



## Full wwPDB EM Validation Report ⓘ

Jun 17, 2026 – 06:42 PM EDT

PDB ID : 9ZJT / pdb\_00009zjt  
EMDB ID : EMD-74341  
Title : PSI-IsiA Complex from Anabaena 7120  
Authors : Mazor, Y.M.; Maqdisi, R.M.; Gorski, C.G.; Pakrasi, H.P.; Biswas, S.B.;  
Niedzwiedzki, D.N.  
Deposited on : 2025-12-05  
Resolution : 2.22 Å(reported)

This is a Full wwPDB EM Validation 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

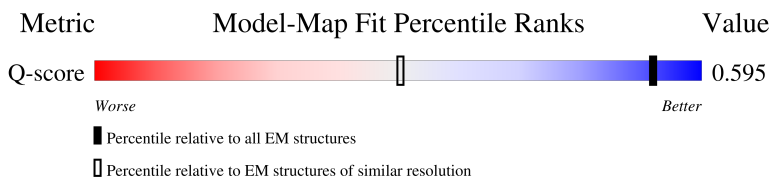
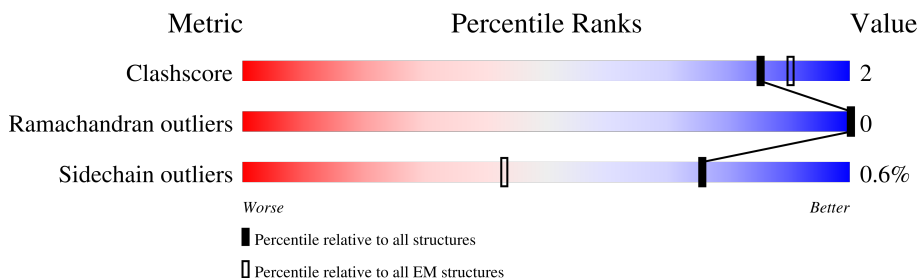
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*


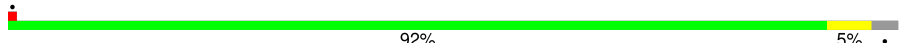
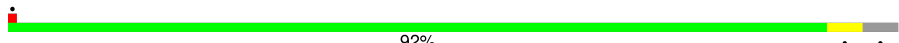

The reported resolution of this entry is 2.22 Å.

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	3277 ( 1.73 - 2.72 )

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	1	476	 91% 7% .
2	2	342	 92% 5% .
3	3	320	 92% . .
4	4	342	 96% .

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Mol	Chain	Length	Quality of chain
4	5	342	
4	6	342	
4	7	342	
5	A	752	
6	B	740	
7	C	81	
8	D	139	
9	E	70	
10	F	164	
11	I	46	
12	J	49	
13	K	84	
14	M	32	
15	X	44	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	LUT	1	518	X	-	-	-

## 2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 49418 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 reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	465	Total	C	N	O	S	0	0
			3583	2375	577	623	8		

- Molecule 2 is a protein called Photosystem II CP43 protein PsbC homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	333	Total	C	N	O	S	0	0
			2607	1742	427	434	4		

- Molecule 3 is a protein called Photosystem II CP43 protein PsbC homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	306	Total	C	N	O	S	0	0
			2394	1595	396	399	4		

- Molecule 4 is a protein called Iron stress-induced chlorophyll-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	341	Total	C	N	O	S	0	0
			2660	1770	440	445	5		
4	5	332	Total	C	N	O	S	0	0
			2593	1728	429	431	5		
4	6	319	Total	C	N	O	S	0	0
			2469	1647	410	408	4		
4	7	314	Total	C	N	O	S	0	0
			2420	1615	401	400	4		

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	742	Total	C	N	O	S	0	0
			5824	3821	1003	979	21		

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A2 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	739	Total	C	N	O	S	0	0
			5919	3906	990	1005	18		

- Molecule 7 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	80	Total	C	N	O	S	0	0
			599	367	103	118	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	135	Total	C	N	O	S	0	0
			1043	668	179	195	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	E	61	Total	C	N	O	0	0
			490	313	84	93		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	141	Total	C	N	O	S	0	0
			1080	690	184	204	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	I	31	Total	C	N	O	0	0
			253	177	35	41		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	J	43	Total	C	N	O	0	0
			347	236	52	59		

- Molecule 13 is a protein called Photosystem I reaction center subunit Psak.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	72	Total	C	N	O	S	0	0
			524	352	82	89	1		

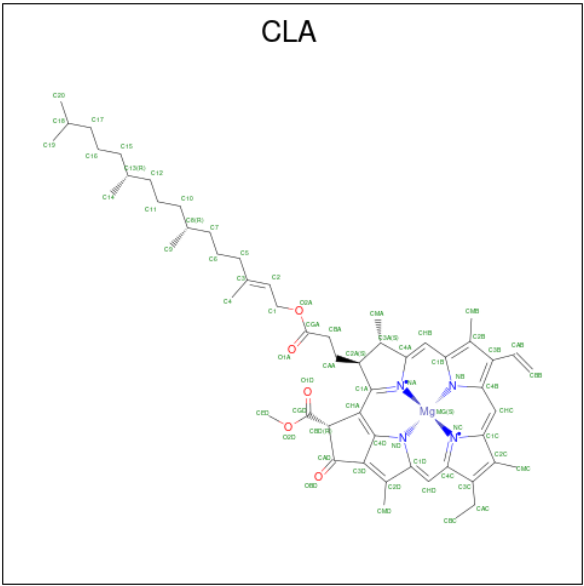
- Molecule 14 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	M	30	Total	C	N	O	0	0
			235	157	36	42		

- Molecule 15 is a protein called Photosystem I 4.8 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	X	29	Total	C	N	O	0	0
			243	170	37	36		

- Molecule 16 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
16	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	6	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	7	1	Total	C	Mg	N	O	0
			44	35	1	3	5	

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Mol	Chain	Residues	Atoms					AltConf
16	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	7	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
16	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	B	1	Total 59	C 49	Mg 1	N 4	O 5	0

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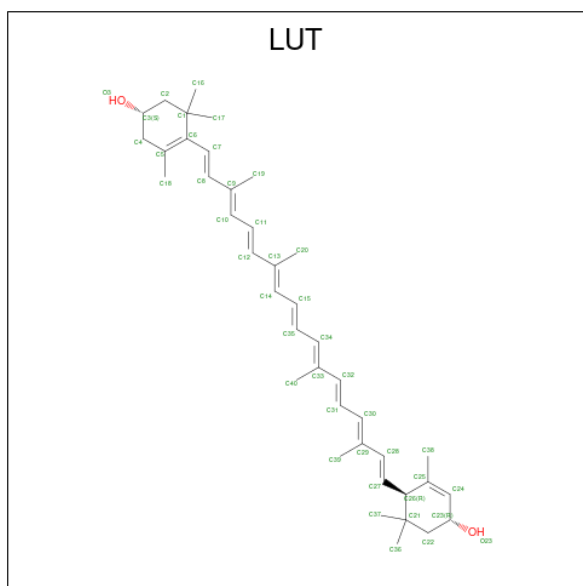
Mol	Chain	Residues	Atoms					AltConf
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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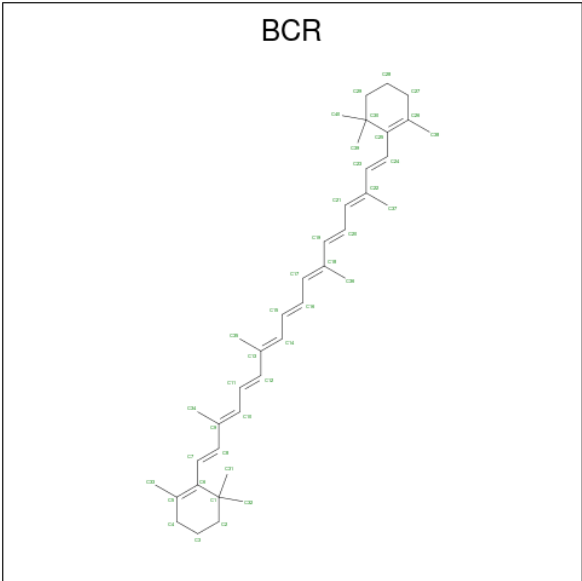
Mol	Chain	Residues	Atoms					AltConf
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	F	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
16	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	K	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 17 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula:  $C_{40}H_{56}O_2$ ).



Mol	Chain	Residues	Atoms			AltConf
17	1	1	Total	C	O	0
			42	40	2	

- Molecule 18 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



Mol	Chain	Residues	Atoms		AltConf
18	1	1	Total	C	0
			40	40	
18	1	1	Total	C	0
			40	40	
18	1	1	Total	C	0
			40	40	
18	1	1	Total	C	0
			40	40	
18	1	1	Total	C	0
			40	40	
18	2	1	Total	C	0
			40	40	
18	2	1	Total	C	0
			40	40	
18	2	1	Total	C	0
			40	40	
18	3	1	Total	C	0
			40	40	
18	3	1	Total	C	0
			40	40	
18	3	1	Total	C	0
			40	40	

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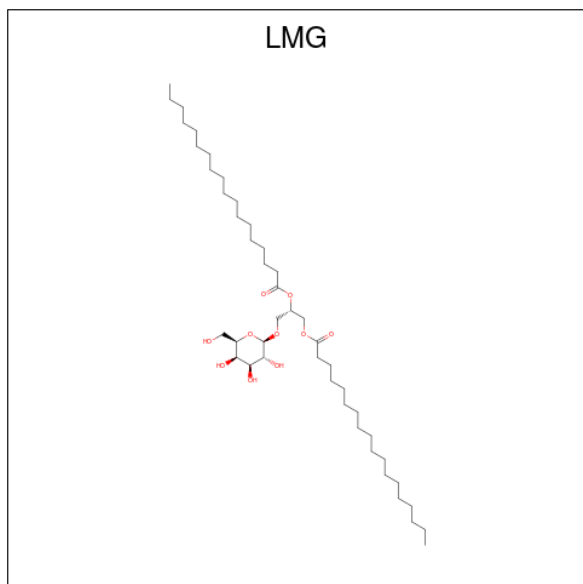
Mol	Chain	Residues	Atoms	AltConf
18	4	1	Total C 40 40	0
18	4	1	Total C 40 40	0
18	5	1	Total C 40 40	0
18	5	1	Total C 40 40	0
18	5	1	Total C 40 40	0
18	5	1	Total C 40 40	0
18	5	1	Total C 40 40	0
18	5	1	Total C 40 40	0
18	6	1	Total C 40 40	0
18	6	1	Total C 40 40	0
18	6	1	Total C 40 40	0
18	6	1	Total C 40 40	0
18	7	1	Total C 40 40	0
18	7	1	Total C 40 40	0
18	A	1	Total C 40 40	0
18	A	1	Total C 40 40	0
18	A	1	Total C 40 40	0
18	A	1	Total C 40 40	0
18	A	1	Total C 40 40	0
18	B	1	Total C 40 40	0
18	B	1	Total C 40 40	0

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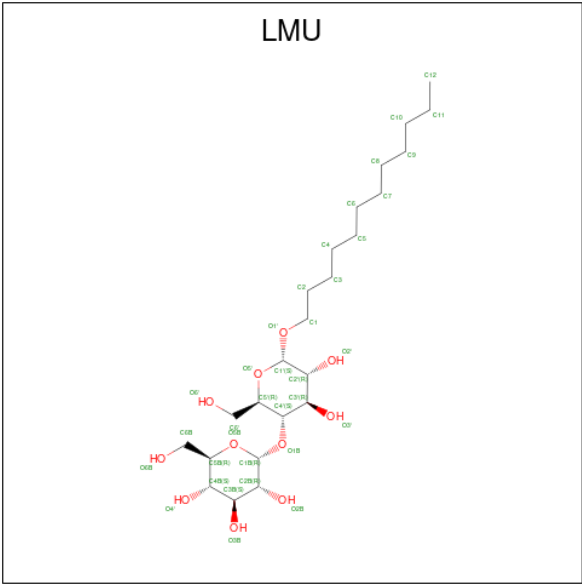
Mol	Chain	Residues	Atoms	AltConf
18	B	1	Total C 40 40	0
18	B	1	Total C 40 40	0
18	B	1	Total C 40 40	0
18	B	1	Total C 40 40	0
18	F	1	Total C 40 40	0
18	F	1	Total C 40 40	0
18	I	1	Total C 40 40	0
18	I	1	Total C 40 40	0
18	J	1	Total C 40 40	0
18	K	1	Total C 40 40	0
18	M	1	Total C 40 40	0

- Molecule 19 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



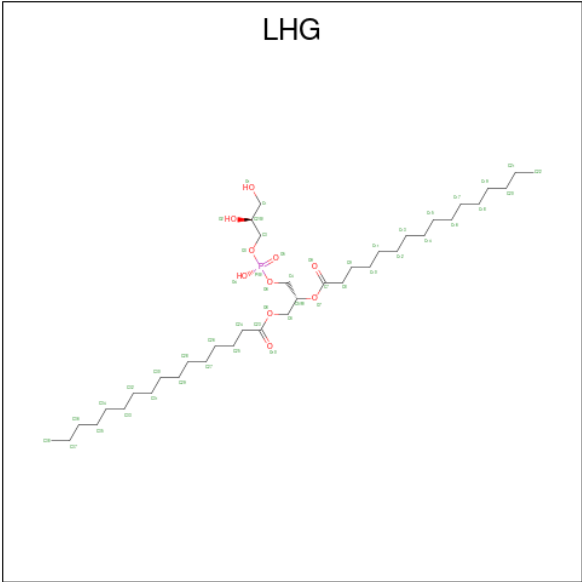
Mol	Chain	Residues	Atoms			AltConf
19	1	1	Total	C	O	0
			40	30	10	
19	5	1	Total	C	O	0
			43	33	10	
19	A	1	Total	C	O	0
			39	29	10	
19	B	1	Total	C	O	0
			54	44	10	

- Molecule 20 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



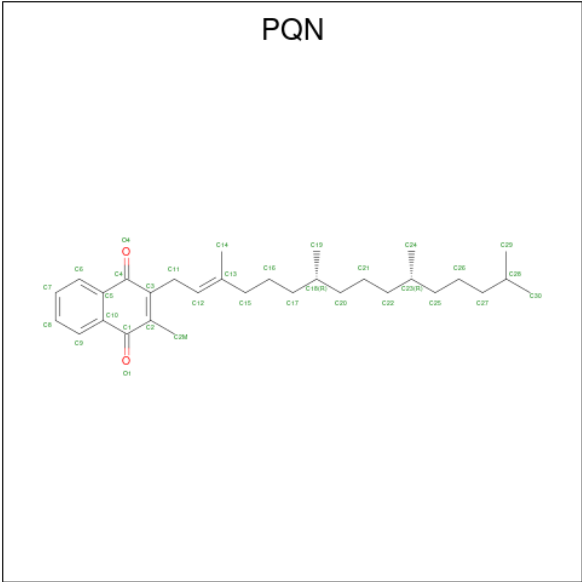
Mol	Chain	Residues	Atoms			AltConf
20	1	1	Total	C	O	0
			35	24	11	
20	4	1	Total	C	O	0
			35	24	11	

- Molecule 21 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



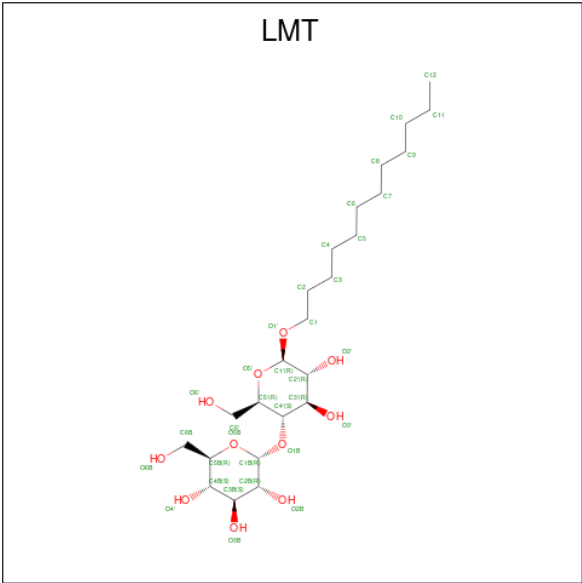
Mol	Chain	Residues	Atoms				AltConf
21	3	1	Total	C	O	P	0
			23	12	10	1	
21	4	1	Total	C	O	P	0
			23	12	10	1	
21	5	1	Total	C	O	P	0
			23	12	10	1	
21	5	1	Total	C	O	P	0
			23	12	10	1	
21	A	1	Total	C	O	P	0
			49	38	10	1	
21	A	1	Total	C	O	P	0
			27	16	10	1	
21	B	1	Total	C	O	P	0
			45	34	10	1	

- Molecule 22 is PHYLLOQUINONE (CCD ID: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>) (labeled as "Lig- and of Interest" by depositor).



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

- Molecule 23 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



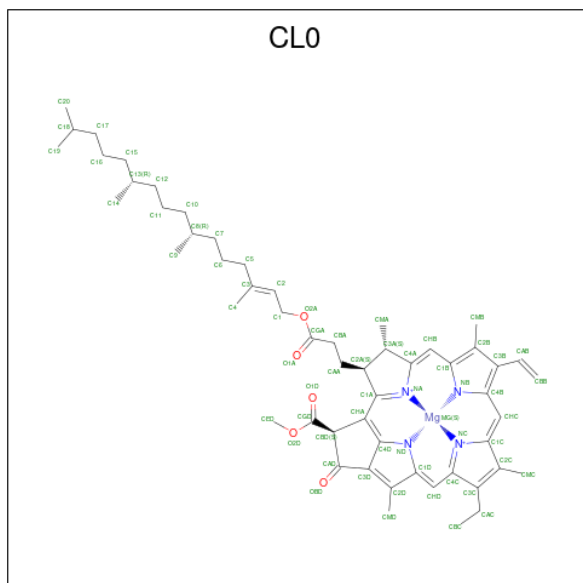
Mol	Chain	Residues	Atoms			AltConf
23	A	1	Total	C	O	0
			35	24	11	
23	B	1	Total	C	O	0
			35	24	11	

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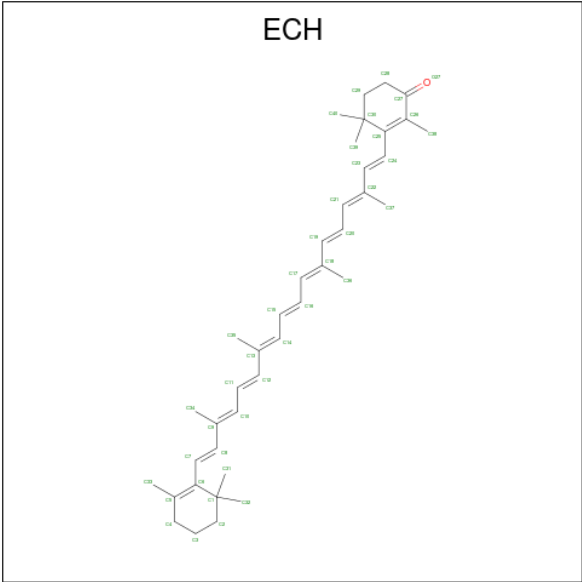
Mol	Chain	Residues	Atoms			AltConf
23	B	1	Total	C	O	0
			35	24	11	
23	I	1	Total	C	O	0
			35	24	11	

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



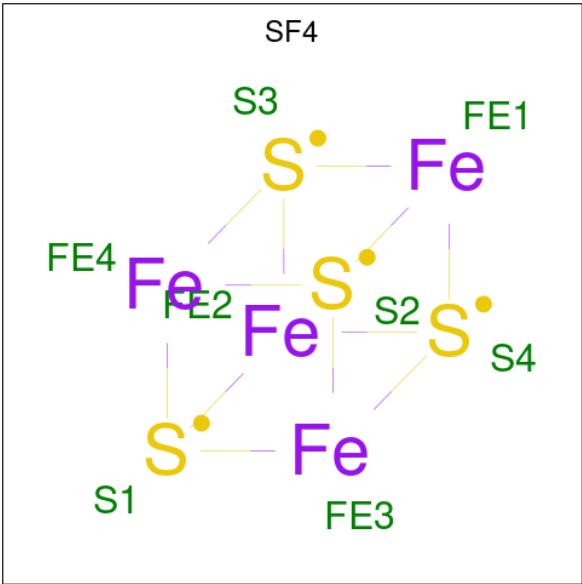
Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 25 is beta,beta-caroten-4-one (CCD ID: ECH) (formula:  $C_{40}H_{54}O$ ).



Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	C	O	0
			41	40	1	
25	A	1	Total	C	O	0
			41	40	1	
25	B	1	Total	C	O	0
			41	40	1	

- Molecule 26 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).

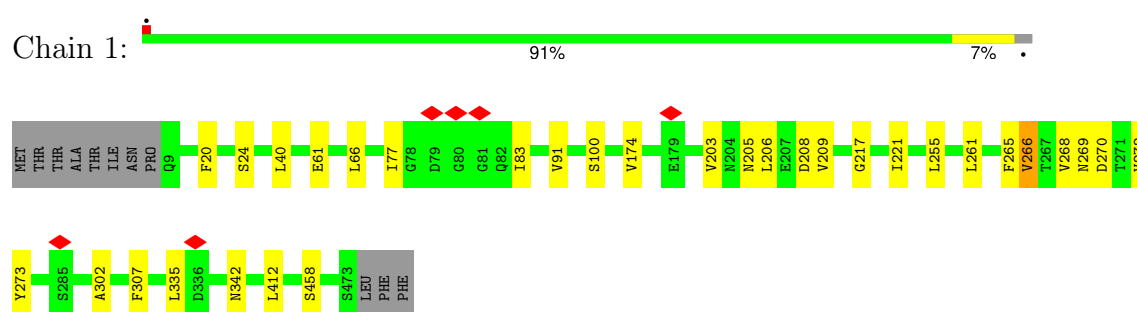


Mol	Chain	Residues	Atoms			AltConf
26	B	1	Total 8	Fe 4	S 4	0
26	C	1	Total 8	Fe 4	S 4	0
26	C	1	Total 8	Fe 4	S 4	0

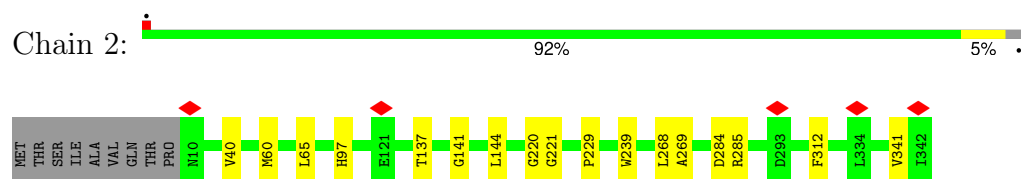
### 3 Residue-property plots

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

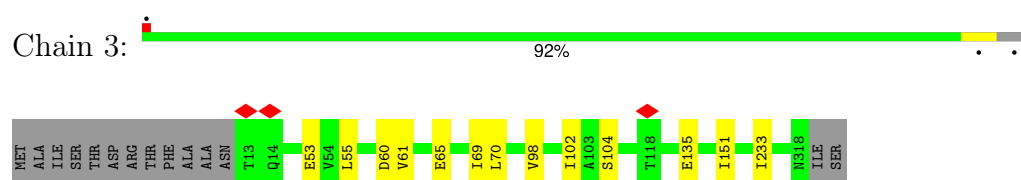
- Molecule 1: Photosystem I reaction center subunit XI



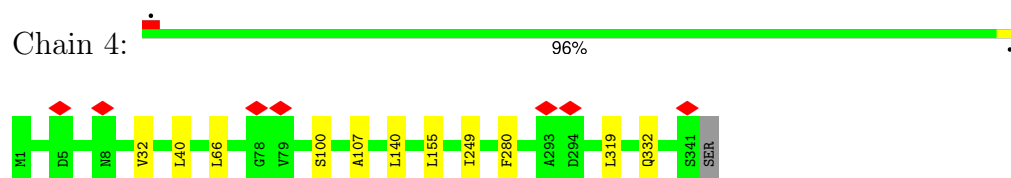
- Molecule 2: Photosystem II CP43 protein PsbC homolog



- Molecule 3: Photosystem II CP43 protein PsbC homolog



- Molecule 4: Iron stress-induced chlorophyll-binding protein



- Molecule 4: Iron stress-induced chlorophyll-binding protein





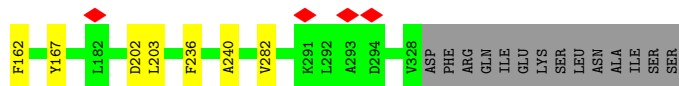
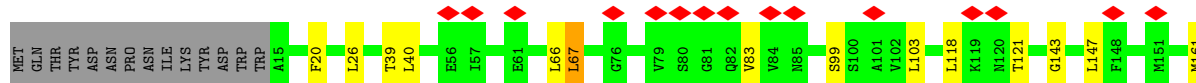
- Molecule 4: Iron stress-induced chlorophyll-binding protein

Chain 6: 89% 7%



- Molecule 4: Iron stress-induced chlorophyll-binding protein

Chain 7: 6% 86% 6% 8%



- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1

Chain A: 96%



- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2 1

Chain B: 95% 5%



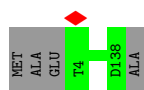
- Molecule 7: Photosystem I iron-sulfur center

Chain C: 99%



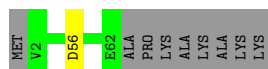
- Molecule 8: Photosystem I reaction center subunit II

Chain D: 97%



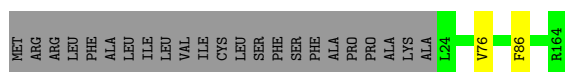
- Molecule 9: Photosystem I reaction center subunit IV

Chain E: 86% 13%



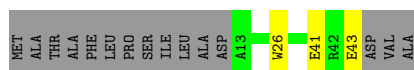
- Molecule 10: Photosystem I reaction center subunit III

Chain F: 85% 14%



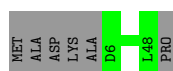
- Molecule 11: Photosystem I reaction center subunit VIII

Chain I: 61% 7% 33%



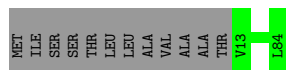
- Molecule 12: Photosystem I reaction center subunit IX

Chain J: 88% 12%



- Molecule 13: Photosystem I reaction center subunit PsaK

Chain K: 86% 14%



- Molecule 14: Photosystem I reaction center subunit XII

Chain M: 94% 6%



- Molecule 15: Photosystem I 4.8 kDa protein

Chain X: 61% 5% 34%

MET	ALA	LYS	ALA	LYS	ILE	SER	PRO	VAL	ALA	ASN	THR	GLY	ALA	LYS	P16	L34	I43	Q44
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	96842	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 ( $e^-/\text{\AA}^2$ )	35	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	34.681	Depositor
Minimum map value	-14.026	Depositor
Average map value	0.021	Depositor
Map value standard deviation	1.154	Depositor
Recommended contour level	4.34	Depositor
Map size ( $\text{\AA}$ )	321.536, 321.536, 321.536	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.628, 0.628, 0.628	Depositor

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, CLA, LHG, LUT, BCR, LMG, ECH, CL0, LMT, PQN, 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	1	0.10	0/3694	0.22	0/5048
2	2	0.09	0/2697	0.21	0/3680
3	3	0.11	0/2471	0.22	0/3379
4	4	0.11	0/2748	0.22	0/3747
4	5	0.12	0/2681	0.25	0/3657
4	6	0.11	0/2550	0.25	0/3476
4	7	0.09	0/2499	0.23	0/3407
5	A	0.12	0/6023	0.23	0/8216
6	B	0.11	0/6143	0.24	0/8398
7	C	0.10	0/609	0.24	0/826
8	D	0.09	0/1067	0.22	0/1441
9	E	0.09	0/499	0.21	0/677
10	F	0.10	0/1104	0.24	0/1500
11	I	0.13	0/262	0.29	0/358
12	J	0.10	0/358	0.20	0/490
13	K	0.10	0/539	0.23	0/739
14	M	0.09	0/239	0.18	0/326
15	X	0.09	0/253	0.22	0/347
All	All	0.11	0/36436	0.23	0/49712

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	3583	0	3560	23	0
2	2	2607	0	2581	10	0
3	3	2394	0	2396	8	0
4	4	2660	0	2643	9	0
4	5	2593	0	2570	8	0
4	6	2469	0	2465	8	0
4	7	2420	0	2414	16	0
5	A	5824	0	5703	17	0
6	B	5919	0	5679	22	0
7	C	599	0	585	0	0
8	D	1043	0	1049	0	0
9	E	490	0	484	1	0
10	F	1080	0	1076	1	0
11	I	253	0	255	4	0
12	J	347	0	352	0	0
13	K	524	0	558	0	0
14	M	235	0	251	0	0
15	X	243	0	244	1	0
16	1	1031	0	941	16	0
16	2	830	0	777	10	0
16	3	730	0	698	5	0
16	4	965	0	930	9	0
16	5	925	0	856	5	0
16	6	915	0	836	3	0
16	7	817	0	649	5	0
16	A	2379	0	2397	22	0
16	B	2493	0	2588	20	0
16	F	96	0	74	0	0
16	J	155	0	138	0	0
16	K	115	0	111	0	0
16	X	45	0	33	0	0
17	1	42	0	55	6	0
18	1	200	0	280	7	0
18	2	120	0	168	1	0
18	3	120	0	168	4	0
18	4	80	0	112	3	0
18	5	240	0	336	1	0
18	6	160	0	224	3	0
18	7	80	0	112	1	0
18	A	200	0	280	3	0
18	B	240	0	336	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	F	80	0	112	1	0
18	I	80	0	112	2	0
18	J	40	0	56	0	0
18	K	40	0	56	2	0
18	M	40	0	56	2	0
19	1	40	0	50	0	0
19	5	43	0	56	0	0
19	A	39	0	48	0	0
19	B	54	0	81	0	0
20	1	35	0	46	1	0
20	4	35	0	46	0	0
21	3	23	0	16	0	0
21	4	23	0	16	0	0
21	5	46	0	32	0	0
21	A	76	0	98	1	0
21	B	45	0	63	1	0
22	A	33	0	46	1	0
22	B	33	0	46	1	0
23	A	35	0	46	0	0
23	B	70	0	92	0	0
23	I	35	0	46	0	0
24	A	65	0	72	6	0
25	A	82	0	108	2	0
25	B	41	0	54	0	0
26	B	8	0	0	0	0
26	C	16	0	0	0	0
All	All	49418	0	49418	218	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 2.

All (218) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1:518:LUT:H371	17:1:518:LUT:H28	1.66	0.75
4:5:291:LYS:HA	4:5:291:LYS:HE2	1.72	0.71
16:A:835:CLA:H143	22:B:803:PQN:H191	1.74	0.69
1:1:272:VAL:HG21	16:1:504:CLA:HMA2	1.76	0.65
4:6:258:TYR:O	4:6:262:VAL:HG22	1.97	0.65
1:1:272:VAL:HG13	1:1:273:TYR:CD1	2.31	0.65
16:A:806:CLA:HBB1	16:A:806:CLA:HMB1	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:831:CLA:HMB1	16:A:831:CLA:HBB1	1.81	0.63
4:7:20:PHE:CG	4:7:26:LEU:HD22	2.34	0.63
1:1:91:VAL:HG23	18:1:519:BCR:H313	1.83	0.58
16:2:414:CLA:HHD	16:2:414:CLA:HBC3	1.84	0.58
16:A:839:CLA:HBB1	16:A:839:CLA:HMB1	1.87	0.57
6:B:49:THR:HG21	16:B:812:CLA:CAB	2.35	0.57
1:1:40:LEU:HD22	18:1:520:BCR:H362	1.86	0.57
4:4:249:ILE:HD12	16:4:410:CLA:HED1	1.86	0.57
16:7:511:CLA:HBB1	16:7:511:CLA:HMB1	1.87	0.56
16:1:517:CLA:HBC1	18:1:522:BCR:H372	1.88	0.56
21:A:803:LHG:HC32	16:A:827:CLA:HMB3	1.88	0.56
16:2:406:CLA:HBB1	16:2:406:CLA:HMB1	1.87	0.56
4:7:143:GLY:O	4:7:147:LEU:HD23	2.06	0.55
16:B:844:CLA:HMB1	16:B:844:CLA:HBB1	1.88	0.55
4:5:214:LEU:HD21	16:5:412:CLA:H93	1.87	0.55
18:M:101:BCR:HC8	18:M:101:BCR:H311	1.88	0.55
16:3:508:CLA:HBB1	16:3:508:CLA:HMB1	1.88	0.54
4:7:26:LEU:HD21	16:7:512:CLA:HMA3	1.89	0.54
4:7:26:LEU:HD23	4:7:26:LEU:O	2.08	0.54
4:4:249:ILE:CD1	16:4:410:CLA:HED1	2.37	0.54
5:A:197:MET:HE1	16:A:828:CLA:H142	1.89	0.54
16:B:846:CLA:HBB1	16:B:846:CLA:HMB1	1.90	0.54
18:4:419:BCR:HC8	18:4:419:BCR:H311	1.91	0.53
1:1:266:VAL:HG23	1:1:273:TYR:CD2	2.42	0.53
5:A:399:GLY:HA3	5:A:603:LEU:HD11	1.89	0.53
4:6:32:VAL:HG13	4:6:107:ALA:HB2	1.89	0.53
4:7:83:VAL:HG23	4:7:83:VAL:O	2.09	0.53
4:7:202:ASP:OD1	4:7:203:LEU:N	2.41	0.53
4:6:172:GLN:OE1	4:6:172:GLN:N	2.41	0.53
24:A:805:CL0:H30	24:A:805:CL0:H36	1.91	0.52
16:4:410:CLA:H2A	16:4:410:CLA:HED3	1.91	0.52
6:B:526:VAL:HG21	6:B:600:TYR:HB2	1.91	0.52
11:I:41:GLU:HA	11:I:41:GLU:OE1	2.10	0.52
20:1:527:LMU:H123	25:A:848:ECH:H33	1.92	0.52
16:1:505:CLA:HBB1	16:1:505:CLA:HMB1	1.91	0.52
5:A:605:ILE:HG13	24:A:805:CL0:H69	1.91	0.52
4:4:32:VAL:HG13	4:4:107:ALA:HB2	1.92	0.51
16:A:852:CLA:HMB1	16:A:852:CLA:HBB1	1.92	0.51
16:1:506:CLA:HBB1	16:1:506:CLA:HMB1	1.93	0.51
1:1:270:ASP:C	1:1:270:ASP:OD2	2.54	0.51
2:2:144:LEU:HG	16:2:409:CLA:HED1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1:507:CLA:HBB1	16:1:507:CLA:HMB1	1.91	0.51
16:A:828:CLA:H171	16:A:828:CLA:H141	1.93	0.51
2:2:268:LEU:HD23	2:2:269:ALA:N	2.25	0.50
6:B:638:LEU:HD22	6:B:731:PHE:HA	1.93	0.50
18:2:418:BCR:HC8	18:2:418:BCR:H311	1.93	0.50
16:A:808:CLA:HBB1	16:A:808:CLA:HMB1	1.93	0.50
4:5:61:GLU:OE2	4:5:61:GLU:N	2.45	0.50
6:B:536:THR:HG21	6:B:589:TRP:CE2	2.46	0.50
1:1:66:LEU:HB3	16:1:503:CLA:HED1	1.93	0.49
5:A:430:VAL:HG11	16:A:841:CLA:H202	1.94	0.49
5:A:121:ILE:HG23	5:A:122:VAL:HG22	1.94	0.49
1:1:268:VAL:HG23	1:1:269:ASN:N	2.28	0.49
6:B:387:MET:HE1	18:B:852:BCR:H361	1.93	0.49
3:3:55:LEU:HD12	4:4:280:PHE:HB2	1.95	0.49
4:4:332:GLN:HA	4:4:332:GLN:OE1	2.12	0.49
6:B:458:LEU:HD22	6:B:621:THR:HG21	1.96	0.48
18:1:521:BCR:H403	18:1:521:BCR:H23C	1.95	0.48
16:5:411:CLA:C15	16:5:412:CLA:HMD2	2.44	0.48
3:3:70:LEU:HD22	16:3:504:CLA:OBD	2.13	0.48
3:3:135:GLU:HA	3:3:135:GLU:OE2	2.13	0.48
4:5:50:ILE:HD11	4:5:89:TYR:HB2	1.95	0.48
22:A:801:PQN:H172	18:F:203:BCR:H382	1.95	0.48
6:B:343:ALA:HB2	18:B:852:BCR:H372	1.94	0.48
16:B:835:CLA:H191	18:B:850:BCR:C32	2.44	0.48
4:4:40:LEU:HD21	16:5:410:CLA:H42	1.94	0.48
4:6:45:PHE:O	4:6:49:GLU:HG3	2.14	0.48
16:B:814:CLA:HHB	16:B:815:CLA:HHB	1.96	0.48
4:7:236:PHE:O	4:7:240:ALA:HB3	2.14	0.48
16:2:408:CLA:HBB1	16:2:408:CLA:HMB1	1.95	0.47
16:B:801:CLA:HBB1	16:B:801:CLA:HMB1	1.95	0.47
16:5:411:CLA:HAA2	16:5:411:CLA:H93	1.96	0.47
16:A:830:CLA:HMB1	16:A:830:CLA:HBB1	1.95	0.47
1:1:203:VAL:HG23	1:1:208:ASP:HB2	1.97	0.47
5:A:538:ILE:HD12	24:A:805:CL0:H62	1.96	0.47
16:4:410:CLA:C15	16:4:411:CLA:HMD2	2.45	0.47
4:5:194:PHE:O	4:5:195:ALA:HB3	2.14	0.47
4:7:40:LEU:C	4:7:40:LEU:HD13	2.40	0.47
5:A:197:MET:HB2	16:A:816:CLA:HBC2	1.96	0.47
16:A:818:CLA:HBB1	16:A:818:CLA:HMB1	1.97	0.47
16:B:829:CLA:HBB1	16:B:829:CLA:HMB1	1.97	0.47
4:6:140:LEU:HD11	16:6:501:CLA:HMA3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:77:ILE:HG22	1:1:174:VAL:HG21	1.96	0.47
4:5:50:ILE:HD11	4:5:89:TYR:CB	2.45	0.47
6:B:697:LEU:C	6:B:697:LEU:HD23	2.41	0.46
18:K:101:BCR:H392	18:K:101:BCR:H23C	1.98	0.46
1:1:255:LEU:HD11	16:1:507:CLA:HED2	1.98	0.46
18:1:521:BCR:C23	18:1:521:BCR:H392	2.45	0.46
16:B:832:CLA:H191	15:X:34:LEU:HD23	1.96	0.46
16:1:506:CLA:HAA2	16:1:507:CLA:HMB3	1.97	0.46
4:7:202:ASP:OD1	4:7:202:ASP:C	2.59	0.46
1:1:412:LEU:HD13	1:1:458:SER:HB2	1.97	0.46
6:B:188:LEU:HD21	18:B:849:BCR:H331	1.97	0.45
16:B:820:CLA:HMB1	16:B:820:CLA:HBB1	1.97	0.45
4:5:45:PHE:O	4:5:49:GLU:HG3	2.16	0.45
18:6:518:BCR:C8	18:6:518:BCR:H321	2.47	0.45
1:1:261:LEU:HD23	16:1:504:CLA:H43	1.99	0.45
18:6:518:BCR:C23	18:6:518:BCR:H403	2.46	0.45
5:A:506:VAL:HG21	16:A:837:CLA:HMA2	1.98	0.45
6:B:438:LEU:HD23	16:B:801:CLA:H92	1.98	0.45
21:B:806:LHG:H381	16:B:832:CLA:H42	1.97	0.45
18:3:515:BCR:H321	18:3:515:BCR:HC8	1.97	0.45
6:B:74:PHE:O	6:B:78:ILE:HD13	2.17	0.45
1:1:307:PHE:CZ	16:1:506:CLA:HMB3	2.52	0.45
6:B:381:TYR:O	6:B:384:ILE:HG13	2.16	0.45
1:1:307:PHE:CE2	16:1:506:CLA:HMB3	2.52	0.45
4:7:67:LEU:HD13	4:7:67:LEU:O	2.17	0.45
18:6:521:BCR:H403	18:6:521:BCR:H23C	1.98	0.45
4:7:99:SER:O	4:7:103:LEU:HG	2.17	0.45
3:3:60:ASP:O	3:3:61:VAL:HG23	2.17	0.44
6:B:434:GLY:HA2	6:B:532:LEU:HD22	1.98	0.44
4:4:319:LEU:HD21	16:4:416:CLA:HMB3	1.98	0.44
18:4:419:BCR:C23	18:4:419:BCR:H403	2.48	0.44
18:5:420:BCR:H311	18:5:420:BCR:C8	2.47	0.44
16:6:506:CLA:HBB1	16:6:506:CLA:HMB1	1.99	0.44
6:B:587:LEU:HD23	6:B:717:LEU:HD21	1.98	0.44
1:1:217:GLY:O	1:1:221:ILE:HG12	2.18	0.44
18:1:523:BCR:H331	18:1:523:BCR:C8	2.47	0.44
5:A:220:VAL:HG13	5:A:240:PRO:HB3	1.99	0.44
24:A:805:CL0:H60	24:A:805:CL0:H53	1.35	0.44
16:B:832:CLA:H152	16:B:841:CLA:H142	1.99	0.44
4:4:66:LEU:HB3	16:4:405:CLA:HED3	2.00	0.44
16:1:509:CLA:H102	17:1:518:LUT:H30	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:414:CLA:HBC3	16:2:414:CLA:CHD	2.47	0.44
3:3:102:ILE:HG21	18:3:514:BCR:C12	2.48	0.43
5:A:91:MET:HE1	16:A:811:CLA:HMA2	1.99	0.43
16:5:404:CLA:CAD	16:5:411:CLA:H92	2.48	0.43
5:A:395:ILE:HG22	5:A:603:LEU:HD13	2.00	0.43
17:1:518:LUT:C28	17:1:518:LUT:H361	2.48	0.43
18:B:853:BCR:H24C	18:B:853:BCR:H371	1.88	0.43
1:1:302:ALA:HB1	17:1:518:LUT:H12	2.01	0.43
18:7:518:BCR:H311	18:7:518:BCR:HC8	2.00	0.43
5:A:222:ALA:HB3	5:A:223:PRO:HD3	2.01	0.43
16:B:837:CLA:H62	16:B:837:CLA:H41	1.81	0.43
16:1:525:CLA:HBB1	16:1:525:CLA:HMB1	2.00	0.43
2:2:137:THR:HG21	2:2:229:PRO:HD3	2.01	0.43
16:7:511:CLA:HMB1	16:7:511:CLA:CBB	2.48	0.43
11:I:26:TRP:HZ2	18:I:102:BCR:H333	1.83	0.43
16:3:504:CLA:H3A	16:3:506:CLA:H142	1.99	0.42
4:5:32:VAL:HG13	4:5:107:ALA:HB2	2.01	0.42
16:1:509:CLA:HBC2	17:1:518:LUT:H392	2.01	0.42
4:6:147:LEU:HD11	4:6:219:ILE:HG13	2.00	0.42
9:E:56:ASP:OD2	9:E:56:ASP:C	2.62	0.42
1:1:335:LEU:HD11	1:1:342:ASN:HB3	2.01	0.42
4:7:118:LEU:O	4:7:121:THR:HG22	2.19	0.42
6:B:481:LEU:O	6:B:482:LEU:HB2	2.20	0.42
6:B:580:TRP:HZ2	6:B:714:VAL:HG22	1.83	0.42
16:3:507:CLA:HBB1	16:3:507:CLA:HMB1	2.01	0.42
5:A:545:VAL:HG11	5:A:598:TRP:CE2	2.54	0.42
16:6:509:CLA:HBB1	16:6:509:CLA:HMB1	2.01	0.42
1:1:206:LEU:O	1:1:209:VAL:HG22	2.19	0.42
16:B:810:CLA:HMB1	16:B:810:CLA:HBB1	2.01	0.42
6:B:189:ALA:HB2	16:B:835:CLA:H193	2.01	0.42
1:1:272:VAL:HG21	16:1:504:CLA:CMA	2.46	0.42
6:B:65:LEU:HD12	6:B:142:LEU:HD12	2.01	0.42
6:B:74:PHE:CZ	6:B:78:ILE:HD11	2.55	0.42
2:2:141:GLY:HA2	2:2:221:GLY:HA2	2.02	0.41
16:4:403:CLA:CAD	16:4:410:CLA:H92	2.49	0.41
16:4:411:CLA:O2A	16:4:411:CLA:C4	2.68	0.41
4:6:294:ASP:OD2	4:6:294:ASP:C	2.62	0.41
5:A:506:VAL:HG13	16:A:837:CLA:HED3	2.02	0.41
18:1:520:BCR:H24C	18:1:520:BCR:H371	1.93	0.41
11:I:43:GLU:HA	11:I:43:GLU:OE2	2.20	0.41
2:2:239:TRP:CD1	2:2:341:VAL:HG22	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:140:LEU:HD11	16:4:402:CLA:HMA3	2.01	0.41
3:3:151:ILE:HD11	3:3:233:ILE:HG13	2.03	0.41
18:4:419:BCR:H23C	18:4:419:BCR:H392	2.03	0.41
4:6:152:ALA:O	4:6:155:LEU:HG	2.20	0.41
3:3:98:VAL:HG13	18:3:516:BCR:H332	2.01	0.41
16:B:832:CLA:H43	16:B:845:CLA:HBA1	2.02	0.41
18:B:853:BCR:H20C	18:B:853:BCR:H361	1.89	0.41
18:I:102:BCR:C8	18:I:102:BCR:H311	2.50	0.41
2:2:40:VAL:HG12	2:2:97:HIS:O	2.21	0.41
16:2:405:CLA:HBB1	16:2:405:CLA:HMB1	2.02	0.41
4:7:161:MET:HE2	4:7:162:PHE:N	2.35	0.41
24:A:805:CL0:H61	16:A:806:CLA:HMA1	2.03	0.41
18:A:845:BCR:H24C	18:A:845:BCR:H371	1.90	0.41
6:B:653:TRP:CZ2	6:B:733:ILE:HG21	2.55	0.41
18:B:804:BCR:H24C	18:B:804:BCR:H371	1.92	0.41
16:B:822:CLA:HMB1	16:B:822:CLA:HBB1	2.03	0.41
2:2:60:MET:HG3	2:2:65:LEU:HD12	2.03	0.41
16:3:506:CLA:HBB1	16:3:506:CLA:HMB1	2.03	0.41
5:A:310:HIS:CE1	18:A:845:BCR:H363	2.56	0.41
10:F:76:VAL:HG12	10:F:86:PHE:HB2	2.02	0.41
4:7:26:LEU:CD2	16:7:512:CLA:HMA3	2.50	0.41
16:A:852:CLA:H43	6:B:442:VAL:HG22	2.02	0.41
18:K:101:BCR:H20C	18:K:101:BCR:H361	1.91	0.41
18:M:101:BCR:H24C	18:M:101:BCR:H371	1.92	0.41
4:7:167:TYR:CD1	4:7:167:TYR:C	2.99	0.41
16:A:809:CLA:HBB1	16:A:809:CLA:HMB1	2.03	0.41
16:B:817:CLA:H2A	16:B:817:CLA:O2A	2.21	0.41
1:1:302:ALA:CB	17:1:518:LUT:H12	2.51	0.40
2:2:284:ASP:O	2:2:285:ARG:C	2.63	0.40
3:3:53:GLU:OE2	3:3:69:ILE:O	2.39	0.40
4:7:282:VAL:O	4:7:282:VAL:HG12	2.21	0.40
5:A:678:PHE:CG	18:A:850:BCR:H363	2.55	0.40
6:B:377:THR:HG23	6:B:598:THR:HG21	2.04	0.40
1:1:20:PHE:HB3	16:1:510:CLA:HED1	2.03	0.40
18:3:516:BCR:C8	18:3:516:BCR:H331	2.51	0.40
16:B:814:CLA:HHC	16:B:814:CLA:HBB1	2.03	0.40
11:I:43:GLU:OE2	11:I:43:GLU:CA	2.69	0.40
5:A:605:ILE:HD12	24:A:805:CL0:H53	2.04	0.40
16:A:844:CLA:HMC2	16:B:847:CLA:H42	2.03	0.40
1:1:40:LEU:HD21	16:2:407:CLA:H43	2.03	0.40
2:2:312:PHE:CZ	16:2:406:CLA:HMB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:406:CLA:HMB1	16:2:406:CLA:CBB	2.51	0.40
16:7:510:CLA:HBB1	16:7:510:CLA:HMB1	2.03	0.40
16:A:828:CLA:H141	16:A:828:CLA:C17	2.50	0.40
25:A:853:ECH:C8	25:A:853:ECH:H32	2.51	0.40
2:2:220:GLY:HA2	16:2:414:CLA:HBC2	2.04	0.40
16:A:807:CLA:H2	16:A:814:CLA:H92	2.03	0.40

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	1	463/476 (97%)	458 (99%)	5 (1%)	0	100	100
2	2	331/342 (97%)	321 (97%)	10 (3%)	0	100	100
3	3	304/320 (95%)	297 (98%)	7 (2%)	0	100	100
4	4	339/342 (99%)	330 (97%)	9 (3%)	0	100	100
4	5	330/342 (96%)	324 (98%)	6 (2%)	0	100	100
4	6	317/342 (93%)	312 (98%)	5 (2%)	0	100	100
4	7	312/342 (91%)	305 (98%)	7 (2%)	0	100	100
5	A	740/752 (98%)	726 (98%)	14 (2%)	0	100	100
6	B	737/740 (100%)	723 (98%)	14 (2%)	0	100	100
7	C	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
8	D	133/139 (96%)	132 (99%)	1 (1%)	0	100	100
9	E	59/70 (84%)	57 (97%)	2 (3%)	0	100	100
10	F	139/164 (85%)	136 (98%)	3 (2%)	0	100	100
11	I	29/46 (63%)	29 (100%)	0	0	100	100
12	J	41/49 (84%)	41 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	K	70/84 (83%)	68 (97%)	2 (3%)	0	100	100
14	M	28/32 (88%)	28 (100%)	0	0	100	100
15	X	27/44 (61%)	27 (100%)	0	0	100	100
All	All	4477/4707 (95%)	4389 (98%)	88 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	1	363/373 (97%)	356 (98%)	7 (2%)	50	64
2	2	263/271 (97%)	263 (100%)	0	100	100
3	3	243/254 (96%)	241 (99%)	2 (1%)	73	84
4	4	264/265 (100%)	262 (99%)	2 (1%)	73	84
4	5	256/265 (97%)	255 (100%)	1 (0%)	84	91
4	6	243/265 (92%)	242 (100%)	1 (0%)	84	91
4	7	237/265 (89%)	234 (99%)	3 (1%)	61	75
5	A	595/605 (98%)	595 (100%)	0	100	100
6	B	601/602 (100%)	598 (100%)	3 (0%)	81	89
7	C	68/69 (99%)	68 (100%)	0	100	100
8	D	108/110 (98%)	108 (100%)	0	100	100
9	E	54/60 (90%)	54 (100%)	0	100	100
10	F	110/129 (85%)	110 (100%)	0	100	100
11	I	28/39 (72%)	28 (100%)	0	100	100
12	J	38/42 (90%)	38 (100%)	0	100	100
13	K	57/66 (86%)	57 (100%)	0	100	100
14	M	25/27 (93%)	25 (100%)	0	100	100
15	X	24/34 (71%)	23 (96%)	1 (4%)	26	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3577/3741 (96%)	3557 (99%)	20 (1%)	76	88

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	24	SER
1	1	61	GLU
1	1	83	ILE
1	1	100	SER
1	1	205	ASN
1	1	265	PHE
1	1	266	VAL
3	3	65	GLU
3	3	104	SER
4	4	100	SER
4	4	155	LEU
4	5	282	VAL
4	6	147	LEU
4	7	39	THR
4	7	66	LEU
4	7	67	LEU
6	B	283	LEU
6	B	319	PHE
6	B	583	PHE
15	X	43	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	22	ASN
1	1	34	HIS
1	1	54	ASN
1	1	96	HIS
1	1	314	HIS
1	1	401	ASN
2	2	10	ASN
2	2	23	HIS
2	2	177	HIS
2	2	193	HIS
2	2	314	GLN
3	3	86	GLN

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Mol	Chain	Res	Type
3	3	114	HIS
3	3	131	GLN
4	4	193	HIS
4	4	221	HIS
4	5	117	ASN
4	6	144	HIS
4	7	144	HIS
5	A	94	HIS
5	A	310	HIS
5	A	627	ASN
5	A	715	GLN
6	B	711	GLN
7	C	16	GLN
8	D	128	GLN
10	F	34	ASN
10	F	38	GLN
15	X	32	ASN
15	X	41	HIS

### 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](#)

274 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	$\# Z  > 2$
16	CLA	4	404	4	49,53,73	1.17	4 (8%)	58,89,113	0.98	2 (3%)
16	CLA	7	515	4	64,70,73	0.94	4 (6%)	74,108,113	0.95	4 (5%)
16	CLA	B	809	6	69,73,73	1.00	4 (5%)	82,113,113	0.91	3 (3%)
16	CLA	7	508	-	54,58,73	1.14	4 (7%)	64,95,113	1.08	5 (7%)
16	CLA	6	510	-	69,73,73	0.99	4 (5%)	82,113,113	0.86	1 (1%)
16	CLA	7	517	-	49,53,73	1.19	4 (8%)	58,89,113	1.06	4 (6%)
16	CLA	A	825	-	61,65,73	1.07	4 (6%)	72,103,113	1.00	3 (4%)
18	BCR	3	515	-	41,41,41	0.29	0	56,56,56	0.67	0
21	LHG	5	425	16	22,22,48	0.70	0	25,28,54	0.63	0
16	CLA	6	515	4	69,73,73	1.00	4 (5%)	82,113,113	0.90	3 (3%)
16	CLA	7	502	-	49,53,73	1.21	5 (10%)	58,89,113	1.00	4 (6%)
16	CLA	5	403	4	49,53,73	1.19	4 (8%)	58,89,113	0.98	2 (3%)
16	CLA	7	507	-	49,53,73	1.19	4 (8%)	58,89,113	1.06	4 (6%)
21	LHG	A	803	16	26,26,48	0.67	0	29,32,54	0.61	0
16	CLA	B	838	6	69,73,73	0.99	4 (5%)	82,113,113	0.95	5 (6%)
16	CLA	3	502	3	59,63,73	1.08	5 (8%)	70,101,113	0.90	2 (2%)
16	CLA	7	503	-	49,53,73	1.19	4 (8%)	58,89,113	1.15	5 (8%)
16	CLA	3	503	3	49,53,73	1.18	4 (8%)	58,89,113	0.92	1 (1%)
16	CLA	6	507	4	69,73,73	0.99	5 (7%)	82,113,113	0.93	4 (4%)
16	CLA	B	834	6	69,73,73	1.00	4 (5%)	82,113,113	0.91	3 (3%)
16	CLA	2	407	2	59,63,73	1.07	5 (8%)	70,101,113	1.08	6 (8%)
16	CLA	4	414	-	49,53,73	1.18	4 (8%)	58,89,113	1.13	3 (5%)
18	BCR	6	521	-	41,41,41	0.30	0	56,56,56	0.45	0
16	CLA	B	819	6	49,53,73	1.18	4 (8%)	58,89,113	0.95	1 (1%)
16	CLA	B	847	-	69,73,73	1.00	4 (5%)	82,113,113	0.96	6 (7%)
16	CLA	B	843	-	49,53,73	1.17	4 (8%)	58,89,113	0.98	1 (1%)
18	BCR	A	847	-	41,41,41	0.29	0	56,56,56	0.44	0
16	CLA	4	408	4	69,73,73	0.99	4 (5%)	82,113,113	0.95	4 (4%)
16	CLA	3	511	3	49,53,73	1.18	4 (8%)	58,89,113	1.03	2 (3%)
16	CLA	5	412	-	69,73,73	1.01	5 (7%)	82,113,113	0.89	3 (3%)
16	CLA	A	819	-	49,53,73	1.19	4 (8%)	58,89,113	0.97	0
16	CLA	6	512	-	49,53,73	1.20	4 (8%)	58,89,113	1.01	3 (5%)
16	CLA	4	416	4	69,73,73	1.00	4 (5%)	82,113,113	0.99	6 (7%)
16	CLA	6	505	4	69,73,73	1.00	5 (7%)	82,113,113	0.98	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	CLA	A	822	5	69,73,73	0.97	4 (5%)	82,113,113	0.92	2 (2%)
16	CLA	A	826	5	55,59,73	1.11	4 (7%)	64,96,113	0.99	4 (6%)
16	CLA	1	526	21	49,53,73	1.18	4 (8%)	58,89,113	0.99	2 (3%)
16	CLA	4	410	4	64,68,73	1.04	4 (6%)	76,107,113	0.90	4 (5%)
16	CLA	A	837	5	55,59,73	1.10	4 (7%)	64,96,113	0.97	3 (4%)
18	BCR	1	519	-	41,41,41	0.27	0	56,56,56	0.61	0
18	BCR	3	516	-	41,41,41	0.29	0	56,56,56	0.52	0
16	CLA	A	810	5	54,58,73	1.11	4 (7%)	64,95,113	0.99	4 (6%)
18	BCR	6	520	-	41,41,41	0.29	0	56,56,56	0.60	0
18	BCR	M	101	-	41,41,41	0.30	0	56,56,56	0.60	0
16	CLA	4	413	4	49,53,73	1.18	4 (8%)	58,89,113	1.05	2 (3%)
16	CLA	7	509	4	64,68,73	1.04	4 (6%)	76,107,113	0.91	3 (3%)
16	CLA	1	511	1	49,53,73	1.20	4 (8%)	58,89,113	1.10	5 (8%)
16	CLA	A	833	5	69,73,73	0.98	5 (7%)	82,113,113	0.89	2 (2%)
16	CLA	B	813	6	69,73,73	0.99	4 (5%)	82,113,113	0.95	4 (4%)
16	CLA	1	515	1	50,54,73	1.16	4 (8%)	59,90,113	0.97	2 (3%)
16	CLA	4	403	4	59,63,73	1.08	4 (6%)	70,101,113	0.93	2 (2%)
16	CLA	B	824	6	63,67,73	1.03	4 (6%)	74,105,113	0.99	5 (6%)
16	CLA	B	829	-	59,63,73	1.08	4 (6%)	70,101,113	0.95	5 (7%)
16	CLA	1	517	-	59,63,73	1.08	4 (6%)	70,101,113	0.96	4 (5%)
16	CLA	B	841	6	69,73,73	0.99	4 (5%)	82,113,113	0.95	3 (3%)
16	CLA	J	1102	12	49,53,73	1.18	4 (8%)	58,89,113	1.00	4 (6%)
16	CLA	3	504	3	69,73,73	1.01	5 (7%)	82,113,113	1.00	6 (7%)
16	CLA	A	827	5	51,55,73	1.15	4 (7%)	60,91,113	0.97	3 (5%)
16	CLA	B	839	6	69,73,73	0.99	4 (5%)	82,113,113	0.92	4 (4%)
16	CLA	2	406	-	69,73,73	1.00	4 (5%)	82,113,113	0.94	3 (3%)
16	CLA	3	512	3	49,53,73	1.20	4 (8%)	58,89,113	0.98	3 (5%)
16	CLA	1	503	-	69,73,73	1.00	4 (5%)	82,113,113	0.86	1 (1%)
16	CLA	B	820	6	69,73,73	0.99	4 (5%)	82,113,113	0.94	3 (3%)
16	CLA	B	826	-	69,73,73	1.00	5 (7%)	82,113,113	0.91	4 (4%)
16	CLA	B	828	6	49,53,73	1.21	4 (8%)	58,89,113	1.03	2 (3%)
16	CLA	A	842	5	69,73,73	0.98	3 (4%)	82,113,113	0.98	4 (4%)
18	BCR	4	419	-	41,41,41	0.31	0	56,56,56	0.56	0
21	LHG	4	421	-	22,22,48	0.69	0	25,28,54	0.66	0
26	SF4	C	102	-	0,12,12	-	-	-	-	-
16	CLA	A	828	-	69,73,73	1.00	3 (4%)	82,113,113	1.03	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	CLA	A	840	5	69,73,73	1.00	5 (7%)	82,113,113	0.95	4 (4%)
16	CLA	B	812	6	69,73,73	0.99	4 (5%)	82,113,113	0.95	4 (4%)
16	CLA	4	411	-	69,73,73	1.00	4 (5%)	82,113,113	0.86	2 (2%)
16	CLA	6	508	4	59,63,73	1.08	4 (6%)	70,101,113	0.98	4 (5%)
16	CLA	6	514	-	49,53,73	1.19	4 (8%)	58,89,113	1.00	1 (1%)
16	CLA	A	841	5	69,73,73	0.98	3 (4%)	82,113,113	0.94	3 (3%)
18	BCR	F	203	-	41,41,41	0.30	0	56,56,56	0.82	1 (1%)
16	CLA	4	409	4	59,63,73	1.08	5 (8%)	70,101,113	1.01	4 (5%)
18	BCR	2	416	-	41,41,41	0.31	0	56,56,56	0.53	0
16	CLA	4	402	4	54,58,73	1.11	4 (7%)	64,95,113	1.01	3 (4%)
16	CLA	A	811	5	69,73,73	0.99	4 (5%)	82,113,113	1.04	5 (6%)
23	LMT	I	103	-	36,36,36	0.52	0	47,47,47	0.70	0
16	CLA	1	525	5	59,63,73	1.07	5 (8%)	70,101,113	0.98	3 (4%)
16	CLA	5	410	21,4	59,63,73	1.07	4 (6%)	70,101,113	1.03	5 (7%)
26	SF4	B	802	-	0,12,12	-	-	-	-	-
16	CLA	2	404	2	69,73,73	0.99	4 (5%)	82,113,113	0.91	2 (2%)
16	CLA	4	406	4	69,73,73	0.99	4 (5%)	82,113,113	1.00	4 (4%)
16	CLA	B	844	6	64,68,73	1.03	3 (4%)	76,107,113	0.99	6 (7%)
16	CLA	A	809	5	69,73,73	1.00	4 (5%)	82,113,113	0.95	3 (3%)
18	BCR	B	854	-	41,41,41	0.30	0	56,56,56	0.68	0
16	CLA	1	516	1	64,68,73	1.02	4 (6%)	76,107,113	0.94	1 (1%)
16	CLA	2	412	-	49,53,73	1.18	4 (8%)	58,89,113	1.00	2 (3%)
16	CLA	1	505	-	64,68,73	1.04	5 (7%)	76,107,113	1.03	6 (7%)
18	BCR	2	418	-	41,41,41	0.28	0	56,56,56	0.52	0
21	LHG	5	424	-	22,22,48	0.71	0	25,28,54	0.63	0
16	CLA	4	417	-	64,68,73	1.04	4 (6%)	76,107,113	0.95	5 (6%)
16	CLA	A	823	5	54,58,73	1.13	5 (9%)	64,95,113	1.06	6 (9%)
16	CLA	B	816	6	69,73,73	0.99	4 (5%)	82,113,113	0.88	1 (1%)
16	CLA	B	835	6	69,73,73	0.99	4 (5%)	82,113,113	0.94	6 (7%)
16	CLA	2	405	2	69,73,73	0.99	4 (5%)	82,113,113	0.98	4 (4%)
16	CLA	3	507	-	59,63,73	1.08	4 (6%)	70,101,113	0.92	3 (4%)
16	CLA	7	505	4	49,53,73	1.19	4 (8%)	58,89,113	0.98	3 (5%)
16	CLA	7	510	-	49,53,73	1.19	4 (8%)	58,89,113	0.98	3 (5%)
16	CLA	5	418	4	49,53,73	1.18	4 (8%)	58,89,113	1.06	5 (8%)
16	CLA	B	814	6	69,73,73	1.01	6 (8%)	82,113,113	0.94	4 (4%)
16	CLA	6	504	4	69,73,73	1.00	5 (7%)	82,113,113	0.98	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	BCR	5	421	-	41,41,41	0.28	0	56,56,56	0.71	0
18	BCR	5	422	-	41,41,41	0.28	0	56,56,56	0.68	2 (3%)
16	CLA	A	852	-	69,73,73	1.00	4 (5%)	82,113,113	0.94	4 (4%)
18	BCR	5	402	-	41,41,41	0.29	0	56,56,56	0.46	0
19	LMG	A	851	-	39,39,55	0.55	0	47,47,63	0.62	0
16	CLA	B	833	6	69,73,73	1.00	4 (5%)	82,113,113	0.90	4 (4%)
16	CLA	A	818	5	49,53,73	1.18	4 (8%)	58,89,113	0.97	3 (5%)
16	CLA	2	414	2	49,53,73	1.18	5 (10%)	58,89,113	1.04	1 (1%)
16	CLA	1	510	1	64,68,73	1.04	4 (6%)	76,107,113	0.98	4 (5%)
20	LMU	4	401	-	36,36,36	0.45	0	47,47,47	0.81	1 (2%)
16	CLA	B	825	6	69,73,73	0.99	4 (5%)	82,113,113	0.92	3 (3%)
16	CLA	4	415	-	69,73,73	1.01	4 (5%)	82,113,113	0.92	4 (4%)
16	CLA	A	843	5	69,73,73	0.99	4 (5%)	82,113,113	0.91	5 (6%)
16	CLA	A	806	-	69,73,73	1.01	4 (5%)	82,113,113	0.93	5 (6%)
16	CLA	2	408	2	64,68,73	1.05	4 (6%)	76,107,113	0.89	3 (3%)
16	CLA	1	506	1	69,73,73	0.99	4 (5%)	82,113,113	0.89	4 (4%)
16	CLA	5	417	4	69,73,73	1.00	5 (7%)	82,113,113	0.94	4 (4%)
16	CLA	6	509	4	64,68,73	1.05	5 (7%)	76,107,113	0.95	2 (2%)
16	CLA	2	410	2	64,68,73	1.04	5 (7%)	76,107,113	1.09	5 (6%)
16	CLA	7	512	4	49,53,73	1.18	4 (8%)	58,89,113	1.05	1 (1%)
25	ECH	A	853	-	42,42,42	0.35	0	55,58,58	0.69	0
16	CLA	B	815	6	69,73,73	0.99	4 (5%)	82,113,113	1.00	4 (4%)
18	BCR	B	853	-	41,41,41	0.29	0	56,56,56	0.44	0
18	BCR	B	850	-	41,41,41	0.29	0	56,56,56	0.54	0
21	LHG	B	806	-	44,44,48	0.53	0	47,50,54	0.51	0
16	CLA	B	846	6	69,73,73	0.99	4 (5%)	82,113,113	0.92	4 (4%)
16	CLA	2	403	-	69,73,73	1.01	4 (5%)	82,113,113	0.93	3 (3%)
18	BCR	A	845	-	41,41,41	0.32	0	56,56,56	0.71	1 (1%)
16	CLA	1	512	-	49,53,73	1.19	4 (8%)	58,89,113	1.01	3 (5%)
18	BCR	K	101	-	41,41,41	0.30	0	56,56,56	0.44	0
16	CLA	F	201	-	55,59,73	1.10	4 (7%)	64,96,113	1.02	5 (7%)
25	ECH	A	848	-	42,42,42	0.35	0	55,58,58	0.71	0
16	CLA	A	832	5	69,73,73	0.99	5 (7%)	82,113,113	0.94	5 (6%)
25	ECH	B	851	-	42,42,42	0.36	0	55,58,58	0.92	2 (3%)
16	CLA	3	508	3	64,68,73	1.04	4 (6%)	76,107,113	0.91	2 (2%)
16	CLA	B	830	6	69,73,73	1.00	4 (5%)	82,113,113	1.02	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	CLA	A	808	5	69,73,73	0.99	4 (5%)	82,113,113	0.96	4 (4%)
16	CLA	5	408	4	64,68,73	1.03	5 (7%)	76,107,113	0.94	1 (1%)
16	CLA	B	801	-	69,73,73	0.99	4 (5%)	82,113,113	0.90	2 (2%)
16	CLA	5	407	4	69,73,73	0.99	4 (5%)	82,113,113	0.90	3 (3%)
16	CLA	6	513	-	49,53,73	1.18	5 (10%)	58,89,113	1.06	4 (6%)
16	CLA	A	812	5	69,73,73	0.98	4 (5%)	82,113,113	0.92	2 (2%)
16	CLA	2	411	2	49,53,73	1.17	4 (8%)	58,89,113	1.02	3 (5%)
16	CLA	6	501	4	54,58,73	1.12	4 (7%)	64,95,113	1.06	5 (7%)
18	BCR	4	420	-	41,41,41	0.29	0	56,56,56	0.54	0
19	LMG	B	805	-	54,54,55	0.50	0	62,62,63	0.57	0
24	CL0	A	805	5	58,73,73	1.87	6 (10%)	60,113,113	1.48	9 (15%)
16	CLA	1	504	1	69,73,73	1.00	4 (5%)	82,113,113	1.00	2 (2%)
16	CLA	2	402	2	49,53,73	1.20	5 (10%)	58,89,113	1.07	3 (5%)
16	CLA	6	506	4	64,68,73	1.02	4 (6%)	76,107,113	0.95	4 (5%)
18	BCR	1	523	-	41,41,41	0.31	0	56,56,56	0.50	0
18	BCR	5	423	-	41,41,41	0.29	0	56,56,56	0.46	0
16	CLA	B	842	-	49,53,73	1.18	4 (8%)	58,89,113	0.97	3 (5%)
20	LMU	1	527	-	36,36,36	0.46	0	47,47,47	0.62	0
16	CLA	5	405	4	49,53,73	1.19	4 (8%)	58,89,113	0.95	0
16	CLA	5	414	4	49,53,73	1.19	4 (8%)	58,89,113	1.07	2 (3%)
16	CLA	B	837	6	69,73,73	0.98	4 (5%)	82,113,113	0.99	5 (6%)
16	CLA	A	814	5,16	69,73,73	0.99	4 (5%)	82,113,113	0.97	4 (4%)
21	LHG	A	802	-	48,48,48	0.51	0	51,54,54	0.49	0
16	CLA	5	419	4	49,53,73	1.18	4 (8%)	58,89,113	1.00	2 (3%)
16	CLA	B	836	6	69,73,73	0.98	4 (5%)	82,113,113	0.98	5 (6%)
18	BCR	I	102	-	41,41,41	0.29	0	56,56,56	0.49	0
23	LMT	B	807	-	36,36,36	0.52	0	47,47,47	0.71	0
22	PQN	A	801	-	34,34,34	0.36	0	43,45,45	0.66	1 (2%)
18	BCR	6	518	-	41,41,41	0.32	0	56,56,56	0.51	0
18	BCR	A	850	-	41,41,41	0.28	0	56,56,56	0.48	0
16	CLA	A	829	-	59,63,73	1.06	4 (6%)	70,101,113	0.95	5 (7%)
16	CLA	A	836	5	69,73,73	0.99	4 (5%)	82,113,113	0.95	5 (6%)
18	BCR	5	420	-	41,41,41	0.32	0	56,56,56	0.68	1 (1%)
16	CLA	5	406	4	69,73,73	1.00	4 (5%)	82,113,113	0.95	5 (6%)
16	CLA	J	1103	12	49,53,73	1.19	4 (8%)	58,89,113	1.03	2 (3%)
16	CLA	K	103	13	69,73,73	1.00	4 (5%)	82,113,113	0.91	3 (3%)
16	CLA	A	807	5,16	58,62,73	1.08	4 (6%)	68,99,113	0.99	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	CLA	4	405	4	69,73,73	0.99	4 (5%)	82,113,113	0.94	3 (3%)
16	CLA	7	516	4	49,53,73	1.20	5 (10%)	58,89,113	1.04	3 (5%)
16	CLA	A	839	5	55,59,73	1.11	4 (7%)	64,96,113	1.00	3 (4%)
18	BCR	3	514	-	41,41,41	0.28	0	56,56,56	0.56	0
17	LUT	1	518	-	42,43,43	0.81	0	51,60,60	1.61	9 (17%)
16	CLA	3	509	-	69,73,73	1.00	5 (7%)	82,113,113	1.02	7 (8%)
16	CLA	5	411	4	64,68,73	1.04	5 (7%)	76,107,113	0.96	5 (6%)
16	CLA	K	102	-	54,58,73	1.12	4 (7%)	64,95,113	1.01	4 (6%)
16	CLA	4	412	4	54,58,73	1.13	4 (7%)	64,95,113	1.01	3 (4%)
23	LMT	B	808	-	36,36,36	0.53	0	47,47,47	0.78	1 (2%)
16	CLA	B	832	-	69,73,73	0.98	4 (5%)	82,113,113	0.91	3 (3%)
16	CLA	5	409	4	69,73,73	1.00	4 (5%)	82,113,113	0.93	5 (6%)
23	LMT	A	804	-	36,36,36	0.53	0	47,47,47	0.74	0
16	CLA	A	821	5	58,62,73	1.07	5 (8%)	68,99,113	0.97	3 (4%)
16	CLA	7	504	4	49,53,73	1.19	4 (8%)	58,89,113	0.99	2 (3%)
16	CLA	2	413	2	64,68,73	1.04	4 (6%)	76,107,113	0.98	4 (5%)
19	LMG	5	426	-	43,43,55	0.54	0	51,51,63	0.64	0
21	LHG	3	517	-	22,22,48	0.70	0	25,28,54	0.64	0
16	CLA	3	505	3	69,73,73	0.99	5 (7%)	82,113,113	1.00	3 (3%)
16	CLA	A	816	5	69,73,73	0.99	5 (7%)	82,113,113	0.97	4 (4%)
16	CLA	A	838	5	59,63,73	1.08	4 (6%)	70,101,113	0.96	4 (5%)
16	CLA	1	502	1	59,63,73	1.09	4 (6%)	70,101,113	0.89	3 (4%)
16	CLA	A	835	5	69,73,73	1.00	5 (7%)	82,113,113	0.97	4 (4%)
16	CLA	B	818	6	69,73,73	1.01	4 (5%)	82,113,113	0.91	1 (1%)
16	CLA	1	509	1	64,68,73	1.03	4 (6%)	76,107,113	0.94	3 (3%)
16	CLA	2	415	2	49,53,73	1.17	4 (8%)	58,89,113	1.03	2 (3%)
16	CLA	B	845	-	69,73,73	0.98	4 (5%)	82,113,113	0.91	4 (4%)
19	LMG	1	524	-	40,40,55	0.56	0	48,48,63	0.62	0
18	BCR	1	520	-	41,41,41	0.28	0	56,56,56	0.68	1 (1%)
16	CLA	6	502	4	54,58,73	1.11	4 (7%)	64,95,113	1.02	5 (7%)
16	CLA	1	514	1	54,58,73	1.14	4 (7%)	64,95,113	0.94	5 (7%)
16	CLA	5	404	4	54,58,73	1.12	4 (7%)	64,95,113	0.99	4 (6%)
18	BCR	6	519	-	41,41,41	0.31	0	56,56,56	0.43	0
16	CLA	A	831	5	69,73,73	1.00	5 (7%)	82,113,113	0.93	5 (6%)
18	BCR	A	849	-	41,41,41	0.29	0	56,56,56	0.61	0
18	BCR	A	846	-	41,41,41	0.28	0	56,56,56	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	BCR	B	804	-	41,41,41	0.29	0	56,56,56	0.53	0
18	BCR	1	521	-	41,41,41	0.30	0	56,56,56	0.58	1 (1%)
16	CLA	4	418	4	49,53,73	1.19	5 (10%)	58,89,113	1.06	5 (8%)
18	BCR	2	417	-	41,41,41	0.28	0	56,56,56	0.54	0
16	CLA	B	810	-	69,73,73	1.00	5 (7%)	82,113,113	0.97	4 (4%)
16	CLA	3	506	-	69,73,73	1.00	3 (4%)	82,113,113	0.87	4 (4%)
16	CLA	1	508	-	69,73,73	1.01	4 (5%)	82,113,113	1.03	6 (7%)
16	CLA	6	511	4	49,53,73	1.18	5 (10%)	58,89,113	0.96	2 (3%)
16	CLA	4	407	4	69,73,73	0.99	5 (7%)	82,113,113	1.03	5 (6%)
16	CLA	6	517	4	49,53,73	1.18	4 (8%)	58,89,113	1.06	3 (5%)
18	BCR	F	204	-	41,41,41	0.29	0	56,56,56	0.49	0
16	CLA	5	413	4	64,68,73	1.05	5 (7%)	76,107,113	0.99	5 (6%)
16	CLA	3	513	3	49,53,73	1.18	4 (8%)	58,89,113	0.96	1 (1%)
16	CLA	A	830	5	69,73,73	1.01	4 (5%)	82,113,113	0.92	5 (6%)
16	CLA	J	1101	5	69,73,73	1.00	4 (5%)	82,113,113	0.84	3 (3%)
16	CLA	A	813	5	59,63,73	1.06	4 (6%)	70,101,113	1.04	4 (5%)
16	CLA	6	503	4	49,53,73	1.18	4 (8%)	58,89,113	0.98	0
16	CLA	1	501	1	49,53,73	1.18	4 (8%)	58,89,113	0.96	2 (3%)
18	BCR	5	401	-	41,41,41	0.29	0	56,56,56	0.70	0
16	CLA	7	514	-	49,53,73	1.19	4 (8%)	58,89,113	1.04	2 (3%)
16	CLA	A	834	5	64,68,73	1.03	4 (6%)	76,107,113	0.88	2 (2%)
18	BCR	1	522	-	41,41,41	0.30	0	56,56,56	0.74	0
16	CLA	A	844	-	69,73,73	0.98	4 (5%)	82,113,113	1.02	5 (6%)
16	CLA	B	822	6	49,53,73	1.18	4 (8%)	58,89,113	0.98	3 (5%)
16	CLA	A	815	5	64,68,73	1.03	5 (7%)	76,107,113	1.08	7 (9%)
16	CLA	B	821	6	60,64,73	1.06	4 (6%)	71,102,113	0.98	5 (7%)
18	BCR	I	101	-	41,41,41	0.30	0	56,56,56	0.66	0
16	CLA	B	840	6	62,66,73	1.04	4 (6%)	73,104,113	0.92	1 (1%)
26	SF4	C	101	-	0,12,12	-	-	-	-	-
16	CLA	7	501	-	49,53,73	1.22	5 (10%)	58,89,113	0.99	2 (3%)
16	CLA	3	510	3	59,63,73	1.09	4 (6%)	70,101,113	1.06	5 (7%)
16	CLA	7	506	4	64,68,73	1.06	5 (7%)	76,107,113	0.94	4 (5%)
16	CLA	3	501	3	69,73,73	1.00	4 (5%)	82,113,113	0.98	3 (3%)
16	CLA	7	511	4	41,50,73	1.40	3 (7%)	49,79,113	1.22	2 (4%)
16	CLA	2	401	2	59,63,73	1.08	5 (8%)	70,101,113	0.92	3 (4%)
16	CLA	5	415	-	49,53,73	1.19	4 (8%)	58,89,113	1.00	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	CLA	7	513	-	49,53,73	1.19	5 (10%)	58,89,113	1.10	4 (6%)
16	CLA	B	817	6	64,68,73	1.04	4 (6%)	76,107,113	0.90	2 (2%)
18	BCR	B	849	-	41,41,41	0.32	0	56,56,56	0.85	3 (5%)
16	CLA	B	848	6	69,73,73	0.98	3 (4%)	82,113,113	1.07	6 (7%)
16	CLA	B	823	6	59,63,73	1.06	4 (6%)	70,101,113	1.00	4 (5%)
16	CLA	1	507	1	49,53,73	1.17	5 (10%)	58,89,113	0.98	3 (5%)
16	CLA	6	516	4	49,53,73	1.16	4 (8%)	58,89,113	0.99	1 (1%)
16	CLA	1	513	1	49,53,73	1.19	4 (8%)	58,89,113	0.99	1 (1%)
16	CLA	B	827	6	60,64,73	1.07	4 (6%)	71,102,113	0.92	4 (5%)
16	CLA	B	811	6	58,62,73	1.07	4 (6%)	68,99,113	0.94	2 (2%)
16	CLA	A	817	5	59,63,73	1.07	5 (8%)	70,101,113	0.96	3 (4%)
16	CLA	2	409	-	59,63,73	1.08	4 (6%)	70,101,113	1.01	3 (4%)
16	CLA	A	820	5	58,62,73	1.08	4 (6%)	68,99,113	0.97	4 (5%)
16	CLA	X	101	15	49,53,73	1.19	4 (8%)	58,89,113	0.99	2 (3%)
18	BCR	B	852	-	41,41,41	0.28	0	56,56,56	0.68	0
18	BCR	J	1104	-	41,41,41	0.29	0	56,56,56	0.64	0
18	BCR	7	519	-	41,41,41	0.29	0	56,56,56	0.51	0
18	BCR	7	518	-	41,41,41	0.30	0	56,56,56	0.44	0
22	PQN	B	803	-	34,34,34	0.37	0	43,45,45	0.69	1 (2%)
16	CLA	F	202	-	49,53,73	1.18	4 (8%)	58,89,113	0.94	2 (3%)
16	CLA	B	831	6	69,73,73	1.00	5 (7%)	82,113,113	0.95	3 (3%)
16	CLA	5	416	-	49,53,73	1.18	4 (8%)	58,89,113	1.04	2 (3%)
16	CLA	A	824	-	69,73,73	0.97	4 (5%)	82,113,113	0.95	4 (4%)

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
16	CLA	4	404	4	-	2/15/91/115	-
16	CLA	7	515	4	-	12/33/109/115	-
16	CLA	B	809	6	-	7/39/115/115	-
16	CLA	7	508	-	-	10/21/97/115	-
16	CLA	6	510	-	-	9/39/115/115	-
16	CLA	7	517	-	-	4/15/91/115	-
16	CLA	A	825	-	-	2/30/106/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	3	515	-	-	10/29/63/63	0/2/2/2
21	LHG	5	425	16	-	2/27/27/53	-
16	CLA	6	515	4	-	11/39/115/115	-
16	CLA	7	502	-	-	5/15/91/115	-
16	CLA	5	403	4	-	4/15/91/115	-
16	CLA	7	507	-	-	6/15/91/115	-
21	LHG	A	803	16	-	5/31/31/53	-
16	CLA	B	838	6	-	9/39/115/115	-
16	CLA	3	502	3	-	4/27/103/115	-
16	CLA	7	503	-	-	5/15/91/115	-
16	CLA	3	503	3	-	4/15/91/115	-
16	CLA	6	507	4	-	12/39/115/115	-
16	CLA	B	834	6	-	9/39/115/115	-
16	CLA	2	407	2	-	11/27/103/115	-
16	CLA	4	414	-	-	7/15/91/115	-
18	BCR	6	521	-	-	8/29/63/63	0/2/2/2
16	CLA	B	819	6	-	5/15/91/115	-
16	CLA	B	847	-	-	8/39/115/115	-
16	CLA	B	843	-	-	5/15/91/115	-
18	BCR	A	847	-	-	3/29/63/63	0/2/2/2
16	CLA	4	408	4	-	9/39/115/115	-
16	CLA	3	511	3	-	7/15/91/115	-
16	CLA	5	412	-	-	14/39/115/115	-
16	CLA	A	819	-	-	3/15/91/115	-
16	CLA	6	512	-	-	7/15/91/115	-
16	CLA	4	416	4	-	9/39/115/115	-
16	CLA	6	505	4	-	11/39/115/115	-
16	CLA	A	822	5	-	5/39/115/115	-
16	CLA	A	826	5	-	2/23/99/115	-
16	CLA	1	526	21	-	4/15/91/115	-
16	CLA	4	410	4	-	9/33/109/115	-
16	CLA	A	837	5	-	7/23/99/115	-
18	BCR	1	519	-	-	3/29/63/63	0/2/2/2
18	BCR	3	516	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	A	810	5	-	6/21/97/115	-
18	BCR	6	520	-	-	3/29/63/63	0/2/2/2
18	BCR	M	101	-	-	5/29/63/63	0/2/2/2
16	CLA	4	413	4	-	2/15/91/115	-
16	CLA	7	509	4	-	12/33/109/115	-
16	CLA	1	511	1	-	5/15/91/115	-
16	CLA	A	833	5	-	10/39/115/115	-
16	CLA	B	813	6	-	11/39/115/115	-
16	CLA	1	515	1	-	8/17/93/115	-
16	CLA	4	403	4	-	5/27/103/115	-
16	CLA	B	824	6	-	5/32/108/115	-
16	CLA	B	829	-	-	4/27/103/115	-
16	CLA	1	517	-	-	10/27/103/115	-
16	CLA	B	841	6	-	11/39/115/115	-
16	CLA	J	1102	12	-	3/15/91/115	-
16	CLA	3	504	3	-	10/39/115/115	-
16	CLA	A	827	5	-	8/18/94/115	-
16	CLA	B	839	6	-	12/39/115/115	-
16	CLA	2	406	-	-	15/39/115/115	-
16	CLA	3	512	3	-	10/15/91/115	-
16	CLA	1	503	-	-	10/39/115/115	-
16	CLA	B	820	6	-	6/39/115/115	-
16	CLA	B	826	-	-	6/39/115/115	-
16	CLA	B	828	6	-	6/15/91/115	-
16	CLA	A	842	5	-	16/39/115/115	-
18	BCR	4	419	-	-	11/29/63/63	0/2/2/2
21	LHG	4	421	-	-	5/27/27/53	-
26	SF4	C	102	-	-	-	0/6/5/5
16	CLA	A	828	-	-	14/39/115/115	-
16	CLA	A	840	5	-	15/39/115/115	-
16	CLA	B	812	6	-	8/39/115/115	-
16	CLA	4	411	-	-	16/39/115/115	-
16	CLA	6	508	4	-	15/27/103/115	-
16	CLA	6	514	-	-	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	A	841	5	-	15/39/115/115	-
18	BCR	F	203	-	-	6/29/63/63	0/2/2/2
16	CLA	4	409	4	-	9/27/103/115	-
18	BCR	2	416	-	-	7/29/63/63	0/2/2/2
16	CLA	4	402	4	-	6/21/97/115	-
16	CLA	A	811	5	-	11/39/115/115	-
23	LMT	I	103	-	-	10/21/61/61	0/2/2/2
16	CLA	1	525	5	-	4/27/103/115	-
16	CLA	5	410	21,4	-	7/27/103/115	-
26	SF4	B	802	-	-	-	0/6/5/5
16	CLA	2	404	2	-	14/39/115/115	-
16	CLA	4	406	4	-	15/39/115/115	-
16	CLA	B	844	6	-	5/33/109/115	-
16	CLA	A	809	5	-	12/39/115/115	-
18	BCR	B	854	-	-	0/29/63/63	0/2/2/2
16	CLA	1	516	1	-	9/33/109/115	-
16	CLA	2	412	-	-	7/15/91/115	-
16	CLA	1	505	-	-	13/33/109/115	-
18	BCR	2	418	-	-	7/29/63/63	0/2/2/2
21	LHG	5	424	-	-	8/27/27/53	-
16	CLA	4	417	-	-	10/33/109/115	-
16	CLA	A	823	5	-	4/21/97/115	-
16	CLA	B	816	6	-	16/39/115/115	-
16	CLA	B	835	6	-	11/39/115/115	-
16	CLA	2	405	2	-	5/39/115/115	-
16	CLA	3	507	-	-	6/27/103/115	-
16	CLA	7	505	4	-	8/15/91/115	-
16	CLA	7	510	-	-	8/15/91/115	-
16	CLA	5	418	4	-	7/15/91/115	-
16	CLA	B	814	6	-	9/39/115/115	-
16	CLA	6	504	4	-	12/39/115/115	-
18	BCR	5	421	-	-	4/29/63/63	0/2/2/2
18	BCR	5	422	-	-	2/29/63/63	0/2/2/2
16	CLA	A	852	-	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	5	402	-	-	2/29/63/63	0/2/2/2
19	LMG	A	851	-	-	9/34/54/70	0/1/1/1
16	CLA	B	833	6	-	3/39/115/115	-
16	CLA	A	818	5	-	4/15/91/115	-
16	CLA	2	414	2	-	8/15/91/115	-
16	CLA	1	510	1	-	8/33/109/115	-
20	LMU	4	401	-	-	5/21/61/61	0/2/2/2
16	CLA	B	825	6	-	14/39/115/115	-
16	CLA	4	415	-	-	13/39/115/115	-
16	CLA	A	843	5	-	6/39/115/115	-
16	CLA	A	806	-	-	5/39/115/115	-
16	CLA	2	408	2	-	13/33/109/115	-
16	CLA	1	506	1	-	6/39/115/115	-
16	CLA	5	417	4	-	14/39/115/115	-
16	CLA	6	509	4	-	9/33/109/115	-
16	CLA	2	410	2	-	11/33/109/115	-
16	CLA	7	512	4	-	4/15/91/115	-
25	ECH	A	853	-	-	8/29/66/66	0/2/2/2
16	CLA	B	815	6	-	11/39/115/115	-
18	BCR	B	853	-	-	6/29/63/63	0/2/2/2
18	BCR	B	850	-	-	9/29/63/63	0/2/2/2
21	LHG	B	806	-	-	7/49/49/53	-
16	CLA	B	846	6	-	11/39/115/115	-
16	CLA	2	403	-	-	10/39/115/115	-
18	BCR	A	845	-	-	5/29/63/63	0/2/2/2
16	CLA	1	512	-	-	4/15/91/115	-
18	BCR	K	101	-	-	4/29/63/63	0/2/2/2
16	CLA	F	201	-	-	5/23/99/115	-
25	ECH	A	848	-	-	3/29/66/66	0/2/2/2
16	CLA	A	832	5	-	3/39/115/115	-
25	ECH	B	851	-	-	11/29/66/66	0/2/2/2
16	CLA	3	508	3	-	7/33/109/115	-
16	CLA	B	830	6	-	9/39/115/115	-
16	CLA	A	808	5	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	5	408	4	-	11/33/109/115	-
16	CLA	B	801	-	-	2/39/115/115	-
16	CLA	5	407	4	-	15/39/115/115	-
16	CLA	6	513	-	-	6/15/91/115	-
16	CLA	A	812	5	-	14/39/115/115	-
16	CLA	2	411	2	-	5/15/91/115	-
16	CLA	6	501	4	-	5/21/97/115	-
18	BCR	4	420	-	-	2/29/63/63	0/2/2/2
19	LMG	B	805	-	-	11/49/69/70	0/1/1/1
24	CL0	A	805	5	-	9/37/135/135	-
16	CLA	1	504	1	-	7/39/115/115	-
16	CLA	2	402	2	-	4/15/91/115	-
16	CLA	6	506	4	-	6/33/109/115	-
18	BCR	1	523	-	-	5/29/63/63	0/2/2/2
18	BCR	5	423	-	-	3/29/63/63	0/2/2/2
16	CLA	B	842	-	-	1/15/91/115	-
20	LMU	1	527	-	-	9/21/61/61	0/2/2/2
16	CLA	5	405	4	-	3/15/91/115	-
16	CLA	5	414	4	-	6/15/91/115	-
16	CLA	B	837	6	-	17/39/115/115	-
16	CLA	A	814	5,16	-	12/39/115/115	-
21	LHG	A	802	-	-	15/53/53/53	-
16	CLA	5	419	4	-	2/15/91/115	-
16	CLA	B	836	6	-	10/39/115/115	-
18	BCR	I	102	-	-	9/29/63/63	0/2/2/2
23	LMT	B	807	-	-	6/21/61/61	0/2/2/2
22	PQN	A	801	-	-	3/23/43/43	0/2/2/2
18	BCR	6	518	-	-	9/29/63/63	0/2/2/2
18	BCR	A	850	-	-	10/29/63/63	0/2/2/2
16	CLA	A	829	-	-	6/27/103/115	-
16	CLA	A	836	5	-	7/39/115/115	-
18	BCR	5	420	-	-	9/29/63/63	0/2/2/2
16	CLA	5	406	4	-	9/39/115/115	-
16	CLA	J	1103	12	-	3/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	K	103	13	-	6/39/115/115	-
16	CLA	A	807	5,16	-	6/26/102/115	-
16	CLA	4	405	4	-	9/39/115/115	-
16	CLA	7	516	4	-	6/15/91/115	-
16	CLA	A	839	5	-	5/23/99/115	-
18	BCR	3	514	-	-	6/29/63/63	0/2/2/2
17	LUT	1	518	-	1/1/12/27	9/29/67/67	0/2/2/2
16	CLA	3	509	-	-	19/39/115/115	-
16	CLA	5	411	4	-	10/33/109/115	-
16	CLA	K	102	-	-	5/21/97/115	-
16	CLA	4	412	4	-	8/21/97/115	-
23	LMT	B	808	-	-	5/21/61/61	0/2/2/2
16	CLA	B	832	-	-	10/39/115/115	-
16	CLA	5	409	4	-	9/39/115/115	-
23	LMT	A	804	-	-	5/21/61/61	0/2/2/2
16	CLA	A	821	5	-	5/26/102/115	-
16	CLA	7	504	4	-	6/15/91/115	-
16	CLA	2	413	2	-	16/33/109/115	-
19	LMG	5	426	-	-	6/38/58/70	0/1/1/1
21	LHG	3	517	-	-	7/27/27/53	-
16	CLA	3	505	3	-	14/39/115/115	-
16	CLA	A	816	5	-	11/39/115/115	-
16	CLA	A	838	5	-	5/27/103/115	-
16	CLA	1	502	1	-	7/27/103/115	-
16	CLA	A	835	5	-	8/39/115/115	-
16	CLA	B	818	6	-	9/39/115/115	-
16	CLA	1	509	1	-	10/33/109/115	-
16	CLA	2	415	2	-	4/15/91/115	-
16	CLA	B	845	-	-	8/39/115/115	-
19	LMG	1	524	-	-	5/35/55/70	0/1/1/1
18	BCR	1	520	-	-	2/29/63/63	0/2/2/2
16	CLA	6	502	4	-	5/21/97/115	-
16	CLA	1	514	1	-	5/21/97/115	-
16	CLA	5	404	4	-	6/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	6	519	-	-	8/29/63/63	0/2/2/2
16	CLA	A	831	5	-	8/39/115/115	-
18	BCR	A	849	-	-	2/29/63/63	0/2/2/2
18	BCR	A	846	-	-	3/29/63/63	0/2/2/2
18	BCR	B	804	-	-	10/29/63/63	0/2/2/2
18	BCR	1	521	-	-	4/29/63/63	0/2/2/2
16	CLA	4	418	4	-	4/15/91/115	-
18	BCR	2	417	-	-	5/29/63/63	0/2/2/2
16	CLA	B	810	-	-	11/39/115/115	-
16	CLA	3	506	-	-	15/39/115/115	-
16	CLA	1	508	-	-	12/39/115/115	-
16	CLA	6	511	4	-	6/15/91/115	-
16	CLA	4	407	4	-	10/39/115/115	-
16	CLA	6	517	4	-	4/15/91/115	-
18	BCR	F	204	-	-	6/29/63/63	0/2/2/2
16	CLA	5	413	4	-	14/33/109/115	-
16	CLA	3	513	3	-	4/15/91/115	-
16	CLA	A	830	5	-	10/39/115/115	-
16	CLA	J	1101	5	-	15/39/115/115	-
16	CLA	A	813	5	-	9/27/103/115	-
16	CLA	6	503	4	-	4/15/91/115	-
16	CLA	1	501	1	-	5/15/91/115	-
18	BCR	5	401	-	-	1/29/63/63	0/2/2/2
16	CLA	7	514	-	-	7/15/91/115	-
16	CLA	A	834	5	-	2/33/109/115	-
18	BCR	1	522	-	-	9/29/63/63	0/2/2/2
16	CLA	A	844	-	-	10/39/115/115	-
16	CLA	B	822	6	-	7/15/91/115	-
16	CLA	A	815	5	-	5/33/109/115	-
16	CLA	B	821	6	-	9/29/105/115	-
18	BCR	I	101	-	-	8/29/63/63	0/2/2/2
16	CLA	B	840	6	-	9/31/107/115	-
26	SF4	C	101	-	-	-	0/6/5/5
16	CLA	7	501	-	-	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	3	510	3	-	10/27/103/115	-
16	CLA	7	506	4	-	7/33/109/115	-
16	CLA	3	501	3	-	9/39/115/115	-
16	CLA	7	511	4	-	10/27/77/115	-
16	CLA	2	401	2	-	7/27/103/115	-
16	CLA	5	415	-	-	1/15/91/115	-
16	CLA	7	513	-	-	6/15/91/115	-
16	CLA	B	817	6	-	4/33/109/115	-
18	BCR	B	849	-	-	6/29/63/63	0/2/2/2
16	CLA	B	848	6	-	10/39/115/115	-
16	CLA	B	823	6	-	4/27/103/115	-
16	CLA	1	507	1	-	4/15/91/115	-
16	CLA	6	516	4	-	4/15/91/115	-
16	CLA	1	513	1	-	8/15/91/115	-
16	CLA	B	827	6	-	10/29/105/115	-
16	CLA	B	811	6	-	3/26/102/115	-
16	CLA	A	817	5	-	6/27/103/115	-
16	CLA	2	409	-	-	10/27/103/115	-
16	CLA	A	820	5	-	7/26/102/115	-
16	CLA	X	101	15	-	8/15/91/115	-
18	BCR	B	852	-	-	6/29/63/63	0/2/2/2
18	BCR	J	1104	-	-	4/29/63/63	0/2/2/2
18	BCR	7	519	-	-	2/29/63/63	0/2/2/2
18	BCR	7	518	-	-	5/29/63/63	0/2/2/2
22	PQN	B	803	-	-	3/23/43/43	0/2/2/2
16	CLA	F	202	-	-	1/15/91/115	-
16	CLA	B	831	6	-	14/39/115/115	-
16	CLA	5	416	-	-	6/15/91/115	-
16	CLA	A	824	-	-	12/39/115/115	-

All (861) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	805	CL0	C1B-C2B	8.60	1.49	1.39
24	A	805	CL0	C3B-C4B	8.12	1.49	1.41
16	7	511	CLA	C1B-C2B	5.54	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	805	CL0	C3D-C4D	3.90	1.47	1.41
16	J	1101	CLA	C1D-ND	3.64	1.42	1.37
16	1	508	CLA	C1D-ND	3.61	1.42	1.37
16	2	409	CLA	C1D-ND	3.60	1.42	1.37
16	7	511	CLA	C4B-C3B	3.59	1.49	1.38
16	1	512	CLA	C1D-ND	3.55	1.42	1.37
16	1	514	CLA	C1D-ND	3.55	1.42	1.37
16	B	842	CLA	C1D-ND	3.54	1.42	1.37
16	B	828	CLA	C1D-ND	3.54	1.42	1.37
16	7	501	CLA	C1D-ND	3.54	1.42	1.37
16	1	513	CLA	C1D-ND	3.54	1.42	1.37
16	5	405	CLA	C1D-ND	3.54	1.42	1.37
16	B	833	CLA	C1D-ND	3.53	1.42	1.37
16	X	101	CLA	C1D-ND	3.53	1.42	1.37
16	A	834	CLA	C1D-ND	3.53	1.42	1.37
16	7	510	CLA	C1D-ND	3.53	1.42	1.37
16	3	504	CLA	C1D-ND	3.53	1.42	1.37
16	6	514	CLA	C1D-ND	3.53	1.42	1.37
16	4	417	CLA	C1D-ND	3.52	1.42	1.37
16	6	512	CLA	C1D-ND	3.52	1.42	1.37
16	5	403	CLA	C1D-ND	3.52	1.42	1.37
16	7	514	CLA	C1D-ND	3.51	1.42	1.37
16	A	814	CLA	C1D-ND	3.51	1.42	1.37
16	F	202	CLA	C1D-ND	3.51	1.42	1.37
16	A	811	CLA	C1D-ND	3.50	1.42	1.37
16	7	508	CLA	C1D-ND	3.50	1.42	1.37
16	A	825	CLA	C1D-ND	3.50	1.42	1.37
16	2	408	CLA	C1D-ND	3.49	1.42	1.37
16	3	512	CLA	C1D-ND	3.49	1.42	1.37
16	A	806	CLA	C1D-ND	3.49	1.42	1.37
16	B	818	CLA	C1D-ND	3.49	1.42	1.37
16	B	834	CLA	C1D-ND	3.49	1.42	1.37
16	1	502	CLA	C1D-ND	3.48	1.42	1.37
16	3	513	CLA	C1D-ND	3.48	1.42	1.37
16	A	830	CLA	C1D-ND	3.48	1.42	1.37
16	B	827	CLA	C1D-ND	3.48	1.42	1.37
16	1	510	CLA	C1D-ND	3.47	1.42	1.37
16	1	517	CLA	C1D-ND	3.47	1.42	1.37
16	3	510	CLA	C1D-ND	3.46	1.42	1.37
16	7	513	CLA	C1D-ND	3.46	1.42	1.37
16	B	830	CLA	C1D-ND	3.46	1.42	1.37
16	B	847	CLA	C1D-ND	3.46	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	3	506	CLA	C1D-ND	3.45	1.42	1.37
16	J	1103	CLA	C1D-ND	3.45	1.42	1.37
16	A	809	CLA	C1D-ND	3.45	1.42	1.37
16	3	503	CLA	C1D-ND	3.45	1.42	1.37
16	2	406	CLA	C1D-ND	3.44	1.42	1.37
16	4	415	CLA	C1D-ND	3.44	1.42	1.37
16	2	413	CLA	C1D-ND	3.43	1.42	1.37
16	A	831	CLA	C1D-ND	3.43	1.42	1.37
16	6	503	CLA	C1D-ND	3.43	1.42	1.37
16	7	512	CLA	C1D-ND	3.43	1.42	1.37
16	5	410	CLA	C1D-ND	3.43	1.42	1.37
16	A	818	CLA	C1D-ND	3.43	1.42	1.37
16	A	826	CLA	C1D-ND	3.43	1.42	1.37
16	1	515	CLA	C1D-ND	3.42	1.42	1.37
16	3	507	CLA	C1D-ND	3.42	1.42	1.37
16	4	410	CLA	C1D-ND	3.42	1.42	1.37
16	5	404	CLA	C1D-ND	3.42	1.42	1.37
16	4	411	CLA	C1D-ND	3.42	1.42	1.37
16	7	509	CLA	C1D-ND	3.42	1.42	1.37
16	B	822	CLA	C1D-ND	3.42	1.42	1.37
16	A	808	CLA	C1D-ND	3.42	1.42	1.37
16	4	413	CLA	C1D-ND	3.42	1.42	1.37
16	5	414	CLA	C1D-ND	3.42	1.42	1.37
16	2	410	CLA	C1D-ND	3.42	1.42	1.37
16	4	405	CLA	C1D-ND	3.42	1.42	1.37
16	A	838	CLA	C1D-ND	3.41	1.42	1.37
16	B	835	CLA	C1D-ND	3.41	1.42	1.37
16	7	504	CLA	C1D-ND	3.41	1.42	1.37
16	7	516	CLA	C1D-ND	3.41	1.42	1.37
16	A	827	CLA	C1D-ND	3.41	1.42	1.37
16	A	836	CLA	C1D-ND	3.41	1.42	1.37
16	B	819	CLA	C1D-ND	3.40	1.42	1.37
16	B	820	CLA	C1D-ND	3.40	1.42	1.37
16	B	810	CLA	C1D-ND	3.40	1.42	1.37
16	4	408	CLA	C1D-ND	3.40	1.42	1.37
16	4	412	CLA	C1D-ND	3.40	1.42	1.37
16	B	824	CLA	C1D-ND	3.40	1.42	1.37
16	7	505	CLA	C1D-ND	3.40	1.42	1.37
16	4	416	CLA	C1D-ND	3.40	1.42	1.37
16	6	517	CLA	C1D-ND	3.40	1.42	1.37
16	A	819	CLA	C1D-ND	3.40	1.42	1.37
16	A	841	CLA	C1D-ND	3.40	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	K	102	CLA	C1D-ND	3.40	1.42	1.37
16	4	402	CLA	C1D-ND	3.40	1.42	1.37
16	1	526	CLA	C1D-ND	3.39	1.42	1.37
16	5	416	CLA	C1D-ND	3.39	1.42	1.37
16	7	507	CLA	C1D-ND	3.39	1.42	1.37
16	4	403	CLA	C1D-ND	3.39	1.42	1.37
16	2	412	CLA	C1D-ND	3.39	1.42	1.37
16	5	412	CLA	C1D-ND	3.39	1.42	1.37
16	K	103	CLA	C1D-ND	3.39	1.42	1.37
16	1	511	CLA	C1D-ND	3.39	1.42	1.37
16	5	406	CLA	C1D-ND	3.39	1.42	1.37
16	1	504	CLA	C1D-ND	3.38	1.42	1.37
16	5	408	CLA	C1D-ND	3.38	1.42	1.37
16	B	811	CLA	C1D-ND	3.38	1.42	1.37
16	2	403	CLA	C1D-ND	3.38	1.42	1.37
16	A	835	CLA	C1D-ND	3.38	1.42	1.37
16	B	844	CLA	C1D-ND	3.37	1.42	1.37
16	6	508	CLA	C1D-ND	3.37	1.42	1.37
16	3	511	CLA	C1D-ND	3.37	1.42	1.37
16	7	517	CLA	C1D-ND	3.36	1.42	1.37
16	1	501	CLA	C1D-ND	3.36	1.42	1.37
16	4	418	CLA	C1D-ND	3.36	1.42	1.37
16	1	505	CLA	C1D-ND	3.36	1.42	1.37
16	6	509	CLA	C1D-ND	3.36	1.42	1.37
16	4	409	CLA	C1D-ND	3.36	1.42	1.37
16	A	852	CLA	C1D-ND	3.36	1.42	1.37
16	A	828	CLA	C1D-ND	3.35	1.42	1.37
16	6	510	CLA	C1D-ND	3.35	1.42	1.37
16	A	822	CLA	C1D-ND	3.35	1.42	1.37
16	J	1102	CLA	C1D-ND	3.35	1.42	1.37
16	B	825	CLA	C1D-ND	3.34	1.42	1.37
16	6	501	CLA	C1D-ND	3.34	1.42	1.37
16	A	821	CLA	C1D-ND	3.34	1.42	1.37
16	B	812	CLA	C1D-ND	3.34	1.42	1.37
16	3	502	CLA	C1D-ND	3.34	1.42	1.37
16	1	503	CLA	C1D-ND	3.34	1.42	1.37
16	5	413	CLA	C1D-ND	3.34	1.42	1.37
16	5	411	CLA	C1D-ND	3.34	1.42	1.37
16	B	839	CLA	C1D-ND	3.34	1.42	1.37
16	F	201	CLA	C1D-ND	3.34	1.42	1.37
16	B	831	CLA	C1D-ND	3.34	1.42	1.37
16	1	509	CLA	C1D-ND	3.33	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	3	508	CLA	C1D-ND	3.33	1.42	1.37
16	6	505	CLA	C1D-ND	3.33	1.42	1.37
16	A	820	CLA	C1D-ND	3.33	1.42	1.37
16	B	845	CLA	C1D-ND	3.33	1.42	1.37
16	5	407	CLA	C1D-ND	3.33	1.42	1.37
16	B	816	CLA	C1D-ND	3.33	1.42	1.37
16	6	504	CLA	C1D-ND	3.33	1.42	1.37
16	A	837	CLA	C1D-ND	3.33	1.42	1.37
16	A	807	CLA	C1D-ND	3.32	1.42	1.37
16	5	418	CLA	C1D-ND	3.32	1.42	1.37
16	A	844	CLA	C1D-ND	3.32	1.42	1.37
16	6	515	CLA	C1D-ND	3.32	1.42	1.37
16	B	829	CLA	C1D-ND	3.32	1.42	1.37
16	A	813	CLA	C1D-ND	3.32	1.42	1.37
16	A	843	CLA	C1D-ND	3.32	1.42	1.37
16	B	815	CLA	C1D-ND	3.31	1.42	1.37
16	7	506	CLA	C1D-ND	3.31	1.42	1.37
16	7	502	CLA	C1D-ND	3.31	1.42	1.37
16	7	503	CLA	C1D-ND	3.31	1.42	1.37
16	B	837	CLA	C1D-ND	3.30	1.42	1.37
16	6	516	CLA	C1D-ND	3.30	1.42	1.37
16	A	842	CLA	C1D-ND	3.30	1.42	1.37
16	2	405	CLA	C1D-ND	3.30	1.42	1.37
16	B	813	CLA	C1D-ND	3.30	1.42	1.37
16	A	839	CLA	C1D-ND	3.30	1.42	1.37
16	2	411	CLA	C1D-ND	3.29	1.42	1.37
16	4	406	CLA	C1D-ND	3.29	1.42	1.37
16	4	414	CLA	C1D-ND	3.29	1.42	1.37
16	B	801	CLA	C1D-ND	3.29	1.42	1.37
16	2	402	CLA	C1D-ND	3.29	1.42	1.37
16	B	848	CLA	C1D-ND	3.29	1.42	1.37
16	B	843	CLA	C1D-ND	3.28	1.42	1.37
16	5	419	CLA	C1D-ND	3.28	1.42	1.37
16	B	809	CLA	C1D-ND	3.28	1.42	1.37
16	6	511	CLA	C1D-ND	3.28	1.42	1.37
16	B	817	CLA	C1D-ND	3.28	1.42	1.37
16	2	401	CLA	C1D-ND	3.28	1.42	1.37
16	A	823	CLA	C1D-ND	3.27	1.42	1.37
16	3	501	CLA	C1D-ND	3.27	1.42	1.37
16	2	415	CLA	C1D-ND	3.27	1.42	1.37
16	4	407	CLA	C1D-ND	3.27	1.42	1.37
16	B	841	CLA	C1D-ND	3.26	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	846	CLA	C1D-ND	3.26	1.42	1.37
16	1	525	CLA	C1D-ND	3.26	1.42	1.37
16	A	816	CLA	C1D-ND	3.26	1.42	1.37
16	1	516	CLA	C1D-ND	3.25	1.42	1.37
16	B	821	CLA	C1D-ND	3.25	1.42	1.37
16	B	823	CLA	C1D-ND	3.25	1.42	1.37
16	5	409	CLA	C1D-ND	3.25	1.42	1.37
16	6	513	CLA	C1D-ND	3.25	1.42	1.37
16	4	404	CLA	C1D-ND	3.24	1.42	1.37
16	B	838	CLA	C1D-ND	3.23	1.42	1.37
16	A	829	CLA	C1D-ND	3.23	1.42	1.37
16	A	817	CLA	C1D-ND	3.23	1.42	1.37
16	5	415	CLA	C1D-ND	3.23	1.42	1.37
16	3	505	CLA	C1D-ND	3.23	1.42	1.37
16	A	810	CLA	C1D-ND	3.23	1.42	1.37
16	A	812	CLA	C1D-ND	3.23	1.42	1.37
16	A	832	CLA	C1D-ND	3.22	1.42	1.37
16	6	502	CLA	C1D-ND	3.22	1.42	1.37
16	1	507	CLA	C1D-ND	3.22	1.42	1.37
16	2	404	CLA	C1D-ND	3.22	1.42	1.37
16	A	824	CLA	C1D-ND	3.21	1.42	1.37
16	B	826	CLA	C1D-ND	3.20	1.42	1.37
16	B	832	CLA	C1D-ND	3.19	1.42	1.37
16	1	506	CLA	C1D-ND	3.19	1.42	1.37
16	2	407	CLA	C1D-ND	3.18	1.42	1.37
16	B	814	CLA	C1D-ND	3.18	1.42	1.37
16	A	840	CLA	C1D-ND	3.18	1.42	1.37
16	A	833	CLA	C1D-ND	3.17	1.42	1.37
16	A	815	CLA	C1D-ND	3.17	1.42	1.37
16	B	836	CLA	C1D-ND	3.17	1.42	1.37
16	B	840	CLA	C1D-ND	3.16	1.42	1.37
16	3	509	CLA	C1D-ND	3.14	1.42	1.37
16	6	507	CLA	C1D-ND	3.13	1.42	1.37
16	7	511	CLA	C4D-ND	-3.12	1.33	1.37
16	5	417	CLA	C1D-ND	3.09	1.41	1.37
16	2	414	CLA	C1D-ND	3.08	1.41	1.37
16	6	506	CLA	C1D-ND	3.05	1.41	1.37
16	7	508	CLA	C1B-C2B	2.67	1.49	1.43
16	B	842	CLA	C1B-C2B	2.67	1.49	1.43
16	6	501	CLA	C1B-C2B	2.67	1.49	1.43
16	1	510	CLA	C1B-C2B	2.67	1.49	1.43
16	A	815	CLA	C1B-C2B	2.66	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	2	402	CLA	C1B-C2B	2.66	1.49	1.43
16	2	405	CLA	C1B-C2B	2.65	1.49	1.43
16	7	517	CLA	C1B-C2B	2.65	1.49	1.43
16	7	501	CLA	C1B-C2B	2.65	1.49	1.43
16	6	512	CLA	C1B-C2B	2.64	1.49	1.43
16	3	506	CLA	C1B-C2B	2.64	1.49	1.43
16	7	503	CLA	C1B-C2B	2.64	1.49	1.43
16	4	418	CLA	C1B-C2B	2.64	1.49	1.43
16	4	416	CLA	C1B-C2B	2.63	1.49	1.43
16	5	415	CLA	C1B-C2B	2.63	1.49	1.43
24	A	805	CL0	C1D-C2D	2.63	1.42	1.39
16	B	830	CLA	C1B-C2B	2.62	1.49	1.43
16	5	414	CLA	C1B-C2B	2.62	1.49	1.43
16	7	515	CLA	C1B-C2B	2.62	1.49	1.43
16	A	842	CLA	C1B-C2B	2.62	1.49	1.43
16	5	405	CLA	C1B-C2B	2.62	1.49	1.43
16	6	504	CLA	C1B-C2B	2.62	1.49	1.43
16	A	826	CLA	C1B-C2B	2.62	1.49	1.43
16	3	501	CLA	C1B-C2B	2.61	1.49	1.43
16	5	409	CLA	C1B-C2B	2.61	1.49	1.43
16	5	419	CLA	C1B-C2B	2.61	1.49	1.43
16	B	841	CLA	C1B-C2B	2.61	1.49	1.43
16	A	825	CLA	C1B-C2B	2.61	1.49	1.43
16	2	407	CLA	C1B-C2B	2.61	1.49	1.43
16	3	512	CLA	C1B-C2B	2.61	1.49	1.43
16	7	510	CLA	C1B-C2B	2.61	1.49	1.43
16	4	415	CLA	C1B-C2B	2.60	1.49	1.43
16	A	810	CLA	C1B-C2B	2.60	1.49	1.43
16	2	403	CLA	C1B-C2B	2.60	1.49	1.43
16	5	417	CLA	C1B-C2B	2.60	1.49	1.43
16	A	807	CLA	C1B-C2B	2.60	1.49	1.43
16	A	852	CLA	C1B-C2B	2.60	1.49	1.43
16	B	848	CLA	C1B-C2B	2.60	1.49	1.43
16	B	809	CLA	C1B-C2B	2.60	1.49	1.43
16	5	418	CLA	C1B-C2B	2.60	1.49	1.43
16	6	515	CLA	C1B-C2B	2.60	1.49	1.43
16	7	504	CLA	C1B-C2B	2.59	1.49	1.43
16	B	844	CLA	C1B-C2B	2.59	1.49	1.43
16	1	503	CLA	C1B-C2B	2.59	1.49	1.43
16	7	506	CLA	C1B-C2B	2.59	1.49	1.43
16	5	403	CLA	C1B-C2B	2.59	1.49	1.43
16	1	517	CLA	C1B-C2B	2.59	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	2	415	CLA	C1B-C2B	2.59	1.49	1.43
16	A	840	CLA	C1B-C2B	2.59	1.49	1.43
16	7	516	CLA	C1B-C2B	2.59	1.49	1.43
16	1	511	CLA	C1B-C2B	2.59	1.49	1.43
16	B	814	CLA	C3B-C4B	2.59	1.50	1.42
16	5	416	CLA	C1B-C2B	2.59	1.49	1.43
16	B	847	CLA	C1B-C2B	2.59	1.49	1.43
16	6	514	CLA	C1B-C2B	2.58	1.49	1.43
16	7	514	CLA	C1B-C2B	2.58	1.49	1.43
16	B	811	CLA	C1B-C2B	2.58	1.49	1.43
16	1	509	CLA	C1B-C2B	2.58	1.49	1.43
16	1	512	CLA	C1B-C2B	2.58	1.49	1.43
16	3	509	CLA	C1B-C2B	2.58	1.49	1.43
16	4	409	CLA	C1B-C2B	2.58	1.49	1.43
16	7	505	CLA	C1B-C2B	2.58	1.49	1.43
16	3	513	CLA	C1B-C2B	2.58	1.49	1.43
16	B	815	CLA	C1B-C2B	2.57	1.49	1.43
16	4	402	CLA	C1B-C2B	2.57	1.49	1.43
16	B	836	CLA	C1B-C2B	2.57	1.49	1.43
16	B	829	CLA	C1B-C2B	2.57	1.49	1.43
16	B	827	CLA	C1B-C2B	2.57	1.49	1.43
16	1	513	CLA	C1B-C2B	2.57	1.49	1.43
16	7	512	CLA	C1B-C2B	2.57	1.49	1.43
16	1	504	CLA	C1B-C2B	2.56	1.49	1.43
16	1	502	CLA	C1B-C2B	2.56	1.49	1.43
16	A	836	CLA	C1B-C2B	2.56	1.49	1.43
16	4	414	CLA	C1B-C2B	2.56	1.49	1.43
16	6	513	CLA	C1B-C2B	2.56	1.49	1.43
16	B	828	CLA	C1B-C2B	2.56	1.49	1.43
16	B	823	CLA	C1B-C2B	2.56	1.49	1.43
16	B	835	CLA	C1B-C2B	2.56	1.49	1.43
16	A	806	CLA	C1B-C2B	2.56	1.49	1.43
16	6	517	CLA	C1B-C2B	2.56	1.49	1.43
16	A	839	CLA	C1B-C2B	2.56	1.49	1.43
16	1	525	CLA	C1B-C2B	2.56	1.49	1.43
16	K	103	CLA	C1B-C2B	2.56	1.49	1.43
16	2	414	CLA	C1B-C2B	2.56	1.49	1.43
16	A	835	CLA	C1B-C2B	2.55	1.49	1.43
16	2	408	CLA	C1B-C2B	2.55	1.49	1.43
16	2	406	CLA	C1B-C2B	2.55	1.49	1.43
16	B	826	CLA	C1B-C2B	2.55	1.49	1.43
16	2	404	CLA	C1B-C2B	2.55	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	3	510	CLA	C1B-C2B	2.55	1.49	1.43
16	7	507	CLA	C1B-C2B	2.55	1.49	1.43
16	6	516	CLA	C1B-C2B	2.55	1.49	1.43
16	B	846	CLA	C1B-C2B	2.55	1.49	1.43
16	A	823	CLA	C1B-C2B	2.55	1.49	1.43
16	1	505	CLA	C1B-C2B	2.55	1.49	1.43
16	J	1102	CLA	C1B-C2B	2.55	1.49	1.43
16	1	526	CLA	C1B-C2B	2.55	1.49	1.43
16	A	838	CLA	C1B-C2B	2.55	1.49	1.43
16	2	401	CLA	C1B-C2B	2.55	1.49	1.43
16	3	511	CLA	C1B-C2B	2.54	1.49	1.43
16	2	410	CLA	C1B-C2B	2.54	1.49	1.43
16	1	514	CLA	C1B-C2B	2.54	1.49	1.43
16	2	411	CLA	C1B-C2B	2.54	1.49	1.43
16	6	509	CLA	C1B-C2B	2.54	1.49	1.43
16	A	832	CLA	C1B-C2B	2.54	1.49	1.43
16	A	819	CLA	C1B-C2B	2.54	1.49	1.43
16	A	818	CLA	C1B-C2B	2.54	1.49	1.43
16	B	818	CLA	C1B-C2B	2.54	1.49	1.43
16	B	838	CLA	C1B-C2B	2.54	1.49	1.43
16	3	508	CLA	C1B-C2B	2.54	1.49	1.43
16	7	502	CLA	C1B-C2B	2.54	1.49	1.43
16	B	817	CLA	C1B-C2B	2.54	1.49	1.43
16	A	820	CLA	C1B-C2B	2.53	1.49	1.43
16	A	828	CLA	C1B-C2B	2.53	1.49	1.43
16	3	504	CLA	C1B-C2B	2.53	1.49	1.43
16	F	201	CLA	C1B-C2B	2.53	1.49	1.43
16	B	845	CLA	C1B-C2B	2.53	1.49	1.43
16	A	808	CLA	C1B-C2B	2.53	1.49	1.43
16	6	508	CLA	C1B-C2B	2.53	1.49	1.43
16	6	505	CLA	C3B-C4B	2.53	1.50	1.42
16	5	412	CLA	C1B-C2B	2.53	1.49	1.43
16	3	507	CLA	C1B-C2B	2.53	1.49	1.43
16	5	404	CLA	C1B-C2B	2.53	1.49	1.43
16	4	407	CLA	C1B-C2B	2.53	1.49	1.43
16	6	502	CLA	C1B-C2B	2.53	1.49	1.43
16	6	506	CLA	C1B-C2B	2.53	1.49	1.43
16	B	822	CLA	C1B-C2B	2.53	1.49	1.43
16	B	840	CLA	C1B-C2B	2.53	1.49	1.43
16	A	844	CLA	C1B-C2B	2.52	1.49	1.43
16	B	821	CLA	C1B-C2B	2.52	1.49	1.43
16	B	832	CLA	C1B-C2B	2.52	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	6	511	CLA	C1B-C2B	2.52	1.49	1.43
16	A	809	CLA	C1B-C2B	2.52	1.49	1.43
16	3	505	CLA	C1B-C2B	2.52	1.49	1.43
16	4	412	CLA	C1B-C2B	2.52	1.49	1.43
16	6	510	CLA	C1B-C2B	2.52	1.49	1.43
16	7	513	CLA	C1B-C2B	2.52	1.49	1.43
16	5	413	CLA	C1B-C2B	2.52	1.49	1.43
16	A	830	CLA	C1B-C2B	2.52	1.49	1.43
16	B	825	CLA	C1B-C2B	2.52	1.49	1.43
16	5	408	CLA	C1B-C2B	2.52	1.49	1.43
16	A	811	CLA	C1B-C2B	2.52	1.49	1.43
16	A	827	CLA	C1B-C2B	2.52	1.49	1.43
16	4	405	CLA	C1B-C2B	2.51	1.49	1.43
16	5	406	CLA	C1B-C2B	2.51	1.49	1.43
16	1	507	CLA	C1B-C2B	2.51	1.49	1.43
16	4	403	CLA	C1B-C2B	2.51	1.49	1.43
16	2	409	CLA	C1B-C2B	2.51	1.49	1.43
16	B	843	CLA	C1B-C2B	2.51	1.49	1.43
16	5	410	CLA	C1B-C2B	2.51	1.49	1.43
16	B	816	CLA	C1B-C2B	2.51	1.49	1.43
16	6	507	CLA	C1B-C2B	2.50	1.49	1.43
16	1	515	CLA	C1B-C2B	2.50	1.49	1.43
16	J	1101	CLA	C1B-C2B	2.50	1.49	1.43
16	4	410	CLA	C1B-C2B	2.50	1.49	1.43
16	4	417	CLA	C1B-C2B	2.50	1.49	1.43
16	A	829	CLA	C1B-C2B	2.50	1.49	1.43
16	B	833	CLA	C3B-C4B	2.50	1.50	1.42
16	A	817	CLA	C1B-C2B	2.50	1.49	1.43
16	4	404	CLA	C1B-C2B	2.50	1.49	1.43
16	4	413	CLA	C1B-C2B	2.50	1.49	1.43
16	1	516	CLA	C1B-C2B	2.50	1.49	1.43
16	J	1103	CLA	C1B-C2B	2.50	1.49	1.43
16	3	502	CLA	C1B-C2B	2.50	1.49	1.43
16	B	839	CLA	C1B-C2B	2.50	1.49	1.43
16	B	801	CLA	C1B-C2B	2.50	1.49	1.43
16	3	503	CLA	C1B-C2B	2.50	1.49	1.43
16	A	812	CLA	C1B-C2B	2.50	1.49	1.43
16	X	101	CLA	C1B-C2B	2.50	1.49	1.43
16	K	102	CLA	C1B-C2B	2.49	1.49	1.43
16	4	411	CLA	C1B-C2B	2.49	1.49	1.43
16	B	810	CLA	C1B-C2B	2.49	1.49	1.43
16	7	509	CLA	C1B-C2B	2.49	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	819	CLA	C1B-C2B	2.49	1.49	1.43
16	2	413	CLA	C1B-C2B	2.49	1.49	1.43
16	A	814	CLA	C1B-C2B	2.49	1.49	1.43
16	2	412	CLA	C1B-C2B	2.49	1.49	1.43
16	F	202	CLA	C1B-C2B	2.48	1.49	1.43
16	B	813	CLA	C1B-C2B	2.48	1.49	1.43
16	5	407	CLA	C3B-C4B	2.48	1.50	1.42
16	1	506	CLA	C1B-C2B	2.48	1.49	1.43
16	A	837	CLA	C1B-C2B	2.48	1.48	1.43
16	A	841	CLA	C1B-C2B	2.48	1.48	1.43
16	3	503	CLA	C3B-C4B	2.48	1.50	1.42
24	A	805	CL0	C1A-CHA	-2.48	1.37	1.40
16	B	814	CLA	C1B-C2B	2.47	1.48	1.43
16	A	833	CLA	C1B-C2B	2.47	1.48	1.43
16	B	834	CLA	C1B-C2B	2.47	1.48	1.43
16	6	503	CLA	C1B-C2B	2.47	1.48	1.43
16	A	831	CLA	C1B-C2B	2.47	1.48	1.43
16	A	843	CLA	C1B-C2B	2.46	1.48	1.43
16	F	202	CLA	C3B-C4B	2.46	1.49	1.42
16	A	820	CLA	C3B-C4B	2.46	1.49	1.42
16	B	831	CLA	C1B-C2B	2.46	1.48	1.43
16	B	819	CLA	C3B-C4B	2.46	1.49	1.42
16	A	834	CLA	C1B-C2B	2.46	1.48	1.43
16	1	501	CLA	C1B-C2B	2.46	1.48	1.43
16	B	820	CLA	C1B-C2B	2.46	1.48	1.43
16	B	824	CLA	C1B-C2B	2.45	1.48	1.43
16	4	408	CLA	C1B-C2B	2.45	1.48	1.43
16	2	413	CLA	C3B-C4B	2.45	1.49	1.42
16	5	407	CLA	C1B-C2B	2.44	1.48	1.43
16	1	508	CLA	C1B-C2B	2.44	1.48	1.43
16	7	502	CLA	C3B-C4B	2.44	1.49	1.42
16	B	817	CLA	C3B-C4B	2.44	1.49	1.42
16	5	417	CLA	C3B-C4B	2.44	1.49	1.42
16	B	837	CLA	C1B-C2B	2.44	1.48	1.43
16	4	406	CLA	C1B-C2B	2.43	1.48	1.43
16	6	505	CLA	C1B-C2B	2.43	1.48	1.43
16	A	816	CLA	C3B-C4B	2.43	1.49	1.42
16	4	416	CLA	C3B-C4B	2.43	1.49	1.42
16	A	822	CLA	C1B-C2B	2.43	1.48	1.43
16	7	509	CLA	C3B-C4B	2.43	1.49	1.42
16	B	840	CLA	C3B-C4B	2.43	1.49	1.42
16	7	513	CLA	C3B-C4B	2.43	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	821	CLA	C1B-C2B	2.43	1.48	1.43
16	J	1103	CLA	C3B-C4B	2.43	1.49	1.42
16	4	417	CLA	C3B-C4B	2.43	1.49	1.42
16	A	813	CLA	C1B-C2B	2.43	1.48	1.43
16	6	503	CLA	C3B-C4B	2.43	1.49	1.42
16	1	508	CLA	C3B-C4B	2.42	1.49	1.42
16	B	839	CLA	C3B-C4B	2.42	1.49	1.42
16	5	411	CLA	C1B-C2B	2.42	1.48	1.43
16	B	812	CLA	C1B-C2B	2.42	1.48	1.43
16	J	1101	CLA	C3B-C4B	2.42	1.49	1.42
16	X	101	CLA	C3B-C4B	2.42	1.49	1.42
16	A	824	CLA	C1B-C2B	2.42	1.48	1.43
16	A	813	CLA	C3B-C4B	2.42	1.49	1.42
16	B	843	CLA	C3B-C4B	2.41	1.49	1.42
16	A	841	CLA	C3B-C4B	2.41	1.49	1.42
16	A	843	CLA	C3B-C4B	2.41	1.49	1.42
16	6	515	CLA	C3B-C4B	2.41	1.49	1.42
16	B	801	CLA	C3B-C4B	2.41	1.49	1.42
16	A	816	CLA	C1B-C2B	2.41	1.48	1.43
16	5	410	CLA	C3B-C4B	2.41	1.49	1.42
16	A	822	CLA	C3B-C4B	2.40	1.49	1.42
16	K	102	CLA	C3B-C4B	2.40	1.49	1.42
16	5	415	CLA	C3B-C4B	2.40	1.49	1.42
16	A	831	CLA	C3B-C4B	2.40	1.49	1.42
16	B	833	CLA	C1B-C2B	2.40	1.48	1.43
16	B	815	CLA	C3B-C4B	2.40	1.49	1.42
16	1	511	CLA	C3B-C4B	2.40	1.49	1.42
16	6	514	CLA	C3B-C4B	2.40	1.49	1.42
16	7	515	CLA	C3B-C4B	2.39	1.49	1.42
16	1	501	CLA	C3B-C4B	2.39	1.49	1.42
16	A	837	CLA	C3B-C4B	2.39	1.49	1.42
16	1	514	CLA	C3B-C4B	2.38	1.49	1.42
16	3	504	CLA	C3B-C4B	2.38	1.49	1.42
16	6	513	CLA	C3B-C4B	2.38	1.49	1.42
16	2	414	CLA	C3B-C4B	2.38	1.49	1.42
16	B	829	CLA	C3B-C4B	2.38	1.49	1.42
16	1	506	CLA	C3B-C4B	2.38	1.49	1.42
16	7	512	CLA	C3B-C4B	2.38	1.49	1.42
16	B	834	CLA	C3B-C4B	2.38	1.49	1.42
16	2	412	CLA	C3B-C4B	2.38	1.49	1.42
16	A	830	CLA	C3B-C4B	2.38	1.49	1.42
16	4	414	CLA	C3B-C4B	2.38	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	4	408	CLA	C3B-C4B	2.38	1.49	1.42
16	3	513	CLA	C3B-C4B	2.38	1.49	1.42
16	7	501	CLA	C3B-C4B	2.38	1.49	1.42
16	4	406	CLA	C3B-C4B	2.37	1.49	1.42
16	A	806	CLA	C3B-C4B	2.37	1.49	1.42
16	1	504	CLA	C3B-C4B	2.37	1.49	1.42
16	2	409	CLA	C3B-C4B	2.37	1.49	1.42
16	5	404	CLA	C3B-C4B	2.37	1.49	1.42
16	A	838	CLA	C3B-C4B	2.37	1.49	1.42
16	B	818	CLA	C3B-C4B	2.37	1.49	1.42
16	2	410	CLA	C3B-C4B	2.37	1.49	1.42
16	1	513	CLA	C3B-C4B	2.37	1.49	1.42
16	7	508	CLA	C3B-C4B	2.37	1.49	1.42
16	7	514	CLA	C3B-C4B	2.36	1.49	1.42
16	3	512	CLA	C3B-C4B	2.36	1.49	1.42
16	5	413	CLA	C3B-C4B	2.36	1.49	1.42
16	7	507	CLA	C3B-C4B	2.36	1.49	1.42
16	3	507	CLA	C3B-C4B	2.36	1.49	1.42
16	5	411	CLA	C3B-C4B	2.36	1.49	1.42
16	1	502	CLA	C3B-C4B	2.36	1.49	1.42
16	1	512	CLA	C3B-C4B	2.36	1.49	1.42
16	B	810	CLA	C3B-C4B	2.36	1.49	1.42
16	6	512	CLA	C3B-C4B	2.36	1.49	1.42
16	A	832	CLA	C3B-C4B	2.35	1.49	1.42
16	2	401	CLA	C3B-C4B	2.35	1.49	1.42
16	B	828	CLA	C3B-C4B	2.35	1.49	1.42
16	1	516	CLA	C3B-C4B	2.35	1.49	1.42
16	3	511	CLA	C3B-C4B	2.35	1.49	1.42
16	1	505	CLA	C3B-C4B	2.35	1.49	1.42
16	2	408	CLA	C3B-C4B	2.35	1.49	1.42
16	7	516	CLA	C3B-C4B	2.35	1.49	1.42
16	F	201	CLA	C3B-C4B	2.35	1.49	1.42
16	B	847	CLA	C3B-C4B	2.35	1.49	1.42
16	B	848	CLA	C3B-C4B	2.35	1.49	1.42
16	3	510	CLA	C3B-C4B	2.35	1.49	1.42
16	4	403	CLA	C3B-C4B	2.35	1.49	1.42
16	J	1102	CLA	C3B-C4B	2.35	1.49	1.42
16	5	403	CLA	C3B-C4B	2.34	1.49	1.42
16	7	503	CLA	C3B-C4B	2.34	1.49	1.42
16	4	405	CLA	C3B-C4B	2.34	1.49	1.42
16	5	412	CLA	C3B-C4B	2.34	1.49	1.42
16	A	811	CLA	C3B-C4B	2.34	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	5	405	CLA	C3B-C4B	2.34	1.49	1.42
16	A	829	CLA	C3B-C4B	2.34	1.49	1.42
16	B	823	CLA	C3B-C4B	2.34	1.49	1.42
16	6	507	CLA	C3B-C4B	2.34	1.49	1.42
16	2	415	CLA	C3B-C4B	2.34	1.49	1.42
16	2	402	CLA	C3B-C4B	2.34	1.49	1.42
16	7	504	CLA	C3B-C4B	2.34	1.49	1.42
16	A	823	CLA	C3B-C4B	2.34	1.49	1.42
16	B	822	CLA	C3B-C4B	2.34	1.49	1.42
16	2	406	CLA	C3B-C4B	2.33	1.49	1.42
16	B	846	CLA	C3B-C4B	2.33	1.49	1.42
16	1	503	CLA	C3B-C4B	2.33	1.49	1.42
16	1	515	CLA	C3B-C4B	2.33	1.49	1.42
16	B	820	CLA	C3B-C4B	2.33	1.49	1.42
16	4	415	CLA	C3B-C4B	2.33	1.49	1.42
16	4	418	CLA	C3B-C4B	2.33	1.49	1.42
16	2	404	CLA	C3B-C4B	2.33	1.49	1.42
16	A	844	CLA	C3B-C4B	2.33	1.49	1.42
16	B	838	CLA	C3B-C4B	2.33	1.49	1.42
16	3	508	CLA	C3B-C4B	2.33	1.49	1.42
16	A	807	CLA	C3B-C4B	2.33	1.49	1.42
16	B	814	CLA	CHC-C1C	2.33	1.43	1.38
16	B	827	CLA	C3B-C4B	2.33	1.49	1.42
16	7	506	CLA	C3B-C4B	2.33	1.49	1.42
16	4	404	CLA	C3B-C4B	2.33	1.49	1.42
16	2	403	CLA	C3B-C4B	2.33	1.49	1.42
16	6	501	CLA	C3B-C4B	2.33	1.49	1.42
16	B	821	CLA	C3B-C4B	2.33	1.49	1.42
16	5	406	CLA	C3B-C4B	2.32	1.49	1.42
16	3	502	CLA	C3B-C4B	2.32	1.49	1.42
16	A	808	CLA	C3B-C4B	2.32	1.49	1.42
16	3	501	CLA	C3B-C4B	2.32	1.49	1.42
16	6	508	CLA	C3B-C4B	2.32	1.49	1.42
16	4	407	CLA	C3B-C4B	2.32	1.49	1.42
16	A	852	CLA	C3B-C4B	2.32	1.49	1.42
16	1	509	CLA	C3B-C4B	2.32	1.49	1.42
16	A	818	CLA	C3B-C4B	2.32	1.49	1.42
16	2	407	CLA	C3B-C4B	2.32	1.49	1.42
16	5	416	CLA	C3B-C4B	2.32	1.49	1.42
16	4	411	CLA	C3B-C4B	2.32	1.49	1.42
16	B	825	CLA	C3B-C4B	2.32	1.49	1.42
16	A	814	CLA	C3B-C4B	2.32	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	813	CLA	C3B-C4B	2.32	1.49	1.42
16	5	418	CLA	C3B-C4B	2.32	1.49	1.42
16	2	411	CLA	C3B-C4B	2.32	1.49	1.42
16	6	509	CLA	C3B-C4B	2.32	1.49	1.42
16	1	517	CLA	C3B-C4B	2.32	1.49	1.42
16	B	835	CLA	C3B-C4B	2.32	1.49	1.42
16	A	821	CLA	C3B-C4B	2.32	1.49	1.42
16	B	832	CLA	C3B-C4B	2.32	1.49	1.42
16	A	833	CLA	C3B-C4B	2.31	1.49	1.42
16	A	836	CLA	C3B-C4B	2.31	1.49	1.42
16	B	812	CLA	C3B-C4B	2.31	1.49	1.42
16	1	526	CLA	C3B-C4B	2.31	1.49	1.42
16	4	402	CLA	C3B-C4B	2.31	1.49	1.42
16	A	809	CLA	C3B-C4B	2.31	1.49	1.42
16	4	413	CLA	C3B-C4B	2.31	1.49	1.42
16	5	408	CLA	C3B-C4B	2.31	1.49	1.42
16	A	824	CLA	C3B-C4B	2.31	1.49	1.42
16	6	516	CLA	C3B-C4B	2.31	1.49	1.42
16	6	511	CLA	C3B-C4B	2.31	1.49	1.42
16	A	817	CLA	C3B-C4B	2.31	1.49	1.42
16	7	505	CLA	C3B-C4B	2.31	1.49	1.42
16	7	510	CLA	C3B-C4B	2.30	1.49	1.42
16	B	816	CLA	C3B-C4B	2.30	1.49	1.42
16	B	826	CLA	C3B-C4B	2.30	1.49	1.42
16	A	812	CLA	C3B-C4B	2.30	1.49	1.42
16	6	517	CLA	C3B-C4B	2.30	1.49	1.42
16	4	410	CLA	C3B-C4B	2.30	1.49	1.42
16	5	414	CLA	C3B-C4B	2.30	1.49	1.42
16	3	509	CLA	C3B-C4B	2.30	1.49	1.42
16	B	842	CLA	C3B-C4B	2.30	1.49	1.42
16	B	837	CLA	C3B-C4B	2.29	1.49	1.42
16	A	834	CLA	C3B-C4B	2.29	1.49	1.42
16	B	830	CLA	C3B-C4B	2.29	1.49	1.42
16	B	841	CLA	C3B-C4B	2.29	1.49	1.42
16	2	405	CLA	C3B-C4B	2.29	1.49	1.42
16	B	845	CLA	C3B-C4B	2.29	1.49	1.42
16	A	827	CLA	C3B-C4B	2.28	1.49	1.42
16	6	506	CLA	C3B-C4B	2.28	1.49	1.42
16	A	826	CLA	C3B-C4B	2.28	1.49	1.42
16	6	510	CLA	C3B-C4B	2.28	1.49	1.42
16	B	809	CLA	C3B-C4B	2.28	1.49	1.42
16	K	103	CLA	C3B-C4B	2.28	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	1	510	CLA	C3B-C4B	2.28	1.49	1.42
16	4	412	CLA	C3B-C4B	2.28	1.49	1.42
16	B	811	CLA	C3B-C4B	2.28	1.49	1.42
16	5	419	CLA	C3B-C4B	2.28	1.49	1.42
16	5	409	CLA	C3B-C4B	2.28	1.49	1.42
16	1	507	CLA	C3B-C4B	2.27	1.49	1.42
16	A	810	CLA	C3B-C4B	2.27	1.49	1.42
16	6	502	CLA	C3B-C4B	2.27	1.49	1.42
16	A	839	CLA	C3B-C4B	2.27	1.49	1.42
16	4	409	CLA	C3B-C4B	2.27	1.49	1.42
16	B	836	CLA	C3B-C4B	2.27	1.49	1.42
16	A	835	CLA	C3B-C4B	2.26	1.49	1.42
16	A	840	CLA	C3B-C4B	2.26	1.49	1.42
16	3	505	CLA	C3B-C4B	2.26	1.49	1.42
16	5	417	CLA	CHC-C1C	2.26	1.43	1.38
16	A	825	CLA	C3B-C4B	2.26	1.49	1.42
16	3	504	CLA	CHC-C1C	2.26	1.43	1.38
16	B	844	CLA	C3B-C4B	2.25	1.49	1.42
16	7	517	CLA	C3B-C4B	2.25	1.49	1.42
16	B	831	CLA	C3B-C4B	2.25	1.49	1.42
16	1	525	CLA	C3B-C4B	2.24	1.49	1.42
16	7	508	CLA	CHC-C1C	2.24	1.43	1.38
16	3	506	CLA	C3B-C4B	2.24	1.49	1.42
16	A	842	CLA	C3B-C4B	2.23	1.49	1.42
16	B	824	CLA	C3B-C4B	2.23	1.49	1.42
16	1	514	CLA	CHC-C1C	2.22	1.42	1.38
16	A	820	CLA	CHC-C1C	2.22	1.42	1.38
16	A	819	CLA	C3B-C4B	2.22	1.49	1.42
16	7	505	CLA	CHC-C1C	2.22	1.42	1.38
16	6	504	CLA	C3B-C4B	2.22	1.49	1.42
16	3	510	CLA	CHC-C1C	2.21	1.42	1.38
16	A	812	CLA	CHC-C1C	2.21	1.42	1.38
16	B	801	CLA	CHC-C1C	2.21	1.42	1.38
16	6	508	CLA	CHC-C1C	2.21	1.42	1.38
16	A	828	CLA	C3B-C4B	2.20	1.49	1.42
16	X	101	CLA	CHC-C1C	2.20	1.42	1.38
16	2	406	CLA	CHC-C1C	2.20	1.42	1.38
16	5	413	CLA	CHC-C1C	2.20	1.42	1.38
16	1	512	CLA	CHC-C1C	2.20	1.42	1.38
16	7	515	CLA	CHC-C1C	2.20	1.42	1.38
16	1	511	CLA	CHC-C1C	2.20	1.42	1.38
16	B	819	CLA	CHC-C1C	2.20	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	7	517	CLA	CHC-C1C	2.19	1.42	1.38
16	7	501	CLA	CHC-C1C	2.19	1.42	1.38
16	B	826	CLA	CHC-C1C	2.19	1.42	1.38
16	A	815	CLA	C3B-C4B	2.19	1.49	1.42
16	7	504	CLA	CHC-C1C	2.18	1.42	1.38
16	7	514	CLA	CHC-C1C	2.18	1.42	1.38
16	A	817	CLA	CHC-C1C	2.18	1.42	1.38
16	A	813	CLA	CHC-C1C	2.18	1.42	1.38
16	B	822	CLA	CHC-C1C	2.18	1.42	1.38
16	J	1103	CLA	CHC-C1C	2.18	1.42	1.38
16	A	840	CLA	MG-ND	-2.17	2.01	2.05
16	2	402	CLA	CHC-C1C	2.17	1.42	1.38
16	6	511	CLA	CHC-C1C	2.17	1.42	1.38
16	A	810	CLA	CHC-C1C	2.17	1.42	1.38
16	K	102	CLA	CHC-C1C	2.16	1.42	1.38
16	B	834	CLA	CHC-C1C	2.16	1.42	1.38
16	3	505	CLA	CHC-C1C	2.16	1.42	1.38
16	2	414	CLA	CHC-C1C	2.16	1.42	1.38
16	7	502	CLA	CHC-C1C	2.16	1.42	1.38
16	2	410	CLA	CHC-C1C	2.16	1.42	1.38
16	B	817	CLA	CHC-C1C	2.16	1.42	1.38
16	7	516	CLA	CHC-C1C	2.16	1.42	1.38
16	B	818	CLA	CHC-C1C	2.16	1.42	1.38
16	B	823	CLA	CHC-C1C	2.15	1.42	1.38
16	6	505	CLA	CHC-C1C	2.15	1.42	1.38
16	B	810	CLA	CHC-C1C	2.15	1.42	1.38
16	A	806	CLA	CHC-C1C	2.15	1.42	1.38
16	B	824	CLA	CHC-C1C	2.15	1.42	1.38
16	A	831	CLA	CHC-C1C	2.15	1.42	1.38
16	B	829	CLA	CHC-C1C	2.15	1.42	1.38
16	7	515	CLA	MG-ND	-2.15	2.01	2.05
16	5	407	CLA	CHC-C1C	2.15	1.42	1.38
16	2	413	CLA	CHC-C1C	2.15	1.42	1.38
16	A	838	CLA	CHC-C1C	2.15	1.42	1.38
16	B	812	CLA	CHC-C1C	2.15	1.42	1.38
16	A	815	CLA	CHC-C1C	2.15	1.42	1.38
16	A	807	CLA	CHC-C1C	2.14	1.42	1.38
16	B	821	CLA	CHC-C1C	2.14	1.42	1.38
16	1	515	CLA	CHC-C1C	2.14	1.42	1.38
16	4	418	CLA	CHC-C1C	2.14	1.42	1.38
16	B	816	CLA	CHC-C1C	2.14	1.42	1.38
16	B	847	CLA	CHC-C1C	2.14	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	852	CLA	CHC-C1C	2.13	1.42	1.38
16	3	509	CLA	CHC-C1C	2.13	1.42	1.38
16	7	506	CLA	CHC-C1C	2.13	1.42	1.38
16	1	502	CLA	CHC-C1C	2.13	1.42	1.38
16	4	416	CLA	CHC-C1C	2.13	1.42	1.38
16	7	512	CLA	CHC-C1C	2.13	1.42	1.38
16	1	504	CLA	CHC-C1C	2.13	1.42	1.38
16	A	821	CLA	CHC-C1C	2.13	1.42	1.38
16	1	509	CLA	CHC-C1C	2.13	1.42	1.38
16	5	415	CLA	CHC-C1C	2.13	1.42	1.38
16	2	403	CLA	CHC-C1C	2.13	1.42	1.38
16	B	831	CLA	CHC-C1C	2.13	1.42	1.38
16	5	418	CLA	CHC-C1C	2.13	1.42	1.38
24	A	805	CL0	MG-NB	-2.13	2.01	2.05
16	2	415	CLA	CHC-C1C	2.12	1.42	1.38
16	7	503	CLA	CHC-C1C	2.12	1.42	1.38
16	1	517	CLA	CHC-C1C	2.12	1.42	1.38
16	1	508	CLA	CHC-C1C	2.12	1.42	1.38
16	1	516	CLA	CHC-C1C	2.12	1.42	1.38
16	2	407	CLA	CHC-C1C	2.12	1.42	1.38
16	5	408	CLA	CHC-C1C	2.12	1.42	1.38
16	5	411	CLA	CHC-C1C	2.12	1.42	1.38
16	5	417	CLA	MG-ND	-2.12	2.01	2.05
16	B	815	CLA	CHC-C1C	2.12	1.42	1.38
16	B	828	CLA	CHC-C1C	2.12	1.42	1.38
16	B	838	CLA	CHC-C1C	2.12	1.42	1.38
16	1	505	CLA	CHC-C1C	2.12	1.42	1.38
16	A	811	CLA	CHC-C1C	2.12	1.42	1.38
16	A	823	CLA	MG-ND	-2.12	2.01	2.05
16	A	823	CLA	CHC-C1C	2.11	1.42	1.38
16	B	840	CLA	CHC-C1C	2.11	1.42	1.38
16	B	814	CLA	MG-ND	-2.11	2.01	2.05
16	7	513	CLA	CHC-C1C	2.11	1.42	1.38
16	B	833	CLA	CHC-C1C	2.11	1.42	1.38
16	4	412	CLA	CHC-C1C	2.11	1.42	1.38
16	A	818	CLA	CHC-C1C	2.11	1.42	1.38
16	4	406	CLA	CHC-C1C	2.11	1.42	1.38
16	B	813	CLA	CHC-C1C	2.11	1.42	1.38
16	B	846	CLA	CHC-C1C	2.11	1.42	1.38
16	B	835	CLA	CHC-C1C	2.11	1.42	1.38
16	A	829	CLA	CHC-C1C	2.11	1.42	1.38
16	A	843	CLA	CHC-C1C	2.11	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	840	CLA	CHC-C1C	2.10	1.42	1.38
16	5	416	CLA	CHC-C1C	2.10	1.42	1.38
16	2	404	CLA	CHC-C1C	2.10	1.42	1.38
16	6	506	CLA	CHC-C1C	2.10	1.42	1.38
16	5	412	CLA	CHC-C1C	2.10	1.42	1.38
16	A	835	CLA	CHC-C1C	2.10	1.42	1.38
16	6	512	CLA	CHC-C1C	2.10	1.42	1.38
16	6	513	CLA	CHC-C1C	2.10	1.42	1.38
16	1	506	CLA	CHC-C1C	2.10	1.42	1.38
16	2	411	CLA	CHC-C1C	2.10	1.42	1.38
16	J	1102	CLA	CHC-C1C	2.10	1.42	1.38
16	4	417	CLA	CHC-C1C	2.10	1.42	1.38
16	A	827	CLA	CHC-C1C	2.10	1.42	1.38
16	6	517	CLA	CHC-C1C	2.10	1.42	1.38
16	F	201	CLA	CHC-C1C	2.10	1.42	1.38
16	B	825	CLA	CHC-C1C	2.10	1.42	1.38
16	3	512	CLA	CHC-C1C	2.09	1.42	1.38
16	5	414	CLA	CHC-C1C	2.09	1.42	1.38
16	A	832	CLA	CHC-C1C	2.09	1.42	1.38
16	B	843	CLA	CHC-C1C	2.09	1.42	1.38
16	5	406	CLA	CHC-C1C	2.09	1.42	1.38
16	1	501	CLA	CHC-C1C	2.09	1.42	1.38
16	6	501	CLA	CHC-C1C	2.09	1.42	1.38
16	4	415	CLA	CHC-C1C	2.09	1.42	1.38
16	B	839	CLA	CHC-C1C	2.09	1.42	1.38
16	B	830	CLA	CHC-C1C	2.09	1.42	1.38
16	6	507	CLA	CHC-C1C	2.09	1.42	1.38
16	A	844	CLA	CHC-C1C	2.09	1.42	1.38
16	B	845	CLA	CHC-C1C	2.09	1.42	1.38
16	1	525	CLA	CHC-C1C	2.09	1.42	1.38
16	A	808	CLA	CHC-C1C	2.09	1.42	1.38
16	7	507	CLA	CHC-C1C	2.08	1.42	1.38
16	6	514	CLA	CHC-C1C	2.08	1.42	1.38
16	K	103	CLA	CHC-C1C	2.08	1.42	1.38
16	5	403	CLA	CHC-C1C	2.08	1.42	1.38
16	5	405	CLA	CHC-C1C	2.08	1.42	1.38
16	6	515	CLA	CHC-C1C	2.08	1.42	1.38
16	5	413	CLA	MG-ND	-2.08	2.01	2.05
16	3	511	CLA	CHC-C1C	2.08	1.42	1.38
16	A	830	CLA	CHC-C1C	2.08	1.42	1.38
16	B	832	CLA	CHC-C1C	2.08	1.42	1.38
16	1	507	CLA	CHC-C1C	2.08	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	2	412	CLA	CHC-C1C	2.08	1.42	1.38
16	B	837	CLA	CHC-C1C	2.08	1.42	1.38
16	7	506	CLA	MG-ND	-2.08	2.01	2.05
16	A	826	CLA	CHC-C1C	2.07	1.42	1.38
16	A	814	CLA	CHC-C1C	2.07	1.42	1.38
16	J	1101	CLA	CHC-C1C	2.07	1.42	1.38
16	2	407	CLA	MG-ND	-2.07	2.01	2.05
16	6	516	CLA	CHC-C1C	2.07	1.42	1.38
16	3	513	CLA	CHC-C1C	2.07	1.42	1.38
16	1	503	CLA	CHC-C1C	2.07	1.42	1.38
16	6	513	CLA	MG-ND	-2.07	2.01	2.05
16	5	410	CLA	CHC-C1C	2.07	1.42	1.38
16	1	525	CLA	MG-ND	-2.07	2.01	2.05
16	B	831	CLA	MG-ND	-2.07	2.01	2.05
16	4	403	CLA	CHC-C1C	2.07	1.42	1.38
16	A	816	CLA	CHC-C1C	2.06	1.42	1.38
16	A	824	CLA	CHC-C1C	2.06	1.42	1.38
16	3	509	CLA	MG-ND	-2.06	2.01	2.05
16	4	407	CLA	CHC-C1C	2.06	1.42	1.38
16	7	509	CLA	CHC-C1C	2.06	1.42	1.38
16	1	507	CLA	MG-ND	-2.06	2.01	2.05
16	A	832	CLA	MG-ND	-2.06	2.01	2.05
16	3	503	CLA	CHC-C1C	2.06	1.42	1.38
16	B	809	CLA	CHC-C1C	2.06	1.42	1.38
16	3	504	CLA	MG-ND	-2.06	2.01	2.05
16	B	814	CLA	MG-NB	-2.06	2.01	2.05
16	3	501	CLA	CHC-C1C	2.06	1.42	1.38
16	4	402	CLA	CHC-C1C	2.06	1.42	1.38
16	4	418	CLA	MG-ND	-2.06	2.01	2.05
16	2	410	CLA	MG-ND	-2.06	2.01	2.05
16	1	510	CLA	CHC-C1C	2.06	1.42	1.38
16	1	513	CLA	CHC-C1C	2.06	1.42	1.38
16	4	404	CLA	CHC-C1C	2.06	1.42	1.38
16	B	810	CLA	MG-ND	-2.06	2.01	2.05
16	2	401	CLA	CHC-C1C	2.06	1.42	1.38
16	A	834	CLA	CHC-C1C	2.06	1.42	1.38
16	6	503	CLA	CHC-C1C	2.06	1.42	1.38
16	B	820	CLA	CHC-C1C	2.06	1.42	1.38
16	4	410	CLA	CHC-C1C	2.05	1.42	1.38
16	4	414	CLA	CHC-C1C	2.05	1.42	1.38
16	5	409	CLA	CHC-C1C	2.05	1.42	1.38
16	B	841	CLA	CHC-C1C	2.05	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	6	507	CLA	MG-ND	-2.05	2.01	2.05
16	A	817	CLA	MG-ND	-2.05	2.01	2.05
16	7	510	CLA	CHC-C1C	2.05	1.42	1.38
16	B	811	CLA	CHC-C1C	2.05	1.42	1.38
16	2	409	CLA	CHC-C1C	2.05	1.42	1.38
16	A	833	CLA	CHC-C1C	2.05	1.42	1.38
16	6	504	CLA	MG-ND	-2.05	2.01	2.05
16	6	505	CLA	MG-ND	-2.05	2.01	2.05
16	A	836	CLA	CHC-C1C	2.05	1.42	1.38
16	4	409	CLA	CHC-C1C	2.05	1.42	1.38
16	1	505	CLA	MG-ND	-2.05	2.01	2.05
16	6	502	CLA	CHC-C1C	2.05	1.42	1.38
16	2	401	CLA	MG-ND	-2.05	2.01	2.05
16	A	809	CLA	CHC-C1C	2.04	1.42	1.38
16	4	408	CLA	CHC-C1C	2.04	1.42	1.38
16	F	202	CLA	CHC-C1C	2.04	1.42	1.38
16	A	837	CLA	CHC-C1C	2.04	1.42	1.38
16	6	509	CLA	MG-ND	-2.04	2.01	2.05
16	2	405	CLA	CHC-C1C	2.04	1.42	1.38
16	1	526	CLA	CHC-C1C	2.04	1.42	1.38
16	4	413	CLA	CHC-C1C	2.04	1.42	1.38
16	B	836	CLA	CHC-C1C	2.04	1.42	1.38
16	A	831	CLA	MG-ND	-2.04	2.01	2.05
16	6	509	CLA	CHC-C1C	2.04	1.42	1.38
16	A	815	CLA	MG-ND	-2.03	2.01	2.05
16	A	819	CLA	CHC-C1C	2.03	1.42	1.38
16	2	414	CLA	MG-ND	-2.03	2.01	2.05
16	7	502	CLA	MG-ND	-2.03	2.01	2.05
16	3	507	CLA	CHC-C1C	2.03	1.42	1.38
16	B	826	CLA	MG-ND	-2.03	2.01	2.05
16	3	508	CLA	CHC-C1C	2.03	1.42	1.38
16	2	408	CLA	CHC-C1C	2.03	1.42	1.38
16	5	419	CLA	CHC-C1C	2.03	1.42	1.38
16	7	501	CLA	MG-ND	-2.03	2.01	2.05
16	4	405	CLA	CHC-C1C	2.03	1.42	1.38
16	5	412	CLA	MG-ND	-2.02	2.01	2.05
16	A	822	CLA	CHC-C1C	2.02	1.42	1.38
16	A	825	CLA	CHC-C1C	2.02	1.42	1.38
16	B	827	CLA	CHC-C1C	2.02	1.42	1.38
16	A	816	CLA	MG-ND	-2.02	2.01	2.05
16	4	411	CLA	CHC-C1C	2.02	1.42	1.38
16	A	839	CLA	CHC-C1C	2.02	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	2	402	CLA	MG-ND	-2.01	2.01	2.05
16	3	505	CLA	MG-ND	-2.01	2.01	2.05
16	7	516	CLA	MG-ND	-2.01	2.01	2.05
16	6	504	CLA	CHC-C1C	2.01	1.42	1.38
16	6	511	CLA	MG-ND	-2.01	2.01	2.05
16	A	835	CLA	MG-ND	-2.01	2.01	2.05
16	4	409	CLA	MG-ND	-2.01	2.01	2.05
16	4	407	CLA	MG-ND	-2.01	2.01	2.05
16	7	513	CLA	MG-ND	-2.01	2.01	2.05
16	5	404	CLA	CHC-C1C	2.01	1.42	1.38
16	3	502	CLA	CHC-C1C	2.01	1.42	1.38
16	B	842	CLA	CHC-C1C	2.01	1.42	1.38
16	5	411	CLA	MG-ND	-2.01	2.01	2.05
16	5	408	CLA	MG-ND	-2.01	2.01	2.05
16	A	833	CLA	MG-ND	-2.00	2.01	2.05
16	6	510	CLA	CHC-C1C	2.00	1.42	1.38
16	A	821	CLA	MG-ND	-2.00	2.01	2.05
16	3	502	CLA	MG-ND	-2.00	2.01	2.05

