



wwPDB EM Validation Summary Report ⓘ

Apr 6, 2026 – 04:00 AM UTC

PDB ID : 9UOV / pdb_00009uov
EMDB ID : EMD-64383
Title : PSI-8 FCPI supercomplex from haptophyte *Chrysotila roscoffensis*
Authors : La Rocca, R.; Tsai, P.-C.; Kato, K.; Nakajima, Y.; Akita, F.; Shen, J.-R.
Deposited on : 2025-04-26
Resolution : 2.33 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

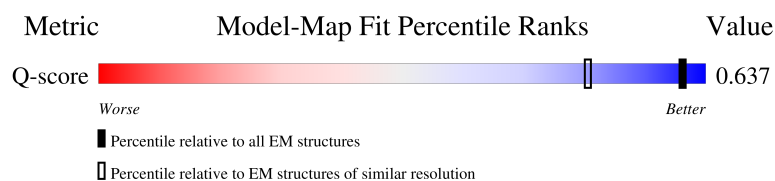
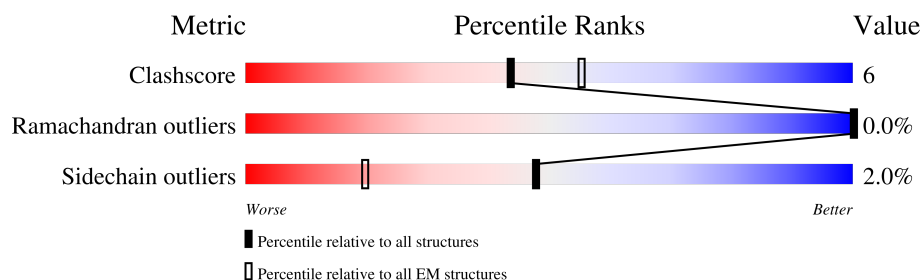
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

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

The reported resolution of this entry is 2.33 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	4434 (1.83 - 2.83)

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	 87% 12% .
2	B	734	 90% 10%
3	C	81	 93% 6% .
4	D	142	 91% 6% . .

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Mol	Chain	Length	Quality of chain
5	E	67	
6	F	184	
7	I	35	
8	J	39	
9	L	141	
10	M	29	
11	O	201	
12	P	231	
13	Q	197	
14	R	90	
15	S	215	
16	U	191	
17	G	209	
18	H	169	
19	T	202	

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
20	CLA	A	802	X	-	-	-
20	CLA	A	803	X	-	-	-
20	CLA	A	804	X	-	-	-
20	CLA	A	805	X	-	-	-
20	CLA	A	806	X	-	-	-
20	CLA	A	808	X	-	-	-
20	CLA	A	810	X	-	-	-
20	CLA	A	811	X	-	-	-
20	CLA	A	812	X	-	-	-
20	CLA	A	814	X	-	-	-
20	CLA	A	815	X	-	-	-
20	CLA	A	816	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	A	817	X	-	-	-
20	CLA	A	818	X	-	-	-
20	CLA	A	820	X	-	-	-
20	CLA	A	821	X	-	-	-
20	CLA	A	822	X	-	-	-
20	CLA	A	823	X	-	-	-
20	CLA	A	824	X	-	-	-
20	CLA	A	825	X	-	-	-
20	CLA	A	828	X	-	-	-
20	CLA	A	829	X	-	-	-
20	CLA	A	831	X	-	-	-
20	CLA	A	832	X	-	-	-
20	CLA	A	833	X	-	-	-
20	CLA	A	834	X	-	-	-
20	CLA	A	835	X	-	-	-
20	CLA	A	836	X	-	-	-
20	CLA	A	838	X	-	-	-
20	CLA	A	845	X	-	-	-
20	CLA	A	849	X	-	-	-
20	CLA	A	851	X	-	-	-
20	CLA	A	852	X	-	-	-
20	CLA	A	853	X	-	-	-
20	CLA	A	854	X	-	-	-
20	CLA	B	801	X	-	-	-
20	CLA	B	802	X	-	-	-
20	CLA	B	803	X	-	-	-
20	CLA	B	804	X	-	-	-
20	CLA	B	805	X	-	-	-
20	CLA	B	806	X	-	-	-
20	CLA	B	807	X	-	-	-
20	CLA	B	808	X	-	-	-
20	CLA	B	809	X	-	-	-
20	CLA	B	812	X	-	-	-
20	CLA	B	815	X	-	-	-
20	CLA	B	816	X	-	-	-
20	CLA	B	817	X	-	-	-
20	CLA	B	820	X	-	-	-
20	CLA	B	821	X	-	-	-
20	CLA	B	822	X	-	-	-
20	CLA	B	823	X	-	-	-
20	CLA	B	827	X	-	-	-
20	CLA	B	829	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	B	830	X	-	-	-
20	CLA	B	831	X	-	-	-
20	CLA	B	832	X	-	-	-
20	CLA	B	833	X	-	-	-
20	CLA	B	834	X	-	-	-
20	CLA	B	835	X	-	-	-
20	CLA	B	843	X	-	-	-
20	CLA	B	844	X	-	-	-
20	CLA	B	845	X	-	-	-
20	CLA	B	846	X	-	-	-
20	CLA	B	848	X	-	-	-
20	CLA	F	802	X	-	-	-
20	CLA	F	803	X	-	-	-
20	CLA	G	202	X	-	-	-
20	CLA	G	203	X	-	-	-
20	CLA	G	205	X	-	-	-
20	CLA	G	206	X	-	-	-
20	CLA	G	207	X	-	-	-
20	CLA	G	208	X	-	-	-
20	CLA	G	210	X	-	-	-
20	CLA	G	215	X	-	-	-
20	CLA	H	201	X	-	-	-
20	CLA	H	202	X	-	-	-
20	CLA	H	203	X	-	-	-
20	CLA	H	204	X	-	-	-
20	CLA	H	205	X	-	-	-
20	CLA	H	206	X	-	-	-
20	CLA	H	207	X	-	-	-
20	CLA	H	208	X	-	-	-
20	CLA	H	209	X	-	-	-
20	CLA	J	103	X	-	-	-
20	CLA	L	202	X	-	-	-
20	CLA	O	203	X	-	-	-
20	CLA	O	204	X	-	-	-
20	CLA	O	205	X	-	-	-
20	CLA	O	206	X	-	-	-
20	CLA	O	207	X	-	-	-
20	CLA	O	208	X	-	-	-
20	CLA	P	207	X	-	-	-
20	CLA	P	208	X	-	-	-
20	CLA	P	209	X	-	-	-
20	CLA	P	213	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	P	214	X	-	-	-
20	CLA	P	216	X	-	-	-
20	CLA	Q	204	X	-	-	-
20	CLA	Q	205	X	-	-	-
20	CLA	Q	206	X	-	-	-
20	CLA	Q	207	X	-	-	-
20	CLA	Q	208	X	-	-	-
20	CLA	Q	211	X	-	-	-
20	CLA	Q	213	X	-	-	-
20	CLA	R	101	X	-	-	-
20	CLA	S	205	X	-	-	-
20	CLA	S	206	X	-	-	-
20	CLA	S	207	X	-	-	-
20	CLA	S	214	X	-	-	-
20	CLA	S	215	X	-	-	-
20	CLA	T	201	X	-	-	-
20	CLA	T	202	X	-	-	-
20	CLA	T	203	X	-	-	-
20	CLA	T	205	X	-	-	-
20	CLA	T	206	X	-	-	-
20	CLA	T	211	X	-	-	-
20	CLA	U	204	X	-	-	-
20	CLA	U	206	X	-	-	-
20	CLA	U	208	X	-	-	-
20	CLA	U	209	X	-	-	-
20	CLA	U	211	X	-	-	-

2 Entry composition [i](#)

There are 32 unique types of molecules in this entry. The entry contains 39964 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 (psaA).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	741	Total	C	N	O	S	0	0
			5813	3807	984	994	28		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	732	Total	C	N	O	S	0	0
			5805	3823	977	984	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			599	366	106	116	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	138	Total	C	N	O	S	0	0
			1092	697	188	204	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	64	Total	C	N	O	S	0	0
			494	314	86	93	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	161	Total	C	N	O	S	0	0
			1246	802	209	229	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	34	Total	C	N	O	S	0	0
			266	183	35	46	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	39	Total	C	N	O	S	0	0
			305	204	45	54	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	140	Total	C	N	O	S	0	0
			1056	693	168	194	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	29	Total	C	N	O	S	0	0
			216	144	34	37	1		

- Molecule 11 is a protein called Fucoxanthin chlorophyll a/c binding protein III (FCPI-3).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	O	176	Total	C	N	O	S	0	0
			1341	872	217	244	8		

- Molecule 12 is a protein called Fucoxanthin chlorophyll a/c binding protein VI (FCPI-6).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	193	Total	C	N	O	S	0	0
			1441	927	239	264	11		

- Molecule 13 is a protein called Fucoxanthin chlorophyll a/c binding protein IV (FCPI-4).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	167	Total	C	N	O	S	0	0
			1257	809	202	234	12		

- Molecule 14 is a protein called Photosystem I reaction center subunit psaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	88	Total	C	N	O	S	0	0
			664	434	106	123	1		

- Molecule 15 is a protein called Fucoxanthin chlorophyll a/c binding protein II (FCPI-2).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	165	Total	C	N	O	S	0	0
			1238	802	204	226	6		

- Molecule 16 is a protein called Fucoxanthin chlorophyll a/c binding protein I (FCPI-1).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	141	Total	C	N	O	S	0	0
			1082	692	183	198	9		

- Molecule 17 is a protein called Fucoxanthin chlorophyll a/c binding protein VII (FCPI-7).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	G	155	Total	C	N	O	S	0	0
			1179	756	190	224	9		

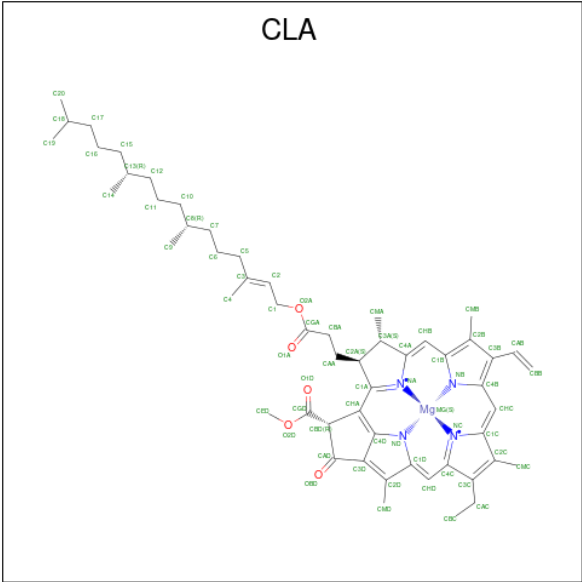
- Molecule 18 is a protein called Fucoxanthin chlorophyll a/c binding protein VIII (FCPI-8).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	H	149	Total	C	N	O	S	0	0
			1128	725	185	206	12		

- Molecule 19 is a protein called Fucoxanthin chlorophyll a/c binding protein V (FCPI-5).

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	99	Total	C	N	O	S	0	0
			731	471	122	130	8		

- Molecule 20 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 43	C 35	Mg 1	N 4	O 3	0
20	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 62	C 52	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
20	B	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	F	1	Total 48	C 38	Mg 1	N 4	O 5	0
20	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
20	L	1	Total 49	C 39	Mg 1	N 4	O 5	0
20	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	O	1	Total 43	C 35	Mg 1	N 4	O 3	0
20	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	O	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	O	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	O	1	Total 41	C 33	Mg 1	N 4	O 3	0
20	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	P	1	Total 56	C 46	Mg 1	N 4	O 5	0
20	P	1	Total 52	C 42	Mg 1	N 4	O 5	0
20	P	1	Total 47	C 37	Mg 1	N 4	O 5	0
20	P	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	P	1	Total 41	C 33	Mg 1	N 4	O 3	0
20	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	P	1	Total 47	C 37	Mg 1	N 4	O 5	0
20	Q	1	Total 48	C 38	Mg 1	N 4	O 5	0
20	Q	1	Total 61	C 51	Mg 1	N 4	O 5	0
20	Q	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	Q	1	Total 51	C 41	Mg 1	N 4	O 5	0
20	Q	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	Q	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	Q	1	Total 41	C 33	Mg 1	N 4	O 3	0
20	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	Q	1	Total 57	C 47	Mg 1	N 4	O 5	0
20	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	S	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	S	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	S	1	Total 52	C 42	Mg 1	N 4	O 5	0
20	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	U	1	Total 61	C 51	Mg 1	N 4	O 5	0
20	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	U	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	U	1	Total 42	C 34	Mg 1	N 4	O 3	0
20	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	U	1	Total 52	C 42	Mg 1	N 4	O 5	0
20	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	G	1	Total 41	C 33	Mg 1	N 4	O 3	0
20	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	G	1	Total 43	C 35	Mg 1	N 4	O 3	0

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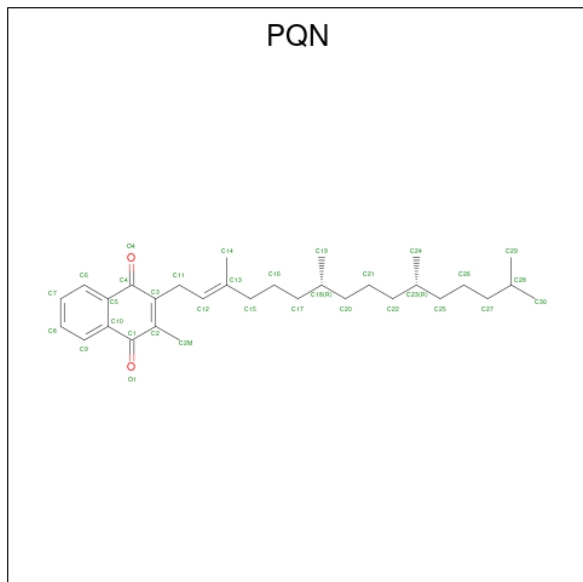
Mol	Chain	Residues	Atoms					AltConf
20	G	1	Total 61	C 51	Mg 1	N 4	O 5	0
20	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	G	1	Total 56	C 46	Mg 1	N 4	O 5	0
20	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	H	1	Total 40	C 32	Mg 1	N 4	O 3	0
20	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	H	1	Total 61	C 51	Mg 1	N 4	O 5	0
20	H	1	Total 44	C 35	Mg 1	N 4	O 4	0
20	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	H	1	Total 58	C 48	Mg 1	N 4	O 5	0
20	H	1	Total 41	C 33	Mg 1	N 4	O 3	0
20	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	T	1	Total 42	C 34	Mg 1	N 4	O 3	0
20	T	1	Total 41	C 33	Mg 1	N 4	O 3	0
20	T	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	T	1	Total 57	C 47	Mg 1	N 4	O 5	0
20	T	1	Total 46	C 36	Mg 1	N 4	O 5	0

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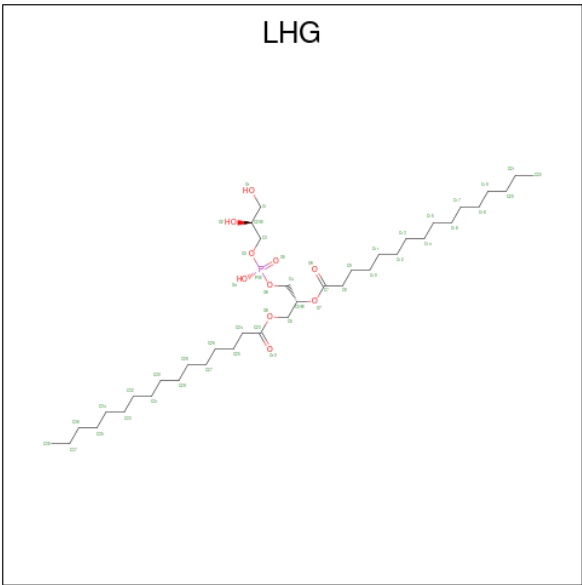
Mol	Chain	Residues	Atoms					AltConf
20	T	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
20	T	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	T	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
20	T	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	T	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

- Molecule 21 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



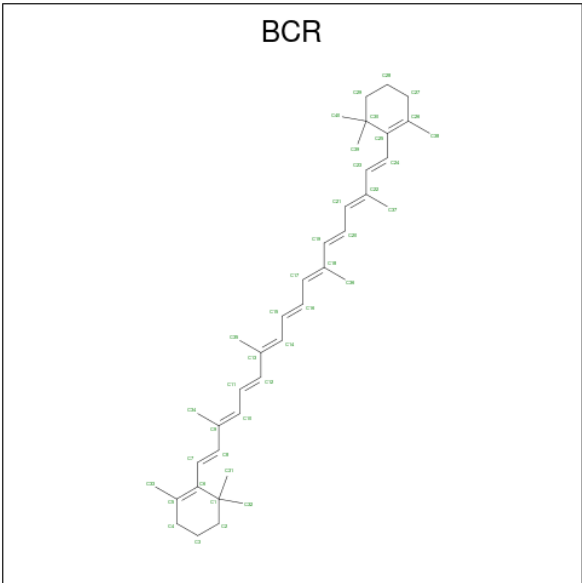
Mol	Chain	Residues	Atoms			AltConf
21	A	1	Total	C	O	0
			33	31	2	
21	B	1	Total	C	O	0
			33	31	2	

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
22	A	1	Total	C	O	P	0
			48	37	10	1	
22	A	1	Total	C	O	P	0
			27	16	10	1	
22	P	1	Total	C	O	P	0
			49	38	10	1	
22	G	1	Total	C	O	P	0
			27	16	10	1	

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
23	A	1	Total 40	C 40	0
23	A	1	Total 40	C 40	0
23	A	1	Total 40	C 40	0
23	A	1	Total 40	C 40	0
23	B	1	Total 40	C 40	0
23	B	1	Total 40	C 40	0
23	B	1	Total 40	C 40	0
23	B	1	Total 40	C 40	0
23	B	1	Total 40	C 40	0
23	F	1	Total 40	C 40	0
23	F	1	Total 40	C 40	0
23	I	1	Total 40	C 40	0
23	I	1	Total 40	C 40	0
23	J	1	Total 40	C 40	0
23	L	1	Total 40	C 40	0
23	L	1	Total 40	C 40	0
23	M	1	Total 40	C 40	0
23	R	1	Total 39	C 39	0

- Molecule 24 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 25 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



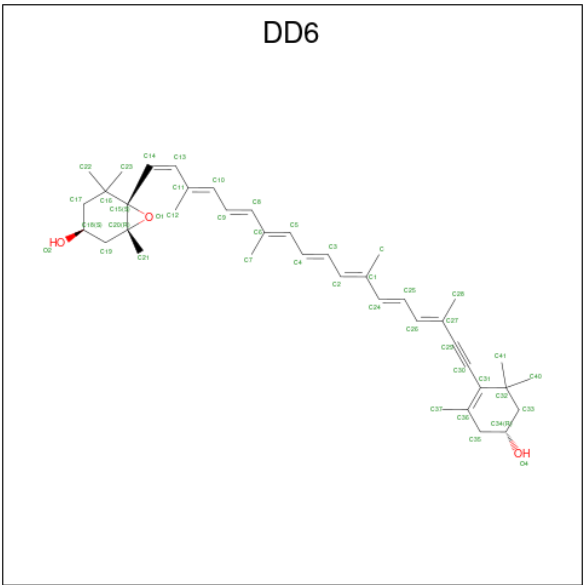
Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total 8	Fe 4	S 4	0
25	C	1	Total 8	Fe 4	S 4	0

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

- Molecule 26 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: C₄₀H₅₄O₃) (labeled as "Ligand of Interest" by depositor).



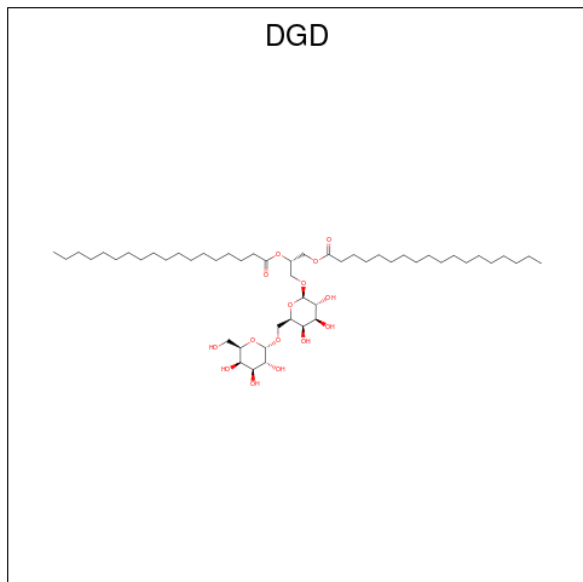
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			43	40	3	
26	J	1	Total	C	O	0
			43	40	3	
26	O	1	Total	C	O	0
			43	40	3	
26	O	1	Total	C	O	0
			43	40	3	
26	O	1	Total	C	O	0
			43	40	3	
26	O	1	Total	C	O	0
			43	40	3	
26	P	1	Total	C	O	0
			43	40	3	
26	P	1	Total	C	O	0
			43	40	3	

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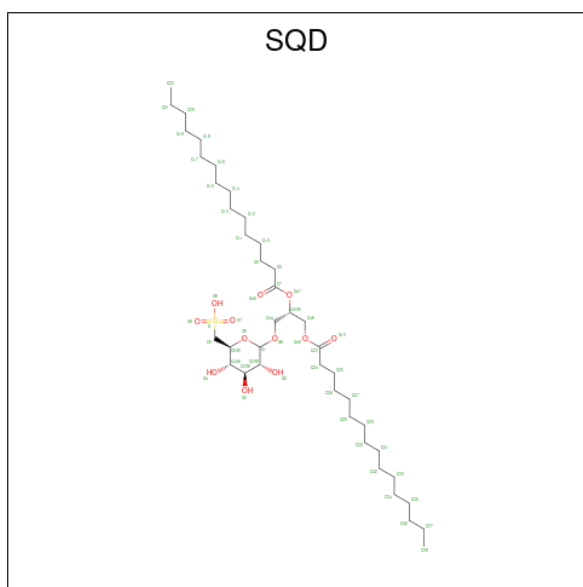
Mol	Chain	Residues	Atoms			AltConf
26	P	1	Total 43	C 40	O 3	0
26	P	1	Total 43	C 40	O 3	0
26	Q	1	Total 43	C 40	O 3	0
26	Q	1	Total 43	C 40	O 3	0
26	S	1	Total 43	C 40	O 3	0
26	S	1	Total 43	C 40	O 3	0
26	S	1	Total 43	C 40	O 3	0
26	S	1	Total 43	C 40	O 3	0
26	S	1	Total 43	C 40	O 3	0
26	U	1	Total 43	C 40	O 3	0
26	U	1	Total 43	C 40	O 3	0
26	U	1	Total 26	C 25	O 1	0
26	G	1	Total 43	C 40	O 3	0
26	G	1	Total 43	C 40	O 3	0
26	G	1	Total 43	C 40	O 3	0
26	G	1	Total 43	C 40	O 3	0
26	G	1	Total 43	C 40	O 3	0
26	H	1	Total 43	C 40	O 3	0
26	H	1	Total 43	C 40	O 3	0
26	T	1	Total 43	C 40	O 3	0
26	T	1	Total 43	C 40	O 3	0

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



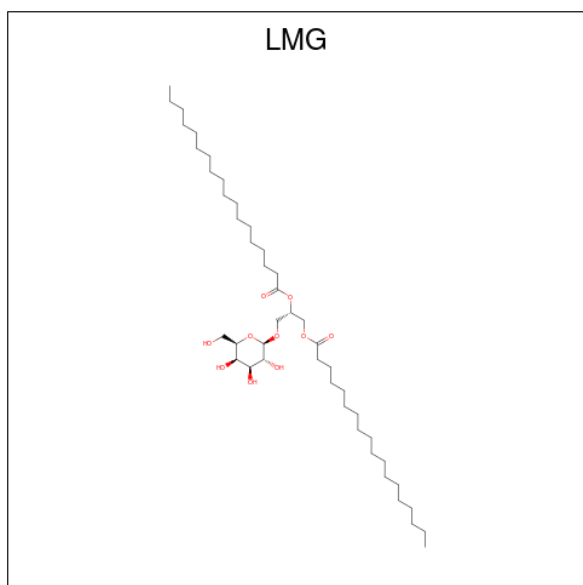
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
27	B	1	60	45	15	0

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



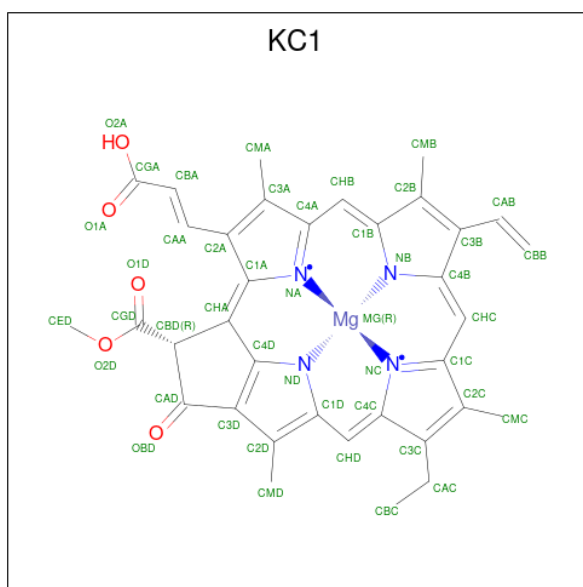
Mol	Chain	Residues	Atoms				AltConf
28	B	1	Total	C	O	S	0
			50	37	12	1	
28	S	1	Total	C	O	S	0
			46	33	12	1	

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



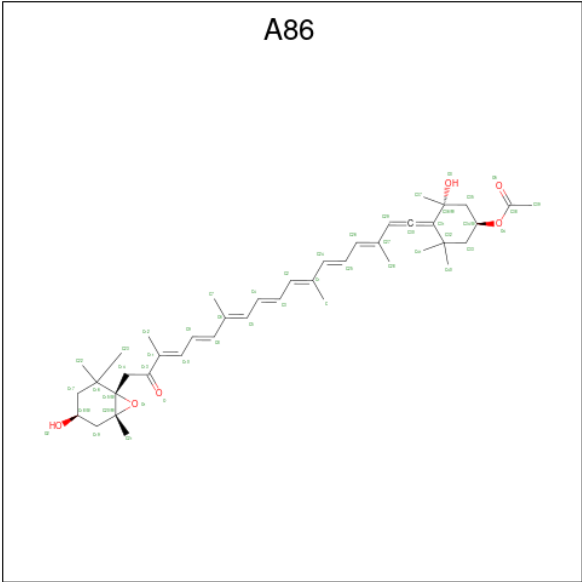
Mol	Chain	Residues	Atoms			AltConf
29	I	1	Total	C	O	0
			49	39	10	
29	J	1	Total	C	O	0
			39	29	10	
29	P	1	Total	C	O	0
			34	24	10	
29	P	1	Total	C	O	0
			25	15	10	
29	Q	1	Total	C	O	0
			55	45	10	
29	U	1	Total	C	O	0
			32	22	10	

- Molecule 30 is Chlorophyll c1 (CCD ID: KC1) (formula: $C_{35}H_{30}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
30	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	P	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
30	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	T	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: $C_{42}H_{58}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
31	P	1	Total	C	O	0
			48	42	6	
31	Q	1	Total	C	O	0
			48	42	6	
31	Q	1	Total	C	O	0
			48	42	6	
31	Q	1	Total	C	O	0
			48	42	6	
31	R	1	Total	C	O	0
			44	40	4	
31	R	1	Total	C	O	0
			48	42	6	
31	U	1	Total	C	O	0
			48	42	6	

- Molecule 32 is water.

Mol	Chain	Residues	Atoms		AltConf
32	A	55	Total	O	0
			55	55	
32	B	91	Total	O	0
			91	91	
32	C	9	Total	O	0
			9	9	
32	D	8	Total	O	0
			8	8	
32	E	5	Total	O	0
			5	5	

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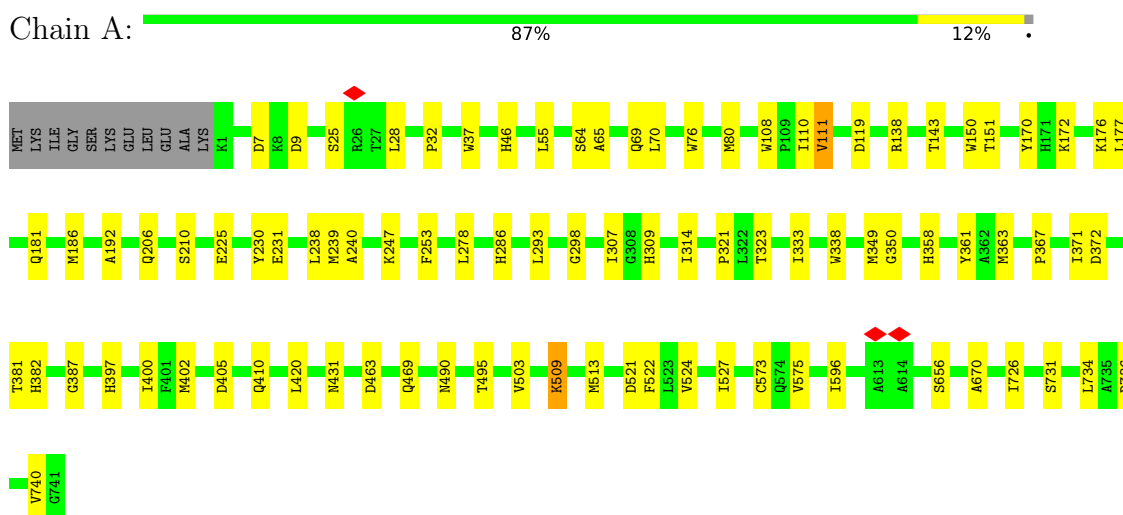
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Mol	Chain	Residues	Atoms		AltConf
32	F	9	Total 9	O 9	0
32	I	1	Total 1	O 1	0
32	J	4	Total 4	O 4	0
32	L	5	Total 5	O 5	0
32	M	1	Total 1	O 1	0
32	O	7	Total 7	O 7	0
32	P	8	Total 8	O 8	0
32	Q	3	Total 3	O 3	0
32	R	4	Total 4	O 4	0
32	S	5	Total 5	O 5	0
32	U	4	Total 4	O 4	0
32	G	6	Total 6	O 6	0
32	H	2	Total 2	O 2	0
32	T	2	Total 2	O 2	0

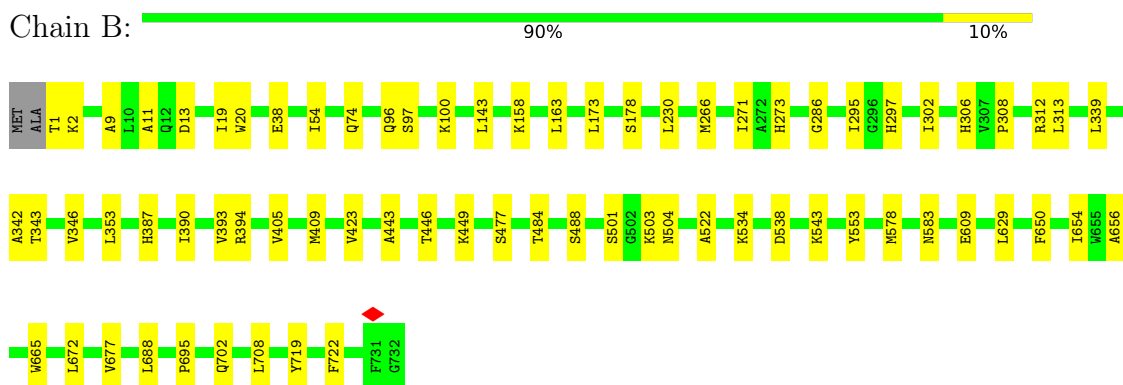
3 Residue-property plots

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

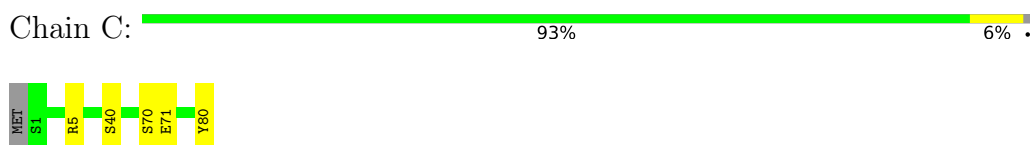
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1 (psaA)




- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 (psaB)



- Molecule 3: Photosystem I iron-sulfur center (psaC)




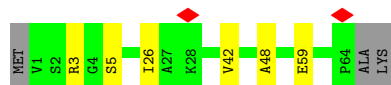
- Molecule 4: Photosystem I reaction center subunit II (psaD)

Chain D:  91% 6% ..




- Molecule 5: Photosystem I reaction center subunit IV (psaE)

Chain E:  87% 9% .



- Molecule 6: Photosystem I reaction center subunit III (psaF)

Chain F:  78% 9% 12%




- Molecule 7: Photosystem I reaction center subunit VIII (psaI)

Chain I:  69% 26% ..



- Molecule 8: Photosystem I reaction center subunit IX (psaJ)

Chain J:  82% 18%



- Molecule 9: Photosystem I reaction center subunit XI (psaL)

Chain L:  87% 11% ..




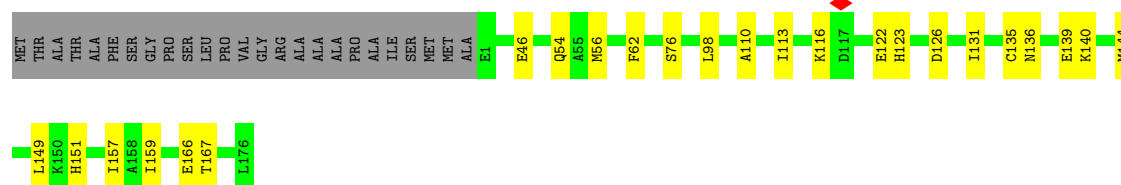
- Molecule 10: Photosystem I reaction center subunit XII (psaM)

Chain M:  97% .



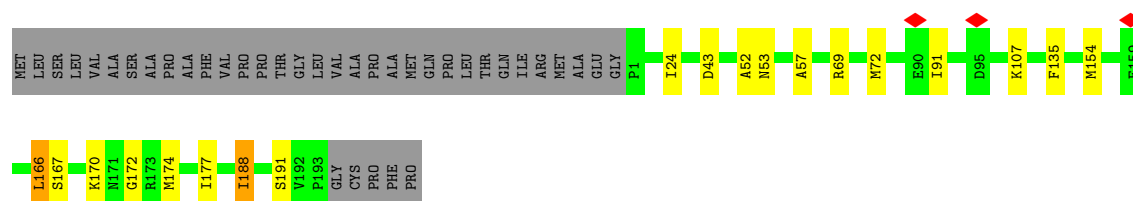
- Molecule 11: Fucoxanthin chlorophyll a/c binding protein III (FCPI-3)

Chain O:  76% 12% 12%



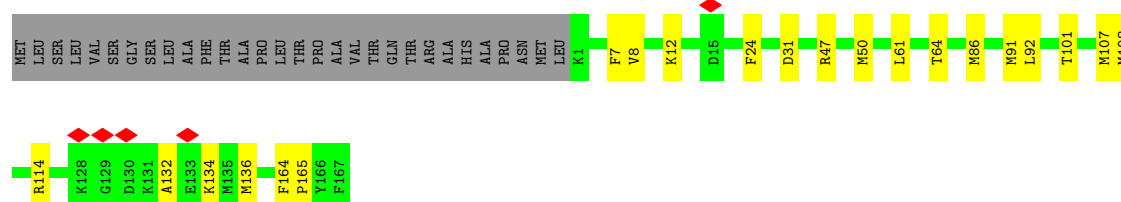
- Molecule 12: Fucoxanthin chlorophyll a/c binding protein VI (FCPI-6)

Chain P:  75% 7% 16%




- Molecule 13: Fucoxanthin chlorophyll a/c binding protein IV (FCPI-4)

Chain Q:  74% 11% 15%



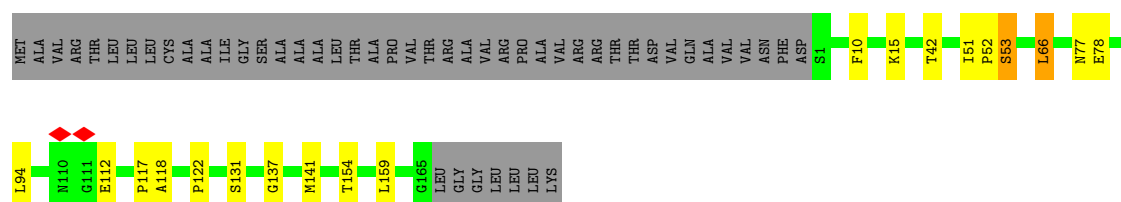
- Molecule 14: Photosystem I reaction center subunit psaR

Chain R:  89% 9% 0%



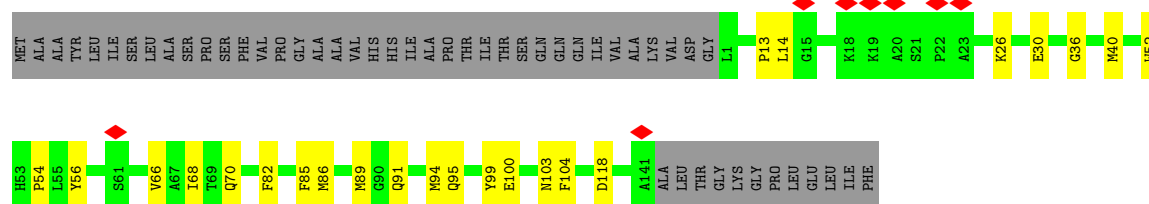
- Molecule 15: Fucoxanthin chlorophyll a/c binding protein II (FCPI-2)

Chain S:  68% 8% 23%



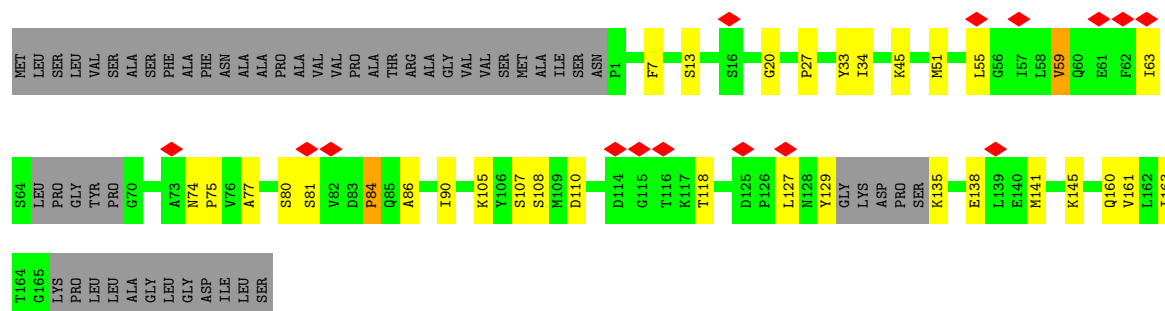
- Molecule 16: Fucoxanthin chlorophyll a/c binding protein I (FCPI-1)

Chain U: 



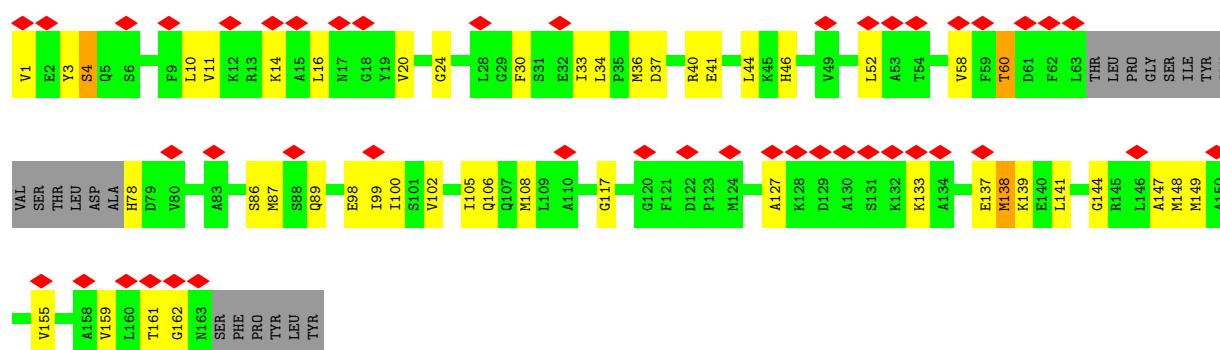
- Molecule 17: Fucoxanthin chlorophyll a/c binding protein VII (FCPI-7)

Chain G: 




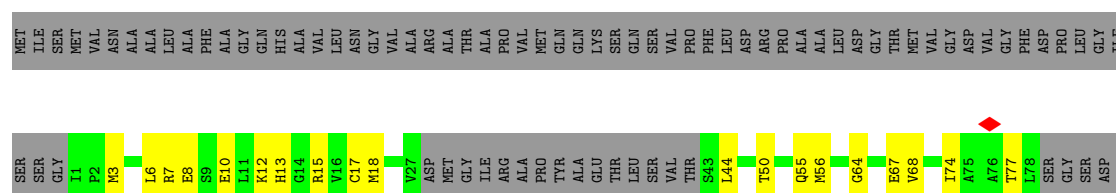
- Molecule 18: Fucoxanthin chlorophyll a/c binding protein VIII (FCPI-8)

Chain H: 



- Molecule 19: Fucoxanthin chlorophyll a/c binding protein V (FCPI-5)

Chain T: 





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	17450	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.480	Depositor
Minimum map value	-0.232	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	436.2, 436.2, 436.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.727, 0.727, 0.727	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/6007	0.45	0/8185
2	B	0.23	0/6015	0.46	0/8205
3	C	0.20	0/609	0.44	0/826
4	D	0.24	0/1116	0.51	0/1503
5	E	0.21	0/505	0.38	0/689
6	F	0.22	0/1275	0.44	0/1728
7	I	0.25	0/273	0.53	0/373
8	J	0.23	0/313	0.53	0/427
9	L	0.29	0/1081	0.56	0/1470
10	M	0.19	0/218	0.30	0/295
11	O	0.29	0/1376	0.57	0/1865
12	P	0.25	0/1480	0.47	0/2010
13	Q	0.36	0/1285	0.65	1/1736 (0.1%)
14	R	0.23	0/681	0.40	0/930
15	S	0.23	0/1272	0.46	0/1732
16	U	0.26	0/1109	0.57	0/1499
17	G	1.35	1/1204 (0.1%)	0.80	2/1624 (0.1%)
18	H	0.44	0/1149	0.83	2/1546 (0.1%)
19	T	0.32	0/741	0.57	0/999
All	All	0.38	1/27709 (0.0%)	0.52	5/37642 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
13	Q	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	G	84	PRO	N-CD	45.36	2.11	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	G	84	PRO	N-CD-CG	-18.97	74.75	103.20
13	Q	165	PRO	CB-CA-C	-10.53	97.53	111.12
17	G	84	PRO	CA-N-CD	-9.21	99.11	112.00
18	H	159	VAL	N-CA-C	-8.01	105.39	112.12
18	H	155	VAL	N-CA-C	-6.60	106.40	111.62

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	Q	164	PHE	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	5813	0	5698	60	0
2	B	5805	0	5634	52	0
3	C	599	0	577	4	0
4	D	1092	0	1096	6	0
5	E	494	0	488	3	0
6	F	1246	0	1256	11	0
7	I	266	0	278	9	0
8	J	305	0	310	6	0
9	L	1056	0	1068	17	0
10	M	216	0	234	1	0
11	O	1341	0	1347	21	0
12	P	1441	0	1421	14	0
13	Q	1257	0	1260	15	0
14	R	664	0	668	4	0
15	S	1238	0	1217	13	0
16	U	1082	0	1058	16	0
17	G	1179	0	1166	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	H	1128	0	1134	34	0
19	T	731	0	749	23	0
20	A	2669	0	2699	70	0
20	B	2409	0	2457	61	0
20	F	94	0	69	4	0
20	G	561	0	486	17	0
20	H	459	0	403	15	0
20	J	42	0	31	1	0
20	L	164	0	150	2	0
20	O	495	0	475	11	0
20	P	403	0	337	9	0
20	Q	609	0	566	12	0
20	R	110	0	105	3	0
20	S	384	0	358	12	0
20	T	473	0	379	17	0
20	U	441	0	417	11	0
21	A	33	0	46	4	0
21	B	33	0	46	4	0
22	A	75	0	93	1	0
22	G	27	0	24	1	0
22	P	49	0	74	1	0
23	A	160	0	224	9	0
23	B	200	0	280	14	0
23	F	80	0	112	2	0
23	I	80	0	112	3	0
23	J	40	0	56	1	0
23	L	80	0	112	5	0
23	M	40	0	56	4	0
23	R	39	0	53	1	0
24	A	65	0	72	2	0
25	A	8	0	0	0	0
25	C	16	0	0	0	0
26	A	43	0	0	0	0
26	G	215	0	0	1	0
26	H	86	0	0	0	0
26	J	43	0	0	0	0
26	O	215	0	0	0	0
26	P	172	0	0	0	0
26	Q	86	0	0	0	0
26	S	215	0	0	0	0
26	T	86	0	0	0	0
26	U	112	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	B	60	0	81	0	0
28	B	50	0	67	0	0
28	S	46	0	56	5	0
29	I	49	0	68	2	0
29	J	39	0	48	1	0
29	P	59	0	57	5	0
29	Q	55	0	86	3	0
29	U	32	0	34	1	0
30	O	45	0	0	0	0
30	P	179	0	0	1	0
30	Q	45	0	0	0	0
30	S	90	0	0	0	0
30	T	45	0	0	0	0
30	U	45	0	0	0	0
31	P	48	0	0	0	0
31	Q	144	0	0	0	0
31	R	92	0	0	0	0
31	U	48	0	0	0	0
32	A	55	0	0	1	0
32	B	91	0	0	1	0
32	C	9	0	0	0	0
32	D	8	0	0	0	0
32	E	5	0	0	0	0
32	F	9	0	0	0	0
32	G	6	0	0	0	0
32	H	2	0	0	0	0
32	I	1	0	0	0	0
32	J	4	0	0	0	0
32	L	5	0	0	0	0
32	M	1	0	0	0	0
32	O	7	0	0	0	0
32	P	8	0	0	0	0
32	Q	3	0	0	0	0
32	R	4	0	0	0	0
32	S	5	0	0	0	0
32	T	2	0	0	0	0
32	U	4	0	0	0	0
All	All	39964	0	37448	499	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 499 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)
17:G:84:PRO:N	17:G:84:PRO:CD	2.11	1.02
18:H:161:THR:HG22	18:H:162:GLY:H	1.29	0.95
18:H:161:THR:HG22	18:H:162:GLY:N	1.83	0.92
9:L:47:LEU:HG	9:L:51:MET:HE2	1.58	0.85
18:H:161:THR:CG2	18:H:162:GLY:H	1.93	0.82

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/752 (98%)	718 (97%)	20 (3%)	1 (0%)	48	57
2	B	730/734 (100%)	713 (98%)	17 (2%)	0	100	100
3	C	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
4	D	136/142 (96%)	127 (93%)	9 (7%)	0	100	100
5	E	62/67 (92%)	62 (100%)	0	0	100	100
6	F	159/184 (86%)	156 (98%)	3 (2%)	0	100	100
7	I	32/35 (91%)	32 (100%)	0	0	100	100
8	J	37/39 (95%)	37 (100%)	0	0	100	100
9	L	138/141 (98%)	136 (99%)	2 (1%)	0	100	100
10	M	27/29 (93%)	27 (100%)	0	0	100	100
11	O	174/201 (87%)	172 (99%)	2 (1%)	0	100	100
12	P	191/231 (83%)	186 (97%)	5 (3%)	0	100	100
13	Q	165/197 (84%)	160 (97%)	5 (3%)	0	100	100
14	R	86/90 (96%)	85 (99%)	1 (1%)	0	100	100
15	S	163/215 (76%)	156 (96%)	7 (4%)	0	100	100
16	U	139/191 (73%)	135 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	G	149/209 (71%)	144 (97%)	5 (3%)	0	100	100
18	H	145/169 (86%)	133 (92%)	12 (8%)	0	100	100
19	T	91/202 (45%)	90 (99%)	1 (1%)	0	100	100
All	All	3441/3909 (88%)	3346 (97%)	94 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	603/612 (98%)	594 (98%)	9 (2%)	57	69
2	B	590/591 (100%)	584 (99%)	6 (1%)	68	79
3	C	68/69 (99%)	67 (98%)	1 (2%)	57	69
4	D	118/122 (97%)	117 (99%)	1 (1%)	73	82
5	E	53/55 (96%)	53 (100%)	0	100	100
6	F	133/152 (88%)	131 (98%)	2 (2%)	57	69
7	I	31/32 (97%)	29 (94%)	2 (6%)	15	17
8	J	32/32 (100%)	32 (100%)	0	100	100
9	L	111/112 (99%)	110 (99%)	1 (1%)	70	80
10	M	21/21 (100%)	21 (100%)	0	100	100
11	O	145/161 (90%)	143 (99%)	2 (1%)	59	71
12	P	144/173 (83%)	140 (97%)	4 (3%)	38	50
13	Q	133/157 (85%)	132 (99%)	1 (1%)	73	82
14	R	71/73 (97%)	70 (99%)	1 (1%)	59	71
15	S	125/162 (77%)	121 (97%)	4 (3%)	34	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	U	110/148 (74%)	108 (98%)	2 (2%)	51 64
17	G	127/167 (76%)	121 (95%)	6 (5%)	23 30
18	H	119/137 (87%)	108 (91%)	11 (9%)	8 8
19	T	73/153 (48%)	70 (96%)	3 (4%)	27 35
All	All	2807/3129 (90%)	2751 (98%)	56 (2%)	48 61

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	Q	64	THR
19	T	110	ILE
16	U	118	ASP
19	T	44	LEU
18	H	99	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
14	R	52	ASN
16	U	93	ASN
17	G	146	ASN
16	U	120	GLN
2	B	641	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

250 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
20	CLA	G	203	17	49,53,73	1.43	8 (16%)	58,89,113	1.03	3 (5%)
20	CLA	B	824	2	69,73,73	1.21	7 (10%)	82,113,113	0.97	5 (6%)
20	CLA	T	201	-	46,50,73	1.42	8 (17%)	53,85,113	1.08	3 (5%)
20	CLA	A	830	1	54,58,73	1.31	6 (11%)	64,95,113	0.97	4 (6%)
20	CLA	A	852	1	69,73,73	1.18	8 (11%)	82,113,113	0.92	4 (4%)
26	DD6	U	212	-	40,45,45	1.30	7 (17%)	51,67,67	1.71	13 (25%)
20	CLA	O	202	11	47,51,73	1.40	6 (12%)	55,86,113	1.10	4 (7%)
20	CLA	B	822	2	69,73,73	1.23	7 (10%)	82,113,113	0.92	3 (3%)
20	CLA	A	814	32	49,53,73	1.40	7 (14%)	58,89,113	1.15	5 (8%)
20	CLA	A	815	1	69,73,73	1.20	7 (10%)	82,113,113	0.93	4 (4%)
20	CLA	T	207	19	69,73,73	1.12	6 (8%)	82,113,113	1.01	5 (6%)
23	BCR	R	102	-	40,40,41	1.13	2 (5%)	54,54,56	1.39	9 (16%)
26	DD6	G	214	-	40,45,45	1.32	7 (17%)	51,67,67	1.68	14 (27%)
20	CLA	U	208	16	50,54,73	1.32	6 (12%)	59,90,113	1.17	5 (8%)
20	CLA	B	810	2	58,62,73	1.43	9 (15%)	71,100,113	0.91	3 (4%)
20	CLA	B	815	2	63,67,73	1.24	7 (11%)	74,105,113	1.00	5 (6%)
20	CLA	B	820	-	67,71,73	1.21	8 (11%)	79,110,113	0.98	6 (7%)
20	CLA	G	202	-	45,49,73	1.45	6 (13%)	54,84,113	1.07	4 (7%)
20	CLA	A	817	1	49,53,73	1.42	7 (14%)	58,89,113	1.11	4 (6%)
20	CLA	A	826	1	69,73,73	1.28	8 (11%)	82,113,113	0.82	2 (2%)
20	CLA	G	201	17	49,53,73	1.36	7 (14%)	58,89,113	1.10	4 (6%)
20	CLA	A	835	1	69,73,73	1.24	8 (11%)	82,113,113	1.07	5 (6%)
22	LHG	A	840	20	26,26,48	0.83	1 (3%)	29,32,54	1.35	3 (10%)
30	KC1	U	213	16	49,53,53	1.62	9 (18%)	61,89,89	1.17	5 (8%)
20	CLA	B	835	-	69,73,73	1.22	7 (10%)	82,113,113	0.95	5 (6%)
20	CLA	Q	216	-	69,73,73	1.13	7 (10%)	82,113,113	0.88	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	BCR	I	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.25	5 (8%)
31	A86	U	202	-	47,50,50	1.37	5 (10%)	51,76,76	1.37	7 (13%)
26	DD6	T	213	-	40,45,45	1.34	8 (20%)	51,67,67	1.66	12 (23%)
20	CLA	A	820	1	55,59,73	1.37	8 (14%)	64,96,113	1.02	3 (4%)
26	DD6	T	212	-	40,45,45	1.31	7 (17%)	51,67,67	1.76	12 (23%)
23	BCR	F	804	-	41,41,41	1.05	2 (4%)	56,56,56	1.28	4 (7%)
26	DD6	S	213	-	40,45,45	1.29	6 (15%)	51,67,67	1.81	12 (23%)
26	DD6	U	203	-	40,45,45	1.38	9 (22%)	51,67,67	2.12	15 (29%)
20	CLA	B	809	2	69,73,73	1.19	8 (11%)	82,113,113	0.92	4 (4%)
20	CLA	B	821	32	68,72,73	1.14	7 (10%)	80,111,113	0.93	4 (5%)
20	CLA	A	804	1	69,73,73	1.15	7 (10%)	82,113,113	0.90	4 (4%)
20	CLA	U	210	16	69,73,73	1.15	6 (8%)	82,113,113	0.90	5 (6%)
20	CLA	A	813	1	54,58,73	1.39	7 (12%)	64,95,113	1.07	4 (6%)
20	CLA	A	834	1	69,73,73	1.27	8 (11%)	82,113,113	0.98	4 (4%)
20	CLA	A	819	1	47,51,73	1.39	7 (14%)	55,86,113	1.10	4 (7%)
20	CLA	Q	209	13	69,73,73	1.15	7 (10%)	82,113,113	0.90	4 (4%)
20	CLA	L	204	32	54,58,73	1.30	7 (12%)	64,95,113	1.24	7 (10%)
25	SF4	C	101	3	0,12,12	-	-	-	-	-
30	KC1	Q	210	13	49,53,53	1.65	9 (18%)	61,89,89	1.14	7 (11%)
30	KC1	S	211	15	49,53,53	1.51	7 (14%)	61,89,89	1.12	6 (9%)
20	CLA	B	807	2	69,73,73	1.20	8 (11%)	82,113,113	0.89	3 (3%)
26	DD6	S	204	-	40,45,45	1.44	9 (22%)	51,67,67	1.68	13 (25%)
20	CLA	A	806	1	69,73,73	1.16	8 (11%)	82,113,113	0.88	4 (4%)
20	CLA	T	205	-	50,54,73	1.31	6 (12%)	59,90,113	1.20	7 (11%)
20	CLA	S	206	15	50,54,73	1.49	8 (16%)	59,90,113	1.10	4 (6%)
20	CLA	S	214	-	69,73,73	1.14	7 (10%)	82,113,113	0.93	4 (4%)
20	CLA	B	801	-	69,73,73	1.19	7 (10%)	82,113,113	0.93	4 (4%)
20	CLA	B	843	2	69,73,73	1.22	7 (10%)	82,113,113	0.92	4 (4%)
20	CLA	S	215	15	69,73,73	1.17	7 (10%)	82,113,113	0.90	3 (3%)
26	DD6	G	217	-	40,45,45	1.24	7 (17%)	51,67,67	1.48	10 (19%)
20	CLA	G	207	17	64,68,73	1.16	7 (10%)	76,107,113	1.01	4 (5%)
20	CLA	A	823	1	69,73,73	1.23	6 (8%)	82,113,113	0.92	4 (4%)
20	CLA	L	202	9	53,57,73	1.33	8 (15%)	61,93,113	1.16	6 (9%)
26	DD6	H	211	-	40,45,45	1.28	7 (17%)	51,67,67	1.54	10 (19%)
20	CLA	T	210	19	50,54,73	1.45	8 (16%)	59,90,113	1.13	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	KC1	T	208	-	49,53,53	1.67	9 (18%)	61,89,89	1.12	5 (8%)
20	CLA	L	203	9	69,73,73	1.16	7 (10%)	82,113,113	0.87	4 (4%)
20	CLA	G	206	17	69,73,73	1.26	7 (10%)	82,113,113	0.88	3 (3%)
20	CLA	S	205	15	50,54,73	1.39	7 (14%)	59,90,113	1.07	4 (6%)
20	CLA	A	809	1	66,70,73	1.24	7 (10%)	78,109,113	0.89	3 (3%)
20	CLA	A	803	1	69,73,73	1.15	7 (10%)	82,113,113	0.93	4 (4%)
26	DD6	G	212	-	40,45,45	1.32	7 (17%)	51,67,67	1.58	10 (19%)
20	CLA	O	206	-	69,73,73	1.15	7 (10%)	82,113,113	0.97	5 (6%)
23	BCR	B	838	-	41,41,41	1.07	2 (4%)	56,56,56	1.24	6 (10%)
20	CLA	A	829	1	69,73,73	1.22	7 (10%)	82,113,113	0.91	4 (4%)
30	KC1	P	206	12	49,53,53	1.55	8 (16%)	61,89,89	1.02	3 (4%)
20	CLA	F	803	6	50,54,73	1.37	7 (14%)	59,90,113	1.06	4 (6%)
20	CLA	U	207	-	69,73,73	1.13	7 (10%)	82,113,113	1.08	9 (10%)
20	CLA	P	213	12	45,49,73	1.42	6 (13%)	54,84,113	1.31	7 (12%)
20	CLA	H	205	18	49,53,73	1.52	8 (16%)	58,89,113	0.97	3 (5%)
30	KC1	O	210	11	49,53,53	1.67	11 (22%)	61,89,89	0.99	4 (6%)
20	CLA	A	851	1	69,73,73	1.18	7 (10%)	82,113,113	0.90	3 (3%)
20	CLA	B	812	2	58,62,73	1.30	6 (10%)	68,99,113	0.93	4 (5%)
28	SQD	S	201	-	44,46,54	1.02	4 (9%)	54,57,65	1.55	9 (16%)
29	LMG	Q	217	-	55,55,55	0.70	0	63,63,63	1.29	6 (9%)
26	DD6	O	214	-	40,45,45	1.25	8 (20%)	51,67,67	1.56	9 (17%)
20	CLA	G	209	17	60,64,73	1.22	7 (11%)	71,102,113	0.95	4 (5%)
20	CLA	O	211	11	45,49,73	1.45	6 (13%)	54,84,113	1.21	6 (11%)
20	CLA	G	215	17	49,53,73	1.34	7 (14%)	58,89,113	1.11	4 (6%)
20	CLA	Q	213	32	61,65,73	1.21	7 (11%)	72,103,113	1.10	6 (8%)
20	CLA	G	208	-	59,63,73	1.20	7 (11%)	70,101,113	1.04	4 (5%)
20	CLA	R	104	14	69,73,73	1.45	9 (13%)	82,113,113	0.93	4 (4%)
20	CLA	B	805	2	69,73,73	1.18	8 (11%)	82,113,113	0.89	4 (4%)
31	A86	Q	218	-	47,50,50	1.42	6 (12%)	51,76,76	1.41	9 (17%)
31	A86	R	105	-	47,50,50	1.39	5 (10%)	51,76,76	1.37	8 (15%)
20	CLA	J	103	8	46,50,73	1.39	7 (15%)	53,85,113	1.03	3 (5%)
26	DD6	S	203	-	40,45,45	1.30	8 (20%)	51,67,67	1.57	10 (19%)
26	DD6	O	212	-	40,45,45	1.30	7 (17%)	51,67,67	1.64	11 (21%)
20	CLA	A	808	1	60,64,73	1.28	7 (11%)	71,102,113	0.94	3 (4%)
26	DD6	O	213	-	40,45,45	1.29	8 (20%)	51,67,67	1.42	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	DD6	P	218	-	40,45,45	1.40	8 (20%)	51,67,67	1.75	11 (21%)
23	BCR	M	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.30	6 (10%)
26	DD6	G	213	-	40,45,45	1.36	8 (20%)	51,67,67	1.54	9 (17%)
20	CLA	B	831	2	69,73,73	1.19	7 (10%)	82,113,113	0.87	4 (4%)
20	CLA	A	807	1	58,62,73	1.30	8 (13%)	68,99,113	1.07	5 (7%)
25	SF4	A	850	1,2	0,12,12	-	-	-		
20	CLA	Q	203	13	52,56,73	1.39	8 (15%)	61,92,113	1.19	6 (9%)
26	DD6	P	205	-	40,45,45	1.30	8 (20%)	51,67,67	1.62	9 (17%)
20	CLA	B	808	2	69,73,73	1.22	7 (10%)	82,113,113	0.88	2 (2%)
20	CLA	G	205	17	65,69,73	1.14	7 (10%)	77,108,113	1.15	8 (10%)
20	CLA	O	205	11	69,73,73	1.19	5 (7%)	82,113,113	0.90	4 (4%)
20	CLA	A	828	1	69,73,73	1.22	6 (8%)	82,113,113	0.88	3 (3%)
20	CLA	H	207	-	62,66,73	1.23	7 (11%)	73,104,113	1.19	8 (10%)
20	CLA	H	206	18	69,73,73	1.17	8 (11%)	82,113,113	1.28	9 (10%)
23	BCR	A	844	-	41,41,41	1.12	2 (4%)	56,56,56	1.21	5 (8%)
20	CLA	B	848	2	54,58,73	1.33	8 (14%)	64,95,113	1.02	3 (4%)
20	CLA	O	209	11	69,73,73	1.15	6 (8%)	82,113,113	1.04	5 (6%)
20	CLA	B	814	2	59,63,73	1.35	8 (13%)	70,101,113	0.95	3 (4%)
20	CLA	A	825	1	69,73,73	1.23	7 (10%)	82,113,113	0.89	3 (3%)
26	DD6	O	215	-	40,45,45	1.41	9 (22%)	51,67,67	1.56	13 (25%)
20	CLA	G	204	17	47,51,73	1.38	7 (14%)	55,86,113	1.02	3 (5%)
20	CLA	A	846	1	64,68,73	1.31	6 (9%)	76,107,113	0.95	4 (5%)
20	CLA	U	204	-	65,69,73	1.21	7 (10%)	77,108,113	0.89	4 (5%)
21	PQN	A	837	-	34,34,34	0.39	0	43,45,45	0.59	1 (2%)
29	LMG	J	102	-	39,39,55	0.88	0	47,47,63	1.24	4 (8%)
30	KC1	P	219	12	49,53,53	1.53	7 (14%)	61,89,89	1.02	2 (3%)
28	SQD	B	847	-	48,50,54	1.00	5 (10%)	58,61,65	1.52	9 (15%)
26	DD6	O	201	-	40,45,45	1.31	9 (22%)	51,67,67	1.47	8 (15%)
20	CLA	A	824	1	66,70,73	1.21	7 (10%)	78,109,113	0.96	3 (3%)
23	BCR	A	841	-	41,41,41	1.05	2 (4%)	56,56,56	1.29	5 (8%)
26	DD6	P	215	-	40,45,45	1.33	8 (20%)	51,67,67	1.50	9 (17%)
31	A86	P	204	-	47,50,50	1.36	4 (8%)	51,76,76	1.70	11 (21%)
23	BCR	F	801	-	41,41,41	1.05	2 (4%)	56,56,56	1.23	4 (7%)
22	LHG	A	839	-	47,47,48	0.61	0	50,53,54	1.20	5 (10%)
20	CLA	A	812	1	49,53,73	1.44	6 (12%)	58,89,113	1.11	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	T	209	19	45,49,73	1.40	5 (11%)	54,84,113	1.15	5 (9%)
20	CLA	B	818	2	50,54,73	1.39	7 (14%)	59,90,113	1.13	4 (6%)
31	A86	Q	214	-	47,50,50	1.41	5 (10%)	51,76,76	1.67	10 (19%)
20	CLA	P	209	-	56,60,73	1.27	6 (10%)	65,97,113	0.95	3 (4%)
20	CLA	P	216	12	51,55,73	1.38	7 (13%)	60,91,113	1.12	5 (8%)
20	CLA	B	811	2	59,63,73	1.24	7 (11%)	70,101,113	0.95	4 (5%)
20	CLA	H	202	18	64,68,73	1.18	7 (10%)	76,107,113	1.01	3 (3%)
20	CLA	B	845	2	69,73,73	1.26	8 (11%)	82,113,113	0.97	4 (4%)
20	CLA	Q	208	13	54,58,73	1.32	9 (16%)	64,95,113	1.00	4 (6%)
26	DD6	J	101	-	40,45,45	1.28	7 (17%)	51,67,67	1.52	9 (17%)
20	CLA	T	202	19	45,49,73	1.43	8 (17%)	54,84,113	1.16	4 (7%)
20	CLA	O	204	11	69,73,73	1.18	8 (11%)	82,113,113	0.89	3 (3%)
20	CLA	P	214	12	49,53,73	1.45	8 (16%)	58,89,113	1.09	3 (5%)
20	CLA	U	211	16	56,60,73	1.33	8 (14%)	65,97,113	1.06	4 (6%)
26	DD6	Q	215	-	40,45,45	1.29	7 (17%)	51,67,67	1.51	9 (17%)
24	CL0	A	848	1	58,73,73	0.89	4 (6%)	60,113,113	1.74	8 (13%)
31	A86	R	103	-	44,46,50	1.43	4 (9%)	49,70,76	1.63	10 (20%)
25	SF4	C	102	3	0,12,12	-	-	-	-	-
20	CLA	A	827	1	54,58,73	1.39	7 (12%)	64,95,113	1.00	4 (6%)
20	CLA	B	819	2	57,61,73	1.30	7 (12%)	67,98,113	0.96	4 (5%)
20	CLA	A	833	1	69,73,73	1.23	7 (10%)	82,113,113	0.98	4 (4%)
20	CLA	T	203	19	50,54,73	1.43	8 (16%)	59,90,113	0.98	3 (5%)
20	CLA	B	827	2	53,57,73	1.36	8 (15%)	61,93,113	0.98	3 (4%)
20	CLA	A	849	1	69,73,73	1.20	6 (8%)	82,113,113	0.93	4 (4%)
20	CLA	H	201	-	44,48,73	1.45	6 (13%)	51,82,113	1.35	7 (13%)
26	DD6	A	855	-	40,45,45	1.29	8 (20%)	51,67,67	1.54	10 (19%)
20	CLA	A	838	22	56,60,73	1.28	6 (10%)	65,97,113	1.07	4 (6%)
20	CLA	B	828	2	62,66,73	1.27	6 (9%)	73,104,113	0.93	3 (4%)
20	CLA	Q	204	-	65,69,73	1.19	6 (9%)	77,108,113	1.02	5 (6%)
20	CLA	R	101	32	49,53,73	1.41	7 (14%)	58,89,113	1.10	4 (6%)
20	CLA	U	209	16	46,50,73	1.35	6 (13%)	53,85,113	1.15	6 (11%)
26	DD6	Q	202	-	40,45,45	1.30	7 (17%)	51,67,67	1.72	14 (27%)
26	DD6	S	212	-	40,45,45	1.32	7 (17%)	51,67,67	1.64	10 (19%)
20	CLA	P	208	12	60,64,73	1.31	8 (13%)	71,102,113	0.97	4 (5%)
20	CLA	B	825	2	69,73,73	1.22	9 (13%)	82,113,113	0.91	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	F	802	-	52,56,73	1.38	8 (15%)	61,92,113	1.18	7 (11%)
23	BCR	I	102	-	41,41,41	1.11	2 (4%)	56,56,56	1.24	5 (8%)
31	A86	Q	201	-	47,50,50	1.31	5 (10%)	51,76,76	1.45	10 (19%)
20	CLA	A	836	-	69,73,73	1.19	8 (11%)	82,113,113	1.03	6 (7%)
20	CLA	U	205	16	69,73,73	1.17	7 (10%)	82,113,113	0.98	3 (3%)
20	CLA	U	206	16	49,53,73	1.45	7 (14%)	58,89,113	0.97	3 (5%)
23	BCR	B	841	-	41,41,41	1.09	2 (4%)	56,56,56	1.13	3 (5%)
20	CLA	B	816	2	64,68,73	1.24	8 (12%)	76,107,113	0.93	4 (5%)
26	DD6	G	211	-	40,45,45	1.29	6 (15%)	51,67,67	1.40	7 (13%)
20	CLA	A	818	32	69,73,73	1.17	8 (11%)	82,113,113	0.87	3 (3%)
30	KC1	S	209	15	49,53,53	1.56	7 (14%)	61,89,89	1.22	7 (11%)
20	CLA	B	802	2	69,73,73	1.24	7 (10%)	82,113,113	0.80	3 (3%)
21	PQN	B	836	-	34,34,34	0.41	0	43,45,45	0.57	1 (2%)
20	CLA	A	816	1	69,73,73	1.17	8 (11%)	82,113,113	0.95	4 (4%)
20	CLA	S	207	15	49,53,73	1.36	7 (14%)	58,89,113	1.04	5 (8%)
20	CLA	Q	206	13	54,59,73	1.41	6 (11%)	62,96,113	0.95	3 (4%)
20	CLA	A	854	-	69,73,73	1.16	5 (7%)	82,113,113	1.29	9 (10%)
20	CLA	O	207	11	50,54,73	1.36	7 (14%)	59,90,113	1.07	4 (6%)
20	CLA	Q	212	13	69,73,73	1.23	7 (10%)	82,113,113	1.01	8 (9%)
20	CLA	A	811	1	69,73,73	1.21	8 (11%)	82,113,113	0.93	3 (3%)
20	CLA	A	845	32	69,73,73	1.18	7 (10%)	82,113,113	0.96	3 (3%)
20	CLA	P	210	32	51,55,73	1.33	6 (11%)	60,91,113	1.05	4 (6%)
20	CLA	Q	211	13	45,49,73	1.48	7 (15%)	54,84,113	1.22	6 (11%)
20	CLA	B	823	2	69,73,73	1.23	7 (10%)	82,113,113	0.96	5 (6%)
23	BCR	B	837	-	41,41,41	1.16	3 (7%)	56,56,56	1.26	7 (12%)
30	KC1	P	212	12	46,52,53	1.72	10 (21%)	59,87,89	1.11	6 (10%)
20	CLA	T	206	19	46,50,73	1.41	6 (13%)	53,85,113	1.09	4 (7%)
26	DD6	P	220	-	40,45,45	1.33	8 (20%)	51,67,67	1.79	12 (23%)
20	CLA	A	822	32	69,73,73	1.14	6 (8%)	82,113,113	0.94	4 (4%)
20	CLA	B	833	32	69,73,73	1.17	7 (10%)	82,113,113	0.98	6 (7%)
20	CLA	B	830	2	62,66,73	1.29	7 (11%)	73,104,113	0.96	3 (4%)
20	CLA	B	817	32	69,73,73	1.19	7 (10%)	82,113,113	0.95	5 (6%)
20	CLA	B	829	-	69,73,73	1.17	7 (10%)	82,113,113	0.95	4 (4%)
23	BCR	L	205	-	41,41,41	1.09	2 (4%)	56,56,56	1.35	5 (8%)
20	CLA	A	810	1	58,62,73	1.30	7 (12%)	68,99,113	1.06	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	P	207	12	69,73,73	1.15	7 (10%)	82,113,113	0.94	4 (4%)
26	DD6	H	210	-	40,45,45	1.33	5 (12%)	51,67,67	1.57	10 (19%)
20	CLA	A	853	32	69,73,73	1.17	7 (10%)	82,113,113	0.97	4 (4%)
20	CLA	O	208	11	64,68,73	1.18	6 (9%)	76,107,113	0.97	4 (5%)
20	CLA	T	204	-	61,65,73	1.19	5 (8%)	72,103,113	1.00	5 (6%)
23	BCR	B	839	-	41,41,41	1.09	3 (7%)	56,56,56	1.29	10 (17%)
20	CLA	P	211	12	54,58,73	1.28	6 (11%)	64,95,113	1.06	3 (4%)
20	CLA	H	209	18	49,53,73	1.40	7 (14%)	58,89,113	1.08	4 (6%)
20	CLA	A	802	1	59,63,73	1.35	7 (11%)	70,101,113	0.96	3 (4%)
29	LMG	U	201	-	32,32,55	0.97	1 (3%)	40,40,63	1.21	3 (7%)
20	CLA	H	208	18	45,49,73	1.43	7 (15%)	54,84,113	1.29	7 (12%)
23	BCR	B	840	-	41,41,41	1.07	2 (4%)	56,56,56	1.28	7 (12%)
20	CLA	H	203	18	65,69,73	1.19	5 (7%)	77,108,113	1.01	5 (6%)
23	BCR	L	201	-	41,41,41	1.11	2 (4%)	56,56,56	1.25	5 (8%)
20	CLA	B	826	2	54,58,73	1.39	7 (12%)	64,95,113	0.96	3 (4%)
30	KC1	P	203	12	49,53,53	1.68	10 (20%)	61,89,89	1.12	7 (11%)
20	CLA	G	210	17	49,53,73	1.42	7 (14%)	58,89,113	1.01	3 (5%)
20	CLA	B	846	2	69,73,73	1.18	7 (10%)	82,113,113	1.04	5 (6%)
20	CLA	B	803	-	69,73,73	1.15	7 (10%)	82,113,113	0.99	7 (8%)
20	CLA	S	208	15	56,60,73	1.25	6 (10%)	65,97,113	1.09	4 (6%)
23	BCR	A	843	-	41,41,41	1.10	2 (4%)	56,56,56	1.22	5 (8%)
27	DGD	B	842	-	61,61,67	0.89	1 (1%)	75,75,81	1.36	9 (12%)
20	CLA	A	805	1	53,57,73	1.38	6 (11%)	61,93,113	1.04	4 (6%)
20	CLA	A	832	1	55,59,73	1.37	8 (14%)	64,96,113	1.04	5 (7%)
20	CLA	S	202	32	69,73,73	1.14	5 (7%)	82,113,113	1.06	6 (7%)
26	DD6	U	214	-	24,26,45	1.50	5 (20%)	29,35,67	1.63	7 (24%)
23	BCR	A	842	-	41,41,41	1.05	2 (4%)	56,56,56	1.16	3 (5%)
20	CLA	A	821	32	69,73,73	1.21	7 (10%)	82,113,113	1.00	6 (7%)
20	CLA	B	832	2	51,55,73	1.40	6 (11%)	60,91,113	1.03	4 (6%)
20	CLA	Q	205	13	64,68,73	1.22	8 (12%)	76,107,113	0.94	3 (3%)
20	CLA	B	806	2	69,73,73	1.21	7 (10%)	82,113,113	0.89	3 (3%)
29	LMG	P	217	-	25,25,55	1.34	5 (20%)	33,33,63	1.28	4 (12%)
20	CLA	Q	207	13	50,54,73	1.39	7 (14%)	59,90,113	1.22	6 (10%)
29	LMG	P	202	-	34,34,55	1.04	3 (8%)	42,42,63	1.23	4 (9%)
20	CLA	B	844	2	69,73,73	1.21	6 (8%)	82,113,113	0.89	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	BCR	J	104	-	41,41,41	1.12	2 (4%)	56,56,56	1.29	5 (8%)
20	CLA	B	813	2	63,67,73	1.30	8 (12%)	74,105,113	1.09	7 (9%)
20	CLA	B	834	2	69,73,73	1.12	6 (8%)	82,113,113	0.90	4 (4%)
29	LMG	I	103	-	49,49,55	0.79	1 (2%)	57,57,63	1.24	6 (10%)
20	CLA	T	211	-	51,55,73	1.35	7 (13%)	60,91,113	1.18	4 (6%)
20	CLA	B	804	2	49,53,73	1.45	8 (16%)	58,89,113	1.05	4 (6%)
20	CLA	A	801	-	69,73,73	1.17	8 (11%)	82,113,113	0.86	4 (4%)
20	CLA	O	203	-	49,53,73	1.39	7 (14%)	58,89,113	1.07	4 (6%)
22	LHG	G	216	-	26,26,48	0.85	1 (3%)	29,32,54	1.26	2 (6%)
20	CLA	H	204	18	47,52,73	1.40	7 (14%)	55,87,113	1.07	3 (5%)
26	DD6	S	210	-	40,45,45	1.31	7 (17%)	51,67,67	1.46	10 (19%)
22	LHG	P	201	-	48,48,48	0.63	1 (2%)	51,54,54	1.23	6 (11%)
20	CLA	A	831	1	49,53,73	1.37	6 (12%)	58,89,113	1.10	4 (6%)
20	CLA	A	847	1	69,73,73	1.23	8 (11%)	82,113,113	1.06	6 (7%)

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
20	CLA	G	203	17	1/1/11/20	7/15/91/115	-
20	CLA	B	824	2	-	3/39/115/115	-
20	CLA	T	201	-	1/1/10/20	0/12/88/115	-
20	CLA	A	830	1	-	1/21/97/115	-
20	CLA	A	852	1	1/1/15/20	7/39/115/115	-
26	DD6	U	212	-	-	10/26/80/80	0/3/3/3
20	CLA	O	202	11	-	2/13/89/115	-
20	CLA	B	822	2	1/1/15/20	0/39/115/115	-
20	CLA	A	814	32	1/1/11/20	4/15/91/115	-
20	CLA	A	815	1	1/1/15/20	10/39/115/115	-
20	CLA	T	207	19	-	5/39/115/115	-
23	BCR	R	102	-	-	9/27/61/63	0/2/2/2
26	DD6	G	214	-	-	12/26/80/80	0/3/3/3
20	CLA	U	208	16	1/1/11/20	2/17/93/115	-
20	CLA	B	815	2	1/1/13/20	8/32/108/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	810	2	-	2/25/101/115	-
20	CLA	B	820	-	1/1/14/20	4/37/113/115	-
20	CLA	G	202	-	1/1/10/20	0/10/86/115	-
20	CLA	A	817	1	1/1/11/20	0/15/91/115	-
20	CLA	A	826	1	-	3/39/115/115	-
20	CLA	G	201	17	-	2/15/91/115	-
20	CLA	A	835	1	1/1/15/20	11/39/115/115	-
22	LHG	A	840	20	-	8/31/31/53	-
30	KC1	U	213	16	-	2/15/71/71	-
20	CLA	B	835	-	1/1/15/20	0/39/115/115	-
20	CLA	Q	216	-	-	11/39/115/115	-
23	BCR	I	101	-	-	8/29/63/63	0/2/2/2
31	A86	U	202	-	-	15/34/90/90	0/3/3/3
26	DD6	T	213	-	-	19/26/80/80	0/3/3/3
20	CLA	A	820	1	1/1/12/20	0/23/99/115	-
26	DD6	T	212	-	-	14/26/80/80	0/3/3/3
23	BCR	F	804	-	-	10/29/63/63	0/2/2/2
26	DD6	S	213	-	-	16/26/80/80	0/3/3/3
26	DD6	U	203	-	-	16/26/80/80	0/3/3/3
20	CLA	B	809	2	1/1/15/20	8/39/115/115	-
20	CLA	B	821	32	1/1/14/20	6/38/114/115	-
20	CLA	A	804	1	1/1/15/20	5/39/115/115	-
20	CLA	U	210	16	-	8/39/115/115	-
20	CLA	A	813	1	-	0/21/97/115	-
20	CLA	A	834	1	1/1/15/20	5/39/115/115	-
20	CLA	A	819	1	-	0/13/89/115	-
20	CLA	Q	209	13	-	10/39/115/115	-
20	CLA	L	204	32	-	6/21/97/115	-
30	KC1	Q	210	13	-	2/15/71/71	-
25	SF4	C	101	3	-	-	0/6/5/5
30	KC1	S	211	15	-	6/15/71/71	-
20	CLA	B	807	2	1/1/15/20	3/39/115/115	-
26	DD6	S	204	-	-	13/26/80/80	0/3/3/3
20	CLA	A	806	1	1/1/15/20	3/39/115/115	-
20	CLA	T	205	-	1/1/11/20	5/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	S	206	15	1/1/11/20	2/17/93/115	-
20	CLA	S	214	-	1/1/15/20	7/39/115/115	-
20	CLA	B	801	-	1/1/15/20	3/39/115/115	-
20	CLA	B	843	2	1/1/15/20	6/39/115/115	-
20	CLA	S	215	15	1/1/15/20	6/39/115/115	-
26	DD6	G	217	-	-	12/26/80/80	0/3/3/3
20	CLA	G	207	17	1/1/14/20	5/33/109/115	-
20	CLA	A	823	1	1/1/15/20	6/39/115/115	-
20	CLA	L	202	9	1/1/11/20	6/20/96/115	-
26	DD6	H	211	-	-	11/26/80/80	0/3/3/3
20	CLA	T	210	19	-	3/17/93/115	-
30	KC1	T	208	-	-	3/15/71/71	-
20	CLA	L	203	9	-	2/39/115/115	-
20	CLA	G	206	17	1/1/15/20	11/39/115/115	-
20	CLA	S	205	15	1/1/11/20	0/17/93/115	-
20	CLA	A	809	1	-	2/36/112/115	-
20	CLA	A	803	1	1/1/15/20	5/39/115/115	-
26	DD6	G	212	-	-	13/26/80/80	0/3/3/3
20	CLA	O	206	-	1/1/15/20	7/39/115/115	-
23	BCR	B	838	-	-	7/29/63/63	0/2/2/2
20	CLA	A	829	1	1/1/15/20	3/39/115/115	-
30	KC1	P	206	12	-	3/15/71/71	-
20	CLA	F	803	6	1/1/11/20	4/17/93/115	-
20	CLA	U	207	-	-	9/39/115/115	-
20	CLA	P	213	12	1/1/10/20	2/10/86/115	-
20	CLA	H	205	18	1/1/11/20	3/15/91/115	-
30	KC1	O	210	11	-	0/15/71/71	-
20	CLA	A	851	1	1/1/15/20	11/39/115/115	-
20	CLA	B	812	2	1/1/12/20	1/26/102/115	-
28	SQD	S	201	-	-	16/41/61/69	0/1/1/1
29	LMG	Q	217	-	-	16/50/70/70	0/1/1/1
26	DD6	O	214	-	-	11/26/80/80	0/3/3/3
20	CLA	G	209	17	-	5/29/105/115	-
20	CLA	O	211	11	-	1/10/86/115	-
20	CLA	G	215	17	1/1/11/20	2/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	Q	213	32	1/1/13/20	7/30/106/115	-
20	CLA	G	208	-	1/1/13/20	6/27/103/115	-
20	CLA	R	104	14	-	12/39/115/115	-
20	CLA	B	805	2	1/1/15/20	7/39/115/115	-
31	A86	Q	218	-	-	21/34/90/90	0/3/3/3
31	A86	R	105	-	-	15/34/90/90	0/3/3/3
20	CLA	J	103	8	1/1/10/20	2/12/88/115	-
26	DD6	S	203	-	-	4/26/80/80	0/3/3/3
26	DD6	O	212	-	-	6/26/80/80	0/3/3/3
20	CLA	A	808	1	1/1/13/20	4/29/105/115	-
26	DD6	O	213	-	-	9/26/80/80	0/3/3/3
26	DD6	P	218	-	-	14/26/80/80	0/3/3/3
23	BCR	M	101	-	-	8/29/63/63	0/2/2/2
26	DD6	G	213	-	-	10/26/80/80	0/3/3/3
20	CLA	B	831	2	1/1/15/20	8/39/115/115	-
20	CLA	A	807	1	-	6/26/102/115	-
25	SF4	A	850	1,2	-	-	0/6/5/5
20	CLA	Q	203	13	-	5/19/95/115	-
26	DD6	P	205	-	-	6/26/80/80	0/3/3/3
20	CLA	B	808	2	1/1/15/20	7/39/115/115	-
20	CLA	G	205	17	1/1/14/20	10/35/111/115	-
20	CLA	O	205	11	1/1/15/20	5/39/115/115	-
20	CLA	A	828	1	1/1/15/20	3/39/115/115	-
20	CLA	H	207	-	1/1/13/20	5/31/107/115	-
20	CLA	H	206	18	1/1/15/20	16/39/115/115	-
23	BCR	A	844	-	-	9/29/63/63	0/2/2/2
20	CLA	B	848	2	1/1/12/20	3/21/97/115	-
20	CLA	O	209	11	-	7/39/115/115	-
20	CLA	B	814	2	-	2/27/103/115	-
20	CLA	A	825	1	1/1/15/20	7/39/115/115	-
26	DD6	O	215	-	-	14/26/80/80	0/3/3/3
20	CLA	G	204	17	-	3/13/89/115	-
20	CLA	A	846	1	-	3/33/109/115	-
20	CLA	U	204	-	1/1/14/20	4/35/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	PQN	A	837	-	-	4/23/43/43	0/2/2/2
29	LMG	J	102	-	-	14/34/54/70	0/1/1/1
30	KC1	P	219	12	-	4/15/71/71	-
28	SQD	B	847	-	-	18/45/65/69	0/1/1/1
26	DD6	O	201	-	-	8/26/80/80	0/3/3/3
20	CLA	A	824	1	1/1/14/20	9/36/112/115	-
23	BCR	A	841	-	-	7/29/63/63	0/2/2/2
26	DD6	P	215	-	-	5/26/80/80	0/3/3/3
31	A86	P	204	-	-	17/34/90/90	0/3/3/3
23	BCR	F	801	-	-	6/29/63/63	0/2/2/2
22	LHG	A	839	-	-	24/52/52/53	-
20	CLA	A	812	1	1/1/11/20	1/15/91/115	-
20	CLA	T	209	19	-	1/10/86/115	-
20	CLA	B	818	2	-	0/17/93/115	-
31	A86	Q	214	-	-	13/34/90/90	0/3/3/3
20	CLA	P	209	-	1/1/12/20	1/24/100/115	-
20	CLA	P	216	12	1/1/11/20	0/18/94/115	-
20	CLA	B	811	2	-	1/27/103/115	-
20	CLA	H	202	18	1/1/14/20	7/33/109/115	-
20	CLA	B	845	2	1/1/15/20	4/39/115/115	-
20	CLA	Q	208	13	1/1/12/20	2/21/97/115	-
26	DD6	J	101	-	-	6/26/80/80	0/3/3/3
20	CLA	T	202	19	1/1/10/20	0/10/86/115	-
20	CLA	O	204	11	1/1/15/20	2/39/115/115	-
20	CLA	P	214	12	1/1/11/20	5/15/91/115	-
20	CLA	U	211	16	1/1/12/20	3/24/100/115	-
26	DD6	Q	215	-	-	12/26/80/80	0/3/3/3
24	CL0	A	848	1	-	3/37/135/135	-
31	A86	R	103	-	-	12/30/84/90	0/3/3/3
25	SF4	C	102	3	-	-	0/6/5/5
20	CLA	A	827	1	-	3/21/97/115	-
20	CLA	B	819	2	-	1/25/101/115	-
20	CLA	A	833	1	1/1/15/20	7/39/115/115	-
20	CLA	T	203	19	1/1/11/20	3/17/93/115	-
20	CLA	B	827	2	1/1/11/20	3/20/96/115	-
20	CLA	A	849	1	1/1/15/20	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	H	201	-	1/1/9/20	0/10/82/115	-
26	DD6	A	855	-	-	14/26/80/80	0/3/3/3
20	CLA	A	838	22	1/1/12/20	5/24/100/115	-
20	CLA	Q	204	-	1/1/14/20	0/35/111/115	-
20	CLA	B	828	2	-	7/31/107/115	-
20	CLA	R	101	32	1/1/11/20	2/15/91/115	-
20	CLA	U	209	16	1/1/10/20	0/12/88/115	-
26	DD6	Q	202	-	-	6/26/80/80	0/3/3/3
26	DD6	S	212	-	-	13/26/80/80	0/3/3/3
20	CLA	P	208	12	1/1/13/20	6/29/105/115	-
20	CLA	B	825	2	-	8/39/115/115	-
20	CLA	F	802	-	1/1/11/20	3/19/95/115	-
23	BCR	I	102	-	-	8/29/63/63	0/2/2/2
31	A86	Q	201	-	-	16/34/90/90	0/3/3/3
20	CLA	A	836	-	1/1/15/20	3/39/115/115	-
20	CLA	U	206	16	1/1/11/20	3/15/91/115	-
20	CLA	U	205	16	-	3/39/115/115	-
23	BCR	B	841	-	-	7/29/63/63	0/2/2/2
20	CLA	B	816	2	1/1/14/20	3/33/109/115	-
26	DD6	G	211	-	-	6/26/80/80	0/3/3/3
20	CLA	A	818	32	1/1/15/20	6/39/115/115	-
30	KC1	S	209	15	-	1/15/71/71	-
20	CLA	B	802	2	1/1/15/20	2/39/115/115	-
21	PQN	B	836	-	-	4/23/43/43	0/2/2/2
20	CLA	A	816	1	1/1/15/20	0/39/115/115	-
20	CLA	S	207	15	1/1/11/20	2/15/91/115	-
20	CLA	Q	206	13	1/1/12/20	3/22/98/115	-
20	CLA	A	854	-	1/1/15/20	9/39/115/115	-
20	CLA	O	207	11	1/1/11/20	0/17/93/115	-
20	CLA	Q	212	13	-	3/39/115/115	-
20	CLA	A	811	1	1/1/15/20	8/39/115/115	-
20	CLA	A	845	32	1/1/15/20	8/39/115/115	-
20	CLA	P	210	32	-	4/18/94/115	-
20	CLA	Q	211	13	1/1/10/20	3/10/86/115	-
20	CLA	B	823	2	1/1/15/20	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	B	837	-	-	9/29/63/63	0/2/2/2
30	KC1	P	212	12	-	4/12/68/71	-
20	CLA	T	206	19	1/1/10/20	1/12/88/115	-
26	DD6	P	220	-	-	15/26/80/80	0/3/3/3
20	CLA	A	822	32	1/1/15/20	6/39/115/115	-
20	CLA	B	833	32	1/1/15/20	2/39/115/115	-
20	CLA	B	830	2	1/1/13/20	1/31/107/115	-
20	CLA	B	817	32	1/1/15/20	4/39/115/115	-
20	CLA	B	829	-	1/1/15/20	1/39/115/115	-
23	BCR	L	205	-	-	7/29/63/63	0/2/2/2
20	CLA	A	810	1	1/1/12/20	3/26/102/115	-
20	CLA	P	207	12	1/1/15/20	7/39/115/115	-
26	DD6	H	210	-	-	14/26/80/80	0/3/3/3
20	CLA	A	853	32	1/1/15/20	2/39/115/115	-
20	CLA	O	208	11	1/1/14/20	2/33/109/115	-
20	CLA	T	204	-	-	9/30/106/115	-
23	BCR	B	839	-	-	2/29/63/63	0/2/2/2
20	CLA	H	209	18	1/1/11/20	4/15/91/115	-
20	CLA	P	211	12	-	2/21/97/115	-
20	CLA	A	802	1	1/1/13/20	1/27/103/115	-
29	LMG	U	201	-	-	14/27/47/70	0/1/1/1
20	CLA	H	208	18	1/1/10/20	2/10/86/115	-
23	BCR	B	840	-	-	5/29/63/63	0/2/2/2
20	CLA	H	203	18	1/1/14/20	6/35/111/115	-
23	BCR	L	201	-	-	11/29/63/63	0/2/2/2
20	CLA	B	826	2	-	0/21/97/115	-
30	KC1	P	203	12	-	1/15/71/71	-
20	CLA	G	210	17	1/1/11/20	4/15/91/115	-
20	CLA	B	846	2	1/1/15/20	5/39/115/115	-
20	CLA	B	803	-	1/1/15/20	5/39/115/115	-
20	CLA	S	208	15	-	5/24/100/115	-
23	BCR	A	843	-	-	4/29/63/63	0/2/2/2
27	DGD	B	842	-	-	19/49/89/95	0/2/2/2
20	CLA	A	805	1	1/1/11/20	1/20/96/115	-
20	CLA	A	832	1	1/1/12/20	0/23/99/115	-
20	CLA	S	202	32	-	3/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	DD6	U	214	-	-	10/14/37/80	0/1/1/3
23	BCR	A	842	-	-	7/29/63/63	0/2/2/2
20	CLA	A	821	32	1/1/15/20	5/39/115/115	-
20	CLA	B	832	2	1/1/11/20	1/18/94/115	-
20	CLA	Q	205	13	1/1/14/20	5/33/109/115	-
20	CLA	B	806	2	1/1/15/20	9/39/115/115	-
29	LMG	P	217	-	-	8/19/39/70	0/1/1/1
20	CLA	Q	207	13	1/1/11/20	4/17/93/115	-
29	LMG	P	202	-	-	15/29/49/70	0/1/1/1
20	CLA	B	844	2	1/1/15/20	5/39/115/115	-
23	BCR	J	104	-	-	13/29/63/63	0/2/2/2
20	CLA	B	813	2	-	13/32/108/115	-
20	CLA	B	834	2	1/1/15/20	20/39/115/115	-
29	LMG	I	103	-	-	16/44/64/70	0/1/1/1
20	CLA	T	211	-	1/1/11/20	6/18/94/115	-
20	CLA	B	804	2	1/1/11/20	5/15/91/115	-
20	CLA	O	203	-	1/1/11/20	0/15/91/115	-
20	CLA	A	801	-	-	4/39/115/115	-
22	LHG	G	216	-	-	20/31/31/53	-
20	CLA	H	204	18	1/1/10/20	0/14/90/115	-
26	DD6	S	210	-	-	7/26/80/80	0/3/3/3
22	LHG	P	201	-	-	25/53/53/53	-
20	CLA	A	831	1	1/1/11/20	4/15/91/115	-
20	CLA	A	847	1	-	6/39/115/115	-

The worst 5 of 1573 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	Q	214	A86	C13-C11	-6.76	1.36	1.49
31	Q	218	A86	C13-C11	-6.75	1.36	1.49
31	R	105	A86	C13-C11	-6.62	1.37	1.49
31	U	202	A86	C13-C11	-6.44	1.37	1.49
31	P	204	A86	C13-C11	-6.37	1.37	1.49

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	848	CL0	C1B-CHB-C4A	9.49	127.43	121.32
31	Q	214	A86	C29-C30-C31	-5.98	170.60	177.66
31	P	204	A86	C26-C25-C24	5.79	139.97	123.20
26	U	203	DD6	C4-C3-C2	5.70	135.18	123.52
26	P	220	DD6	C10-C9-C8	5.46	139.01	123.20

5 of 122 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	A	802	CLA	ND
20	A	803	CLA	ND
20	A	804	CLA	ND
20	A	805	CLA	ND
20	A	806	CLA	ND

5 of 1527 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	806	CLA	CHA-CBD-CGD-O1D
20	A	806	CLA	CHA-CBD-CGD-O2D
20	A	815	CLA	C3A-C2A-CAA-CBA
20	A	826	CLA	CHA-CBD-CGD-O1D
20	A	826	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

