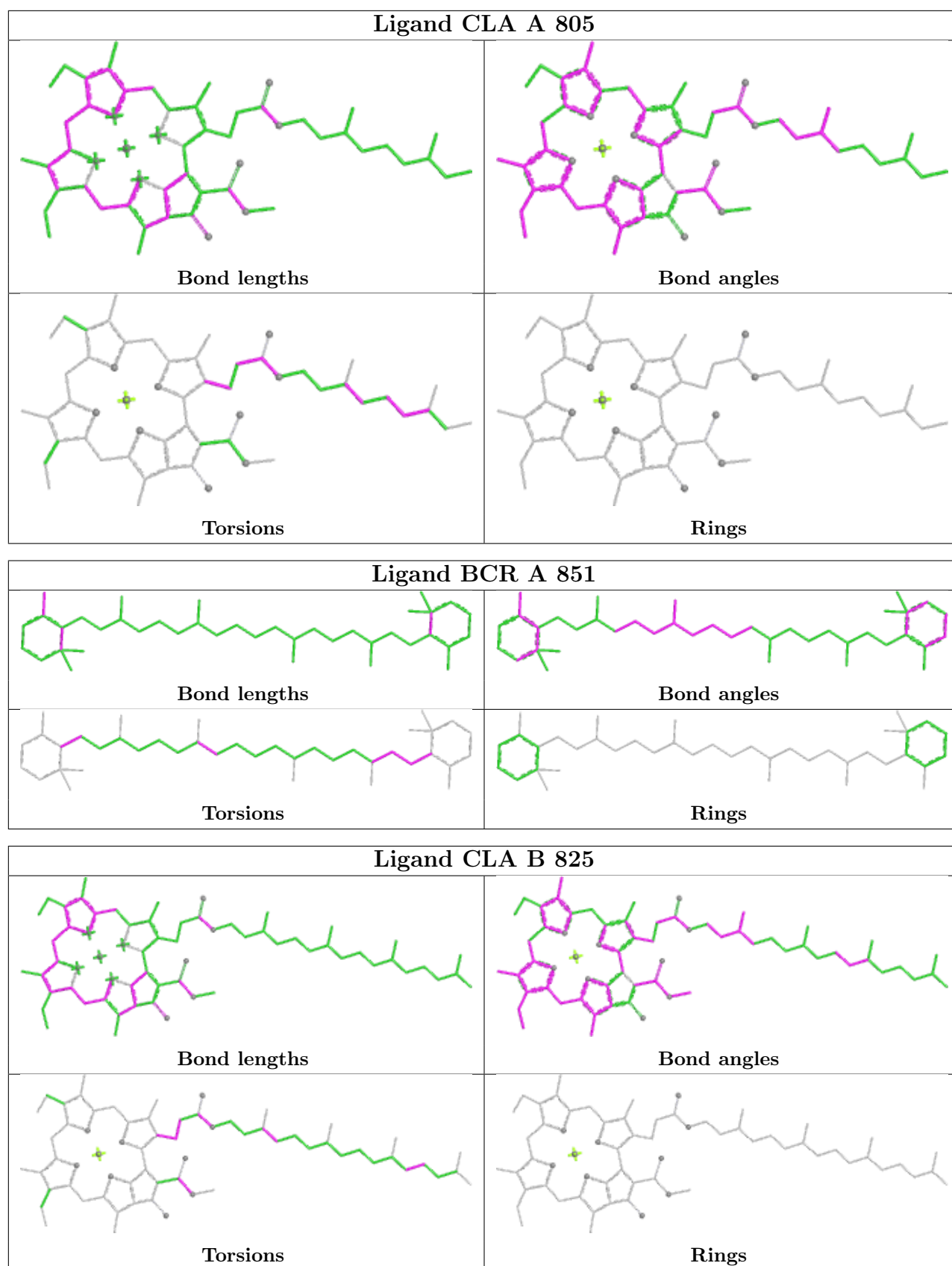


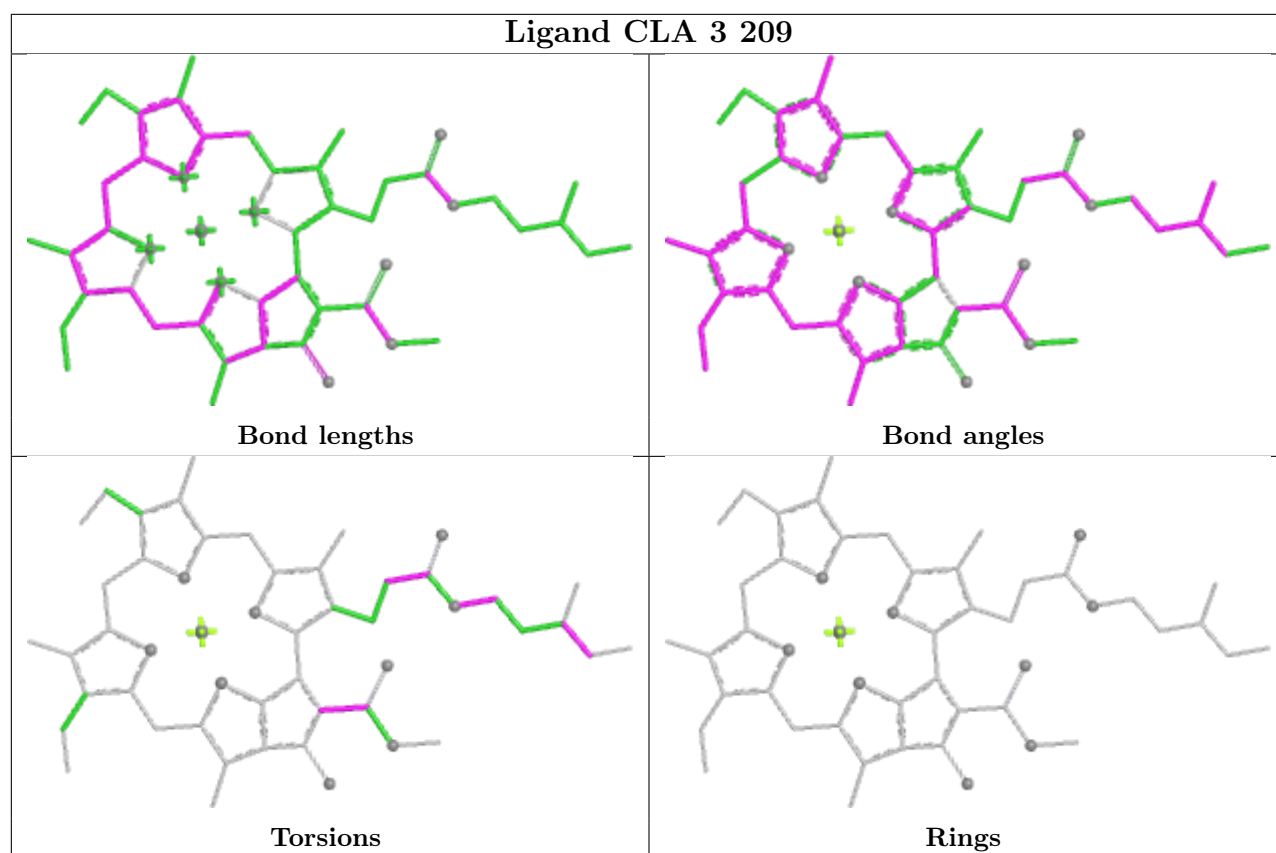
Ligand CLA B 831	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR J 104	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand A86 2 218	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 830**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 804****Bond lengths****Bond angles****Torsions****Rings**

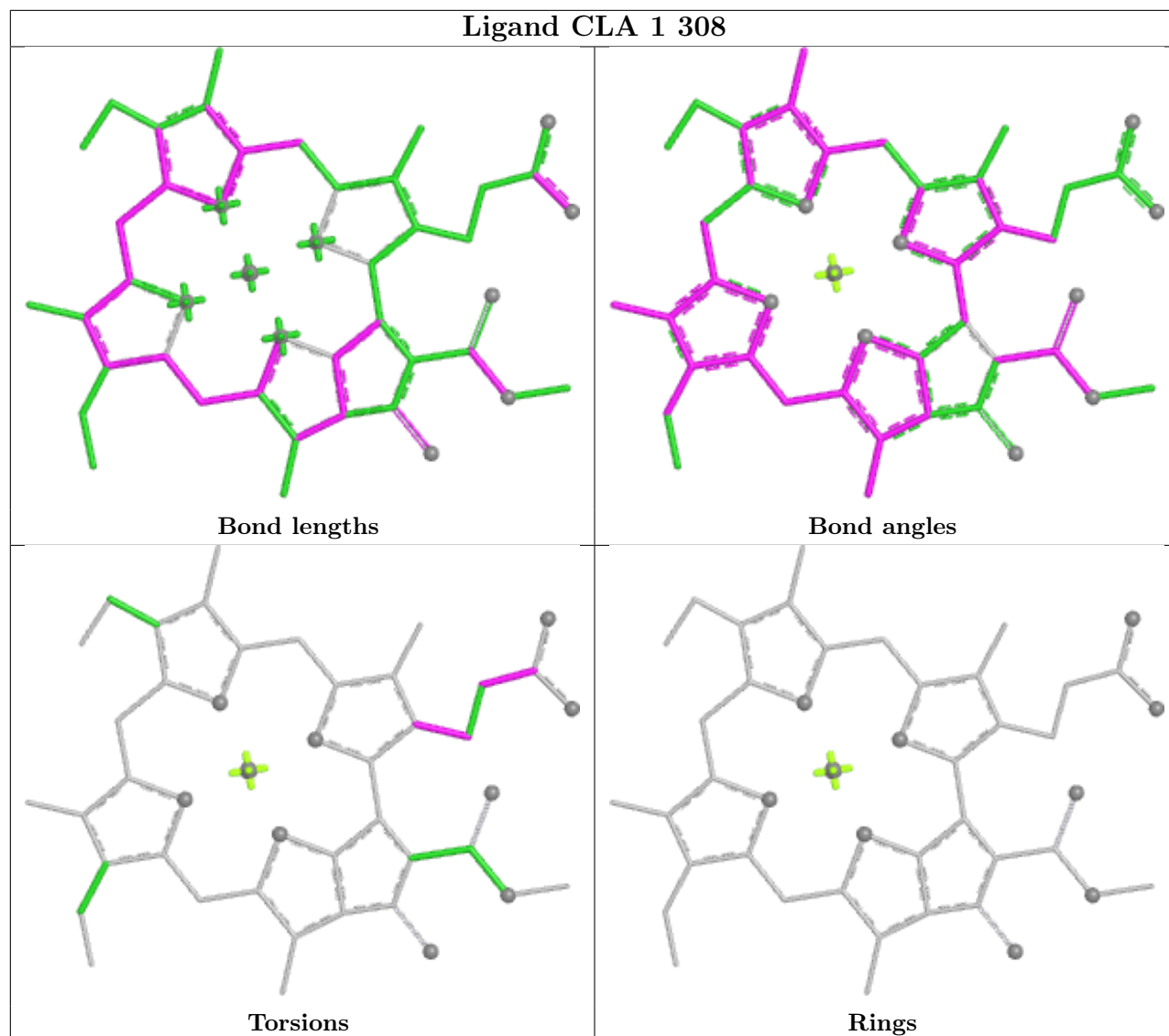




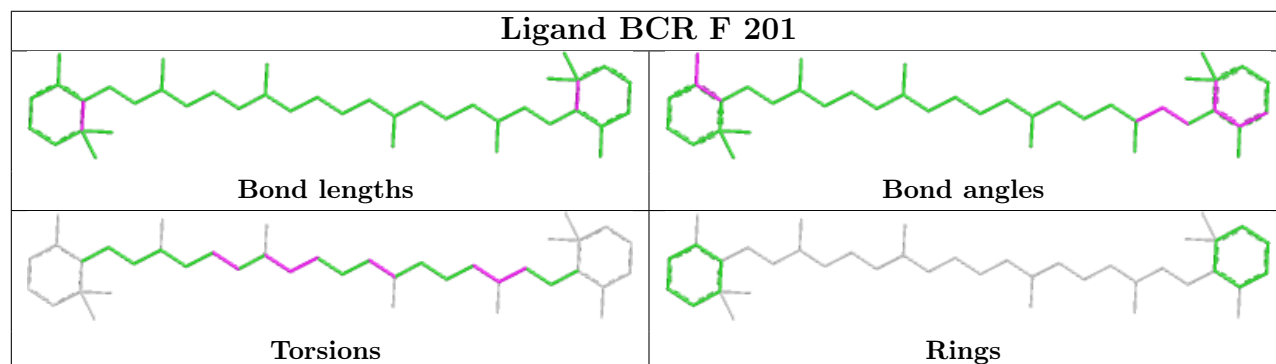


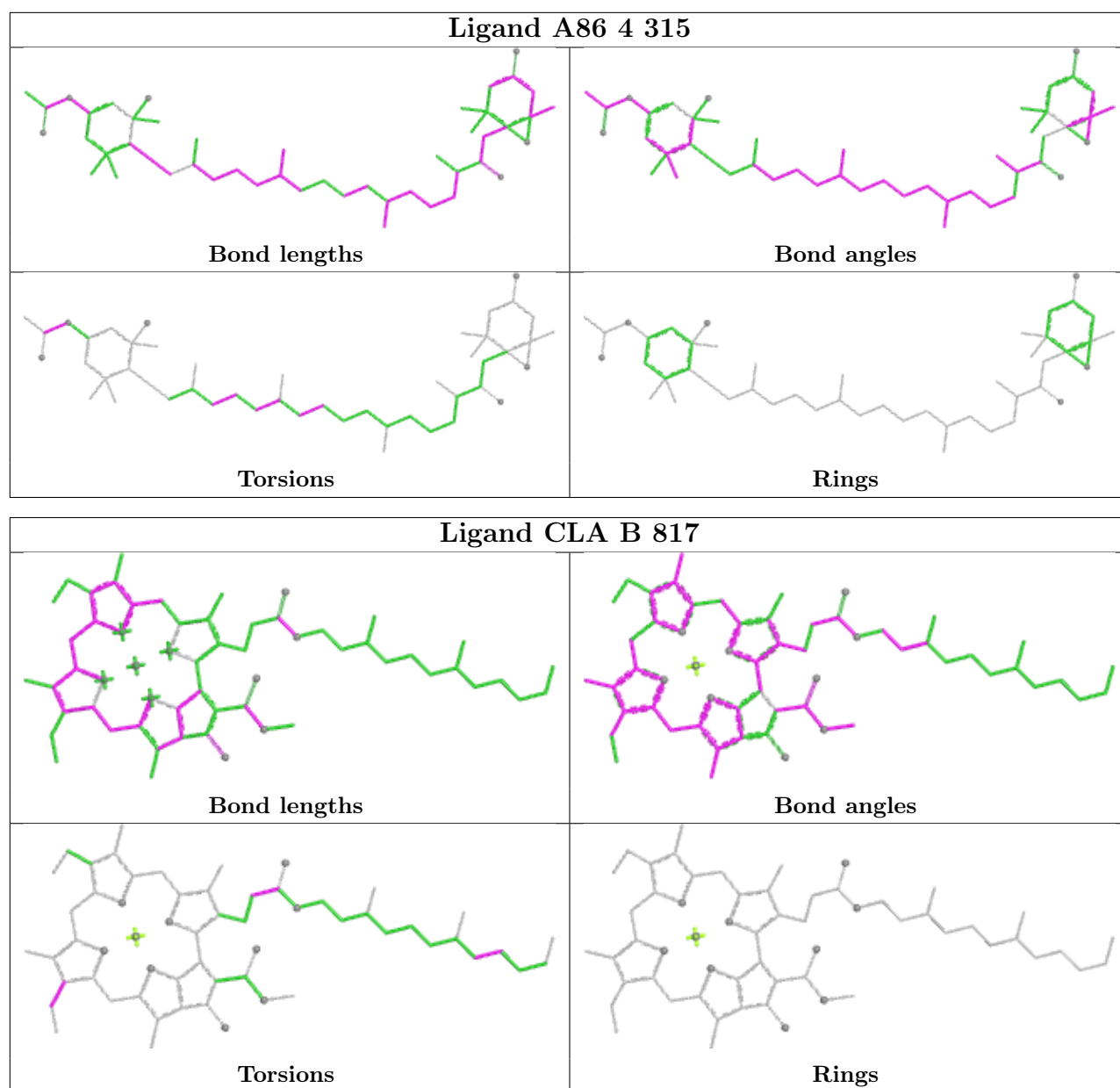


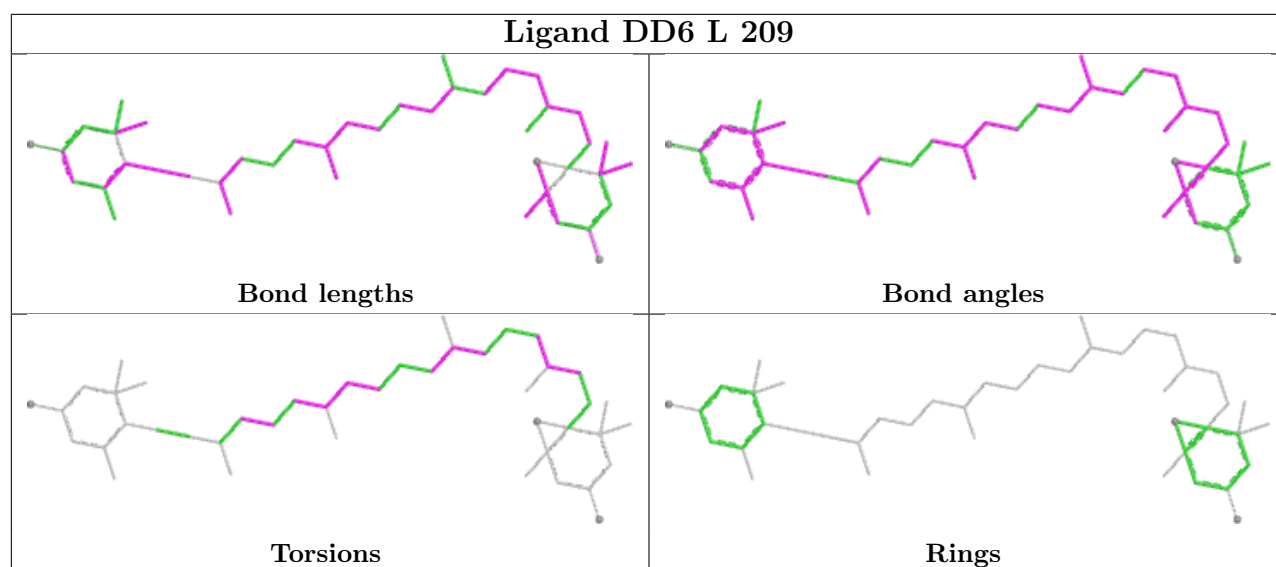
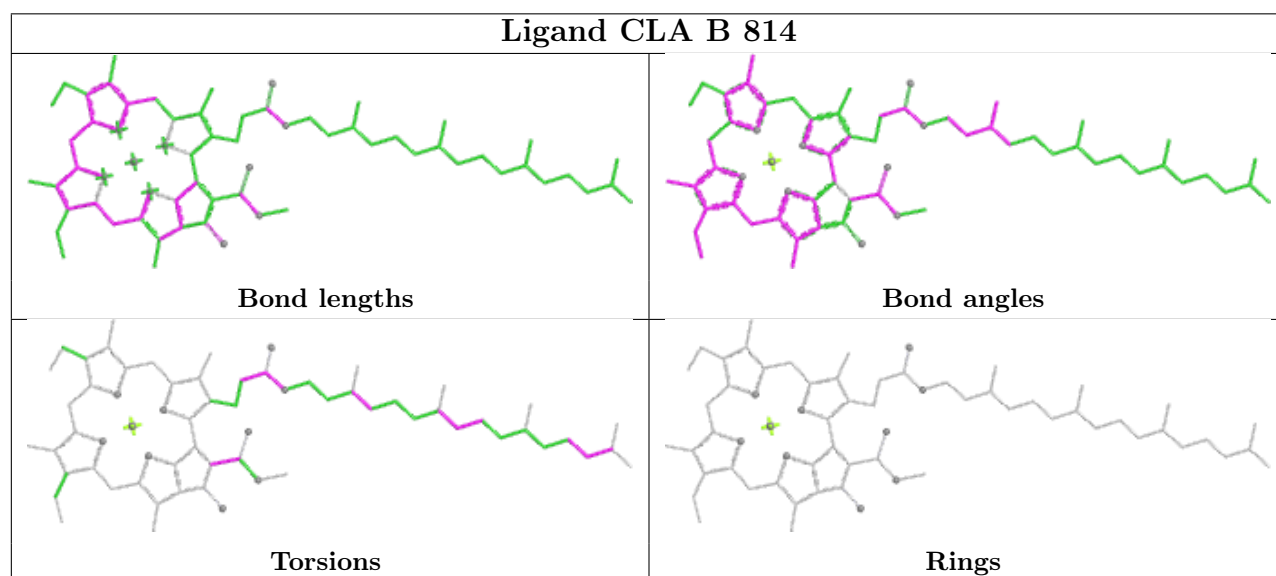
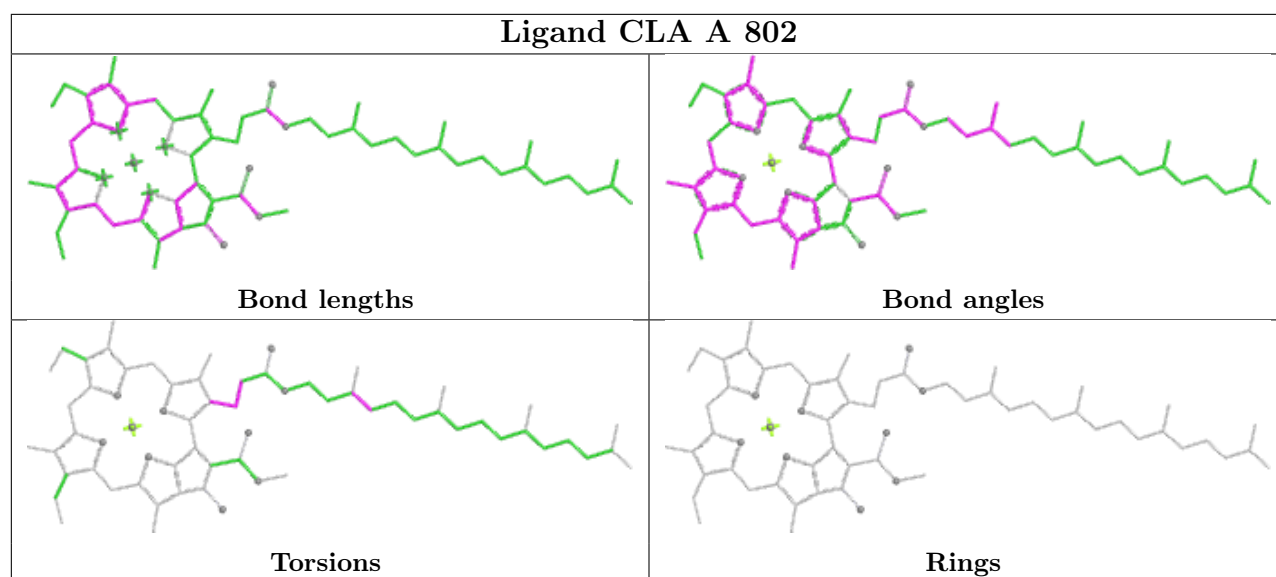
Ligand CLA 1 308



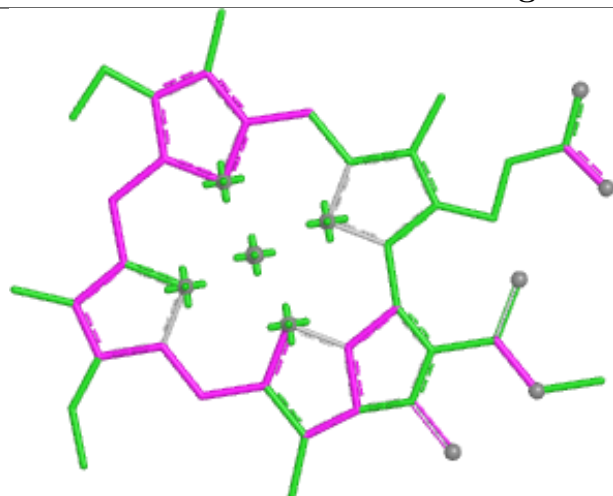
Ligand BCR F 201



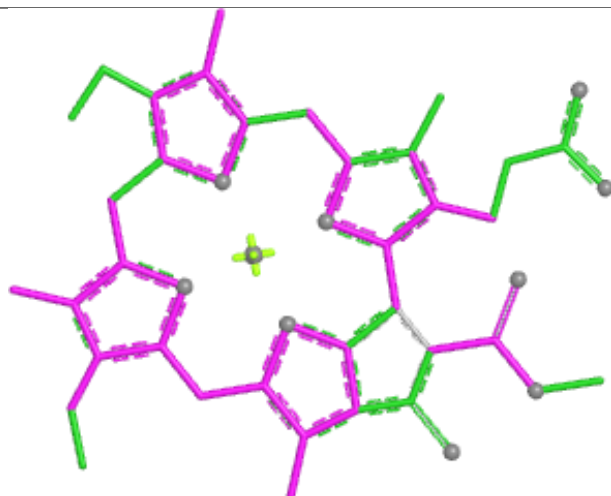




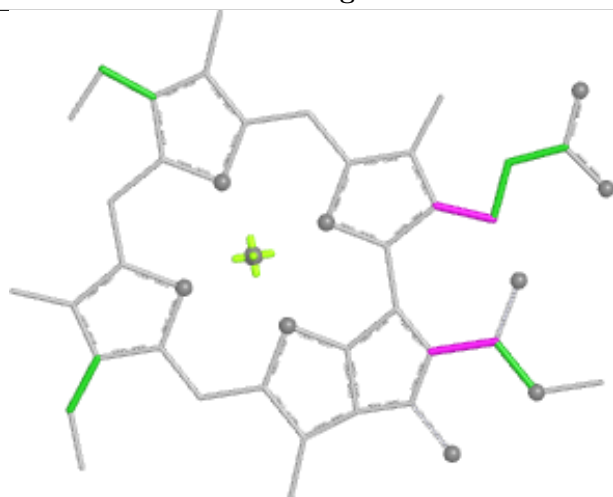
Ligand CLA 5 215



Bond lengths



Bond angles

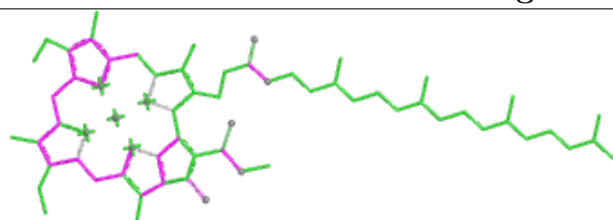


Torsions

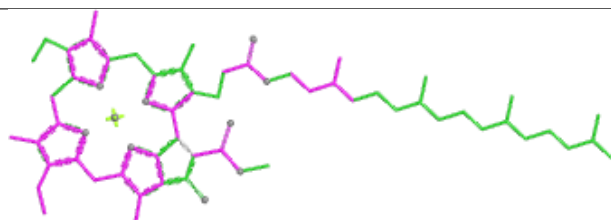


Rings

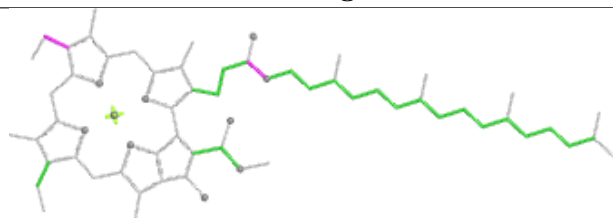
Ligand CLA L 203



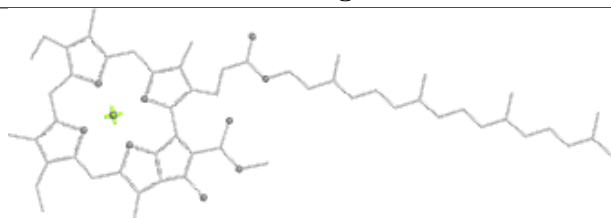
Bond lengths



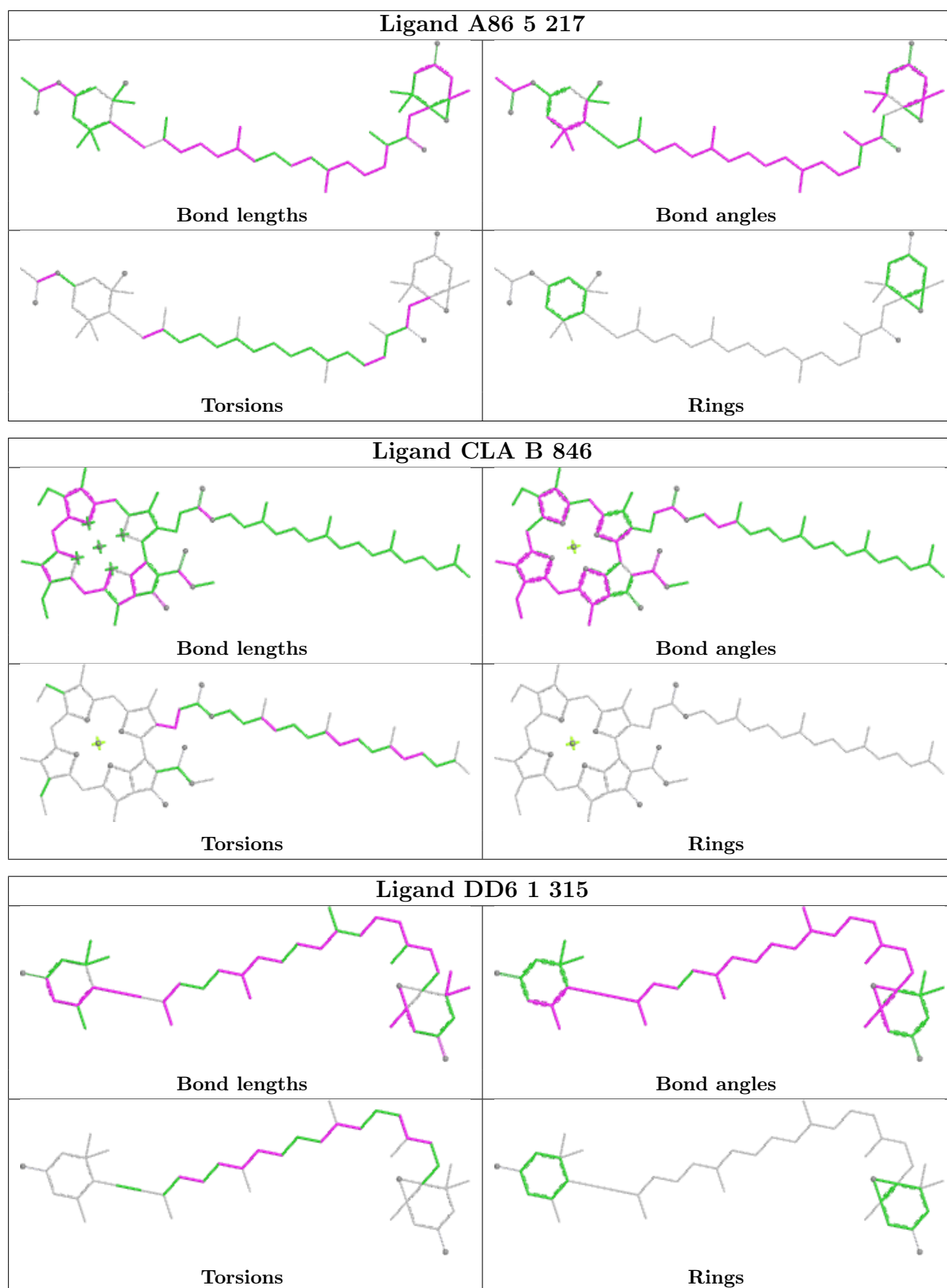
Bond angles

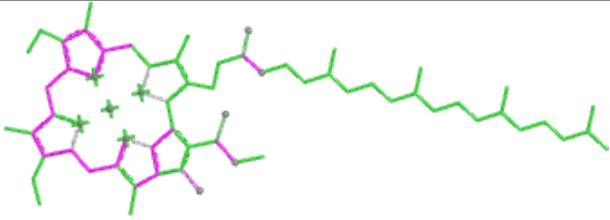
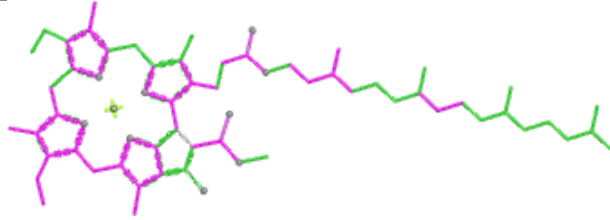
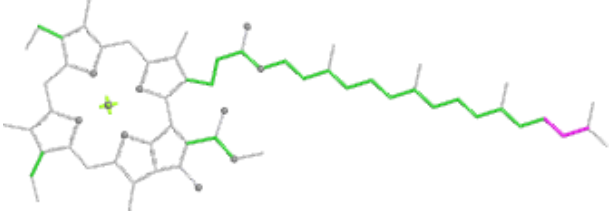
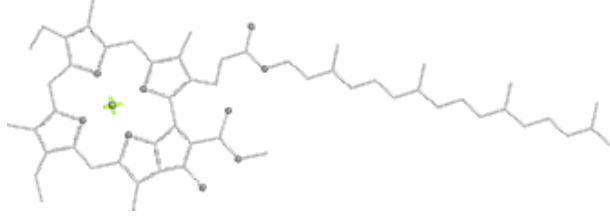