All (733) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	805	CL0	C1B-CHB-C4A	6.30	125.38	121.32
17	1	518	LUT	C7-C8-C9	-5.72	117.77	126.23
16	7	511	CLA	CMB-C2B-C3B	4.62	123.98	116.53
16	2	410	CLA	C4A-NA-C1A	4.39	108.68	106.68
17	1	518	LUT	C21-C26-C27	4.37	117.85	112.83
16	B	848	CLA	C4A-NA-C1A	4.10	108.55	106.68
16	7	503	CLA	C4A-NA-C1A	3.95	108.48	106.68
16	A	828	CLA	C4A-NA-C1A	3.94	108.47	106.68
16	4	414	CLA	C4A-NA-C1A	3.90	108.46	106.68
16	B	815	CLA	C4A-NA-C1A	3.87	108.44	106.68
16	A	811	CLA	C4A-NA-C1A	3.79	108.41	106.68
16	B	830	CLA	C4A-NA-C1A	3.58	108.31	106.68
16	A	844	CLA	C4A-NA-C1A	3.55	108.30	106.68
16	3	510	CLA	C4A-NA-C1A	3.52	108.28	106.68
22	B	803	PQN	C11-C3-C4	-3.46	114.94	118.58
16	2	409	CLA	C4A-NA-C1A	3.36	108.21	106.68
16	7	513	CLA	C4A-NA-C1A	3.31	108.19	106.68
16	4	407	CLA	C4-C3-C5	3.29	120.94	115.23
16	5	414	CLA	C4A-NA-C1A	3.25	108.16	106.68
25	B	851	ECH	C11-C10-C9	3.23	131.81	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	4	409	CLA	C4A-NA-C1A	3.20	108.14	106.68
16	4	413	CLA	C4A-NA-C1A	3.18	108.13	106.68
16	6	517	CLA	C4A-NA-C1A	3.18	108.13	106.68
16	A	840	CLA	C4A-NA-C1A	3.13	108.11	106.68
24	A	805	CL0	CHA-C1A-C2A	-3.13	125.96	133.31
16	2	407	CLA	C4-C3-C5	3.10	120.61	115.23
16	B	837	CLA	C4A-NA-C1A	3.07	108.08	106.68
16	A	837	CLA	C4A-NA-C1A	3.03	108.06	106.68
16	B	810	CLA	C4A-NA-C1A	3.01	108.05	106.68
16	3	511	CLA	C4A-NA-C1A	2.98	108.04	106.68
16	1	525	CLA	C4A-NA-C1A	2.98	108.04	106.68
24	A	805	CL0	C1C-CHC-C4B	2.96	126.67	116.07
16	2	414	CLA	CHD-C1D-ND	-2.93	120.68	124.80
22	A	801	PQN	C11-C3-C4	-2.92	115.50	118.58
16	2	405	CLA	C4A-NA-C1A	2.92	108.01	106.68
16	3	505	CLA	C4A-NA-C1A	2.89	108.00	106.68
24	A	805	CL0	C4D-CHA-CBD	-2.87	106.08	108.97
17	1	518	LUT	C26-C27-C28	-2.86	120.13	124.58
17	1	518	LUT	C38-C25-C24	-2.85	116.62	123.36
16	1	508	CLA	C3B-C2B-C1B	-2.84	103.83	107.17
16	5	410	CLA	C4A-NA-C1A	2.83	107.97	106.68
16	2	415	CLA	C3B-C2B-C1B	-2.82	103.84	107.17
16	6	504	CLA	C3B-C2B-C1B	-2.82	103.84	107.17
16	1	508	CLA	C4A-NA-C1A	2.82	107.97	106.68
18	B	849	BCR	C2-C1-C6	2.82	114.53	110.44
16	A	835	CLA	C1-C2-C3	-2.81	121.58	126.20
16	A	844	CLA	C3B-C2B-C1B	-2.81	103.86	107.17
16	A	815	CLA	C3B-C4B-NB	-2.79	108.04	110.53
16	A	813	CLA	C3B-C2B-C1B	-2.79	103.89	107.17
16	A	823	CLA	C4A-NA-C1A	2.78	107.95	106.68
16	2	411	CLA	C4A-NA-C1A	2.77	107.94	106.68
16	6	502	CLA	C1-C2-C3	-2.76	122.29	126.76
16	5	416	CLA	CHD-C1D-ND	-2.76	120.92	124.80
16	2	403	CLA	C3B-C2B-C1B	-2.75	103.93	107.17
16	A	815	CLA	C4A-NA-C1A	2.75	107.93	106.68
16	7	507	CLA	C3B-C2B-C1B	-2.75	103.93	107.17
16	A	825	CLA	C1-C2-C3	-2.73	121.72	126.20
16	3	504	CLA	C4A-NA-C1A	2.72	107.92	106.68
16	1	507	CLA	C3B-C2B-C1B	-2.71	103.97	107.17
16	1	511	CLA	CHD-C1D-ND	-2.70	121.00	124.80
16	3	509	CLA	C4A-NA-C1A	2.70	107.91	106.68
16	7	514	CLA	CHD-C1D-ND	-2.68	121.03	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	814	CLA	C3B-C4B-NB	-2.68	108.14	110.53
16	1	501	CLA	C3B-C2B-C1B	-2.68	104.01	107.17
16	1	508	CLA	CHD-C1D-ND	-2.67	121.04	124.80
16	K	102	CLA	C1-C2-C3	-2.67	122.44	126.76
16	1	505	CLA	C3B-C2B-C1B	-2.66	104.03	107.17
24	A	805	CL0	C4C-CHD-C1D	2.66	125.58	116.07
16	3	501	CLA	C4A-NA-C1A	2.65	107.89	106.68
16	5	411	CLA	C4A-NA-C1A	2.65	107.89	106.68
16	A	834	CLA	C3B-C2B-C1B	-2.64	104.05	107.17
16	A	806	CLA	O2A-CGA-O1A	-2.64	117.03	123.63
16	4	406	CLA	CHD-C1D-ND	-2.64	121.09	124.80
16	4	416	CLA	CMB-C2B-C1B	2.63	129.42	125.42
16	A	829	CLA	C3B-C2B-C1B	-2.61	104.09	107.17
16	B	844	CLA	C4A-NA-C1A	2.61	107.87	106.68
16	A	811	CLA	CHD-C1D-ND	-2.61	121.13	124.80
16	A	826	CLA	C3B-C2B-C1B	-2.61	104.10	107.17
16	5	404	CLA	C1C-C2C-C3C	-2.61	104.24	106.98
16	A	852	CLA	C3B-C4B-NB	-2.59	108.22	110.53
16	7	502	CLA	C3B-C4B-NB	-2.59	108.22	110.53
16	6	504	CLA	C1-C2-C3	-2.59	121.96	126.20
16	6	509	CLA	C3B-C2B-C1B	-2.58	104.12	107.17
16	B	822	CLA	C3B-C2B-C1B	-2.58	104.13	107.17
16	7	513	CLA	CHD-C1D-ND	-2.58	121.18	124.80
16	7	508	CLA	C3B-C4B-NB	-2.58	108.23	110.53
16	B	847	CLA	C3B-C4B-NB	-2.58	108.23	110.53
16	B	831	CLA	C3B-C4B-NB	-2.57	108.23	110.53
16	A	842	CLA	CHD-C1D-ND	-2.57	121.18	124.80
16	B	838	CLA	C3B-C2B-C1B	-2.57	104.14	107.17
16	6	514	CLA	CHD-C1D-ND	-2.57	121.19	124.80
16	A	811	CLA	CHA-C1A-NA	-2.56	120.59	126.39
16	A	839	CLA	C4A-NA-C1A	2.56	107.85	106.68
16	B	821	CLA	C4A-NA-C1A	2.56	107.85	106.68
16	3	505	CLA	CHD-C1D-ND	-2.56	121.20	124.80
16	4	414	CLA	CHD-C1D-ND	-2.55	121.22	124.80
16	1	504	CLA	C1-C2-C3	-2.54	122.03	126.20
16	5	411	CLA	C3B-C4B-NB	-2.54	108.26	110.53
16	7	504	CLA	CHD-C1D-ND	-2.54	121.23	124.80
16	A	818	CLA	C3B-C2B-C1B	-2.53	104.18	107.17
18	B	849	BCR	C4-C5-C6	-2.53	119.29	122.70
16	3	509	CLA	CHD-C1D-ND	-2.52	121.25	124.80
16	A	814	CLA	C4A-NA-C1A	2.52	107.83	106.68
16	1	509	CLA	O2A-CGA-O1A	-2.52	117.32	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	5	406	CLA	C1-C2-C3	-2.52	122.07	126.20
16	A	813	CLA	CHD-C1D-ND	-2.52	121.26	124.80
16	A	831	CLA	C1-C2-C3	-2.51	122.08	126.20
16	B	836	CLA	C1-C2-C3	-2.51	122.09	126.20
16	7	505	CLA	CHD-C1D-ND	-2.51	121.28	124.80
16	2	402	CLA	C3B-C4B-NB	-2.51	108.29	110.53
16	B	824	CLA	C4A-NA-C1A	2.51	107.82	106.68
16	B	813	CLA	C3B-C2B-C1B	-2.50	104.22	107.17
16	A	842	CLA	C1-C2-C3	-2.50	122.10	126.20
16	A	810	CLA	CHD-C1D-ND	-2.50	121.28	124.80
16	4	413	CLA	CHD-C1D-ND	-2.50	121.29	124.80
16	B	820	CLA	C3B-C2B-C1B	-2.50	104.22	107.17
16	6	505	CLA	C1-C2-C3	-2.50	122.11	126.20
16	6	505	CLA	C3B-C4B-NB	-2.49	108.31	110.53
16	6	508	CLA	CHD-C1D-ND	-2.49	121.30	124.80
16	4	406	CLA	C4A-NA-C1A	2.49	107.81	106.68
16	4	417	CLA	C3B-C2B-C1B	-2.49	104.24	107.17
16	4	417	CLA	C3B-C4B-NB	-2.48	108.32	110.53
17	1	518	LUT	C18-C5-C6	-2.48	121.78	124.48
16	A	809	CLA	C3B-C2B-C1B	-2.47	104.26	107.17
18	5	422	BCR	C4-C5-C6	-2.47	119.37	122.70
16	B	841	CLA	C4A-NA-C1A	2.46	107.80	106.68
24	A	805	CL0	C3D-C4D-CHA	2.46	112.28	108.54
16	B	831	CLA	C3B-C2B-C1B	-2.46	104.27	107.17
16	5	407	CLA	CHD-C1D-ND	-2.46	121.35	124.80
16	B	848	CLA	C3B-C2B-C1B	-2.46	104.28	107.17
16	2	406	CLA	C3B-C4B-NB	-2.45	108.34	110.53
16	1	505	CLA	CHD-C1D-ND	-2.45	121.35	124.80
16	A	814	CLA	CHA-C1A-NA	-2.45	120.84	126.39
16	2	404	CLA	CHD-C1D-ND	-2.45	121.36	124.80
16	5	410	CLA	CHA-C1A-NA	-2.45	120.85	126.39
16	B	813	CLA	C1-C2-C3	-2.44	122.19	126.20
16	4	406	CLA	C1-C2-C3	-2.44	122.19	126.20
16	6	515	CLA	C3B-C2B-C1B	-2.44	104.29	107.17
16	A	816	CLA	C3B-C2B-C1B	-2.44	104.29	107.17
16	J	1102	CLA	C3B-C4B-NB	-2.44	108.35	110.53
16	5	418	CLA	C3B-C2B-C1B	-2.44	104.29	107.17
16	A	841	CLA	CHD-C1D-ND	-2.44	121.37	124.80
16	7	501	CLA	C3B-C4B-NB	-2.44	108.35	110.53
16	B	836	CLA	C4A-NA-C1A	2.44	107.79	106.68
16	5	418	CLA	C3B-C4B-NB	-2.43	108.36	110.53
16	5	419	CLA	CHD-C1D-ND	-2.43	121.38	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	823	CLA	CHD-C1D-ND	-2.43	121.38	124.80
16	B	847	CLA	C4-C3-C5	2.43	119.44	115.23
16	A	828	CLA	C1-C2-C3	-2.42	122.22	126.20
16	B	821	CLA	CHD-C1D-ND	-2.42	121.39	124.80
16	2	410	CLA	CHA-C1A-NA	-2.42	120.90	126.39
16	A	842	CLA	C3B-C2B-C1B	-2.42	104.31	107.17
16	6	515	CLA	CHD-C1D-ND	-2.42	121.39	124.80
16	B	846	CLA	CHD-C1D-ND	-2.42	121.39	124.80
16	A	821	CLA	CHB-C4A-NA	2.42	127.89	124.40
16	B	826	CLA	C3B-C4B-NB	-2.42	108.37	110.53
16	1	502	CLA	CHD-C1D-ND	-2.42	121.40	124.80
16	A	840	CLA	C3B-C2B-C1B	-2.42	104.32	107.17
16	A	843	CLA	C3B-C2B-C1B	-2.42	104.32	107.17
16	A	822	CLA	CHD-C1D-ND	-2.41	121.41	124.80
16	5	403	CLA	CHB-C4A-NA	2.41	127.88	124.40
16	A	820	CLA	C3B-C4B-NB	-2.41	108.38	110.53
16	7	511	CLA	CHD-C1D-ND	-2.41	121.41	124.80
20	4	401	LMU	C1B-O1B-C4'	2.41	123.69	117.98
16	4	415	CLA	CHD-C1D-ND	-2.41	121.42	124.80
16	6	501	CLA	C1-C2-C3	-2.41	122.87	126.76
16	5	410	CLA	CHD-C1D-ND	-2.41	121.42	124.80
16	6	501	CLA	CHD-C1D-ND	-2.41	121.42	124.80
16	A	808	CLA	C3B-C2B-C1B	-2.41	104.33	107.17
16	6	506	CLA	C3B-C2B-C1B	-2.40	104.34	107.17
16	B	809	CLA	CHD-C1D-ND	-2.40	121.42	124.80
16	2	412	CLA	CHD-C1D-ND	-2.40	121.42	124.80
16	A	830	CLA	C3B-C2B-C1B	-2.40	104.34	107.17
16	1	505	CLA	C1-C2-C3	-2.40	122.26	126.20
16	B	829	CLA	C3B-C2B-C1B	-2.40	104.34	107.17
16	B	834	CLA	O2A-CGA-O1A	-2.40	117.62	123.63
16	F	201	CLA	C3B-C2B-C1B	-2.40	104.34	107.17
16	4	402	CLA	C3B-C2B-C1B	-2.40	104.34	107.17
16	7	517	CLA	C3B-C4B-NB	-2.40	108.39	110.53
17	1	518	LUT	C31-C32-C33	-2.40	119.80	126.36
16	1	509	CLA	CHA-C1A-NA	-2.39	120.97	126.39
16	J	1103	CLA	C3B-C2B-C1B	-2.39	104.35	107.17
16	7	517	CLA	CHD-C1D-ND	-2.39	121.43	124.80
16	K	103	CLA	C3B-C2B-C1B	-2.39	104.35	107.17
16	6	513	CLA	CHD-C1D-ND	-2.39	121.44	124.80
16	B	813	CLA	CHD-C1D-ND	-2.39	121.44	124.80
16	4	417	CLA	CMB-C2B-C1B	2.39	129.06	125.42
16	1	504	CLA	CHD-C1D-ND	-2.39	121.44	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	4	408	CLA	CHD-C1D-ND	-2.39	121.44	124.80
16	B	834	CLA	CHB-C4A-NA	2.39	127.85	124.40
16	A	808	CLA	C1-C2-C3	-2.39	122.29	126.20
17	1	518	LUT	C22-C23-C24	-2.38	107.64	111.18
16	4	418	CLA	C3B-C2B-C1B	-2.38	104.36	107.17
16	2	408	CLA	CHD-C1D-ND	-2.38	121.45	124.80
16	4	408	CLA	CMB-C2B-C1B	2.38	129.05	125.42
16	F	201	CLA	CHB-C4A-NA	2.38	127.84	124.40
16	4	402	CLA	C1-C2-C3	-2.38	122.91	126.76
16	5	418	CLA	CHD-C1D-ND	-2.38	121.45	124.80
16	2	409	CLA	CHD-C1D-ND	-2.38	121.45	124.80
16	5	417	CLA	C3B-C2B-C1B	-2.37	104.37	107.17
16	5	412	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
16	2	413	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
16	B	828	CLA	C4A-NA-C1A	2.37	107.76	106.68
16	A	833	CLA	CHD-C1D-ND	-2.37	121.47	124.80
16	2	401	CLA	C1-C2-C3	-2.37	122.32	126.20
16	A	812	CLA	CHD-C1D-ND	-2.36	121.48	124.80
16	1	511	CLA	C3B-C4B-NB	-2.36	108.42	110.53
16	4	416	CLA	CHD-C1D-ND	-2.36	121.48	124.80
16	A	807	CLA	CHD-C1D-ND	-2.36	121.48	124.80
16	A	825	CLA	C3B-C4B-NB	-2.36	108.42	110.53
16	B	824	CLA	C1-C2-C3	-2.36	122.33	126.20
18	A	845	BCR	C2-C1-C6	2.36	113.86	110.44
16	7	513	CLA	C3B-C2B-C1B	-2.36	104.39	107.17
16	6	508	CLA	C1-C2-C3	-2.36	122.34	126.20
16	3	504	CLA	C3B-C2B-C1B	-2.36	104.39	107.17
16	1	509	CLA	CHD-C1D-ND	-2.36	121.49	124.80
16	A	835	CLA	C3B-C4B-NB	-2.35	108.43	110.53
16	3	508	CLA	C3B-C2B-C1B	-2.35	104.40	107.17
16	A	815	CLA	CHD-C1D-ND	-2.35	121.50	124.80
16	A	807	CLA	C3B-C4B-NB	-2.35	108.43	110.53
16	B	828	CLA	C3B-C4B-NB	-2.35	108.43	110.53
16	6	517	CLA	CHD-C1D-ND	-2.35	121.50	124.80
16	2	402	CLA	CHB-C4A-NA	2.35	127.79	124.40
16	5	409	CLA	CHD-C1D-ND	-2.35	121.50	124.80
16	1	506	CLA	C3B-C2B-C1B	-2.35	104.40	107.17
16	4	418	CLA	CHD-C1D-ND	-2.34	121.50	124.80
16	B	830	CLA	C3B-C4B-NB	-2.34	108.44	110.53
16	B	836	CLA	CHD-C1D-ND	-2.34	121.51	124.80
16	B	822	CLA	CHD-C1D-ND	-2.34	121.51	124.80
16	A	829	CLA	C1-C2-C3	-2.34	122.37	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	841	CLA	C3B-C2B-C1B	-2.33	104.42	107.17
16	7	515	CLA	CHD-C1D-ND	-2.33	121.55	124.84
16	A	828	CLA	O2A-CGA-O1A	-2.33	117.79	123.63
16	B	847	CLA	CHA-C1A-NA	-2.33	121.11	126.39
16	4	416	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
16	B	819	CLA	C3B-C2B-C1B	-2.33	104.42	107.17
16	5	415	CLA	CHD-C1D-ND	-2.33	121.52	124.80
16	A	809	CLA	C1-C2-C3	-2.33	122.38	126.20
16	A	815	CLA	C2A-C1A-CHA	2.33	127.91	123.87
16	6	506	CLA	C3B-C4B-NB	-2.33	108.45	110.53
16	7	516	CLA	C3B-C4B-NB	-2.33	108.45	110.53
16	5	415	CLA	C3B-C4B-NB	-2.33	108.45	110.53
16	6	505	CLA	CHD-C1D-ND	-2.32	121.53	124.80
16	A	842	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
16	2	415	CLA	CHD-C1D-ND	-2.32	121.53	124.80
25	B	851	ECH	C8-C9-C10	2.32	122.66	119.01
16	A	821	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
16	4	411	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
16	A	808	CLA	CHD-C1D-ND	-2.32	121.54	124.80
16	6	506	CLA	CHD-C1D-ND	-2.32	121.54	124.80
16	B	844	CLA	C3B-C2B-C1B	-2.32	104.43	107.17
16	1	503	CLA	CHD-C1D-ND	-2.32	121.54	124.80
16	A	806	CLA	C3B-C4B-NB	-2.32	108.46	110.53
16	4	409	CLA	CHD-C1D-ND	-2.31	121.55	124.80
16	7	513	CLA	C3B-C4B-NB	-2.31	108.46	110.53
16	B	829	CLA	C3B-C4B-NB	-2.31	108.47	110.53
16	4	408	CLA	C1-C2-C3	-2.31	122.41	126.20
16	A	823	CLA	C1-C2-C3	-2.31	123.03	126.76
16	B	839	CLA	CHD-C1D-ND	-2.31	121.56	124.80
16	5	409	CLA	C3B-C4B-NB	-2.30	108.47	110.53
16	B	843	CLA	CHD-C1D-ND	-2.30	121.56	124.80
16	B	836	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
16	A	816	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
16	1	512	CLA	CHD-C1D-ND	-2.30	121.56	124.80
16	A	817	CLA	CHD-C1D-ND	-2.30	121.56	124.80
16	B	832	CLA	CHD-C1D-ND	-2.30	121.56	124.80
16	A	824	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
16	B	827	CLA	C1-C2-C3	-2.30	122.43	126.20
16	3	513	CLA	CHD-C1D-ND	-2.30	121.57	124.80
16	6	512	CLA	CHD-C1D-ND	-2.30	121.57	124.80
16	4	409	CLA	C3B-C4B-NB	-2.30	108.48	110.53
16	2	404	CLA	O2A-CGA-O1A	-2.30	117.88	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	825	CLA	CHD-C1D-ND	-2.30	121.57	124.80
16	B	845	CLA	CHD-C1D-ND	-2.29	121.57	124.80
16	6	504	CLA	CHB-C4A-NA	2.29	127.71	124.40
16	X	101	CLA	CHD-C1D-ND	-2.29	121.58	124.80
18	1	520	BCR	C27-C26-C25	-2.29	119.61	122.70
16	3	509	CLA	CHA-C1A-NA	-2.29	121.20	126.39
16	3	504	CLA	C3B-C4B-NB	-2.29	108.49	110.53
16	2	413	CLA	CHD-C1D-ND	-2.29	121.59	124.80
16	A	820	CLA	CHD-C1D-ND	-2.28	121.59	124.80
16	B	824	CLA	O2A-CGA-O1A	-2.28	117.91	123.63
16	B	842	CLA	CMB-C2B-C1B	2.28	128.90	125.42
16	A	817	CLA	C3B-C4B-NB	-2.28	108.49	110.53
16	B	811	CLA	CHD-C1D-ND	-2.28	121.59	124.80
16	5	410	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
16	A	810	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
16	5	404	CLA	C1-C2-C3	-2.28	123.07	126.76
16	5	410	CLA	C3B-C2B-C1B	-2.28	104.48	107.17
16	A	810	CLA	C3B-C4B-NB	-2.28	108.50	110.53
16	A	843	CLA	CHD-C1D-ND	-2.28	121.60	124.80
16	1	506	CLA	CHD-C1D-ND	-2.27	121.60	124.80
16	1	501	CLA	CHD-C1D-ND	-2.27	121.61	124.80
16	3	511	CLA	CHD-C1D-ND	-2.27	121.61	124.80
16	6	507	CLA	CHD-C1D-ND	-2.27	121.61	124.80
16	1	510	CLA	CHD-C1D-ND	-2.27	121.61	124.80
16	B	841	CLA	CHD-C1D-ND	-2.27	121.61	124.80
16	1	513	CLA	C3B-C4B-NB	-2.27	108.50	110.53
16	3	503	CLA	CHD-C1D-ND	-2.27	121.61	124.80
16	7	504	CLA	CHB-C4A-NA	2.27	127.67	124.40
16	B	823	CLA	CHD-C1D-ND	-2.26	121.62	124.80
16	1	525	CLA	C3B-C4B-NB	-2.26	108.51	110.53
16	2	412	CLA	C3B-C2B-C1B	-2.26	104.50	107.17
16	A	814	CLA	C3B-C2B-C1B	-2.26	104.50	107.17
16	A	826	CLA	CHD-C1D-ND	-2.26	121.62	124.80
16	B	826	CLA	C1-C2-C3	-2.26	122.49	126.20
16	1	512	CLA	C3B-C4B-NB	-2.26	108.51	110.53
16	6	513	CLA	C3B-C4B-NB	-2.26	108.51	110.53
16	7	506	CLA	C3B-C4B-NB	-2.26	108.51	110.53
16	A	828	CLA	CHA-C1A-NA	-2.26	121.28	126.39
16	6	502	CLA	C4A-NA-C1A	2.26	107.71	106.68
16	J	1101	CLA	CHD-C1D-ND	-2.26	121.63	124.80
16	7	503	CLA	C3B-C4B-NB	-2.25	108.52	110.53
16	B	838	CLA	CHB-C4A-NA	2.25	127.65	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	824	CLA	C3B-C2B-C1B	-2.25	104.51	107.17
16	A	831	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
16	A	816	CLA	C1-C2-C3	-2.25	122.51	126.20
16	7	509	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
18	F	203	BCR	C12-C13-C14	-2.25	115.47	119.01
16	7	506	CLA	CHD-C1D-ND	-2.25	121.64	124.80
16	F	202	CLA	CHD-C1D-ND	-2.25	121.64	124.80
16	A	822	CLA	C1-C2-C3	-2.25	122.51	126.20
16	B	844	CLA	C3B-C4B-NB	-2.24	108.53	110.53
16	5	406	CLA	CHD-C1D-ND	-2.24	121.64	124.80
16	A	832	CLA	CHB-C4A-NA	2.24	127.64	124.40
16	2	406	CLA	C1-C2-C3	-2.24	122.52	126.20
16	1	510	CLA	CMB-C2B-C1B	2.24	128.84	125.42
16	A	839	CLA	CHD-C1D-ND	-2.24	121.65	124.80
16	6	501	CLA	CHB-C4A-NA	2.24	127.64	124.40
16	5	417	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
16	7	515	CLA	C3B-C4B-NB	-2.24	108.53	110.53
16	5	419	CLA	CHB-C4A-NA	2.24	127.63	124.40
16	6	517	CLA	C3B-C2B-C1B	-2.23	104.53	107.17
16	2	405	CLA	CHD-C1D-ND	-2.23	121.66	124.80
16	4	403	CLA	C1-C2-C3	-2.23	122.54	126.20
16	7	502	CLA	CHD-C1D-ND	-2.23	121.66	124.80
16	A	830	CLA	C1-C2-C3	-2.23	122.54	126.20
16	B	827	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
16	6	509	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
16	4	410	CLA	C3B-C2B-C1B	-2.23	104.55	107.17
16	B	817	CLA	CHD-C1D-ND	-2.23	121.67	124.80
16	A	811	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
16	1	511	CLA	C3B-C2B-C1B	-2.23	104.55	107.17
16	5	403	CLA	CHD-C1D-ND	-2.22	121.67	124.80
16	7	503	CLA	CHD-C1D-ND	-2.22	121.67	124.80
16	4	418	CLA	C4A-NA-C1A	2.22	107.69	106.68
16	B	840	CLA	CHD-C1D-ND	-2.22	121.68	124.80
16	6	501	CLA	C3B-C4B-NB	-2.22	108.55	110.53
16	B	844	CLA	CMB-C2B-C1B	2.22	128.79	125.42
16	1	511	CLA	C4A-NA-C1A	2.22	107.69	106.68
16	3	509	CLA	C3B-C2B-C1B	-2.22	104.56	107.17
16	A	838	CLA	CHD-C1D-ND	-2.21	121.69	124.80
16	7	503	CLA	C3B-C2B-C1B	-2.21	104.56	107.17
16	B	844	CLA	CHD-C1D-ND	-2.21	121.69	124.80
16	A	833	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
16	B	810	CLA	CHD-C1D-ND	-2.21	121.69	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	J	1102	CLA	C3B-C2B-C1B	-2.21	104.56	107.17
16	K	103	CLA	CHD-C1D-ND	-2.21	121.69	124.80
16	3	510	CLA	C3B-C2B-C1B	-2.21	104.56	107.17
16	B	829	CLA	C1-C2-C3	-2.21	122.58	126.20
16	B	825	CLA	CHB-C4A-NA	2.21	127.59	124.40
16	B	814	CLA	C1-C2-C3	-2.21	122.58	126.20
16	F	201	CLA	CHD-C1D-ND	-2.21	121.70	124.80
16	5	411	CLA	CHA-C1A-NA	-2.21	121.39	126.39
18	B	849	BCR	C20-C21-C22	-2.20	124.19	127.28
16	6	505	CLA	CHB-C4A-NA	2.20	127.58	124.40
16	B	846	CLA	C3B-C2B-C1B	-2.20	104.57	107.17
16	6	506	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
16	F	201	CLA	C1-C2-C3	-2.20	122.59	126.20
16	4	417	CLA	CHD-C1D-ND	-2.20	121.71	124.80
16	4	418	CLA	CHB-C4A-NA	2.20	127.58	124.40
16	1	508	CLA	C3B-C4B-NB	-2.20	108.57	110.53
16	A	831	CLA	C3B-C4B-NB	-2.20	108.57	110.53
16	6	507	CLA	C1-C2-C3	-2.20	122.59	126.20
16	A	852	CLA	CHB-C4A-NA	2.20	127.57	124.40
16	6	512	CLA	C4A-NA-C1A	2.20	107.68	106.68
16	1	505	CLA	C4-C3-C5	2.20	119.04	115.23
16	A	812	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
16	A	844	CLA	C3B-C4B-NB	-2.20	108.57	110.53
16	7	510	CLA	CMB-C2B-C1B	2.20	128.76	125.42
18	5	422	BCR	C2-C1-C6	2.20	113.63	110.44
16	B	814	CLA	CHD-C1D-ND	-2.20	121.71	124.80
16	A	831	CLA	CHD-C1D-ND	-2.19	121.71	124.80
16	4	410	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
16	A	809	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
16	A	835	CLA	CHD-C1D-ND	-2.19	121.72	124.80
16	A	811	CLA	C1-C2-C3	-2.19	122.61	126.20
16	B	839	CLA	C1-C2-C3	-2.19	122.61	126.20
16	A	844	CLA	CHD-C1D-ND	-2.19	121.72	124.80
16	6	504	CLA	CHD-C1D-ND	-2.19	121.72	124.80
16	4	412	CLA	CHB-C4A-NA	2.19	127.56	124.40
16	5	417	CLA	C3B-C4B-NB	-2.19	108.58	110.53
16	B	811	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
16	3	510	CLA	CHD-C1D-ND	-2.19	121.73	124.80
16	3	504	CLA	CHD-C1D-ND	-2.18	121.73	124.80
16	4	416	CLA	C1-C2-C3	-2.18	122.62	126.20
24	A	805	CL0	C3C-C4C-NC	-2.18	109.32	114.65
18	1	521	BCR	C30-C25-C26	-2.18	119.66	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	K	102	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
16	1	502	CLA	CHB-C4A-NA	2.18	127.55	124.40
16	A	821	CLA	CHD-C1D-ND	-2.18	121.73	124.80
16	5	404	CLA	C3B-C4B-NB	-2.18	108.58	110.53
16	2	406	CLA	CHD-C1D-ND	-2.18	121.74	124.80
17	1	518	LUT	C11-C12-C13	-2.18	120.39	126.36
16	A	836	CLA	CHA-C1A-NA	-2.18	121.46	126.39
16	A	824	CLA	C1-C2-C3	-2.18	122.63	126.20
16	5	414	CLA	CHD-C1D-ND	-2.18	121.74	124.80
16	1	502	CLA	O2A-CGA-O1A	-2.18	118.19	123.63
16	4	415	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
16	4	405	CLA	C1-C2-C3	-2.17	122.64	126.20
16	B	812	CLA	C3B-C2B-C1B	-2.17	104.61	107.17
16	B	809	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
16	A	818	CLA	CHD-C1D-ND	-2.17	121.75	124.80
16	1	514	CLA	C1-C2-C3	-2.17	123.26	126.76
16	A	806	CLA	CHB-C4A-NA	2.16	127.52	124.40
16	A	830	CLA	CHD-C1D-ND	-2.16	121.76	124.80
16	B	848	CLA	O2A-CGA-O1A	-2.16	118.21	123.63
16	B	845	CLA	C3B-C2B-C1B	-2.16	104.62	107.17
16	7	509	CLA	CHD-C1D-ND	-2.16	121.76	124.80
16	A	830	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
16	2	401	CLA	CHD-C1D-ND	-2.16	121.76	124.80
16	B	844	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
16	4	407	CLA	CHD-C1D-ND	-2.16	121.76	124.80
24	A	805	CL0	CMD-C2D-C3D	2.16	129.00	124.68
16	X	101	CLA	C3B-C2B-C1B	-2.16	104.62	107.17
16	3	506	CLA	CHB-C4A-NA	2.16	127.52	124.40
16	7	516	CLA	CHB-C4A-NA	2.16	127.52	124.40
16	B	834	CLA	CHD-C1D-ND	-2.16	121.77	124.80
16	1	510	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
16	2	407	CLA	CHD-C1D-ND	-2.16	121.77	124.80
16	A	831	CLA	CHB-C4A-NA	2.16	127.51	124.40
23	B	808	LMT	O1B-C4'-C3'	2.16	112.71	107.23
16	4	412	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
16	3	505	CLA	CHA-C1A-NA	-2.16	121.51	126.39
16	2	410	CLA	C1-C2-C3	-2.16	122.67	126.20
16	5	413	CLA	CHD-C1D-ND	-2.16	121.77	124.80
16	2	405	CLA	O2A-CGA-O1A	-2.16	118.24	123.63
16	A	829	CLA	CHD-C1D-ND	-2.15	121.77	124.80
16	B	823	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
16	7	516	CLA	CHD-C1D-ND	-2.15	121.77	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	815	CLA	CMB-C2B-C1B	2.15	128.70	125.42
16	4	410	CLA	CHD-C1D-ND	-2.15	121.77	124.80
16	B	836	CLA	C3B-C2B-C1B	-2.15	104.63	107.17
16	B	833	CLA	C1-C2-C3	-2.15	122.67	126.20
16	4	402	CLA	CHA-C1A-NA	-2.15	121.52	126.39
16	B	848	CLA	C1-C2-C3	-2.15	122.67	126.20
16	7	509	CLA	C3B-C2B-C1B	-2.15	104.64	107.17
16	B	821	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
16	B	835	CLA	C4A-NA-C1A	2.15	107.66	106.68
16	B	846	CLA	C4A-NA-C1A	2.15	107.66	106.68
16	2	408	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
16	2	403	CLA	C1-C2-C3	-2.15	122.68	126.20
16	A	837	CLA	CHD-C1D-ND	-2.14	121.78	124.80
16	B	847	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
16	1	526	CLA	C3B-C2B-C1B	-2.14	104.64	107.17
16	A	836	CLA	CHD-C1D-ND	-2.14	121.79	124.80
16	B	831	CLA	CHB-C4A-NA	2.14	127.49	124.40
16	B	820	CLA	CHD-C1D-ND	-2.14	121.79	124.80
16	1	517	CLA	CHB-C4A-NA	2.14	127.49	124.40
16	B	830	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
16	3	509	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
16	1	517	CLA	C1-C2-C3	-2.14	122.69	126.20
16	K	102	CLA	CHD-C1D-ND	-2.14	121.80	124.80
16	3	509	CLA	C4-C3-C5	2.14	118.94	115.23
16	A	807	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
16	3	502	CLA	CHD-C1D-ND	-2.14	121.80	124.80
16	A	813	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
16	A	832	CLA	CHD-C1D-ND	-2.14	121.80	124.80
16	A	828	CLA	C3B-C2B-C1B	-2.14	104.65	107.17
16	A	841	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
16	2	409	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
16	3	506	CLA	CHD-C1D-ND	-2.13	121.80	124.80
16	B	835	CLA	C3B-C2B-C1B	-2.13	104.66	107.17
16	A	834	CLA	CHD-C1D-ND	-2.13	121.80	124.80
16	B	815	CLA	CHD-C1D-ND	-2.13	121.80	124.80
16	7	508	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
16	5	408	CLA	CHD-C1D-ND	-2.13	121.81	124.80
16	6	501	CLA	C3B-C2B-C1B	-2.13	104.66	107.17
16	A	806	CLA	CHD-C1D-ND	-2.13	121.81	124.80
16	7	502	CLA	C3B-C2B-C1B	-2.13	104.66	107.17
16	B	841	CLA	CAA-C2A-C3A	2.13	118.74	113.00
16	B	826	CLA	CHD-C1D-ND	-2.13	121.81	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	816	CLA	C3B-C4B-NB	-2.13	108.63	110.53
16	B	835	CLA	CHD-C1D-ND	-2.12	121.81	124.80
16	6	513	CLA	C4A-NA-C1A	2.12	107.65	106.68
16	B	837	CLA	CHD-C1D-ND	-2.12	121.81	124.80
16	5	409	CLA	C1-C2-C3	-2.12	122.72	126.20
16	5	413	CLA	C3B-C4B-NB	-2.12	108.64	110.53
16	7	502	CLA	C2B-C1B-NB	-2.12	108.12	110.33
16	B	824	CLA	C3B-C4B-NB	-2.12	108.64	110.53
16	3	501	CLA	C1-C2-C3	-2.12	122.72	126.20
16	3	510	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
16	4	404	CLA	C3B-C2B-C1B	-2.12	104.67	107.17
16	B	847	CLA	CHB-C4A-NA	2.12	127.46	124.40
16	5	413	CLA	C4A-NA-C1A	2.12	107.65	106.68
16	1	512	CLA	CHB-C4A-NA	2.12	127.46	124.40
16	6	507	CLA	CMB-C2B-C1B	2.12	128.65	125.42
16	3	504	CLA	C1-C2-C3	-2.12	122.73	126.20
16	A	835	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
16	5	416	CLA	C3B-C4B-NB	-2.12	108.64	110.53
16	A	826	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
16	B	812	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
16	A	820	CLA	C1-C2-C3	-2.12	122.73	126.20
16	2	413	CLA	C2A-C1A-CHA	2.12	127.54	123.87
16	B	829	CLA	CHD-C1D-ND	-2.12	121.82	124.80
16	A	820	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
16	1	514	CLA	CMB-C2B-C1B	2.12	128.64	125.42
16	4	415	CLA	CHB-C4A-NA	2.11	127.45	124.40
16	6	515	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
16	A	838	CLA	C1-C2-C3	-2.11	122.73	126.20
16	7	517	CLA	CMB-C2B-C1B	2.11	128.64	125.42
16	A	823	CLA	C3B-C2B-C1B	-2.11	104.68	107.17
16	2	405	CLA	CHA-C1A-NA	-2.11	121.61	126.39
16	1	505	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
16	A	843	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
16	A	852	CLA	CHD-C1D-ND	-2.11	121.83	124.80
16	B	801	CLA	C3B-C4B-NB	-2.11	108.65	110.53
16	2	407	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
16	3	501	CLA	CHD-C1D-ND	-2.11	121.83	124.80
16	4	412	CLA	C3B-C4B-NB	-2.11	108.65	110.53
16	1	516	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
16	5	412	CLA	C3B-C2B-C1B	-2.11	104.69	107.17
16	B	810	CLA	CHA-C1A-NA	-2.11	121.62	126.39
16	B	809	CLA	CHB-C4A-NA	2.11	127.44	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	1	514	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
16	6	511	CLA	CHD-C1D-ND	-2.10	121.84	124.80
16	A	830	CLA	C3B-C4B-NB	-2.10	108.65	110.53
16	A	815	CLA	CHA-C1A-NA	-2.10	121.63	126.39
16	A	829	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
16	5	413	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
16	B	825	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
16	5	418	CLA	C4A-NA-C1A	2.10	107.64	106.68
16	A	827	CLA	C3B-C4B-NB	-2.10	108.65	110.53
16	3	508	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
16	4	411	CLA	CHD-C1D-ND	-2.10	121.85	124.80
16	3	502	CLA	C1-C2-C3	-2.10	122.75	126.20
16	6	504	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
16	7	508	CLA	CHB-C4A-NA	2.10	127.43	124.40
16	5	411	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
16	B	848	CLA	CHD-C1D-ND	-2.10	121.85	124.80
16	6	516	CLA	C3B-C2B-C1B	-2.10	104.70	107.17
16	B	832	CLA	CMB-C2B-C1B	2.10	128.61	125.42
18	5	420	BCR	C2-C1-C6	2.10	113.48	110.44
16	3	509	CLA	C3B-C4B-NB	-2.10	108.66	110.53
16	7	503	CLA	CHA-C1A-NA	-2.10	121.64	126.39
16	7	505	CLA	C3B-C4B-NB	-2.09	108.66	110.53
16	A	824	CLA	CHD-C1D-ND	-2.09	121.86	124.80
16	A	837	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
16	5	417	CLA	CHD-C1D-ND	-2.09	121.86	124.80
16	B	837	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
16	B	837	CLA	C3B-C2B-C1B	-2.09	104.70	107.17
16	3	506	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
16	B	826	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
16	4	415	CLA	C3B-C4B-NB	-2.09	108.66	110.53
16	B	812	CLA	C1-C2-C3	-2.09	122.77	126.20
16	3	512	CLA	C3B-C4B-NB	-2.09	108.66	110.53
16	1	517	CLA	C3B-C2B-C1B	-2.09	104.70	107.17
16	5	406	CLA	C4A-NA-C1A	2.09	107.63	106.68
16	B	835	CLA	CHB-C4A-NA	2.09	127.42	124.40
16	6	508	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
16	7	510	CLA	CHD-C1D-ND	-2.09	121.86	124.80
16	A	839	CLA	C3B-C2B-C1B	-2.09	104.71	107.17
16	1	515	CLA	CHD-C1D-ND	-2.09	121.86	124.80
16	B	845	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
16	2	413	CLA	C1-C2-C3	-2.09	122.78	126.20
16	B	837	CLA	CHA-C1A-NA	-2.09	121.66	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	828	CLA	C3B-C4B-NB	-2.09	108.67	110.53
16	B	814	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
16	2	407	CLA	C4A-NA-C1A	2.09	107.63	106.68
16	7	501	CLA	CHD-C1D-ND	-2.09	121.87	124.80
16	A	840	CLA	CHD-C1D-ND	-2.09	121.87	124.80
16	7	506	CLA	C3B-C2B-C1B	-2.09	104.71	107.17
16	B	817	CLA	C3B-C4B-NB	-2.09	108.67	110.53
16	4	409	CLA	C1-C2-C3	-2.08	122.78	126.20
16	2	410	CLA	O2A-CGA-O1A	-2.08	118.41	123.63
16	4	404	CLA	CHD-C1D-ND	-2.08	121.87	124.80
16	1	514	CLA	CHB-C4A-NA	2.08	127.41	124.40
16	3	510	CLA	C3B-C4B-NB	-2.08	108.67	110.53
16	4	405	CLA	CHD-C1D-ND	-2.08	121.87	124.80
16	2	403	CLA	C3B-C4B-NB	-2.08	108.67	110.53
16	A	814	CLA	CHD-C1D-ND	-2.08	121.87	124.80
16	B	838	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
16	6	505	CLA	CMB-C2B-C1B	2.08	128.58	125.42
16	K	102	CLA	C3B-C2B-C1B	-2.08	104.72	107.17
16	A	827	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
16	A	838	CLA	C1C-C2C-C3C	-2.08	104.79	106.98
16	A	840	CLA	C3B-C4B-NB	-2.08	108.67	110.53
16	1	510	CLA	C4A-NA-C1A	2.08	107.63	106.68
16	B	838	CLA	CHD-C1D-ND	-2.08	121.88	124.80
16	B	847	CLA	CHD-C1D-ND	-2.08	121.88	124.80
16	1	517	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
16	A	815	CLA	O2A-CGA-O1A	-2.08	118.44	123.63
16	B	827	CLA	CHD-C1D-ND	-2.08	121.88	124.80
16	1	507	CLA	C3B-C4B-NB	-2.08	108.68	110.53
16	5	413	CLA	C1-C2-C3	-2.07	122.80	126.20
16	7	507	CLA	C4A-NA-C1A	2.07	107.62	106.68
16	A	843	CLA	C3B-C4B-NB	-2.07	108.68	110.53
16	A	832	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
16	3	504	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
16	B	813	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
16	A	806	CLA	C3B-C2B-C1B	-2.07	104.73	107.17
16	B	824	CLA	CHD-C1D-ND	-2.07	121.89	124.80
16	B	835	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
16	A	815	CLA	C1-C2-C3	-2.07	122.80	126.20
16	1	505	CLA	C2D-C1D-ND	-2.07	108.08	110.13
24	A	805	CL0	O2A-CGA-O1A	-2.07	118.45	123.63
16	B	835	CLA	C1-C2-C3	-2.07	122.81	126.20
16	K	103	CLA	O2A-CGA-O1A	-2.07	118.45	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	827	CLA	C3B-C2B-C1B	-2.07	104.73	107.17
16	4	410	CLA	CHB-C4A-NA	2.07	127.38	124.40
16	B	820	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
16	J	1101	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
16	B	832	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
16	4	406	CLA	CHA-C1A-NA	-2.06	121.72	126.39
16	B	823	CLA	C1-C2-C3	-2.06	122.81	126.20
16	B	830	CLA	CHD-C1D-ND	-2.06	121.90	124.80
16	B	830	CLA	CHA-C1A-NA	-2.06	121.72	126.39
16	4	407	CLA	CHB-C4A-NA	2.06	127.38	124.40
16	5	407	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
16	7	515	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
16	6	508	CLA	CMB-C2B-C1B	2.06	128.56	125.42
16	A	844	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
16	2	408	CLA	C3B-C2B-C1B	-2.06	104.74	107.17
16	7	508	CLA	C3B-C2B-C1B	-2.06	104.74	107.17
16	5	412	CLA	CHD-C1D-ND	-2.06	121.90	124.80
16	A	817	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
16	5	411	CLA	CHD-C1D-ND	-2.06	121.90	124.80
16	7	507	CLA	CHD-C1D-ND	-2.06	121.90	124.80
16	3	506	CLA	C3B-C4B-NB	-2.06	108.69	110.53
16	J	1102	CLA	C4A-NA-C1A	2.06	107.62	106.68
16	F	201	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
16	7	514	CLA	C4A-NA-C1A	2.05	107.62	106.68
16	4	417	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
16	B	818	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
16	B	810	CLA	C3B-C4B-NB	-2.05	108.70	110.53
16	1	526	CLA	CHD-C1D-ND	-2.05	121.92	124.80
16	6	502	CLA	CHD-C1D-ND	-2.05	121.92	124.80
16	2	402	CLA	CHD-C1D-ND	-2.05	121.92	124.80
16	7	517	CLA	C4A-NA-C1A	2.05	107.61	106.68
16	7	505	CLA	C3B-C2B-C1B	-2.05	104.75	107.17
16	3	507	CLA	CHD-C1D-ND	-2.05	121.92	124.80
16	7	508	CLA	CHD-C1D-ND	-2.05	121.92	124.80
16	B	833	CLA	CHD-C1D-ND	-2.05	121.92	124.80
16	6	502	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
16	B	801	CLA	C3B-C2B-C1B	-2.05	104.76	107.17
16	5	409	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
16	B	848	CLA	CHB-C4A-NA	2.04	127.35	124.40
16	4	407	CLA	CMB-C2B-C1B	2.04	128.53	125.42
16	4	418	CLA	CHA-C1A-NA	-2.04	121.77	126.39
16	1	508	CLA	C1-C2-C3	-2.04	122.85	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	823	CLA	C3B-C4B-NB	-2.04	108.71	110.53
16	5	418	CLA	CHB-C4A-NA	2.04	127.34	124.40
16	6	510	CLA	C3B-C2B-C1B	-2.04	104.76	107.17
16	A	823	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
16	B	812	CLA	CHD-C1D-ND	-2.04	121.93	124.80
16	5	406	CLA	CHB-C4A-NA	2.04	127.34	124.40
16	J	1103	CLA	CHD-C1D-ND	-2.04	121.93	124.80
16	A	836	CLA	C4A-NA-C1A	2.04	107.61	106.68
16	2	407	CLA	C4-C3-C2	-2.04	118.39	123.63
17	1	518	LUT	C19-C9-C10	-2.04	119.51	122.82
16	3	512	CLA	O2A-CGA-O1A	-2.04	118.09	123.33
16	1	515	CLA	CHB-C4A-NA	2.04	127.34	124.40
16	B	845	CLA	CHB-C4A-NA	2.04	127.34	124.40
16	4	408	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
16	A	843	CLA	C1-C2-C3	-2.04	122.86	126.20
16	A	827	CLA	CHD-C1D-ND	-2.04	121.94	124.80
16	1	514	CLA	CHD-C1D-ND	-2.04	121.94	124.80
16	7	515	CLA	C3B-C2B-C1B	-2.04	104.77	107.17
16	6	513	CLA	C3B-C2B-C1B	-2.03	104.77	107.17
16	5	406	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
16	7	510	CLA	C3B-C4B-NB	-2.03	108.72	110.53
16	4	403	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
16	5	409	CLA	CHB-C4A-NA	2.03	127.33	124.40
16	B	842	CLA	CHB-C4A-NA	2.03	127.33	124.40
16	B	839	CLA	CHB-C4A-NA	2.03	127.33	124.40
16	A	832	CLA	C1-C2-C3	-2.03	122.87	126.20
16	2	411	CLA	CHD-C1D-ND	-2.03	121.94	124.80
16	3	512	CLA	CHD-C1D-ND	-2.03	121.94	124.80
16	F	202	CLA	CHB-C4A-NA	2.03	127.33	124.40
16	A	852	CLA	C3B-C2B-C1B	-2.03	104.78	107.17
16	1	507	CLA	CHD-C1D-ND	-2.03	121.94	124.80
16	4	407	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
16	7	506	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
16	3	507	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
16	1	506	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
16	1	508	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
16	B	838	CLA	C4A-NA-C1A	2.03	107.60	106.68
16	7	512	CLA	CHD-C1D-ND	-2.03	121.95	124.80
16	B	833	CLA	C3B-C4B-NB	-2.03	108.72	110.53
16	6	505	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
16	A	826	CLA	C1-C2-C3	-2.03	122.88	126.20
16	2	407	CLA	C3B-C4B-NB	-2.02	108.72	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	825	CLA	O2A-CGA-O1A	-2.02	118.56	123.63
16	A	810	CLA	C1-C2-C3	-2.02	123.49	126.76
16	B	821	CLA	C1-C2-C3	-2.02	122.88	126.20
16	A	832	CLA	C3B-C4B-NB	-2.02	108.72	110.53
16	B	839	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
16	B	829	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
16	B	815	CLA	C3B-C4B-NB	-2.02	108.73	110.53
16	2	401	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
16	A	813	CLA	C3B-C4B-NB	-2.02	108.73	110.53
16	1	511	CLA	CHB-C4A-NA	2.02	127.31	124.40
16	B	833	CLA	CHB-C4A-NA	2.02	127.31	124.40
16	2	411	CLA	CMB-C2B-C1B	2.02	128.49	125.42
16	4	414	CLA	C3B-C4B-NB	-2.02	108.73	110.53
16	A	836	CLA	O2A-CGA-O1A	-2.02	118.59	123.63
16	B	816	CLA	CHD-C1D-ND	-2.01	121.97	124.80
16	A	808	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
16	J	1102	CLA	CHD-C1D-ND	-2.01	121.97	124.80
16	5	407	CLA	C4-C3-C5	2.01	118.72	115.23
16	J	1101	CLA	C1-C2-C3	-2.01	122.90	126.20
16	2	410	CLA	CHD-C1D-ND	-2.01	121.97	124.80
16	B	842	CLA	O2A-CGA-O1A	-2.01	118.16	123.33
16	A	829	CLA	C3B-C4B-NB	-2.01	108.73	110.53
16	1	525	CLA	CHD-C1D-ND	-2.01	121.97	124.80
16	4	416	CLA	C3B-C2B-C1B	-2.01	104.80	107.17
16	4	405	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
16	6	502	CLA	C3B-C4B-NB	-2.01	108.74	110.53
16	4	416	CLA	CHB-C4A-NA	2.01	127.30	124.40
16	B	823	CLA	C3B-C2B-C1B	-2.01	104.80	107.17
16	5	404	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
16	A	838	CLA	C3B-C4B-NB	-2.01	108.74	110.53
16	6	511	CLA	C3B-C4B-NB	-2.01	108.74	110.53
16	B	821	CLA	C3B-C4B-NB	-2.01	108.74	110.53
16	3	507	CLA	CHB-C4A-NA	2.01	127.30	124.40
16	B	846	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
16	6	507	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
16	6	512	CLA	C1C-C2C-C3C	-2.00	104.87	106.98
16	7	507	CLA	C3B-C4B-NB	-2.00	108.74	110.53
16	B	822	CLA	C3B-C4B-NB	-2.00	108.74	110.53
16	A	818	CLA	C3B-C4B-NB	-2.00	108.74	110.53
16	A	836	CLA	C3B-C2B-C1B	-2.00	104.81	107.17
16	1	506	CLA	CMB-C2B-C1B	2.00	128.47	125.42

