



## wwPDB EM Validation Summary Report ⓘ

Apr 12, 2026 – 12:26 PM UTC

PDB ID : 9UH3 / pdb\_00009uh3  
EMDB ID : EMD-64153  
Title : PSI-9 FCPI supercomplex from haptophyte *Chrysotila roscoffensis*  
Authors : La Rocca, R.; Tsai, P.-C.; Kato, K.; Nakajima, Y.; Akita, F.; Shen, J.-R.  
Deposited on : 2025-04-14  
Resolution : 1.74 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

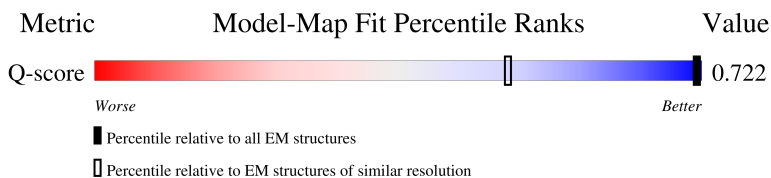
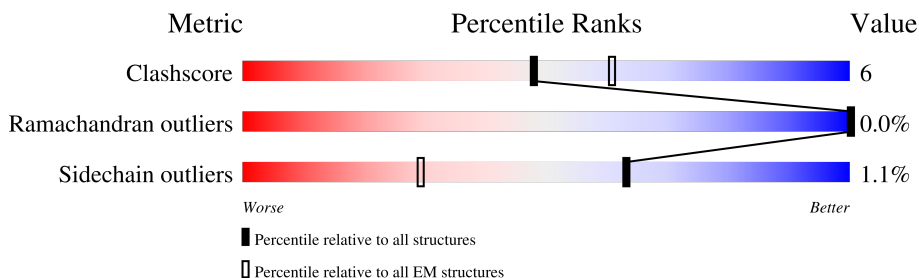
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 1.74 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.








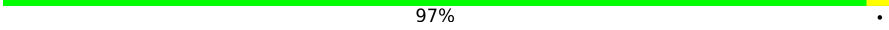





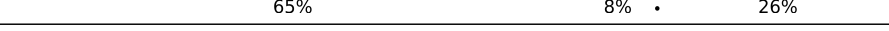





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	645 ( 1.25 - 2.24 )

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

Mol	Chain	Length	Quality of chain
1	A	752	 90% 9% .
2	B	734	 92% 7% .
3	C	81	 94% 5% .
4	D	142	 92% 5% .

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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	K	200	
20	T	202	
21	k	89	

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
22	CLA	A	802	X	-	-	-
22	CLA	A	803	X	-	-	-
22	CLA	A	804	X	-	-	-
22	CLA	A	805	X	-	-	-
22	CLA	A	806	X	-	-	-
22	CLA	A	809	X	-	-	-
22	CLA	A	810	X	-	-	-
22	CLA	A	811	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	812	X	-	-	-
22	CLA	A	815	X	-	-	-
22	CLA	A	816	X	-	-	-
22	CLA	A	817	X	-	-	-
22	CLA	A	818	X	-	-	-
22	CLA	A	820	X	-	-	-
22	CLA	A	821	X	-	-	-
22	CLA	A	822	X	-	-	-
22	CLA	A	823	X	-	-	-
22	CLA	A	824	X	-	-	-
22	CLA	A	825	X	-	-	-
22	CLA	A	828	X	-	-	-
22	CLA	A	829	X	-	-	-
22	CLA	A	831	X	-	-	-
22	CLA	A	832	X	-	-	-
22	CLA	A	833	X	-	-	-
22	CLA	A	835	X	-	-	-
22	CLA	A	836	X	-	-	-
22	CLA	A	838	X	-	-	-
22	CLA	A	845	X	-	-	-
22	CLA	A	850	X	-	-	-
22	CLA	A	853	X	-	-	-
22	CLA	A	854	X	-	-	-
22	CLA	A	855	X	-	-	-
22	CLA	A	856	X	-	-	-
22	CLA	B	801	X	-	-	-
22	CLA	B	802	X	-	-	-
22	CLA	B	803	X	-	-	-
22	CLA	B	804	X	-	-	-
22	CLA	B	805	X	-	-	-
22	CLA	B	807	X	-	-	-
22	CLA	B	808	X	-	-	-
22	CLA	B	811	X	-	-	-
22	CLA	B	815	X	-	-	-
22	CLA	B	816	X	-	-	-
22	CLA	B	819	X	-	-	-
22	CLA	B	820	X	-	-	-
22	CLA	B	821	X	-	-	-
22	CLA	B	822	X	-	-	-
22	CLA	B	826	X	-	-	-
22	CLA	B	828	X	-	-	-
22	CLA	B	829	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	830	X	-	-	-
22	CLA	B	831	X	-	-	-
22	CLA	B	832	X	-	-	-
22	CLA	B	834	X	-	-	-
22	CLA	B	842	X	-	-	-
22	CLA	B	843	X	-	-	-
22	CLA	B	844	X	-	-	-
22	CLA	B	845	X	-	-	-
22	CLA	B	847	X	-	-	-
22	CLA	F	802	X	-	-	-
22	CLA	F	803	X	-	-	-
22	CLA	F	804	X	-	-	-
22	CLA	G	202	X	-	-	-
22	CLA	G	203	X	-	-	-
22	CLA	G	206	X	-	-	-
22	CLA	G	208	X	-	-	-
22	CLA	G	209	X	-	-	-
22	CLA	G	210	X	-	-	-
22	CLA	G	215	X	-	-	-
22	CLA	H	202	X	-	-	-
22	CLA	H	203	X	-	-	-
22	CLA	H	204	X	-	-	-
22	CLA	H	205	X	-	-	-
22	CLA	H	206	X	-	-	-
22	CLA	H	208	X	-	-	-
22	CLA	H	209	X	-	-	-
22	CLA	H	213	X	-	-	-
22	CLA	J	103	X	-	-	-
22	CLA	K	203	X	-	-	-
22	CLA	K	205	X	-	-	-
22	CLA	K	206	X	-	-	-
22	CLA	L	204	X	-	-	-
22	CLA	O	205	X	-	-	-
22	CLA	O	206	X	-	-	-
22	CLA	O	207	X	-	-	-
22	CLA	O	208	X	-	-	-
22	CLA	P	207	X	-	-	-
22	CLA	P	208	X	-	-	-
22	CLA	P	209	X	-	-	-
22	CLA	P	213	X	-	-	-
22	CLA	P	214	X	-	-	-
22	CLA	P	216	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	Q	204	X	-	-	-
22	CLA	Q	205	X	-	-	-
22	CLA	Q	206	X	-	-	-
22	CLA	Q	207	X	-	-	-
22	CLA	Q	208	X	-	-	-
22	CLA	Q	211	X	-	-	-
22	CLA	Q	213	X	-	-	-
22	CLA	R	101	X	-	-	-
22	CLA	S	202	X	-	-	-
22	CLA	S	206	X	-	-	-
22	CLA	S	207	X	-	-	-
22	CLA	S	208	X	-	-	-
22	CLA	S	216	X	-	-	-
22	CLA	S	217	X	-	-	-
22	CLA	T	201	X	-	-	-
22	CLA	T	202	X	-	-	-
22	CLA	T	203	X	-	-	-
22	CLA	T	204	X	-	-	-
22	CLA	T	205	X	-	-	-
22	CLA	T	211	X	-	-	-
22	CLA	U	204	X	-	-	-
22	CLA	U	206	X	-	-	-
22	CLA	U	207	X	-	-	-
22	CLA	U	208	X	-	-	-
22	CLA	U	211	X	-	-	-
22	CLA	k	102	X	-	-	-
22	CLA	k	103	X	-	-	-

## 2 Entry composition [i](#)

There are 35 unique types of molecules in this entry. The entry contains 42258 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 IX (FCPI-9).

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	97	Total	C	N	O	S	0	0
			748	495	121	125	7		

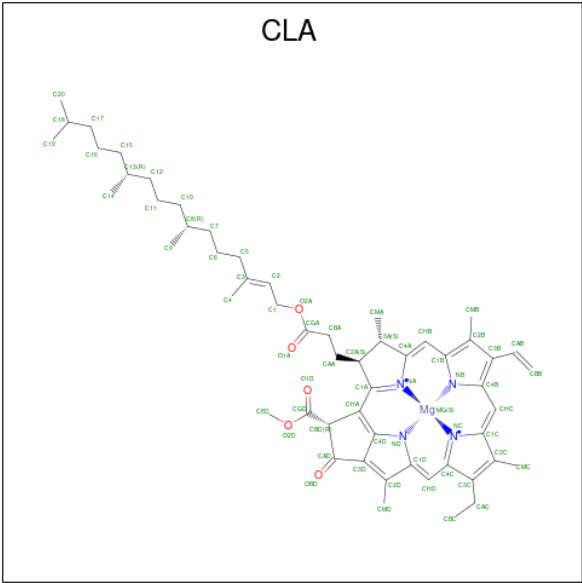
- Molecule 20 is a protein called Fucoxanthin chlorophyll a/c binding protein V (FCPI-5).

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

- Molecule 21 is a protein called Photosystem I reaction center subunit psaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	k	55	Total	C	N	O	S	0	0
			379	247	62	67	3		

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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

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

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 40	C 32	Mg 1	N 4	O 3	0
22	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	F	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
22	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	L	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	O	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
22	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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

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Mol	Chain	Residues	Atoms					AltConf
22	Q	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	Q	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	S	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	S	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	S	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	U	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	U	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	U	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	U	1	Total 52	C 42	Mg 1	N 4	O 5	0

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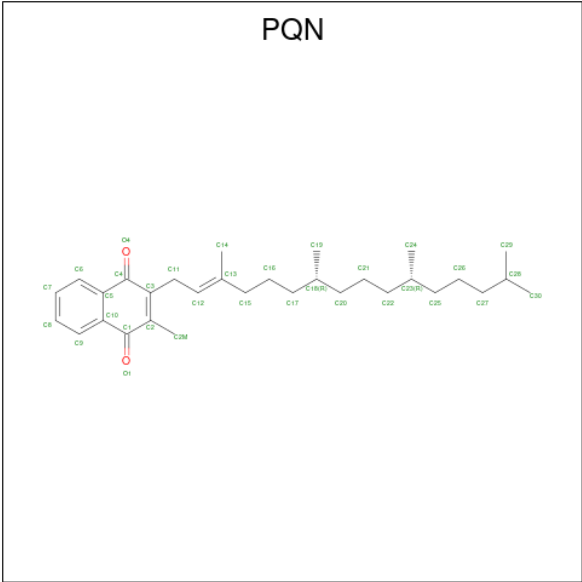
Mol	Chain	Residues	Atoms					AltConf
22	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	G	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	G	1	Total 43	C 35	Mg 1	N 4	O 3	0
22	G	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	G	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	H	1	Total 40	C 32	Mg 1	N 4	O 3	0
22	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	H	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	H	1	Total 44	C 35	Mg 1	N 4	O 4	0
22	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	H	1	Total 58	C 48	Mg 1	N 4	O 5	0
22	H	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	H	1	Total 65	C 55	Mg 1	N 4	O 5	0

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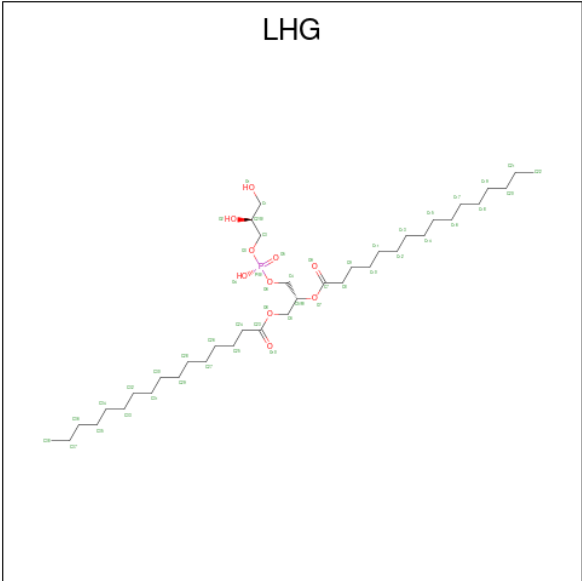
Mol	Chain	Residues	Atoms					AltConf
22	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	T	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	T	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	T	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	T	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	T	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	T	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	T	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	T	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	T	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	T	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
22	k	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	k	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

- Molecule 23 is PHYLLOQUINONE (CCD ID: PQN) (formula:  $C_{31}H_{46}O_2$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



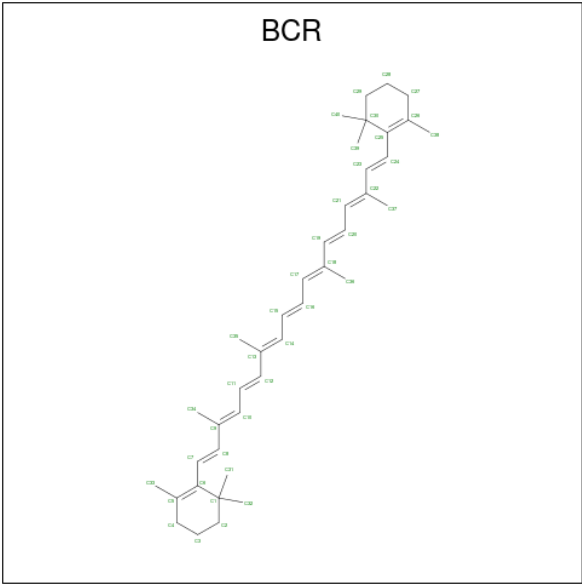
Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	P	0
			48	37	10	1	

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

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



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

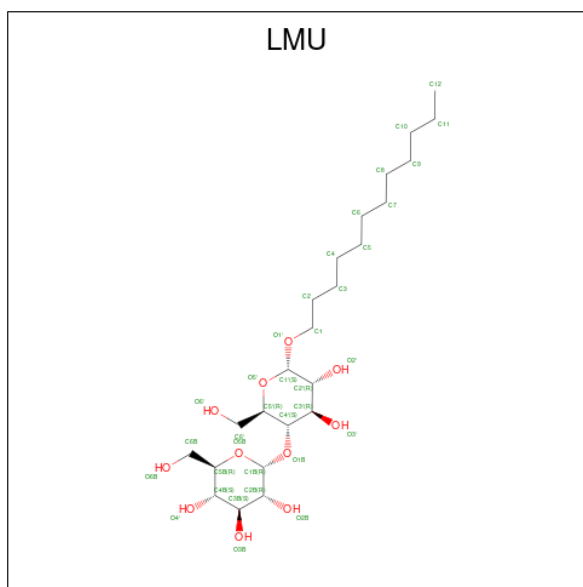
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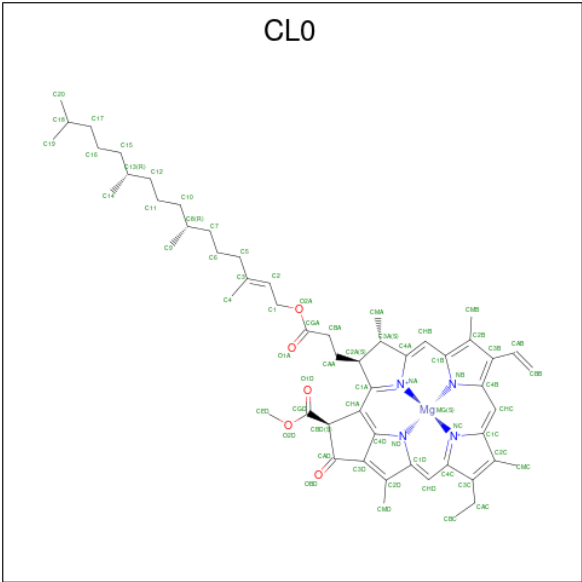
Mol	Chain	Residues	Atoms	AltConf
25	B	1	Total C 40 40	0
25	F	1	Total C 40 40	0
25	F	1	Total C 40 40	0
25	I	1	Total C 40 40	0
25	I	1	Total C 40 40	0
25	J	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	M	1	Total C 40 40	0
25	R	1	Total C 39 39	0
25	k	1	Total C 40 40	0

- Molecule 26 is DODECYL-ALPHA-D-MALTOSE (CCD ID: LMU) (formula:  $C_{24}H_{46}O_{11}$ ).



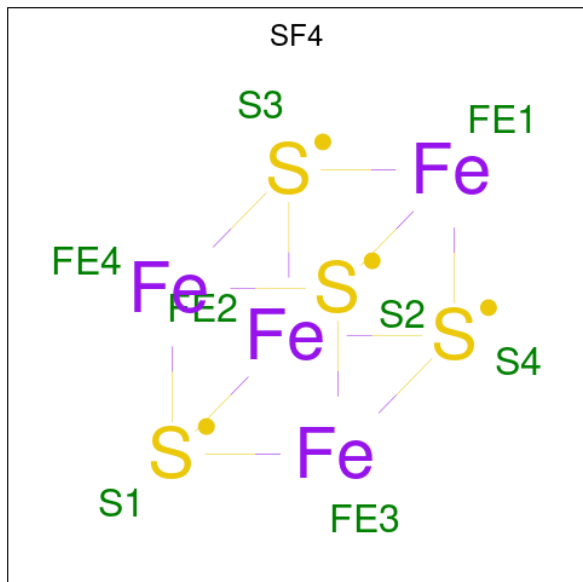
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			35	24	11	
26	A	1	Total	C	O	0
			35	24	11	
26	F	1	Total	C	O	0
			35	24	11	
26	F	1	Total	C	O	0
			35	24	11	
26	L	1	Total	C	O	0
			35	24	11	
26	M	1	Total	C	O	0
			35	24	11	
26	O	1	Total	C	O	0
			35	24	11	
26	P	1	Total	C	O	0
			25	14	11	
26	S	1	Total	C	O	0
			31	20	11	
26	K	1	Total	C	O	0
			35	24	11	
26	K	1	Total	C	O	0
			24	13	11	

- Molecule 27 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



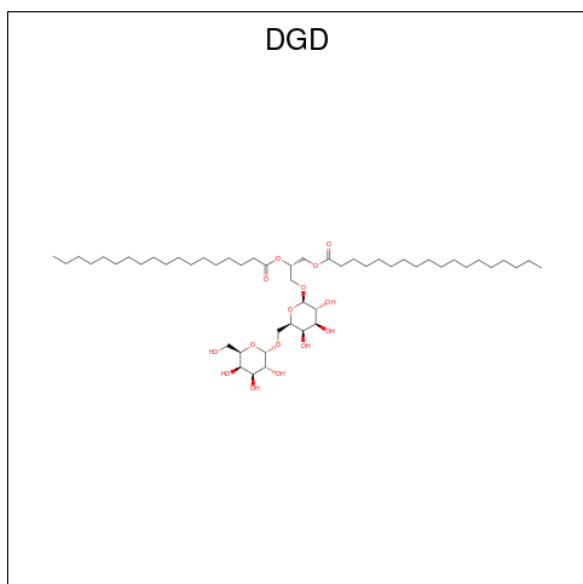
Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 28 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).



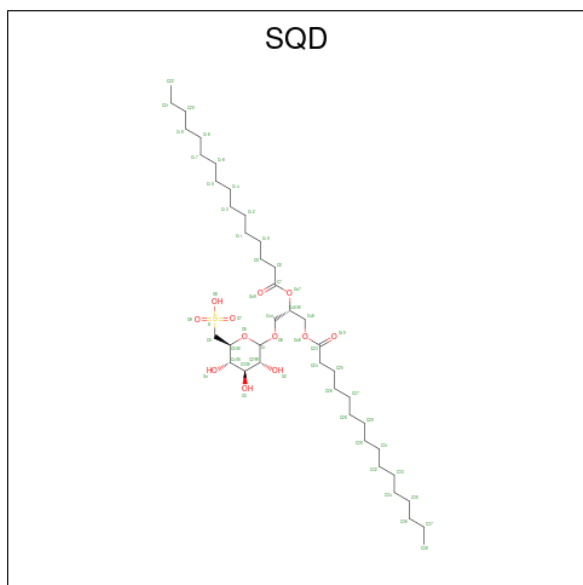
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	Fe	S	0
			8	4	4	
28	C	1	Total	Fe	S	0
			8	4	4	
28	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $\text{C}_{51}\text{H}_{96}\text{O}_{15}$ ).



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

- Molecule 30 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
30	B	1	Total	C	O	S	0
			50	37	12	1	
30	S	1	Total	C	O	S	0
			46	33	12	1	

- Molecule 31 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene -3,3'-diol (CCD ID: DD6) (formula:  $C_{40}H_{54}O_3$ ).

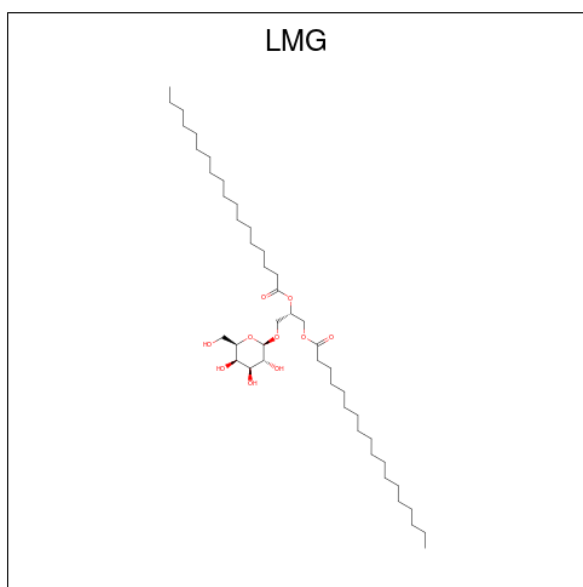


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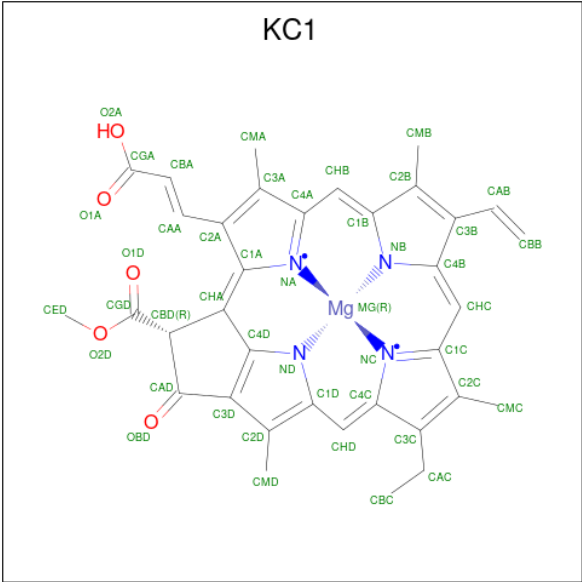
Mol	Chain	Residues	Atoms			AltConf
31	S	1	Total 43	C 40	O 3	0
31	S	1	Total 43	C 40	O 3	0
31	S	1	Total 43	C 40	O 3	0
31	U	1	Total 43	C 40	O 3	0
31	U	1	Total 43	C 40	O 3	0
31	U	1	Total 26	C 25	O 1	0
31	G	1	Total 43	C 40	O 3	0
31	G	1	Total 43	C 40	O 3	0
31	G	1	Total 43	C 40	O 3	0
31	G	1	Total 43	C 40	O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

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



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

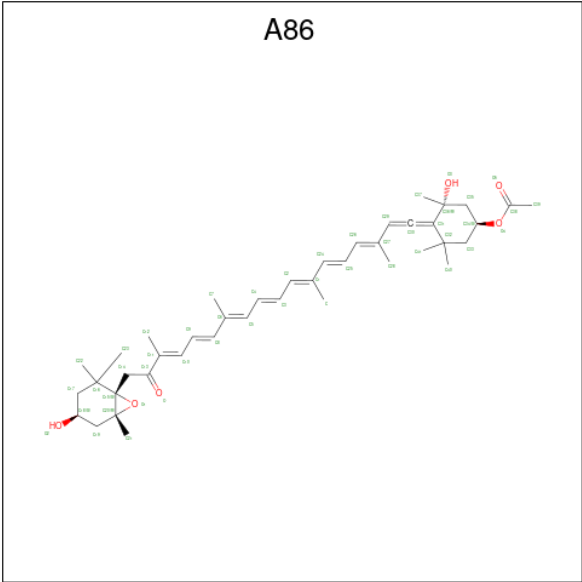
- Molecule 33 is Chlorophyll c1 (CCD ID: KC1) (formula:  $C_{35}H_{30}MgN_4O_5$ ).



Mol	Chain	Residues	Atoms					AltConf
33	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	P	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
33	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 34 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<sub>42</sub>H<sub>58</sub>O<sub>6</sub>).





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

- Molecule 35 is water.

Mol	Chain	Residues	Atoms		AltConf
35	A	117	Total	O	0
			117	117	
35	B	211	Total	O	0
			211	211	
35	C	46	Total	O	0
			46	46	
35	D	21	Total	O	0
			21	21	
35	E	14	Total	O	0
			14	14	

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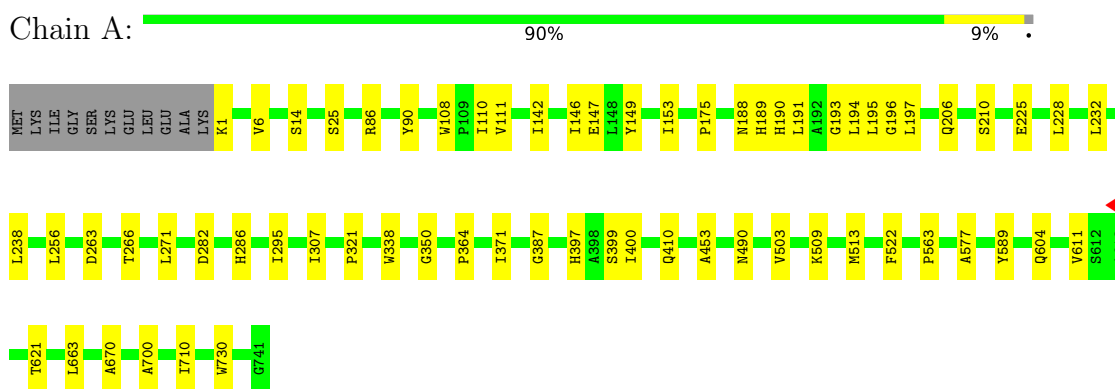
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Mol	Chain	Residues	Atoms		AltConf
35	F	21	Total 21	O 21	0
35	I	2	Total 2	O 2	0
35	J	3	Total 3	O 3	0
35	L	18	Total 18	O 18	0
35	M	2	Total 2	O 2	0
35	O	11	Total 11	O 11	0
35	P	18	Total 18	O 18	0
35	Q	9	Total 9	O 9	0
35	R	4	Total 4	O 4	0
35	S	11	Total 11	O 11	0
35	U	5	Total 5	O 5	0
35	k	1	Total 1	O 1	0

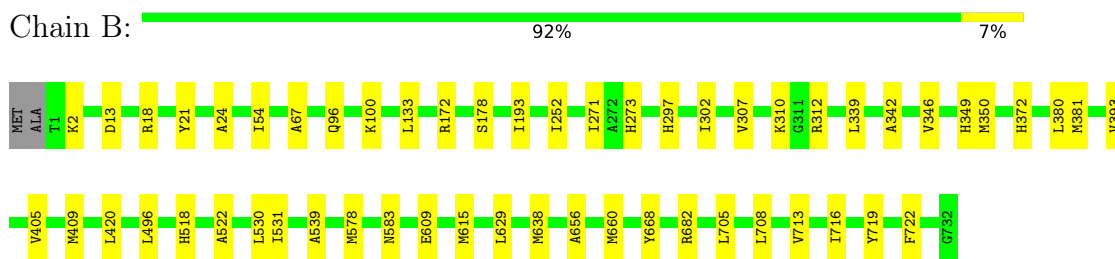
### 3 Residue-property plots

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.

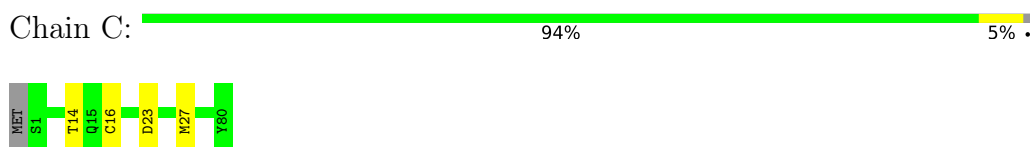
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1 (psaA)



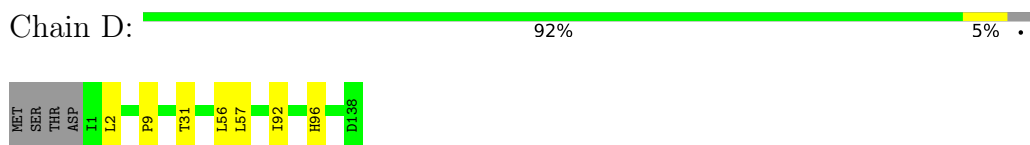
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 (psaB)



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



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




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

Chain E:  90% . . .




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

Chain F:  80% 8% 12%




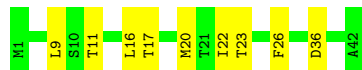
- Molecule 7: Photosystem I reaction center subunit VIII (psaI)

Chain I:  86% 11% .



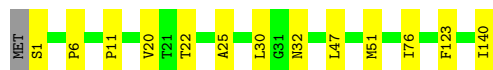
- Molecule 8: Photosystem I reaction center subunit IX (psaJ)

Chain J:  77% 23%



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

Chain L:  90% 9% .




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

Chain M:  97% .




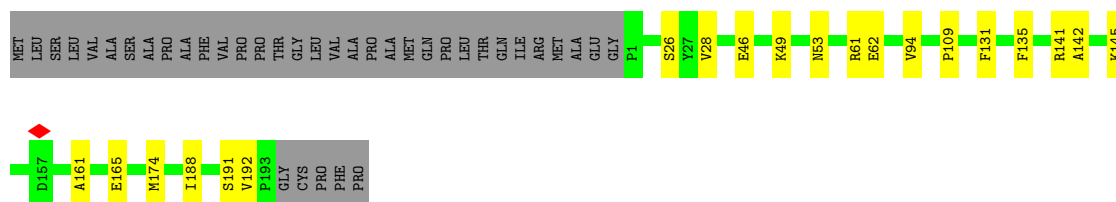
- Molecule 11: Fucoxanthin chlorophyll a/c binding protein III (FCPI-3)

Chain O:  81% 7% 12%




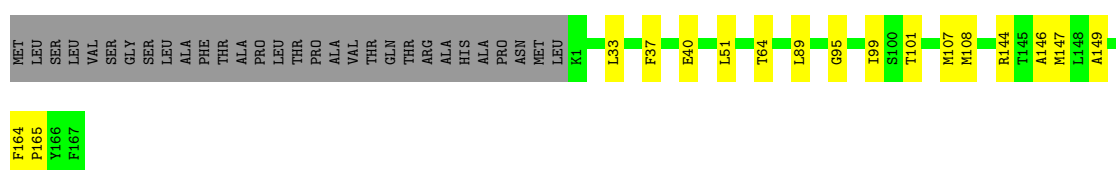
- Molecule 12: Fucoxanthin chlorophyll a/c binding protein VI (FCPI-6)

Chain P:  75% 9% 16%



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

Chain Q:  76% 9% 15%



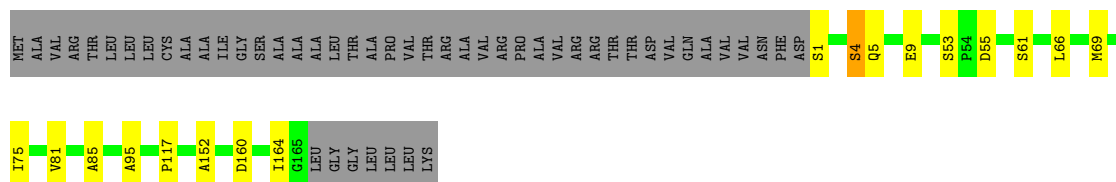
- Molecule 14: Photosystem I reaction center subunit psaR

Chain R:  88% 10% .



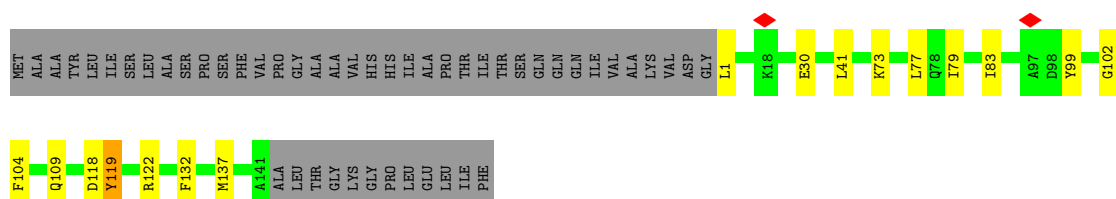
- Molecule 15: Fucoxanthin chlorophyll a/c binding protein II (FCPI-2)

Chain S:  69% 7% 23%



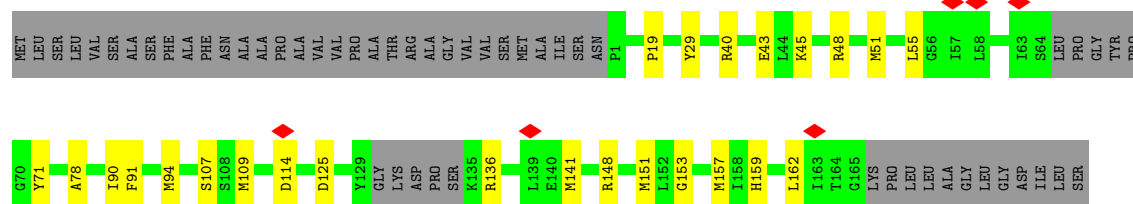
- Molecule 16: Fucoxanthin chlorophyll a/c binding protein I (FCPI-1)

Chain U:  65% 8% . 26%



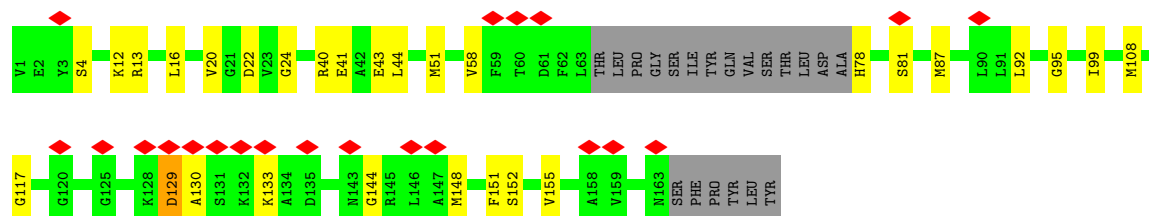
- Molecule 17: Fucoxanthin chlorophyll a/c binding protein VII (FCPI-7)

Chain G:  62% 12% 26%




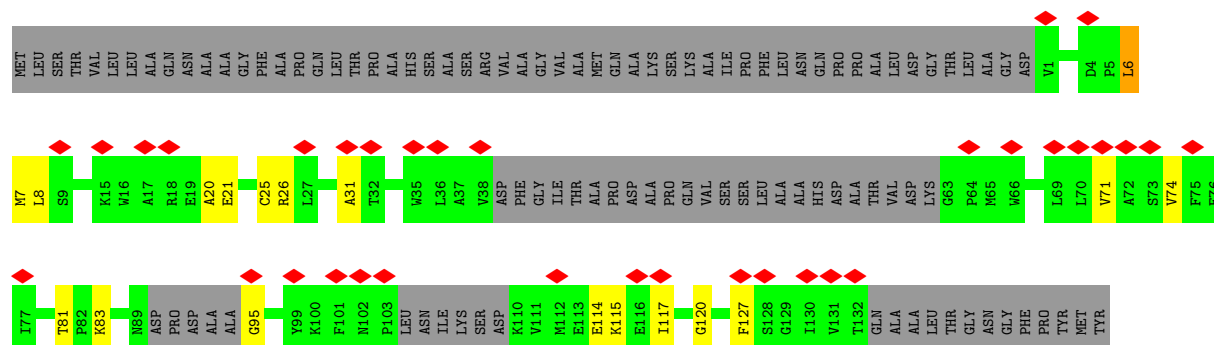
- Molecule 18: Fucoxanthin chlorophyll a/c binding protein VIII (FCPI-8)

Chain H:  12% 71% 17% 12%



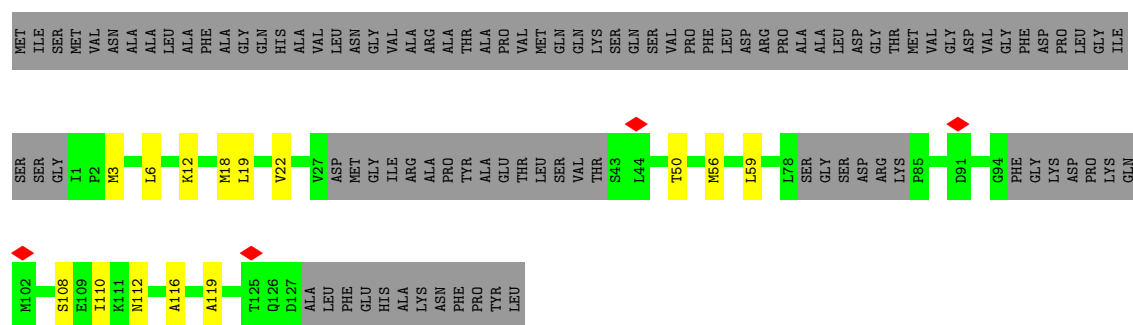
- Molecule 19: Fucoxanthin chlorophyll a/c binding protein IX (FCPI-9)

Chain K:  17% 40% 8% 52%



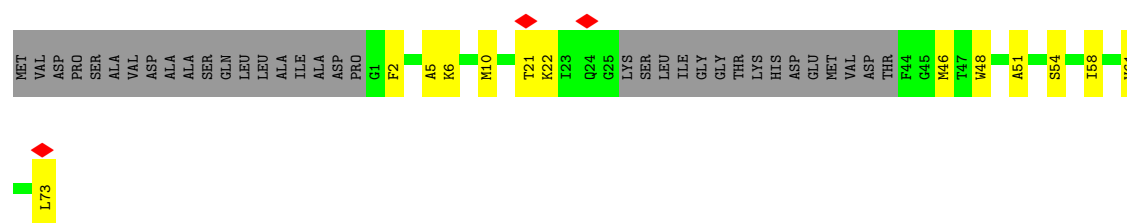
- Molecule 20: Fucoxanthin chlorophyll a/c binding protein V (FCPI-5)

Chain T:  42% 7% 51%



- Molecule 21: Photosystem I reaction center subunit psaK

Frequency	Percentage
Daily	47%
Weekly	15%
Monthly	38%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	191444	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	1.885	Depositor
Minimum map value	-0.618	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.065	Depositor
Map size ( $\text{\AA}$ )	436.2, 436.2, 436.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.727, 0.727, 0.727	Depositor



## 5 Model quality

### 5.1 Standard geometry

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

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	0.20	0/6007	0.40	0/8185
2	B	0.22	0/6015	0.41	0/8205
3	C	0.16	0/609	0.38	0/826
4	D	0.15	0/1116	0.38	0/1503
5	E	0.16	0/505	0.31	0/689
6	F	0.21	0/1275	0.42	0/1728
7	I	0.22	0/273	0.48	0/373
8	J	0.43	0/313	0.70	0/427
9	L	0.20	0/1081	0.43	0/1470
10	M	0.19	0/218	0.30	0/295
11	O	0.18	0/1376	0.39	0/1865
12	P	0.20	0/1480	0.37	0/2010
13	Q	0.16	0/1285	0.37	0/1736
14	R	0.19	0/681	0.35	0/930
15	S	0.14	0/1272	0.32	0/1732
16	U	0.24	0/1109	0.47	2/1499 (0.1%)
17	G	0.17	0/1204	0.39	0/1624
18	H	0.20	0/1149	0.41	0/1546
19	K	0.25	0/764	0.52	0/1029
20	T	0.24	0/741	0.44	0/999
21	k	0.14	0/383	0.30	0/519
All	All	0.20	0/28856	0.41	2/39190 (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
11	O	0	1
13	Q	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
19	K	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	U	119	TYR	CA-C-N	5.81	128.54	120.29
16	U	119	TYR	C-N-CA	5.81	128.54	120.29

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	K	20	ALA	Peptide
11	O	173	VAL	Peptide
13	Q	164	PHE	Peptide
13	Q	165	PRO	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5813	0	5698	49	0
2	B	5805	0	5635	49	0
3	C	599	0	577	3	0
4	D	1092	0	1096	4	0
5	E	494	0	488	2	0
6	F	1246	0	1256	12	0
7	I	266	0	278	4	0
8	J	305	0	310	8	0
9	L	1056	0	1068	10	0
10	M	216	0	234	1	0
11	O	1341	0	1347	14	0
12	P	1441	0	1421	16	0
13	Q	1257	0	1260	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	R	664	0	668	5	0
15	S	1238	0	1217	13	0
16	U	1082	0	1058	12	0
17	G	1179	0	1166	22	0
18	H	1128	0	1134	18	0
19	K	748	0	777	12	0
20	T	731	0	749	23	0
21	k	379	0	409	10	0
22	A	2701	0	2712	65	0
22	B	2344	0	2385	79	0
22	F	159	0	141	4	0
22	G	561	0	486	20	0
22	H	524	0	475	14	0
22	J	42	0	31	1	0
22	K	245	0	201	7	0
22	L	164	0	150	4	0
22	O	495	0	475	13	0
22	P	403	0	337	8	0
22	Q	609	0	566	8	0
22	R	110	0	105	5	0
22	S	384	0	358	9	0
22	T	473	0	379	22	0
22	U	441	0	417	14	0
22	k	97	0	80	4	0
23	A	33	0	46	2	0
23	B	33	0	46	1	0
24	A	75	0	93	3	0
24	G	27	0	24	1	0
24	P	49	0	74	4	0
25	A	160	0	224	5	0
25	B	200	0	280	14	0
25	F	80	0	112	4	0
25	I	80	0	112	5	0
25	J	40	0	56	1	0
25	L	80	0	112	2	0
25	M	40	0	56	1	0
25	R	39	0	53	3	0
25	k	40	0	56	2	0
26	A	70	0	92	1	0
26	F	70	0	92	1	0
26	K	59	0	67	2	0
26	L	35	0	46	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	M	35	0	46	1	0
26	O	35	0	46	0	0
26	P	25	0	23	0	0
26	S	31	0	35	1	0
27	A	65	0	72	3	0
28	A	8	0	0	0	0
28	C	16	0	0	1	0
29	B	60	0	81	9	0
30	B	50	0	67	1	0
30	S	46	0	56	1	0
31	G	172	0	0	3	0
31	H	129	0	0	0	0
31	J	43	0	0	0	0
31	K	43	0	0	0	0
31	O	215	0	0	2	0
31	P	172	0	0	0	0
31	Q	86	0	0	0	0
31	S	215	0	0	0	0
31	T	86	0	0	0	0
31	U	112	0	0	1	0
31	k	43	0	0	0	0
32	J	39	0	48	3	0
32	P	59	0	58	4	0
32	Q	55	0	86	3	0
32	S	49	0	68	2	0
32	U	32	0	34	1	0
33	O	45	0	0	0	0
33	P	179	0	0	0	0
33	Q	45	0	0	0	0
33	S	90	0	0	0	0
33	T	45	0	0	1	0
33	U	45	0	0	0	0
34	P	48	0	0	0	0
34	Q	144	0	0	0	0
34	R	92	0	0	1	0
34	U	48	0	0	0	0
35	A	117	0	0	1	0
35	B	211	0	0	0	0
35	C	46	0	0	0	0
35	D	21	0	0	0	0
35	E	14	0	0	0	0
35	F	21	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	I	2	0	0	0	0
35	J	3	0	0	0	0
35	L	18	0	0	0	0
35	M	2	0	0	0	0
35	O	11	0	0	0	0
35	P	18	0	0	0	0
35	Q	9	0	0	0	0
35	R	4	0	0	0	0
35	S	11	0	0	0	0
35	U	5	0	0	0	0
35	k	1	0	0	0	0
All	All	42258	0	39505	480	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 480 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)
19:K:8:LEU:HD21	21:k:46:MET:SD	2.05	0.96
17:G:90:ILE:HG22	17:G:94:MET:HE2	1.50	0.94
12:P:46:GLU:OE2	12:P:49:LYS:HE3	1.68	0.93
20:T:56:MET:HE2	20:T:56:MET:HA	1.56	0.87
22:B:830:CLA:H152	25:F:805:BCR:H23C	1.65	0.78

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%)	719 (97%)	20 (3%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	730/734 (100%)	712 (98%)	18 (2%)	0	100	100
3	C	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
4	D	136/142 (96%)	132 (97%)	4 (3%)	0	100	100
5	E	62/67 (92%)	61 (98%)	1 (2%)	0	100	100
6	F	159/184 (86%)	155 (98%)	4 (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%)	137 (99%)	1 (1%)	0	100	100
10	M	27/29 (93%)	27 (100%)	0	0	100	100
11	O	174/201 (87%)	170 (98%)	3 (2%)	1 (1%)	21	8
12	P	191/231 (83%)	188 (98%)	3 (2%)	0	100	100
13	Q	165/197 (84%)	157 (95%)	8 (5%)	0	100	100
14	R	86/90 (96%)	84 (98%)	2 (2%)	0	100	100
15	S	163/215 (76%)	160 (98%)	3 (2%)	0	100	100
16	U	139/191 (73%)	138 (99%)	1 (1%)	0	100	100
17	G	149/209 (71%)	146 (98%)	3 (2%)	0	100	100
18	H	145/169 (86%)	140 (97%)	5 (3%)	0	100	100
19	K	89/200 (44%)	87 (98%)	2 (2%)	0	100	100
20	T	91/202 (45%)	89 (98%)	2 (2%)	0	100	100
21	k	51/89 (57%)	50 (98%)	1 (2%)	0	100	100
All	All	3581/4198 (85%)	3498 (98%)	82 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	O	174	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	603/612 (98%)	598 (99%)	5 (1%)	73	64
2	B	590/591 (100%)	589 (100%)	1 (0%)	87	84
3	C	68/69 (99%)	68 (100%)	0	100	100
4	D	118/122 (97%)	118 (100%)	0	100	100
5	E	53/55 (96%)	52 (98%)	1 (2%)	50	28
6	F	133/152 (88%)	132 (99%)	1 (1%)	73	64
7	I	31/32 (97%)	31 (100%)	0	100	100
8	J	32/32 (100%)	32 (100%)	0	100	100
9	L	111/112 (99%)	110 (99%)	1 (1%)	70	59
10	M	21/21 (100%)	21 (100%)	0	100	100
11	O	145/161 (90%)	145 (100%)	0	100	100
12	P	144/173 (83%)	141 (98%)	3 (2%)	47	24
13	Q	133/157 (85%)	132 (99%)	1 (1%)	73	64
14	R	71/73 (97%)	70 (99%)	1 (1%)	59	41
15	S	125/162 (77%)	121 (97%)	4 (3%)	34	11
16	U	110/148 (74%)	108 (98%)	2 (2%)	51	30
17	G	127/167 (76%)	127 (100%)	0	100	100
18	H	119/137 (87%)	115 (97%)	4 (3%)	32	10
19	K	78/153 (51%)	75 (96%)	3 (4%)	29	8
20	T	73/153 (48%)	70 (96%)	3 (4%)	27	6
21	k	38/65 (58%)	36 (95%)	2 (5%)	20	4
All	All	2923/3347 (87%)	2891 (99%)	32 (1%)	63	50

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	T	22	VAL
20	T	110	ILE
13	Q	64	THR
12	P	192	VAL
21	k	2	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
6	F	44	GLN
9	L	32	ASN
18	H	157	GLN
17	G	3	ASN
17	G	102	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

272 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
22	CLA	A	807	1	69,73,73	1.17	8 (11%)	82,113,113	0.94	4 (4%)
22	CLA	B	828	35	69,73,73	1.17	7 (10%)	82,113,113	0.98	5 (6%)
26	LMU	K	201	-	36,36,36	1.19	3 (8%)	47,47,47	1.61	9 (19%)
22	CLA	P	213	12	45,49,73	1.48	7 (15%)	54,84,113	1.21	4 (7%)
22	CLA	G	208	-	59,63,73	1.24	6 (10%)	70,101,113	1.08	6 (8%)
25	BCR	B	838	-	41,41,41	1.09	3 (7%)	56,56,56	1.27	6 (10%)
22	CLA	S	206	15	50,54,73	1.34	6 (12%)	59,90,113	1.08	4 (6%)
22	CLA	F	803	35	52,56,73	1.40	7 (13%)	61,92,113	1.20	6 (9%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	BCR	L	205	-	41,41,41	1.04	2 (4%)	56,56,56	1.31	5 (8%)
22	CLA	Q	205	13	64,68,73	1.21	8 (12%)	76,107,113	0.91	3 (3%)
22	CLA	Q	213	35	61,65,73	1.24	7 (11%)	72,103,113	1.06	7 (9%)
22	CLA	A	822	35	69,73,73	1.12	6 (8%)	82,113,113	0.91	4 (4%)
22	CLA	B	804	2	69,73,73	1.16	7 (10%)	82,113,113	0.91	4 (4%)
25	BCR	J	104	-	41,41,41	1.08	2 (4%)	56,56,56	1.20	4 (7%)
22	CLA	U	211	16	56,60,73	1.33	7 (12%)	65,97,113	1.08	5 (7%)
22	CLA	A	812	1	49,53,73	1.42	8 (16%)	58,89,113	1.04	4 (6%)
31	DD6	J	101	-	40,45,45	1.27	8 (20%)	51,67,67	1.57	9 (17%)
22	CLA	O	205	11	69,73,73	1.22	7 (10%)	82,113,113	0.91	4 (4%)
31	DD6	O	214	-	40,45,45	1.24	7 (17%)	51,67,67	1.54	9 (17%)
25	BCR	F	801	-	41,41,41	1.03	2 (4%)	56,56,56	1.22	2 (3%)
22	CLA	G	210	17	49,53,73	1.51	8 (16%)	58,89,113	1.03	4 (6%)
22	CLA	A	806	1	69,73,73	1.14	8 (11%)	82,113,113	1.00	4 (4%)
22	CLA	B	807	2	69,73,73	1.23	7 (10%)	82,113,113	0.90	3 (3%)
22	CLA	B	813	2	59,63,73	1.40	8 (13%)	70,101,113	0.94	3 (4%)
22	CLA	H	207	18	69,73,73	1.14	8 (11%)	82,113,113	1.13	7 (8%)
23	PQN	B	835	-	34,34,34	0.41	0	43,45,45	0.55	1 (2%)
22	CLA	A	835	1	69,73,73	1.23	7 (10%)	82,113,113	0.92	3 (3%)
31	DD6	O	213	-	40,45,45	1.33	8 (20%)	51,67,67	1.38	8 (15%)
34	A86	Q	214	-	47,50,50	1.37	5 (10%)	51,76,76	1.41	8 (15%)
24	LHG	G	216	-	26,26,48	0.86	1 (3%)	29,32,54	1.20	2 (6%)
22	CLA	A	838	24	56,60,73	1.33	8 (14%)	65,97,113	1.06	5 (7%)
25	BCR	B	839	-	41,41,41	1.06	2 (4%)	56,56,56	1.20	5 (8%)
25	BCR	I	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.29	6 (10%)
26	LMU	O	216	-	36,36,36	1.23	2 (5%)	47,47,47	1.07	2 (4%)
22	CLA	O	204	11	69,73,73	1.19	8 (11%)	82,113,113	0.90	4 (4%)
22	CLA	B	827	2	62,66,73	1.30	7 (11%)	73,104,113	1.00	6 (8%)
22	CLA	A	854	1	69,73,73	1.14	6 (8%)	82,113,113	0.93	6 (7%)
22	CLA	A	816	1	69,73,73	1.17	8 (11%)	82,113,113	0.95	4 (4%)
22	CLA	B	810	2	59,63,73	1.22	7 (11%)	70,101,113	0.96	5 (7%)
22	CLA	A	818	35	69,73,73	1.14	7 (10%)	82,113,113	0.96	5 (6%)
22	CLA	k	103	35	59,63,73	1.30	7 (11%)	70,101,113	0.98	3 (4%)
31	DD6	U	214	-	24,26,45	1.52	5 (20%)	29,35,67	1.59	6 (20%)
32	LMG	P	217	-	25,25,55	1.38	4 (16%)	33,33,63	1.47	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	B	806	2	69,73,73	1.17	7 (10%)	82,113,113	0.90	3 (3%)
22	CLA	Q	204	-	65,69,73	1.18	6 (9%)	77,108,113	0.99	4 (5%)
22	CLA	P	216	12	51,55,73	1.39	7 (13%)	60,91,113	1.14	5 (8%)
22	CLA	k	102	21	46,50,73	1.44	7 (15%)	53,85,113	1.08	3 (5%)
22	CLA	B	803	2	49,53,73	1.46	8 (16%)	58,89,113	1.01	3 (5%)
31	DD6	H	201	-	40,45,45	1.42	9 (22%)	51,67,67	1.67	11 (21%)
22	CLA	U	209	16	46,50,73	1.68	8 (17%)	53,85,113	1.05	3 (5%)
31	DD6	P	220	-	40,45,45	1.30	7 (17%)	51,67,67	1.70	12 (23%)
22	CLA	A	848	1	69,73,73	1.20	8 (11%)	82,113,113	1.04	6 (7%)
22	CLA	B	805	2	69,73,73	1.20	8 (11%)	82,113,113	0.86	4 (4%)
22	CLA	B	845	2	69,73,73	1.19	8 (11%)	82,113,113	1.21	9 (10%)
32	LMG	P	202	-	34,34,55	1.02	2 (5%)	42,42,63	1.28	4 (9%)
33	KC1	T	208	20	49,53,53	1.77	10 (20%)	61,89,89	1.06	2 (3%)
26	LMU	M	102	-	36,36,36	1.18	2 (5%)	47,47,47	1.03	2 (4%)
22	CLA	P	207	12	69,73,73	1.14	7 (10%)	82,113,113	0.97	4 (4%)
26	LMU	P	221	-	26,26,36	1.28	2 (7%)	37,37,47	1.36	4 (10%)
22	CLA	T	201	-	46,50,73	1.48	8 (17%)	53,85,113	1.03	3 (5%)
22	CLA	O	211	11	45,49,73	1.45	7 (15%)	54,84,113	1.20	5 (9%)
22	CLA	Q	216	35	69,73,73	1.13	7 (10%)	82,113,113	0.88	4 (4%)
22	CLA	A	830	1	54,58,73	1.34	7 (12%)	64,95,113	0.94	3 (4%)
32	LMG	Q	217	-	55,55,55	0.70	0	63,63,63	1.32	6 (9%)
22	CLA	B	823	2	69,73,73	1.25	7 (10%)	82,113,113	0.97	5 (6%)
22	CLA	S	207	15	50,54,73	1.49	7 (14%)	59,90,113	1.07	5 (8%)
22	CLA	Q	203	13	52,56,73	1.33	7 (13%)	61,92,113	1.04	4 (6%)
25	BCR	F	805	-	41,41,41	1.05	2 (4%)	56,56,56	1.18	5 (8%)
22	CLA	A	819	1	47,51,73	1.42	7 (14%)	55,86,113	1.04	3 (5%)
22	CLA	B	826	2	53,57,73	1.39	7 (13%)	61,93,113	0.99	3 (4%)
22	CLA	L	204	35	54,58,73	1.32	7 (12%)	64,95,113	1.11	6 (9%)
22	CLA	B	812	2	63,67,73	1.27	9 (14%)	74,105,113	0.92	4 (5%)
22	CLA	B	824	2	69,73,73	1.25	7 (10%)	82,113,113	0.85	2 (2%)
26	LMU	A	857	-	36,36,36	0.42	0	47,47,47	0.74	1 (2%)
22	CLA	A	824	1	66,70,73	1.22	7 (10%)	78,109,113	0.97	3 (3%)
31	DD6	U	212	-	40,45,45	1.30	7 (17%)	51,67,67	1.66	10 (19%)
22	CLA	A	820	1	55,59,73	1.36	7 (12%)	64,96,113	1.12	5 (7%)
30	SQD	B	846	-	48,50,54	1.00	5 (10%)	58,61,65	1.55	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	G	202	-	45,49,73	1.42	6 (13%)	54,84,113	1.12	5 (9%)
22	CLA	A	833	1	69,73,73	1.22	7 (10%)	82,113,113	0.92	4 (4%)
22	CLA	Q	212	13	69,73,73	1.23	7 (10%)	82,113,113	0.99	7 (8%)
25	BCR	M	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.29	7 (12%)
28	SF4	A	852	1,2	0,12,12	-	-	-	-	-
31	DD6	O	201	-	40,45,45	1.29	7 (17%)	51,67,67	1.46	10 (19%)
22	CLA	Q	209	13	69,73,73	1.21	7 (10%)	82,113,113	0.86	3 (3%)
25	BCR	R	102	-	40,40,41	1.18	2 (5%)	54,54,56	1.43	11 (20%)
22	CLA	A	811	1	69,73,73	1.18	8 (11%)	82,113,113	0.92	3 (3%)
22	CLA	G	205	17	65,69,73	1.15	6 (9%)	77,108,113	1.06	8 (10%)
22	CLA	B	847	2	54,58,73	1.33	7 (12%)	64,95,113	1.02	3 (4%)
22	CLA	H	213	-	69,73,73	1.15	5 (7%)	82,113,113	1.11	7 (8%)
22	CLA	T	206	20	46,50,73	1.83	8 (17%)	53,85,113	1.03	3 (5%)
22	CLA	A	827	1	54,58,73	1.40	7 (12%)	64,95,113	0.97	4 (6%)
22	CLA	A	834	1	69,73,73	1.30	9 (13%)	82,113,113	0.88	4 (4%)
22	CLA	P	210	35	51,55,73	1.35	6 (11%)	60,91,113	1.06	4 (6%)
22	CLA	A	856	-	50,54,73	1.33	7 (14%)	59,90,113	1.04	4 (6%)
29	DGD	B	841	-	61,61,67	0.95	1 (1%)	75,75,81	1.33	7 (9%)
31	DD6	T	213	-	40,45,45	1.33	6 (15%)	51,67,67	2.05	12 (23%)
22	CLA	B	843	2	69,73,73	1.27	6 (8%)	82,113,113	0.88	3 (3%)
31	DD6	G	211	-	40,45,45	1.31	8 (20%)	51,67,67	1.45	7 (13%)
22	CLA	A	814	35	49,53,73	1.39	7 (14%)	58,89,113	1.11	6 (10%)
22	CLA	P	211	12	54,58,73	1.27	7 (12%)	64,95,113	1.01	4 (6%)
31	DD6	k	101	-	40,45,45	1.30	8 (20%)	51,67,67	1.47	10 (19%)
22	CLA	B	821	2	69,73,73	1.24	7 (10%)	82,113,113	0.90	4 (4%)
22	CLA	U	205	16	69,73,73	1.18	7 (10%)	82,113,113	0.91	3 (3%)
22	CLA	A	810	1	58,62,73	1.27	6 (10%)	68,99,113	1.06	4 (5%)
22	CLA	A	823	1	69,73,73	1.22	7 (10%)	82,113,113	0.87	3 (3%)
33	KC1	P	219	12	49,53,53	1.55	9 (18%)	61,89,89	0.86	1 (1%)
22	CLA	B	808	2	69,73,73	1.19	8 (11%)	82,113,113	0.91	5 (6%)
25	BCR	A	843	-	41,41,41	1.06	2 (4%)	56,56,56	1.23	4 (7%)
26	LMU	F	807	-	36,36,36	1.21	2 (5%)	47,47,47	0.97	2 (4%)
22	CLA	B	814	2	63,67,73	1.20	6 (9%)	74,105,113	1.01	5 (6%)
22	CLA	U	206	16	49,53,73	1.39	7 (14%)	58,89,113	0.99	3 (5%)
22	CLA	H	209	18	45,49,73	1.43	7 (15%)	54,84,113	1.22	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	B	829	2	62,66,73	1.27	8 (12%)	73,104,113	1.03	4 (5%)
22	CLA	A	804	1	69,73,73	1.16	7 (10%)	82,113,113	0.91	6 (7%)
27	CL0	A	849	1	58,73,73	0.97	4 (6%)	60,113,113	1.83	10 (16%)
34	A86	Q	201	-	47,50,50	1.32	5 (10%)	51,76,76	1.41	8 (15%)
22	CLA	F	804	6	50,54,73	1.38	7 (14%)	59,90,113	1.06	4 (6%)
32	LMG	J	102	-	39,39,55	0.87	0	47,47,63	1.24	4 (8%)
22	CLA	A	845	35	69,73,73	1.19	7 (10%)	82,113,113	0.87	3 (3%)
22	CLA	A	851	1	69,73,73	1.20	7 (10%)	82,113,113	0.91	3 (3%)
22	CLA	B	815	2	64,68,73	1.23	7 (10%)	76,107,113	0.95	4 (5%)
25	BCR	B	836	-	41,41,41	1.09	2 (4%)	56,56,56	1.18	5 (8%)
22	CLA	B	844	2	69,73,73	1.24	7 (10%)	82,113,113	1.01	4 (4%)
22	CLA	L	203	9	69,73,73	1.15	7 (10%)	82,113,113	0.88	4 (4%)
34	A86	R	103	-	44,46,50	1.50	3 (6%)	49,70,76	1.69	14 (28%)
22	CLA	B	822	2	69,73,73	1.21	6 (8%)	82,113,113	0.92	3 (3%)
22	CLA	Q	208	13	54,58,73	1.33	8 (14%)	64,95,113	1.41	7 (10%)
22	CLA	K	205	19	59,63,73	1.25	7 (11%)	70,101,113	0.98	4 (5%)
31	DD6	S	214	-	40,45,45	1.24	7 (17%)	51,67,67	1.69	10 (19%)
22	CLA	B	818	2	57,61,73	1.26	8 (14%)	67,98,113	0.97	5 (7%)
22	CLA	T	211	-	51,55,73	1.35	7 (13%)	60,91,113	1.16	5 (8%)
25	BCR	k	104	-	41,41,41	1.06	2 (4%)	56,56,56	1.29	6 (10%)
22	CLA	A	831	1	49,53,73	1.38	7 (14%)	58,89,113	1.14	4 (6%)
22	CLA	A	801	-	69,73,73	1.16	8 (11%)	82,113,113	0.86	4 (4%)
22	CLA	T	210	20	50,54,73	1.42	7 (14%)	59,90,113	1.11	5 (8%)
22	CLA	R	101	35	49,53,73	1.43	8 (16%)	58,89,113	1.08	4 (6%)
22	CLA	S	209	15	56,60,73	1.25	4 (7%)	65,97,113	1.04	4 (6%)
22	CLA	H	205	18	47,52,73	1.43	8 (17%)	55,87,113	1.06	3 (5%)
22	CLA	T	202	20	45,49,73	1.41	7 (15%)	54,84,113	1.14	5 (9%)
22	CLA	O	207	11	50,54,73	1.37	7 (14%)	59,90,113	1.11	6 (10%)
22	CLA	S	216	35	69,73,73	1.13	7 (10%)	82,113,113	0.91	4 (4%)
25	BCR	A	842	-	41,41,41	1.08	2 (4%)	56,56,56	1.13	4 (7%)
33	KC1	P	206	12	49,53,53	1.64	11 (22%)	61,89,89	0.80	1 (1%)
31	DD6	P	218	-	40,45,45	1.33	8 (20%)	51,67,67	1.91	11 (21%)
22	CLA	P	208	12	60,64,73	1.27	8 (13%)	71,102,113	0.98	4 (5%)
22	CLA	O	202	11	47,51,73	1.39	6 (12%)	55,86,113	1.14	5 (9%)
32	LMG	U	201	-	32,32,55	0.99	0	40,40,63	1.13	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	DD6	K	208	-	40,45,45	1.37	9 (22%)	51,67,67	1.60	9 (17%)
22	CLA	F	802	35	69,73,73	1.19	8 (11%)	82,113,113	0.98	4 (4%)
34	A86	P	204	-	47,50,50	1.36	5 (10%)	51,76,76	1.45	9 (17%)
22	CLA	B	825	2	54,58,73	1.42	8 (14%)	64,95,113	0.96	4 (6%)
31	DD6	G	214	-	40,45,45	1.33	7 (17%)	51,67,67	1.63	13 (25%)
22	CLA	B	820	35	68,72,73	1.14	6 (8%)	80,111,113	0.92	4 (5%)
22	CLA	P	214	12	49,53,73	1.46	7 (14%)	58,89,113	1.11	4 (6%)
34	A86	Q	218	-	47,50,50	1.40	5 (10%)	51,76,76	1.42	9 (17%)
22	CLA	A	817	1	49,53,73	1.40	7 (14%)	58,89,113	1.13	4 (6%)
22	CLA	A	836	35	69,73,73	1.16	8 (11%)	82,113,113	0.96	4 (4%)
31	DD6	P	205	-	40,45,45	1.26	7 (17%)	51,67,67	1.58	10 (19%)
22	CLA	A	855	-	44,48,73	1.47	8 (18%)	51,82,113	1.33	7 (13%)
22	CLA	A	850	35	69,73,73	1.14	7 (10%)	82,113,113	0.92	4 (4%)
22	CLA	U	208	16	50,54,73	1.36	7 (14%)	59,90,113	1.16	6 (10%)
22	CLA	A	853	1	69,73,73	1.17	7 (10%)	82,113,113	0.90	3 (3%)
22	CLA	G	215	17	49,53,73	1.35	5 (10%)	58,89,113	1.17	4 (6%)
22	CLA	O	209	11	69,73,73	1.19	7 (10%)	82,113,113	1.03	5 (6%)
22	CLA	S	202	35	69,73,73	1.11	5 (7%)	82,113,113	1.08	6 (7%)
22	CLA	A	825	1	69,73,73	1.21	7 (10%)	82,113,113	0.87	4 (4%)
22	CLA	G	203	17	49,53,73	1.45	7 (14%)	58,89,113	1.12	4 (6%)
22	CLA	B	809	2	58,62,73	1.40	9 (15%)	71,100,113	0.94	4 (5%)
22	CLA	O	208	11	64,68,73	1.17	7 (10%)	76,107,113	0.93	4 (5%)
22	CLA	P	209	-	56,60,73	1.29	6 (10%)	65,97,113	0.98	5 (7%)
22	CLA	H	210	18	49,53,73	1.49	7 (14%)	58,89,113	1.08	5 (8%)
22	CLA	G	209	17	60,64,73	1.22	6 (10%)	71,102,113	1.08	6 (8%)
22	CLA	G	207	17	64,68,73	1.15	6 (9%)	76,107,113	1.03	4 (5%)
23	PQN	A	837	-	34,34,34	0.40	0	43,45,45	0.59	1 (2%)
28	SF4	C	102	3	0,12,12	-	-	-	-	-
33	KC1	P	212	12	46,52,53	1.70	9 (19%)	59,87,89	1.18	6 (10%)
22	CLA	B	817	2	50,54,73	1.37	7 (14%)	59,90,113	1.08	4 (6%)
24	LHG	A	839	-	47,47,48	0.65	2 (4%)	50,53,54	1.22	5 (10%)
22	CLA	A	805	1	53,57,73	1.40	7 (13%)	61,93,113	0.99	4 (6%)
26	LMU	A	847	-	36,36,36	1.21	2 (5%)	47,47,47	0.89	1 (2%)
25	BCR	L	201	-	41,41,41	1.09	2 (4%)	56,56,56	1.19	4 (7%)
22	CLA	A	826	1	69,73,73	1.29	8 (11%)	82,113,113	0.81	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	K	207	19	62,66,73	1.21	6 (9%)	73,104,113	1.18	6 (8%)
22	CLA	B	819	35	67,71,73	1.21	7 (10%)	79,110,113	1.00	5 (6%)
22	CLA	B	811	2	58,62,73	1.32	7 (12%)	68,99,113	0.96	4 (5%)
31	DD6	G	212	-	40,45,45	1.31	7 (17%)	51,67,67	1.53	10 (19%)
33	KC1	S	210	15	49,53,53	1.61	9 (18%)	61,89,89	1.09	4 (6%)
25	BCR	B	840	-	41,41,41	1.08	2 (4%)	56,56,56	1.18	5 (8%)
22	CLA	H	204	18	65,69,73	1.16	6 (9%)	77,108,113	0.98	4 (5%)
22	CLA	K	206	19	49,53,73	1.54	8 (16%)	58,89,113	0.98	3 (5%)
22	CLA	B	801	2	69,73,73	1.24	6 (8%)	82,113,113	0.79	3 (3%)
25	BCR	A	841	-	41,41,41	1.02	2 (4%)	56,56,56	1.26	2 (3%)
22	CLA	B	802	-	69,73,73	1.16	7 (10%)	82,113,113	0.97	7 (8%)
22	CLA	L	202	9	53,57,73	1.35	8 (15%)	61,93,113	1.13	6 (9%)
22	CLA	Q	207	13	50,54,73	1.37	8 (16%)	59,90,113	1.19	7 (11%)
25	BCR	I	102	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	4 (7%)
22	CLA	G	201	17	49,53,73	1.38	6 (12%)	58,89,113	1.07	4 (6%)
31	DD6	S	204	-	40,45,45	1.28	7 (17%)	51,67,67	1.51	9 (17%)
31	DD6	G	213	-	40,45,45	1.29	8 (20%)	51,67,67	1.42	7 (13%)
33	KC1	Q	210	13	49,53,53	1.59	9 (18%)	61,89,89	1.12	6 (9%)
31	DD6	P	215	-	40,45,45	1.35	7 (17%)	51,67,67	1.83	11 (21%)
22	CLA	A	846	1	64,68,73	1.31	7 (10%)	76,107,113	0.91	4 (5%)
22	CLA	H	202	-	44,48,73	1.43	6 (13%)	51,82,113	1.44	7 (13%)
31	DD6	T	212	-	40,45,45	1.32	7 (17%)	51,67,67	1.67	9 (17%)
22	CLA	B	831	2	51,55,73	1.39	6 (11%)	60,91,113	1.02	4 (6%)
22	CLA	B	816	35	69,73,73	1.18	7 (10%)	82,113,113	0.90	4 (4%)
26	LMU	F	806	-	36,36,36	1.28	3 (8%)	47,47,47	1.55	8 (17%)
22	CLA	A	802	1	59,63,73	1.24	8 (13%)	70,101,113	0.95	4 (5%)
31	DD6	U	203	-	40,45,45	1.34	7 (17%)	51,67,67	1.74	12 (23%)
22	CLA	A	828	1	69,73,73	1.26	7 (10%)	82,113,113	0.85	3 (3%)
22	CLA	A	832	1	55,59,73	1.35	8 (14%)	64,96,113	1.07	5 (7%)
22	CLA	T	209	20	45,49,73	1.46	7 (15%)	54,84,113	1.18	5 (9%)
22	CLA	R	104	14	69,73,73	1.31	8 (11%)	82,113,113	0.92	5 (6%)
22	CLA	T	207	20	69,73,73	1.11	5 (7%)	82,113,113	0.95	5 (6%)
22	CLA	H	203	18	64,68,73	1.24	8 (12%)	76,107,113	0.97	5 (6%)
22	CLA	O	203	-	49,53,73	1.40	8 (16%)	58,89,113	1.11	4 (6%)
34	A86	R	105	-	47,50,50	1.40	5 (10%)	51,76,76	1.28	8 (15%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	S	217	15	69,73,73	1.16	7 (10%)	82,113,113	1.03	6 (7%)
22	CLA	T	205	-	50,54,73	1.34	6 (12%)	59,90,113	1.14	5 (8%)
32	LMG	S	213	-	49,49,55	0.73	1 (2%)	57,57,63	1.29	6 (10%)
33	KC1	S	212	15	49,53,53	1.56	7 (14%)	61,89,89	1.20	6 (9%)
22	CLA	B	832	35	69,73,73	1.19	8 (11%)	82,113,113	0.95	4 (4%)
22	CLA	B	833	2	69,73,73	1.23	7 (10%)	82,113,113	0.90	4 (4%)
22	CLA	A	815	1	69,73,73	1.21	7 (10%)	82,113,113	0.98	5 (6%)
22	CLA	A	809	1	66,70,73	1.19	7 (10%)	78,109,113	0.88	4 (5%)
22	CLA	T	203	20	50,54,73	1.40	7 (14%)	59,90,113	1.00	3 (5%)
34	A86	U	202	-	47,50,50	1.36	5 (10%)	51,76,76	1.39	7 (13%)
25	BCR	B	837	-	41,41,41	1.04	2 (4%)	56,56,56	1.20	3 (5%)
22	CLA	J	103	8	46,50,73	1.40	7 (15%)	53,85,113	1.03	4 (7%)
31	DD6	Q	202	-	40,45,45	1.31	8 (20%)	51,67,67	1.70	14 (27%)
31	DD6	O	215	-	40,45,45	1.29	7 (17%)	51,67,67	1.60	11 (21%)
22	CLA	U	207	35	69,73,73	1.10	6 (8%)	82,113,113	1.08	8 (9%)
31	DD6	H	212	-	40,45,45	1.31	7 (17%)	51,67,67	1.55	11 (21%)
26	LMU	K	202	-	25,25,36	1.24	3 (12%)	36,36,47	1.82	11 (30%)
24	LHG	P	201	-	48,48,48	0.61	2 (4%)	51,54,54	1.26	5 (9%)
24	LHG	A	840	22	26,26,48	0.88	1 (3%)	29,32,54	1.32	3 (10%)
22	CLA	U	204	35	65,69,73	1.19	7 (10%)	77,108,113	0.96	4 (5%)
22	CLA	A	803	1	69,73,73	1.14	7 (10%)	82,113,113	0.93	4 (4%)
22	CLA	A	813	1	54,58,73	1.40	6 (11%)	64,95,113	1.10	5 (7%)
22	CLA	G	204	17	47,51,73	1.39	7 (14%)	55,86,113	1.08	3 (5%)
31	DD6	S	215	-	40,45,45	1.28	7 (17%)	51,67,67	1.66	10 (19%)
22	CLA	G	206	17	69,73,73	1.31	7 (10%)	82,113,113	0.92	4 (4%)
22	CLA	U	210	16	69,73,73	1.14	6 (8%)	82,113,113	0.92	5 (6%)
22	CLA	A	821	35	69,73,73	1.20	7 (10%)	82,113,113	0.95	4 (4%)
33	KC1	O	210	11	49,53,53	1.60	10 (20%)	61,89,89	1.19	5 (8%)
22	CLA	Q	211	13	45,49,73	1.48	7 (15%)	54,84,113	1.22	5 (9%)
22	CLA	K	204	19	46,50,73	1.42	7 (15%)	53,85,113	1.17	5 (9%)
28	SF4	C	101	3	0,12,12	-	-	-	-	-
31	DD6	Q	215	-	40,45,45	1.27	8 (20%)	51,67,67	1.52	10 (19%)
31	DD6	S	205	-	40,45,45	1.29	8 (20%)	51,67,67	1.49	10 (19%)
22	CLA	K	203	19	49,53,73	1.69	9 (18%)	58,89,113	1.84	12 (20%)
31	DD6	H	211	-	40,45,45	1.29	6 (15%)	51,67,67	1.71	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	B	834	35	69,73,73	1.19	8 (11%)	82,113,113	0.95	6 (7%)
33	KC1	U	213	16	49,53,53	1.65	11 (22%)	61,89,89	0.90	3 (4%)
22	CLA	B	842	2	69,73,73	1.23	9 (13%)	82,113,113	0.92	3 (3%)
25	BCR	A	844	-	41,41,41	1.10	2 (4%)	56,56,56	1.21	6 (10%)
22	CLA	S	208	15	49,53,73	1.31	5 (10%)	58,89,113	1.10	5 (8%)
22	CLA	H	208	-	62,66,73	1.20	6 (9%)	73,104,113	0.96	4 (5%)
22	CLA	T	204	-	61,65,73	1.20	5 (8%)	72,103,113	0.98	4 (5%)
33	KC1	P	203	-	49,53,53	1.70	11 (22%)	61,89,89	0.87	1 (1%)
30	SQD	S	201	-	44,46,54	1.03	4 (9%)	54,57,65	1.51	9 (16%)
22	CLA	B	830	2	69,73,73	1.20	6 (8%)	82,113,113	0.88	4 (4%)
31	DD6	O	212	-	40,45,45	1.34	9 (22%)	51,67,67	1.66	10 (19%)
22	CLA	A	808	1	60,64,73	1.27	8 (13%)	71,102,113	0.93	3 (4%)
31	DD6	S	211	-	40,45,45	1.26	7 (17%)	51,67,67	1.45	7 (13%)
26	LMU	S	203	-	32,32,36	1.35	4 (12%)	43,43,47	1.62	6 (13%)
22	CLA	Q	206	13	54,59,73	1.42	7 (12%)	62,96,113	0.96	3 (4%)
22	CLA	H	206	18	49,53,73	1.48	7 (14%)	58,89,113	0.95	3 (5%)
22	CLA	O	206	35	69,73,73	1.17	7 (10%)	82,113,113	0.92	5 (6%)
22	CLA	A	829	1	69,73,73	1.19	6 (8%)	82,113,113	0.90	4 (4%)
26	LMU	L	206	-	36,36,36	1.18	2 (5%)	47,47,47	1.22	3 (6%)

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
22	CLA	A	807	1	-	3/39/115/115	-
22	CLA	B	828	35	1/1/15/20	1/39/115/115	-
26	LMU	K	201	-	-	9/21/61/61	0/2/2/2
22	CLA	P	213	12	1/1/10/20	2/10/86/115	-
22	CLA	G	208	-	1/1/13/20	2/27/103/115	-
25	BCR	B	838	-	-	3/29/63/63	0/2/2/2
22	CLA	S	206	15	1/1/11/20	0/17/93/115	-
22	CLA	F	803	35	1/1/11/20	3/19/95/115	-
25	BCR	L	205	-	-	8/29/63/63	0/2/2/2
22	CLA	Q	205	13	1/1/14/20	4/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	Q	213	35	1/1/13/20	7/30/106/115	-
22	CLA	A	822	35	1/1/15/20	3/39/115/115	-
22	CLA	B	804	2	1/1/15/20	8/39/115/115	-
25	BCR	J	104	-	-	7/29/63/63	0/2/2/2
22	CLA	U	211	16	1/1/12/20	6/24/100/115	-
22	CLA	A	812	1	1/1/11/20	0/15/91/115	-
31	DD6	J	101	-	-	5/26/80/80	0/3/3/3
22	CLA	O	205	11	1/1/15/20	9/39/115/115	-
31	DD6	O	214	-	-	8/26/80/80	0/3/3/3
25	BCR	F	801	-	-	4/29/63/63	0/2/2/2
22	CLA	G	210	17	1/1/11/20	4/15/91/115	-
22	CLA	A	806	1	1/1/15/20	7/39/115/115	-
22	CLA	B	807	2	1/1/15/20	5/39/115/115	-
22	CLA	B	813	2	-	2/27/103/115	-
22	CLA	H	207	18	-	11/39/115/115	-
23	PQN	B	835	-	-	1/23/43/43	0/2/2/2
22	CLA	A	835	1	1/1/15/20	1/39/115/115	-
31	DD6	O	213	-	-	11/26/80/80	0/3/3/3
34	A86	Q	214	-	-	11/34/90/90	0/3/3/3
24	LHG	G	216	-	-	14/31/31/53	-
22	CLA	A	838	24	1/1/12/20	2/24/100/115	-
25	BCR	B	839	-	-	4/29/63/63	0/2/2/2
25	BCR	I	101	-	-	3/29/63/63	0/2/2/2
26	LMU	O	216	-	-	14/21/61/61	0/2/2/2
22	CLA	O	204	11	-	1/39/115/115	-
22	CLA	A	854	1	1/1/15/20	6/39/115/115	-
22	CLA	k	103	35	1/1/13/20	3/27/103/115	-
22	CLA	A	816	1	1/1/15/20	0/39/115/115	-
22	CLA	B	810	2	-	1/27/103/115	-
22	CLA	A	818	35	1/1/15/20	2/39/115/115	-
22	CLA	B	827	2	-	4/31/107/115	-
31	DD6	U	214	-	-	8/14/37/80	0/1/1/3
32	LMG	P	217	-	-	12/19/39/70	0/1/1/1
22	CLA	B	806	2	-	3/39/115/115	-
22	CLA	Q	204	-	1/1/14/20	5/35/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	P	216	12	1/1/11/20	0/18/94/115	-
22	CLA	k	102	21	1/1/10/20	0/12/88/115	-
22	CLA	B	803	2	1/1/11/20	4/15/91/115	-
31	DD6	H	201	-	-	12/26/80/80	0/3/3/3
22	CLA	U	209	16	-	0/12/88/115	-
31	DD6	P	220	-	-	11/26/80/80	0/3/3/3
22	CLA	B	805	2	1/1/15/20	4/39/115/115	-
22	CLA	B	845	2	1/1/15/20	7/39/115/115	-
22	CLA	A	848	1	-	5/39/115/115	-
32	LMG	P	202	-	-	12/29/49/70	0/1/1/1
33	KC1	T	208	20	-	1/15/71/71	-
26	LMU	M	102	-	-	9/21/61/61	0/2/2/2
22	CLA	P	207	12	1/1/15/20	8/39/115/115	-
26	LMU	P	221	-	-	6/11/51/61	0/2/2/2
22	CLA	T	201	-	1/1/10/20	1/12/88/115	-
22	CLA	O	211	11	-	0/10/86/115	-
22	CLA	Q	216	35	-	7/39/115/115	-
22	CLA	A	830	1	-	1/21/97/115	-
32	LMG	Q	217	-	-	24/50/70/70	0/1/1/1
22	CLA	B	823	2	-	3/39/115/115	-
22	CLA	S	207	15	1/1/11/20	3/17/93/115	-
22	CLA	Q	203	13	-	2/19/95/115	-
25	BCR	F	805	-	-	6/29/63/63	0/2/2/2
22	CLA	A	819	1	-	0/13/89/115	-
22	CLA	B	826	2	1/1/11/20	2/20/96/115	-
22	CLA	L	204	35	1/1/12/20	7/21/97/115	-
22	CLA	B	812	2	-	2/32/108/115	-
22	CLA	B	824	2	-	3/39/115/115	-
26	LMU	A	857	-	-	12/21/61/61	0/2/2/2
22	CLA	A	824	1	1/1/14/20	4/36/112/115	-
31	DD6	U	212	-	-	13/26/80/80	0/3/3/3
22	CLA	A	820	1	1/1/12/20	4/23/99/115	-
30	SQD	B	846	-	-	17/45/65/69	0/1/1/1
22	CLA	G	202	-	1/1/10/20	0/10/86/115	-
22	CLA	A	833	1	1/1/15/20	3/39/115/115	-
22	CLA	Q	212	13	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	M	101	-	-	6/29/63/63	0/2/2/2
31	DD6	O	201	-	-	6/26/80/80	0/3/3/3
28	SF4	A	852	1,2	-	-	0/6/5/5
22	CLA	Q	209	13	-	10/39/115/115	-
25	BCR	R	102	-	-	10/27/61/63	0/2/2/2
22	CLA	A	811	1	1/1/15/20	3/39/115/115	-
22	CLA	H	213	-	1/1/15/20	10/39/115/115	-
22	CLA	B	847	2	1/1/12/20	4/21/97/115	-
22	CLA	G	205	17	-	9/35/111/115	-
22	CLA	T	206	20	-	0/12/88/115	-
22	CLA	A	827	1	-	3/21/97/115	-
22	CLA	A	834	1	-	5/39/115/115	-
22	CLA	P	210	35	-	4/18/94/115	-
22	CLA	A	856	-	1/1/11/20	4/17/93/115	-
29	DGD	B	841	-	-	19/49/89/95	0/2/2/2
31	DD6	T	213	-	-	12/26/80/80	0/3/3/3
22	CLA	B	843	2	1/1/15/20	3/39/115/115	-
31	DD6	G	211	-	-	8/26/80/80	0/3/3/3
22	CLA	A	814	35	-	5/15/91/115	-
22	CLA	P	211	12	-	2/21/97/115	-
31	DD6	k	101	-	-	10/26/80/80	0/3/3/3
22	CLA	B	821	2	1/1/15/20	0/39/115/115	-
22	CLA	U	205	16	-	4/39/115/115	-
22	CLA	A	810	1	1/1/12/20	0/26/102/115	-
22	CLA	A	823	1	1/1/15/20	2/39/115/115	-
33	KC1	P	219	12	-	3/15/71/71	-
22	CLA	B	808	2	1/1/15/20	4/39/115/115	-
25	BCR	A	843	-	-	3/29/63/63	0/2/2/2
26	LMU	F	807	-	-	7/21/61/61	0/2/2/2
22	CLA	H	209	18	1/1/10/20	2/10/86/115	-
22	CLA	U	206	16	1/1/11/20	3/15/91/115	-
22	CLA	B	814	2	-	6/32/108/115	-
22	CLA	B	829	2	1/1/13/20	3/31/107/115	-
22	CLA	A	804	1	1/1/15/20	9/39/115/115	-
27	CL0	A	849	1	-	8/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	A86	Q	201	-	-	13/34/90/90	0/3/3/3
22	CLA	F	804	6	1/1/11/20	3/17/93/115	-
32	LMG	J	102	-	-	27/34/54/70	0/1/1/1
22	CLA	A	845	35	1/1/15/20	6/39/115/115	-
22	CLA	B	815	2	1/1/14/20	2/33/109/115	-
22	CLA	A	851	1	-	4/39/115/115	-
25	BCR	B	836	-	-	8/29/63/63	0/2/2/2
22	CLA	B	844	2	1/1/15/20	2/39/115/115	-
22	CLA	L	203	9	-	0/39/115/115	-
34	A86	R	103	-	-	8/30/84/90	0/3/3/3
22	CLA	B	822	2	1/1/15/20	5/39/115/115	-
22	CLA	Q	208	13	1/1/12/20	1/21/97/115	-
22	CLA	K	205	19	1/1/13/20	4/27/103/115	-
31	DD6	S	214	-	-	16/26/80/80	0/3/3/3
22	CLA	B	818	2	-	1/25/101/115	-
22	CLA	T	211	-	1/1/11/20	4/18/94/115	-
25	BCR	k	104	-	-	8/29/63/63	0/2/2/2
22	CLA	A	831	1	1/1/11/20	2/15/91/115	-
22	CLA	A	801	-	-	3/39/115/115	-
22	CLA	T	210	20	-	4/17/93/115	-
22	CLA	R	101	35	1/1/11/20	0/15/91/115	-
22	CLA	S	209	15	-	3/24/100/115	-
22	CLA	H	205	18	1/1/10/20	2/14/90/115	-
22	CLA	T	202	20	1/1/10/20	1/10/86/115	-
22	CLA	O	207	11	1/1/11/20	4/17/93/115	-
22	CLA	S	216	35	1/1/15/20	0/39/115/115	-
25	BCR	A	842	-	-	8/29/63/63	0/2/2/2
33	KC1	P	206	12	-	2/15/71/71	-
31	DD6	P	218	-	-	11/26/80/80	0/3/3/3
22	CLA	P	208	12	1/1/13/20	5/29/105/115	-
22	CLA	O	202	11	-	1/13/89/115	-
32	LMG	U	201	-	-	14/27/47/70	0/1/1/1
31	DD6	K	208	-	-	10/26/80/80	0/3/3/3
22	CLA	F	802	35	1/1/15/20	0/39/115/115	-
34	A86	P	204	-	-	9/34/90/90	0/3/3/3
22	CLA	B	825	2	-	0/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DD6	G	214	-	-	10/26/80/80	0/3/3/3
22	CLA	B	820	35	1/1/14/20	2/38/114/115	-
22	CLA	P	214	12	1/1/11/20	2/15/91/115	-
34	A86	Q	218	-	-	13/34/90/90	0/3/3/3
22	CLA	A	817	1	1/1/11/20	0/15/91/115	-
22	CLA	A	836	35	1/1/15/20	5/39/115/115	-
31	DD6	P	205	-	-	4/26/80/80	0/3/3/3
22	CLA	A	855	-	1/1/9/20	1/10/82/115	-
22	CLA	A	850	35	1/1/15/20	2/39/115/115	-
22	CLA	U	208	16	1/1/11/20	4/17/93/115	-
22	CLA	A	853	1	1/1/15/20	9/39/115/115	-
22	CLA	G	215	17	1/1/11/20	3/15/91/115	-
22	CLA	G	203	17	1/1/11/20	4/15/91/115	-
22	CLA	S	202	35	1/1/15/20	4/39/115/115	-
22	CLA	A	825	1	1/1/15/20	6/39/115/115	-
22	CLA	O	209	11	-	8/39/115/115	-
22	CLA	P	209	-	1/1/12/20	1/24/100/115	-
22	CLA	O	208	11	1/1/14/20	2/33/109/115	-
22	CLA	B	809	2	-	2/25/101/115	-
22	CLA	H	210	18	-	4/15/91/115	-
22	CLA	G	209	17	1/1/13/20	4/29/105/115	-
22	CLA	G	207	17	-	5/33/109/115	-
23	PQN	A	837	-	-	3/23/43/43	0/2/2/2
33	KC1	P	212	12	-	4/12/68/71	-
28	SF4	C	102	3	-	-	0/6/5/5
22	CLA	B	817	2	-	1/17/93/115	-
24	LHG	A	839	-	-	15/52/52/53	-
22	CLA	A	805	1	1/1/11/20	3/20/96/115	-
26	LMU	A	847	-	-	10/21/61/61	0/2/2/2
25	BCR	L	201	-	-	10/29/63/63	0/2/2/2
22	CLA	A	826	1	-	3/39/115/115	-
22	CLA	K	207	19	-	7/31/107/115	-
22	CLA	B	819	35	1/1/14/20	4/37/113/115	-
22	CLA	B	811	2	1/1/12/20	2/26/102/115	-
31	DD6	G	212	-	-	5/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	KC1	S	210	15	-	1/15/71/71	-
25	BCR	B	840	-	-	8/29/63/63	0/2/2/2
22	CLA	H	204	18	1/1/14/20	3/35/111/115	-
22	CLA	K	206	19	1/1/11/20	4/15/91/115	-
22	CLA	B	801	2	1/1/15/20	3/39/115/115	-
25	BCR	A	841	-	-	7/29/63/63	0/2/2/2
22	CLA	B	802	-	1/1/15/20	4/39/115/115	-
22	CLA	Q	207	13	1/1/11/20	5/17/93/115	-
22	CLA	L	202	9	-	6/20/96/115	-
25	BCR	I	102	-	-	10/29/63/63	0/2/2/2
22	CLA	G	201	17	-	2/15/91/115	-
31	DD6	S	204	-	-	7/26/80/80	0/3/3/3
31	DD6	G	213	-	-	9/26/80/80	0/3/3/3
33	KC1	Q	210	13	-	2/15/71/71	-
31	DD6	P	215	-	-	12/26/80/80	0/3/3/3
22	CLA	A	846	1	-	2/33/109/115	-
22	CLA	H	202	-	1/1/9/20	0/10/82/115	-
31	DD6	T	212	-	-	9/26/80/80	0/3/3/3
22	CLA	B	831	2	1/1/11/20	0/18/94/115	-
22	CLA	B	816	35	1/1/15/20	6/39/115/115	-
26	LMU	F	806	-	-	15/21/61/61	0/2/2/2
22	CLA	A	802	1	1/1/13/20	3/27/103/115	-
31	DD6	U	203	-	-	12/26/80/80	0/3/3/3
22	CLA	A	828	1	1/1/15/20	3/39/115/115	-
22	CLA	A	832	1	1/1/12/20	1/23/99/115	-
22	CLA	T	209	20	-	0/10/86/115	-
22	CLA	R	104	14	-	6/39/115/115	-
22	CLA	T	207	20	-	5/39/115/115	-
22	CLA	H	203	18	1/1/14/20	9/33/109/115	-
22	CLA	O	203	-	-	0/15/91/115	-
34	A86	R	105	-	-	11/34/90/90	0/3/3/3
22	CLA	S	217	15	1/1/15/20	2/39/115/115	-
22	CLA	T	205	-	1/1/11/20	2/17/93/115	-
32	LMG	S	213	-	-	22/44/64/70	0/1/1/1
33	KC1	S	212	15	-	5/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	832	35	1/1/15/20	3/39/115/115	-
22	CLA	B	833	2	-	4/39/115/115	-
22	CLA	A	815	1	1/1/15/20	7/39/115/115	-
22	CLA	A	809	1	1/1/14/20	2/36/112/115	-
22	CLA	T	203	20	1/1/11/20	5/17/93/115	-
34	A86	U	202	-	-	17/34/90/90	0/3/3/3
25	BCR	B	837	-	-	8/29/63/63	0/2/2/2
22	CLA	J	103	8	1/1/10/20	2/12/88/115	-
31	DD6	Q	202	-	-	5/26/80/80	0/3/3/3
31	DD6	O	215	-	-	15/26/80/80	0/3/3/3
22	CLA	U	207	35	1/1/15/20	3/39/115/115	-
31	DD6	H	212	-	-	10/26/80/80	0/3/3/3
26	LMU	K	202	-	-	4/10/50/61	0/2/2/2
24	LHG	P	201	-	-	38/53/53/53	-
24	LHG	A	840	22	-	12/31/31/53	-
22	CLA	U	204	35	1/1/14/20	7/35/111/115	-
22	CLA	A	803	1	1/1/15/20	4/39/115/115	-
22	CLA	A	813	1	-	0/21/97/115	-
22	CLA	G	204	17	-	4/13/89/115	-
31	DD6	S	215	-	-	13/26/80/80	0/3/3/3
22	CLA	G	206	17	1/1/15/20	15/39/115/115	-
22	CLA	U	210	16	-	3/39/115/115	-
22	CLA	A	821	35	1/1/15/20	8/39/115/115	-
33	KC1	O	210	11	-	0/15/71/71	-
22	CLA	Q	211	13	1/1/10/20	2/10/86/115	-
22	CLA	K	204	19	-	0/12/88/115	-
31	DD6	Q	215	-	-	9/26/80/80	0/3/3/3
31	DD6	H	211	-	-	13/26/80/80	0/3/3/3
31	DD6	S	205	-	-	10/26/80/80	0/3/3/3
22	CLA	K	203	19	1/1/11/20	2/15/91/115	-
28	SF4	C	101	3	-	-	0/6/5/5
22	CLA	B	834	35	1/1/15/20	1/39/115/115	-
33	KC1	U	213	16	-	0/15/71/71	-
22	CLA	B	842	2	1/1/15/20	4/39/115/115	-
25	BCR	A	844	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	S	208	15	1/1/11/20	0/15/91/115	-
22	CLA	H	208	-	1/1/13/20	5/31/107/115	-
22	CLA	T	204	-	1/1/13/20	10/30/106/115	-
33	KC1	P	203	-	-	1/15/71/71	-
30	SQD	S	201	-	-	21/41/61/69	0/1/1/1
22	CLA	B	830	2	1/1/15/20	1/39/115/115	-
31	DD6	O	212	-	-	10/26/80/80	0/3/3/3
22	CLA	A	808	1	-	2/29/105/115	-
31	DD6	S	211	-	-	13/26/80/80	0/3/3/3
26	LMU	S	203	-	-	10/17/57/61	0/2/2/2
22	CLA	Q	206	13	1/1/12/20	3/22/98/115	-
22	CLA	H	206	18	1/1/11/20	2/15/91/115	-
22	CLA	O	206	35	1/1/15/20	5/39/115/115	-
22	CLA	A	829	1	1/1/15/20	3/39/115/115	-
26	LMU	L	206	-	-	7/21/61/61	0/2/2/2

The worst 5 of 1680 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	R	103	A86	C13-C11	-6.84	1.36	1.49
34	R	105	A86	C13-C11	-6.74	1.36	1.49
34	Q	218	A86	C13-C11	-6.70	1.37	1.49
34	Q	214	A86	C13-C11	-6.52	1.37	1.49
22	K	203	CLA	MG-NA	6.36	2.21	2.06

The worst 5 of 1406 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	849	CL0	C1B-CHB-C4A	9.33	127.33	121.32
31	T	213	DD6	C10-C9-C8	6.72	142.68	123.20
22	Q	208	CLA	C1-O2A-CGA	6.47	132.31	116.65
22	K	203	CLA	CAA-C2A-C3A	-6.14	96.40	113.00
31	P	218	DD6	C10-C9-C8	5.49	139.10	123.20

5 of 119 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	802	CLA	ND
22	A	803	CLA	ND

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Mol	Chain	Res	Type	Atom
22	A	804	CLA	ND
22	A	805	CLA	ND
22	A	806	CLA	ND

5 of 1495 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	803	CLA	CAD-CBD-CGD-O2D
22	A	804	CLA	C1A-C2A-CAA-CBA
22	A	804	CLA	C3A-C2A-CAA-CBA
22	A	806	CLA	CBA-CGA-O2A-C1
22	A	806	CLA	O1A-CGA-O2A-C1

There are no ring outliers.