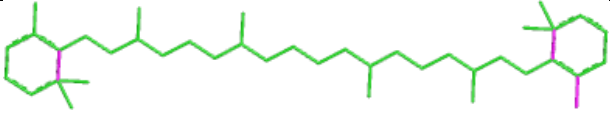
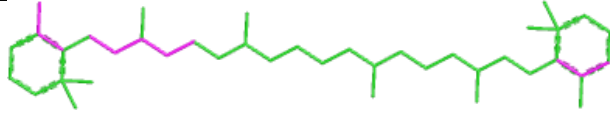
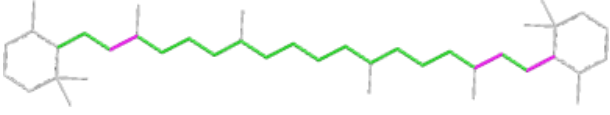
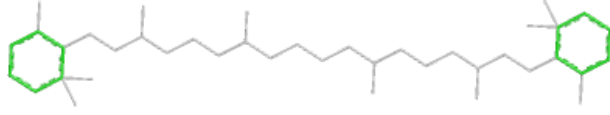
Torsions



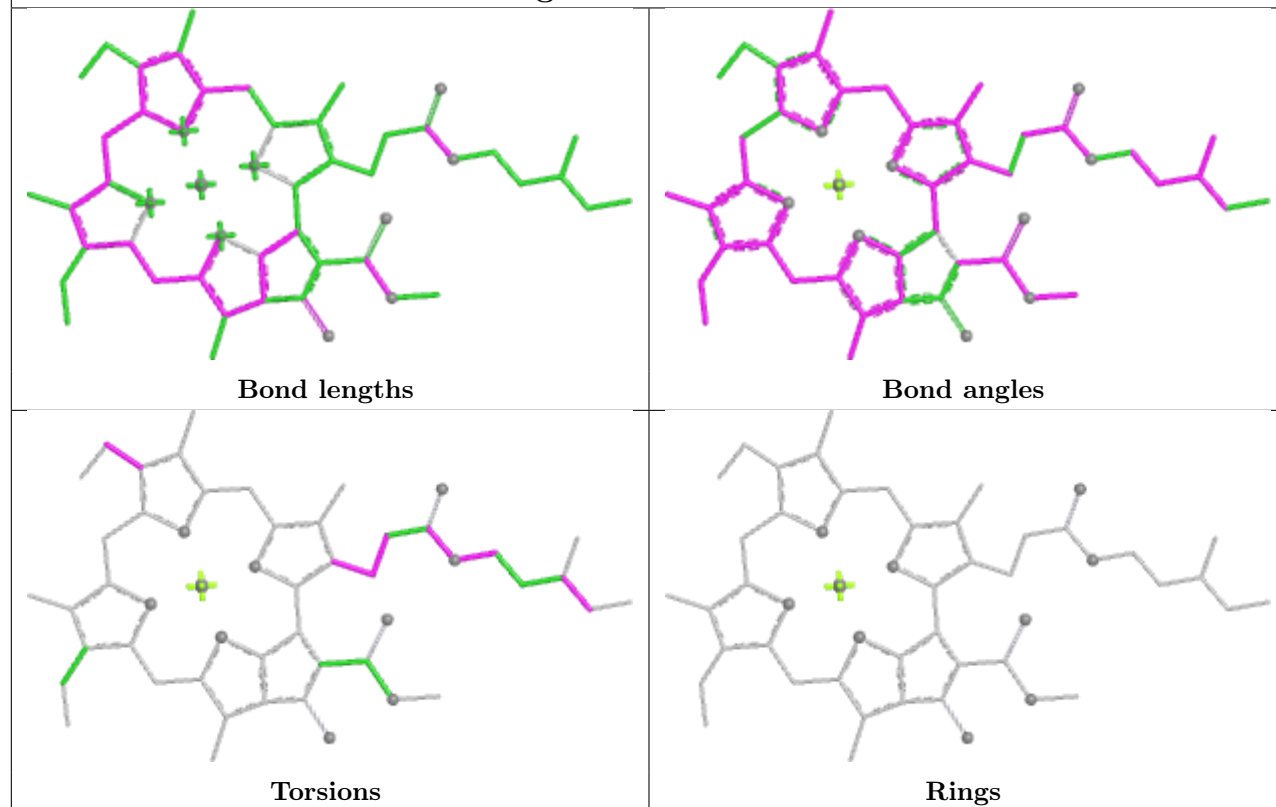
Rings



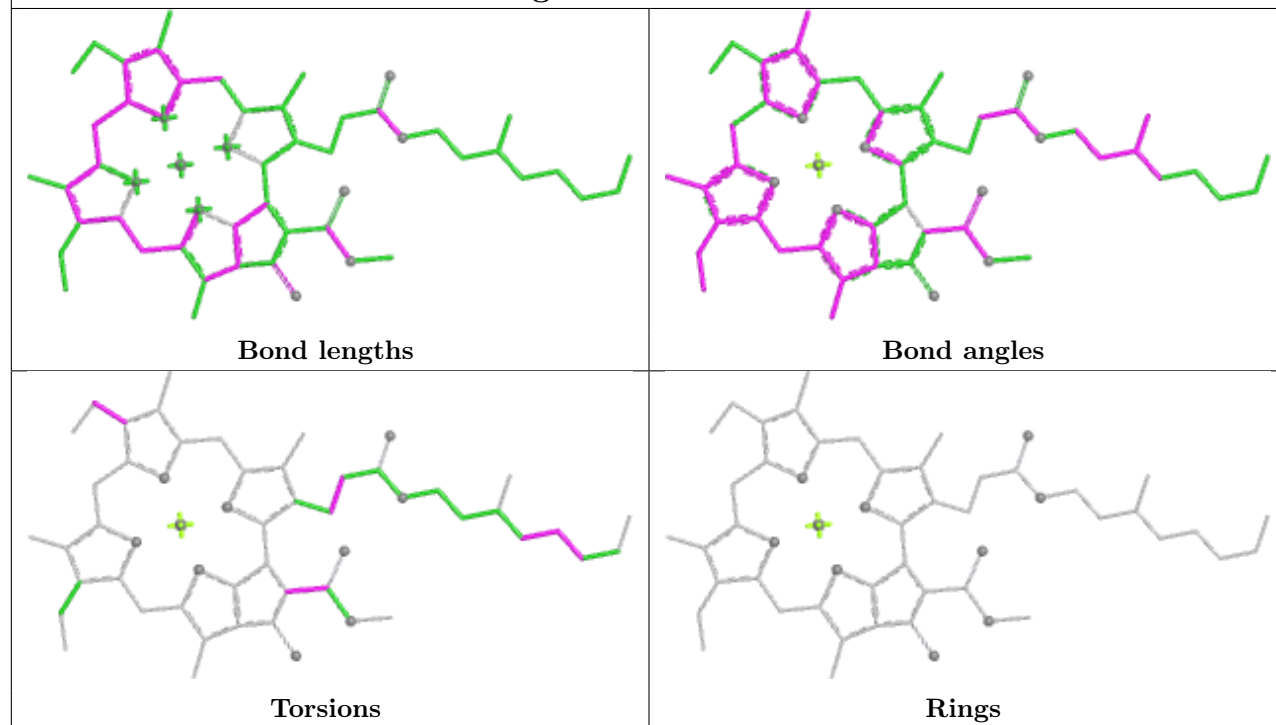
Ligand CLA A 880			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

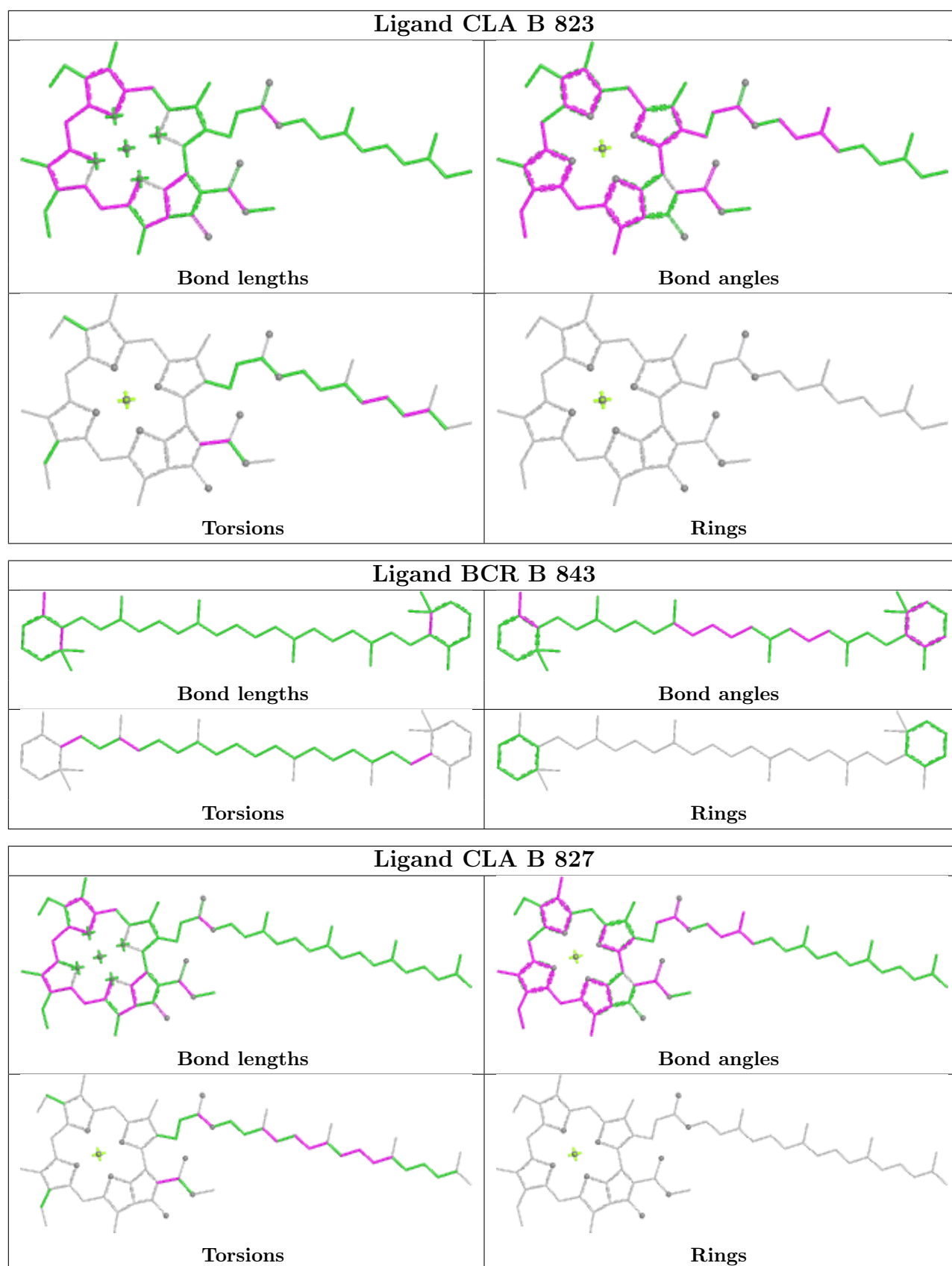
Ligand BCR L 205			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

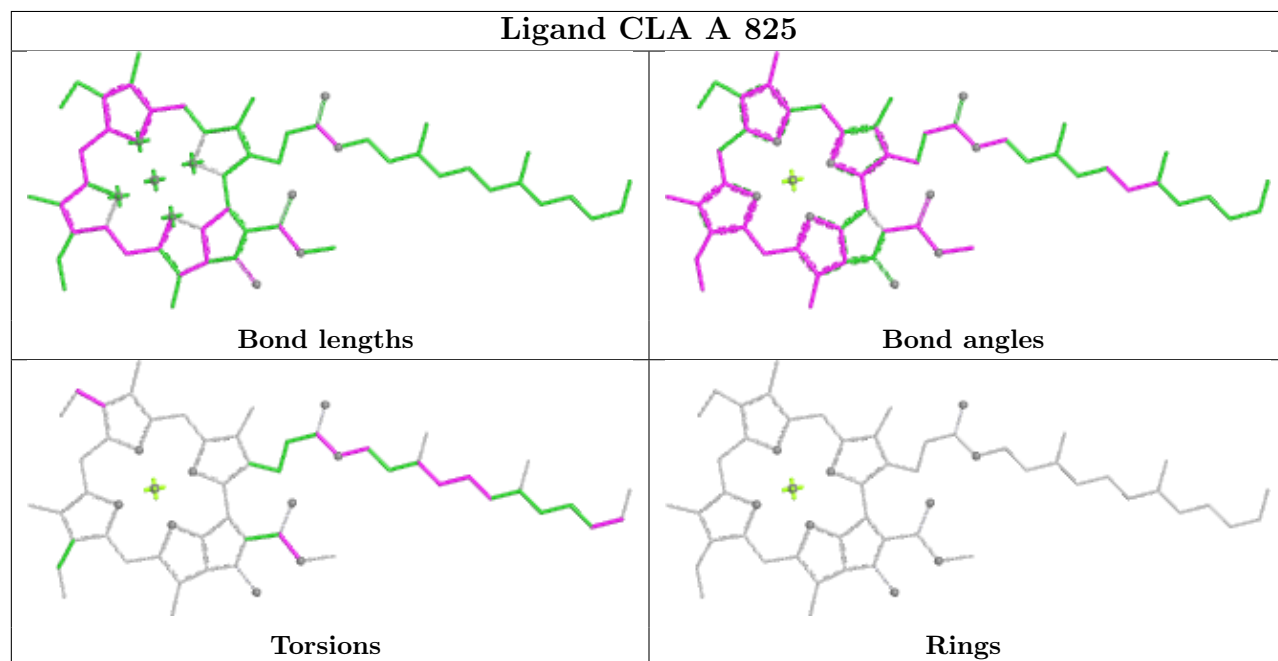
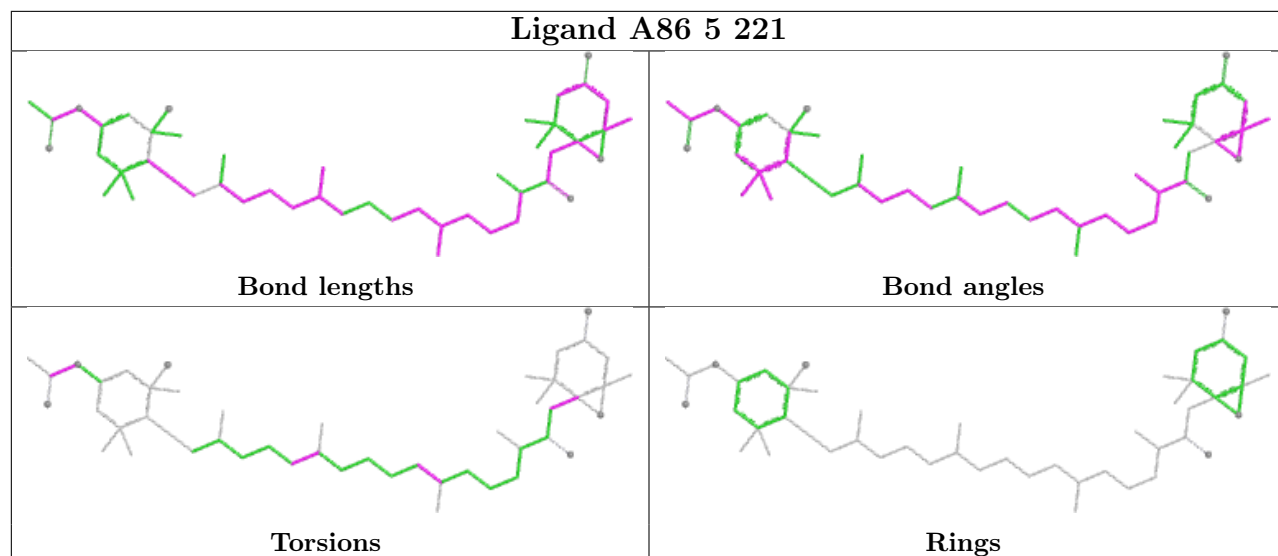
Ligand CLA 1 306



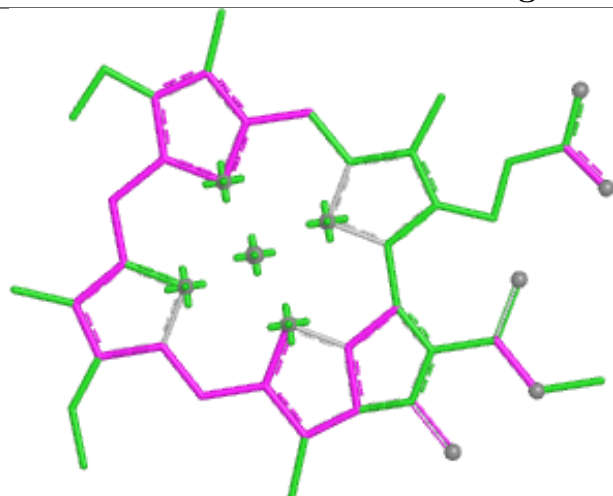
Ligand CLA B 822



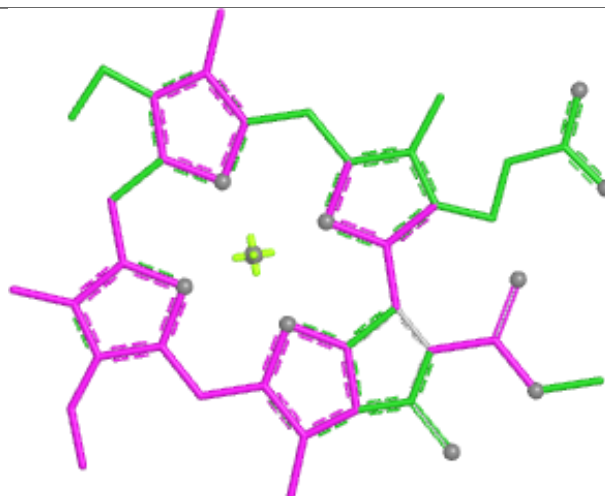




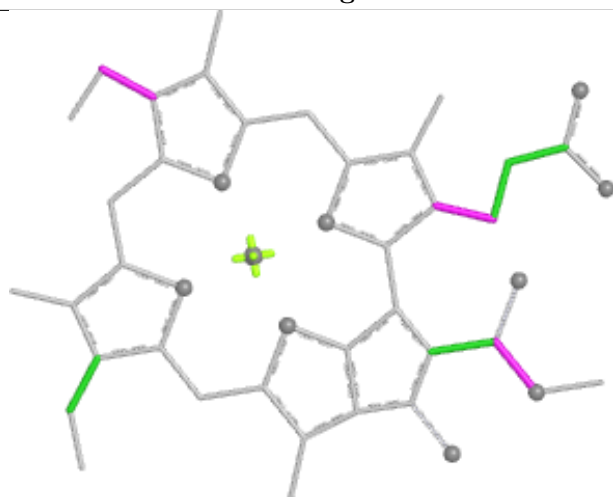
Ligand CLA 3 210



Bond lengths



Bond angles

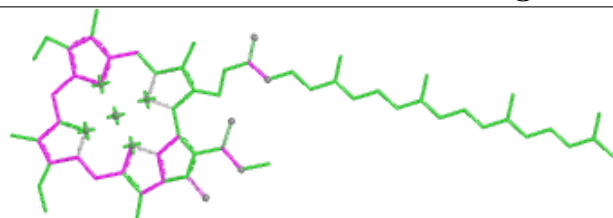


Torsions

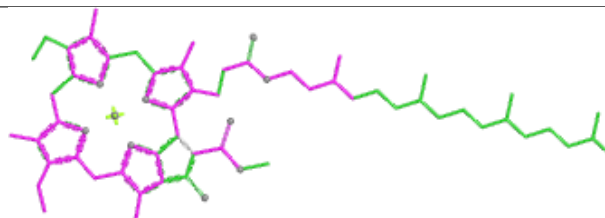


Rings

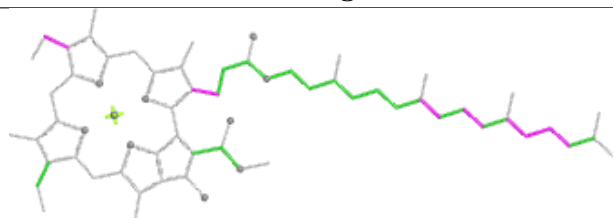
Ligand CLA B 811



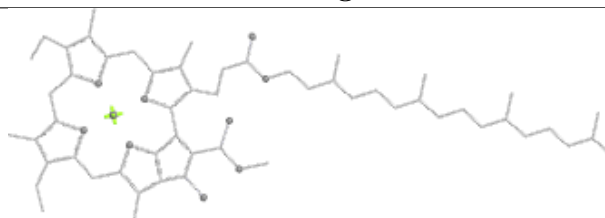
Bond lengths



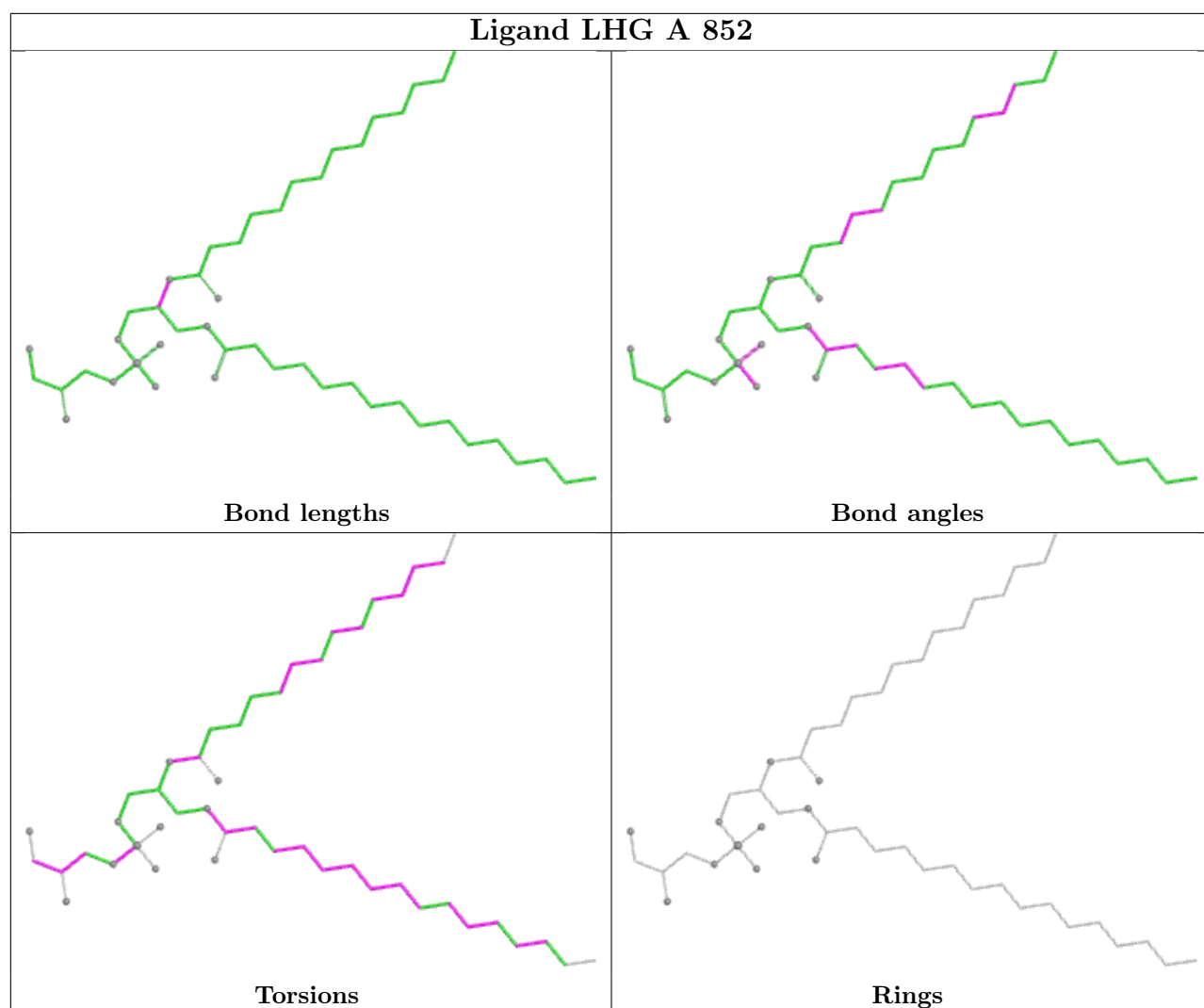
Bond angles



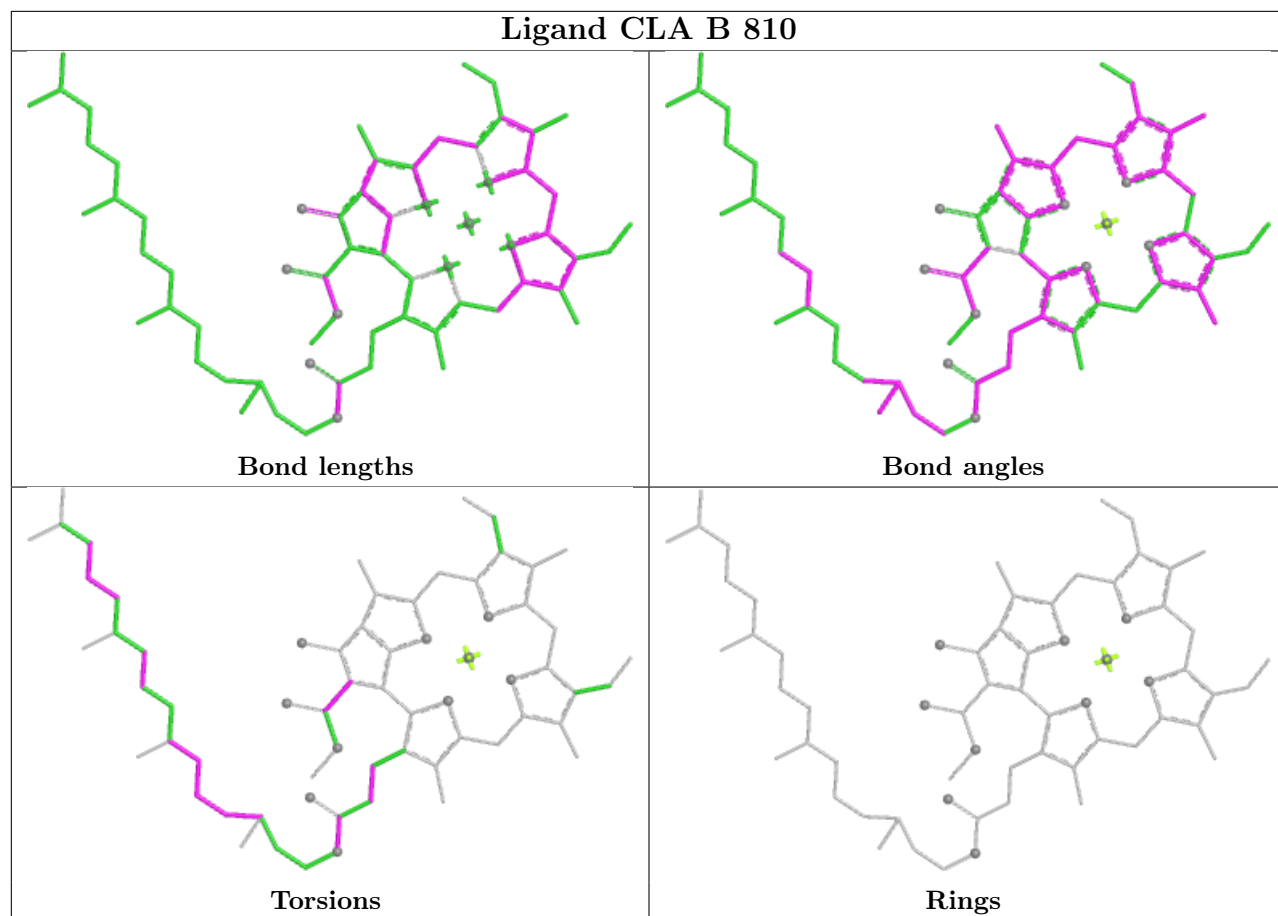
Torsions



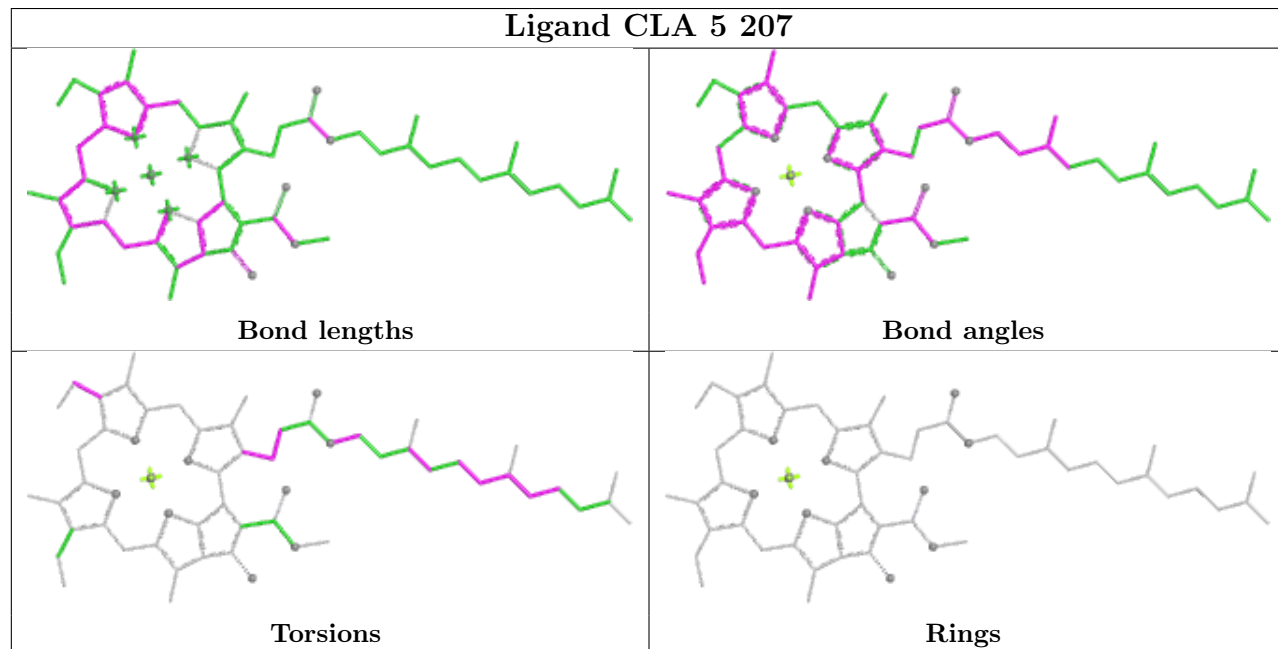
Rings

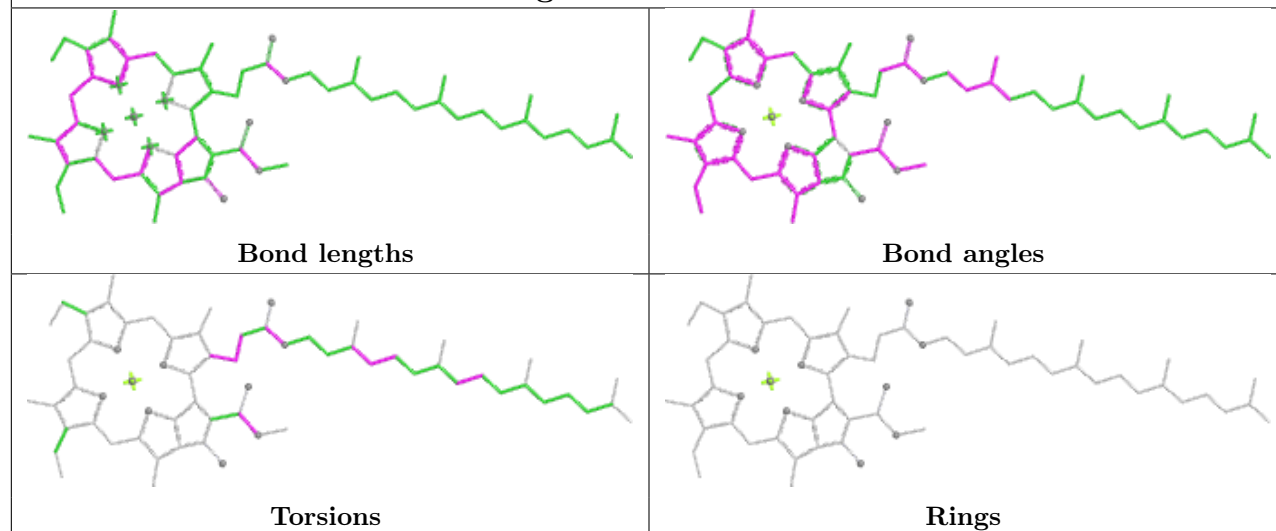
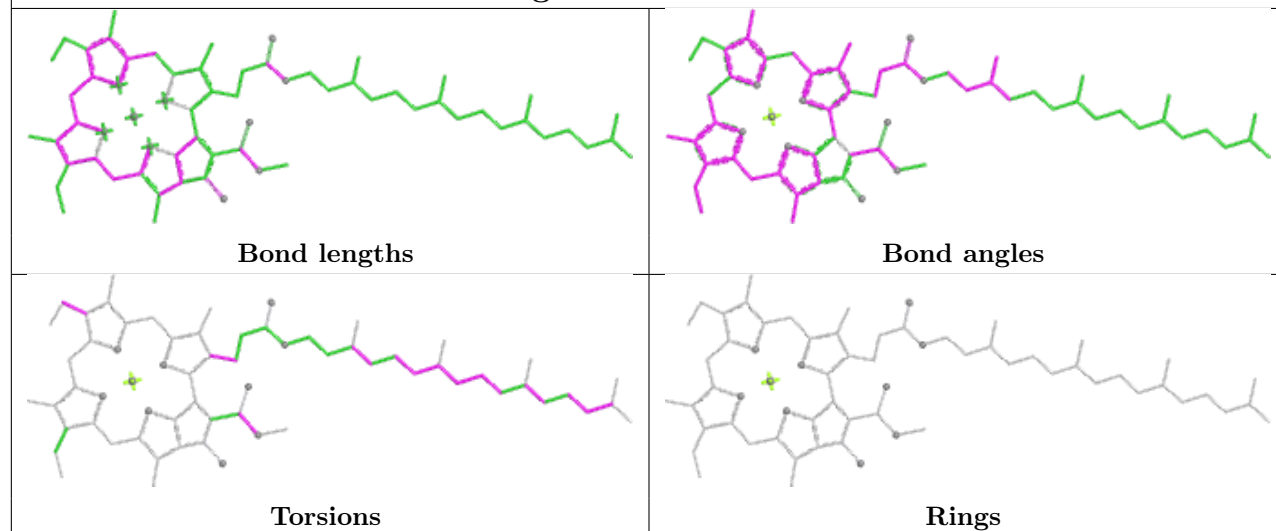
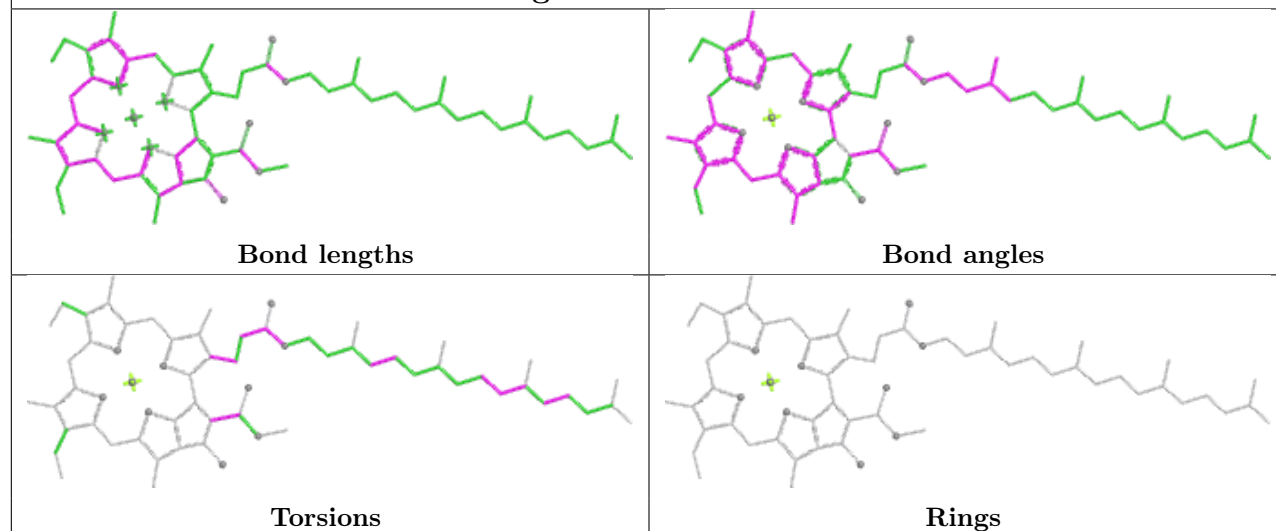