167 monomers are involved in 289 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	G	203	CLA	1	0
20	B	824	CLA	3	0
20	T	201	CLA	3	0
20	A	852	CLA	2	0
20	O	202	CLA	1	0
20	B	822	CLA	2	0
20	A	814	CLA	2	0
20	A	815	CLA	2	0
20	T	207	CLA	3	0
23	R	102	BCR	1	0
26	G	214	DD6	1	0
20	U	208	CLA	1	0
20	B	810	CLA	1	0
20	B	815	CLA	4	0
20	B	820	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	G	202	CLA	1	0
20	A	817	CLA	1	0
20	A	826	CLA	1	0
20	G	201	CLA	1	0
20	A	835	CLA	4	0
22	A	840	LHG	1	0
20	B	835	CLA	6	0
20	Q	216	CLA	3	0
23	I	101	BCR	1	0
20	A	820	CLA	1	0
23	F	804	BCR	1	0
26	U	203	DD6	2	0
20	B	809	CLA	3	0
20	B	821	CLA	1	0
20	A	804	CLA	2	0
20	U	210	CLA	2	0
20	A	813	CLA	1	0
20	A	834	CLA	1	0
20	B	807	CLA	2	0
20	T	205	CLA	1	0
20	S	206	CLA	2	0
20	S	214	CLA	4	0
20	S	215	CLA	1	0
20	G	207	CLA	1	0
20	A	823	CLA	1	0
20	L	202	CLA	2	0
20	T	210	CLA	2	0
20	G	206	CLA	3	0
20	S	205	CLA	2	0
20	A	803	CLA	6	0
23	B	838	BCR	5	0
20	A	829	CLA	2	0
30	P	206	KC1	1	0
20	F	803	CLA	3	0
20	U	207	CLA	1	0
20	P	213	CLA	2	0
20	H	205	CLA	2	0
20	A	851	CLA	1	0
20	B	812	CLA	1	0
28	S	201	SQD	5	0
29	Q	217	LMG	3	0
20	G	209	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	O	211	CLA	2	0
20	G	215	CLA	1	0
20	Q	213	CLA	1	0
20	G	208	CLA	2	0
20	R	104	CLA	2	0
20	J	103	CLA	1	0
20	A	808	CLA	1	0
23	M	101	BCR	4	0
20	B	831	CLA	2	0
20	A	807	CLA	1	0
20	Q	203	CLA	2	0
20	B	808	CLA	4	0
20	G	205	CLA	2	0
20	O	205	CLA	2	0
20	A	828	CLA	1	0
20	H	207	CLA	3	0
20	H	206	CLA	4	0
23	A	844	BCR	2	0
20	B	848	CLA	4	0
20	O	209	CLA	1	0
20	B	814	CLA	1	0
20	A	825	CLA	2	0
20	G	204	CLA	1	0
20	A	846	CLA	1	0
21	A	837	PQN	4	0
29	J	102	LMG	1	0
20	A	824	CLA	4	0
23	A	841	BCR	2	0
23	F	801	BCR	1	0
20	B	818	CLA	2	0
20	B	811	CLA	1	0
20	B	845	CLA	1	0
20	Q	208	CLA	1	0
20	T	202	CLA	2	0
20	P	214	CLA	2	0
20	U	211	CLA	1	0
24	A	848	CL0	2	0
20	B	819	CLA	4	0
20	A	833	CLA	5	0
20	B	827	CLA	1	0
20	A	849	CLA	2	0
20	H	201	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	838	CLA	3	0
20	B	828	CLA	1	0
20	Q	204	CLA	1	0
20	R	101	CLA	1	0
20	U	209	CLA	1	0
20	P	208	CLA	2	0
20	B	825	CLA	1	0
20	F	802	CLA	1	0
23	I	102	BCR	2	0
20	A	836	CLA	1	0
20	U	205	CLA	5	0
20	U	206	CLA	2	0
23	B	841	BCR	1	0
20	B	816	CLA	2	0
20	A	818	CLA	3	0
20	B	802	CLA	2	0
21	B	836	PQN	4	0
20	A	816	CLA	2	0
20	Q	206	CLA	1	0
20	A	854	CLA	4	0
20	O	207	CLA	2	0
20	Q	212	CLA	2	0
20	A	811	CLA	5	0
20	A	845	CLA	2	0
20	P	210	CLA	1	0
23	B	837	BCR	5	0
20	T	206	CLA	2	0
20	A	822	CLA	1	0
20	B	833	CLA	5	0
20	B	830	CLA	3	0
20	B	829	CLA	2	0
23	L	205	BCR	2	0
20	A	810	CLA	2	0
20	P	207	CLA	1	0
20	A	853	CLA	2	0
20	O	208	CLA	3	0
20	T	204	CLA	3	0
23	B	839	BCR	2	0
20	P	211	CLA	1	0
20	A	802	CLA	1	0
29	U	201	LMG	1	0
20	H	208	CLA	2	0

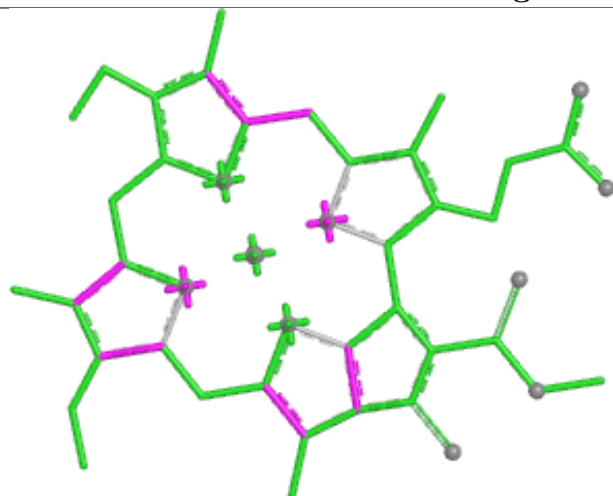
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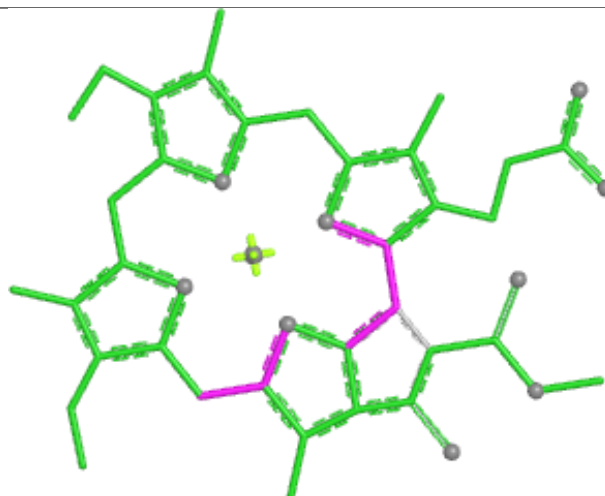
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	840	BCR	1	0
20	H	203	CLA	1	0
23	L	201	BCR	3	0
20	B	826	CLA	1	0
20	G	210	CLA	1	0
20	B	846	CLA	3	0
20	B	803	CLA	1	0
23	A	843	BCR	3	0
20	S	202	CLA	4	0
23	A	842	BCR	2	0
20	A	821	CLA	2	0
20	Q	205	CLA	1	0
29	P	217	LMG	5	0
20	Q	207	CLA	1	0
20	B	844	CLA	3	0
23	J	104	BCR	1	0
20	B	813	CLA	1	0
20	B	834	CLA	1	0
29	I	103	LMG	2	0
20	T	211	CLA	1	0
20	A	801	CLA	1	0
22	G	216	LHG	1	0
20	H	204	CLA	2	0
22	P	201	LHG	1	0
20	A	831	CLA	2	0
20	A	847	CLA	5	0

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

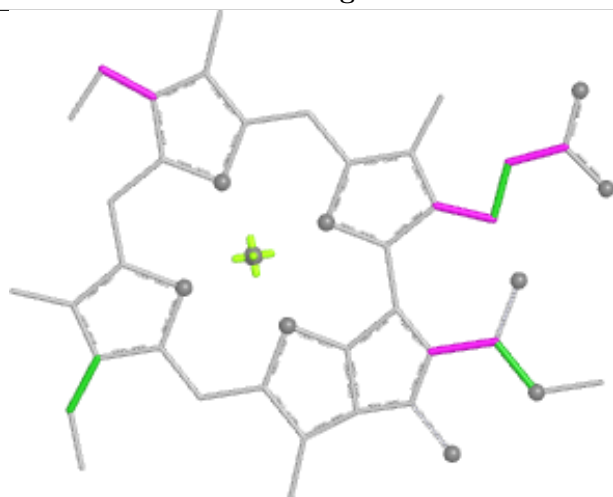
Ligand CLA G 203



Bond lengths



Bond angles

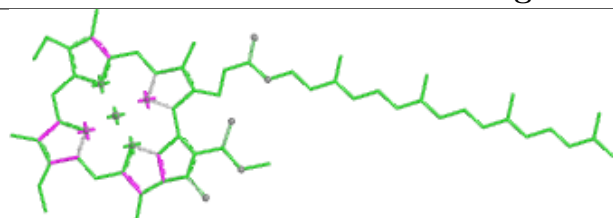


Torsions

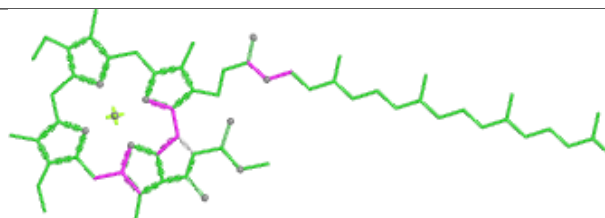


Rings

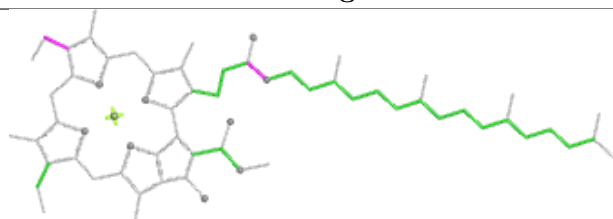
Ligand CLA B 824



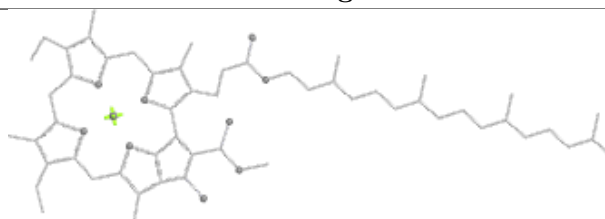
Bond lengths



Bond angles

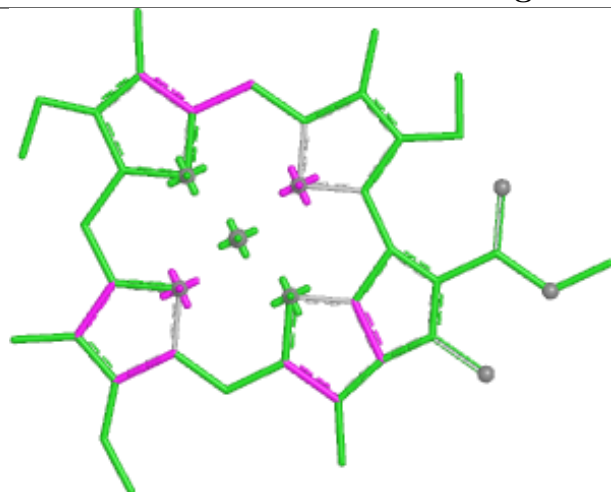


Torsions

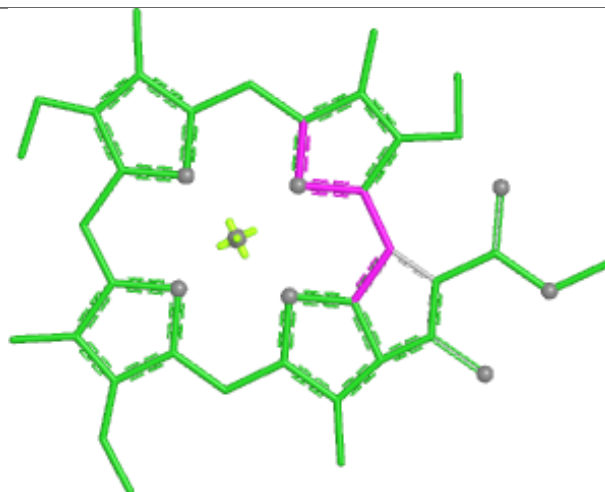


Rings

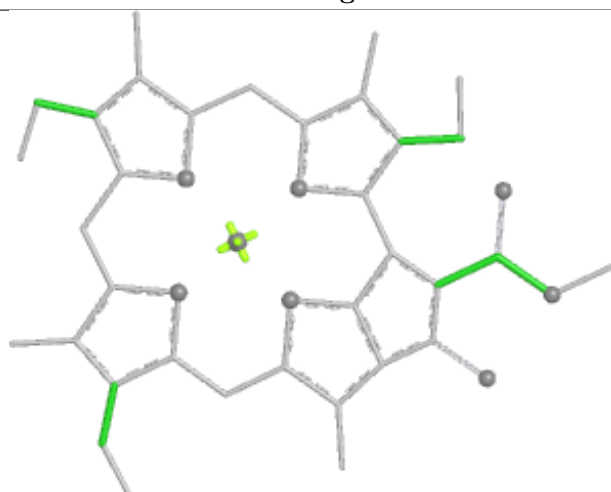
Ligand CLA T 201



Bond lengths



Bond angles

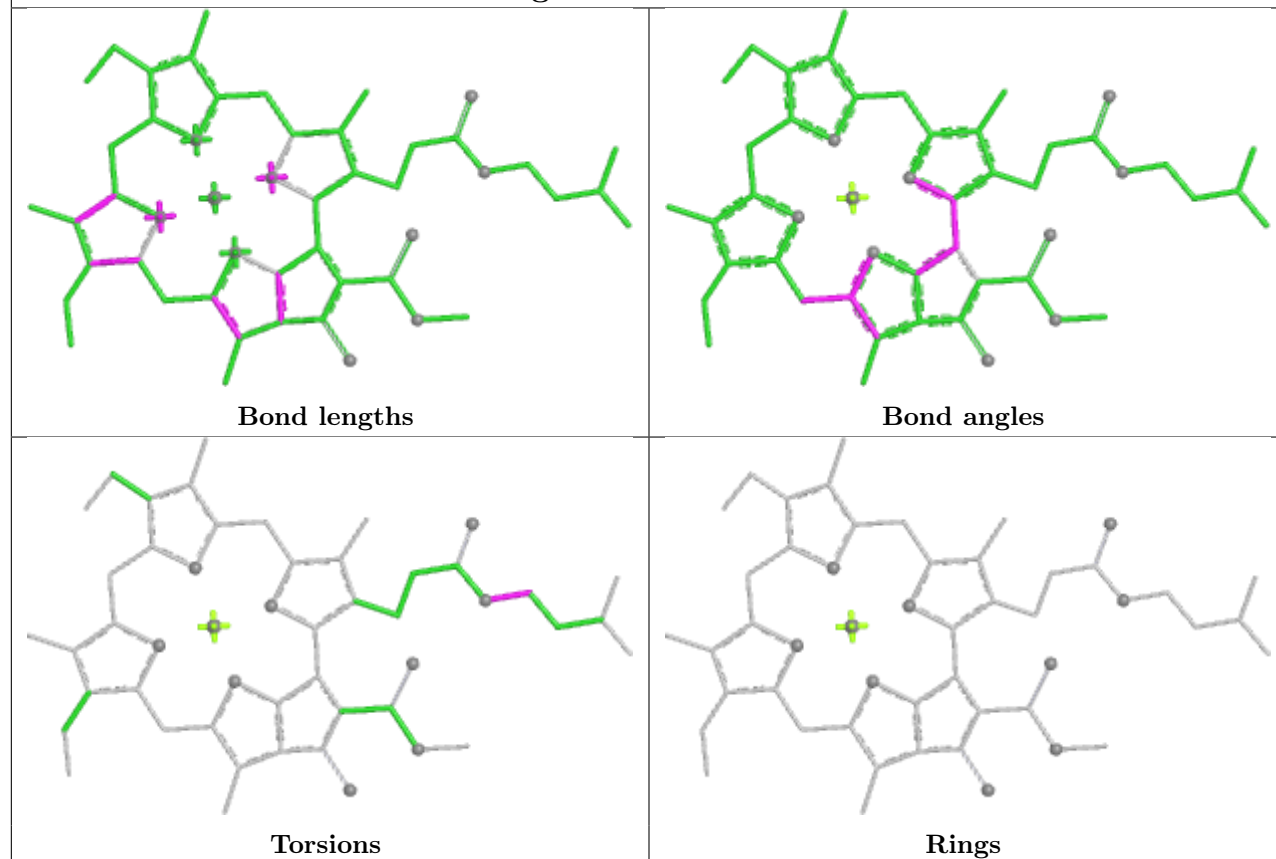


Torsions

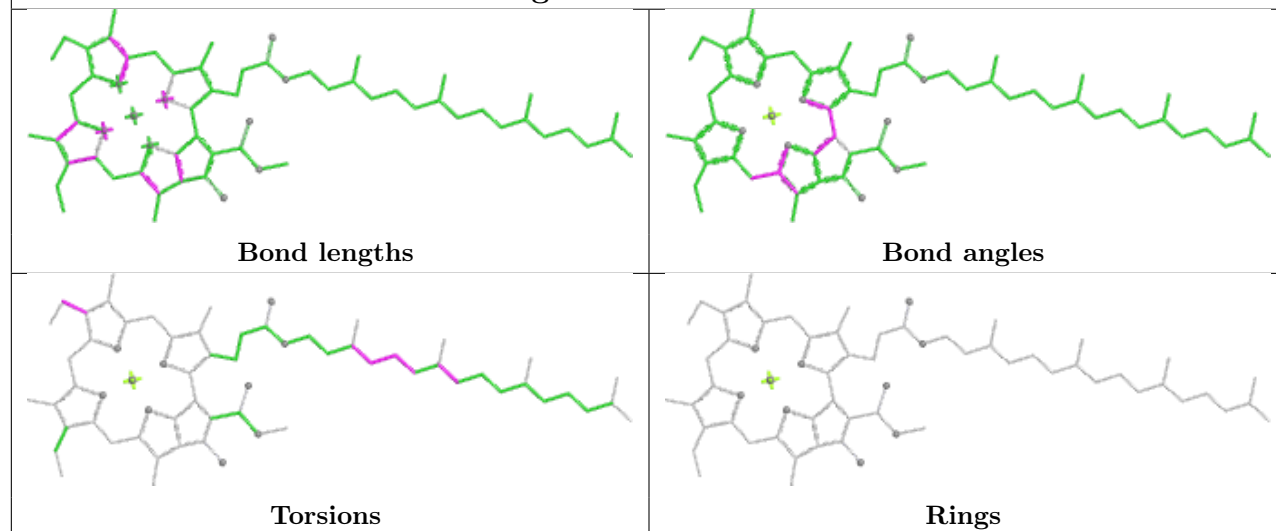


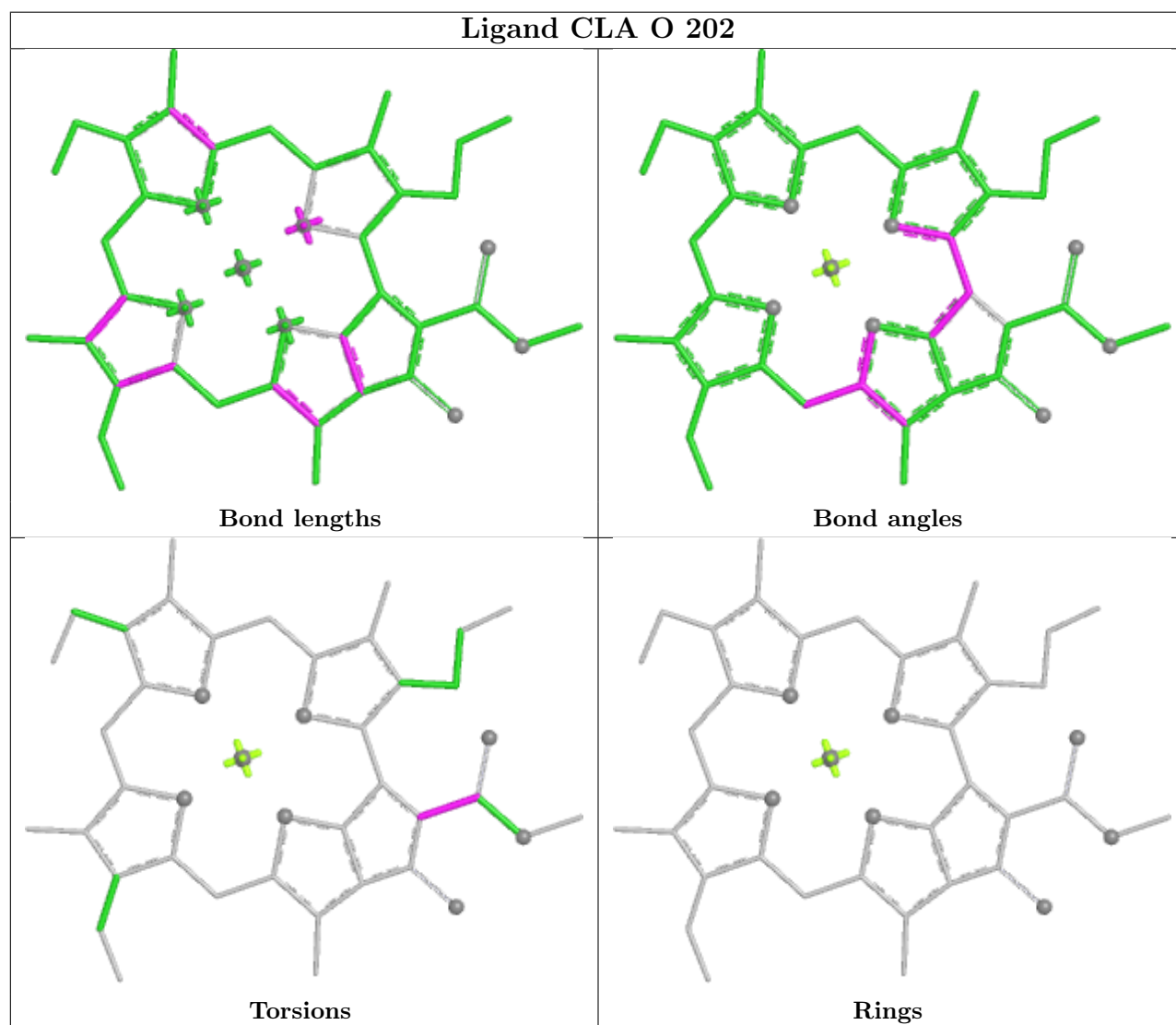
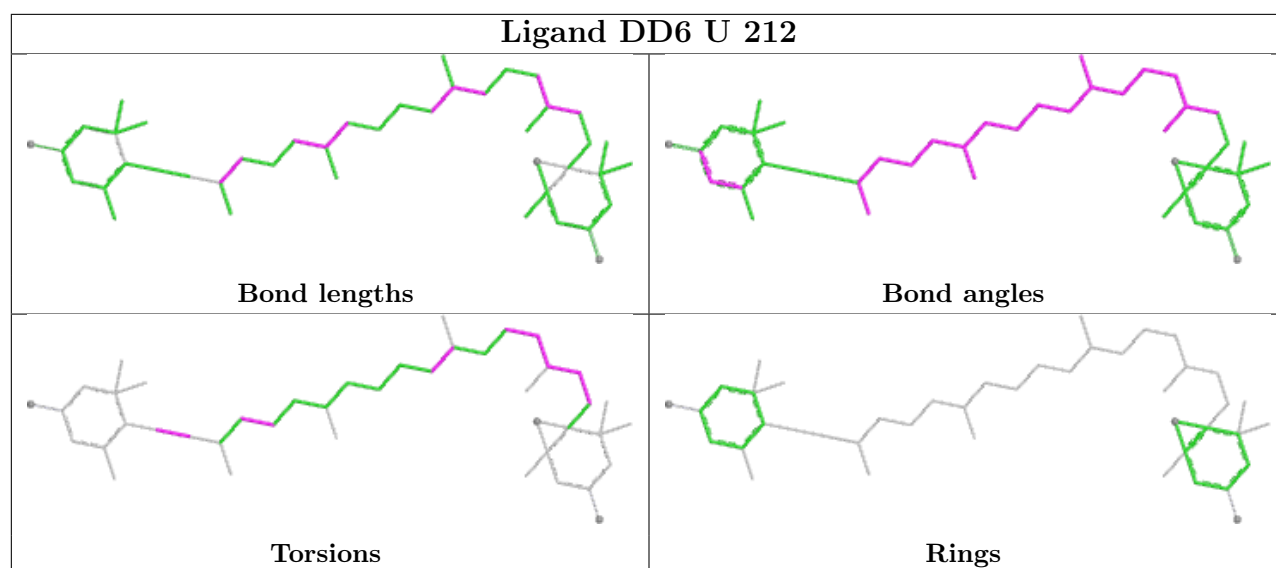
Rings

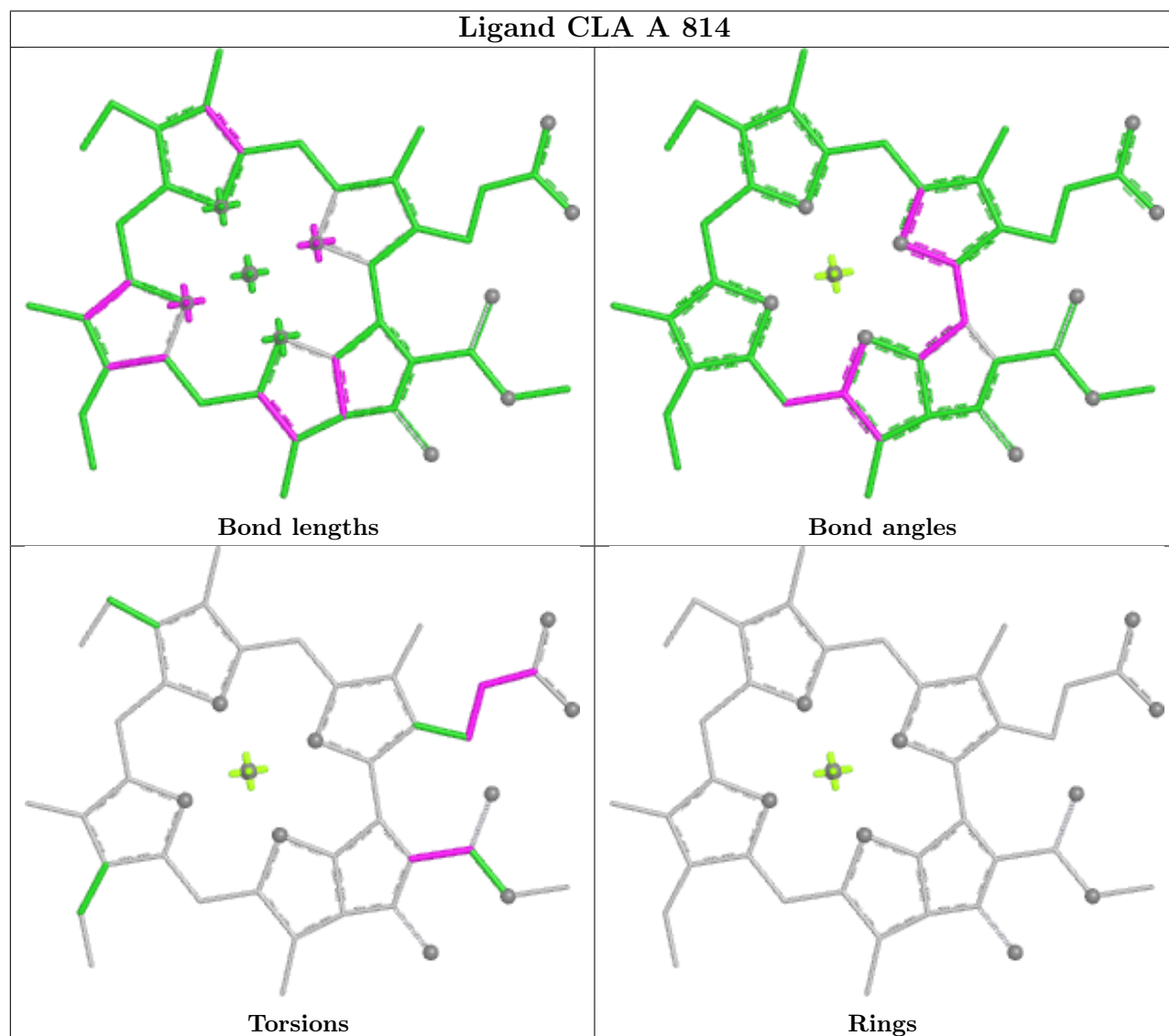
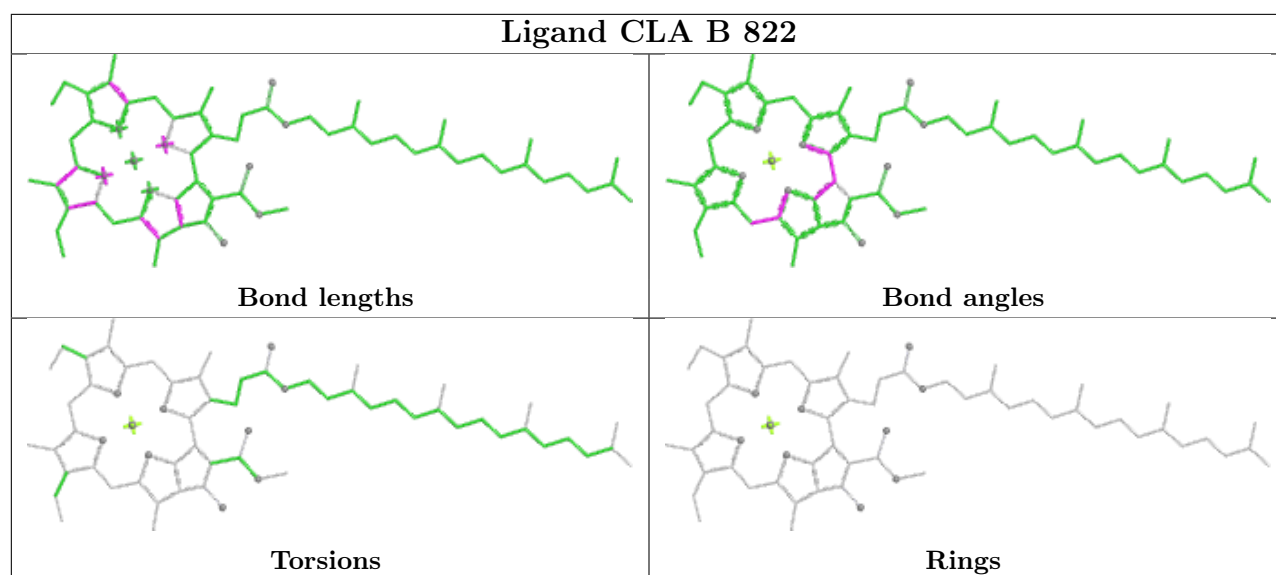
Ligand CLA A 830

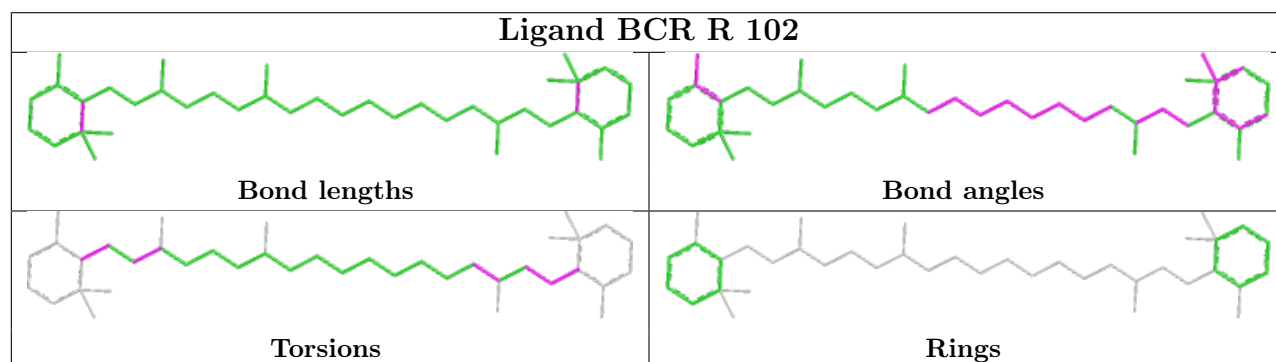
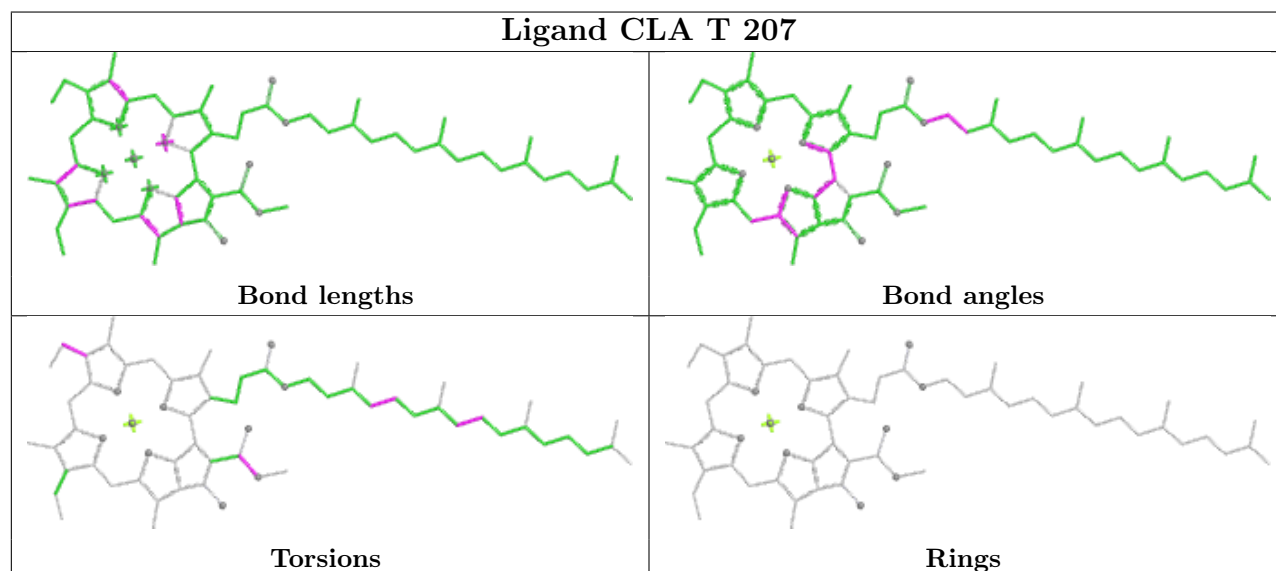
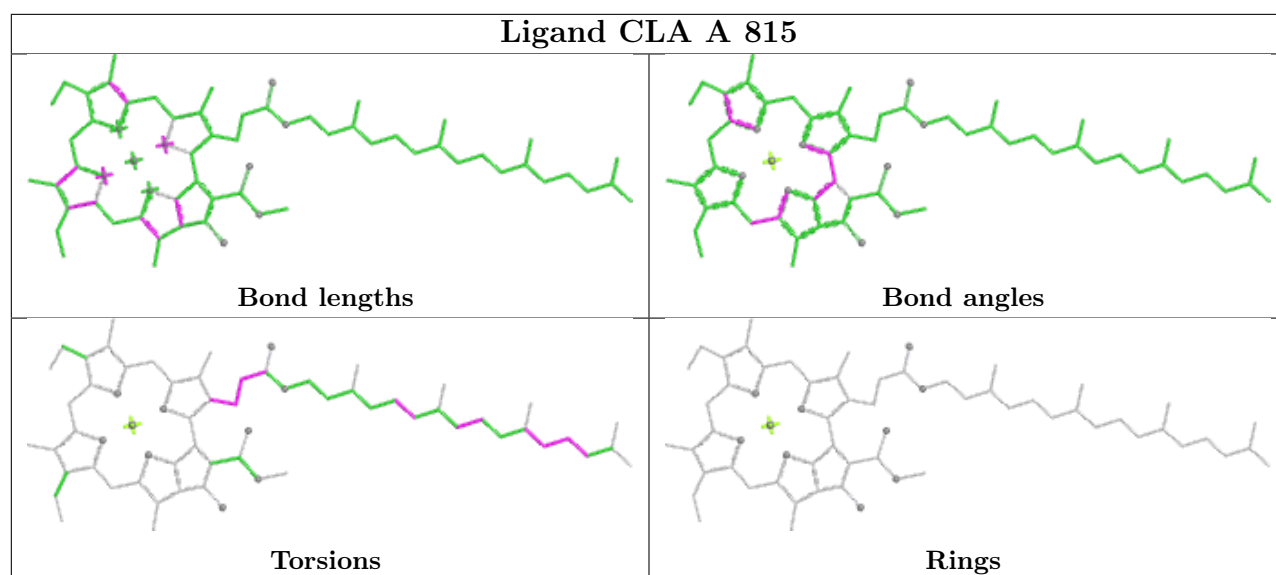


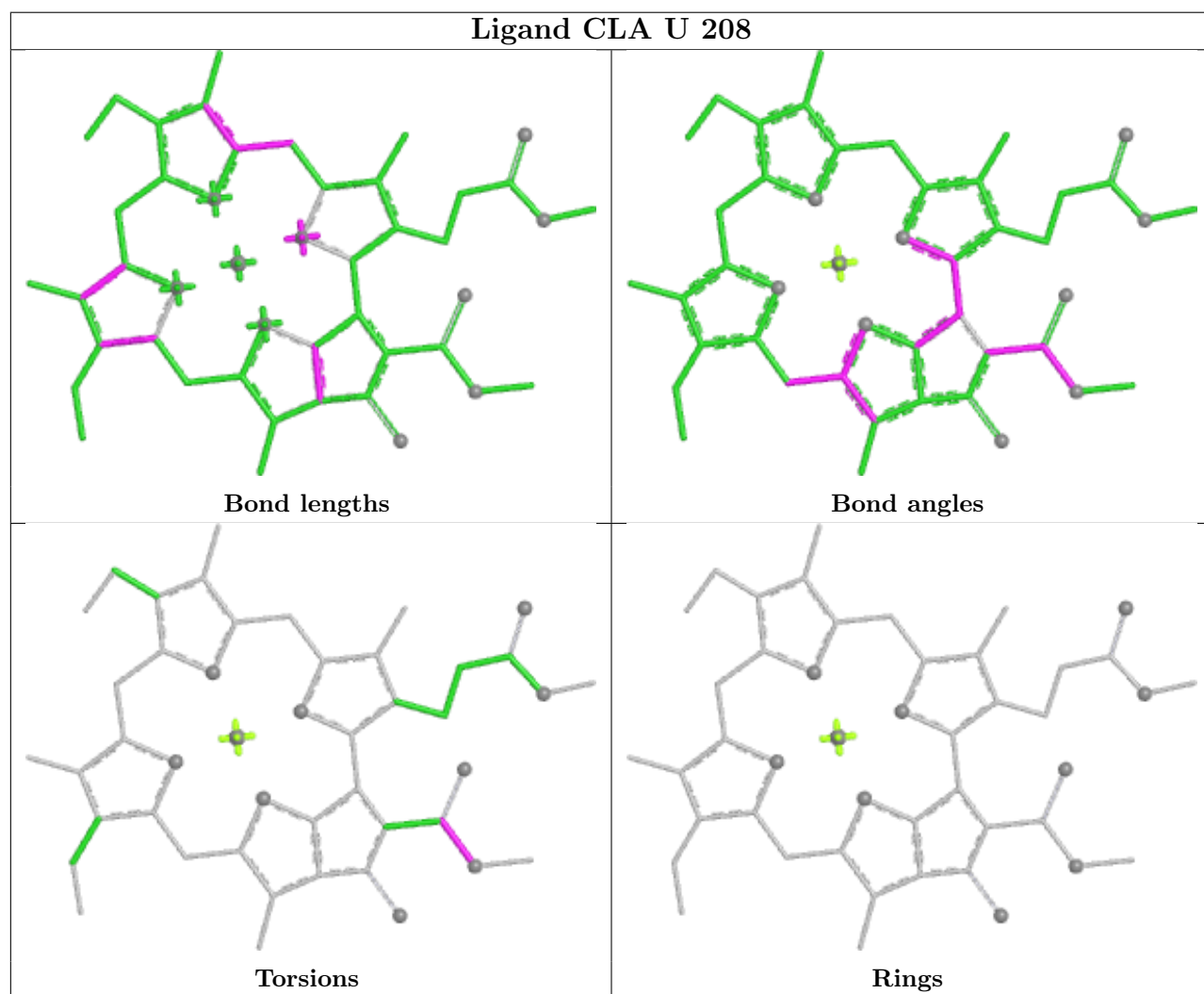
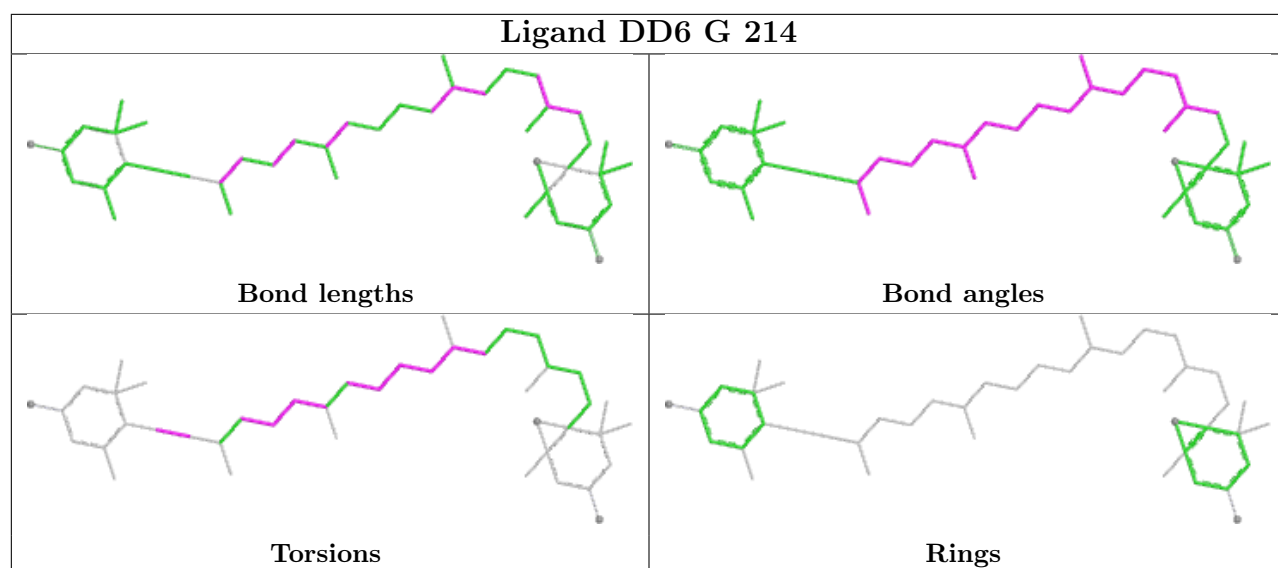
Ligand CLA A 852



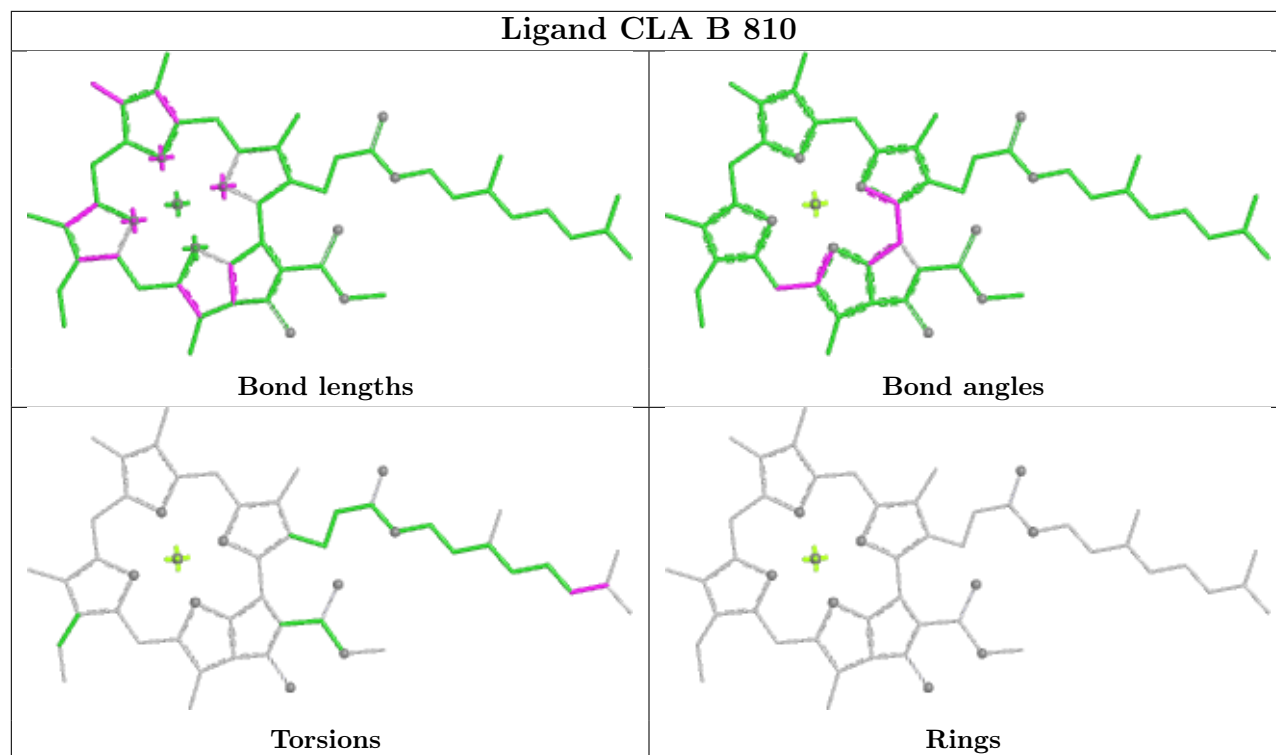




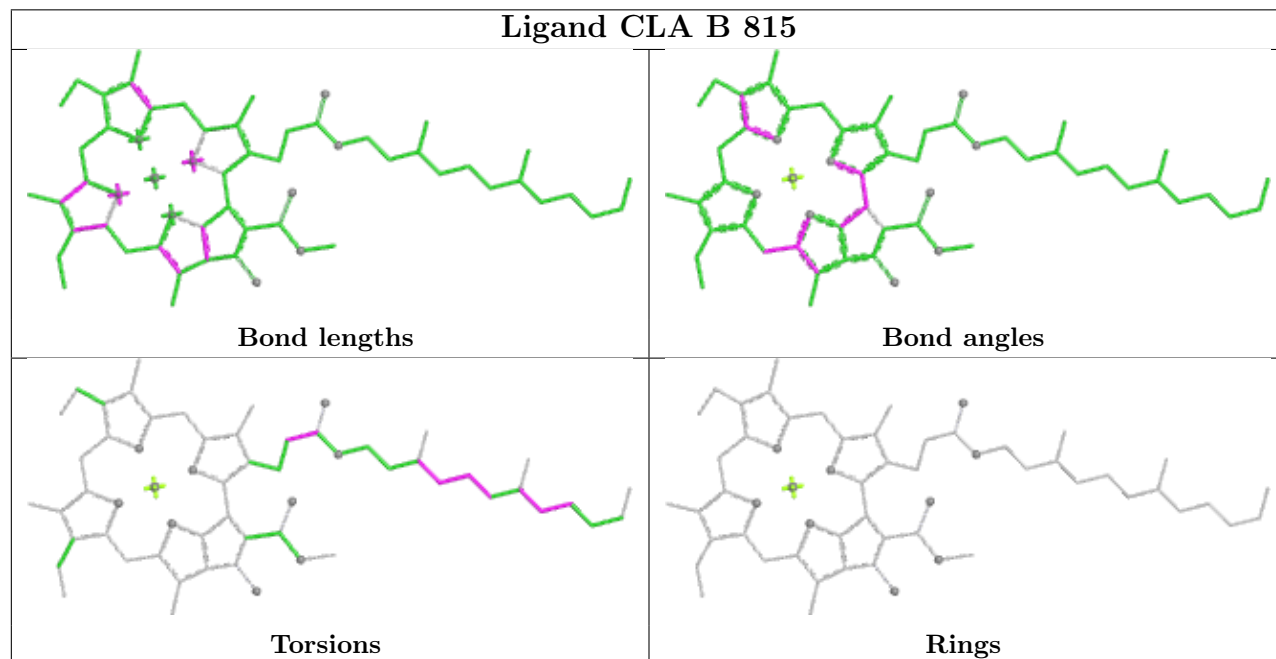


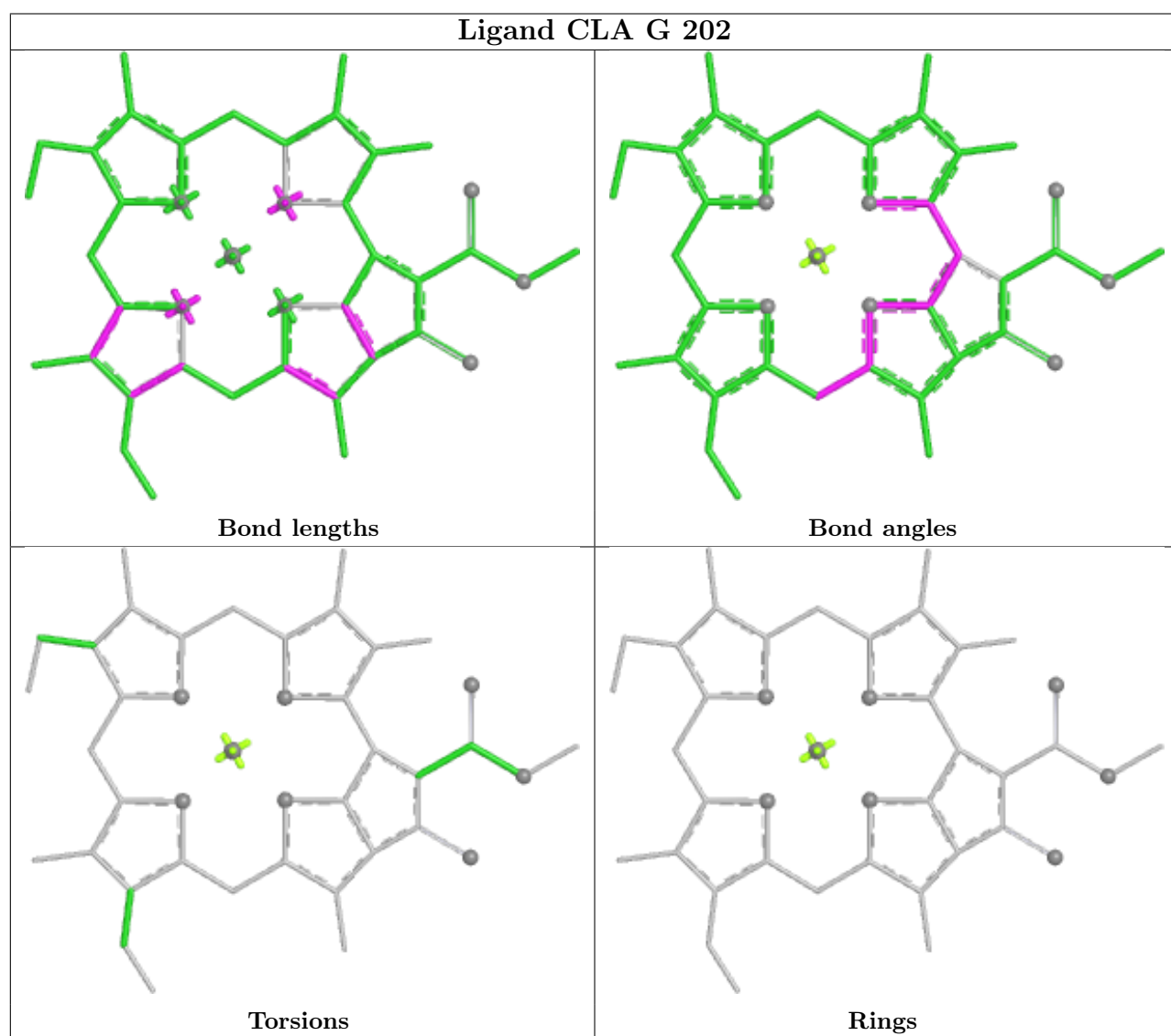
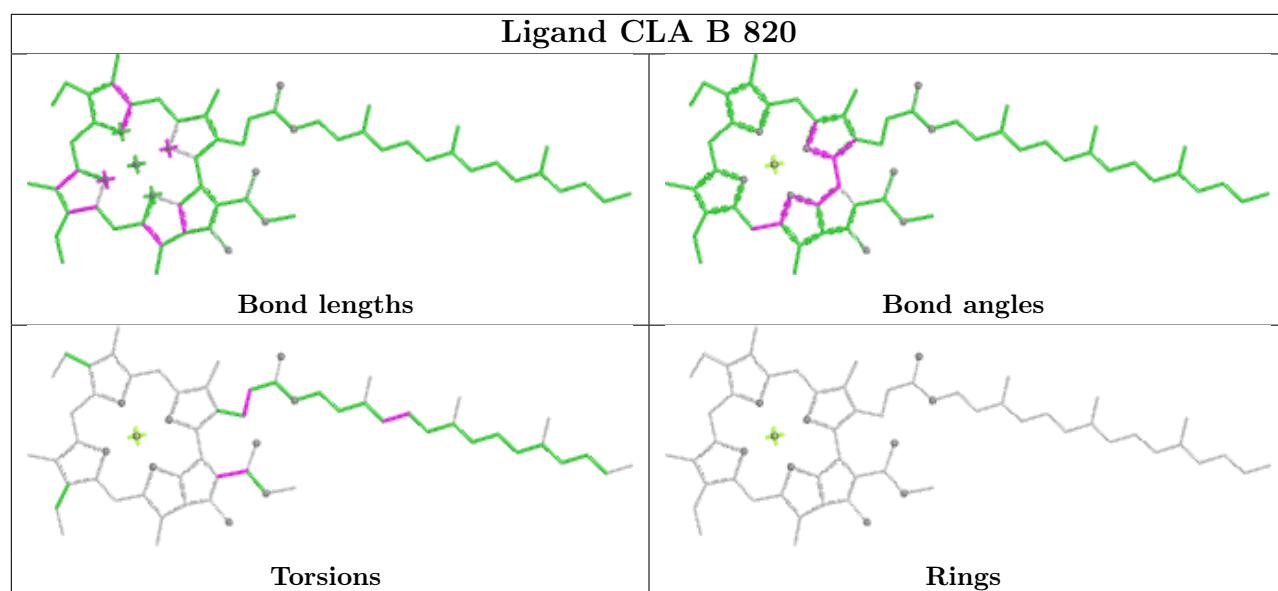


Ligand CLA B 810

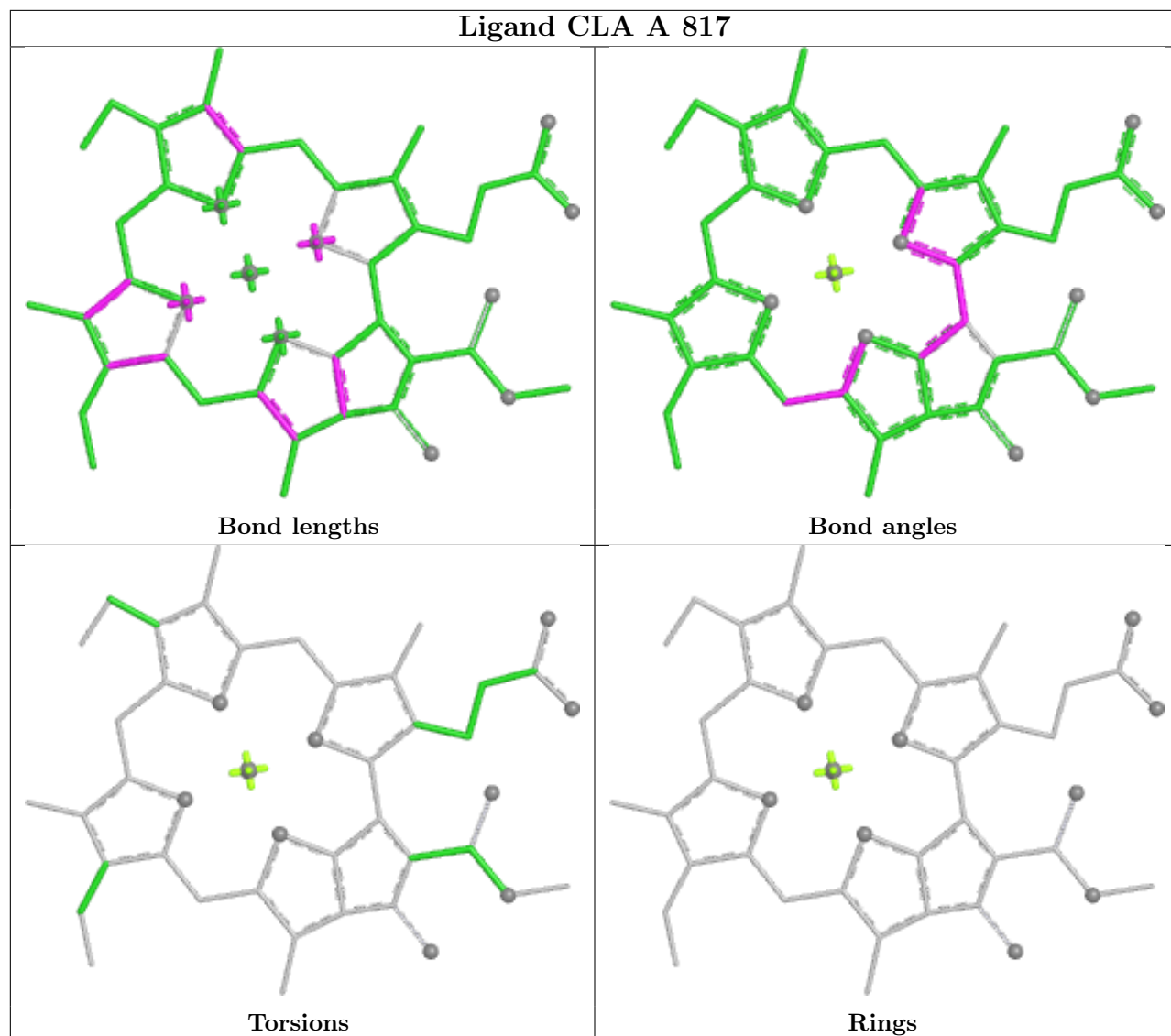


Ligand CLA B 815

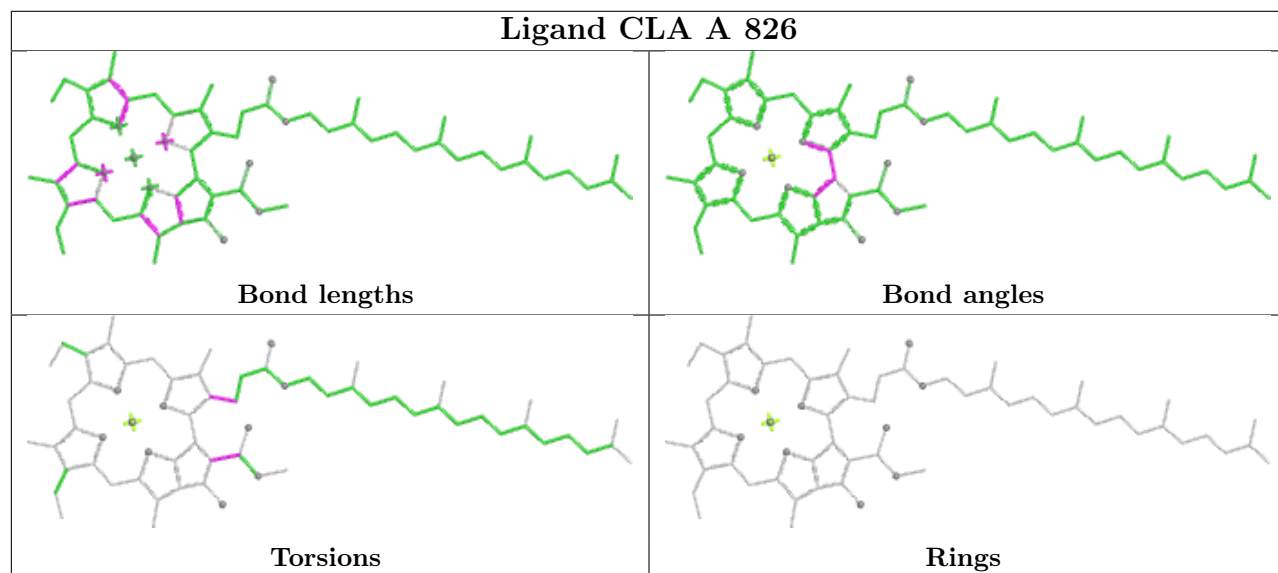


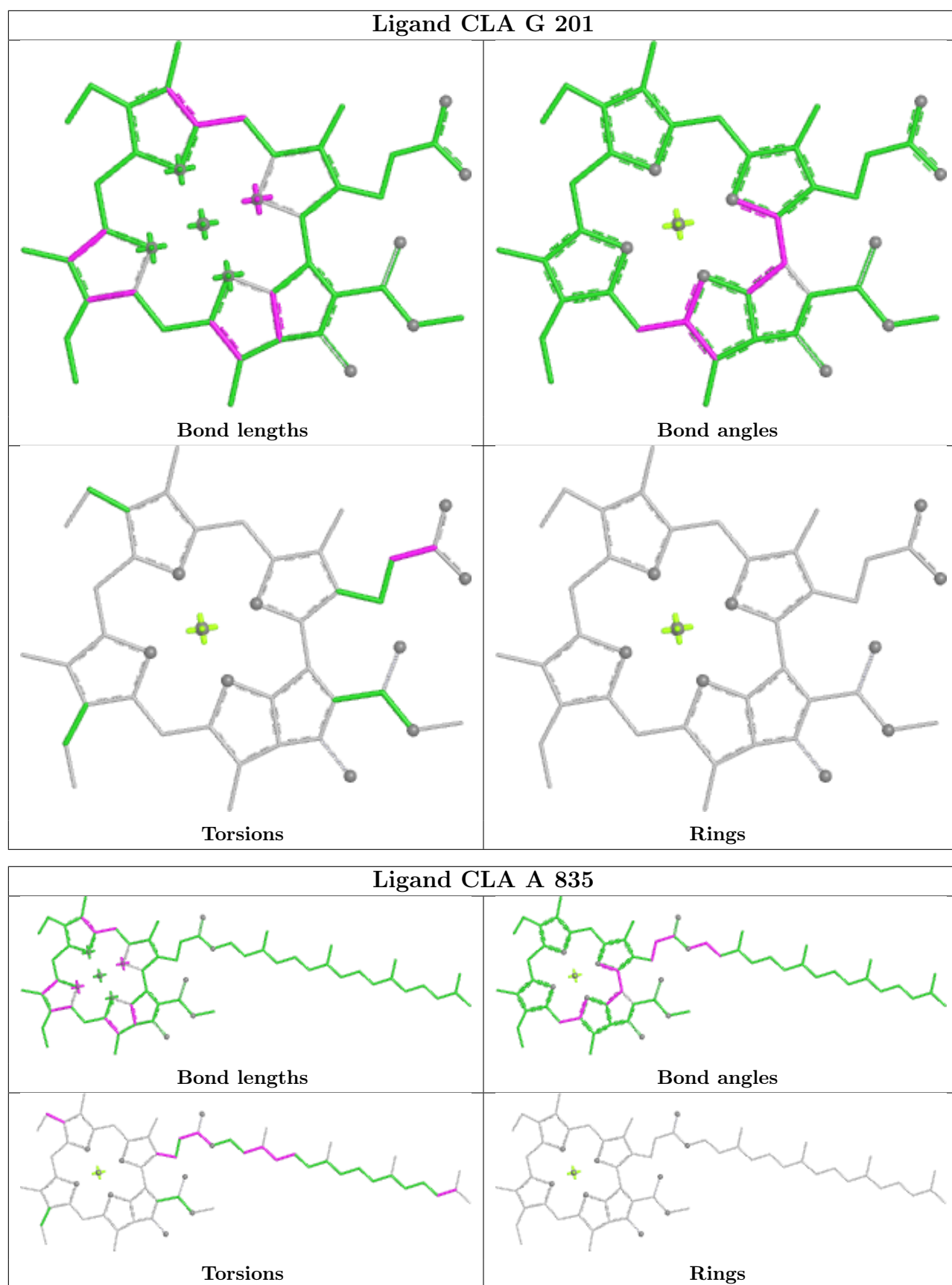


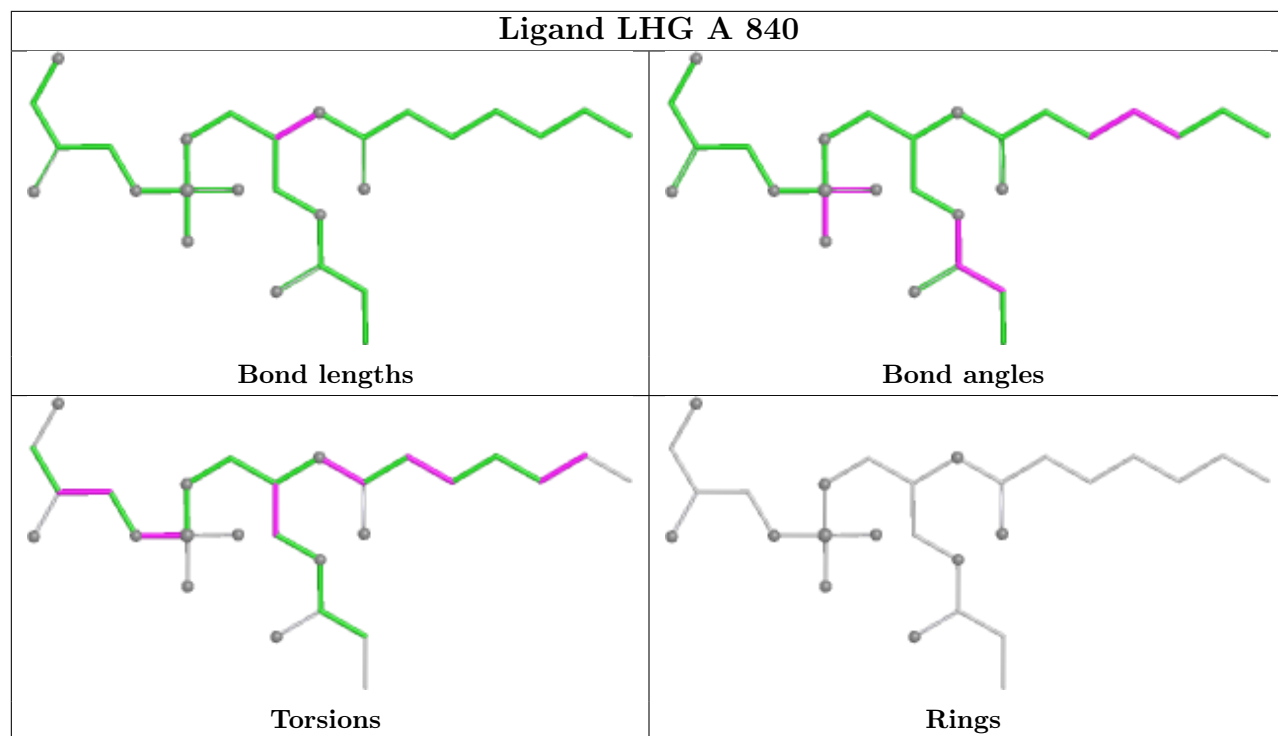
Ligand CLA A 817



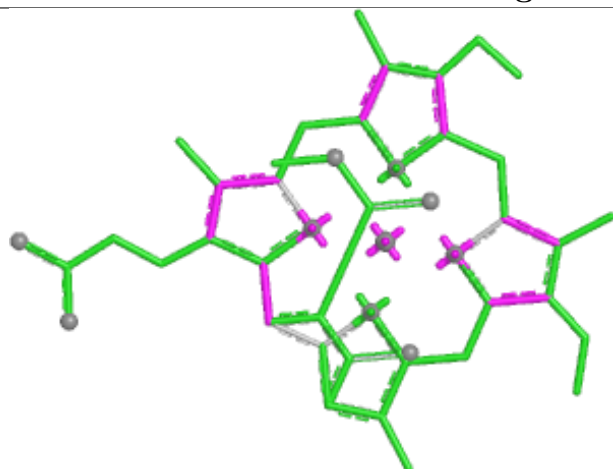
Ligand CLA A 826



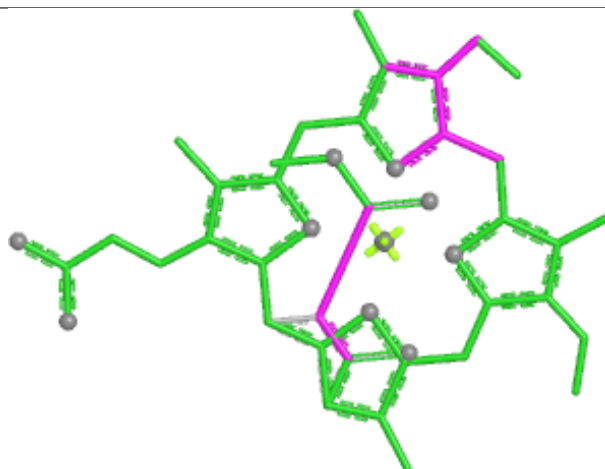




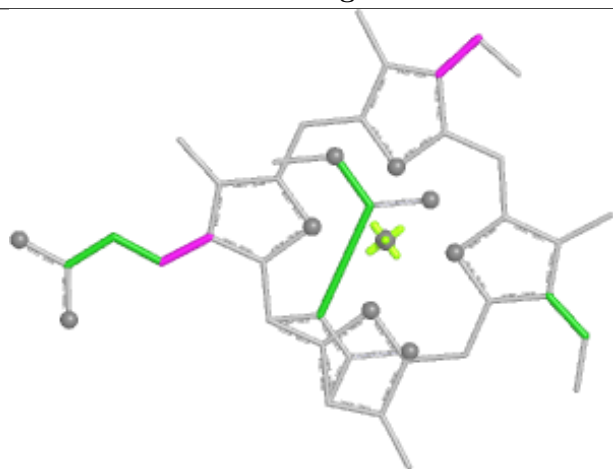
Ligand KC1 U 213



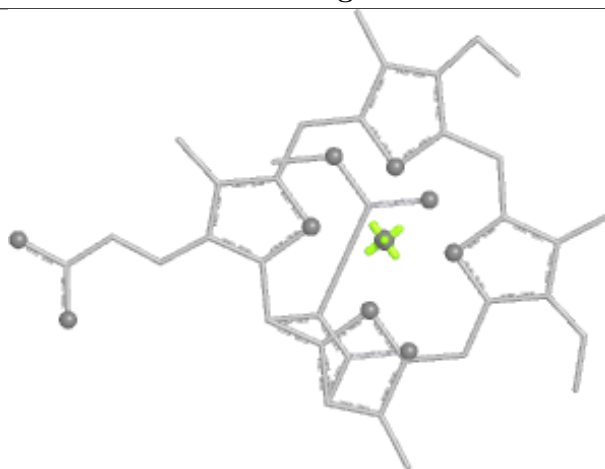
Bond lengths



Bond angles

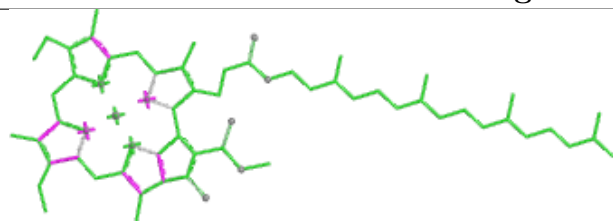


Torsions

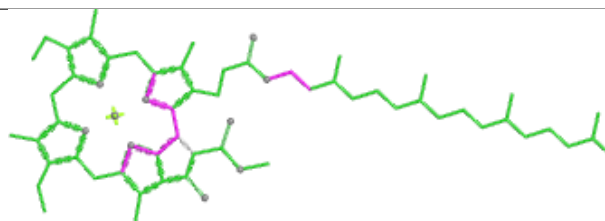


Rings

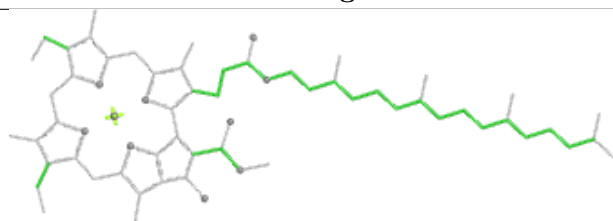
Ligand CLA B 835



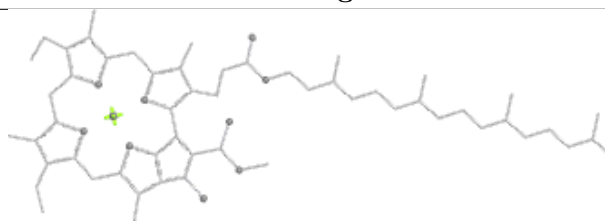
Bond lengths



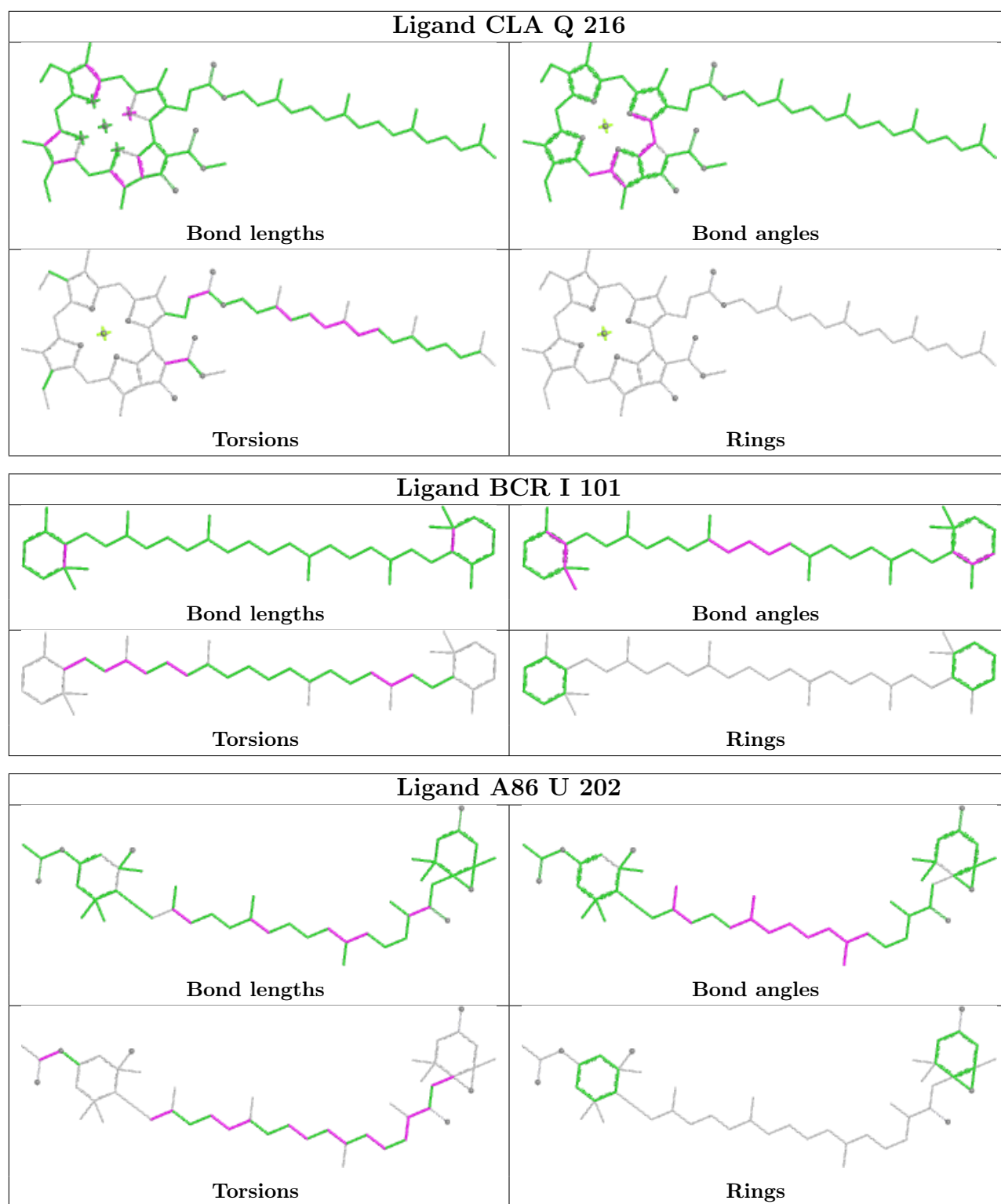
Bond angles

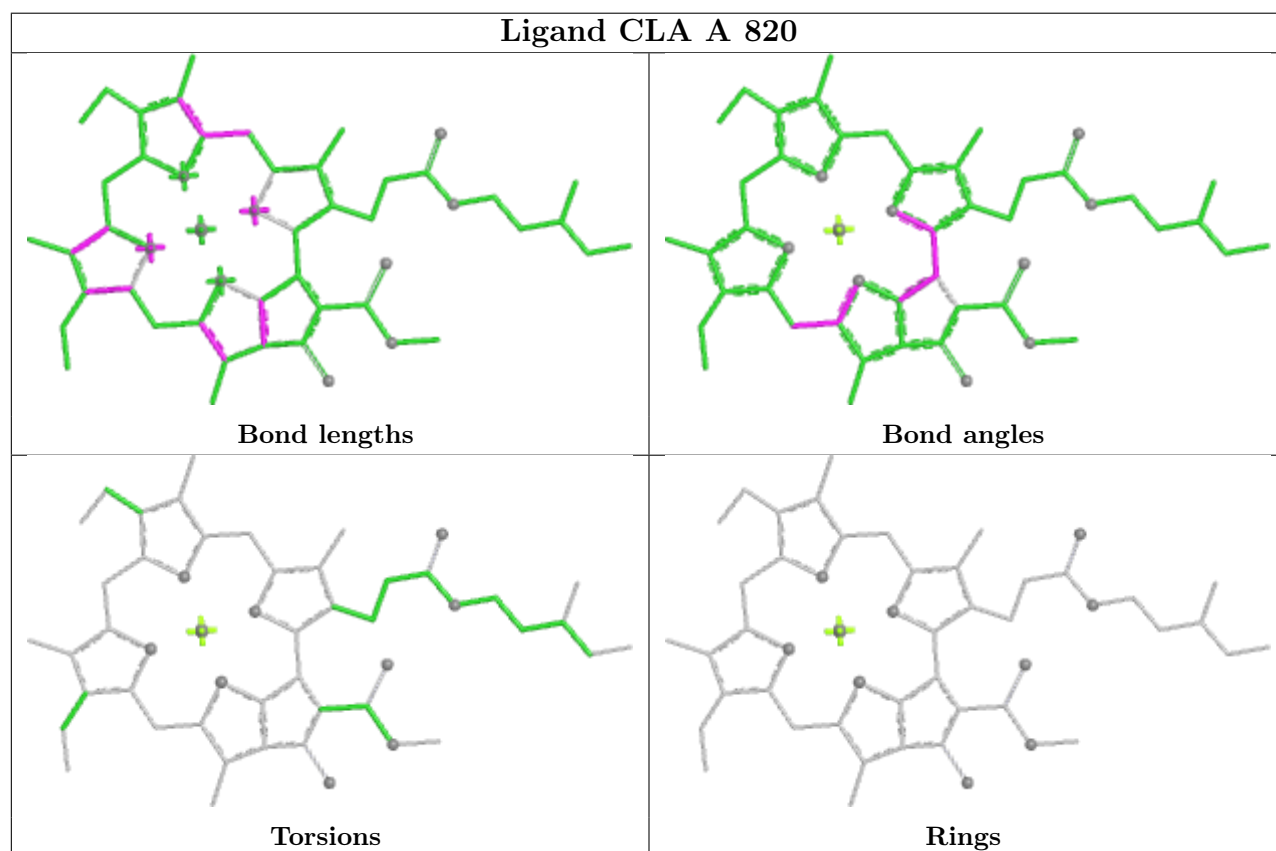
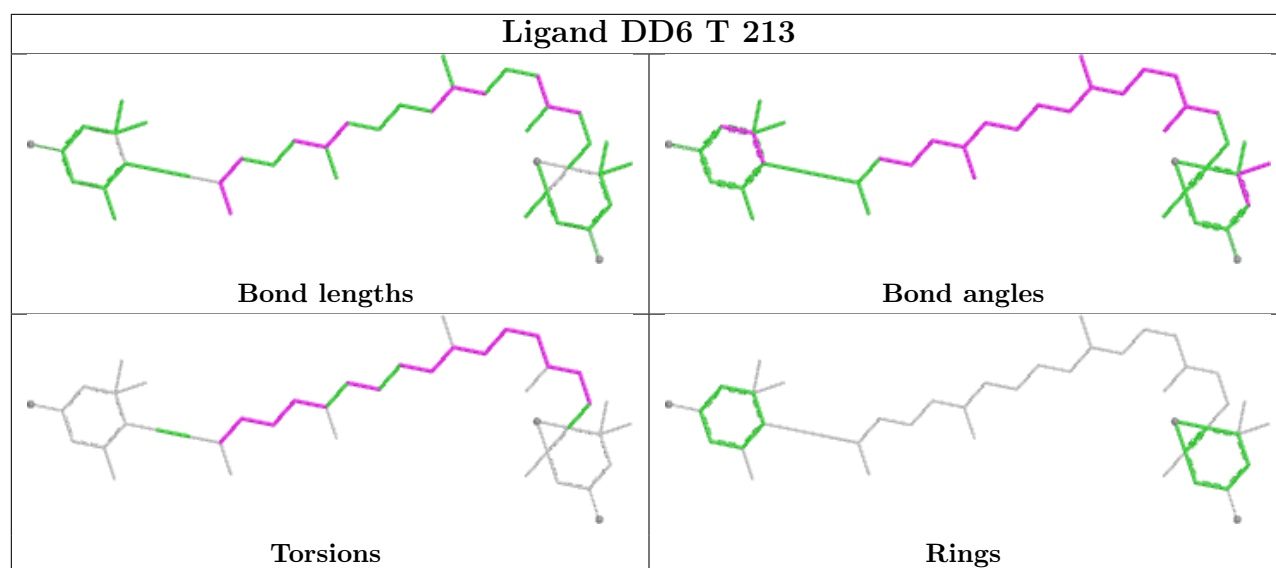


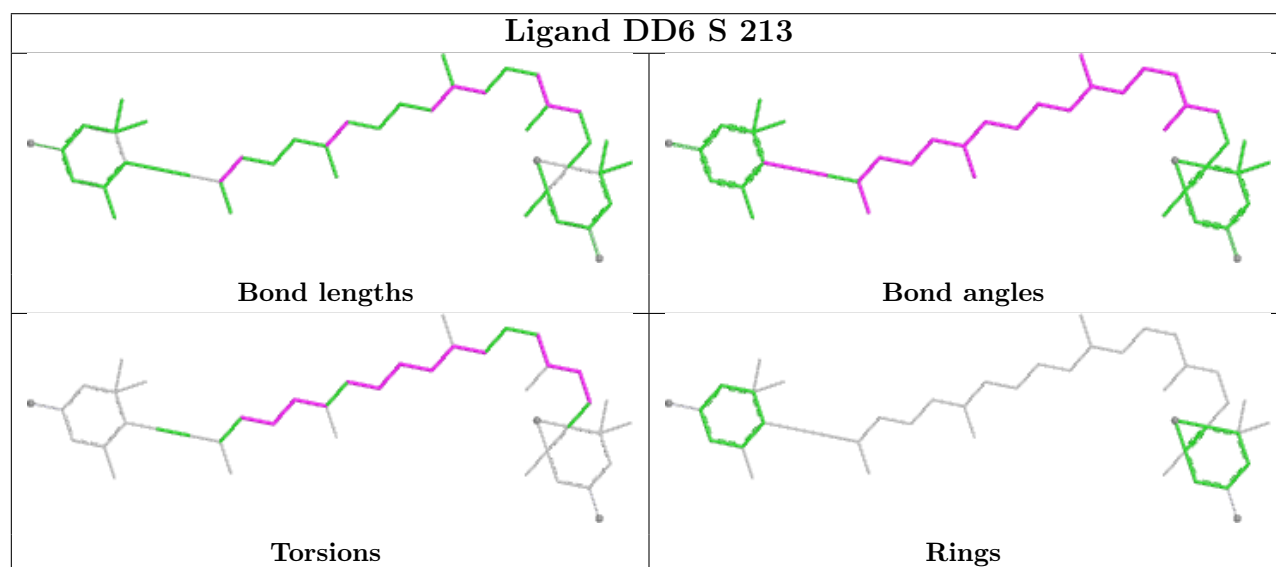
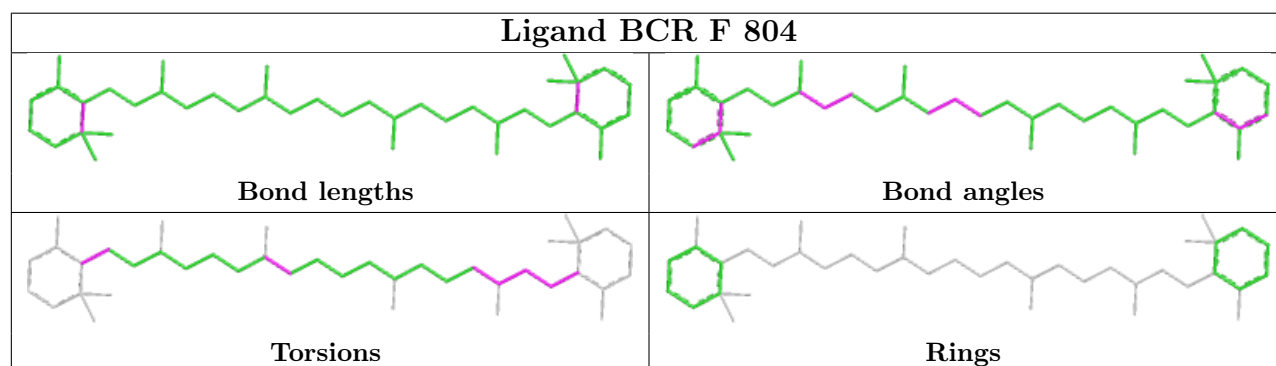
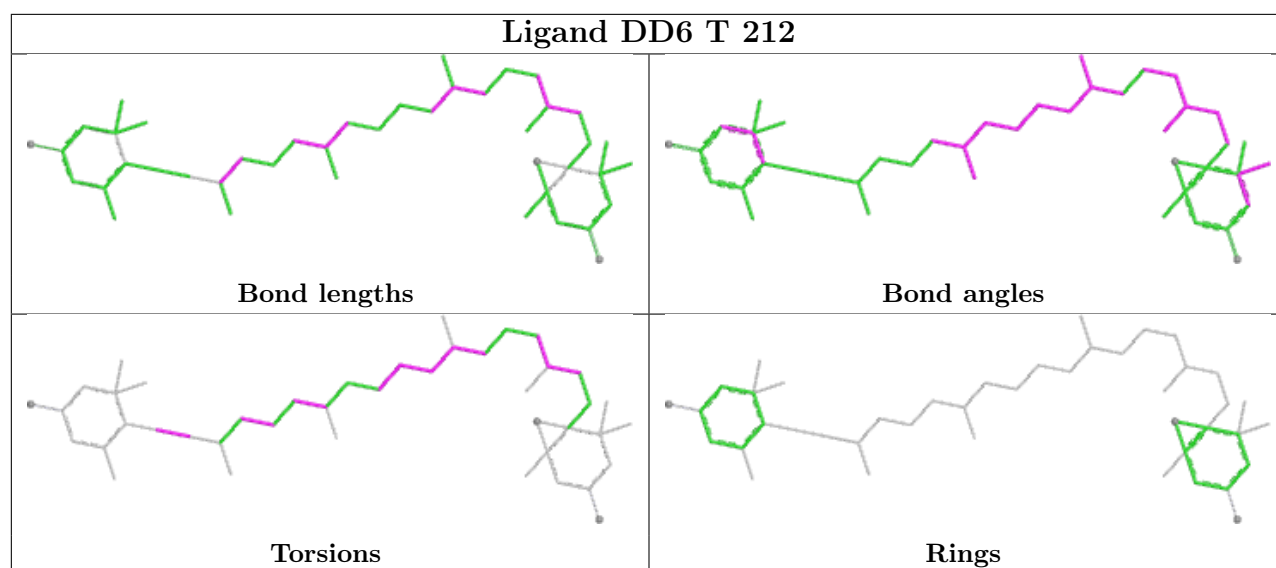
Torsions

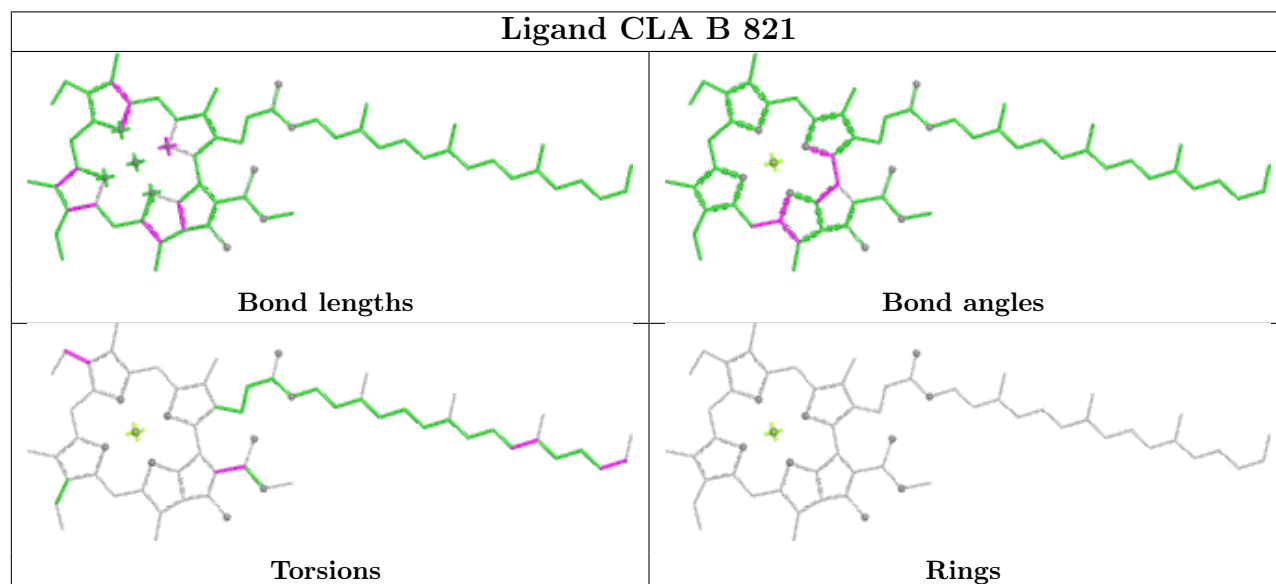
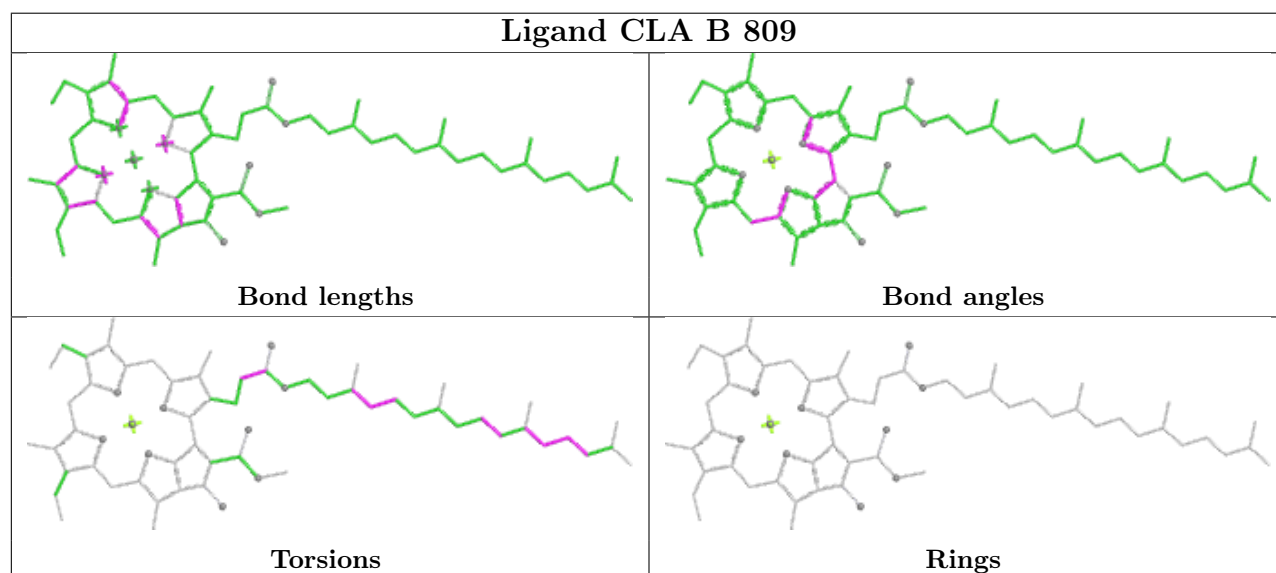
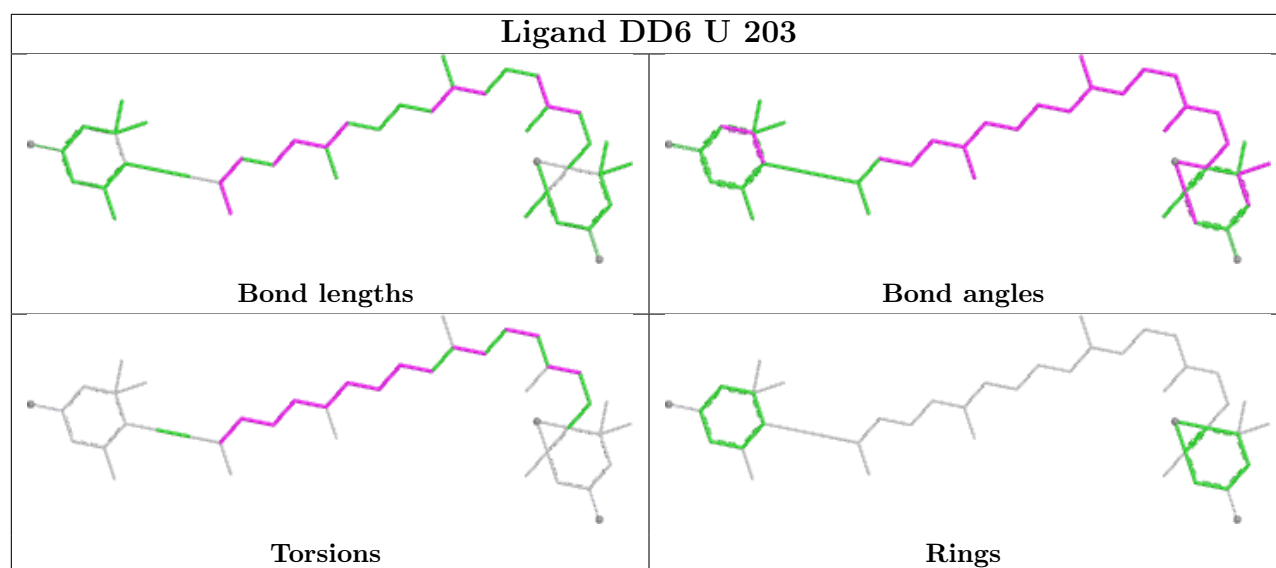