190 monomers are involved in 325 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	807	CLA	2	0
22	B	828	CLA	4	0
26	K	201	LMU	2	0
22	P	213	CLA	1	0
22	G	208	CLA	1	0
25	B	838	BCR	2	0
22	S	206	CLA	3	0
25	L	205	BCR	1	0
22	Q	213	CLA	1	0
22	A	822	CLA	1	0
22	B	804	CLA	2	0
25	J	104	BCR	1	0
22	U	211	CLA	4	0
22	O	205	CLA	4	0
25	F	801	BCR	1	0
22	B	807	CLA	2	0
22	H	207	CLA	2	0
23	B	835	PQN	1	0
22	A	835	CLA	4	0
24	G	216	LHG	1	0
22	A	838	CLA	1	0
25	B	839	BCR	4	0
25	I	101	BCR	3	0
22	B	827	CLA	1	0
22	A	854	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	816	CLA	6	0
22	B	810	CLA	1	0
22	k	103	CLA	2	0
32	P	217	LMG	3	0
22	B	806	CLA	4	0
22	Q	204	CLA	2	0
22	k	102	CLA	2	0
22	B	803	CLA	1	0
22	U	209	CLA	2	0
22	A	848	CLA	3	0
22	B	805	CLA	3	0
22	B	845	CLA	6	0
32	P	202	LMG	1	0
33	T	208	KC1	1	0
26	M	102	LMU	1	0
22	P	207	CLA	2	0
22	T	201	CLA	1	0
22	Q	216	CLA	1	0
32	Q	217	LMG	3	0
22	B	823	CLA	3	0
22	Q	203	CLA	1	0
25	F	805	BCR	3	0
22	B	826	CLA	5	0
22	L	204	CLA	1	0
22	B	812	CLA	2	0
22	B	824	CLA	3	0
22	A	824	CLA	4	0
31	U	212	DD6	1	0
22	A	820	CLA	1	0
30	B	846	SQD	1	0
22	G	202	CLA	1	0
22	A	833	CLA	2	0
22	Q	212	CLA	1	0
25	M	101	BCR	1	0
25	R	102	BCR	3	0
22	A	811	CLA	2	0
22	G	205	CLA	4	0
22	B	847	CLA	3	0
22	H	213	CLA	7	0
22	T	206	CLA	2	0
22	P	210	CLA	2	0
29	B	841	DGD	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	G	211	DD6	1	0
22	A	814	CLA	2	0
22	P	211	CLA	1	0
22	B	821	CLA	2	0
22	U	205	CLA	2	0
22	A	810	CLA	3	0
22	A	823	CLA	1	0
22	B	808	CLA	1	0
25	A	843	BCR	2	0
22	B	814	CLA	3	0
22	U	206	CLA	1	0
22	H	209	CLA	1	0
22	B	829	CLA	2	0
27	A	849	CL0	3	0
22	F	804	CLA	2	0
32	J	102	LMG	3	0
22	A	845	CLA	3	0
22	A	851	CLA	2	0
22	B	815	CLA	2	0
25	B	836	BCR	2	0
22	B	844	CLA	2	0
22	L	203	CLA	1	0
34	R	103	A86	1	0
22	B	822	CLA	1	0
22	Q	208	CLA	2	0
22	K	205	CLA	1	0
22	B	818	CLA	4	0
22	T	211	CLA	1	0
25	k	104	BCR	2	0
22	A	831	CLA	3	0
22	A	801	CLA	4	0
22	T	210	CLA	7	0
22	R	101	CLA	1	0
22	S	209	CLA	1	0
22	H	205	CLA	1	0
22	O	207	CLA	1	0
22	S	216	CLA	3	0
25	A	842	BCR	1	0
22	P	208	CLA	1	0
22	O	202	CLA	2	0
32	U	201	LMG	1	0
22	F	802	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	G	214	DD6	2	0
22	B	820	CLA	3	0
22	P	214	CLA	1	0
22	A	817	CLA	2	0
22	A	836	CLA	4	0
22	A	855	CLA	1	0
22	A	850	CLA	2	0
22	U	208	CLA	2	0
22	A	853	CLA	3	0
22	G	215	CLA	1	0
22	O	209	CLA	4	0
22	S	202	CLA	2	0
22	A	825	CLA	2	0
22	G	203	CLA	1	0
22	B	809	CLA	2	0
22	O	208	CLA	1	0
22	H	210	CLA	1	0
22	G	209	CLA	6	0
22	G	207	CLA	1	0
23	A	837	PQN	2	0
28	C	102	SF4	1	0
22	B	817	CLA	2	0
24	A	839	LHG	2	0
22	A	805	CLA	1	0
26	A	847	LMU	1	0
25	L	201	BCR	1	0
22	A	826	CLA	3	0
22	K	207	CLA	3	0
22	B	819	CLA	2	0
25	B	840	BCR	2	0
22	K	206	CLA	1	0
22	B	801	CLA	2	0
25	A	841	BCR	1	0
22	B	802	CLA	4	0
22	L	202	CLA	2	0
25	I	102	BCR	2	0
22	G	201	CLA	1	0
22	A	846	CLA	2	0
22	H	202	CLA	1	0
22	B	831	CLA	1	0
22	B	816	CLA	3	0
26	F	806	LMU	1	0

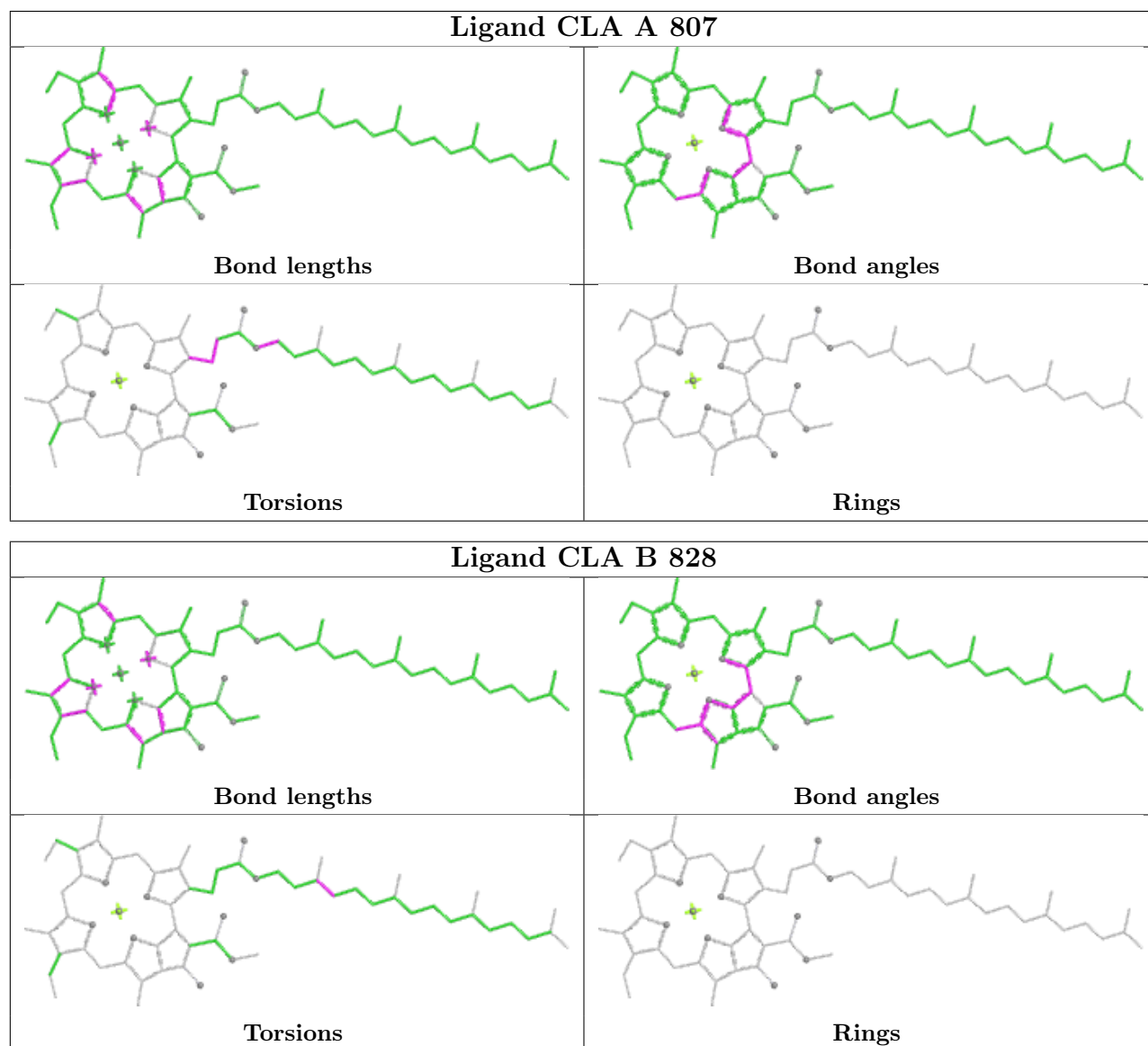
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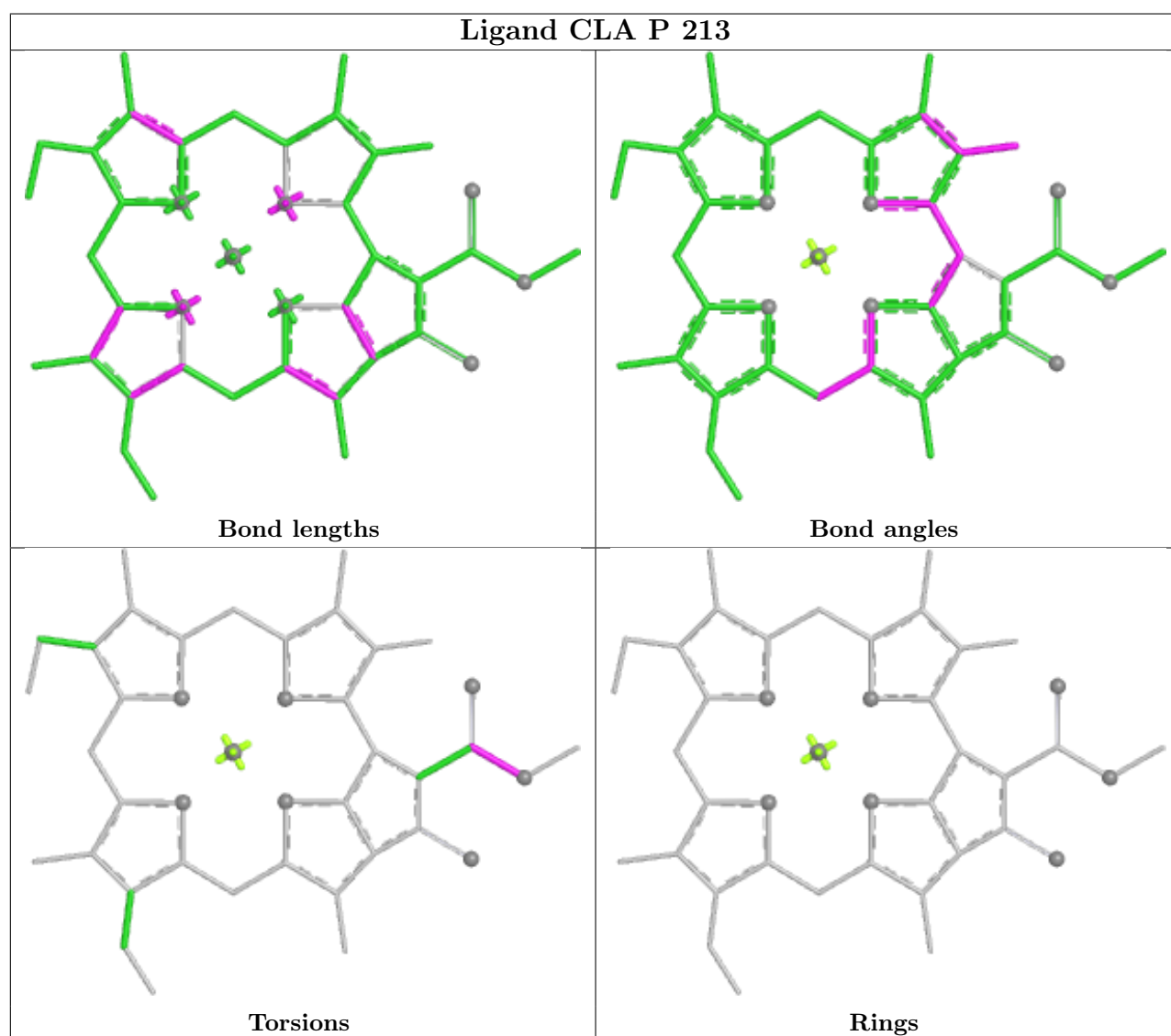
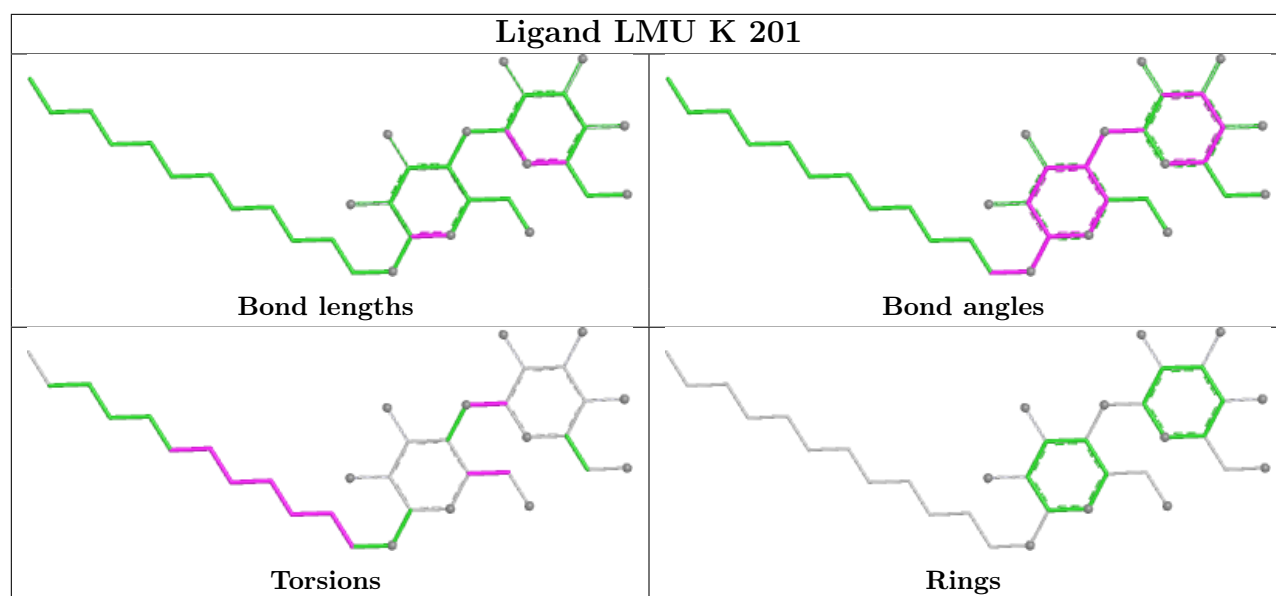
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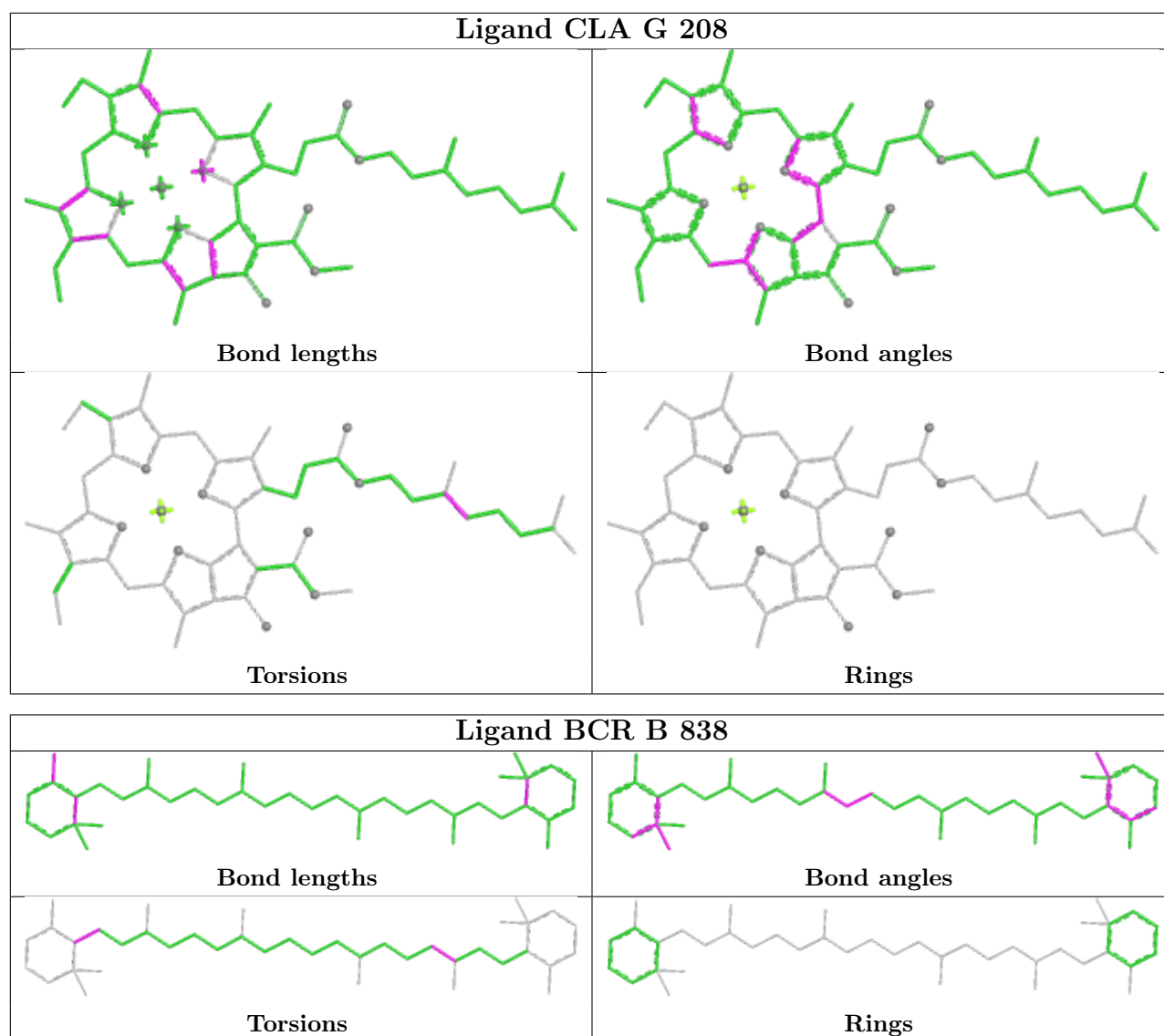
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	802	CLA	1	0
22	A	828	CLA	1	0
22	T	209	CLA	1	0
22	R	104	CLA	4	0
22	T	207	CLA	2	0
22	H	203	CLA	1	0
22	O	203	CLA	1	0
22	S	217	CLA	2	0
22	T	205	CLA	1	0
32	S	213	LMG	2	0
22	B	832	CLA	2	0
22	B	833	CLA	2	0
22	A	815	CLA	1	0
25	B	837	BCR	4	0
22	J	103	CLA	1	0
22	U	207	CLA	2	0
24	P	201	LHG	4	0
24	A	840	LHG	1	0
22	U	204	CLA	1	0
22	A	803	CLA	2	0
22	A	813	CLA	1	0
22	G	204	CLA	1	0
22	G	206	CLA	5	0
22	U	210	CLA	3	0
22	K	204	CLA	2	0
22	K	203	CLA	1	0
22	B	834	CLA	7	0
22	B	842	CLA	2	0
25	A	844	BCR	1	0
22	S	208	CLA	2	0
22	T	204	CLA	7	0
30	S	201	SQD	1	0
22	B	830	CLA	4	0
31	O	212	DD6	2	0
22	A	808	CLA	2	0
26	S	203	LMU	1	0
22	H	206	CLA	1	0
22	A	829	CLA	1	0
26	L	206	LMU	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

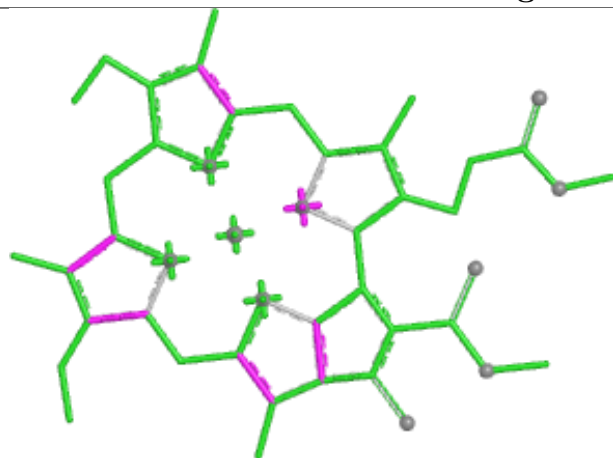




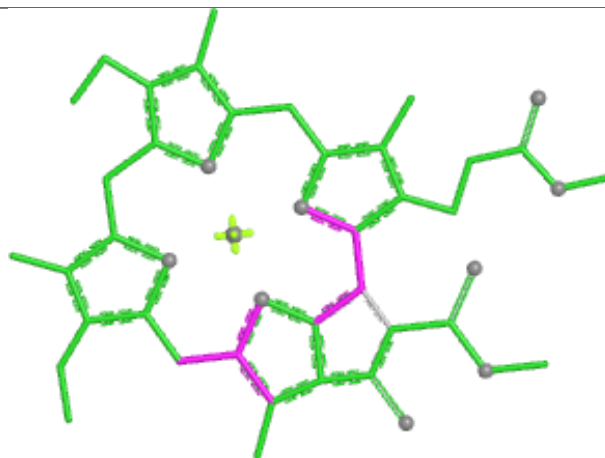




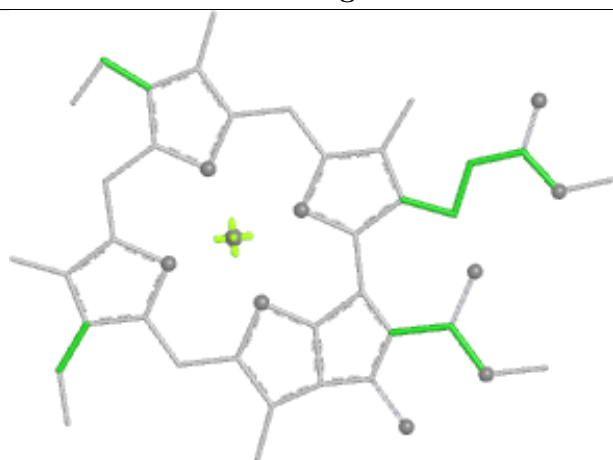
## Ligand CLA S 206



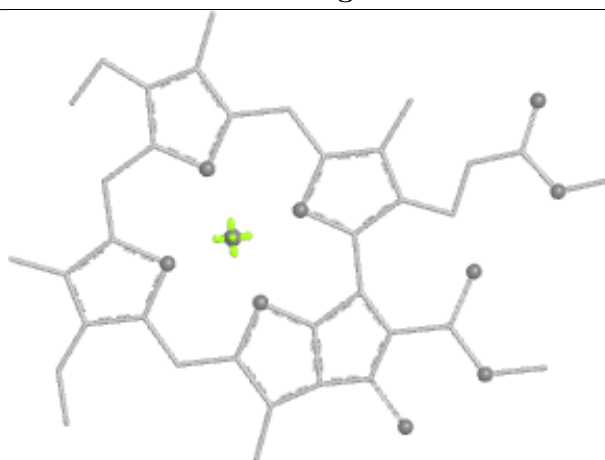
Bond lengths



Bond angles

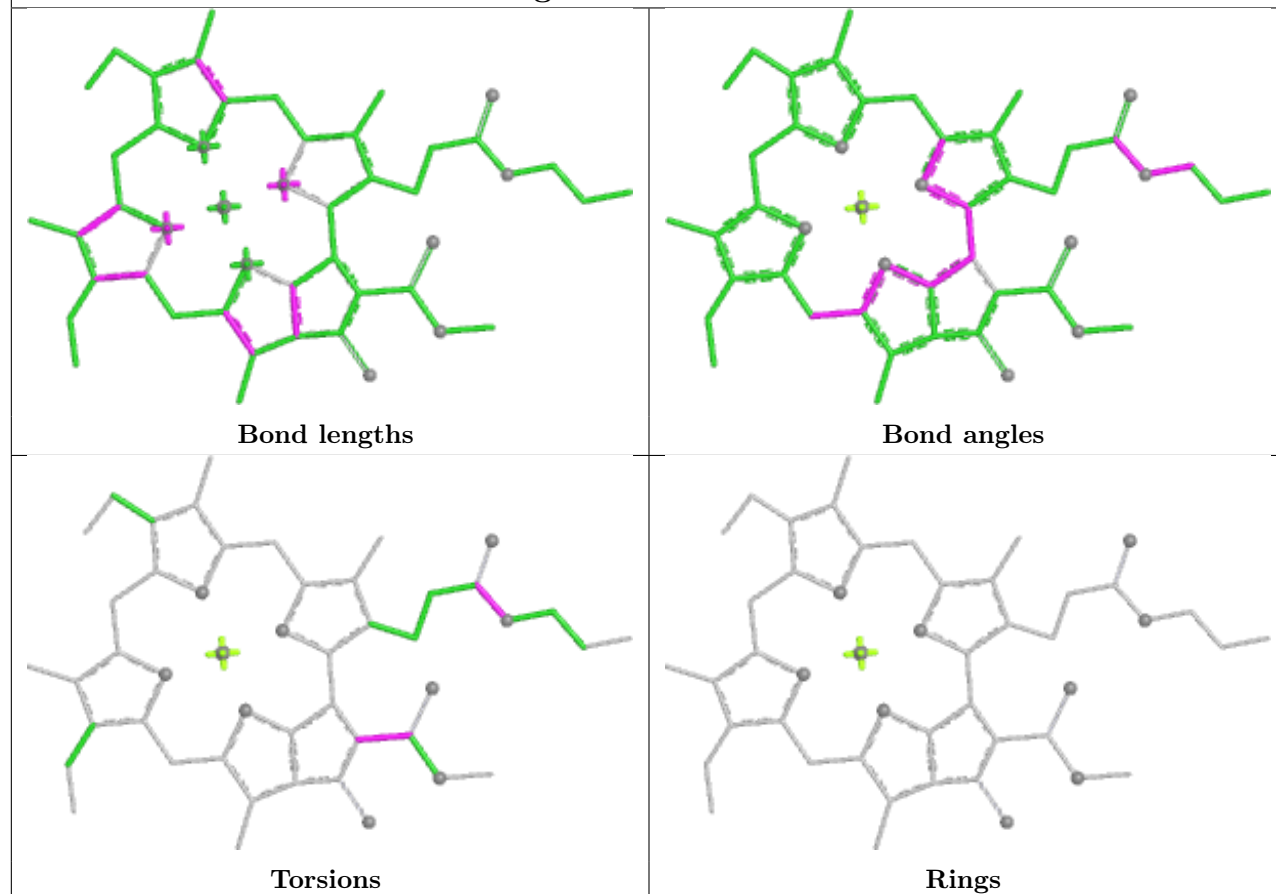


Torsions

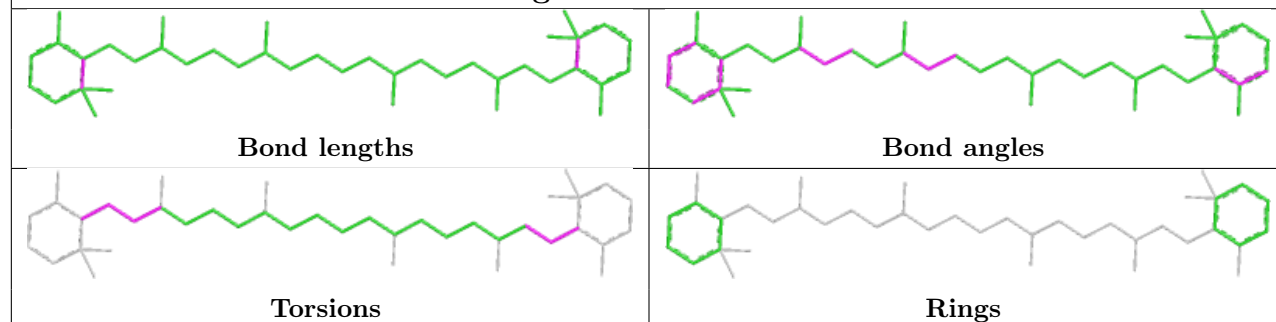


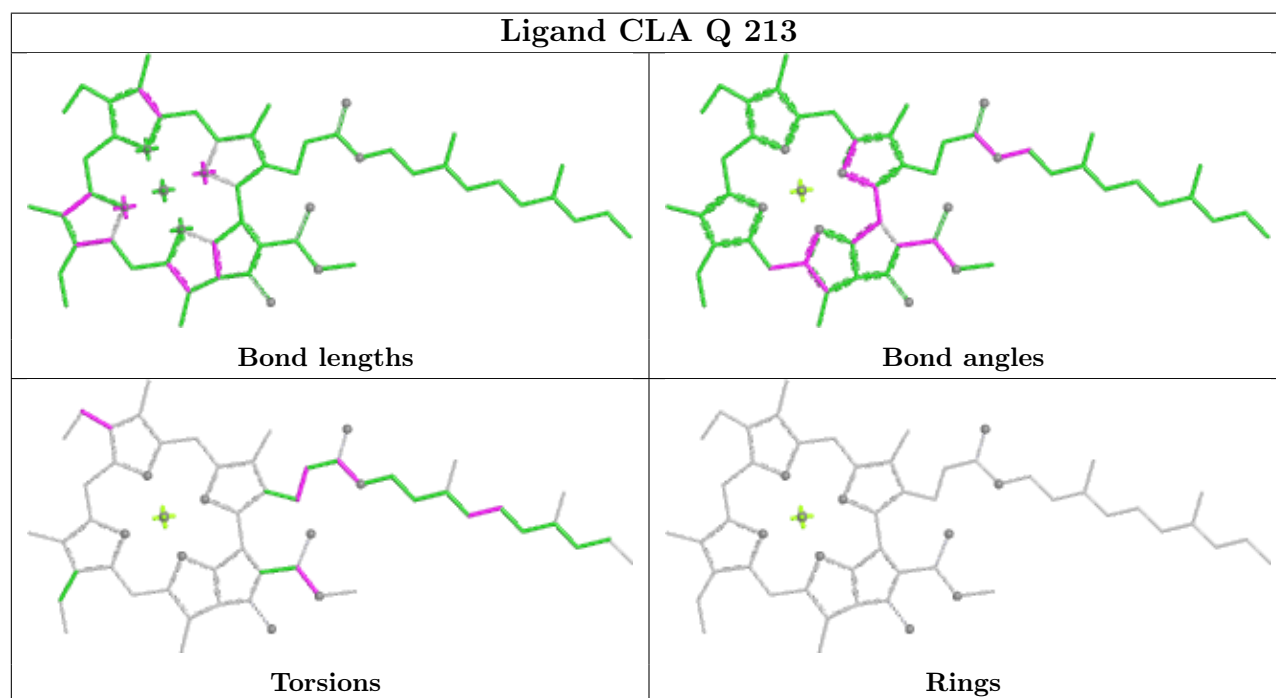
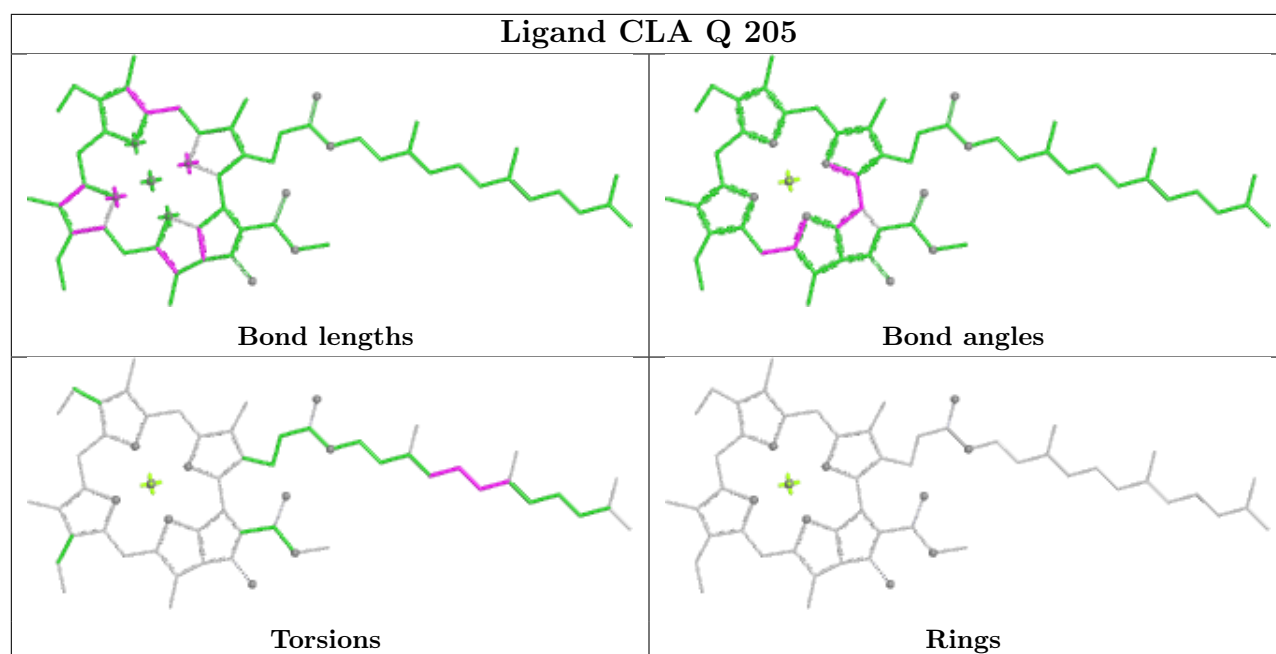
Rings

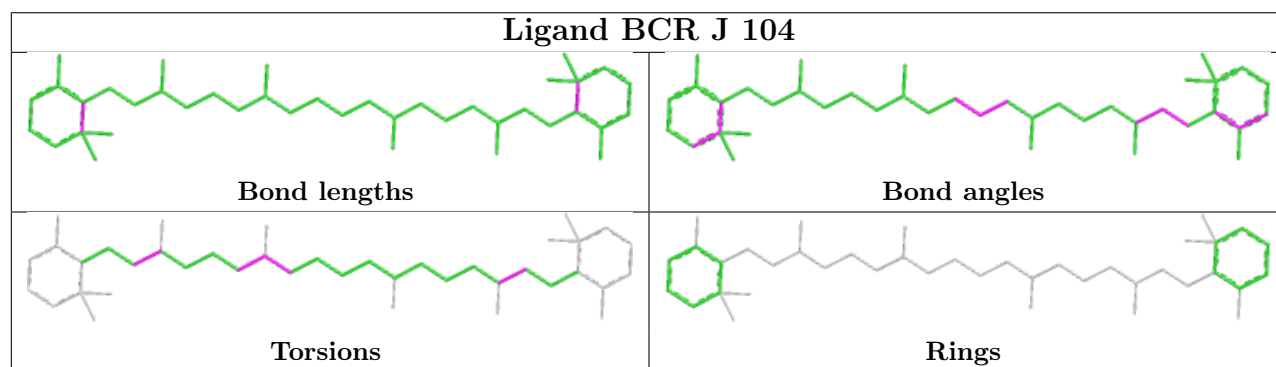
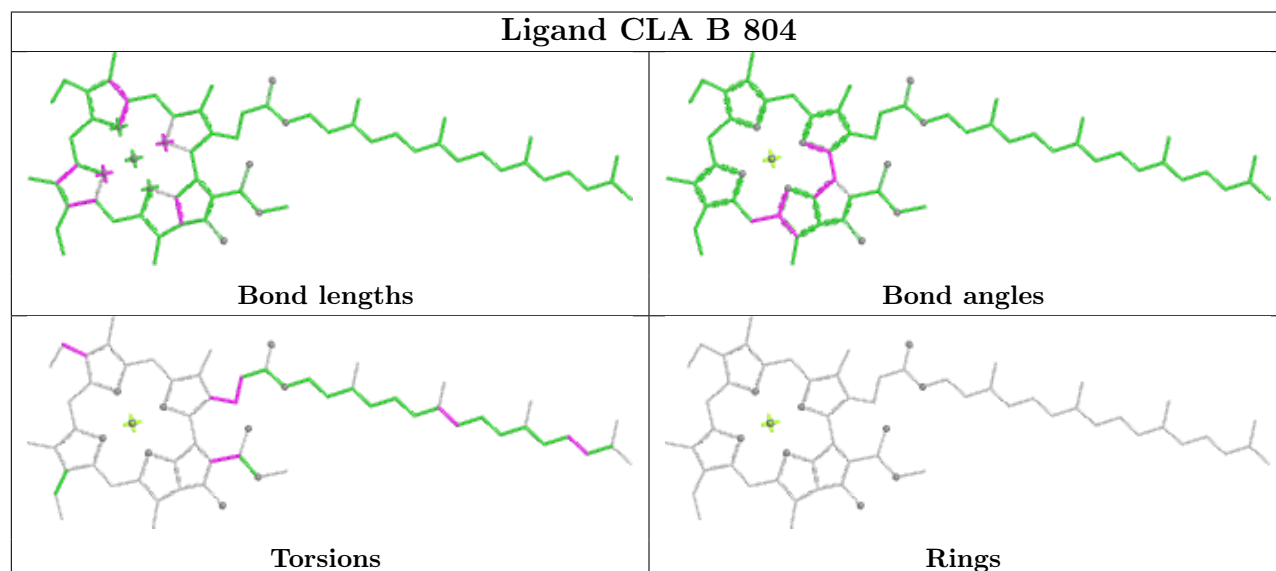
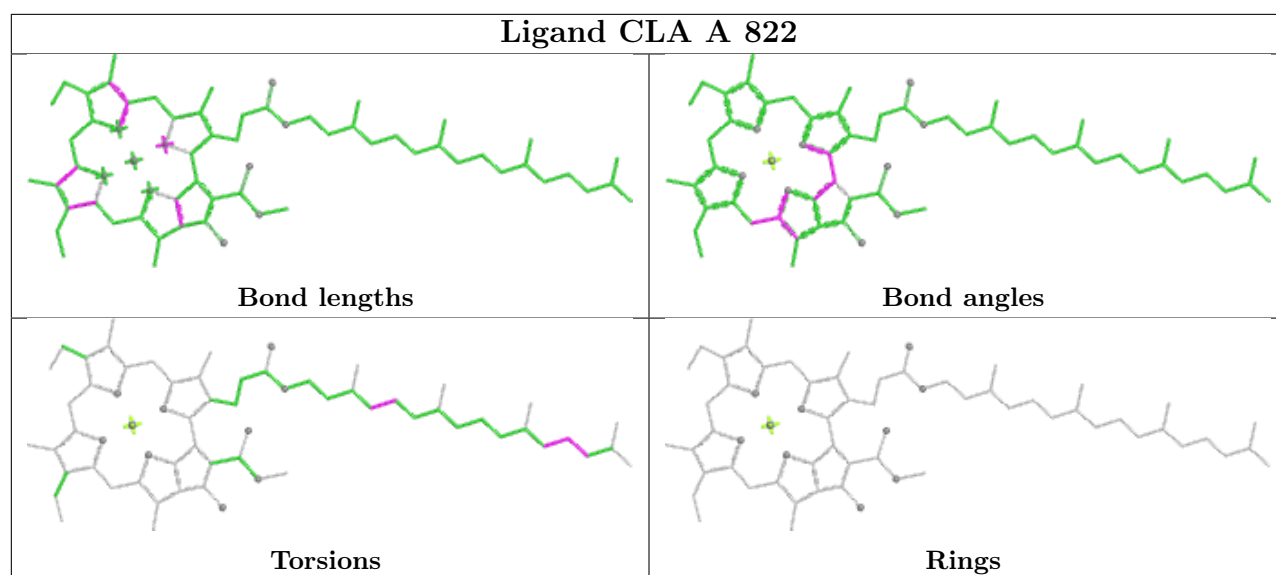
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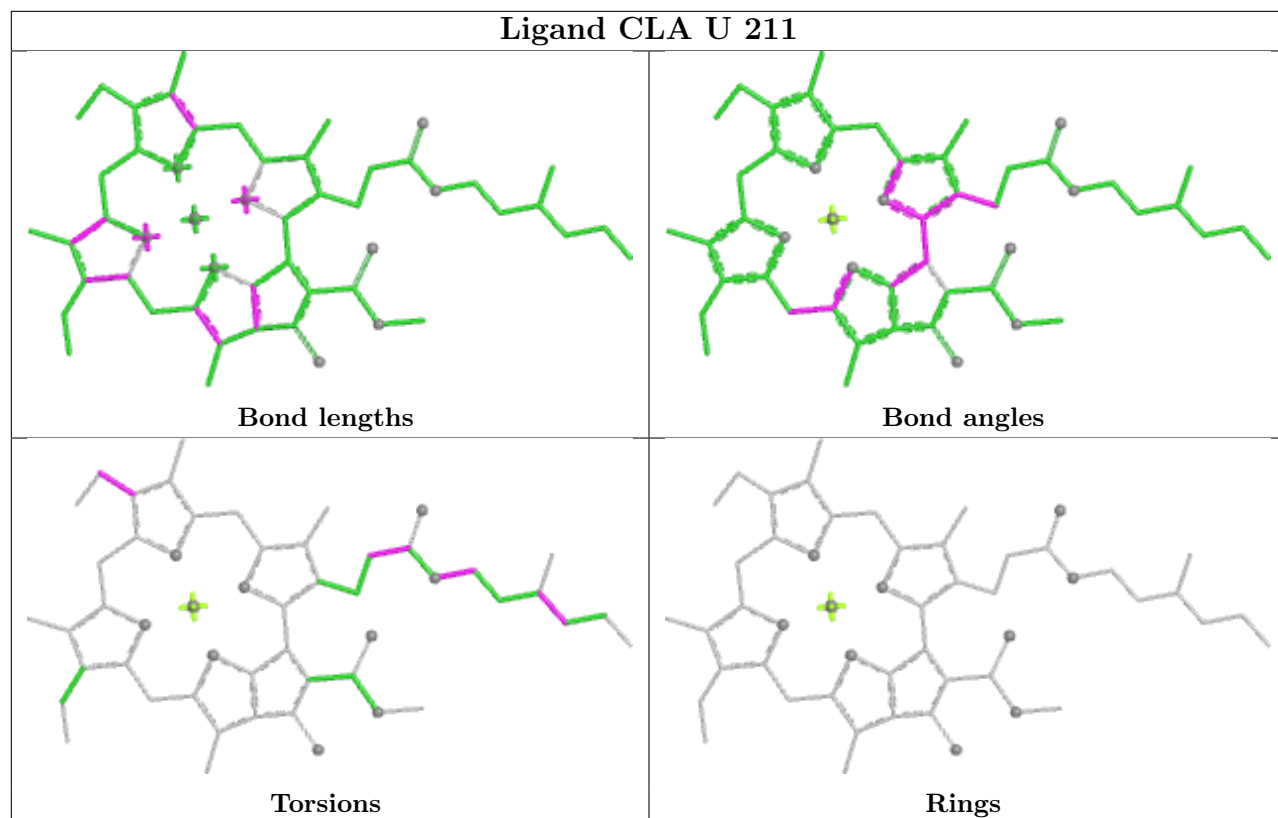


## Ligand BCR L 205

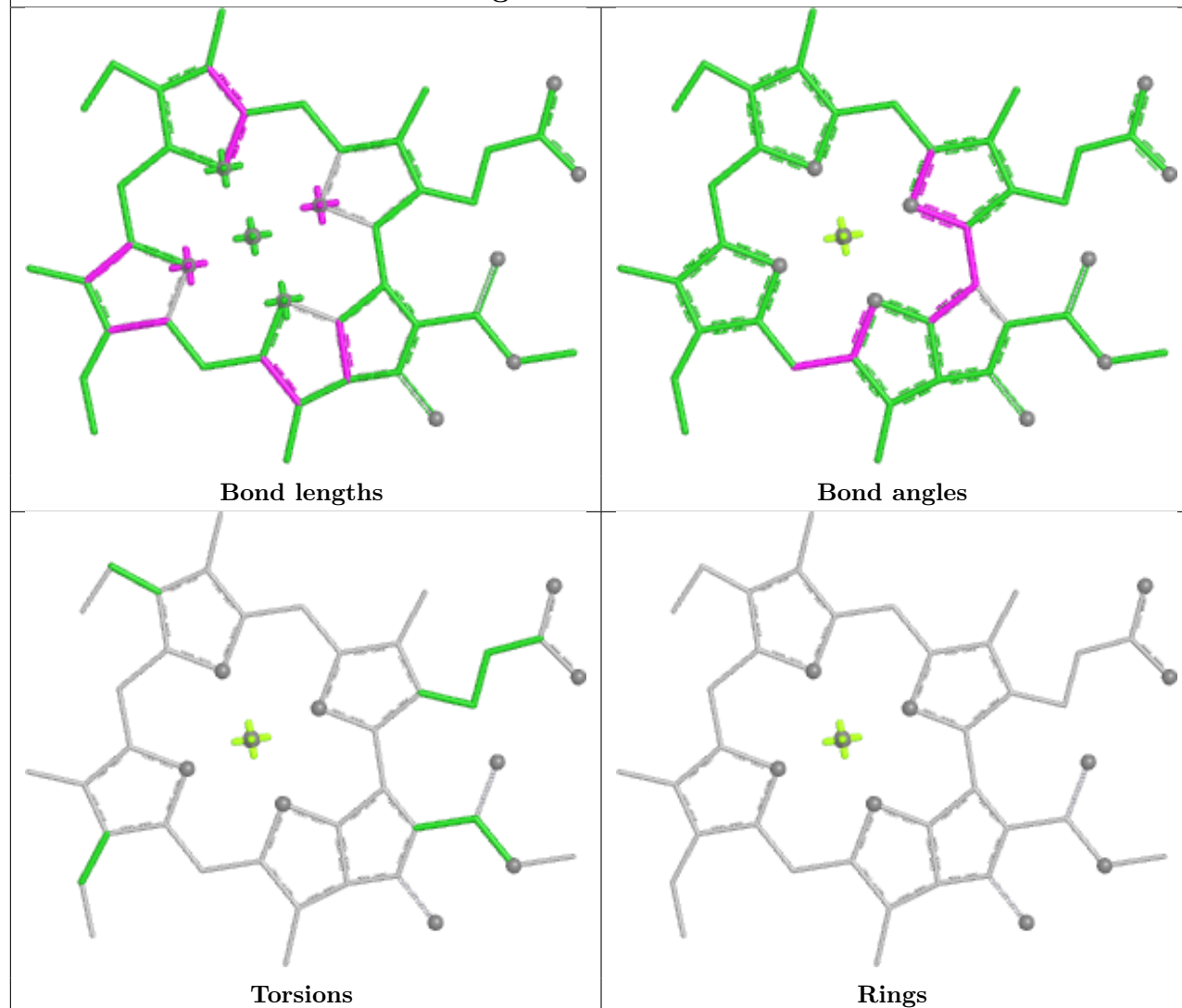




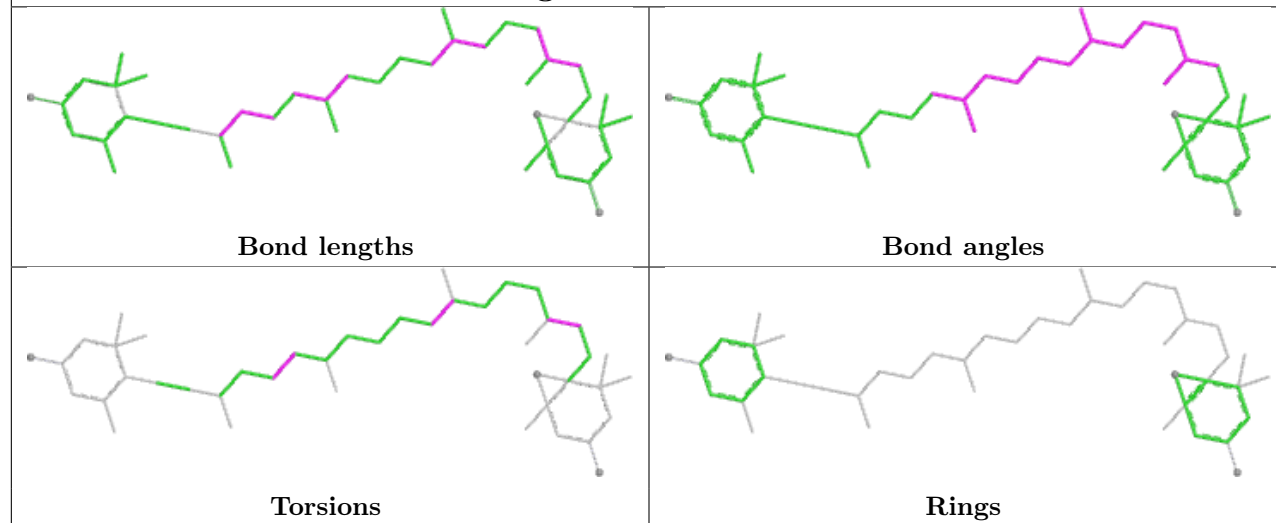


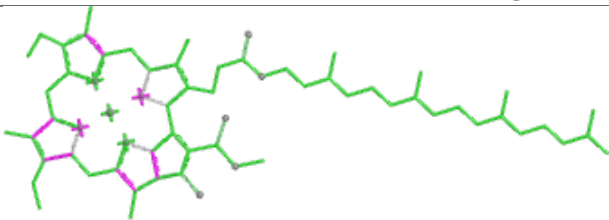
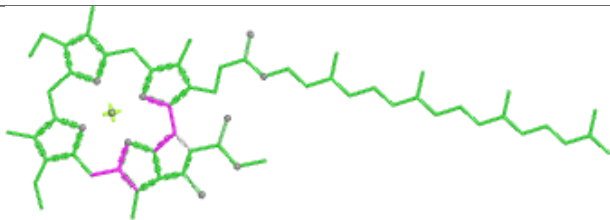
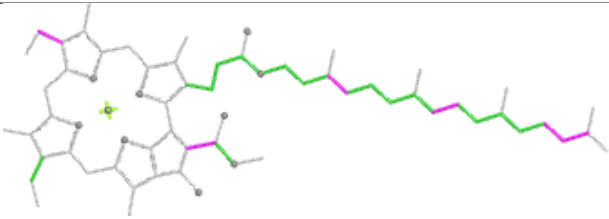
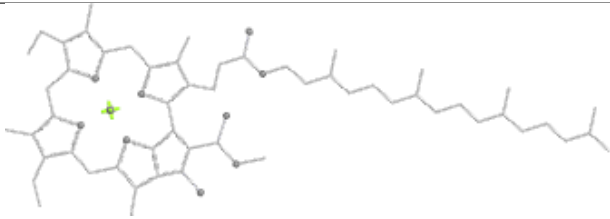


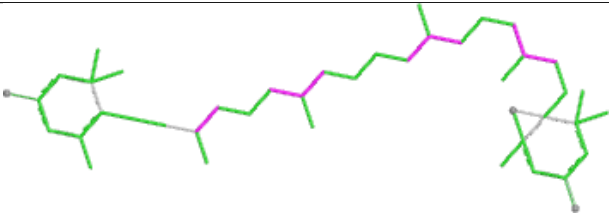
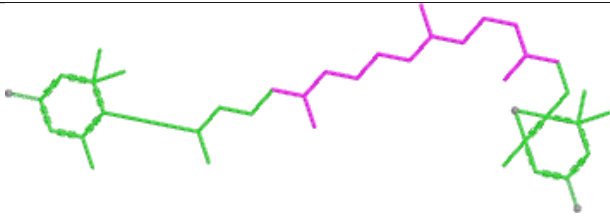
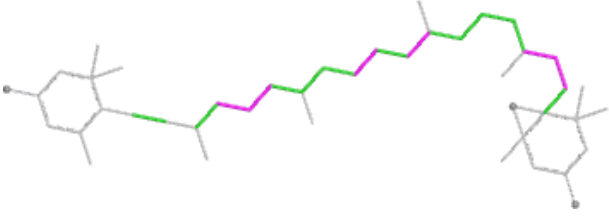
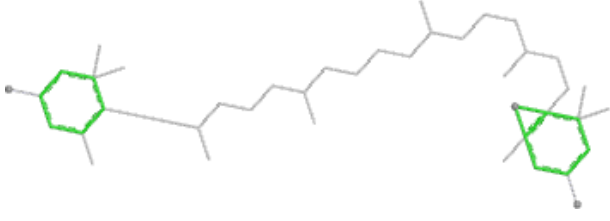
## Ligand CLA A 812

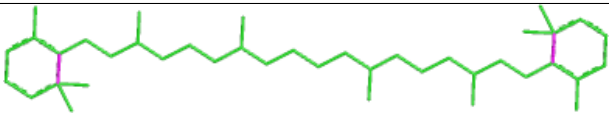
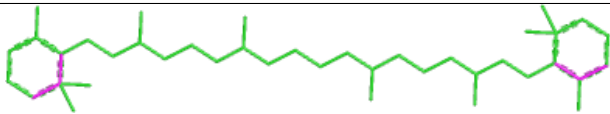
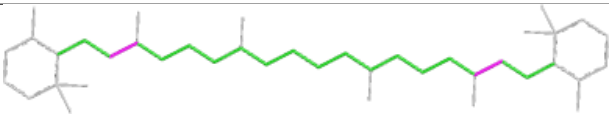
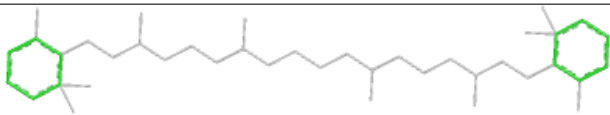


## Ligand DD6 J 101

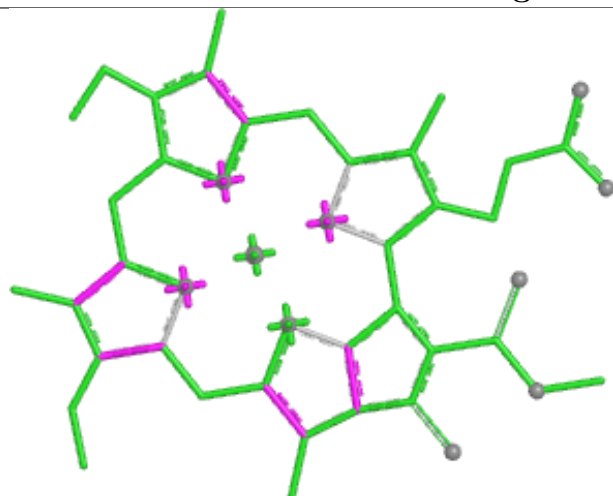


Ligand CLA O 205	
	
Bond lengths	Bond angles
	
Torsions	Rings

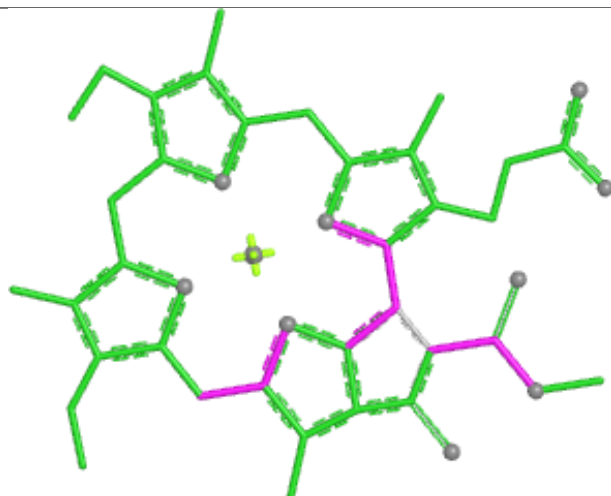
Ligand DD6 O 214	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR F 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

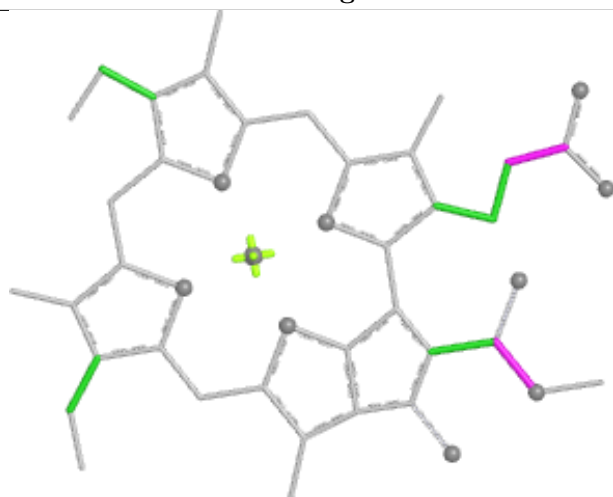
## Ligand CLA G 210



Bond lengths



Bond angles

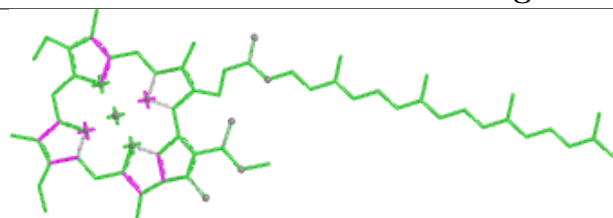


Torsions

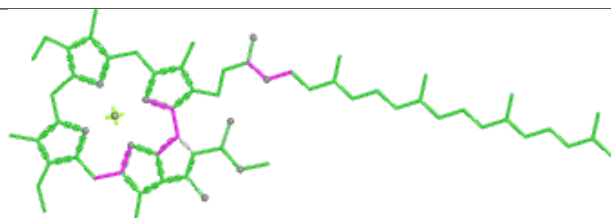


Rings

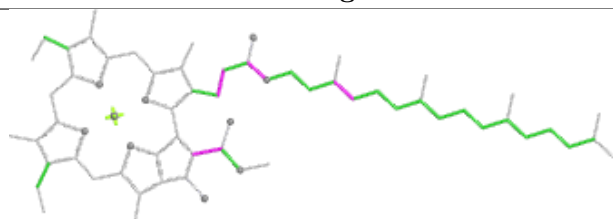
## Ligand CLA A 806



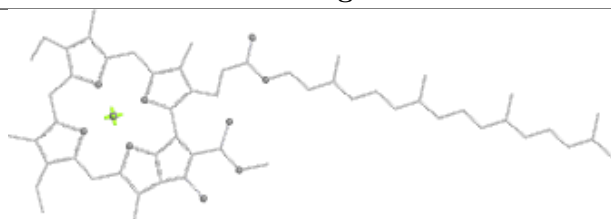
Bond lengths



Bond angles

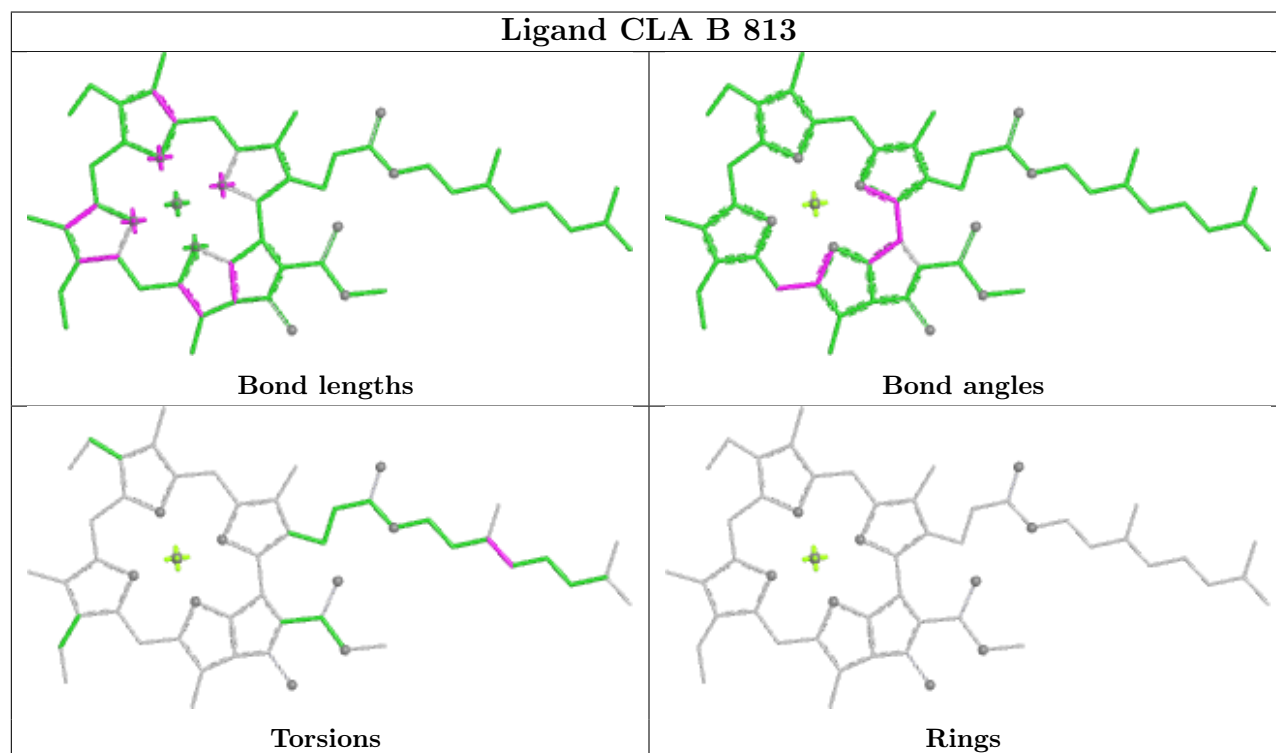
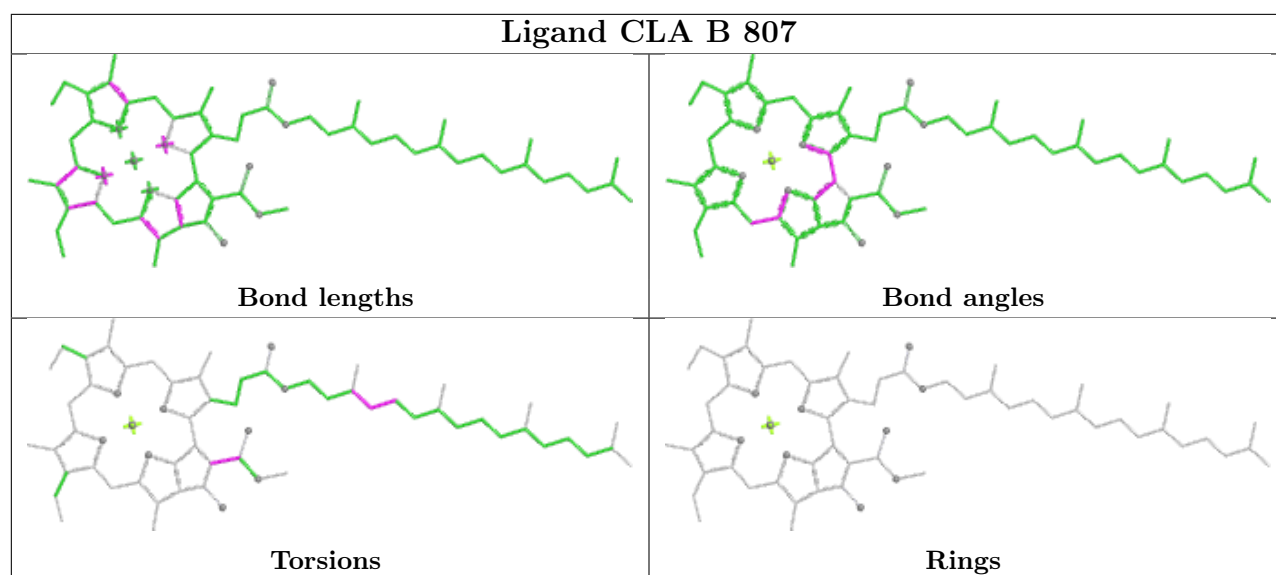


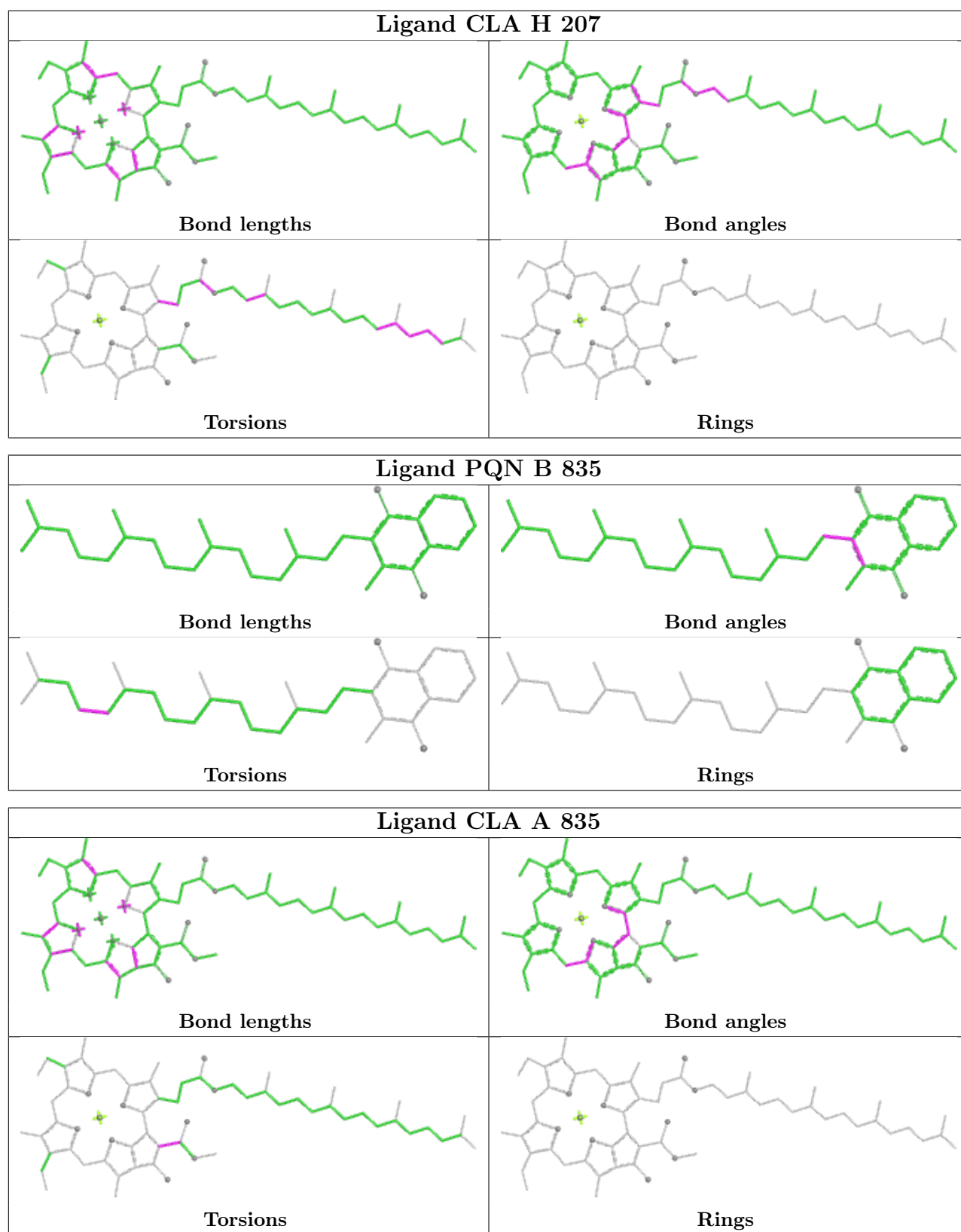
Torsions

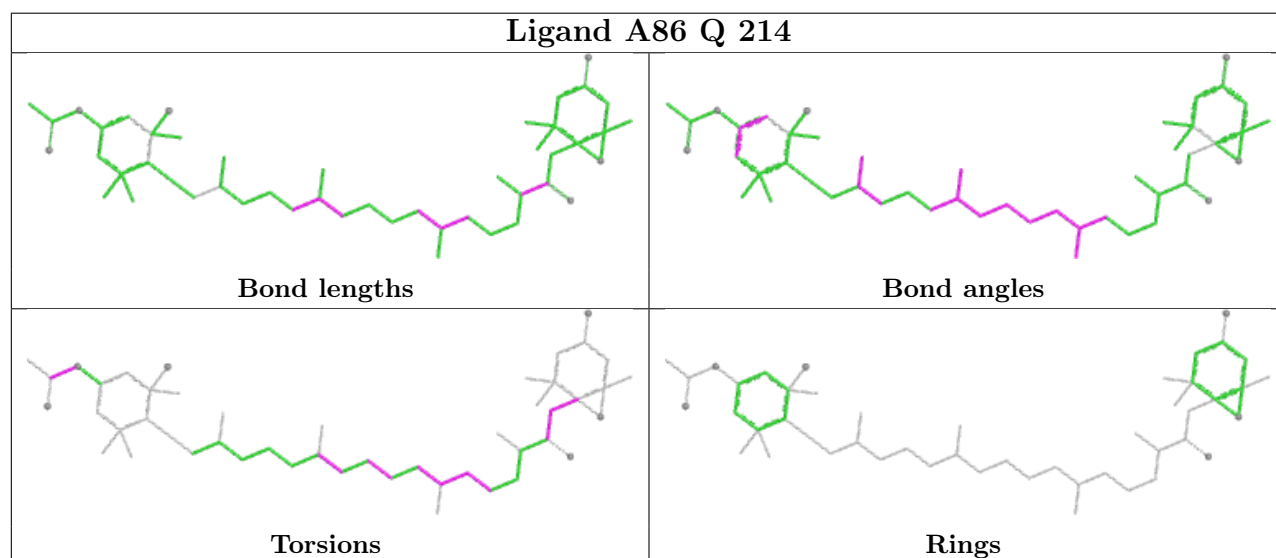
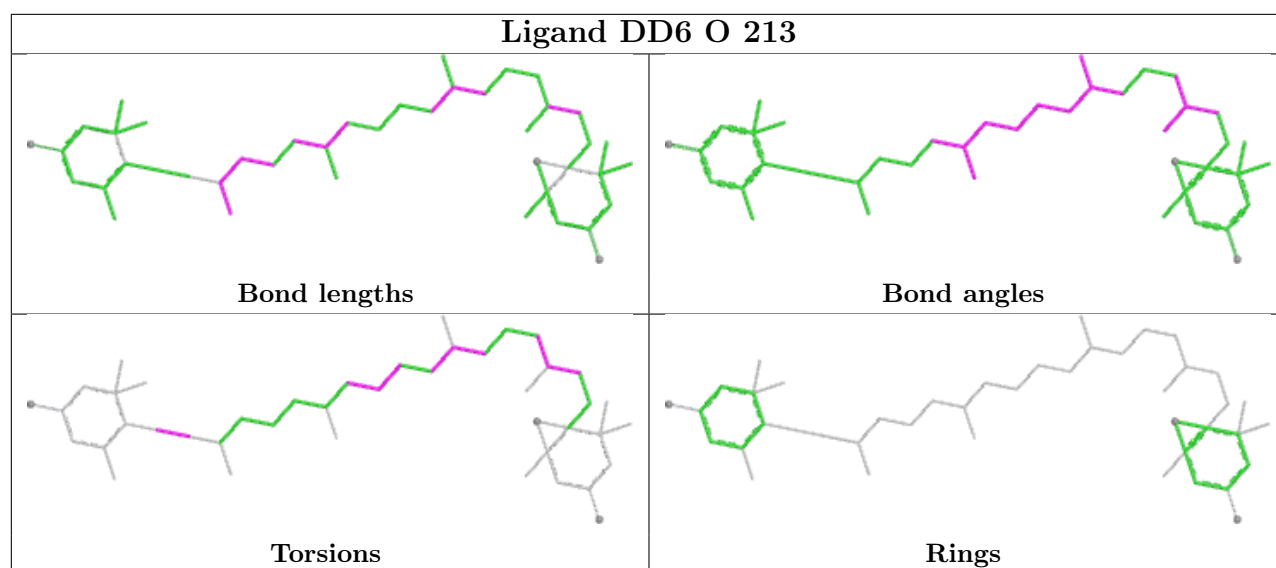


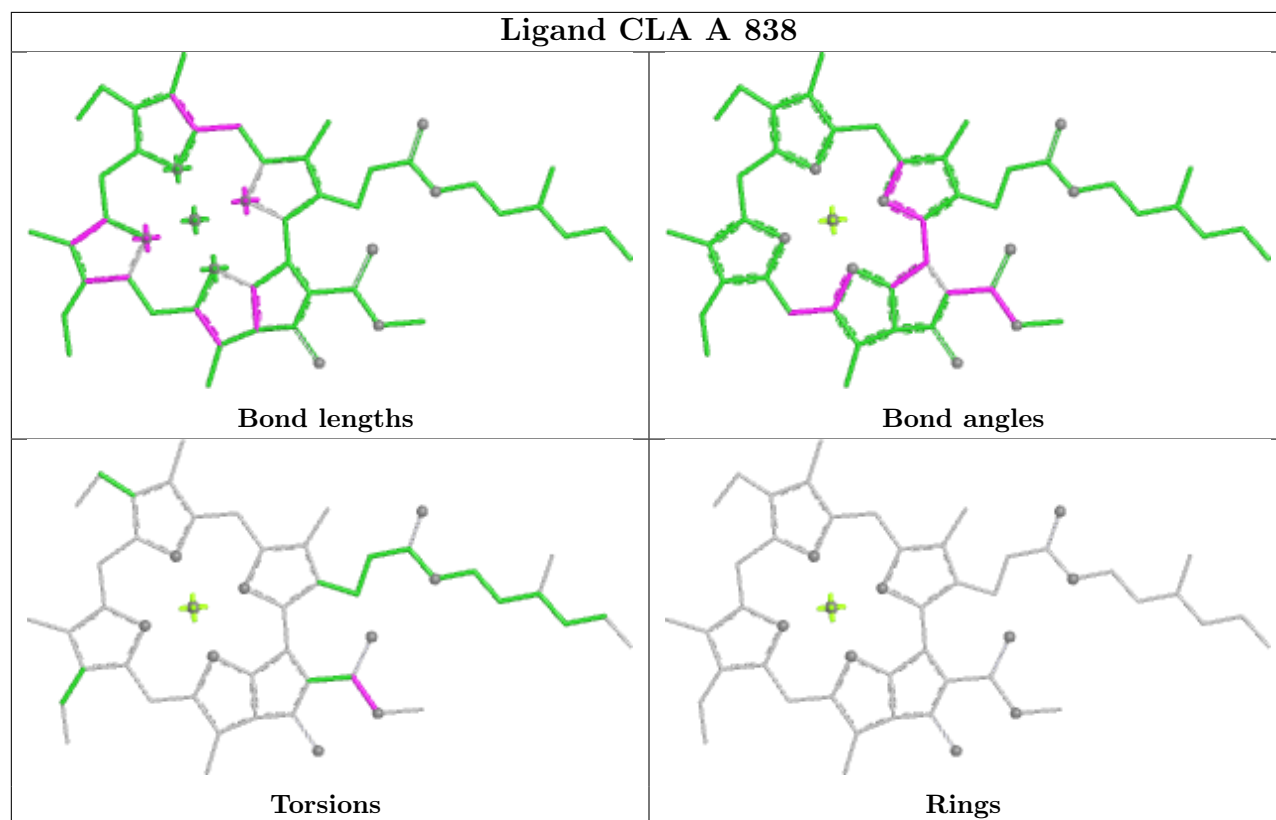
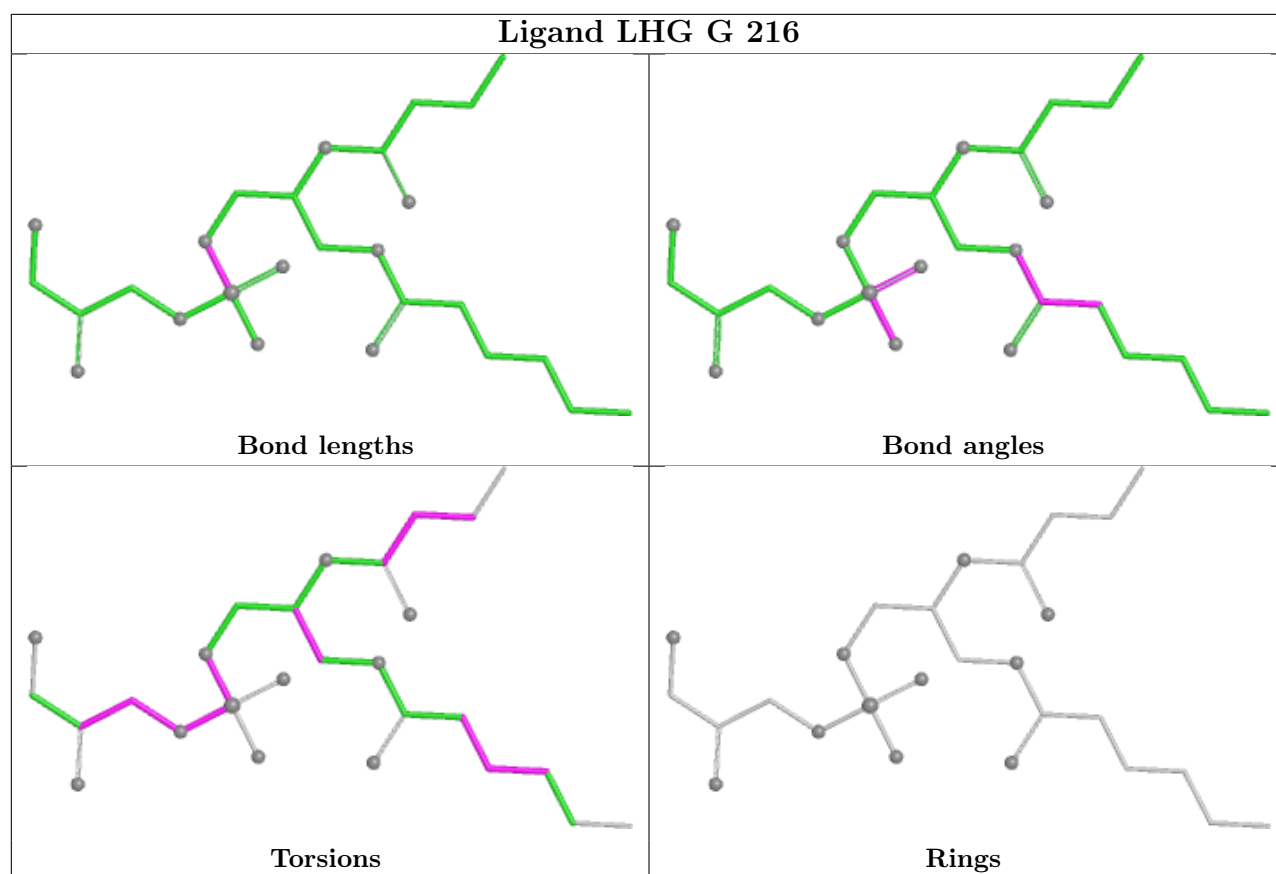
Rings

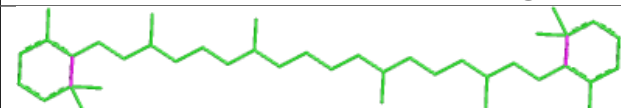
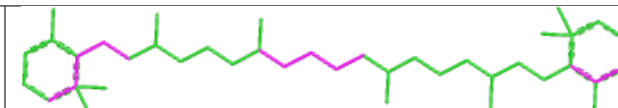
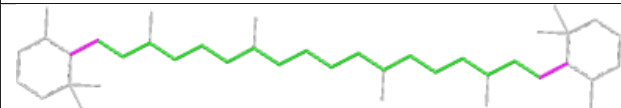
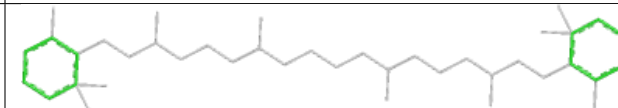



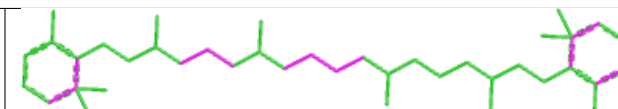
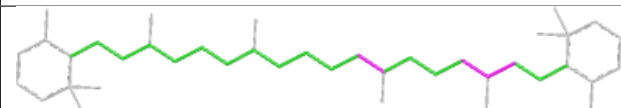
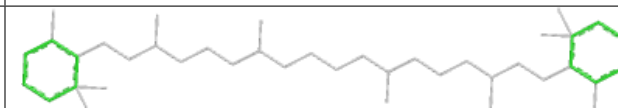


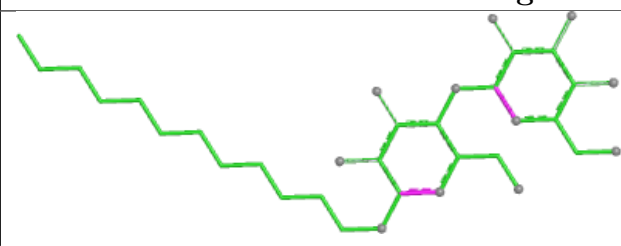
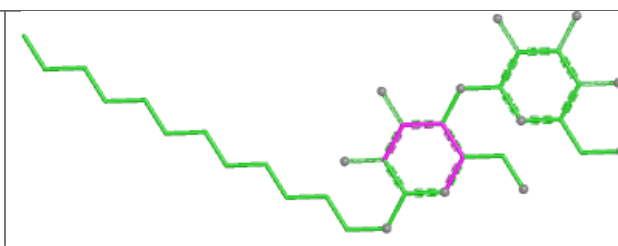
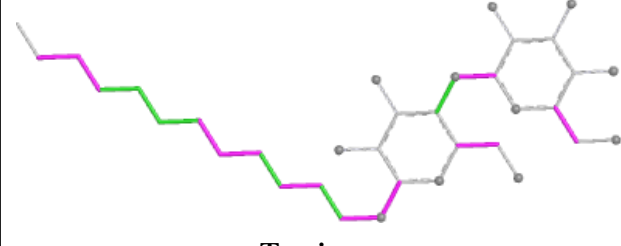
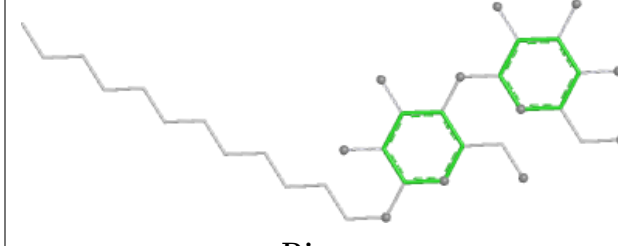


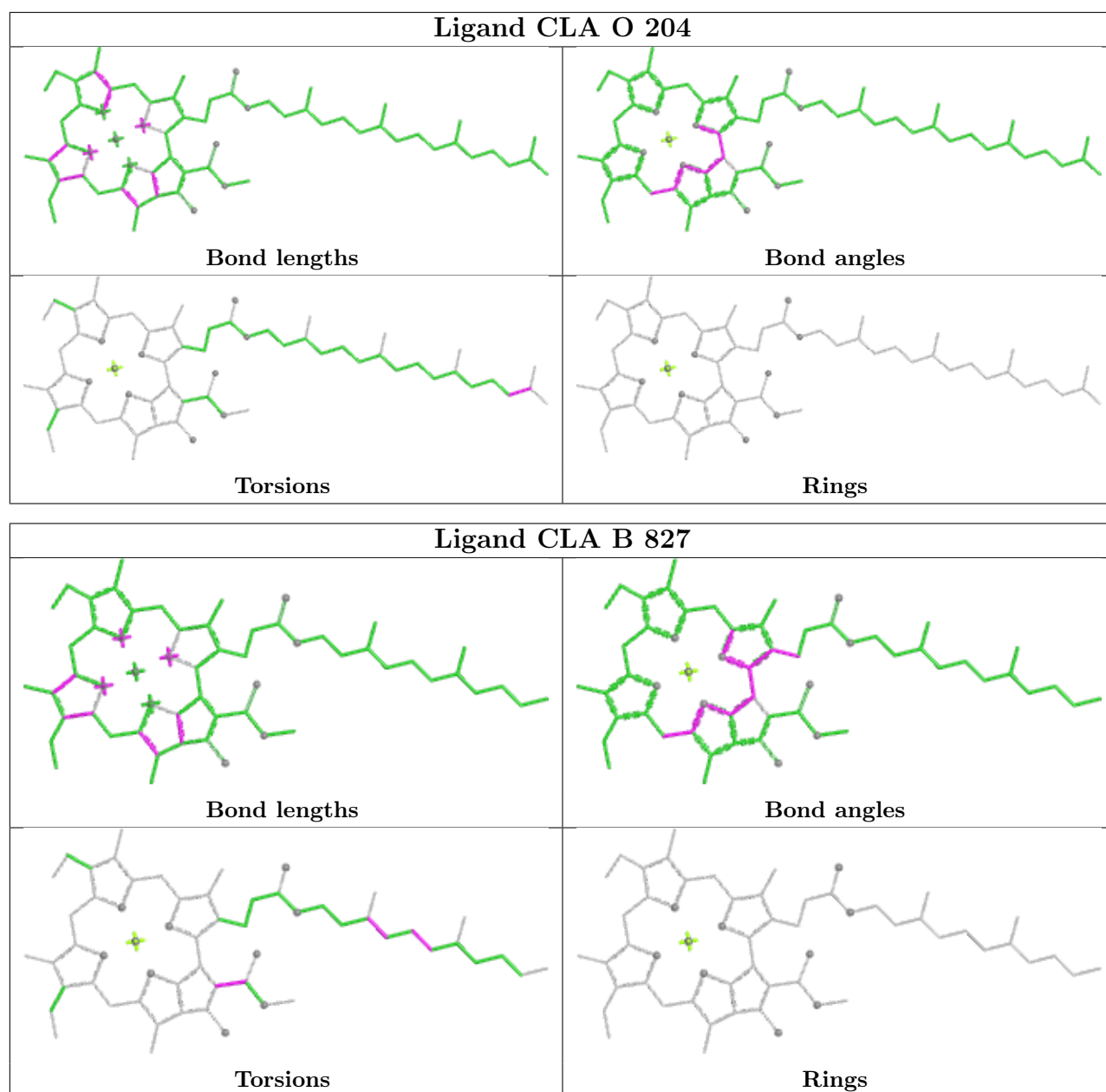


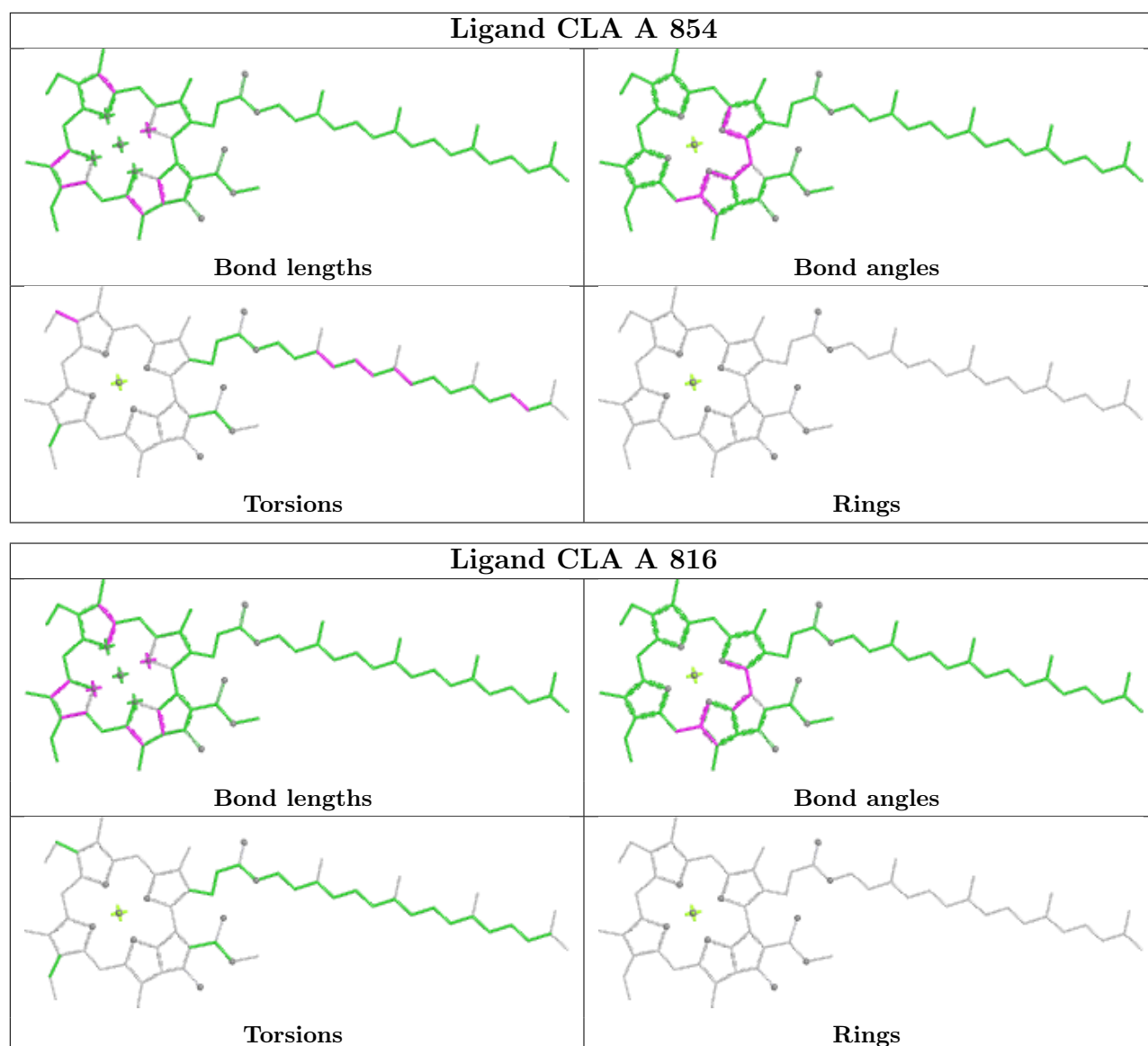


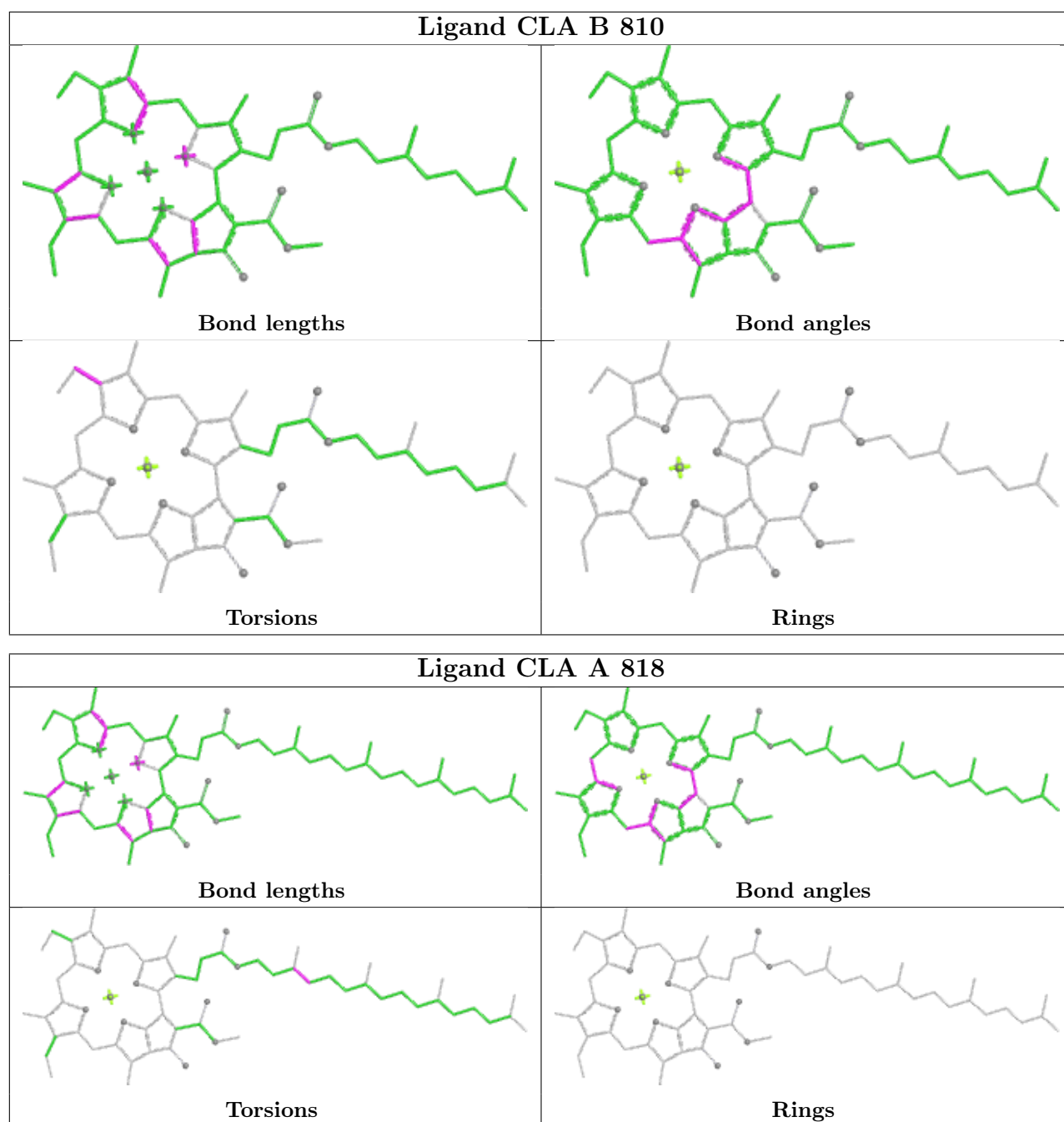
Ligand BCR B 839	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR I 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

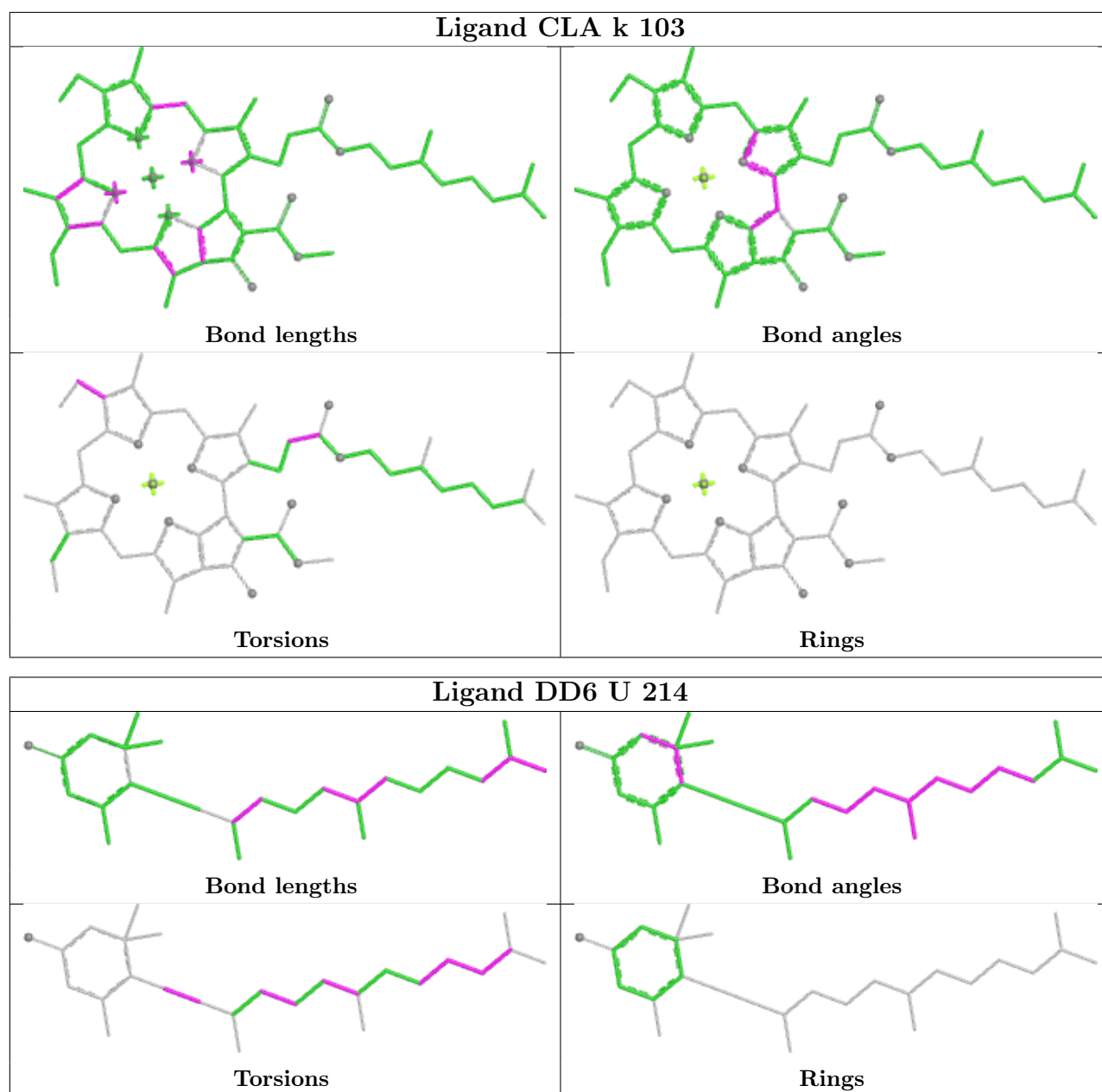
Ligand LMU O 216	
	
Bond lengths	Bond angles
	
Torsions	Rings

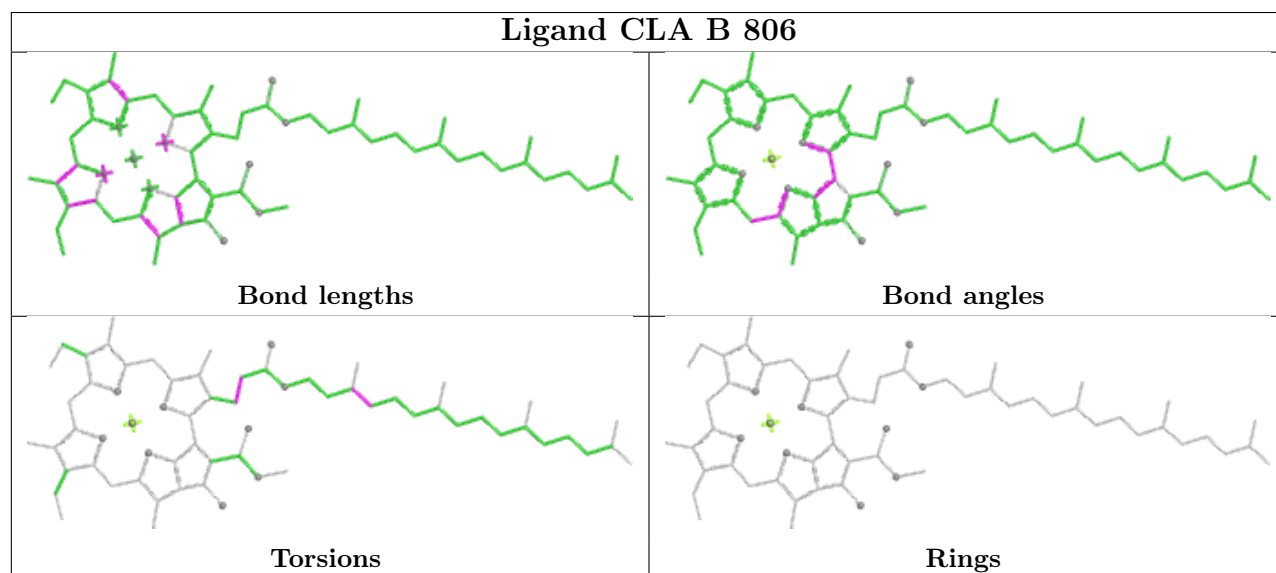
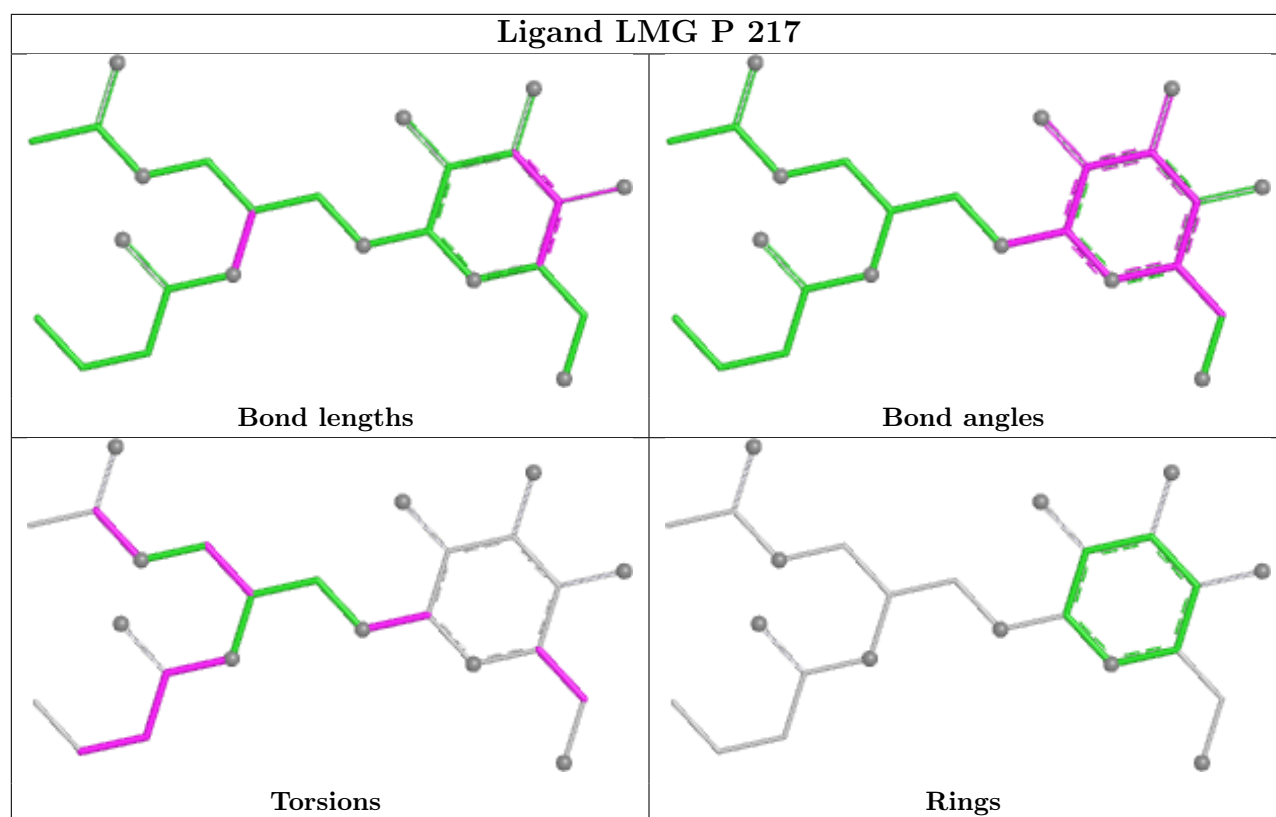


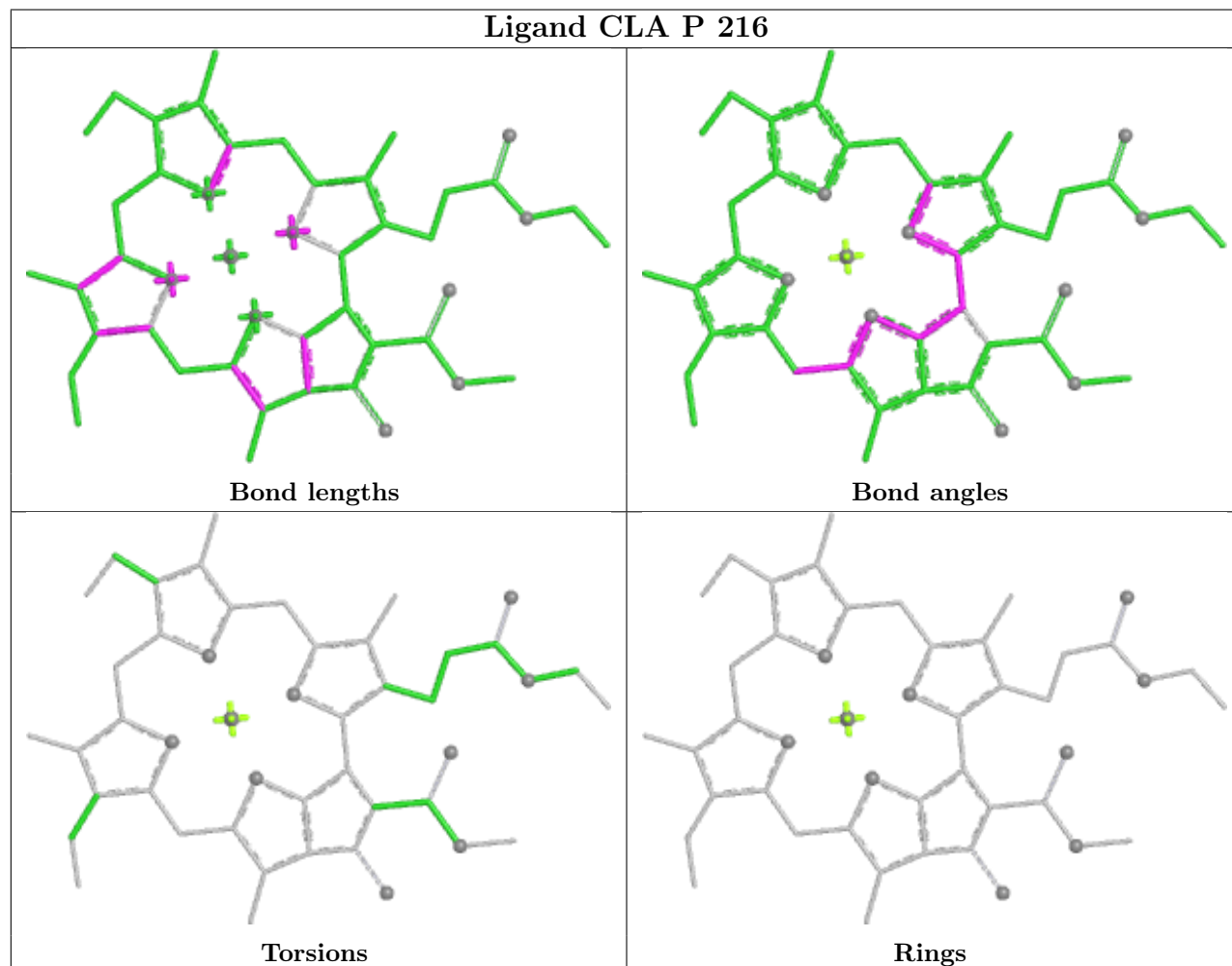
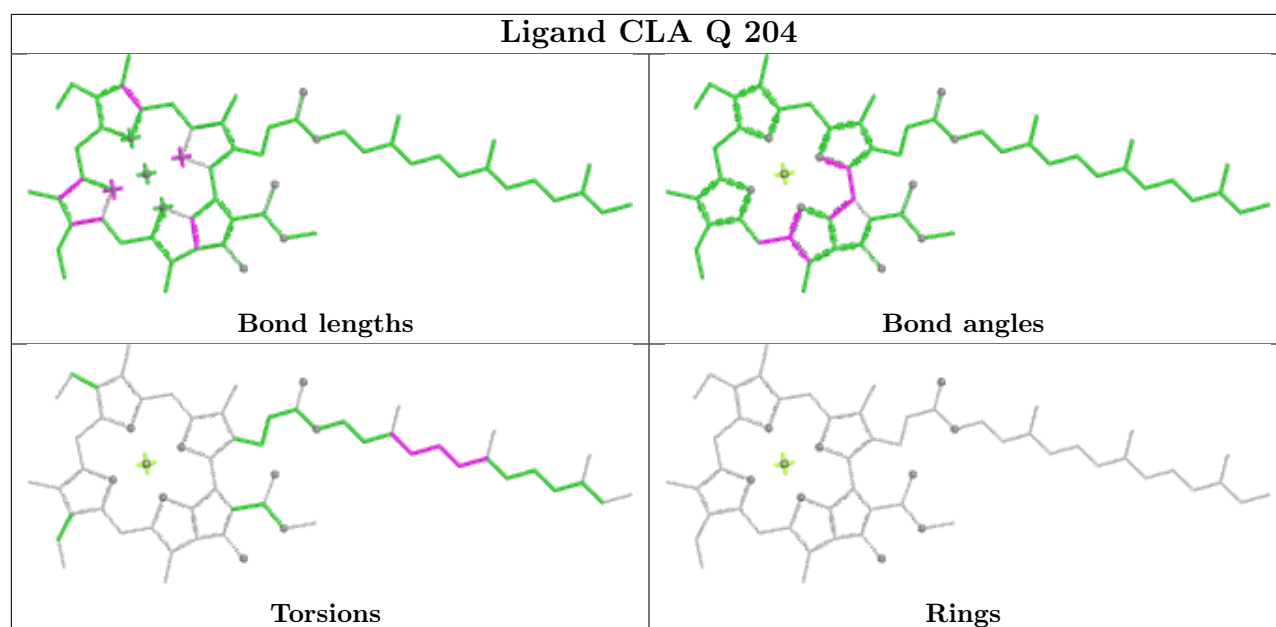