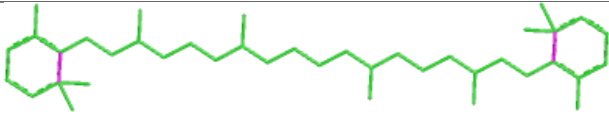
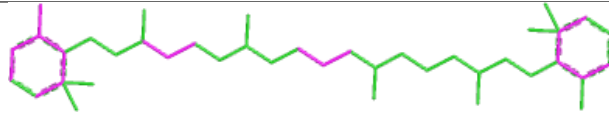
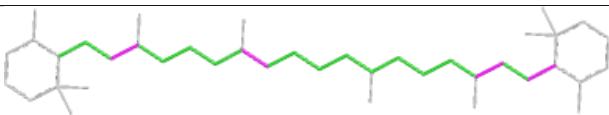
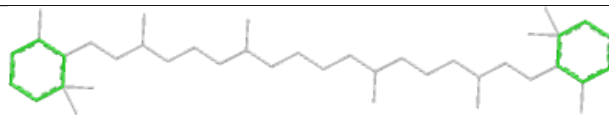
Ligand CLA B 810

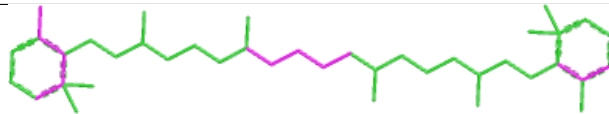
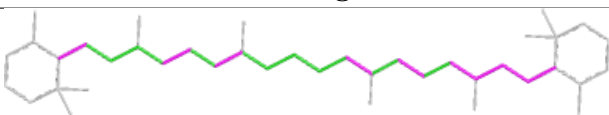
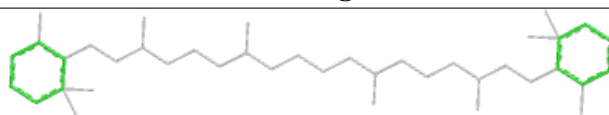


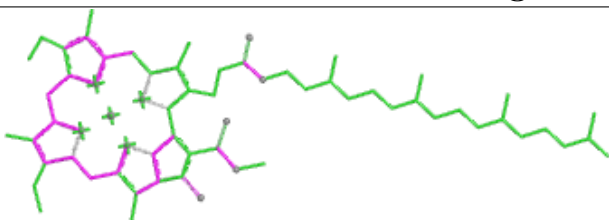
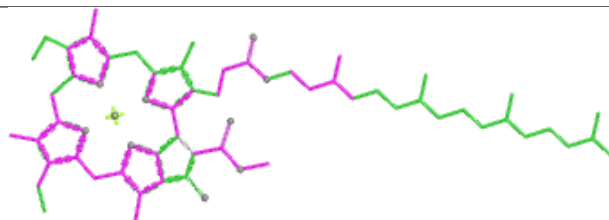
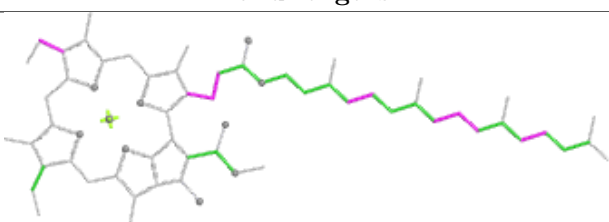
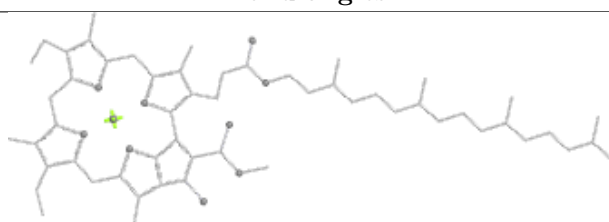
Ligand CLA 5 207

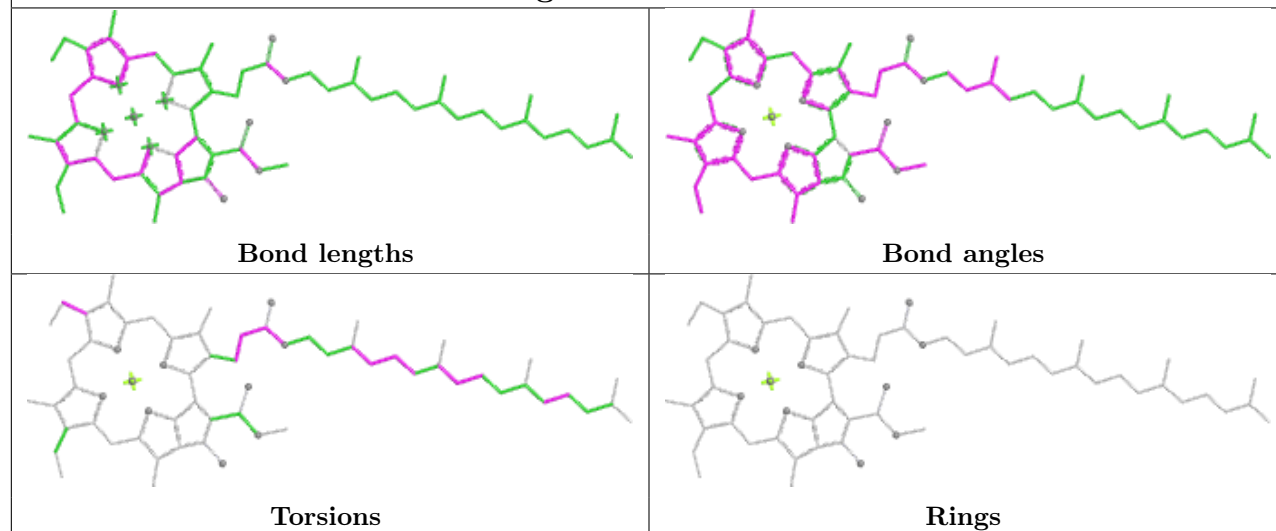
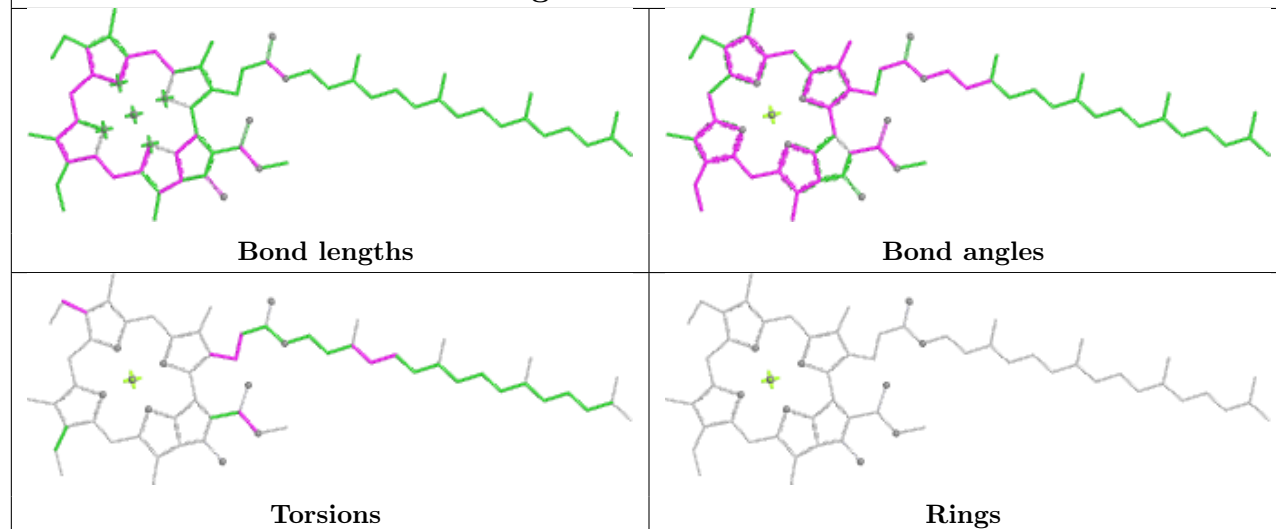
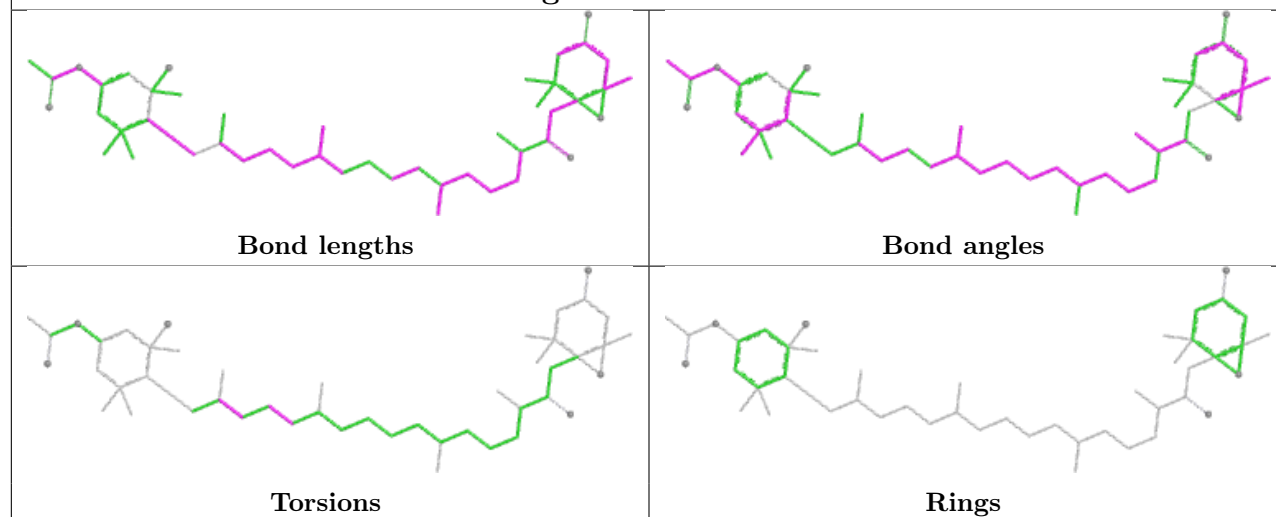


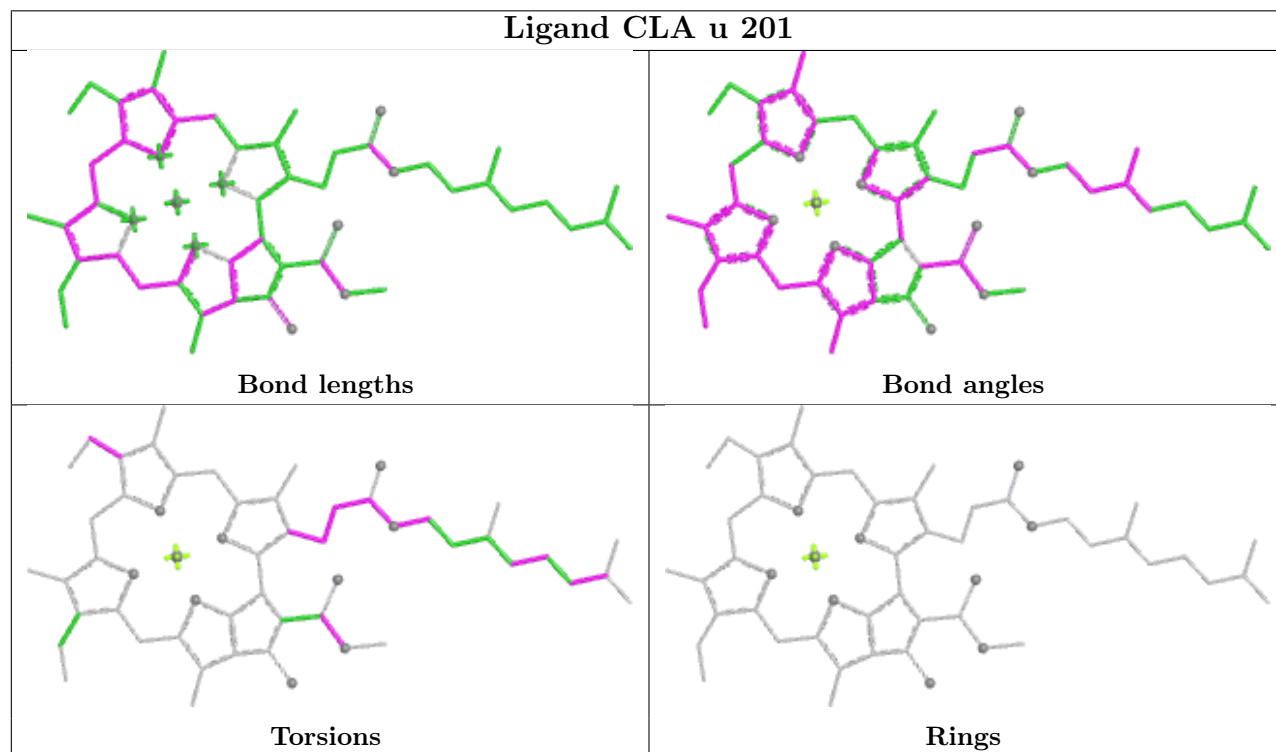
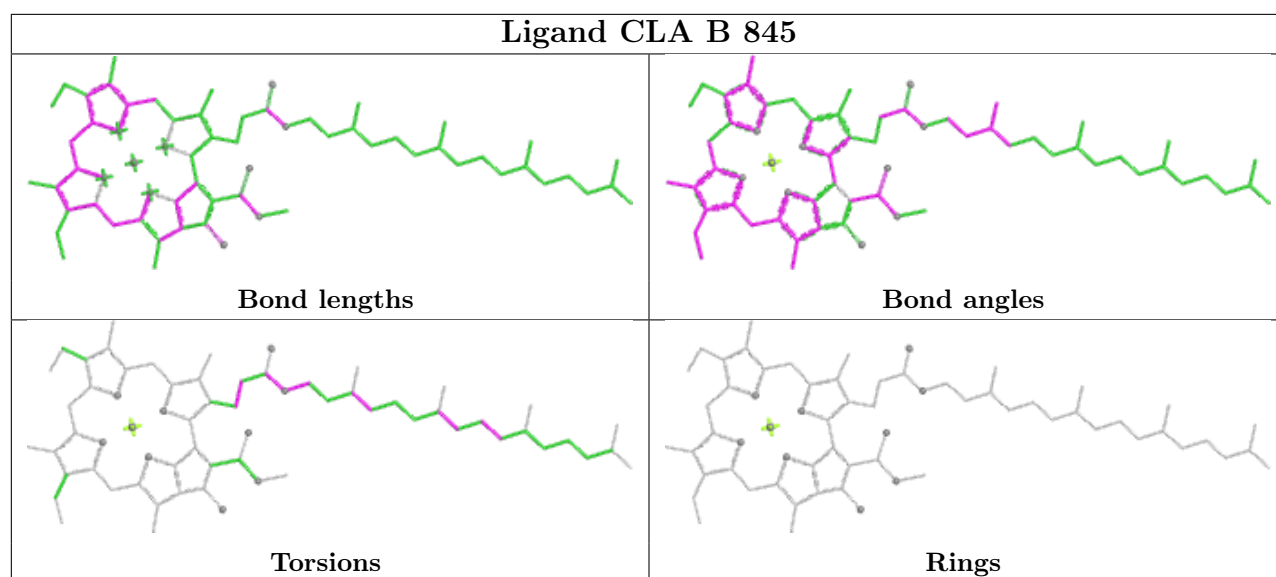
Ligand CLA 3 202**Ligand CLA B 821****Ligand CLA B 805**

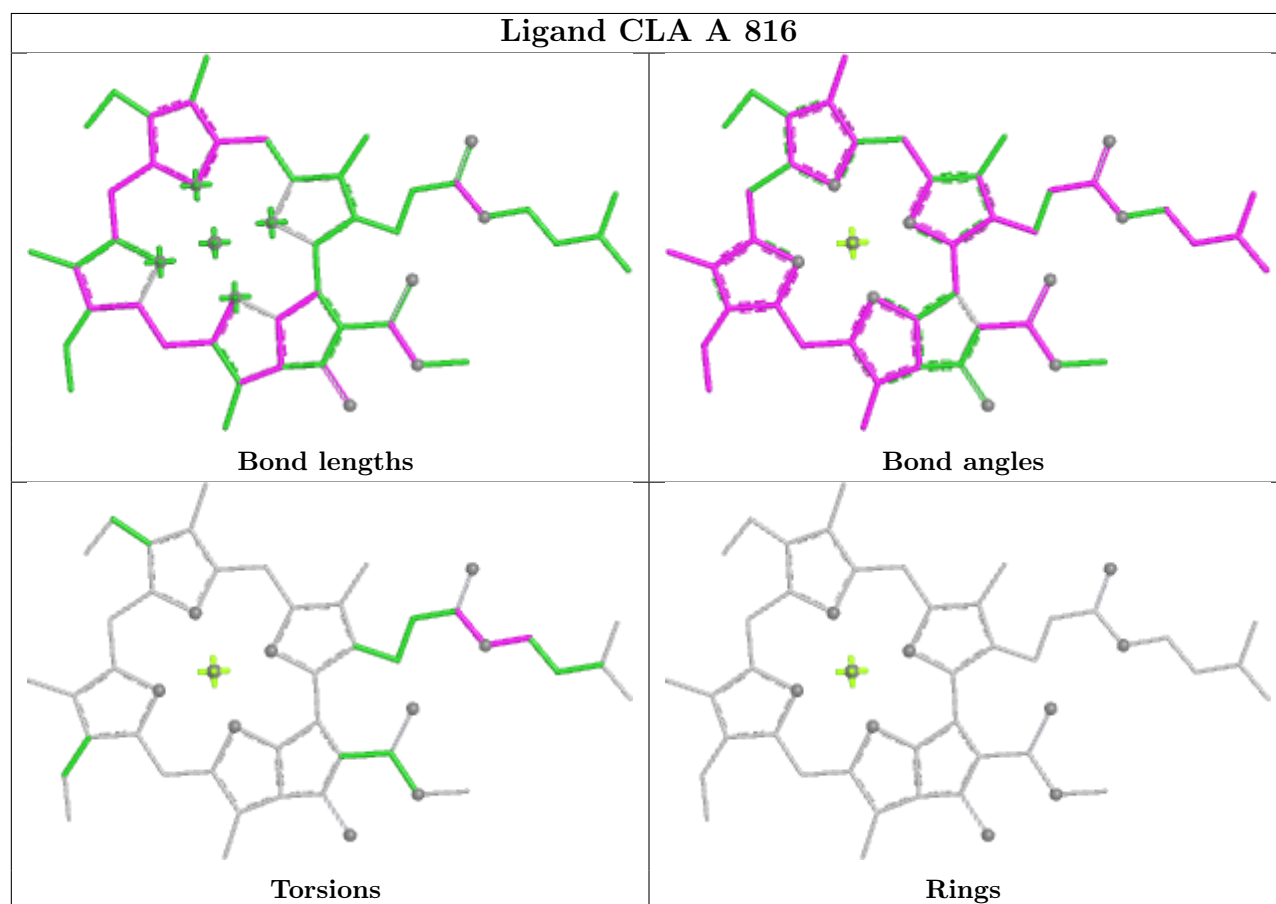
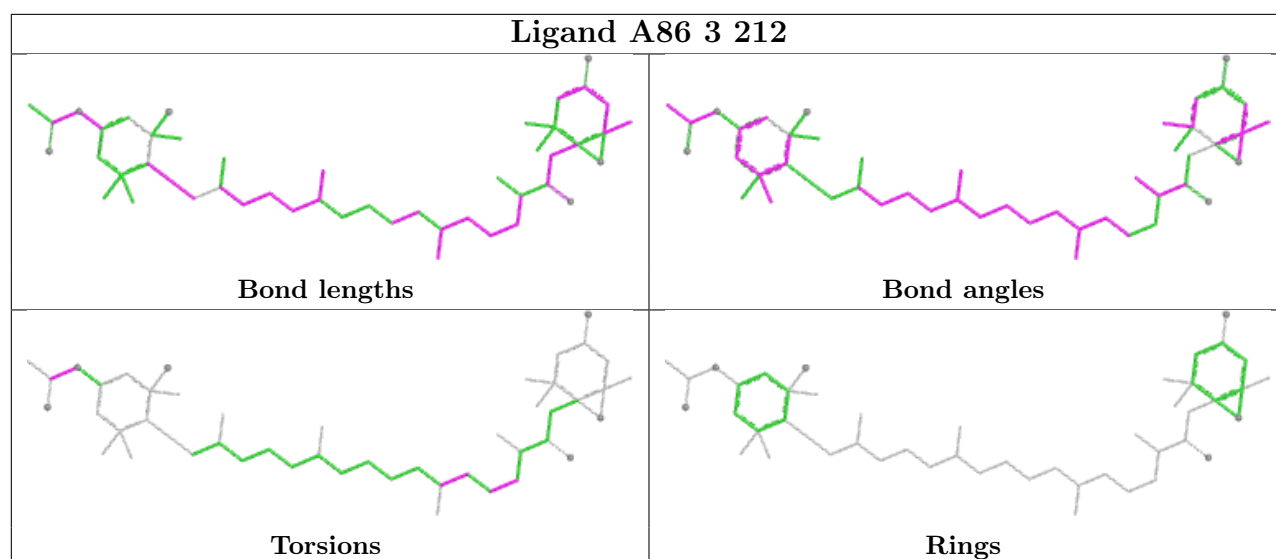
Ligand BCR I 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

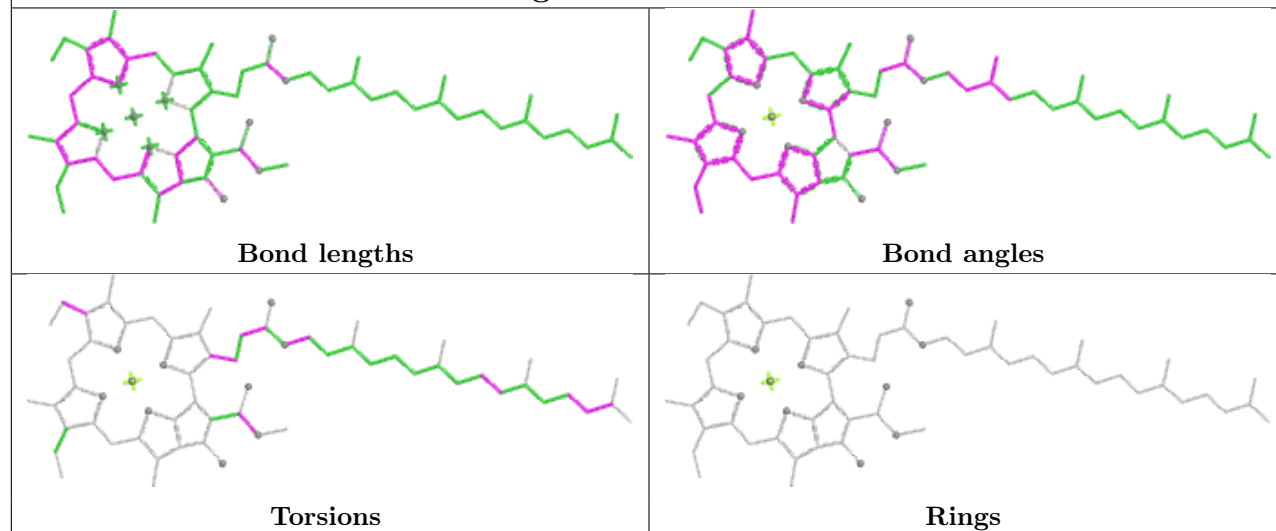
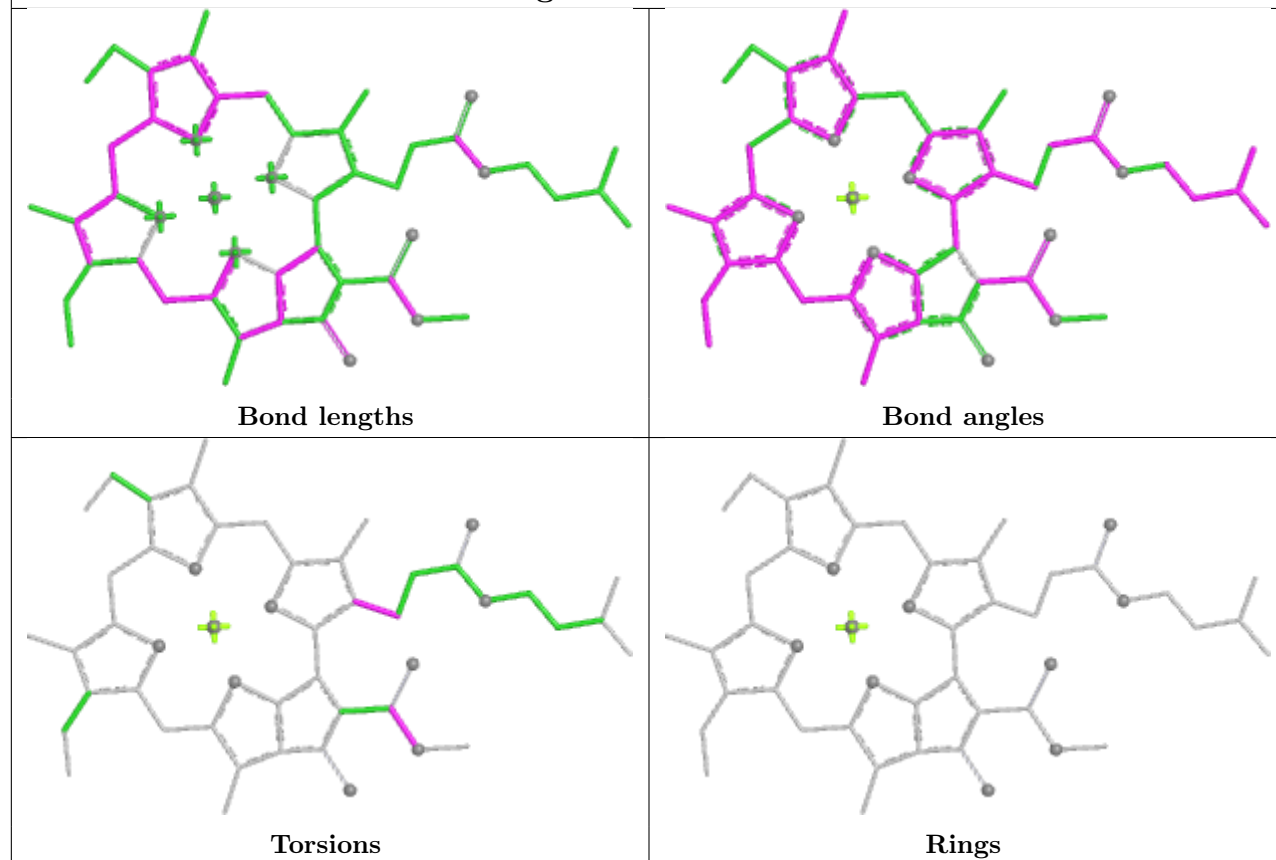
Ligand BCR 1 314	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 810	
	
Bond lengths	Bond angles
	
Torsions	Rings

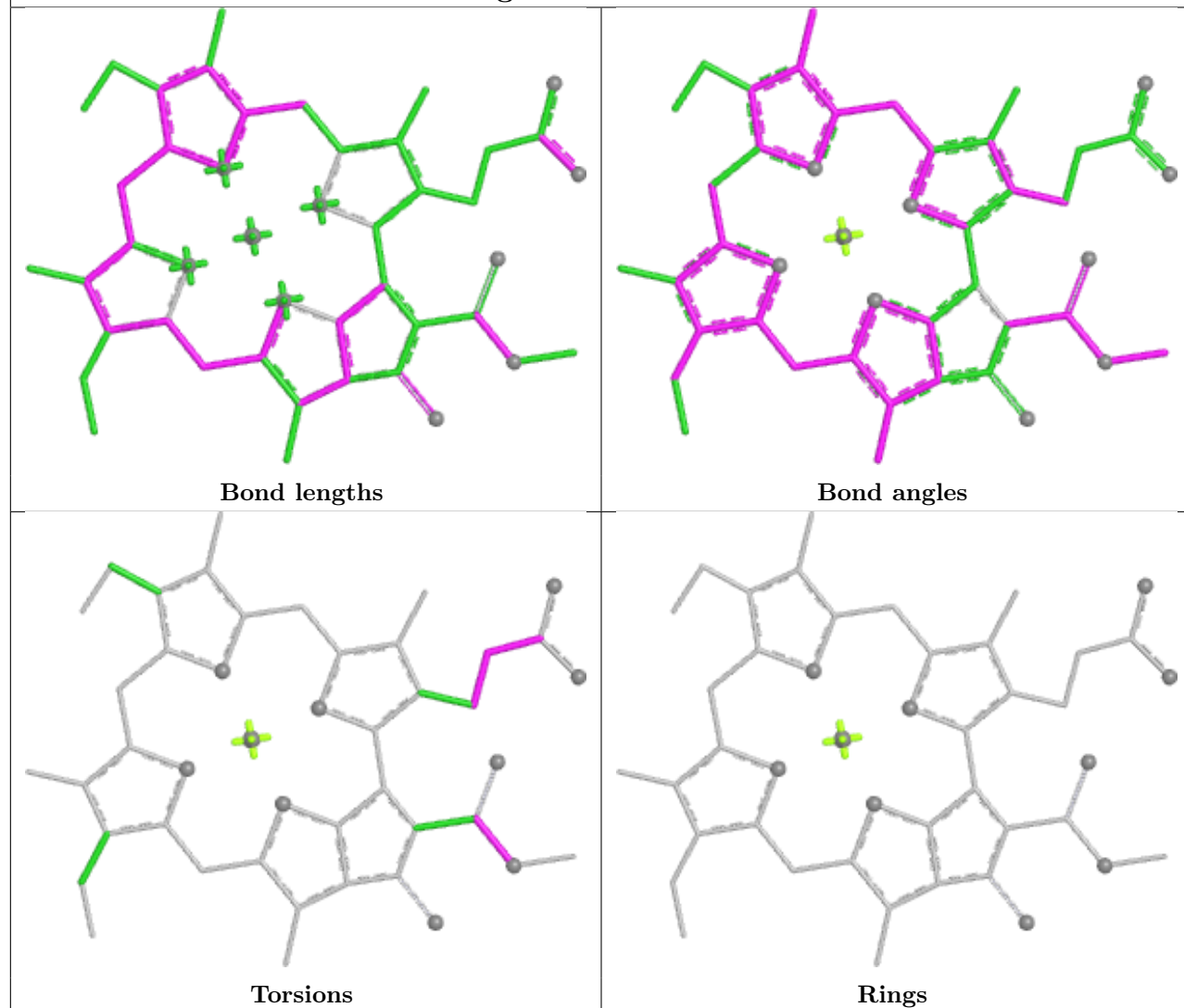
Ligand CLA 1 310**Ligand CLA A 822****Ligand A86 5 219**



