



Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 03:14 AM UTC

PDB ID : 7ZQC / pdb_00007zqc
EMDB ID : EMD-14870
Title : Monomeric PSI of Chlamydomonas reinhardtii at 2.31 Å resolution
Authors : Naschberger, A.; Amunts, A.
Deposited on : 2022-04-29
Resolution : 2.31 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

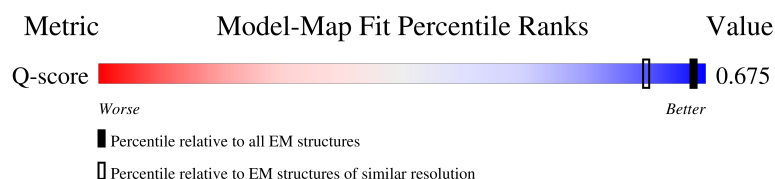
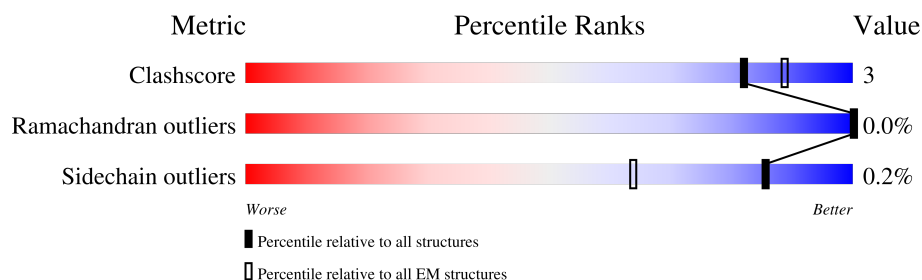
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.31 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	4306 (1.81 - 2.81)

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

Mol	Chain	Length	Quality of chain
1	A	751	 95%
2	B	735	 95% 5%
3	C	81	 83% 16% 15%
4	D	196	 69% 27% 15%

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Mol	Chain	Length	Quality of chain
5	E	97	
6	F	227	
7	G	126	
8	I	106	
9	J	40	
10	L	196	
11	K	113	
12	1	228	
12	Z	228	
13	3	298	
14	7	241	
15	8	243	
16	4	264	
17	5	257	
18	6	257	
19	9	213	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CL0	A	801	X	-	-	-
21	CLA	1	602	X	-	-	-
21	CLA	1	603	X	-	-	-
21	CLA	1	604	X	-	-	-
21	CLA	1	608	X	-	-	-
21	CLA	1	609	X	-	-	-
21	CLA	1	610	X	-	-	-
21	CLA	1	611	X	-	-	-
21	CLA	1	612	X	-	-	-
21	CLA	1	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	1	614	X	-	-	-
21	CLA	1	616	X	-	-	-
21	CLA	3	602	X	-	-	-
21	CLA	3	603	X	-	-	-
21	CLA	3	604	X	-	-	-
21	CLA	3	606	X	-	-	-
21	CLA	3	607	X	-	-	-
21	CLA	3	609	X	-	-	-
21	CLA	3	610	X	-	-	-
21	CLA	3	611	X	-	-	-
21	CLA	3	612	X	-	-	-
21	CLA	3	613	X	-	-	-
21	CLA	3	614	X	-	-	-
21	CLA	3	615	X	-	-	-
21	CLA	3	617	X	-	-	-
21	CLA	4	602	X	-	-	-
21	CLA	4	603	X	-	-	-
21	CLA	4	604	X	-	-	-
21	CLA	4	609	X	-	-	-
21	CLA	4	610	X	-	-	-
21	CLA	4	611	X	-	-	-
21	CLA	4	612	X	-	-	-
21	CLA	4	613	X	-	-	-
21	CLA	4	614	X	-	-	-
21	CLA	4	616	X	-	-	-
21	CLA	5	601	X	-	-	-
21	CLA	5	602	X	-	-	-
21	CLA	5	603	X	-	-	-
21	CLA	5	604	X	-	-	-
21	CLA	5	609	X	-	-	-
21	CLA	5	610	X	-	-	-
21	CLA	5	611	X	-	-	-
21	CLA	5	612	X	-	-	-
21	CLA	5	613	X	-	-	-
21	CLA	5	614	X	-	-	-
21	CLA	5	616	X	-	-	-
21	CLA	5	617	X	-	-	-
21	CLA	5	621	X	-	-	-
21	CLA	6	602	X	-	-	-
21	CLA	6	603	X	-	-	-
21	CLA	6	604	X	-	-	-
21	CLA	6	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	6	610	X	-	-	-
21	CLA	6	611	X	-	-	-
21	CLA	6	612	X	-	-	-
21	CLA	6	613	X	-	-	-
21	CLA	6	614	X	-	-	-
21	CLA	6	617	X	-	-	-
21	CLA	6	622	X	-	-	-
21	CLA	7	602	X	-	-	-
21	CLA	7	603	X	-	-	-
21	CLA	7	604	X	-	-	-
21	CLA	7	608	X	-	-	-
21	CLA	7	609	X	-	-	-
21	CLA	7	610	X	-	-	-
21	CLA	7	611	X	-	-	-
21	CLA	7	612	X	-	-	-
21	CLA	7	613	X	-	-	-
21	CLA	7	614	X	-	-	-
21	CLA	7	616	X	-	-	-
21	CLA	7	620	X	-	-	-
21	CLA	8	602	X	-	-	-
21	CLA	8	603	X	-	-	-
21	CLA	8	604	X	-	-	-
21	CLA	8	608	X	-	-	-
21	CLA	8	609	X	-	-	-
21	CLA	8	610	X	-	-	-
21	CLA	8	611	X	-	-	-
21	CLA	8	612	X	-	-	-
21	CLA	8	613	X	-	-	-
21	CLA	8	614	X	-	-	-
21	CLA	8	616	X	-	-	-
21	CLA	9	601	X	-	-	-
21	CLA	9	602	X	-	-	-
21	CLA	9	603	X	-	-	-
21	CLA	9	604	X	-	-	-
21	CLA	9	609	X	-	-	-
21	CLA	9	610	X	-	-	-
21	CLA	9	611	X	-	-	-
21	CLA	9	612	X	-	-	-
21	CLA	9	613	X	-	-	-
21	CLA	9	614	X	-	-	-
21	CLA	A	802	X	-	-	-
21	CLA	A	803	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	A	804	X	-	-	-
21	CLA	A	805	X	-	-	-
21	CLA	A	806	X	-	-	-
21	CLA	A	807	X	-	-	-
21	CLA	A	808	X	-	-	-
21	CLA	A	809	X	-	-	-
21	CLA	A	810	X	-	-	-
21	CLA	A	811	X	-	-	-
21	CLA	A	812	X	-	-	-
21	CLA	A	813	X	-	-	-
21	CLA	A	814	X	-	-	-
21	CLA	A	815	X	-	-	-
21	CLA	A	816	X	-	-	-
21	CLA	A	817	X	-	-	-
21	CLA	A	818	X	-	-	-
21	CLA	A	819	X	-	-	-
21	CLA	A	820	X	-	-	-
21	CLA	A	821	X	-	-	-
21	CLA	A	822	X	-	-	-
21	CLA	A	823	X	-	-	-
21	CLA	A	824	X	-	-	-
21	CLA	A	825	X	-	-	-
21	CLA	A	826	X	-	-	-
21	CLA	A	827	X	-	-	-
21	CLA	A	828	X	-	-	-
21	CLA	A	829	X	-	-	-
21	CLA	A	830	X	-	-	-
21	CLA	A	831	X	-	-	-
21	CLA	A	832	X	-	-	-
21	CLA	A	833	X	-	-	-
21	CLA	A	834	X	-	-	-
21	CLA	A	835	X	-	-	-
21	CLA	A	836	X	-	-	-
21	CLA	A	837	X	-	-	-
21	CLA	A	838	X	-	-	-
21	CLA	A	839	X	-	-	-
21	CLA	A	840	X	-	-	-
21	CLA	A	841	X	-	-	-
21	CLA	A	842	X	-	-	-
21	CLA	A	843	X	-	-	-
21	CLA	A	845	X	-	-	-
21	CLA	A	854	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	B	802	X	-	-	-
21	CLA	B	803	X	-	-	-
21	CLA	B	804	X	-	-	-
21	CLA	B	805	X	-	-	-
21	CLA	B	806	X	-	-	-
21	CLA	B	807	X	-	-	-
21	CLA	B	808	X	-	-	-
21	CLA	B	809	X	-	-	-
21	CLA	B	810	X	-	-	-
21	CLA	B	811	X	-	-	-
21	CLA	B	812	X	-	-	-
21	CLA	B	813	X	-	-	-
21	CLA	B	814	X	-	-	-
21	CLA	B	815	X	-	-	-
21	CLA	B	816	X	-	-	-
21	CLA	B	817	X	-	-	-
21	CLA	B	818	X	-	-	-
21	CLA	B	819	X	-	-	-
21	CLA	B	820	X	-	-	-
21	CLA	B	821	X	-	-	-
21	CLA	B	822	X	-	-	-
21	CLA	B	823	X	-	-	-
21	CLA	B	824	X	-	-	-
21	CLA	B	825	X	-	-	-
21	CLA	B	826	X	-	-	-
21	CLA	B	827	X	-	-	-
21	CLA	B	828	X	-	-	-
21	CLA	B	829	X	-	-	-
21	CLA	B	830	X	-	-	-
21	CLA	B	831	X	-	-	-
21	CLA	B	832	X	-	-	-
21	CLA	B	833	X	-	-	-
21	CLA	B	834	X	-	-	-
21	CLA	B	835	X	-	-	-
21	CLA	B	836	X	-	-	-
21	CLA	B	837	X	-	-	-
21	CLA	B	838	X	-	-	-
21	CLA	B	839	X	-	-	-
21	CLA	B	840	X	-	-	-
21	CLA	B	841	X	-	-	-
21	CLA	F	301	X	-	-	-
21	CLA	F	303	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	F	304	X	-	-	-
21	CLA	G	203	X	-	-	-
21	CLA	G	204	X	-	-	-
21	CLA	J	101	X	-	-	-
21	CLA	K	201	X	-	-	-
21	CLA	K	203	X	-	-	-
21	CLA	K	204	X	-	-	-
21	CLA	K	206	X	-	-	-
21	CLA	L	203	X	-	-	-
21	CLA	L	204	X	-	-	-
21	CLA	Z	602	X	-	-	-
21	CLA	Z	603	X	-	-	-
21	CLA	Z	604	X	-	-	-
21	CLA	Z	608	X	-	-	-
21	CLA	Z	609	X	-	-	-
21	CLA	Z	610	X	-	-	-
21	CLA	Z	611	X	-	-	-
21	CLA	Z	612	X	-	-	-
21	CLA	Z	613	X	-	-	-
21	CLA	Z	614	X	-	-	-
21	CLA	Z	616	X	-	-	-
30	CHL	1	601	X	-	-	-
30	CHL	1	606	X	-	-	-
30	CHL	1	607	X	-	-	-
30	CHL	3	608	X	-	-	-
30	CHL	4	601	X	-	-	-
30	CHL	4	606	X	-	-	-
30	CHL	4	607	X	-	-	-
30	CHL	4	608	X	-	-	-
30	CHL	4	618	X	-	-	-
30	CHL	5	606	X	-	-	-
30	CHL	5	607	X	-	-	-
30	CHL	5	608	X	-	-	-
30	CHL	5	618	X	-	-	-
30	CHL	6	601	X	-	-	-
30	CHL	6	606	X	-	-	-
30	CHL	6	607	X	-	-	-
30	CHL	6	608	X	-	-	-
30	CHL	6	616	X	-	-	-
30	CHL	6	618	X	-	-	-
30	CHL	7	601	X	-	-	-
30	CHL	7	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CHL	7	607	X	-	-	-
30	CHL	8	601	X	-	-	-
30	CHL	8	606	X	-	-	-
30	CHL	8	607	X	-	-	-
30	CHL	9	606	X	-	-	-
30	CHL	9	607	X	-	-	-
30	CHL	Z	601	X	-	-	-
30	CHL	Z	606	X	-	-	-
30	CHL	Z	607	X	-	-	-
31	XAT	1	618	X	-	-	-

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 101000 atoms, of which 50501 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	742	Total	C	H	N	O	S	0	0
			11498	3808	5673	994	1001	22		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	733	Total	C	H	N	O	S	0	0
			11400	3824	5576	977	1005	18		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	80	Total	C	H	N	O	S	0	0
			1183	369	582	103	117	12		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	144	Total	C	H	N	O	S	0	0
			2284	725	1151	200	201	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	64	Total	C	H	N	O	0	0
			1011	322	505	89	95		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	165	Total	C	H	N	O	S	0	0
			2568	817	1302	213	233	3		

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	80	Total	C	H	N	O	0	0
			1177	379	583	103	112		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	37	Total	C	H	N	O S	0	0
			573	195	292	39	46 1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	40	Total	C	H	N	O S	0	0
			657	224	328	46	58 1		

- Molecule 10 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	124	Total	C	H	N	O S	0	0
			1806	586	907	146	164 3		

- Molecule 11 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	86	Total	C	H	N	O S	0	0
			1203	370	620	100	111 2		

- Molecule 12 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1	194	Total	C	H	N	O S	0	0
			2842	941	1397	240	261 3		
12	Z	194	Total	C	H	N	O S	0	0
			2842	941	1397	240	261 3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	3	227	Total	C	H	N	O S	0	0
			3431	1128	1695	283	317 8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
14	7	213	Total	C	H	N	O	S	0	0
			3240	1072	1590	274	298	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
15	8	217	Total	C	H	N	O	S	0	0
			3279	1073	1629	280	293	4		

- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic (Lhca4).

Mol	Chain	Residues	Atoms						AltConf	Trace
16	4	212	Total	C	H	N	O	S	0	0
			3251	1080	1603	268	295	5		

- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	5	227	Total	C	H	N	O	S	0	0
			3522	1154	1747	297	316	8		

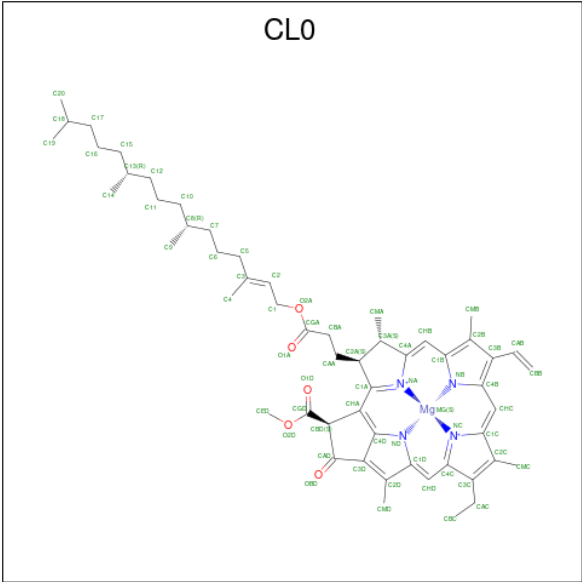
- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	6	230	Total	C	H	N	O	S	0	0
			3542	1167	1770	293	306	6		

- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

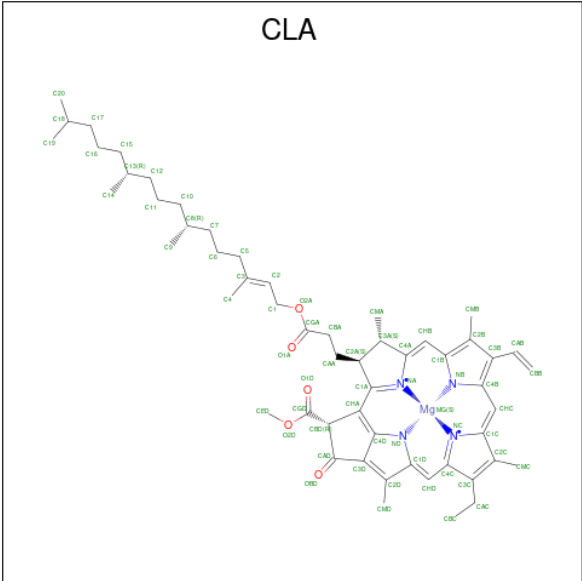
Mol	Chain	Residues	Atoms						AltConf	Trace
19	9	156	Total	C	H	N	O	S	0	0
			2386	775	1196	201	208	6		

- Molecule 20 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
20	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

- Molecule 21 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	A	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			110	47	53	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			117	49	58	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			113	48	55	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	F	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	F	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	F	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	G	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	G	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	J	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	L	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	L	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	K	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	K	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	K	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	K	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	1	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	1	1	Total	C	H	Mg	N	O	0
			110	47	53	1	4	5	
21	1	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	1	1	Total	C	H	Mg	N	O	0
			122	51	61	1	4	5	
21	1	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	1	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	1	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	3	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	3	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	3	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	3	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
21	3	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	3	1	Total	C	H	Mg	N	O	0
			122	51	61	1	4	5	
21	3	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	3	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	3	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	3	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	3	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	3	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	3	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	7	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	7	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	
21	7	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
21	7	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	7	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	7	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	7	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	7	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	7	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	7	1	Total	C	H	Mg	N	O	0
			76	35	33	1	4	3	
21	7	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	7	1	Total	C	H	Mg	N	O	0
			98	43	45	1	4	5	
21	8	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	8	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	8	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	8	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	8	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	8	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	8	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	8	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	8	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	8	1	Total	C	H	Mg	N	O	0
			110	47	53	1	4	5	
21	8	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	Z	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	Z	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	Z	1	Total	C	H	Mg	N	O	0
			110	47	53	1	4	5	
21	Z	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	Z	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	Z	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	Z	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	Z	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	Z	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	Z	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	Z	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	4	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	4	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	4	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	4	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	4	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	4	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	4	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	4	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	4	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	4	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	4	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	5	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	5	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	5	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	5	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	5	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	5	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	

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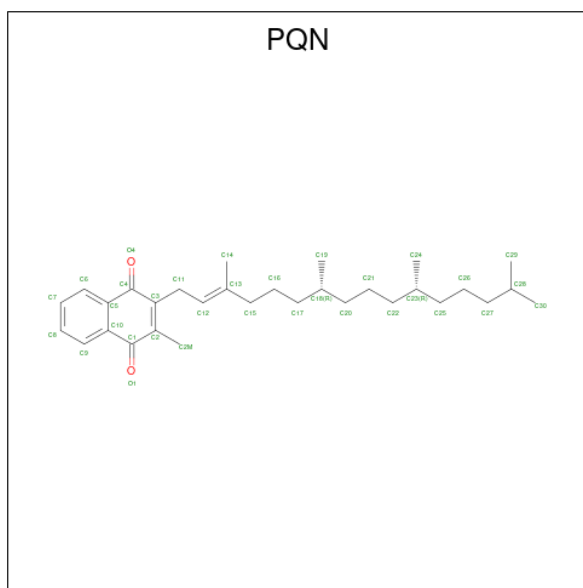
Mol	Chain	Residues	Atoms						AltConf
21	5	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	5	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	5	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
21	5	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	5	1	Total	C	H	Mg	N	O	0
			98	43	45	1	4	5	
21	5	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	5	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	6	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	6	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	6	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	6	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	6	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	6	1	Total	C	H	Mg	N	O	0
			113	48	55	1	4	5	
21	6	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	6	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	6	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	6	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	6	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	9	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	9	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	9	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	

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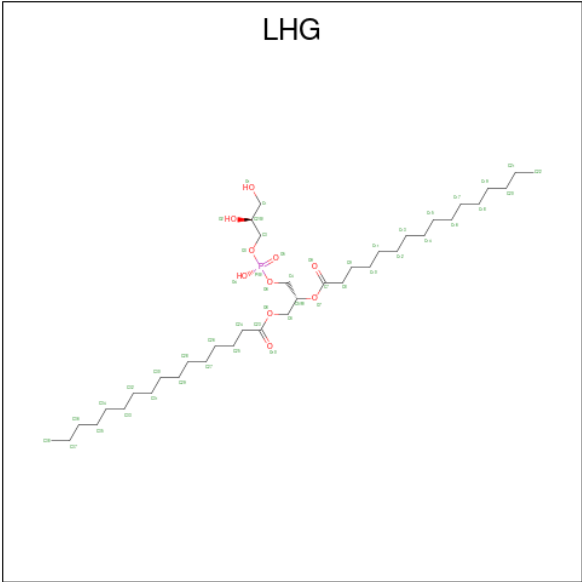
Mol	Chain	Residues	Atoms						AltConf
21	9	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	9	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
21	9	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	9	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	9	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	9	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	9	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	

- Molecule 22 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
22	A	1	Total	C	H	O	0
			79	31	46	2	
22	B	1	Total	C	H	O	0
			79	31	46	2	

- Molecule 23 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



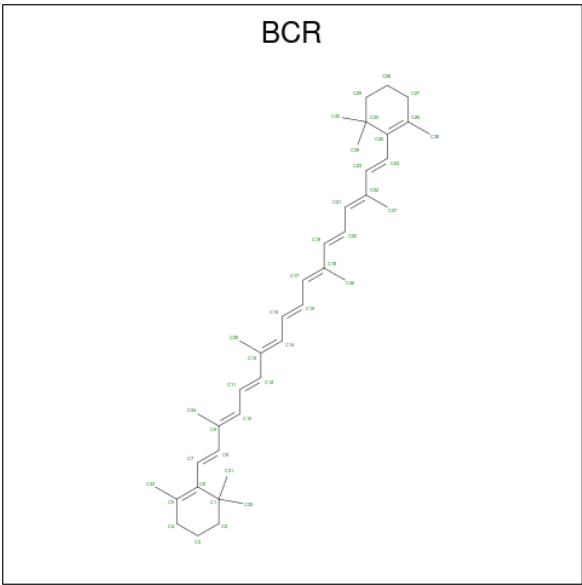
Mol	Chain	Residues	Atoms					AltConf
23	A	1	Total	C	H	O	P	0
			123	38	74	10	1	
23	A	1	Total	C	H	O	P	0
			87	27	49	10	1	
23	B	1	Total	C	H	O	P	0
			108	34	63	10	1	
23	1	1	Total	C	H	O	P	0
			102	33	58	10	1	
23	3	1	Total	C	H	O	P	0
			114	36	67	10	1	
23	3	1	Total	C	H	O	P	0
			63	20	32	10	1	
23	7	1	Total	C	H	O	P	0
			123	38	74	10	1	
23	8	1	Total	C	H	O	P	0
			105	33	61	10	1	
23	Z	1	Total	C	H	O	P	0
			87	28	48	10	1	
23	4	1	Total	C	H	O	P	0
			123	38	74	10	1	
23	4	1	Total	C	H	O	P	0
			87	27	49	10	1	
23	5	1	Total	C	H	O	P	0
			81	26	44	10	1	
23	6	1	Total	C	H	O	P	0
			123	38	74	10	1	
23	6	1	Total	C	H	O	P	0
			78	25	42	10	1	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
23	9	1	72	23	38	10	1	0

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



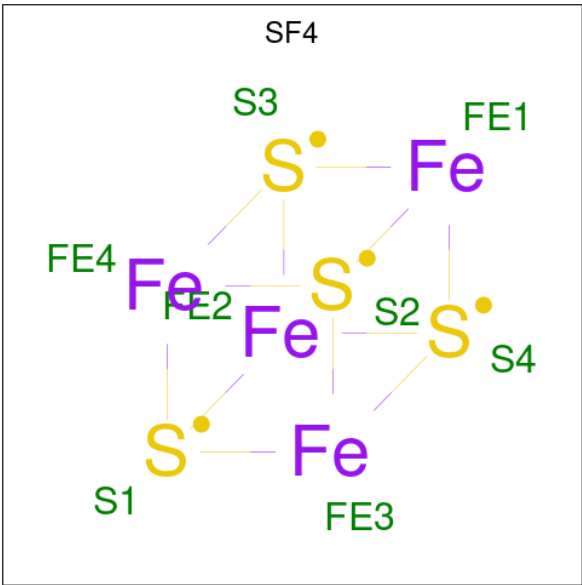
Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total	C	H	0
			96	40	56	
24	A	1	Total	C	H	0
			96	40	56	
24	A	1	Total	C	H	0
			96	40	56	
24	A	1	Total	C	H	0
			96	40	56	
24	A	1	Total	C	H	0
			96	40	56	
24	B	1	Total	C	H	0
			96	40	56	
24	B	1	Total	C	H	0
			96	40	56	
24	B	1	Total	C	H	0
			96	40	56	
24	B	1	Total	C	H	0
			96	40	56	

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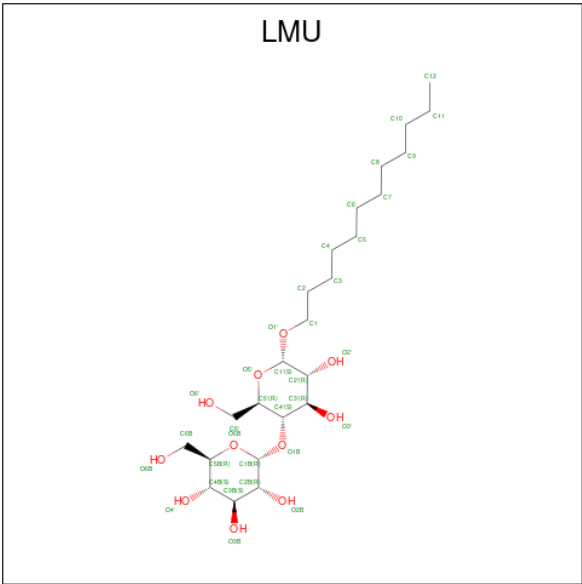
Mol	Chain	Residues	Atoms			AltConf
24	B	1	Total	C	H	0
			96	40	56	
24	B	1	Total	C	H	0
			96	40	56	
24	G	1	Total	C	H	0
			96	40	56	
24	I	1	Total	C	H	0
			96	40	56	
24	J	1	Total	C	H	0
			96	40	56	
24	L	1	Total	C	H	0
			96	40	56	
24	L	1	Total	C	H	0
			96	40	56	
24	K	1	Total	C	H	0
			96	40	56	
24	K	1	Total	C	H	0
			96	40	56	
24	3	1	Total	C	H	0
			96	40	56	
24	3	1	Total	C	H	0
			96	40	56	
24	3	1	Total	C	H	0
			96	40	56	
24	7	1	Total	C	H	0
			96	40	56	
24	8	1	Total	C	H	0
			96	40	56	
24	4	1	Total	C	H	0
			96	40	56	
24	5	1	Total	C	H	0
			96	40	56	
24	6	1	Total	C	H	0
			96	40	56	

- Molecule 25 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 26 is DODECYL-ALPHA-D-MALTOSE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁) (labeled as "Ligand of Interest" by depositor).



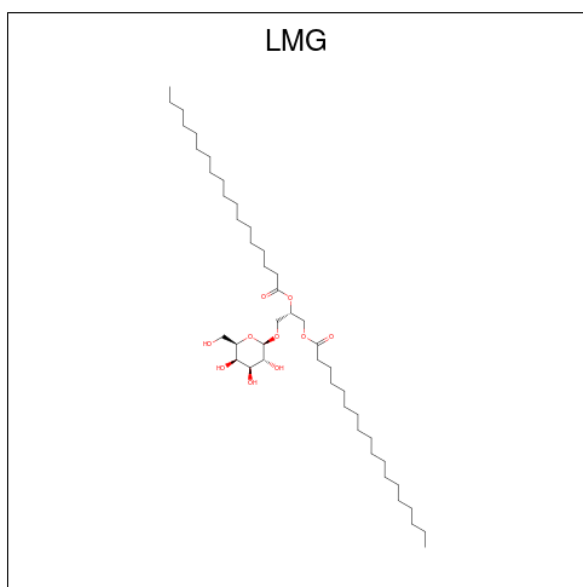
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	H	O	0
			75	23	41	11	
26	A	1	Total	C	H	O	0
			81	24	46	11	
26	A	1	Total	C	H	O	0
			44	14	24	6	
26	A	1	Total	C	H	O	0
			59	18	35	6	
26	A	1	Total	C	H	O	0
			81	24	46	11	
26	A	1	Total	C	H	O	0
			59	18	35	6	
26	A	1	Total	C	H	O	0
			59	18	35	6	
26	B	1	Total	C	H	O	0
			81	24	46	11	
26	G	1	Total	C	H	O	0
			59	18	35	6	
26	K	1	Total	C	H	O	0
			59	18	35	6	
26	1	1	Total	C	H	O	0
			81	24	46	11	
26	1	1	Total	C	H	O	0
			41	13	22	6	
26	1	1	Total	C	H	O	0
			59	18	35	6	
26	1	1	Total	C	H	O	0
			50	16	28	6	
26	1	1	Total	C	H	O	0
			59	18	35	6	
26	1	1	Total	C	H	O	0
			59	18	35	6	
26	7	1	Total	C	H	O	0
			69	21	37	11	
26	7	1	Total	C	H	O	0
			50	16	28	6	
26	7	1	Total	C	H	O	0
			54	16	27	11	
26	8	1	Total	C	H	O	0
			59	18	35	6	
26	8	1	Total	C	H	O	0
			59	18	35	6	
26	8	1	Total	C	H	O	0
			81	24	46	11	

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Mol	Chain	Residues	Atoms				AltConf
26	8	1	Total	C	H	O	0
			59	18	35	6	
26	Z	1	Total	C	H	O	0
			66	20	35	11	
26	Z	1	Total	C	H	O	0
			50	16	28	6	
26	4	1	Total	C	H	O	0
			72	22	39	11	
26	4	1	Total	C	H	O	0
			44	14	24	6	
26	5	1	Total	C	H	O	0
			59	18	35	6	
26	6	1	Total	C	H	O	0
			44	14	24	6	
26	6	1	Total	C	H	O	0
			59	18	35	6	
26	6	1	Total	C	H	O	0
			59	18	35	6	
26	6	1	Total	C	H	O	0
			59	18	35	6	

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



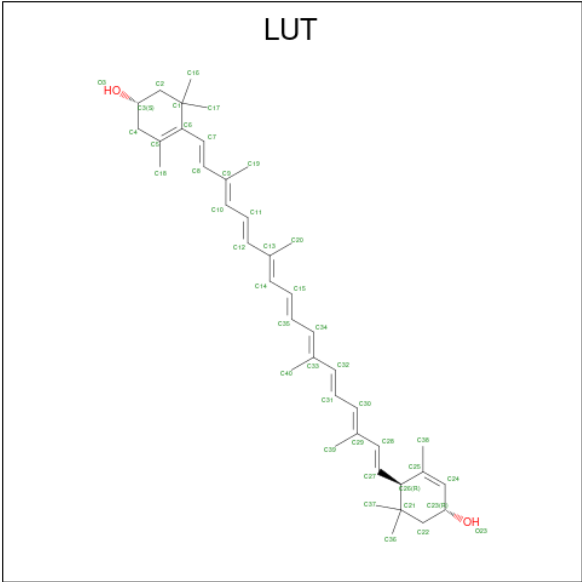
Mol	Chain	Residues	Atoms				AltConf
27	A	1	Total	C	H	O	0
			90	30	50	10	

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Mol	Chain	Residues	Atoms				AltConf
27	A	1	Total	C	H	O	0
			66	22	34	10	
27	B	1	Total	C	H	O	0
			99	33	56	10	
27	B	1	Total	C	H	O	0
			78	26	42	10	
27	J	1	Total	C	H	O	0
			75	25	40	10	
27	J	1	Total	C	H	O	0
			99	32	57	10	
27	1	1	Total	C	H	O	0
			78	26	42	10	
27	1	1	Total	C	H	O	0
			120	39	71	10	
27	3	1	Total	C	H	O	0
			120	40	75	5	
27	7	1	Total	C	H	O	0
			81	27	44	10	
27	8	1	Total	C	H	O	0
			66	22	34	10	
27	8	1	Total	C	H	O	0
			99	32	57	10	
27	4	1	Total	C	H	O	0
			96	31	55	10	
27	4	1	Total	C	H	O	0
			60	22	33	5	
27	6	1	Total	C	H	O	0
			55	18	35	2	

- Molecule 28 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂) (labeled as "Ligand of Interest" by depositor).



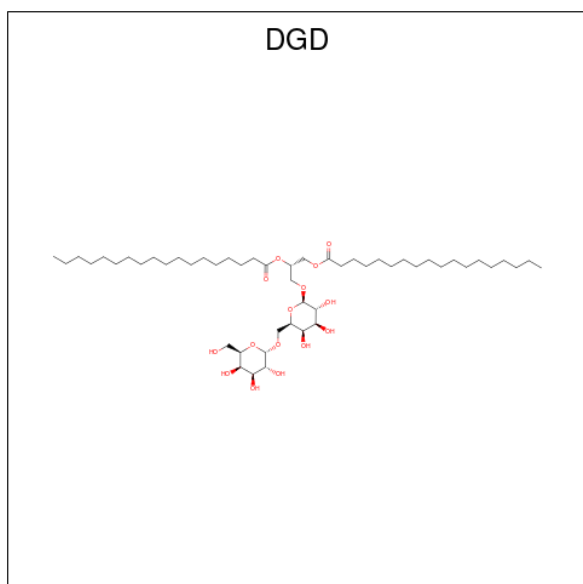
Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	H	O	0
			98	40	56	2	
28	F	1	Total	C	H	O	0
			98	40	56	2	
28	1	1	Total	C	H	O	0
			98	40	56	2	
28	1	1	Total	C	H	O	0
			98	40	56	2	
28	3	1	Total	C	H	O	0
			98	40	56	2	
28	3	1	Total	C	H	O	0
			98	40	56	2	
28	3	1	Total	C	H	O	0
			98	40	56	2	
28	7	1	Total	C	H	O	0
			98	40	56	2	
28	7	1	Total	C	H	O	0
			98	40	56	2	
28	8	1	Total	C	H	O	0
			98	40	56	2	
28	Z	1	Total	C	H	O	0
			98	40	56	2	
28	Z	1	Total	C	H	O	0
			59	25	33	1	
28	4	1	Total	C	H	O	0
			98	40	56	2	
28	5	1	Total	C	H	O	0
			98	40	56	2	

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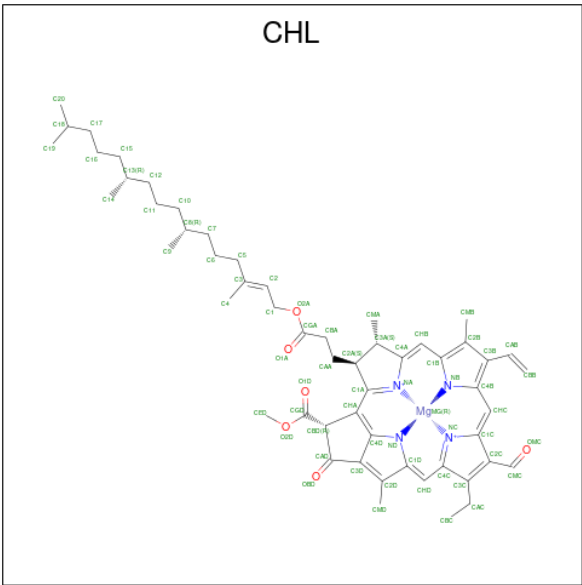
Mol	Chain	Residues	Atoms				AltConf
28	5	1	Total	C	H	O	0
			98	40	56	2	
28	6	1	Total	C	H	O	0
			98	40	56	2	
28	9	1	Total	C	H	O	0
			98	40	56	2	
28	9	1	Total	C	H	O	0
			98	40	56	2	

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
29	B	1	Total	C	H	O	0
			138	44	79	15	

- Molecule 30 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



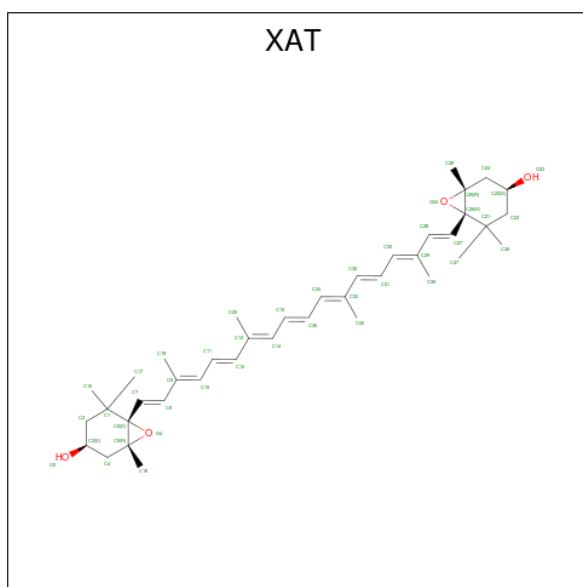
Mol	Chain	Residues	Atoms						AltConf
30	1	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
30	1	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
30	1	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	3	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	7	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	7	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
30	7	1	Total	C	H	Mg	N	O	0
			97	43	43	1	4	6	
30	8	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	8	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	8	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	Z	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	Z	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
30	Z	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	4	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	

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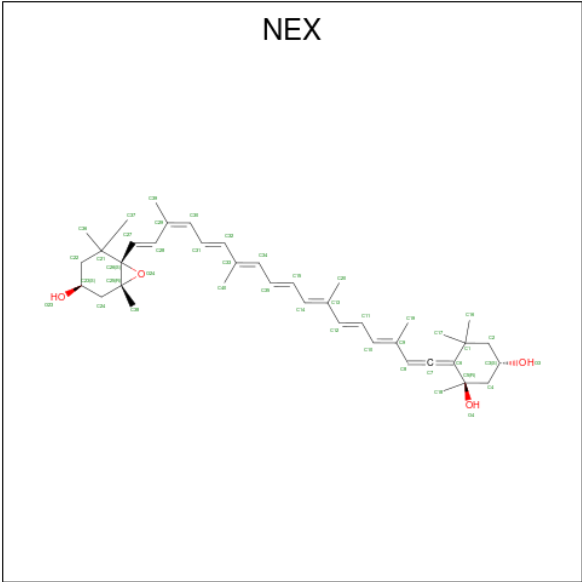
Mol	Chain	Residues	Atoms						AltConf
30	4	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	4	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	4	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	4	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
30	5	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
30	5	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	5	1	Total	C	H	Mg	N	O	0
			88	40	37	1	4	6	
30	5	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
30	6	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	6	1	Total	C	H	Mg	N	O	0
			109	47	51	1	4	6	
30	6	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	6	1	Total	C	H	Mg	N	O	0
			88	40	37	1	4	6	
30	6	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	6	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
30	9	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
30	9	1	Total	C	H	Mg	N	O	0
			88	40	37	1	4	6	

- Molecule 31 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
31	1	1	Total	C	H	O	0
			100	40	56	4	
31	7	1	Total	C	H	O	0
			100	40	56	4	
31	8	1	Total	C	H	O	0
			100	40	56	4	
31	Z	1	Total	C	H	O	0
			100	40	56	4	
31	4	1	Total	C	H	O	0
			100	40	56	4	
31	5	1	Total	C	H	O	0
			100	40	56	4	
31	6	1	Total	C	H	O	0
			100	40	56	4	

- Molecule 32 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
32	5	1	Total	C	H	O	0
			100	40	56	4	
32	6	1	Total	C	H	O	0
			100	40	56	4	

- Molecule 33 is water.

Mol	Chain	Residues	Atoms		AltConf
33	H	184	Total	O	0
			184	184	
33	H	171	Total	O	0
			171	171	
33	H	35	Total	O	0
			35	35	
33	H	23	Total	O	0
			23	23	
33	H	9	Total	O	0
			9	9	
33	H	28	Total	O	0
			28	28	
33	H	6	Total	O	0
			6	6	
33	H	2	Total	O	0
			2	2	
33	H	2	Total	O	0
			2	2	
33	H	21	Total	O	0
			21	21	

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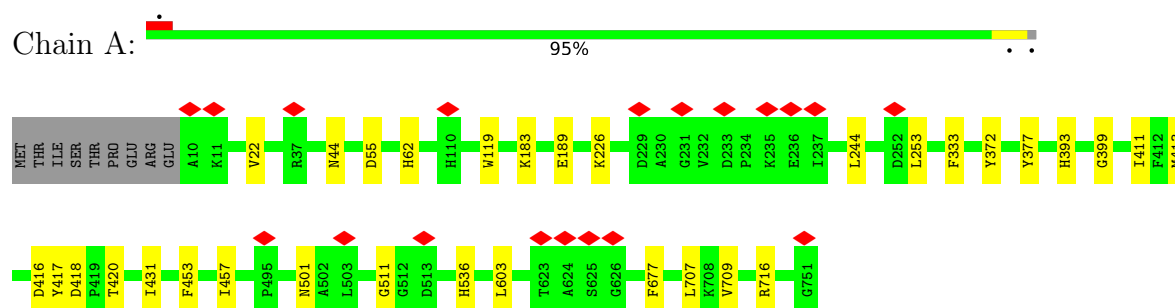
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Mol	Chain	Residues	Atoms		AltConf
33	H	28	Total 28	O 28	0
33	H	33	Total 33	O 33	0
33	H	28	Total 28	O 28	0
33	H	11	Total 11	O 11	0
33	H	12	Total 12	O 12	0
33	H	14	Total 14	O 14	0
33	H	14	Total 14	O 14	0

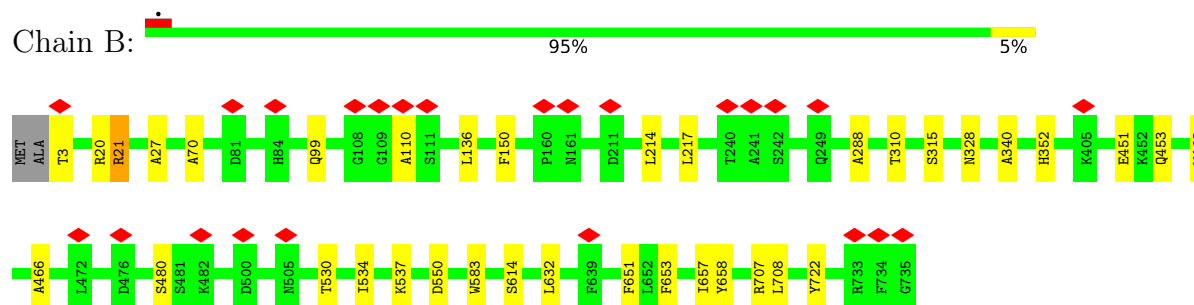
3 Residue-property plots

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

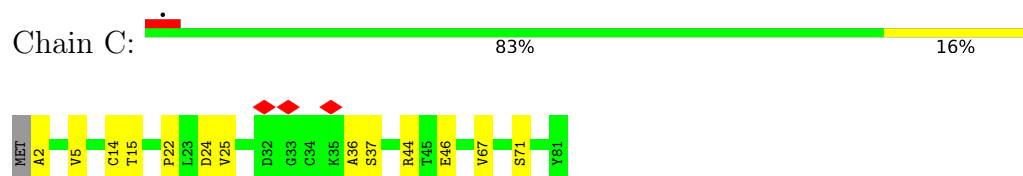
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



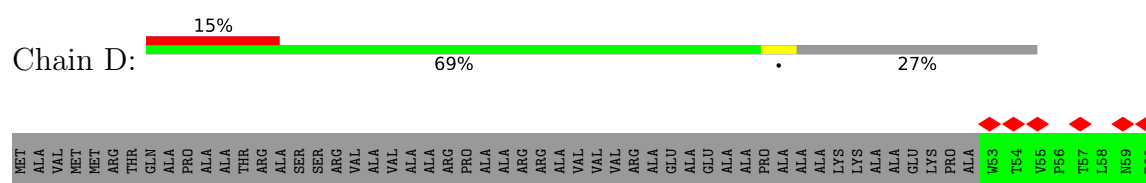
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

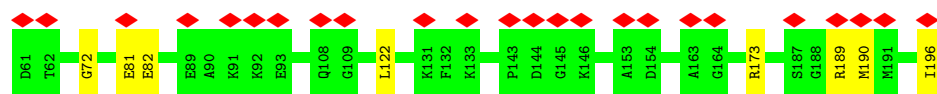


- Molecule 3: Photosystem I iron-sulfur center

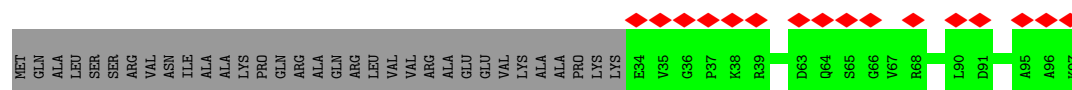


- Molecule 4: Photosystem I reaction center subunit II, chloroplastic

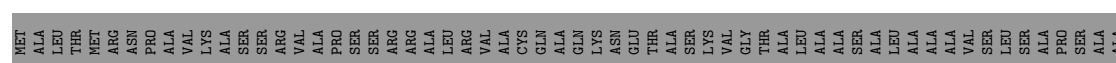




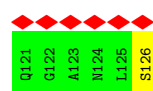
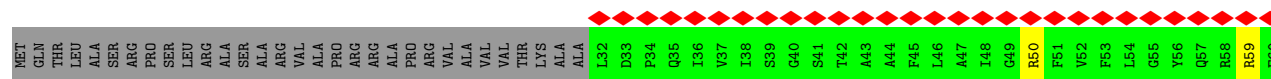
- Molecule 5: Photosystem I reaction center subunit IV, chloroplastic



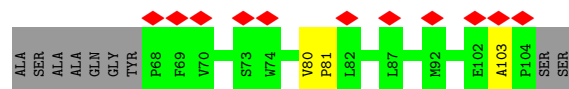
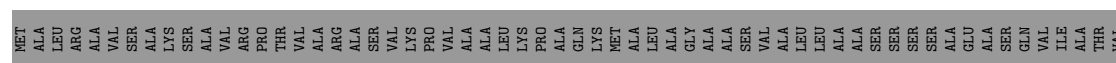
- Molecule 6: Photosystem I reaction center subunit III, chloroplastic



- Molecule 7: Photosystem I reaction center subunit V, chloroplastic

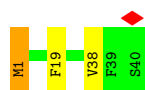


- Molecule 8: Photosystem I reaction center subunit VIII

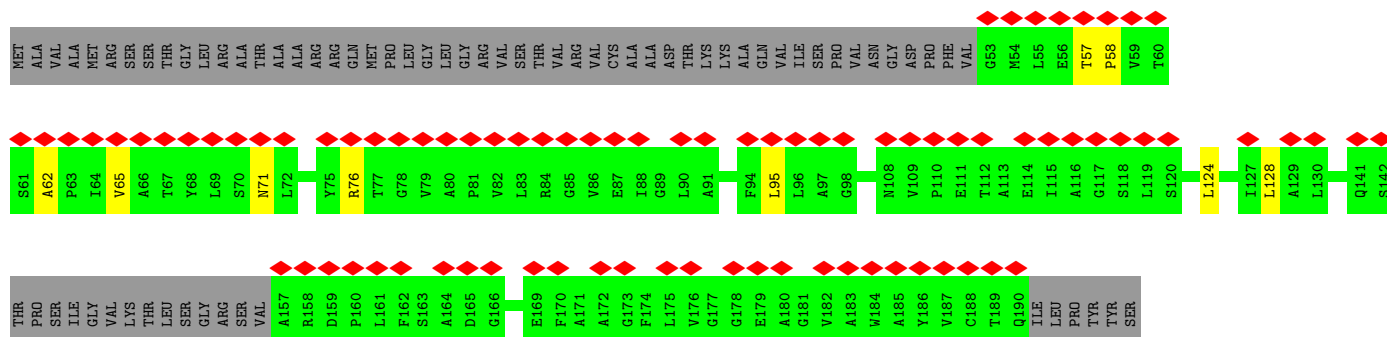
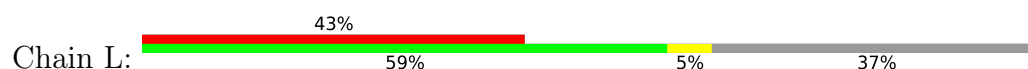


- Molecule 9: Photosystem I reaction center subunit IX

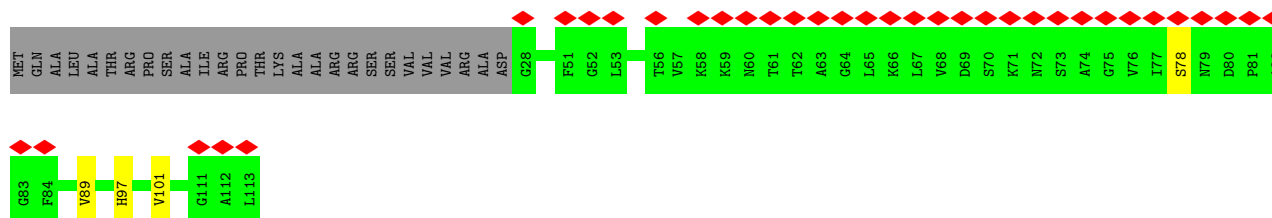
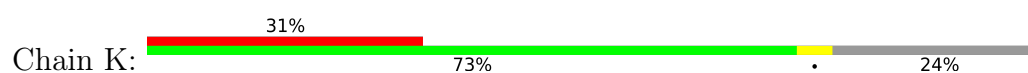




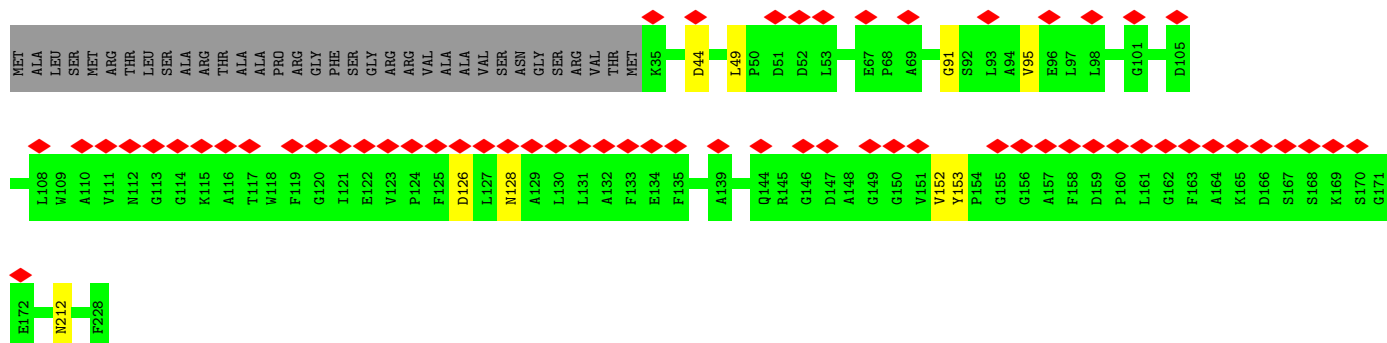
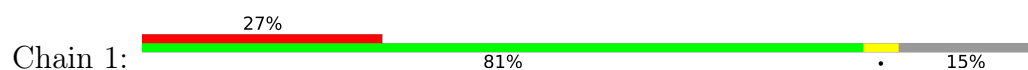
- Molecule 10: PSI subunit V



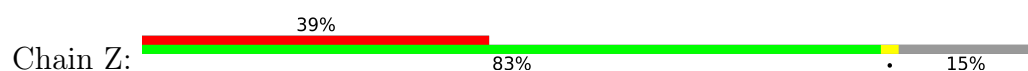
- Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic

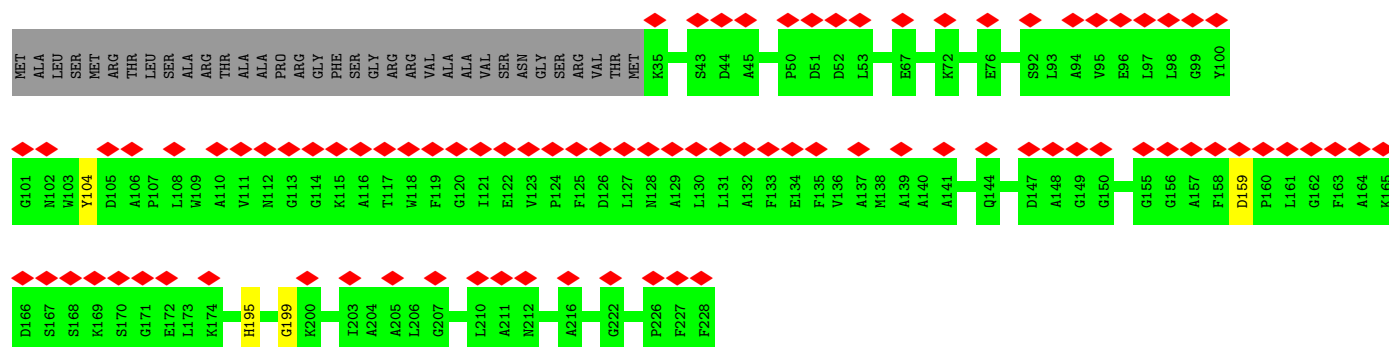


- Molecule 12: Chlorophyll a-b binding protein, chloroplastic

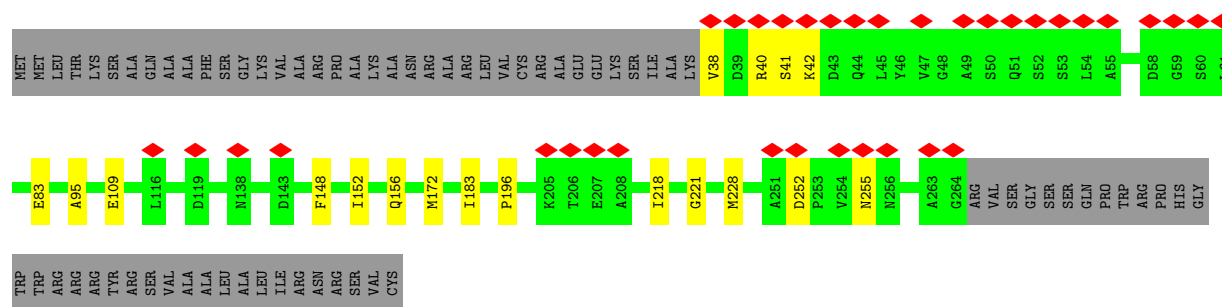


- Molecule 12: Chlorophyll a-b binding protein, chloroplastic

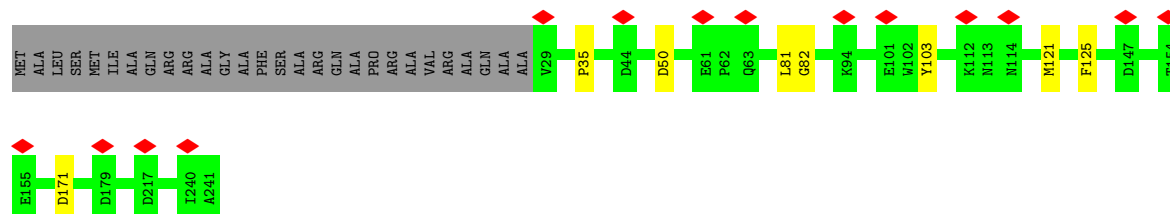
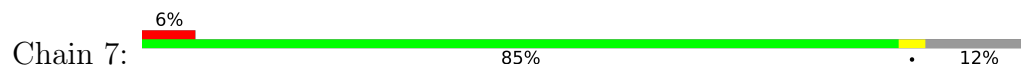




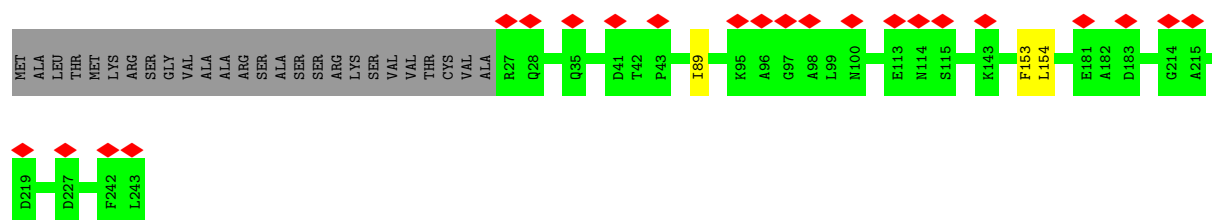
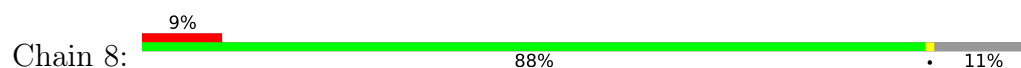
- Molecule 13: Chlorophyll a-b binding protein, chloroplastic



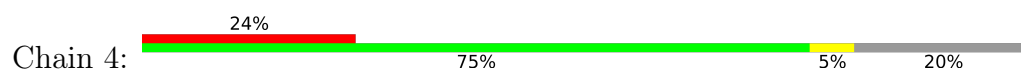
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic

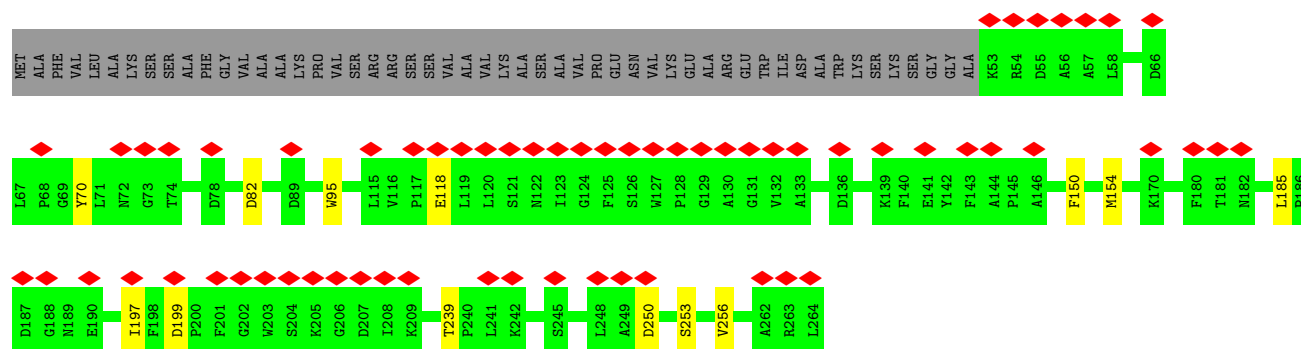


- Molecule 15: Chlorophyll a-b binding protein, chloroplastic



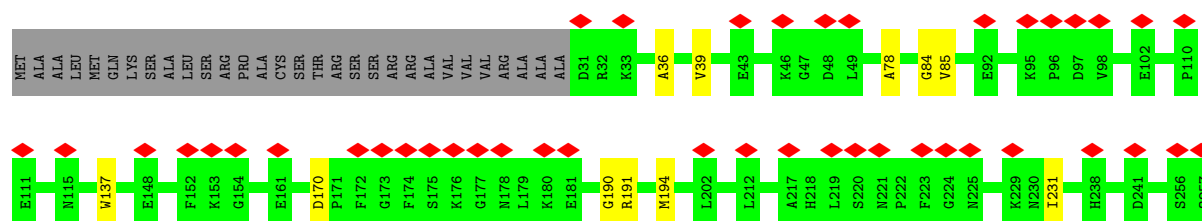
- Molecule 16: Chlorophyll a-b binding protein, chloroplastic (Lhca4)





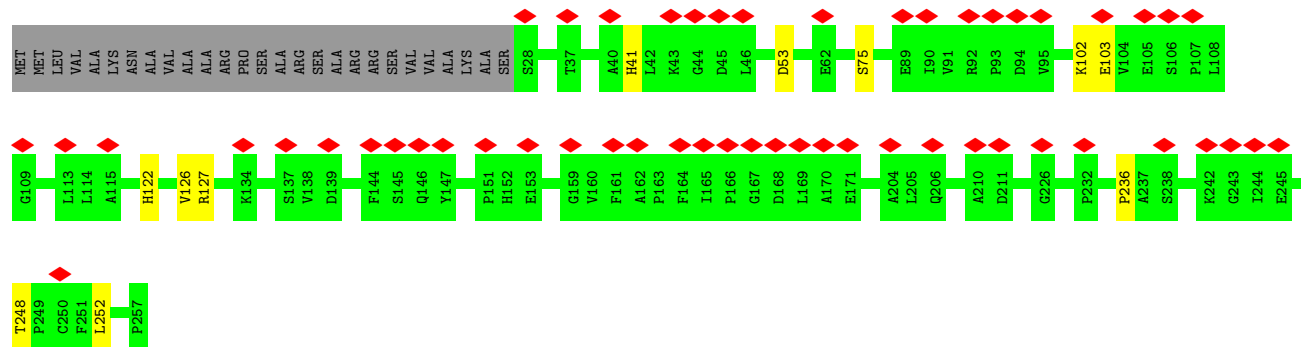
- Molecule 17: Chlorophyll a-b binding protein, chloroplastic

Chain 5: 17% 84% 12%



- Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 6: 21% 85% 11%



- Molecule 19: Chlorophyll a-b binding protein, chloroplastic

Chain 9: 73% 68% 5% 27%



F121	L122	E123	I124	K125	R126	Y127	Q128	G129	F130	K131	GLN	THR	GLY	THR	GLY	SER	PHE	ILE	ASN	SER	PHE	PRO	PHE	ASP	PRO	ALA	GLY	MET	ASN	SER	PRO	S153	M154	A155	T156	K157	E158	V159	K160	N161	G162	R163	L164	A165	M166	V167	A168	F169	I170	G171	F172	C173	V174	Q175	A176	L177	A178	T179	R180																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
T181	Q182	P183	I184	E185	G186	L187	T188	A189	H190	L191	A192	D193	P194	F195	G196	K197	N198	I199	T200	Y201	Y202	L203	T204	H205	L206	P207	E208	T209	L210	G211	S212	ALA																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	</

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	74209	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.321	Depositor
Minimum map value	-0.124	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.055	Depositor
Map size ($\text{\AA}$)	420.0, 420.0, 420.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.84, 0.84, 0.84	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.15	0/6021	0.26	0/8208
2	B	0.15	0/6036	0.26	0/8240
3	C	0.16	0/611	0.29	0/826
4	D	0.14	0/1161	0.26	0/1567
5	E	0.14	0/516	0.21	0/700
6	F	0.13	0/1292	0.23	0/1747
7	G	0.10	0/604	0.17	0/818
8	I	0.12	0/293	0.23	0/406
9	J	0.13	0/329	0.22	0/452
10	L	0.12	0/920	0.19	0/1257
11	K	0.14	0/588	0.18	0/795
12	1	0.13	0/1491	0.21	0/2028
12	Z	0.12	0/1491	0.19	0/2028
13	3	0.14	0/1784	0.24	0/2420
14	7	0.15	0/1702	0.23	0/2310
15	8	0.14	0/1701	0.22	0/2315
16	4	0.13	0/1703	0.20	0/2321
17	5	0.14	0/1830	0.21	0/2492
18	6	0.14	0/1834	0.23	0/2505
19	9	0.09	0/1221	0.17	0/1657
All	All	0.14	0/33128	0.23	0/45092

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 ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5825	5673	5675	27	0
2	B	5824	5576	5577	29	0
3	C	601	582	581	9	0
4	D	1133	1151	1150	6	0
5	E	506	505	504	0	0
6	F	1266	1302	1301	9	0
7	G	594	583	581	7	0
8	I	281	292	292	2	0
9	J	329	328	328	4	0
10	L	899	907	905	7	0
11	K	583	620	620	3	0
12	1	1445	1397	1396	6	0
12	Z	1445	1397	1396	3	0
13	3	1736	1695	1694	11	0
14	7	1650	1590	1589	9	0
15	8	1650	1629	1629	2	0
16	4	1648	1603	1602	9	0
17	5	1775	1747	1746	9	0
18	6	1772	1770	1770	6	0
19	9	1190	1196	1192	9	0
20	A	65	72	72	0	0
21	1	639	625	625	3	0
21	3	730	695	695	7	0
21	4	565	534	534	5	0
21	5	740	712	712	9	0
21	6	628	605	605	2	0
21	7	652	598	598	4	0
21	8	617	587	587	4	0
21	9	517	445	445	2	0
21	A	2718	2856	2856	27	0
21	B	2463	2580	2580	22	0
21	F	175	177	177	1	0
21	G	106	92	92	1	0
21	J	55	49	49	1	0
21	K	196	158	158	2	0
21	L	110	105	105	1	0
21	Z	637	616	616	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	A	33	46	46	1	0
22	B	33	46	46	0	0
23	1	44	58	58	0	0
23	3	78	99	99	2	0
23	4	87	123	123	0	0
23	5	37	44	44	0	0
23	6	85	116	116	0	0
23	7	49	74	74	1	0
23	8	44	61	61	0	0
23	9	34	38	38	0	0
23	A	87	123	123	0	0
23	B	45	63	63	0	0
23	Z	39	48	48	1	0
24	3	120	168	168	2	0
24	4	40	56	56	1	0
24	5	40	56	56	1	0
24	6	40	56	56	3	0
24	7	40	56	56	0	0
24	8	40	56	56	0	0
24	A	200	280	280	11	0
24	B	280	392	392	9	0
24	G	40	56	56	2	0
24	I	40	56	56	0	0
24	J	40	56	56	2	0
24	K	80	112	112	4	0
24	L	80	112	112	2	0
25	A	8	0	0	0	0
25	C	16	0	0	0	0
26	1	148	201	201	1	0
26	4	53	63	63	0	0
26	5	24	35	35	0	0
26	6	92	129	129	0	0
26	7	81	92	92	0	0
26	8	107	151	151	0	0
26	A	196	262	262	3	0
26	B	35	46	46	2	0
26	G	24	35	35	0	0
26	K	24	35	35	0	0
26	Z	53	63	63	0	0
27	1	85	113	113	1	0
27	3	45	75	75	0	0
27	4	68	88	88	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	6	20	35	35	0	0
27	7	37	44	44	0	0
27	8	74	91	91	0	0
27	A	72	84	84	4	0
27	B	79	98	98	0	0
27	J	77	97	97	1	0
28	1	84	112	112	0	0
28	3	126	168	168	1	0
28	4	42	56	56	1	0
28	5	84	112	112	4	0
28	6	42	56	56	1	0
28	7	84	112	112	1	0
28	8	42	56	56	0	0
28	9	84	112	112	4	0
28	A	42	56	56	0	0
28	F	42	56	56	4	0
28	Z	68	89	89	2	0
29	B	59	79	79	1	0
30	1	158	132	132	0	0
30	3	66	70	70	0	0
30	4	310	311	311	2	0
30	5	206	167	167	2	0
30	6	350	327	327	2	0
30	7	166	144	144	0	0
30	8	198	210	210	1	0
30	9	93	64	64	0	0
30	Z	178	171	171	1	0
31	1	44	56	56	0	0
31	4	44	56	56	0	0
31	5	44	56	56	1	0
31	6	44	56	56	0	0
31	7	44	56	56	1	0
31	8	44	56	56	0	0
31	Z	44	56	56	0	0
32	5	44	56	56	0	0
32	6	44	56	56	0	0
33	H	621	0	0	25	0
All	All	50499	50501	50486	252	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 3.