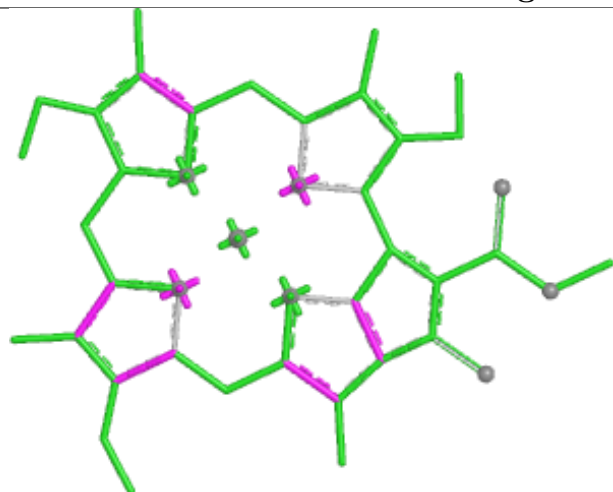




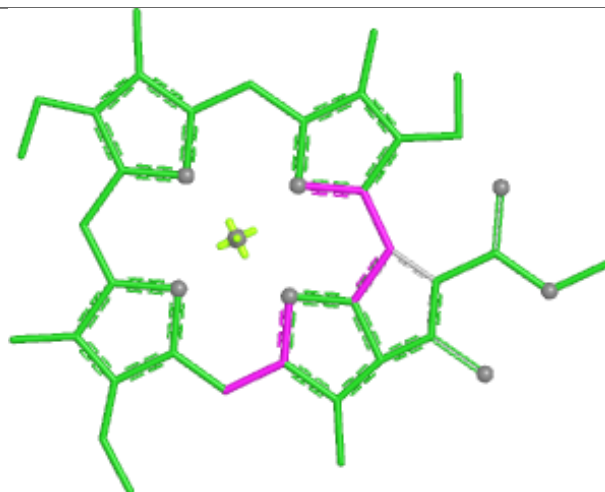




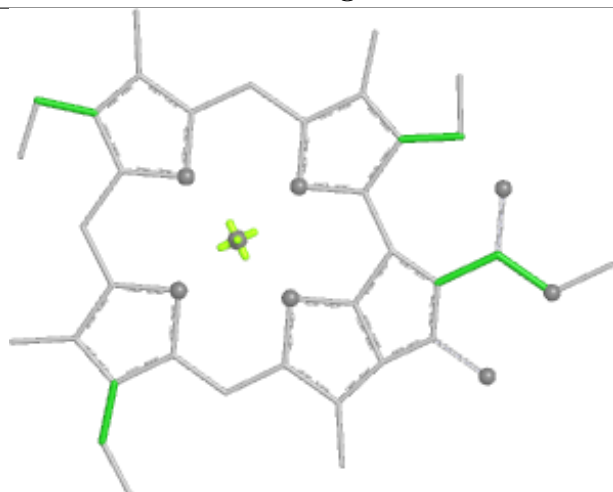
## Ligand CLA k 102



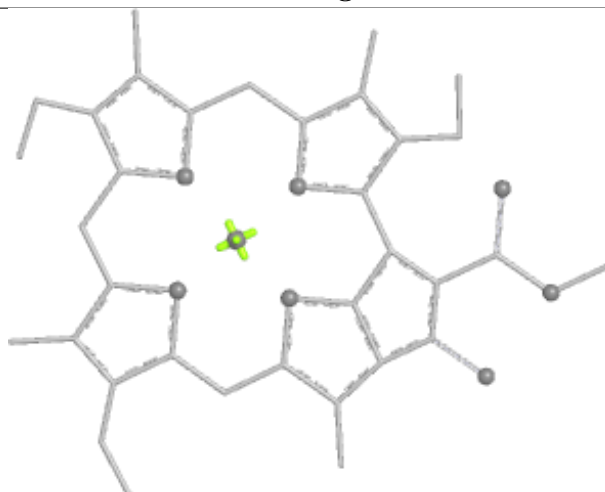
Bond lengths



Bond angles

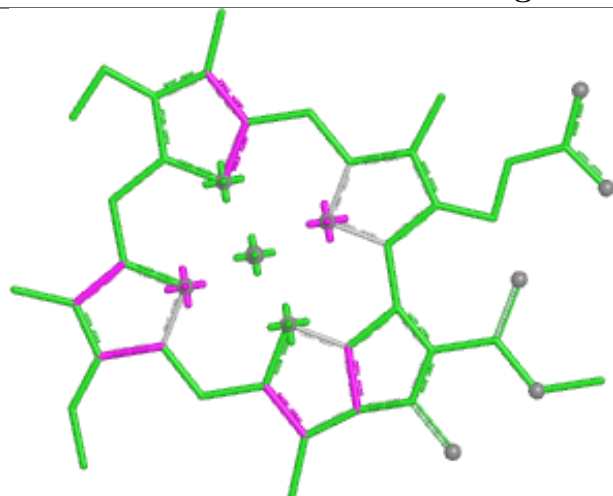


Torsions

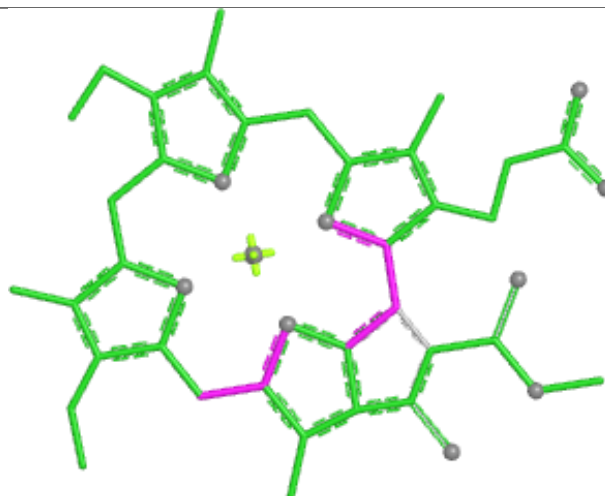


Rings

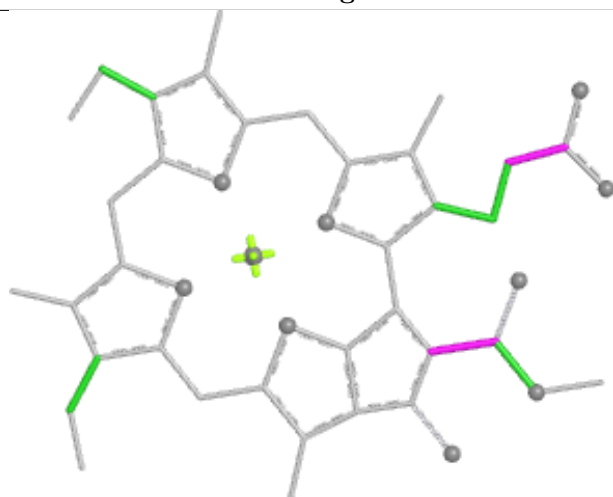
## Ligand CLA B 803



Bond lengths



Bond angles

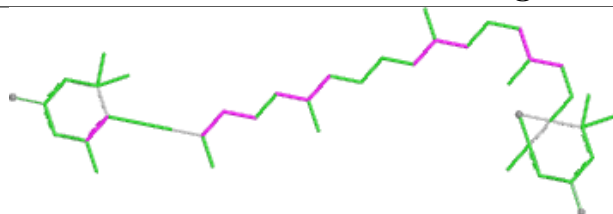


Torsions

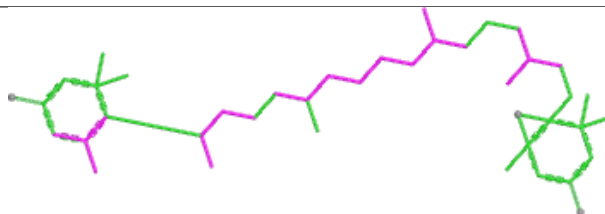


Rings

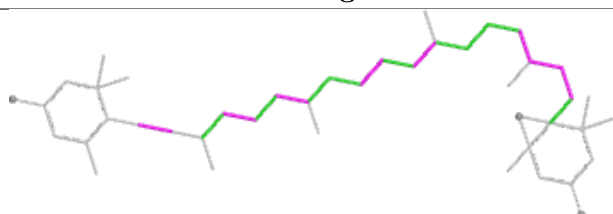
## Ligand DD6 H 201



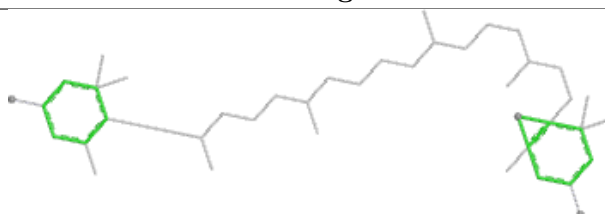
Bond lengths



Bond angles

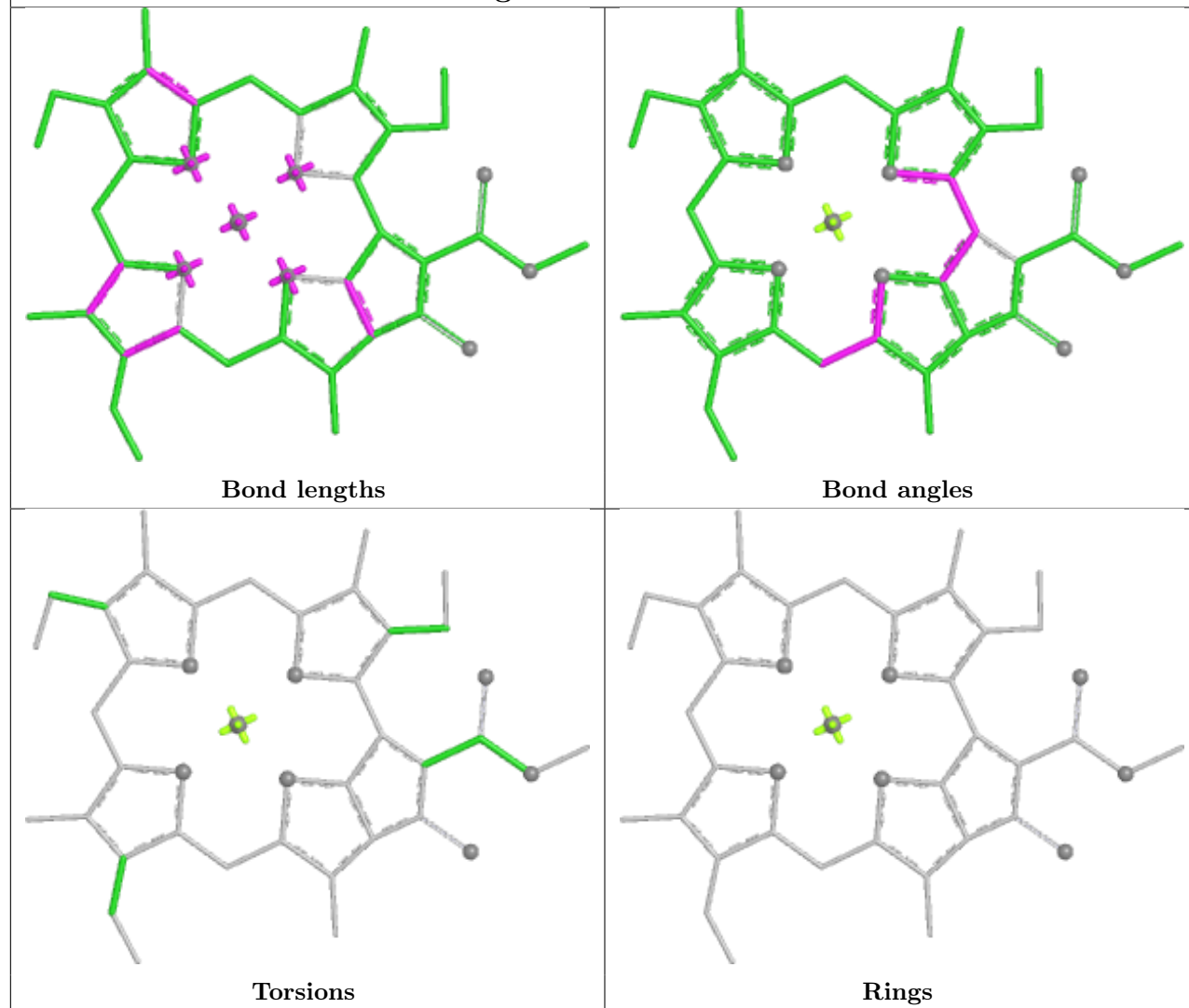


Torsions

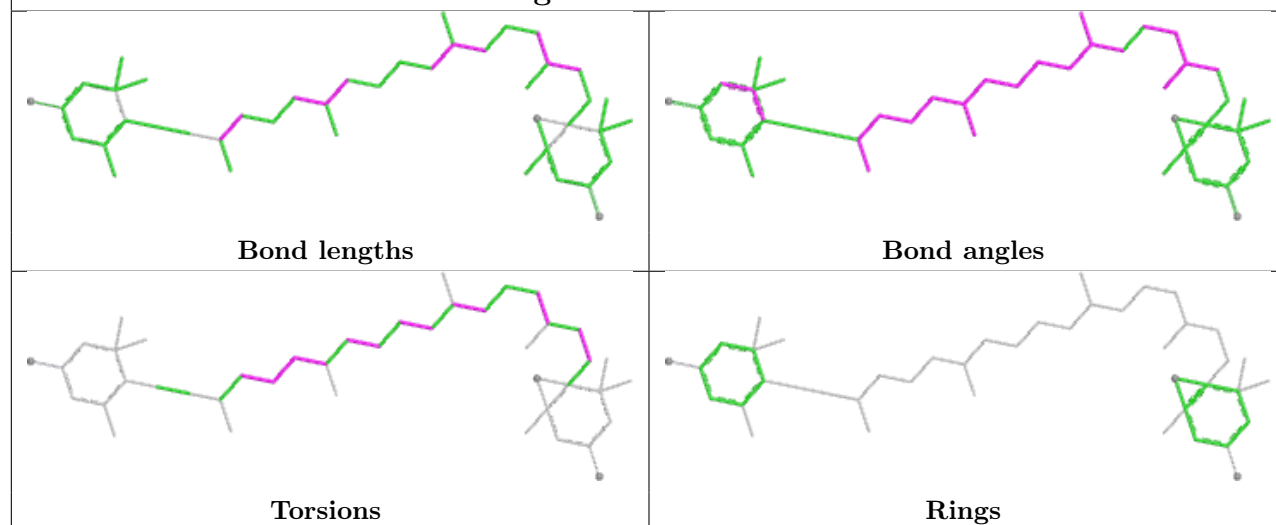


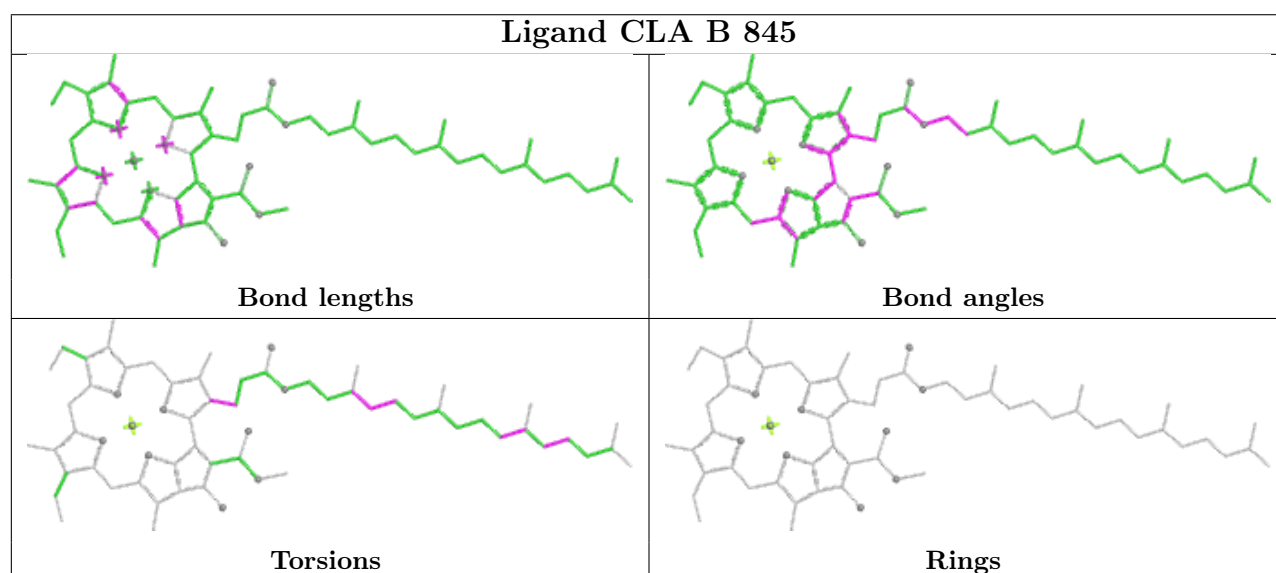
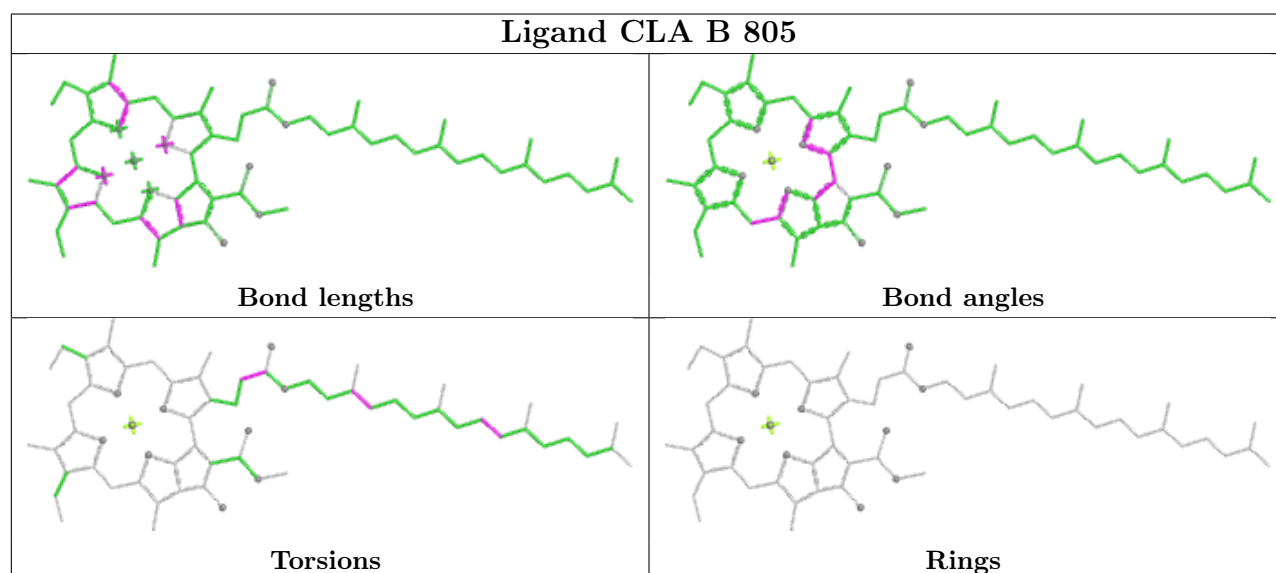
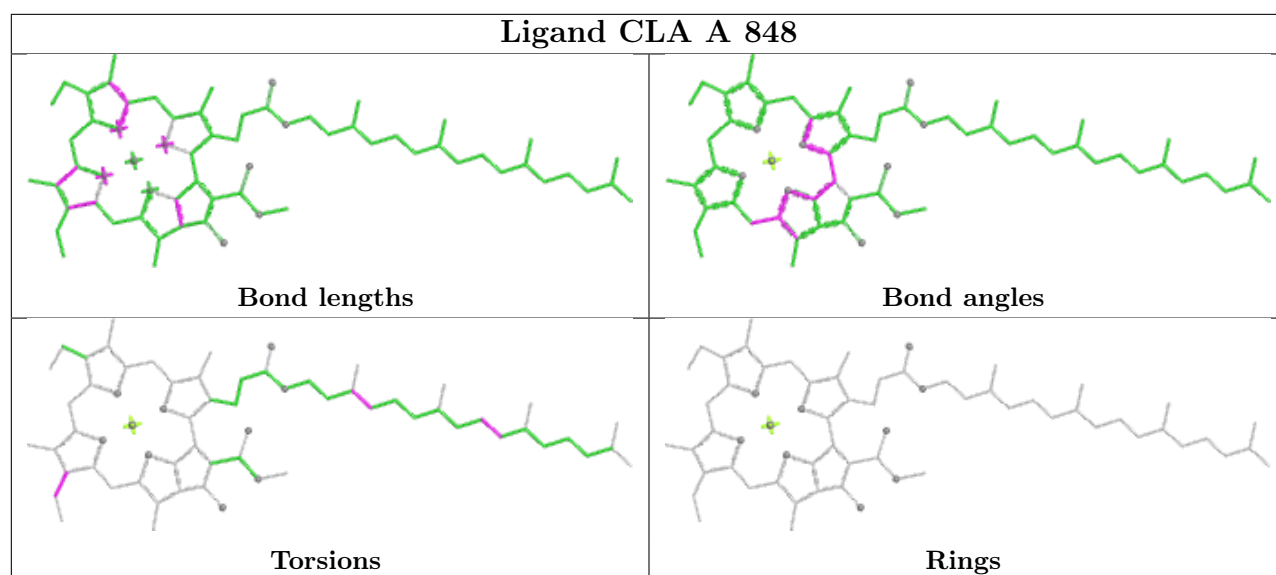
Rings

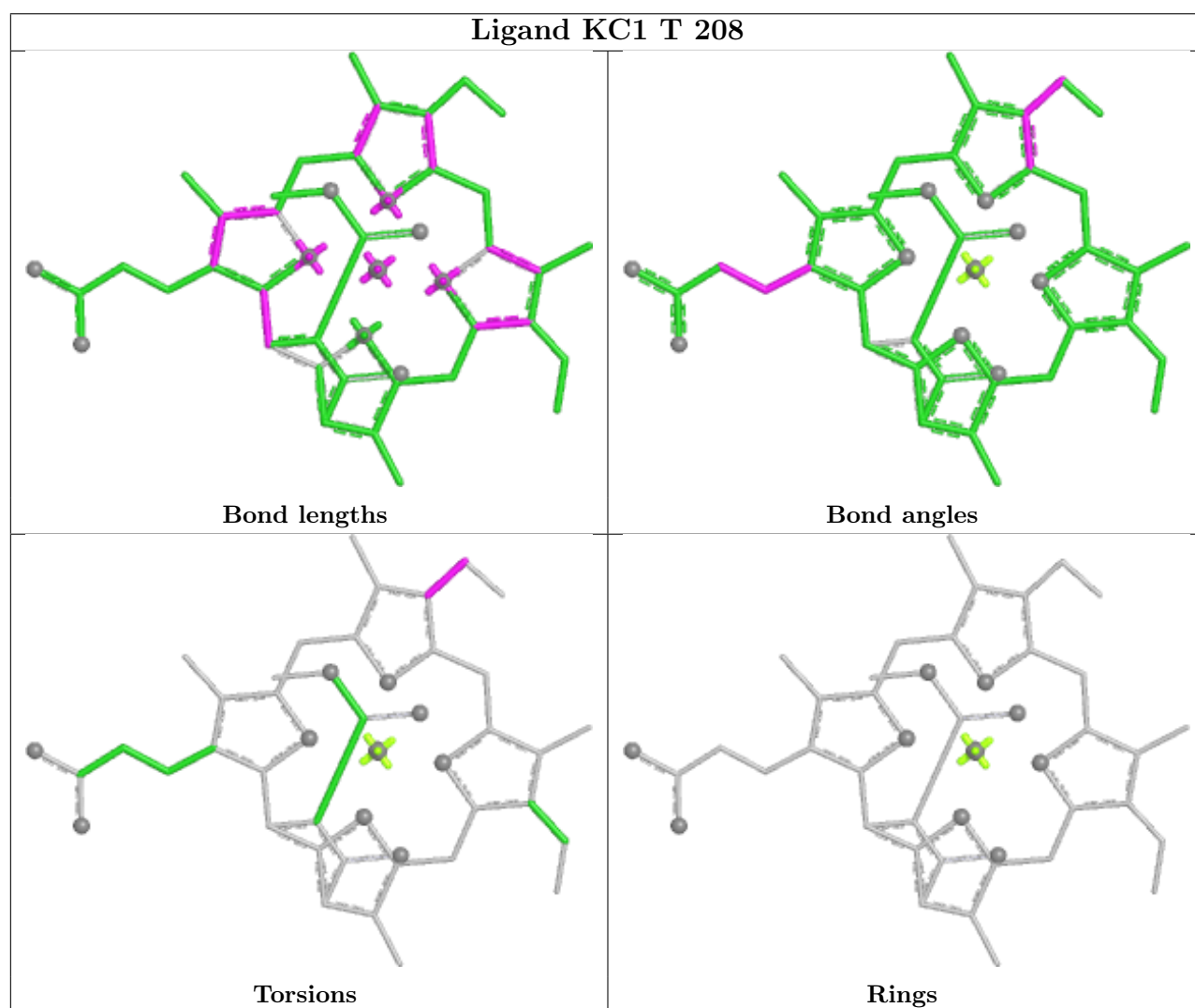
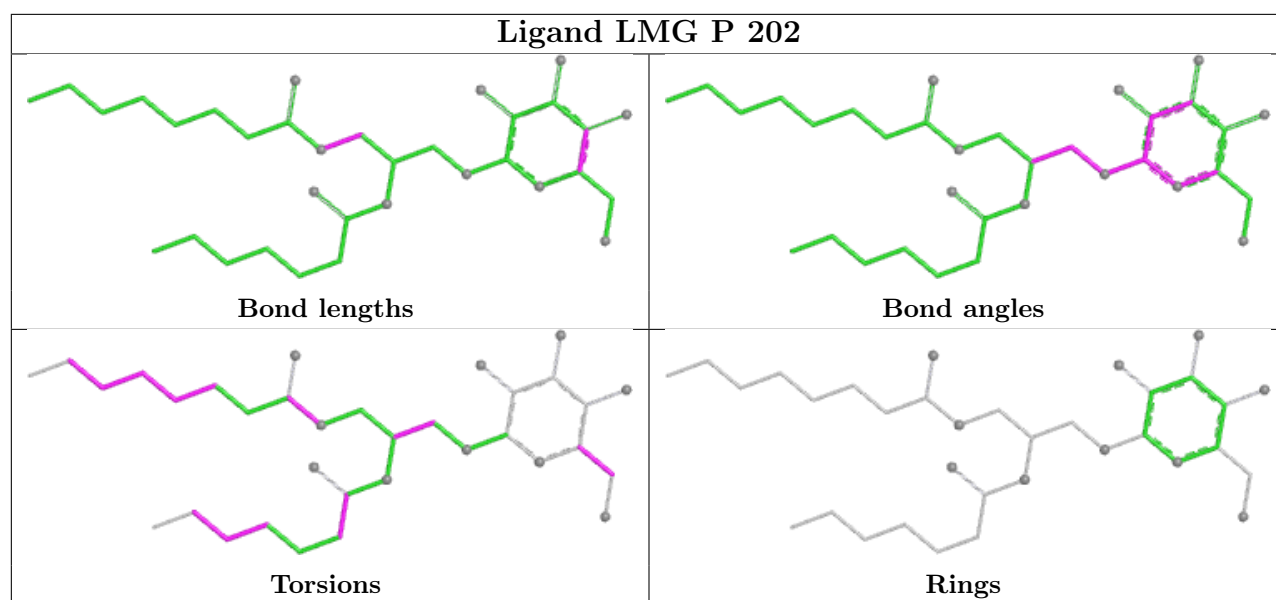
## Ligand CLA U 209



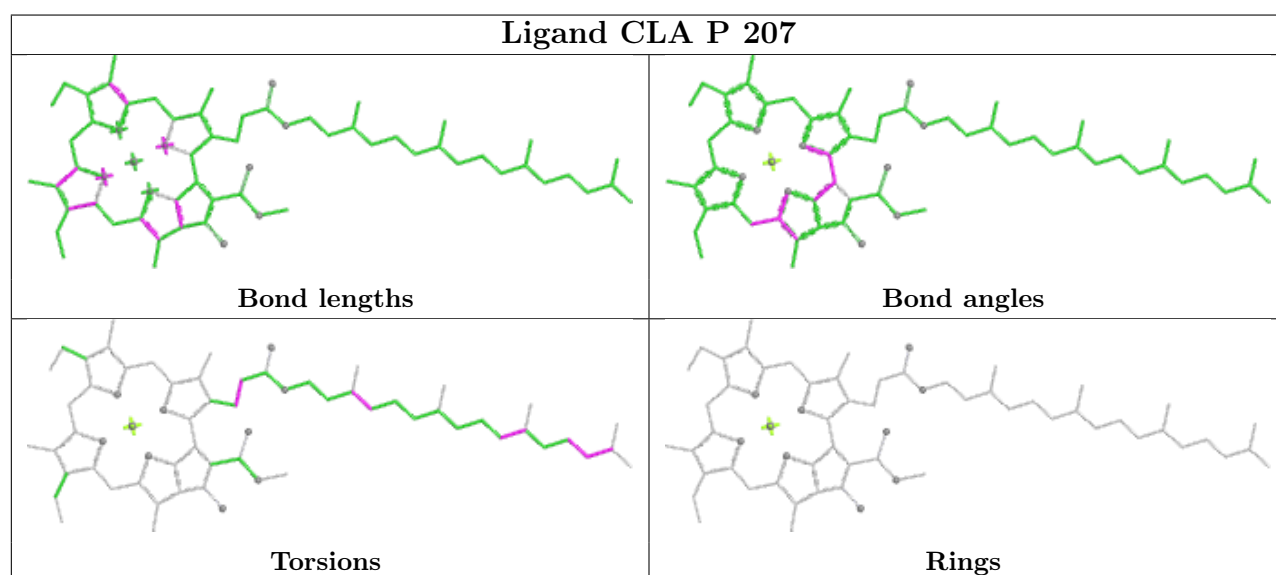
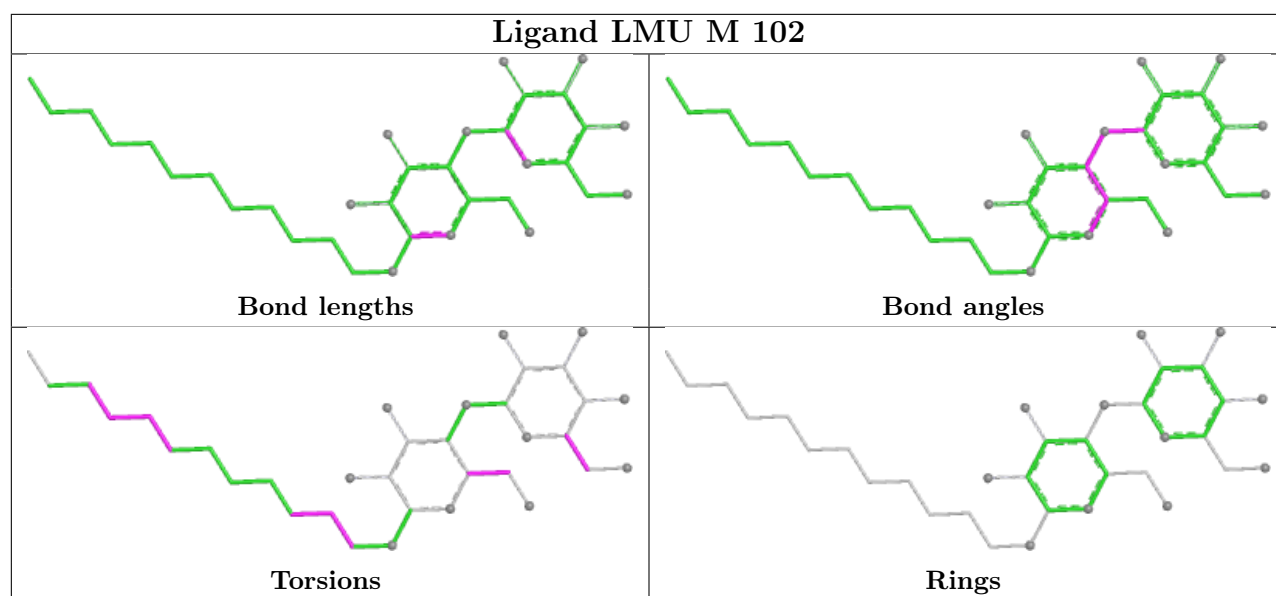
## Ligand DD6 P 220

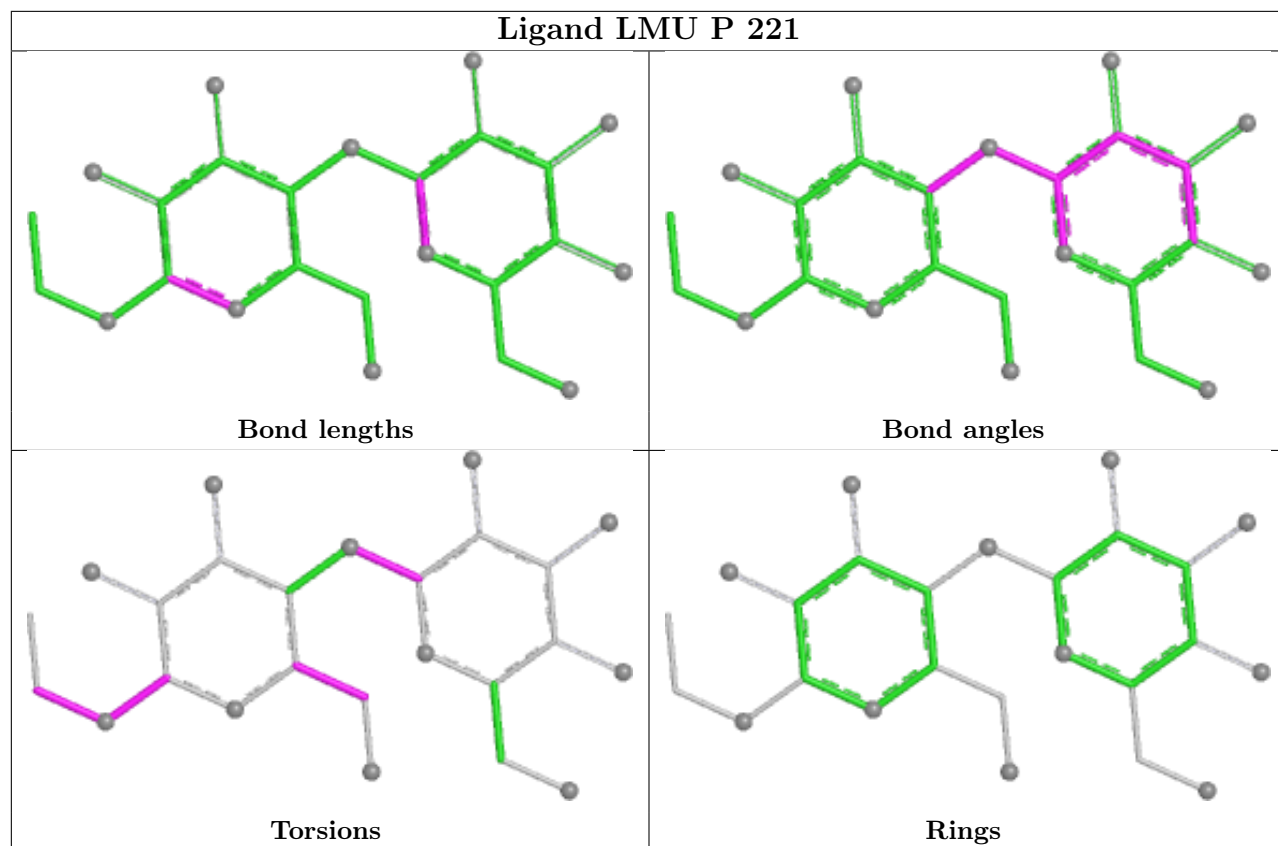




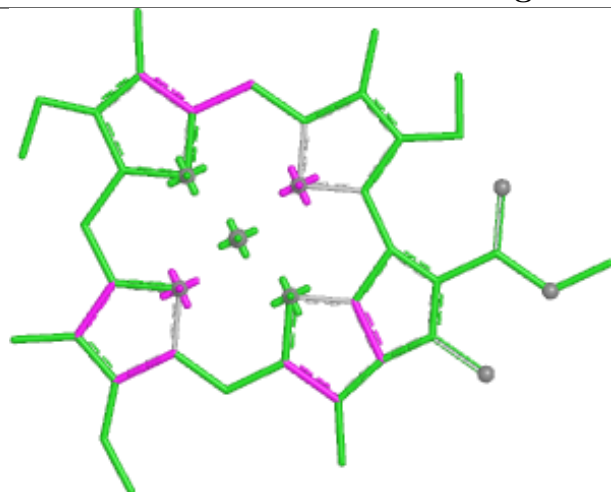




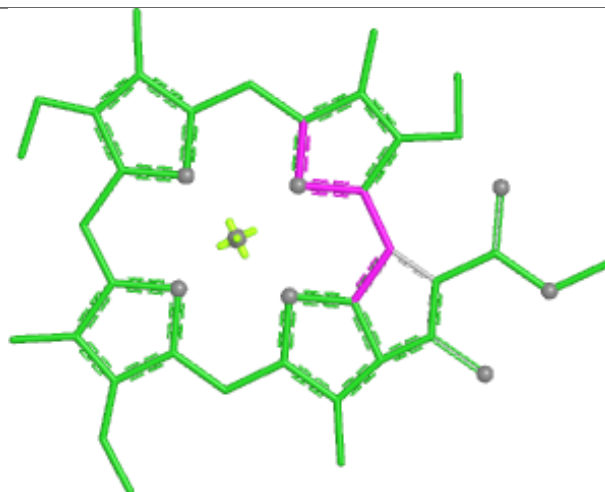




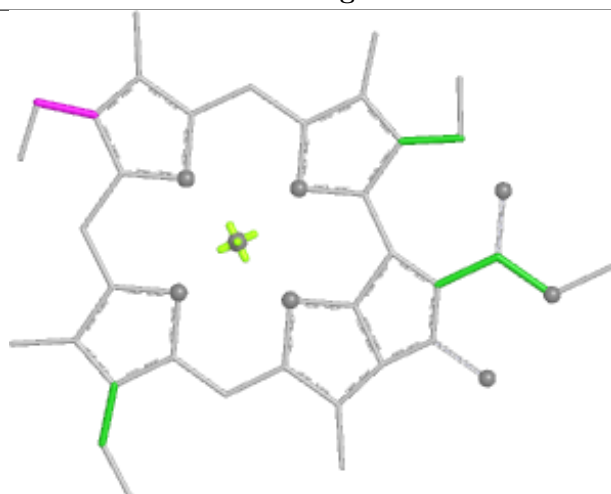
## Ligand CLA T 201



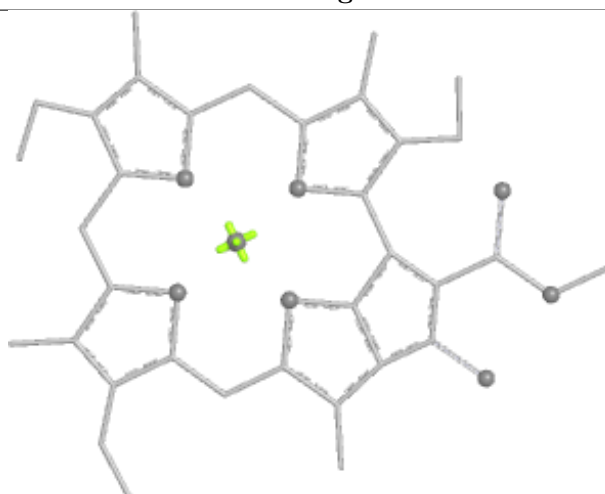
Bond lengths



Bond angles

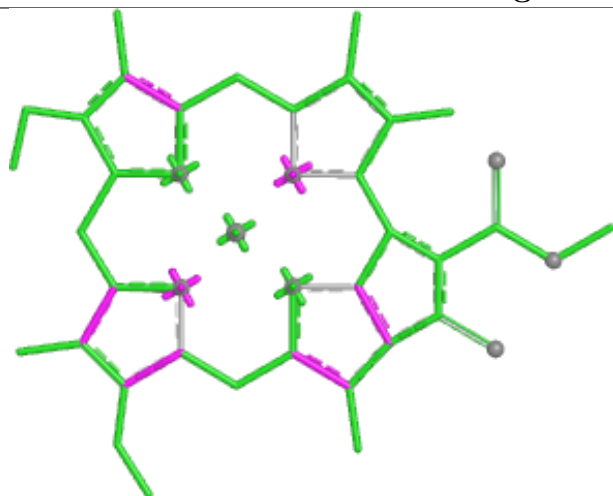


Torsions

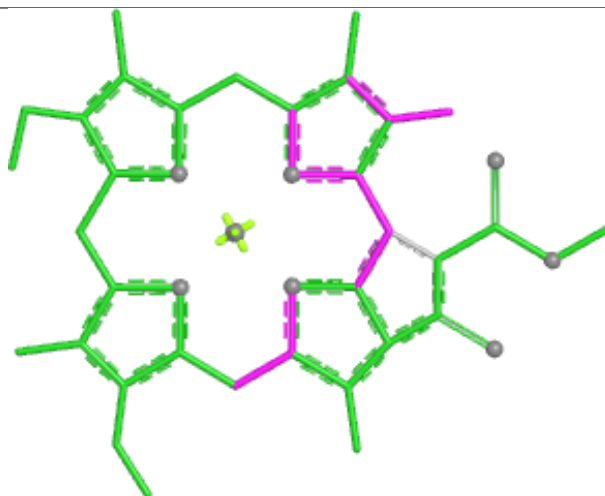


Rings

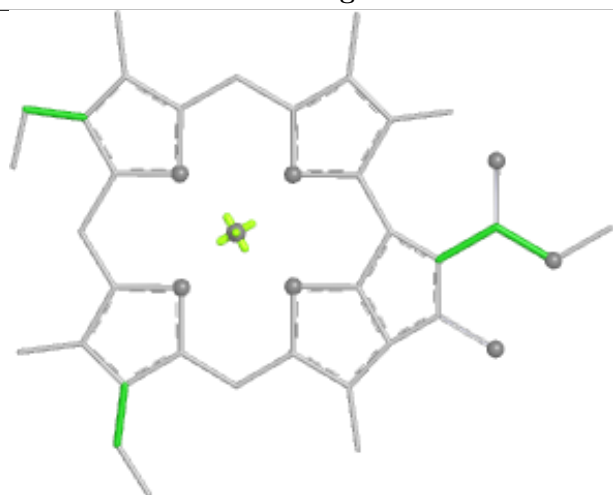
## Ligand CLA O 211



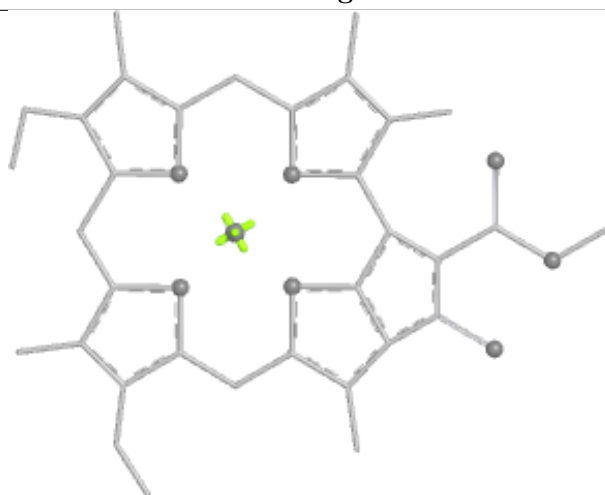
Bond lengths



Bond angles

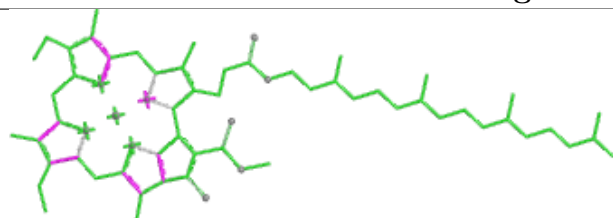


Torsions

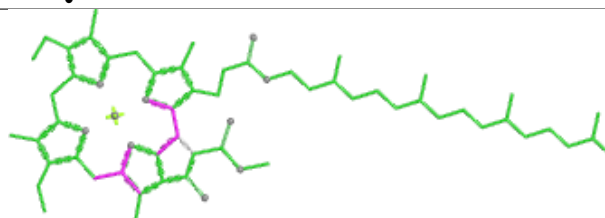


Rings

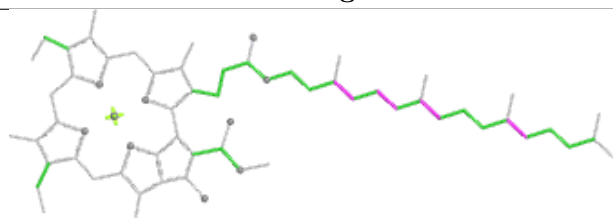
## Ligand CLA Q 216



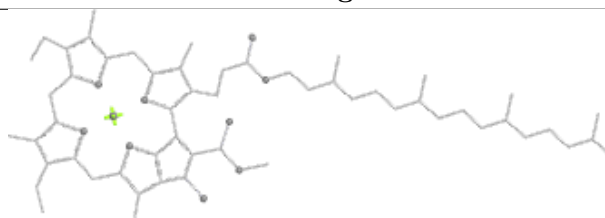
Bond lengths



Bond angles

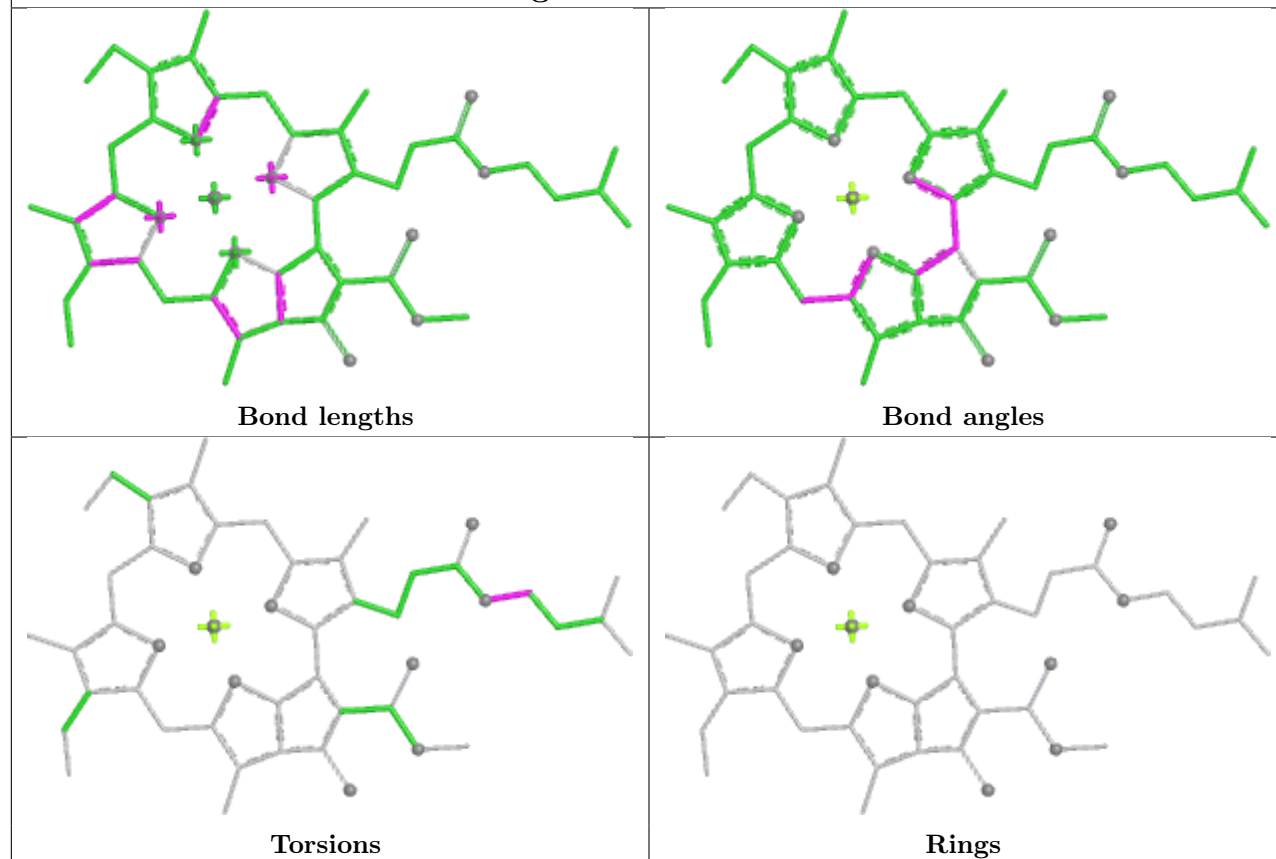


Torsions

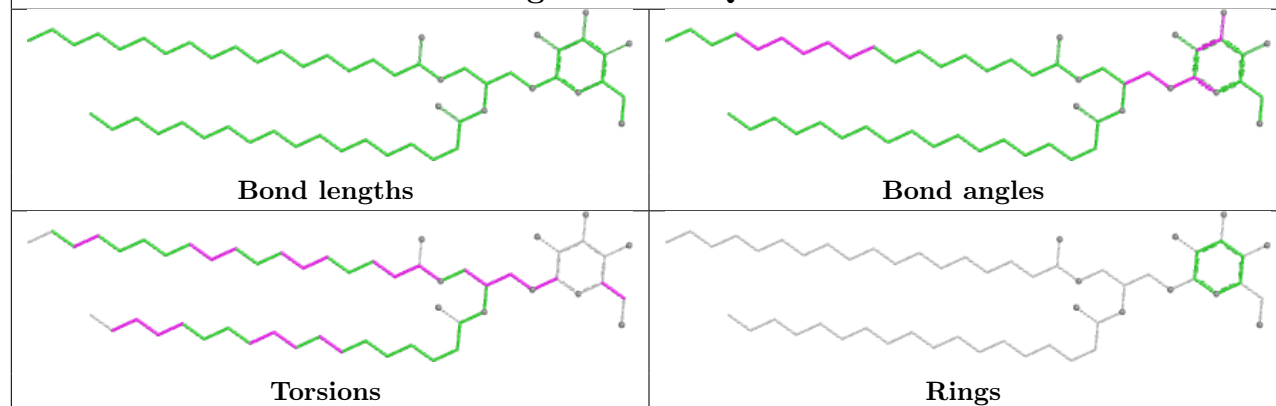


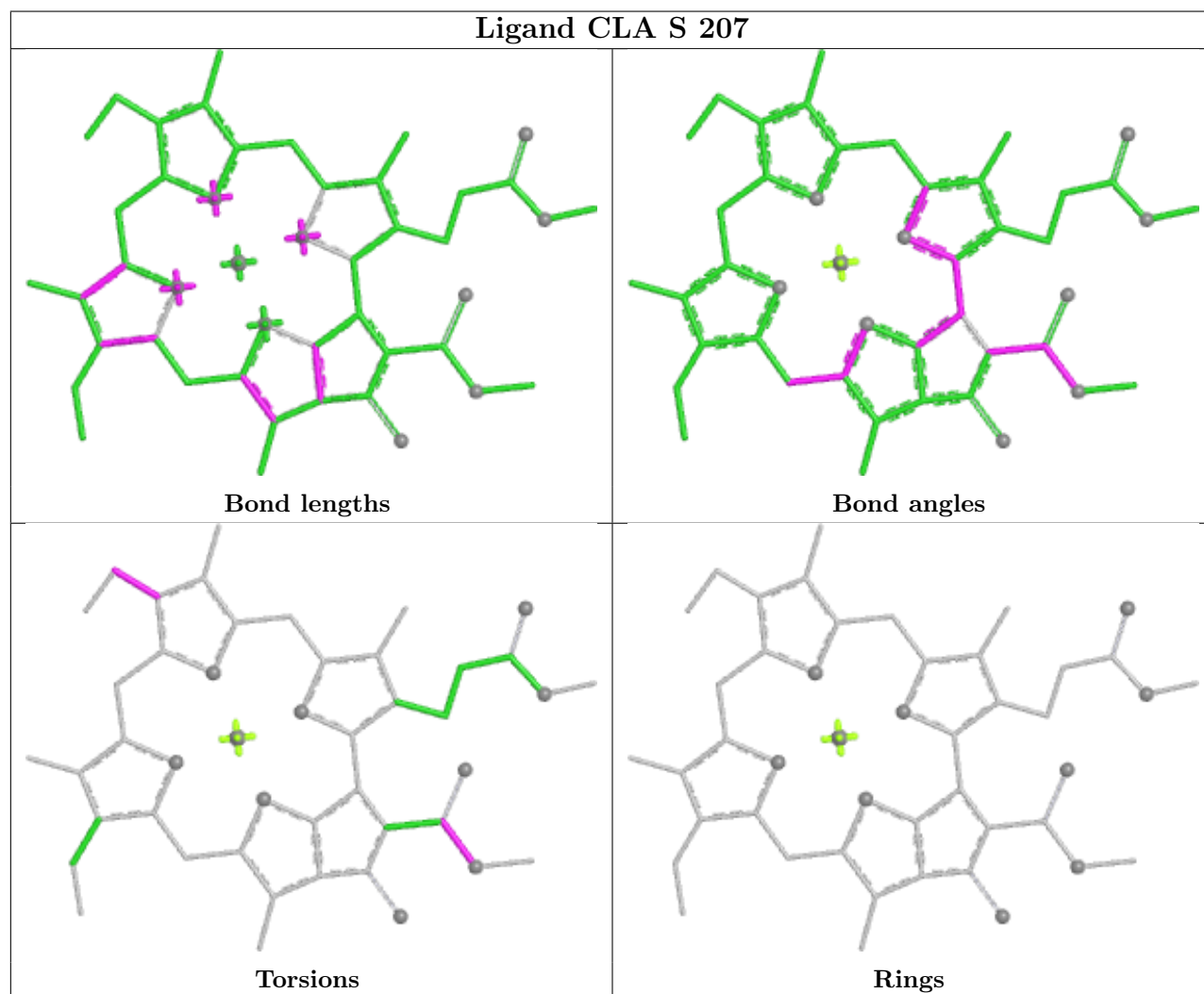
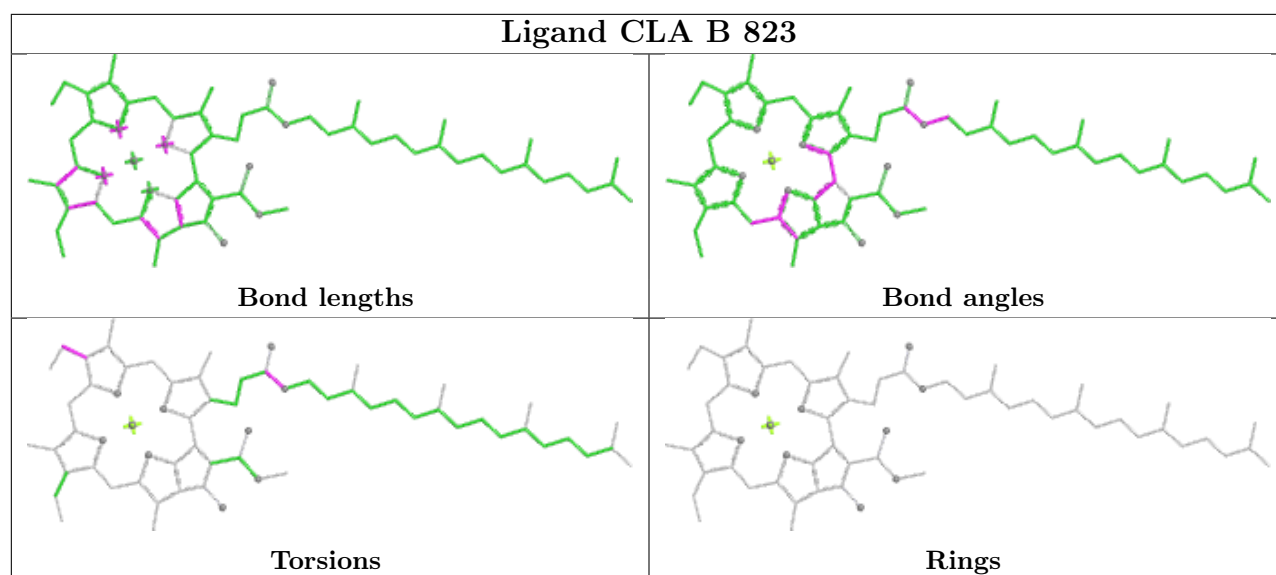
Rings

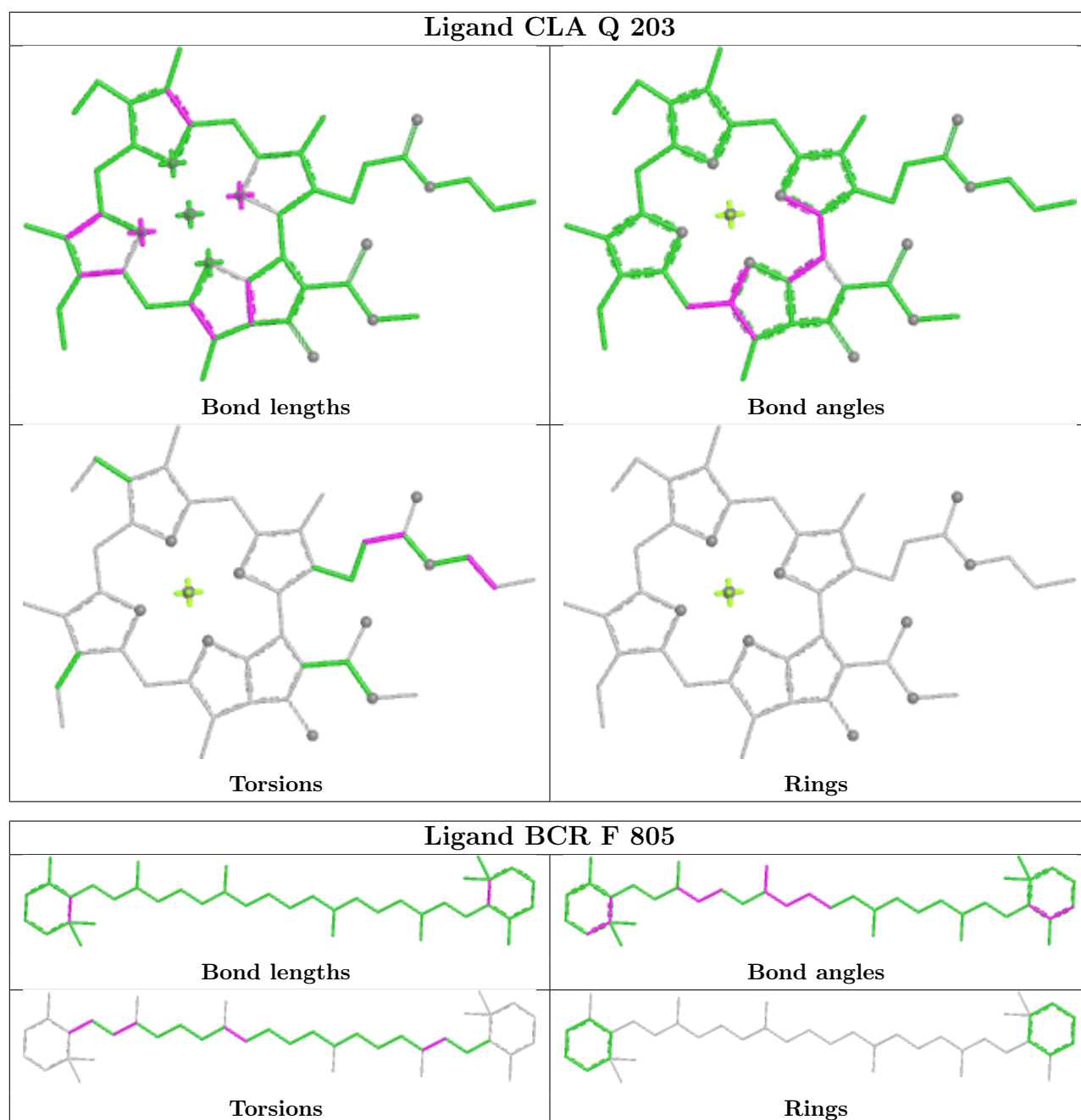
## Ligand CLA A 830



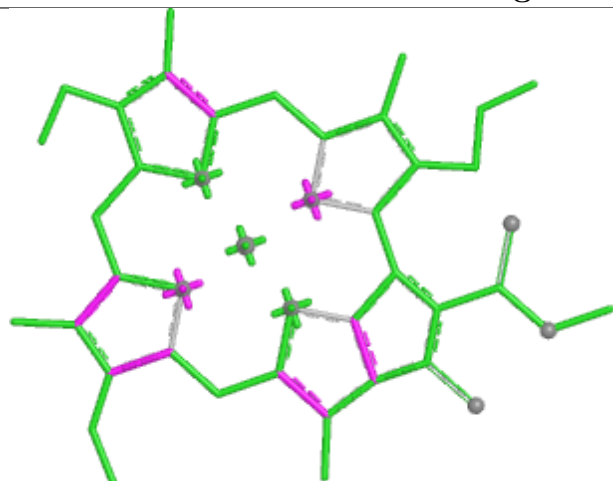
## Ligand LMG Q 217



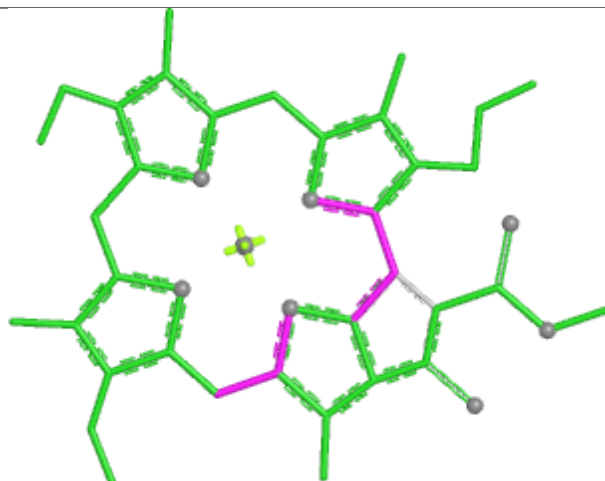




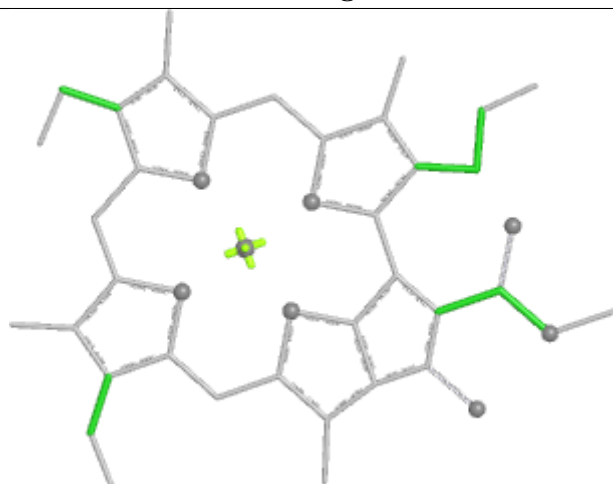
## Ligand CLA A 819



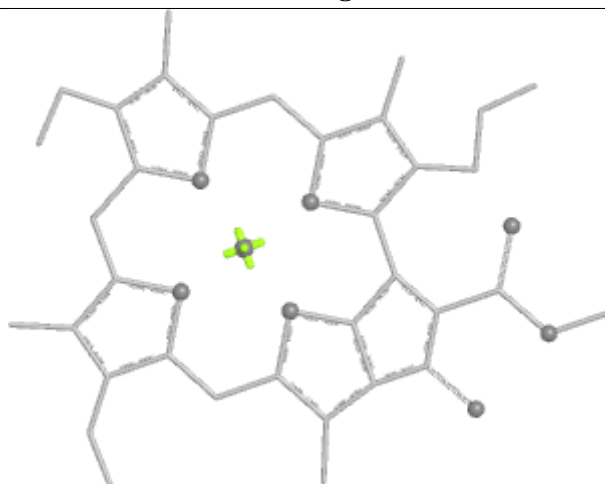
Bond lengths



Bond angles



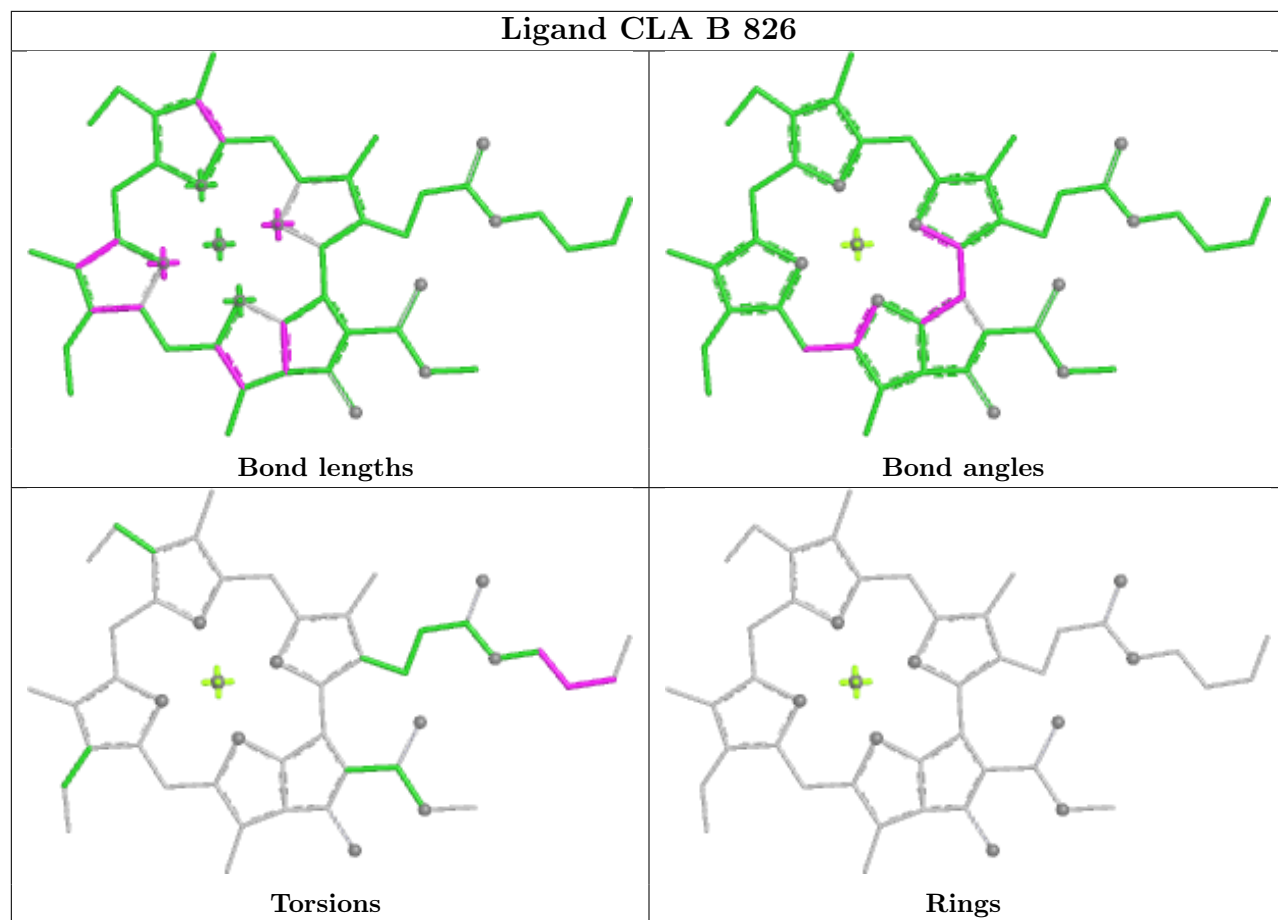
Torsions



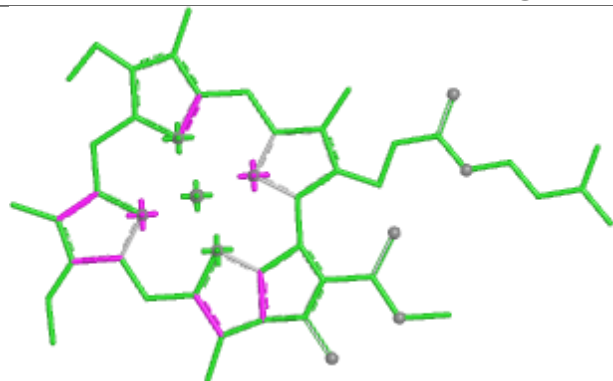
Rings



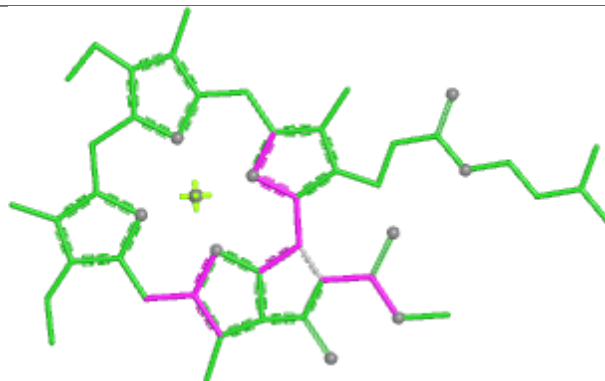
## Ligand CLA B 826



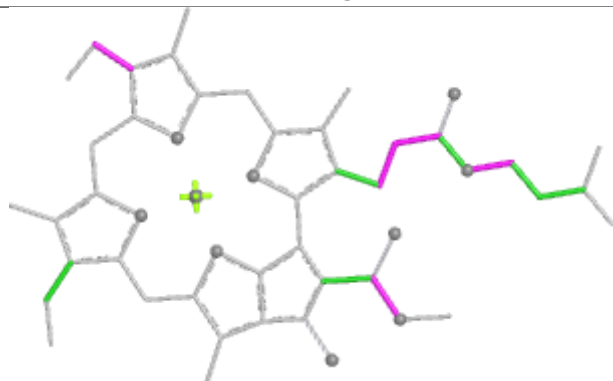
## Ligand CLA L 204



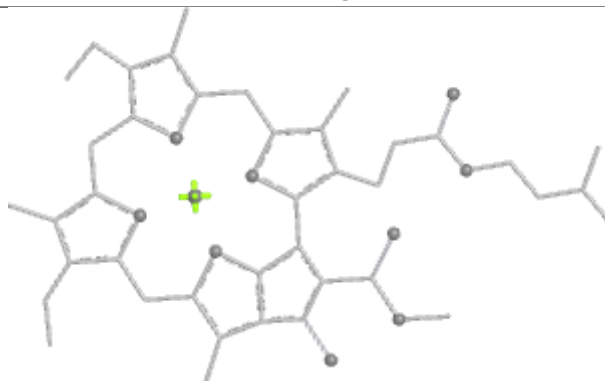
Bond lengths



Bond angles

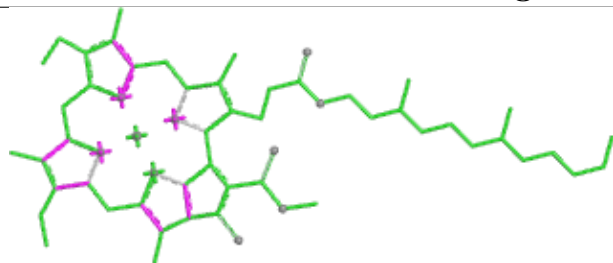


Torsions

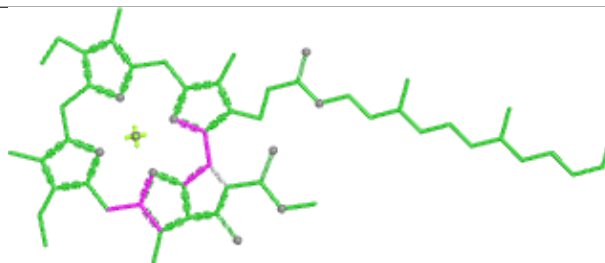


Rings

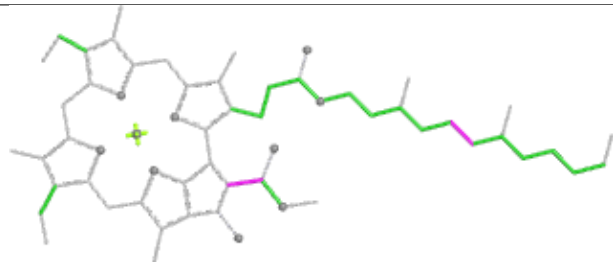
## Ligand CLA B 812



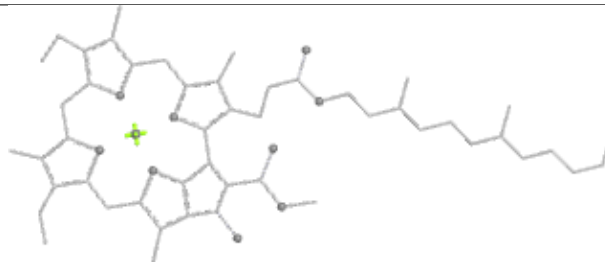
Bond lengths



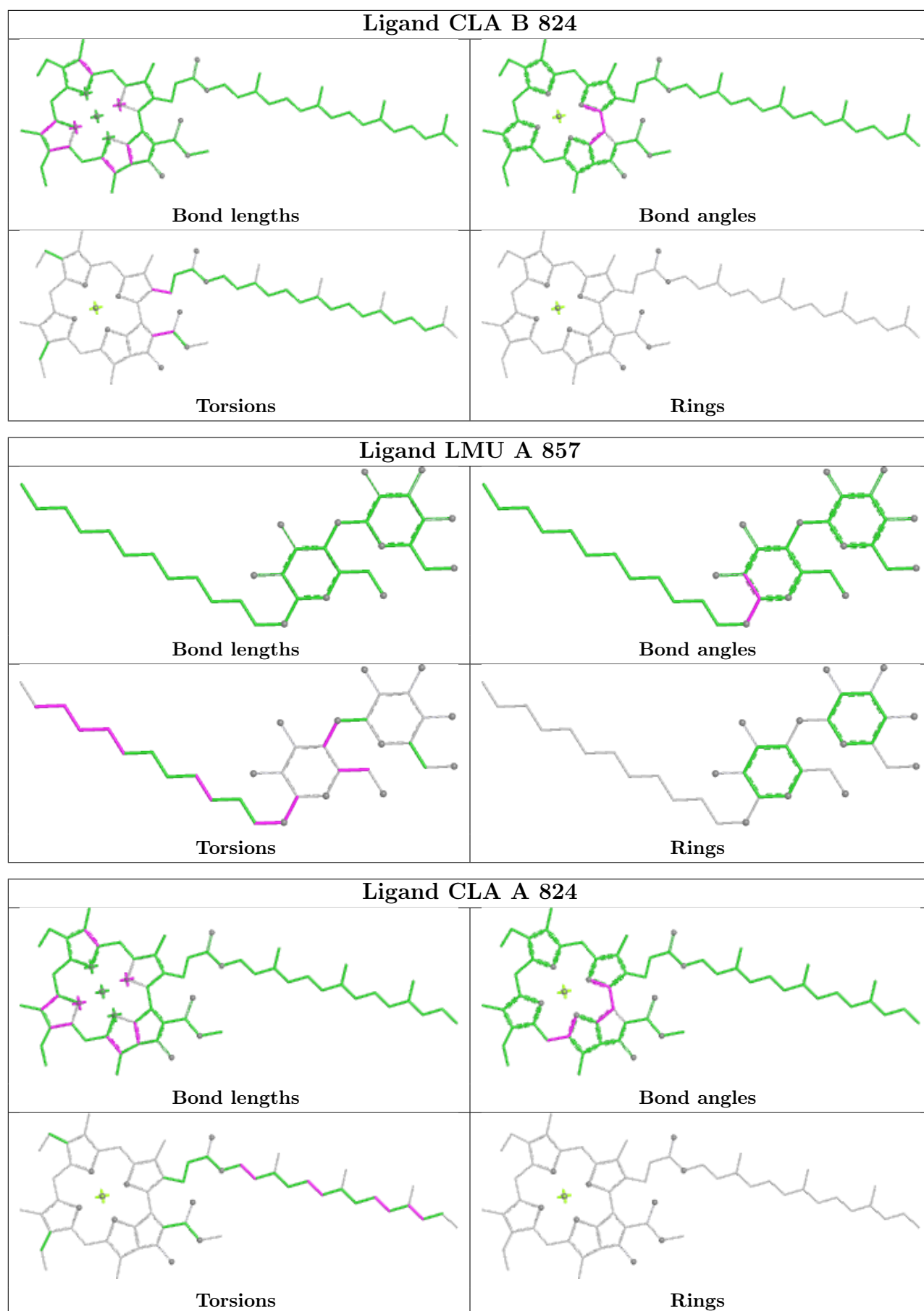
Bond angles

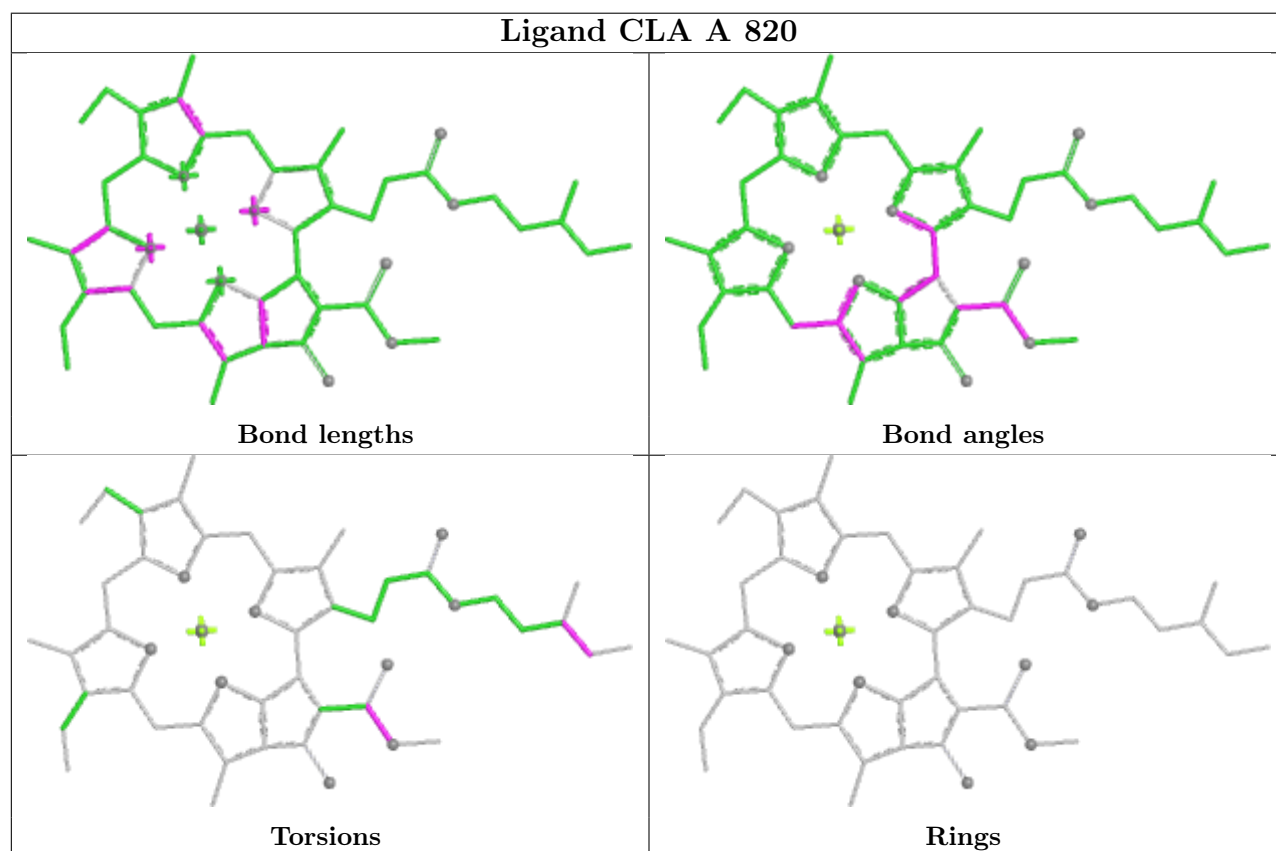
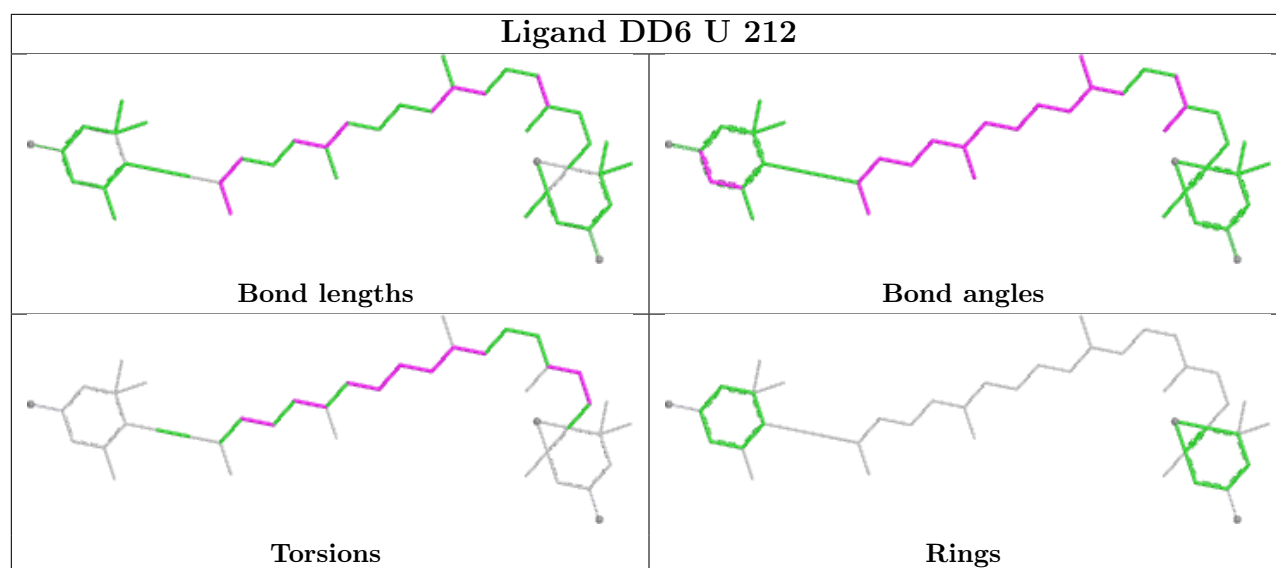


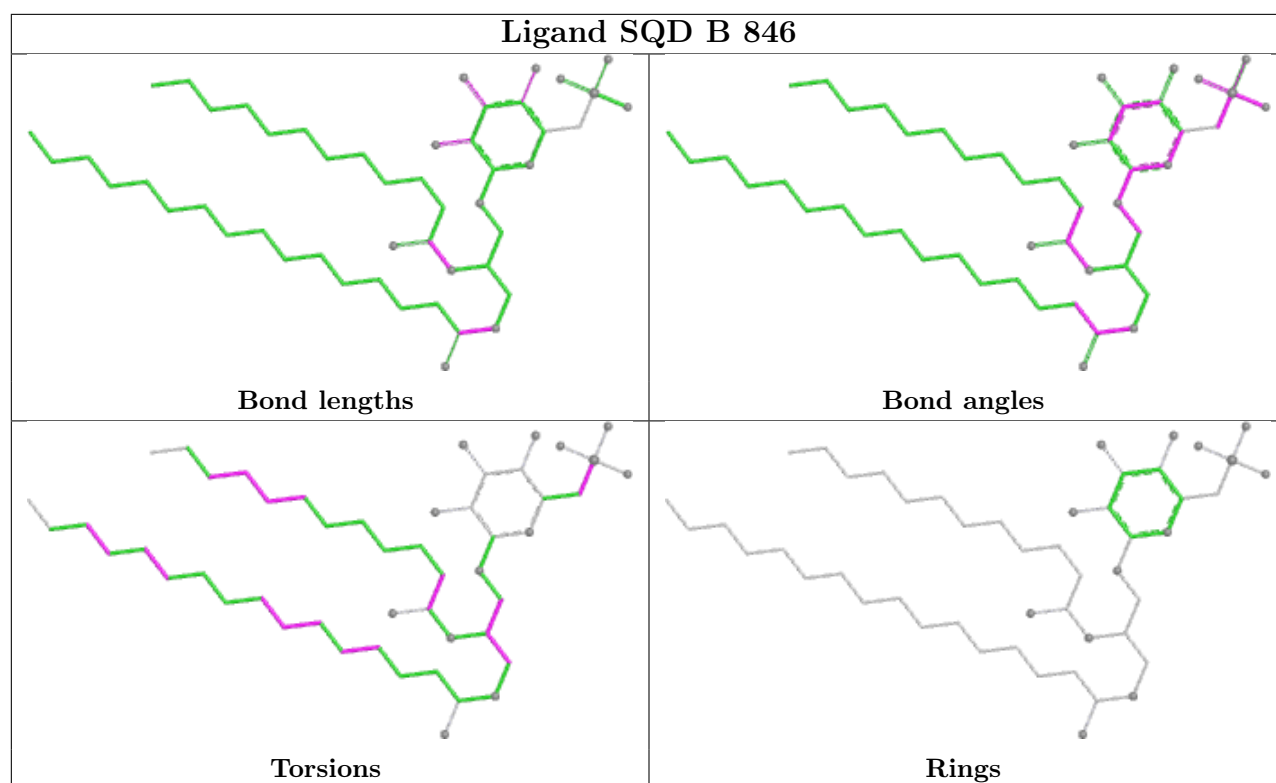
Torsions



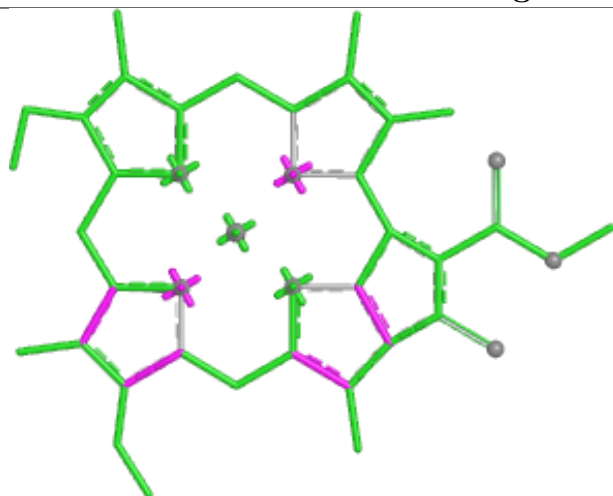
Rings



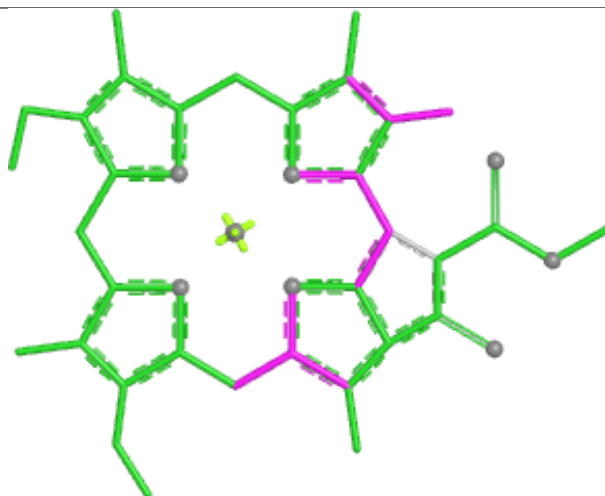




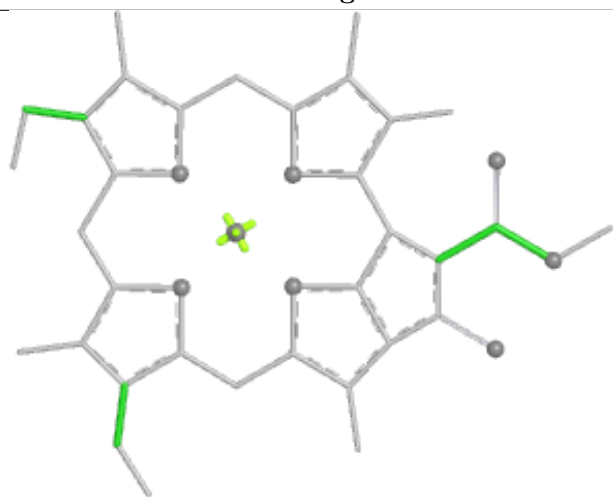
## Ligand CLA G 202



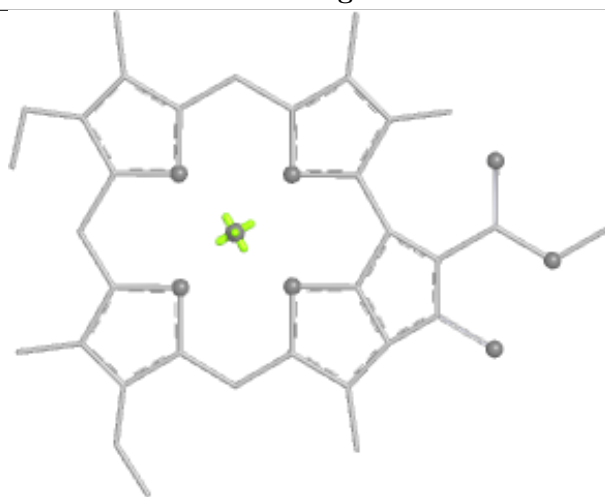
Bond lengths



Bond angles

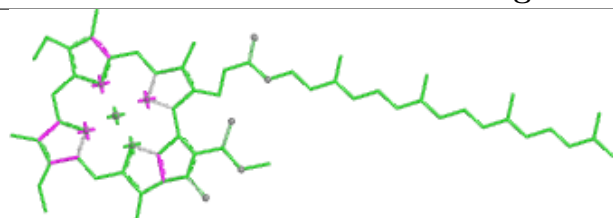


Torsions

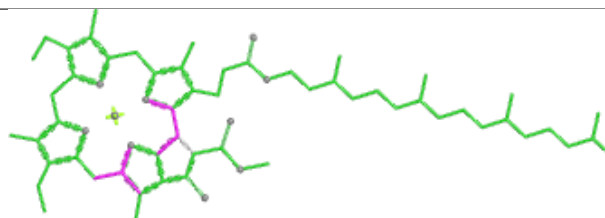


Rings

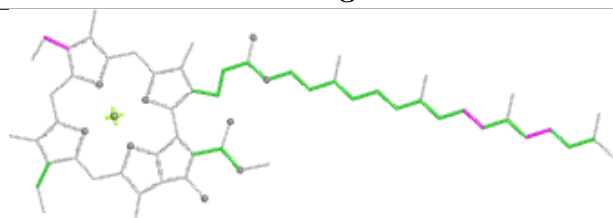
## Ligand CLA A 833



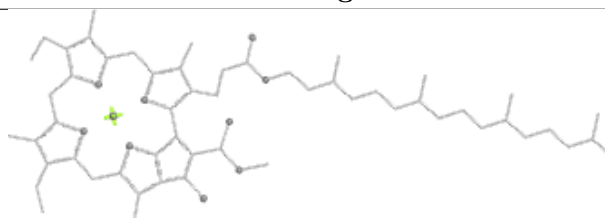
Bond lengths



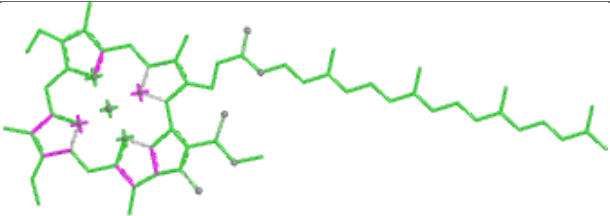
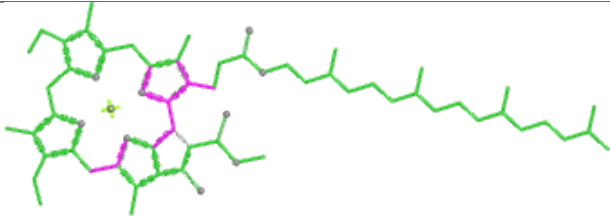
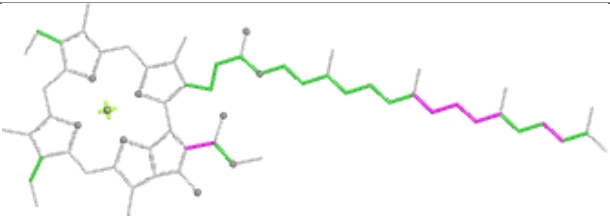
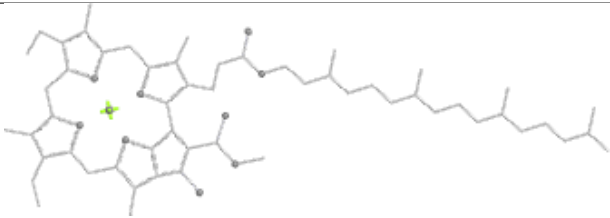
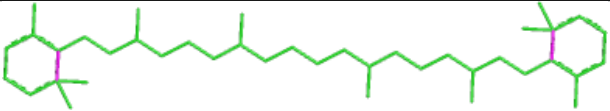
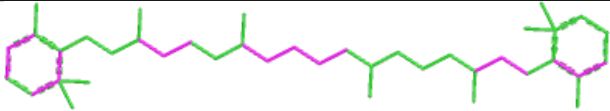

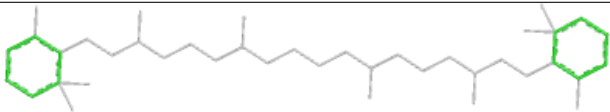
Bond angles

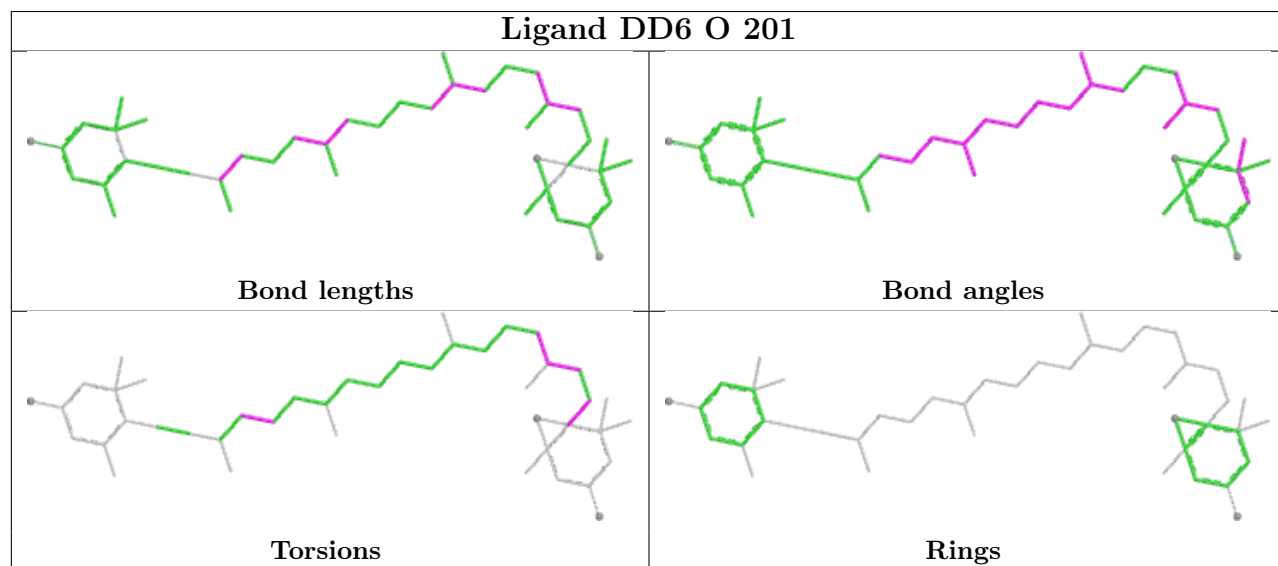
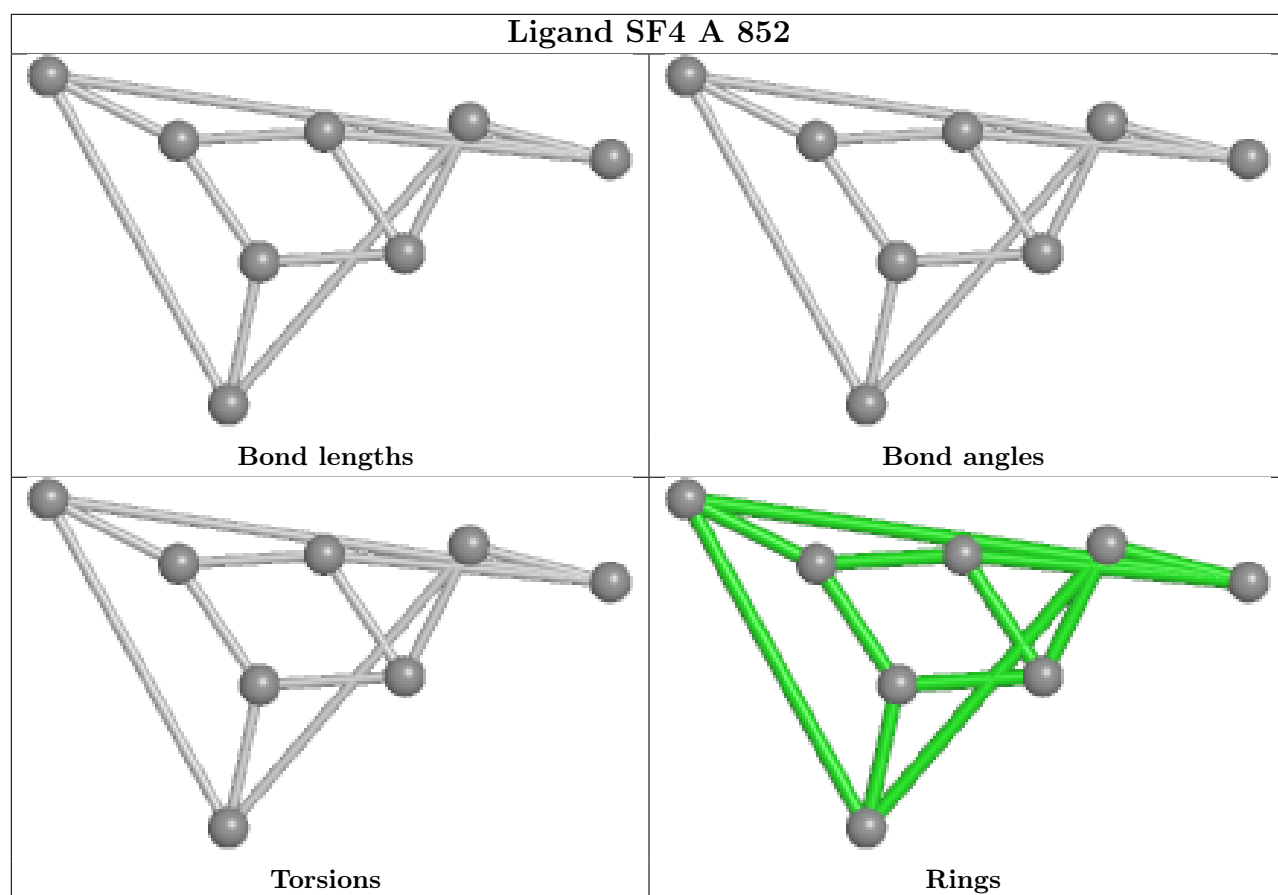


Torsions

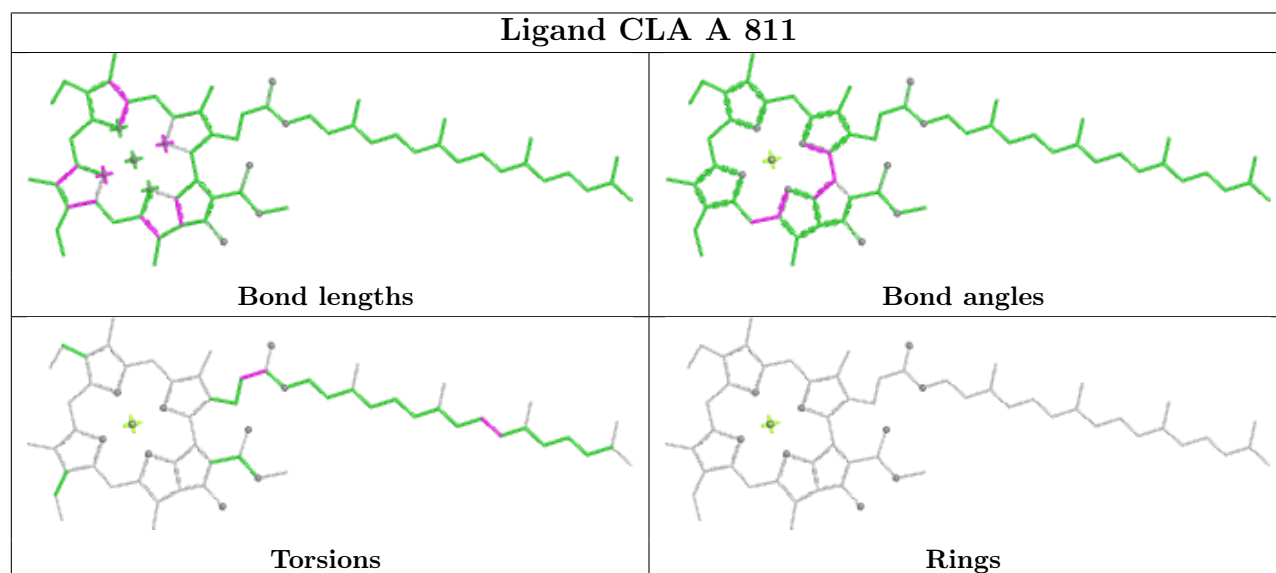
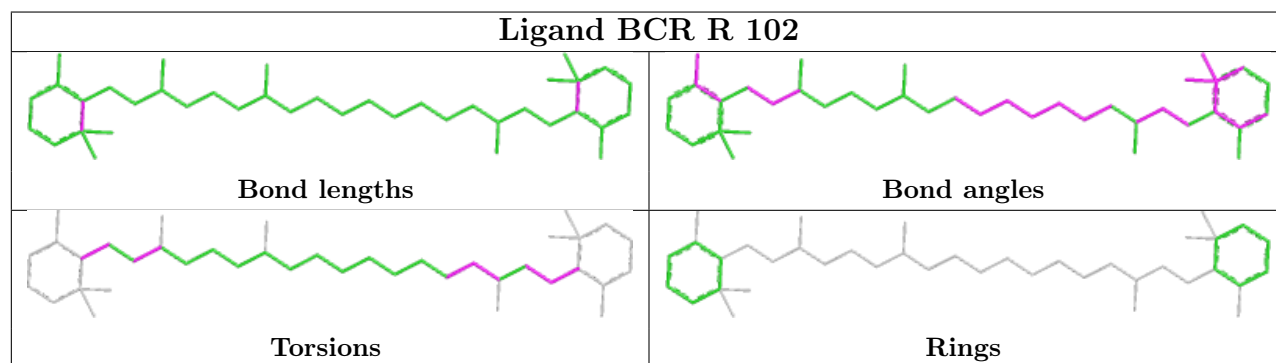
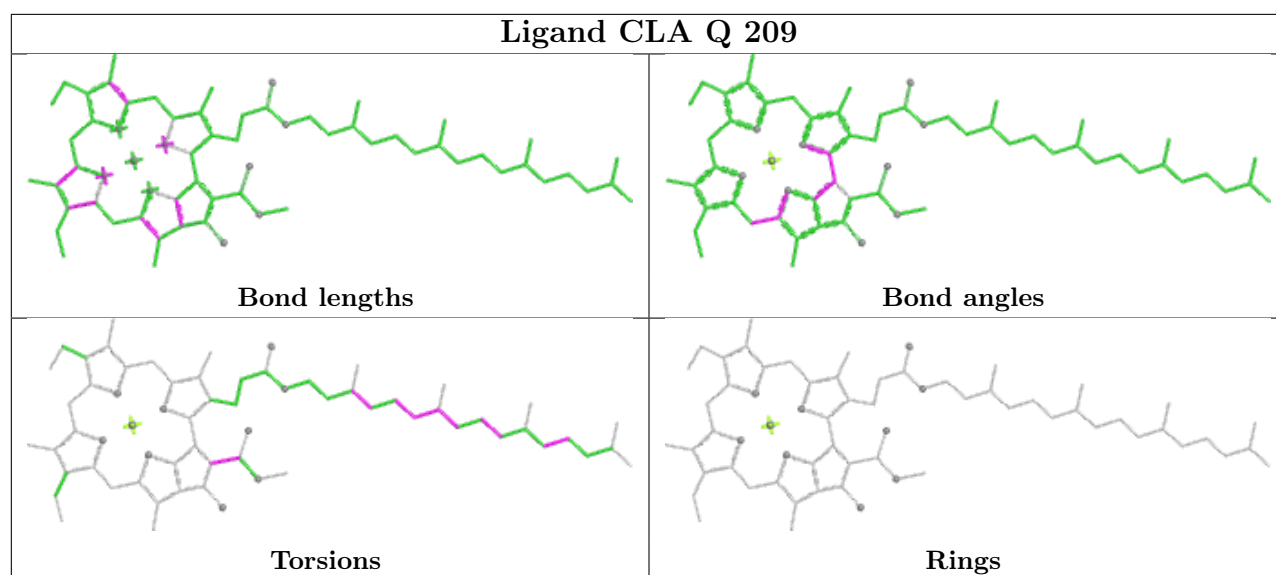