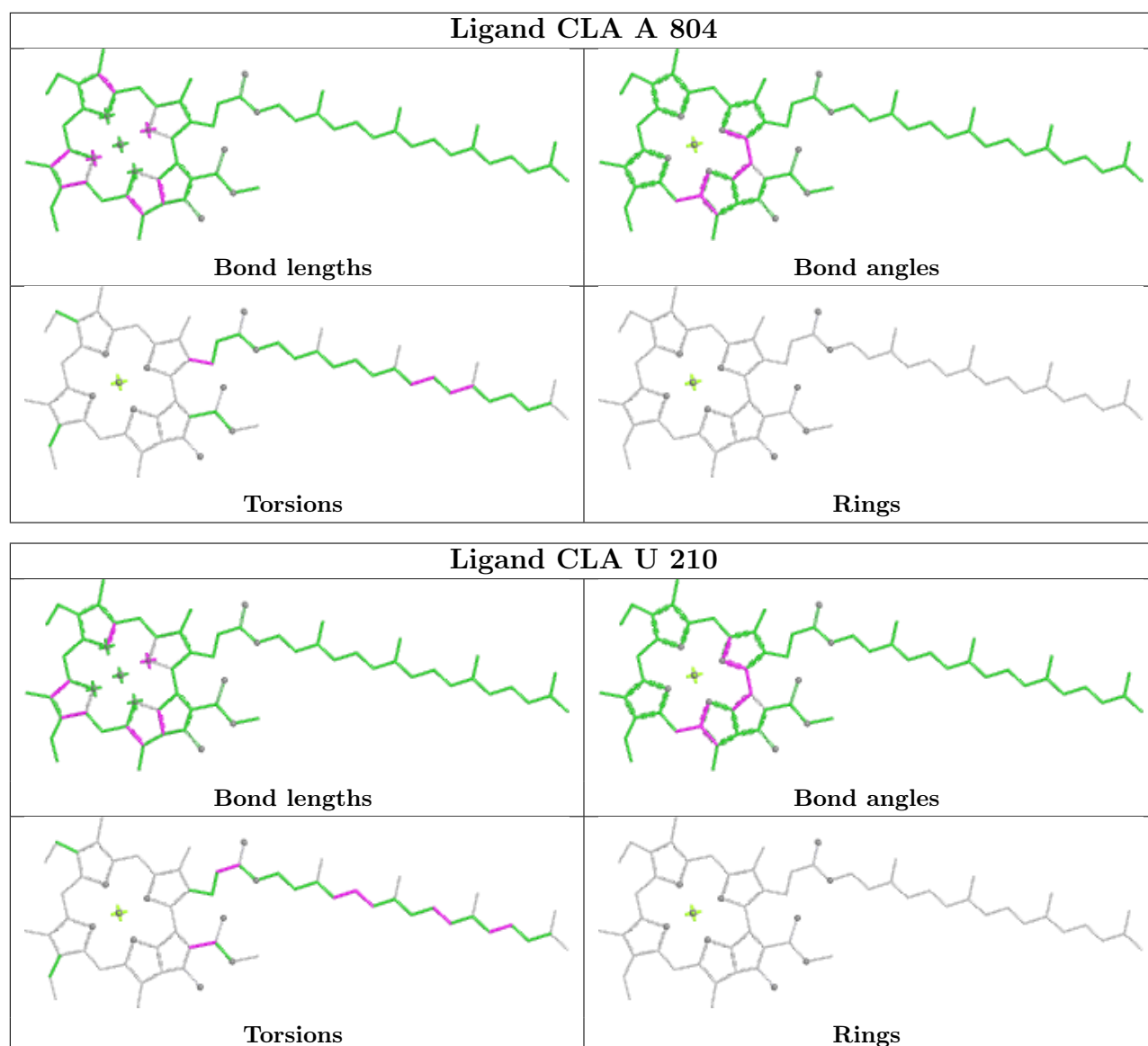
Rings



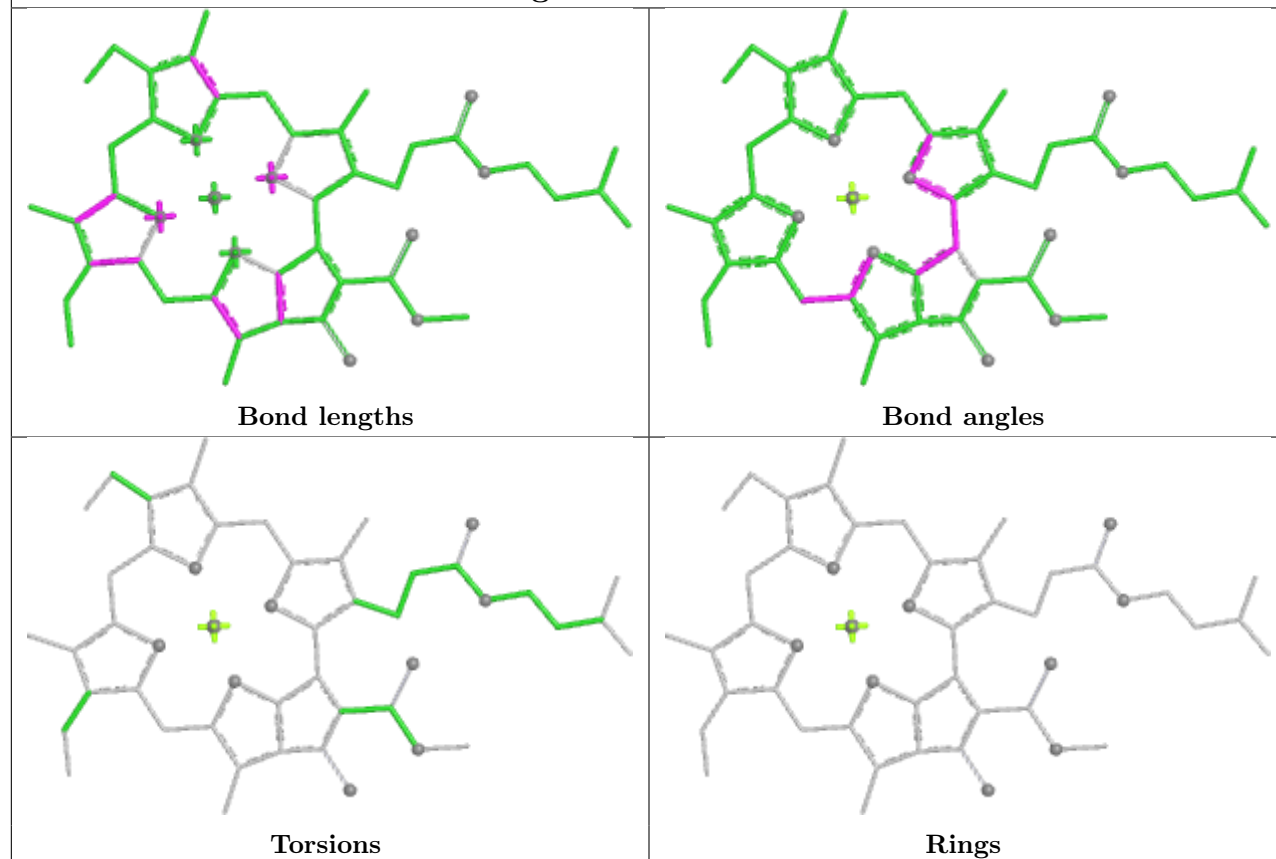




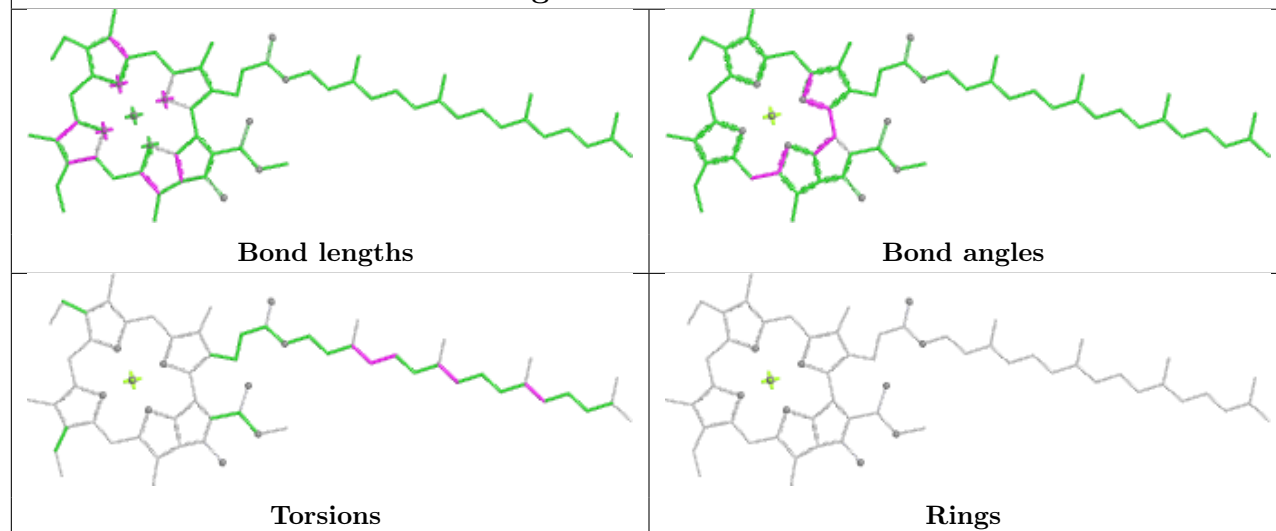




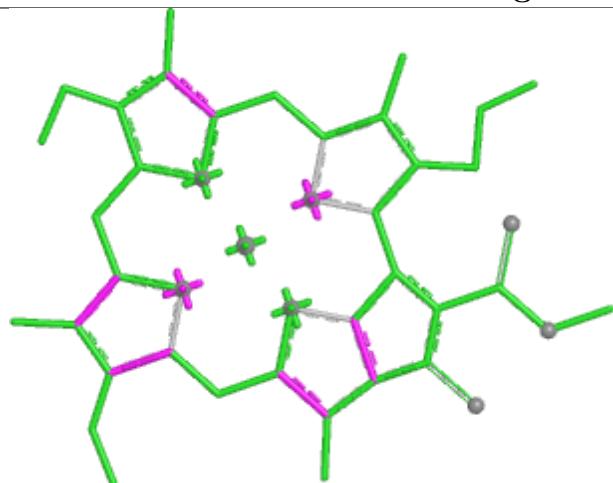
Ligand CLA A 813



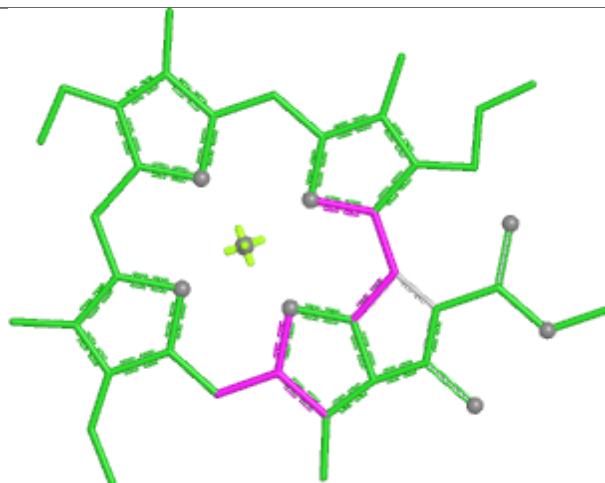
Ligand CLA A 834



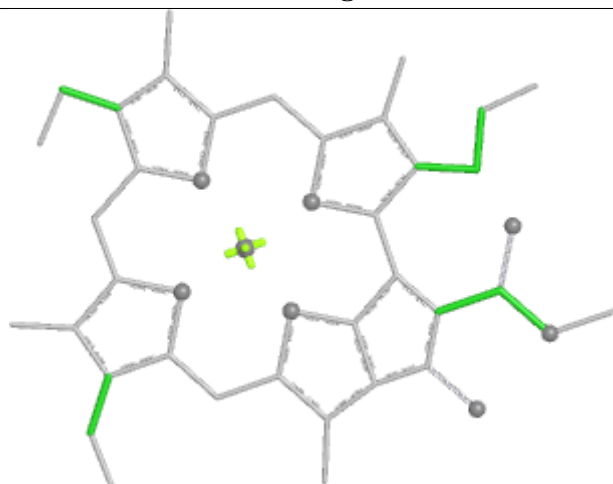
Ligand CLA A 819



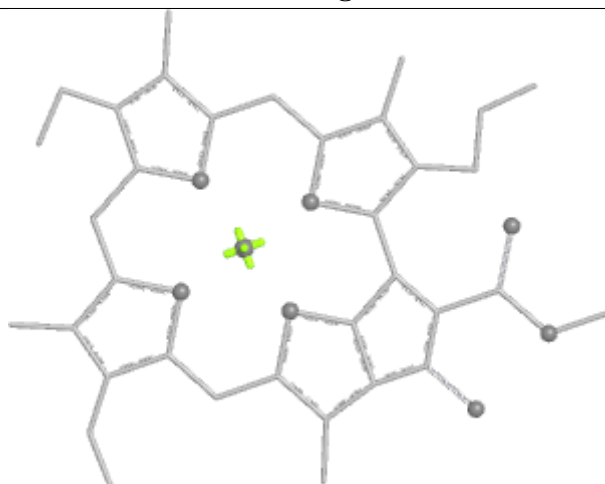
Bond lengths



Bond angles

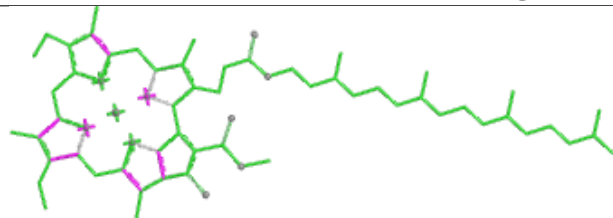


Torsions

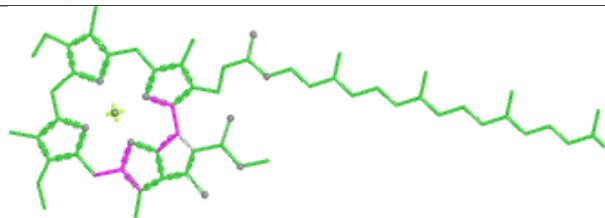


Rings

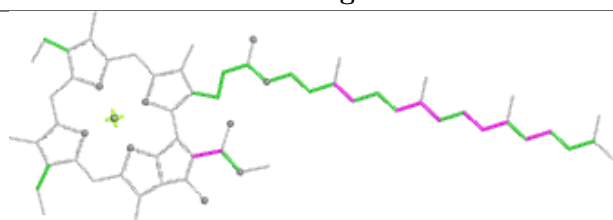
Ligand CLA Q 209



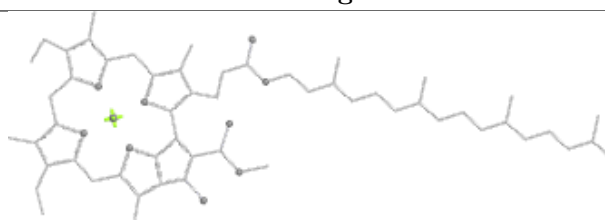
Bond lengths



Bond angles

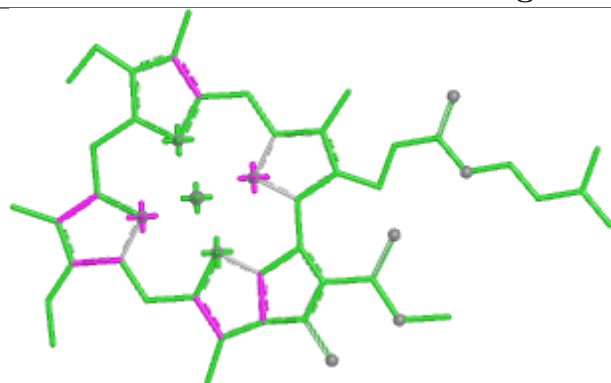


Torsions

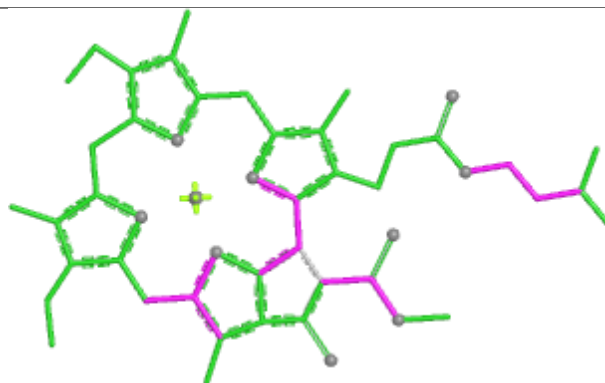


Rings

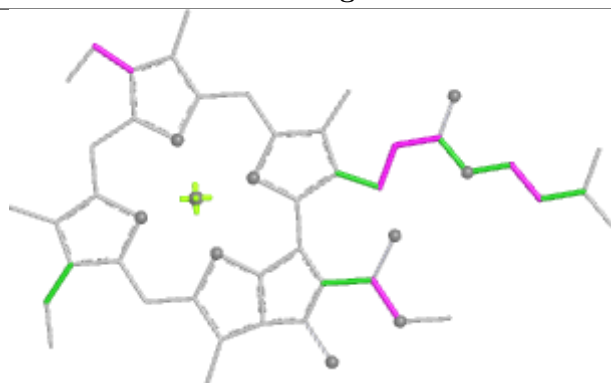
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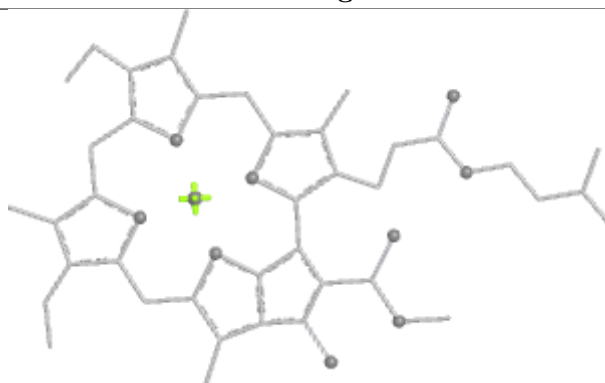
Bond lengths



Bond angles

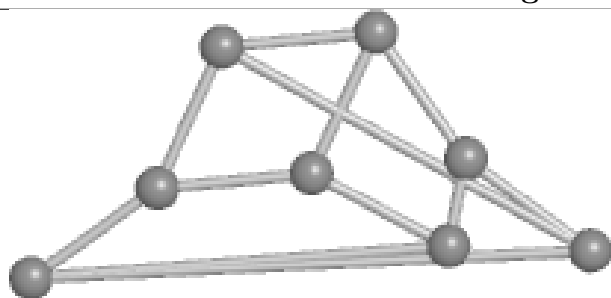


Torsions

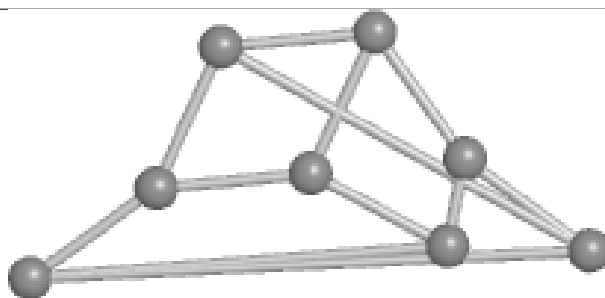


Rings

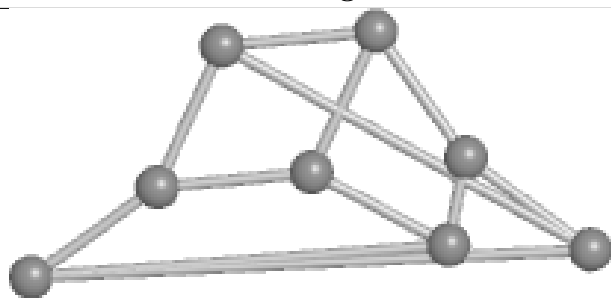
Ligand SF4 C 101



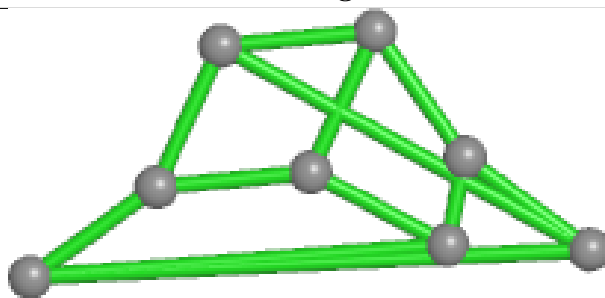
Bond lengths



Bond angles

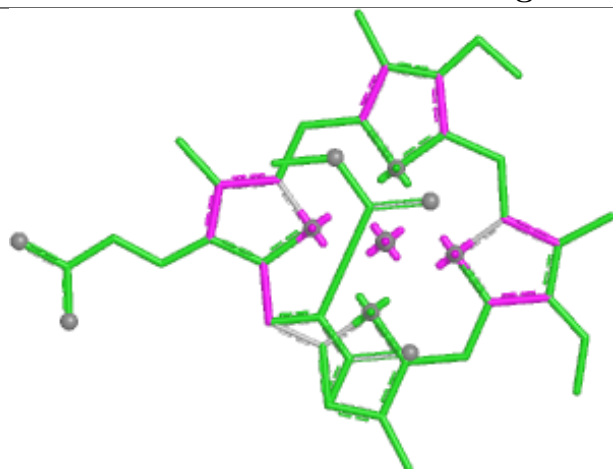


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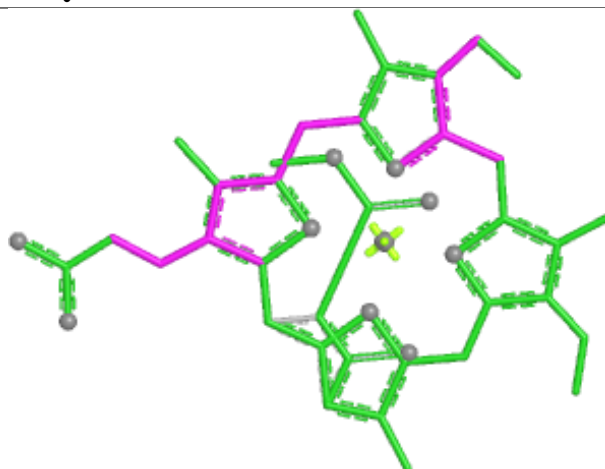


Rings

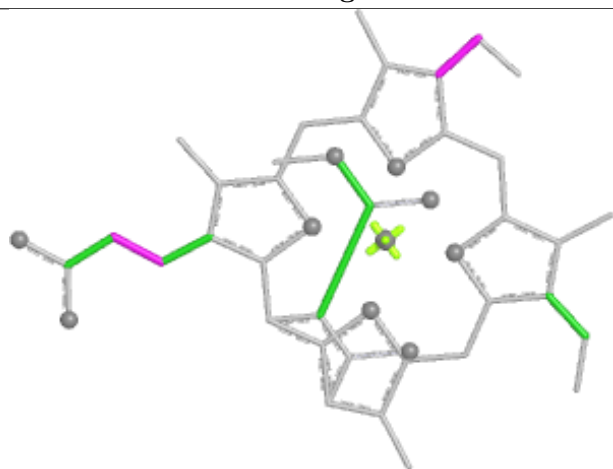
Ligand KC1 Q 210



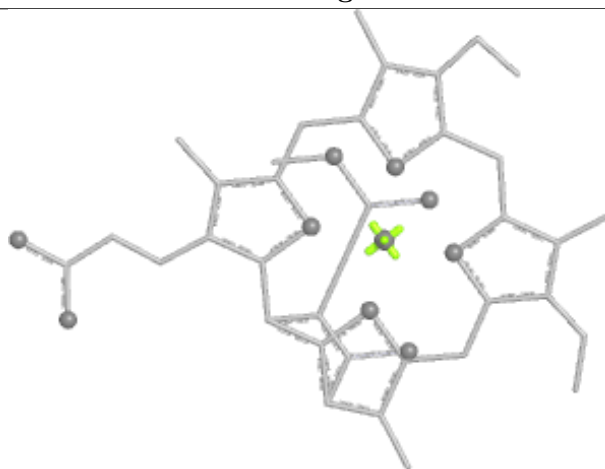
Bond lengths



Bond angles

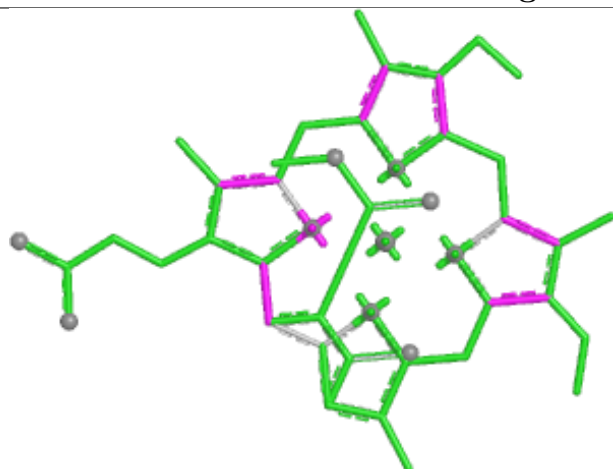


Torsions

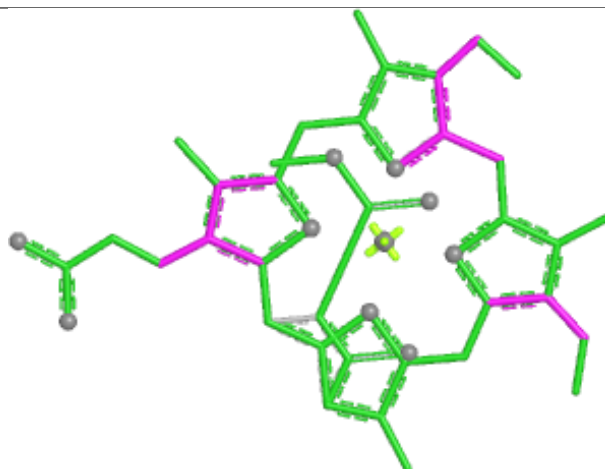


Rings

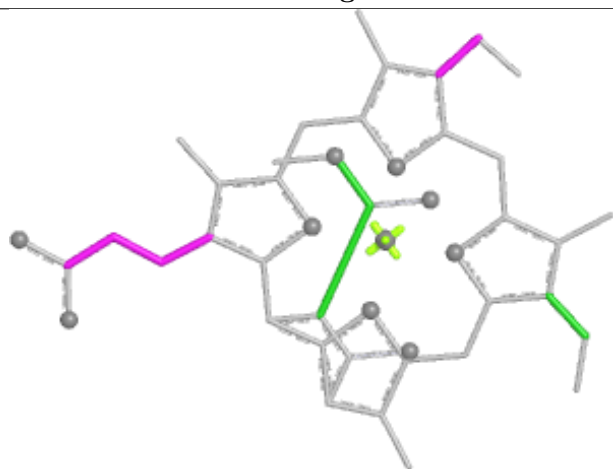
Ligand KC1 S 211



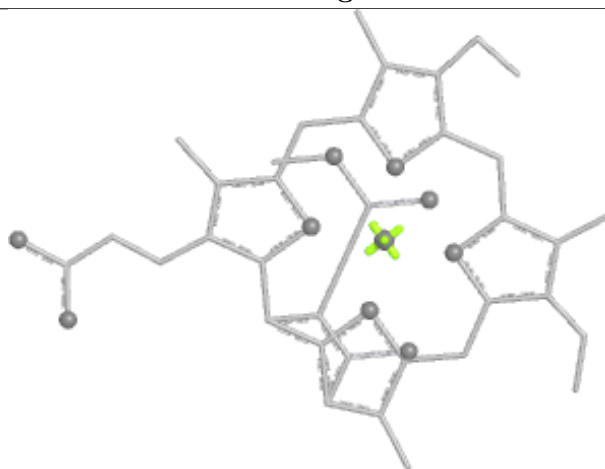
Bond lengths



Bond angles

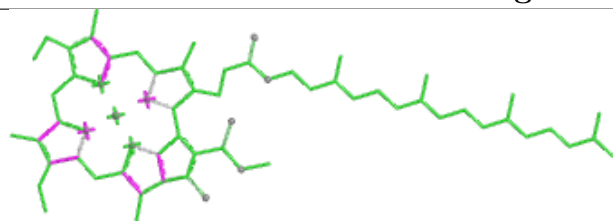


Torsions

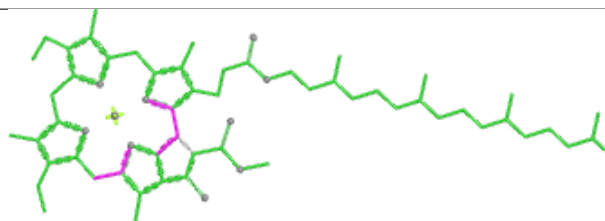


Rings

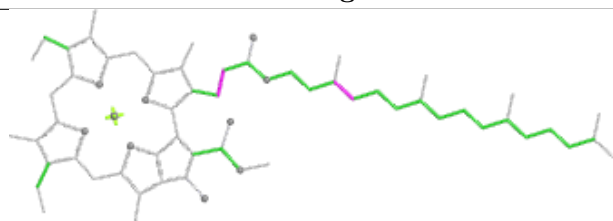
Ligand CLA B 807



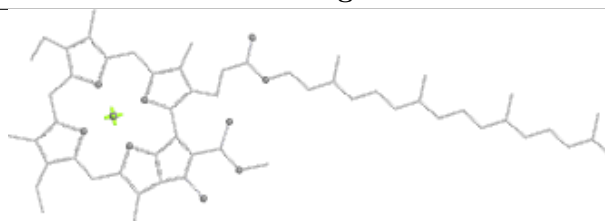
Bond lengths



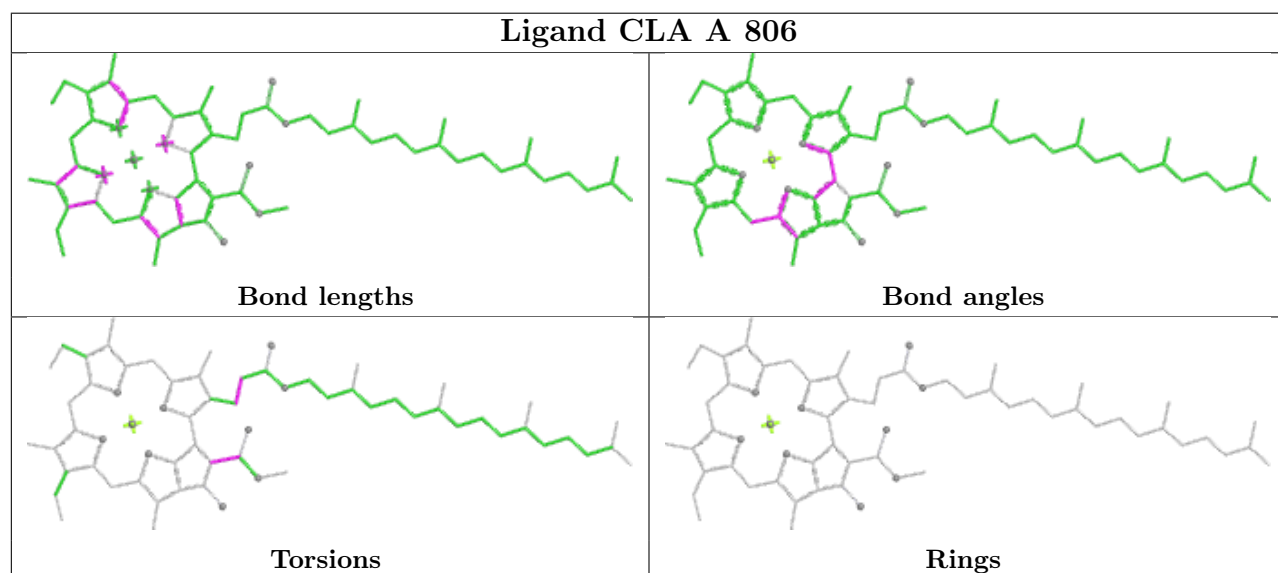
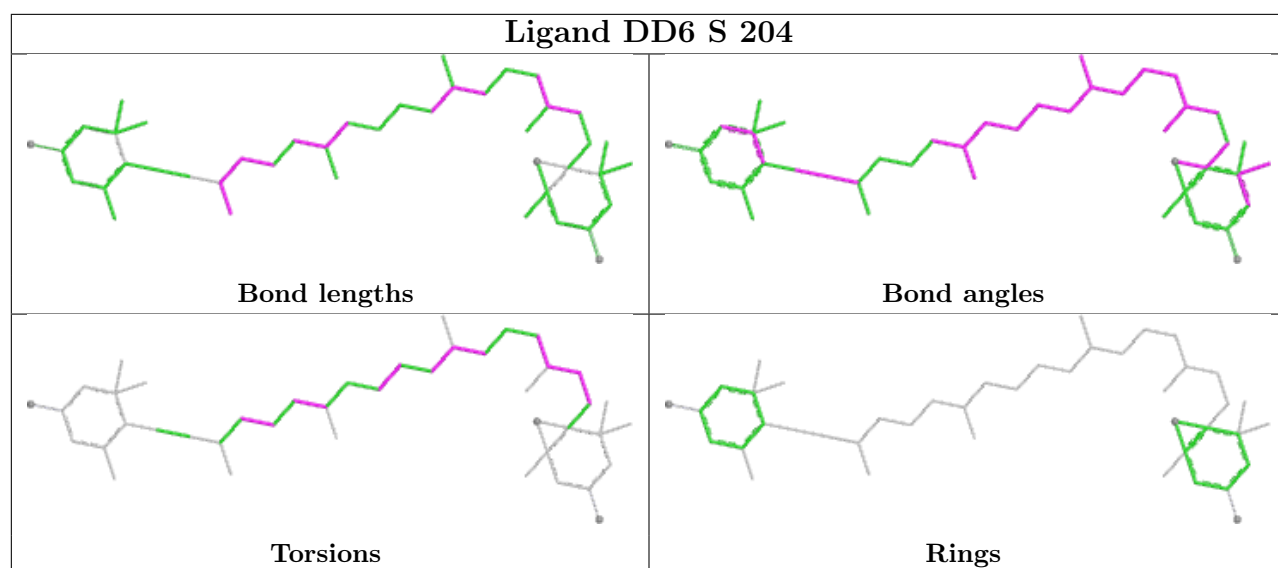
Bond angles



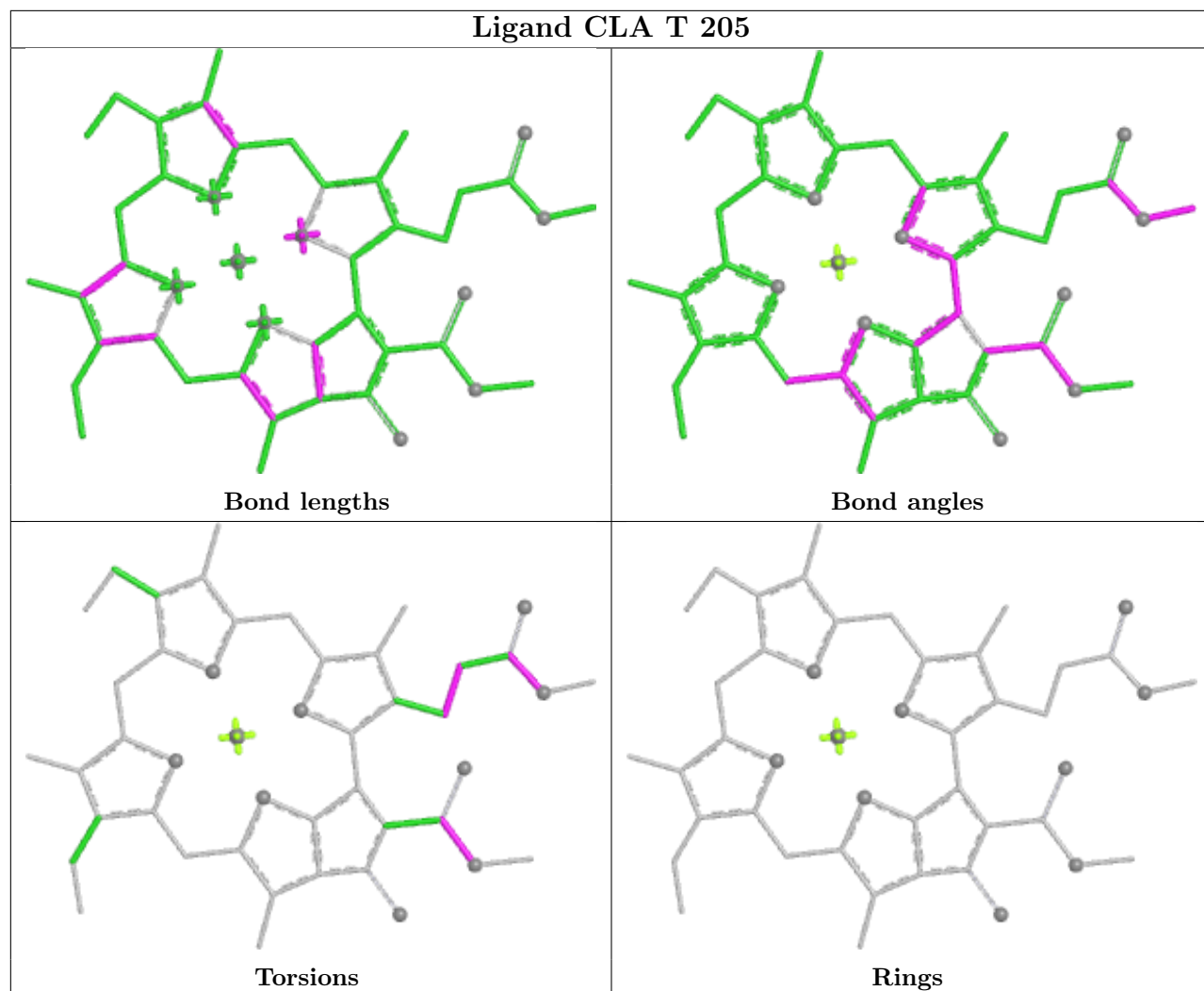
Torsions



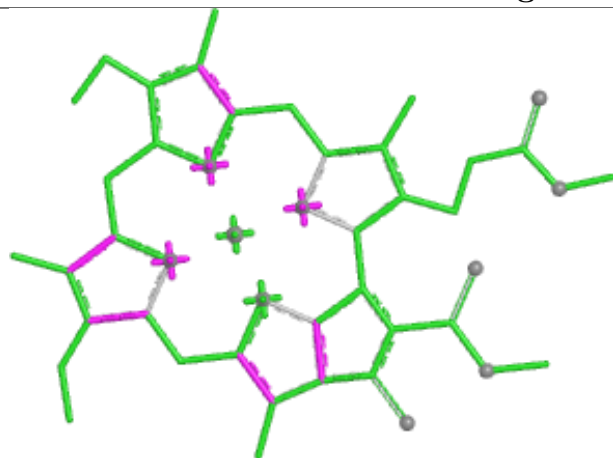
Rings



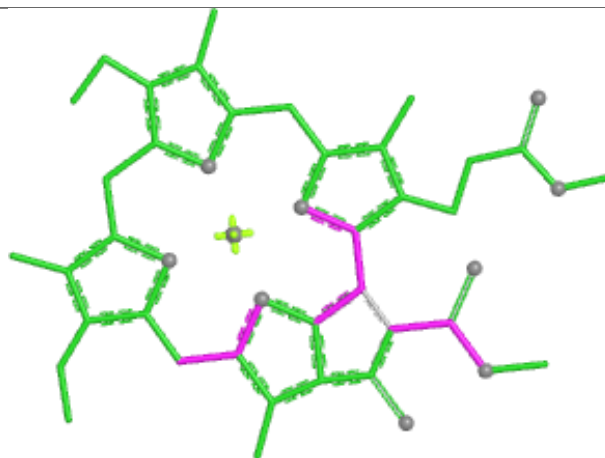
Ligand CLA T 205



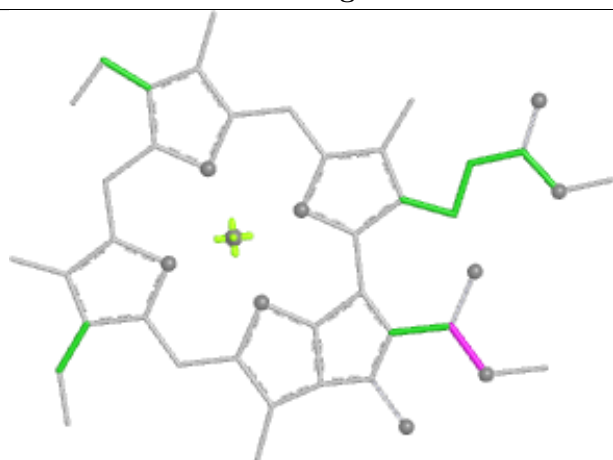
Ligand CLA S 206



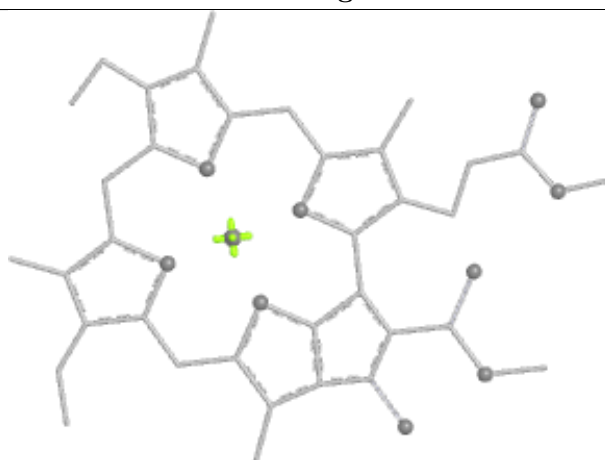
Bond lengths



Bond angles

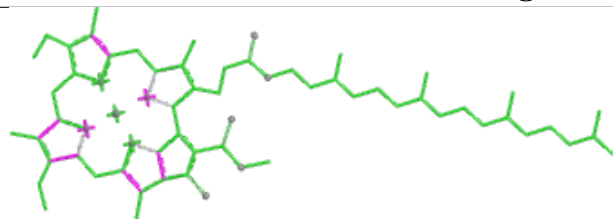


Torsions

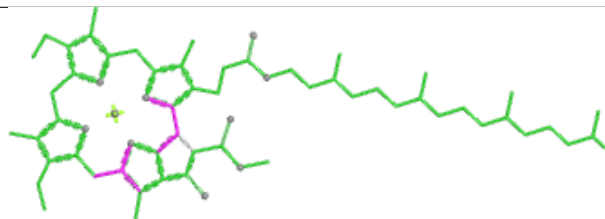


Rings

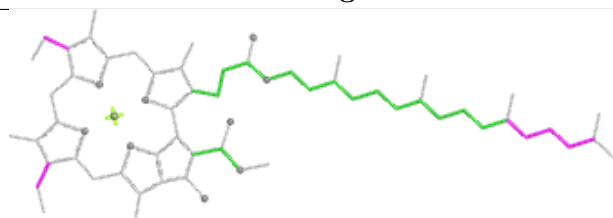
Ligand CLA S 214



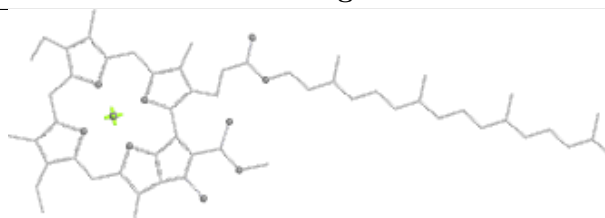
Bond lengths



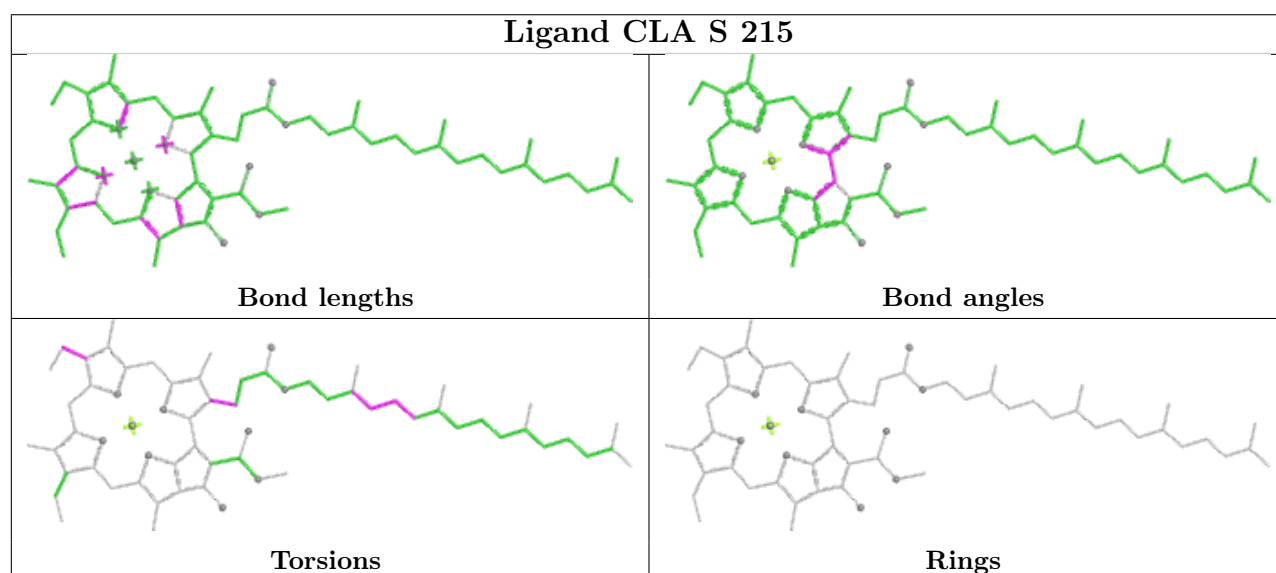
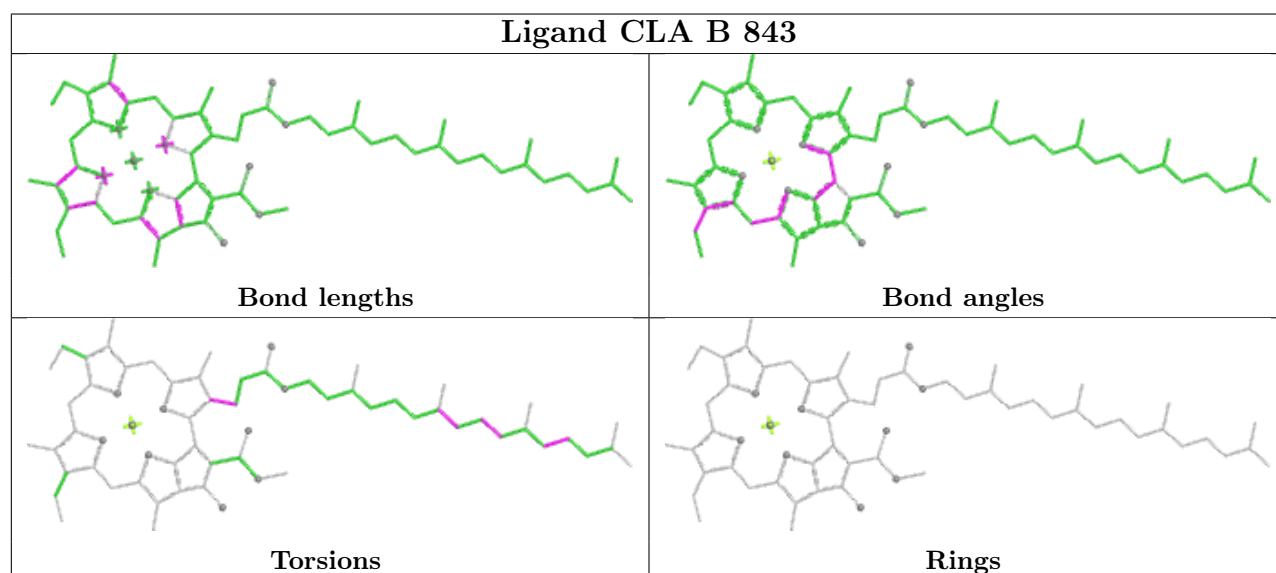
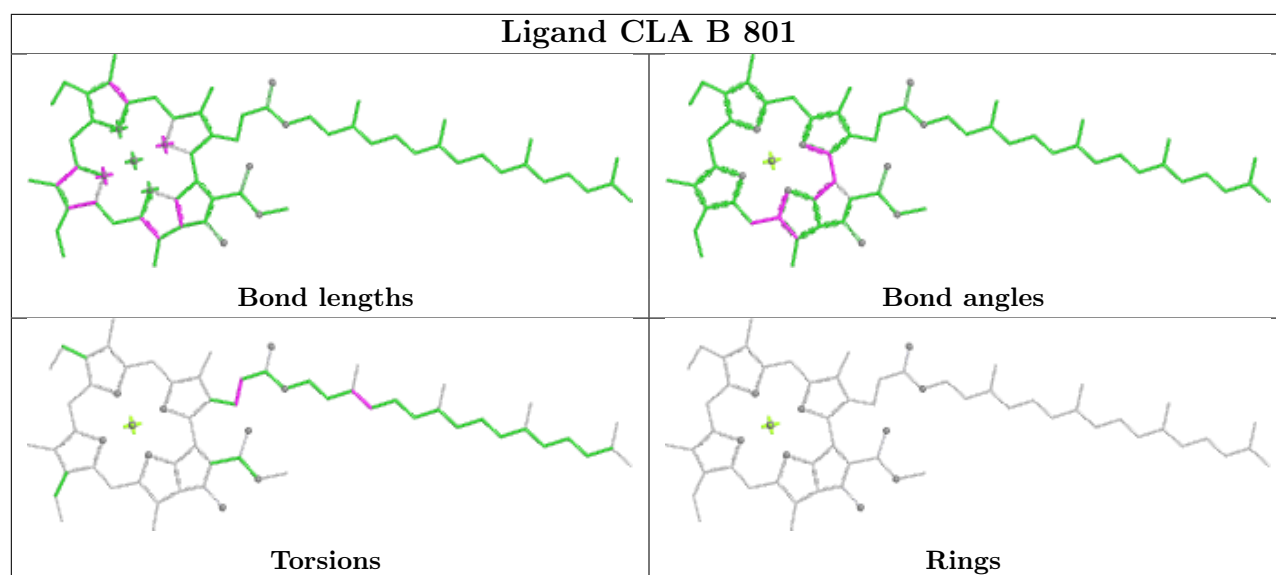
Bond angles

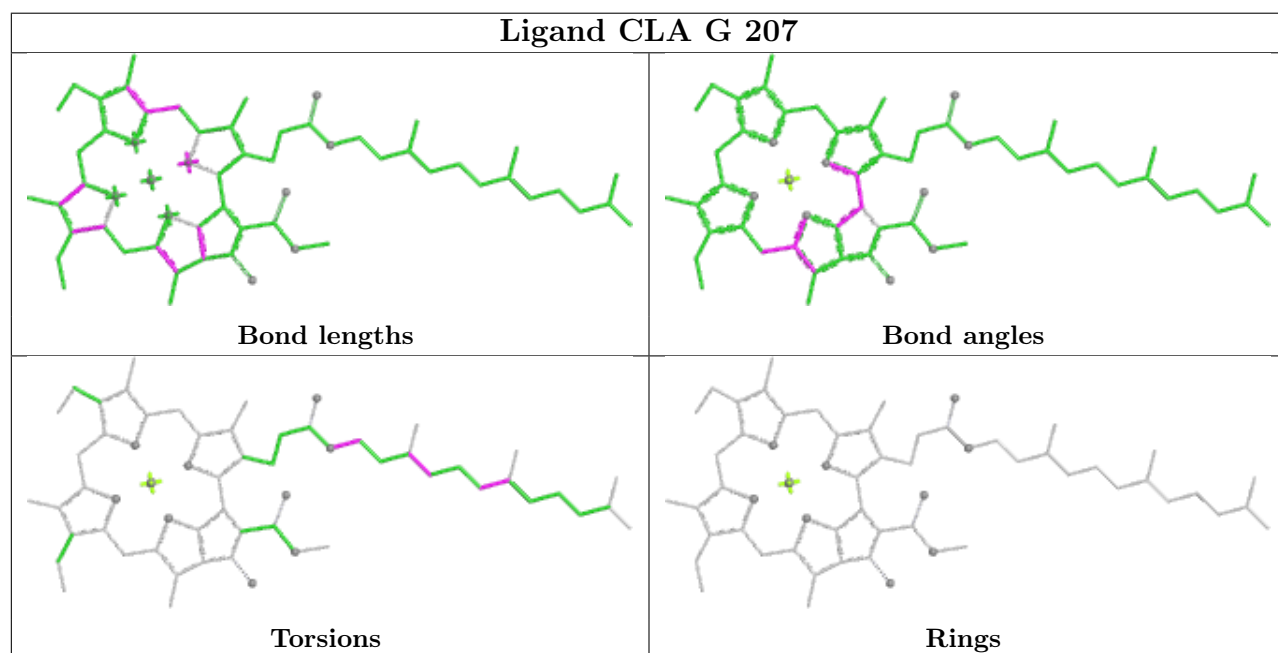
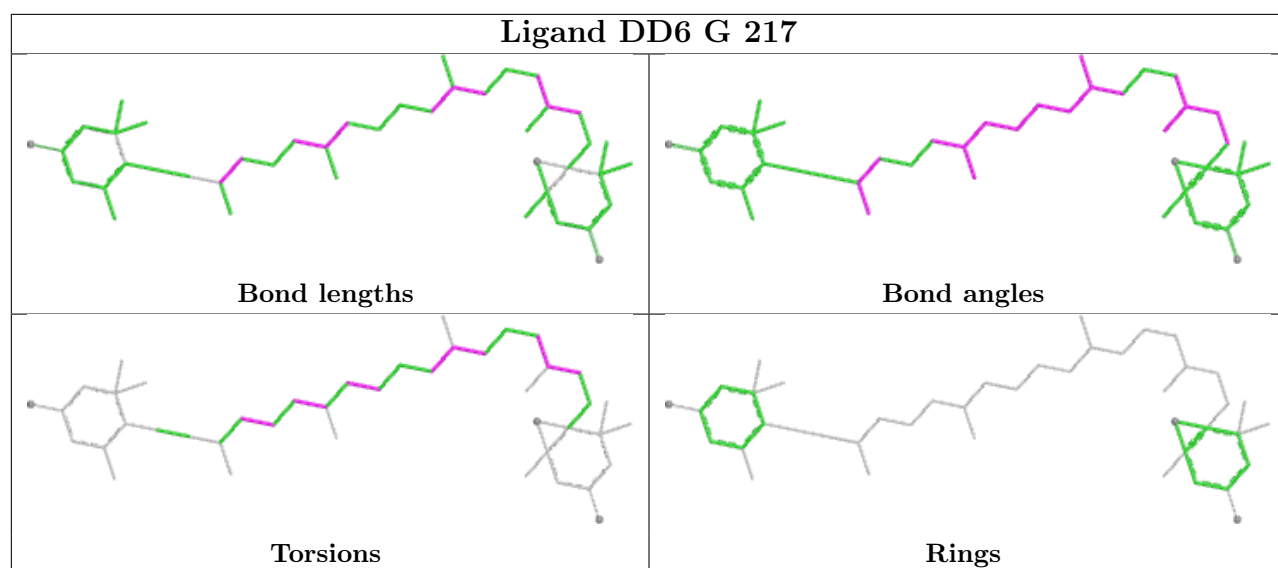


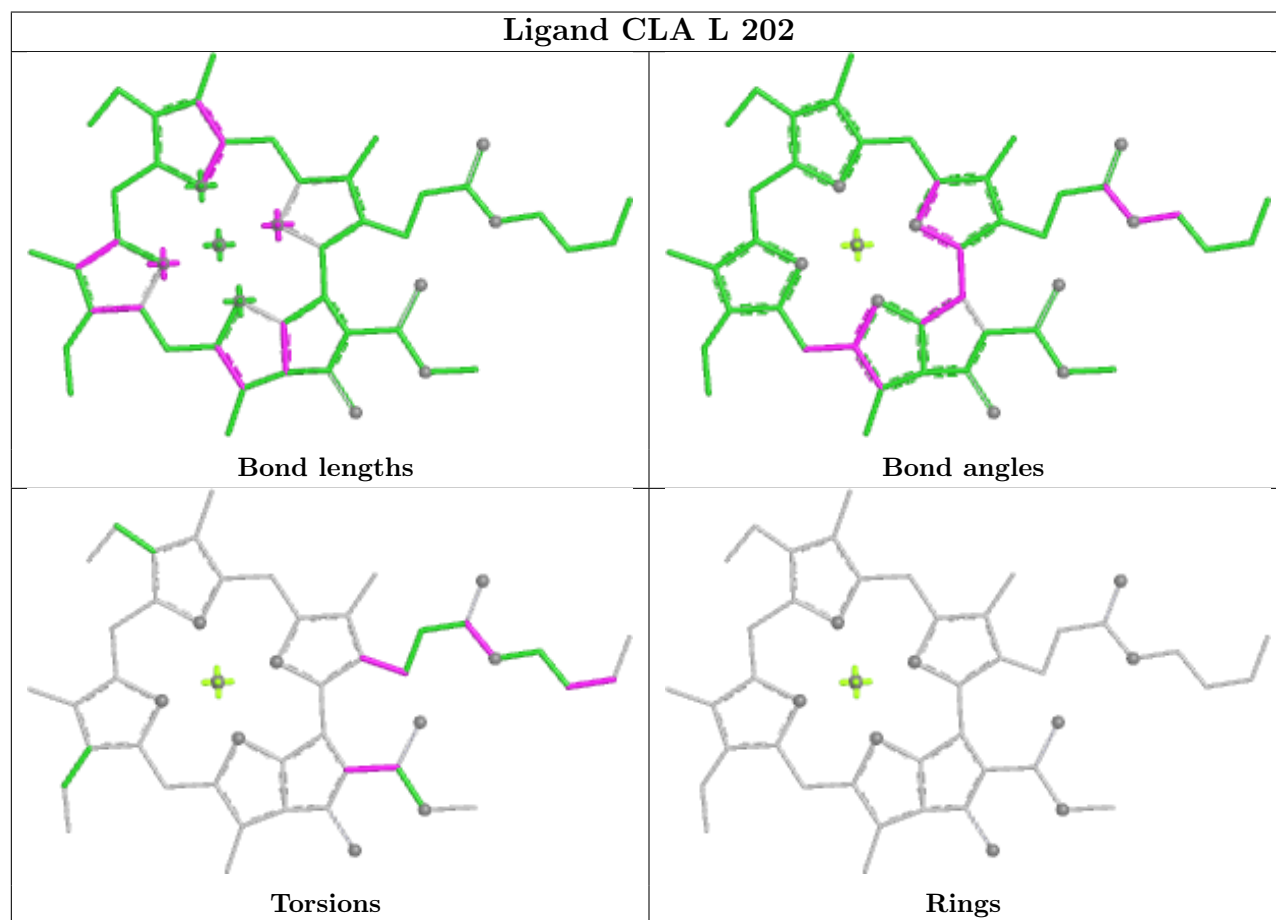
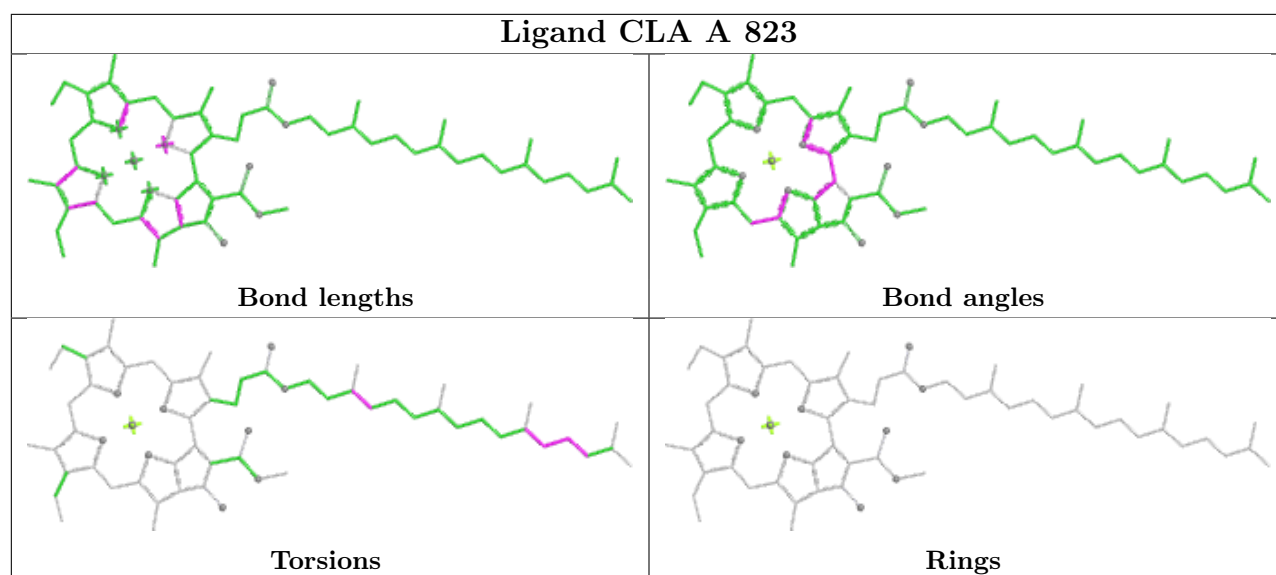
Torsions

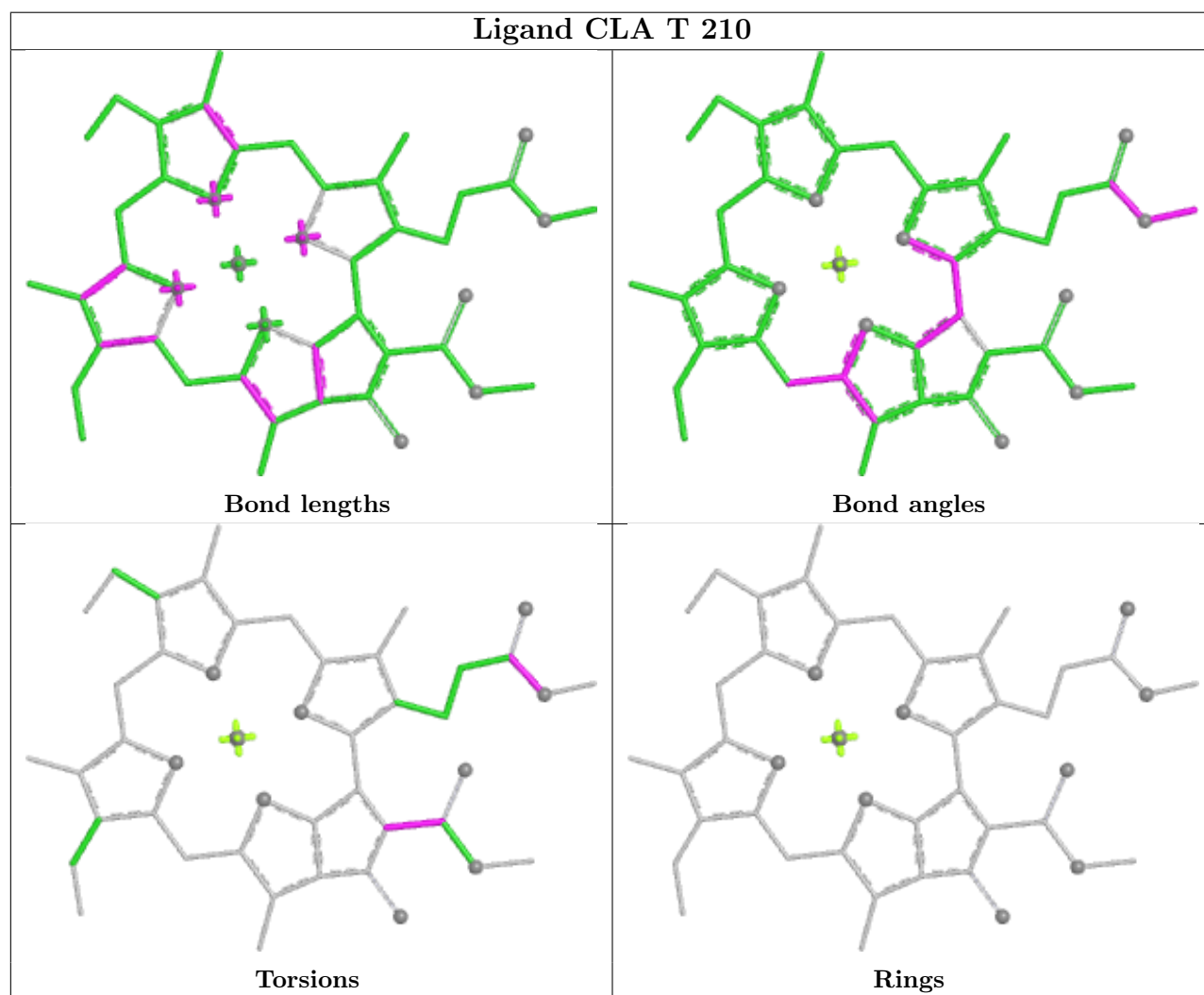
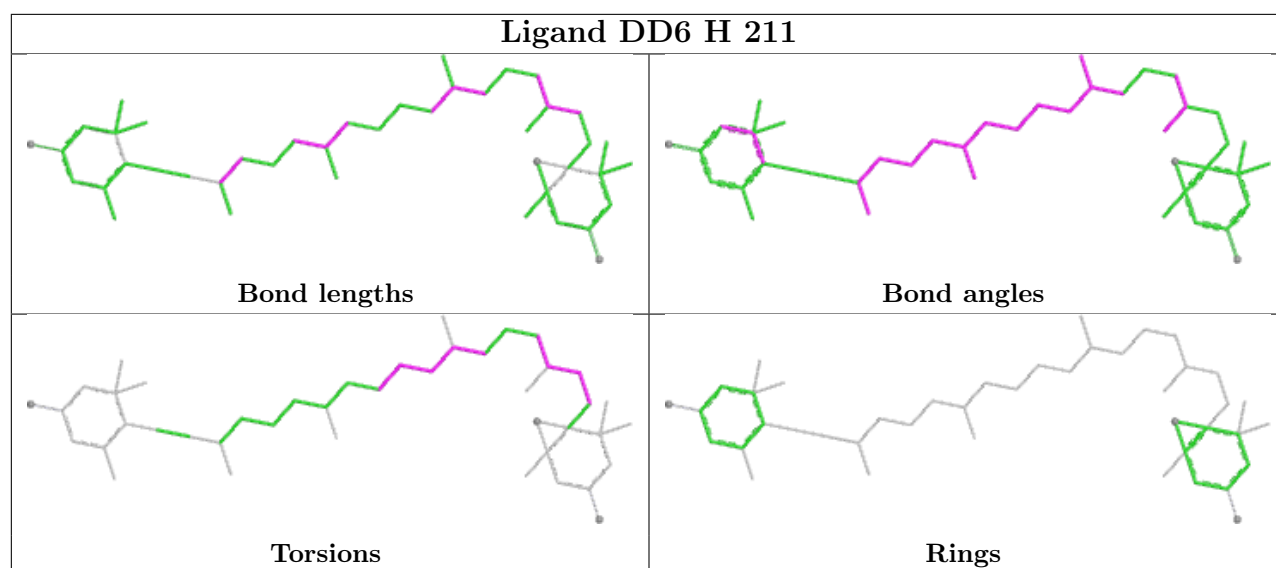


Rings

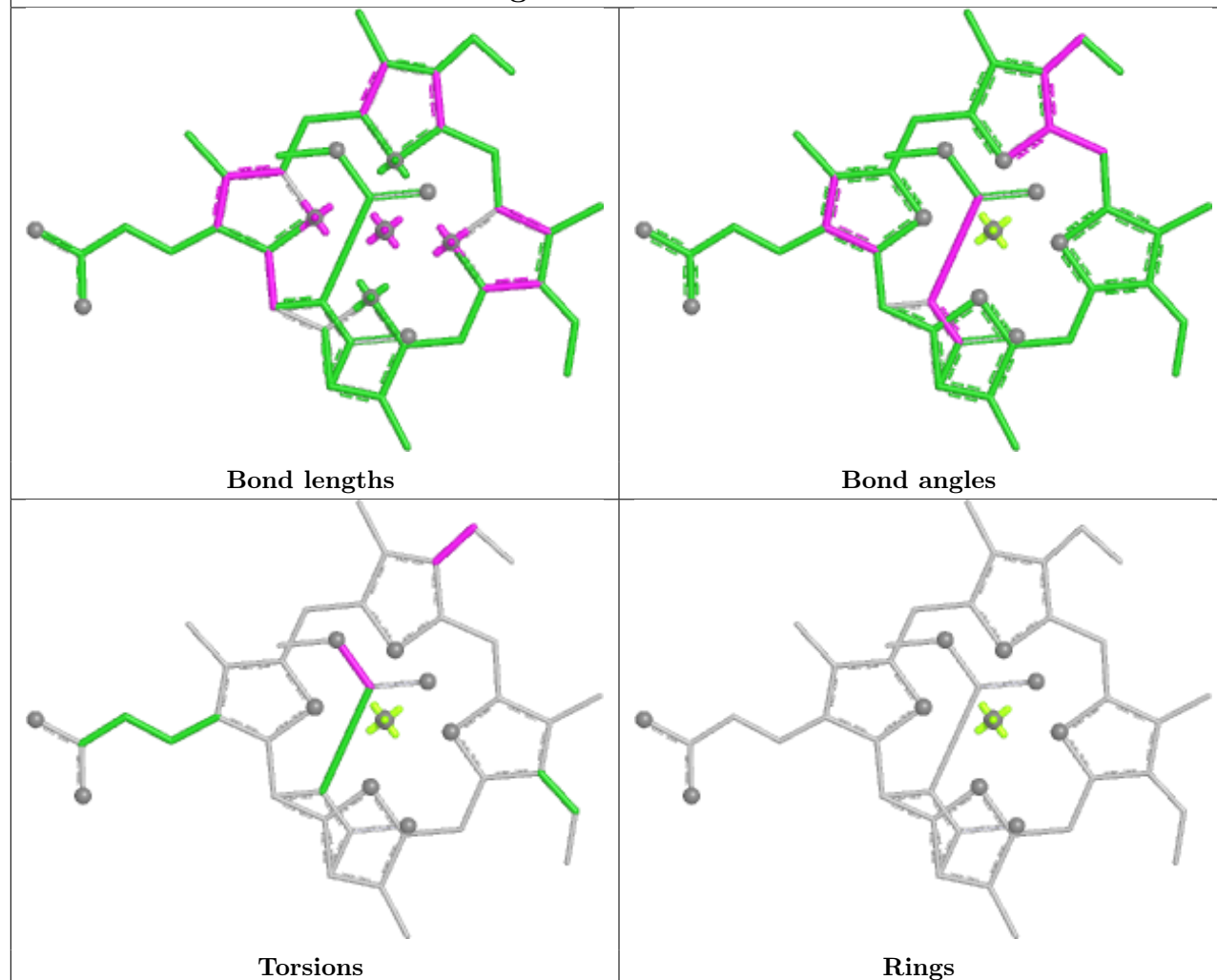




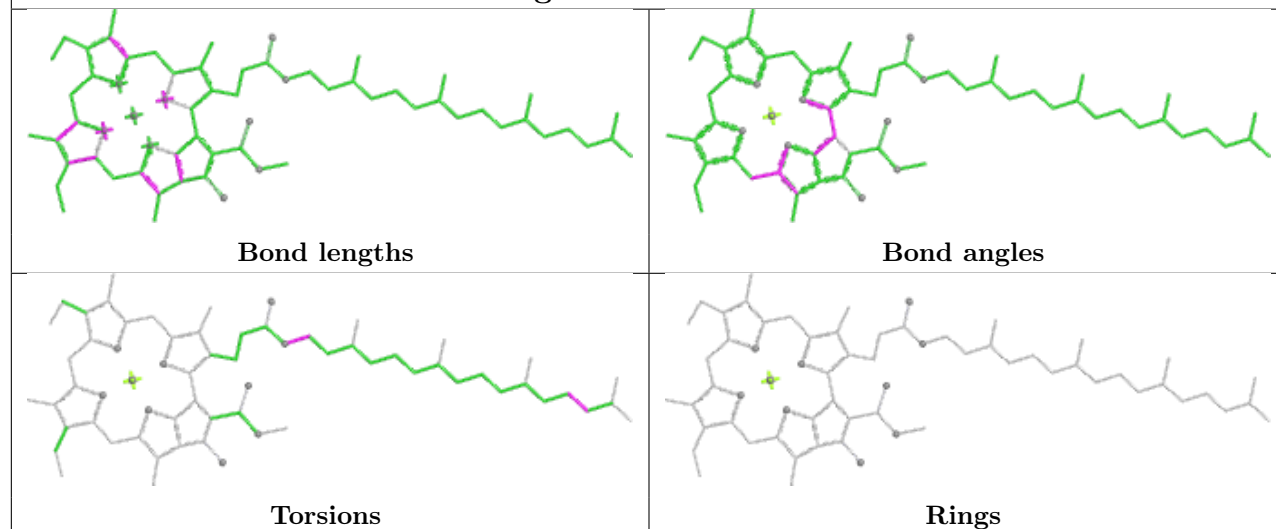


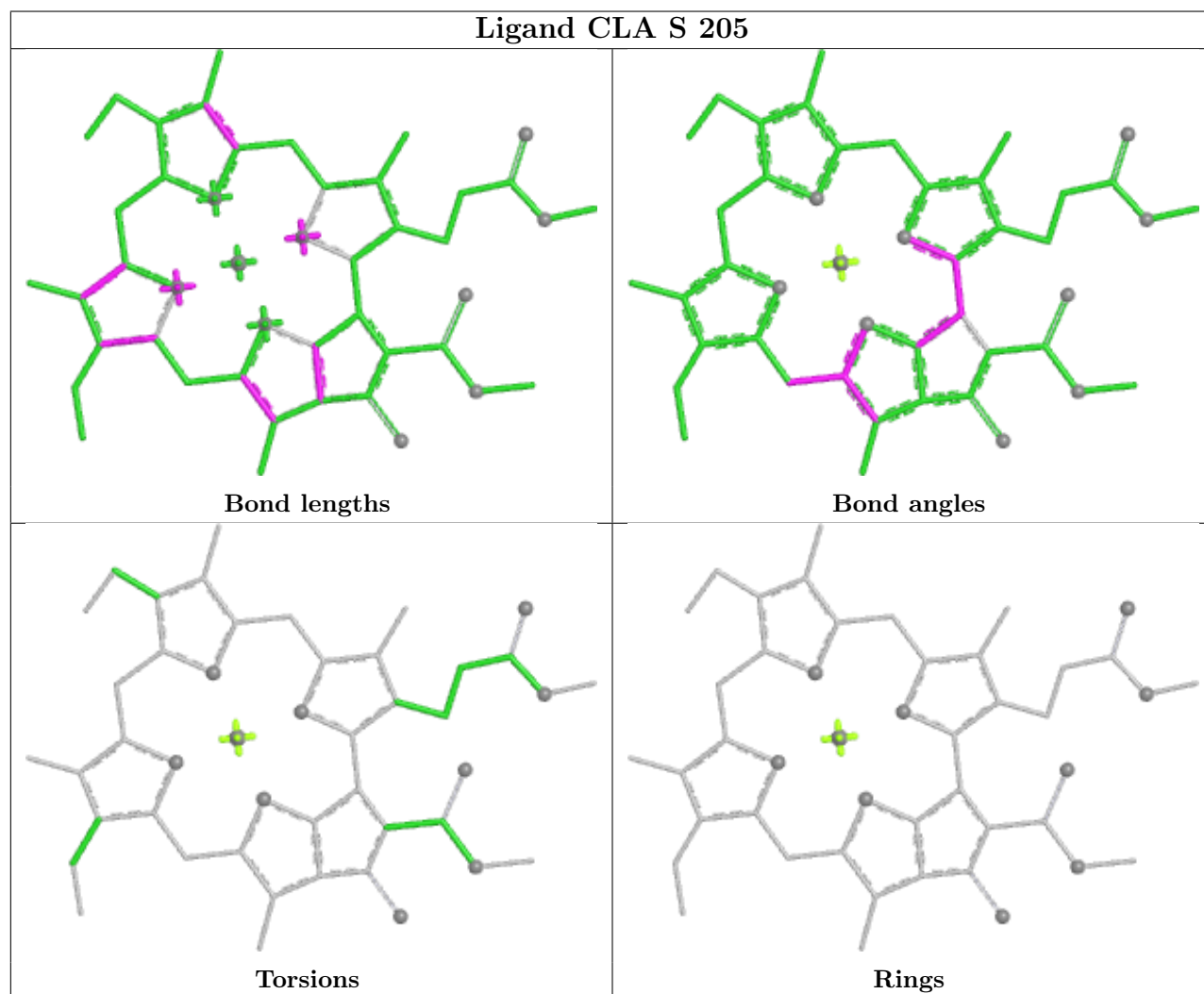
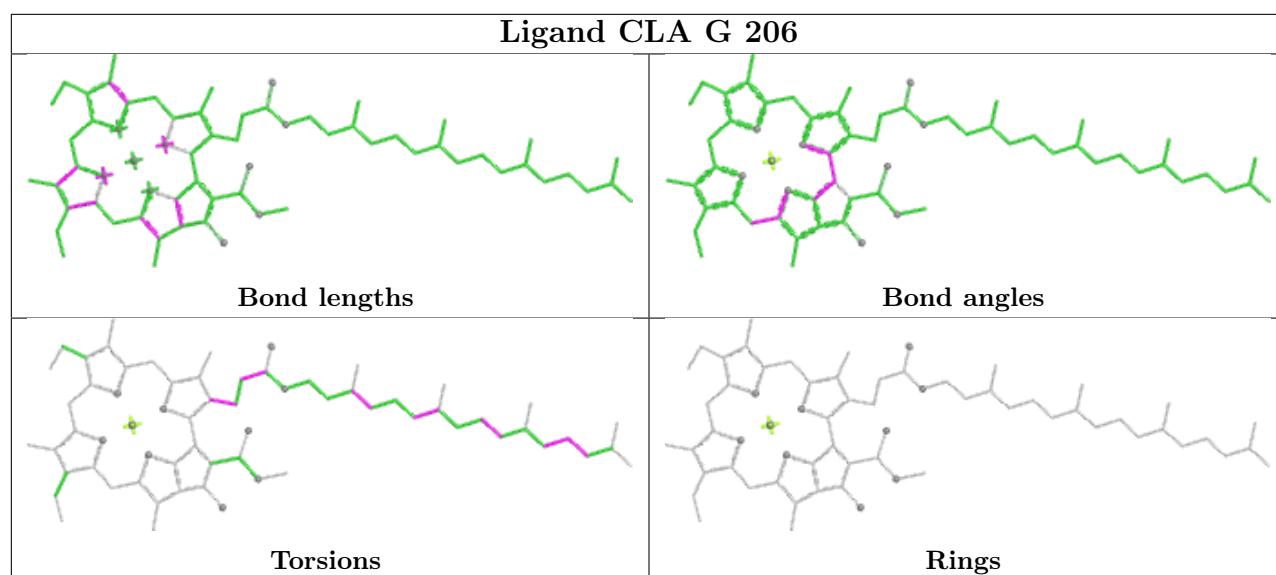


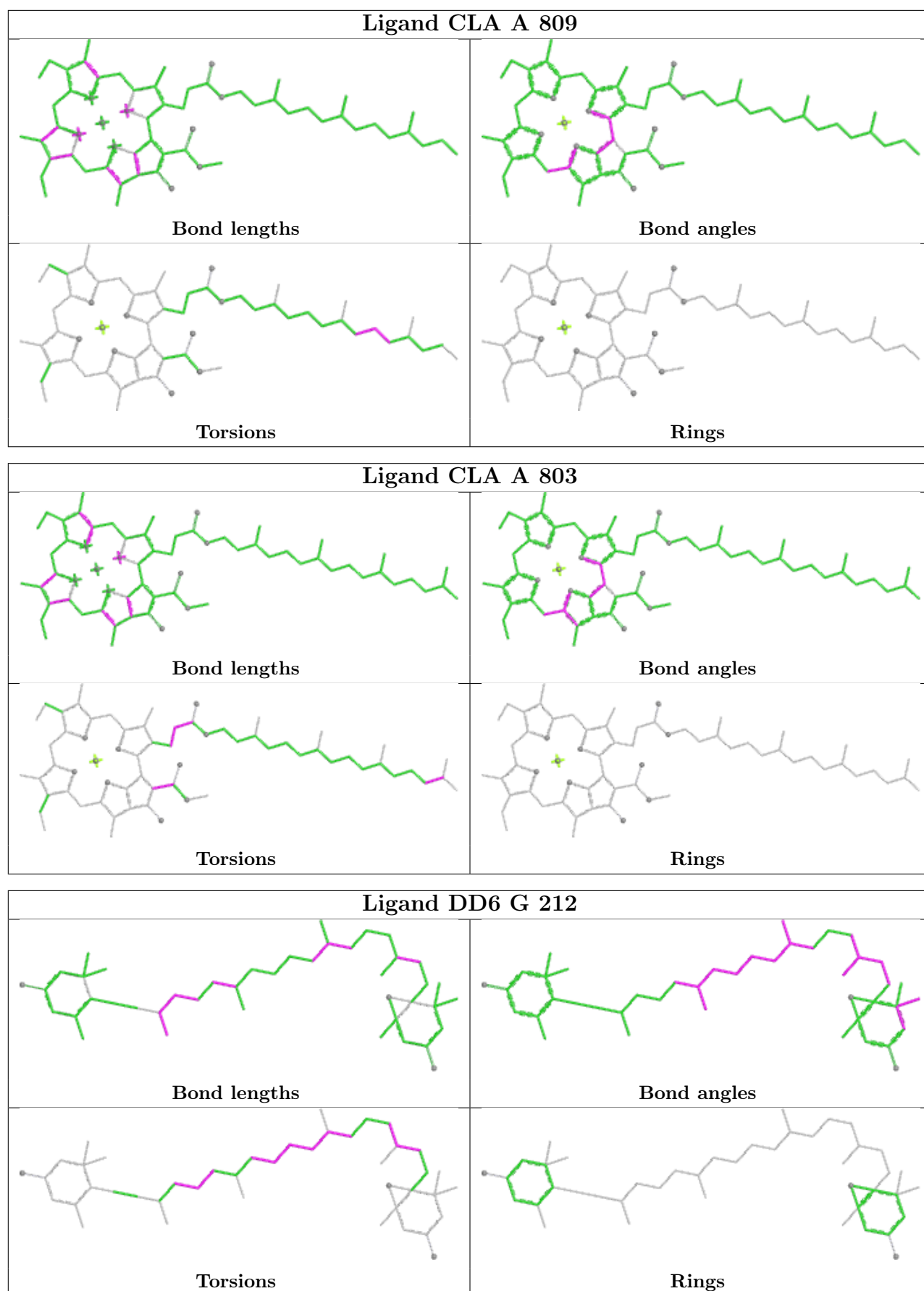
Ligand KC1 T 208

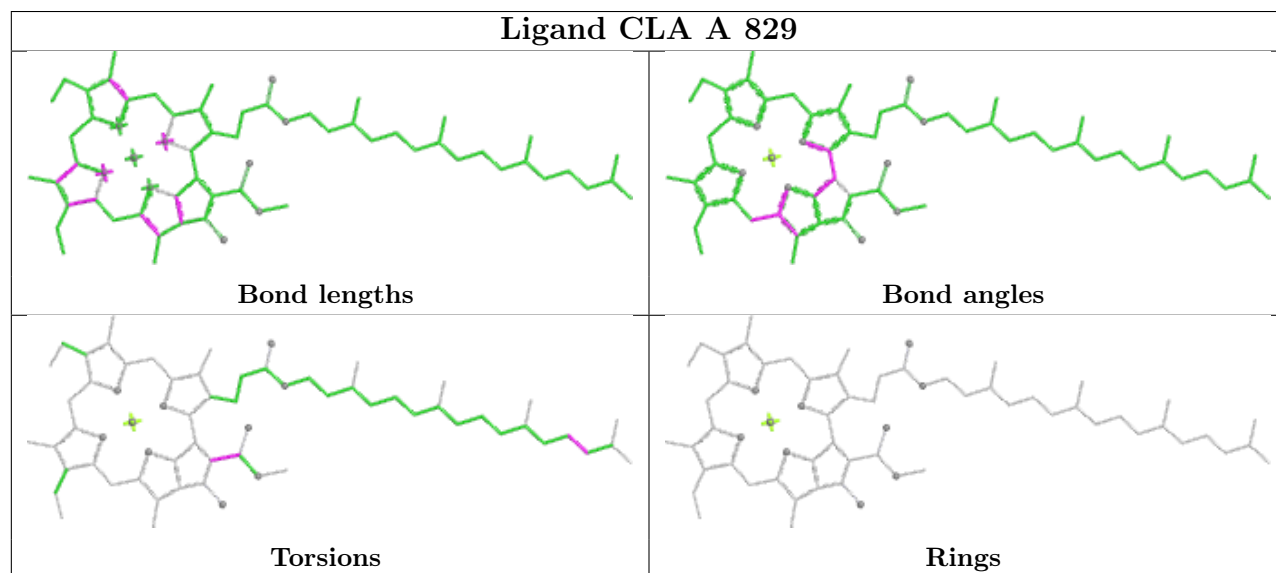
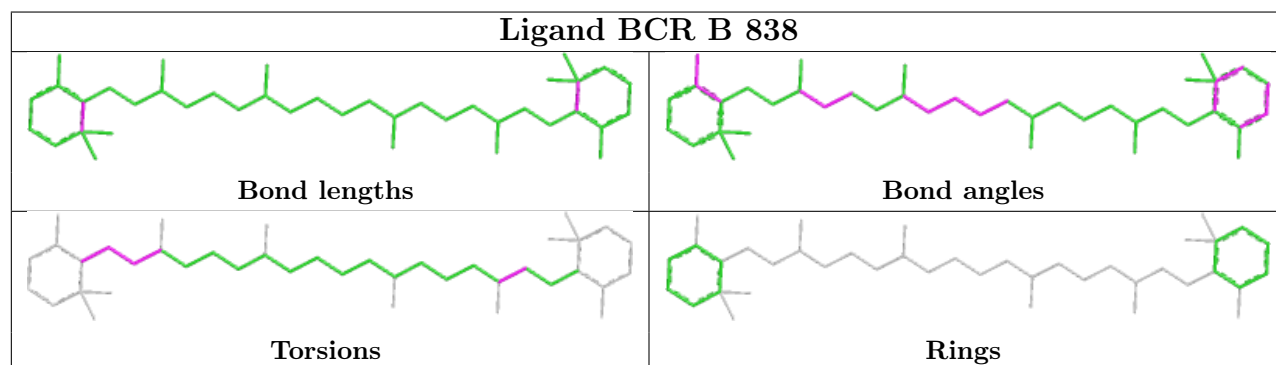
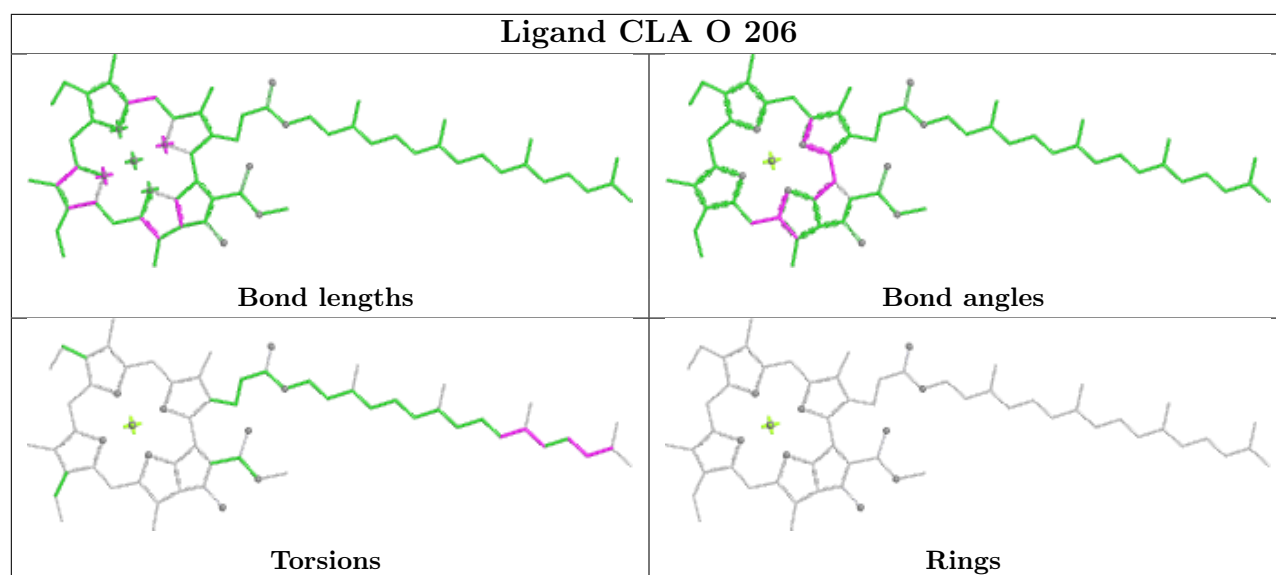