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	1	518	LUT	C26

All (2026) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	1	501	CLA	C4B-C3B-CAB-CBB
16	1	502	CLA	C2B-C3B-CAB-CBB
16	1	502	CLA	C4B-C3B-CAB-CBB
16	1	505	CLA	C1A-C2A-CAA-CBA
16	1	505	CLA	CBD-CGD-O2D-CED
16	1	506	CLA	C1A-C2A-CAA-CBA
16	1	508	CLA	C1A-C2A-CAA-CBA
16	1	508	CLA	C3A-C2A-CAA-CBA
16	1	508	CLA	CAD-CBD-CGD-O1D
16	1	508	CLA	CAD-CBD-CGD-O2D
16	1	510	CLA	CHA-CBD-CGD-O2D
16	1	511	CLA	C1A-C2A-CAA-CBA
16	1	511	CLA	C3A-C2A-CAA-CBA
16	1	512	CLA	CHA-CBD-CGD-O1D
16	1	512	CLA	CHA-CBD-CGD-O2D
16	1	514	CLA	CBD-CGD-O2D-CED
16	1	515	CLA	C1A-C2A-CAA-CBA
16	1	515	CLA	C3A-C2A-CAA-CBA
16	1	515	CLA	C4B-C3B-CAB-CBB
16	1	526	CLA	CAD-CBD-CGD-O1D
16	1	526	CLA	CAD-CBD-CGD-O2D
16	2	403	CLA	C1A-C2A-CAA-CBA
16	2	404	CLA	C4B-C3B-CAB-CBB
16	2	406	CLA	CBD-CGD-O2D-CED
16	2	408	CLA	CBD-CGD-O2D-CED
16	2	408	CLA	C4-C3-C5-C6
16	2	409	CLA	C1A-C2A-CAA-CBA
16	2	410	CLA	CBD-CGD-O2D-CED
16	2	412	CLA	C1A-C2A-CAA-CBA
16	2	412	CLA	C3A-C2A-CAA-CBA
16	2	412	CLA	CBD-CGD-O2D-CED
16	2	413	CLA	C1A-C2A-CAA-CBA
16	2	414	CLA	CBD-CGD-O2D-CED
16	2	415	CLA	CHA-CBD-CGD-O1D
16	2	415	CLA	CHA-CBD-CGD-O2D
16	3	501	CLA	CHA-CBD-CGD-O1D
16	3	501	CLA	CHA-CBD-CGD-O2D
16	3	501	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	3	503	CLA	CBD-CGD-O2D-CED
16	3	504	CLA	C1A-C2A-CAA-CBA
16	3	504	CLA	C3A-C2A-CAA-CBA
16	3	504	CLA	CBD-CGD-O2D-CED
16	3	505	CLA	C1A-C2A-CAA-CBA
16	3	505	CLA	C3A-C2A-CAA-CBA
16	3	506	CLA	CHA-CBD-CGD-O1D
16	3	506	CLA	CHA-CBD-CGD-O2D
16	3	508	CLA	C6-C7-C8-C9
16	3	509	CLA	CHA-CBD-CGD-O1D
16	3	509	CLA	CHA-CBD-CGD-O2D
16	3	509	CLA	C2-C3-C5-C6
16	3	509	CLA	C4-C3-C5-C6
16	3	510	CLA	C1A-C2A-CAA-CBA
16	3	512	CLA	C1A-C2A-CAA-CBA
16	3	512	CLA	C3A-C2A-CAA-CBA
16	3	512	CLA	CAD-CBD-CGD-O1D
16	3	512	CLA	CAD-CBD-CGD-O2D
16	4	402	CLA	C1A-C2A-CAA-CBA
16	4	405	CLA	C1A-C2A-CAA-CBA
16	4	405	CLA	CBD-CGD-O2D-CED
16	4	406	CLA	C1A-C2A-CAA-CBA
16	4	406	CLA	C3A-C2A-CAA-CBA
16	4	410	CLA	CBD-CGD-O2D-CED
16	4	411	CLA	O2A-C1-C2-C3
16	4	412	CLA	C1A-C2A-CAA-CBA
16	4	416	CLA	C1A-C2A-CAA-CBA
16	5	404	CLA	CHA-CBD-CGD-O1D
16	5	404	CLA	CHA-CBD-CGD-O2D
16	5	406	CLA	C1A-C2A-CAA-CBA
16	5	406	CLA	C3A-C2A-CAA-CBA
16	5	406	CLA	CBD-CGD-O2D-CED
16	5	407	CLA	CAD-CBD-CGD-O1D
16	5	407	CLA	CAD-CBD-CGD-O2D
16	5	409	CLA	CBD-CGD-O2D-CED
16	5	410	CLA	CHA-CBD-CGD-O1D
16	5	410	CLA	CHA-CBD-CGD-O2D
16	5	411	CLA	C4B-C3B-CAB-CBB
16	5	411	CLA	CBD-CGD-O2D-CED
16	5	412	CLA	CAD-CBD-CGD-O2D
16	5	413	CLA	C1A-C2A-CAA-CBA
16	5	413	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	6	502	CLA	CHA-CBD-CGD-O1D
16	6	502	CLA	CHA-CBD-CGD-O2D
16	6	503	CLA	CBD-CGD-O2D-CED
16	6	504	CLA	C1A-C2A-CAA-CBA
16	6	504	CLA	CHA-CBD-CGD-O1D
16	6	504	CLA	CHA-CBD-CGD-O2D
16	6	505	CLA	C1A-C2A-CAA-CBA
16	6	505	CLA	C3A-C2A-CAA-CBA
16	6	506	CLA	CBD-CGD-O2D-CED
16	6	509	CLA	CBD-CGD-O2D-CED
16	6	510	CLA	CAD-CBD-CGD-O1D
16	6	510	CLA	CAD-CBD-CGD-O2D
16	6	512	CLA	CBD-CGD-O2D-CED
16	6	514	CLA	CBD-CGD-O2D-CED
16	6	515	CLA	C1A-C2A-CAA-CBA
16	6	515	CLA	CBD-CGD-O2D-CED
16	7	501	CLA	CBD-CGD-O2D-CED
16	7	502	CLA	CHA-CBD-CGD-O1D
16	7	502	CLA	CHA-CBD-CGD-O2D
16	7	503	CLA	CBD-CGD-O2D-CED
16	7	504	CLA	CHA-CBD-CGD-O1D
16	7	504	CLA	CHA-CBD-CGD-O2D
16	7	504	CLA	CBD-CGD-O2D-CED
16	7	505	CLA	CBD-CGD-O2D-CED
16	7	506	CLA	C4B-C3B-CAB-CBB
16	7	506	CLA	CBD-CGD-O2D-CED
16	7	507	CLA	CBD-CGD-O2D-CED
16	7	508	CLA	CHA-CBD-CGD-O1D
16	7	508	CLA	CHA-CBD-CGD-O2D
16	7	511	CLA	NA-C4A-CHB-C1B
16	7	511	CLA	C2C-C1C-CHC-C4B
16	7	511	CLA	C1B-C2B-C3B-C4B
16	7	511	CLA	CMB-C2B-C3B-C4B
16	7	511	CLA	C2B-C3B-C4B-CHC
16	7	511	CLA	CBD-CGD-O2D-CED
16	7	512	CLA	CBD-CGD-O2D-CED
16	7	514	CLA	CBD-CGD-O2D-CED
16	7	515	CLA	C1A-C2A-CAA-CBA
16	7	515	CLA	CBD-CGD-O2D-CED
16	7	516	CLA	CBD-CGD-O2D-CED
16	A	807	CLA	CHA-CBD-CGD-O1D
16	A	807	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
16	A	808	CLA	C1A-C2A-CAA-CBA
16	A	808	CLA	C3A-C2A-CAA-CBA
16	A	809	CLA	C1A-C2A-CAA-CBA
16	A	809	CLA	CHA-CBD-CGD-O1D
16	A	809	CLA	CHA-CBD-CGD-O2D
16	A	809	CLA	CBD-CGD-O2D-CED
16	A	810	CLA	C2-C1-O2A-CGA
16	A	811	CLA	CHA-CBD-CGD-O1D
16	A	811	CLA	CHA-CBD-CGD-O2D
16	A	814	CLA	C1A-C2A-CAA-CBA
16	A	814	CLA	C3A-C2A-CAA-CBA
16	A	817	CLA	C1A-C2A-CAA-CBA
16	A	821	CLA	C3A-C2A-CAA-CBA
16	A	824	CLA	O1A-CGA-O2A-C1
16	A	830	CLA	C1A-C2A-CAA-CBA
16	A	830	CLA	C11-C10-C8-C9
16	A	835	CLA	C2B-C3B-CAB-CBB
16	A	835	CLA	C4B-C3B-CAB-CBB
16	A	836	CLA	CHA-CBD-CGD-O1D
16	A	836	CLA	CHA-CBD-CGD-O2D
16	A	837	CLA	C2-C3-C5-C6
16	A	839	CLA	C2-C3-C5-C6
16	A	839	CLA	C4-C3-C5-C6
16	A	840	CLA	C1A-C2A-CAA-CBA
16	B	815	CLA	C1A-C2A-CAA-CBA
16	B	815	CLA	CHA-CBD-CGD-O1D
16	B	815	CLA	CHA-CBD-CGD-O2D
16	B	822	CLA	C1A-C2A-CAA-CBA
16	B	822	CLA	CHA-CBD-CGD-O1D
16	B	822	CLA	CHA-CBD-CGD-O2D
16	B	823	CLA	C1A-C2A-CAA-CBA
16	B	824	CLA	C2B-C3B-CAB-CBB
16	B	825	CLA	C1A-C2A-CAA-CBA
16	B	825	CLA	C3A-C2A-CAA-CBA
16	B	831	CLA	CHA-CBD-CGD-O1D
16	B	831	CLA	CHA-CBD-CGD-O2D
16	B	832	CLA	CHA-CBD-CGD-O1D
16	B	832	CLA	CHA-CBD-CGD-O2D
16	B	834	CLA	C1A-C2A-CAA-CBA
16	B	834	CLA	C3A-C2A-CAA-CBA
16	B	836	CLA	CHA-CBD-CGD-O1D
16	B	836	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
16	B	837	CLA	C1A-C2A-CAA-CBA
16	B	837	CLA	C3A-C2A-CAA-CBA
16	B	837	CLA	CBD-CGD-O2D-CED
16	B	841	CLA	C3A-C2A-CAA-CBA
16	J	1101	CLA	C1A-C2A-CAA-CBA
16	J	1101	CLA	C3A-C2A-CAA-CBA
16	J	1101	CLA	CHA-CBD-CGD-O1D
16	J	1101	CLA	CHA-CBD-CGD-O2D
16	K	102	CLA	C4B-C3B-CAB-CBB
16	K	103	CLA	CBD-CGD-O2D-CED
17	1	518	LUT	C7-C8-C9-C10
17	1	518	LUT	C21-C26-C27-C28
17	1	518	LUT	C27-C28-C29-C30
17	1	518	LUT	C27-C28-C29-C39
17	1	518	LUT	C29-C30-C31-C32
18	1	522	BCR	C11-C12-C13-C14
18	1	522	BCR	C19-C20-C21-C22
18	1	523	BCR	C7-C8-C9-C10
18	2	416	BCR	C5-C6-C7-C8
18	2	416	BCR	C21-C22-C23-C24
18	2	416	BCR	C37-C22-C23-C24
18	2	418	BCR	C1-C6-C7-C8
18	2	418	BCR	C5-C6-C7-C8
18	2	418	BCR	C21-C22-C23-C24
18	2	418	BCR	C23-C24-C25-C26
18	3	515	BCR	C1-C6-C7-C8
18	3	515	BCR	C5-C6-C7-C8
18	3	516	BCR	C17-C18-C19-C20
18	4	419	BCR	C1-C6-C7-C8
18	4	419	BCR	C5-C6-C7-C8
18	4	419	BCR	C9-C10-C11-C12
18	4	419	BCR	C11-C12-C13-C14
18	4	419	BCR	C21-C22-C23-C24
18	4	419	BCR	C37-C22-C23-C24
18	4	419	BCR	C23-C24-C25-C30
18	5	420	BCR	C5-C6-C7-C8
18	5	420	BCR	C17-C18-C19-C20
18	5	420	BCR	C36-C18-C19-C20
18	6	518	BCR	C1-C6-C7-C8
18	6	518	BCR	C17-C18-C19-C20
18	6	518	BCR	C21-C22-C23-C24
18	6	518	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
18	6	521	BCR	C23-C24-C25-C26
18	6	521	BCR	C23-C24-C25-C30
18	7	518	BCR	C1-C6-C7-C8
18	7	518	BCR	C5-C6-C7-C8
18	A	845	BCR	C11-C12-C13-C14
18	A	845	BCR	C11-C12-C13-C35
18	A	845	BCR	C17-C18-C19-C20
18	A	850	BCR	C7-C8-C9-C10
18	B	804	BCR	C5-C6-C7-C8
18	B	804	BCR	C7-C8-C9-C10
18	B	804	BCR	C7-C8-C9-C34
18	B	804	BCR	C17-C18-C19-C20
18	B	849	BCR	C11-C12-C13-C14
18	B	849	BCR	C11-C12-C13-C35
18	B	850	BCR	C11-C12-C13-C14
18	B	852	BCR	C21-C22-C23-C24
18	B	853	BCR	C11-C12-C13-C14
18	F	203	BCR	C11-C12-C13-C14
18	F	203	BCR	C17-C18-C19-C20
18	F	203	BCR	C36-C18-C19-C20
18	F	203	BCR	C21-C22-C23-C24
18	F	203	BCR	C37-C22-C23-C24
18	I	101	BCR	C17-C18-C19-C20
18	I	101	BCR	C21-C22-C23-C24
18	I	101	BCR	C37-C22-C23-C24
18	I	101	BCR	C23-C24-C25-C26
18	I	102	BCR	C5-C6-C7-C8
18	K	101	BCR	C23-C24-C25-C26
18	K	101	BCR	C23-C24-C25-C30
18	M	101	BCR	C17-C18-C19-C20
19	A	851	LMG	O6-C1-O1-C7
21	3	517	LHG	C2-C3-O3-P
21	4	421	LHG	C2-C3-O3-P
21	5	424	LHG	C2-C3-O3-P
21	5	424	LHG	C4-O6-P-O3
21	5	424	LHG	C4-O6-P-O4
21	A	802	LHG	C3-O3-P-O5
21	B	806	LHG	C4-O6-P-O4
23	B	807	LMT	O5'-C1'-O1'-C1
23	I	103	LMT	C2'-C1'-O1'-C1
23	I	103	LMT	O5'-C1'-O1'-C1
25	A	853	ECH	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	A	853	ECH	C7-C8-C9-C10
25	A	853	ECH	C7-C8-C9-C34
25	A	853	ECH	C11-C12-C13-C14
25	A	853	ECH	C11-C12-C13-C35
25	B	851	ECH	C21-C22-C23-C24
25	B	851	ECH	C37-C22-C23-C24
16	2	414	CLA	C2C-C3C-CAC-CBC
16	2	404	CLA	O1D-CGD-O2D-CED
16	6	504	CLA	O1D-CGD-O2D-CED
16	3	512	CLA	O1D-CGD-O2D-CED
16	4	405	CLA	O1D-CGD-O2D-CED
16	5	406	CLA	O1D-CGD-O2D-CED
16	5	411	CLA	O1D-CGD-O2D-CED
16	6	512	CLA	O1D-CGD-O2D-CED
16	6	515	CLA	O1D-CGD-O2D-CED
16	7	503	CLA	O1D-CGD-O2D-CED
16	7	505	CLA	O1D-CGD-O2D-CED
16	7	515	CLA	O1D-CGD-O2D-CED
16	B	837	CLA	O1D-CGD-O2D-CED
16	1	507	CLA	CBD-CGD-O2D-CED
16	1	513	CLA	CBD-CGD-O2D-CED
16	1	515	CLA	CBD-CGD-O2D-CED
16	2	404	CLA	CBD-CGD-O2D-CED
16	3	506	CLA	CBD-CGD-O2D-CED
16	3	512	CLA	CBD-CGD-O2D-CED
16	4	418	CLA	CBD-CGD-O2D-CED
16	5	418	CLA	CBD-CGD-O2D-CED
16	6	504	CLA	CBD-CGD-O2D-CED
16	7	510	CLA	CBD-CGD-O2D-CED
16	A	814	CLA	CBD-CGD-O2D-CED
16	A	826	CLA	CBD-CGD-O2D-CED
16	B	809	CLA	CBD-CGD-O2D-CED
16	B	813	CLA	CBD-CGD-O2D-CED
16	B	848	CLA	CBD-CGD-O2D-CED
16	J	1102	CLA	CBD-CGD-O2D-CED
16	1	510	CLA	O1A-CGA-O2A-C1
16	2	409	CLA	O1A-CGA-O2A-C1
16	4	415	CLA	O1A-CGA-O2A-C1
16	7	509	CLA	O1A-CGA-O2A-C1
16	A	811	CLA	O1A-CGA-O2A-C1
16	A	828	CLA	O1A-CGA-O2A-C1
16	B	812	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	B	837	CLA	O1A-CGA-O2A-C1
16	B	848	CLA	O1A-CGA-O2A-C1
16	2	408	CLA	O1D-CGD-O2D-CED
16	2	412	CLA	O1D-CGD-O2D-CED
16	5	418	CLA	O1D-CGD-O2D-CED
16	6	503	CLA	O1D-CGD-O2D-CED
16	6	514	CLA	O1D-CGD-O2D-CED
16	7	501	CLA	O1D-CGD-O2D-CED
16	7	504	CLA	O1D-CGD-O2D-CED
16	K	103	CLA	O1D-CGD-O2D-CED
21	4	421	LHG	C5-C6-O8-C23
16	2	414	CLA	C4C-C3C-CAC-CBC
16	1	515	CLA	O1D-CGD-O2D-CED
16	4	411	CLA	CBA-CGA-O2A-C1
16	A	824	CLA	CBA-CGA-O2A-C1
16	1	504	CLA	CBD-CGD-O2D-CED
16	1	506	CLA	CBD-CGD-O2D-CED
16	6	516	CLA	CBD-CGD-O2D-CED
16	A	822	CLA	CBD-CGD-O2D-CED
16	1	502	CLA	O1A-CGA-O2A-C1
16	1	509	CLA	O1A-CGA-O2A-C1
16	2	401	CLA	O1A-CGA-O2A-C1
16	4	411	CLA	O1A-CGA-O2A-C1
16	5	412	CLA	O1A-CGA-O2A-C1
16	6	502	CLA	O1A-CGA-O2A-C1
16	6	504	CLA	O1A-CGA-O2A-C1
16	6	515	CLA	O1A-CGA-O2A-C1
16	7	515	CLA	O1A-CGA-O2A-C1
16	A	806	CLA	O1A-CGA-O2A-C1
16	A	808	CLA	O1A-CGA-O2A-C1
16	A	815	CLA	O1A-CGA-O2A-C1
16	A	816	CLA	O1A-CGA-O2A-C1
16	A	825	CLA	O1A-CGA-O2A-C1
16	B	821	CLA	O1A-CGA-O2A-C1
16	B	838	CLA	O1A-CGA-O2A-C1
16	K	103	CLA	O1A-CGA-O2A-C1
19	A	851	LMG	O10-C28-O8-C9
21	5	424	LHG	O10-C23-O8-C6
23	B	808	LMT	C3'-C4'-O1B-C1B
16	1	514	CLA	O1D-CGD-O2D-CED
16	2	410	CLA	O1D-CGD-O2D-CED
16	3	504	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	5	413	CLA	O1D-CGD-O2D-CED
16	6	506	CLA	O1D-CGD-O2D-CED
16	6	509	CLA	O1D-CGD-O2D-CED
16	7	507	CLA	O1D-CGD-O2D-CED
16	7	514	CLA	O1D-CGD-O2D-CED
16	7	516	CLA	O1D-CGD-O2D-CED
23	A	804	LMT	C3'-C4'-O1B-C1B
16	2	406	CLA	O1D-CGD-O2D-CED
16	2	414	CLA	O1D-CGD-O2D-CED
16	4	410	CLA	O1D-CGD-O2D-CED
16	5	409	CLA	O1D-CGD-O2D-CED
16	7	506	CLA	O1D-CGD-O2D-CED
16	7	511	CLA	O1D-CGD-O2D-CED
16	A	809	CLA	O1D-CGD-O2D-CED
16	6	511	CLA	CBD-CGD-O2D-CED
16	1	508	CLA	C3-C5-C6-C7
16	2	409	CLA	C3-C5-C6-C7
16	2	410	CLA	C3-C5-C6-C7
16	3	510	CLA	C3-C5-C6-C7
16	4	410	CLA	C3-C5-C6-C7
16	4	411	CLA	C3-C5-C6-C7
16	4	417	CLA	C3-C5-C6-C7
16	6	505	CLA	C3-C5-C6-C7
16	A	814	CLA	C3-C5-C6-C7
16	A	840	CLA	C3-C5-C6-C7
21	5	424	LHG	C5-C6-O8-C23
16	3	501	CLA	O1D-CGD-O2D-CED
16	1	502	CLA	CBA-CGA-O2A-C1
16	1	503	CLA	CBA-CGA-O2A-C1
16	1	510	CLA	CBA-CGA-O2A-C1
16	2	409	CLA	CBA-CGA-O2A-C1
16	4	415	CLA	CBA-CGA-O2A-C1
16	5	411	CLA	CBA-CGA-O2A-C1
16	5	412	CLA	CBA-CGA-O2A-C1
16	6	504	CLA	CBA-CGA-O2A-C1
16	7	509	CLA	CBA-CGA-O2A-C1
16	A	806	CLA	CBA-CGA-O2A-C1
16	A	811	CLA	CBA-CGA-O2A-C1
16	A	815	CLA	CBA-CGA-O2A-C1
16	A	828	CLA	CBA-CGA-O2A-C1
16	A	837	CLA	CBA-CGA-O2A-C1
16	A	841	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	B	812	CLA	CBA-CGA-O2A-C1
16	B	837	CLA	CBA-CGA-O2A-C1
16	B	848	CLA	CBA-CGA-O2A-C1
19	A	851	LMG	C29-C28-O8-C9
21	5	424	LHG	C24-C23-O8-C6
20	4	401	LMU	C5'-C4'-O1B-C1B
16	3	510	CLA	CBD-CGD-O2D-CED
16	4	408	CLA	CBD-CGD-O2D-CED
16	4	414	CLA	CBD-CGD-O2D-CED
16	5	414	CLA	CBD-CGD-O2D-CED
16	A	812	CLA	CBD-CGD-O2D-CED
16	B	811	CLA	CBD-CGD-O2D-CED
16	B	825	CLA	CBD-CGD-O2D-CED
16	B	835	CLA	CBD-CGD-O2D-CED
16	K	102	CLA	CBD-CGD-O2D-CED
16	X	101	CLA	CBD-CGD-O2D-CED
16	1	505	CLA	O1D-CGD-O2D-CED
16	1	507	CLA	O1D-CGD-O2D-CED
16	3	503	CLA	O1D-CGD-O2D-CED
16	A	826	CLA	O1D-CGD-O2D-CED
16	B	823	CLA	O1A-CGA-O2A-C1
16	7	512	CLA	O1D-CGD-O2D-CED
16	1	505	CLA	C4-C3-C5-C6
16	4	407	CLA	C4-C3-C5-C6
16	5	408	CLA	C4-C3-C5-C6
16	B	837	CLA	C4-C3-C5-C6
16	2	408	CLA	C2-C3-C5-C6
16	4	407	CLA	C2-C3-C5-C6
16	5	408	CLA	C2-C3-C5-C6
16	B	837	CLA	C2-C3-C5-C6
16	3	507	CLA	CBD-CGD-O2D-CED
16	4	415	CLA	CBD-CGD-O2D-CED
16	A	814	CLA	O1D-CGD-O2D-CED
16	J	1102	CLA	O1D-CGD-O2D-CED
21	5	425	LHG	O10-C23-O8-C6
16	3	507	CLA	C3-C5-C6-C7
16	4	406	CLA	C3-C5-C6-C7
16	B	815	CLA	C3-C5-C6-C7
16	1	509	CLA	CBA-CGA-O2A-C1
16	2	401	CLA	CBA-CGA-O2A-C1
16	3	506	CLA	CBA-CGA-O2A-C1
16	4	410	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	5	404	CLA	CBA-CGA-O2A-C1
16	5	407	CLA	CBA-CGA-O2A-C1
16	6	502	CLA	CBA-CGA-O2A-C1
16	6	515	CLA	CBA-CGA-O2A-C1
16	7	515	CLA	CBA-CGA-O2A-C1
16	A	808	CLA	CBA-CGA-O2A-C1
16	A	816	CLA	CBA-CGA-O2A-C1
16	A	825	CLA	CBA-CGA-O2A-C1
16	A	829	CLA	CBA-CGA-O2A-C1
16	A	831	CLA	CBA-CGA-O2A-C1
16	A	840	CLA	CBA-CGA-O2A-C1
16	B	809	CLA	CBA-CGA-O2A-C1
16	B	821	CLA	CBA-CGA-O2A-C1
16	B	823	CLA	CBA-CGA-O2A-C1
16	B	838	CLA	CBA-CGA-O2A-C1
16	B	839	CLA	CBA-CGA-O2A-C1
16	B	846	CLA	CBA-CGA-O2A-C1
16	K	103	CLA	CBA-CGA-O2A-C1
18	7	518	BCR	C19-C20-C21-C22
16	1	503	CLA	O1A-CGA-O2A-C1
16	2	408	CLA	O1A-CGA-O2A-C1
16	3	506	CLA	O1A-CGA-O2A-C1
16	4	410	CLA	O1A-CGA-O2A-C1
16	4	417	CLA	O1A-CGA-O2A-C1
16	5	407	CLA	O1A-CGA-O2A-C1
16	5	411	CLA	O1A-CGA-O2A-C1
16	7	508	CLA	O1A-CGA-O2A-C1
16	A	810	CLA	O1A-CGA-O2A-C1
16	A	829	CLA	O1A-CGA-O2A-C1
16	A	837	CLA	O1A-CGA-O2A-C1
16	B	836	CLA	O1A-CGA-O2A-C1
16	B	839	CLA	O1A-CGA-O2A-C1
21	3	517	LHG	O10-C23-O8-C6
16	3	506	CLA	O1D-CGD-O2D-CED
16	B	813	CLA	O1D-CGD-O2D-CED
16	B	848	CLA	O1D-CGD-O2D-CED
16	5	407	CLA	C3-C5-C6-C7
16	B	825	CLA	C3-C5-C6-C7
16	B	841	CLA	C3-C5-C6-C7
16	B	845	CLA	C3-C5-C6-C7
16	2	411	CLA	CBD-CGD-O2D-CED
16	4	412	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	6	517	CLA	CBD-CGD-O2D-CED
16	A	838	CLA	CBD-CGD-O2D-CED
16	B	810	CLA	CBD-CGD-O2D-CED
21	A	803	LHG	O2-C2-C3-O3
16	4	418	CLA	O1D-CGD-O2D-CED
16	B	809	CLA	O1D-CGD-O2D-CED
16	2	410	CLA	CBA-CGA-O2A-C1
16	4	407	CLA	CBA-CGA-O2A-C1
16	6	507	CLA	CBA-CGA-O2A-C1
16	A	809	CLA	CBA-CGA-O2A-C1
16	B	836	CLA	CBA-CGA-O2A-C1
16	J	1101	CLA	CBA-CGA-O2A-C1
16	1	504	CLA	O1A-CGA-O2A-C1
16	A	831	CLA	O1A-CGA-O2A-C1
16	A	840	CLA	O1A-CGA-O2A-C1
16	A	841	CLA	O1A-CGA-O2A-C1
21	3	517	LHG	C8-C7-O7-C5
23	B	807	LMT	C3'-C4'-O1B-C1B
16	5	404	CLA	O1A-CGA-O2A-C1
16	7	510	CLA	O1D-CGD-O2D-CED
16	2	404	CLA	C3-C5-C6-C7
16	3	509	CLA	C3-C5-C6-C7
16	5	408	CLA	C3-C5-C6-C7
16	5	412	CLA	CBD-CGD-O2D-CED
16	B	826	CLA	CBD-CGD-O2D-CED
16	1	504	CLA	CBA-CGA-O2A-C1
16	2	408	CLA	CBA-CGA-O2A-C1
16	4	417	CLA	CBA-CGA-O2A-C1
16	7	508	CLA	CBA-CGA-O2A-C1
16	A	810	CLA	CBA-CGA-O2A-C1
21	3	517	LHG	C24-C23-O8-C6
21	5	425	LHG	C24-C23-O8-C6
16	B	847	CLA	C4-C3-C5-C6
16	1	505	CLA	C2-C3-C5-C6
16	B	847	CLA	C2-C3-C5-C6
16	4	407	CLA	O1A-CGA-O2A-C1
16	A	809	CLA	O1A-CGA-O2A-C1
16	B	809	CLA	O1A-CGA-O2A-C1
16	J	1101	CLA	O1A-CGA-O2A-C1
16	2	407	CLA	CBD-CGD-O2D-CED
16	6	508	CLA	CBD-CGD-O2D-CED
16	F	201	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	4	407	CLA	C2A-CAA-CBA-CGA
16	A	824	CLA	C2A-CAA-CBA-CGA
16	A	830	CLA	C2A-CAA-CBA-CGA
16	A	832	CLA	C2A-CAA-CBA-CGA
16	1	513	CLA	O1D-CGD-O2D-CED
16	2	410	CLA	O1A-CGA-O2A-C1
16	B	846	CLA	O1A-CGA-O2A-C1
16	6	508	CLA	C3-C5-C6-C7
22	A	801	PQN	C13-C15-C16-C17
16	A	827	CLA	CBA-CGA-O2A-C1
16	B	814	CLA	CBA-CGA-O2A-C1
16	B	815	CLA	CBA-CGA-O2A-C1
16	1	502	CLA	CBD-CGD-O2D-CED
16	5	403	CLA	CBD-CGD-O2D-CED
16	7	513	CLA	CBD-CGD-O2D-CED
16	A	807	CLA	CBD-CGD-O2D-CED
16	A	813	CLA	CBD-CGD-O2D-CED
16	A	840	CLA	CBD-CGD-O2D-CED
16	B	831	CLA	CBD-CGD-O2D-CED
16	B	840	CLA	CBD-CGD-O2D-CED
16	6	507	CLA	O1A-CGA-O2A-C1
16	1	506	CLA	O1D-CGD-O2D-CED
16	6	516	CLA	O1D-CGD-O2D-CED
16	A	822	CLA	O1D-CGD-O2D-CED
16	1	517	CLA	CBD-CGD-O2D-CED
16	4	402	CLA	CBD-CGD-O2D-CED
16	6	513	CLA	CBD-CGD-O2D-CED
16	7	508	CLA	CBD-CGD-O2D-CED
16	A	833	CLA	CBD-CGD-O2D-CED
16	B	832	CLA	CBD-CGD-O2D-CED
16	B	814	CLA	O1A-CGA-O2A-C1
16	B	815	CLA	O1A-CGA-O2A-C1
21	A	803	LHG	C1-C2-C3-O3
16	1	504	CLA	O1D-CGD-O2D-CED
16	2	407	CLA	CBA-CGA-O2A-C1
16	3	509	CLA	CBA-CGA-O2A-C1
16	4	402	CLA	CBA-CGA-O2A-C1
16	4	403	CLA	CBA-CGA-O2A-C1
16	4	408	CLA	CBA-CGA-O2A-C1
16	4	416	CLA	CBA-CGA-O2A-C1
16	6	509	CLA	CBA-CGA-O2A-C1
16	A	813	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	A	844	CLA	CBA-CGA-O2A-C1
16	B	813	CLA	CBA-CGA-O2A-C1
16	B	829	CLA	CBA-CGA-O2A-C1
16	B	830	CLA	CBA-CGA-O2A-C1
16	B	835	CLA	CBA-CGA-O2A-C1
16	B	840	CLA	CBA-CGA-O2A-C1
16	B	841	CLA	CBA-CGA-O2A-C1
21	4	421	LHG	C24-C23-O8-C6
16	1	512	CLA	CBD-CGD-O2D-CED
16	4	411	CLA	CBD-CGD-O2D-CED
16	5	417	CLA	CBD-CGD-O2D-CED
16	6	511	CLA	O1D-CGD-O2D-CED
16	2	407	CLA	C4-C3-C5-C6
16	2	407	CLA	C2-C3-C5-C6
16	B	838	CLA	CBD-CGD-O2D-CED
16	1	516	CLA	C11-C10-C8-C9
16	2	413	CLA	C6-C7-C8-C9
16	5	417	CLA	C11-C12-C13-C14
16	7	509	CLA	C11-C10-C8-C9
16	A	830	CLA	C11-C12-C13-C14
16	A	844	CLA	C14-C13-C15-C16
16	B	810	CLA	C11-C12-C13-C14
16	B	815	CLA	C11-C12-C13-C14
16	B	832	CLA	C14-C13-C15-C16
16	B	838	CLA	C11-C12-C13-C14
16	B	846	CLA	C11-C10-C8-C9
16	A	812	CLA	O1D-CGD-O2D-CED
16	B	825	CLA	O1D-CGD-O2D-CED
16	X	101	CLA	O1D-CGD-O2D-CED
23	B	807	LMT	C2'-C1'-O1'-C1
16	5	408	CLA	CBA-CGA-O2A-C1
16	A	813	CLA	O1A-CGA-O2A-C1
16	B	840	CLA	O1A-CGA-O2A-C1
17	1	518	LUT	C7-C8-C9-C19
18	1	521	BCR	C37-C22-C23-C24
18	1	522	BCR	C11-C12-C13-C35
18	1	522	BCR	C36-C18-C19-C20
18	1	523	BCR	C7-C8-C9-C34
18	2	417	BCR	C36-C18-C19-C20
18	2	418	BCR	C37-C22-C23-C24
18	3	515	BCR	C37-C22-C23-C24
18	3	516	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
18	4	419	BCR	C11-C12-C13-C35
18	5	420	BCR	C7-C8-C9-C34
18	6	518	BCR	C36-C18-C19-C20
18	6	521	BCR	C37-C22-C23-C24
18	7	518	BCR	C7-C8-C9-C34
18	A	845	BCR	C36-C18-C19-C20
18	A	850	BCR	C7-C8-C9-C34
18	A	850	BCR	C37-C22-C23-C24
18	B	804	BCR	C36-C18-C19-C20
18	B	850	BCR	C7-C8-C9-C34
18	B	850	BCR	C11-C12-C13-C35
18	B	852	BCR	C11-C12-C13-C35
18	B	852	BCR	C37-C22-C23-C24
18	B	853	BCR	C7-C8-C9-C34
18	B	853	BCR	C11-C12-C13-C35
18	F	203	BCR	C11-C12-C13-C35
18	I	101	BCR	C36-C18-C19-C20
18	I	102	BCR	C7-C8-C9-C34
18	I	102	BCR	C37-C22-C23-C24
18	K	101	BCR	C37-C22-C23-C24
18	M	101	BCR	C7-C8-C9-C34
18	M	101	BCR	C36-C18-C19-C20
25	A	848	ECH	C7-C8-C9-C34
18	1	522	BCR	C17-C18-C19-C20
18	6	521	BCR	C21-C22-C23-C24
18	K	101	BCR	C21-C22-C23-C24
18	M	101	BCR	C7-C8-C9-C10
25	A	848	ECH	C7-C8-C9-C10
16	2	403	CLA	C2A-CAA-CBA-CGA
16	B	816	CLA	C2A-CAA-CBA-CGA
16	B	838	CLA	C2A-CAA-CBA-CGA
16	K	102	CLA	C2A-CAA-CBA-CGA
16	6	509	CLA	O1A-CGA-O2A-C1
16	2	401	CLA	CBD-CGD-O2D-CED
16	A	842	CLA	CBD-CGD-O2D-CED
16	4	415	CLA	C2-C1-O2A-CGA
16	4	408	CLA	O1D-CGD-O2D-CED
16	5	414	CLA	O1D-CGD-O2D-CED
16	6	505	CLA	CBD-CGD-O2D-CED
16	2	408	CLA	C8-C10-C11-C12
16	4	410	CLA	C5-C6-C7-C8
16	B	814	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	A	801	PQN	C25-C26-C27-C28
16	5	417	CLA	C3-C5-C6-C7
16	A	817	CLA	C3-C5-C6-C7
16	B	813	CLA	O1A-CGA-O2A-C1
16	5	404	CLA	CBD-CGD-O2D-CED
24	A	805	CL0	C12-C13-C15-C16
16	6	508	CLA	CBA-CGA-O2A-C1
23	I	103	LMT	O5'-C5'-C6'-O6'
16	B	834	CLA	C8-C10-C11-C12
18	B	849	BCR	C19-C20-C21-C22
18	I	102	BCR	C15-C16-C17-C18
21	3	517	LHG	O9-C7-O7-C5
16	B	811	CLA	O1D-CGD-O2D-CED
20	1	527	LMU	O5B-C1B-O1B-C4'
16	4	416	CLA	O1A-CGA-O2A-C1
16	A	844	CLA	O1A-CGA-O2A-C1
16	B	829	CLA	O1A-CGA-O2A-C1
16	B	841	CLA	O1A-CGA-O2A-C1
21	4	421	LHG	O10-C23-O8-C6
16	3	510	CLA	O1D-CGD-O2D-CED
16	3	506	CLA	C8-C10-C11-C12
16	5	410	CLA	C5-C6-C7-C8
16	B	837	CLA	C10-C11-C12-C13
16	1	508	CLA	C2A-CAA-CBA-CGA
16	3	506	CLA	C2A-CAA-CBA-CGA
16	3	510	CLA	C2A-CAA-CBA-CGA
16	5	408	CLA	C2A-CAA-CBA-CGA
16	A	811	CLA	C2A-CAA-CBA-CGA
16	B	831	CLA	C2A-CAA-CBA-CGA
16	B	836	CLA	C2A-CAA-CBA-CGA
16	B	839	CLA	C2A-CAA-CBA-CGA
16	5	412	CLA	C13-C15-C16-C17
16	A	808	CLA	C8-C10-C11-C12
16	A	828	CLA	C5-C6-C7-C8
16	B	848	CLA	C15-C16-C17-C18
16	4	414	CLA	O1D-CGD-O2D-CED
16	2	407	CLA	O1A-CGA-O2A-C1
16	3	509	CLA	O1A-CGA-O2A-C1
16	4	402	CLA	O1A-CGA-O2A-C1
16	4	403	CLA	O1A-CGA-O2A-C1
16	4	408	CLA	O1A-CGA-O2A-C1
16	B	830	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	B	835	CLA	O1A-CGA-O2A-C1
16	1	526	CLA	CBD-CGD-O2D-CED
16	B	835	CLA	O1D-CGD-O2D-CED
16	B	832	CLA	CBA-CGA-O2A-C1
16	2	413	CLA	CBD-CGD-O2D-CED
16	A	827	CLA	O1A-CGA-O2A-C1
19	1	524	LMG	C10-C11-C12-C13
16	A	822	CLA	C5-C6-C7-C8
16	5	411	CLA	C3-C5-C6-C7
16	3	507	CLA	O1D-CGD-O2D-CED
16	4	415	CLA	O1D-CGD-O2D-CED
16	B	810	CLA	O1D-CGD-O2D-CED
16	K	102	CLA	O1D-CGD-O2D-CED
16	B	846	CLA	C10-C11-C12-C13
16	A	818	CLA	CBD-CGD-O2D-CED
16	5	408	CLA	O1A-CGA-O2A-C1
16	2	411	CLA	O1D-CGD-O2D-CED
16	4	412	CLA	O1D-CGD-O2D-CED
16	6	517	CLA	O1D-CGD-O2D-CED
21	A	802	LHG	C12-C13-C14-C15
24	A	805	CL0	C13-C15-C16-C17
16	6	505	CLA	CBA-CGA-O2A-C1
16	A	833	CLA	CBA-CGA-O2A-C1
16	3	511	CLA	CBD-CGD-O2D-CED
16	A	827	CLA	CBD-CGD-O2D-CED
16	A	841	CLA	CBD-CGD-O2D-CED
16	B	816	CLA	CBD-CGD-O2D-CED
16	A	838	CLA	O1D-CGD-O2D-CED
16	A	809	CLA	C3-C5-C6-C7
16	3	512	CLA	C2A-CAA-CBA-CGA
16	A	810	CLA	C2A-CAA-CBA-CGA
16	2	404	CLA	CBA-CGA-O2A-C1
16	5	409	CLA	CBA-CGA-O2A-C1
16	A	830	CLA	CBA-CGA-O2A-C1
16	1	503	CLA	C13-C15-C16-C17
16	1	504	CLA	C13-C15-C16-C17
16	3	509	CLA	C13-C15-C16-C17
16	4	411	CLA	C13-C15-C16-C17
16	A	808	CLA	C10-C11-C12-C13
16	B	814	CLA	C5-C6-C7-C8
16	7	511	CLA	CAB-C3B-C4B-CHC
16	1	509	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	3	513	CLA	CBD-CGD-O2D-CED
16	6	508	CLA	O1A-CGA-O2A-C1
16	3	505	CLA	C3-C5-C6-C7
16	2	404	CLA	C5-C6-C7-C8
16	4	410	CLA	C10-C11-C12-C13
16	B	818	CLA	C5-C6-C7-C8
16	7	511	CLA	NC-C1C-CHC-C4B
23	B	807	LMT	O1'-C1-C2-C3
16	7	509	CLA	C3-C5-C6-C7
16	2	405	CLA	C8-C10-C11-C12
16	5	411	CLA	C5-C6-C7-C8
16	B	809	CLA	C15-C16-C17-C18
16	6	510	CLA	CBA-CGA-O2A-C1
21	B	806	LHG	C23-C24-C25-C26
18	1	523	BCR	C37-C22-C23-C24
18	2	416	BCR	C7-C8-C9-C34
18	5	423	BCR	C7-C8-C9-C34
18	6	519	BCR	C7-C8-C9-C34
18	6	519	BCR	C36-C18-C19-C20
18	6	519	BCR	C37-C22-C23-C24
18	6	521	BCR	C7-C8-C9-C34
18	A	850	BCR	C36-C18-C19-C20
18	B	852	BCR	C36-C18-C19-C20
18	F	204	BCR	C36-C18-C19-C20
25	A	853	ECH	C36-C18-C19-C20
18	1	523	BCR	C21-C22-C23-C24
18	2	416	BCR	C7-C8-C9-C10
18	2	417	BCR	C17-C18-C19-C20
18	3	515	BCR	C21-C22-C23-C24
18	6	519	BCR	C7-C8-C9-C10
18	6	519	BCR	C21-C22-C23-C24
18	B	852	BCR	C11-C12-C13-C14
18	I	102	BCR	C7-C8-C9-C10
18	I	102	BCR	C21-C22-C23-C24
16	5	409	CLA	O1A-CGA-O2A-C1
16	B	822	CLA	C2A-CAA-CBA-CGA
16	2	407	CLA	O1D-CGD-O2D-CED
16	7	515	CLA	C11-C10-C8-C9
16	B	844	CLA	C11-C12-C13-C14
16	5	412	CLA	O1D-CGD-O2D-CED
16	B	826	CLA	O1D-CGD-O2D-CED
16	A	833	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	6	508	CLA	O1D-CGD-O2D-CED
16	F	201	CLA	O1D-CGD-O2D-CED
16	5	413	CLA	CBA-CGA-O2A-C1
16	4	407	CLA	C13-C15-C16-C17
16	4	404	CLA	CBD-CGD-O2D-CED
16	A	828	CLA	C2-C1-O2A-CGA
16	B	821	CLA	C2-C1-O2A-CGA
16	4	417	CLA	C11-C12-C13-C14
16	4	417	CLA	C11-C12-C13-C15
16	5	407	CLA	C16-C17-C18-C20
16	6	505	CLA	C16-C17-C18-C19
16	7	515	CLA	C11-C10-C8-C7
16	A	833	CLA	C16-C17-C18-C19
16	A	835	CLA	C16-C17-C18-C19
16	B	841	CLA	C16-C17-C18-C19
16	B	841	CLA	C16-C17-C18-C20
16	2	404	CLA	O1A-CGA-O2A-C1
16	A	815	CLA	C5-C6-C7-C8
16	B	815	CLA	C5-C6-C7-C8
16	B	832	CLA	O1A-CGA-O2A-C1
16	B	827	CLA	CBA-CGA-O2A-C1
21	A	802	LHG	C26-C27-C28-C29
16	1	502	CLA	O1D-CGD-O2D-CED
16	A	813	CLA	O1D-CGD-O2D-CED
16	2	407	CLA	C4B-C3B-CAB-CBB
16	6	507	CLA	C4B-C3B-CAB-CBB
16	A	827	CLA	C4B-C3B-CAB-CBB
16	B	824	CLA	C4B-C3B-CAB-CBB
16	B	828	CLA	C4B-C3B-CAB-CBB
19	A	851	LMG	C12-C13-C14-C15
16	2	408	CLA	C11-C12-C13-C14
16	2	408	CLA	C11-C12-C13-C15
16	B	844	CLA	C11-C12-C13-C15
16	B	846	CLA	C16-C17-C18-C19
16	A	830	CLA	O1A-CGA-O2A-C1
16	7	501	CLA	C2A-CAA-CBA-CGA
16	A	812	CLA	C2A-CAA-CBA-CGA
16	5	409	CLA	C11-C10-C8-C7
21	B	806	LHG	C7-C8-C9-C10
16	1	503	CLA	C5-C6-C7-C8
16	6	505	CLA	O1A-CGA-O2A-C1
16	B	813	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
16	1	506	CLA	C3A-C2A-CAA-CBA
16	2	401	CLA	C3A-C2A-CAA-CBA
16	2	409	CLA	C3A-C2A-CAA-CBA
16	2	411	CLA	C3A-C2A-CAA-CBA
16	3	511	CLA	C3A-C2A-CAA-CBA
16	4	412	CLA	C3A-C2A-CAA-CBA
16	4	413	CLA	C3A-C2A-CAA-CBA
16	4	415	CLA	C3A-C2A-CAA-CBA
16	5	414	CLA	C3A-C2A-CAA-CBA
16	5	416	CLA	C3A-C2A-CAA-CBA
16	6	512	CLA	C3A-C2A-CAA-CBA
16	6	514	CLA	C3A-C2A-CAA-CBA
16	6	515	CLA	C3A-C2A-CAA-CBA
16	7	510	CLA	C3A-C2A-CAA-CBA
16	7	515	CLA	C3A-C2A-CAA-CBA
16	A	809	CLA	C3A-C2A-CAA-CBA
16	A	812	CLA	C3A-C2A-CAA-CBA
16	A	813	CLA	C3A-C2A-CAA-CBA
16	A	840	CLA	C3A-C2A-CAA-CBA
16	A	852	CLA	C3A-C2A-CAA-CBA
16	B	812	CLA	C3A-C2A-CAA-CBA
16	B	815	CLA	C3A-C2A-CAA-CBA
16	B	823	CLA	C3A-C2A-CAA-CBA
16	B	827	CLA	C3A-C2A-CAA-CBA
16	B	831	CLA	C3A-C2A-CAA-CBA
16	B	840	CLA	C3A-C2A-CAA-CBA
16	B	843	CLA	C3A-C2A-CAA-CBA
16	X	101	CLA	C3A-C2A-CAA-CBA
16	B	801	CLA	C15-C16-C17-C18
16	7	513	CLA	O1D-CGD-O2D-CED
16	1	516	CLA	CBD-CGD-O2D-CED
16	A	807	CLA	O1D-CGD-O2D-CED
16	2	413	CLA	CBA-CGA-O2A-C1
16	A	814	CLA	CBA-CGA-O2A-C1
20	1	527	LMU	C6-C7-C8-C9
16	4	409	CLA	C3-C5-C6-C7
16	B	831	CLA	C3-C5-C6-C7
16	A	840	CLA	O1D-CGD-O2D-CED
16	6	510	CLA	O1A-CGA-O2A-C1
16	1	504	CLA	C15-C16-C17-C18
16	B	840	CLA	O1D-CGD-O2D-CED
23	B	807	LMT	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
16	2	413	CLA	C11-C12-C13-C15
16	6	505	CLA	C16-C17-C18-C20
17	1	518	LUT	C1-C6-C7-C8
17	1	518	LUT	C5-C6-C7-C8
18	1	519	BCR	C1-C6-C7-C8
18	1	521	BCR	C23-C24-C25-C26
18	1	521	BCR	C23-C24-C25-C30
18	2	416	BCR	C1-C6-C7-C8
18	2	417	BCR	C23-C24-C25-C30
18	2	418	BCR	C23-C24-C25-C30
18	3	514	BCR	C1-C6-C7-C8
18	3	515	BCR	C23-C24-C25-C26
18	3	515	BCR	C23-C24-C25-C30
18	4	419	BCR	C23-C24-C25-C26
18	4	420	BCR	C23-C24-C25-C26
18	4	420	BCR	C23-C24-C25-C30
18	5	420	BCR	C1-C6-C7-C8
18	5	422	BCR	C23-C24-C25-C26
18	5	422	BCR	C23-C24-C25-C30
18	6	518	BCR	C5-C6-C7-C8
18	6	518	BCR	C23-C24-C25-C26
18	6	518	BCR	C23-C24-C25-C30
18	6	519	BCR	C1-C6-C7-C8
18	6	519	BCR	C5-C6-C7-C8
18	7	519	BCR	C23-C24-C25-C26
18	7	519	BCR	C23-C24-C25-C30
18	A	845	BCR	C5-C6-C7-C8
18	B	853	BCR	C23-C24-C25-C26
18	I	102	BCR	C1-C6-C7-C8
18	J	1104	BCR	C1-C6-C7-C8
18	M	101	BCR	C1-C6-C7-C8
25	A	853	ECH	C5-C6-C7-C8
25	B	851	ECH	C5-C6-C7-C8
16	5	403	CLA	O1D-CGD-O2D-CED
16	3	505	CLA	CBA-CGA-O2A-C1
16	B	818	CLA	CBA-CGA-O2A-C1
16	B	816	CLA	C3-C5-C6-C7
16	1	517	CLA	O1D-CGD-O2D-CED
16	7	508	CLA	O1D-CGD-O2D-CED
16	B	831	CLA	O1D-CGD-O2D-CED
16	2	407	CLA	C2A-CAA-CBA-CGA
16	3	508	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
21	A	802	LHG	C16-C17-C18-C19
16	5	413	CLA	O1A-CGA-O2A-C1
16	B	827	CLA	O1A-CGA-O2A-C1
16	4	409	CLA	CBD-CGD-O2D-CED
16	B	817	CLA	C4-C3-C5-C6
16	3	510	CLA	CBA-CGA-O2A-C1
16	6	509	CLA	C6-C7-C8-C9
16	6	510	CLA	C11-C10-C8-C9
16	6	513	CLA	O1D-CGD-O2D-CED
19	B	805	LMG	C38-C39-C40-C41
16	2	413	CLA	C8-C10-C11-C12
16	1	505	CLA	CBA-CGA-O2A-C1
16	4	406	CLA	CBA-CGA-O2A-C1
16	A	835	CLA	C16-C17-C18-C20
16	A	842	CLA	C5-C6-C7-C8
16	2	413	CLA	O1A-CGA-O2A-C1
18	1	522	BCR	C37-C22-C23-C24
18	3	514	BCR	C37-C22-C23-C24
18	5	420	BCR	C37-C22-C23-C24
18	5	421	BCR	C37-C22-C23-C24
18	J	1104	BCR	C7-C8-C9-C34
25	B	851	ECH	C7-C8-C9-C34
23	B	807	LMT	C5'-C4'-O1B-C1B
21	B	806	LHG	C13-C14-C15-C16
18	5	420	BCR	C7-C8-C9-C10
18	5	420	BCR	C21-C22-C23-C24
18	B	853	BCR	C7-C8-C9-C10
18	J	1104	BCR	C7-C8-C9-C10
25	B	851	ECH	C7-C8-C9-C10
16	2	413	CLA	C11-C12-C13-C14
16	5	407	CLA	C16-C17-C18-C19
16	A	833	CLA	C16-C17-C18-C20
16	A	840	CLA	C16-C17-C18-C19
16	A	840	CLA	C16-C17-C18-C20
16	B	846	CLA	C16-C17-C18-C20
16	B	813	CLA	C4-C3-C5-C6
16	B	845	CLA	C4-C3-C5-C6
16	B	813	CLA	C2-C3-C5-C6
16	B	817	CLA	C2-C3-C5-C6
19	A	851	LMG	C15-C16-C17-C18
16	4	402	CLA	O1D-CGD-O2D-CED
16	6	509	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
16	B	832	CLA	O1D-CGD-O2D-CED
16	3	505	CLA	O1A-CGA-O2A-C1
16	A	814	CLA	O1A-CGA-O2A-C1
22	B	803	PQN	C13-C15-C16-C17
16	6	504	CLA	C10-C11-C12-C13
16	1	509	CLA	C5-C6-C7-C8
16	4	407	CLA	C15-C16-C17-C18
16	5	407	CLA	C8-C10-C11-C12
22	A	801	PQN	C15-C16-C17-C18
16	A	833	CLA	O1D-CGD-O2D-CED
16	4	409	CLA	C5-C6-C7-C8
16	B	845	CLA	C2-C3-C5-C6
16	1	513	CLA	C2A-CAA-CBA-CGA
16	2	402	CLA	C2A-CAA-CBA-CGA
16	2	410	CLA	C2A-CAA-CBA-CGA
16	B	827	CLA	C2A-CAA-CBA-CGA
16	A	824	CLA	CBD-CGD-O2D-CED
16	4	411	CLA	O1D-CGD-O2D-CED
16	5	417	CLA	O1D-CGD-O2D-CED
19	B	805	LMG	O6-C5-C6-O5
20	4	401	LMU	O1'-C1-C2-C3
16	1	512	CLA	O1D-CGD-O2D-CED
16	4	406	CLA	C16-C17-C18-C20
20	1	527	LMU	O5'-C5'-C6'-O6'
16	B	838	CLA	O1D-CGD-O2D-CED
16	B	818	CLA	O1A-CGA-O2A-C1
16	1	517	CLA	C3-C5-C6-C7
16	2	401	CLA	C1A-C2A-CAA-CBA
16	2	411	CLA	C1A-C2A-CAA-CBA
16	2	414	CLA	C1A-C2A-CAA-CBA
16	3	511	CLA	C1A-C2A-CAA-CBA
16	4	409	CLA	C1A-C2A-CAA-CBA
16	4	413	CLA	C1A-C2A-CAA-CBA
16	4	414	CLA	C1A-C2A-CAA-CBA
16	4	415	CLA	C1A-C2A-CAA-CBA
16	5	414	CLA	C1A-C2A-CAA-CBA
16	5	416	CLA	C1A-C2A-CAA-CBA
16	6	501	CLA	C1A-C2A-CAA-CBA
16	6	506	CLA	C1A-C2A-CAA-CBA
16	6	512	CLA	C1A-C2A-CAA-CBA
16	6	513	CLA	C1A-C2A-CAA-CBA
16	6	514	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
16	7	510	CLA	C1A-C2A-CAA-CBA
16	7	513	CLA	C1A-C2A-CAA-CBA
16	A	812	CLA	C1A-C2A-CAA-CBA
16	A	821	CLA	C1A-C2A-CAA-CBA
16	A	852	CLA	C1A-C2A-CAA-CBA
16	B	814	CLA	C1A-C2A-CAA-CBA
16	B	827	CLA	C1A-C2A-CAA-CBA
16	B	831	CLA	C1A-C2A-CAA-CBA
16	B	840	CLA	C1A-C2A-CAA-CBA
16	B	841	CLA	C1A-C2A-CAA-CBA
16	B	843	CLA	C1A-C2A-CAA-CBA
16	B	848	CLA	C1A-C2A-CAA-CBA
16	X	101	CLA	C1A-C2A-CAA-CBA
16	3	502	CLA	CBA-CGA-O2A-C1
16	3	510	CLA	O1A-CGA-O2A-C1
19	5	426	LMG	O6-C5-C6-O5
16	2	404	CLA	C11-C12-C13-C15
16	3	501	CLA	C11-C12-C13-C15
16	5	407	CLA	C12-C13-C15-C16
16	A	830	CLA	C11-C10-C8-C7
16	A	833	CLA	C12-C13-C15-C16
16	A	840	CLA	C12-C13-C15-C16
16	A	841	CLA	C11-C10-C8-C7
16	A	844	CLA	C12-C13-C15-C16
16	B	810	CLA	C11-C12-C13-C15
16	B	814	CLA	C6-C7-C8-C10
16	B	818	CLA	C11-C10-C8-C7
16	B	820	CLA	C11-C10-C8-C7
16	B	825	CLA	C11-C10-C8-C7
16	B	837	CLA	C12-C13-C15-C16
16	B	845	CLA	C11-C10-C8-C7
16	J	1101	CLA	C12-C13-C15-C16
16	A	841	CLA	C16-C17-C18-C19
16	4	406	CLA	O1A-CGA-O2A-C1
16	1	515	CLA	CBA-CGA-O2A-C1
16	A	831	CLA	C15-C16-C17-C18
19	1	524	LMG	O6-C5-C6-O5
16	A	842	CLA	C15-C16-C17-C18
16	B	847	CLA	C15-C16-C17-C18
16	4	416	CLA	C2A-CAA-CBA-CGA
16	6	508	CLA	C2A-CAA-CBA-CGA
16	7	508	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
16	B	821	CLA	C2A-CAA-CBA-CGA
16	1	508	CLA	C6-C7-C8-C9
16	1	510	CLA	C11-C10-C8-C9
16	2	406	CLA	C14-C13-C15-C16
16	3	509	CLA	C6-C7-C8-C9
16	5	409	CLA	C11-C10-C8-C9
16	A	814	CLA	C11-C12-C13-C14
16	A	841	CLA	C11-C12-C13-C14
16	B	818	CLA	C11-C12-C13-C14
16	B	831	CLA	C6-C7-C8-C9
16	1	517	CLA	CBA-CGA-O2A-C1
16	2	406	CLA	CBA-CGA-O2A-C1
16	1	516	CLA	C10-C11-C12-C13
16	A	820	CLA	CBD-CGD-O2D-CED
16	2	401	CLA	O1D-CGD-O2D-CED
16	A	842	CLA	O1D-CGD-O2D-CED
16	B	813	CLA	C5-C6-C7-C8
16	4	409	CLA	CBA-CGA-O2A-C1
16	6	501	CLA	CBA-CGA-O2A-C1
20	1	527	LMU	O5B-C5B-C6B-O6B
16	4	406	CLA	C16-C17-C18-C19
16	A	841	CLA	C16-C17-C18-C20
16	5	404	CLA	O1D-CGD-O2D-CED
19	B	805	LMG	C28-C29-C30-C31
23	B	808	LMT	O5B-C5B-C6B-O6B
16	1	505	CLA	O1A-CGA-O2A-C1
18	1	522	BCR	C21-C22-C23-C24
18	A	850	BCR	C21-C22-C23-C24
18	B	849	BCR	C21-C22-C23-C24
18	B	850	BCR	C7-C8-C9-C10
16	2	406	CLA	O1A-CGA-O2A-C1
16	5	407	CLA	C5-C6-C7-C8
16	5	411	CLA	C10-C11-C12-C13
16	6	505	CLA	O1D-CGD-O2D-CED
16	4	410	CLA	O2A-C1-C2-C3
16	7	509	CLA	O2A-C1-C2-C3
16	A	844	CLA	O2A-C1-C2-C3
16	B	831	CLA	O2A-C1-C2-C3
16	3	502	CLA	O1A-CGA-O2A-C1
19	A	851	LMG	C17-C18-C19-C20
16	1	516	CLA	CBA-CGA-O2A-C1
16	7	506	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	A	812	CLA	CBA-CGA-O2A-C1
16	A	838	CLA	CBA-CGA-O2A-C1
16	1	526	CLA	O1D-CGD-O2D-CED
16	4	416	CLA	CAA-CBA-CGA-O2A
23	I	103	LMT	C4'-C5'-C6'-O6'
16	A	806	CLA	C2-C1-O2A-CGA
16	1	516	CLA	C11-C12-C13-C15
16	2	413	CLA	O1D-CGD-O2D-CED
16	B	834	CLA	CAA-CBA-CGA-O2A
16	A	829	CLA	CBD-CGD-O2D-CED
16	1	525	CLA	C5-C6-C7-C8
16	A	818	CLA	O1D-CGD-O2D-CED
16	B	816	CLA	O1D-CGD-O2D-CED
16	B	834	CLA	C4-C3-C5-C6
16	A	823	CLA	CBA-CGA-O2A-C1
20	1	527	LMU	C2-C1-O1'-C1'
20	4	401	LMU	C2-C1-O1'-C1'
23	A	804	LMT	C2-C1-O1'-C1'
16	1	505	CLA	C11-C10-C8-C9
16	2	404	CLA	C11-C12-C13-C14
16	3	501	CLA	C11-C12-C13-C14
16	4	406	CLA	C14-C13-C15-C16
16	5	407	CLA	C14-C13-C15-C16
16	A	816	CLA	C11-C12-C13-C14
16	A	831	CLA	C11-C12-C13-C14
16	A	833	CLA	C14-C13-C15-C16
16	A	840	CLA	C14-C13-C15-C16
16	A	841	CLA	C11-C10-C8-C9
16	B	814	CLA	C6-C7-C8-C9
16	B	818	CLA	C11-C10-C8-C9
16	B	820	CLA	C11-C10-C8-C9
16	B	825	CLA	C11-C10-C8-C9
16	B	836	CLA	C11-C10-C8-C9
16	B	837	CLA	C14-C13-C15-C16
16	B	839	CLA	C14-C13-C15-C16
16	B	845	CLA	C11-C10-C8-C9
16	J	1101	CLA	C14-C13-C15-C16
24	A	805	CL0	C14-C13-C15-C16
16	3	511	CLA	O1D-CGD-O2D-CED
16	A	841	CLA	O1D-CGD-O2D-CED
16	1	510	CLA	C5-C6-C7-C8
16	4	409	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	2	402	CLA	C4B-C3B-CAB-CBB
16	3	510	CLA	C4B-C3B-CAB-CBB
16	4	409	CLA	C4B-C3B-CAB-CBB
16	4	412	CLA	C4B-C3B-CAB-CBB
16	4	416	CLA	C4B-C3B-CAB-CBB
16	5	405	CLA	C4B-C3B-CAB-CBB
16	5	408	CLA	C4B-C3B-CAB-CBB
16	5	416	CLA	C4B-C3B-CAB-CBB
16	6	511	CLA	C4B-C3B-CAB-CBB
16	7	514	CLA	C4B-C3B-CAB-CBB
16	7	517	CLA	C4B-C3B-CAB-CBB
16	A	813	CLA	C4B-C3B-CAB-CBB
16	A	821	CLA	C4B-C3B-CAB-CBB
16	X	101	CLA	C4B-C3B-CAB-CBB
16	A	827	CLA	O1D-CGD-O2D-CED
16	A	828	CLA	C8-C10-C11-C12
16	A	852	CLA	C13-C15-C16-C17
19	5	426	LMG	C14-C15-C16-C17
16	2	403	CLA	CBA-CGA-O2A-C1
16	1	517	CLA	O1A-CGA-O2A-C1
16	1	501	CLA	C2A-CAA-CBA-CGA
16	1	505	CLA	C2A-CAA-CBA-CGA
16	1	505	CLA	C11-C10-C8-C7
16	1	508	CLA	C6-C7-C8-C10
16	1	510	CLA	C11-C10-C8-C7
16	2	405	CLA	C12-C13-C15-C16
16	2	406	CLA	C12-C13-C15-C16
16	3	509	CLA	C11-C12-C13-C15
16	4	406	CLA	C12-C13-C15-C16
16	4	408	CLA	C11-C10-C8-C7
16	A	814	CLA	C11-C12-C13-C15
16	A	816	CLA	C11-C12-C13-C15
16	A	831	CLA	C11-C12-C13-C15
16	A	836	CLA	C12-C13-C15-C16
16	A	841	CLA	C11-C12-C13-C15
16	B	816	CLA	C11-C12-C13-C15
16	B	818	CLA	C11-C12-C13-C15
16	B	831	CLA	C6-C7-C8-C10
16	B	832	CLA	C12-C13-C15-C16
16	B	836	CLA	C11-C10-C8-C7
16	B	839	CLA	C12-C13-C15-C16
16	A	844	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
16	1	517	CLA	C4-C3-C5-C6
16	2	414	CLA	C3A-C2A-CAA-CBA
16	4	405	CLA	C3A-C2A-CAA-CBA
16	5	413	CLA	C3A-C2A-CAA-CBA
16	6	504	CLA	C3A-C2A-CAA-CBA
16	7	505	CLA	C3A-C2A-CAA-CBA
16	A	830	CLA	C3A-C2A-CAA-CBA
16	B	814	CLA	C3A-C2A-CAA-CBA
16	B	816	CLA	C3A-C2A-CAA-CBA
16	B	822	CLA	C3A-C2A-CAA-CBA
16	1	509	CLA	O1D-CGD-O2D-CED
16	6	501	CLA	O1A-CGA-O2A-C1
17	1	518	LUT	C9-C10-C11-C12
18	2	418	BCR	C19-C20-C21-C22
18	6	521	BCR	C15-C16-C17-C18
18	B	804	BCR	C19-C20-C21-C22
25	A	848	ECH	C13-C14-C15-C16
18	3	515	BCR	C7-C8-C9-C34
18	A	846	BCR	C37-C22-C23-C24
16	J	1101	CLA	C5-C6-C7-C8
18	7	518	BCR	C7-C8-C9-C10
16	3	513	CLA	O1D-CGD-O2D-CED
16	1	516	CLA	C11-C12-C13-C14
16	1	517	CLA	C2-C3-C5-C6
16	4	416	CLA	C3-C5-C6-C7
16	A	843	CLA	C16-C17-C18-C19
16	A	840	CLA	C8-C10-C11-C12
16	4	404	CLA	O1D-CGD-O2D-CED
18	6	520	BCR	C23-C24-C25-C30
18	B	804	BCR	C23-C24-C25-C30
18	B	853	BCR	C23-C24-C25-C30
18	F	204	BCR	C1-C6-C7-C8
25	B	851	ECH	C23-C24-C25-C26
16	B	824	CLA	CBA-CGA-O2A-C1
16	A	835	CLA	C5-C6-C7-C8
16	2	409	CLA	CBD-CGD-O2D-CED
16	5	405	CLA	CBD-CGD-O2D-CED
24	A	805	CL0	CAA-CBA-CGA-O2A
16	7	505	CLA	C2A-CAA-CBA-CGA
16	4	405	CLA	C8-C10-C11-C12
16	B	813	CLA	C10-C11-C12-C13
21	A	802	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
16	B	827	CLA	C11-C10-C8-C7
16	4	415	CLA	C4-C3-C5-C6
16	A	822	CLA	C4-C3-C5-C6
16	B	821	CLA	C4-C3-C5-C6
16	B	844	CLA	C4-C3-C5-C6
16	B	810	CLA	C13-C15-C16-C17
16	B	844	CLA	C2-C3-C5-C6
16	1	509	CLA	C11-C12-C13-C15
16	A	843	CLA	C16-C17-C18-C20
16	5	417	CLA	CBA-CGA-O2A-C1
16	A	838	CLA	O1A-CGA-O2A-C1
16	1	508	CLA	C11-C10-C8-C9
16	2	405	CLA	C14-C13-C15-C16
16	2	406	CLA	C11-C10-C8-C9
16	3	509	CLA	C11-C12-C13-C14
16	5	413	CLA	C6-C7-C8-C9
16	A	834	CLA	C11-C10-C8-C9
16	A	842	CLA	C11-C10-C8-C9
22	B	803	PQN	C25-C26-C27-C28
16	1	516	CLA	O1D-CGD-O2D-CED
16	B	816	CLA	C8-C10-C11-C12
16	B	826	CLA	C15-C16-C17-C18
18	6	521	BCR	C13-C14-C15-C16
16	B	821	CLA	C2-C3-C5-C6
16	B	834	CLA	C2-C3-C5-C6
16	B	816	CLA	C16-C17-C18-C19
16	1	503	CLA	CBD-CGD-O2D-CED
20	1	527	LMU	C7-C8-C9-C10
16	J	1101	CLA	C13-C15-C16-C17
16	7	506	CLA	O1A-CGA-O2A-C1
16	A	812	CLA	O1A-CGA-O2A-C1
16	A	821	CLA	CAA-CBA-CGA-O2A
16	1	514	CLA	CBA-CGA-O2A-C1
20	4	401	LMU	C3'-C4'-O1B-C1B
16	6	515	CLA	C13-C15-C16-C17
16	A	812	CLA	C15-C16-C17-C18
16	A	828	CLA	C13-C15-C16-C17
16	2	406	CLA	C15-C16-C17-C18
16	A	833	CLA	C5-C6-C7-C8
18	B	849	BCR	C37-C22-C23-C24
18	I	101	BCR	C11-C12-C13-C35
16	1	508	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
16	1	516	CLA	C11-C10-C8-C7
16	2	406	CLA	C11-C10-C8-C7
16	4	411	CLA	C6-C7-C8-C10
16	4	415	CLA	C11-C12-C13-C15
16	5	406	CLA	C11-C10-C8-C7
16	5	417	CLA	C11-C12-C13-C15
16	A	812	CLA	C12-C13-C15-C16
16	A	814	CLA	C6-C7-C8-C10
16	A	824	CLA	C12-C13-C15-C16
16	A	841	CLA	C6-C7-C8-C10
16	A	842	CLA	C11-C10-C8-C7
16	B	826	CLA	C11-C10-C8-C7
16	B	838	CLA	C11-C12-C13-C15
16	B	846	CLA	C6-C7-C8-C10
16	B	847	CLA	C12-C13-C15-C16
18	1	521	BCR	C21-C22-C23-C24
18	5	423	BCR	C7-C8-C9-C10
18	6	521	BCR	C7-C8-C9-C10
18	A	850	BCR	C17-C18-C19-C20
18	B	852	BCR	C17-C18-C19-C20
18	F	204	BCR	C17-C18-C19-C20
25	A	853	ECH	C17-C18-C19-C20
16	A	839	CLA	CBA-CGA-O2A-C1
16	2	405	CLA	C4C-C3C-CAC-CBC
16	4	409	CLA	O1D-CGD-O2D-CED
16	1	508	CLA	C8-C10-C11-C12
16	B	827	CLA	C11-C10-C8-C9
16	5	417	CLA	CAA-CBA-CGA-O2A
16	1	516	CLA	O1A-CGA-O2A-C1
16	2	403	CLA	O1A-CGA-O2A-C1
16	A	823	CLA	O1A-CGA-O2A-C1
16	4	415	CLA	C2-C3-C5-C6
16	A	822	CLA	C2-C3-C5-C6
16	1	509	CLA	C10-C11-C12-C13
16	2	404	CLA	C8-C10-C11-C12
16	4	409	CLA	O2A-C1-C2-C3
16	5	411	CLA	O2A-C1-C2-C3
16	5	412	CLA	O2A-C1-C2-C3
16	6	507	CLA	O2A-C1-C2-C3
16	6	509	CLA	O2A-C1-C2-C3
18	A	847	BCR	C19-C20-C21-C22
16	3	505	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	4	406	CLA	C10-C11-C12-C13
16	B	811	CLA	C5-C6-C7-C8
23	I	103	LMT	C2-C3-C4-C5
16	B	835	CLA	C4-C3-C5-C6
16	2	403	CLA	C5-C6-C7-C8
16	4	408	CLA	C8-C10-C11-C12
16	6	508	CLA	C5-C6-C7-C8
16	B	832	CLA	C5-C6-C7-C8
16	B	834	CLA	C10-C11-C12-C13
16	A	814	CLA	C6-C7-C8-C9
16	A	836	CLA	C14-C13-C15-C16
16	B	847	CLA	C14-C13-C15-C16
16	A	824	CLA	C16-C17-C18-C20
21	B	806	LHG	C10-C11-C12-C13
16	5	417	CLA	O1A-CGA-O2A-C1
16	B	824	CLA	O1A-CGA-O2A-C1
16	A	840	CLA	C10-C11-C12-C13
16	1	514	CLA	O1A-CGA-O2A-C1
16	B	848	CLA	C2-C1-O2A-CGA
18	1	523	BCR	C9-C10-C11-C12
23	B	808	LMT	C4-C5-C6-C7
16	A	807	CLA	C6-C7-C8-C9
16	A	827	CLA	C4C-C3C-CAC-CBC
16	5	407	CLA	C4-C3-C5-C6
16	B	835	CLA	C13-C15-C16-C17
21	B	806	LHG	C9-C10-C11-C12
16	3	506	CLA	C16-C17-C18-C20
16	A	836	CLA	C5-C6-C7-C8
16	A	824	CLA	O1D-CGD-O2D-CED
16	A	839	CLA	O1A-CGA-O2A-C1
16	A	817	CLA	C6-C7-C8-C10
16	A	842	CLA	C3-C5-C6-C7
18	5	402	BCR	C36-C18-C19-C20
18	A	849	BCR	C11-C12-C13-C35
16	1	502	CLA	C1A-C2A-CAA-CBA
16	1	509	CLA	C1A-C2A-CAA-CBA
16	1	513	CLA	C4B-C3B-CAB-CBB
16	1	514	CLA	C4B-C3B-CAB-CBB
16	3	502	CLA	C4B-C3B-CAB-CBB
16	3	512	CLA	C4B-C3B-CAB-CBB
16	4	403	CLA	C4B-C3B-CAB-CBB
16	4	406	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
16	4	414	CLA	C4B-C3B-CAB-CBB
16	5	410	CLA	C4B-C3B-CAB-CBB
16	5	415	CLA	C4B-C3B-CAB-CBB
16	5	417	CLA	C4B-C3B-CAB-CBB
16	6	502	CLA	C4B-C3B-CAB-CBB
16	6	503	CLA	C4B-C3B-CAB-CBB
16	6	515	CLA	C4B-C3B-CAB-CBB
16	7	505	CLA	C1A-C2A-CAA-CBA
16	7	513	CLA	C4B-C3B-CAB-CBB
16	7	514	CLA	C1A-C2A-CAA-CBA
16	7	515	CLA	C4B-C3B-CAB-CBB
16	7	516	CLA	C1A-C2A-CAA-CBA
16	A	813	CLA	C1A-C2A-CAA-CBA
16	A	838	CLA	C4B-C3B-CAB-CBB
16	B	815	CLA	C4B-C3B-CAB-CBB
16	B	816	CLA	C1A-C2A-CAA-CBA
16	B	833	CLA	C1A-C2A-CAA-CBA
16	B	839	CLA	C4B-C3B-CAB-CBB
16	B	842	CLA	C4B-C3B-CAB-CBB
16	B	843	CLA	C4B-C3B-CAB-CBB
16	B	848	CLA	C4B-C3B-CAB-CBB
16	J	1101	CLA	C4B-C3B-CAB-CBB
16	J	1103	CLA	C4B-C3B-CAB-CBB
16	A	820	CLA	O1D-CGD-O2D-CED
16	6	510	CLA	C5-C6-C7-C8
18	5	421	BCR	C21-C22-C23-C24
18	6	519	BCR	C17-C18-C19-C20
18	A	849	BCR	C11-C12-C13-C14
18	I	101	BCR	C11-C12-C13-C14
16	7	511	CLA	CHB-C1B-C2B-CMB
16	6	507	CLA	CBD-CGD-O2D-CED
16	3	501	CLA	C11-C10-C8-C7
16	3	504	CLA	C11-C10-C8-C7
16	3	509	CLA	C11-C10-C8-C7
16	4	405	CLA	C11-C10-C8-C7
16	4	417	CLA	C11-C10-C8-C7
16	6	505	CLA	C11-C12-C13-C15
16	6	507	CLA	C11-C10-C8-C7
16	A	809	CLA	C12-C13-C15-C16
16	A	828	CLA	C11-C10-C8-C7
16	A	830	CLA	C11-C12-C13-C15
16	A	844	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
16	B	816	CLA	C6-C7-C8-C10
16	B	825	CLA	C6-C7-C8-C10
16	B	845	CLA	C11-C12-C13-C15
23	I	103	LMT	C7-C8-C9-C10
16	1	509	CLA	C11-C12-C13-C14
16	B	844	CLA	C8-C10-C11-C12
16	B	820	CLA	C4C-C3C-CAC-CBC
16	B	816	CLA	C16-C17-C18-C20
16	A	829	CLA	O1D-CGD-O2D-CED
16	6	504	CLA	C5-C6-C7-C8
16	B	830	CLA	C5-C6-C7-C8
16	7	503	CLA	C2A-CAA-CBA-CGA
16	4	415	CLA	C11-C12-C13-C14
16	5	406	CLA	C11-C10-C8-C9
16	A	812	CLA	C14-C13-C15-C16
16	A	824	CLA	C14-C13-C15-C16
16	A	841	CLA	C6-C7-C8-C9
16	B	826	CLA	C11-C10-C8-C9
16	B	846	CLA	C6-C7-C8-C9
18	1	519	BCR	C9-C10-C11-C12
18	5	423	BCR	C13-C14-C15-C16
18	B	849	BCR	C13-C14-C15-C16
19	5	426	LMG	C39-C40-C41-C42
24	A	805	CL0	C3-C5-C6-C7
16	3	505	CLA	C13-C15-C16-C17
16	5	405	CLA	O1D-CGD-O2D-CED
16	3	506	CLA	C16-C17-C18-C19
16	A	824	CLA	C16-C17-C18-C19
16	A	816	CLA	C15-C16-C17-C18
16	6	509	CLA	C3-C5-C6-C7
16	1	513	CLA	CAD-CBD-CGD-O2D
16	2	413	CLA	CAD-CBD-CGD-O2D
16	3	505	CLA	CAD-CBD-CGD-O2D
16	4	406	CLA	CAD-CBD-CGD-O2D
16	4	407	CLA	CAD-CBD-CGD-O2D
16	4	411	CLA	CAD-CBD-CGD-O2D
16	4	417	CLA	CAD-CBD-CGD-O2D
16	5	414	CLA	CAD-CBD-CGD-O2D
16	5	418	CLA	CAD-CBD-CGD-O2D
16	7	510	CLA	CAD-CBD-CGD-O2D
16	7	515	CLA	CAD-CBD-CGD-O2D
16	A	816	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
16	A	812	CLA	C10-C11-C12-C13
21	A	803	LHG	C24-C23-O8-C6
16	4	405	CLA	C5-C6-C7-C8
16	1	505	CLA	C11-C12-C13-C15
16	A	824	CLA	C3-C5-C6-C7
16	B	828	CLA	C2A-CAA-CBA-CGA
22	B	803	PQN	C23-C25-C26-C27
16	1	510	CLA	CHA-CBD-CGD-O1D
16	1	513	CLA	CAD-CBD-CGD-O1D
16	2	413	CLA	CAD-CBD-CGD-O1D
16	3	504	CLA	CHA-CBD-CGD-O1D
16	3	504	CLA	CHA-CBD-CGD-O2D
16	3	505	CLA	CAD-CBD-CGD-O1D
16	4	406	CLA	CAD-CBD-CGD-O1D
16	4	407	CLA	CAD-CBD-CGD-O1D
16	4	411	CLA	CAD-CBD-CGD-O1D
16	4	417	CLA	CAD-CBD-CGD-O1D
16	5	412	CLA	CAD-CBD-CGD-O1D
16	5	413	CLA	CAD-CBD-CGD-O1D
16	5	414	CLA	CAD-CBD-CGD-O1D
16	5	418	CLA	CAD-CBD-CGD-O1D
16	6	503	CLA	CHA-CBD-CGD-O1D
16	6	506	CLA	CHA-CBD-CGD-O1D
16	6	506	CLA	CHA-CBD-CGD-O2D
16	7	505	CLA	CHA-CBD-CGD-O1D
16	7	507	CLA	CAD-CBD-CGD-O1D
16	7	510	CLA	CAD-CBD-CGD-O1D
16	7	515	CLA	CAD-CBD-CGD-O1D
16	A	816	CLA	CAD-CBD-CGD-O1D
16	B	812	CLA	CAD-CBD-CGD-O1D
16	B	813	CLA	CHA-CBD-CGD-O1D
16	B	813	CLA	CHA-CBD-CGD-O2D
16	B	828	CLA	CHA-CBD-CGD-O1D
16	B	828	CLA	CHA-CBD-CGD-O2D
18	1	519	BCR	C13-C14-C15-C16
18	5	401	BCR	C13-C14-C15-C16
18	6	518	BCR	C13-C14-C15-C16
18	F	204	BCR	C19-C20-C21-C22
21	A	803	LHG	C4-O6-P-O4
21	B	806	LHG	C4-O6-P-O3
16	B	837	CLA	C15-C16-C17-C18
16	5	411	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
16	7	506	CLA	C2B-C3B-CAB-CBB
16	7	517	CLA	C2B-C3B-CAB-CBB
18	B	804	BCR	C1-C6-C7-C8
18	I	101	BCR	C23-C24-C25-C30
25	B	851	ECH	C23-C24-C25-C30
16	B	835	CLA	C2-C3-C5-C6
16	1	503	CLA	O1D-CGD-O2D-CED
18	4	419	BCR	C36-C18-C19-C20
18	A	847	BCR	C37-C22-C23-C24
16	X	101	CLA	C2C-C3C-CAC-CBC
16	3	505	CLA	O1D-CGD-O2D-CED
23	I	103	LMT	C9-C10-C11-C12
19	B	805	LMG	C34-C35-C36-C37
16	6	504	CLA	C3-C5-C6-C7
16	7	506	CLA	C2C-C3C-CAC-CBC
16	1	515	CLA	O1A-CGA-O2A-C1
16	B	846	CLA	C8-C10-C11-C12
16	2	401	CLA	O2A-C1-C2-C3
16	3	508	CLA	O2A-C1-C2-C3
16	2	413	CLA	CAA-CBA-CGA-O2A
23	A	804	LMT	C5'-C4'-O1B-C1B
21	A	802	LHG	C10-C11-C12-C13
16	B	825	CLA	C15-C16-C17-C18
16	3	504	CLA	C11-C10-C8-C9
16	4	408	CLA	C11-C10-C8-C9
16	4	411	CLA	C6-C7-C8-C9
16	4	417	CLA	C6-C7-C8-C9
16	B	820	CLA	C11-C12-C13-C14
16	2	413	CLA	C6-C7-C8-C10
16	B	815	CLA	C11-C12-C13-C15
23	A	804	LMT	C4-C5-C6-C7
16	4	412	CLA	O1A-CGA-O2A-C1
16	A	806	CLA	C16-C17-C18-C19
21	A	803	LHG	O10-C23-O8-C6
16	4	412	CLA	CBA-CGA-O2A-C1
16	B	825	CLA	C16-C17-C18-C19
16	B	824	CLA	CAA-CBA-CGA-O2A
19	5	426	LMG	C15-C16-C17-C18
16	2	403	CLA	C8-C10-C11-C12
16	5	410	CLA	CBA-CGA-O2A-C1
16	A	841	CLA	C4-C3-C5-C6
16	5	412	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
16	5	417	CLA	C16-C17-C18-C19
16	A	813	CLA	CAA-CBA-CGA-O2A
19	B	805	LMG	C41-C42-C43-C44
16	4	403	CLA	C3-C5-C6-C7
16	6	510	CLA	C13-C15-C16-C17
16	2	404	CLA	CAA-CBA-CGA-O2A
18	3	514	BCR	C36-C18-C19-C20
16	2	409	CLA	O1D-CGD-O2D-CED
18	3	514	BCR	C21-C22-C23-C24
16	1	510	CLA	C10-C11-C12-C13
16	A	806	CLA	C2A-CAA-CBA-CGA
16	B	810	CLA	C2A-CAA-CBA-CGA
16	B	829	CLA	C2A-CAA-CBA-CGA
18	1	520	BCR	C9-C10-C11-C12
18	J	1104	BCR	C13-C14-C15-C16
16	A	832	CLA	C8-C10-C11-C12
16	6	507	CLA	O1D-CGD-O2D-CED
23	B	808	LMT	C2-C1-O1'-C1'
16	3	501	CLA	C6-C7-C8-C9
16	3	505	CLA	C14-C13-C15-C16
16	A	828	CLA	C11-C10-C8-C9
16	B	816	CLA	C6-C7-C8-C9
16	B	825	CLA	C6-C7-C8-C9
16	2	410	CLA	C4B-C3B-CAB-CBB
16	2	413	CLA	C4B-C3B-CAB-CBB
16	3	505	CLA	C4B-C3B-CAB-CBB
16	5	413	CLA	C4B-C3B-CAB-CBB
16	6	508	CLA	C4B-C3B-CAB-CBB
16	6	513	CLA	C4B-C3B-CAB-CBB
16	A	811	CLA	C4B-C3B-CAB-CBB
16	A	819	CLA	C4B-C3B-CAB-CBB
16	B	821	CLA	C4B-C3B-CAB-CBB
16	B	833	CLA	C4B-C3B-CAB-CBB
16	A	828	CLA	C15-C16-C17-C18
16	5	418	CLA	CAA-CBA-CGA-O2A
16	A	828	CLA	C16-C17-C18-C19
16	A	820	CLA	CBA-CGA-O2A-C1
21	A	802	LHG	C24-C23-O8-C6
16	5	410	CLA	O1A-CGA-O2A-C1
16	A	841	CLA	C2-C3-C5-C6
16	6	513	CLA	CAA-CBA-CGA-O2A
16	A	835	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
16	B	846	CLA	C11-C10-C8-C7
21	A	802	LHG	O10-C23-O8-C6
16	1	511	CLA	CAA-CBA-CGA-O2A
16	1	505	CLA	C11-C12-C13-C14
16	5	417	CLA	C16-C17-C18-C20
16	B	825	CLA	C16-C17-C18-C20
16	A	820	CLA	O1A-CGA-O2A-C1
16	2	403	CLA	C3A-C2A-CAA-CBA
16	3	510	CLA	C3A-C2A-CAA-CBA
16	7	508	CLA	C3A-C2A-CAA-CBA
16	7	514	CLA	C3A-C2A-CAA-CBA
16	A	817	CLA	C3A-C2A-CAA-CBA
16	A	842	CLA	C3A-C2A-CAA-CBA
16	B	833	CLA	C3A-C2A-CAA-CBA
18	A	850	BCR	C11-C10-C9-C34
18	A	850	BCR	C16-C17-C18-C36
18	B	850	BCR	C11-C10-C9-C34
18	F	204	BCR	C35-C13-C14-C15
18	I	102	BCR	C20-C21-C22-C37
19	1	524	LMG	O6-C1-O1-C7
25	B	851	ECH	C11-C10-C9-C34
25	B	851	ECH	C20-C21-C22-C37
16	5	406	CLA	C5-C6-C7-C8
16	6	513	CLA	CAA-CBA-CGA-O1A
16	7	514	CLA	CAA-CBA-CGA-O2A
16	A	842	CLA	C8-C10-C11-C12
16	3	509	CLA	C2-C1-O2A-CGA
18	1	522	BCR	C13-C14-C15-C16
18	2	416	BCR	C19-C20-C21-C22
18	B	804	BCR	C9-C10-C11-C12
16	3	508	CLA	C10-C11-C12-C13
16	1	511	CLA	CAA-CBA-CGA-O1A
16	2	402	CLA	CAA-CBA-CGA-O1A
16	7	513	CLA	CAA-CBA-CGA-O1A
16	J	1103	CLA	CAA-CBA-CGA-O2A
20	1	527	LMU	O1'-C1-C2-C3
16	3	509	CLA	C16-C17-C18-C20
16	K	103	CLA	C16-C17-C18-C19
16	5	418	CLA	CAA-CBA-CGA-O1A
16	3	506	CLA	C4C-C3C-CAC-CBC
16	4	416	CLA	CAA-CBA-CGA-O1A
16	B	834	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
19	B	805	LMG	C13-C14-C15-C16
16	4	405	CLA	C11-C10-C8-C9
16	4	417	CLA	C11-C10-C8-C9
16	5	408	CLA	C6-C7-C8-C9
16	6	515	CLA	C11-C10-C8-C9
16	7	509	CLA	C6-C7-C8-C9
16	A	811	CLA	C6-C7-C8-C9
16	A	835	CLA	C11-C10-C8-C9
16	A	844	CLA	C6-C7-C8-C9
16	B	810	CLA	C11-C10-C8-C9
16	B	816	CLA	C11-C12-C13-C14
16	B	816	CLA	C14-C13-C15-C16
16	B	825	CLA	C11-C12-C13-C14
16	B	837	CLA	C6-C7-C8-C9
16	B	845	CLA	C11-C12-C13-C14
16	B	847	CLA	C11-C12-C13-C14
16	1	517	CLA	C6-C7-C8-C9
16	6	508	CLA	C6-C7-C8-C10
23	I	103	LMT	O5B-C1B-O1B-C4'
16	7	516	CLA	CAA-CBA-CGA-O2A
21	A	802	LHG	C6-C5-O7-C7
16	B	818	CLA	C3-C5-C6-C7
16	7	503	CLA	CAA-CBA-CGA-O2A
16	5	412	CLA	C16-C17-C18-C19
16	2	414	CLA	CAA-CBA-CGA-O2A
16	7	502	CLA	CAA-CBA-CGA-O2A
16	7	514	CLA	CAA-CBA-CGA-O1A
16	A	823	CLA	C2A-CAA-CBA-CGA
16	7	515	CLA	C10-C11-C12-C13
16	6	508	CLA	C1A-C2A-CAA-CBA
16	6	511	CLA	C1A-C2A-CAA-CBA
16	7	508	CLA	C1A-C2A-CAA-CBA
16	A	815	CLA	C1A-C2A-CAA-CBA
16	A	836	CLA	C1A-C2A-CAA-CBA
16	A	842	CLA	C1A-C2A-CAA-CBA
16	B	812	CLA	C1A-C2A-CAA-CBA
16	B	820	CLA	C1A-C2A-CAA-CBA
16	B	835	CLA	C1A-C2A-CAA-CBA
16	F	201	CLA	C1A-C2A-CAA-CBA
18	A	850	BCR	C11-C10-C9-C8
18	A	850	BCR	C16-C17-C18-C19
18	B	850	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
18	F	204	BCR	C12-C13-C14-C15
18	I	102	BCR	C20-C21-C22-C23
25	B	851	ECH	C11-C10-C9-C8
25	B	851	ECH	C20-C21-C22-C23
16	B	830	CLA	C16-C17-C18-C19
16	4	414	CLA	CAA-CBA-CGA-O2A
16	B	810	CLA	C8-C10-C11-C12
16	1	501	CLA	C2B-C3B-CAB-CBB
16	1	515	CLA	C2B-C3B-CAB-CBB
16	A	840	CLA	C2B-C3B-CAB-CBB
16	B	812	CLA	C2B-C3B-CAB-CBB
16	K	102	CLA	C2B-C3B-CAB-CBB
18	2	417	BCR	C5-C6-C7-C8
18	2	417	BCR	C23-C24-C25-C26
18	3	514	BCR	C5-C6-C7-C8
18	5	421	BCR	C1-C6-C7-C8
18	5	421	BCR	C23-C24-C25-C30
18	6	520	BCR	C5-C6-C7-C8
18	A	846	BCR	C5-C6-C7-C8
16	2	414	CLA	CAA-CBA-CGA-O1A
16	4	414	CLA	CAA-CBA-CGA-O1A
16	7	513	CLA	CAA-CBA-CGA-O2A
16	7	516	CLA	CAA-CBA-CGA-O1A
16	A	812	CLA	C16-C17-C18-C19
16	A	834	CLA	C10-C11-C12-C13
16	1	507	CLA	CAA-CBA-CGA-O2A
16	A	812	CLA	C4-C3-C5-C6
19	B	805	LMG	C29-C30-C31-C32
16	2	402	CLA	CAA-CBA-CGA-O2A
16	3	512	CLA	CAA-CBA-CGA-O1A
16	J	1103	CLA	CAA-CBA-CGA-O1A
19	A	851	LMG	C29-C30-C31-C32
16	3	505	CLA	C12-C13-C15-C16
16	3	506	CLA	C11-C10-C8-C7
16	7	509	CLA	C6-C7-C8-C10
16	A	831	CLA	C12-C13-C15-C16
16	A	843	CLA	C11-C10-C8-C7
16	B	810	CLA	C11-C10-C8-C7
16	B	835	CLA	C12-C13-C15-C16
16	B	839	CLA	C11-C10-C8-C7
16	J	1101	CLA	C16-C17-C18-C20
16	6	509	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
16	A	816	CLA	C2A-CAA-CBA-CGA
16	A	820	CLA	C2A-CAA-CBA-CGA
16	7	502	CLA	CAA-CBA-CGA-O1A
16	J	1101	CLA	CBD-CGD-O2D-CED
16	B	836	CLA	C8-C10-C11-C12
16	5	413	CLA	C11-C12-C13-C15
16	B	837	CLA	C16-C17-C18-C19
18	B	850	BCR	C37-C22-C23-C24
16	7	507	CLA	CAA-CBA-CGA-O2A
16	1	525	CLA	C4-C3-C5-C6
16	A	852	CLA	C4-C3-C5-C6
16	A	824	CLA	C13-C15-C16-C17
16	5	407	CLA	C2-C3-C5-C6
16	6	512	CLA	C2C-C3C-CAC-CBC
20	1	527	LMU	C9-C10-C11-C12
16	2	409	CLA	C6-C7-C8-C9
16	3	503	CLA	CAA-CBA-CGA-O2A
16	7	501	CLA	CAA-CBA-CGA-O2A
16	B	828	CLA	CAA-CBA-CGA-O2A
16	2	406	CLA	C6-C7-C8-C9
16	2	408	CLA	C6-C7-C8-C9
16	3	501	CLA	C11-C10-C8-C9
16	3	506	CLA	C11-C10-C8-C9
16	A	828	CLA	C10-C11-C12-C13
16	4	415	CLA	C13-C15-C16-C17
16	6	507	CLA	C8-C10-C11-C12
16	2	404	CLA	C4-C3-C5-C6
16	5	412	CLA	C4-C3-C5-C6
16	A	836	CLA	C4-C3-C5-C6
16	7	507	CLA	CAA-CBA-CGA-O1A
23	B	808	LMT	C5'-C4'-O1B-C1B
16	5	412	CLA	C15-C16-C17-C18
16	A	829	CLA	C6-C7-C8-C10
16	A	820	CLA	C5-C6-C7-C8
16	5	403	CLA	CAA-CBA-CGA-O2A
16	7	503	CLA	CAA-CBA-CGA-O1A
21	A	802	LHG	C24-C25-C26-C27
16	3	509	CLA	C15-C16-C17-C18
16	4	411	CLA	C15-C16-C17-C18
16	1	507	CLA	CAA-CBA-CGA-O1A
16	7	509	CLA	C10-C11-C12-C13
16	2	415	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
16	5	416	CLA	CAA-CBA-CGA-O2A
16	7	512	CLA	CAA-CBA-CGA-O2A
16	B	822	CLA	CAA-CBA-CGA-O2A
16	5	406	CLA	C8-C10-C11-C12
16	1	509	CLA	C4B-C3B-CAB-CBB
16	3	511	CLA	C4B-C3B-CAB-CBB
16	4	407	CLA	C4B-C3B-CAB-CBB
16	5	406	CLA	C4B-C3B-CAB-CBB
16	5	418	CLA	C4B-C3B-CAB-CBB
16	7	507	CLA	C4B-C3B-CAB-CBB
16	7	516	CLA	C4B-C3B-CAB-CBB
16	A	837	CLA	C4B-C3B-CAB-CBB
16	A	842	CLA	C4B-C3B-CAB-CBB
16	A	843	CLA	C4B-C3B-CAB-CBB
16	B	830	CLA	C4B-C3B-CAB-CBB
16	A	842	CLA	O1A-CGA-O2A-C1
16	4	418	CLA	CAA-CBA-CGA-O2A
16	7	510	CLA	CAA-CBA-CGA-O2A
16	X	101	CLA	CAA-CBA-CGA-O2A
16	J	1101	CLA	O1D-CGD-O2D-CED
16	B	831	CLA	O1A-CGA-O2A-C1
16	3	512	CLA	CAA-CBA-CGA-O2A
16	B	843	CLA	CAA-CBA-CGA-O2A
16	3	509	CLA	C16-C17-C18-C19
16	A	828	CLA	C16-C17-C18-C20
16	K	103	CLA	C16-C17-C18-C20
24	A	805	CL0	CHA-CBD-CGD-O1D
24	A	805	CL0	CHA-CBD-CGD-O2D
16	A	840	CLA	C5-C6-C7-C8
16	A	817	CLA	CAA-CBA-CGA-O2A
16	3	513	CLA	CAA-CBA-CGA-O2A
16	6	516	CLA	CAA-CBA-CGA-O2A
16	7	504	CLA	CAA-CBA-CGA-O2A
16	3	510	CLA	C6-C7-C8-C10
21	5	424	LHG	O7-C7-C8-C9
16	3	503	CLA	CAA-CBA-CGA-O1A
16	B	809	CLA	CAA-CBA-CGA-O2A
16	A	852	CLA	C2-C3-C5-C6
16	B	835	CLA	C15-C16-C17-C18
16	3	508	CLA	C6-C7-C8-C10
16	7	510	CLA	CAA-CBA-CGA-O1A
18	5	420	BCR	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
16	A	816	CLA	C16-C17-C18-C19
16	5	419	CLA	CAA-CBA-CGA-O2A
16	6	511	CLA	CAA-CBA-CGA-O2A
18	3	515	BCR	C7-C8-C9-C10
18	A	846	BCR	C21-C22-C23-C24
16	3	504	CLA	C6-C7-C8-C9
21	5	424	LHG	O9-C7-C8-C9
16	2	412	CLA	CAA-CBA-CGA-O2A
16	7	501	CLA	CAA-CBA-CGA-O1A
16	A	819	CLA	CAA-CBA-CGA-O2A
16	B	827	CLA	C5-C6-C7-C8
16	A	844	CLA	C2A-CAA-CBA-CGA
16	B	847	CLA	C2A-CAA-CBA-CGA
16	2	409	CLA	C2-C1-O2A-CGA
16	3	505	CLA	C2-C1-O2A-CGA
16	4	406	CLA	C2-C1-O2A-CGA
16	A	811	CLA	C2-C1-O2A-CGA
16	A	831	CLA	C2-C1-O2A-CGA
16	B	846	CLA	C2-C1-O2A-CGA
16	1	517	CLA	C6-C7-C8-C10
16	4	411	CLA	C16-C17-C18-C20
16	6	508	CLA	C6-C7-C8-C9
16	B	830	CLA	C16-C17-C18-C20
16	4	402	CLA	C3A-C2A-CAA-CBA
16	6	508	CLA	C3A-C2A-CAA-CBA
16	A	810	CLA	C3A-C2A-CAA-CBA
16	B	820	CLA	C3A-C2A-CAA-CBA
16	1	501	CLA	CAA-CBA-CGA-O2A
16	2	415	CLA	CAA-CBA-CGA-O1A
16	6	512	CLA	CAA-CBA-CGA-O2A
16	6	517	CLA	CAA-CBA-CGA-O2A
16	7	517	CLA	CAA-CBA-CGA-O2A
16	B	819	CLA	CAA-CBA-CGA-O2A
16	B	828	CLA	CAA-CBA-CGA-O1A
16	B	827	CLA	CAA-CBA-CGA-O2A
19	5	426	LMG	O10-C28-O8-C9
23	A	804	LMT	O1'-C1-C2-C3
16	B	827	CLA	C3-C5-C6-C7
16	2	410	CLA	C10-C11-C12-C13
16	3	511	CLA	CAA-CBA-CGA-O2A
16	7	512	CLA	CAA-CBA-CGA-O1A
16	B	843	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
16	A	842	CLA	CBA-CGA-O2A-C1
16	5	409	CLA	O2A-C1-C2-C3
16	5	410	CLA	O2A-C1-C2-C3
16	6	508	CLA	O2A-C1-C2-C3
16	A	815	CLA	O2A-C1-C2-C3
16	B	830	CLA	O2A-C1-C2-C3
21	A	802	LHG	C4-C5-O7-C7
16	5	403	CLA	CAA-CBA-CGA-O1A
16	A	807	CLA	C3-C5-C6-C7
16	B	831	CLA	CBA-CGA-O2A-C1
24	A	805	CL0	CAA-CBA-CGA-O1A
16	A	812	CLA	C16-C17-C18-C20
16	3	513	CLA	CAA-CBA-CGA-O1A
16	B	822	CLA	CAA-CBA-CGA-O1A
16	A	813	CLA	C5-C6-C7-C8
19	A	851	LMG	C28-C29-C30-C31
16	5	416	CLA	CAA-CBA-CGA-O1A
16	6	516	CLA	CAA-CBA-CGA-O1A
16	X	101	CLA	CAA-CBA-CGA-O1A
19	5	426	LMG	C29-C28-O8-C9
19	1	524	LMG	C30-C31-C32-C33
16	2	408	CLA	C10-C11-C12-C13
16	4	418	CLA	CAA-CBA-CGA-O1A
16	5	419	CLA	CAA-CBA-CGA-O1A
16	6	511	CLA	CAA-CBA-CGA-O1A
16	A	852	CLA	C8-C10-C11-C12
16	B	810	CLA	C3-C5-C6-C7
16	7	504	CLA	CAA-CBA-CGA-O1A
16	B	826	CLA	C13-C15-C16-C17
16	2	412	CLA	CAA-CBA-CGA-O1A
16	A	811	CLA	C4-C3-C5-C6
16	A	816	CLA	C4-C3-C5-C6
16	6	517	CLA	CAA-CBA-CGA-O1A
16	A	819	CLA	CAA-CBA-CGA-O1A
18	1	520	BCR	C13-C14-C15-C16
16	5	408	CLA	C2C-C3C-CAC-CBC
16	A	811	CLA	C16-C17-C18-C19
16	B	841	CLA	C8-C10-C11-C12
24	A	805	CL0	C15-C16-C17-C18
16	3	511	CLA	CAA-CBA-CGA-O1A
16	7	505	CLA	CAA-CBA-CGA-O2A
16	2	407	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
16	B	840	CLA	CAA-CBA-CGA-O2A
16	B	847	CLA	C5-C6-C7-C8
16	1	505	CLA	C6-C7-C8-C9
16	6	507	CLA	C11-C10-C8-C9
16	A	809	CLA	C14-C13-C15-C16
16	2	409	CLA	C6-C7-C8-C10
16	B	837	CLA	C16-C17-C18-C20
16	6	501	CLA	CAA-CBA-CGA-O2A
16	7	509	CLA	CAA-CBA-CGA-O2A
18	4	419	BCR	C17-C18-C19-C20
18	5	402	BCR	C17-C18-C19-C20
16	4	415	CLA	C3-C5-C6-C7
16	6	514	CLA	C4C-C3C-CAC-CBC
16	B	834	CLA	C2A-CAA-CBA-CGA
16	1	506	CLA	C6-C7-C8-C10
16	2	406	CLA	C6-C7-C8-C10
16	3	504	CLA	C6-C7-C8-C10
16	6	515	CLA	C11-C10-C8-C7
16	7	509	CLA	C11-C10-C8-C7
16	A	808	CLA	C12-C13-C15-C16
16	A	842	CLA	C11-C12-C13-C15
16	B	801	CLA	C11-C10-C8-C7
16	B	825	CLA	C11-C12-C13-C15
16	B	830	CLA	C6-C7-C8-C10
16	B	840	CLA	C6-C7-C8-C10
21	A	802	LHG	C19-C20-C21-C22
16	1	504	CLA	C2B-C3B-CAB-CBB
16	2	412	CLA	C2B-C3B-CAB-CBB
16	A	823	CLA	C2B-C3B-CAB-CBB
16	A	824	CLA	C2B-C3B-CAB-CBB
18	1	522	BCR	C5-C6-C7-C8
18	6	520	BCR	C23-C24-C25-C26
18	B	850	BCR	C5-C6-C7-C8
21	3	517	LHG	O7-C7-C8-C9
21	4	421	LHG	O7-C7-C8-C9
16	5	409	CLA	CAA-CBA-CGA-O2A
16	5	412	CLA	C2-C1-O2A-CGA
16	A	817	CLA	C2-C1-O2A-CGA
16	A	844	CLA	C2-C1-O2A-CGA
16	B	831	CLA	C2-C1-O2A-CGA
16	6	507	CLA	CAA-CBA-CGA-O2A
16	B	830	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
16	1	525	CLA	C6-C7-C8-C9
16	6	515	CLA	C16-C17-C18-C20
16	B	839	CLA	C2-C3-C5-C6
19	B	805	LMG	C31-C32-C33-C34
16	1	501	CLA	CAA-CBA-CGA-O1A
16	2	410	CLA	CAA-CBA-CGA-O2A
16	1	503	CLA	C3-C5-C6-C7
16	4	411	CLA	C16-C17-C18-C19
16	A	821	CLA	CAA-CBA-CGA-O1A
16	A	833	CLA	C8-C10-C11-C12
16	A	835	CLA	C13-C15-C16-C17
16	B	819	CLA	CAA-CBA-CGA-O1A
16	B	839	CLA	C4-C3-C5-C6
16	4	411	CLA	CAA-CBA-CGA-O2A
16	5	413	CLA	CAA-CBA-CGA-O2A
16	A	808	CLA	CAA-CBA-CGA-O2A
16	6	512	CLA	CAA-CBA-CGA-O1A
16	4	406	CLA	C8-C10-C11-C12
16	7	517	CLA	CAA-CBA-CGA-O1A
16	A	818	CLA	CAA-CBA-CGA-O2A
16	5	417	CLA	CAA-CBA-CGA-O1A
16	A	831	CLA	C14-C13-C15-C16
16	B	835	CLA	C14-C13-C15-C16
16	B	839	CLA	C11-C10-C8-C9
18	3	515	BCR	C11-C12-C13-C35
16	B	812	CLA	CAA-CBA-CGA-O2A
16	1	503	CLA	C4B-C3B-CAB-CBB
16	1	511	CLA	C4B-C3B-CAB-CBB
16	2	407	CLA	C1A-C2A-CAA-CBA
16	2	411	CLA	C4B-C3B-CAB-CBB
16	7	502	CLA	C4B-C3B-CAB-CBB
16	A	810	CLA	C1A-C2A-CAA-CBA
16	A	820	CLA	C4B-C3B-CAB-CBB
16	A	828	CLA	C1A-C2A-CAA-CBA
16	A	839	CLA	C1A-C2A-CAA-CBA
16	B	809	CLA	C4B-C3B-CAB-CBB
16	B	816	CLA	C4B-C3B-CAB-CBB
16	B	817	CLA	C4B-C3B-CAB-CBB
16	B	819	CLA	C4B-C3B-CAB-CBB
16	F	201	CLA	C4B-C3B-CAB-CBB
16	1	513	CLA	CAA-CBA-CGA-O2A
16	A	830	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
16	3	506	CLA	CAA-CBA-CGA-O2A
16	3	509	CLA	CAA-CBA-CGA-O2A
16	A	837	CLA	CAA-CBA-CGA-O2A
16	B	821	CLA	CAA-CBA-CGA-O2A
19	1	524	LMG	O7-C8-C9-O8
18	3	514	BCR	C17-C18-C19-C20
18	3	515	BCR	C11-C12-C13-C14
18	A	847	BCR	C21-C22-C23-C24
16	6	506	CLA	C11-C12-C13-C14
16	A	811	CLA	C16-C17-C18-C20
16	A	816	CLA	C16-C17-C18-C20
16	J	1101	CLA	C16-C17-C18-C19
16	2	408	CLA	CAA-CBA-CGA-O2A
16	3	507	CLA	CAA-CBA-CGA-O2A
16	6	508	CLA	CAA-CBA-CGA-O2A
16	A	827	CLA	CAA-CBA-CGA-O2A
19	B	805	LMG	O7-C10-C11-C12
16	2	413	CLA	C2A-CAA-CBA-CGA
16	A	832	CLA	C5-C6-C7-C8
16	2	405	CLA	C2C-C3C-CAC-CBC
16	1	503	CLA	C4C-C3C-CAC-CBC
16	7	505	CLA	CAA-CBA-CGA-O1A
16	4	408	CLA	CAA-CBA-CGA-O2A
19	A	851	LMG	C30-C31-C32-C33
16	2	410	CLA	C2-C1-O2A-CGA
16	2	403	CLA	C6-C7-C8-C10
16	4	405	CLA	C6-C7-C8-C10
16	5	412	CLA	C11-C12-C13-C15
16	B	836	CLA	C12-C13-C15-C16
16	6	504	CLA	C15-C16-C17-C18
16	5	413	CLA	C11-C12-C13-C14
16	6	510	CLA	C15-C16-C17-C18
16	B	839	CLA	C13-C15-C16-C17
23	I	103	LMT	C2B-C1B-O1B-C4'
16	1	517	CLA	C4C-C3C-CAC-CBC
19	B	805	LMG	C30-C31-C32-C33
16	2	406	CLA	CAA-CBA-CGA-O2A
16	B	841	CLA	CAA-CBA-CGA-O2A
16	2	404	CLA	C2A-CAA-CBA-CGA
16	5	407	CLA	C2A-CAA-CBA-CGA
16	A	843	CLA	C2A-CAA-CBA-CGA
16	A	852	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
16	5	408	CLA	C11-C12-C13-C14
16	B	810	CLA	C15-C16-C17-C18
16	B	832	CLA	C15-C16-C17-C18
16	6	501	CLA	CAA-CBA-CGA-O1A
16	2	413	CLA	C3A-C2A-CAA-CBA
16	4	414	CLA	C3A-C2A-CAA-CBA
16	4	416	CLA	C3A-C2A-CAA-CBA
16	5	417	CLA	C3A-C2A-CAA-CBA
16	A	828	CLA	C3A-C2A-CAA-CBA
16	B	819	CLA	C3A-C2A-CAA-CBA
16	B	848	CLA	C3A-C2A-CAA-CBA
16	F	201	CLA	C3A-C2A-CAA-CBA
16	2	403	CLA	C15-C16-C17-C18
16	3	508	CLA	CAA-CBA-CGA-O2A
16	7	508	CLA	CAA-CBA-CGA-O2A
16	1	508	CLA	C5-C6-C7-C8
16	B	840	CLA	CAA-CBA-CGA-O1A
16	A	818	CLA	CAA-CBA-CGA-O1A
16	2	407	CLA	CAA-CBA-CGA-O1A
16	B	812	CLA	CAA-CBA-CGA-O1A
16	1	503	CLA	C10-C11-C12-C13
16	2	403	CLA	C6-C7-C8-C9
16	3	509	CLA	C11-C10-C8-C9
16	6	505	CLA	C11-C12-C13-C14
16	A	808	CLA	C14-C13-C15-C16
16	A	814	CLA	C11-C10-C8-C9
16	A	843	CLA	C11-C10-C8-C9
16	2	408	CLA	CAA-CBA-CGA-O1A
16	2	406	CLA	C8-C10-C11-C12
16	B	837	CLA	C8-C10-C11-C12
16	2	410	CLA	CAA-CBA-CGA-O1A
16	A	827	CLA	CAA-CBA-CGA-O1A
16	4	410	CLA	CAA-CBA-CGA-O2A
16	2	404	CLA	C2-C3-C5-C6
16	A	837	CLA	C4-C3-C5-C6
16	F	202	CLA	CAA-CBA-CGA-O2A
16	5	409	CLA	CAA-CBA-CGA-O1A
16	7	509	CLA	CAA-CBA-CGA-O1A
16	A	842	CLA	CAA-CBA-CGA-O2A
16	3	507	CLA	C5-C6-C7-C8
18	B	804	BCR	C11-C12-C13-C14
18	B	850	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
21	3	517	LHG	O9-C7-C8-C9
16	3	507	CLA	CAA-CBA-CGA-O1A
16	6	507	CLA	CAA-CBA-CGA-O1A
16	5	416	CLA	C4C-C3C-CAC-CBC
16	B	841	CLA	C5-C6-C7-C8
16	A	837	CLA	CAA-CBA-CGA-O1A
16	B	821	CLA	CAA-CBA-CGA-O1A
16	B	841	CLA	CAA-CBA-CGA-O1A
16	4	412	CLA	CAA-CBA-CGA-O2A
16	B	836	CLA	CAA-CBA-CGA-O2A
16	A	809	CLA	C2A-CAA-CBA-CGA
21	A	802	LHG	C4-C5-C6-O8
16	1	513	CLA	CAA-CBA-CGA-O1A
16	3	506	CLA	CAA-CBA-CGA-O1A
16	5	413	CLA	CAA-CBA-CGA-O1A
16	6	508	CLA	CAA-CBA-CGA-O1A
23	I	103	LMT	C1-C2-C3-C4
21	A	802	LHG	O8-C23-C24-C25
16	2	406	CLA	CAA-CBA-CGA-O1A
16	4	408	CLA	CAA-CBA-CGA-O1A
16	A	841	CLA	C4C-C3C-CAC-CBC
16	1	506	CLA	CAD-CBD-CGD-O2D
16	4	403	CLA	CAD-CBD-CGD-O2D
16	5	413	CLA	CAD-CBD-CGD-O2D
16	5	417	CLA	CAD-CBD-CGD-O2D
16	6	507	CLA	CAD-CBD-CGD-O2D
16	7	509	CLA	CAD-CBD-CGD-O2D
16	A	829	CLA	CAD-CBD-CGD-O2D
16	B	817	CLA	CAD-CBD-CGD-O2D
16	B	818	CLA	CAD-CBD-CGD-O2D
16	B	819	CLA	CAD-CBD-CGD-O2D
16	J	1102	CLA	CAD-CBD-CGD-O2D
16	5	407	CLA	C15-C16-C17-C18
16	B	829	CLA	CAA-CBA-CGA-O2A
16	B	848	CLA	CAA-CBA-CGA-O2A
19	B	805	LMG	O9-C10-C11-C12
16	B	839	CLA	C15-C16-C17-C18
16	B	838	CLA	C10-C11-C12-C13
16	A	808	CLA	CAA-CBA-CGA-O1A
16	3	502	CLA	CAA-CBA-CGA-O2A
16	2	406	CLA	C16-C17-C18-C20
16	B	814	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
16	B	845	CLA	C16-C17-C18-C19
21	A	802	LHG	C25-C26-C27-C28
16	4	411	CLA	CAA-CBA-CGA-O1A
16	6	510	CLA	CAA-CBA-CGA-O2A
16	1	525	CLA	C2-C3-C5-C6
20	1	527	LMU	C5'-C4'-O1B-C1B
16	3	508	CLA	CAA-CBA-CGA-O1A
16	B	838	CLA	C8-C10-C11-C12
20	4	401	LMU	C6-C7-C8-C9
16	5	408	CLA	CAA-CBA-CGA-O2A
16	B	816	CLA	CAA-CBA-CGA-O2A
16	B	837	CLA	CAA-CBA-CGA-O2A
16	3	509	CLA	CAA-CBA-CGA-O1A
16	A	842	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

104 monomers are involved in 140 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	3	515	BCR	1	0
21	A	803	LHG	1	0
16	2	407	CLA	1	0
18	6	521	BCR	1	0
16	B	847	CLA	1	0
16	5	412	CLA	2	0
16	4	416	CLA	1	0
16	4	410	CLA	5	0
16	A	837	CLA	2	0
18	1	519	BCR	1	0
18	3	516	BCR	2	0
18	M	101	BCR	2	0
16	4	403	CLA	1	0
16	B	829	CLA	1	0
16	1	517	CLA	1	0
16	B	841	CLA	1	0
16	3	504	CLA	2	0
16	A	827	CLA	1	0
16	2	406	CLA	3	0
16	1	503	CLA	1	0
16	B	820	CLA	1	0
18	4	419	BCR	3	0
16	A	828	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	812	CLA	1	0
16	4	411	CLA	2	0
16	A	841	CLA	1	0
18	F	203	BCR	1	0
16	4	402	CLA	1	0
16	A	811	CLA	1	0
16	1	525	CLA	1	0
16	5	410	CLA	1	0
16	B	844	CLA	1	0
16	A	809	CLA	1	0
16	1	505	CLA	1	0
18	2	418	BCR	1	0
16	B	835	CLA	2	0
16	2	405	CLA	1	0
16	3	507	CLA	1	0
16	7	510	CLA	1	0
16	B	814	CLA	2	0
16	A	852	CLA	2	0
16	A	818	CLA	1	0
16	2	414	CLA	3	0
16	1	510	CLA	1	0
16	A	806	CLA	2	0
16	2	408	CLA	1	0
16	1	506	CLA	4	0
16	6	509	CLA	1	0
16	7	512	CLA	2	0
25	A	853	ECH	1	0
16	B	815	CLA	1	0
18	B	853	BCR	2	0
18	B	850	BCR	1	0
21	B	806	LHG	1	0
16	B	846	CLA	1	0
18	A	845	BCR	2	0
18	K	101	BCR	2	0
25	A	848	ECH	1	0
16	3	508	CLA	1	0
16	A	808	CLA	1	0
16	B	801	CLA	2	0
16	6	501	CLA	1	0
24	A	805	CL0	6	0
16	1	504	CLA	3	0
16	6	506	CLA	1	0

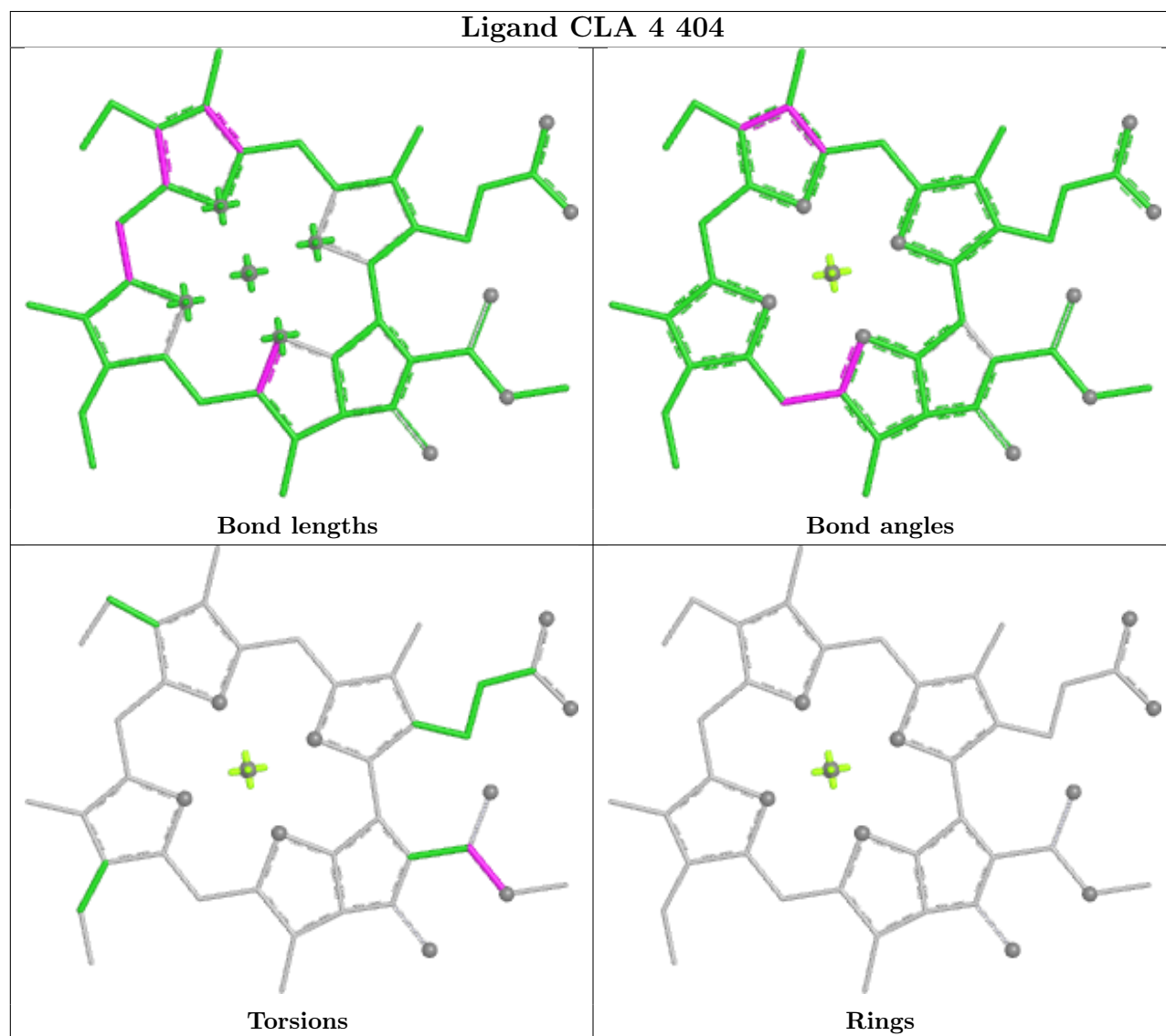
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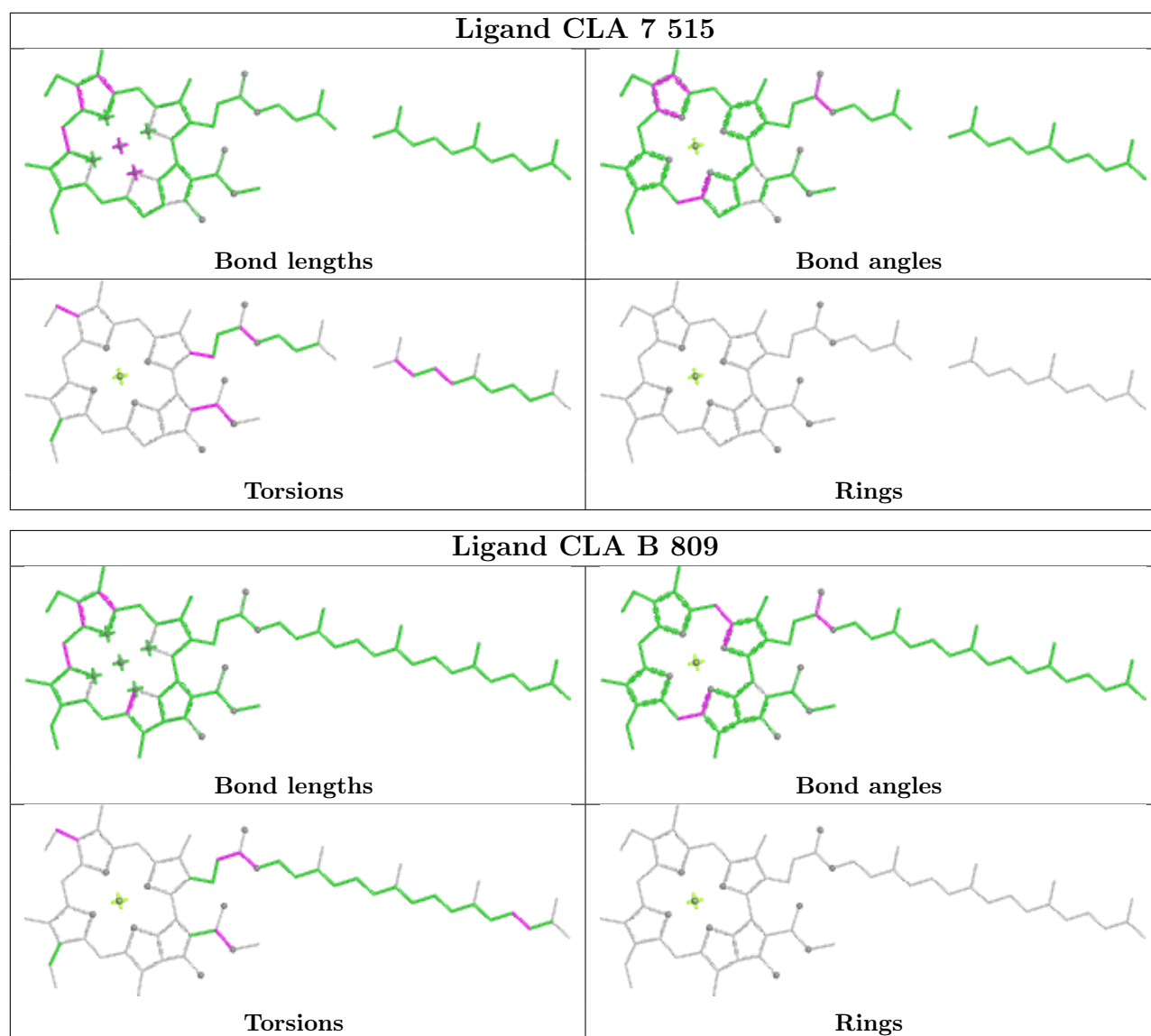
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	1	523	BCR	1	0
20	1	527	LMU	1	0
16	B	837	CLA	1	0
16	A	814	CLA	1	0
18	I	102	BCR	2	0
22	A	801	PQN	1	0
18	6	518	BCR	2	0
18	A	850	BCR	1	0
18	5	420	BCR	1	0
16	A	807	CLA	1	0
16	4	405	CLA	1	0
16	A	839	CLA	1	0
18	3	514	BCR	1	0
17	1	518	LUT	6	0
16	5	411	CLA	3	0
16	B	832	CLA	4	0
16	A	816	CLA	1	0
16	A	835	CLA	1	0
16	1	509	CLA	2	0
16	B	845	CLA	1	0
18	1	520	BCR	2	0
16	5	404	CLA	1	0
16	A	831	CLA	1	0
18	B	804	BCR	1	0
18	1	521	BCR	2	0
16	B	810	CLA	1	0
16	3	506	CLA	2	0
16	A	830	CLA	1	0
18	1	522	BCR	1	0
16	A	844	CLA	1	0
16	B	822	CLA	1	0
16	7	511	CLA	2	0
16	B	817	CLA	1	0
18	B	849	BCR	1	0
16	1	507	CLA	3	0
16	2	409	CLA	1	0
18	B	852	BCR	2	0
18	7	518	BCR	1	0
22	B	803	PQN	1	0

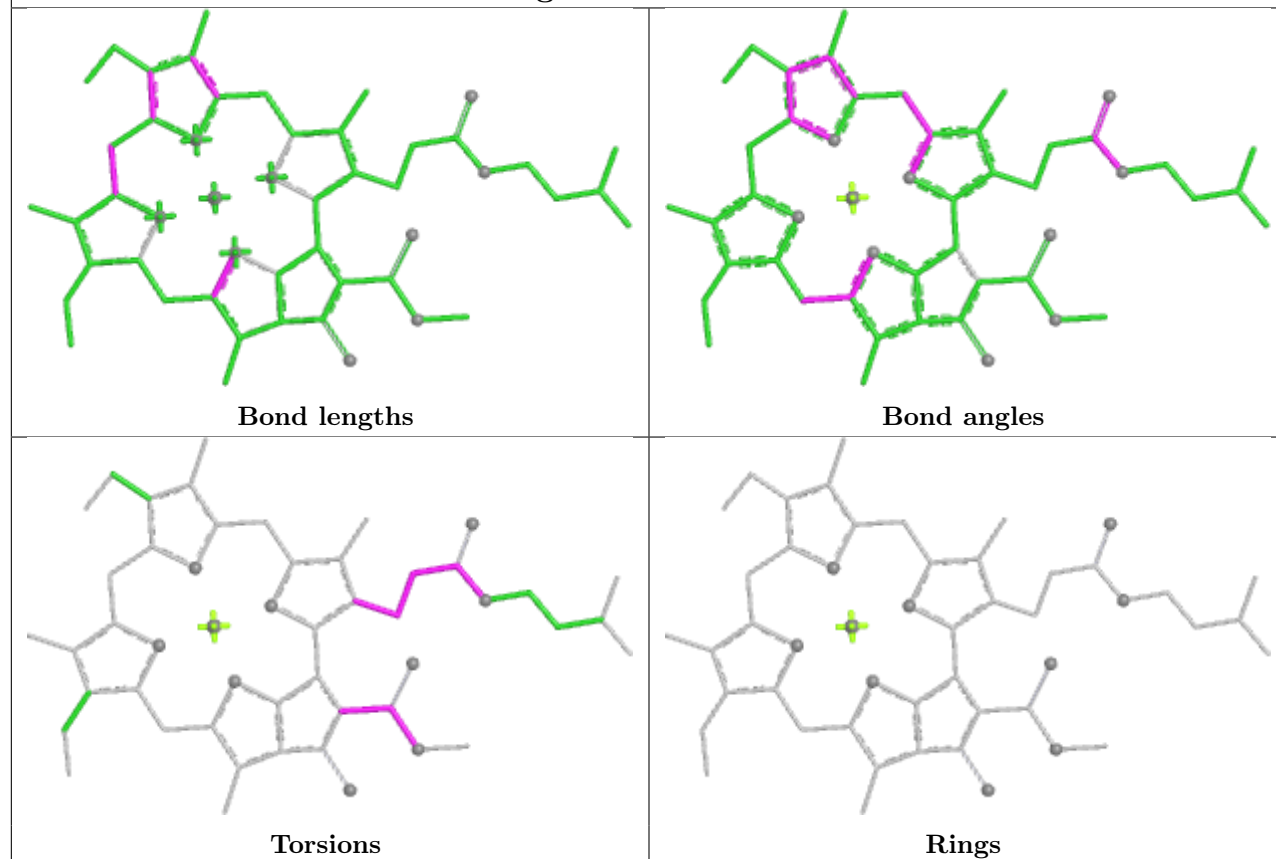
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

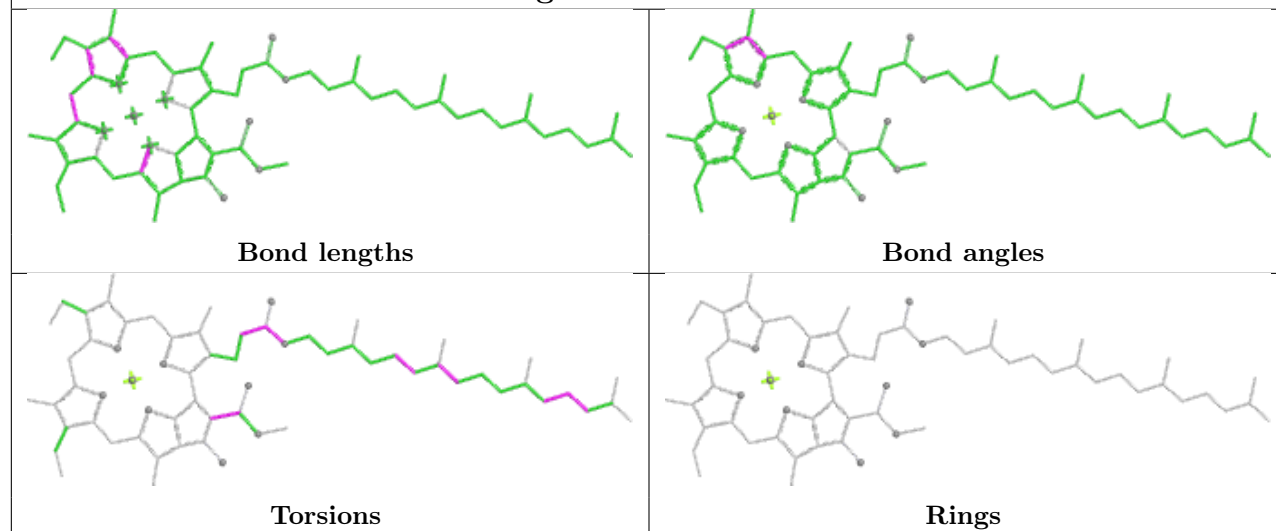




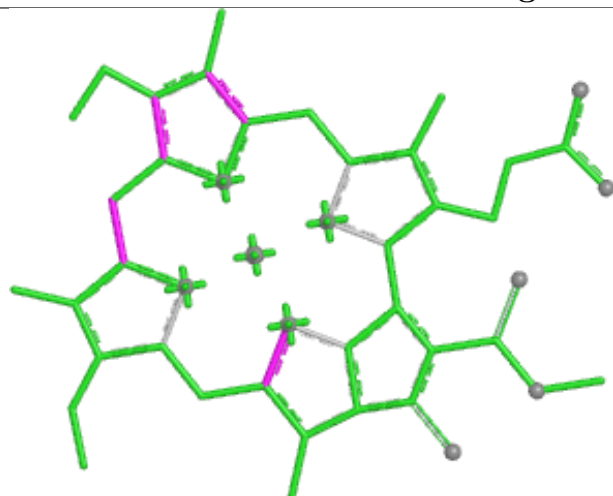
## Ligand CLA 7 508



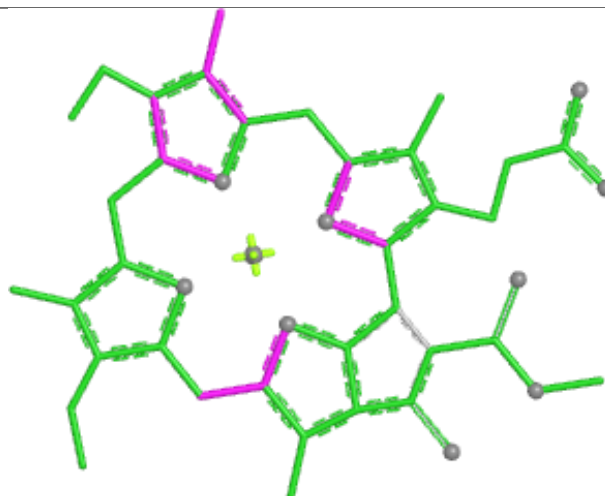
## Ligand CLA 6 510



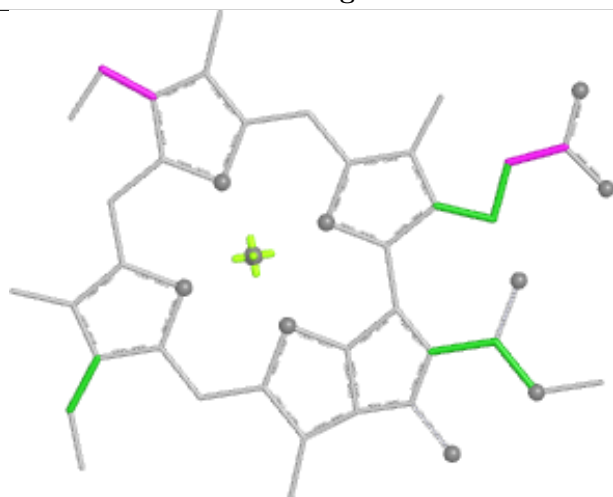
## Ligand CLA 7 517



Bond lengths



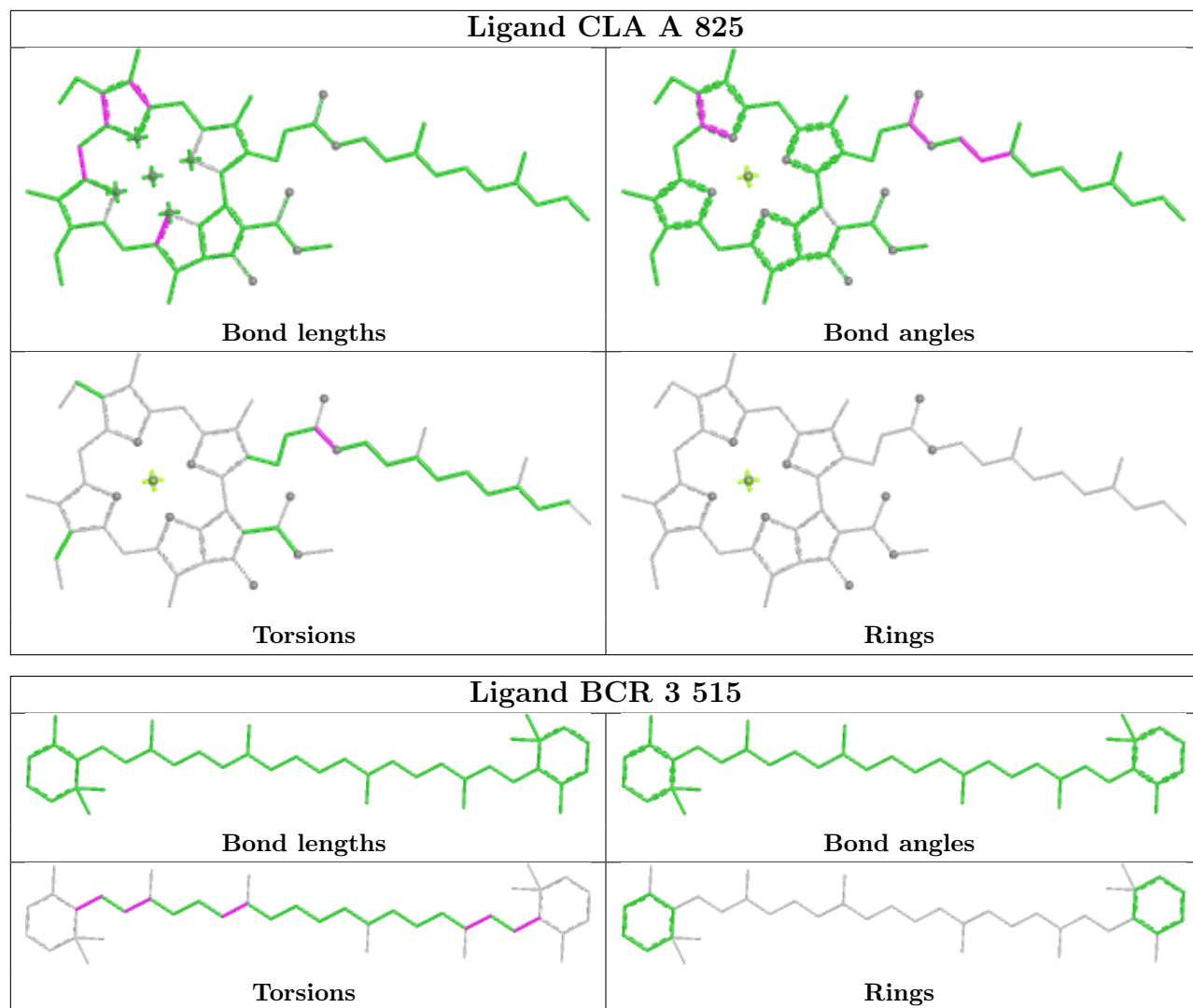
Bond angles

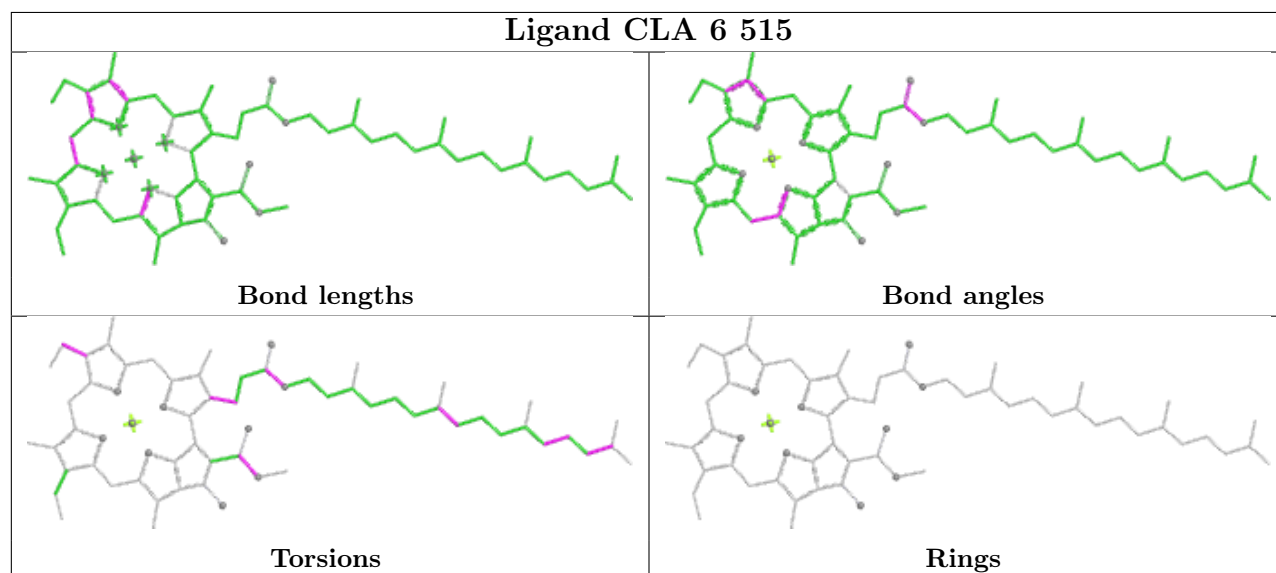
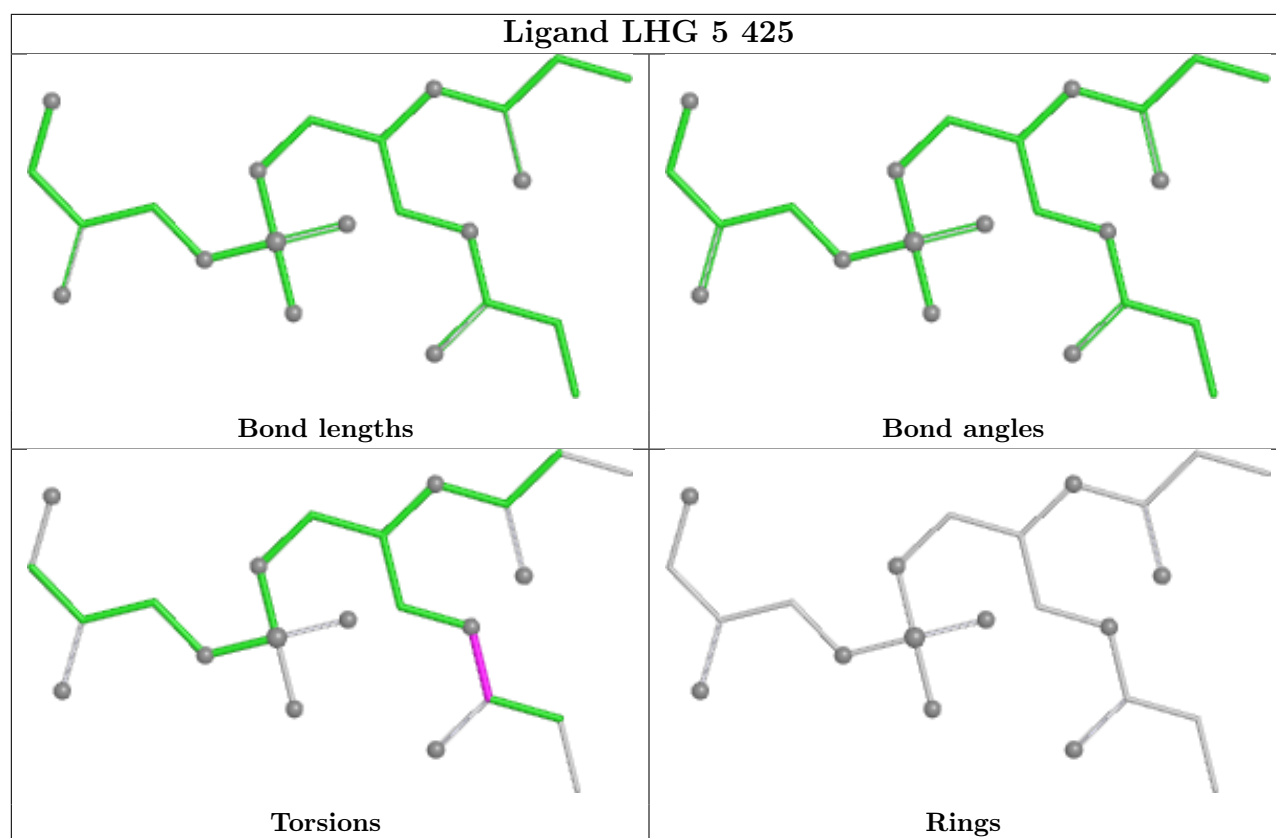


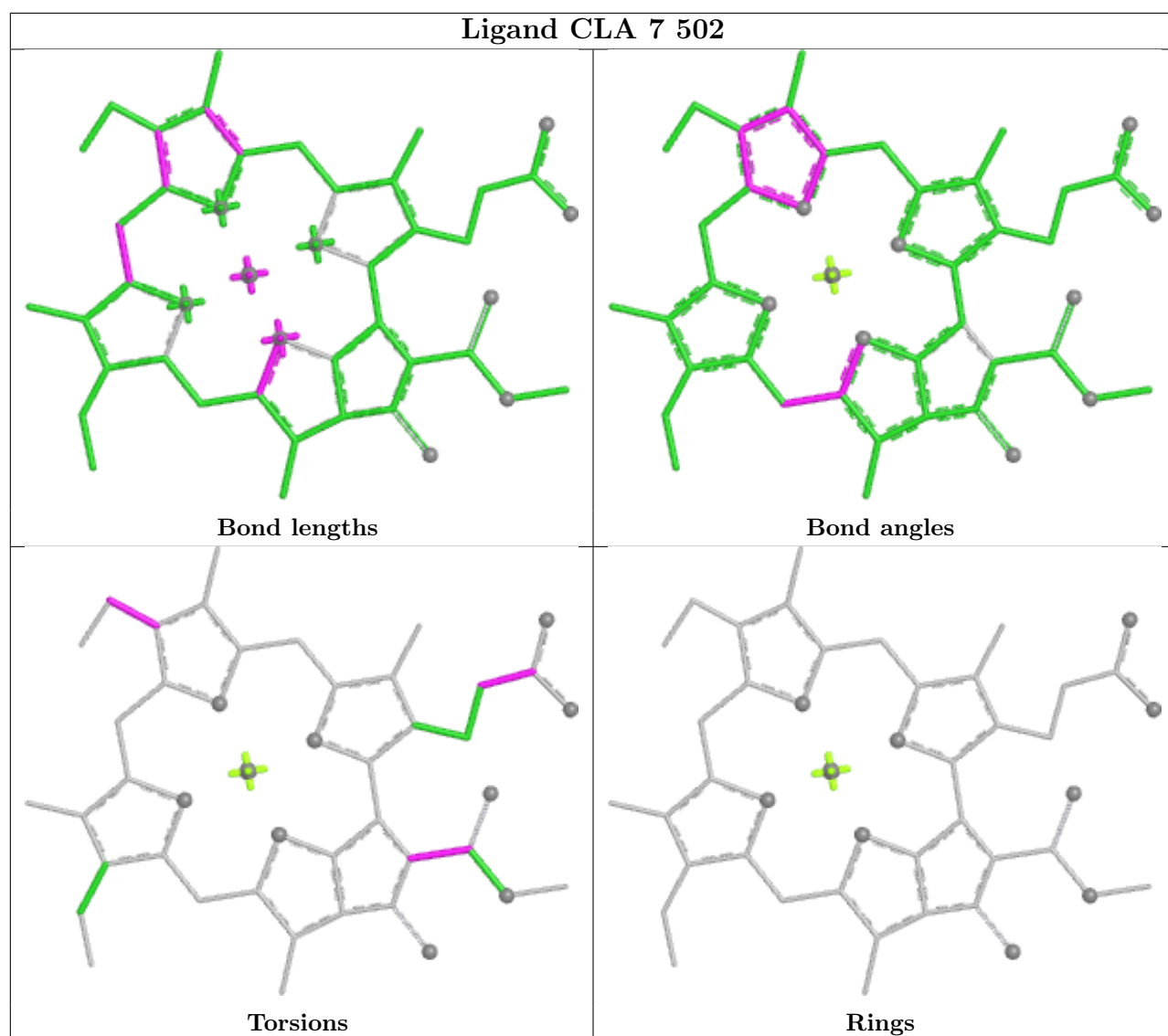
Torsions



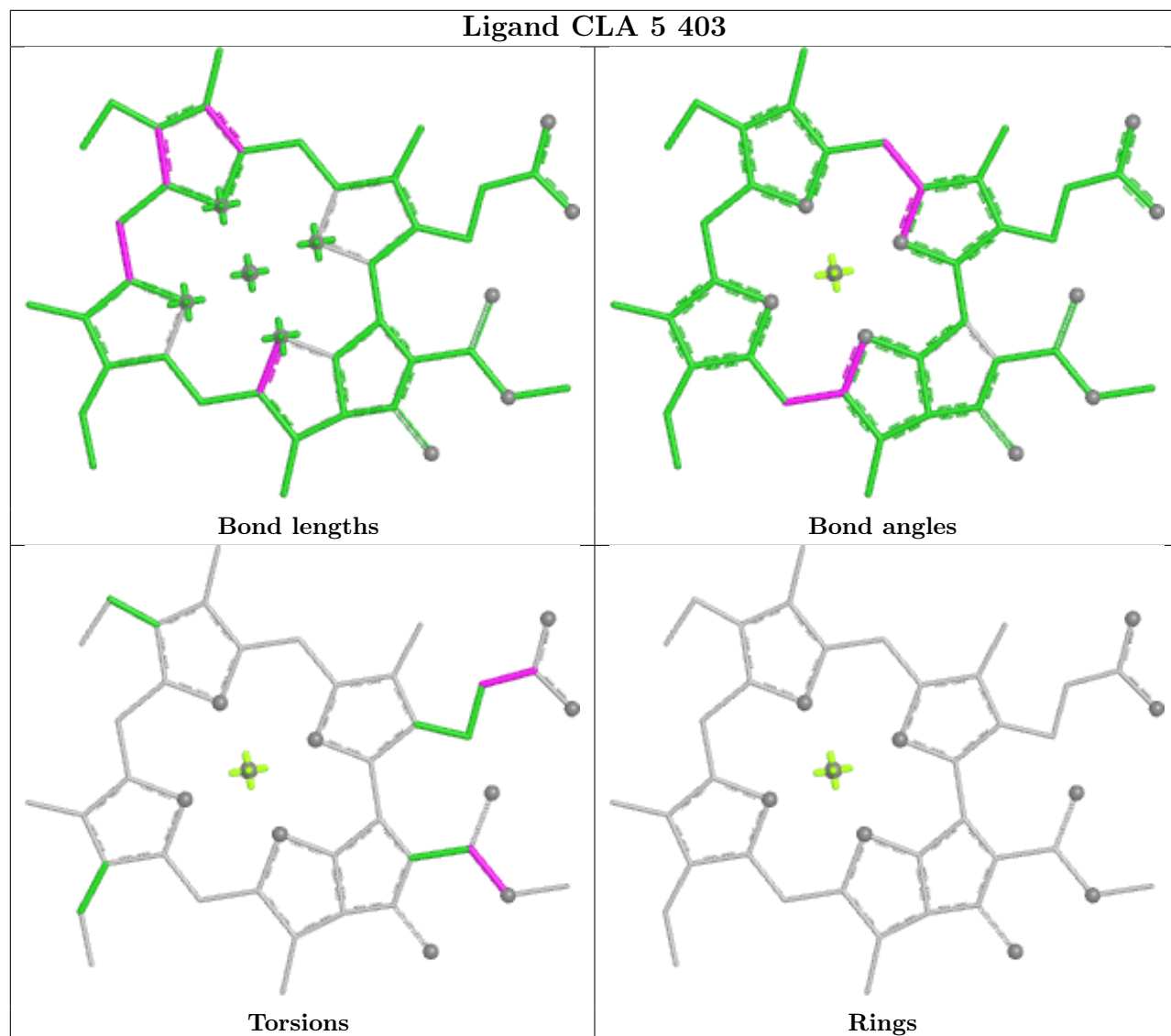
Rings



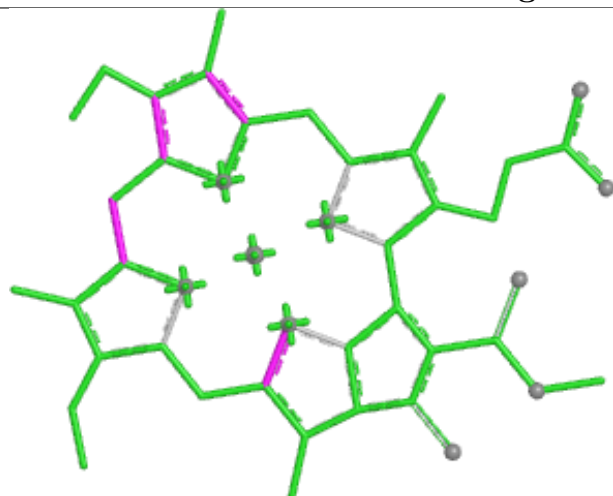




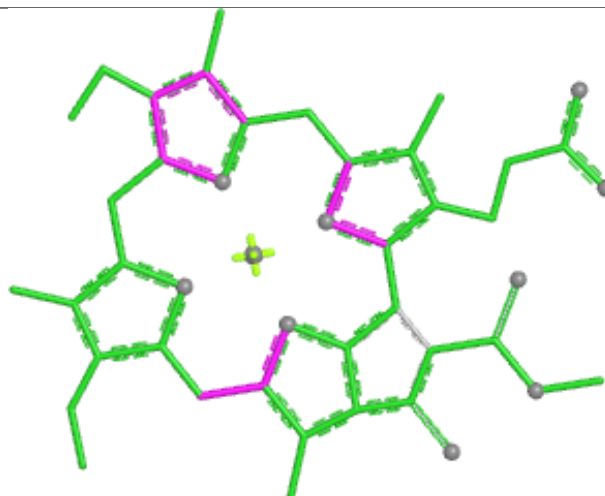
## Ligand CLA 5 403



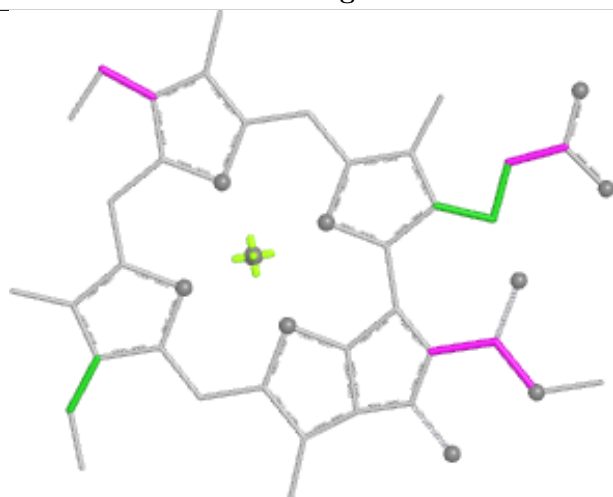
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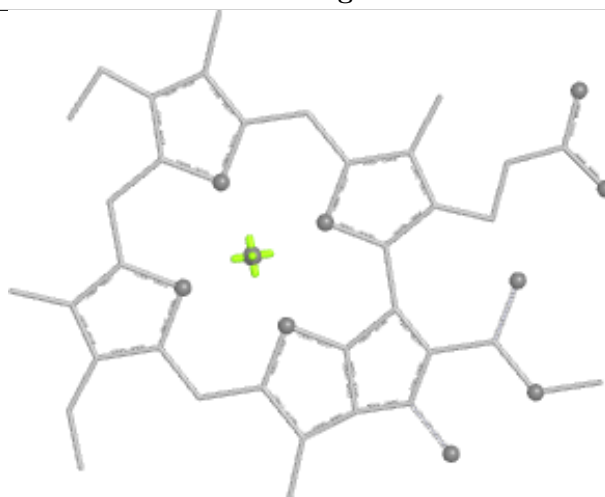
Bond lengths



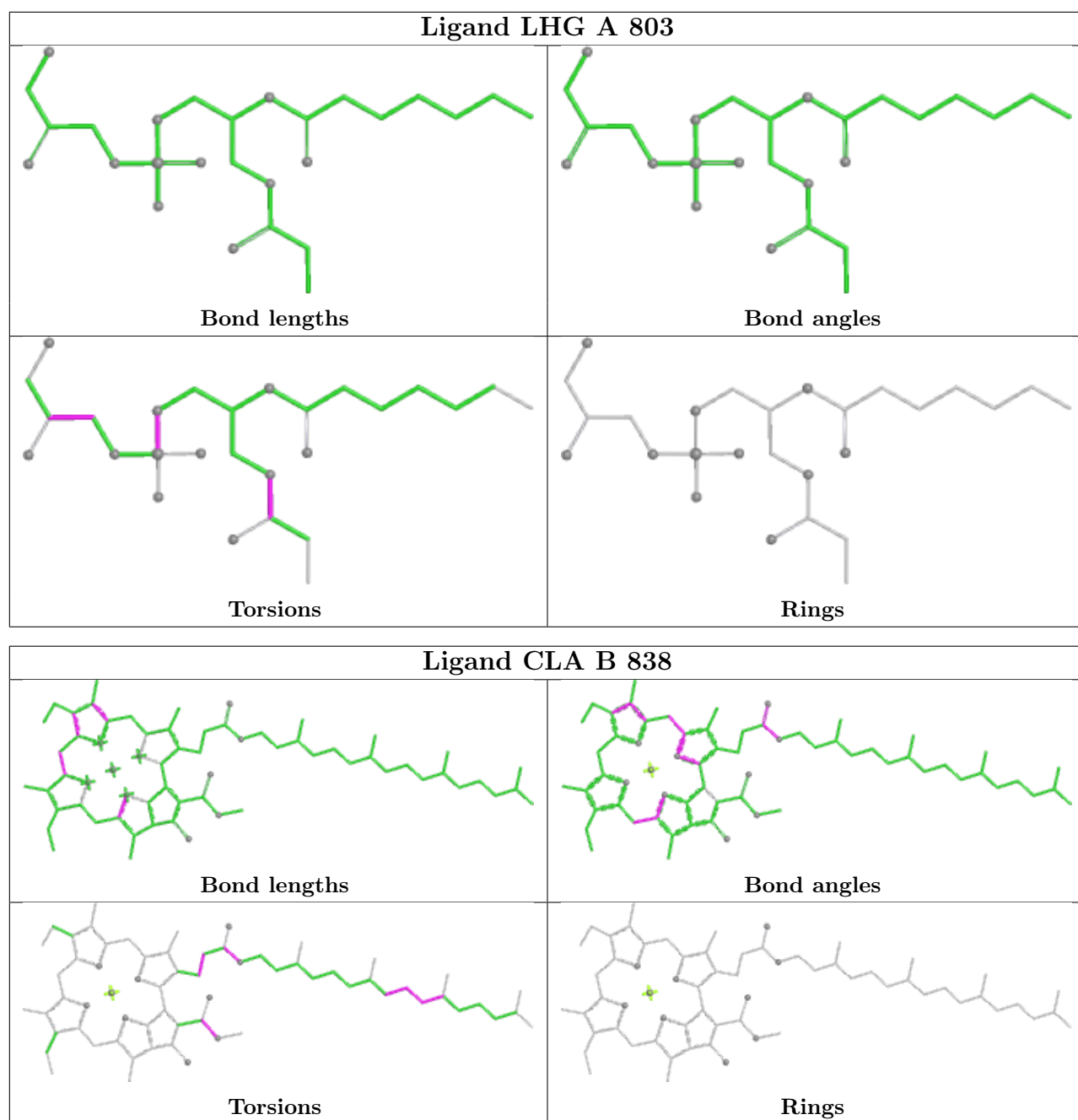
Bond angles

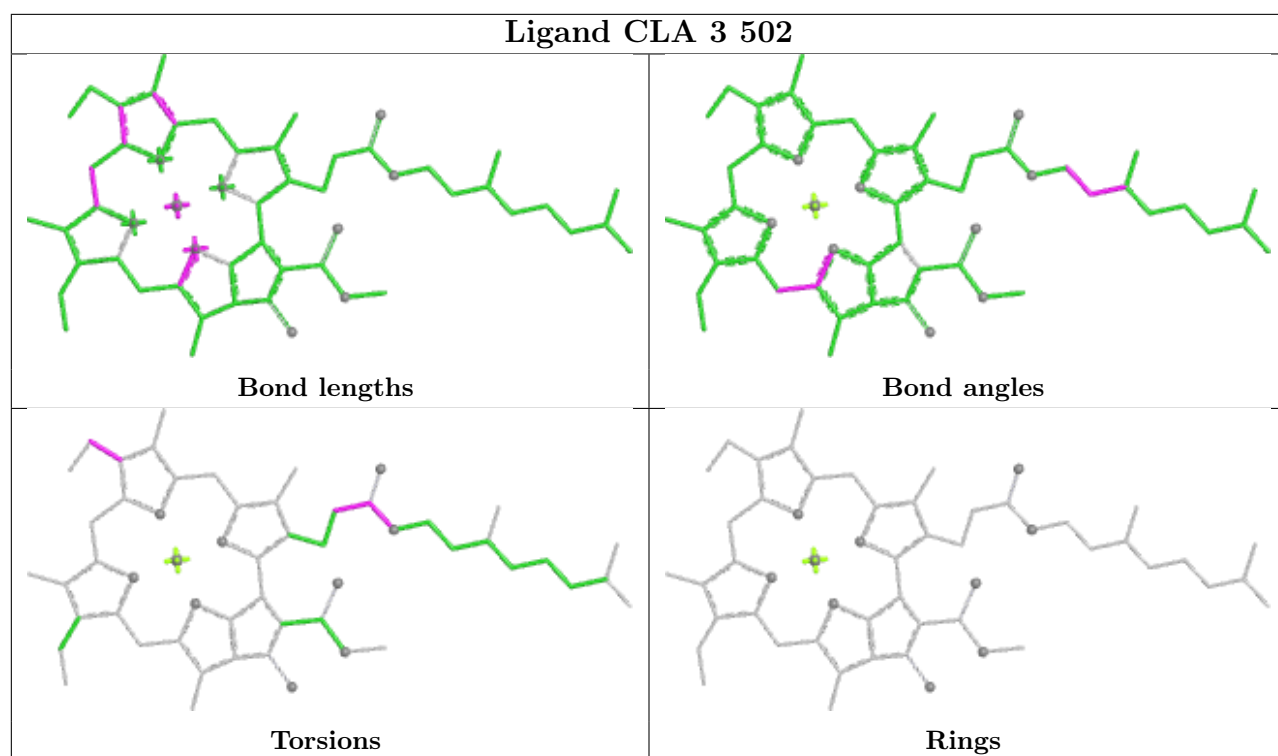


Torsions

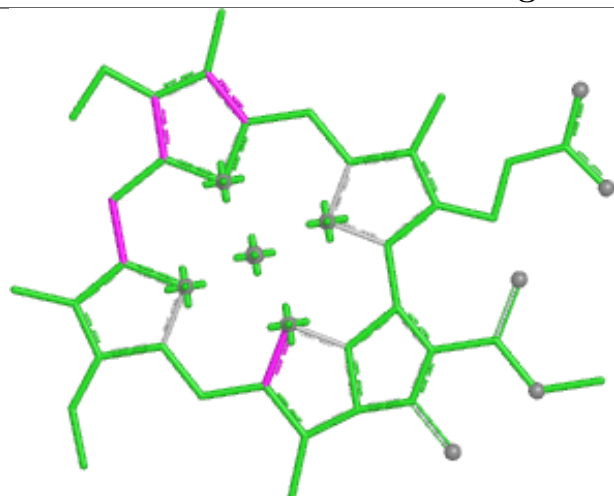


Rings

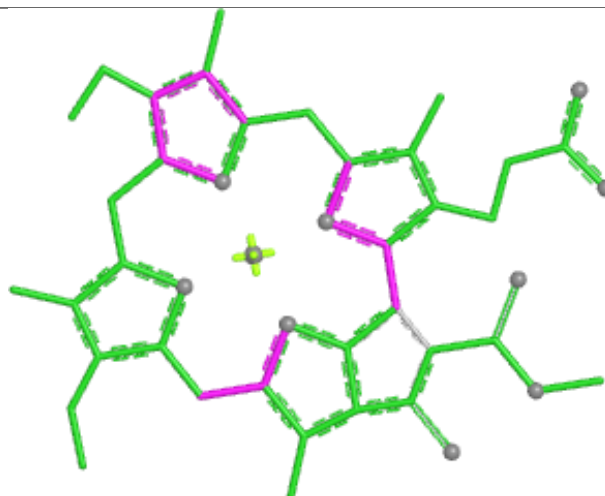




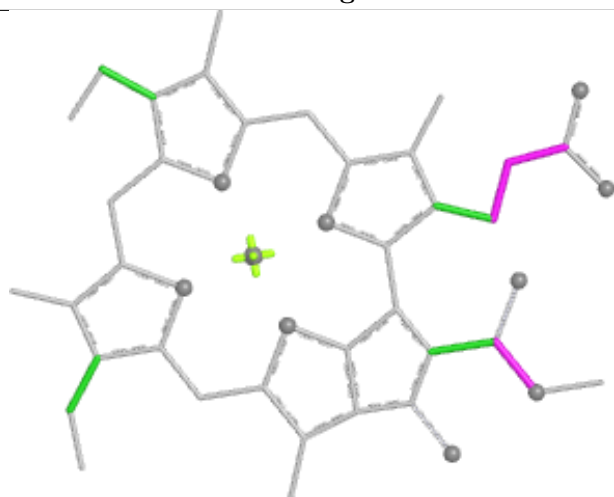
## Ligand CLA 7 503



Bond lengths



Bond angles

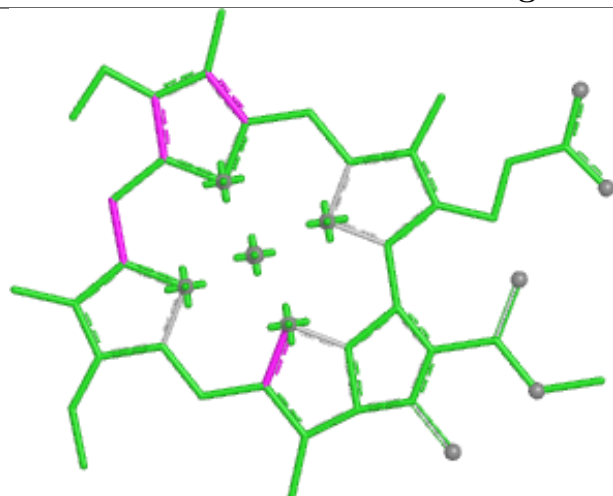


Torsions

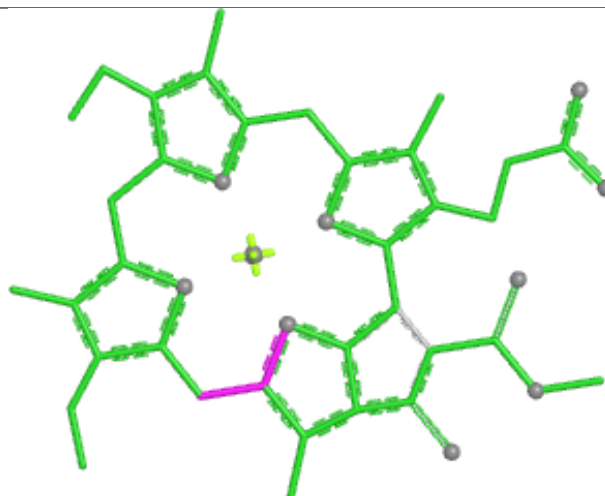


Rings

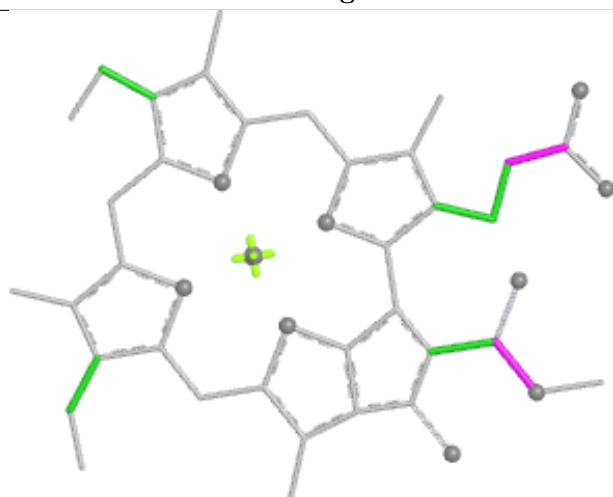
## Ligand CLA 3 503



Bond lengths



Bond angles

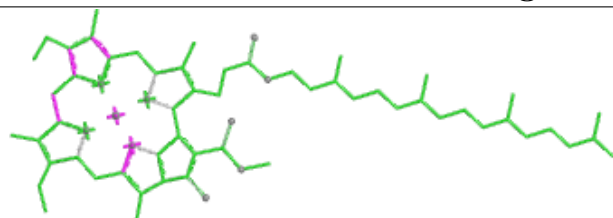


Torsions

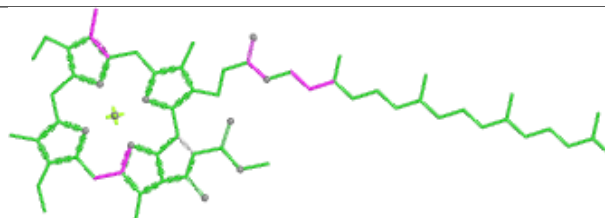


Rings

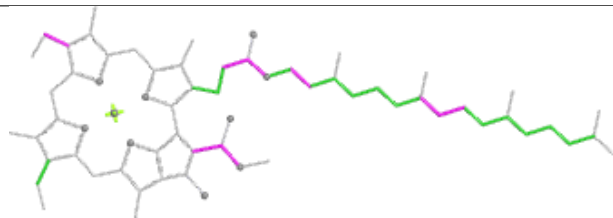
## Ligand CLA 6 507



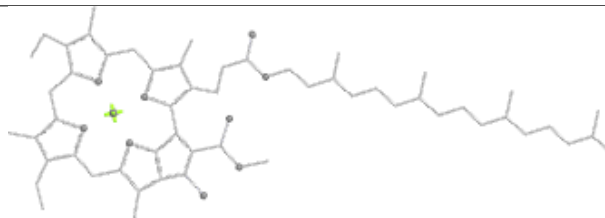
Bond lengths



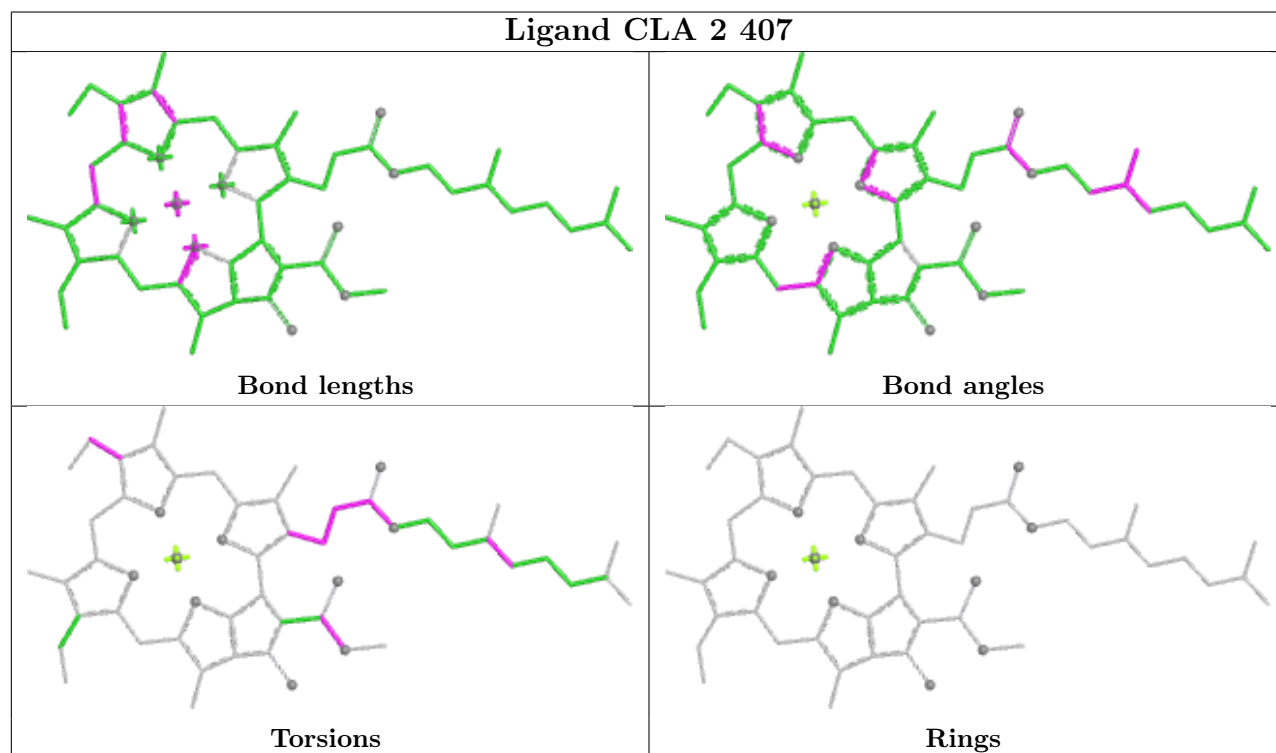
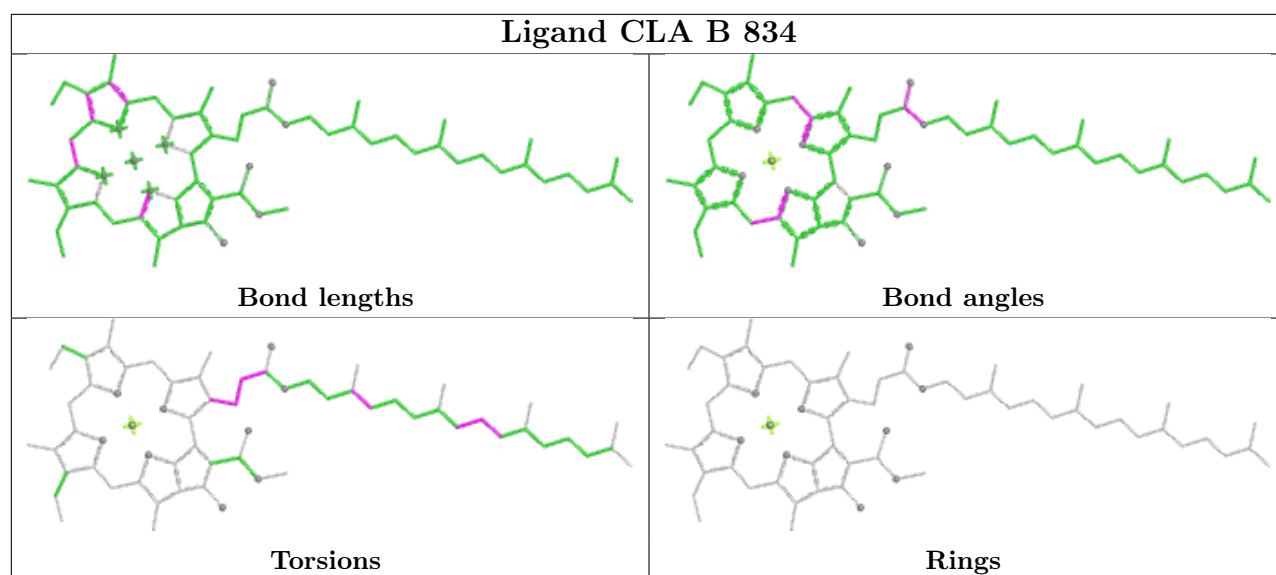
Bond angles