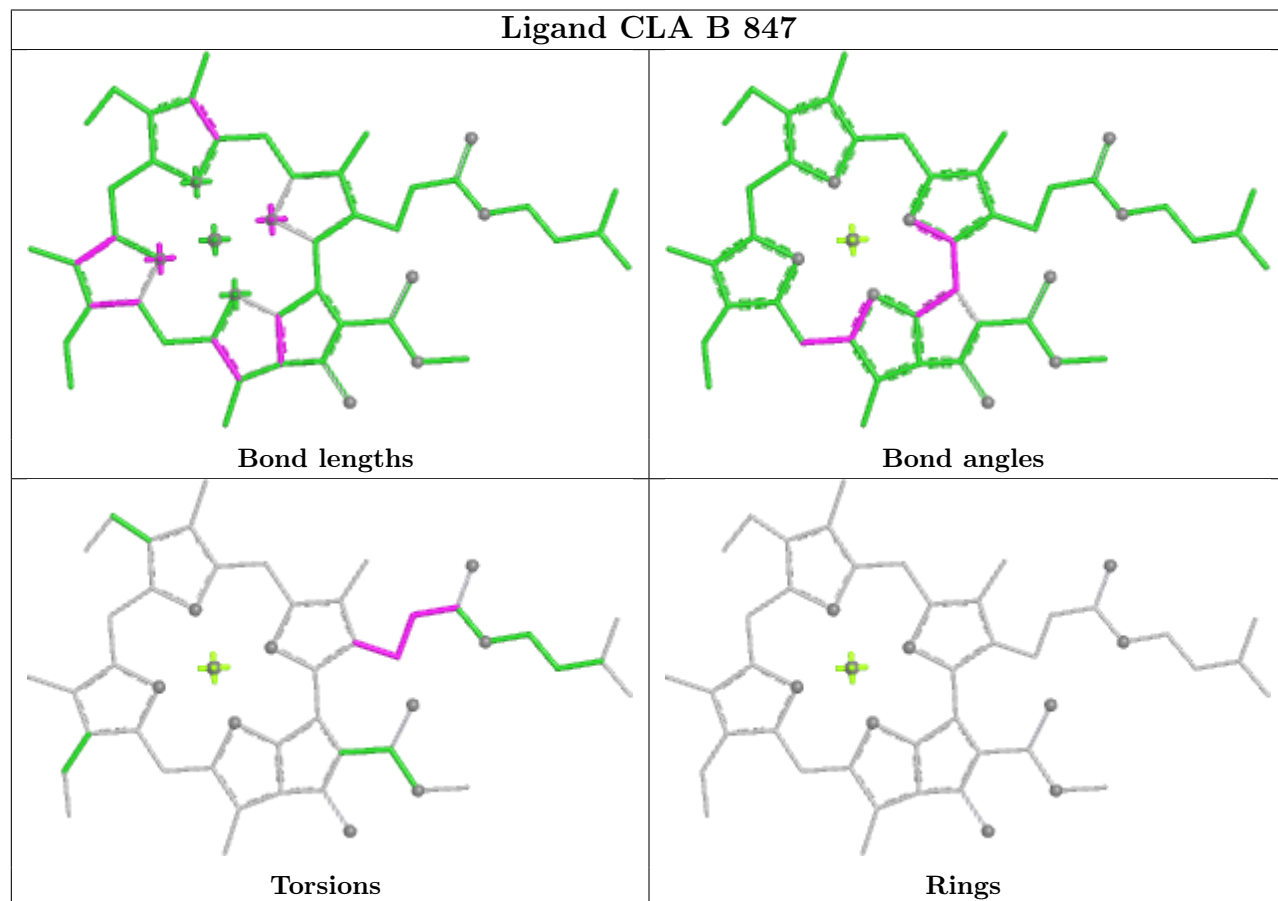
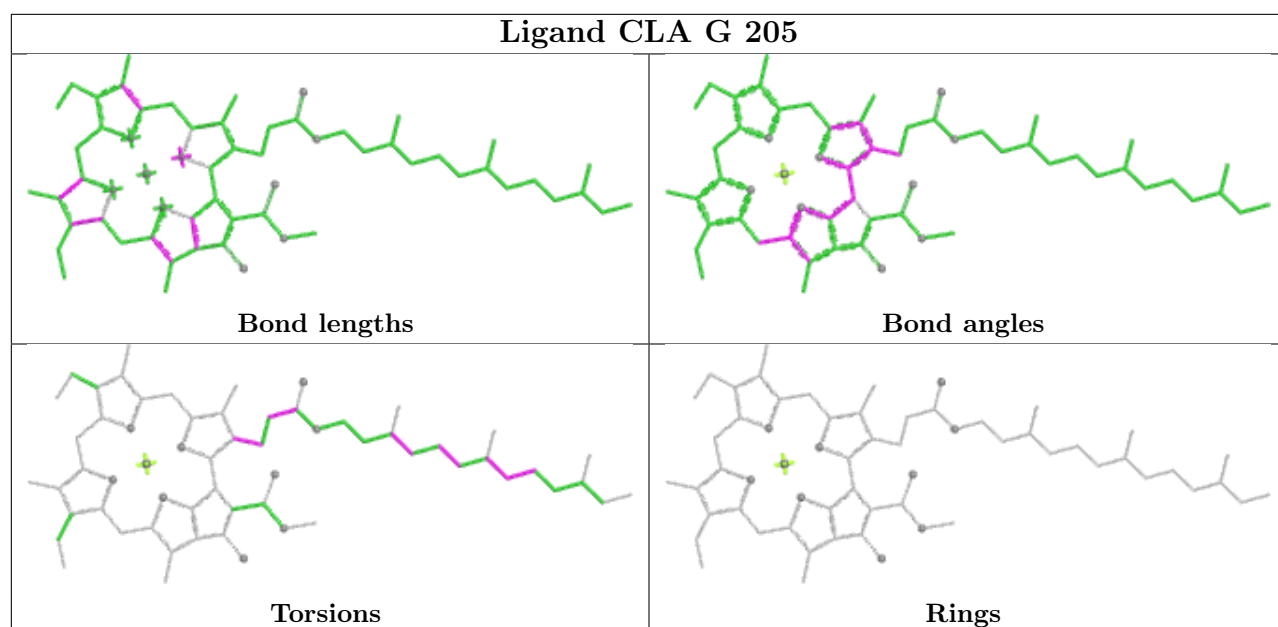
Rings

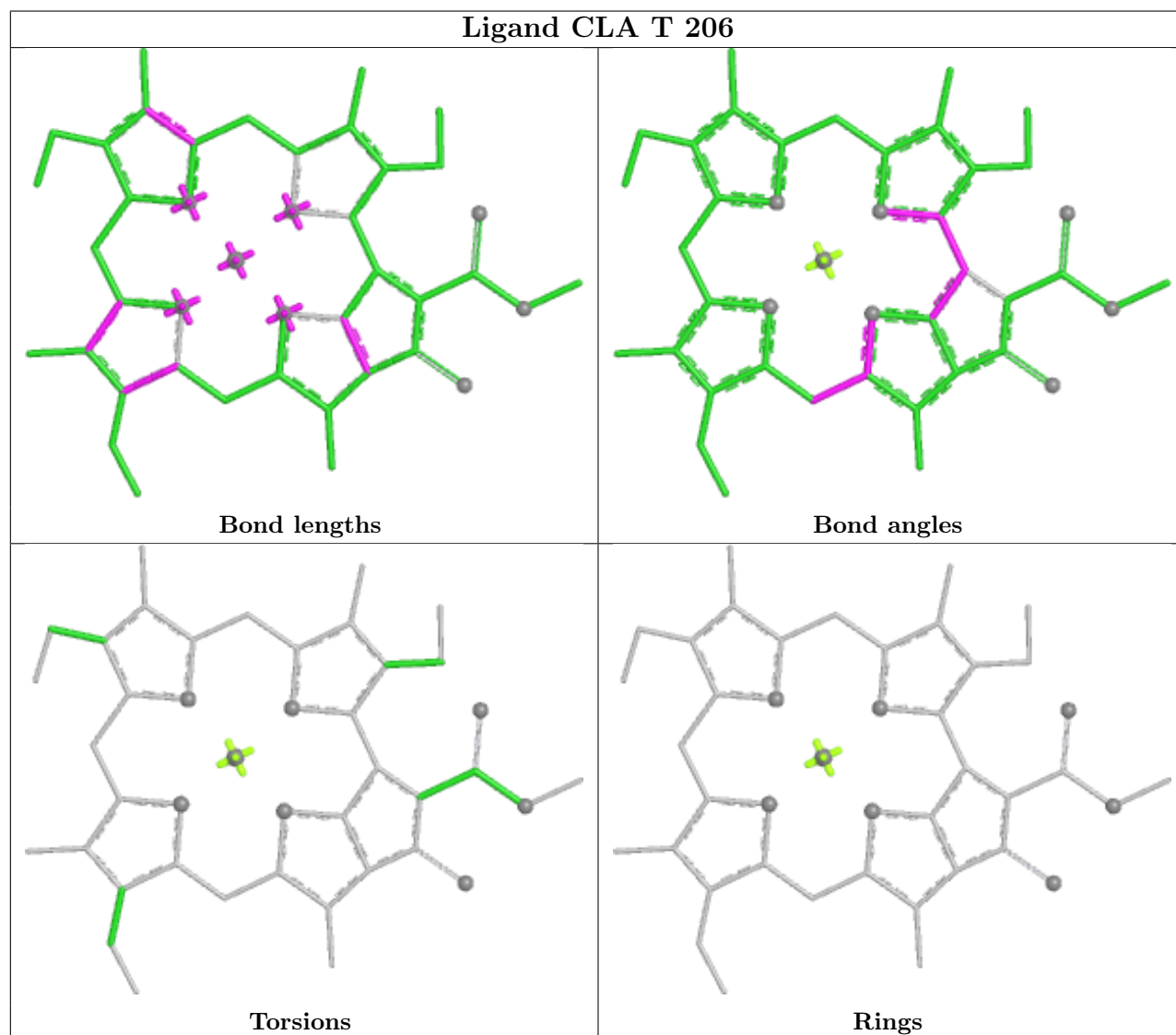
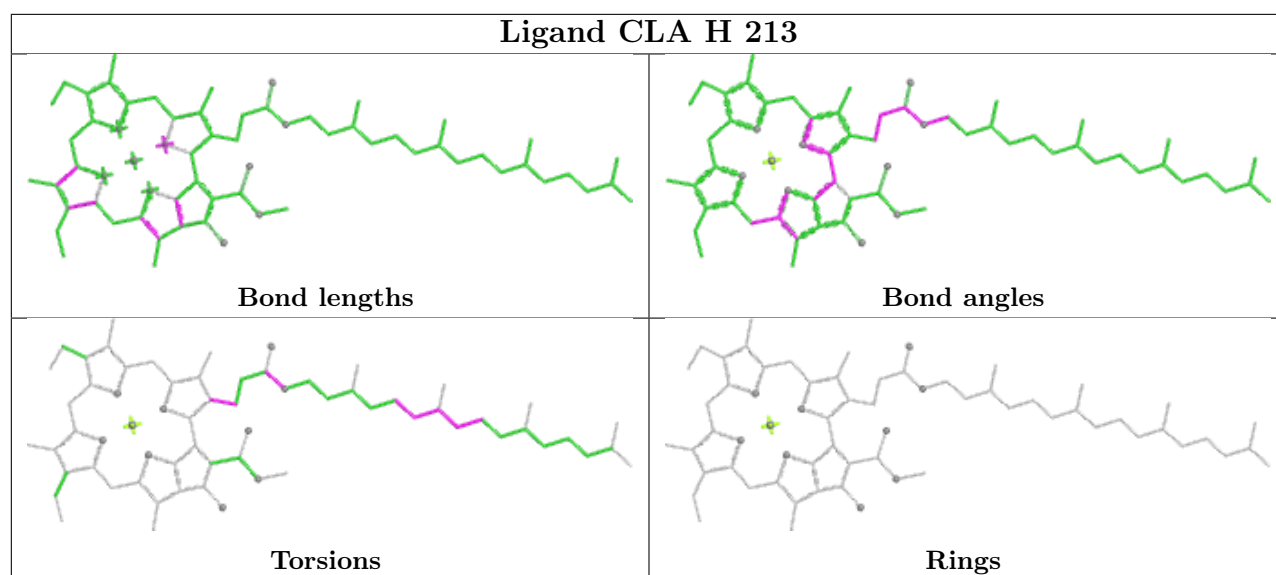
Ligand CLA Q 212	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR M 101	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



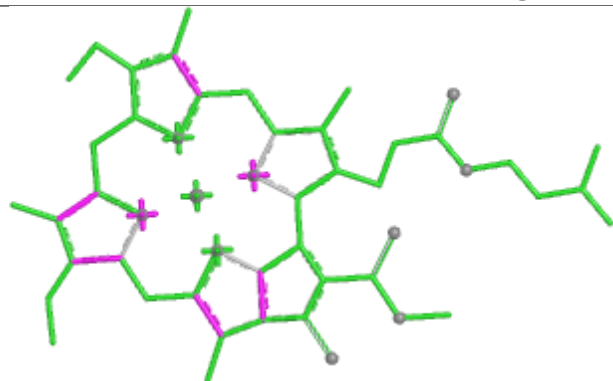




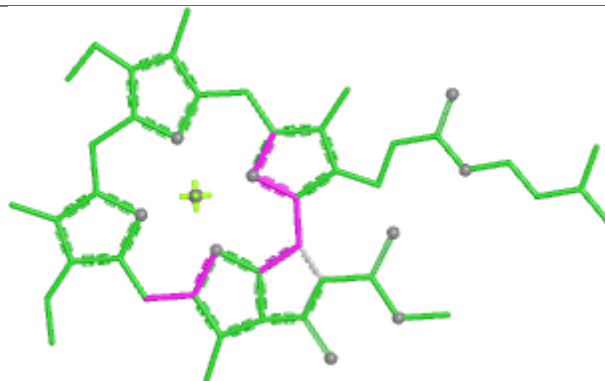




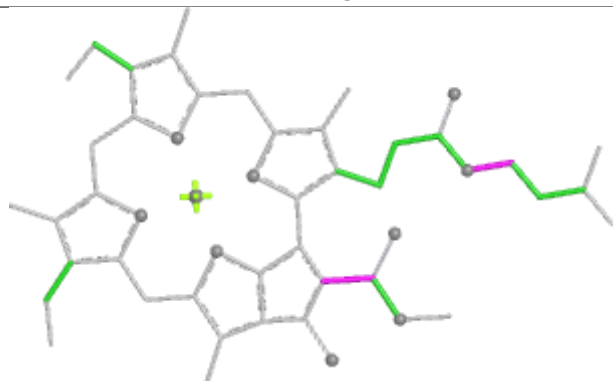
## Ligand CLA A 827



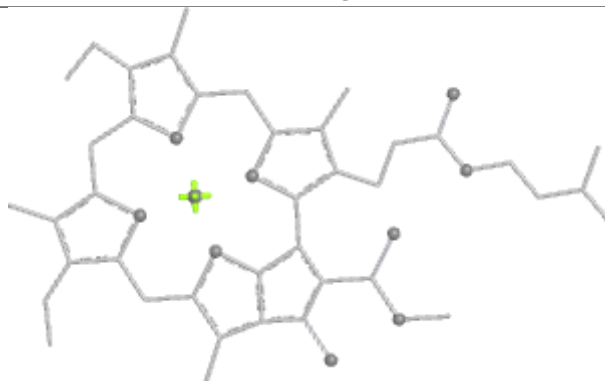
Bond lengths



Bond angles

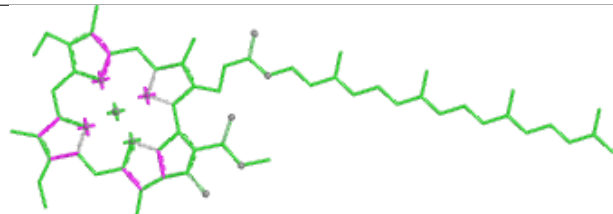


Torsions

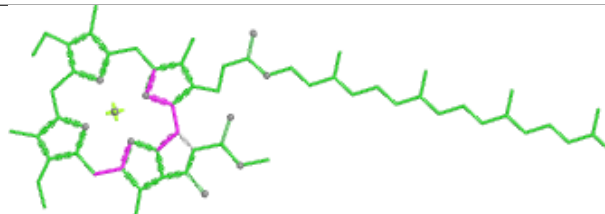


Rings

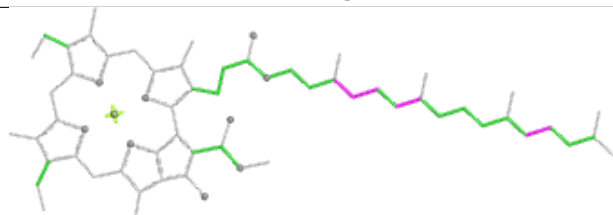
## Ligand CLA A 834



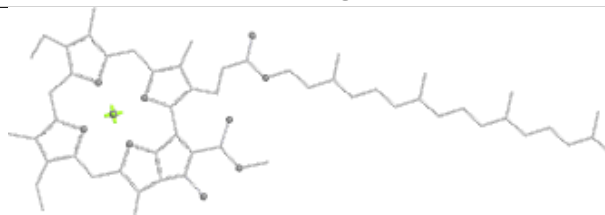
Bond lengths



Bond angles

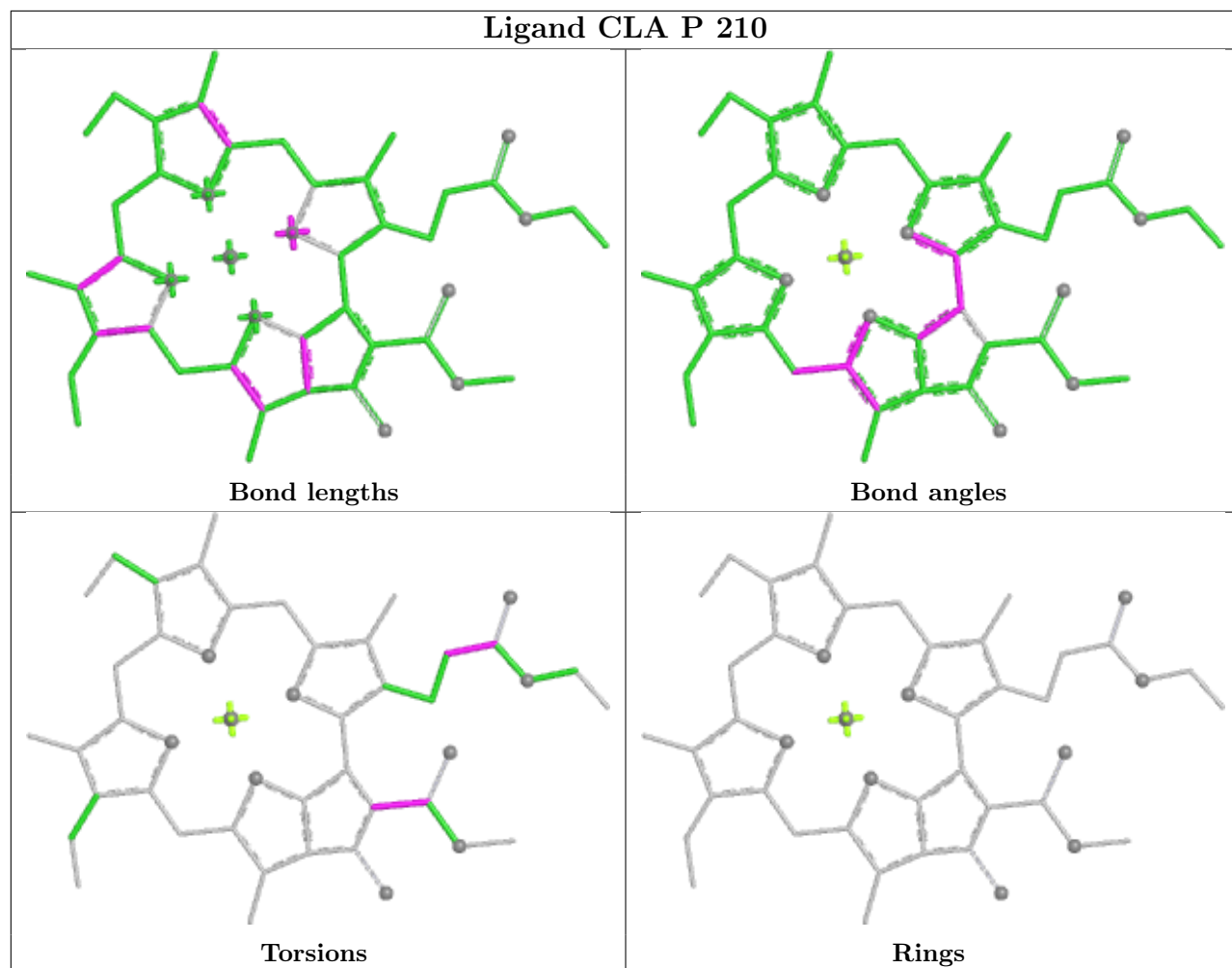


Torsions

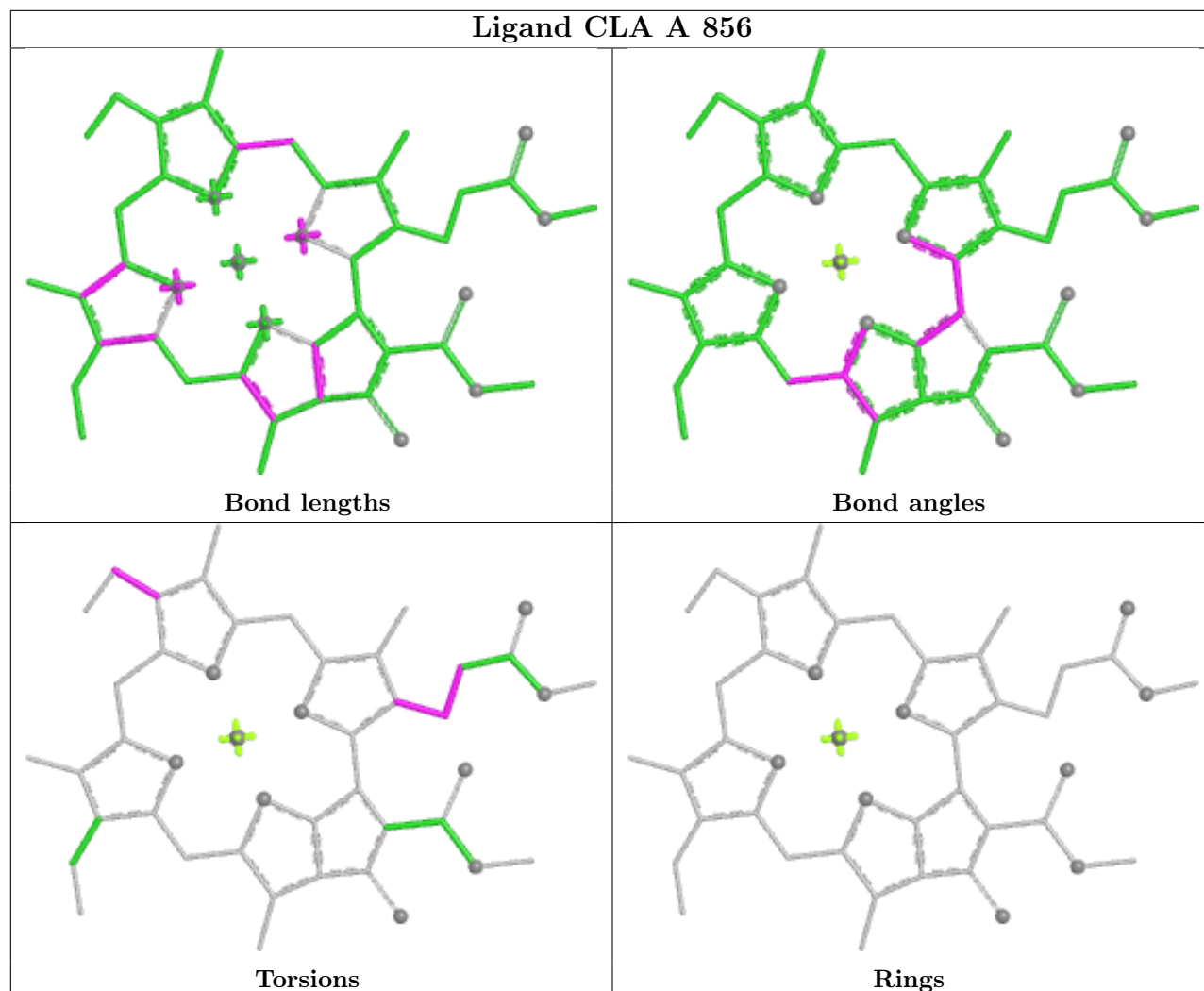


Rings

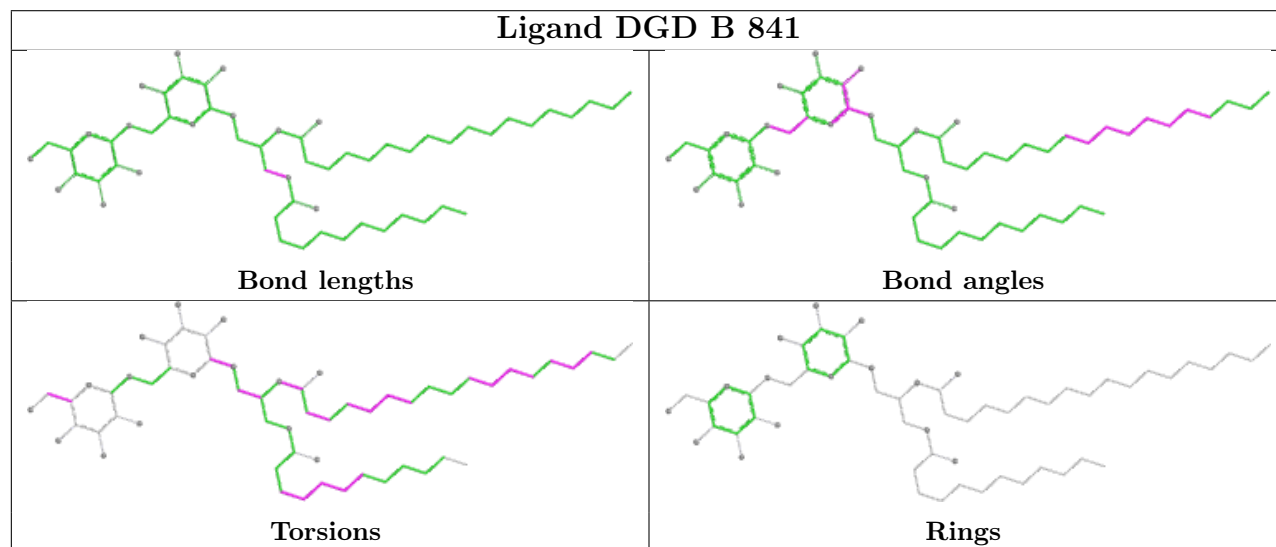
## Ligand CLA P 210

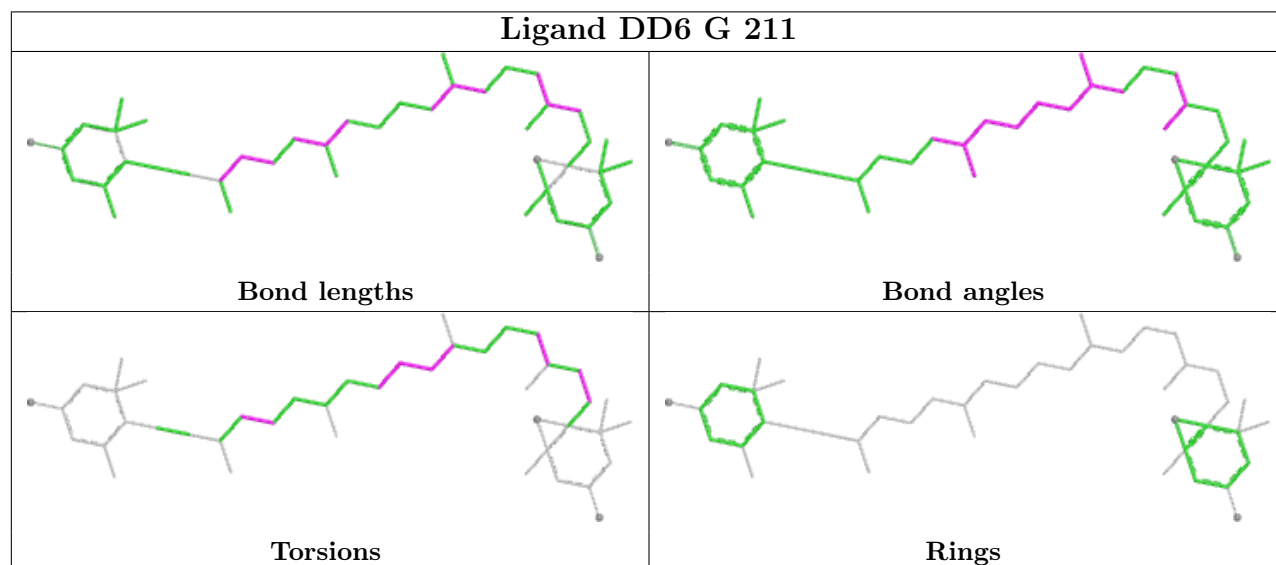
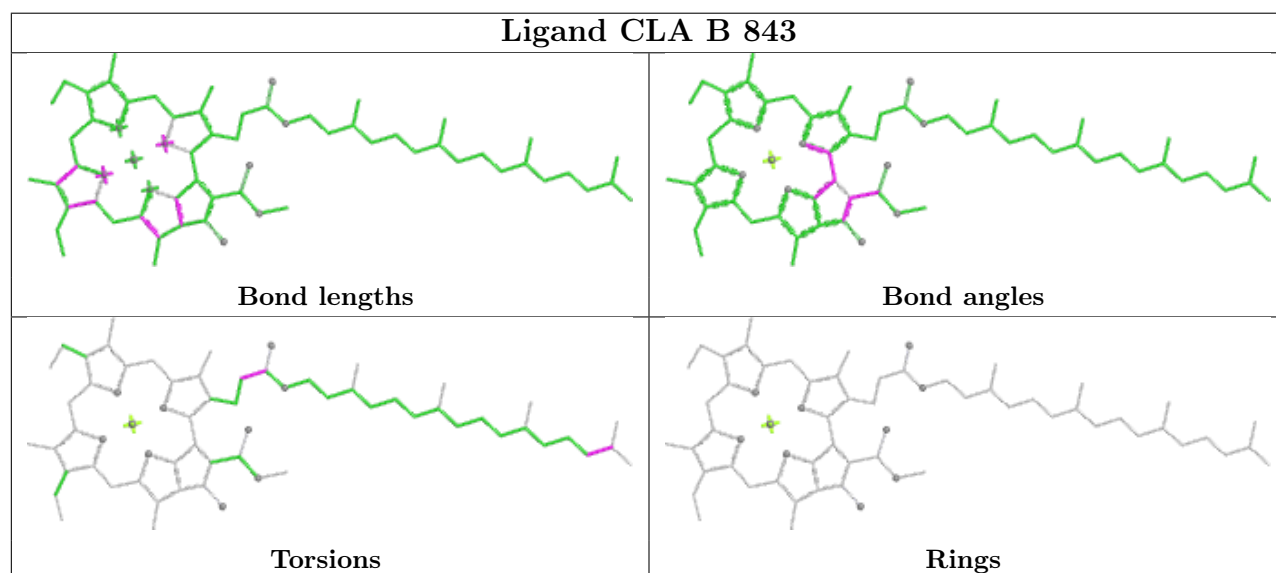
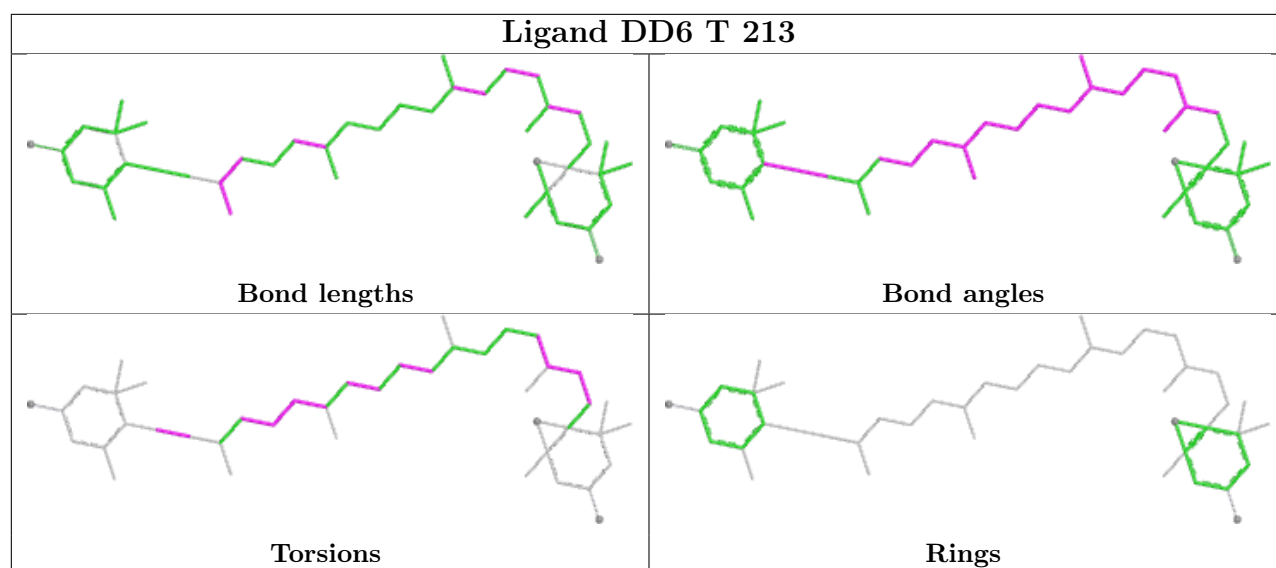


## Ligand CLA A 856

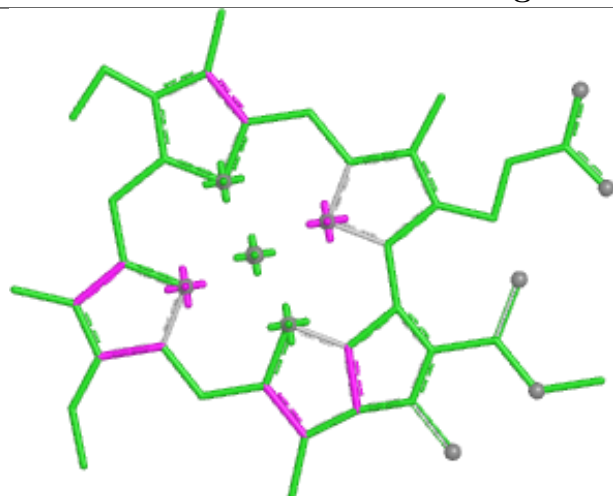


## Ligand DGD B 841

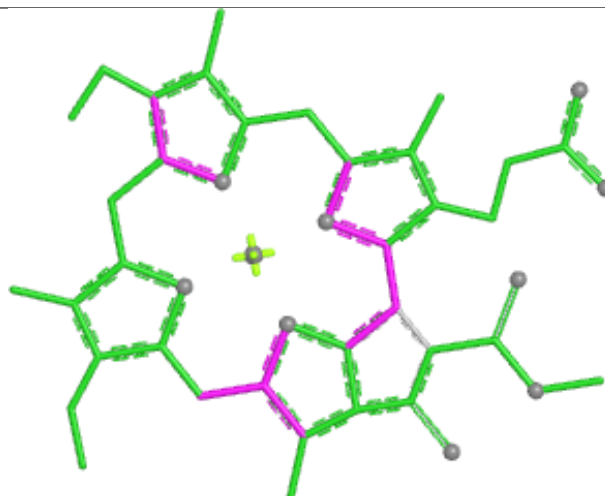




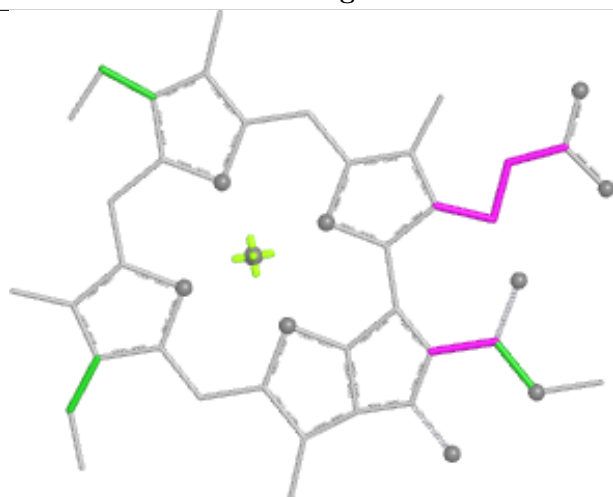
## Ligand CLA A 814



Bond lengths



Bond angles



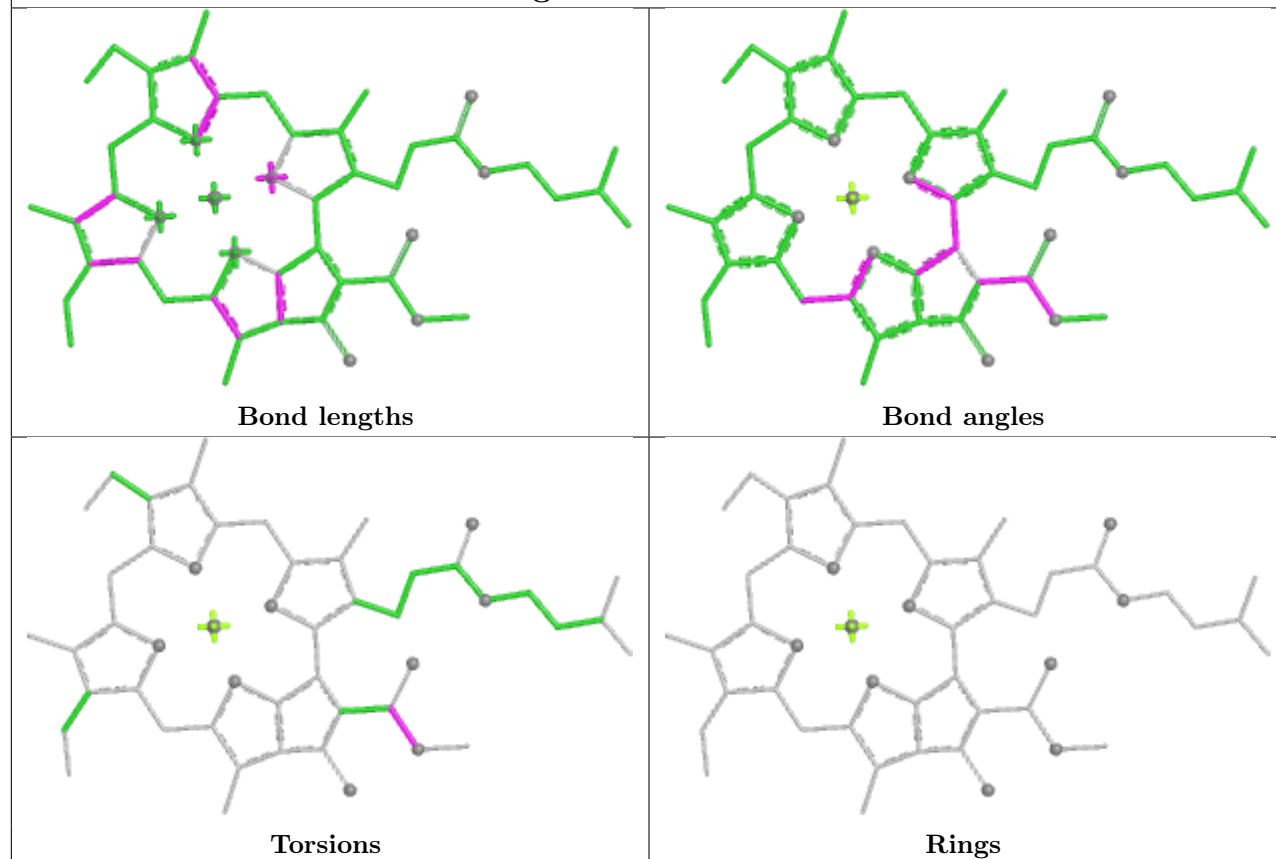
Torsions



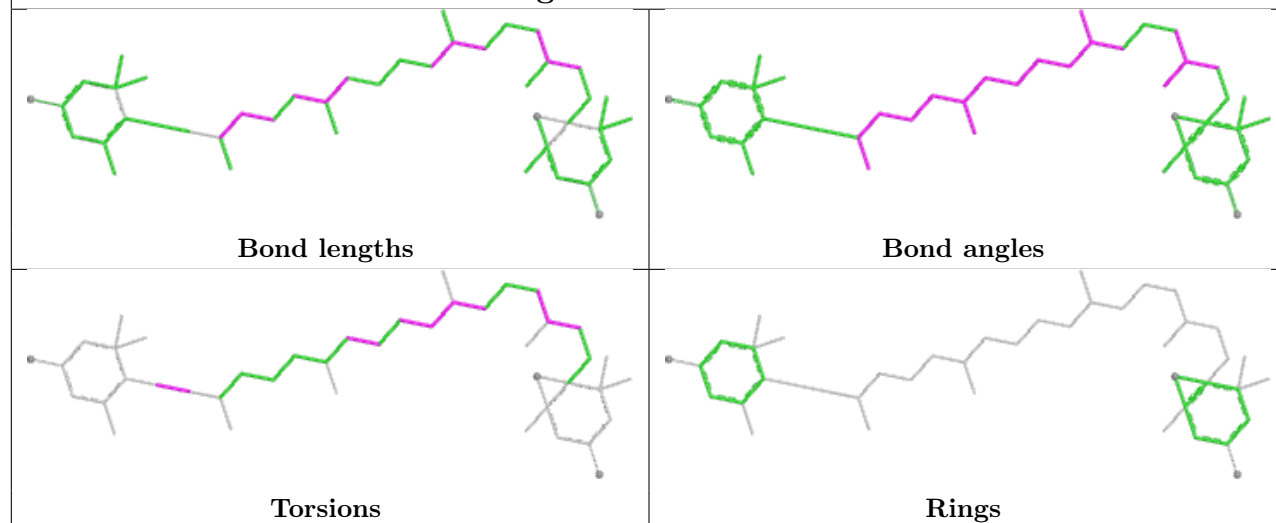
Rings

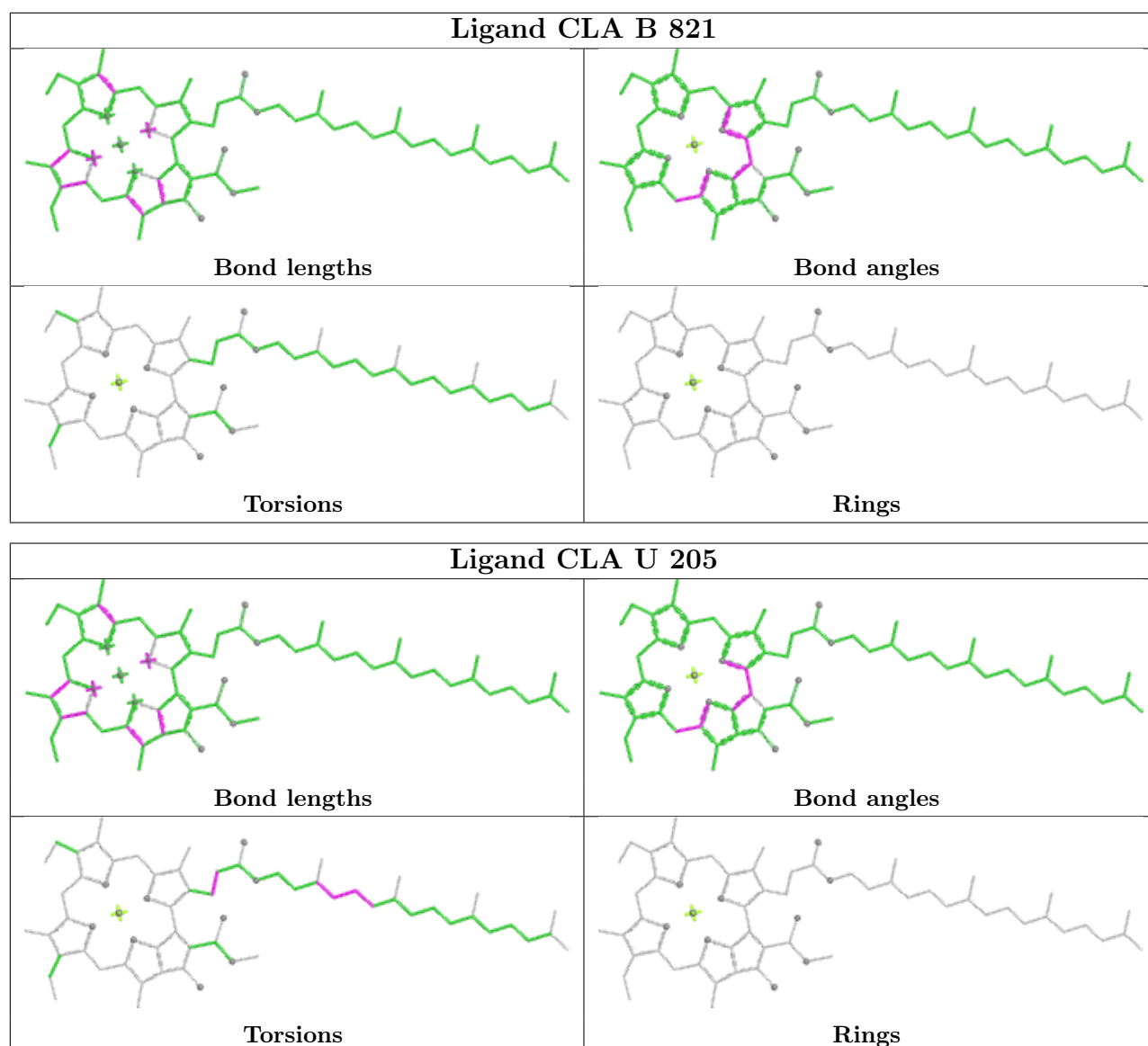


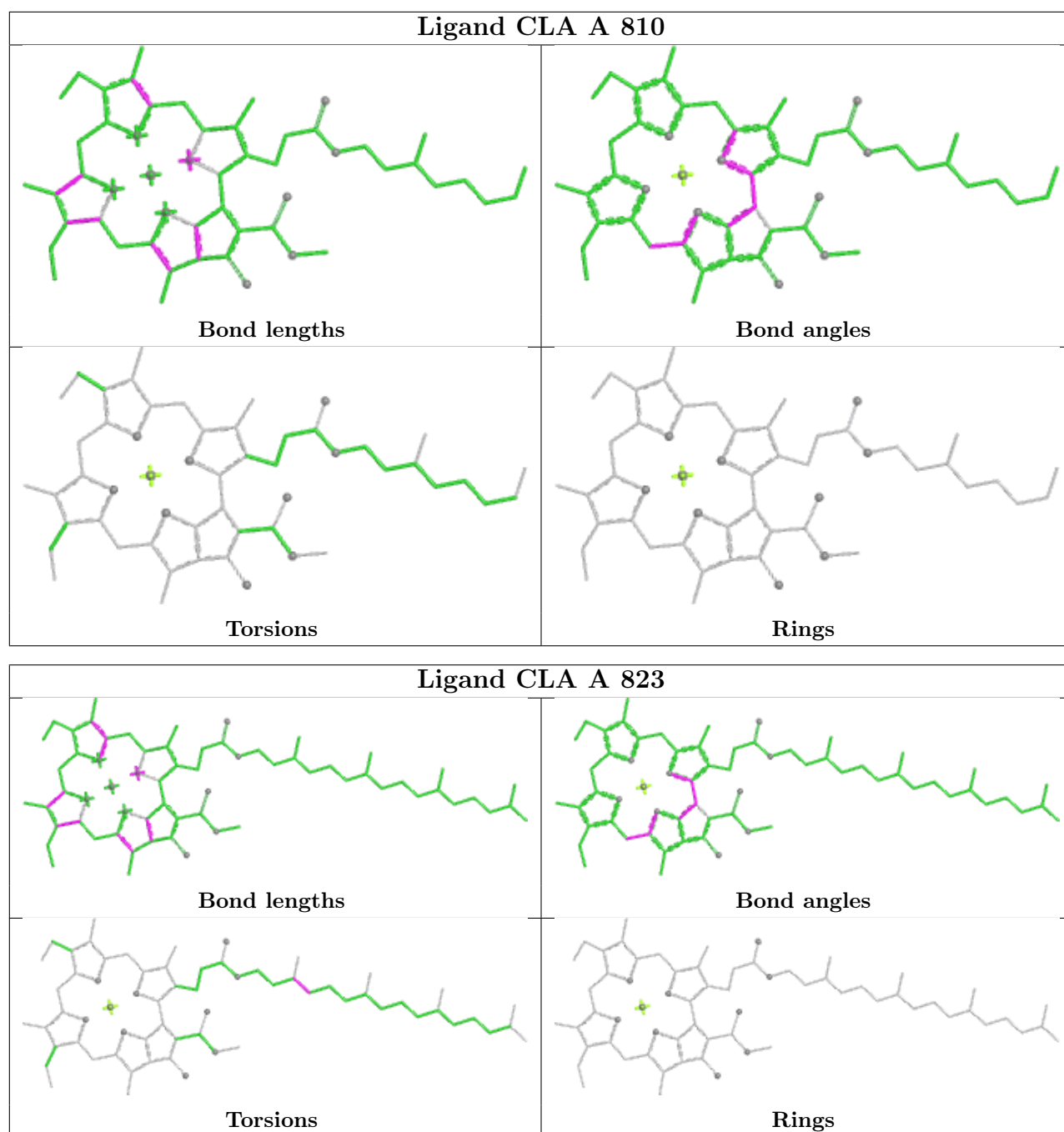
## Ligand CLA P 211



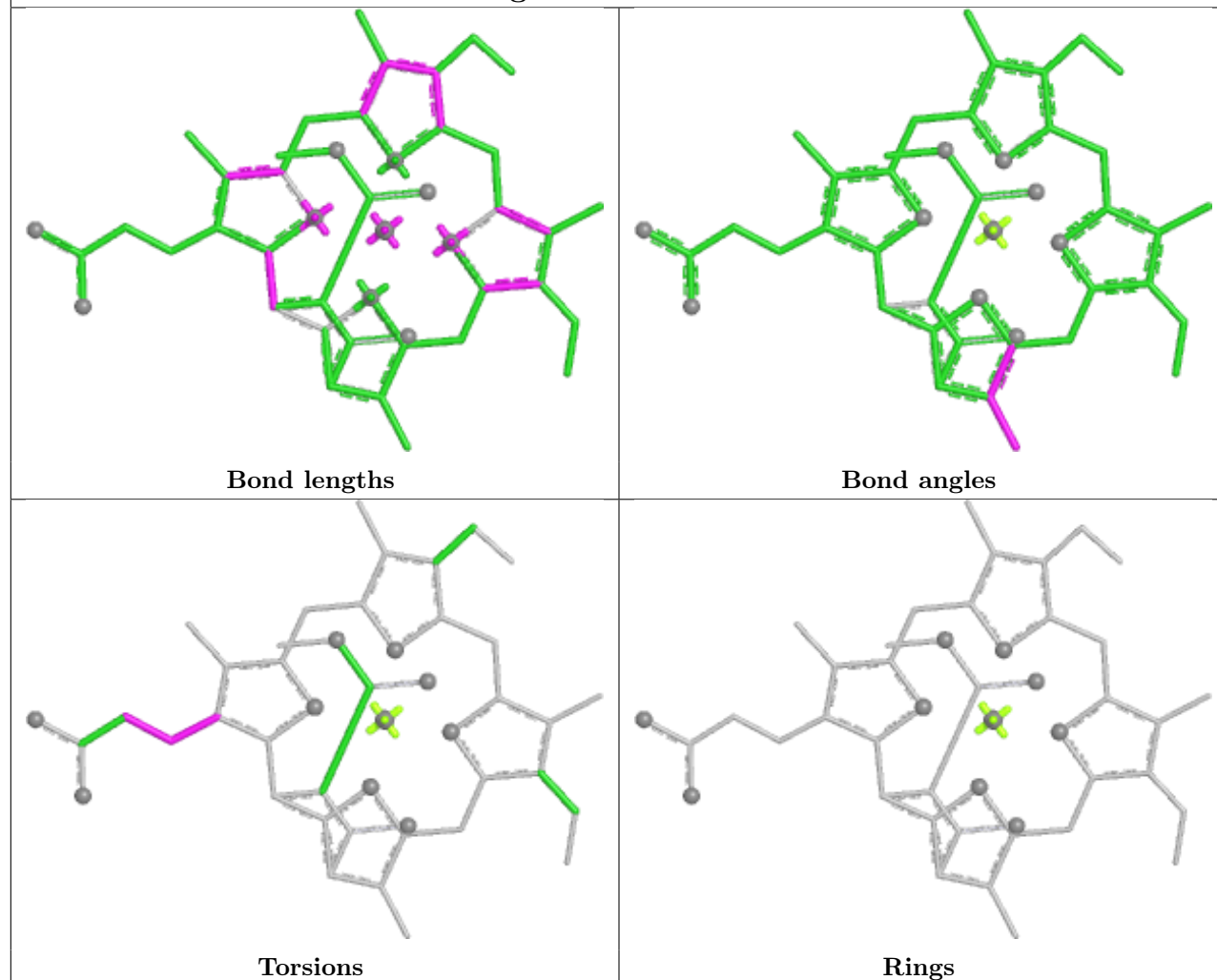
## Ligand DD6 k 101



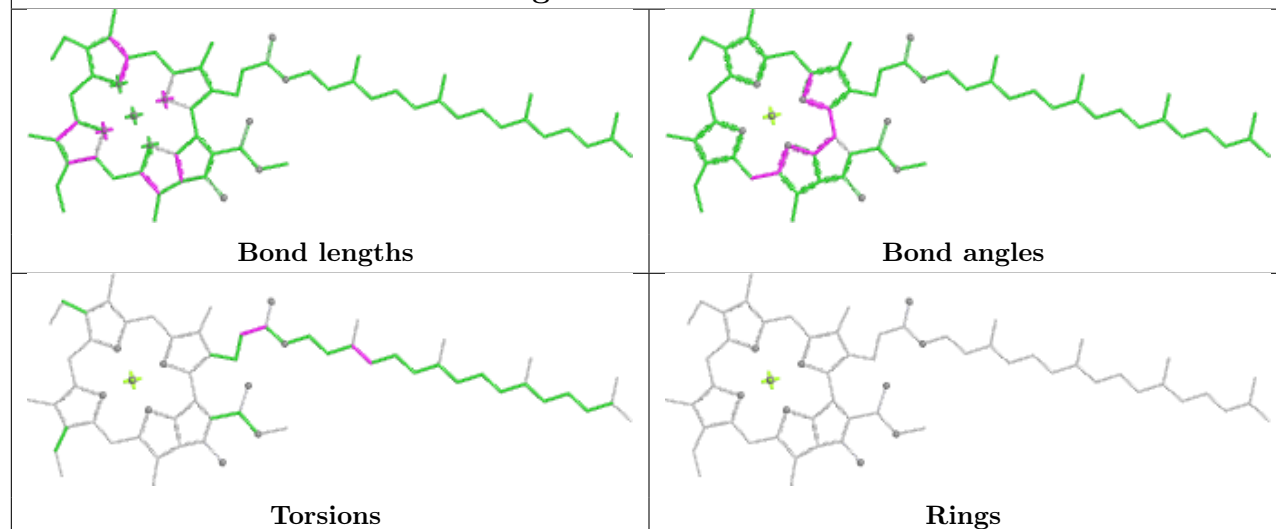


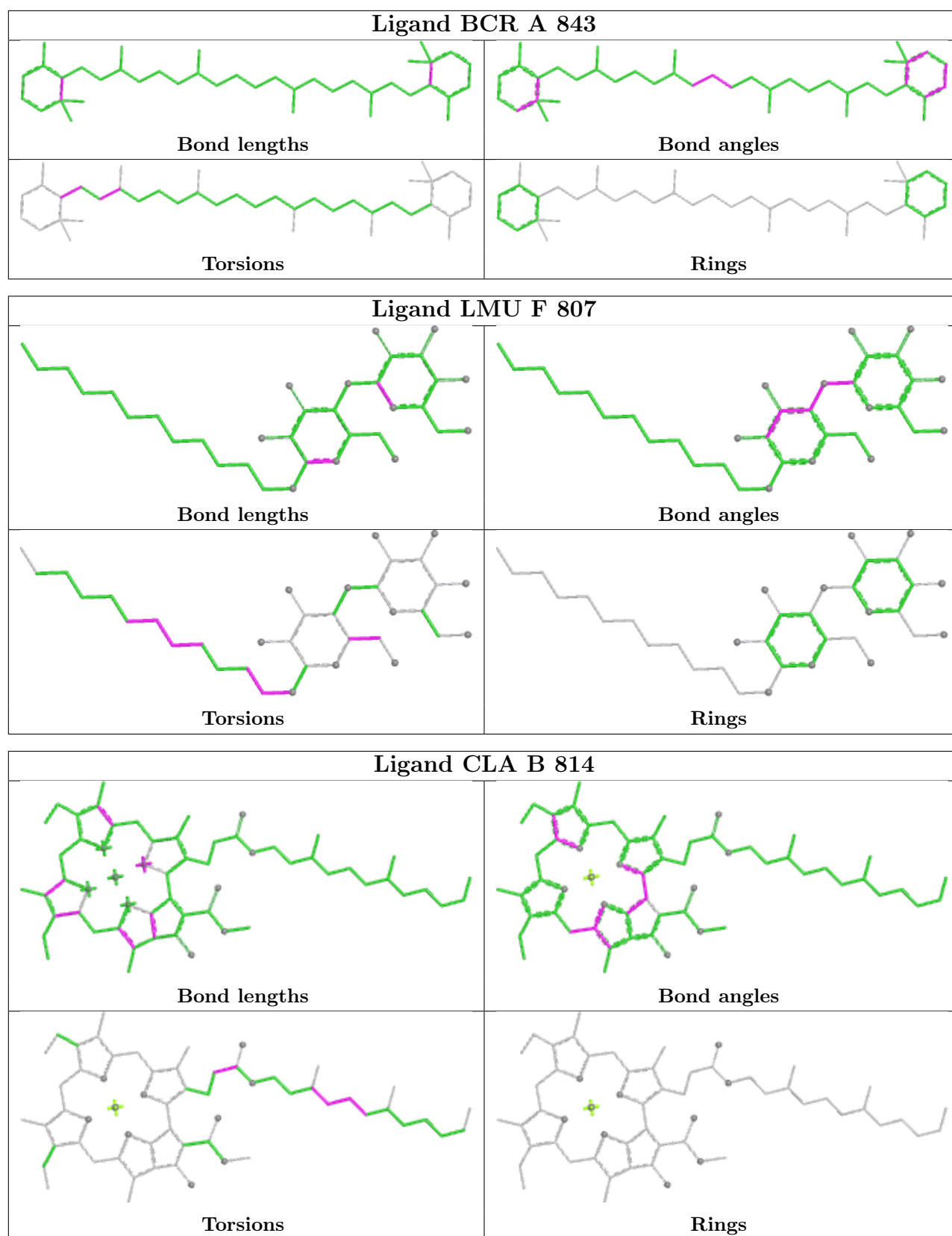


## Ligand KC1 P 219

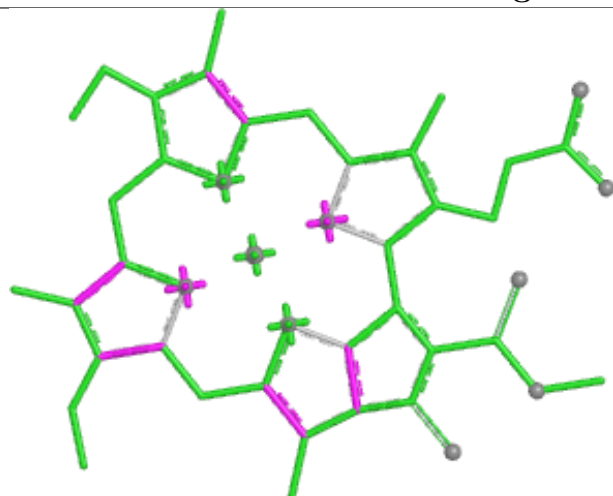


## Ligand CLA B 808

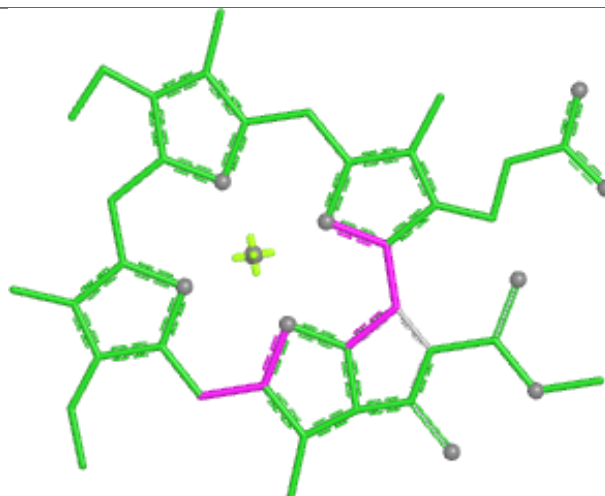




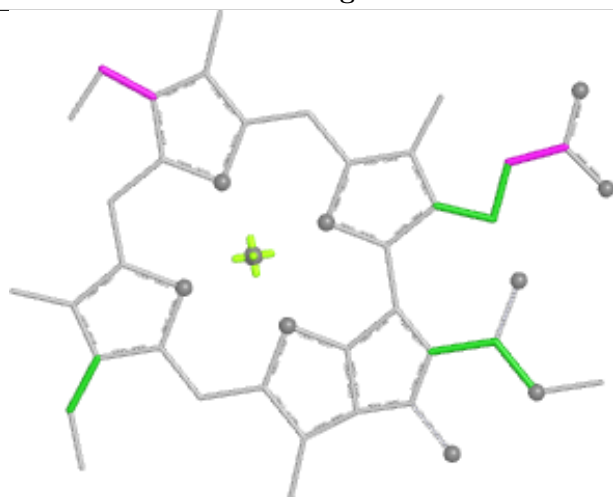
## Ligand CLA U 206



Bond lengths



Bond angles

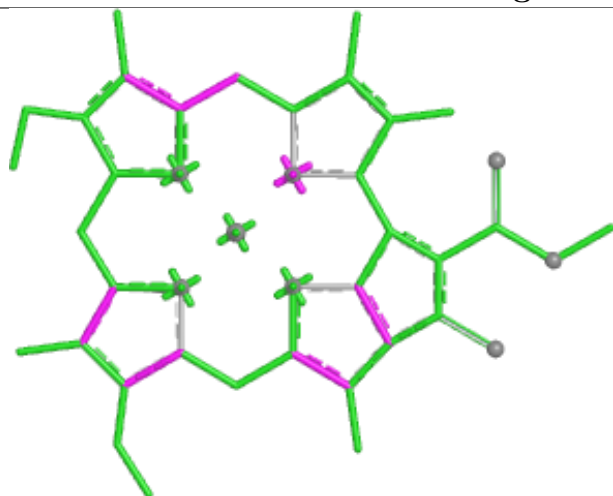


Torsions

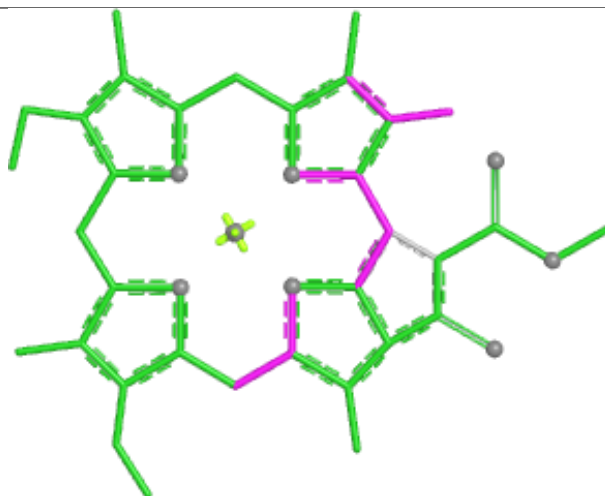


Rings

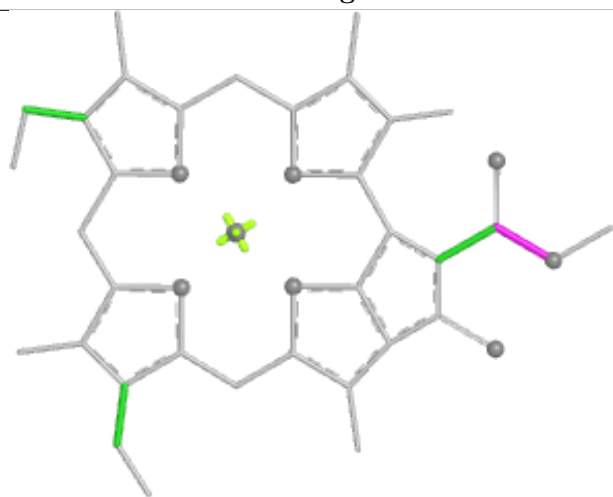
## Ligand CLA H 209



Bond lengths



Bond angles

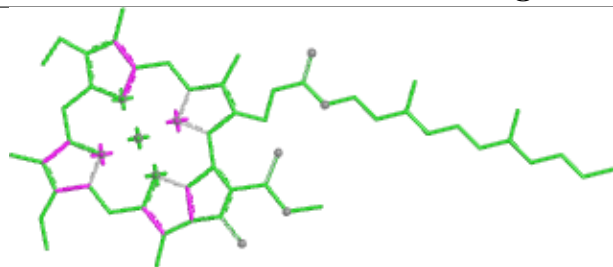


Torsions

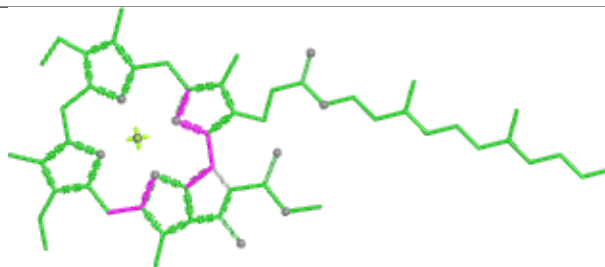


Rings

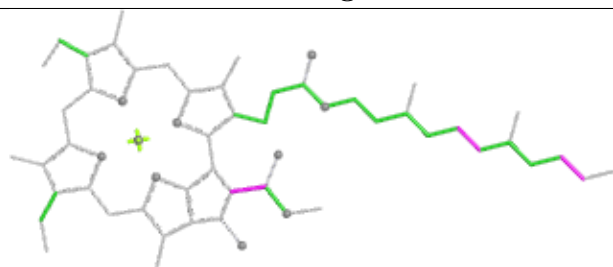
## Ligand CLA B 829



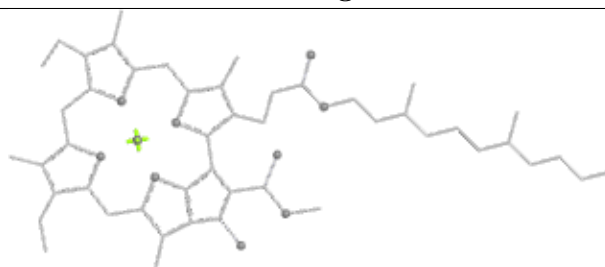
Bond lengths



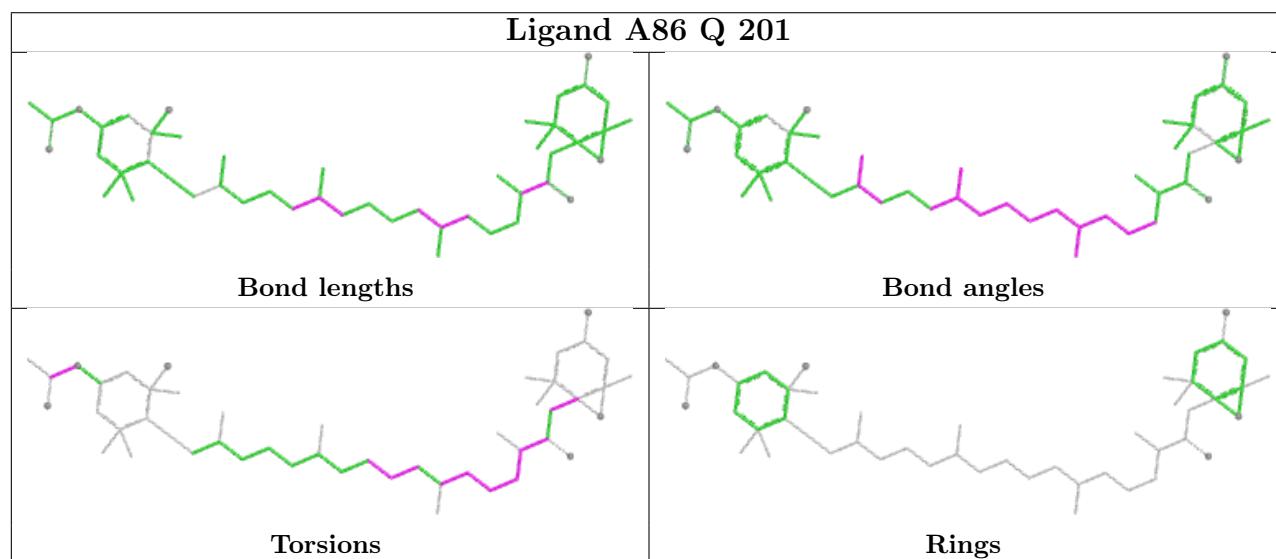
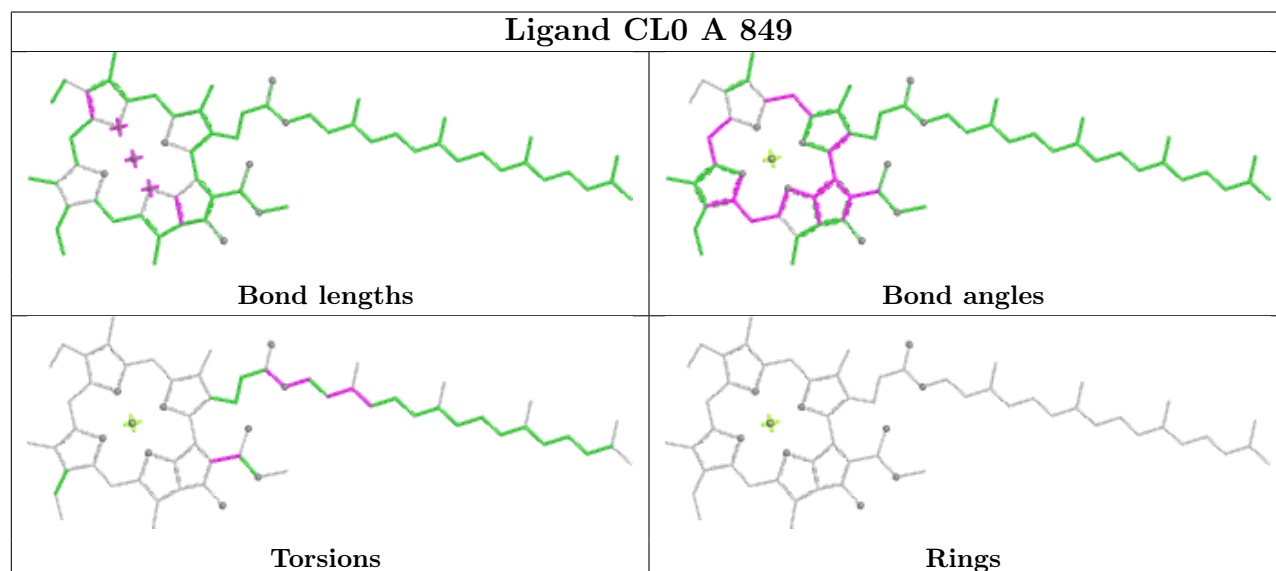
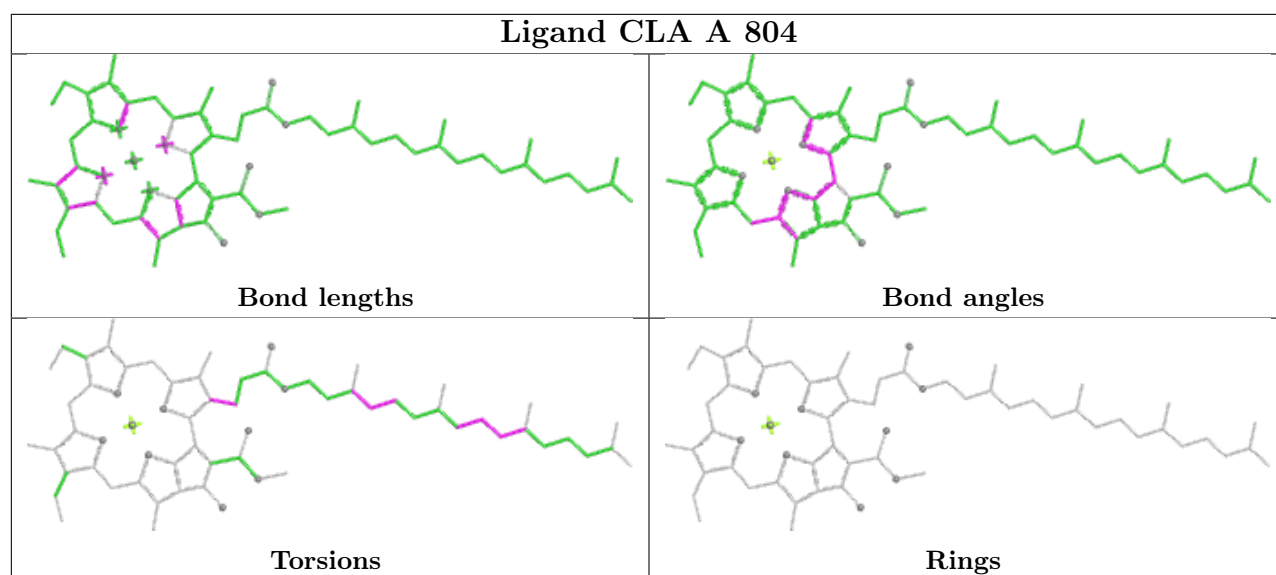
Bond angles



Torsions

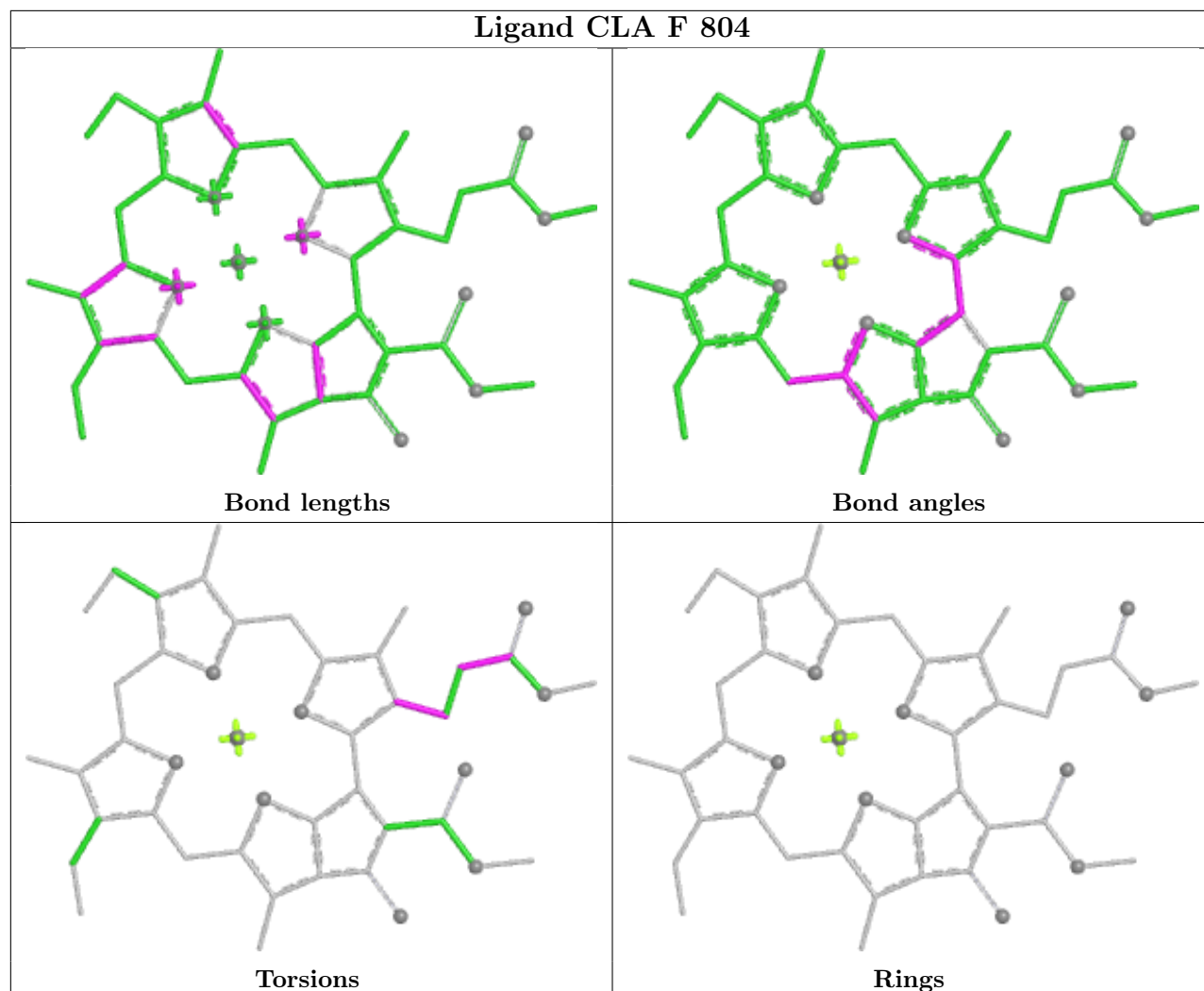


Rings

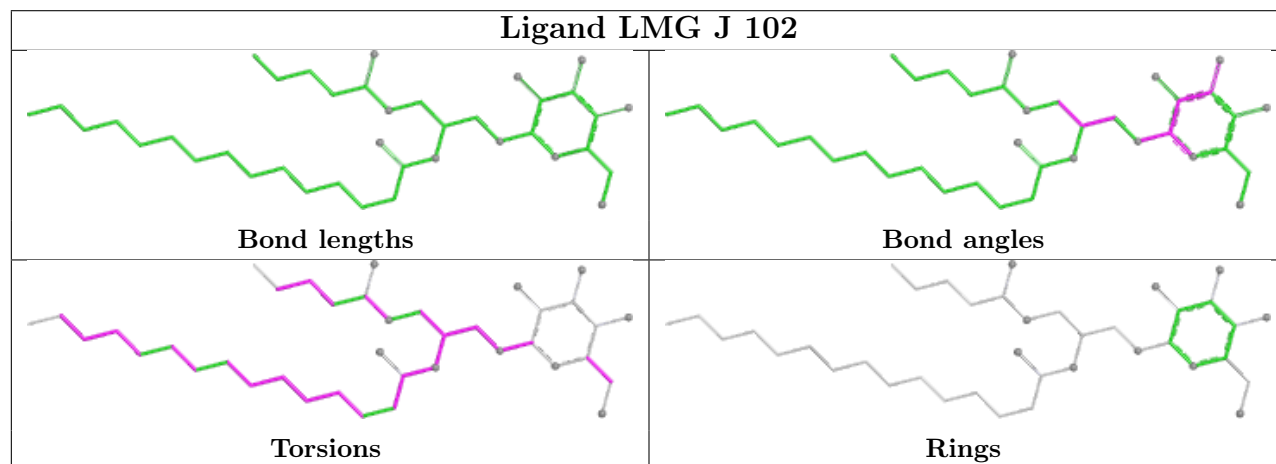


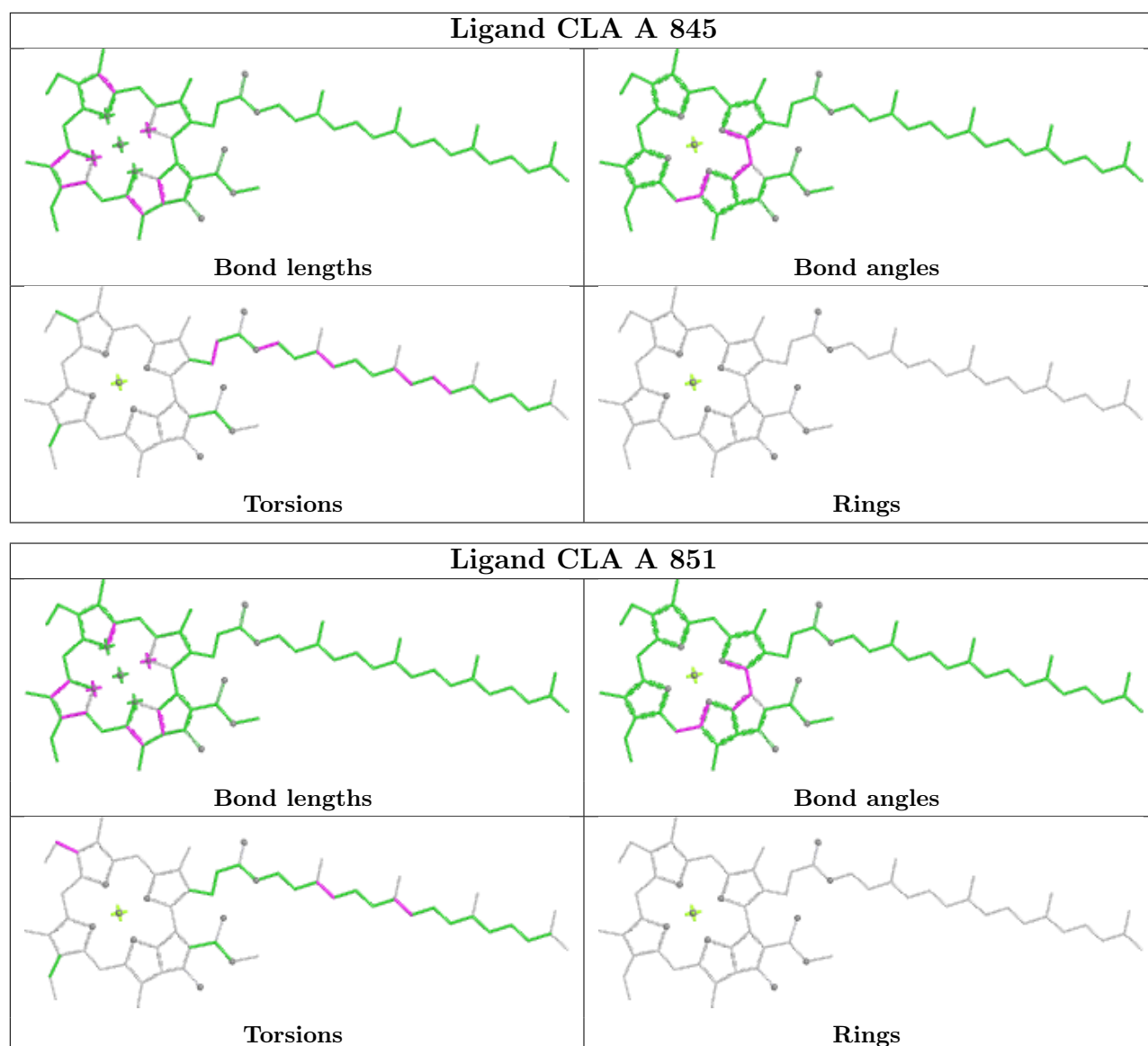


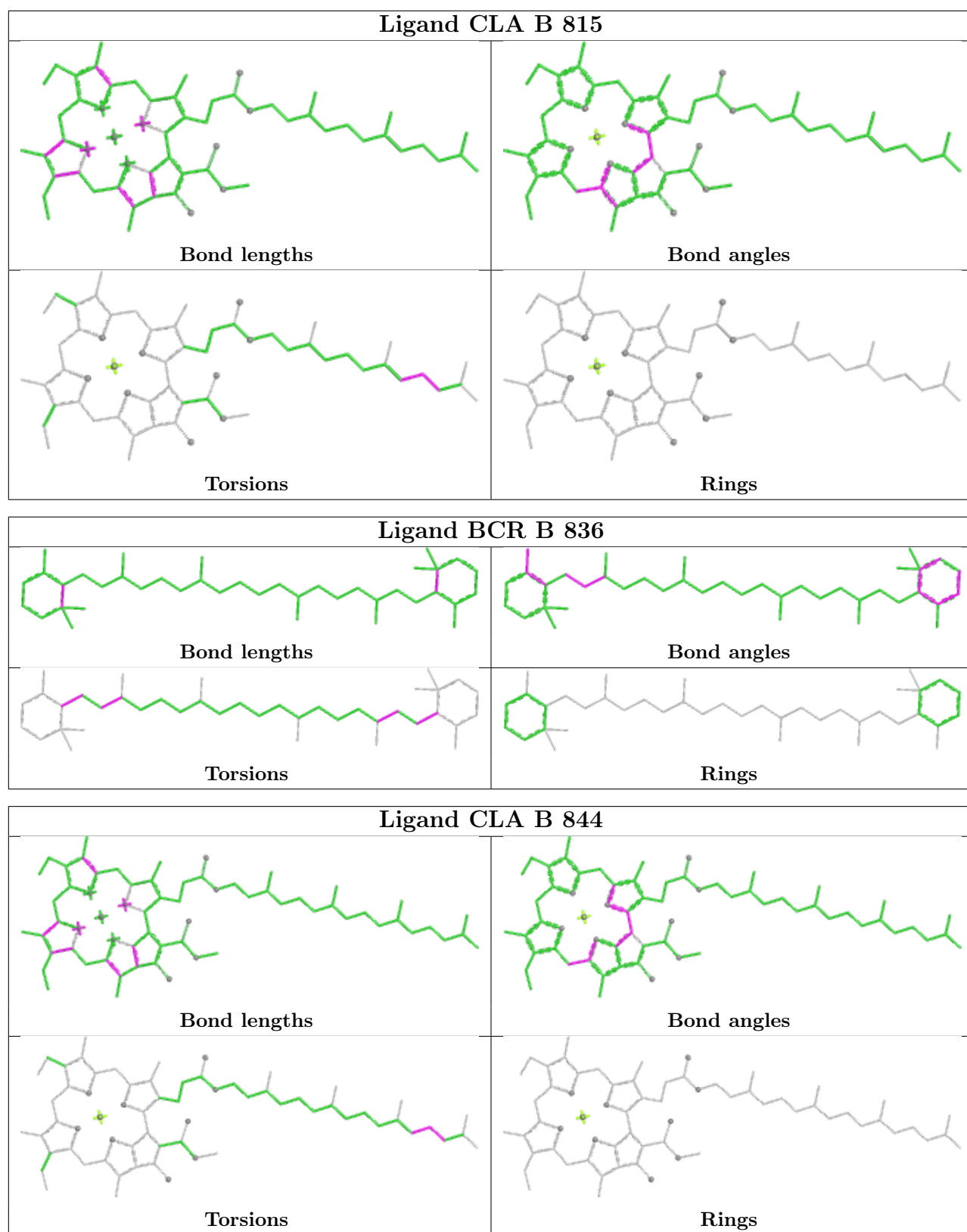
## Ligand CLA F 804



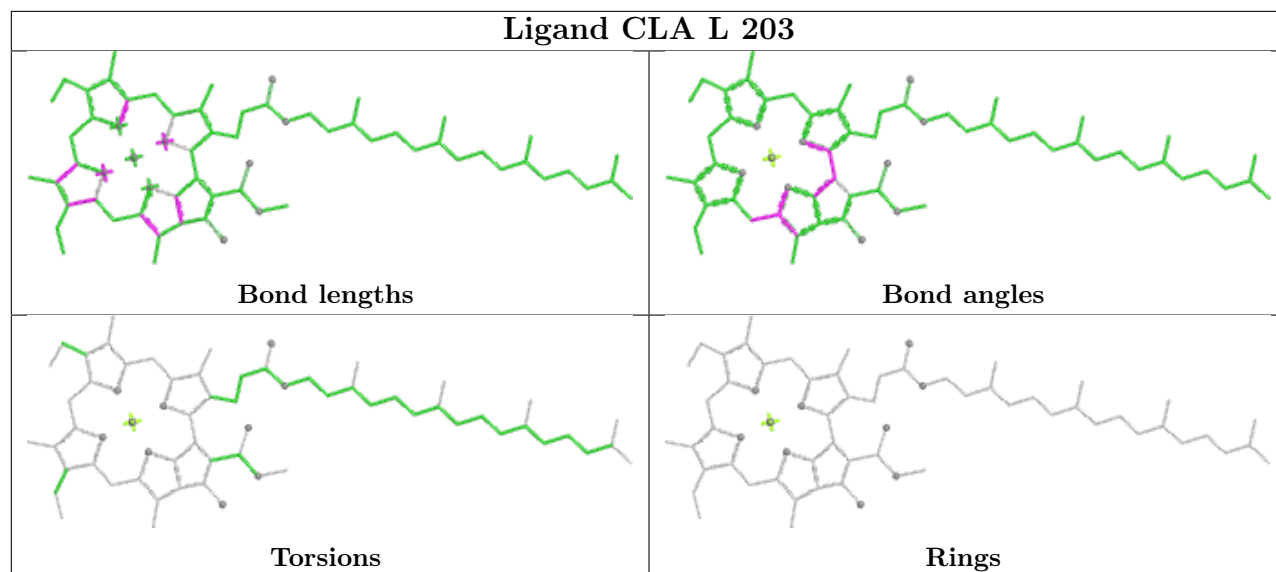
## Ligand LMG J 102



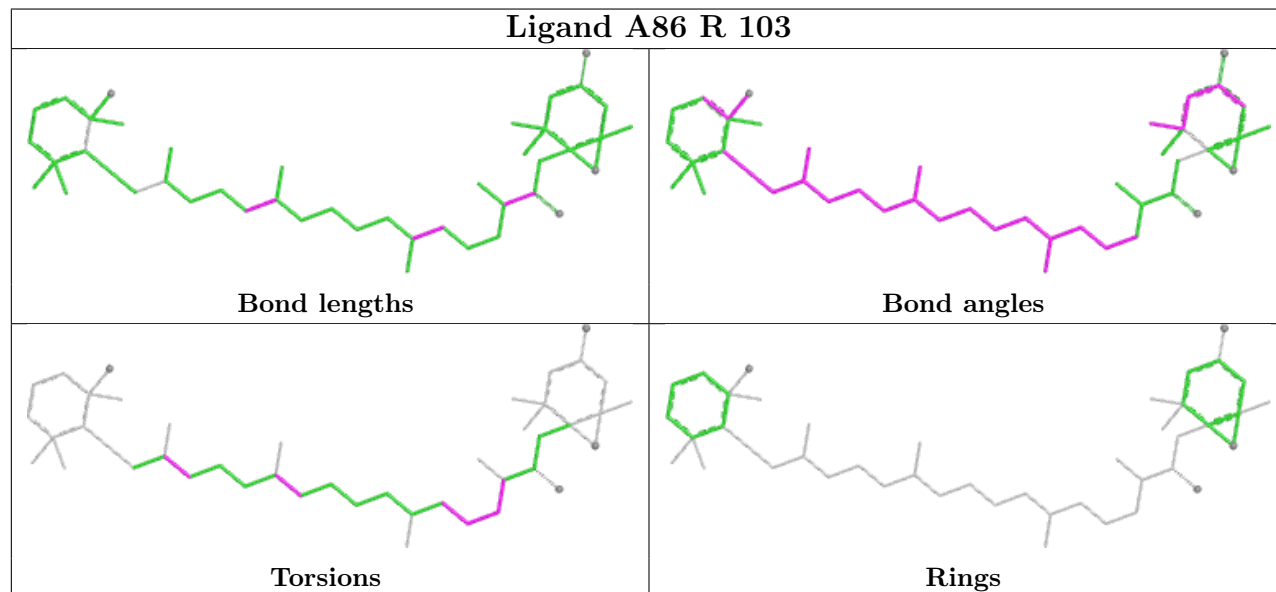




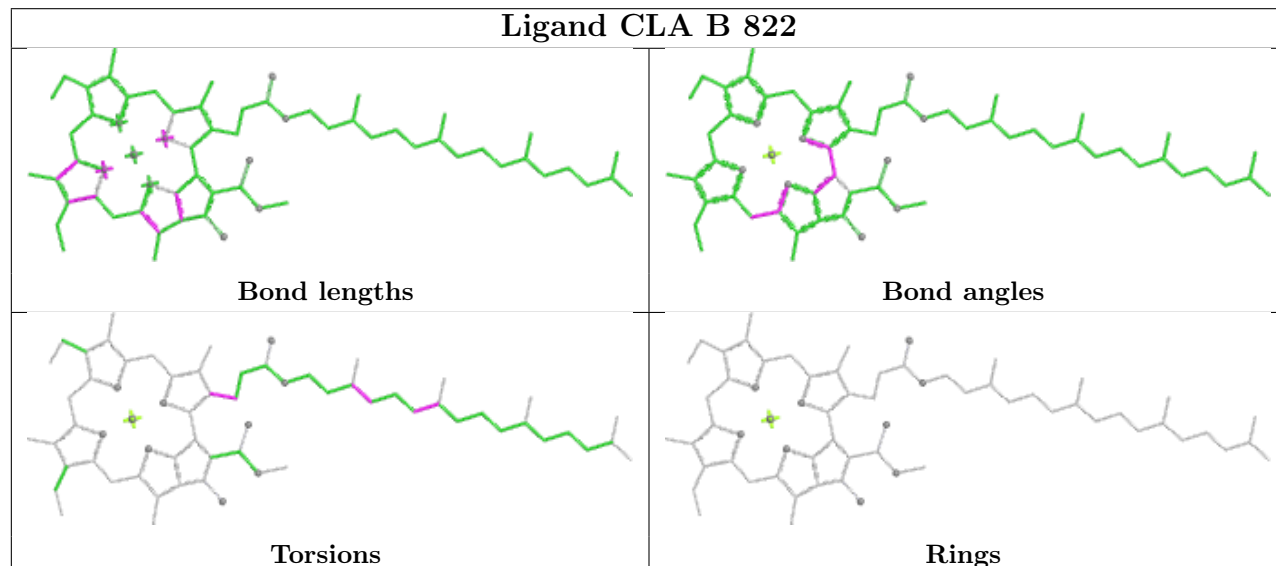
## Ligand CLA L 203



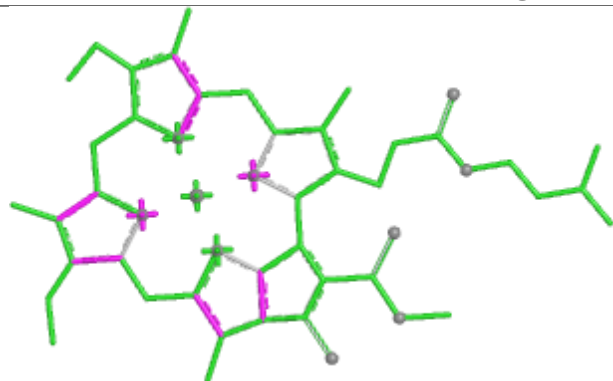
## Ligand A86 R 103



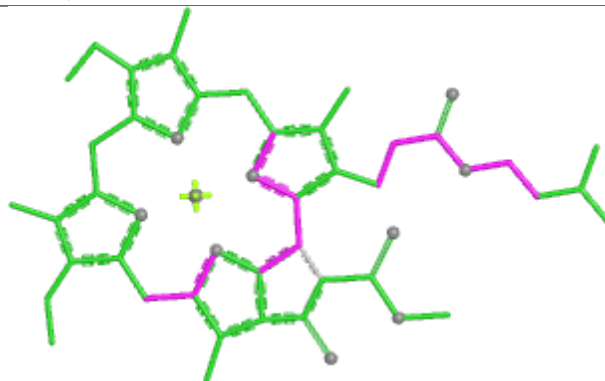
## Ligand CLA B 822



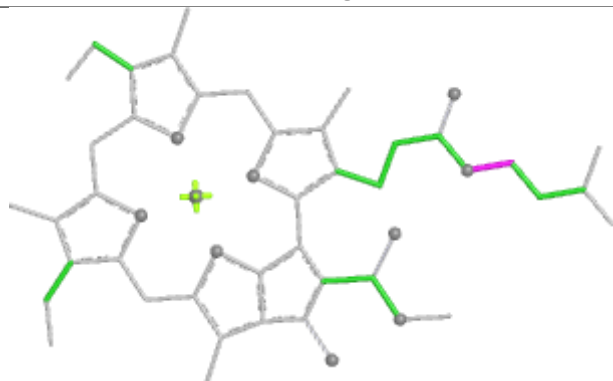
## Ligand CLA Q 208



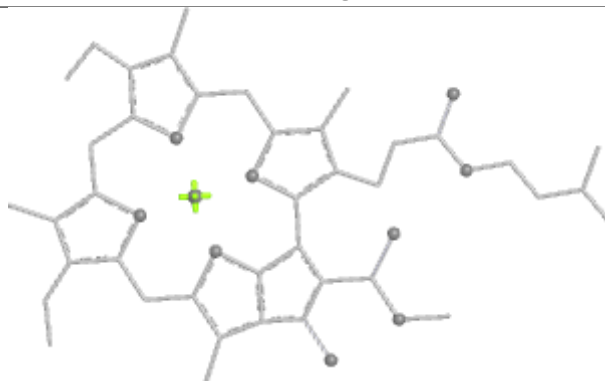
Bond lengths



Bond angles

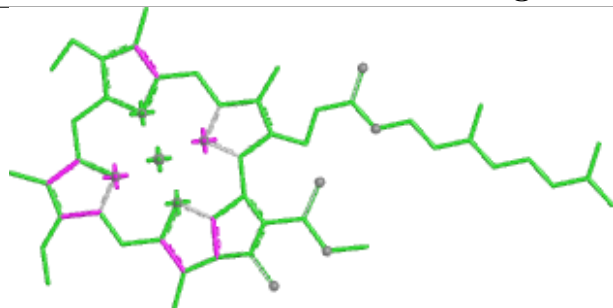


Torsions

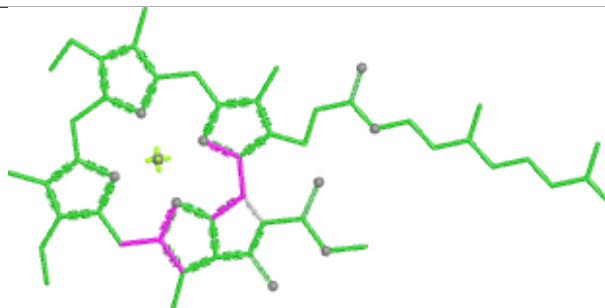


Rings

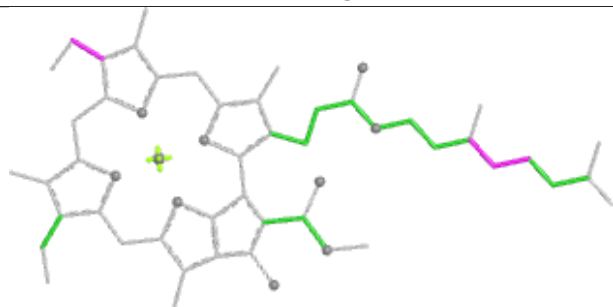
## Ligand CLA K 205



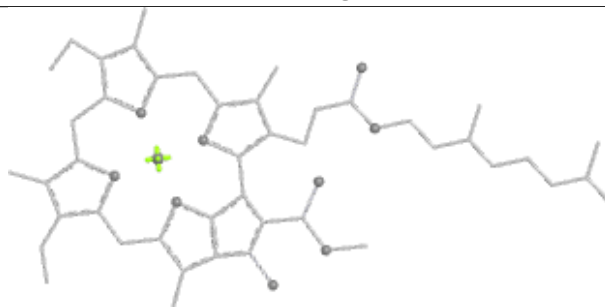
Bond lengths



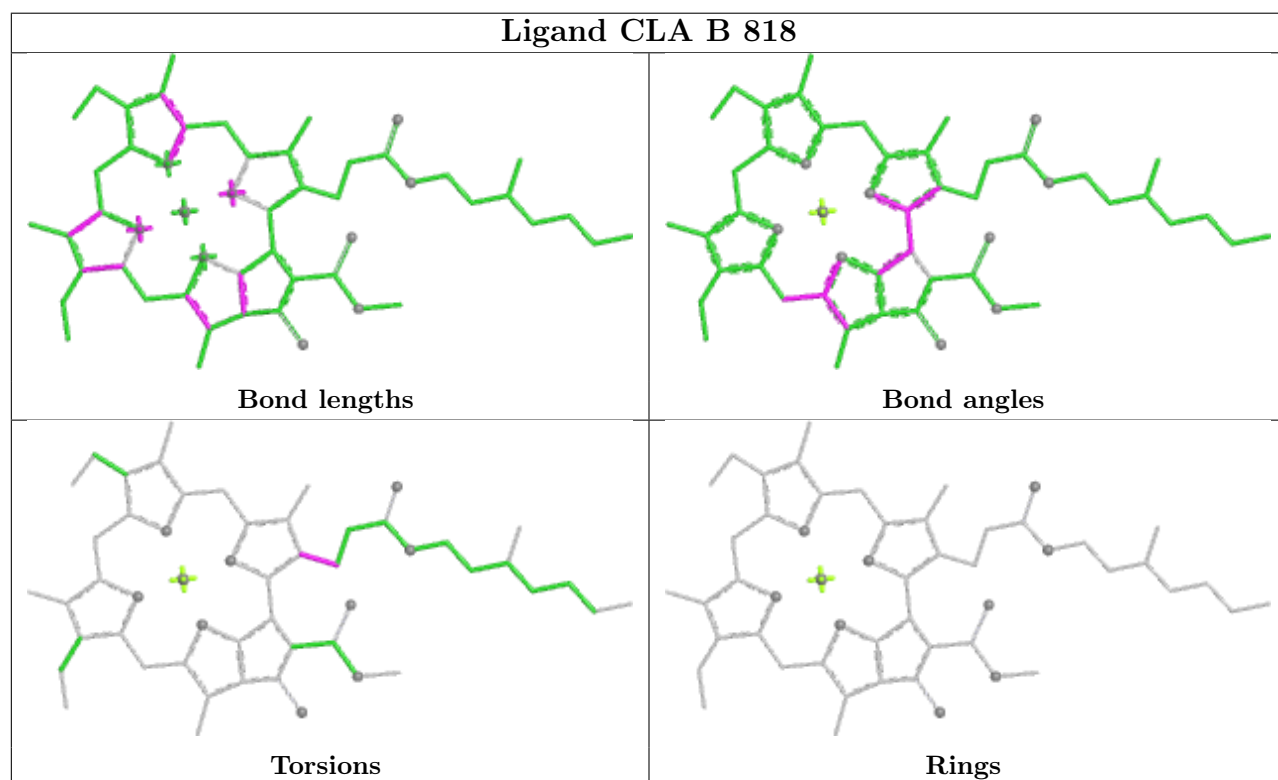
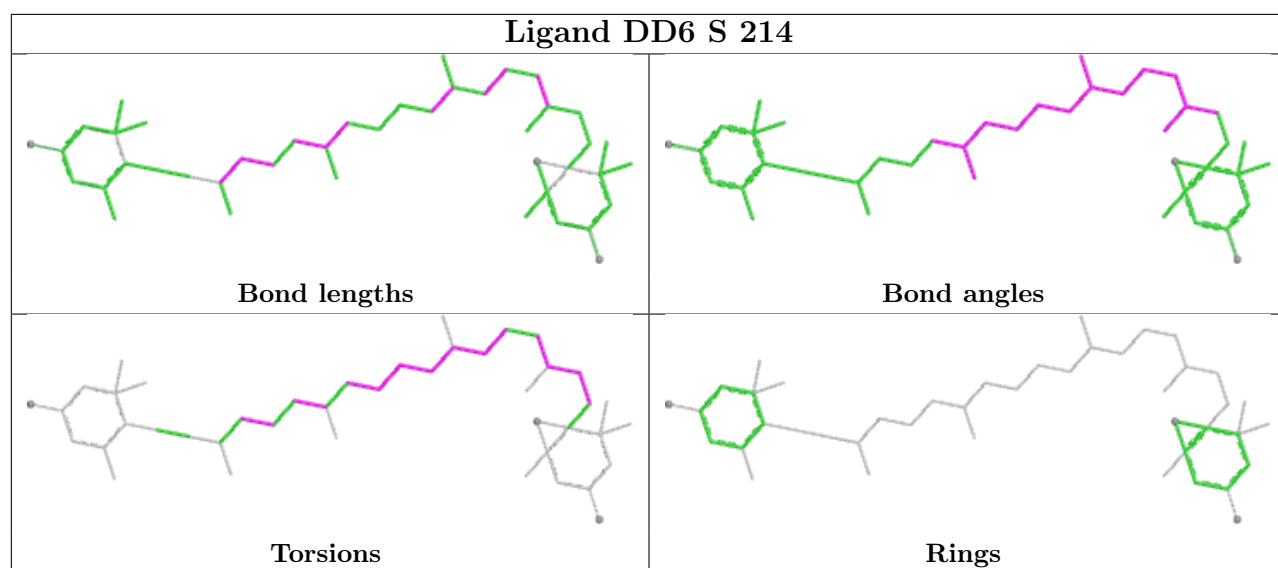
Bond angles