Ligand CLA L 203

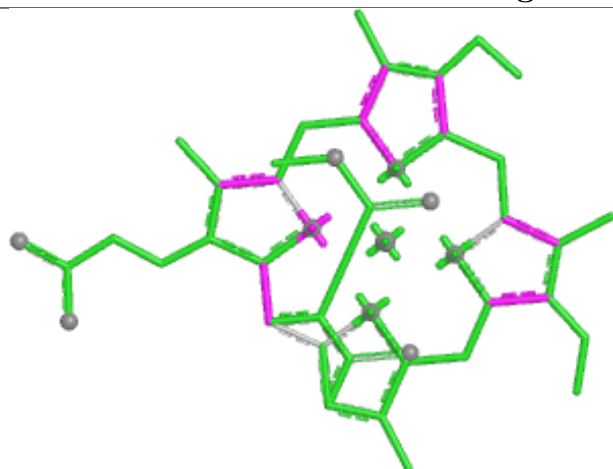




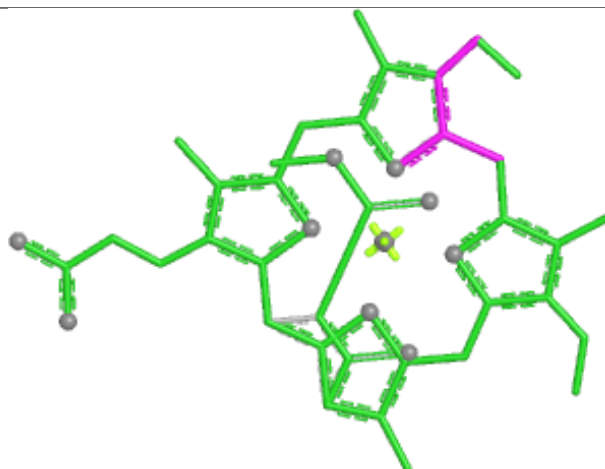




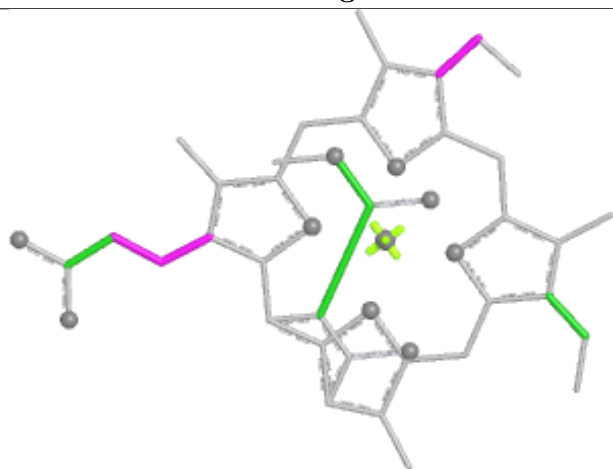
Ligand KC1 P 206



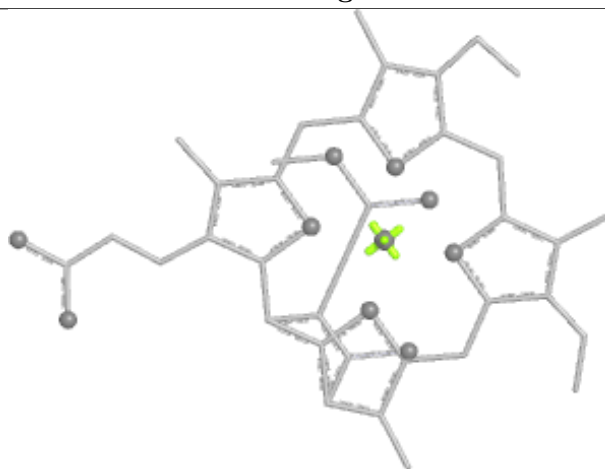
Bond lengths



Bond angles

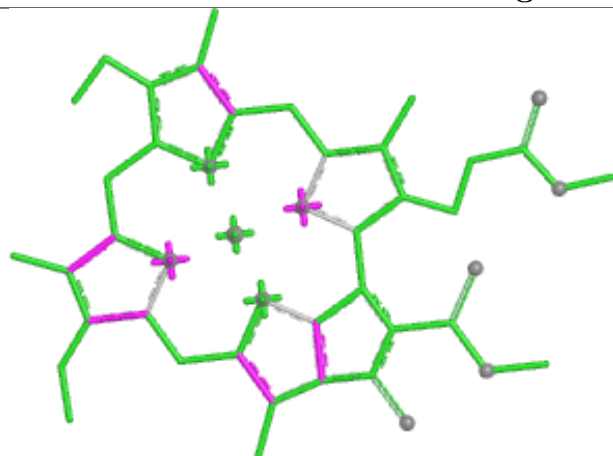


Torsions

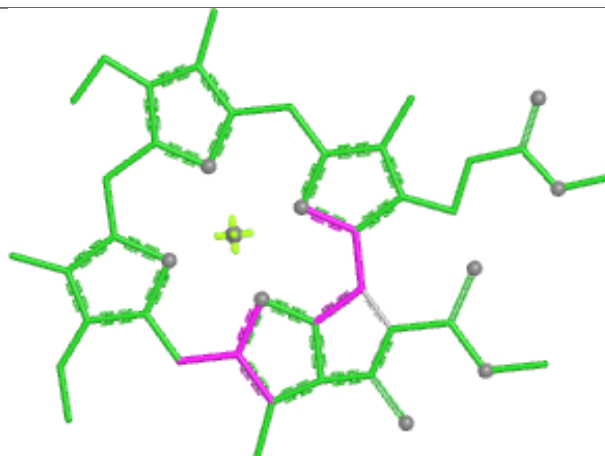


Rings

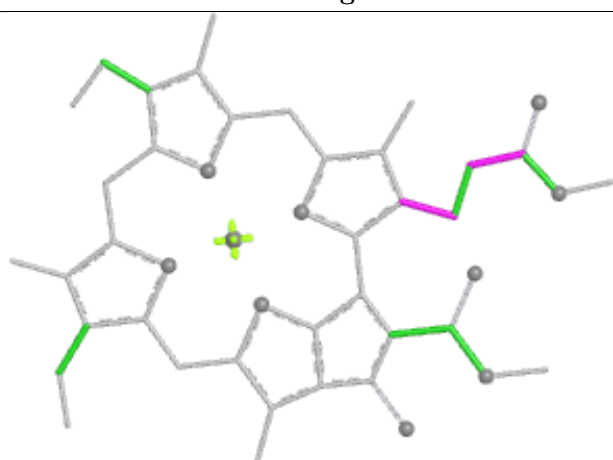
Ligand CLA F 803



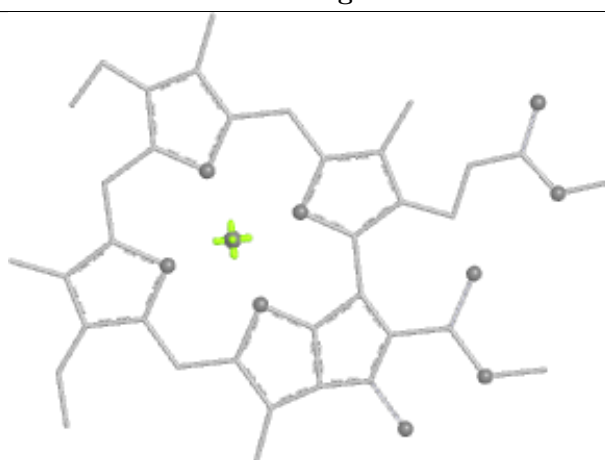
Bond lengths



Bond angles

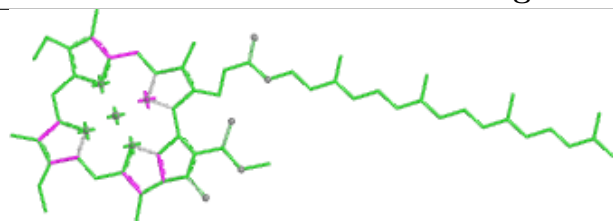


Torsions

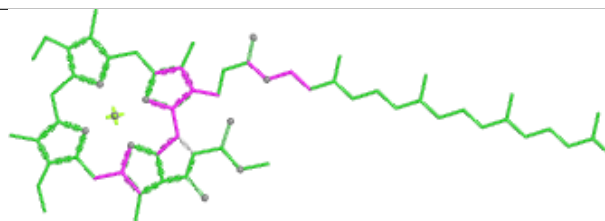


Rings

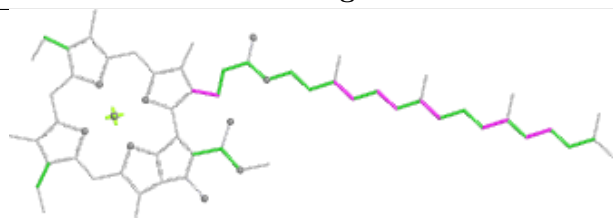
Ligand CLA U 207



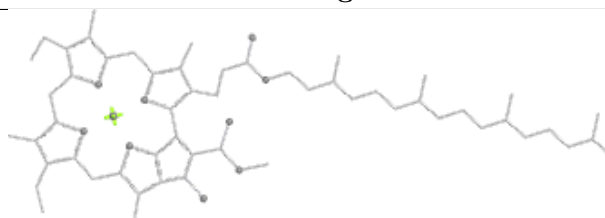
Bond lengths



Bond angles

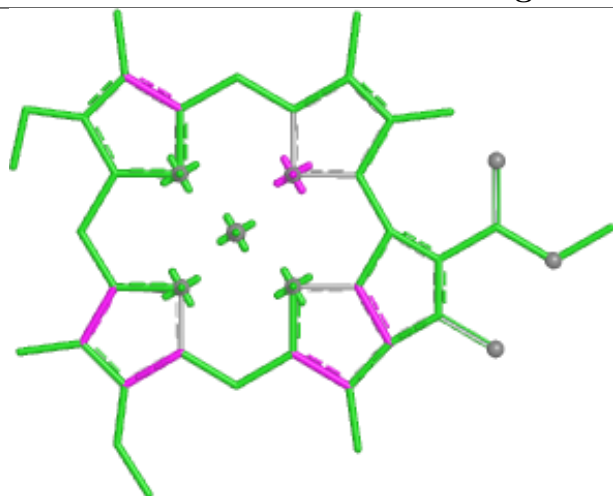


Torsions

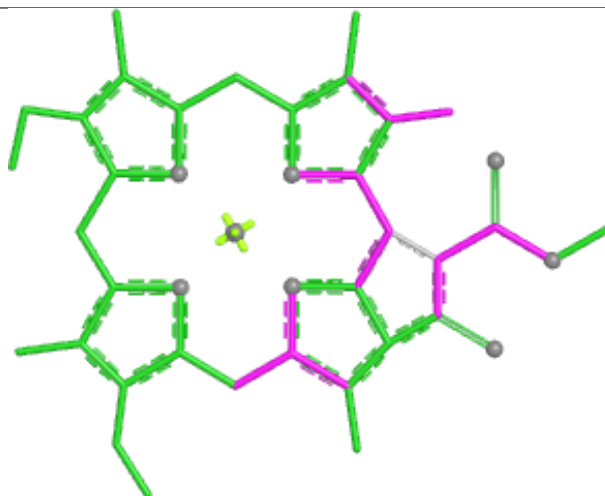


Rings

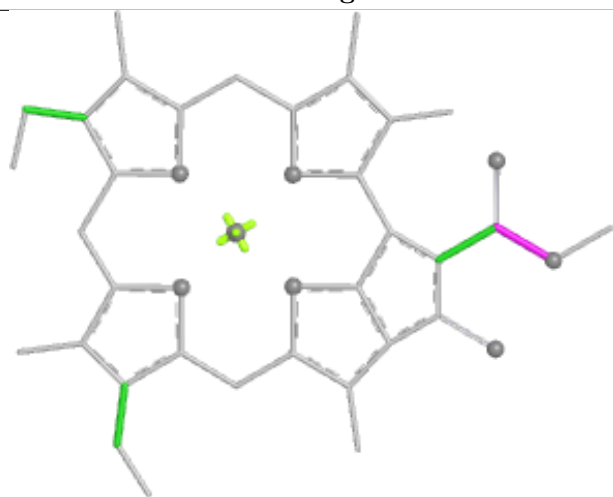
Ligand CLA P 213



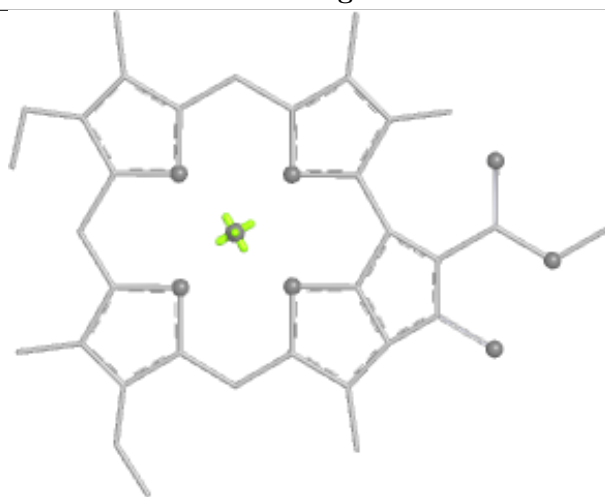
Bond lengths



Bond angles

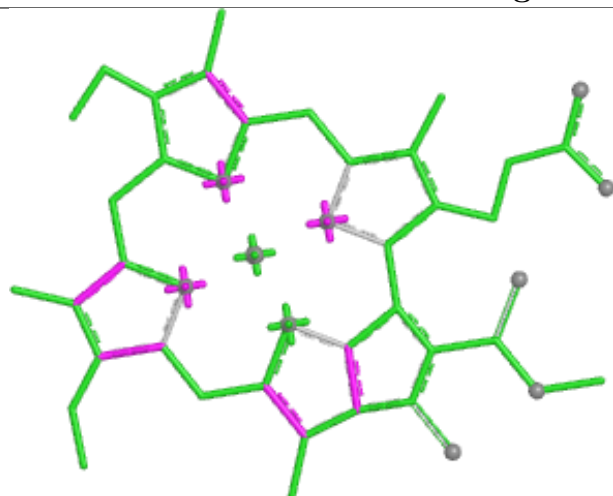


Torsions

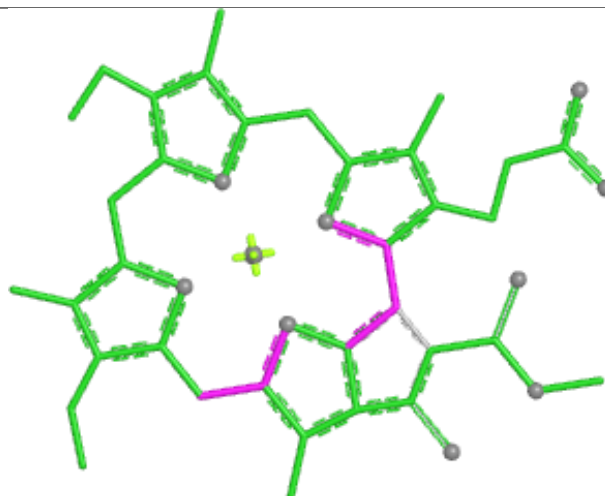


Rings

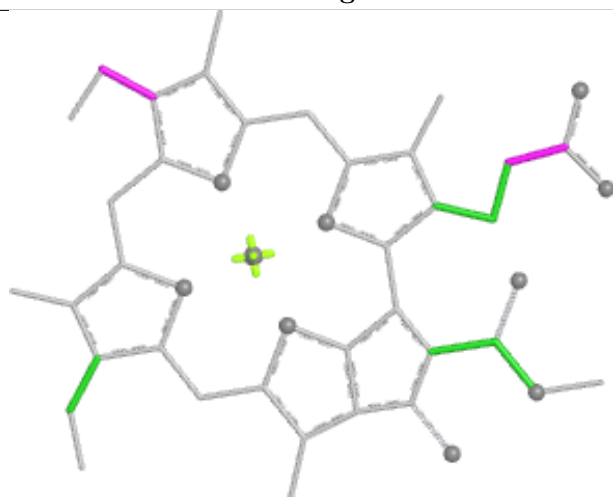
Ligand CLA H 205



Bond lengths



Bond angles

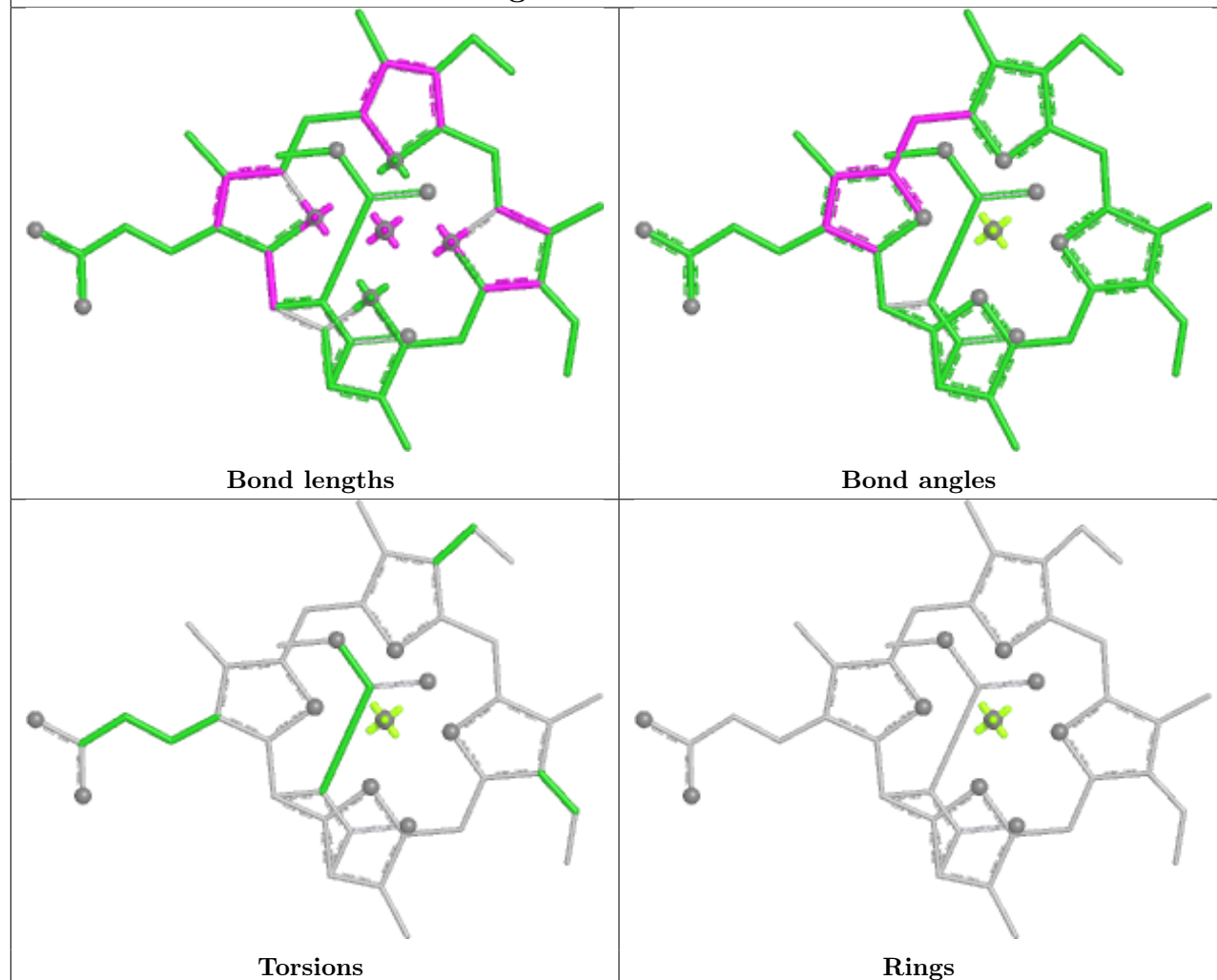


Torsions

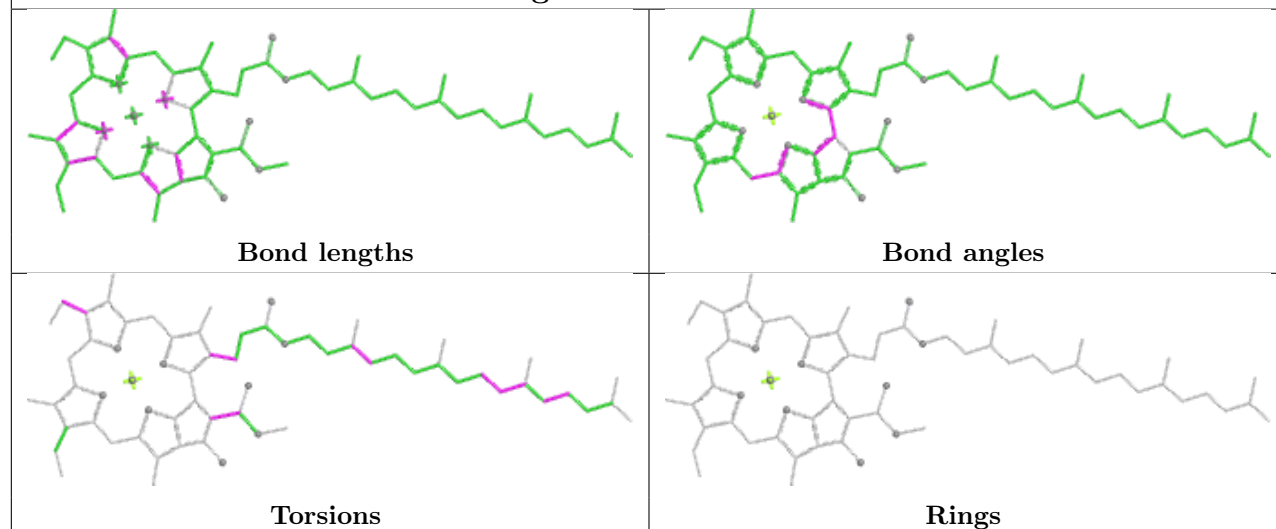


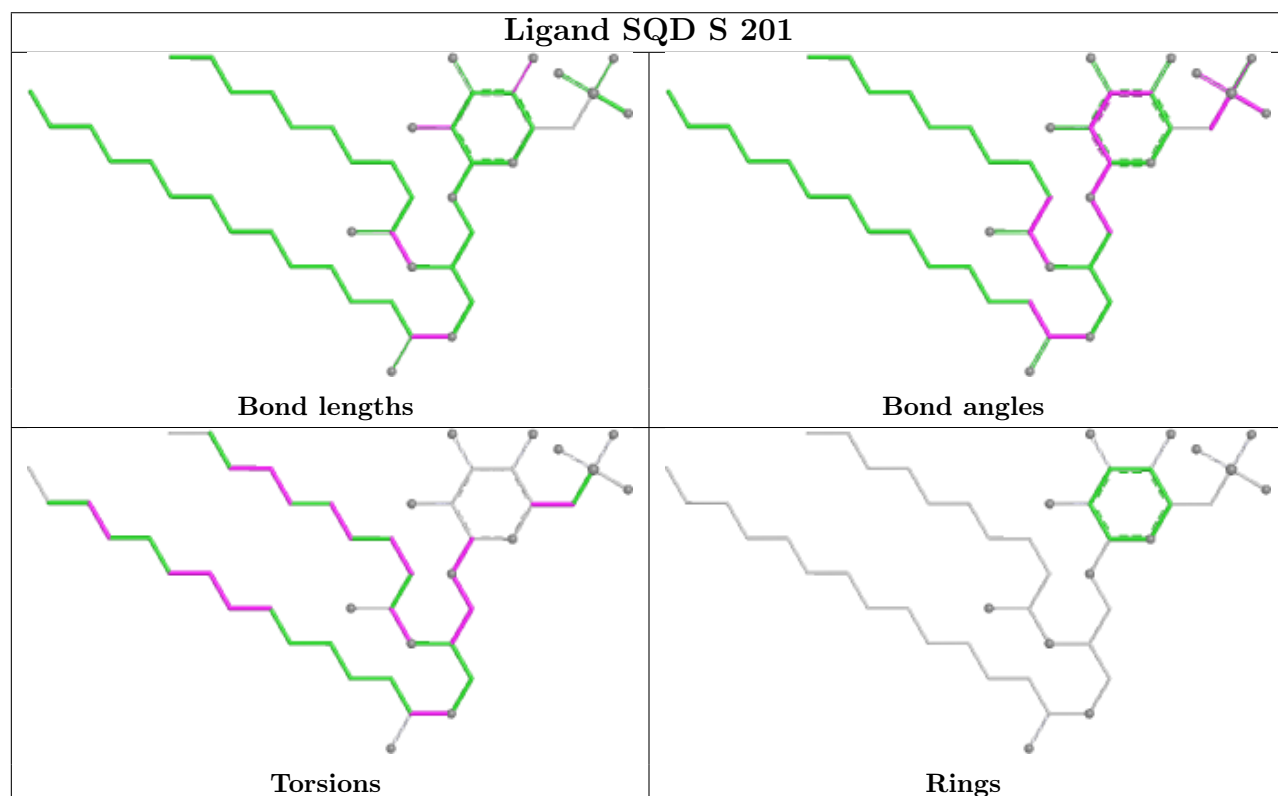
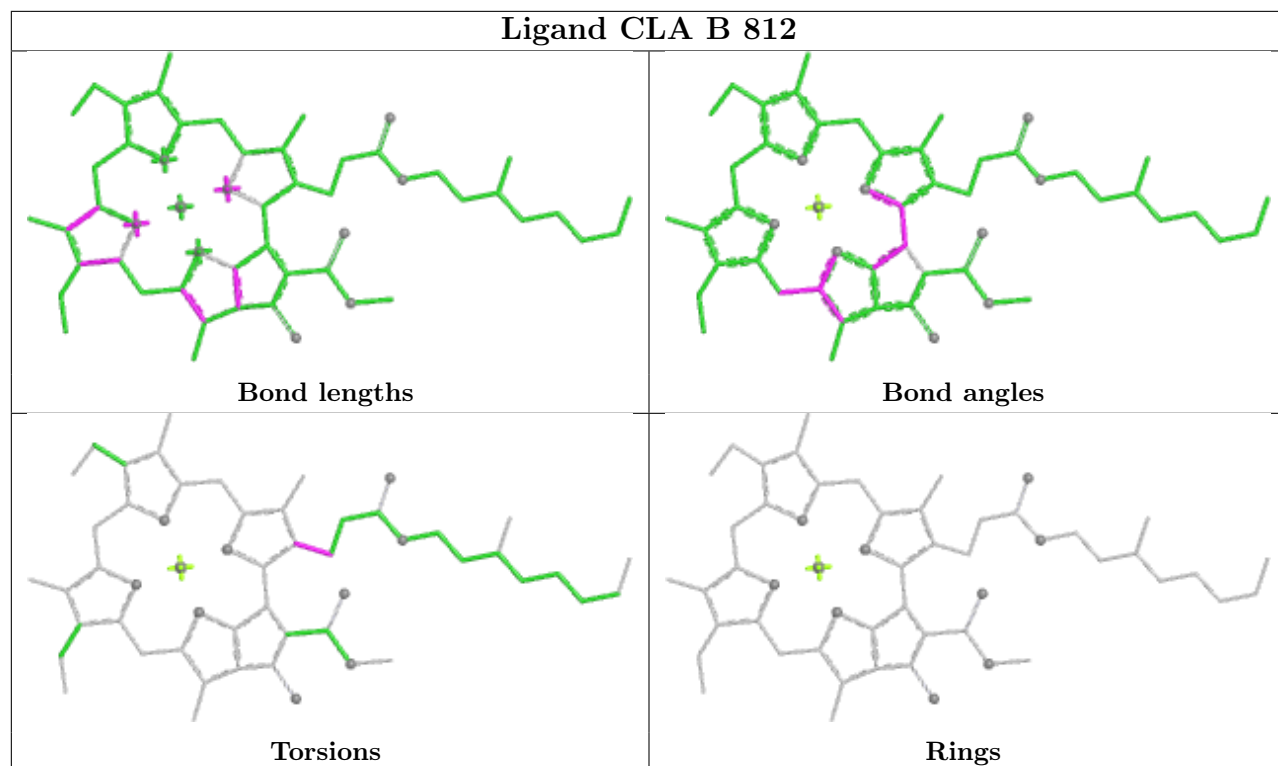
Rings

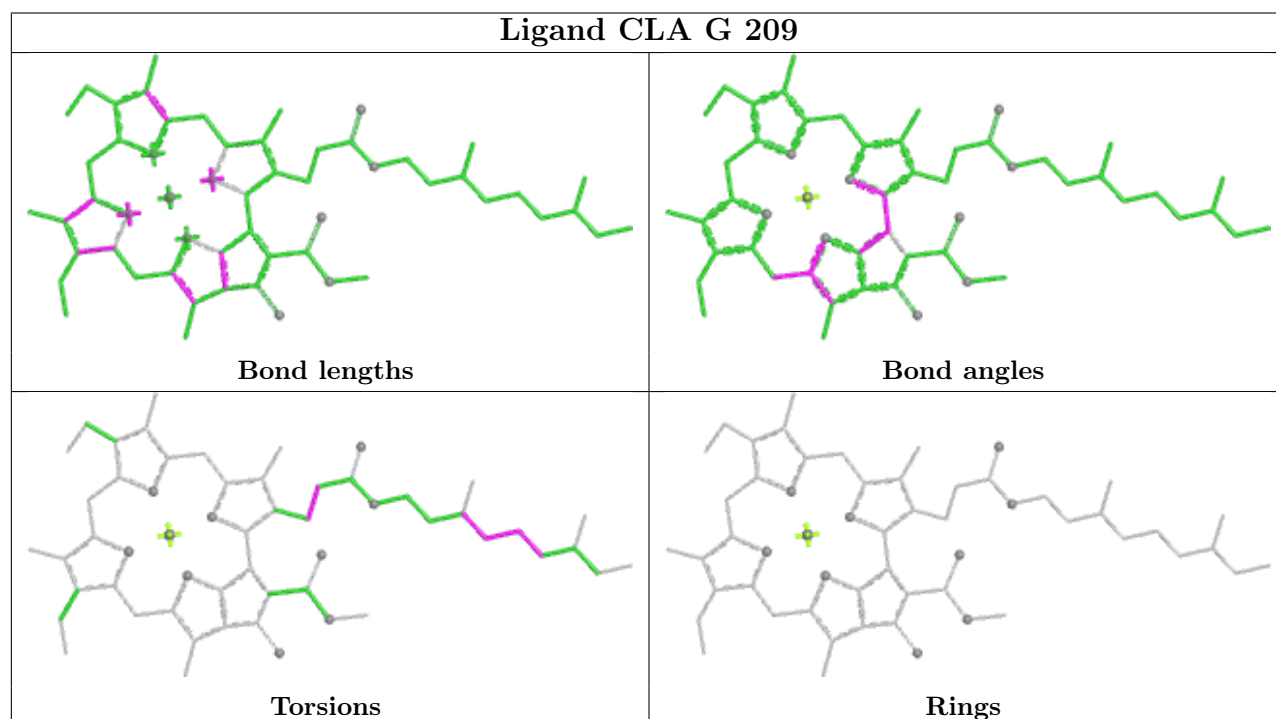
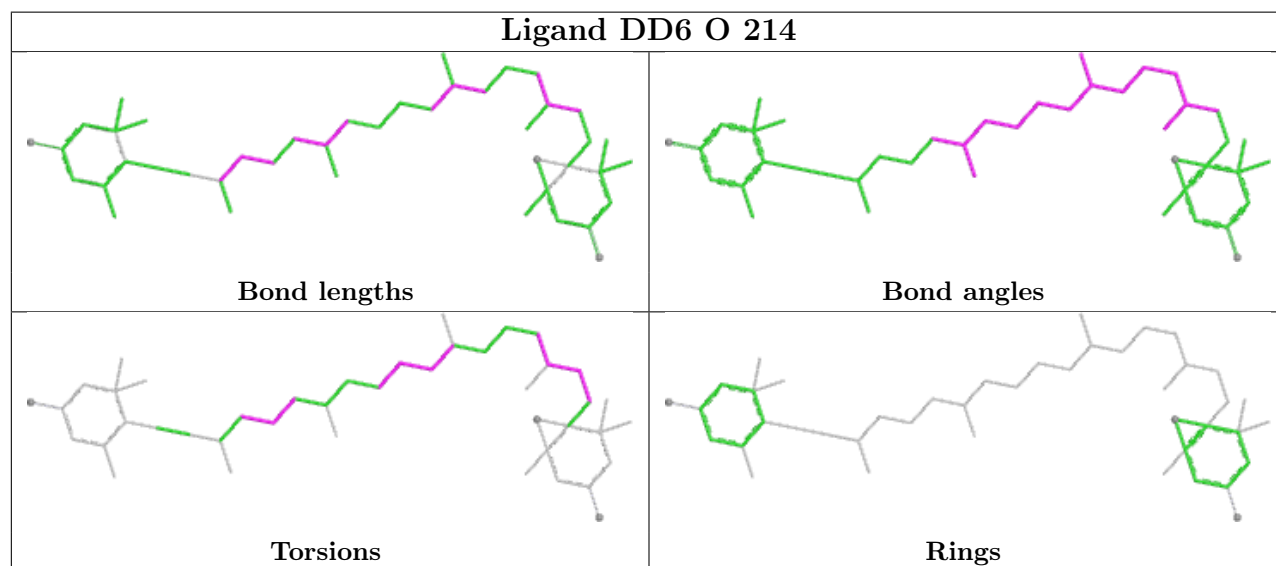
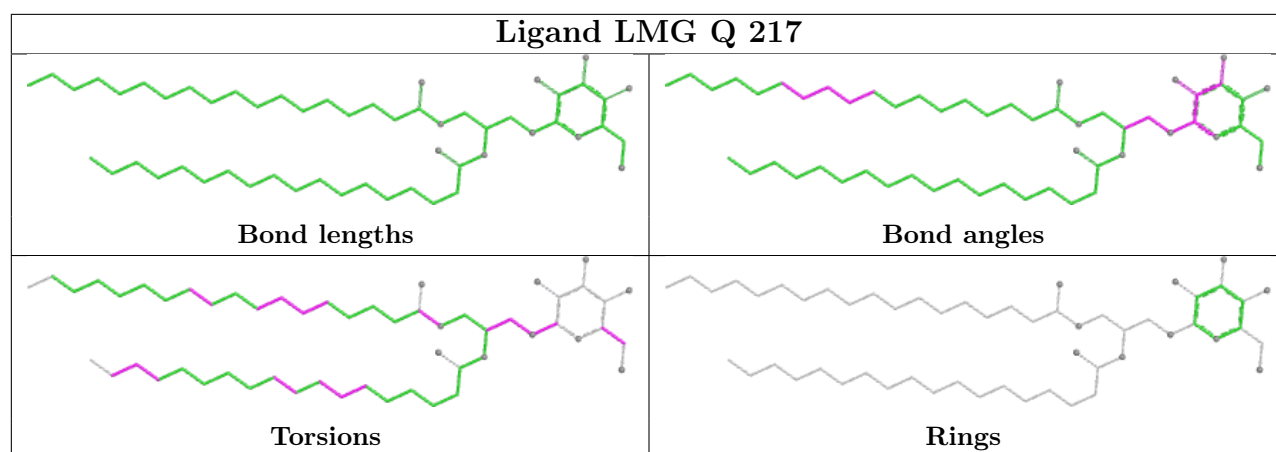
Ligand KC1 O 210



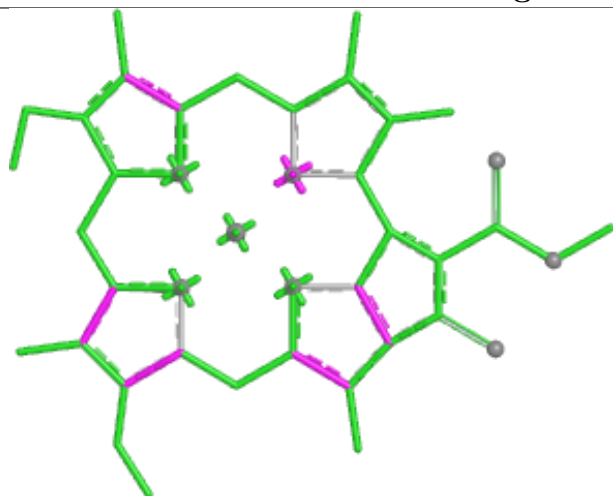
Ligand CLA A 851



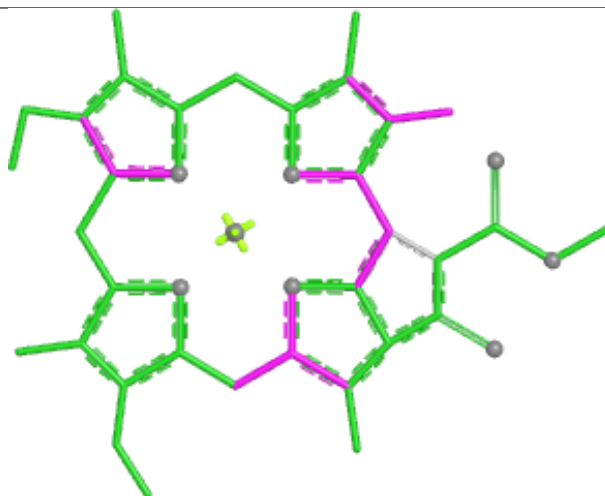




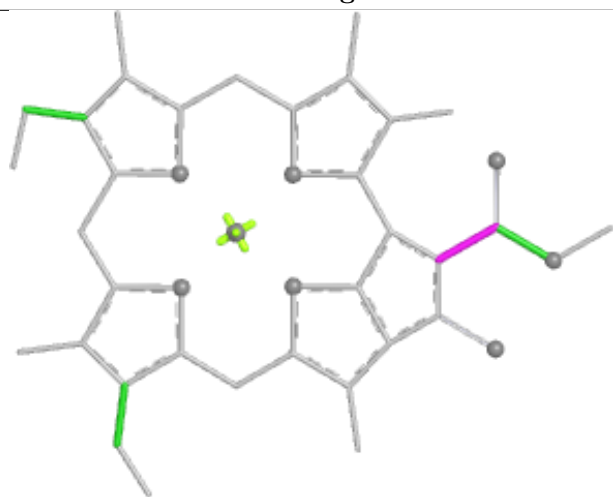
Ligand CLA O 211



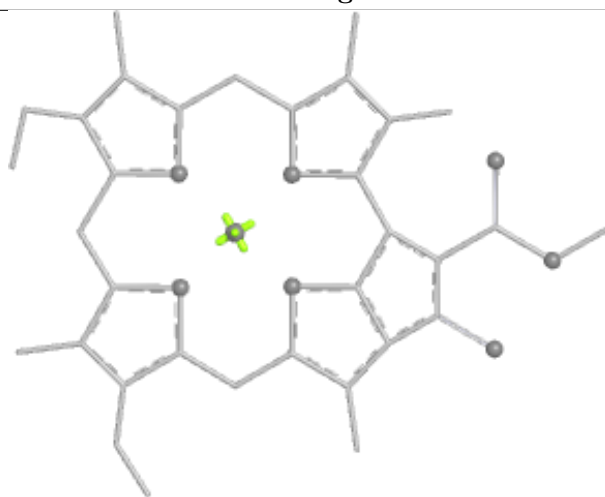
Bond lengths



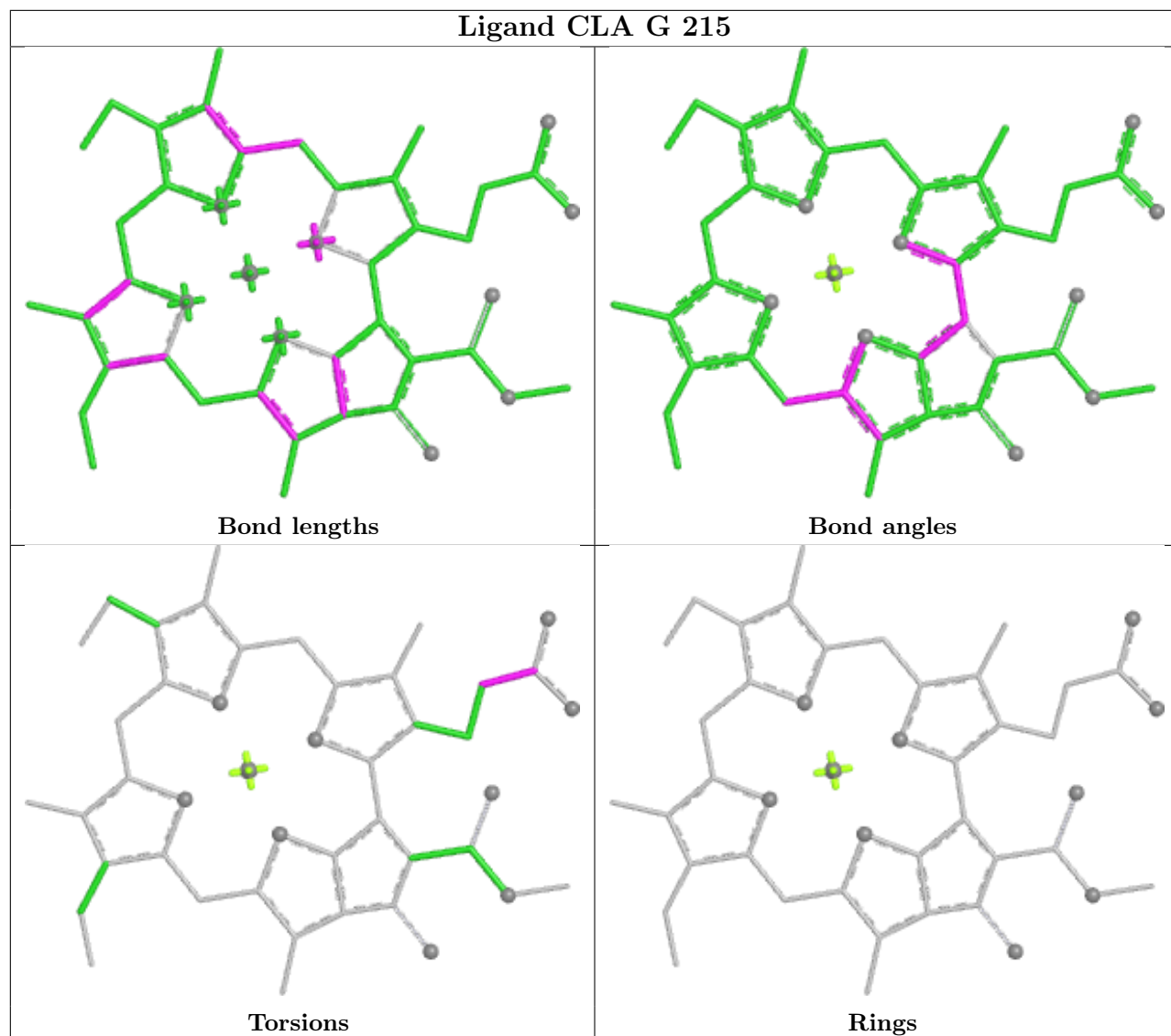
Bond angles



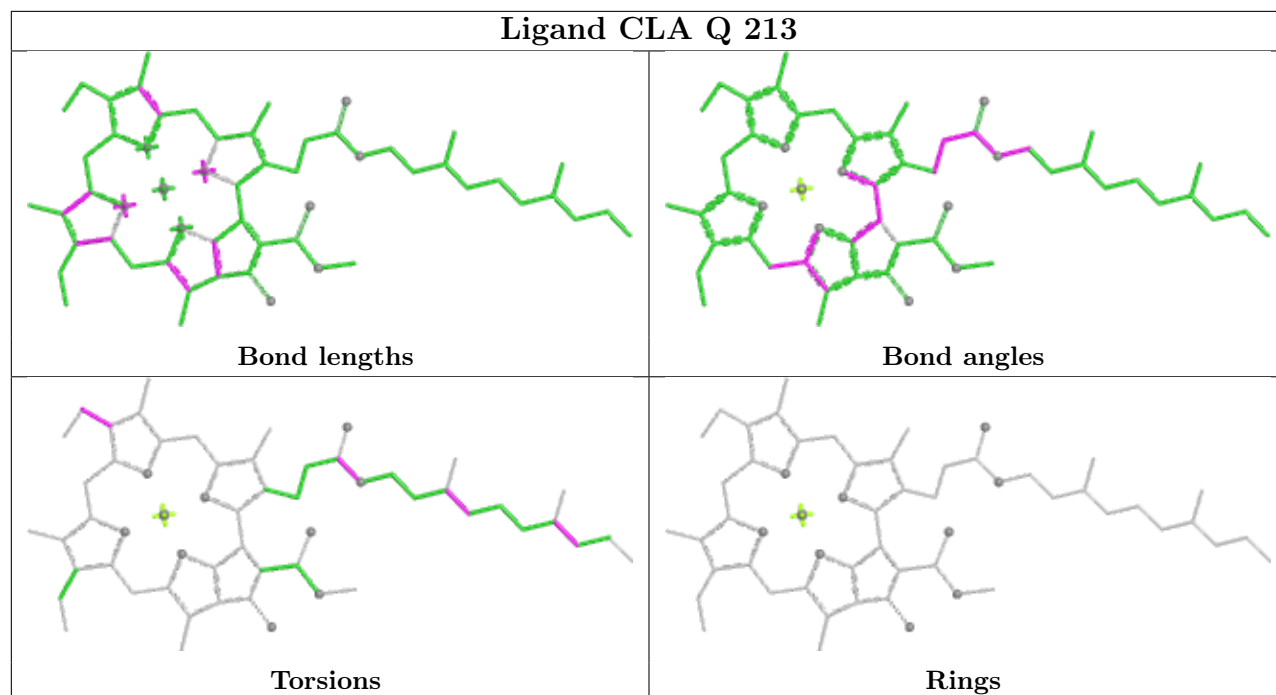
Torsions



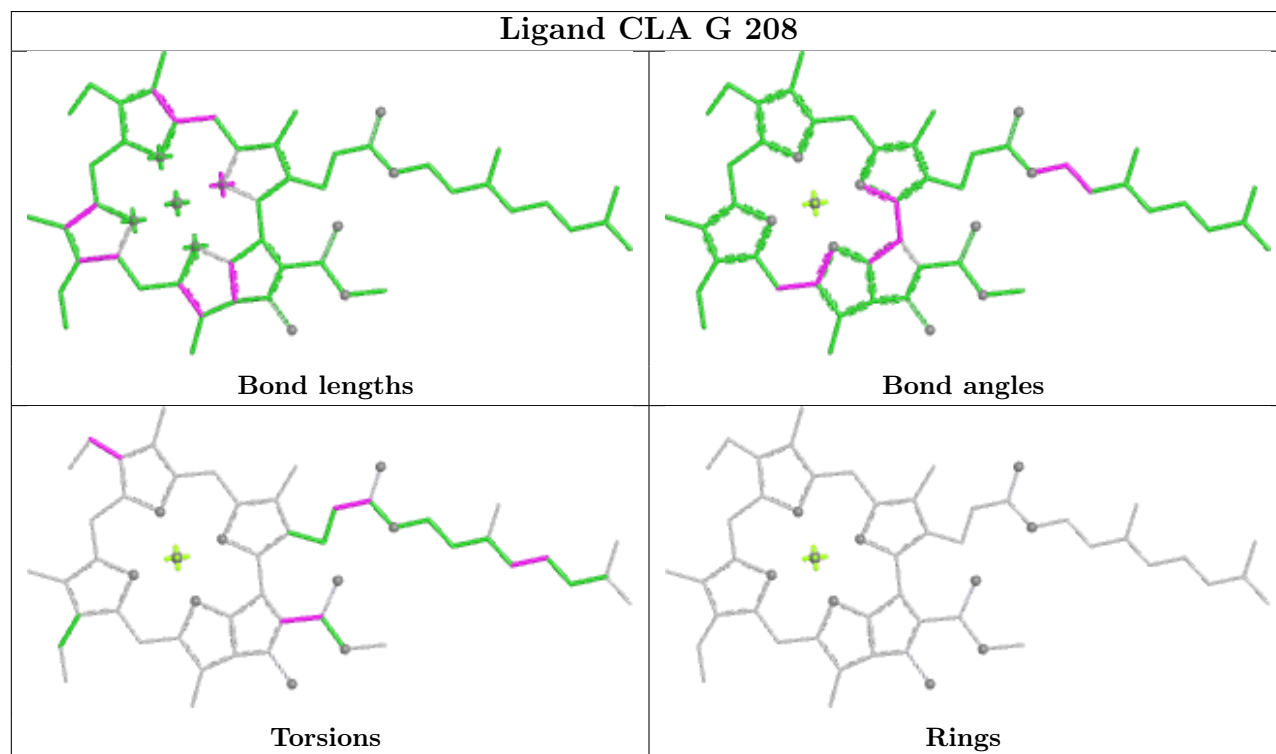
Rings

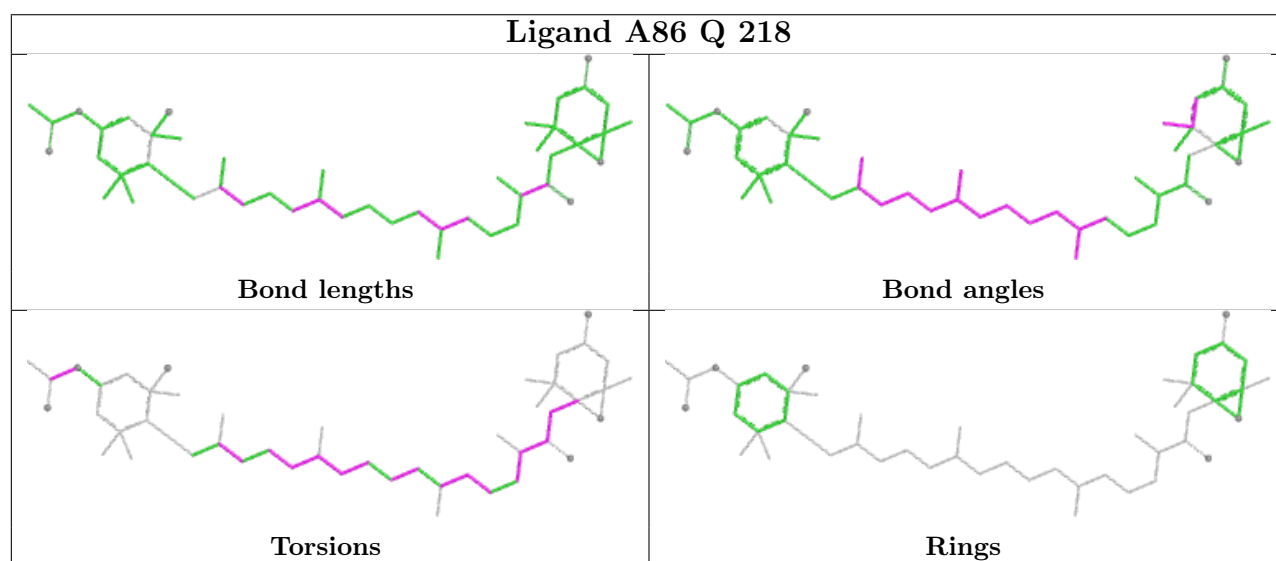
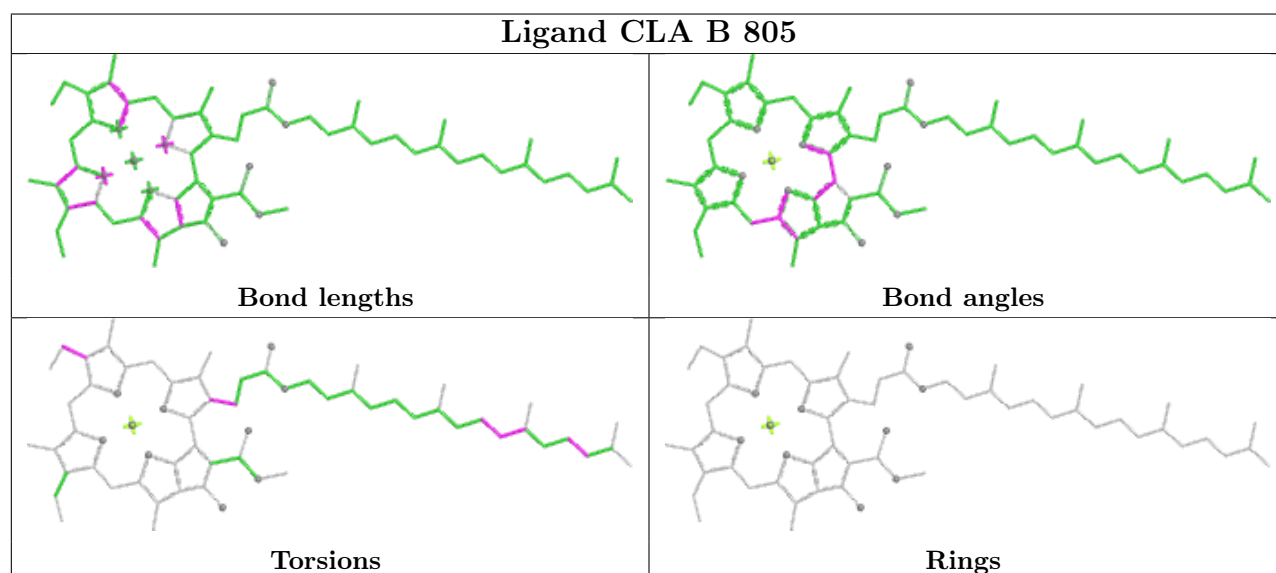
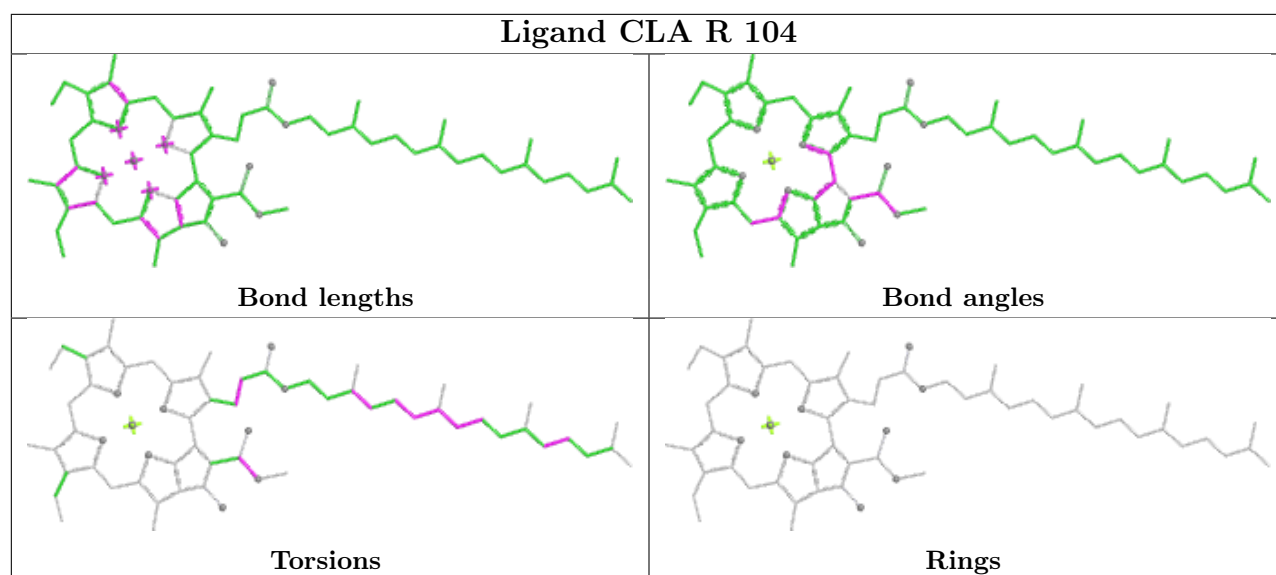


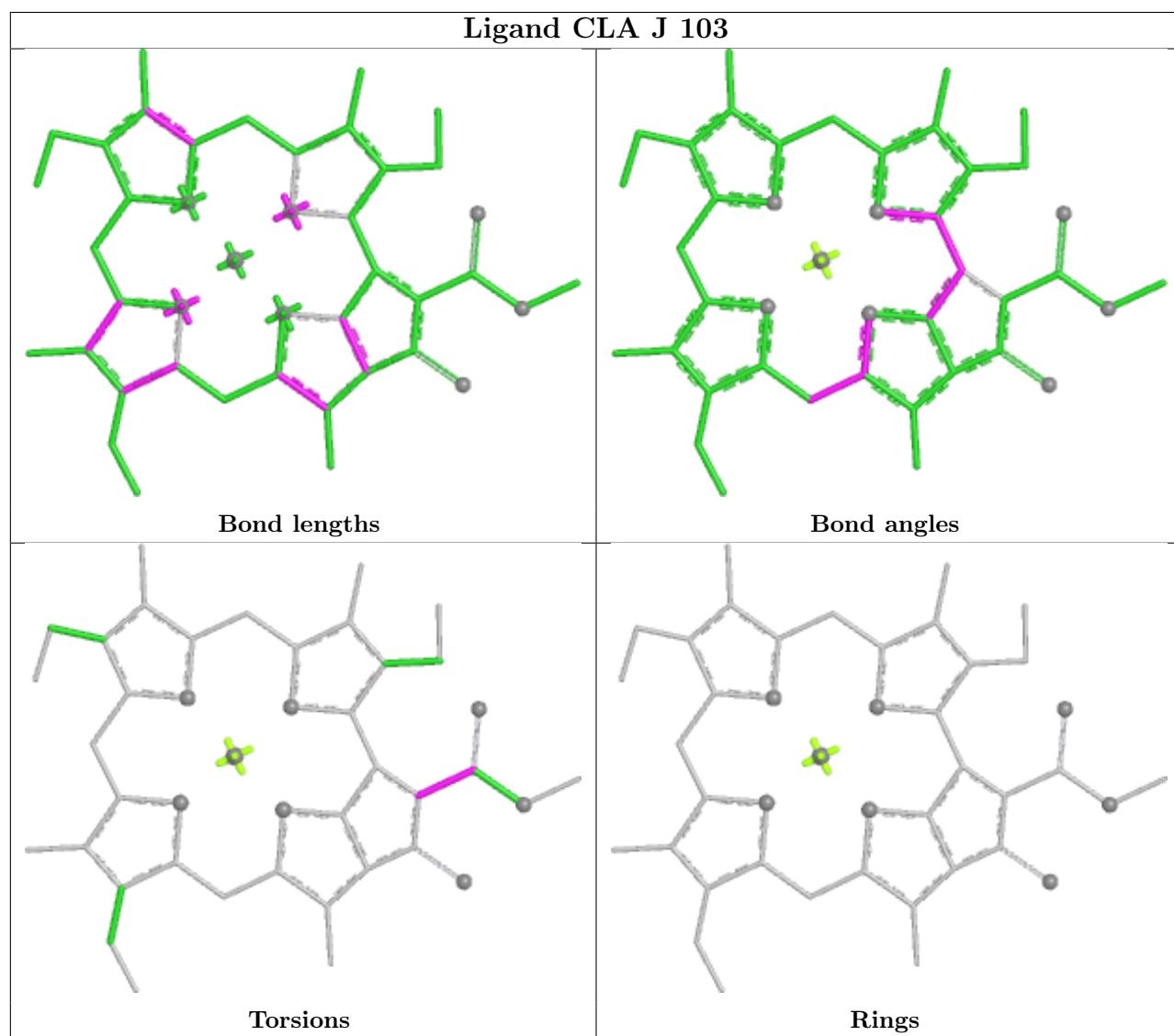
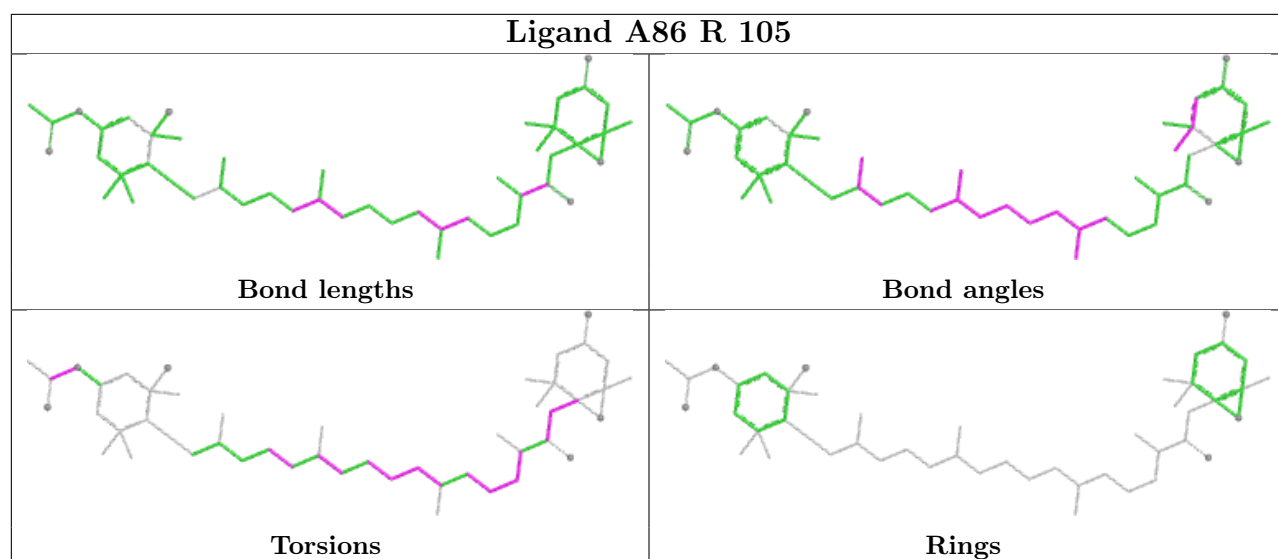
Ligand CLA Q 213

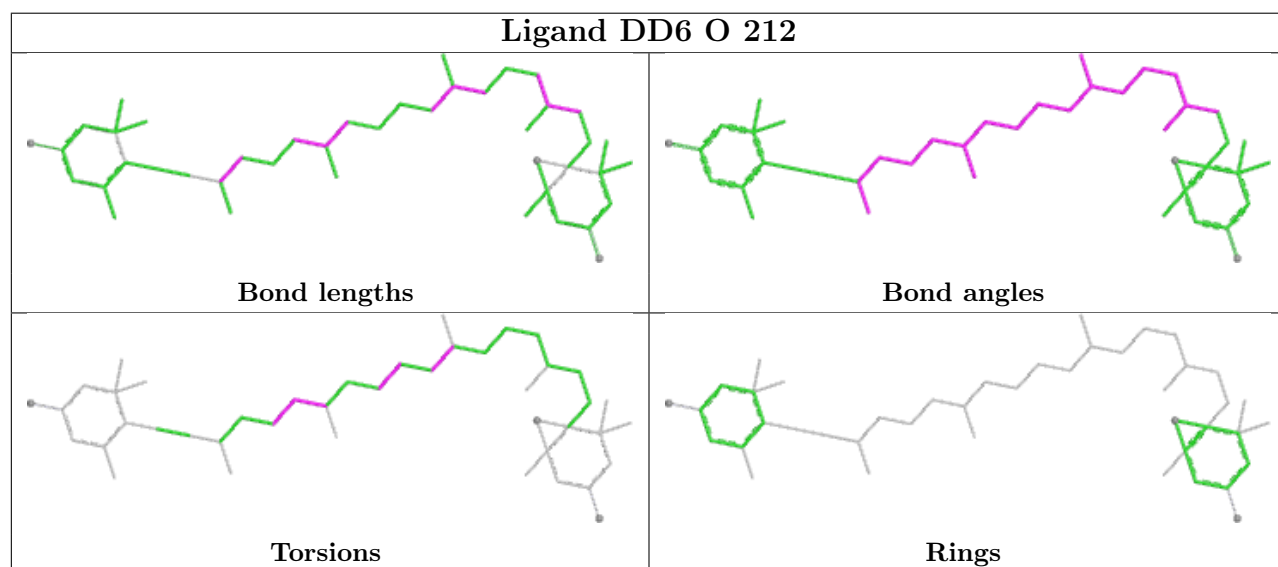
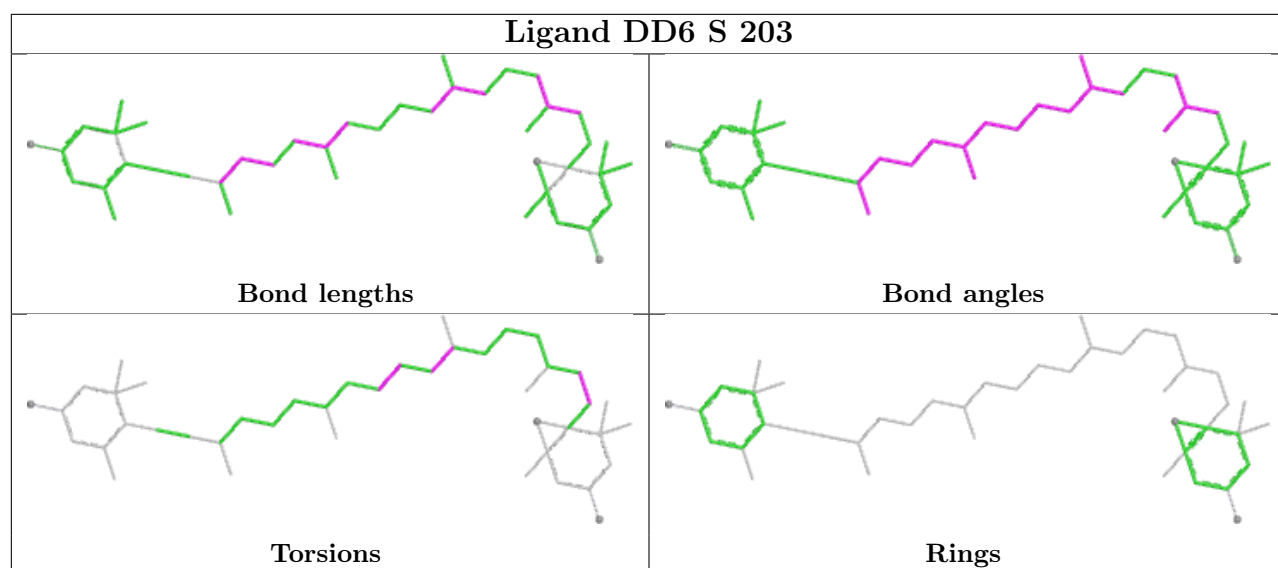


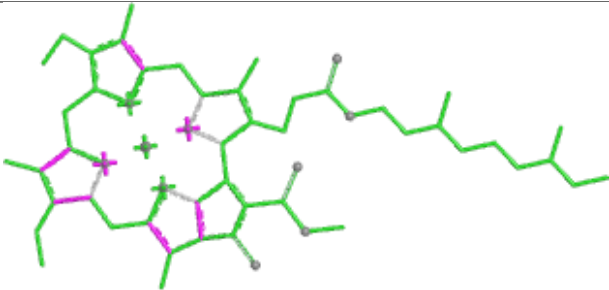
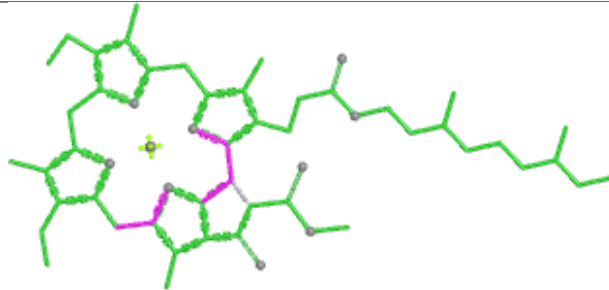
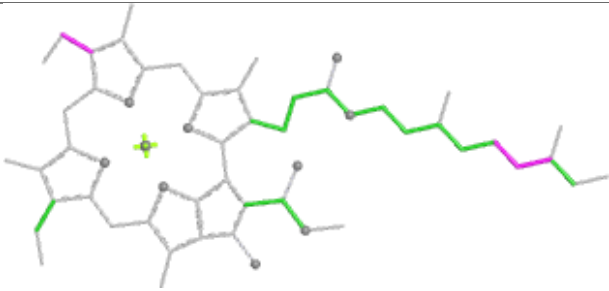
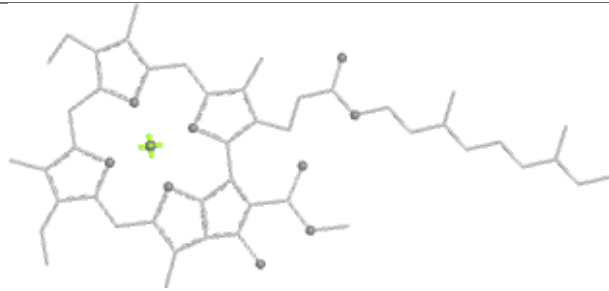
Ligand CLA G 208

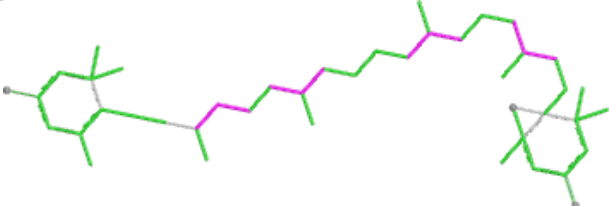
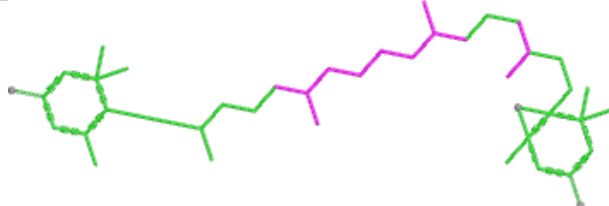
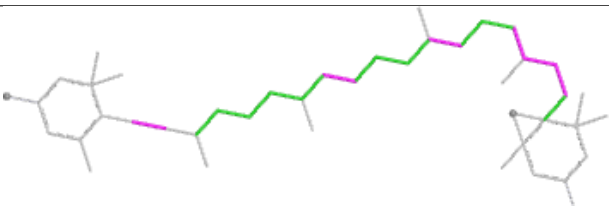
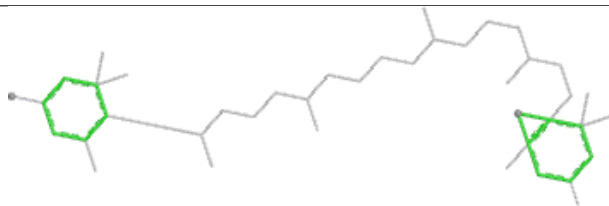


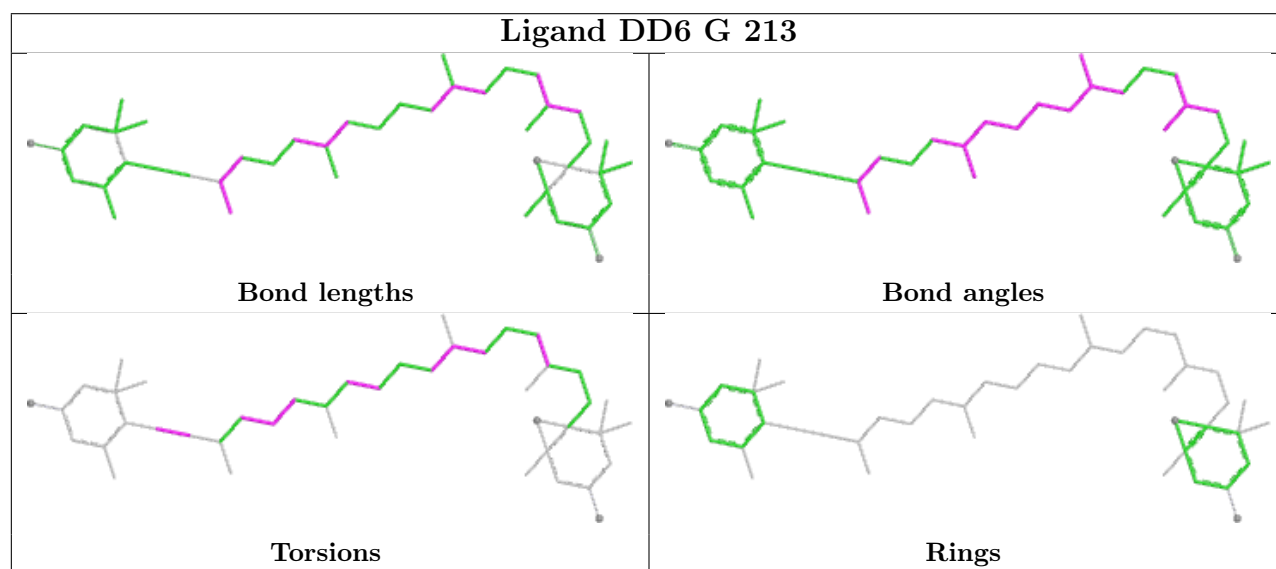
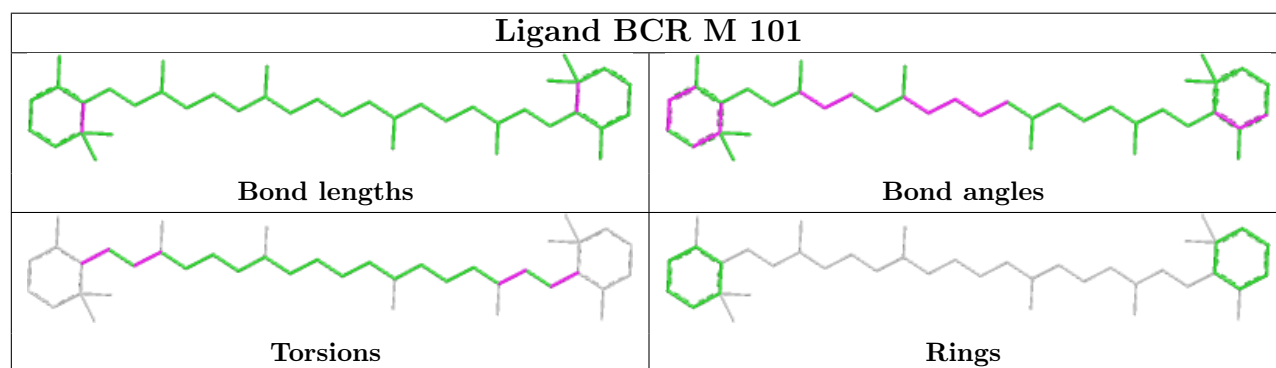
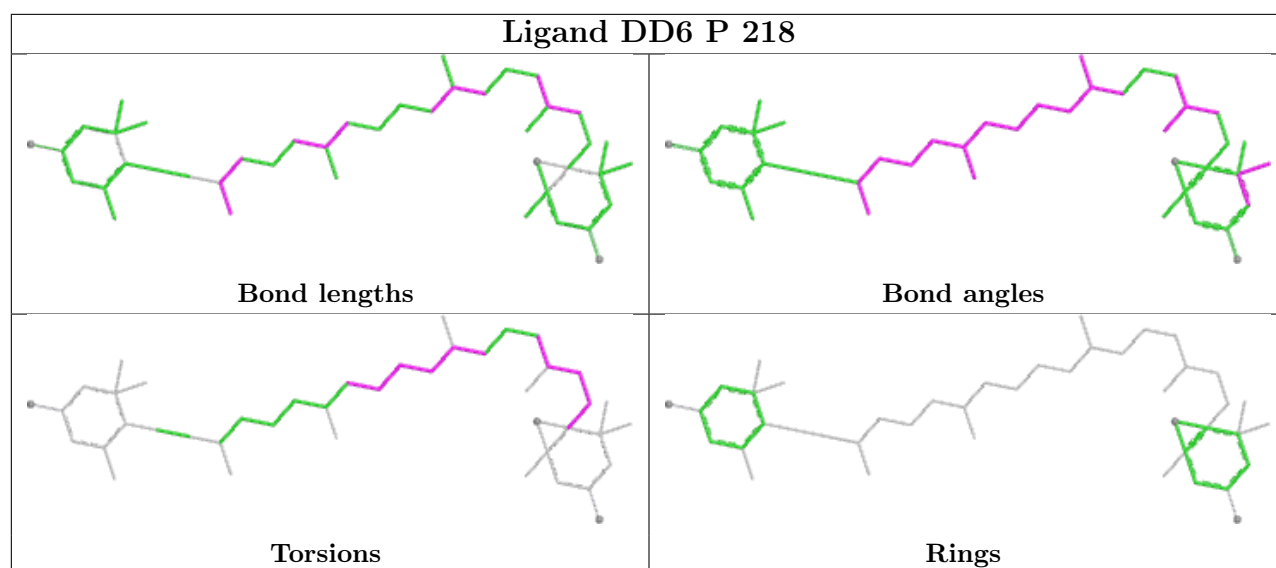


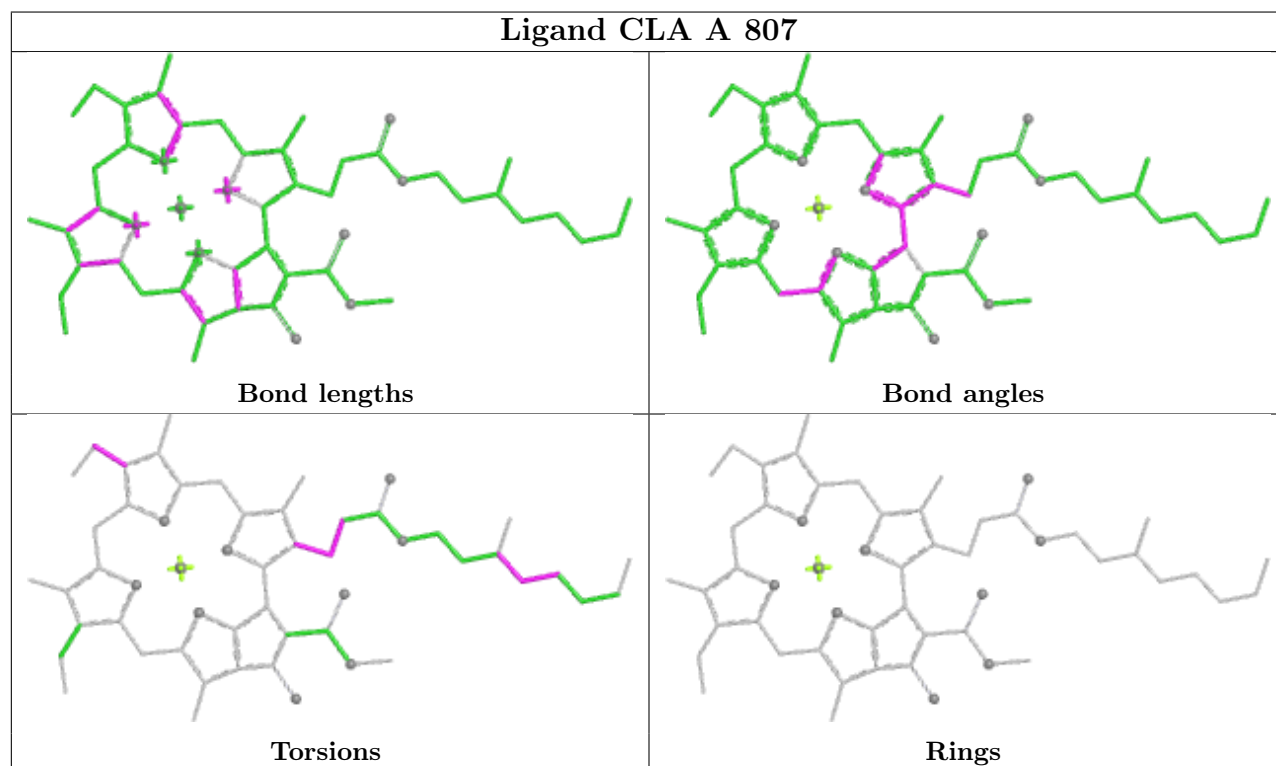
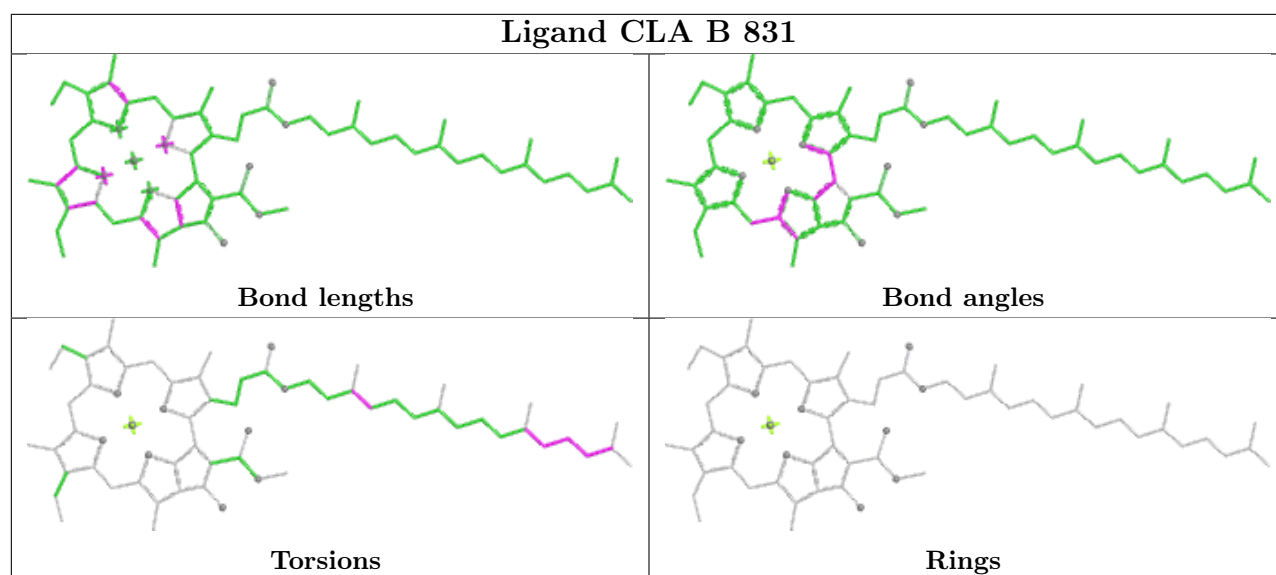


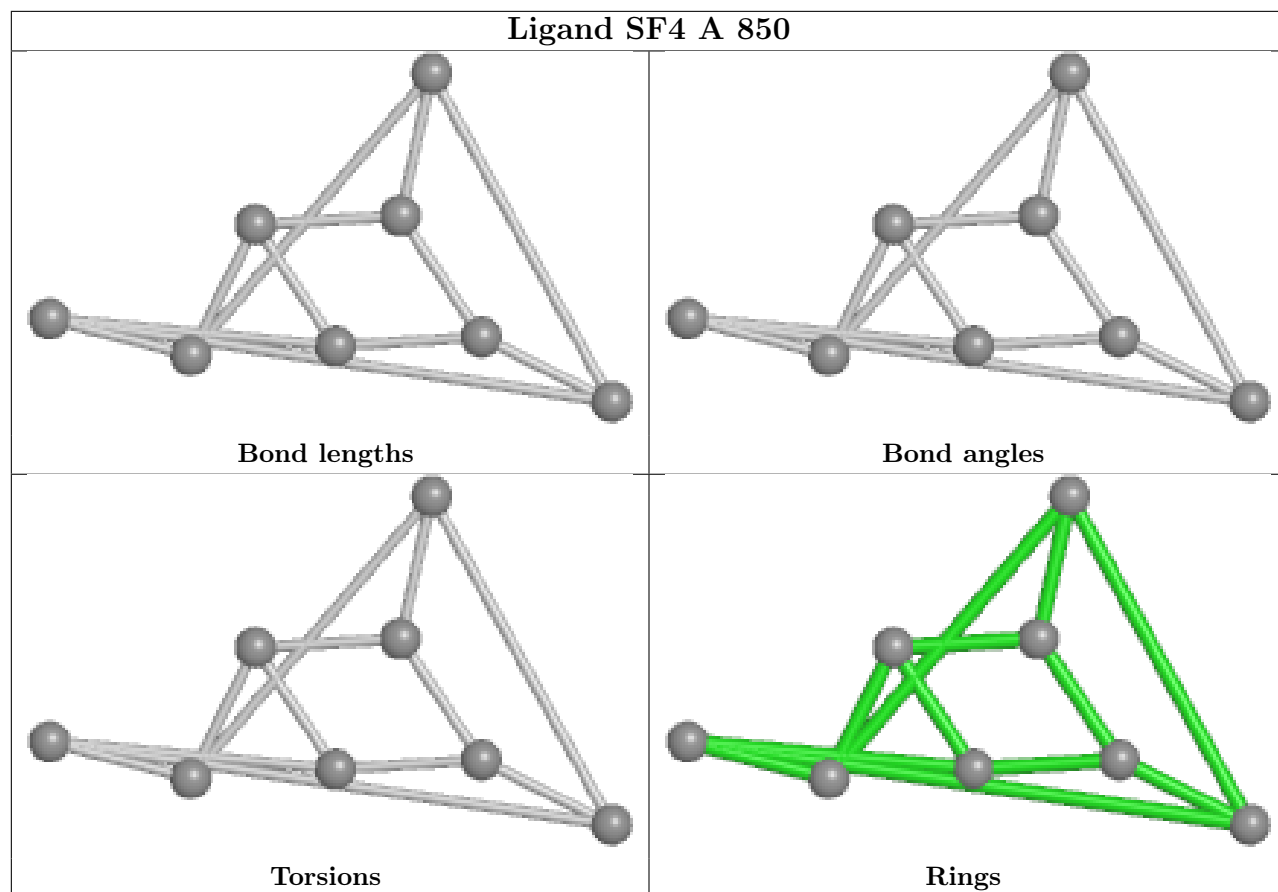


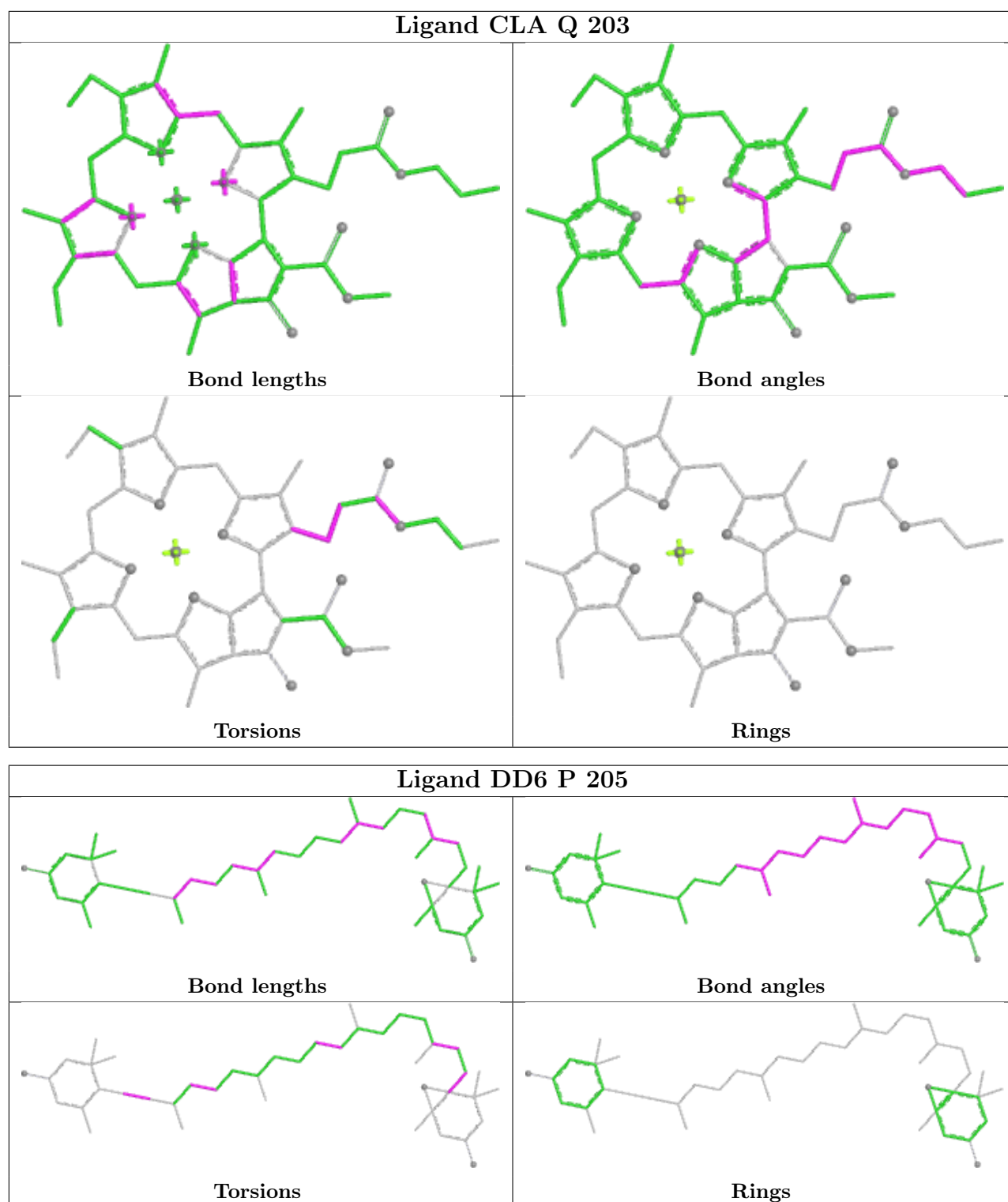
Ligand CLA A 808	
	
Bond lengths	Bond angles
	
Torsions	Rings

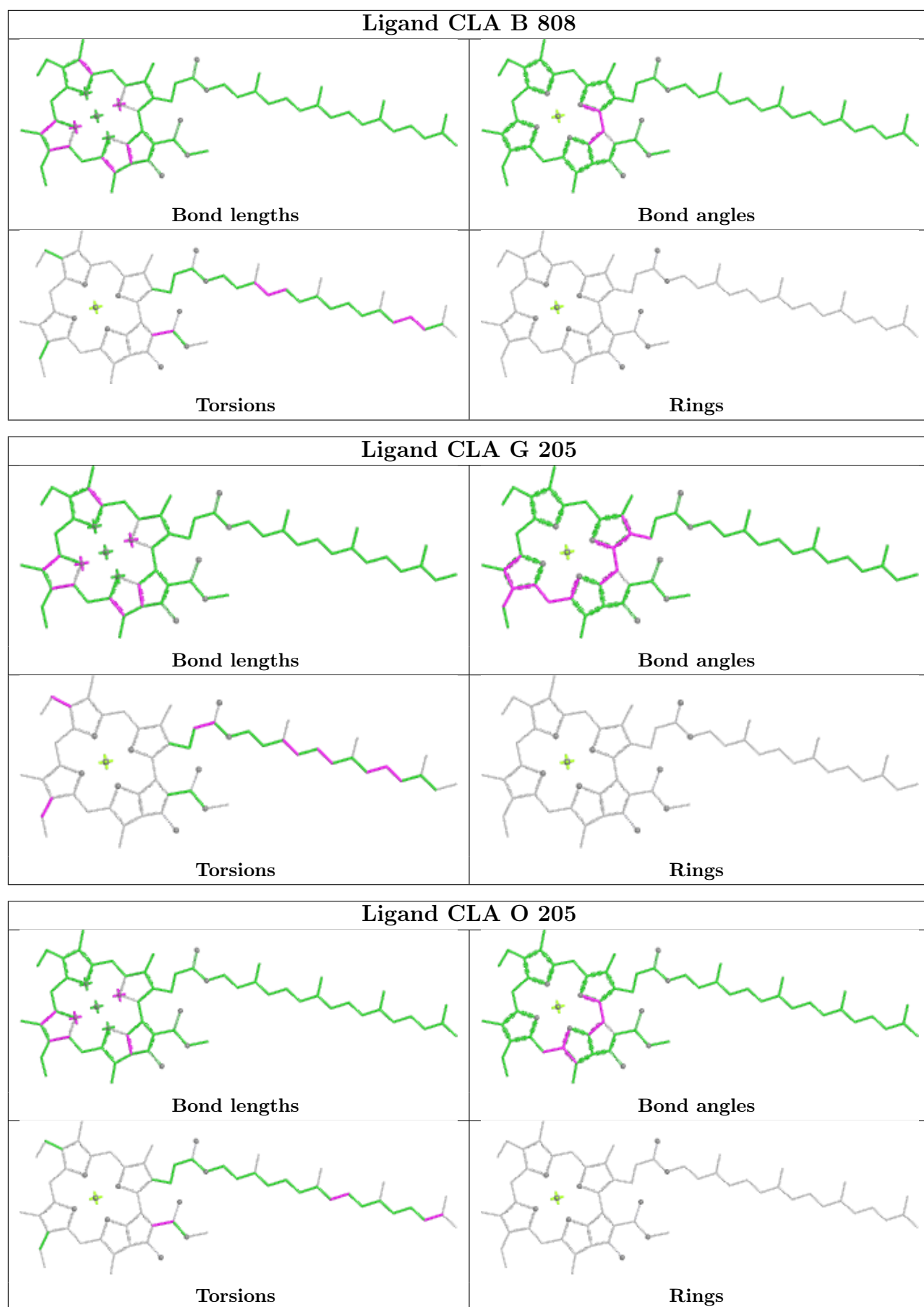
Ligand DD6 O 213	
	
Bond lengths	Bond angles
	
Torsions	Rings

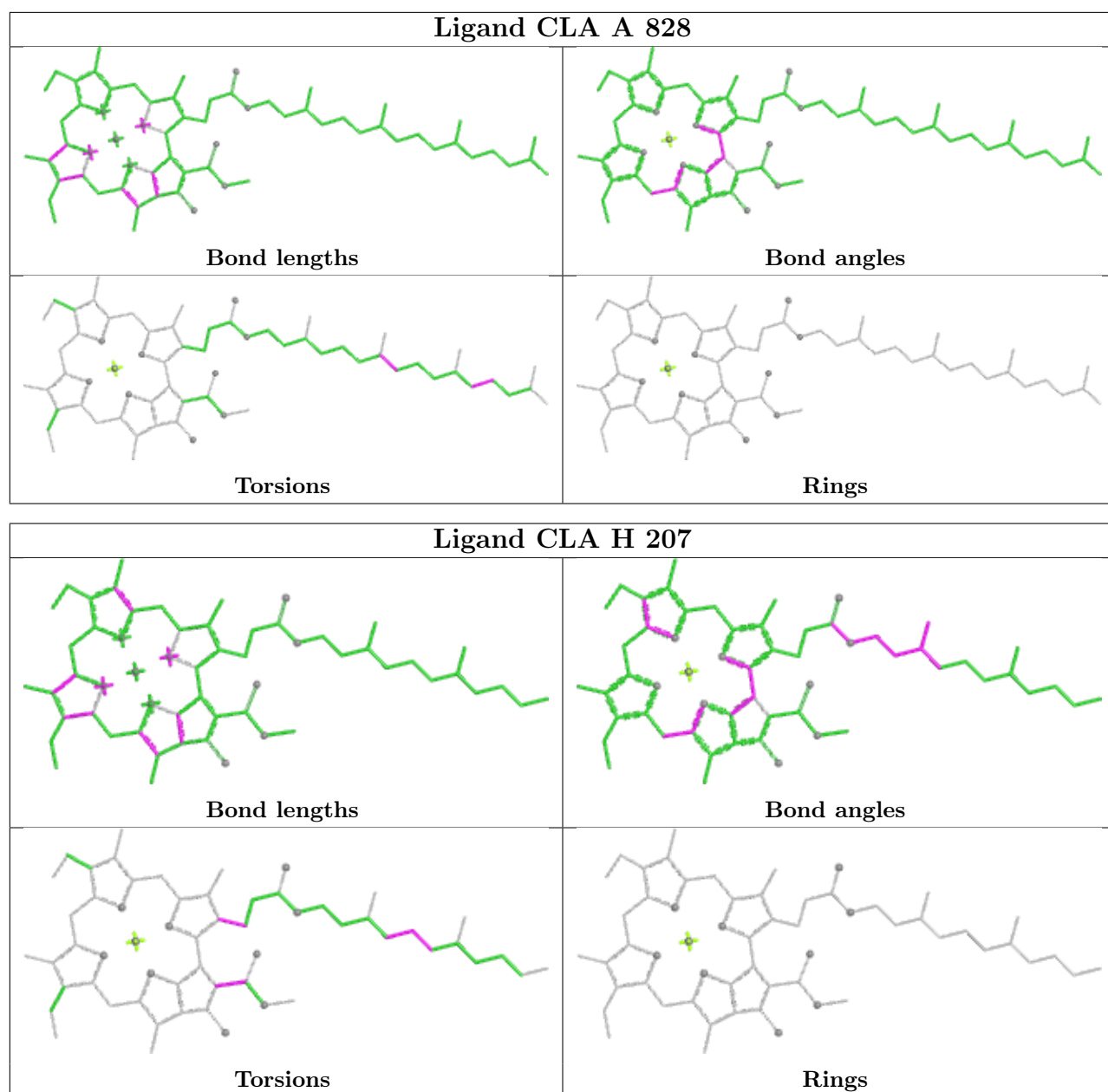


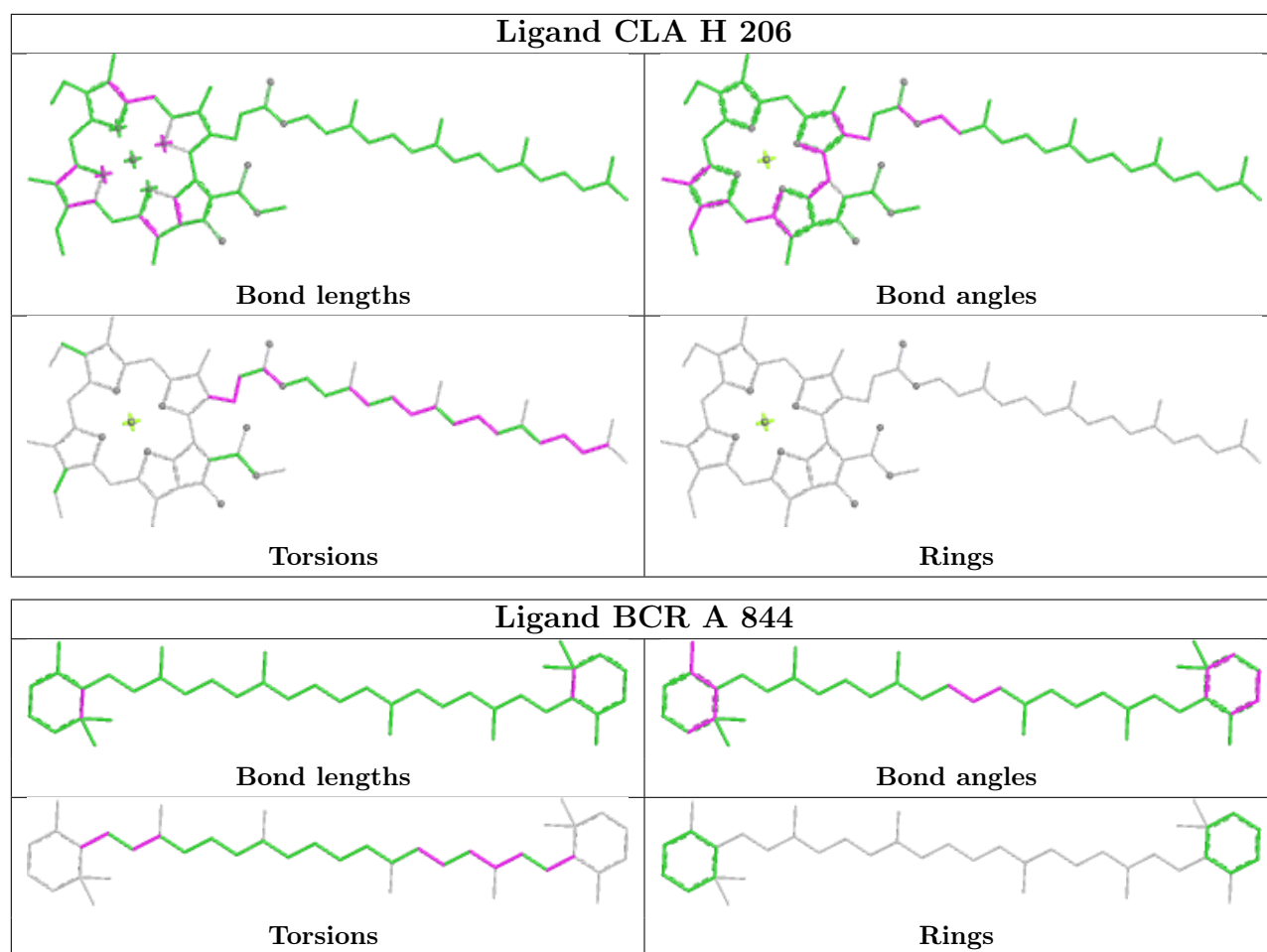




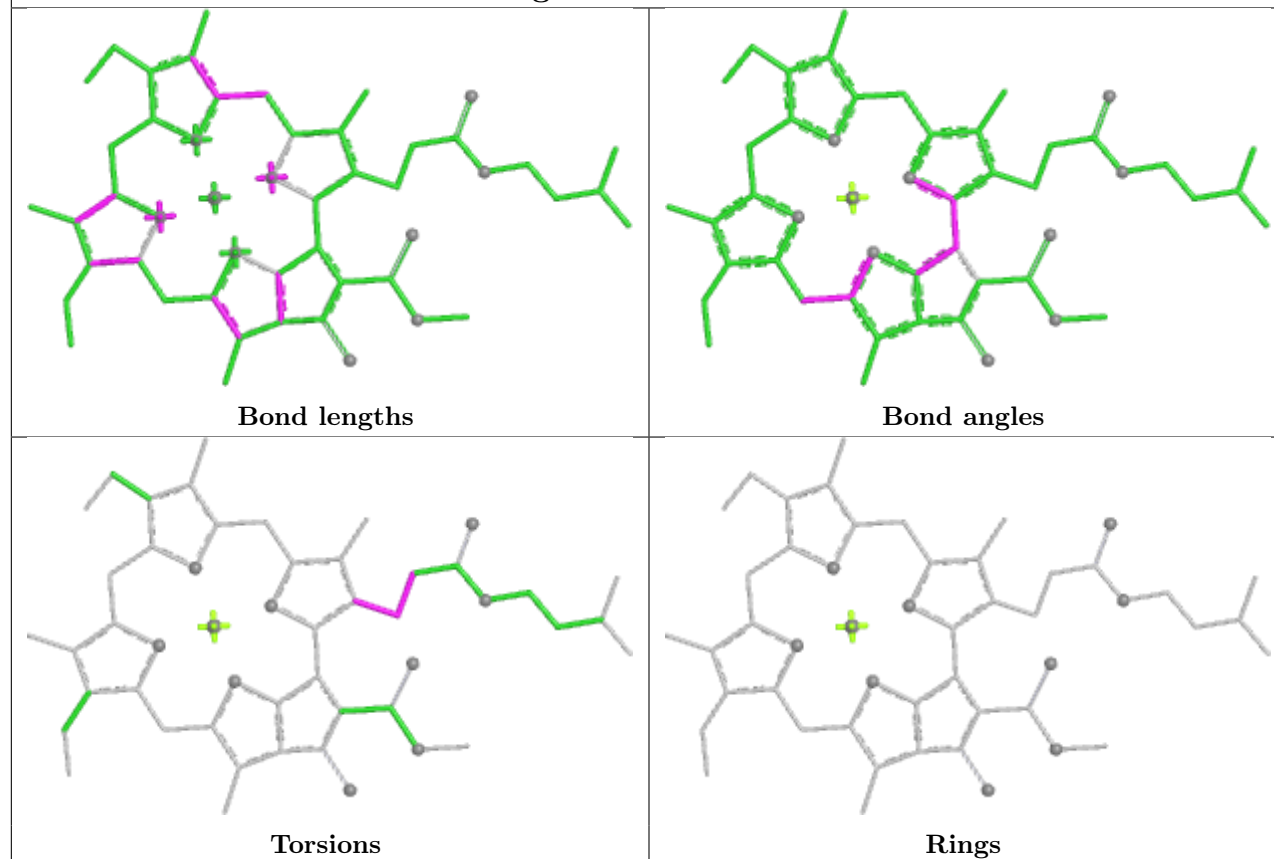




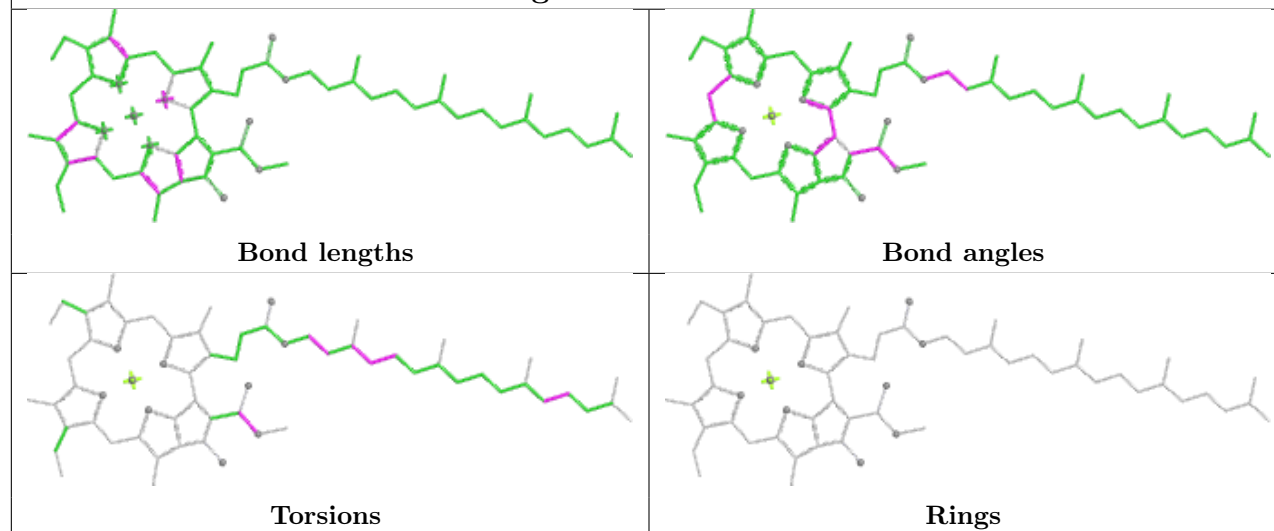


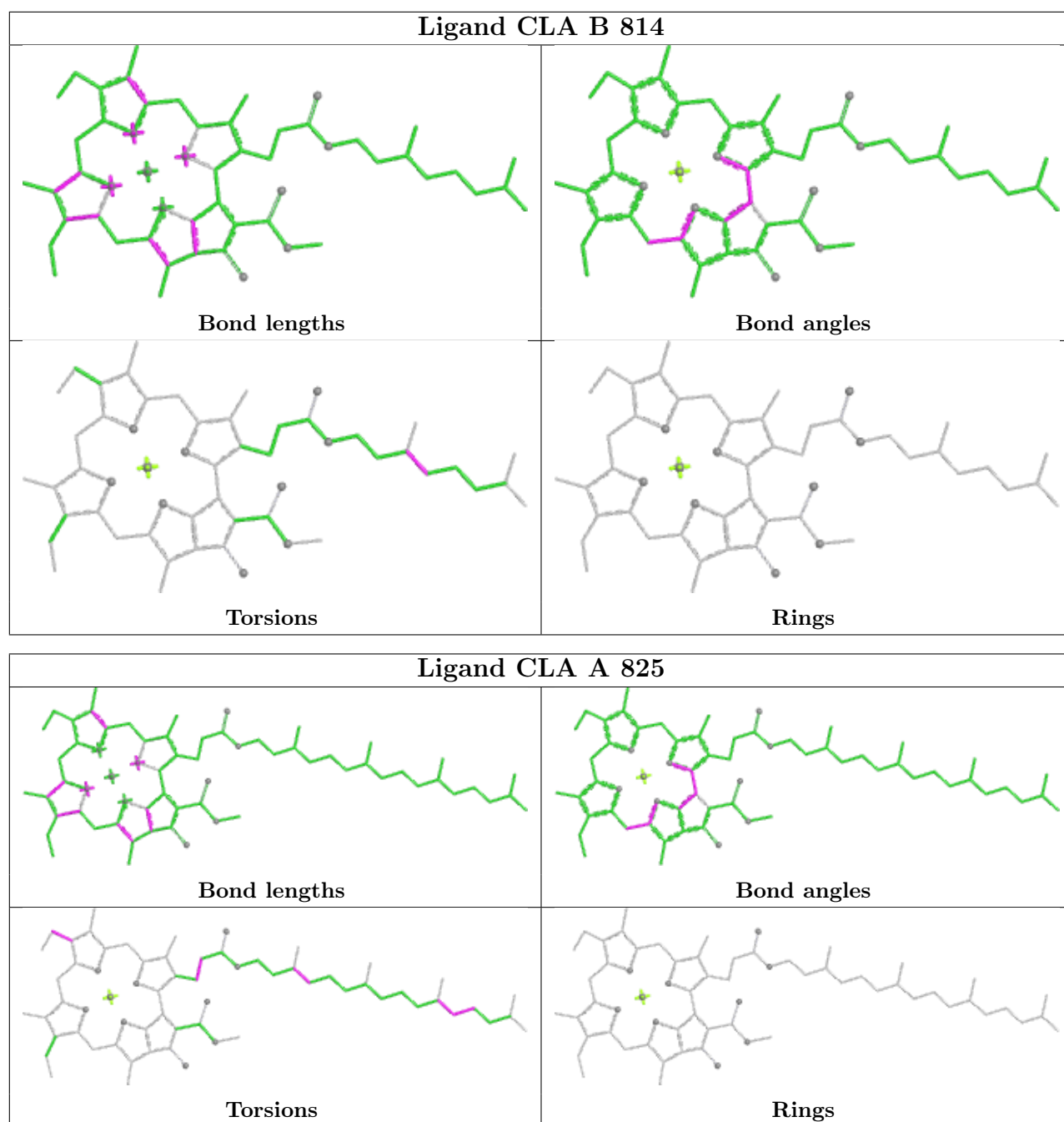


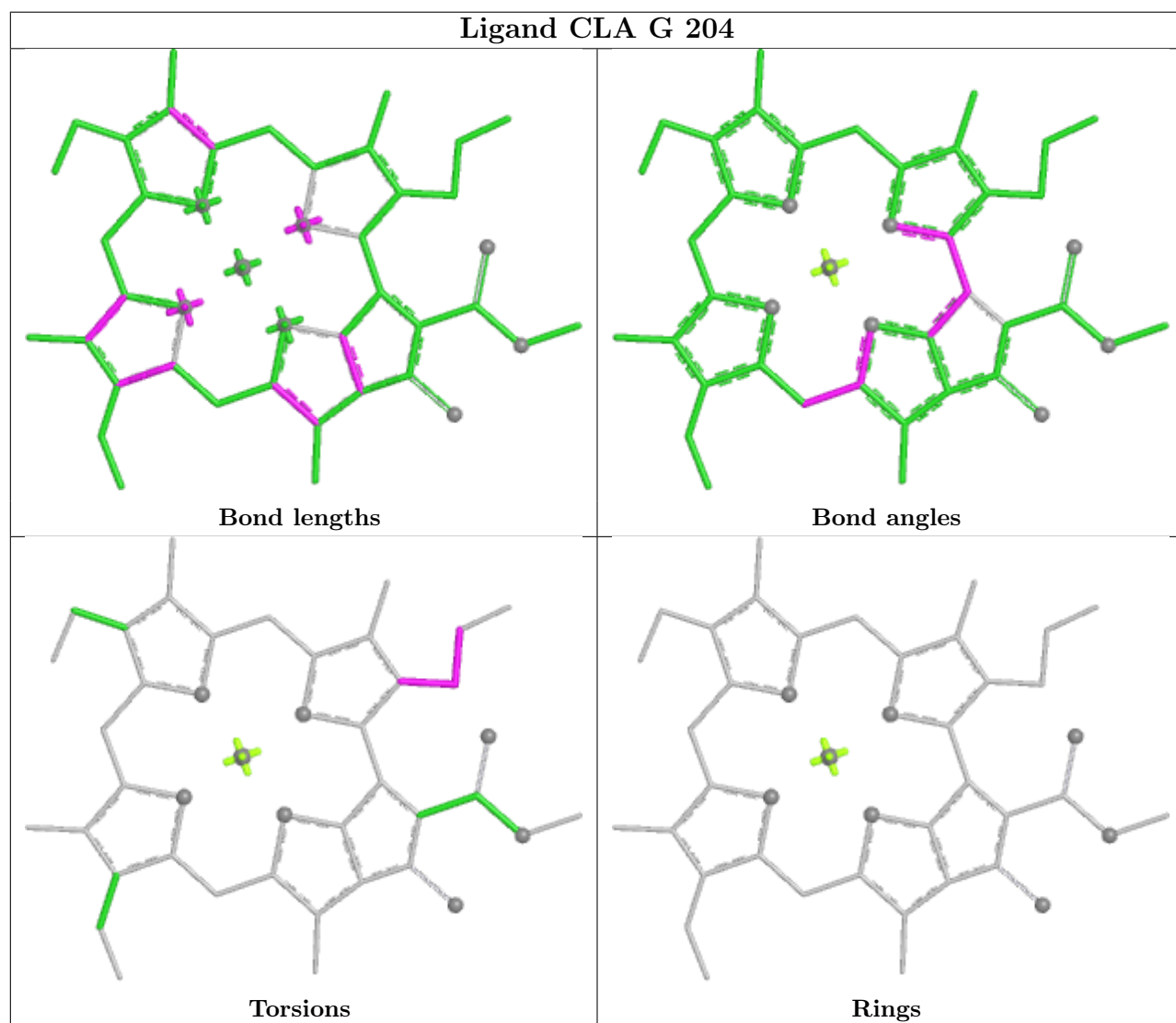
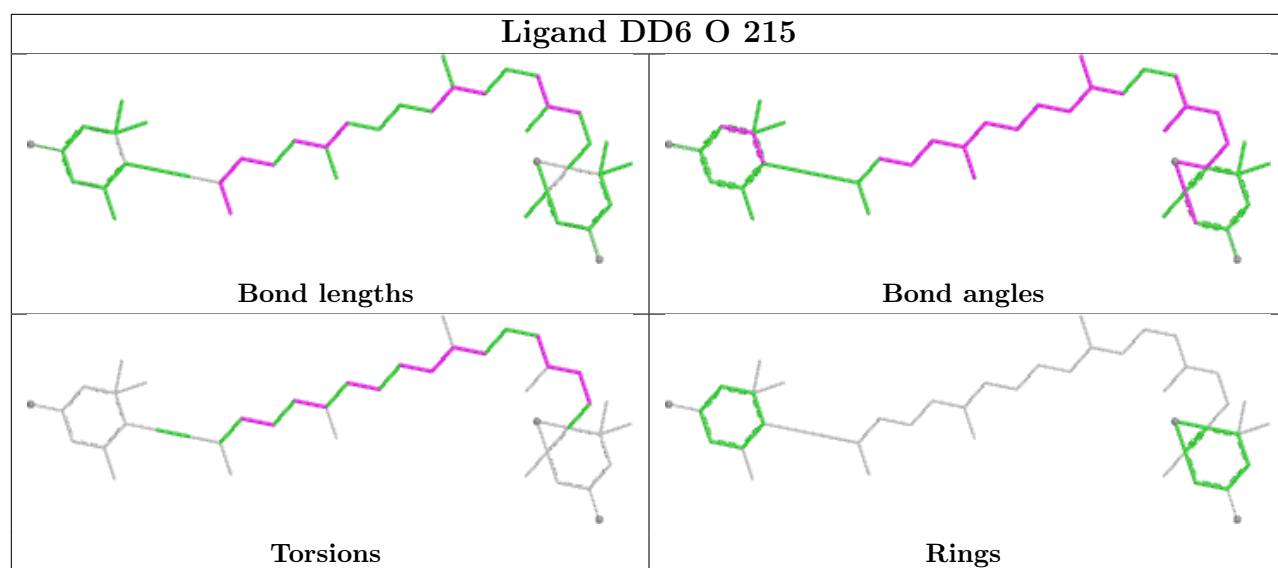
Ligand CLA B 848