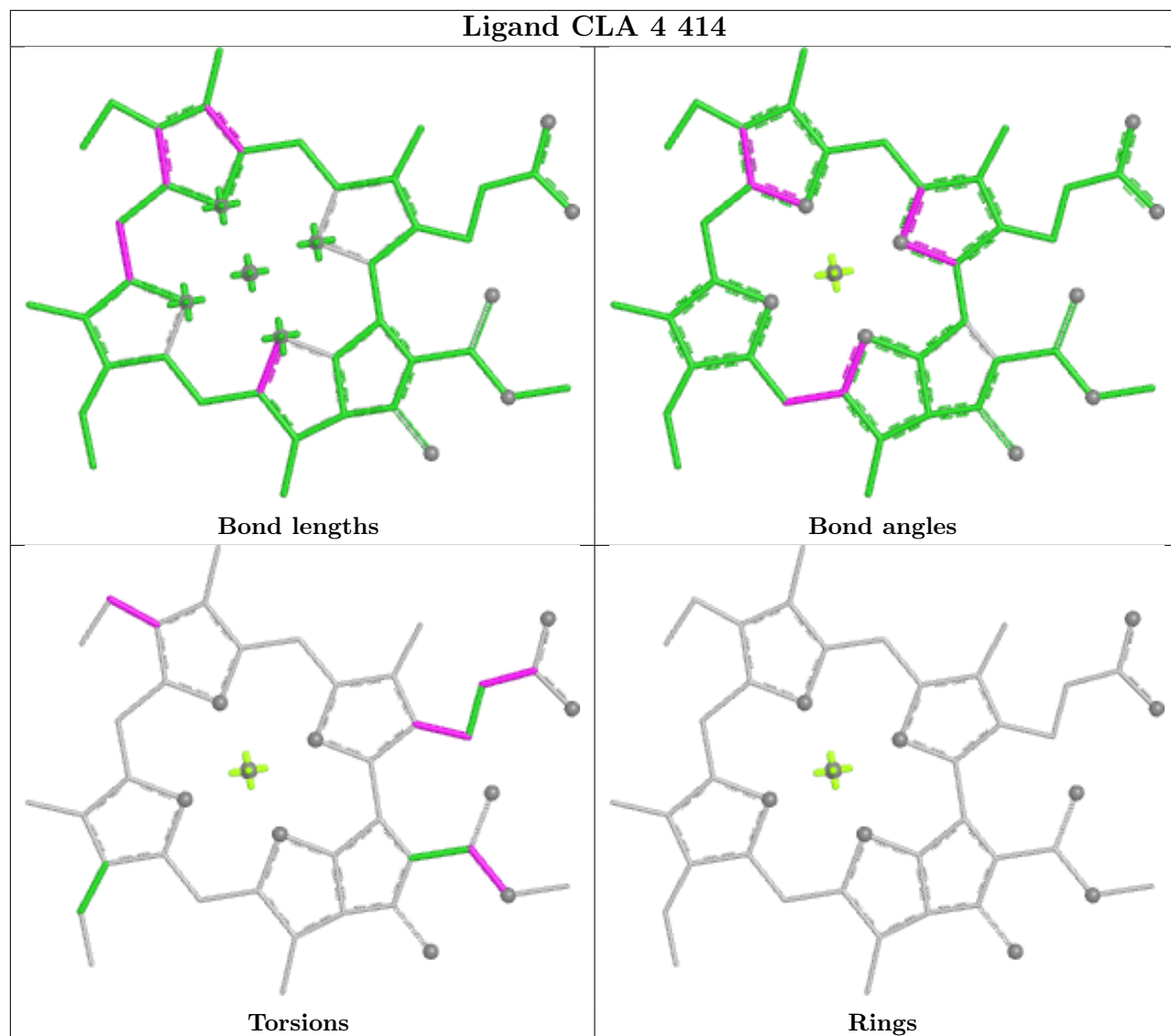
Torsions



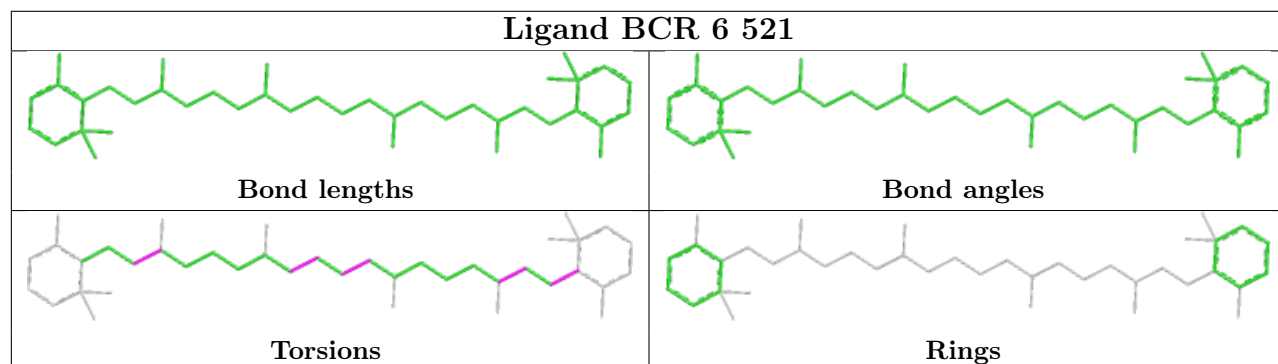
Rings



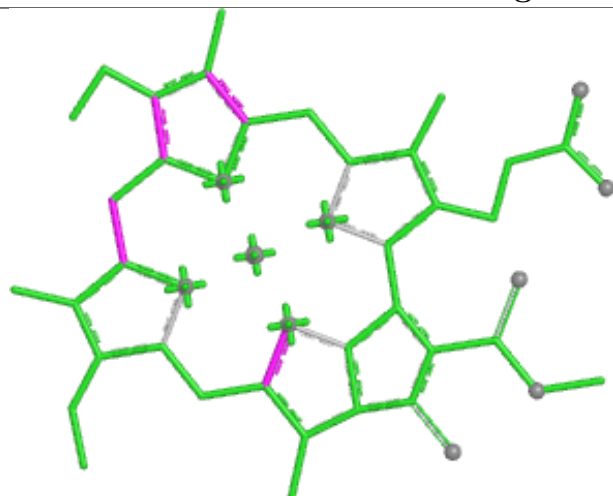
## Ligand CLA 4 414



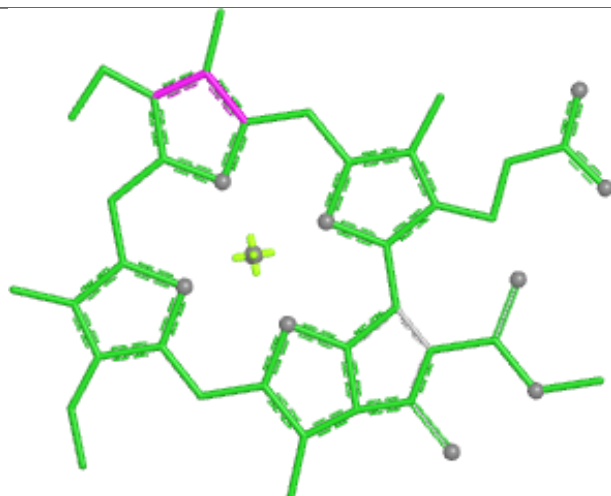
## Ligand BCR 6 521



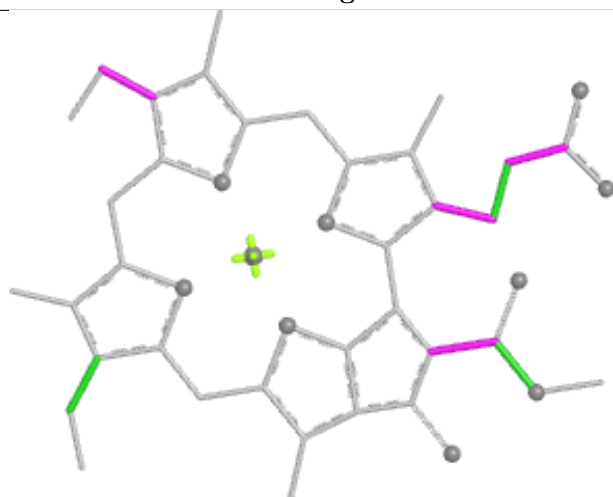
## Ligand CLA B 819



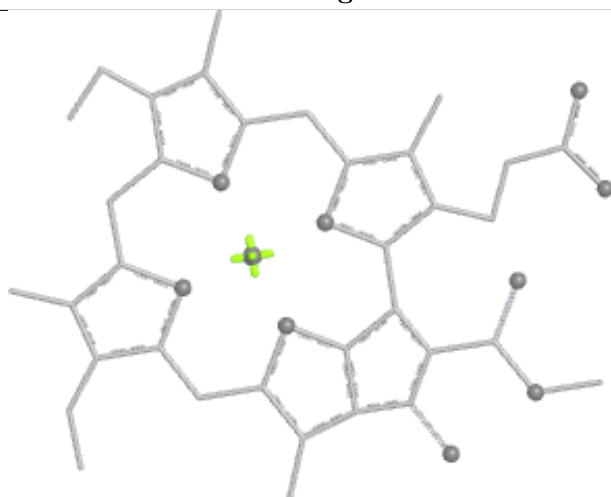
Bond lengths



Bond angles

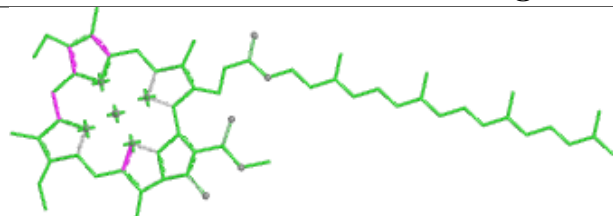


Torsions

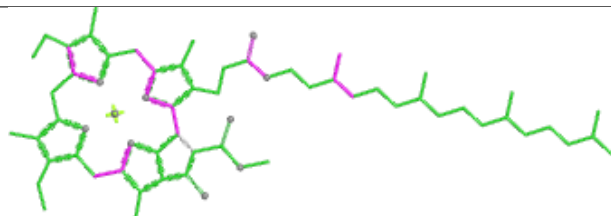


Rings

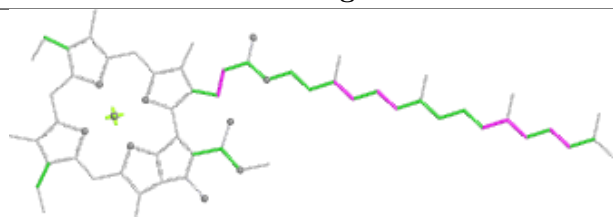
## Ligand CLA B 847



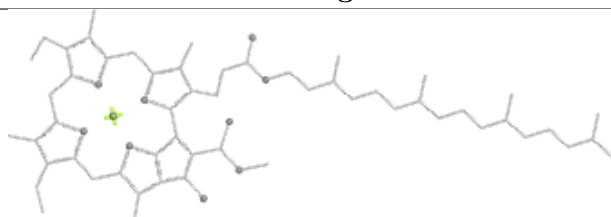
Bond lengths



Bond angles

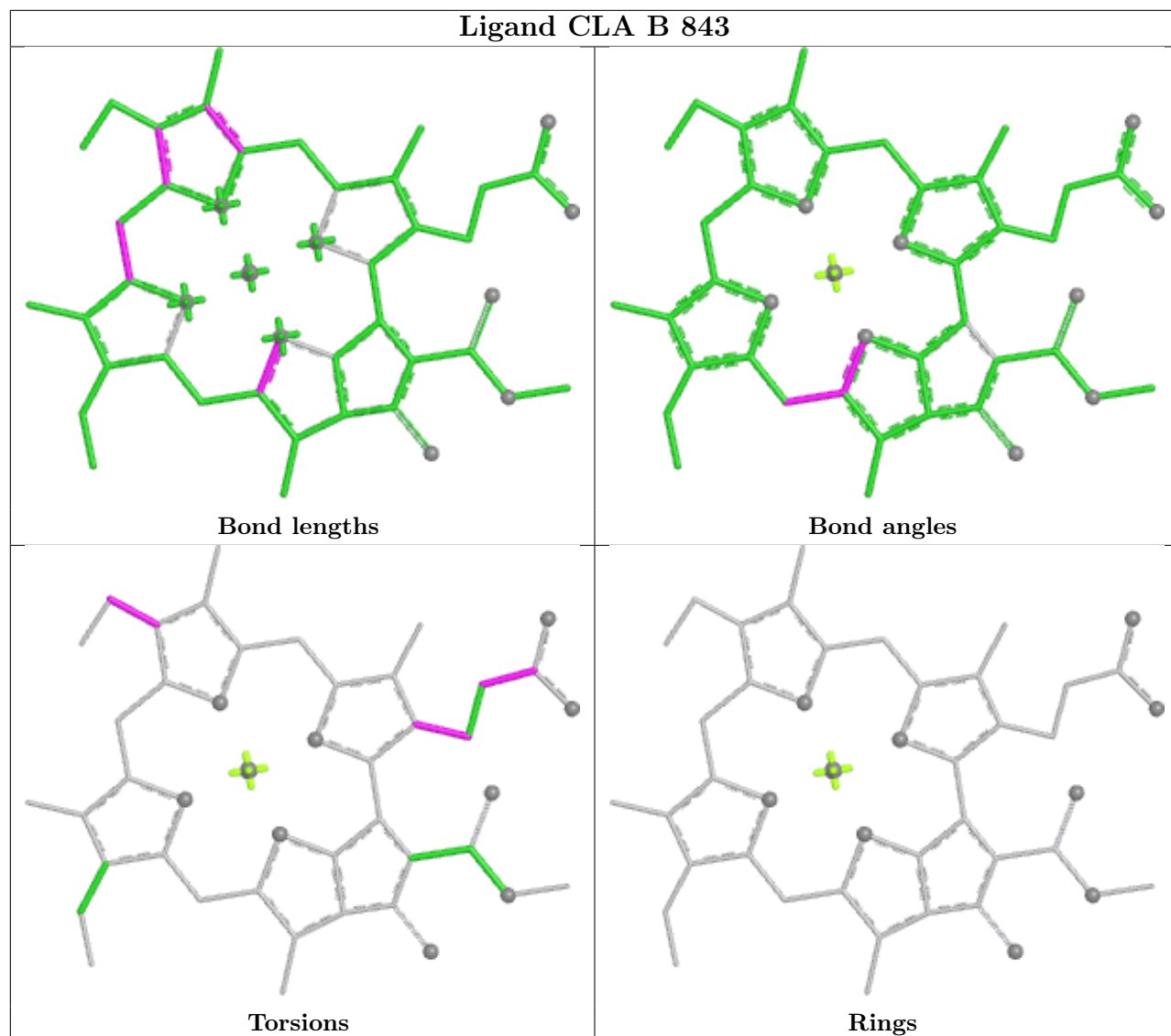


Torsions

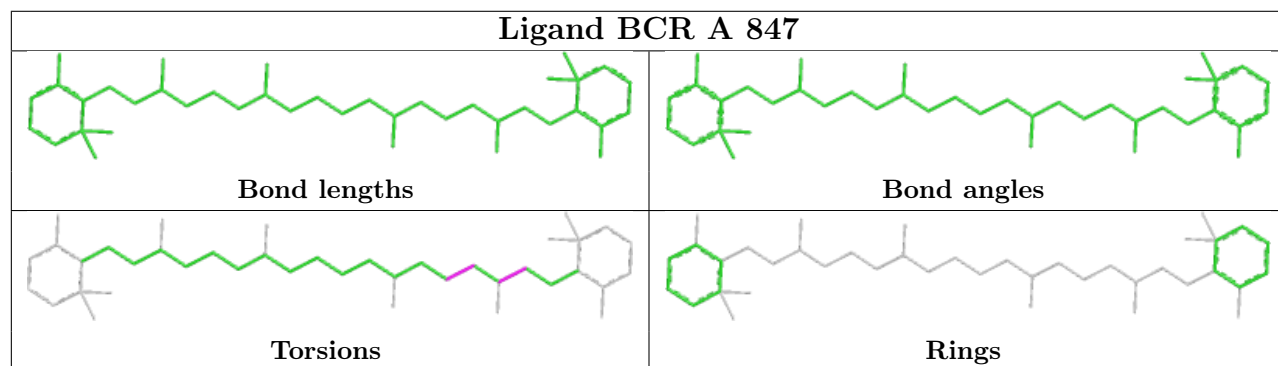


Rings

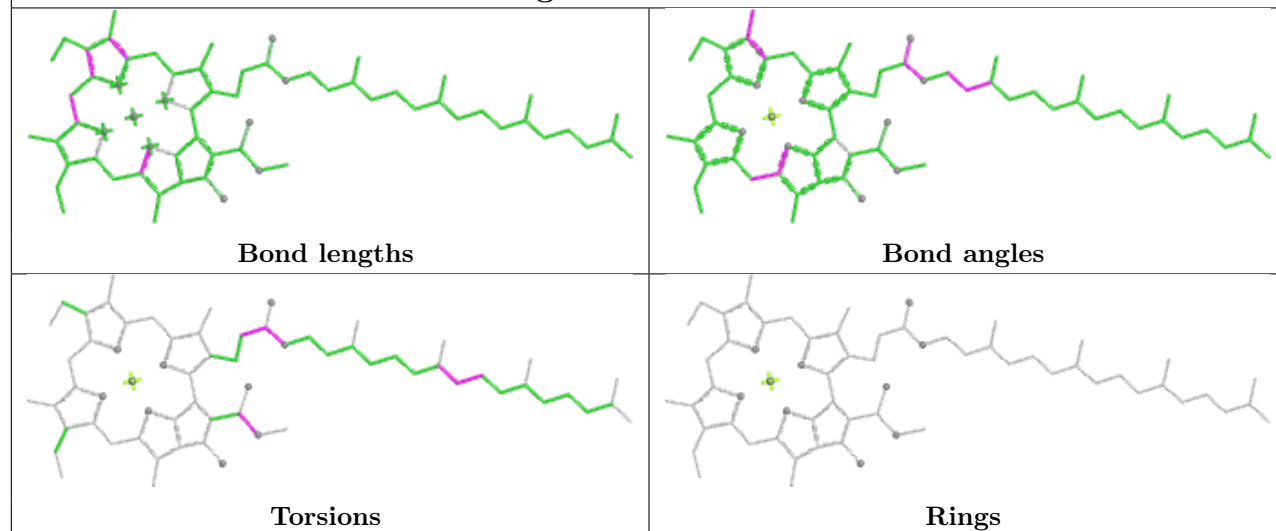
## Ligand CLA B 843



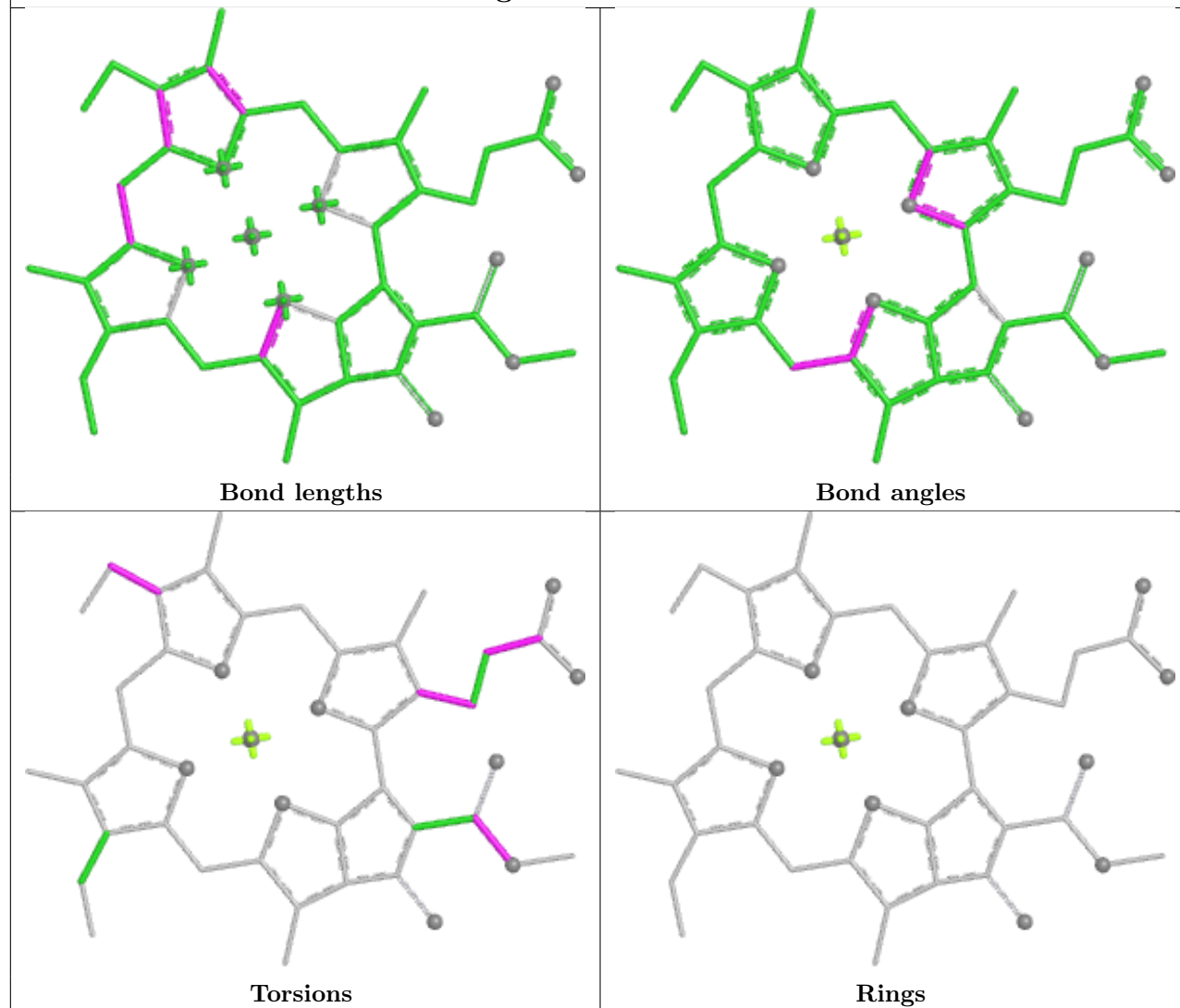
## Ligand BCR A 847

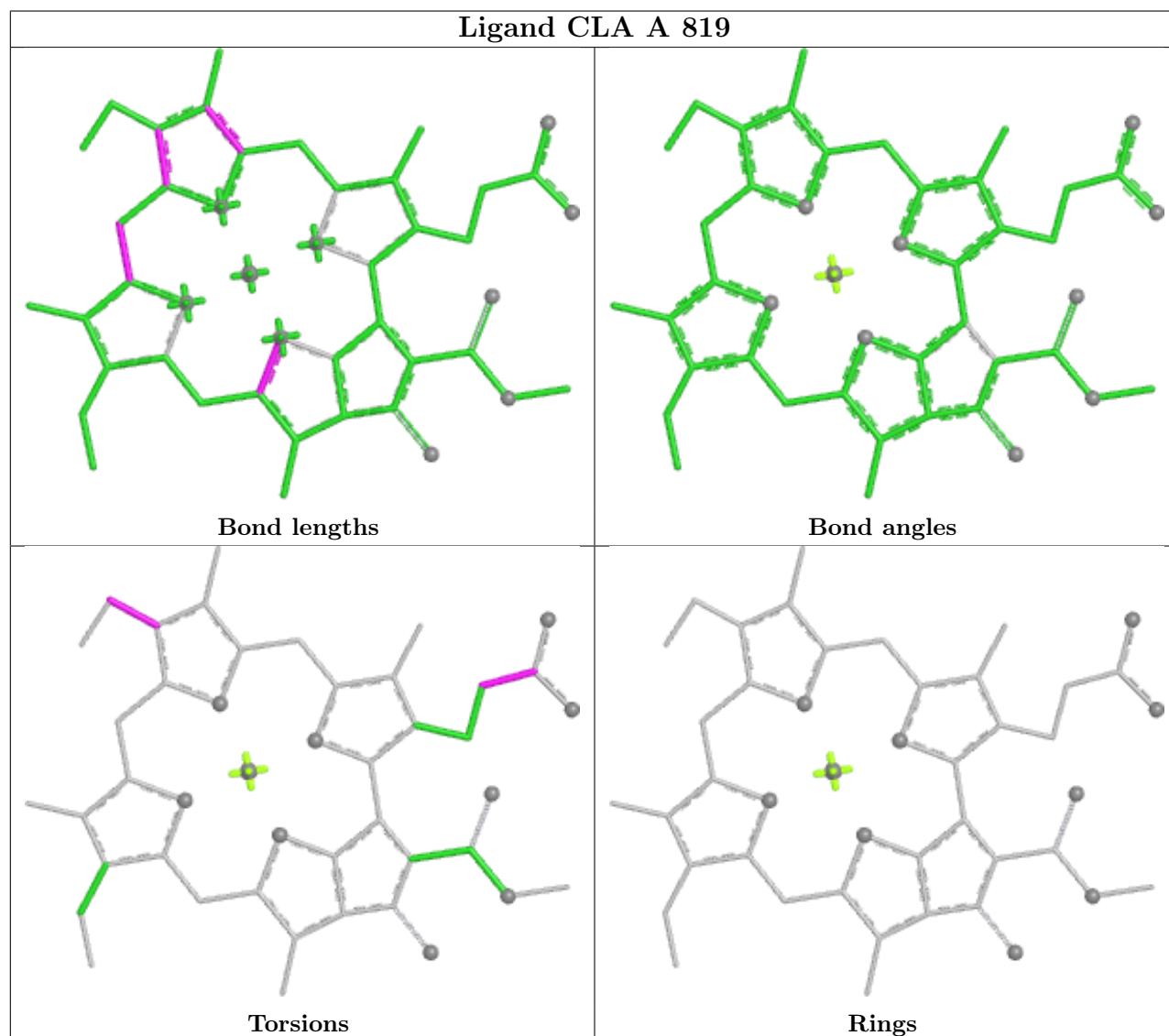
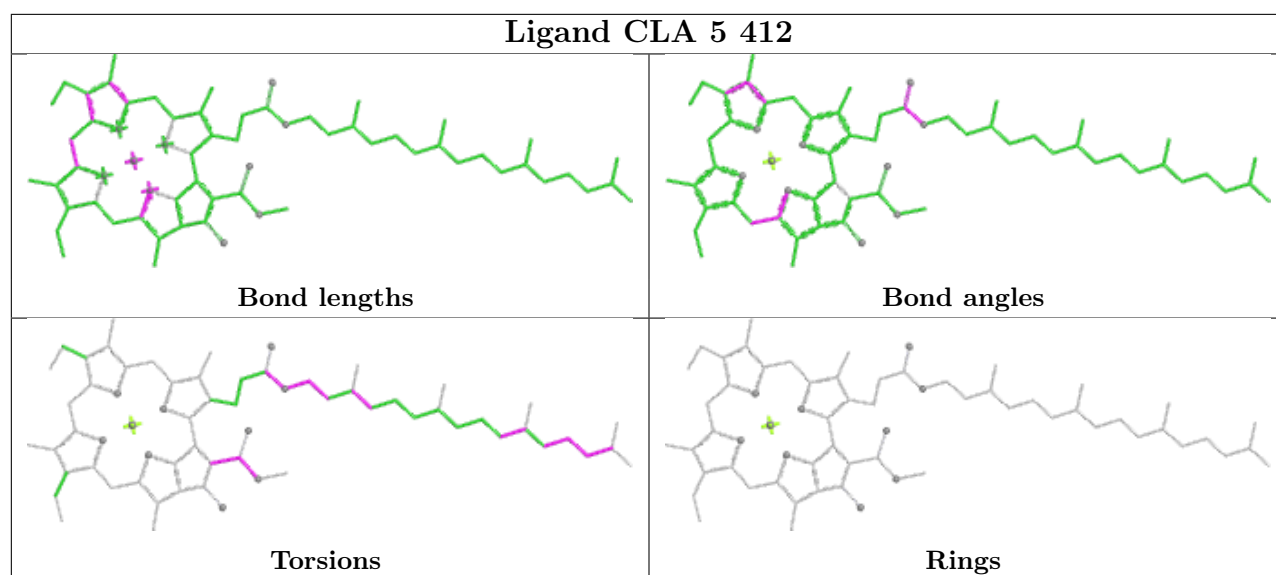


## Ligand CLA 4 408

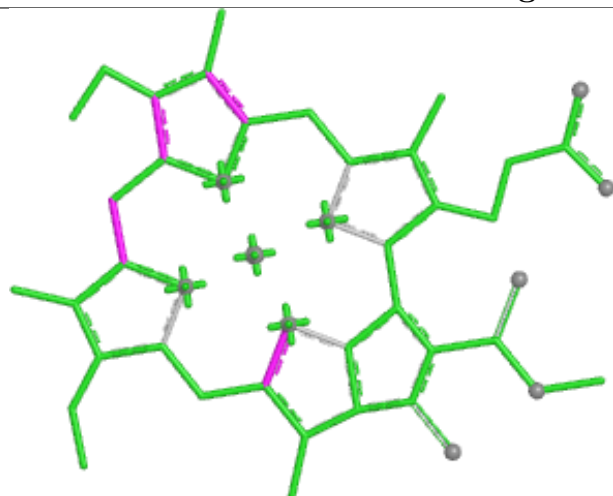


## Ligand CLA 3 511

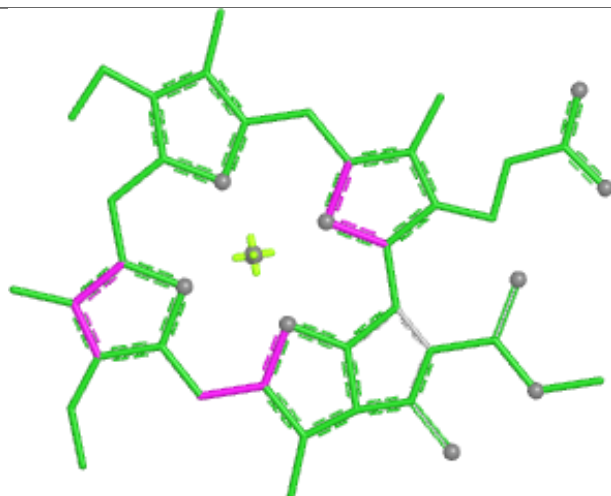




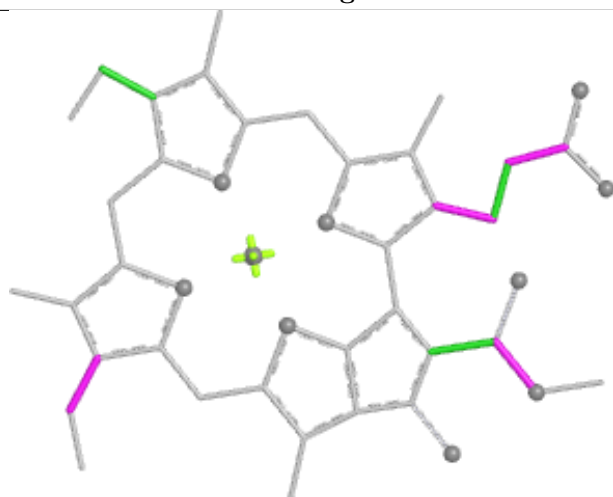
## Ligand CLA 6 512



Bond lengths



Bond angles

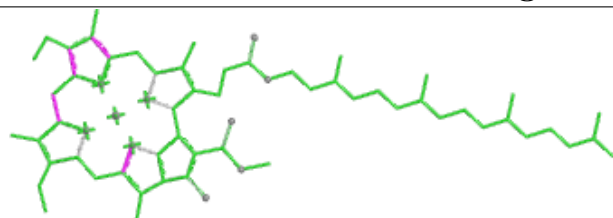


Torsions

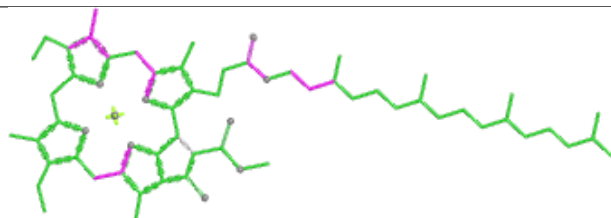


Rings

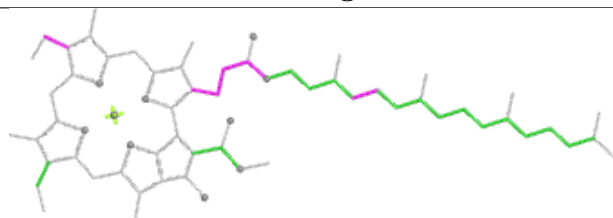
## Ligand CLA 4 416



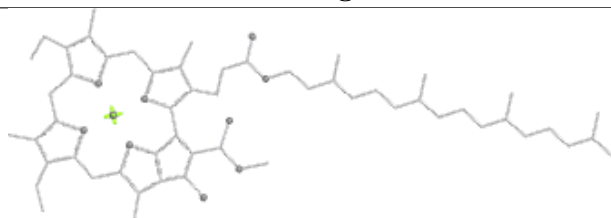
Bond lengths



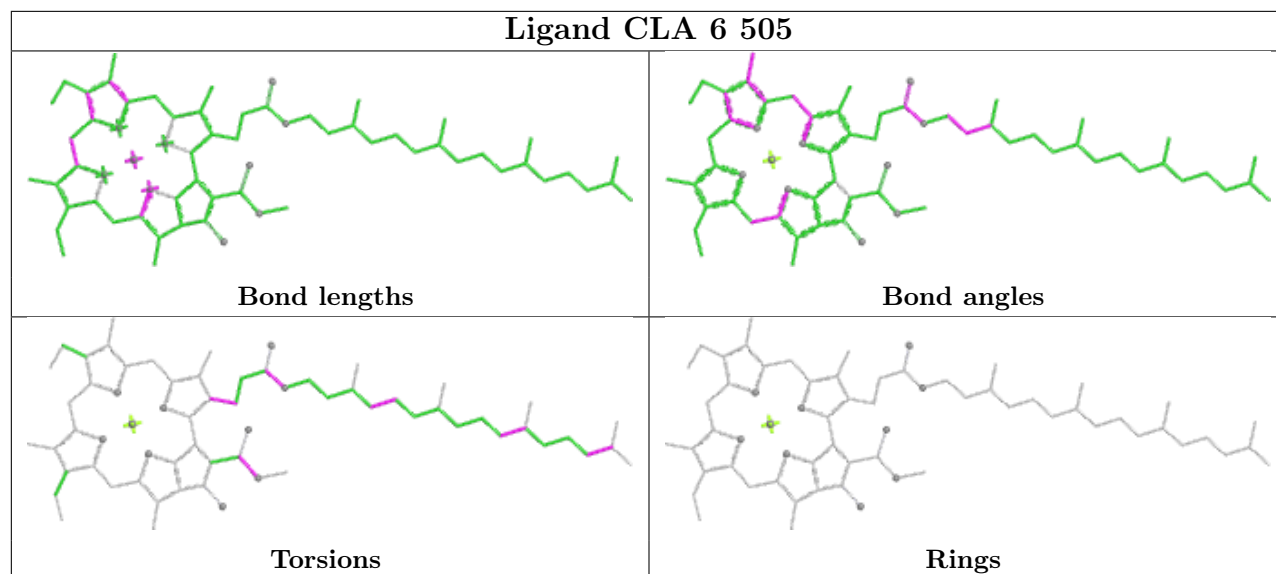
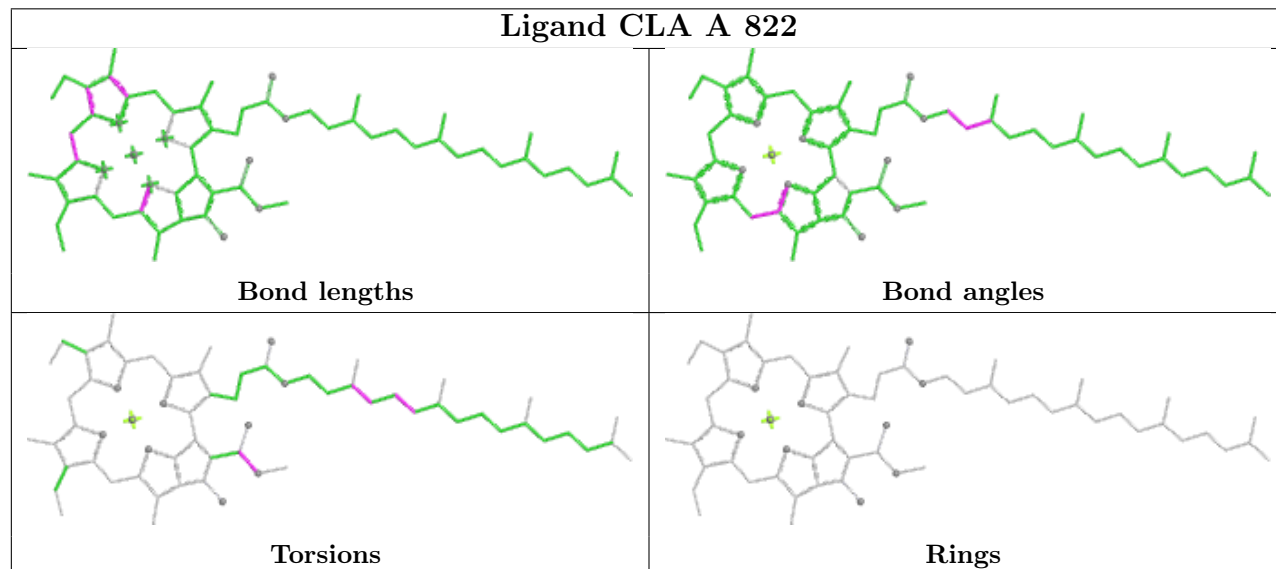
Bond angles

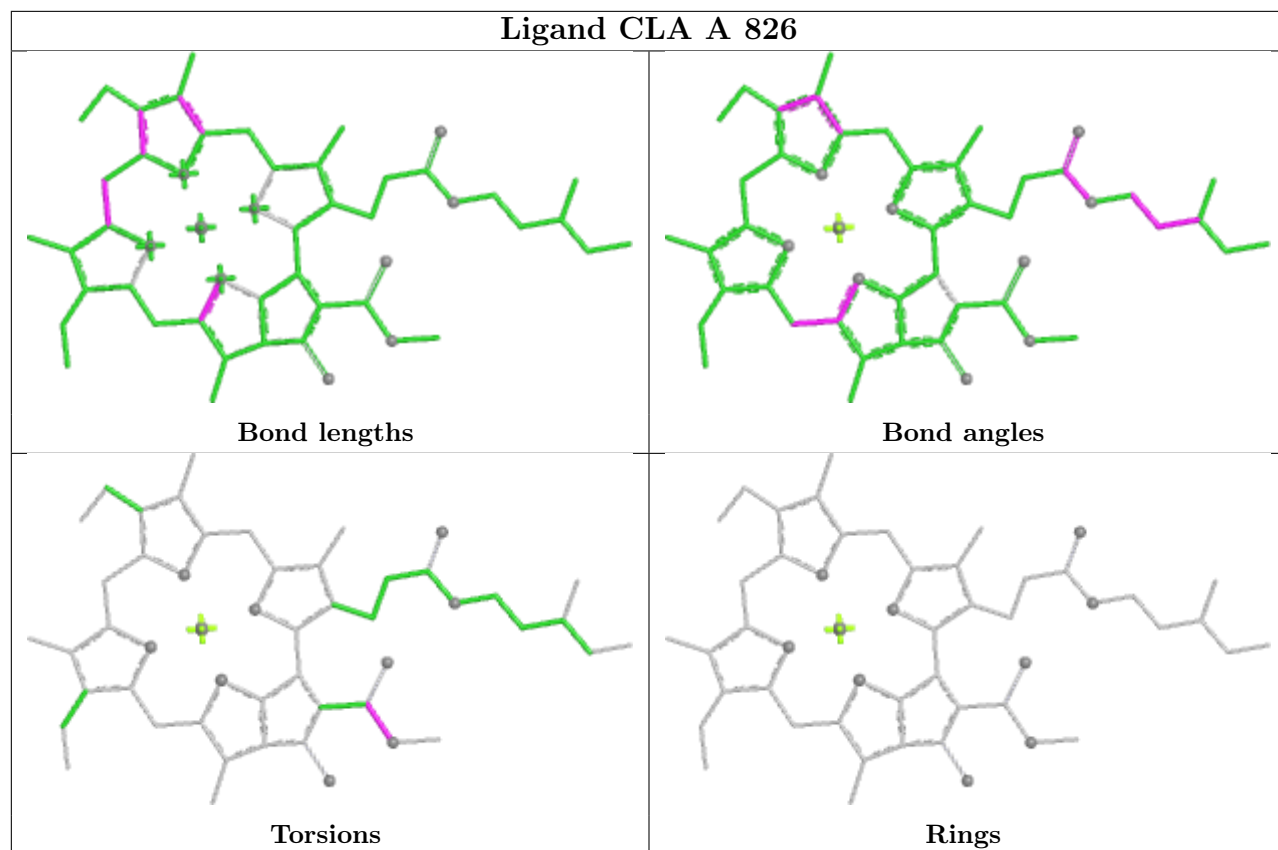


Torsions

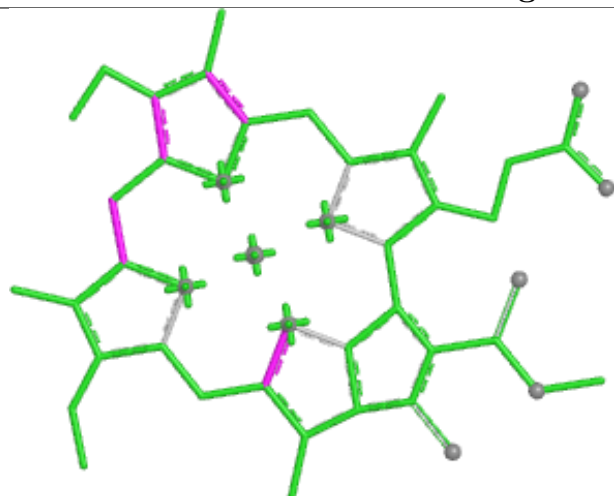


Rings

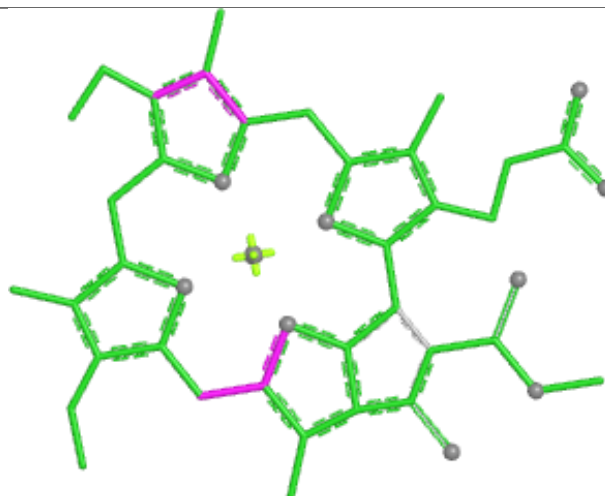
**Ligand CLA 6 505****Ligand CLA A 822**



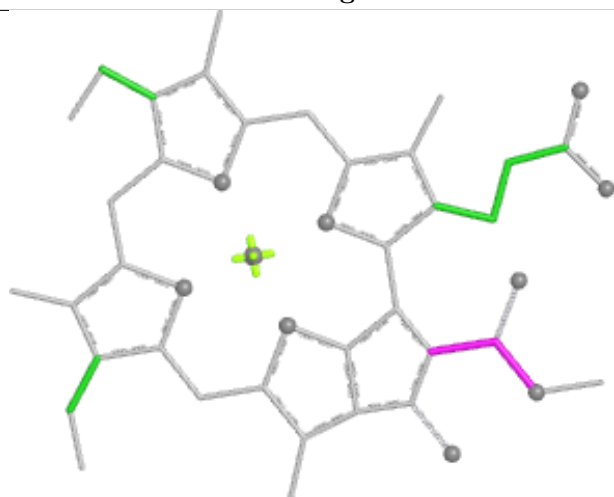
## Ligand CLA 1 526



Bond lengths



Bond angles

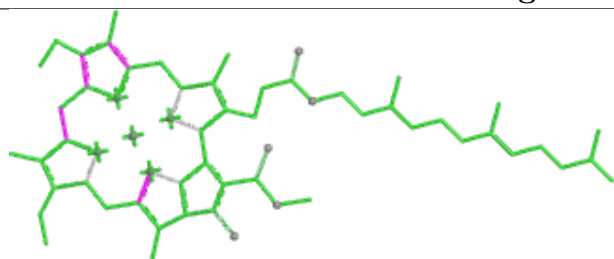


Torsions

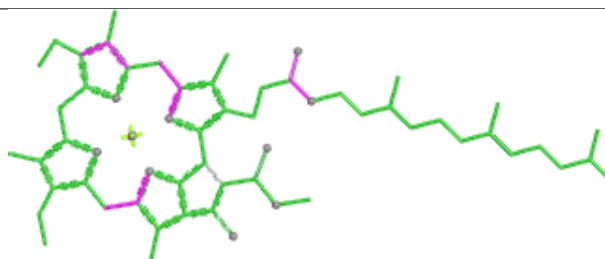


Rings

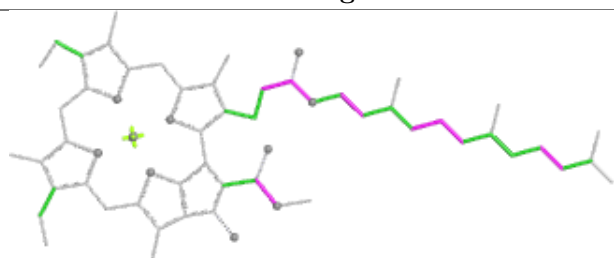
## Ligand CLA 4 410



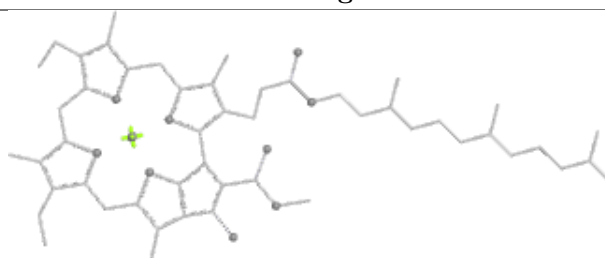
Bond lengths



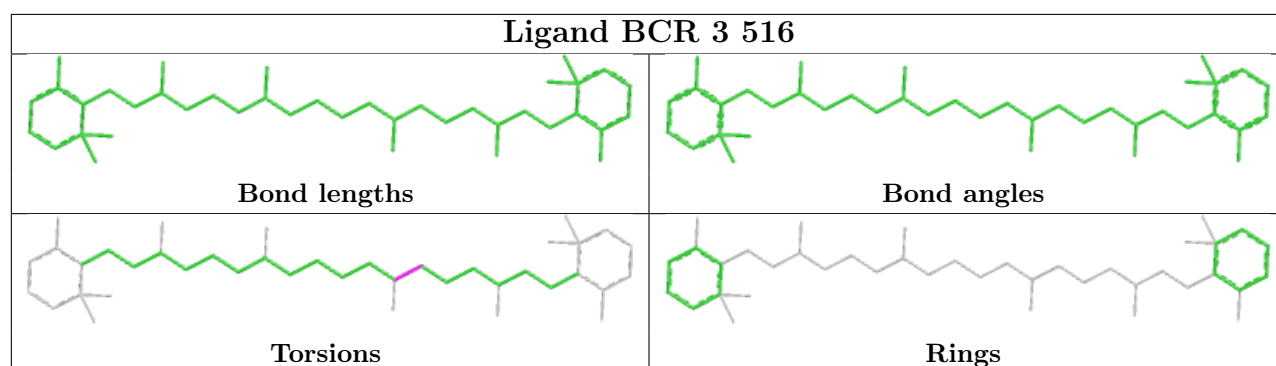
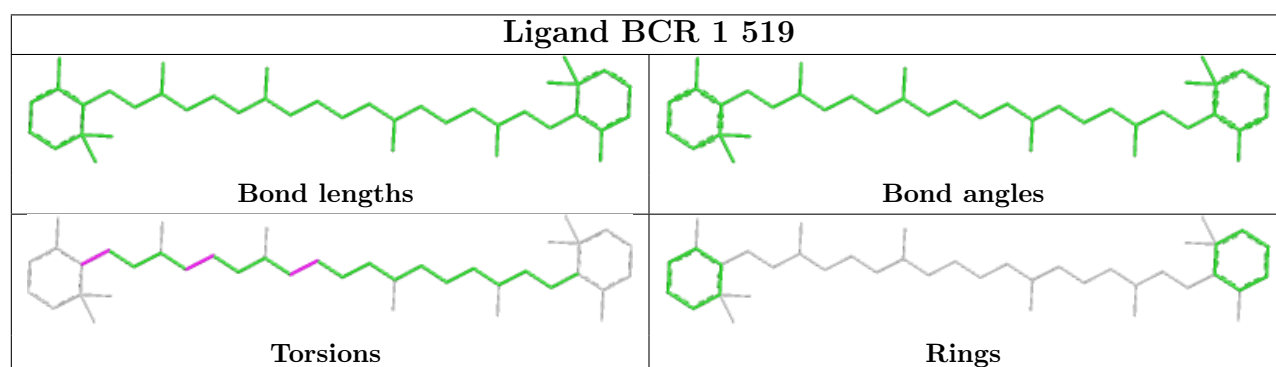
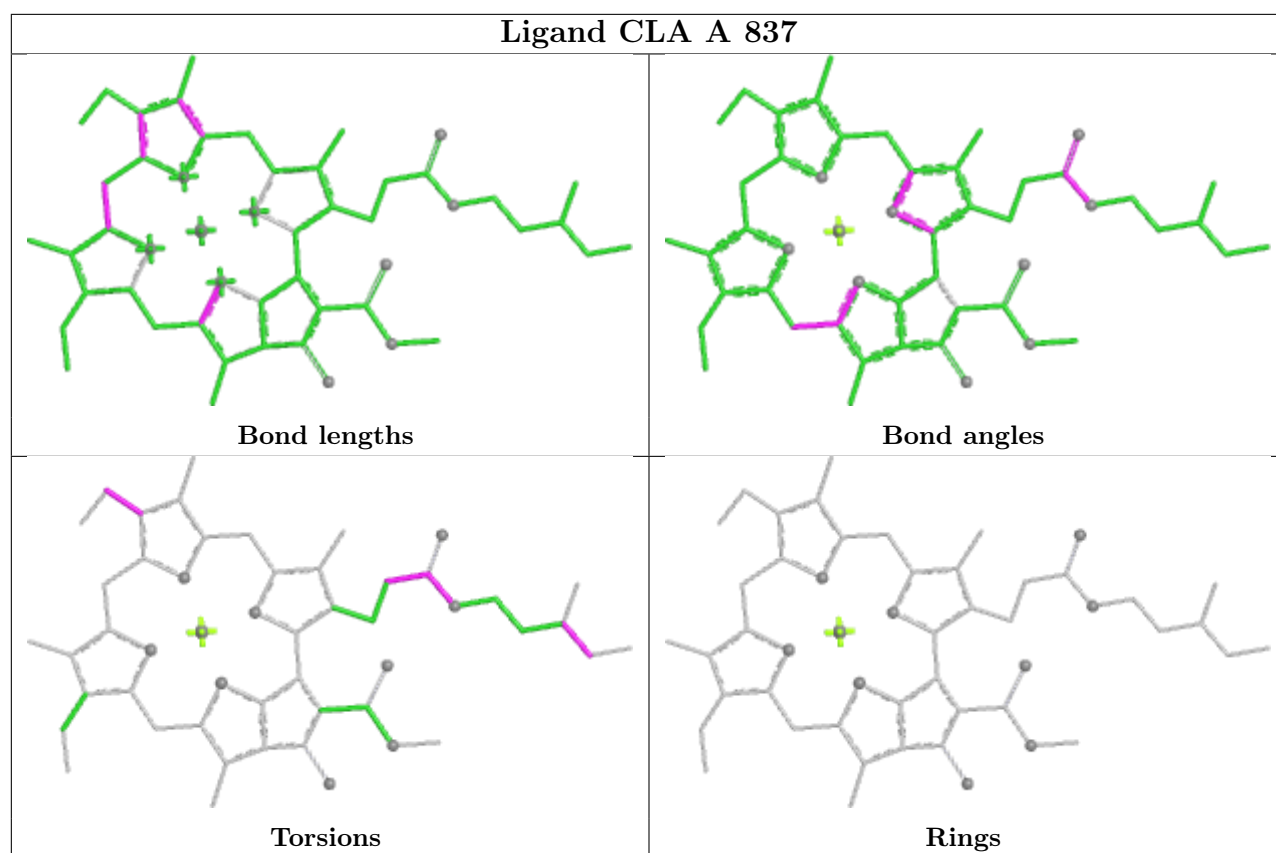
Bond angles

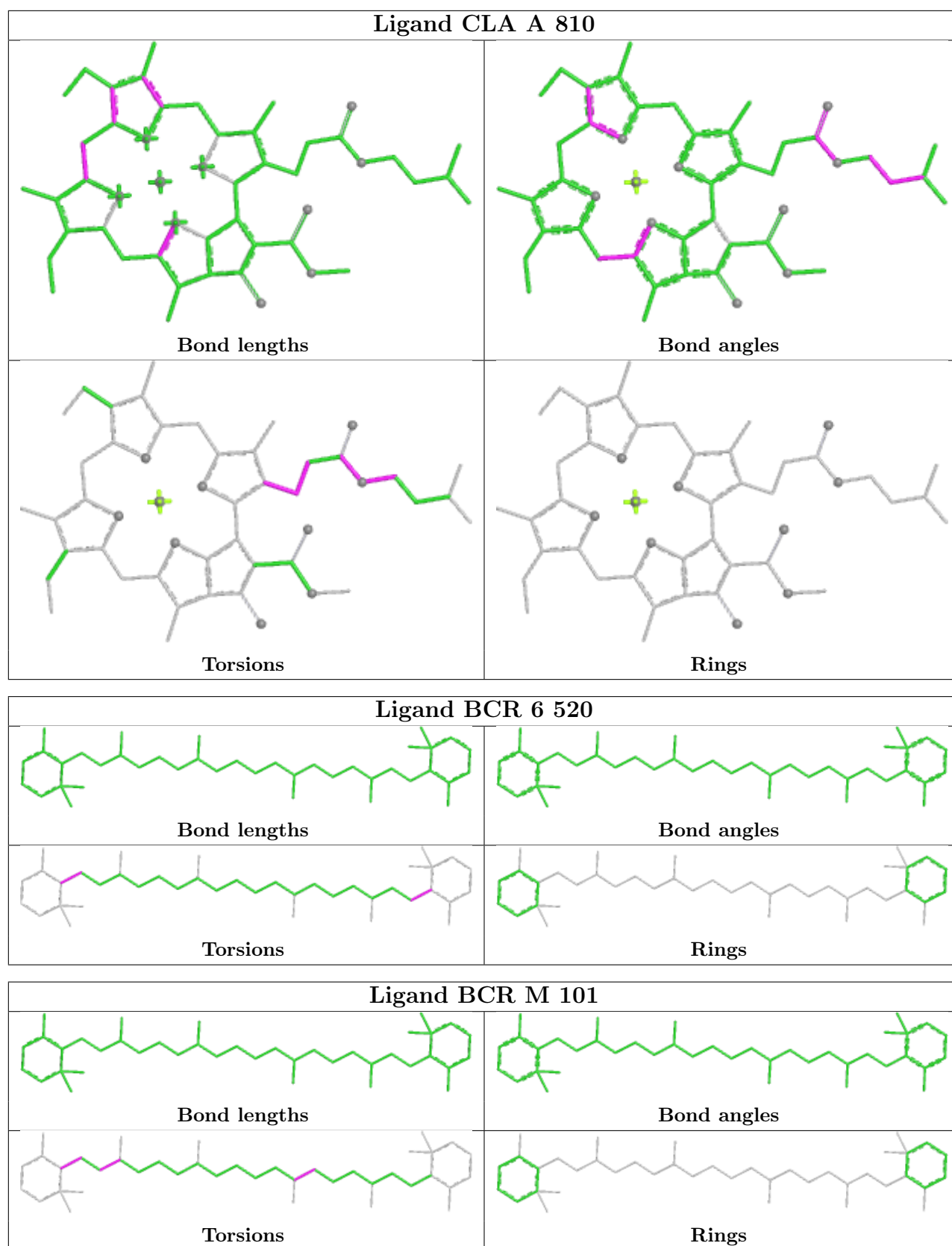


Torsions

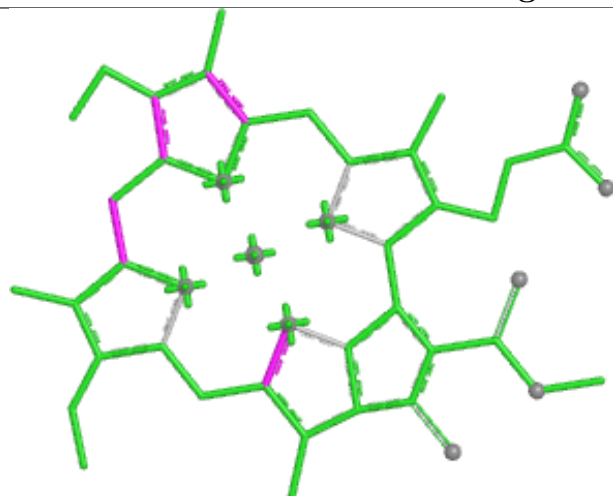


Rings

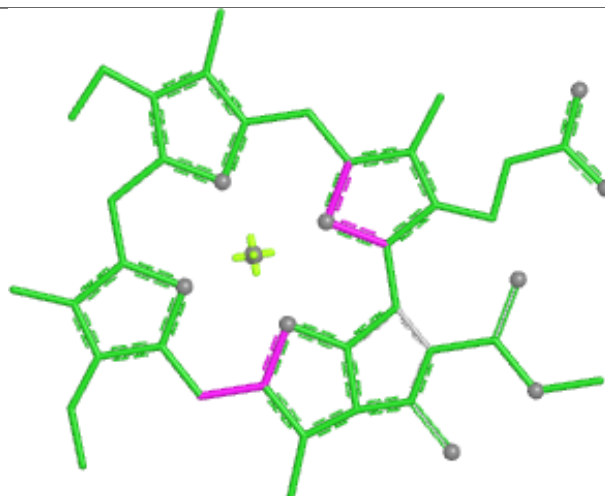




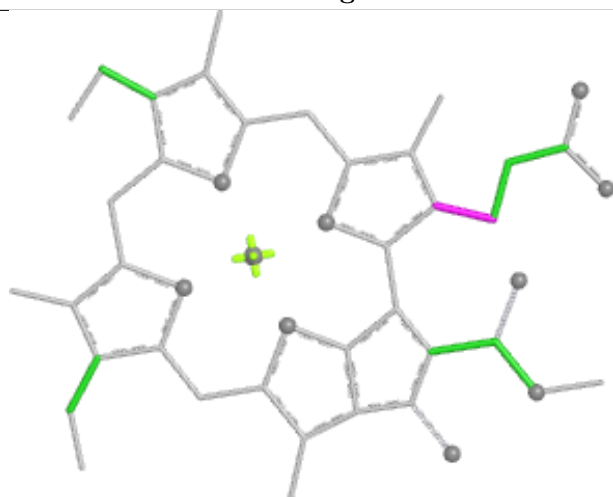
## Ligand CLA 4 413



Bond lengths



Bond angles

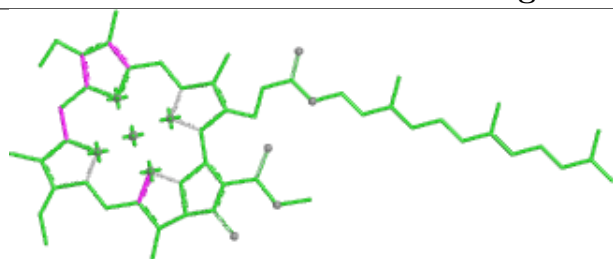


Torsions

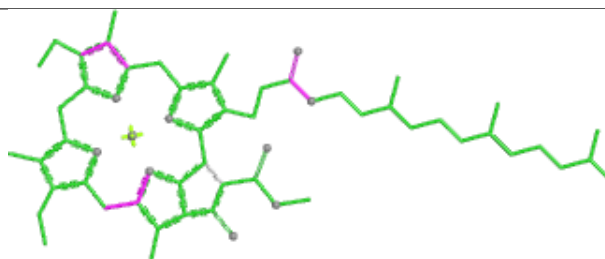


Rings

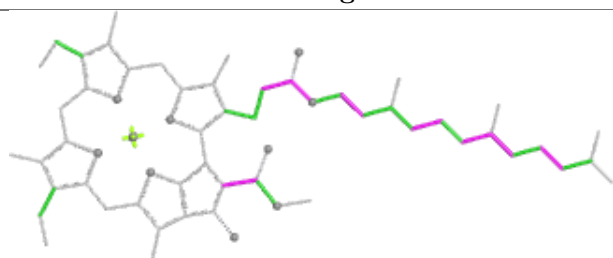
## Ligand CLA 7 509



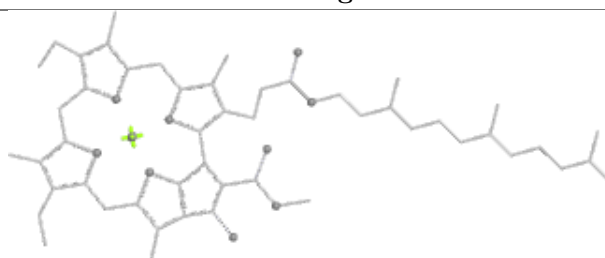
Bond lengths



Bond angles

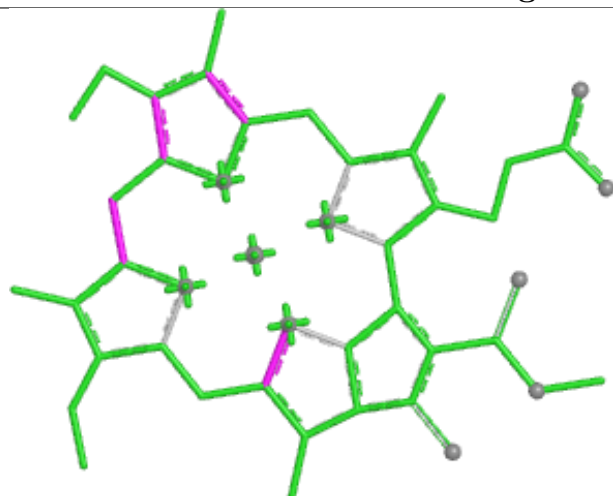


Torsions

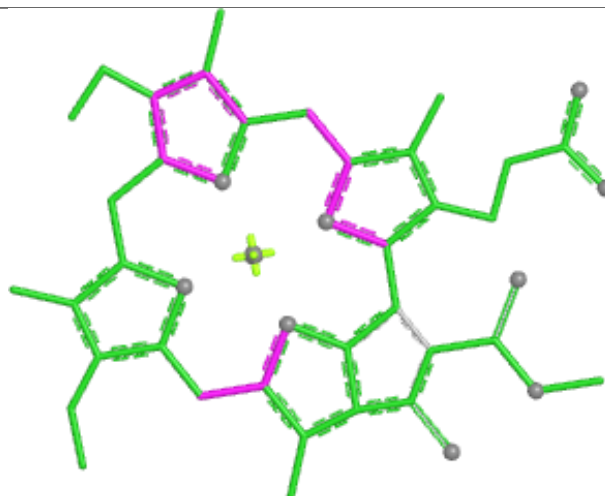


Rings

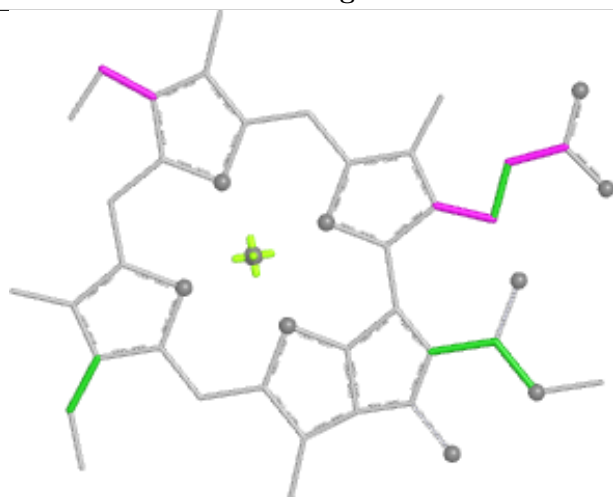
## Ligand CLA 1 511



Bond lengths



Bond angles

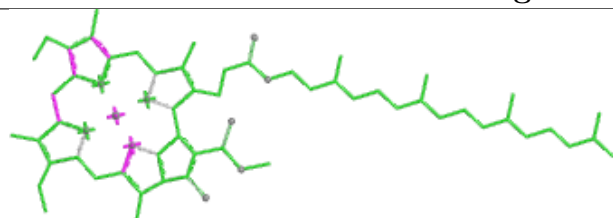


Torsions

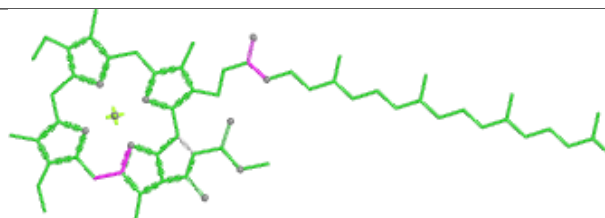


Rings

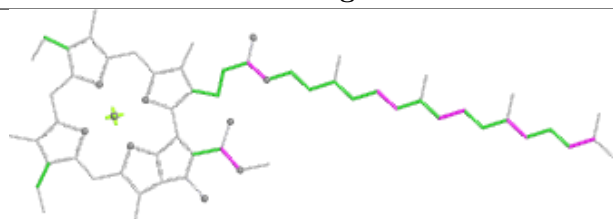
## Ligand CLA A 833



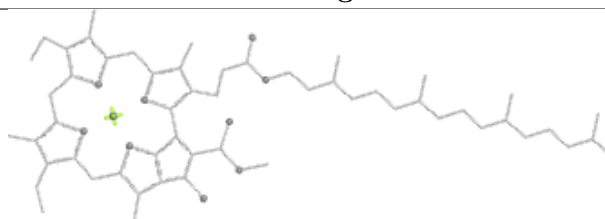
Bond lengths



Bond angles

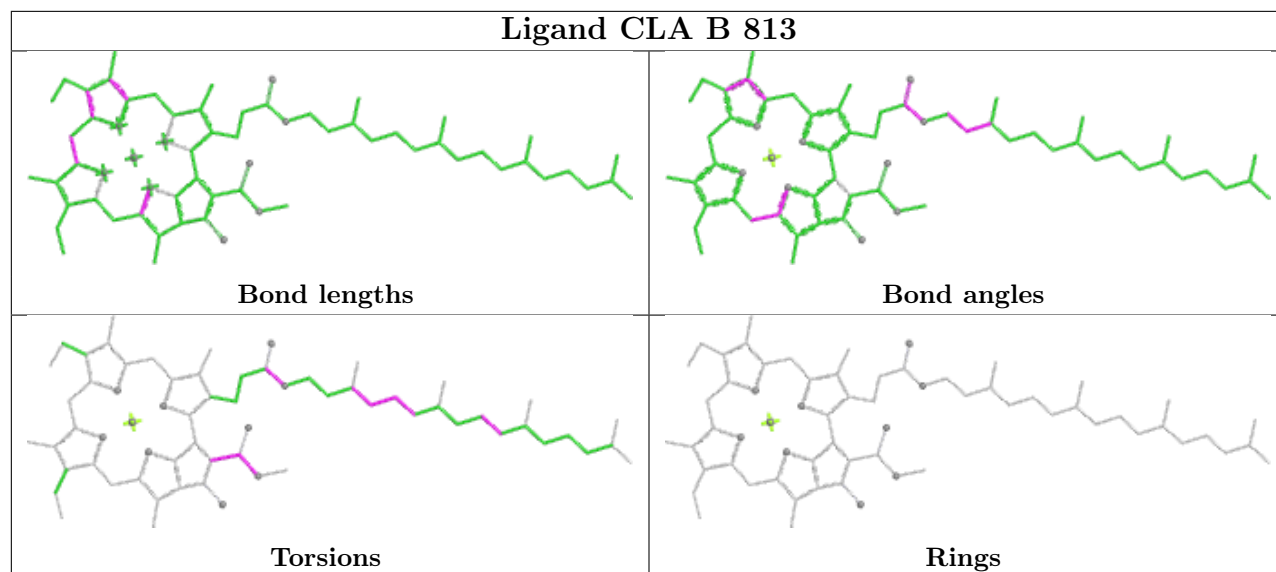


Torsions

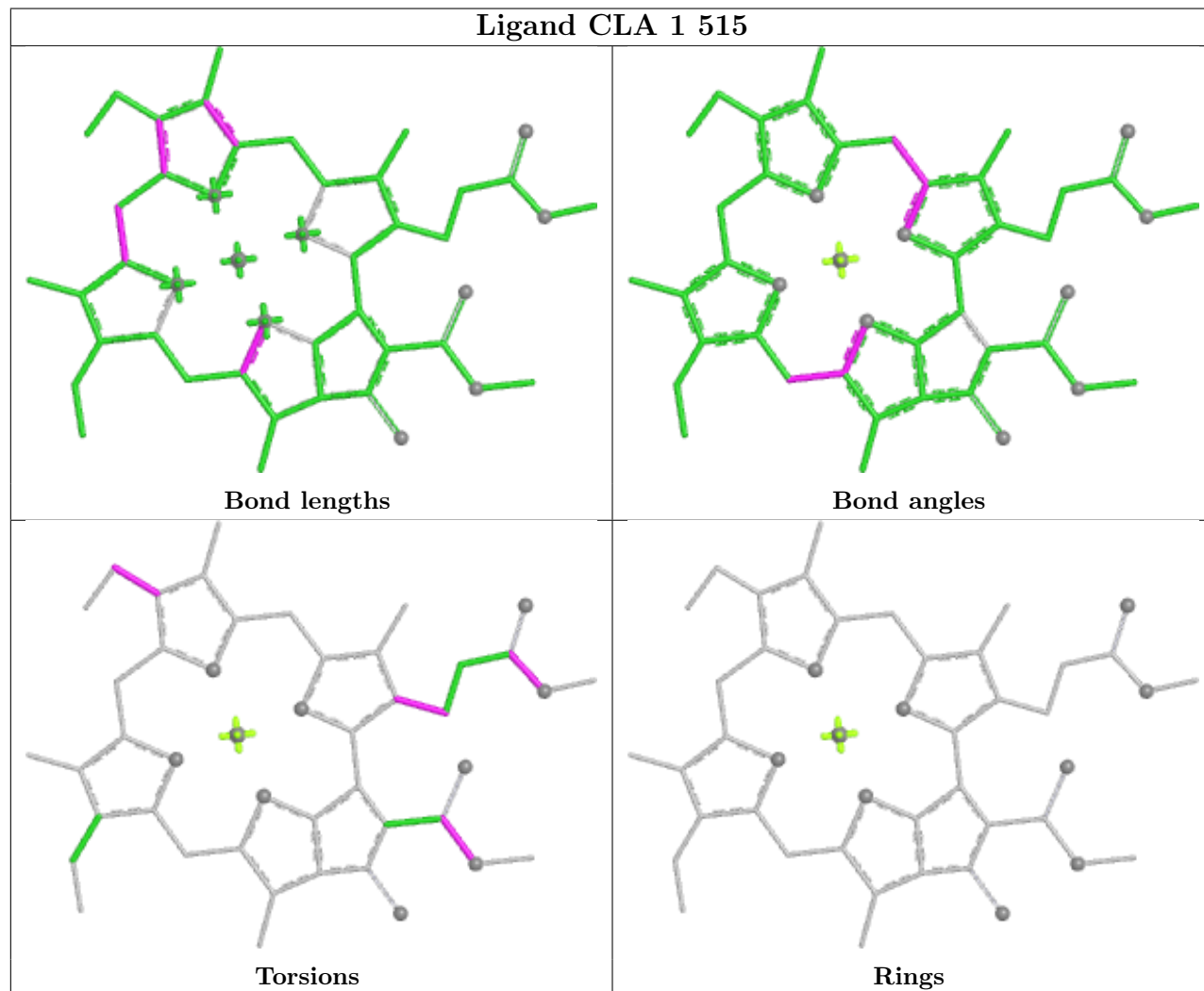


Rings

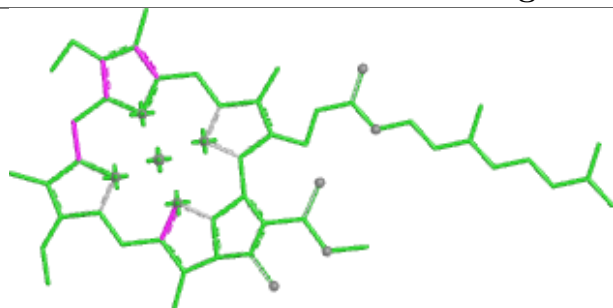
## Ligand CLA B 813



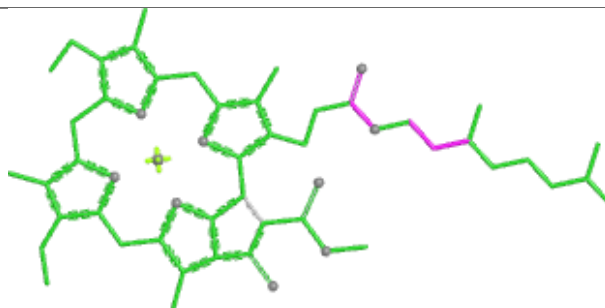
## Ligand CLA 1 515



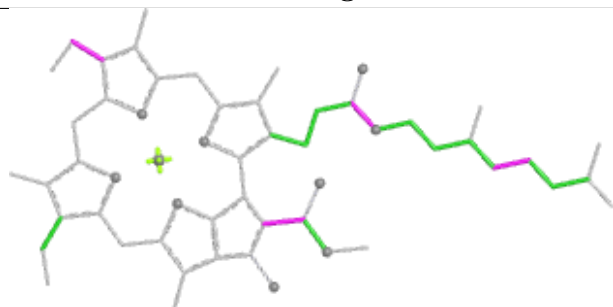
## Ligand CLA 4 403



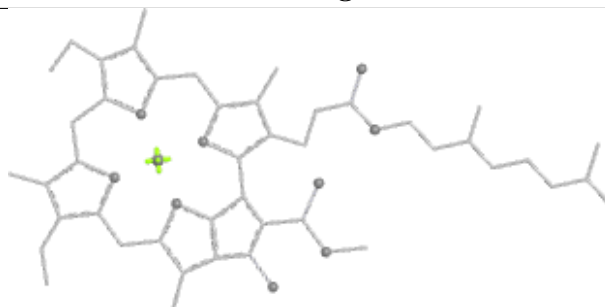
Bond lengths



Bond angles

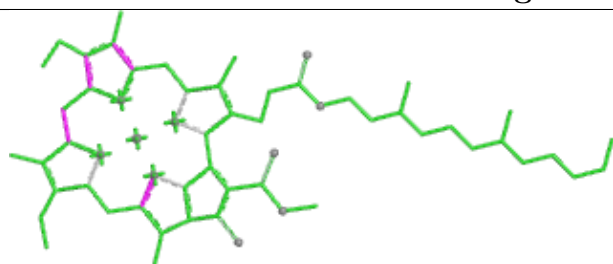


Torsions

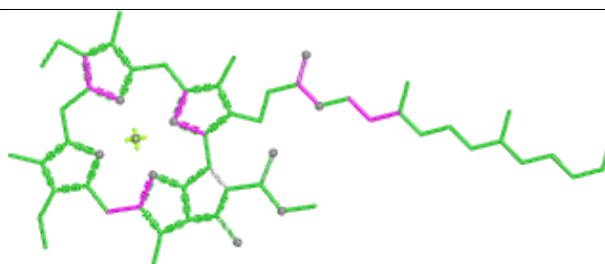


Rings

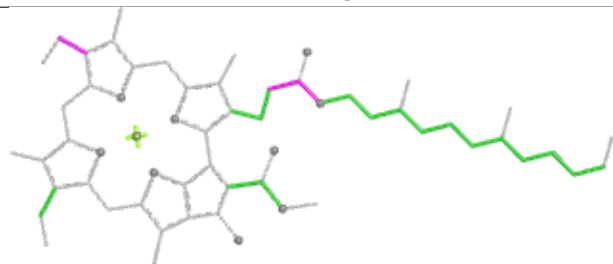
## Ligand CLA B 824



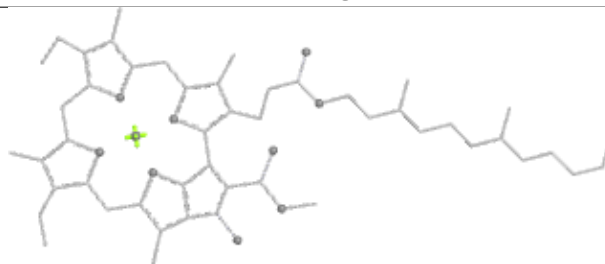
Bond lengths



Bond angles

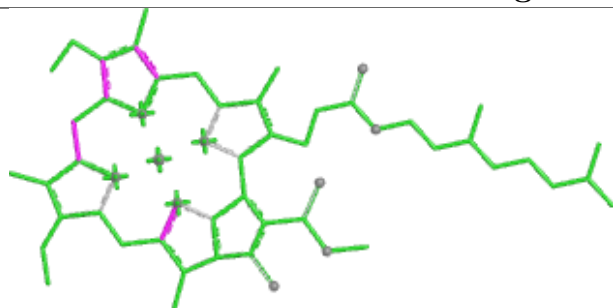


Torsions

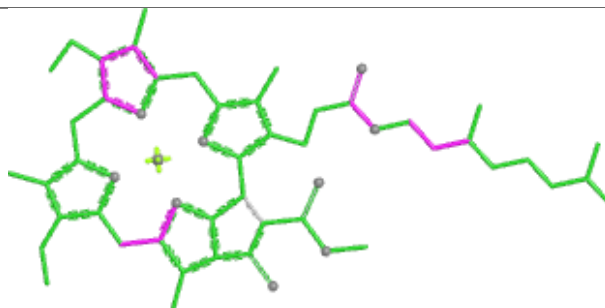


Rings

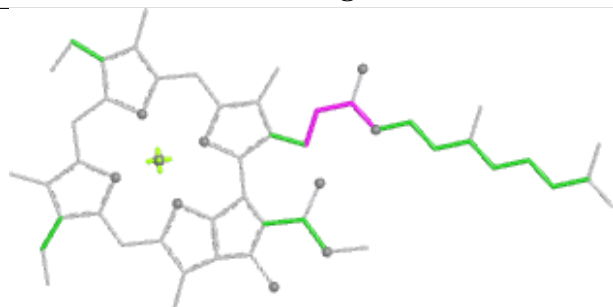
## Ligand CLA B 829



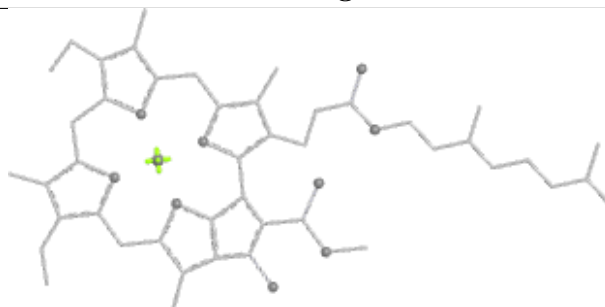
Bond lengths



Bond angles

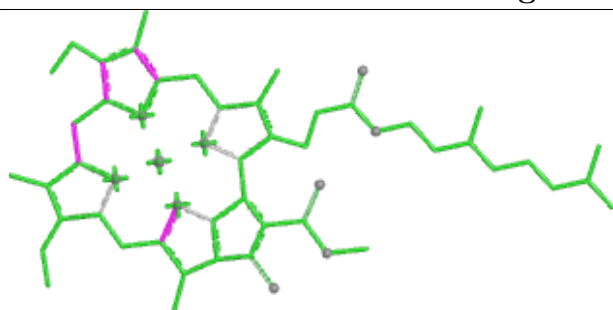


Torsions

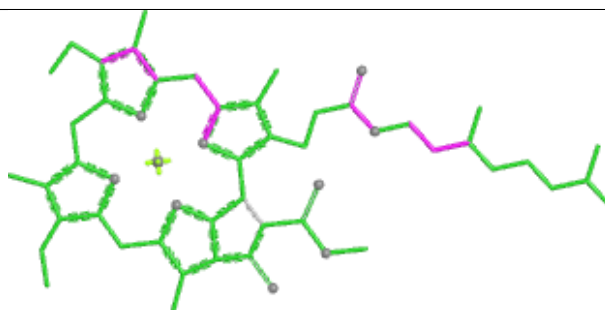


Rings

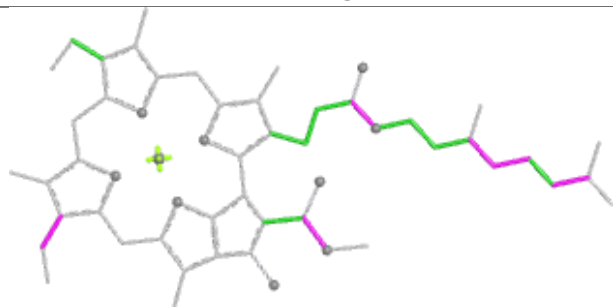
## Ligand CLA 1 517



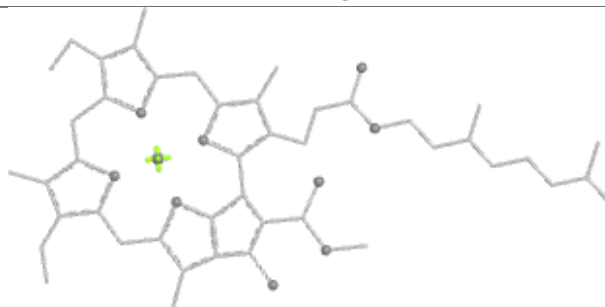
Bond lengths



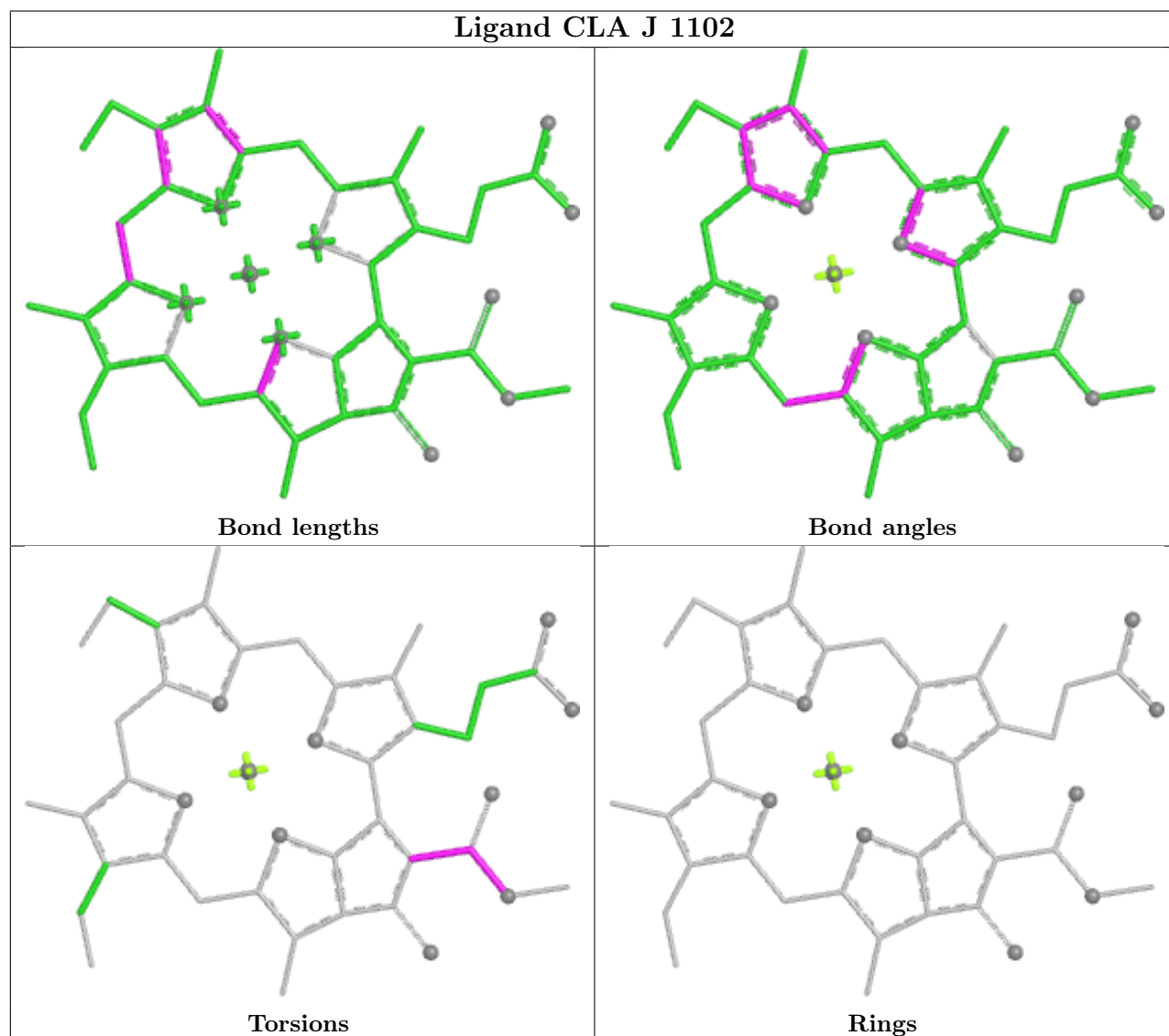
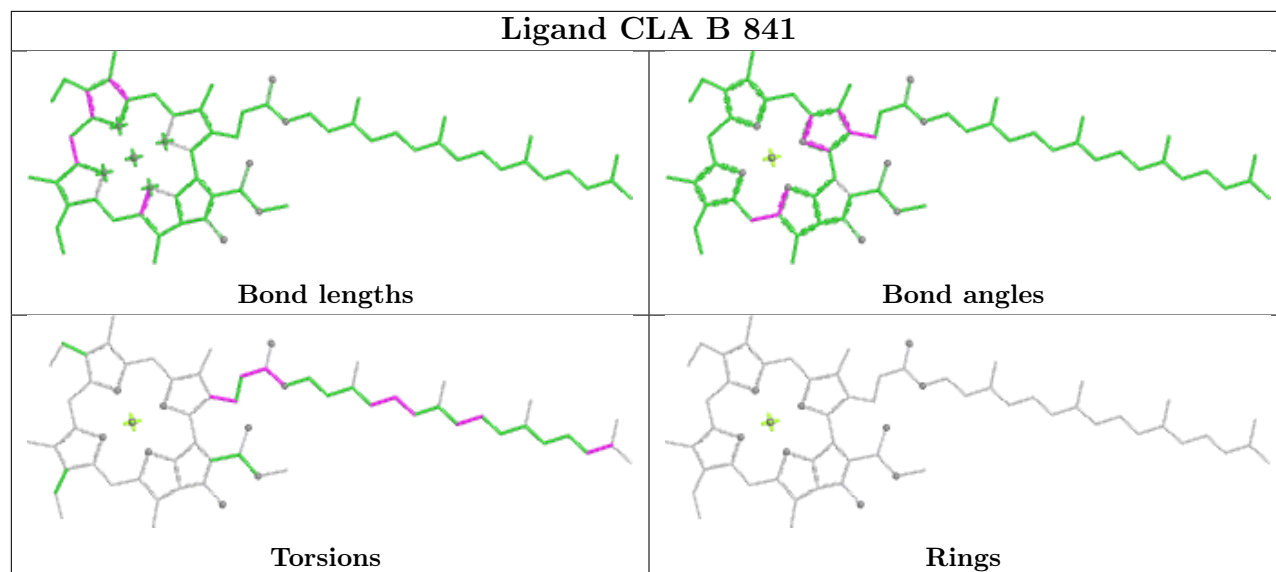
Bond angles



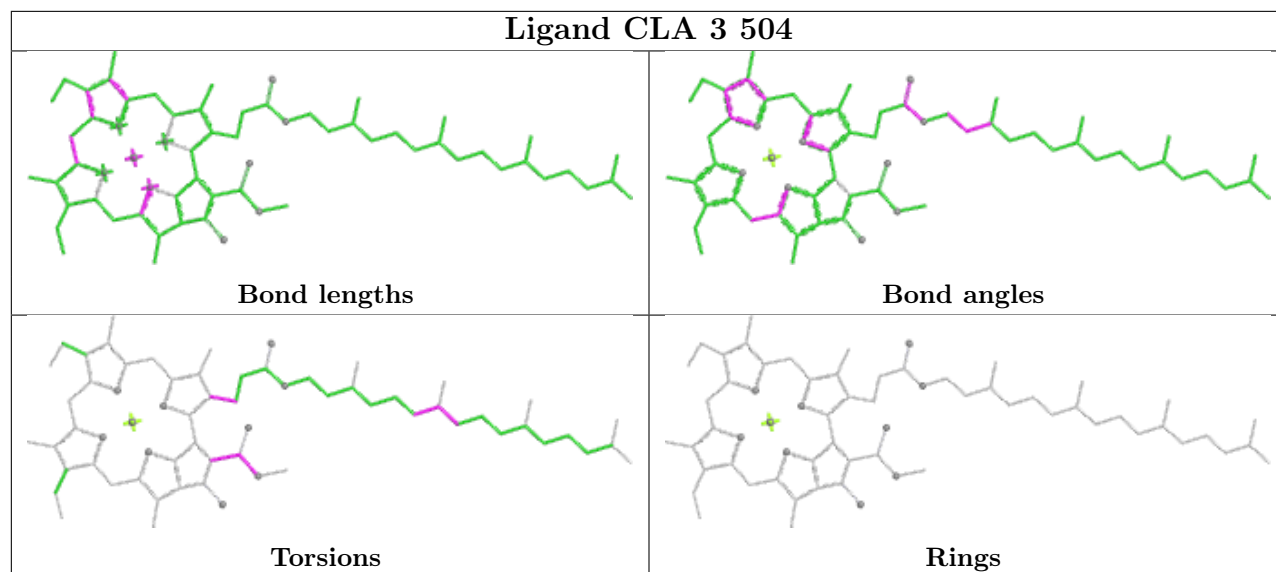
Torsions



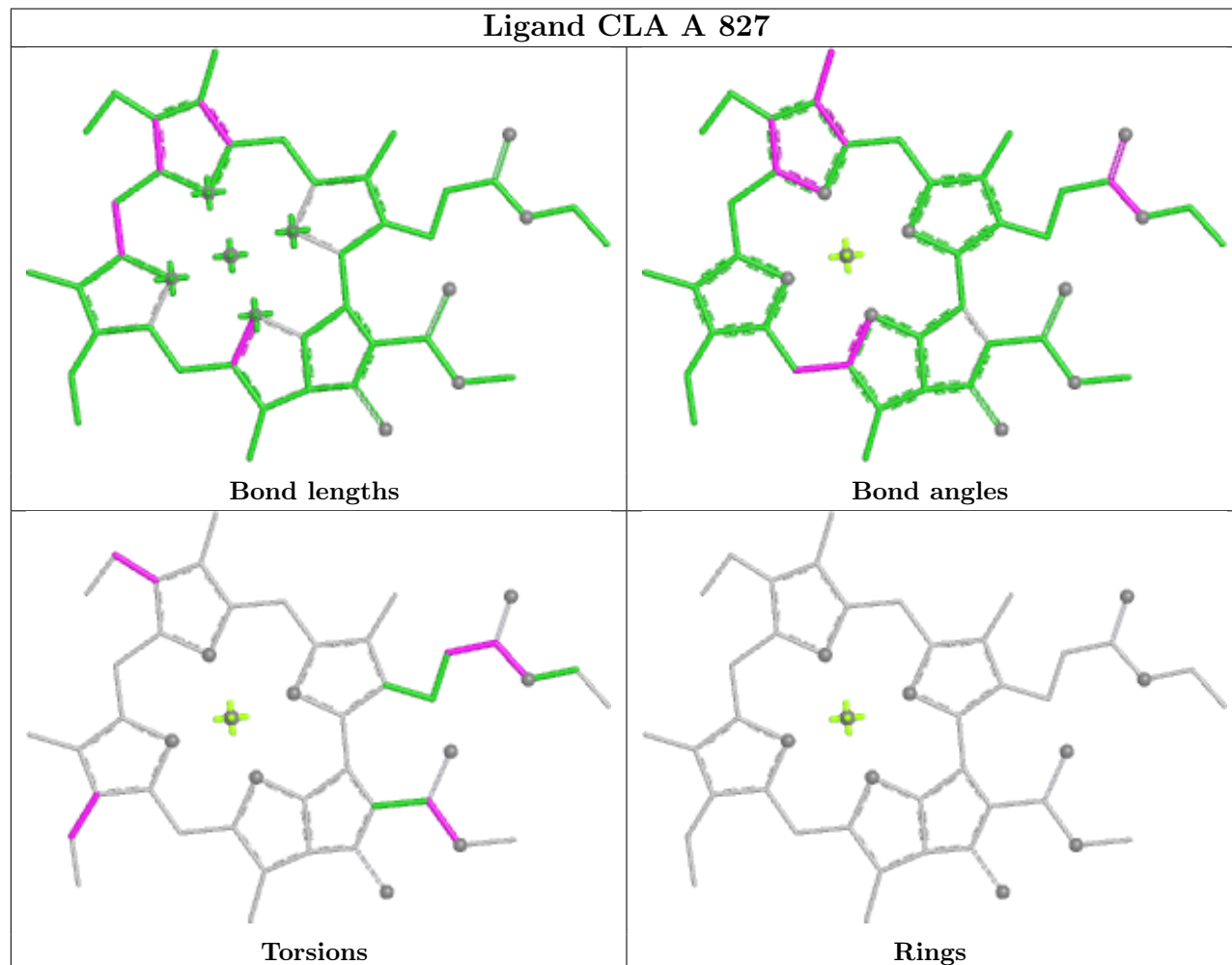
Rings

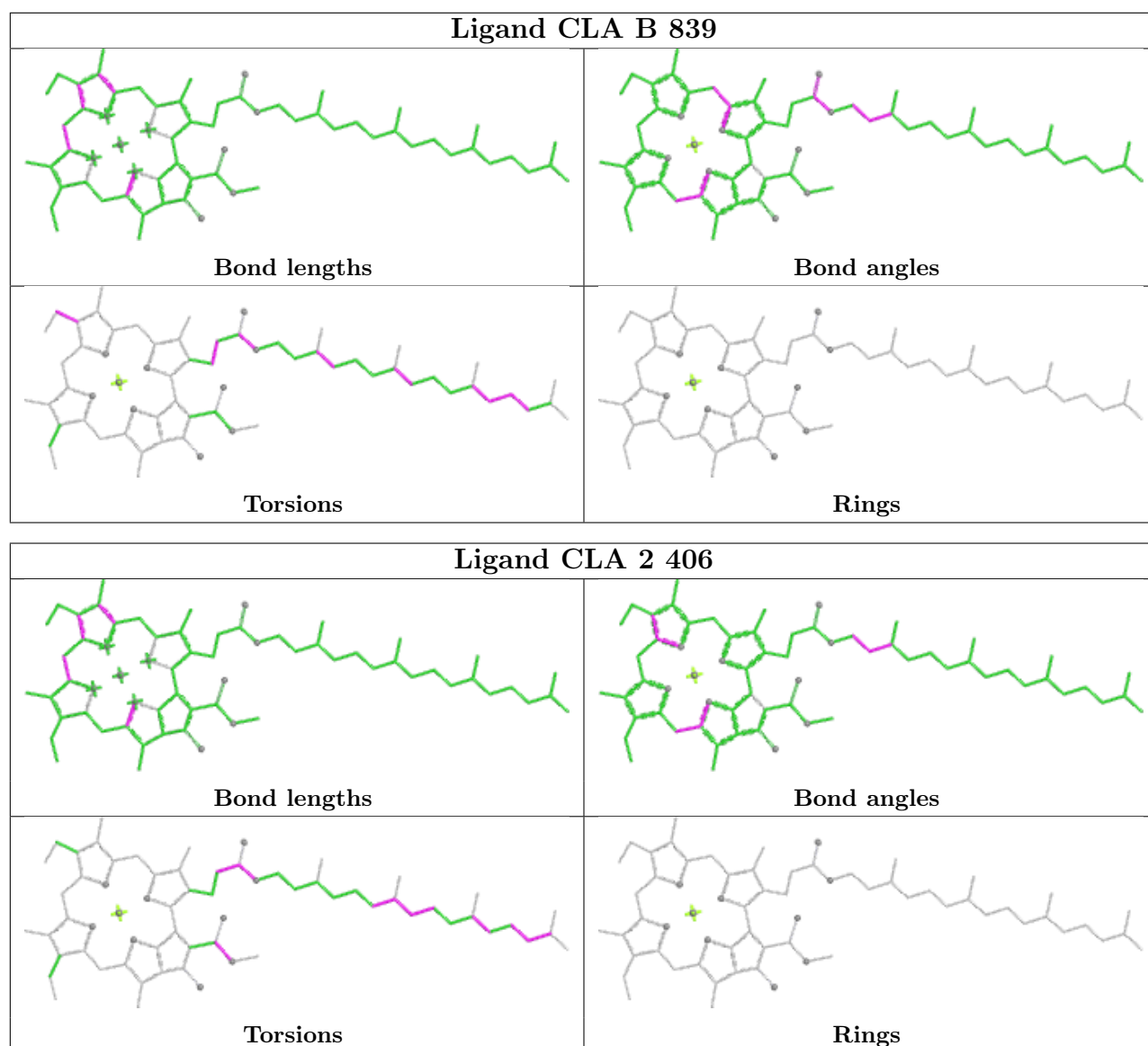


## Ligand CLA 3 504

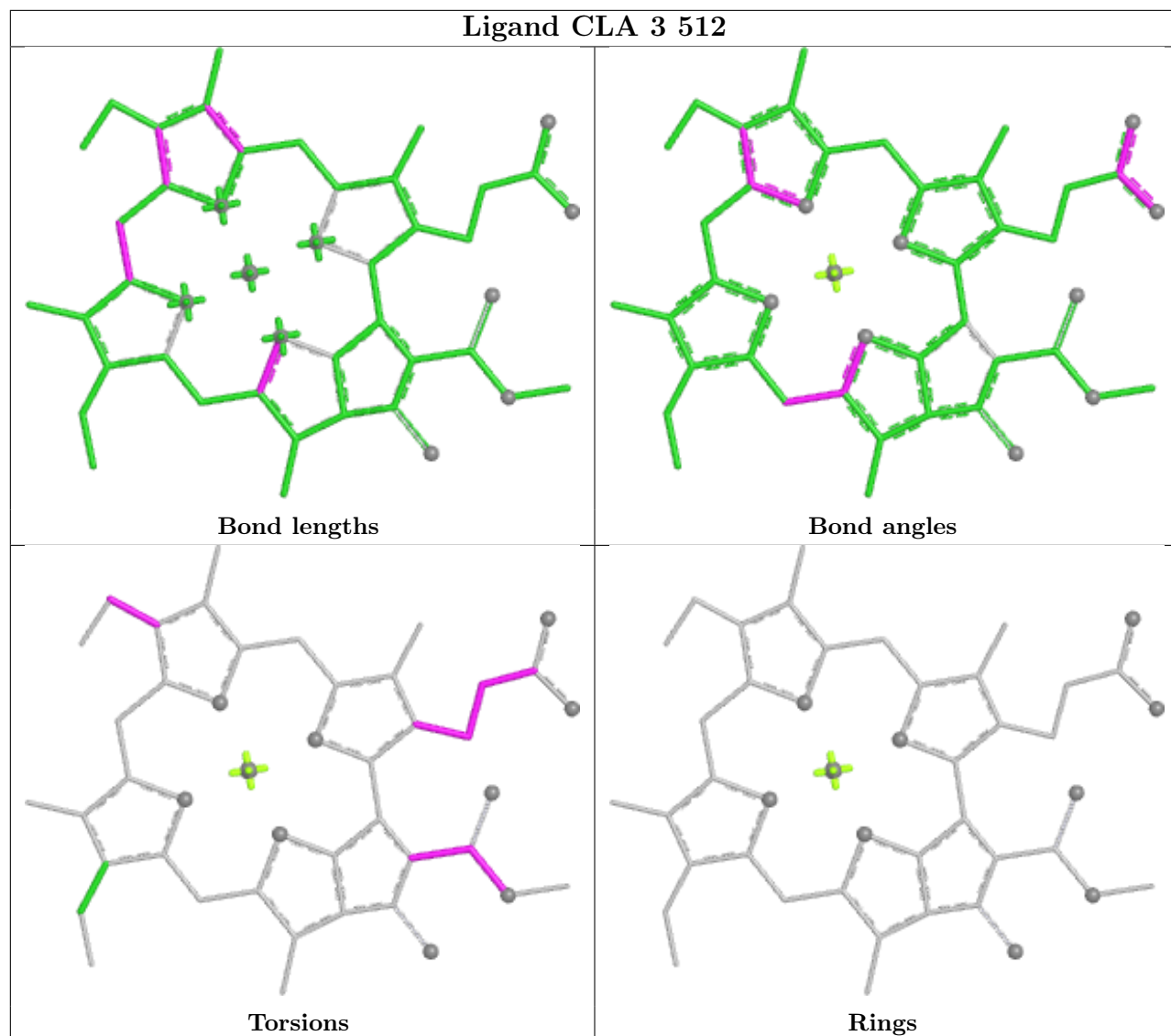


## Ligand CLA A 827

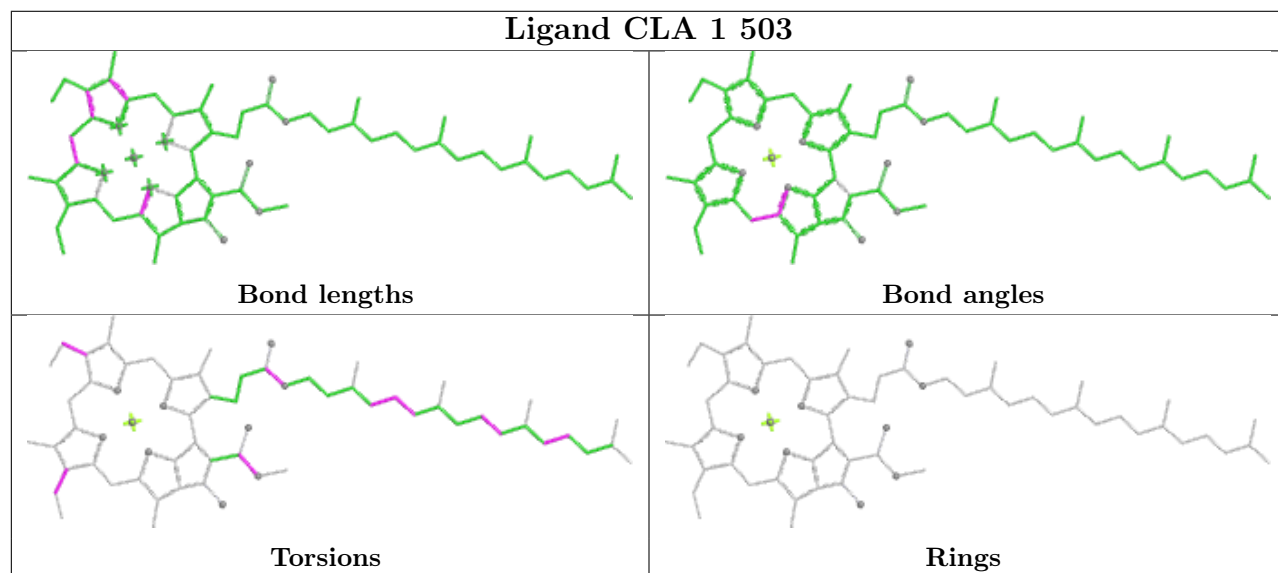


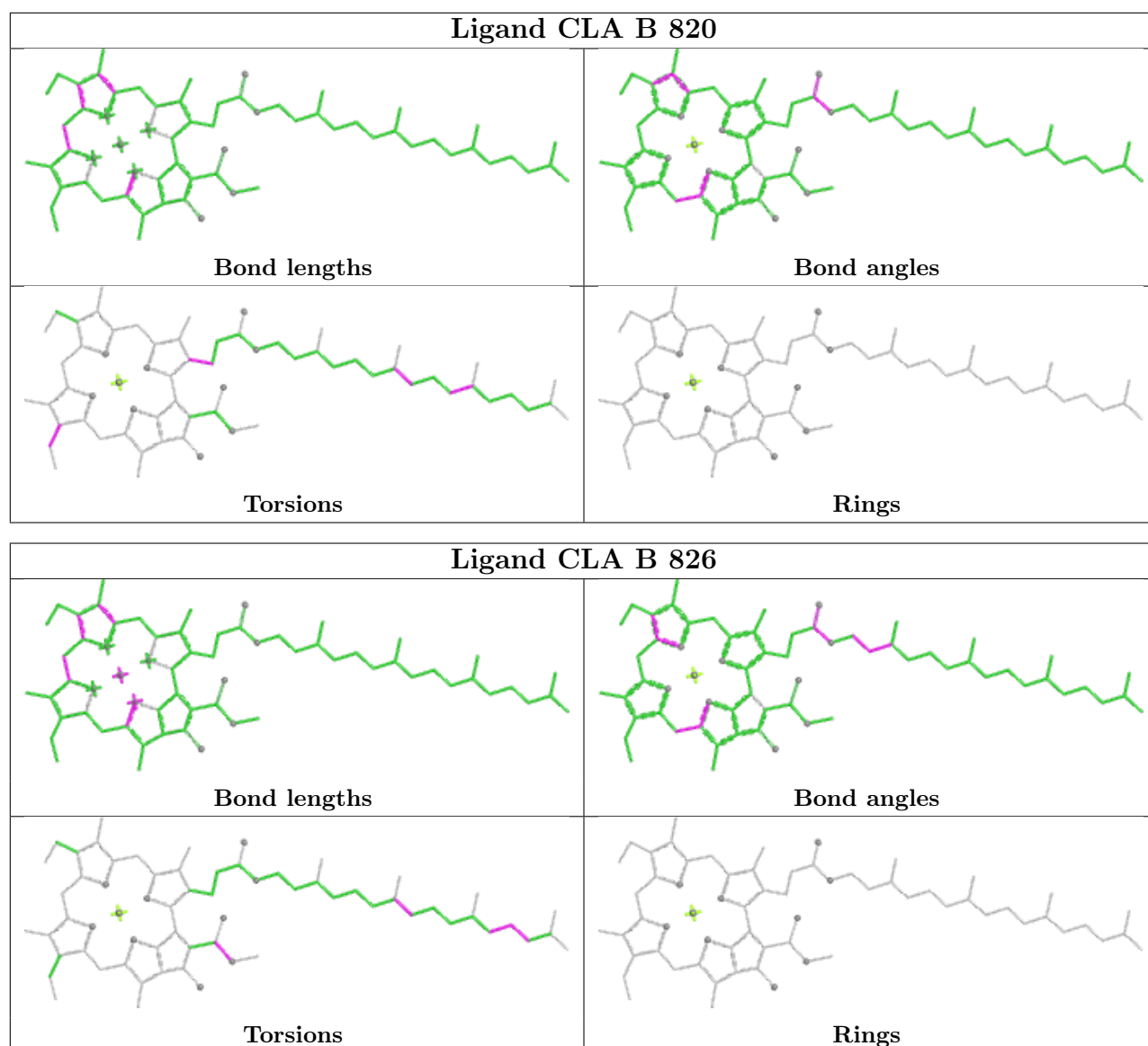


## Ligand CLA 3 512

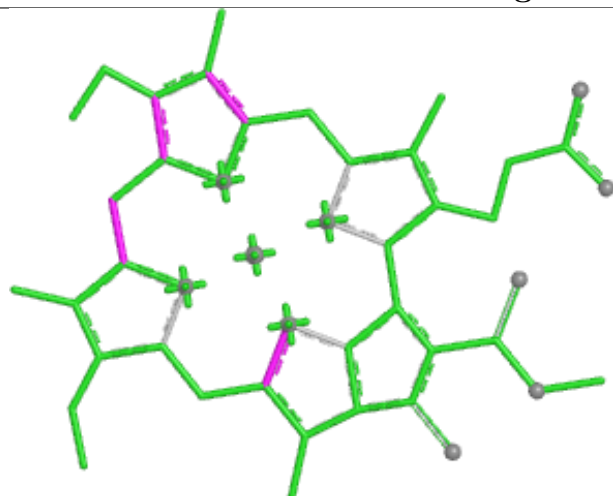


## Ligand CLA 1 503

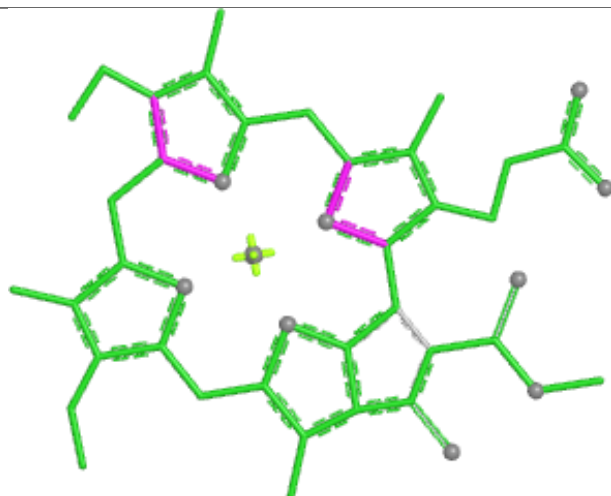




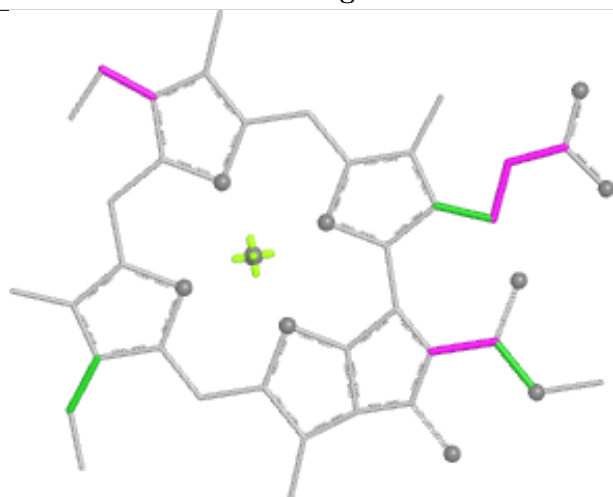
## Ligand CLA B 828



Bond lengths



Bond angles

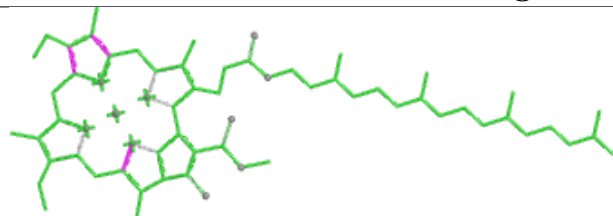


Torsions

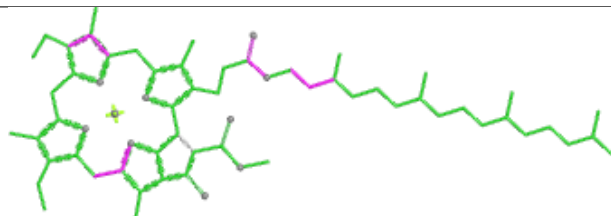


Rings

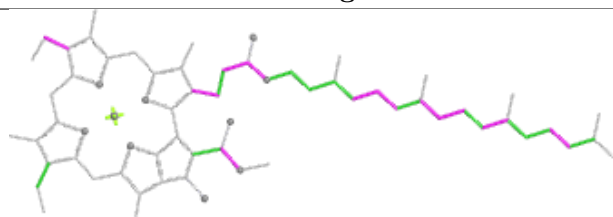
## Ligand CLA A 842



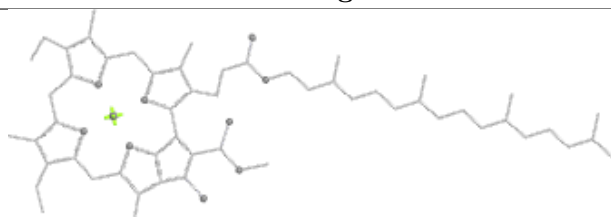
Bond lengths



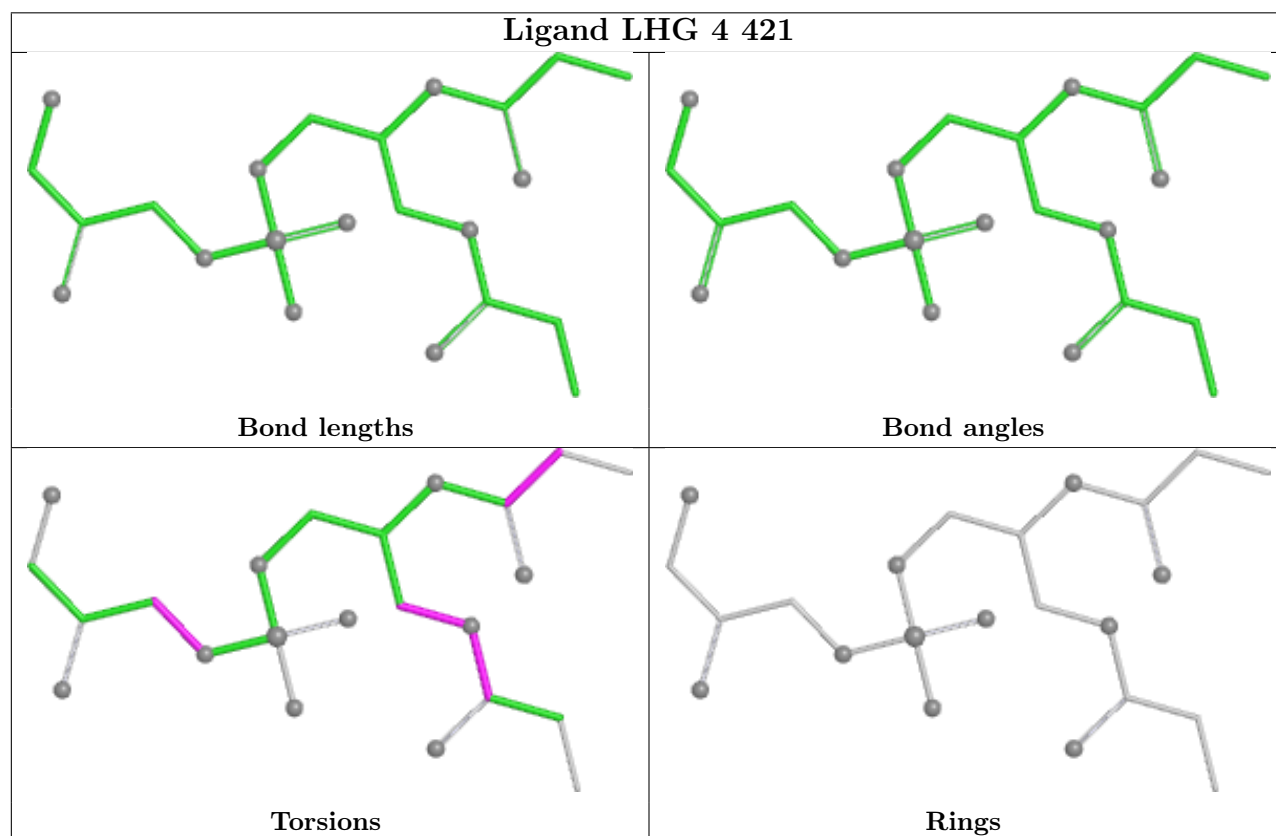
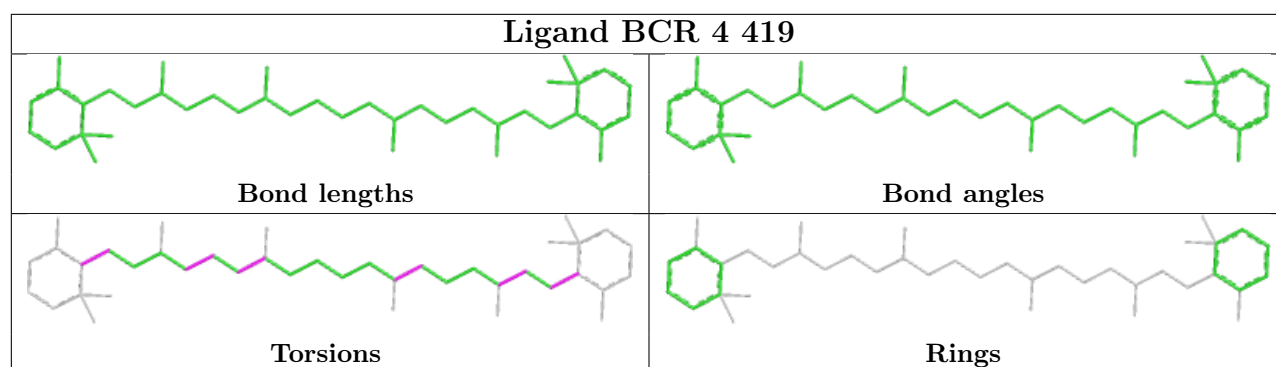
Bond angles

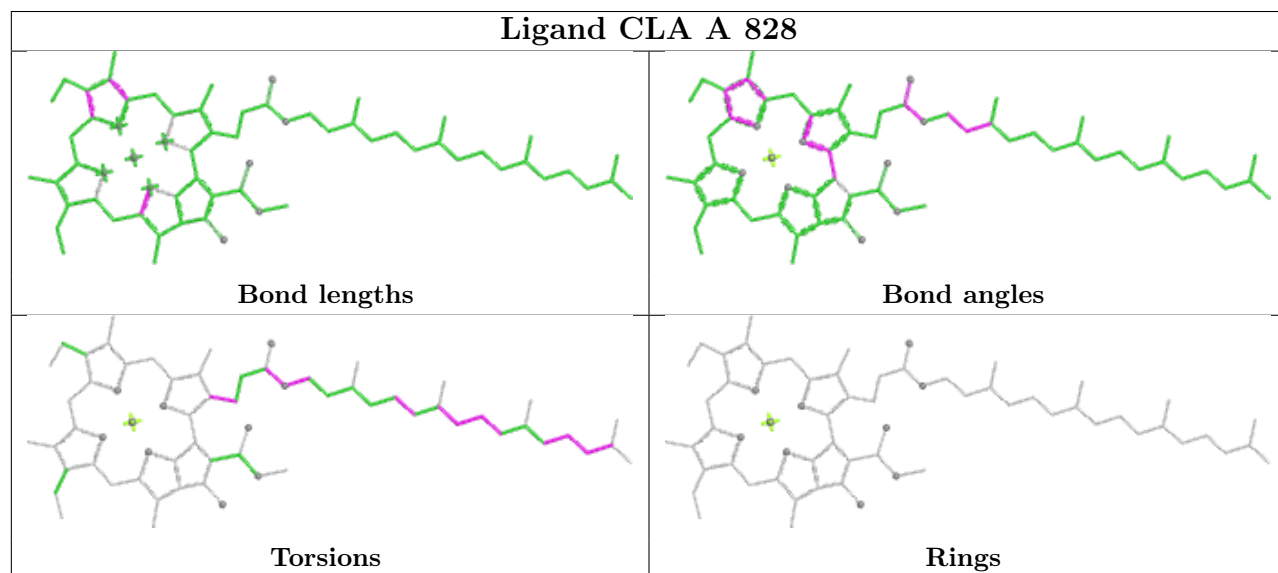
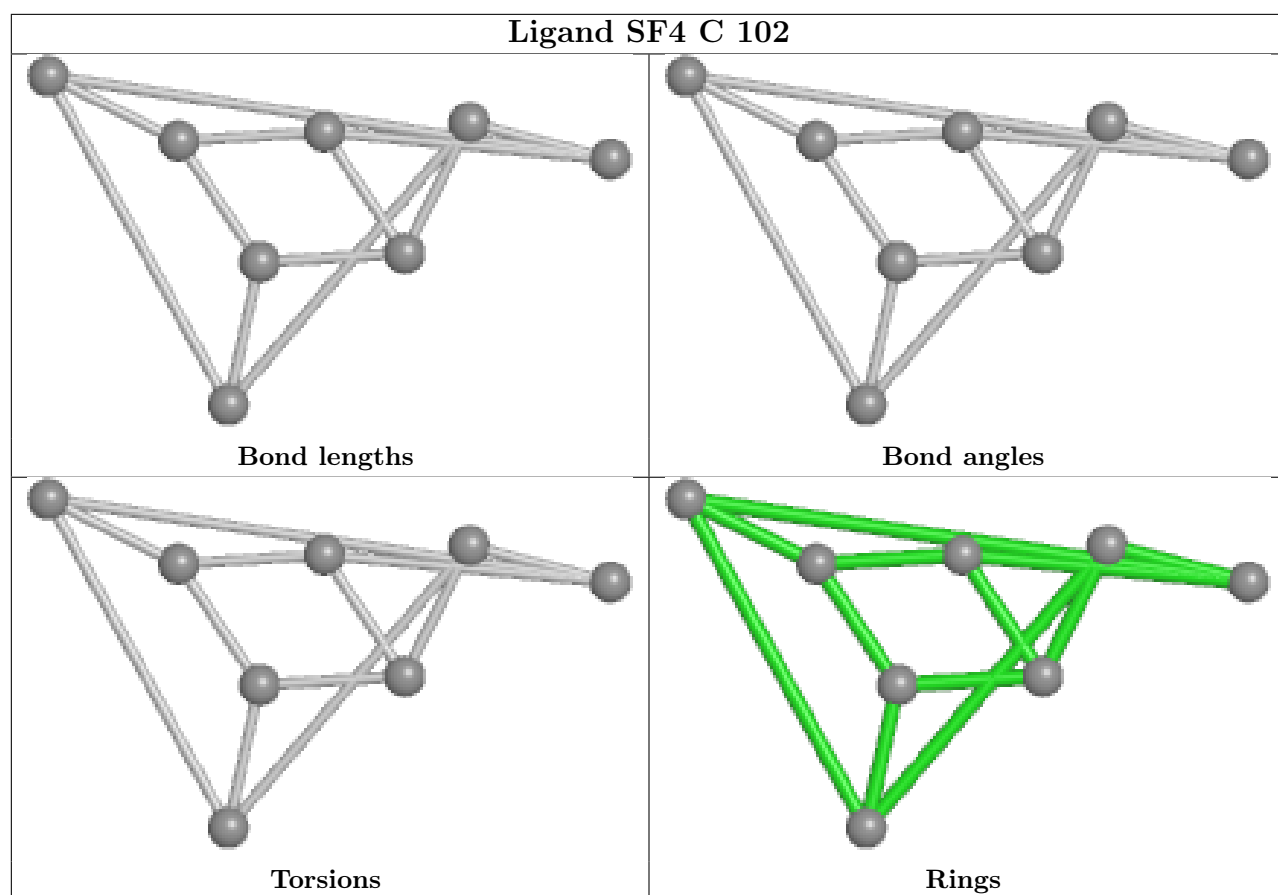


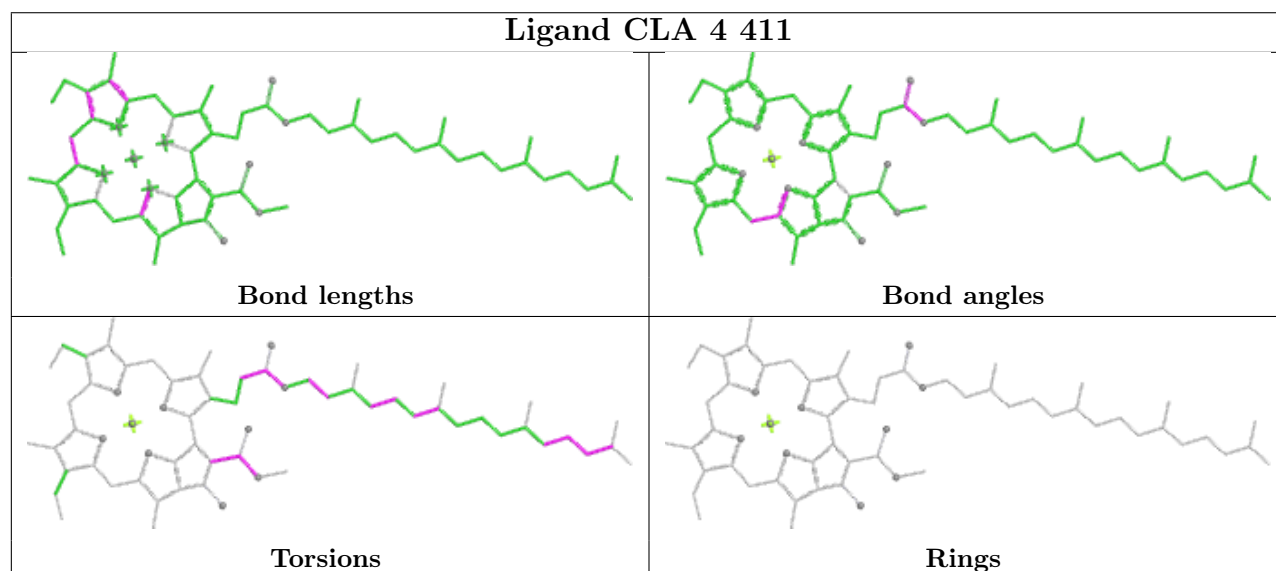
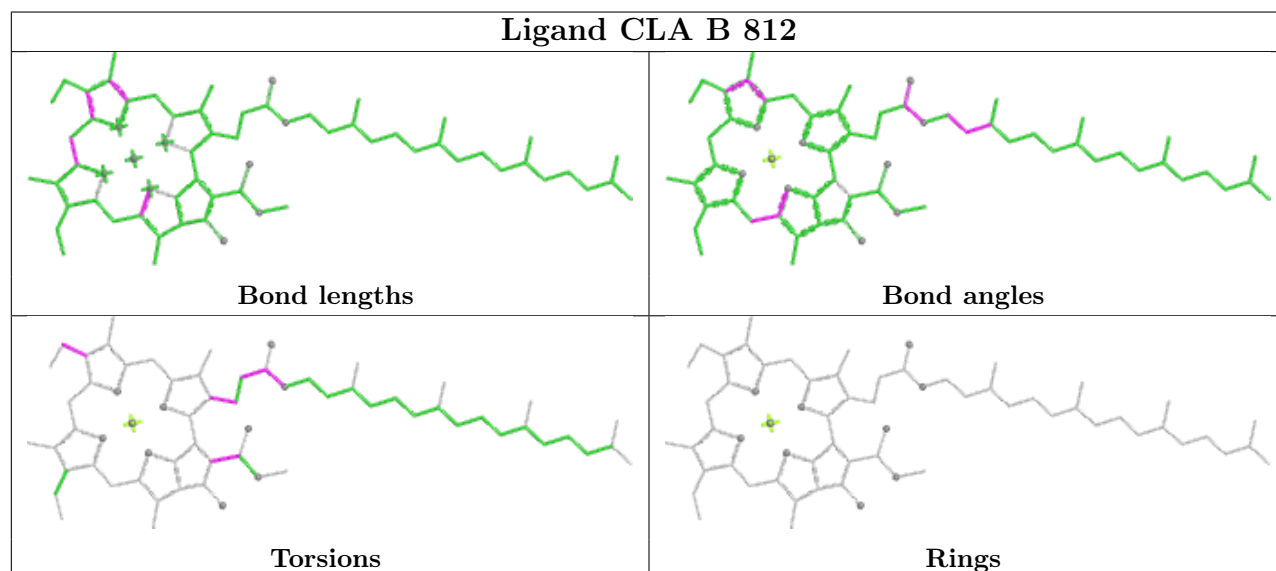
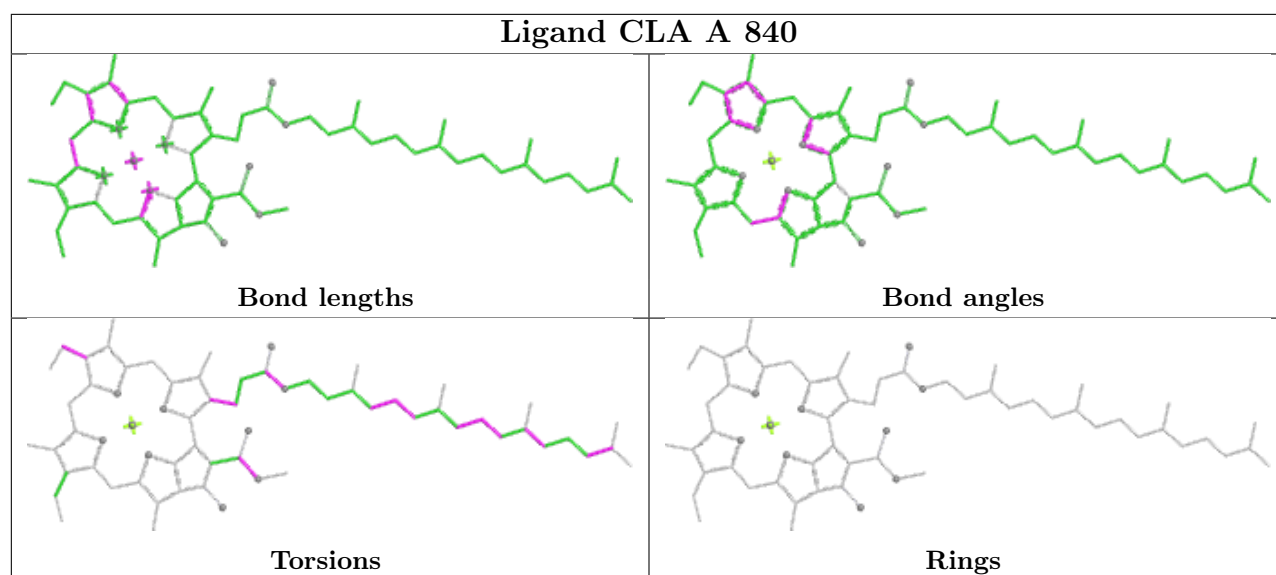
Torsions