All (252) 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)
21:A:810:CLA:H143	21:A:812:CLA:H142	1.59	0.84
3:C:24:ASP:OD2	33:H:590:HOH:O	1.96	0.83
1:A:189:GLU:OE1	33:H:554:HOH:O	1.96	0.83
27:A:860:LMG:O2	9:J:1:AME:OT	1.97	0.82
27:A:859:LMG:O1	27:A:859:LMG:O4	2.00	0.79
19:9:52:ASP:OD1	28:9:617:LUT:O23	1.99	0.79
7:G:59:ARG:NH1	26:1:621:LMU:O2B	2.16	0.79
12:1:49:LEU:O	33:H:638:HOH:O	2.04	0.76
14:7:50:ASP:OD2	33:H:645:HOH:O	2.04	0.75
2:B:310:THR:OG1	33:H:352:HOH:O	1.98	0.74
2:B:214:LEU:O	19:9:180:ARG:NH2	2.21	0.74
17:5:170:ASP:OD1	28:5:620:LUT:O23	2.05	0.73
21:Z:603:CLA:HED2	21:Z:603:CLA:H43	1.69	0.73
10:L:71:ASN:O	10:L:76:ARG:NH2	2.20	0.73
13:3:109:GLU:OE2	33:H:640:HOH:O	2.07	0.72
1:A:44:ASN:OD1	33:H:439:HOH:O	2.07	0.72
23:7:625:LHG:O1	33:H:544:HOH:O	2.08	0.72
2:B:550:ASP:OD2	33:H:424:HOH:O	2.07	0.72
21:Z:616:CLA:H72	21:Z:616:CLA:H41	1.72	0.71
1:A:416:ASP:OD1	33:H:299:HOH:O	2.07	0.71
16:4:250:ASP:OD2	16:4:253:SER:OG	2.08	0.71
14:7:103:TYR:O	33:H:533:HOH:O	2.09	0.71
16:4:199:ASP:OD1	28:4:619:LUT:O23	2.09	0.70
30:5:607:CHL:H42	30:6:616:CHL:HED2	1.74	0.70
21:A:833:CLA:H42	10:L:65:VAL:HG13	1.75	0.69
12:Z:159:ASP:OD1	28:Z:617:LUT:O23	2.10	0.69
12:1:212:ASN:OD1	33:H:632:HOH:O	2.10	0.69
19:9:123:GLU:OE1	19:9:126:ARG:NH2	2.26	0.68
2:B:110:ALA:O	33:H:247:HOH:O	2.12	0.67
2:B:707:ARG:NH1	33:H:456:HOH:O	2.26	0.67
13:3:148:PHE:CE2	13:3:152:ILE:HD11	2.30	0.67
1:A:511:GLY:O	33:H:341:HOH:O	2.12	0.66
23:Z:620:LHG:O10	33:H:511:HOH:O	2.14	0.66
2:B:328:ASN:O	33:H:537:HOH:O	2.14	0.66
21:1:603:CLA:HED2	21:1:603:CLA:H43	1.78	0.65
2:B:614:SER:O	33:H:466:HOH:O	2.14	0.65
12:1:44:ASP:O	27:1:628:LMG:O4	2.16	0.64
13:3:252:ASP:OD2	13:3:255:ASN:ND2	2.33	0.61
6:F:175:LYS:NZ	33:H:618:HOH:O	2.33	0.60
3:C:2:ALA:N	3:C:71:SER:HG	2.00	0.60
16:4:256:VAL:N	21:4:613:CLA:O1A	2.34	0.60
23:3:721:LHG:O6	23:3:721:LHG:O2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:716:ARG:O	33:H:440:HOH:O	2.16	0.60
21:1:603:CLA:H43	21:1:603:CLA:CED	2.32	0.60
30:6:608:CHL:H11	28:6:621:LUT:H383	1.83	0.60
1:A:119:TRP:CD2	21:A:810:CLA:HED3	2.37	0.59
28:F:305:LUT:C28	28:F:305:LUT:H381	2.31	0.59
13:3:95:ALA:HB1	13:3:221:GLY:HA3	1.82	0.59
26:B:853:LMU:O5B	26:B:853:LMU:O3'	2.20	0.59
14:7:121:MET:HA	14:7:121:MET:HE3	1.85	0.58
14:7:171:ASP:OD1	28:7:621:LUT:O23	2.20	0.58
3:C:22:PRO:O	4:D:122:LEU:HD23	2.04	0.58
21:A:843:CLA:H141	10:L:124:LEU:HD11	1.85	0.58
18:6:236:PRO:O	18:6:248:THR:OG1	2.21	0.57
2:B:288:ALA:HB2	21:B:819:CLA:HBC2	1.86	0.57
21:B:826:CLA:HBB1	21:B:826:CLA:HMB1	1.87	0.56
6:F:204:LEU:HA	21:8:603:CLA:H42	1.85	0.56
11:K:89:VAL:HG22	21:K:201:CLA:HMD2	1.87	0.56
30:4:601:CHL:OBD	18:6:127:ARG:NH1	2.39	0.56
19:9:96:TRP:O	28:9:617:LUT:O3	2.24	0.56
1:A:226:LYS:NZ	1:A:253:LEU:O	2.39	0.55
2:B:150:PHE:CZ	21:B:811:CLA:H142	2.40	0.55
24:B:844:BCR:H321	24:B:844:BCR:HC8	1.87	0.55
14:7:121:MET:HE2	14:7:125:PHE:CE1	2.40	0.55
24:A:852:BCR:H362	21:A:854:CLA:H2	1.88	0.55
24:A:851:BCR:H23C	24:A:851:BCR:H403	1.88	0.55
1:A:183:LYS:NZ	26:A:865:LMU:O2'	2.32	0.55
12:1:126:ASP:OD2	12:1:128:ASN:ND2	2.38	0.54
21:5:601:CLA:C14	21:5:603:CLA:H41	2.36	0.54
1:A:377:TYR:O	33:H:187:HOH:O	2.18	0.54
21:A:803:CLA:HMB1	21:A:803:CLA:HBB1	1.89	0.54
12:1:91:GLY:O	12:1:95:VAL:HG23	2.08	0.54
13:3:172:MET:HE2	13:3:172:MET:HA	1.89	0.54
30:8:601:CHL:H41	21:8:614:CLA:H42	1.89	0.54
27:A:859:LMG:HO4	27:A:859:LMG:C1	2.18	0.53
1:A:333:PHE:CZ	21:A:845:CLA:HED2	2.43	0.53
13:3:40:ARG:O	13:3:41:SER:OG	2.18	0.53
21:B:819:CLA:HMB2	21:B:824:CLA:HMA3	1.91	0.53
21:B:832:CLA:H61	28:F:305:LUT:H182	1.91	0.53
21:B:819:CLA:HMB1	21:B:824:CLA:HED1	1.91	0.53
24:B:843:BCR:H331	24:B:843:BCR:C8	2.39	0.53
7:G:79:ASP:O	19:9:58:GLN:NE2	2.39	0.53
2:B:653:PHE:CZ	2:B:657:ILE:HD11	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:613:CLA:H102	21:1:613:CLA:H143	1.90	0.52
21:A:832:CLA:HMA2	10:L:57:THR:HG21	1.90	0.52
26:A:863:LMU:O5B	26:A:863:LMU:O3'	2.18	0.52
6:F:208:GLN:OE1	6:F:212:ARG:NH2	2.43	0.52
2:B:3:THR:O	8:I:103:ALA:N	2.42	0.51
2:B:466:ALA:O	2:B:480:SER:OG	2.19	0.51
21:A:809:CLA:H91	21:A:812:CLA:H201	1.92	0.51
6:F:123:LEU:HD21	9:J:38:VAL:HG11	1.93	0.51
14:7:81:LEU:HD22	21:7:610:CLA:H201	1.92	0.51
21:A:854:CLA:HBB1	21:A:854:CLA:HMB1	1.92	0.51
24:A:852:BCR:H331	24:A:852:BCR:C8	2.40	0.51
13:3:228:MET:HE2	28:3:622:LUT:H10	1.93	0.51
1:A:677:PHE:CD2	24:A:852:BCR:H363	2.46	0.50
24:A:848:BCR:H362	24:A:849:BCR:H21C	1.92	0.50
10:L:95:LEU:HD22	21:L:204:CLA:CHD	2.42	0.50
13:3:172:MET:HE1	14:7:35:PRO:HB2	1.94	0.50
21:5:612:CLA:HBC2	21:5:612:CLA:HHD	1.94	0.50
21:B:816:CLA:H43	7:G:117:ILE:HG13	1.94	0.50
21:A:843:CLA:H13	10:L:128:LEU:HD21	1.94	0.50
2:B:27:ALA:HA	21:B:829:CLA:H42	1.94	0.50
24:J:102:BCR:H331	24:J:102:BCR:C8	2.41	0.49
21:3:607:CLA:HBC1	24:3:719:BCR:H361	1.94	0.49
16:4:118:GLU:OE2	16:4:239:THR:OG1	2.28	0.49
21:A:811:CLA:HBA1	21:A:813:CLA:HMD2	1.95	0.49
3:C:25:VAL:HG13	3:C:44:ARG:O	2.13	0.49
3:C:22:PRO:C	4:D:122:LEU:HD23	2.37	0.49
10:L:58:PRO:O	10:L:62:ALA:HB2	2.13	0.49
21:3:615:CLA:C3	21:5:616:CLA:HED3	2.43	0.49
30:4:608:CHL:O1A	21:4:610:CLA:HMD1	2.12	0.48
21:A:833:CLA:HBB1	21:A:833:CLA:HMB3	1.95	0.48
16:4:95:TRP:CD1	27:4:624:LMG:HO4	2.30	0.48
21:7:614:CLA:HAB	28:5:626:LUT:H192	1.96	0.48
21:A:823:CLA:H101	21:A:823:CLA:H142	1.95	0.48
24:B:801:BCR:H331	24:B:801:BCR:C8	2.44	0.48
19:9:208:GLU:OE1	19:9:208:GLU:N	2.43	0.48
2:B:20:ARG:O	2:B:21:ARG:CB	2.62	0.47
21:A:810:CLA:HMB1	21:A:810:CLA:HBB1	1.95	0.47
2:B:722:TYR:HB2	21:B:802:CLA:HED2	1.94	0.47
24:L:205:BCR:H331	24:L:205:BCR:C8	2.44	0.47
21:9:613:CLA:C4C	21:9:613:CLA:H42	2.44	0.47
1:A:677:PHE:CG	24:A:852:BCR:H363	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:3:183:ILE:HG22	13:3:196:PRO:HG2	1.97	0.47
12:Z:195:HIS:O	12:Z:199:GLY:N	2.46	0.47
24:4:621:BCR:H331	24:4:621:BCR:C8	2.44	0.47
27:A:859:LMG:O1	27:A:859:LMG:C4	2.63	0.47
17:5:191:ARG:HA	17:5:194:MET:HE3	1.97	0.47
21:5:602:CLA:H41	21:5:603:CLA:O1A	2.14	0.47
30:5:608:CHL:H12	28:5:620:LUT:H383	1.96	0.47
1:A:418:ASP:OD2	1:A:420:THR:OG1	2.28	0.47
1:A:501:ASN:HB2	21:A:837:CLA:HED2	1.95	0.47
4:D:72:GLY:O	33:H:240:HOH:O	2.21	0.47
24:L:205:BCR:C23	24:L:205:BCR:H403	2.44	0.46
1:A:399:GLY:HA3	1:A:603:LEU:HD11	1.97	0.46
2:B:70:ALA:HB2	2:B:136:LEU:HB2	1.96	0.46
21:B:814:CLA:H61	21:B:814:CLA:H41	1.75	0.46
21:4:613:CLA:H42	21:4:616:CLA:HBC2	1.96	0.46
1:A:453:PHE:CZ	1:A:457:ILE:HD11	2.50	0.46
24:B:846:BCR:H331	24:B:846:BCR:C8	2.45	0.46
16:4:150:PHE:CE1	16:4:154:MET:HE3	2.50	0.46
7:G:78:ASP:OD1	7:G:78:ASP:N	2.48	0.46
24:K:202:BCR:H23C	24:K:202:BCR:H403	1.98	0.46
2:B:453:GLN:HE21	6:F:130:LEU:HD13	1.81	0.46
1:A:413:MET:HE1	1:A:431:ILE:HD11	1.98	0.45
17:5:85:VAL:HG11	28:5:620:LUT:H12	1.98	0.45
24:A:849:BCR:H331	24:A:849:BCR:C8	2.45	0.45
21:B:803:CLA:H42	21:B:803:CLA:O1A	2.16	0.45
21:B:808:CLA:C1A	21:B:808:CLA:CGA	2.94	0.45
6:F:64:ILE:HD11	6:F:143:TYR:CD2	2.51	0.45
28:9:617:LUT:C28	28:9:617:LUT:H381	2.46	0.45
1:A:22:VAL:HG11	21:A:812:CLA:HED1	1.97	0.45
24:3:719:BCR:H331	24:3:719:BCR:C8	2.47	0.45
24:B:844:BCR:H382	24:B:844:BCR:H23C	1.98	0.45
12:1:152:VAL:HG13	12:1:153:TYR:CD2	2.52	0.45
23:3:623:LHG:HC62	21:5:616:CLA:HMD3	1.99	0.45
21:A:802:CLA:HMD3	2:B:534:ILE:HG12	1.99	0.45
21:7:610:CLA:H13	21:6:603:CLA:H142	1.98	0.45
15:8:89:ILE:CD1	21:8:610:CLA:H142	2.47	0.45
24:A:851:BCR:H392	24:A:851:BCR:C23	2.47	0.44
21:A:811:CLA:H13	24:A:849:BCR:H372	1.99	0.44
21:Z:608:CLA:H12	28:Z:617:LUT:H383	1.99	0.44
14:7:121:MET:HE2	14:7:125:PHE:HE1	1.80	0.44
24:B:843:BCR:H362	24:G:205:BCR:H312	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:173:ARG:NH2	4:D:196:ILE:OXT	2.48	0.44
21:A:841:CLA:HAA2	21:B:831:CLA:HMB1	2.00	0.44
1:A:55:ASP:O	1:A:62:HIS:NE2	2.51	0.44
17:5:78:ALA:HB1	17:5:190:GLY:HA3	2.00	0.44
1:A:707:LEU:HD21	28:F:305:LUT:H192	1.99	0.44
2:B:530:THR:HG21	2:B:583:TRP:CE2	2.53	0.44
14:7:82:GLY:HA2	31:7:622:XAT:H181	1.99	0.44
21:3:615:CLA:H42	17:5:231:ILE:HG13	2.00	0.43
21:3:615:CLA:H43	21:5:616:CLA:HED3	1.99	0.43
21:3:615:CLA:H42	17:5:231:ILE:CG1	2.47	0.43
21:5:617:CLA:H61	21:5:617:CLA:H41	1.90	0.43
17:5:137:TRP:CG	21:5:617:CLA:HBC1	2.53	0.43
24:K:202:BCR:C8	24:K:202:BCR:H331	2.47	0.43
18:6:102:LYS:NZ	18:6:103:GLU:OE2	2.35	0.43
17:5:84:GLY:HA2	31:5:624:XAT:H181	2.01	0.43
2:B:217:LEU:HD11	19:9:207:PRO:HA	2.01	0.43
13:3:42:LYS:HG2	21:3:611:CLA:HMA1	2.01	0.43
2:B:537:LYS:NZ	33:H:577:HOH:O	2.52	0.43
11:K:97:HIS:O	11:K:101:VAL:HG23	2.19	0.43
21:5:621:CLA:CBD	21:5:621:CLA:HAA2	2.49	0.43
1:A:707:LEU:HD23	6:F:216:LEU:HD23	2.00	0.43
21:A:818:CLA:H61	21:A:818:CLA:H41	1.86	0.43
2:B:632:LEU:HD21	2:B:651:PHE:CD1	2.54	0.43
7:G:50:ARG:NH2	7:G:91:ASP:OD1	2.52	0.43
1:A:709:VAL:O	1:A:709:VAL:HG22	2.18	0.43
21:B:816:CLA:HED1	7:G:126:SER:HB2	2.01	0.43
21:4:613:CLA:H42	21:4:616:CLA:CBC	2.49	0.42
7:G:97:ILE:N	21:G:204:CLA:O2A	2.53	0.42
21:7:620:CLA:O1A	18:6:252:LEU:N	2.52	0.42
12:Z:104:TYR:O	30:Z:607:CHL:HED1	2.19	0.42
21:B:837:CLA:H41	28:F:305:LUT:H371	2.01	0.42
9:J:1:AME:C	9:J:1:AME:HT23	2.49	0.42
27:J:103:LMG:O1	27:J:103:LMG:HC61	2.19	0.42
1:A:411:ILE:HD13	21:A:831:CLA:CED	2.50	0.42
15:8:154:LEU:HB2	21:Z:603:CLA:H42	2.00	0.42
21:9:613:CLA:H61	21:9:613:CLA:H41	1.80	0.42
19:9:175:GLN:O	19:9:179:THR:OG1	2.12	0.42
24:5:622:BCR:H20C	24:5:622:BCR:H361	1.93	0.42
6:F:207:VAL:HG21	21:8:603:CLA:H41	2.01	0.42
1:A:244:LEU:O	26:A:857:LMU:O2'	2.36	0.42
2:B:352:HIS:CE1	21:B:826:CLA:NB	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:463:TRP:CG	21:F:304:CLA:HMA3	2.55	0.42
4:D:189:ARG:NH1	4:D:190:MET:O	2.53	0.42
11:K:78:SER:OG	21:K:201:CLA:O1D	2.37	0.42
18:6:41:HIS:NE2	18:6:53:ASP:OD2	2.46	0.42
24:6:623:BCR:H24C	24:6:623:BCR:H371	1.94	0.42
16:4:95:TRP:CG	27:4:624:LMG:HO4	2.38	0.42
22:A:844:PQN:H301	9:J:19:PHE:CZ	2.54	0.41
2:B:708:LEU:HD22	29:B:850:DGD:HB22	2.02	0.41
21:6:604:CLA:C1B	24:6:623:BCR:H402	2.50	0.41
24:A:850:BCR:H24C	24:A:850:BCR:H371	1.86	0.41
2:B:658:TYR:CD2	21:B:802:CLA:HMA1	2.56	0.41
21:B:831:CLA:H62	21:B:831:CLA:H41	1.91	0.41
3:C:5:VAL:HG22	3:C:67:VAL:HG22	2.02	0.41
2:B:315:SER:OG	21:B:841:CLA:O1A	2.20	0.41
21:A:802:CLA:CGA	21:A:802:CLA:H3A	2.50	0.41
21:A:821:CLA:HBB1	24:K:207:BCR:H342	2.02	0.41
13:3:38:VAL:HB	21:3:613:CLA:H141	2.03	0.41
21:4:613:CLA:H61	21:4:613:CLA:H41	1.80	0.41
2:B:340:ALA:HB2	24:B:847:BCR:H372	2.02	0.41
21:B:824:CLA:HAA2	21:B:824:CLA:HBD	2.01	0.41
3:C:14:CYS:O	3:C:15:THR:OG1	2.30	0.41
3:C:36:ALA:O	3:C:37:SER:OG	2.34	0.41
24:6:623:BCR:C8	24:6:623:BCR:H331	2.51	0.41
3:C:46:GLU:O	33:H:594:HOH:O	2.22	0.41
21:A:820:CLA:CAD	21:A:830:CLA:H41	2.51	0.41
24:B:848:BCR:H20C	24:B:848:BCR:H361	1.93	0.41
4:D:81:GLU:O	4:D:82:GLU:HB3	2.20	0.41
8:I:80:VAL:HB	8:I:81:PRO:HD3	2.03	0.41
21:J:101:CLA:H62	21:J:101:CLA:H41	1.89	0.41
1:A:417:TYR:OH	33:H:561:HOH:O	2.20	0.41
24:G:205:BCR:H24C	24:G:205:BCR:H371	1.87	0.41
26:B:853:LMU:H3O2	26:B:853:LMU:C1B	2.32	0.40
24:K:202:BCR:C11	24:K:207:BCR:H333	2.51	0.40
18:6:122:HIS:O	18:6:126:VAL:HG23	2.21	0.40
1:A:393:HIS:HB2	21:A:829:CLA:CHB	2.51	0.40
1:A:536:HIS:CG	21:A:839:CLA:HED3	2.56	0.40
24:J:102:BCR:H20C	24:J:102:BCR:H361	1.90	0.40
17:5:36:ALA:O	17:5:39:VAL:HG22	2.21	0.40
2:B:451:GLU:OE2	6:F:114:ARG:NH1	2.53	0.40
16:4:70:TYR:OH	16:4:82:ASP:OD2	2.38	0.40
19:9:172:PHE:CE1	28:9:616:LUT:H182	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:851:BCR:H24C	24:A:851:BCR:H371	1.90	0.40
21:B:819:CLA:CMB	21:B:824:CLA:HED1	2.51	0.40
21:B:832:CLA:H152	21:B:832:CLA:H193	2.04	0.40
24:B:845:BCR:C8	24:B:845:BCR:H331	2.49	0.40
16:4:185:LEU:HD21	16:4:197:ILE:HG22	2.02	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	A	740/751 (98%)	724 (98%)	16 (2%)	0	100	100
2	B	731/735 (100%)	710 (97%)	20 (3%)	1 (0%)	48	59
3	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
4	D	142/196 (72%)	138 (97%)	4 (3%)	0	100	100
5	E	62/97 (64%)	61 (98%)	1 (2%)	0	100	100
6	F	163/227 (72%)	162 (99%)	1 (1%)	0	100	100
7	G	76/126 (60%)	73 (96%)	3 (4%)	0	100	100
8	I	35/106 (33%)	34 (97%)	1 (3%)	0	100	100
9	J	38/40 (95%)	38 (100%)	0	0	100	100
10	L	120/196 (61%)	118 (98%)	2 (2%)	0	100	100
11	K	84/113 (74%)	84 (100%)	0	0	100	100
12	1	192/228 (84%)	191 (100%)	1 (0%)	0	100	100
12	Z	192/228 (84%)	188 (98%)	4 (2%)	0	100	100
13	3	225/298 (76%)	218 (97%)	7 (3%)	0	100	100
14	7	211/241 (88%)	205 (97%)	6 (3%)	0	100	100
15	8	215/243 (88%)	212 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	4	210/264 (80%)	209 (100%)	1 (0%)	0	100	100
17	5	225/257 (88%)	222 (99%)	3 (1%)	0	100	100
18	6	228/257 (89%)	223 (98%)	5 (2%)	0	100	100
19	9	148/213 (70%)	145 (98%)	3 (2%)	0	100	100
All	All	4115/4897 (84%)	4031 (98%)	83 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	601/610 (98%)	600 (100%)	1 (0%)	87	94
2	B	596/597 (100%)	595 (100%)	1 (0%)	87	94
3	C	69/70 (99%)	69 (100%)	0	100	100
4	D	121/152 (80%)	121 (100%)	0	100	100
5	E	55/81 (68%)	55 (100%)	0	100	100
6	F	127/169 (75%)	127 (100%)	0	100	100
7	G	59/94 (63%)	58 (98%)	1 (2%)	53	70
8	I	31/76 (41%)	31 (100%)	0	100	100
9	J	35/35 (100%)	35 (100%)	0	100	100
10	L	90/148 (61%)	90 (100%)	0	100	100
11	K	59/80 (74%)	59 (100%)	0	100	100
12	1	137/162 (85%)	137 (100%)	0	100	100
12	Z	137/162 (85%)	137 (100%)	0	100	100
13	3	174/230 (76%)	171 (98%)	3 (2%)	53	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	7	164/181 (91%)	164 (100%)	0	100	100
15	8	163/183 (89%)	162 (99%)	1 (1%)	78	88
16	4	166/205 (81%)	166 (100%)	0	100	100
17	5	184/206 (89%)	184 (100%)	0	100	100
18	6	184/203 (91%)	183 (100%)	1 (0%)	81	89
19	9	117/159 (74%)	117 (100%)	0	100	100
All	All	3269/3803 (86%)	3261 (100%)	8 (0%)	85	94

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	372	TYR
2	B	99	GLN
7	G	78	ASP
13	3	83	GLU
13	3	156	GLN
13	3	218	ILE
15	8	153	PHE
18	6	75	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	387	GLN
2	B	77	GLN
2	B	99	GLN
2	B	453	GLN
4	D	148	GLN
6	F	169	GLN
7	G	121	GLN
12	1	180	ASN
12	1	194	GLN
13	3	220	ASN
14	7	162	ASN
14	7	218	ASN
16	4	166	GLN
16	4	182	ASN
19	9	40	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
9	AME	J	1	9	9,10,11	0.52	0	9,11,13	0.95	1 (11%)

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
9	AME	J	1	9	-	5/9/10/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	1	AME	O-C-CA	-2.64	117.97	124.77

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	J	1	AME	C-CA-CB-CG
9	J	1	AME	N-CA-CB-CG
9	J	1	AME	CT2-CT1-N-CA
9	J	1	AME	OT-CT1-N-CA
9	J	1	AME	CB-CA-N-CT1

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	J	1	AME	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

351 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
21	CLA	5	610	17	64,68,73	1.20	4 (6%)	76,107,113	0.81	2 (2%)
27	LMG	J	104	-	35,35,55	0.19	0	43,43,63	0.17	0
21	CLA	A	813	-	69,73,73	1.17	5 (7%)	82,113,113	0.79	2 (2%)
30	CHL	6	618	18	37,51,74	2.48	10 (27%)	30,86,114	1.54	5 (16%)
31	XAT	6	624	-	41,47,47	0.14	0	54,74,74	0.70	1 (1%)
23	LHG	9	622	21	33,33,48	0.26	0	36,39,54	0.29	0
21	CLA	A	808	-	54,58,73	1.28	5 (9%)	64,95,113	0.90	2 (3%)
31	XAT	7	622	-	41,47,47	0.15	0	54,74,74	0.62	1 (1%)
21	CLA	B	805	-	69,73,73	1.13	4 (5%)	82,113,113	0.80	2 (2%)
21	CLA	B	830	-	49,53,73	1.34	4 (8%)	58,89,113	0.96	2 (3%)
26	LMU	4	625	-	34,34,36	0.11	0	45,45,47	0.26	0
30	CHL	8	601	15	60,74,74	1.89	10 (16%)	58,114,114	1.10	4 (6%)
21	CLA	B	836	-	64,68,73	1.16	5 (7%)	76,107,113	0.84	2 (2%)
21	CLA	Z	613	33	69,73,73	1.16	5 (7%)	82,113,113	0.83	3 (3%)
21	CLA	B	812	-	69,73,73	1.17	5 (7%)	82,113,113	0.81	2 (2%)
21	CLA	Z	602	12	64,68,73	1.22	5 (7%)	76,107,113	0.88	2 (2%)
21	CLA	7	616	14	50,54,73	1.37	5 (10%)	59,90,113	0.94	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	LMU	1	625	-	24,24,36	0.10	0	29,29,47	0.31	0
28	LUT	9	616	-	42,43,43	0.23	0	51,60,60	0.34	0
21	CLA	A	804	-	69,73,73	1.14	5 (7%)	82,113,113	0.79	2 (2%)
20	CL0	A	801	-	58,73,73	1.35	7 (12%)	60,113,113	1.52	4 (6%)
21	CLA	3	613	13	64,68,73	1.20	5 (7%)	76,107,113	0.83	2 (2%)
28	LUT	7	624	-	42,43,43	0.24	0	51,60,60	0.32	0
21	CLA	B	807	-	59,63,73	1.28	4 (6%)	70,101,113	0.87	2 (2%)
29	DGD	B	850	-	60,60,67	0.17	0	74,74,81	0.37	1 (1%)
26	LMU	8	624	-	24,24,36	0.11	0	29,29,47	0.25	0
21	CLA	Z	614	-	54,58,73	1.33	4 (7%)	64,95,113	0.93	3 (4%)
30	CHL	6	606	33	52,66,74	2.07	10 (19%)	48,104,114	1.18	5 (10%)
21	CLA	3	610	13	69,73,73	1.15	5 (7%)	82,113,113	0.80	2 (2%)
21	CLA	A	826	33	69,73,73	1.15	4 (5%)	82,113,113	0.83	2 (2%)
23	LHG	4	623	-	37,37,48	0.25	0	40,43,54	0.31	0
21	CLA	B	841	23	69,73,73	1.19	5 (7%)	82,113,113	0.83	2 (2%)
21	CLA	F	304	6	69,73,73	1.16	5 (7%)	82,113,113	0.84	2 (2%)
21	CLA	9	601	19	50,54,73	1.38	4 (8%)	59,90,113	0.96	3 (5%)
28	LUT	6	621	-	42,43,43	0.26	0	51,60,60	0.44	0
28	LUT	5	626	-	42,43,43	0.29	0	51,60,60	0.42	0
21	CLA	8	613	15	69,73,73	1.14	5 (7%)	82,113,113	0.81	3 (3%)
26	LMU	4	626	-	20,20,36	0.15	0	25,25,47	0.29	0
21	CLA	L	204	33	49,53,73	1.40	4 (8%)	58,89,113	0.99	3 (5%)
31	XAT	Z	618	-	41,47,47	0.13	0	54,74,74	0.73	1 (1%)
24	BCR	B	844	-	41,41,41	0.16	0	56,56,56	0.42	0
24	BCR	L	201	-	41,41,41	0.12	0	56,56,56	0.39	0
26	LMU	8	625	-	24,24,36	0.13	0	29,29,47	0.30	0
21	CLA	5	601	17	69,73,73	1.18	4 (5%)	82,113,113	0.82	2 (2%)
26	LMU	G	206	-	24,24,36	0.12	0	29,29,47	0.26	0
26	LMU	7	628	-	22,22,36	0.12	0	27,27,47	0.32	0
21	CLA	1	610	12	69,73,73	1.14	5 (7%)	82,113,113	0.82	3 (3%)
21	CLA	A	831	-	69,73,73	1.09	4 (5%)	82,113,113	0.82	2 (2%)
21	CLA	A	806	-	69,73,73	1.09	5 (7%)	82,113,113	0.89	2 (2%)
21	CLA	A	817	33	59,63,73	1.26	5 (8%)	70,101,113	0.88	2 (2%)
21	CLA	7	614	-	47,51,73	1.41	5 (10%)	55,86,113	0.97	2 (3%)
28	LUT	3	621	-	42,43,43	0.23	0	51,60,60	0.37	0
24	BCR	B	847	-	41,41,41	0.17	0	56,56,56	0.46	0
21	CLA	6	611	23	62,66,73	1.26	4 (6%)	73,104,113	0.86	2 (2%)
21	CLA	A	816	-	69,73,73	1.13	5 (7%)	82,113,113	0.81	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	Z	608	33	54,58,73	1.33	4 (7%)	64,95,113	0.94	2 (3%)
21	CLA	B	810	-	69,73,73	1.15	5 (7%)	82,113,113	0.82	3 (3%)
21	CLA	B	814	-	64,68,73	1.18	4 (6%)	76,107,113	0.87	3 (3%)
30	CHL	7	607	33	48,62,74	2.16	10 (20%)	43,99,114	1.26	5 (11%)
30	CHL	Z	607	33	60,74,74	1.96	10 (16%)	58,114,114	1.04	4 (6%)
21	CLA	9	610	19	64,68,73	1.21	4 (6%)	76,107,113	0.84	3 (3%)
21	CLA	K	204	-	50,54,73	1.37	5 (10%)	59,90,113	0.97	3 (5%)
21	CLA	A	802	-	69,73,73	1.09	5 (7%)	82,113,113	0.77	2 (2%)
27	LMG	7	626	-	37,37,55	0.20	0	45,45,63	0.33	0
21	CLA	A	819	-	64,68,73	1.17	5 (7%)	76,107,113	0.87	2 (2%)
24	BCR	B	843	-	41,41,41	0.14	0	56,56,56	0.29	0
21	CLA	A	820	-	69,73,73	1.12	5 (7%)	82,113,113	0.81	3 (3%)
30	CHL	9	606	-	36,50,74	2.48	10 (27%)	29,85,114	1.36	4 (13%)
21	CLA	B	833	-	62,66,73	1.17	5 (8%)	73,104,113	0.89	3 (4%)
21	CLA	A	838	-	55,59,73	1.27	4 (7%)	64,96,113	0.91	2 (3%)
26	LMU	8	628	-	24,24,36	0.14	0	29,29,47	0.28	0
27	LMG	A	859	-	40,40,55	0.19	0	48,48,63	0.26	0
28	LUT	F	305	-	42,43,43	0.30	0	51,60,60	0.76	1 (1%)
21	CLA	B	828	-	69,73,73	1.12	5 (7%)	82,113,113	0.81	3 (3%)
21	CLA	B	821	-	69,73,73	1.18	5 (7%)	82,113,113	0.83	3 (3%)
28	LUT	3	622	-	42,43,43	0.21	0	51,60,60	0.38	0
28	LUT	3	720	-	42,43,43	0.23	0	51,60,60	0.31	0
21	CLA	8	609	15	49,53,73	1.36	5 (10%)	58,89,113	0.95	2 (3%)
21	CLA	3	603	-	69,73,73	1.15	5 (7%)	82,113,113	0.81	2 (2%)
21	CLA	J	101	9	59,63,73	1.24	4 (6%)	70,101,113	0.89	2 (2%)
24	BCR	K	202	-	41,41,41	0.18	0	56,56,56	0.40	0
27	LMG	B	852	-	43,43,55	0.18	0	51,51,63	0.21	0
21	CLA	8	614	-	61,65,73	1.26	4 (6%)	72,103,113	0.86	2 (2%)
21	CLA	8	612	15	59,63,73	1.23	4 (6%)	70,101,113	0.87	2 (2%)
21	CLA	B	803	-	69,73,73	1.18	4 (5%)	82,113,113	0.82	3 (3%)
21	CLA	3	614	-	49,53,73	1.39	4 (8%)	58,89,113	0.98	3 (5%)
21	CLA	A	840	-	69,73,73	1.17	5 (7%)	82,113,113	0.83	2 (2%)
21	CLA	7	603	-	56,60,73	1.31	5 (8%)	65,97,113	0.92	3 (4%)
21	CLA	A	836	-	69,73,73	1.14	4 (5%)	82,113,113	0.80	2 (2%)
30	CHL	8	607	33	60,74,74	1.88	10 (16%)	58,114,114	1.13	5 (8%)
26	LMU	A	863	-	36,36,36	0.08	0	47,47,47	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CHL	5	608	33	45,59,74	2.30	10 (22%)	40,96,114	1.31	5 (12%)
22	PQN	A	844	-	34,34,34	0.31	0	43,45,45	0.48	0
21	CLA	A	835	-	69,73,73	1.16	4 (5%)	82,113,113	0.81	2 (2%)
23	LHG	A	846	-	48,48,48	0.26	0	51,54,54	0.34	0
21	CLA	A	812	-	69,73,73	1.09	4 (5%)	82,113,113	0.79	2 (2%)
21	CLA	B	824	33	69,73,73	1.21	4 (5%)	82,113,113	0.84	2 (2%)
21	CLA	6	612	18	49,53,73	1.37	4 (8%)	58,89,113	0.96	3 (5%)
21	CLA	B	834	-	64,68,73	1.18	5 (7%)	76,107,113	0.86	2 (2%)
30	CHL	7	601	14	60,74,74	1.89	10 (16%)	58,114,114	1.05	5 (8%)
21	CLA	5	617	-	69,73,73	1.12	5 (7%)	82,113,113	0.82	2 (2%)
27	LMG	4	624	-	41,41,55	0.20	0	49,49,63	0.47	0
26	LMU	A	858	-	36,36,36	0.09	0	47,47,47	0.19	0
21	CLA	F	303	33	49,53,73	1.36	5 (10%)	58,89,113	0.95	2 (3%)
21	CLA	5	614	-	49,53,73	1.39	4 (8%)	58,89,113	0.97	3 (5%)
21	CLA	5	612	17	49,53,73	1.38	4 (8%)	58,89,113	0.96	2 (3%)
27	LMG	1	624	-	36,36,55	0.19	0	44,44,63	0.16	0
30	CHL	4	601	16	60,74,74	1.98	10 (16%)	58,114,114	1.01	3 (5%)
21	CLA	Z	604	33	61,65,73	1.25	5 (8%)	72,103,113	0.88	3 (4%)
21	CLA	A	837	1	61,65,73	1.28	5 (8%)	72,103,113	0.89	2 (2%)
24	BCR	A	852	-	41,41,41	0.15	0	56,56,56	0.38	0
21	CLA	A	807	1	69,73,73	1.13	5 (7%)	82,113,113	0.76	2 (2%)
21	CLA	6	610	18	64,68,73	1.21	5 (7%)	76,107,113	0.84	2 (2%)
30	CHL	1	601	12	60,74,74	1.90	10 (16%)	58,114,114	1.06	4 (6%)
21	CLA	F	301	33	69,73,73	1.13	5 (7%)	82,113,113	0.82	2 (2%)
31	XAT	8	618	-	41,47,47	0.17	0	54,74,74	0.68	2 (3%)
21	CLA	A	810	1	69,73,73	1.19	5 (7%)	82,113,113	0.86	3 (3%)
24	BCR	3	620	-	41,41,41	0.21	0	56,56,56	0.41	0
21	CLA	9	614	-	49,53,73	1.38	4 (8%)	58,89,113	0.95	3 (5%)
31	XAT	5	624	-	41,47,47	0.13	0	54,74,74	0.76	1 (1%)
21	CLA	4	604	33	54,58,73	1.32	5 (9%)	64,95,113	0.93	3 (4%)
24	BCR	8	619	-	41,41,41	0.13	0	56,56,56	0.31	0
21	CLA	K	201	11	49,53,73	1.43	4 (8%)	58,89,113	0.96	1 (1%)
26	LMU	1	622	-	19,19,36	0.13	0	24,24,47	0.31	0
26	LMU	A	861	-	24,24,36	0.12	0	29,29,47	0.33	0
21	CLA	4	616	16	49,53,73	1.37	5 (10%)	58,89,113	0.98	3 (5%)
23	LHG	7	625	21	48,48,48	0.24	0	51,54,54	0.27	0
26	LMU	A	864	-	24,24,36	0.12	0	29,29,47	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	4	602	16	64,68,73	1.20	5 (7%)	76,107,113	0.88	3 (3%)
21	CLA	Z	609	12	69,73,73	1.13	5 (7%)	82,113,113	0.90	4 (4%)
21	CLA	1	614	-	64,68,73	1.21	5 (7%)	76,107,113	0.85	3 (3%)
21	CLA	B	813	-	69,73,73	1.15	4 (5%)	82,113,113	0.82	2 (2%)
21	CLA	Z	616	12	64,68,73	1.22	5 (7%)	76,107,113	0.86	3 (3%)
21	CLA	4	614	-	59,63,73	1.29	4 (6%)	70,101,113	0.89	2 (2%)
24	BCR	A	851	-	41,41,41	0.16	0	56,56,56	0.38	0
21	CLA	B	806	2	69,73,73	1.15	4 (5%)	82,113,113	0.77	2 (2%)
21	CLA	3	617	13	50,54,73	1.37	5 (10%)	59,90,113	0.96	2 (3%)
24	BCR	6	623	-	41,41,41	0.20	0	56,56,56	0.44	0
21	CLA	A	821	-	59,63,73	1.25	5 (8%)	70,101,113	0.86	2 (2%)
21	CLA	B	808	-	69,73,73	1.12	5 (7%)	82,113,113	0.81	2 (2%)
21	CLA	5	611	23	59,63,73	1.27	4 (6%)	70,101,113	0.86	2 (2%)
21	CLA	4	613	16	69,73,73	1.19	4 (5%)	82,113,113	0.82	2 (2%)
26	LMU	7	629	-	28,28,36	0.11	0	39,39,47	0.28	0
21	CLA	8	608	33	54,58,73	1.32	5 (9%)	64,95,113	0.93	2 (3%)
21	CLA	B	840	-	69,73,73	1.11	5 (7%)	82,113,113	0.83	2 (2%)
23	LHG	8	620	21	43,43,48	0.27	0	46,49,54	0.28	0
21	CLA	6	622	33	59,63,73	1.28	4 (6%)	70,101,113	0.88	2 (2%)
24	BCR	A	849	-	41,41,41	0.17	0	56,56,56	0.29	0
24	BCR	L	205	-	41,41,41	0.23	0	56,56,56	0.44	0
21	CLA	9	611	23	49,53,73	1.41	4 (8%)	58,89,113	0.98	3 (5%)
28	LUT	A	856	-	42,43,43	0.26	0	51,60,60	0.56	1 (1%)
27	LMG	1	628	-	49,49,55	0.17	0	57,57,63	0.19	0
21	CLA	3	607	13	59,63,73	1.24	5 (8%)	70,101,113	0.86	3 (4%)
26	LMU	1	626	-	24,24,36	0.12	0	29,29,47	0.26	0
30	CHL	6	608	33	45,59,74	2.27	10 (22%)	40,96,114	1.30	5 (12%)
21	CLA	6	613	33	69,73,73	1.18	5 (7%)	82,113,113	0.84	2 (2%)
21	CLA	3	609	13	65,69,73	1.20	5 (7%)	77,108,113	0.83	2 (2%)
26	LMU	6	632	-	20,20,36	0.14	0	25,25,47	0.27	0
21	CLA	A	811	-	69,73,73	1.09	5 (7%)	82,113,113	0.82	3 (3%)
21	CLA	1	611	23	65,69,73	1.18	5 (7%)	77,108,113	0.83	3 (3%)
31	XAT	1	618	-	41,47,47	0.13	0	54,74,74	0.76	3 (5%)
21	CLA	A	805	-	59,63,73	1.19	4 (6%)	70,101,113	0.85	2 (2%)
21	CLA	9	602	19	64,68,73	1.22	4 (6%)	76,107,113	0.86	3 (3%)
30	CHL	8	606	33	60,74,74	1.93	10 (16%)	58,114,114	1.12	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CHL	5	618	17	37,51,74	2.46	10 (27%)	30,86,114	1.49	5 (16%)
28	LUT	8	617	-	42,43,43	0.28	0	51,60,60	0.41	0
21	CLA	B	818	-	69,73,73	1.17	4 (5%)	82,113,113	0.82	2 (2%)
21	CLA	A	814	-	69,73,73	1.14	5 (7%)	82,113,113	0.79	2 (2%)
21	CLA	8	602	15	69,73,73	1.14	5 (7%)	82,113,113	0.82	2 (2%)
21	CLA	A	809	1	69,73,73	1.12	4 (5%)	82,113,113	0.81	3 (3%)
21	CLA	A	824	-	49,53,73	1.42	5 (10%)	58,89,113	0.97	2 (3%)
21	CLA	7	610	14	69,73,73	1.12	5 (7%)	82,113,113	0.95	4 (4%)
21	CLA	5	609	17	69,73,73	1.13	5 (7%)	82,113,113	0.80	3 (3%)
21	CLA	B	826	-	69,73,73	1.13	5 (7%)	82,113,113	0.83	3 (3%)
24	BCR	4	621	-	41,41,41	0.13	0	56,56,56	0.35	0
21	CLA	B	820	-	60,64,73	1.26	5 (8%)	71,102,113	0.87	2 (2%)
21	CLA	A	845	23	49,53,73	1.36	4 (8%)	58,89,113	0.95	2 (3%)
26	LMU	6	630	-	24,24,36	0.14	0	29,29,47	0.24	0
21	CLA	A	827	33	69,73,73	1.14	5 (7%)	82,113,113	0.80	2 (2%)
23	LHG	6	619	21	48,48,48	0.24	0	51,54,54	0.35	0
30	CHL	4	607	33	60,74,74	1.94	10 (16%)	58,114,114	1.04	4 (6%)
21	CLA	9	613	19	69,73,73	1.16	4 (5%)	82,113,113	0.82	3 (3%)
26	LMU	6	631	-	24,24,36	0.12	0	29,29,47	0.26	0
23	LHG	3	721	-	30,30,48	0.28	0	33,36,54	0.33	0
24	BCR	A	848	-	41,41,41	0.18	0	56,56,56	0.35	0
21	CLA	7	611	23	69,73,73	1.16	5 (7%)	82,113,113	0.80	2 (2%)
21	CLA	3	615	33	69,73,73	1.18	5 (7%)	82,113,113	0.84	2 (2%)
21	CLA	4	603	16	69,73,73	1.16	5 (7%)	82,113,113	0.79	2 (2%)
23	LHG	5	623	21	36,36,48	0.27	0	39,42,54	0.29	0
24	BCR	5	622	-	41,41,41	0.19	0	56,56,56	0.35	0
23	LHG	4	622	21	48,48,48	0.23	0	51,54,54	0.38	0
26	LMU	8	627	-	36,36,36	0.09	0	47,47,47	0.37	0
21	CLA	1	609	12	69,73,73	1.19	4 (5%)	82,113,113	0.79	2 (2%)
21	CLA	1	602	12	64,68,73	1.20	5 (7%)	76,107,113	0.88	3 (3%)
21	CLA	Z	603	-	69,73,73	1.19	5 (7%)	82,113,113	0.82	2 (2%)
21	CLA	3	604	33	69,73,73	1.16	5 (7%)	82,113,113	0.83	3 (3%)
21	CLA	B	837	-	69,73,73	1.12	5 (7%)	82,113,113	0.82	2 (2%)
21	CLA	3	612	13	50,54,73	1.37	5 (10%)	59,90,113	0.96	3 (5%)
26	LMU	Z	622	-	32,32,36	0.10	0	43,43,47	0.20	0
21	CLA	B	802	-	69,73,73	1.12	5 (7%)	82,113,113	0.77	2 (2%)
24	BCR	B	801	-	41,41,41	0.11	0	56,56,56	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	B	832	-	69,73,73	1.14	5 (7%)	82,113,113	0.83	2 (2%)
21	CLA	3	602	13	64,68,73	1.17	5 (7%)	76,107,113	0.84	3 (3%)
24	BCR	I	172	-	41,41,41	0.18	0	56,56,56	0.39	0
21	CLA	B	809	2	69,73,73	1.16	4 (5%)	82,113,113	0.79	2 (2%)
21	CLA	A	833	-	69,73,73	1.18	5 (7%)	82,113,113	0.80	3 (3%)
21	CLA	B	819	33	64,68,73	1.20	5 (7%)	76,107,113	0.83	3 (3%)
32	NEX	6	625	-	40,46,46	0.29	0	50,70,70	0.88	3 (6%)
21	CLA	B	817	-	69,73,73	1.13	5 (7%)	82,113,113	0.83	3 (3%)
21	CLA	6	602	18	69,73,73	1.17	4 (5%)	82,113,113	0.83	3 (3%)
25	SF4	A	853	1,2	0,12,12	-	-	-	-	-
21	CLA	B	827	-	69,73,73	1.14	5 (7%)	82,113,113	0.85	2 (2%)
30	CHL	Z	601	12	60,74,74	1.92	10 (16%)	58,114,114	1.08	5 (8%)
21	CLA	A	815	-	59,63,73	1.23	5 (8%)	70,101,113	0.88	2 (2%)
21	CLA	B	825	33	69,73,73	1.13	5 (7%)	82,113,113	0.77	2 (2%)
21	CLA	5	602	17	69,73,73	1.17	5 (7%)	82,113,113	0.83	3 (3%)
30	CHL	4	618	16	40,54,74	2.40	10 (25%)	34,90,114	1.35	5 (14%)
24	BCR	B	845	-	41,41,41	0.15	0	56,56,56	0.36	0
21	CLA	L	203	-	69,73,73	1.15	4 (5%)	82,113,113	0.80	3 (3%)
23	LHG	Z	620	21	38,38,48	0.26	0	41,44,54	0.30	0
28	LUT	1	619	-	42,43,43	0.22	0	51,60,60	0.39	0
24	BCR	3	718	-	41,41,41	0.23	0	56,56,56	0.32	0
26	LMU	A	862	-	20,20,36	0.12	0	25,25,47	0.28	0
26	LMU	5	627	-	24,24,36	0.12	0	29,29,47	0.24	0
21	CLA	A	841	-	69,73,73	1.11	5 (7%)	82,113,113	0.81	2 (2%)
27	LMG	8	626	-	32,32,55	0.21	0	40,40,63	0.16	0
30	CHL	6	616	18	60,74,74	1.94	10 (16%)	58,114,114	1.08	5 (8%)
21	CLA	5	613	17	60,64,73	1.23	4 (6%)	71,102,113	0.88	3 (4%)
30	CHL	9	607	-	45,59,74	2.24	10 (22%)	40,96,114	1.31	5 (12%)
21	CLA	Z	612	12	49,53,73	1.37	4 (8%)	58,89,113	0.95	3 (5%)
26	LMU	Z	621	-	22,22,36	0.13	0	27,27,47	0.27	0
26	LMU	1	621	-	36,36,36	0.09	0	47,47,47	0.27	0
27	LMG	A	860	-	32,32,55	0.22	0	40,40,63	0.46	0
28	LUT	Z	619	-	26,26,43	0.38	0	33,35,60	0.36	0
21	CLA	A	834	-	69,73,73	1.18	5 (7%)	82,113,113	0.89	3 (3%)
24	BCR	J	102	-	41,41,41	0.14	0	56,56,56	0.32	0
27	LMG	8	629	-	42,42,55	0.18	0	50,50,63	0.16	0
23	LHG	1	620	21	43,43,48	0.25	0	46,49,54	0.27	0
21	CLA	7	612	14	56,60,73	1.27	5 (8%)	65,97,113	0.92	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LMG	3	722	-	44,44,55	0.22	0	46,46,63	0.27	0
21	CLA	A	822	33	69,73,73	1.14	5 (7%)	82,113,113	0.84	3 (3%)
21	CLA	A	803	33	69,73,73	1.23	4 (5%)	82,113,113	0.82	3 (3%)
21	CLA	1	608	33	69,73,73	1.18	5 (7%)	82,113,113	0.83	3 (3%)
21	CLA	Z	610	12	64,68,73	1.21	5 (7%)	76,107,113	0.82	3 (3%)
21	CLA	4	612	16	49,53,73	1.37	4 (8%)	58,89,113	0.95	2 (3%)
23	LHG	A	847	21	37,37,48	0.28	0	40,43,54	0.31	0
31	XAT	4	620	-	41,47,47	0.13	0	54,74,74	0.73	1 (1%)
21	CLA	9	609	19	55,59,73	1.31	4 (7%)	64,96,113	0.94	3 (4%)
26	LMU	1	623	-	24,24,36	0.14	0	29,29,47	0.27	0
21	CLA	A	829	-	69,73,73	1.15	4 (5%)	82,113,113	0.80	4 (4%)
24	BCR	B	848	-	41,41,41	0.15	0	56,56,56	0.48	0
21	CLA	4	609	16	64,68,73	1.25	4 (6%)	76,107,113	0.89	3 (3%)
21	CLA	B	816	-	69,73,73	1.16	5 (7%)	82,113,113	0.82	2 (2%)
26	LMU	1	627	-	22,22,36	0.13	0	27,27,47	0.36	0
21	CLA	B	815	-	69,73,73	1.17	4 (5%)	82,113,113	0.80	2 (2%)
26	LMU	K	208	-	24,24,36	0.12	0	29,29,47	0.28	0
21	CLA	A	842	-	69,73,73	1.10	5 (7%)	82,113,113	0.83	2 (2%)
23	LHG	B	851	21	44,44,48	0.26	0	47,50,54	0.30	0
21	CLA	1	613	33	69,73,73	1.15	5 (7%)	82,113,113	0.82	3 (3%)
24	BCR	B	846	-	41,41,41	0.15	0	56,56,56	0.37	0
21	CLA	4	610	16	64,68,73	1.20	5 (7%)	76,107,113	0.85	3 (3%)
28	LUT	9	617	-	42,43,43	0.19	0	51,60,60	0.35	0
21	CLA	B	829	-	69,73,73	1.08	4 (5%)	82,113,113	0.78	2 (2%)
26	LMU	A	857	-	35,35,36	0.09	0	46,46,47	0.22	0
21	CLA	5	621	33	50,54,73	1.41	4 (8%)	59,90,113	1.09	6 (10%)
21	CLA	6	617	-	49,53,73	1.38	5 (10%)	58,89,113	0.98	3 (5%)
21	CLA	8	603	-	69,73,73	1.18	5 (7%)	82,113,113	0.81	2 (2%)
27	LMG	B	854	-	36,36,55	0.19	0	44,44,63	0.15	0
30	CHL	3	608	33	60,74,74	1.98	10 (16%)	58,114,114	1.12	5 (8%)
26	LMU	A	865	-	24,24,36	0.12	0	29,29,47	0.43	0
21	CLA	9	612	19	49,53,73	1.37	4 (8%)	58,89,113	0.96	2 (3%)
26	LMU	6	628	-	24,24,36	0.12	0	29,29,47	0.29	0
21	CLA	A	843	33	69,73,73	1.15	5 (7%)	82,113,113	0.87	3 (3%)
30	CHL	4	606	33	60,74,74	1.95	10 (16%)	58,114,114	1.07	5 (8%)
21	CLA	8	616	15	49,53,73	1.38	5 (10%)	58,89,113	0.97	2 (3%)
21	CLA	K	206	11	49,53,73	1.40	4 (8%)	58,89,113	0.97	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	NEX	5	625	-	40,46,46	0.20	0	50,70,70	1.37	5 (10%)
25	SF4	C	102	3	0,12,12	-	-	-		
21	CLA	B	804	-	49,53,73	1.36	5 (10%)	58,89,113	0.94	2 (3%)
27	LMG	4	627	-	26,26,55	0.26	0	28,28,63	0.18	0
21	CLA	A	854	33	69,73,73	1.16	5 (7%)	82,113,113	0.80	2 (2%)
30	CHL	Z	606	33	40,54,74	2.37	10 (25%)	34,90,114	1.41	5 (14%)
21	CLA	9	603	19	59,63,73	1.26	4 (6%)	70,101,113	0.89	3 (4%)
21	CLA	9	604	19	49,53,73	1.37	4 (8%)	58,89,113	0.98	3 (5%)
21	CLA	7	609	14	49,53,73	1.37	5 (10%)	58,89,113	0.97	3 (5%)
30	CHL	5	607	33	60,74,74	1.96	10 (16%)	58,114,114	1.05	5 (8%)
30	CHL	6	607	33	60,74,74	1.96	10 (16%)	58,114,114	1.12	6 (10%)
21	CLA	5	603	-	69,73,73	1.17	5 (7%)	82,113,113	0.82	3 (3%)
27	LMG	J	103	-	42,42,55	0.17	0	50,50,63	0.41	0
24	BCR	7	623	-	41,41,41	0.16	0	56,56,56	0.33	0
26	LMU	7	627	-	33,33,36	0.11	0	44,44,47	0.18	0
21	CLA	G	204	7	50,54,73	1.38	4 (8%)	59,90,113	0.94	2 (3%)
21	CLA	A	823	-	69,73,73	1.16	5 (7%)	82,113,113	0.81	3 (3%)
21	CLA	6	614	-	54,58,73	1.31	4 (7%)	64,95,113	0.92	2 (3%)
21	CLA	5	616	17	57,61,73	1.26	4 (7%)	67,98,113	0.89	3 (4%)
21	CLA	7	613	14	69,73,73	1.15	5 (7%)	82,113,113	0.85	3 (3%)
21	CLA	1	616	12	50,54,73	1.40	5 (10%)	59,90,113	0.99	3 (5%)
21	CLA	6	609	18	59,63,73	1.27	5 (8%)	70,101,113	0.86	3 (4%)
21	CLA	1	604	33	54,58,73	1.33	4 (7%)	64,95,113	0.93	3 (4%)
21	CLA	B	838	-	54,58,73	1.32	4 (7%)	64,95,113	0.95	3 (4%)
21	CLA	A	825	-	59,63,73	1.25	5 (8%)	70,101,113	0.88	2 (2%)
24	BCR	G	205	-	41,41,41	0.12	0	56,56,56	0.30	0
21	CLA	1	612	12	49,53,73	1.37	4 (8%)	58,89,113	0.95	2 (3%)
21	CLA	7	620	33	57,61,73	1.28	5 (8%)	67,98,113	0.88	2 (2%)
21	CLA	A	828	-	69,73,73	1.12	5 (7%)	82,113,113	0.77	2 (2%)
22	PQN	B	842	-	34,34,34	0.32	0	43,45,45	0.43	0
24	BCR	A	850	-	41,41,41	0.13	0	56,56,56	0.30	0
28	LUT	7	621	-	42,43,43	0.24	0	51,60,60	0.36	0
21	CLA	8	604	33	64,68,73	1.21	5 (7%)	76,107,113	0.86	2 (2%)
21	CLA	3	611	-	59,63,73	1.27	4 (6%)	70,101,113	0.89	3 (4%)
27	LMG	6	633	-	19,19,55	0.31	0	19,19,63	0.29	0
21	CLA	A	818	-	69,73,73	1.12	5 (7%)	82,113,113	0.79	2 (2%)
21	CLA	B	811	-	69,73,73	1.16	5 (7%)	82,113,113	0.82	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	LUT	1	617	-	42,43,43	0.27	0	51,60,60	0.44	0
30	CHL	1	607	33	40,54,74	2.38	10 (25%)	34,90,114	1.24	4 (11%)
30	CHL	5	606	33	40,54,74	2.40	10 (25%)	34,90,114	1.39	5 (14%)
21	CLA	A	839	-	69,73,73	1.14	5 (7%)	82,113,113	0.85	3 (3%)
21	CLA	B	835	33	49,53,73	1.39	4 (8%)	58,89,113	0.95	2 (3%)
21	CLA	1	603	-	61,65,73	1.23	5 (8%)	72,103,113	0.88	3 (4%)
30	CHL	6	601	18	60,74,74	1.95	10 (16%)	58,114,114	1.11	5 (8%)
21	CLA	K	203	33	64,68,73	1.24	4 (6%)	76,107,113	0.88	3 (3%)
21	CLA	7	608	33	54,58,73	1.30	5 (9%)	64,95,113	0.91	2 (3%)
21	CLA	B	839	33	69,73,73	1.16	4 (5%)	82,113,113	0.81	3 (3%)
28	LUT	5	620	-	42,43,43	0.24	0	51,60,60	0.49	0
21	CLA	B	831	-	59,63,73	1.24	5 (8%)	70,101,113	0.88	3 (4%)
21	CLA	7	604	33	55,59,73	1.27	5 (9%)	64,96,113	0.91	3 (4%)
21	CLA	B	822	-	63,67,73	1.21	5 (7%)	74,105,113	0.87	3 (4%)
21	CLA	6	603	-	69,73,73	1.18	5 (7%)	82,113,113	0.80	2 (2%)
30	CHL	4	608	33	60,74,74	1.99	10 (16%)	58,114,114	1.10	5 (8%)
28	LUT	Z	617	-	42,43,43	0.24	0	51,60,60	0.39	0
21	CLA	6	604	-	69,73,73	1.17	5 (7%)	82,113,113	0.82	3 (3%)
26	LMU	B	853	-	36,36,36	0.09	0	47,47,47	0.35	0
21	CLA	8	610	15	69,73,73	1.13	5 (7%)	82,113,113	0.79	2 (2%)
21	CLA	7	602	14	69,73,73	1.13	5 (7%)	82,113,113	0.82	2 (2%)
24	BCR	3	719	-	41,41,41	0.12	0	56,56,56	0.36	0
30	CHL	1	606	33	40,54,74	2.39	10 (25%)	34,90,114	1.39	5 (14%)
21	CLA	Z	611	23	64,68,73	1.20	5 (7%)	76,107,113	0.85	3 (3%)
21	CLA	5	604	33	59,63,73	1.27	4 (6%)	70,101,113	0.88	2 (2%)
21	CLA	A	830	-	69,73,73	1.13	4 (5%)	82,113,113	0.78	2 (2%)
21	CLA	G	203	-	64,68,73	1.21	4 (6%)	76,107,113	0.84	2 (2%)
21	CLA	8	611	23	49,53,73	1.36	5 (10%)	58,89,113	0.94	3 (5%)
23	LHG	6	629	-	35,35,48	0.27	0	38,41,54	0.32	0
21	CLA	A	832	-	59,63,73	1.26	5 (8%)	70,101,113	0.86	2 (2%)
28	LUT	4	619	-	42,43,43	0.29	0	51,60,60	0.46	0
21	CLA	B	823	-	69,73,73	1.16	5 (7%)	82,113,113	0.80	2 (2%)
25	SF4	C	101	3	0,12,12	-	-	-	-	-
21	CLA	4	611	23	64,68,73	1.23	5 (7%)	76,107,113	0.84	3 (3%)
23	LHG	3	623	-	46,46,48	0.23	0	49,52,54	0.28	0
24	BCR	K	207	-	41,41,41	0.14	0	56,56,56	0.23	0
21	CLA	3	606	33	46,50,73	1.43	5 (10%)	53,85,113	1.02	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CHL	7	606	33	40,54,74	2.38	10 (25%)	34,90,114	1.43	5 (14%)