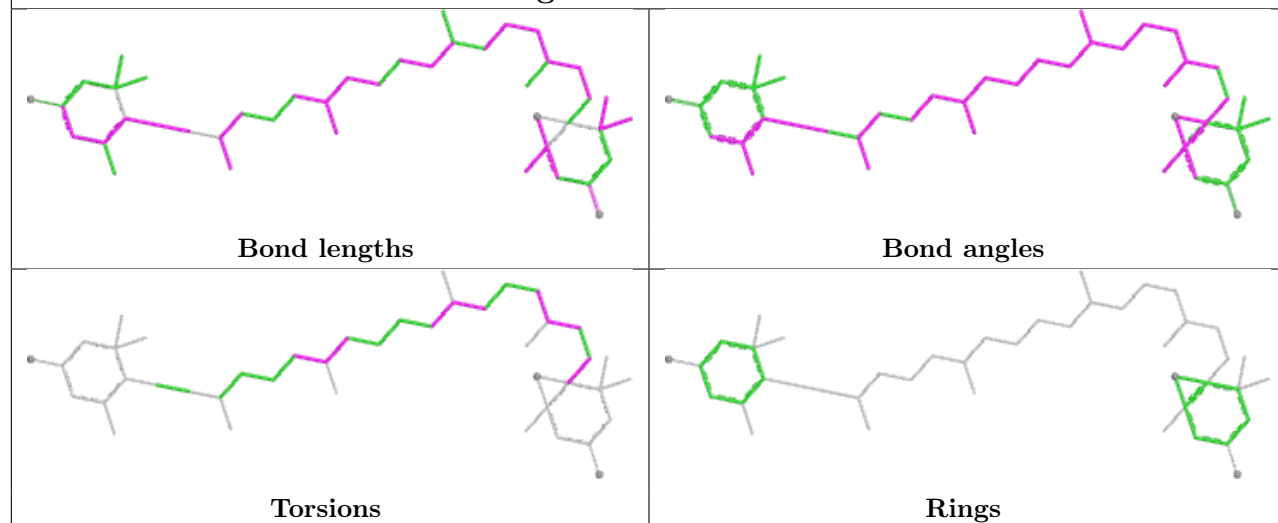


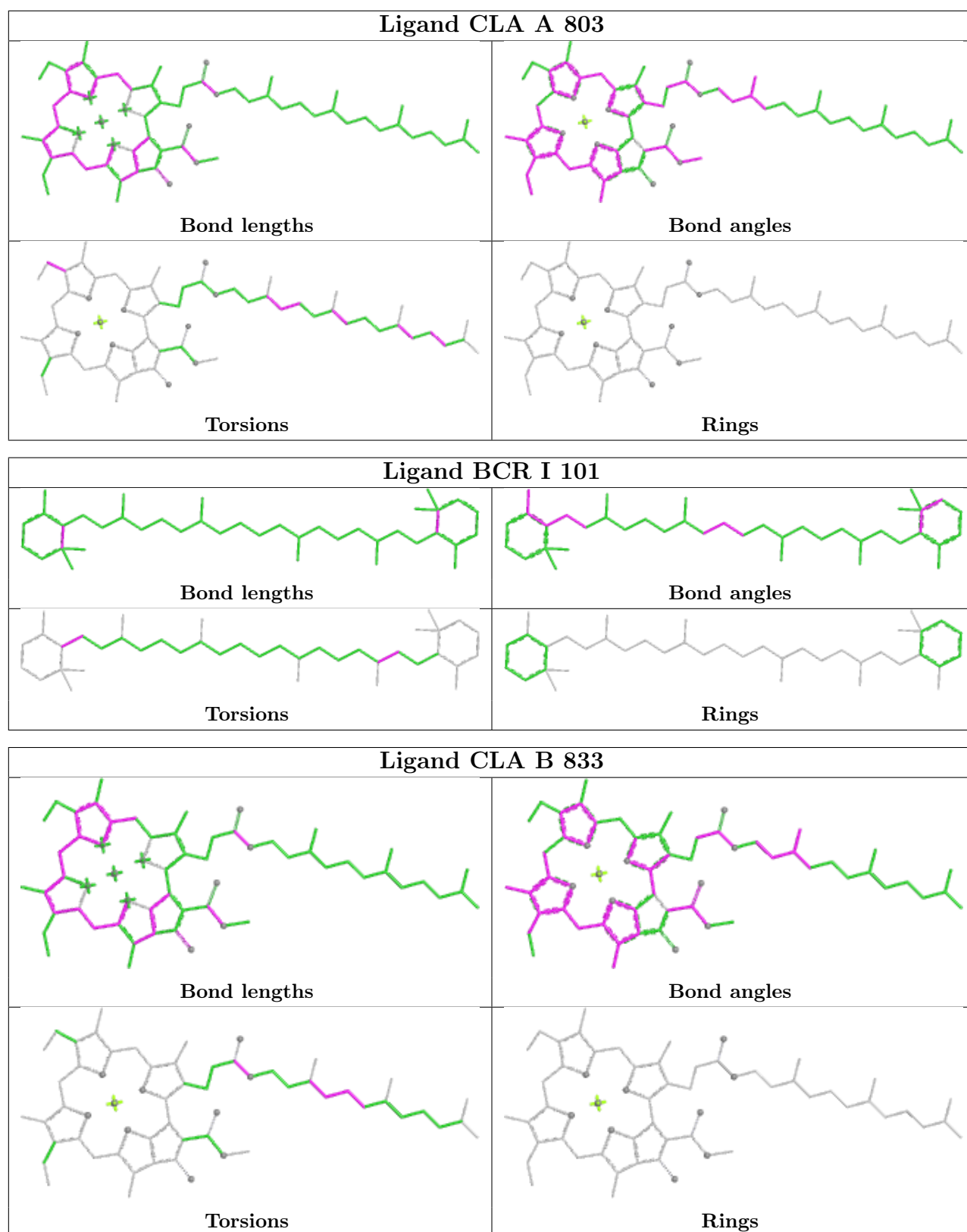
Ligand CLA B 838**Ligand CLA 4 304**

Ligand CLA 5 213

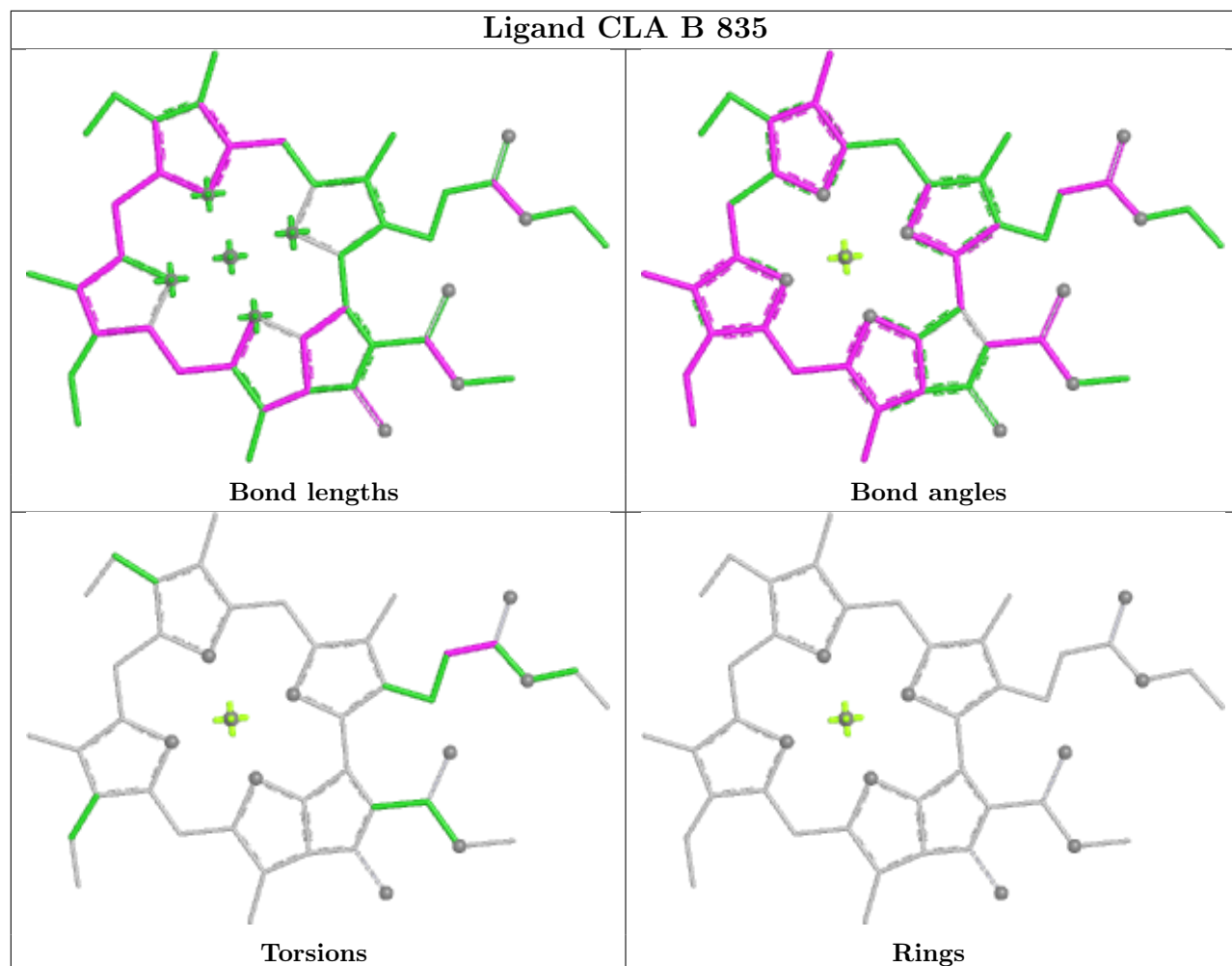


Ligand DD6 3 213

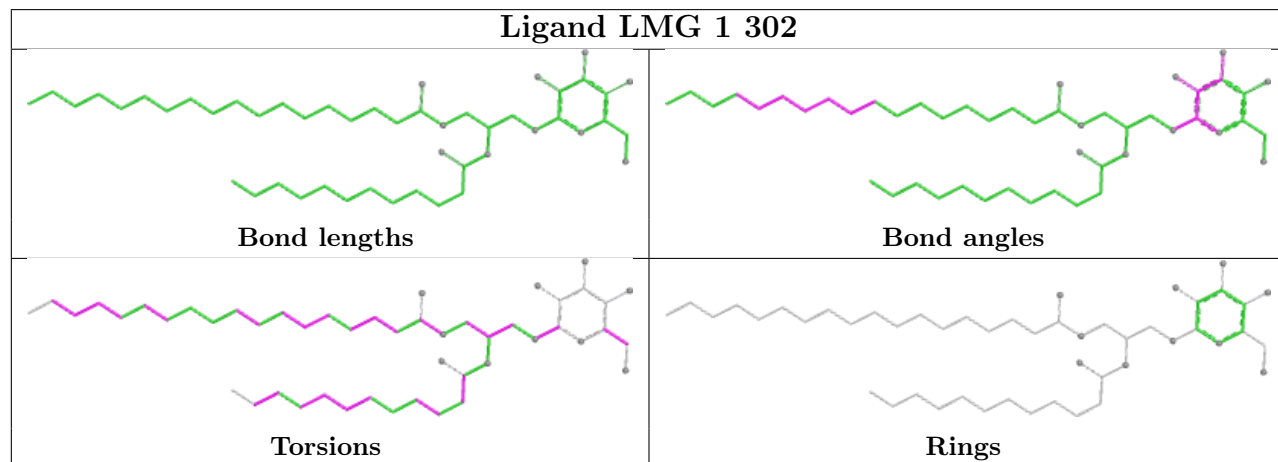


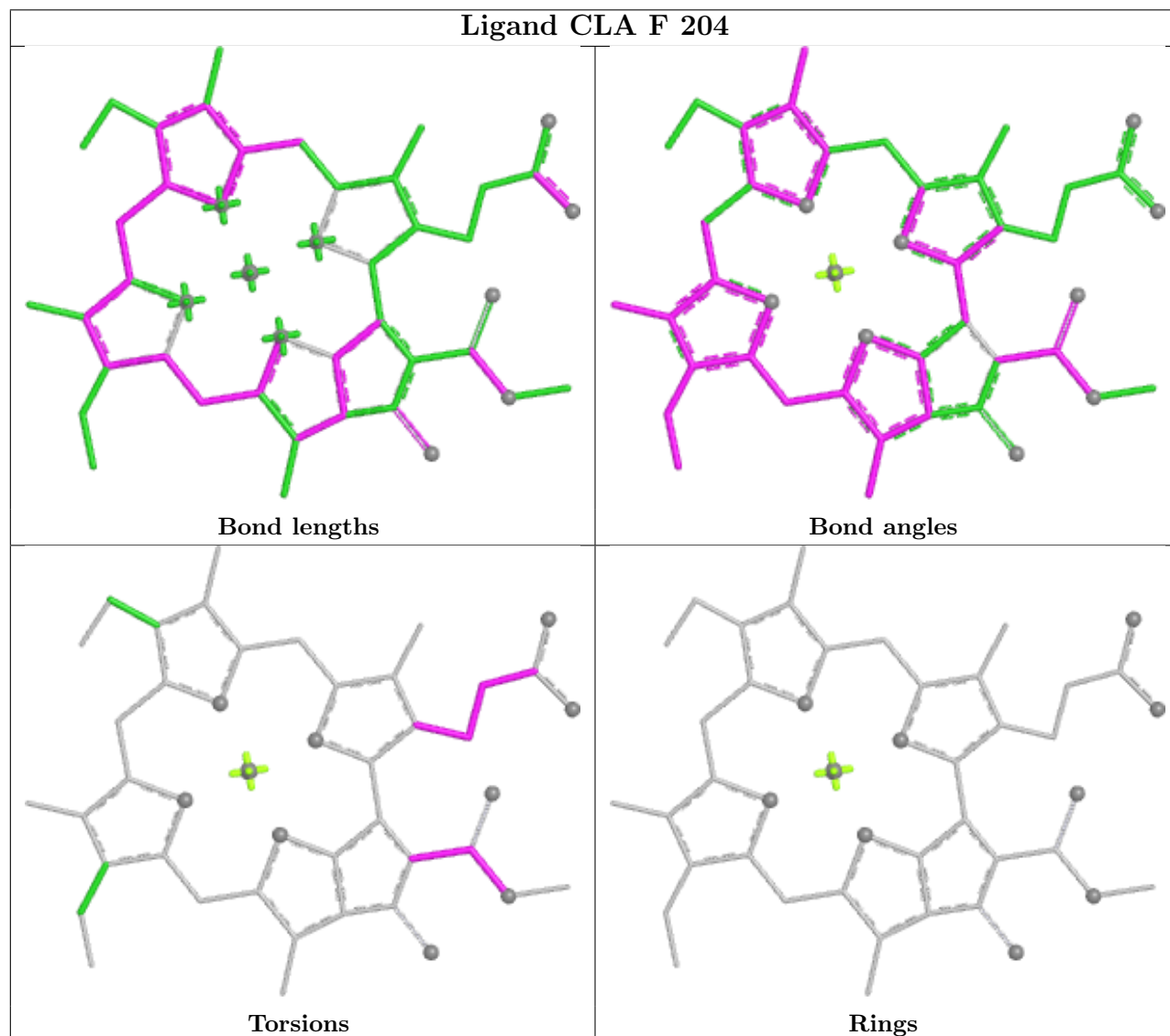
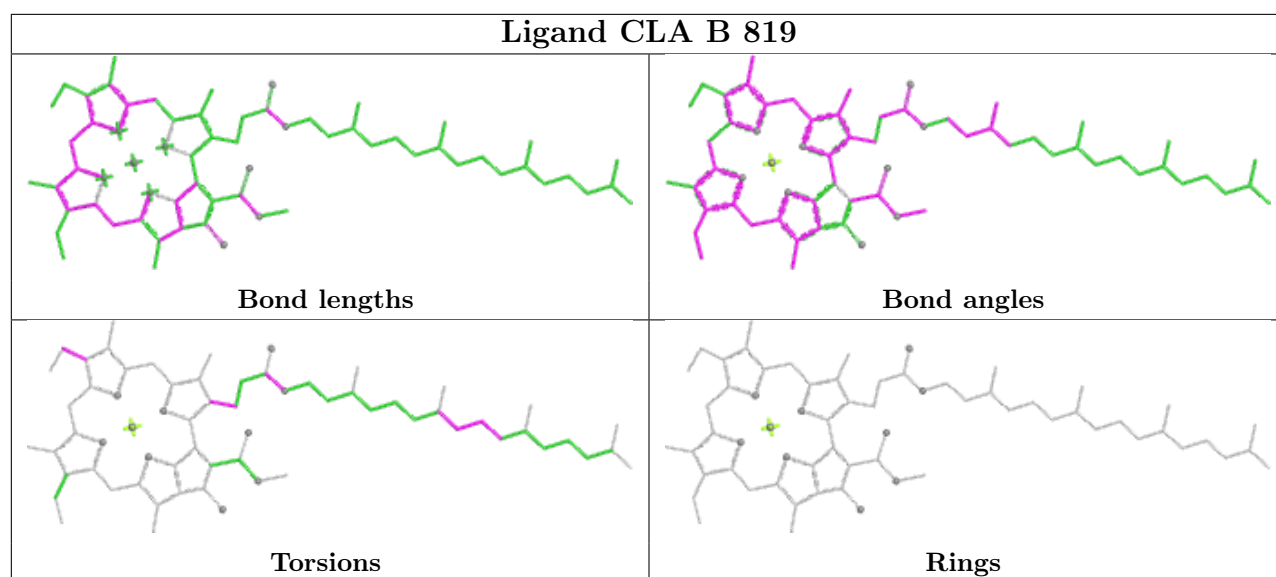


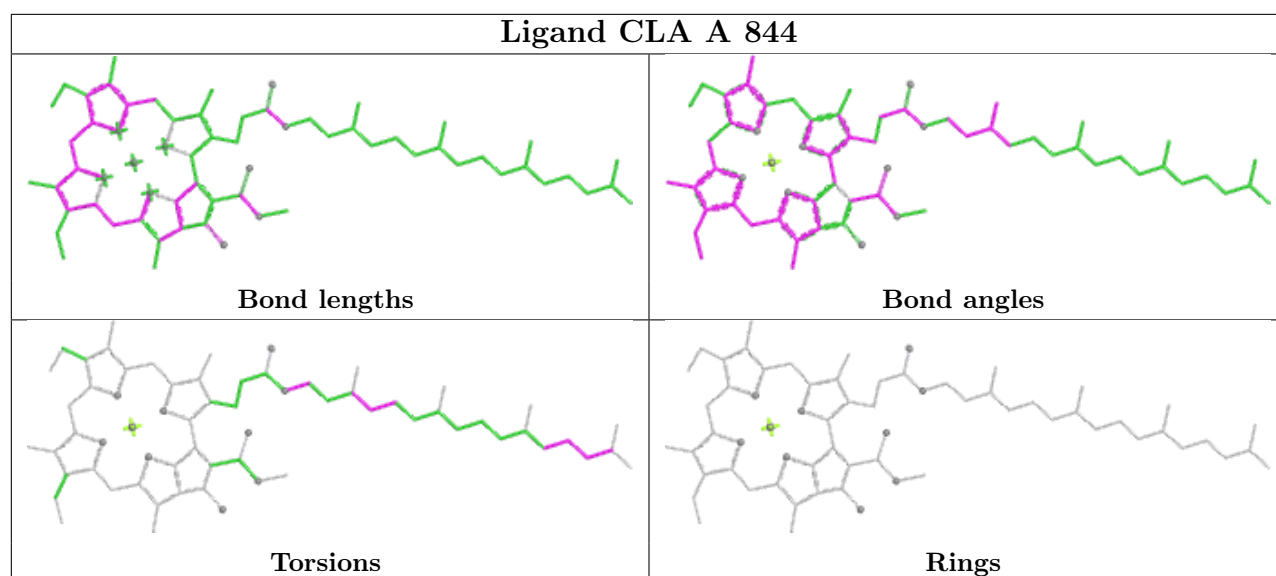
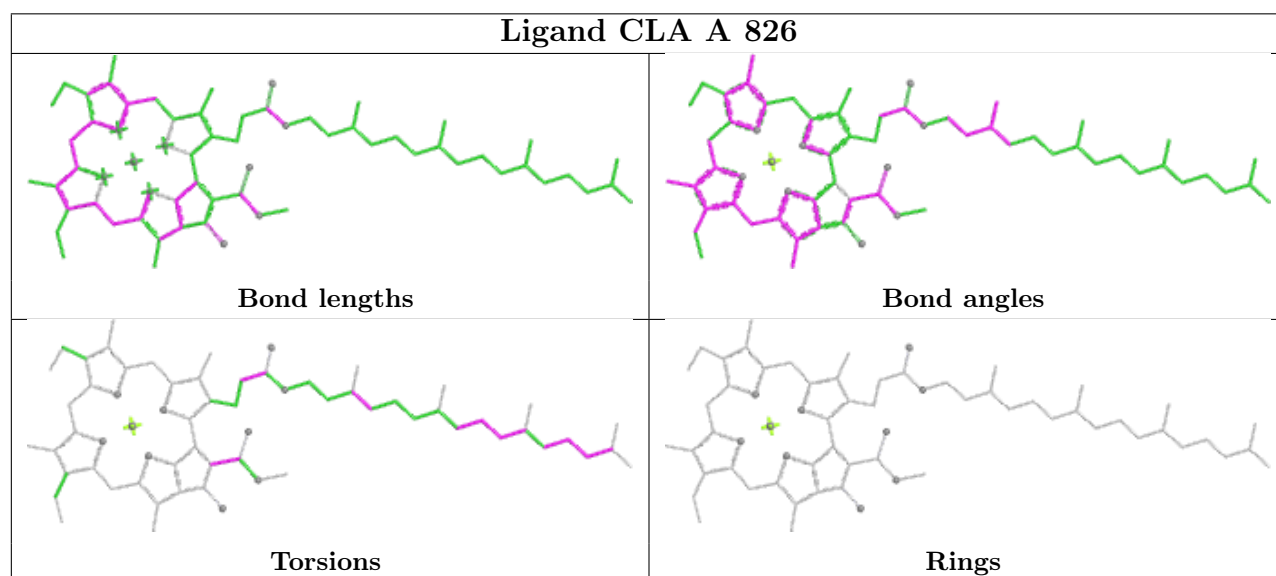
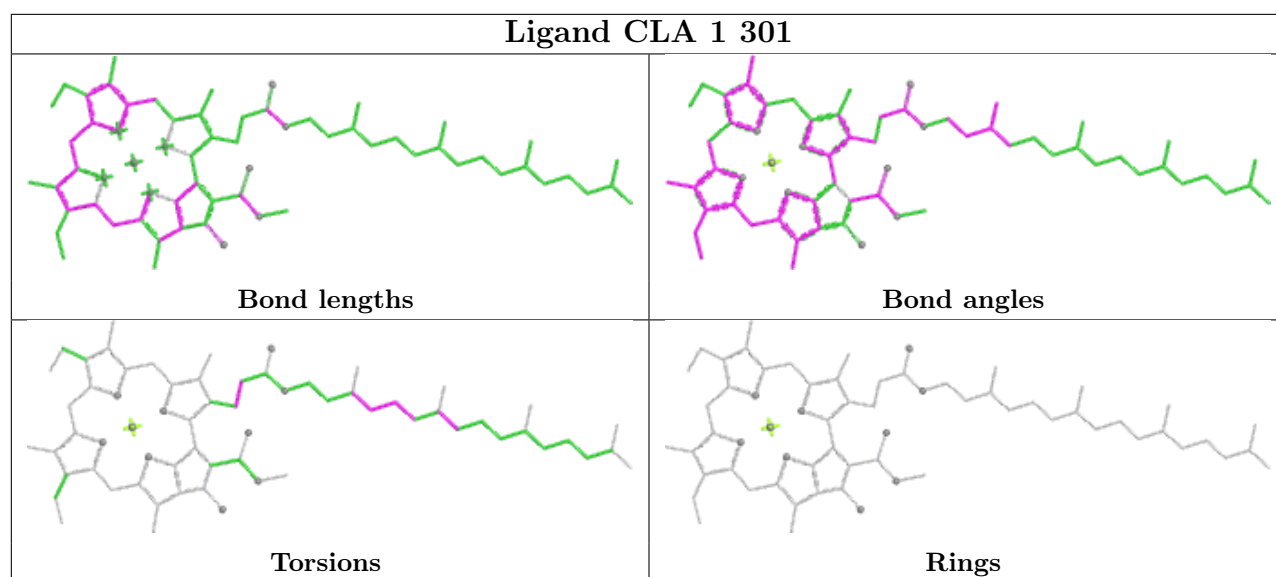
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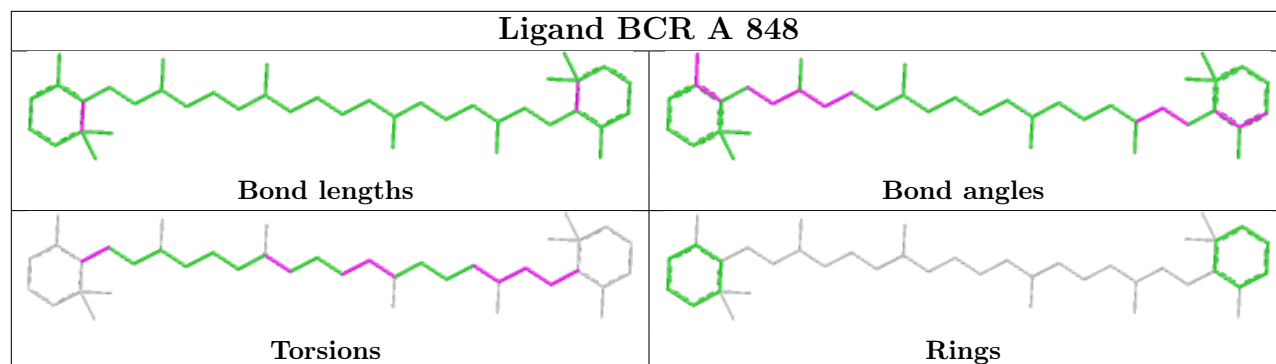
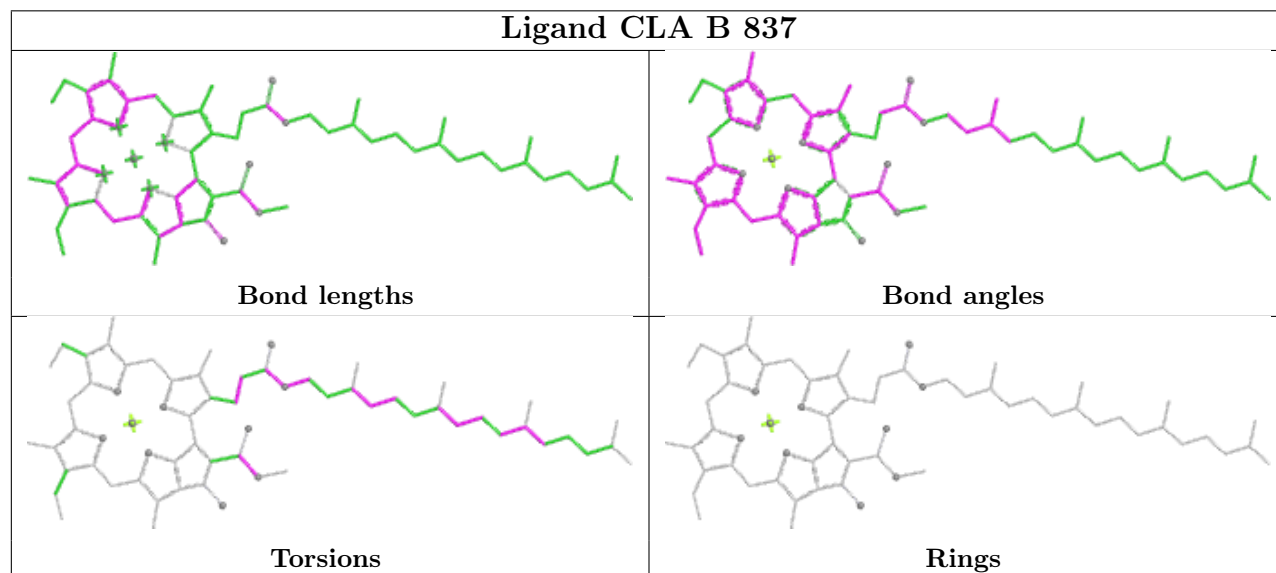
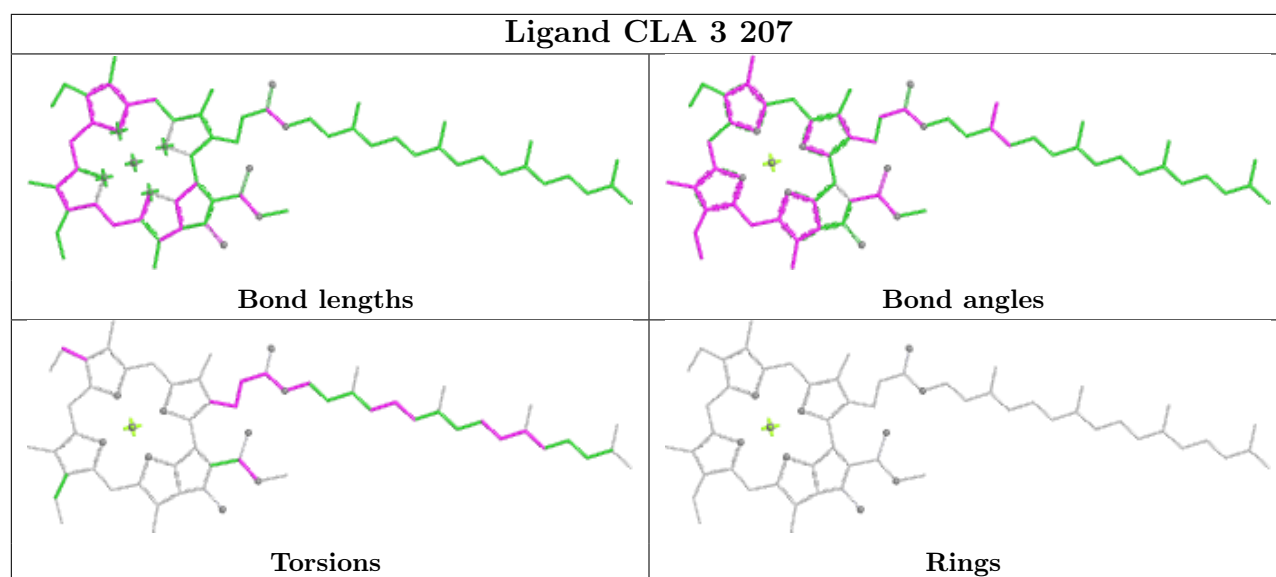