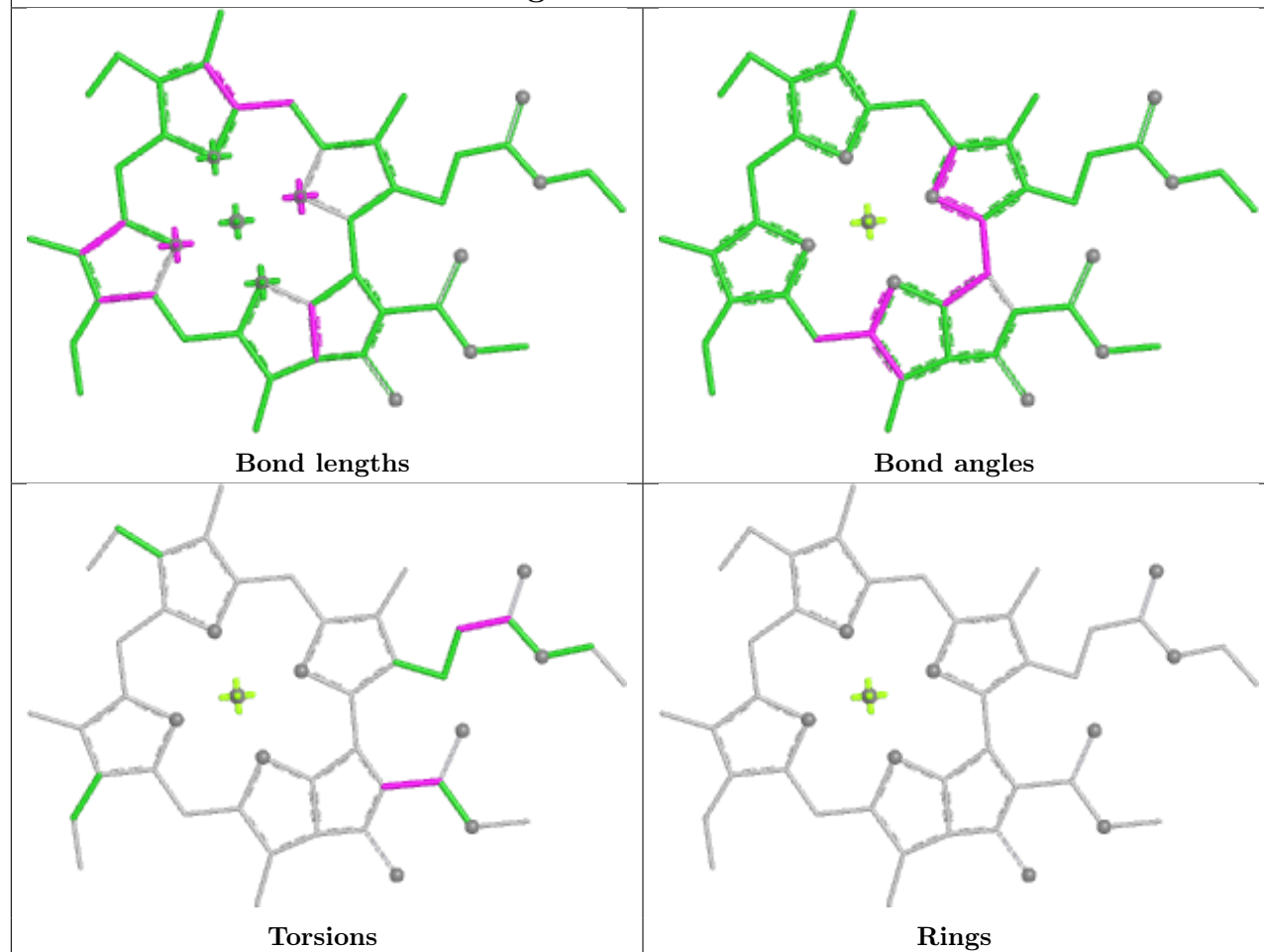
Torsions



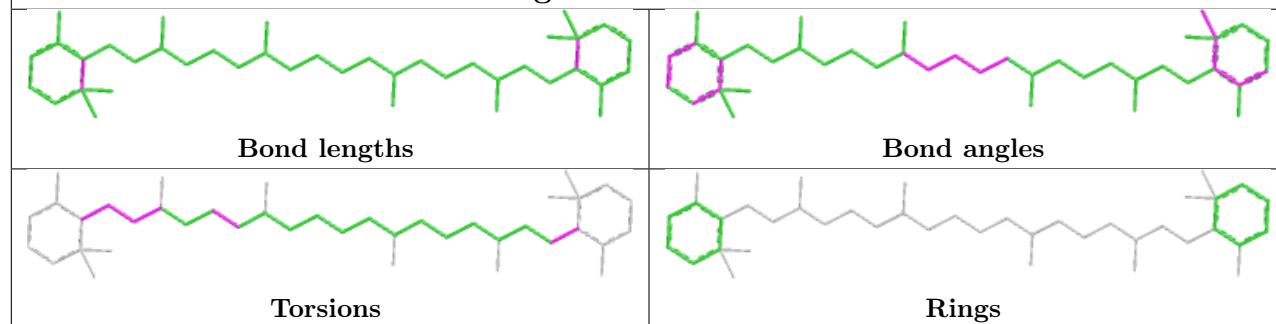
Rings



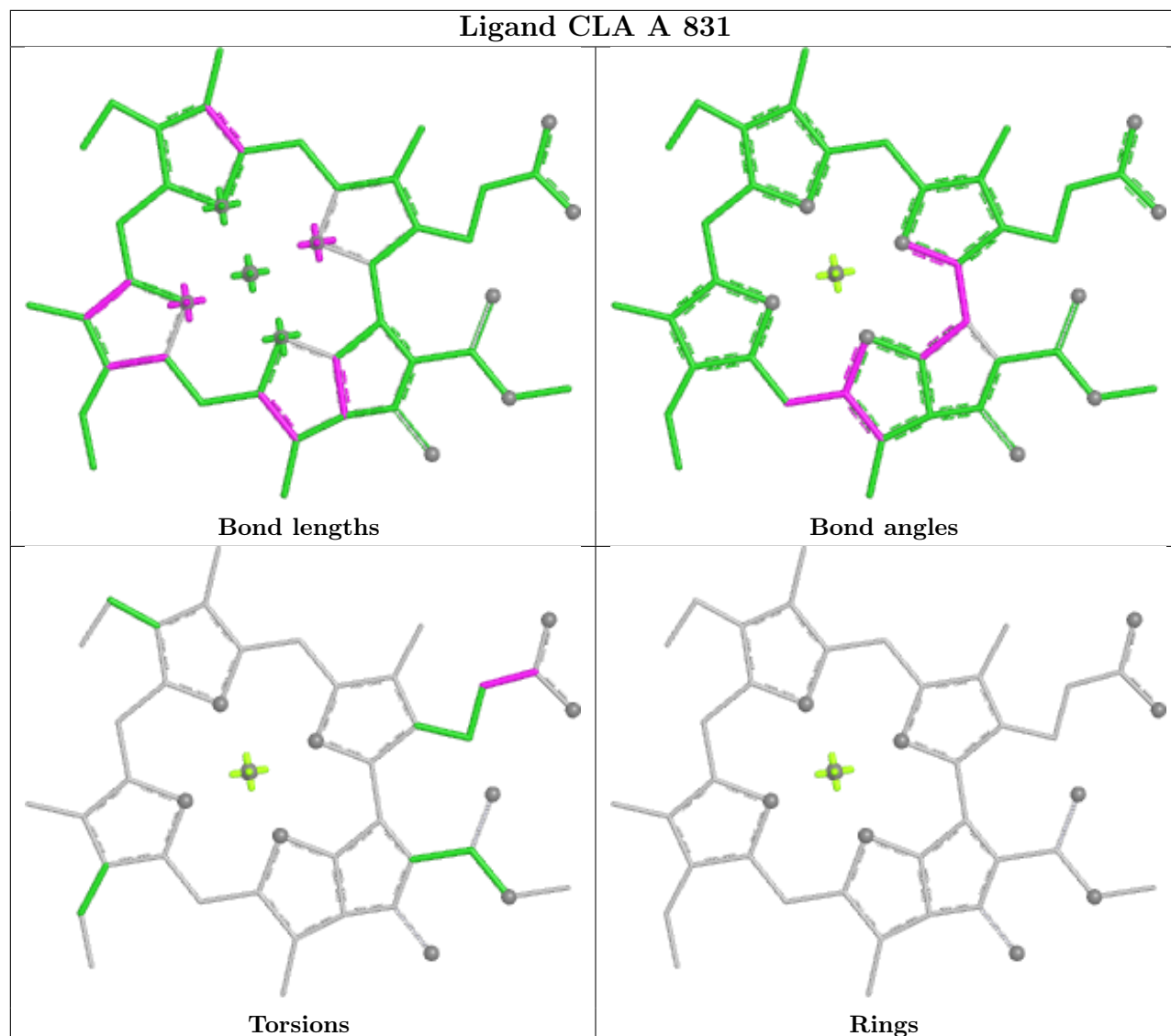
## Ligand CLA T 211



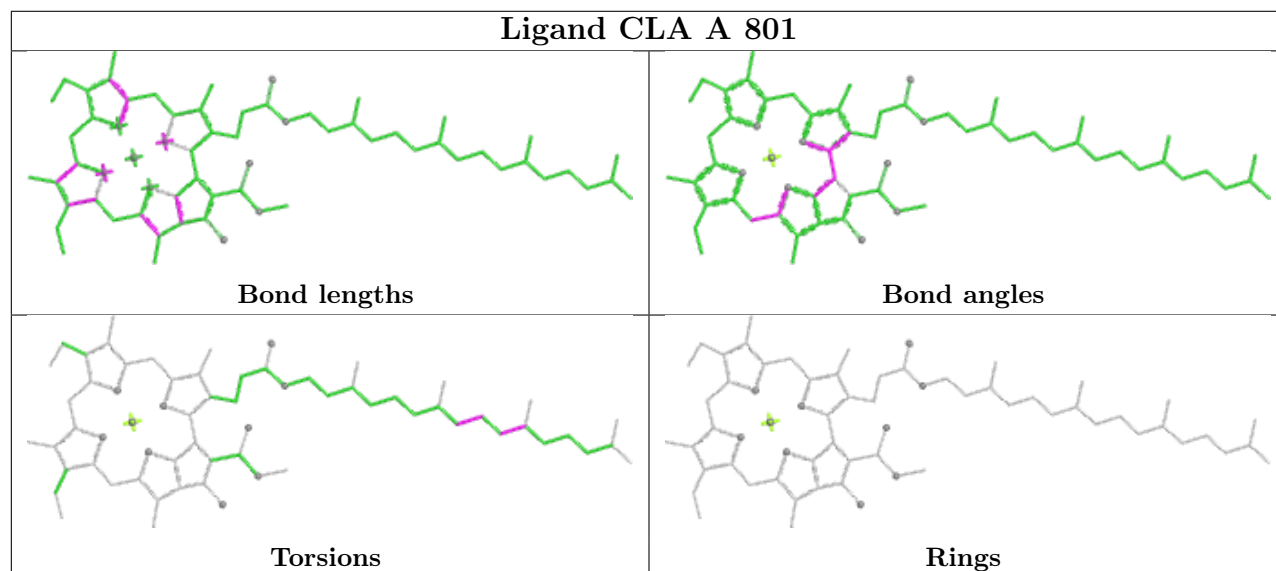
## Ligand BCR k 104



## Ligand CLA A 831

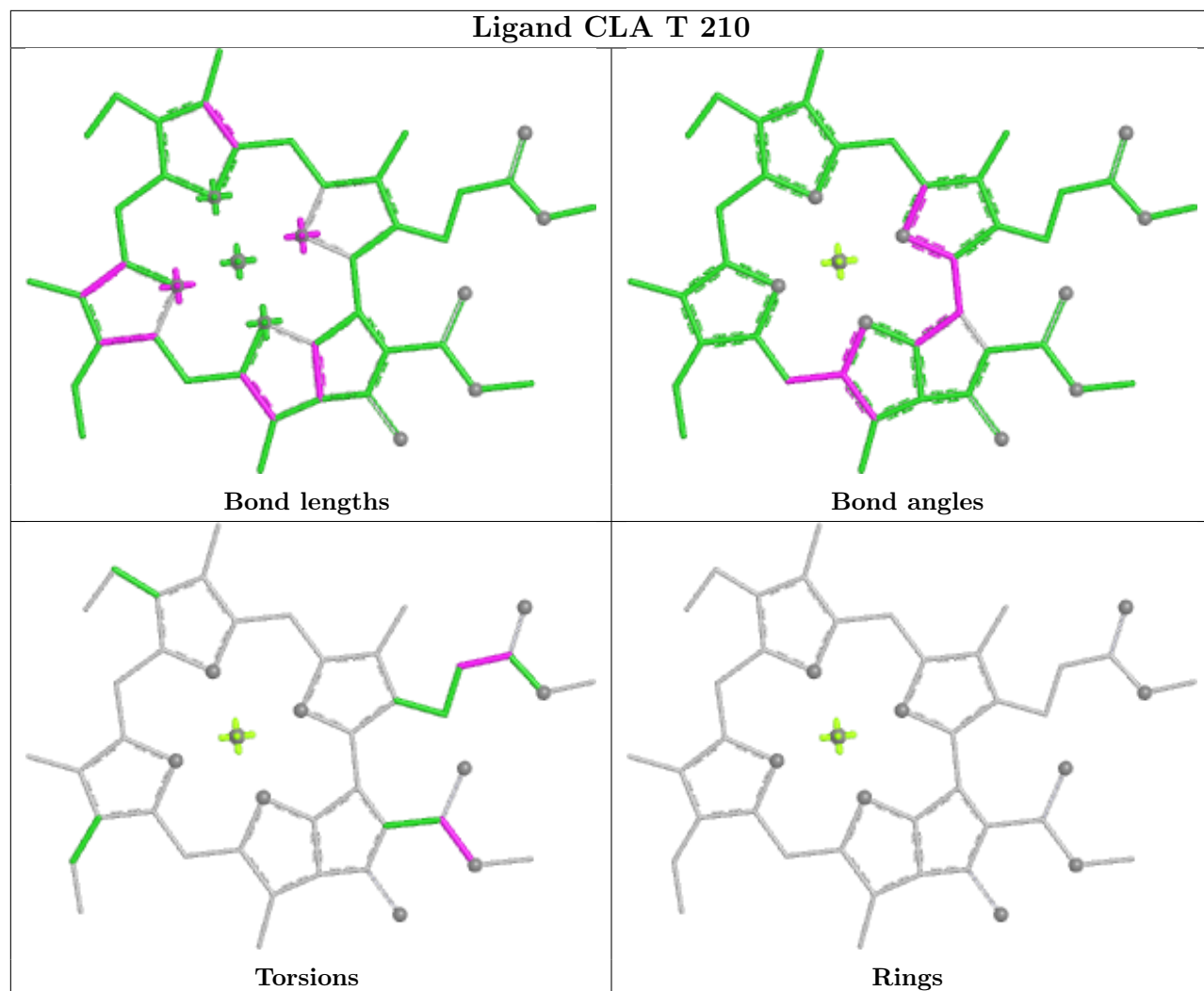


## Ligand CLA A 801

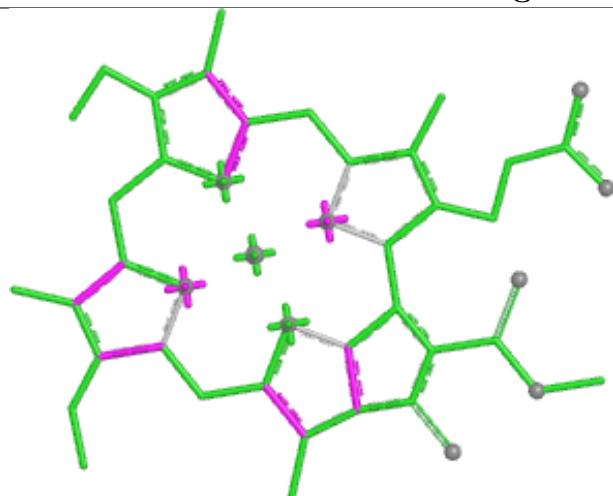




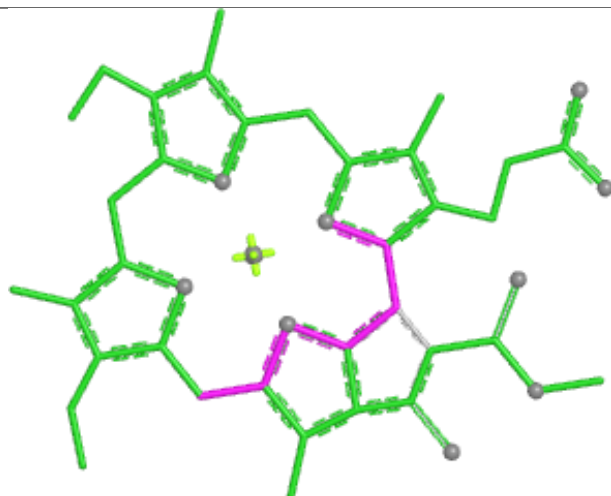
## Ligand CLA T 210



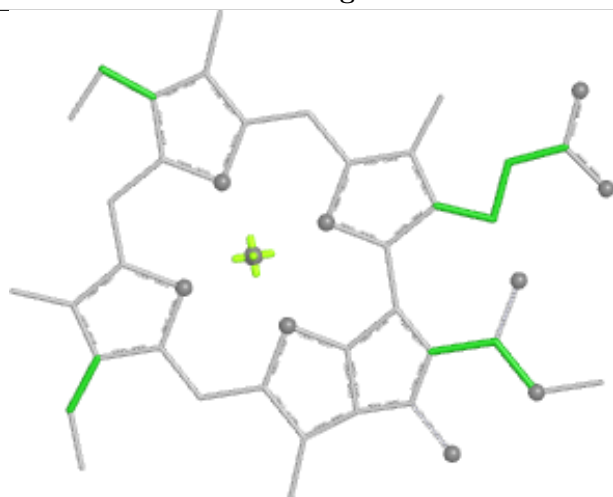
## Ligand CLA R 101



Bond lengths



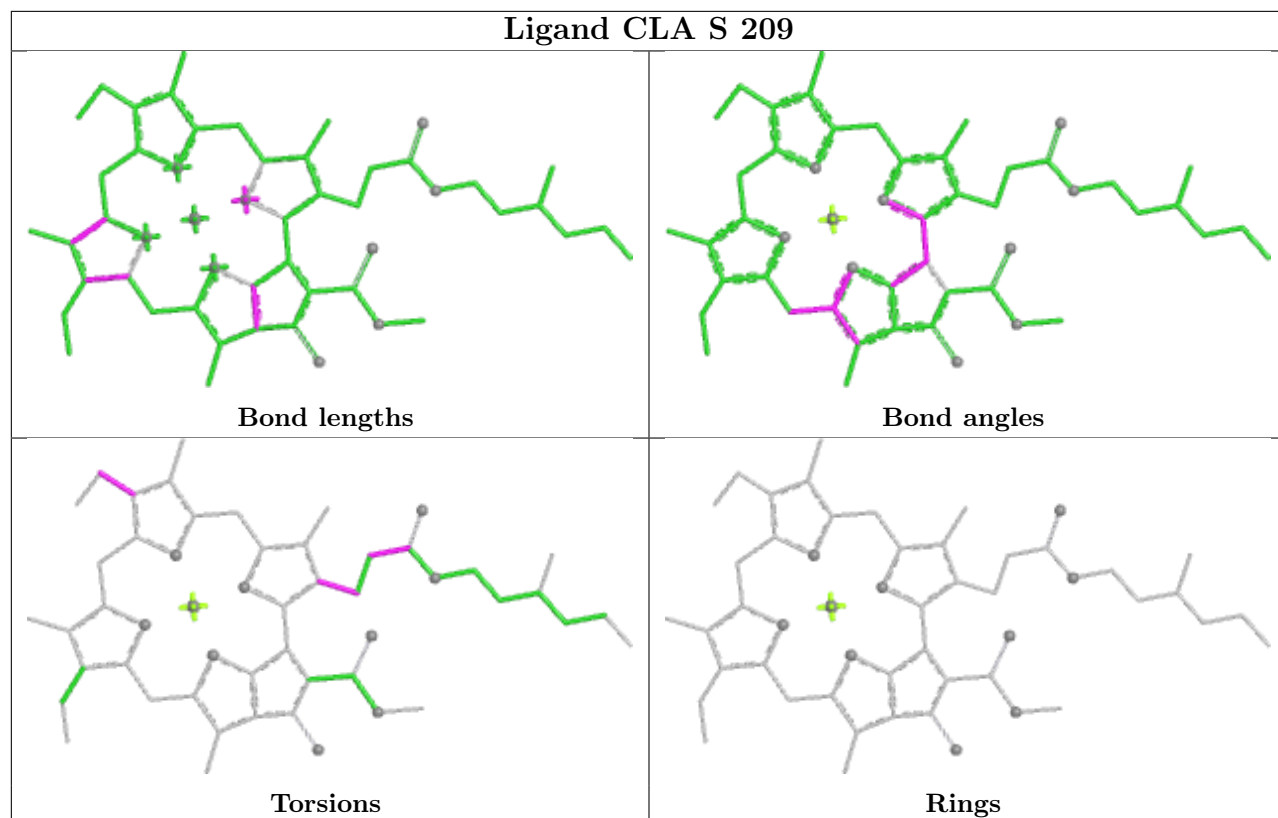
Bond angles



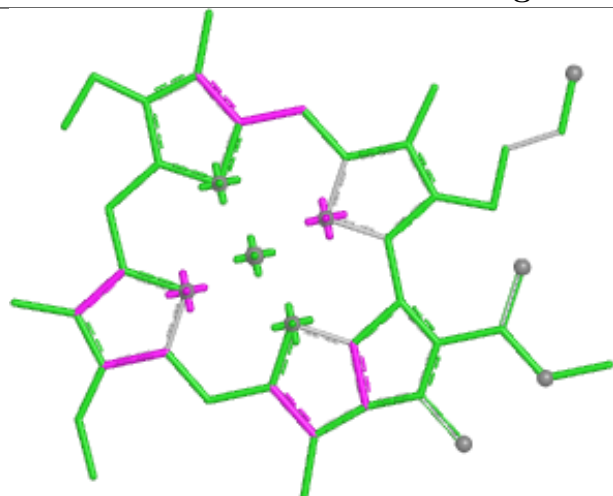
Torsions



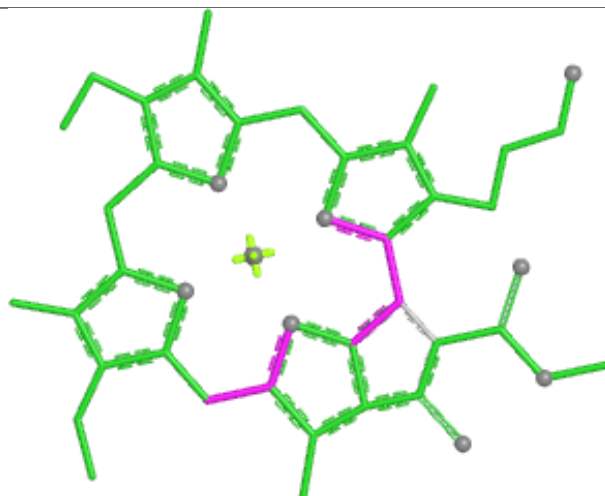
Rings



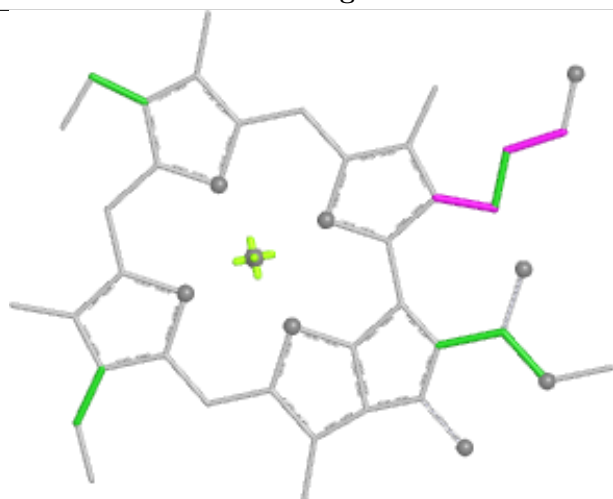
## Ligand CLA H 205



Bond lengths



Bond angles

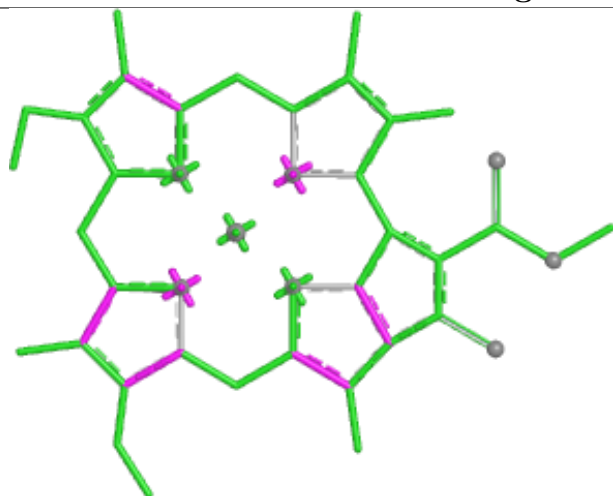


Torsions

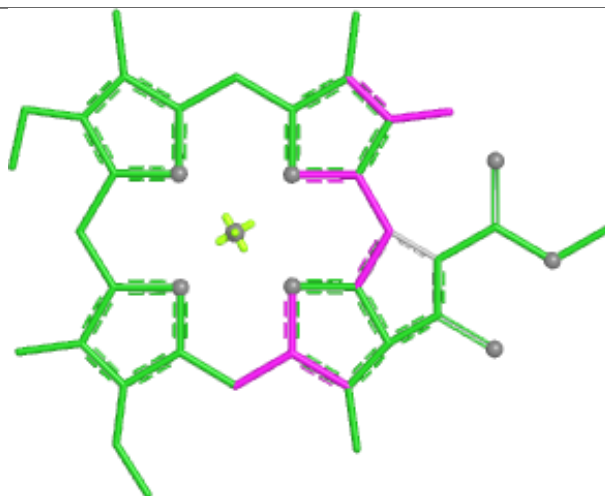


Rings

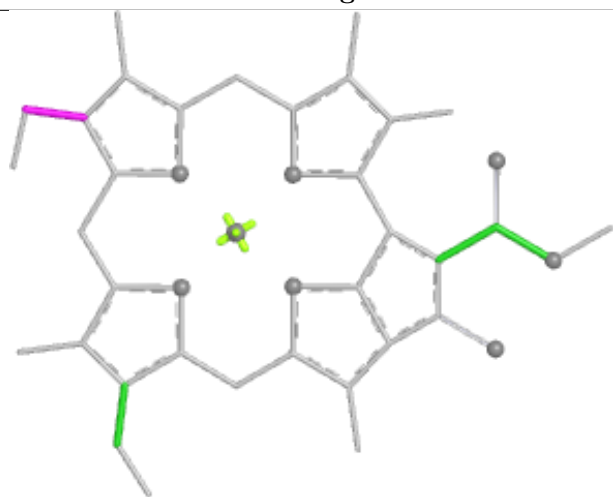
## Ligand CLA T 202



Bond lengths



Bond angles

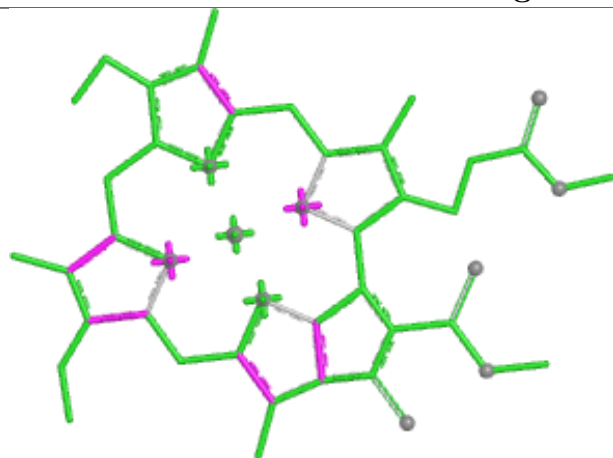


Torsions

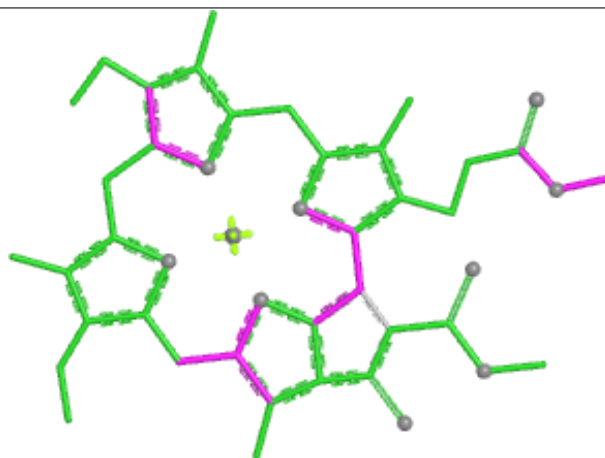


Rings

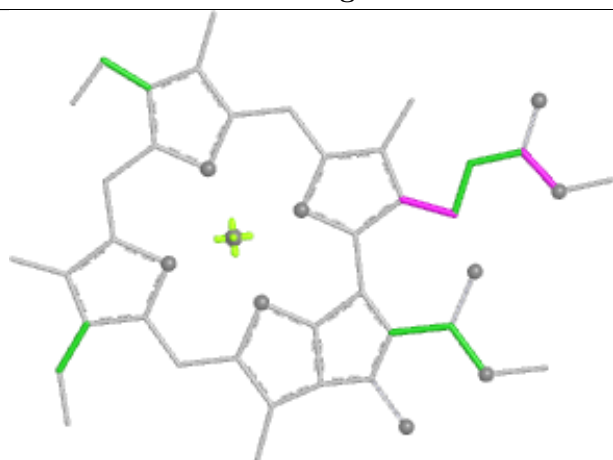
## Ligand CLA O 207



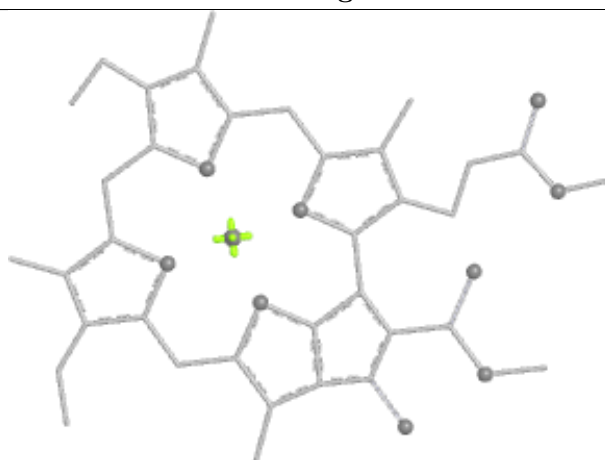
Bond lengths



Bond angles

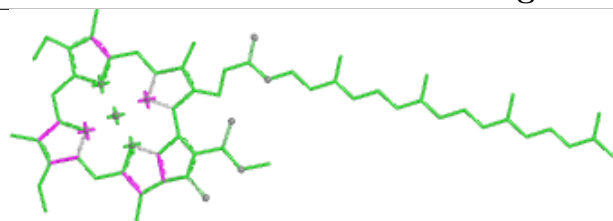


Torsions

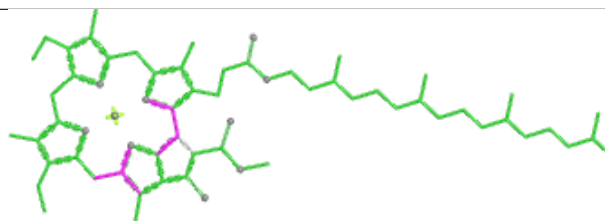


Rings

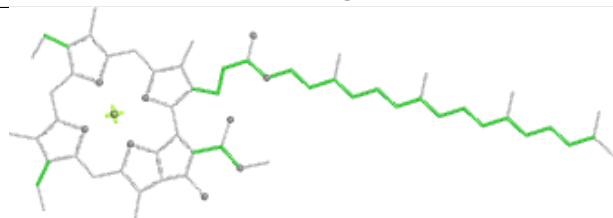
## Ligand CLA S 216



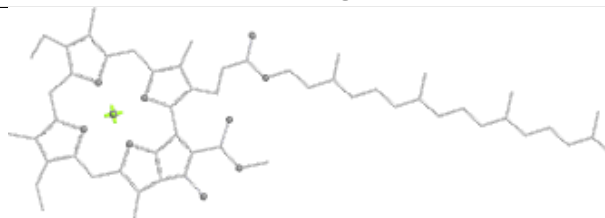
Bond lengths



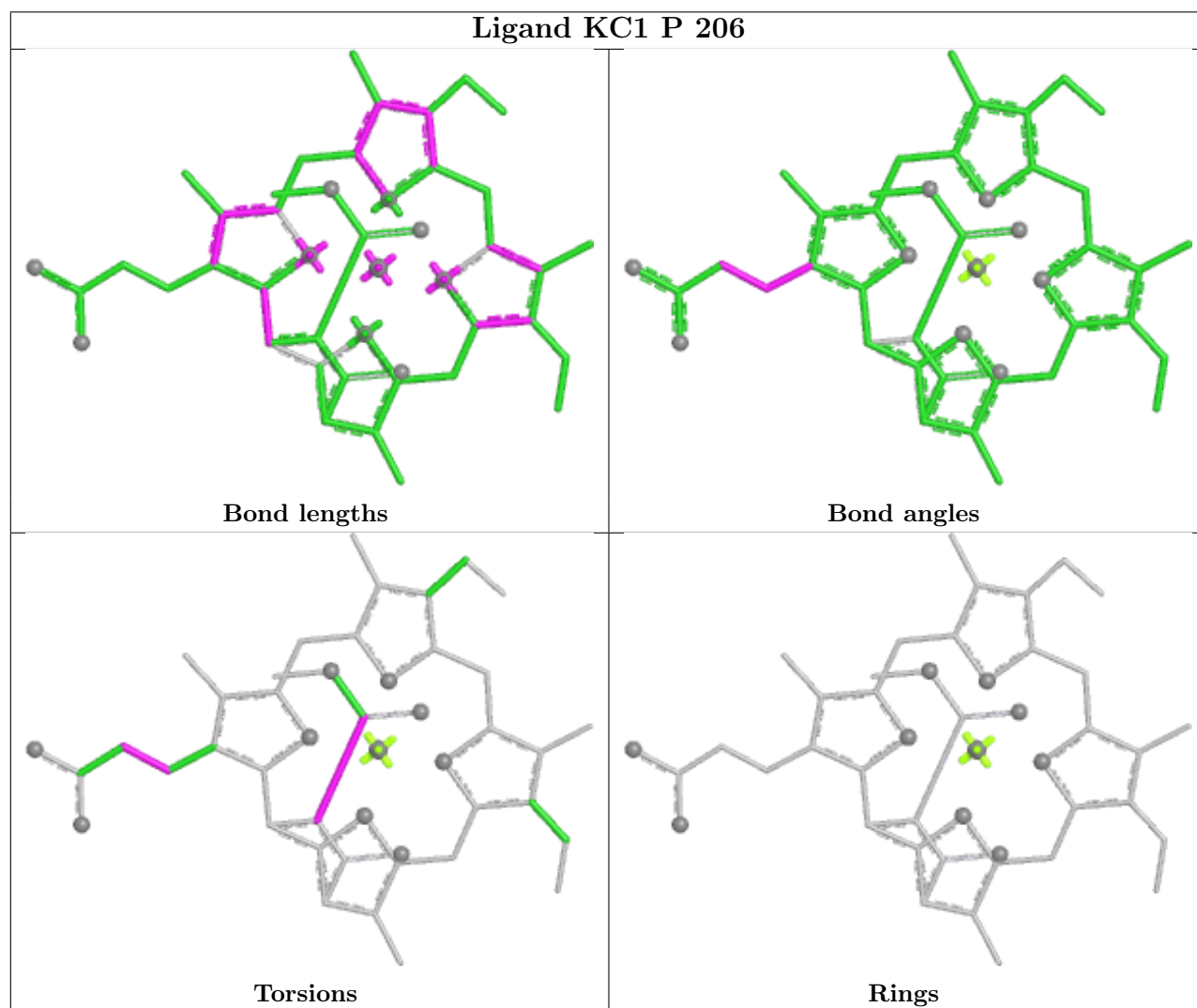
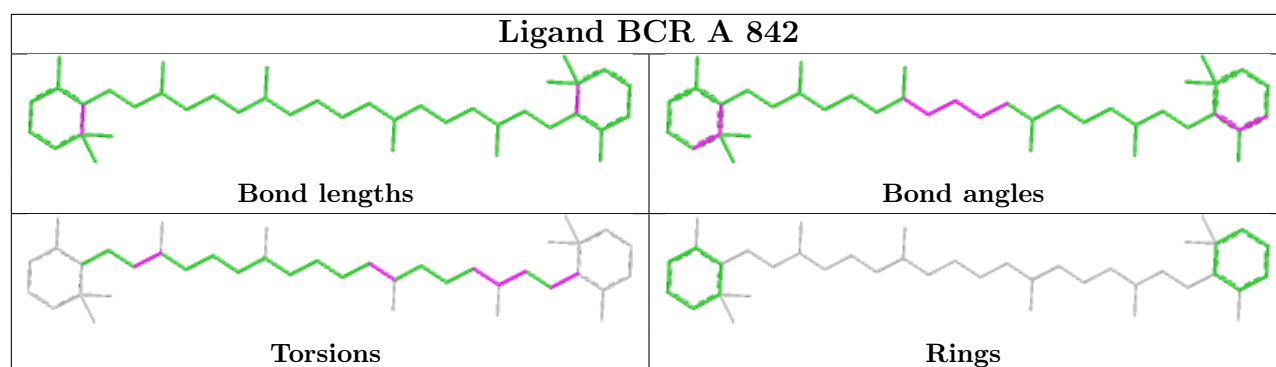
Bond angles

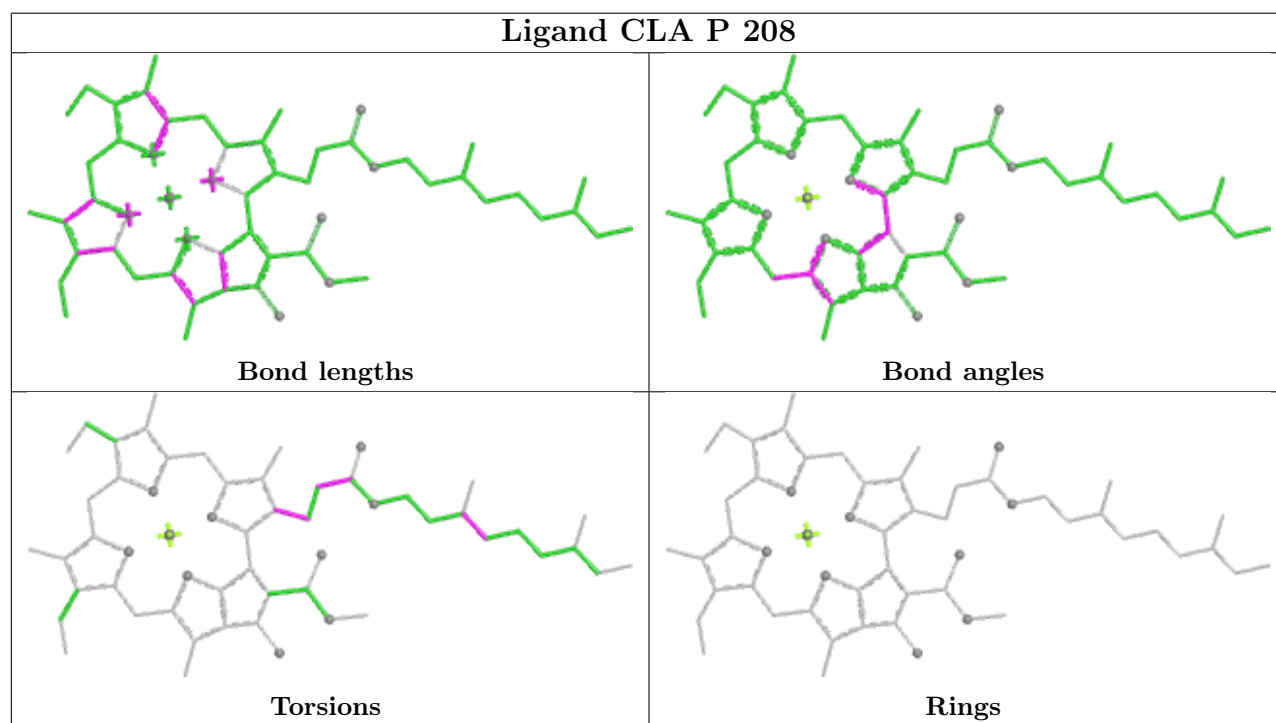
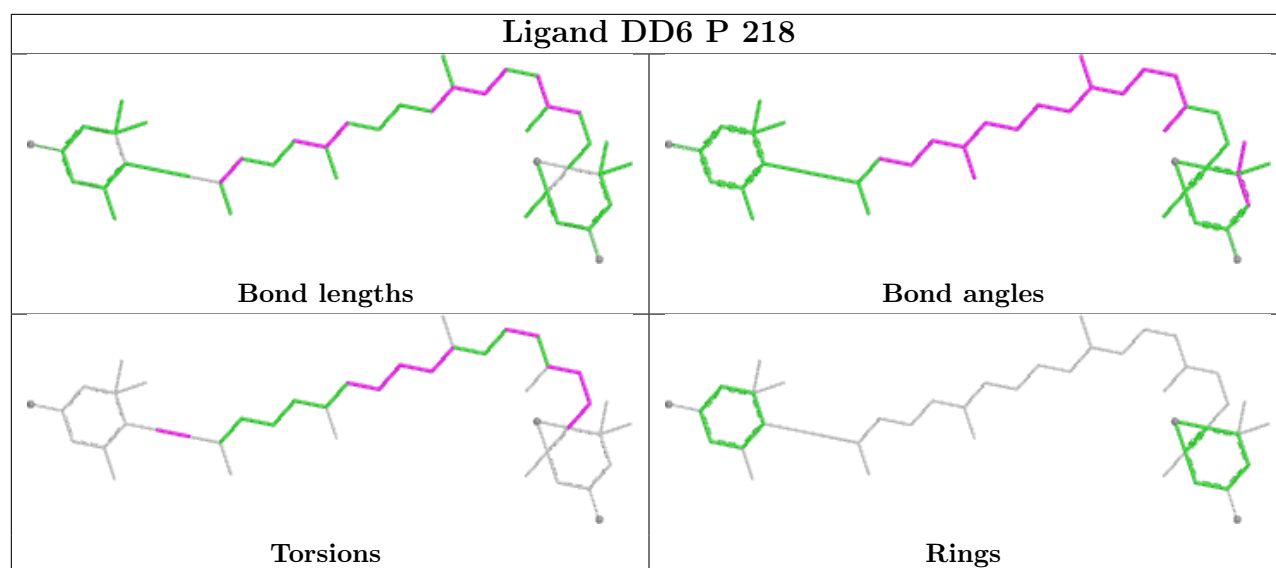


Torsions



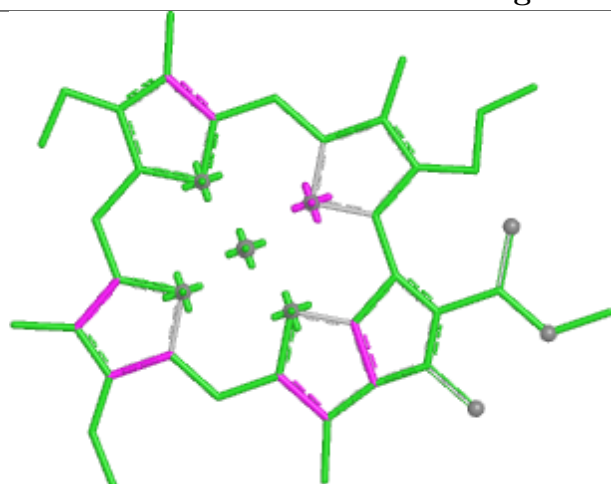
Rings



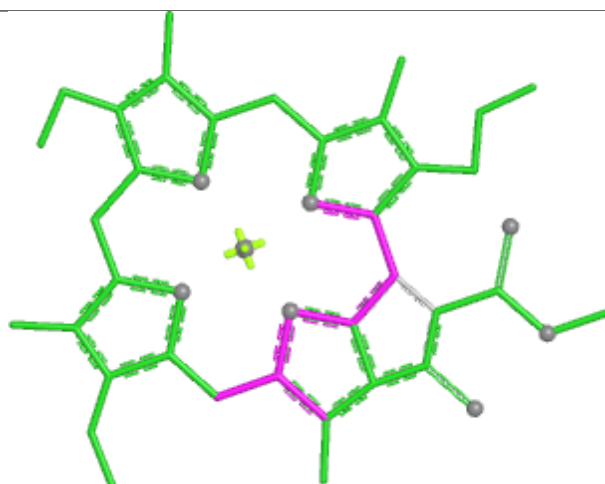




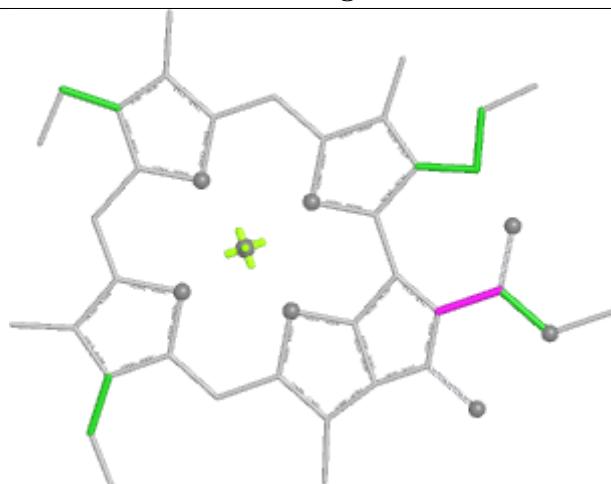
## Ligand CLA O 202



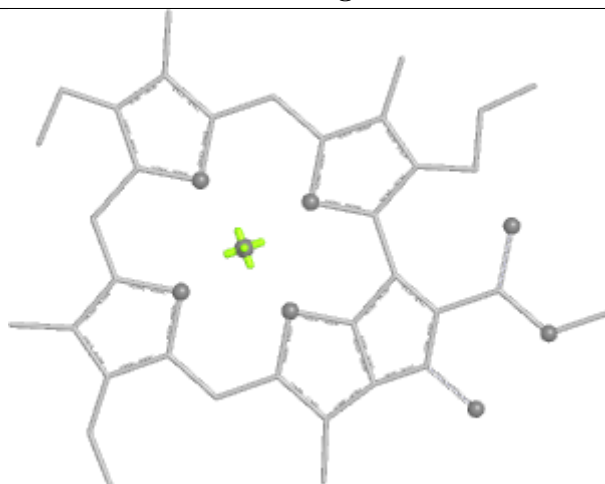
Bond lengths



Bond angles

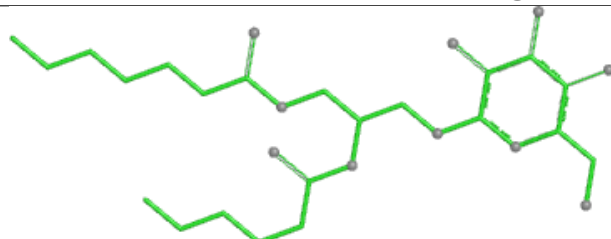


Torsions

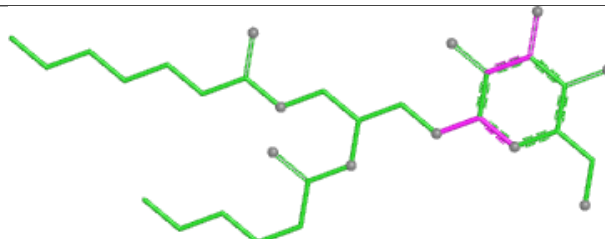


Rings

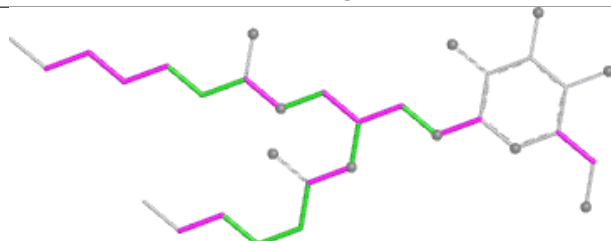
## Ligand LMG U 201



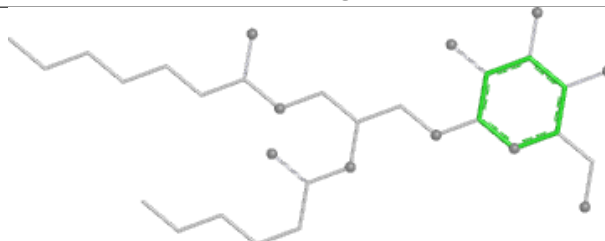
Bond lengths



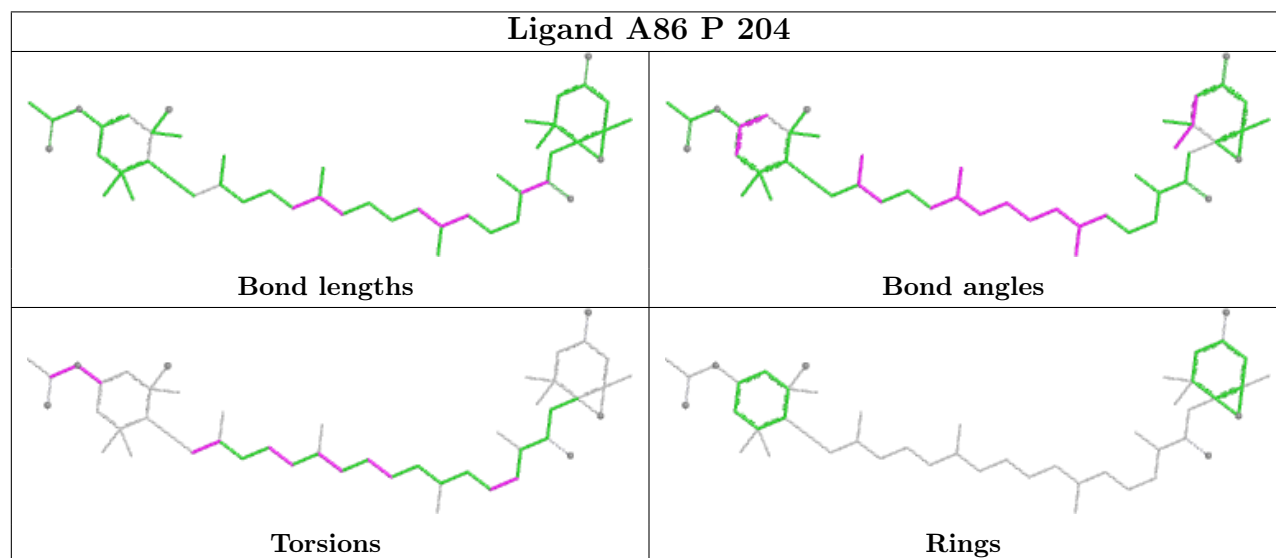
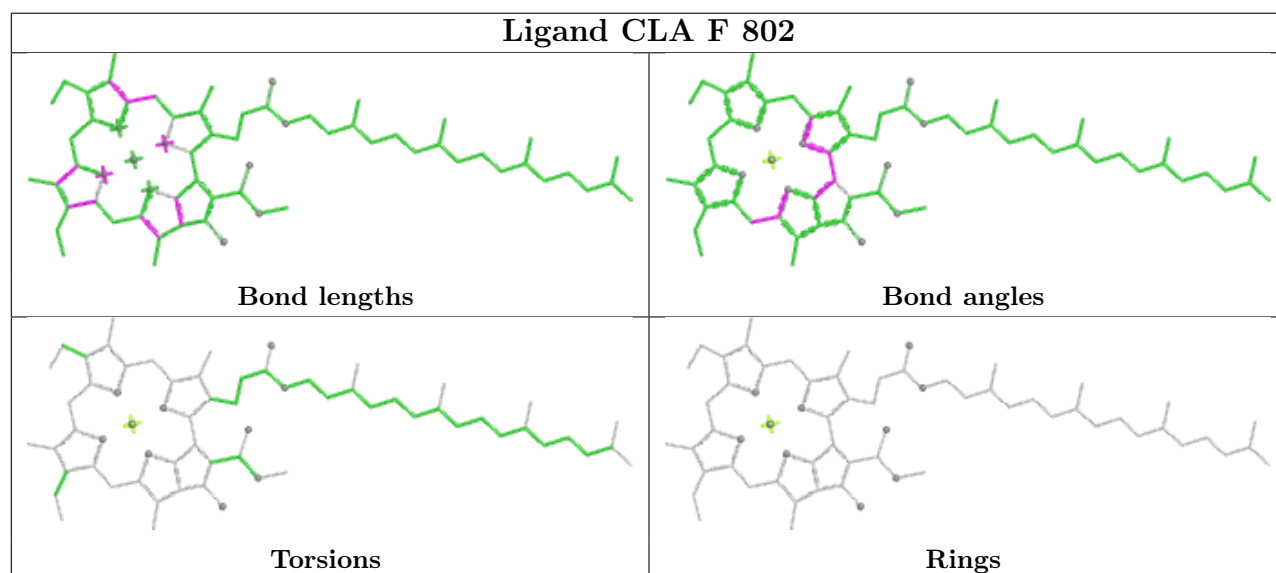
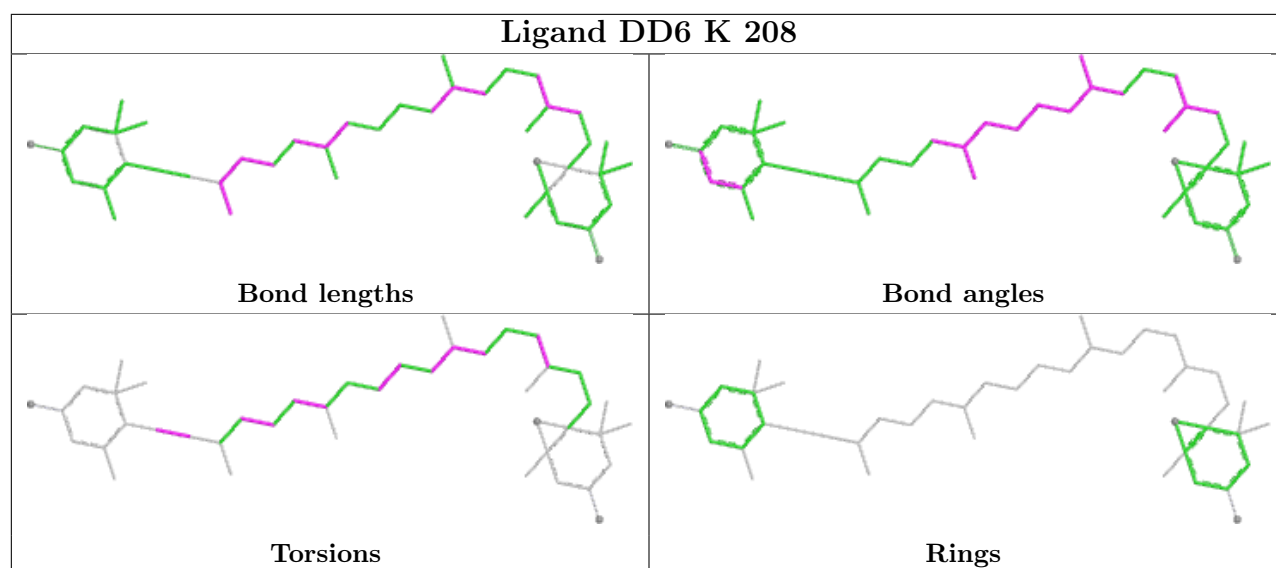
Bond angles



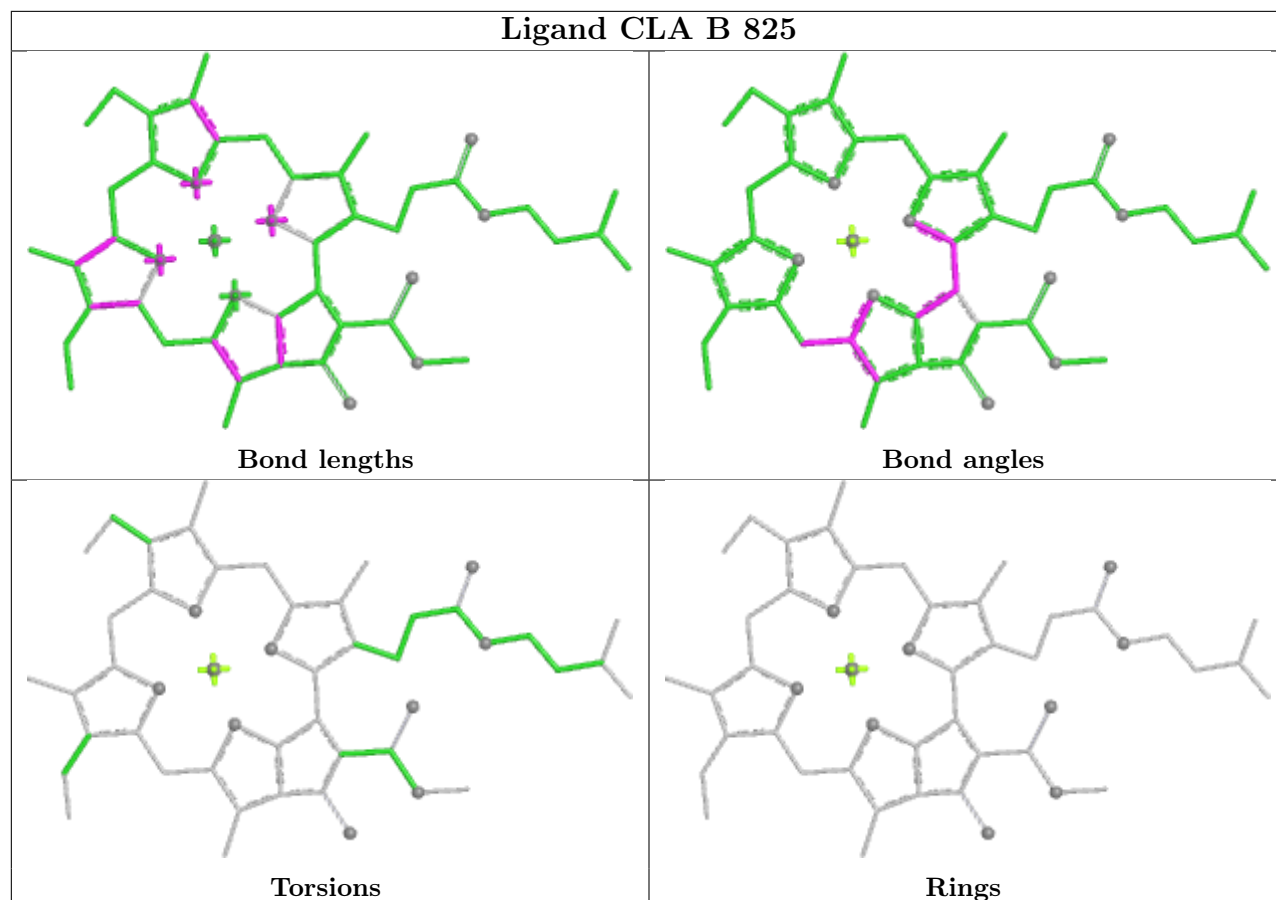
Torsions



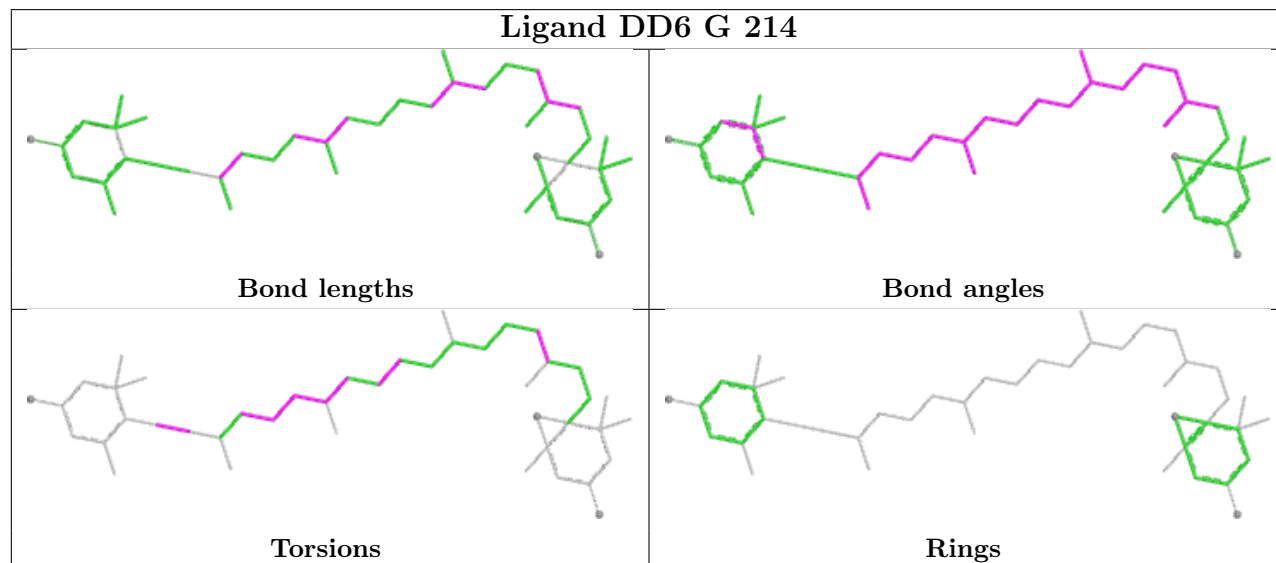
Rings

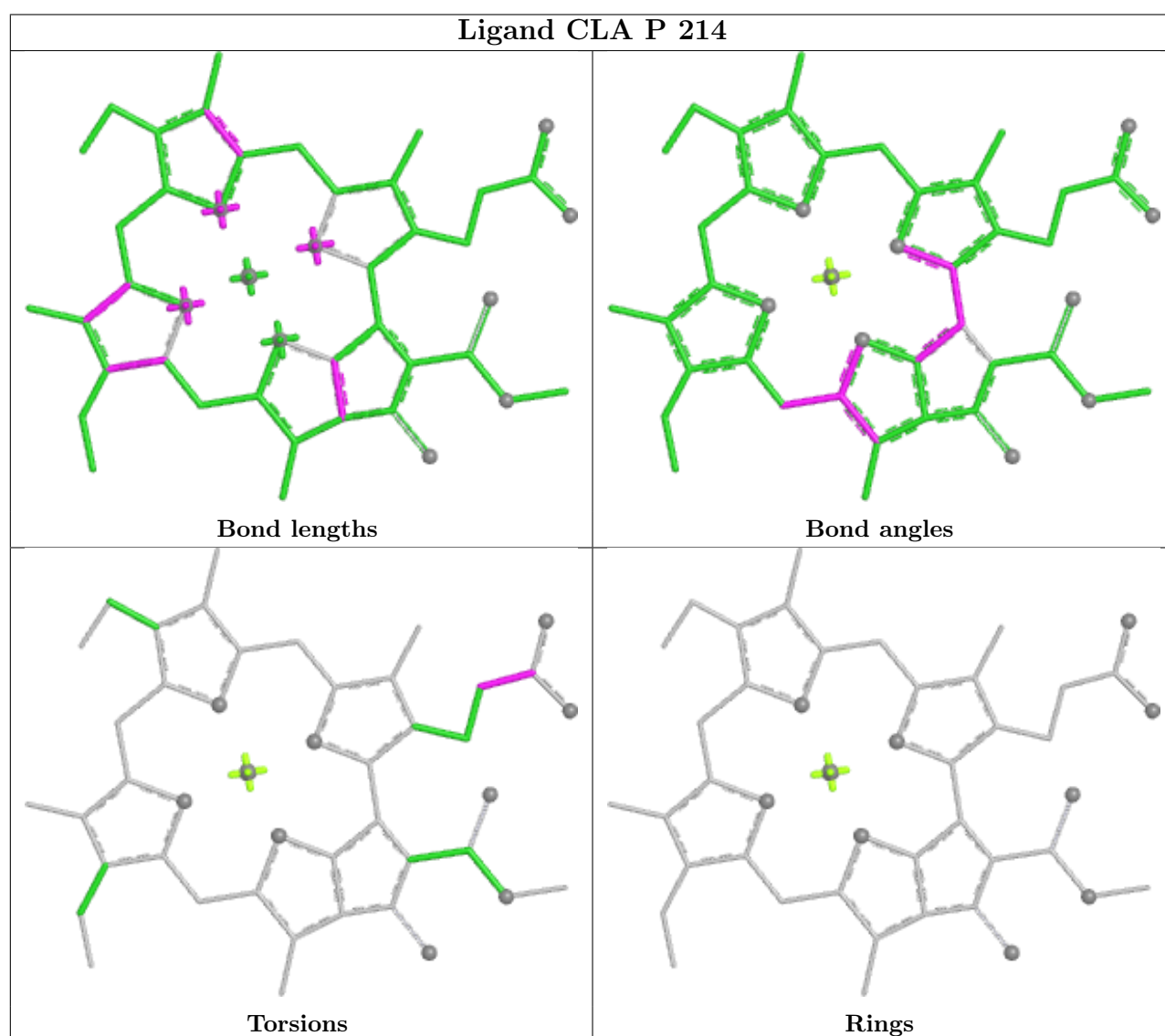
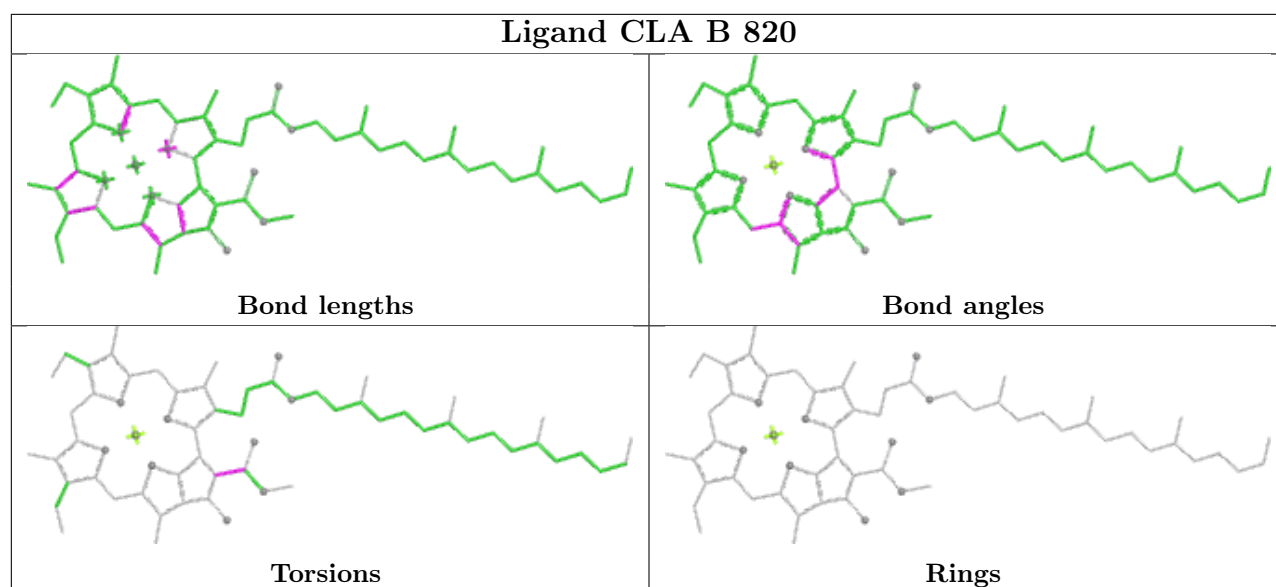


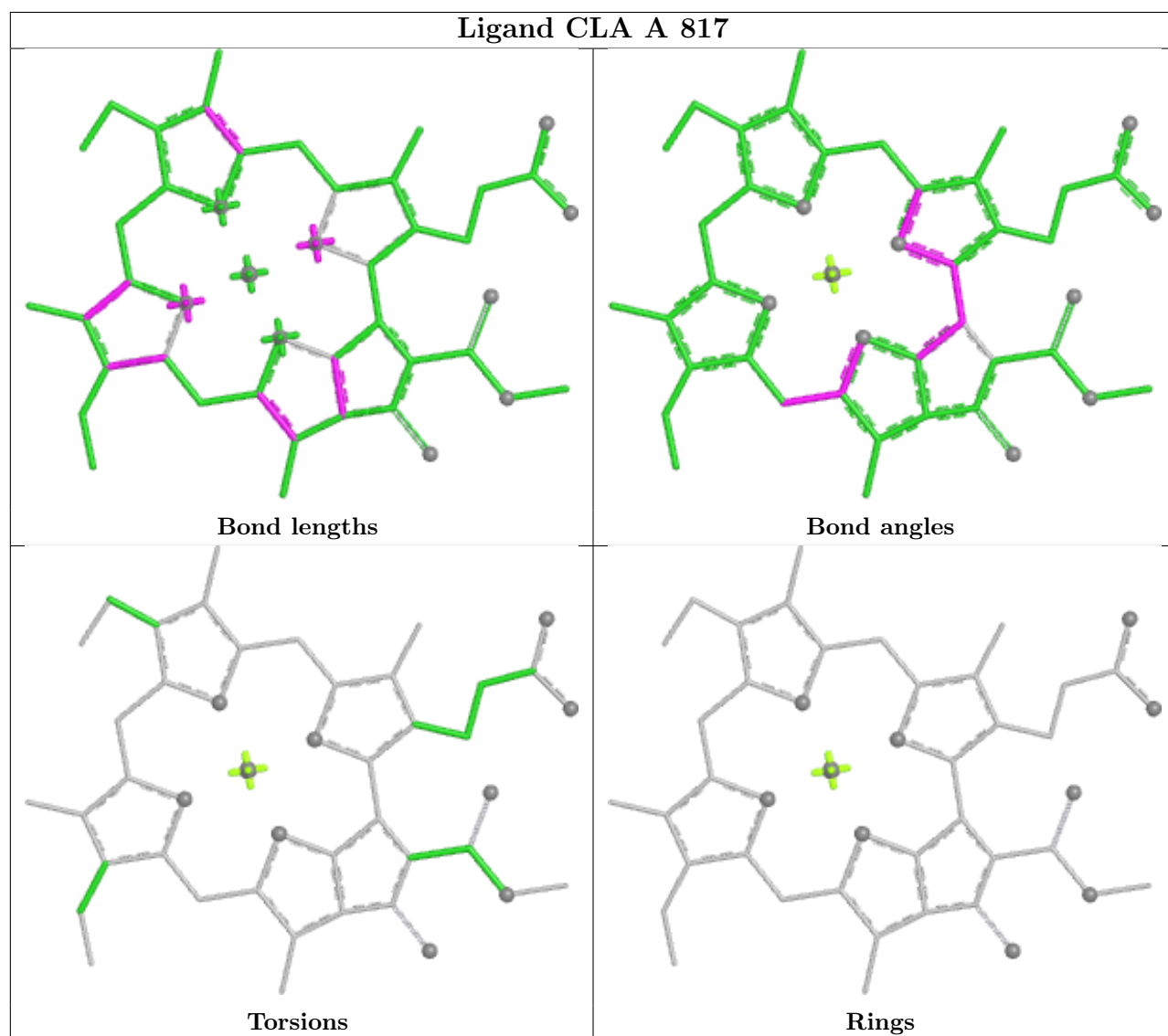
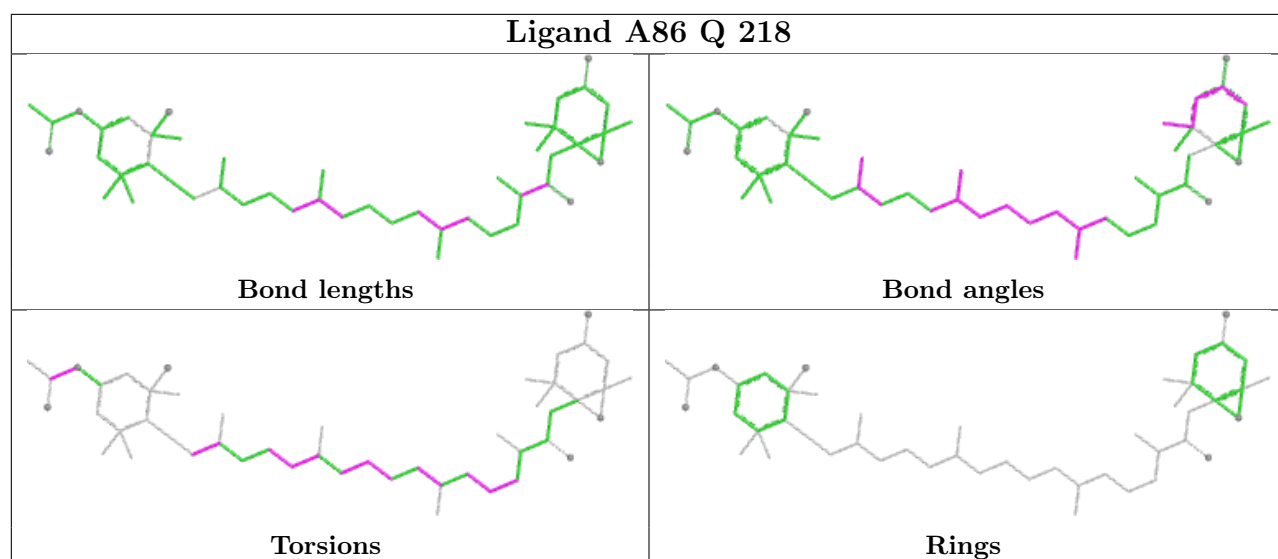
## Ligand CLA B 825

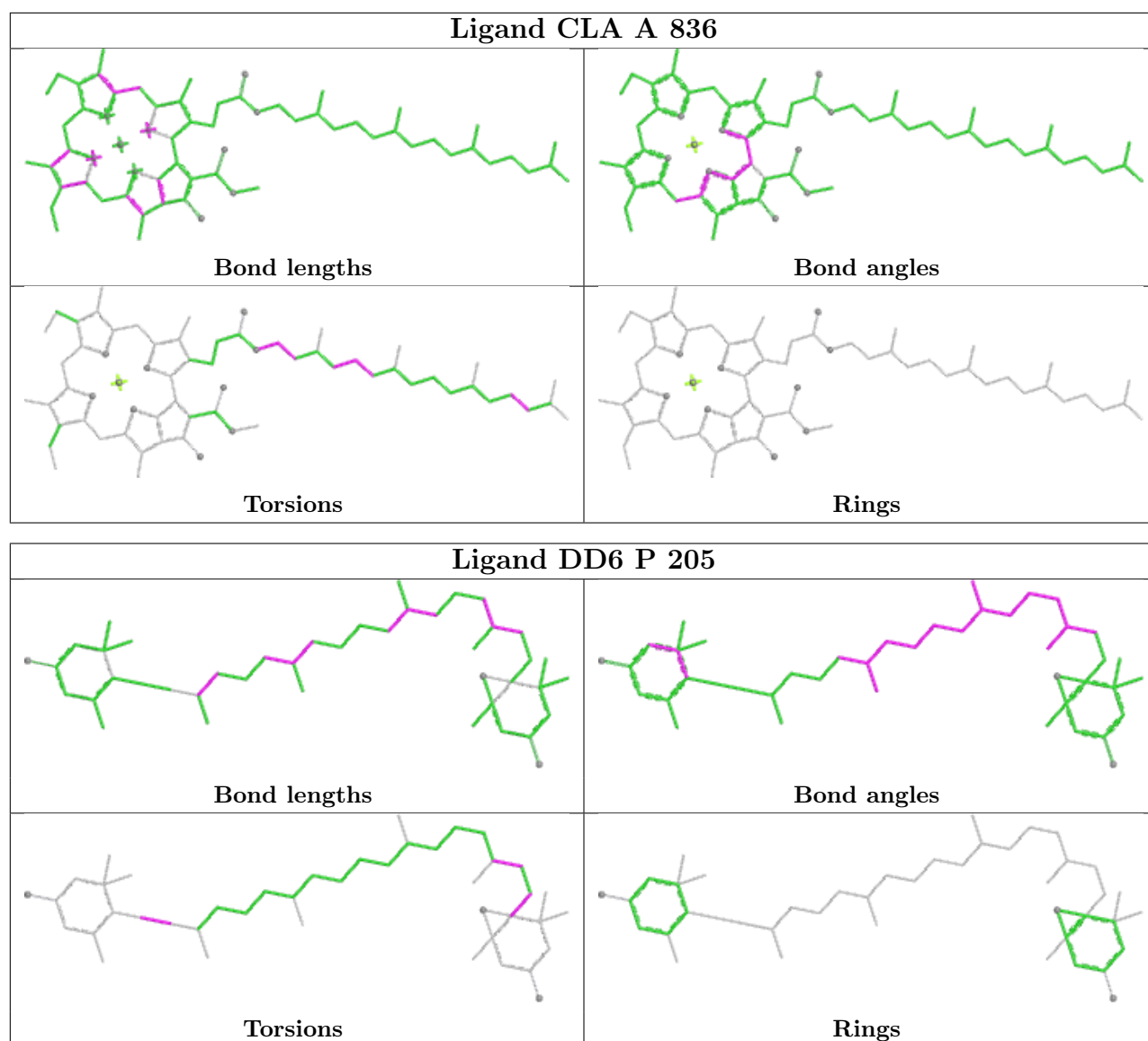


## Ligand DD6 G 214

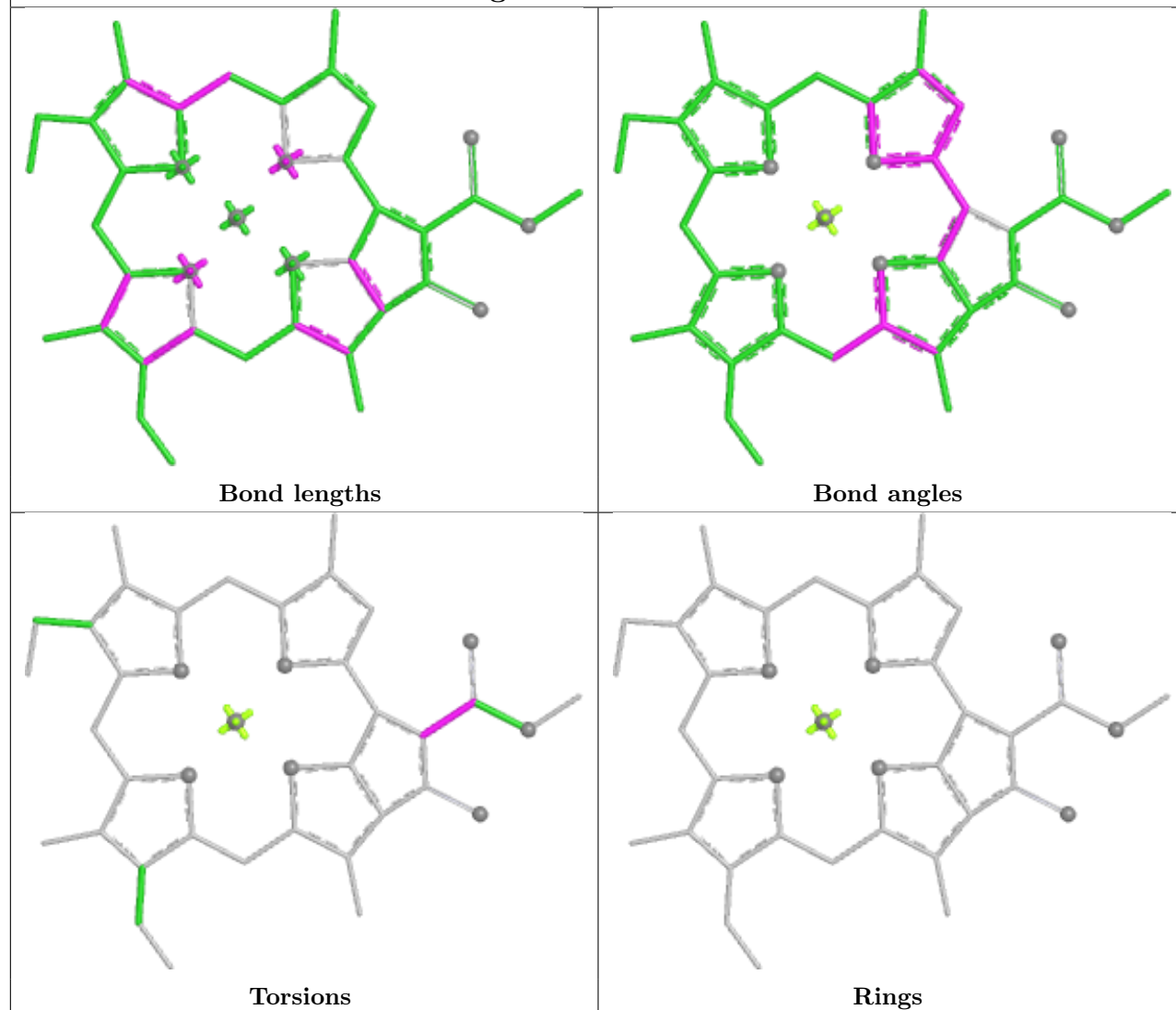




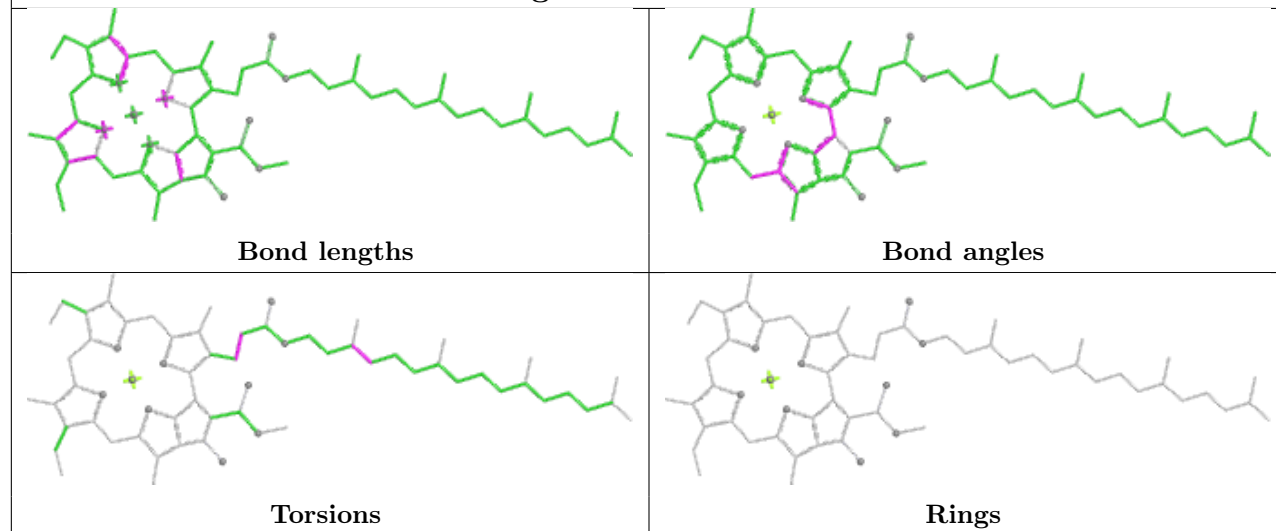




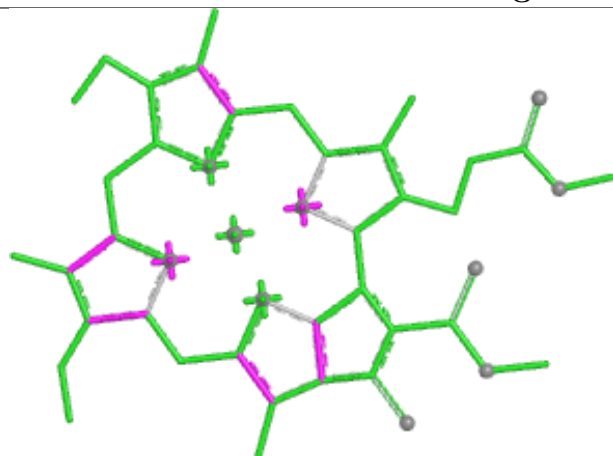
## Ligand CLA A 855



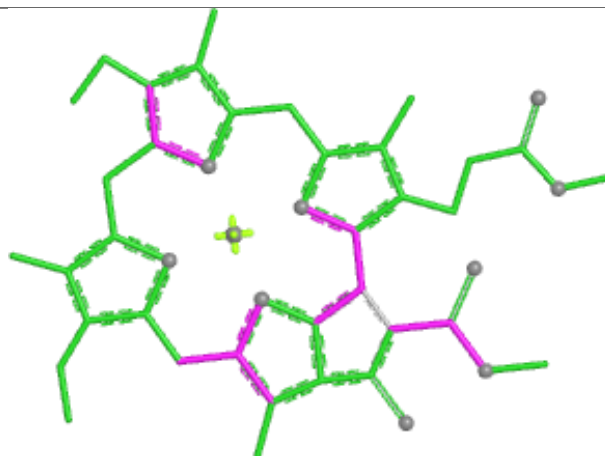
## Ligand CLA A 850



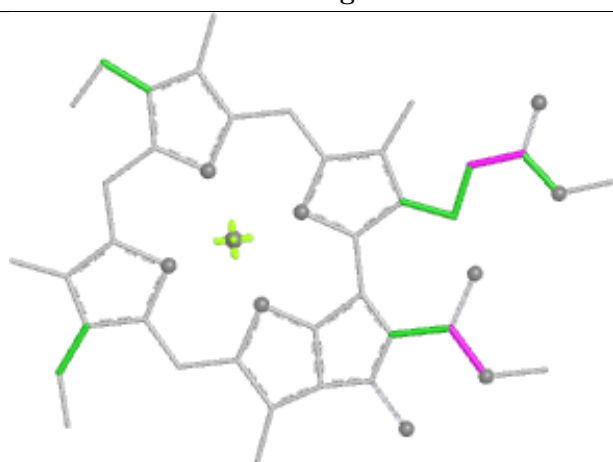
## Ligand CLA U 208



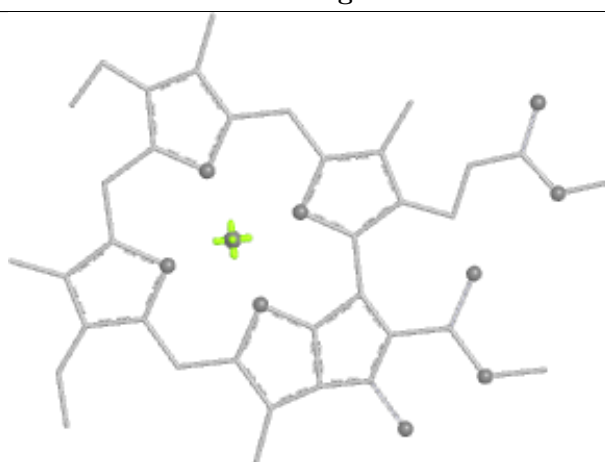
Bond lengths



Bond angles

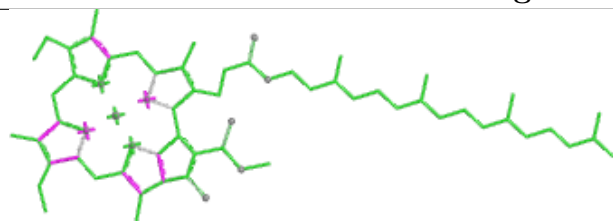


Torsions

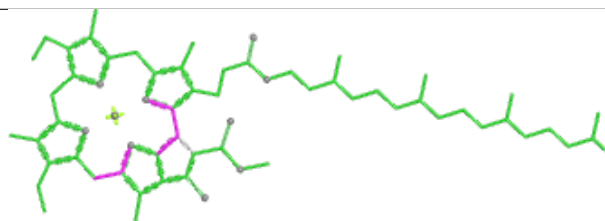


Rings

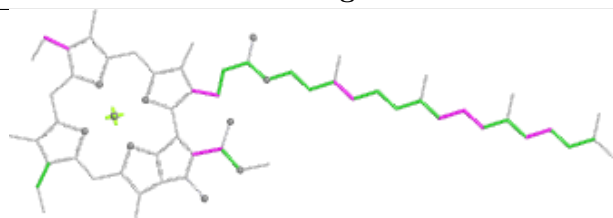
## Ligand CLA A 853



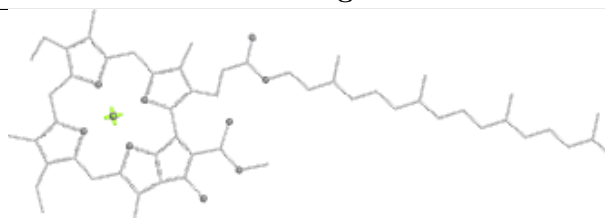
Bond lengths



Bond angles



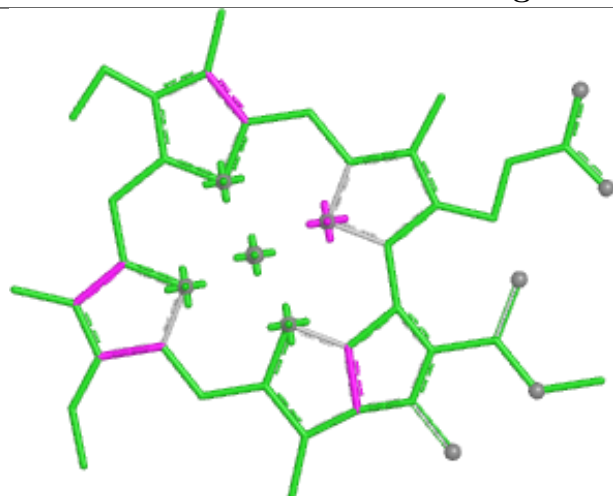
Torsions



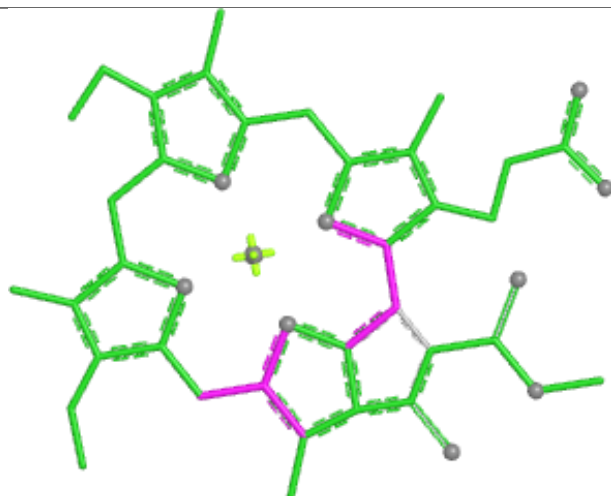
Rings



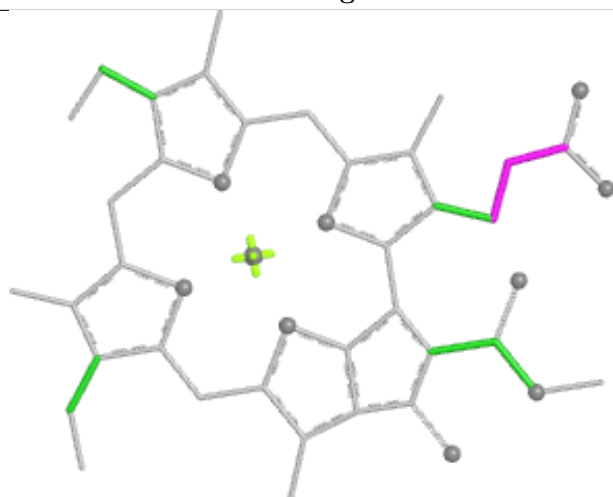
## Ligand CLA G 215



Bond lengths



Bond angles

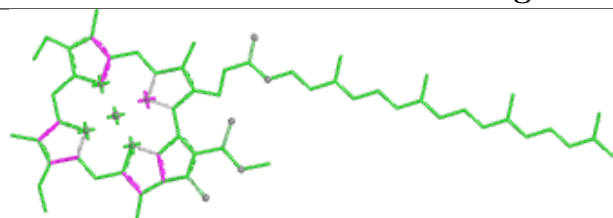


Torsions

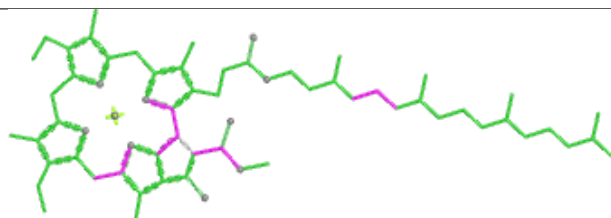


Rings

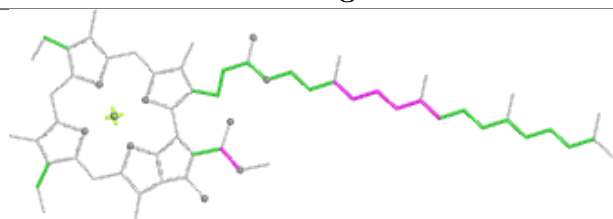
## Ligand CLA O 209



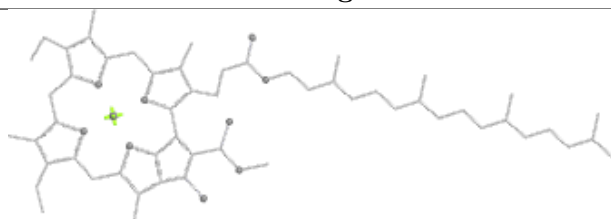
Bond lengths



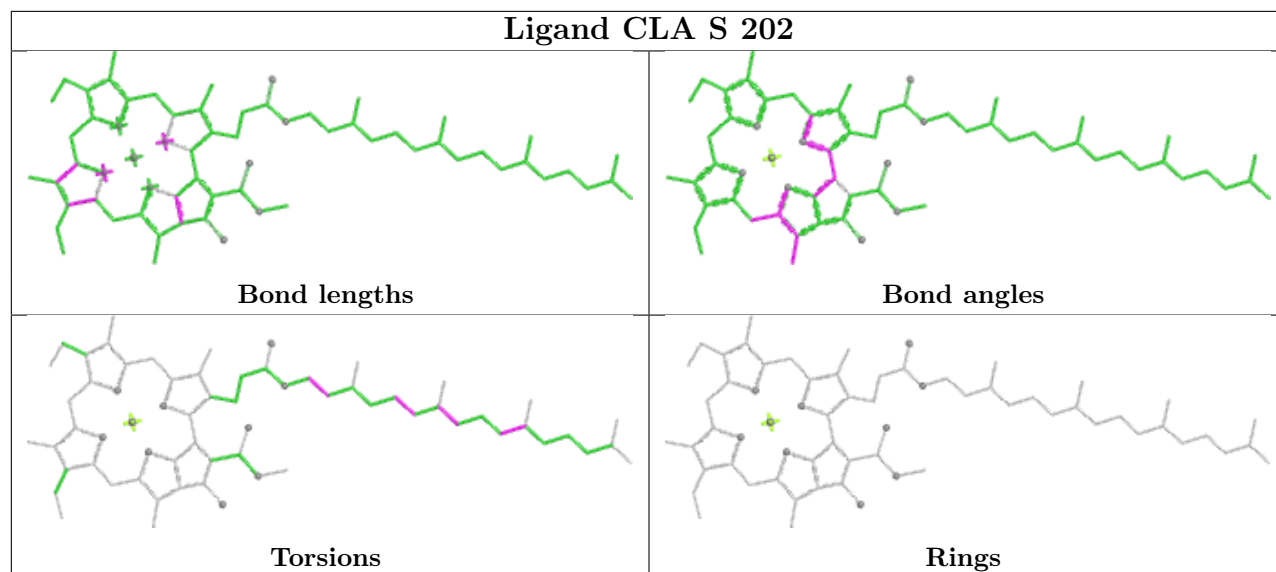
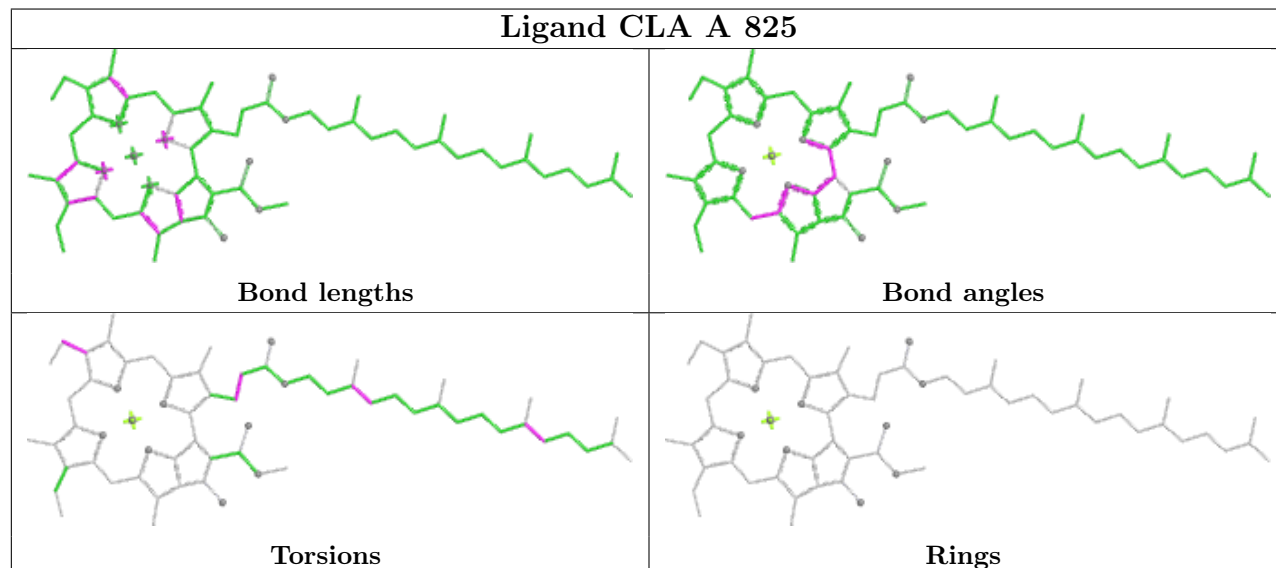
Bond angles