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
21	CLA	5	610	17	1/1/19/20	2/33/109/115	-
27	LMG	J	104	-	-	9/30/50/70	0/1/1/1
21	CLA	A	813	-	1/1/20/20	3/39/115/115	-
30	CHL	6	618	18	3/3/20/26	0/12/110/137	-
31	XAT	6	624	-	-	0/31/93/93	0/4/4/4
23	LHG	9	622	21	-	8/38/38/53	-
21	CLA	A	808	-	1/1/17/20	0/21/97/115	-
31	XAT	7	622	-	-	0/31/93/93	0/4/4/4
21	CLA	B	805	-	1/1/20/20	7/39/115/115	-
21	CLA	B	830	-	1/1/15/20	0/15/91/115	-
26	LMU	4	625	-	-	4/19/59/61	0/2/2/2
30	CHL	8	601	15	3/3/26/26	6/39/137/137	-
21	CLA	B	836	-	1/1/19/20	3/33/109/115	-
21	CLA	Z	613	33	1/1/20/20	2/39/115/115	-
21	CLA	B	812	-	1/1/20/20	2/39/115/115	-
21	CLA	Z	602	12	1/1/19/20	3/33/109/115	-
21	CLA	7	616	14	1/1/15/20	3/17/93/115	-
26	LMU	1	625	-	-	3/15/35/61	0/1/1/2
28	LUT	9	616	-	-	2/29/67/67	0/2/2/2
21	CLA	A	804	-	1/1/20/20	2/39/115/115	-
20	CL0	A	801	-	3/3/25/25	4/37/135/135	-
21	CLA	3	613	13	1/1/19/20	6/33/109/115	-
28	LUT	7	624	-	-	2/29/67/67	0/2/2/2
21	CLA	B	807	-	1/1/18/20	4/27/103/115	-
29	DGD	B	850	-	-	10/48/88/95	0/2/2/2
26	LMU	8	624	-	-	1/15/35/61	0/1/1/2
21	CLA	Z	614	-	1/1/17/20	2/21/97/115	-
30	CHL	6	606	33	3/3/24/26	5/30/128/137	-
21	CLA	3	610	13	1/1/20/20	0/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	826	33	1/1/20/20	5/39/115/115	-
23	LHG	4	623	-	-	15/42/42/53	-
21	CLA	B	841	23	1/1/20/20	10/39/115/115	-
21	CLA	F	304	6	1/1/20/20	6/39/115/115	-
21	CLA	9	601	19	1/1/15/20	2/17/93/115	-
28	LUT	6	621	-	-	2/29/67/67	0/2/2/2
28	LUT	5	626	-	-	2/29/67/67	0/2/2/2
21	CLA	8	613	15	1/1/20/20	5/39/115/115	-
26	LMU	4	626	-	-	0/11/31/61	0/1/1/2
21	CLA	L	204	33	1/1/15/20	3/15/91/115	-
31	XAT	Z	618	-	-	0/31/93/93	0/4/4/4
24	BCR	B	844	-	-	2/29/63/63	0/2/2/2
24	BCR	L	201	-	-	3/29/63/63	0/2/2/2
26	LMU	8	625	-	-	2/15/35/61	0/1/1/2
21	CLA	5	601	17	1/1/20/20	6/39/115/115	-
26	LMU	G	206	-	-	5/15/35/61	0/1/1/2
26	LMU	7	628	-	-	3/13/33/61	0/1/1/2
21	CLA	1	610	12	1/1/20/20	0/39/115/115	-
21	CLA	A	831	-	1/1/20/20	2/39/115/115	-
21	CLA	A	806	-	1/1/20/20	12/39/115/115	-
21	CLA	A	817	33	1/1/18/20	2/27/103/115	-
21	CLA	7	614	-	1/1/14/20	3/13/89/115	-
28	LUT	3	621	-	-	2/29/67/67	0/2/2/2
24	BCR	B	847	-	-	2/29/63/63	0/2/2/2
21	CLA	6	611	23	1/1/18/20	2/31/107/115	-
21	CLA	A	816	-	1/1/20/20	3/39/115/115	-
21	CLA	Z	608	33	1/1/17/20	3/21/97/115	-
21	CLA	B	810	-	1/1/20/20	2/39/115/115	-
21	CLA	B	814	-	1/1/19/20	5/33/109/115	-
30	CHL	7	607	33	3/3/23/26	0/25/123/137	-
30	CHL	Z	607	33	3/3/26/26	2/39/137/137	-
21	CLA	9	610	19	1/1/19/20	3/33/109/115	-
21	CLA	K	204	-	1/1/15/20	2/17/93/115	-
21	CLA	A	802	-	1/1/20/20	0/39/115/115	-
27	LMG	7	626	-	-	3/32/52/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	819	-	1/1/19/20	5/33/109/115	-
24	BCR	B	843	-	-	0/29/63/63	0/2/2/2
21	CLA	A	820	-	1/1/20/20	4/39/115/115	-
30	CHL	9	606	-	3/3/20/26	0/10/108/137	-
21	CLA	B	833	-	1/1/18/20	4/31/107/115	-
21	CLA	A	838	-	1/1/17/20	3/23/99/115	-
26	LMU	8	628	-	-	4/15/35/61	0/1/1/2
27	LMG	A	859	-	-	7/35/55/70	0/1/1/1
28	LUT	F	305	-	-	6/29/67/67	0/2/2/2
21	CLA	B	828	-	1/1/20/20	2/39/115/115	-
21	CLA	B	821	-	1/1/20/20	7/39/115/115	-
28	LUT	3	622	-	-	2/29/67/67	0/2/2/2
28	LUT	3	720	-	-	0/29/67/67	0/2/2/2
21	CLA	8	609	15	1/1/15/20	2/15/91/115	-
21	CLA	3	603	-	1/1/20/20	6/39/115/115	-
21	CLA	J	101	9	1/1/18/20	4/27/103/115	-
24	BCR	K	202	-	-	2/29/63/63	0/2/2/2
27	LMG	B	852	-	-	9/38/58/70	0/1/1/1
21	CLA	8	614	-	1/1/18/20	7/30/106/115	-
21	CLA	8	612	15	1/1/18/20	4/27/103/115	-
21	CLA	B	803	-	1/1/20/20	1/39/115/115	-
21	CLA	3	614	-	1/1/15/20	2/15/91/115	-
21	CLA	A	840	-	1/1/20/20	5/39/115/115	-
21	CLA	7	603	-	1/1/17/20	2/24/100/115	-
21	CLA	A	836	-	1/1/20/20	4/39/115/115	-
30	CHL	8	607	33	3/3/26/26	11/39/137/137	-
26	LMU	A	863	-	-	5/21/61/61	0/2/2/2
30	CHL	5	608	33	3/3/23/26	0/21/119/137	-
22	PQN	A	844	-	-	4/23/43/43	0/2/2/2
21	CLA	A	835	-	1/1/20/20	3/39/115/115	-
23	LHG	A	846	-	-	6/53/53/53	-
21	CLA	A	812	-	1/1/20/20	7/39/115/115	-
21	CLA	B	824	33	1/1/20/20	3/39/115/115	-
21	CLA	6	612	18	1/1/15/20	4/15/91/115	-
21	CLA	B	834	-	1/1/19/20	2/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	7	601	14	3/3/26/26	3/39/137/137	-
21	CLA	5	617	-	1/1/20/20	4/39/115/115	-
27	LMG	4	624	-	-	7/36/56/70	0/1/1/1
26	LMU	A	858	-	-	7/21/61/61	0/2/2/2
21	CLA	F	303	33	1/1/15/20	2/15/91/115	-
21	CLA	5	614	-	1/1/15/20	2/15/91/115	-
21	CLA	5	612	17	1/1/15/20	7/15/91/115	-
27	LMG	1	624	-	-	0/31/51/70	0/1/1/1
30	CHL	4	601	16	3/3/26/26	6/39/137/137	-
21	CLA	Z	604	33	1/1/18/20	1/30/106/115	-
21	CLA	A	837	1	1/1/18/20	1/30/106/115	-
24	BCR	A	852	-	-	4/29/63/63	0/2/2/2
21	CLA	A	807	1	1/1/20/20	5/39/115/115	-
21	CLA	6	610	18	1/1/19/20	0/33/109/115	-
30	CHL	1	601	12	3/3/26/26	9/39/137/137	-
21	CLA	F	301	33	1/1/20/20	2/39/115/115	-
31	XAT	8	618	-	-	0/31/93/93	0/4/4/4
21	CLA	A	810	1	1/1/20/20	6/39/115/115	-
24	BCR	3	620	-	-	4/29/63/63	0/2/2/2
21	CLA	9	614	-	1/1/15/20	4/15/91/115	-
31	XAT	5	624	-	-	0/31/93/93	0/4/4/4
21	CLA	4	604	33	1/1/17/20	0/21/97/115	-
24	BCR	8	619	-	-	4/29/63/63	0/2/2/2
21	CLA	K	201	11	1/1/15/20	2/15/91/115	-
26	LMU	1	622	-	-	3/10/30/61	0/1/1/2
26	LMU	A	861	-	-	3/15/35/61	0/1/1/2
21	CLA	4	616	16	1/1/15/20	2/15/91/115	-
23	LHG	7	625	21	-	8/53/53/53	-
26	LMU	A	864	-	-	2/15/35/61	0/1/1/2
21	CLA	4	602	16	1/1/19/20	2/33/109/115	-
21	CLA	Z	609	12	1/1/20/20	12/39/115/115	-
21	CLA	1	614	-	1/1/19/20	4/33/109/115	-
21	CLA	B	813	-	1/1/20/20	7/39/115/115	-
21	CLA	Z	616	12	1/1/19/20	2/33/109/115	-
21	CLA	4	614	-	1/1/18/20	6/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	A	851	-	-	2/29/63/63	0/2/2/2
21	CLA	B	806	2	1/1/20/20	3/39/115/115	-
21	CLA	3	617	13	1/1/15/20	2/17/93/115	-
24	BCR	6	623	-	-	2/29/63/63	0/2/2/2
21	CLA	A	821	-	1/1/18/20	4/27/103/115	-
21	CLA	B	808	-	1/1/20/20	7/39/115/115	-
21	CLA	5	611	23	1/1/18/20	0/27/103/115	-
21	CLA	4	613	16	1/1/20/20	8/39/115/115	-
26	LMU	7	629	-	-	3/13/53/61	0/2/2/2
21	CLA	8	608	33	1/1/17/20	1/21/97/115	-
21	CLA	B	840	-	1/1/20/20	4/39/115/115	-
23	LHG	8	620	21	-	10/48/48/53	-
21	CLA	6	622	33	1/1/18/20	1/27/103/115	-
24	BCR	A	849	-	-	0/29/63/63	0/2/2/2
24	BCR	L	205	-	-	2/29/63/63	0/2/2/2
21	CLA	9	611	23	1/1/15/20	2/15/91/115	-
28	LUT	A	856	-	-	4/29/67/67	0/2/2/2
27	LMG	1	628	-	-	5/44/64/70	0/1/1/1
21	CLA	3	607	13	1/1/18/20	4/27/103/115	-
30	CHL	6	608	33	3/3/23/26	2/21/119/137	-
26	LMU	1	626	-	-	0/15/35/61	0/1/1/2
21	CLA	6	613	33	1/1/20/20	4/39/115/115	-
21	CLA	3	609	13	1/1/19/20	1/35/111/115	-
26	LMU	6	632	-	-	3/11/31/61	0/1/1/2
21	CLA	A	811	-	1/1/20/20	5/39/115/115	-
21	CLA	1	611	23	1/1/19/20	7/35/111/115	-
31	XAT	1	618	-	1/1/26/26	0/31/93/93	0/4/4/4
21	CLA	A	805	-	1/1/18/20	3/27/103/115	-
21	CLA	9	602	19	1/1/19/20	2/33/109/115	-
30	CHL	8	606	33	3/3/26/26	9/39/137/137	-
30	CHL	5	618	17	3/3/20/26	0/12/110/137	-
28	LUT	8	617	-	-	2/29/67/67	0/2/2/2
21	CLA	B	818	-	1/1/20/20	3/39/115/115	-
21	CLA	A	814	-	1/1/20/20	3/39/115/115	-
21	CLA	8	602	15	1/1/20/20	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	809	1	1/1/20/20	5/39/115/115	-
21	CLA	A	824	-	1/1/15/20	2/15/91/115	-
21	CLA	7	610	14	1/1/20/20	4/39/115/115	-
21	CLA	5	609	17	1/1/20/20	2/39/115/115	-
21	CLA	B	826	-	1/1/20/20	0/39/115/115	-
24	BCR	4	621	-	-	2/29/63/63	0/2/2/2
21	CLA	B	820	-	1/1/18/20	2/29/105/115	-
21	CLA	A	845	23	1/1/15/20	2/15/91/115	-
26	LMU	6	630	-	-	4/15/35/61	0/1/1/2
21	CLA	A	827	33	1/1/20/20	0/39/115/115	-
23	LHG	6	619	21	-	10/53/53/53	-
30	CHL	4	607	33	3/3/26/26	4/39/137/137	-
21	CLA	9	613	19	1/1/20/20	6/39/115/115	-
26	LMU	6	631	-	-	2/15/35/61	0/1/1/2
23	LHG	3	721	-	-	9/35/35/53	-
24	BCR	A	848	-	-	2/29/63/63	0/2/2/2
21	CLA	7	611	23	1/1/20/20	3/39/115/115	-
21	CLA	3	615	33	1/1/20/20	8/39/115/115	-
21	CLA	4	603	16	1/1/20/20	5/39/115/115	-
23	LHG	5	623	21	-	8/41/41/53	-
24	BCR	5	622	-	-	2/29/63/63	0/2/2/2
23	LHG	4	622	21	-	14/53/53/53	-
26	LMU	8	627	-	-	10/21/61/61	0/2/2/2
21	CLA	1	609	12	1/1/20/20	5/39/115/115	-
21	CLA	1	602	12	1/1/19/20	2/33/109/115	-
21	CLA	Z	603	-	1/1/20/20	3/39/115/115	-
21	CLA	3	604	33	1/1/20/20	2/39/115/115	-
21	CLA	B	837	-	1/1/20/20	5/39/115/115	-
21	CLA	3	612	13	1/1/15/20	6/17/93/115	-
26	LMU	Z	622	-	-	4/17/57/61	0/2/2/2
21	CLA	B	802	-	1/1/20/20	0/39/115/115	-
24	BCR	B	801	-	-	0/29/63/63	0/2/2/2
21	CLA	B	832	-	1/1/20/20	4/39/115/115	-
21	CLA	3	602	13	1/1/19/20	2/33/109/115	-
24	BCR	I	172	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	809	2	1/1/20/20	9/39/115/115	-
21	CLA	A	833	-	1/1/20/20	1/39/115/115	-
21	CLA	B	819	33	1/1/19/20	3/33/109/115	-
32	NEX	6	625	-	-	5/27/83/83	0/3/3/3
21	CLA	B	817	-	1/1/20/20	8/39/115/115	-
21	CLA	6	602	18	1/1/20/20	2/39/115/115	-
25	SF4	A	853	1,2	-	-	0/6/5/5
21	CLA	B	827	-	1/1/20/20	4/39/115/115	-
30	CHL	Z	601	12	3/3/26/26	5/39/137/137	-
21	CLA	A	815	-	1/1/18/20	2/27/103/115	-
21	CLA	B	825	33	1/1/20/20	3/39/115/115	-
21	CLA	5	602	17	1/1/20/20	0/39/115/115	-
30	CHL	4	618	16	3/3/21/26	2/15/113/137	-
24	BCR	B	845	-	-	4/29/63/63	0/2/2/2
21	CLA	L	203	-	1/1/20/20	5/39/115/115	-
23	LHG	Z	620	21	-	8/43/43/53	-
28	LUT	1	619	-	-	2/29/67/67	0/2/2/2
24	BCR	3	718	-	-	1/29/63/63	0/2/2/2
26	LMU	A	862	-	-	1/11/31/61	0/1/1/2
26	LMU	5	627	-	-	1/15/35/61	0/1/1/2
21	CLA	A	841	-	1/1/20/20	4/39/115/115	-
27	LMG	8	626	-	-	1/27/47/70	0/1/1/1
30	CHL	6	616	18	3/3/26/26	2/39/137/137	-
21	CLA	5	613	17	1/1/18/20	1/29/105/115	-
30	CHL	9	607	-	3/3/23/26	0/21/119/137	-
21	CLA	Z	612	12	1/1/15/20	5/15/91/115	-
26	LMU	Z	621	-	-	2/13/33/61	0/1/1/2
26	LMU	1	621	-	-	6/21/61/61	0/2/2/2
27	LMG	A	860	-	-	7/27/47/70	0/1/1/1
28	LUT	Z	619	-	-	2/18/37/67	0/1/1/2
21	CLA	A	834	-	1/1/20/20	3/39/115/115	-
24	BCR	J	102	-	-	2/29/63/63	0/2/2/2
27	LMG	8	629	-	-	8/37/57/70	0/1/1/1
23	LHG	1	620	21	-	4/48/48/53	-
21	CLA	7	612	14	1/1/17/20	3/24/100/115	-
27	LMG	3	722	-	-	11/46/46/70	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	822	33	1/1/20/20	2/39/115/115	-
21	CLA	A	803	33	1/1/20/20	1/39/115/115	-
21	CLA	1	608	33	1/1/20/20	5/39/115/115	-
21	CLA	Z	610	12	1/1/19/20	0/33/109/115	-
21	CLA	4	612	16	1/1/15/20	2/15/91/115	-
23	LHG	A	847	21	-	3/42/42/53	-
31	XAT	4	620	-	-	0/31/93/93	0/4/4/4
21	CLA	9	609	19	1/1/17/20	5/23/99/115	-
26	LMU	1	623	-	-	2/15/35/61	0/1/1/2
21	CLA	A	829	-	1/1/20/20	3/39/115/115	-
24	BCR	B	848	-	-	2/29/63/63	0/2/2/2
21	CLA	4	609	16	1/1/19/20	8/33/109/115	-
21	CLA	B	816	-	1/1/20/20	1/39/115/115	-
26	LMU	1	627	-	-	3/13/33/61	0/1/1/2
21	CLA	B	815	-	1/1/20/20	5/39/115/115	-
26	LMU	K	208	-	-	3/15/35/61	0/1/1/2
21	CLA	A	842	-	1/1/20/20	4/39/115/115	-
23	LHG	B	851	21	-	12/49/49/53	-
21	CLA	1	613	33	1/1/20/20	7/39/115/115	-
24	BCR	B	846	-	-	2/29/63/63	0/2/2/2
21	CLA	4	610	16	1/1/19/20	0/33/109/115	-
28	LUT	9	617	-	-	0/29/67/67	0/2/2/2
21	CLA	B	829	-	1/1/20/20	3/39/115/115	-
26	LMU	A	857	-	-	5/20/60/61	0/2/2/2
21	CLA	5	621	33	1/1/15/20	7/17/93/115	-
21	CLA	6	617	-	1/1/15/20	0/15/91/115	-
21	CLA	8	603	-	1/1/20/20	3/39/115/115	-
27	LMG	B	854	-	-	2/31/51/70	0/1/1/1
30	CHL	3	608	33	3/3/26/26	3/39/137/137	-
26	LMU	A	865	-	-	2/15/35/61	0/1/1/2
21	CLA	9	612	19	1/1/15/20	4/15/91/115	-
26	LMU	6	628	-	-	2/15/35/61	0/1/1/2
21	CLA	A	843	33	1/1/20/20	7/39/115/115	-
30	CHL	4	606	33	3/3/26/26	5/39/137/137	-
21	CLA	8	616	15	1/1/15/20	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	K	206	11	1/1/15/20	4/15/91/115	-
32	NEX	5	625	-	-	2/27/83/83	0/3/3/3
25	SF4	C	102	3	-	-	0/6/5/5
21	CLA	B	804	-	1/1/15/20	0/15/91/115	-
27	LMG	4	627	-	-	2/28/28/70	-
21	CLA	A	854	33	1/1/20/20	6/39/115/115	-
30	CHL	Z	606	33	3/3/21/26	4/15/113/137	-
21	CLA	9	603	19	1/1/18/20	8/27/103/115	-
21	CLA	9	604	19	1/1/15/20	0/15/91/115	-
21	CLA	7	609	14	1/1/15/20	0/15/91/115	-
30	CHL	5	607	33	3/3/26/26	5/39/137/137	-
30	CHL	6	607	33	3/3/26/26	9/39/137/137	-
21	CLA	5	603	-	1/1/20/20	14/39/115/115	-
27	LMG	J	103	-	-	2/37/57/70	0/1/1/1
24	BCR	7	623	-	-	2/29/63/63	0/2/2/2
26	LMU	7	627	-	-	2/18/58/61	0/2/2/2
21	CLA	G	204	7	1/1/15/20	3/17/93/115	-
21	CLA	A	823	-	1/1/20/20	10/39/115/115	-
21	CLA	6	614	-	1/1/17/20	0/21/97/115	-
21	CLA	5	616	17	1/1/17/20	2/25/101/115	-
21	CLA	7	613	14	1/1/20/20	3/39/115/115	-
21	CLA	1	616	12	1/1/15/20	2/17/93/115	-
21	CLA	6	609	18	1/1/18/20	1/27/103/115	-
21	CLA	1	604	33	1/1/17/20	0/21/97/115	-
21	CLA	B	838	-	1/1/17/20	3/21/97/115	-
21	CLA	A	825	-	1/1/18/20	2/27/103/115	-
24	BCR	G	205	-	-	1/29/63/63	0/2/2/2
21	CLA	1	612	12	1/1/15/20	3/15/91/115	-
21	CLA	7	620	33	1/1/17/20	0/25/101/115	-
21	CLA	A	828	-	1/1/20/20	2/39/115/115	-
22	PQN	B	842	-	-	2/23/43/43	0/2/2/2
24	BCR	A	850	-	-	0/29/63/63	0/2/2/2
28	LUT	7	621	-	-	2/29/67/67	0/2/2/2
21	CLA	8	604	33	1/1/19/20	2/33/109/115	-
21	CLA	3	611	-	1/1/18/20	3/27/103/115	-
27	LMG	6	633	-	-	4/17/17/70	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	818	-	1/1/20/20	2/39/115/115	-
21	CLA	B	811	-	1/1/20/20	3/39/115/115	-
28	LUT	1	617	-	-	2/29/67/67	0/2/2/2
30	CHL	1	607	33	3/3/21/26	3/15/113/137	-
30	CHL	5	606	33	3/3/21/26	2/15/113/137	-
21	CLA	A	839	-	1/1/20/20	3/39/115/115	-
21	CLA	B	835	33	1/1/15/20	0/15/91/115	-
21	CLA	1	603	-	1/1/18/20	4/30/106/115	-
30	CHL	6	601	18	3/3/26/26	3/39/137/137	-
21	CLA	K	203	33	1/1/19/20	6/33/109/115	-
21	CLA	7	608	33	1/1/17/20	0/21/97/115	-
21	CLA	B	839	33	1/1/20/20	7/39/115/115	-
28	LUT	5	620	-	-	2/29/67/67	0/2/2/2
21	CLA	B	831	-	1/1/18/20	3/27/103/115	-
21	CLA	7	604	33	1/1/17/20	1/23/99/115	-
21	CLA	B	822	-	1/1/18/20	3/32/108/115	-
21	CLA	6	603	-	1/1/20/20	6/39/115/115	-
30	CHL	4	608	33	3/3/26/26	5/39/137/137	-
28	LUT	Z	617	-	-	2/29/67/67	0/2/2/2
21	CLA	6	604	-	1/1/20/20	4/39/115/115	-
26	LMU	B	853	-	-	7/21/61/61	0/2/2/2
21	CLA	8	610	15	1/1/20/20	0/39/115/115	-
21	CLA	7	602	14	1/1/20/20	2/39/115/115	-
24	BCR	3	719	-	-	2/29/63/63	0/2/2/2
30	CHL	1	606	33	3/3/21/26	0/15/113/137	-
21	CLA	Z	611	23	1/1/19/20	6/33/109/115	-
21	CLA	5	604	33	1/1/18/20	5/27/103/115	-
21	CLA	A	830	-	1/1/20/20	4/39/115/115	-
21	CLA	G	203	-	1/1/19/20	5/33/109/115	-
21	CLA	8	611	23	1/1/15/20	0/15/91/115	-
23	LHG	6	629	-	-	12/40/40/53	-
21	CLA	A	832	-	1/1/18/20	1/27/103/115	-
28	LUT	4	619	-	-	2/29/67/67	0/2/2/2
21	CLA	B	823	-	1/1/20/20	6/39/115/115	-
25	SF4	C	101	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	4	611	23	1/1/19/20	4/33/109/115	-
23	LHG	3	623	-	-	14/51/51/53	-
24	BCR	K	207	-	-	2/29/63/63	0/2/2/2
21	CLA	3	606	33	1/1/14/20	0/12/88/115	-
30	CHL	7	606	33	3/3/21/26	0/15/113/137	-