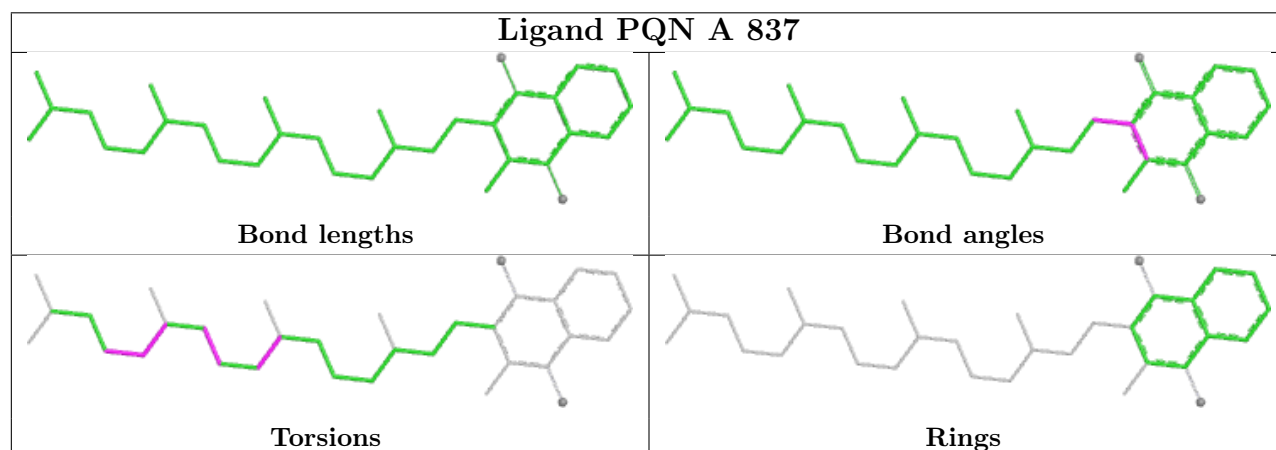
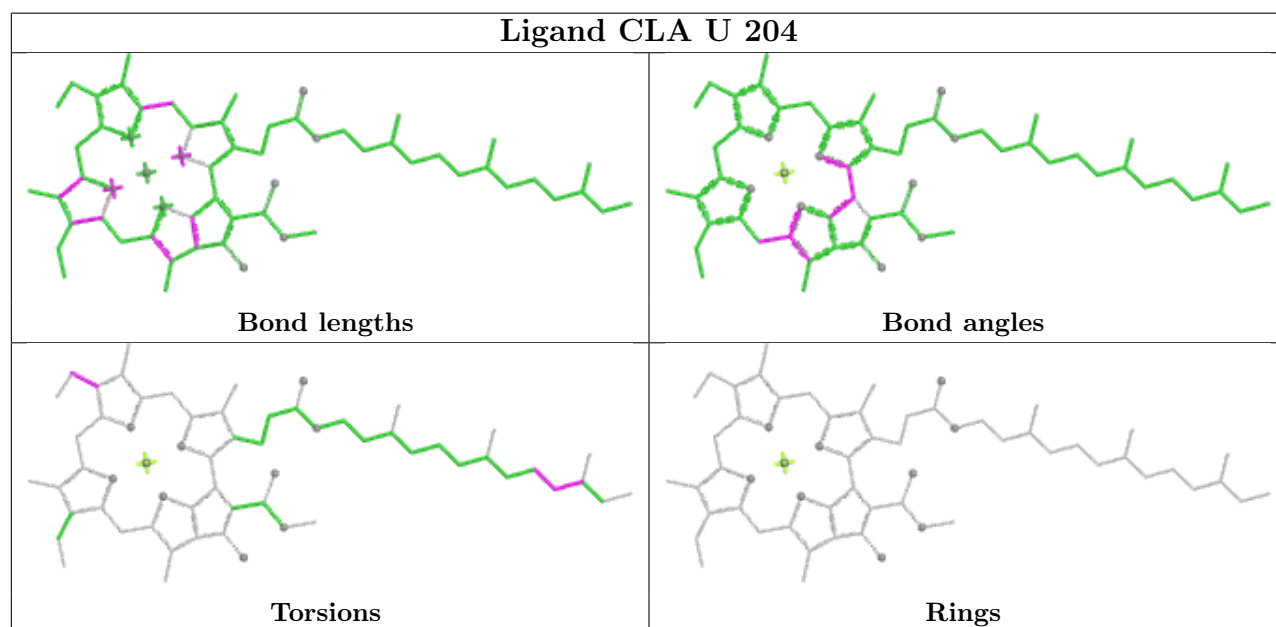
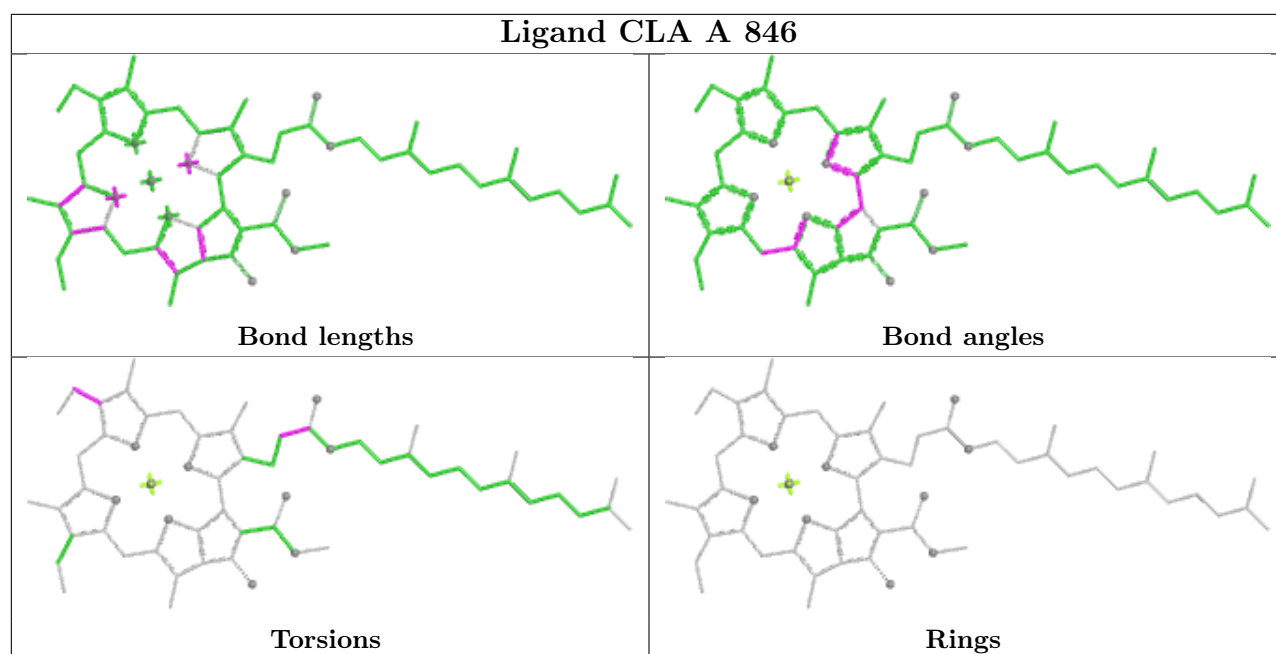


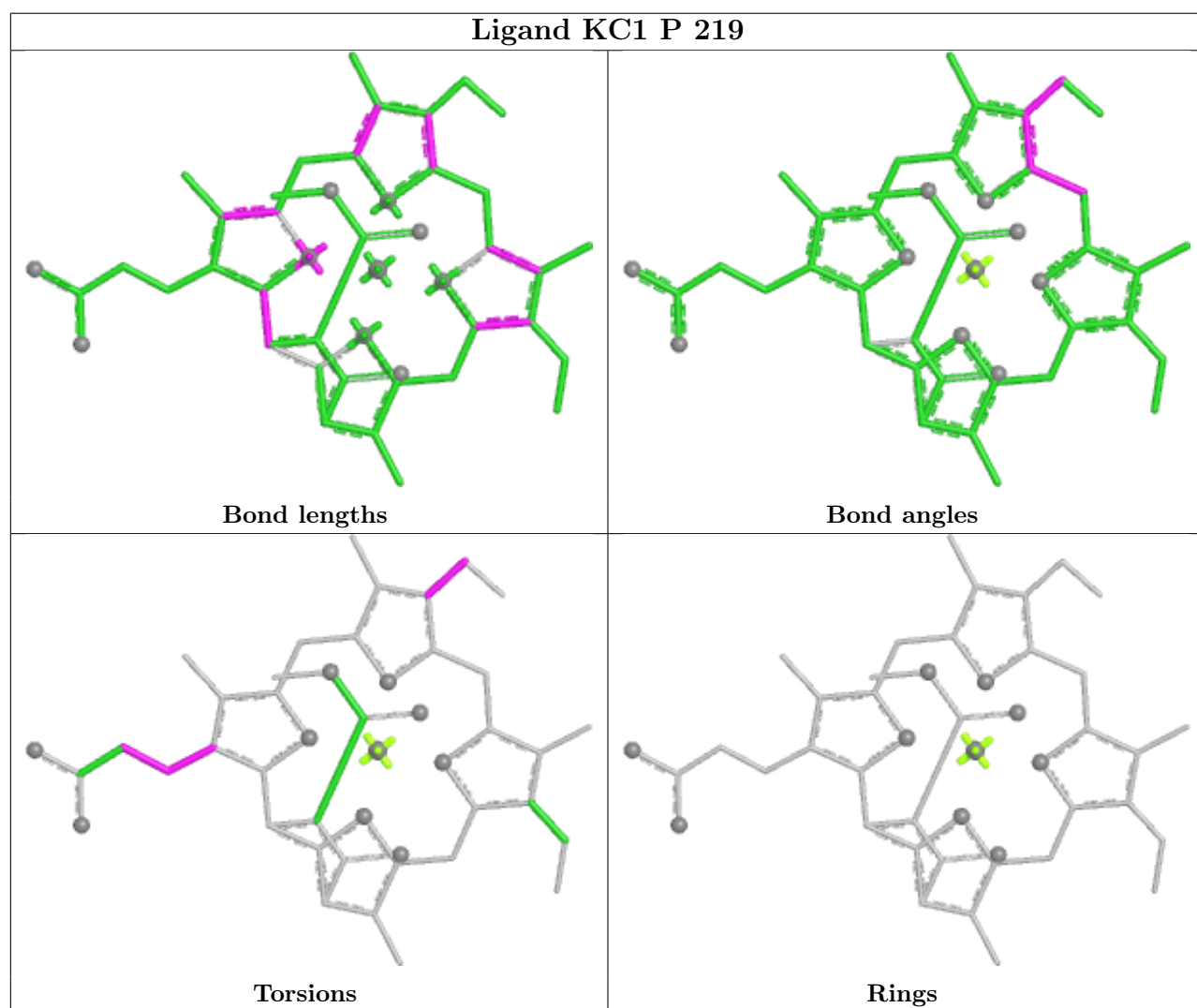
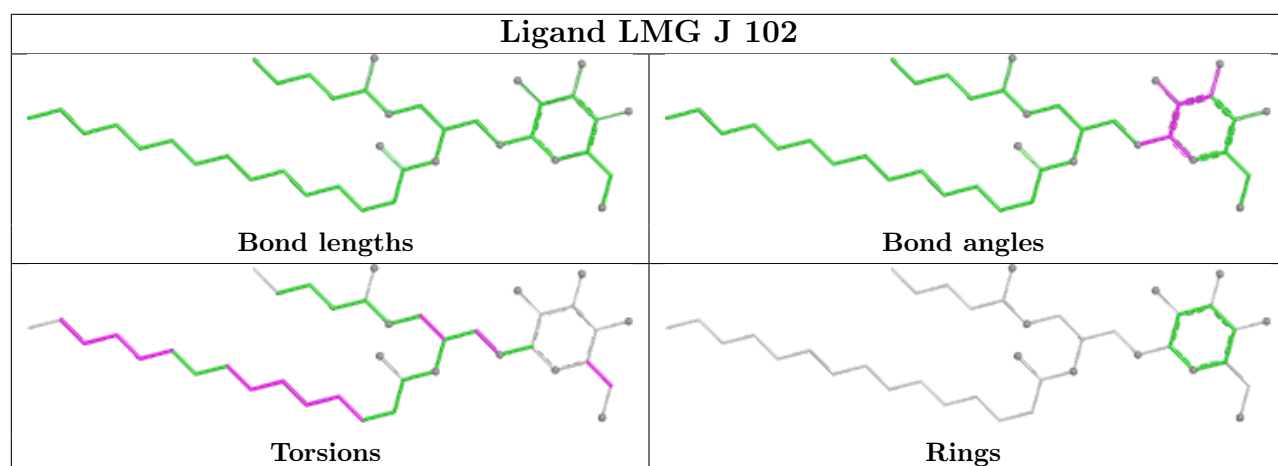
Ligand CLA O 209

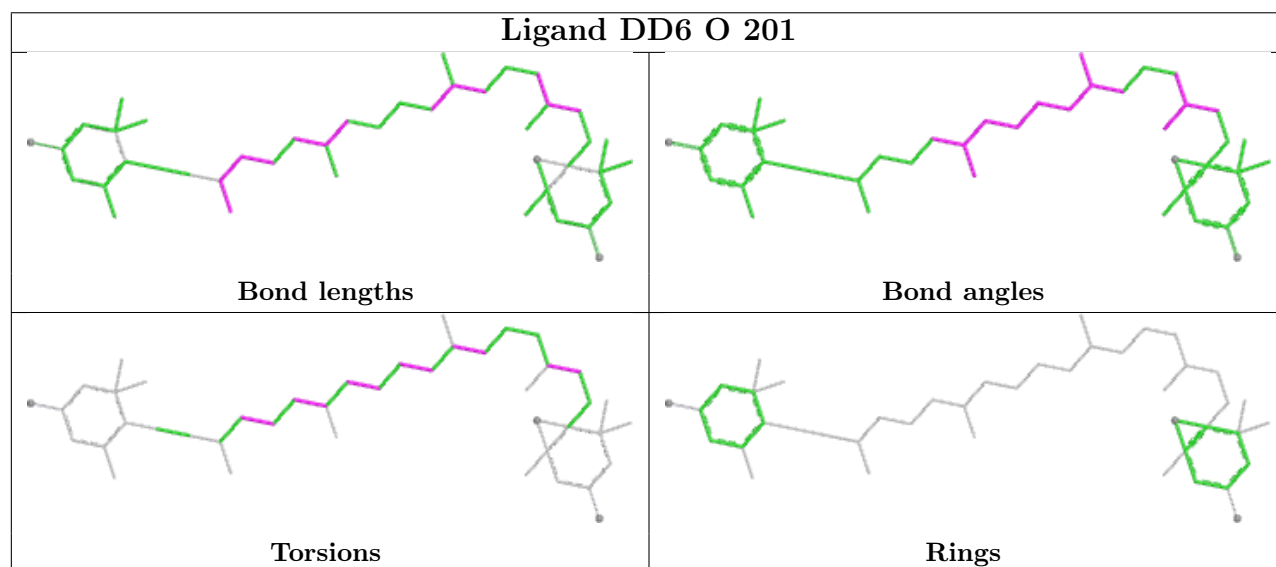
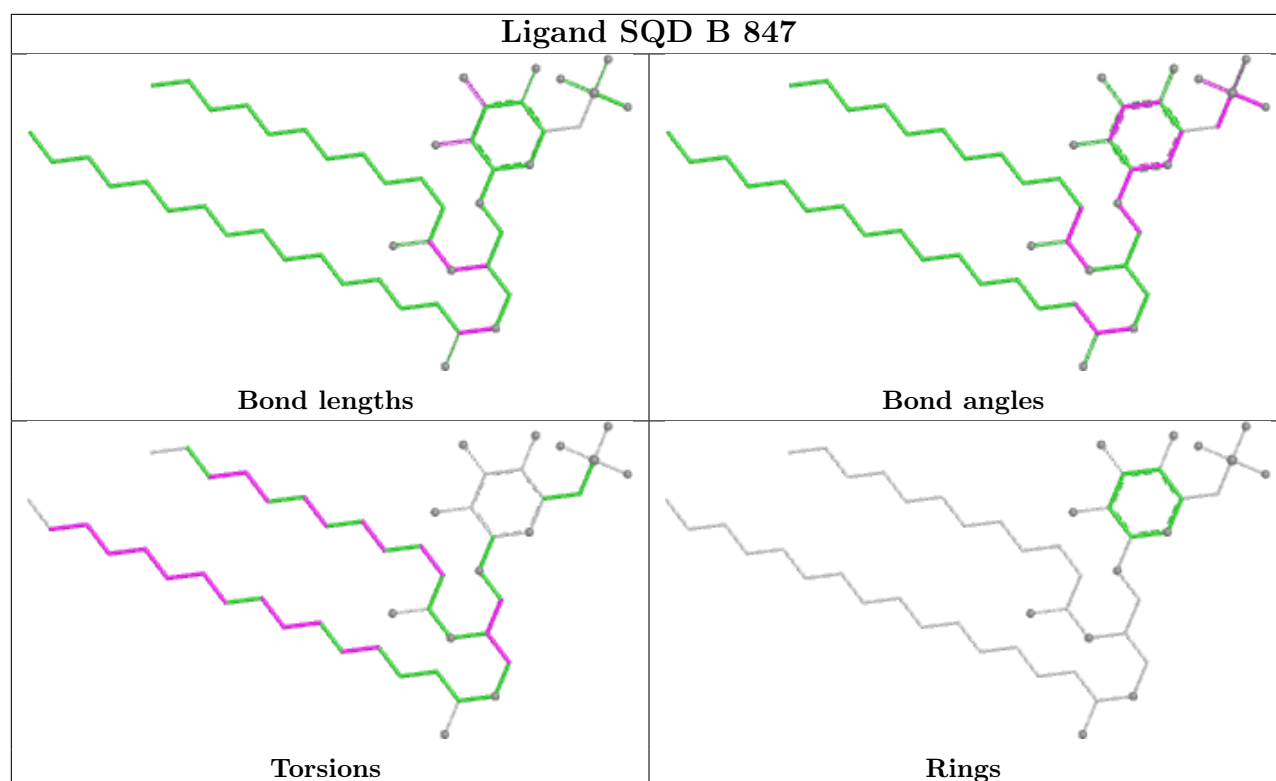


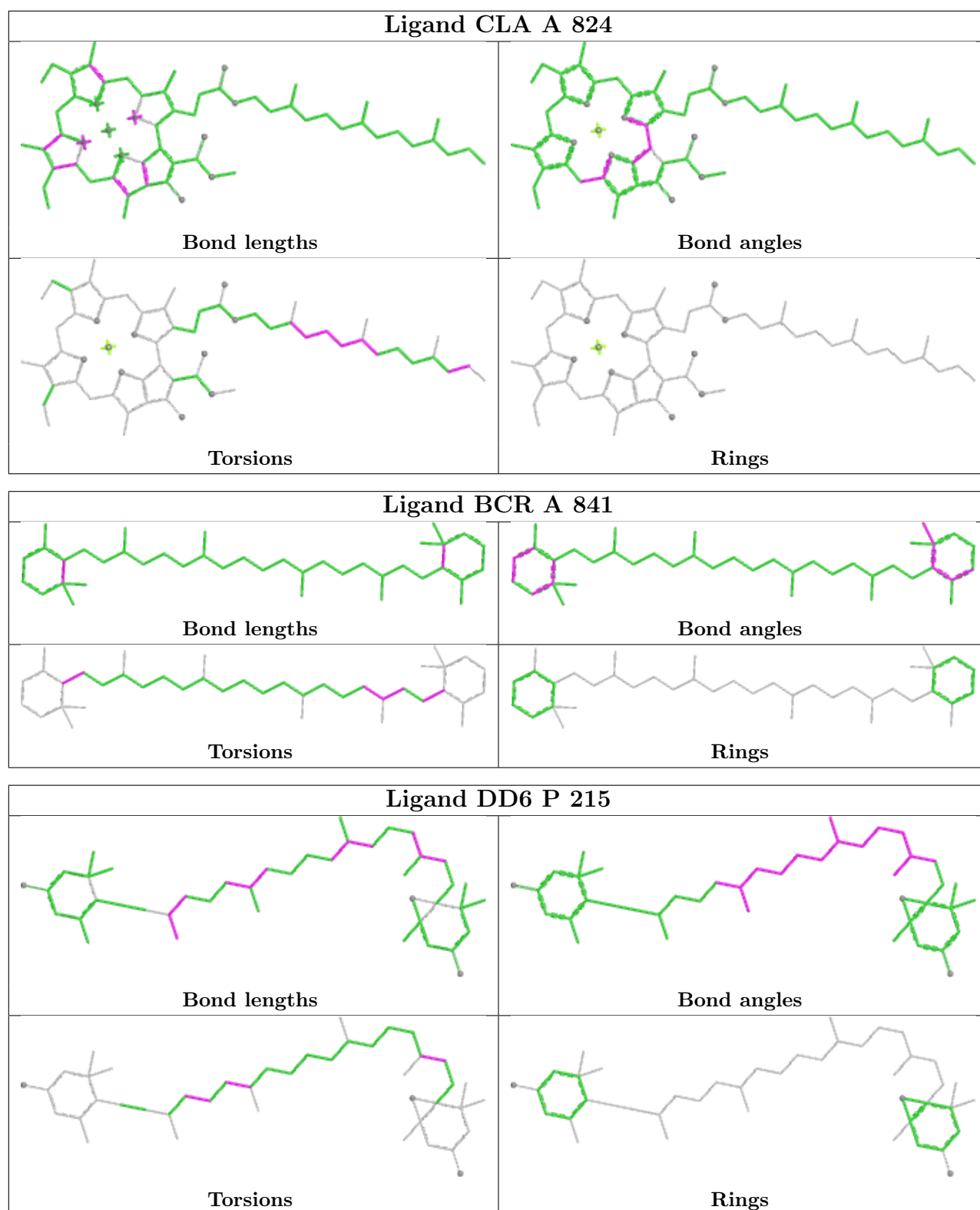


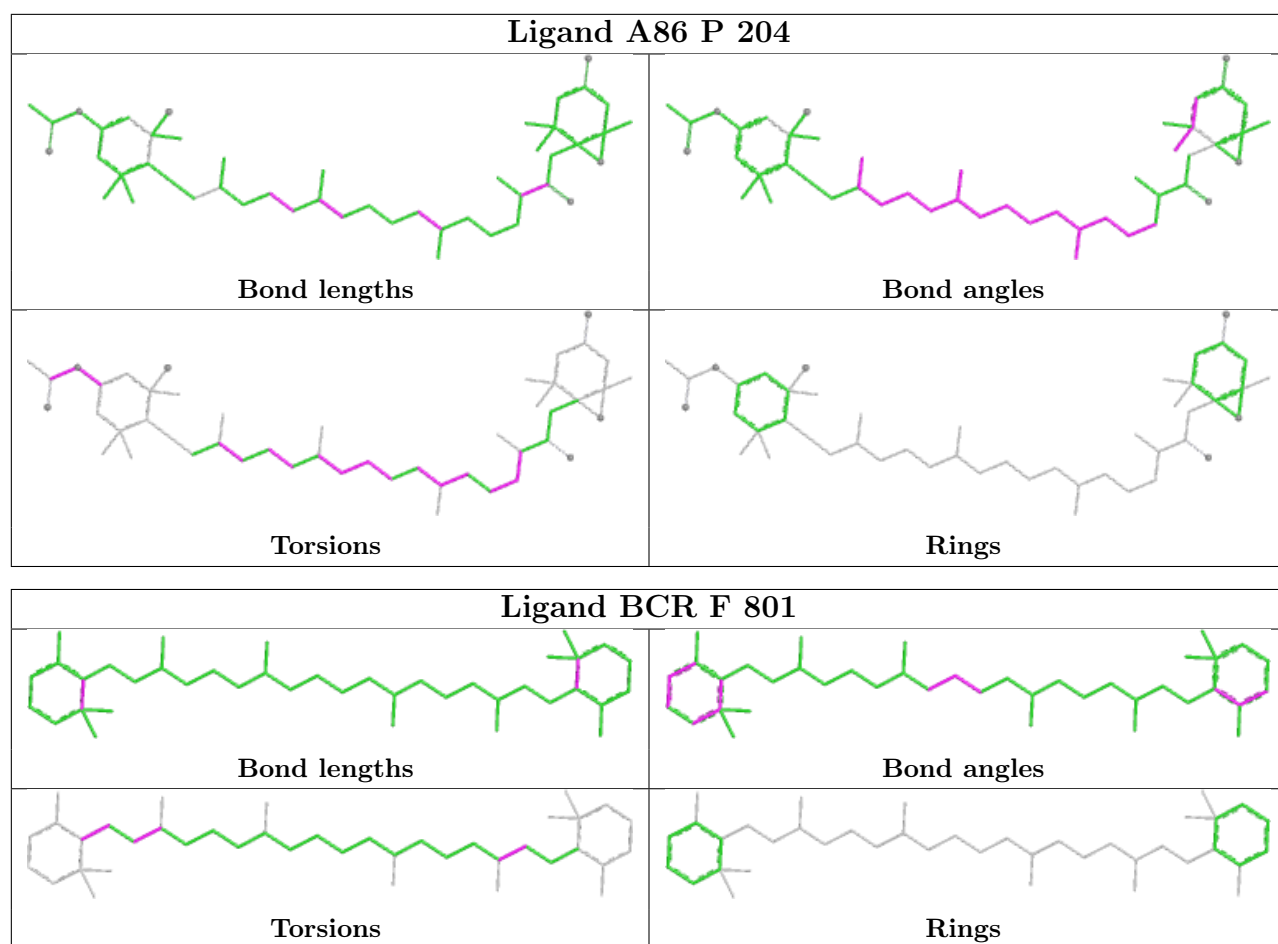


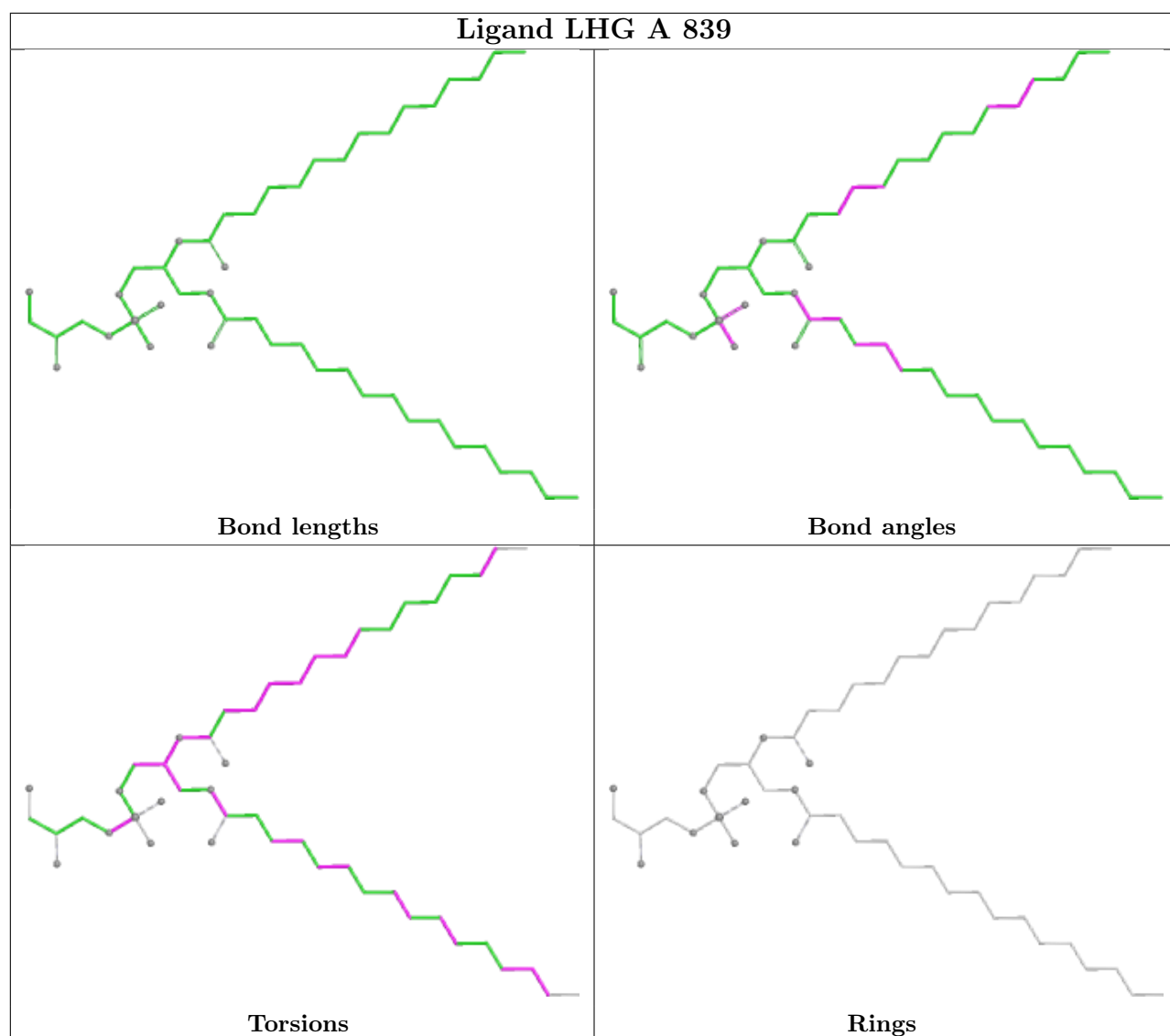




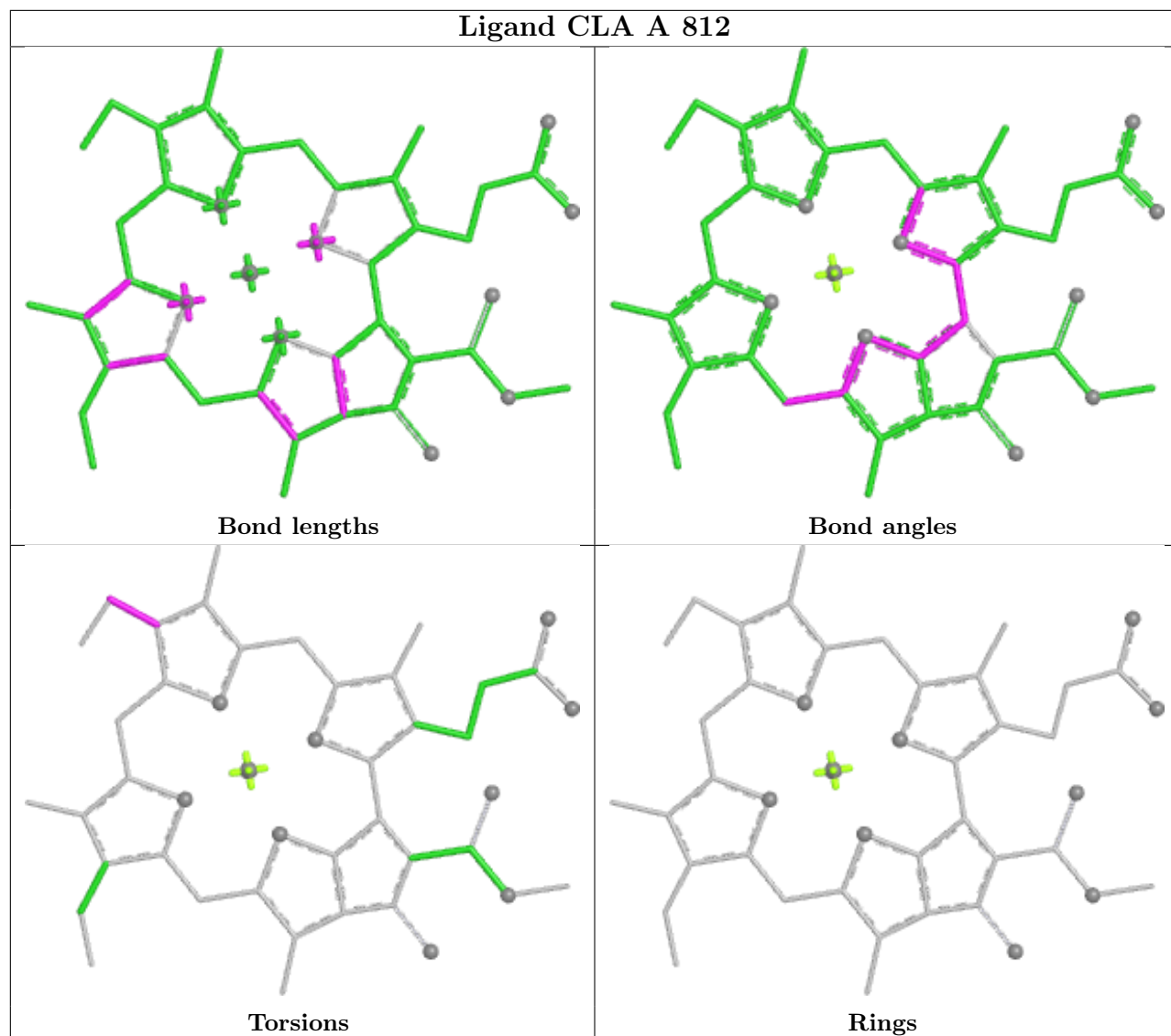




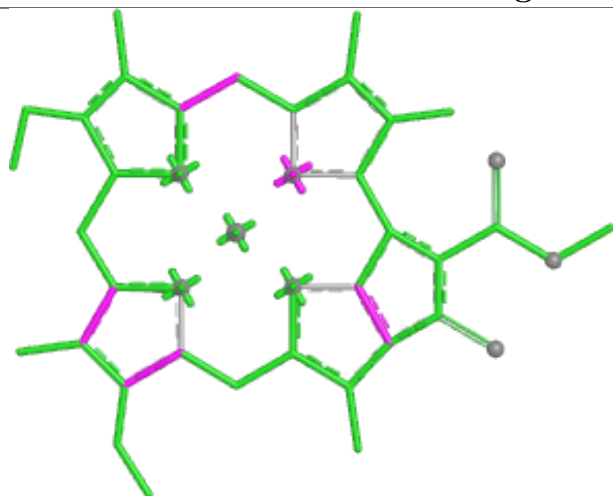




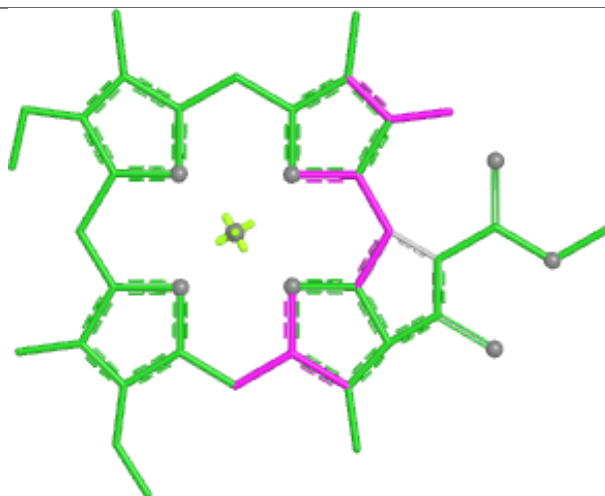
Ligand CLA A 812



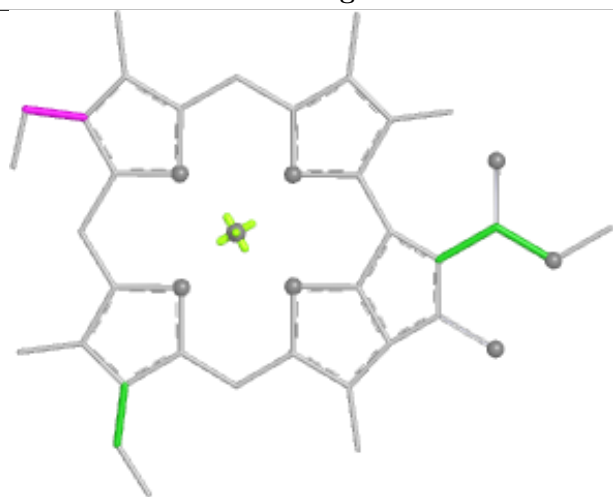
Ligand CLA T 209



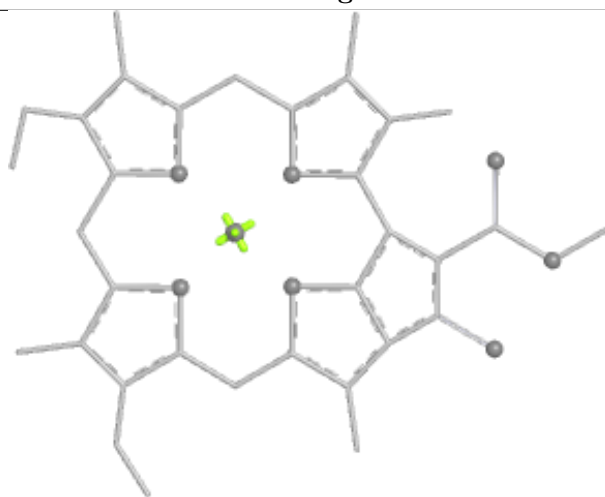
Bond lengths



Bond angles

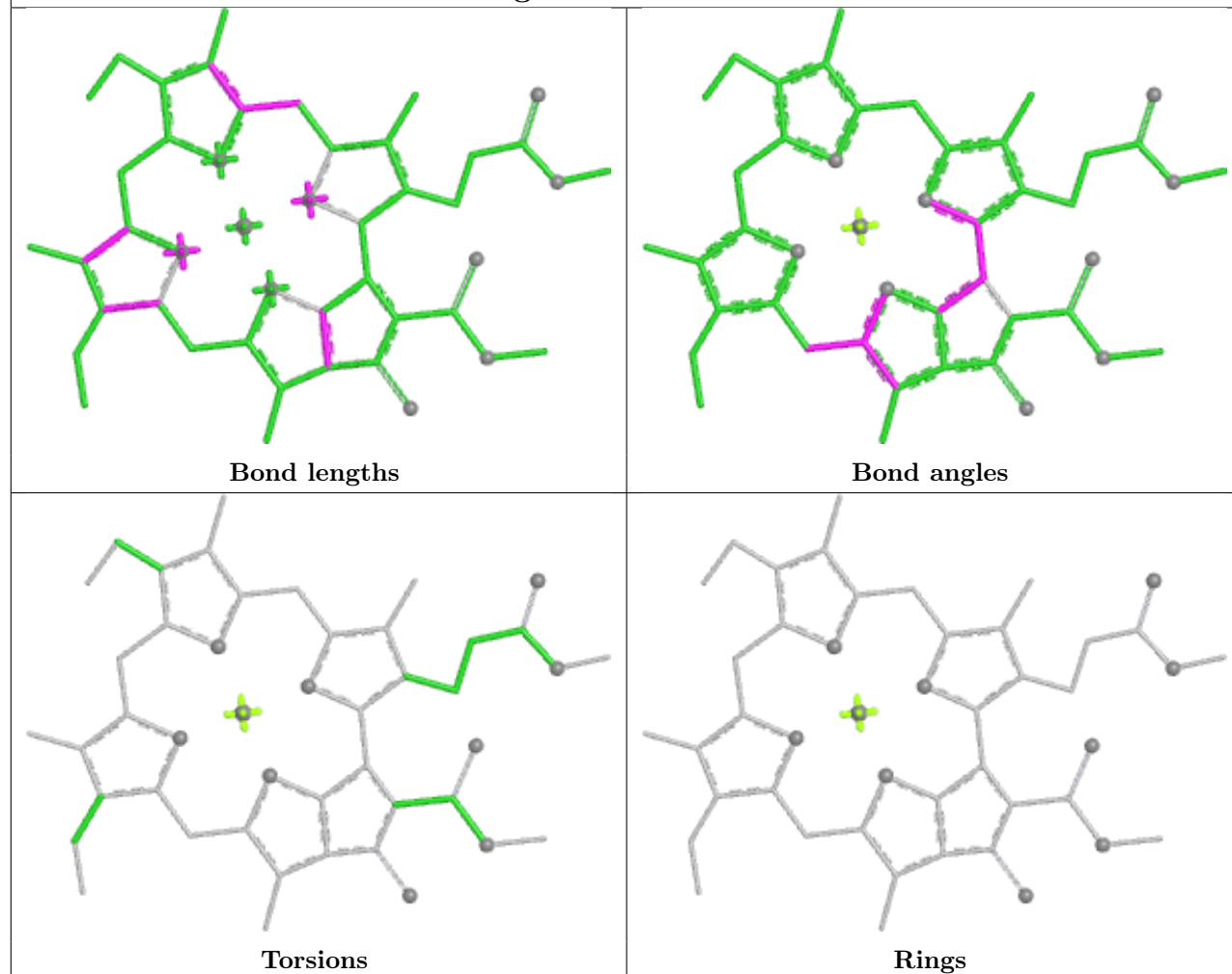


Torsions

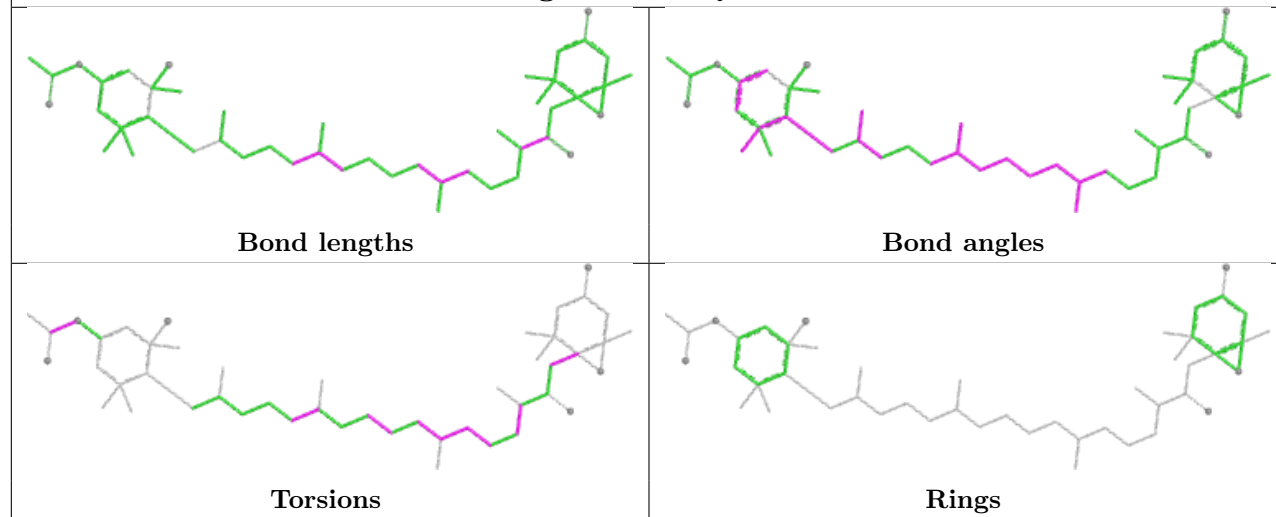


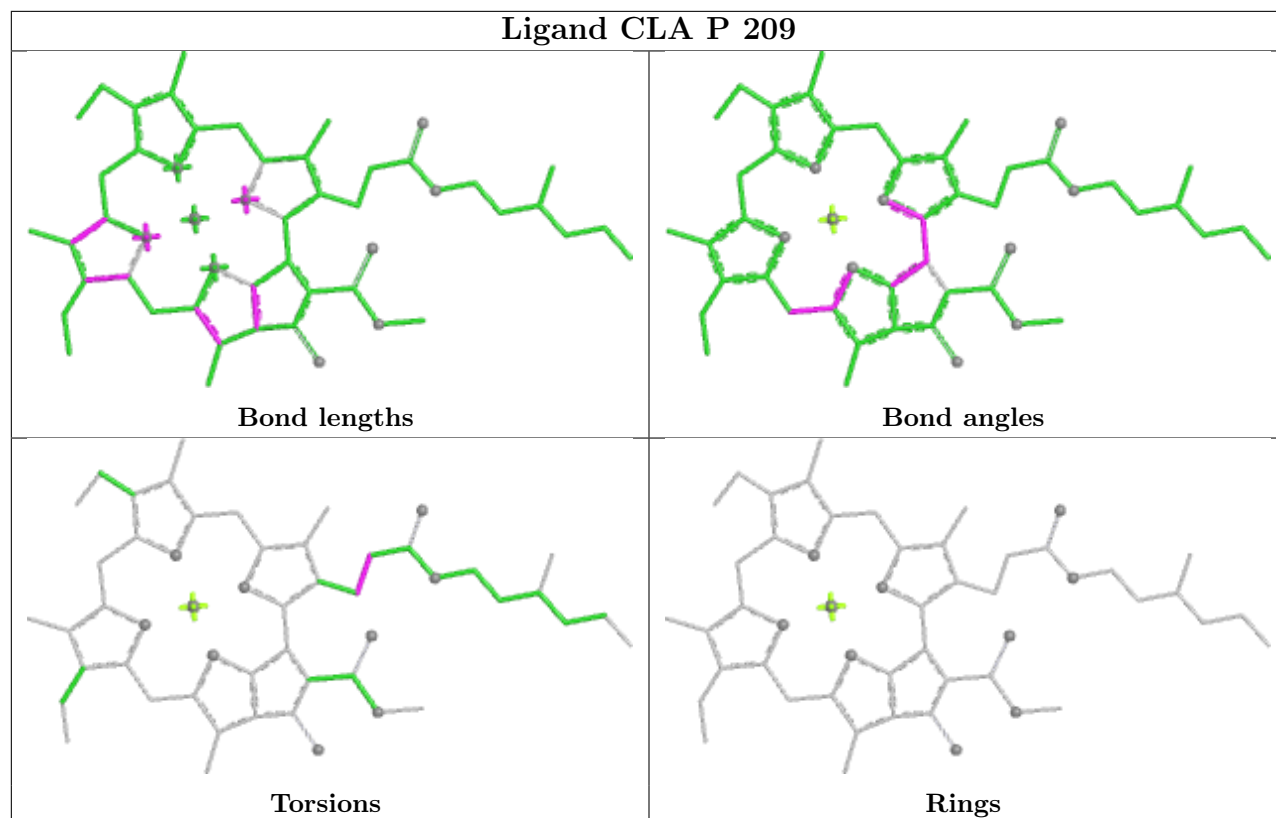
Rings

Ligand CLA B 818

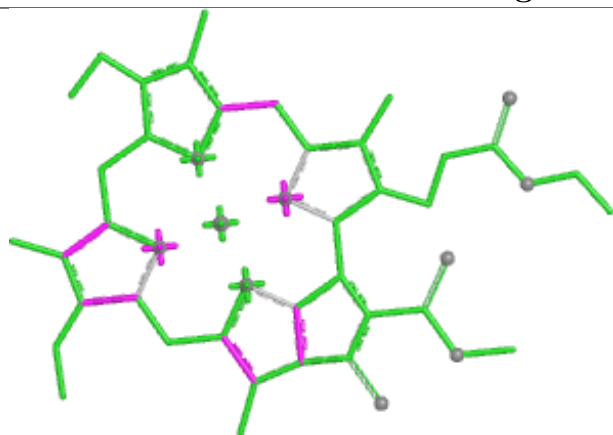


Ligand A86 Q 214

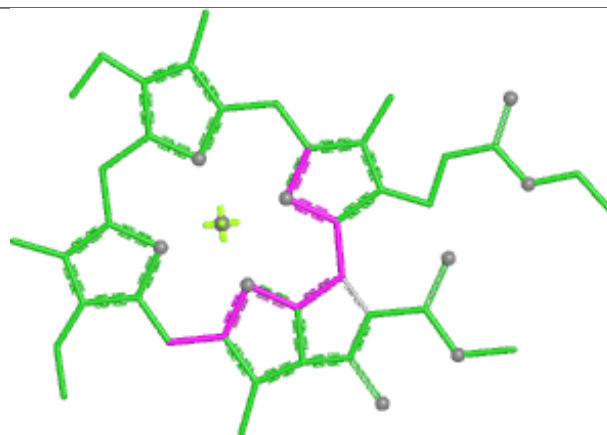




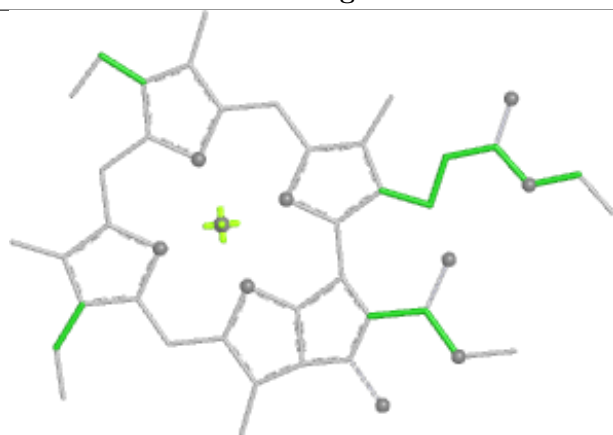
Ligand CLA P 216



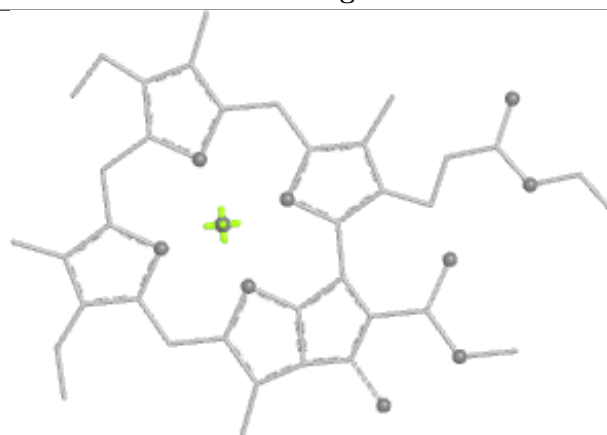
Bond lengths



Bond angles

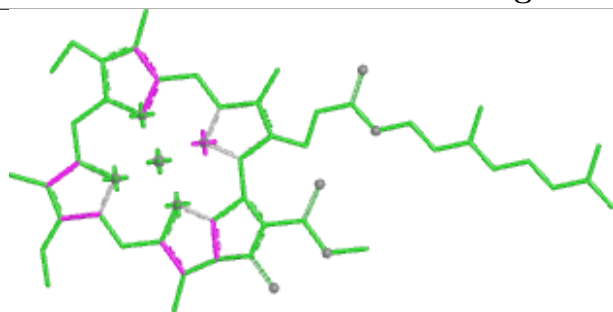


Torsions

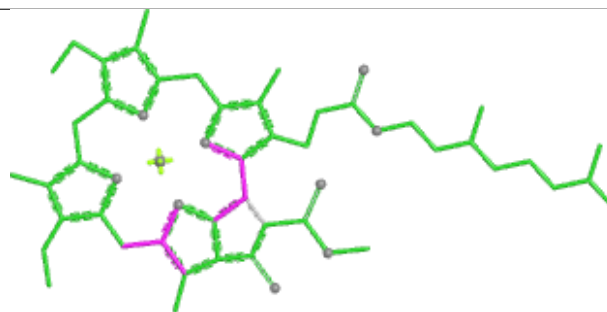


Rings

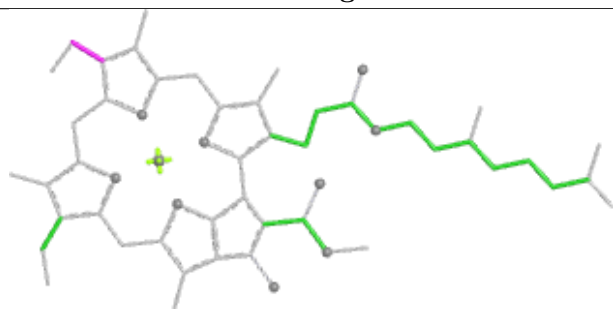
Ligand CLA B 811



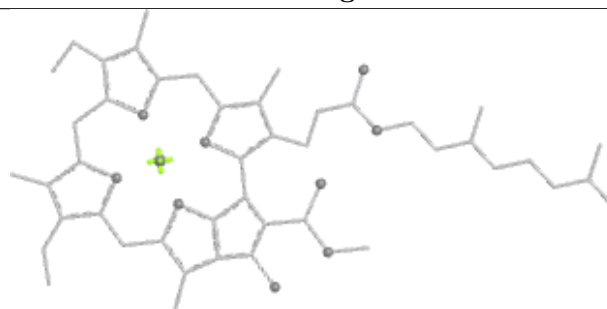
Bond lengths



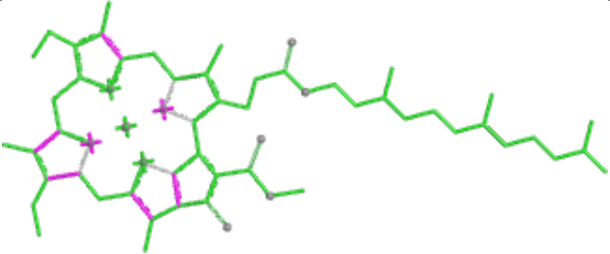
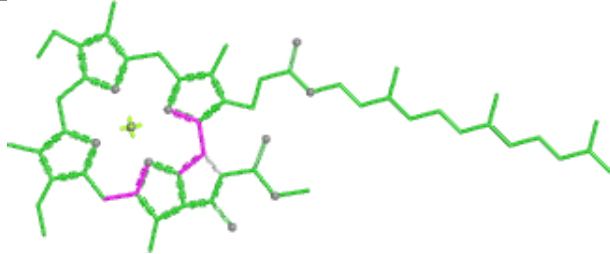
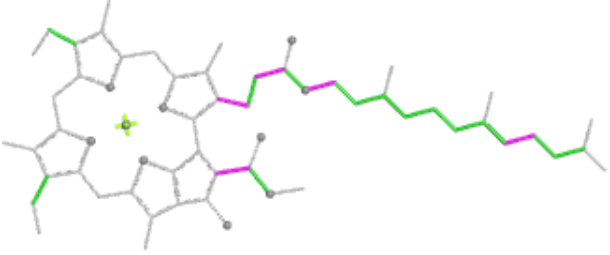
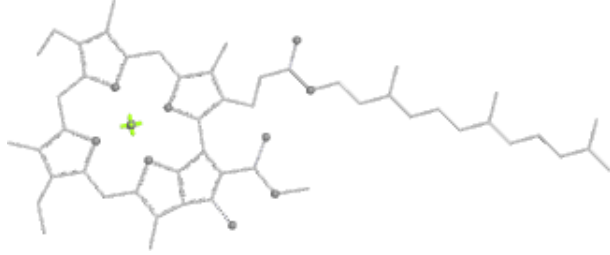
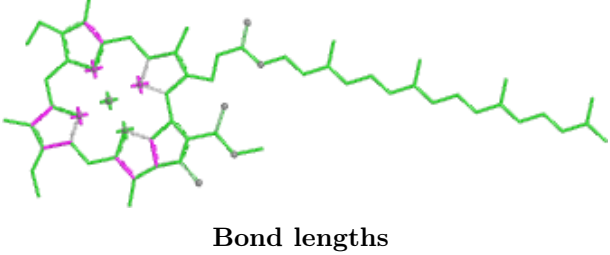
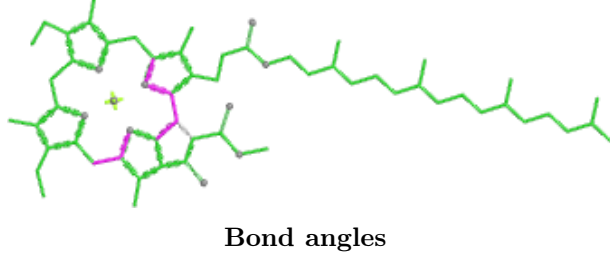
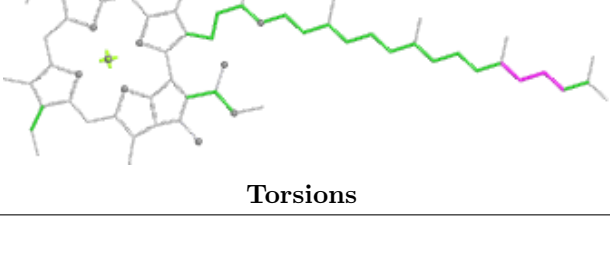
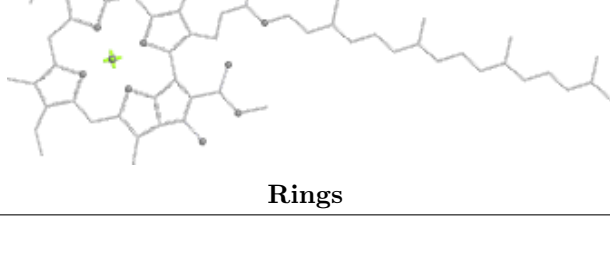
Bond angles



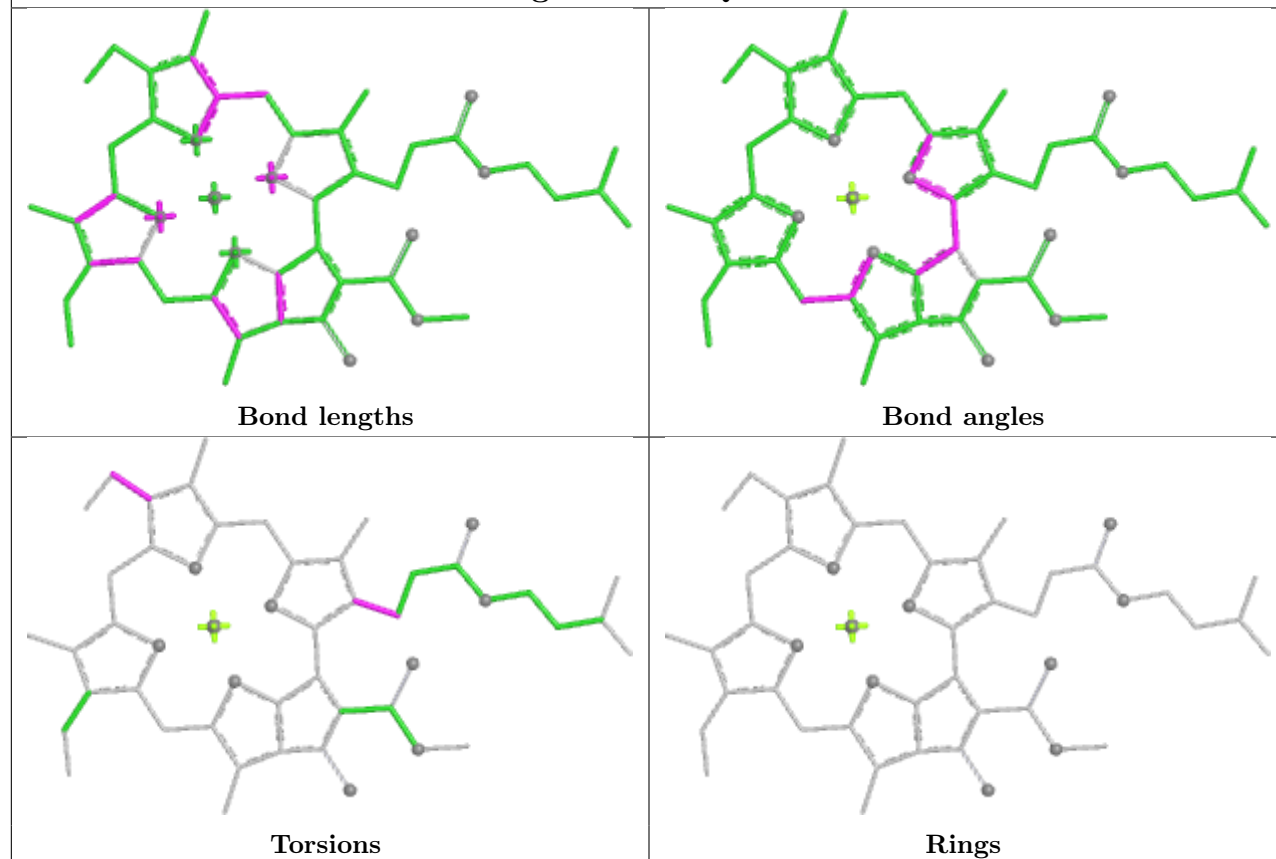
Torsions



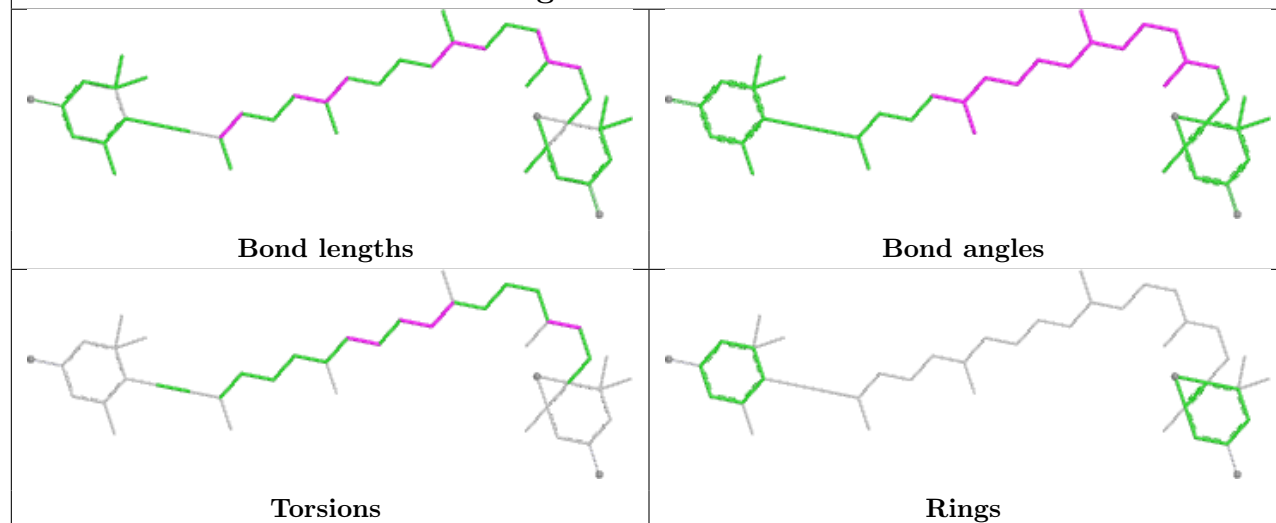
Rings

Ligand CLA H 202	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA B 845	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

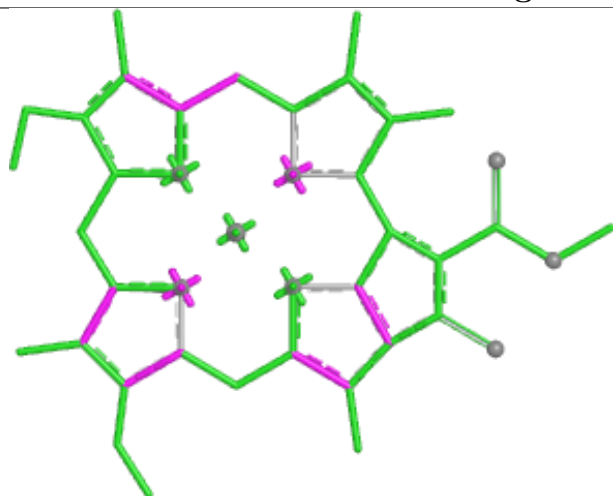
Ligand CLA Q 208



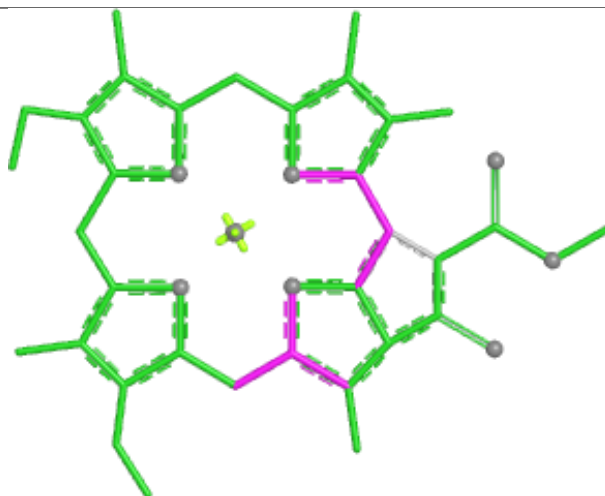
Ligand DD6 J 101



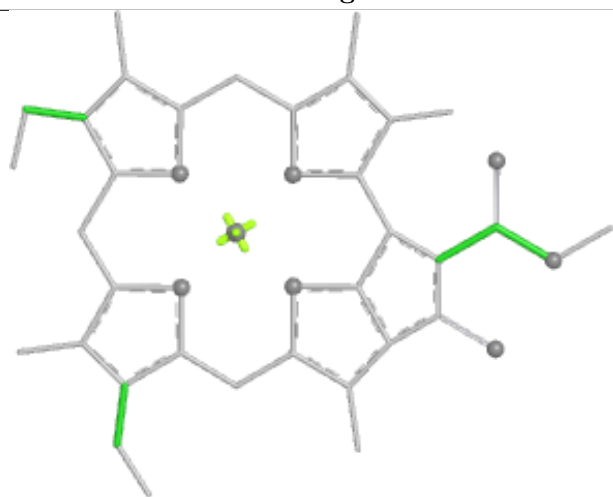
Ligand CLA T 202



Bond lengths



Bond angles

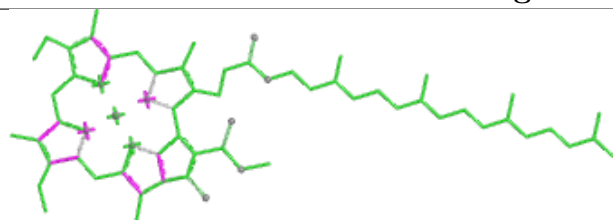


Torsions

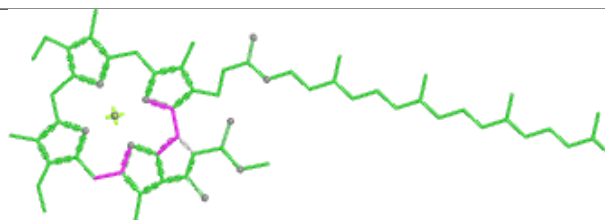


Rings

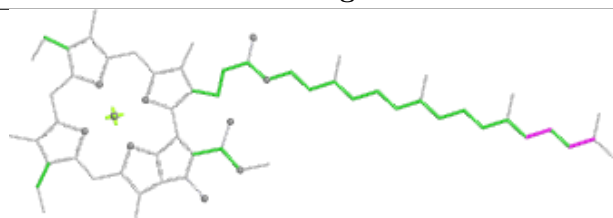
Ligand CLA O 204



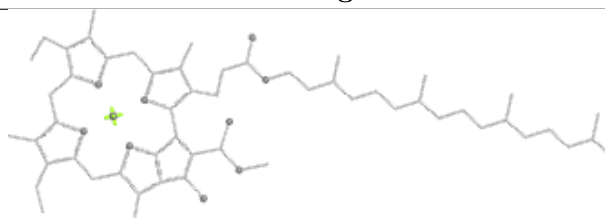
Bond lengths



Bond angles

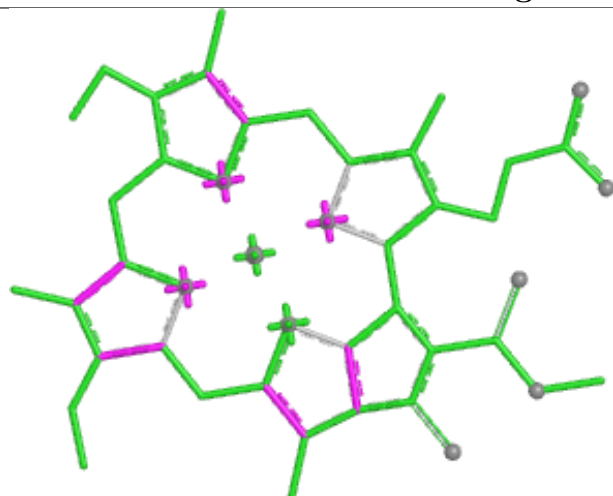


Torsions

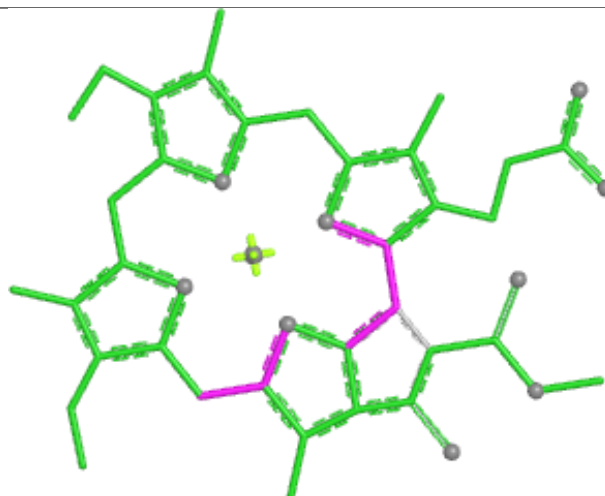


Rings

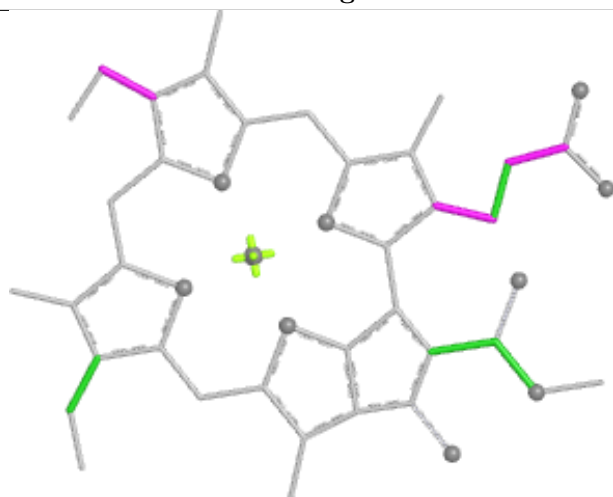
Ligand CLA P 214



Bond lengths



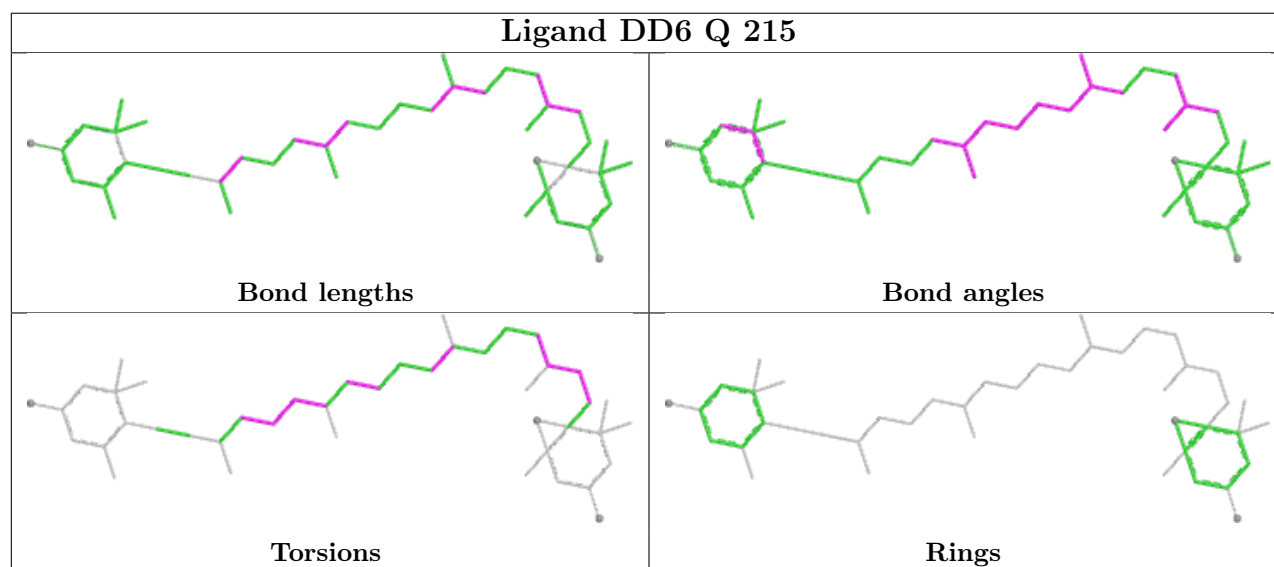
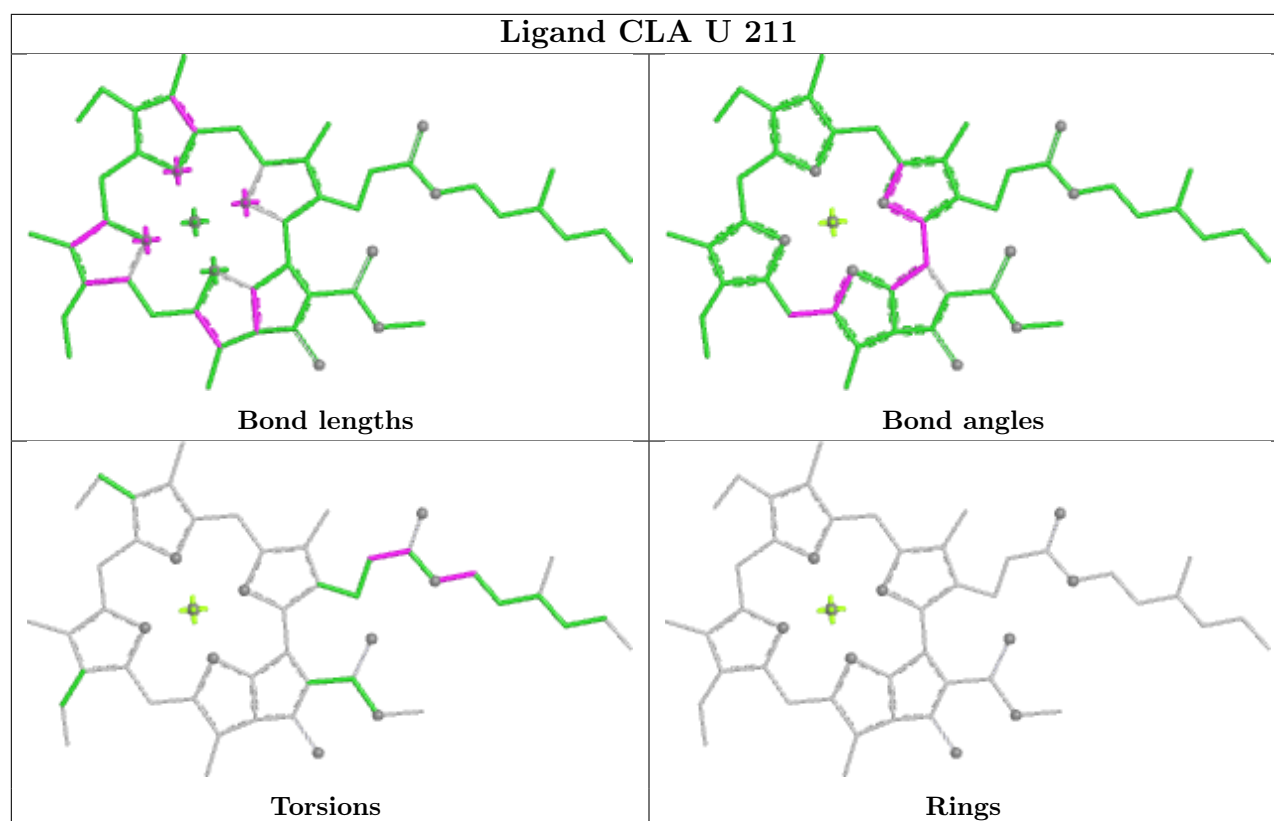
Bond angles