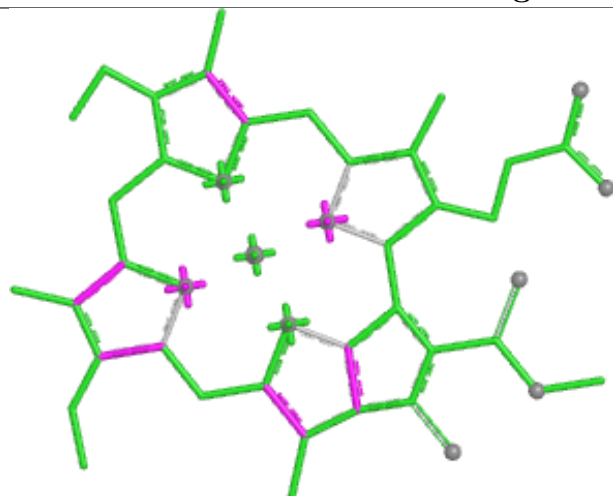
Torsions



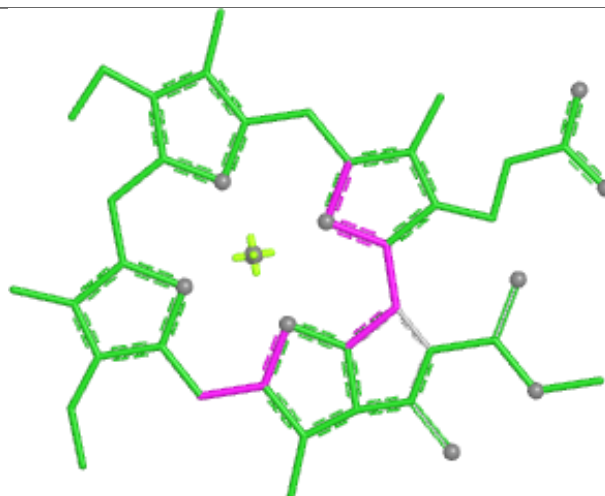
Rings

**Ligand CLA S 202****Ligand CLA A 825**

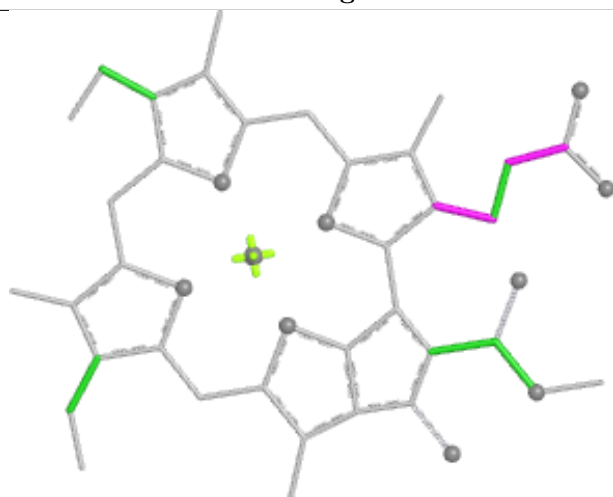
## Ligand CLA G 203



Bond lengths



Bond angles

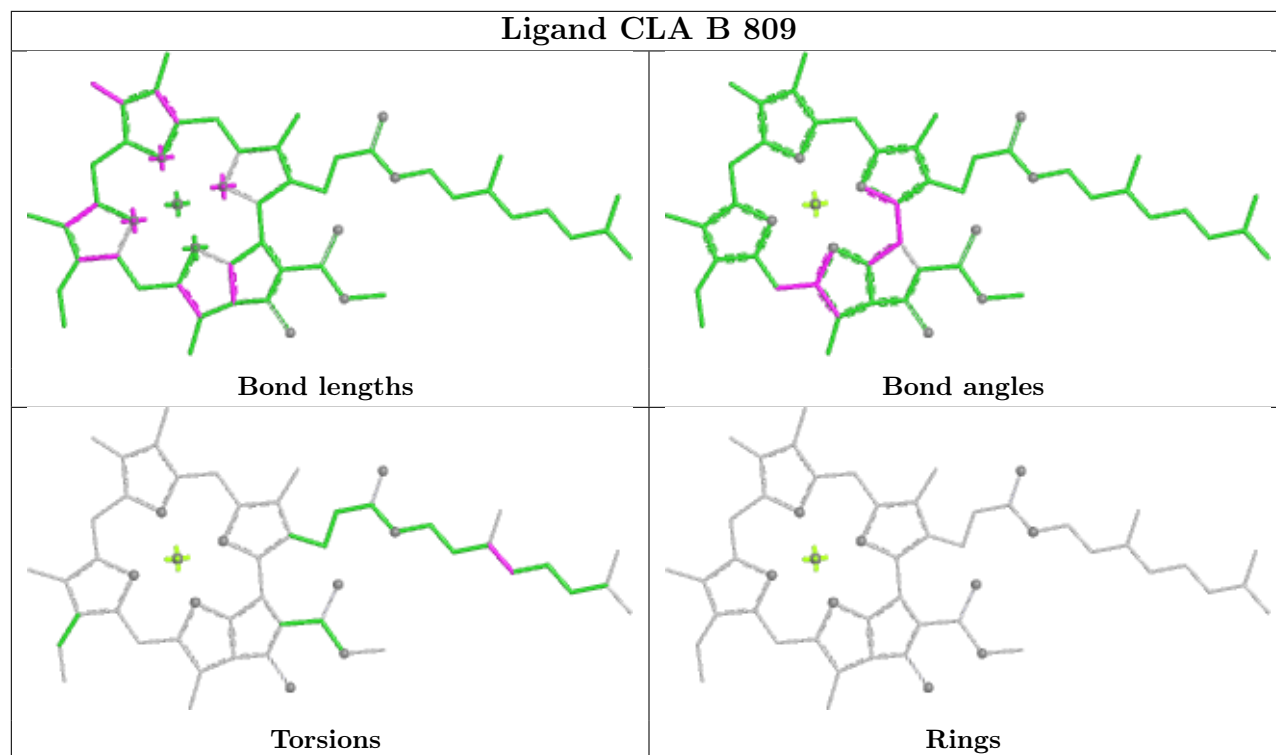


Torsions

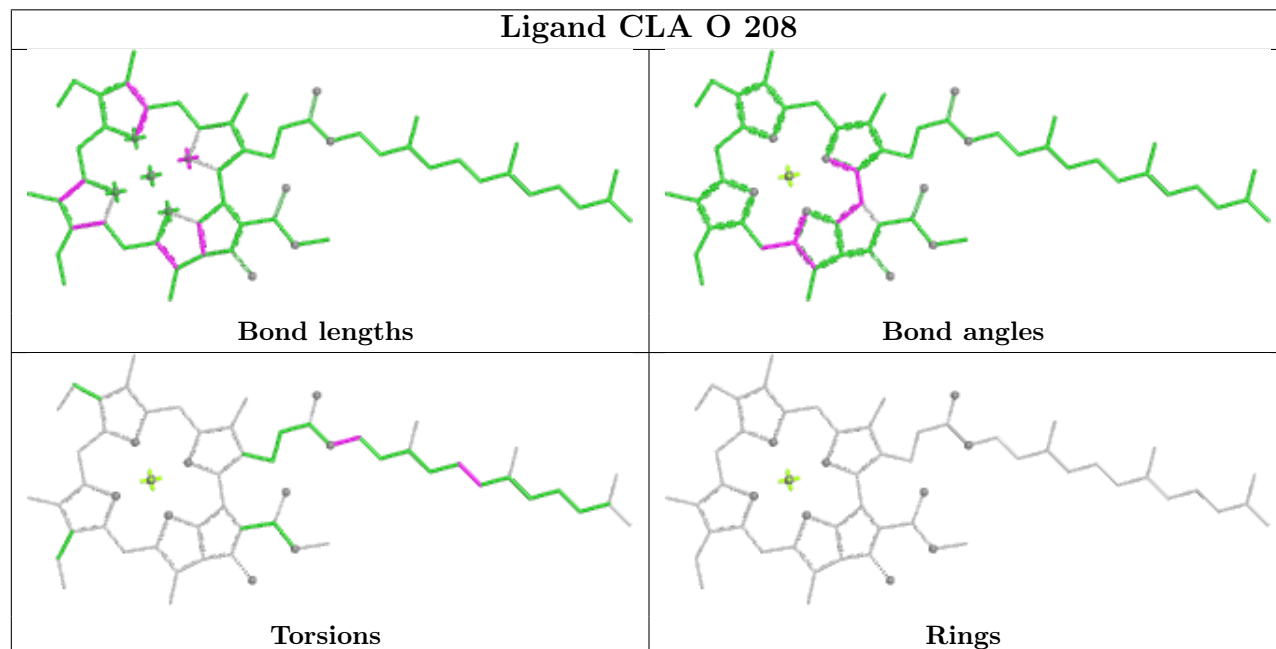


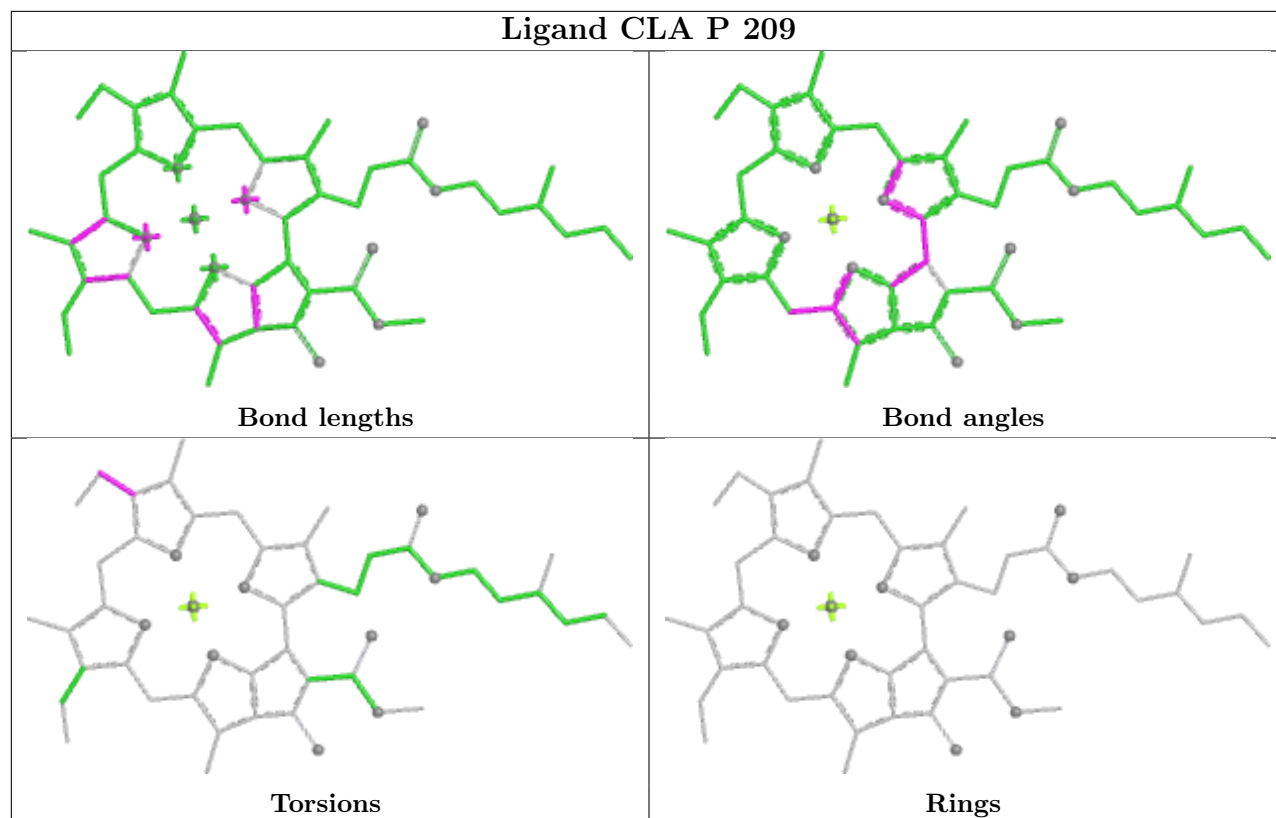
Rings

## Ligand CLA B 809

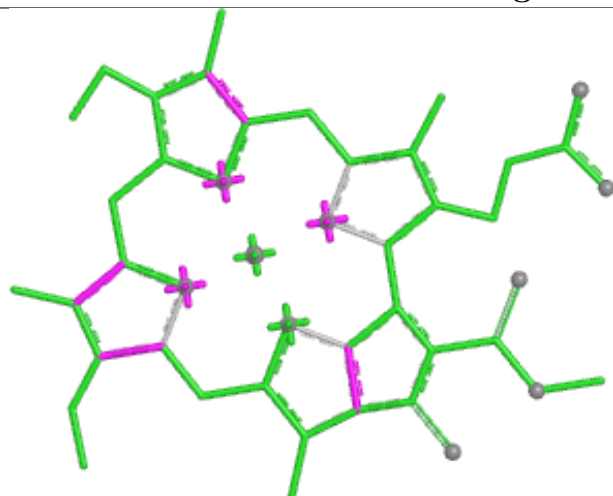


## Ligand CLA O 208

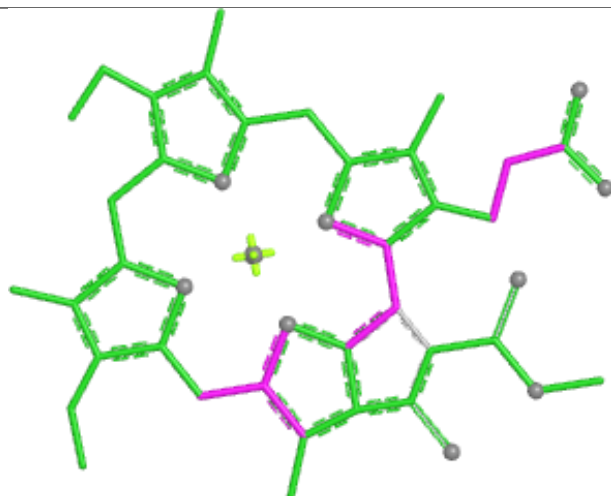




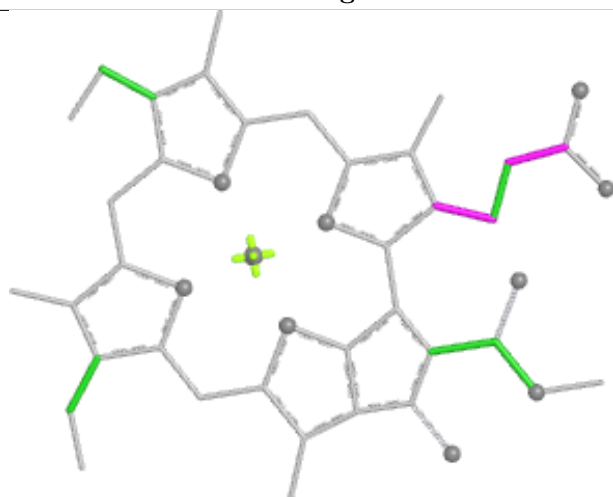
## Ligand CLA H 210



Bond lengths



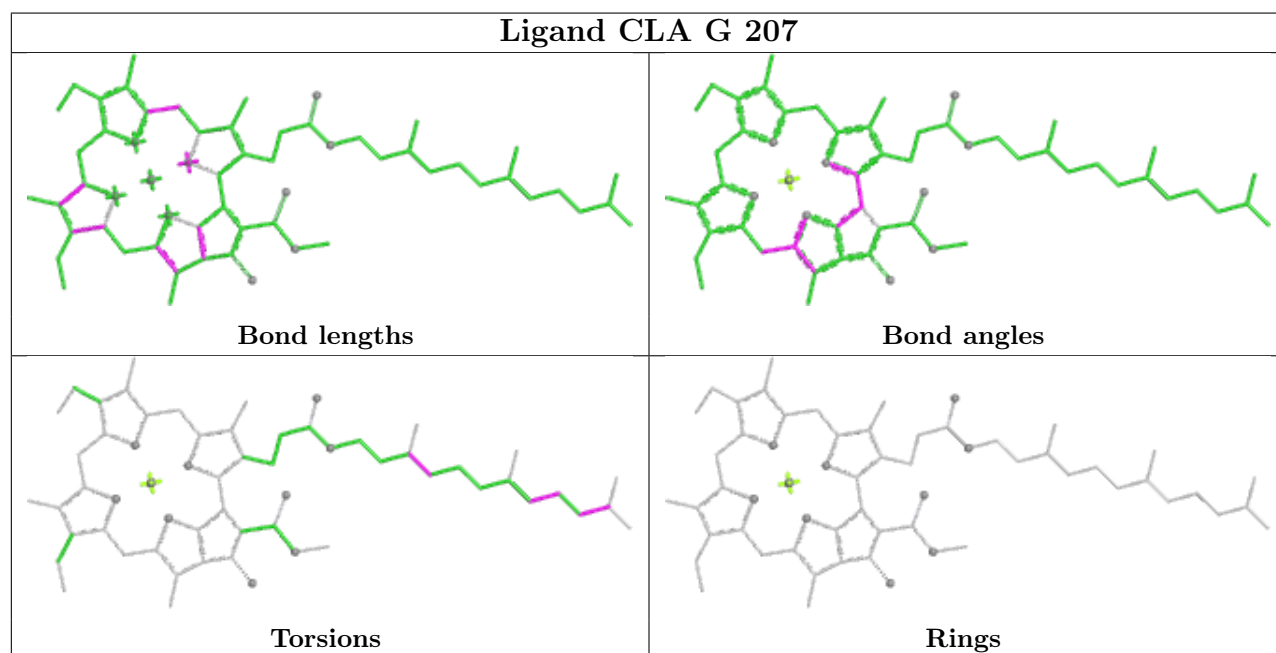
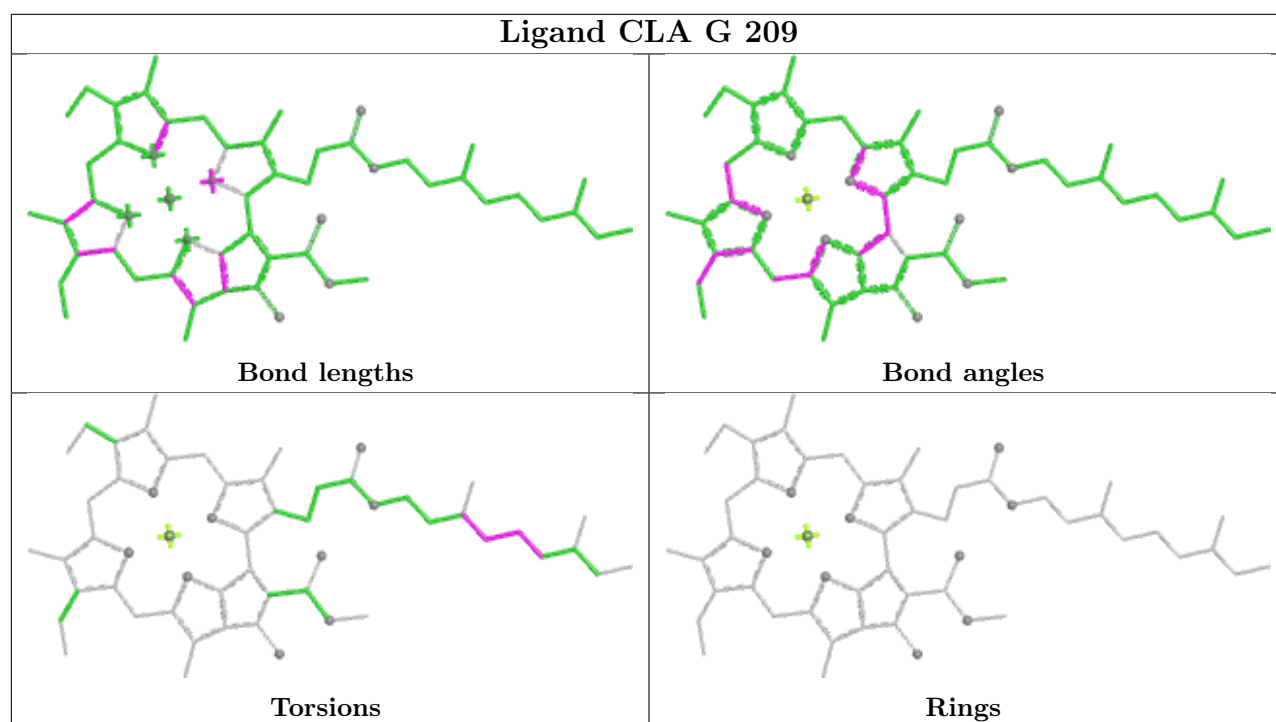
Bond angles

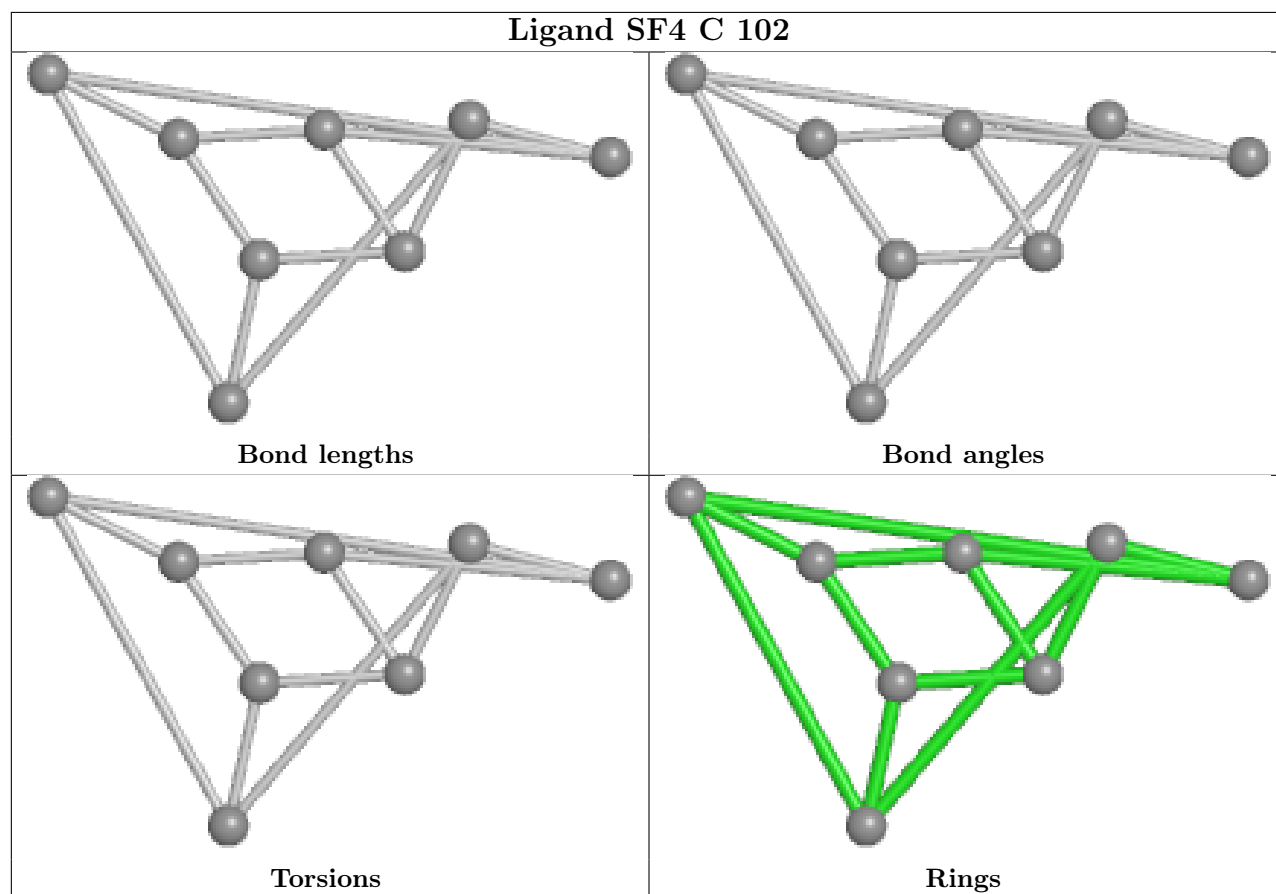
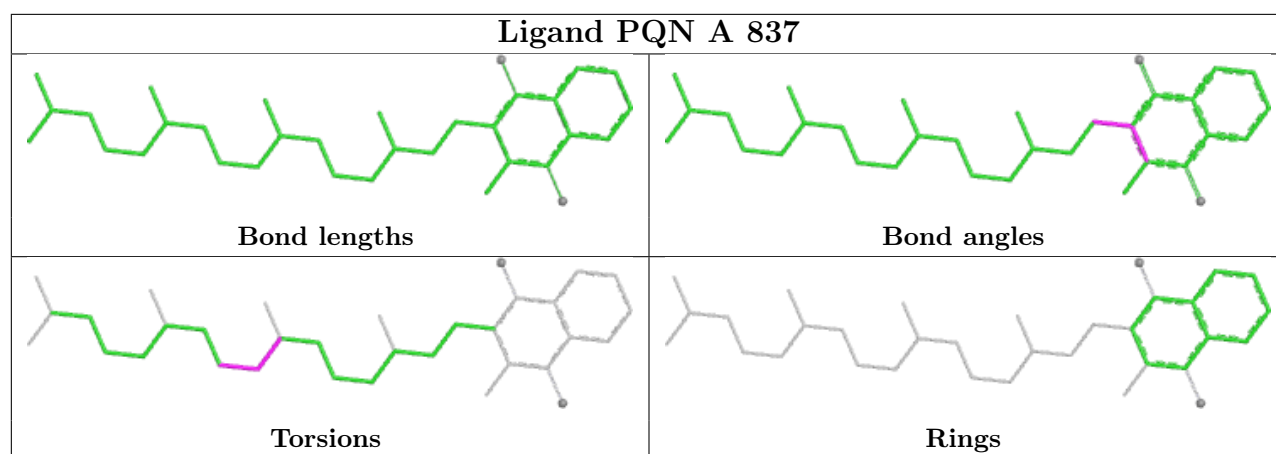


Torsions



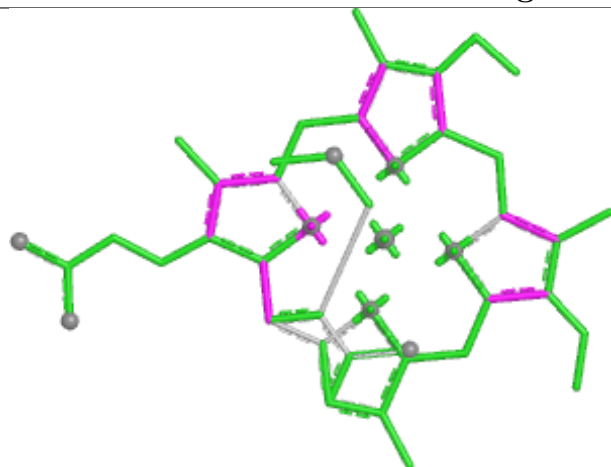
Rings



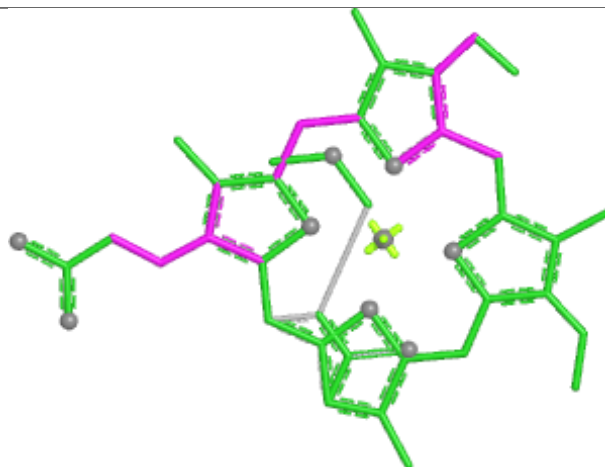




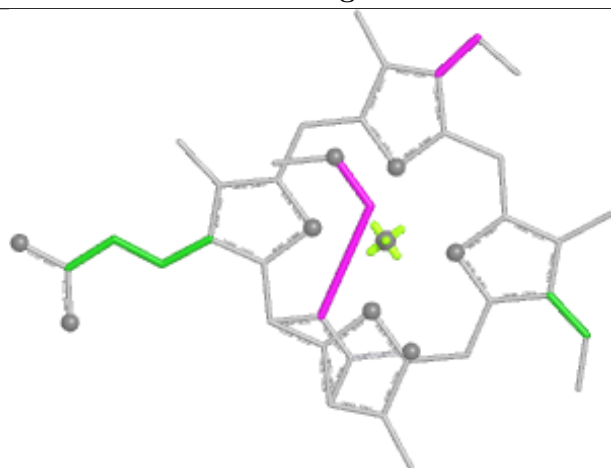
## Ligand KC1 P 212



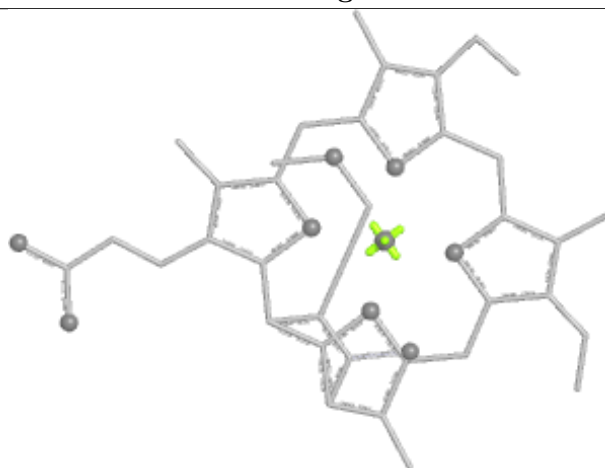
Bond lengths



Bond angles

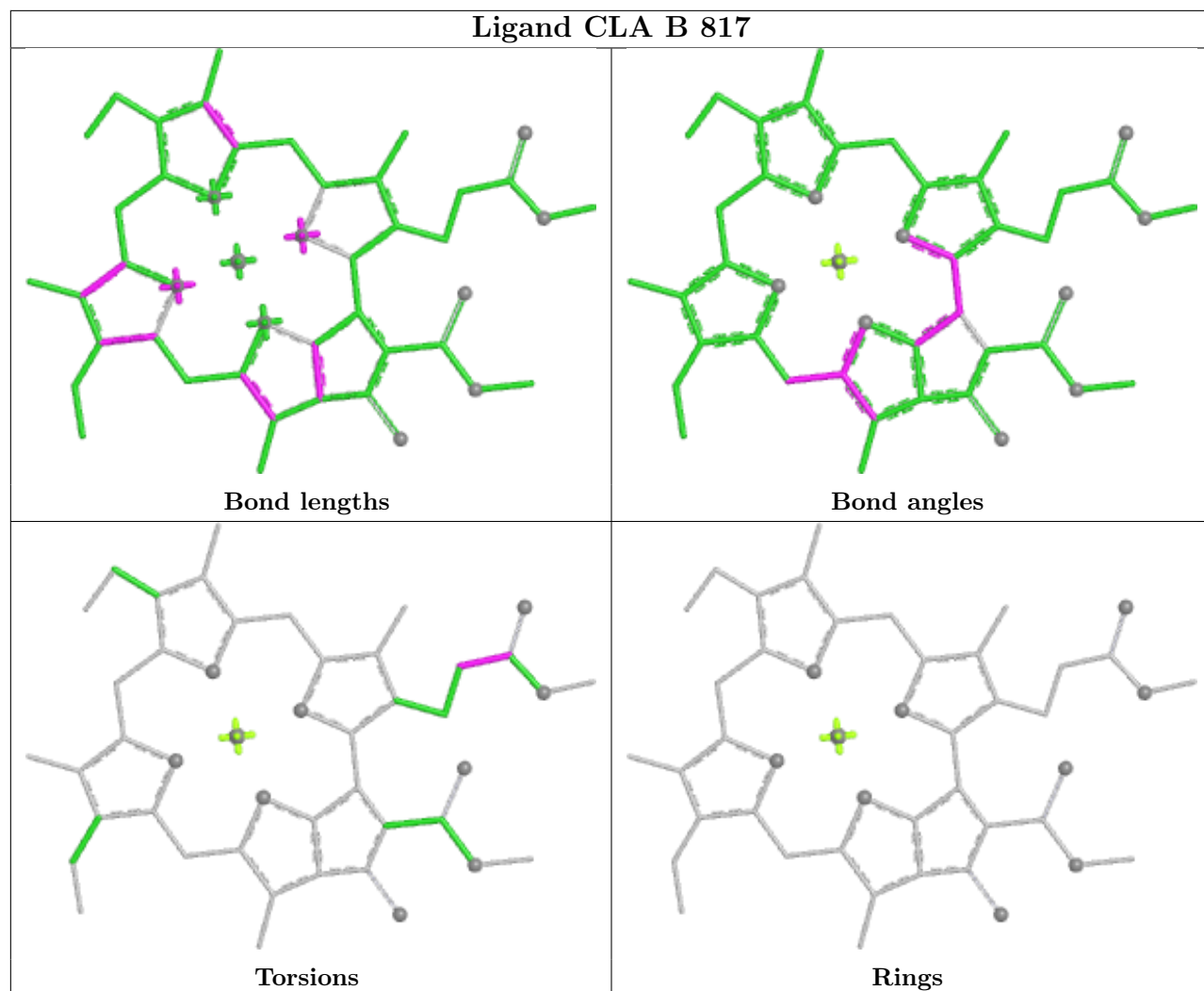


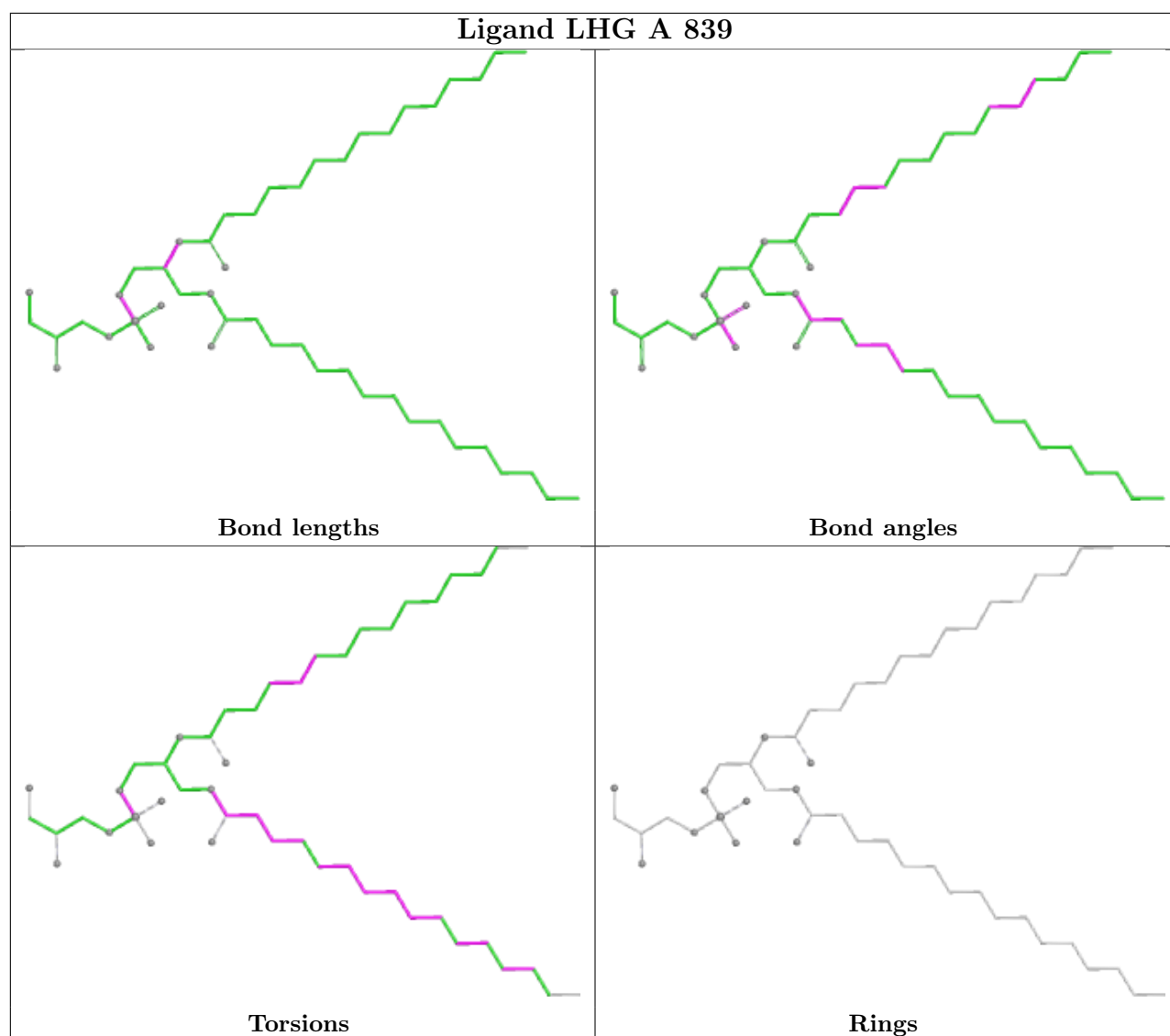
Torsions



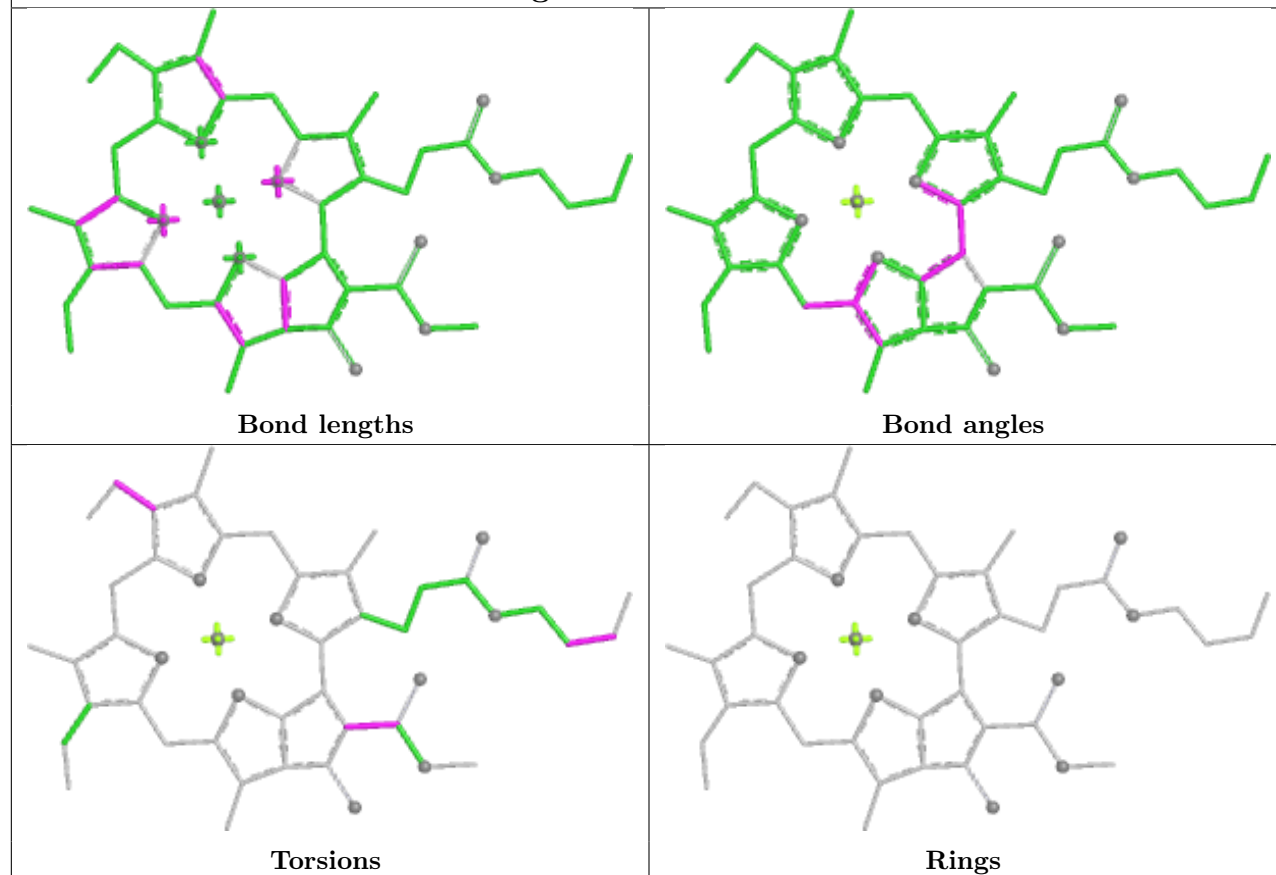
Rings

## Ligand CLA B 817

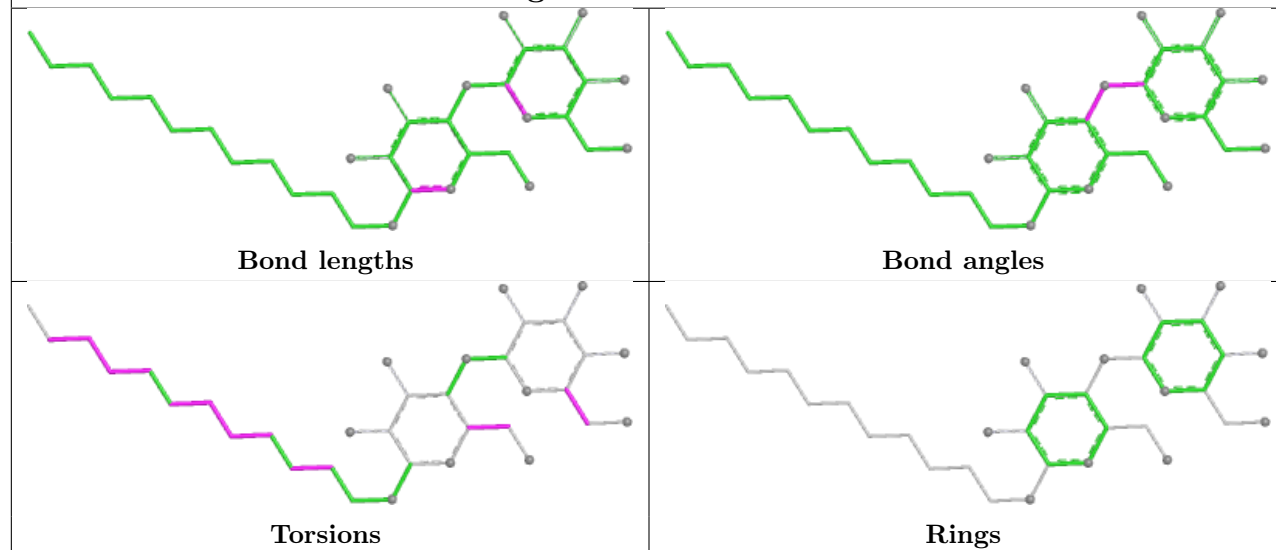


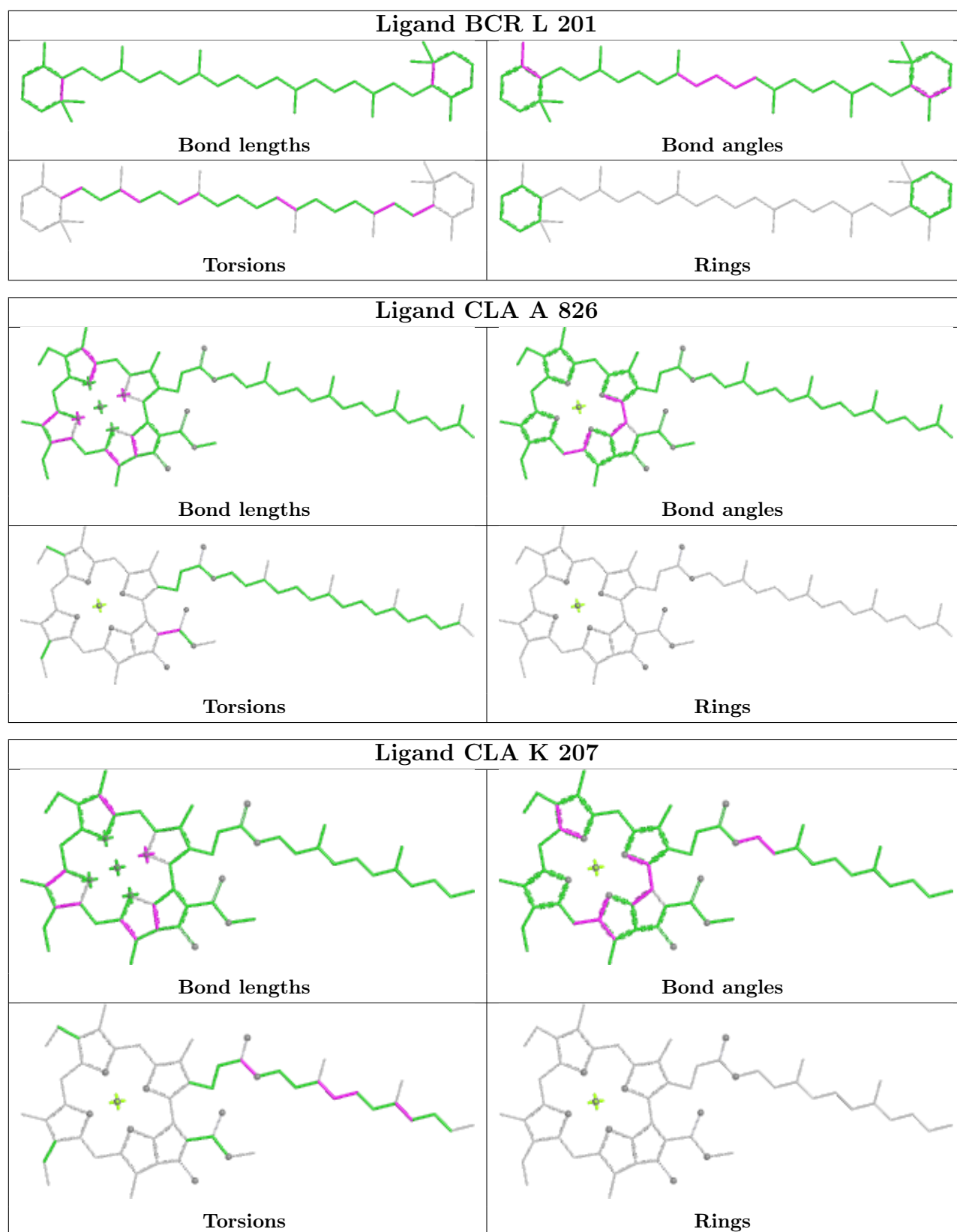


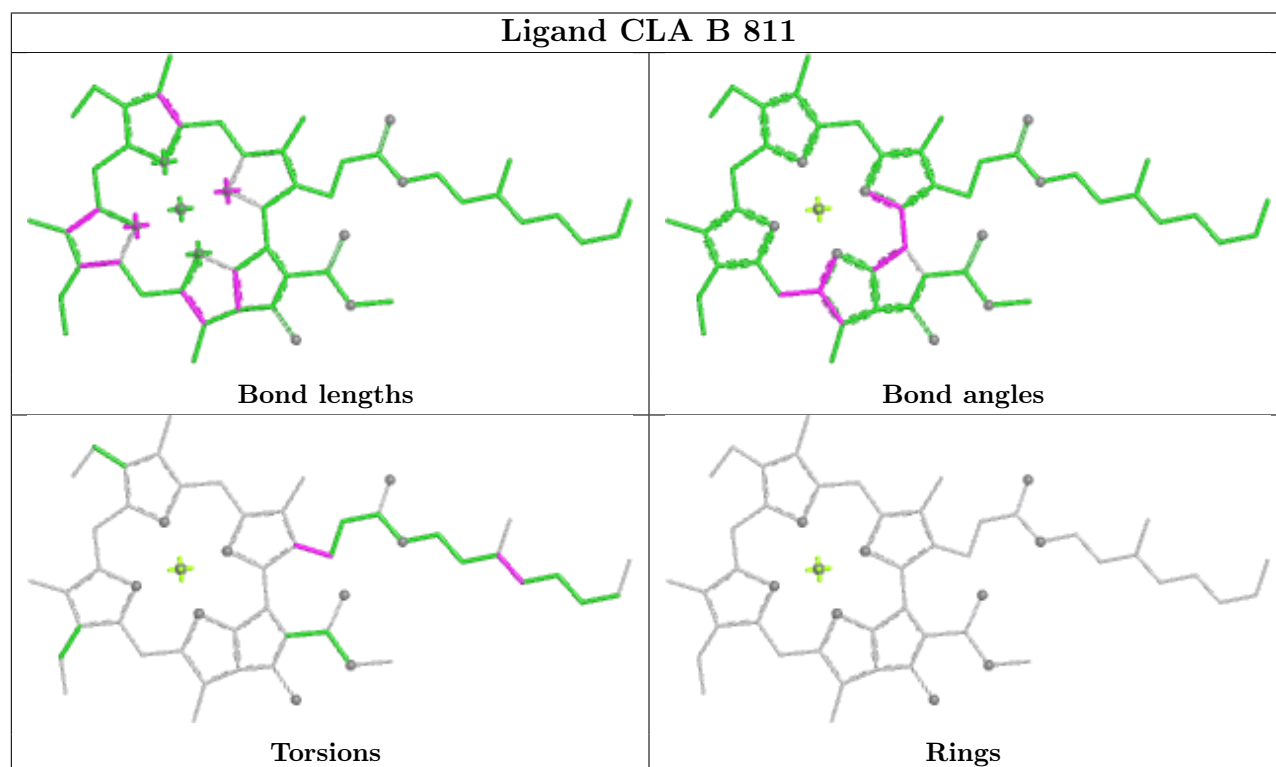
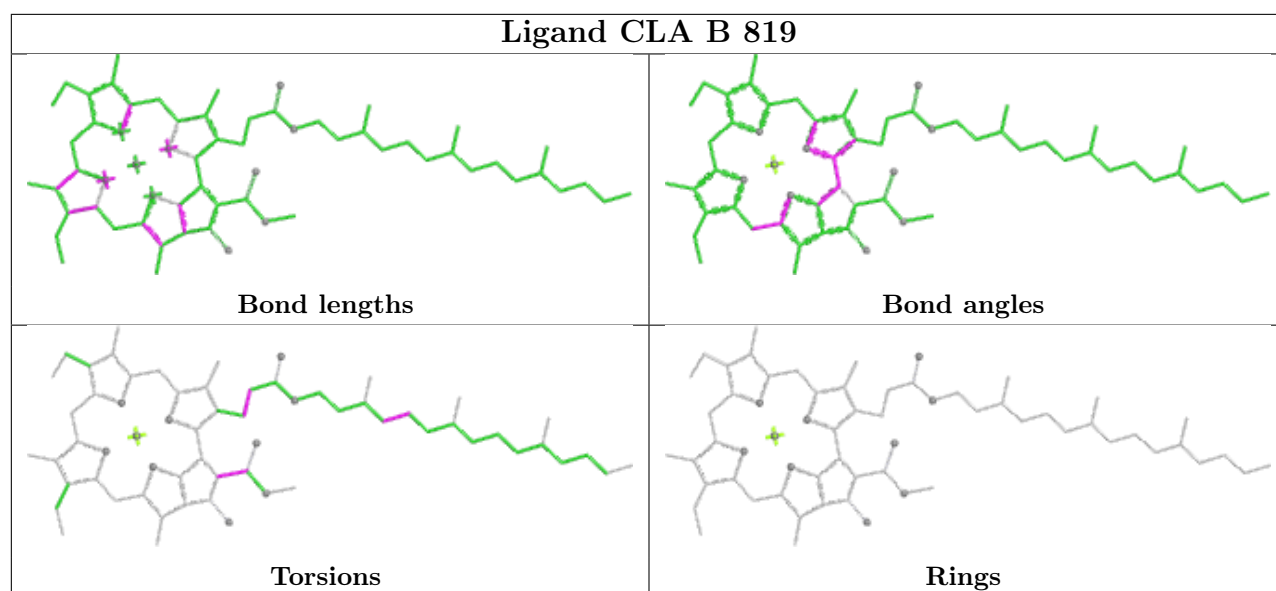
## Ligand CLA A 805

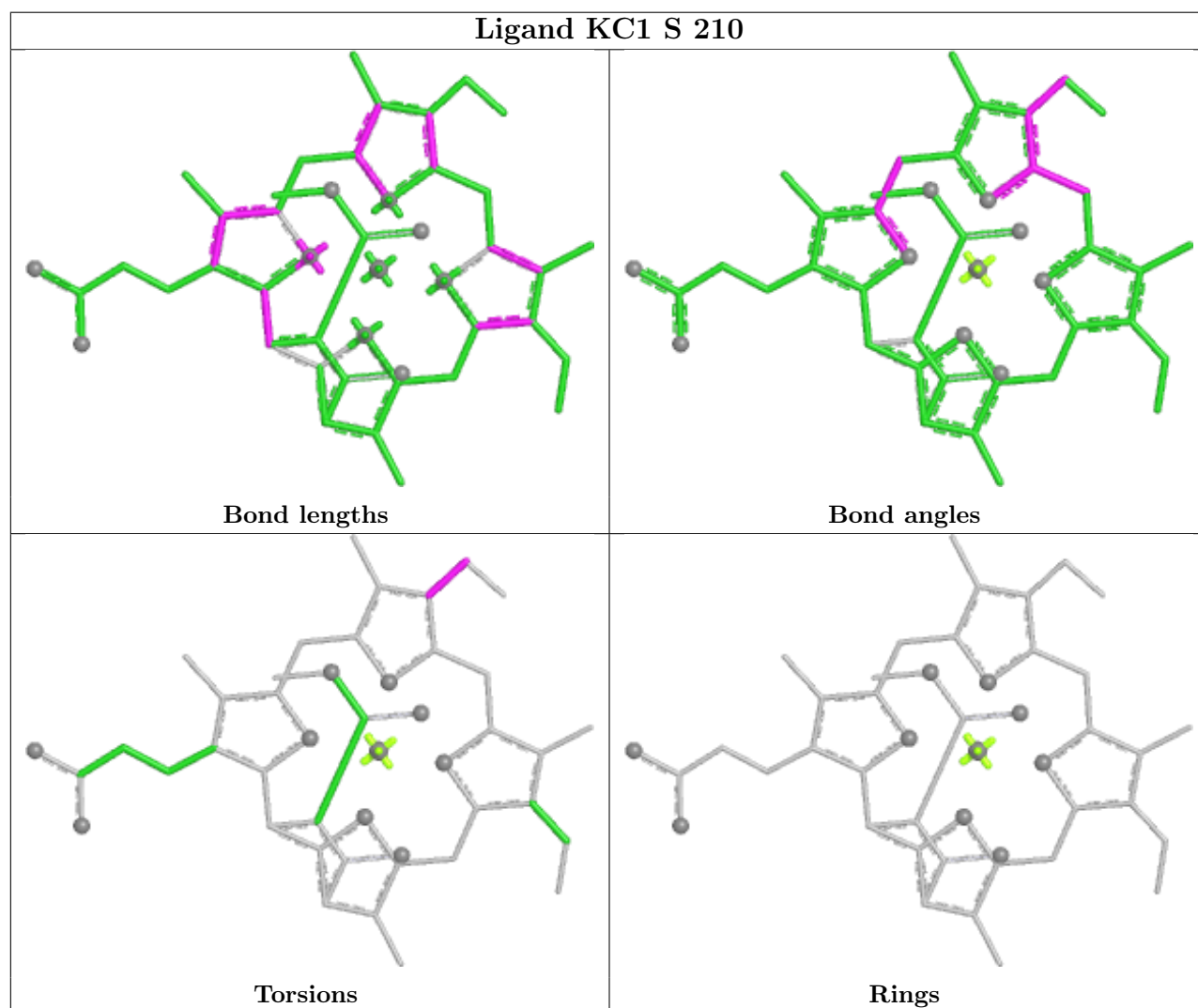
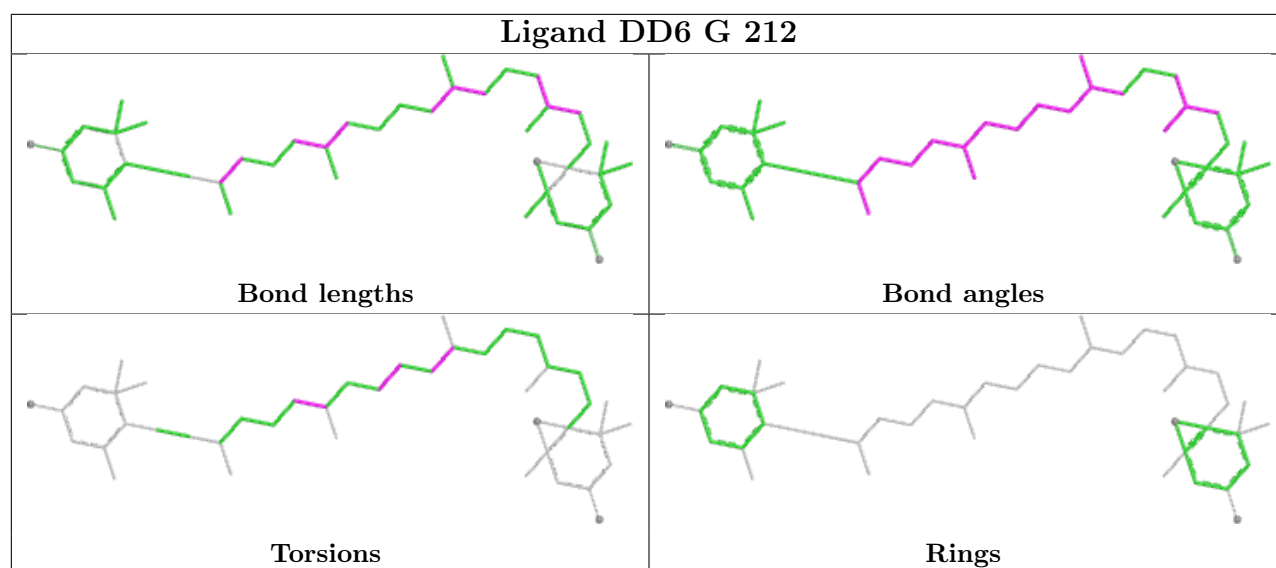


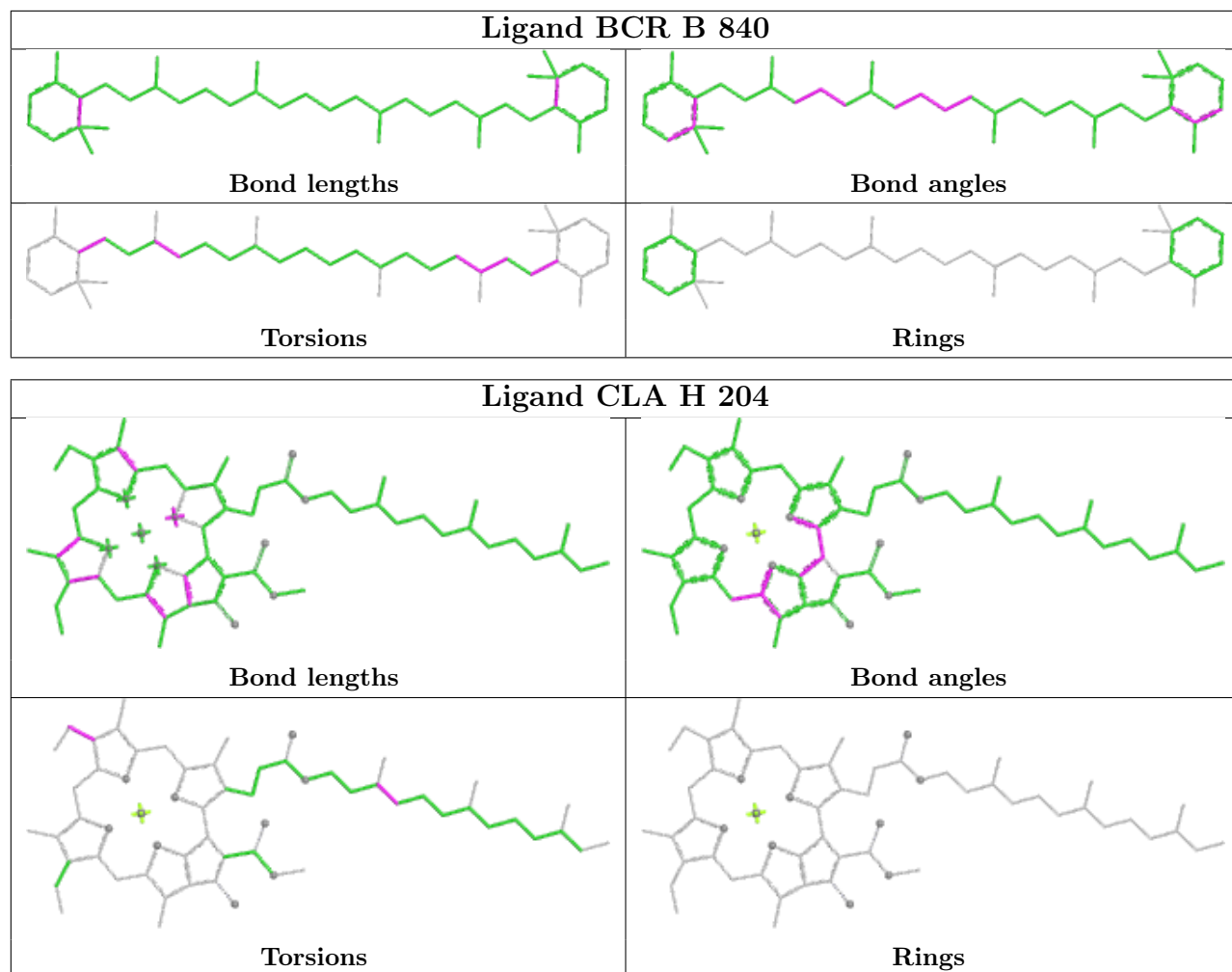
## Ligand LMU A 847





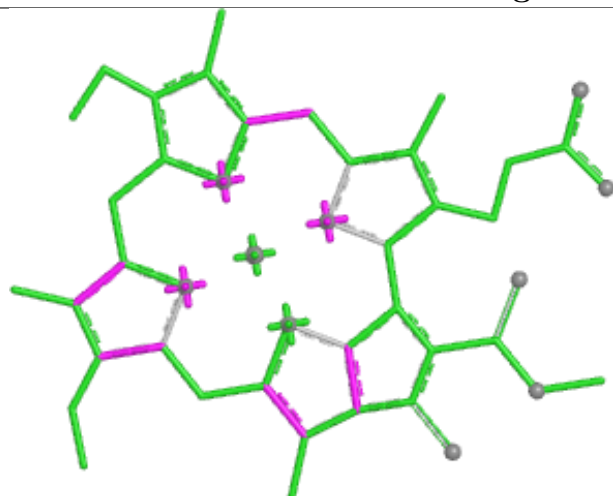




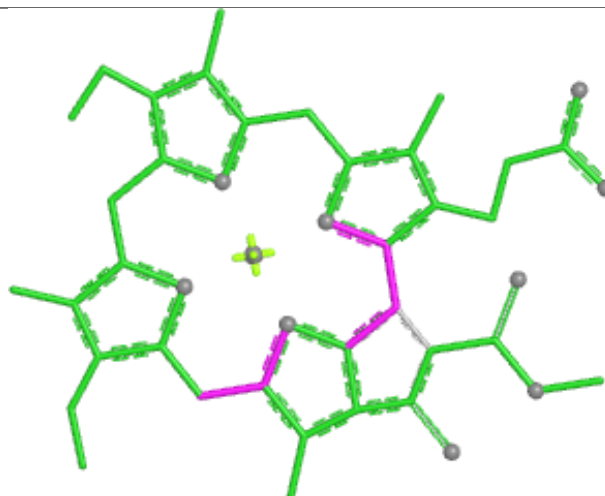




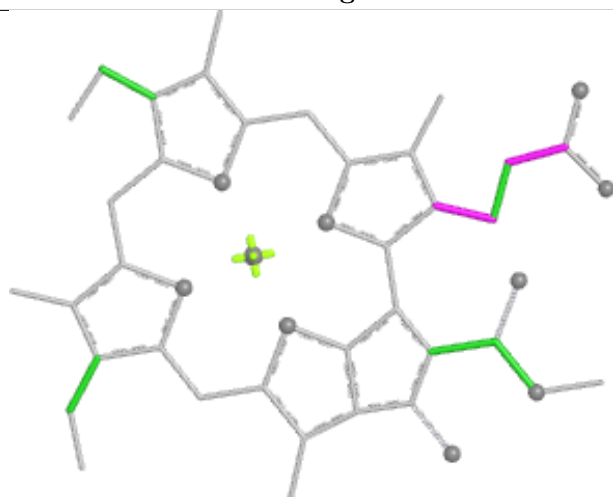
## Ligand CLA K 206



Bond lengths



Bond angles

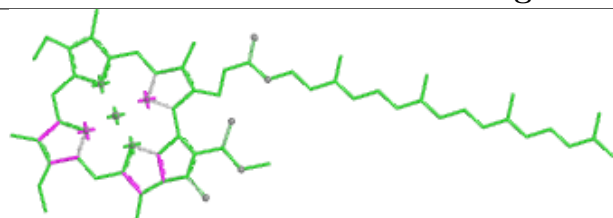


Torsions

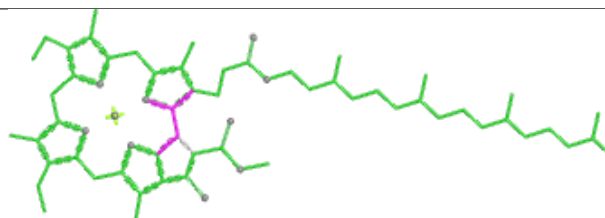


Rings

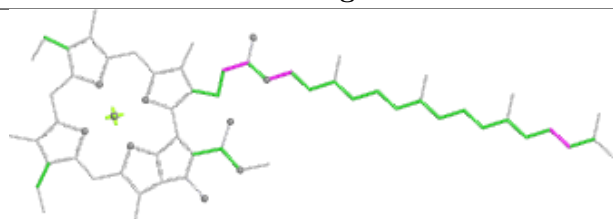
## Ligand CLA B 801



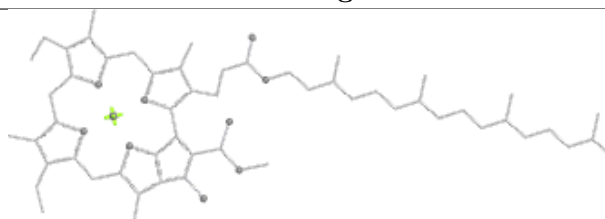
Bond lengths



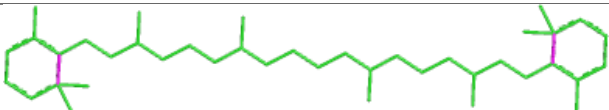
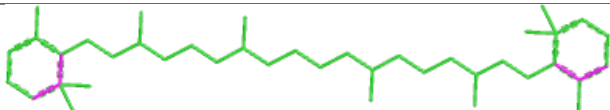
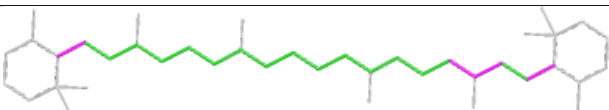
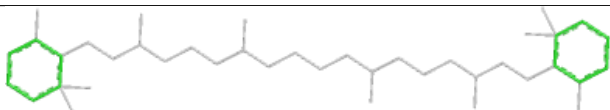
Bond angles

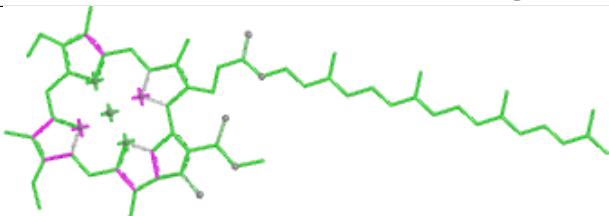
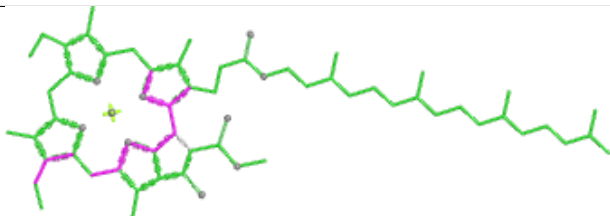
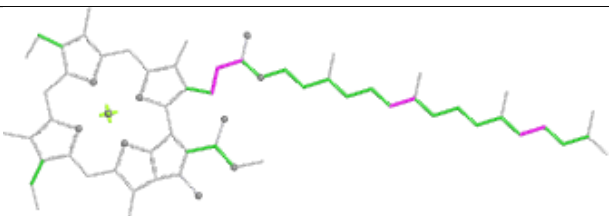
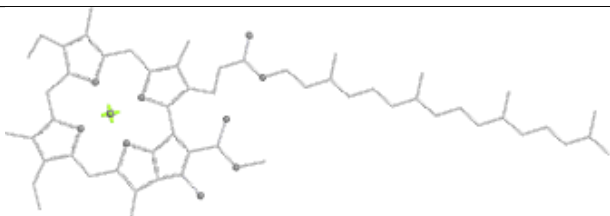


Torsions

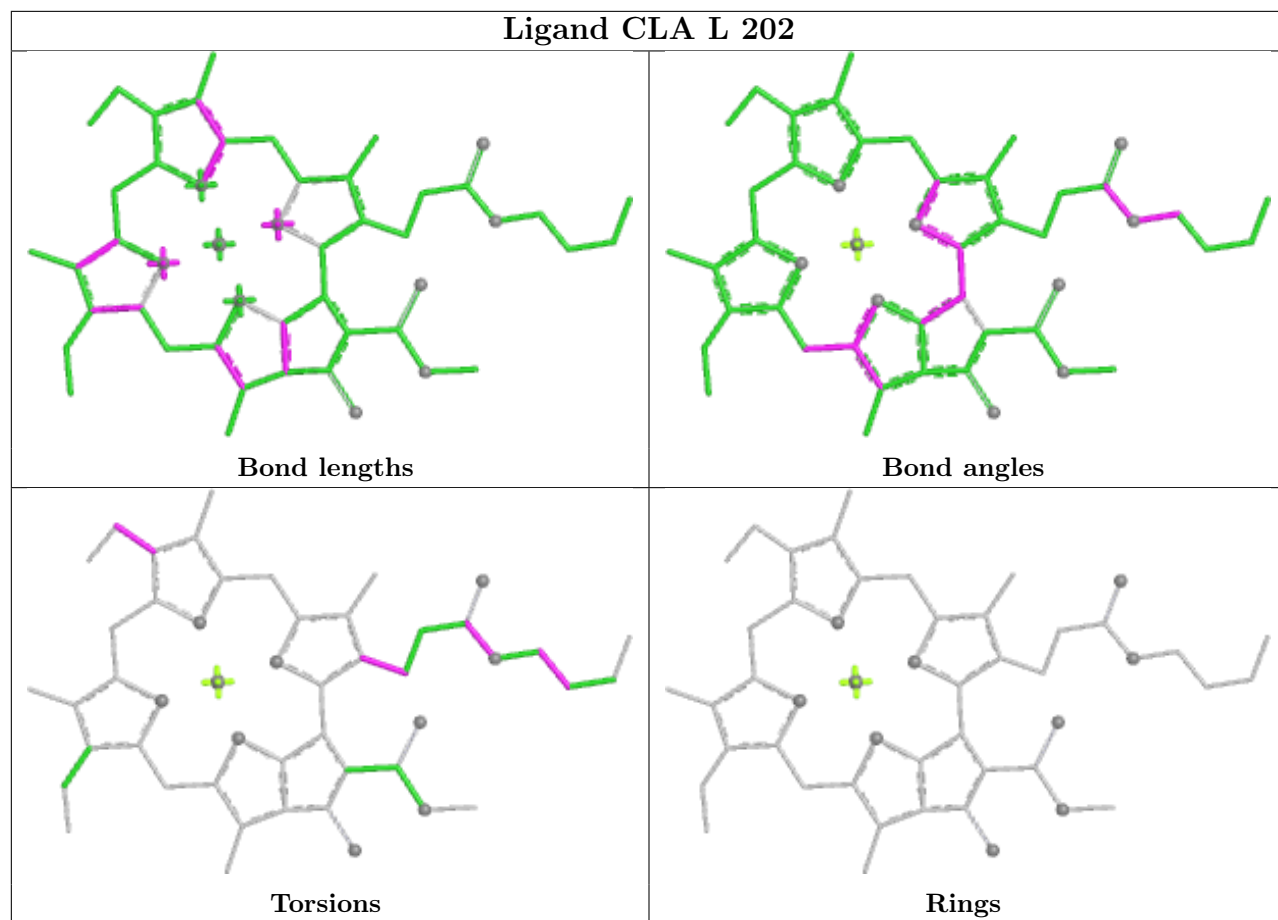


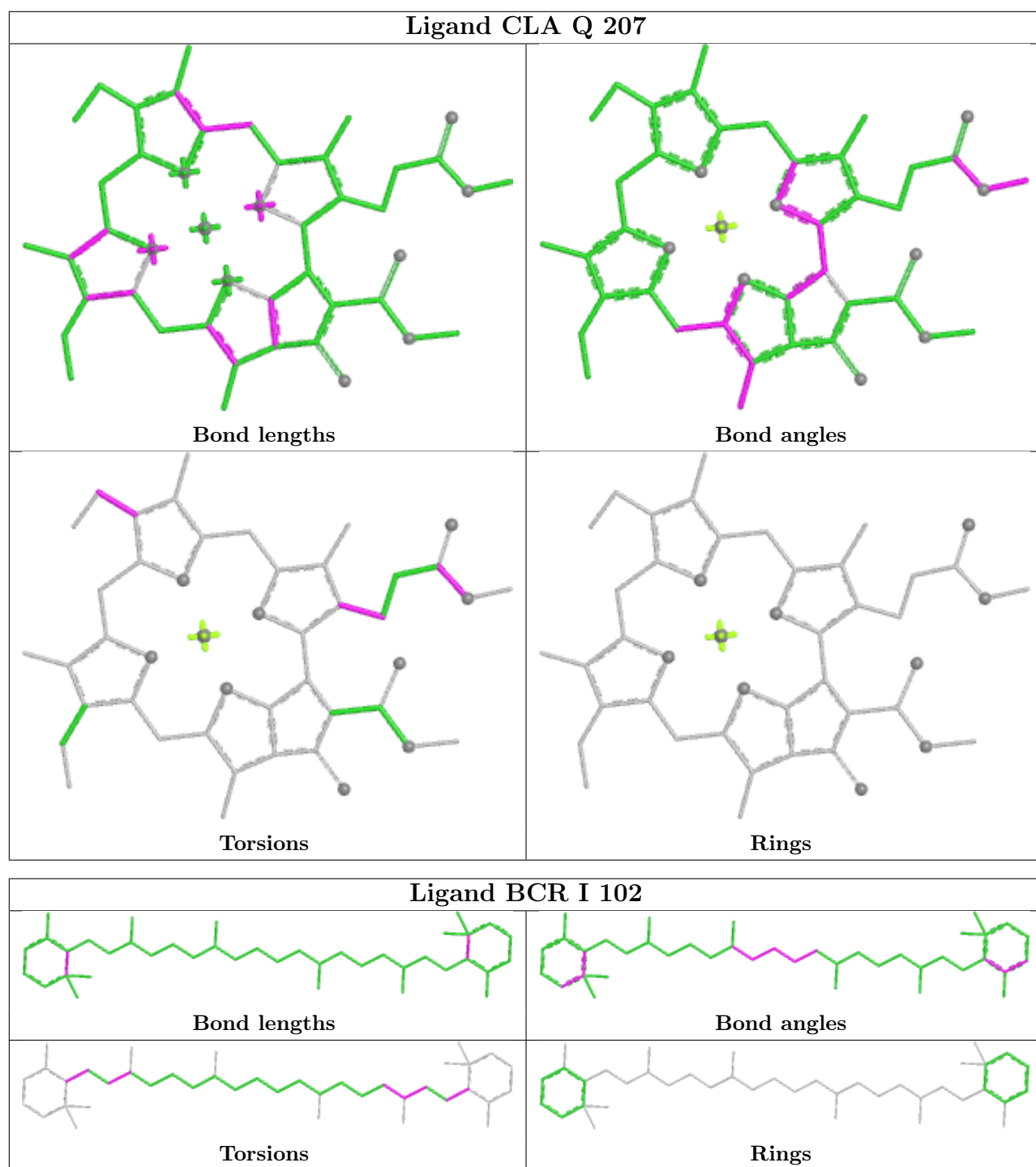
Rings

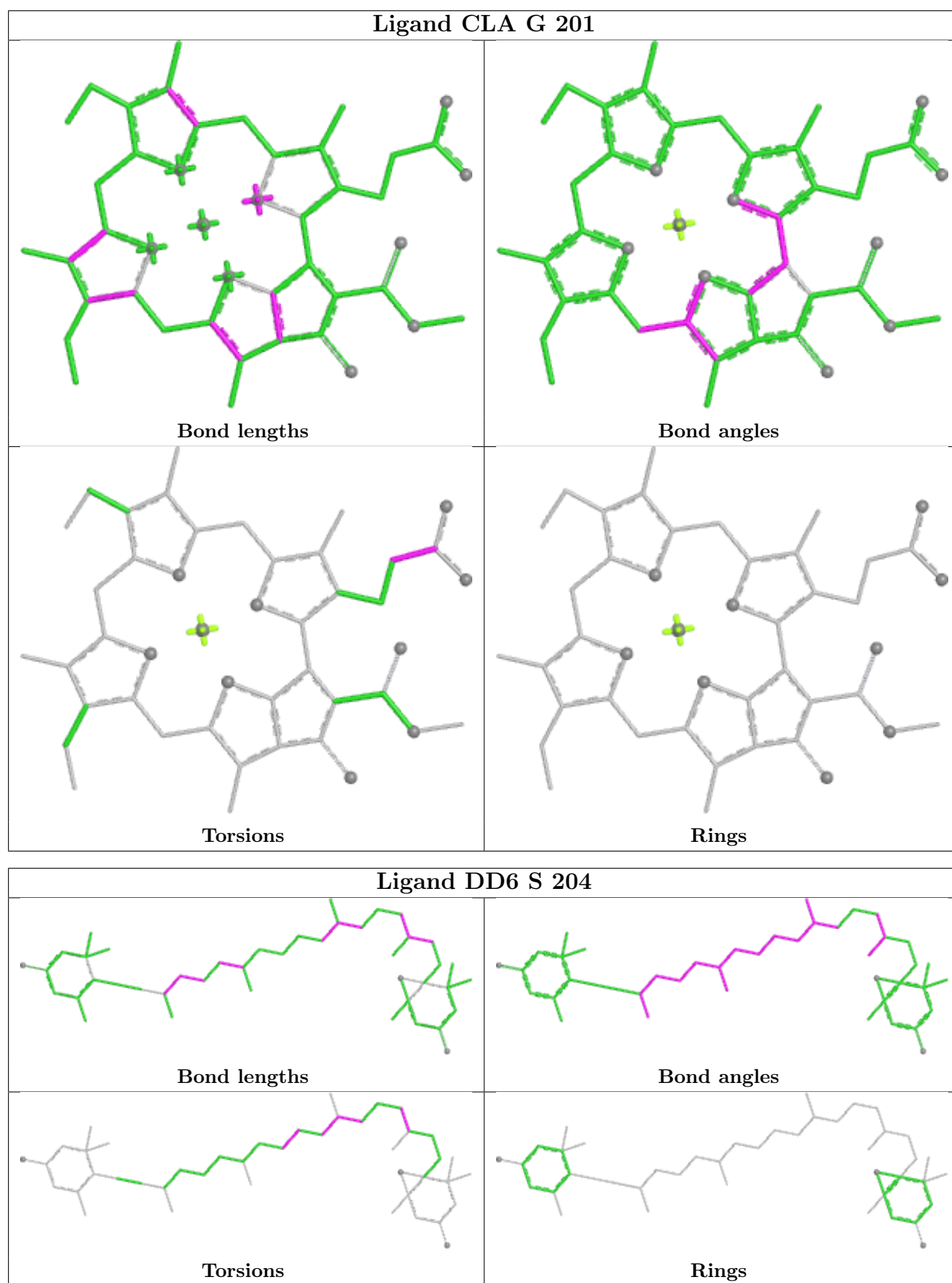
Ligand BCR A 841	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 802	
	
Bond lengths	Bond angles
	
Torsions	Rings

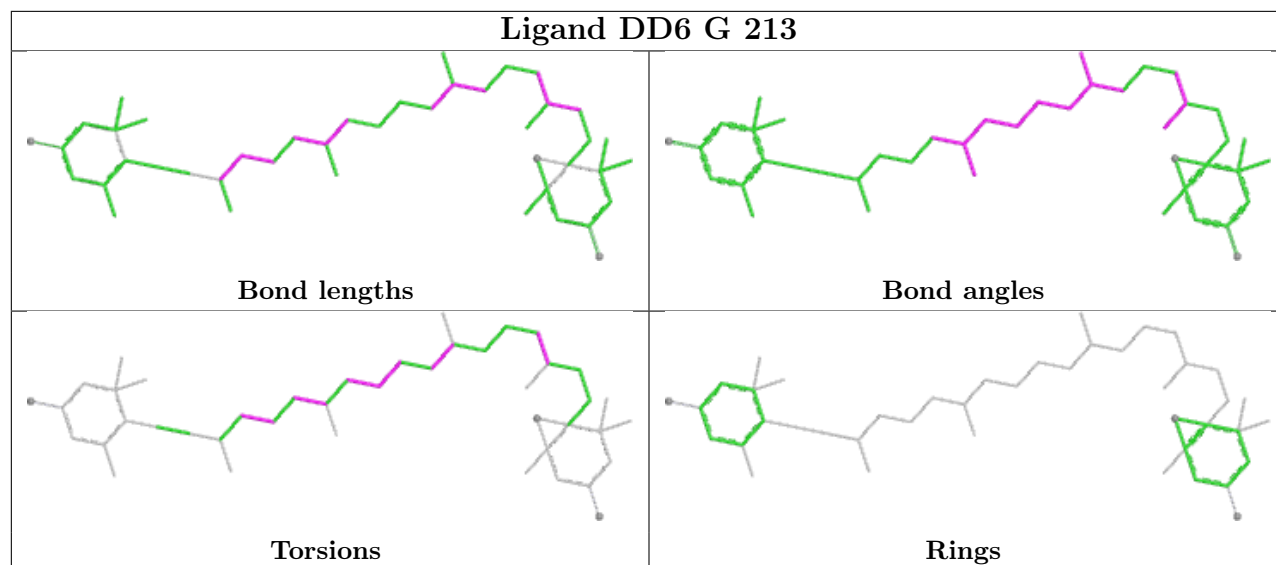
## Ligand CLA L 202



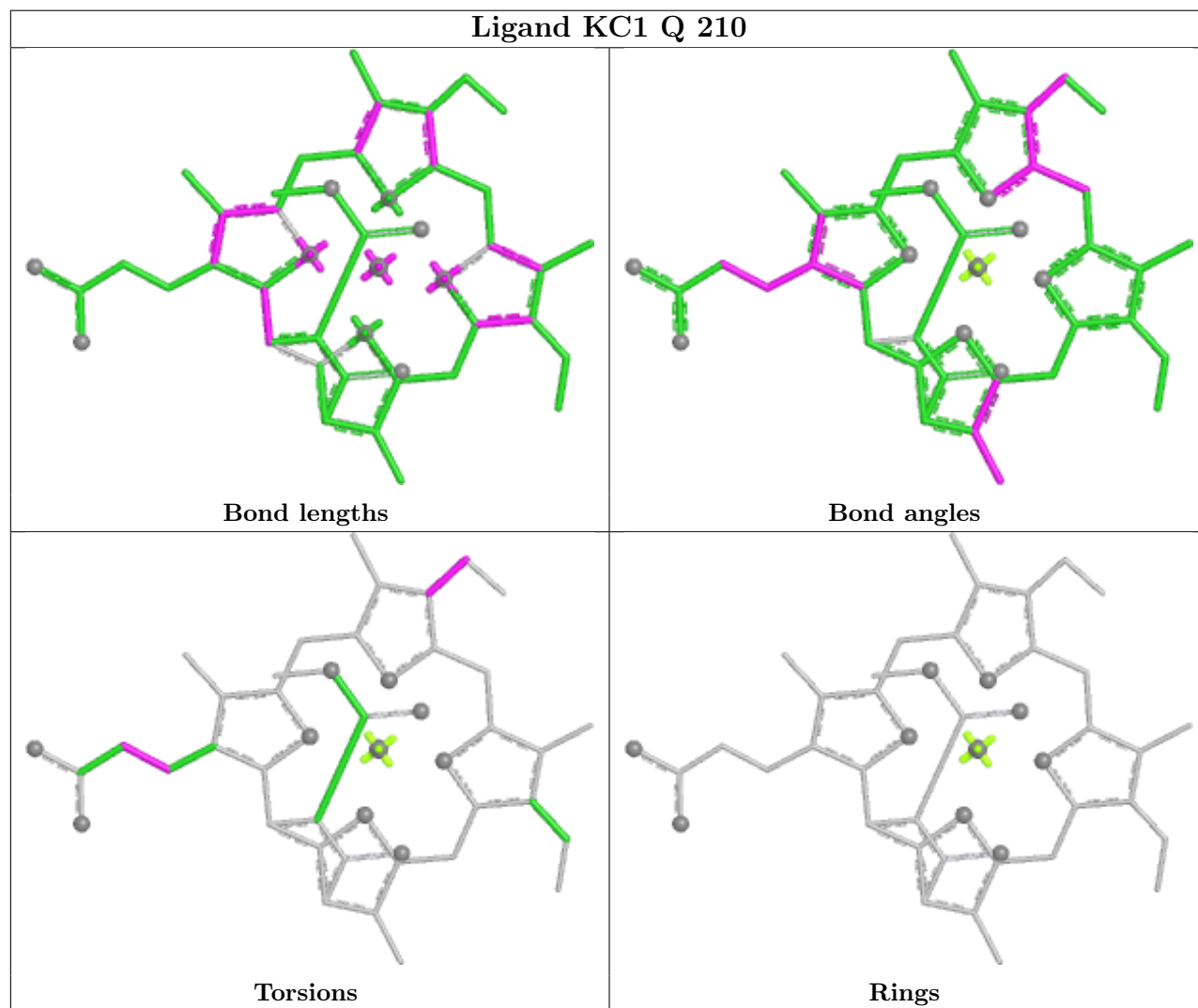




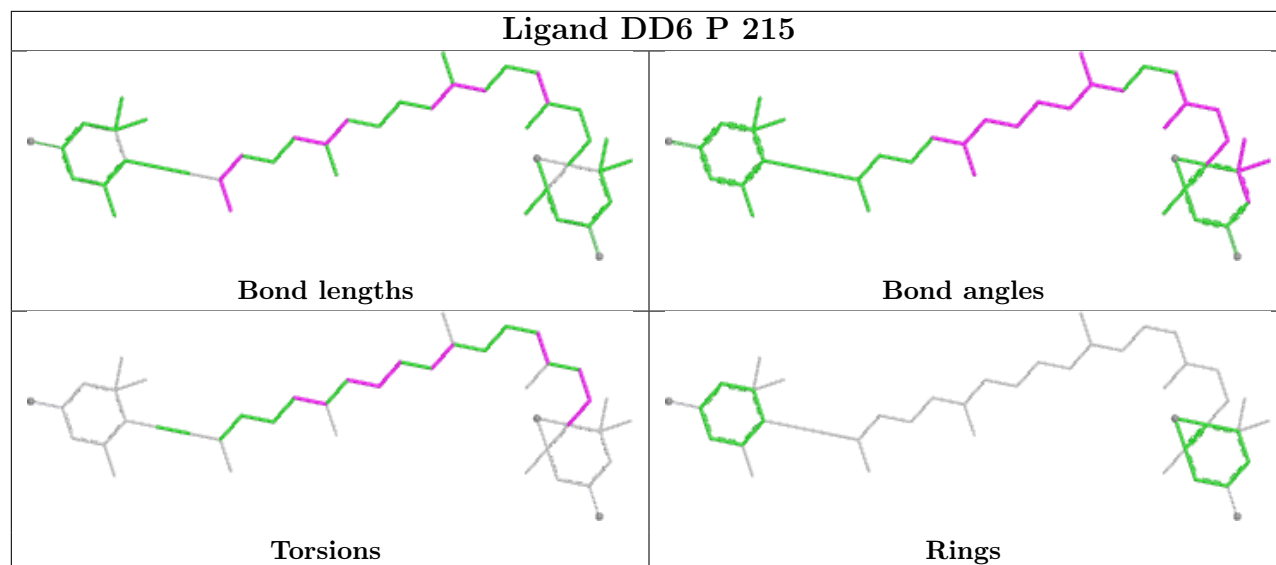
## Ligand DD6 G 213



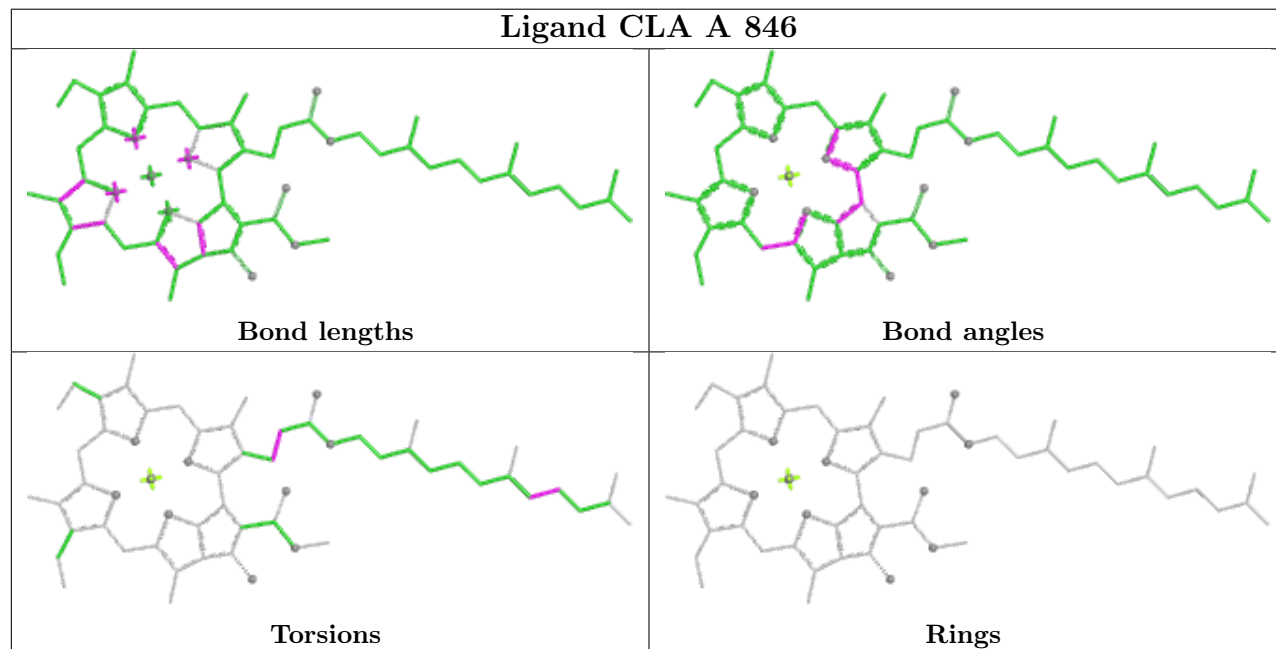
## Ligand KC1 Q 210



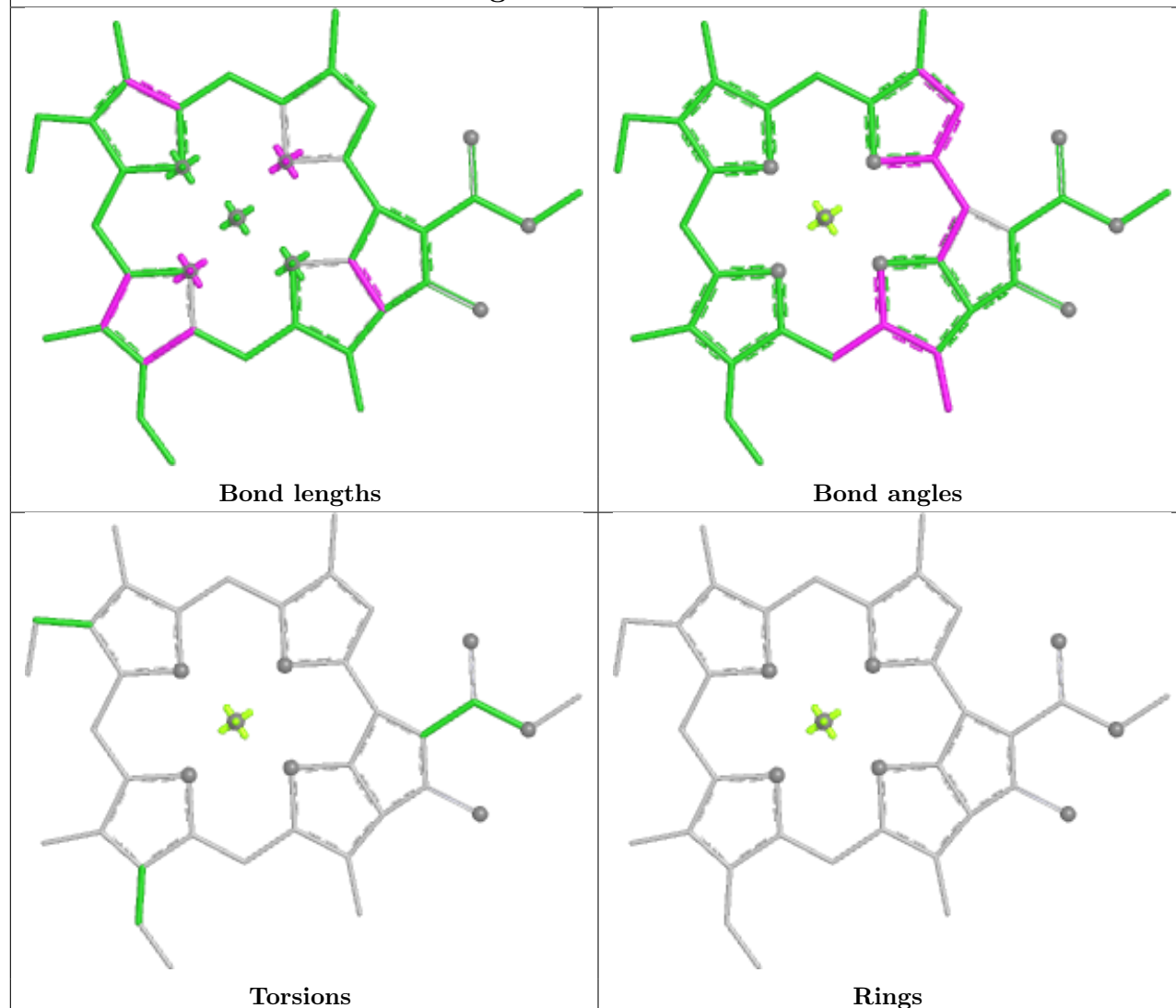
## Ligand DD6 P 215



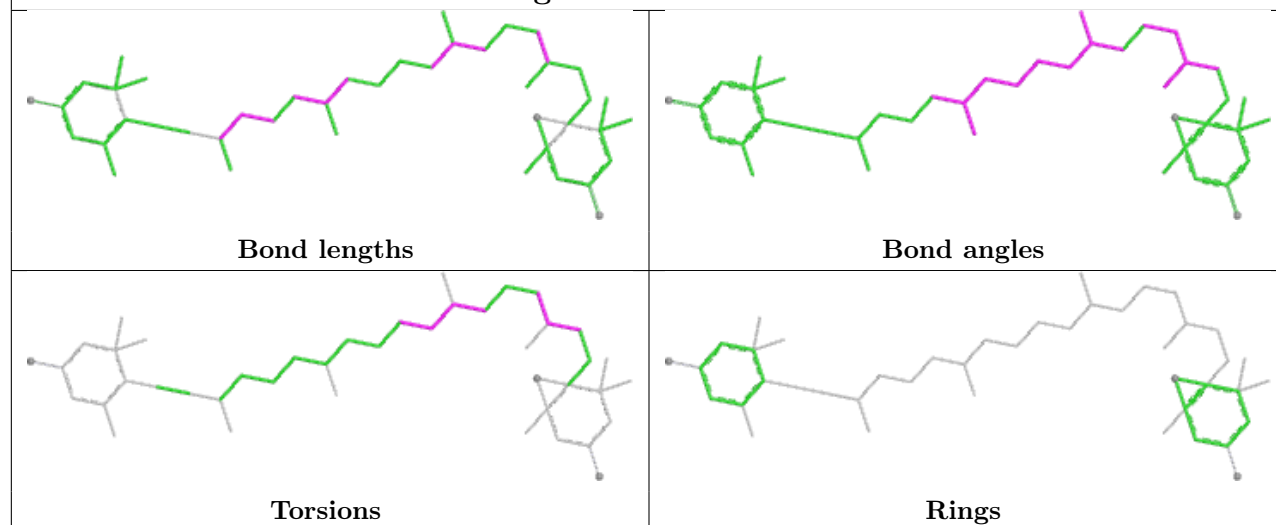
## Ligand CLA A 846



## Ligand CLA H 202

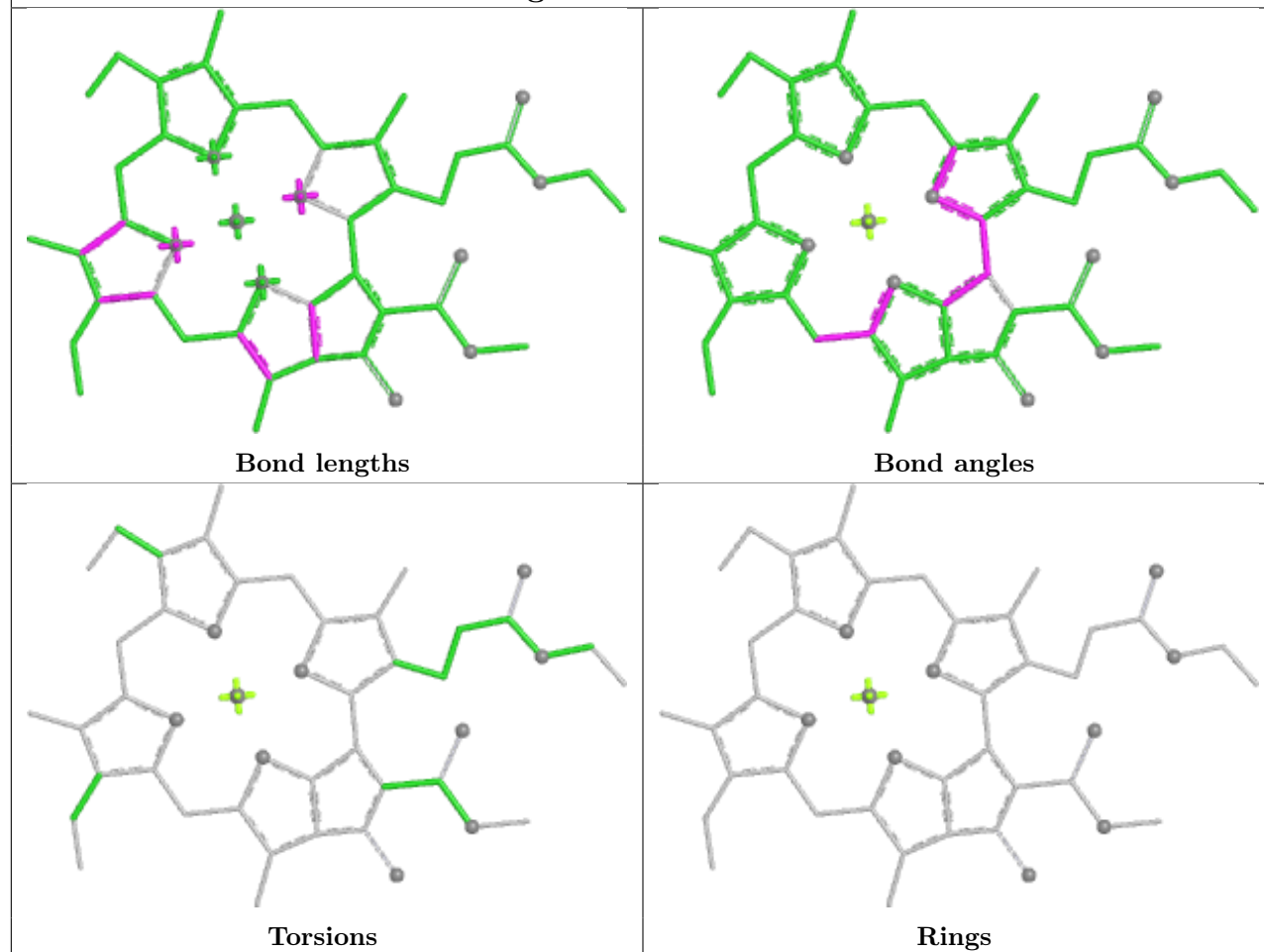


## Ligand DD6 T 212

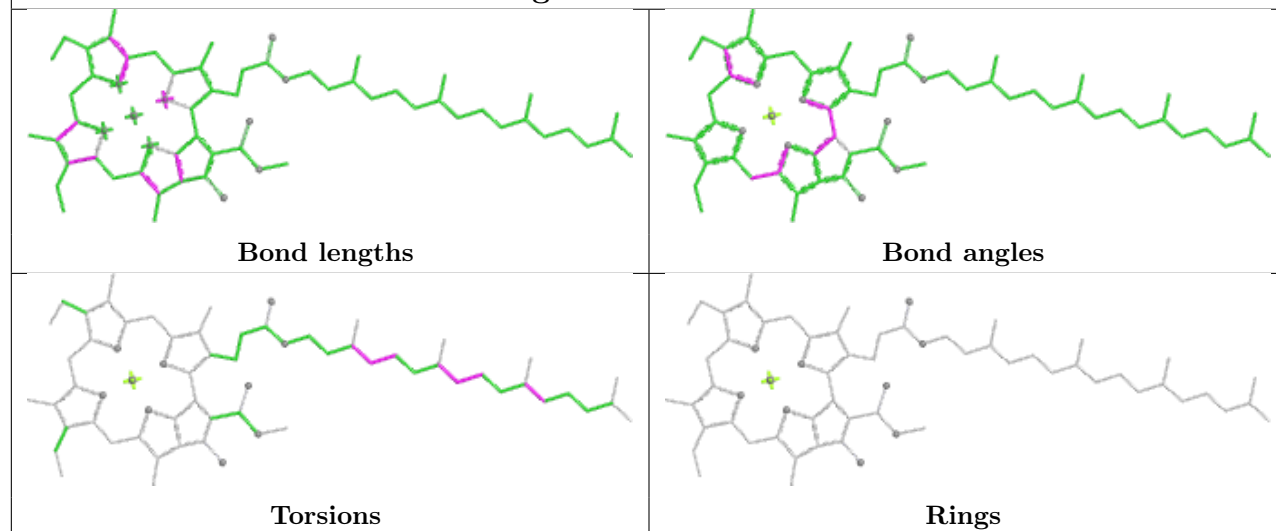


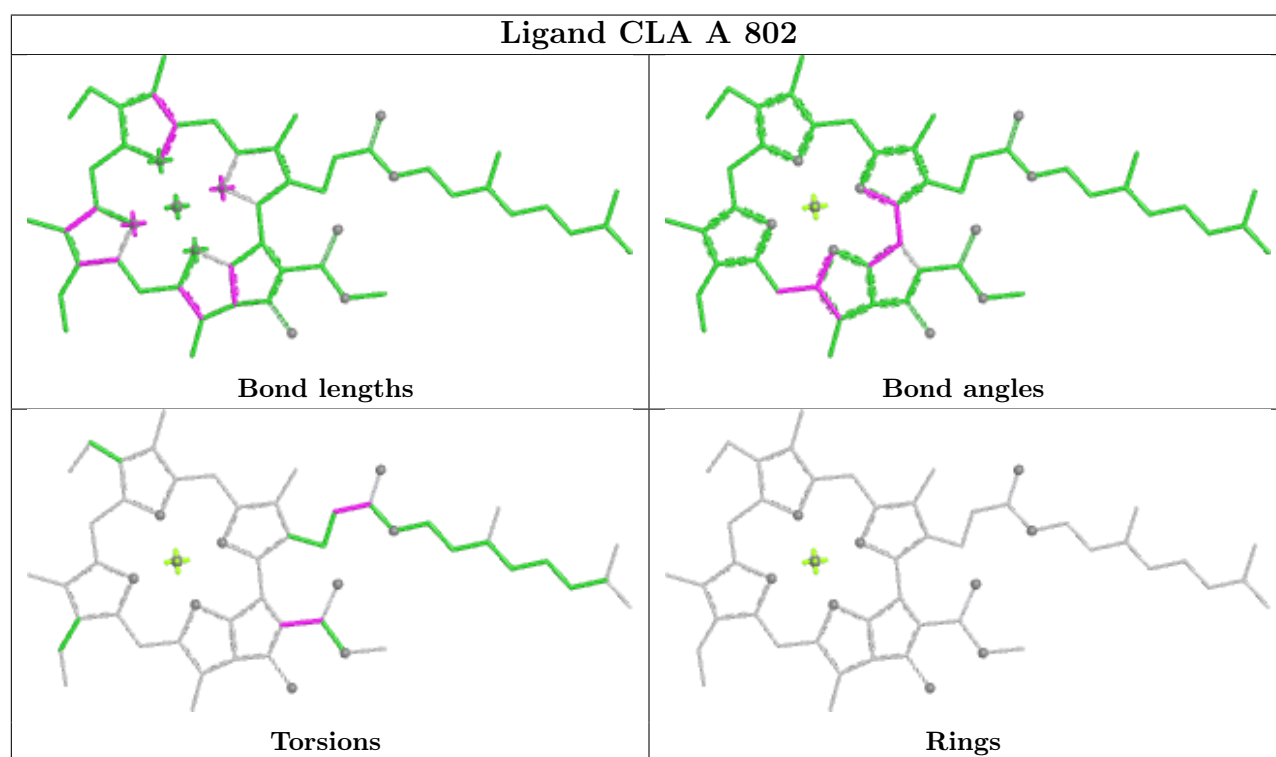
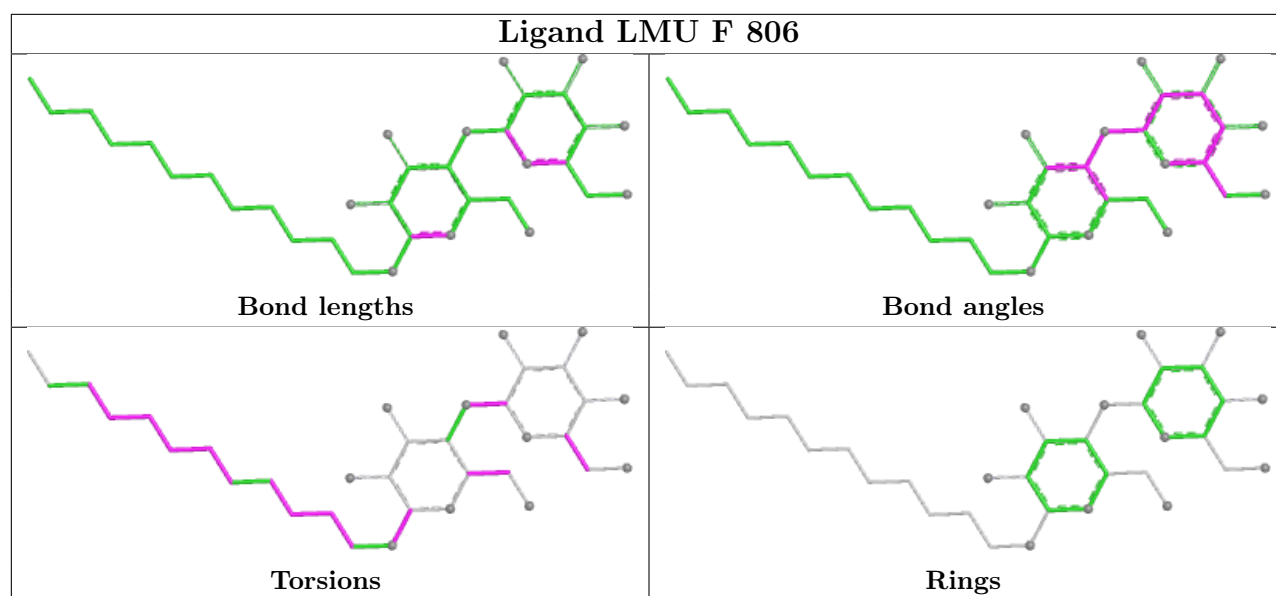