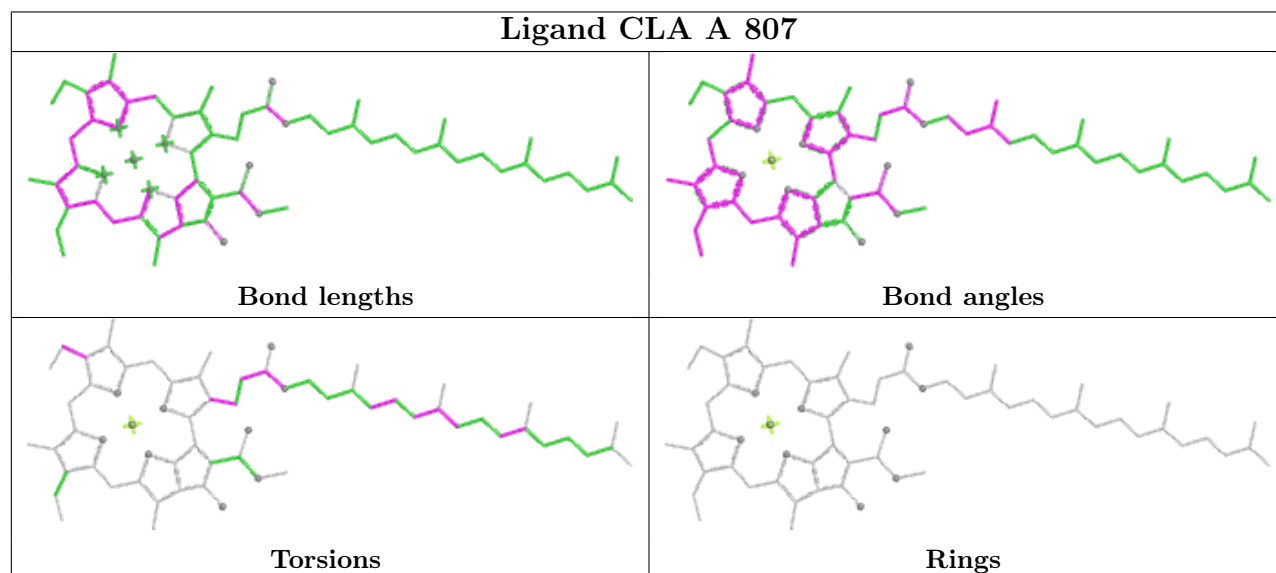
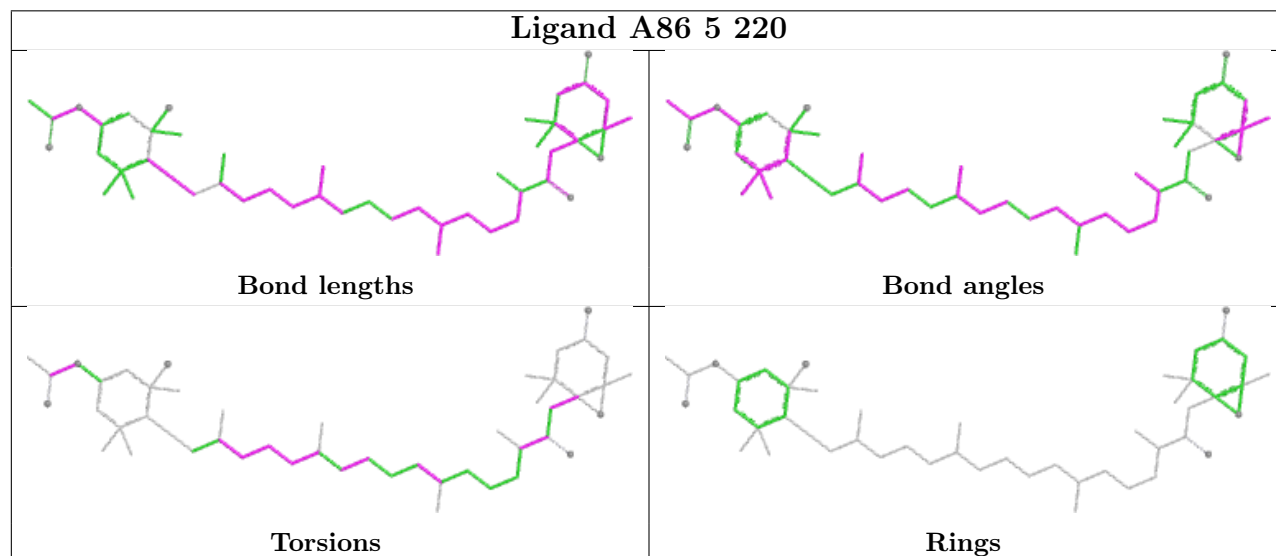
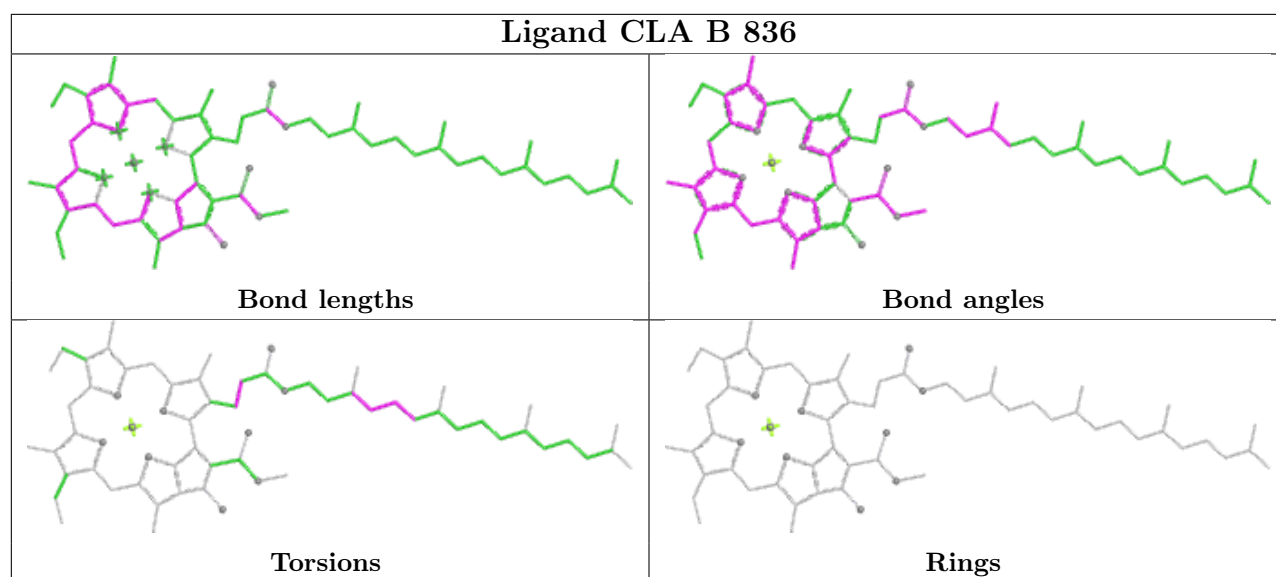
Ligand LMG 1 302

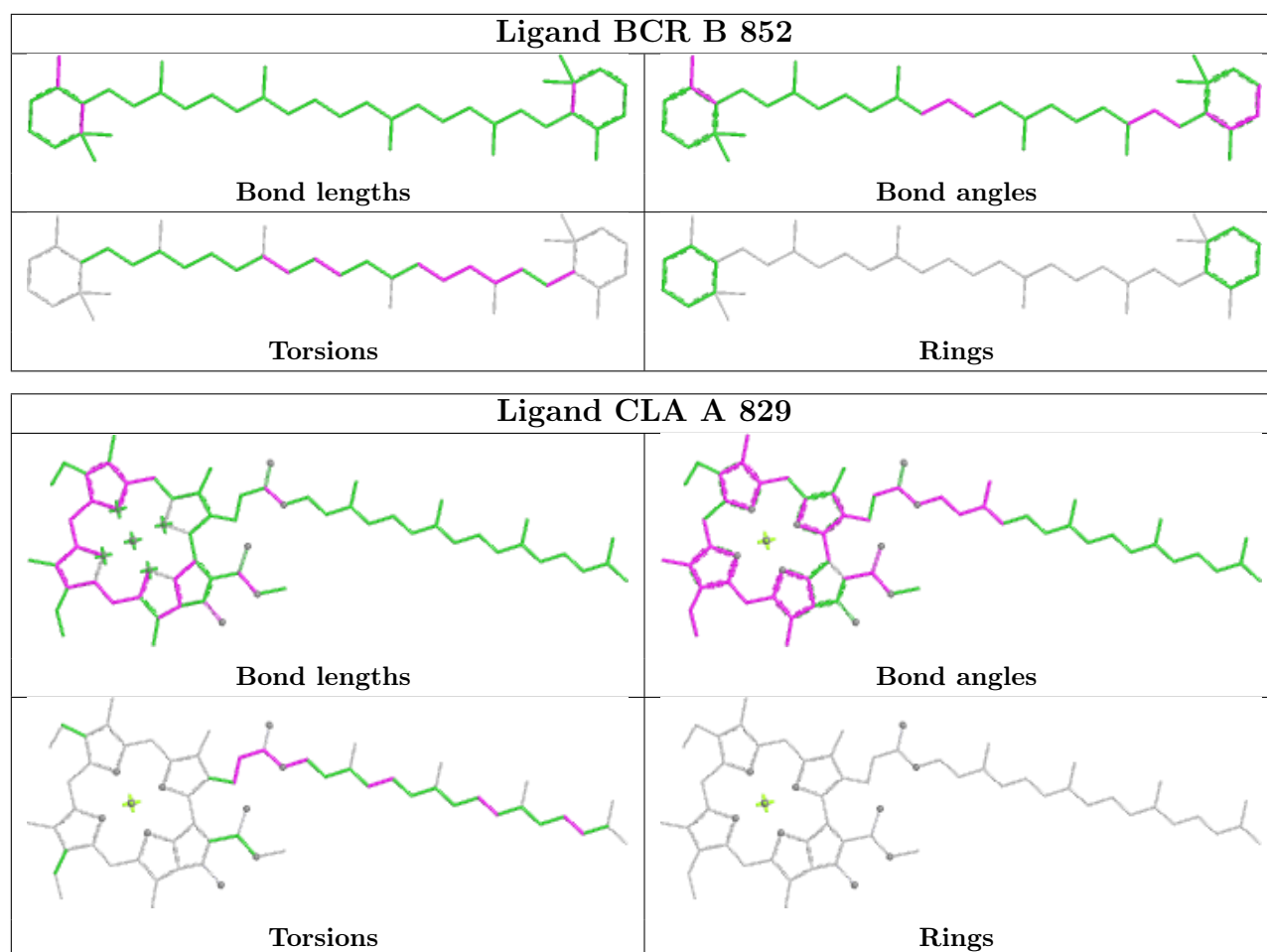




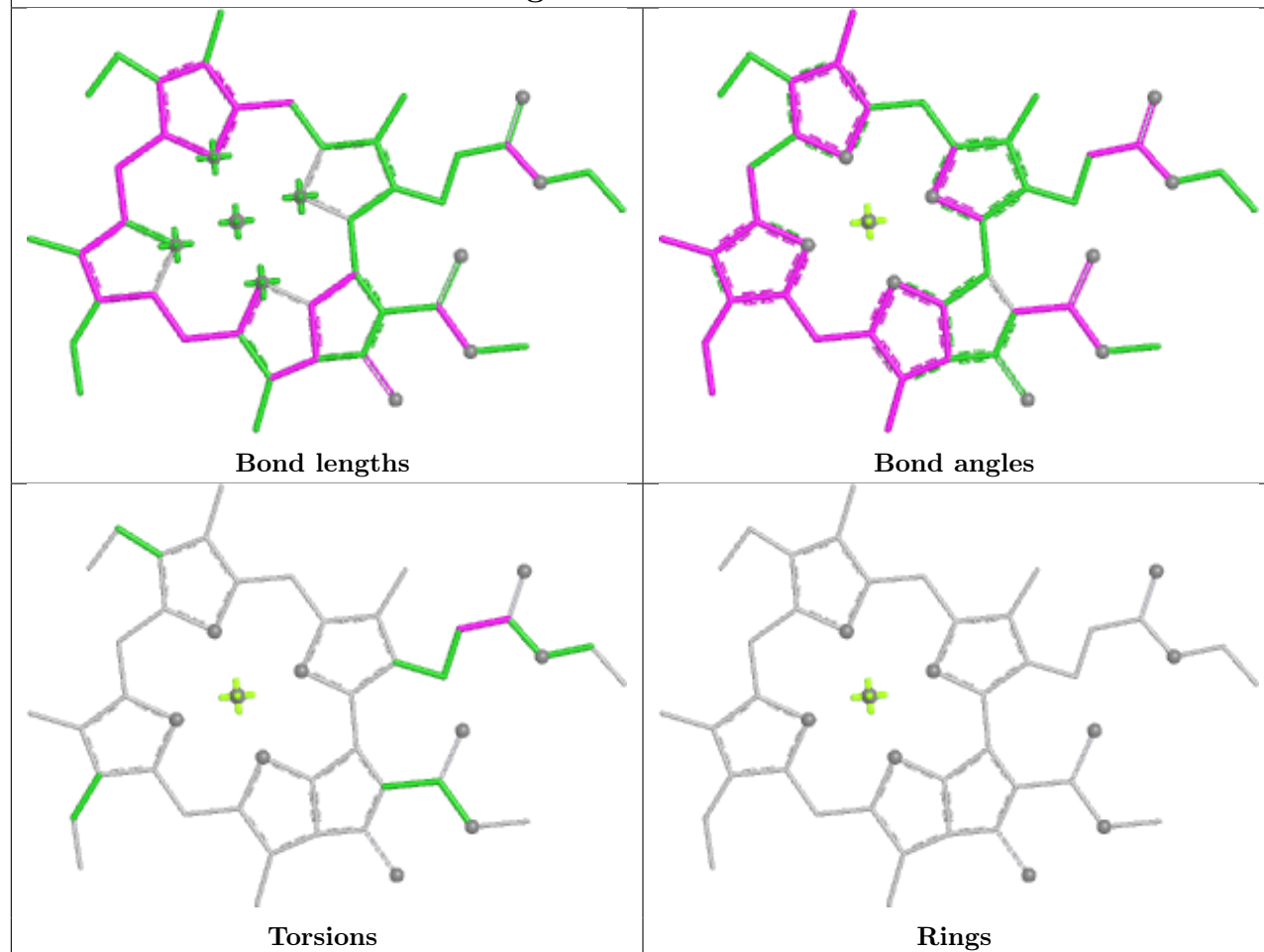




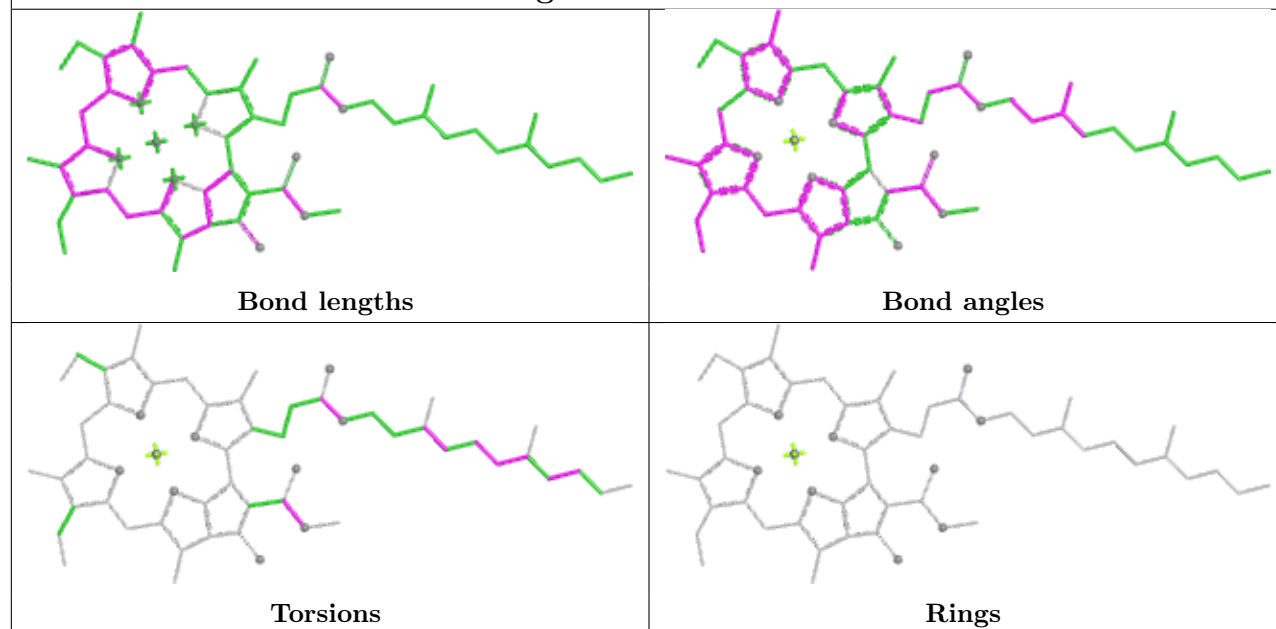




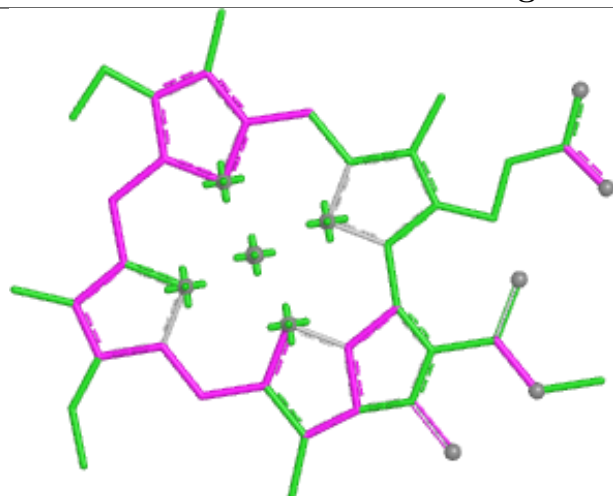
Ligand CLA A 840



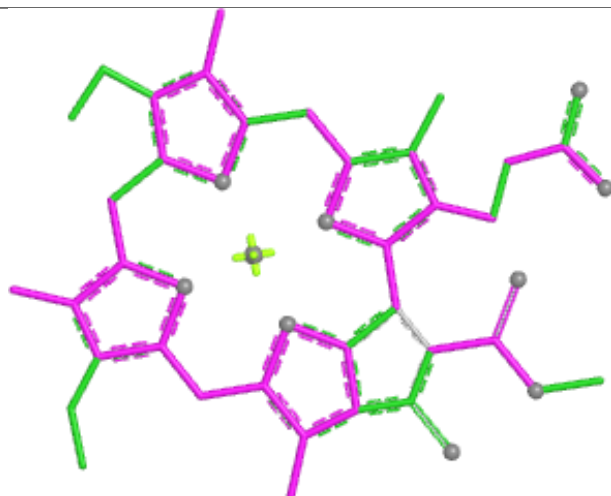
Ligand CLA 5 211



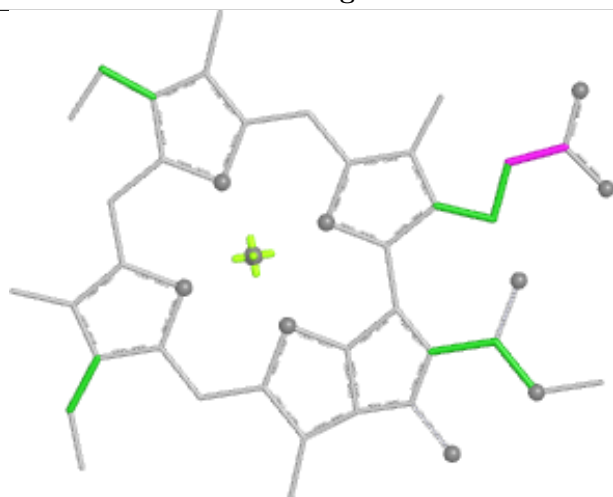
Ligand CLA J 103



Bond lengths



Bond angles

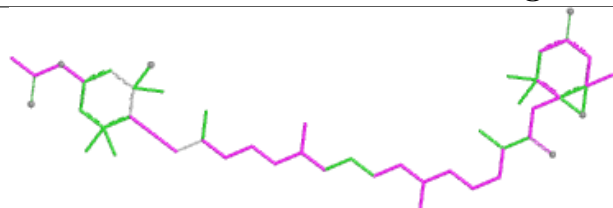


Torsions

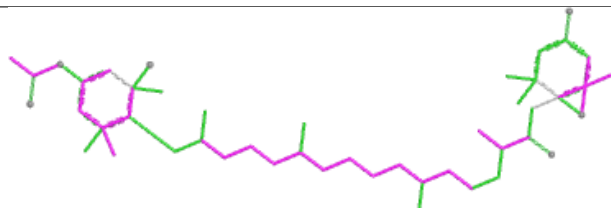


Rings

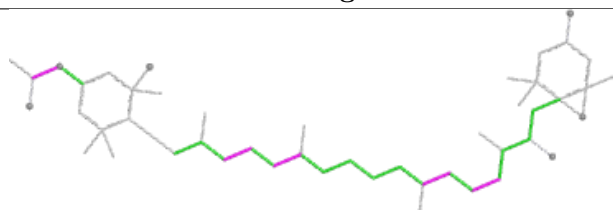
Ligand A86 4 316



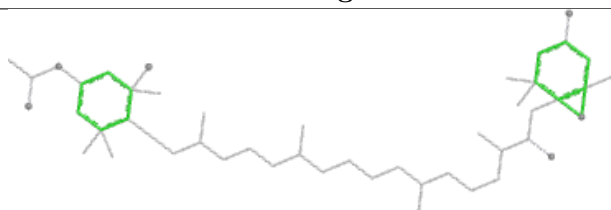
Bond lengths



Bond angles

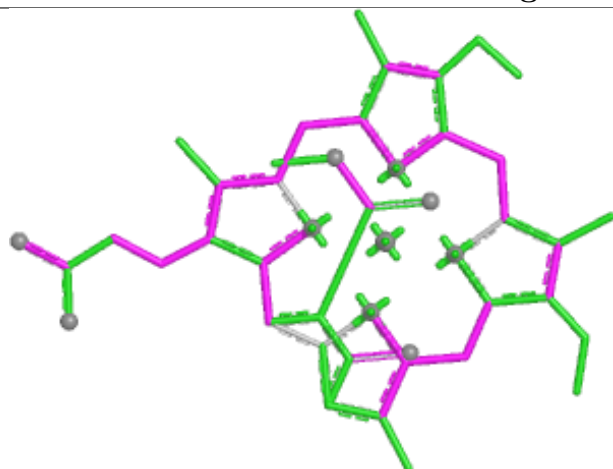


Torsions

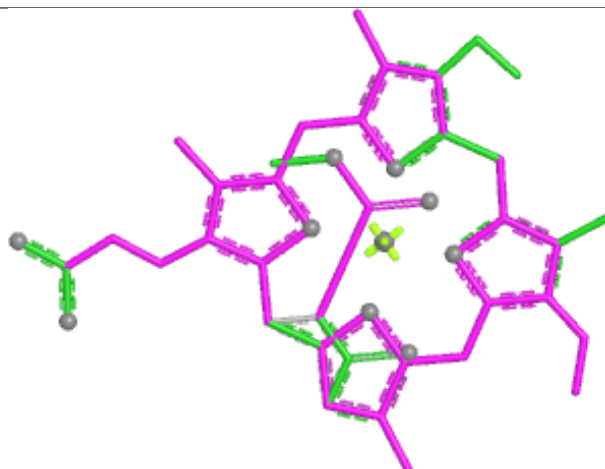


Rings

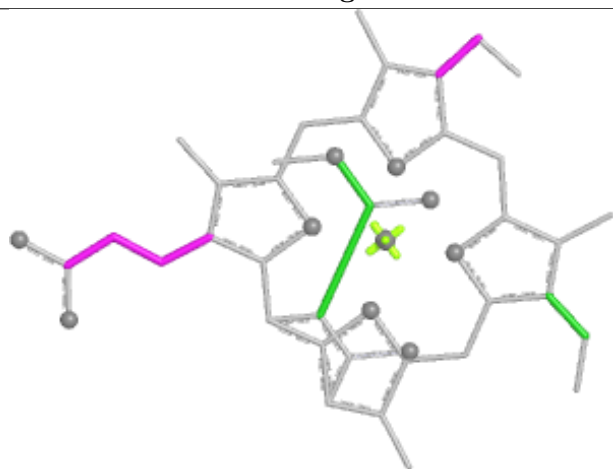
Ligand KC1 4 302



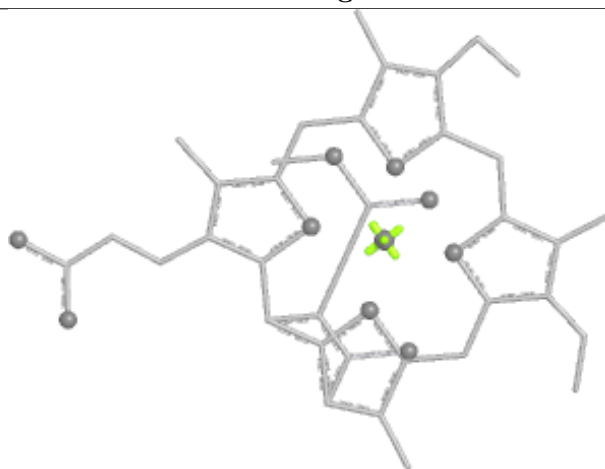
Bond lengths



Bond angles

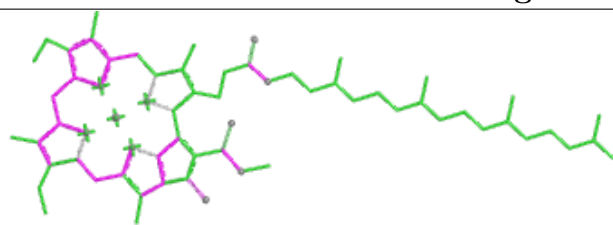


Torsions

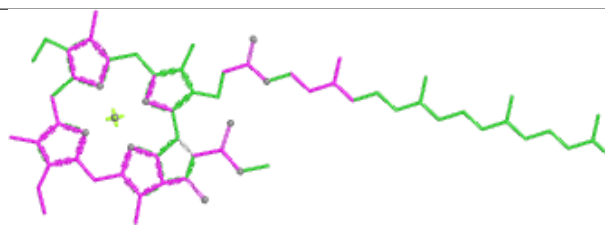


Rings

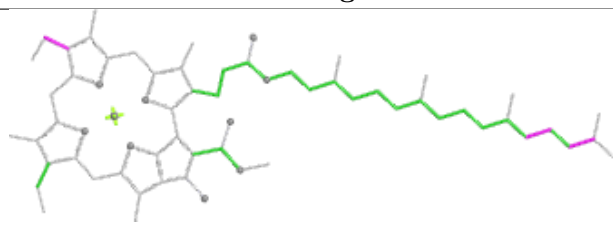
Ligand CLA B 824



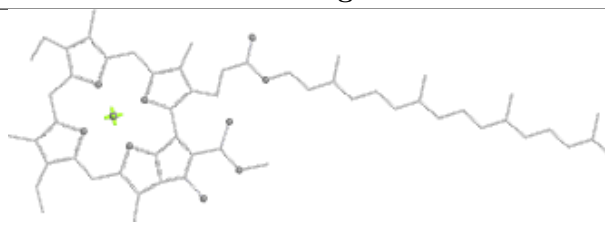
Bond lengths



Bond angles

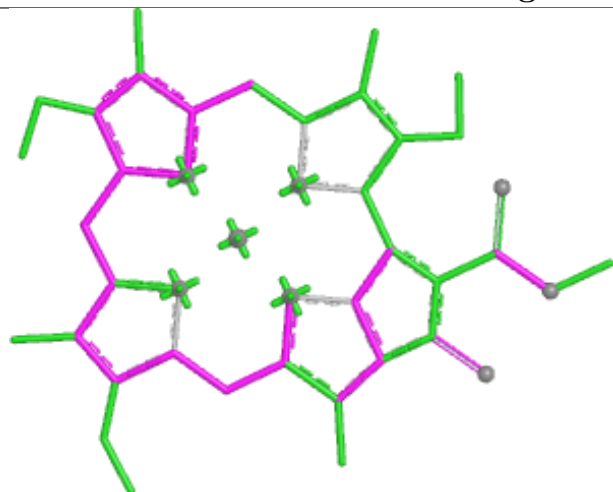


Torsions

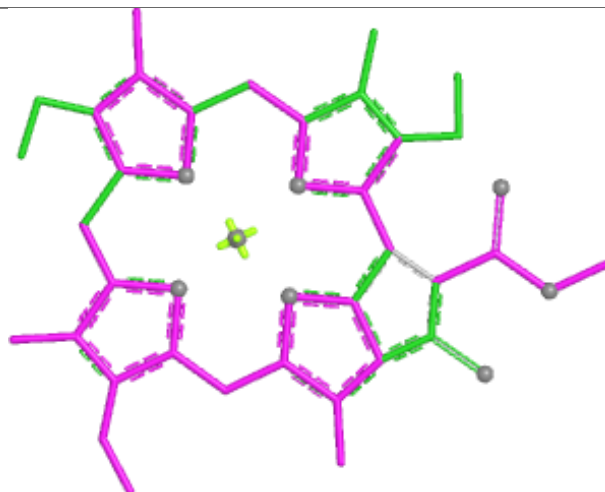


Rings

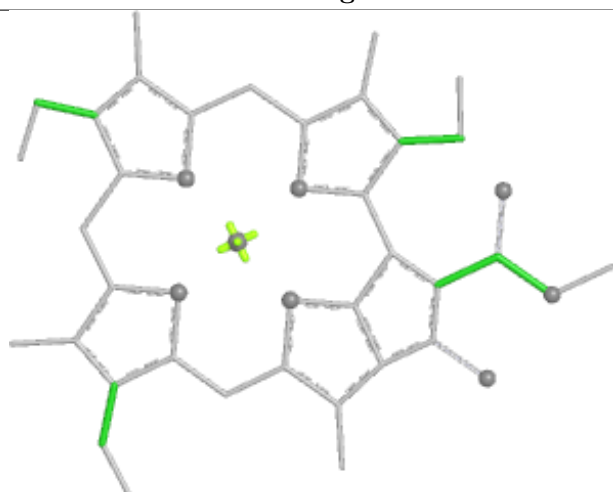
Ligand CLA 2 215



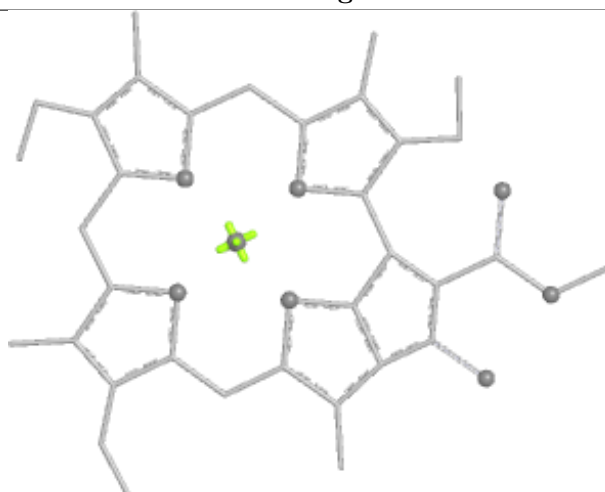
Bond lengths



Bond angles

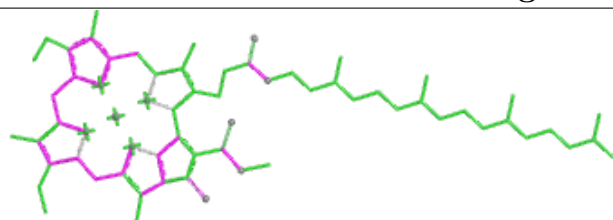


Torsions

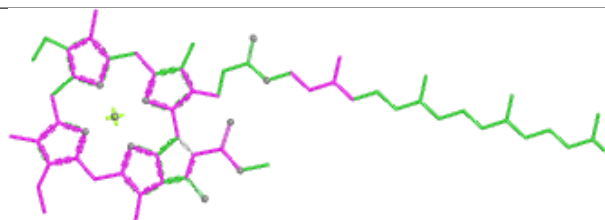


Rings

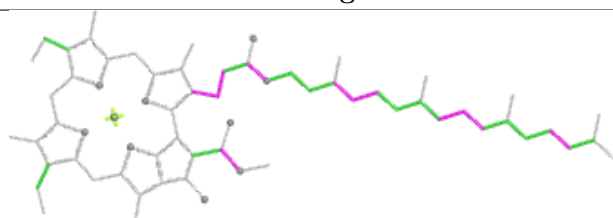
Ligand CLA 5 210



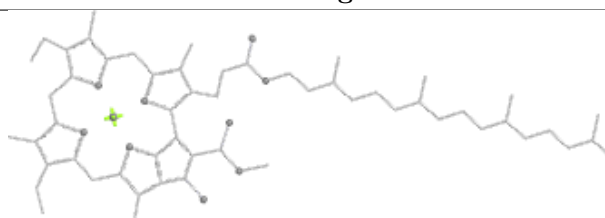
Bond lengths



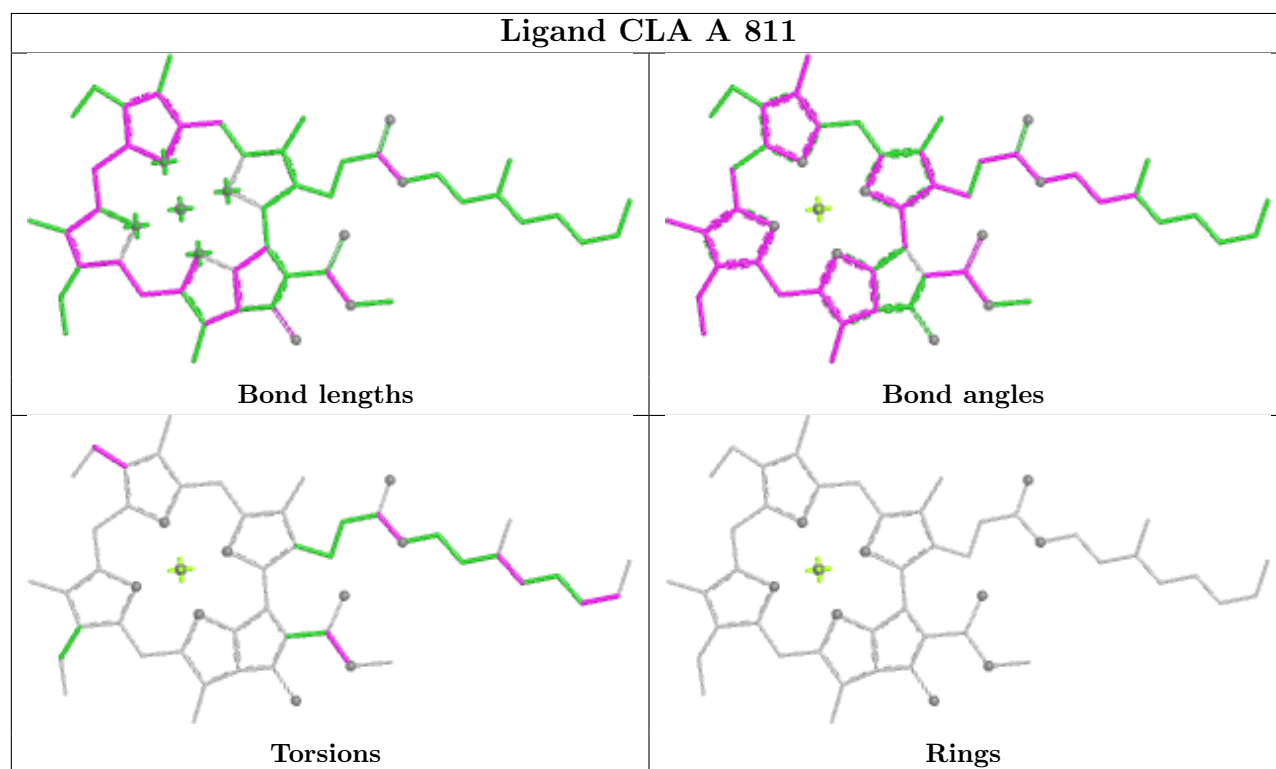
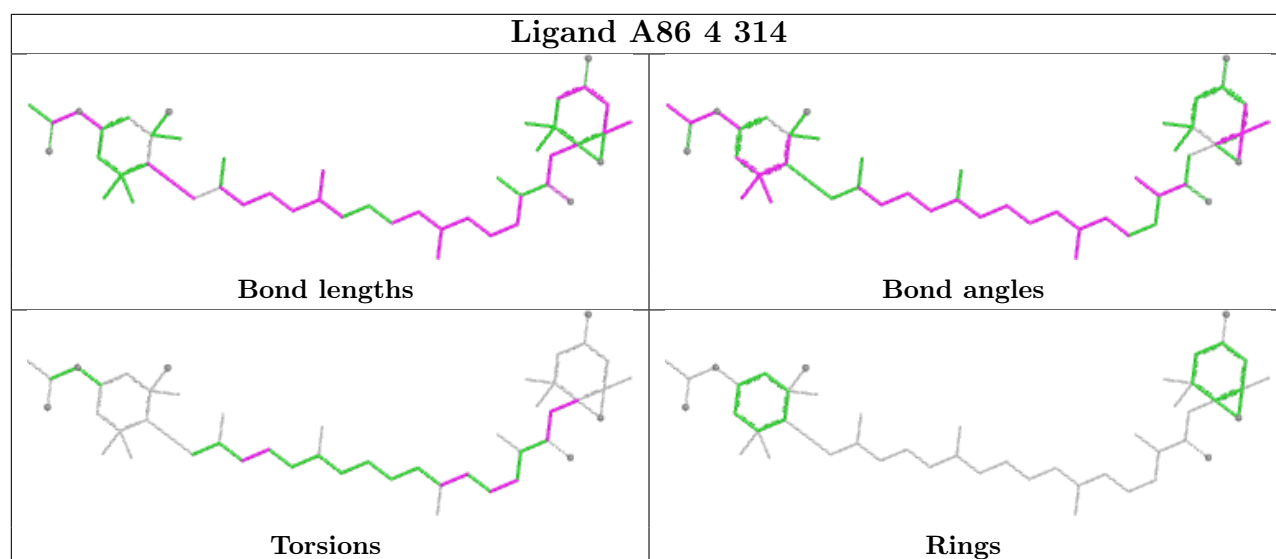
Bond angles