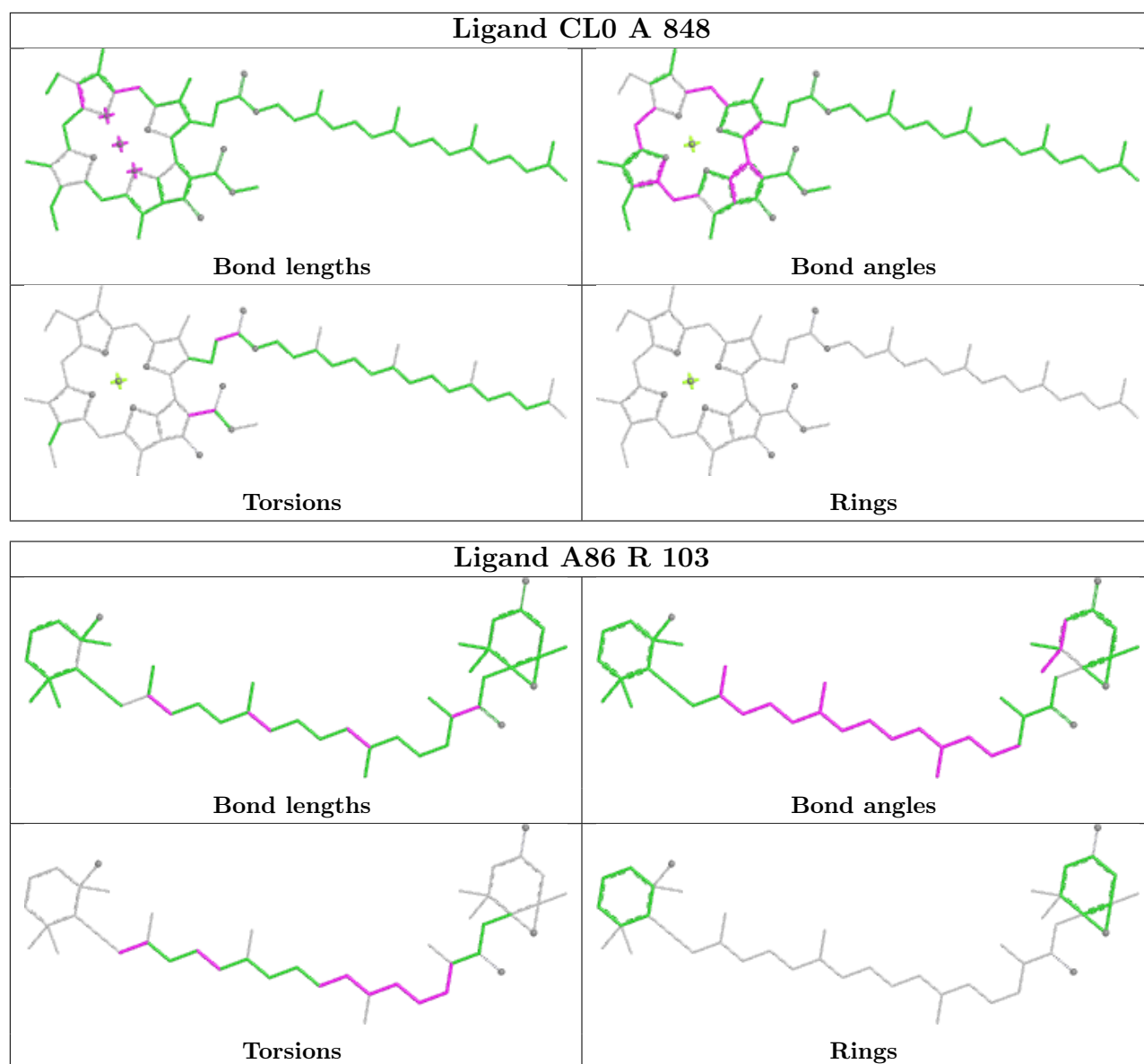


Torsions

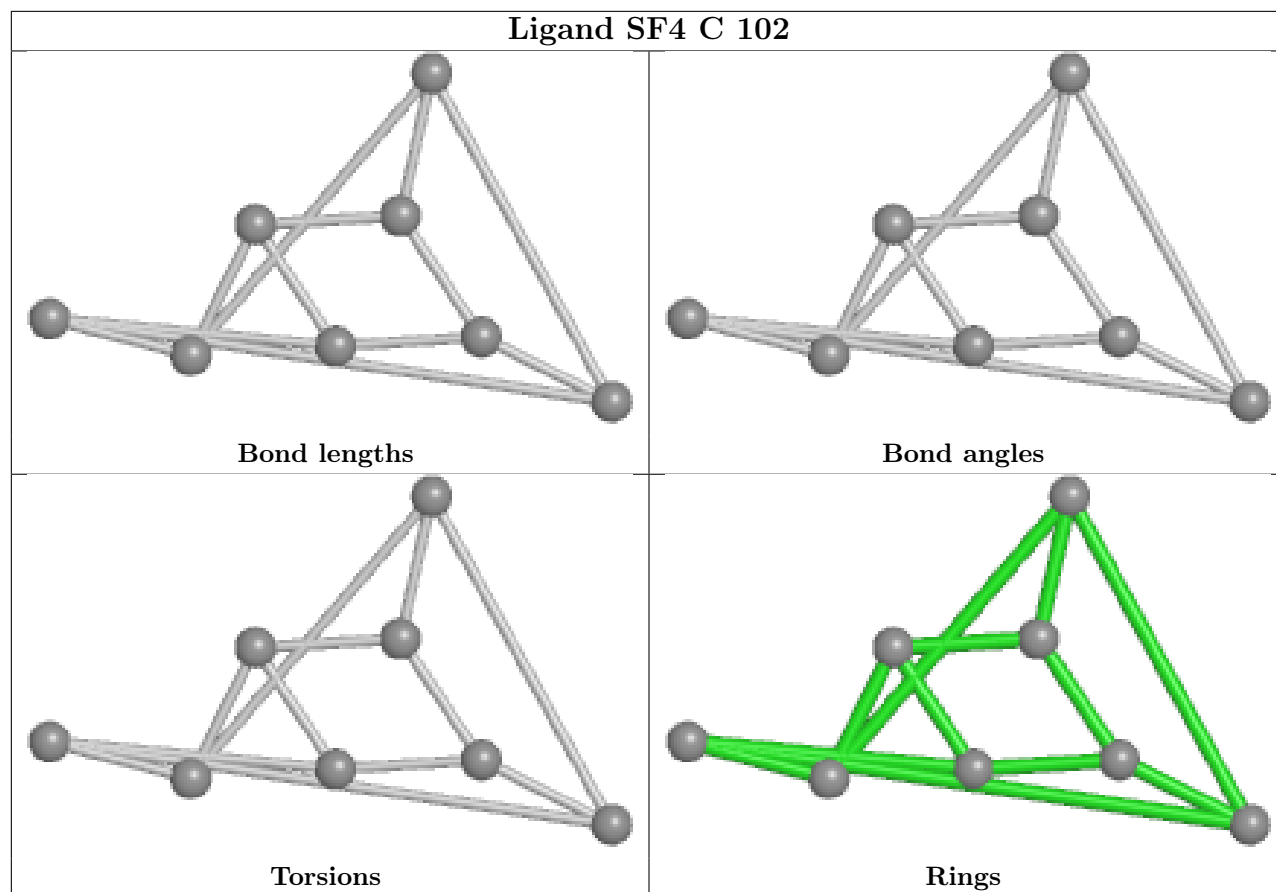


Rings

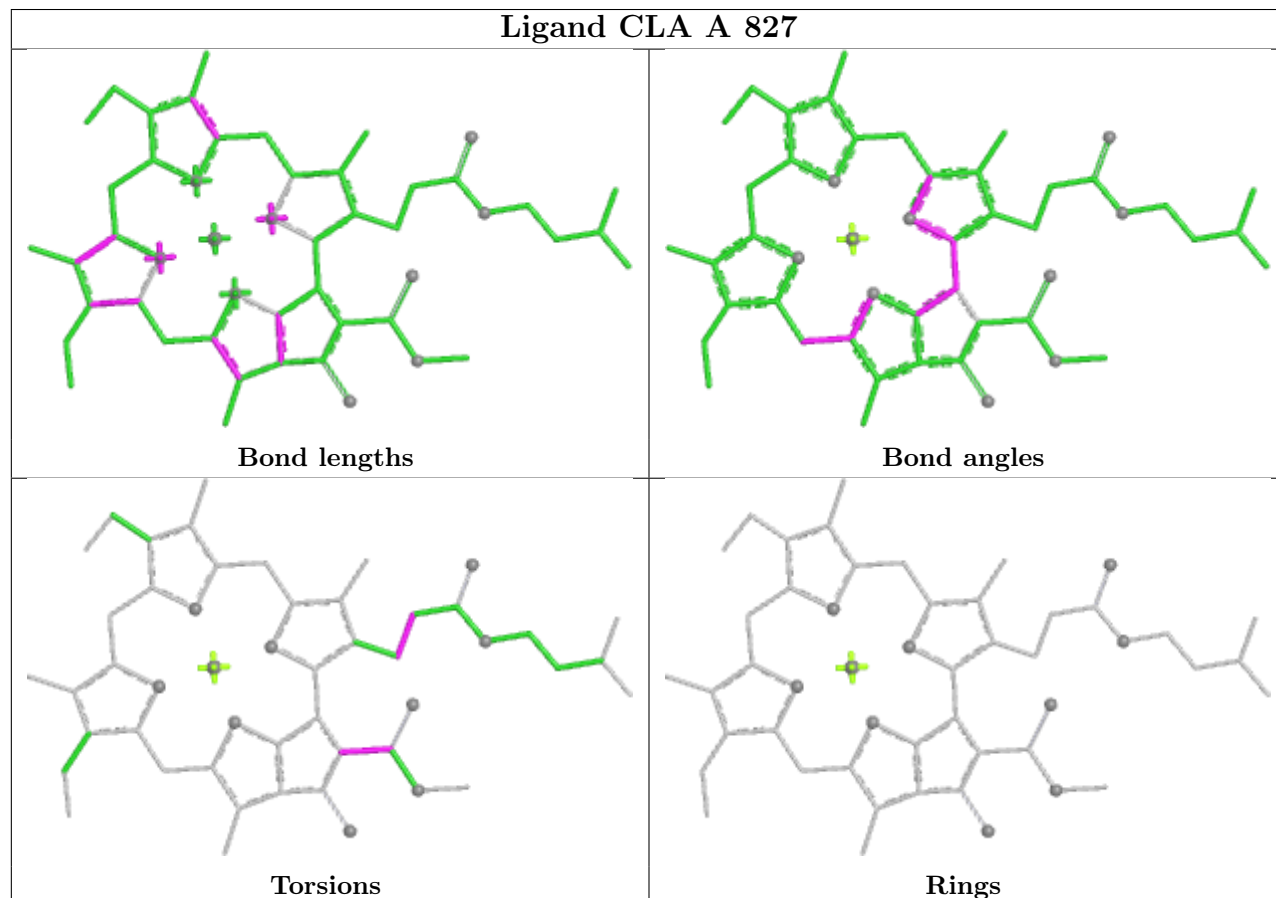


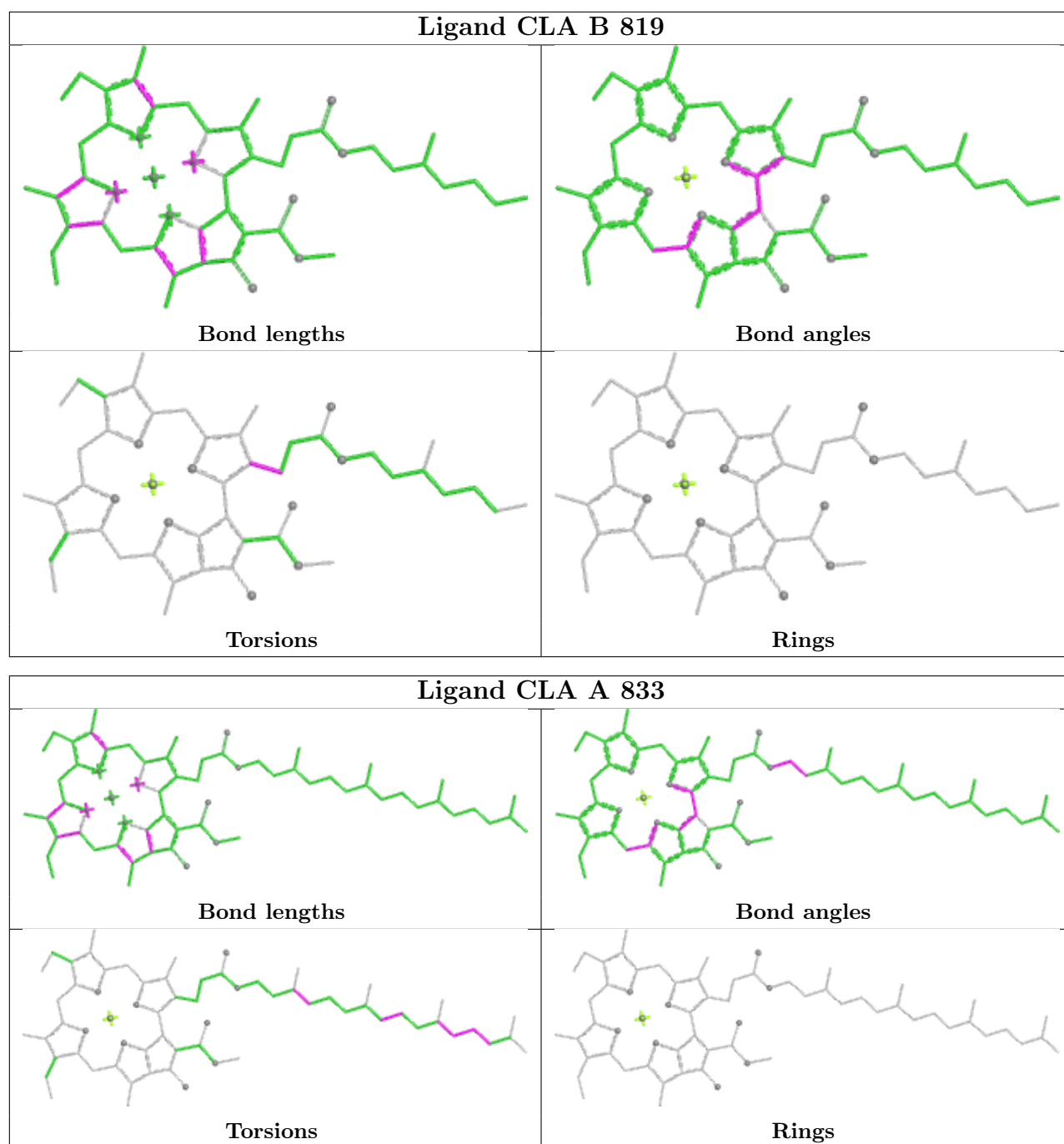


Ligand SF4 C 102

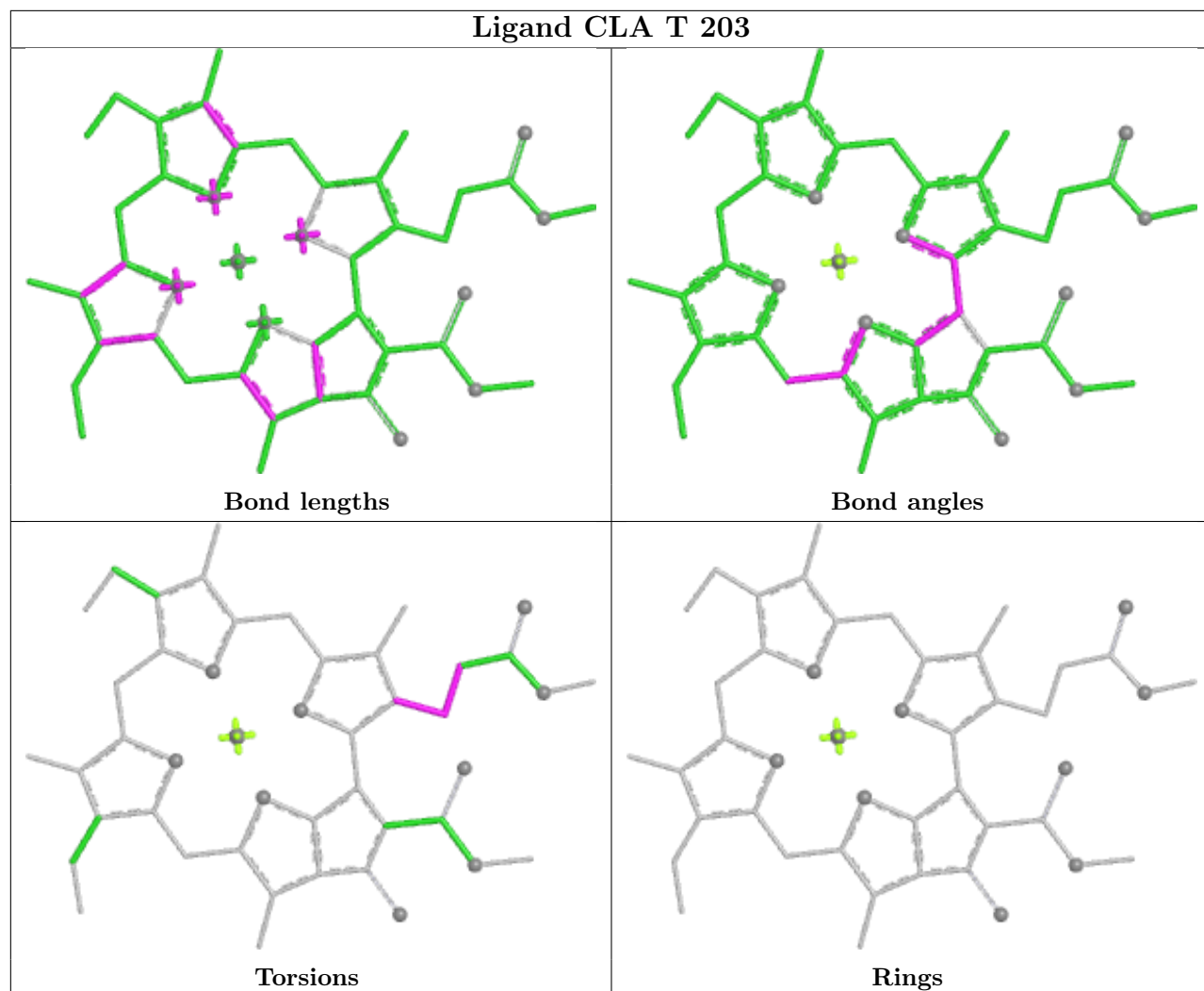


Ligand CLA A 827

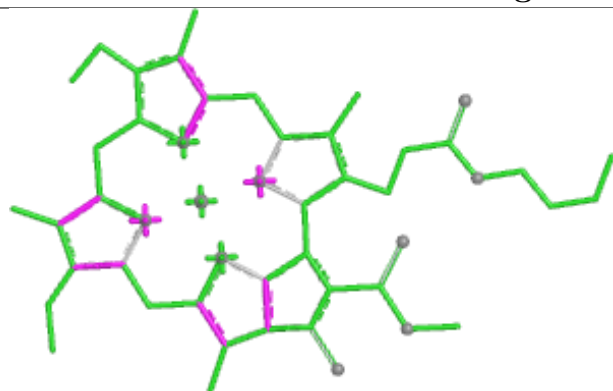




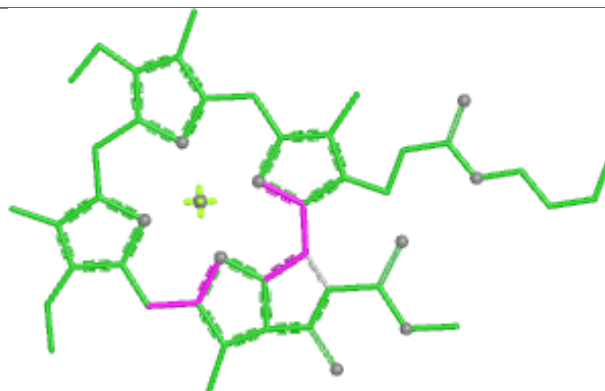
Ligand CLA T 203



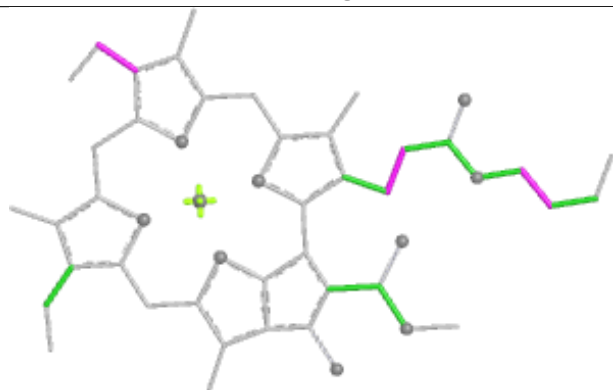
Ligand CLA B 827



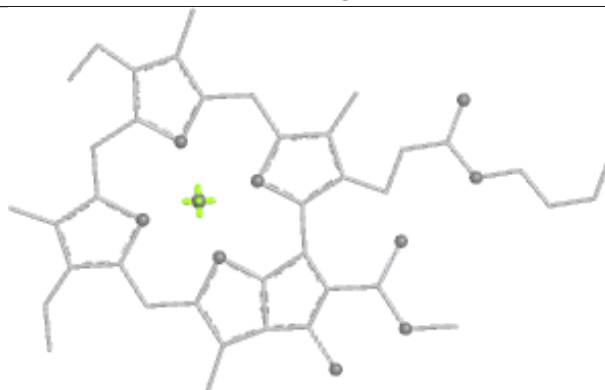
Bond lengths



Bond angles

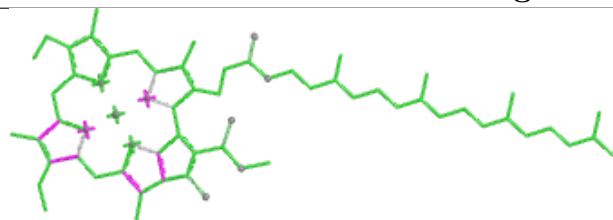


Torsions

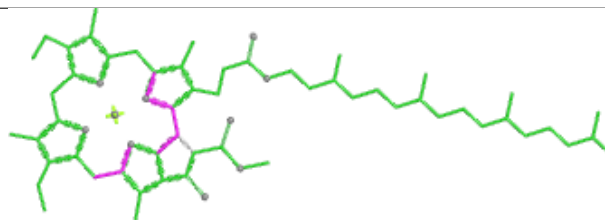


Rings

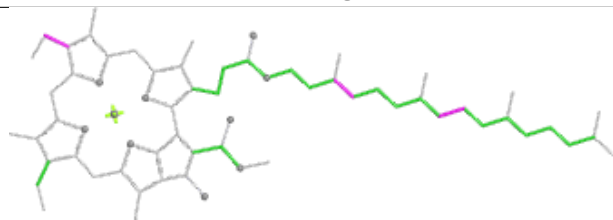
Ligand CLA A 849



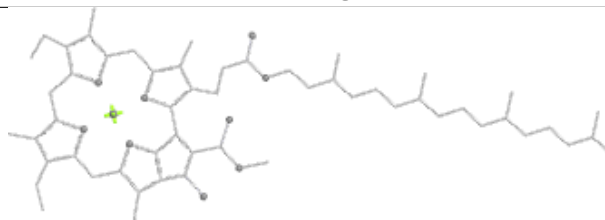
Bond lengths



Bond angles

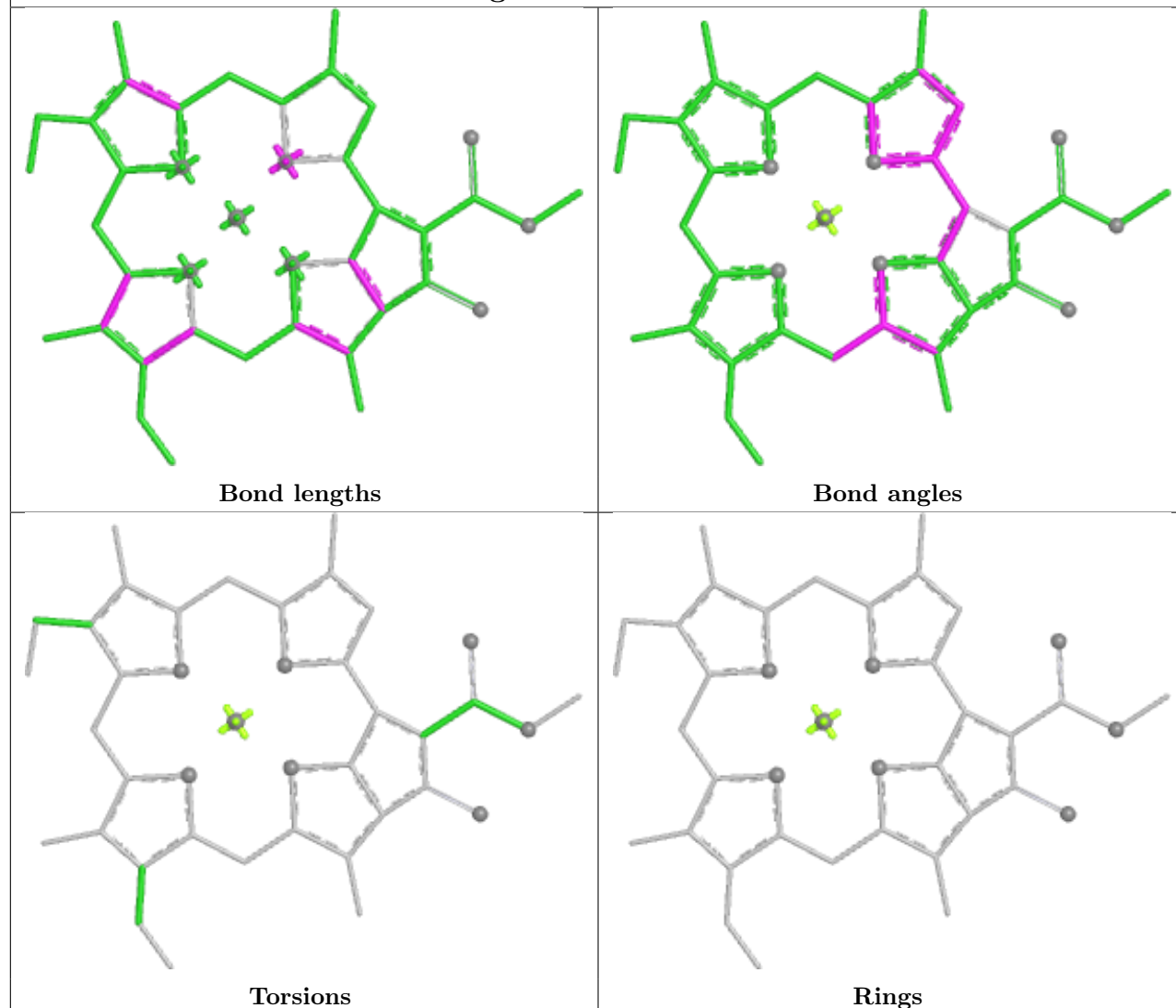


Torsions

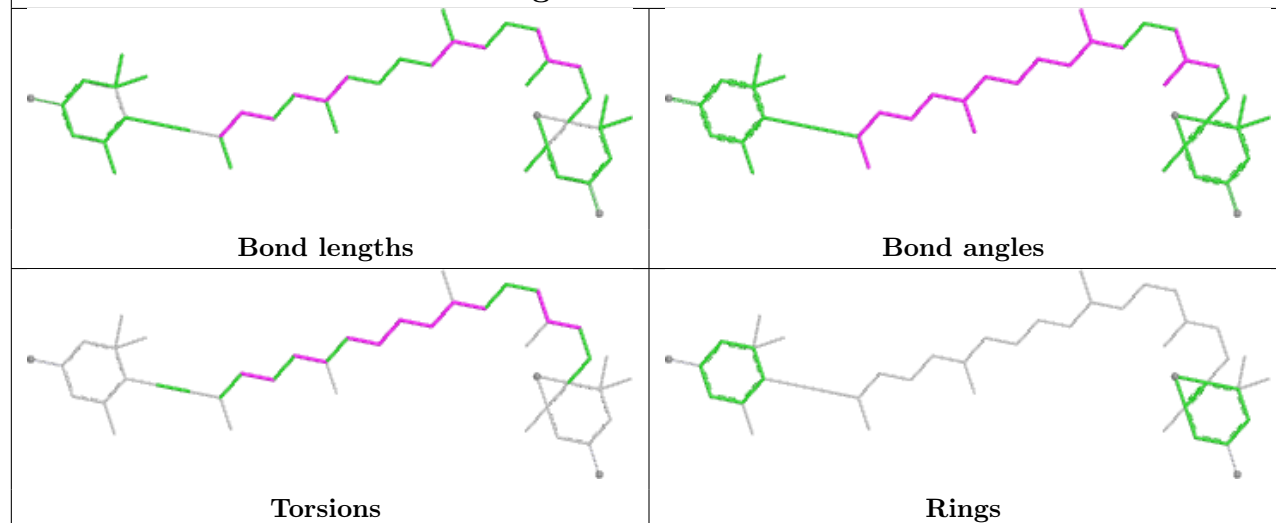


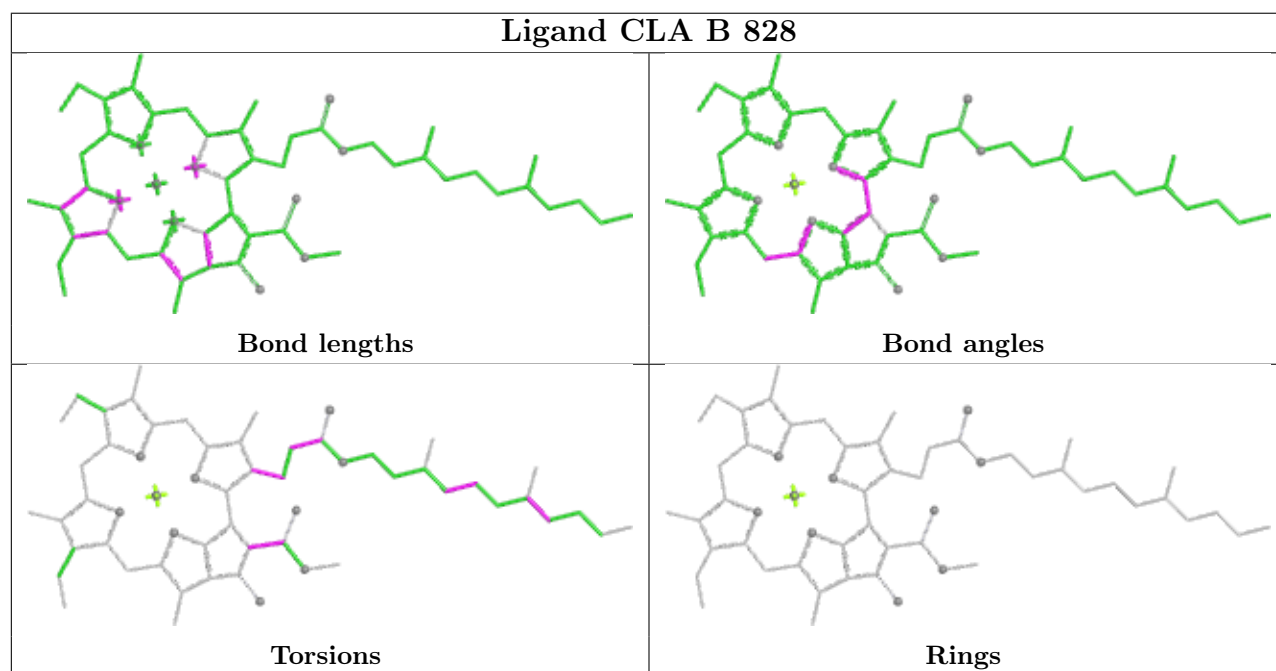
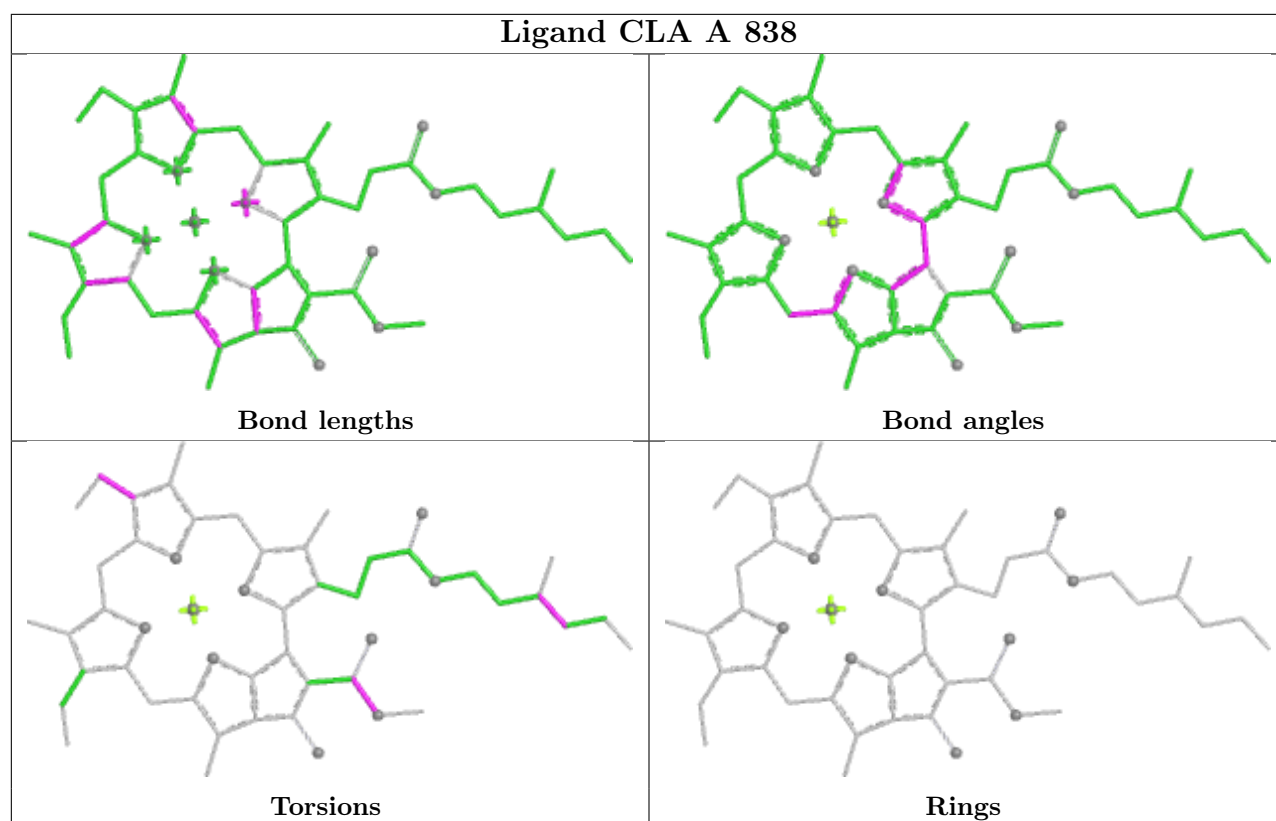
Rings

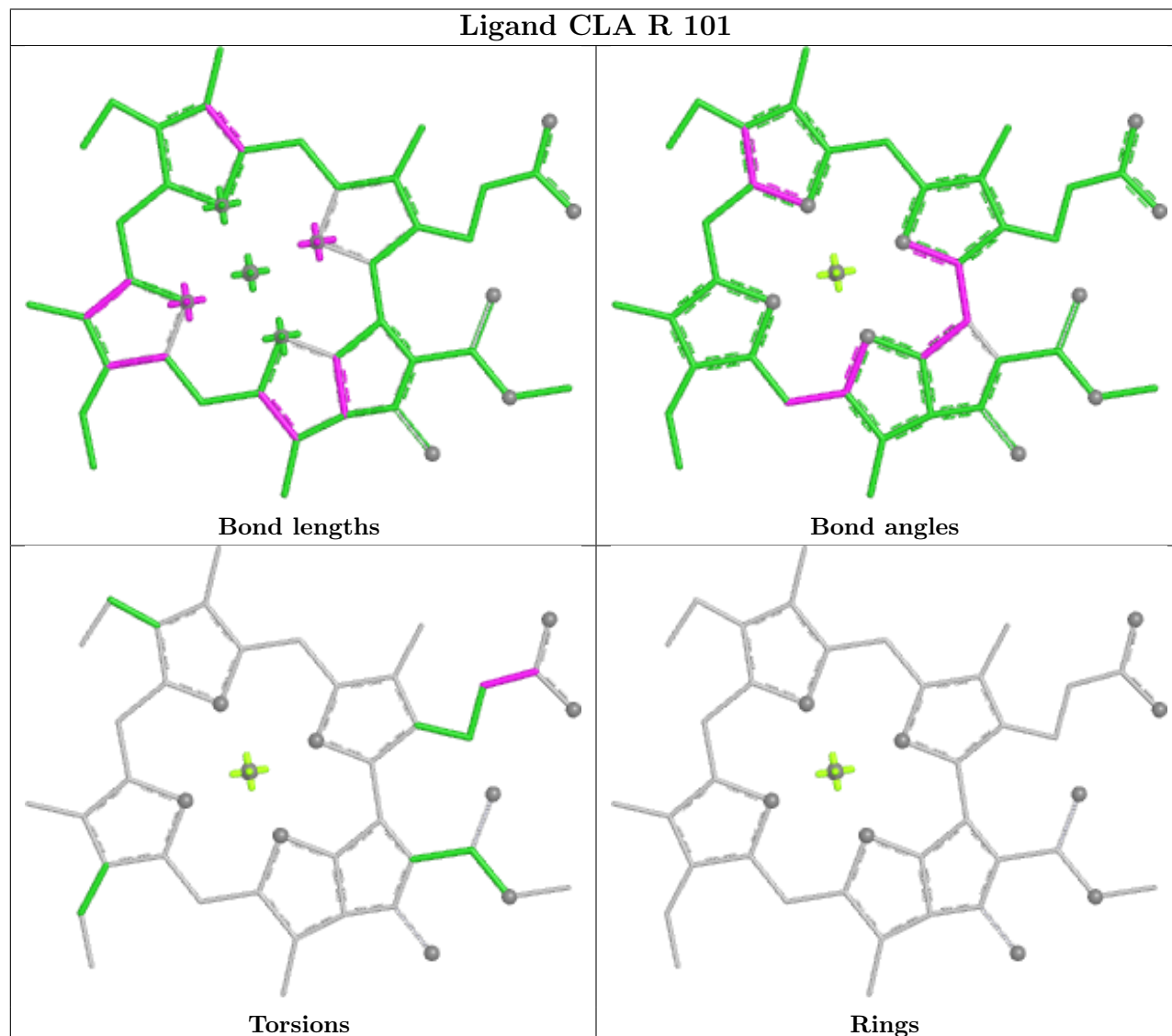
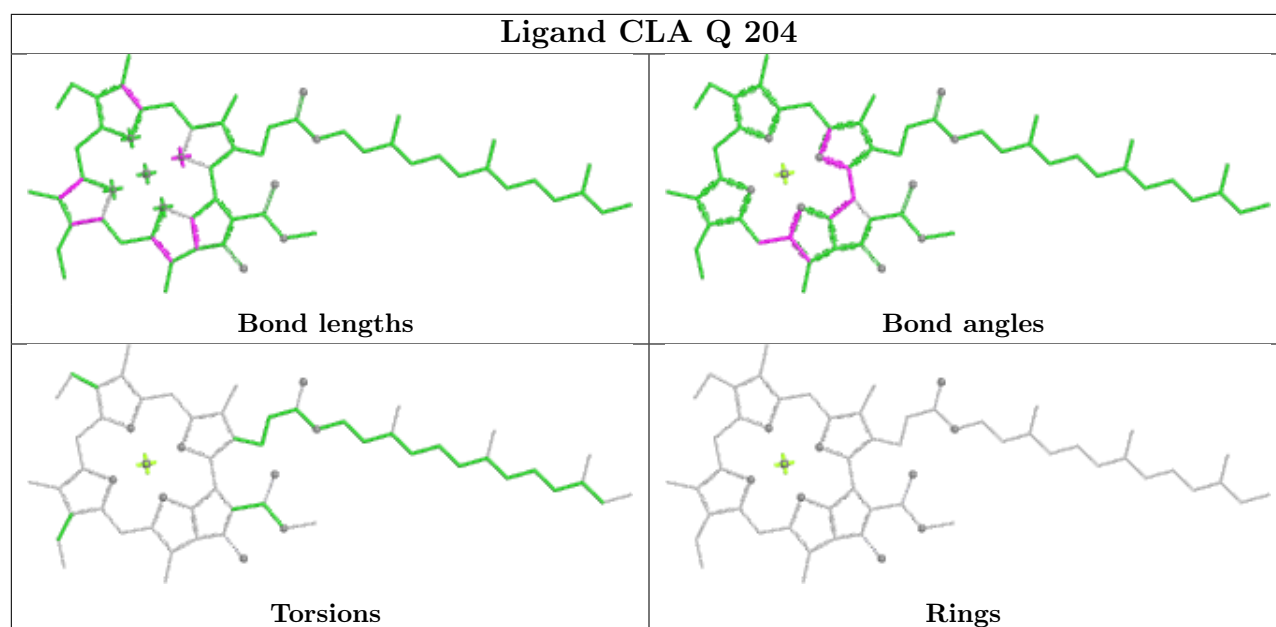
Ligand CLA H 201



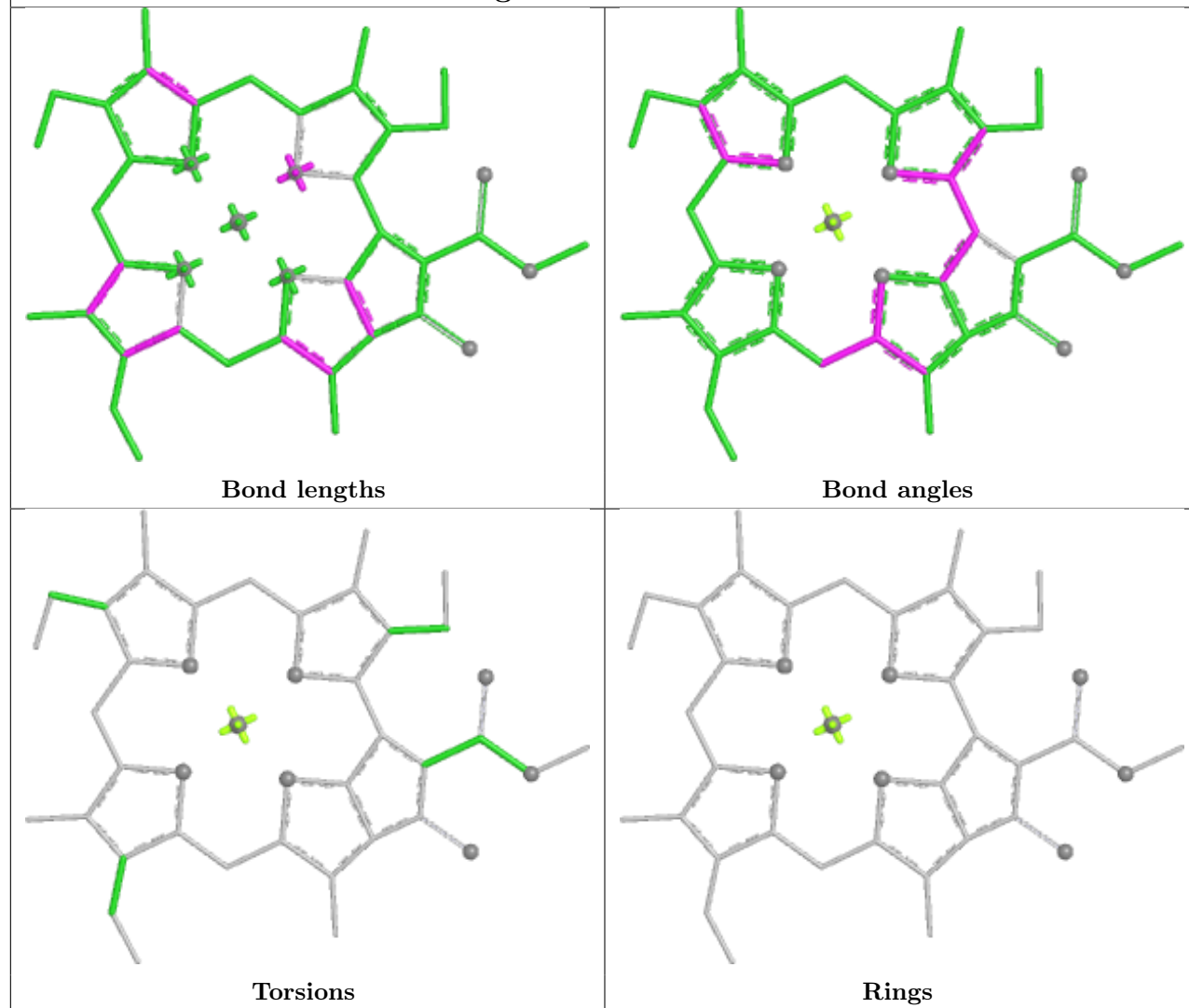
Ligand DD6 A 855



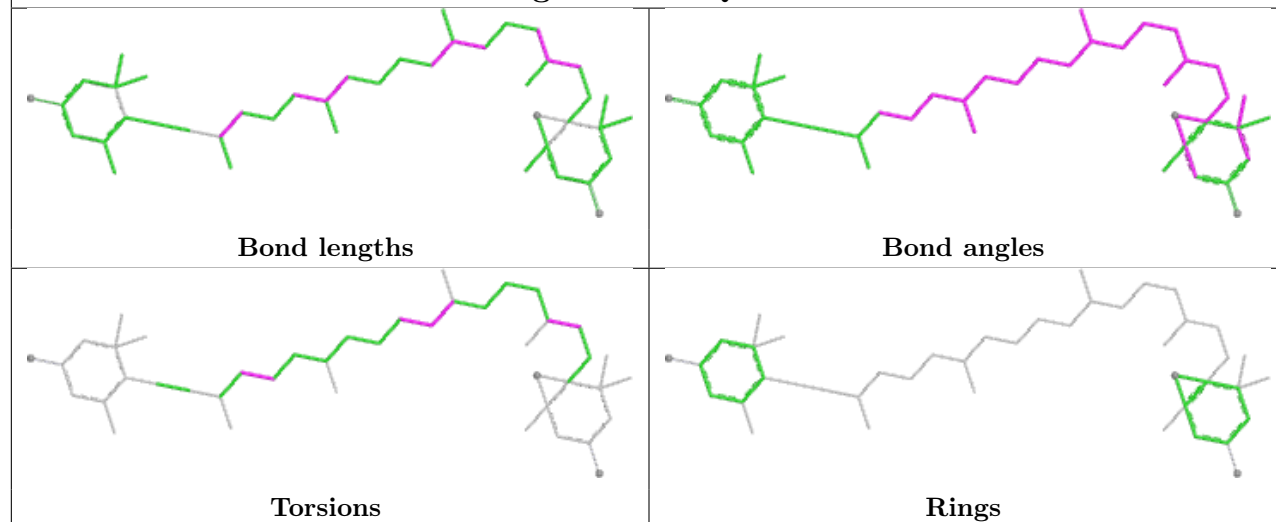


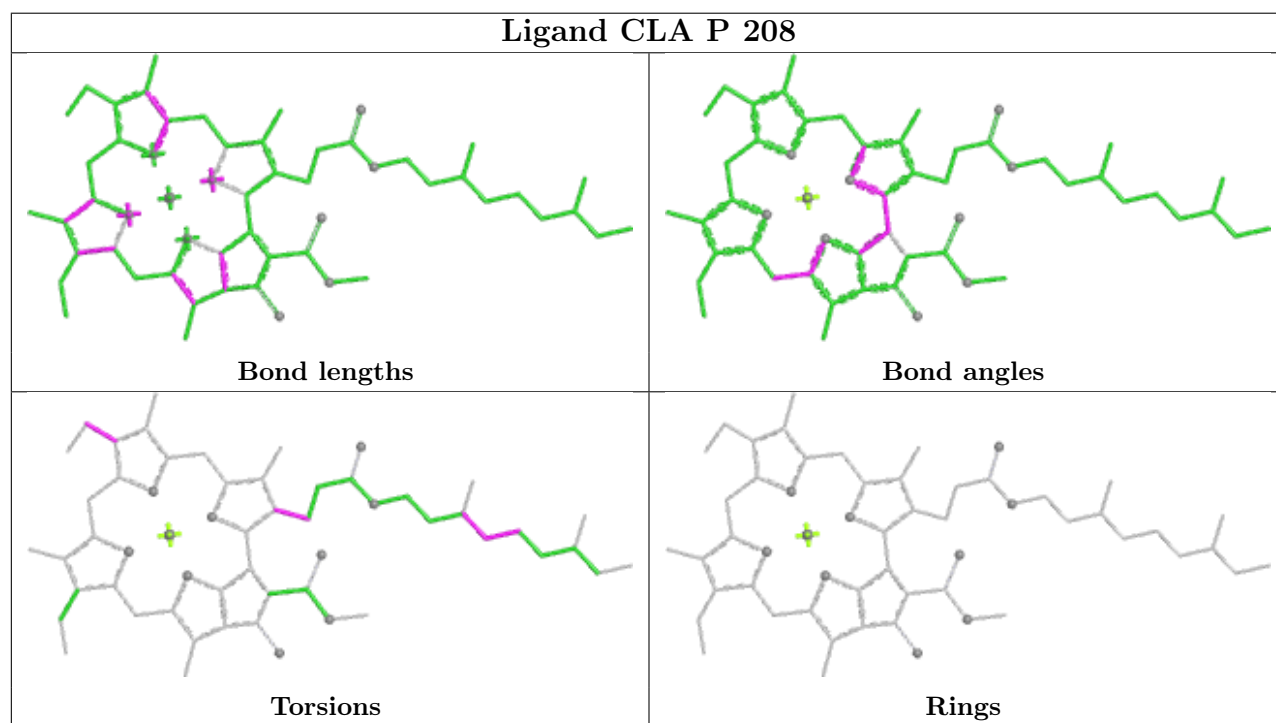
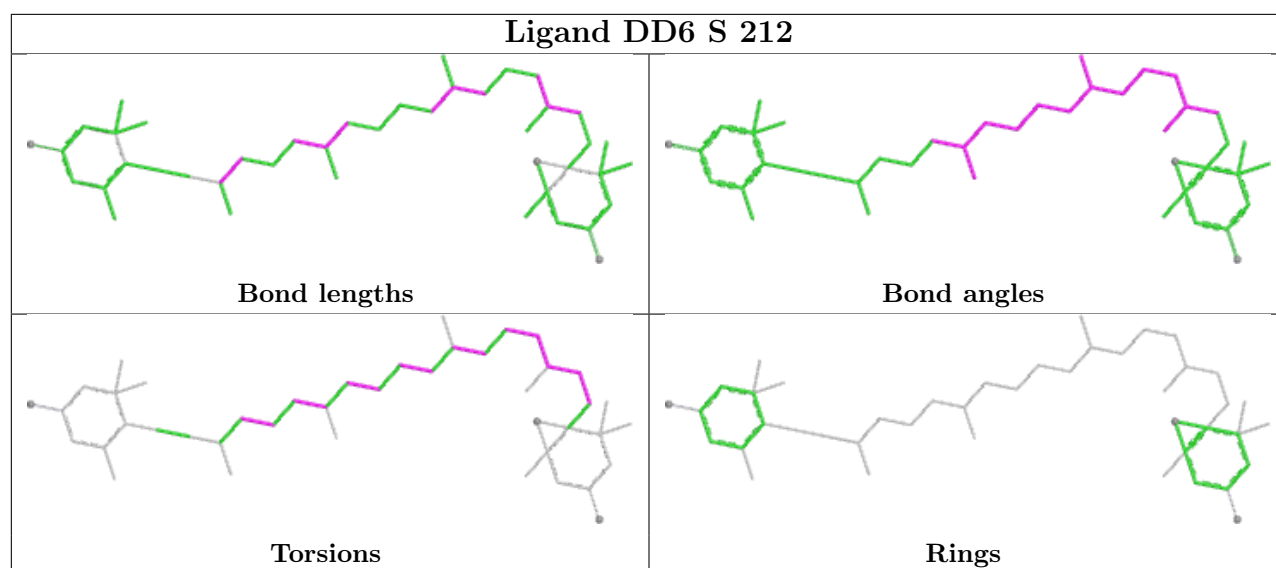


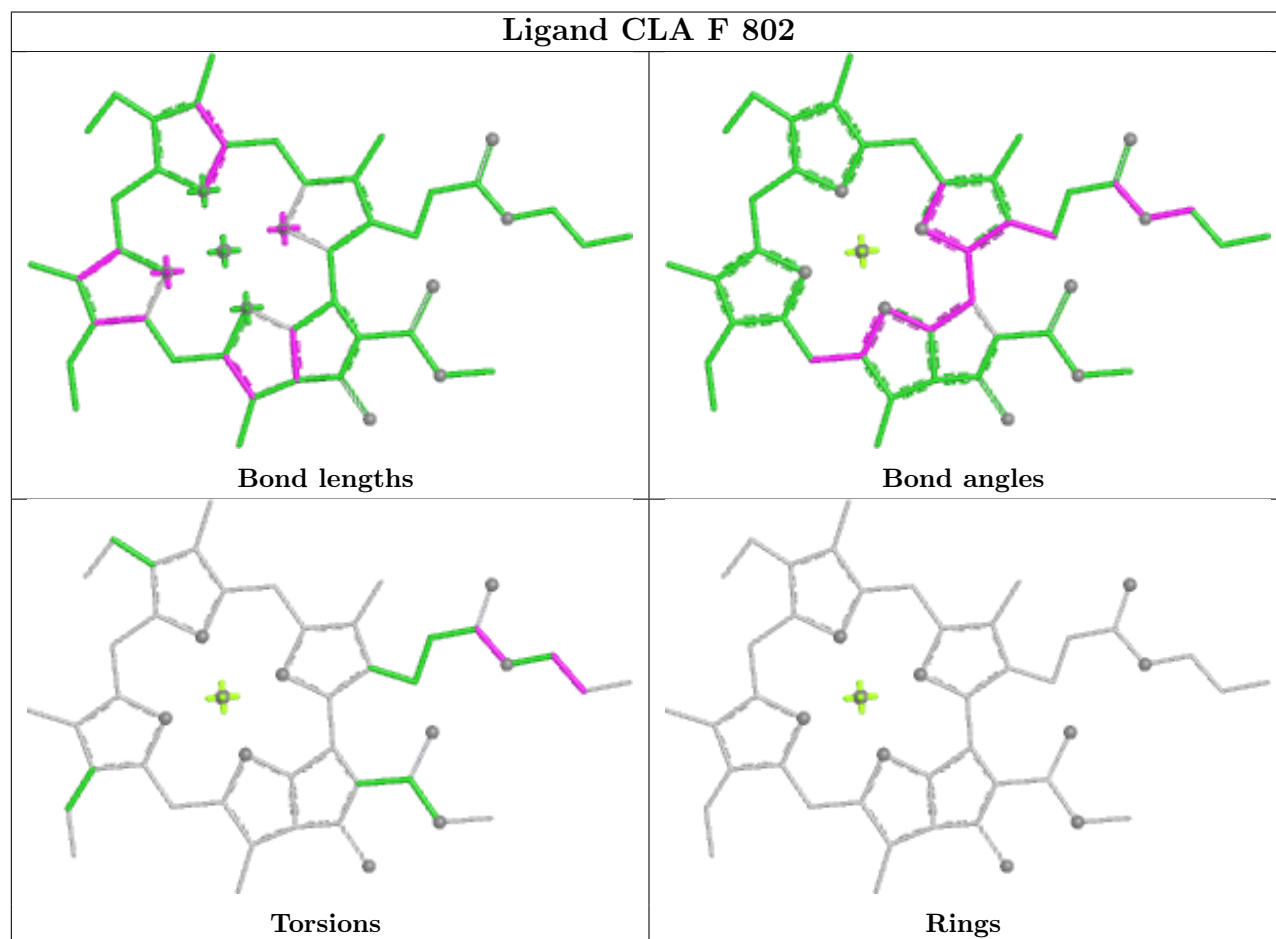
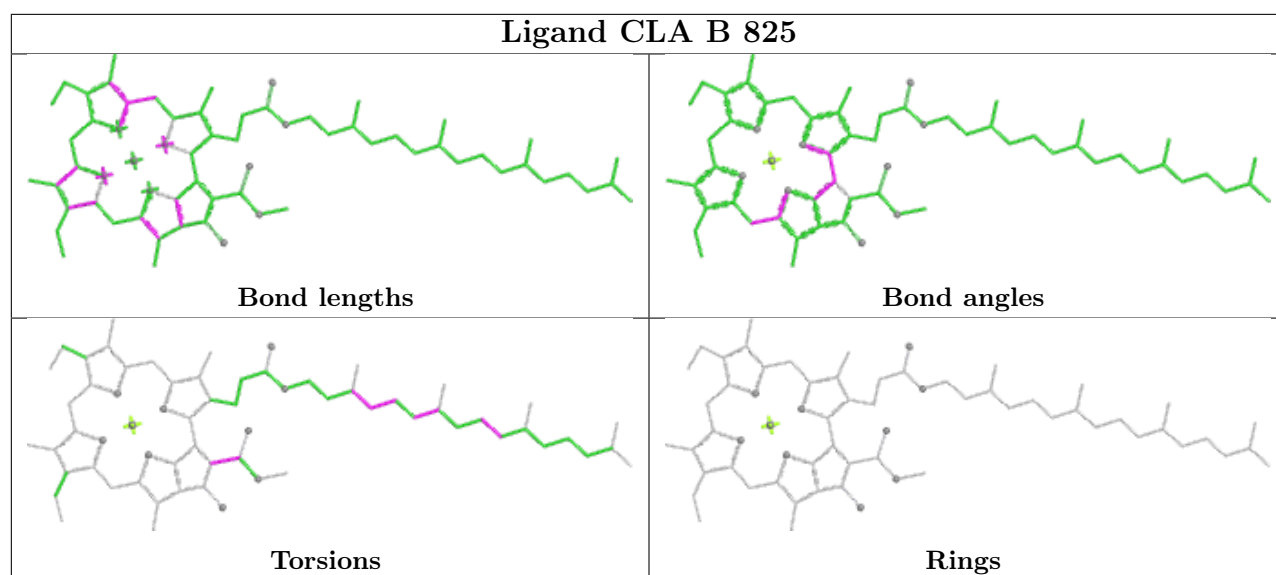
Ligand CLA U 209

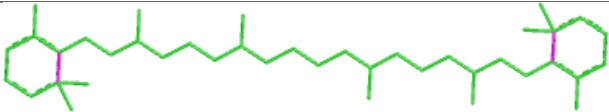
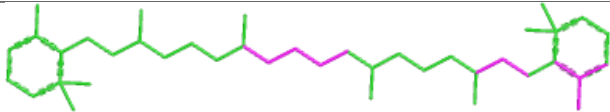
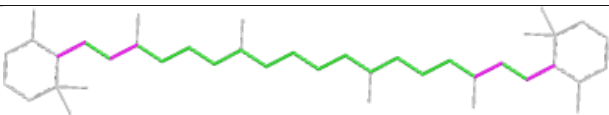
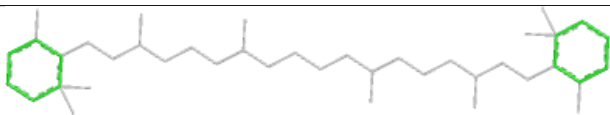


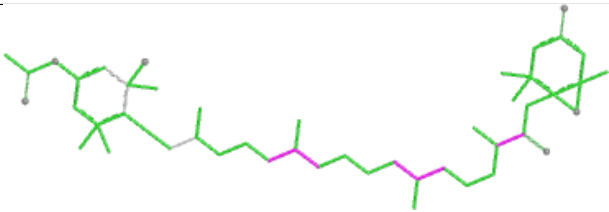
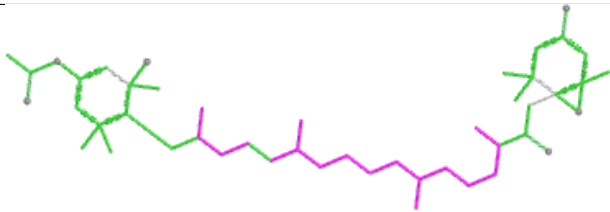
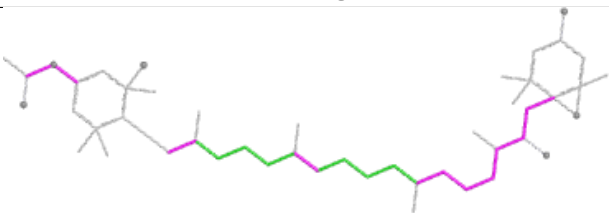
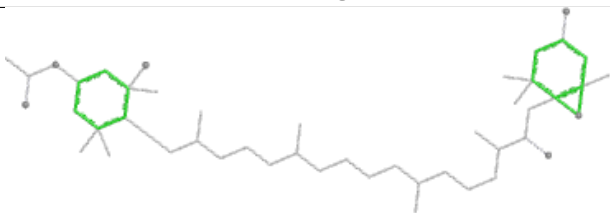
Ligand DD6 Q 202

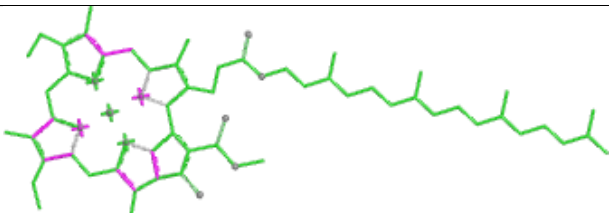
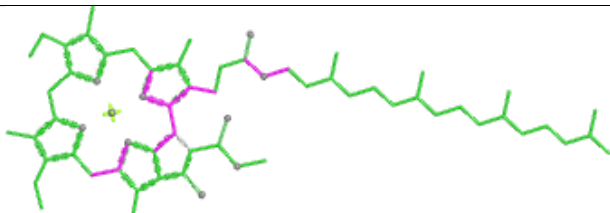
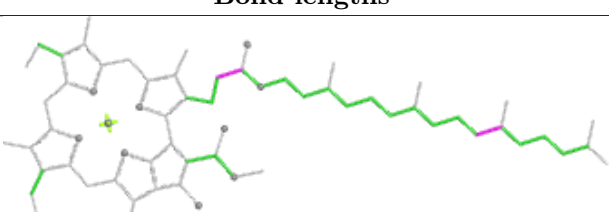
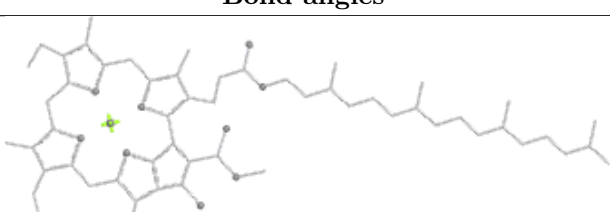


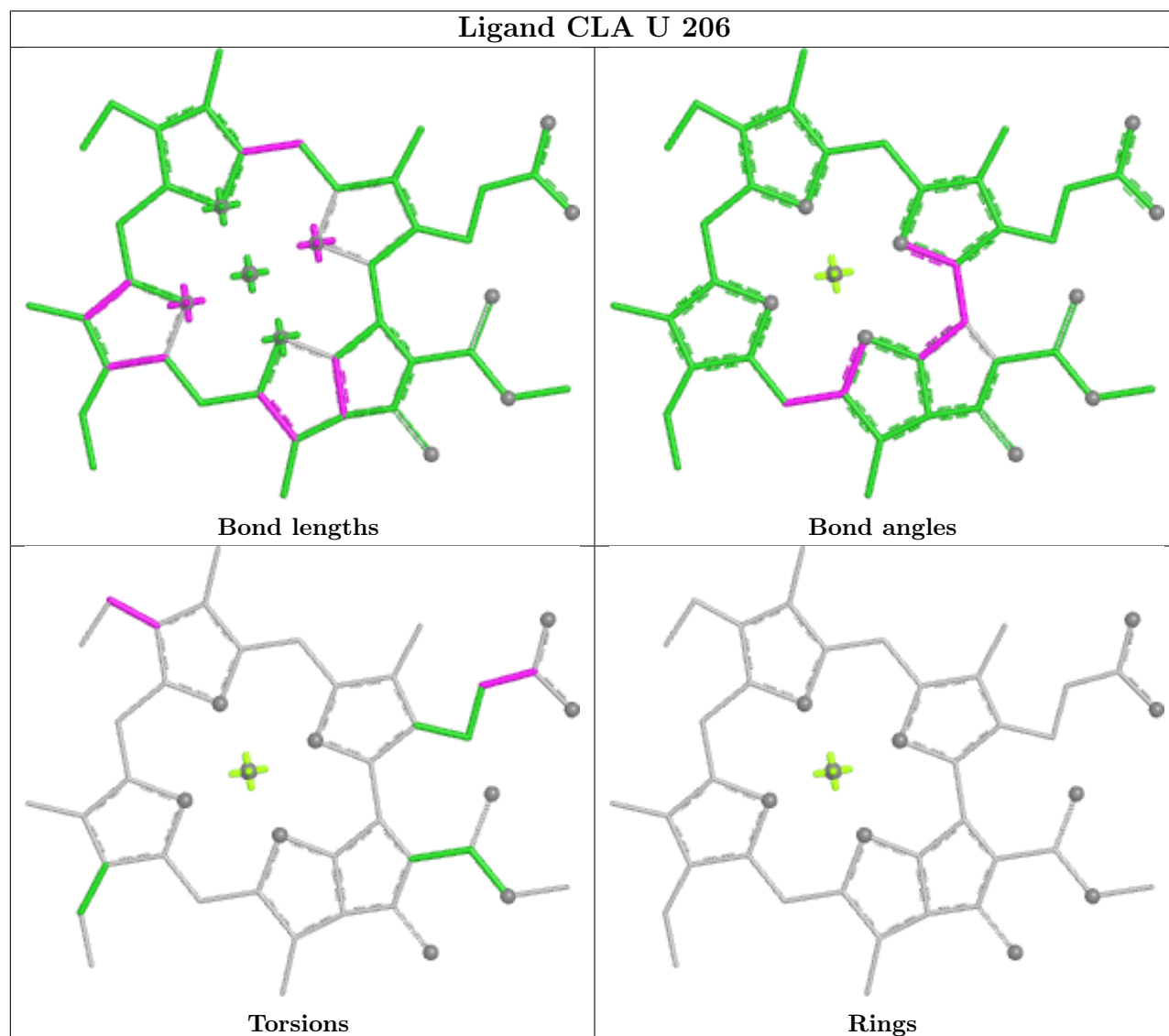
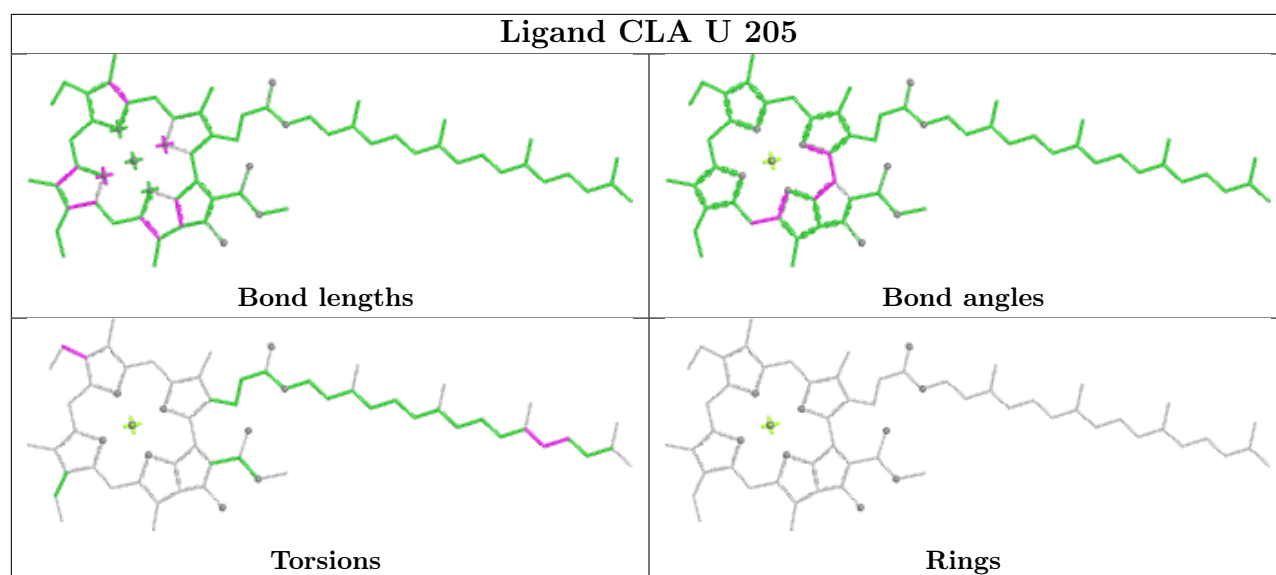


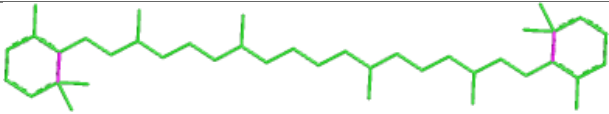
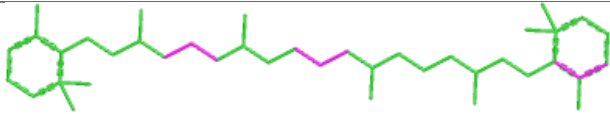
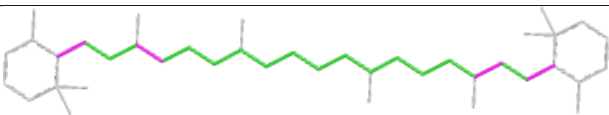
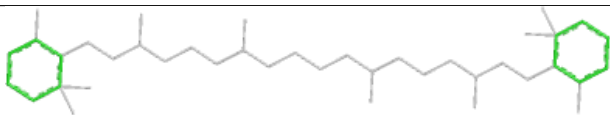


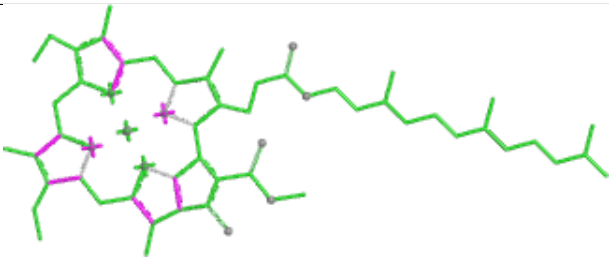
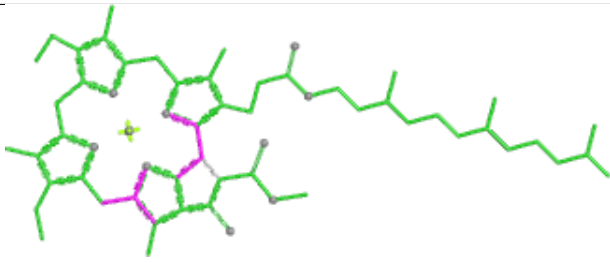
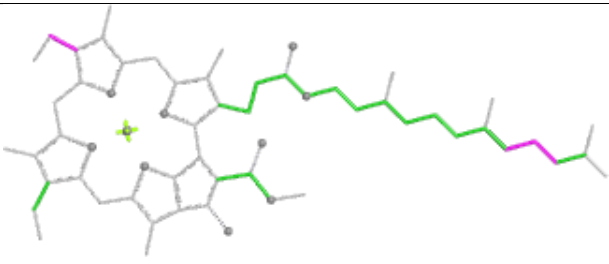
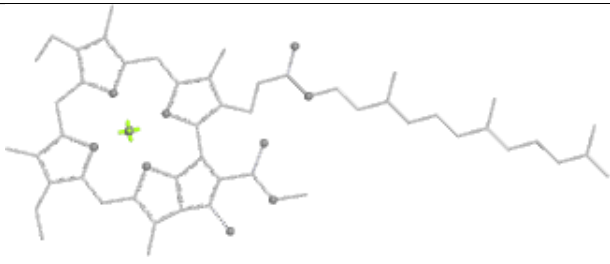
Ligand BCR I 102	
	
Bond lengths	Bond angles
	
Torsions	Rings


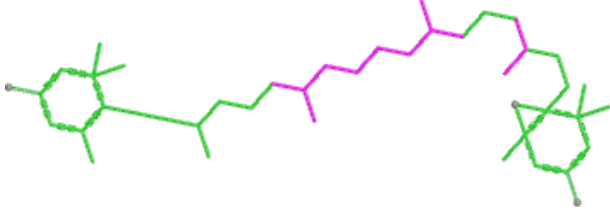
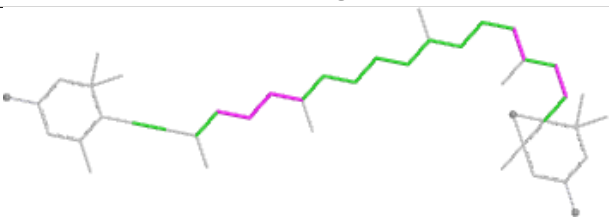
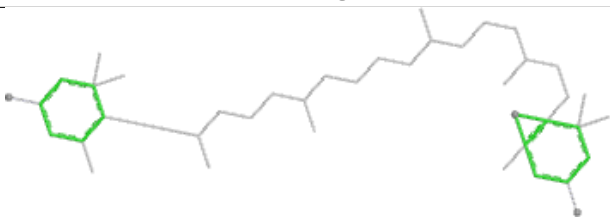
Ligand A86 Q 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

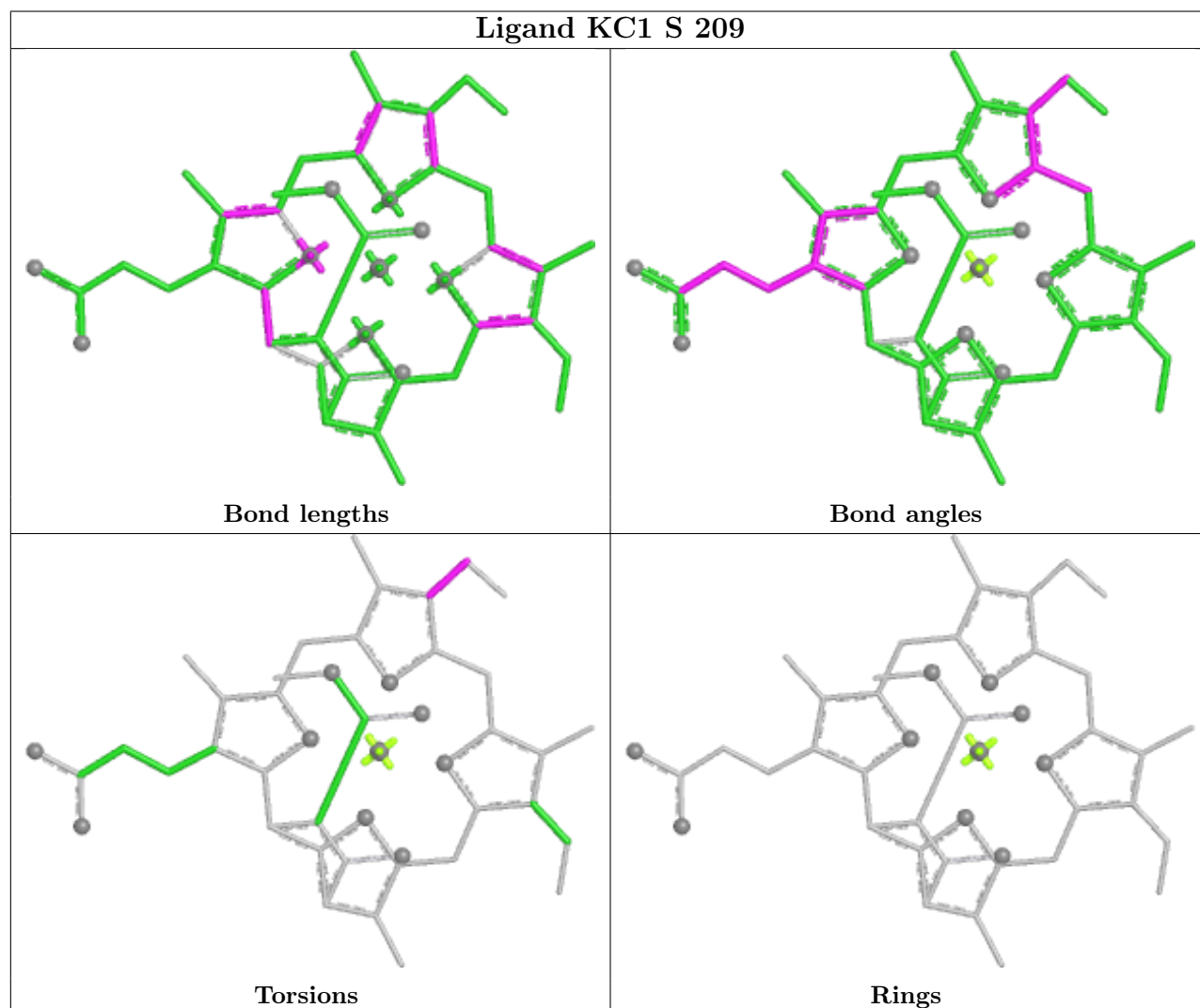
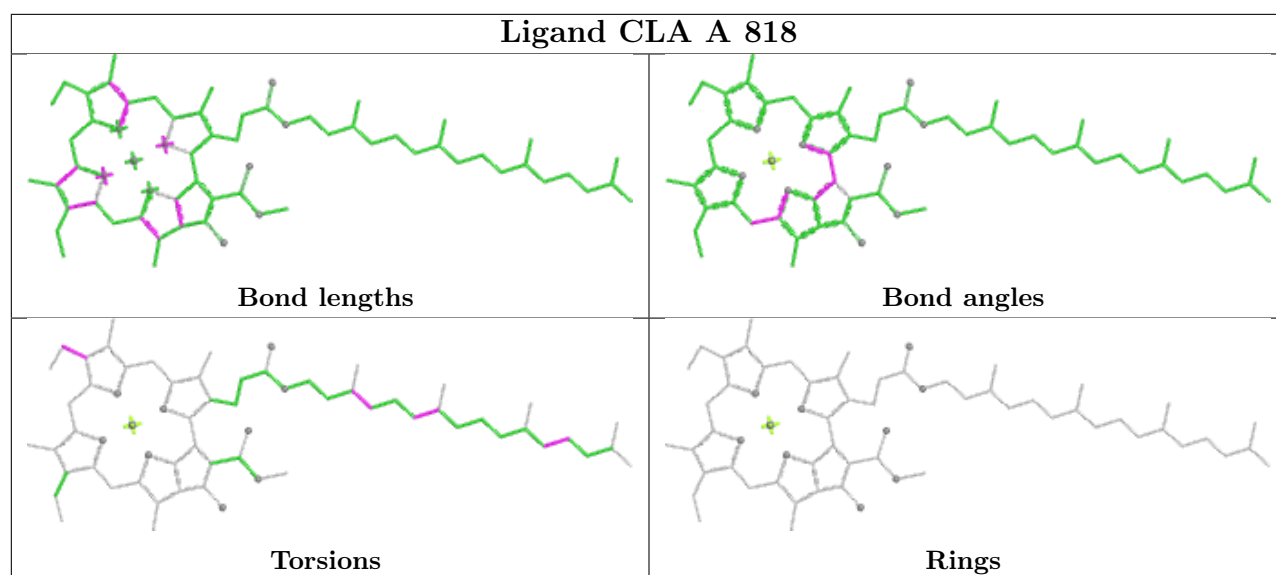
Ligand CLA A 836	
	
Bond lengths	Bond angles
	
Torsions	Rings

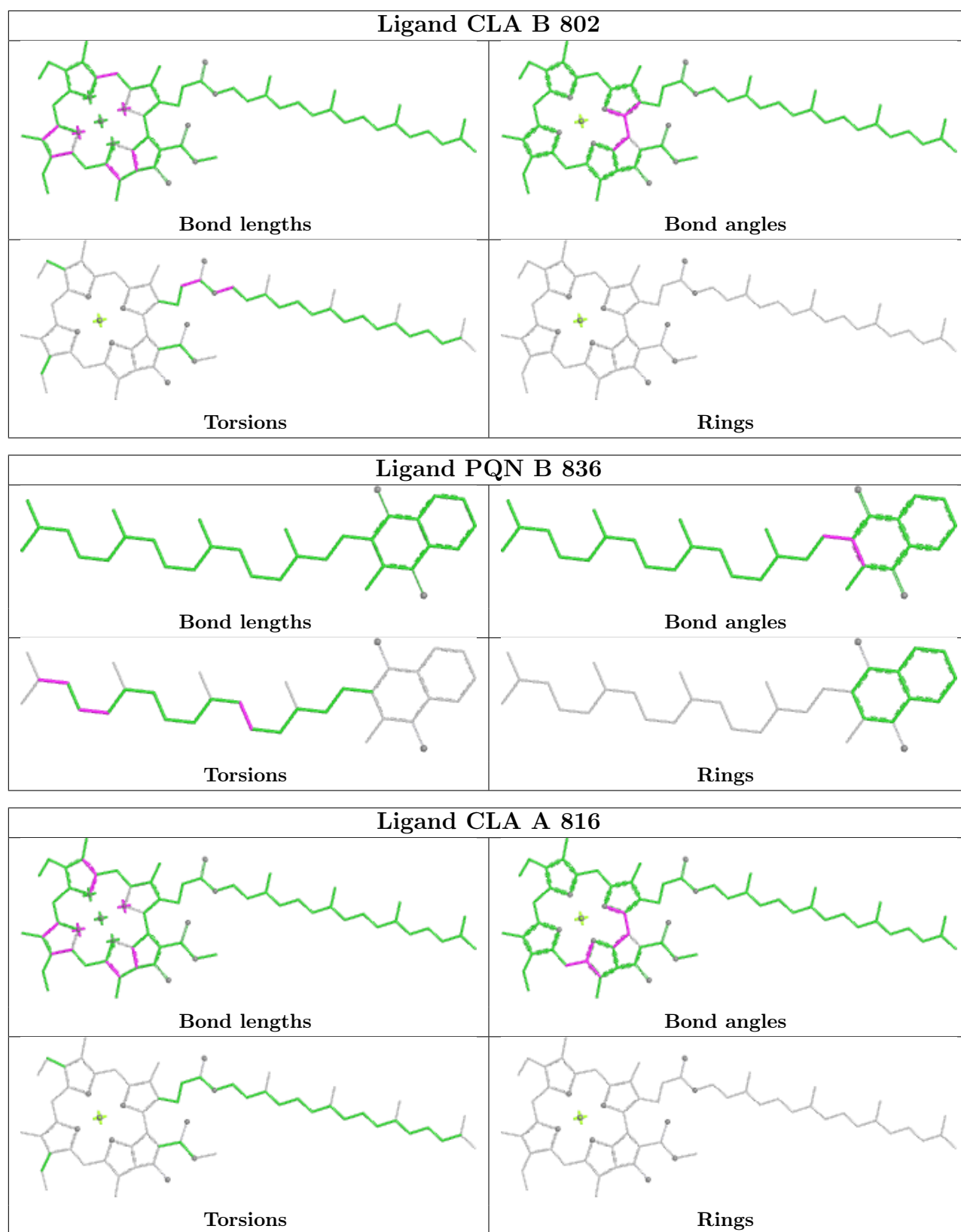


Ligand BCR B 841	
	
Bond lengths	Bond angles
	
Torsions	Rings

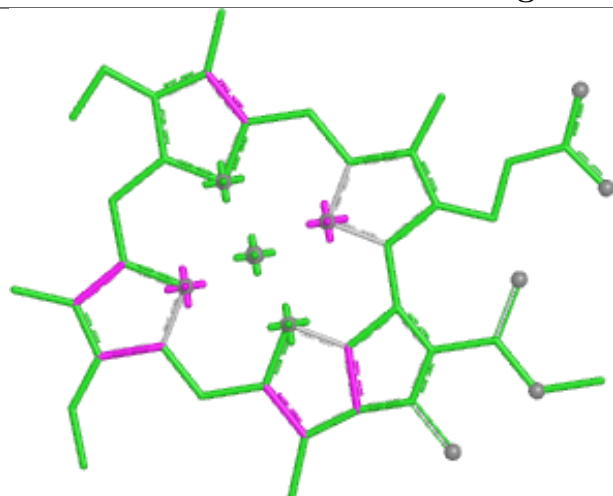
Ligand CLA B 816	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DD6 G 211	
	
Bond lengths	Bond angles
	
Torsions	Rings

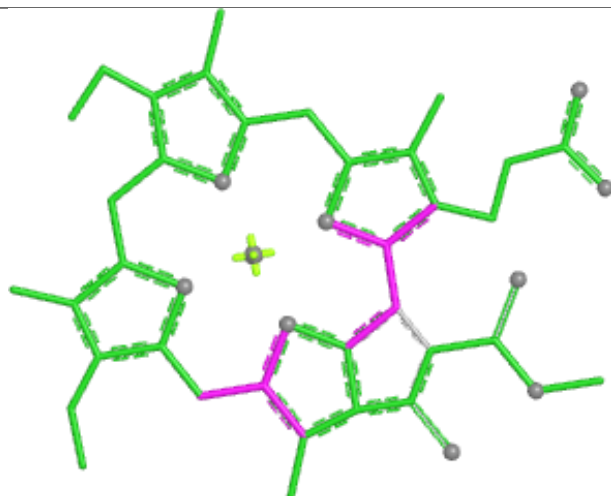




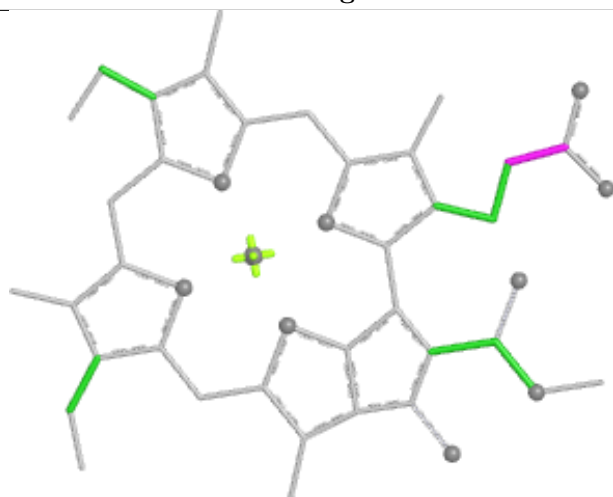
Ligand CLA S 207



Bond lengths



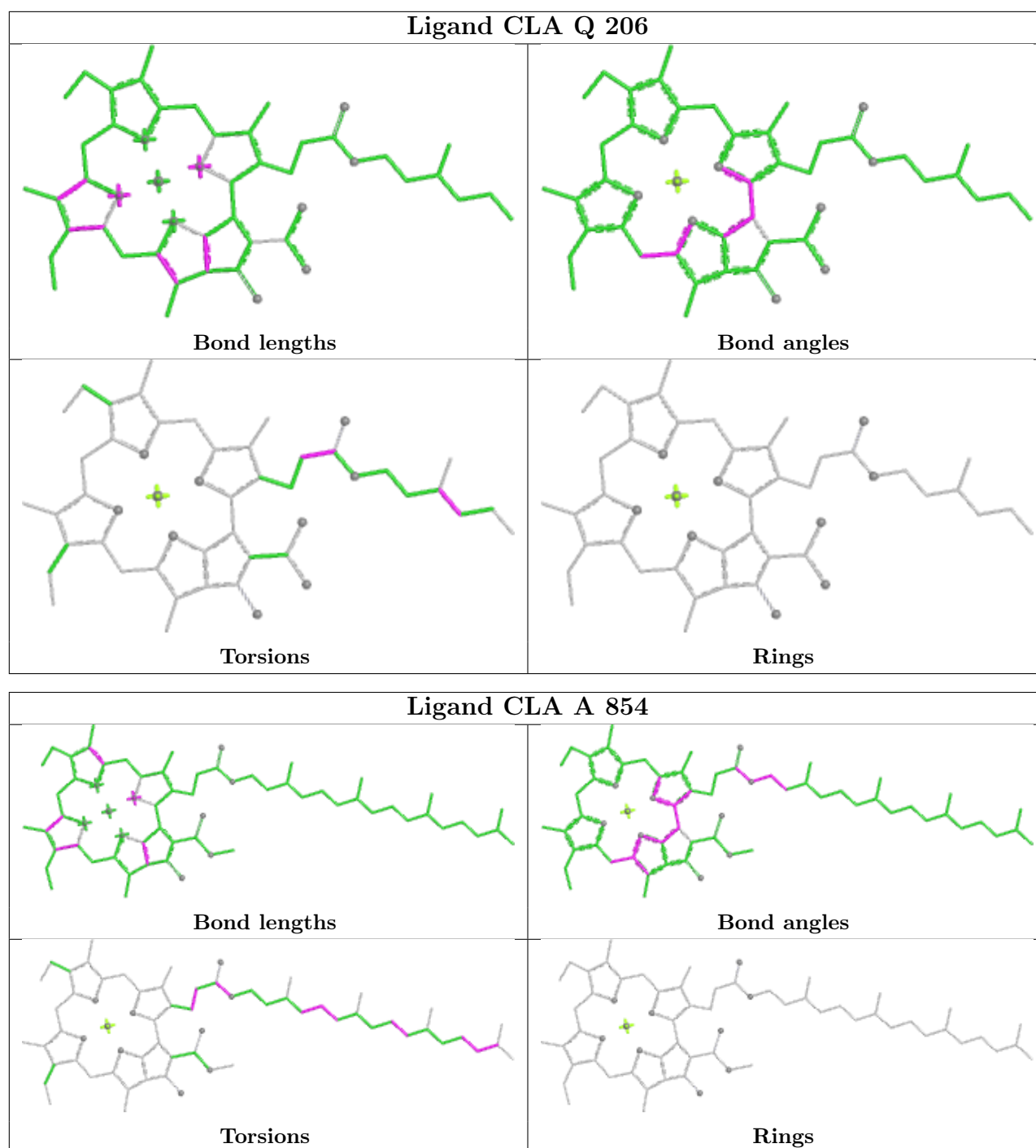
Bond angles



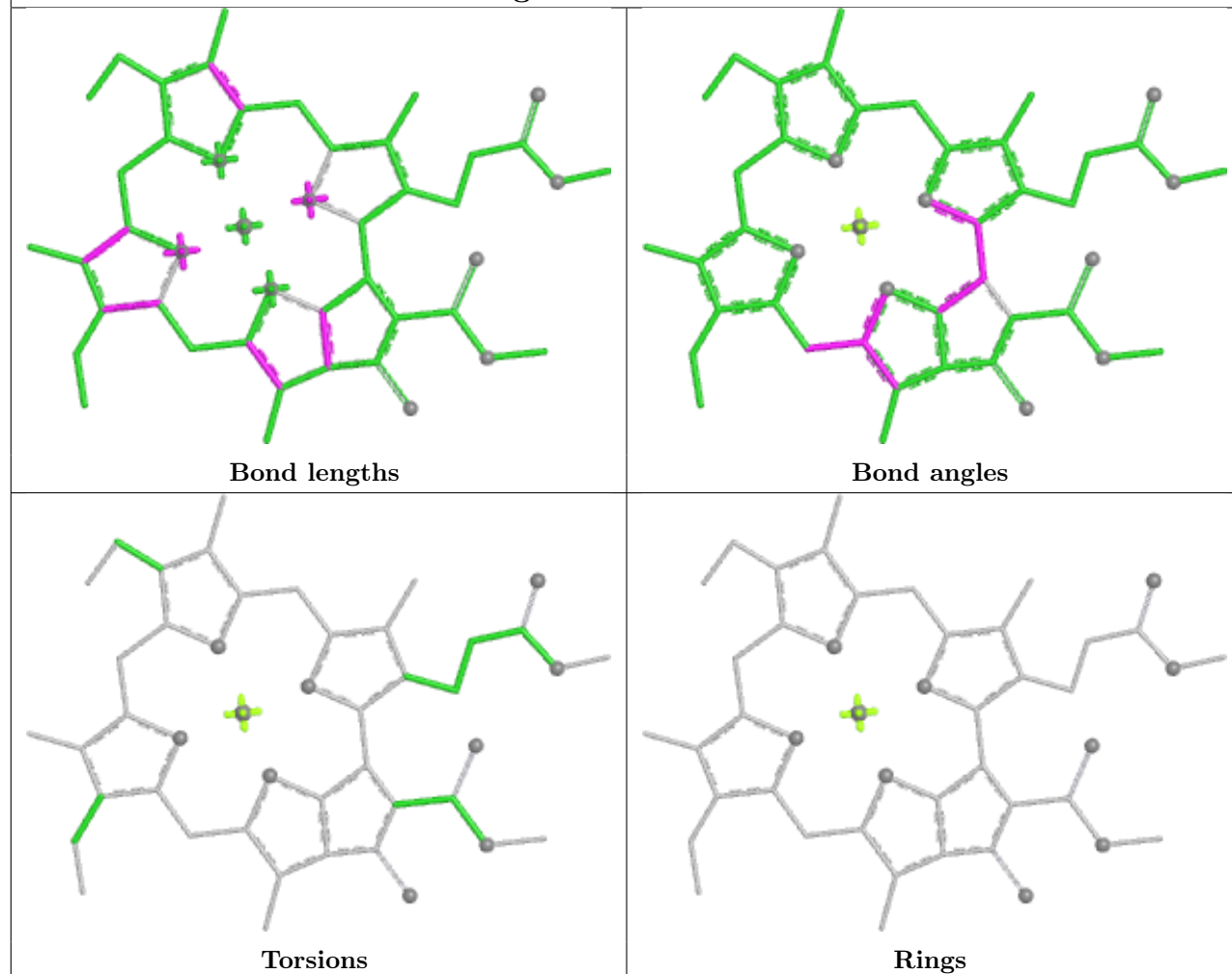
Torsions



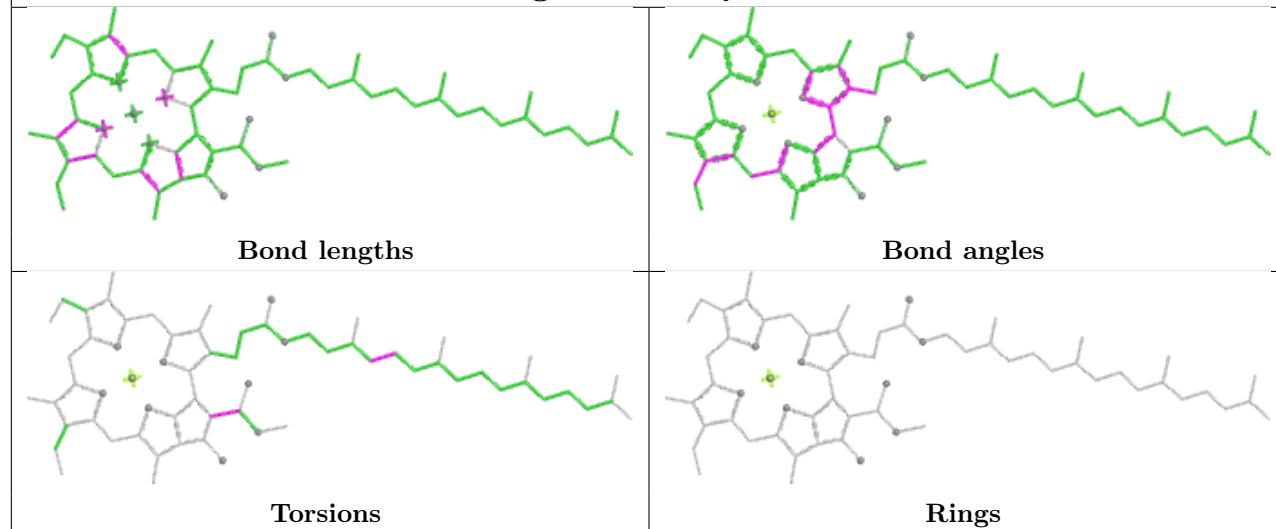
Rings

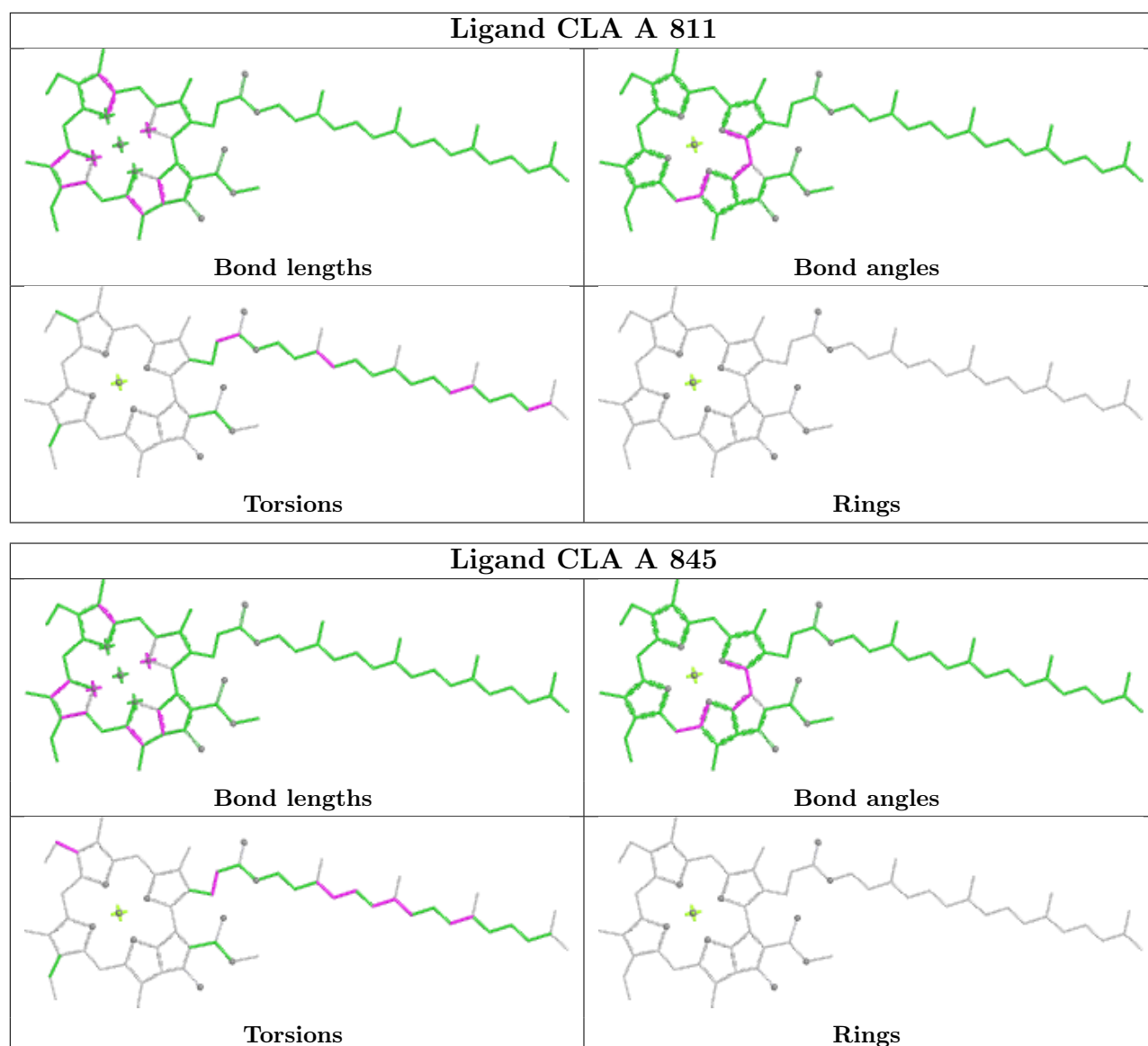


Ligand CLA O 207

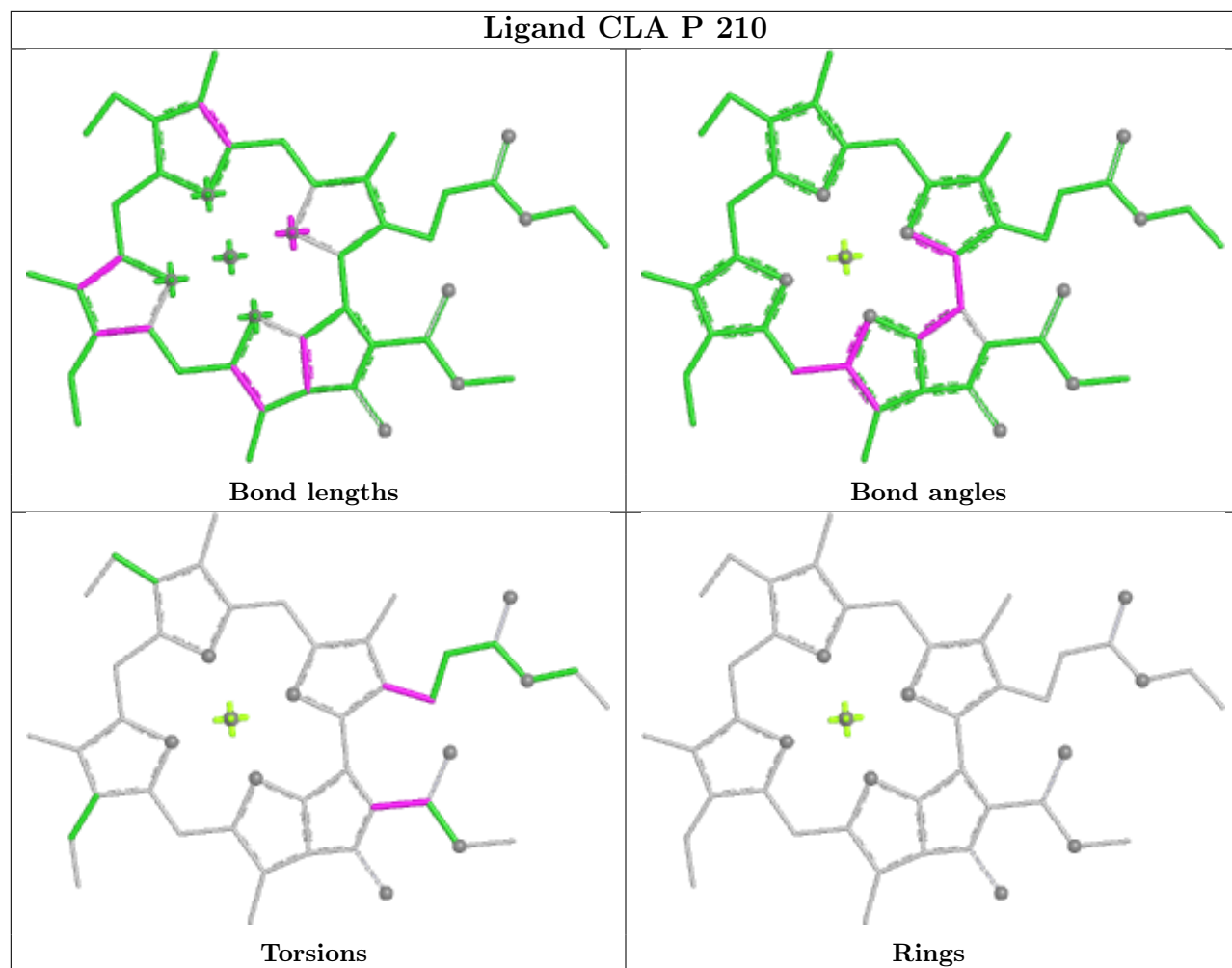


Ligand CLA Q 212

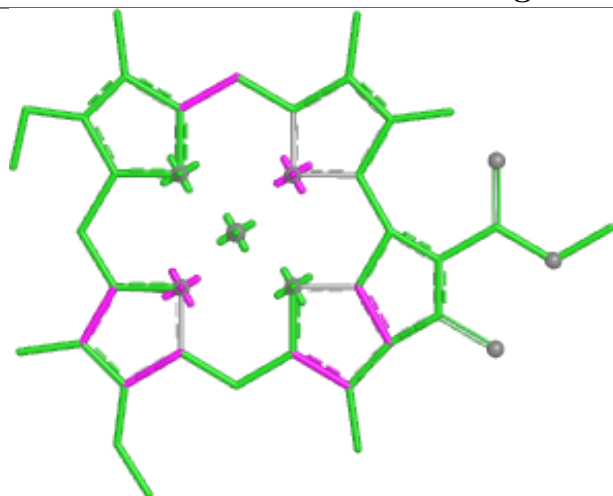




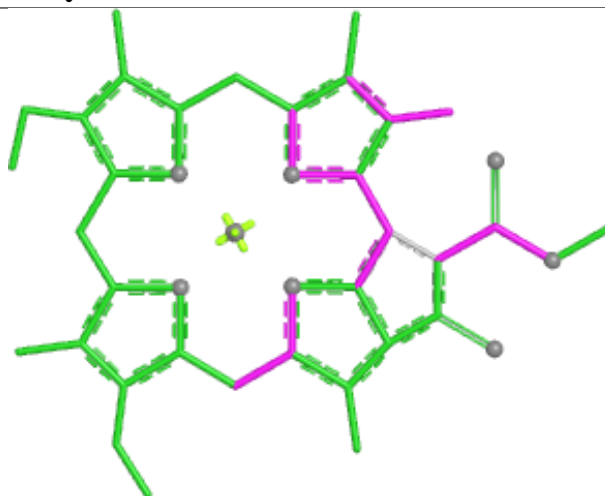
Ligand CLA P 210



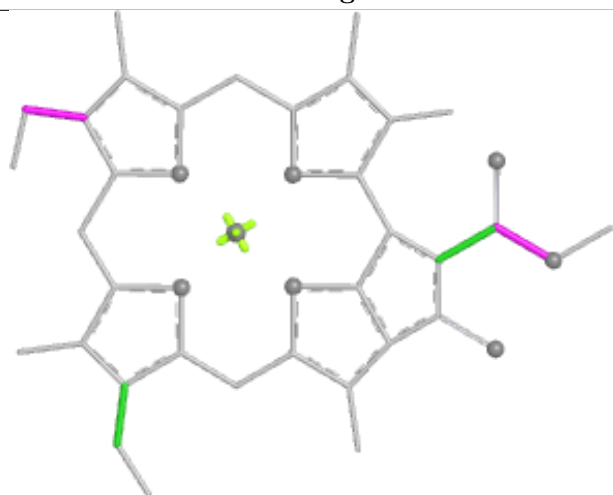
Ligand CLA Q 211



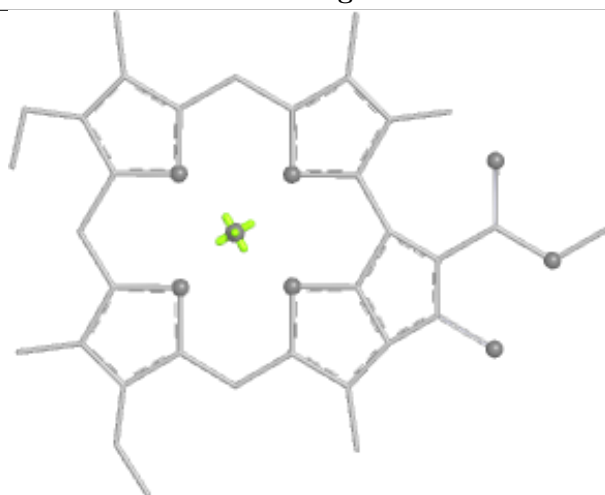
Bond lengths



Bond angles

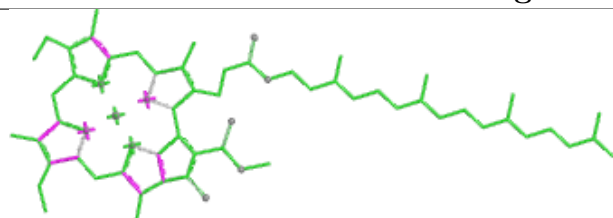


Torsions

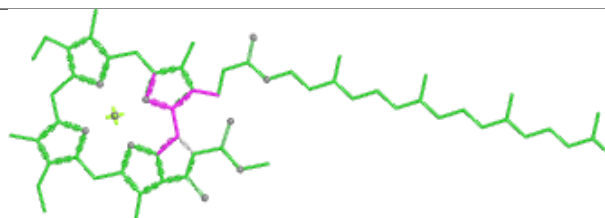


Rings

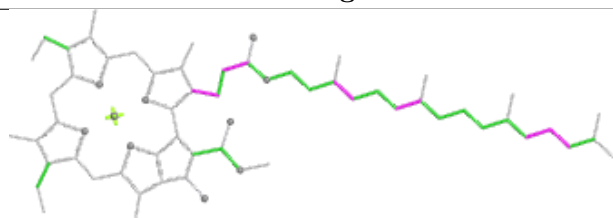
Ligand CLA B 823



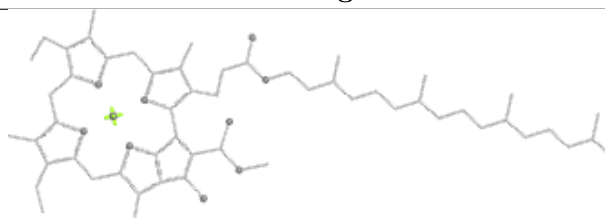
Bond lengths



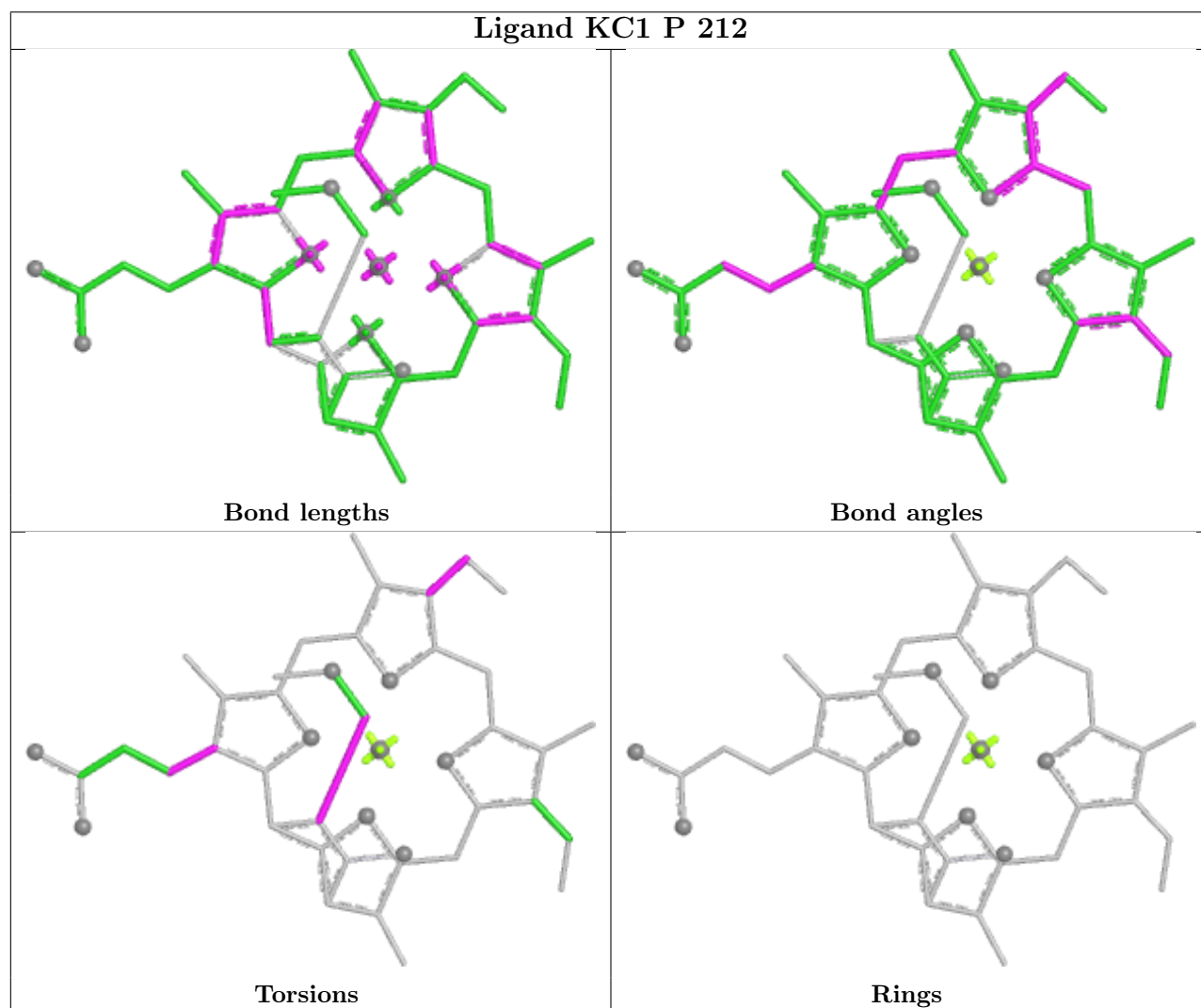
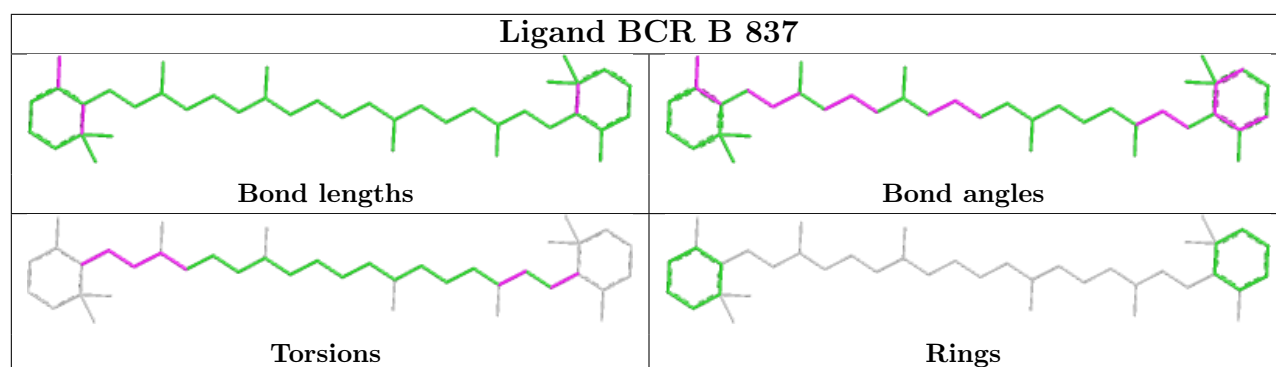
Bond angles