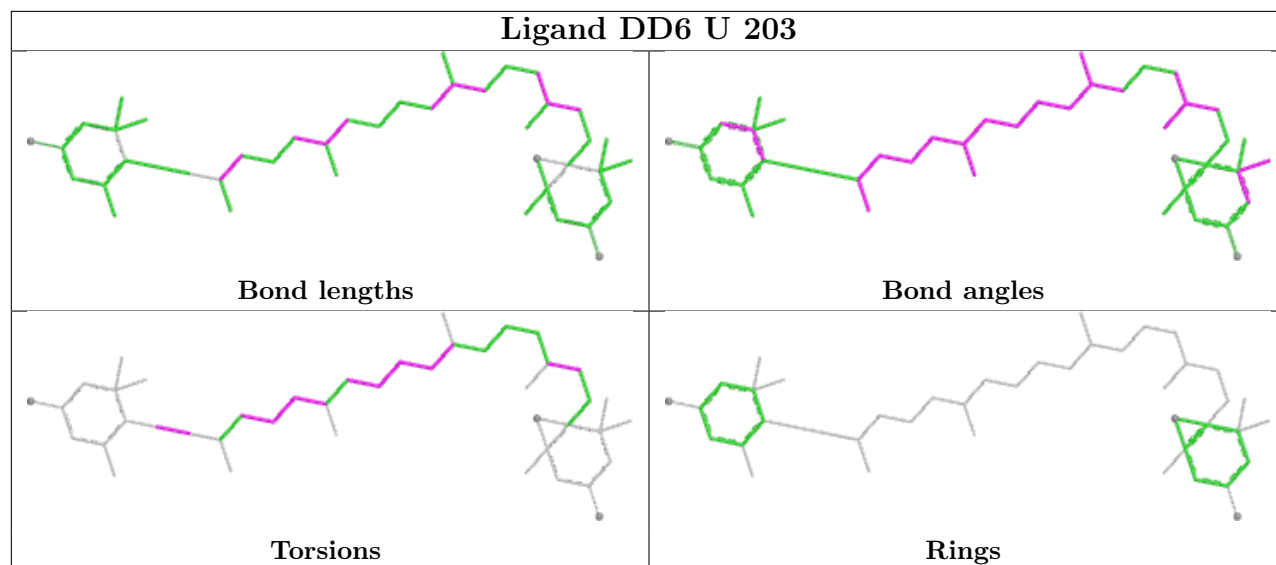
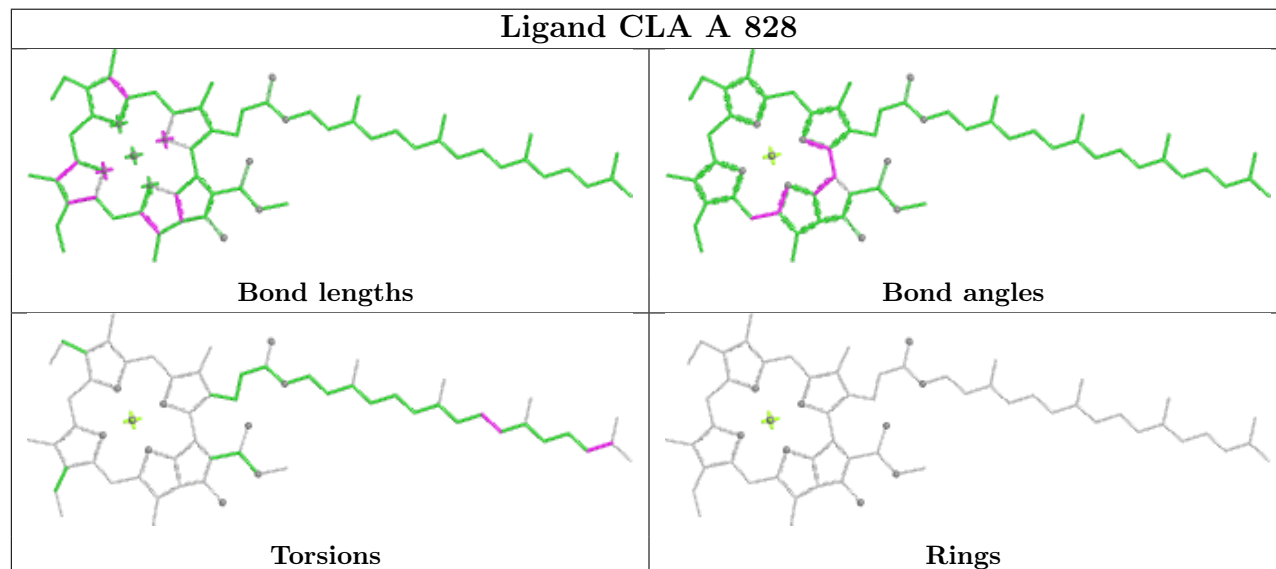
## Ligand CLA B 831



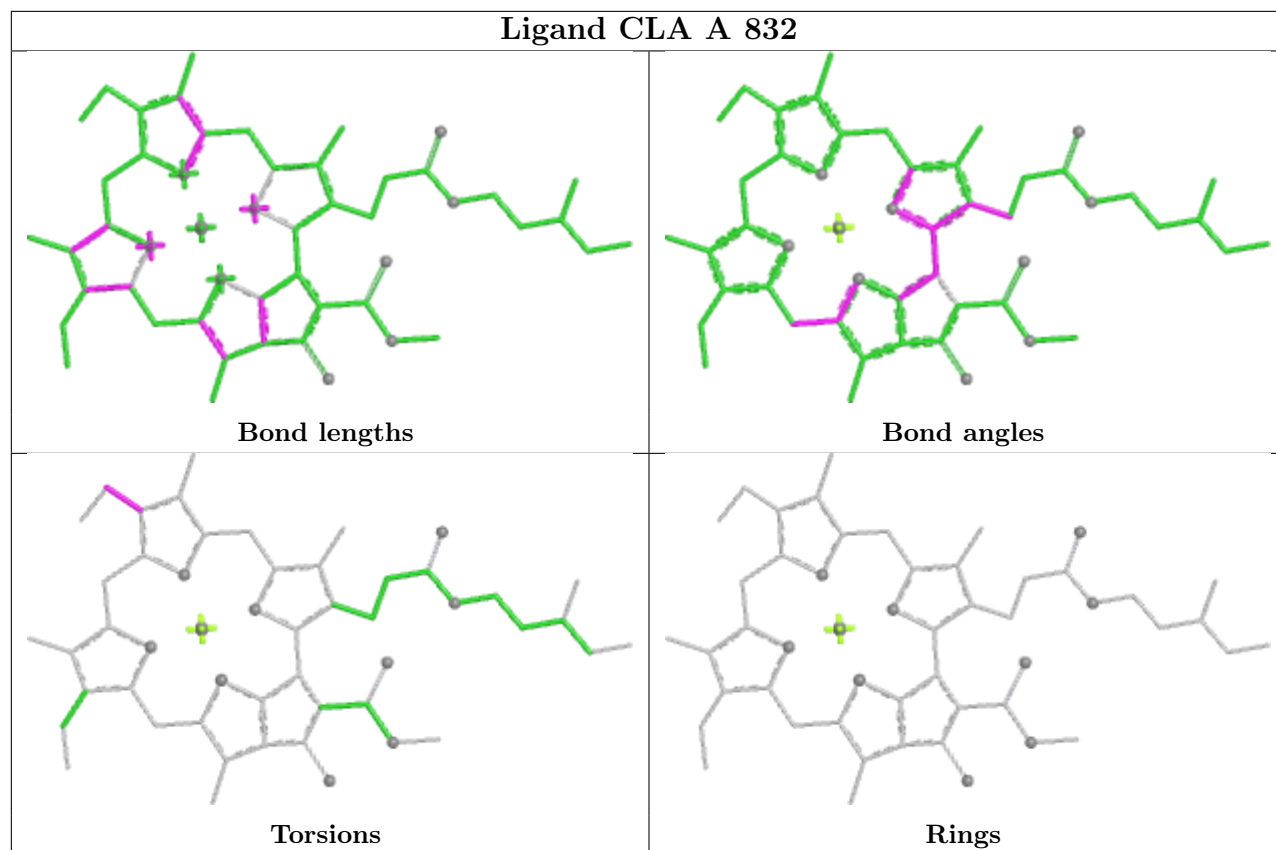
## Ligand CLA B 816



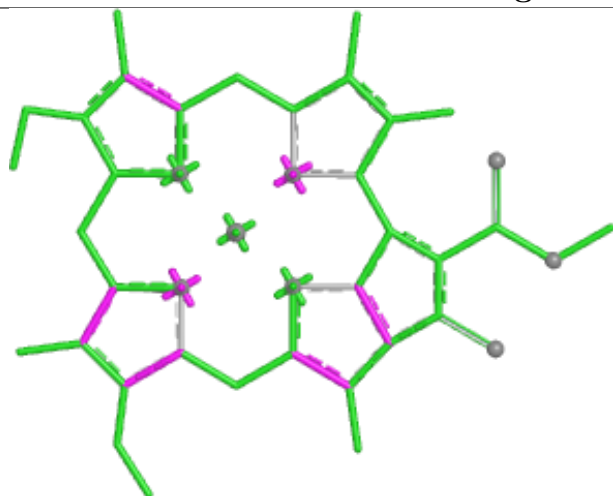


**Ligand DD6 U 203****Ligand CLA A 828**

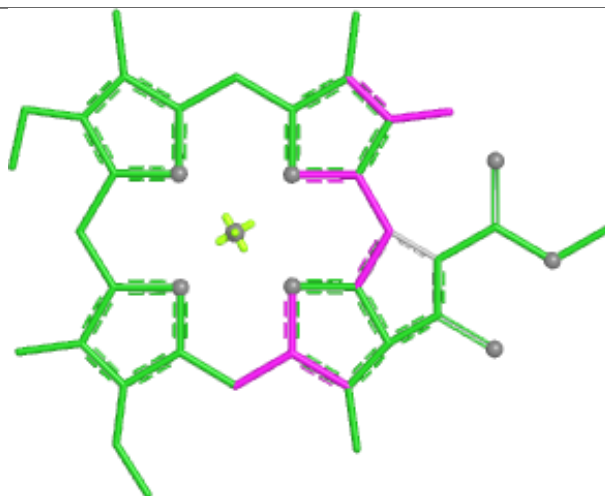
## Ligand CLA A 832



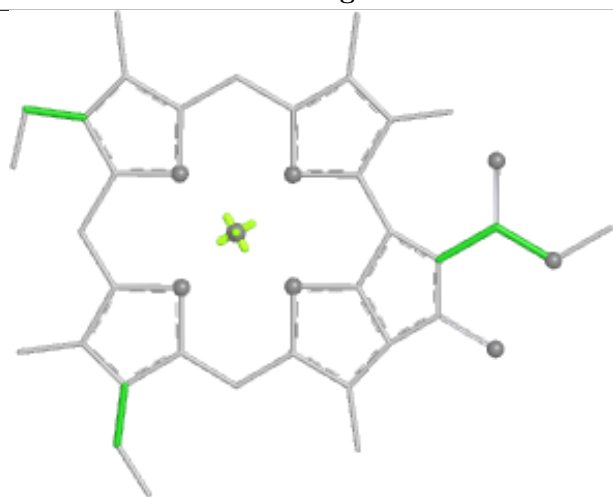
## Ligand CLA T 209



Bond lengths



Bond angles

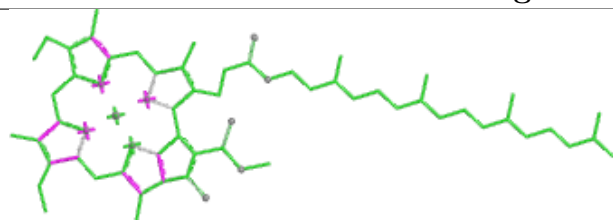


Torsions

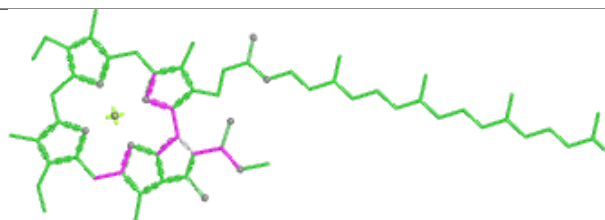


Rings

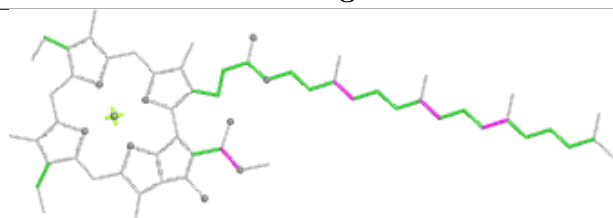
## Ligand CLA R 104



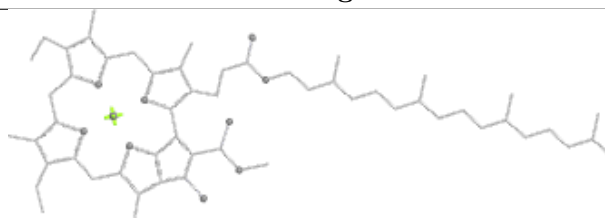
Bond lengths



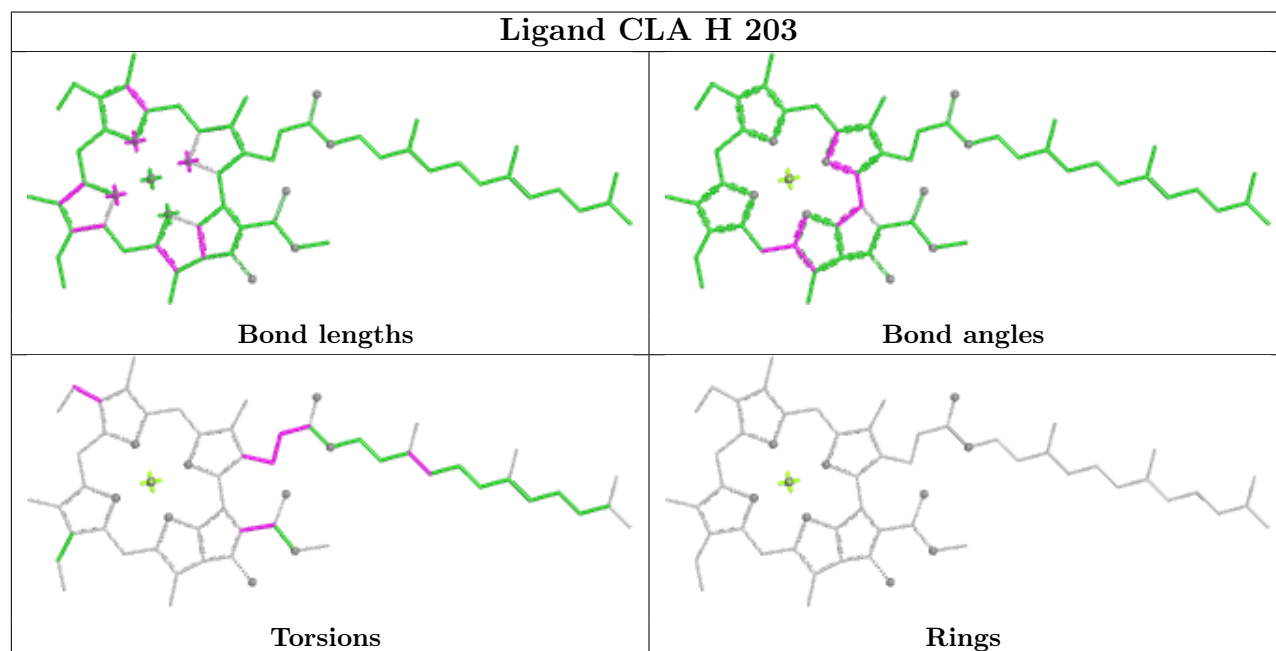
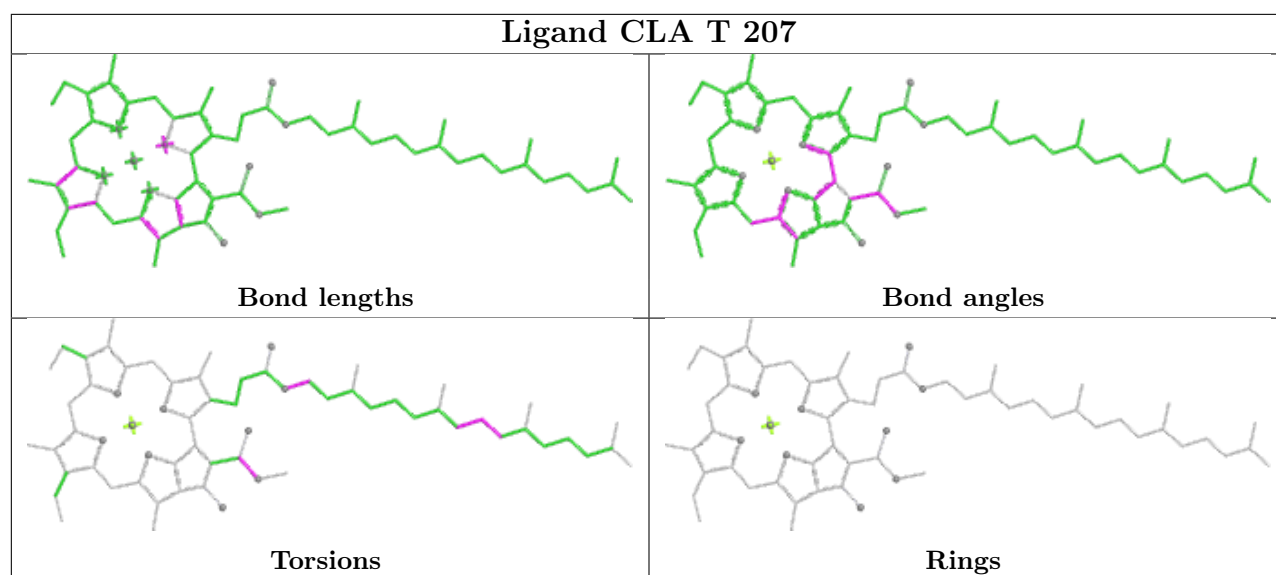
Bond angles



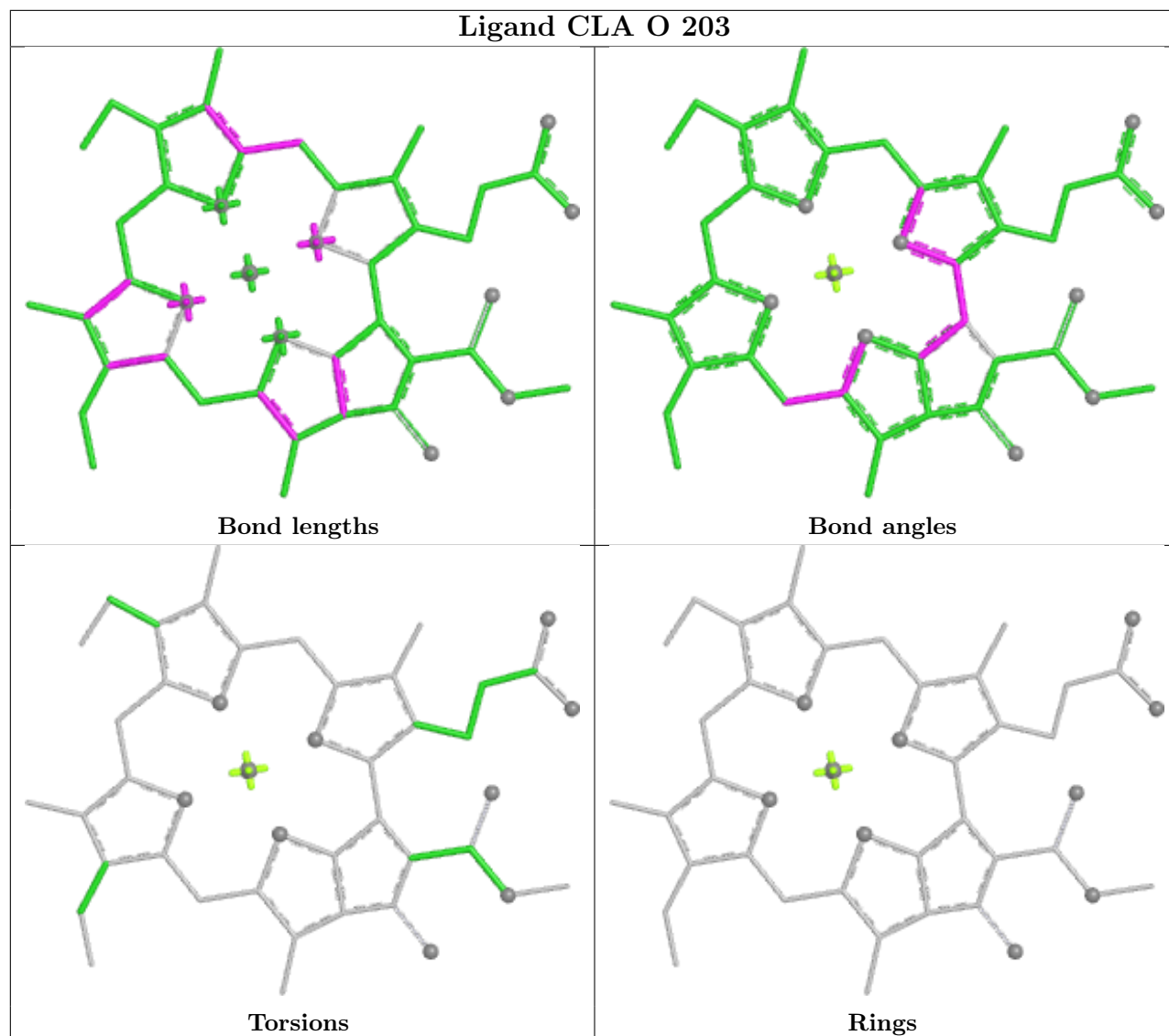
Torsions



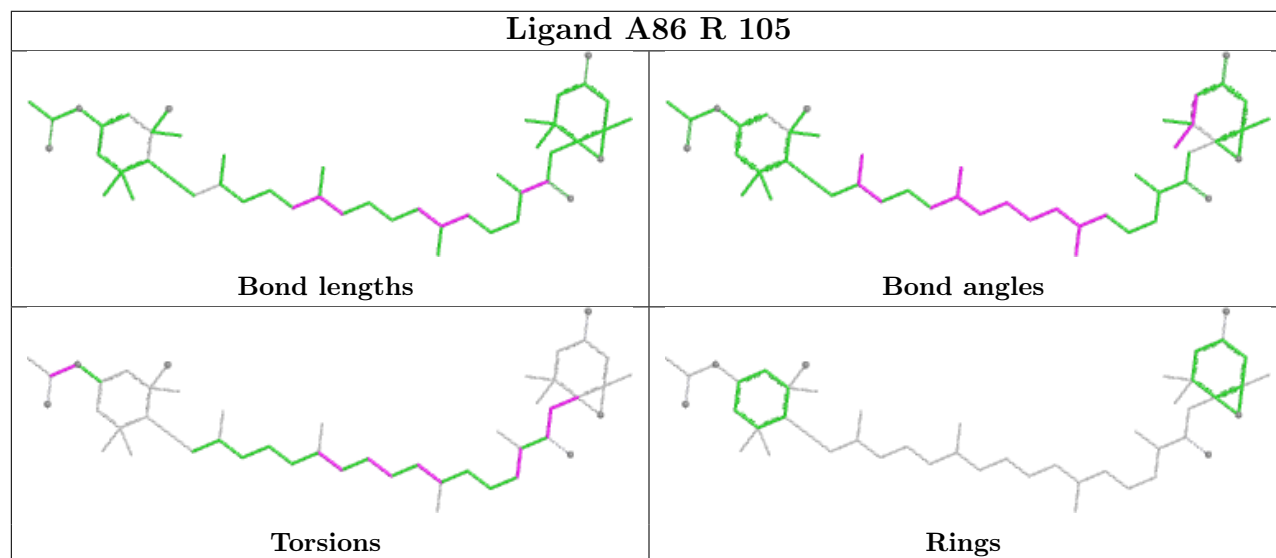
Rings



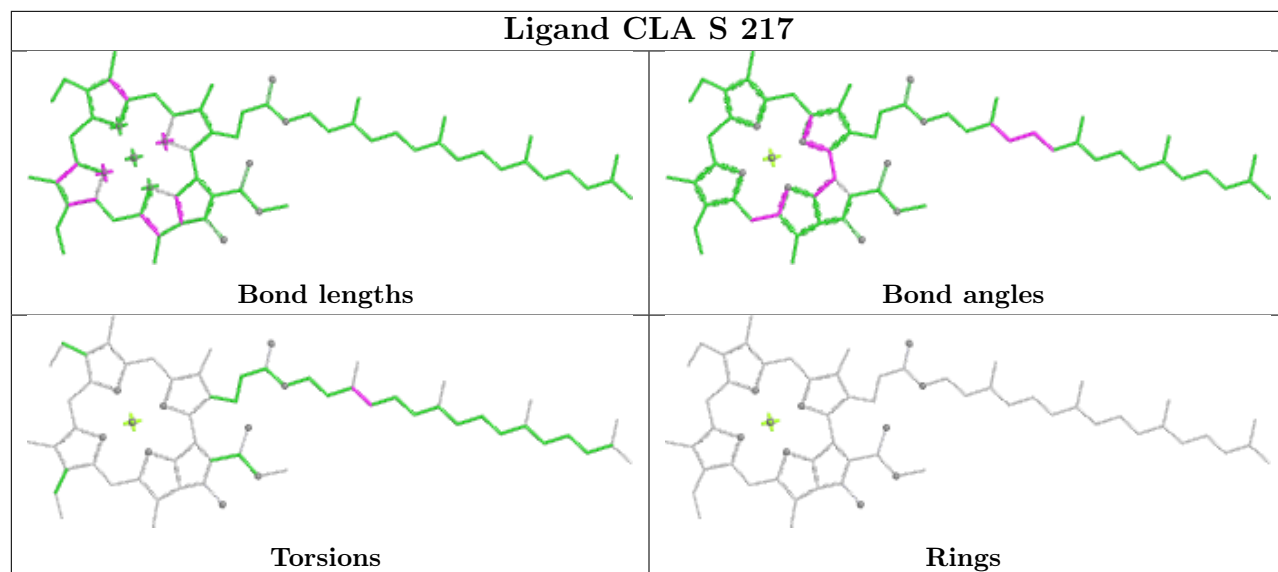
## Ligand CLA O 203



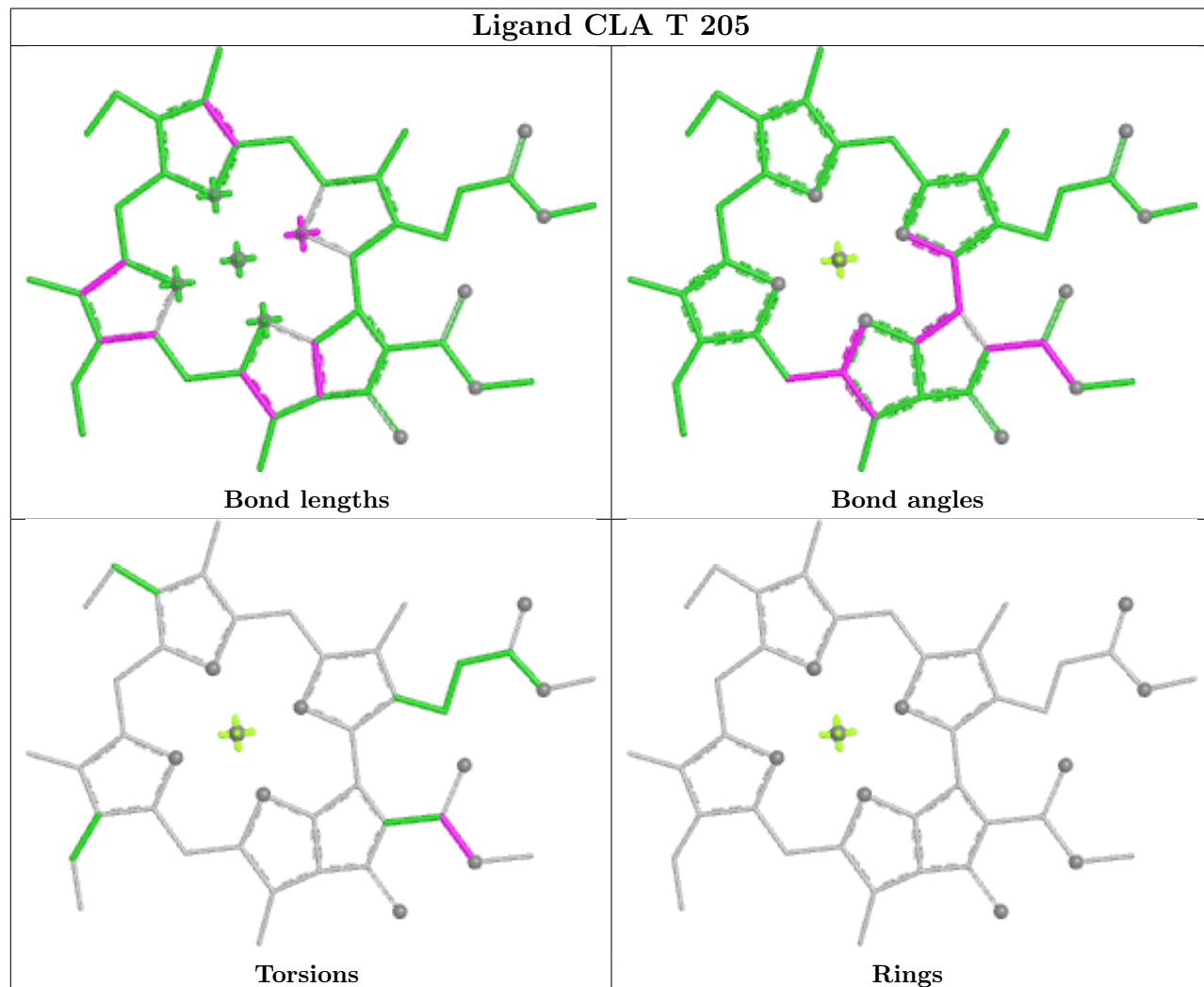
## Ligand A86 R 105



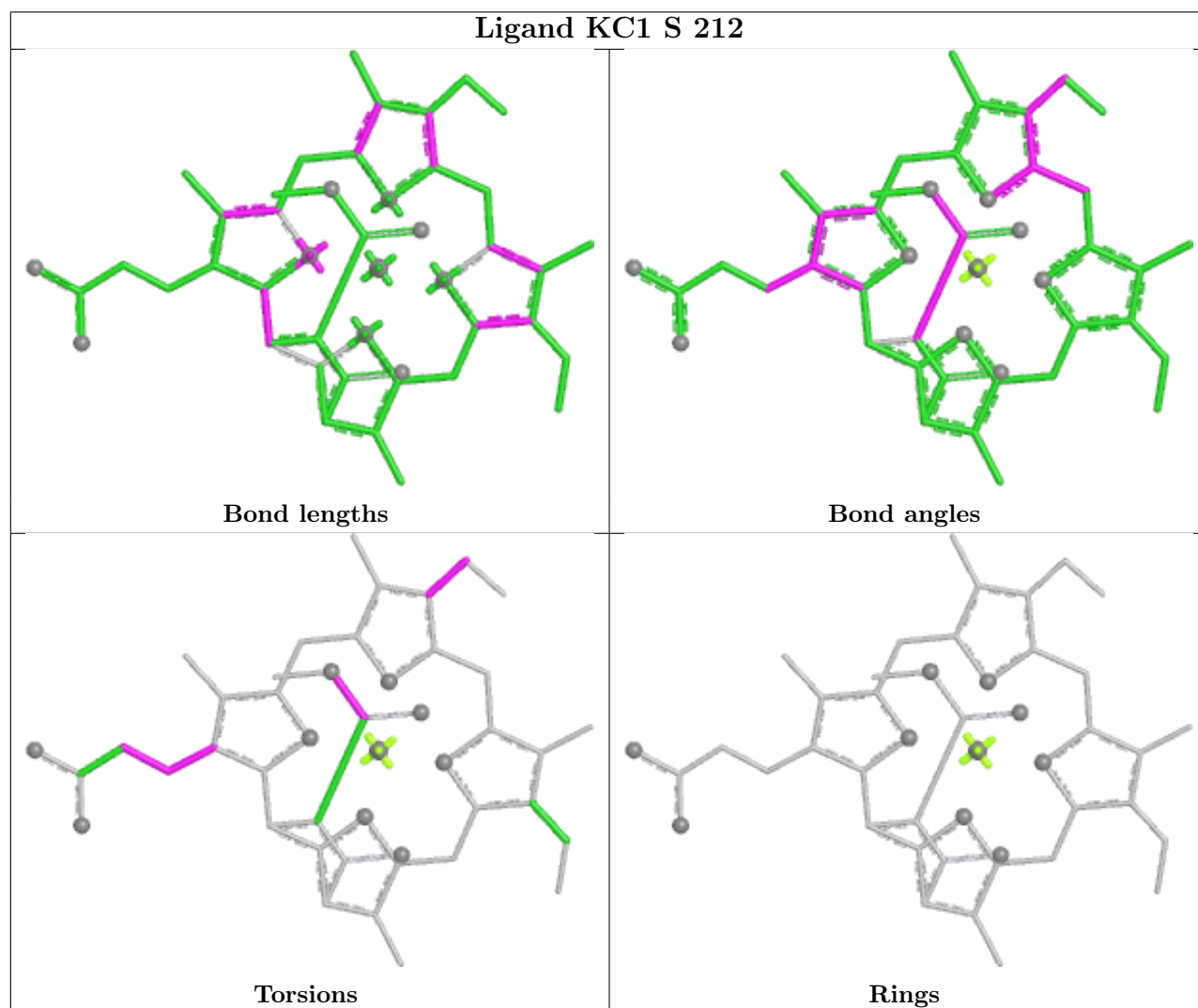
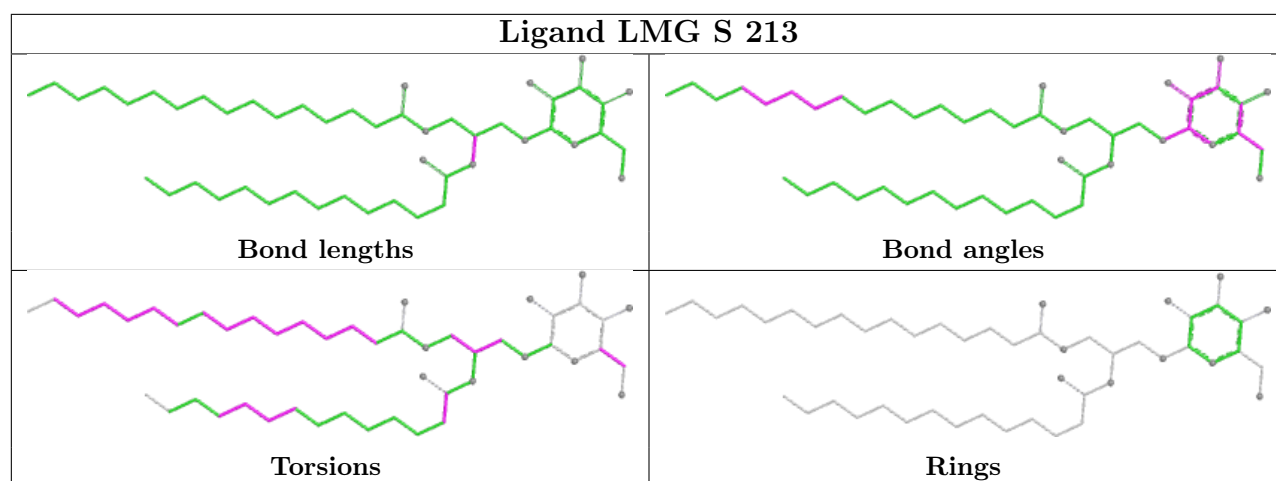
## Ligand CLA S 217

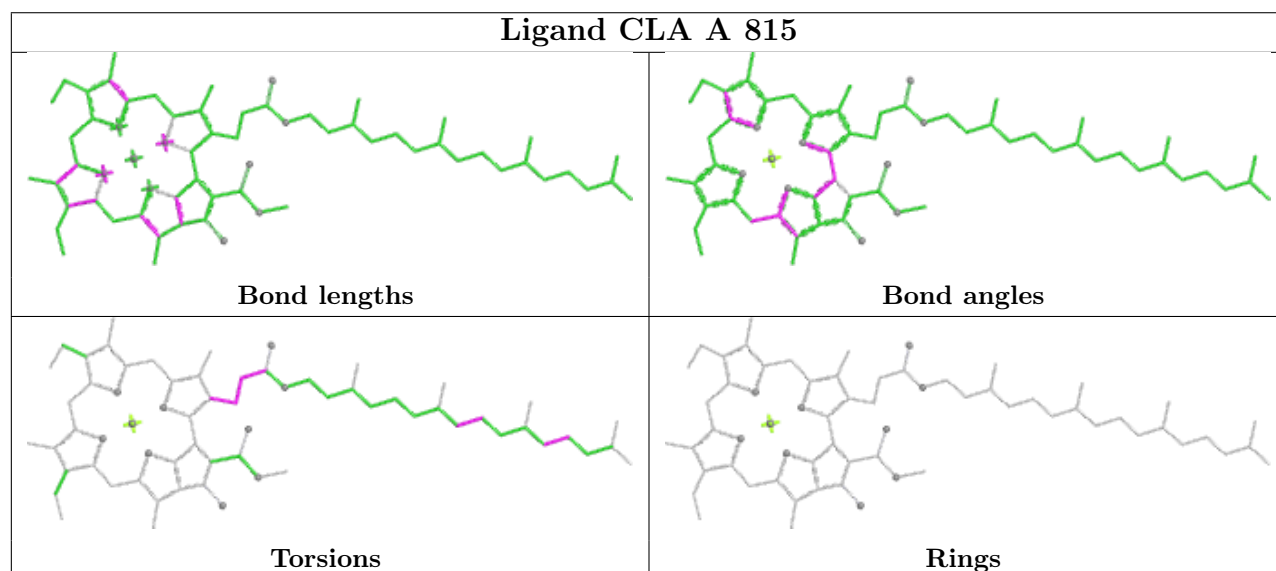
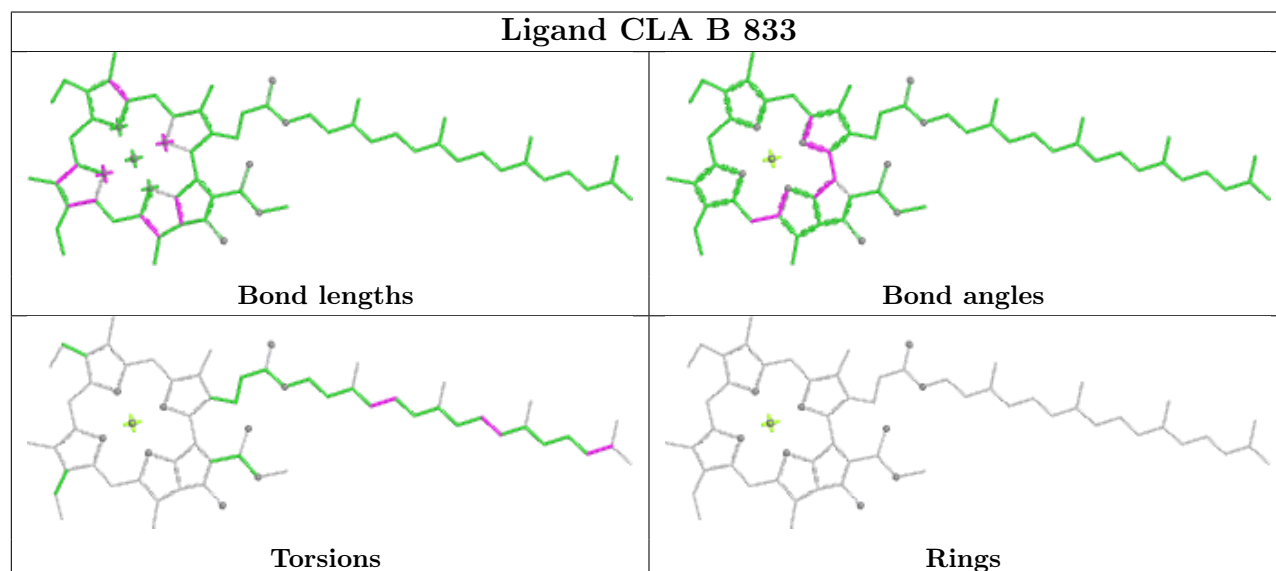
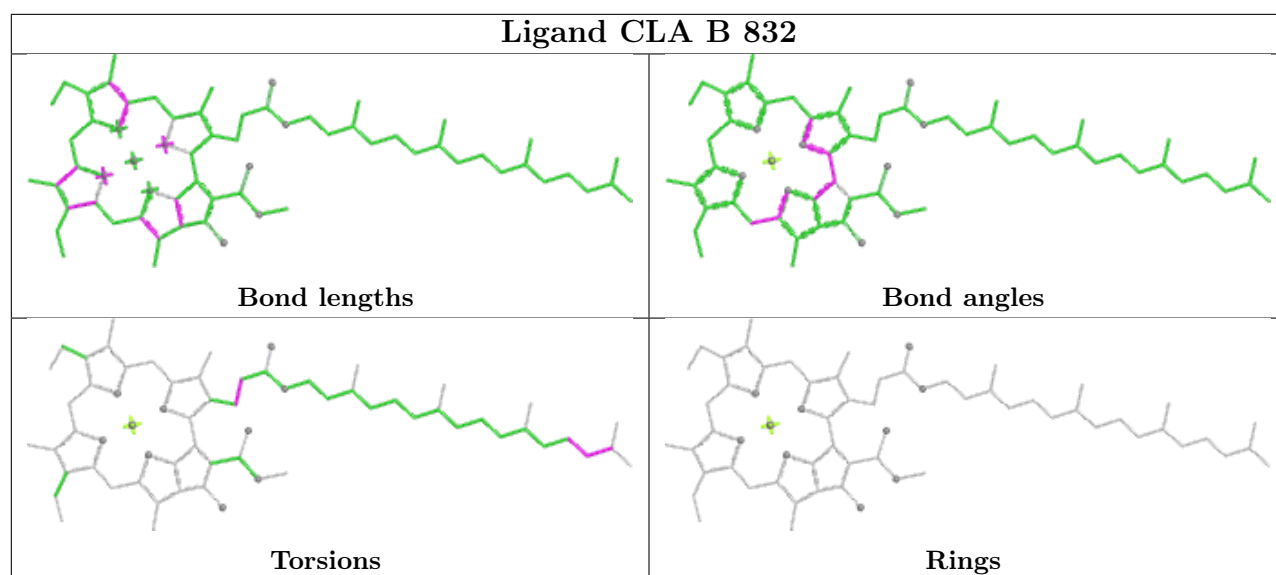


## Ligand CLA T 205

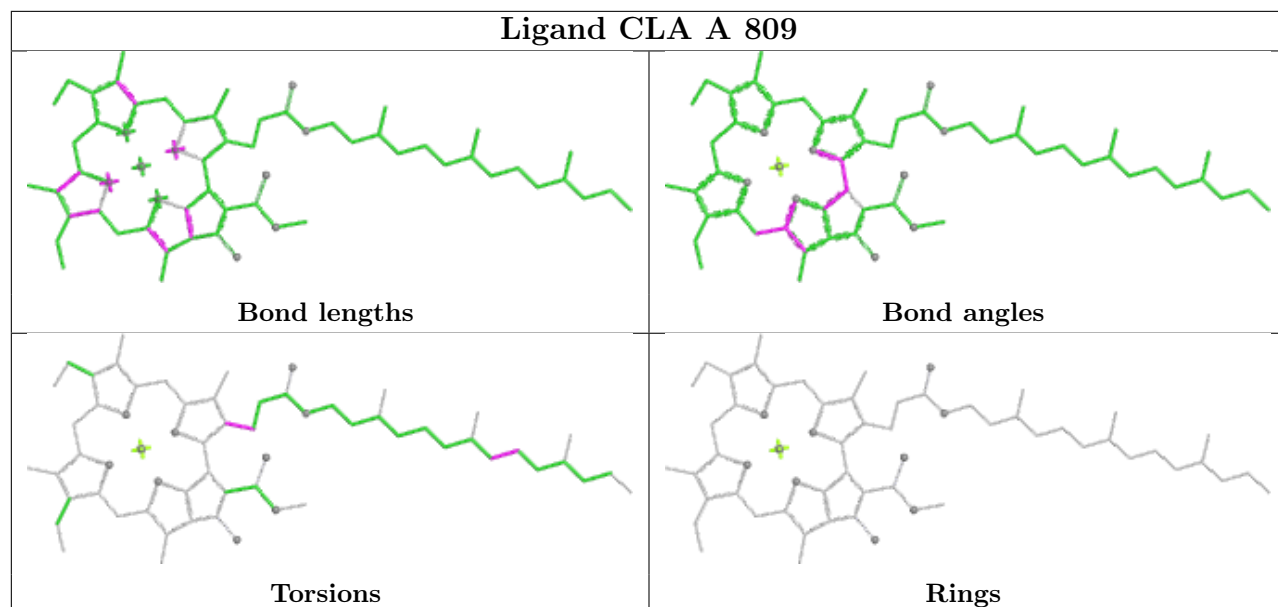




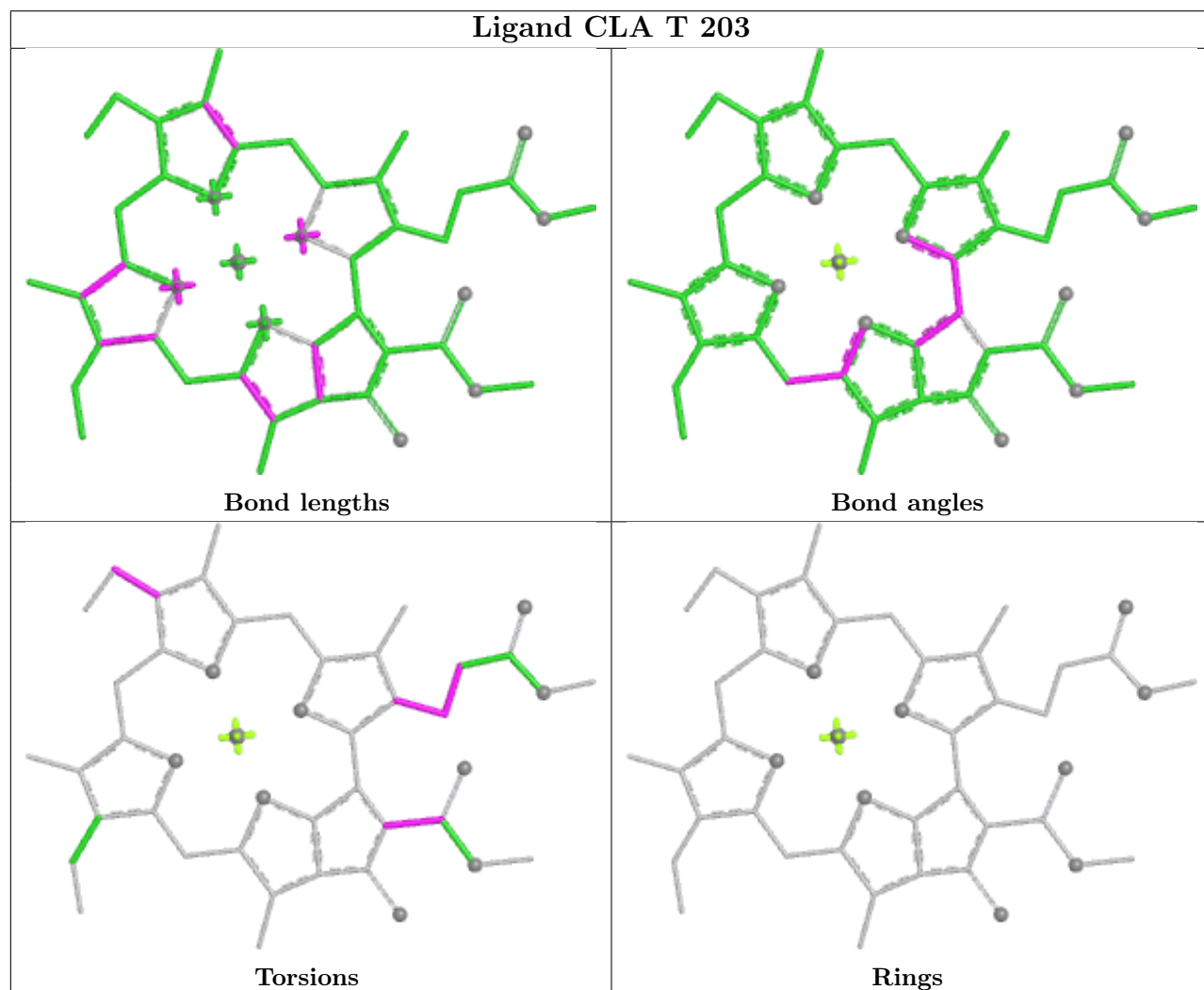


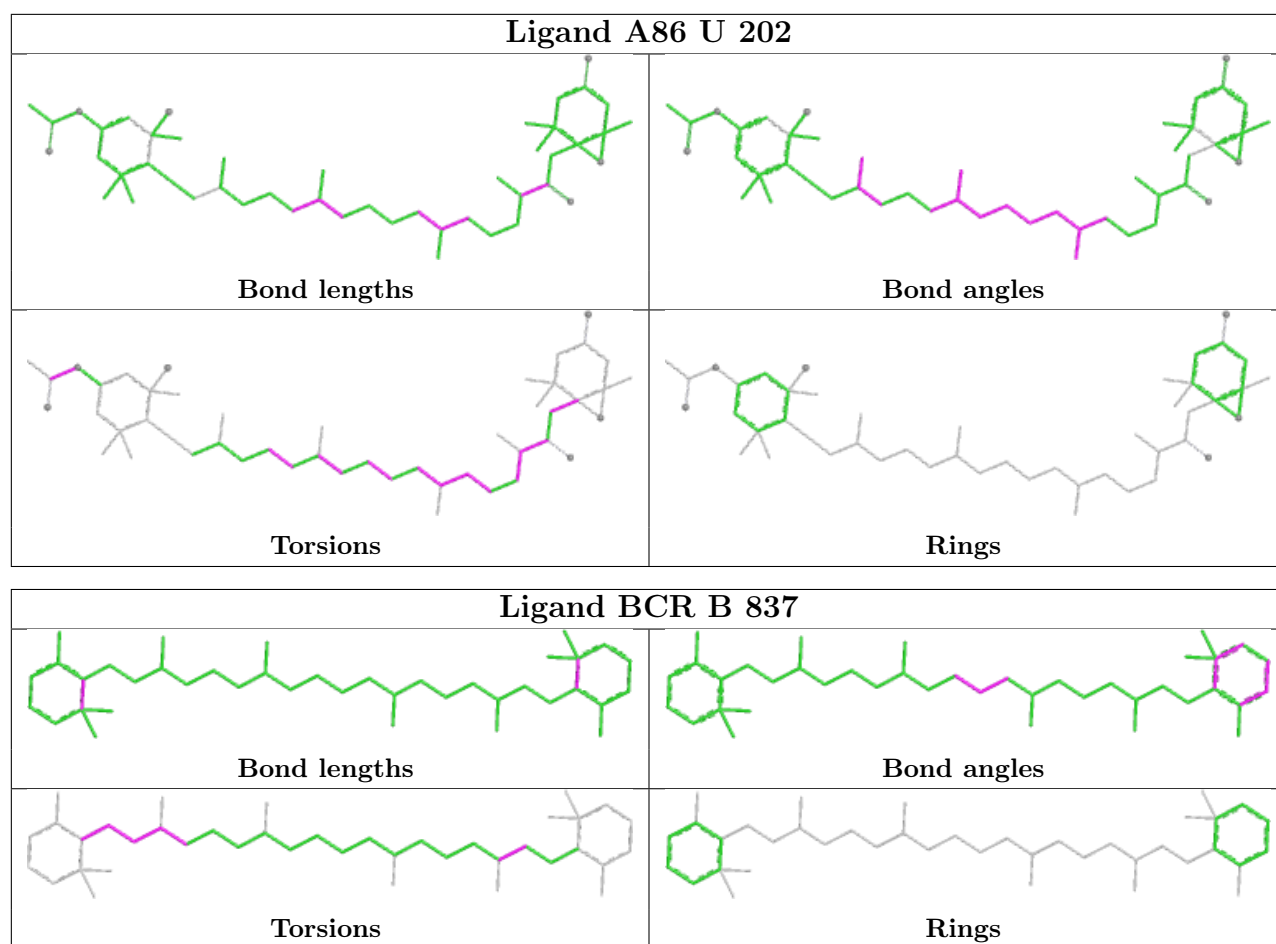


## Ligand CLA A 809

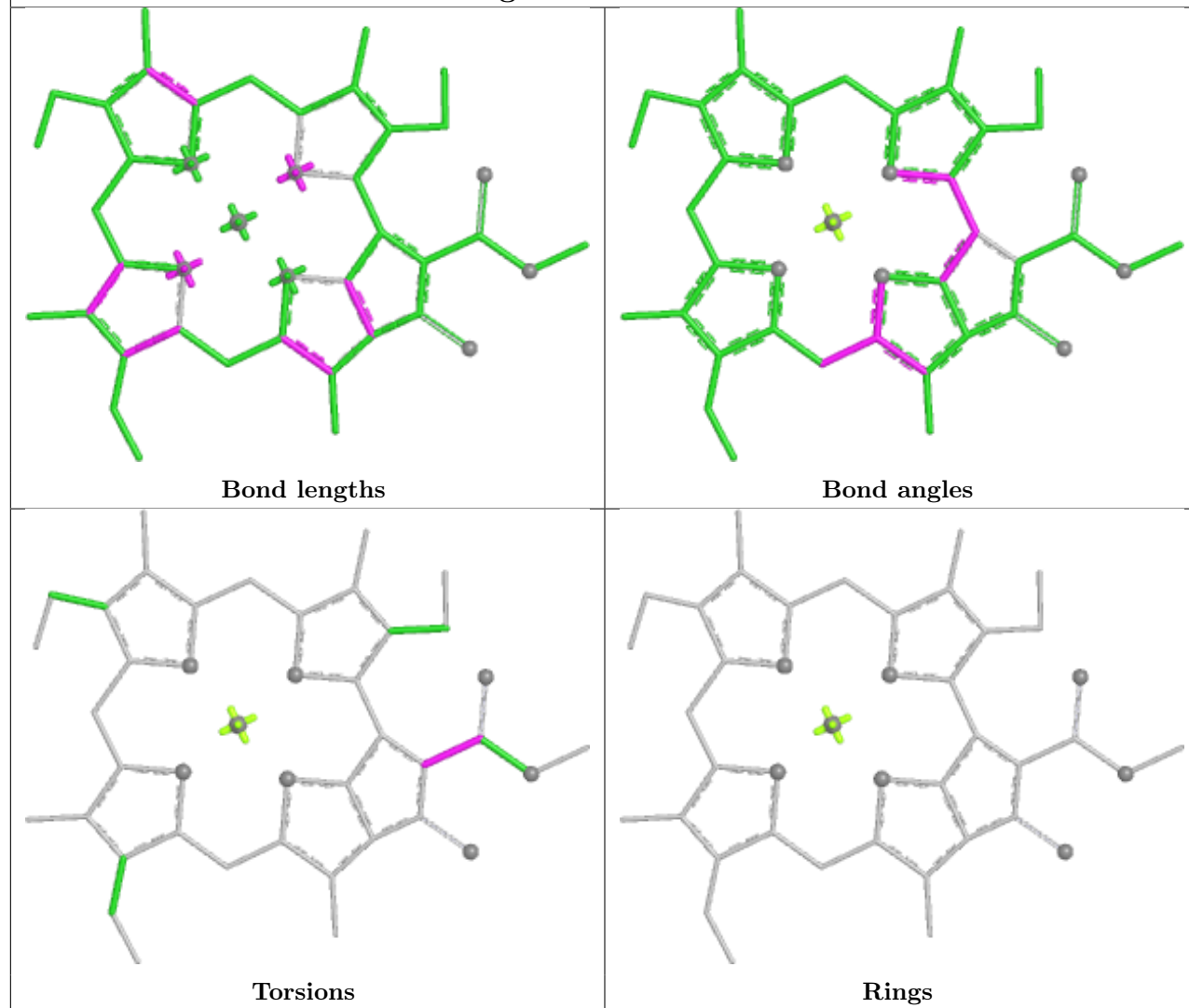


## Ligand CLA T 203

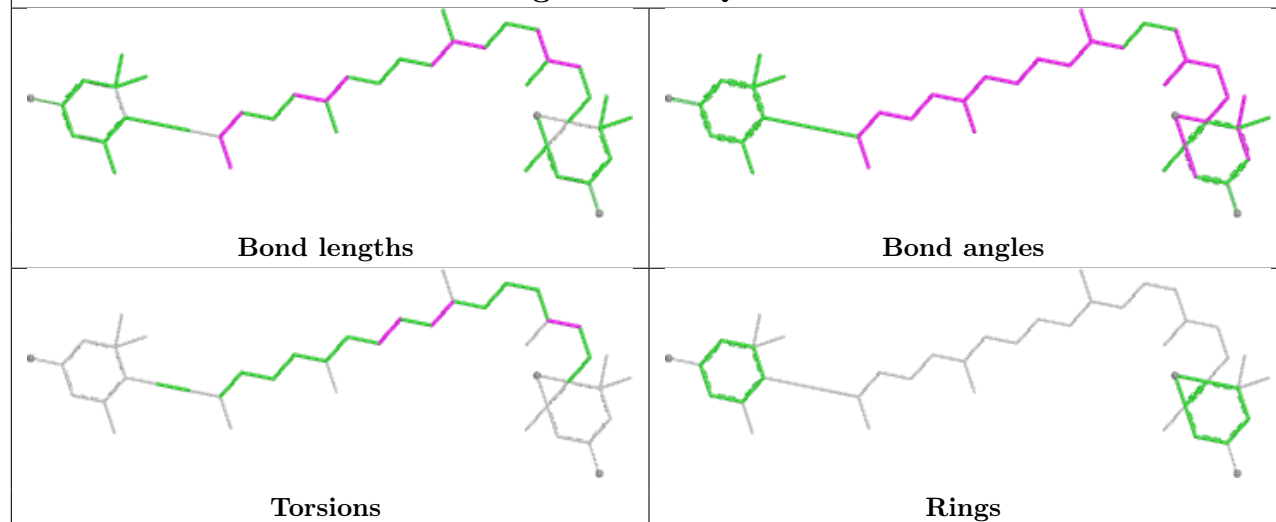


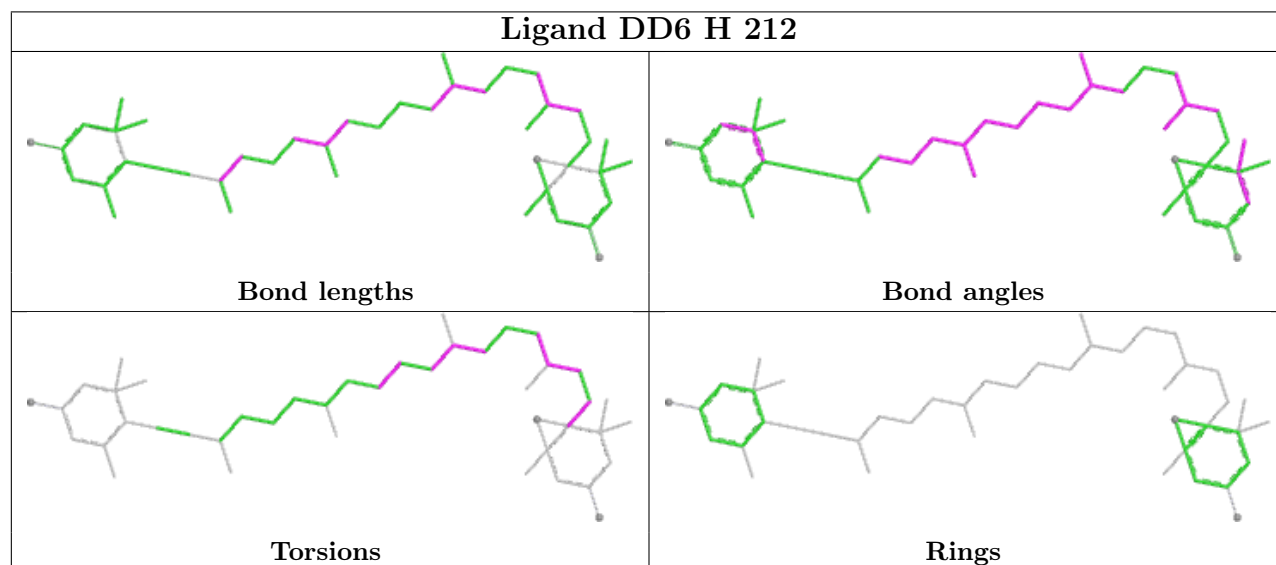
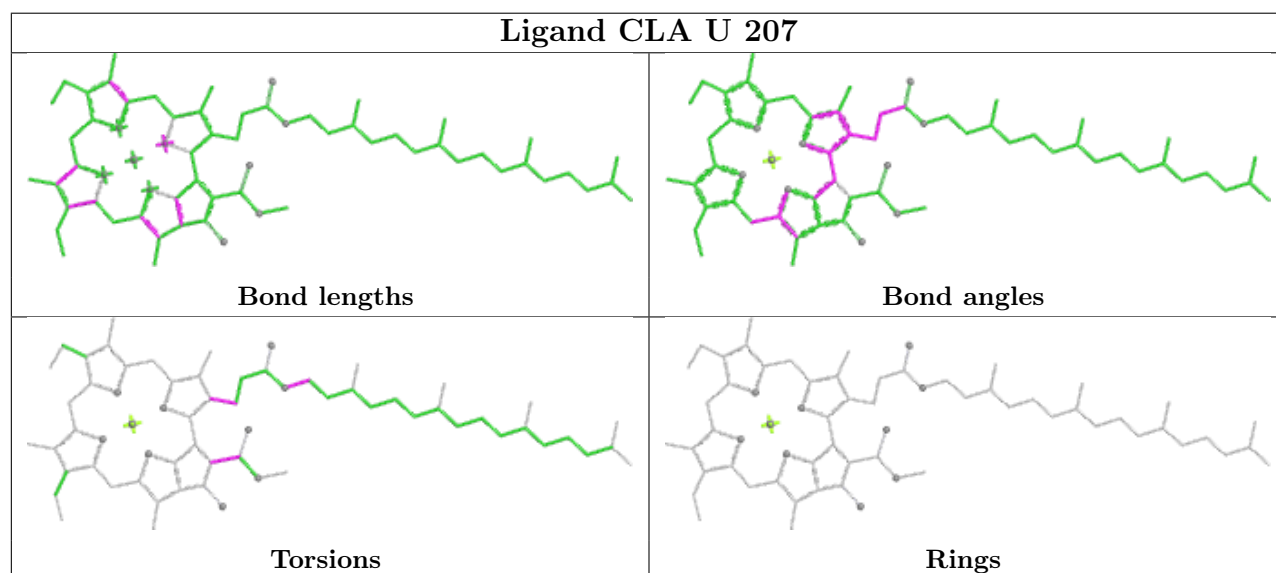
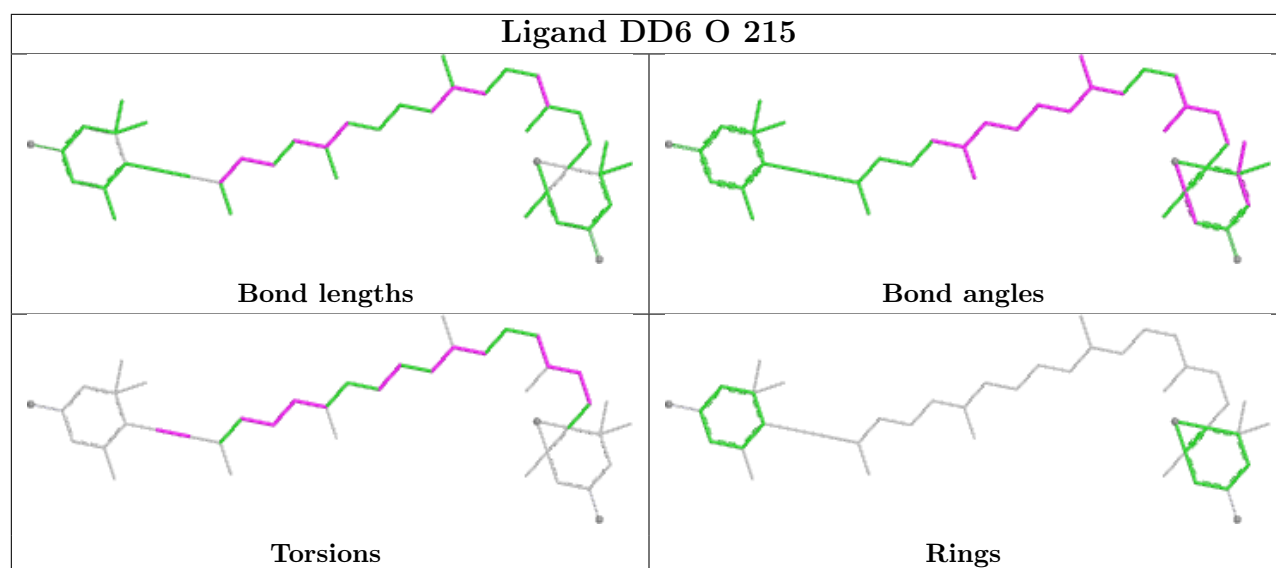


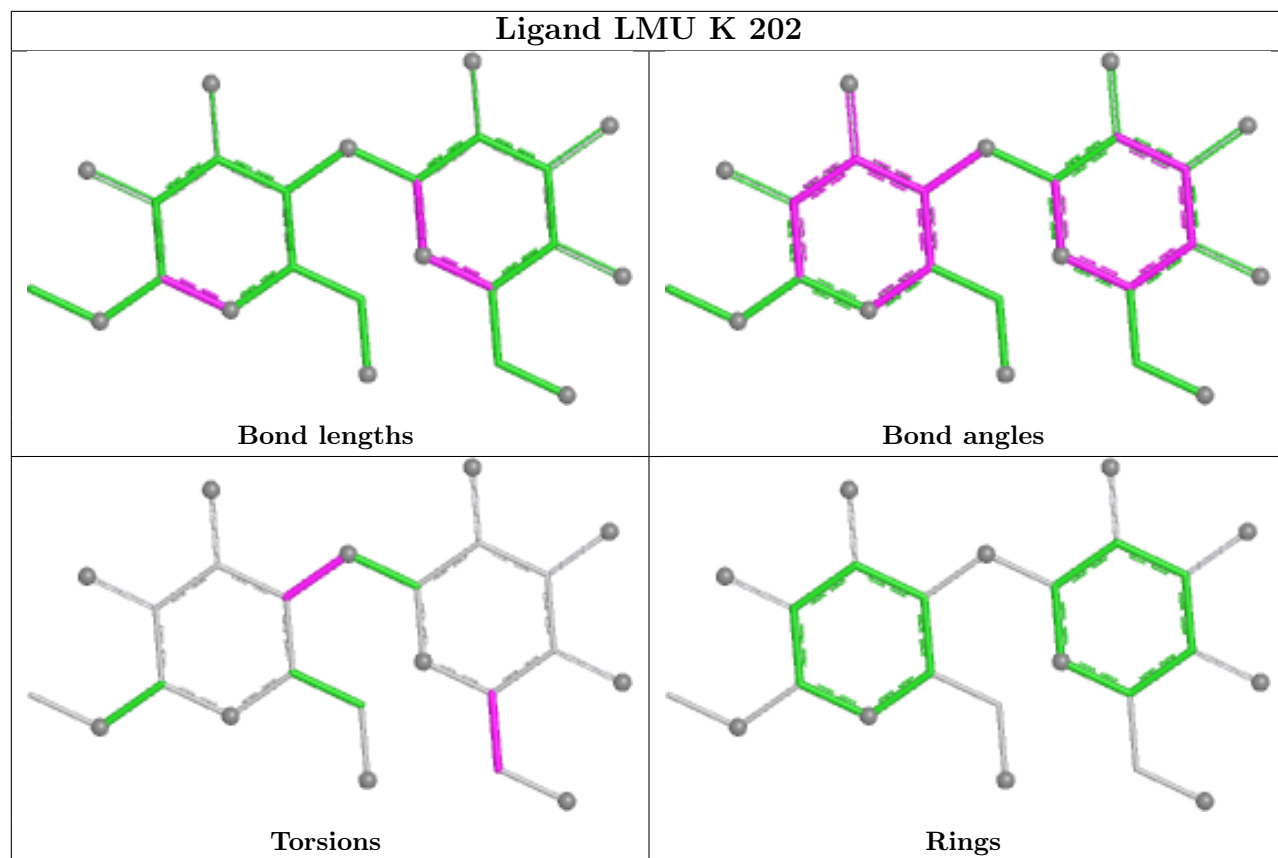
## Ligand CLA J 103

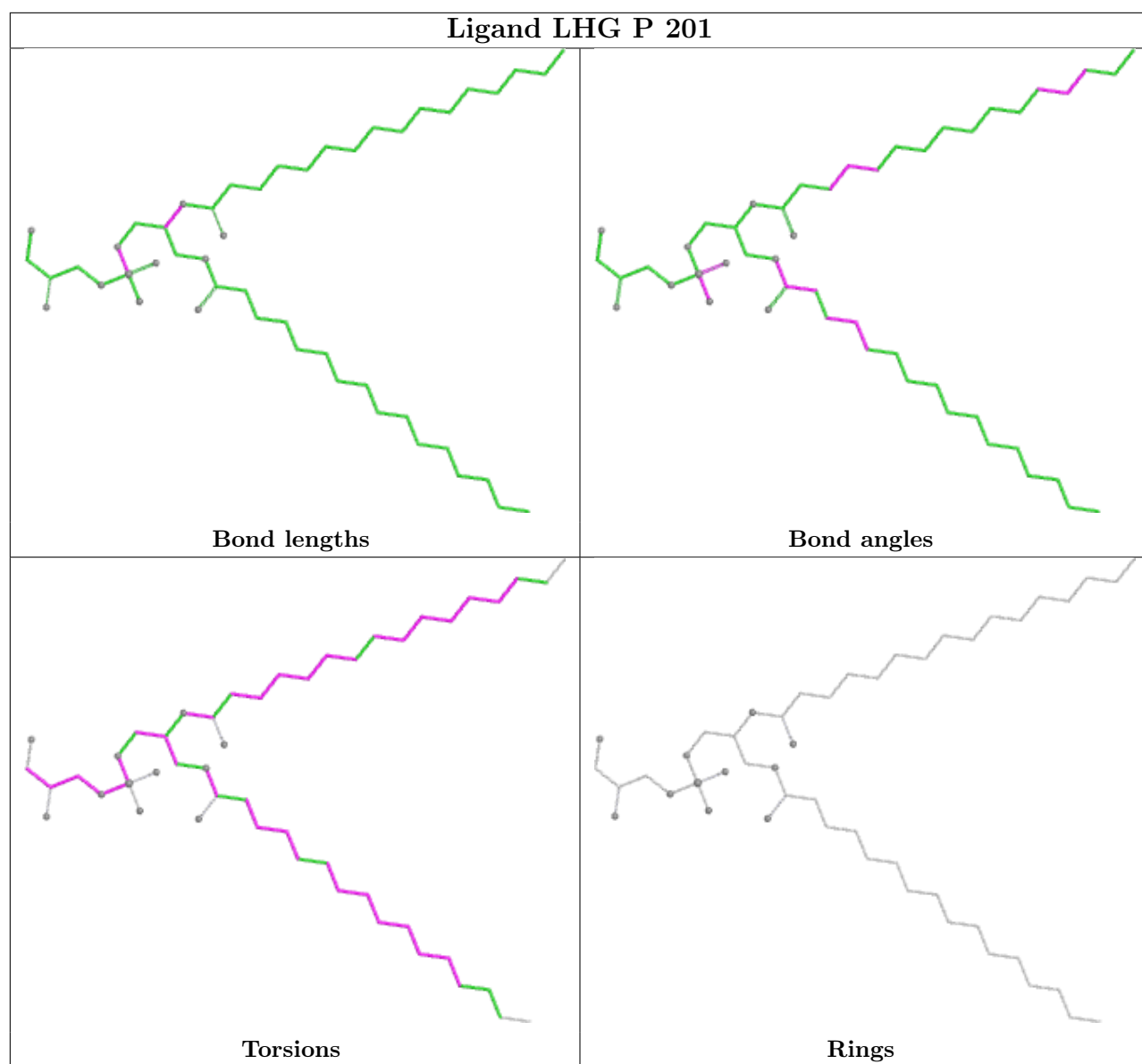


## Ligand DD6 Q 202

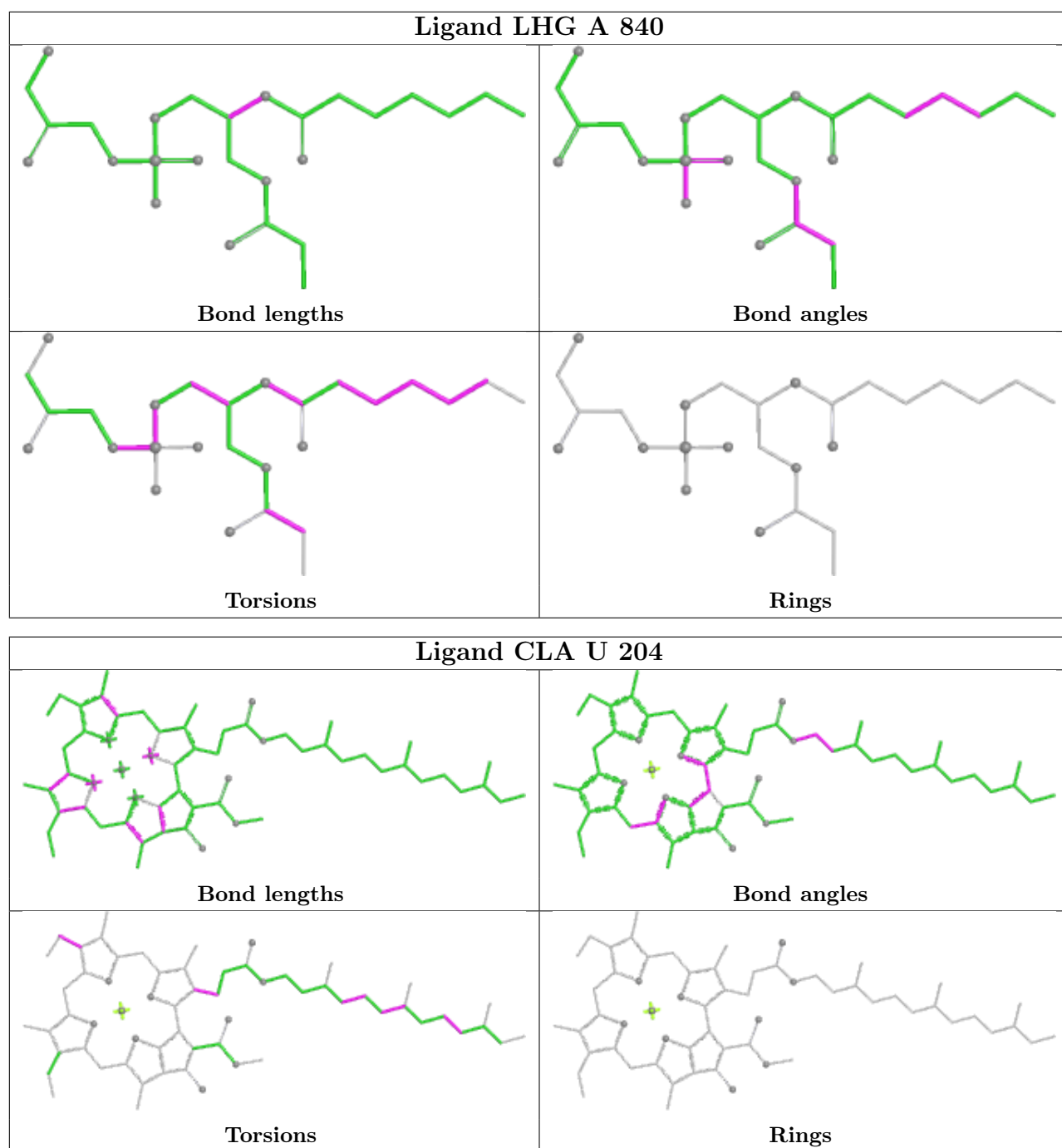




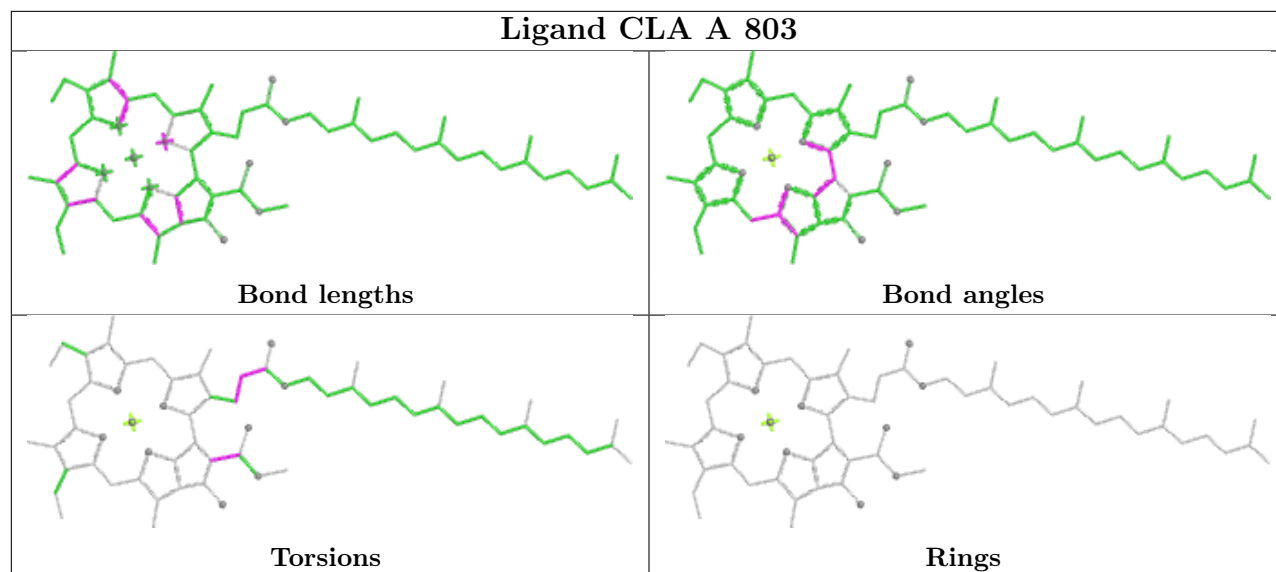




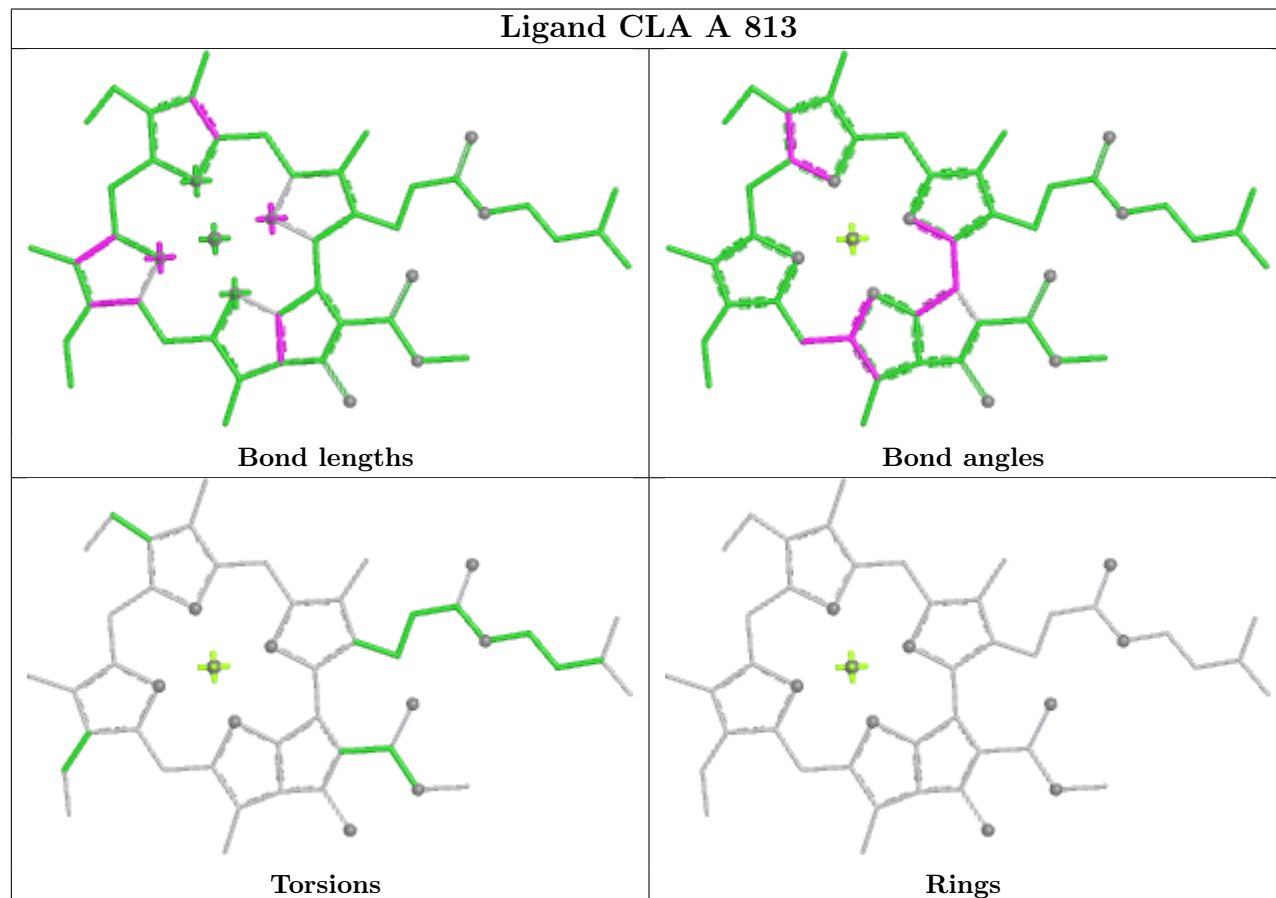


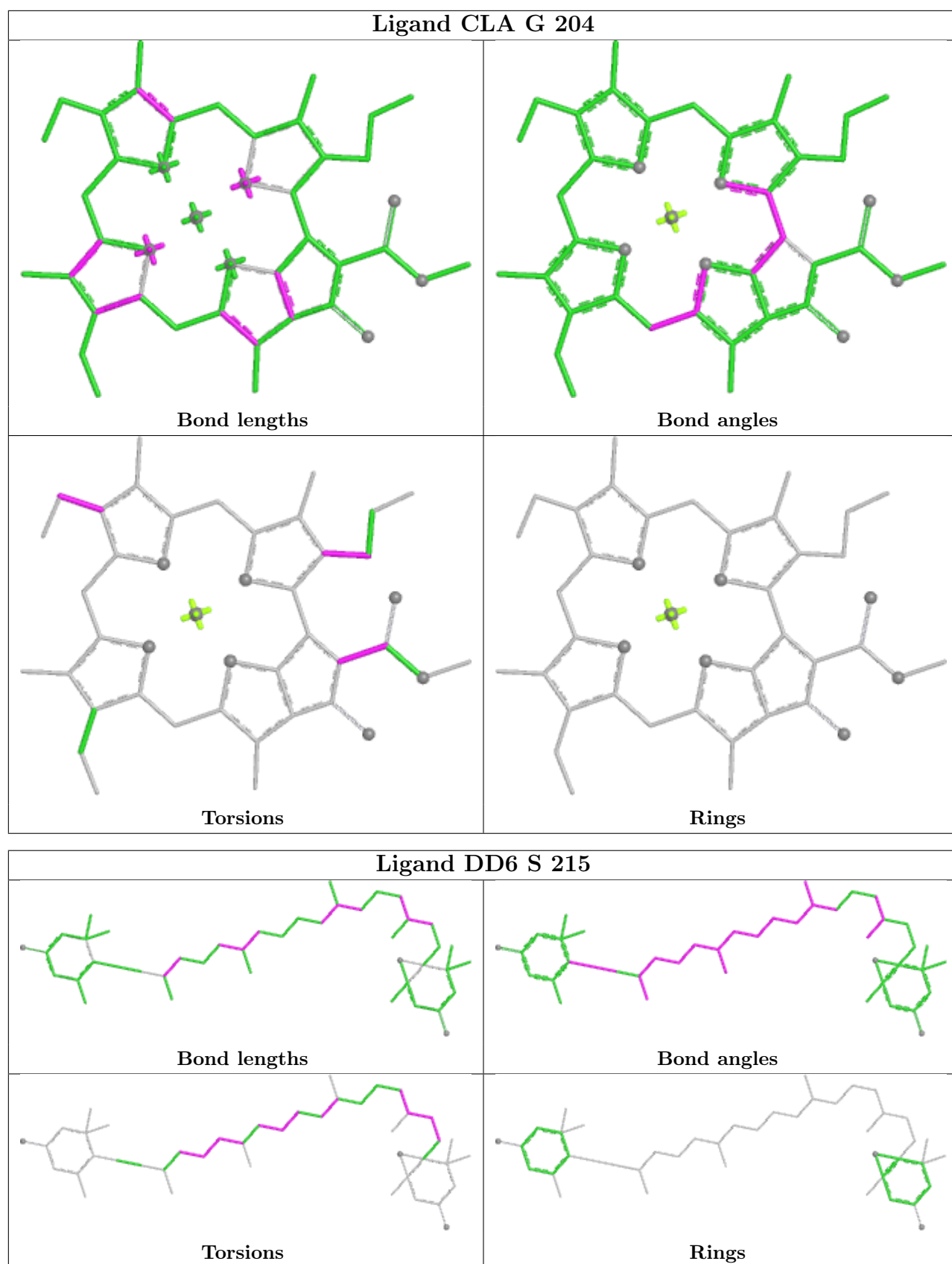


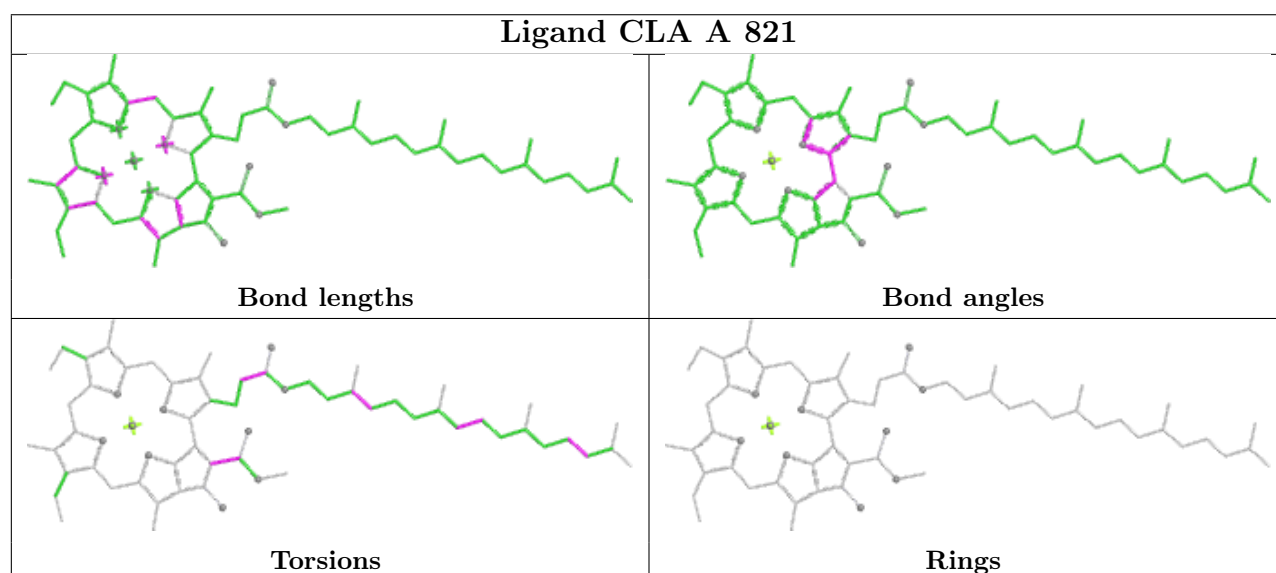
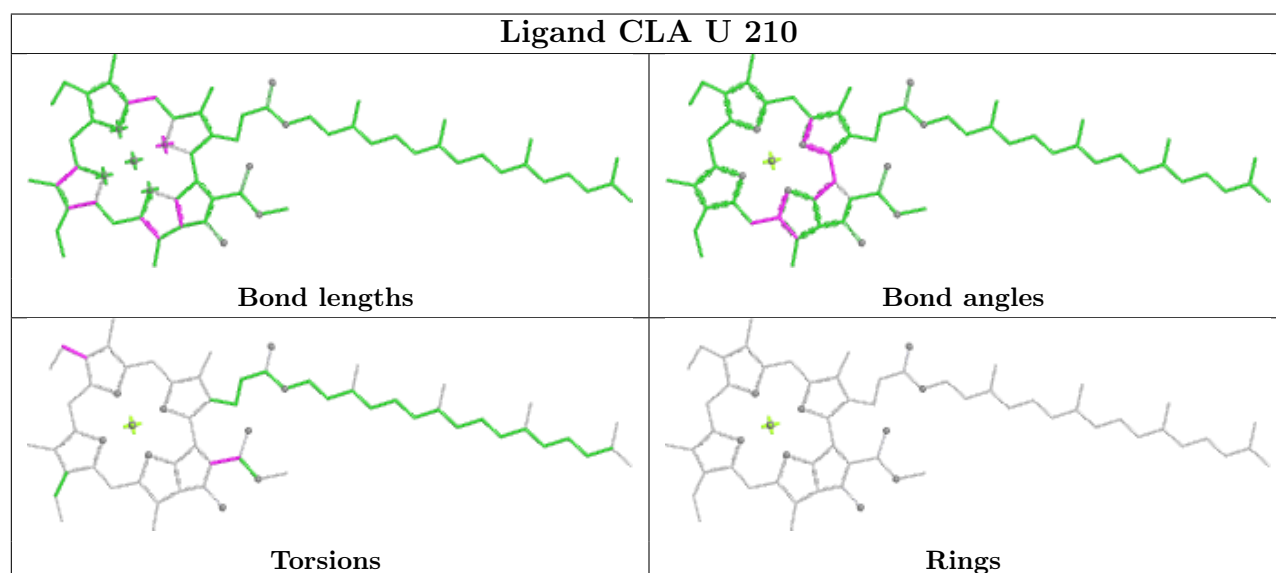
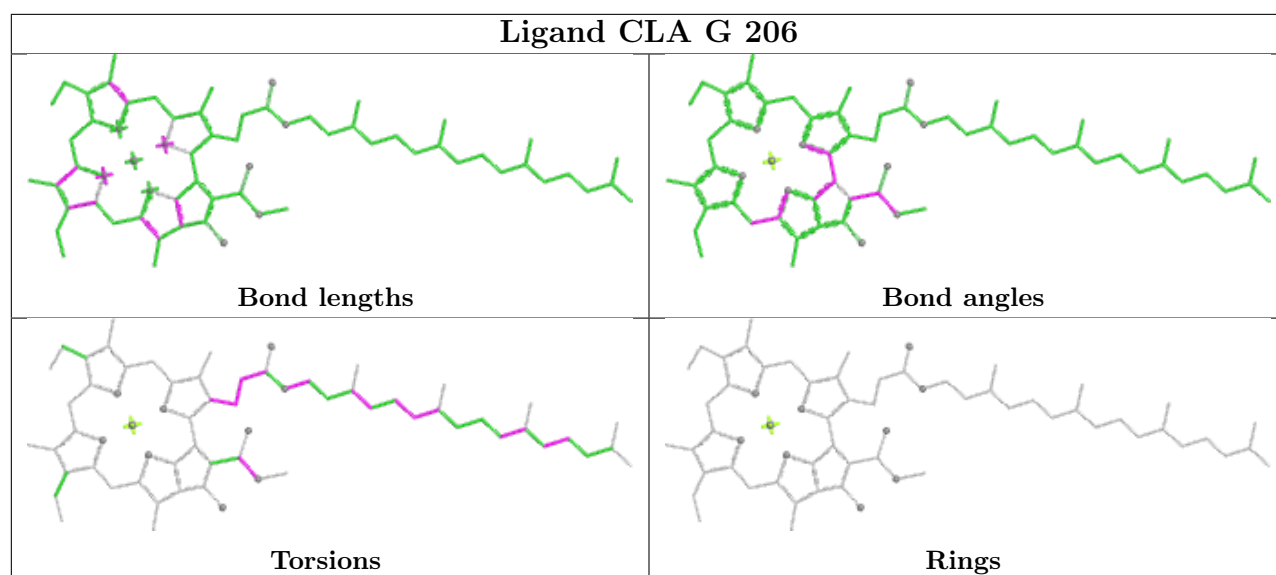
## Ligand CLA A 803



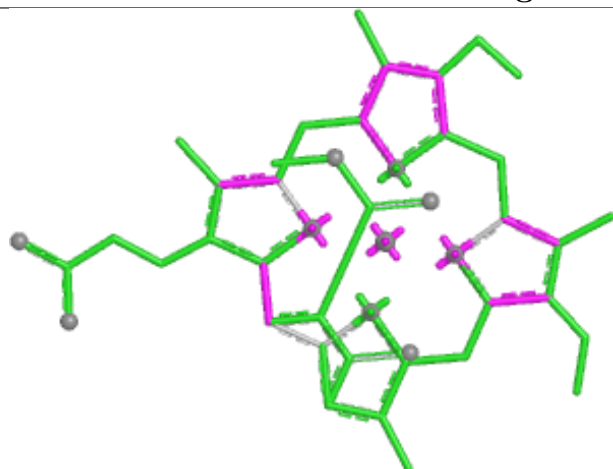
## Ligand CLA A 813



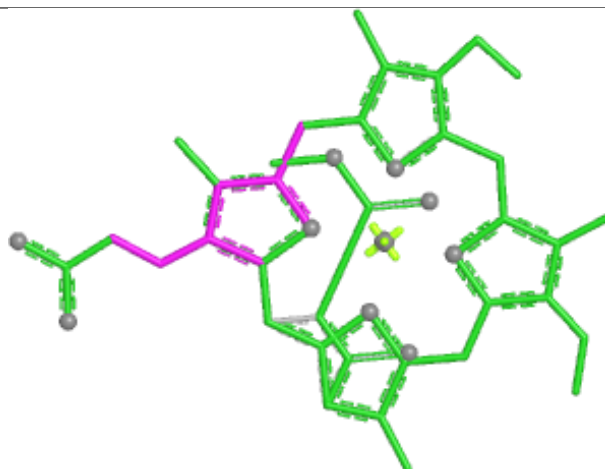




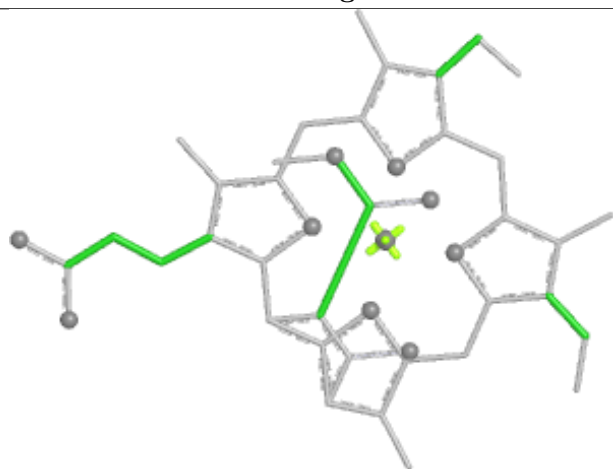
## Ligand KC1 O 210



Bond lengths



Bond angles

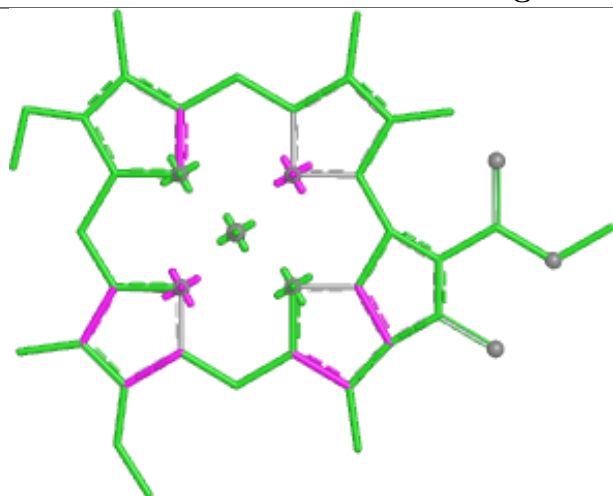


Torsions

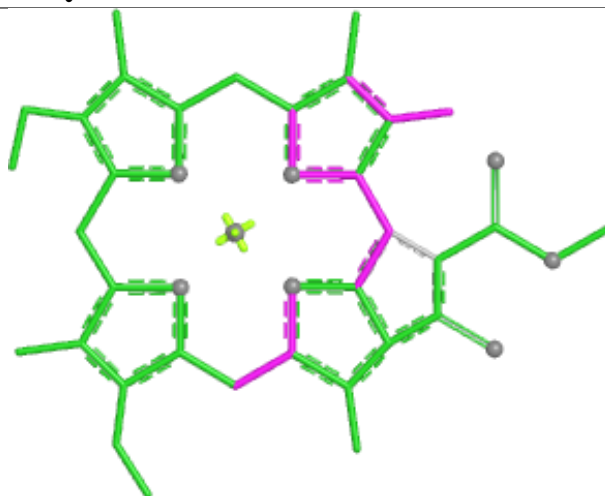


Rings

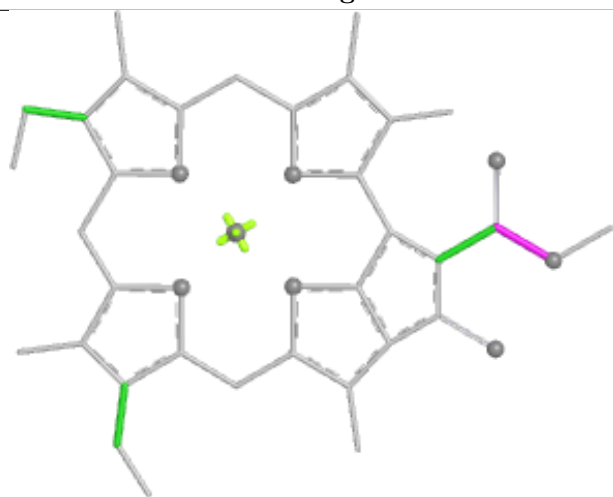
## Ligand CLA Q 211



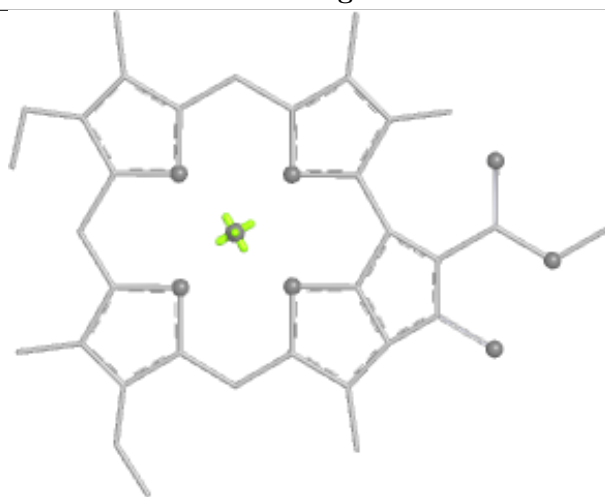
Bond lengths



Bond angles

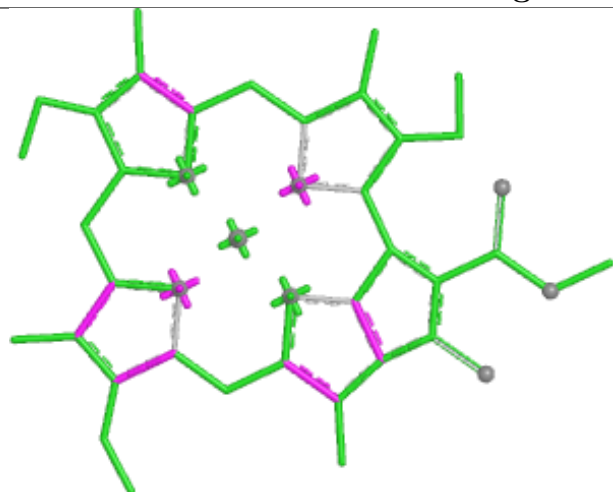


Torsions

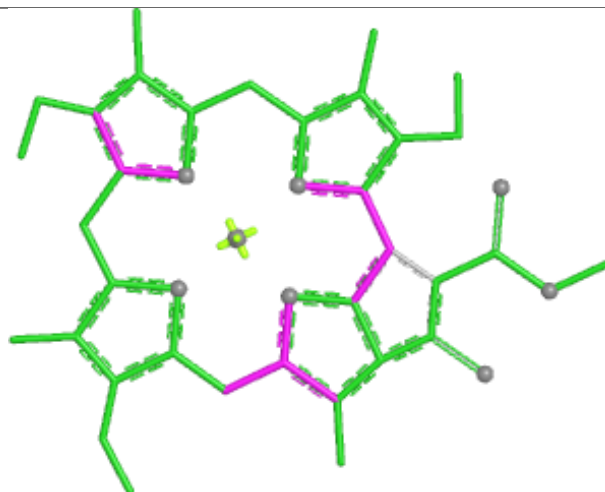


Rings

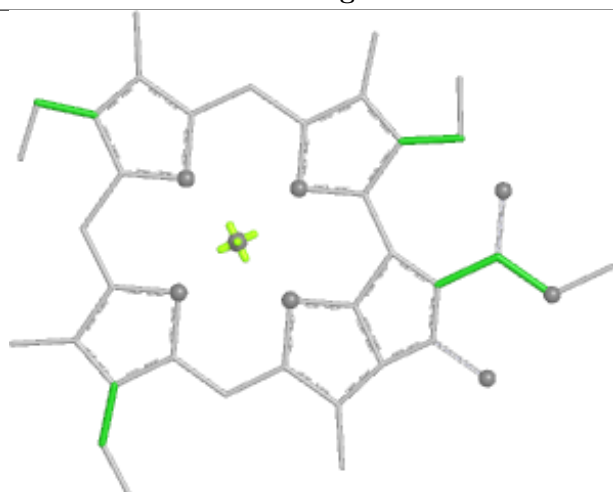
## Ligand CLA K 204



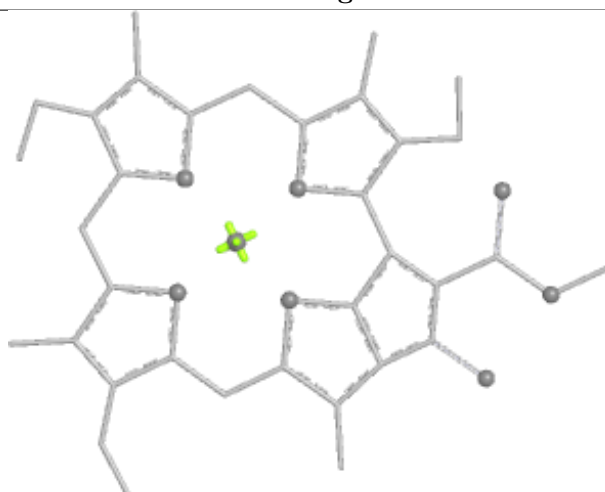
Bond lengths



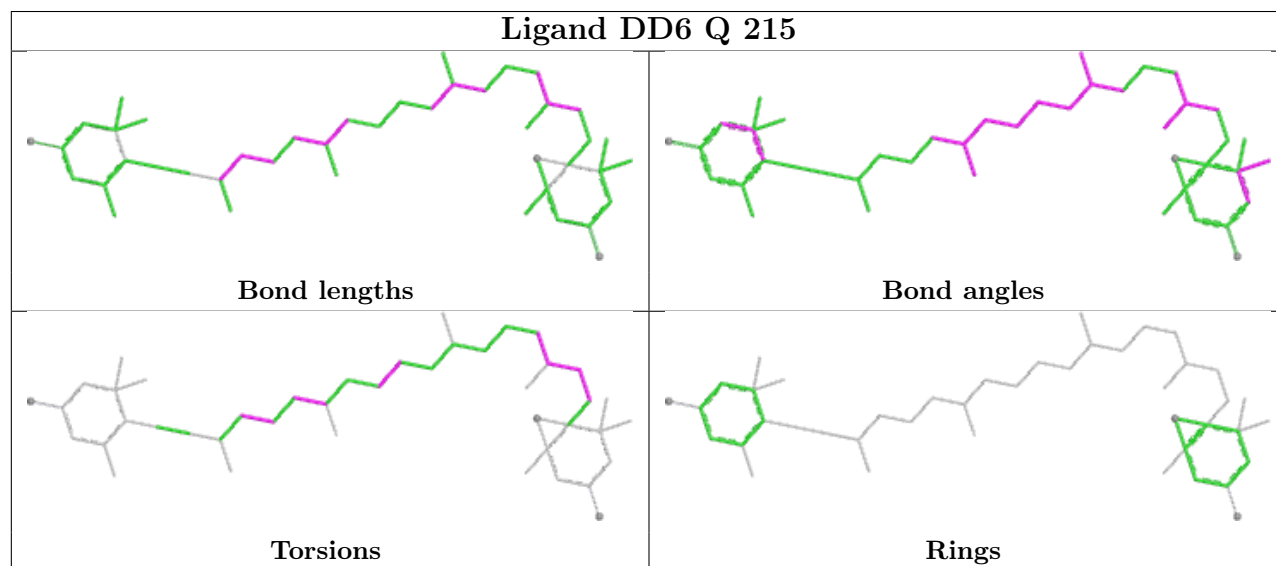
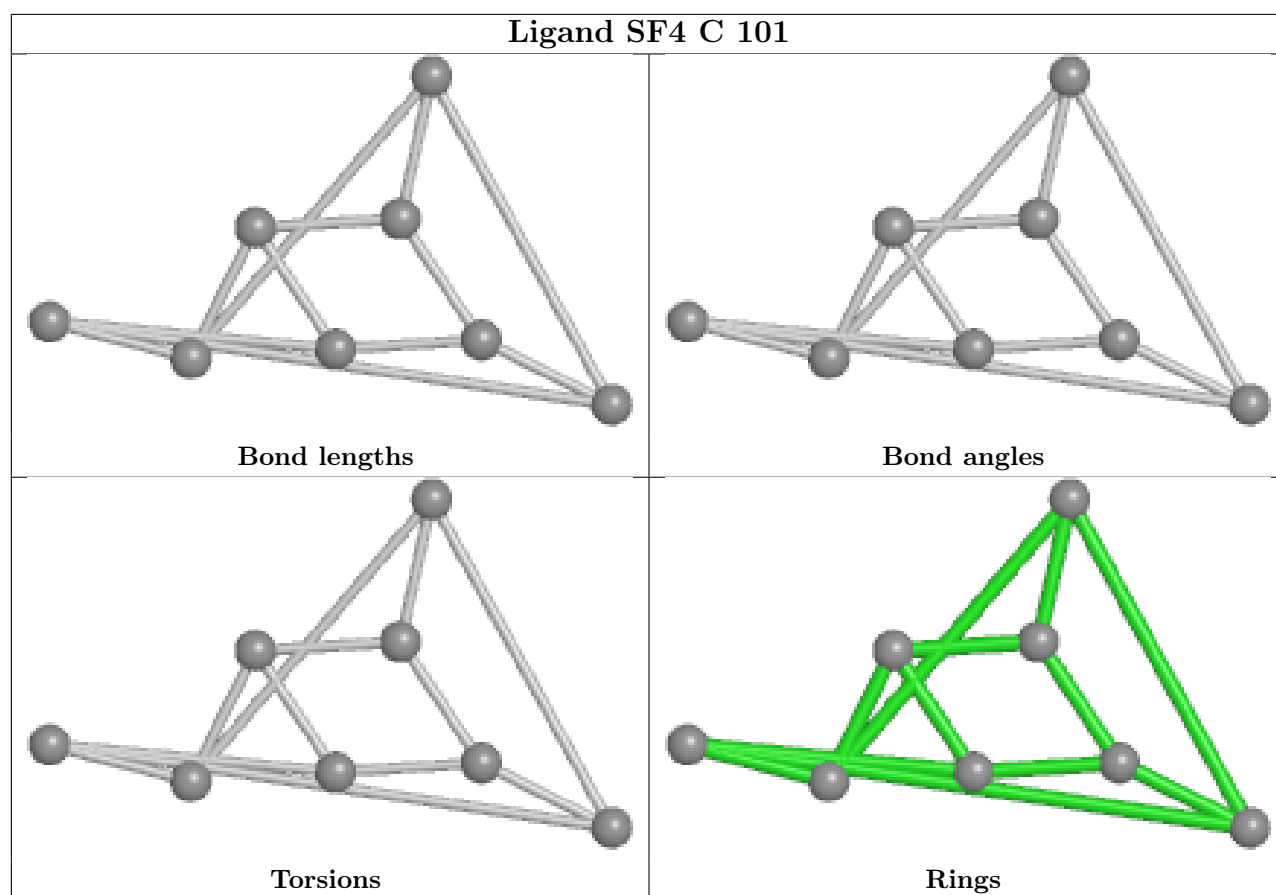
Bond angles