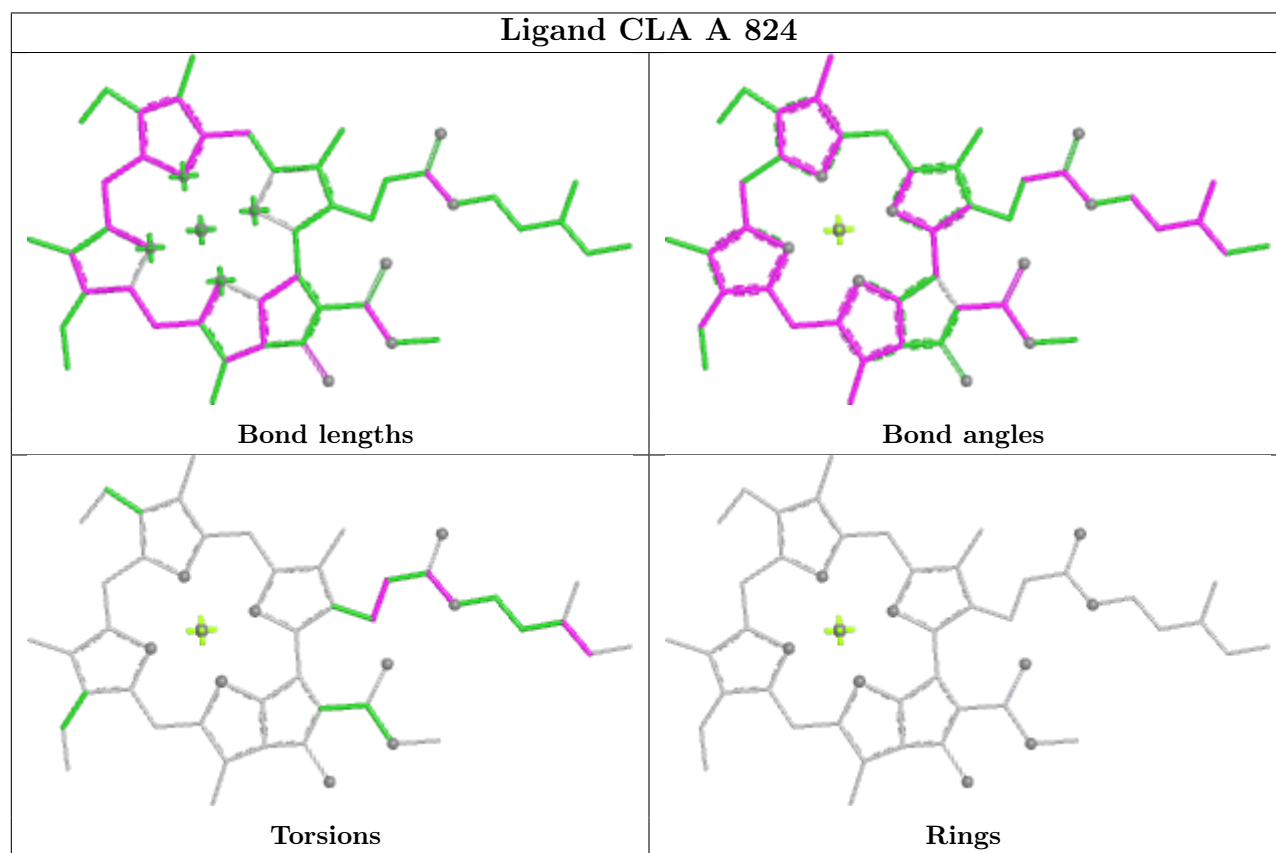
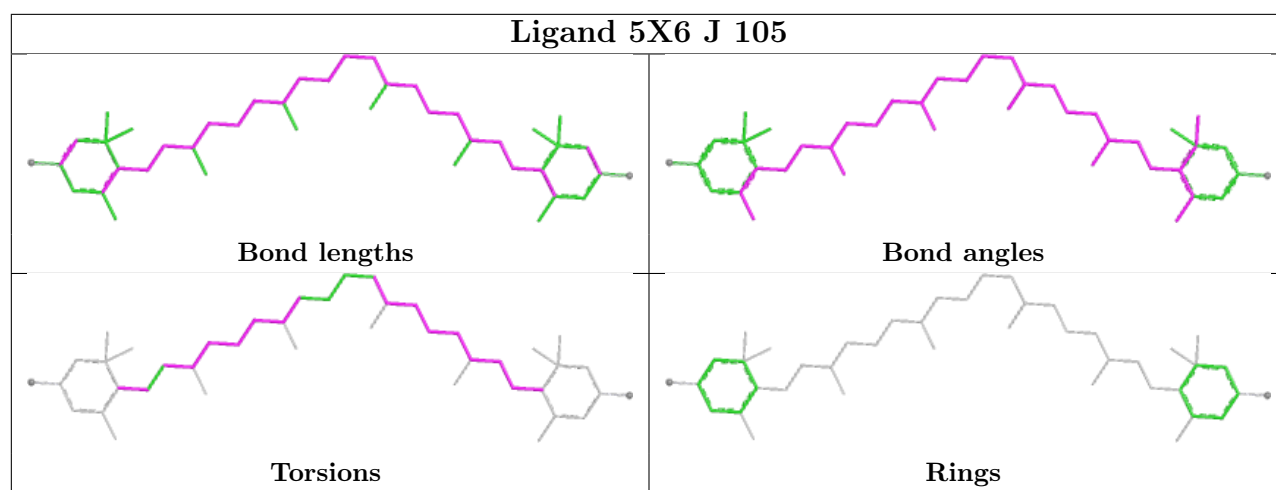


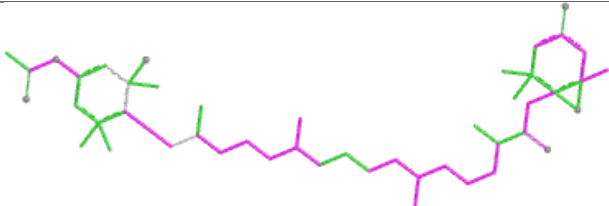
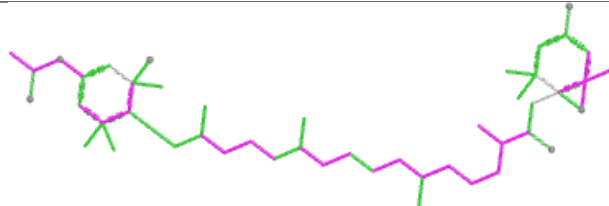
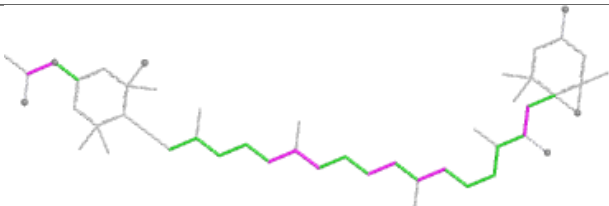
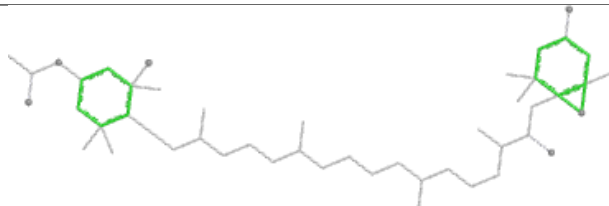
Torsions

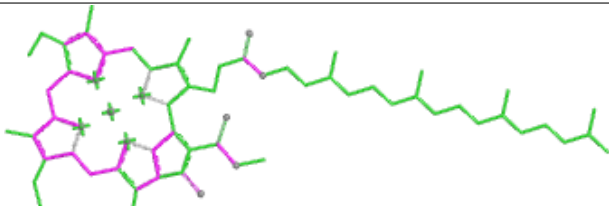
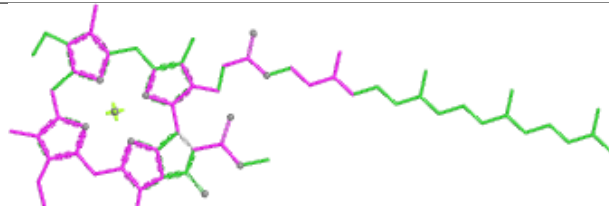
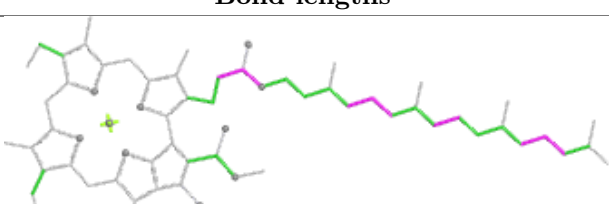
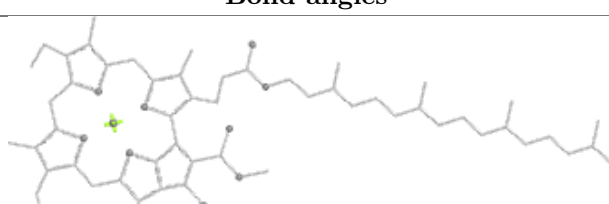


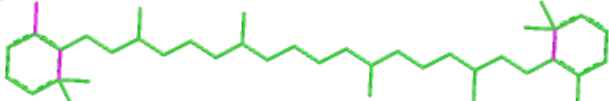
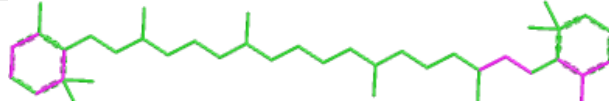
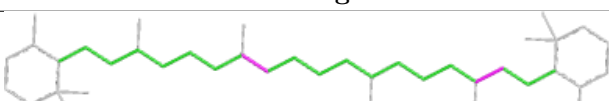
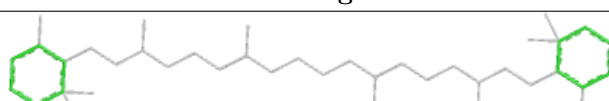
Rings

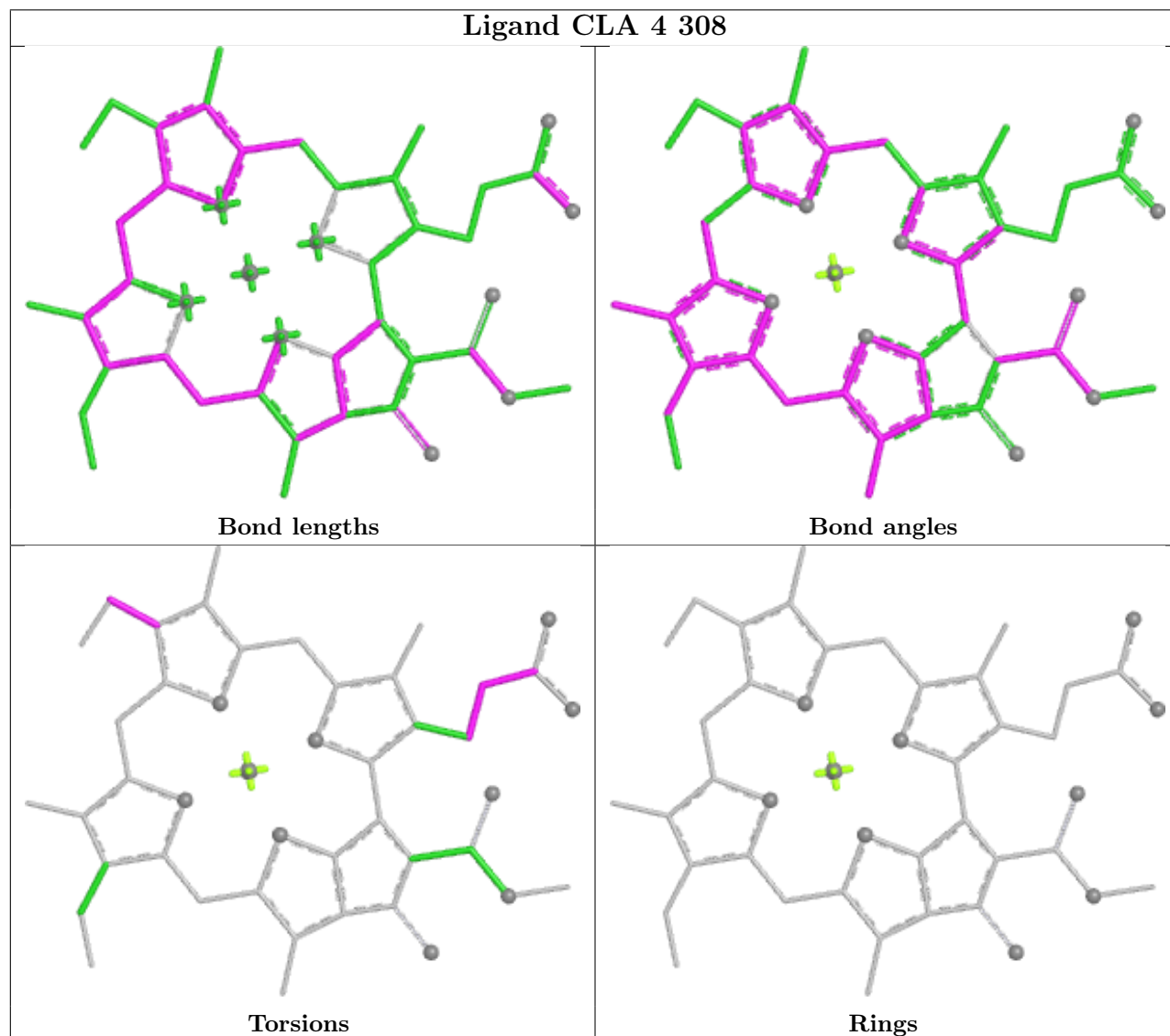
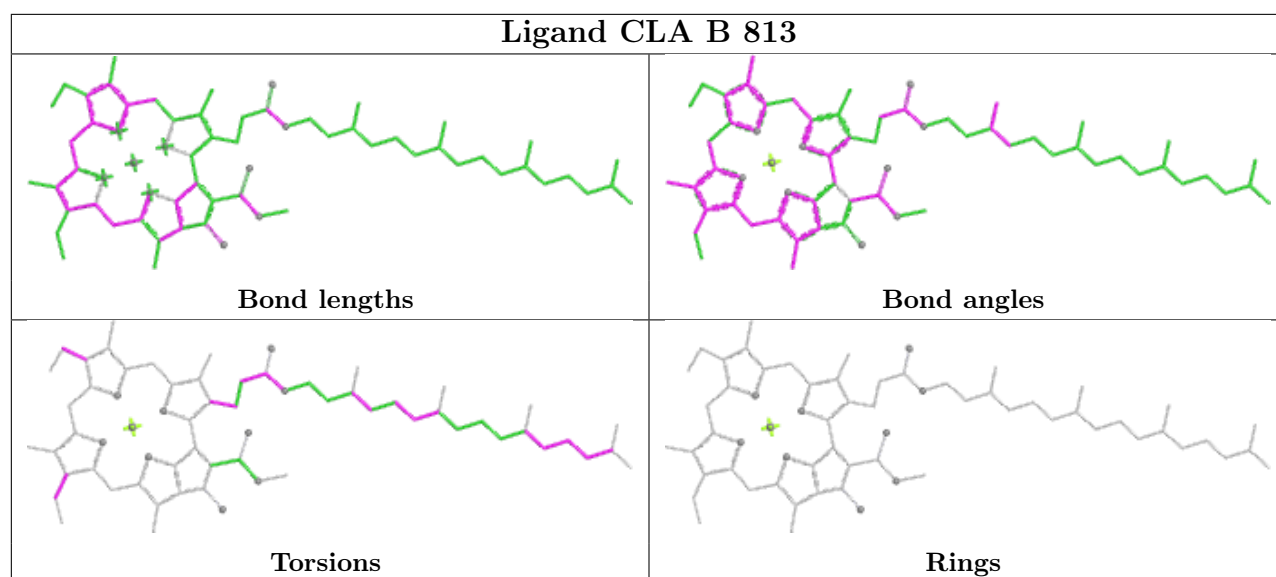


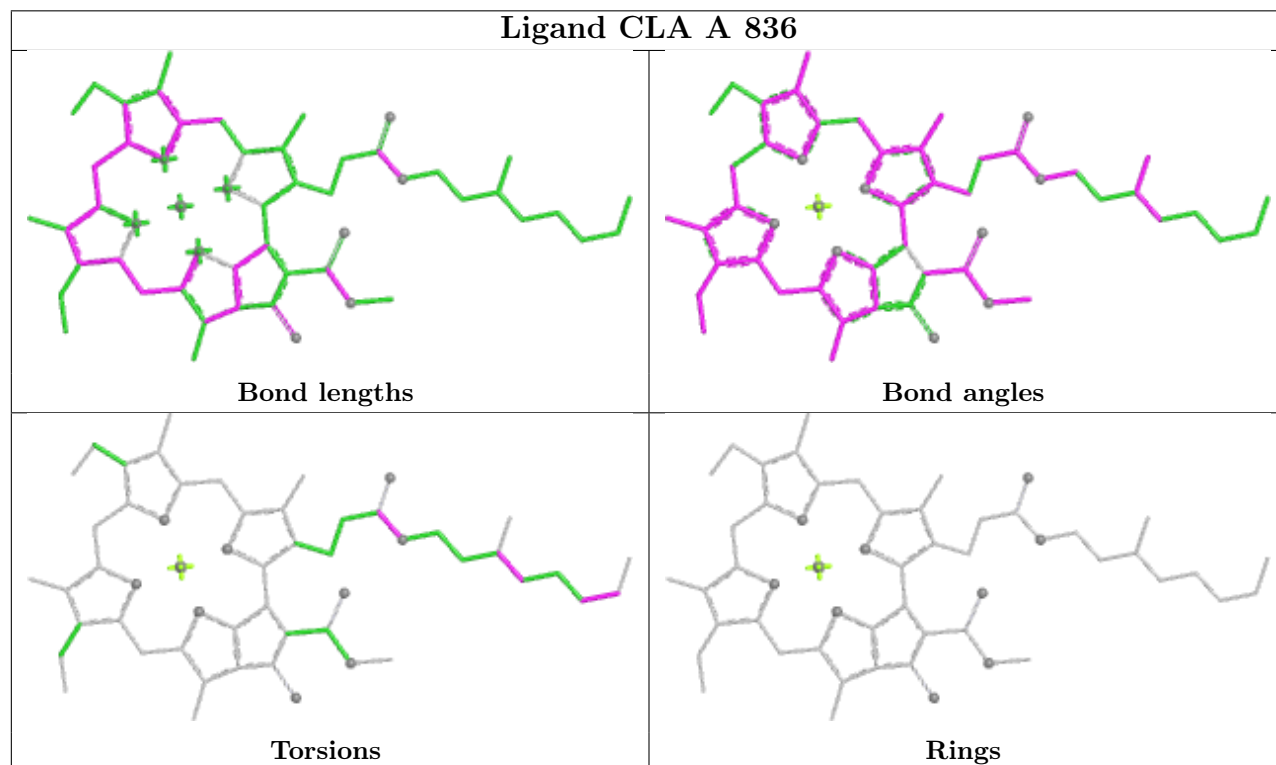
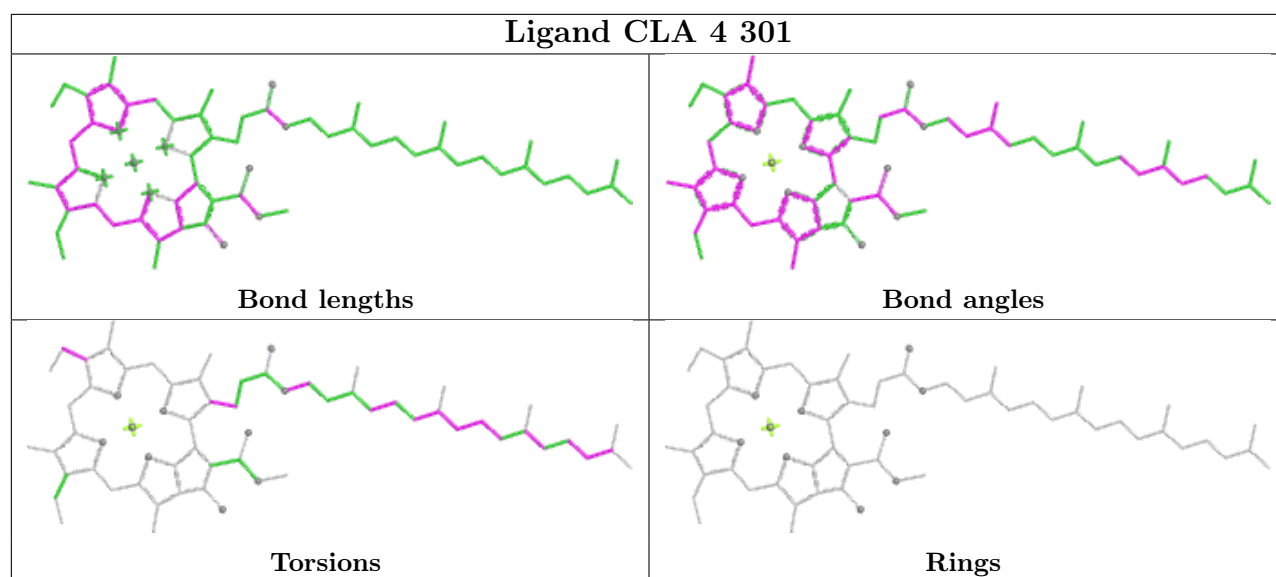


Ligand A86 3 228	
	
Bond lengths	Bond angles
	
Torsions	Rings

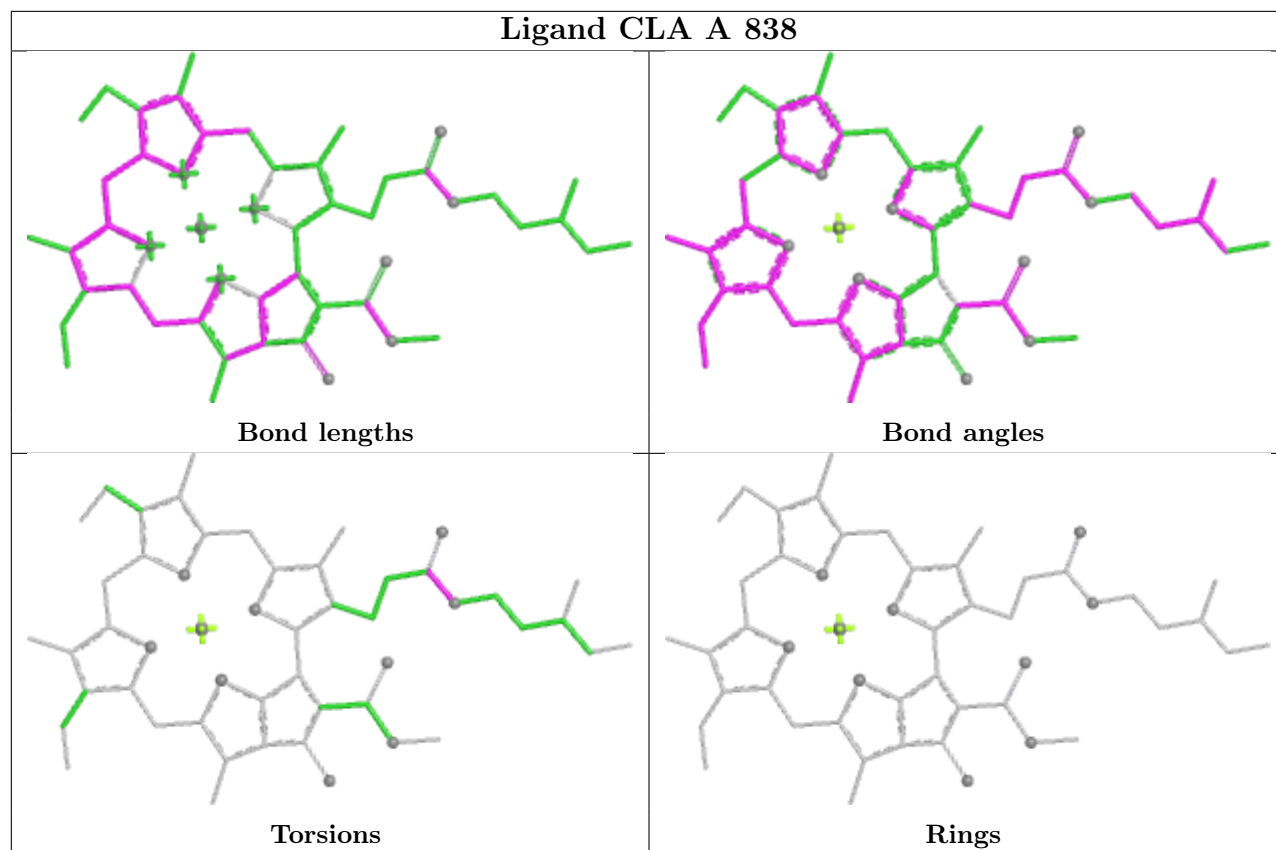
Ligand CLA A 839	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR F 205	
	
Bond lengths	Bond angles
	
Torsions	Rings

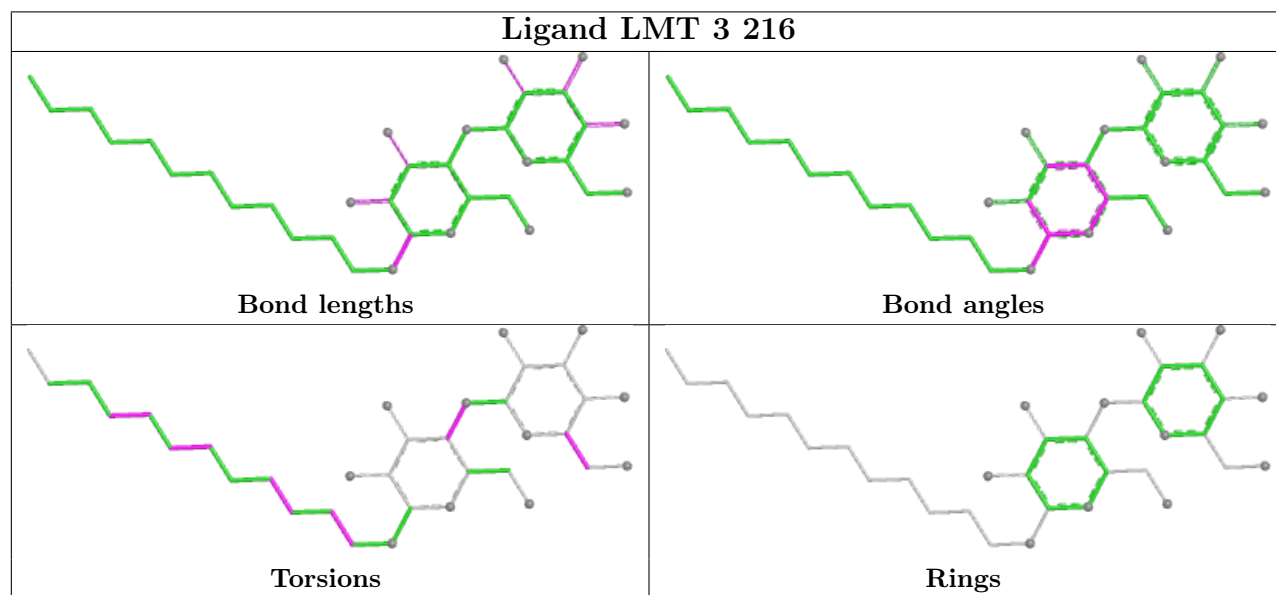


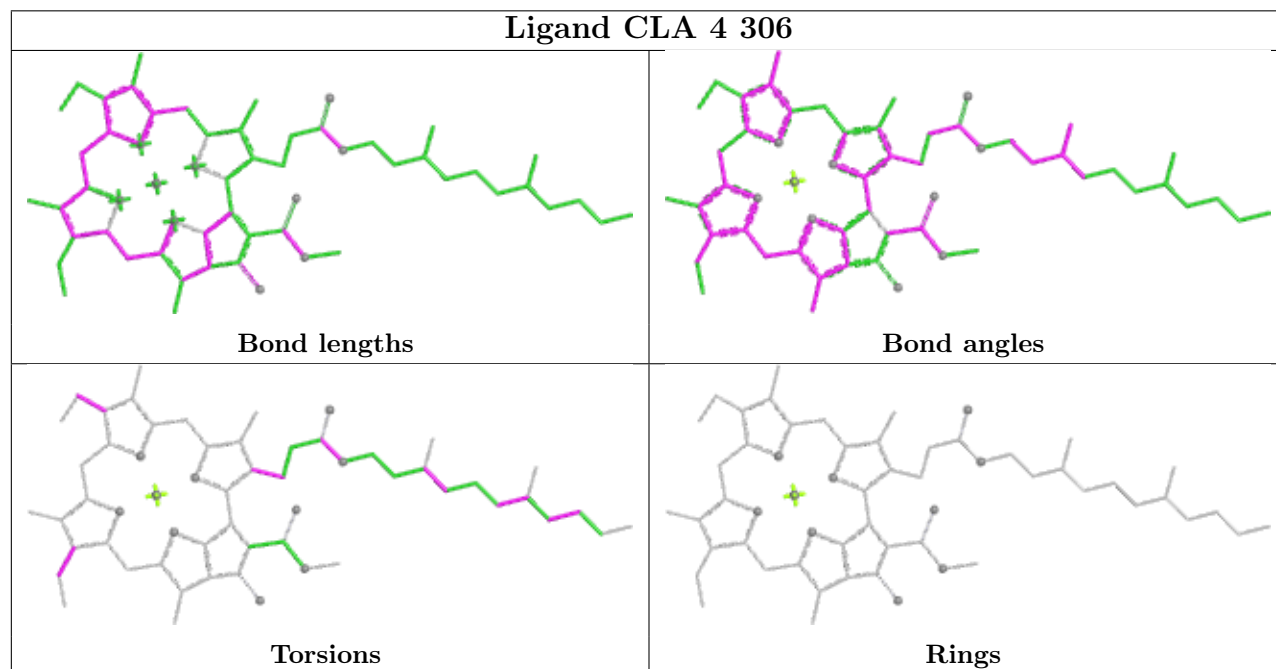
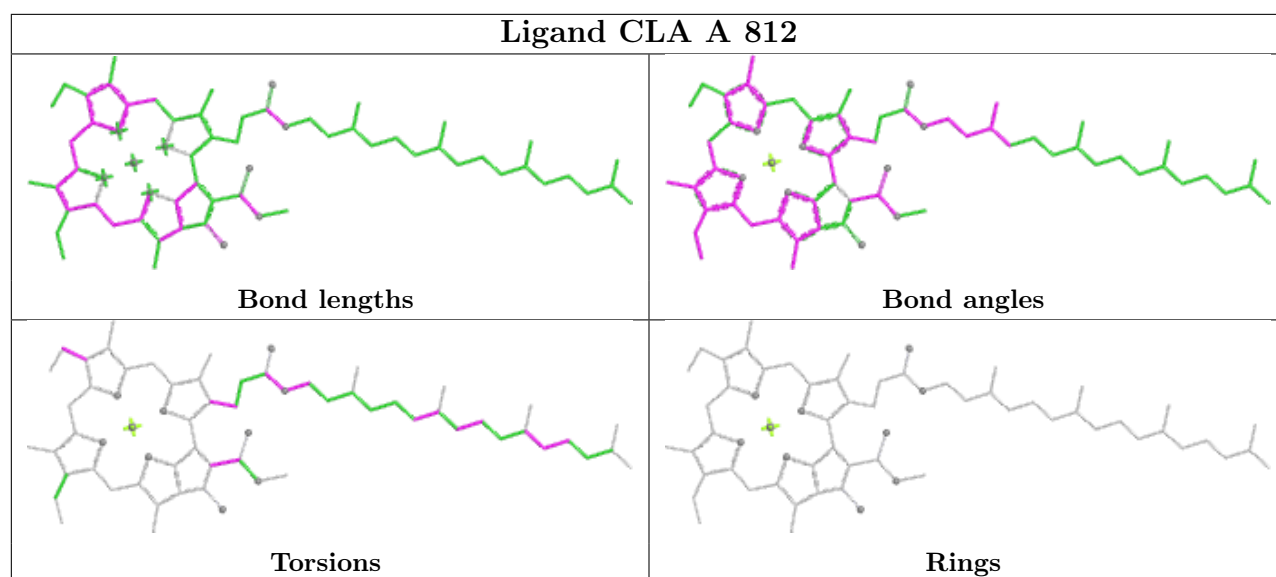