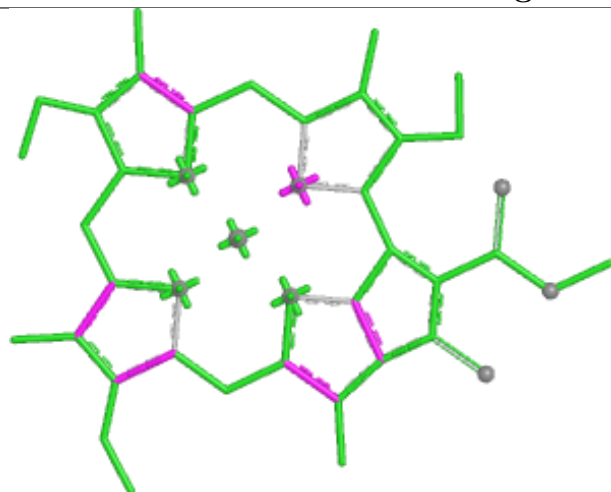
Torsions



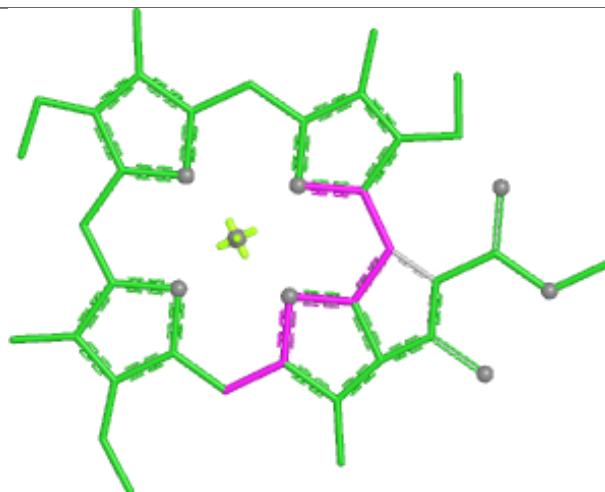
Rings



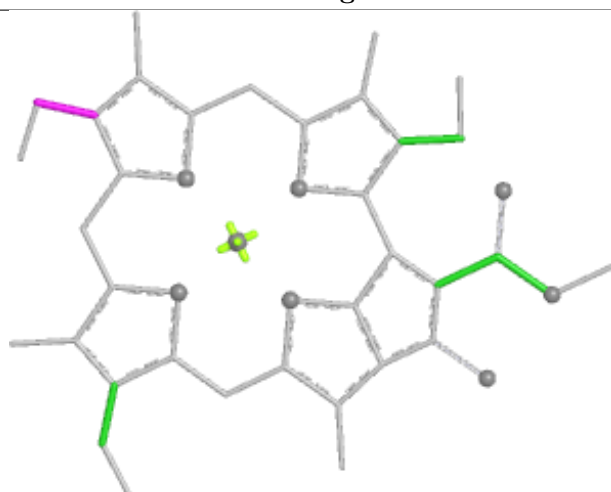
Ligand CLA T 206



Bond lengths



Bond angles

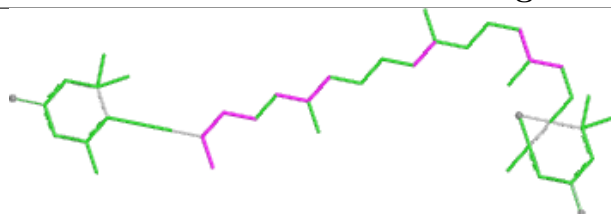


Torsions

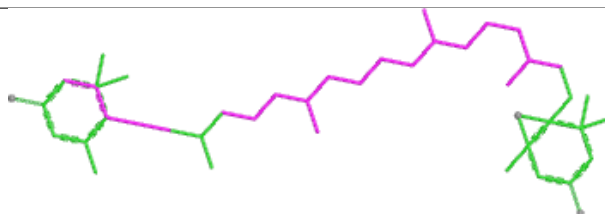


Rings

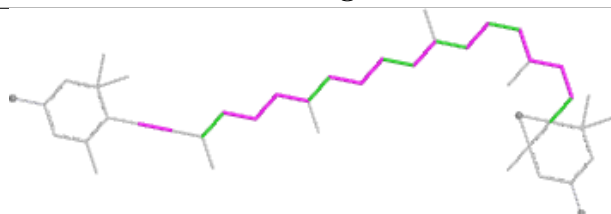
Ligand DD6 P 220



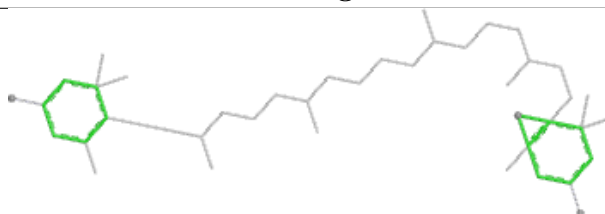
Bond lengths



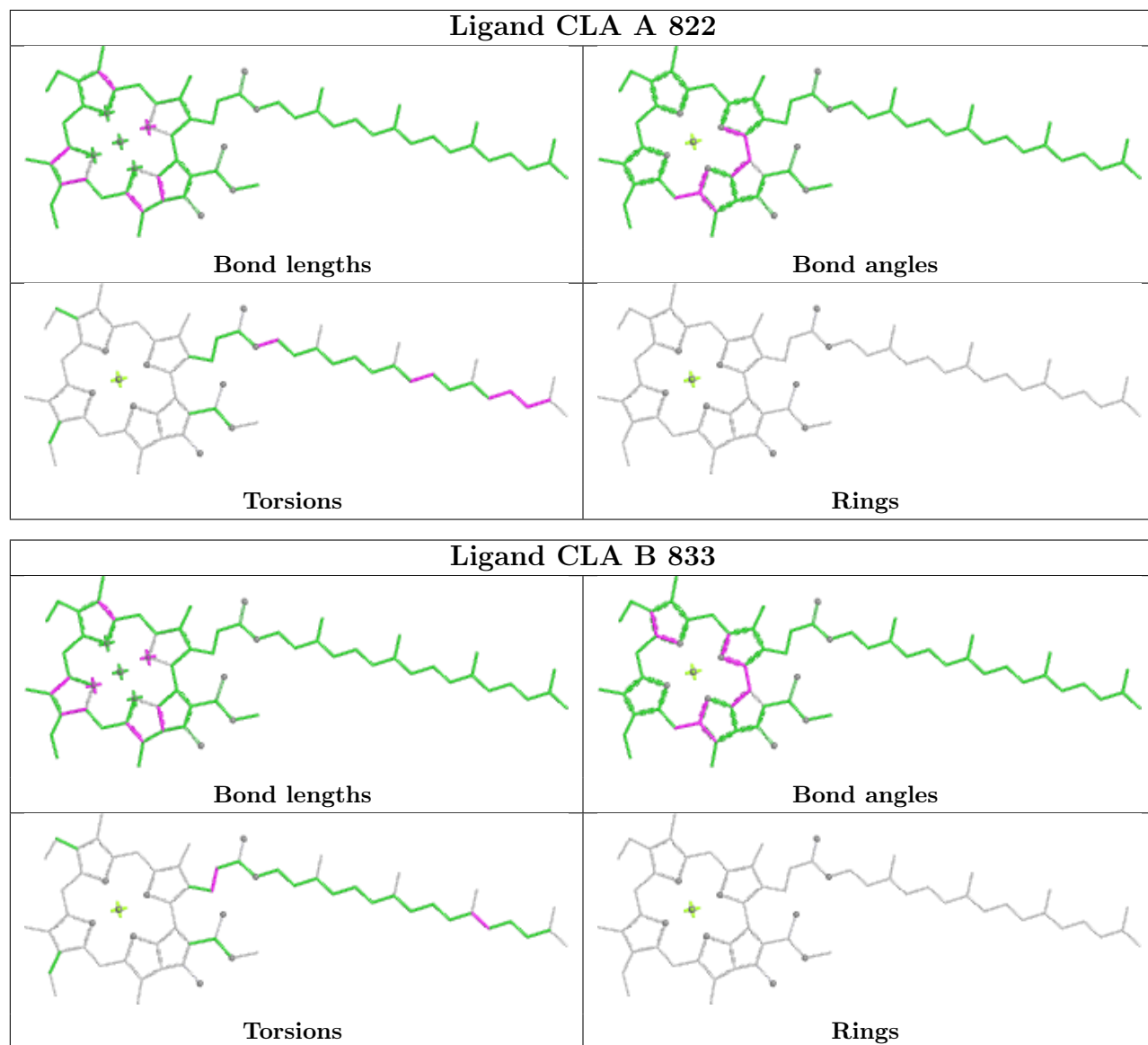
Bond angles

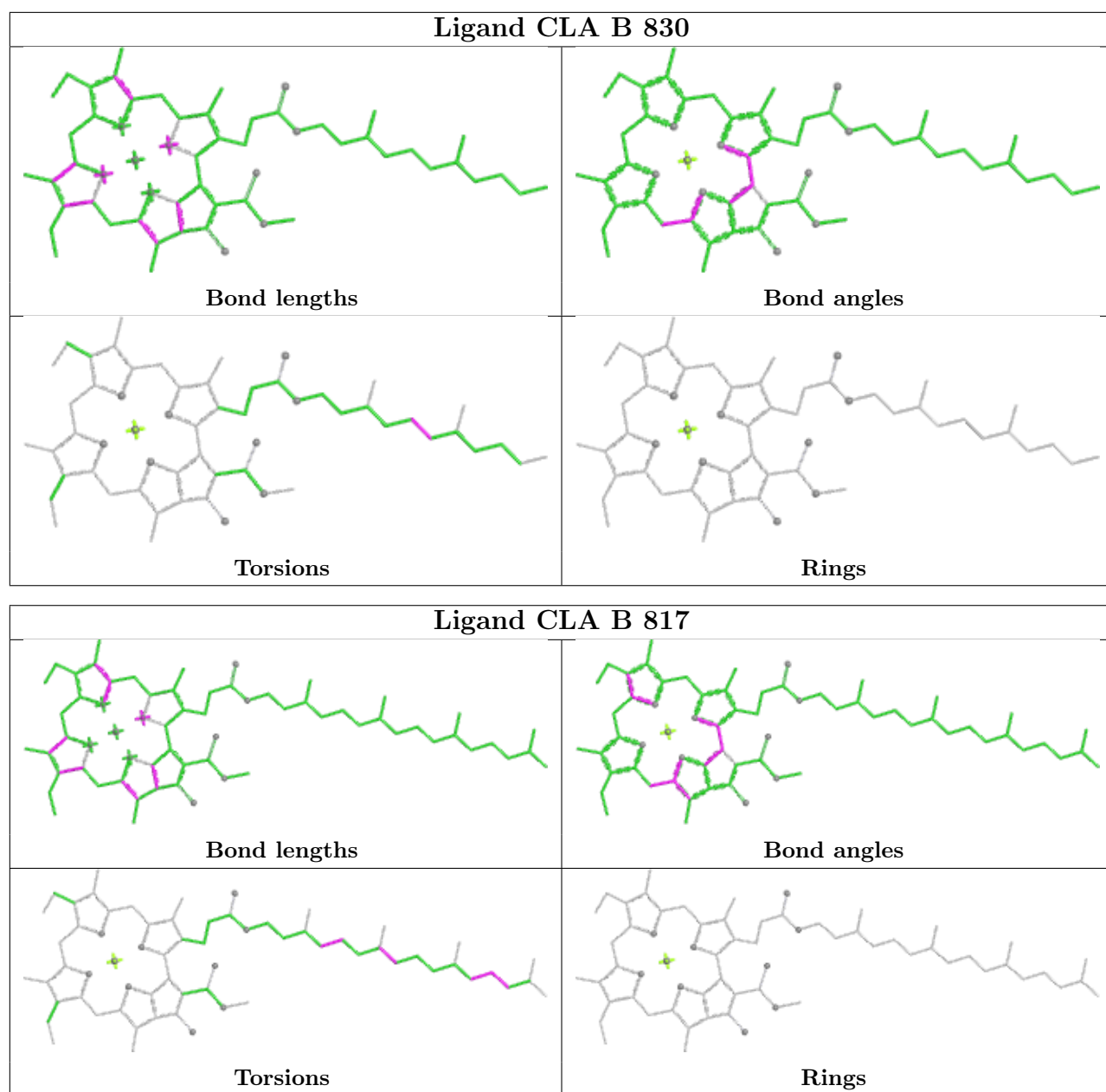


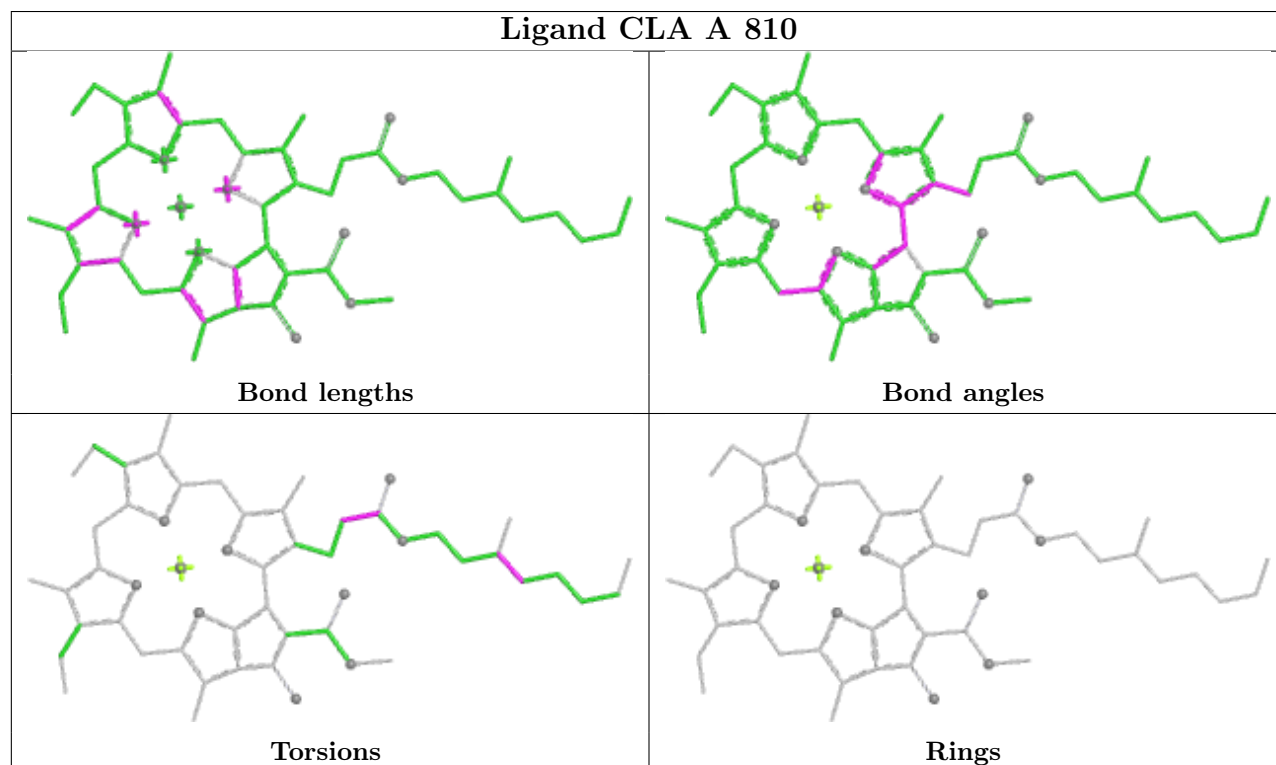
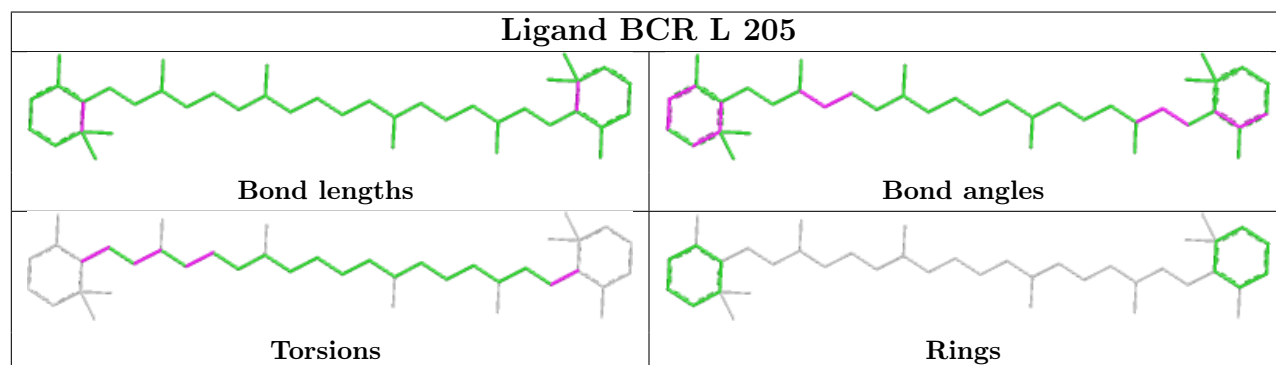
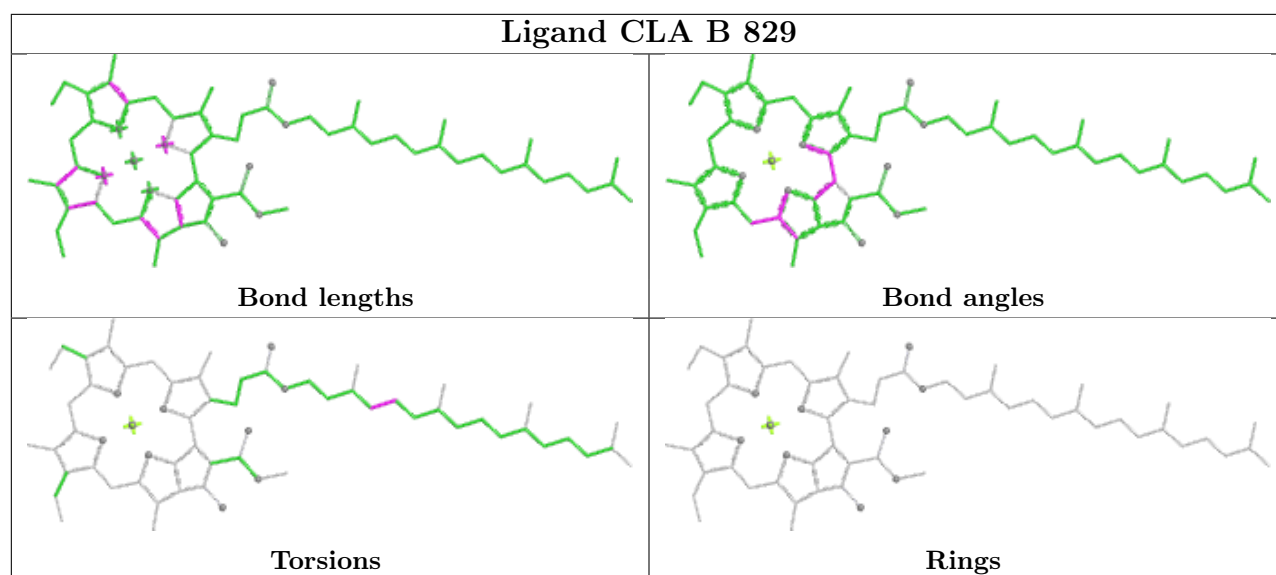
Torsions



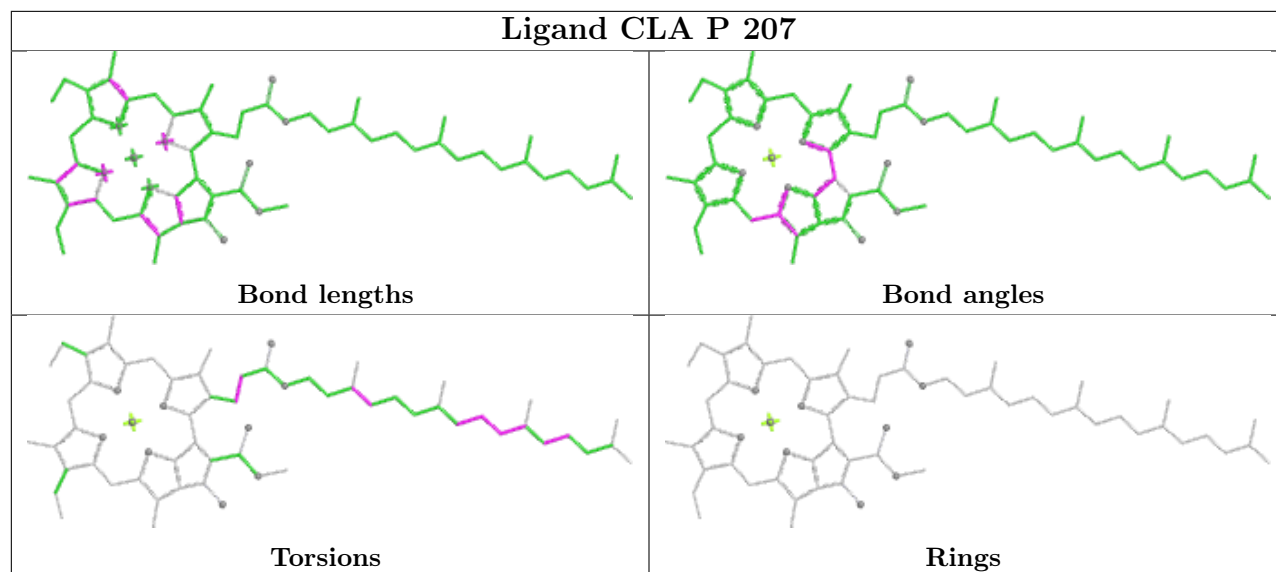
Rings



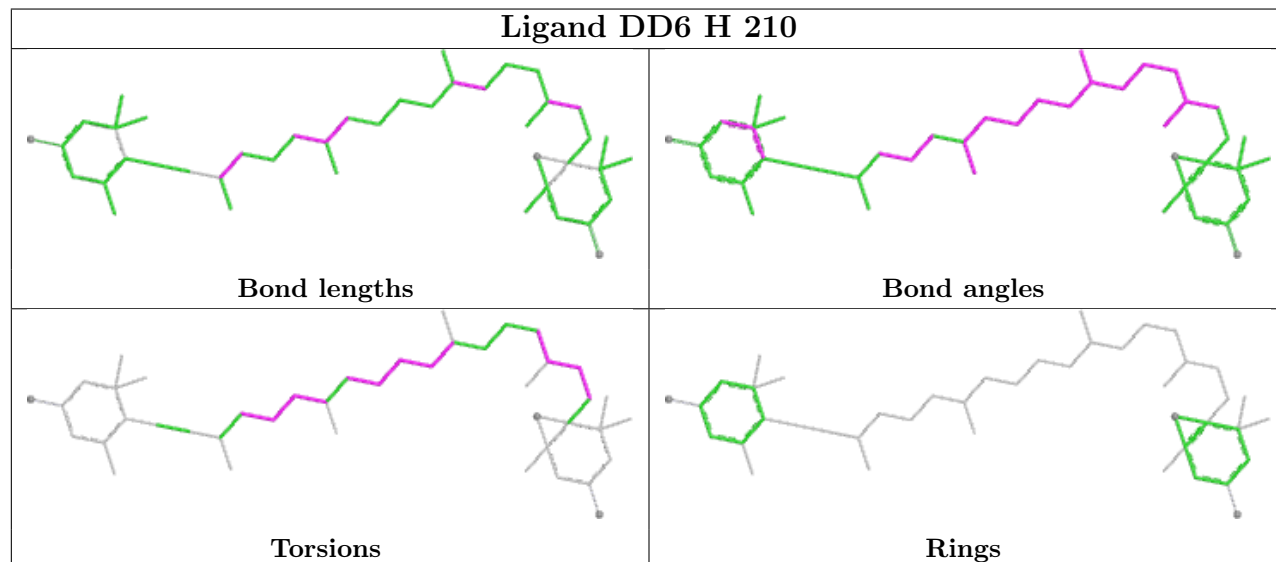




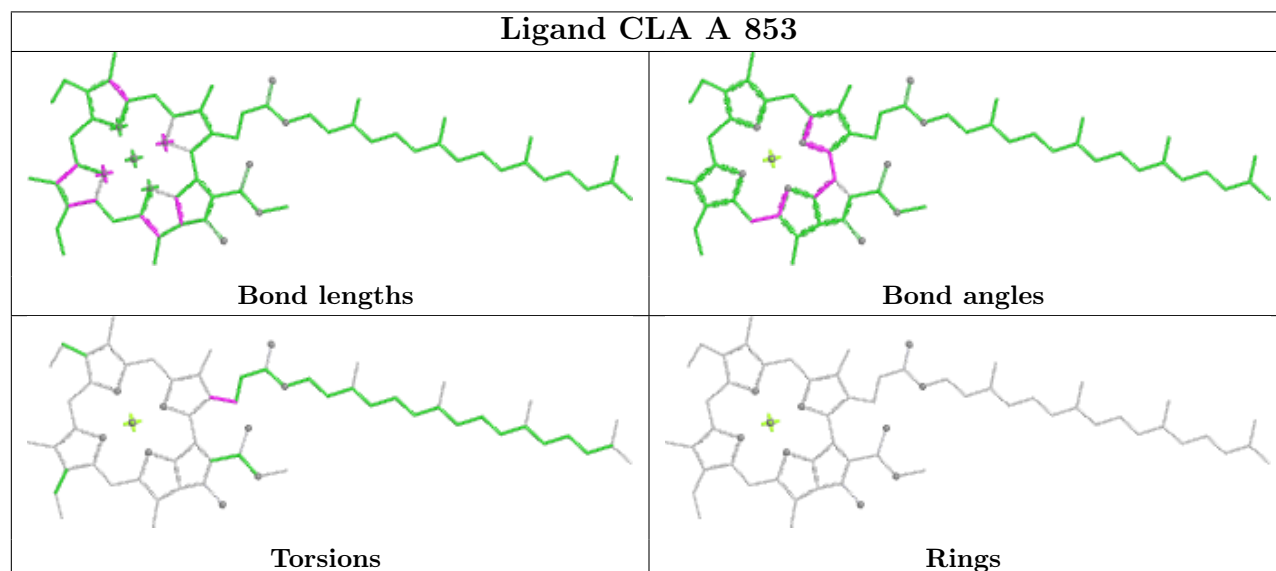
Ligand CLA P 207

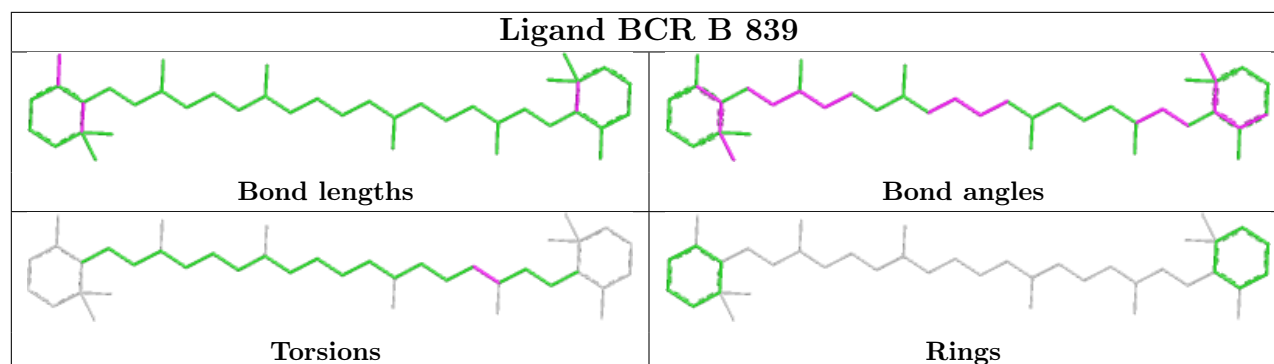
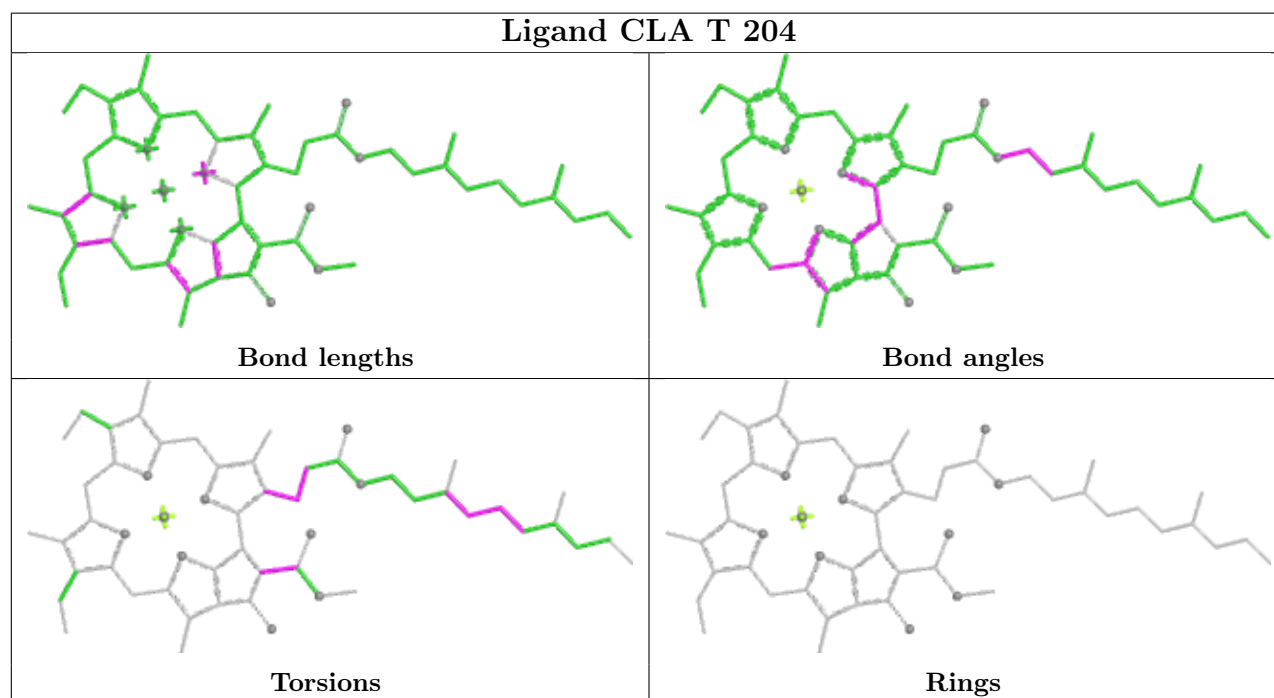
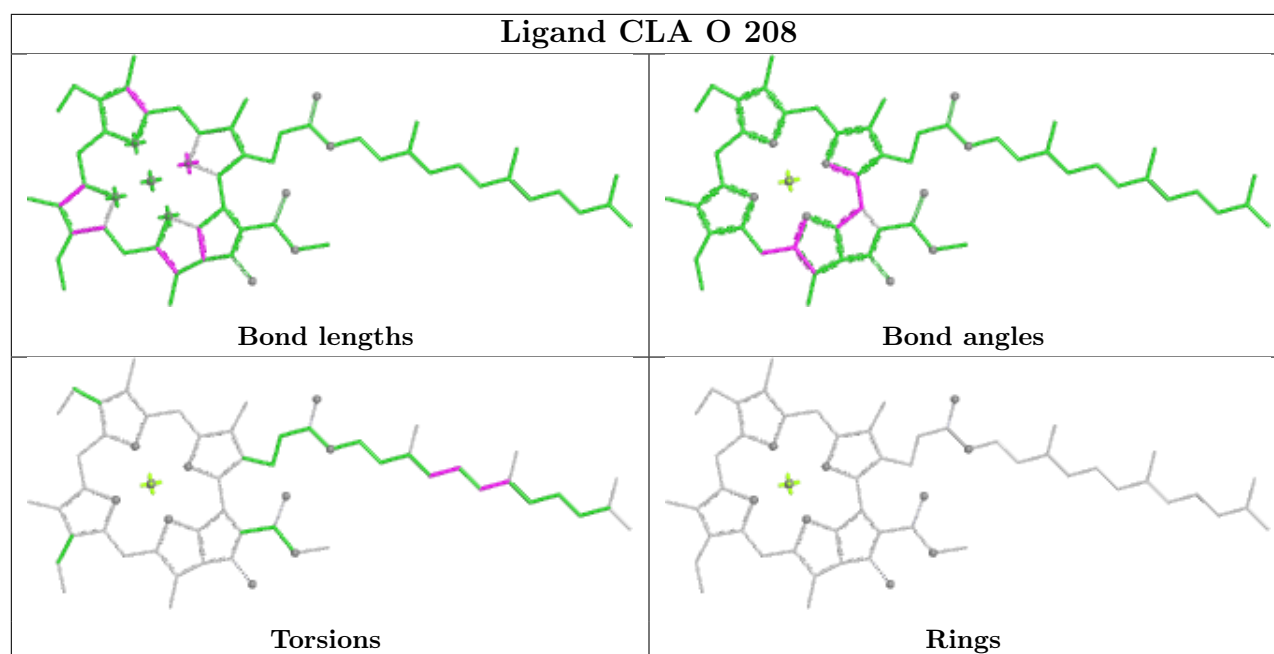


Ligand DD6 H 210

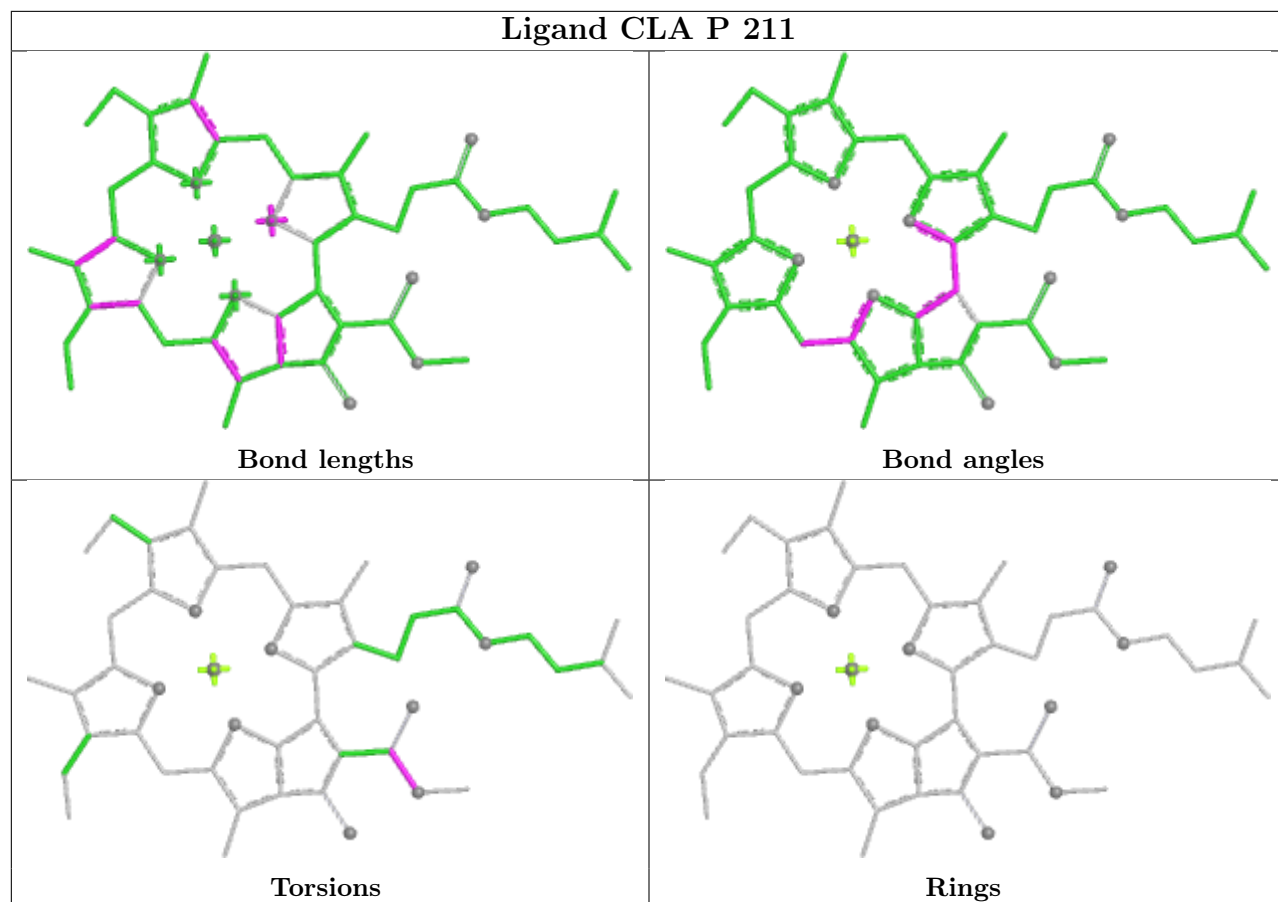


Ligand CLA A 853

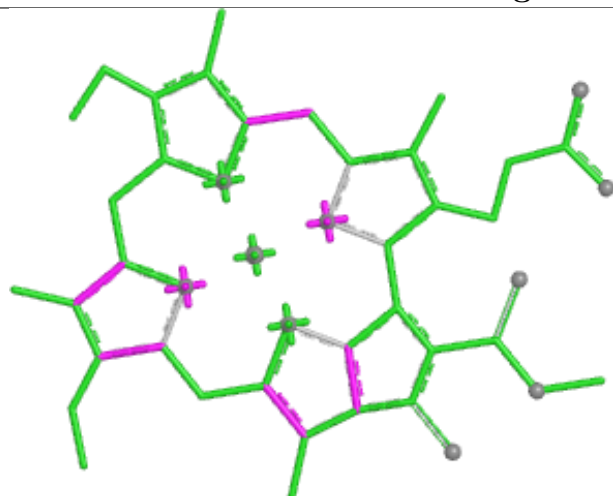




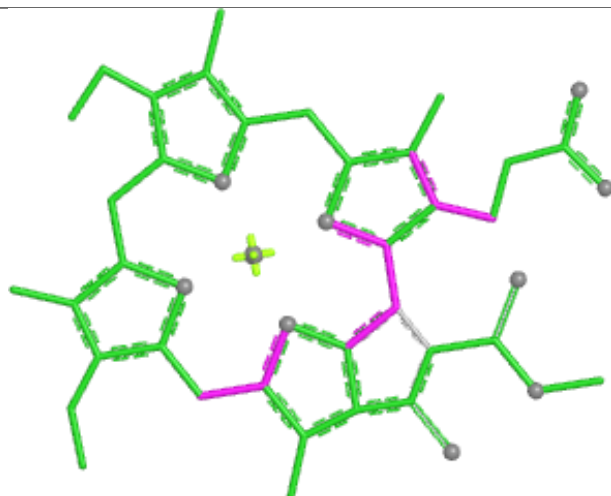
Ligand CLA P 211



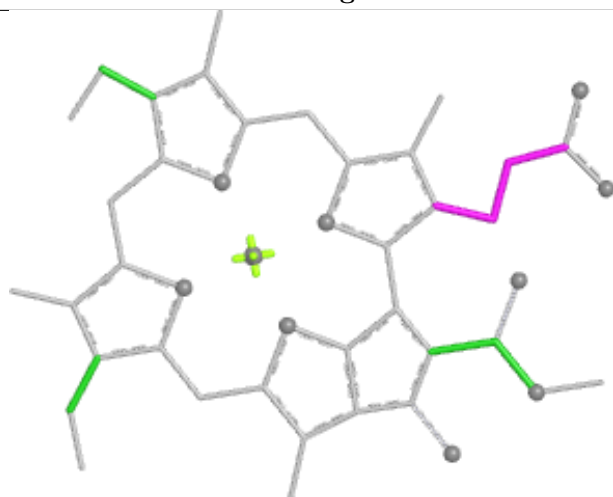
Ligand CLA H 209



Bond lengths



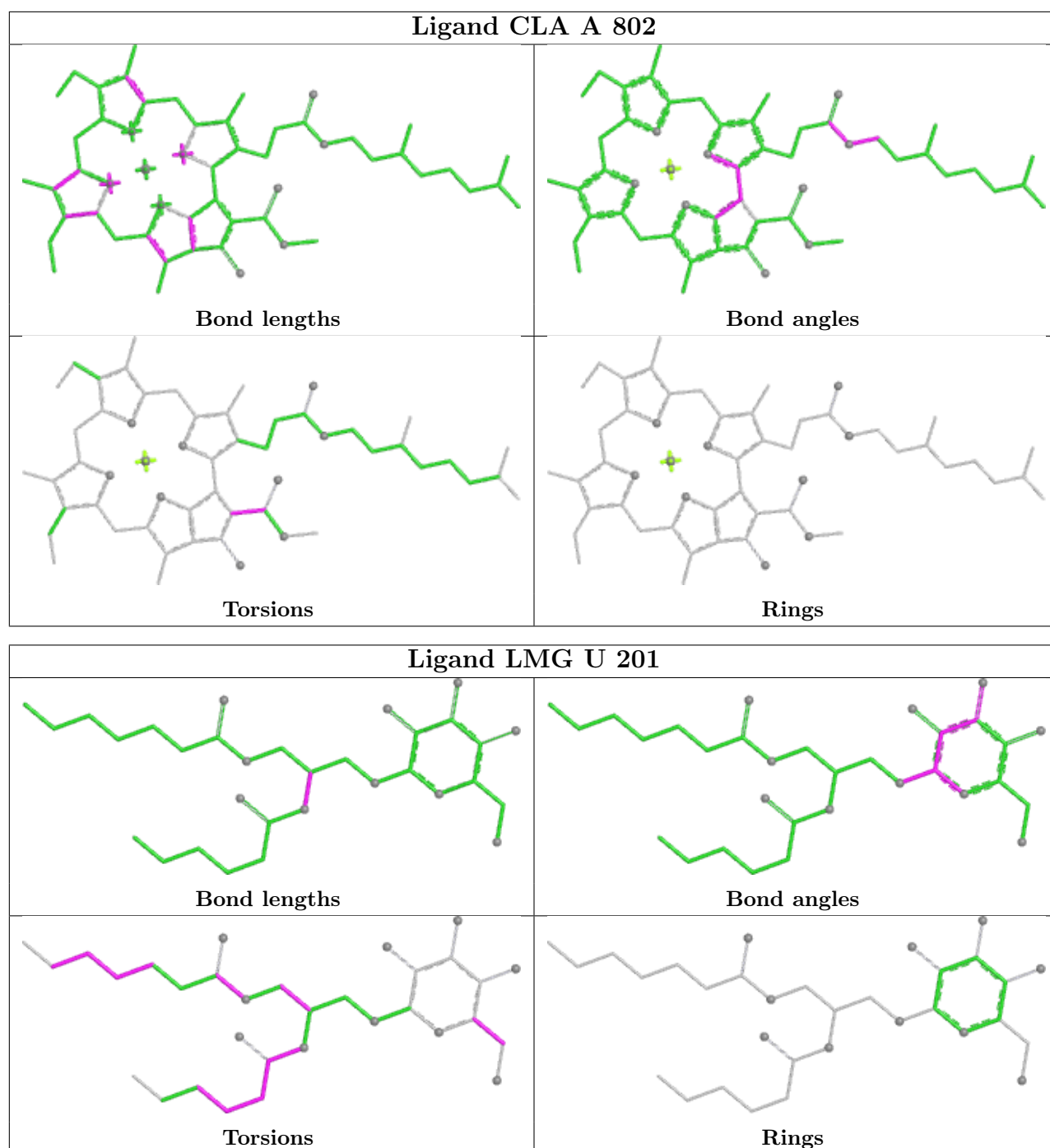
Bond angles



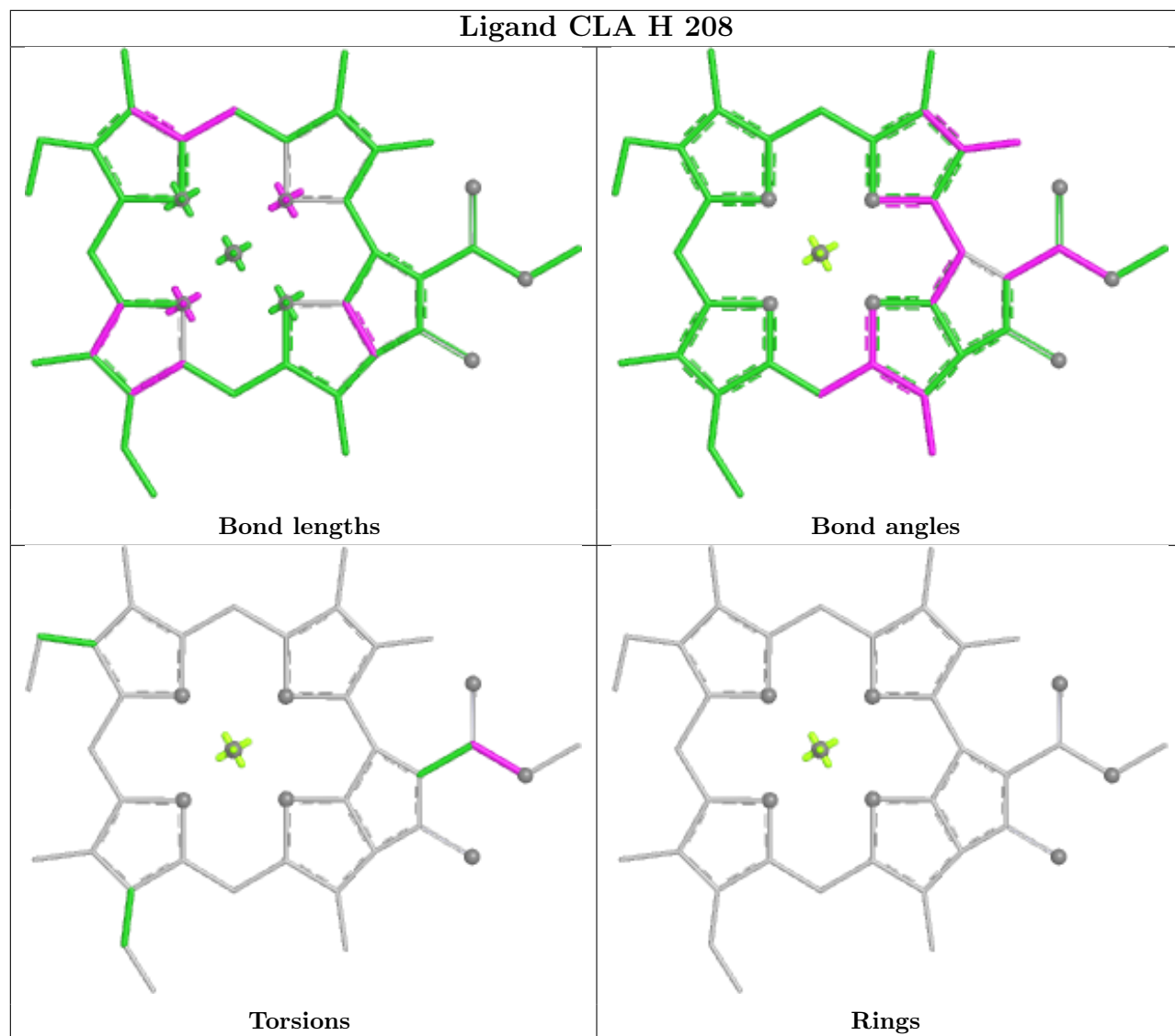
Torsions



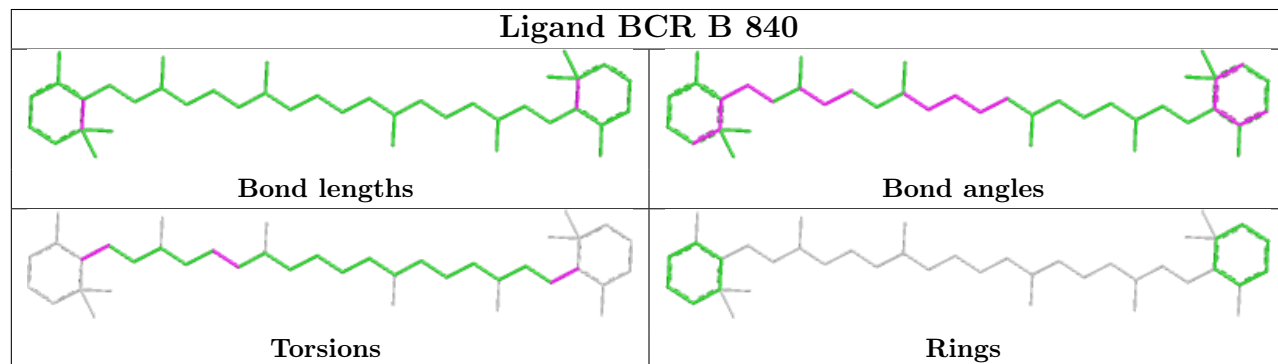
Rings

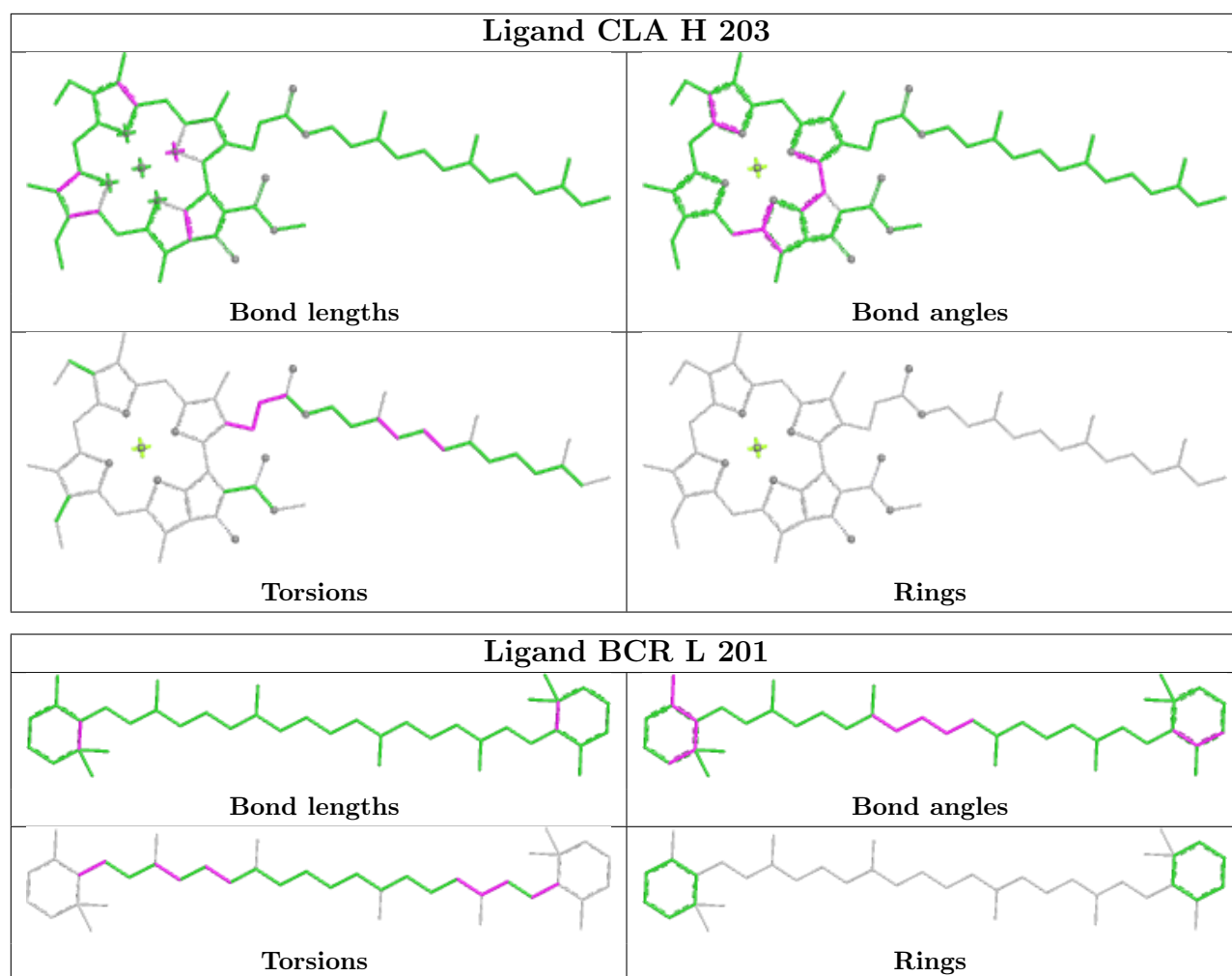


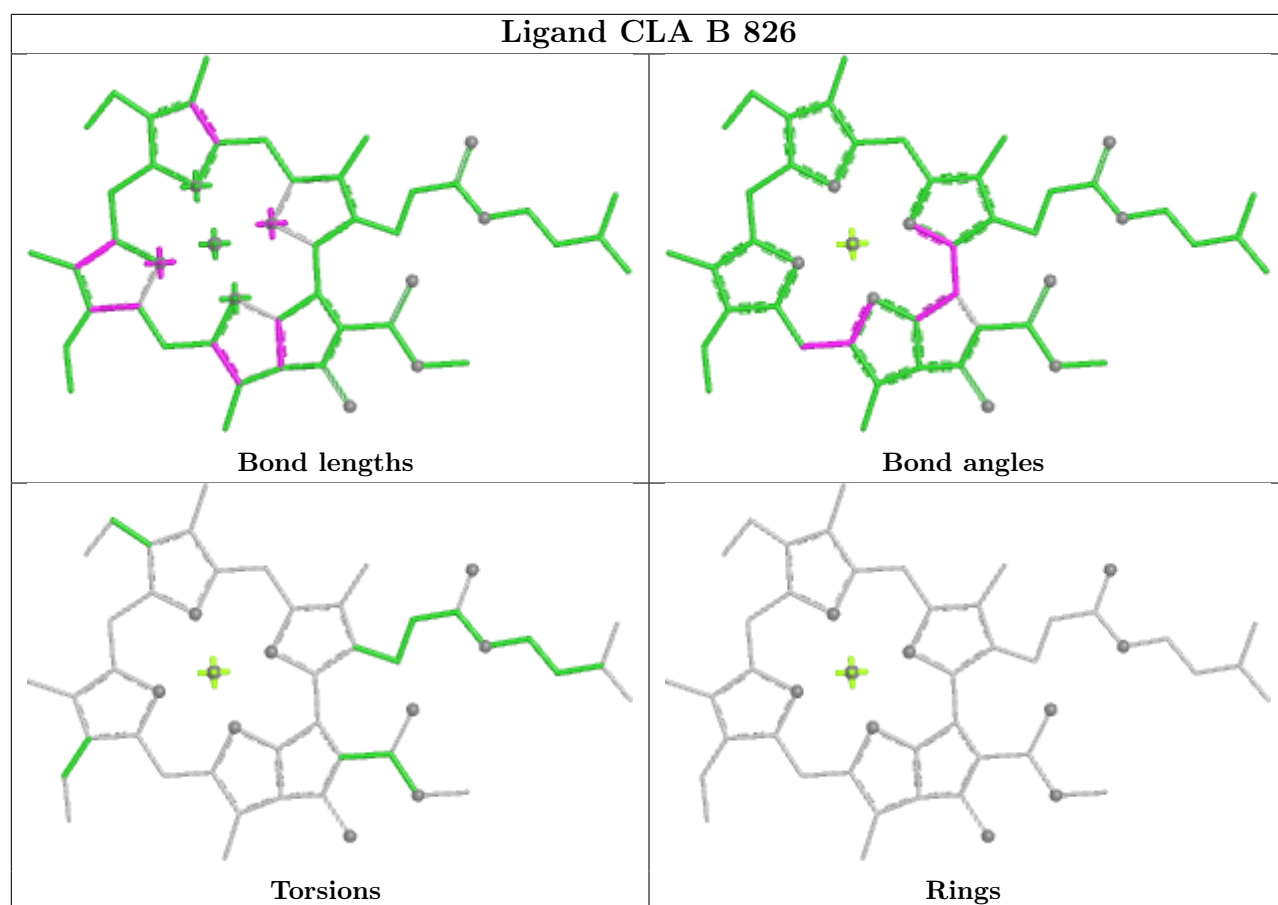
Ligand CLA H 208



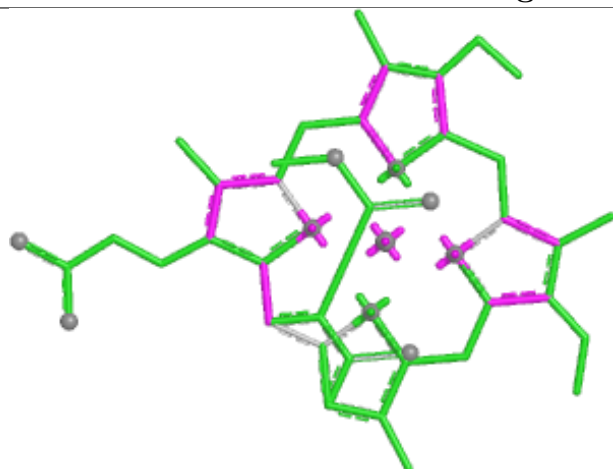
Ligand BCR B 840



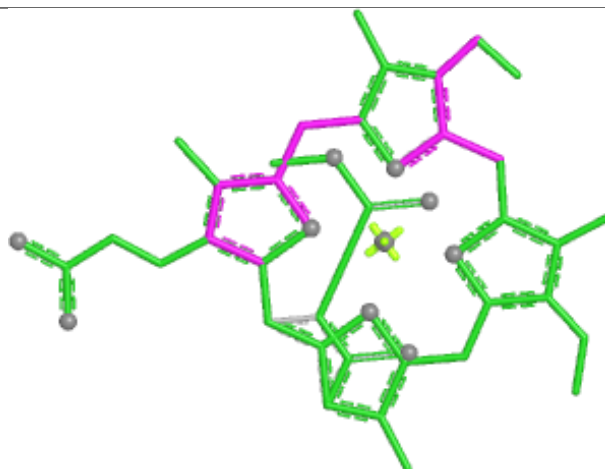




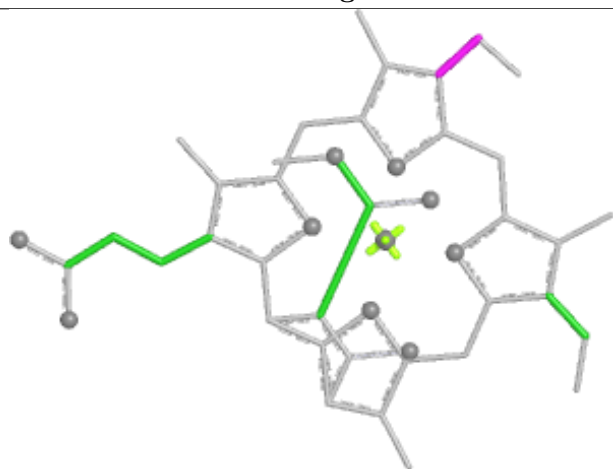
Ligand KC1 P 203



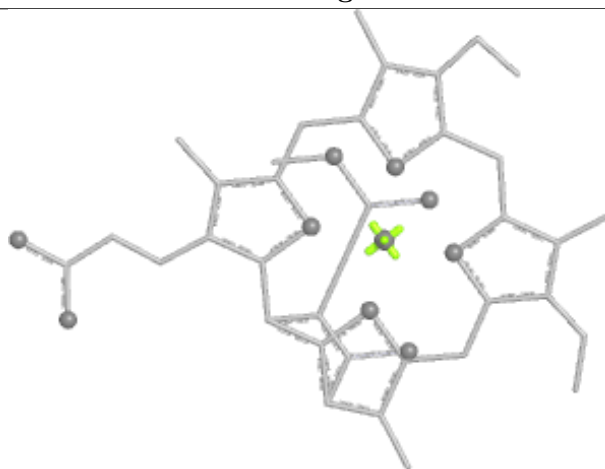
Bond lengths



Bond angles

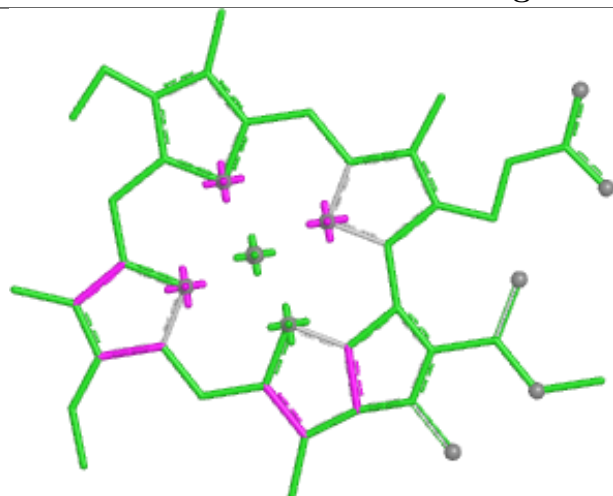


Torsions

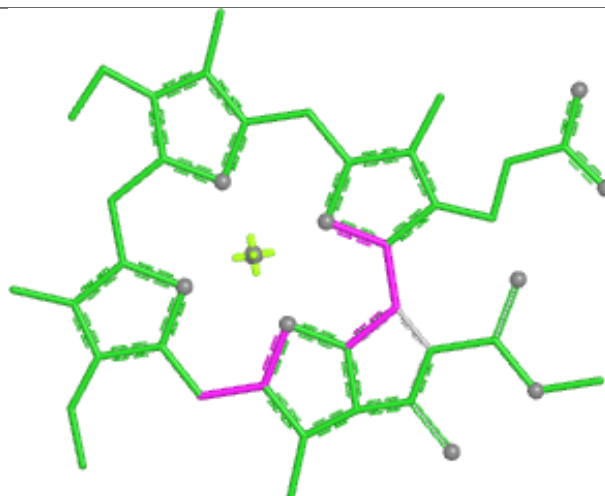


Rings

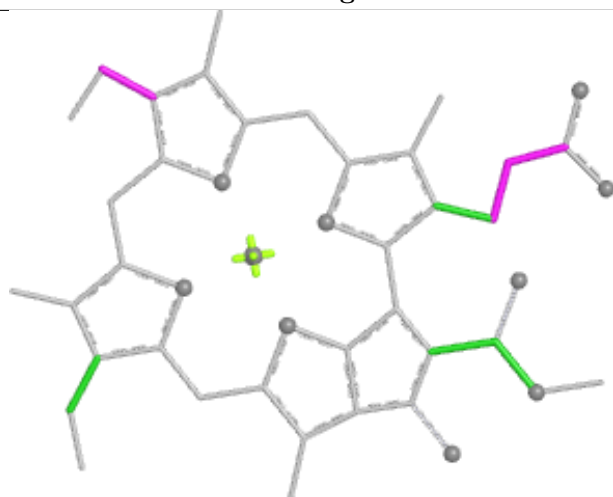
Ligand CLA G 210



Bond lengths



Bond angles

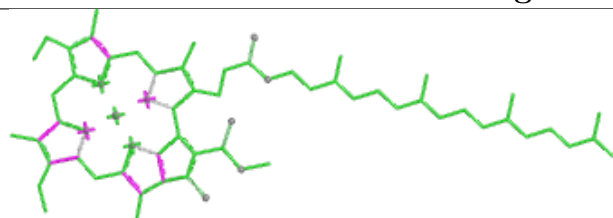


Torsions

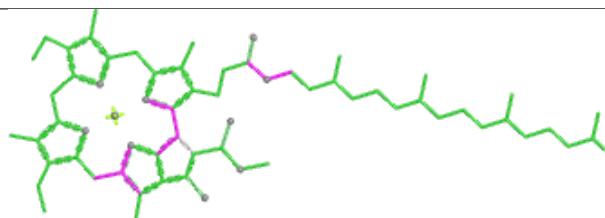


Rings

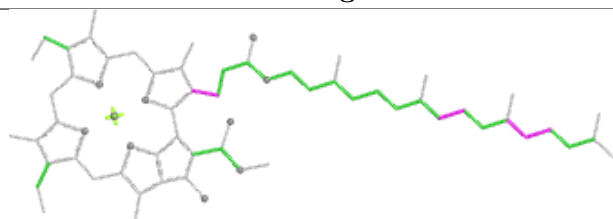
Ligand CLA B 846



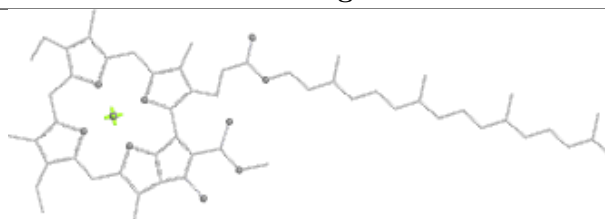
Bond lengths



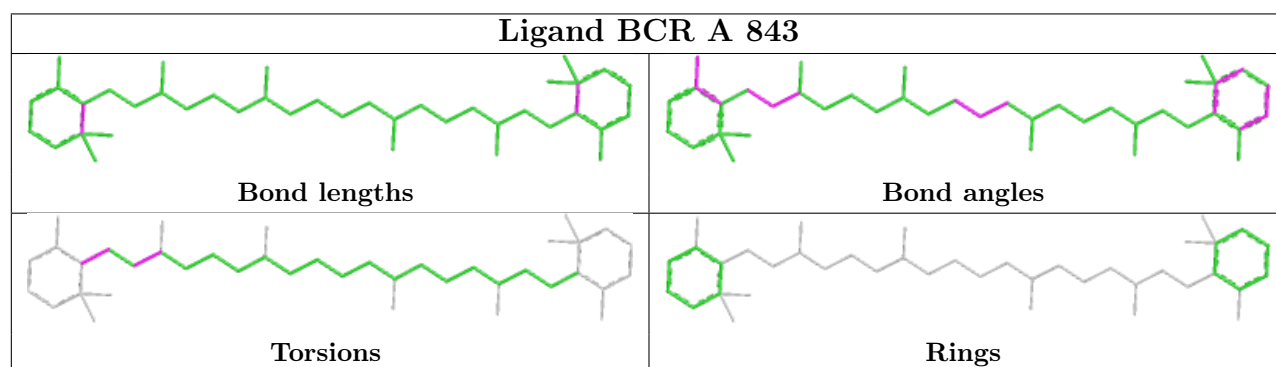
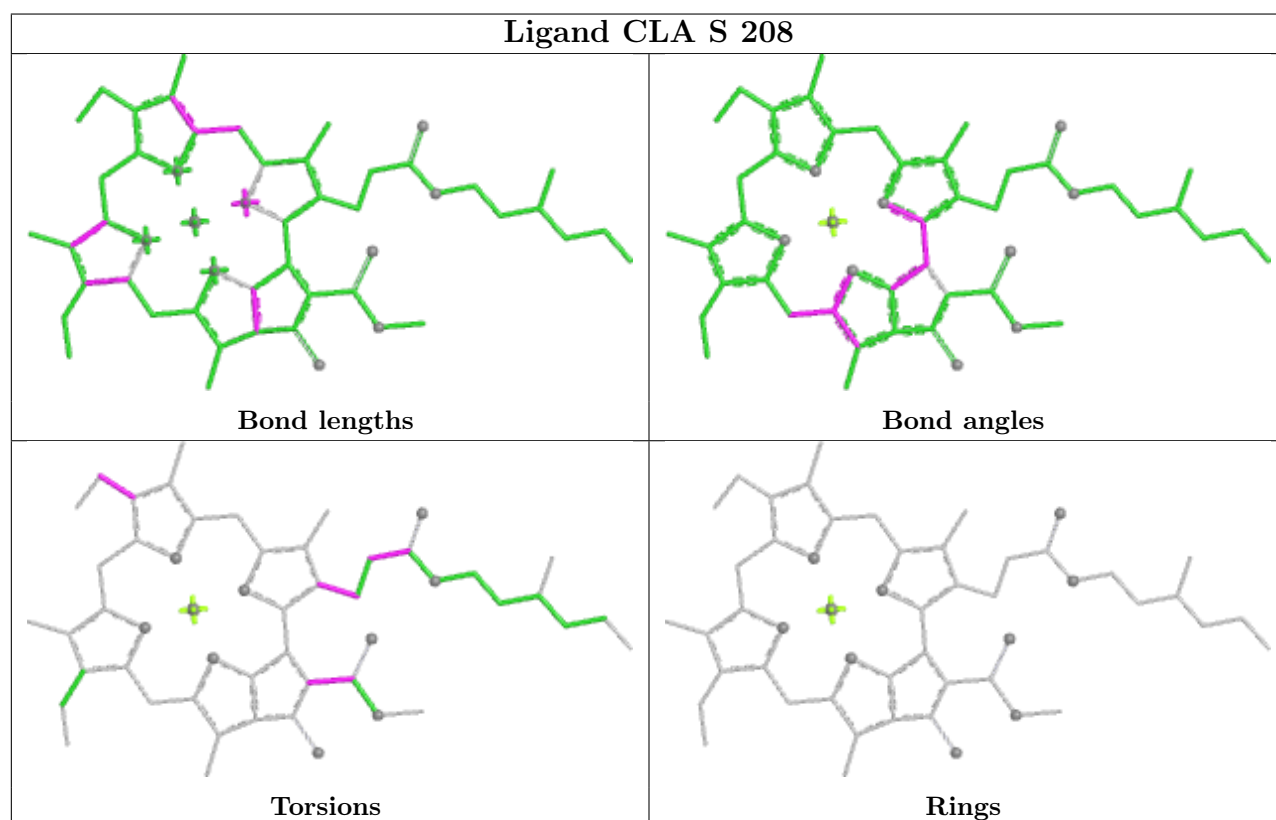
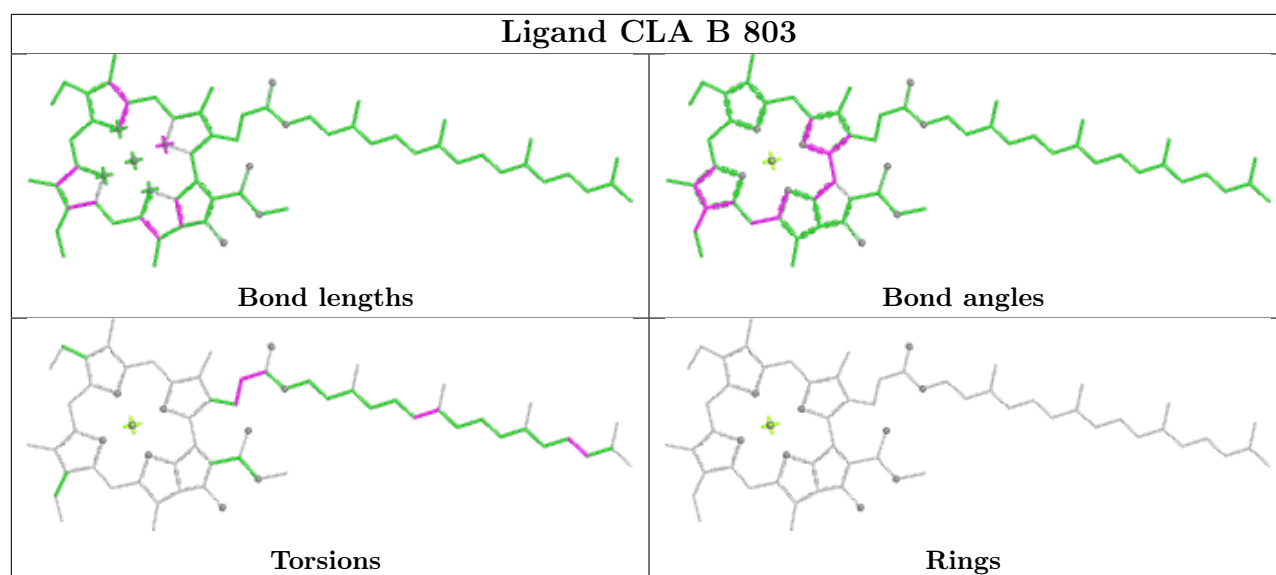
Bond angles

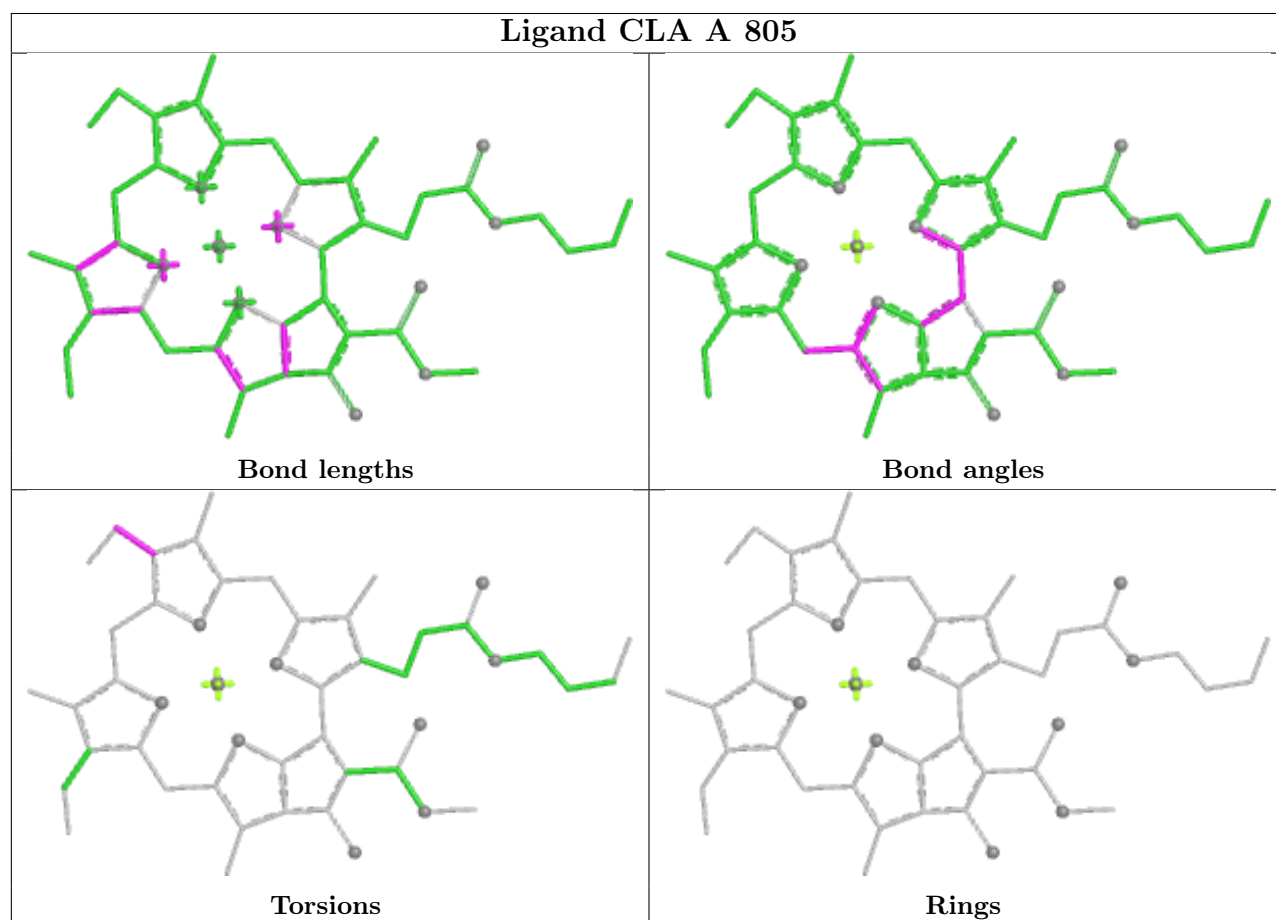
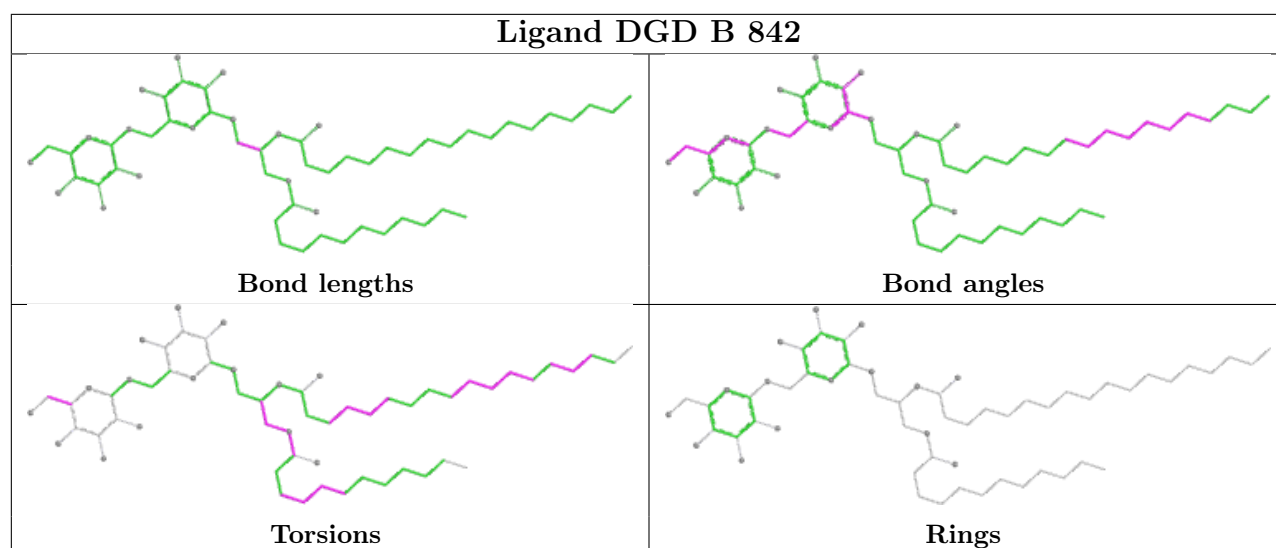


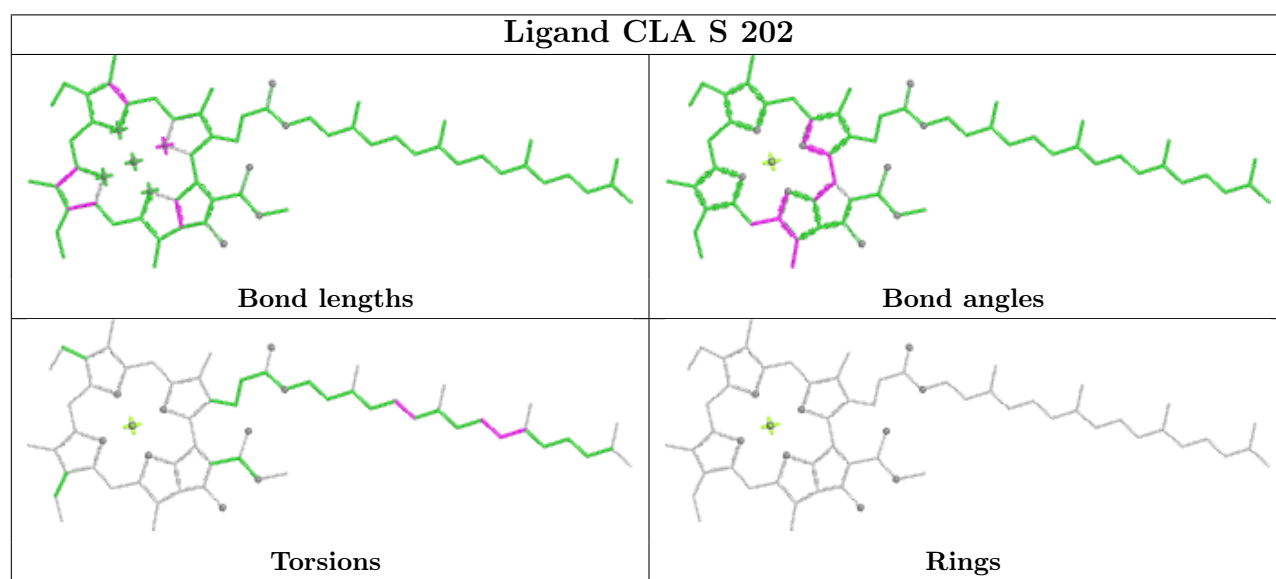
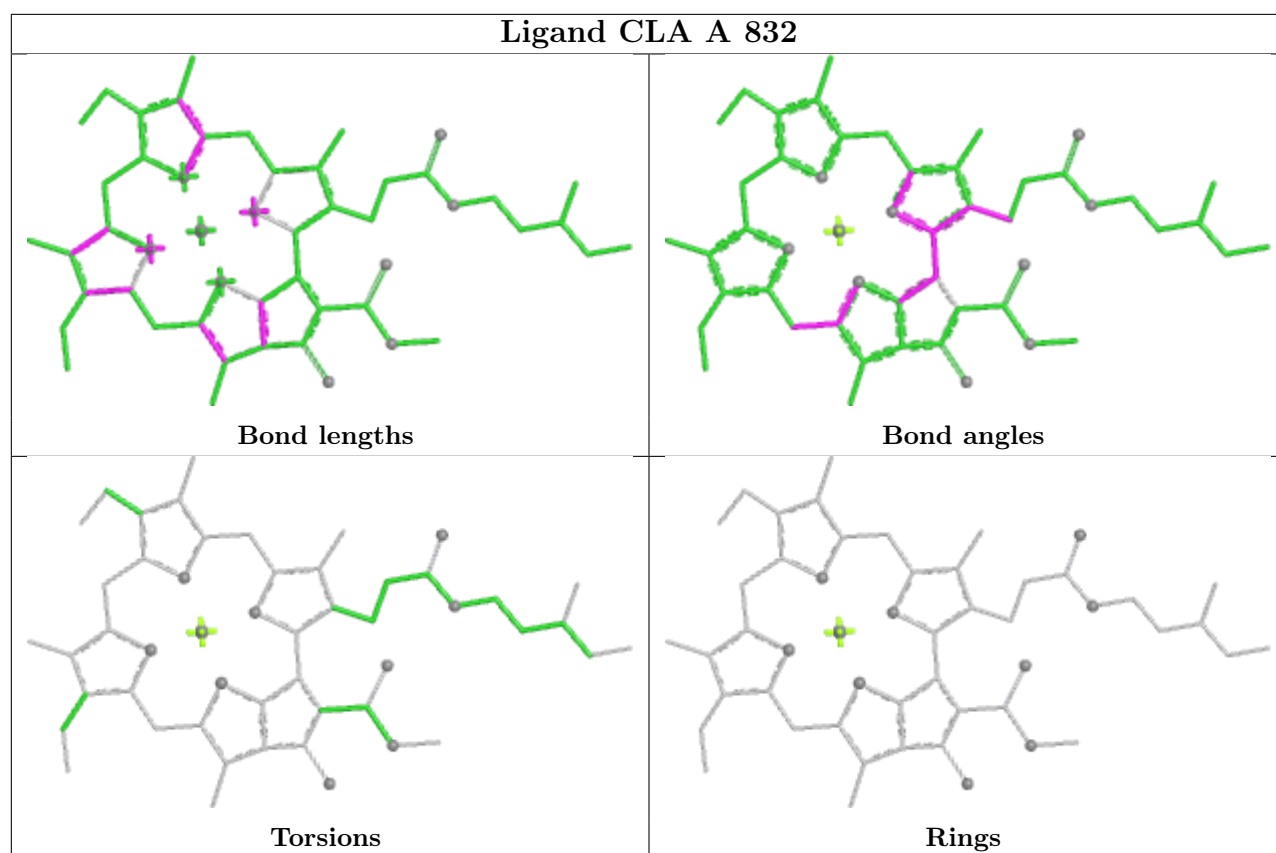
Torsions