All (1224) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	4	601	CHL	MG-NB	-7.47	1.91	2.05
30	6	601	CHL	MG-NB	-7.37	1.91	2.05
30	6	616	CHL	MG-NB	-7.31	1.91	2.05
30	1	607	CHL	MG-NB	-7.29	1.91	2.05
30	4	607	CHL	MG-NB	-7.26	1.91	2.05
30	Z	607	CHL	MG-NB	-7.26	1.91	2.05
30	4	618	CHL	MG-NB	-7.25	1.91	2.05
30	5	607	CHL	MG-NB	-7.24	1.91	2.05
30	5	618	CHL	MG-NB	-7.23	1.91	2.05
30	4	608	CHL	MG-NB	-7.22	1.91	2.05
30	6	606	CHL	MG-NB	-7.22	1.91	2.05
30	5	606	CHL	MG-NB	-7.21	1.91	2.05
30	6	607	CHL	MG-NB	-7.20	1.91	2.05
30	7	601	CHL	MG-NB	-7.20	1.91	2.05
30	3	608	CHL	MG-NB	-7.19	1.91	2.05
30	6	608	CHL	MG-NB	-7.18	1.91	2.05
30	Z	606	CHL	MG-NB	-7.16	1.91	2.05
30	9	607	CHL	MG-NB	-7.16	1.91	2.05
30	7	607	CHL	MG-NB	-7.15	1.91	2.05
30	5	608	CHL	MG-NB	-7.15	1.91	2.05
30	1	606	CHL	MG-NB	-7.15	1.91	2.05
30	4	606	CHL	MG-NB	-7.15	1.91	2.05
30	6	618	CHL	MG-NB	-7.13	1.91	2.05
30	8	606	CHL	MG-NB	-7.12	1.91	2.05
30	9	606	CHL	MG-NB	-7.10	1.91	2.05
30	Z	601	CHL	MG-NB	-7.08	1.91	2.05
30	1	601	CHL	MG-NB	-7.08	1.91	2.05
30	8	607	CHL	MG-NB	-7.08	1.91	2.05
30	8	601	CHL	MG-NB	-7.06	1.91	2.05
30	9	607	CHL	C1B-C2B	7.02	1.47	1.39
30	7	606	CHL	C1B-C2B	6.99	1.47	1.39
30	7	606	CHL	MG-NB	-6.98	1.92	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	9	606	CHL	C1B-C2B	6.96	1.47	1.39
30	4	618	CHL	C1B-C2B	6.92	1.47	1.39
30	4	608	CHL	C1B-C2B	6.83	1.47	1.39
30	Z	606	CHL	C1B-C2B	6.74	1.47	1.39
30	4	601	CHL	C1B-C2B	6.73	1.47	1.39
30	3	608	CHL	C1B-C2B	6.72	1.47	1.39
30	5	618	CHL	C1B-C2B	6.67	1.47	1.39
30	4	607	CHL	C1B-C2B	6.67	1.47	1.39
30	7	601	CHL	C1B-C2B	6.65	1.47	1.39
30	6	606	CHL	C1B-C2B	6.64	1.47	1.39
30	4	606	CHL	C1B-C2B	6.63	1.47	1.39
30	1	601	CHL	C1B-C2B	6.60	1.47	1.39
30	6	601	CHL	C1B-C2B	6.57	1.47	1.39
30	6	608	CHL	C1B-C2B	6.54	1.47	1.39
30	8	607	CHL	C1B-C2B	6.51	1.47	1.39
30	8	606	CHL	C1B-C2B	6.50	1.46	1.39
30	1	606	CHL	C1B-C2B	6.49	1.46	1.39
30	6	618	CHL	C1B-C2B	6.44	1.46	1.39
30	7	607	CHL	C1B-C2B	6.43	1.46	1.39
30	Z	607	CHL	C1B-C2B	6.41	1.46	1.39
30	6	616	CHL	C1B-C2B	6.38	1.46	1.39
30	5	608	CHL	C1B-C2B	6.37	1.46	1.39
30	5	607	CHL	C1B-C2B	6.30	1.46	1.39
30	5	606	CHL	C1B-C2B	6.26	1.46	1.39
30	Z	601	CHL	C1B-C2B	6.23	1.46	1.39
30	6	607	CHL	C1B-C2B	6.20	1.46	1.39
30	1	607	CHL	C1B-C2B	6.13	1.46	1.39
30	4	601	CHL	MG-ND	-6.09	1.93	2.05
30	1	607	CHL	MG-ND	-6.08	1.93	2.05
30	Z	607	CHL	MG-ND	-6.05	1.93	2.05
30	4	607	CHL	MG-ND	-5.99	1.93	2.05
21	A	803	CLA	MG-NB	-5.99	1.93	2.05
30	6	607	CHL	MG-ND	-5.98	1.93	2.05
30	5	607	CHL	MG-ND	-5.98	1.93	2.05
30	8	606	CHL	MG-ND	-5.96	1.94	2.05
30	6	616	CHL	MG-ND	-5.91	1.94	2.05
30	7	606	CHL	MG-ND	-5.90	1.94	2.05
30	8	601	CHL	MG-ND	-5.89	1.94	2.05
30	6	601	CHL	MG-ND	-5.88	1.94	2.05
30	4	608	CHL	MG-ND	-5.87	1.94	2.05
30	7	607	CHL	MG-ND	-5.86	1.94	2.05
30	5	606	CHL	MG-ND	-5.85	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	1	606	CHL	MG-ND	-5.84	1.94	2.05
30	6	606	CHL	MG-ND	-5.83	1.94	2.05
30	8	601	CHL	C1B-C2B	5.83	1.46	1.39
30	6	618	CHL	MG-ND	-5.82	1.94	2.05
30	1	601	CHL	MG-ND	-5.81	1.94	2.05
30	5	608	CHL	MG-ND	-5.81	1.94	2.05
30	Z	601	CHL	MG-ND	-5.80	1.94	2.05
30	7	601	CHL	MG-ND	-5.77	1.94	2.05
30	4	606	CHL	MG-ND	-5.75	1.94	2.05
30	3	608	CHL	MG-ND	-5.74	1.94	2.05
30	8	607	CHL	MG-ND	-5.74	1.94	2.05
30	6	608	CHL	MG-ND	-5.73	1.94	2.05
30	5	618	CHL	MG-ND	-5.73	1.94	2.05
30	4	618	CHL	MG-ND	-5.72	1.94	2.05
30	9	606	CHL	MG-ND	-5.71	1.94	2.05
30	9	607	CHL	MG-ND	-5.68	1.94	2.05
30	Z	606	CHL	MG-ND	-5.68	1.94	2.05
21	1	616	CLA	MG-NB	-5.56	1.94	2.05
21	A	837	CLA	MG-NB	-5.54	1.94	2.05
21	7	603	CLA	MG-NB	-5.49	1.94	2.05
21	B	803	CLA	MG-NB	-5.46	1.95	2.05
21	B	807	CLA	MG-NB	-5.44	1.95	2.05
21	B	841	CLA	MG-NB	-5.42	1.95	2.05
30	5	608	CHL	C3A-C2A	-5.41	1.50	1.54
21	A	810	CLA	MG-NB	-5.41	1.95	2.05
21	1	609	CLA	MG-NB	-5.41	1.95	2.05
21	B	824	CLA	MG-NB	-5.39	1.95	2.05
21	B	821	CLA	MG-NB	-5.39	1.95	2.05
21	6	622	CLA	MG-NB	-5.37	1.95	2.05
21	A	834	CLA	MG-NB	-5.36	1.95	2.05
21	3	617	CLA	MG-NB	-5.36	1.95	2.05
21	6	611	CLA	MG-NB	-5.35	1.95	2.05
21	K	203	CLA	MG-NB	-5.34	1.95	2.05
21	A	833	CLA	MG-NB	-5.33	1.95	2.05
21	A	824	CLA	MG-NB	-5.33	1.95	2.05
21	6	610	CLA	MG-NB	-5.31	1.95	2.05
21	Z	616	CLA	MG-NB	-5.31	1.95	2.05
21	B	809	CLA	MG-NB	-5.30	1.95	2.05
21	9	603	CLA	C1D-ND	5.30	1.44	1.37
21	6	602	CLA	MG-NB	-5.30	1.95	2.05
21	4	613	CLA	MG-NB	-5.29	1.95	2.05
21	4	609	CLA	MG-NB	-5.28	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	K	206	CLA	MG-NB	-5.28	1.95	2.05
20	A	801	CL0	MG-NB	-5.27	1.95	2.05
21	A	827	CLA	MG-NB	-5.27	1.95	2.05
21	5	602	CLA	MG-NB	-5.27	1.95	2.05
21	6	604	CLA	MG-NB	-5.27	1.95	2.05
21	A	829	CLA	MG-NB	-5.26	1.95	2.05
21	B	820	CLA	MG-NB	-5.26	1.95	2.05
21	Z	602	CLA	MG-NB	-5.26	1.95	2.05
21	3	606	CLA	MG-NB	-5.26	1.95	2.05
21	9	602	CLA	MG-NB	-5.25	1.95	2.05
21	G	203	CLA	C1D-ND	5.25	1.44	1.37
30	3	608	CHL	C3A-C2A	-5.25	1.50	1.54
21	5	611	CLA	MG-NB	-5.24	1.95	2.05
21	6	603	CLA	MG-NB	-5.24	1.95	2.05
21	B	818	CLA	MG-NB	-5.23	1.95	2.05
21	1	608	CLA	MG-NB	-5.23	1.95	2.05
21	Z	604	CLA	MG-NB	-5.23	1.95	2.05
21	Z	610	CLA	MG-NB	-5.22	1.95	2.05
21	A	823	CLA	MG-NB	-5.22	1.95	2.05
21	K	201	CLA	MG-NB	-5.22	1.95	2.05
21	B	823	CLA	MG-NB	-5.22	1.95	2.05
21	G	204	CLA	C1D-ND	5.22	1.44	1.37
21	5	621	CLA	C1D-ND	5.21	1.44	1.37
21	B	812	CLA	MG-NB	-5.21	1.95	2.05
21	3	611	CLA	MG-NB	-5.21	1.95	2.05
21	8	603	CLA	MG-NB	-5.20	1.95	2.05
21	7	614	CLA	MG-NB	-5.20	1.95	2.05
21	1	604	CLA	MG-NB	-5.20	1.95	2.05
21	6	609	CLA	MG-NB	-5.20	1.95	2.05
21	8	609	CLA	MG-NB	-5.20	1.95	2.05
21	6	614	CLA	C1D-ND	5.19	1.44	1.37
21	4	611	CLA	MG-NB	-5.19	1.95	2.05
21	Z	608	CLA	MG-NB	-5.18	1.95	2.05
21	Z	614	CLA	MG-NB	-5.18	1.95	2.05
21	9	613	CLA	C1D-ND	5.18	1.44	1.37
21	5	614	CLA	MG-NB	-5.18	1.95	2.05
21	9	611	CLA	MG-NB	-5.18	1.95	2.05
21	9	612	CLA	C1D-ND	5.17	1.44	1.37
21	B	824	CLA	C1D-ND	5.17	1.44	1.37
21	B	835	CLA	MG-NB	-5.17	1.95	2.05
21	B	810	CLA	MG-NB	-5.16	1.95	2.05
21	Z	612	CLA	C1D-ND	5.16	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	603	CLA	MG-NB	-5.16	1.95	2.05
21	L	204	CLA	MG-NB	-5.16	1.95	2.05
21	1	602	CLA	MG-NB	-5.16	1.95	2.05
21	5	610	CLA	MG-NB	-5.16	1.95	2.05
21	8	604	CLA	MG-NB	-5.15	1.95	2.05
21	7	616	CLA	MG-NB	-5.15	1.95	2.05
21	5	604	CLA	MG-NB	-5.15	1.95	2.05
21	9	601	CLA	MG-NB	-5.15	1.95	2.05
21	8	608	CLA	MG-NB	-5.15	1.95	2.05
21	4	616	CLA	MG-NB	-5.15	1.95	2.05
21	9	609	CLA	C1D-ND	5.15	1.44	1.37
21	3	615	CLA	MG-NB	-5.15	1.95	2.05
21	A	843	CLA	MG-NB	-5.14	1.95	2.05
21	1	614	CLA	MG-NB	-5.14	1.95	2.05
21	4	604	CLA	MG-NB	-5.14	1.95	2.05
21	3	604	CLA	MG-NB	-5.13	1.95	2.05
21	7	620	CLA	C1D-ND	5.13	1.44	1.37
21	A	840	CLA	MG-NB	-5.13	1.95	2.05
21	A	832	CLA	MG-NB	-5.12	1.95	2.05
21	8	610	CLA	MG-NB	-5.12	1.95	2.05
21	9	611	CLA	C1D-ND	5.12	1.44	1.37
21	5	601	CLA	C1D-ND	5.12	1.44	1.37
21	8	616	CLA	MG-NB	-5.12	1.95	2.05
21	Z	603	CLA	MG-NB	-5.12	1.95	2.05
21	5	601	CLA	MG-NB	-5.12	1.95	2.05
21	6	613	CLA	MG-NB	-5.12	1.95	2.05
21	9	601	CLA	C1D-ND	5.11	1.44	1.37
21	9	610	CLA	MG-NB	-5.11	1.95	2.05
21	9	609	CLA	MG-NB	-5.11	1.95	2.05
21	1	603	CLA	MG-NB	-5.10	1.95	2.05
21	4	602	CLA	MG-NB	-5.10	1.95	2.05
21	4	614	CLA	MG-NB	-5.10	1.95	2.05
21	6	617	CLA	MG-NB	-5.10	1.95	2.05
21	3	614	CLA	MG-NB	-5.10	1.95	2.05
21	8	611	CLA	MG-NB	-5.10	1.95	2.05
21	L	203	CLA	MG-NB	-5.10	1.95	2.05
21	B	834	CLA	MG-NB	-5.10	1.95	2.05
21	Z	611	CLA	MG-NB	-5.10	1.95	2.05
21	B	811	CLA	MG-NB	-5.09	1.95	2.05
21	9	604	CLA	C1D-ND	5.08	1.44	1.37
21	Z	613	CLA	MG-NB	-5.08	1.95	2.05
21	B	839	CLA	MG-NB	-5.08	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	826	CLA	MG-NB	-5.08	1.95	2.05
21	3	613	CLA	MG-NB	-5.08	1.95	2.05
21	4	610	CLA	MG-NB	-5.07	1.95	2.05
21	B	822	CLA	MG-NB	-5.07	1.95	2.05
21	3	609	CLA	MG-NB	-5.06	1.95	2.05
21	3	603	CLA	MG-NB	-5.06	1.95	2.05
21	B	804	CLA	MG-NB	-5.06	1.95	2.05
21	K	204	CLA	MG-NB	-5.06	1.95	2.05
21	G	204	CLA	MG-NB	-5.06	1.95	2.05
21	F	304	CLA	C1D-ND	5.06	1.44	1.37
21	8	614	CLA	C1D-ND	5.06	1.44	1.37
21	4	611	CLA	C1D-ND	5.05	1.44	1.37
21	4	603	CLA	C1D-ND	5.05	1.44	1.37
21	6	612	CLA	C1D-ND	5.05	1.44	1.37
21	7	602	CLA	MG-NB	-5.05	1.95	2.05
21	Z	603	CLA	C1D-ND	5.05	1.44	1.37
21	A	805	CLA	MG-NB	-5.05	1.95	2.05
21	7	608	CLA	MG-NB	-5.05	1.95	2.05
21	5	621	CLA	MG-NB	-5.05	1.95	2.05
21	A	854	CLA	MG-NB	-5.05	1.95	2.05
21	4	614	CLA	C1D-ND	5.05	1.44	1.37
21	A	821	CLA	MG-NB	-5.04	1.95	2.05
21	7	611	CLA	MG-NB	-5.04	1.95	2.05
21	8	614	CLA	MG-NB	-5.03	1.95	2.05
21	3	614	CLA	C1D-ND	5.03	1.44	1.37
21	B	815	CLA	MG-NB	-5.03	1.95	2.05
21	9	613	CLA	MG-NB	-5.03	1.95	2.05
21	1	613	CLA	MG-NB	-5.03	1.95	2.05
21	3	610	CLA	MG-NB	-5.02	1.95	2.05
21	A	822	CLA	MG-NB	-5.02	1.95	2.05
21	9	614	CLA	C1D-ND	5.02	1.44	1.37
21	J	101	CLA	MG-NB	-5.02	1.95	2.05
21	9	614	CLA	MG-NB	-5.01	1.95	2.05
21	A	826	CLA	C1D-ND	5.01	1.44	1.37
21	B	838	CLA	MG-NB	-5.00	1.95	2.05
21	6	611	CLA	C1D-ND	5.00	1.44	1.37
21	A	804	CLA	MG-NB	-5.00	1.95	2.05
21	B	827	CLA	MG-NB	-5.00	1.95	2.05
21	A	819	CLA	MG-NB	-5.00	1.95	2.05
21	A	813	CLA	C1D-ND	5.00	1.44	1.37
21	B	819	CLA	MG-NB	-4.99	1.95	2.05
21	7	609	CLA	MG-NB	-4.99	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	7	620	CLA	MG-NB	-4.99	1.95	2.05
21	7	610	CLA	MG-NB	-4.99	1.95	2.05
21	L	204	CLA	C1D-ND	4.99	1.44	1.37
21	8	602	CLA	MG-NB	-4.99	1.95	2.05
21	F	303	CLA	C1D-ND	4.98	1.44	1.37
21	B	813	CLA	C1D-ND	4.98	1.44	1.37
21	4	612	CLA	C1D-ND	4.98	1.44	1.37
21	9	610	CLA	C1D-ND	4.98	1.44	1.37
21	A	815	CLA	MG-NB	-4.98	1.95	2.05
21	5	613	CLA	MG-NB	-4.98	1.95	2.05
21	9	602	CLA	C1D-ND	4.98	1.44	1.37
30	5	606	CHL	C3A-C2A	-4.97	1.50	1.54
21	8	612	CLA	C1D-ND	4.97	1.44	1.37
21	B	832	CLA	C1D-ND	4.97	1.44	1.37
21	3	612	CLA	C1D-ND	4.97	1.44	1.37
21	1	611	CLA	MG-NB	-4.97	1.95	2.05
21	A	836	CLA	MG-NB	-4.97	1.95	2.05
21	9	604	CLA	MG-NB	-4.97	1.95	2.05
21	7	612	CLA	C1D-ND	4.97	1.44	1.37
21	9	603	CLA	MG-NB	-4.96	1.95	2.05
21	A	817	CLA	MG-NB	-4.96	1.96	2.05
21	A	835	CLA	MG-NB	-4.96	1.96	2.05
21	7	613	CLA	MG-NB	-4.95	1.96	2.05
21	Z	614	CLA	C1D-ND	4.95	1.44	1.37
21	6	622	CLA	C1D-ND	4.94	1.44	1.37
21	B	806	CLA	C1D-ND	4.94	1.44	1.37
21	A	842	CLA	MG-NB	-4.94	1.96	2.05
21	Z	602	CLA	C1D-ND	4.94	1.44	1.37
21	B	831	CLA	MG-NB	-4.93	1.96	2.05
21	K	204	CLA	C1D-ND	4.93	1.44	1.37
21	B	813	CLA	MG-NB	-4.93	1.96	2.05
21	1	612	CLA	C1D-ND	4.93	1.44	1.37
21	A	841	CLA	MG-NB	-4.93	1.96	2.05
21	3	602	CLA	MG-NB	-4.93	1.96	2.05
21	A	817	CLA	C1D-ND	4.92	1.44	1.37
21	5	612	CLA	C1D-ND	4.92	1.44	1.37
21	A	839	CLA	MG-NB	-4.92	1.96	2.05
21	A	845	CLA	C1D-ND	4.92	1.44	1.37
21	F	304	CLA	MG-NB	-4.92	1.96	2.05
21	B	806	CLA	MG-NB	-4.91	1.96	2.05
21	B	816	CLA	C1D-ND	4.91	1.44	1.37
21	1	609	CLA	C1D-ND	4.91	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	K	206	CLA	C1D-ND	4.90	1.44	1.37
21	A	830	CLA	MG-NB	-4.90	1.96	2.05
21	1	610	CLA	MG-NB	-4.90	1.96	2.05
21	7	604	CLA	MG-NB	-4.90	1.96	2.05
21	Z	604	CLA	C1D-ND	4.89	1.44	1.37
21	B	817	CLA	MG-NB	-4.89	1.96	2.05
21	A	813	CLA	MG-NB	-4.89	1.96	2.05
21	5	616	CLA	C1D-ND	4.89	1.44	1.37
21	B	816	CLA	MG-NB	-4.89	1.96	2.05
21	1	604	CLA	C1D-ND	4.88	1.44	1.37
21	B	827	CLA	C1D-ND	4.88	1.44	1.37
30	6	607	CHL	CHB-C4A	-4.88	1.32	1.38
21	5	612	CLA	MG-NB	-4.87	1.96	2.05
21	4	612	CLA	MG-NB	-4.87	1.96	2.05
21	Z	613	CLA	C1D-ND	4.87	1.44	1.37
21	5	614	CLA	C1D-ND	4.86	1.44	1.37
21	B	814	CLA	MG-NB	-4.86	1.96	2.05
21	A	845	CLA	MG-NB	-4.86	1.96	2.05
21	K	201	CLA	C1D-ND	4.85	1.44	1.37
21	G	203	CLA	MG-NB	-4.85	1.96	2.05
21	6	612	CLA	MG-NB	-4.85	1.96	2.05
21	4	609	CLA	C1D-ND	4.85	1.44	1.37
21	8	608	CLA	C1D-ND	4.85	1.44	1.37
21	7	611	CLA	C1D-ND	4.85	1.44	1.37
21	8	603	CLA	C1D-ND	4.85	1.44	1.37
21	A	808	CLA	MG-NB	-4.84	1.96	2.05
21	Z	609	CLA	MG-NB	-4.84	1.96	2.05
21	5	616	CLA	MG-NB	-4.84	1.96	2.05
21	3	604	CLA	C1D-ND	4.84	1.44	1.37
21	F	303	CLA	MG-NB	-4.84	1.96	2.05
21	5	611	CLA	C1D-ND	4.84	1.44	1.37
21	6	613	CLA	C1D-ND	4.83	1.44	1.37
21	B	832	CLA	MG-NB	-4.83	1.96	2.05
21	B	815	CLA	C1D-ND	4.83	1.44	1.37
21	5	609	CLA	MG-NB	-4.83	1.96	2.05
21	K	203	CLA	C1D-ND	4.83	1.44	1.37
21	3	607	CLA	MG-NB	-4.83	1.96	2.05
21	B	805	CLA	MG-NB	-4.83	1.96	2.05
21	1	612	CLA	MG-NB	-4.83	1.96	2.05
21	6	604	CLA	C1D-ND	4.83	1.44	1.37
21	3	612	CLA	MG-NB	-4.83	1.96	2.05
21	8	613	CLA	MG-NB	-4.83	1.96	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	828	CLA	MG-NB	-4.82	1.96	2.05
21	F	301	CLA	MG-NB	-4.82	1.96	2.05
21	6	609	CLA	C1D-ND	4.82	1.44	1.37
21	5	603	CLA	C1D-ND	4.82	1.44	1.37
30	6	608	CHL	C3A-C2A	-4.82	1.50	1.54
21	A	825	CLA	C1D-ND	4.82	1.44	1.37
21	6	614	CLA	MG-NB	-4.82	1.96	2.05
21	B	811	CLA	C1D-ND	4.82	1.44	1.37
21	7	614	CLA	C1D-ND	4.82	1.44	1.37
21	4	602	CLA	C1D-ND	4.81	1.44	1.37
21	8	613	CLA	C1D-ND	4.81	1.44	1.37
21	A	826	CLA	MG-NB	-4.81	1.96	2.05
21	B	835	CLA	C1D-ND	4.81	1.44	1.37
21	9	612	CLA	MG-NB	-4.81	1.96	2.05
21	A	816	CLA	MG-NB	-4.80	1.96	2.05
21	B	803	CLA	C1D-ND	4.80	1.44	1.37
21	1	608	CLA	C1D-ND	4.80	1.44	1.37
21	B	814	CLA	C1D-ND	4.80	1.44	1.37
21	B	830	CLA	MG-NB	-4.80	1.96	2.05
21	A	831	CLA	C1D-ND	4.80	1.44	1.37
21	B	820	CLA	C1D-ND	4.80	1.44	1.37
21	B	831	CLA	C1D-ND	4.79	1.44	1.37
21	A	825	CLA	MG-NB	-4.79	1.96	2.05
21	3	609	CLA	C1D-ND	4.79	1.44	1.37
21	A	840	CLA	C1D-ND	4.78	1.44	1.37
21	B	805	CLA	C1D-ND	4.78	1.44	1.37
21	3	606	CLA	C1D-ND	4.77	1.44	1.37
21	A	809	CLA	MG-NB	-4.77	1.96	2.05
21	B	828	CLA	MG-NB	-4.77	1.96	2.05
21	7	616	CLA	C1D-ND	4.77	1.44	1.37
21	B	837	CLA	MG-NB	-4.77	1.96	2.05
21	B	807	CLA	C1D-ND	4.76	1.44	1.37
21	A	814	CLA	MG-NB	-4.76	1.96	2.05
21	1	614	CLA	C1D-ND	4.76	1.44	1.37
21	Z	609	CLA	C1D-ND	4.76	1.44	1.37
21	Z	611	CLA	C1D-ND	4.76	1.44	1.37
21	7	609	CLA	C1D-ND	4.76	1.44	1.37
21	Z	616	CLA	C1D-ND	4.75	1.44	1.37
21	7	613	CLA	C1D-ND	4.75	1.44	1.37
21	3	607	CLA	C1D-ND	4.75	1.44	1.37
21	B	838	CLA	C1D-ND	4.75	1.44	1.37
21	A	810	CLA	C1D-ND	4.75	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	825	CLA	MG-NB	-4.75	1.96	2.05
21	A	835	CLA	C1D-ND	4.75	1.44	1.37
21	A	816	CLA	C1D-ND	4.74	1.44	1.37
21	F	301	CLA	C1D-ND	4.74	1.44	1.37
21	5	617	CLA	MG-NB	-4.74	1.96	2.05
21	Z	608	CLA	C1D-ND	4.74	1.44	1.37
21	B	828	CLA	C1D-ND	4.73	1.44	1.37
21	4	604	CLA	C1D-ND	4.73	1.44	1.37
21	A	812	CLA	MG-NB	-4.73	1.96	2.05
21	J	101	CLA	C1D-ND	4.73	1.44	1.37
21	6	603	CLA	C1D-ND	4.73	1.44	1.37
21	A	838	CLA	C1D-ND	4.73	1.44	1.37
21	6	617	CLA	C1D-ND	4.73	1.44	1.37
21	A	807	CLA	MG-NB	-4.72	1.96	2.05
21	B	802	CLA	MG-NB	-4.72	1.96	2.05
21	5	602	CLA	C1D-ND	4.72	1.44	1.37
21	A	839	CLA	C1D-ND	4.72	1.44	1.37
21	B	808	CLA	C1D-ND	4.72	1.44	1.37
21	5	604	CLA	C1D-ND	4.72	1.44	1.37
21	B	822	CLA	C1D-ND	4.71	1.44	1.37
21	B	837	CLA	C1D-ND	4.71	1.44	1.37
21	7	608	CLA	C1D-ND	4.71	1.44	1.37
21	B	819	CLA	C1D-ND	4.70	1.44	1.37
21	4	613	CLA	C1D-ND	4.70	1.44	1.37
21	6	602	CLA	C1D-ND	4.70	1.44	1.37
21	A	818	CLA	C1D-ND	4.70	1.44	1.37
21	B	812	CLA	C1D-ND	4.70	1.44	1.37
21	B	839	CLA	C1D-ND	4.70	1.44	1.37
21	3	615	CLA	C1D-ND	4.69	1.44	1.37
21	B	804	CLA	C1D-ND	4.69	1.44	1.37
21	7	604	CLA	C1D-ND	4.69	1.44	1.37
21	4	603	CLA	MG-NB	-4.69	1.96	2.05
21	8	604	CLA	C1D-ND	4.69	1.44	1.37
21	A	838	CLA	MG-NB	-4.69	1.96	2.05
21	A	837	CLA	C1D-ND	4.68	1.44	1.37
21	A	854	CLA	C1D-ND	4.67	1.44	1.37
20	A	801	CL0	MG-ND	-4.67	1.96	2.05
21	A	820	CLA	MG-NB	-4.67	1.96	2.05
21	1	603	CLA	C1D-ND	4.66	1.44	1.37
21	B	809	CLA	C1D-ND	4.65	1.44	1.37
21	5	613	CLA	C1D-ND	4.65	1.44	1.37
21	3	611	CLA	C1D-ND	4.64	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	836	CLA	C1D-ND	4.64	1.44	1.37
21	K	201	CLA	MG-ND	-4.64	1.96	2.05
21	B	810	CLA	C1D-ND	4.63	1.43	1.37
21	1	616	CLA	C1D-ND	4.63	1.43	1.37
21	8	616	CLA	C1D-ND	4.63	1.43	1.37
21	A	806	CLA	MG-NB	-4.63	1.96	2.05
21	A	809	CLA	C1D-ND	4.63	1.43	1.37
21	A	815	CLA	C1D-ND	4.63	1.43	1.37
21	8	602	CLA	C1D-ND	4.63	1.43	1.37
21	A	820	CLA	C1D-ND	4.62	1.43	1.37
21	A	818	CLA	MG-NB	-4.62	1.96	2.05
21	A	802	CLA	MG-NB	-4.62	1.96	2.05
21	7	603	CLA	C1D-ND	4.62	1.43	1.37
21	4	610	CLA	C1D-ND	4.62	1.43	1.37
21	B	808	CLA	MG-NB	-4.62	1.96	2.05
21	8	612	CLA	MG-NB	-4.62	1.96	2.05
21	A	807	CLA	C1D-ND	4.61	1.43	1.37
21	7	612	CLA	MG-NB	-4.61	1.96	2.05
21	1	610	CLA	C1D-ND	4.61	1.43	1.37
21	A	824	CLA	C1D-ND	4.61	1.43	1.37
21	A	834	CLA	C1D-ND	4.61	1.43	1.37
21	A	821	CLA	C1D-ND	4.61	1.43	1.37
21	5	609	CLA	C1D-ND	4.61	1.43	1.37
21	B	840	CLA	C1D-ND	4.60	1.43	1.37
21	A	829	CLA	C1D-ND	4.60	1.43	1.37
21	B	825	CLA	C1D-ND	4.60	1.43	1.37
30	4	601	CHL	C3A-C2A	-4.59	1.50	1.54
21	A	811	CLA	C1D-ND	4.59	1.43	1.37
21	B	833	CLA	MG-NB	-4.59	1.96	2.05
21	B	818	CLA	C1D-ND	4.58	1.43	1.37
21	3	613	CLA	C1D-ND	4.58	1.43	1.37
21	A	832	CLA	C1D-ND	4.58	1.43	1.37
21	1	611	CLA	C1D-ND	4.57	1.43	1.37
21	Z	612	CLA	MG-NB	-4.57	1.96	2.05
21	4	616	CLA	C1D-ND	4.56	1.43	1.37
21	A	803	CLA	C1D-ND	4.56	1.43	1.37
21	A	833	CLA	C1D-ND	4.56	1.43	1.37
21	5	617	CLA	C1D-ND	4.56	1.43	1.37
21	1	602	CLA	C1D-ND	4.56	1.43	1.37
21	B	802	CLA	C1D-ND	4.56	1.43	1.37
21	B	817	CLA	C1D-ND	4.55	1.43	1.37
21	B	841	CLA	C1D-ND	4.55	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	610	CLA	C1D-ND	4.54	1.43	1.37
21	B	829	CLA	MG-NB	-4.54	1.96	2.05
21	1	613	CLA	C1D-ND	4.54	1.43	1.37
21	3	603	CLA	C1D-ND	4.53	1.43	1.37
21	A	836	CLA	C1D-ND	4.53	1.43	1.37
21	7	602	CLA	C1D-ND	4.52	1.43	1.37
21	4	609	CLA	MG-ND	-4.52	1.96	2.05
21	A	808	CLA	C1D-ND	4.52	1.43	1.37
21	A	822	CLA	C1D-ND	4.51	1.43	1.37
30	4	608	CHL	C3A-C2A	-4.51	1.50	1.54
21	A	828	CLA	C1D-ND	4.51	1.43	1.37
21	A	830	CLA	C1D-ND	4.49	1.43	1.37
21	B	836	CLA	MG-NB	-4.48	1.96	2.05
21	A	819	CLA	C1D-ND	4.48	1.43	1.37
21	B	821	CLA	C1D-ND	4.48	1.43	1.37
21	L	203	CLA	C1D-ND	4.48	1.43	1.37
21	6	610	CLA	C1D-ND	4.47	1.43	1.37
21	7	610	CLA	C1D-ND	4.47	1.43	1.37
30	8	606	CHL	CHB-C4A	-4.47	1.33	1.38
21	Z	610	CLA	C1D-ND	4.47	1.43	1.37
30	7	607	CHL	C3A-C2A	-4.46	1.50	1.54
21	A	843	CLA	C1D-ND	4.46	1.43	1.37
21	8	609	CLA	C1D-ND	4.46	1.43	1.37
21	A	806	CLA	C1D-ND	4.46	1.43	1.37
21	A	824	CLA	MG-ND	-4.46	1.96	2.05
21	A	814	CLA	C1D-ND	4.46	1.43	1.37
21	B	821	CLA	MG-ND	-4.45	1.97	2.05
21	A	811	CLA	MG-NB	-4.45	1.97	2.05
21	3	602	CLA	C1D-ND	4.45	1.43	1.37
21	B	830	CLA	C1D-ND	4.45	1.43	1.37
30	5	608	CHL	CHB-C4A	-4.44	1.33	1.38
21	5	621	CLA	MG-ND	-4.44	1.97	2.05
30	5	607	CHL	CHB-C4A	-4.44	1.33	1.38
21	A	804	CLA	C1D-ND	4.44	1.43	1.37
21	B	840	CLA	MG-NB	-4.43	1.97	2.05
30	1	607	CHL	CHB-C4A	-4.41	1.33	1.38
21	8	611	CLA	C1D-ND	4.41	1.43	1.37
30	4	606	CHL	C3A-C2A	-4.40	1.50	1.54
30	6	618	CHL	CHB-C4A	-4.40	1.33	1.38
21	A	803	CLA	MG-ND	-4.39	1.97	2.05
21	5	610	CLA	C1D-ND	4.38	1.43	1.37
21	A	823	CLA	C1D-ND	4.37	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	617	CLA	MG-ND	-4.37	1.97	2.05
21	6	613	CLA	MG-ND	-4.37	1.97	2.05
21	B	833	CLA	C1D-ND	4.37	1.43	1.37
21	1	616	CLA	MG-ND	-4.37	1.97	2.05
30	5	607	CHL	C3A-C2A	-4.37	1.50	1.54
30	1	606	CHL	CHB-C4A	-4.36	1.33	1.38
21	1	608	CLA	MG-ND	-4.36	1.97	2.05
30	6	616	CHL	CHB-C4A	-4.36	1.33	1.38
30	1	606	CHL	C3A-C2A	-4.36	1.50	1.54
21	B	823	CLA	C1D-ND	4.36	1.43	1.37
21	K	203	CLA	MG-ND	-4.35	1.97	2.05
21	3	617	CLA	C1D-ND	4.35	1.43	1.37
21	A	814	CLA	MG-ND	-4.35	1.97	2.05
21	A	832	CLA	MG-ND	-4.35	1.97	2.05
30	Z	607	CHL	CHB-C4A	-4.34	1.33	1.38
21	5	604	CLA	MG-ND	-4.34	1.97	2.05
21	B	834	CLA	C1D-ND	4.34	1.43	1.37
21	B	826	CLA	C1D-ND	4.33	1.43	1.37
21	A	825	CLA	MG-ND	-4.32	1.97	2.05
21	A	842	CLA	C1D-ND	4.32	1.43	1.37
21	A	823	CLA	MG-ND	-4.32	1.97	2.05
21	4	613	CLA	MG-ND	-4.32	1.97	2.05
21	B	818	CLA	MG-ND	-4.32	1.97	2.05
30	4	608	CHL	CHB-C4A	-4.32	1.33	1.38
21	A	837	CLA	MG-ND	-4.31	1.97	2.05
30	1	607	CHL	C3A-C2A	-4.31	1.51	1.54
30	6	607	CHL	C3A-C2A	-4.31	1.51	1.54
30	8	601	CHL	CHB-C4A	-4.30	1.33	1.38
21	A	834	CLA	MG-ND	-4.30	1.97	2.05
21	B	820	CLA	MG-ND	-4.30	1.97	2.05
21	B	830	CLA	MG-ND	-4.29	1.97	2.05
21	A	817	CLA	MG-ND	-4.29	1.97	2.05
21	B	841	CLA	MG-ND	-4.29	1.97	2.05
21	Z	608	CLA	MG-ND	-4.28	1.97	2.05
21	A	812	CLA	C1D-ND	4.28	1.43	1.37
21	B	829	CLA	C1D-ND	4.28	1.43	1.37
21	A	810	CLA	MG-ND	-4.28	1.97	2.05
21	B	823	CLA	MG-ND	-4.27	1.97	2.05
21	5	610	CLA	MG-ND	-4.27	1.97	2.05
30	6	608	CHL	CHB-C4A	-4.27	1.33	1.38
21	A	831	CLA	MG-NB	-4.27	1.97	2.05
21	3	603	CLA	MG-ND	-4.27	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	5	618	CHL	CHB-C4A	-4.26	1.33	1.38
21	3	615	CLA	MG-ND	-4.26	1.97	2.05
21	8	610	CLA	C1D-ND	4.26	1.43	1.37
21	B	812	CLA	MG-ND	-4.26	1.97	2.05
30	6	601	CHL	C3A-C2A	-4.26	1.51	1.54
30	Z	607	CHL	C3A-C2A	-4.25	1.51	1.54
21	5	611	CLA	MG-ND	-4.25	1.97	2.05
21	8	614	CLA	MG-ND	-4.24	1.97	2.05
21	B	824	CLA	MG-ND	-4.24	1.97	2.05
21	3	611	CLA	MG-ND	-4.24	1.97	2.05
21	5	612	CLA	MG-ND	-4.24	1.97	2.05
21	B	838	CLA	MG-ND	-4.24	1.97	2.05
21	Z	603	CLA	MG-ND	-4.24	1.97	2.05
21	3	613	CLA	MG-ND	-4.24	1.97	2.05
21	6	610	CLA	MG-ND	-4.24	1.97	2.05
30	3	608	CHL	CHB-C4A	-4.23	1.33	1.38
21	4	604	CLA	MG-ND	-4.23	1.97	2.05
21	6	602	CLA	MG-ND	-4.23	1.97	2.05
21	A	821	CLA	MG-ND	-4.23	1.97	2.05
21	3	612	CLA	MG-ND	-4.23	1.97	2.05
21	A	833	CLA	MG-ND	-4.23	1.97	2.05
21	5	601	CLA	MG-ND	-4.23	1.97	2.05
21	3	610	CLA	MG-ND	-4.23	1.97	2.05
21	6	603	CLA	MG-ND	-4.22	1.97	2.05
21	A	805	CLA	C1D-ND	4.22	1.43	1.37
21	B	839	CLA	MG-ND	-4.22	1.97	2.05
21	Z	610	CLA	MG-ND	-4.21	1.97	2.05
21	B	815	CLA	MG-ND	-4.21	1.97	2.05
21	K	206	CLA	MG-ND	-4.21	1.97	2.05
21	A	843	CLA	MG-ND	-4.20	1.97	2.05
21	A	807	CLA	MG-ND	-4.20	1.97	2.05
21	8	608	CLA	MG-ND	-4.20	1.97	2.05
30	Z	601	CHL	CHB-C4A	-4.20	1.33	1.38
21	Z	614	CLA	MG-ND	-4.20	1.97	2.05
21	5	613	CLA	MG-ND	-4.20	1.97	2.05
21	A	835	CLA	MG-ND	-4.19	1.97	2.05
21	6	611	CLA	MG-ND	-4.19	1.97	2.05
21	1	609	CLA	MG-ND	-4.19	1.97	2.05
21	B	807	CLA	MG-ND	-4.19	1.97	2.05
21	B	826	CLA	MG-ND	-4.18	1.97	2.05
21	Z	616	CLA	MG-ND	-4.18	1.97	2.05
21	4	614	CLA	MG-ND	-4.18	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	8	604	CLA	MG-ND	-4.18	1.97	2.05
21	A	840	CLA	MG-ND	-4.18	1.97	2.05
30	6	618	CHL	C3A-C2A	-4.18	1.51	1.54
21	A	802	CLA	C1D-ND	4.17	1.43	1.37
21	1	602	CLA	MG-ND	-4.17	1.97	2.05
21	A	813	CLA	MG-ND	-4.17	1.97	2.05
21	6	604	CLA	MG-ND	-4.17	1.97	2.05
21	9	602	CLA	MG-ND	-4.17	1.97	2.05
30	4	618	CHL	C3A-C2A	-4.17	1.51	1.54
21	B	835	CLA	MG-ND	-4.16	1.97	2.05
21	5	602	CLA	MG-ND	-4.16	1.97	2.05
21	7	608	CLA	MG-ND	-4.16	1.97	2.05
21	4	611	CLA	MG-ND	-4.16	1.97	2.05
21	1	604	CLA	MG-ND	-4.16	1.97	2.05
21	L	204	CLA	MG-ND	-4.16	1.97	2.05
30	Z	606	CHL	CHB-C4A	-4.15	1.33	1.38
21	G	204	CLA	MG-ND	-4.15	1.97	2.05
21	1	613	CLA	MG-ND	-4.14	1.97	2.05
21	7	611	CLA	MG-ND	-4.13	1.97	2.05
21	1	611	CLA	MG-ND	-4.13	1.97	2.05
21	8	613	CLA	MG-ND	-4.13	1.97	2.05
21	B	819	CLA	MG-ND	-4.13	1.97	2.05
21	B	840	CLA	MG-ND	-4.13	1.97	2.05
21	8	603	CLA	MG-ND	-4.13	1.97	2.05
21	1	614	CLA	MG-ND	-4.13	1.97	2.05
21	8	616	CLA	MG-ND	-4.13	1.97	2.05
21	A	802	CLA	MG-ND	-4.13	1.97	2.05
21	L	203	CLA	MG-ND	-4.13	1.97	2.05
21	Z	604	CLA	MG-ND	-4.12	1.97	2.05
21	9	611	CLA	MG-ND	-4.12	1.97	2.05
21	4	610	CLA	MG-ND	-4.12	1.97	2.05
21	A	836	CLA	MG-ND	-4.12	1.97	2.05
21	4	616	CLA	MG-ND	-4.12	1.97	2.05
21	8	611	CLA	MG-ND	-4.11	1.97	2.05
21	3	609	CLA	MG-ND	-4.11	1.97	2.05
21	B	834	CLA	MG-ND	-4.11	1.97	2.05
21	A	841	CLA	C1D-ND	4.11	1.43	1.37
21	6	609	CLA	MG-ND	-4.11	1.97	2.05
21	A	804	CLA	MG-ND	-4.11	1.97	2.05
21	K	204	CLA	MG-ND	-4.10	1.97	2.05
21	7	614	CLA	MG-ND	-4.10	1.97	2.05
21	6	622	CLA	MG-ND	-4.10	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	4	618	CHL	CHB-C4A	-4.10	1.33	1.38
21	9	601	CLA	MG-ND	-4.10	1.97	2.05
30	4	606	CHL	CHB-C4A	-4.10	1.33	1.38
30	5	606	CHL	CHB-C4A	-4.10	1.33	1.38
21	B	836	CLA	MG-ND	-4.10	1.97	2.05
30	6	606	CHL	CHB-C4A	-4.09	1.33	1.38
21	Z	602	CLA	MG-ND	-4.09	1.97	2.05
21	B	816	CLA	MG-ND	-4.09	1.97	2.05
21	3	606	CLA	MG-ND	-4.09	1.97	2.05
30	8	607	CHL	CHB-C4A	-4.09	1.33	1.38
21	7	616	CLA	MG-ND	-4.09	1.97	2.05
21	Z	611	CLA	MG-ND	-4.09	1.97	2.05
21	4	603	CLA	MG-ND	-4.08	1.97	2.05
30	Z	606	CHL	C1A-CHA	-4.08	1.35	1.40
21	A	827	CLA	C1D-ND	4.08	1.43	1.37
21	3	607	CLA	MG-ND	-4.08	1.97	2.05
21	5	614	CLA	MG-ND	-4.08	1.97	2.05
21	B	809	CLA	MG-ND	-4.08	1.97	2.05
30	1	601	CHL	CHB-C4A	-4.08	1.33	1.38
21	B	811	CLA	MG-ND	-4.08	1.97	2.05
21	9	612	CLA	MG-ND	-4.07	1.97	2.05
30	4	607	CHL	C1A-CHA	-4.07	1.35	1.40
30	7	606	CHL	CHB-C4A	-4.07	1.33	1.38
21	J	101	CLA	MG-ND	-4.07	1.97	2.05
30	9	607	CHL	CHB-C4A	-4.06	1.33	1.38
21	4	612	CLA	MG-ND	-4.06	1.97	2.05
21	3	614	CLA	MG-ND	-4.06	1.97	2.05
21	6	617	CLA	MG-ND	-4.06	1.97	2.05
21	7	604	CLA	MG-ND	-4.06	1.97	2.05
21	7	613	CLA	MG-ND	-4.06	1.97	2.05
21	G	203	CLA	MG-ND	-4.06	1.97	2.05
21	9	603	CLA	MG-ND	-4.06	1.97	2.05
21	9	614	CLA	MG-ND	-4.05	1.97	2.05
21	A	828	CLA	MG-ND	-4.05	1.97	2.05
21	5	617	CLA	MG-ND	-4.05	1.97	2.05
21	4	602	CLA	MG-ND	-4.05	1.97	2.05
30	6	618	CHL	C1A-CHA	-4.04	1.35	1.40
21	8	609	CLA	MG-ND	-4.04	1.97	2.05
21	A	808	CLA	MG-ND	-4.04	1.97	2.05
21	A	826	CLA	MG-ND	-4.04	1.97	2.05
21	Z	613	CLA	MG-ND	-4.04	1.97	2.05
21	9	610	CLA	MG-ND	-4.04	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	822	CLA	MG-ND	-4.04	1.97	2.05
21	A	822	CLA	MG-ND	-4.04	1.97	2.05
30	Z	601	CHL	C3A-C2A	-4.04	1.51	1.54
30	4	601	CHL	CHB-C4A	-4.04	1.33	1.38
21	B	806	CLA	MG-ND	-4.03	1.97	2.05
21	A	838	CLA	MG-ND	-4.03	1.97	2.05
21	7	603	CLA	MG-ND	-4.03	1.97	2.05
21	7	609	CLA	MG-ND	-4.03	1.97	2.05
30	6	606	CHL	C1A-CHA	-4.03	1.35	1.40
30	7	607	CHL	CHB-C4A	-4.03	1.33	1.38
21	9	613	CLA	MG-ND	-4.03	1.97	2.05
21	A	854	CLA	MG-ND	-4.02	1.97	2.05
21	8	602	CLA	MG-ND	-4.02	1.97	2.05
21	3	604	CLA	MG-ND	-4.02	1.97	2.05
21	1	610	CLA	MG-ND	-4.02	1.97	2.05
21	7	620	CLA	MG-ND	-4.02	1.97	2.05
21	B	833	CLA	MG-ND	-4.02	1.97	2.05
21	B	814	CLA	MG-ND	-4.02	1.97	2.05
21	B	810	CLA	MG-ND	-4.02	1.97	2.05
21	9	604	CLA	MG-ND	-4.01	1.97	2.05
30	7	606	CHL	C1A-CHA	-4.01	1.35	1.40
30	6	616	CHL	C1A-CHA	-4.01	1.35	1.40
21	A	830	CLA	MG-ND	-4.01	1.97	2.05
21	5	616	CLA	MG-ND	-4.01	1.97	2.05
21	B	825	CLA	MG-ND	-4.01	1.97	2.05
21	8	610	CLA	MG-ND	-4.01	1.97	2.05
30	4	608	CHL	C1A-CHA	-4.01	1.35	1.40
30	5	606	CHL	C1A-CHA	-4.01	1.35	1.40
21	B	802	CLA	MG-ND	-4.00	1.97	2.05
21	A	809	CLA	MG-ND	-4.00	1.97	2.05
21	A	841	CLA	MG-ND	-4.00	1.97	2.05
21	3	602	CLA	MG-ND	-4.00	1.97	2.05
21	9	609	CLA	MG-ND	-4.00	1.97	2.05
30	5	608	CHL	C1A-CHA	-4.00	1.35	1.40
30	9	606	CHL	C1A-CHA	-4.00	1.35	1.40
21	F	301	CLA	MG-ND	-4.00	1.97	2.05
21	1	603	CLA	MG-ND	-4.00	1.97	2.05
21	B	805	CLA	MG-ND	-3.99	1.97	2.05
21	B	813	CLA	MG-ND	-3.99	1.97	2.05
21	Z	612	CLA	MG-ND	-3.99	1.97	2.05
21	5	603	CLA	MG-ND	-3.99	1.97	2.05
30	6	601	CHL	CHB-C4A	-3.99	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	4	607	CHL	C3A-C2A	-3.99	1.51	1.54
21	7	602	CLA	MG-ND	-3.99	1.97	2.05
30	7	607	CHL	C1A-CHA	-3.98	1.35	1.40
30	5	607	CHL	C1A-CHA	-3.98	1.35	1.40
21	1	612	CLA	MG-ND	-3.97	1.97	2.05
21	7	612	CLA	MG-ND	-3.97	1.97	2.05
30	5	618	CHL	C1A-CHA	-3.97	1.35	1.40
21	A	839	CLA	MG-ND	-3.97	1.97	2.05
21	5	609	CLA	MG-ND	-3.97	1.97	2.05
30	8	606	CHL	C1A-CHA	-3.97	1.35	1.40
21	B	829	CLA	MG-ND	-3.96	1.97	2.05
21	B	803	CLA	MG-ND	-3.96	1.97	2.05
21	A	815	CLA	MG-ND	-3.96	1.97	2.05
21	F	303	CLA	MG-ND	-3.96	1.97	2.05
21	8	612	CLA	MG-ND	-3.95	1.98	2.05
30	6	601	CHL	C1A-CHA	-3.95	1.35	1.40
30	4	606	CHL	C1A-CHA	-3.95	1.35	1.40
30	9	607	CHL	C1A-CHA	-3.95	1.35	1.40
30	1	607	CHL	C1A-CHA	-3.95	1.35	1.40
30	4	618	CHL	C1A-CHA	-3.95	1.35	1.40
21	Z	609	CLA	MG-ND	-3.94	1.98	2.05
21	B	831	CLA	MG-ND	-3.94	1.98	2.05
30	6	607	CHL	C1A-CHA	-3.93	1.35	1.40
30	9	606	CHL	CHB-C4A	-3.93	1.33	1.38
21	A	812	CLA	MG-ND	-3.93	1.98	2.05
30	1	606	CHL	C1A-CHA	-3.93	1.35	1.40
21	A	827	CLA	MG-ND	-3.93	1.98	2.05
30	9	606	CHL	C2A-C3A	-3.92	1.51	1.54
21	B	817	CLA	MG-ND	-3.92	1.98	2.05
30	6	616	CHL	C3A-C2A	-3.92	1.51	1.54
21	A	820	CLA	MG-ND	-3.92	1.98	2.05
30	6	608	CHL	C1A-CHA	-3.92	1.35	1.40
30	9	607	CHL	C3A-C2A	-3.91	1.51	1.54
30	Z	601	CHL	C1A-CHA	-3.91	1.35	1.40
30	7	606	CHL	C3A-C2A	-3.91	1.51	1.54
21	A	819	CLA	MG-ND	-3.91	1.98	2.05
21	B	804	CLA	MG-ND	-3.91	1.98	2.05
21	6	614	CLA	MG-ND	-3.91	1.98	2.05
30	Z	607	CHL	C1A-CHA	-3.91	1.35	1.40
30	3	608	CHL	C1A-CHA	-3.90	1.35	1.40
21	A	816	CLA	MG-ND	-3.90	1.98	2.05
21	A	845	CLA	MG-ND	-3.89	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	5	618	CHL	C3A-C2A	-3.89	1.51	1.54
21	A	818	CLA	MG-ND	-3.89	1.98	2.05
21	F	304	CLA	MG-ND	-3.88	1.98	2.05
21	6	612	CLA	MG-ND	-3.88	1.98	2.05
21	A	829	CLA	MG-ND	-3.87	1.98	2.05
30	4	607	CHL	CHB-C4A	-3.87	1.34	1.38
21	B	832	CLA	MG-ND	-3.85	1.98	2.05
21	A	806	CLA	MG-ND	-3.83	1.98	2.05
21	B	808	CLA	MG-ND	-3.83	1.98	2.05
21	A	831	CLA	MG-ND	-3.82	1.98	2.05
21	B	828	CLA	MG-ND	-3.82	1.98	2.05
21	B	837	CLA	MG-ND	-3.82	1.98	2.05
30	1	601	CHL	C1A-CHA	-3.82	1.35	1.40
30	7	601	CHL	C1A-CHA	-3.81	1.35	1.40
20	A	801	CL0	C1A-CHA	-3.81	1.35	1.40
21	7	610	CLA	MG-ND	-3.81	1.98	2.05
30	8	601	CHL	C1A-CHA	-3.81	1.35	1.40
30	9	607	CHL	C3B-C4B	3.79	1.45	1.41
30	4	601	CHL	C1A-CHA	-3.75	1.35	1.40
30	8	607	CHL	C1A-CHA	-3.74	1.35	1.40
30	8	606	CHL	C3B-C4B	3.74	1.45	1.41
21	B	827	CLA	MG-ND	-3.74	1.98	2.05
30	Z	606	CHL	C3A-C2A	-3.72	1.51	1.54
30	Z	601	CHL	C3B-C4B	3.68	1.45	1.41
30	9	606	CHL	C3B-C4B	3.67	1.45	1.41
21	A	842	CLA	MG-ND	-3.64	1.98	2.05
21	A	805	CLA	MG-ND	-3.62	1.98	2.05
30	6	616	CHL	C3B-C4B	3.62	1.44	1.41
30	8	601	CHL	C3A-C2A	-3.60	1.51	1.54
30	6	606	CHL	C3A-C2A	-3.60	1.51	1.54
30	1	606	CHL	C3B-C4B	3.60	1.44	1.41
30	4	601	CHL	C3B-C4B	3.59	1.44	1.41
30	Z	606	CHL	C3B-C4B	3.58	1.44	1.41
30	4	608	CHL	C3B-C4B	3.57	1.44	1.41
30	5	607	CHL	C3B-C4B	3.55	1.44	1.41
30	6	618	CHL	C3B-C4B	3.54	1.44	1.41
21	A	811	CLA	MG-ND	-3.53	1.98	2.05
30	4	606	CHL	C3B-C4B	3.53	1.44	1.41
30	6	608	CHL	C3B-C4B	3.50	1.44	1.41
30	Z	607	CHL	C3B-C4B	3.48	1.44	1.41
30	6	607	CHL	C3B-C4B	3.46	1.44	1.41
30	8	601	CHL	C3B-C4B	3.45	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	5	618	CHL	C3B-C4B	3.45	1.44	1.41
30	4	618	CHL	C3B-C4B	3.44	1.44	1.41
30	7	601	CHL	C3A-C2A	-3.41	1.51	1.54
30	1	607	CHL	C3B-C4B	3.41	1.44	1.41
30	5	608	CHL	C3B-C4B	3.41	1.44	1.41
30	6	606	CHL	C3B-C4B	3.40	1.44	1.41
30	7	601	CHL	CHB-C4A	-3.39	1.34	1.38
30	7	607	CHL	C3B-C4B	3.39	1.44	1.41
30	1	601	CHL	C3A-C2A	-3.37	1.51	1.54
30	8	607	CHL	C3B-C4B	3.36	1.44	1.41
30	8	601	CHL	C3B-C2B	-3.35	1.35	1.40
30	5	606	CHL	C3B-C4B	3.35	1.44	1.41
30	7	601	CHL	C3B-C4B	3.31	1.44	1.41
30	1	601	CHL	C3B-C4B	3.29	1.44	1.41
30	5	607	CHL	C3B-C2B	-3.29	1.35	1.40
30	8	606	CHL	C3A-C2A	-3.27	1.51	1.54
30	6	607	CHL	C3B-C2B	-3.24	1.36	1.40
30	4	606	CHL	C3B-C2B	-3.23	1.36	1.40
30	3	608	CHL	C3B-C2B	-3.22	1.36	1.40
30	8	607	CHL	C3B-C2B	-3.21	1.36	1.40
30	5	606	CHL	C3B-C2B	-3.18	1.36	1.40
20	A	801	CL0	C3A-C2A	-3.18	1.52	1.54
30	7	606	CHL	C3B-C4B	3.18	1.44	1.41
30	5	608	CHL	C3B-C2B	-3.17	1.36	1.40
30	6	601	CHL	C3B-C4B	3.16	1.44	1.41
30	7	606	CHL	C3B-C2B	-3.15	1.36	1.40
30	1	606	CHL	C3B-C2B	-3.15	1.36	1.40
30	1	601	CHL	C3B-C2B	-3.11	1.36	1.40
30	6	618	CHL	C3B-C2B	-3.10	1.36	1.40
30	7	607	CHL	C3B-C2B	-3.10	1.36	1.40
30	4	607	CHL	C3B-C4B	3.09	1.44	1.41
30	6	606	CHL	C3B-C2B	-3.09	1.36	1.40
30	Z	607	CHL	C3B-C2B	-3.08	1.36	1.40
30	3	608	CHL	C3B-C4B	3.08	1.44	1.41
30	Z	601	CHL	C3B-C2B	-3.07	1.36	1.40
30	4	608	CHL	C3B-C2B	-3.06	1.36	1.40
30	4	618	CHL	C3B-C2B	-3.06	1.36	1.40
30	6	601	CHL	C3B-C2B	-3.05	1.36	1.40
30	6	616	CHL	C3B-C2B	-3.05	1.36	1.40
30	1	607	CHL	C3B-C2B	-3.04	1.36	1.40
30	4	601	CHL	C3B-C2B	-3.04	1.36	1.40
30	Z	606	CHL	C3B-C2B	-3.03	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	6	608	CHL	C3B-C2B	-3.00	1.36	1.40
30	8	606	CHL	C3B-C2B	-2.99	1.36	1.40
30	4	607	CHL	C3B-C2B	-2.99	1.36	1.40
30	7	601	CHL	C3B-C2B	-2.98	1.36	1.40
30	5	618	CHL	C3B-C2B	-2.97	1.36	1.40
30	9	607	CHL	C3B-C2B	-2.80	1.36	1.40
30	9	606	CHL	C3B-C2B	-2.70	1.36	1.40
21	K	201	CLA	C1D-C2D	-2.62	1.40	1.45
30	7	606	CHL	CHC-C4B	-2.61	1.35	1.39
30	4	607	CHL	CHC-C4B	-2.59	1.35	1.39
21	F	301	CLA	C1D-C2D	-2.54	1.40	1.45
21	A	809	CLA	C1D-C2D	-2.53	1.40	1.45
21	A	829	CLA	C1D-C2D	-2.53	1.40	1.45
21	A	802	CLA	C1D-C2D	-2.53	1.40	1.45
21	B	824	CLA	C1D-C2D	-2.52	1.40	1.45
30	Z	607	CHL	CHC-C4B	-2.51	1.35	1.39
21	B	802	CLA	C1D-C2D	-2.51	1.40	1.45
21	4	609	CLA	C1D-C2D	-2.51	1.40	1.45
21	A	814	CLA	C1D-C2D	-2.51	1.40	1.45
21	A	807	CLA	C1D-C2D	-2.50	1.40	1.45
21	5	621	CLA	C1D-C2D	-2.50	1.40	1.45
30	8	607	CHL	C3A-C2A	-2.50	1.52	1.54
21	B	808	CLA	C1D-C2D	-2.49	1.40	1.45
21	A	838	CLA	C1D-C2D	-2.49	1.40	1.45
30	6	607	CHL	CHB-C1B	-2.48	1.35	1.39
21	1	612	CLA	C1D-C2D	-2.48	1.40	1.45
30	5	608	CHL	CHC-C4B	-2.48	1.35	1.39
21	A	840	CLA	C1D-C2D	-2.47	1.40	1.45
30	6	606	CHL	CHC-C4B	-2.47	1.35	1.39
21	B	813	CLA	C1D-C2D	-2.47	1.40	1.45
30	5	618	CHL	CHC-C4B	-2.47	1.35	1.39
21	B	816	CLA	C1D-C2D	-2.47	1.40	1.45
21	5	601	CLA	C1D-C2D	-2.46	1.40	1.45
30	6	601	CHL	CHC-C4B	-2.46	1.35	1.39
21	5	612	CLA	C1D-C2D	-2.46	1.40	1.45
30	4	608	CHL	CHC-C4B	-2.46	1.35	1.39
21	A	834	CLA	C1D-C2D	-2.46	1.40	1.45
21	3	613	CLA	C1D-C2D	-2.46	1.40	1.45
21	A	804	CLA	C1D-C2D	-2.46	1.40	1.45
21	A	817	CLA	C1D-C2D	-2.45	1.40	1.45
21	8	614	CLA	C1D-C2D	-2.45	1.40	1.45
30	8	607	CHL	CHC-C4B	-2.45	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	1	601	CHL	CHC-C4B	-2.45	1.35	1.39
30	4	618	CHL	CHC-C4B	-2.45	1.35	1.39
21	B	815	CLA	C1D-C2D	-2.45	1.40	1.45
21	4	603	CLA	C1D-C2D	-2.45	1.40	1.45
21	B	838	CLA	C1D-C2D	-2.45	1.40	1.45
21	A	835	CLA	C1D-C2D	-2.45	1.40	1.45
30	6	618	CHL	CHC-C4B	-2.45	1.35	1.39
21	A	826	CLA	C1D-C2D	-2.45	1.40	1.45
21	F	304	CLA	C1D-C2D	-2.45	1.40	1.45
21	5	617	CLA	C1D-C2D	-2.45	1.40	1.45
30	8	606	CHL	CHC-C4B	-2.44	1.35	1.39
21	B	806	CLA	C1D-C2D	-2.44	1.40	1.45
21	Z	612	CLA	C1D-C2D	-2.44	1.40	1.45
20	A	801	CL0	CHB-C4A	-2.44	1.35	1.38
21	B	823	CLA	C1D-C2D	-2.44	1.40	1.45
30	5	606	CHL	CHC-C4B	-2.44	1.35	1.39
21	B	804	CLA	C1D-C2D	-2.44	1.40	1.45
21	7	620	CLA	C1D-C2D	-2.44	1.40	1.45
21	B	820	CLA	C1D-C2D	-2.43	1.40	1.45
30	4	606	CHL	CHC-C4B	-2.43	1.35	1.39
21	A	821	CLA	C1D-C2D	-2.43	1.40	1.45
21	B	809	CLA	C1D-C2D	-2.43	1.40	1.45
21	F	303	CLA	C1D-C2D	-2.43	1.40	1.45
21	1	614	CLA	C1D-C2D	-2.43	1.40	1.45
21	3	610	CLA	C1D-C2D	-2.43	1.40	1.45
21	B	825	CLA	C1D-C2D	-2.43	1.40	1.45
30	7	601	CHL	CHC-C4B	-2.43	1.35	1.39
21	A	845	CLA	C1D-C2D	-2.43	1.40	1.45
30	Z	601	CHL	CHC-C4B	-2.43	1.35	1.39
21	A	805	CLA	C1D-C2D	-2.42	1.40	1.45
21	A	832	CLA	C1D-C2D	-2.42	1.40	1.45
21	B	812	CLA	C1D-C2D	-2.42	1.40	1.45
21	4	613	CLA	C1D-C2D	-2.42	1.40	1.45
21	8	612	CLA	C1D-C2D	-2.42	1.40	1.45
21	A	827	CLA	C1D-C2D	-2.42	1.40	1.45
30	6	607	CHL	CHC-C4B	-2.42	1.35	1.39
21	8	604	CLA	C1D-C2D	-2.42	1.40	1.45
30	Z	601	CHL	CHB-C1B	-2.42	1.35	1.39
21	B	832	CLA	C1D-C2D	-2.42	1.40	1.45
21	A	808	CLA	C1D-C2D	-2.42	1.40	1.45
21	A	813	CLA	C1D-C2D	-2.41	1.40	1.45
21	A	818	CLA	C1D-C2D	-2.41	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Z	603	CLA	C1D-C2D	-2.41	1.40	1.45
21	6	614	CLA	C1D-C2D	-2.41	1.40	1.45
21	B	807	CLA	C1D-C2D	-2.41	1.40	1.45
21	6	611	CLA	C1D-C2D	-2.41	1.40	1.45
21	B	811	CLA	C1D-C2D	-2.41	1.40	1.45
21	3	617	CLA	C1D-C2D	-2.40	1.40	1.45
30	6	618	CHL	CHB-C1B	-2.40	1.35	1.39
21	1	613	CLA	C1D-C2D	-2.40	1.40	1.45
21	B	805	CLA	C1D-C2D	-2.40	1.40	1.45
21	A	824	CLA	C1D-C2D	-2.40	1.40	1.45
21	7	602	CLA	C1D-C2D	-2.40	1.40	1.45
21	B	810	CLA	C1D-C2D	-2.40	1.40	1.45
21	B	830	CLA	C1D-C2D	-2.40	1.40	1.45
21	7	614	CLA	C1D-C2D	-2.40	1.40	1.45
21	B	827	CLA	C1D-C2D	-2.40	1.40	1.45
21	B	835	CLA	C1D-C2D	-2.40	1.40	1.45
21	8	608	CLA	C1D-C2D	-2.40	1.40	1.45
21	6	617	CLA	C1D-C2D	-2.40	1.40	1.45
21	A	836	CLA	C1D-C2D	-2.40	1.40	1.45
21	8	603	CLA	C1D-C2D	-2.39	1.40	1.45
21	8	610	CLA	C1D-C2D	-2.39	1.40	1.45
21	1	609	CLA	C1D-C2D	-2.39	1.40	1.45
21	B	829	CLA	C1D-C2D	-2.39	1.40	1.45
21	A	831	CLA	C1D-C2D	-2.39	1.40	1.45
21	7	612	CLA	C1D-C2D	-2.39	1.40	1.45
21	A	812	CLA	C1D-C2D	-2.39	1.40	1.45
21	K	204	CLA	C1D-C2D	-2.39	1.40	1.45
21	B	818	CLA	C1D-C2D	-2.39	1.40	1.45
21	7	613	CLA	C1D-C2D	-2.39	1.40	1.45
21	1	611	CLA	C1D-C2D	-2.39	1.40	1.45
21	3	603	CLA	C1D-C2D	-2.39	1.40	1.45
21	8	602	CLA	C1D-C2D	-2.39	1.40	1.45
30	6	608	CHL	CHB-C1B	-2.39	1.35	1.39
21	7	616	CLA	C1D-C2D	-2.39	1.40	1.45
30	4	606	CHL	CHB-C1B	-2.39	1.35	1.39
21	8	609	CLA	C1D-C2D	-2.39	1.40	1.45
21	Z	613	CLA	C1D-C2D	-2.39	1.40	1.45
21	5	604	CLA	C1D-C2D	-2.39	1.40	1.45
30	8	607	CHL	CHB-C1B	-2.38	1.35	1.39
21	5	616	CLA	C1D-C2D	-2.38	1.40	1.45
21	6	602	CLA	C1D-C2D	-2.38	1.40	1.45
21	B	840	CLA	C1D-C2D	-2.38	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	Z	606	CHL	CHC-C4B	-2.38	1.35	1.39
21	G	203	CLA	C1D-C2D	-2.38	1.40	1.45
21	1	610	CLA	C1D-C2D	-2.38	1.40	1.45
30	3	608	CHL	CHC-C4B	-2.38	1.35	1.39
21	B	834	CLA	C1D-C2D	-2.38	1.40	1.45
21	A	815	CLA	C1D-C2D	-2.38	1.40	1.45
21	3	615	CLA	C1D-C2D	-2.38	1.40	1.45
21	8	616	CLA	C1D-C2D	-2.38	1.40	1.45
21	5	611	CLA	C1D-C2D	-2.38	1.40	1.45
21	6	603	CLA	C1D-C2D	-2.38	1.40	1.45
30	1	606	CHL	CHB-C1B	-2.38	1.35	1.39
30	6	608	CHL	CHC-C4B	-2.38	1.35	1.39
21	3	612	CLA	C1D-C2D	-2.38	1.40	1.45
30	8	601	CHL	CHB-C1B	-2.38	1.35	1.39
21	3	609	CLA	C1D-C2D	-2.38	1.40	1.45
30	1	606	CHL	CHC-C4B	-2.38	1.35	1.39
21	6	612	CLA	C1D-C2D	-2.37	1.40	1.45
30	5	607	CHL	CHB-C1B	-2.37	1.35	1.39
21	A	833	CLA	C1D-C2D	-2.37	1.40	1.45
30	5	607	CHL	CHC-C4B	-2.37	1.35	1.39
21	4	614	CLA	C1D-C2D	-2.37	1.40	1.45
21	Z	610	CLA	C1D-C2D	-2.37	1.40	1.45
30	1	607	CHL	CHC-C4B	-2.37	1.35	1.39
21	7	610	CLA	C1D-C2D	-2.37	1.40	1.45
21	4	612	CLA	C1D-C2D	-2.37	1.40	1.45
21	A	837	CLA	C1D-C2D	-2.37	1.40	1.45
21	5	602	CLA	C1D-C2D	-2.37	1.40	1.45
30	7	607	CHL	CHC-C4B	-2.37	1.35	1.39
21	A	810	CLA	C1D-C2D	-2.37	1.40	1.45
21	A	843	CLA	C1D-C2D	-2.36	1.40	1.45
21	3	602	CLA	C1D-C2D	-2.36	1.40	1.45
21	6	610	CLA	C1D-C2D	-2.36	1.40	1.45
21	B	841	CLA	C1D-C2D	-2.36	1.40	1.45
21	A	828	CLA	C1D-C2D	-2.36	1.40	1.45
21	B	826	CLA	C1D-C2D	-2.36	1.40	1.45
21	Z	608	CLA	C1D-C2D	-2.36	1.40	1.45
21	B	817	CLA	C1D-C2D	-2.36	1.40	1.45
21	5	610	CLA	C1D-C2D	-2.36	1.40	1.45
21	B	837	CLA	C1D-C2D	-2.36	1.40	1.45
21	G	204	CLA	C1D-C2D	-2.36	1.40	1.45
21	7	608	CLA	C1D-C2D	-2.36	1.40	1.45
21	7	611	CLA	C1D-C2D	-2.36	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	609	CLA	C1D-C2D	-2.36	1.40	1.45
21	7	603	CLA	C1D-C2D	-2.36	1.40	1.45
21	K	206	CLA	C1D-C2D	-2.35	1.40	1.45
21	7	604	CLA	C1D-C2D	-2.35	1.40	1.45
21	A	830	CLA	C1D-C2D	-2.35	1.40	1.45
21	1	603	CLA	C1D-C2D	-2.35	1.40	1.45
21	Z	611	CLA	C1D-C2D	-2.35	1.40	1.45
21	5	613	CLA	C1D-C2D	-2.35	1.40	1.45
21	A	825	CLA	C1D-C2D	-2.35	1.40	1.45
21	Z	609	CLA	C1D-C2D	-2.35	1.40	1.45
21	B	814	CLA	C1D-C2D	-2.35	1.40	1.45
21	B	822	CLA	C1D-C2D	-2.35	1.40	1.45
21	8	613	CLA	C1D-C2D	-2.35	1.40	1.45
30	5	608	CHL	CHB-C1B	-2.35	1.35	1.39
21	A	819	CLA	C1D-C2D	-2.35	1.40	1.45
21	3	606	CLA	C1D-C2D	-2.35	1.40	1.45
21	3	607	CLA	C1D-C2D	-2.35	1.40	1.45
21	B	839	CLA	C1D-C2D	-2.35	1.40	1.45
21	6	613	CLA	C1D-C2D	-2.35	1.40	1.45
30	4	618	CHL	CHB-C1B	-2.35	1.35	1.39
21	A	841	CLA	C1D-C2D	-2.34	1.40	1.45
21	A	816	CLA	C1D-C2D	-2.34	1.40	1.45
21	J	101	CLA	C1D-C2D	-2.34	1.40	1.45
21	1	602	CLA	C1D-C2D	-2.34	1.40	1.45
21	K	203	CLA	C1D-C2D	-2.34	1.40	1.45
21	4	611	CLA	C1D-C2D	-2.34	1.40	1.45
21	B	821	CLA	C1D-C2D	-2.34	1.40	1.45
21	A	803	CLA	C1D-C2D	-2.34	1.40	1.45
21	Z	616	CLA	C1D-C2D	-2.34	1.40	1.45
21	3	614	CLA	C1D-C2D	-2.34	1.40	1.45
21	5	609	CLA	C1D-C2D	-2.34	1.40	1.45
21	9	603	CLA	C1D-C2D	-2.34	1.40	1.45
21	9	602	CLA	C1D-C2D	-2.34	1.40	1.45
30	8	601	CHL	CHC-C4B	-2.33	1.35	1.39
21	6	604	CLA	C1D-C2D	-2.33	1.40	1.45
21	9	612	CLA	C1D-C2D	-2.33	1.40	1.45
21	B	803	CLA	C1D-C2D	-2.33	1.40	1.45
21	1	608	CLA	C1D-C2D	-2.33	1.40	1.45
21	B	836	CLA	C1D-C2D	-2.33	1.40	1.45
21	3	611	CLA	C1D-C2D	-2.33	1.40	1.45
21	4	616	CLA	C1D-C2D	-2.33	1.40	1.45
21	B	831	CLA	C1D-C2D	-2.33	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	602	CLA	C1D-C2D	-2.33	1.40	1.45
21	4	604	CLA	C1D-C2D	-2.33	1.40	1.45
21	L	203	CLA	C1D-C2D	-2.33	1.40	1.45
21	5	614	CLA	C1D-C2D	-2.33	1.40	1.45
21	3	604	CLA	C1D-C2D	-2.33	1.40	1.45
21	6	622	CLA	C1D-C2D	-2.32	1.40	1.45
30	5	618	CHL	CHB-C1B	-2.32	1.35	1.39
21	1	616	CLA	C1D-C2D	-2.32	1.40	1.45
21	A	839	CLA	C1D-C2D	-2.32	1.40	1.45
21	A	854	CLA	C1D-C2D	-2.32	1.40	1.45
21	Z	614	CLA	C1D-C2D	-2.32	1.40	1.45
30	5	606	CHL	CHB-C1B	-2.32	1.35	1.39
30	7	606	CHL	CHB-C1B	-2.31	1.35	1.39
21	8	611	CLA	C1D-C2D	-2.31	1.40	1.45
21	Z	602	CLA	C1D-C2D	-2.31	1.40	1.45
30	6	606	CHL	CHB-C1B	-2.31	1.35	1.39
21	L	204	CLA	C1D-C2D	-2.31	1.40	1.45
21	5	603	CLA	C1D-C2D	-2.31	1.40	1.45
21	A	842	CLA	C1D-C2D	-2.31	1.40	1.45
30	6	616	CHL	CHB-C1B	-2.30	1.35	1.39
30	4	608	CHL	CHB-C1B	-2.30	1.35	1.39
21	9	613	CLA	C1D-C2D	-2.30	1.40	1.45
30	8	606	CHL	CHB-C1B	-2.30	1.35	1.39
30	7	607	CHL	CHB-C1B	-2.30	1.35	1.39
21	9	609	CLA	C1D-C2D	-2.30	1.40	1.45
21	4	610	CLA	C1D-C2D	-2.30	1.40	1.45
21	9	614	CLA	C1D-C2D	-2.30	1.40	1.45
21	A	822	CLA	C1D-C2D	-2.29	1.40	1.45
21	A	823	CLA	C1D-C2D	-2.29	1.40	1.45
30	6	616	CHL	CHC-C4B	-2.29	1.35	1.39
21	9	604	CLA	C1D-C2D	-2.29	1.40	1.45
30	Z	606	CHL	CHB-C1B	-2.29	1.35	1.39
21	9	601	CLA	C1D-C2D	-2.28	1.40	1.45
30	6	601	CHL	CHB-C1B	-2.28	1.35	1.39
21	B	819	CLA	C1D-C2D	-2.28	1.40	1.45
30	9	607	CHL	CHC-C4B	-2.28	1.35	1.39
21	7	609	CLA	C1D-C2D	-2.28	1.40	1.45
21	A	811	CLA	C1D-C2D	-2.27	1.40	1.45
21	A	820	CLA	C1D-C2D	-2.27	1.40	1.45
21	A	806	CLA	C1D-C2D	-2.27	1.40	1.45
21	1	604	CLA	C1D-C2D	-2.27	1.40	1.45
21	B	828	CLA	C1D-C2D	-2.27	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	9	606	CHL	CHB-C1B	-2.26	1.36	1.39
30	Z	607	CHL	CHB-C1B	-2.26	1.36	1.39
21	Z	604	CLA	C1D-C2D	-2.26	1.40	1.45
21	9	610	CLA	C1D-C2D	-2.25	1.40	1.45
30	1	607	CHL	CHB-C1B	-2.24	1.36	1.39
21	9	611	CLA	C1D-C2D	-2.24	1.40	1.45
30	9	606	CHL	CHC-C4B	-2.24	1.36	1.39
30	9	607	CHL	CHB-C1B	-2.24	1.36	1.39
21	B	833	CLA	C1D-C2D	-2.23	1.40	1.45
30	4	601	CHL	CHC-C4B	-2.23	1.36	1.39
30	1	601	CHL	CHB-C1B	-2.22	1.36	1.39
21	B	833	CLA	C3D-C4D	-2.21	1.39	1.44
30	3	608	CHL	CHB-C1B	-2.21	1.36	1.39
20	A	801	CL0	CHD-C4C	-2.17	1.35	1.39
30	4	607	CHL	CHB-C1B	-2.16	1.36	1.39
21	A	854	CLA	C3D-C4D	-2.16	1.39	1.44
21	A	822	CLA	C3D-C4D	-2.15	1.39	1.44
21	7	603	CLA	C3D-C4D	-2.15	1.39	1.44
21	A	814	CLA	C3D-C4D	-2.14	1.39	1.44
21	1	613	CLA	C3D-C4D	-2.14	1.39	1.44
21	A	843	CLA	C3D-C4D	-2.14	1.39	1.44
30	7	601	CHL	CHB-C1B	-2.13	1.36	1.39
21	A	813	CLA	C3D-C4D	-2.12	1.39	1.44
21	A	827	CLA	C3D-C4D	-2.12	1.39	1.44
21	7	610	CLA	C3D-C4D	-2.12	1.39	1.44
21	8	603	CLA	C3D-C4D	-2.11	1.39	1.44
21	6	610	CLA	C3D-C4D	-2.10	1.39	1.44
30	4	601	CHL	CHB-C1B	-2.10	1.36	1.39
21	5	609	CLA	C3D-C4D	-2.10	1.39	1.44
21	A	811	CLA	C3D-C4D	-2.09	1.39	1.44
21	A	815	CLA	C3D-C4D	-2.08	1.39	1.44
21	3	613	CLA	C3D-C4D	-2.08	1.39	1.44
21	8	610	CLA	C3D-C4D	-2.08	1.39	1.44
21	B	817	CLA	C3D-C4D	-2.07	1.39	1.44
21	4	603	CLA	C3D-C4D	-2.07	1.39	1.44
21	A	807	CLA	C3D-C4D	-2.07	1.39	1.44
21	B	823	CLA	C3D-C4D	-2.07	1.39	1.44
21	B	832	CLA	C3D-C4D	-2.07	1.39	1.44
21	B	822	CLA	C3D-C4D	-2.07	1.39	1.44
21	6	609	CLA	C3D-C4D	-2.07	1.39	1.44
21	A	841	CLA	C3D-C4D	-2.07	1.39	1.44
21	7	613	CLA	C3D-C4D	-2.07	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	8	609	CLA	C3D-C4D	-2.07	1.39	1.44
21	A	823	CLA	C3D-C4D	-2.06	1.39	1.44
21	8	608	CLA	C3D-C4D	-2.06	1.39	1.44
21	7	614	CLA	C3D-C4D	-2.06	1.39	1.44
21	7	602	CLA	C3D-C4D	-2.06	1.39	1.44
21	1	602	CLA	C3D-C4D	-2.06	1.39	1.44
21	Z	616	CLA	C3D-C4D	-2.06	1.39	1.44
21	1	603	CLA	C3D-C4D	-2.05	1.39	1.44
21	A	816	CLA	C3D-C4D	-2.05	1.39	1.44
21	7	616	CLA	C3D-C4D	-2.05	1.39	1.44
21	7	608	CLA	C3D-C4D	-2.05	1.39	1.44
21	A	825	CLA	C3D-C4D	-2.05	1.39	1.44
21	A	810	CLA	C3D-C4D	-2.05	1.39	1.44
21	A	821	CLA	C3D-C4D	-2.05	1.39	1.44
21	1	616	CLA	C3D-C4D	-2.05	1.39	1.44
21	8	616	CLA	C3D-C4D	-2.05	1.39	1.44
21	B	836	CLA	C3D-C4D	-2.05	1.39	1.44
21	1	610	CLA	C3D-C4D	-2.05	1.39	1.44
21	3	609	CLA	C3D-C4D	-2.05	1.39	1.44
21	Z	609	CLA	C3D-C4D	-2.05	1.39	1.44
21	B	825	CLA	C3D-C4D	-2.05	1.39	1.44
21	3	607	CLA	C3D-C4D	-2.05	1.39	1.44
21	A	819	CLA	C3D-C4D	-2.05	1.39	1.44
21	A	833	CLA	C3D-C4D	-2.04	1.39	1.44
21	Z	603	CLA	C3D-C4D	-2.04	1.39	1.44
21	A	842	CLA	C3D-C4D	-2.04	1.39	1.44
21	B	826	CLA	C3D-C4D	-2.04	1.39	1.44
21	8	602	CLA	C3D-C4D	-2.04	1.39	1.44
21	B	810	CLA	C3D-C4D	-2.04	1.39	1.44
21	A	817	CLA	C3D-C4D	-2.04	1.39	1.44
21	8	611	CLA	C3D-C4D	-2.04	1.39	1.44
21	A	804	CLA	C3D-C4D	-2.04	1.39	1.44
21	1	614	CLA	C3D-C4D	-2.04	1.39	1.44
21	3	617	CLA	C3D-C4D	-2.04	1.39	1.44
21	7	609	CLA	C3D-C4D	-2.04	1.39	1.44
21	8	604	CLA	C3D-C4D	-2.04	1.39	1.44
21	3	610	CLA	C3D-C4D	-2.04	1.39	1.44
20	A	801	CL0	C1B-C2B	2.04	1.41	1.39
21	A	840	CLA	C3D-C4D	-2.04	1.39	1.44
21	3	612	CLA	C3D-C4D	-2.04	1.39	1.44
21	5	602	CLA	C3D-C4D	-2.03	1.39	1.44
21	B	808	CLA	C3D-C4D	-2.03	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	821	CLA	C3D-C4D	-2.03	1.39	1.44
21	B	827	CLA	C3D-C4D	-2.03	1.39	1.44
21	6	603	CLA	C3D-C4D	-2.03	1.39	1.44
21	A	820	CLA	C3D-C4D	-2.03	1.39	1.44
21	A	834	CLA	C3D-C4D	-2.03	1.39	1.44
21	F	303	CLA	C3D-C4D	-2.03	1.39	1.44
21	A	818	CLA	C3D-C4D	-2.03	1.39	1.44
21	B	831	CLA	C3D-C4D	-2.03	1.39	1.44
21	Z	602	CLA	C3D-C4D	-2.03	1.39	1.44
21	A	808	CLA	C3D-C4D	-2.03	1.39	1.44
21	B	840	CLA	C3D-C4D	-2.03	1.39	1.44
21	K	204	CLA	C3D-C4D	-2.03	1.39	1.44
21	7	612	CLA	C3D-C4D	-2.03	1.39	1.44
21	B	834	CLA	C3D-C4D	-2.03	1.39	1.44
21	A	832	CLA	C3D-C4D	-2.02	1.39	1.44
21	A	839	CLA	C3D-C4D	-2.02	1.39	1.44
21	A	806	CLA	C3D-C4D	-2.02	1.39	1.44
21	B	837	CLA	C3D-C4D	-2.02	1.39	1.44
21	3	606	CLA	C3D-C4D	-2.02	1.39	1.44
21	4	602	CLA	C3D-C4D	-2.02	1.39	1.44
21	8	613	CLA	C3D-C4D	-2.02	1.39	1.44
21	3	603	CLA	C3D-C4D	-2.02	1.39	1.44
21	3	604	CLA	C3D-C4D	-2.02	1.39	1.44
21	7	611	CLA	C3D-C4D	-2.02	1.39	1.44
21	Z	611	CLA	C3D-C4D	-2.02	1.39	1.44
21	B	819	CLA	C3D-C4D	-2.02	1.39	1.44
21	4	604	CLA	C3D-C4D	-2.02	1.39	1.44
21	5	603	CLA	C3D-C4D	-2.02	1.39	1.44
21	A	828	CLA	C3D-C4D	-2.02	1.39	1.44
21	F	301	CLA	C3D-C4D	-2.02	1.39	1.44
21	5	617	CLA	C3D-C4D	-2.02	1.39	1.44
21	7	604	CLA	C3D-C4D	-2.02	1.39	1.44
21	B	802	CLA	C3D-C4D	-2.02	1.39	1.44
21	6	613	CLA	C3D-C4D	-2.02	1.39	1.44
21	F	304	CLA	C3D-C4D	-2.02	1.39	1.44
21	B	811	CLA	C3D-C4D	-2.02	1.39	1.44
21	B	816	CLA	C3D-C4D	-2.02	1.39	1.44
21	6	604	CLA	C3D-C4D	-2.02	1.39	1.44
21	B	812	CLA	C3D-C4D	-2.02	1.39	1.44
21	6	617	CLA	C3D-C4D	-2.01	1.39	1.44
21	A	802	CLA	C3D-C4D	-2.01	1.39	1.44
21	4	610	CLA	C3D-C4D	-2.01	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	615	CLA	C3D-C4D	-2.01	1.39	1.44
21	Z	604	CLA	C3D-C4D	-2.01	1.39	1.44
21	Z	610	CLA	C3D-C4D	-2.01	1.39	1.44
21	A	824	CLA	C3D-C4D	-2.01	1.39	1.44
21	1	608	CLA	C3D-C4D	-2.01	1.39	1.44
21	4	611	CLA	C3D-C4D	-2.01	1.39	1.44
21	3	602	CLA	C3D-C4D	-2.01	1.39	1.44
21	B	841	CLA	C3D-C4D	-2.01	1.39	1.44
21	1	611	CLA	C3D-C4D	-2.01	1.39	1.44
21	Z	613	CLA	C3D-C4D	-2.00	1.39	1.44
21	B	804	CLA	C3D-C4D	-2.00	1.39	1.44
21	A	837	CLA	C3D-C4D	-2.00	1.39	1.44
21	B	828	CLA	C3D-C4D	-2.00	1.39	1.44
21	B	820	CLA	C3D-C4D	-2.00	1.39	1.44
21	7	620	CLA	C3D-C4D	-2.00	1.39	1.44
21	4	616	CLA	C3D-C4D	-2.00	1.39	1.44