Ligand CLA A 838

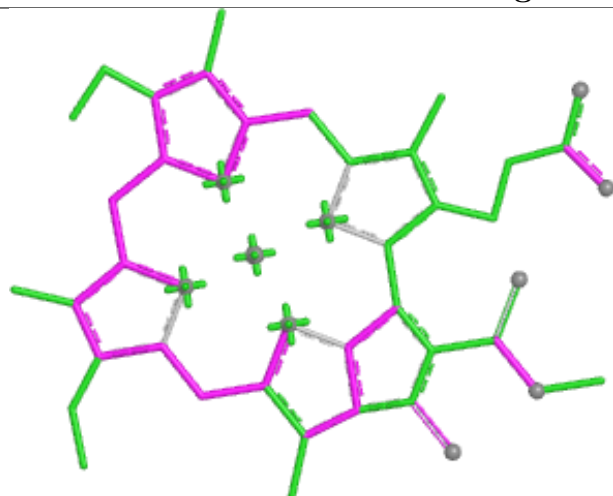


Ligand LMT 3 216

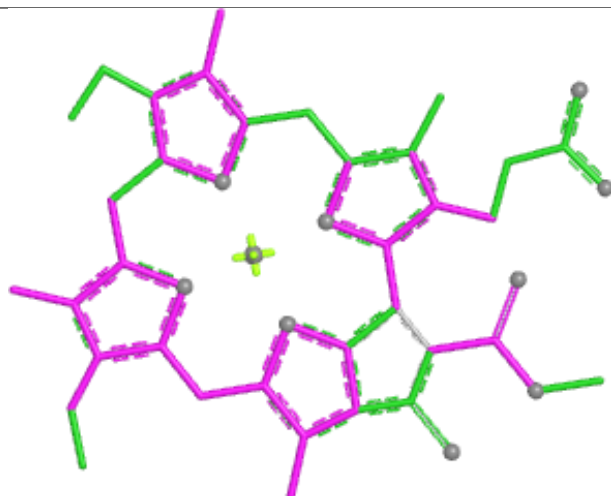




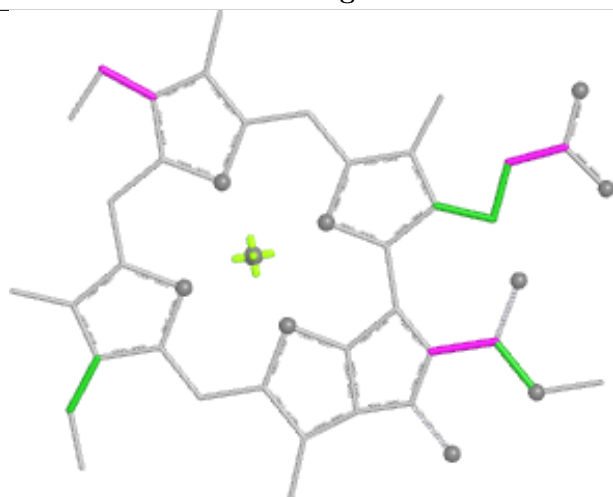
Ligand CLA B 815



Bond lengths



Bond angles

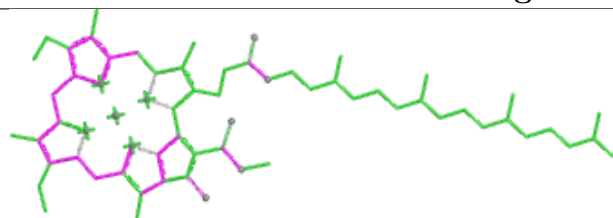


Torsions

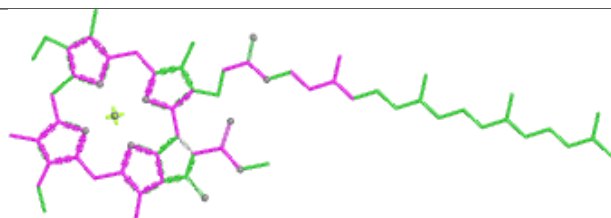


Rings

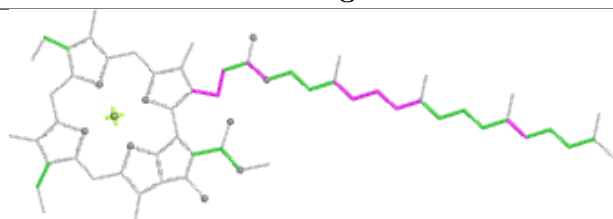
Ligand CLA B 832



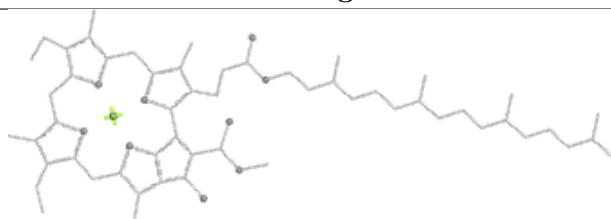
Bond lengths



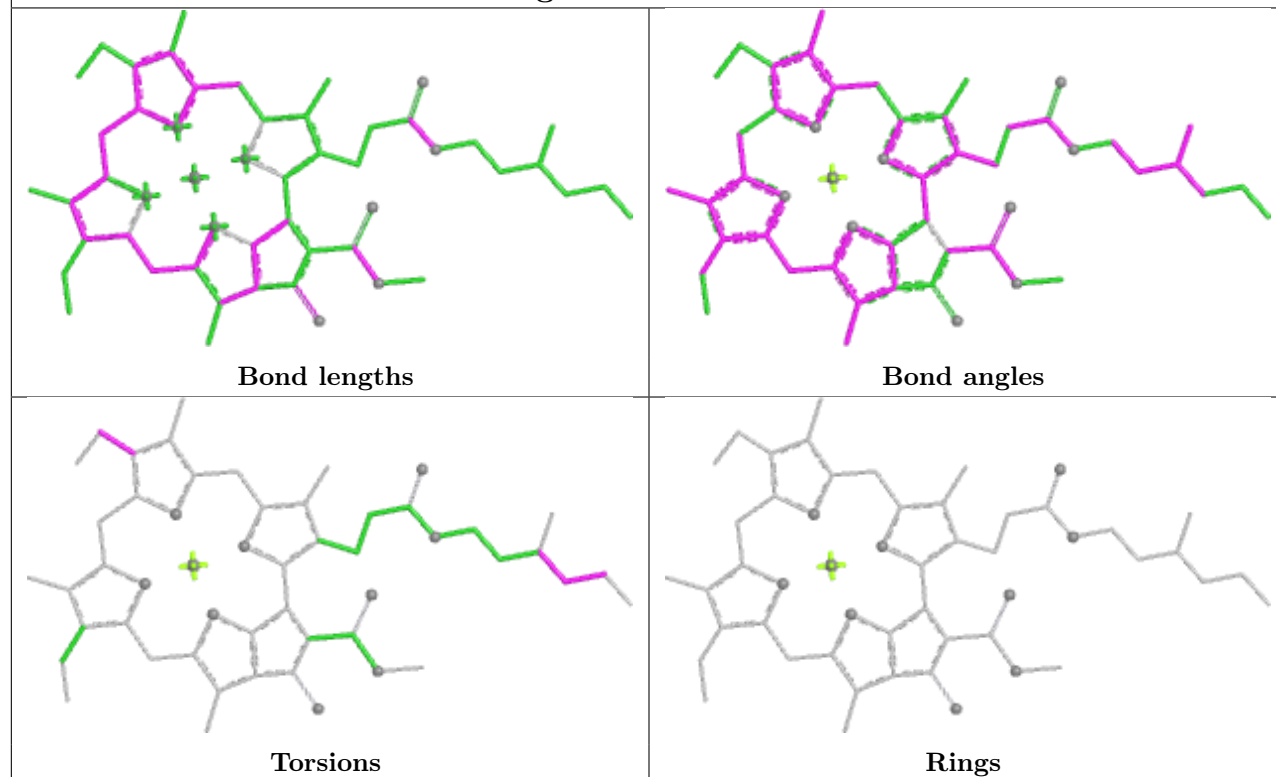
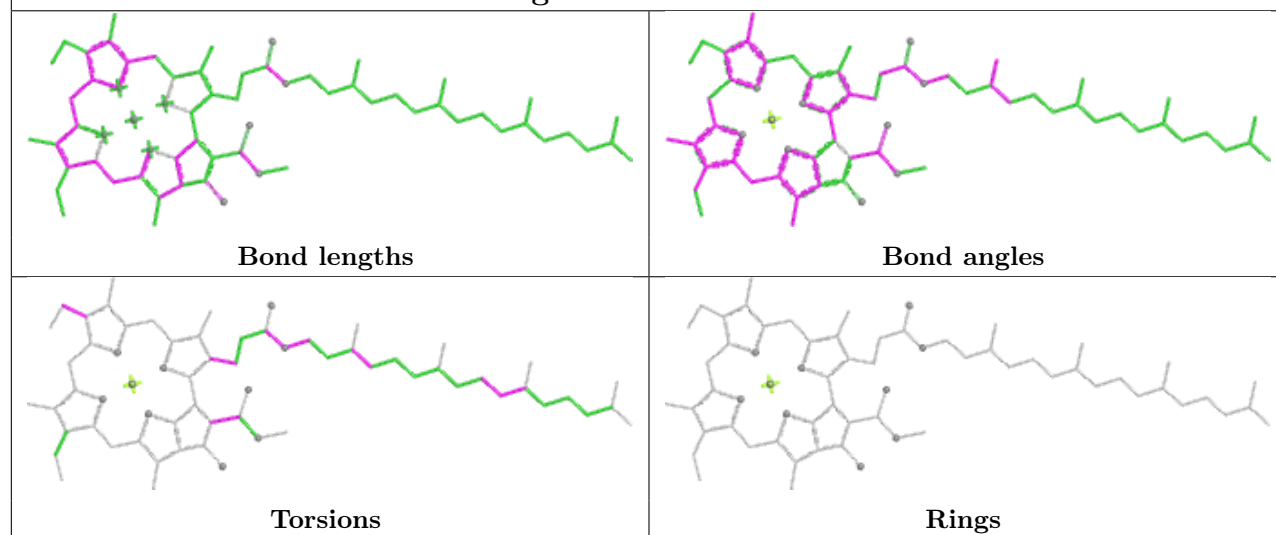
Bond angles

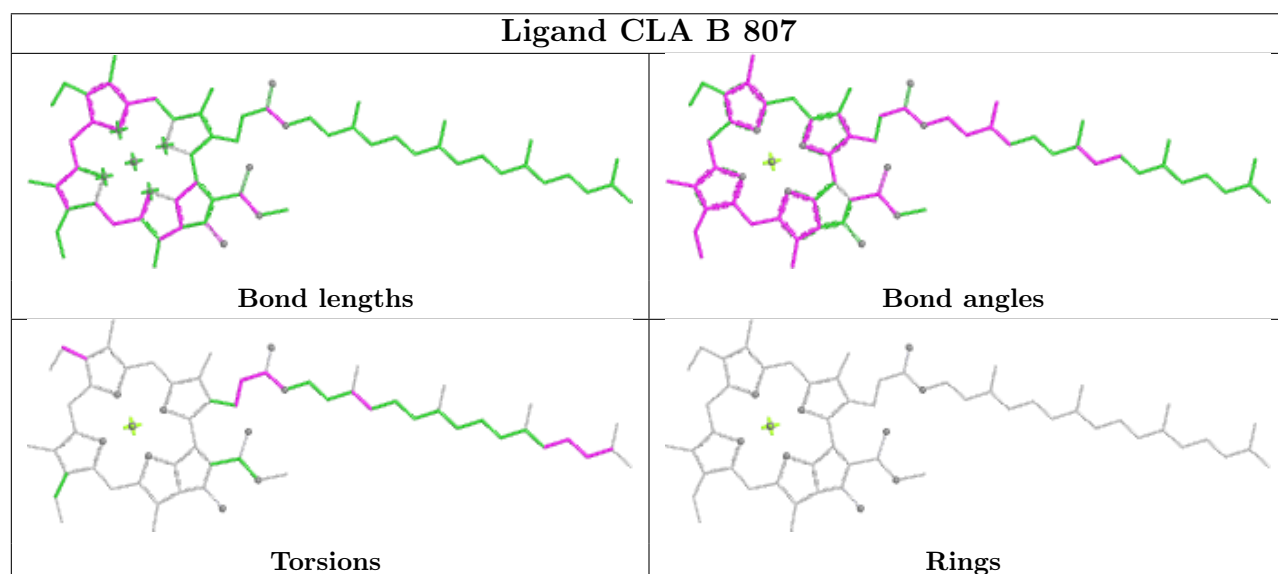
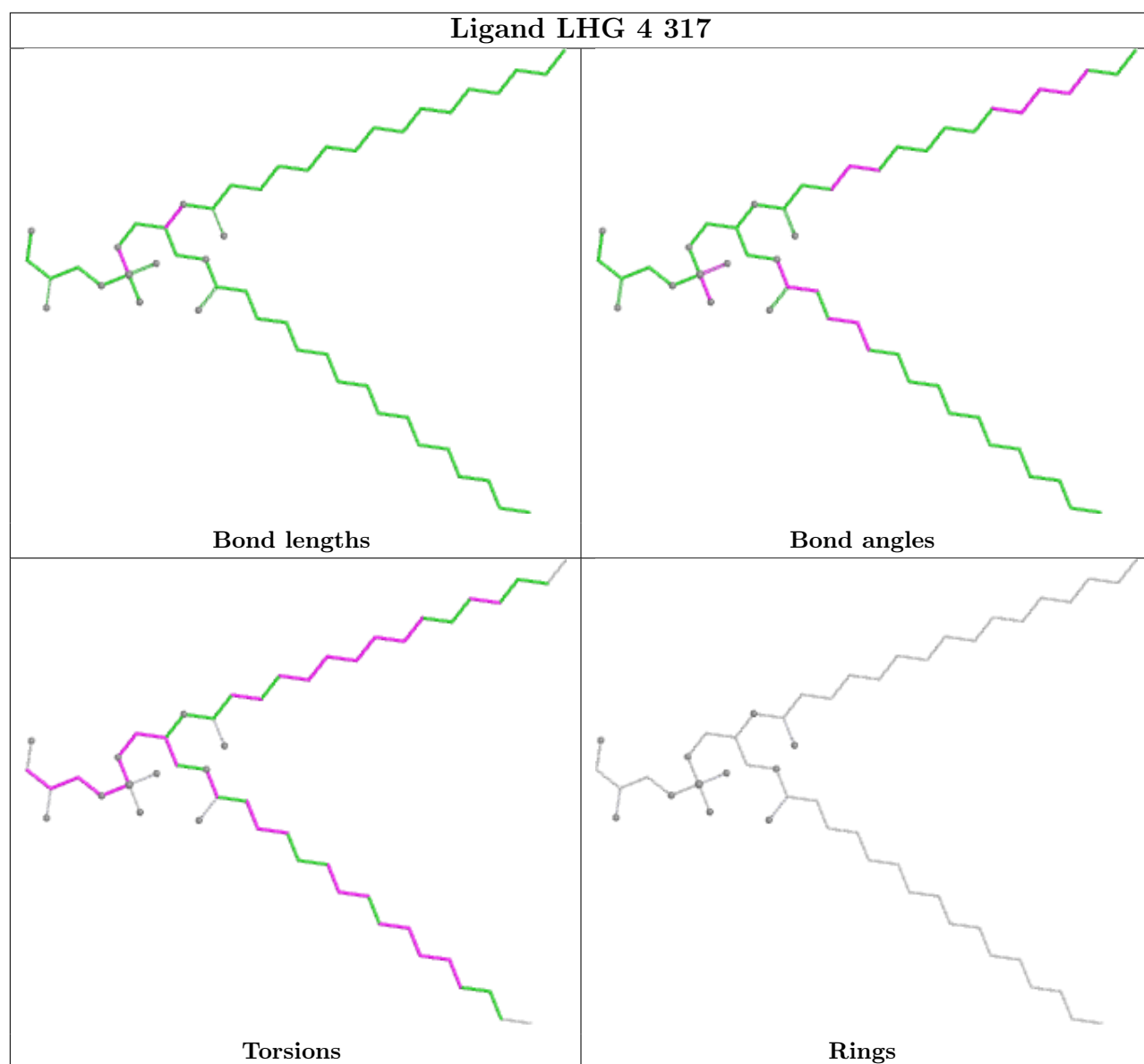


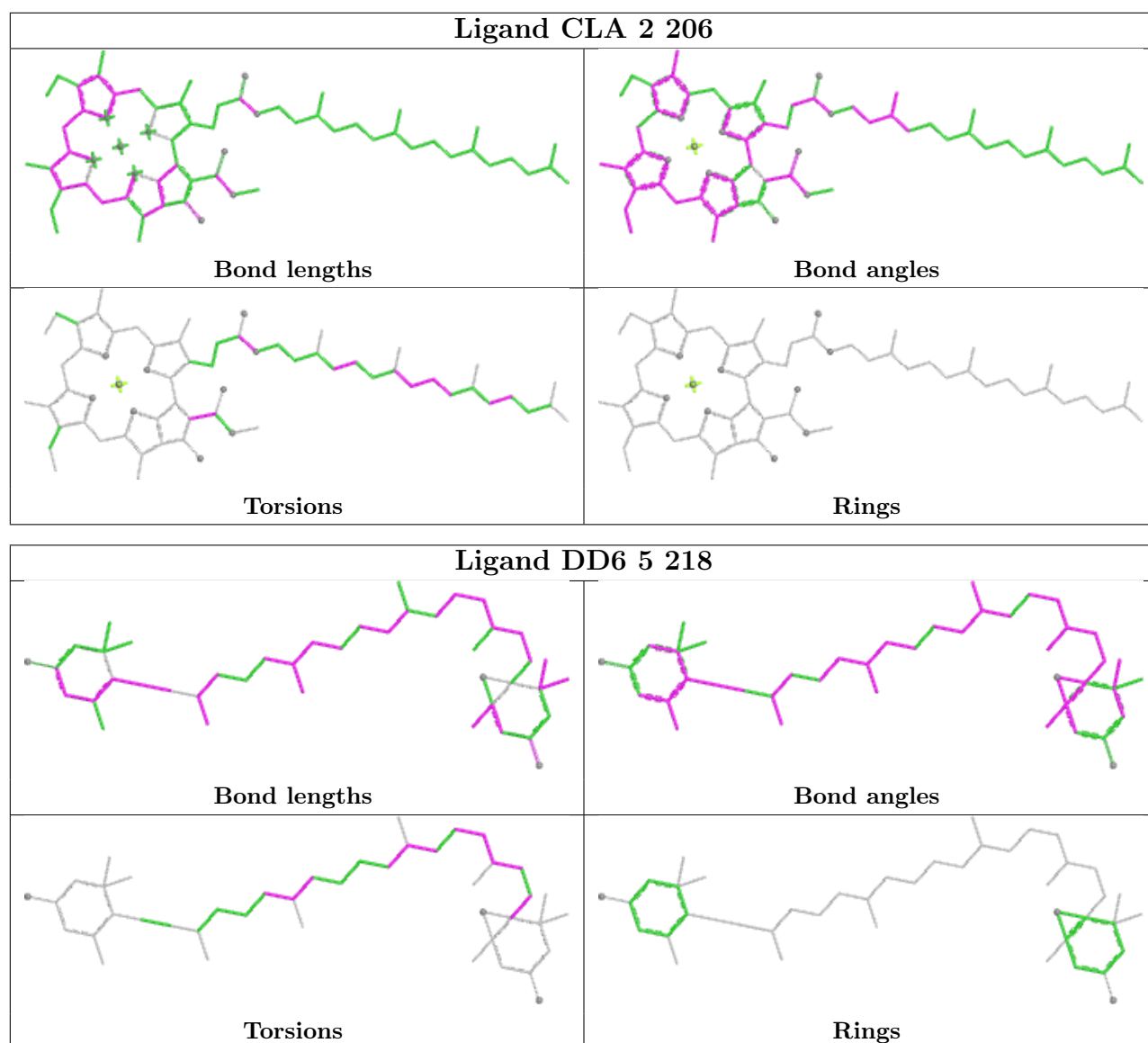
Torsions

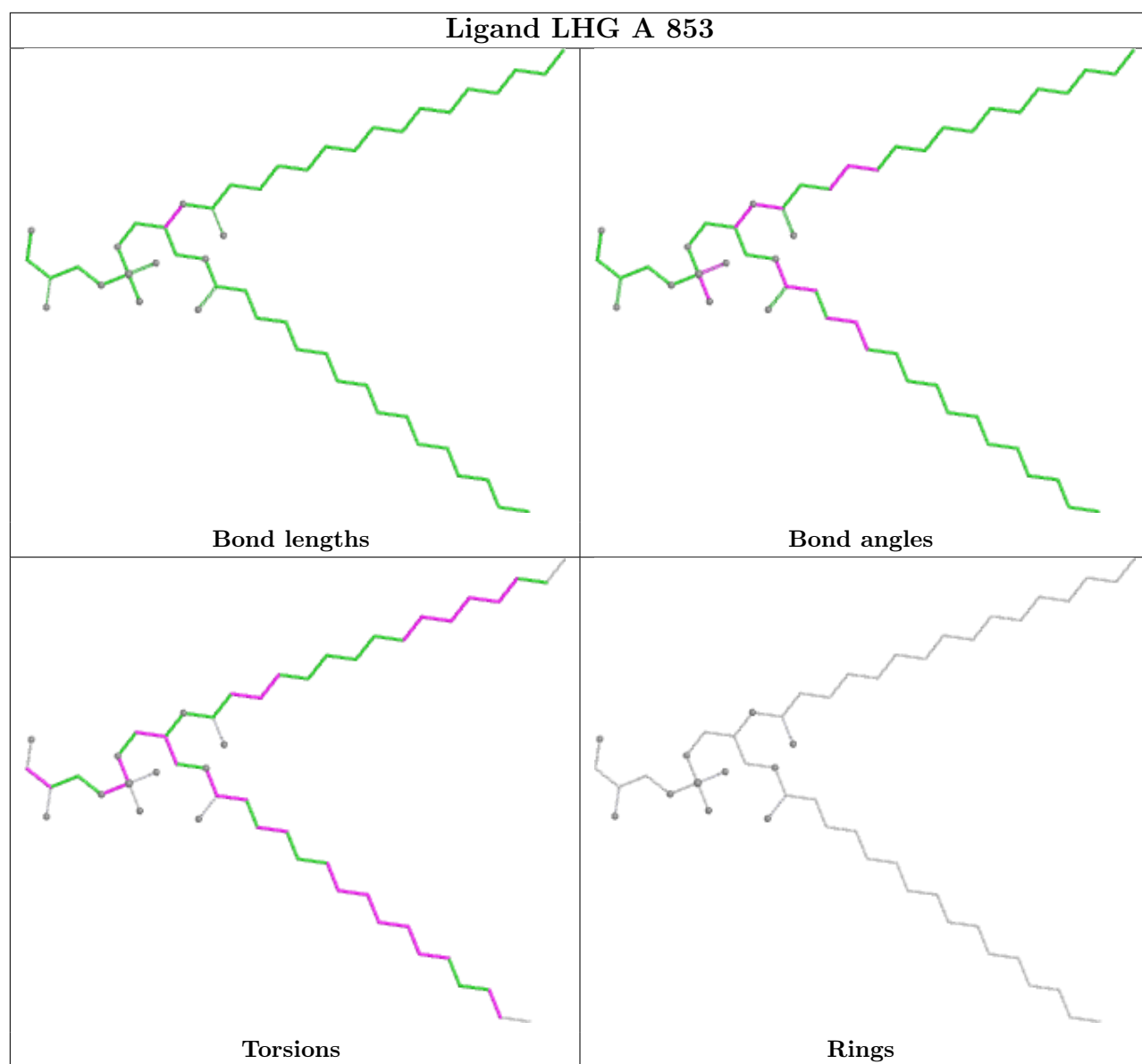


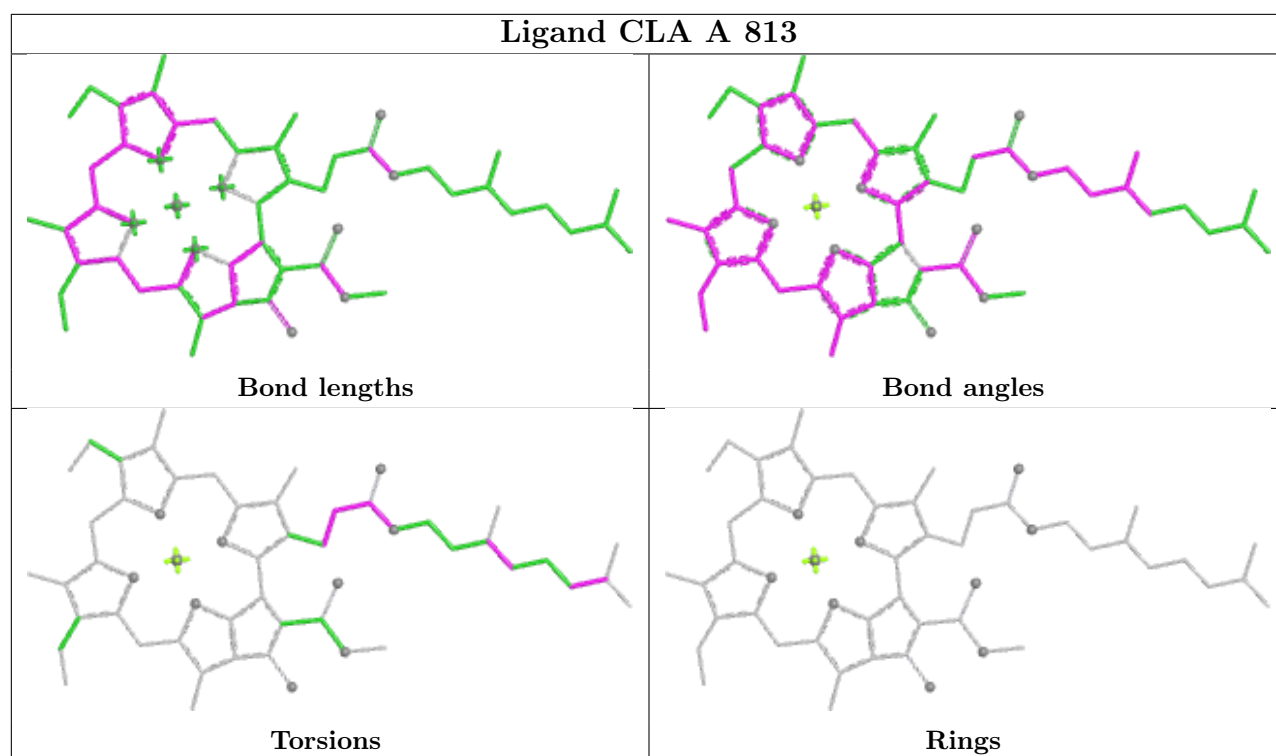
Rings

Ligand CLA 4 312**Ligand CLA A 806**









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

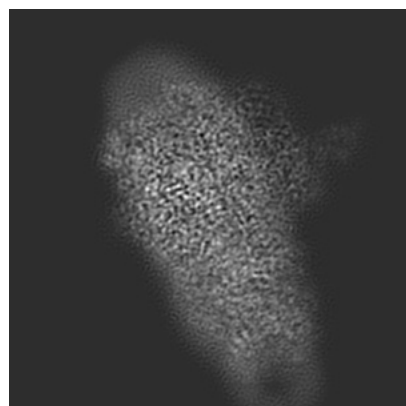
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38457. These allow visual inspection of the internal detail of the map and identification of artifacts.

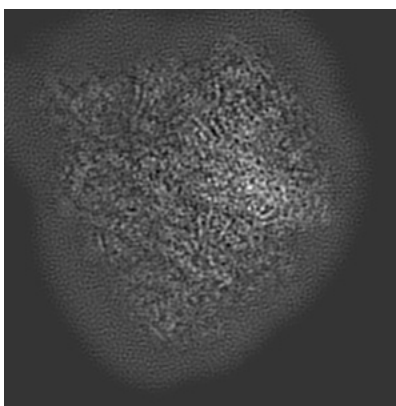
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

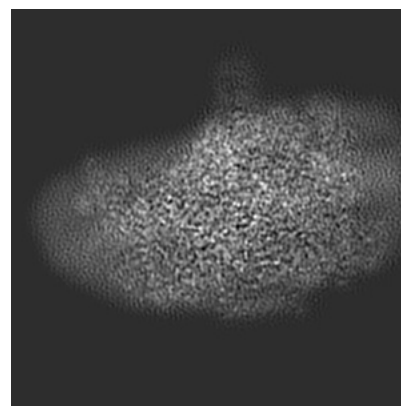
6.1.1 Primary map



X

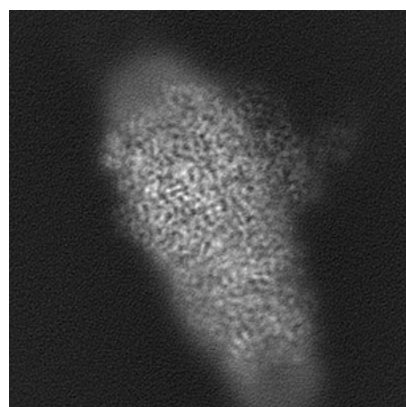


Y

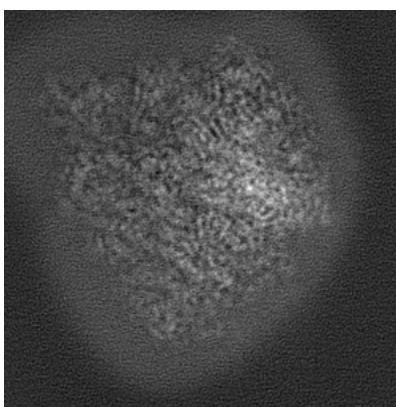


Z

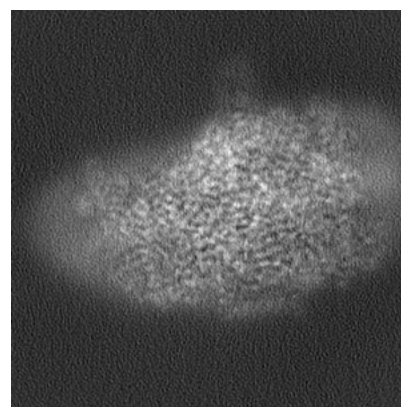
6.1.2 Raw map



X



Y

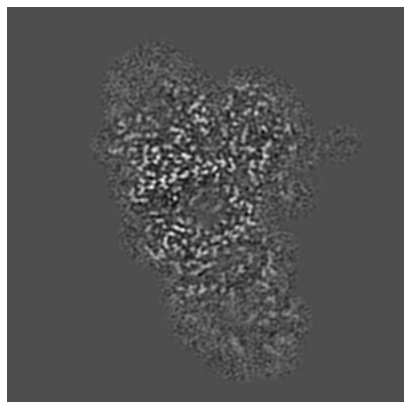


Z

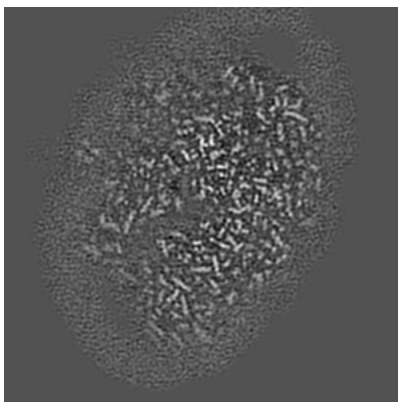
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

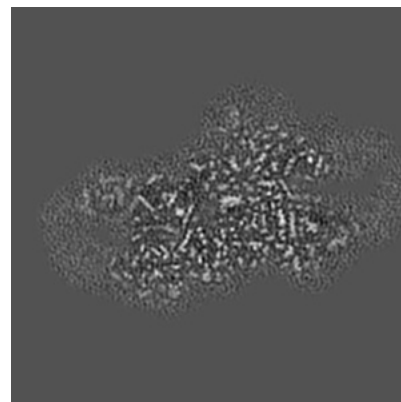
6.2.1 Primary map



X Index: 127

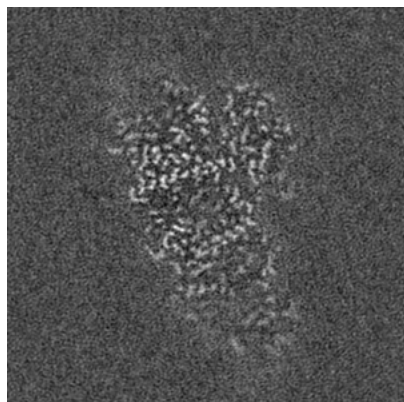


Y Index: 127

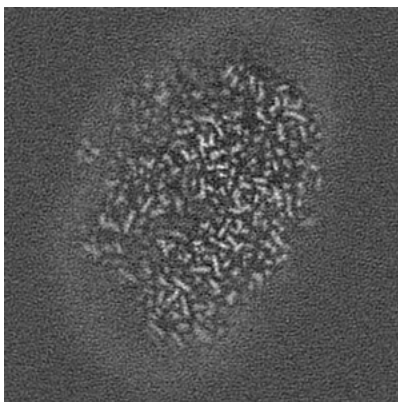


Z Index: 127

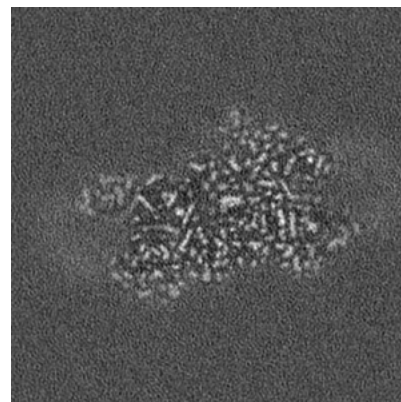
6.2.2 Raw map



X Index: 127



Y Index: 127

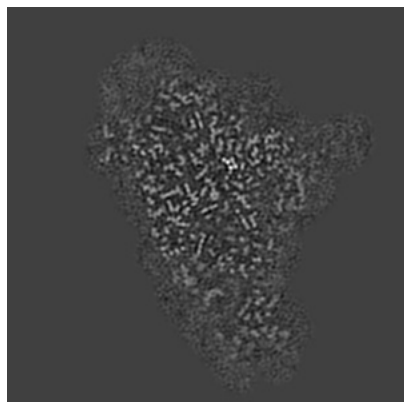


Z Index: 127

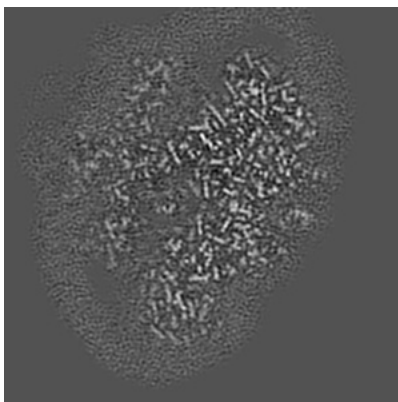
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

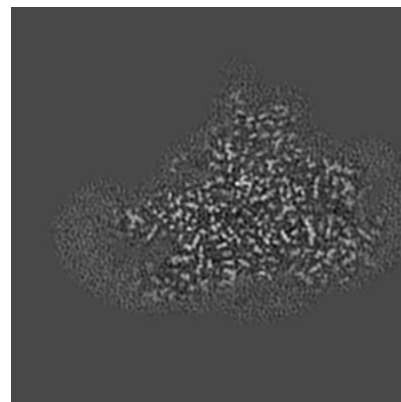
6.3.1 Primary map



X Index: 142

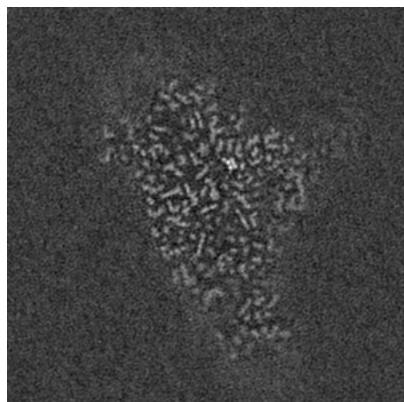


Y Index: 133

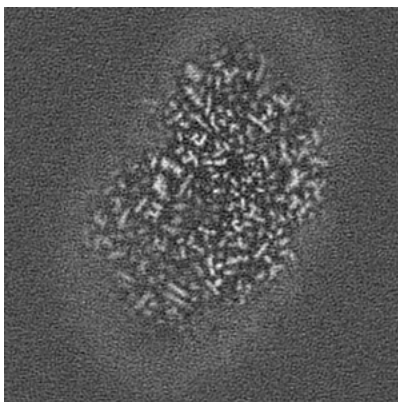


Z Index: 149

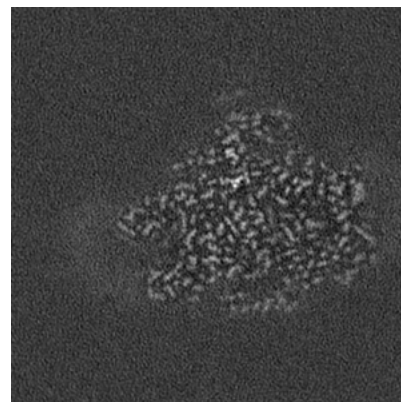
6.3.2 Raw map



X Index: 142



Y Index: 121

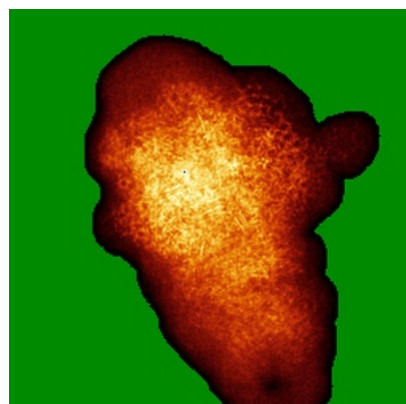


Z Index: 155

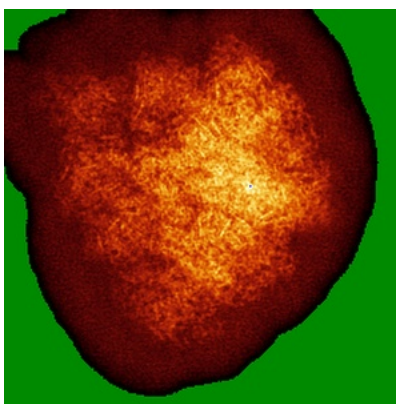
The images above show the largest variance slices of the map in three orthogonal directions.