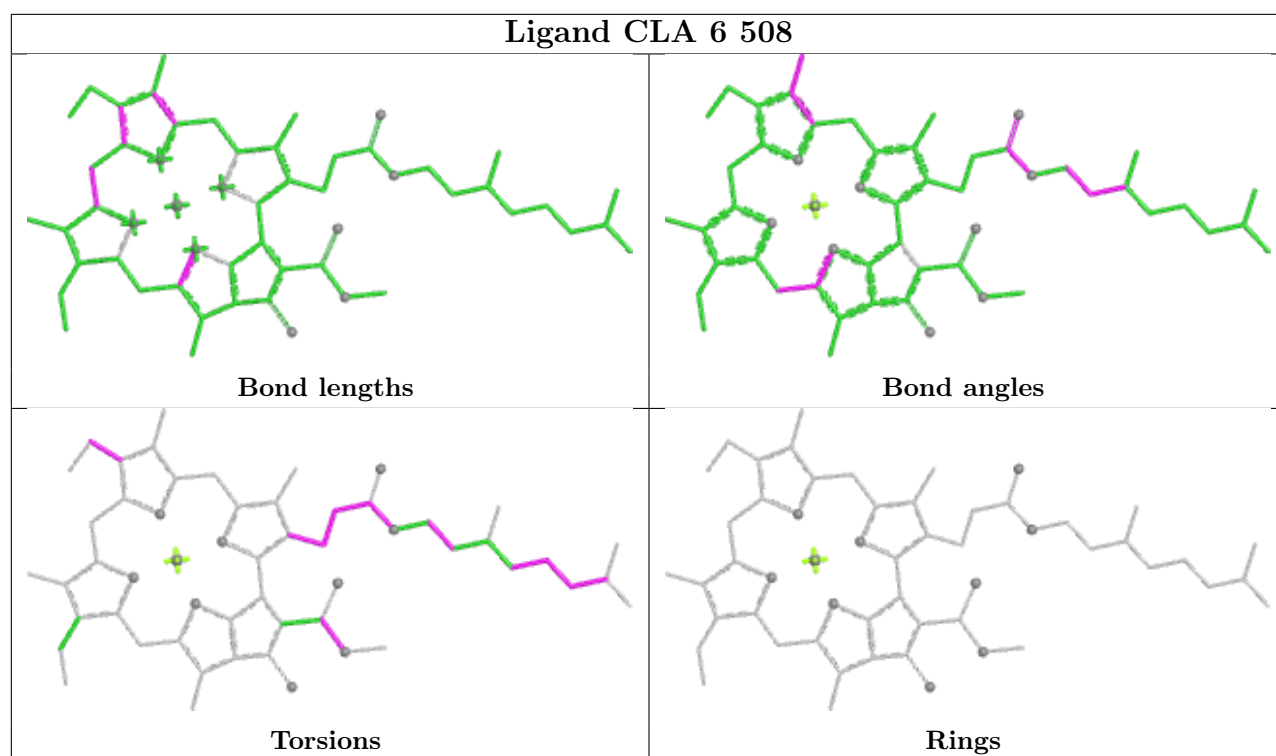


Rings

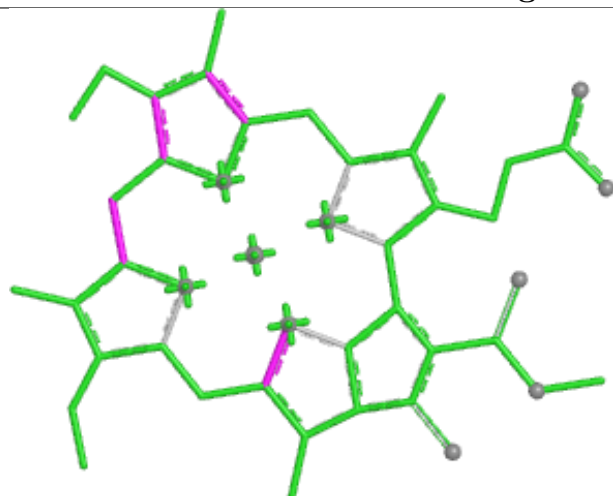




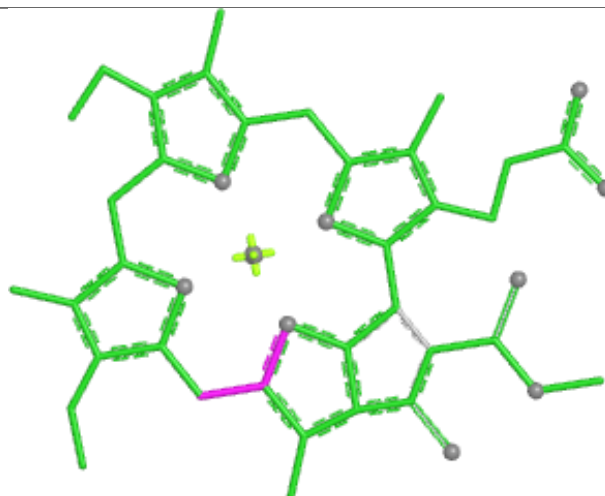




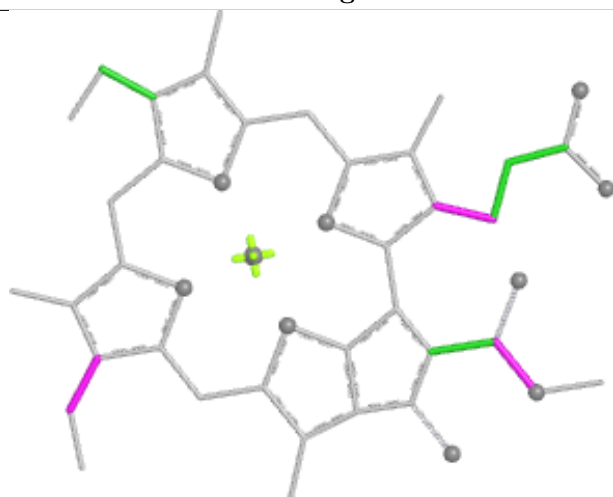
## Ligand CLA 6 514



Bond lengths



Bond angles

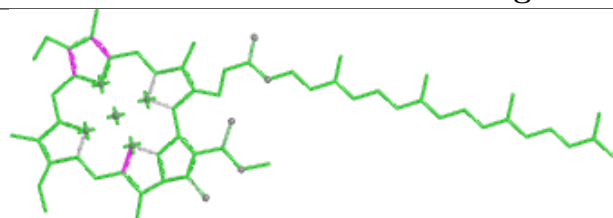


Torsions

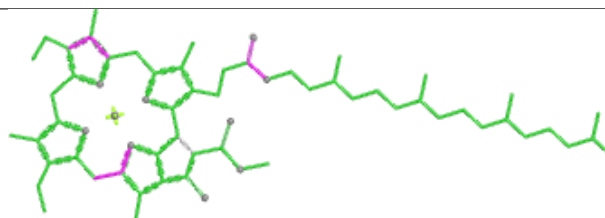


Rings

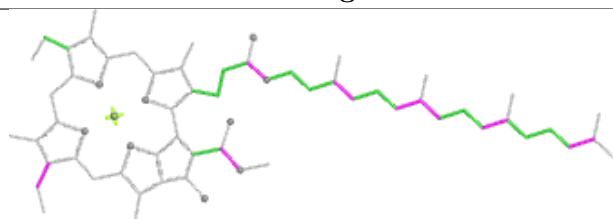
## Ligand CLA A 841



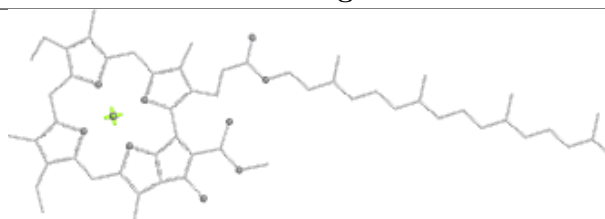
Bond lengths



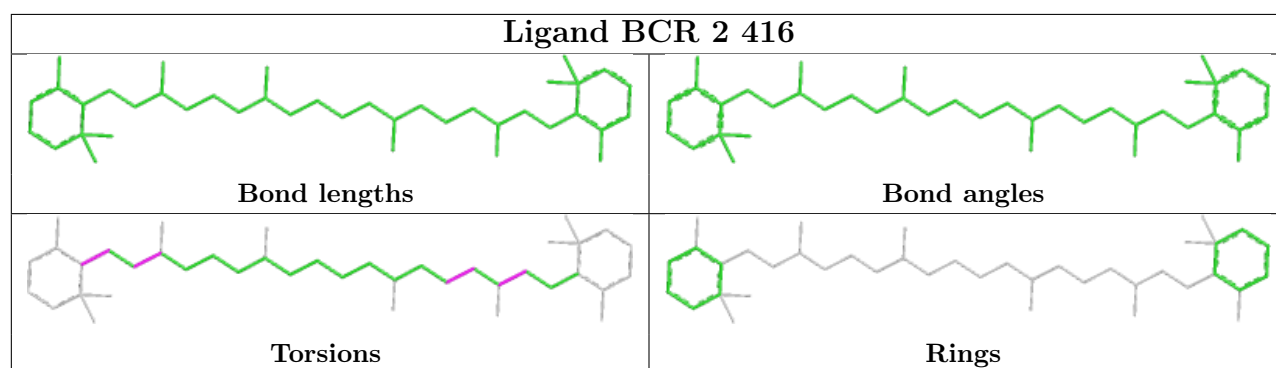
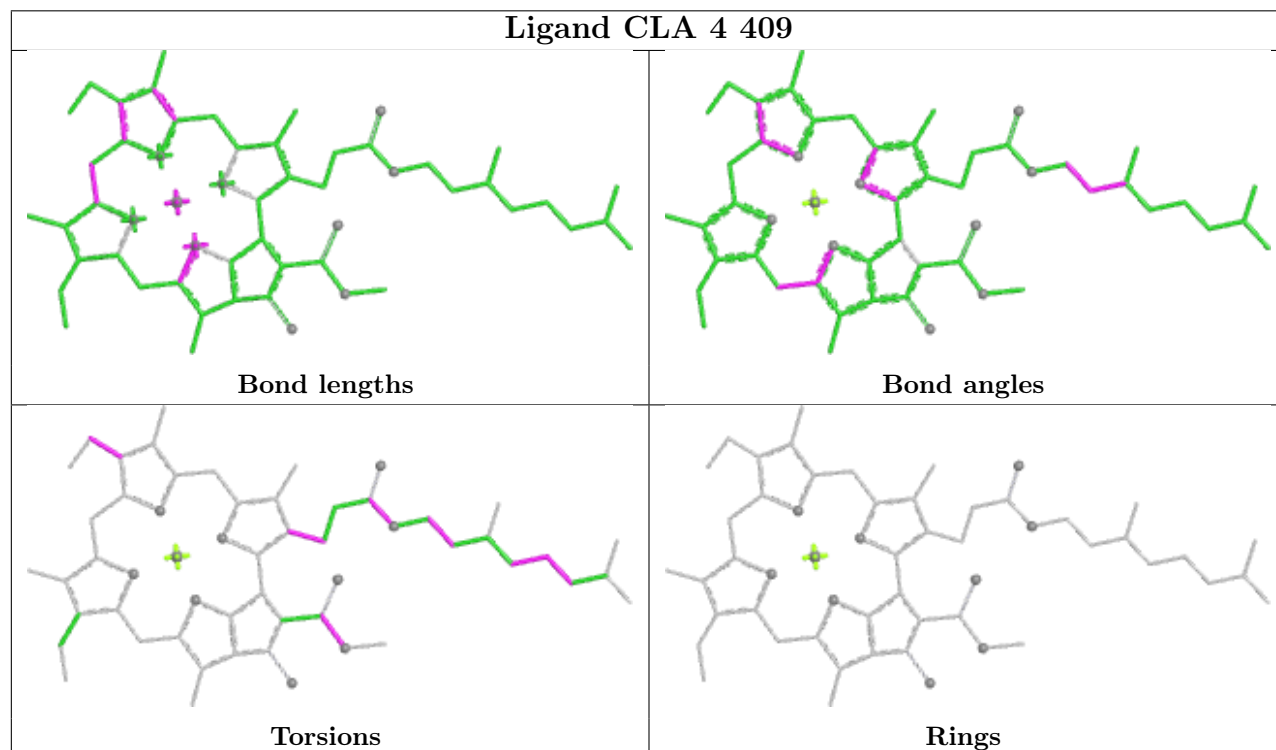
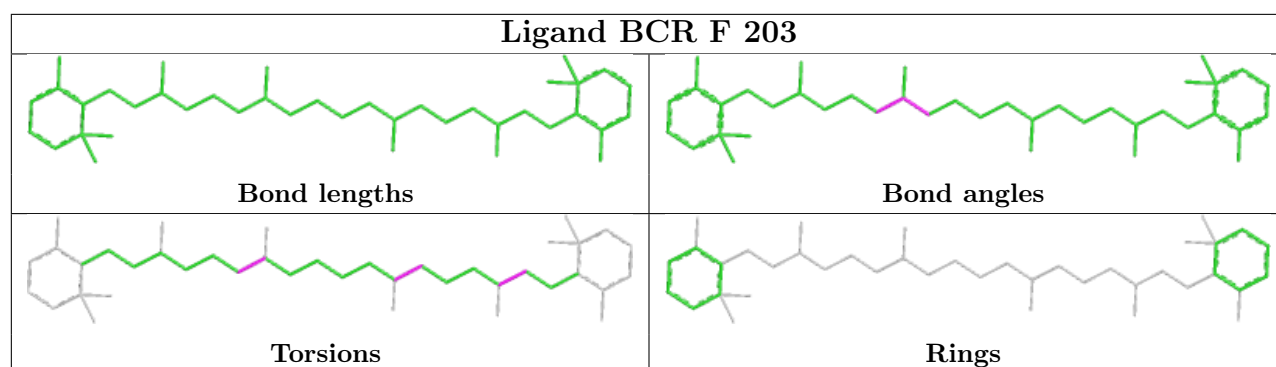
Bond angles



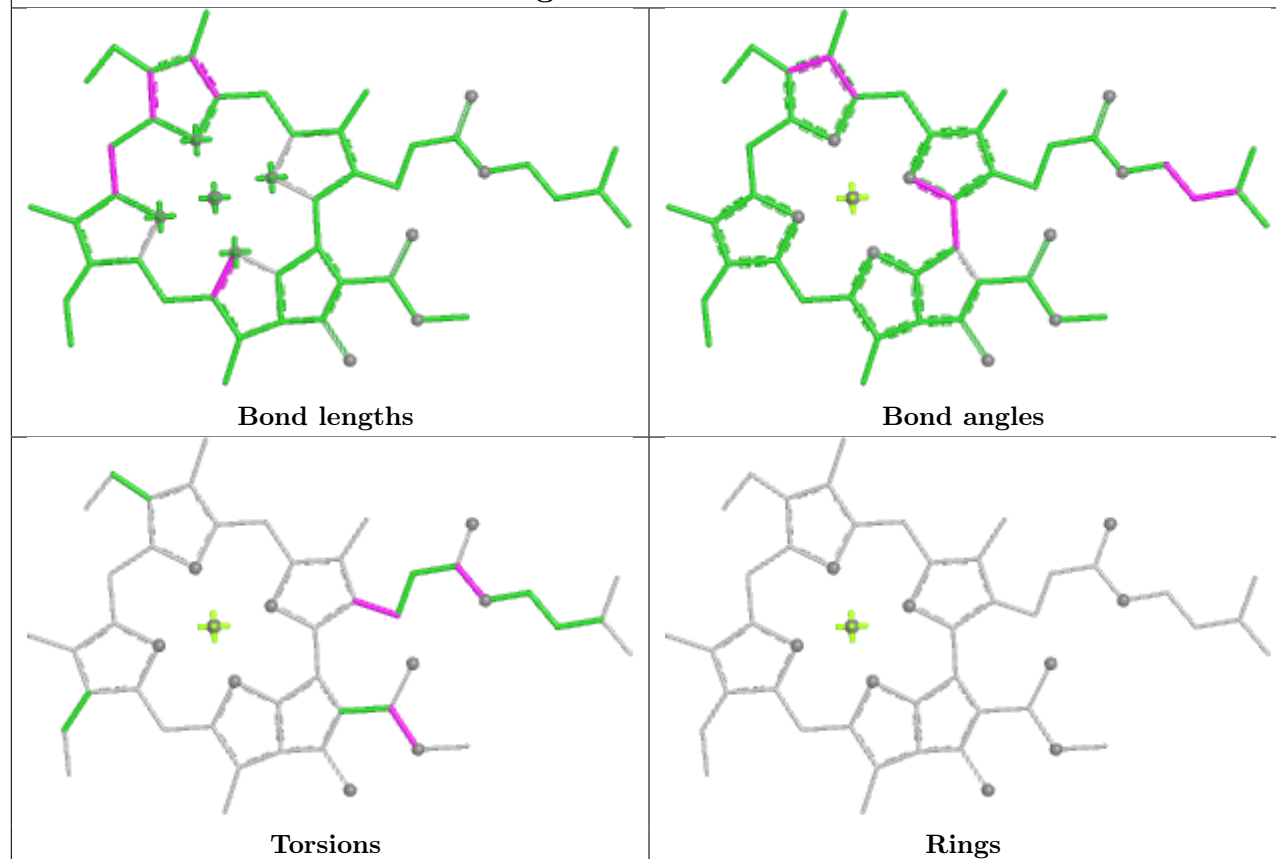
Torsions



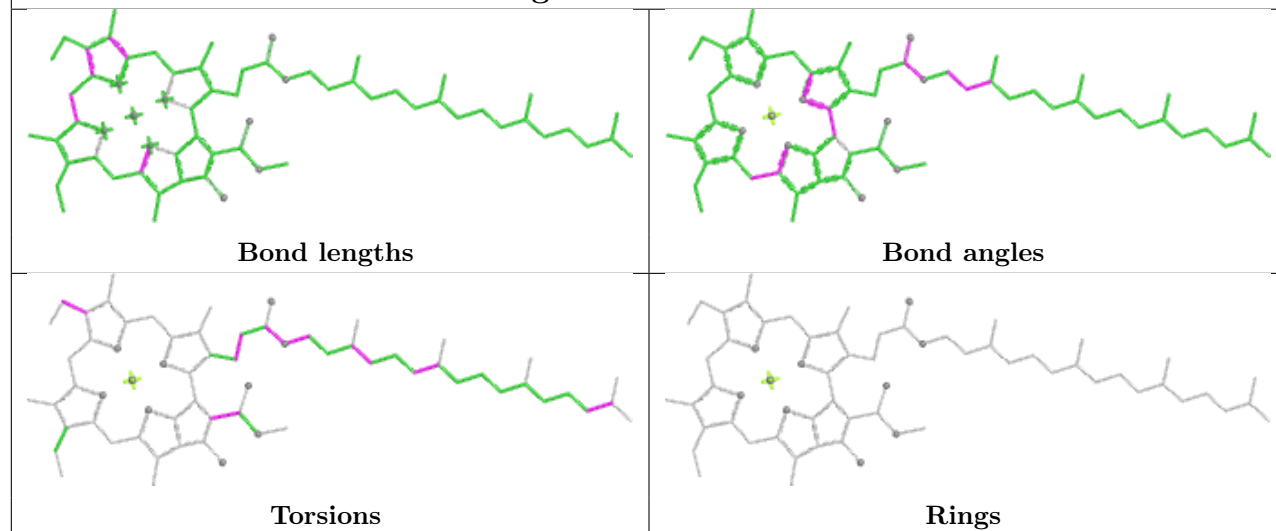
Rings

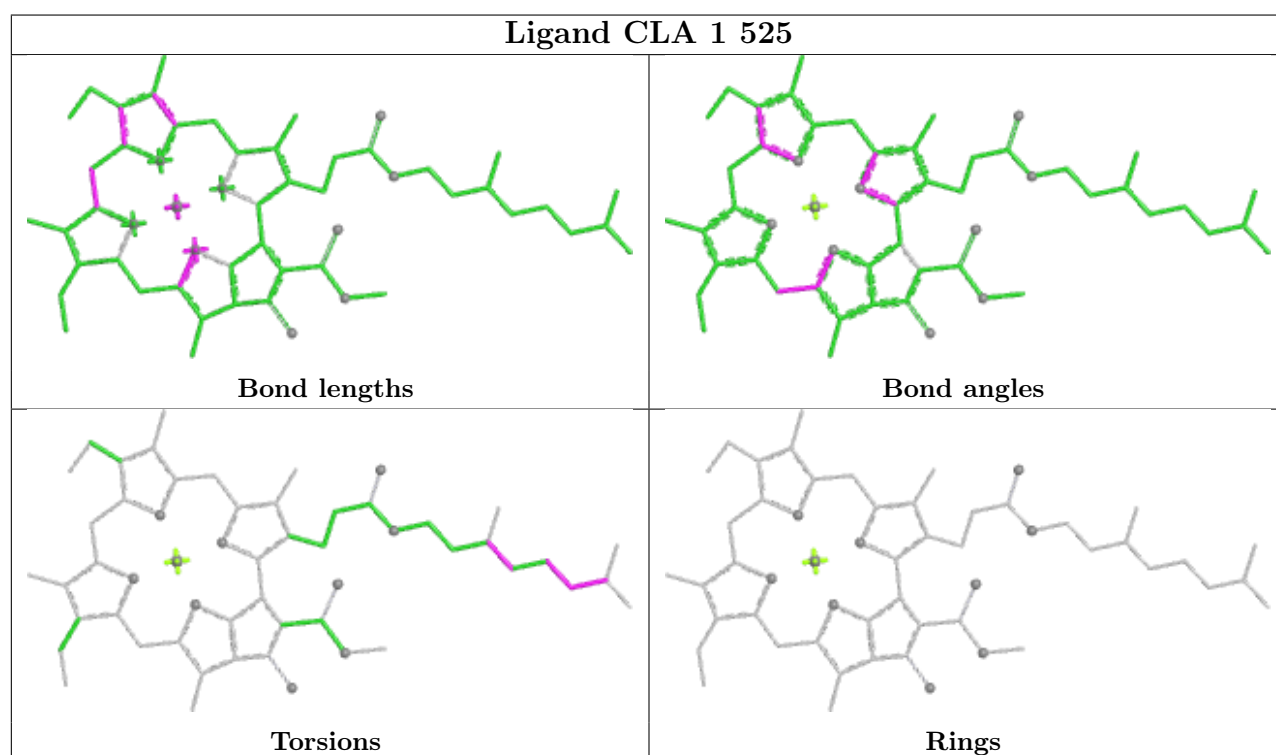
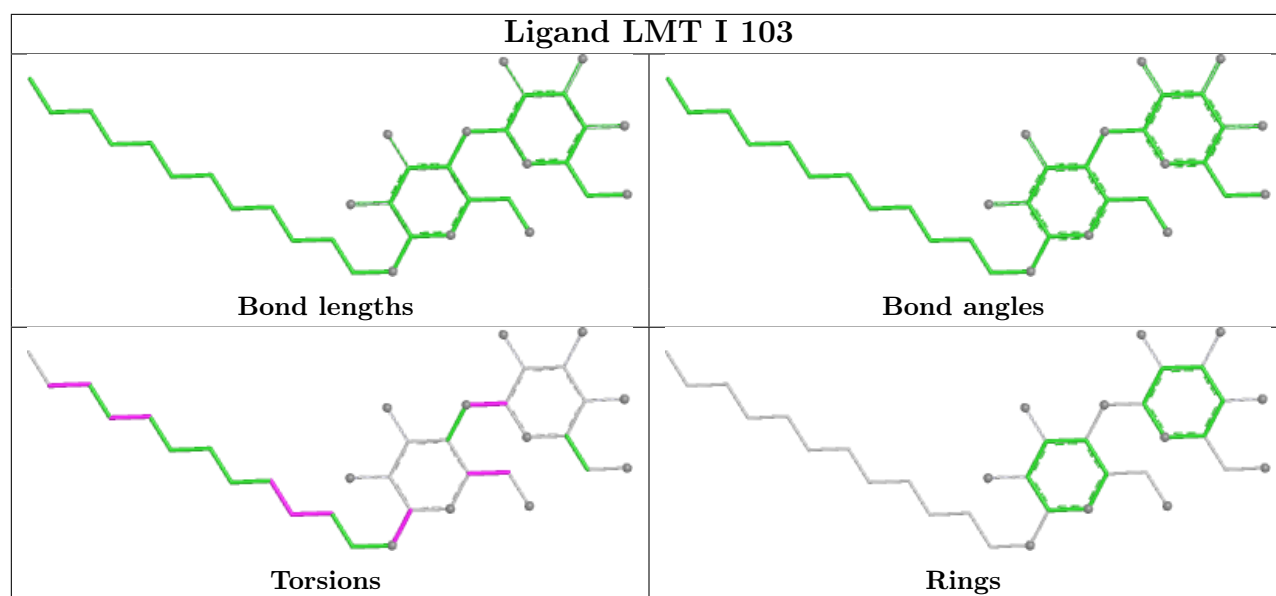


## Ligand CLA 4 402

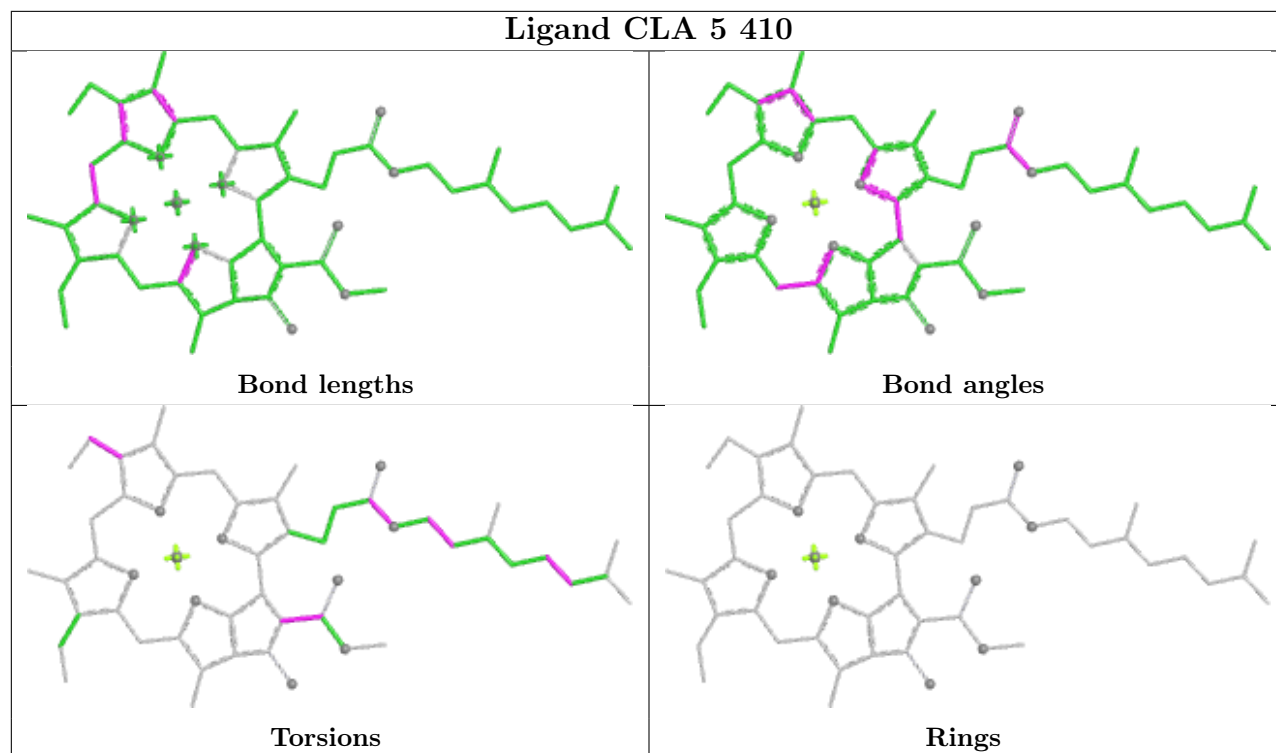


## Ligand CLA A 811

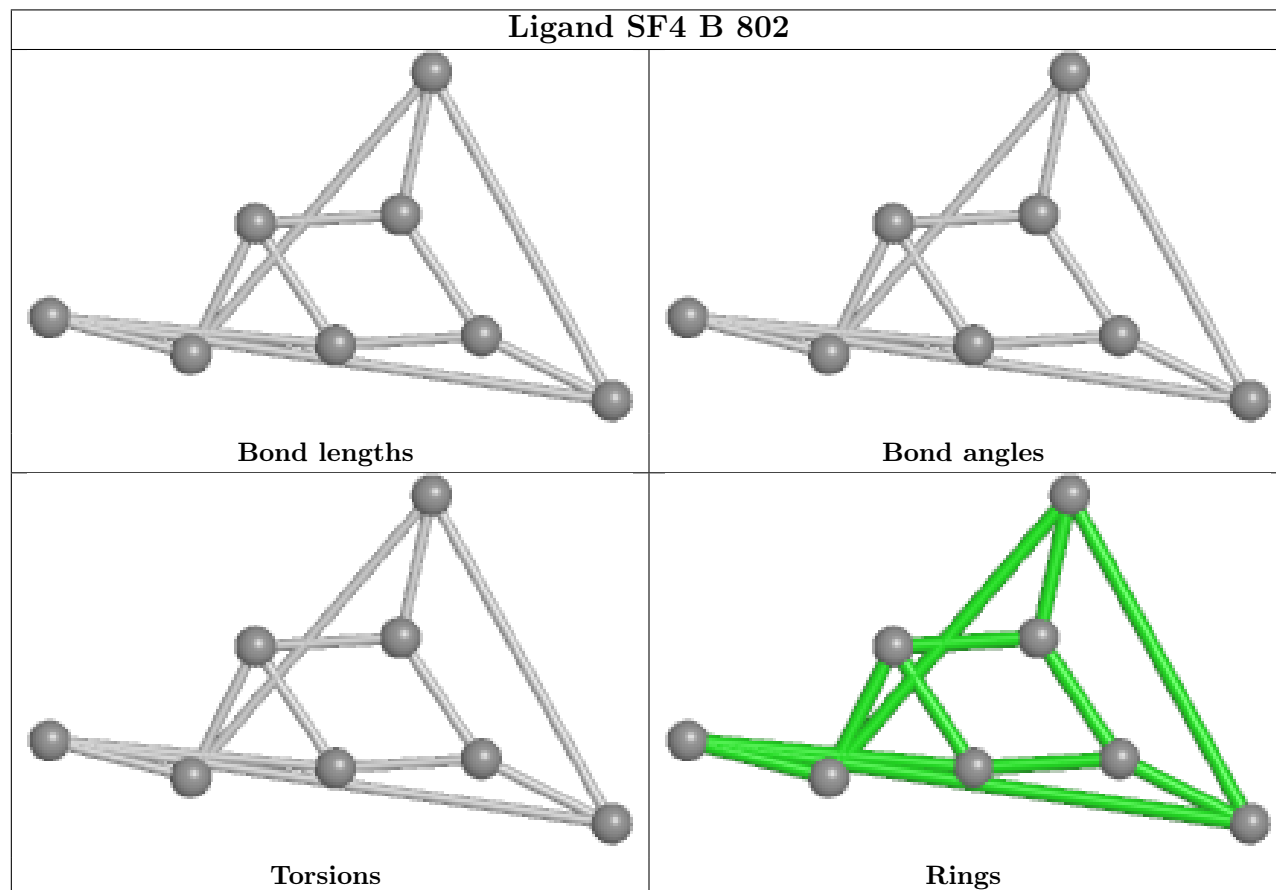


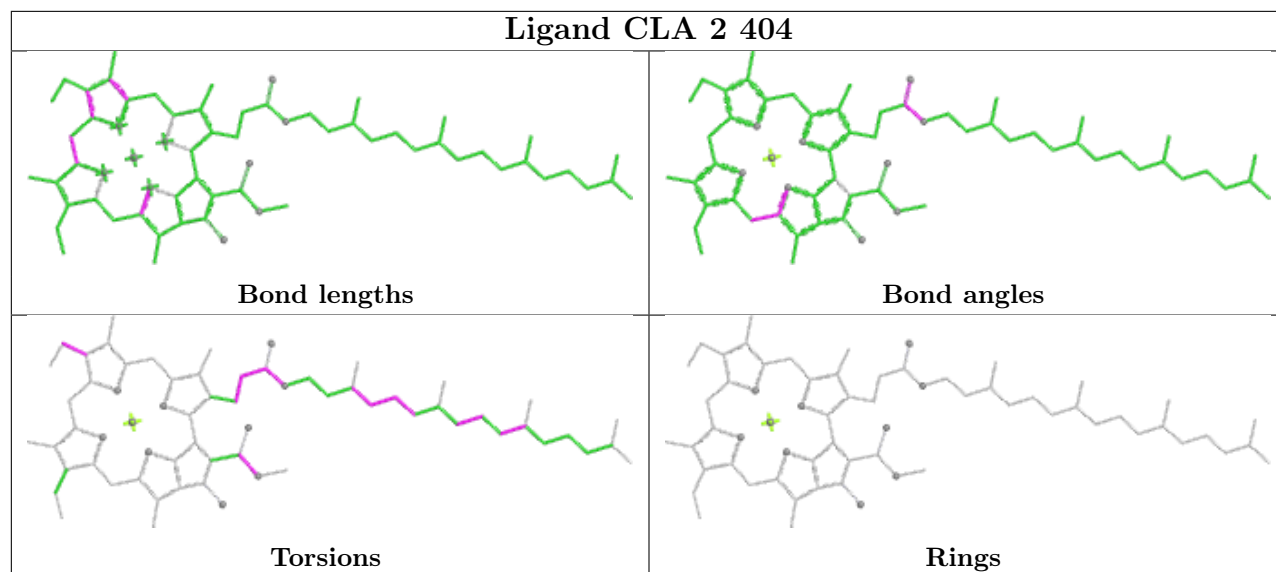
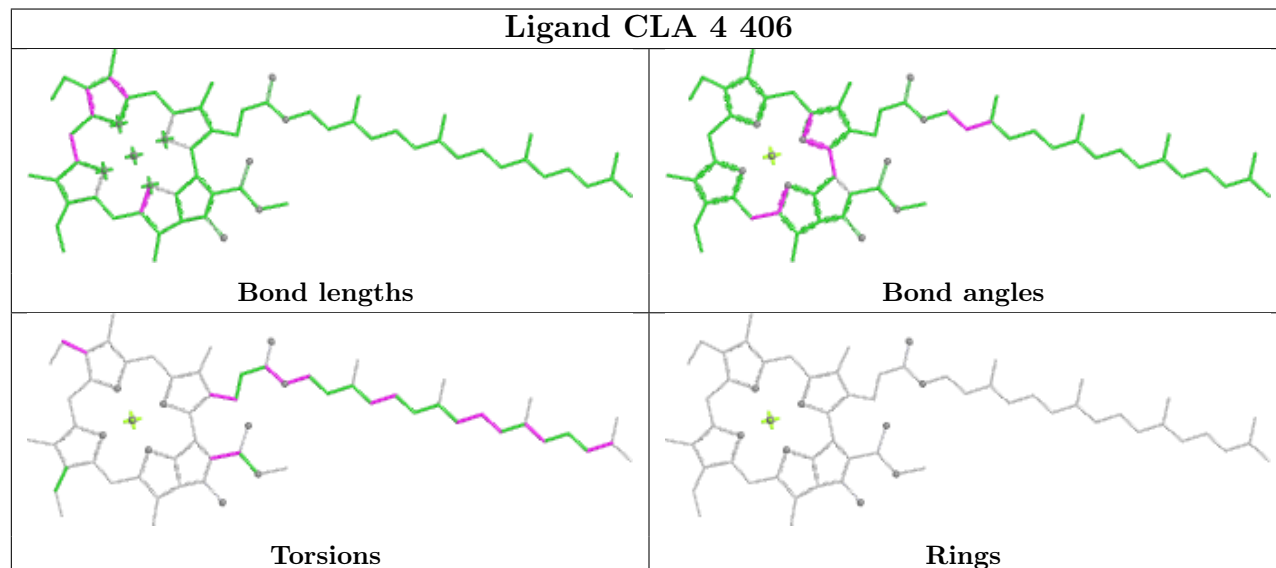


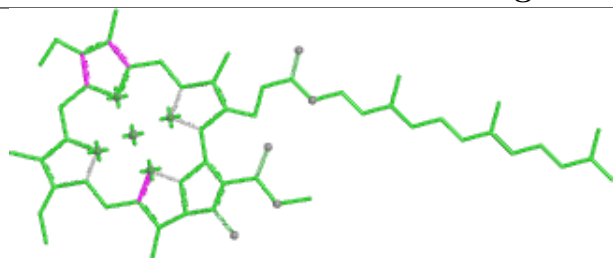
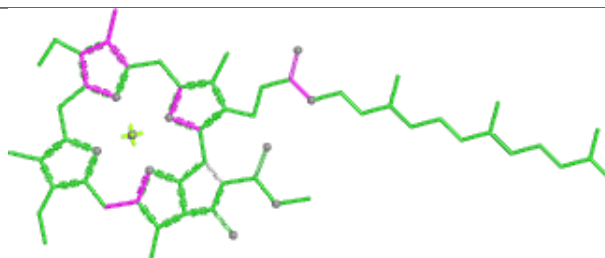
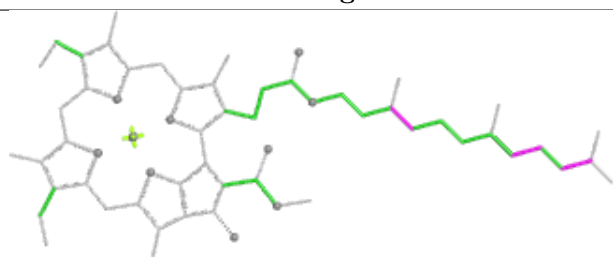
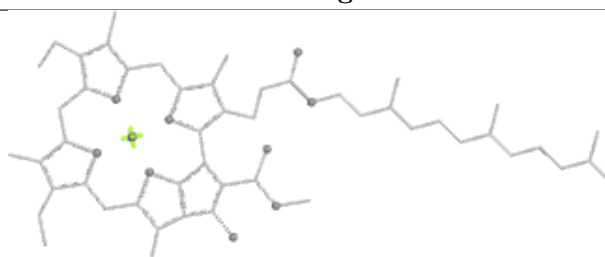
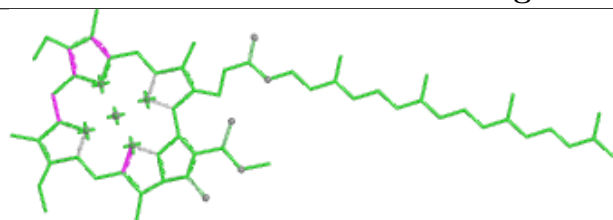
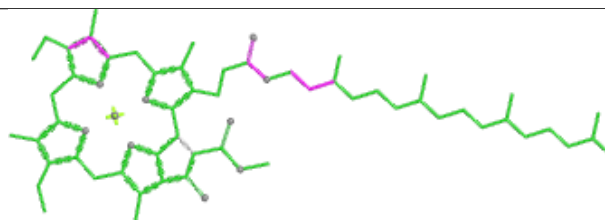
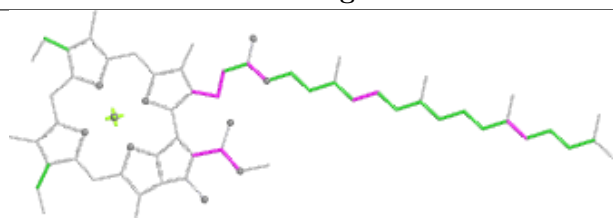
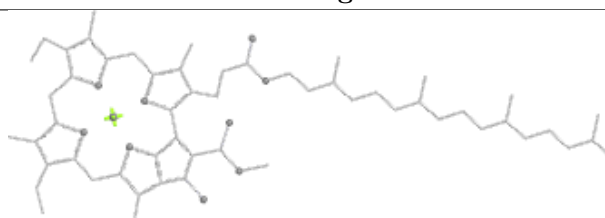
## Ligand CLA 5 410



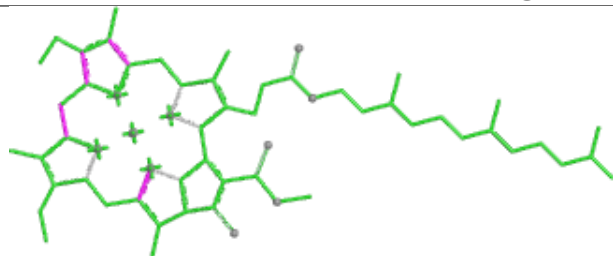
## Ligand SF4 B 802



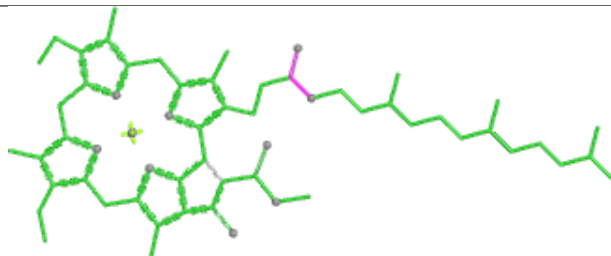
**Ligand CLA 2 404****Ligand CLA 4 406**

**Ligand CLA B 844****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 809****Bond lengths****Bond angles****Torsions****Rings**

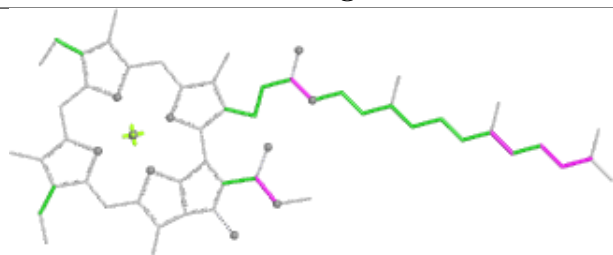
## Ligand CLA 1 516



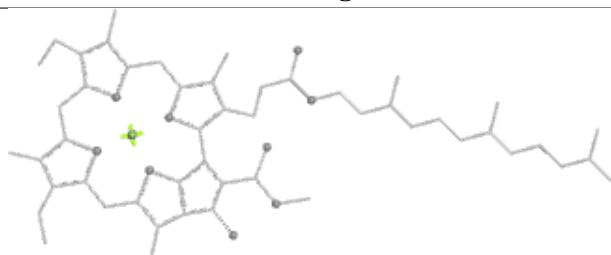
Bond lengths



Bond angles

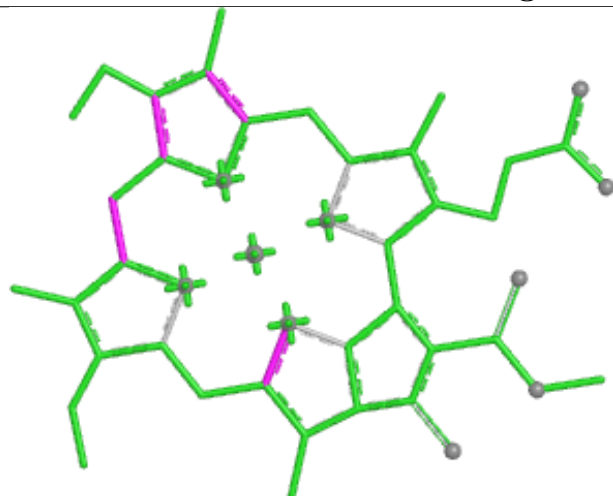


Torsions

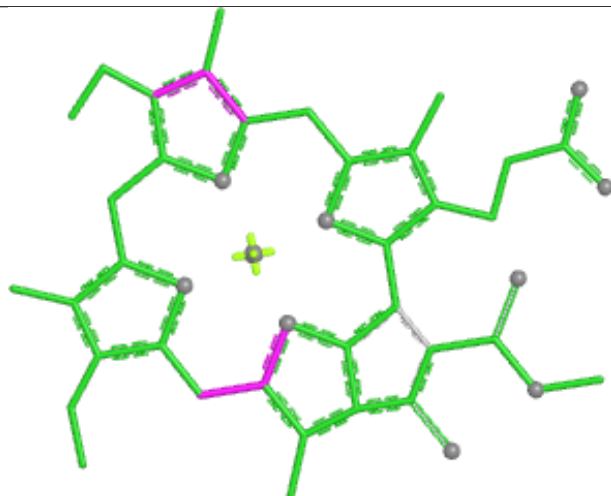


Rings

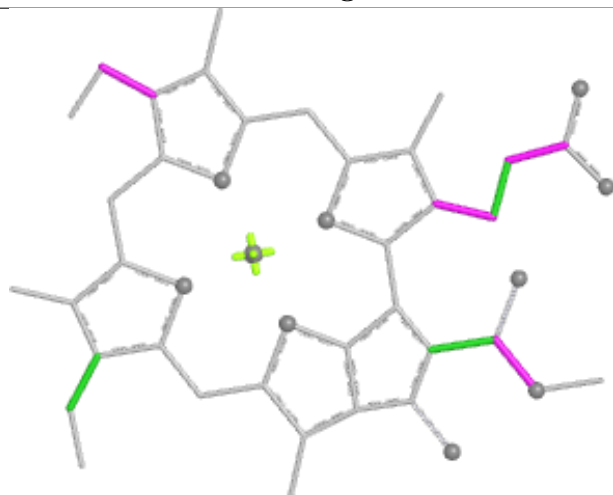
## Ligand CLA 2 412



Bond lengths



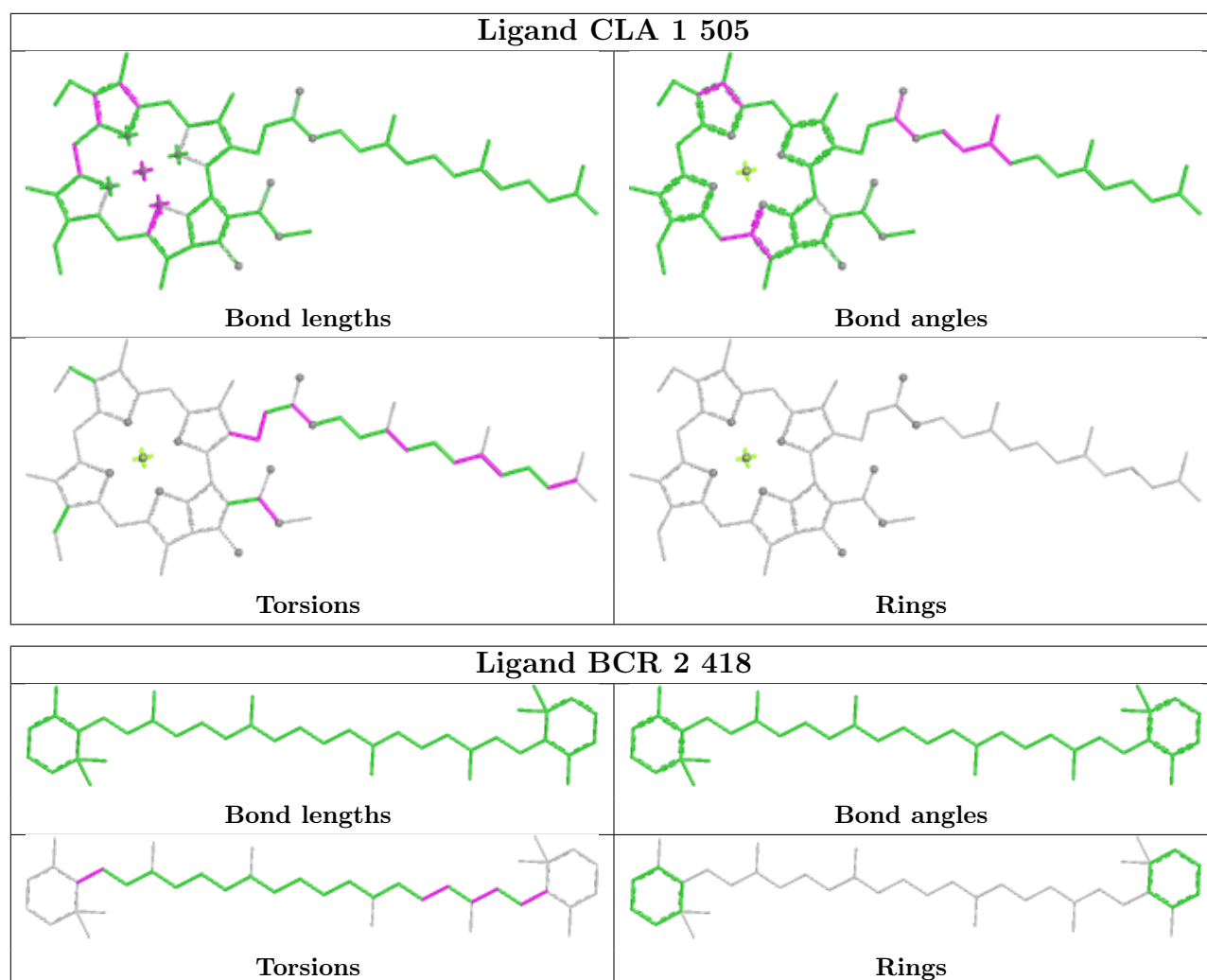
Bond angles

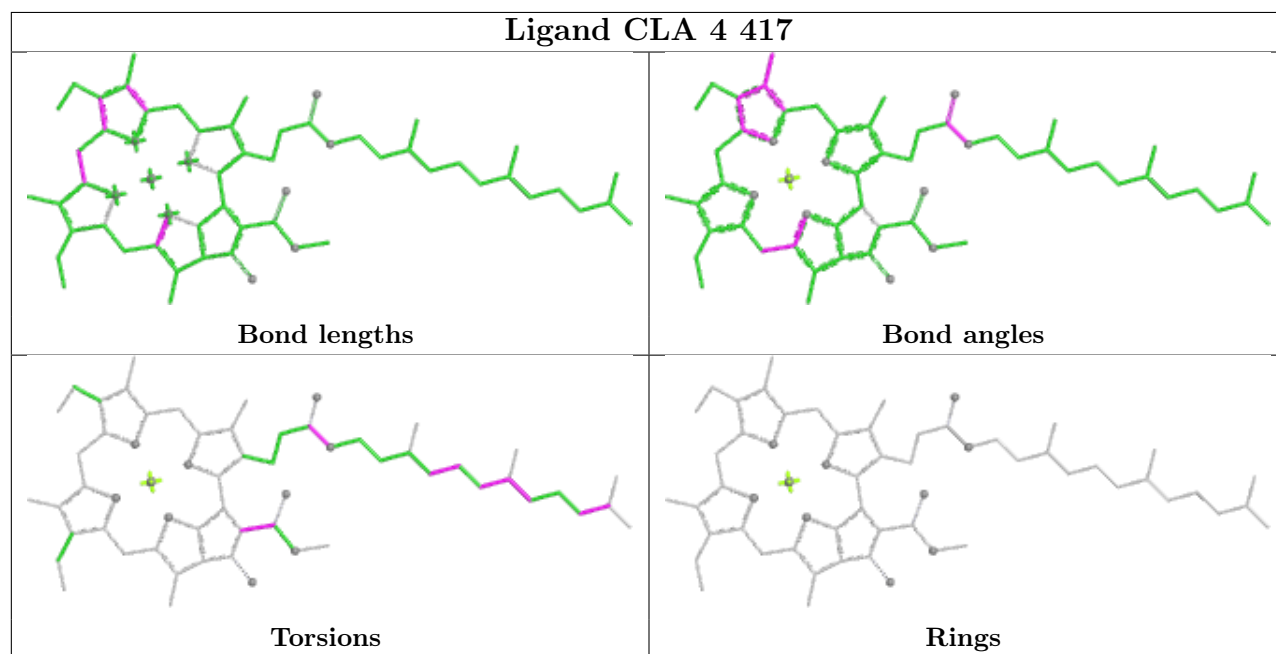
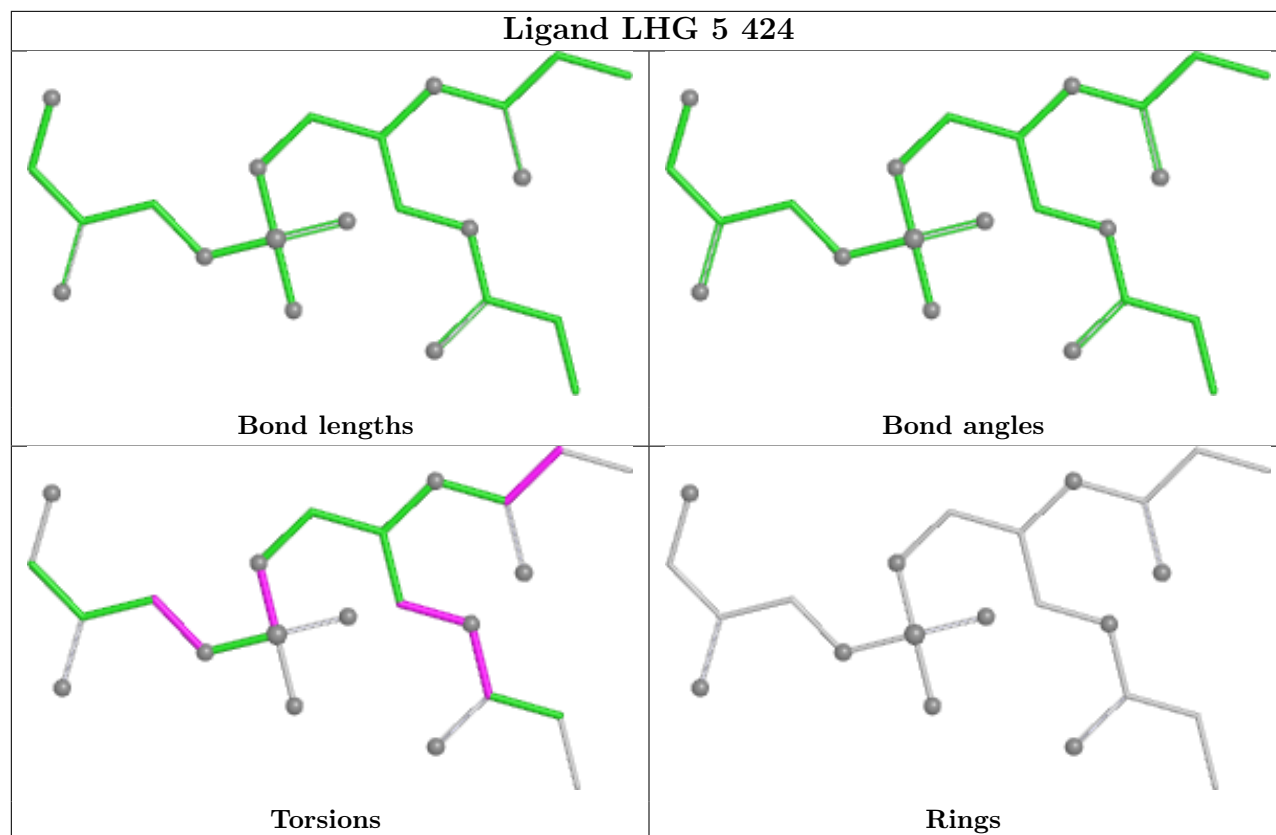


Torsions

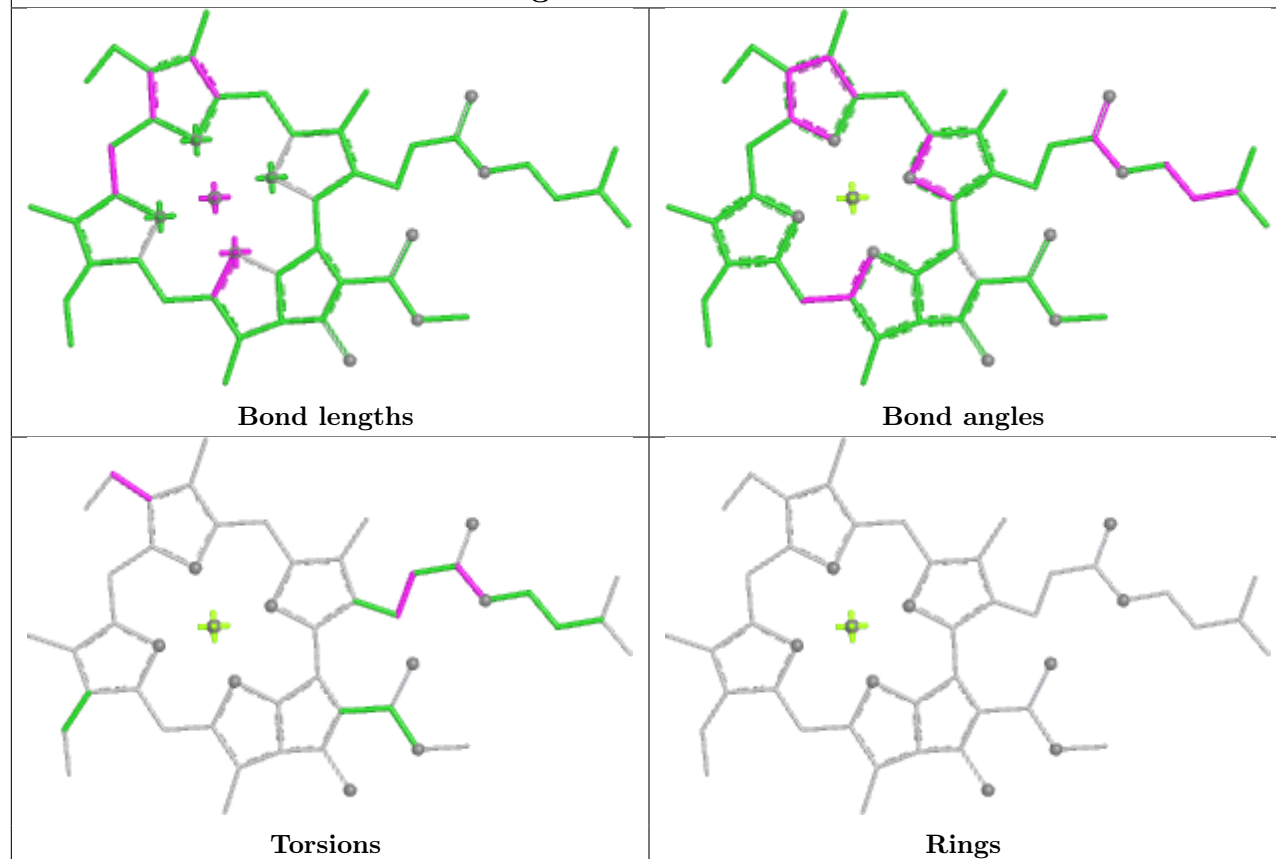


Rings

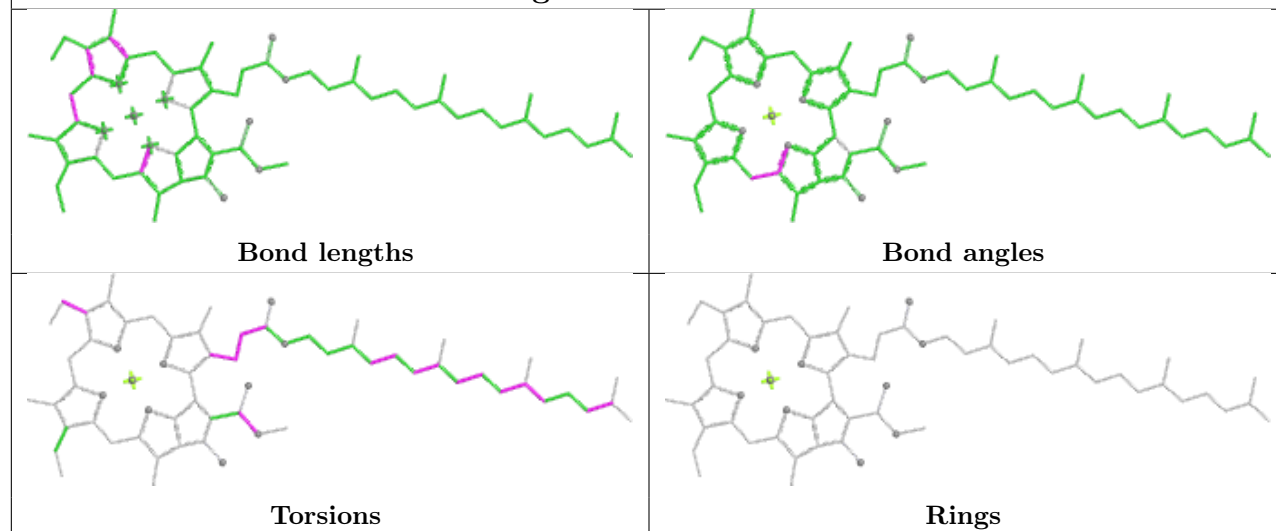


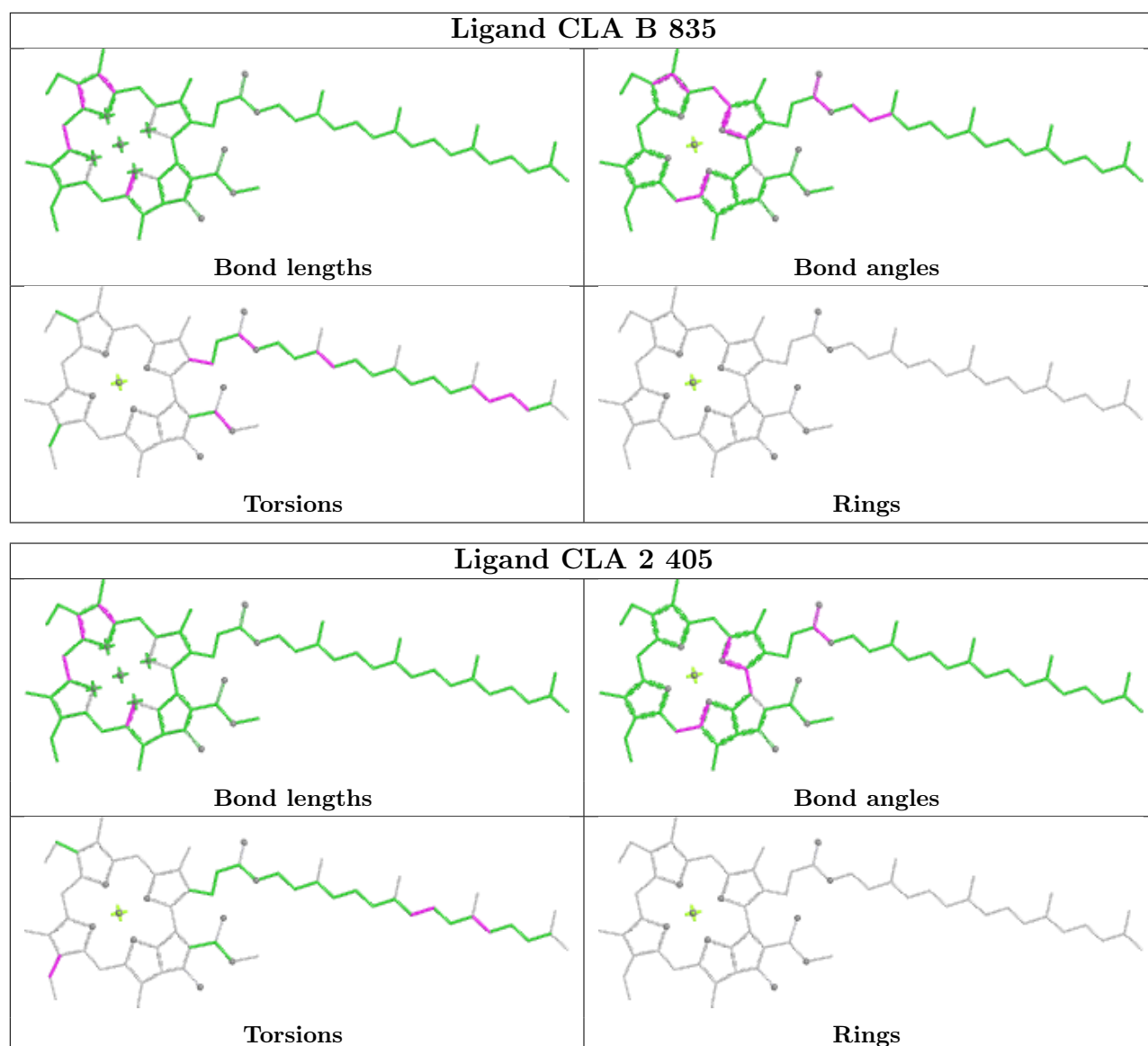


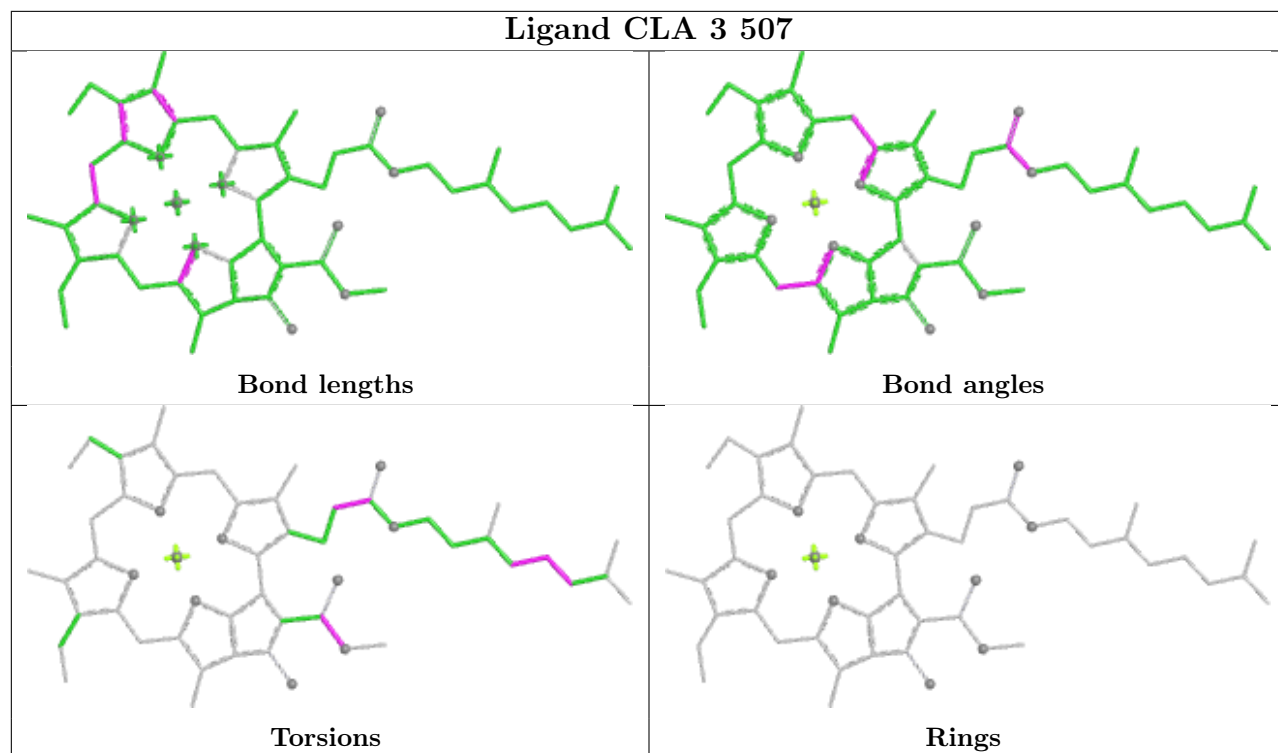
## Ligand CLA A 823

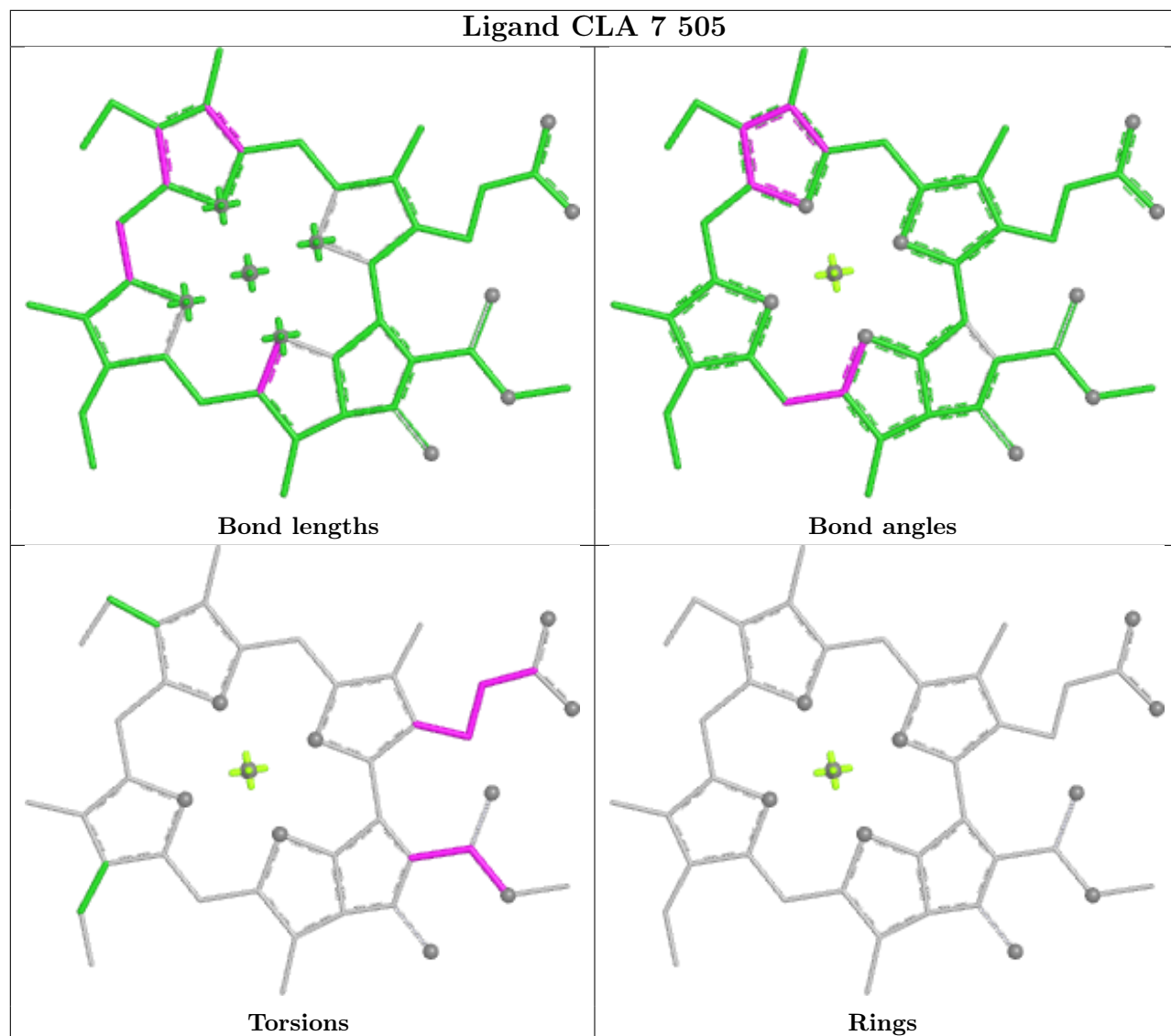


## Ligand CLA B 816

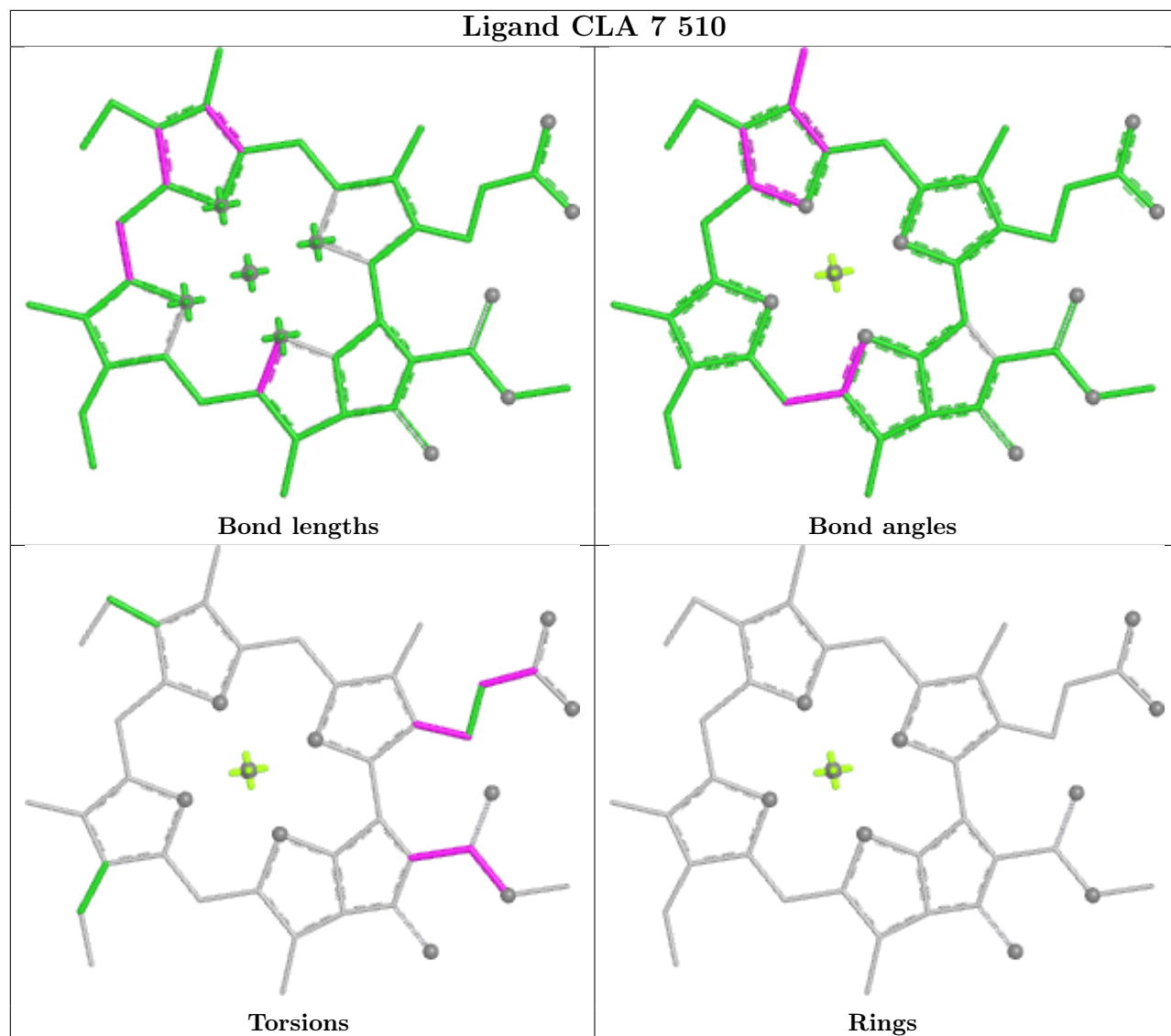




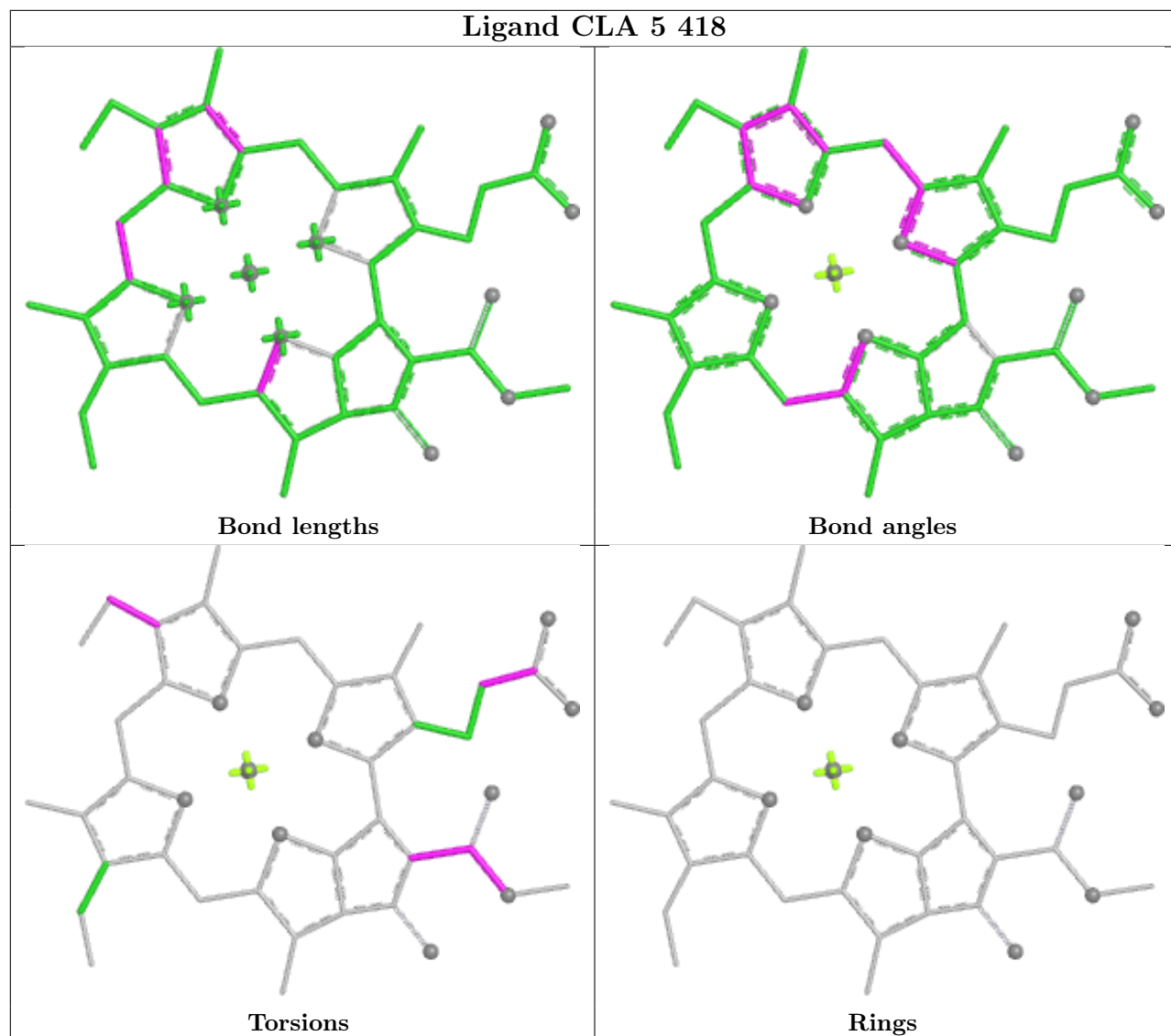




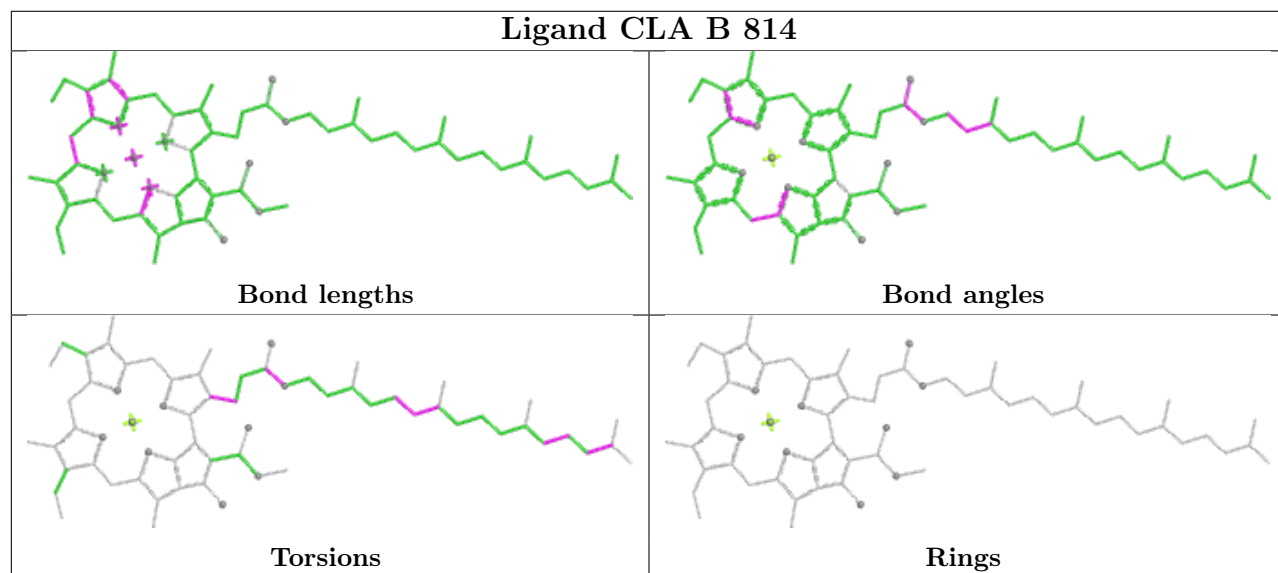
## Ligand CLA 7 510

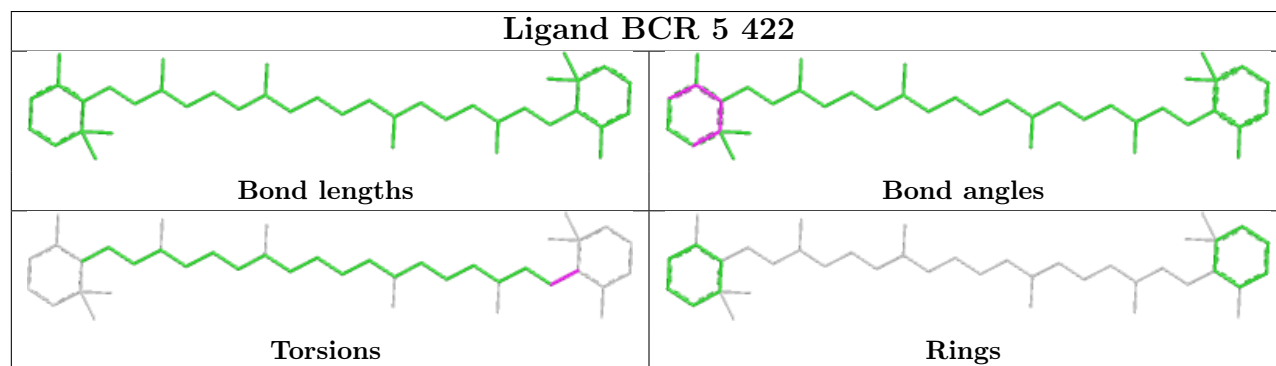
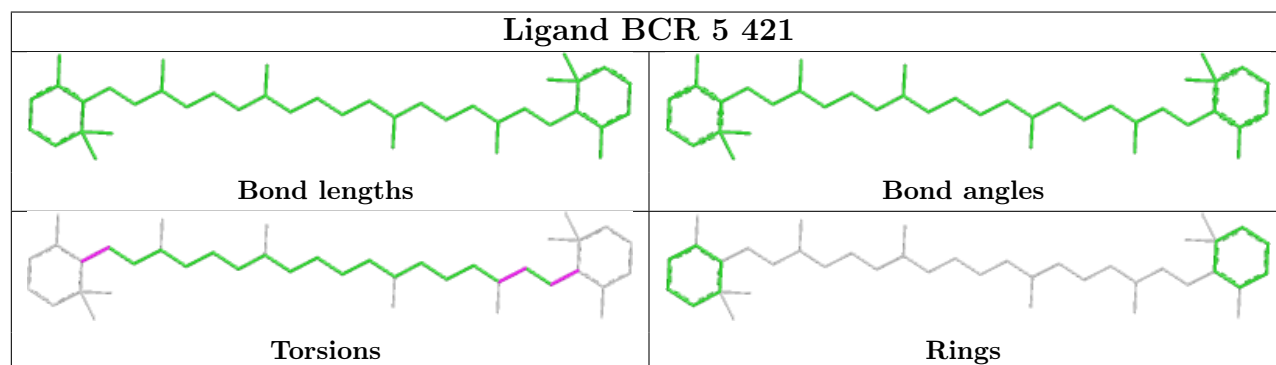
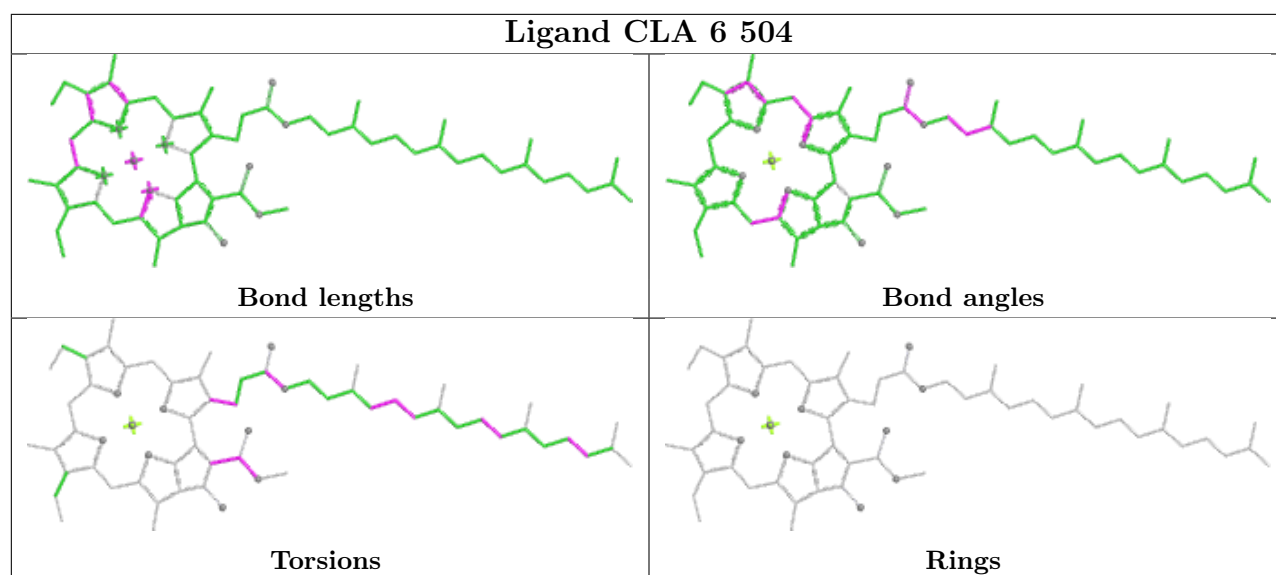


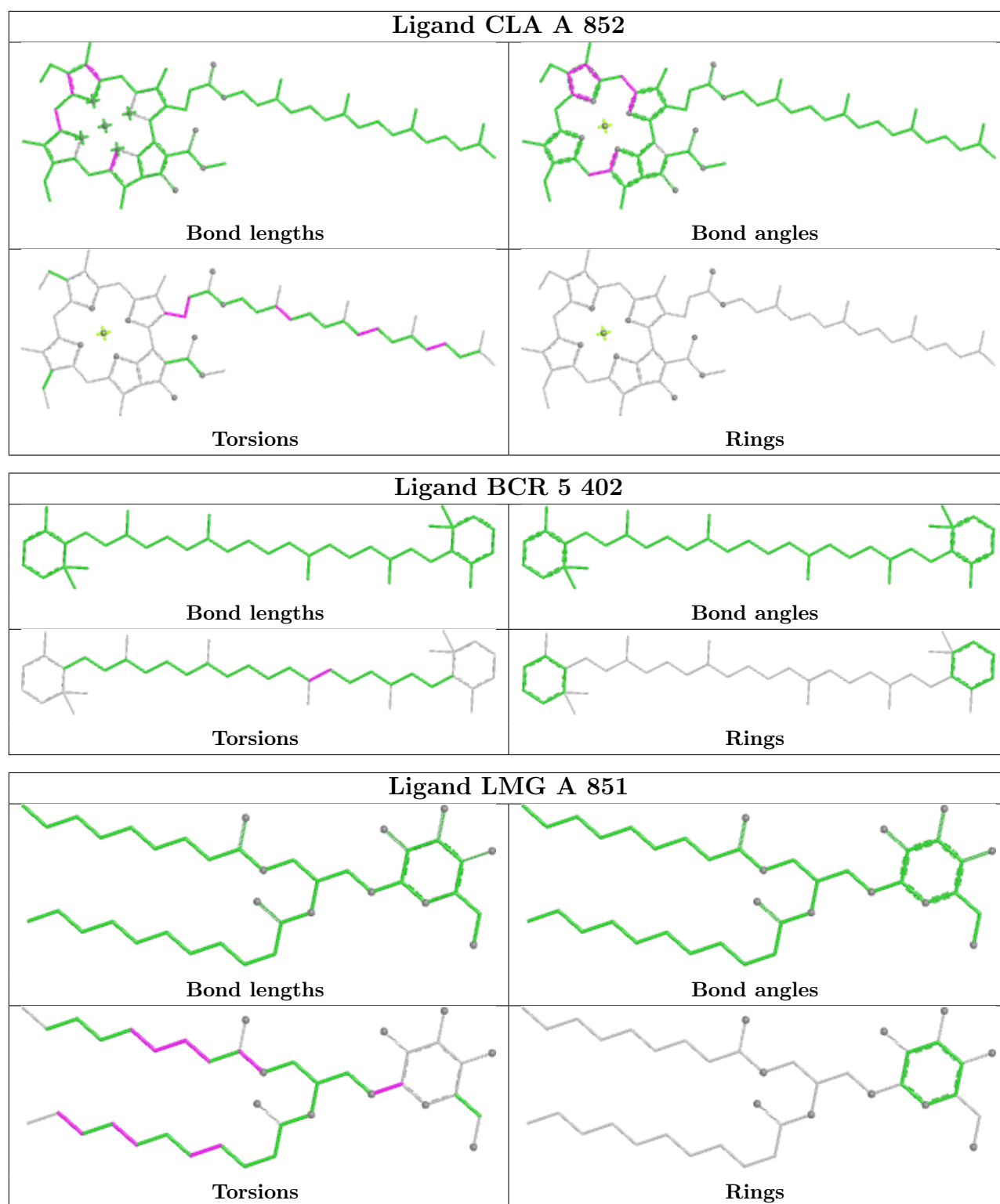
## Ligand CLA 5 418

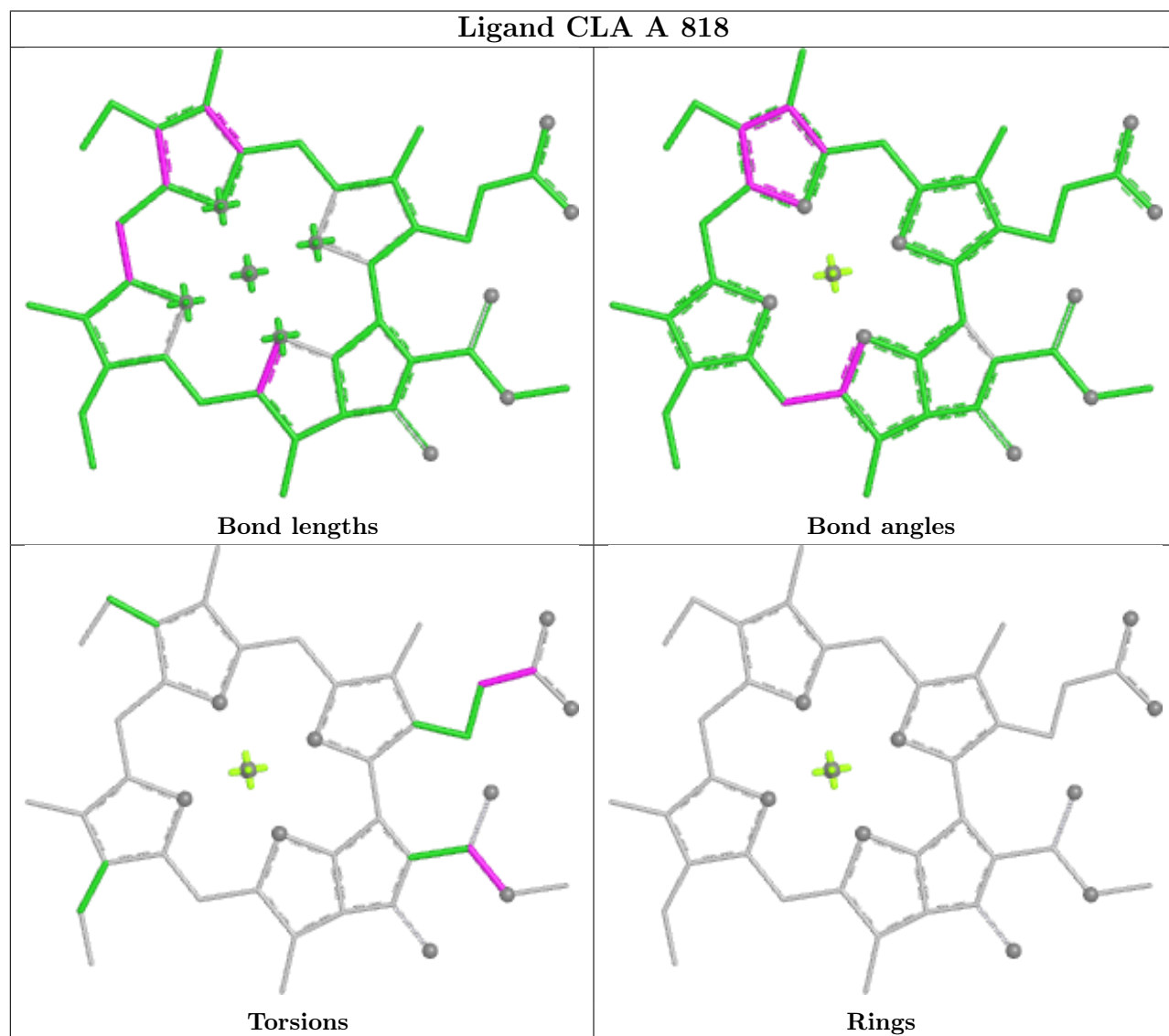
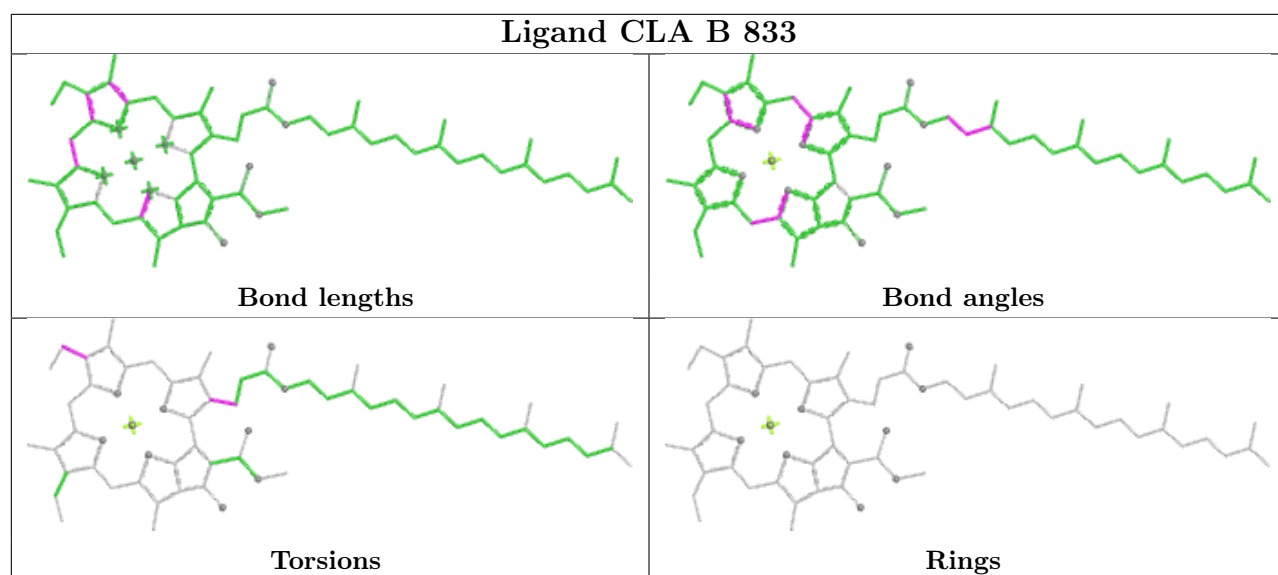


## Ligand CLA B 814

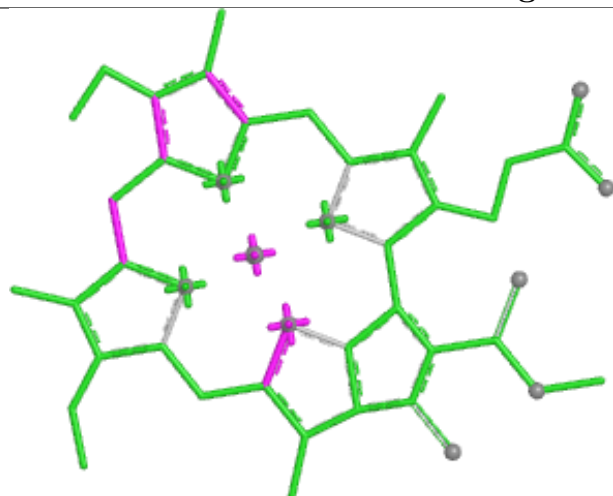




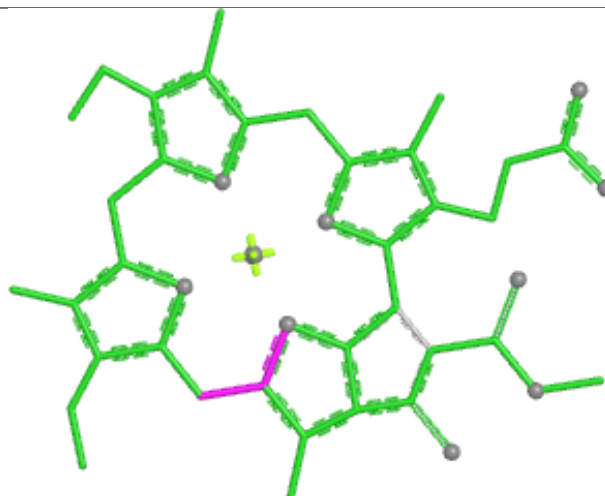




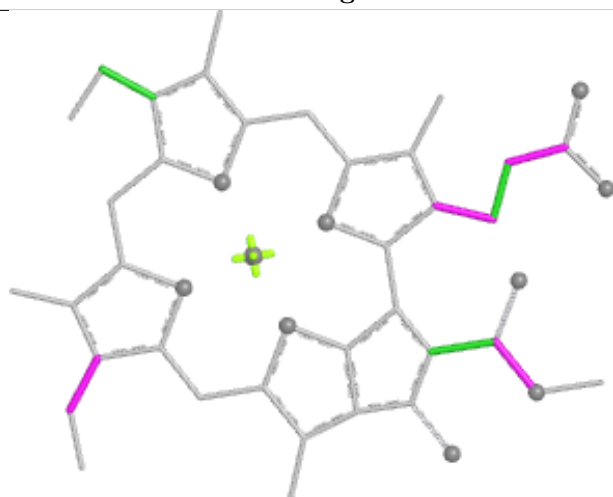
## Ligand CLA 2 414



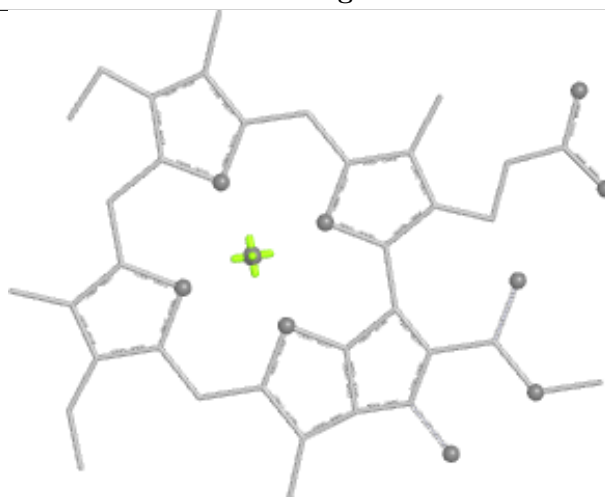
Bond lengths



Bond angles

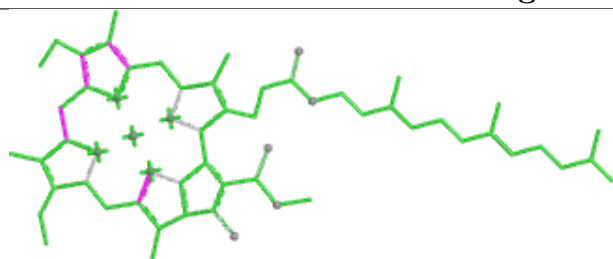


Torsions

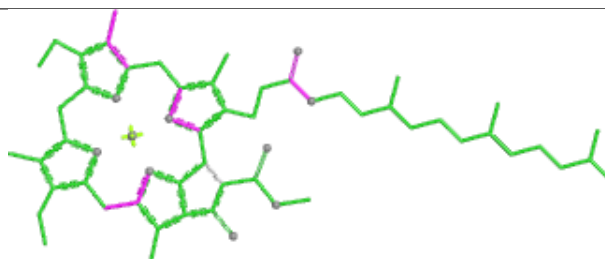


Rings

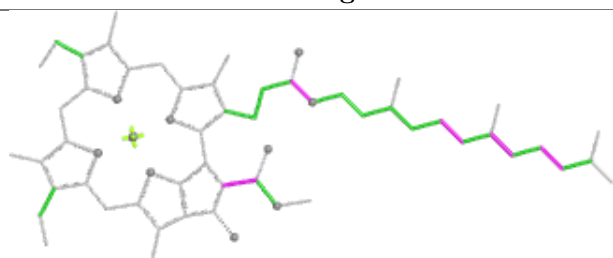
## Ligand CLA 1 510



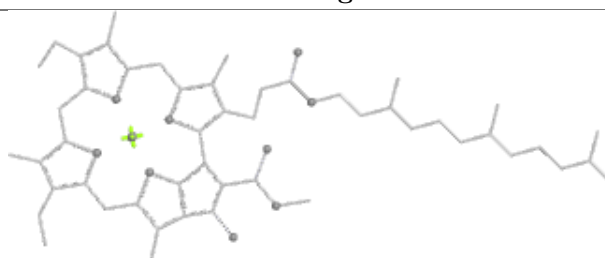
Bond lengths



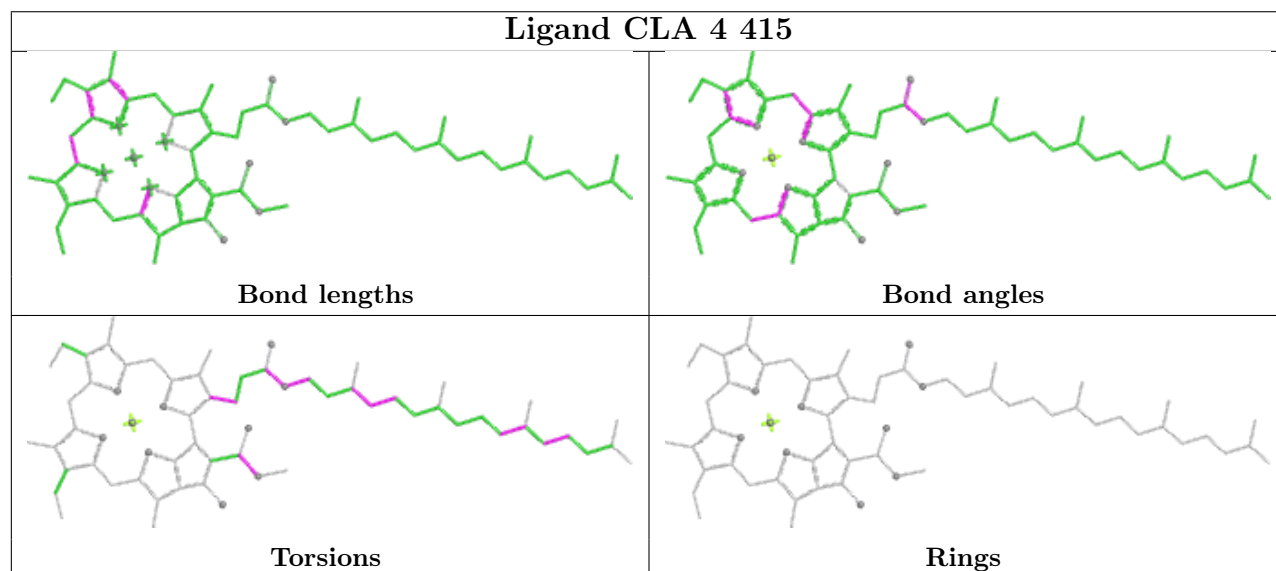
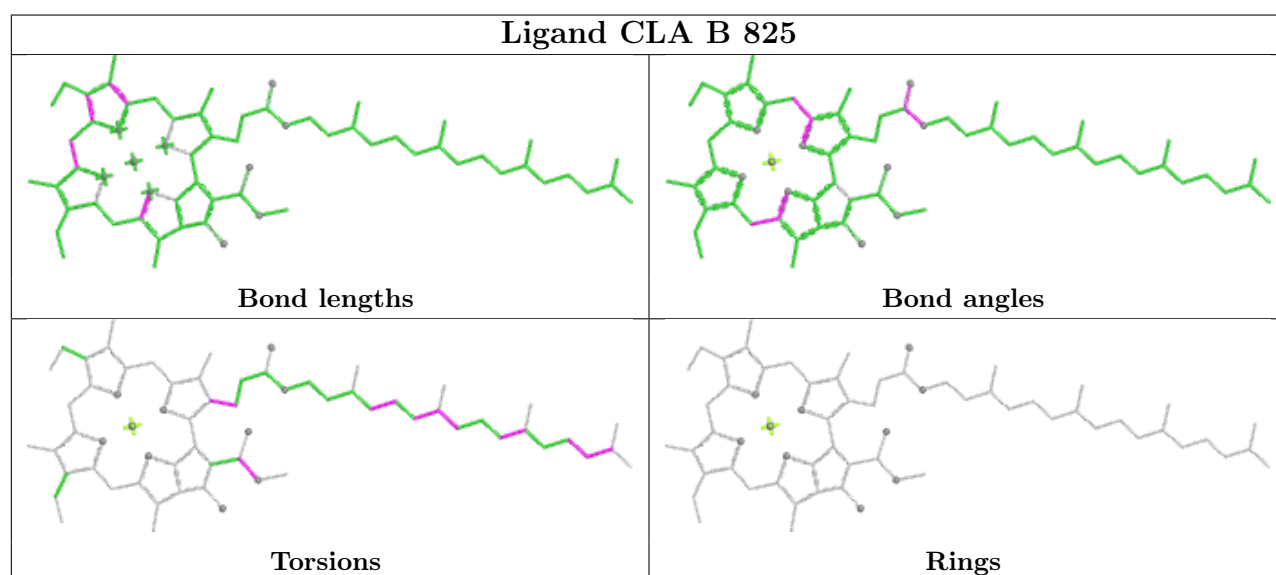
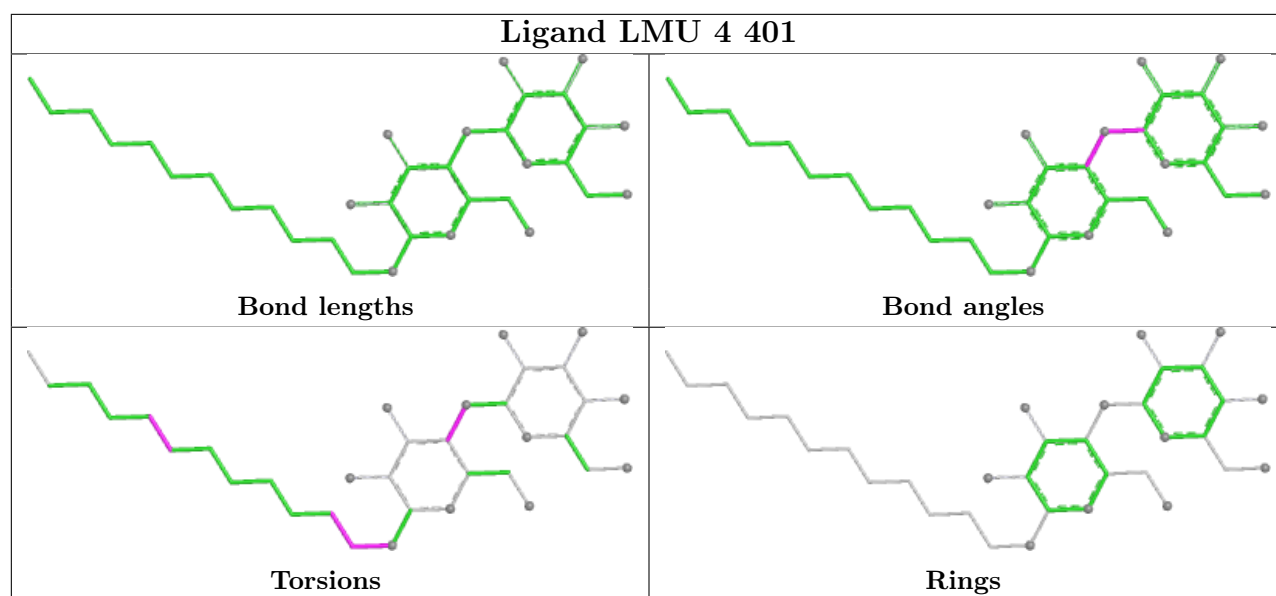
Bond angles

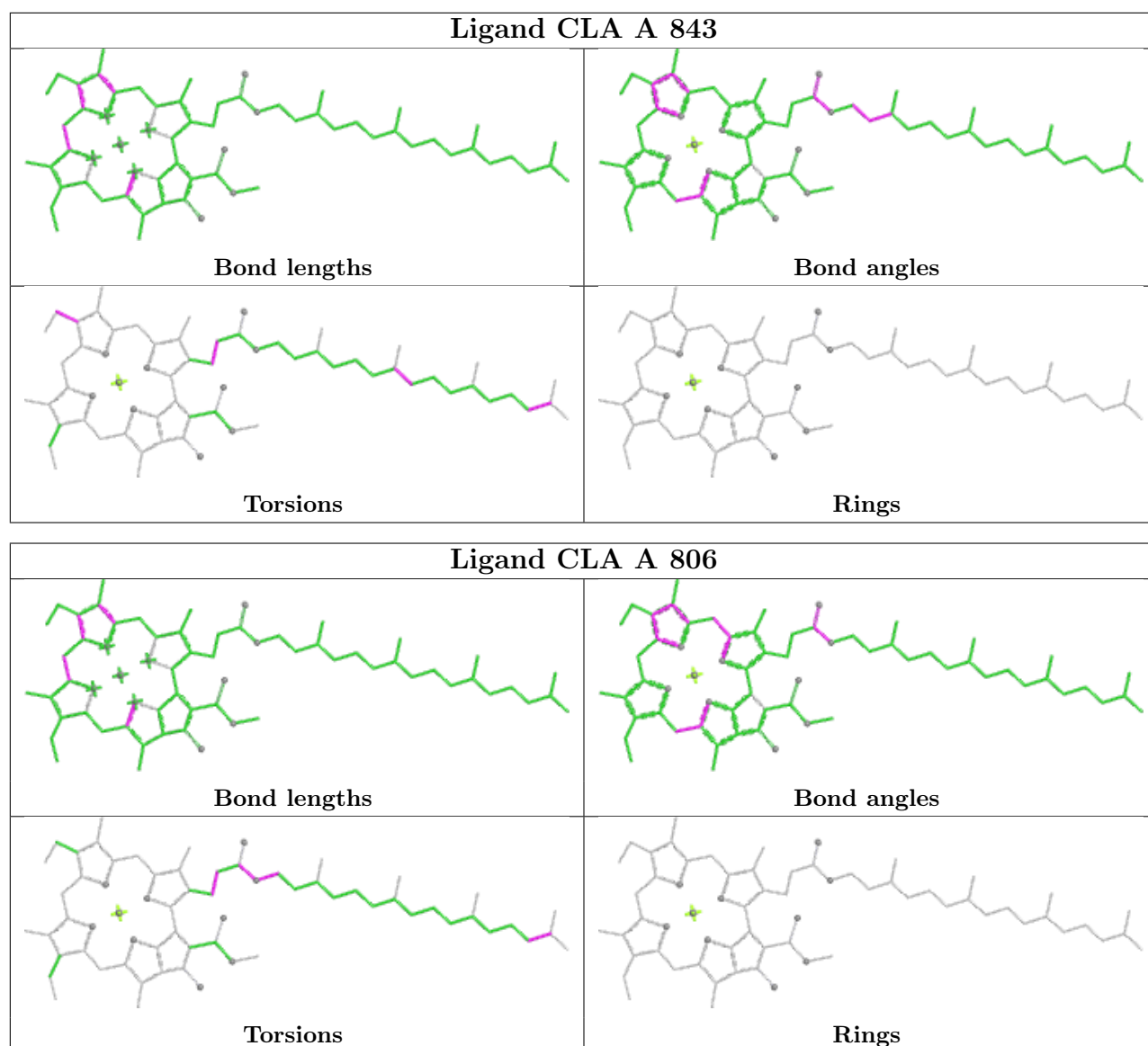


Torsions

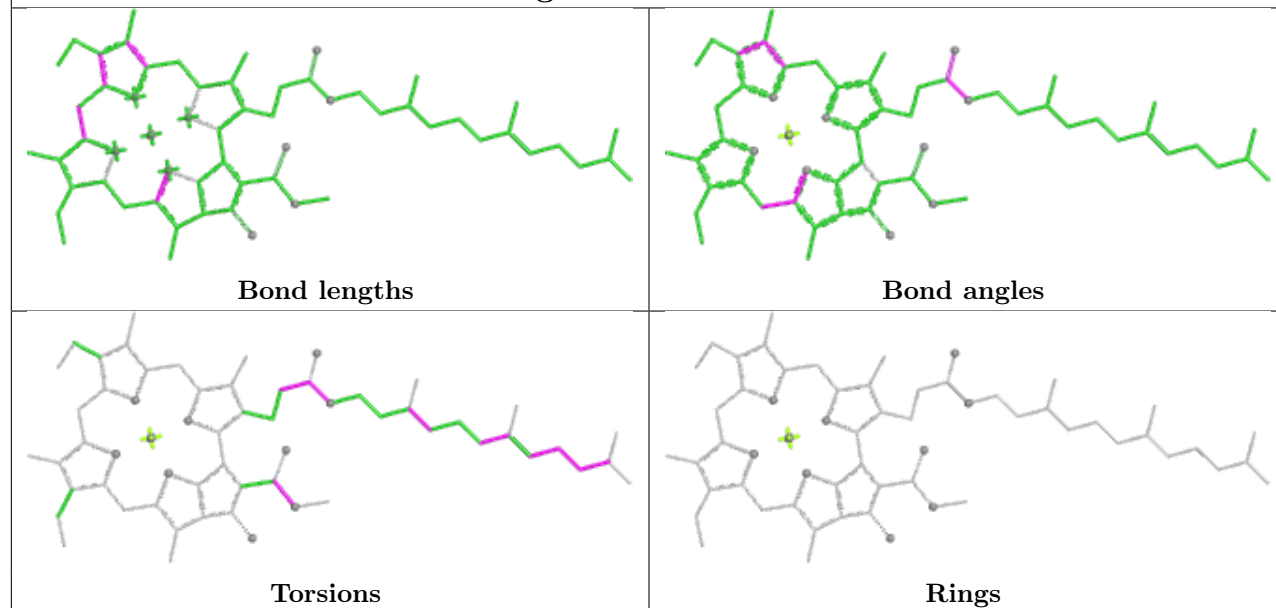


Rings

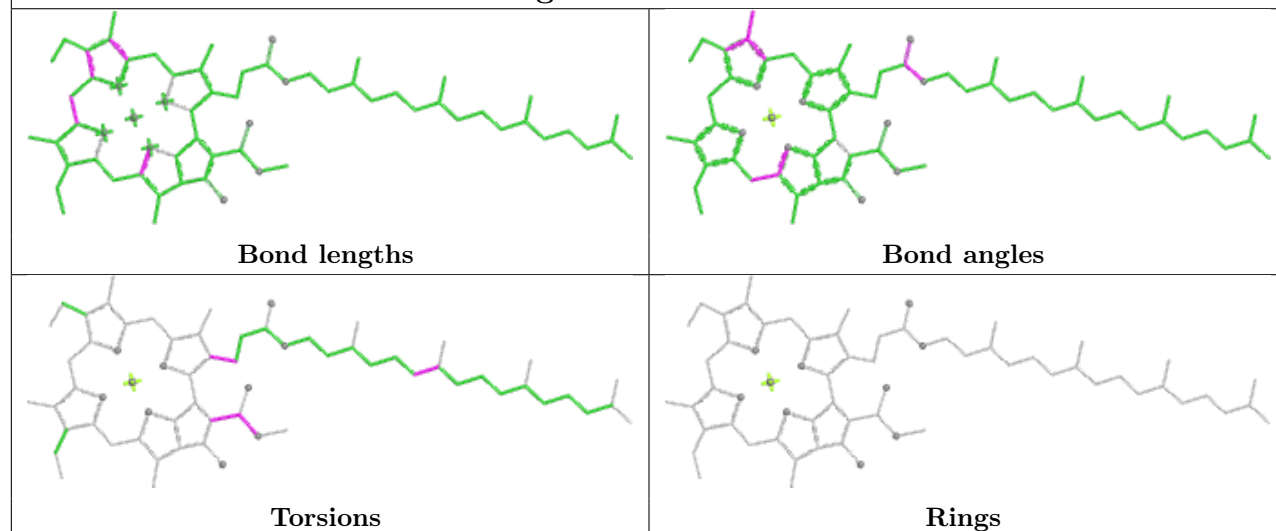


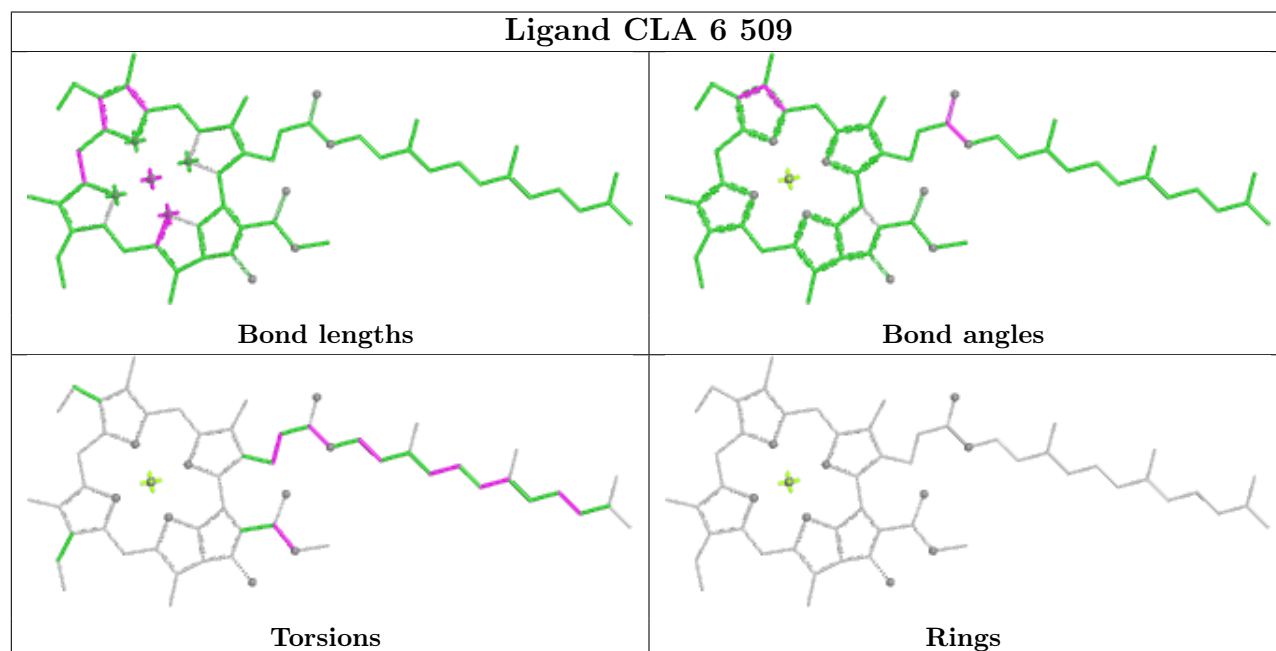
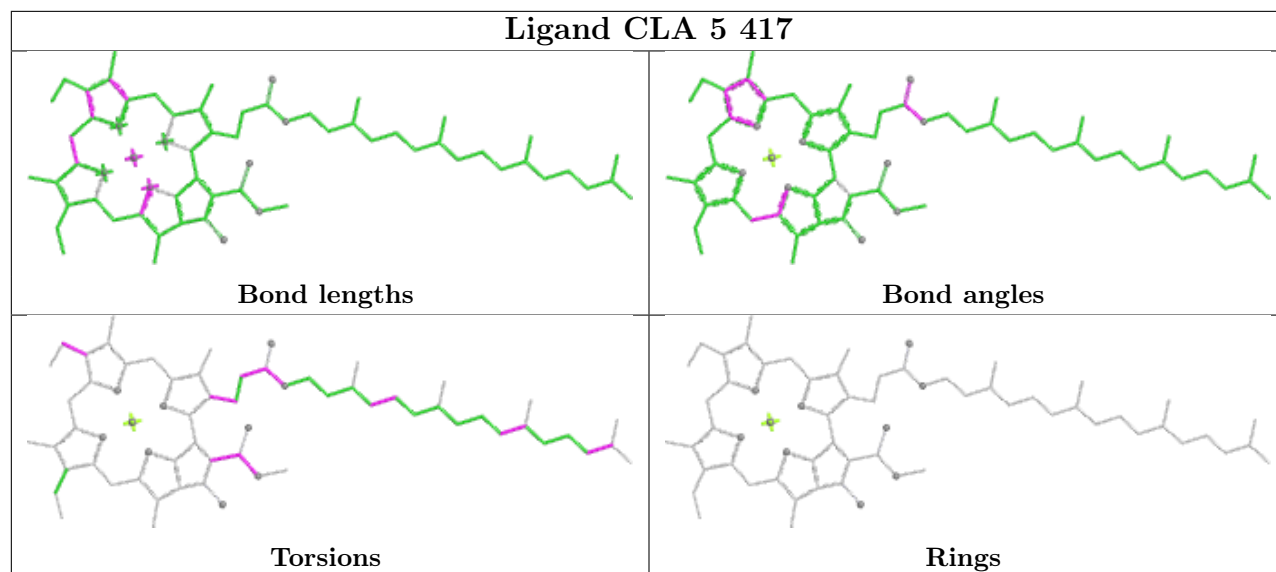