All (658) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	801	CL0	C1B-CHB-C4A	9.47	127.42	121.32
32	5	625	NEX	C5-C6-C1	7.53	127.16	119.70
30	3	608	CHL	C1B-CHB-C4A	4.95	124.51	121.32
30	8	607	CHL	C1B-CHB-C4A	4.93	124.49	121.32
30	8	601	CHL	C1B-CHB-C4A	4.86	124.45	121.32
30	7	606	CHL	C1B-CHB-C4A	4.86	124.45	121.32
30	6	601	CHL	C1B-CHB-C4A	4.85	124.44	121.32
30	8	606	CHL	C1B-CHB-C4A	4.83	124.43	121.32
30	Z	601	CHL	C1B-CHB-C4A	4.70	124.35	121.32
30	6	618	CHL	C1B-CHB-C4A	4.53	124.24	121.32
30	6	616	CHL	C1B-CHB-C4A	4.51	124.22	121.32
30	5	608	CHL	C1B-CHB-C4A	4.45	124.19	121.32
30	4	608	CHL	C1B-CHB-C4A	4.45	124.18	121.32
30	1	601	CHL	C1B-CHB-C4A	4.43	124.17	121.32
30	5	606	CHL	C1B-CHB-C4A	4.40	124.15	121.32
30	5	618	CHL	C1B-CHB-C4A	4.39	124.15	121.32
32	6	625	NEX	C5-C6-C1	4.36	124.03	119.70
21	9	609	CLA	C1D-ND-C4D	-4.32	103.28	106.31
21	Z	613	CLA	C1D-ND-C4D	-4.31	103.29	106.31
21	B	831	CLA	C1D-ND-C4D	-4.30	103.30	106.31
21	9	604	CLA	C1D-ND-C4D	-4.29	103.30	106.31
30	Z	606	CHL	C1B-CHB-C4A	4.29	124.08	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	7	612	CLA	C1D-ND-C4D	-4.28	103.31	106.31
30	6	606	CHL	C1B-CHB-C4A	4.28	124.07	121.32
30	6	608	CHL	C1B-CHB-C4A	4.27	124.07	121.32
30	9	607	CHL	C1B-CHB-C4A	4.27	124.07	121.32
21	3	612	CLA	C1D-ND-C4D	-4.27	103.31	106.31
21	A	811	CLA	C1D-ND-C4D	-4.27	103.32	106.31
21	Z	612	CLA	C1D-ND-C4D	-4.26	103.33	106.31
21	9	603	CLA	C1D-ND-C4D	-4.25	103.33	106.31
21	B	833	CLA	C1D-ND-C4D	-4.25	103.33	106.31
21	1	610	CLA	C1D-ND-C4D	-4.25	103.33	106.31
21	9	610	CLA	C1D-ND-C4D	-4.24	103.33	106.31
21	Z	609	CLA	C1D-ND-C4D	-4.24	103.33	106.31
21	4	604	CLA	C1D-ND-C4D	-4.24	103.33	106.31
21	K	204	CLA	C1D-ND-C4D	-4.24	103.34	106.31
21	3	614	CLA	C1D-ND-C4D	-4.24	103.34	106.31
21	5	603	CLA	C1D-ND-C4D	-4.24	103.34	106.31
21	1	613	CLA	C1D-ND-C4D	-4.23	103.34	106.31
21	9	602	CLA	C1D-ND-C4D	-4.23	103.34	106.31
21	8	612	CLA	C1D-ND-C4D	-4.23	103.34	106.31
30	4	601	CHL	C1B-CHB-C4A	4.23	124.04	121.32
30	1	606	CHL	C1B-CHB-C4A	4.22	124.04	121.32
21	6	617	CLA	C1D-ND-C4D	-4.22	103.35	106.31
21	Z	611	CLA	C1D-ND-C4D	-4.22	103.35	106.31
21	1	612	CLA	C1D-ND-C4D	-4.21	103.36	106.31
21	4	611	CLA	C1D-ND-C4D	-4.20	103.36	106.31
21	B	814	CLA	C1D-ND-C4D	-4.20	103.37	106.31
21	L	203	CLA	C1D-ND-C4D	-4.20	103.37	106.31
21	6	612	CLA	C1D-ND-C4D	-4.19	103.37	106.31
21	A	822	CLA	C1D-ND-C4D	-4.19	103.37	106.31
21	4	602	CLA	C1D-ND-C4D	-4.19	103.37	106.31
30	4	618	CHL	C1B-CHB-C4A	4.19	124.02	121.32
30	4	606	CHL	C1B-CHB-C4A	4.18	124.01	121.32
21	F	304	CLA	C1D-ND-C4D	-4.18	103.38	106.31
21	9	614	CLA	C1D-ND-C4D	-4.18	103.38	106.31
21	B	822	CLA	C1D-ND-C4D	-4.18	103.38	106.31
21	9	601	CLA	C1D-ND-C4D	-4.18	103.38	106.31
21	6	614	CLA	C1D-ND-C4D	-4.18	103.38	106.31
21	B	817	CLA	C1D-ND-C4D	-4.17	103.38	106.31
21	Z	604	CLA	C1D-ND-C4D	-4.17	103.39	106.31
21	1	602	CLA	C1D-ND-C4D	-4.17	103.39	106.31
21	B	808	CLA	C1D-ND-C4D	-4.16	103.39	106.31
21	1	604	CLA	C1D-ND-C4D	-4.16	103.39	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	616	CLA	C1D-ND-C4D	-4.15	103.40	106.31
21	4	610	CLA	C1D-ND-C4D	-4.15	103.40	106.31
21	5	602	CLA	C1D-ND-C4D	-4.15	103.40	106.31
21	5	614	CLA	C1D-ND-C4D	-4.15	103.40	106.31
21	5	613	CLA	C1D-ND-C4D	-4.14	103.41	106.31
21	Z	614	CLA	C1D-ND-C4D	-4.14	103.41	106.31
21	B	816	CLA	C1D-ND-C4D	-4.14	103.41	106.31
21	9	613	CLA	C1D-ND-C4D	-4.13	103.41	106.31
21	6	602	CLA	C1D-ND-C4D	-4.13	103.42	106.31
21	B	811	CLA	C1D-ND-C4D	-4.12	103.42	106.31
21	B	832	CLA	C1D-ND-C4D	-4.12	103.42	106.31
21	8	603	CLA	C1D-ND-C4D	-4.12	103.42	106.31
21	1	614	CLA	C1D-ND-C4D	-4.12	103.42	106.31
21	A	818	CLA	C1D-ND-C4D	-4.12	103.42	106.31
21	7	603	CLA	C1D-ND-C4D	-4.11	103.42	106.31
21	7	616	CLA	C1D-ND-C4D	-4.11	103.42	106.31
21	4	603	CLA	C1D-ND-C4D	-4.11	103.42	106.31
21	K	206	CLA	C1D-ND-C4D	-4.11	103.43	106.31
21	3	602	CLA	C1D-ND-C4D	-4.11	103.43	106.31
21	B	810	CLA	C1D-ND-C4D	-4.11	103.43	106.31
21	4	612	CLA	C1D-ND-C4D	-4.11	103.43	106.31
21	9	612	CLA	C1D-ND-C4D	-4.11	103.43	106.31
21	A	817	CLA	C1D-ND-C4D	-4.11	103.43	106.31
21	4	614	CLA	C1D-ND-C4D	-4.10	103.43	106.31
21	3	607	CLA	C1D-ND-C4D	-4.10	103.43	106.31
21	G	203	CLA	C1D-ND-C4D	-4.10	103.44	106.31
21	G	204	CLA	C1D-ND-C4D	-4.10	103.44	106.31
21	7	609	CLA	C1D-ND-C4D	-4.09	103.44	106.31
21	7	610	CLA	C1D-ND-C4D	-4.09	103.44	106.31
21	9	611	CLA	C1D-ND-C4D	-4.09	103.44	106.31
21	A	816	CLA	C1D-ND-C4D	-4.09	103.44	106.31
21	3	609	CLA	C1D-ND-C4D	-4.09	103.44	106.31
21	7	620	CLA	C1D-ND-C4D	-4.09	103.44	106.31
21	A	839	CLA	C1D-ND-C4D	-4.09	103.44	106.31
21	5	617	CLA	C1D-ND-C4D	-4.08	103.45	106.31
21	7	604	CLA	C1D-ND-C4D	-4.08	103.45	106.31
21	Z	610	CLA	C1D-ND-C4D	-4.08	103.45	106.31
21	6	604	CLA	C1D-ND-C4D	-4.07	103.45	106.31
21	6	611	CLA	C1D-ND-C4D	-4.07	103.45	106.31
21	1	611	CLA	C1D-ND-C4D	-4.07	103.45	106.31
21	3	604	CLA	C1D-ND-C4D	-4.07	103.46	106.31
21	1	608	CLA	C1D-ND-C4D	-4.07	103.46	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	845	CLA	C1D-ND-C4D	-4.07	103.46	106.31
21	J	101	CLA	C1D-ND-C4D	-4.07	103.46	106.31
21	5	609	CLA	C1D-ND-C4D	-4.07	103.46	106.31
21	6	613	CLA	C1D-ND-C4D	-4.07	103.46	106.31
21	1	603	CLA	C1D-ND-C4D	-4.06	103.46	106.31
21	Z	602	CLA	C1D-ND-C4D	-4.06	103.46	106.31
21	5	612	CLA	C1D-ND-C4D	-4.06	103.46	106.31
30	6	607	CHL	C1B-CHB-C4A	4.06	123.94	121.32
21	B	815	CLA	C1D-ND-C4D	-4.06	103.46	106.31
21	B	828	CLA	C1D-ND-C4D	-4.06	103.47	106.31
21	8	613	CLA	C1D-ND-C4D	-4.06	103.47	106.31
21	L	204	CLA	C1D-ND-C4D	-4.05	103.47	106.31
21	Z	616	CLA	C1D-ND-C4D	-4.05	103.47	106.31
21	B	819	CLA	C1D-ND-C4D	-4.05	103.47	106.31
21	A	815	CLA	C1D-ND-C4D	-4.05	103.47	106.31
21	B	804	CLA	C1D-ND-C4D	-4.05	103.47	106.31
21	A	823	CLA	C1D-ND-C4D	-4.04	103.47	106.31
21	6	610	CLA	C1D-ND-C4D	-4.04	103.48	106.31
21	A	820	CLA	C1D-ND-C4D	-4.03	103.48	106.31
21	A	842	CLA	C1D-ND-C4D	-4.02	103.49	106.31
21	6	603	CLA	C1D-ND-C4D	-4.02	103.49	106.31
21	7	614	CLA	C1D-ND-C4D	-4.02	103.49	106.31
21	6	609	CLA	C1D-ND-C4D	-4.02	103.49	106.31
21	A	835	CLA	C1D-ND-C4D	-4.01	103.50	106.31
21	A	840	CLA	C1D-ND-C4D	-4.01	103.50	106.31
21	Z	608	CLA	C1D-ND-C4D	-4.01	103.50	106.31
30	7	607	CHL	C1B-CHB-C4A	4.00	123.90	121.32
21	K	203	CLA	C1D-ND-C4D	-3.99	103.52	106.31
30	7	601	CHL	C1B-CHB-C4A	3.99	123.89	121.32
21	F	303	CLA	C1D-ND-C4D	-3.98	103.52	106.31
21	B	820	CLA	C1D-ND-C4D	-3.98	103.52	106.31
21	B	826	CLA	C1D-ND-C4D	-3.98	103.52	106.31
21	7	613	CLA	C1D-ND-C4D	-3.98	103.52	106.31
21	Z	603	CLA	C1D-ND-C4D	-3.98	103.52	106.31
21	3	611	CLA	C1D-ND-C4D	-3.97	103.52	106.31
21	B	813	CLA	C1D-ND-C4D	-3.97	103.53	106.31
21	A	806	CLA	C1D-ND-C4D	-3.97	103.53	106.31
21	8	616	CLA	C1D-ND-C4D	-3.96	103.53	106.31
21	B	805	CLA	C1D-ND-C4D	-3.96	103.53	106.31
21	3	606	CLA	C1D-ND-C4D	-3.96	103.53	106.31
21	5	611	CLA	C1D-ND-C4D	-3.96	103.53	106.31
21	A	843	CLA	C1D-ND-C4D	-3.96	103.53	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	8	611	CLA	C1D-ND-C4D	-3.96	103.53	106.31
21	B	807	CLA	C1D-ND-C4D	-3.96	103.54	106.31
21	B	827	CLA	C1D-ND-C4D	-3.95	103.54	106.31
30	4	607	CHL	C1B-CHB-C4A	3.95	123.86	121.32
21	3	615	CLA	C1D-ND-C4D	-3.95	103.54	106.31
21	A	813	CLA	C1D-ND-C4D	-3.95	103.54	106.31
21	A	854	CLA	C1D-ND-C4D	-3.95	103.54	106.31
21	B	836	CLA	C1D-ND-C4D	-3.95	103.54	106.31
21	1	616	CLA	C1D-ND-C4D	-3.94	103.55	106.31
21	8	614	CLA	C1D-ND-C4D	-3.94	103.55	106.31
21	8	604	CLA	C1D-ND-C4D	-3.93	103.55	106.31
21	8	609	CLA	C1D-ND-C4D	-3.92	103.56	106.31
21	B	821	CLA	C1D-ND-C4D	-3.92	103.56	106.31
21	5	616	CLA	C1D-ND-C4D	-3.92	103.56	106.31
21	7	611	CLA	C1D-ND-C4D	-3.91	103.57	106.31
21	A	831	CLA	C1D-ND-C4D	-3.91	103.57	106.31
21	A	838	CLA	C1D-ND-C4D	-3.91	103.57	106.31
21	3	613	CLA	C1D-ND-C4D	-3.91	103.57	106.31
21	3	610	CLA	C1D-ND-C4D	-3.91	103.57	106.31
21	B	837	CLA	C1D-ND-C4D	-3.91	103.57	106.31
21	B	823	CLA	C1D-ND-C4D	-3.90	103.57	106.31
21	B	835	CLA	C1D-ND-C4D	-3.90	103.57	106.31
21	5	604	CLA	C1D-ND-C4D	-3.90	103.58	106.31
21	A	819	CLA	C1D-ND-C4D	-3.89	103.58	106.31
21	A	824	CLA	C1D-ND-C4D	-3.89	103.58	106.31
21	A	833	CLA	C1D-ND-C4D	-3.89	103.58	106.31
21	6	622	CLA	C1D-ND-C4D	-3.89	103.58	106.31
21	A	834	CLA	C1D-ND-C4D	-3.89	103.59	106.31
21	7	608	CLA	C1D-ND-C4D	-3.89	103.59	106.31
21	7	602	CLA	C1D-ND-C4D	-3.88	103.59	106.31
21	8	602	CLA	C1D-ND-C4D	-3.88	103.59	106.31
21	A	812	CLA	C1D-ND-C4D	-3.88	103.59	106.31
21	B	818	CLA	C1D-ND-C4D	-3.88	103.59	106.31
21	B	812	CLA	C1D-ND-C4D	-3.88	103.59	106.31
21	A	837	CLA	C1D-ND-C4D	-3.87	103.59	106.31
21	8	608	CLA	C1D-ND-C4D	-3.87	103.60	106.31
21	5	601	CLA	C1D-ND-C4D	-3.87	103.60	106.31
21	B	839	CLA	C1D-ND-C4D	-3.85	103.61	106.31
21	A	821	CLA	C1D-ND-C4D	-3.85	103.61	106.31
21	A	805	CLA	C1D-ND-C4D	-3.84	103.61	106.31
21	A	807	CLA	C1D-ND-C4D	-3.84	103.62	106.31
21	A	827	CLA	C1D-ND-C4D	-3.84	103.62	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	834	CLA	C1D-ND-C4D	-3.83	103.63	106.31
30	Z	607	CHL	C1B-CHB-C4A	3.83	123.78	121.32
21	A	825	CLA	C1D-ND-C4D	-3.83	103.63	106.31
21	1	609	CLA	C1D-ND-C4D	-3.82	103.63	106.31
21	F	301	CLA	C1D-ND-C4D	-3.81	103.64	106.31
21	A	830	CLA	C1D-ND-C4D	-3.81	103.64	106.31
21	A	804	CLA	C1D-ND-C4D	-3.80	103.65	106.31
21	A	803	CLA	C1D-ND-C4D	-3.80	103.65	106.31
21	B	830	CLA	C1D-ND-C4D	-3.80	103.65	106.31
21	4	613	CLA	C1D-ND-C4D	-3.79	103.65	106.31
30	5	607	CHL	C1B-CHB-C4A	3.79	123.76	121.32
21	B	806	CLA	C1D-ND-C4D	-3.79	103.66	106.31
21	B	840	CLA	C1D-ND-C4D	-3.78	103.66	106.31
21	5	610	CLA	C1D-ND-C4D	-3.78	103.66	106.31
32	5	625	NEX	C2-C1-C6	3.77	112.88	109.21
21	A	808	CLA	C1D-ND-C4D	-3.77	103.67	106.31
21	3	617	CLA	C1D-ND-C4D	-3.77	103.67	106.31
21	B	809	CLA	C1D-ND-C4D	-3.76	103.67	106.31
21	A	809	CLA	C1D-ND-C4D	-3.74	103.69	106.31
21	8	610	CLA	C1D-ND-C4D	-3.74	103.69	106.31
21	A	832	CLA	C1D-ND-C4D	-3.74	103.69	106.31
21	A	836	CLA	C1D-ND-C4D	-3.74	103.69	106.31
21	A	828	CLA	C1D-ND-C4D	-3.73	103.69	106.31
21	B	841	CLA	C1D-ND-C4D	-3.72	103.70	106.31
21	A	810	CLA	C1D-ND-C4D	-3.72	103.70	106.31
21	3	603	CLA	C1D-ND-C4D	-3.69	103.72	106.31
21	A	841	CLA	C1D-ND-C4D	-3.69	103.72	106.31
30	9	606	CHL	C1B-CHB-C4A	3.66	123.68	121.32
21	B	824	CLA	C1D-ND-C4D	-3.66	103.75	106.31
21	A	814	CLA	C1D-ND-C4D	-3.63	103.76	106.31
21	A	826	CLA	C1D-ND-C4D	-3.58	103.80	106.31
21	K	201	CLA	C1D-ND-C4D	-3.58	103.80	106.31
21	B	829	CLA	C1D-ND-C4D	-3.57	103.81	106.31
21	B	803	CLA	C1D-ND-C4D	-3.53	103.84	106.31
21	B	838	CLA	C1D-ND-C4D	-3.52	103.84	106.31
21	A	829	CLA	C1D-ND-C4D	-3.52	103.84	106.31
21	4	609	CLA	C1D-ND-C4D	-3.49	103.86	106.31
21	B	825	CLA	C1D-ND-C4D	-3.48	103.87	106.31
21	5	621	CLA	C1D-ND-C4D	-3.48	103.87	106.31
21	B	802	CLA	C1D-ND-C4D	-3.47	103.88	106.31
21	A	802	CLA	C1D-ND-C4D	-3.40	103.92	106.31
30	Z	606	CHL	CHA-C1A-C2A	-3.36	125.41	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	7	610	CLA	C1-C2-C3	-3.28	120.83	126.20
30	1	607	CHL	C1B-CHB-C4A	3.27	123.43	121.32
30	4	608	CHL	CHA-C1A-C2A	-3.24	125.71	133.31
30	6	606	CHL	CHA-C1A-C2A	-3.18	125.83	133.31
30	5	606	CHL	CHA-C1A-C2A	-3.17	125.87	133.31
30	7	606	CHL	CHA-C1A-C2A	-3.17	125.87	133.31
20	A	801	CL0	CHA-C1A-C2A	-3.16	125.88	133.31
30	Z	601	CHL	CHA-C1A-C2A	-3.16	125.88	133.31
30	4	606	CHL	CHA-C1A-C2A	-3.16	125.89	133.31
30	5	608	CHL	CHA-C1A-C2A	-3.14	125.93	133.31
30	6	608	CHL	CHA-C1A-C2A	-3.12	125.97	133.31
30	6	618	CHL	CHA-C1A-C2A	-3.12	125.98	133.31
30	6	601	CHL	CHA-C1A-C2A	-3.09	126.05	133.31
30	7	607	CHL	CHA-C1A-C2A	-3.07	126.10	133.31
30	6	616	CHL	CHA-C1A-C2A	-3.07	126.10	133.31
30	1	606	CHL	CHA-C1A-C2A	-3.06	126.12	133.31
30	9	607	CHL	CHA-C1A-C2A	-3.06	126.12	133.31
31	5	624	XAT	C7-C8-C9	3.05	130.26	125.53
30	8	606	CHL	CHA-C1A-C2A	-3.05	126.15	133.31
30	6	607	CHL	CHA-C1A-C2A	-3.04	126.17	133.31
30	3	608	CHL	CHA-C1A-C2A	-3.02	126.20	133.31
30	7	601	CHL	CHA-C1A-C2A	-3.00	126.27	133.31
21	A	834	CLA	C1-C2-C3	-2.99	121.30	126.20
30	5	618	CHL	CHA-C1A-C2A	-2.99	126.30	133.31
30	1	601	CHL	CHA-C1A-C2A	-2.98	126.31	133.31
30	8	601	CHL	CHA-C1A-C2A	-2.95	126.38	133.31
32	5	625	NEX	O24-C25-C24	-2.91	110.77	113.49
30	4	607	CHL	CHA-C1A-C2A	-2.91	126.48	133.31
30	5	607	CHL	CHA-C1A-C2A	-2.91	126.48	133.31
30	8	607	CHL	CHA-C1A-C2A	-2.87	126.58	133.31
30	7	601	CHL	C3D-C4D-CHA	2.81	112.81	108.54
21	B	803	CLA	CHD-C1D-ND	-2.81	120.85	124.80
30	8	607	CHL	C3D-C4D-CHA	2.80	112.79	108.54
20	A	801	CL0	C3D-C4D-CHA	2.80	112.79	108.54
30	4	618	CHL	CHA-C1A-C2A	-2.77	126.80	133.31
21	4	610	CLA	CHD-C1D-ND	-2.75	120.94	124.80
21	B	833	CLA	CHD-C1D-ND	-2.73	120.96	124.80
30	8	601	CHL	C3D-C4D-CHA	2.73	112.68	108.54
30	Z	607	CHL	C3D-C4D-CHA	2.72	112.67	108.54
21	A	811	CLA	CHD-C1D-ND	-2.72	120.98	124.80
21	A	806	CLA	CHD-C1D-ND	-2.71	120.99	124.80
30	4	618	CHL	C3D-C4D-CHA	2.70	112.65	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	7	607	CHL	C3D-C4D-CHA	2.69	112.63	108.54
30	6	618	CHL	C3D-C4D-CHA	2.69	112.62	108.54
30	1	601	CHL	C3D-C4D-CHA	2.68	112.62	108.54
30	1	607	CHL	C3D-C4D-CHA	2.68	112.61	108.54
30	4	601	CHL	C3D-C4D-CHA	2.68	112.61	108.54
30	9	606	CHL	C3D-C4D-CHA	2.66	112.59	108.54
30	1	606	CHL	C3D-C4D-CHA	2.66	112.58	108.54
30	9	607	CHL	C3D-C4D-CHA	2.66	112.58	108.54
30	6	601	CHL	C3D-C4D-CHA	2.65	112.56	108.54
30	5	607	CHL	C3D-C4D-CHA	2.64	112.56	108.54
30	6	607	CHL	C3D-C4D-CHA	2.64	112.56	108.54
31	1	618	XAT	C7-C8-C9	2.64	129.63	125.53
21	B	829	CLA	CHD-C1D-ND	-2.64	121.09	124.80
30	5	618	CHL	C3D-C4D-CHA	2.64	112.55	108.54
21	5	616	CLA	CHD-C1D-ND	-2.63	121.10	124.80
21	7	610	CLA	CHD-C1D-ND	-2.62	121.11	124.80
21	5	603	CLA	CHD-C1D-ND	-2.61	121.12	124.80
30	4	606	CHL	C3D-C4D-CHA	2.61	112.51	108.54
30	6	616	CHL	C3D-C4D-CHA	2.61	112.51	108.54
30	8	606	CHL	C3D-C4D-CHA	2.61	112.51	108.54
21	B	819	CLA	CHD-C1D-ND	-2.61	121.13	124.80
21	4	602	CLA	CHD-C1D-ND	-2.61	121.13	124.80
21	Z	602	CLA	CHD-C1D-ND	-2.61	121.13	124.80
30	Z	607	CHL	CHA-C1A-C2A	-2.61	127.18	133.31
21	5	621	CLA	C2A-C1A-CHA	2.61	128.39	123.87
30	5	606	CHL	C3D-C4D-CHA	2.60	112.50	108.54
30	6	608	CHL	C3D-C4D-CHA	2.60	112.50	108.54
21	1	604	CLA	CHD-C1D-ND	-2.60	121.14	124.80
21	8	610	CLA	CHD-C1D-ND	-2.60	121.14	124.80
30	4	607	CHL	C3D-C4D-CHA	2.60	112.49	108.54
21	L	203	CLA	CHD-C1D-ND	-2.60	121.15	124.80
21	Z	604	CLA	CHD-C1D-ND	-2.59	121.15	124.80
21	B	828	CLA	CHD-C1D-ND	-2.59	121.16	124.80
21	A	823	CLA	CHD-C1D-ND	-2.59	121.16	124.80
30	7	606	CHL	C3D-C4D-CHA	2.58	112.46	108.54
21	A	815	CLA	CHD-C1D-ND	-2.58	121.18	124.80
21	B	817	CLA	CHD-C1D-ND	-2.57	121.18	124.80
21	4	616	CLA	CHD-C1D-ND	-2.57	121.18	124.80
30	6	606	CHL	C3D-C4D-CHA	2.57	112.45	108.54
21	Z	609	CLA	CAA-C2A-C1A	-2.55	103.61	111.97
30	Z	601	CHL	C3D-C4D-CHA	2.55	112.42	108.54
30	Z	606	CHL	C3D-C4D-CHA	2.55	112.42	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	821	CLA	CHD-C1D-ND	-2.55	121.21	124.80
21	1	608	CLA	CHD-C1D-ND	-2.55	121.22	124.80
30	3	608	CHL	C3D-C4D-CHA	2.55	112.41	108.54
21	7	609	CLA	CHD-C1D-ND	-2.54	121.22	124.80
21	6	610	CLA	CHD-C1D-ND	-2.53	121.24	124.80
21	A	836	CLA	CHD-C1D-ND	-2.53	121.24	124.80
21	A	803	CLA	CHD-C1D-ND	-2.53	121.24	124.80
21	1	602	CLA	CHD-C1D-ND	-2.53	121.25	124.80
31	Z	618	XAT	C7-C8-C9	2.52	129.44	125.53
30	4	608	CHL	C3D-C4D-CHA	2.52	112.37	108.54
21	A	842	CLA	CHD-C1D-ND	-2.52	121.26	124.80
21	A	825	CLA	CHD-C1D-ND	-2.52	121.26	124.80
21	5	610	CLA	CHD-C1D-ND	-2.52	121.26	124.80
21	3	609	CLA	CHD-C1D-ND	-2.51	121.27	124.80
21	Z	610	CLA	CHD-C1D-ND	-2.51	121.27	124.80
21	A	854	CLA	CHD-C1D-ND	-2.51	121.28	124.80
21	8	602	CLA	CHD-C1D-ND	-2.51	121.28	124.80
21	3	604	CLA	CHD-C1D-ND	-2.50	121.29	124.80
30	5	608	CHL	C3D-C4D-CHA	2.50	112.34	108.54
21	3	614	CLA	CHD-C1D-ND	-2.50	121.29	124.80
21	1	603	CLA	CHD-C1D-ND	-2.50	121.29	124.80
21	A	810	CLA	CHD-C1D-ND	-2.50	121.29	124.80
21	6	603	CLA	CHD-C1D-ND	-2.49	121.29	124.80
21	B	834	CLA	CHD-C1D-ND	-2.49	121.30	124.80
21	Z	608	CLA	CHD-C1D-ND	-2.49	121.30	124.80
21	8	603	CLA	CHD-C1D-ND	-2.49	121.30	124.80
21	A	830	CLA	CHD-C1D-ND	-2.49	121.30	124.80
21	A	812	CLA	CHD-C1D-ND	-2.49	121.30	124.80
21	A	802	CLA	CHD-C1D-ND	-2.49	121.31	124.80
21	A	831	CLA	CHD-C1D-ND	-2.48	121.31	124.80
21	4	604	CLA	CHD-C1D-ND	-2.48	121.31	124.80
21	Z	611	CLA	CHD-C1D-ND	-2.48	121.31	124.80
21	6	617	CLA	CHD-C1D-ND	-2.48	121.31	124.80
21	Z	613	CLA	CHD-C1D-ND	-2.48	121.31	124.80
21	9	609	CLA	CHD-C1D-ND	-2.48	121.32	124.80
21	6	602	CLA	CHD-C1D-ND	-2.47	121.32	124.80
21	B	831	CLA	CHD-C1D-ND	-2.47	121.32	124.80
21	9	610	CLA	CHD-C1D-ND	-2.47	121.32	124.80
21	5	614	CLA	CHD-C1D-ND	-2.46	121.33	124.80
21	5	609	CLA	CHD-C1D-ND	-2.46	121.34	124.80
21	5	621	CLA	CAA-C2A-C1A	2.46	120.03	111.97
21	B	803	CLA	C4A-NA-C1A	2.46	107.80	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	9	611	CLA	CHD-C1D-ND	-2.46	121.35	124.80
21	A	822	CLA	CHD-C1D-ND	-2.45	121.35	124.80
21	B	810	CLA	CHD-C1D-ND	-2.45	121.35	124.80
21	9	604	CLA	CHD-C1D-ND	-2.45	121.35	124.80
21	A	820	CLA	CHD-C1D-ND	-2.45	121.35	124.80
21	7	616	CLA	CHD-C1D-ND	-2.45	121.36	124.80
21	5	617	CLA	CHD-C1D-ND	-2.45	121.36	124.80
21	B	809	CLA	CHD-C1D-ND	-2.45	121.36	124.80
21	B	823	CLA	CHD-C1D-ND	-2.44	121.36	124.80
21	5	613	CLA	CHD-C1D-ND	-2.44	121.36	124.80
21	A	837	CLA	CHD-C1D-ND	-2.44	121.36	124.80
21	A	821	CLA	CHD-C1D-ND	-2.44	121.37	124.80
21	A	839	CLA	CHD-C1D-ND	-2.44	121.37	124.80
21	6	613	CLA	CHD-C1D-ND	-2.44	121.37	124.80
21	7	602	CLA	CHD-C1D-ND	-2.44	121.37	124.80
21	4	611	CLA	CHD-C1D-ND	-2.44	121.37	124.80
21	9	602	CLA	CHD-C1D-ND	-2.44	121.37	124.80
21	6	604	CLA	CHD-C1D-ND	-2.43	121.38	124.80
21	L	204	CLA	CHD-C1D-ND	-2.43	121.38	124.80
21	1	613	CLA	CHD-C1D-ND	-2.43	121.38	124.80
21	3	602	CLA	CHD-C1D-ND	-2.43	121.38	124.80
21	A	827	CLA	CHD-C1D-ND	-2.43	121.38	124.80
21	B	827	CLA	CHD-C1D-ND	-2.43	121.38	124.80
21	B	822	CLA	CHD-C1D-ND	-2.43	121.38	124.80
21	4	614	CLA	CHD-C1D-ND	-2.43	121.39	124.80
21	A	816	CLA	CHD-C1D-ND	-2.43	121.39	124.80
21	1	610	CLA	CHD-C1D-ND	-2.43	121.39	124.80
21	9	614	CLA	CHD-C1D-ND	-2.43	121.39	124.80
21	K	203	CLA	CHD-C1D-ND	-2.42	121.40	124.80
21	3	612	CLA	CHD-C1D-ND	-2.42	121.40	124.80
21	B	826	CLA	CHD-C1D-ND	-2.41	121.40	124.80
21	1	616	CLA	CHD-C1D-ND	-2.41	121.41	124.80
21	K	204	CLA	CHD-C1D-ND	-2.41	121.41	124.80
21	8	613	CLA	CHD-C1D-ND	-2.41	121.41	124.80
21	Z	614	CLA	CHD-C1D-ND	-2.41	121.41	124.80
21	6	622	CLA	CHD-C1D-ND	-2.41	121.41	124.80
21	B	811	CLA	CHD-C1D-ND	-2.41	121.41	124.80
21	B	812	CLA	CHD-C1D-ND	-2.41	121.41	124.80
21	F	303	CLA	CHD-C1D-ND	-2.41	121.41	124.80
21	A	843	CLA	O2A-C1-C2	-2.41	98.84	108.11
21	B	832	CLA	CHD-C1D-ND	-2.41	121.41	124.80
21	A	813	CLA	CHD-C1D-ND	-2.41	121.42	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	3	606	CLA	CHD-C1D-ND	-2.41	121.42	124.80
21	6	609	CLA	CHD-C1D-ND	-2.41	121.42	124.80
31	8	618	XAT	C7-C8-C9	2.41	129.26	125.53
21	A	833	CLA	CHD-C1D-ND	-2.41	121.42	124.80
21	7	603	CLA	CHD-C1D-ND	-2.41	121.42	124.80
21	Z	609	CLA	CHD-C1D-ND	-2.40	121.42	124.80
21	A	808	CLA	CHD-C1D-ND	-2.40	121.42	124.80
21	B	841	CLA	CHD-C1D-ND	-2.40	121.42	124.80
21	3	607	CLA	CHD-C1D-ND	-2.40	121.42	124.80
21	3	611	CLA	CHD-C1D-ND	-2.40	121.42	124.80
21	B	830	CLA	CHD-C1D-ND	-2.40	121.42	124.80
21	9	601	CLA	CHD-C1D-ND	-2.40	121.43	124.80
21	8	604	CLA	CHD-C1D-ND	-2.40	121.43	124.80
21	1	611	CLA	CHD-C1D-ND	-2.40	121.43	124.80
21	B	836	CLA	CHD-C1D-ND	-2.40	121.43	124.80
21	8	611	CLA	CHD-C1D-ND	-2.39	121.43	124.80
21	5	604	CLA	CHD-C1D-ND	-2.39	121.43	124.80
21	B	840	CLA	CHD-C1D-ND	-2.39	121.44	124.80
21	8	609	CLA	CHD-C1D-ND	-2.39	121.44	124.80
21	B	815	CLA	CHD-C1D-ND	-2.39	121.44	124.80
21	7	608	CLA	CHD-C1D-ND	-2.39	121.44	124.80
21	7	604	CLA	CHD-C1D-ND	-2.39	121.44	124.80
21	5	602	CLA	CHD-C1D-ND	-2.39	121.44	124.80
21	B	807	CLA	CHD-C1D-ND	-2.39	121.45	124.80
21	3	610	CLA	CHD-C1D-ND	-2.38	121.45	124.80
21	A	805	CLA	CHD-C1D-ND	-2.38	121.45	124.80
21	4	613	CLA	CHD-C1D-ND	-2.38	121.45	124.80
21	B	818	CLA	CHD-C1D-ND	-2.38	121.45	124.80
21	B	804	CLA	CHD-C1D-ND	-2.38	121.45	124.80
28	A	856	LUT	C1-C2-C3	2.38	118.81	113.59
21	A	835	CLA	CHD-C1D-ND	-2.38	121.45	124.80
21	7	612	CLA	CHD-C1D-ND	-2.38	121.45	124.80
21	8	612	CLA	CHD-C1D-ND	-2.38	121.45	124.80
21	A	809	CLA	CHD-C1D-ND	-2.38	121.46	124.80
21	7	611	CLA	CHD-C1D-ND	-2.38	121.46	124.80
21	B	805	CLA	CHD-C1D-ND	-2.37	121.46	124.80
21	K	206	CLA	CHD-C1D-ND	-2.37	121.47	124.80
21	3	603	CLA	CHD-C1D-ND	-2.37	121.47	124.80
31	4	620	XAT	C7-C8-C9	2.37	129.21	125.53
21	8	614	CLA	CHD-C1D-ND	-2.37	121.47	124.80
21	B	814	CLA	CHD-C1D-ND	-2.36	121.48	124.80
21	A	818	CLA	CHD-C1D-ND	-2.35	121.49	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	841	CLA	CHD-C1D-ND	-2.35	121.49	124.80
21	6	614	CLA	CHD-C1D-ND	-2.35	121.50	124.80
21	A	803	CLA	C3B-C4B-NB	-2.35	108.43	110.53
21	J	101	CLA	CHD-C1D-ND	-2.35	121.50	124.80
21	8	608	CLA	CHD-C1D-ND	-2.35	121.50	124.80
21	A	845	CLA	CHD-C1D-ND	-2.35	121.50	124.80
21	4	612	CLA	CHD-C1D-ND	-2.35	121.50	124.80
21	G	203	CLA	CHD-C1D-ND	-2.35	121.50	124.80
21	B	837	CLA	CHD-C1D-ND	-2.35	121.50	124.80
21	A	824	CLA	CHD-C1D-ND	-2.34	121.50	124.80
21	A	817	CLA	CHD-C1D-ND	-2.34	121.51	124.80
21	8	616	CLA	CHD-C1D-ND	-2.34	121.51	124.80
31	6	624	XAT	C7-C8-C9	2.34	129.16	125.53
21	6	611	CLA	CHD-C1D-ND	-2.34	121.51	124.80
21	3	613	CLA	CHD-C1D-ND	-2.34	121.52	124.80
28	F	305	LUT	C27-C28-C29	2.33	131.34	126.32
21	1	614	CLA	CHD-C1D-ND	-2.33	121.52	124.80
21	Z	603	CLA	CHD-C1D-ND	-2.33	121.52	124.80
21	A	804	CLA	CHD-C1D-ND	-2.33	121.52	124.80
21	7	614	CLA	CHD-C1D-ND	-2.33	121.53	124.80
21	Z	616	CLA	CHD-C1D-ND	-2.33	121.53	124.80
21	A	834	CLA	CHD-C1D-ND	-2.33	121.53	124.80
21	9	613	CLA	CHD-C1D-ND	-2.33	121.53	124.80
21	B	820	CLA	CHD-C1D-ND	-2.33	121.53	124.80
21	9	603	CLA	CHD-C1D-ND	-2.33	121.53	124.80
21	B	835	CLA	CHD-C1D-ND	-2.33	121.53	124.80
21	4	603	CLA	CHD-C1D-ND	-2.33	121.53	124.80
21	B	838	CLA	CHD-C1D-ND	-2.32	121.53	124.80
21	F	304	CLA	CHD-C1D-ND	-2.32	121.53	124.80
21	3	615	CLA	CHD-C1D-ND	-2.32	121.54	124.80
21	B	839	CLA	CHD-C1D-ND	-2.32	121.54	124.80
21	G	204	CLA	CHD-C1D-ND	-2.32	121.54	124.80
21	7	613	CLA	CHD-C1D-ND	-2.32	121.54	124.80
21	6	612	CLA	CHD-C1D-ND	-2.31	121.55	124.80
21	A	832	CLA	CHD-C1D-ND	-2.31	121.55	124.80
21	7	620	CLA	CHD-C1D-ND	-2.31	121.55	124.80
21	9	612	CLA	CHD-C1D-ND	-2.31	121.55	124.80
21	A	819	CLA	CHD-C1D-ND	-2.30	121.56	124.80
21	Z	612	CLA	CHD-C1D-ND	-2.30	121.57	124.80
30	8	601	CHL	C4C-CHD-C1D	2.30	124.29	116.07
30	1	601	CHL	C4C-CHD-C1D	2.30	124.29	116.07
21	B	816	CLA	CHD-C1D-ND	-2.29	121.58	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	609	CLA	CHD-C1D-ND	-2.29	121.58	124.80
21	A	829	CLA	C4A-NA-C1A	2.28	107.72	106.68
30	1	607	CHL	CHA-C1A-C2A	-2.28	127.95	133.31
30	8	607	CHL	C1A-CHA-C4D	2.28	122.79	118.98
21	4	609	CLA	CHD-C1D-ND	-2.28	121.60	124.80
21	B	825	CLA	CHD-C1D-ND	-2.28	121.60	124.80
21	5	601	CLA	CHD-C1D-ND	-2.28	121.60	124.80
30	6	601	CHL	C4C-CHD-C1D	2.28	124.21	116.07
21	B	802	CLA	CHD-C1D-ND	-2.27	121.60	124.80
21	F	301	CLA	CHD-C1D-ND	-2.27	121.60	124.80
30	7	607	CHL	C1A-CHA-C4D	2.26	122.76	118.98
30	6	607	CHL	C4C-CHD-C1D	2.26	124.16	116.07
21	5	611	CLA	CHD-C1D-ND	-2.26	121.62	124.80
30	1	606	CHL	C1A-CHA-C4D	2.26	122.75	118.98
21	3	617	CLA	CHD-C1D-ND	-2.26	121.63	124.80
21	B	808	CLA	CHD-C1D-ND	-2.26	121.63	124.80
21	B	838	CLA	CAA-C2A-C3A	-2.25	106.91	113.00
30	9	607	CHL	C4C-CHD-C1D	2.25	124.13	116.07
32	6	625	NEX	O24-C25-C24	-2.25	111.38	113.49
21	A	843	CLA	CHD-C1D-ND	-2.25	121.64	124.80
30	4	607	CHL	C4C-CHD-C1D	2.24	124.10	116.07
30	6	616	CHL	C4C-CHD-C1D	2.24	124.08	116.07
21	A	840	CLA	CHD-C1D-ND	-2.23	121.66	124.80
30	Z	606	CHL	C4C-CHD-C1D	2.23	124.05	116.07
30	1	607	CHL	C4C-CHD-C1D	2.23	124.05	116.07
21	A	828	CLA	CHD-C1D-ND	-2.23	121.67	124.80
30	Z	607	CHL	C4C-CHD-C1D	2.23	124.04	116.07
30	6	618	CHL	C1A-CHA-C4D	2.23	122.70	118.98
30	5	607	CHL	C4C-CHD-C1D	2.23	124.03	116.07
30	6	606	CHL	C4C-CHD-C1D	2.23	124.03	116.07
21	A	826	CLA	CHD-C1D-ND	-2.22	121.67	124.80
30	6	618	CHL	C4C-CHD-C1D	2.22	124.02	116.07
30	3	608	CHL	C4C-CHD-C1D	2.22	124.01	116.07
30	1	606	CHL	C4C-CHD-C1D	2.22	124.01	116.07
30	7	606	CHL	C4C-CHD-C1D	2.22	124.01	116.07
30	4	618	CHL	C4C-CHD-C1D	2.21	123.99	116.07
30	Z	601	CHL	C4C-CHD-C1D	2.21	123.99	116.07
30	8	606	CHL	C1A-CHA-C4D	2.21	122.67	118.98
30	5	608	CHL	C4C-CHD-C1D	2.21	123.98	116.07
21	5	612	CLA	CHD-C1D-ND	-2.21	121.69	124.80
30	5	606	CHL	C4C-CHD-C1D	2.21	123.97	116.07
30	5	618	CHL	C4C-CHD-C1D	2.20	123.96	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	5	607	CHL	C1A-CHA-C4D	2.20	122.66	118.98
30	4	601	CHL	C4C-CHD-C1D	2.20	123.95	116.07
30	7	606	CHL	C1A-CHA-C4D	2.20	122.66	118.98
30	5	606	CHL	C1A-CHA-C4D	2.20	122.65	118.98
30	6	607	CHL	C1A-CHA-C4D	2.19	122.64	118.98
30	4	608	CHL	C4C-CHD-C1D	2.19	123.92	116.07
30	4	606	CHL	C4C-CHD-C1D	2.19	123.92	116.07
30	8	606	CHL	C4C-CHD-C1D	2.19	123.91	116.07
30	6	608	CHL	C4C-CHD-C1D	2.19	123.90	116.07
30	3	608	CHL	C1A-CHA-C4D	2.19	122.63	118.98
30	6	607	CHL	C1-C2-C3	-2.19	122.62	126.20
30	7	607	CHL	C4C-CHD-C1D	2.18	123.89	116.07
30	8	607	CHL	C4C-CHD-C1D	2.18	123.86	116.07
21	9	604	CLA	C3D-C4D-ND	2.17	113.52	109.99
21	B	826	CLA	C3B-C4B-NB	-2.17	108.59	110.53
30	6	616	CHL	C1A-CHA-C4D	2.17	122.61	118.98
21	4	616	CLA	C3D-C4D-ND	2.17	113.52	109.99
21	4	604	CLA	C3D-C4D-ND	2.17	113.51	109.99
30	7	601	CHL	C4C-CHD-C1D	2.17	123.83	116.07
21	A	829	CLA	CHD-C1D-ND	-2.17	121.75	124.80
21	B	806	CLA	CHD-C1D-ND	-2.16	121.76	124.80
21	5	603	CLA	C3D-C4D-ND	2.16	113.50	109.99
21	A	838	CLA	CHD-C1D-ND	-2.16	121.77	124.80
30	4	606	CHL	C1A-CHA-C4D	2.16	122.58	118.98
21	L	203	CLA	C3D-C4D-ND	2.15	113.49	109.99
21	B	833	CLA	C3D-C4D-ND	2.15	113.49	109.99
21	9	610	CLA	C3D-C4D-ND	2.15	113.49	109.99
21	1	612	CLA	CHD-C1D-ND	-2.15	121.78	124.80
30	9	606	CHL	C4C-CHD-C1D	2.15	123.76	116.07
21	9	609	CLA	C3D-C4D-ND	2.15	113.48	109.99
21	A	822	CLA	C3D-C4D-ND	2.14	113.47	109.99
30	Z	601	CHL	C1A-CHA-C4D	2.14	122.56	118.98
21	A	829	CLA	C3B-C4B-NB	-2.14	108.62	110.53
21	A	807	CLA	CHD-C1D-ND	-2.14	121.80	124.80
21	A	814	CLA	CHD-C1D-ND	-2.13	121.80	124.80
21	B	813	CLA	CHD-C1D-ND	-2.13	121.80	124.80
30	9	606	CHL	C1A-CHA-C4D	2.13	122.54	118.98
30	6	606	CHL	C1A-CHA-C4D	2.13	122.54	118.98
29	B	850	DGD	C3G-O3G-C1D	2.13	118.36	113.80
30	Z	606	CHL	C1A-CHA-C4D	2.12	122.52	118.98
30	6	601	CHL	C1A-CHA-C4D	2.12	122.51	118.98
21	B	831	CLA	C3D-C4D-ND	2.11	113.42	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	5	625	NEX	O24-C25-C26	-2.11	57.26	58.93
21	A	820	CLA	C3D-C4D-ND	2.11	113.42	109.99
21	5	614	CLA	C3D-C4D-ND	2.11	113.41	109.99
21	A	811	CLA	C3D-C4D-ND	2.11	113.41	109.99
21	Z	604	CLA	C3D-C4D-ND	2.11	113.41	109.99
30	4	608	CHL	C1A-CHA-C4D	2.11	122.50	118.98
21	Z	613	CLA	C3D-C4D-ND	2.10	113.40	109.99
30	5	608	CHL	C1A-CHA-C4D	2.10	122.48	118.98
21	9	602	CLA	C3D-C4D-ND	2.10	113.39	109.99
21	B	819	CLA	C3D-C4D-ND	2.09	113.39	109.99
21	Z	611	CLA	C3D-C4D-ND	2.09	113.39	109.99
21	Z	614	CLA	C3D-C4D-ND	2.09	113.39	109.99
21	3	614	CLA	C3D-C4D-ND	2.09	113.39	109.99
21	7	610	CLA	O2A-C1-C2	2.09	116.15	108.11
21	1	604	CLA	C3D-C4D-ND	2.09	113.38	109.99
30	6	608	CHL	C1A-CHA-C4D	2.09	122.47	118.98
21	5	616	CLA	CHC-C4B-NB	2.09	127.18	124.05
32	6	625	NEX	O24-C26-C27	-2.09	110.90	116.88
21	B	824	CLA	CHD-C1D-ND	-2.09	121.87	124.80
21	6	617	CLA	C3D-C4D-ND	2.08	113.37	109.99
21	1	613	CLA	C3D-C4D-ND	2.08	113.37	109.99
21	9	601	CLA	C3D-C4D-ND	2.08	113.37	109.99
21	A	823	CLA	C3D-C4D-ND	2.08	113.37	109.99
30	8	606	CHL	C1-C2-C3	-2.08	122.79	126.20
21	5	621	CLA	CHD-C1D-ND	-2.08	121.88	124.80
21	1	610	CLA	C3D-C4D-ND	2.08	113.36	109.99
21	Z	609	CLA	C3D-C4D-ND	2.07	113.36	109.99
21	1	602	CLA	C3D-C4D-ND	2.07	113.36	109.99
21	3	602	CLA	C3D-C4D-ND	2.07	113.35	109.99
21	9	614	CLA	C3D-C4D-ND	2.07	113.35	109.99
21	5	609	CLA	C3D-C4D-ND	2.07	113.35	109.99
21	1	611	CLA	C3D-C4D-ND	2.07	113.35	109.99
20	A	801	CL0	C1C-CHC-C4B	2.07	123.47	116.07
21	A	809	CLA	C4A-NA-C1A	2.07	107.62	106.68
21	B	822	CLA	C3D-C4D-ND	2.07	113.35	109.99
31	7	622	XAT	O4-C5-C6	-2.06	57.29	58.93
21	9	611	CLA	C3D-C4D-ND	2.06	113.34	109.99
21	7	603	CLA	C3D-C4D-ND	2.06	113.34	109.99
21	4	611	CLA	C3D-C4D-ND	2.06	113.33	109.99
21	K	204	CLA	C3D-C4D-ND	2.06	113.33	109.99
21	5	613	CLA	C3D-C4D-ND	2.06	113.33	109.99
21	3	612	CLA	C3D-C4D-ND	2.06	113.33	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	9	603	CLA	C3D-C4D-ND	2.06	113.33	109.99
21	A	810	CLA	C3B-C4B-NB	-2.06	108.69	110.53
21	3	607	CLA	C3D-C4D-ND	2.05	113.32	109.99
30	7	601	CHL	C1A-CHA-C4D	2.05	122.40	118.98
21	A	839	CLA	C3D-C4D-ND	2.05	113.31	109.99
21	1	603	CLA	C3D-C4D-ND	2.05	113.31	109.99
21	1	614	CLA	C3D-C4D-ND	2.05	113.31	109.99
21	4	610	CLA	C3D-C4D-ND	2.05	113.31	109.99
21	4	602	CLA	C3D-C4D-ND	2.05	113.31	109.99
30	5	618	CHL	C1A-CHA-C4D	2.04	122.39	118.98
21	B	817	CLA	C3D-C4D-ND	2.04	113.31	109.99
21	7	613	CLA	CHC-C4B-NB	2.04	127.12	124.05
30	9	607	CHL	C1A-CHA-C4D	2.04	122.39	118.98
21	B	828	CLA	C3D-C4D-ND	2.04	113.31	109.99
21	7	609	CLA	C3D-C4D-ND	2.04	113.31	109.99
21	3	604	CLA	C3D-C4D-ND	2.04	113.30	109.99
21	5	621	CLA	C4A-NA-C1A	2.04	107.61	106.68
21	Z	616	CLA	C3D-C4D-ND	2.04	113.30	109.99
21	Z	610	CLA	C3D-C4D-ND	2.04	113.30	109.99
21	1	608	CLA	C3D-C4D-ND	2.04	113.30	109.99
21	6	604	CLA	C3D-C4D-ND	2.04	113.30	109.99
32	5	625	NEX	O24-C26-C27	-2.04	111.05	116.88
21	L	204	CLA	C3D-C4D-ND	2.03	113.29	109.99
31	1	618	XAT	O4-C6-C7	-2.03	111.05	116.88
21	7	616	CLA	C3D-C4D-ND	2.03	113.29	109.99
21	6	602	CLA	C3D-C4D-ND	2.03	113.29	109.99
21	B	814	CLA	C3D-C4D-ND	2.03	113.29	109.99
21	K	203	CLA	C3D-C4D-ND	2.03	113.29	109.99
31	1	618	XAT	O4-C5-C4	-2.03	111.59	113.49
21	B	821	CLA	C3D-C4D-ND	2.03	113.28	109.99
21	3	611	CLA	C3D-C4D-ND	2.03	113.28	109.99
21	8	611	CLA	C3D-C4D-ND	2.03	113.28	109.99
21	B	839	CLA	CHC-C4B-NB	2.02	127.09	124.05
21	5	602	CLA	C3D-C4D-ND	2.02	113.28	109.99
30	4	618	CHL	C1A-CHA-C4D	2.02	122.35	118.98
21	A	833	CLA	C3D-C4D-ND	2.02	113.26	109.99
21	5	621	CLA	CHA-C1A-NA	-2.02	121.83	126.39
21	1	616	CLA	C3D-C4D-ND	2.01	113.26	109.99
21	7	604	CLA	C3D-C4D-ND	2.01	113.26	109.99
21	9	613	CLA	C3D-C4D-ND	2.01	113.25	109.99
21	6	609	CLA	C3D-C4D-ND	2.01	113.25	109.99
21	4	609	CLA	CAA-C2A-C3A	-2.01	107.58	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	8	618	XAT	O4-C5-C6	-2.01	57.34	58.93
21	6	612	CLA	C3D-C4D-ND	2.01	113.25	109.99
21	K	206	CLA	C3D-C4D-ND	2.00	113.24	109.99
21	Z	612	CLA	C3D-C4D-ND	2.00	113.24	109.99
21	8	613	CLA	C3D-C4D-ND	2.00	113.24	109.99
21	B	810	CLA	C3D-C4D-ND	2.00	113.24	109.99

All (292) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	A	801	CL0	NA
20	A	801	CL0	NC
20	A	801	CL0	ND
21	A	802	CLA	ND
21	A	803	CLA	ND
21	A	804	CLA	ND
21	A	805	CLA	ND
21	A	806	CLA	ND
21	A	807	CLA	ND
21	A	808	CLA	ND
21	A	809	CLA	ND
21	A	810	CLA	ND
21	A	811	CLA	ND
21	A	812	CLA	ND
21	A	813	CLA	ND
21	A	814	CLA	ND
21	A	815	CLA	ND
21	A	816	CLA	ND
21	A	817	CLA	ND
21	A	818	CLA	ND
21	A	819	CLA	ND
21	A	820	CLA	ND
21	A	821	CLA	ND
21	A	822	CLA	ND
21	A	823	CLA	ND
21	A	824	CLA	ND
21	A	825	CLA	ND
21	A	826	CLA	ND
21	A	827	CLA	ND
21	A	828	CLA	ND
21	A	829	CLA	ND
21	A	830	CLA	ND

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Mol	Chain	Res	Type	Atom
21	A	831	CLA	ND
21	A	832	CLA	ND
21	A	833	CLA	ND
21	A	834	CLA	ND
21	A	835	CLA	ND
21	A	836	CLA	ND
21	A	837	CLA	ND
21	A	838	CLA	ND
21	A	839	CLA	ND
21	A	840	CLA	ND
21	A	841	CLA	ND
21	A	842	CLA	ND
21	A	843	CLA	ND
21	A	845	CLA	ND
21	A	854	CLA	ND
21	B	802	CLA	ND
21	B	803	CLA	ND
21	B	804	CLA	ND
21	B	805	CLA	ND
21	B	806	CLA	ND
21	B	807	CLA	ND
21	B	808	CLA	ND
21	B	809	CLA	ND
21	B	810	CLA	ND
21	B	811	CLA	ND
21	B	812	CLA	ND
21	B	813	CLA	ND
21	B	814	CLA	ND
21	B	815	CLA	ND
21	B	816	CLA	ND
21	B	817	CLA	ND
21	B	818	CLA	ND
21	B	819	CLA	ND
21	B	820	CLA	ND
21	B	821	CLA	ND
21	B	822	CLA	ND
21	B	823	CLA	ND
21	B	824	CLA	ND
21	B	825	CLA	ND
21	B	826	CLA	ND
21	B	827	CLA	ND
21	B	828	CLA	ND

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Mol	Chain	Res	Type	Atom
21	B	829	CLA	ND
21	B	830	CLA	ND
21	B	831	CLA	ND
21	B	832	CLA	ND
21	B	833	CLA	ND
21	B	834	CLA	ND
21	B	835	CLA	ND
21	B	836	CLA	ND
21	B	837	CLA	ND
21	B	838	CLA	ND
21	B	839	CLA	ND
21	B	840	CLA	ND
21	B	841	CLA	ND
21	F	301	CLA	ND
21	F	304	CLA	ND
21	F	303	CLA	ND
21	G	203	CLA	ND
21	G	204	CLA	ND
21	J	101	CLA	ND
21	L	203	CLA	ND
21	L	204	CLA	ND
21	K	201	CLA	ND
21	K	203	CLA	ND
21	K	204	CLA	ND
21	K	206	CLA	ND
21	1	602	CLA	ND
21	1	603	CLA	ND
21	1	604	CLA	ND
21	1	608	CLA	ND
21	1	609	CLA	ND
21	1	610	CLA	ND
21	1	611	CLA	ND
21	1	612	CLA	ND
21	1	613	CLA	ND
21	1	614	CLA	ND
21	1	616	CLA	ND
21	3	602	CLA	ND
21	3	603	CLA	ND
21	3	604	CLA	ND
21	3	606	CLA	ND
21	3	607	CLA	ND
21	3	609	CLA	ND

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Mol	Chain	Res	Type	Atom
21	3	610	CLA	ND
21	3	611	CLA	ND
21	3	612	CLA	ND
21	3	613	CLA	ND
21	3	614	CLA	ND
21	3	615	CLA	ND
21	3	617	CLA	ND
21	7	602	CLA	ND
21	7	603	CLA	ND
21	7	604	CLA	ND
21	7	608	CLA	ND
21	7	609	CLA	ND
21	7	610	CLA	ND
21	7	611	CLA	ND
21	7	612	CLA	ND
21	7	613	CLA	ND
21	7	614	CLA	ND
21	7	616	CLA	ND
21	7	620	CLA	ND
21	8	602	CLA	ND
21	8	603	CLA	ND
21	8	604	CLA	ND
21	8	608	CLA	ND
21	8	609	CLA	ND
21	8	610	CLA	ND
21	8	611	CLA	ND
21	8	612	CLA	ND
21	8	613	CLA	ND
21	8	614	CLA	ND
21	8	616	CLA	ND
21	Z	602	CLA	ND
21	Z	603	CLA	ND
21	Z	604	CLA	ND
21	Z	608	CLA	ND
21	Z	609	CLA	ND
21	Z	610	CLA	ND
21	Z	611	CLA	ND
21	Z	612	CLA	ND
21	Z	613	CLA	ND
21	Z	614	CLA	ND
21	Z	616	CLA	ND
21	4	602	CLA	ND

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Mol	Chain	Res	Type	Atom
21	4	603	CLA	ND
21	4	604	CLA	ND
21	4	609	CLA	ND
21	4	610	CLA	ND
21	4	611	CLA	ND
21	4	612	CLA	ND
21	4	613	CLA	ND
21	4	614	CLA	ND
21	4	616	CLA	ND
21	5	601	CLA	ND
21	5	602	CLA	ND
21	5	603	CLA	ND
21	5	604	CLA	ND
21	5	609	CLA	ND
21	5	610	CLA	ND
21	5	611	CLA	ND
21	5	612	CLA	ND
21	5	613	CLA	ND
21	5	614	CLA	ND
21	5	616	CLA	ND
21	5	617	CLA	ND
21	5	621	CLA	ND
21	6	602	CLA	ND
21	6	603	CLA	ND
21	6	604	CLA	ND
21	6	609	CLA	ND
21	6	610	CLA	ND
21	6	611	CLA	ND
21	6	612	CLA	ND
21	6	613	CLA	ND
21	6	614	CLA	ND
21	6	617	CLA	ND
21	6	622	CLA	ND
21	9	601	CLA	ND
21	9	602	CLA	ND
21	9	603	CLA	ND
21	9	604	CLA	ND
21	9	609	CLA	ND
21	9	610	CLA	ND
21	9	611	CLA	ND
21	9	612	CLA	ND
21	9	613	CLA	ND

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Mol	Chain	Res	Type	Atom
21	9	614	CLA	ND
30	1	606	CHL	NA
30	1	606	CHL	NC
30	1	606	CHL	ND
30	1	607	CHL	NA
30	1	607	CHL	NC
30	1	607	CHL	ND
30	1	601	CHL	NA
30	1	601	CHL	NC
30	1	601	CHL	ND
30	3	608	CHL	NA
30	3	608	CHL	NC
30	3	608	CHL	ND
30	7	601	CHL	NA
30	7	601	CHL	NC
30	7	601	CHL	ND
30	7	606	CHL	NA
30	7	606	CHL	NC
30	7	606	CHL	ND
30	7	607	CHL	NA
30	7	607	CHL	NC
30	7	607	CHL	ND
30	8	601	CHL	NA
30	8	601	CHL	NC
30	8	601	CHL	ND
30	8	606	CHL	NA
30	8	606	CHL	NC
30	8	606	CHL	ND
30	8	607	CHL	NA
30	8	607	CHL	NC
30	8	607	CHL	ND
30	Z	601	CHL	NA
30	Z	601	CHL	NC
30	Z	601	CHL	ND
30	Z	606	CHL	NA
30	Z	606	CHL	NC
30	Z	606	CHL	ND
30	Z	607	CHL	NA
30	Z	607	CHL	NC
30	Z	607	CHL	ND
30	4	601	CHL	NA
30	4	601	CHL	NC

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Mol	Chain	Res	Type	Atom
30	4	601	CHL	ND
30	4	606	CHL	NA
30	4	606	CHL	NC
30	4	606	CHL	ND
30	4	607	CHL	NA
30	4	607	CHL	NC
30	4	607	CHL	ND
30	4	608	CHL	NA
30	4	608	CHL	NC
30	4	608	CHL	ND
30	4	618	CHL	NA
30	4	618	CHL	NC
30	4	618	CHL	ND
30	5	606	CHL	NA
30	5	606	CHL	NC
30	5	606	CHL	ND
30	5	607	CHL	NA
30	5	607	CHL	NC
30	5	607	CHL	ND
30	5	608	CHL	NA
30	5	608	CHL	NC
30	5	608	CHL	ND
30	5	618	CHL	NA
30	5	618	CHL	NC
30	5	618	CHL	ND
30	6	601	CHL	NA
30	6	601	CHL	NC
30	6	601	CHL	ND
30	6	606	CHL	NA
30	6	606	CHL	NC
30	6	606	CHL	ND
30	6	607	CHL	NA
30	6	607	CHL	NC
30	6	607	CHL	ND
30	6	608	CHL	NA
30	6	608	CHL	NC
30	6	608	CHL	ND
30	6	616	CHL	NA
30	6	616	CHL	NC
30	6	616	CHL	ND
30	6	618	CHL	NA
30	6	618	CHL	NC