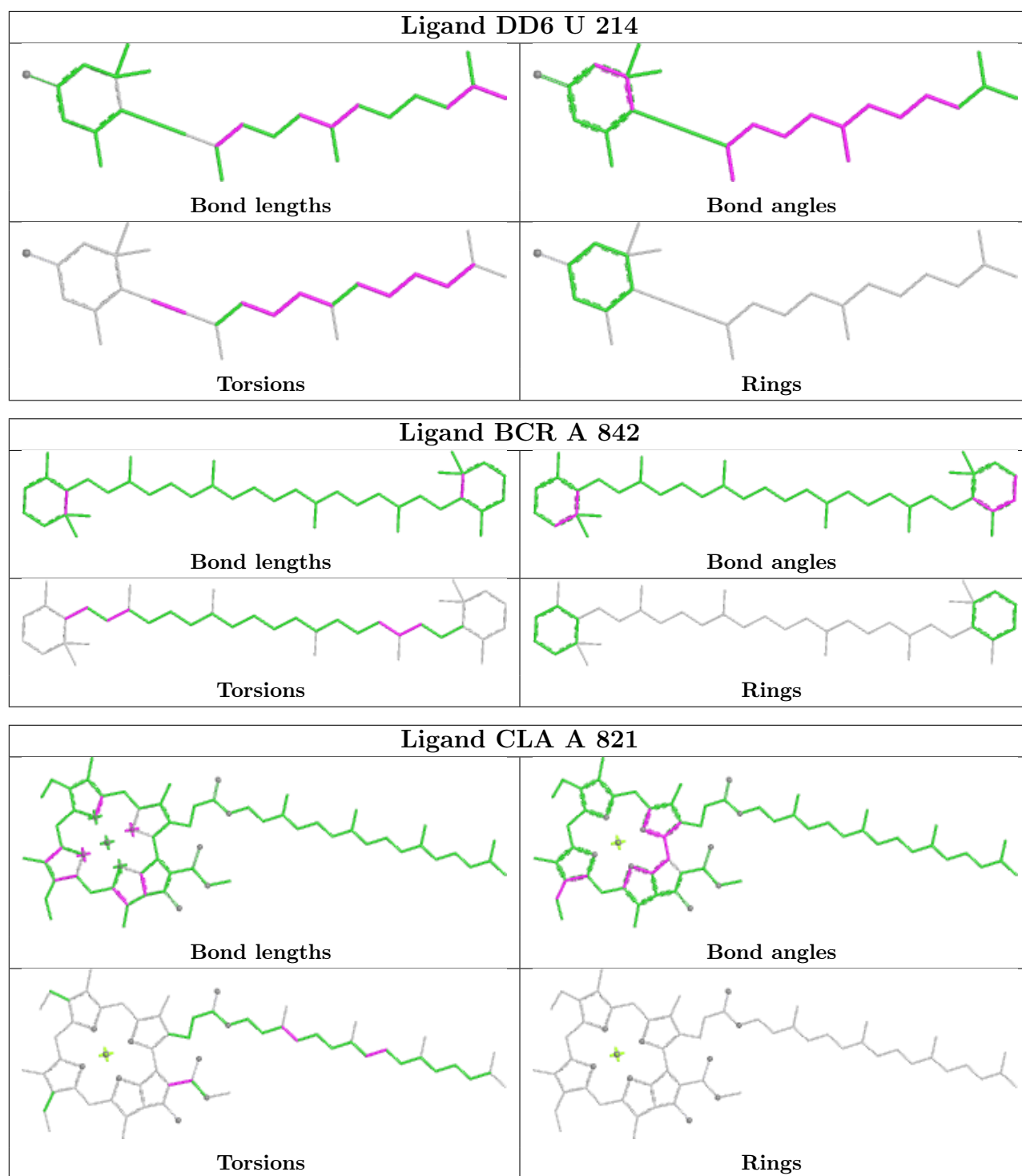


Rings

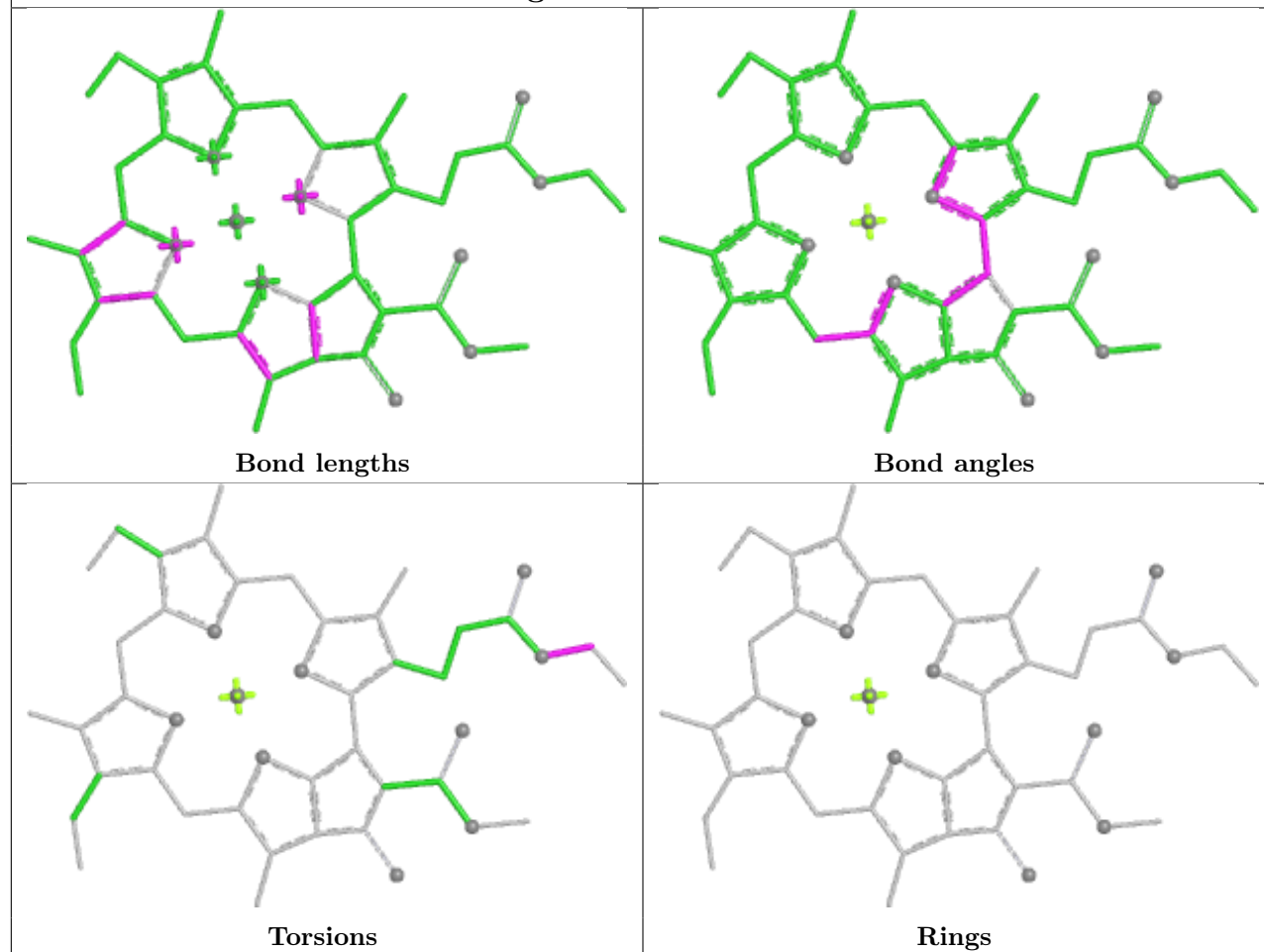




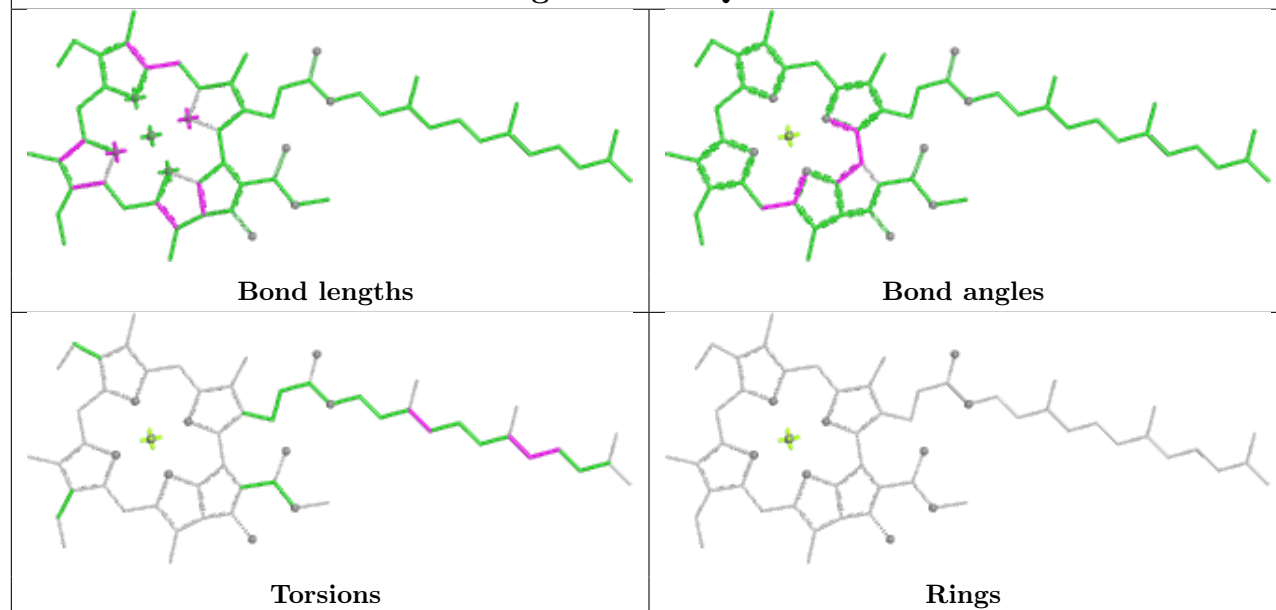


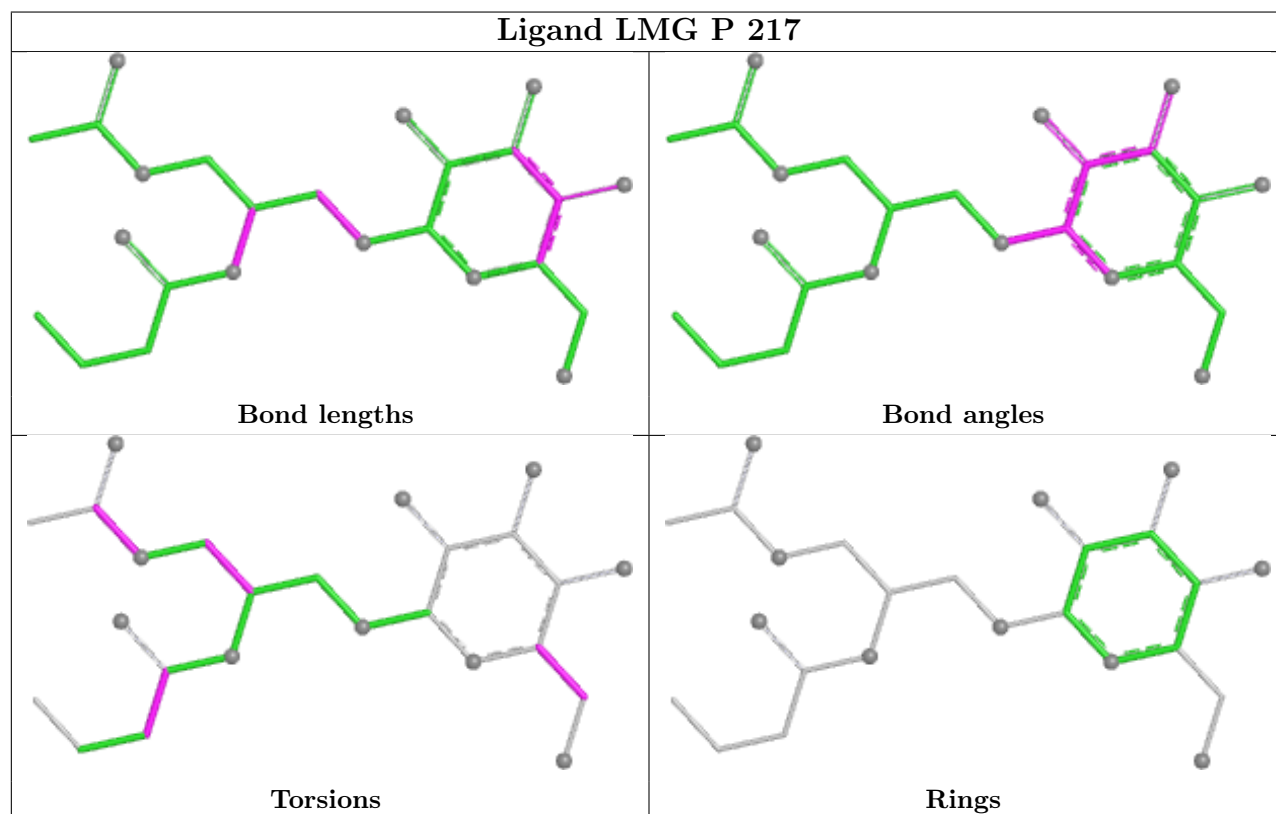
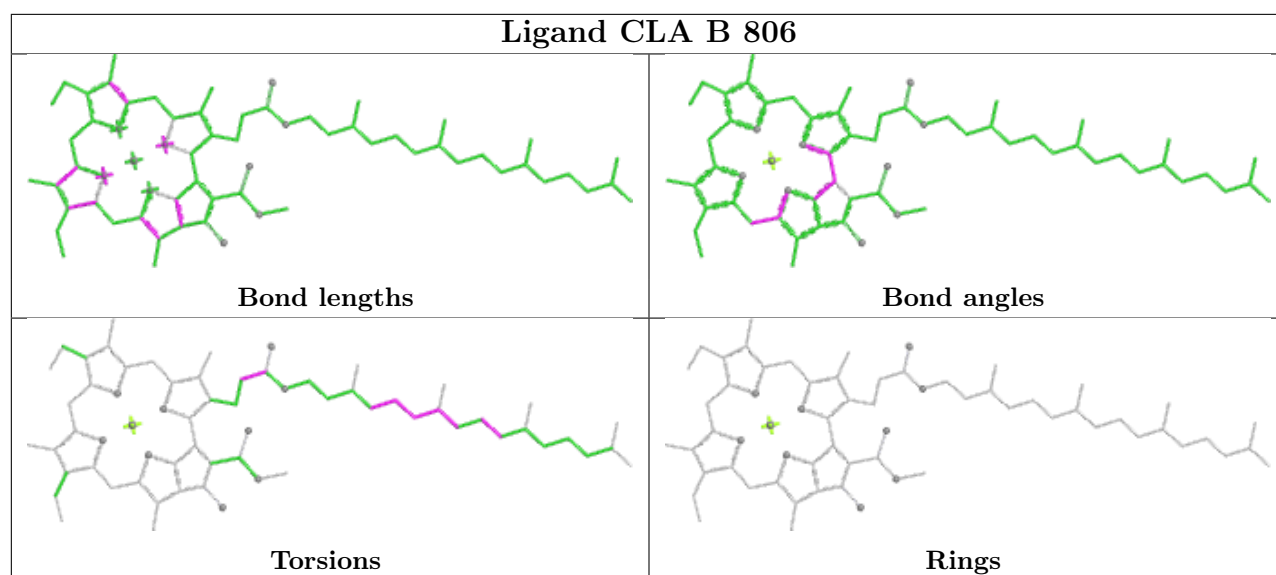


Ligand CLA B 832

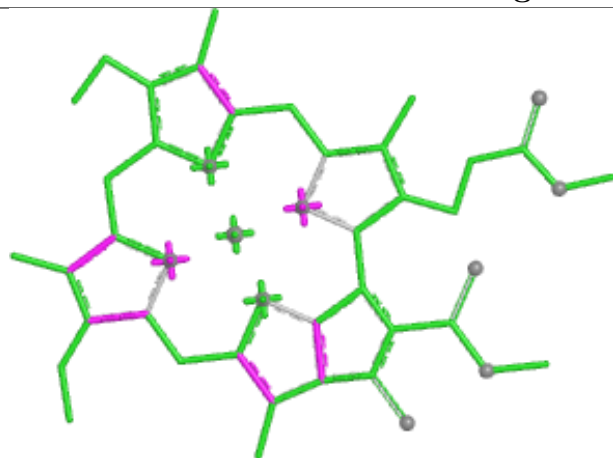


Ligand CLA Q 205

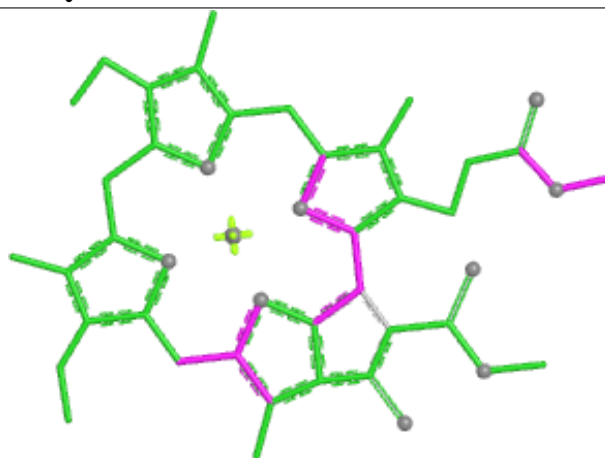




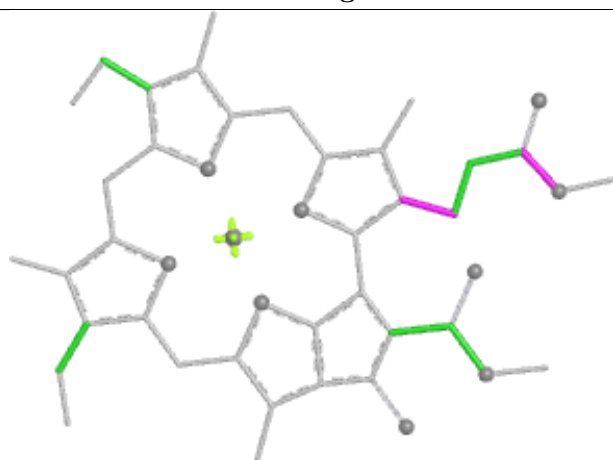
Ligand CLA Q 207



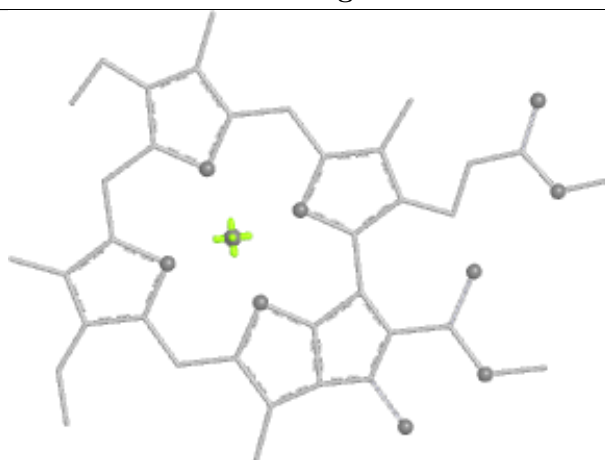
Bond lengths



Bond angles

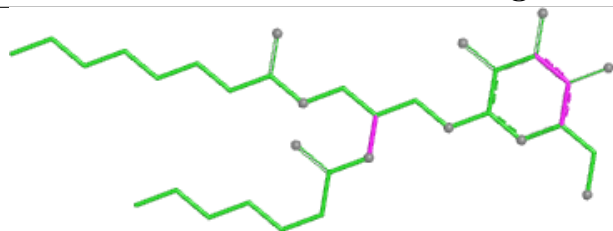


Torsions

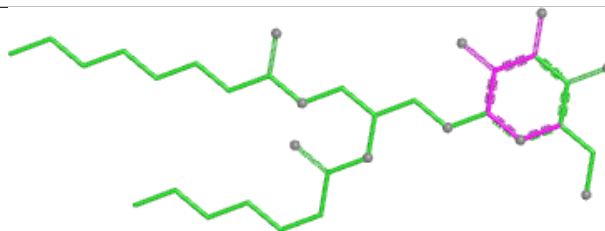


Rings

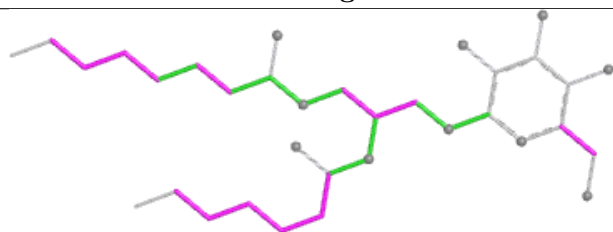
Ligand LMG P 202



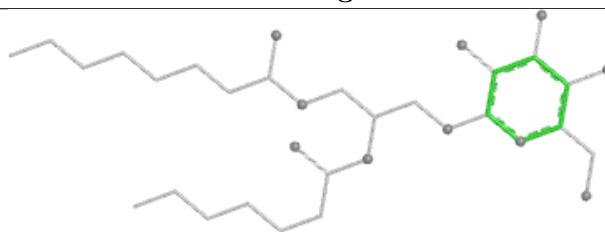
Bond lengths



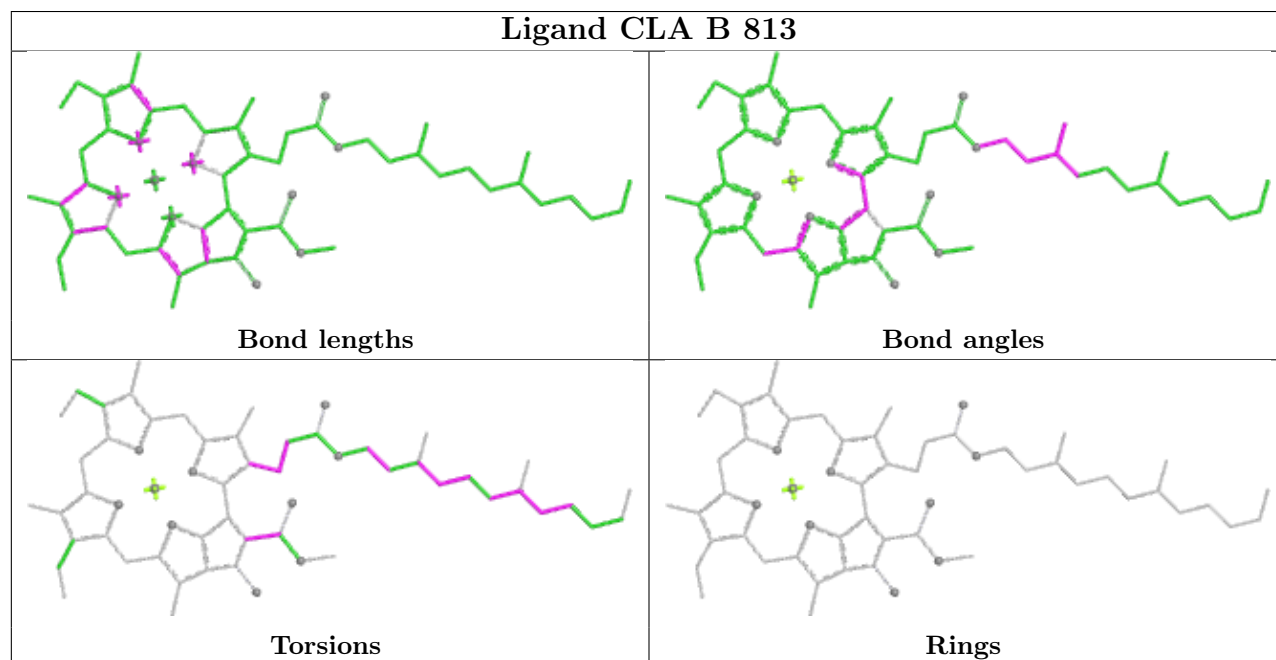
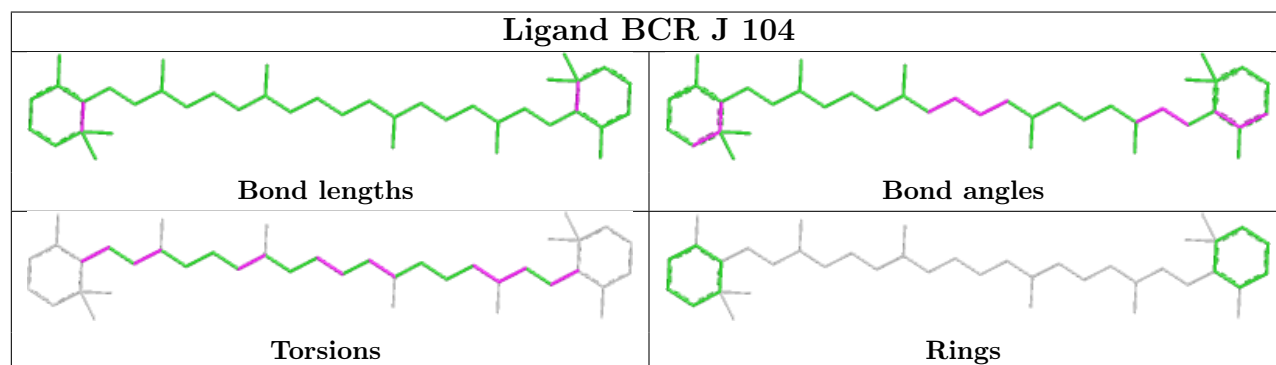
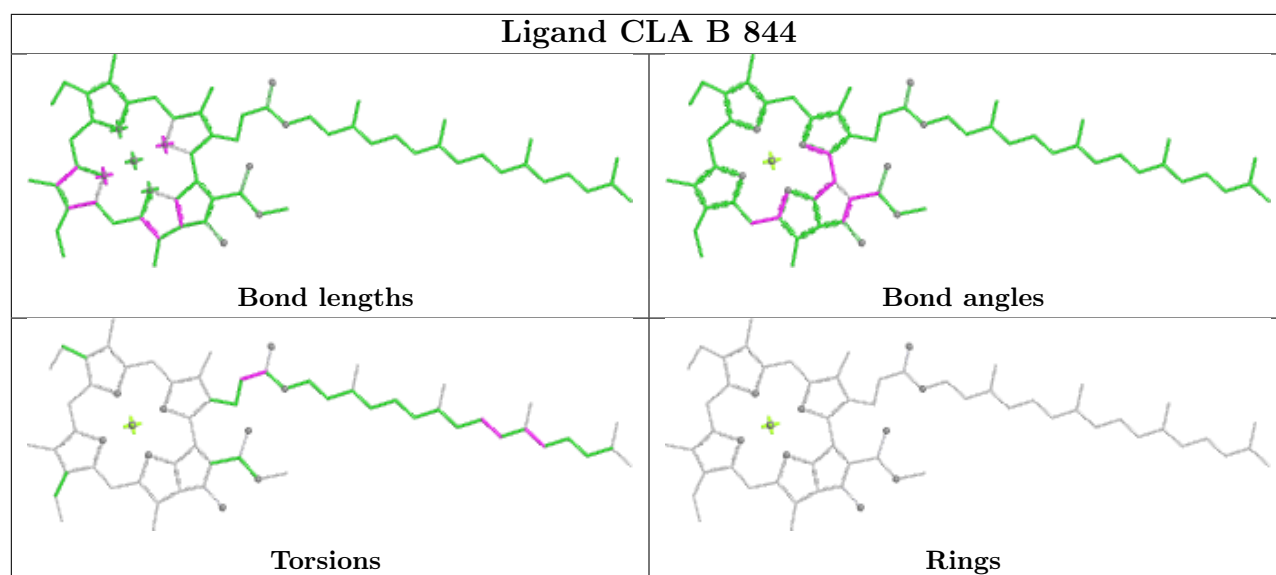
Bond angles

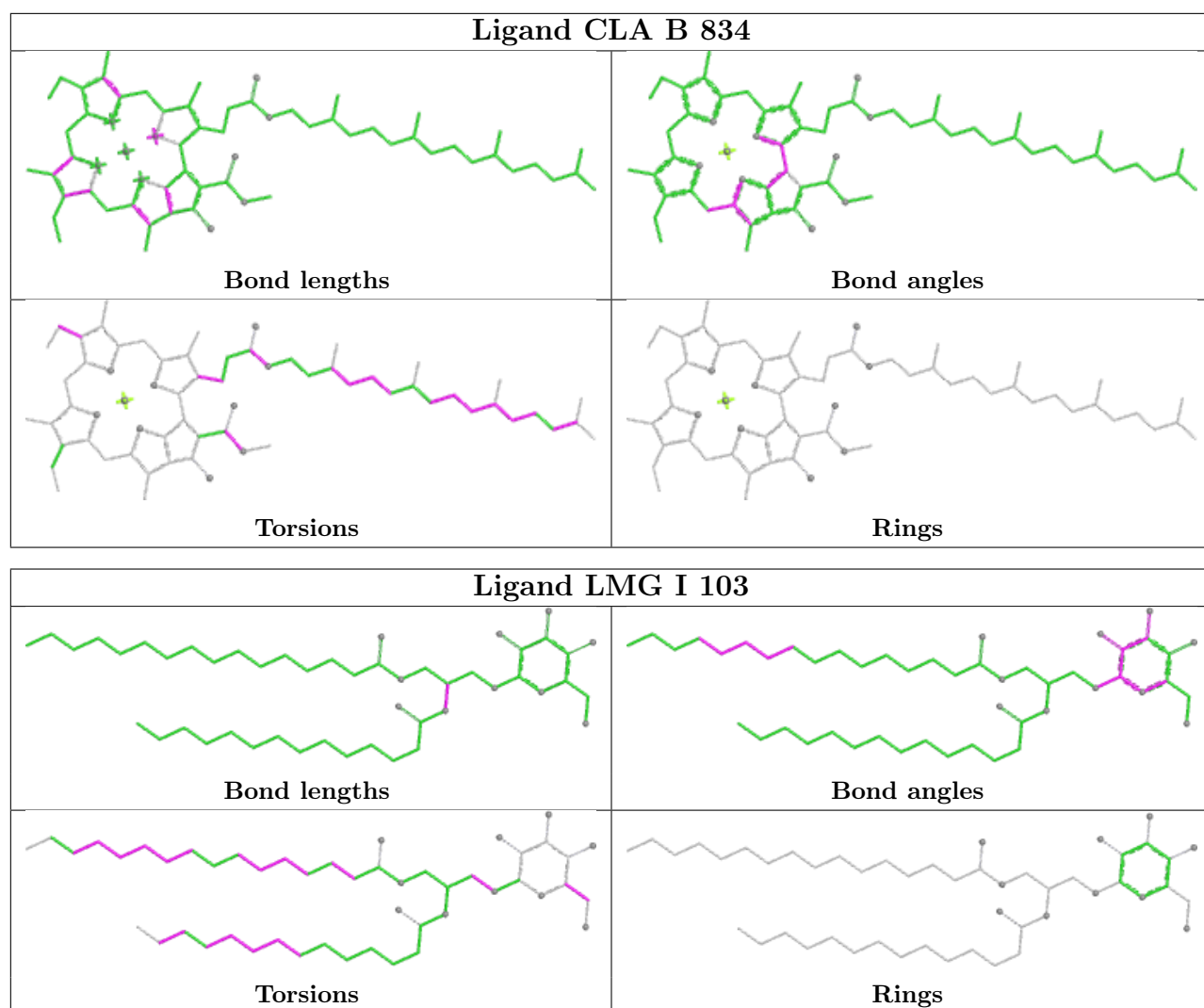


Torsions

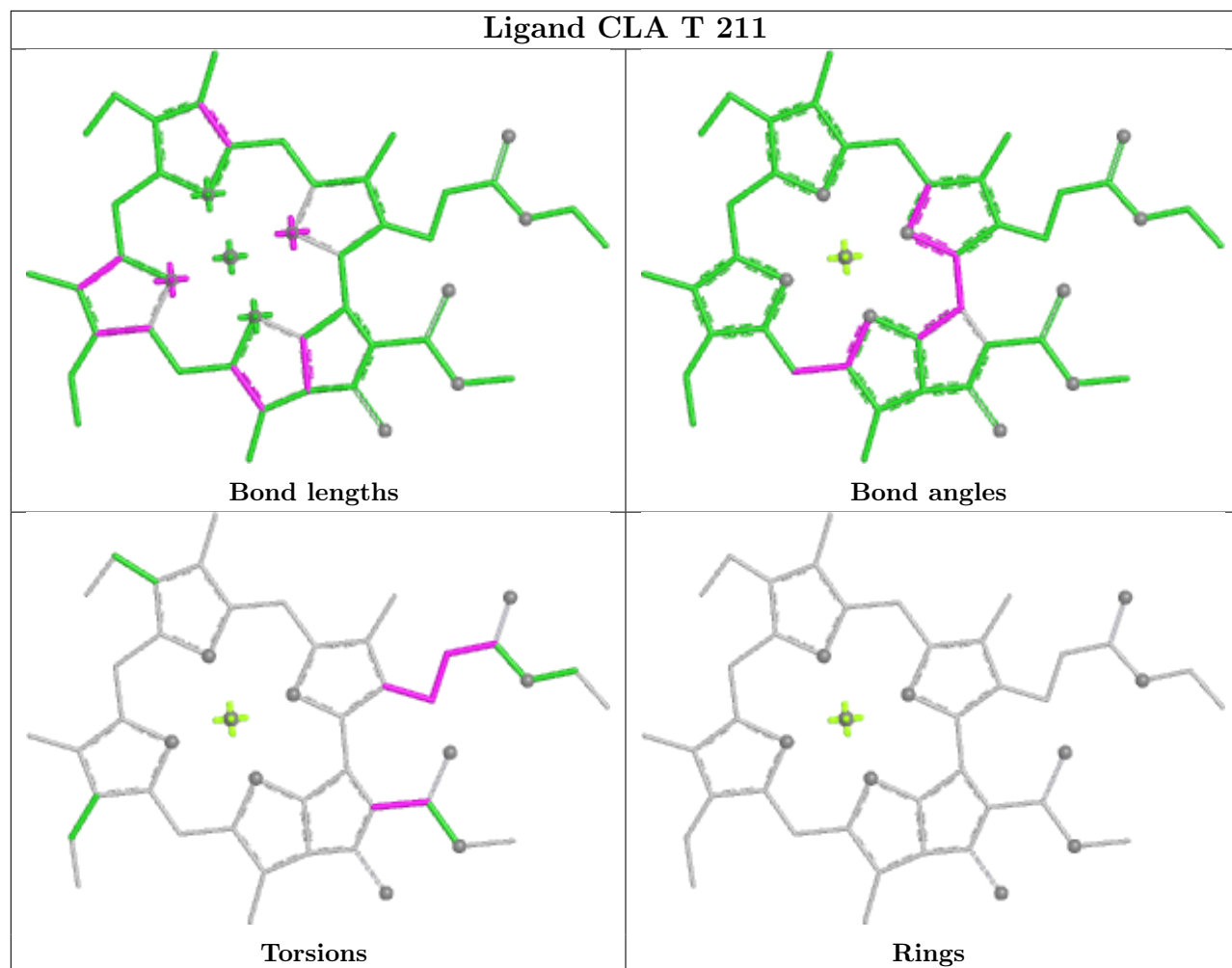


Rings

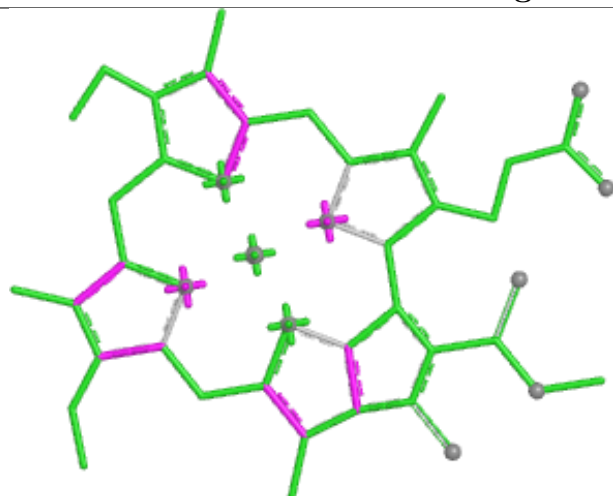




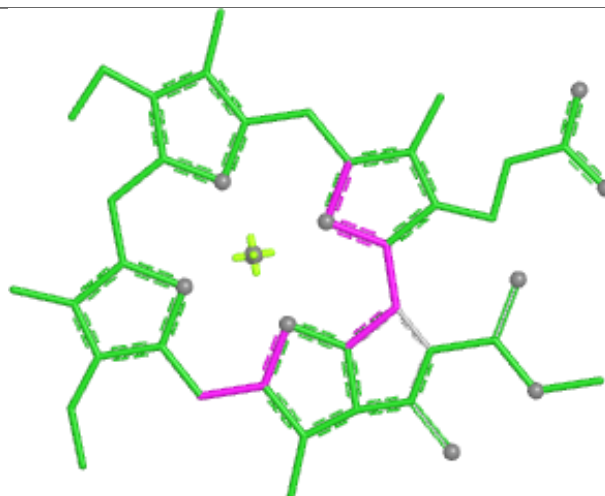
Ligand CLA T 211



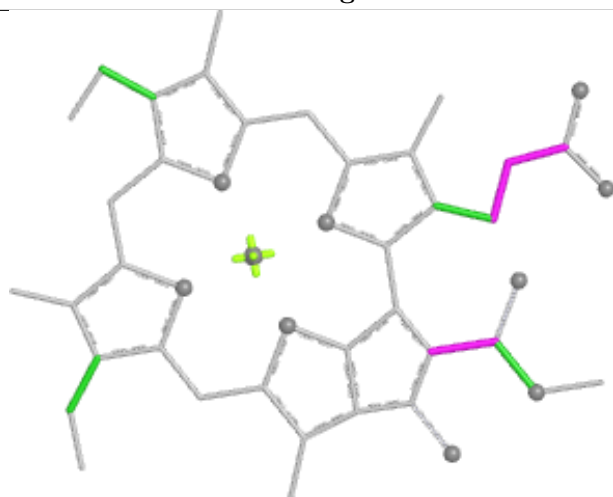
Ligand CLA B 804



Bond lengths



Bond angles

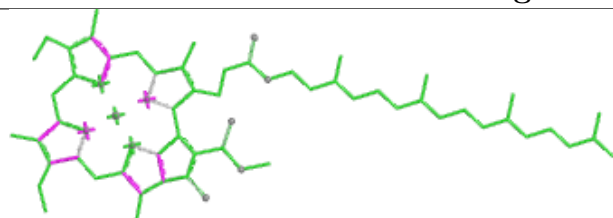


Torsions

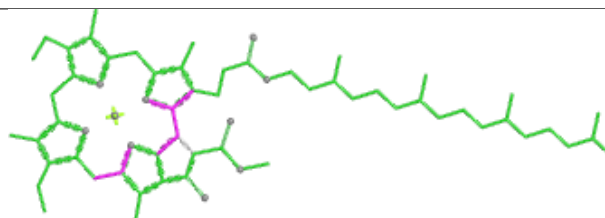


Rings

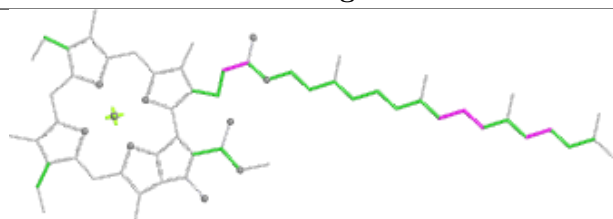
Ligand CLA A 801



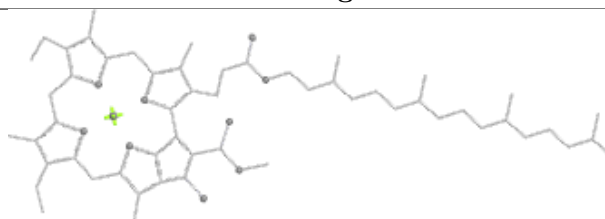
Bond lengths



Bond angles

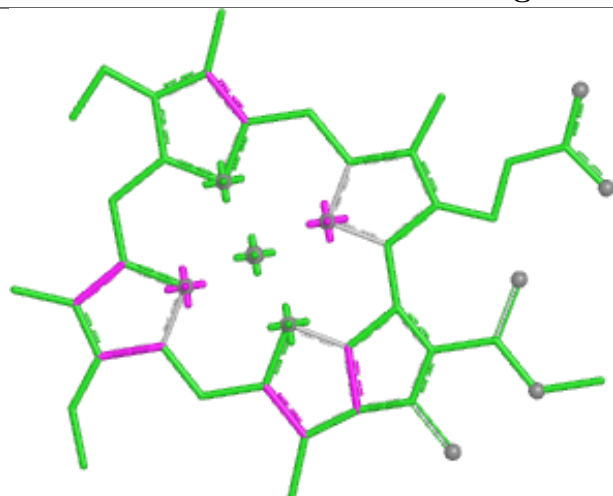


Torsions

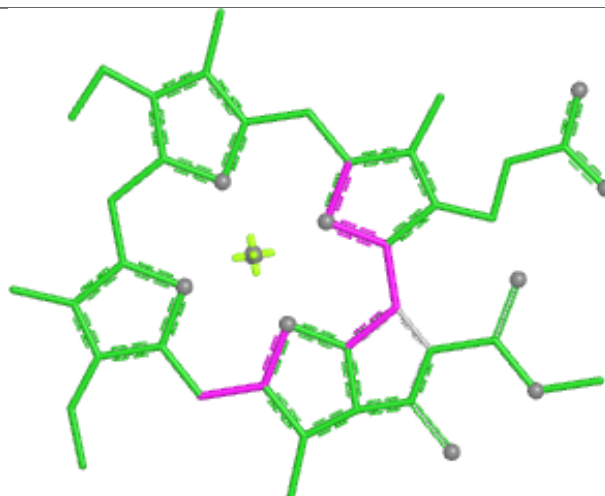


Rings

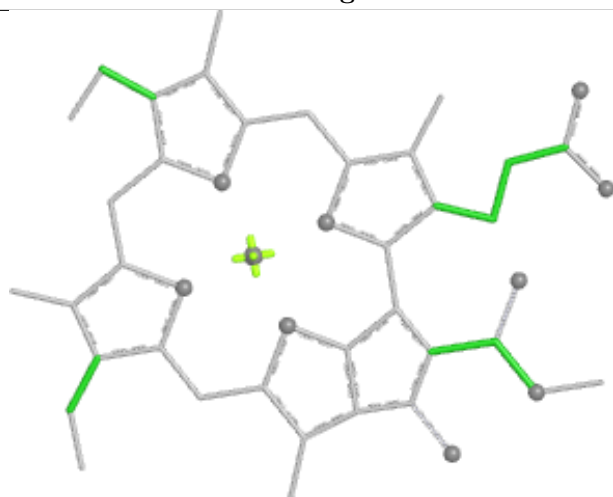
Ligand CLA O 203



Bond lengths



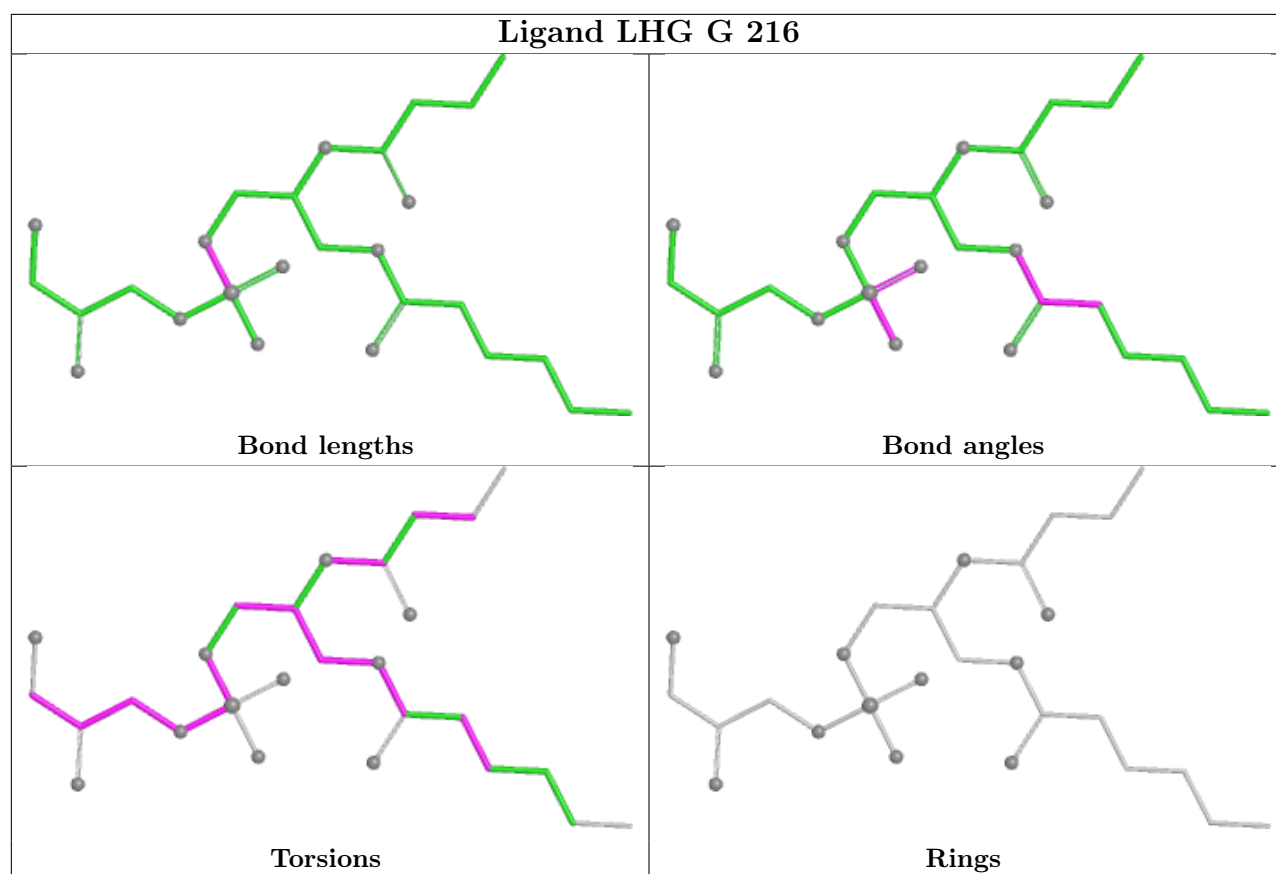
Bond angles

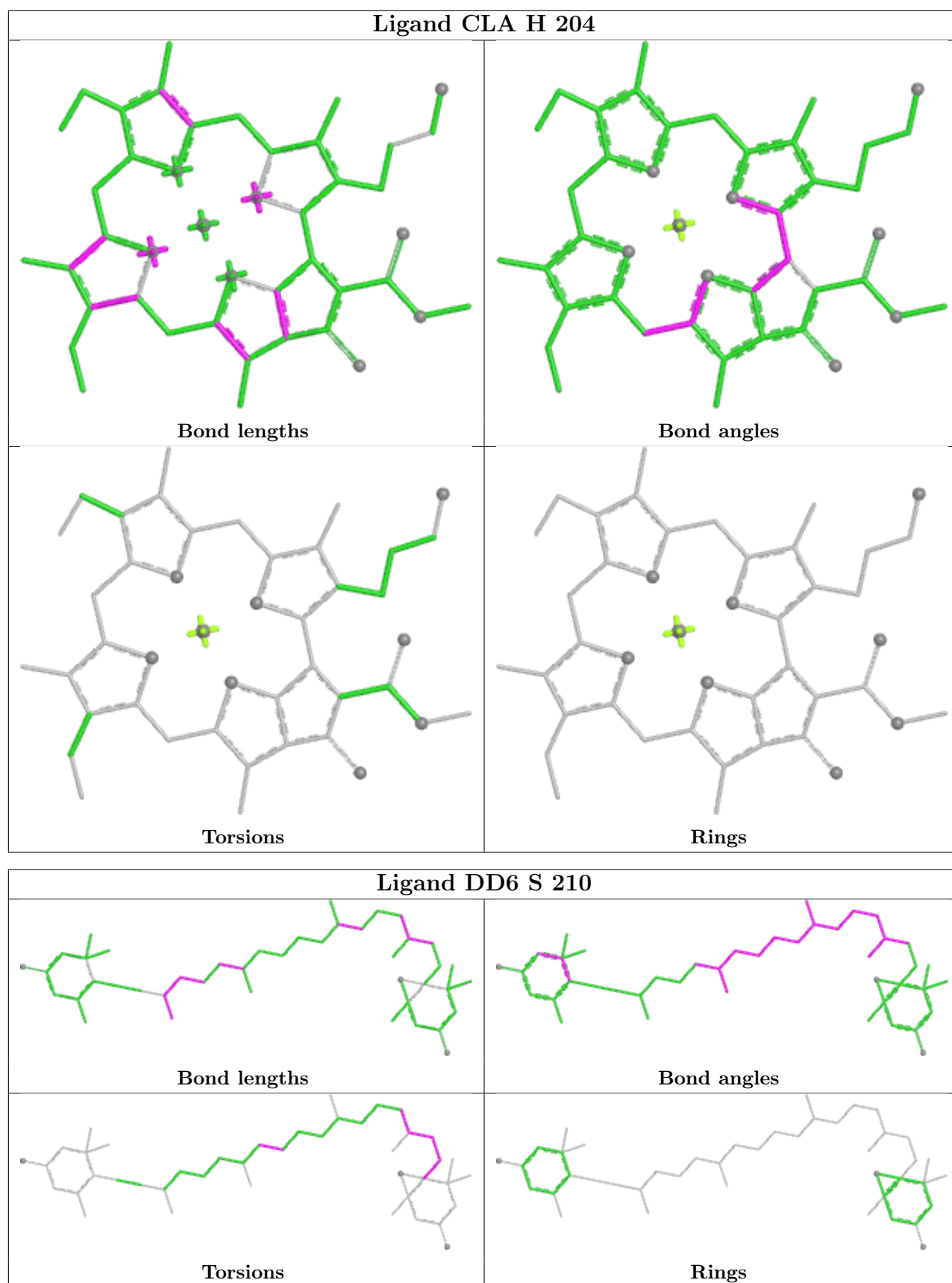


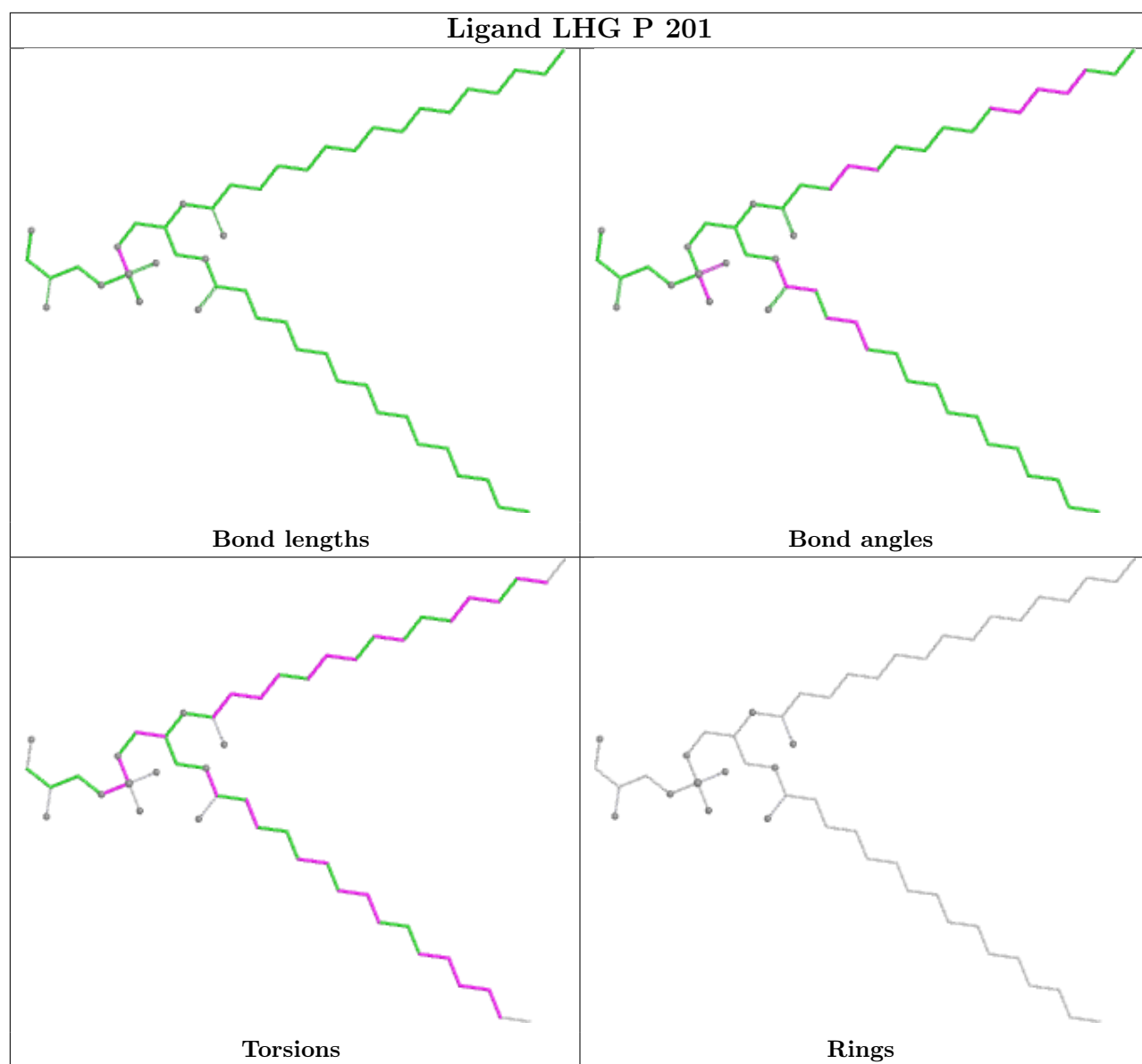
Torsions



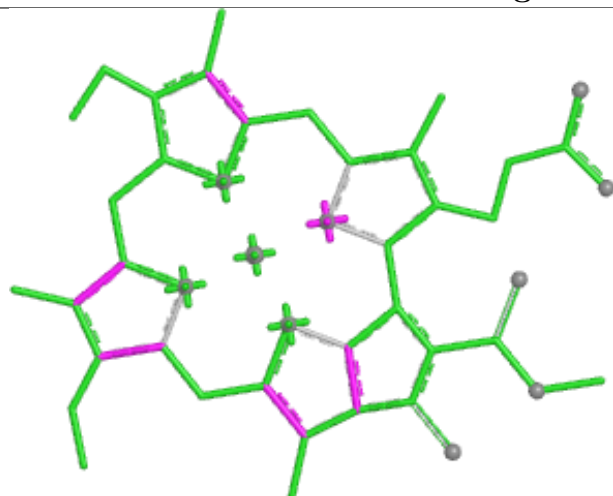
Rings



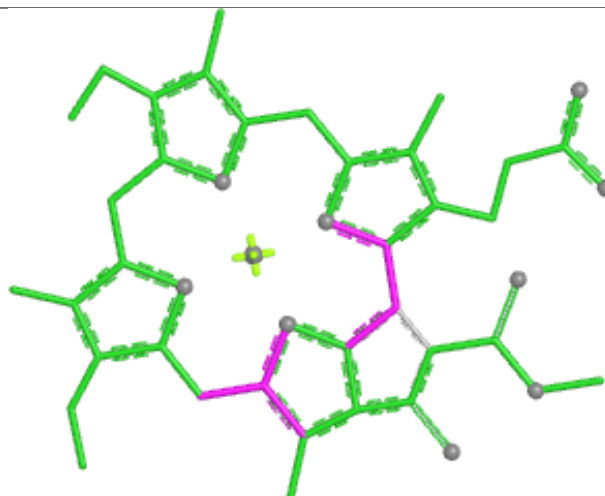




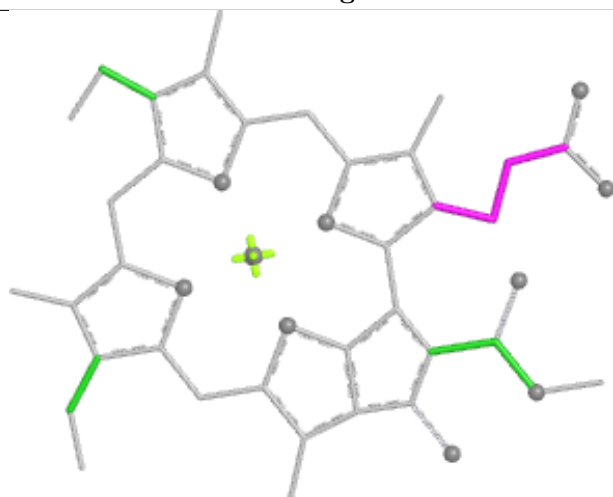
Ligand CLA A 831



Bond lengths



Bond angles

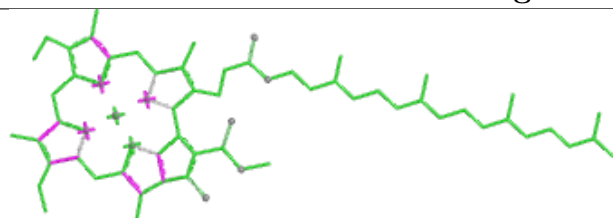


Torsions

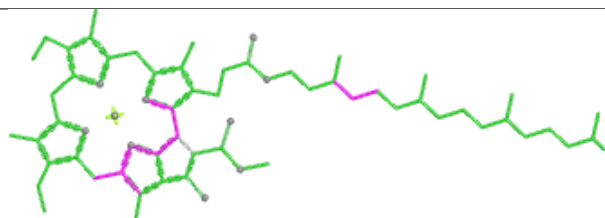


Rings

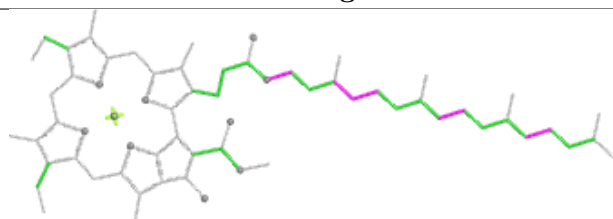
Ligand CLA A 847



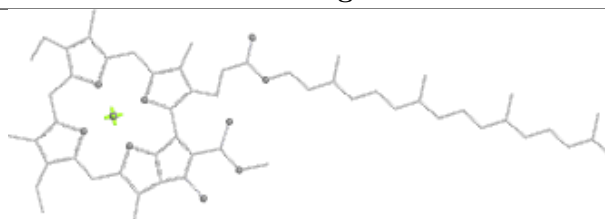
Bond lengths



Bond angles



Torsions



Rings

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.

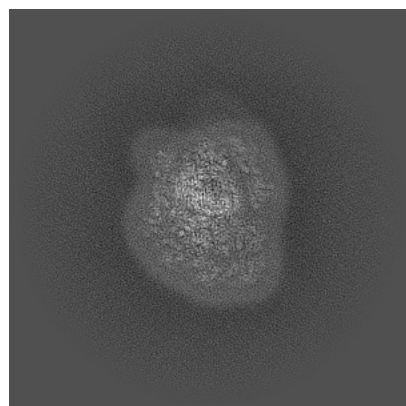
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64383. These allow visual inspection of the internal detail of the map and identification of artifacts.

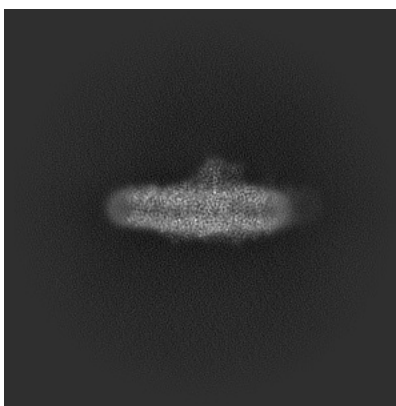
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

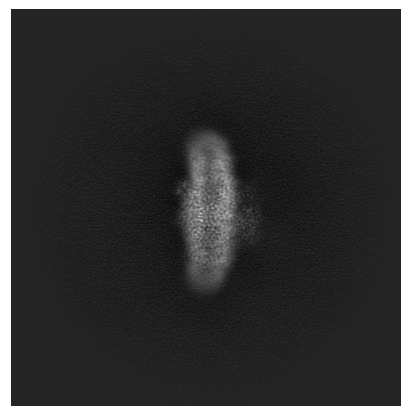
6.1.1 Primary map



X

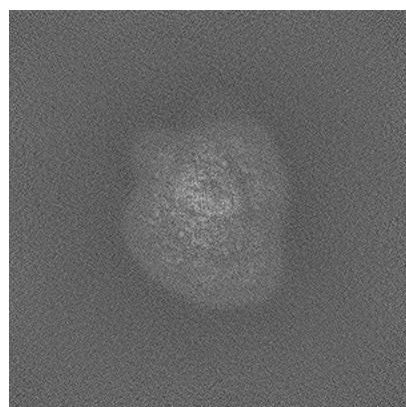


Y

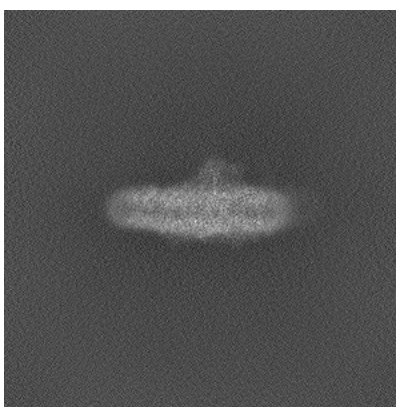


Z

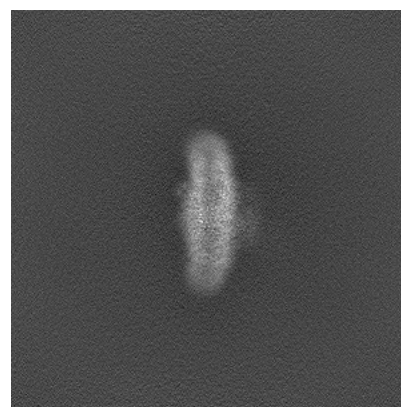
6.1.2 Raw map



X



Y

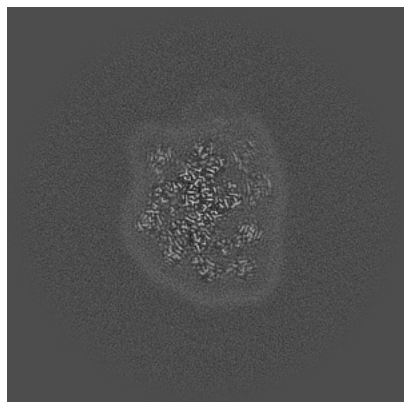


Z

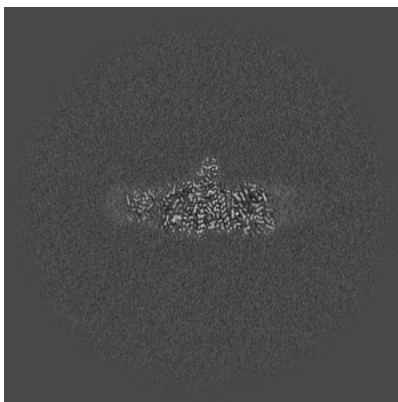
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

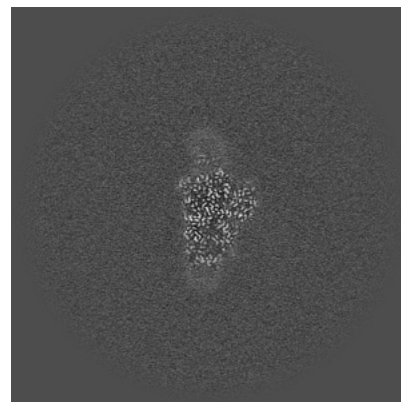
6.2.1 Primary map



X Index: 300

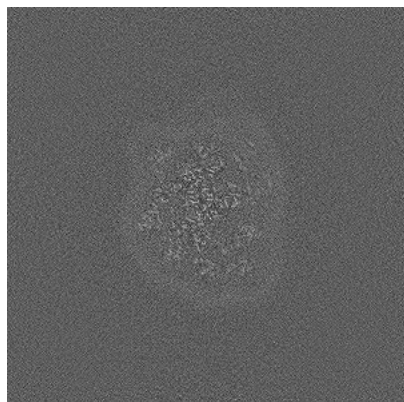


Y Index: 300

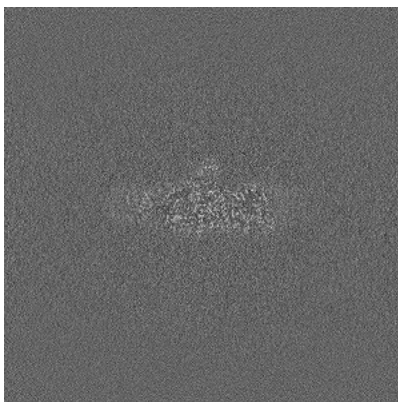


Z Index: 300

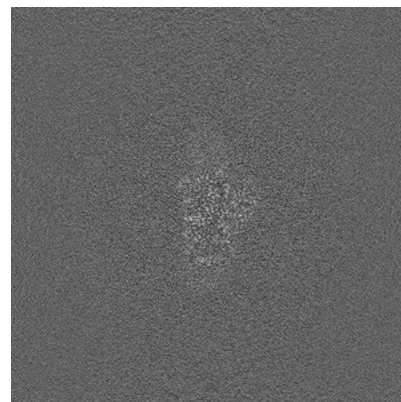
6.2.2 Raw map



X Index: 300



Y Index: 300

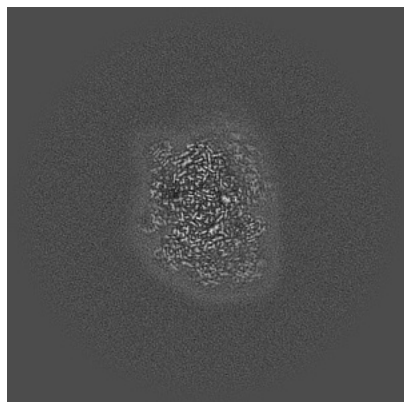


Z Index: 300

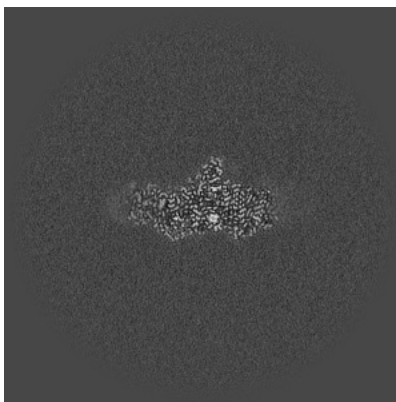
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

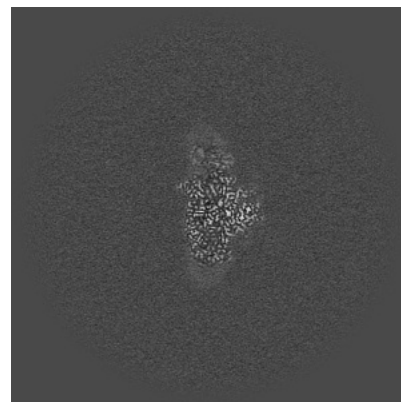
6.3.1 Primary map



X Index: 315

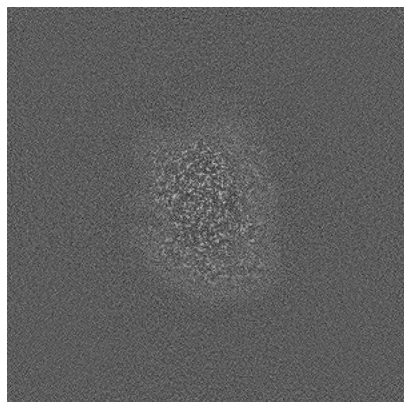


Y Index: 288

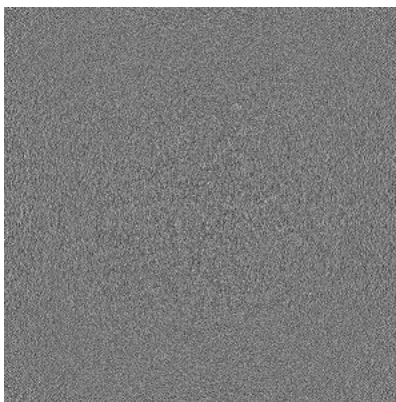


Z Index: 315

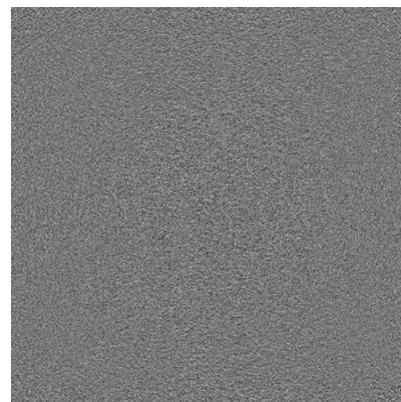
6.3.2 Raw map



X Index: 318



Y Index: 0

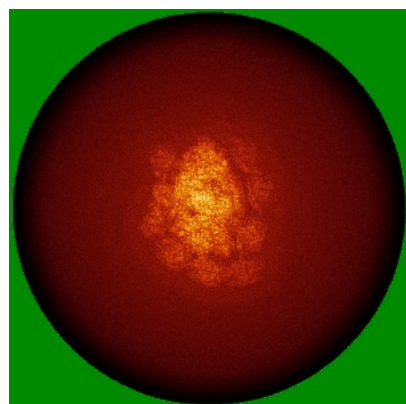


Z Index: 0

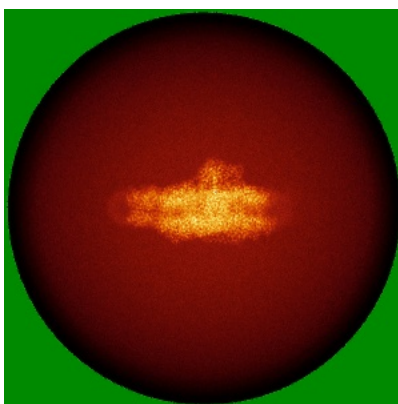
The images above show the largest variance slices of the map in three orthogonal directions.

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

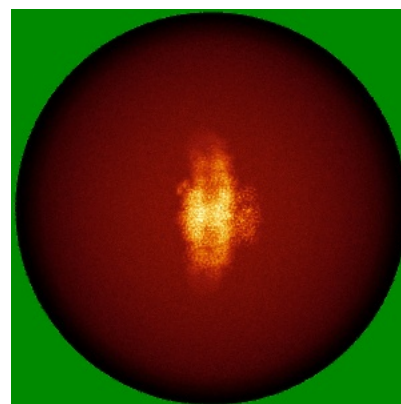
6.4.1 Primary map



X

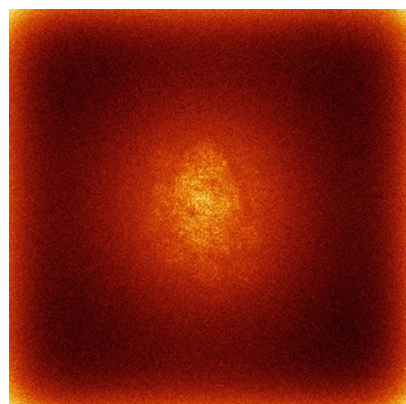


Y

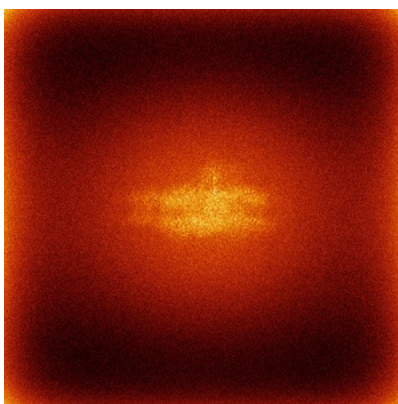


Z

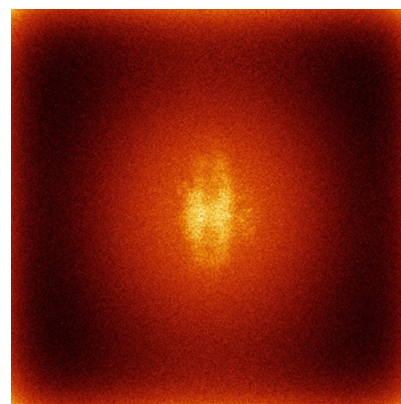
6.4.2 Raw map



X



Y

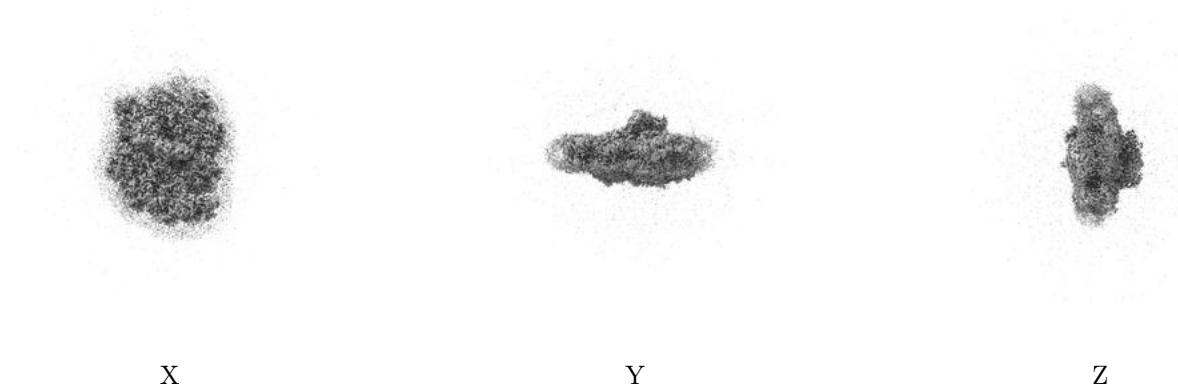


Z

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.

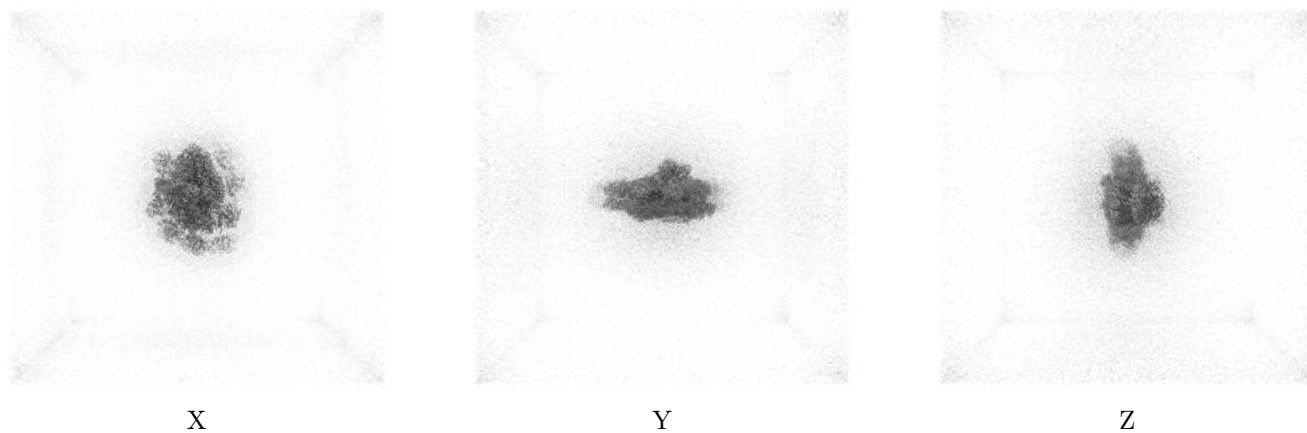
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

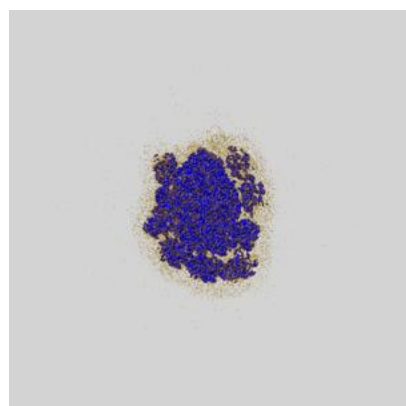
6.6 Mask visualisation [i](#)

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

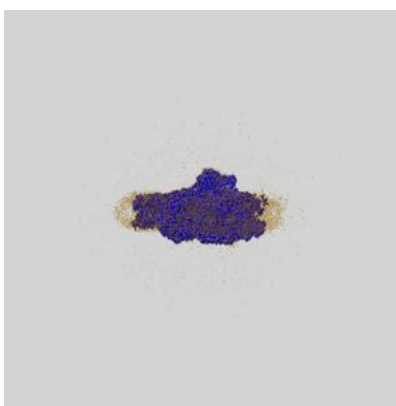
A mask typically either:

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

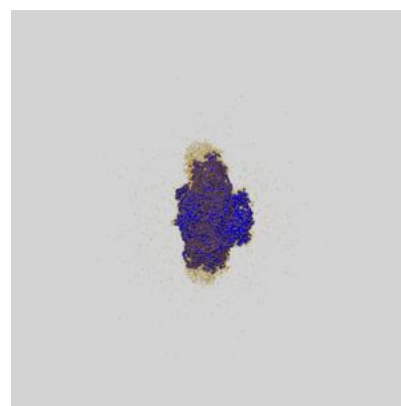
6.6.1 emd_64383_msk_1.map [i](#)



X



Y

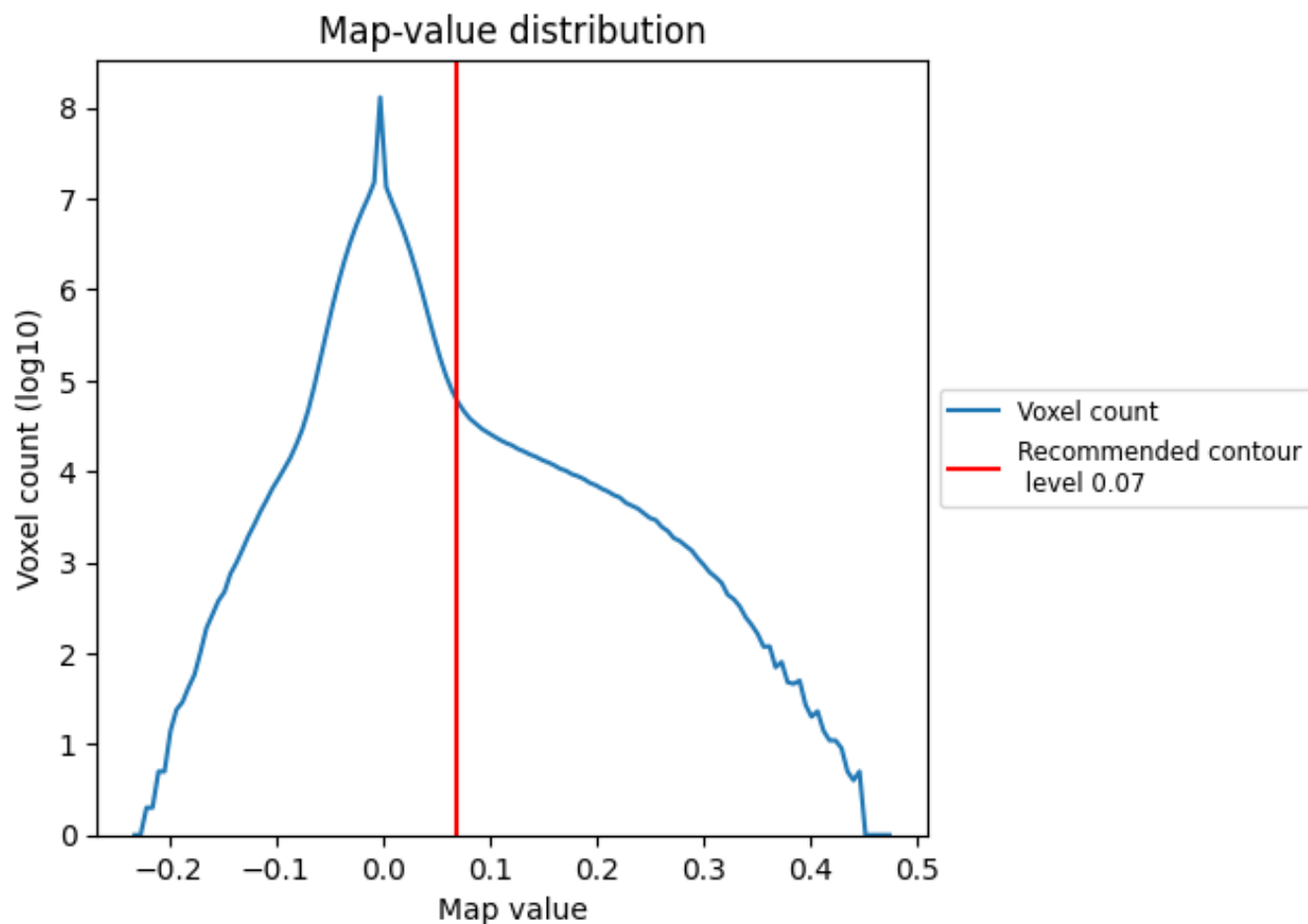


Z

7 Map analysis [i](#)

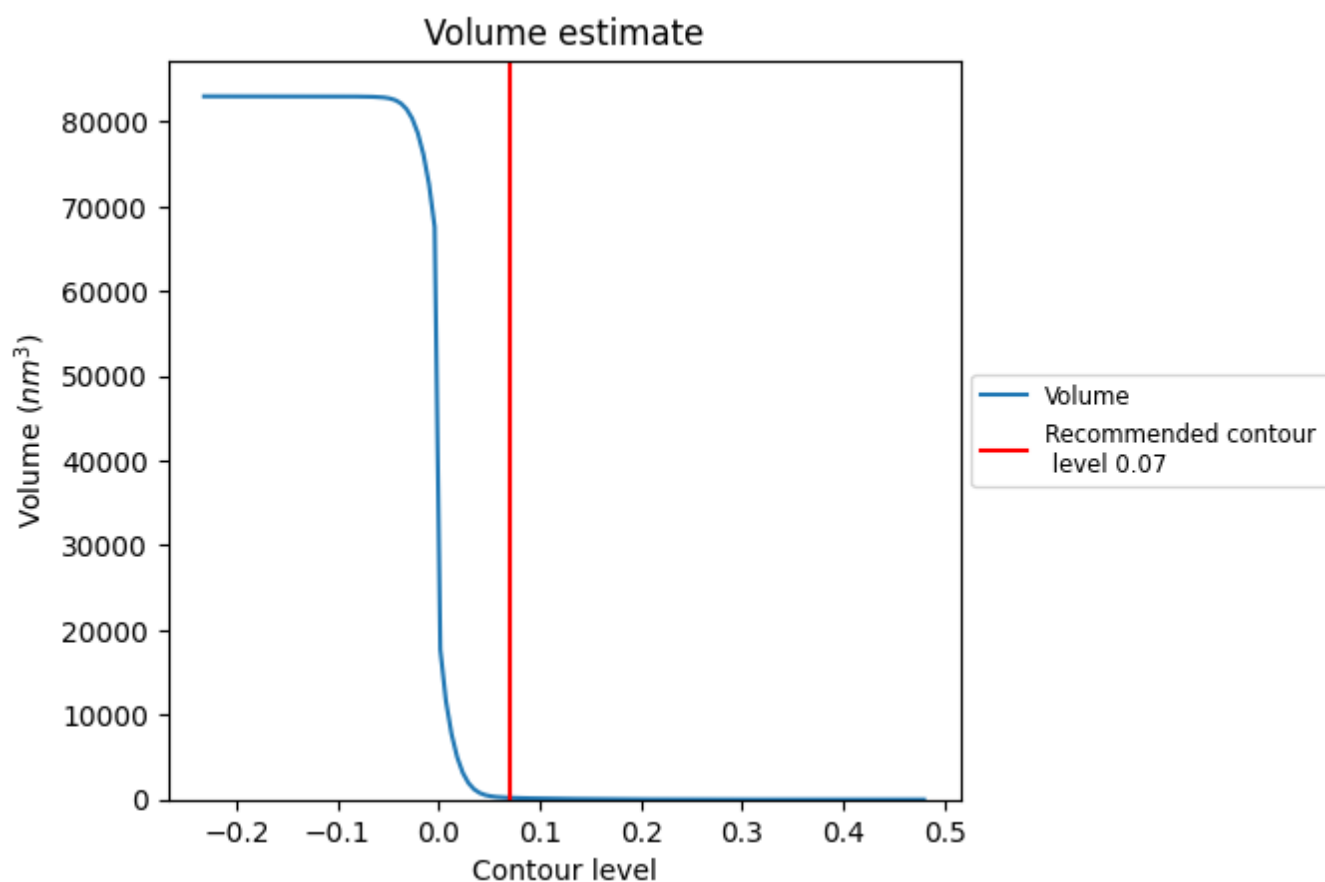
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

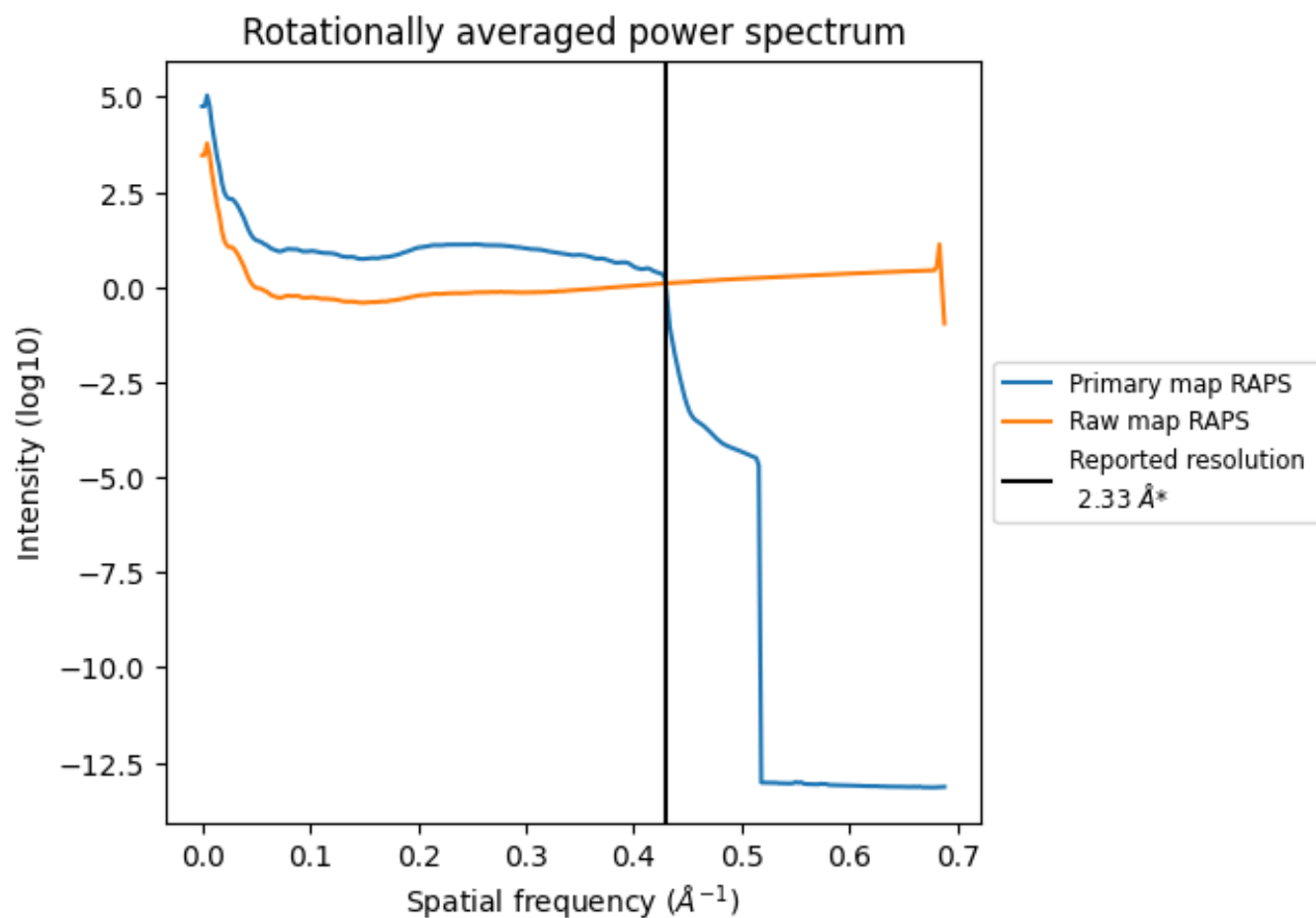
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 212 nm³; this corresponds to an approximate mass of 192 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

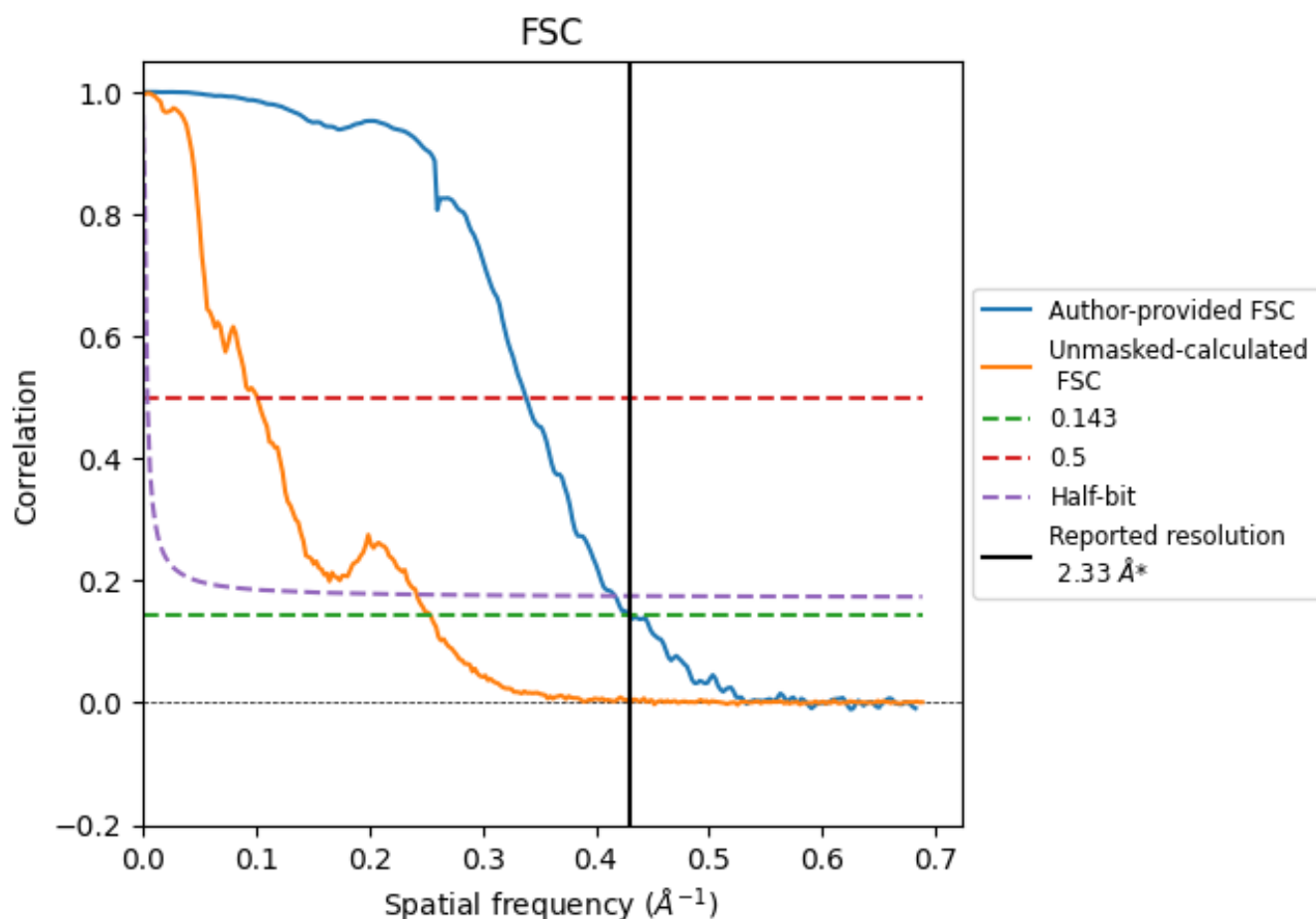


*Reported resolution corresponds to spatial frequency of 0.429 \AA^{-1}

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 0.429 \AA^{-1}

8.2 Resolution estimates [i](#)

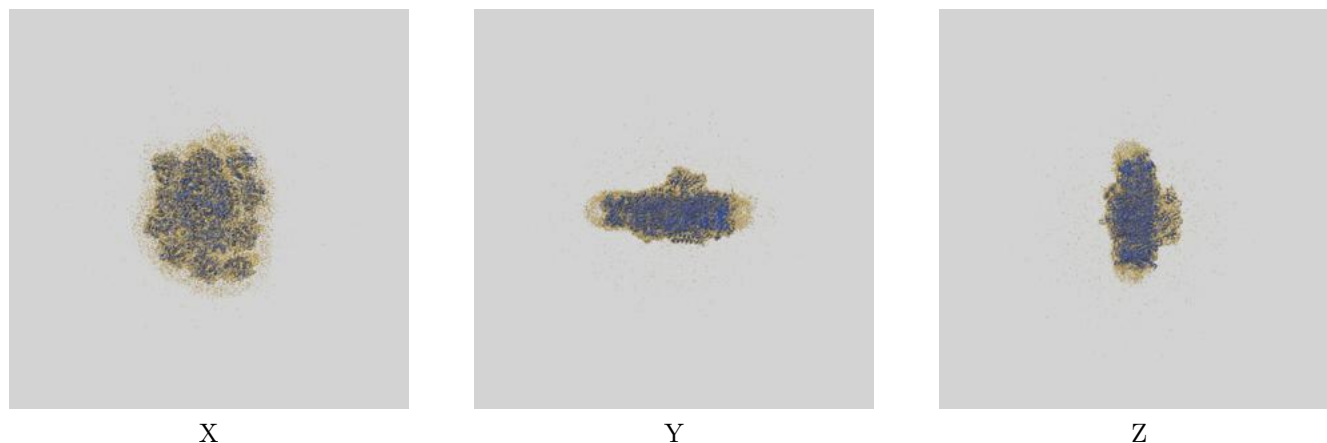
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.33	-	-
Author-provided FSC curve	2.33	2.96	2.40
Unmasked-calculated*	3.94	9.87	4.13

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.94 differs from the reported value 2.33 by more than 10 %

9 Map-model fit [i](#)

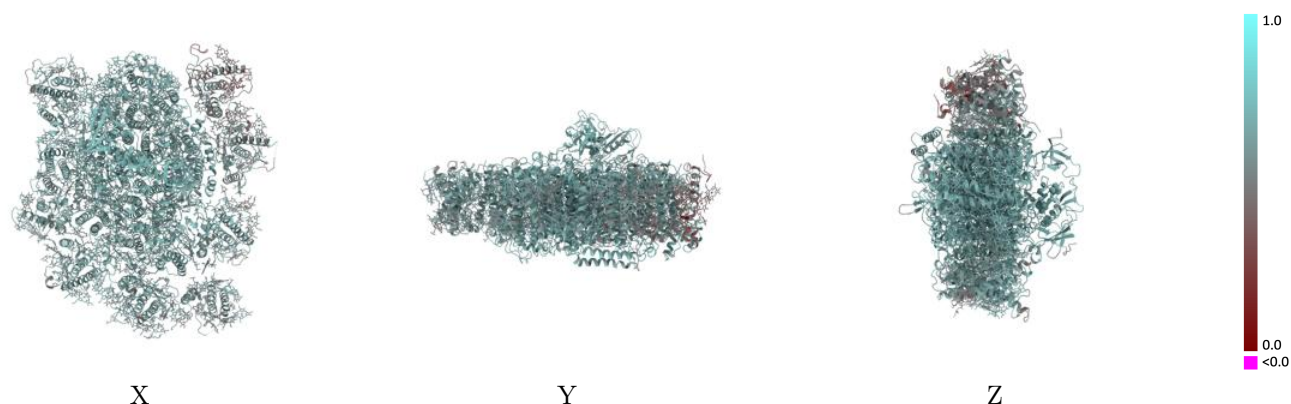
This section contains information regarding the fit between EMDB map EMD-64383 and PDB model 9UOV. Per-residue inclusion information can be found in [section 3](#) on [page 29](#).

9.1 Map-model overlay [i](#)



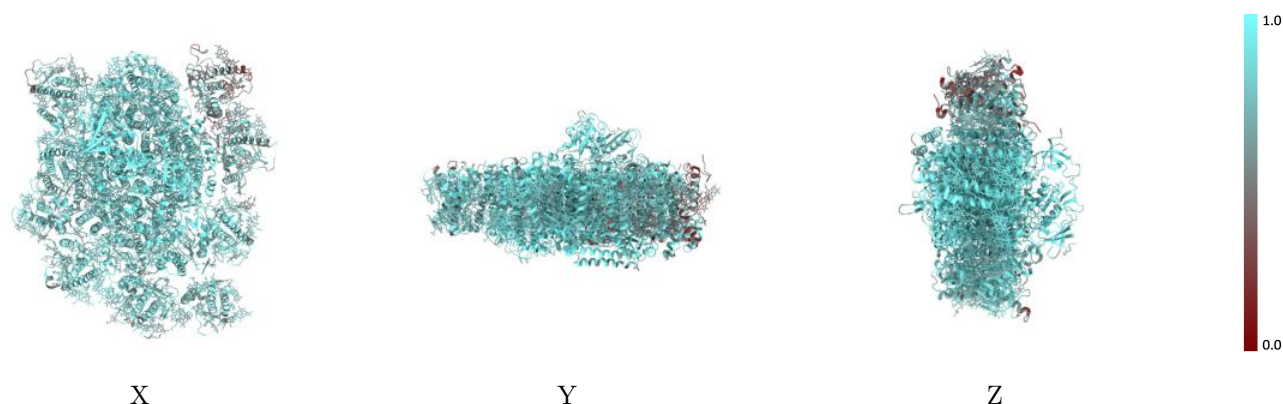
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



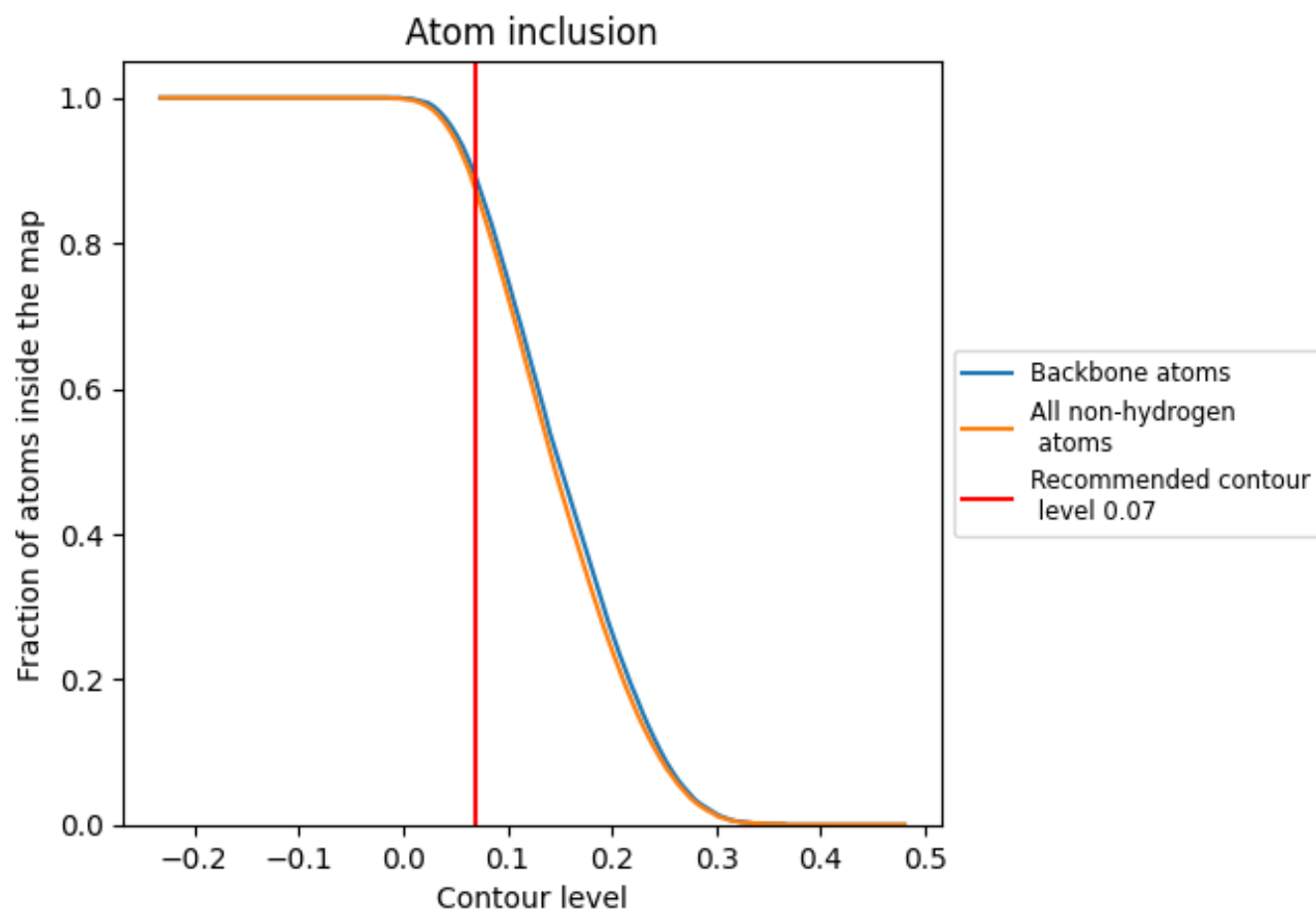
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).









































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 87% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8710	 0.6370
A	 0.9380	 0.6710
B	 0.9610	 0.6850
C	 0.9780	 0.6920
D	 0.9050	 0.6540
E	 0.8960	 0.6650
F	 0.9090	 0.6520
G	 0.6840	 0.5460
H	 0.5310	 0.4690
I	 0.9190	 0.6600
J	 0.9090	 0.6610
L	 0.8980	 0.6530
M	 0.9410	 0.6680
O	 0.8350	 0.6150
P	 0.8390	 0.6080
Q	 0.7970	 0.6030
R	 0.8960	 0.6470
S	 0.8330	 0.6200
T	 0.7510	 0.5660
U	 0.7320	 0.5870