## Ligand CLA 2 408

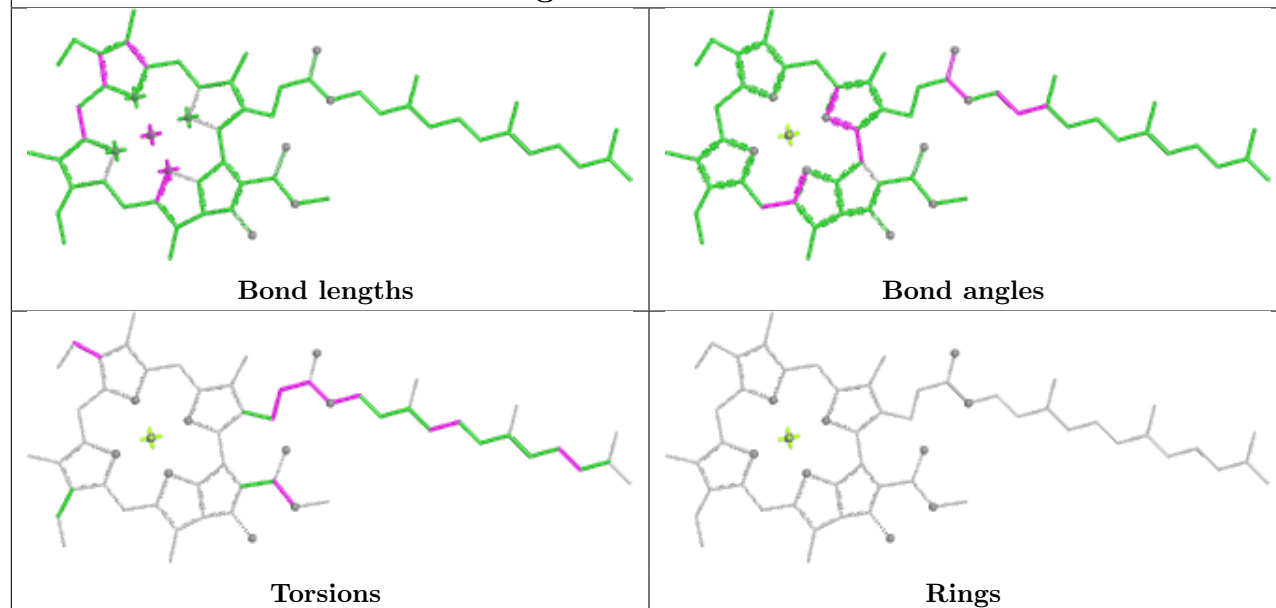


## Ligand CLA 1 506

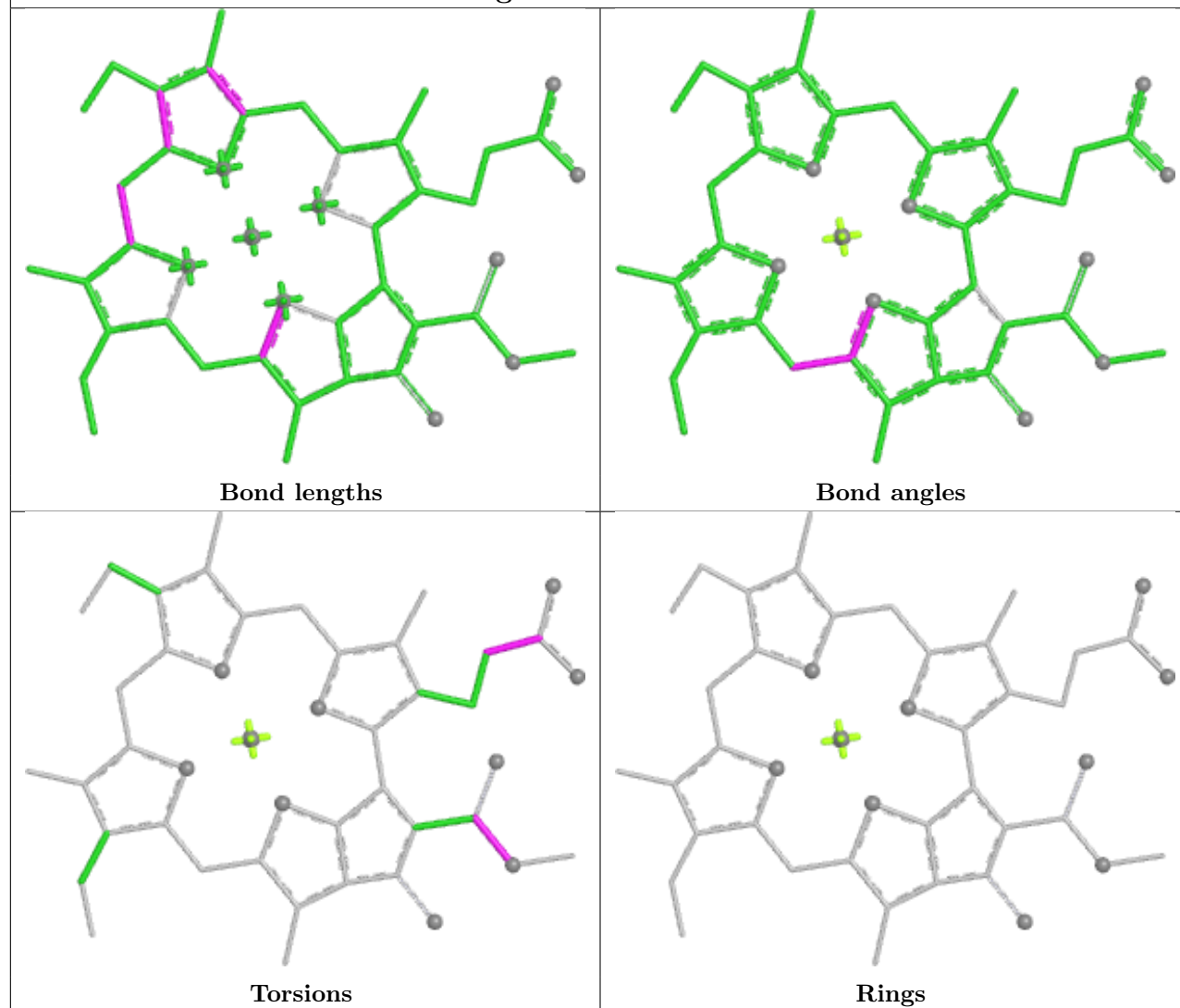


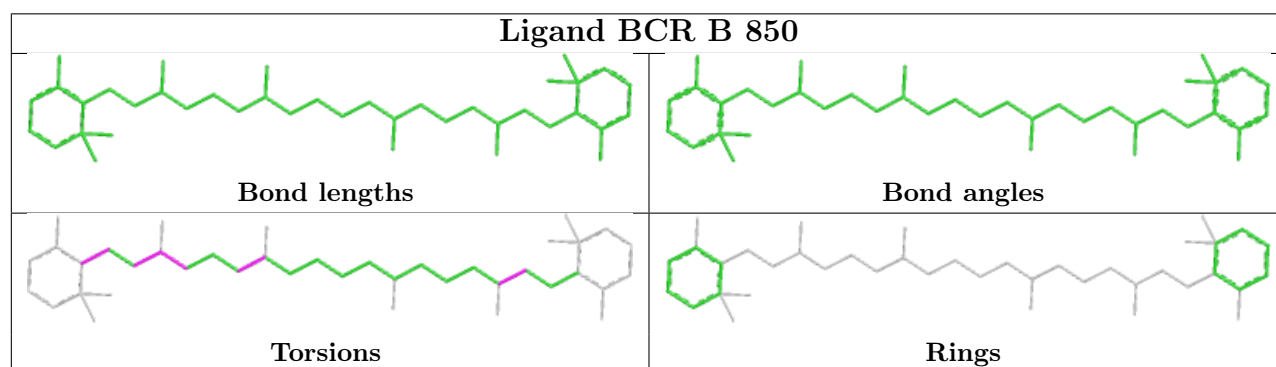
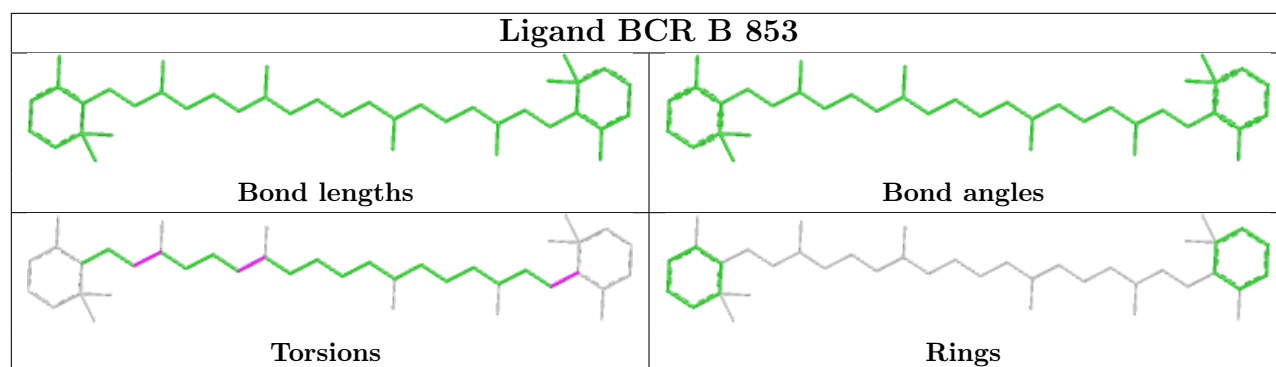
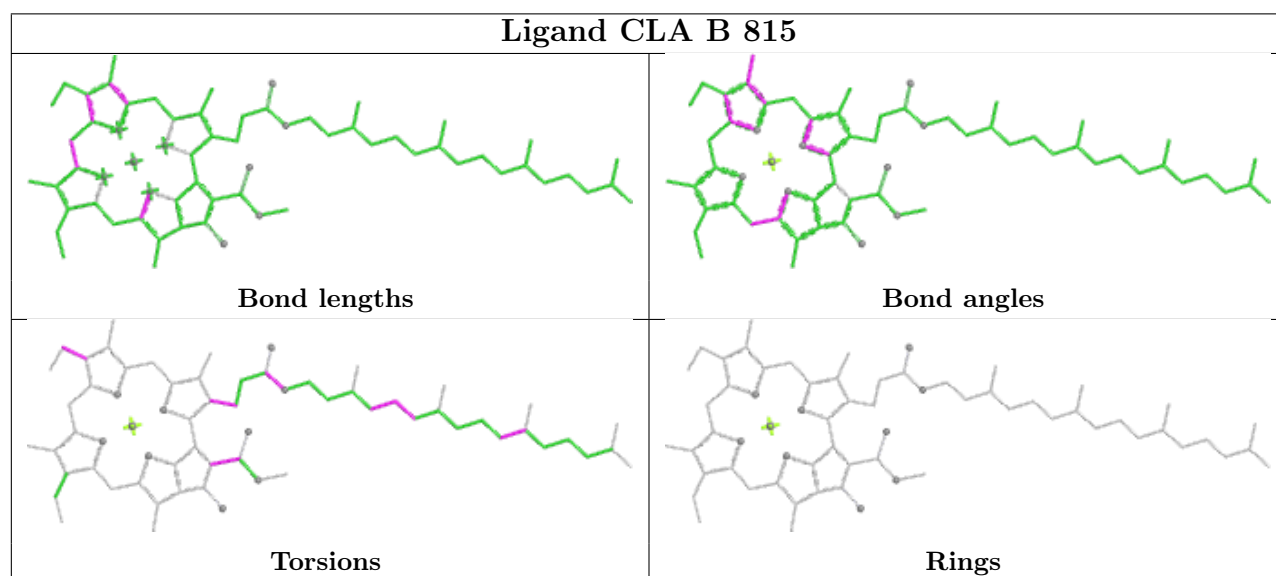
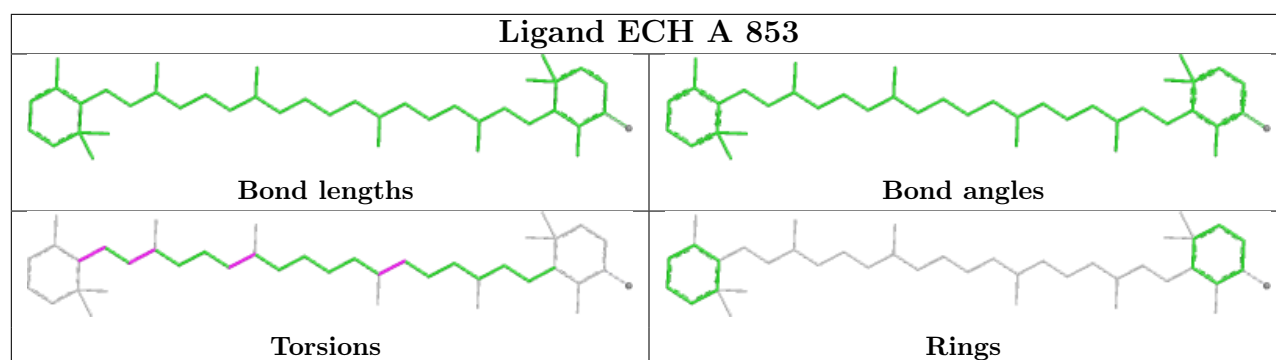


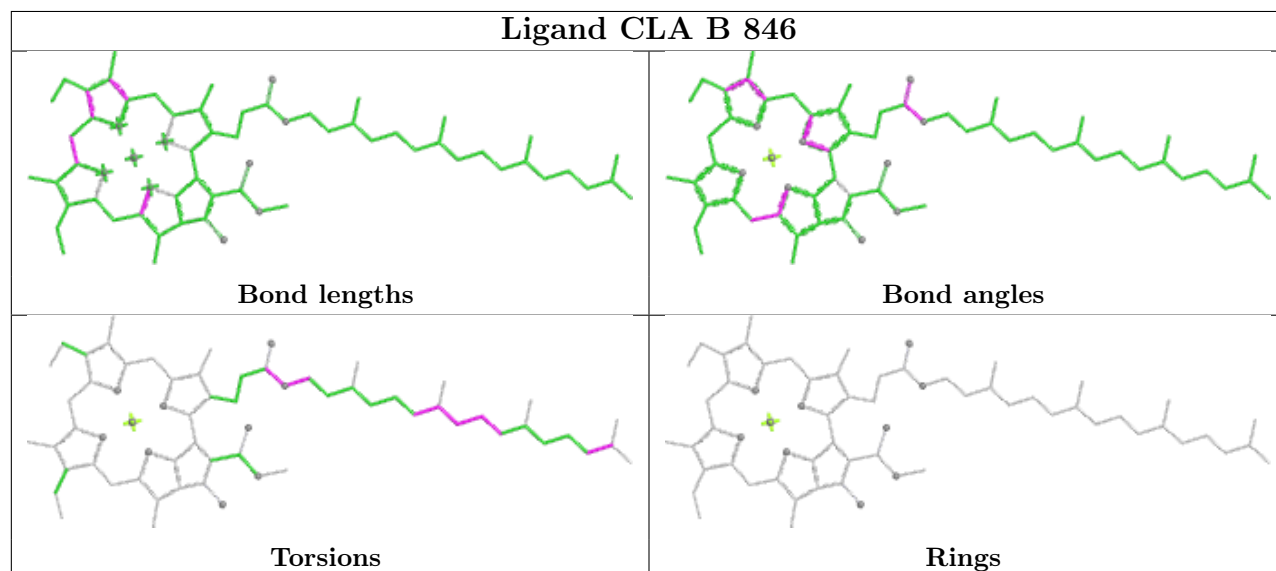
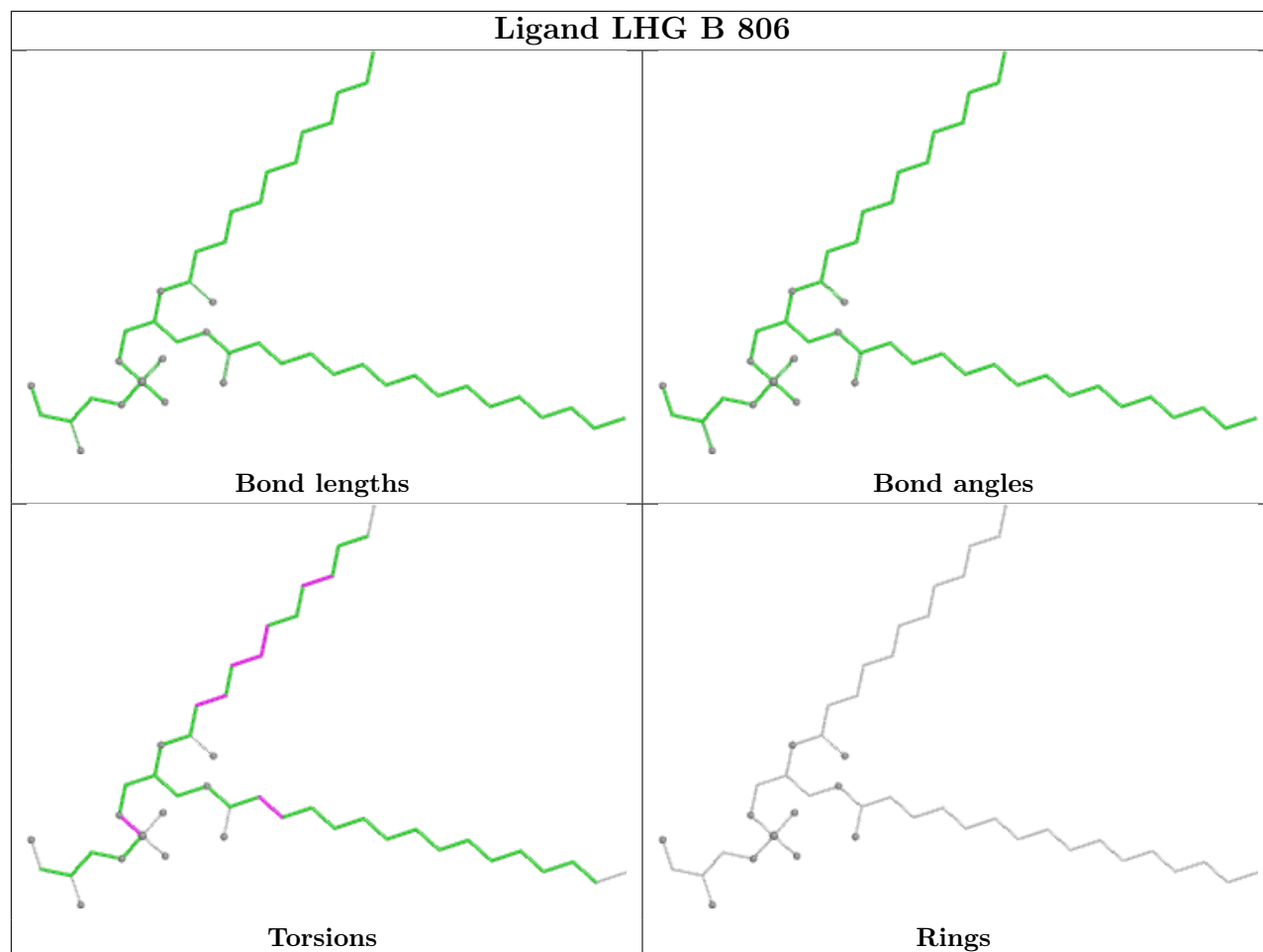
## Ligand CLA 2 410

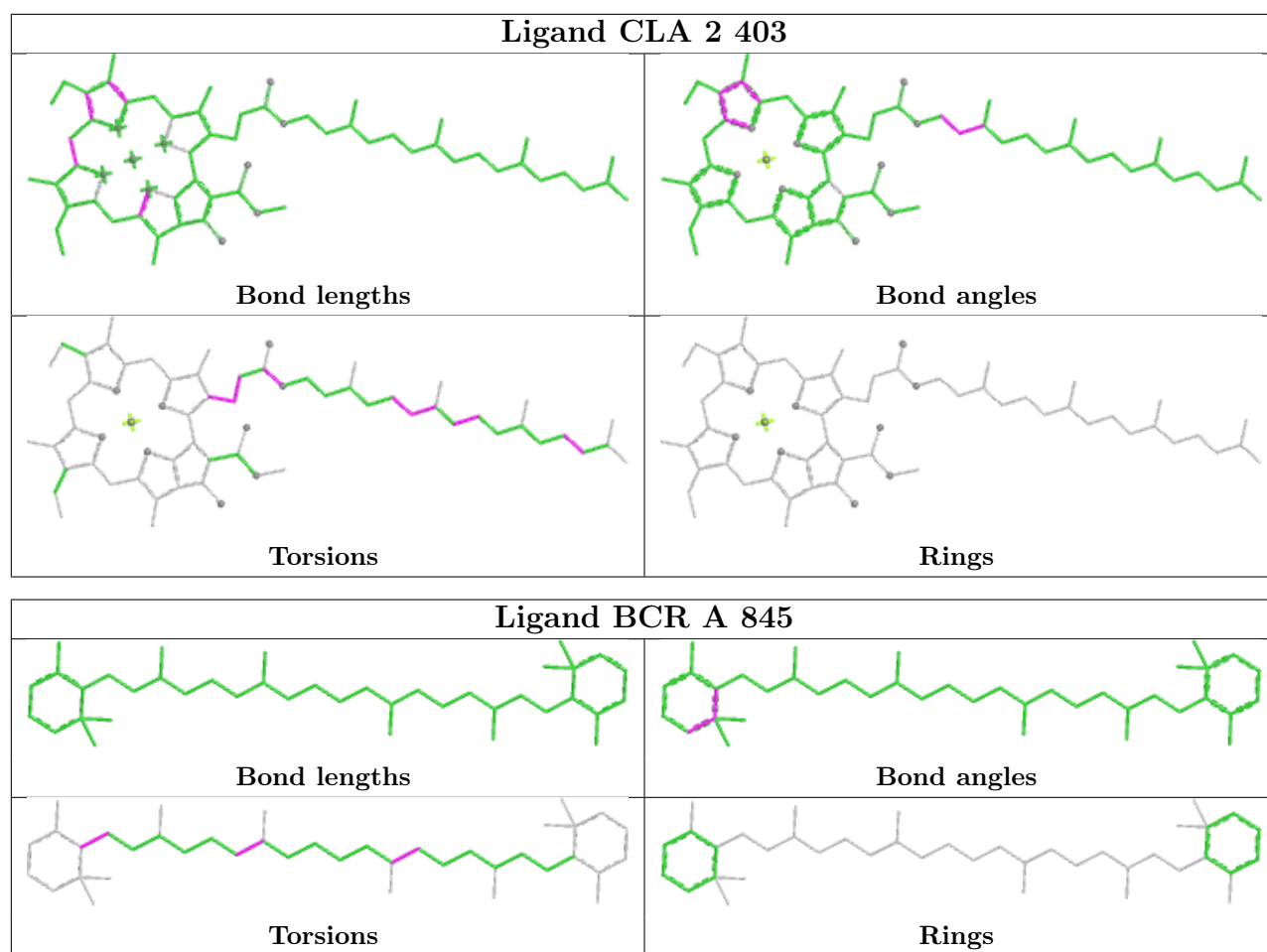


## Ligand CLA 7 512

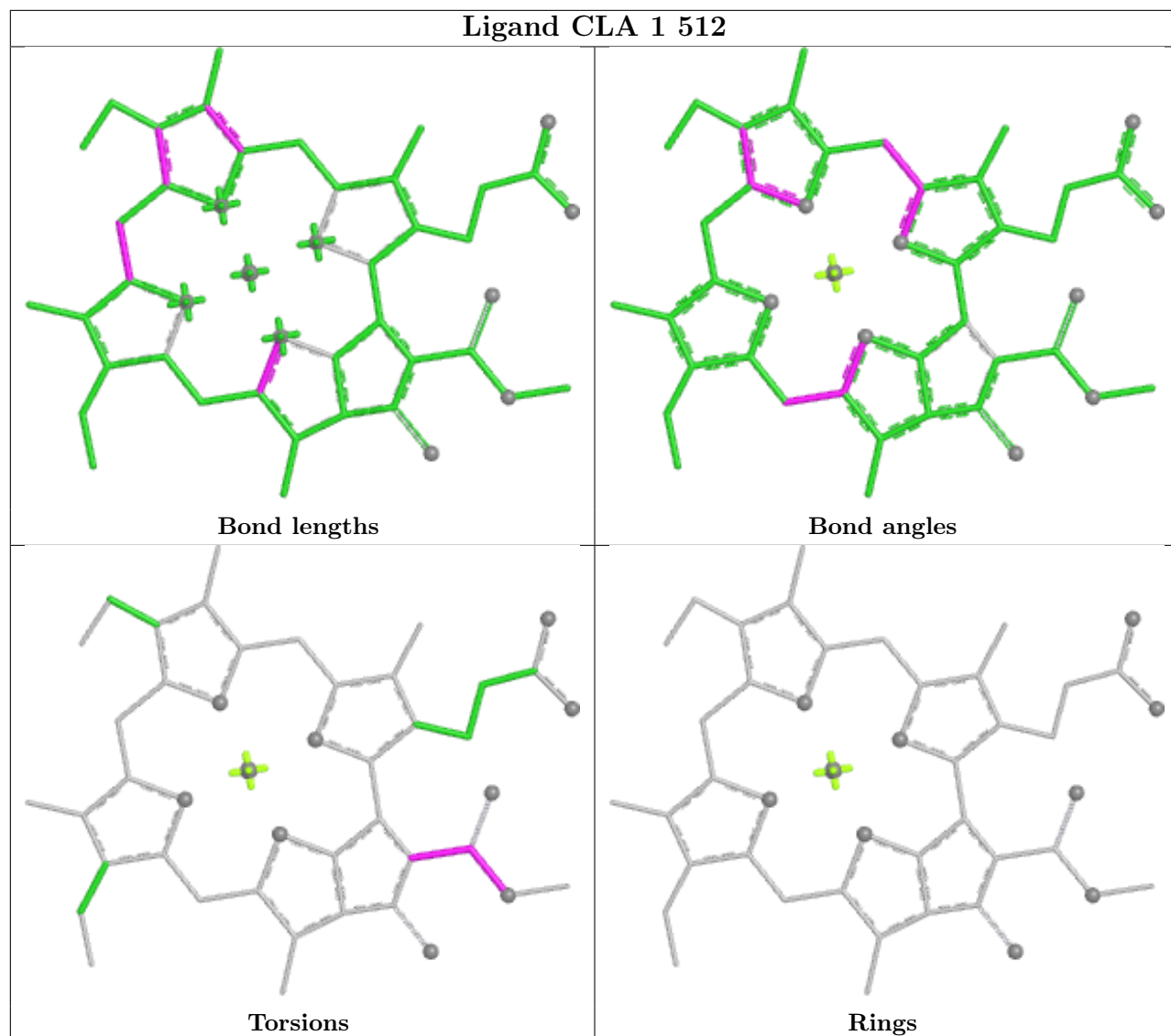




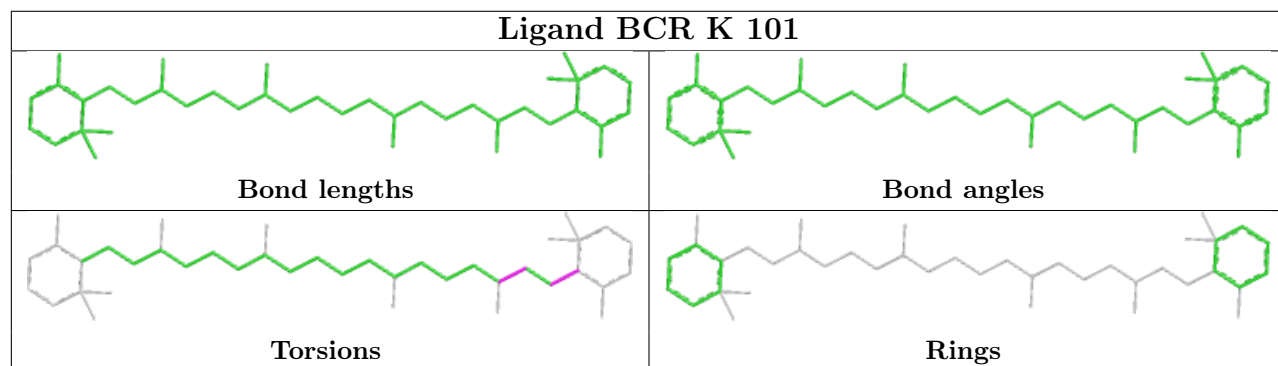


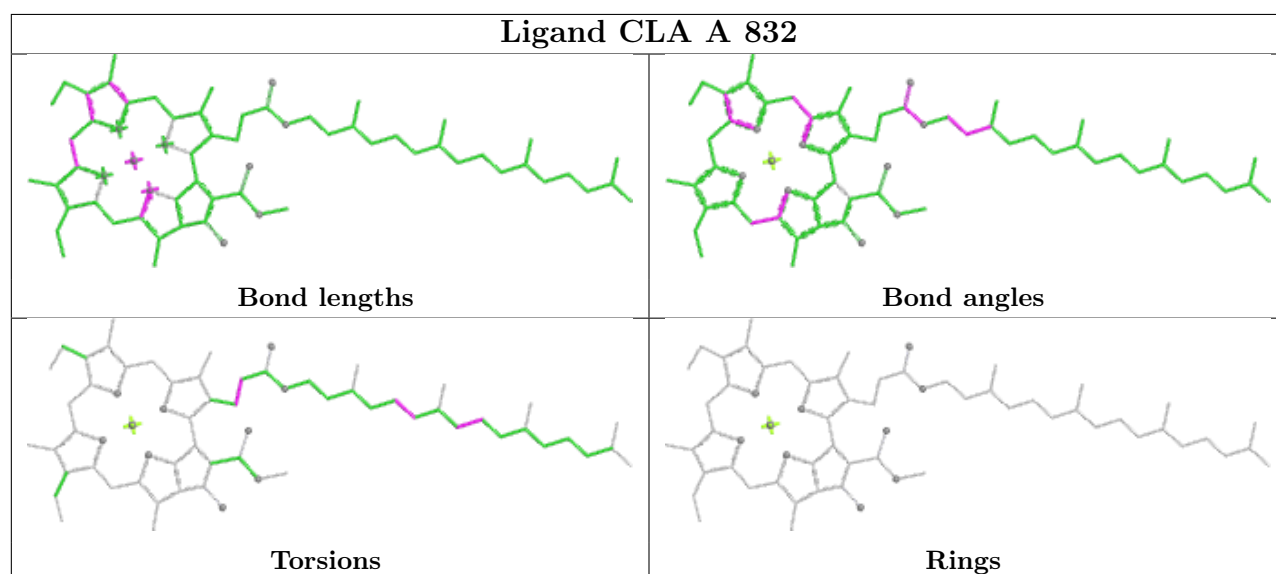
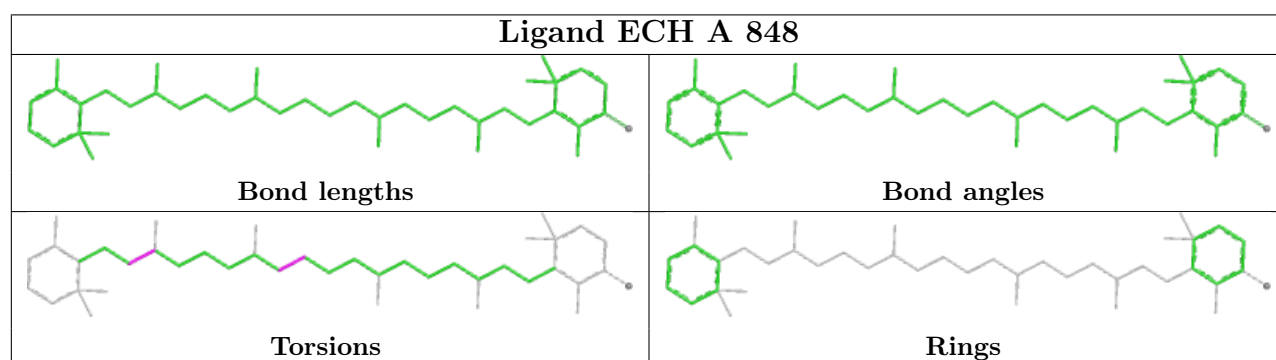
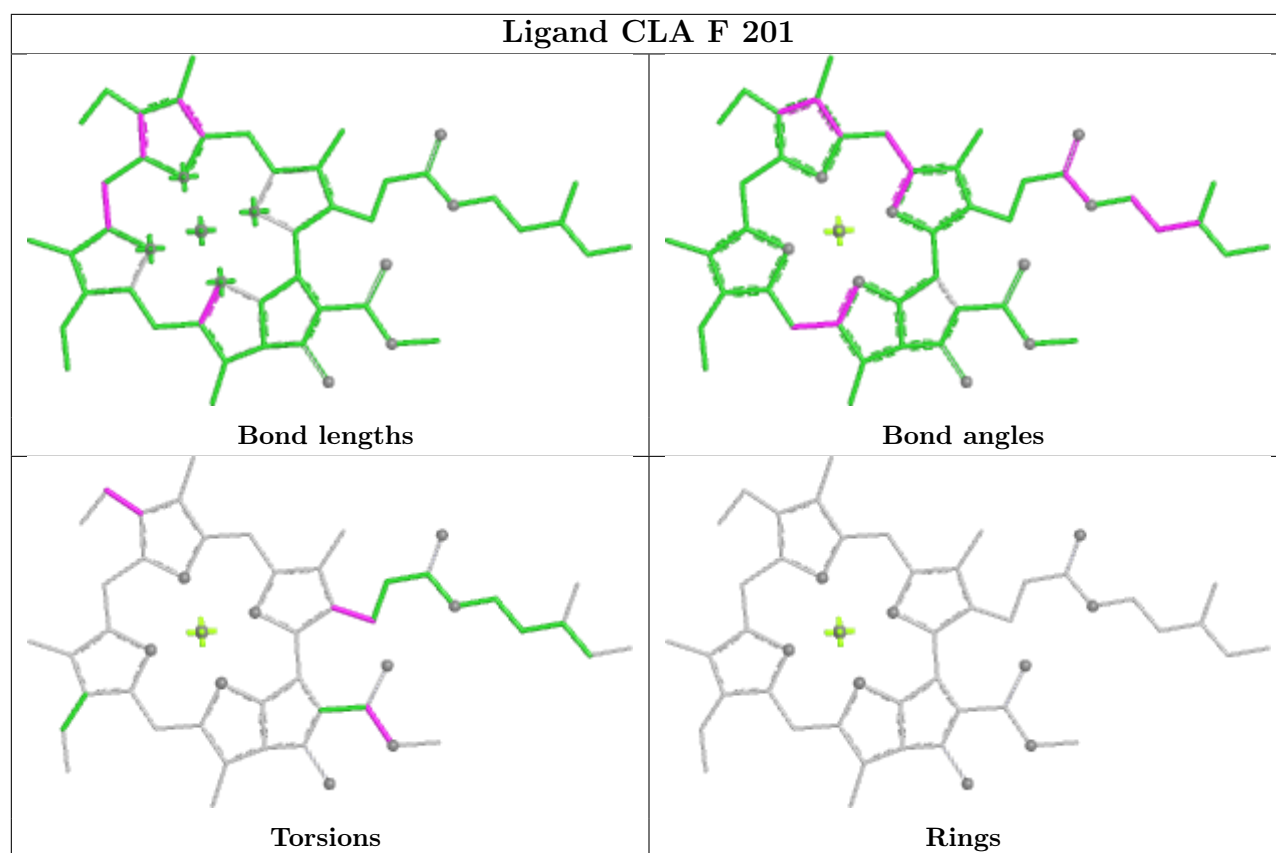


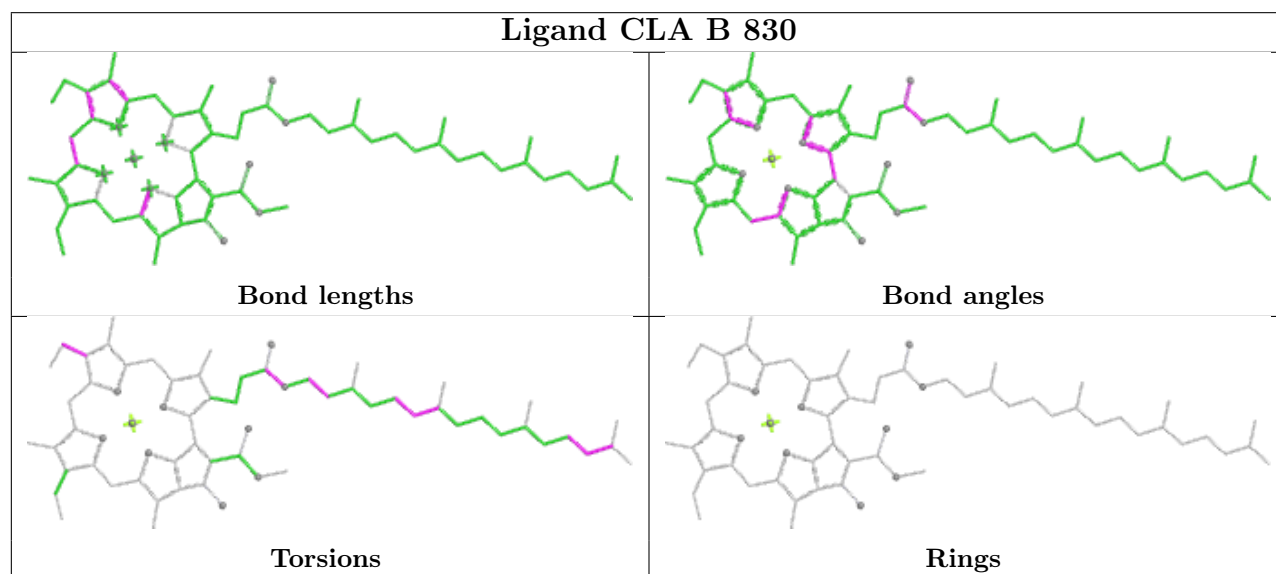
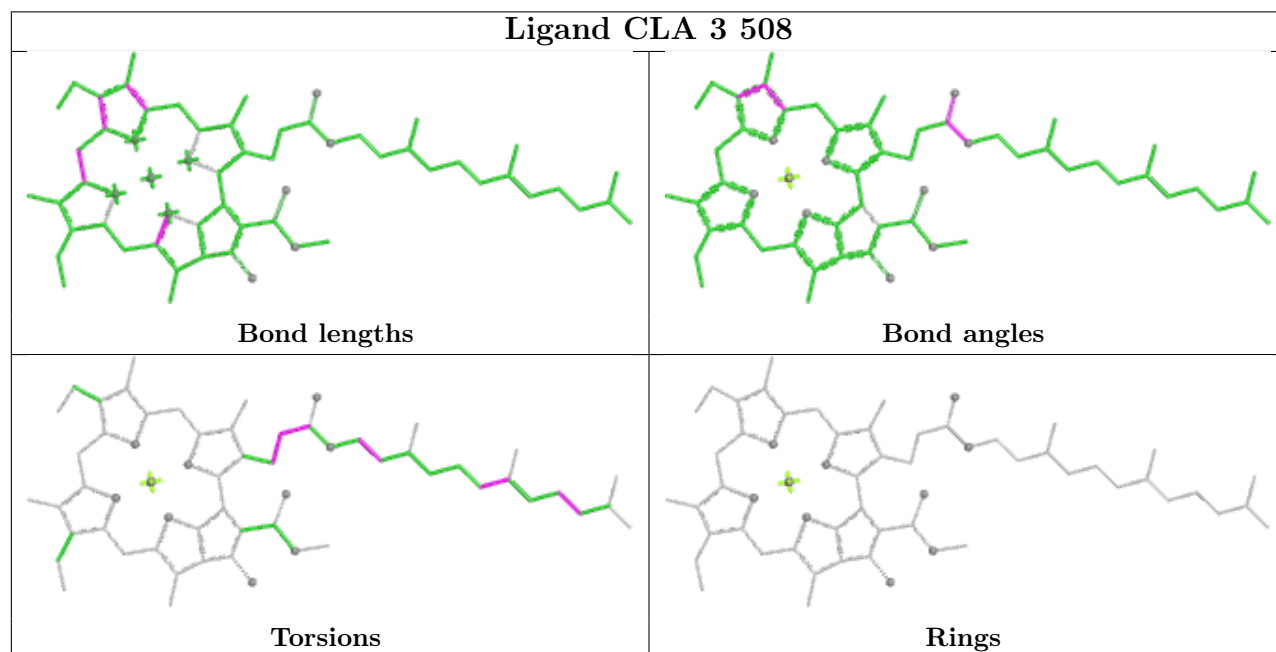
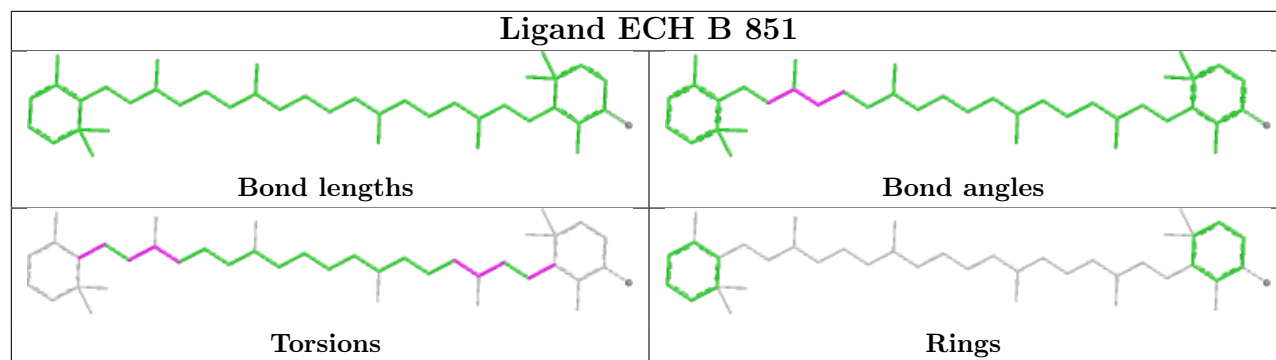
## Ligand CLA 1 512

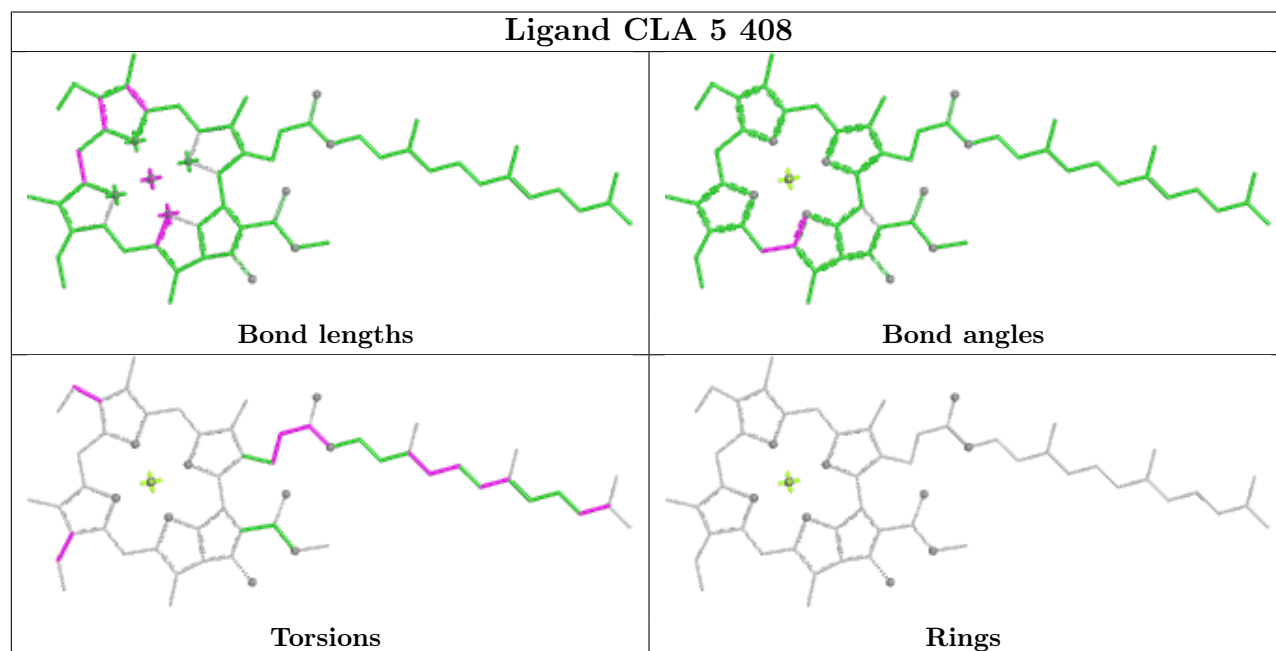
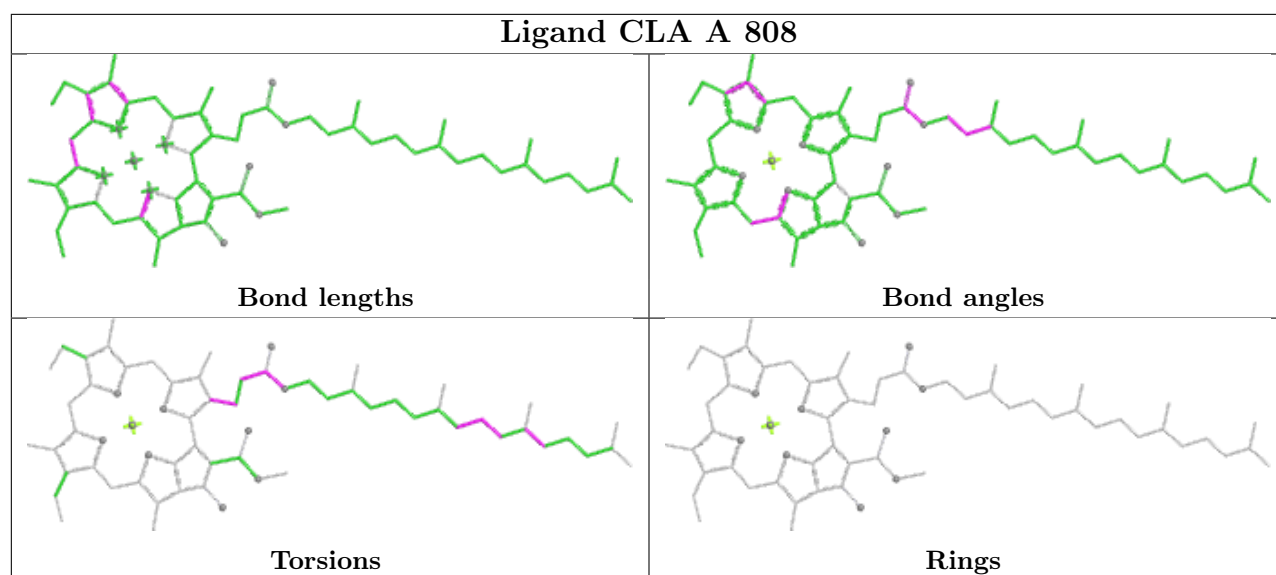


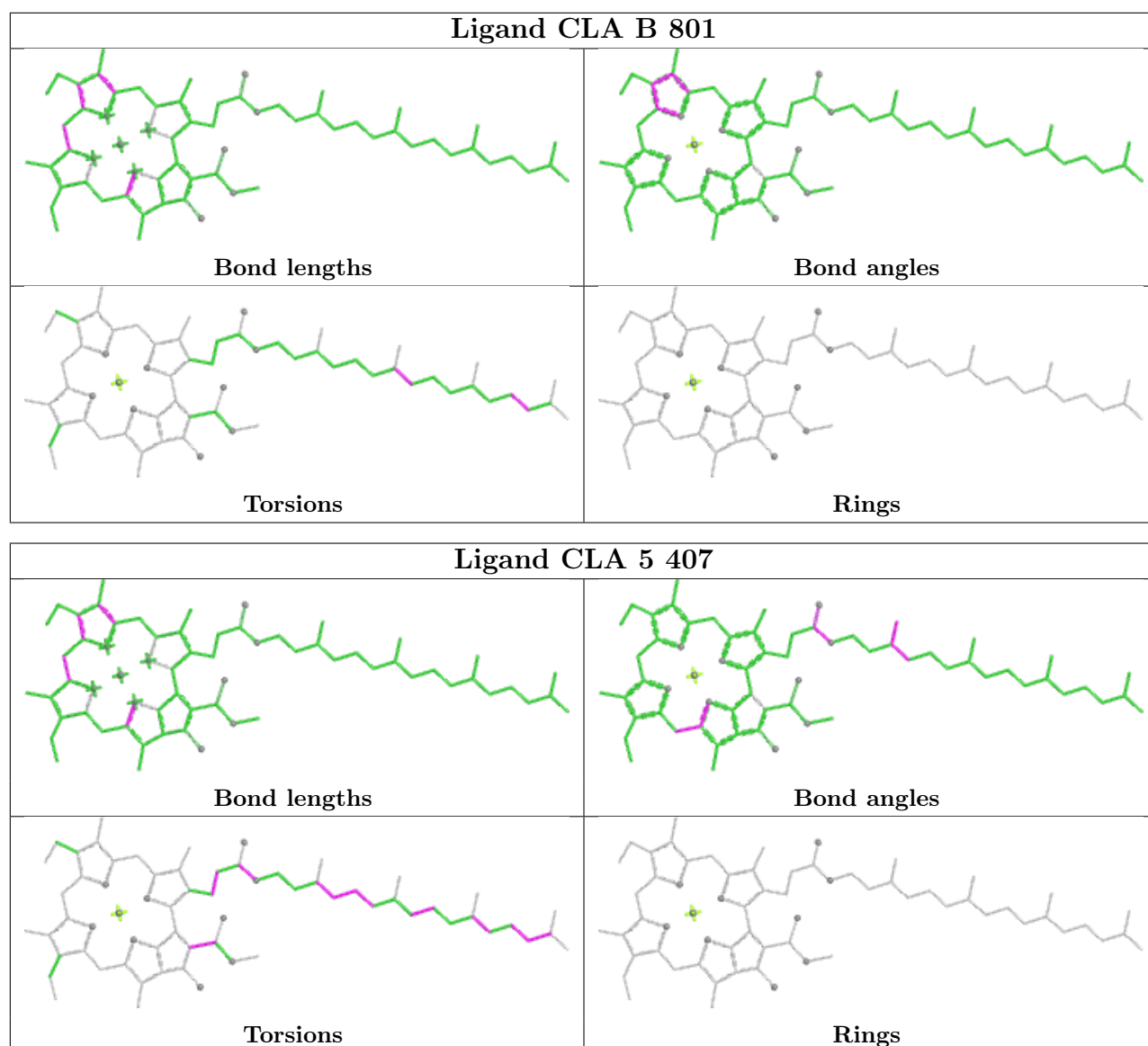
## Ligand BCR K 101



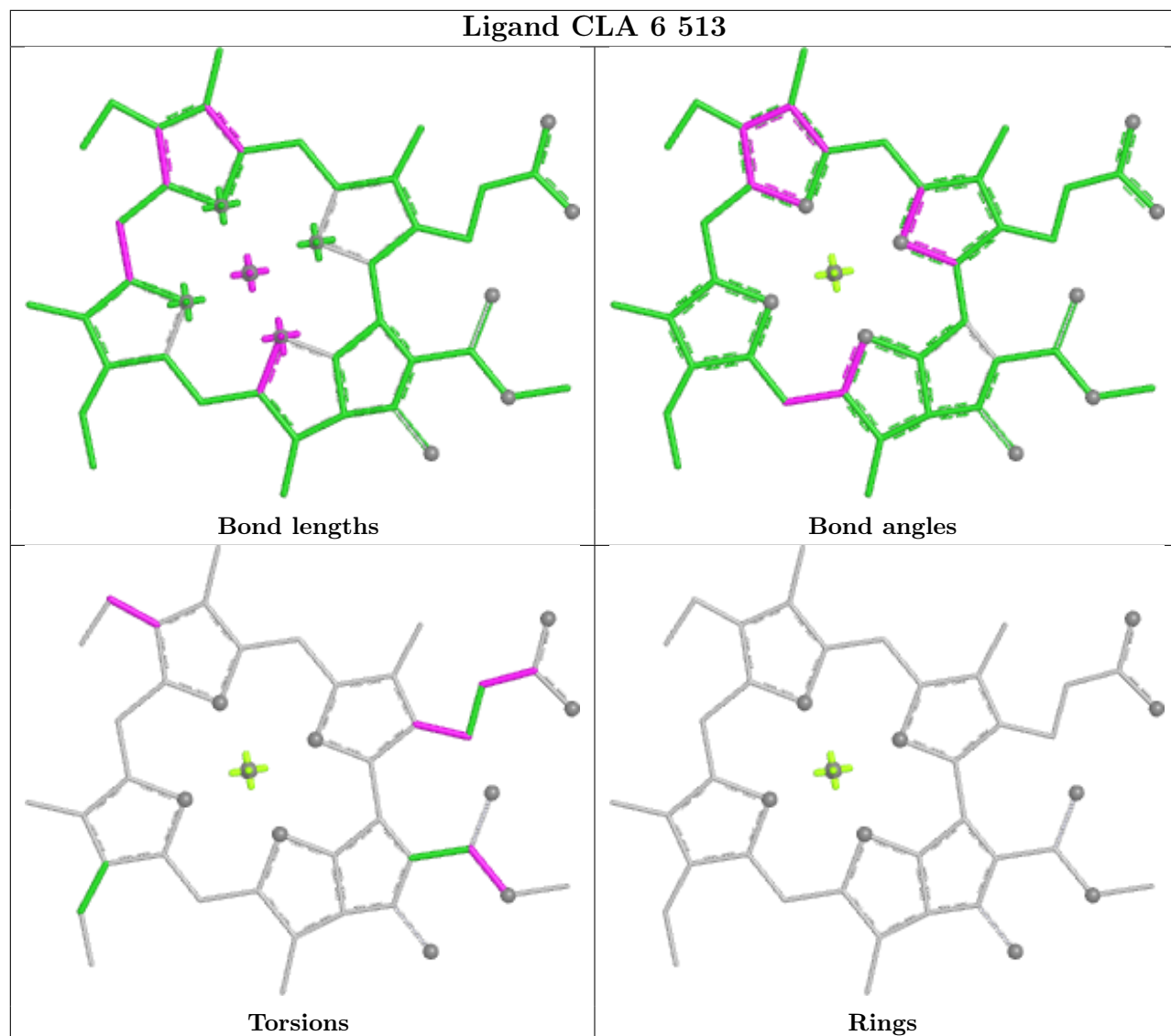




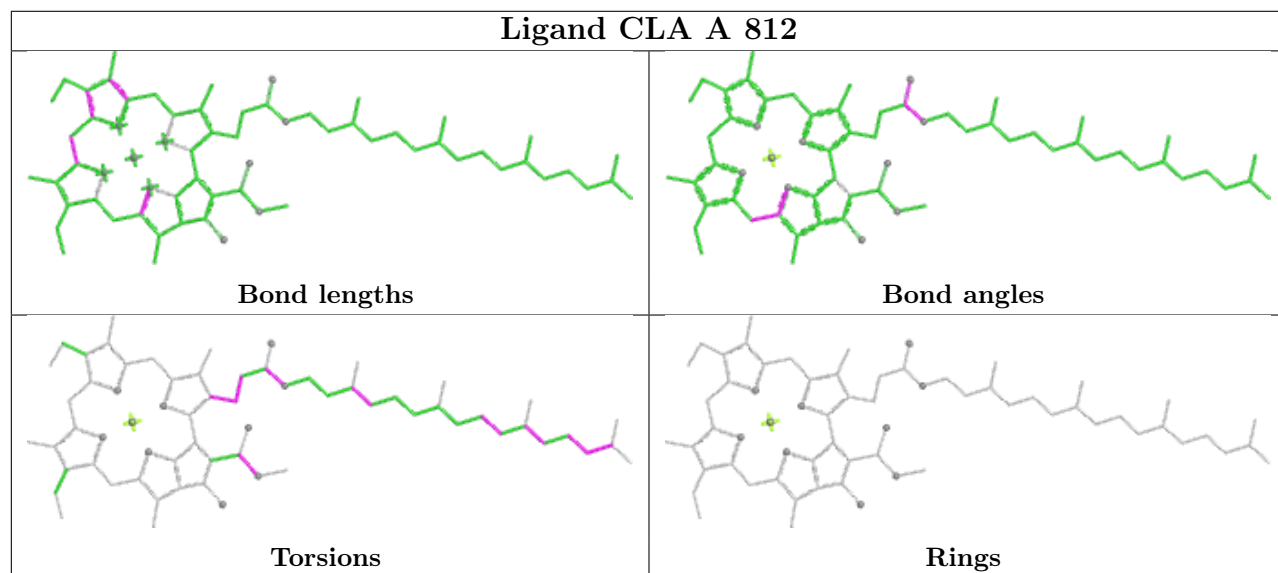


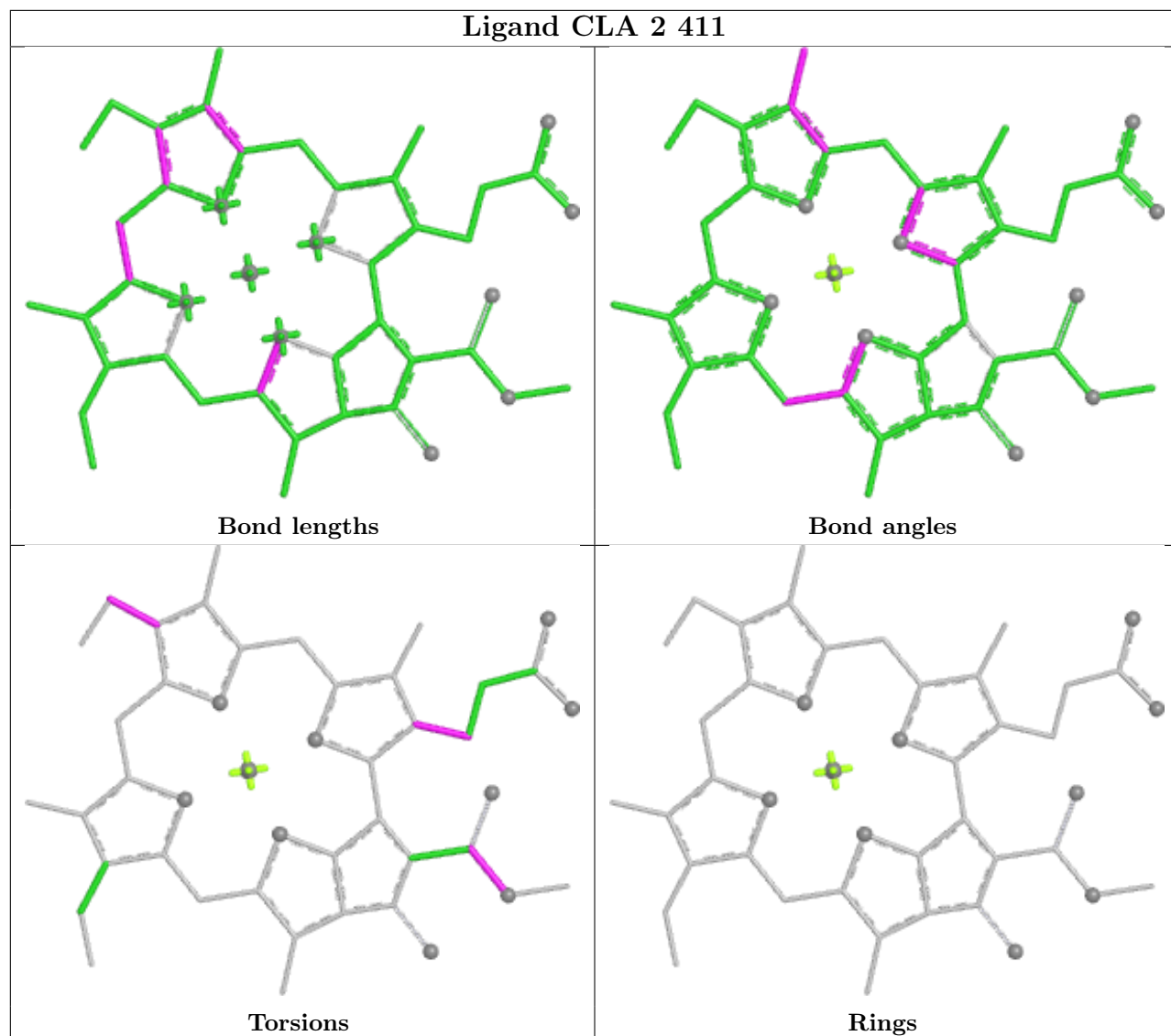


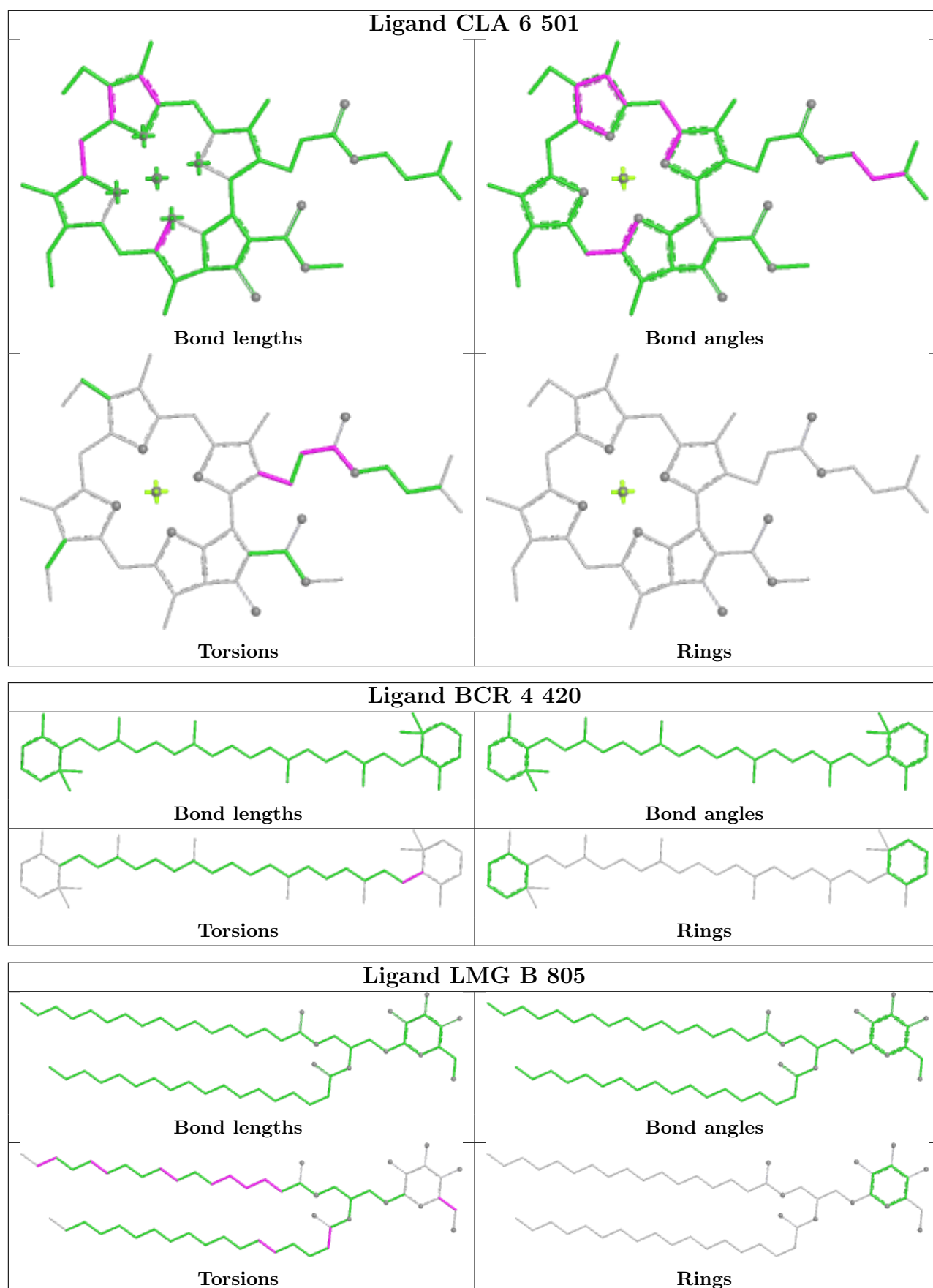
## Ligand CLA 6 513

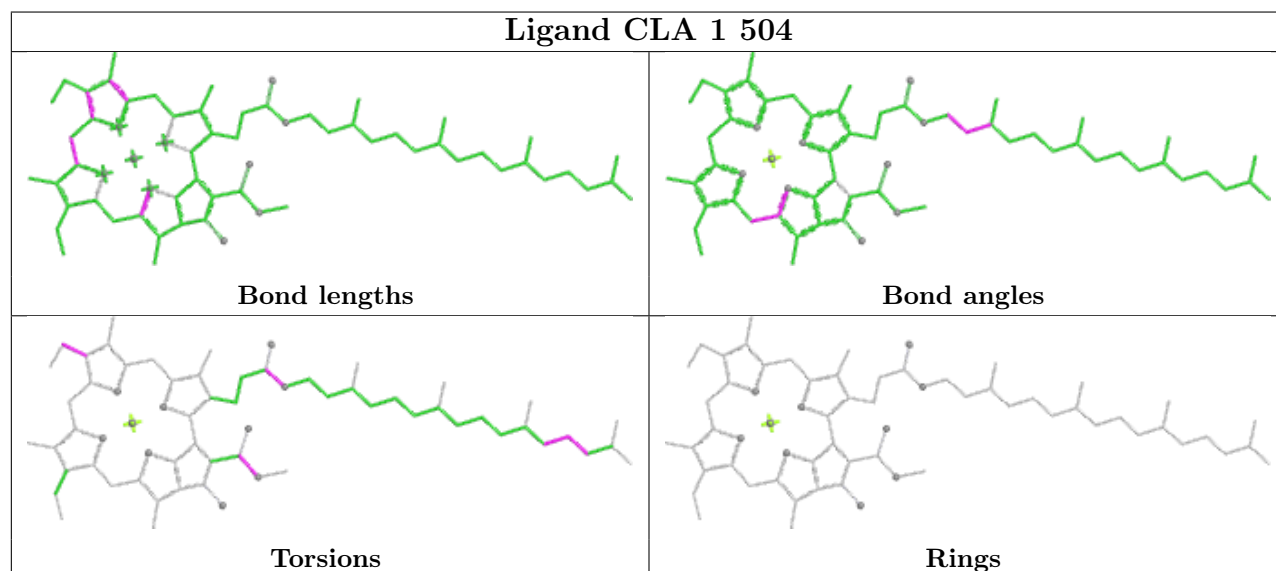
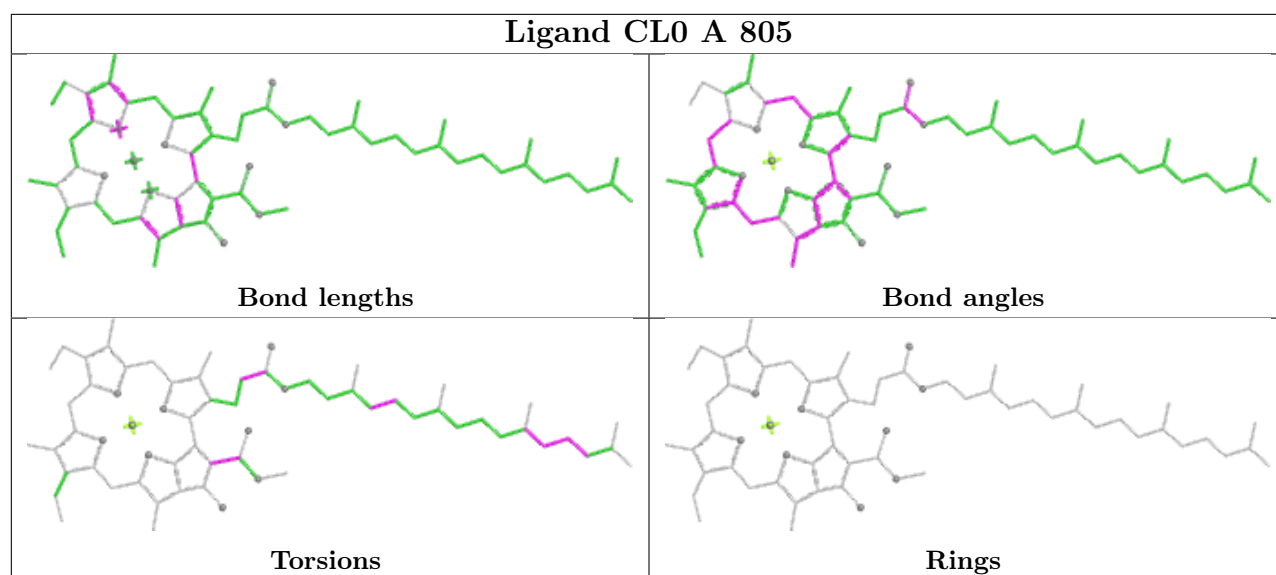


## Ligand CLA A 812

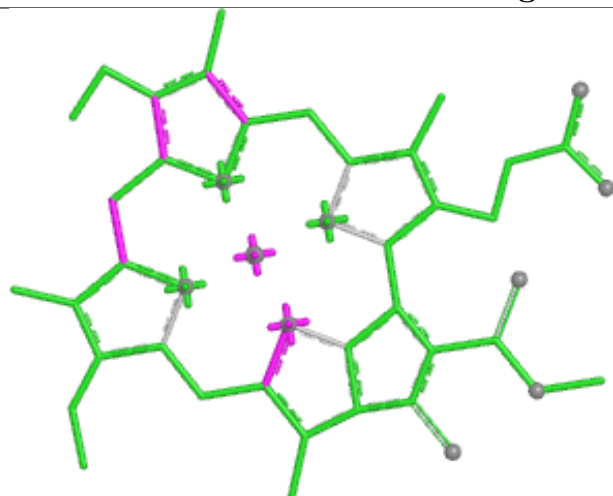




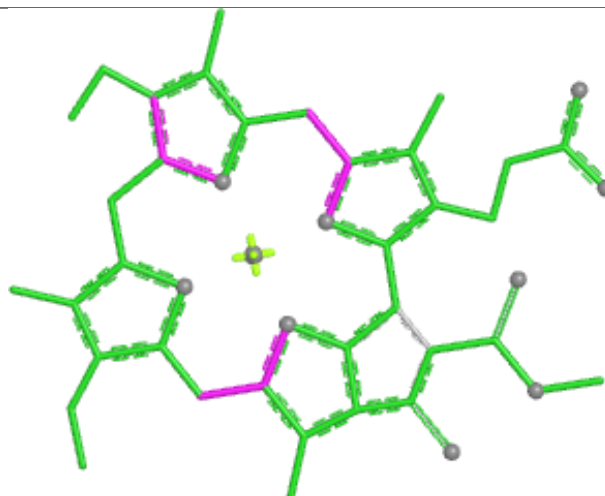




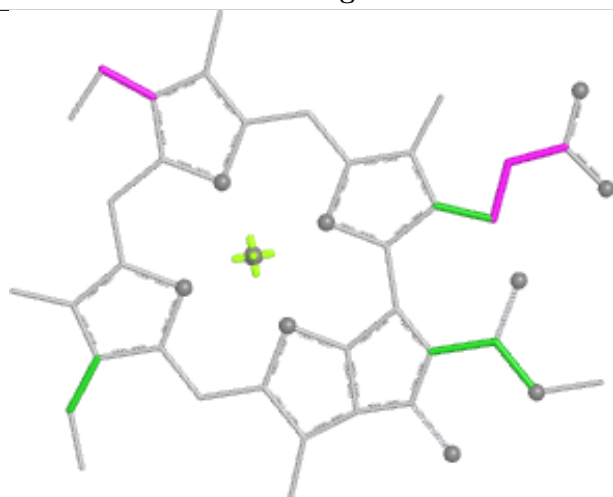
## Ligand CLA 2 402



Bond lengths



Bond angles

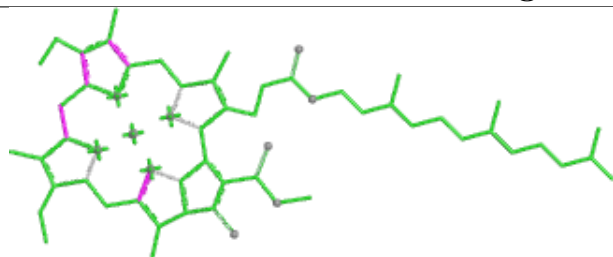


Torsions

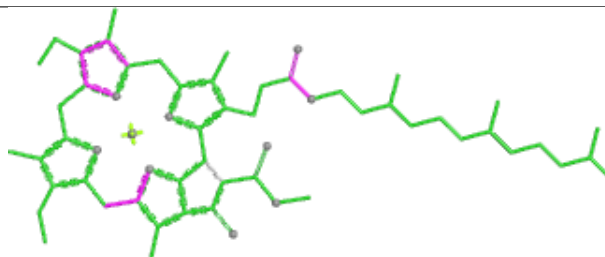


Rings

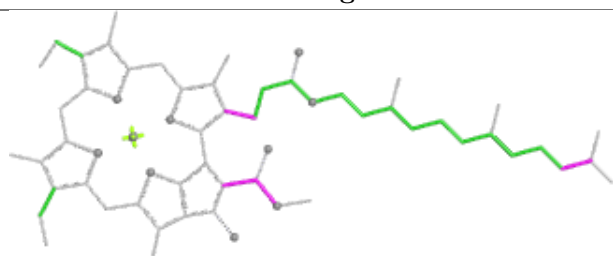
## Ligand CLA 6 506



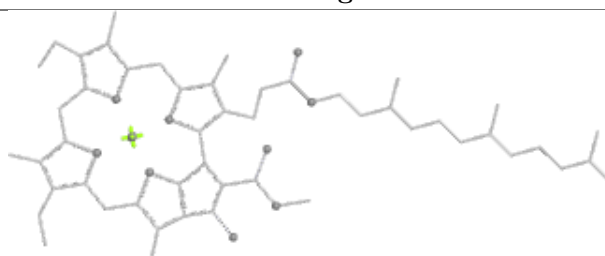
Bond lengths



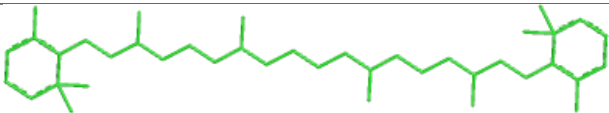
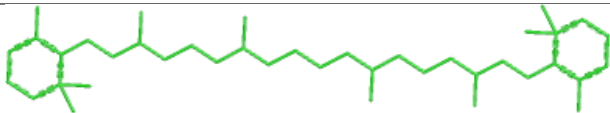
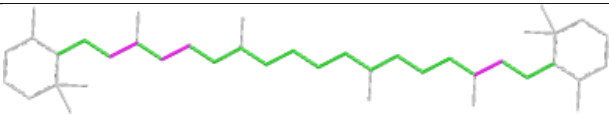
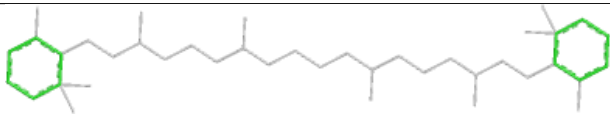
Bond angles



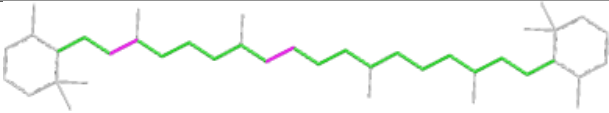
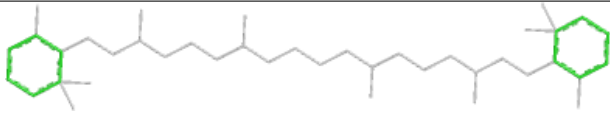


Torsions

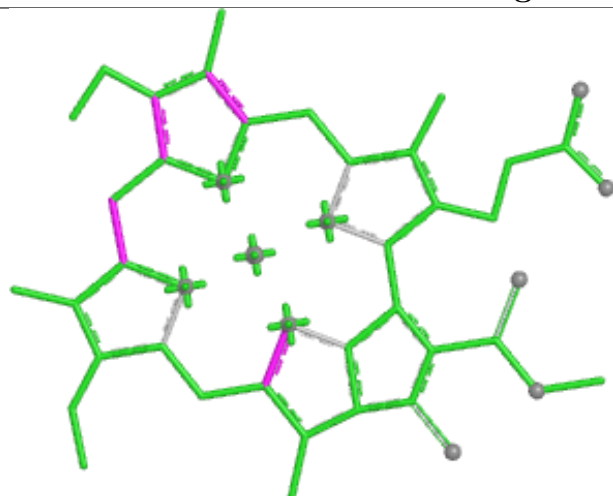


Rings

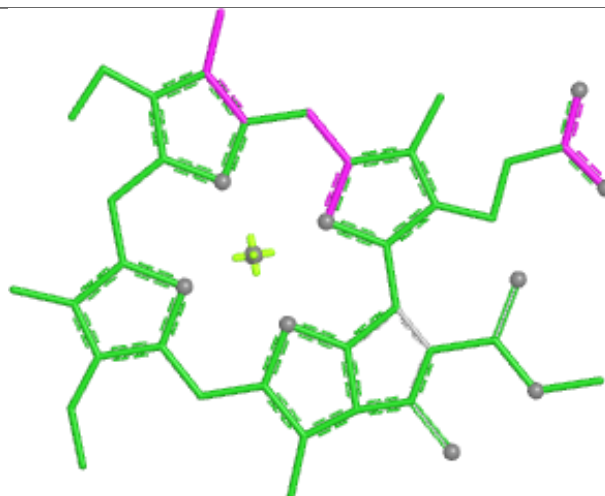
Ligand BCR 1 523	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR 5 423	
 Bond lengths	 Bond angles
 Torsions	 Rings

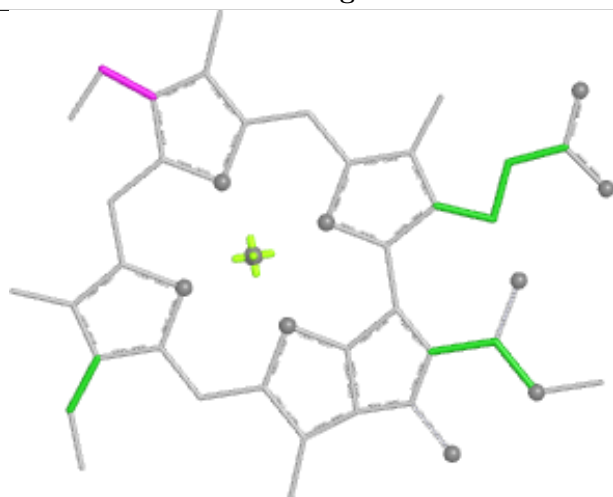
## Ligand CLA B 842



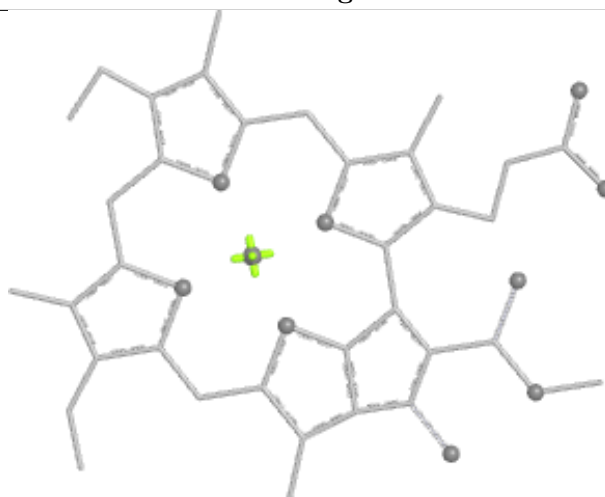
Bond lengths



Bond angles

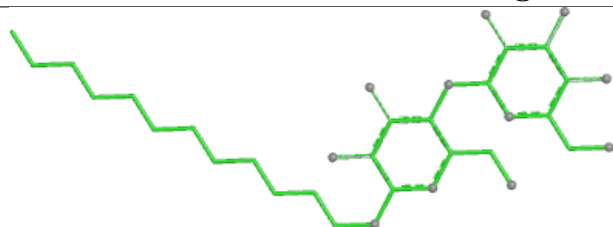


Torsions

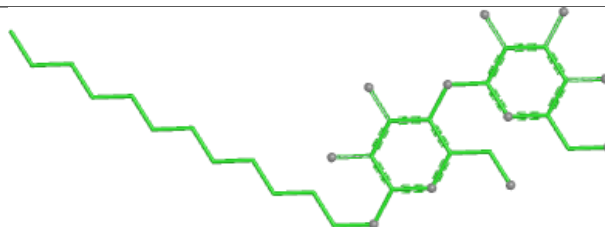


Rings

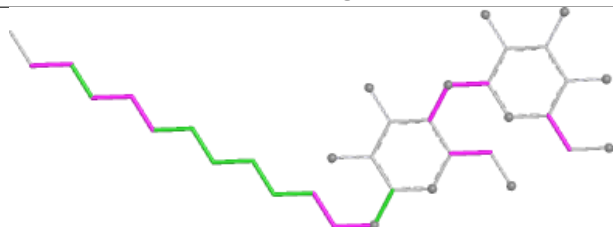
## Ligand LMU 1 527



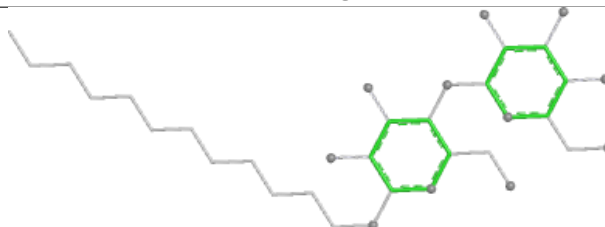
Bond lengths



Bond angles

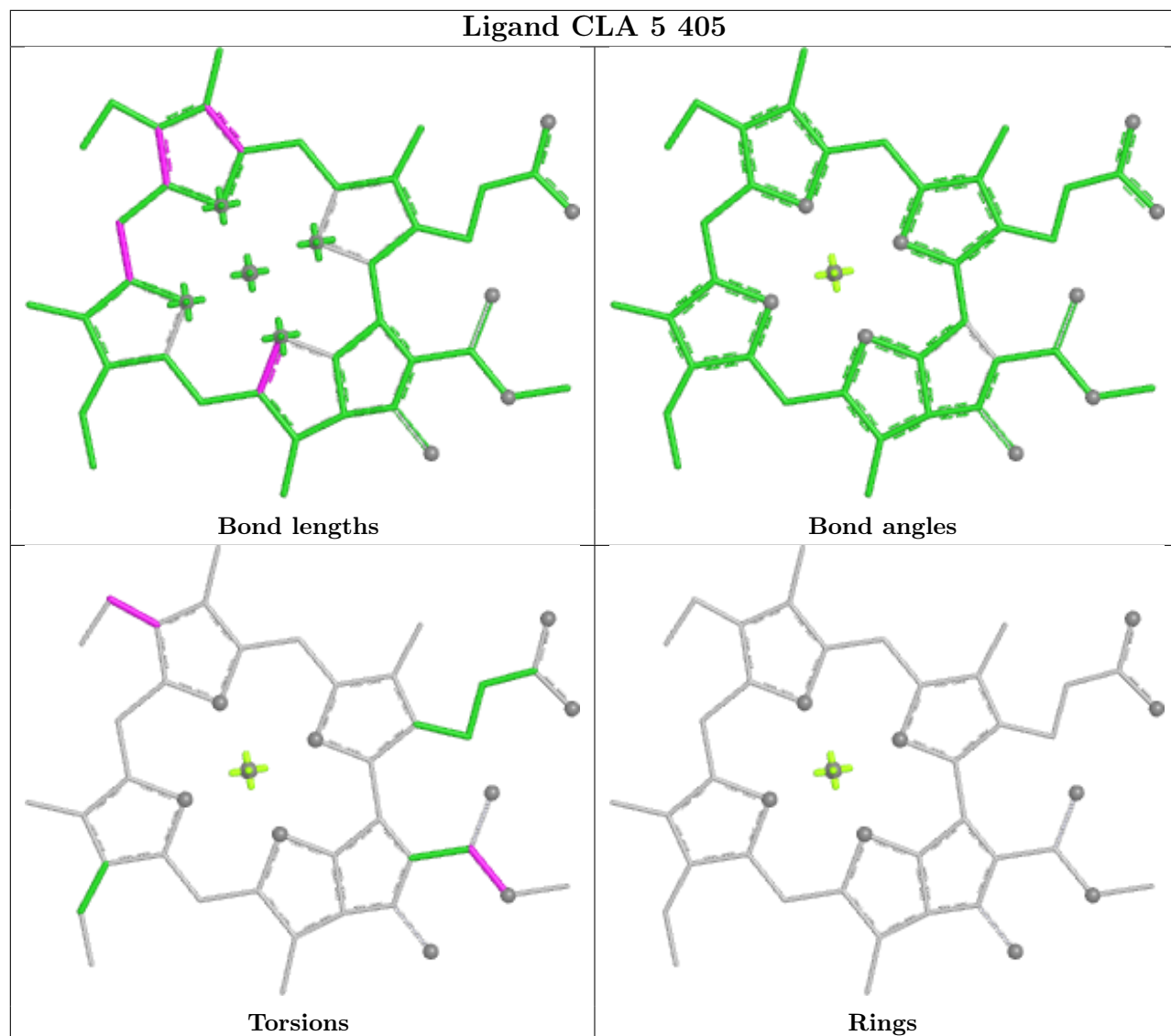


Torsions

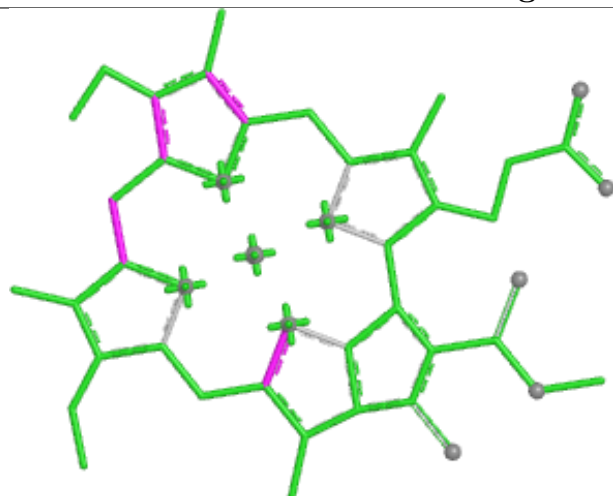


Rings

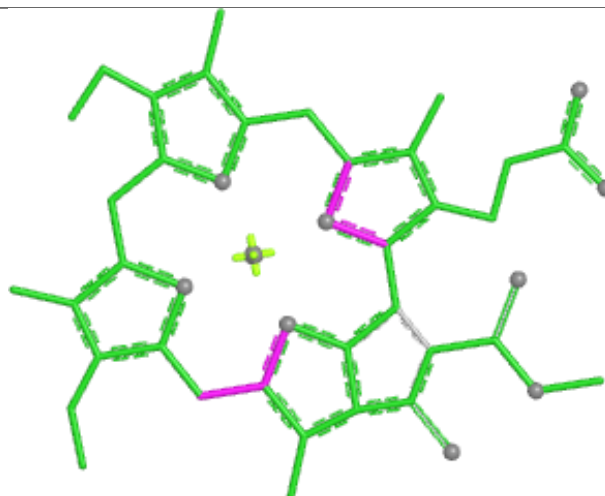
## Ligand CLA 5 405



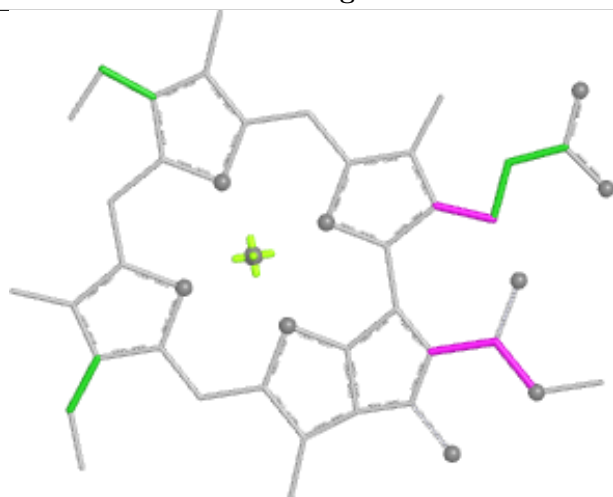
## Ligand CLA 5 414



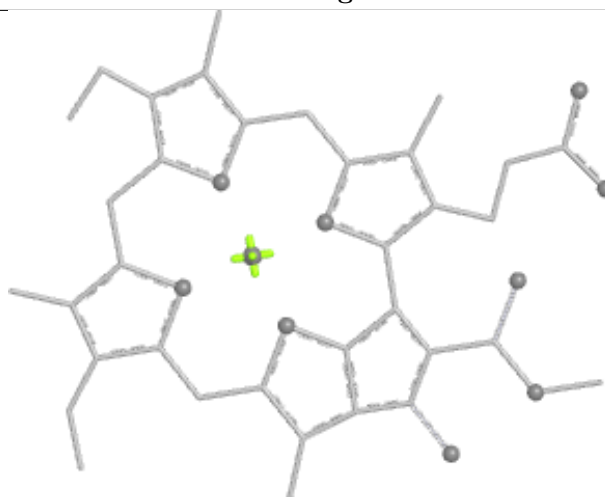
Bond lengths



Bond angles

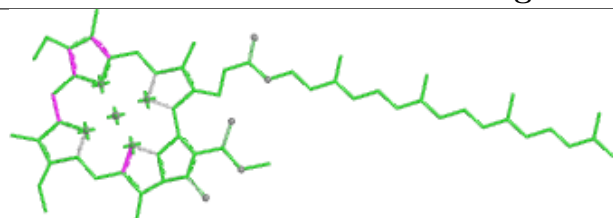


Torsions

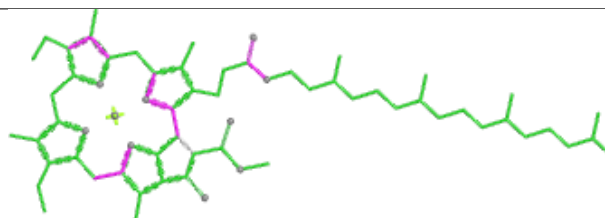


Rings

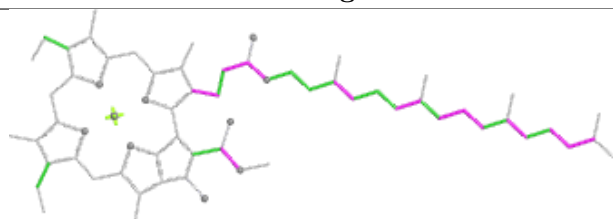
## Ligand CLA B 837



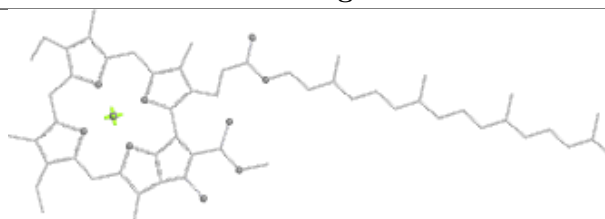
Bond lengths



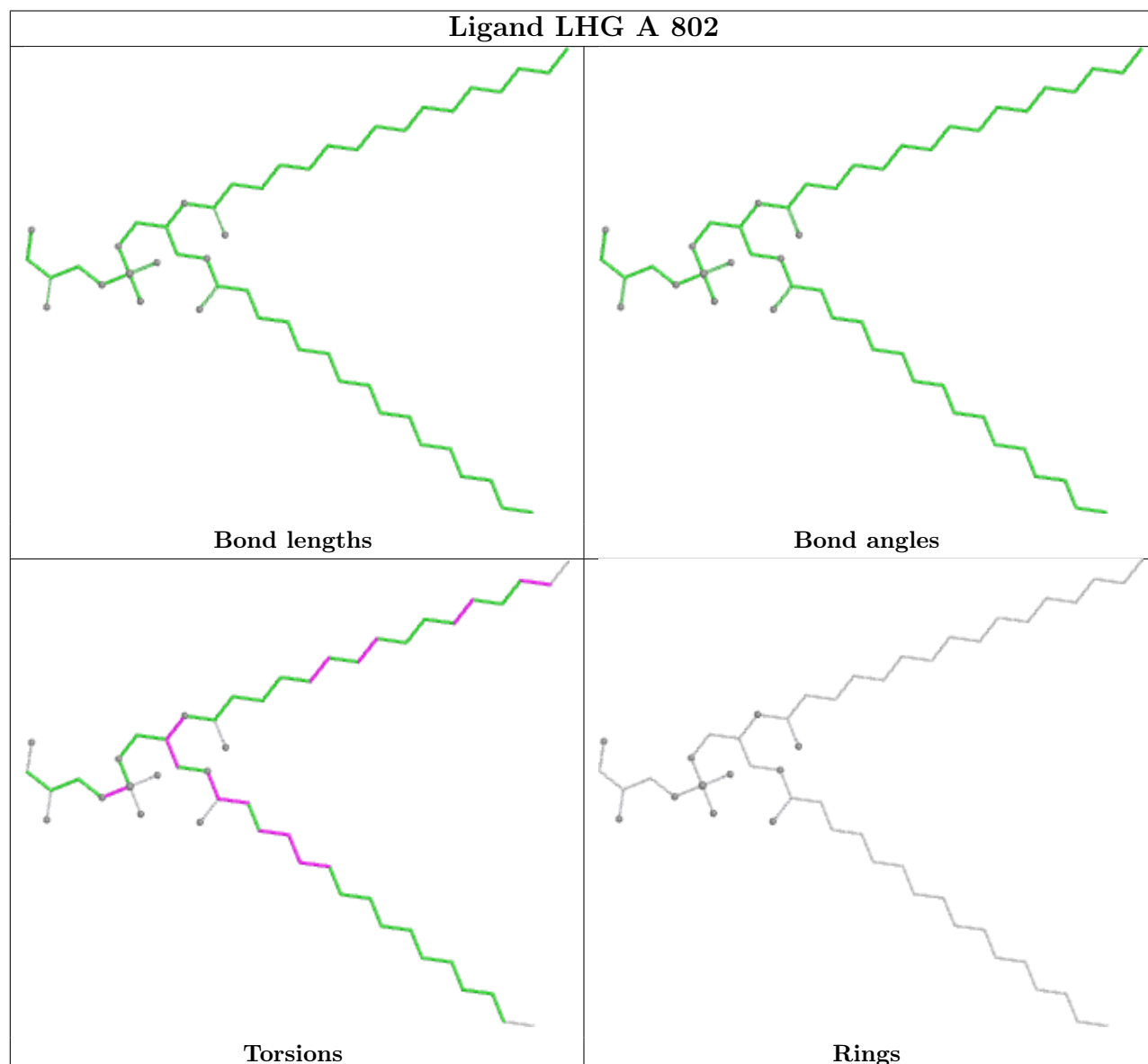
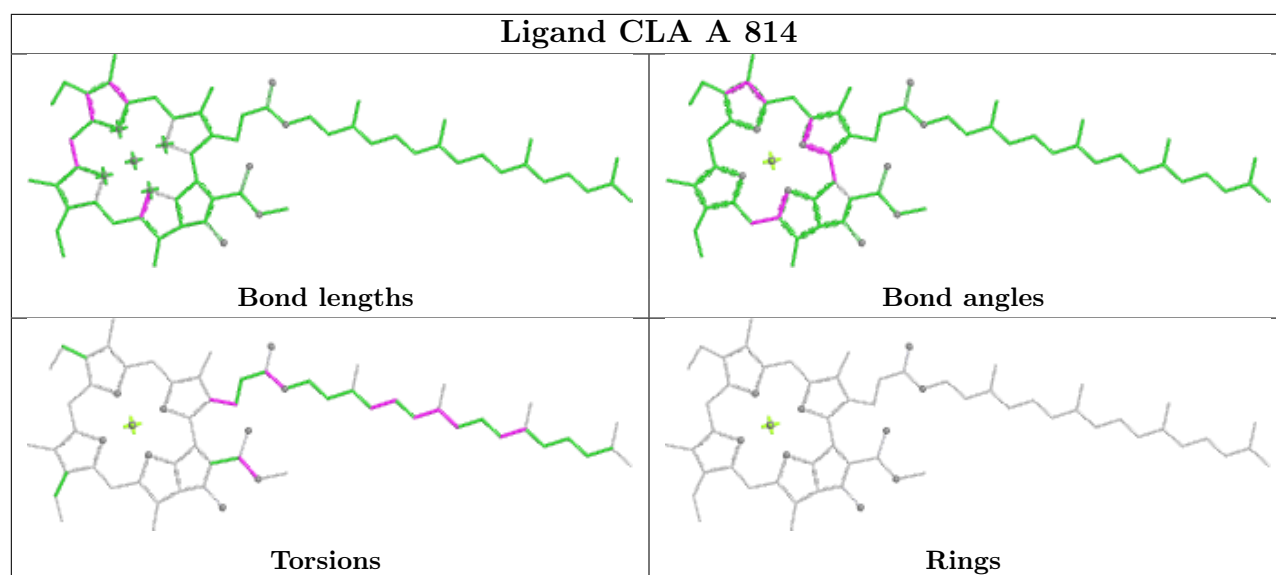
Bond angles



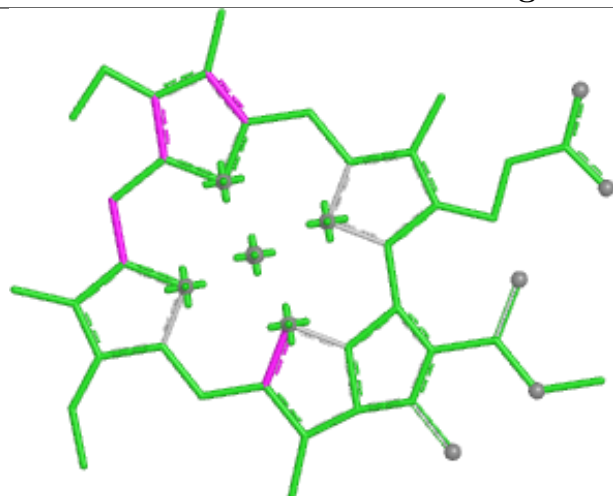
Torsions



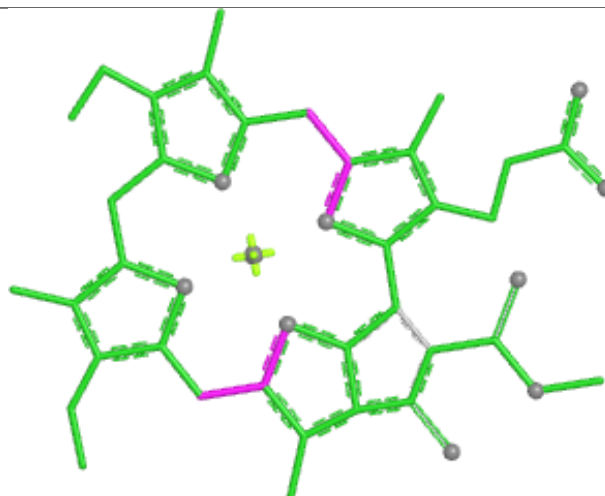
Rings



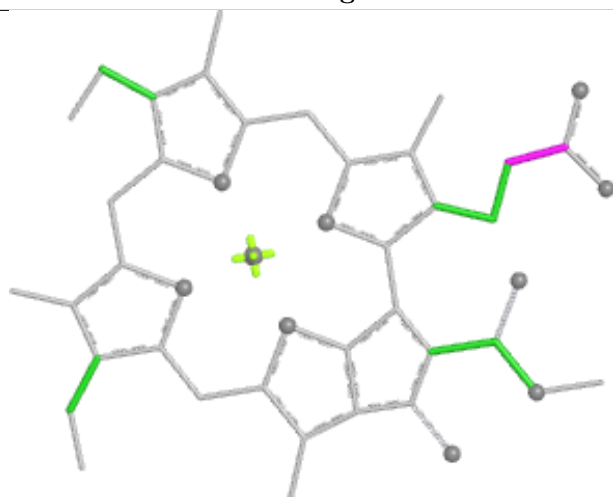
## Ligand CLA 5 419



Bond lengths



Bond angles

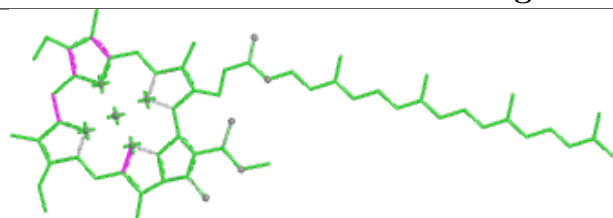


Torsions

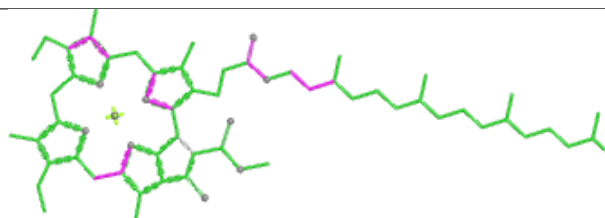


Rings

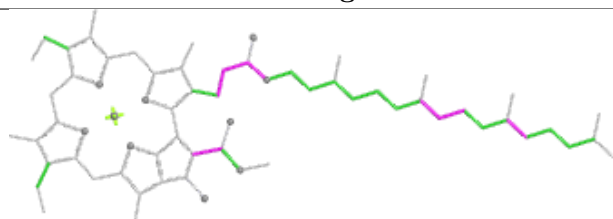
## Ligand CLA B 836



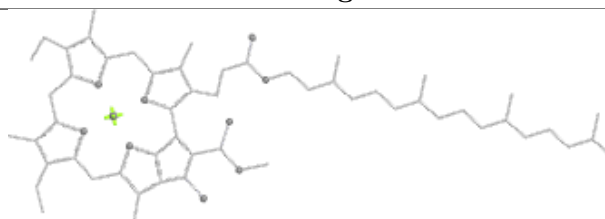
Bond lengths



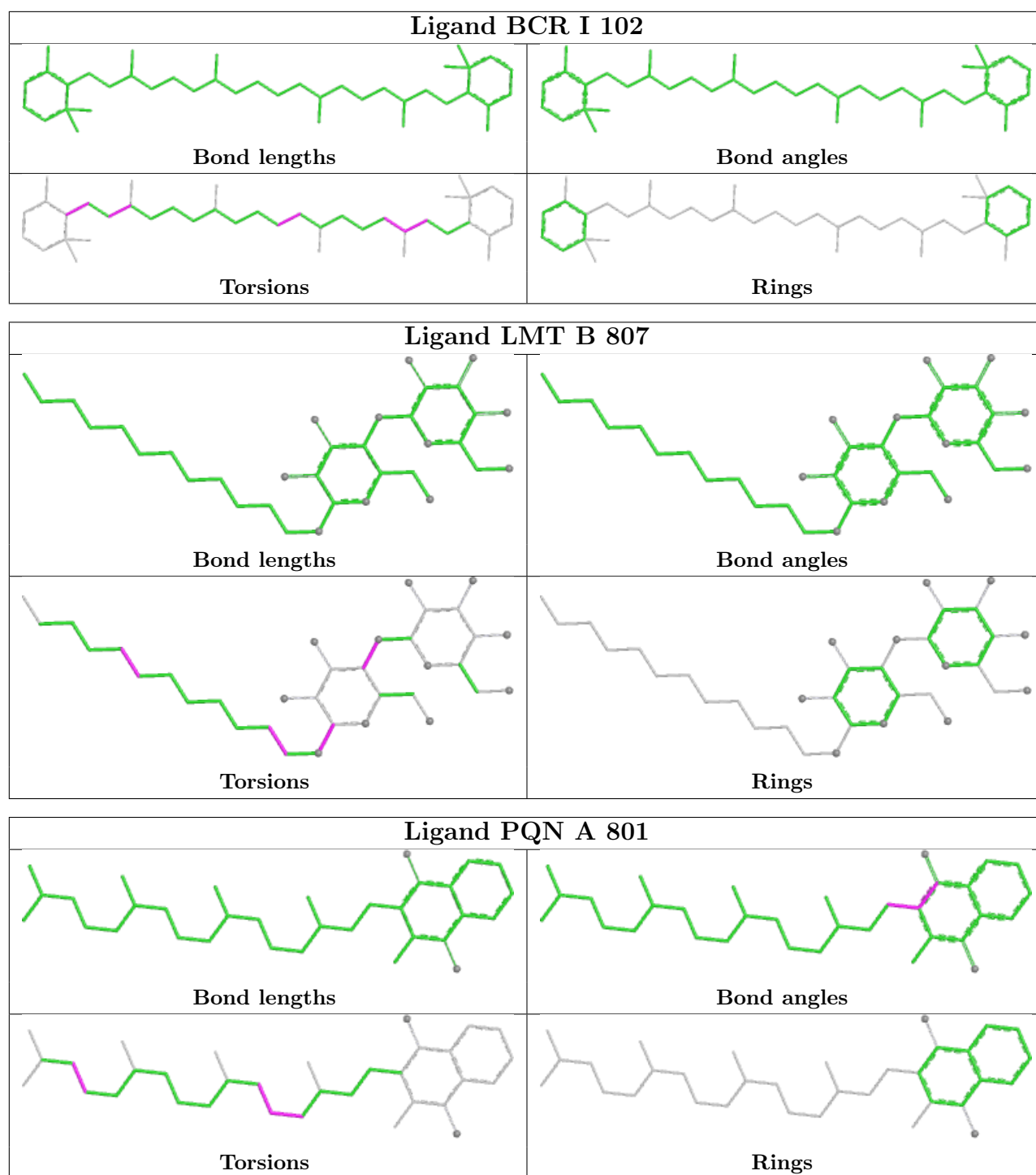
Bond angles

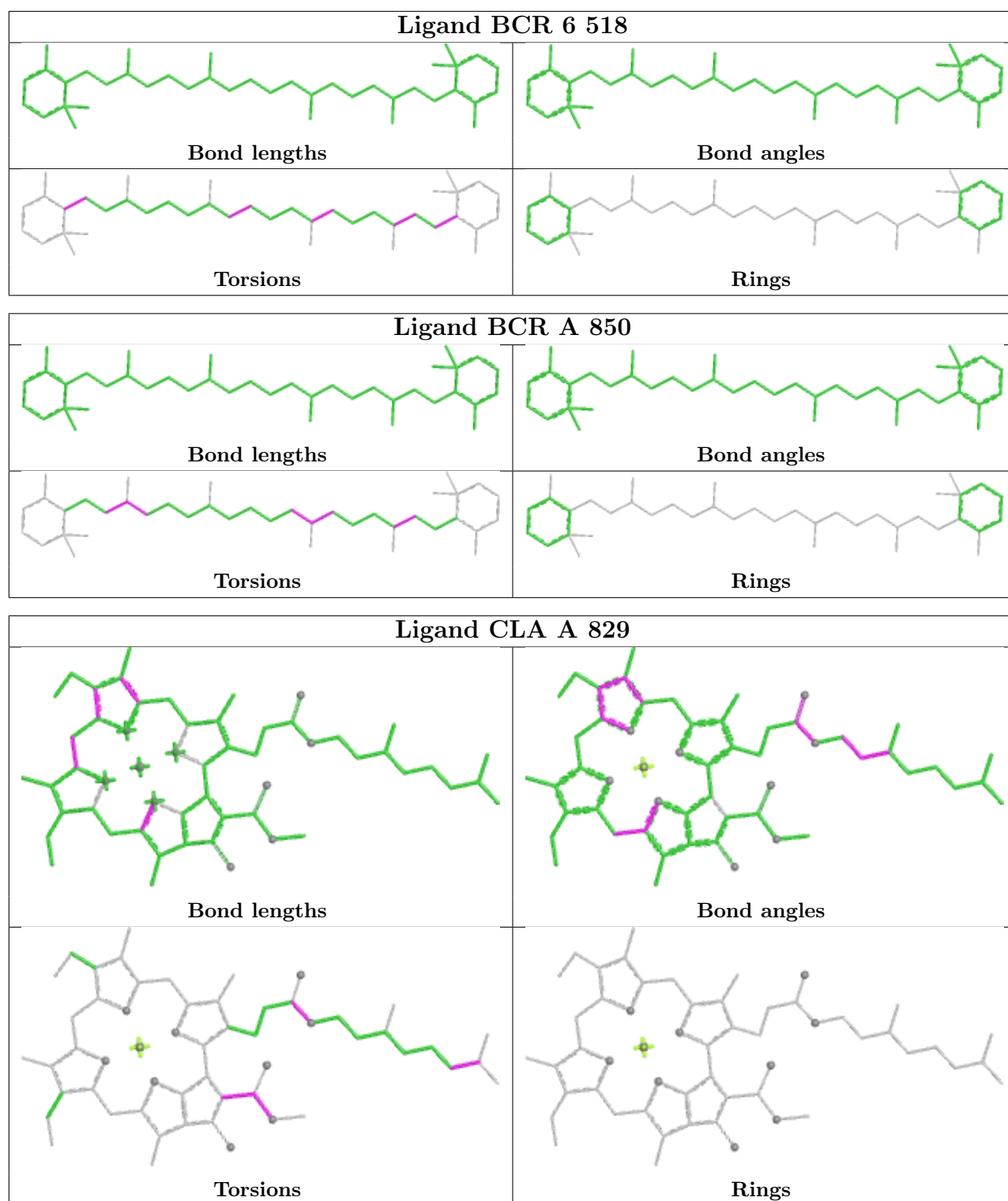


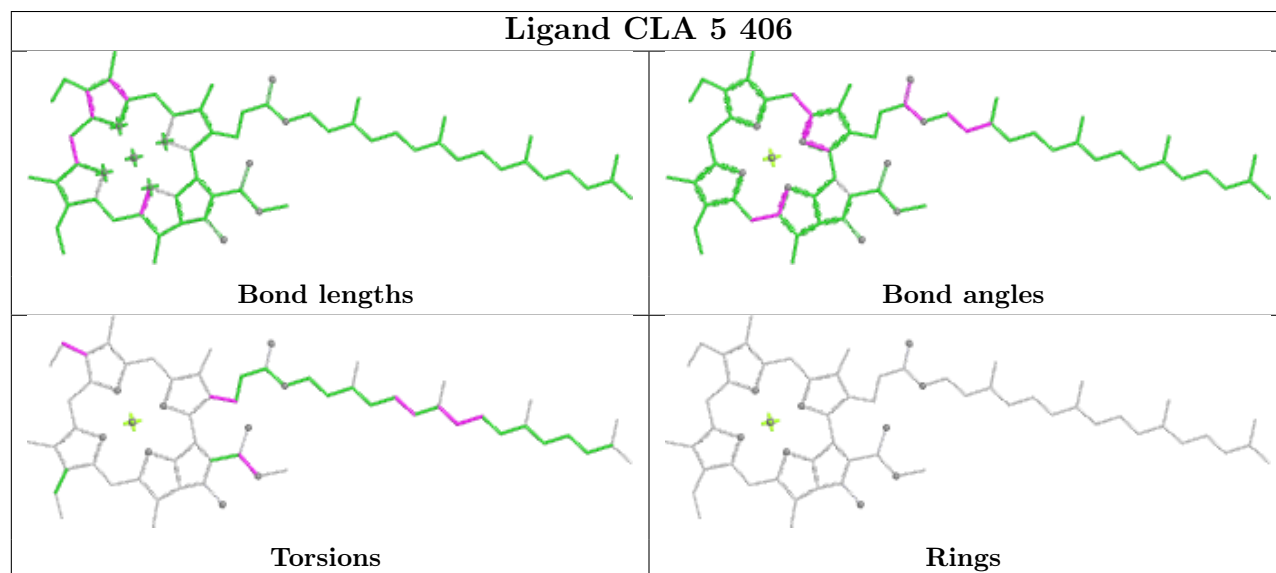
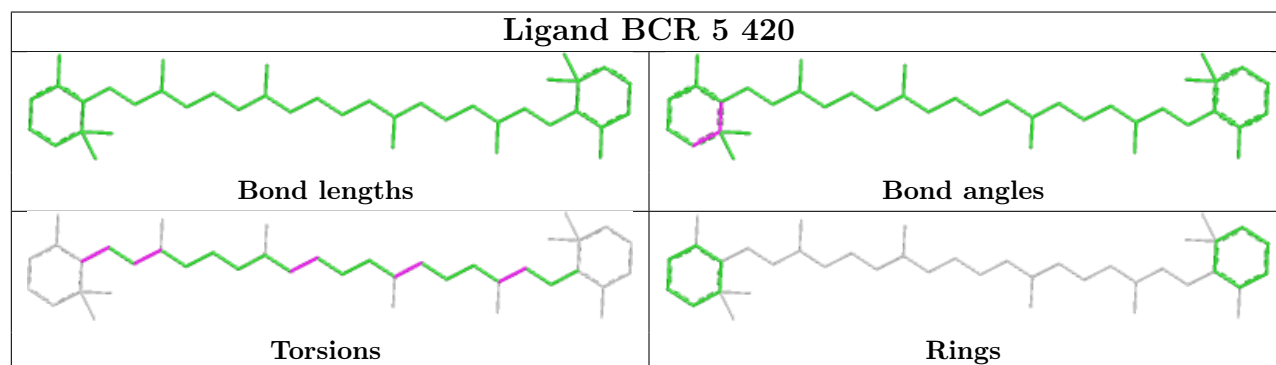
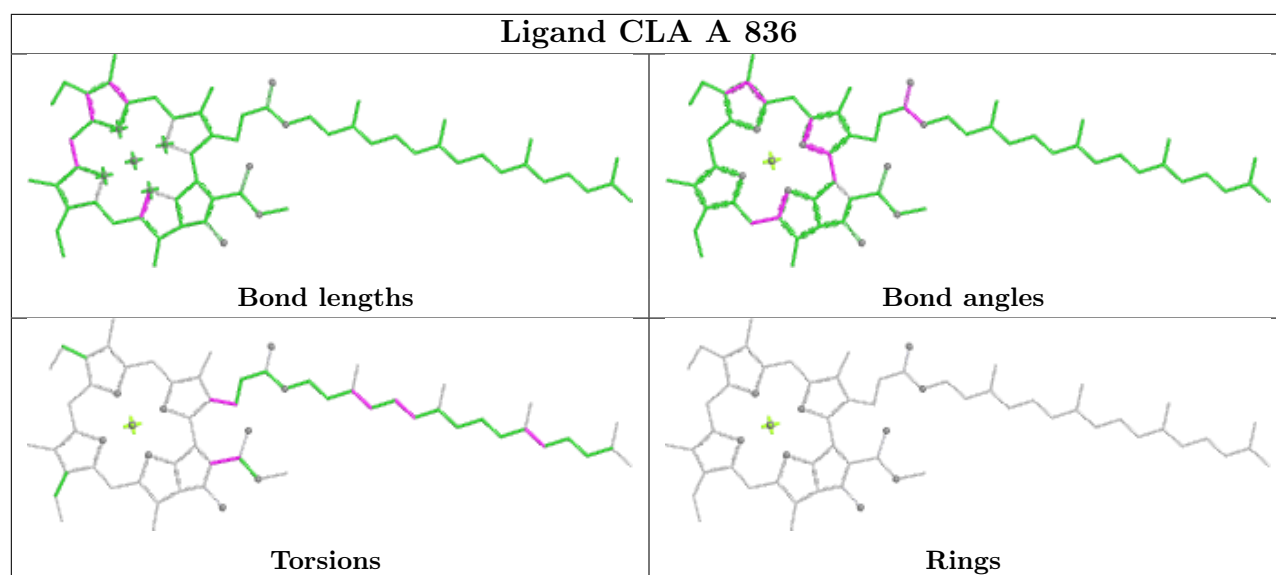
Torsions

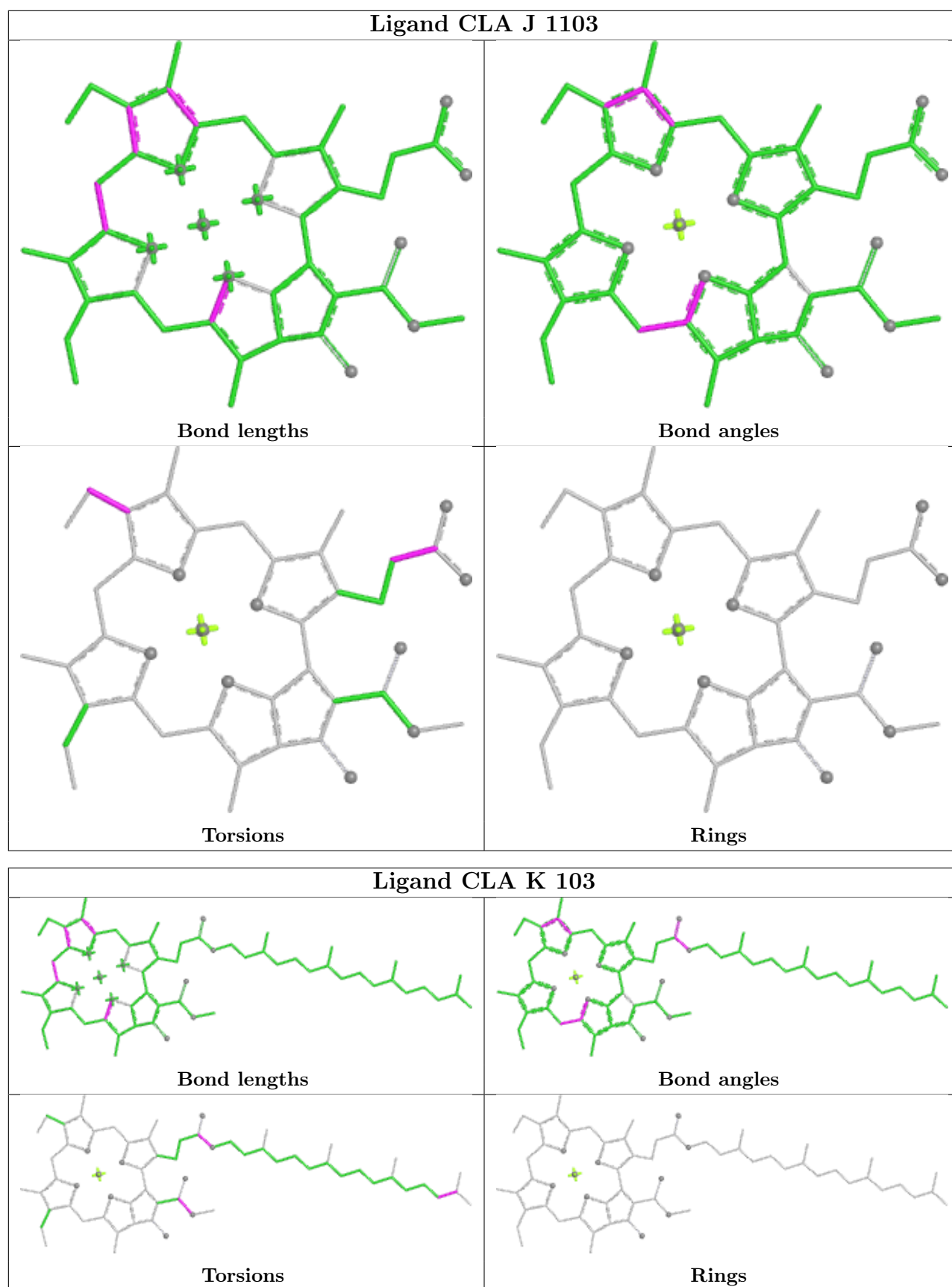


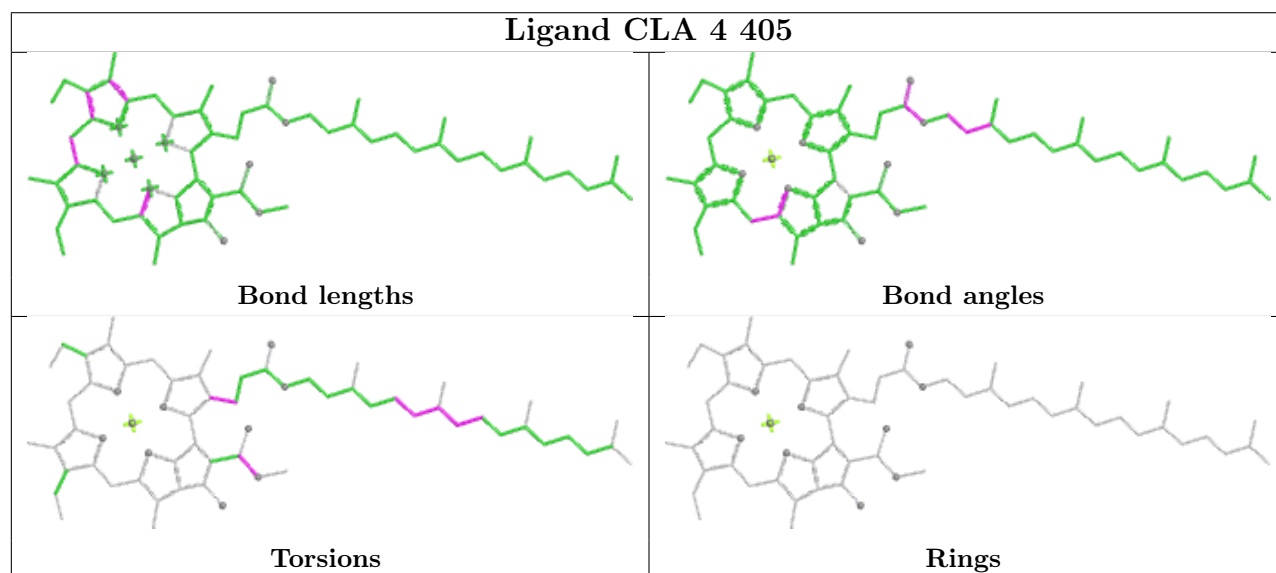
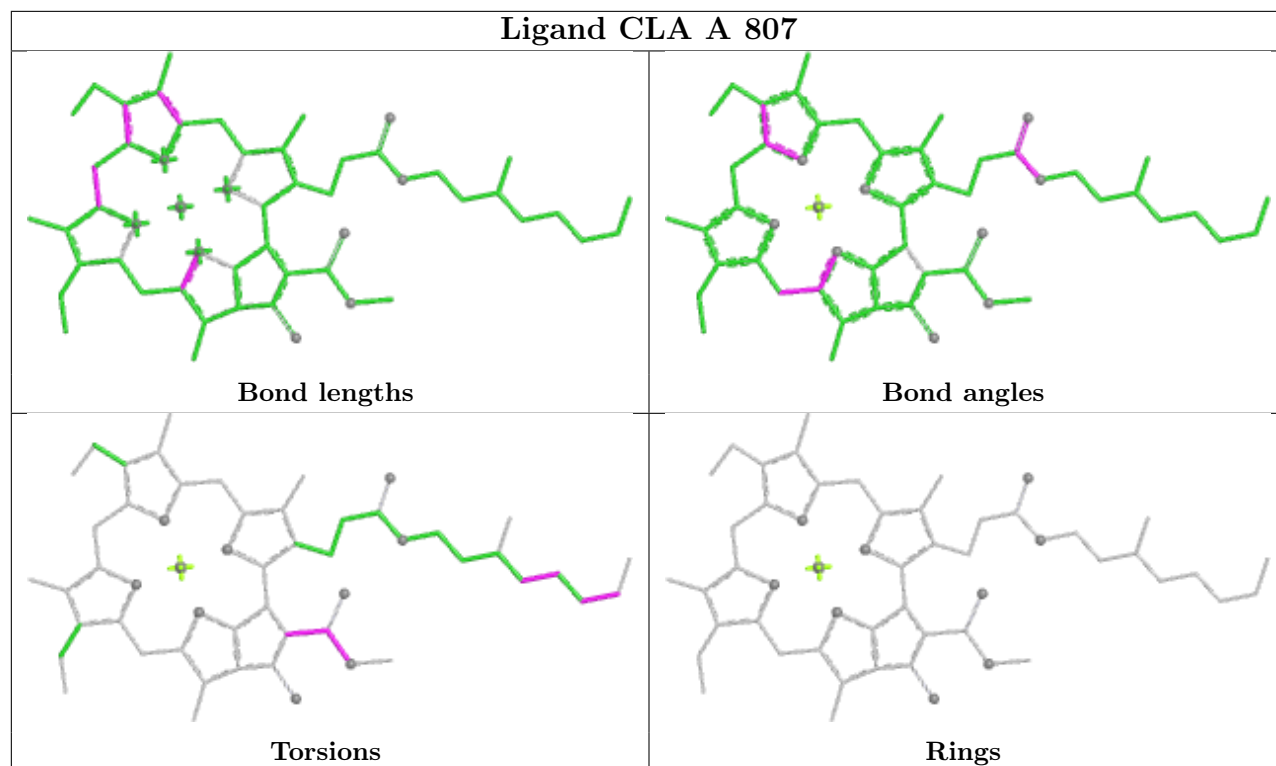
Rings



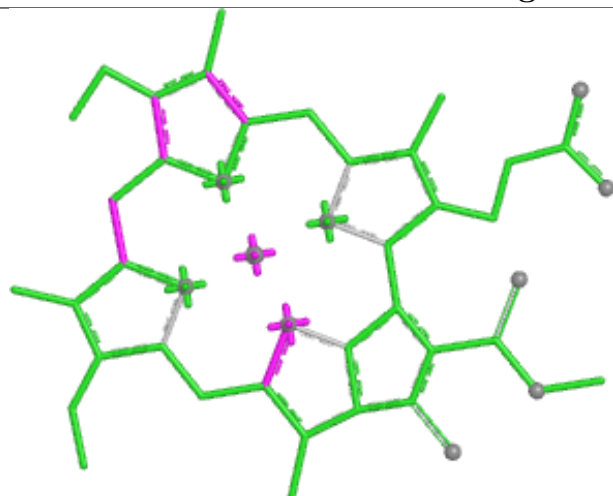




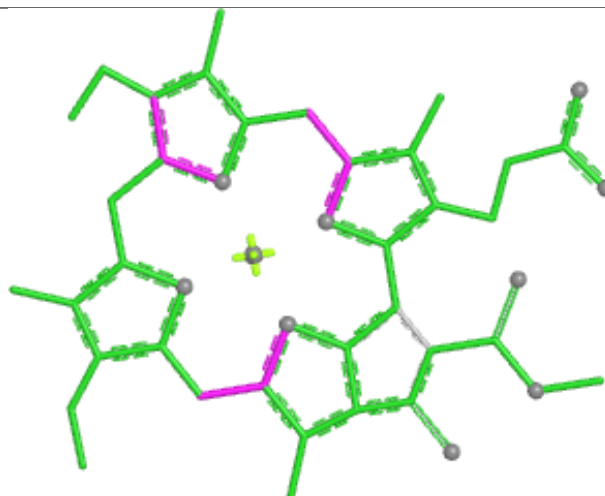




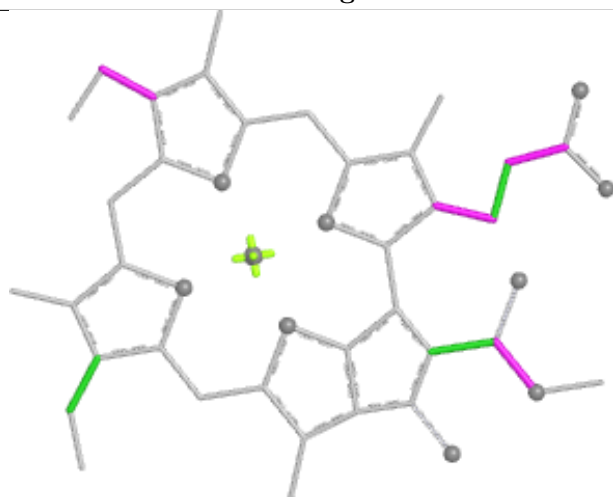
## Ligand CLA 7 516



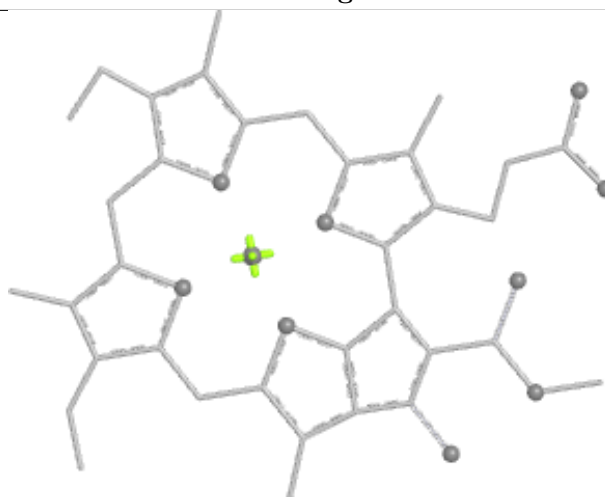
Bond lengths



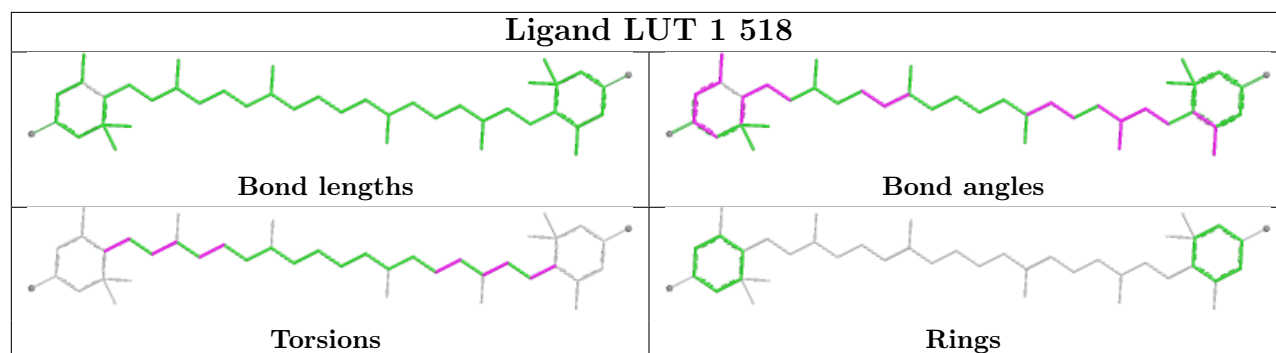
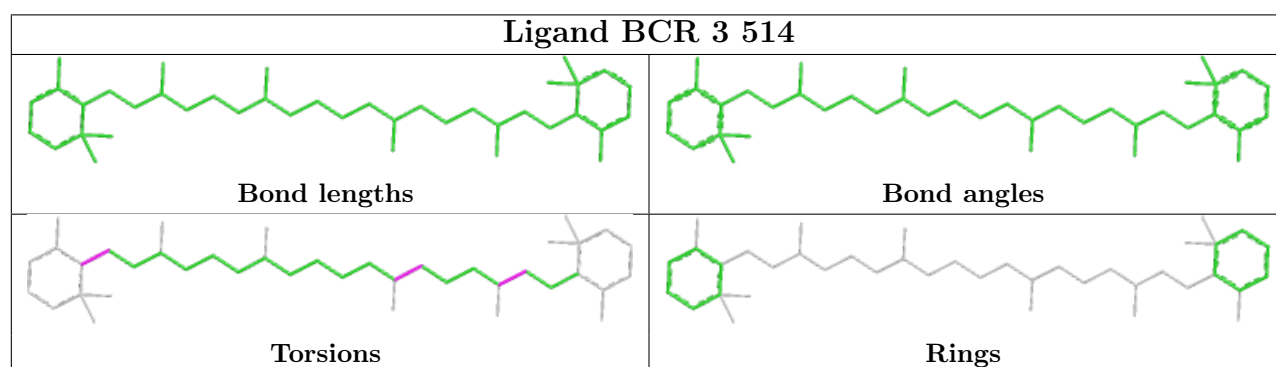
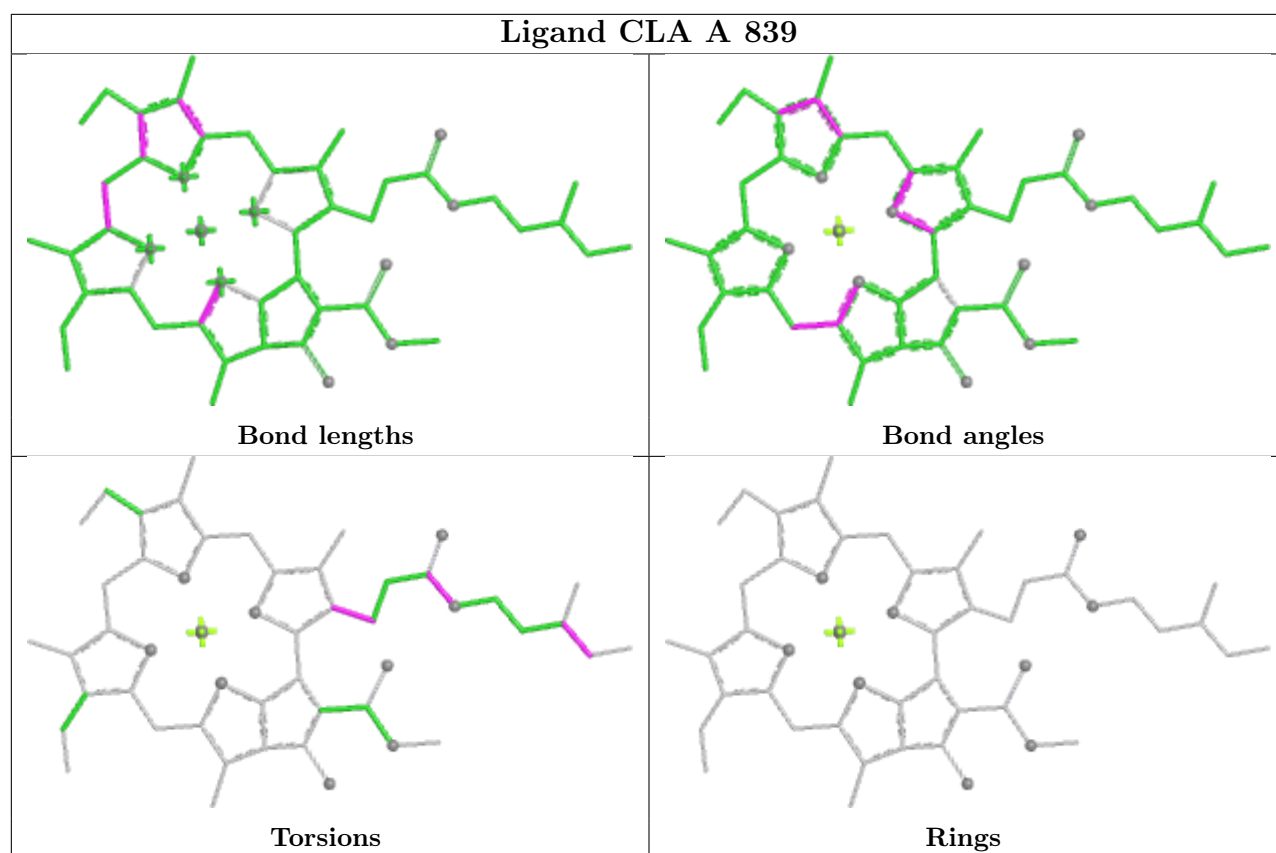
Bond angles