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Mol	Chain	Res	Type	Atom
30	6	618	CHL	ND
30	9	606	CHL	NA
30	9	606	CHL	NC
30	9	606	CHL	ND
30	9	607	CHL	NA
30	9	607	CHL	NC
30	9	607	CHL	ND
31	1	618	XAT	C6

All (1214) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	806	CLA	C1A-C2A-CAA-CBA
21	A	809	CLA	CHA-CBD-CGD-O1D
21	A	809	CLA	CHA-CBD-CGD-O2D
21	A	816	CLA	O2A-C1-C2-C3
21	A	817	CLA	CHA-CBD-CGD-O1D
21	A	817	CLA	CHA-CBD-CGD-O2D
21	A	819	CLA	C1A-C2A-CAA-CBA
21	A	819	CLA	C3A-C2A-CAA-CBA
21	A	819	CLA	C2B-C3B-CAB-CBB
21	A	819	CLA	C4B-C3B-CAB-CBB
21	A	821	CLA	C2B-C3B-CAB-CBB
21	A	821	CLA	C4B-C3B-CAB-CBB
21	A	823	CLA	C4B-C3B-CAB-CBB
21	A	831	CLA	CHA-CBD-CGD-O1D
21	A	831	CLA	CHA-CBD-CGD-O2D
21	A	834	CLA	C2B-C3B-CAB-CBB
21	A	834	CLA	C4B-C3B-CAB-CBB
21	A	835	CLA	CHA-CBD-CGD-O1D
21	A	835	CLA	CHA-CBD-CGD-O2D
21	A	836	CLA	C2B-C3B-CAB-CBB
21	A	836	CLA	C4B-C3B-CAB-CBB
21	A	838	CLA	C2-C3-C5-C6
21	A	838	CLA	C4-C3-C5-C6
21	A	842	CLA	C4B-C3B-CAB-CBB
21	A	845	CLA	CAD-CBD-CGD-O1D
21	A	845	CLA	CAD-CBD-CGD-O2D
21	B	808	CLA	CHA-CBD-CGD-O1D
21	B	808	CLA	CHA-CBD-CGD-O2D
21	B	814	CLA	C4-C3-C5-C6
21	B	817	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
21	B	817	CLA	C4B-C3B-CAB-CBB
21	B	824	CLA	CHA-CBD-CGD-O1D
21	B	824	CLA	CHA-CBD-CGD-O2D
21	B	825	CLA	CHA-CBD-CGD-O1D
21	B	825	CLA	CHA-CBD-CGD-O2D
21	B	829	CLA	CHA-CBD-CGD-O1D
21	B	829	CLA	CHA-CBD-CGD-O2D
21	B	833	CLA	CHA-CBD-CGD-O1D
21	B	833	CLA	CHA-CBD-CGD-O2D
21	B	841	CLA	C1A-C2A-CAA-CBA
21	B	841	CLA	C2B-C3B-CAB-CBB
21	B	841	CLA	C4B-C3B-CAB-CBB
21	F	304	CLA	CAD-CBD-CGD-O1D
21	F	304	CLA	CAD-CBD-CGD-O2D
21	G	203	CLA	CHA-CBD-CGD-O2D
21	G	204	CLA	CHA-CBD-CGD-O2D
21	L	204	CLA	C1A-C2A-CAA-CBA
21	K	201	CLA	C4B-C3B-CAB-CBB
21	K	206	CLA	C2B-C3B-CAB-CBB
21	K	206	CLA	C4B-C3B-CAB-CBB
21	1	603	CLA	C4-C3-C5-C6
21	1	611	CLA	C4B-C3B-CAB-CBB
21	3	602	CLA	CHA-CBD-CGD-O1D
21	3	602	CLA	CHA-CBD-CGD-O2D
21	3	612	CLA	C4B-C3B-CAB-CBB
21	3	614	CLA	C2B-C3B-CAB-CBB
21	3	614	CLA	C4B-C3B-CAB-CBB
21	3	615	CLA	CAD-CBD-CGD-O1D
21	3	615	CLA	CAD-CBD-CGD-O2D
21	3	617	CLA	C2B-C3B-CAB-CBB
21	3	617	CLA	C4B-C3B-CAB-CBB
21	7	602	CLA	CHA-CBD-CGD-O1D
21	7	602	CLA	CHA-CBD-CGD-O2D
21	7	610	CLA	C1A-C2A-CAA-CBA
21	7	610	CLA	C3A-C2A-CAA-CBA
21	7	614	CLA	C2B-C3B-CAB-CBB
21	7	614	CLA	C4B-C3B-CAB-CBB
21	7	616	CLA	C1A-C2A-CAA-CBA
21	7	616	CLA	C3A-C2A-CAA-CBA
21	8	602	CLA	CHA-CBD-CGD-O1D
21	8	602	CLA	CHA-CBD-CGD-O2D
21	8	613	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
21	8	613	CLA	C4B-C3B-CAB-CBB
21	8	614	CLA	C2B-C3B-CAB-CBB
21	8	614	CLA	C4B-C3B-CAB-CBB
21	8	616	CLA	C4B-C3B-CAB-CBB
21	Z	603	CLA	C1A-C2A-CAA-CBA
21	Z	608	CLA	C4B-C3B-CAB-CBB
21	Z	609	CLA	C2B-C3B-CAB-CBB
21	Z	609	CLA	C4B-C3B-CAB-CBB
21	Z	611	CLA	C4B-C3B-CAB-CBB
21	Z	614	CLA	C4B-C3B-CAB-CBB
21	4	613	CLA	C2B-C3B-CAB-CBB
21	4	613	CLA	C4B-C3B-CAB-CBB
21	4	614	CLA	C2B-C3B-CAB-CBB
21	4	614	CLA	C4B-C3B-CAB-CBB
21	5	616	CLA	C2B-C3B-CAB-CBB
21	5	616	CLA	C4B-C3B-CAB-CBB
21	9	601	CLA	C2B-C3B-CAB-CBB
21	9	601	CLA	C4B-C3B-CAB-CBB
21	9	602	CLA	CHA-CBD-CGD-O1D
21	9	602	CLA	CHA-CBD-CGD-O2D
21	9	610	CLA	C2B-C3B-CAB-CBB
21	9	610	CLA	C4B-C3B-CAB-CBB
21	9	613	CLA	C2B-C3B-CAB-CBB
21	9	613	CLA	C4B-C3B-CAB-CBB
21	9	614	CLA	C4B-C3B-CAB-CBB
23	A	846	LHG	C4-O6-P-O5
23	3	623	LHG	C1-C2-C3-O3
23	3	623	LHG	C3-O3-P-O5
23	3	623	LHG	C3-O3-P-O6
23	3	721	LHG	C2-C3-O3-P
23	3	721	LHG	C4-O6-P-O3
23	3	721	LHG	C4-O6-P-O5
23	Z	620	LHG	C3-O3-P-O4
23	Z	620	LHG	C3-O3-P-O6
23	4	622	LHG	C3-O3-P-O5
23	4	622	LHG	C3-O3-P-O6
23	4	622	LHG	C4-O6-P-O4
23	4	622	LHG	C4-O6-P-O5
23	4	623	LHG	C3-O3-P-O4
23	4	623	LHG	C3-O3-P-O5
23	4	623	LHG	C3-O3-P-O6
23	4	623	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
23	4	623	LHG	C4-O6-P-O5
23	5	623	LHG	C4-O6-P-O3
23	5	623	LHG	C4-O6-P-O4
23	6	619	LHG	C4-O6-P-O4
23	6	619	LHG	C4-O6-P-O5
23	6	629	LHG	C3-O3-P-O4
23	6	629	LHG	C3-O3-P-O6
23	6	629	LHG	C4-O6-P-O3
23	6	629	LHG	C4-O6-P-O4
23	9	622	LHG	C4-O6-P-O4
24	J	102	BCR	C23-C24-C25-C26
24	3	620	BCR	C1-C6-C7-C8
24	3	620	BCR	C5-C6-C7-C8
24	8	619	BCR	C1-C6-C7-C8
24	8	619	BCR	C5-C6-C7-C8
26	A	858	LMU	C2'-C1'-O1'-C1
26	A	858	LMU	O5'-C1'-O1'-C1
26	A	865	LMU	C2'-C1'-O1'-C1
26	A	865	LMU	O5'-C1'-O1'-C1
26	A	861	LMU	O5'-C1'-O1'-C1
26	B	853	LMU	C2'-C1'-O1'-C1
26	B	853	LMU	O5'-C1'-O1'-C1
26	K	208	LMU	O5'-C1'-O1'-C1
26	K	208	LMU	C2-C1-O1'-C1'
26	1	625	LMU	C2-C1-O1'-C1'
26	1	627	LMU	O5'-C1'-O1'-C1
26	1	627	LMU	C2-C1-O1'-C1'
26	7	627	LMU	C2'-C1'-O1'-C1
26	7	628	LMU	O5'-C1'-O1'-C1
26	7	629	LMU	C2'-C1'-O1'-C1
26	7	629	LMU	O5'-C1'-O1'-C1
26	Z	622	LMU	C2-C1-O1'-C1'
26	4	625	LMU	O5'-C1'-O1'-C1
26	6	632	LMU	C2'-C1'-O1'-C1
26	6	632	LMU	O5'-C1'-O1'-C1
26	6	628	LMU	O5'-C1'-O1'-C1
26	6	630	LMU	C2'-C1'-O1'-C1
26	6	630	LMU	O5'-C1'-O1'-C1
27	A	860	LMG	O6-C1-O1-C7
27	B	852	LMG	O6-C1-O1-C7
27	B	854	LMG	C2-C1-O1-C7
27	B	854	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
27	4	624	LMG	C2-C1-O1-C7
27	4	624	LMG	O6-C1-O1-C7
28	A	856	LUT	C1-C6-C7-C8
28	A	856	LUT	C5-C6-C7-C8
28	A	856	LUT	C21-C26-C27-C28
28	A	856	LUT	C25-C26-C27-C28
28	F	305	LUT	C21-C26-C27-C28
28	F	305	LUT	C25-C26-C27-C28
28	7	624	LUT	C25-C26-C27-C28
28	5	626	LUT	C21-C26-C27-C28
28	5	626	LUT	C25-C26-C27-C28
29	B	850	DGD	C2D-C1D-O3G-C3G
29	B	850	DGD	O6D-C1D-O3G-C3G
30	8	606	CHL	C1A-C2A-CAA-CBA
30	Z	606	CHL	C1A-C2A-CAA-CBA
30	Z	606	CHL	C3A-C2A-CAA-CBA
30	6	606	CHL	C1A-C2A-CAA-CBA
30	6	606	CHL	C2-C3-C5-C6
30	6	608	CHL	CHA-CBD-CGD-O1D
30	6	608	CHL	CHA-CBD-CGD-O2D
26	B	853	LMU	C3'-C4'-O1B-C1B
26	A	863	LMU	O5B-C1B-O1B-C4'
26	A	858	LMU	O5B-C1B-O1B-C4'
21	A	806	CLA	C3-C5-C6-C7
21	3	604	CLA	C3-C5-C6-C7
30	8	606	CHL	C3-C5-C6-C7
30	5	607	CHL	C3-C5-C6-C7
26	B	853	LMU	O5B-C1B-O1B-C4'
21	B	833	CLA	C4-C3-C5-C6
21	J	101	CLA	C4-C3-C5-C6
21	3	615	CLA	C4-C3-C5-C6
21	5	617	CLA	C4-C3-C5-C6
21	9	613	CLA	C4-C3-C5-C6
30	8	607	CHL	C4-C3-C5-C6
30	6	606	CHL	C4-C3-C5-C6
21	B	814	CLA	C2-C3-C5-C6
21	B	833	CLA	C2-C3-C5-C6
21	J	101	CLA	C2-C3-C5-C6
21	1	603	CLA	C2-C3-C5-C6
21	3	615	CLA	C2-C3-C5-C6
21	5	617	CLA	C2-C3-C5-C6
21	9	613	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
30	8	607	CHL	C2-C3-C5-C6
21	Z	609	CLA	C2A-CAA-CBA-CGA
21	5	603	CLA	C2A-CAA-CBA-CGA
26	A	858	LMU	C2B-C1B-O1B-C4'
21	1	613	CLA	C3-C5-C6-C7
23	3	623	LHG	O2-C2-C3-O3
21	8	612	CLA	C2-C3-C5-C6
30	1	601	CHL	C2-C3-C5-C6
21	A	830	CLA	C2A-CAA-CBA-CGA
26	G	206	LMU	O5'-C1'-O1'-C1
26	1	622	LMU	O5'-C1'-O1'-C1
26	7	627	LMU	O5'-C1'-O1'-C1
26	8	628	LMU	O5'-C1'-O1'-C1
26	Z	621	LMU	O5'-C1'-O1'-C1
27	A	859	LMG	O6-C1-O1-C7
27	7	626	LMG	O6-C1-O1-C7
23	B	851	LHG	C1-C2-C3-O3
23	9	622	LHG	C1-C2-C3-O3
21	5	621	CLA	C2C-C3C-CAC-CBC
21	7	612	CLA	C4-C3-C5-C6
21	8	612	CLA	C4-C3-C5-C6
21	5	610	CLA	C4-C3-C5-C6
30	1	601	CHL	C4-C3-C5-C6
21	7	612	CLA	C2-C3-C5-C6
21	5	610	CLA	C2-C3-C5-C6
21	B	803	CLA	C14-C13-C15-C16
21	B	809	CLA	C6-C7-C8-C9
21	B	823	CLA	C11-C10-C8-C9
21	B	823	CLA	C11-C12-C13-C14
21	1	609	CLA	C11-C10-C8-C9
21	4	609	CLA	C11-C10-C8-C9
21	5	603	CLA	C14-C13-C15-C16
30	1	601	CHL	C6-C7-C8-C9
30	3	608	CHL	C14-C13-C15-C16
30	8	606	CHL	C6-C7-C8-C9
30	6	607	CHL	C6-C7-C8-C9
26	G	206	LMU	C2'-C1'-O1'-C1
26	1	622	LMU	C2'-C1'-O1'-C1
26	1	627	LMU	C2'-C1'-O1'-C1
26	8	628	LMU	C2'-C1'-O1'-C1
26	Z	621	LMU	C2'-C1'-O1'-C1
26	6	628	LMU	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
27	A	859	LMG	C2-C1-O1-C7
27	7	626	LMG	C2-C1-O1-C7
23	B	851	LHG	O2-C2-C3-O3
23	6	629	LHG	O2-C2-C3-O3
23	9	622	LHG	O2-C2-C3-O3
23	B	851	LHG	O7-C5-C6-O8
26	4	625	LMU	O5B-C1B-O1B-C4'
26	8	627	LMU	O5B-C1B-O1B-C4'
21	A	839	CLA	C5-C6-C7-C8
21	5	601	CLA	C11-C12-C13-C15
26	8	627	LMU	C2B-C1B-O1B-C4'
21	B	839	CLA	C2A-CAA-CBA-CGA
30	1	607	CHL	C2A-CAA-CBA-CGA
21	L	203	CLA	C5-C6-C7-C8
30	8	601	CHL	C13-C15-C16-C17
21	B	821	CLA	C8-C10-C11-C12
21	5	603	CLA	C3-C5-C6-C7
21	A	829	CLA	C8-C10-C11-C12
21	4	609	CLA	C2A-CAA-CBA-CGA
21	5	601	CLA	C10-C11-C12-C13
21	5	617	CLA	C8-C10-C11-C12
21	B	817	CLA	C13-C15-C16-C17
21	1	608	CLA	C8-C10-C11-C12
30	Z	601	CHL	C10-C11-C12-C13
21	4	613	CLA	C4-C3-C5-C6
21	1	611	CLA	C5-C6-C7-C8
26	4	625	LMU	C2'-C1'-O1'-C1
27	A	860	LMG	C2-C1-O1-C7
27	8	629	LMG	C2-C1-O1-C7
23	4	622	LHG	O2-C2-C3-O3
23	4	623	LHG	O2-C2-C3-O3
27	B	852	LMG	C10-C11-C12-C13
30	7	601	CHL	C8-C10-C11-C12
21	A	806	CLA	C2A-CAA-CBA-CGA
21	A	843	CLA	C2A-CAA-CBA-CGA
23	B	851	LHG	C23-C24-C25-C26
27	8	629	LMG	O6-C1-O1-C7
27	4	624	LMG	C10-C11-C12-C13
26	A	863	LMU	C2B-C1B-O1B-C4'
21	B	821	CLA	C16-C17-C18-C19
21	5	612	CLA	C2C-C3C-CAC-CBC
27	J	103	LMG	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
23	A	846	LHG	C23-C24-C25-C26
21	4	609	CLA	C5-C6-C7-C8
26	A	863	LMU	C2-C1-O1'-C1'
26	G	206	LMU	C2-C1-O1'-C1'
26	8	624	LMU	C2-C1-O1'-C1'
30	6	601	CHL	C10-C11-C12-C13
21	A	825	CLA	C4B-C3B-CAB-CBB
21	B	821	CLA	C4B-C3B-CAB-CBB
21	B	839	CLA	C4B-C3B-CAB-CBB
21	B	840	CLA	C4B-C3B-CAB-CBB
21	3	611	CLA	C4B-C3B-CAB-CBB
21	Z	613	CLA	C4B-C3B-CAB-CBB
21	4	611	CLA	C4B-C3B-CAB-CBB
21	5	614	CLA	C4B-C3B-CAB-CBB
21	9	611	CLA	C4B-C3B-CAB-CBB
23	6	619	LHG	C9-C10-C11-C12
21	A	805	CLA	C6-C7-C8-C9
21	B	821	CLA	C16-C17-C18-C20
21	B	805	CLA	C2A-CAA-CBA-CGA
21	5	621	CLA	C2A-CAA-CBA-CGA
21	A	814	CLA	C10-C11-C12-C13
21	B	815	CLA	C12-C13-C15-C16
21	A	806	CLA	C3A-C2A-CAA-CBA
21	A	854	CLA	C3A-C2A-CAA-CBA
21	B	840	CLA	C3A-C2A-CAA-CBA
21	9	603	CLA	C3A-C2A-CAA-CBA
30	8	606	CHL	C3A-C2A-CAA-CBA
30	6	606	CHL	C3A-C2A-CAA-CBA
26	7	628	LMU	C1-C2-C3-C4
23	6	619	LHG	C26-C27-C28-C29
29	B	850	DGD	CAB-CBB-CCB-CDB
21	A	823	CLA	C2B-C3B-CAB-CBB
21	A	825	CLA	C2B-C3B-CAB-CBB
21	A	842	CLA	C2B-C3B-CAB-CBB
21	B	821	CLA	C2B-C3B-CAB-CBB
21	B	840	CLA	C2B-C3B-CAB-CBB
21	K	201	CLA	C2B-C3B-CAB-CBB
21	1	611	CLA	C2B-C3B-CAB-CBB
21	3	612	CLA	C2B-C3B-CAB-CBB
21	8	616	CLA	C2B-C3B-CAB-CBB
21	Z	608	CLA	C2B-C3B-CAB-CBB
21	Z	611	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
21	Z	614	CLA	C2B-C3B-CAB-CBB
21	4	611	CLA	C2B-C3B-CAB-CBB
21	6	611	CLA	C2B-C3B-CAB-CBB
21	9	611	CLA	C2B-C3B-CAB-CBB
21	9	614	CLA	C2B-C3B-CAB-CBB
24	A	851	BCR	C23-C24-C25-C26
24	A	851	BCR	C23-C24-C25-C30
24	B	844	BCR	C1-C6-C7-C8
24	B	844	BCR	C5-C6-C7-C8
24	J	102	BCR	C23-C24-C25-C30
24	K	202	BCR	C23-C24-C25-C26
24	K	202	BCR	C23-C24-C25-C30
24	K	207	BCR	C23-C24-C25-C26
24	K	207	BCR	C23-C24-C25-C30
24	3	620	BCR	C23-C24-C25-C26
24	3	620	BCR	C23-C24-C25-C30
24	7	623	BCR	C23-C24-C25-C30
24	8	619	BCR	C23-C24-C25-C30
24	4	621	BCR	C23-C24-C25-C26
24	4	621	BCR	C23-C24-C25-C30
24	5	622	BCR	C23-C24-C25-C26
24	5	622	BCR	C23-C24-C25-C30
24	6	623	BCR	C23-C24-C25-C30
28	F	305	LUT	C1-C6-C7-C8
28	F	305	LUT	C5-C6-C7-C8
28	1	617	LUT	C1-C6-C7-C8
28	Z	617	LUT	C1-C6-C7-C8
28	Z	619	LUT	C1-C6-C7-C8
28	Z	619	LUT	C5-C6-C7-C8
28	9	616	LUT	C1-C6-C7-C8
27	1	628	LMG	C30-C31-C32-C33
21	5	621	CLA	C4C-C3C-CAC-CBC
21	A	839	CLA	C2-C3-C5-C6
21	4	613	CLA	C2-C3-C5-C6
21	A	805	CLA	C6-C7-C8-C10
21	A	807	CLA	C3-C5-C6-C7
21	Z	609	CLA	C11-C10-C8-C9
27	1	628	LMG	C39-C40-C41-C42
26	A	861	LMU	C2'-C1'-O1'-C1
26	K	208	LMU	C2'-C1'-O1'-C1
32	6	625	NEX	C13-C14-C15-C35
27	B	852	LMG	C8-C7-O1-C1

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Mol	Chain	Res	Type	Atoms
21	G	204	CLA	C2A-CAA-CBA-CGA
27	3	722	LMG	C33-C34-C35-C36
21	A	815	CLA	C4-C3-C5-C6
21	B	808	CLA	C4-C3-C5-C6
21	Z	611	CLA	C10-C11-C12-C13
27	1	628	LMG	C32-C33-C34-C35
26	A	861	LMU	O5'-C5'-C6'-O6'
26	B	853	LMU	O5'-C5'-C6'-O6'
26	8	628	LMU	O5'-C5'-C6'-O6'
27	7	626	LMG	O6-C5-C6-O5
27	8	626	LMG	O6-C5-C6-O5
26	1	622	LMU	O5'-C5'-C6'-O6'
27	8	629	LMG	O6-C5-C6-O5
29	B	850	DGD	O6E-C5E-C6E-O5E
26	A	858	LMU	O5'-C5'-C6'-O6'
26	6	630	LMU	O5'-C5'-C6'-O6'
26	6	631	LMU	O5'-C5'-C6'-O6'
21	B	813	CLA	C10-C11-C12-C13
21	Z	604	CLA	C5-C6-C7-C8
27	J	104	LMG	O6-C5-C6-O5
26	A	864	LMU	O5'-C5'-C6'-O6'
26	1	625	LMU	O5'-C5'-C6'-O6'
23	6	629	LHG	C1-C2-C3-O3
21	4	613	CLA	C13-C15-C16-C17
23	Z	620	LHG	C29-C30-C31-C32
21	B	811	CLA	C2A-CAA-CBA-CGA
21	9	613	CLA	C2A-CAA-CBA-CGA
30	8	606	CHL	C2A-CAA-CBA-CGA
26	8	625	LMU	O5'-C5'-C6'-O6'
21	A	854	CLA	C1A-C2A-CAA-CBA
21	B	840	CLA	C1A-C2A-CAA-CBA
21	F	304	CLA	C1A-C2A-CAA-CBA
21	J	101	CLA	C1A-C2A-CAA-CBA
21	1	611	CLA	C1A-C2A-CAA-CBA
21	9	603	CLA	C1A-C2A-CAA-CBA
23	3	721	LHG	O6-C4-C5-C6
23	8	620	LHG	O6-C4-C5-C6
26	G	206	LMU	O5'-C5'-C6'-O6'
21	A	829	CLA	C11-C10-C8-C7
21	F	301	CLA	C11-C12-C13-C15
22	A	844	PQN	C17-C18-C20-C21
21	A	813	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
21	A	828	CLA	C2-C3-C5-C6
27	6	633	LMG	C17-C18-C19-C20
21	6	603	CLA	C5-C6-C7-C8
21	A	809	CLA	C14-C13-C15-C16
21	A	823	CLA	C6-C7-C8-C9
21	L	203	CLA	C14-C13-C15-C16
30	4	601	CHL	C11-C10-C8-C9
21	B	841	CLA	C8-C10-C11-C12
23	A	846	LHG	C27-C28-C29-C30
21	A	843	CLA	CBA-CGA-O2A-C1
26	A	858	LMU	O5B-C5B-C6B-O6B
26	8	627	LMU	O5B-C5B-C6B-O6B
27	4	624	LMG	O6-C5-C6-O5
21	8	602	CLA	C16-C17-C18-C20
23	1	620	LHG	C30-C31-C32-C33
30	5	606	CHL	CHA-CBD-CGD-O1D
30	5	606	CHL	CHA-CBD-CGD-O2D
21	A	815	CLA	C2-C3-C5-C6
21	B	808	CLA	C2-C3-C5-C6
21	B	841	CLA	C10-C11-C12-C13
30	5	607	CHL	C8-C10-C11-C12
30	8	607	CHL	C15-C16-C17-C18
21	A	823	CLA	O2A-C1-C2-C3
21	Z	611	CLA	O2A-C1-C2-C3
21	9	613	CLA	O2A-C1-C2-C3
21	A	813	CLA	C13-C15-C16-C17
21	B	816	CLA	C15-C16-C17-C18
21	8	602	CLA	C15-C16-C17-C18
23	A	847	LHG	C7-C8-C9-C10
26	8	627	LMU	C5'-C4'-O1B-C1B
23	B	851	LHG	O6-C4-C5-O7
26	1	621	LMU	O5'-C1'-O1'-C1
21	A	840	CLA	C15-C16-C17-C18
21	A	818	CLA	C4-C3-C5-C6
30	8	606	CHL	C2-C3-C5-C6
26	1	623	LMU	C11-C10-C9-C8
27	4	627	LMG	C11-C12-C13-C14
23	8	620	LHG	O7-C5-C6-O8
27	A	860	LMG	O7-C8-C9-O8
27	4	624	LMG	O1-C7-C8-O7
30	6	607	CHL	C15-C16-C17-C18
21	A	806	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	A	820	CLA	C4-C3-C5-C6
21	A	830	CLA	C4-C3-C5-C6
21	B	822	CLA	C4-C3-C5-C6
21	B	839	CLA	C4-C3-C5-C6
21	K	203	CLA	C4-C3-C5-C6
21	1	609	CLA	C4-C3-C5-C6
21	1	613	CLA	C4-C3-C5-C6
21	8	614	CLA	C4-C3-C5-C6
21	4	603	CLA	C4-C3-C5-C6
21	4	614	CLA	C4-C3-C5-C6
30	8	606	CHL	C4-C3-C5-C6
30	4	606	CHL	C4-C3-C5-C6
21	B	828	CLA	C2-C3-C5-C6
21	B	832	CLA	C2-C3-C5-C6
23	4	623	LHG	C5-C6-O8-C23
21	7	610	CLA	CBA-CGA-O2A-C1
21	8	603	CLA	C15-C16-C17-C18
26	8	627	LMU	O5'-C5'-C6'-O6'
26	A	858	LMU	C2-C1-O1'-C1'
26	A	862	LMU	C2-C1-O1'-C1'
26	7	629	LMU	C2-C1-O1'-C1'
26	8	627	LMU	C2-C1-O1'-C1'
21	A	810	CLA	C11-C10-C8-C9
21	A	829	CLA	C11-C10-C8-C9
21	B	815	CLA	C14-C13-C15-C16
21	F	301	CLA	C11-C12-C13-C14
22	A	844	PQN	C19-C18-C20-C21
21	F	304	CLA	C4B-C3B-CAB-CBB
21	1	613	CLA	C4B-C3B-CAB-CBB
21	6	604	CLA	C4B-C3B-CAB-CBB
21	6	611	CLA	C4B-C3B-CAB-CBB
21	9	603	CLA	C4B-C3B-CAB-CBB
21	1	608	CLA	C10-C11-C12-C13
23	B	851	LHG	O6-C4-C5-C6
23	5	623	LHG	O6-C4-C5-C6
26	4	625	LMU	C3-C4-C5-C6
21	A	809	CLA	C12-C13-C15-C16
21	A	810	CLA	C11-C10-C8-C7
21	A	822	CLA	C6-C7-C8-C10
21	A	823	CLA	C6-C7-C8-C10
21	7	613	CLA	C11-C12-C13-C15
21	4	609	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
30	4	601	CHL	C11-C10-C8-C7
23	3	623	LHG	C28-C29-C30-C31
30	5	607	CHL	C15-C16-C17-C18
21	A	811	CLA	C4-C3-C5-C6
21	Z	611	CLA	C4-C3-C5-C6
30	6	601	CHL	C4-C3-C5-C6
21	8	614	CLA	C2-C3-C5-C6
21	A	854	CLA	C5-C6-C7-C8
27	3	722	LMG	C36-C37-C38-C39
21	A	841	CLA	C10-C11-C12-C13
21	9	609	CLA	C4-C3-C5-C6
26	8	627	LMU	C3'-C4'-O1B-C1B
27	8	629	LMG	C14-C15-C16-C17
23	4	623	LHG	C1-C2-C3-O3
21	A	806	CLA	C10-C11-C12-C13
23	B	851	LHG	C4-C5-C6-O8
23	8	620	LHG	C4-C5-C6-O8
21	Z	616	CLA	C3-C5-C6-C7
21	A	813	CLA	C16-C17-C18-C19
30	6	607	CHL	C1A-C2A-CAA-CBA
21	A	810	CLA	C4-C3-C5-C6
21	A	828	CLA	C4-C3-C5-C6
21	A	841	CLA	C4-C3-C5-C6
21	B	828	CLA	C4-C3-C5-C6
21	B	832	CLA	C4-C3-C5-C6
21	A	806	CLA	C2-C3-C5-C6
21	A	820	CLA	C2-C3-C5-C6
21	A	830	CLA	C2-C3-C5-C6
21	A	841	CLA	C2-C3-C5-C6
21	B	827	CLA	C2-C3-C5-C6
21	B	839	CLA	C2-C3-C5-C6
21	1	609	CLA	C2-C3-C5-C6
21	4	614	CLA	C2-C3-C5-C6
23	Z	620	LHG	C23-C24-C25-C26
23	A	847	LHG	O6-C4-C5-O7
23	3	623	LHG	O6-C4-C5-O7
23	3	721	LHG	O6-C4-C5-O7
23	8	620	LHG	O6-C4-C5-O7
23	4	622	LHG	O6-C4-C5-O7
23	4	623	LHG	O6-C4-C5-O7
23	6	629	LHG	O6-C4-C5-O7
21	F	304	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	A	848	BCR	C1-C6-C7-C8
24	B	846	BCR	C23-C24-C25-C30
24	B	847	BCR	C23-C24-C25-C30
24	B	848	BCR	C1-C6-C7-C8
24	L	201	BCR	C1-C6-C7-C8
24	3	719	BCR	C23-C24-C25-C30
28	1	619	LUT	C1-C6-C7-C8
28	3	621	LUT	C1-C6-C7-C8
28	3	622	LUT	C1-C6-C7-C8
28	7	621	LUT	C1-C6-C7-C8
28	8	617	LUT	C1-C6-C7-C8
28	5	620	LUT	C1-C6-C7-C8
28	6	621	LUT	C1-C6-C7-C8
30	4	601	CHL	C15-C16-C17-C18
23	3	721	LHG	C5-C4-O6-P
21	A	810	CLA	C2A-CAA-CBA-CGA
21	G	203	CLA	C2A-CAA-CBA-CGA
21	B	812	CLA	C4-C3-C5-C6
21	6	613	CLA	C4-C3-C5-C6
21	B	812	CLA	C2-C3-C5-C6
21	K	203	CLA	C2-C3-C5-C6
21	1	613	CLA	C2-C3-C5-C6
21	Z	611	CLA	C2-C3-C5-C6
21	4	603	CLA	C2-C3-C5-C6
30	4	606	CHL	C2-C3-C5-C6
30	6	601	CHL	C2-C3-C5-C6
21	8	613	CLA	C14-C13-C15-C16
29	B	850	DGD	C2A-C3A-C4A-C5A
27	4	627	LMG	C8-C7-O1-C1
21	B	827	CLA	C4-C3-C5-C6
32	6	625	NEX	C33-C34-C35-C15
21	6	613	CLA	C2-C3-C5-C6
21	B	811	CLA	C15-C16-C17-C18
23	4	623	LHG	C13-C14-C15-C16
21	L	203	CLA	C3-C5-C6-C7
23	Z	620	LHG	O6-C4-C5-C6
23	6	629	LHG	O6-C4-C5-C6
21	B	818	CLA	C6-C7-C8-C10
21	L	203	CLA	C12-C13-C15-C16
21	5	603	CLA	C12-C13-C15-C16
22	A	844	PQN	C21-C22-C23-C25
30	3	608	CHL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
30	8	607	CHL	C6-C7-C8-C10
30	Z	601	CHL	C6-C7-C8-C10
23	6	619	LHG	C25-C26-C27-C28
27	3	722	LMG	C34-C35-C36-C37
27	A	859	LMG	C8-C7-O1-C1
27	A	860	LMG	C8-C7-O1-C1
21	L	203	CLA	C8-C10-C11-C12
21	A	839	CLA	C4-C3-C5-C6
21	A	840	CLA	C4-C3-C5-C6
21	B	807	CLA	C4-C3-C5-C6
21	4	611	CLA	C4-C3-C5-C6
29	B	850	DGD	O2G-C1B-C2B-C3B
21	A	854	CLA	C3-C5-C6-C7
21	B	824	CLA	O2A-C1-C2-C3
30	8	607	CHL	O2A-C1-C2-C3
30	Z	607	CHL	O2A-C1-C2-C3
23	8	620	LHG	C16-C17-C18-C19
23	8	620	LHG	C11-C10-C9-C8
21	A	843	CLA	O1A-CGA-O2A-C1
26	8	627	LMU	O1'-C1-C2-C3
23	1	620	LHG	O6-C4-C5-O7
23	5	623	LHG	O6-C4-C5-O7
26	8	627	LMU	O5'-C1'-O1'-C1
27	B	852	LMG	O1-C7-C8-C9
27	J	104	LMG	O1-C7-C8-C9
27	4	624	LMG	O1-C7-C8-C9
21	8	602	CLA	C16-C17-C18-C19
21	B	823	CLA	C4-C3-C5-C6
21	A	810	CLA	C2-C3-C5-C6
21	B	822	CLA	C2-C3-C5-C6
23	5	623	LHG	O7-C5-C6-O8
27	A	859	LMG	O1-C7-C8-O7
27	B	852	LMG	O1-C7-C8-O7
27	J	104	LMG	O1-C7-C8-O7
21	B	839	CLA	C14-C13-C15-C16
21	7	613	CLA	C11-C12-C13-C14
32	6	625	NEX	C9-C10-C11-C12
26	7	628	LMU	C2'-C1'-O1'-C1
21	B	831	CLA	C4-C3-C5-C6
21	6	604	CLA	C4-C3-C5-C6
23	5	623	LHG	C24-C25-C26-C27
30	5	607	CHL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
30	6	607	CHL	C4C-C3C-CAC-CBC
26	A	857	LMU	O1'-C1-C2-C3
26	A	857	LMU	C2-C1-O1'-C1'
26	6	632	LMU	C2-C1-O1'-C1'
26	A	863	LMU	C5'-C4'-O1B-C1B
27	B	852	LMG	C11-C12-C13-C14
21	A	807	CLA	C4B-C3B-CAB-CBB
21	B	808	CLA	C4B-C3B-CAB-CBB
21	B	819	CLA	C4B-C3B-CAB-CBB
21	G	203	CLA	C4B-C3B-CAB-CBB
21	3	613	CLA	C4B-C3B-CAB-CBB
21	4	603	CLA	C4B-C3B-CAB-CBB
30	4	601	CHL	C4-C3-C5-C6
21	B	832	CLA	C13-C15-C16-C17
23	A	847	LHG	O6-C4-C5-C6
23	1	620	LHG	O6-C4-C5-C6
23	3	623	LHG	O6-C4-C5-C6
23	4	622	LHG	O6-C4-C5-C6
23	4	623	LHG	O6-C4-C5-C6
23	6	619	LHG	O6-C4-C5-C6
23	9	622	LHG	O6-C4-C5-C6
21	A	823	CLA	C11-C12-C13-C15
21	A	840	CLA	C12-C13-C15-C16
21	A	842	CLA	C11-C10-C8-C7
21	B	809	CLA	C11-C10-C8-C7
21	B	813	CLA	C11-C10-C8-C7
21	1	609	CLA	C11-C10-C8-C7
21	5	601	CLA	C11-C10-C8-C7
22	B	842	PQN	C16-C17-C18-C20
30	1	601	CHL	C11-C10-C8-C7
23	Z	620	LHG	O6-C4-C5-O7
23	6	619	LHG	O6-C4-C5-O7
23	9	622	LHG	O6-C4-C5-O7
21	B	818	CLA	C6-C7-C8-C9
21	5	601	CLA	C11-C12-C13-C14
30	Z	601	CHL	C6-C7-C8-C9
26	A	863	LMU	C3'-C4'-O1B-C1B
23	6	629	LHG	C13-C14-C15-C16
21	A	840	CLA	C2-C3-C5-C6
21	B	823	CLA	C2-C3-C5-C6
21	A	804	CLA	CAD-CBD-CGD-O2D
21	A	806	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	B	841	CLA	CAD-CBD-CGD-O2D
21	5	603	CLA	CAD-CBD-CGD-O2D
30	1	601	CHL	CAD-CBD-CGD-O2D
30	Z	601	CHL	CAD-CBD-CGD-O2D
21	7	610	CLA	O1A-CGA-O2A-C1
26	1	621	LMU	O5B-C1B-O1B-C4'
21	A	809	CLA	C2A-CAA-CBA-CGA
23	7	625	LHG	O8-C23-C24-C25
20	A	801	CL0	CHA-CBD-CGD-O2D
21	A	804	CLA	CAD-CBD-CGD-O1D
21	A	806	CLA	CAD-CBD-CGD-O1D
21	A	812	CLA	CHA-CBD-CGD-O1D
21	A	812	CLA	CHA-CBD-CGD-O2D
21	A	816	CLA	CHA-CBD-CGD-O1D
21	A	816	CLA	CHA-CBD-CGD-O2D
21	A	823	CLA	CHA-CBD-CGD-O1D
21	A	823	CLA	CHA-CBD-CGD-O2D
21	A	826	CLA	CHA-CBD-CGD-O1D
21	A	826	CLA	CHA-CBD-CGD-O2D
21	A	838	CLA	CHA-CBD-CGD-O2D
21	B	815	CLA	CHA-CBD-CGD-O1D
21	B	815	CLA	CHA-CBD-CGD-O2D
21	B	821	CLA	CHA-CBD-CGD-O1D
21	B	821	CLA	CHA-CBD-CGD-O2D
21	B	841	CLA	CAD-CBD-CGD-O1D
21	G	203	CLA	CHA-CBD-CGD-O1D
21	G	204	CLA	CHA-CBD-CGD-O1D
21	K	206	CLA	CHA-CBD-CGD-O1D
21	K	206	CLA	CHA-CBD-CGD-O2D
21	1	602	CLA	CHA-CBD-CGD-O1D
21	1	602	CLA	CHA-CBD-CGD-O2D
21	3	612	CLA	CHA-CBD-CGD-O1D
21	3	612	CLA	CHA-CBD-CGD-O2D
21	8	612	CLA	CHA-CBD-CGD-O1D
21	8	612	CLA	CHA-CBD-CGD-O2D
21	Z	602	CLA	CHA-CBD-CGD-O1D
21	Z	602	CLA	CHA-CBD-CGD-O2D
21	Z	612	CLA	CHA-CBD-CGD-O1D
21	Z	612	CLA	CHA-CBD-CGD-O2D
21	4	602	CLA	CHA-CBD-CGD-O1D
21	4	602	CLA	CHA-CBD-CGD-O2D
21	5	603	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
21	5	612	CLA	CHA-CBD-CGD-O1D
21	5	612	CLA	CHA-CBD-CGD-O2D
21	6	602	CLA	CHA-CBD-CGD-O1D
21	6	602	CLA	CHA-CBD-CGD-O2D
21	6	612	CLA	CHA-CBD-CGD-O1D
21	6	612	CLA	CHA-CBD-CGD-O2D
21	9	603	CLA	CHA-CBD-CGD-O1D
21	9	603	CLA	CHA-CBD-CGD-O2D
21	9	612	CLA	CHA-CBD-CGD-O1D
21	9	612	CLA	CHA-CBD-CGD-O2D
23	3	623	LHG	C3-O3-P-O4
23	3	623	LHG	C4-O6-P-O3
23	3	623	LHG	C4-O6-P-O4
23	3	623	LHG	C4-O6-P-O5
23	3	721	LHG	C4-O6-P-O4
23	8	620	LHG	C3-O3-P-O5
23	4	622	LHG	C4-O6-P-O3
23	4	623	LHG	C4-O6-P-O3
23	5	623	LHG	C3-O3-P-O4
23	6	619	LHG	C4-O6-P-O3
23	6	629	LHG	C4-O6-P-O5
23	9	622	LHG	C3-O3-P-O5
23	9	622	LHG	C4-O6-P-O5
30	1	601	CHL	CAD-CBD-CGD-O1D
30	8	607	CHL	CHA-CBD-CGD-O1D
30	8	607	CHL	CHA-CBD-CGD-O2D
30	Z	601	CHL	CAD-CBD-CGD-O1D
30	4	606	CHL	CHA-CBD-CGD-O1D
30	4	606	CHL	CHA-CBD-CGD-O2D
30	4	607	CHL	CHA-CBD-CGD-O2D
30	6	607	CHL	CHA-CBD-CGD-O1D
30	6	607	CHL	CHA-CBD-CGD-O2D
23	7	625	LHG	C24-C25-C26-C27
21	B	805	CLA	C4-C3-C5-C6
21	B	820	CLA	C4-C3-C5-C6
21	B	836	CLA	C4-C3-C5-C6
21	3	613	CLA	C4-C3-C5-C6
21	B	808	CLA	C2B-C3B-CAB-CBB
21	B	819	CLA	C2B-C3B-CAB-CBB
21	B	839	CLA	C2B-C3B-CAB-CBB
21	3	611	CLA	C2B-C3B-CAB-CBB
21	Z	613	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
21	5	614	CLA	C2B-C3B-CAB-CBB
28	4	619	LUT	C1-C6-C7-C8
21	A	811	CLA	C2-C3-C5-C6
21	B	807	CLA	C2-C3-C5-C6
21	4	611	CLA	C2-C3-C5-C6
21	6	604	CLA	C2-C3-C5-C6
30	8	607	CHL	C10-C11-C12-C13
30	6	616	CHL	C13-C15-C16-C17
21	A	819	CLA	CAA-CBA-CGA-O2A
26	1	621	LMU	C2B-C1B-O1B-C4'
23	6	629	LHG	C4-C5-O7-C7
27	3	722	LMG	C7-C8-O7-C10
26	Z	622	LMU	C5'-C4'-O1B-C1B
21	B	817	CLA	CAA-CBA-CGA-O2A
21	B	827	CLA	C13-C15-C16-C17
26	1	621	LMU	C3'-C4'-O1B-C1B
21	Z	603	CLA	CAA-CBA-CGA-O2A
21	A	812	CLA	C14-C13-C15-C16
21	B	837	CLA	C11-C12-C13-C14
21	3	603	CLA	C11-C12-C13-C14
21	5	603	CLA	C6-C7-C8-C9
22	A	844	PQN	C21-C22-C23-C24
30	8	607	CHL	C6-C7-C8-C9
30	5	607	CHL	C11-C10-C8-C9
21	8	613	CLA	C12-C13-C15-C16
23	7	625	LHG	O6-C4-C5-O7
21	A	803	CLA	C2A-CAA-CBA-CGA
21	3	603	CLA	C10-C11-C12-C13
21	A	821	CLA	C4-C3-C5-C6
21	A	818	CLA	C2-C3-C5-C6
26	Z	622	LMU	C3'-C4'-O1B-C1B
23	3	623	LHG	C2-C3-O3-P
23	7	625	LHG	C25-C26-C27-C28
23	4	623	LHG	O7-C5-C6-O8
27	8	629	LMG	O8-C28-C29-C30
23	4	623	LHG	C9-C10-C11-C12
30	8	601	CHL	CAA-CBA-CGA-O2A
21	B	817	CLA	C2A-CAA-CBA-CGA
27	A	859	LMG	O1-C7-C8-C9
27	A	860	LMG	C7-C8-C9-O8
20	A	801	CL0	C5-C6-C7-C8
21	B	807	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
23	B	851	LHG	O7-C7-C8-C9
27	1	628	LMG	C8-C7-O1-C1
21	B	820	CLA	C2-C3-C5-C6
21	5	617	CLA	C10-C11-C12-C13
21	A	854	CLA	C2C-C3C-CAC-CBC
26	B	853	LMU	C2-C1-O1'-C1'
26	1	621	LMU	C2-C1-O1'-C1'
26	8	628	LMU	C2-C1-O1'-C1'
26	8	625	LMU	C2-C1-O1'-C1'
21	A	822	CLA	C6-C7-C8-C9
21	B	809	CLA	C11-C10-C8-C9
21	K	203	CLA	C11-C10-C8-C9
21	7	611	CLA	C11-C12-C13-C14
27	3	722	LMG	C32-C33-C34-C35
23	B	851	LHG	C10-C11-C12-C13
21	A	812	CLA	C4B-C3B-CAB-CBB
21	5	604	CLA	C4-C3-C5-C6
27	8	629	LMG	C15-C16-C17-C18
21	3	609	CLA	C5-C6-C7-C8
21	A	820	CLA	C6-C7-C8-C10
21	B	806	CLA	C6-C7-C8-C10
21	K	203	CLA	C11-C10-C8-C7
21	7	611	CLA	C11-C12-C13-C15
26	1	621	LMU	C5'-C4'-O1B-C1B
23	4	622	LHG	C28-C29-C30-C31
23	8	620	LHG	C18-C19-C20-C21
21	Z	609	CLA	C3A-C2A-CAA-CBA
21	4	609	CLA	C3A-C2A-CAA-CBA
21	5	603	CLA	C4-C3-C5-C6
21	B	805	CLA	C2-C3-C5-C6
21	B	836	CLA	C2-C3-C5-C6
24	A	852	BCR	C11-C10-C9-C34
24	A	852	BCR	C16-C17-C18-C36
24	B	845	BCR	C11-C10-C9-C34
24	B	845	BCR	C20-C21-C22-C37
24	L	201	BCR	C11-C10-C9-C34
28	F	305	LUT	C20-C13-C14-C15
32	5	625	NEX	C39-C29-C30-C31
32	6	625	NEX	C39-C29-C30-C31
21	B	809	CLA	C8-C10-C11-C12
23	6	619	LHG	C11-C10-C9-C8
21	A	832	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
21	A	843	CLA	C2-C1-O2A-CGA
21	7	603	CLA	C2-C1-O2A-CGA
21	8	608	CLA	C2-C1-O2A-CGA
21	Z	608	CLA	C2-C1-O2A-CGA
21	5	603	CLA	C5-C6-C7-C8
21	5	612	CLA	CAA-CBA-CGA-O2A
21	1	614	CLA	C4-C3-C5-C6
21	Z	609	CLA	C4-C3-C5-C6
21	3	613	CLA	C2-C3-C5-C6
30	4	601	CHL	C2-C3-C5-C6
23	4	623	LHG	C4-C5-C6-O8
21	A	843	CLA	C11-C12-C13-C14
21	B	805	CLA	C14-C13-C15-C16
21	B	811	CLA	C11-C10-C8-C9
21	3	603	CLA	C6-C7-C8-C9
21	3	613	CLA	C11-C10-C8-C9
21	3	615	CLA	C11-C10-C8-C9
21	5	603	CLA	C11-C10-C8-C9
21	5	609	CLA	C6-C7-C8-C9
21	6	613	CLA	C11-C10-C8-C9
30	8	601	CHL	C11-C10-C8-C9
30	4	608	CHL	C14-C13-C15-C16
21	4	612	CLA	CAA-CBA-CGA-O2A
30	Z	606	CHL	CAA-CBA-CGA-O2A
29	B	850	DGD	C1G-C2G-O2G-C1B
23	B	851	LHG	C24-C25-C26-C27
21	A	835	CLA	C4-C3-C5-C6
21	1	611	CLA	C4-C3-C5-C6
21	7	603	CLA	C4-C3-C5-C6
23	1	620	LHG	C23-C24-C25-C26
21	A	821	CLA	C2-C3-C5-C6
21	5	603	CLA	C2-C3-C5-C6
26	A	857	LMU	C5'-C4'-O1B-C1B
23	7	625	LHG	C31-C32-C33-C34
21	B	805	CLA	C1A-C2A-CAA-CBA
21	B	822	CLA	C1A-C2A-CAA-CBA
21	Z	609	CLA	C1A-C2A-CAA-CBA
21	5	621	CLA	C1A-C2A-CAA-CBA
24	A	852	BCR	C11-C10-C9-C8
24	A	852	BCR	C16-C17-C18-C19
24	B	845	BCR	C11-C10-C9-C8
24	B	845	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
24	L	201	BCR	C11-C10-C9-C8
28	F	305	LUT	C12-C13-C14-C15
32	5	625	NEX	C28-C29-C30-C31
32	6	625	NEX	C28-C29-C30-C31
21	Z	612	CLA	CAA-CBA-CGA-O1A
21	6	612	CLA	CAA-CBA-CGA-O1A
26	Z	622	LMU	O1'-C1-C2-C3
21	A	807	CLA	C2B-C3B-CAB-CBB
21	B	810	CLA	C2B-C3B-CAB-CBB
21	G	203	CLA	C2B-C3B-CAB-CBB
21	1	613	CLA	C2B-C3B-CAB-CBB
21	3	613	CLA	C2B-C3B-CAB-CBB
21	6	604	CLA	C2B-C3B-CAB-CBB
21	9	603	CLA	C2B-C3B-CAB-CBB
24	A	848	BCR	C5-C6-C7-C8
24	B	847	BCR	C23-C24-C25-C26
24	B	848	BCR	C5-C6-C7-C8
24	3	718	BCR	C23-C24-C25-C30
24	3	719	BCR	C23-C24-C25-C26
24	7	623	BCR	C23-C24-C25-C26
24	8	619	BCR	C23-C24-C25-C26
24	6	623	BCR	C23-C24-C25-C26
28	1	617	LUT	C5-C6-C7-C8
28	1	619	LUT	C5-C6-C7-C8
28	3	621	LUT	C5-C6-C7-C8
28	3	622	LUT	C5-C6-C7-C8
28	7	621	LUT	C5-C6-C7-C8
28	8	617	LUT	C5-C6-C7-C8
28	Z	617	LUT	C5-C6-C7-C8
28	6	621	LUT	C5-C6-C7-C8
28	9	616	LUT	C5-C6-C7-C8
21	Z	612	CLA	CAA-CBA-CGA-O2A
30	Z	606	CHL	CAA-CBA-CGA-O1A
21	B	827	CLA	C3-C5-C6-C7
30	8	601	CHL	C15-C16-C17-C18
21	B	829	CLA	C4-C3-C5-C6
21	3	607	CLA	C4-C3-C5-C6
21	8	613	CLA	C4-C3-C5-C6
21	6	603	CLA	C4-C3-C5-C6
23	7	625	LHG	O6-C4-C5-C6
21	1	614	CLA	C2-C3-C5-C6
21	Z	609	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	B	850	DGD	C9B-CAB-CBB-CCB
21	6	612	CLA	CAA-CBA-CGA-O2A
30	1	607	CHL	CAA-CBA-CGA-O1A
21	A	837	CLA	C6-C7-C8-C10
21	B	819	CLA	C11-C10-C8-C7
21	B	823	CLA	C11-C12-C13-C15
21	B	825	CLA	C11-C10-C8-C7
21	B	837	CLA	C11-C12-C13-C15
30	6	607	CHL	C6-C7-C8-C10
29	B	850	DGD	O1G-C1G-C2G-O2G
21	4	613	CLA	CAA-CBA-CGA-O2A
21	F	303	CLA	CAA-CBA-CGA-O1A
21	A	854	CLA	C4-C3-C5-C6
21	B	809	CLA	C4-C3-C5-C6
21	B	818	CLA	C4-C3-C5-C6
21	1	611	CLA	C2-C3-C5-C6
21	5	604	CLA	C2-C3-C5-C6
27	3	722	LMG	C8-C7-O1-C1
26	G	206	LMU	C7-C8-C9-C10
30	7	601	CHL	C11-C12-C13-C14
21	1	613	CLA	C15-C16-C17-C18
21	4	612	CLA	CAA-CBA-CGA-O1A
21	5	612	CLA	CAA-CBA-CGA-O1A
21	B	837	CLA	C4-C3-C5-C6
21	F	303	CLA	CAA-CBA-CGA-O2A
21	L	204	CLA	CAA-CBA-CGA-O2A
21	5	612	CLA	C4C-C3C-CAC-CBC
21	A	836	CLA	CAA-CBA-CGA-O2A
27	6	633	LMG	C15-C16-C17-C18
21	B	813	CLA	C8-C10-C11-C12
30	3	608	CHL	C2A-CAA-CBA-CGA
21	3	603	CLA	C4-C3-C5-C6
30	4	618	CHL	CAA-CBA-CGA-O2A
21	3	607	CLA	C5-C6-C7-C8
26	1	625	LMU	C2-C3-C4-C5
21	B	807	CLA	C4B-C3B-CAB-CBB
21	1	616	CLA	C4B-C3B-CAB-CBB
21	8	609	CLA	C4B-C3B-CAB-CBB
21	4	616	CLA	C4B-C3B-CAB-CBB
21	B	813	CLA	C2C-C3C-CAC-CBC
26	A	857	LMU	C3'-C4'-O1B-C1B
21	B	817	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
20	A	801	CL0	CHA-CBD-CGD-O1D
23	8	620	LHG	C17-C18-C19-C20
23	3	623	LHG	C32-C33-C34-C35
21	A	814	CLA	C16-C17-C18-C19
23	4	622	LHG	C9-C10-C11-C12
30	1	607	CHL	CAA-CBA-CGA-O2A
21	3	607	CLA	C2-C3-C5-C6
27	J	104	LMG	O6-C1-O1-C7
26	5	627	LMU	C6-C7-C8-C9
26	6	630	LMU	C3-C4-C5-C6
21	1	612	CLA	CAA-CBA-CGA-O1A
21	9	612	CLA	CAA-CBA-CGA-O2A
30	6	607	CHL	C13-C15-C16-C17
21	A	811	CLA	C11-C12-C13-C14
21	A	820	CLA	C11-C12-C13-C14
21	A	826	CLA	C11-C10-C8-C9
21	B	808	CLA	C11-C10-C8-C9
21	1	609	CLA	C14-C13-C15-C16
21	5	609	CLA	C11-C10-C8-C9
21	6	603	CLA	C14-C13-C15-C16
22	B	842	PQN	C16-C17-C18-C19
21	6	622	CLA	C2A-CAA-CBA-CGA
21	5	603	CLA	C2-C1-O2A-CGA
30	1	601	CHL	C2-C1-O2A-CGA
30	8	607	CHL	C2-C1-O2A-CGA
21	B	805	CLA	C3A-C2A-CAA-CBA
21	Z	603	CLA	C3A-C2A-CAA-CBA
21	4	609	CLA	C2C-C3C-CAC-CBC
21	1	612	CLA	CAA-CBA-CGA-O2A
21	A	830	CLA	C5-C6-C7-C8
21	9	614	CLA	CAA-CBA-CGA-O2A
30	4	618	CHL	CAA-CBA-CGA-O1A
21	3	615	CLA	CAA-CBA-CGA-O2A
23	4	622	LHG	O8-C23-C24-C25
27	J	104	LMG	C2-C1-O1-C7
21	9	609	CLA	O2A-C1-C2-C3
21	A	824	CLA	CAA-CBA-CGA-O2A
27	6	633	LMG	O7-C10-C11-C12
27	4	624	LMG	C12-C13-C14-C15
21	1	614	CLA	CAA-CBA-CGA-O2A
21	A	833	CLA	C5-C6-C7-C8
21	L	204	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
21	9	614	CLA	CAA-CBA-CGA-O1A
21	B	831	CLA	C2-C3-C5-C6
21	7	611	CLA	C10-C11-C12-C13
21	B	815	CLA	C4-C3-C5-C6
21	8	603	CLA	CAA-CBA-CGA-O2A
27	A	860	LMG	O7-C10-C11-C12
27	6	633	LMG	O9-C10-C11-C12
21	4	609	CLA	C4C-C3C-CAC-CBC
21	A	806	CLA	C8-C10-C11-C12
21	A	824	CLA	CAA-CBA-CGA-O1A
27	8	629	LMG	C13-C14-C15-C16
21	9	612	CLA	CAA-CBA-CGA-O1A
21	1	608	CLA	C13-C15-C16-C17
21	A	836	CLA	C14-C13-C15-C16
30	1	601	CHL	C11-C10-C8-C9
30	8	607	CHL	C11-C10-C8-C9
30	Z	607	CHL	C6-C7-C8-C9
30	4	606	CHL	C11-C10-C8-C9
27	3	722	LMG	C40-C41-C42-C43
21	B	836	CLA	C3-C5-C6-C7
23	3	721	LHG	O7-C7-C8-C9
21	6	603	CLA	C2-C3-C5-C6
21	A	823	CLA	C2A-CAA-CBA-CGA
30	4	608	CHL	C2A-CAA-CBA-CGA
21	A	811	CLA	C6-C7-C8-C10
21	A	811	CLA	C11-C12-C13-C15
21	A	841	CLA	C11-C10-C8-C7
21	A	843	CLA	C11-C10-C8-C7
21	A	843	CLA	C11-C12-C13-C15
21	B	814	CLA	C6-C7-C8-C10
21	B	837	CLA	C12-C13-C15-C16
21	1	613	CLA	C11-C12-C13-C15
21	3	613	CLA	C11-C10-C8-C7
21	3	615	CLA	C11-C10-C8-C7
21	Z	609	CLA	C11-C10-C8-C7
30	1	601	CHL	C6-C7-C8-C10
30	7	601	CHL	C11-C12-C13-C15
30	8	601	CHL	C11-C10-C8-C7
30	4	608	CHL	C12-C13-C15-C16
21	B	813	CLA	C4C-C3C-CAC-CBC
21	A	812	CLA	C2B-C3B-CAB-CBB
21	K	203	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
21	K	204	CLA	C2B-C3B-CAB-CBB
21	1	608	CLA	C2B-C3B-CAB-CBB
21	8	609	CLA	C2B-C3B-CAB-CBB
21	4	616	CLA	C2B-C3B-CAB-CBB
21	9	609	CLA	C2B-C3B-CAB-CBB
24	B	846	BCR	C23-C24-C25-C26
24	G	205	BCR	C1-C6-C7-C8
24	L	205	BCR	C23-C24-C25-C26
24	L	205	BCR	C23-C24-C25-C30
28	4	619	LUT	C5-C6-C7-C8
28	5	620	LUT	C5-C6-C7-C8
21	A	810	CLA	C2-C1-O2A-CGA
21	6	609	CLA	C2-C1-O2A-CGA
21	4	613	CLA	C5-C6-C7-C8
21	B	838	CLA	CAA-CBA-CGA-O2A
27	3	722	LMG	O8-C28-C29-C30
26	6	631	LMU	O5'-C1'-O1'-C1
21	A	814	CLA	C16-C17-C18-C20
21	Z	602	CLA	C11-C12-C13-C14
21	5	601	CLA	C15-C16-C17-C18
27	B	852	LMG	C28-C29-C30-C31
21	8	604	CLA	C2-C3-C5-C6
21	B	831	CLA	C2A-CAA-CBA-CGA
30	6	606	CHL	C2A-CAA-CBA-CGA
21	A	807	CLA	CAA-CBA-CGA-O2A
21	A	826	CLA	CAA-CBA-CGA-O2A
30	8	606	CHL	CAA-CBA-CGA-O2A
26	A	857	LMU	C2-C3-C4-C5
23	A	846	LHG	C25-C26-C27-C28
21	8	614	CLA	CAA-CBA-CGA-O2A
27	J	104	LMG	O7-C10-C11-C12
21	B	817	CLA	C4C-C3C-CAC-CBC
23	7	625	LHG	C26-C27-C28-C29
21	1	603	CLA	CAA-CBA-CGA-O2A
21	4	603	CLA	CAA-CBA-CGA-O2A
21	1	614	CLA	C2A-CAA-CBA-CGA
21	8	616	CLA	CAA-CBA-CGA-O1A
21	B	806	CLA	CAA-CBA-CGA-O2A
27	J	104	LMG	O8-C28-C29-C30
26	A	864	LMU	C2-C1-O1'-C1'
21	B	837	CLA	C13-C15-C16-C17
21	A	823	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
21	A	840	CLA	C14-C13-C15-C16
21	A	842	CLA	C11-C10-C8-C9
21	5	601	CLA	C11-C10-C8-C9
27	1	628	LMG	C31-C32-C33-C34
21	B	841	CLA	CAA-CBA-CGA-O2A
23	4	622	LHG	O7-C7-C8-C9
21	B	810	CLA	C4B-C3B-CAB-CBB
21	B	813	CLA	C1A-C2A-CAA-CBA
21	K	203	CLA	C4B-C3B-CAB-CBB
21	K	204	CLA	C4B-C3B-CAB-CBB
21	1	608	CLA	C4B-C3B-CAB-CBB
21	3	607	CLA	C4B-C3B-CAB-CBB
21	7	614	CLA	C1A-C2A-CAA-CBA
21	5	603	CLA	C1A-C2A-CAA-CBA
21	5	613	CLA	C4B-C3B-CAB-CBB
21	6	613	CLA	C4B-C3B-CAB-CBB
21	9	609	CLA	C4B-C3B-CAB-CBB
21	B	809	CLA	C3-C5-C6-C7
21	9	610	CLA	C4-C3-C5-C6
21	B	809	CLA	CAA-CBA-CGA-O2A
21	5	621	CLA	CAA-CBA-CGA-O2A
23	Z	620	LHG	O8-C23-C24-C25
23	5	623	LHG	O8-C23-C24-C25
27	3	722	LMG	O7-C10-C11-C12
30	4	607	CHL	CAA-CBA-CGA-O2A
27	3	722	LMG	C18-C19-C20-C21
21	Z	609	CLA	CAA-CBA-CGA-O2A
21	4	614	CLA	CAA-CBA-CGA-O2A
21	6	603	CLA	CAA-CBA-CGA-O2A
23	6	619	LHG	O7-C7-C8-C9
27	B	852	LMG	O7-C10-C11-C12
21	J	101	CLA	C2A-CAA-CBA-CGA
30	4	608	CHL	CAA-CBA-CGA-O2A
21	8	616	CLA	CAA-CBA-CGA-O2A
21	B	832	CLA	C15-C16-C17-C18
30	6	607	CHL	C4-C3-C5-C6
21	1	611	CLA	C2-C1-O2A-CGA
21	7	604	CLA	C2-C1-O2A-CGA
21	9	603	CLA	C2-C1-O2A-CGA
21	3	612	CLA	CAA-CBA-CGA-O2A
21	B	809	CLA	C6-C7-C8-C10
21	B	823	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
21	A	806	CLA	O2A-C1-C2-C3
29	B	850	DGD	O1B-C1B-C2B-C3B
27	8	629	LMG	C20-C21-C22-C23
21	F	304	CLA	CAA-CBA-CGA-O2A
21	5	604	CLA	CAA-CBA-CGA-O2A
21	A	806	CLA	C5-C6-C7-C8
21	Z	616	CLA	C8-C10-C11-C12
21	8	614	CLA	CAA-CBA-CGA-O1A
26	B	853	LMU	C5'-C4'-O1B-C1B
21	B	838	CLA	C3A-C2A-CAA-CBA
21	B	841	CLA	C3A-C2A-CAA-CBA
21	3	604	CLA	C4-C3-C5-C6
21	3	611	CLA	C3A-C2A-CAA-CBA
21	3	615	CLA	C3A-C2A-CAA-CBA
21	8	614	CLA	C3A-C2A-CAA-CBA
21	4	613	CLA	C3A-C2A-CAA-CBA
21	5	603	CLA	C3A-C2A-CAA-CBA
21	5	621	CLA	C3A-C2A-CAA-CBA
21	7	612	CLA	CAA-CBA-CGA-O2A
23	B	851	LHG	O8-C23-C24-C25
30	4	601	CHL	CAA-CBA-CGA-O2A
23	3	623	LHG	C33-C34-C35-C36
21	1	616	CLA	C4C-C3C-CAC-CBC
21	A	807	CLA	CAA-CBA-CGA-O1A
27	3	722	LMG	O9-C10-C11-C12
21	3	603	CLA	CAA-CBA-CGA-O2A
21	1	603	CLA	CAA-CBA-CGA-O1A
21	8	603	CLA	CAA-CBA-CGA-O1A
23	3	721	LHG	O9-C7-C8-C9
30	6	616	CHL	C16-C17-C18-C20
21	B	813	CLA	C11-C10-C8-C9
21	8	604	CLA	C4-C3-C5-C6
21	Z	609	CLA	CAA-CBA-CGA-O1A
27	J	104	LMG	O10-C28-C29-C30
21	B	817	CLA	C10-C11-C12-C13
28	7	624	LUT	C21-C26-C27-C28
21	A	826	CLA	CAA-CBA-CGA-O1A
21	B	838	CLA	CAA-CBA-CGA-O1A
21	5	604	CLA	CAA-CBA-CGA-O1A
23	4	622	LHG	O9-C7-C8-C9
27	B	852	LMG	O9-C10-C11-C12
30	4	608	CHL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
21	Z	609	CLA	C13-C15-C16-C17
21	B	806	CLA	CAA-CBA-CGA-O1A
21	4	603	CLA	CAA-CBA-CGA-O1A
21	5	621	CLA	CAA-CBA-CGA-O1A
27	J	103	LMG	C8-C7-O1-C1
27	A	860	LMG	O9-C10-C11-C12
20	A	801	CL0	CAA-CBA-CGA-O2A
30	4	607	CHL	C2A-CAA-CBA-CGA
27	A	859	LMG	C7-C8-C9-O8
21	B	841	CLA	CAA-CBA-CGA-O1A
23	Z	620	LHG	O10-C23-C24-C25
30	4	607	CHL	CAA-CBA-CGA-O1A
23	9	622	LHG	C5-C4-O6-P
21	9	603	CLA	CAA-CBA-CGA-O2A
23	A	846	LHG	O7-C7-C8-C9
21	A	834	CLA	C8-C10-C11-C12
21	6	603	CLA	CAA-CBA-CGA-O1A
27	J	104	LMG	O9-C10-C11-C12
30	8	606	CHL	CAA-CBA-CGA-O1A
21	A	805	CLA	CAD-CBD-CGD-O2D
21	B	805	CLA	CAD-CBD-CGD-O2D
21	B	834	CLA	CAD-CBD-CGD-O2D
21	B	839	CLA	CAD-CBD-CGD-O2D
21	1	612	CLA	CAD-CBD-CGD-O2D
21	7	616	CLA	CAD-CBD-CGD-O2D
21	Z	612	CLA	CAD-CBD-CGD-O2D
21	5	604	CLA	CAD-CBD-CGD-O2D
21	5	612	CLA	CAD-CBD-CGD-O2D
21	9	609	CLA	CAD-CBD-CGD-O2D
30	8	601	CHL	CAD-CBD-CGD-O2D
23	8	620	LHG	O7-C7-C8-C9
27	A	859	LMG	O8-C28-C29-C30
21	B	834	CLA	C3-C5-C6-C7
21	3	603	CLA	CAA-CBA-CGA-O1A
21	4	614	CLA	CAA-CBA-CGA-O1A
23	4	622	LHG	C30-C31-C32-C33
21	A	812	CLA	C2-C1-O2A-CGA
21	4	609	CLA	C2-C1-O2A-CGA
21	B	809	CLA	CAA-CBA-CGA-O1A
21	3	612	CLA	CAA-CBA-CGA-O1A
21	7	613	CLA	CAA-CBA-CGA-O2A
23	6	629	LHG	O7-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
26	8	627	LMU	C7-C8-C9-C10
23	A	846	LHG	O9-C7-C8-C9
23	B	851	LHG	O10-C23-C24-C25
21	B	814	CLA	CAA-CBA-CGA-O2A
21	A	812	CLA	C10-C11-C12-C13
21	B	814	CLA	CAA-CBA-CGA-O1A
26	1	623	LMU	C7-C8-C9-C10
23	7	625	LHG	O7-C7-C8-C9

There are no ring outliers.