Torsions

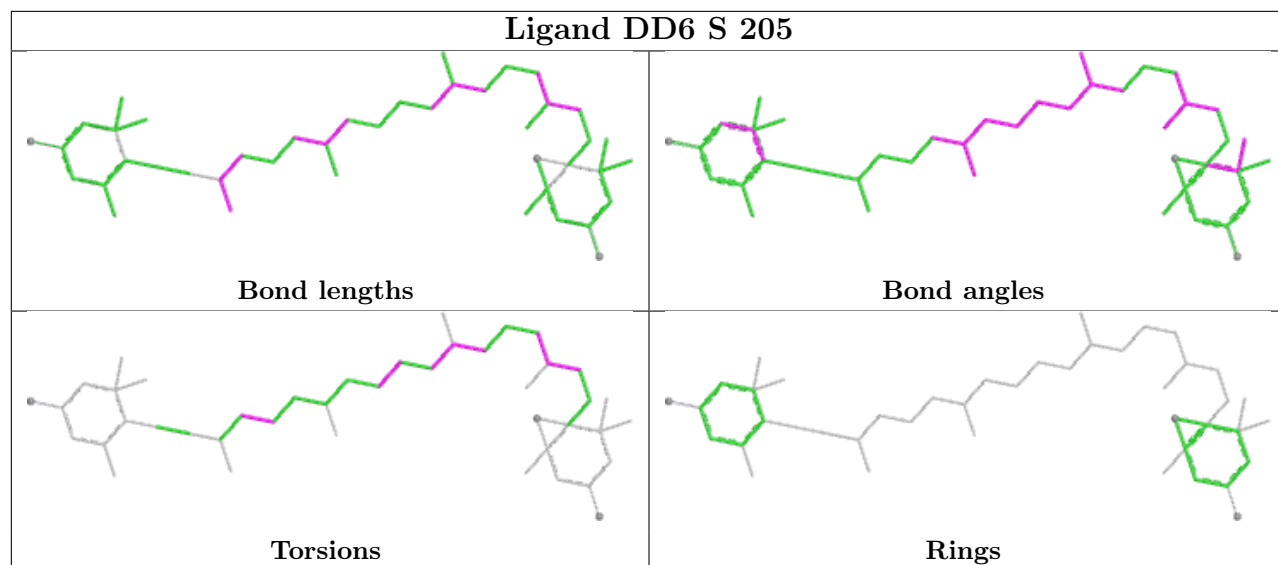


Rings

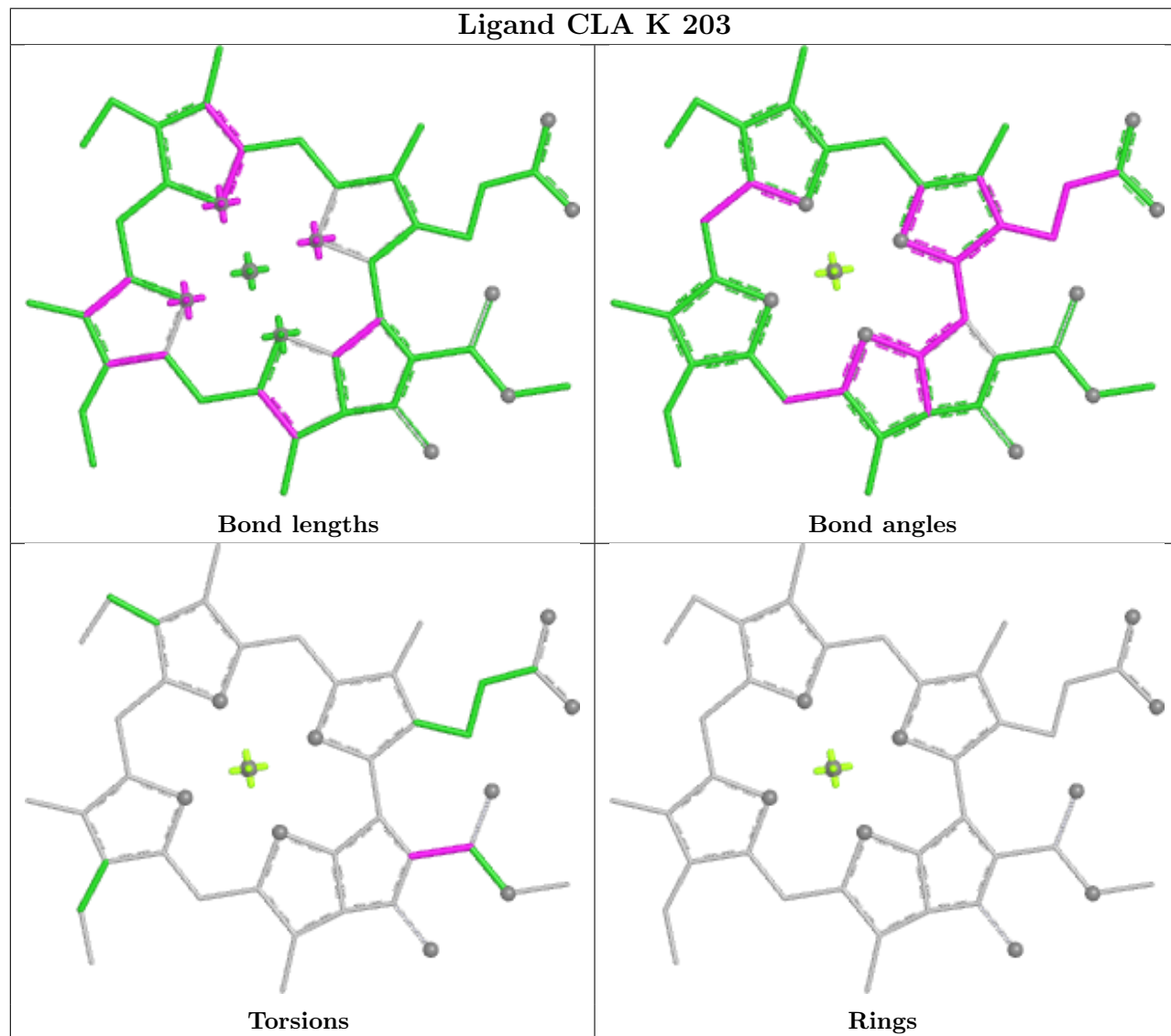


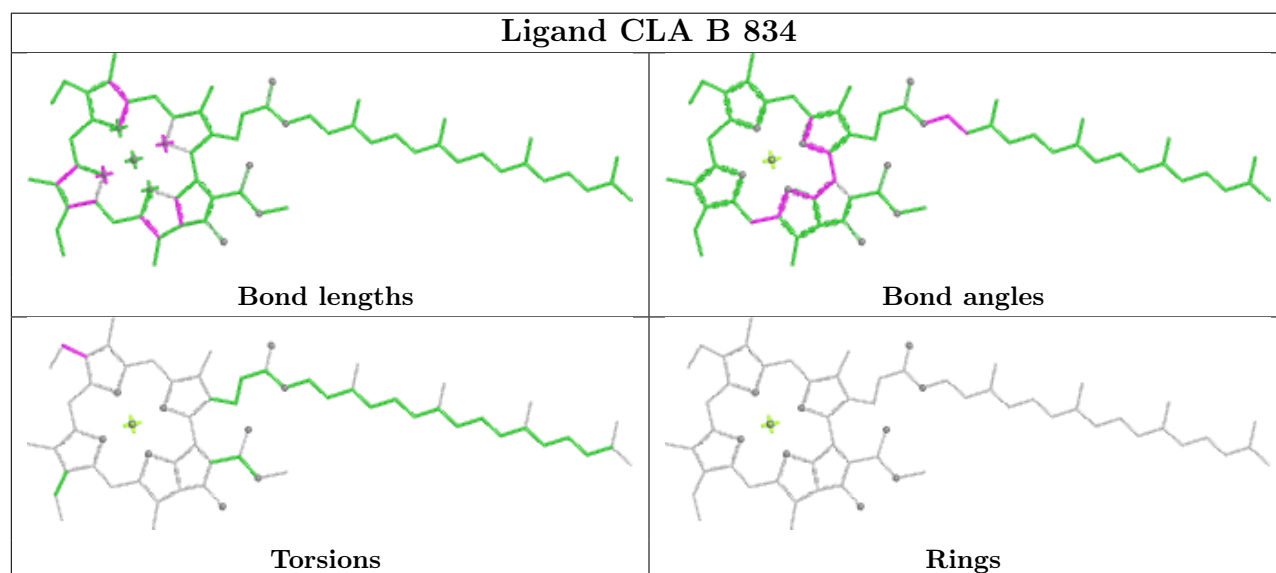
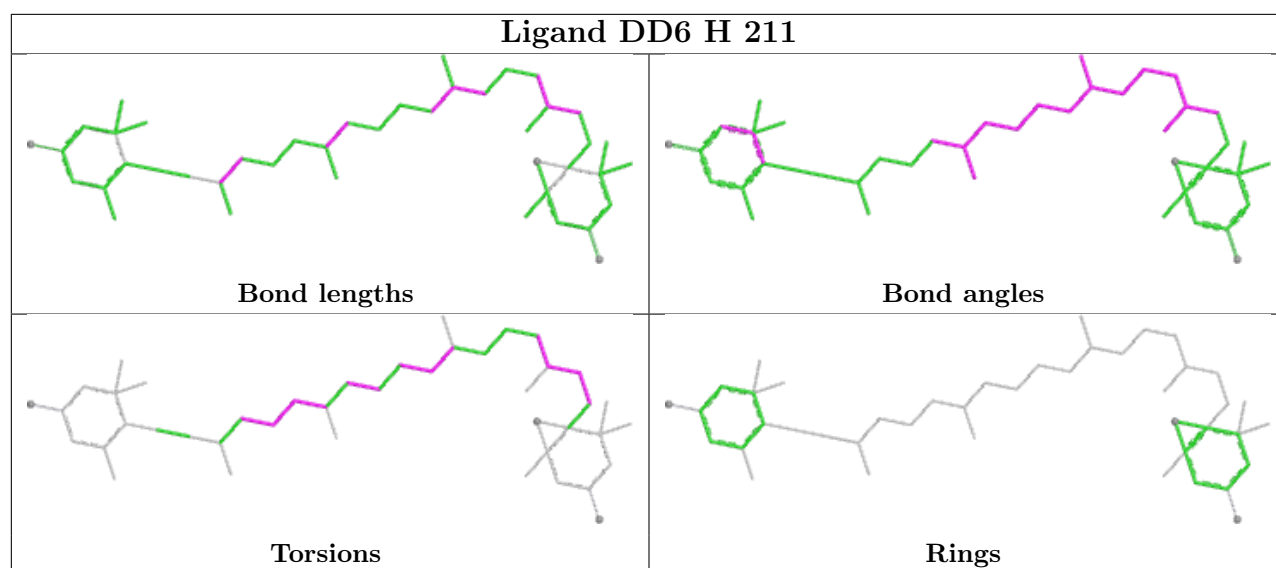


## Ligand DD6 S 205

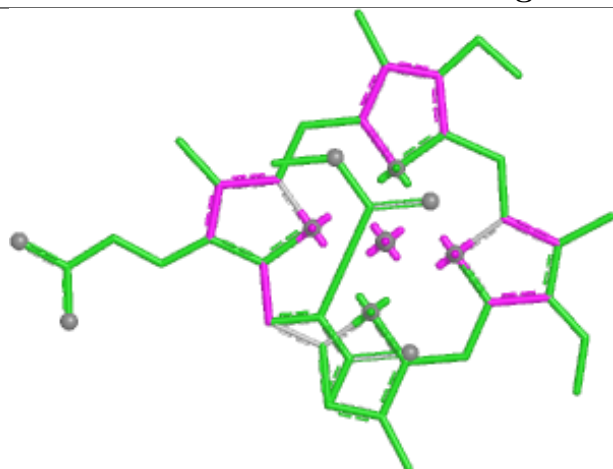


## Ligand CLA K 203

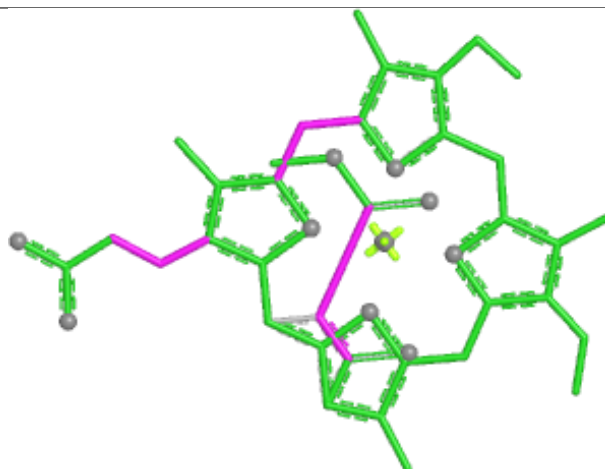




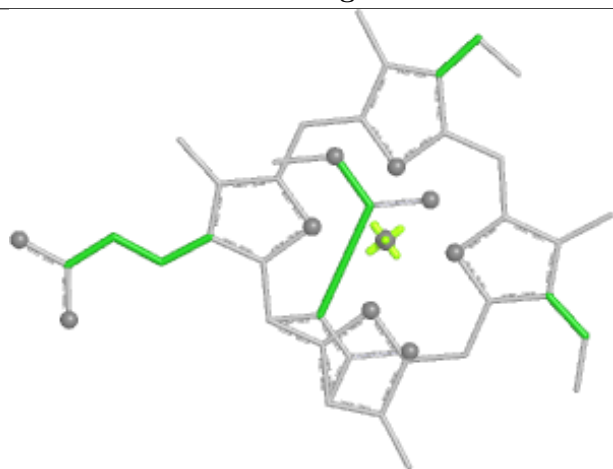
## Ligand KC1 U 213



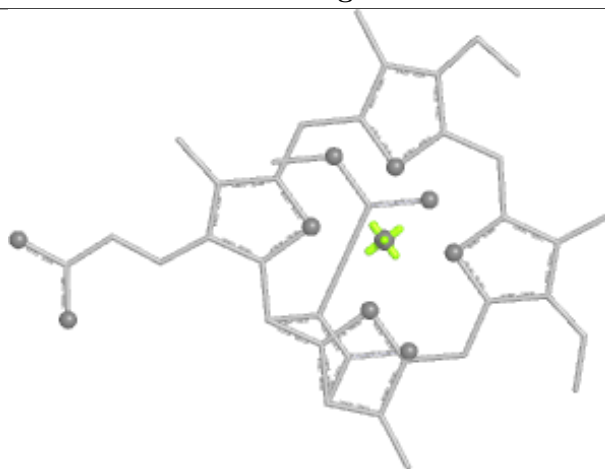
Bond lengths



Bond angles

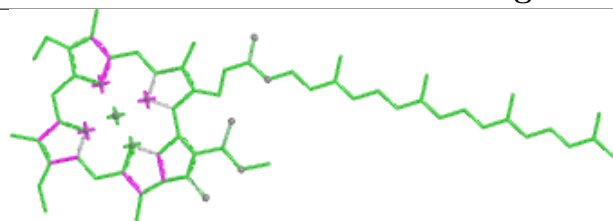


Torsions

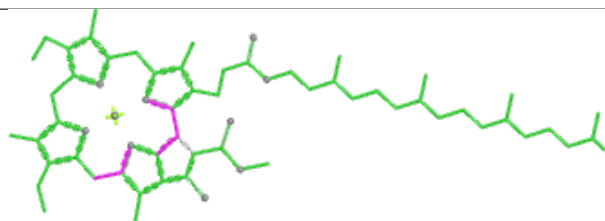


Rings

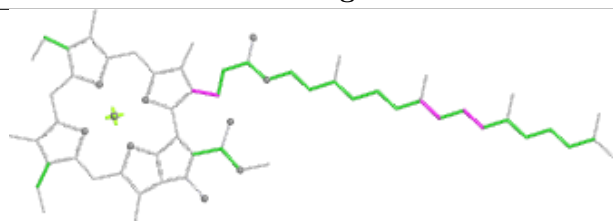
## Ligand CLA B 842



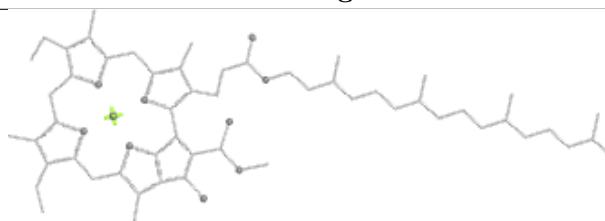
Bond lengths



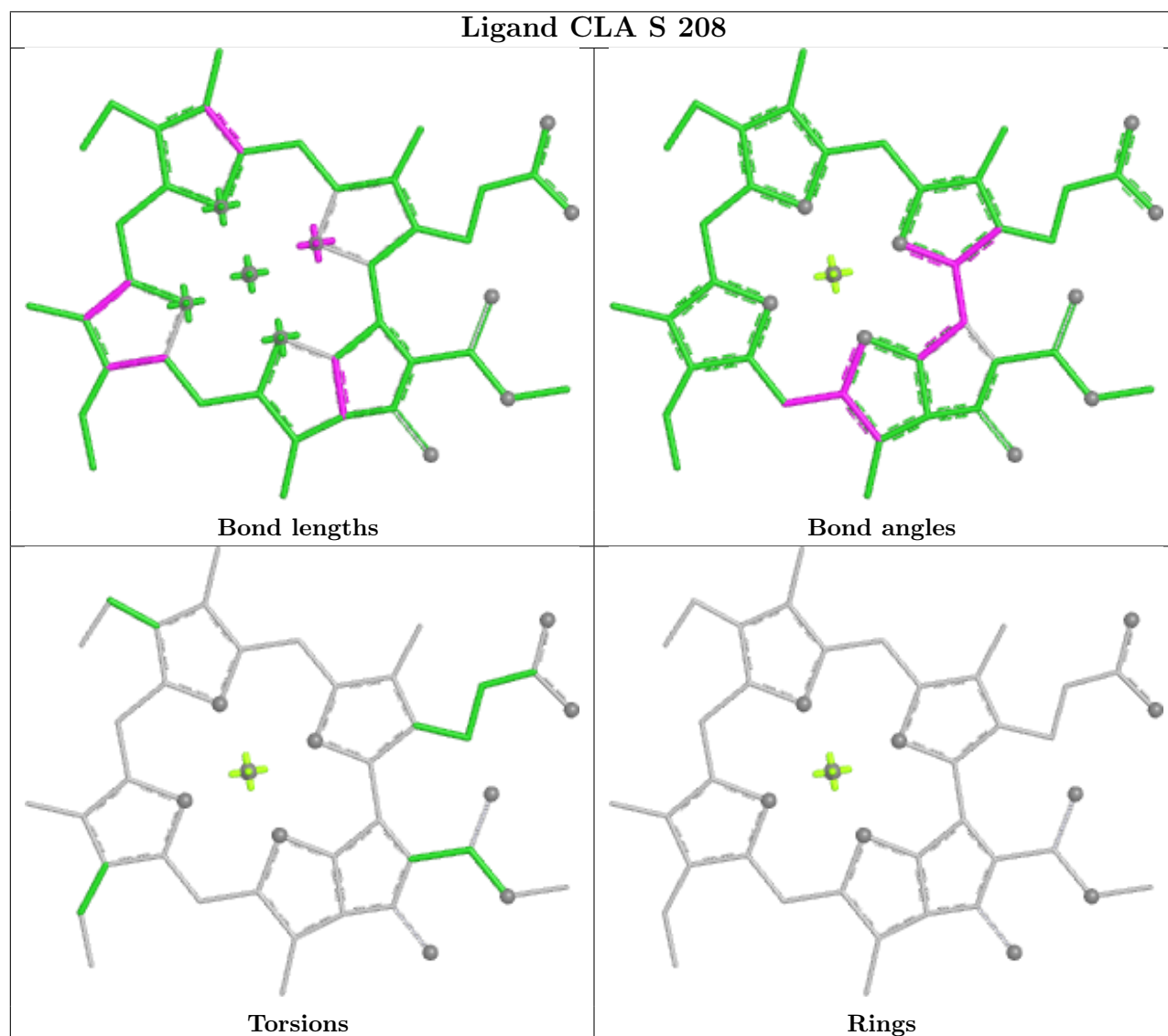
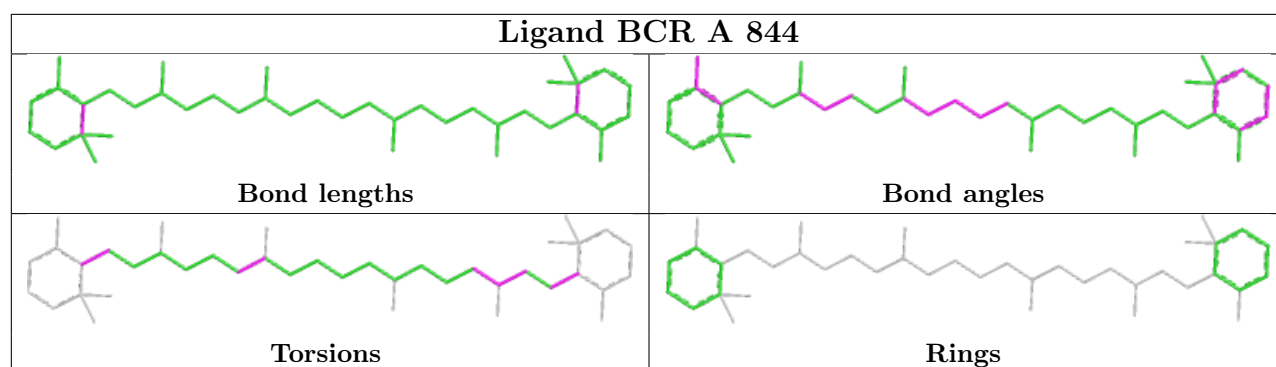
Bond angles



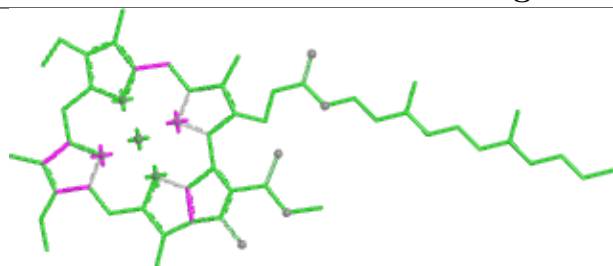
Torsions



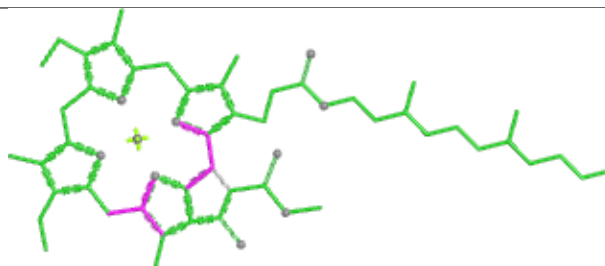
Rings



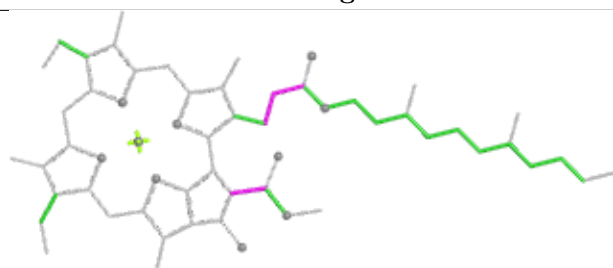
## Ligand CLA H 208



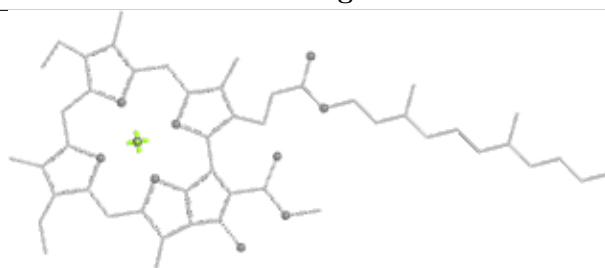
Bond lengths



Bond angles

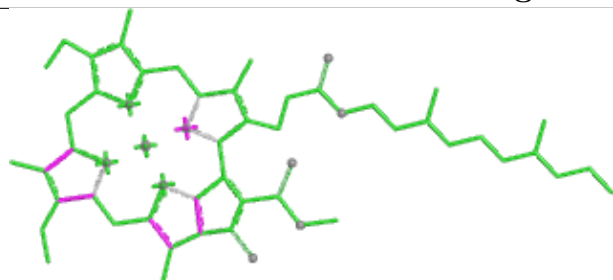


Torsions

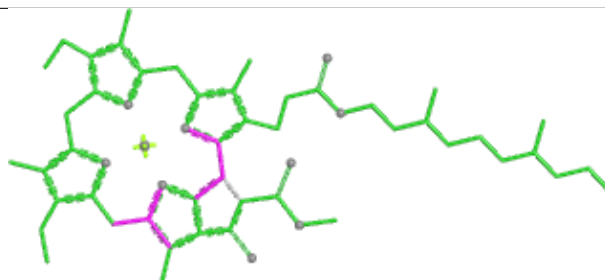


Rings

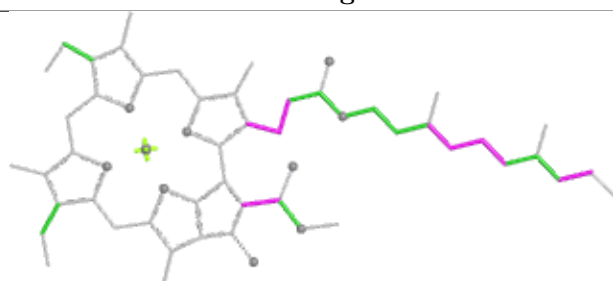
## Ligand CLA T 204



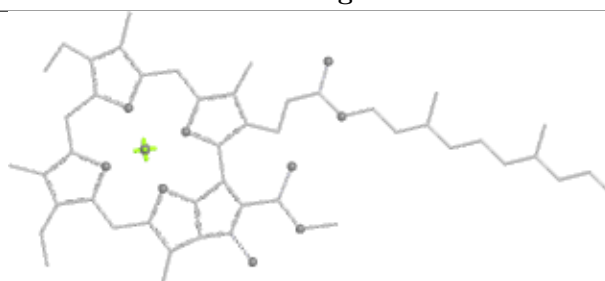
Bond lengths



Bond angles

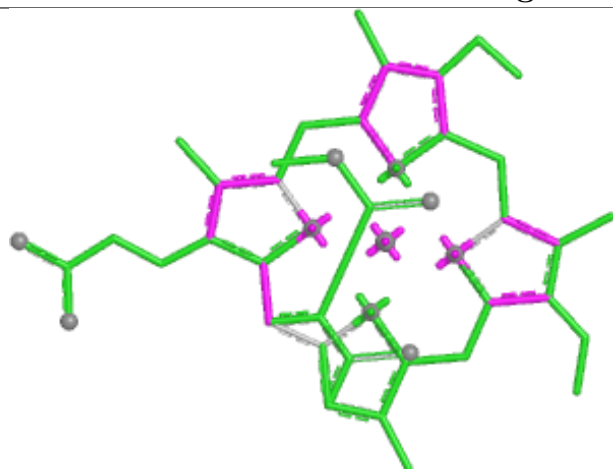


Torsions

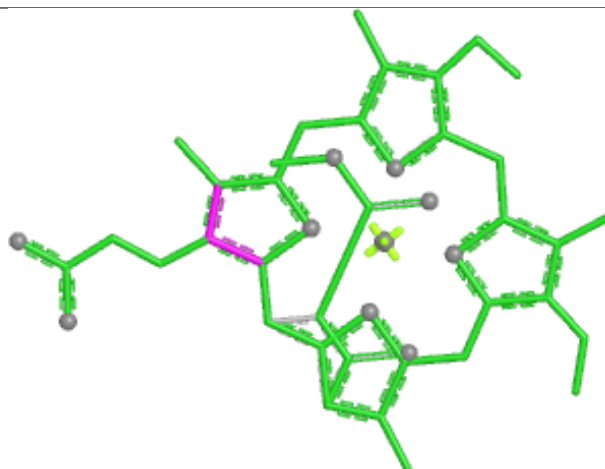


Rings

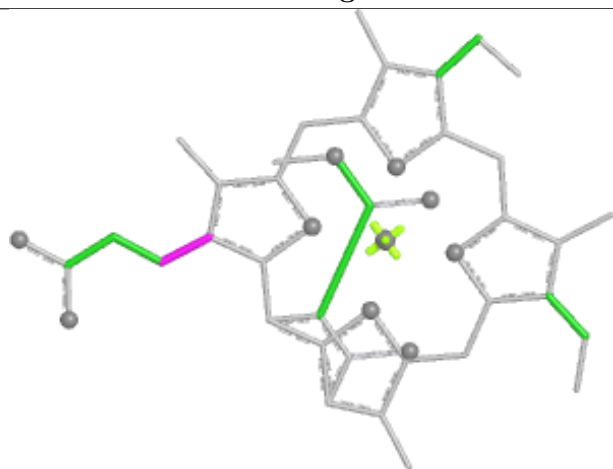
## Ligand KC1 P 203



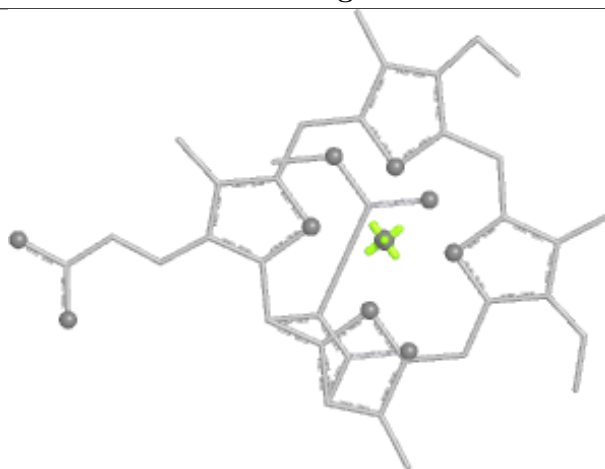
Bond lengths



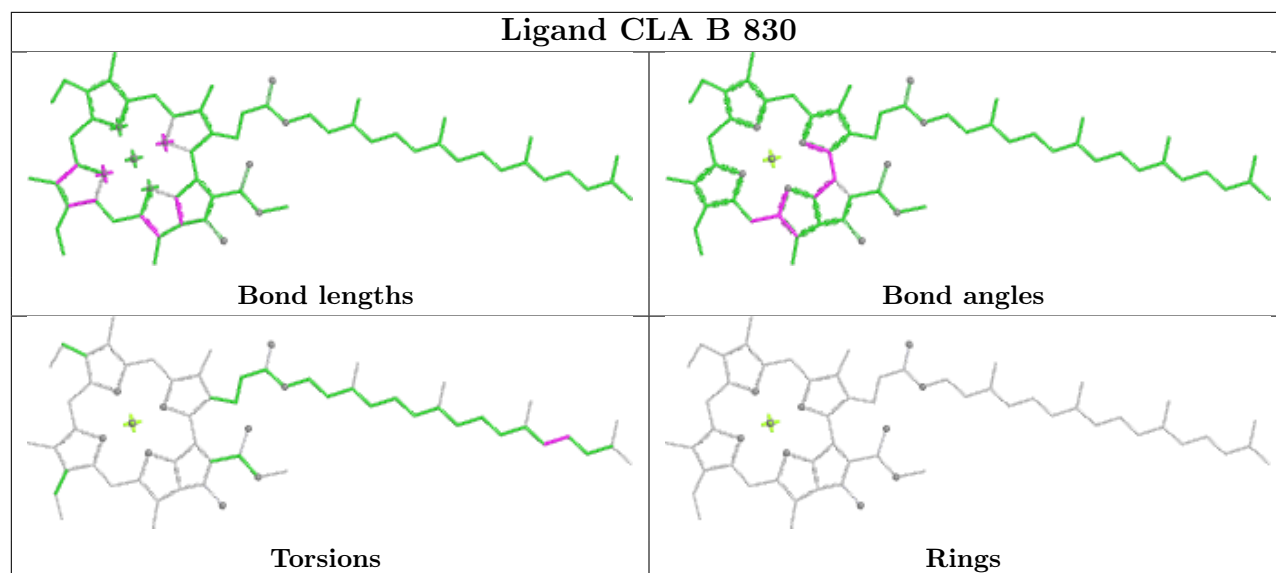
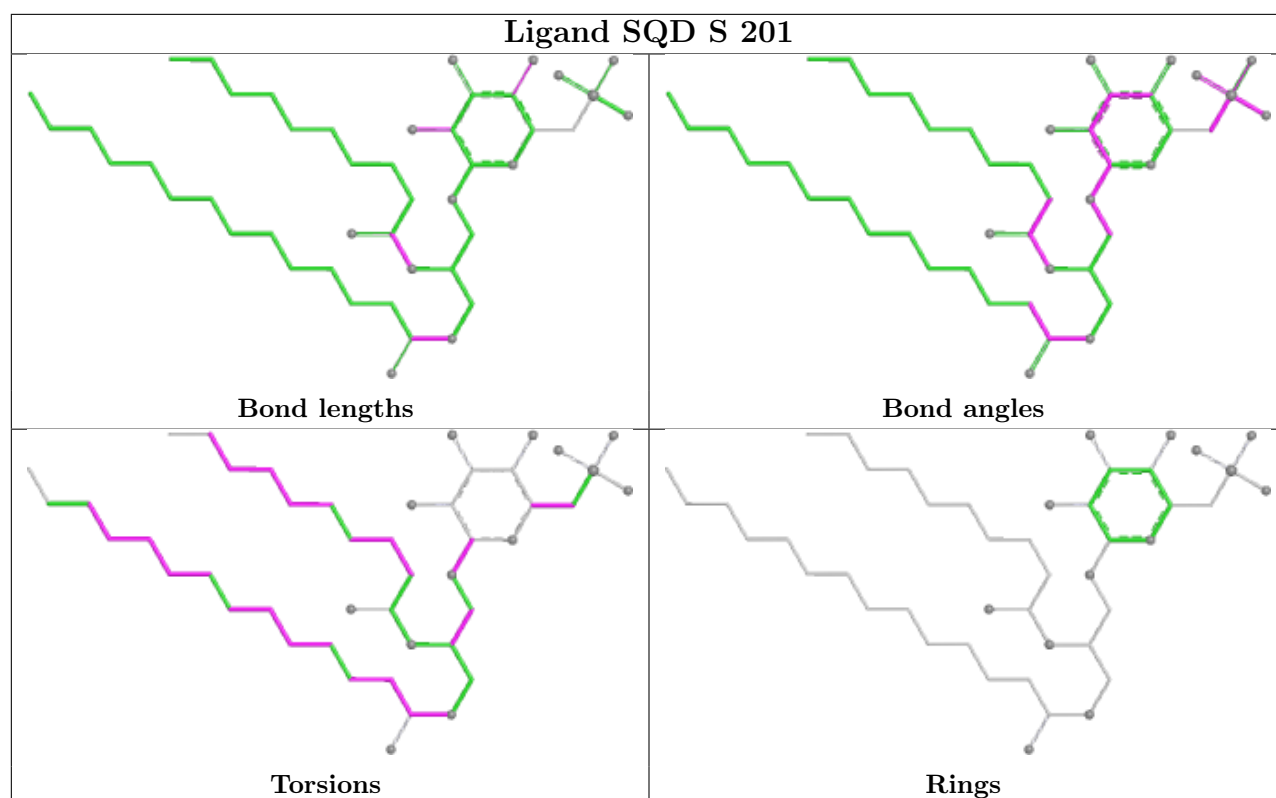
Bond angles

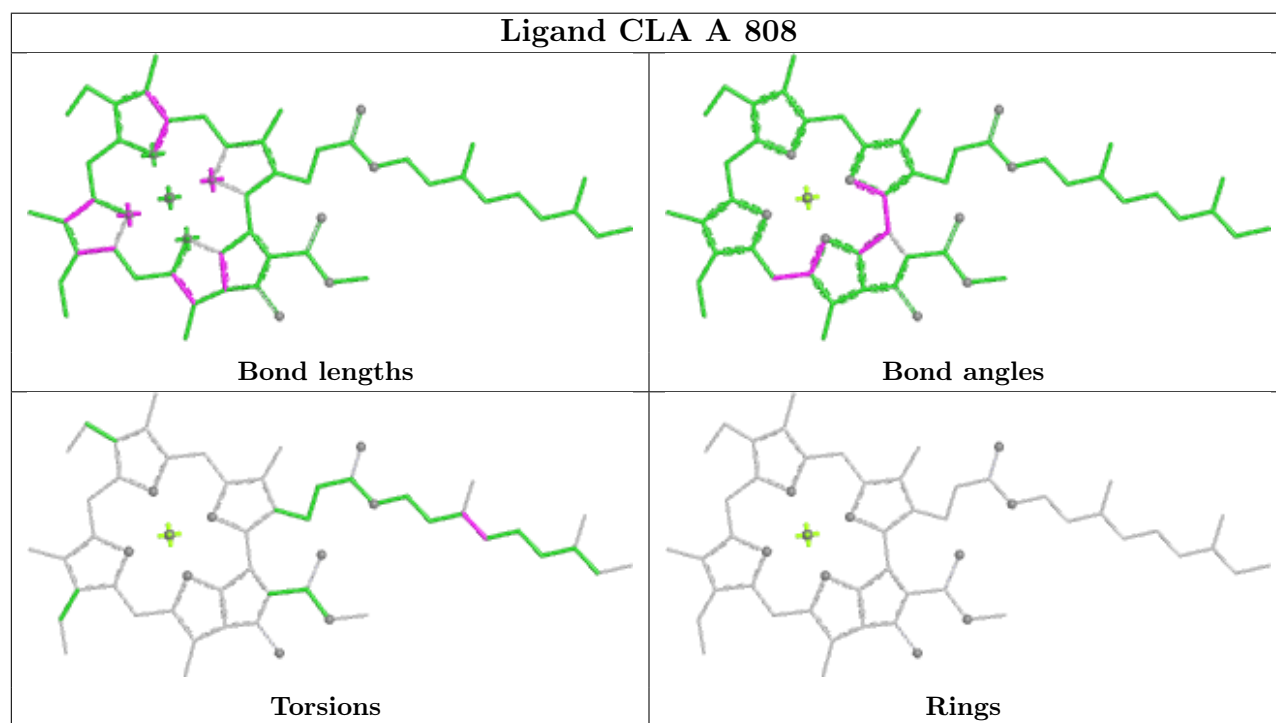
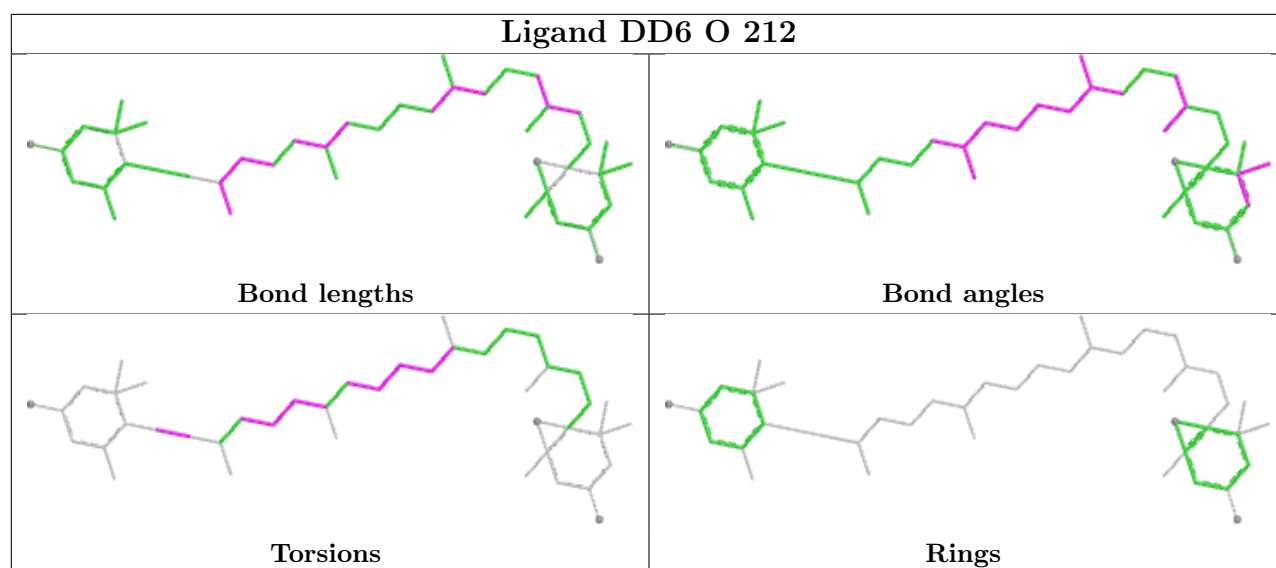


Torsions

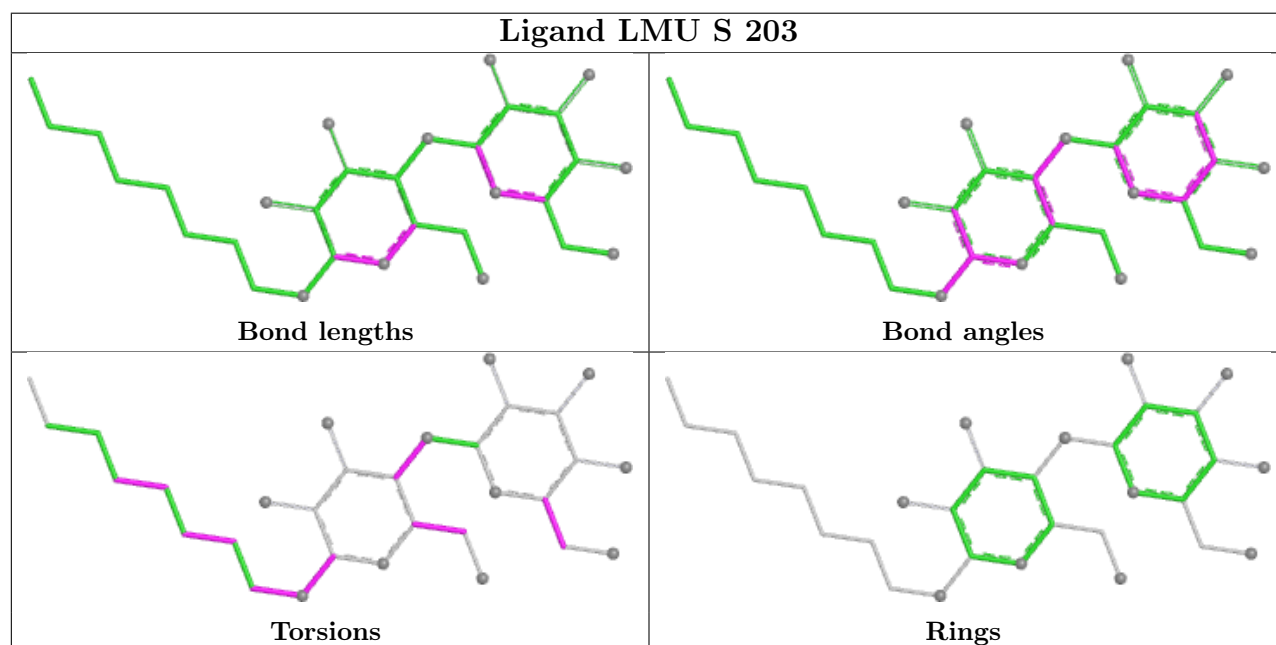
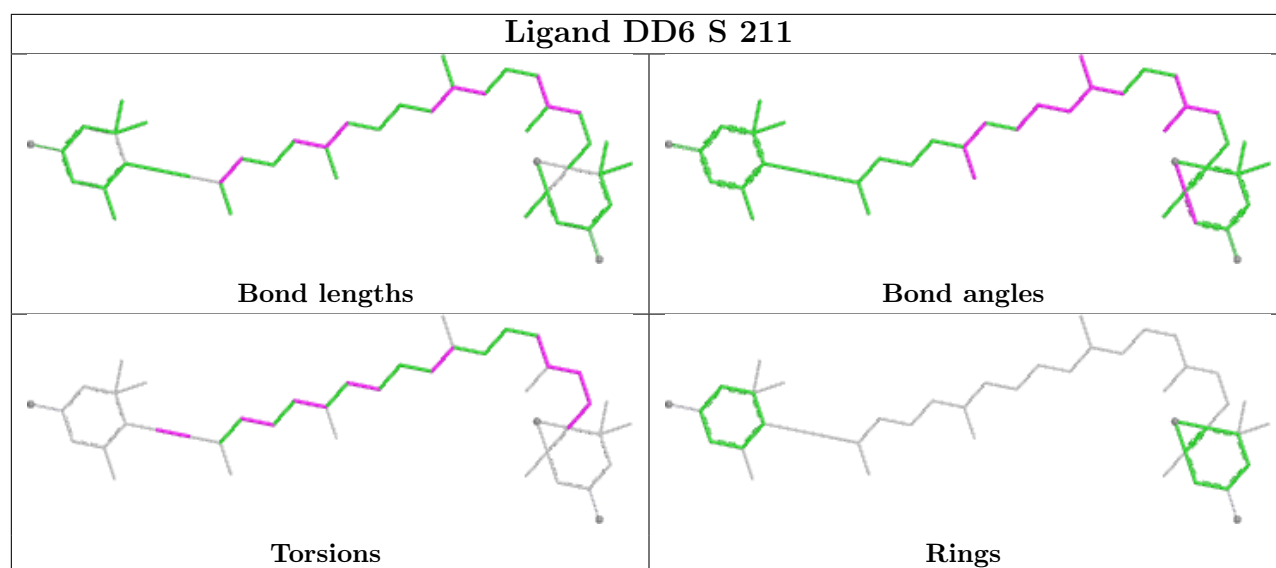


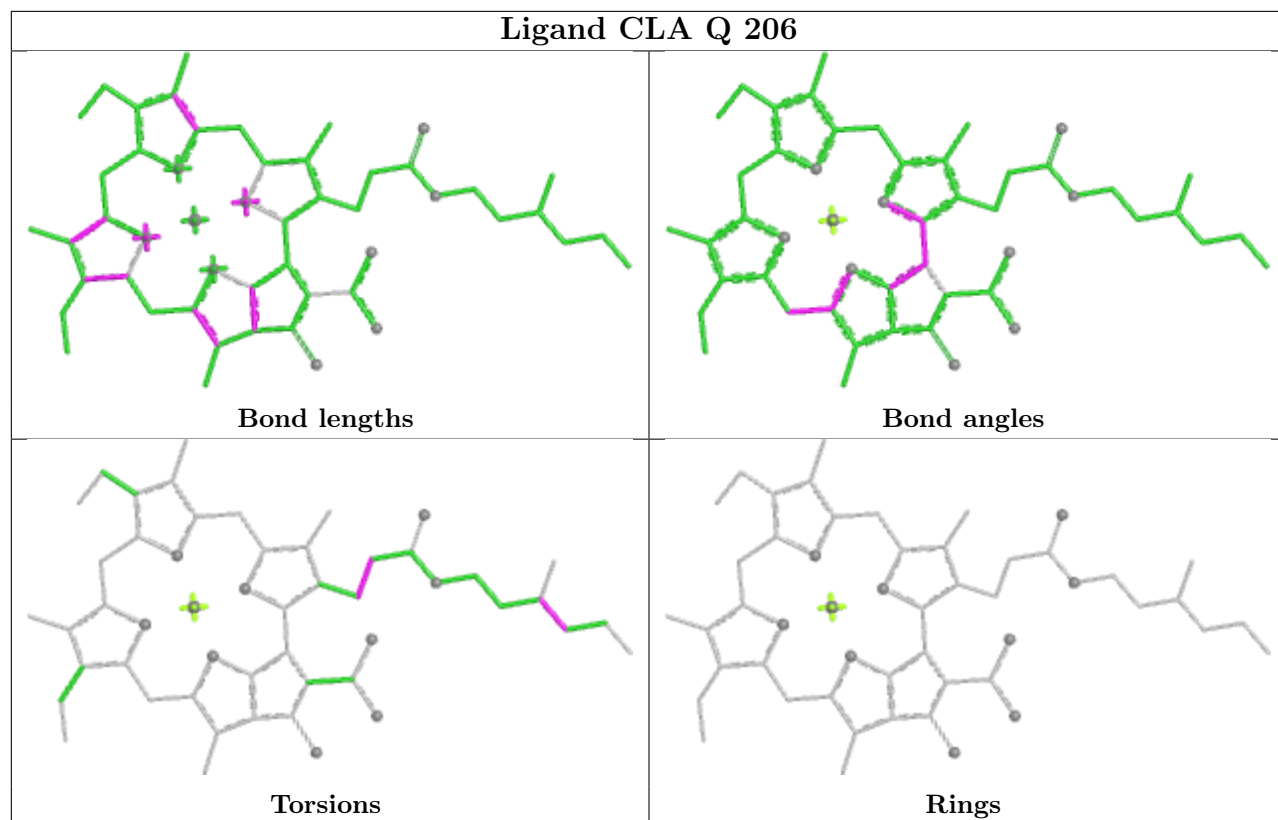
Rings



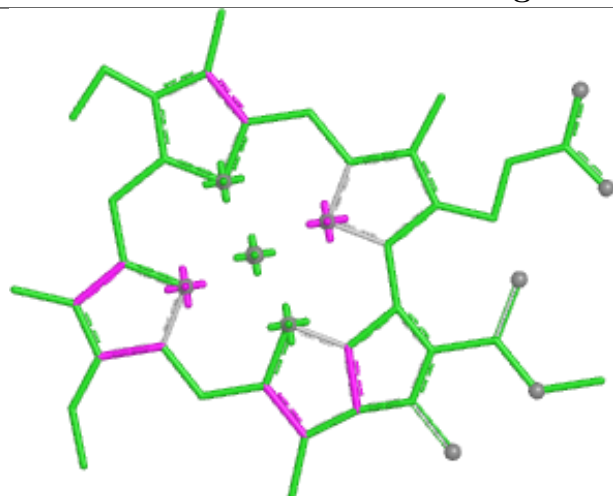




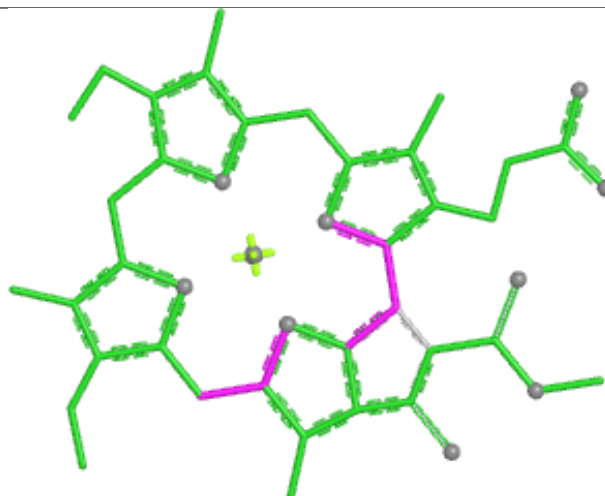




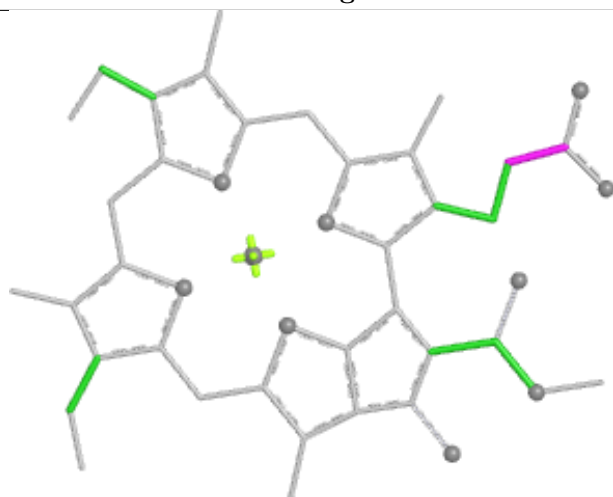
## Ligand CLA H 206



Bond lengths



Bond angles

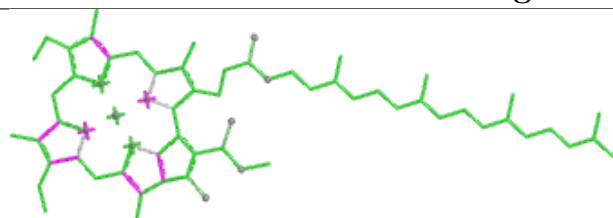


Torsions

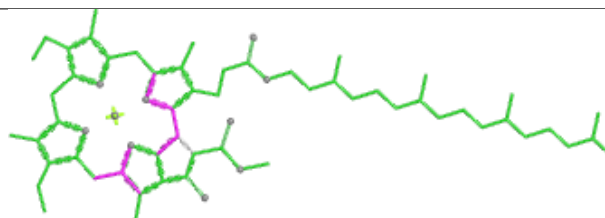


Rings

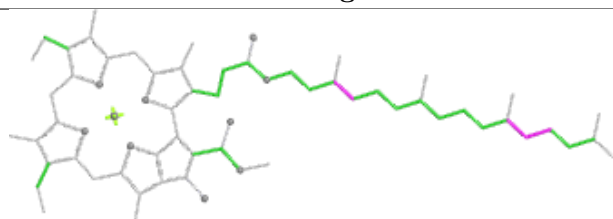
## Ligand CLA O 206



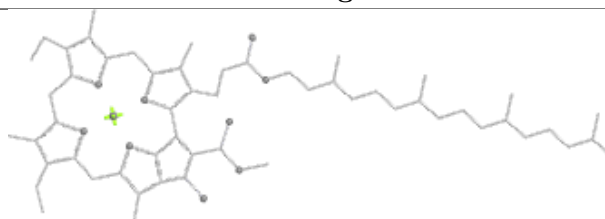
Bond lengths



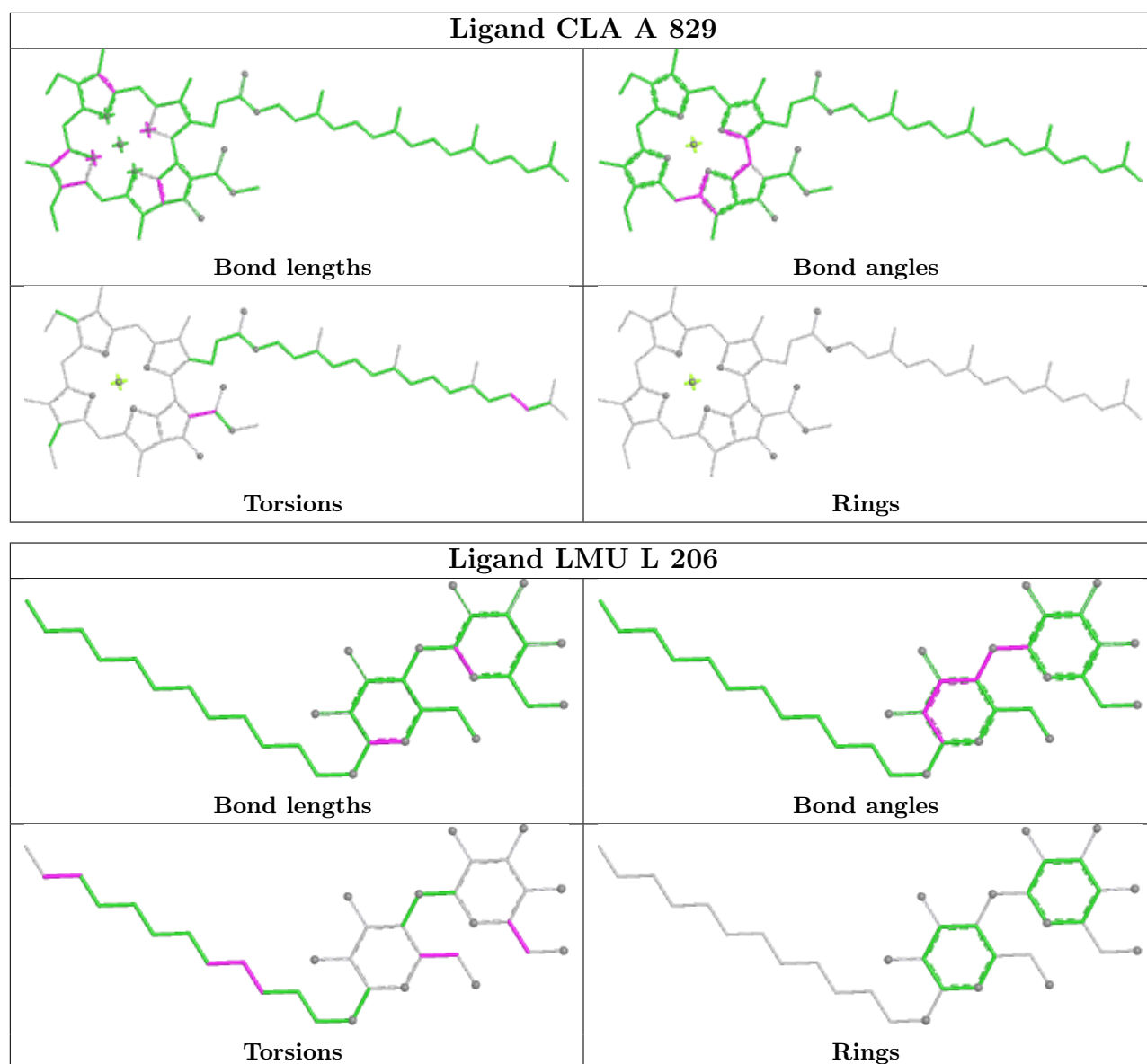
Bond angles



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.

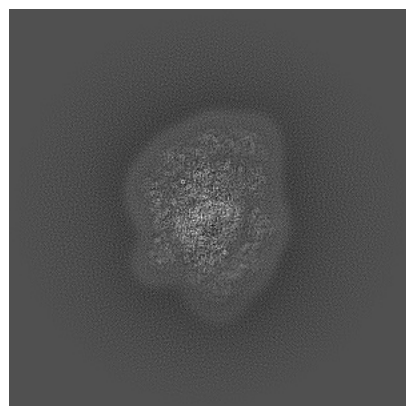
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64153. These allow visual inspection of the internal detail of the map and identification of artifacts.

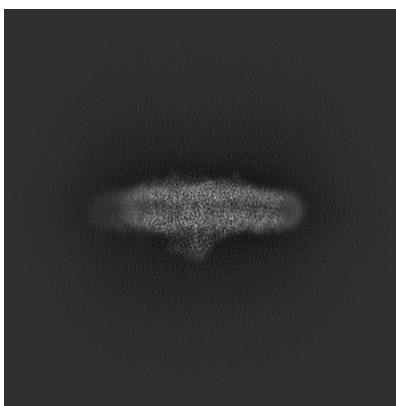
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

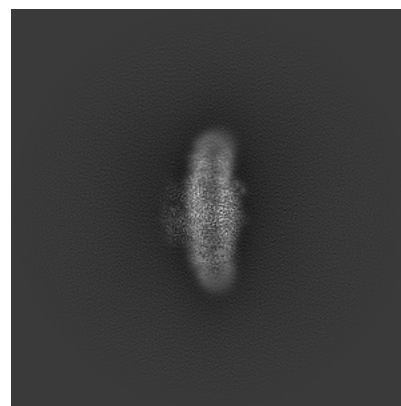
#### 6.1.1 Primary map



X

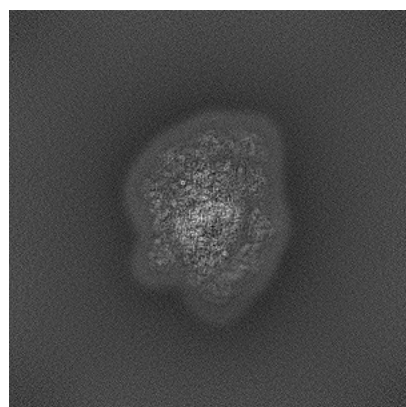


Y

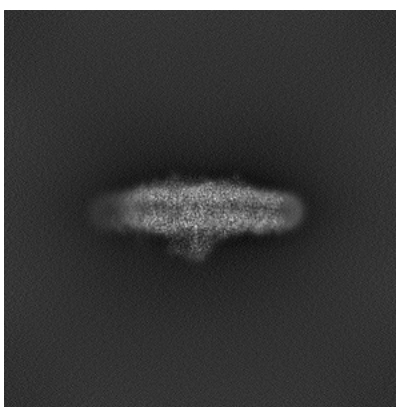


Z

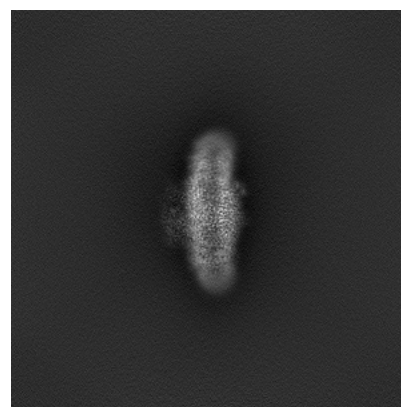
#### 6.1.2 Raw map



X



Y

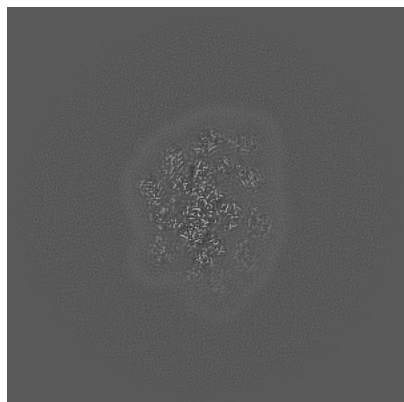


Z

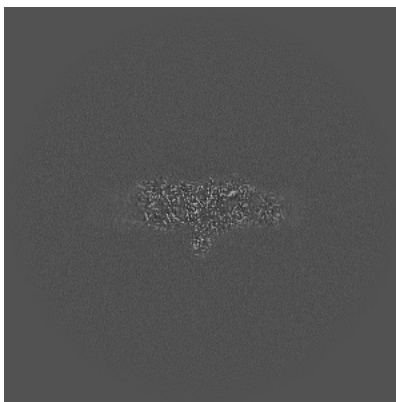
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

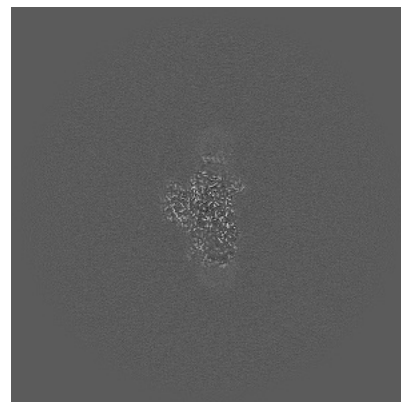
### 6.2.1 Primary map



X Index: 300

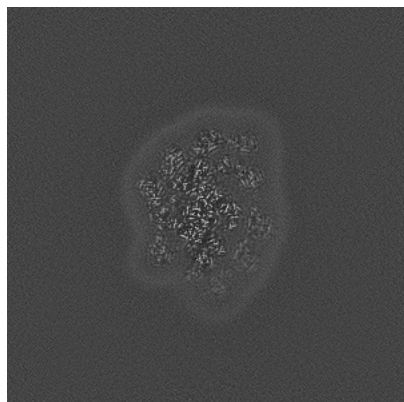


Y Index: 300

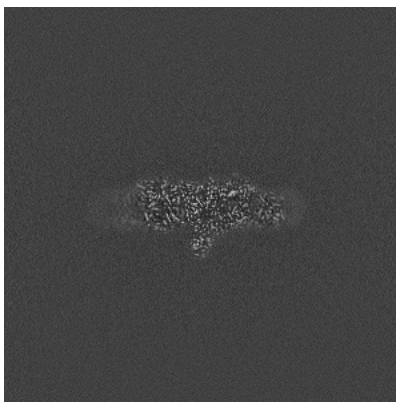


Z Index: 300

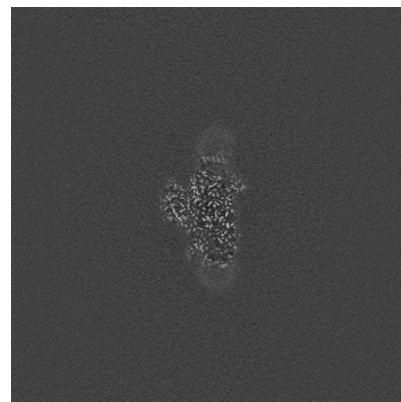
### 6.2.2 Raw map



X Index: 300



Y Index: 300



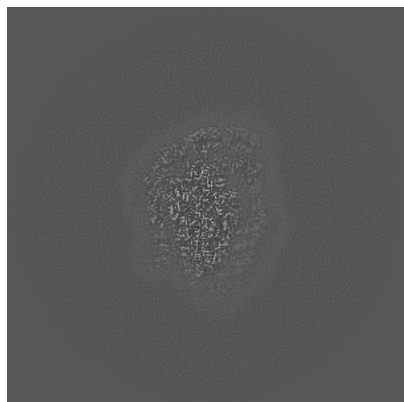
Z Index: 300

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



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

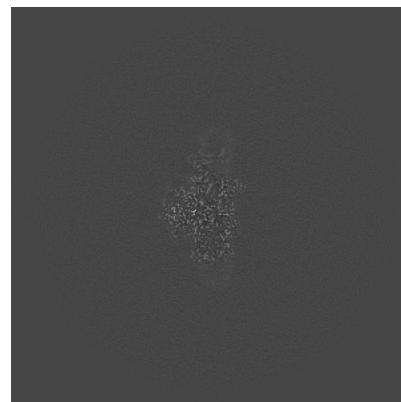
### 6.3.1 Primary map



X Index: 316

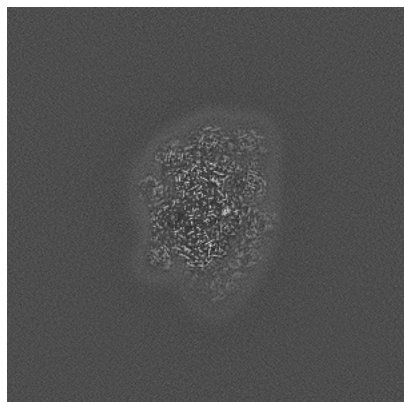


Y Index: 290

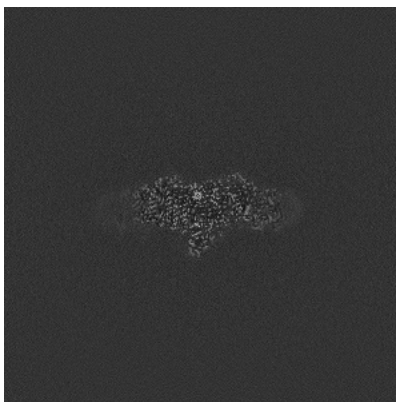


Z Index: 288

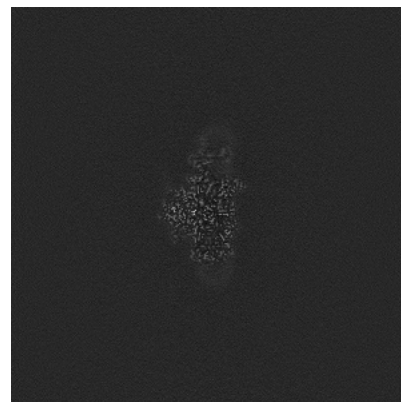
### 6.3.2 Raw map



X Index: 285



Y Index: 289

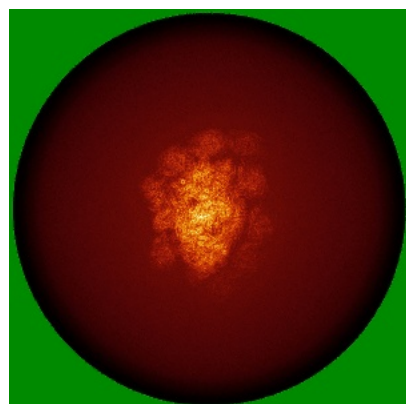


Z Index: 288

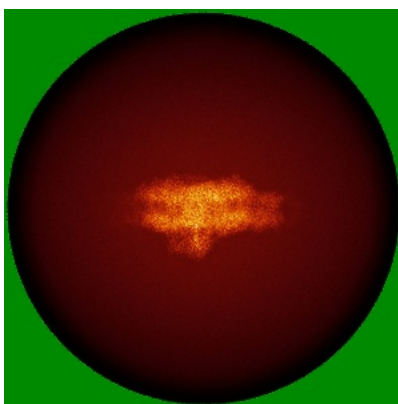
The images above show the largest variance slices of the map in three orthogonal directions.

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

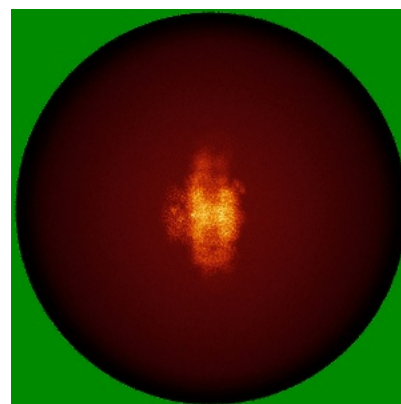
### 6.4.1 Primary map



X

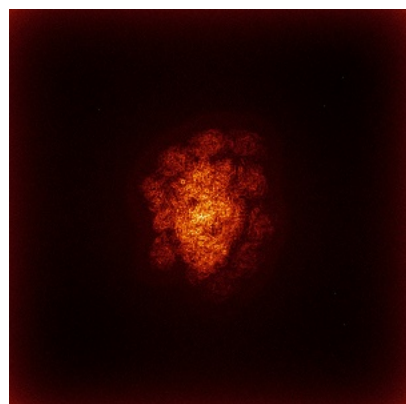


Y



Z

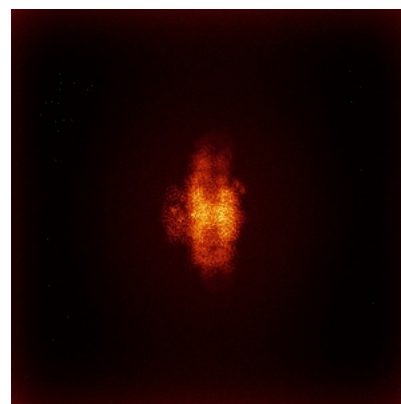
### 6.4.2 Raw map



X



Y



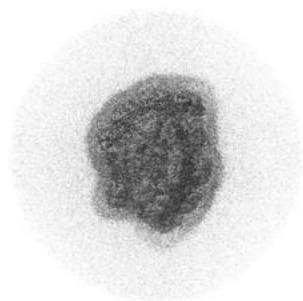
Z

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.

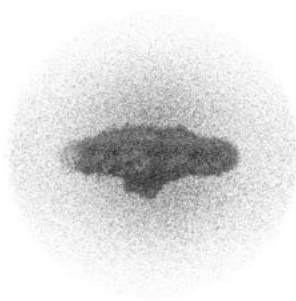


## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



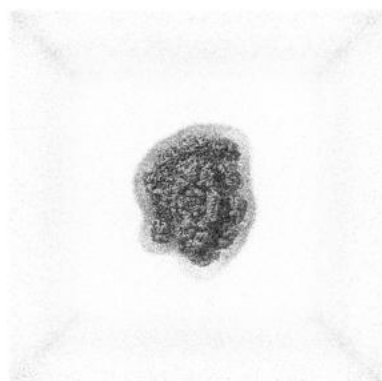
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.065. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

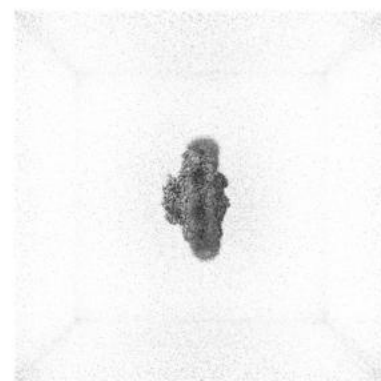
### 6.5.2 Raw map



X



Y



Z

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.

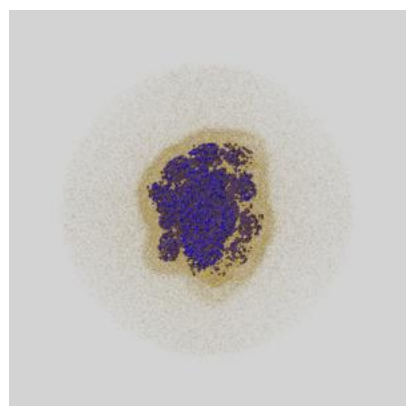
## 6.6 Mask visualisation [i](#)

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

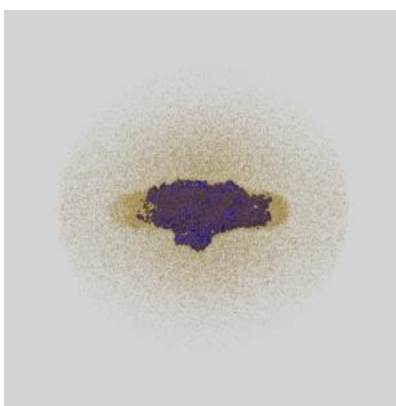
A mask typically either:

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

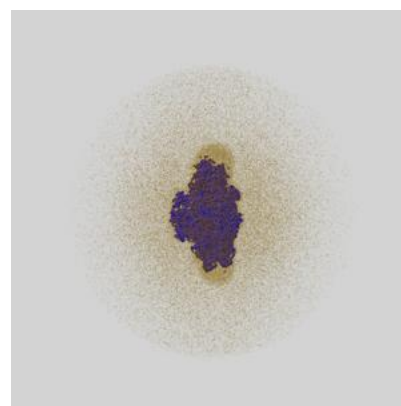
### 6.6.1 emd\_64153\_msk\_1.map [i](#)



X



Y

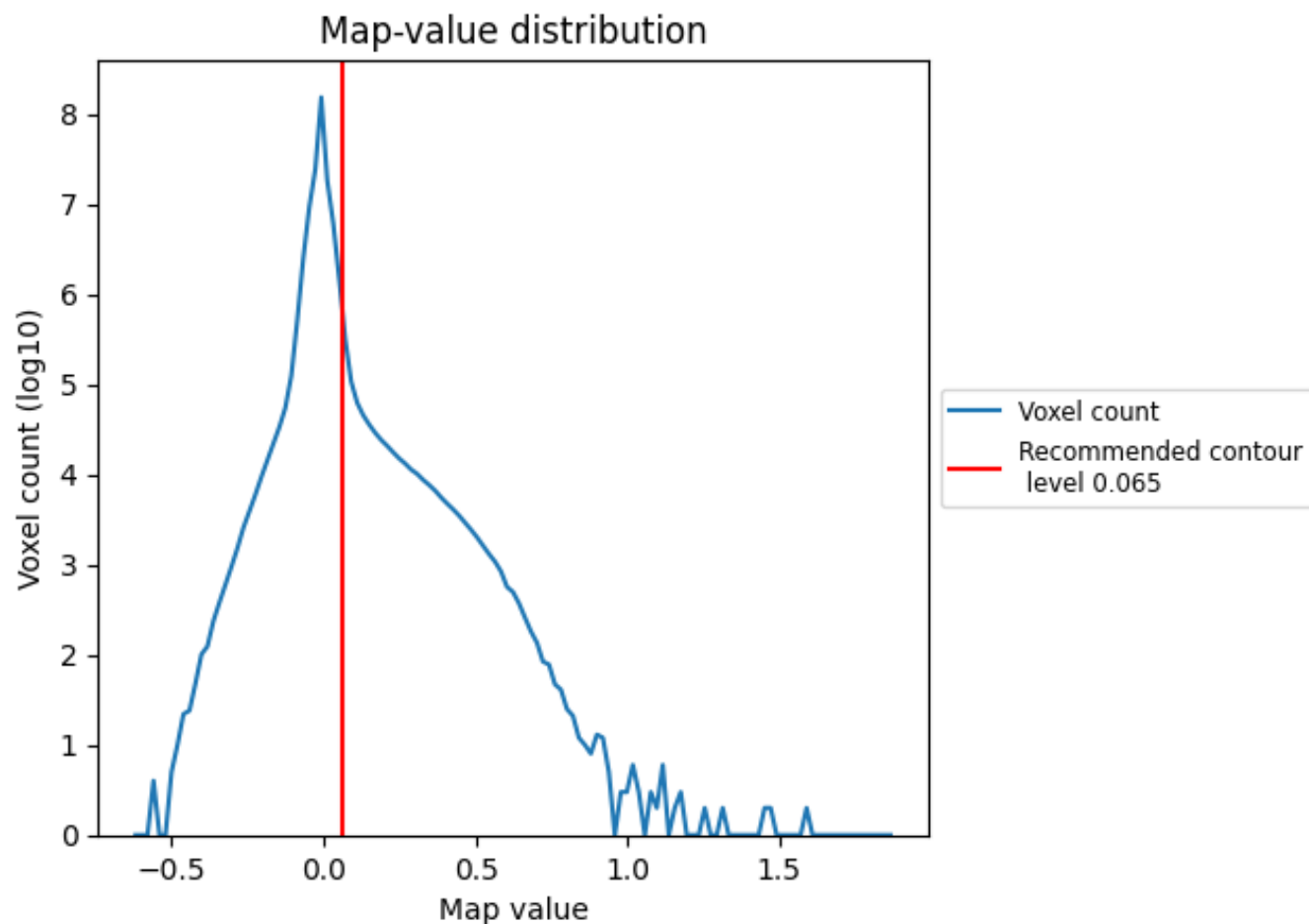


Z

## 7 Map analysis [i](#)

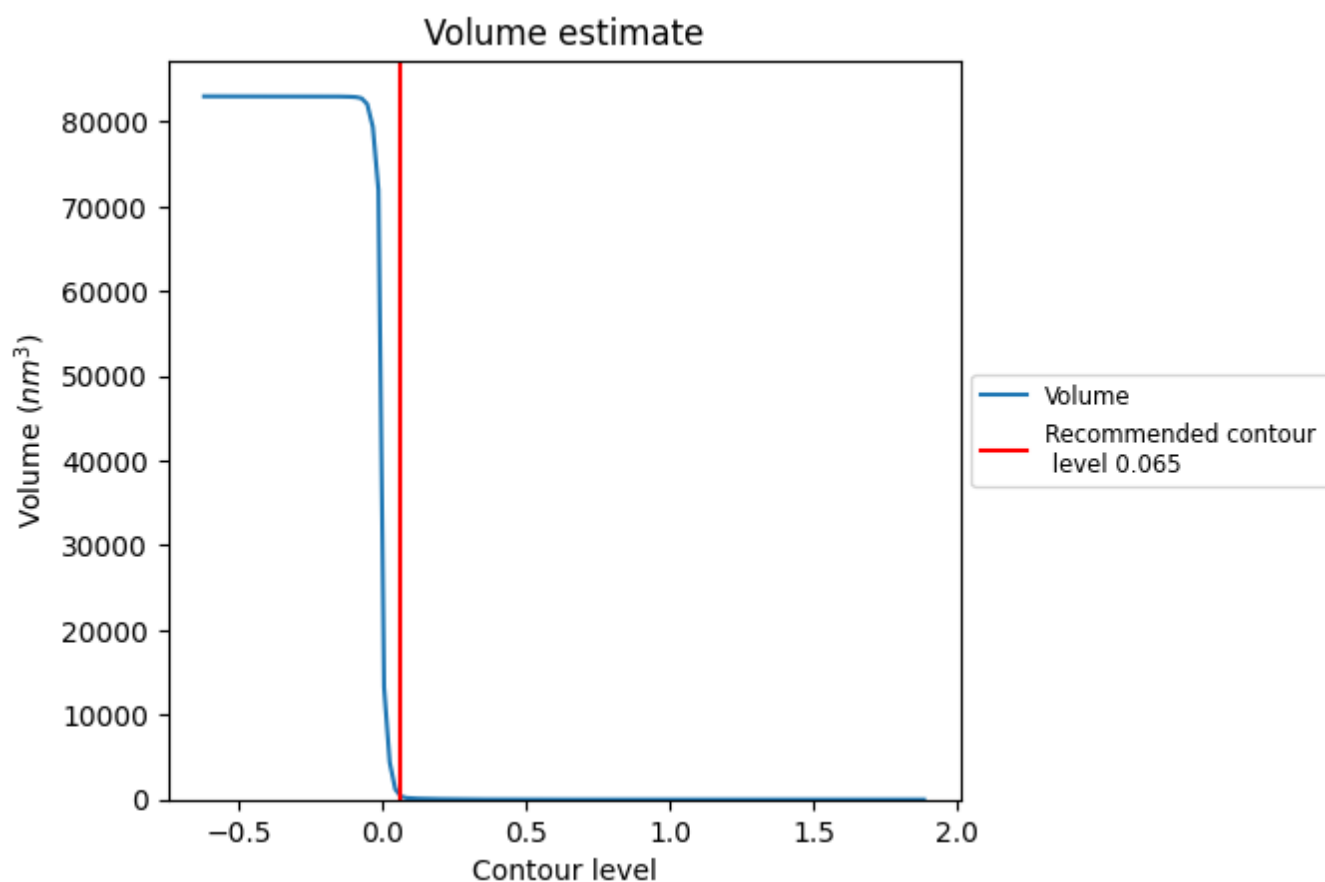
This section contains the results of statistical analysis of the map.

### 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.

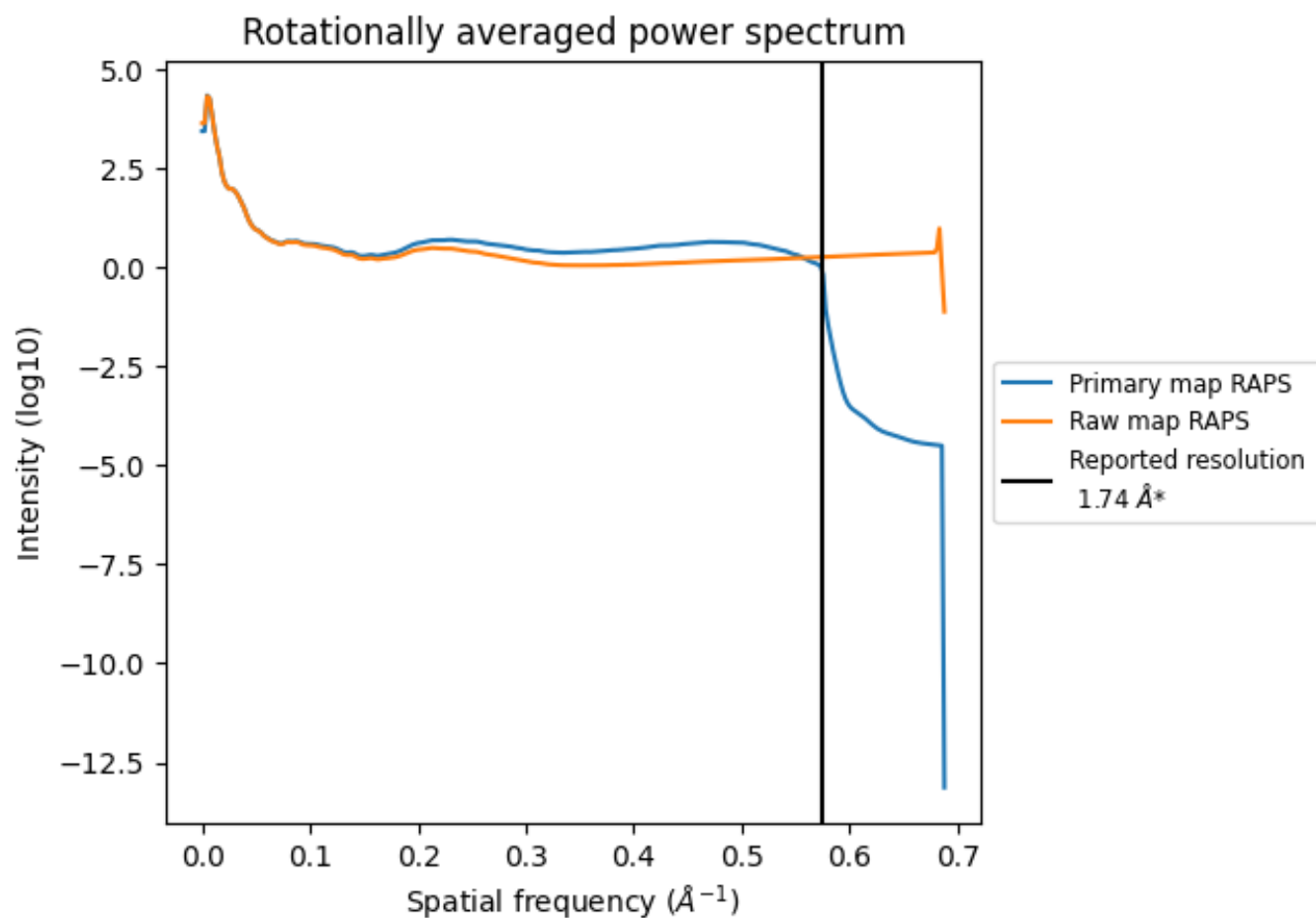
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 416  $\text{nm}^3$ ; this corresponds to an approximate mass of 375 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 ⓘ

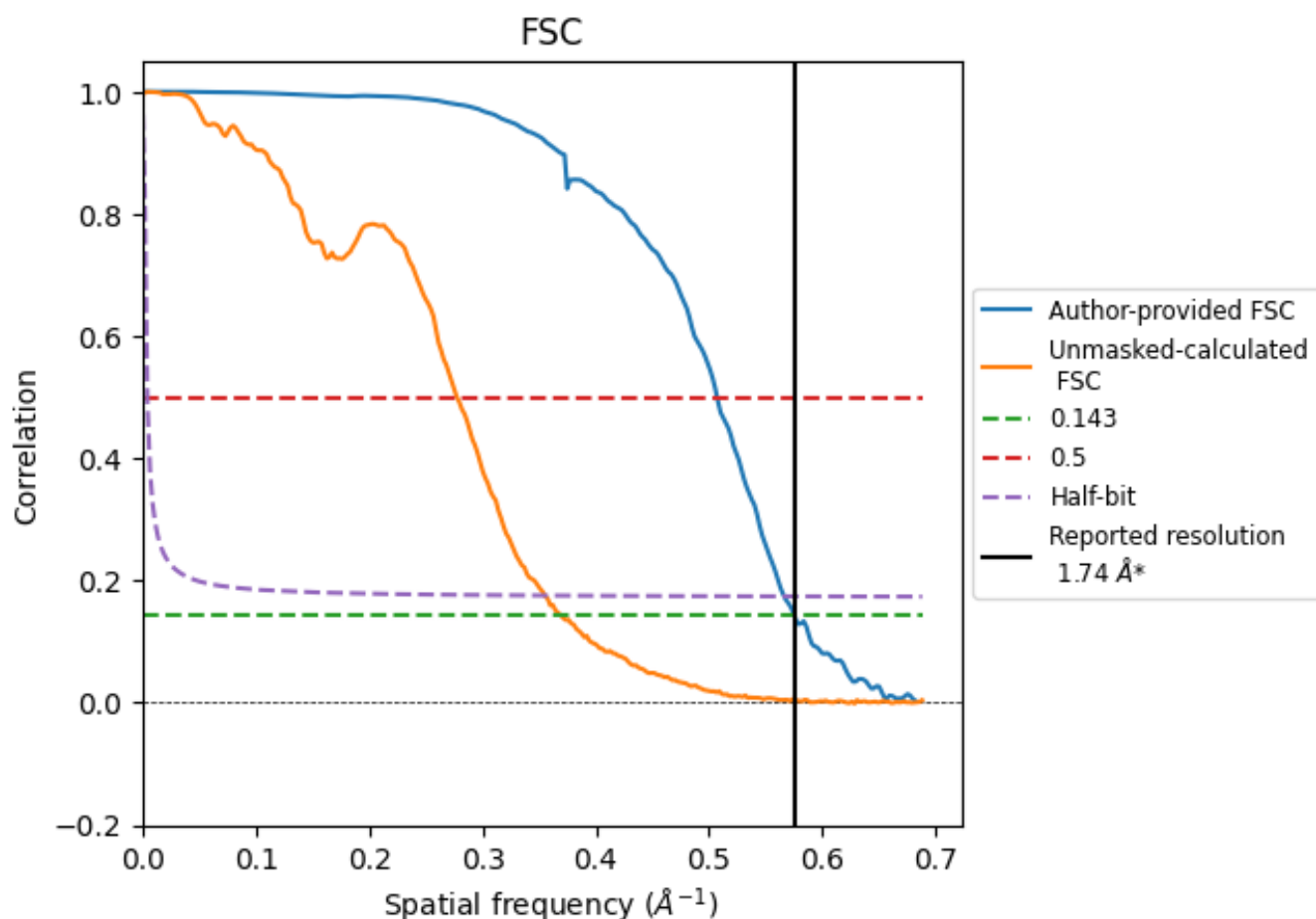


\*Reported resolution corresponds to spatial frequency of 0.575  $\text{\AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.575  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

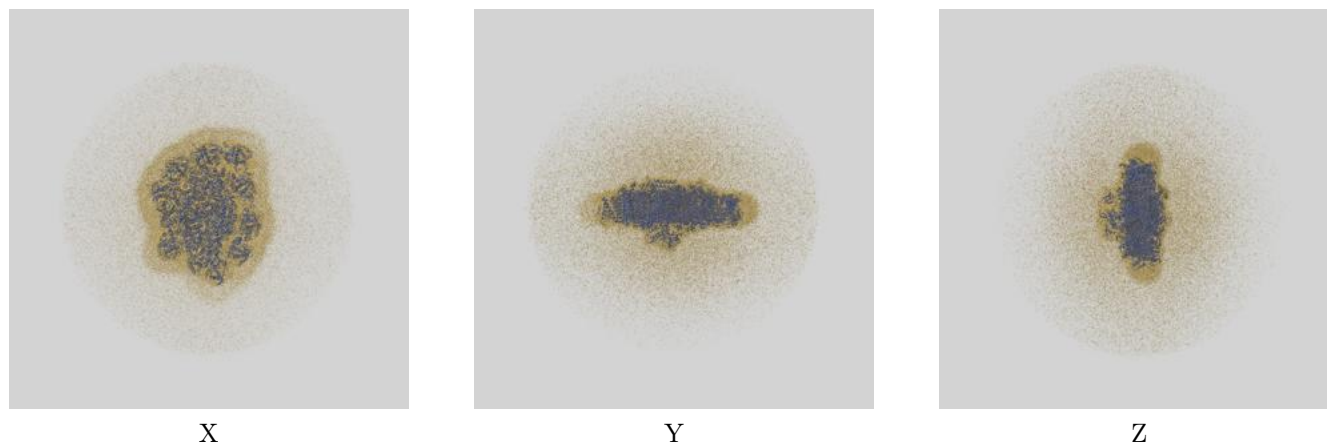
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.74	-	-
Author-provided FSC curve	1.74	1.97	1.77
Unmasked-calculated*	2.71	3.60	2.82

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.71 differs from the reported value 1.74 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-64153 and PDB model 9UH3. Per-residue inclusion information can be found in [section 3](#) on [page 31](#).

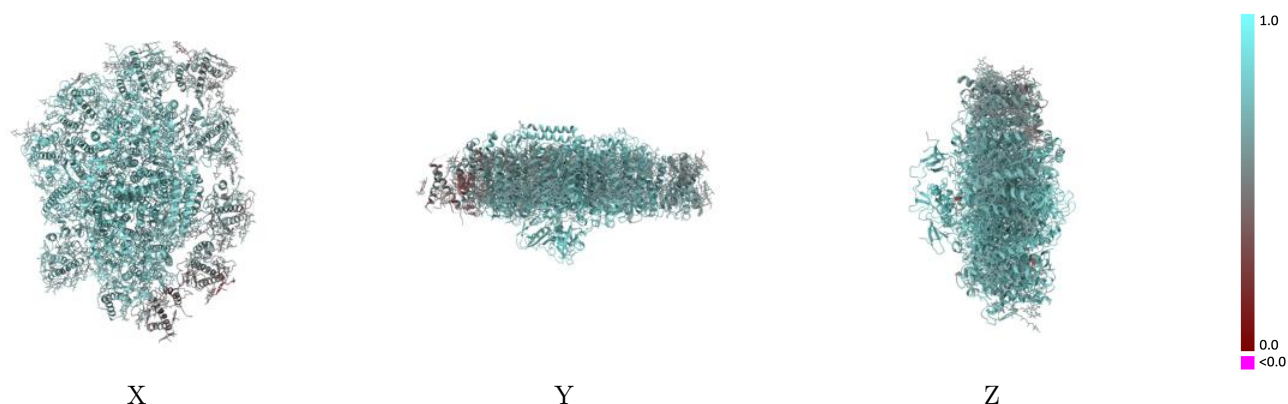
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.065 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.

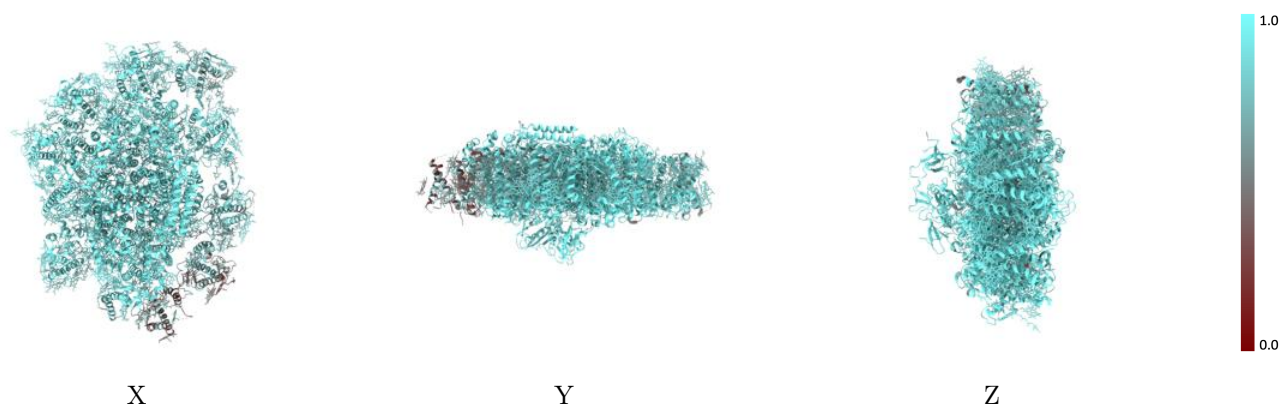


## 9.2 Q-score mapped to coordinate model [i](#)



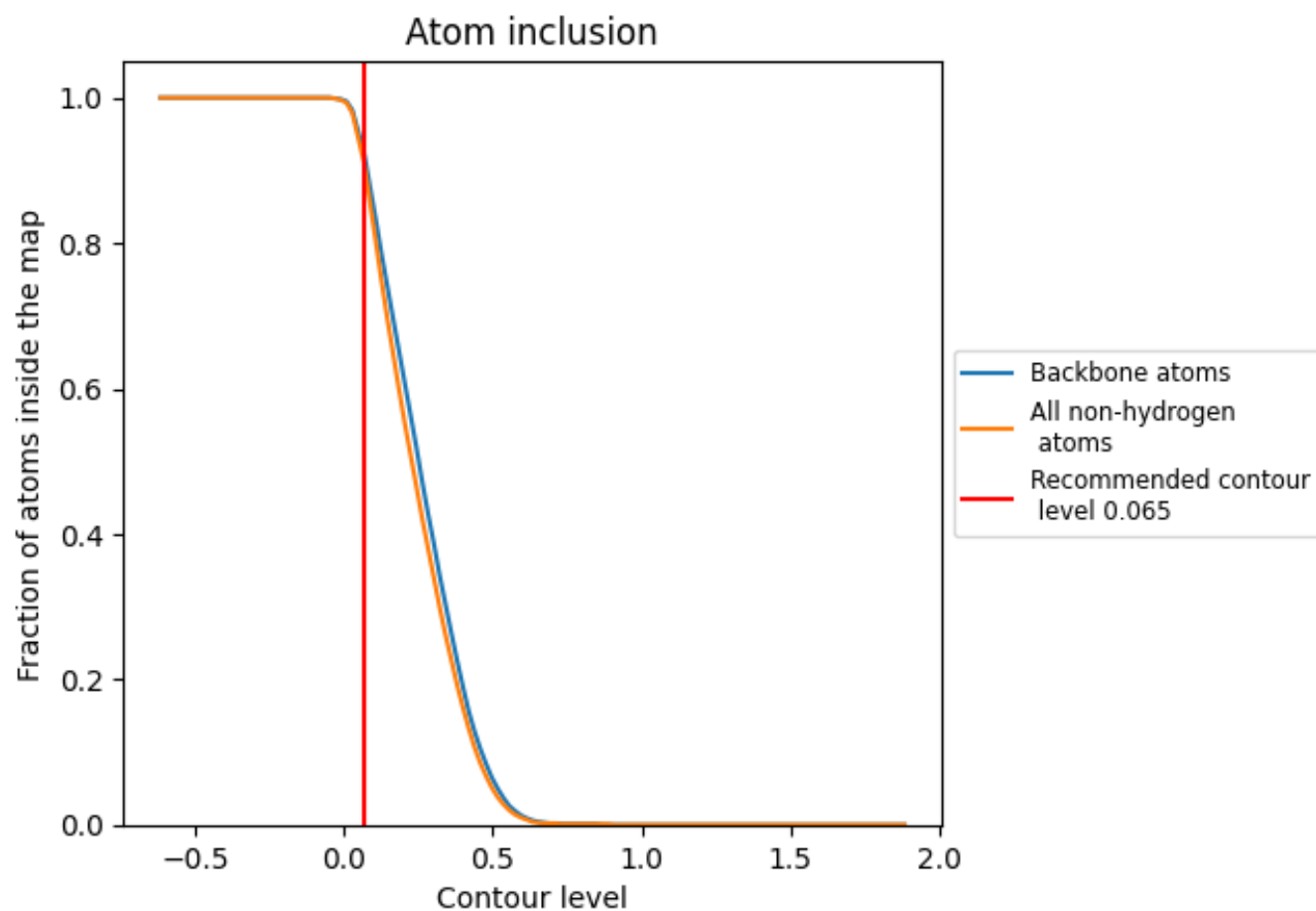
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.065).













































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 91% 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 (0.065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9140	 0.7220
A	 0.9690	 0.7790
B	 0.9840	 0.8090
C	 0.9980	 0.8330
D	 0.9700	 0.7820
E	 0.9520	 0.7730
F	 0.9550	 0.7550
G	 0.7920	 0.5830
H	 0.6390	 0.5150
I	 0.9860	 0.8110
J	 0.9650	 0.7480
K	 0.4900	 0.4410
L	 0.9560	 0.7740
M	 0.9790	 0.7990
O	 0.9340	 0.7160
P	 0.8940	 0.6600
Q	 0.8910	 0.6650
R	 0.9550	 0.7440
S	 0.9440	 0.7330
T	 0.7520	 0.5480
U	 0.8730	 0.6620
k	 0.8200	 0.6270