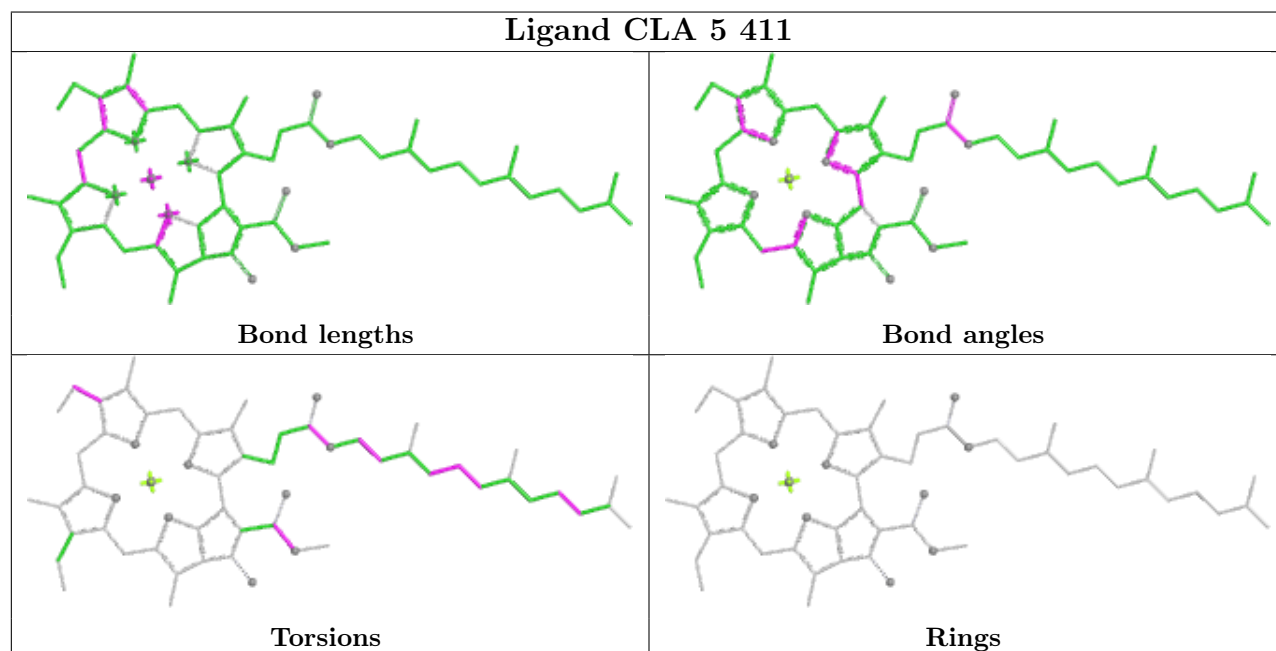
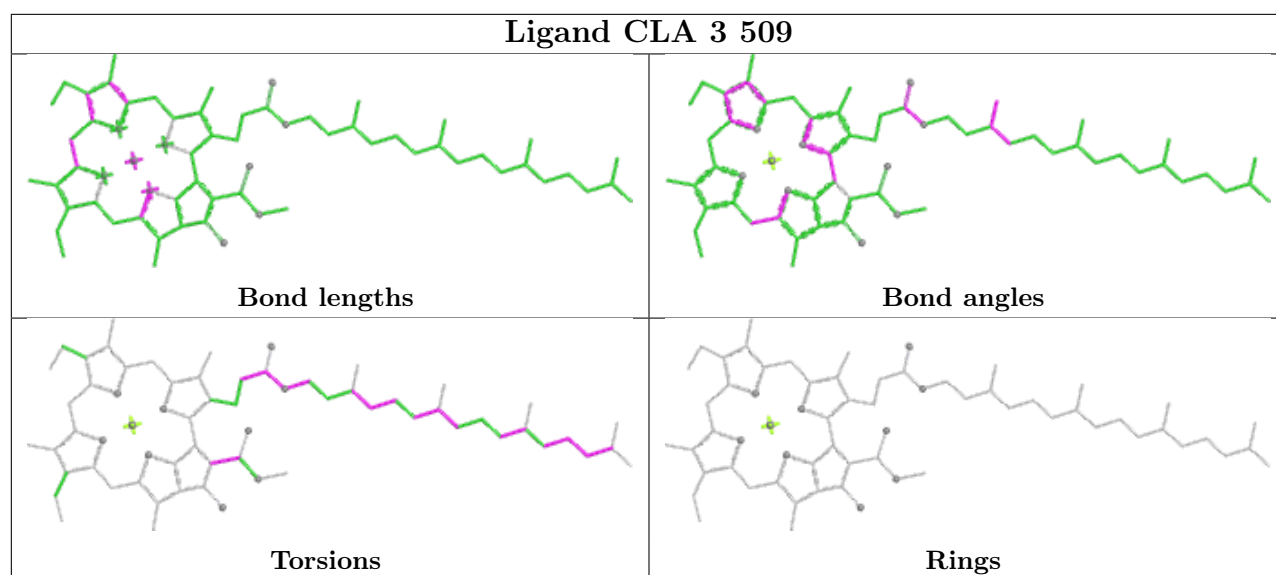


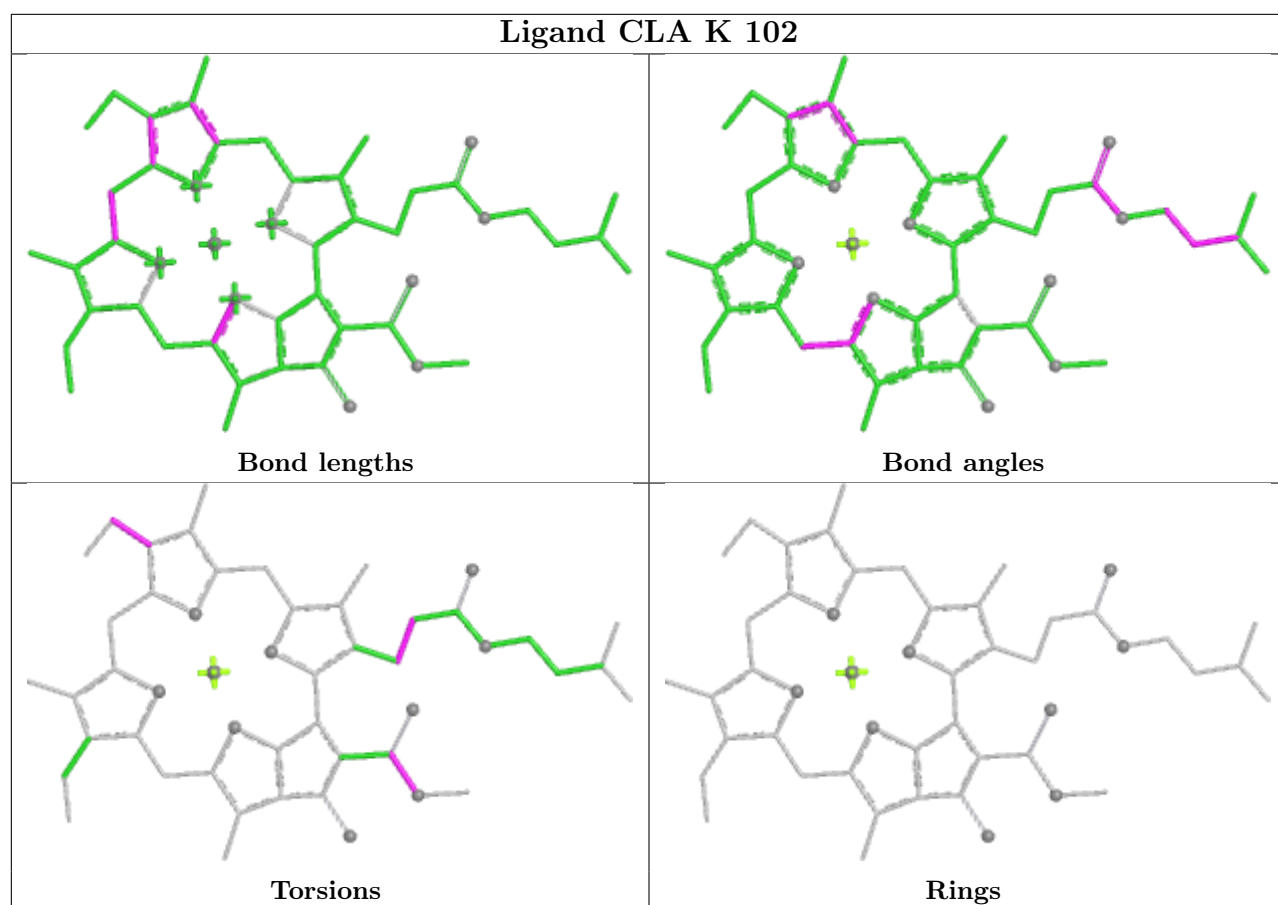
Torsions



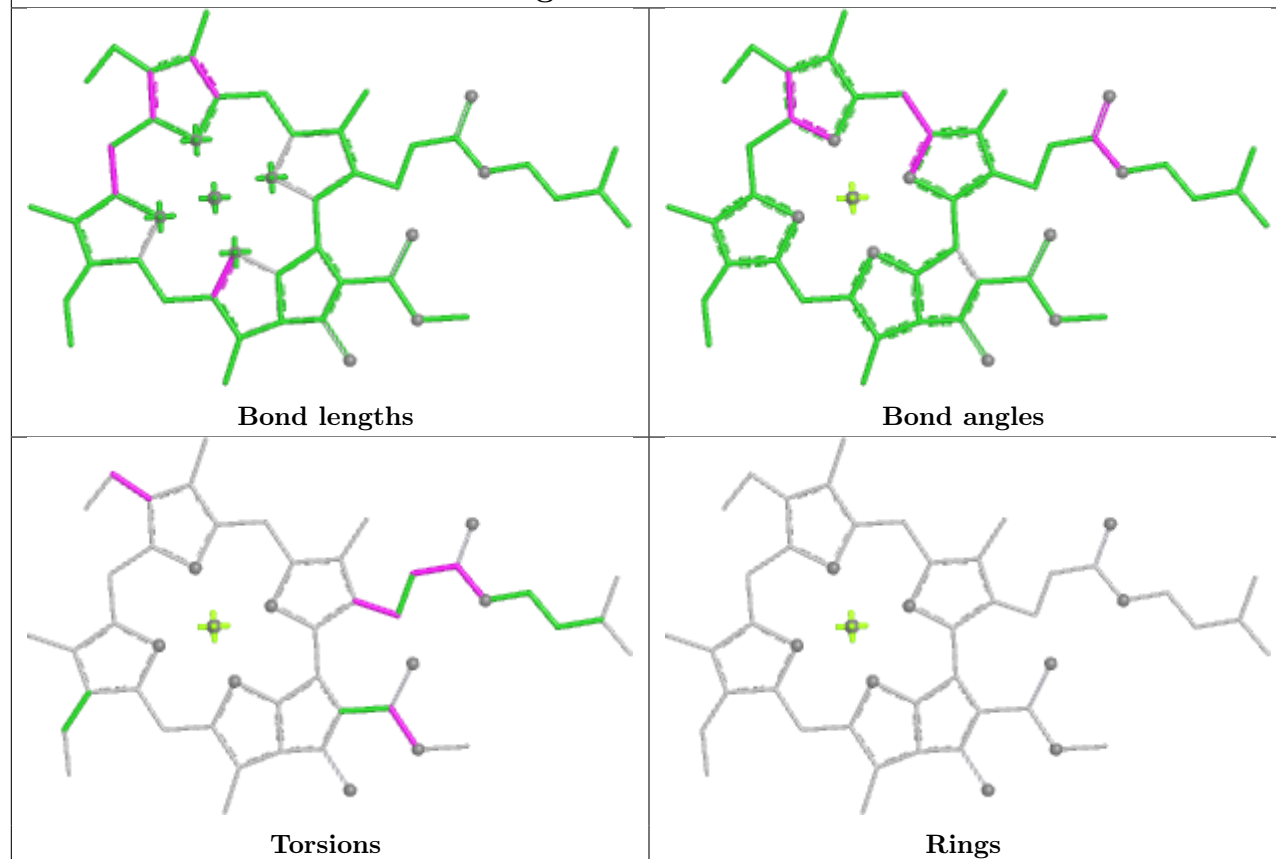
Rings



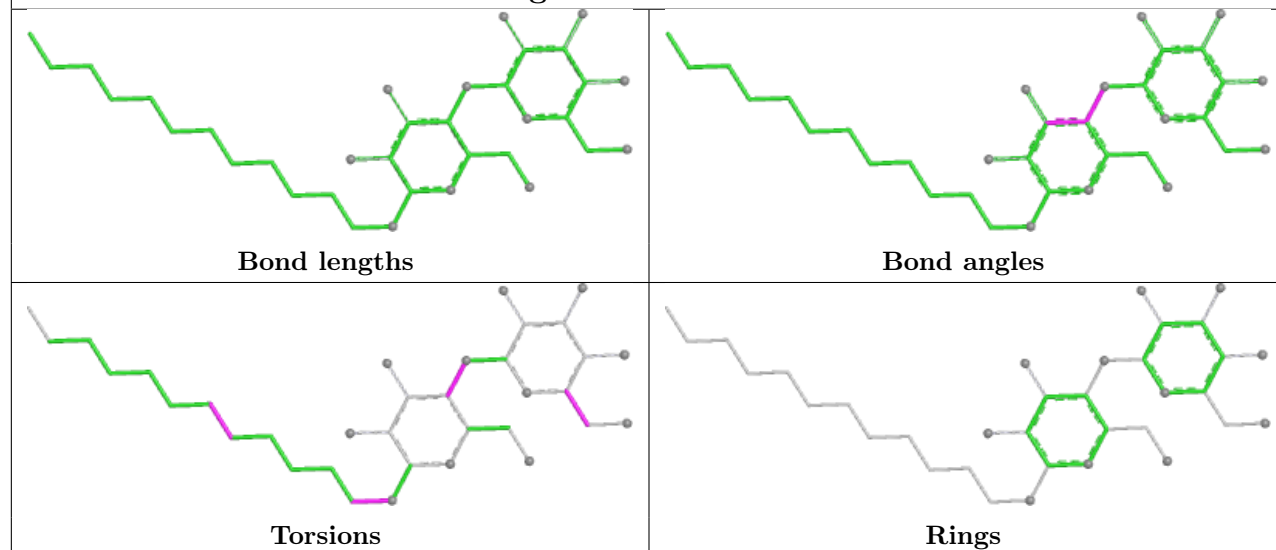


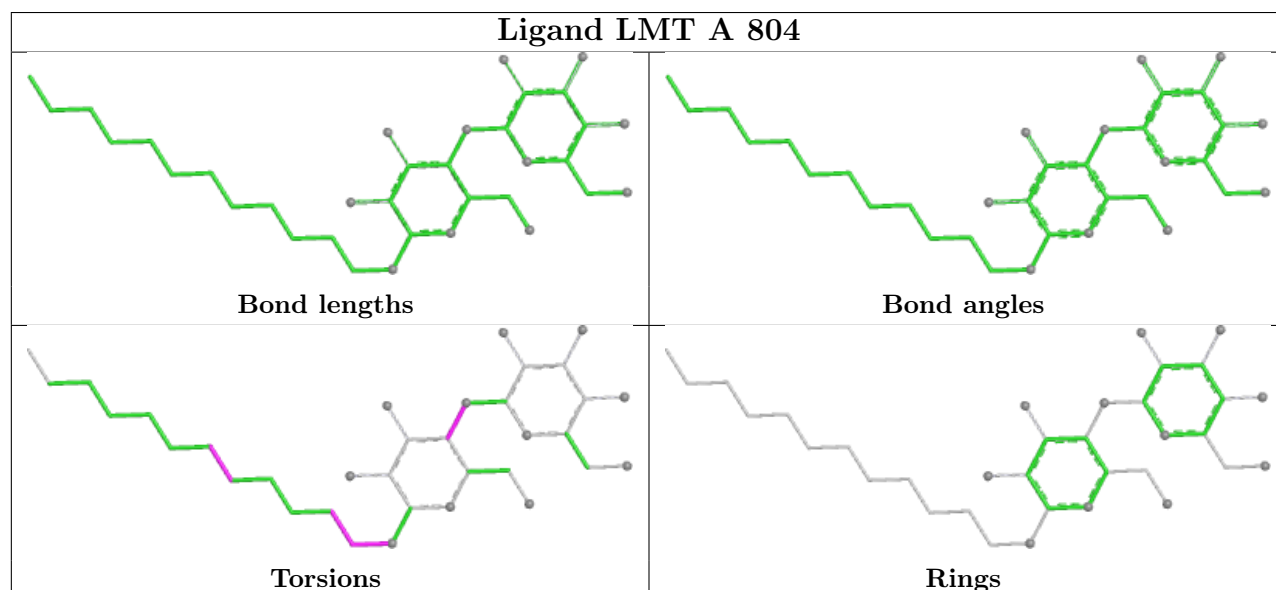
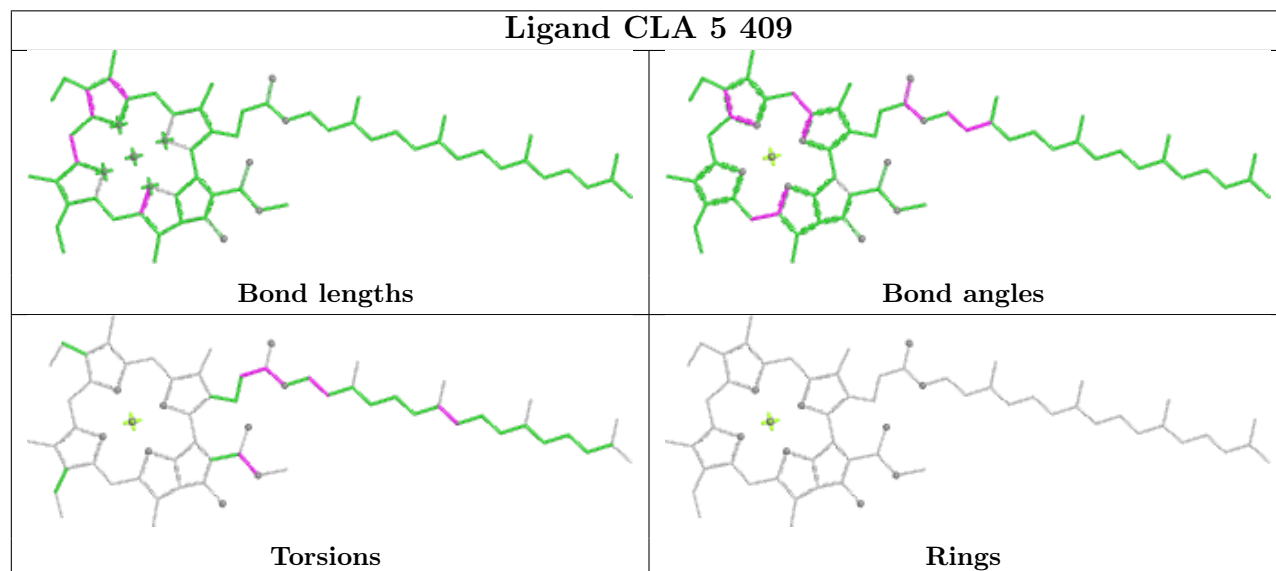
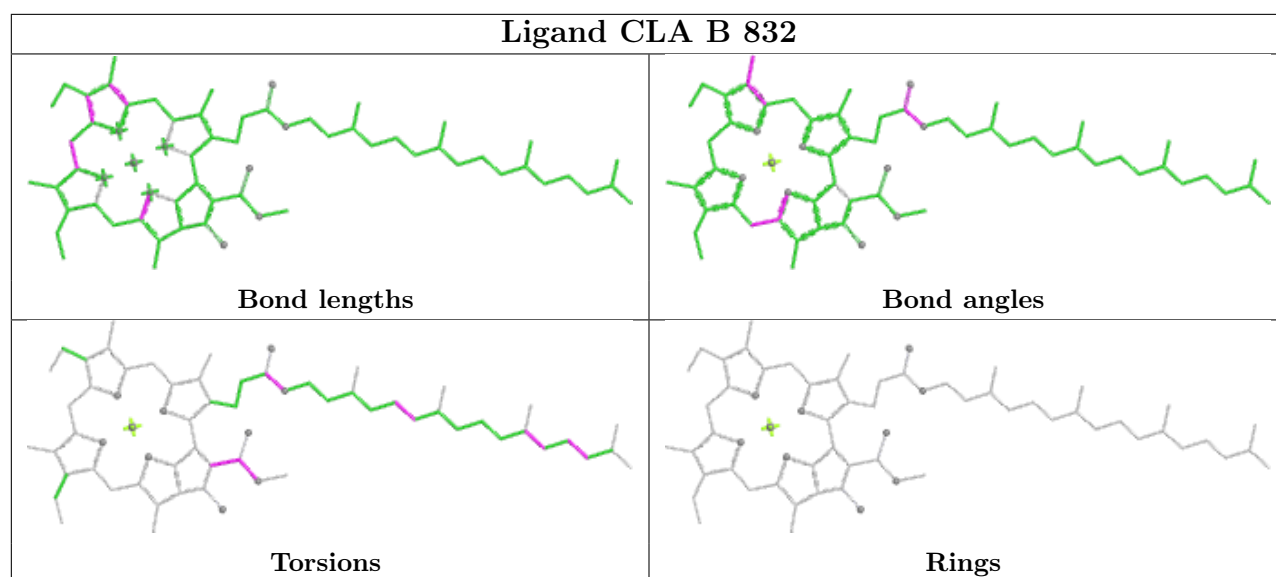


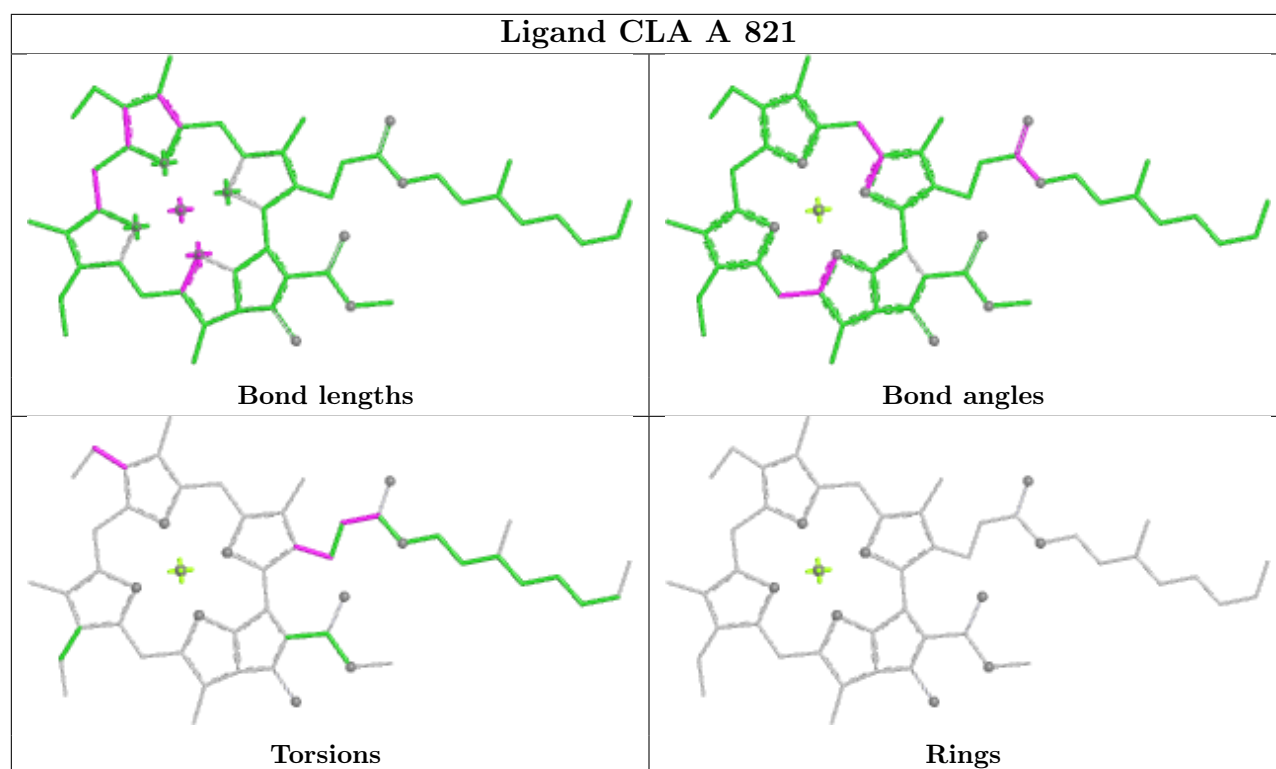
## Ligand CLA 4 412



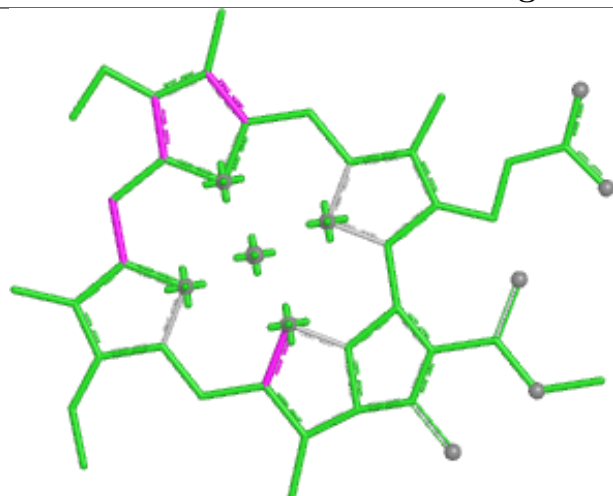
## Ligand LMT B 808



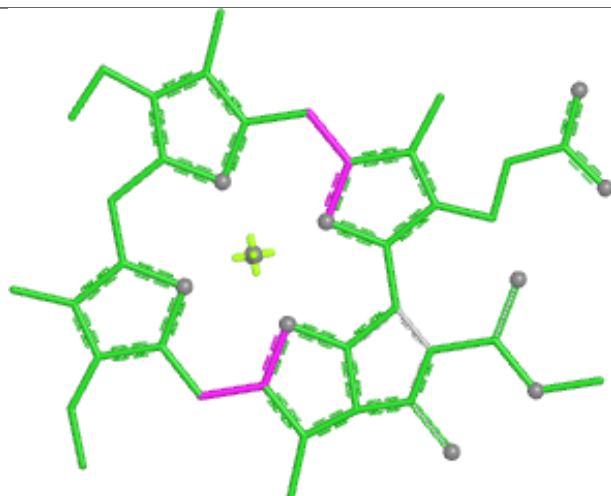




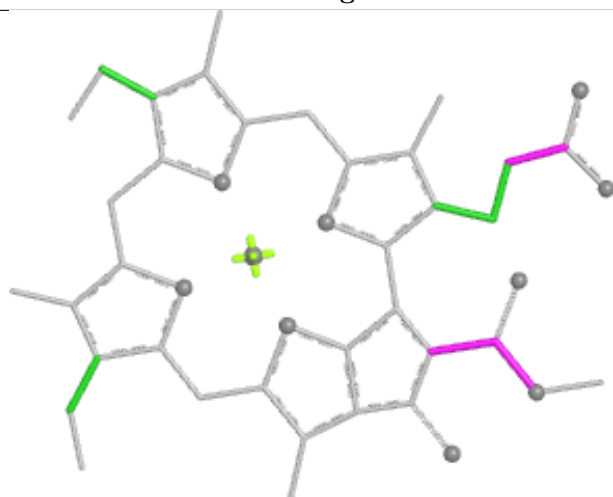
## Ligand CLA 7 504



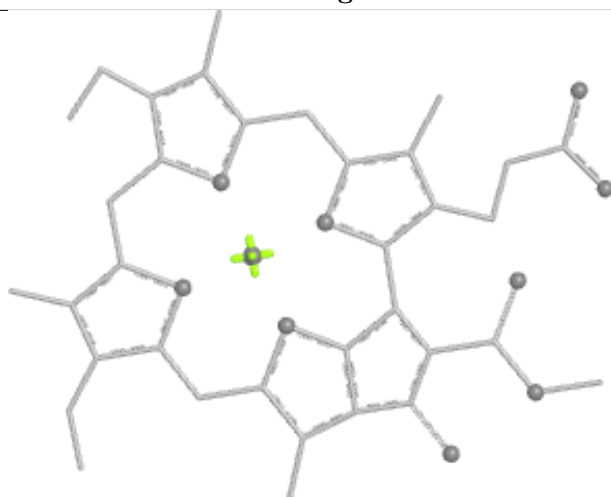
Bond lengths



Bond angles

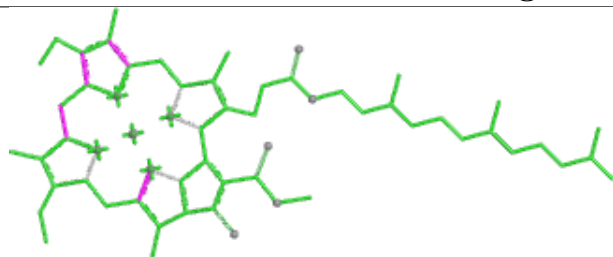


Torsions

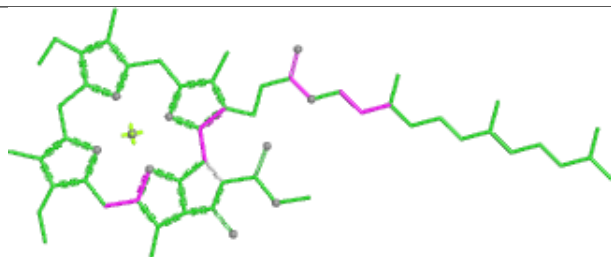


Rings

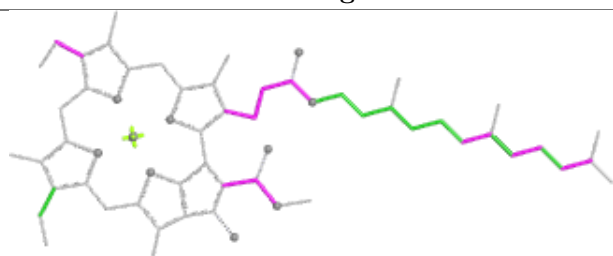
## Ligand CLA 2 413



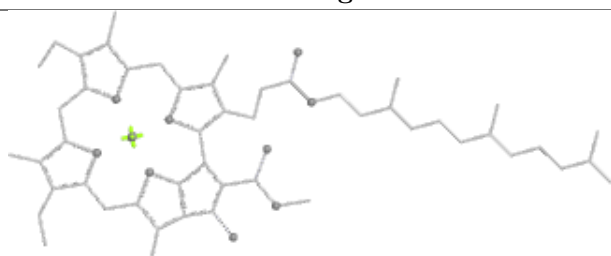
Bond lengths



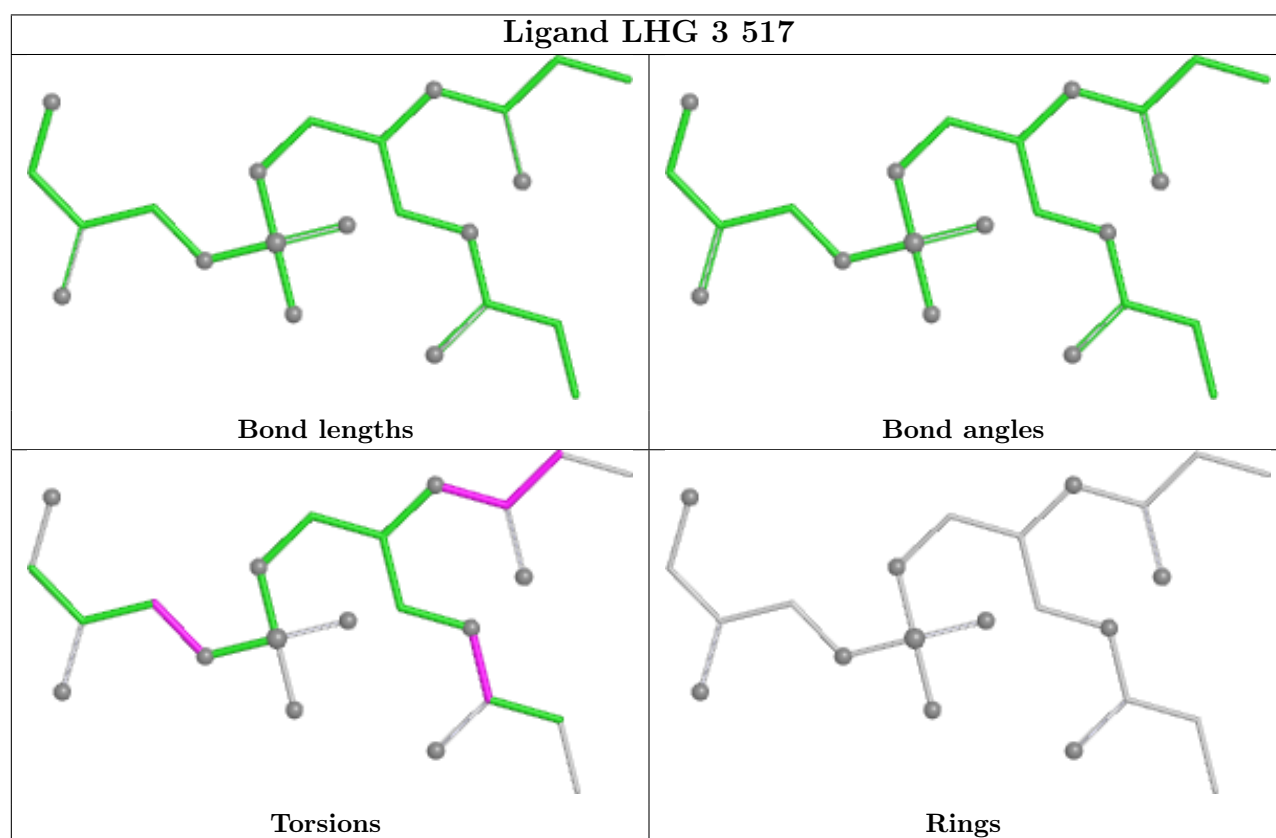
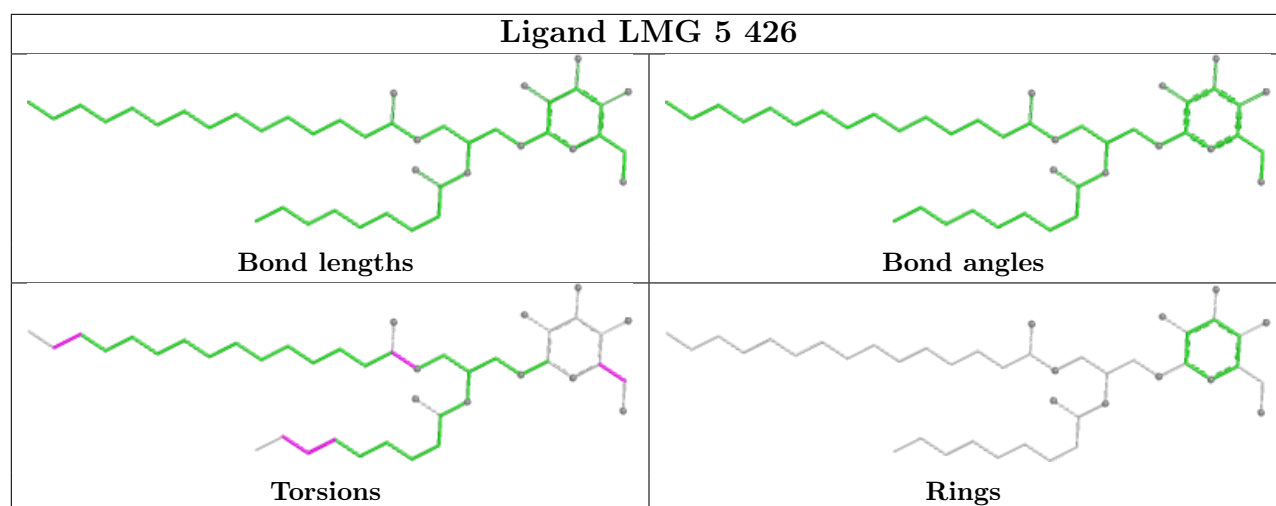
Bond angles

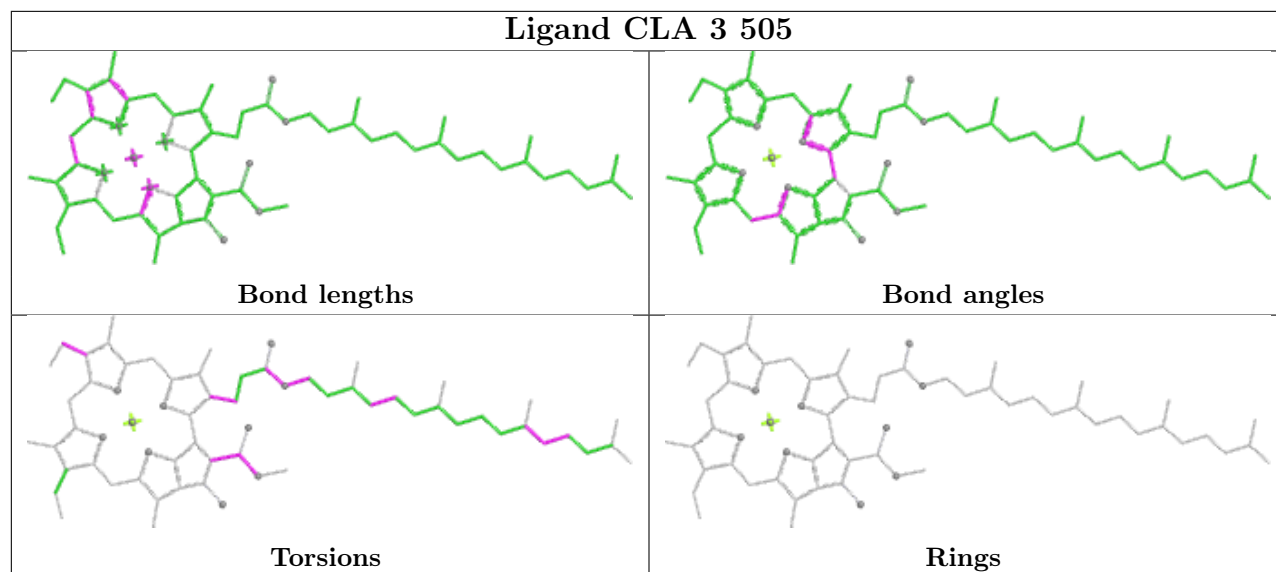
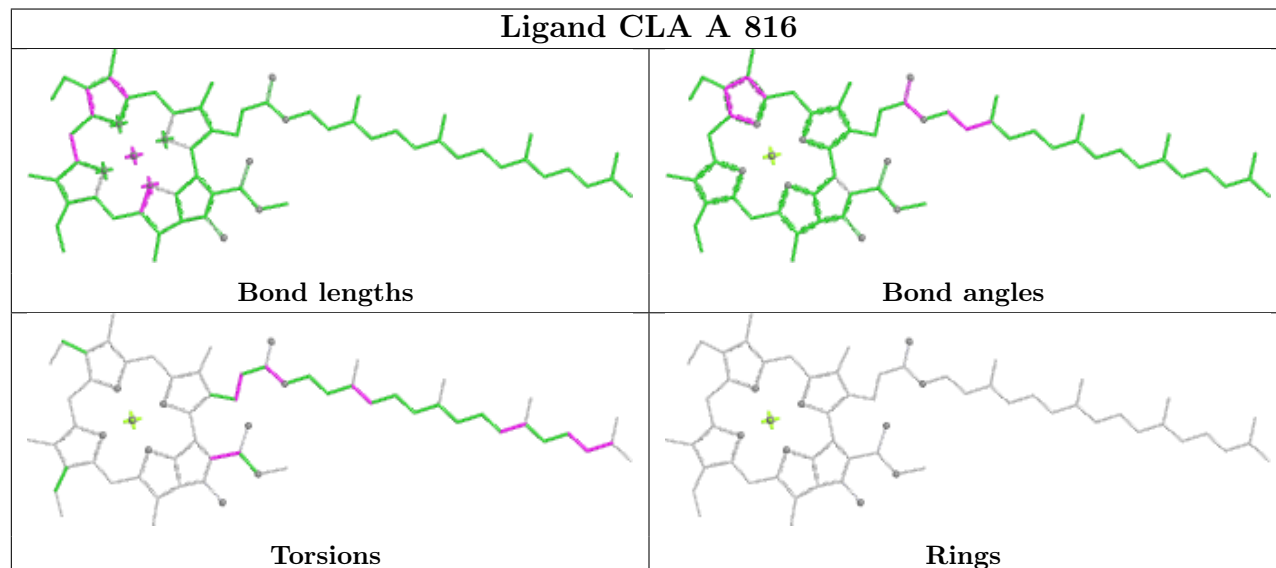


Torsions

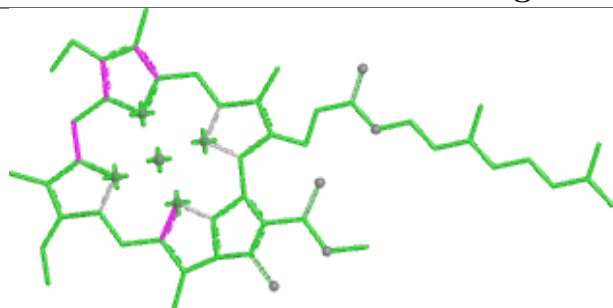


Rings

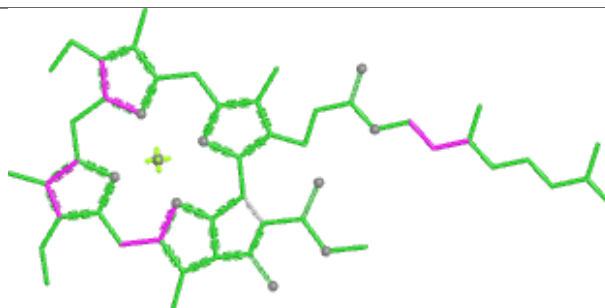


**Ligand CLA 3 505****Ligand CLA A 816**

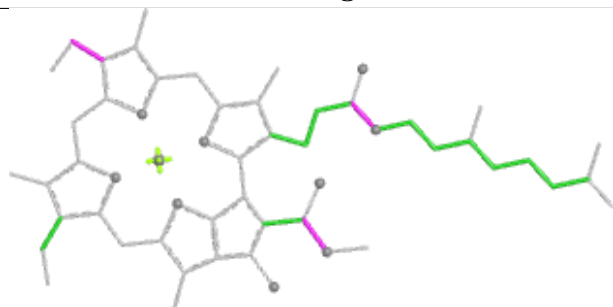
## Ligand CLA A 838



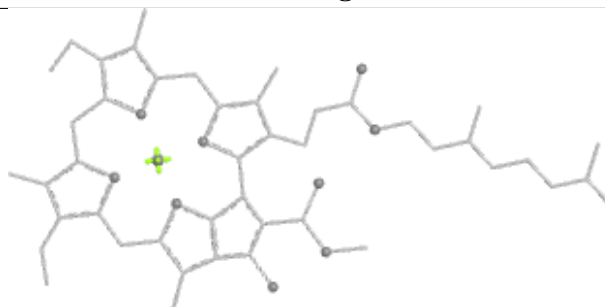
Bond lengths



Bond angles

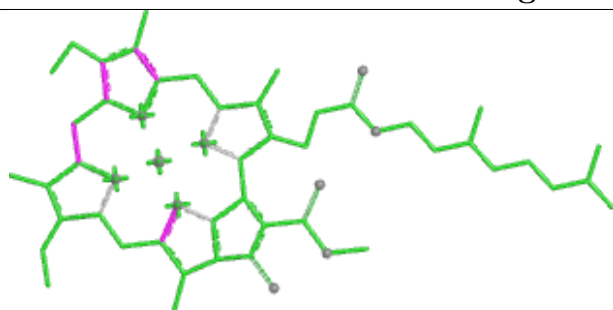


Torsions

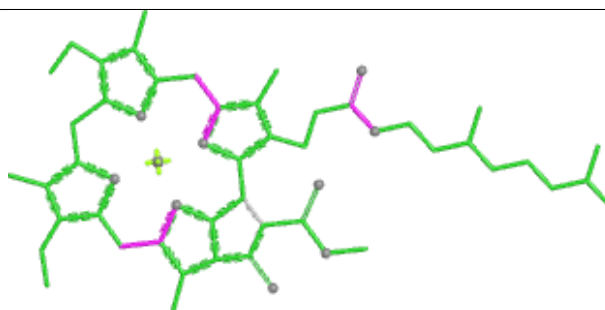


Rings

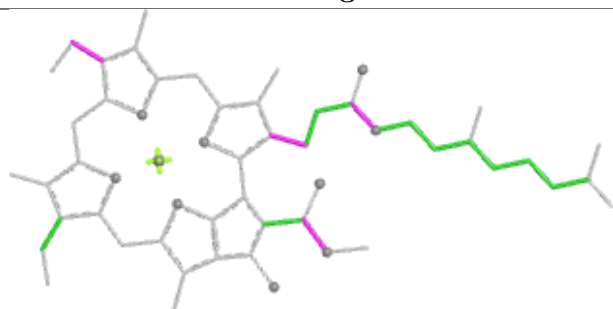
## Ligand CLA 1 502



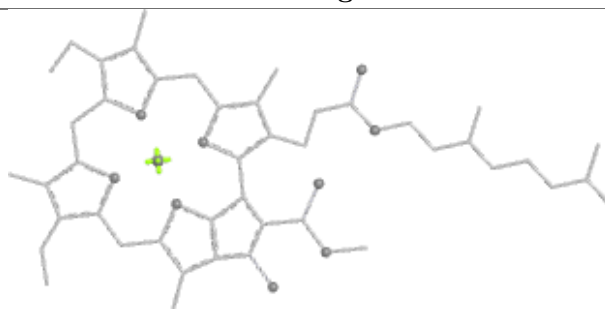
Bond lengths



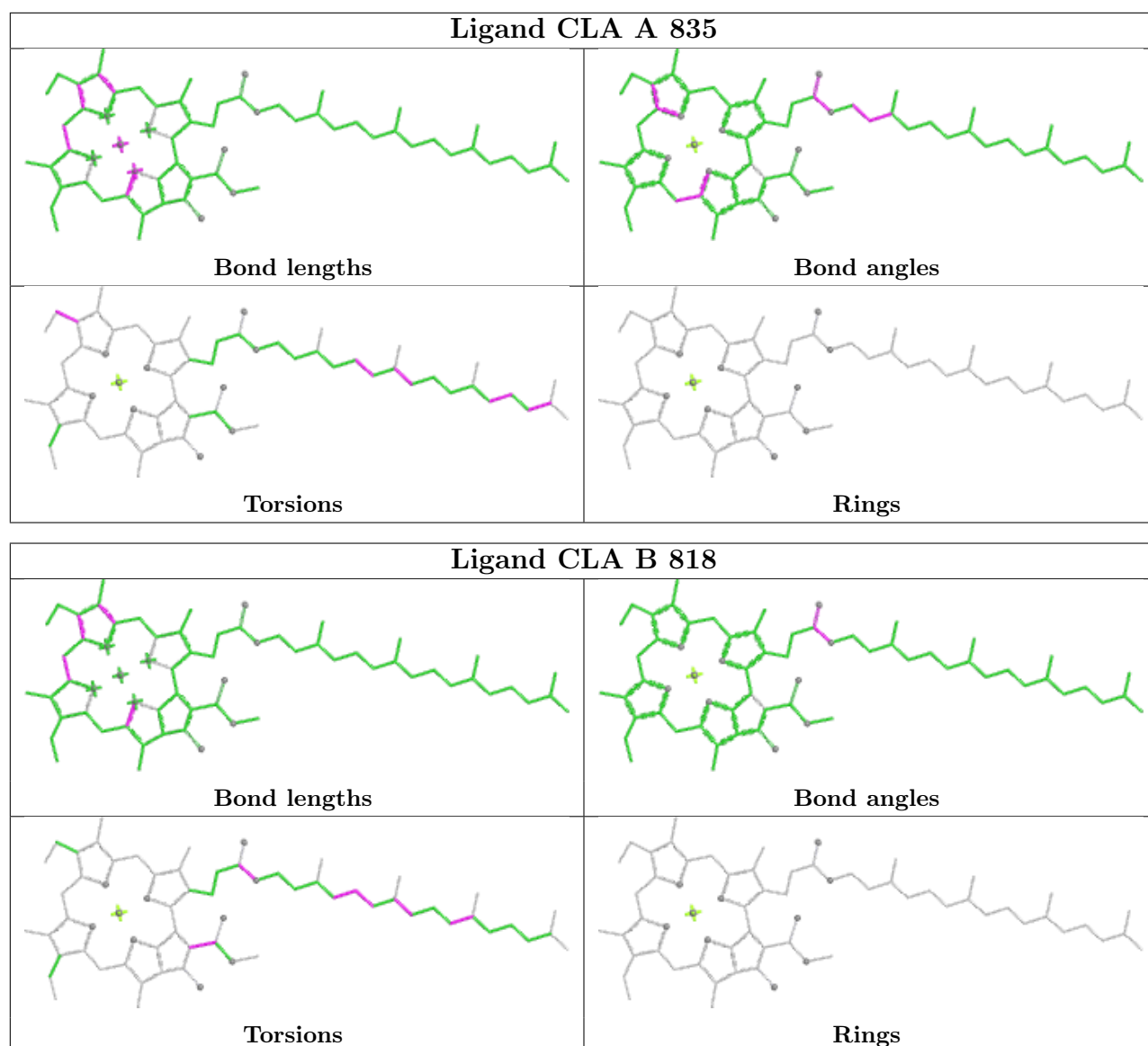
Bond angles



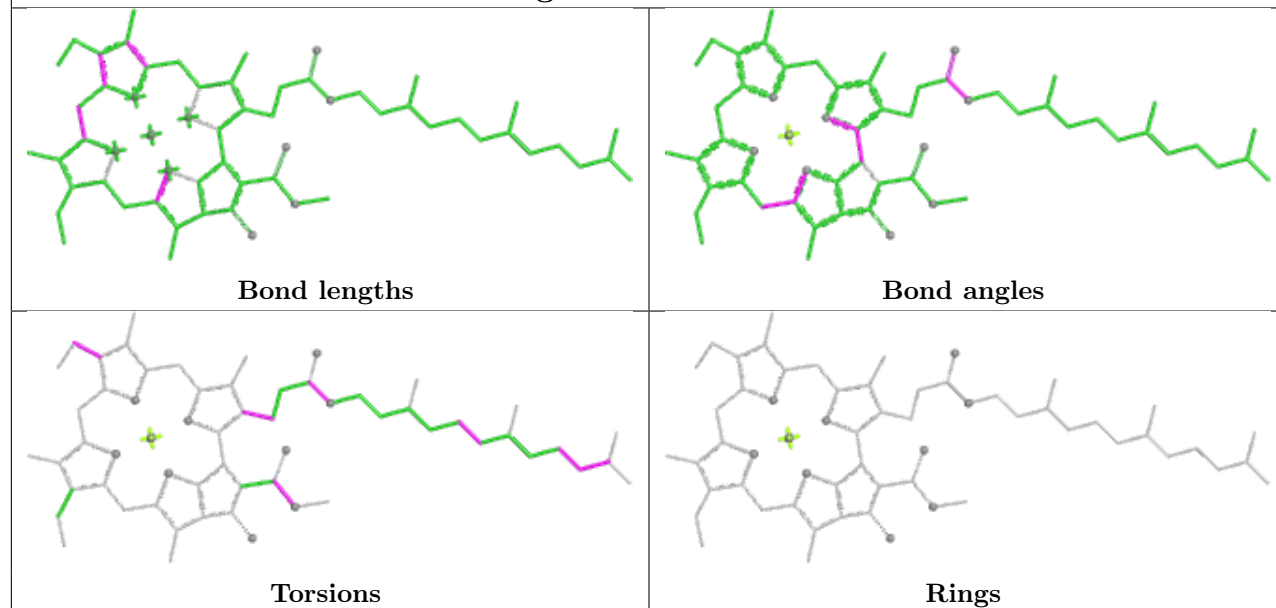
Torsions



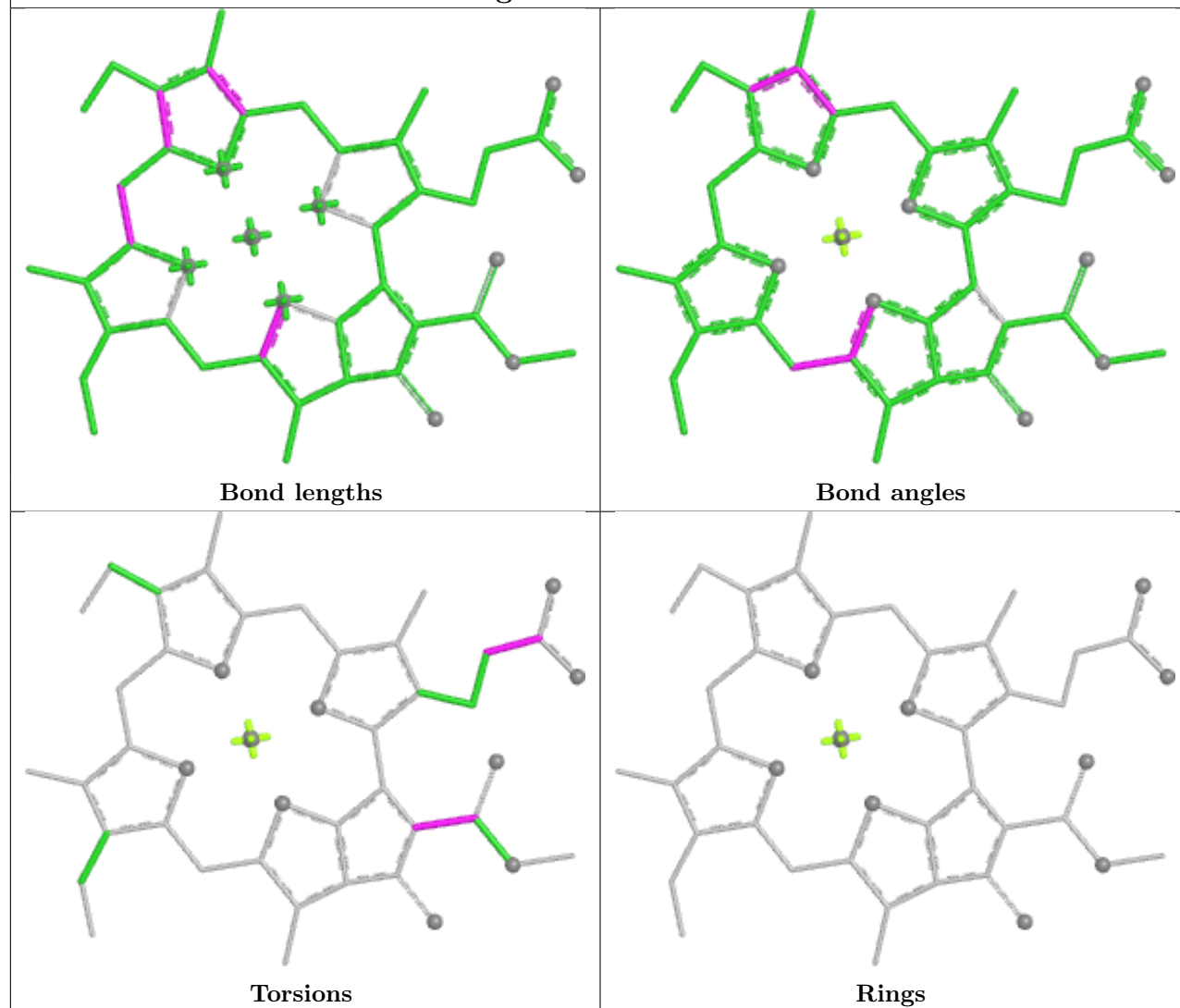
Rings

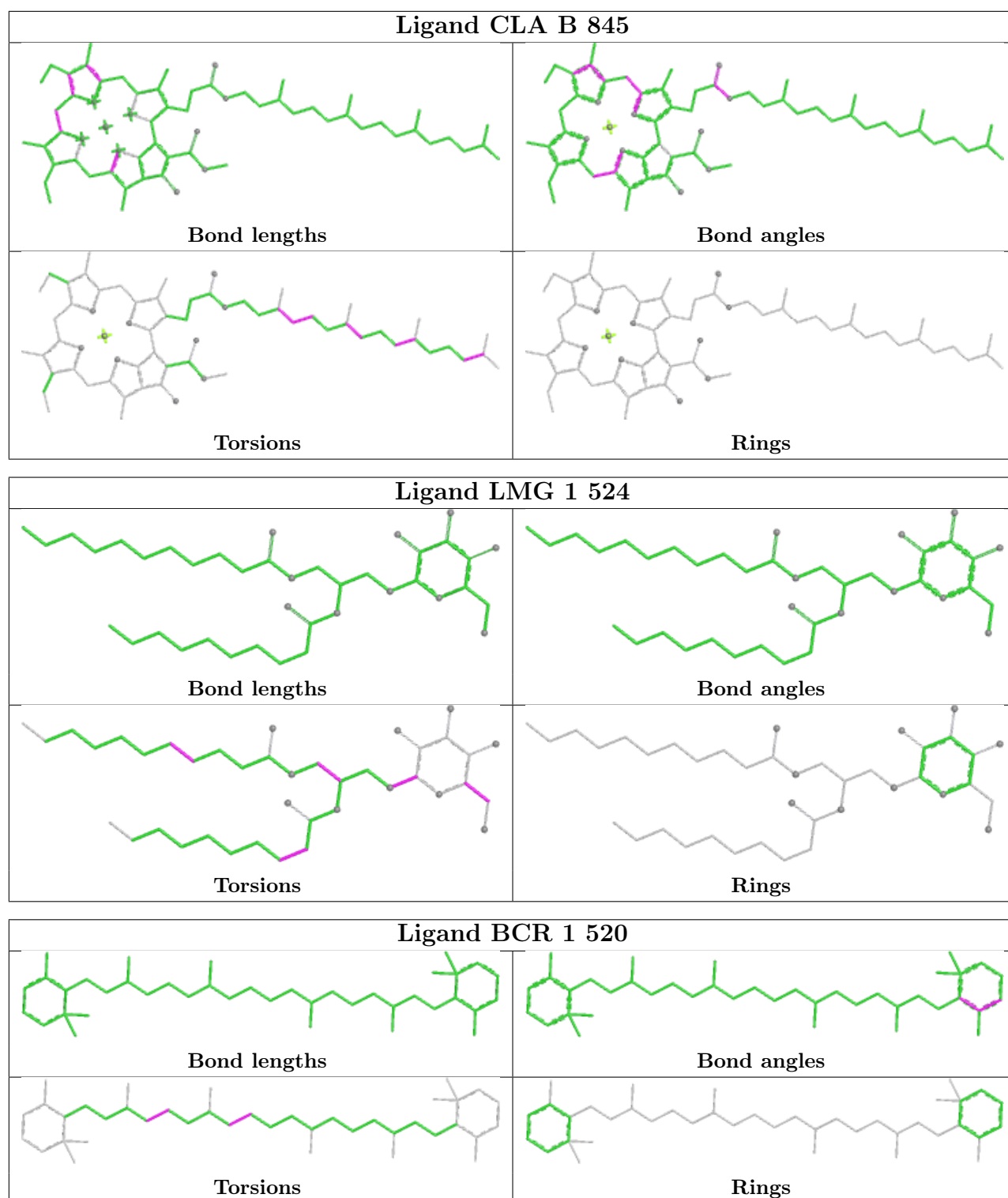


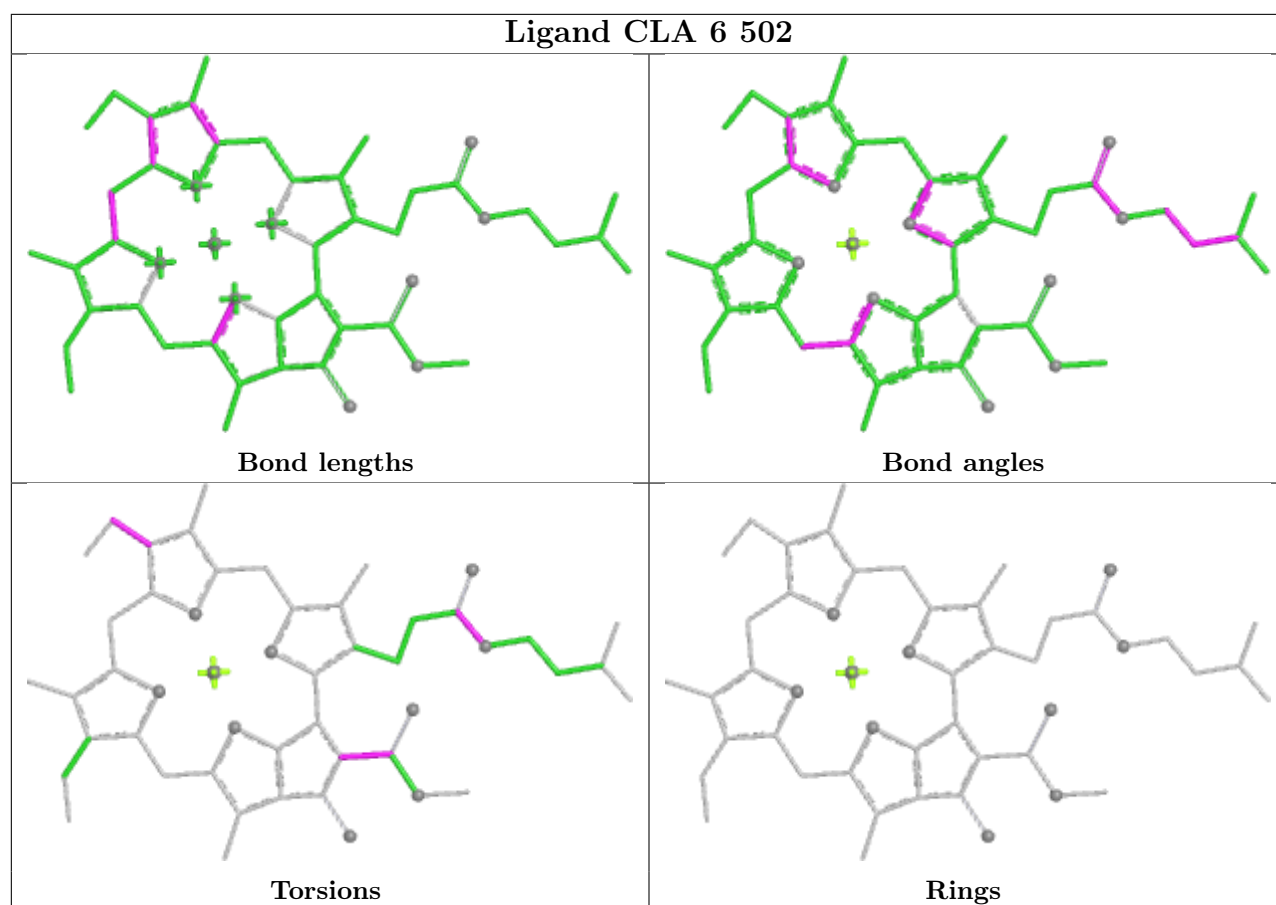
## Ligand CLA 1 509



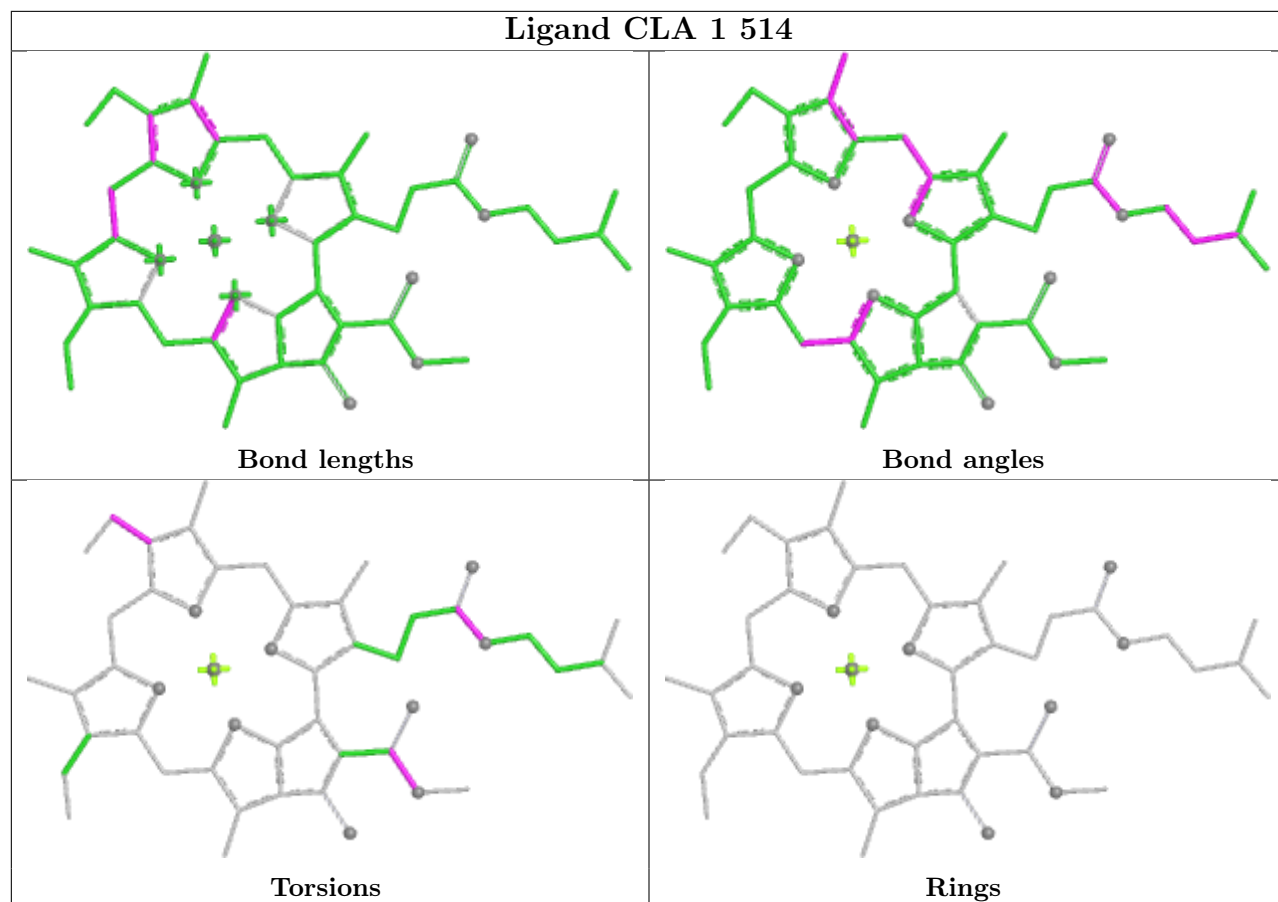
## Ligand CLA 2 415

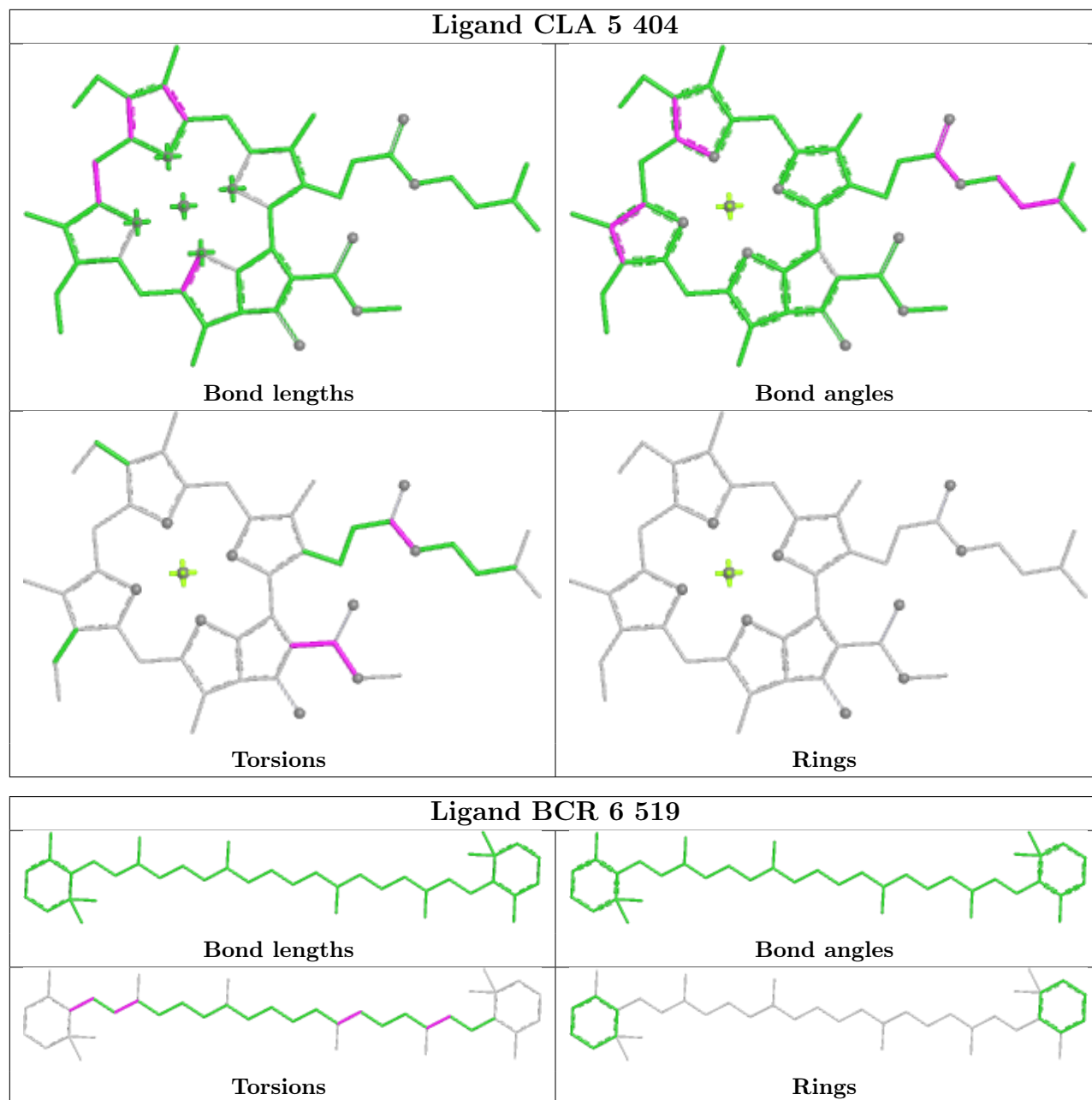


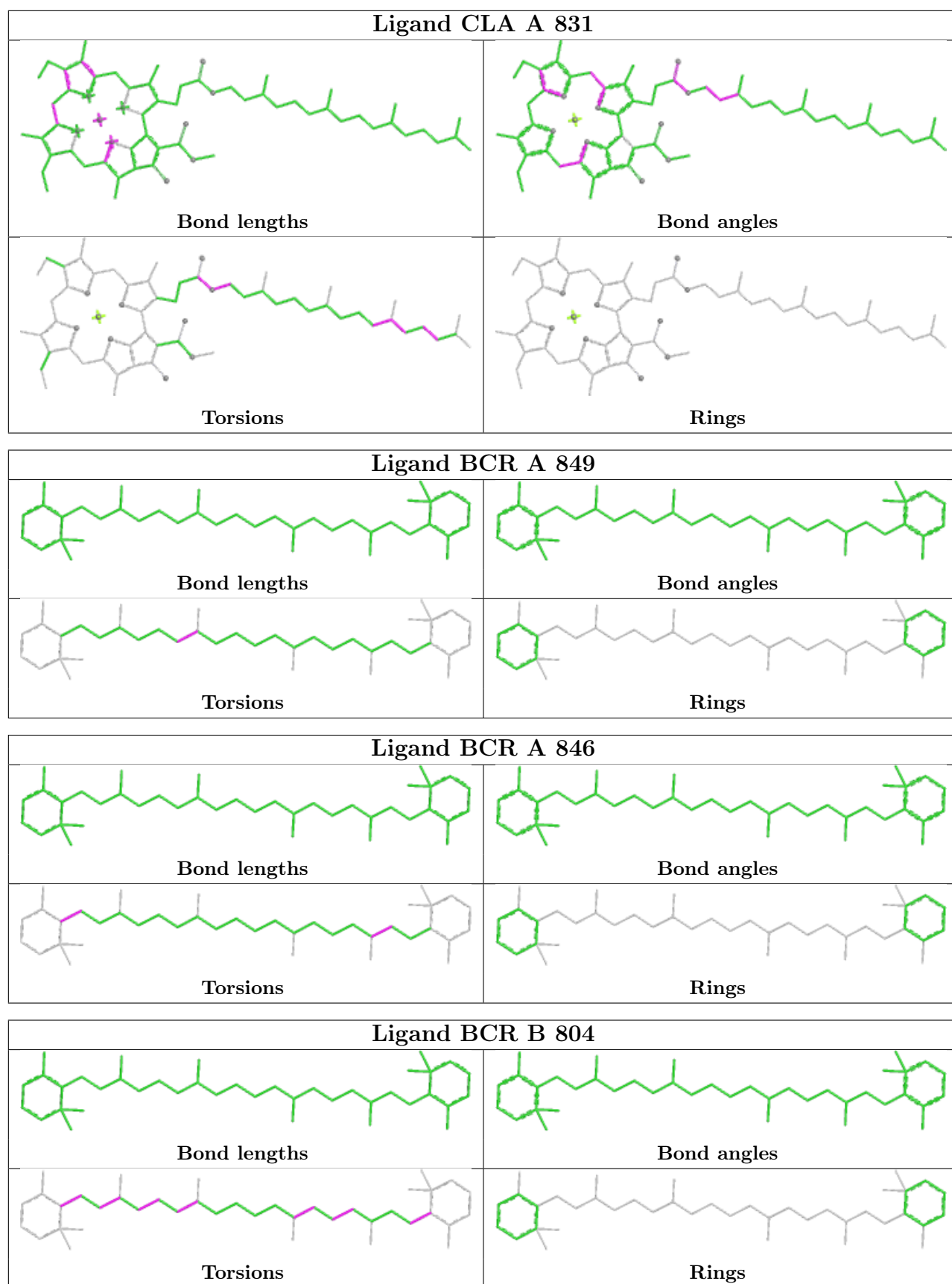


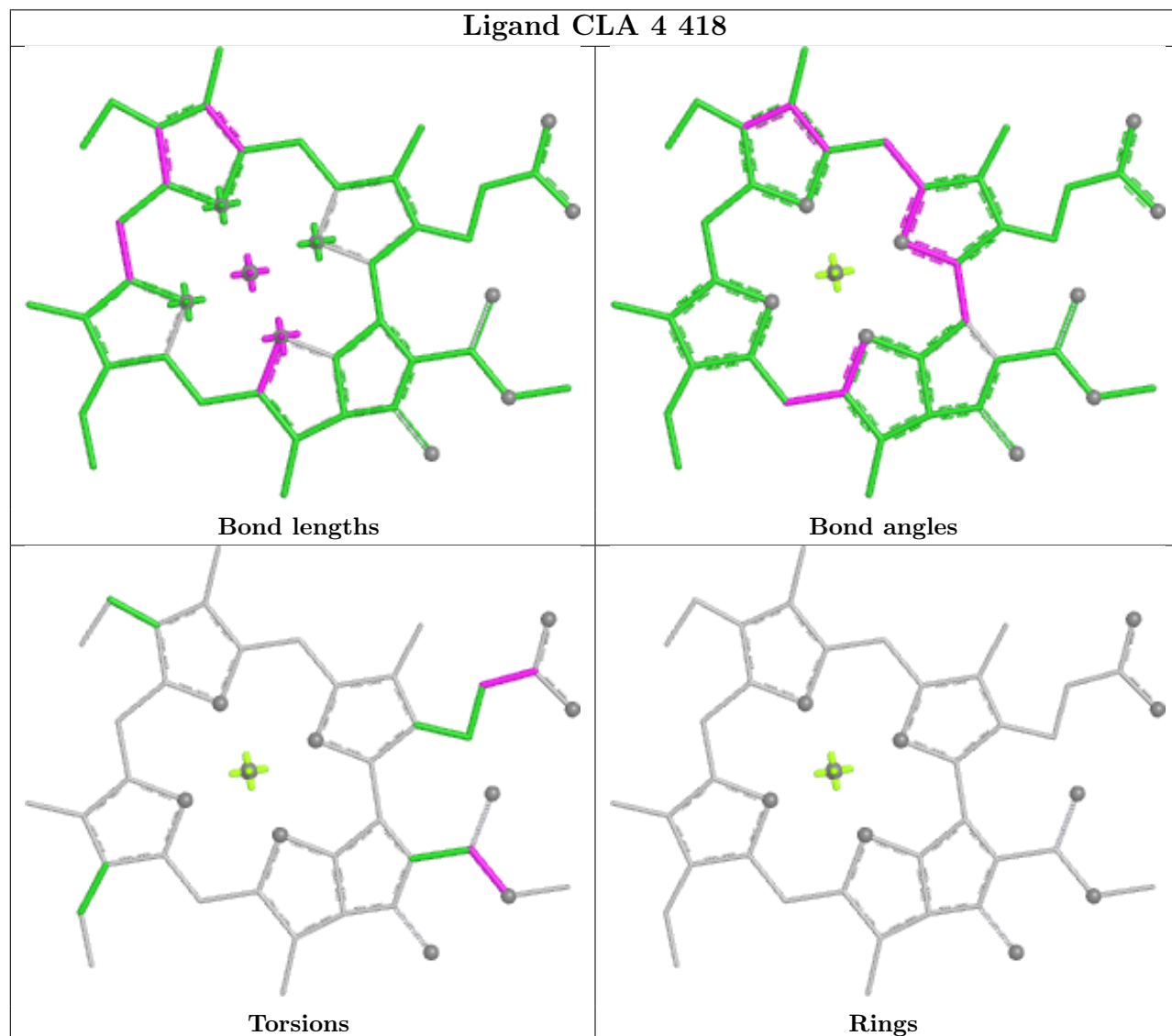
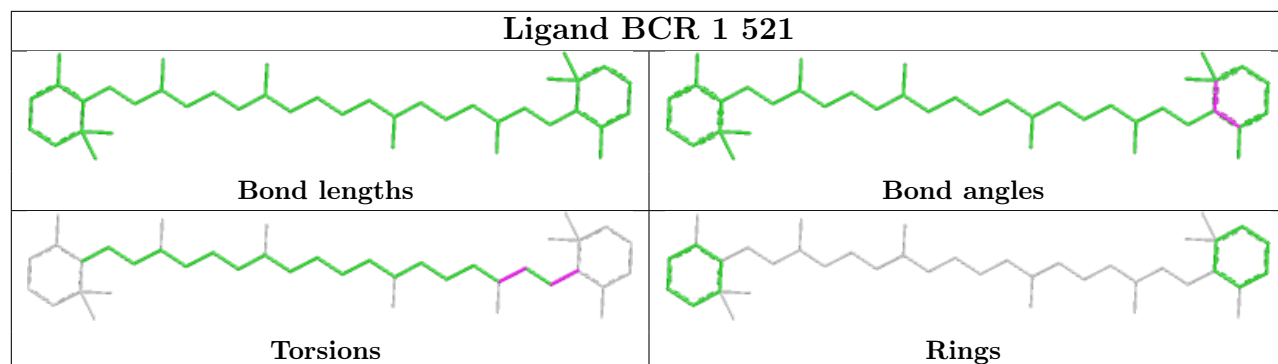


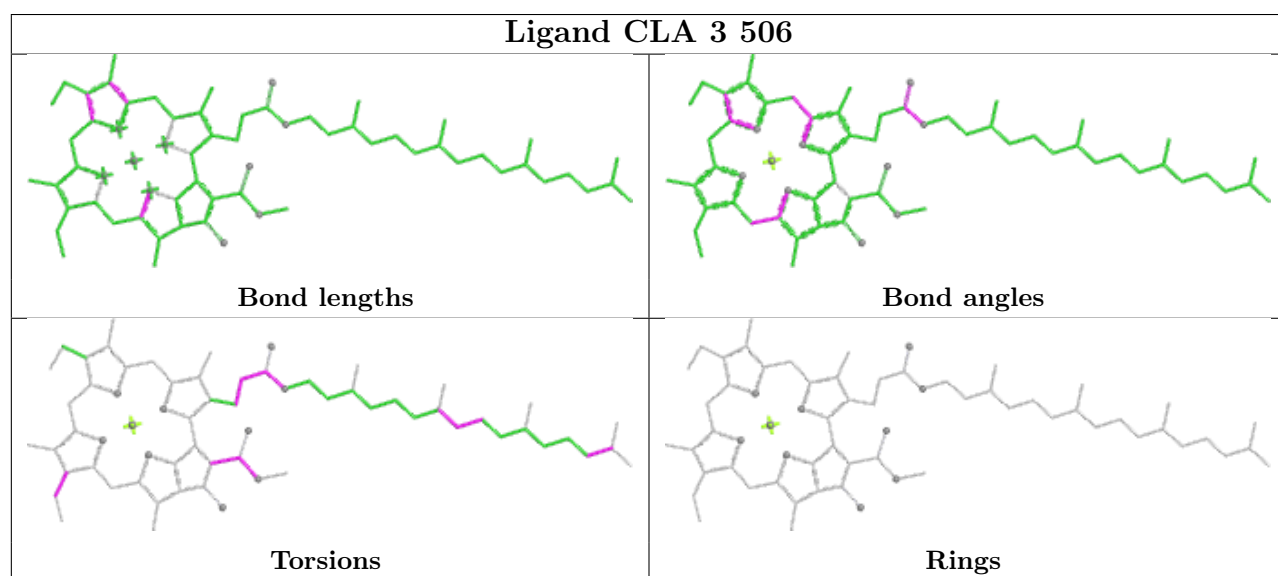
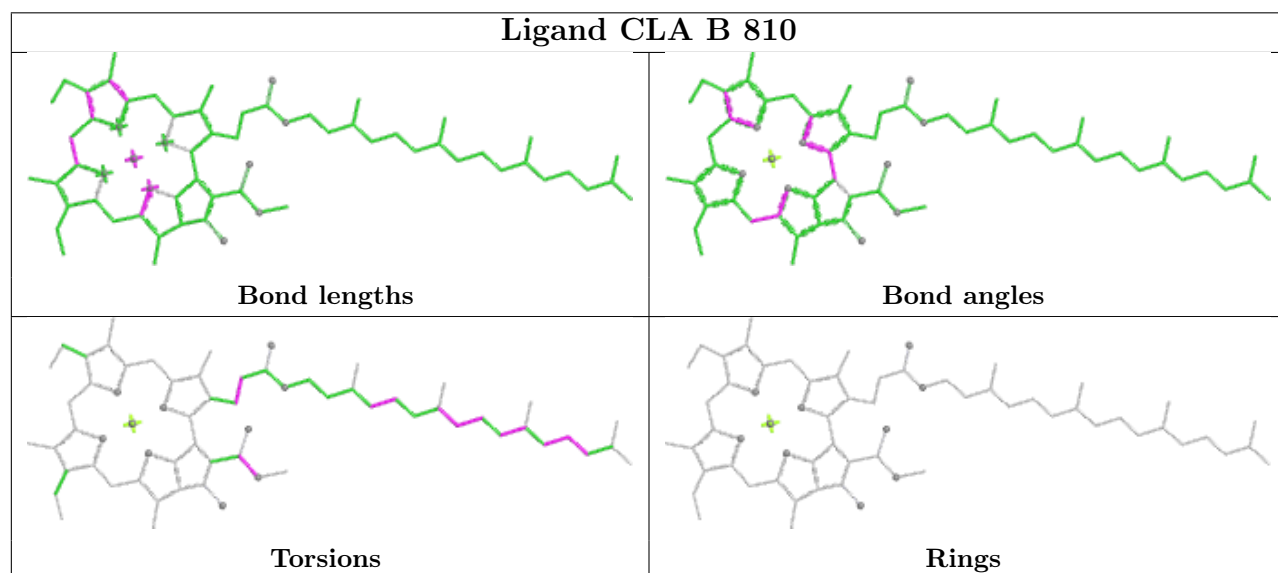
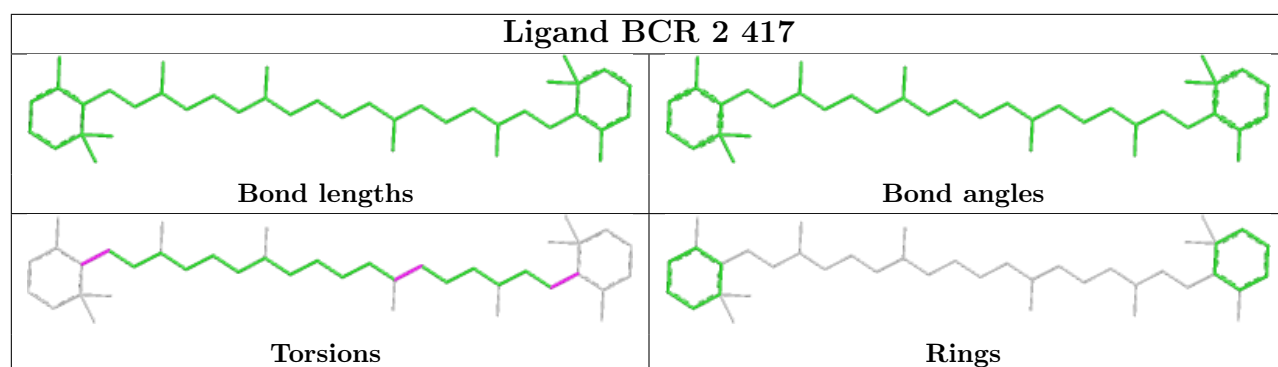
## Ligand CLA 1 514

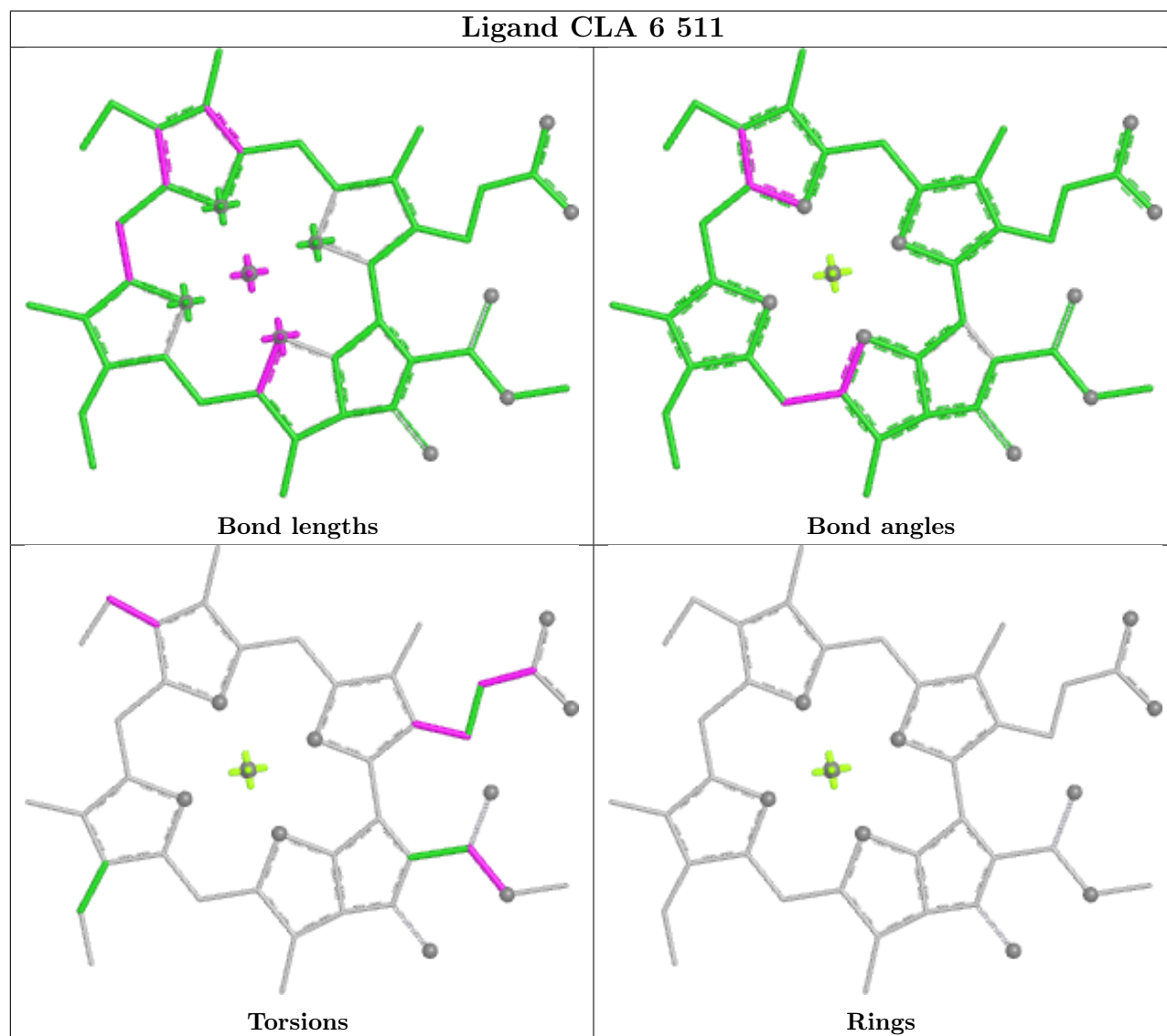
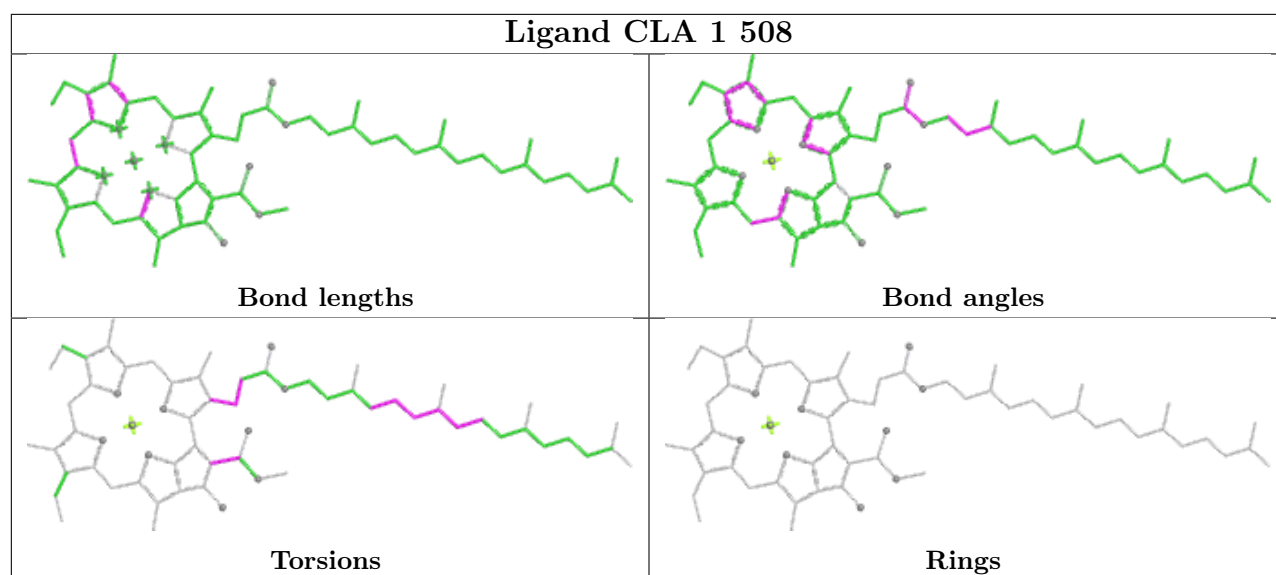




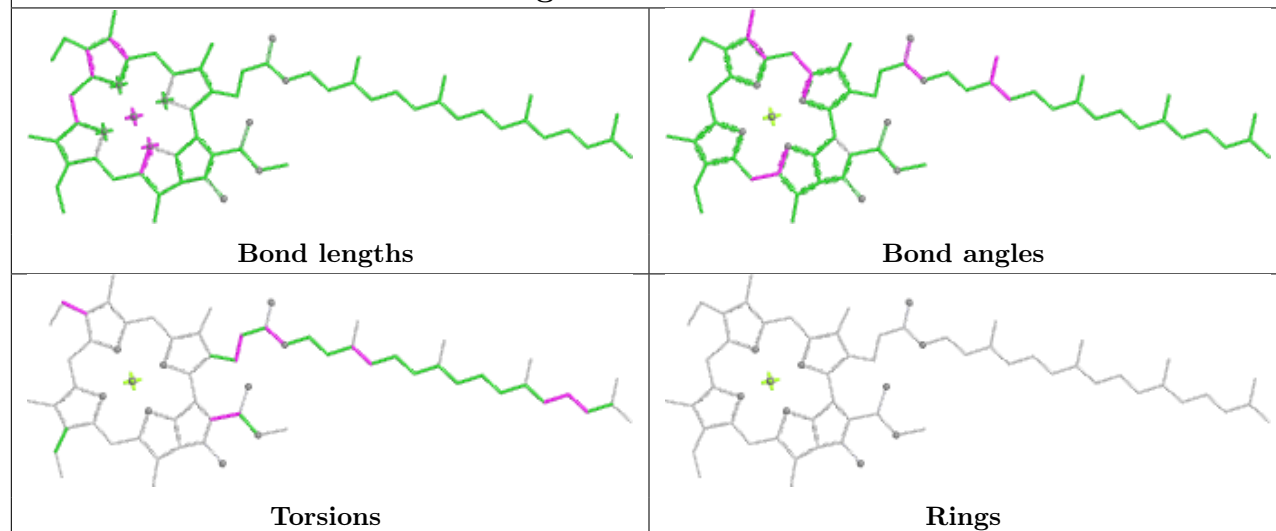




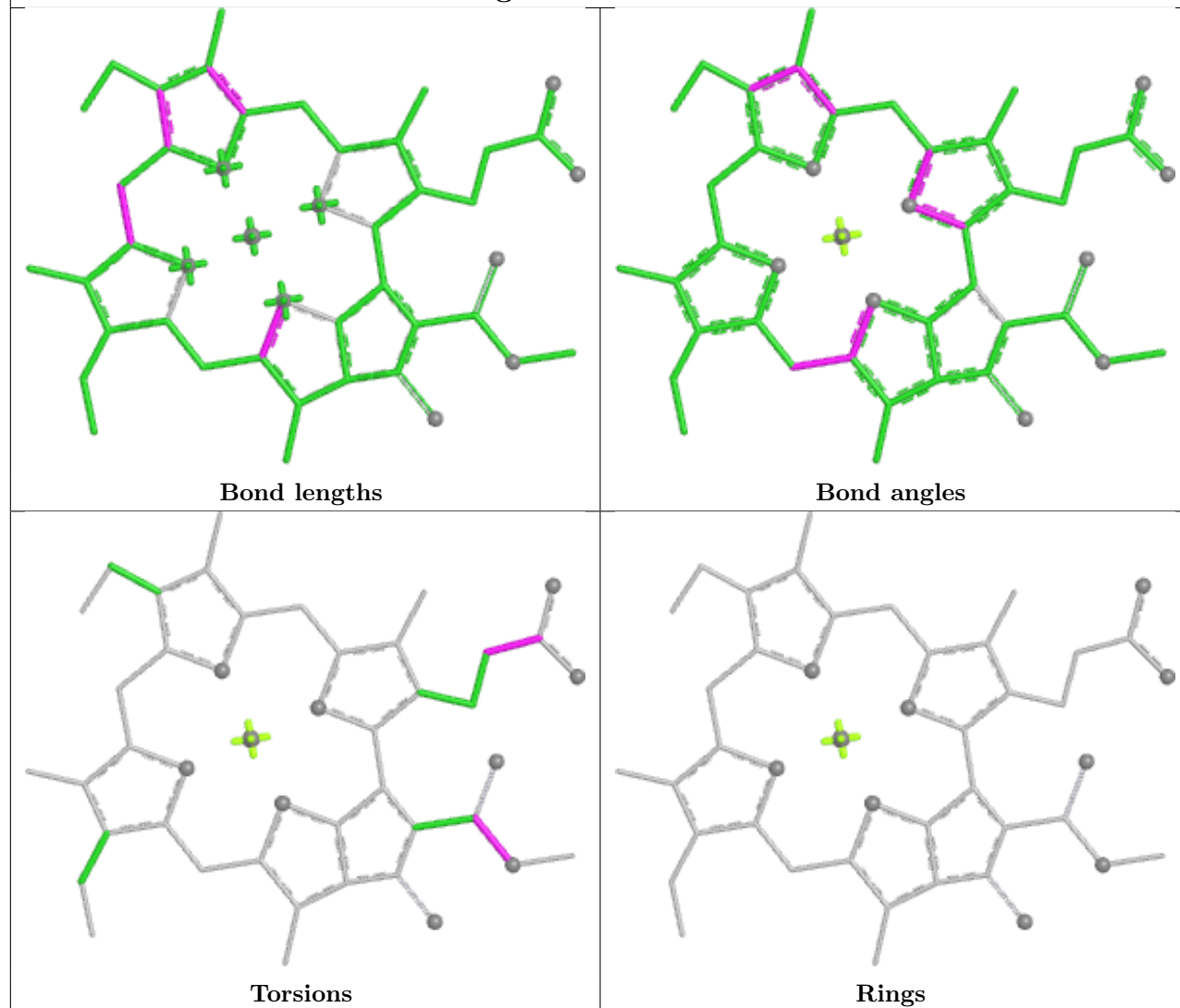


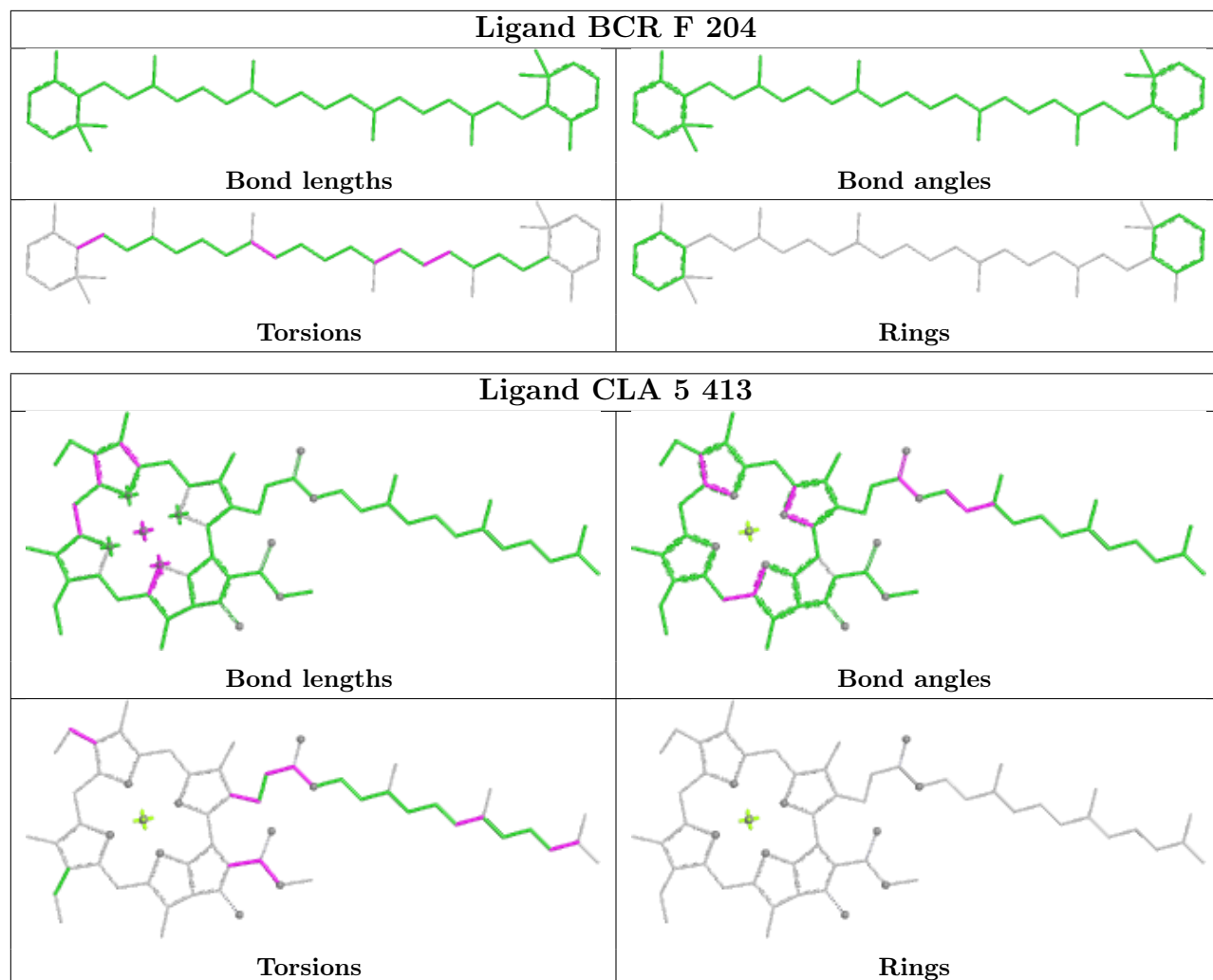


## Ligand CLA 4 407

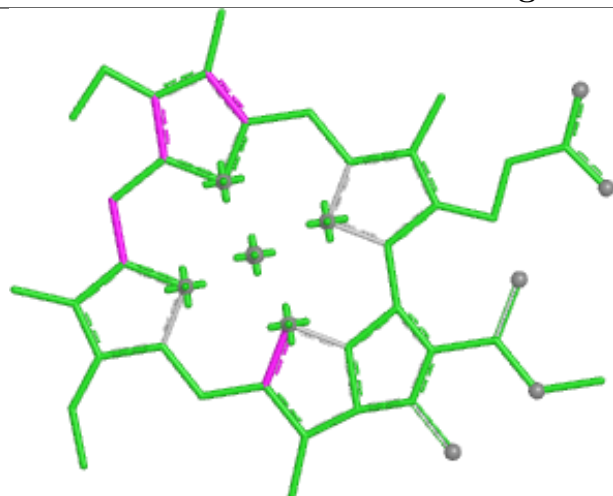


## Ligand CLA 6 517

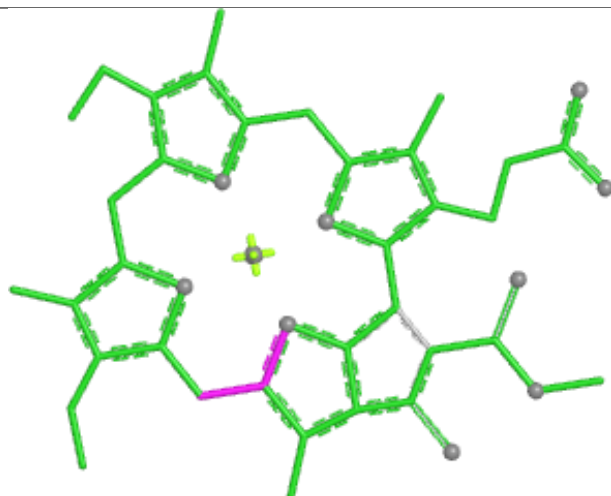




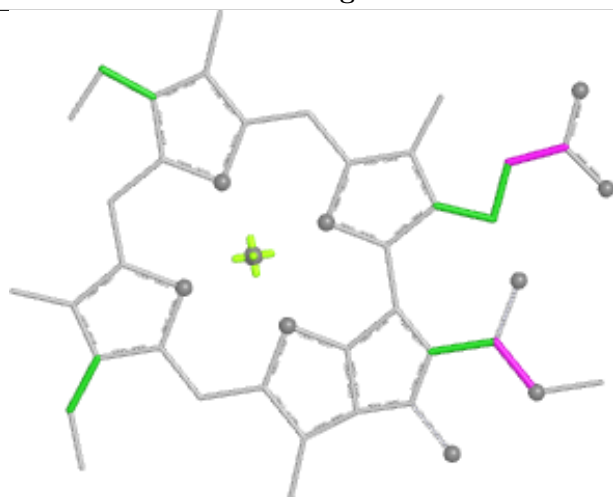
## Ligand CLA 3 513



Bond lengths



Bond angles

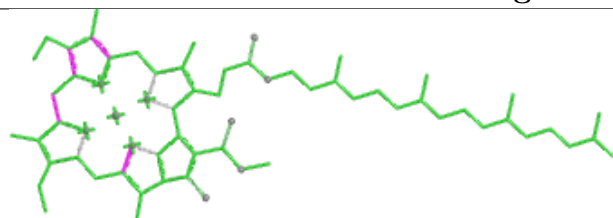


Torsions

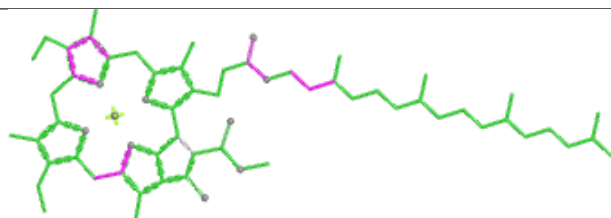


Rings

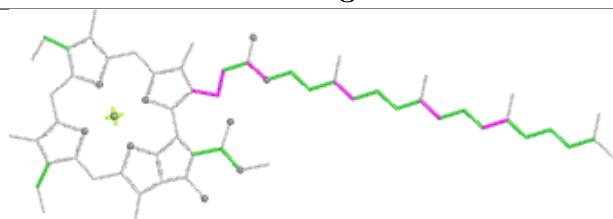
## Ligand CLA A 830



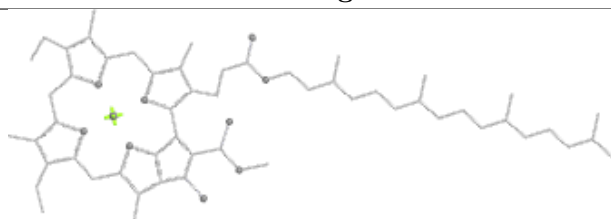
Bond lengths



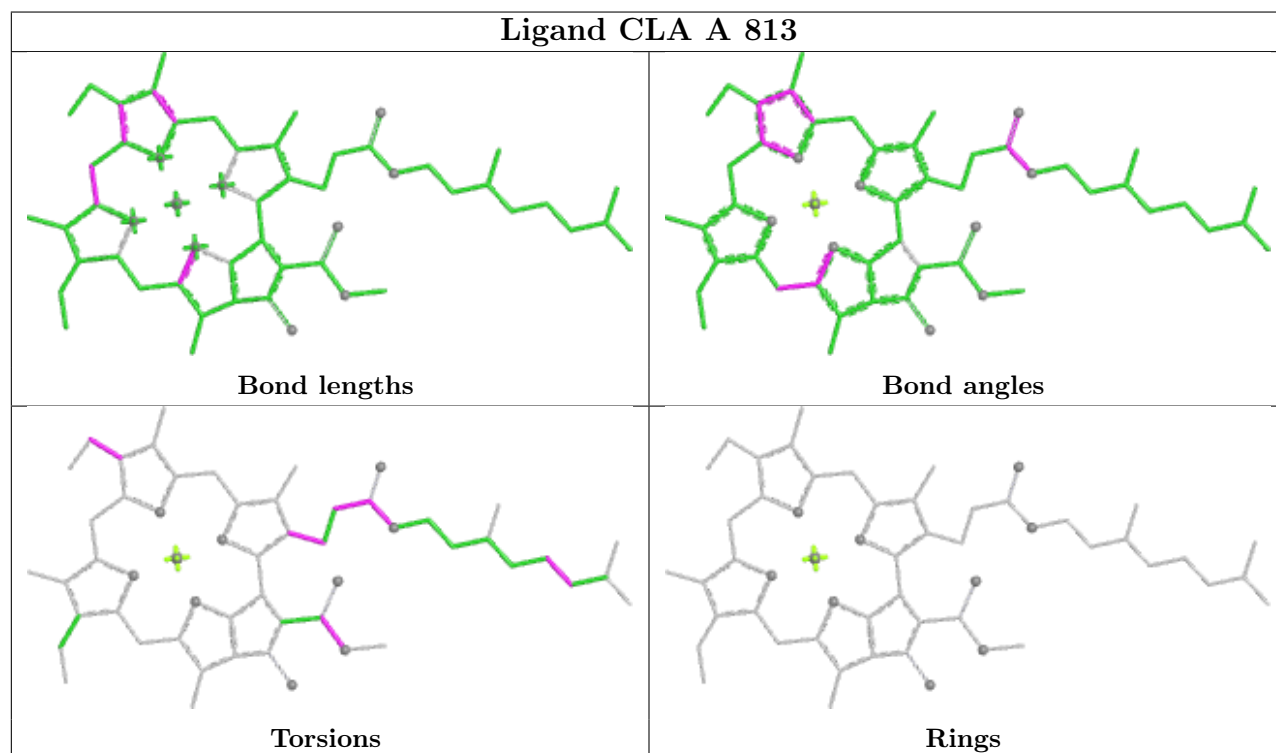
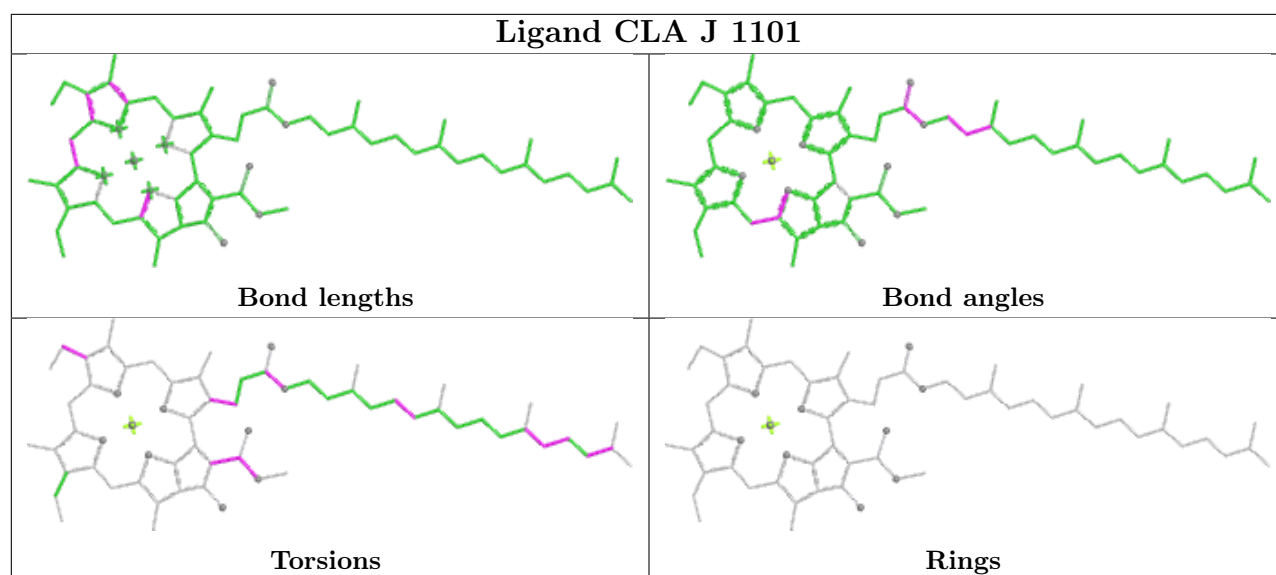
Bond angles



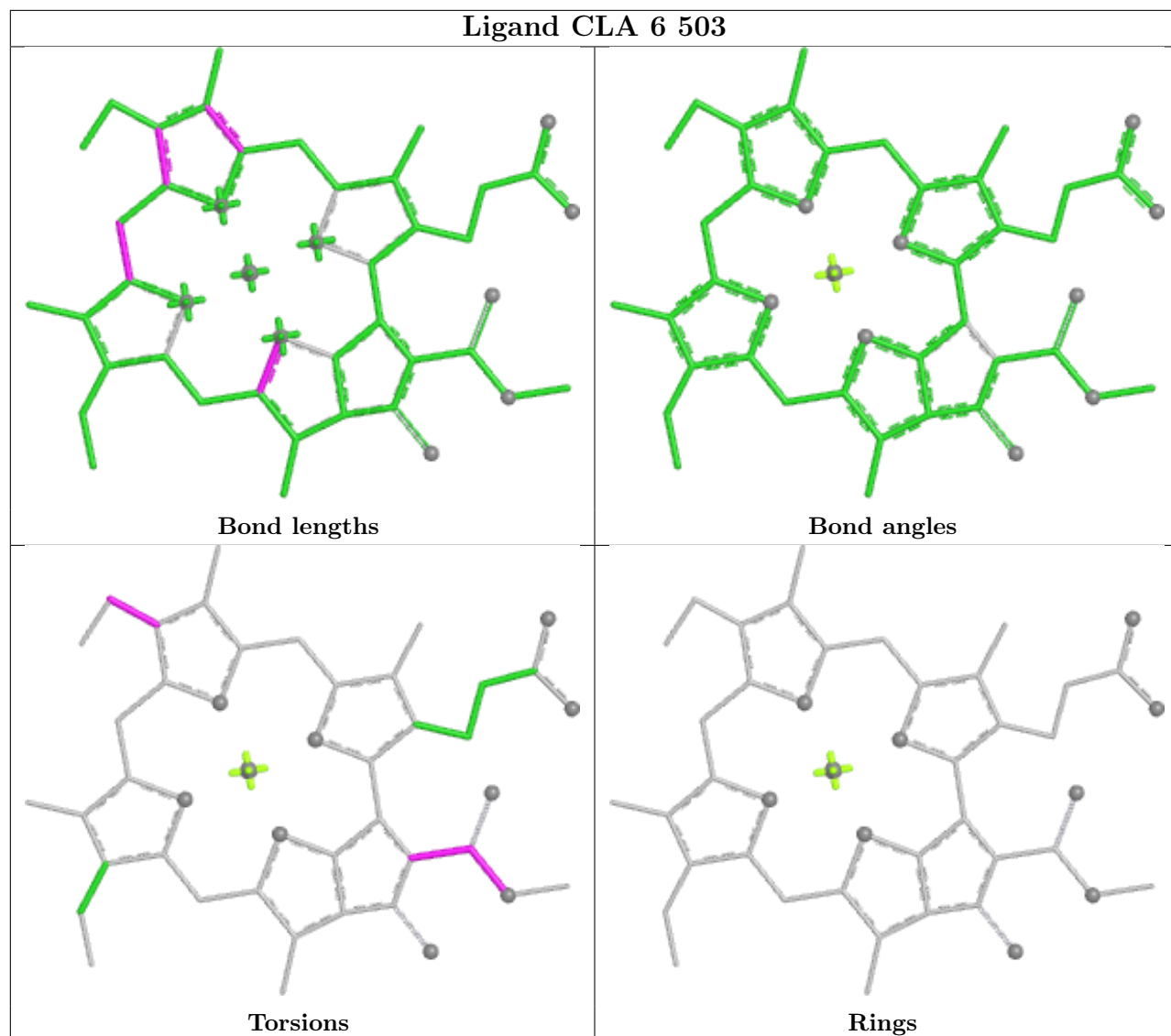
Torsions



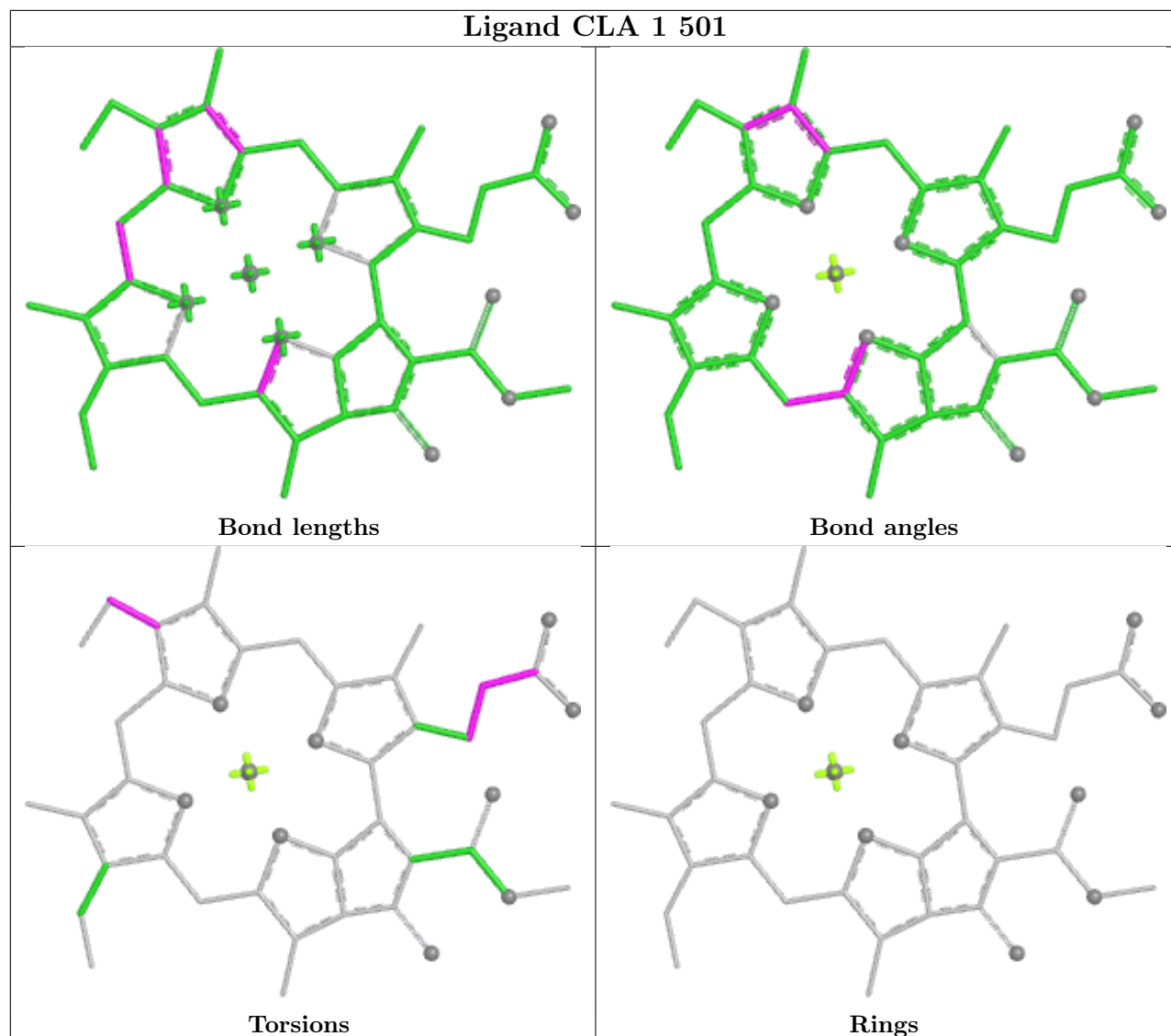
Rings



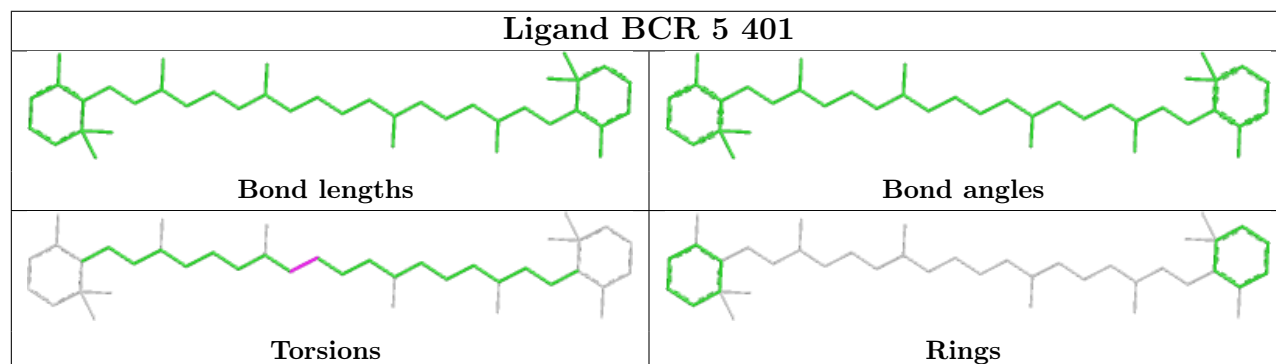
## Ligand CLA 6 503



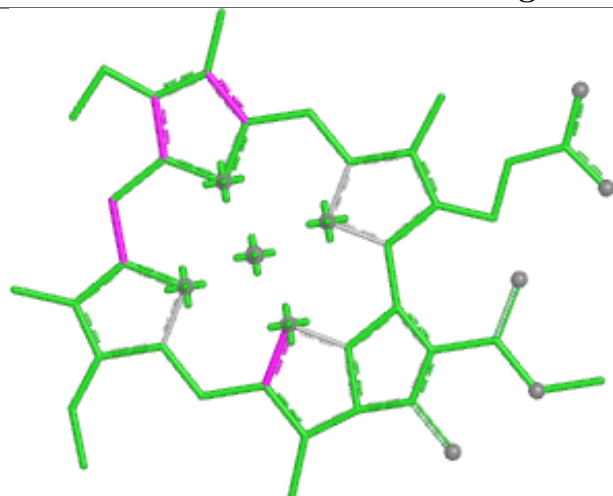
## Ligand CLA 1 501



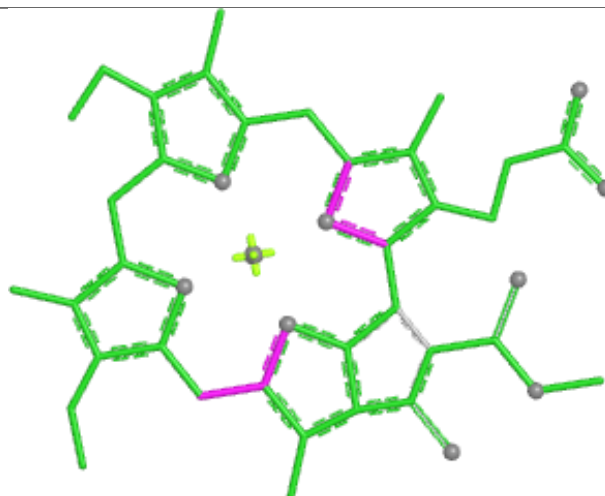
## Ligand BCR 5 401



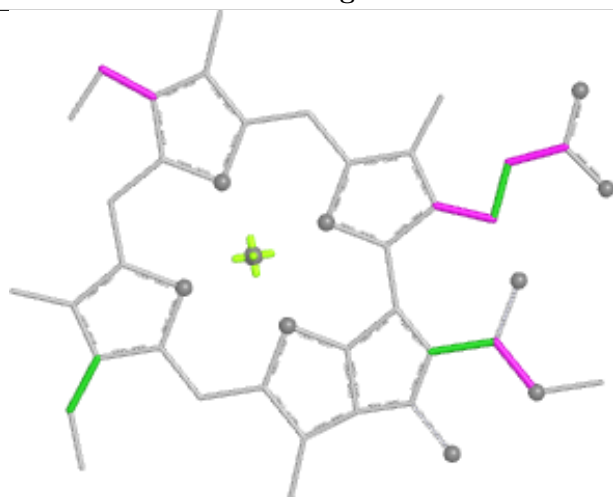
## Ligand CLA 7 514



Bond lengths



Bond angles

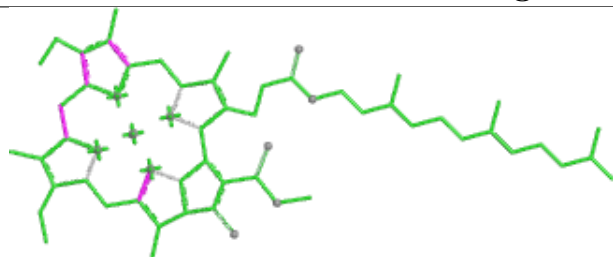


Torsions

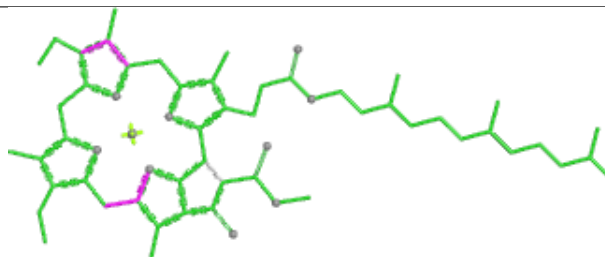


Rings

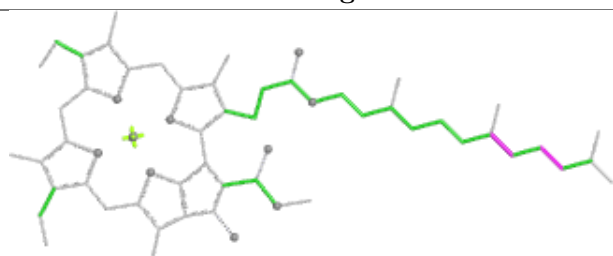
## Ligand CLA A 834



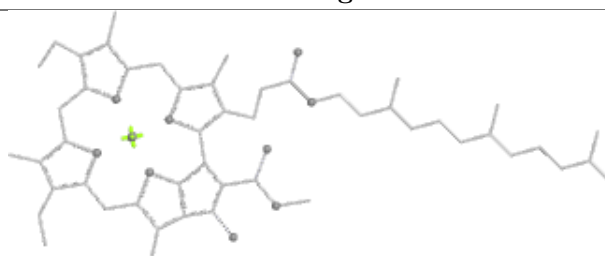
Bond lengths



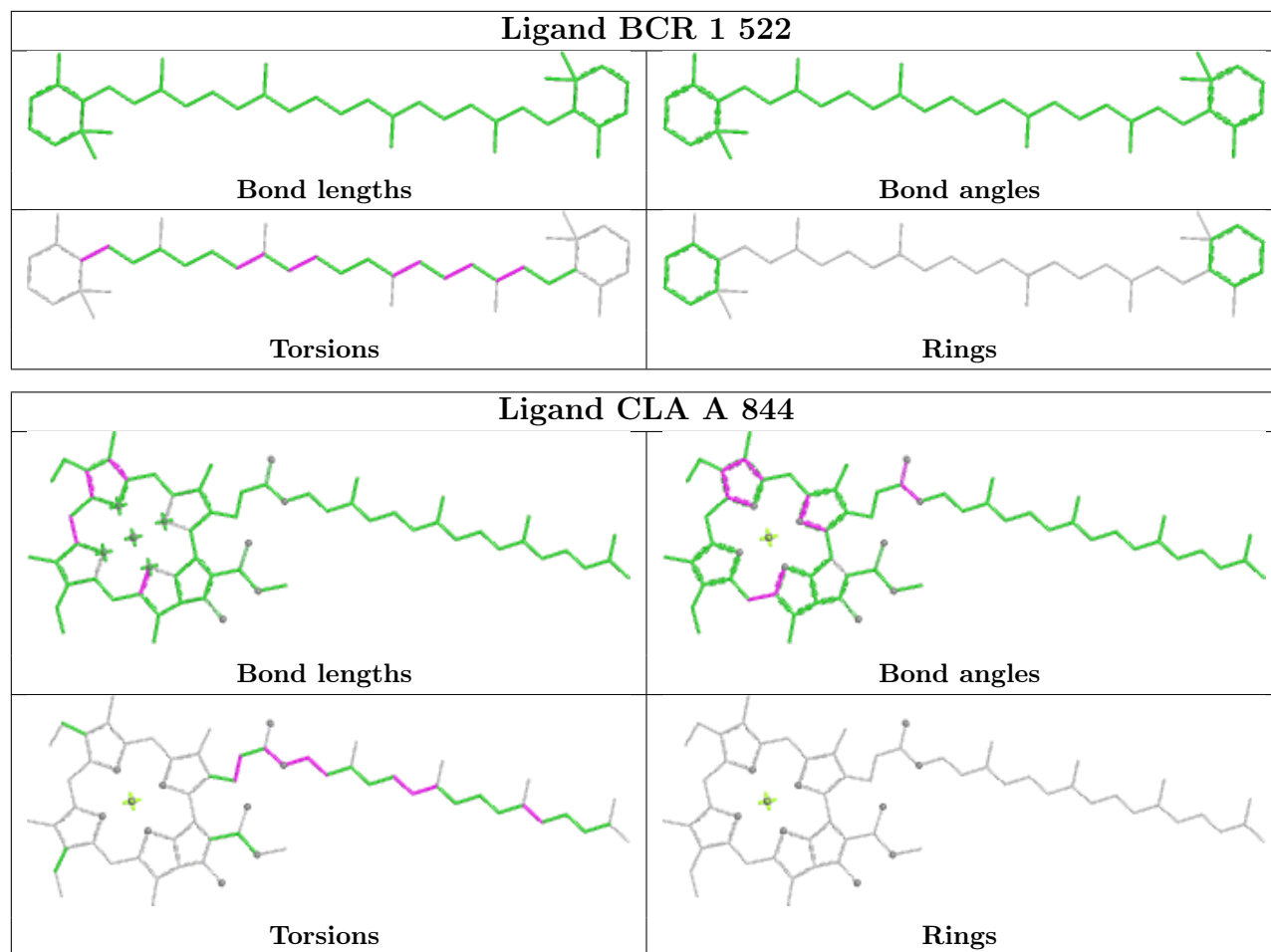
Bond angles



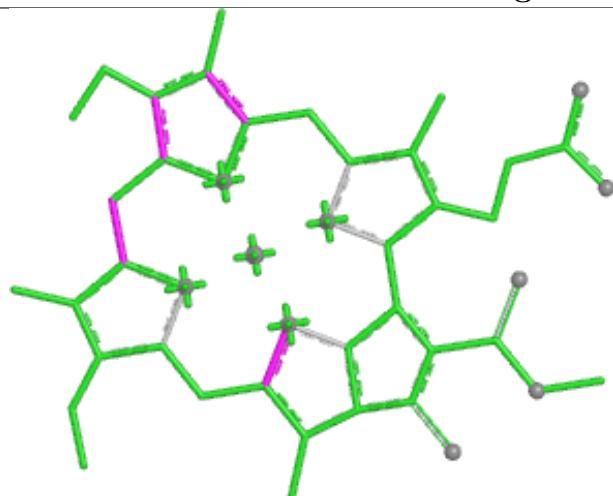
Torsions



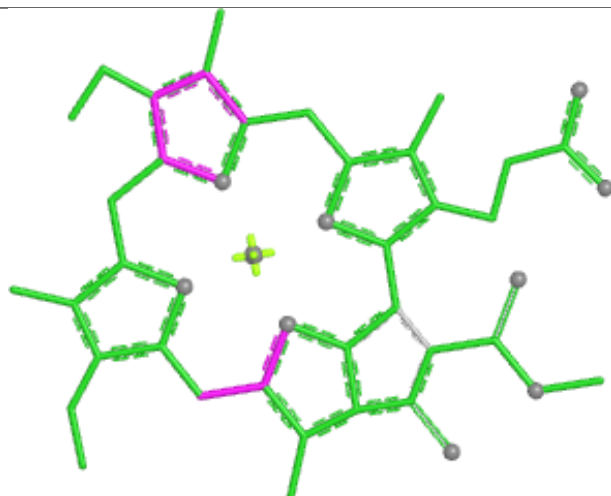
Rings



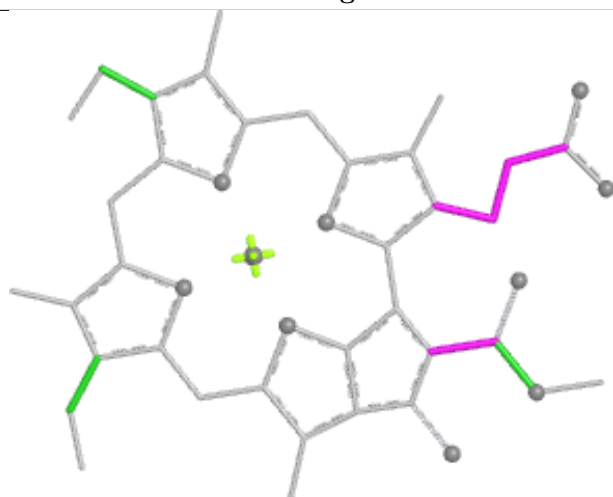
## Ligand CLA B 822



Bond lengths



Bond angles

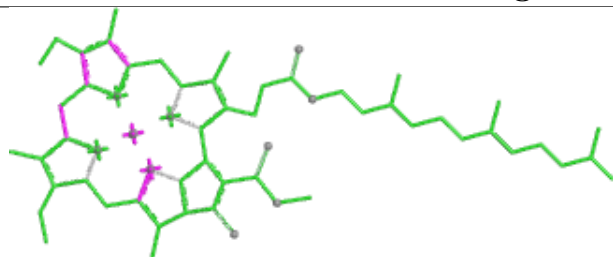


Torsions

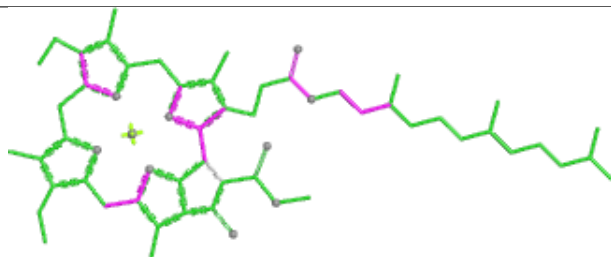


Rings

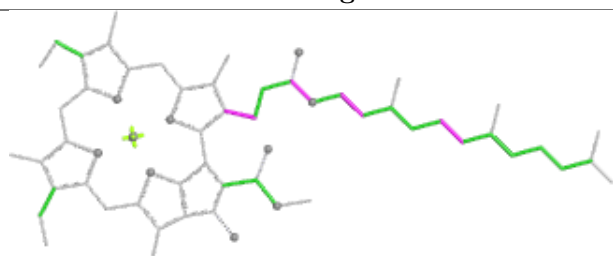
## Ligand CLA A 815



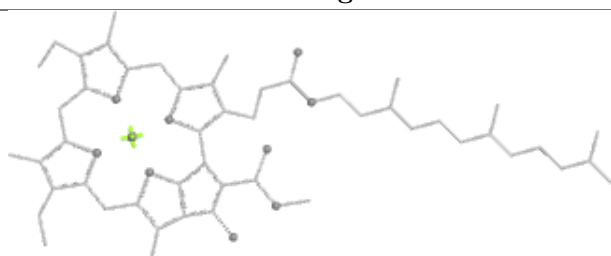
Bond lengths



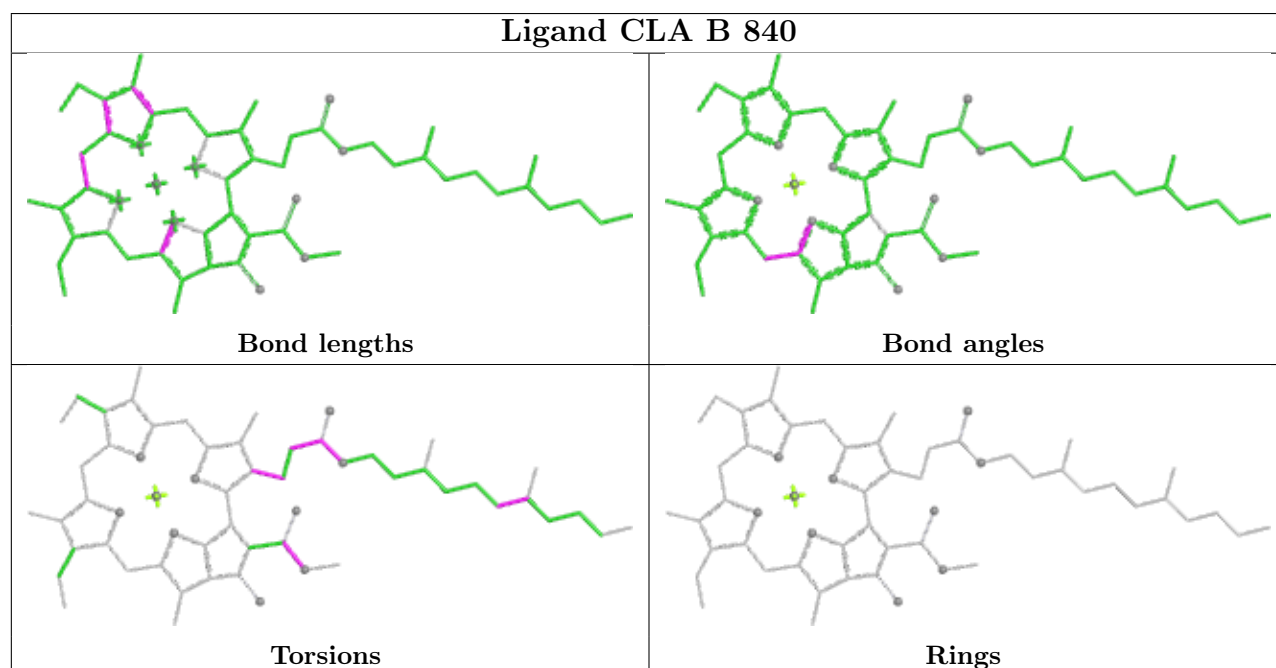
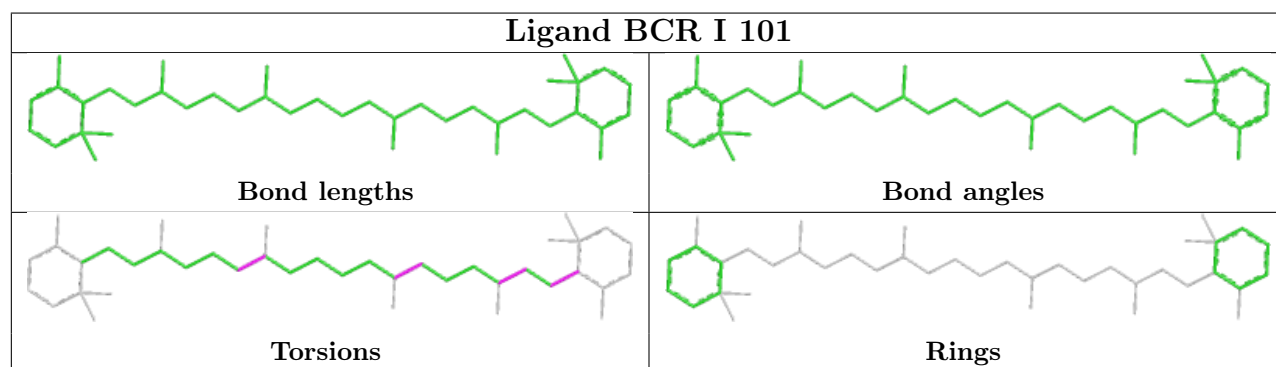
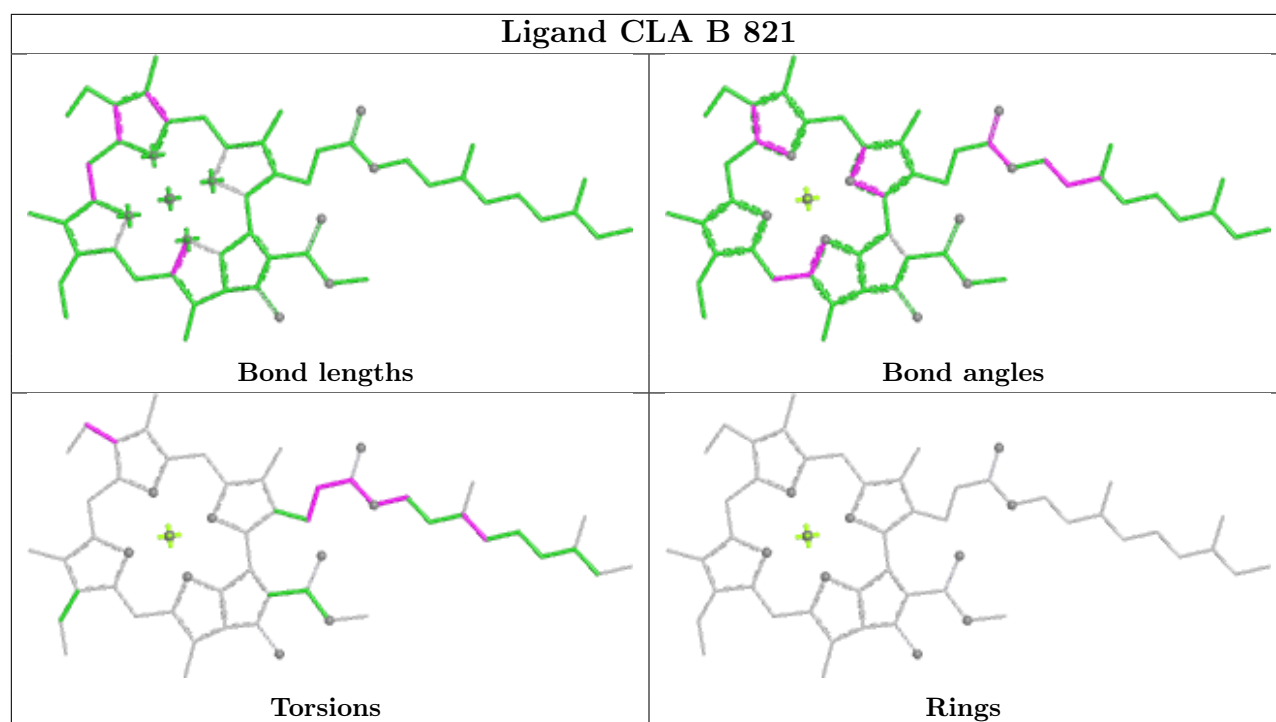
Bond angles