126 monomers are involved in 160 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	813	CLA	1	0
31	7	622	XAT	1	0
30	8	601	CHL	1	0
28	9	616	LUT	1	0
21	3	613	CLA	1	0
29	B	850	DGD	1	0
21	B	841	CLA	1	0
21	F	304	CLA	1	0
28	6	621	LUT	1	0
28	5	626	LUT	1	0
21	L	204	CLA	1	0
24	B	844	BCR	2	0
21	5	601	CLA	1	0
21	A	831	CLA	1	0
21	7	614	CLA	1	0
24	B	847	BCR	1	0
21	Z	608	CLA	1	0
21	B	814	CLA	1	0
30	Z	607	CHL	1	0
21	A	802	CLA	2	0
24	B	843	BCR	2	0
21	A	820	CLA	1	0
27	A	859	LMG	3	0
28	F	305	LUT	4	0
28	3	622	LUT	1	0
21	J	101	CLA	1	0
24	K	202	BCR	3	0
21	8	614	CLA	1	0
21	B	803	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A	863	LMU	1	0
30	5	608	CHL	1	0
22	A	844	PQN	1	0
21	A	812	CLA	3	0
21	B	824	CLA	4	0
21	5	617	CLA	2	0
27	4	624	LMG	2	0
21	5	612	CLA	1	0
30	4	601	CHL	1	0
21	A	837	CLA	1	0
24	A	852	BCR	4	0
21	A	810	CLA	3	0
31	5	624	XAT	1	0
21	K	201	CLA	2	0
21	4	616	CLA	2	0
23	7	625	LHG	1	0
21	Z	616	CLA	1	0
24	A	851	BCR	3	0
24	6	623	BCR	3	0
21	A	821	CLA	1	0
21	B	808	CLA	1	0
21	4	613	CLA	4	0
24	A	849	BCR	3	0
24	L	205	BCR	2	0
27	1	628	LMG	1	0
21	3	607	CLA	1	0
30	6	608	CHL	1	0
21	A	811	CLA	2	0
21	A	809	CLA	1	0
21	7	610	CLA	2	0
21	B	826	CLA	2	0
24	4	621	BCR	1	0
21	A	845	CLA	1	0
21	9	613	CLA	2	0
23	3	721	LHG	1	0
24	A	848	BCR	1	0
21	3	615	CLA	4	0
24	5	622	BCR	1	0
21	Z	603	CLA	2	0
21	B	837	CLA	1	0
21	B	802	CLA	2	0
24	B	801	BCR	1	0

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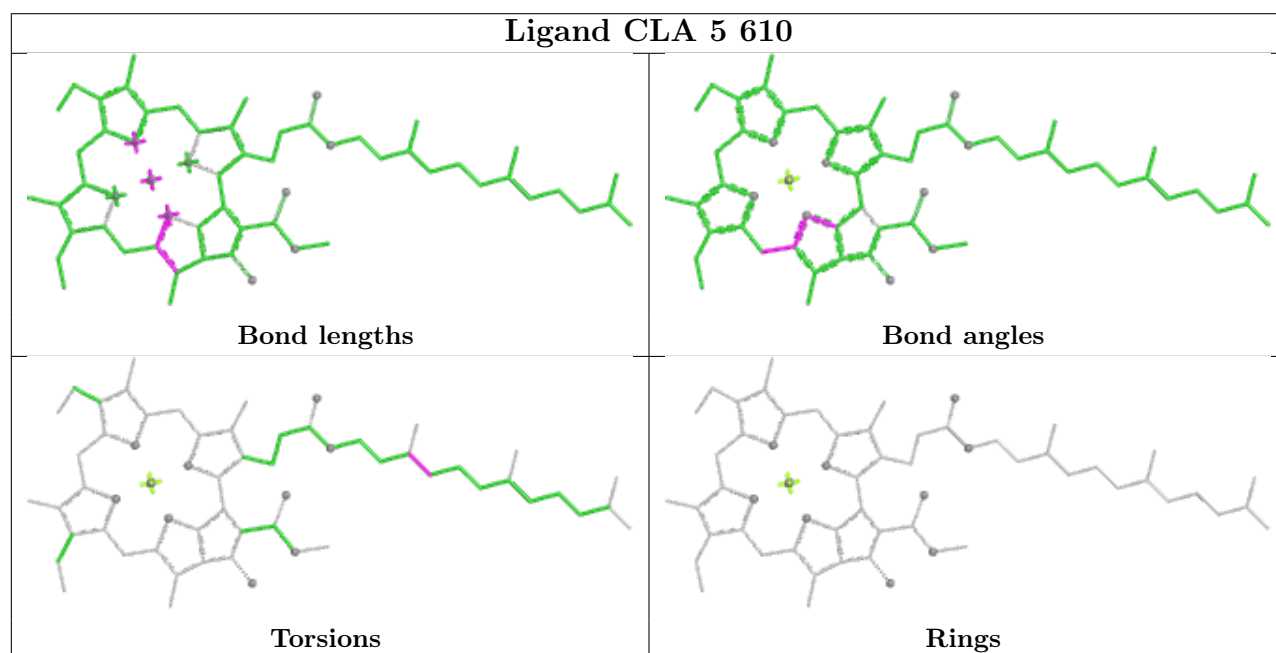
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21	5	602	CLA	1	0
24	B	845	BCR	1	0
23	Z	620	LHG	1	0
21	A	841	CLA	1	0
30	6	616	CHL	1	0
26	1	621	LMU	1	0
27	A	860	LMG	1	0
24	J	102	BCR	2	0
21	A	803	CLA	1	0
21	A	829	CLA	1	0
24	B	848	BCR	1	0
21	B	816	CLA	2	0
21	1	613	CLA	1	0
24	B	846	BCR	1	0
21	4	610	CLA	1	0
28	9	617	LUT	3	0
21	B	829	CLA	1	0
26	A	857	LMU	1	0
21	5	621	CLA	1	0
21	8	603	CLA	2	0
26	A	865	LMU	1	0
21	A	843	CLA	2	0
21	A	854	CLA	2	0
30	5	607	CHL	1	0
21	5	603	CLA	2	0
27	J	103	LMG	1	0
21	G	204	CLA	1	0
21	A	823	CLA	1	0
21	5	616	CLA	3	0
24	G	205	BCR	2	0
21	7	620	CLA	1	0
24	A	850	BCR	1	0
28	7	621	LUT	1	0
21	3	611	CLA	1	0
21	A	818	CLA	1	0
21	B	811	CLA	1	0
21	A	839	CLA	1	0
21	1	603	CLA	2	0
28	5	620	LUT	3	0

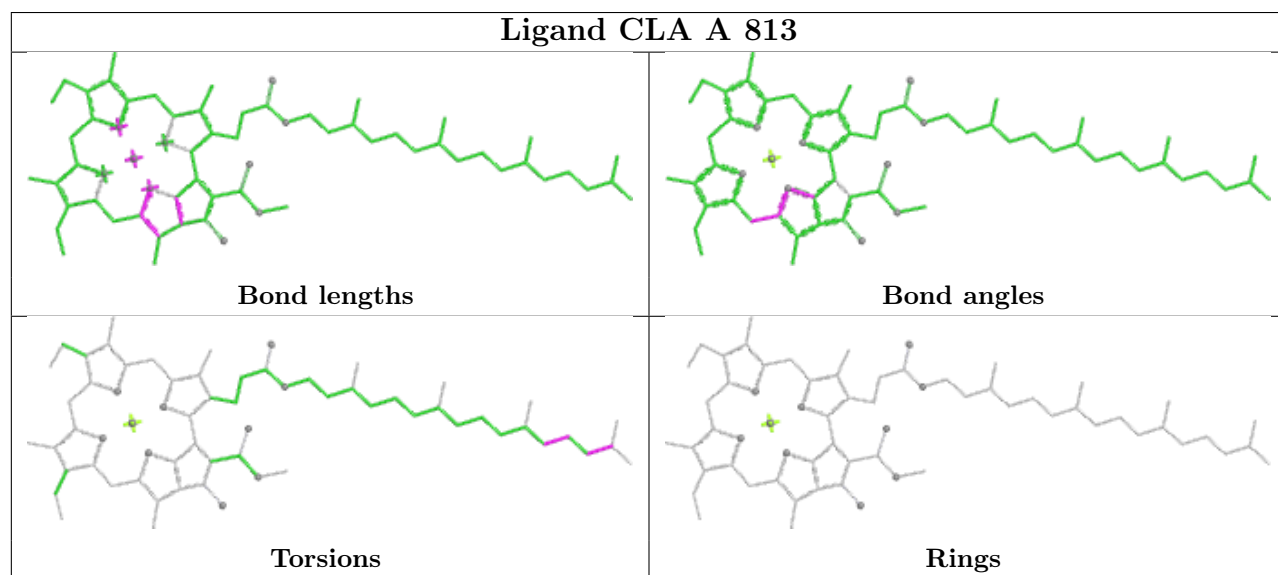
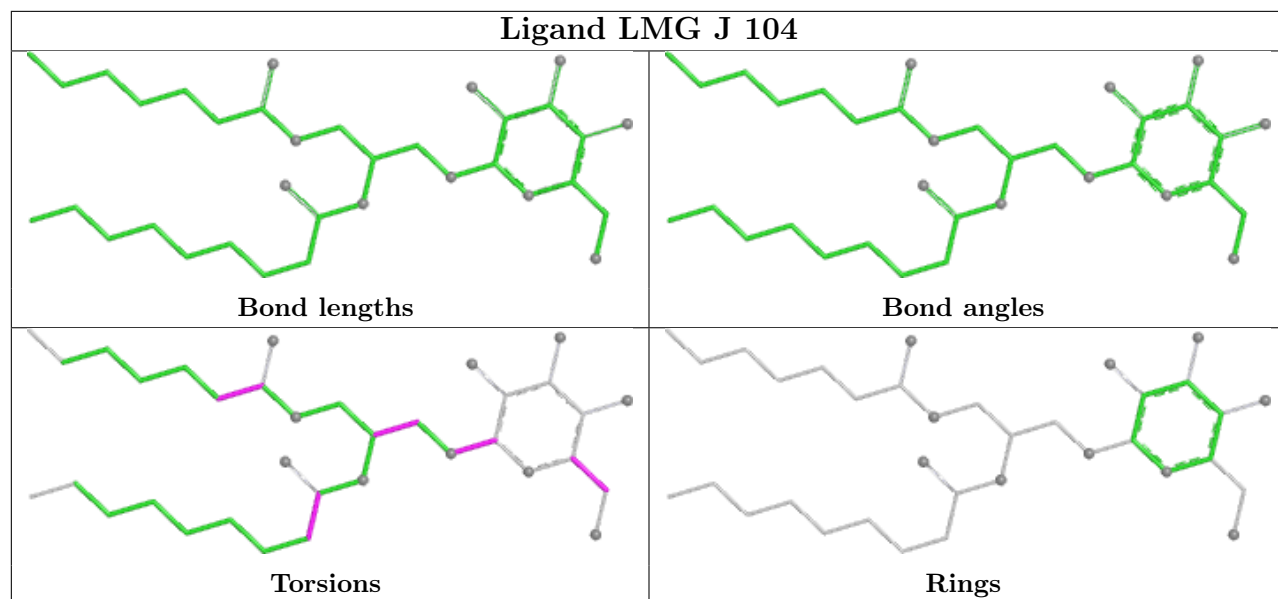
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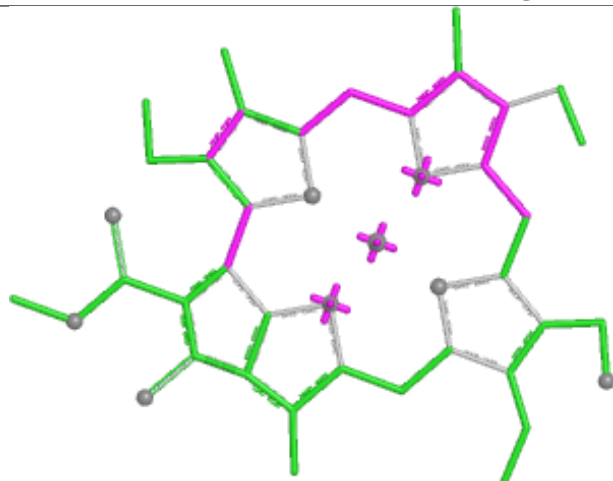
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21	6	603	CLA	1	0
30	4	608	CHL	1	0
28	Z	617	LUT	2	0
21	6	604	CLA	1	0
26	B	853	LMU	2	0
21	8	610	CLA	1	0
24	3	719	BCR	2	0
21	A	830	CLA	1	0
21	A	832	CLA	1	0
28	4	619	LUT	1	0
23	3	623	LHG	1	0
24	K	207	BCR	2	0

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

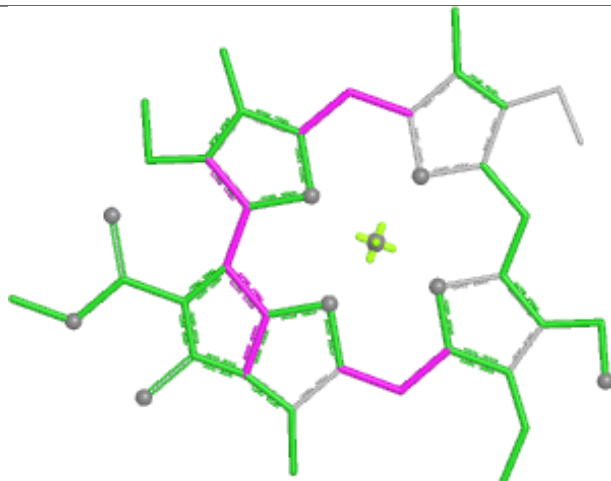




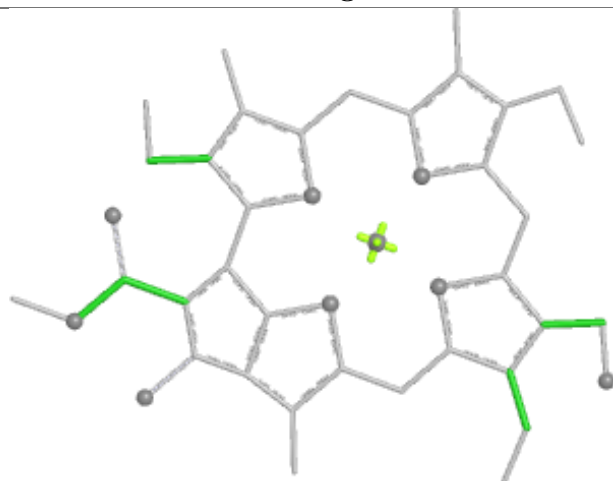
Ligand CHL 6 618



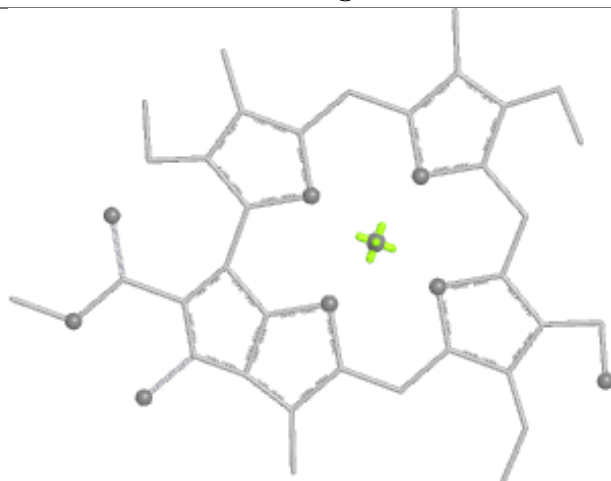
Bond lengths



Bond angles

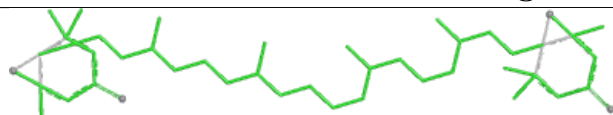


Torsions

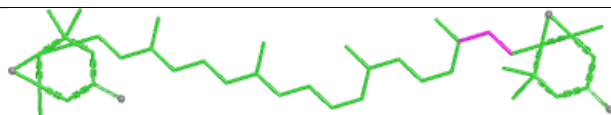


Rings

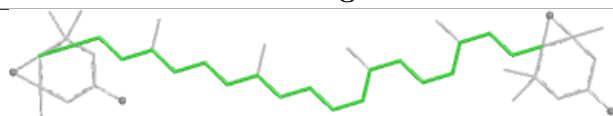
Ligand XAT 6 624



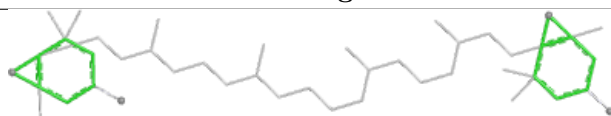
Bond lengths



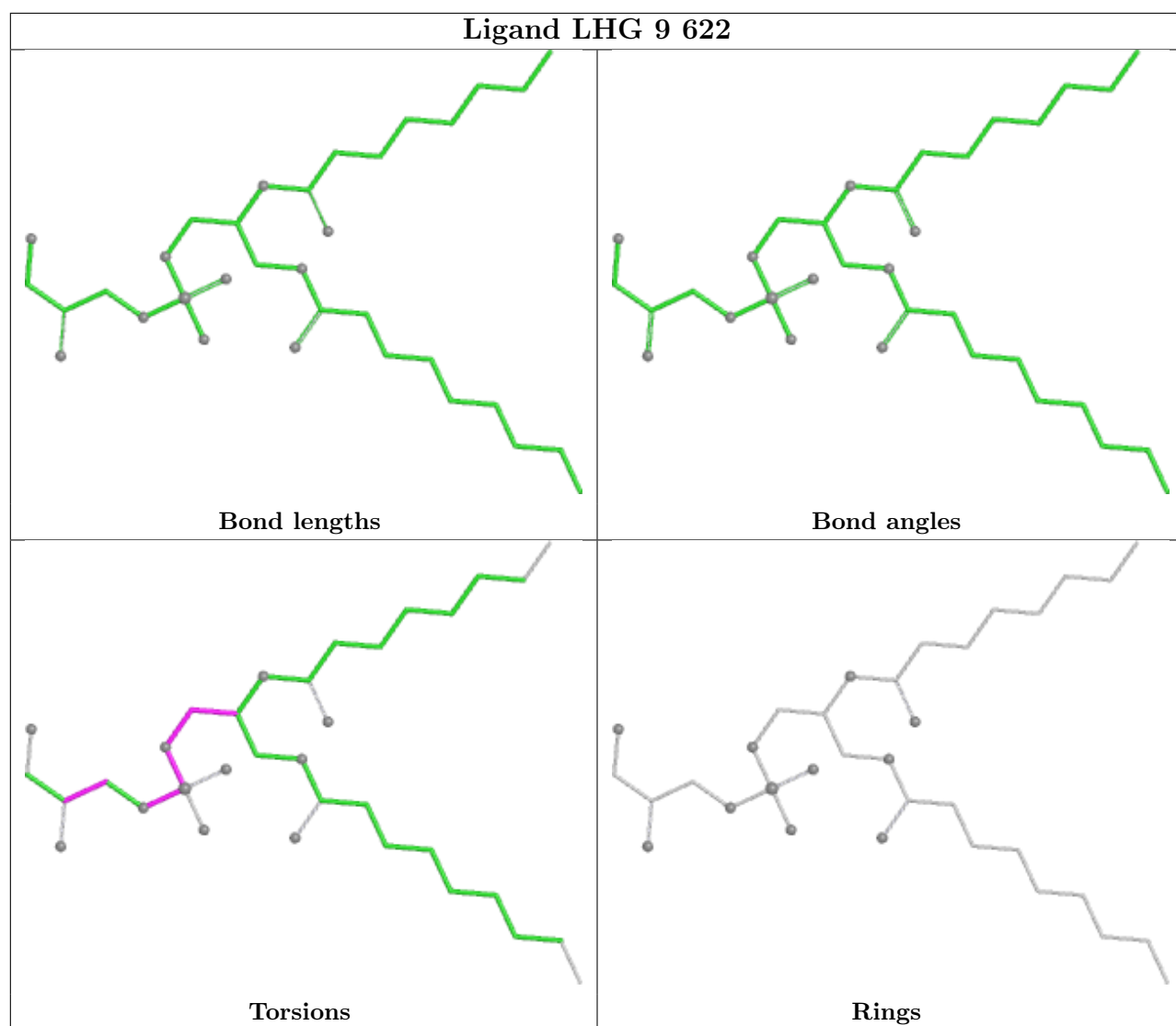
Bond angles

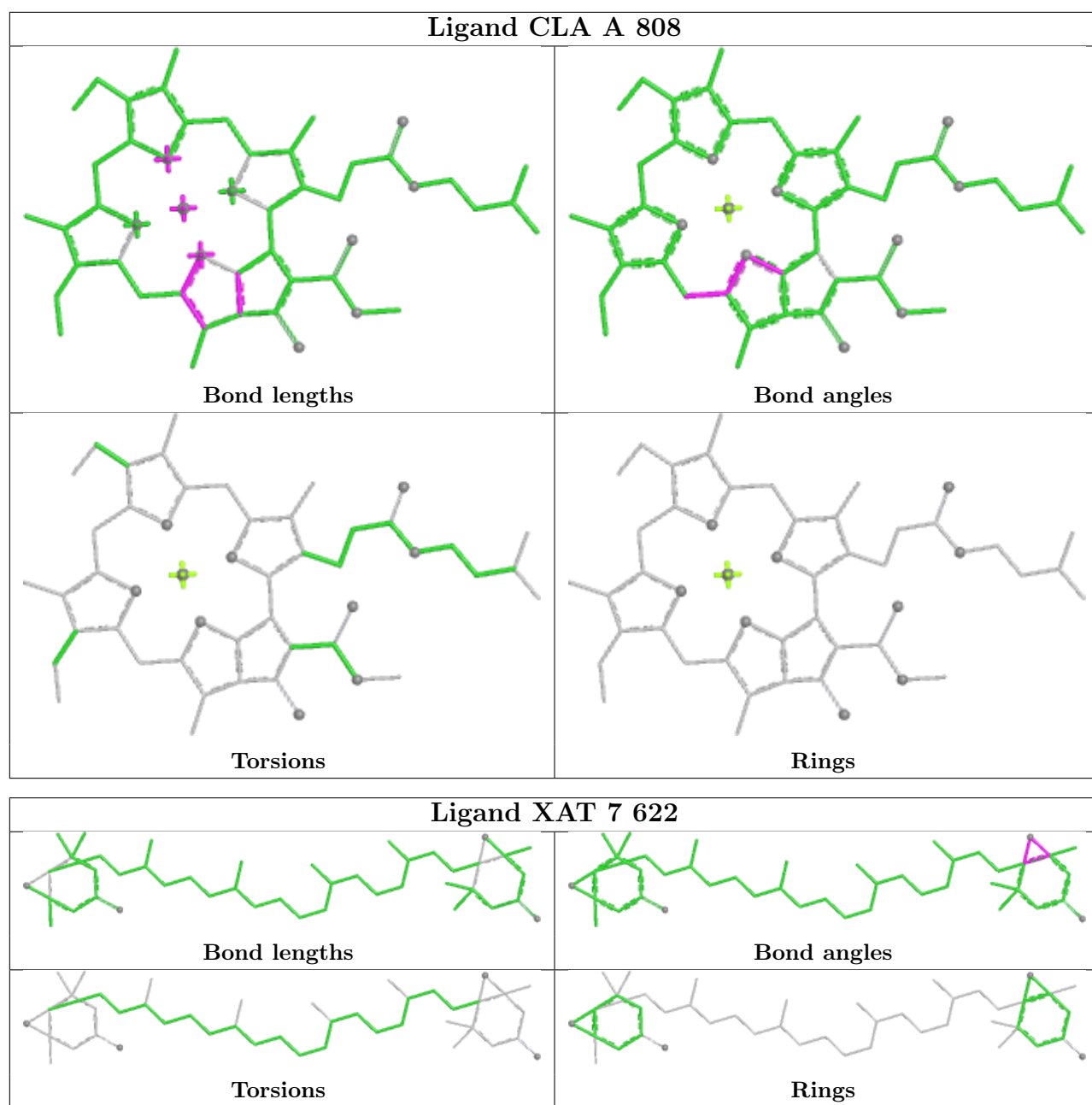


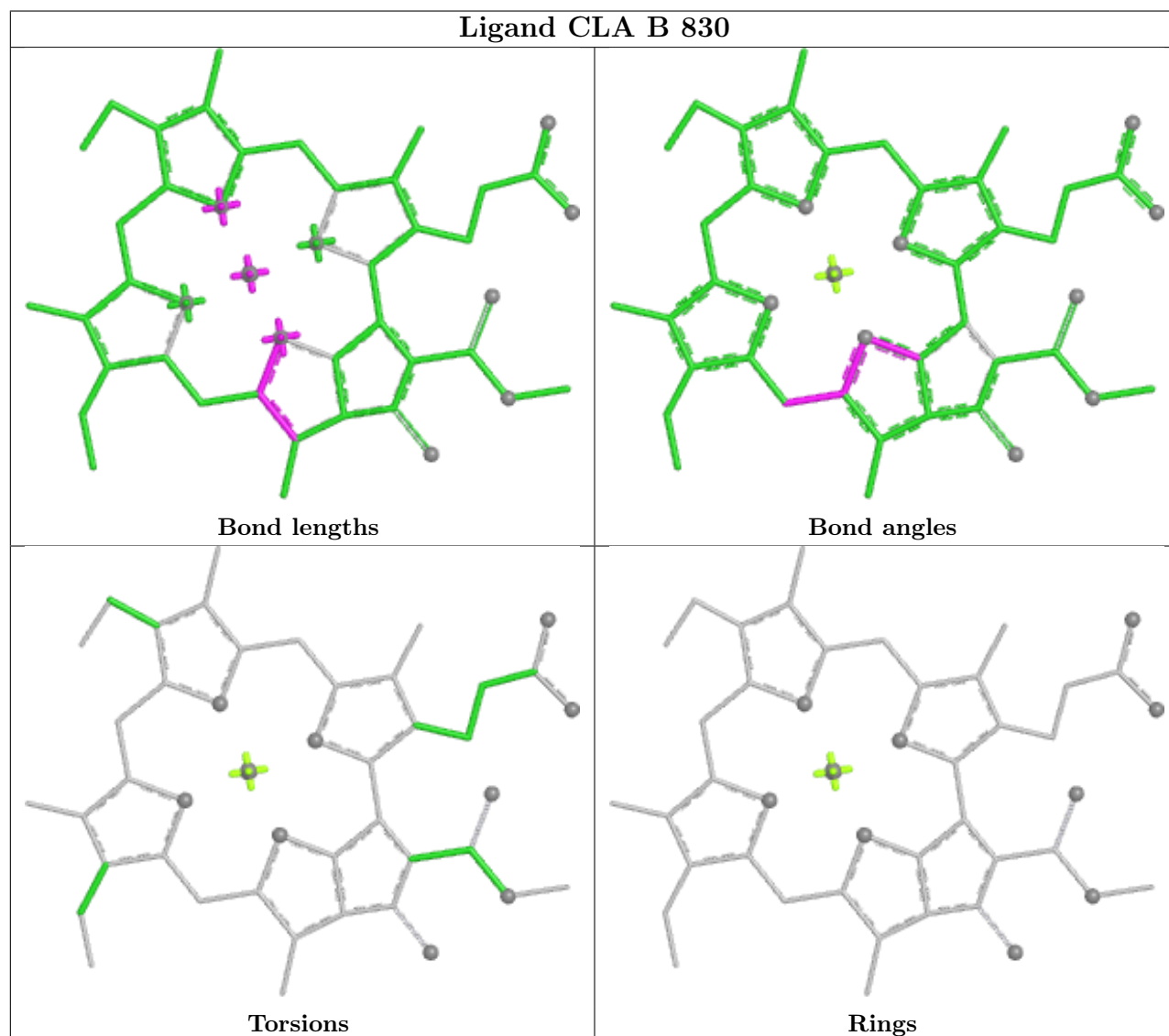
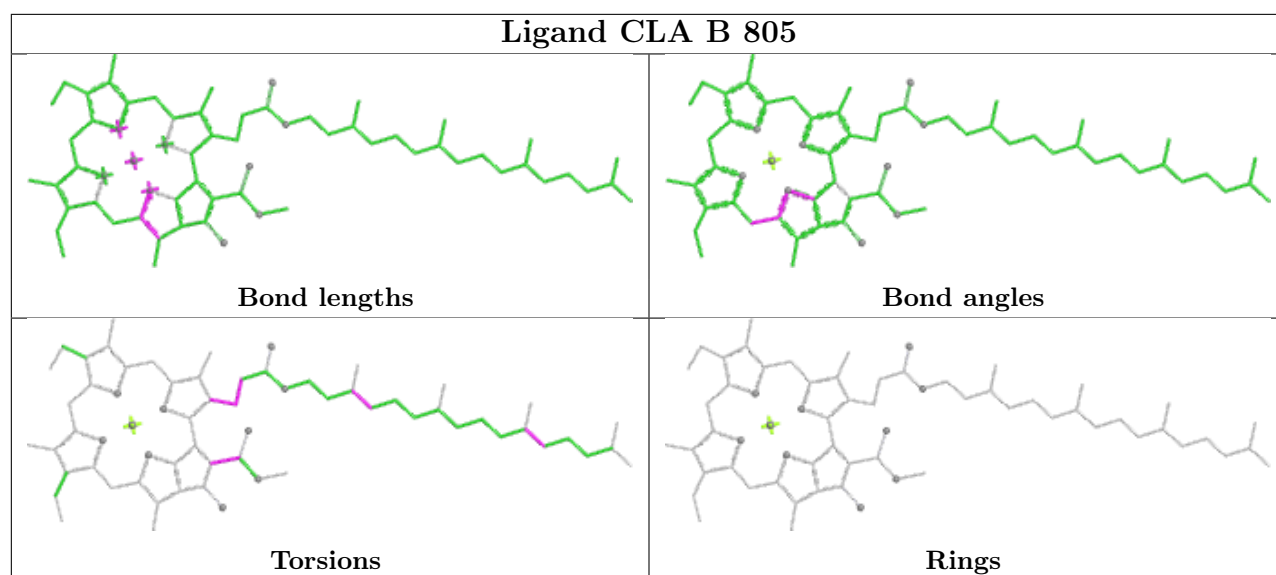
Torsions

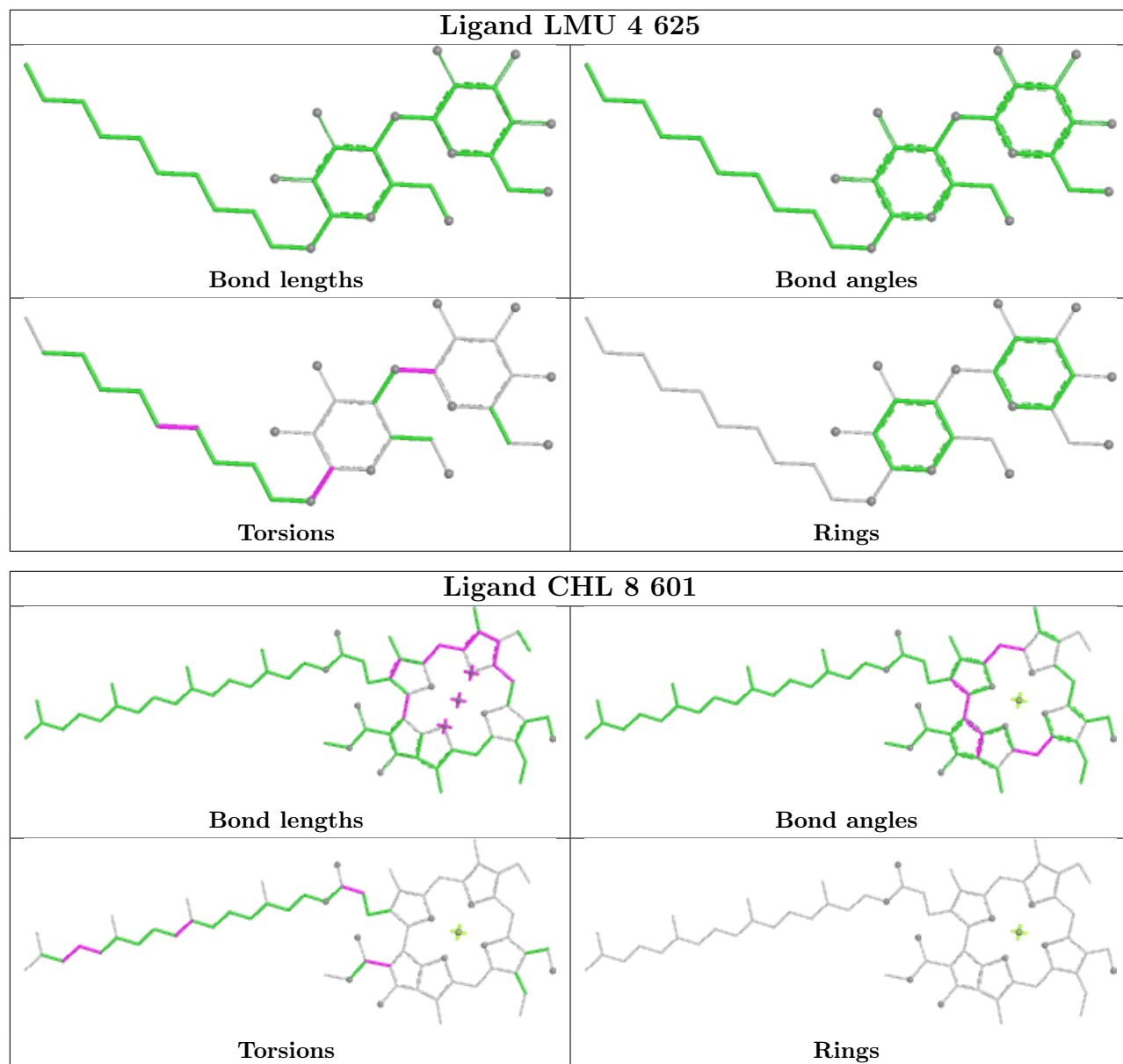


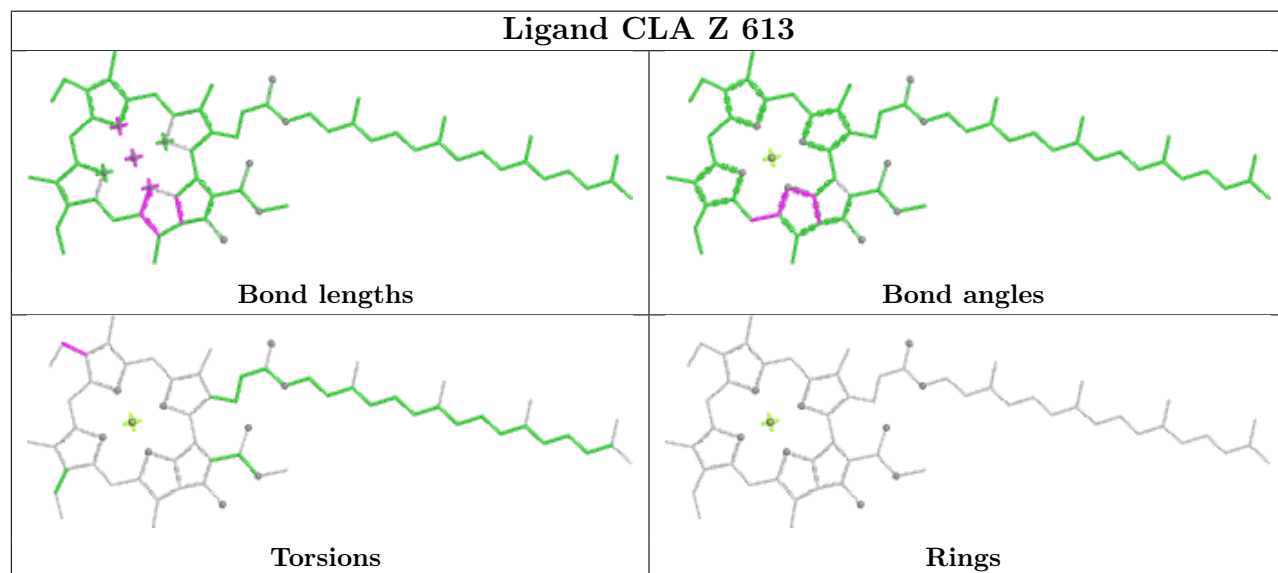
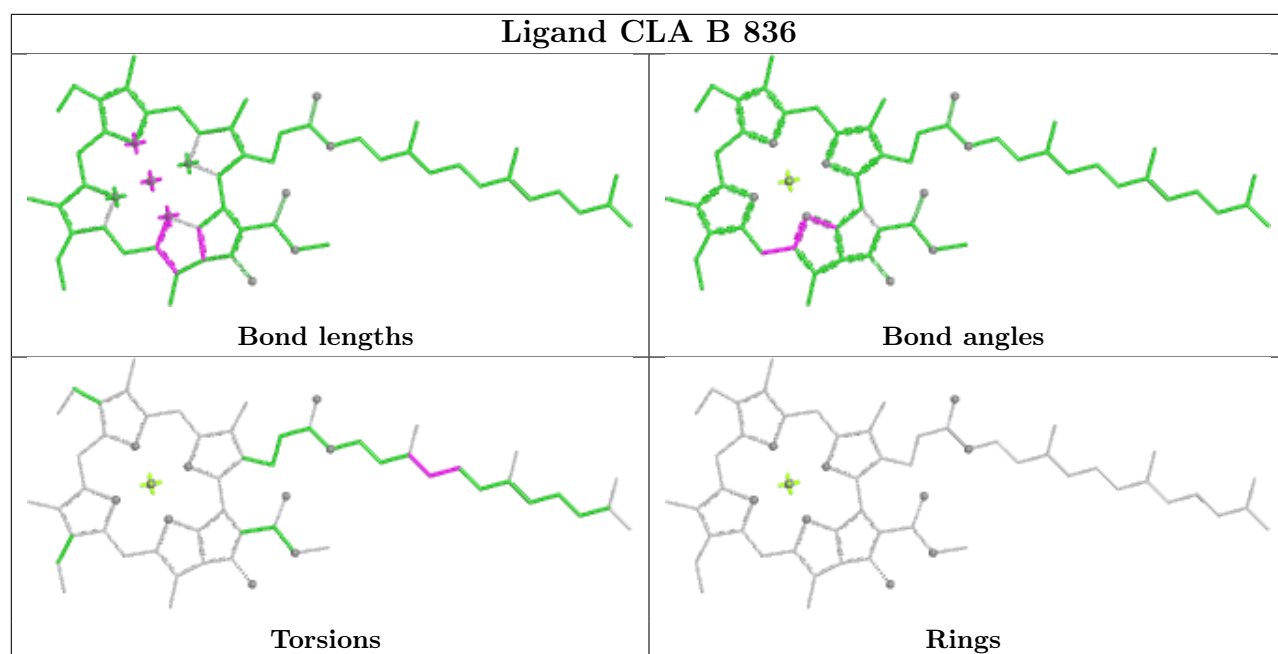
Rings

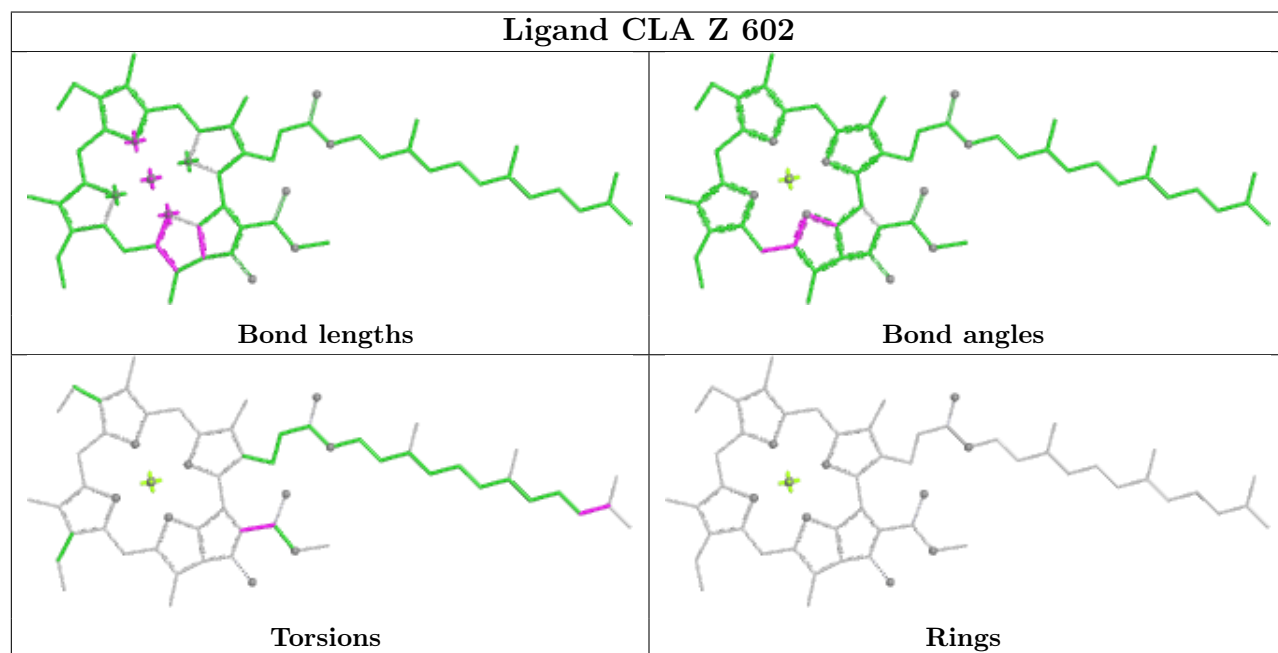
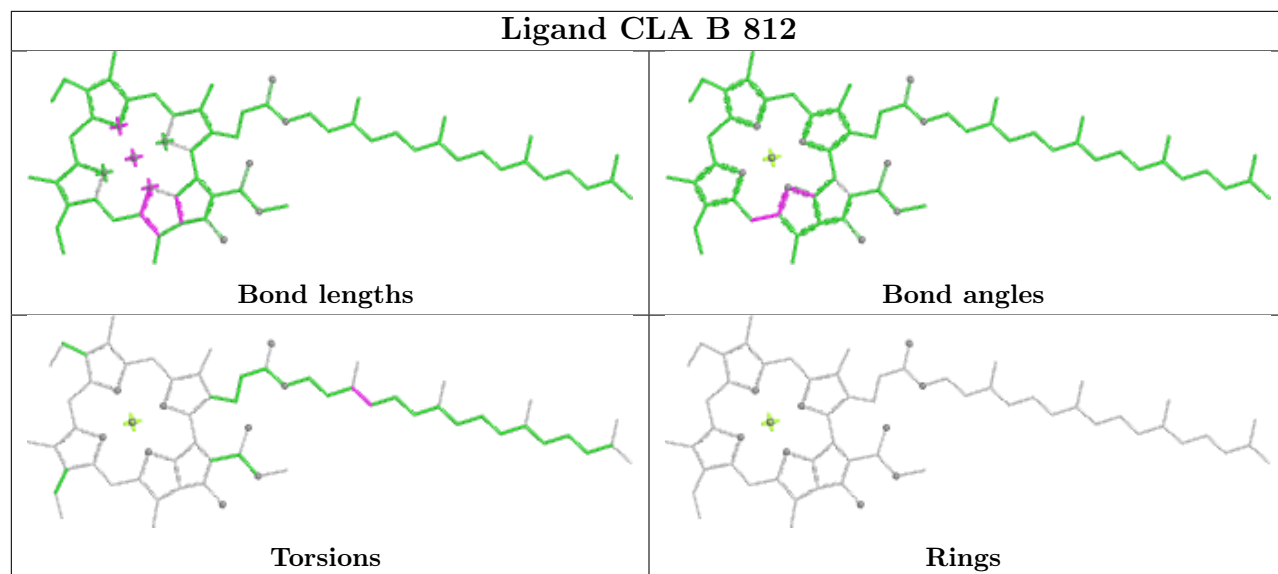




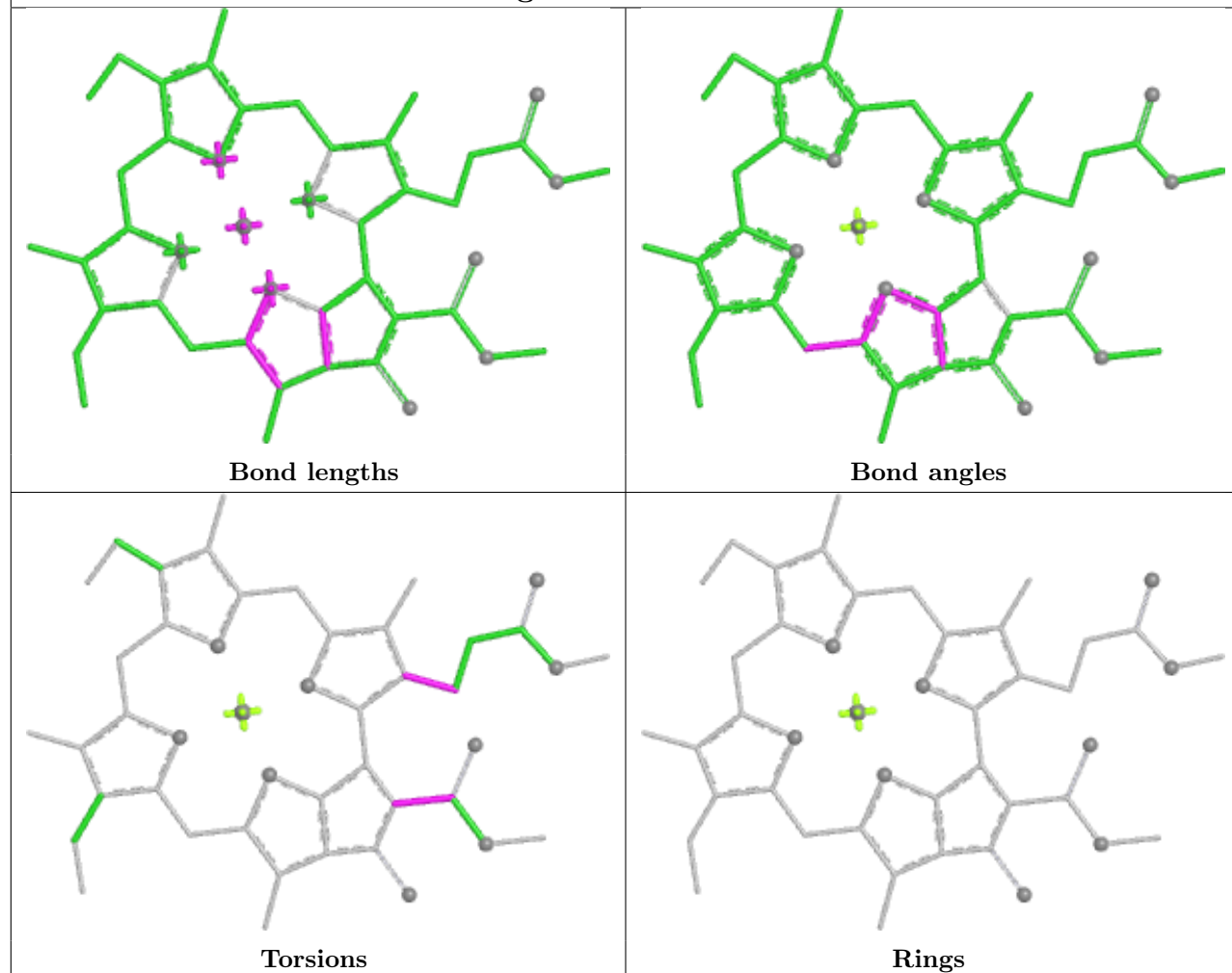




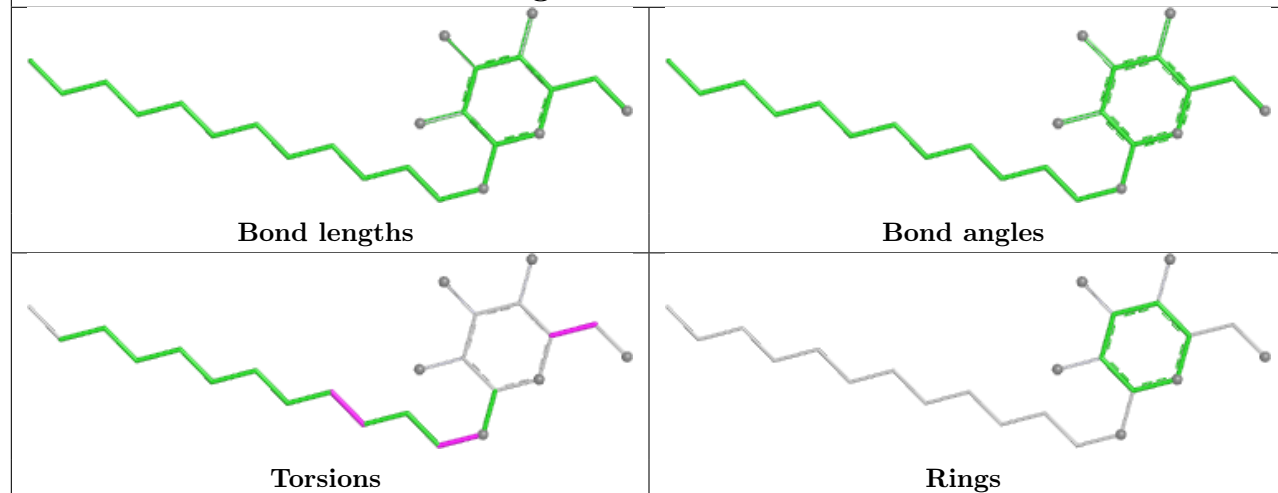


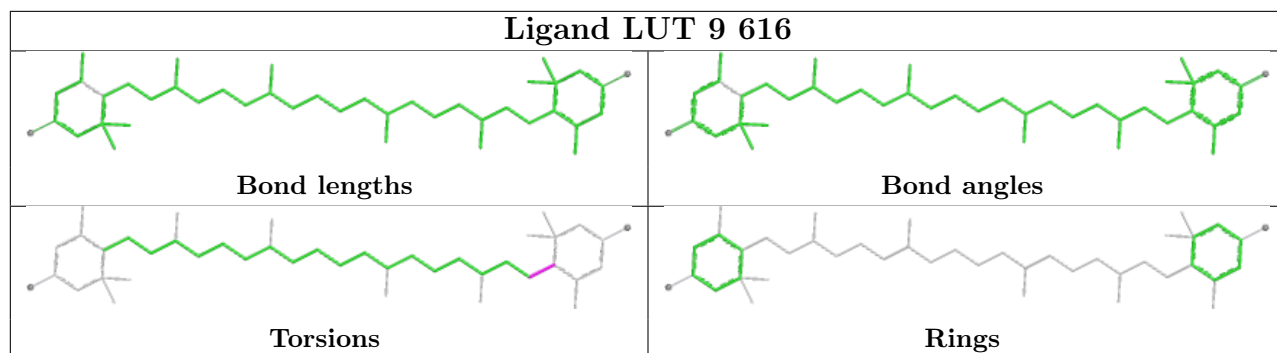
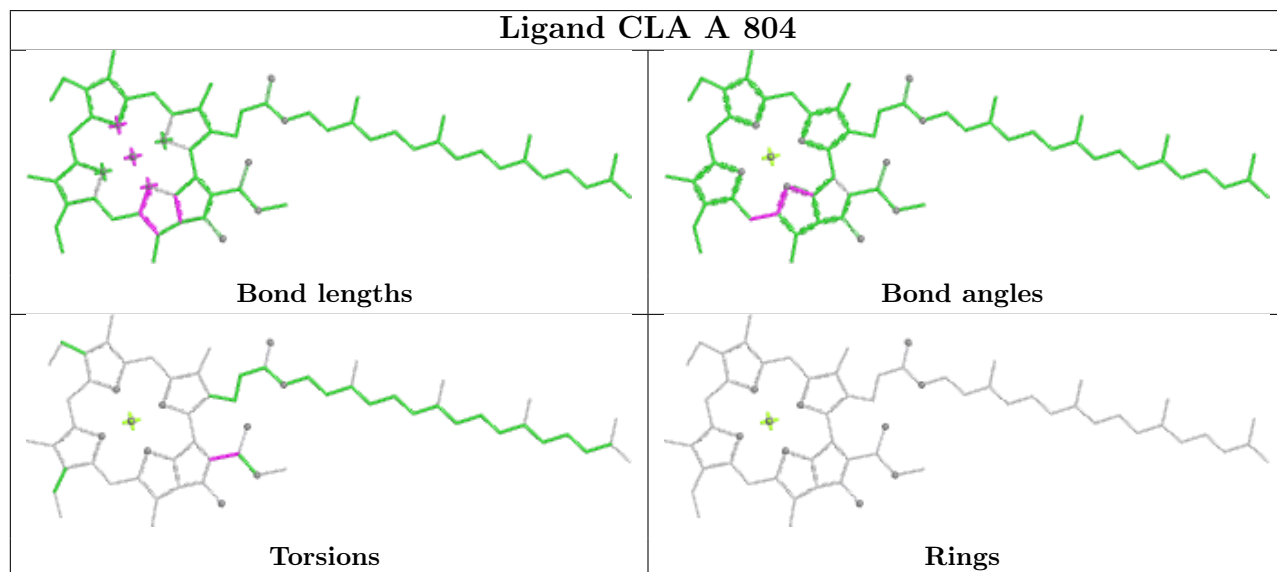
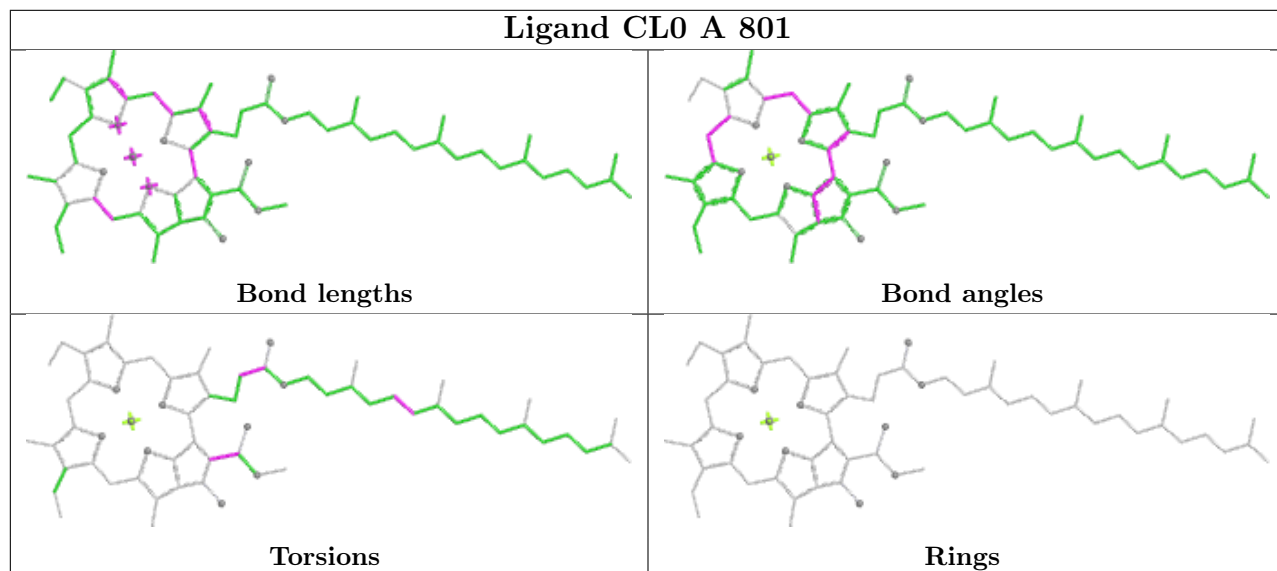