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

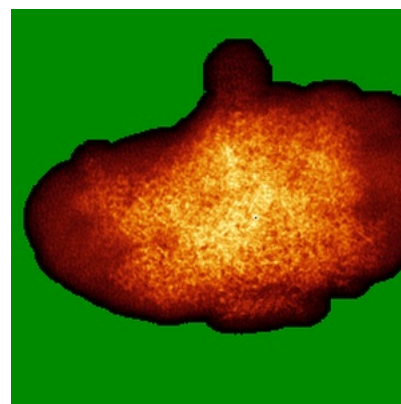
6.4.1 Primary map



X

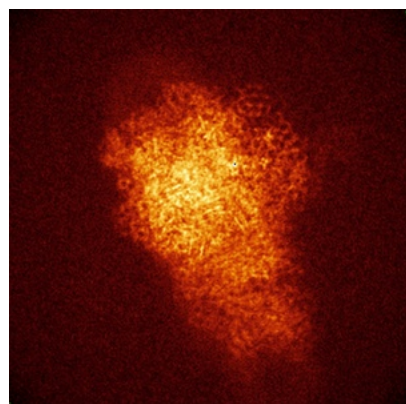


Y

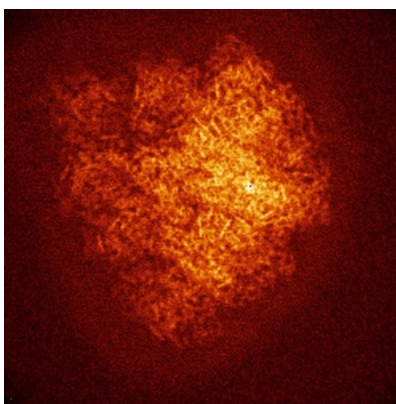


Z

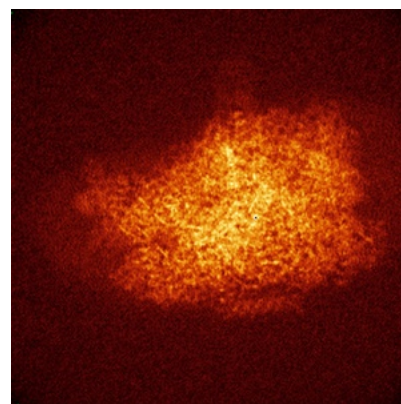
6.4.2 Raw map



X



Y

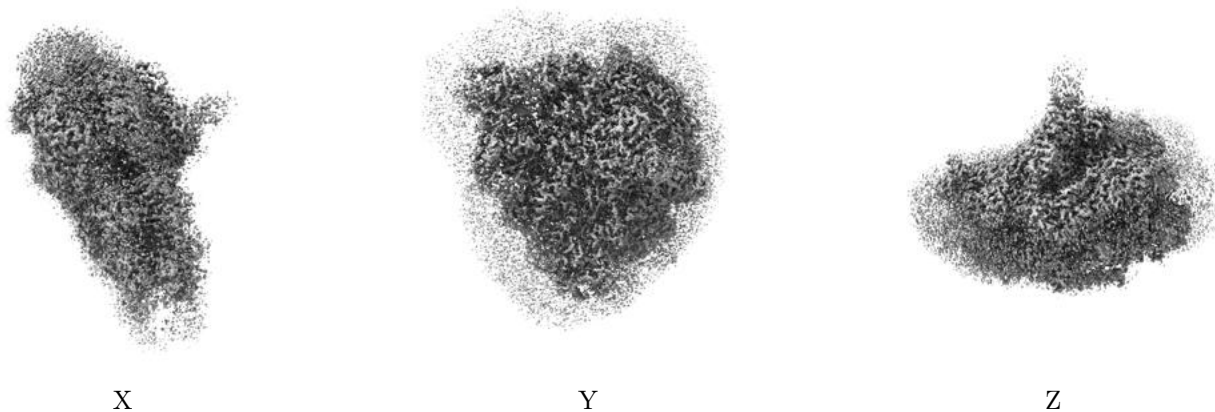


Z

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.

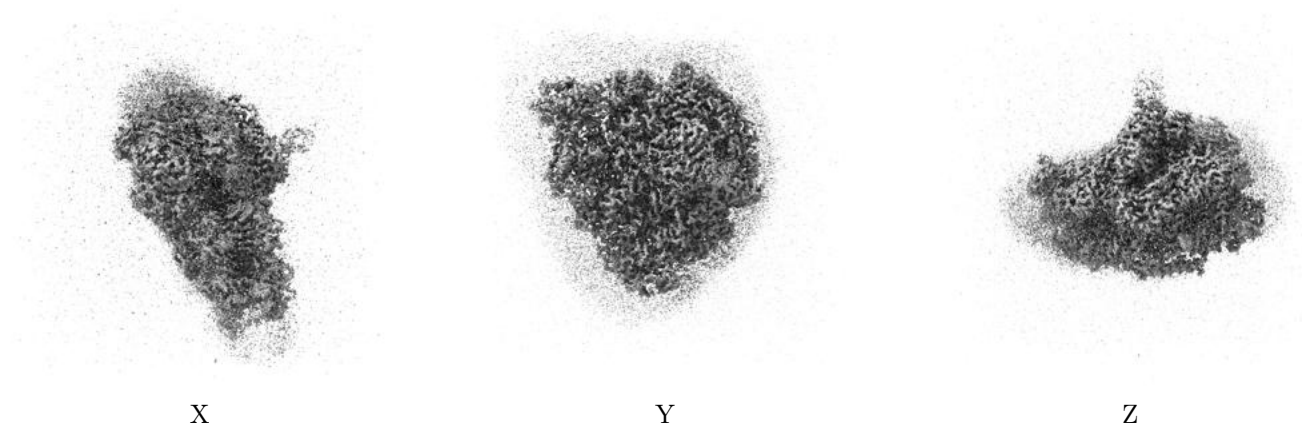
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.012. 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.

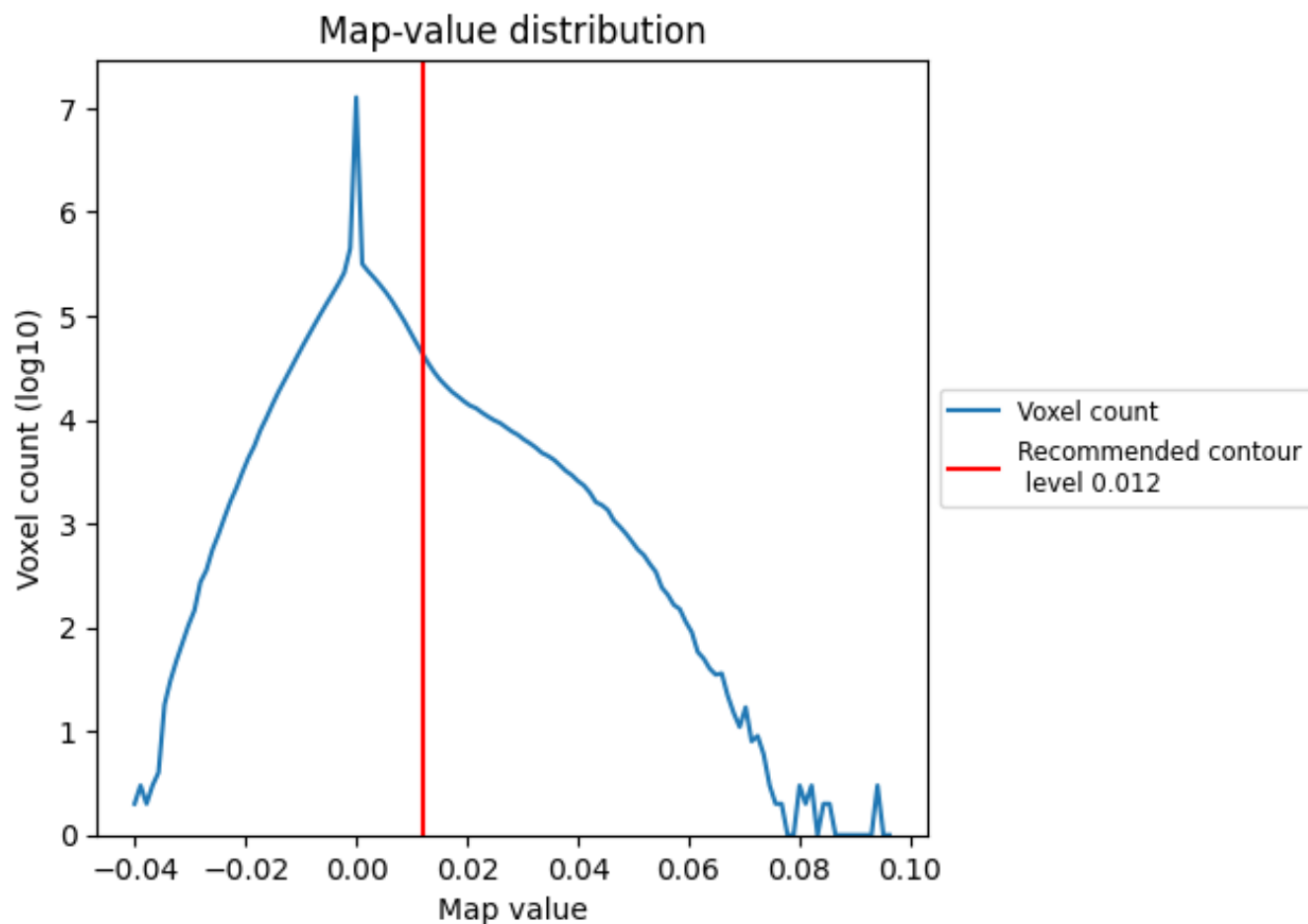
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

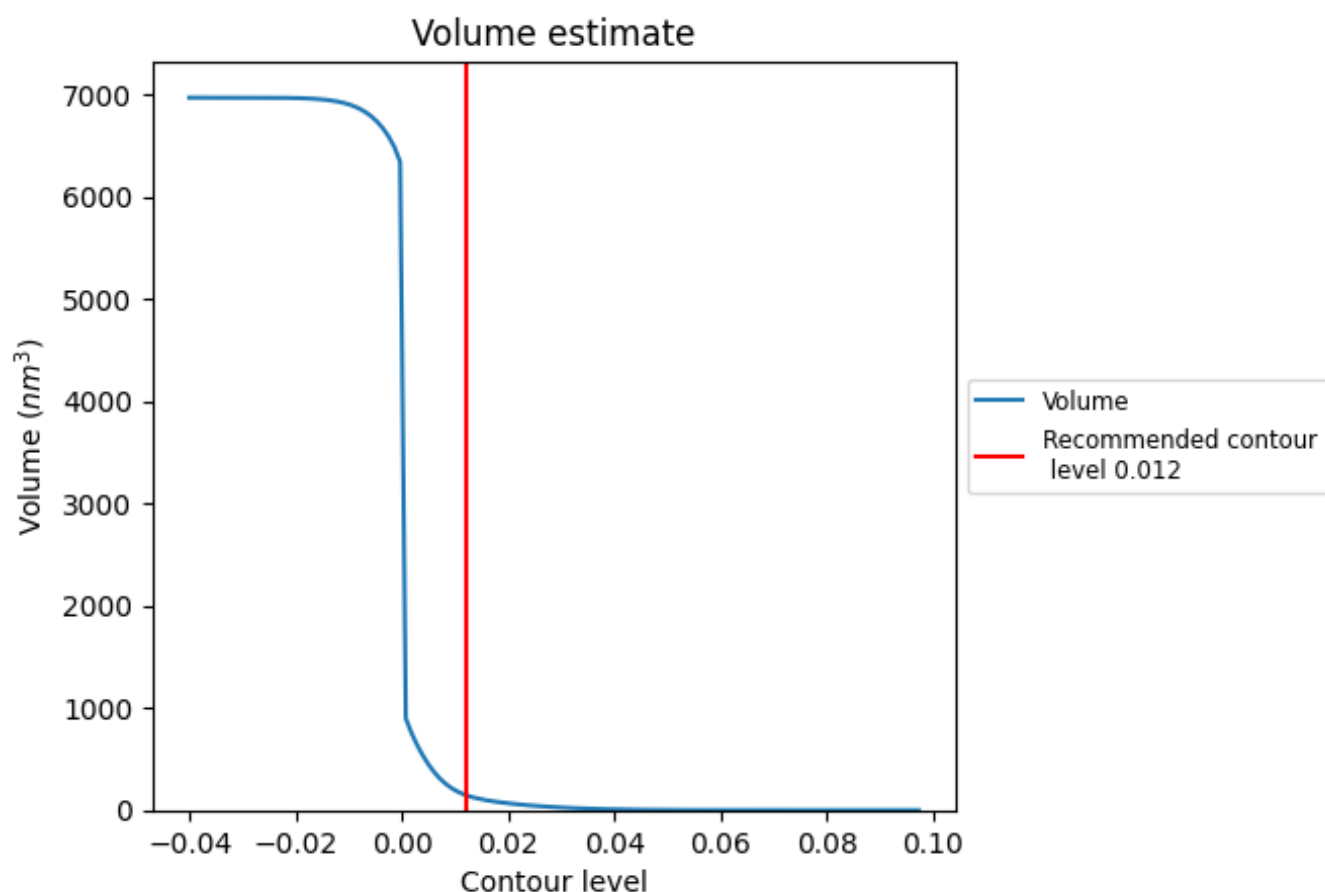
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

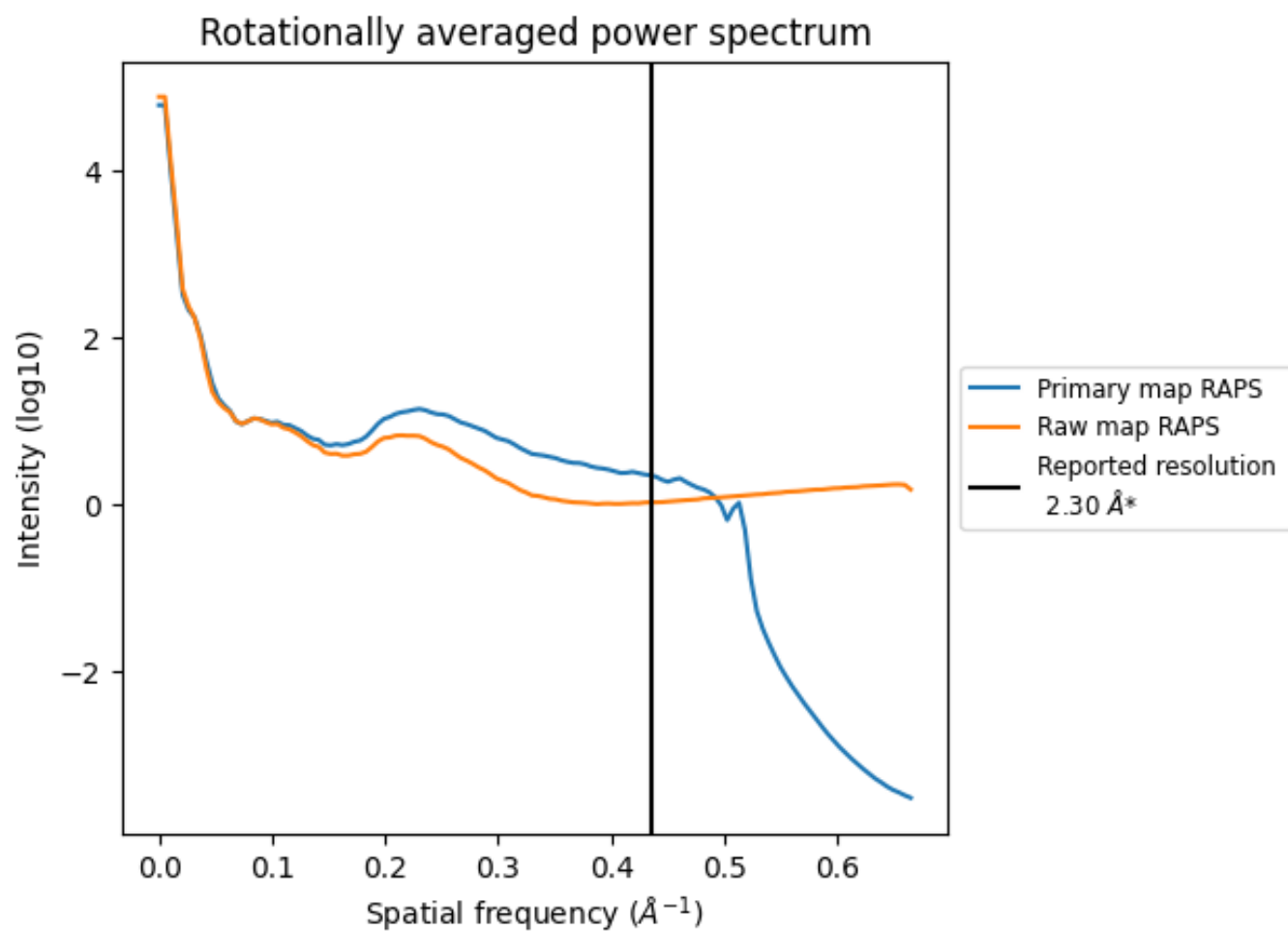
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 149 nm³; this corresponds to an approximate mass of 134 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 [i](#)

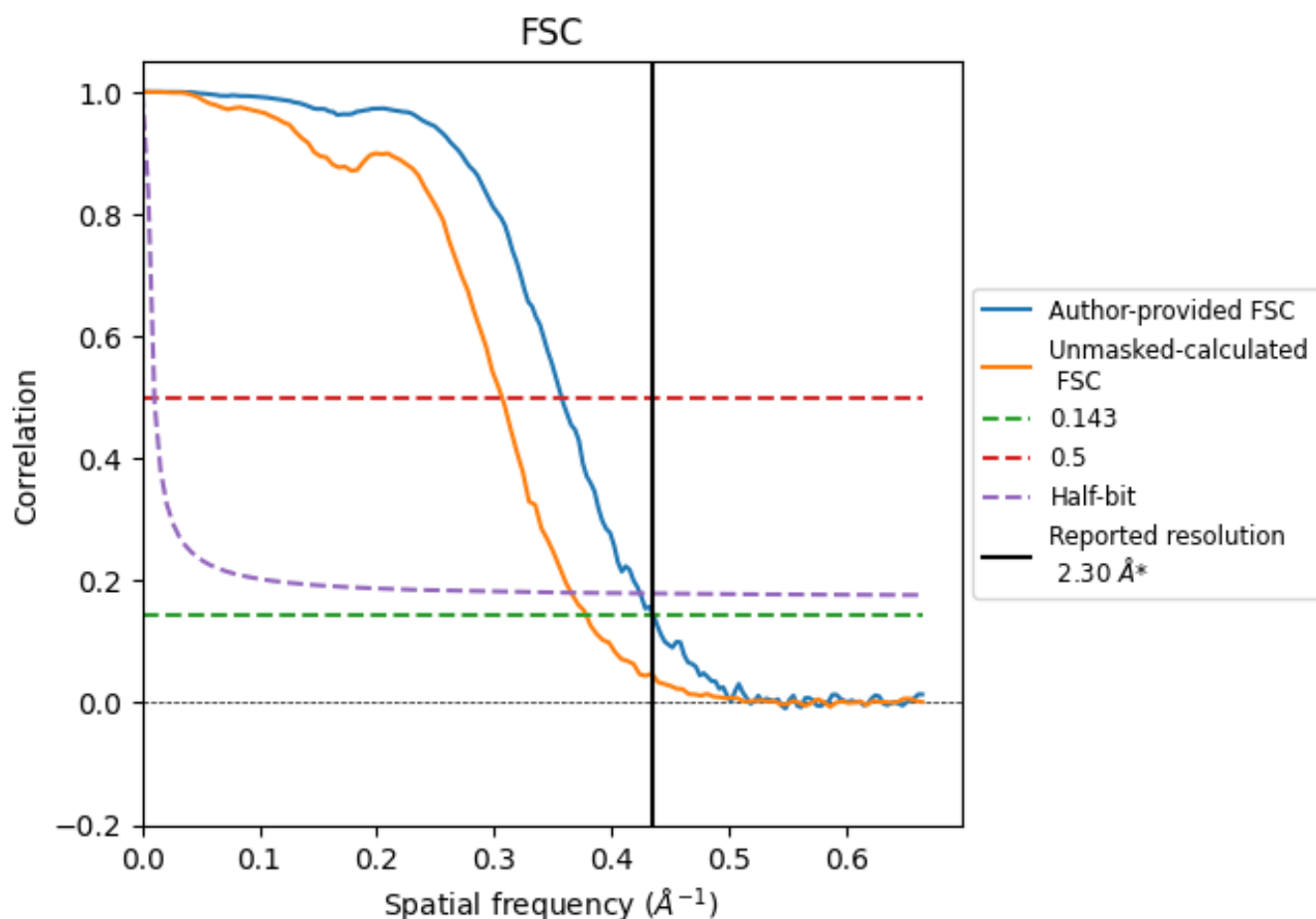


*Reported resolution corresponds to spatial frequency of $0.435 \text{ \AA}^{-1}$

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 0.435 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	2.29	2.80	2.35
Unmasked-calculated*	2.64	3.26	2.73

*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 2.64 differs from the reported value 2.3 by more than 10 %

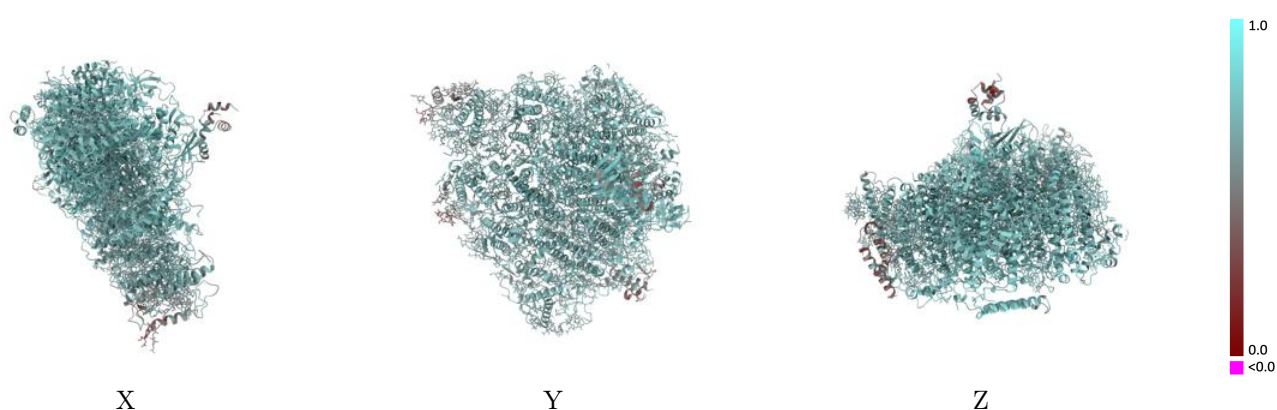
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-38457 and PDB model 8XLS. Per-residue inclusion information can be found in section 3 on page 27.

9.1 Map-model overlay [i](#)

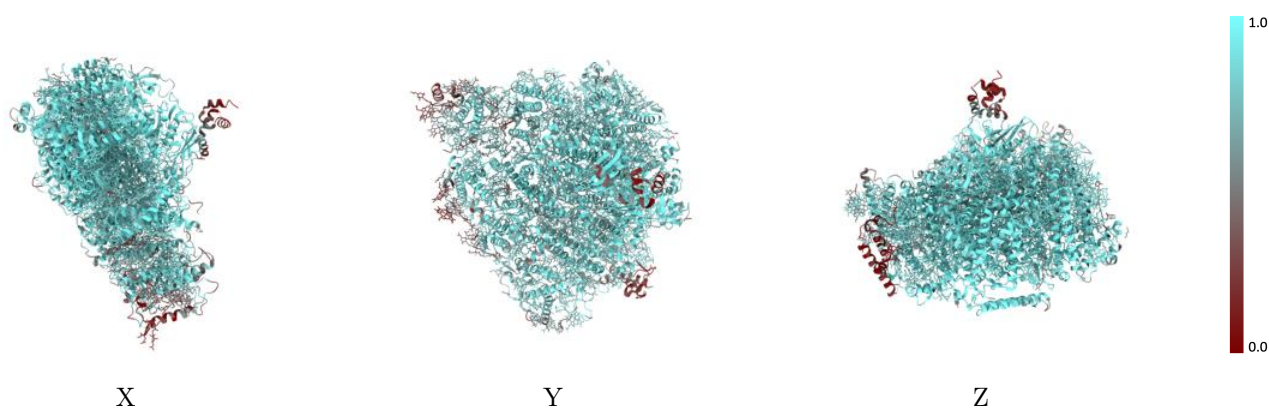
This section was not generated.

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



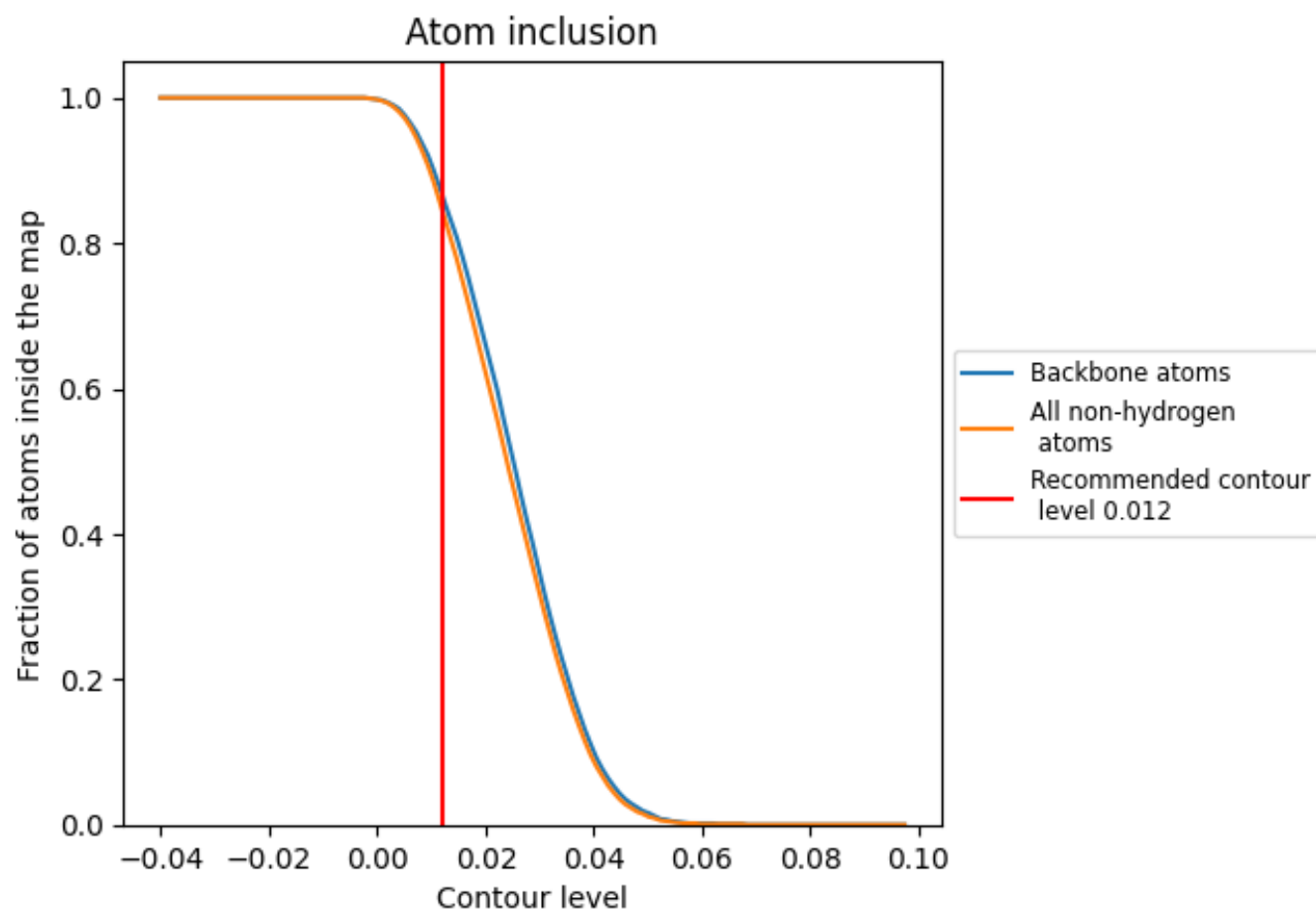
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8450	0.7000
1	0.7930	0.6780
2	0.7590	0.6490
3	0.7860	0.6700
4	0.5900	0.5890
5	0.7560	0.6470
A	0.9140	0.7340
B	0.9300	0.7390
C	0.9780	0.7600
D	0.9360	0.7310
E	0.8460	0.7050
F	0.8780	0.7060
I	0.9350	0.7340
J	0.9060	0.7140
L	0.9040	0.7280
M	0.8620	0.7220
W	0.5100	0.5830
u	0.2160	0.4540