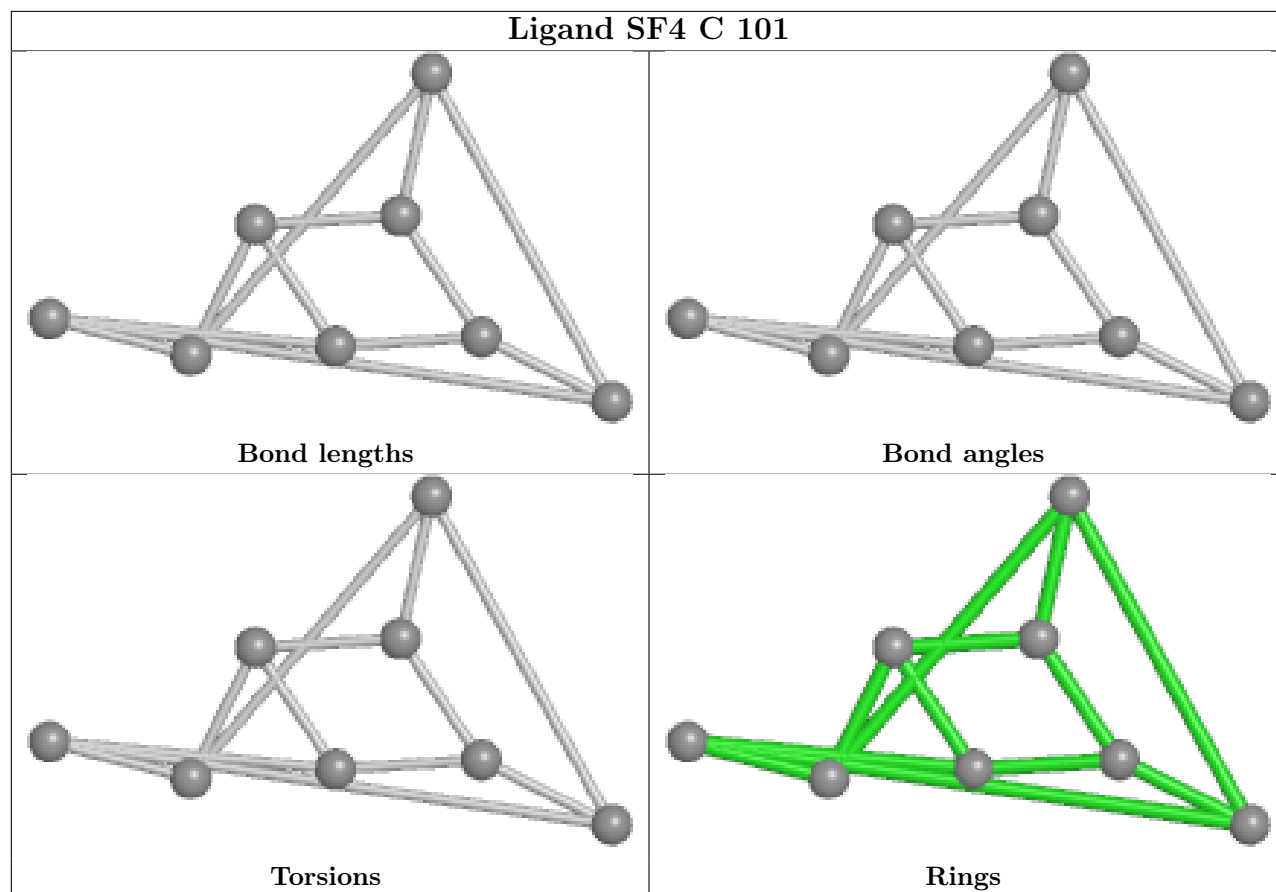


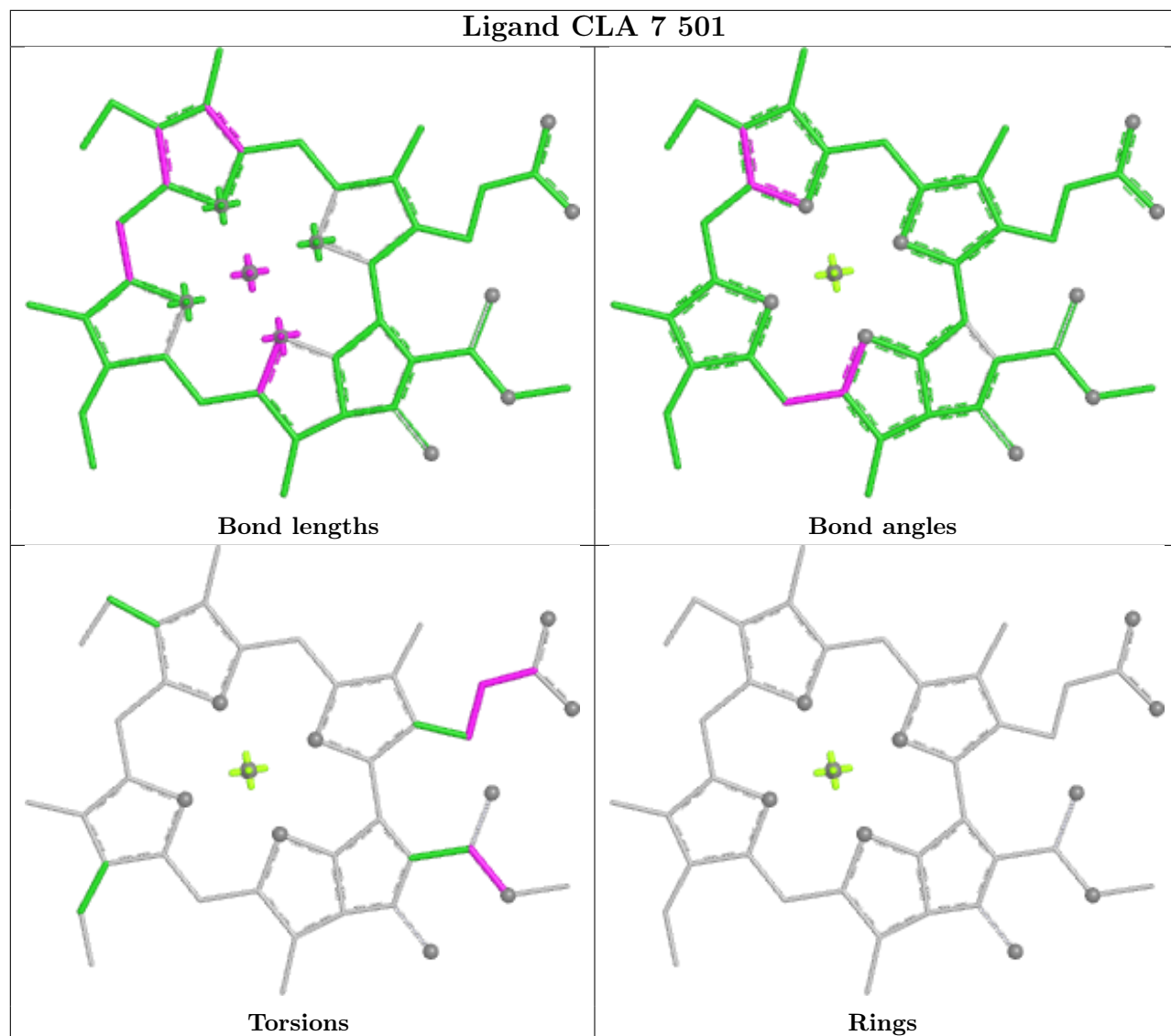
Torsions



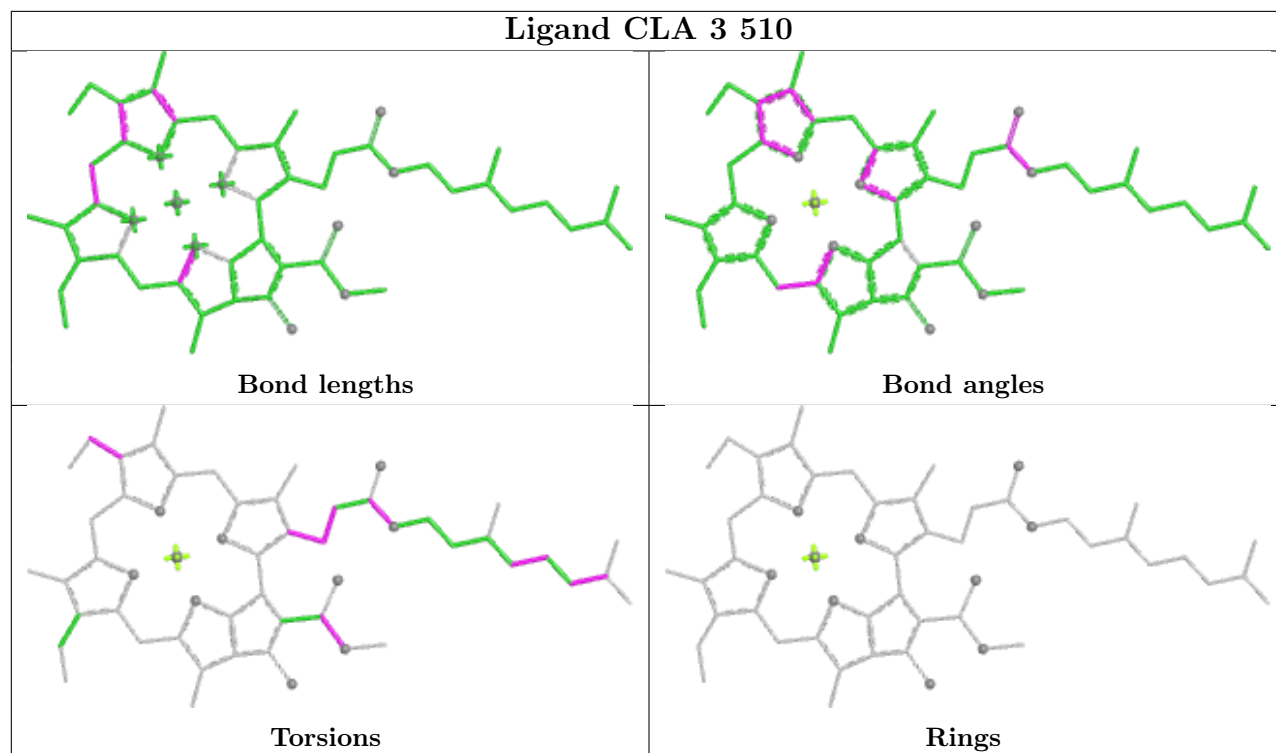
Rings



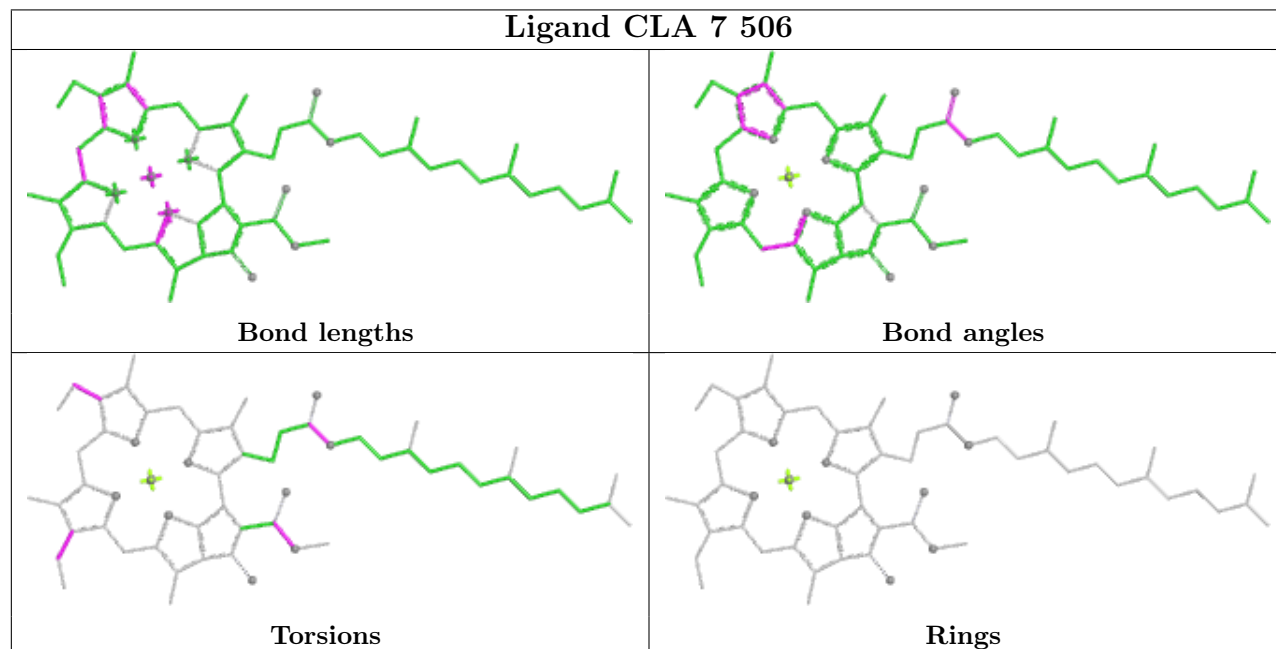




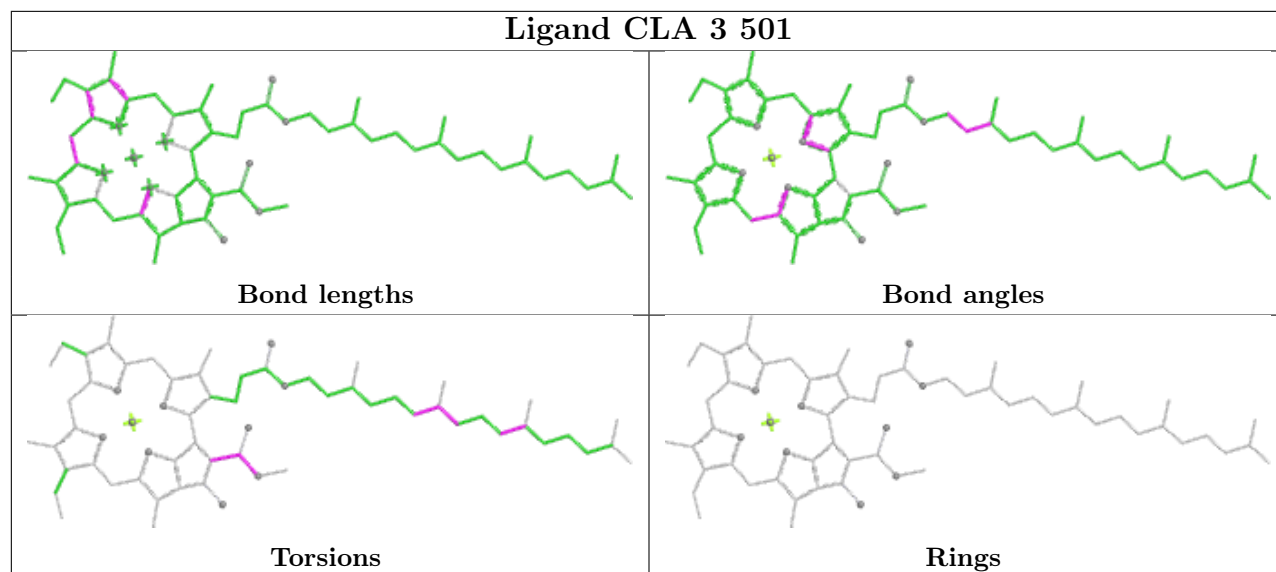
## Ligand CLA 3 510



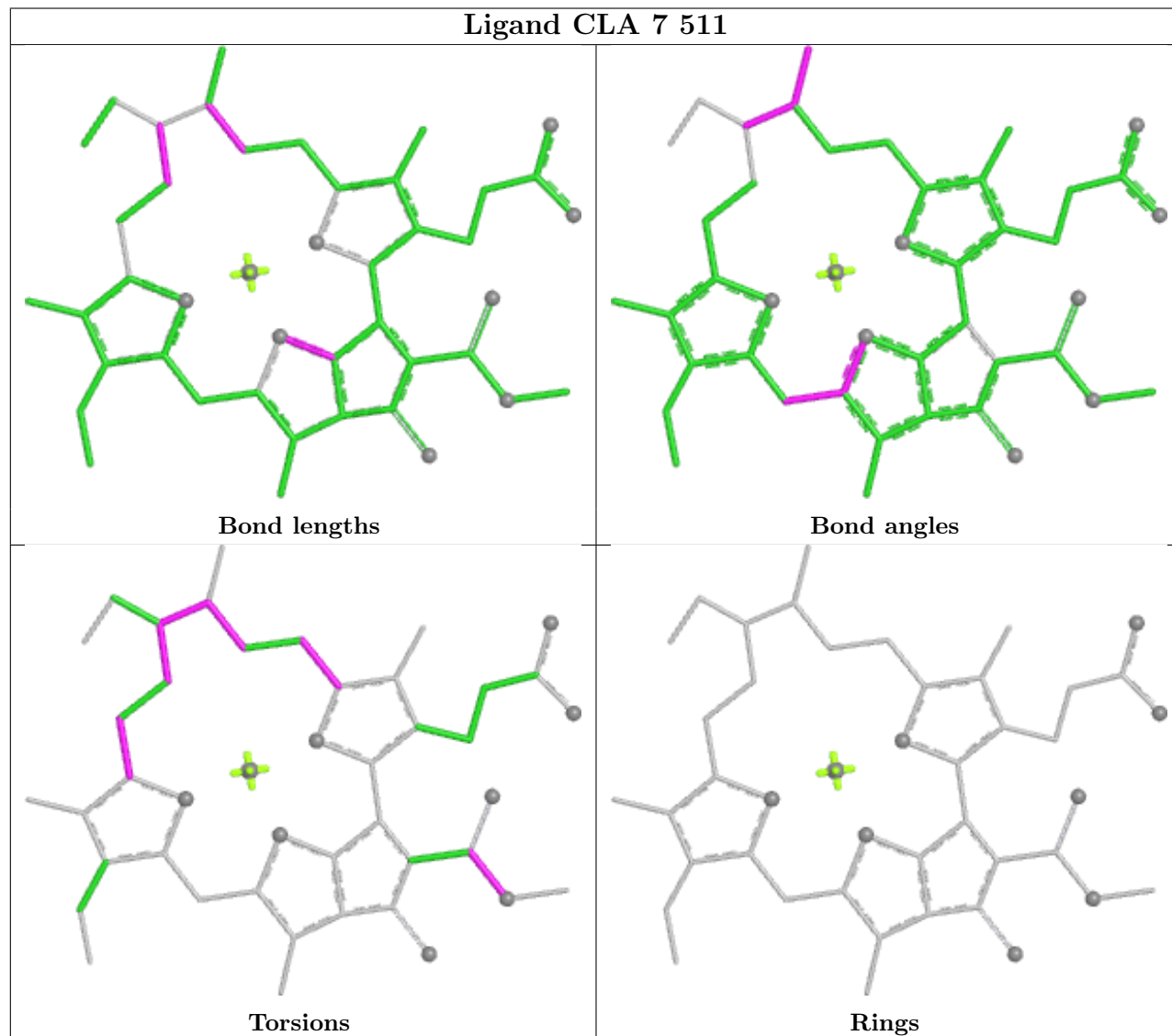
## Ligand CLA 7 506

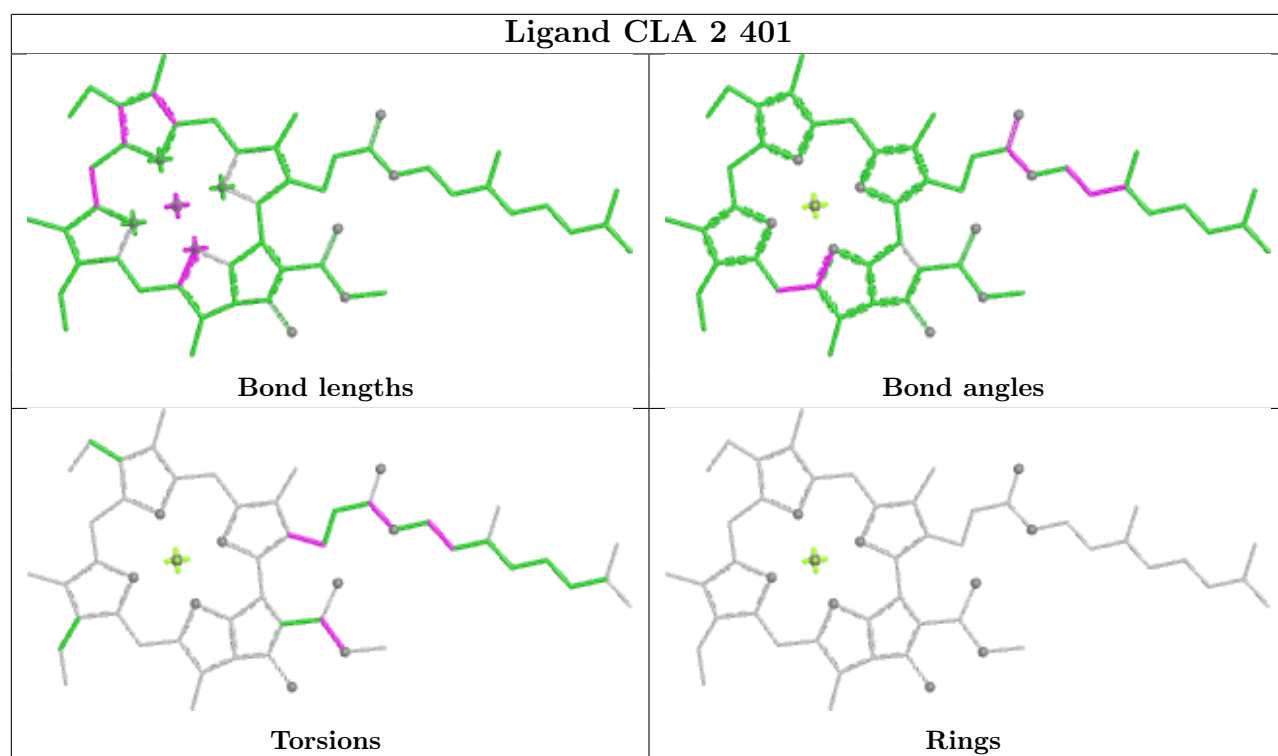


## Ligand CLA 3 501

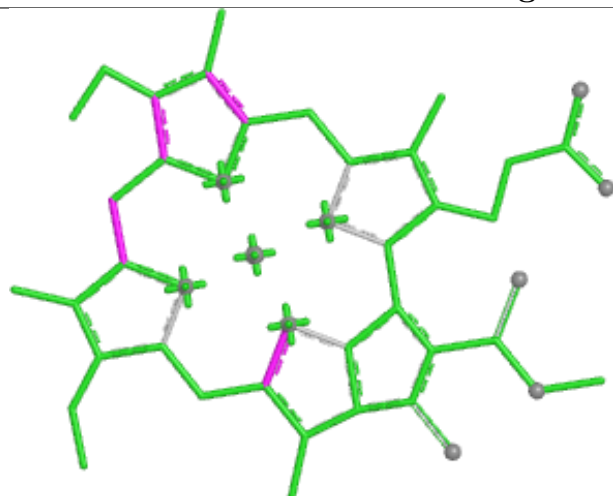


## Ligand CLA 7 511

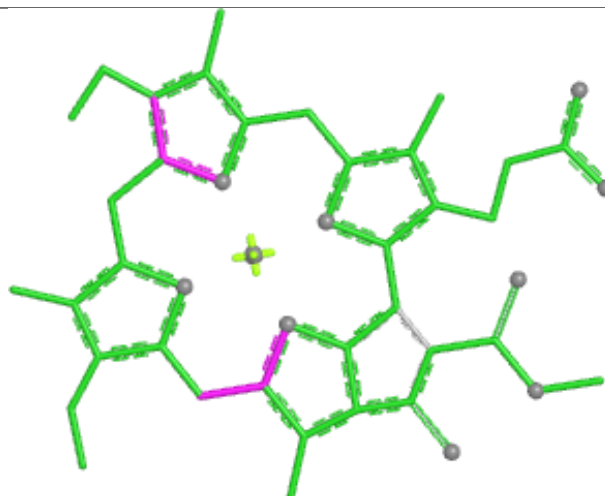




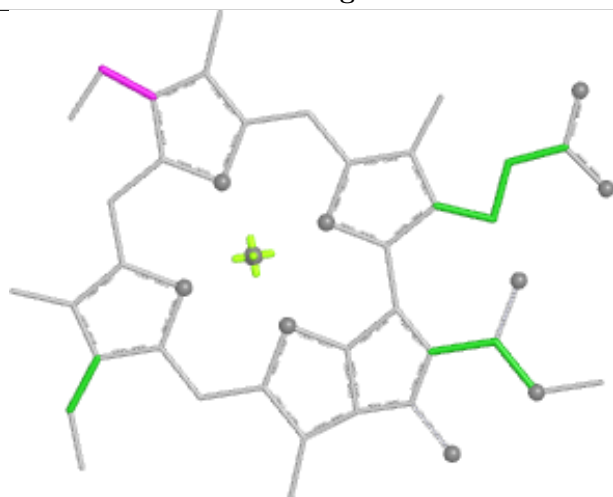
## Ligand CLA 5 415



Bond lengths



Bond angles

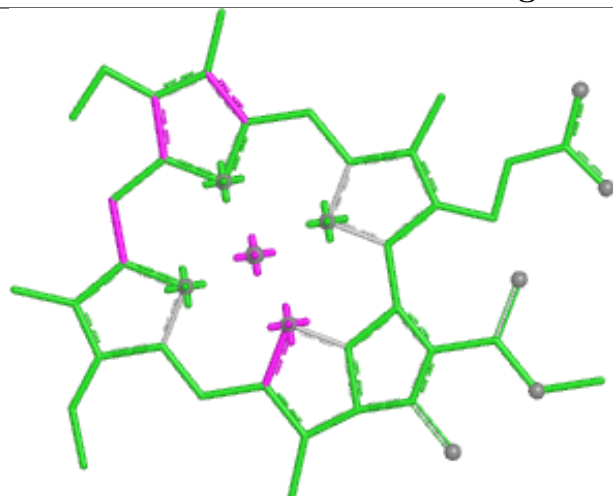


Torsions

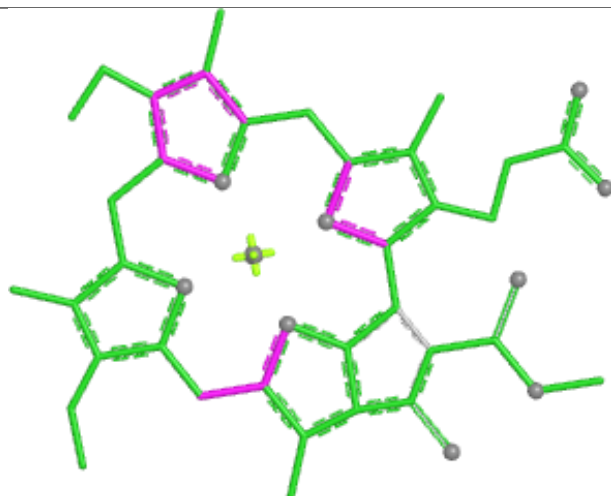


Rings

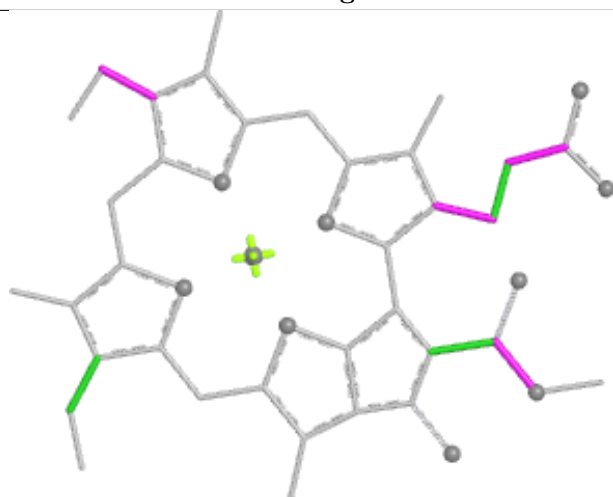
## Ligand CLA 7 513



Bond lengths



Bond angles

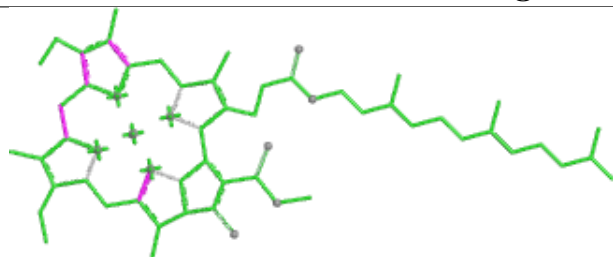


Torsions

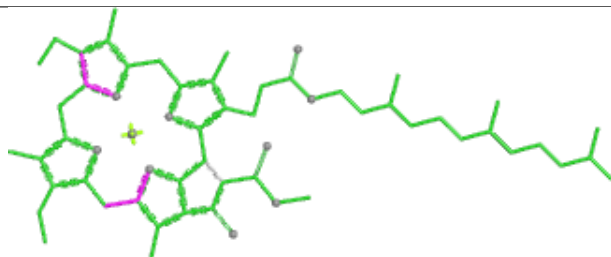


Rings

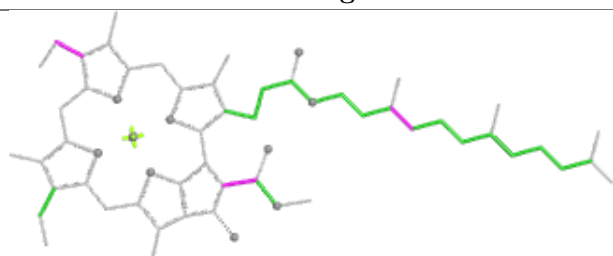
## Ligand CLA B 817



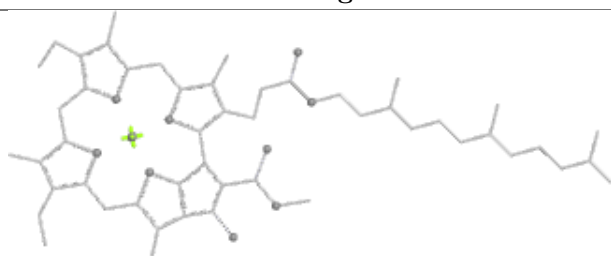
Bond lengths



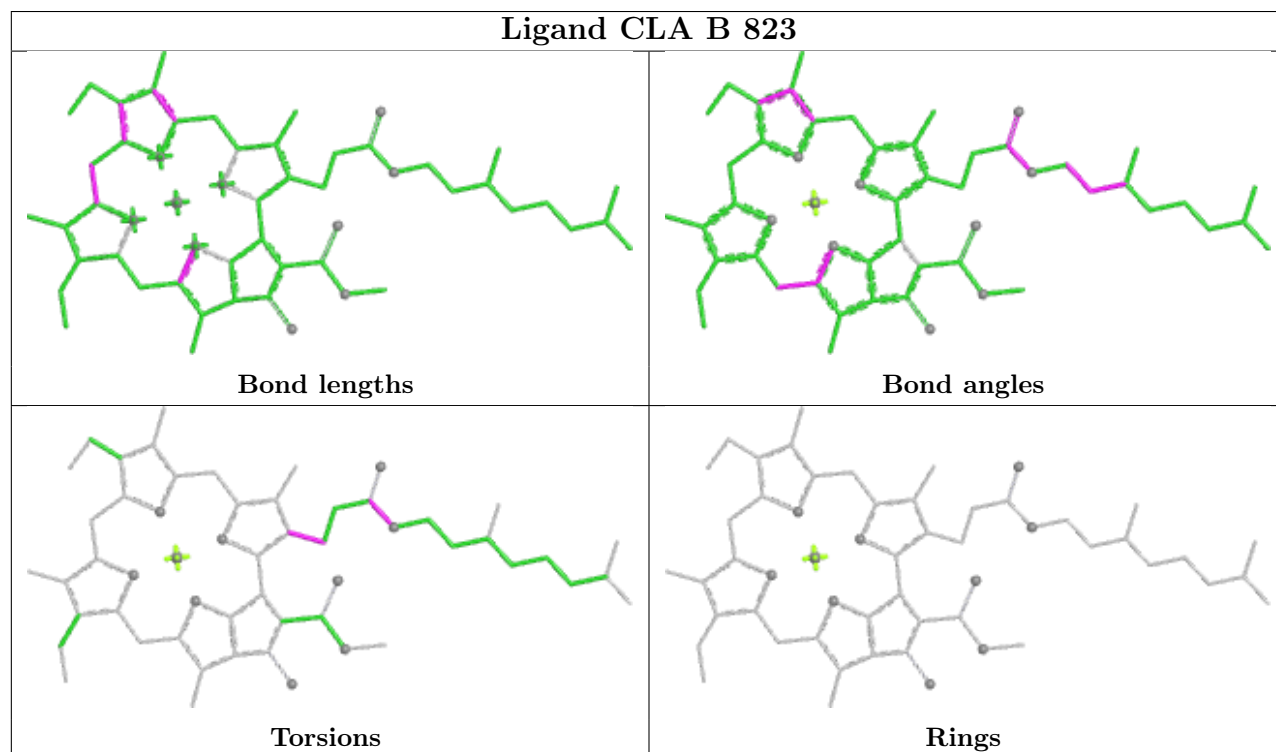
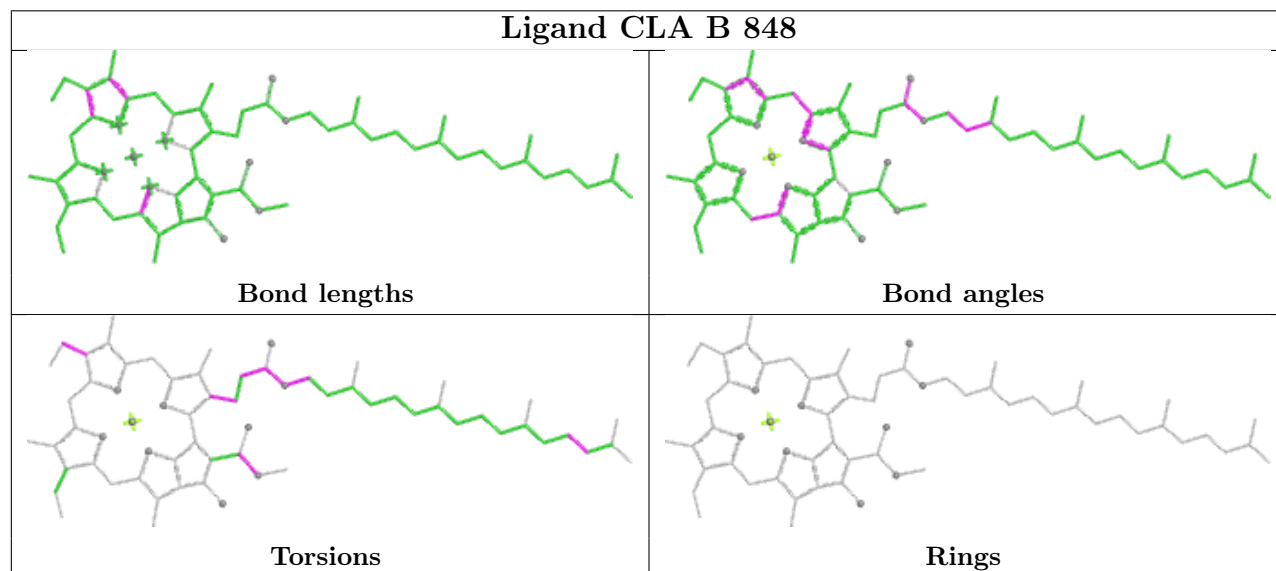
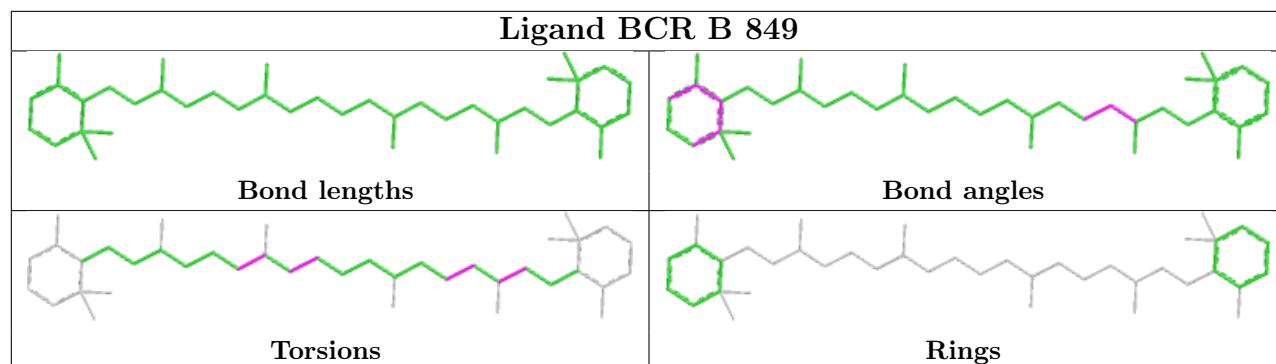
Bond angles



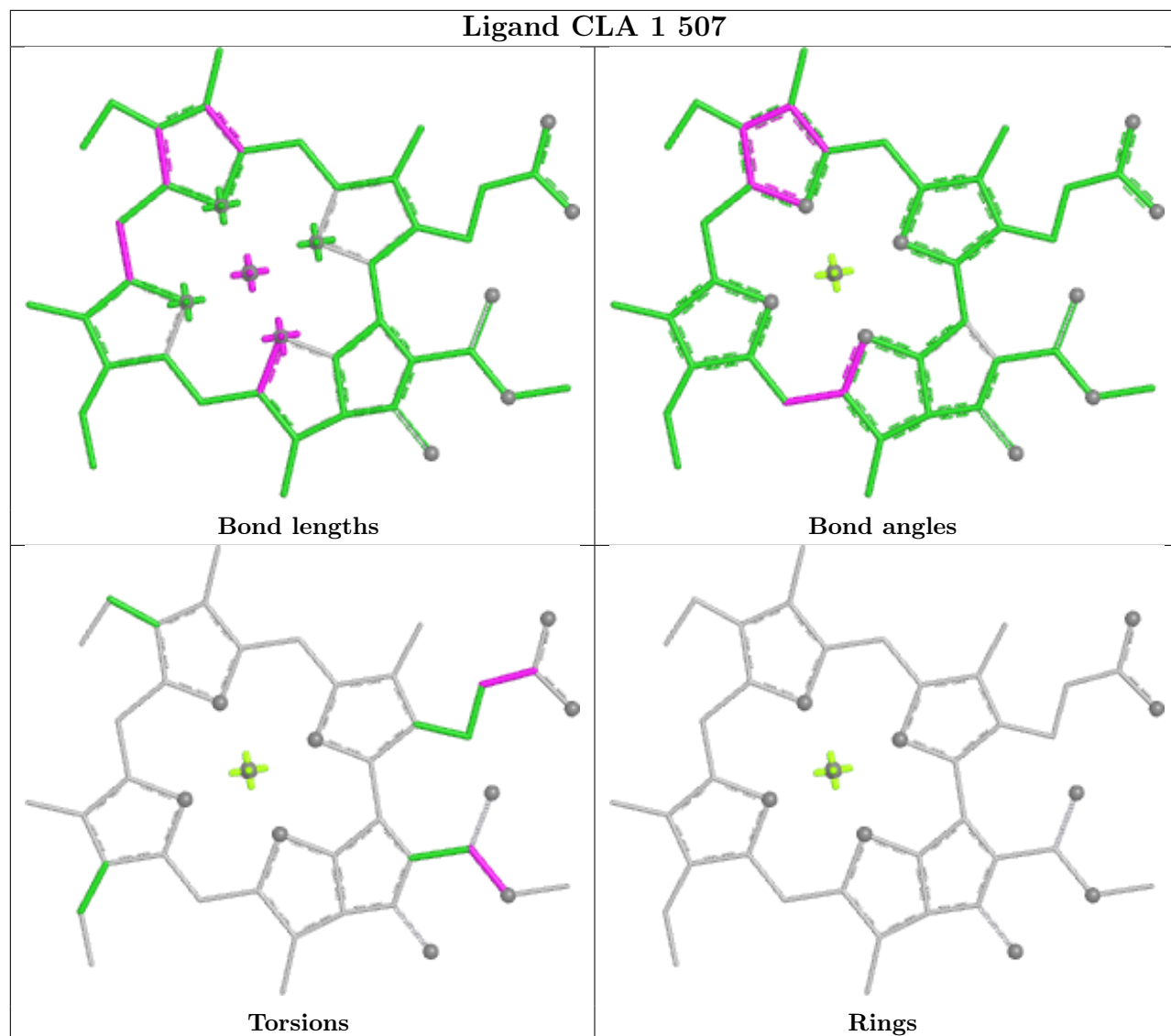
Torsions



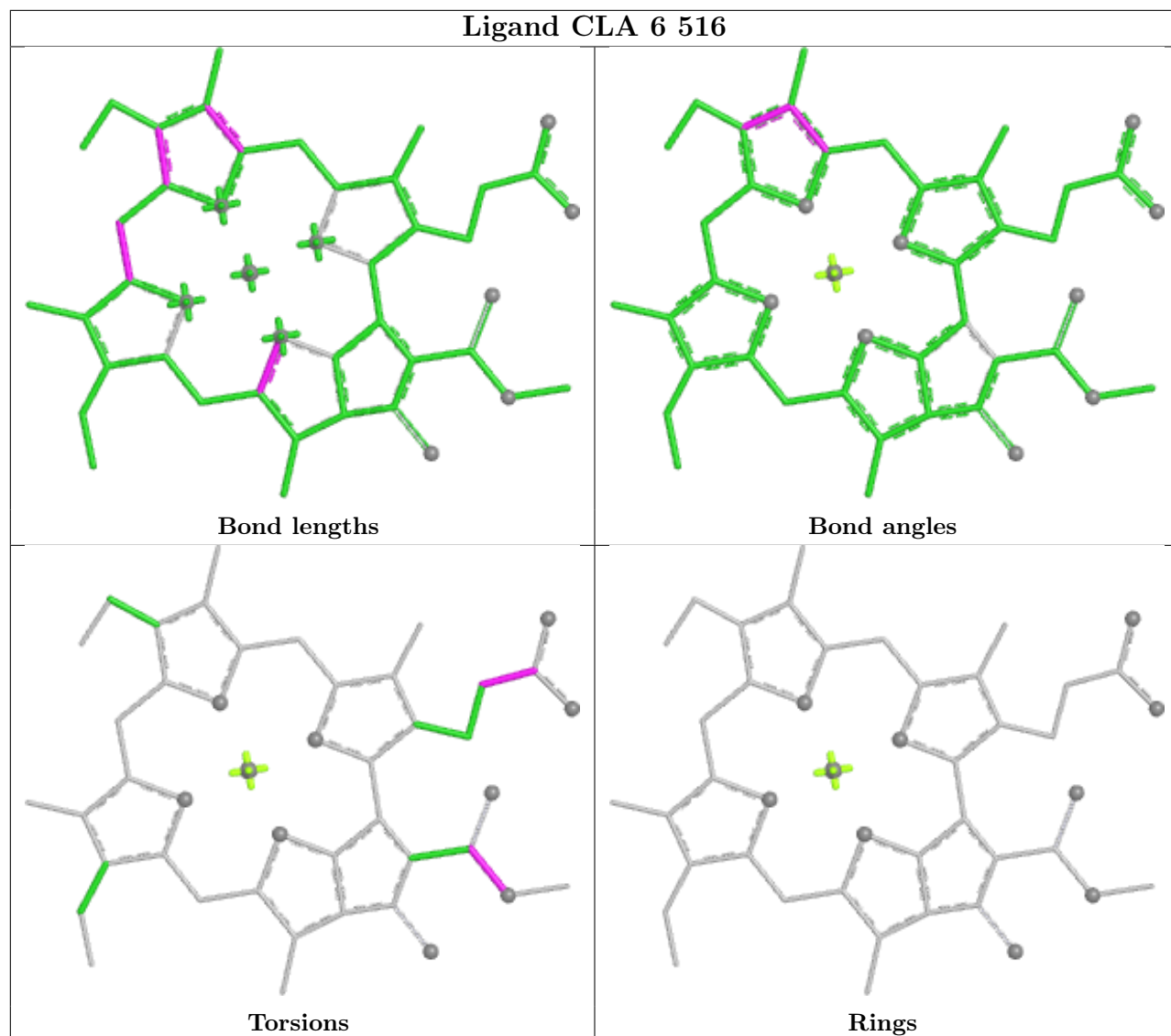
Rings



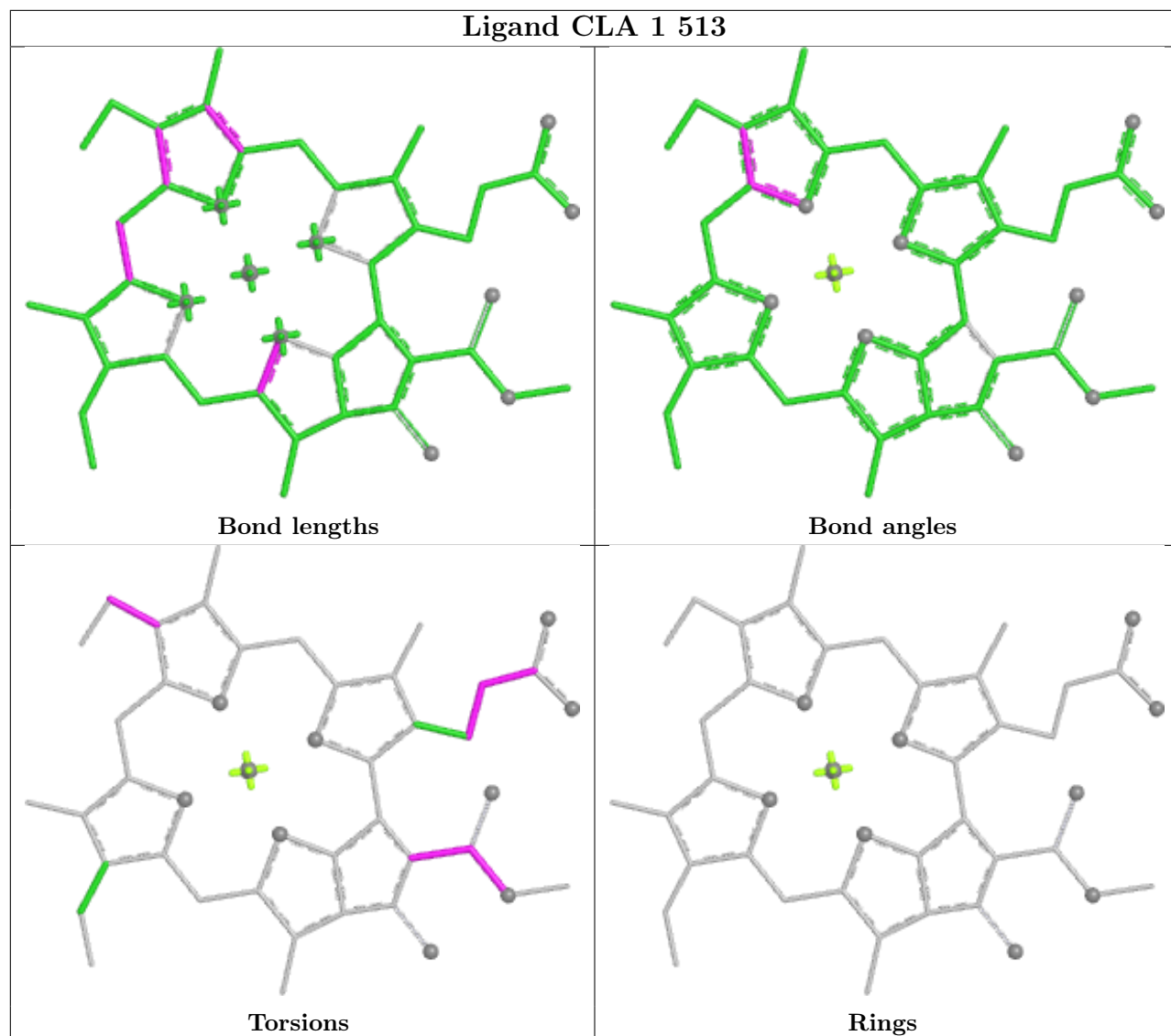
## Ligand CLA 1 507

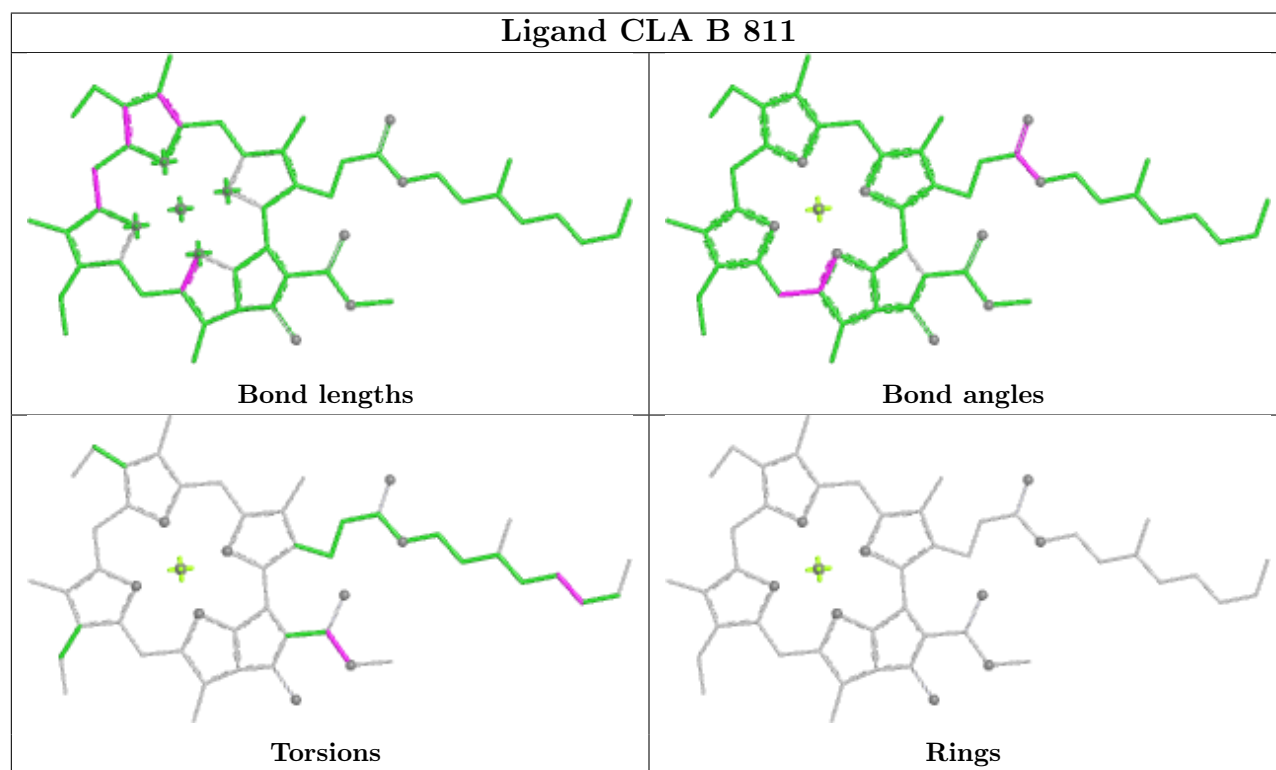
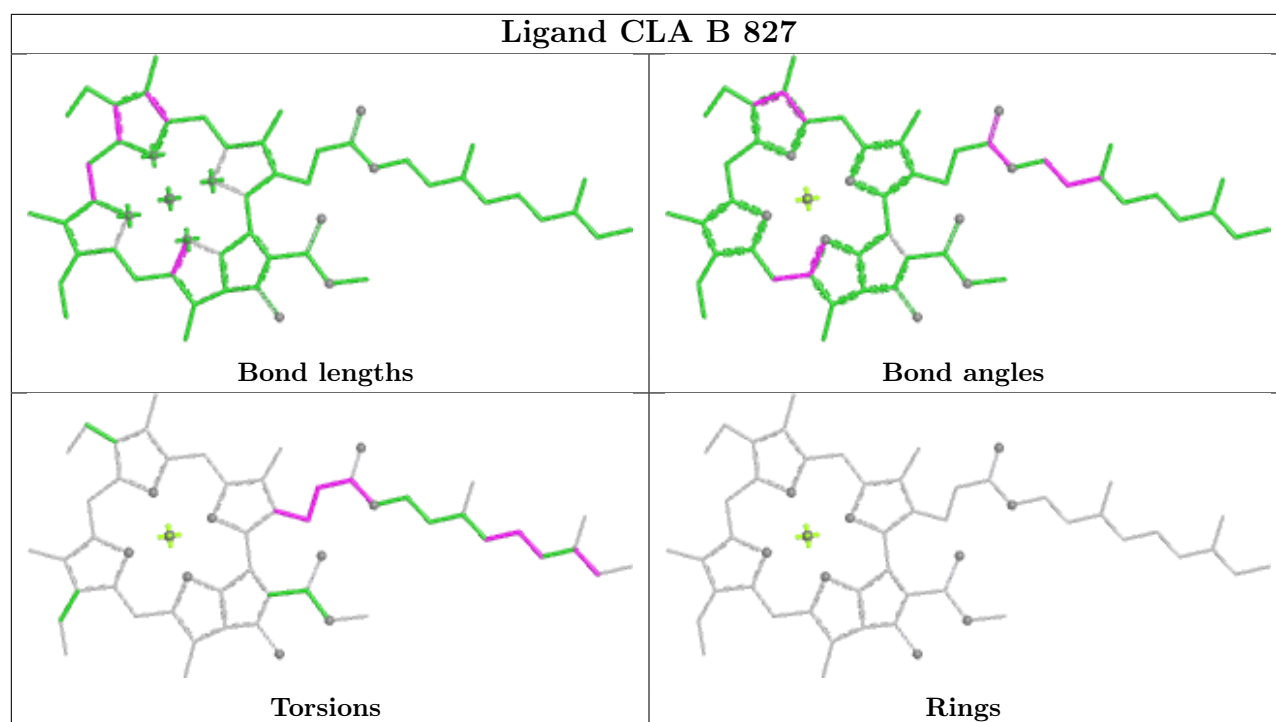


## Ligand CLA 6 516

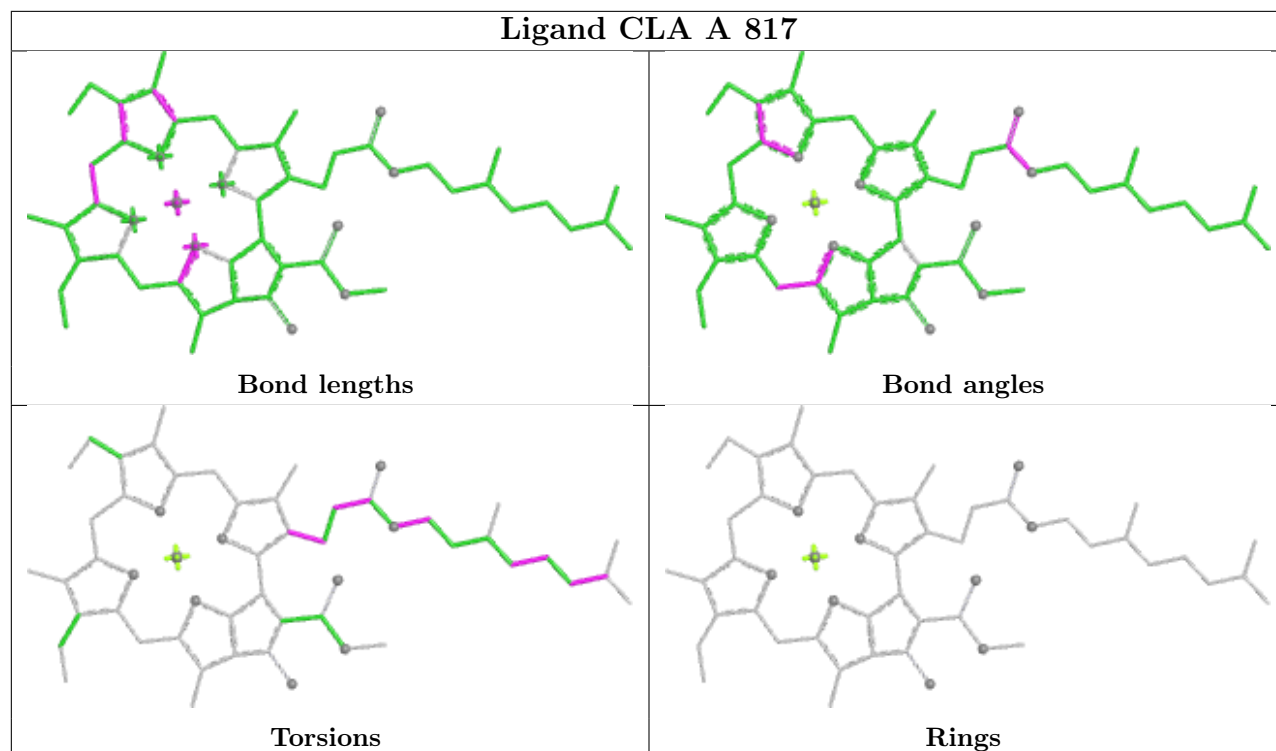


## Ligand CLA 1 513

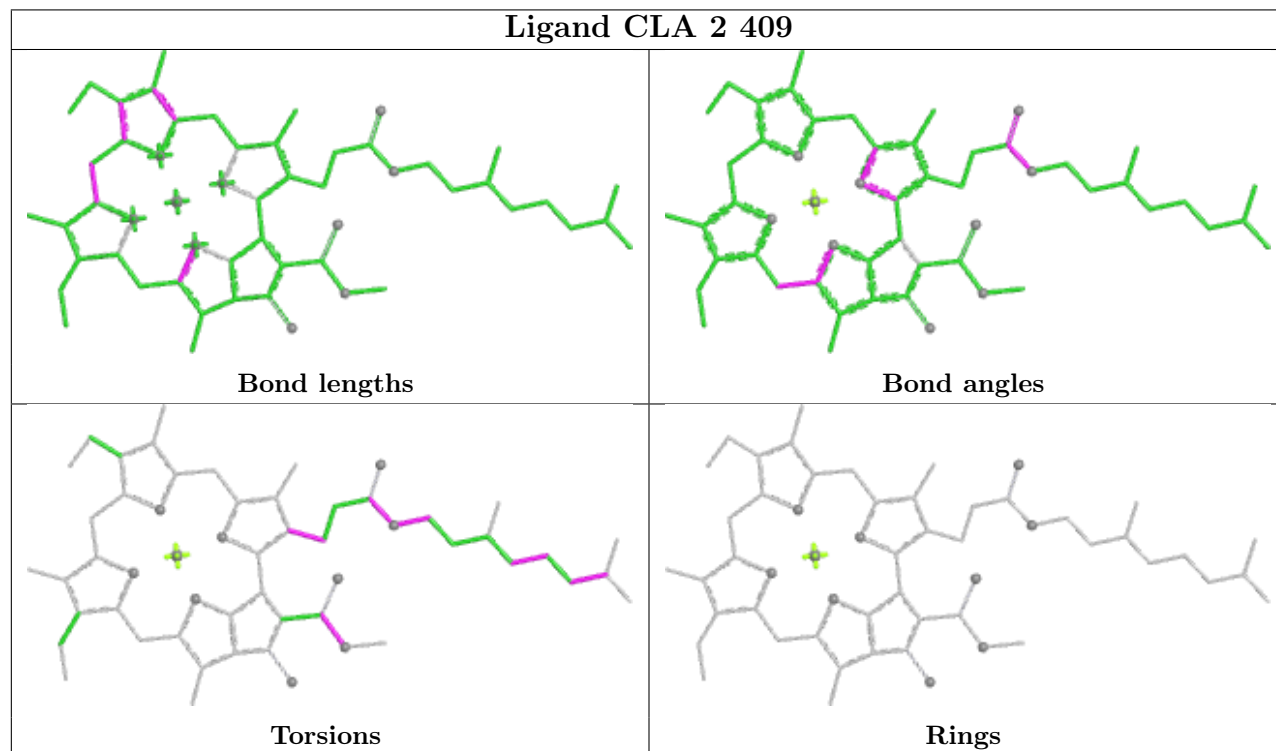


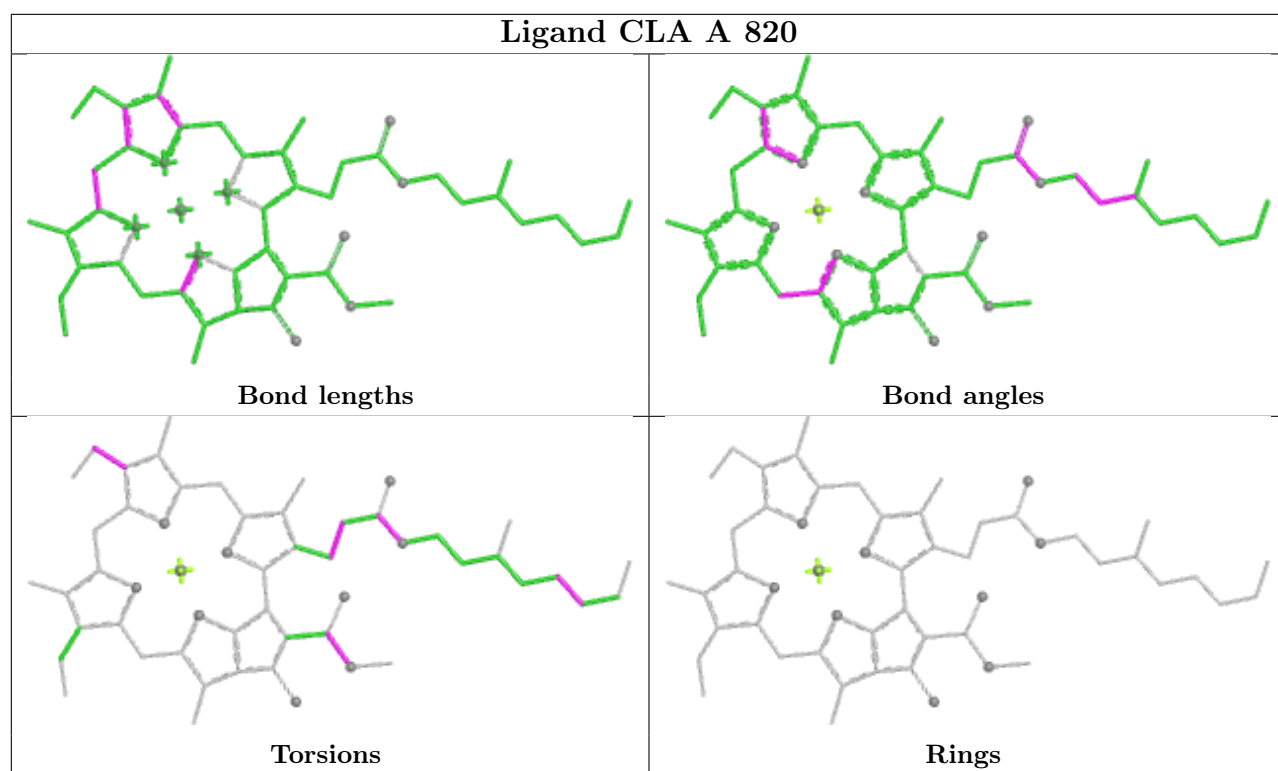


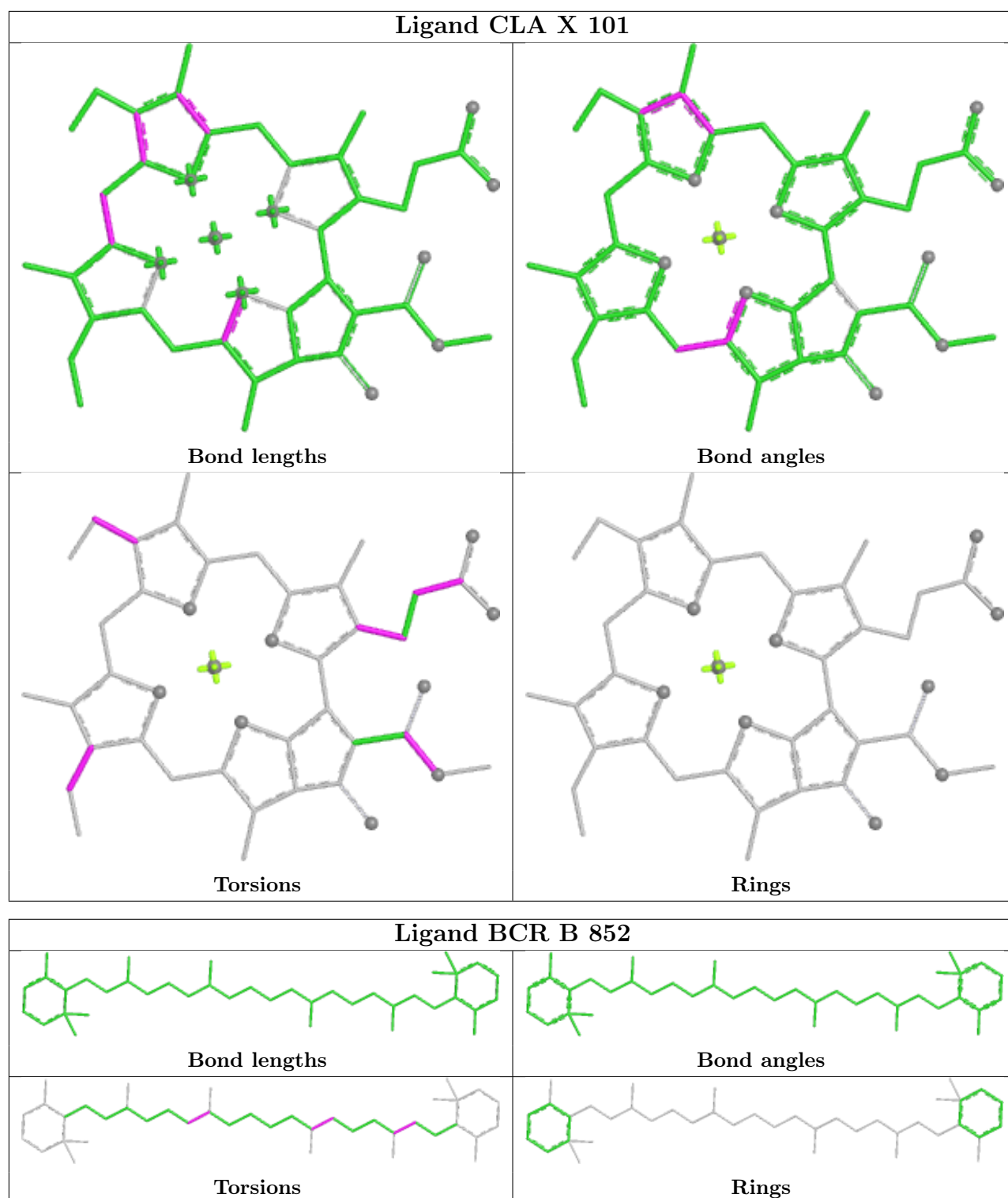
## Ligand CLA A 817

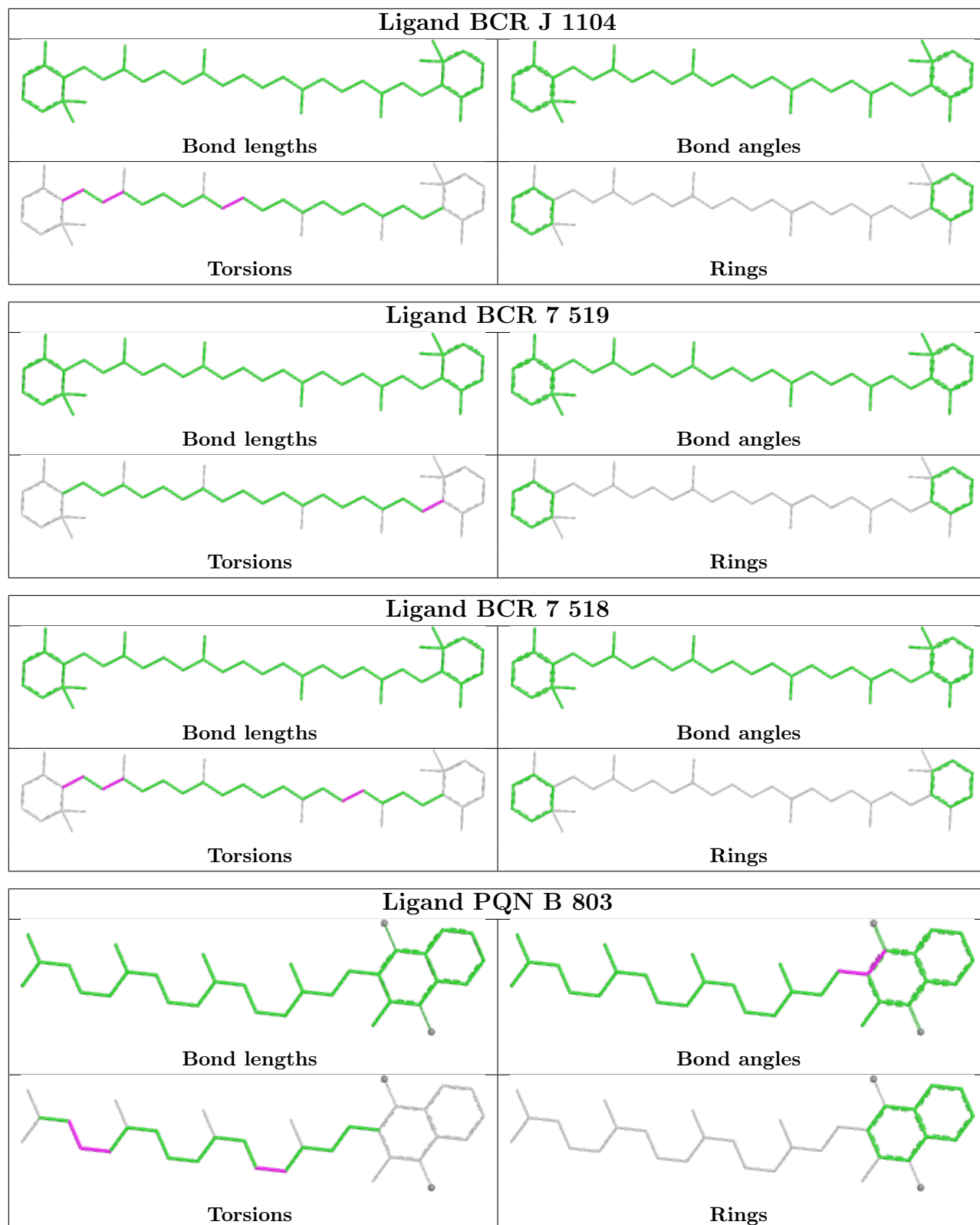


## Ligand CLA 2 409

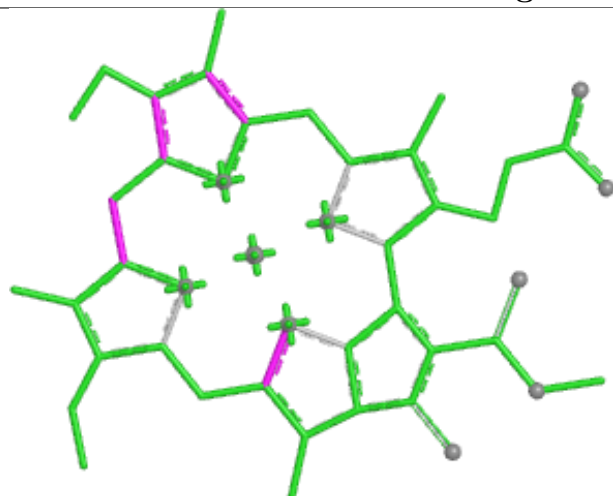




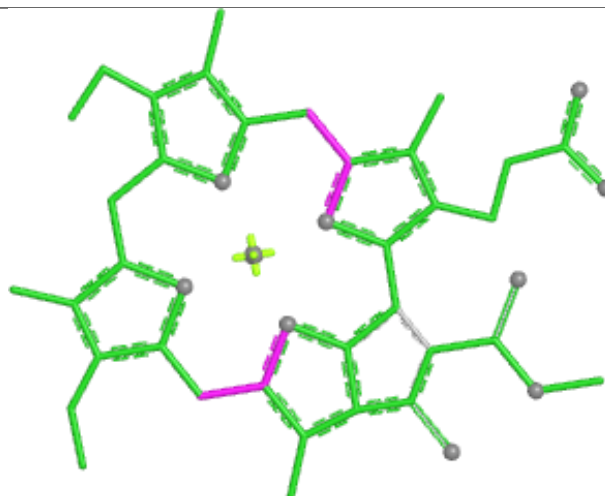




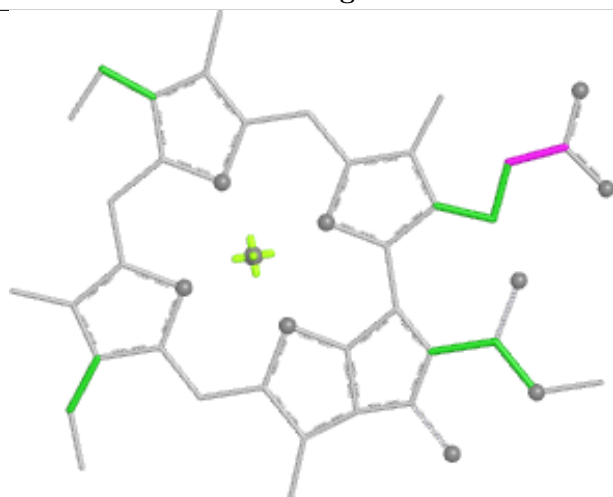
## Ligand CLA F 202



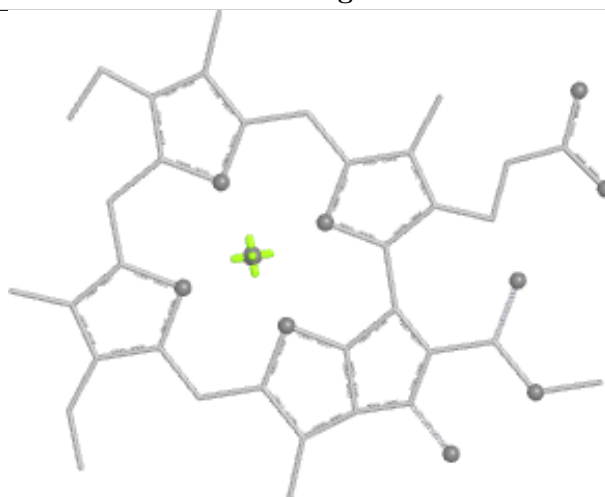
Bond lengths



Bond angles

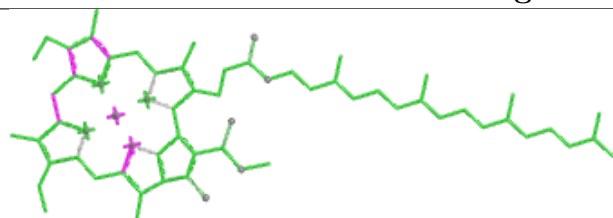


Torsions

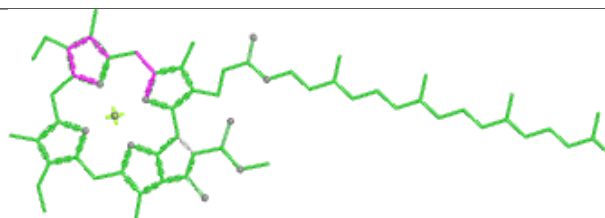


Rings

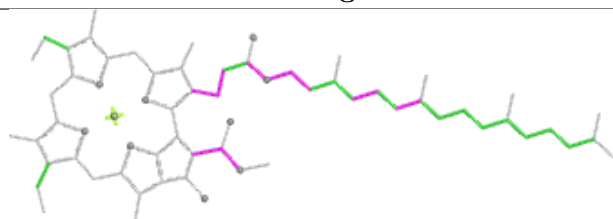
## Ligand CLA B 831



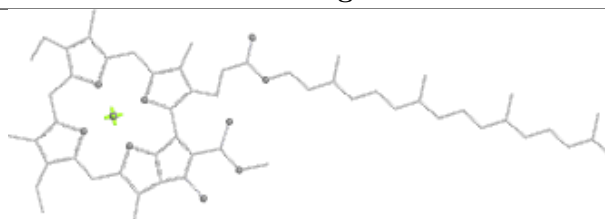
Bond lengths



Bond angles

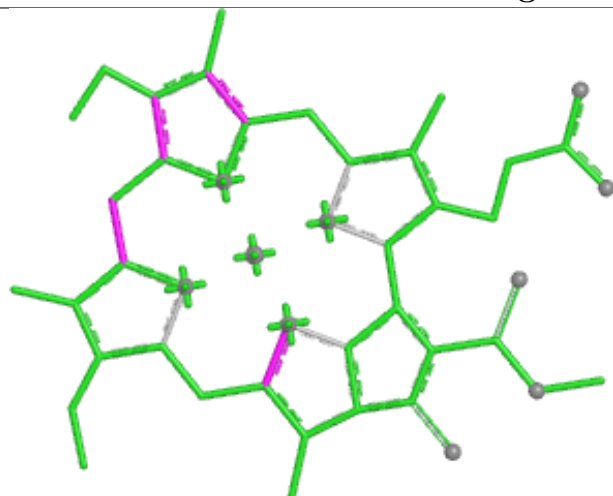


Torsions

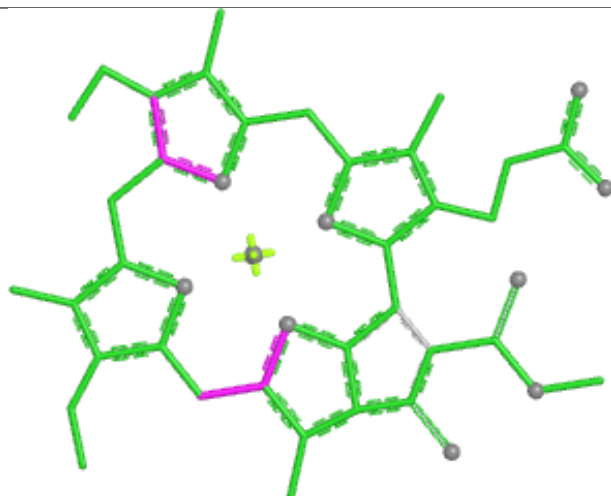


Rings

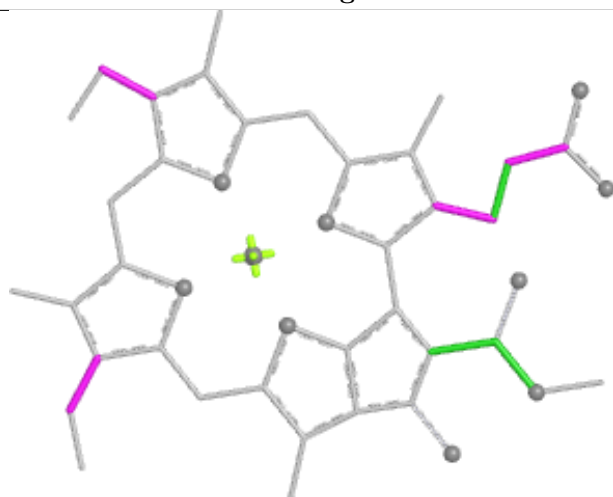
## Ligand CLA 5 416



Bond lengths



Bond angles

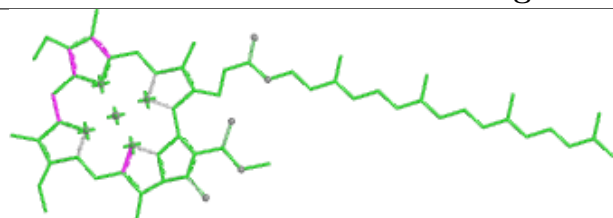


Torsions

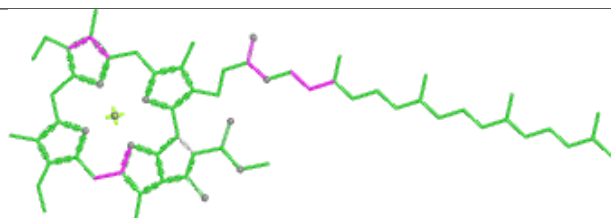


Rings

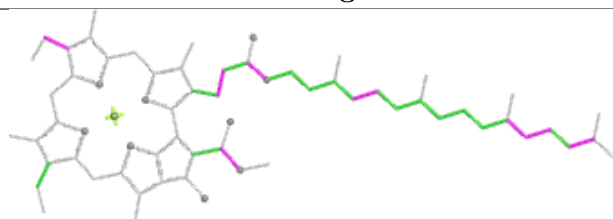
## Ligand CLA A 824



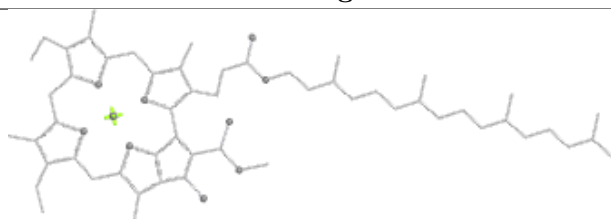
Bond lengths



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.

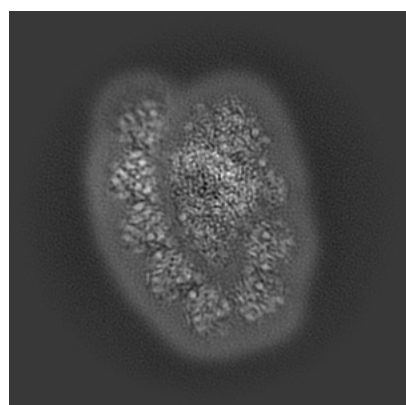
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-74341. These allow visual inspection of the internal detail of the map and identification of artifacts.

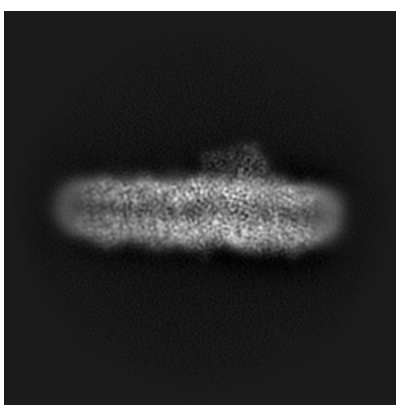
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

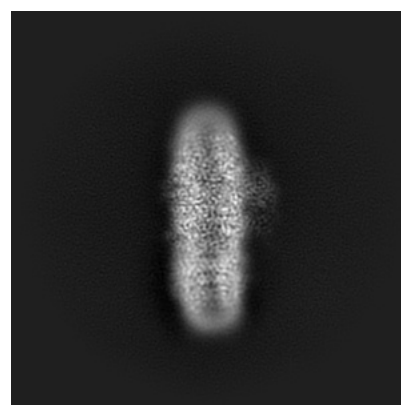
#### 6.1.1 Primary map



X



Y

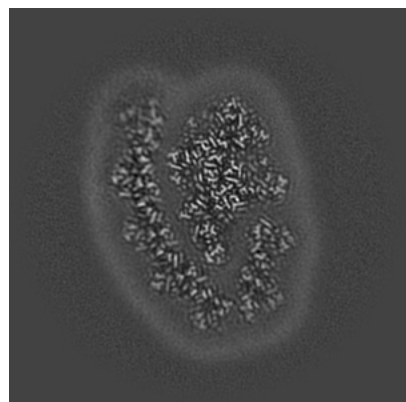


Z

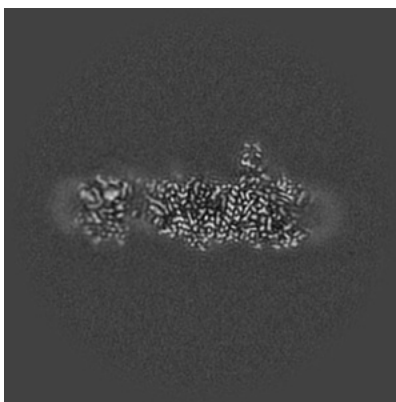
The images above show the map projected in three orthogonal directions.

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

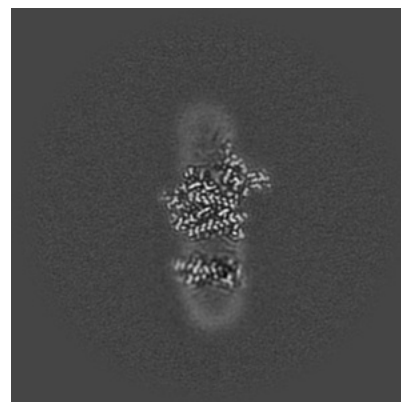
#### 6.2.1 Primary map



X Index: 256



Y Index: 256

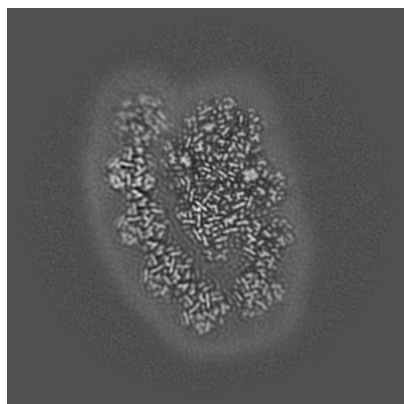


Z Index: 256

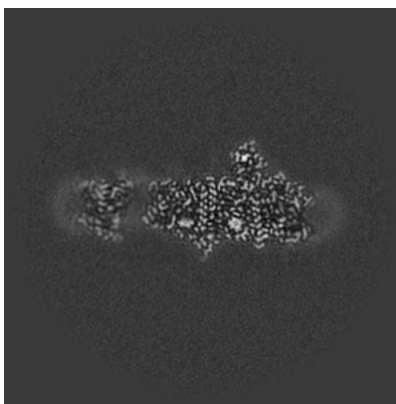
The images above show central slices of the map in three orthogonal directions.

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

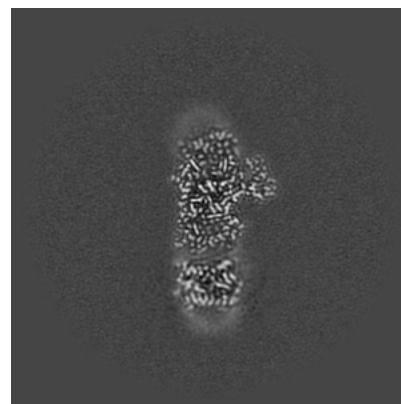
### 6.3.1 Primary map



X Index: 273



Y Index: 266

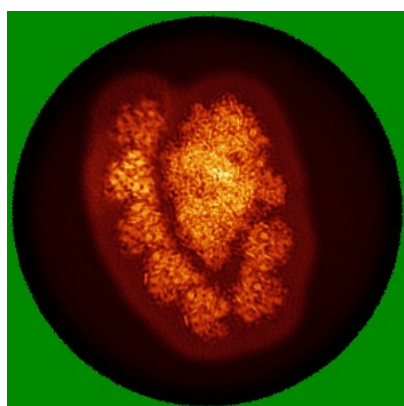


Z Index: 293

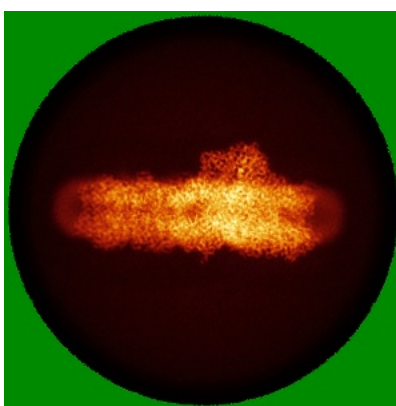
The images above show the largest variance slices of the map in three orthogonal directions.

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

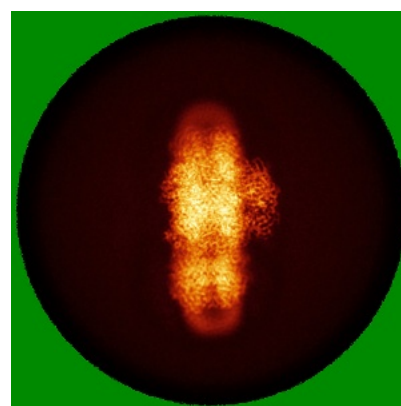
### 6.4.1 Primary map



X



Y

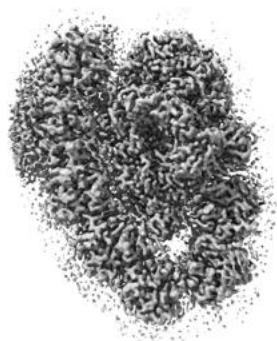


Z

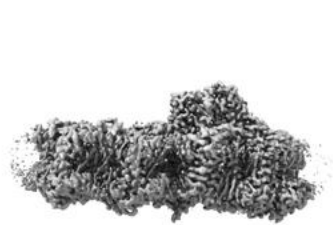
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.34. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

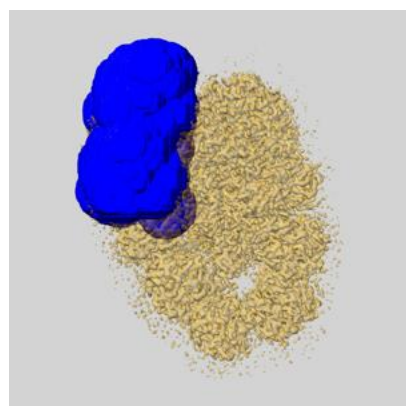
## 6.6 Mask visualisation [i](#)

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

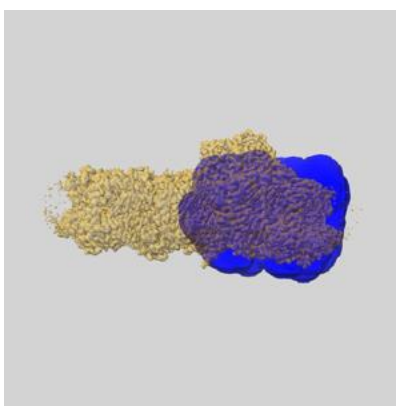
A mask typically either:

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

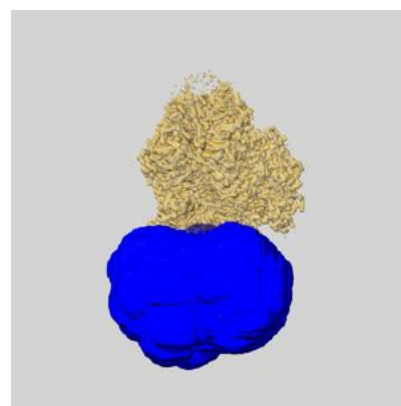
### 6.6.1 emd\_74341\_msk\_1.map [i](#)



X

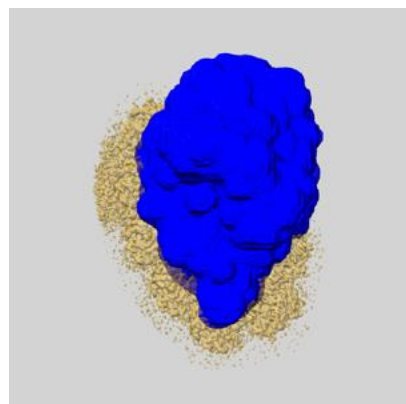


Y

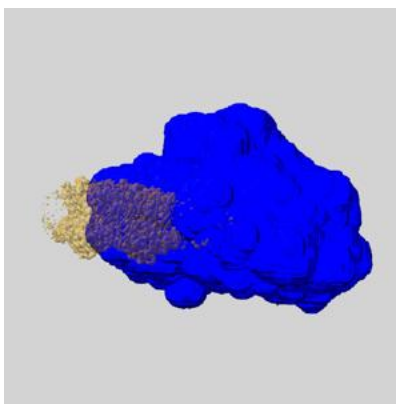


Z

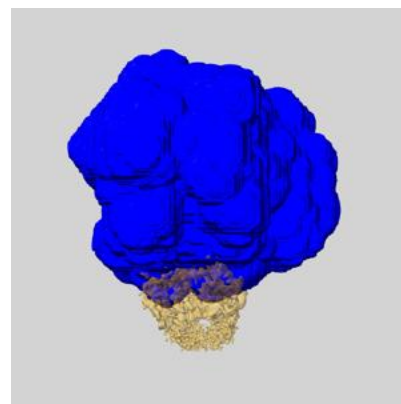
### 6.6.2 emd\_74341\_msk\_2.map [i](#)



X

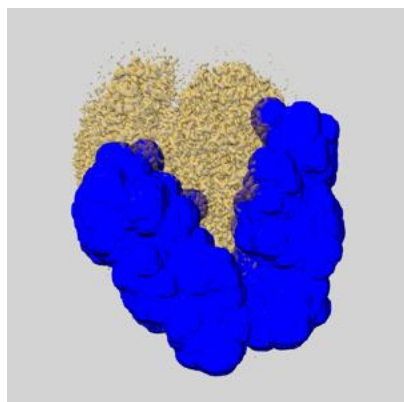


Y

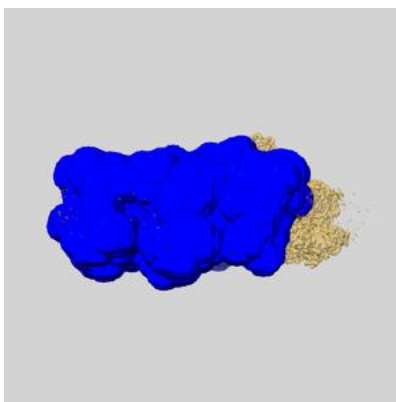


Z

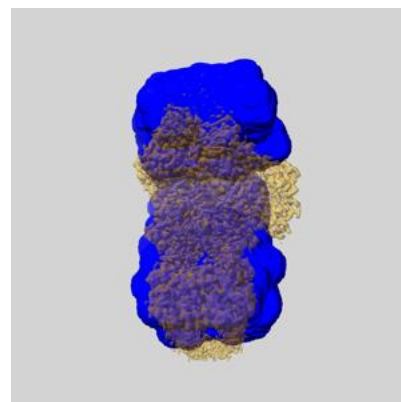
### 6.6.3 emd\_74341\_msk\_3.map ⓘ



X



Y

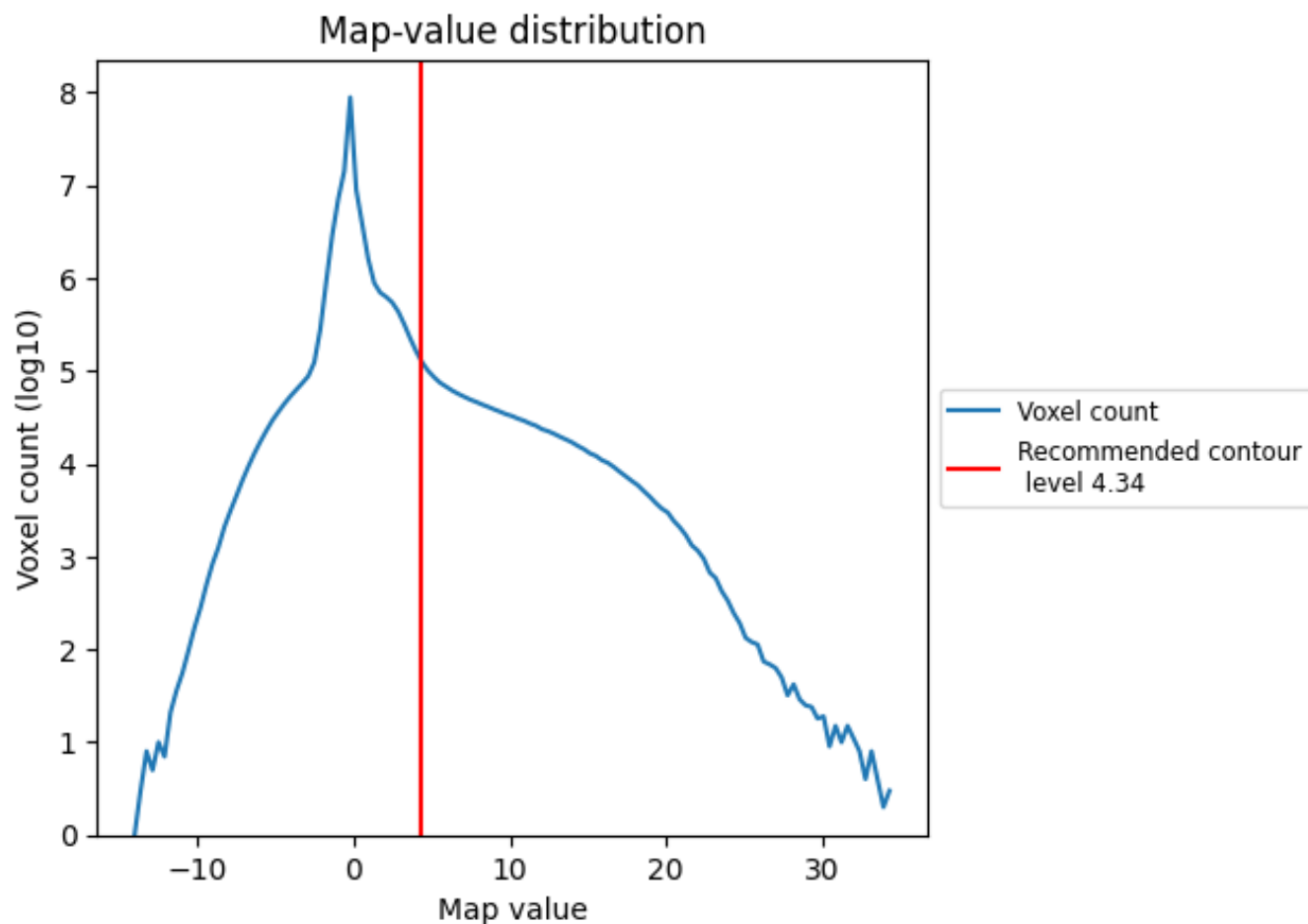


Z

## 7 Map analysis [i](#)

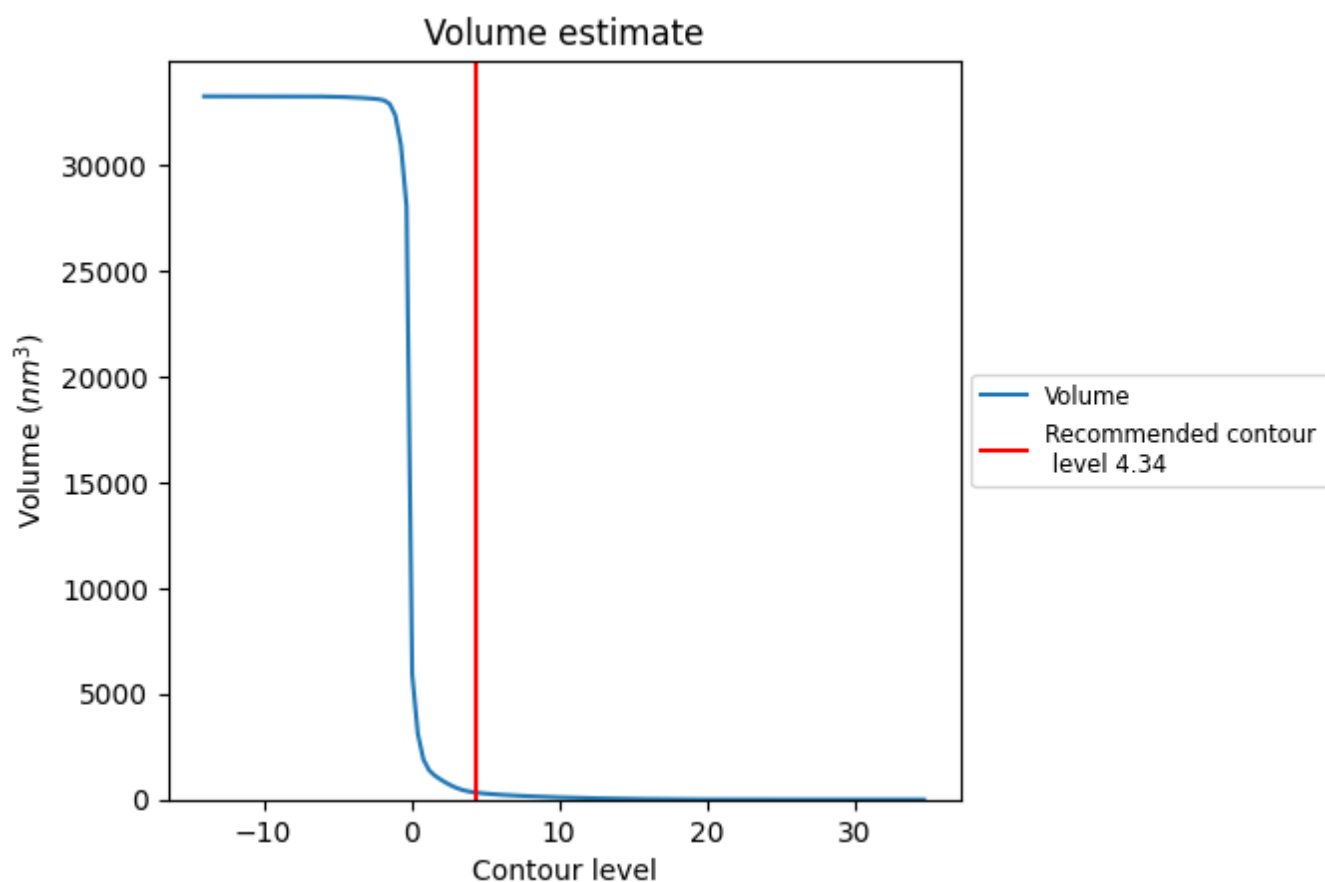
This section contains the results of statistical analysis of the map.

### 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.

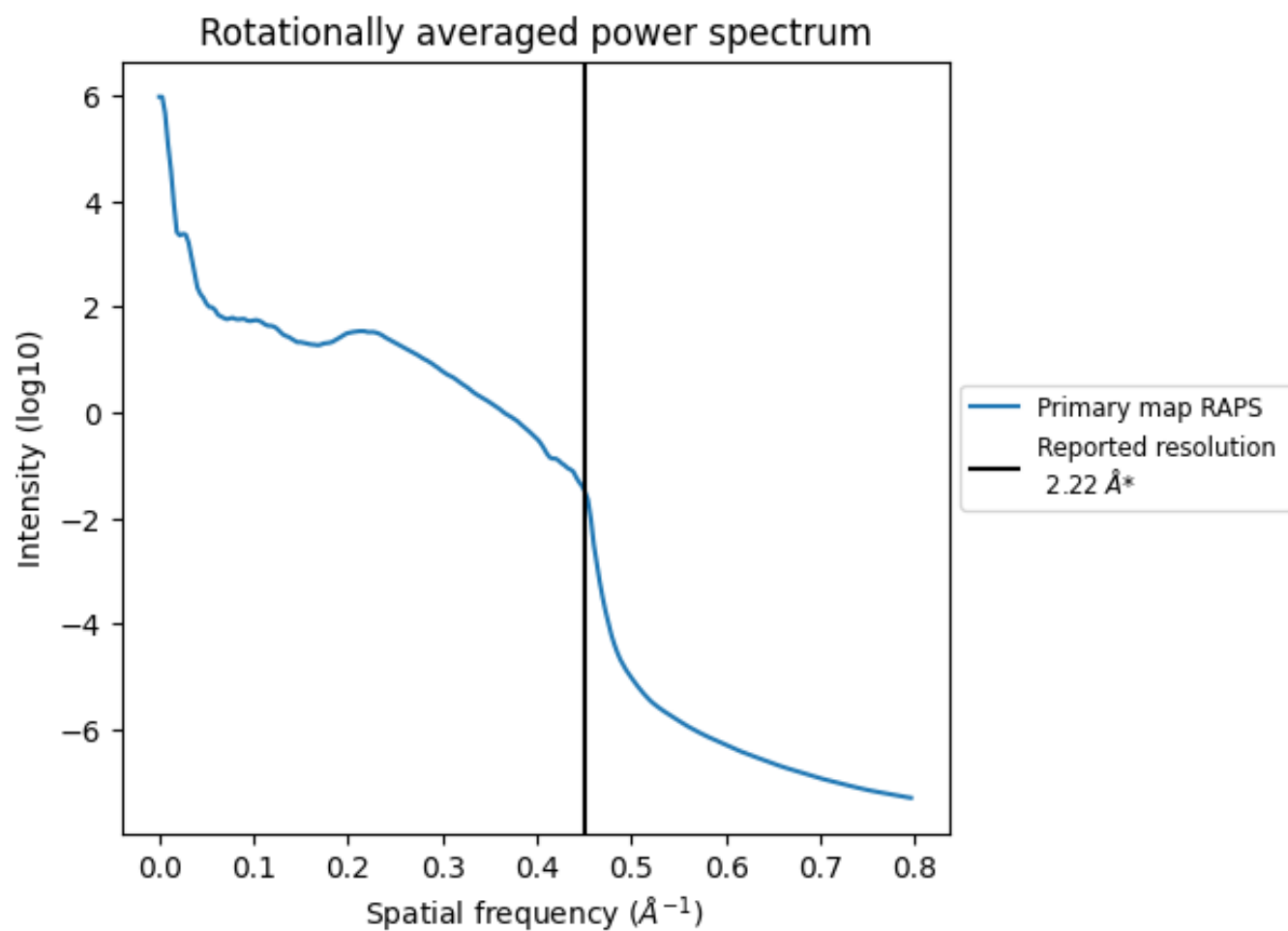
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 333 nm<sup>3</sup>; this corresponds to an approximate mass of 301 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 0.450 Å<sup>-1</sup>

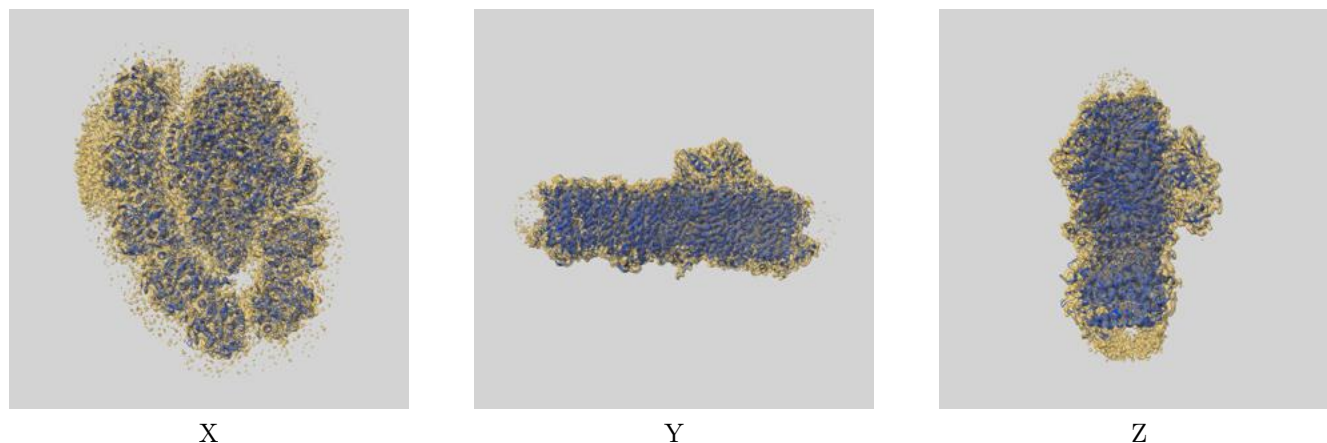
## 8 Fourier-Shell correlation

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

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

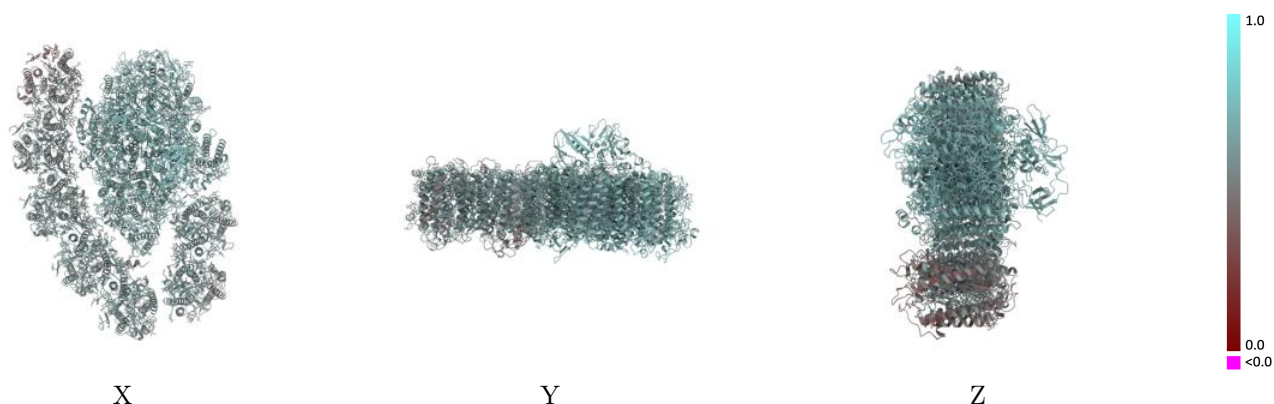
This section contains information regarding the fit between EMDB map EMD-74341 and PDB model 9ZJT. Per-residue inclusion information can be found in section [3](#) on page [26](#).

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



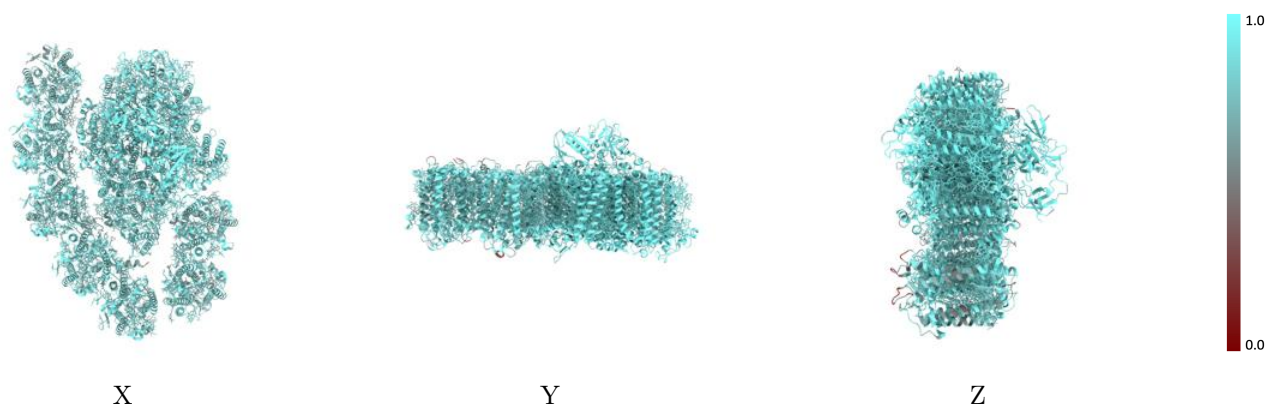
The images above show the 3D surface view of the map at the recommended contour level 4.34 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



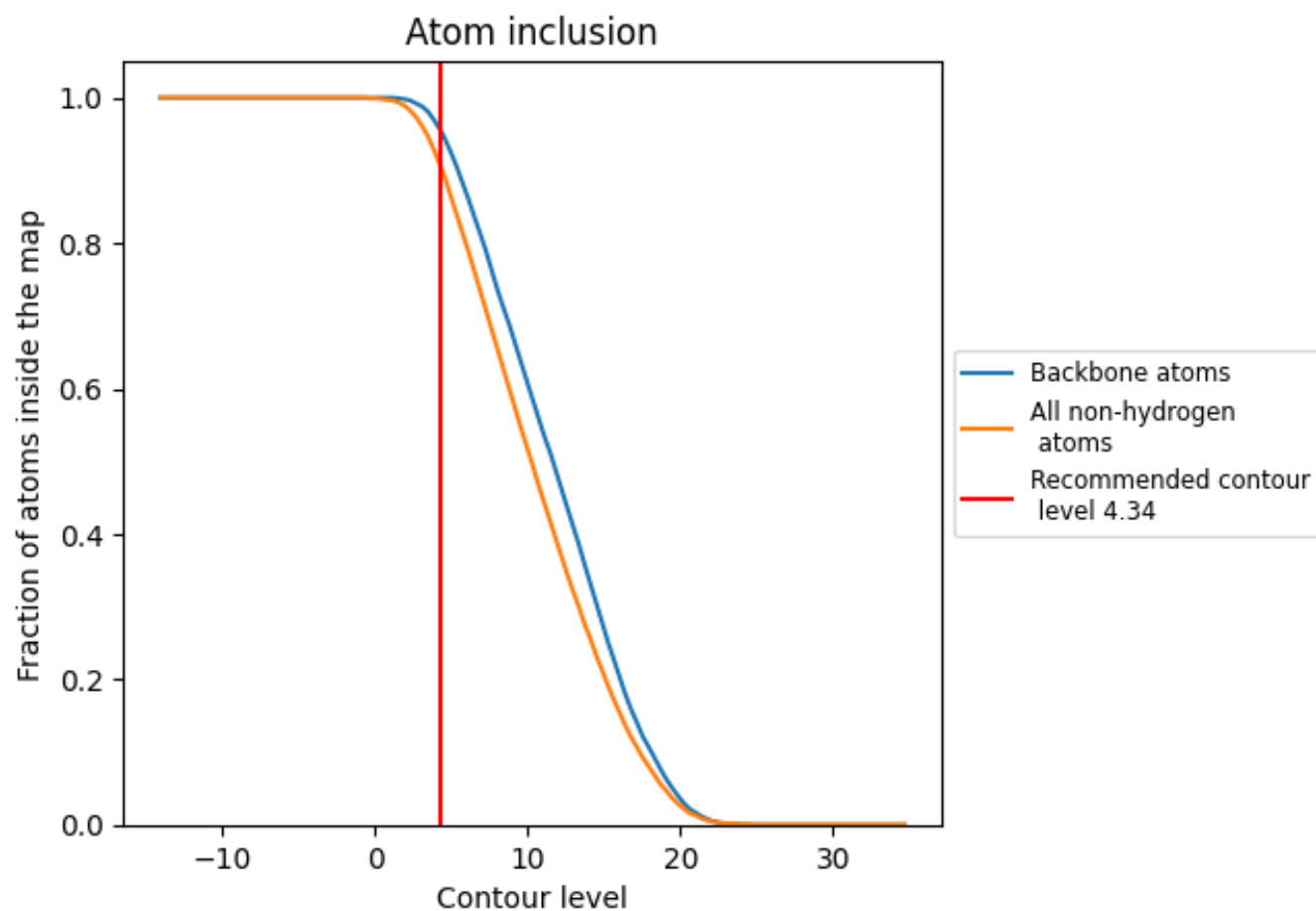
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.34).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 90% 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 (4.34) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9040	<div></div> 0.5950
1	<div></div> 0.8670	<div></div> 0.5670
2	<div></div> 0.8270	<div></div> 0.5480
3	<div></div> 0.8560	<div></div> 0.5600
4	<div></div> 0.8830	<div></div> 0.5690
5	<div></div> 0.8750	<div></div> 0.5580
6	<div></div> 0.9130	<div></div> 0.5280
7	<div></div> 0.7690	<div></div> 0.4610
A	<div></div> 0.9670	<div></div> 0.6610
B	<div></div> 0.9560	<div></div> 0.6520
C	<div></div> 0.9850	<div></div> 0.6620
D	<div></div> 0.9530	<div></div> 0.6440
E	<div></div> 0.9350	<div></div> 0.6350
F	<div></div> 0.9390	<div></div> 0.6410
I	<div></div> 0.9370	<div></div> 0.6230
J	<div></div> 0.9600	<div></div> 0.6390
K	<div></div> 0.9110	<div></div> 0.6230
M	<div></div> 0.9520	<div></div> 0.6390
X	<div></div> 0.9280	<div></div> 0.6300

1.0

0.0

<0.0