Ligand CLA 7 616

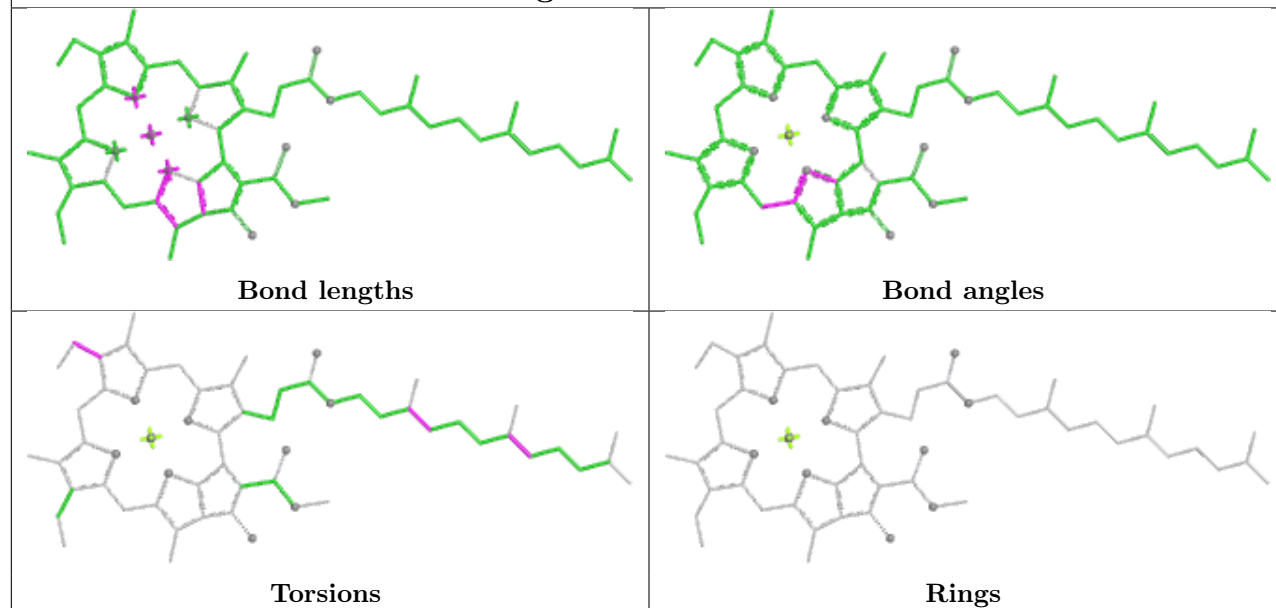


Ligand LMU 1 625

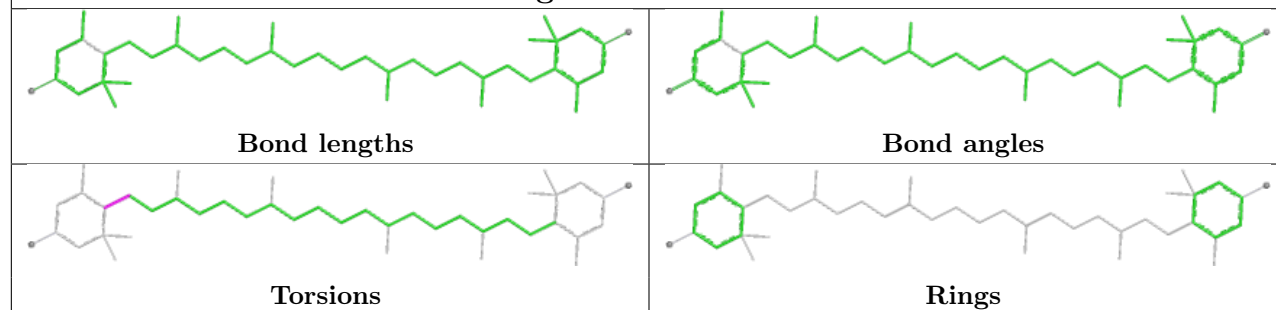


Ligand LUT 9 616**Ligand CLA A 804****Ligand CL0 A 801**

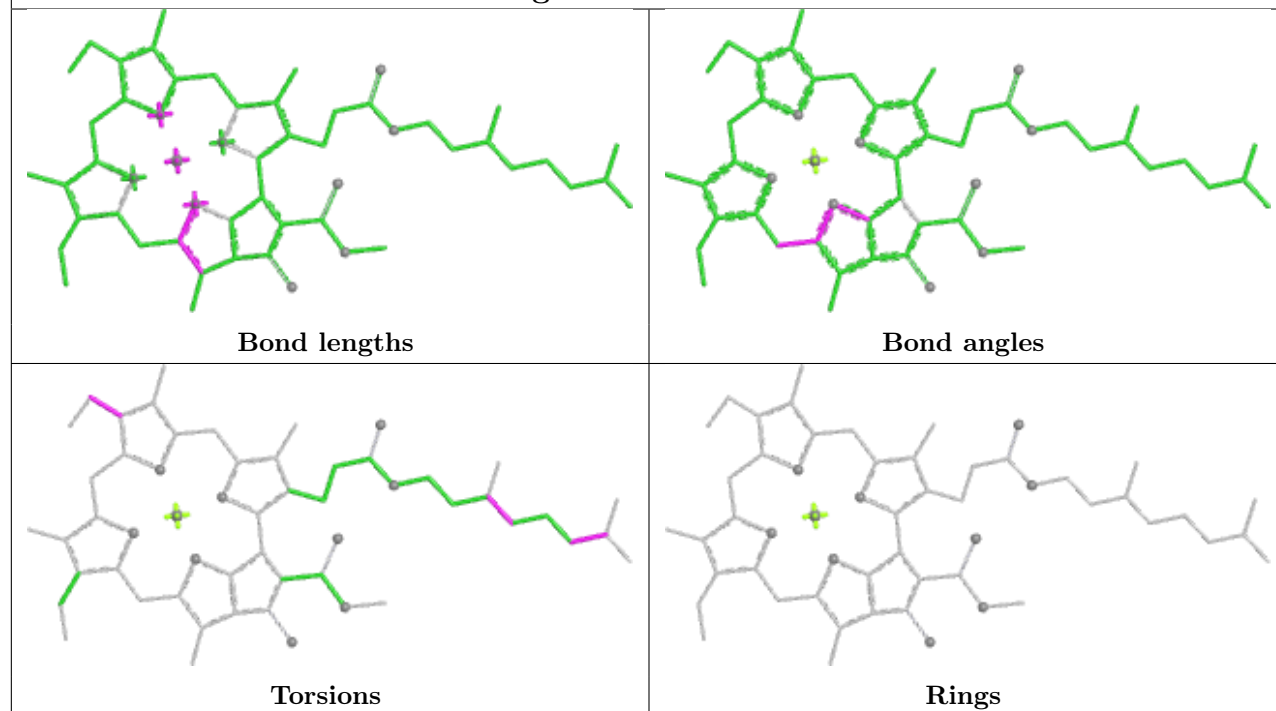
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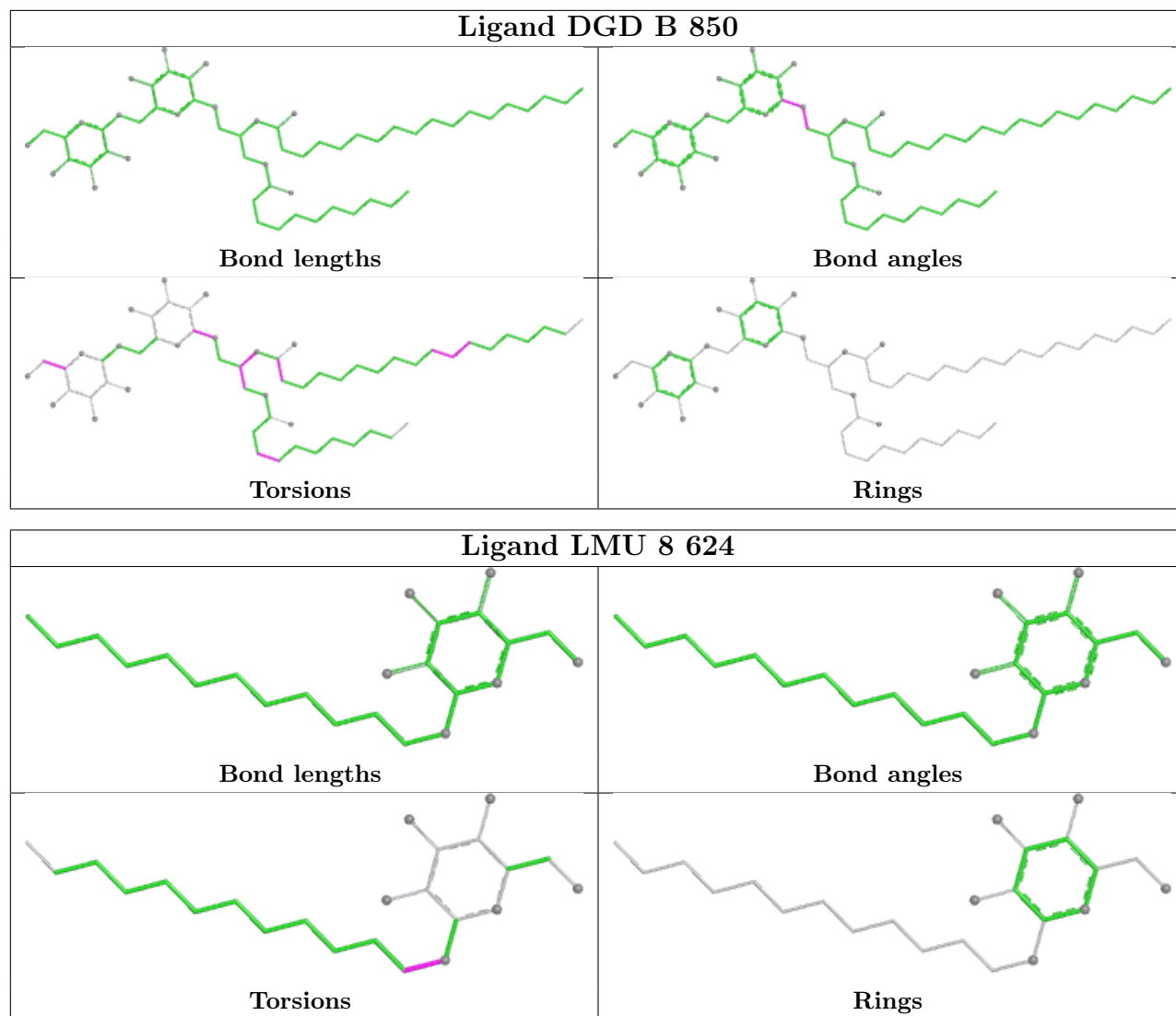


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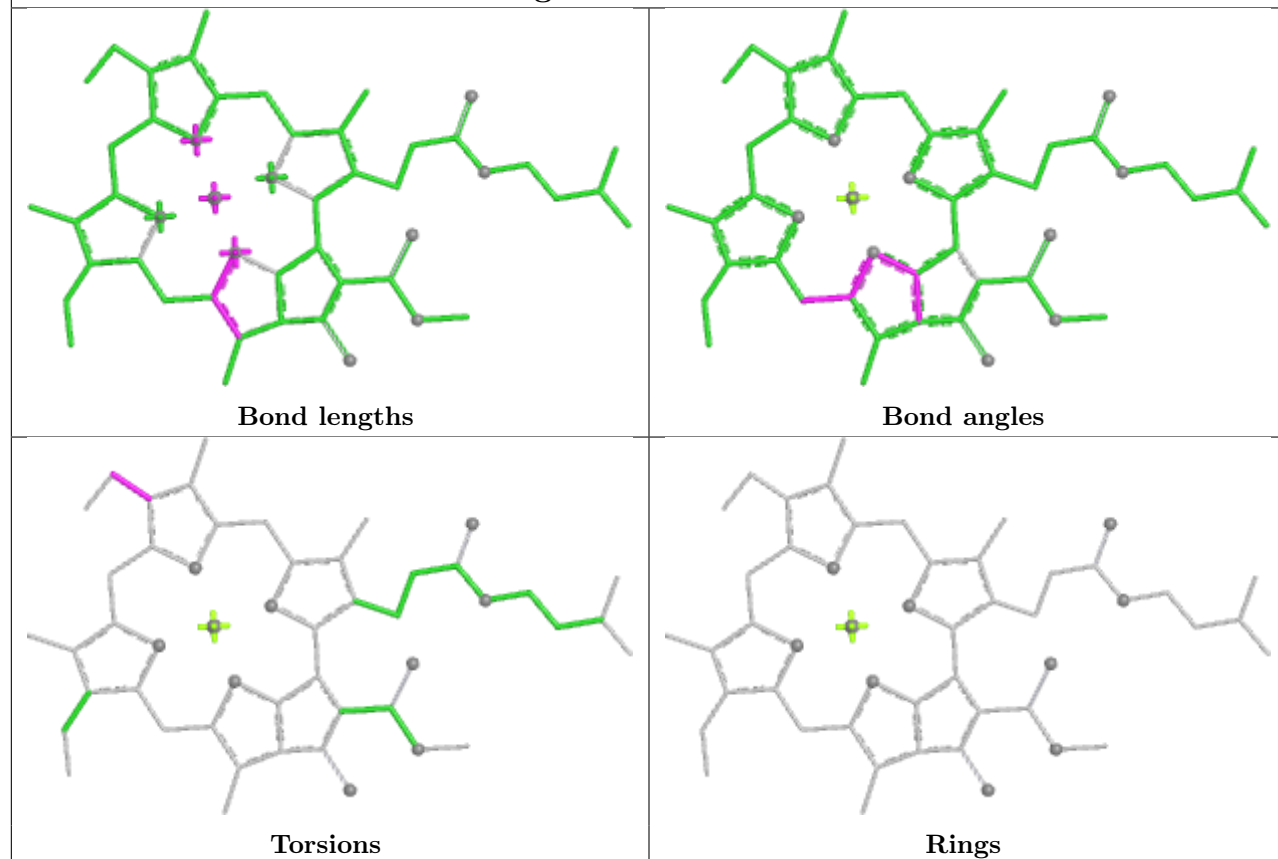


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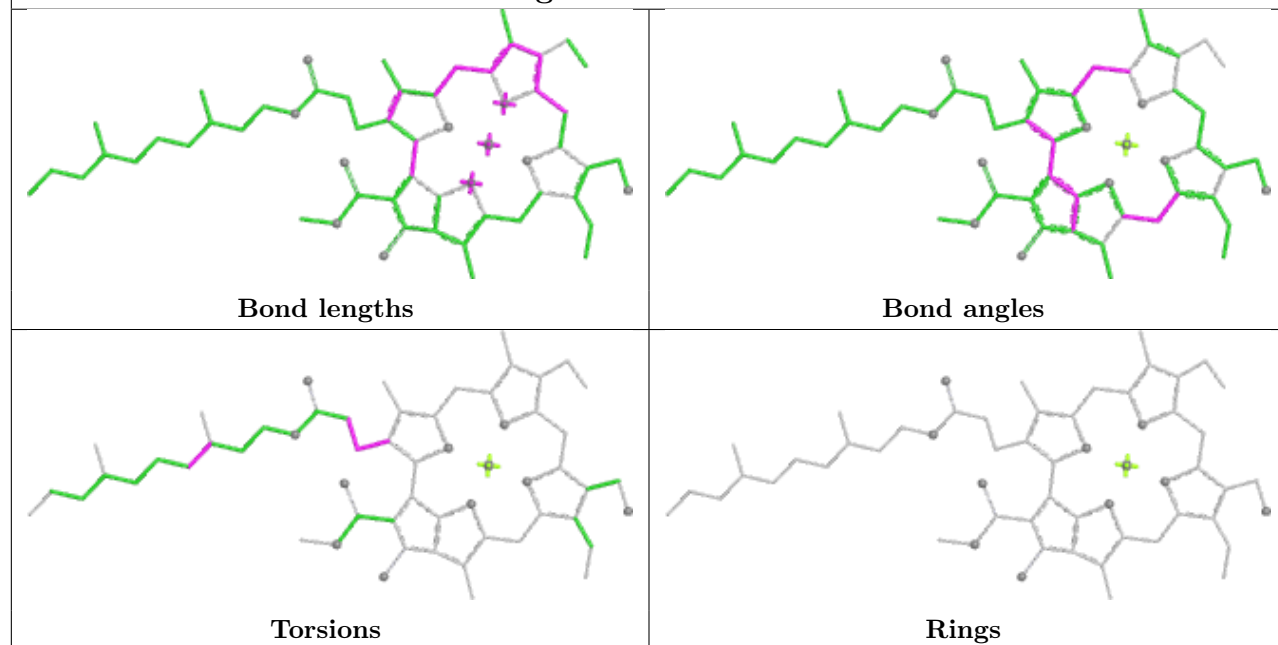


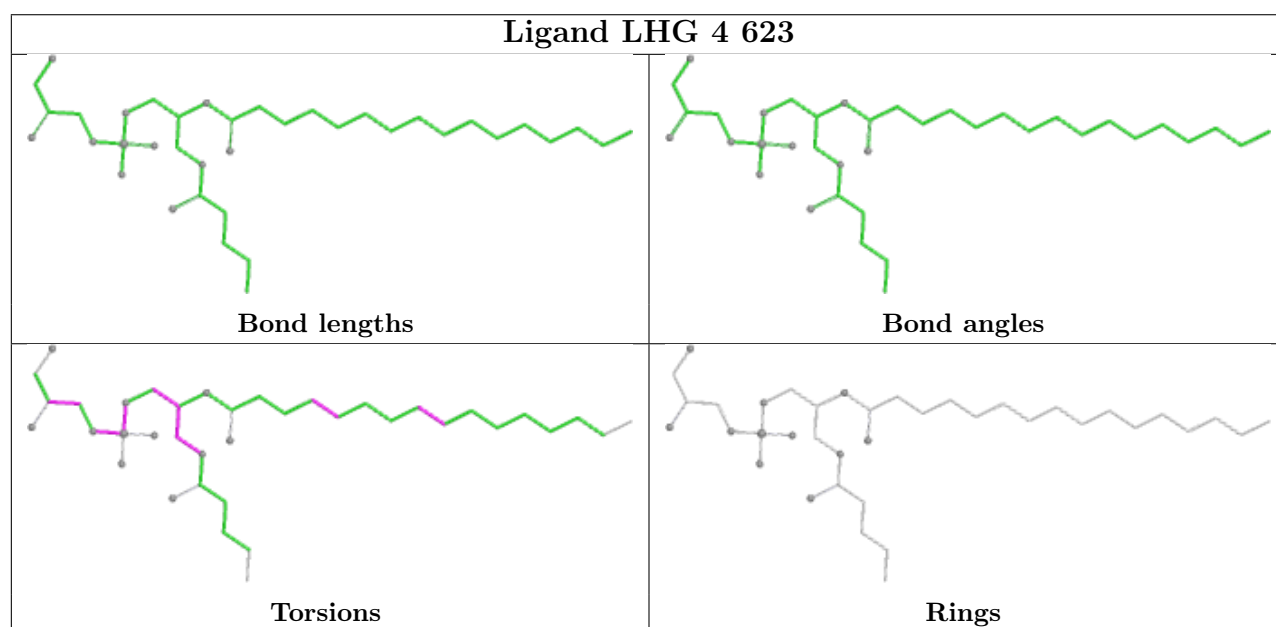
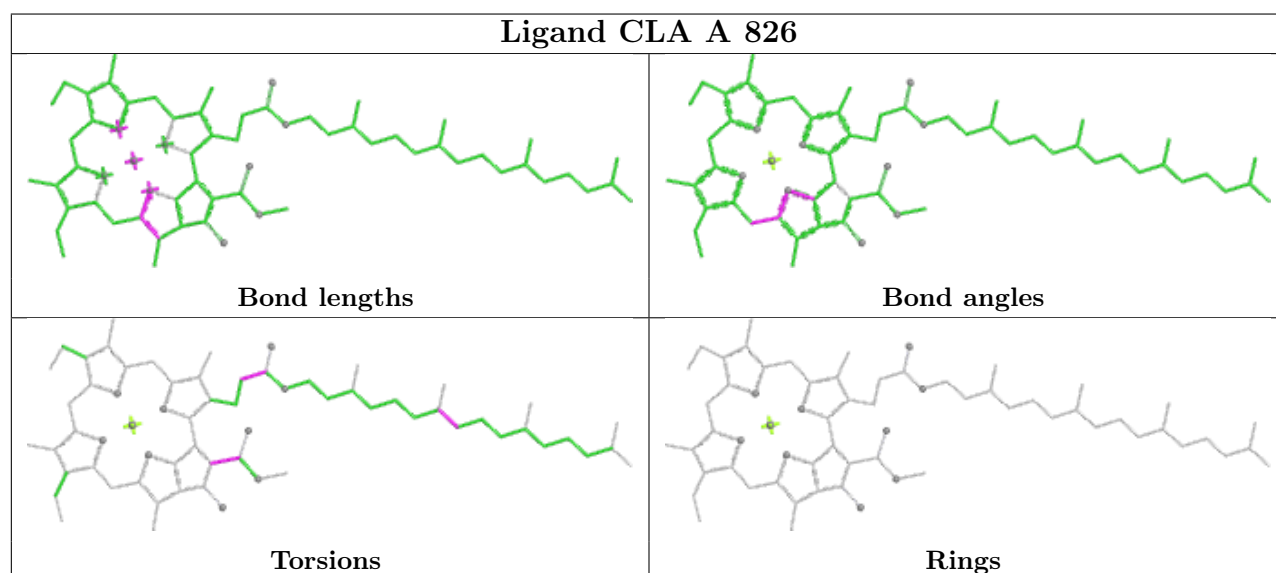
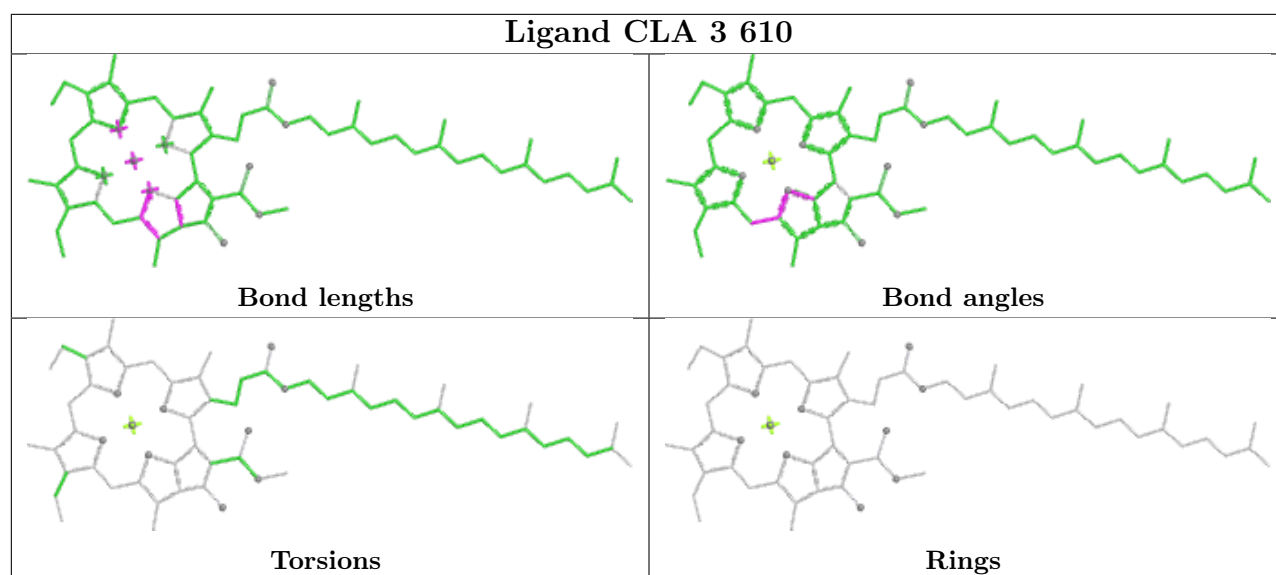


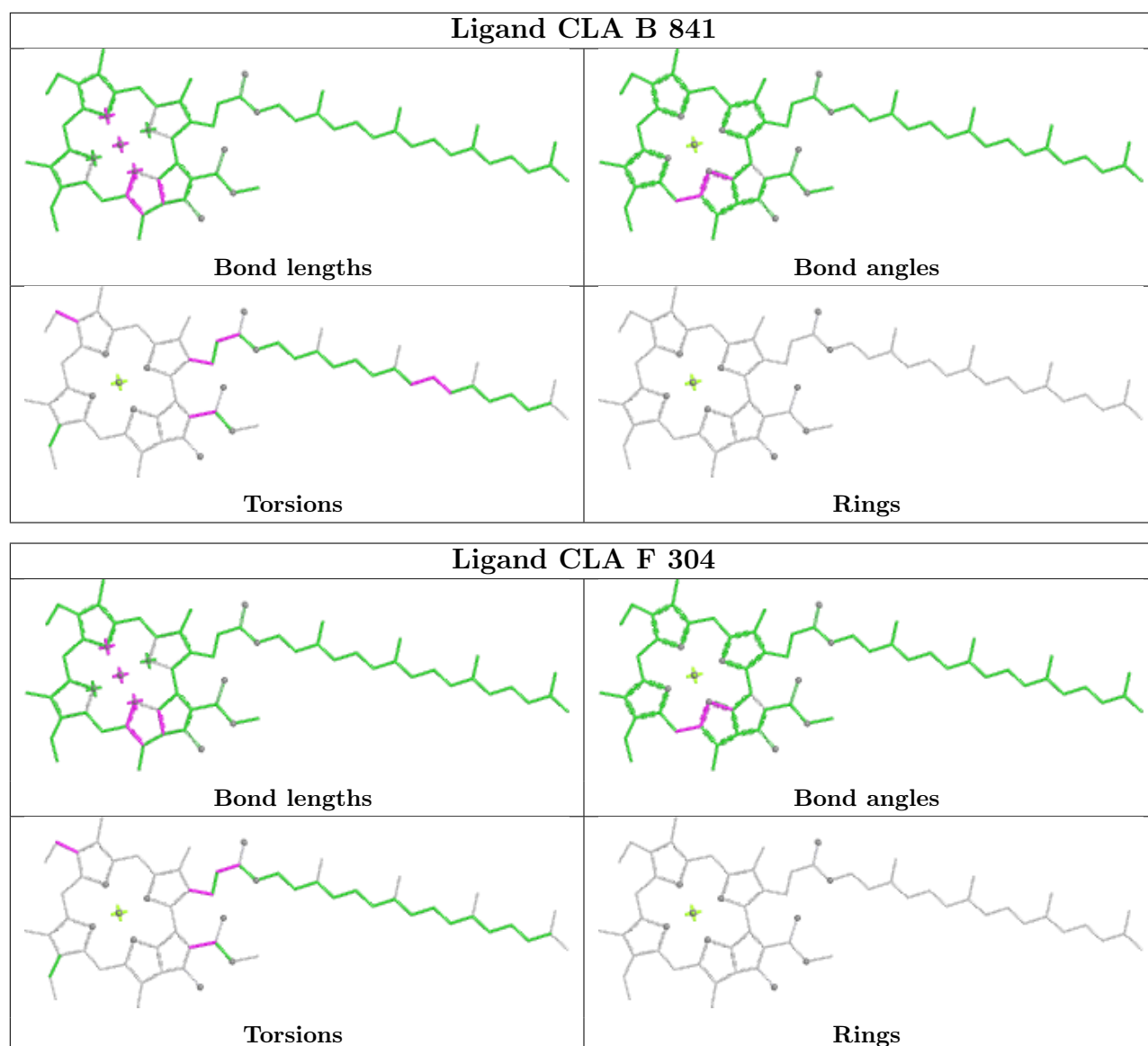
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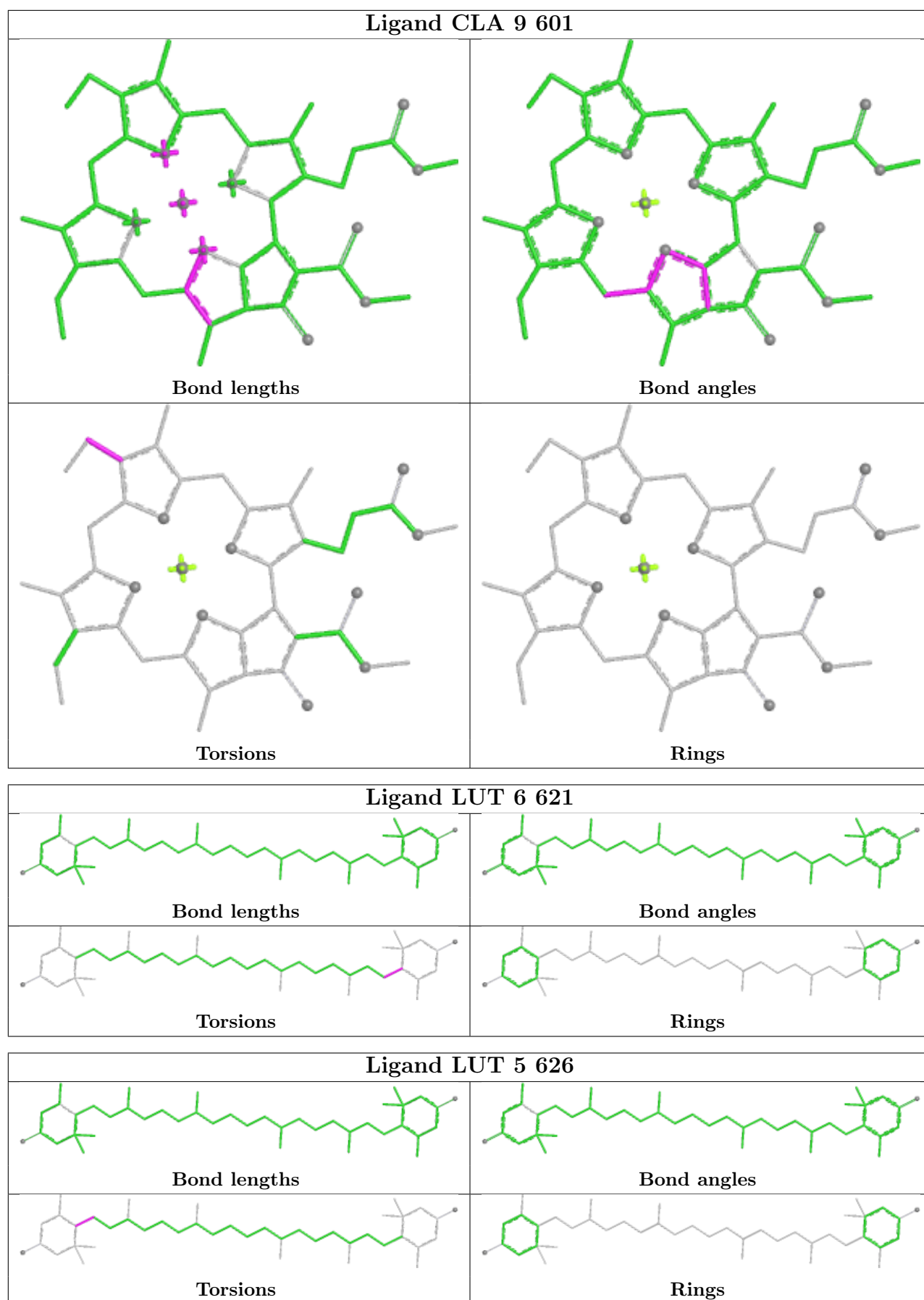


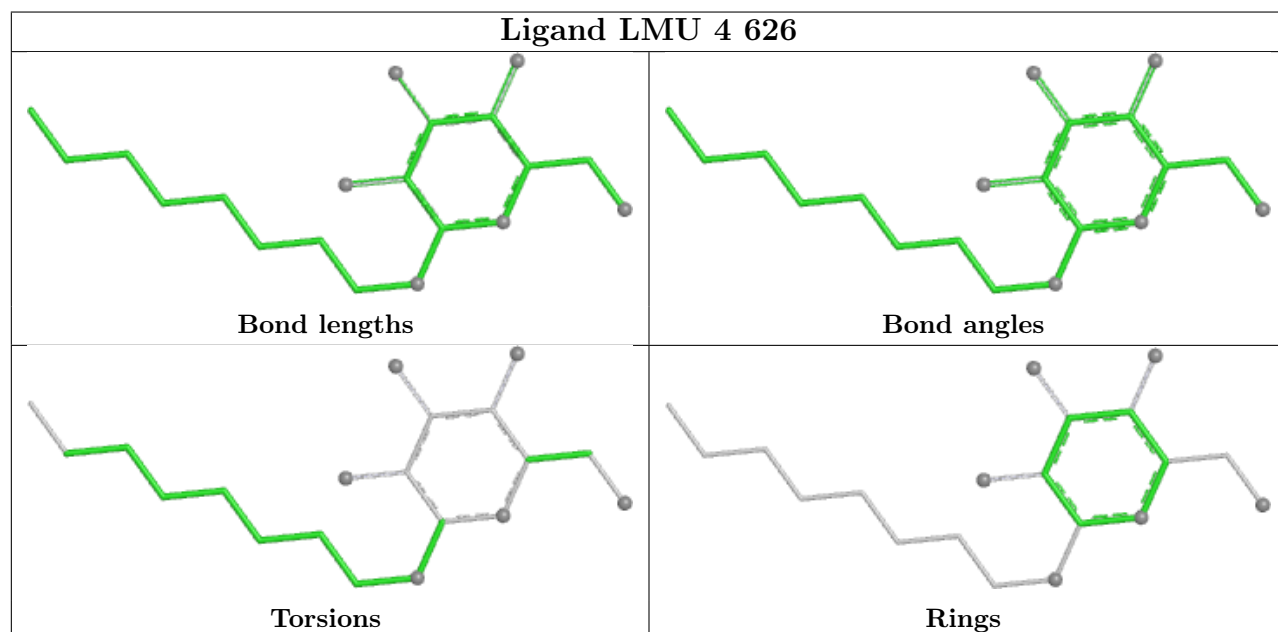
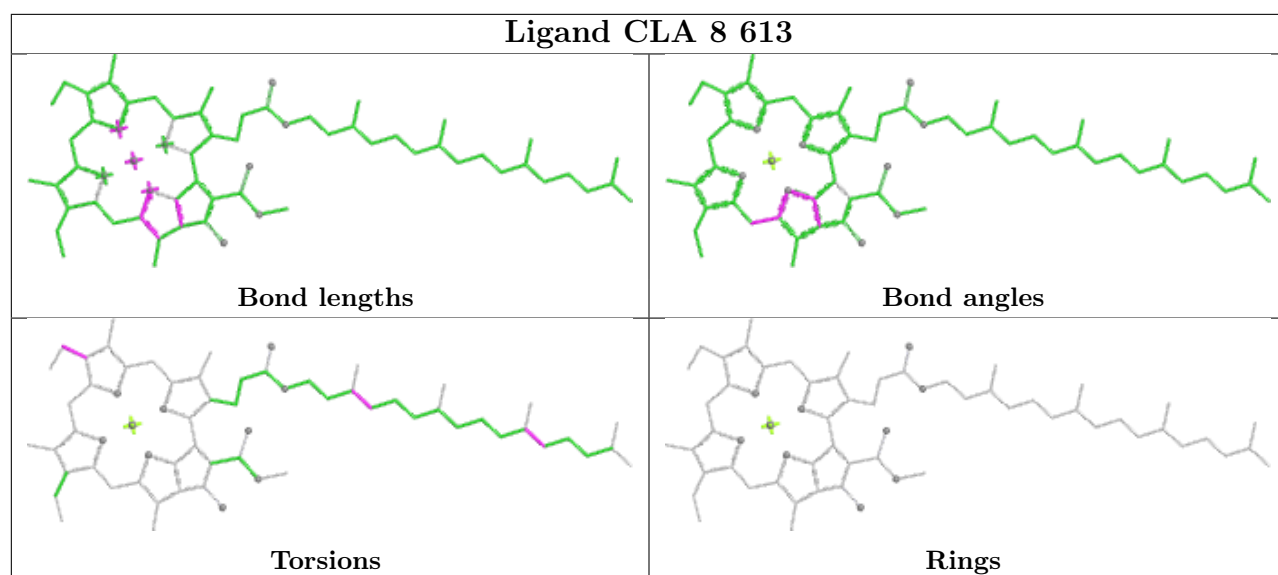
Ligand CHL 6 606



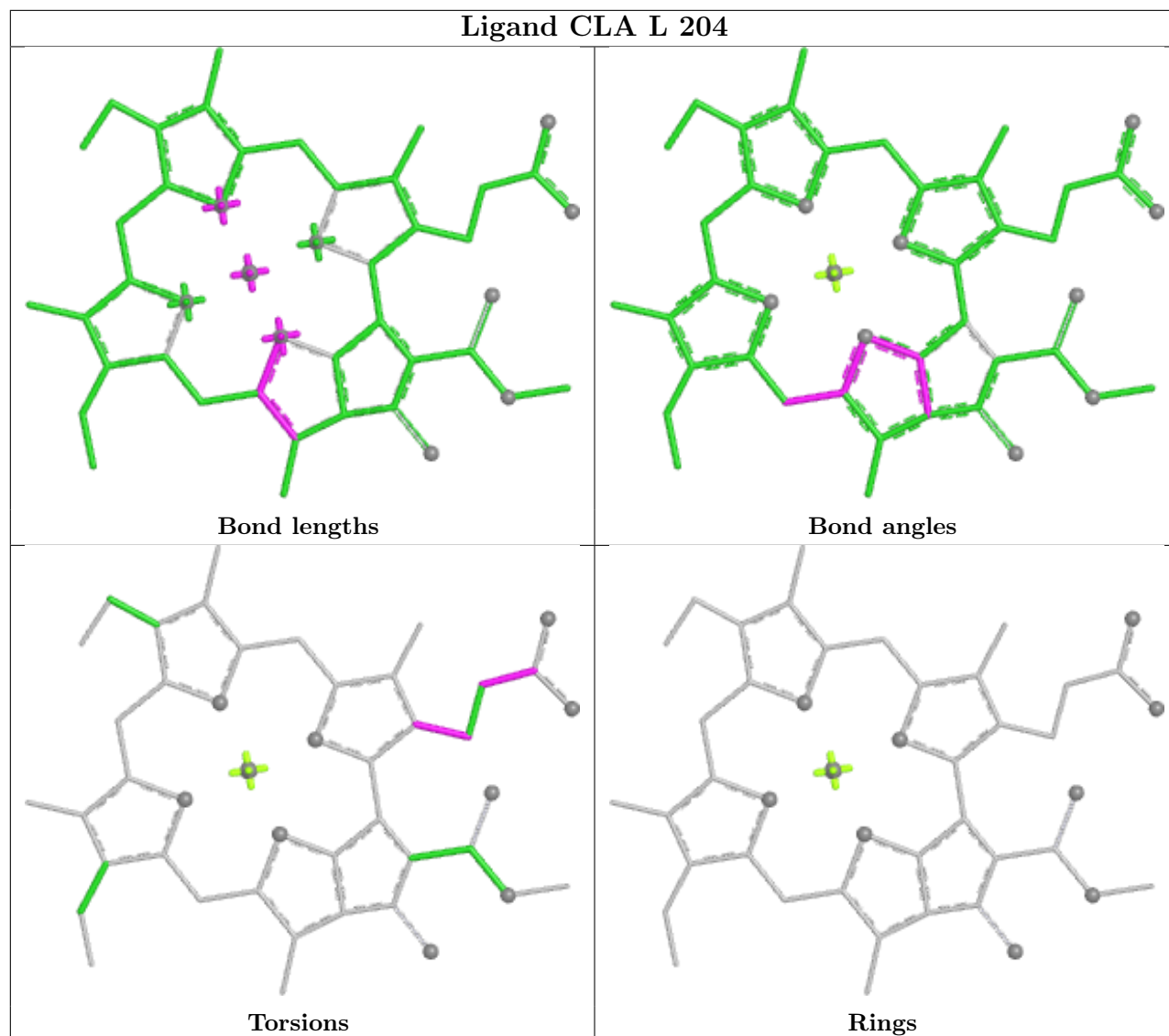




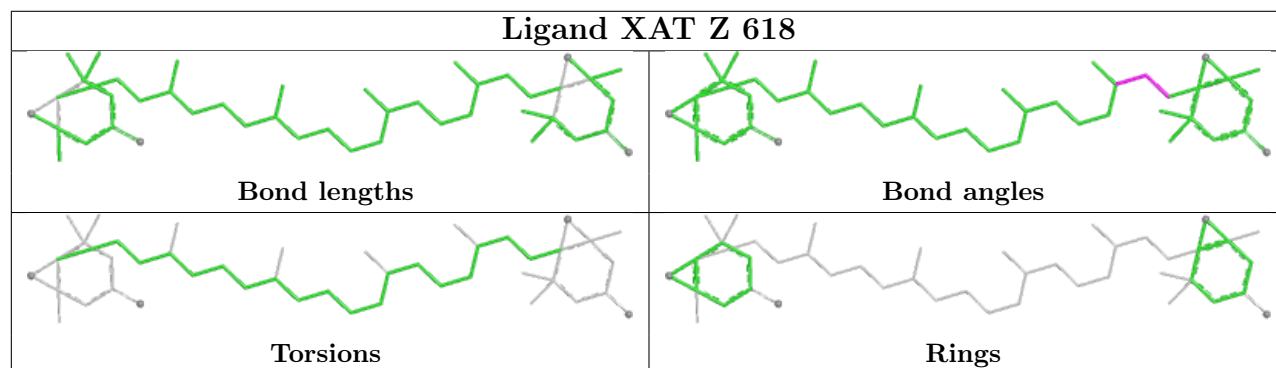


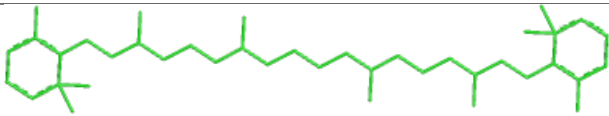
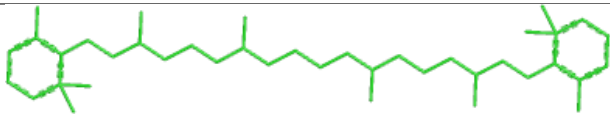
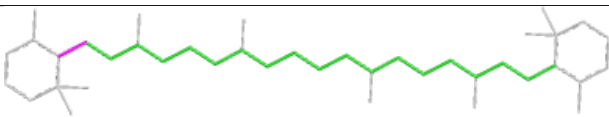
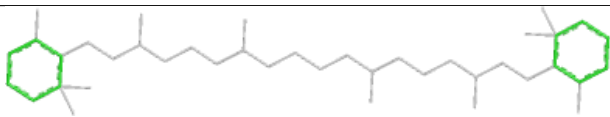


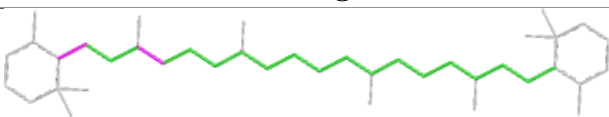
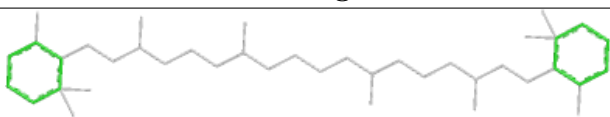
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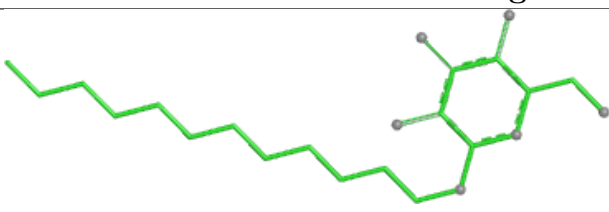
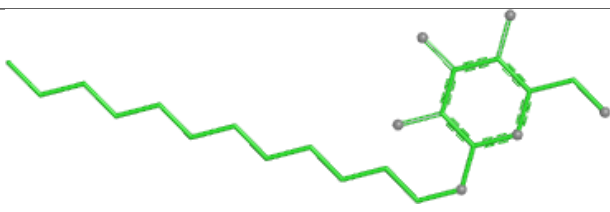
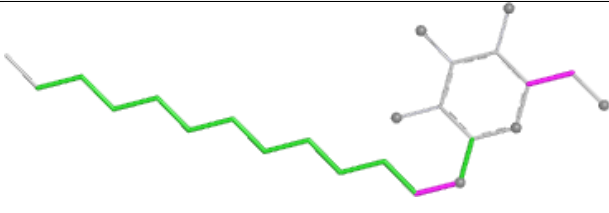
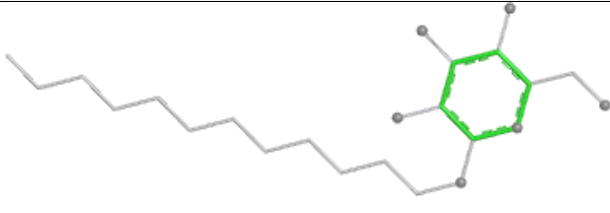


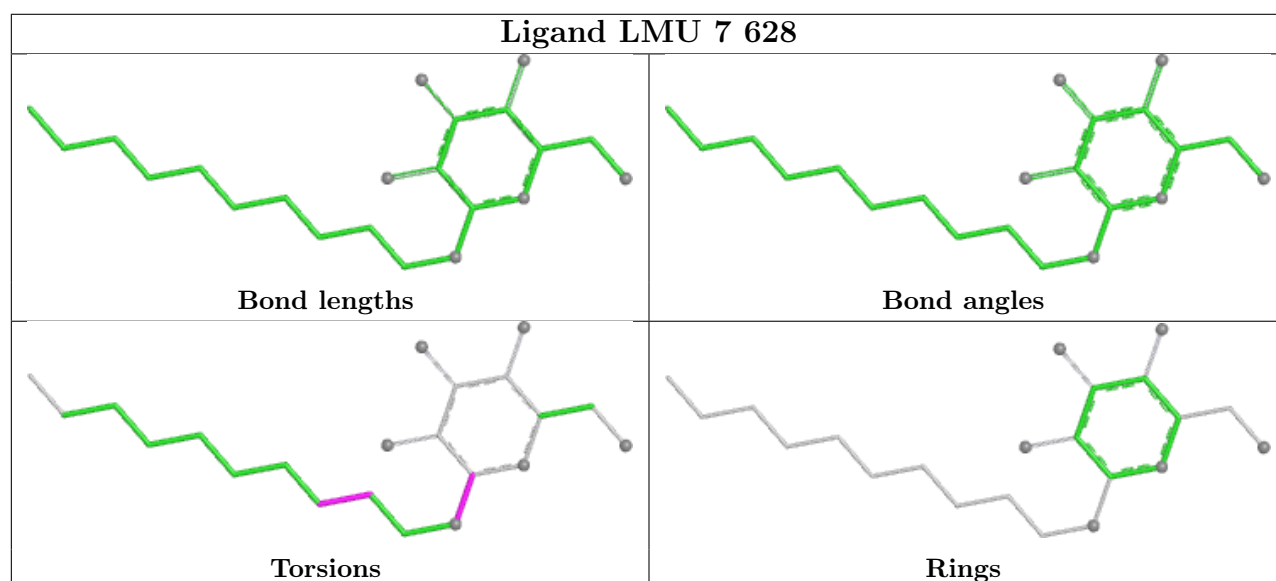
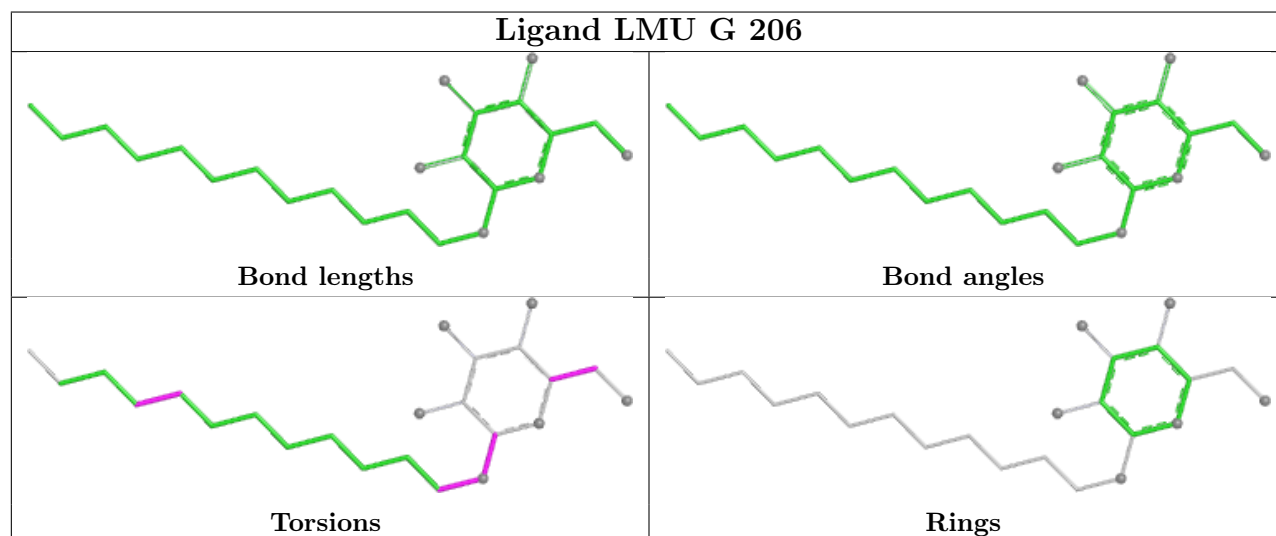
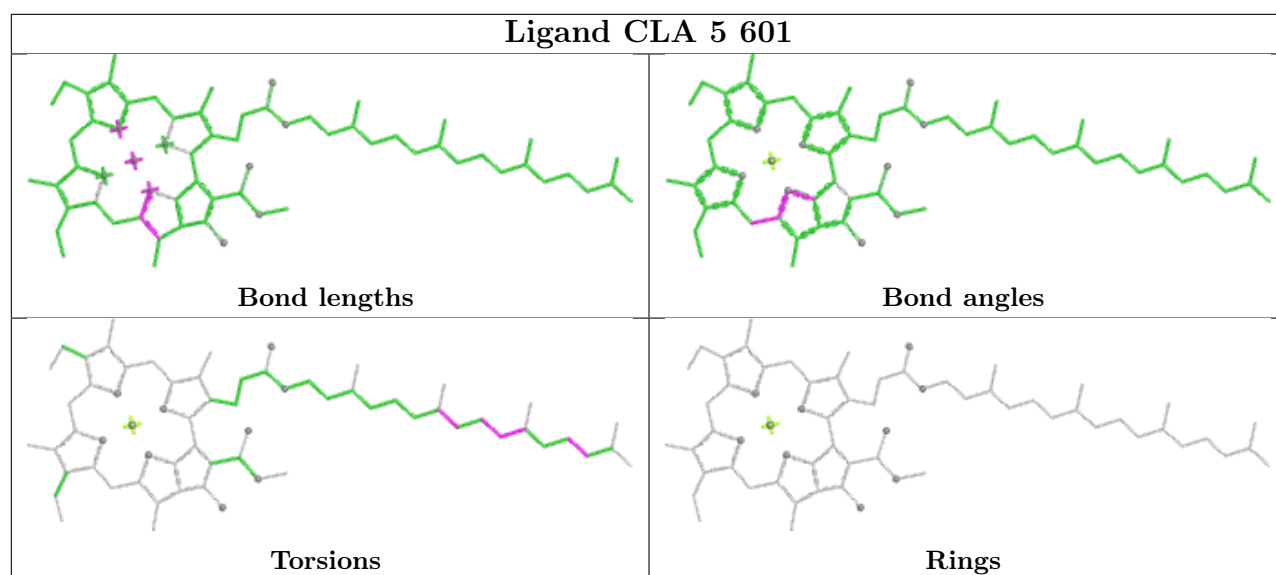
Ligand XAT Z 618

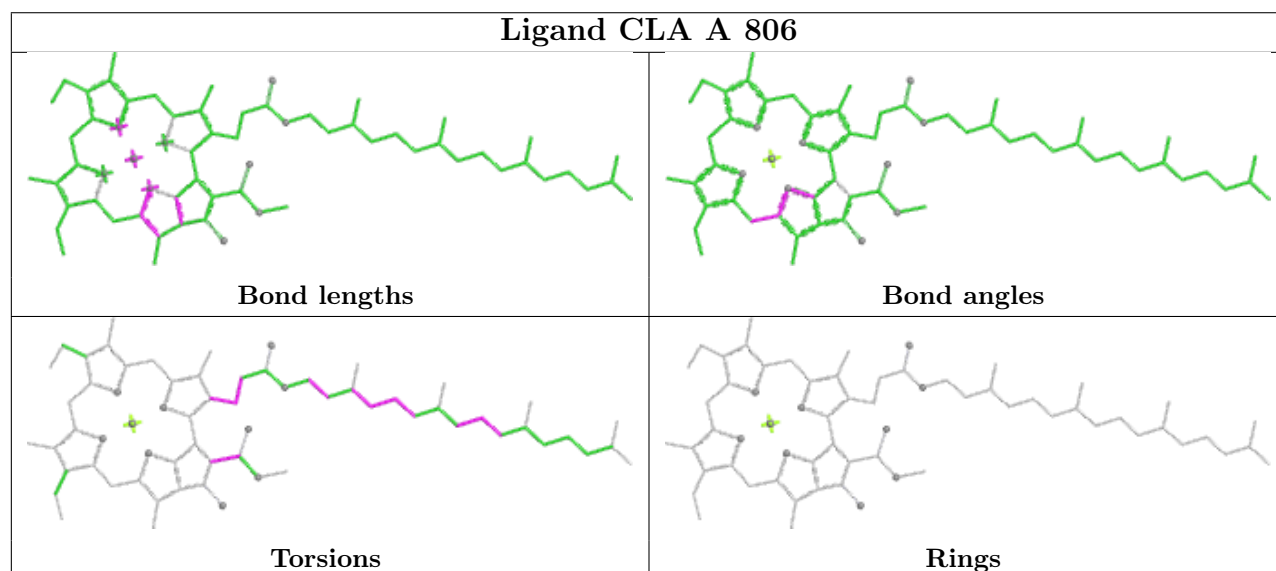
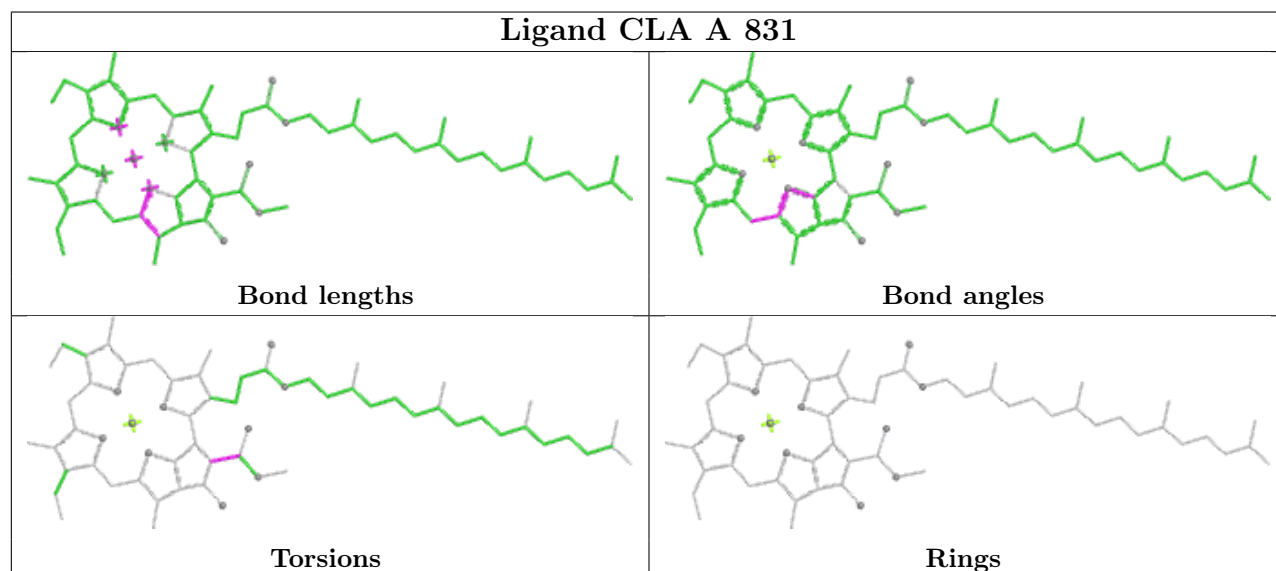
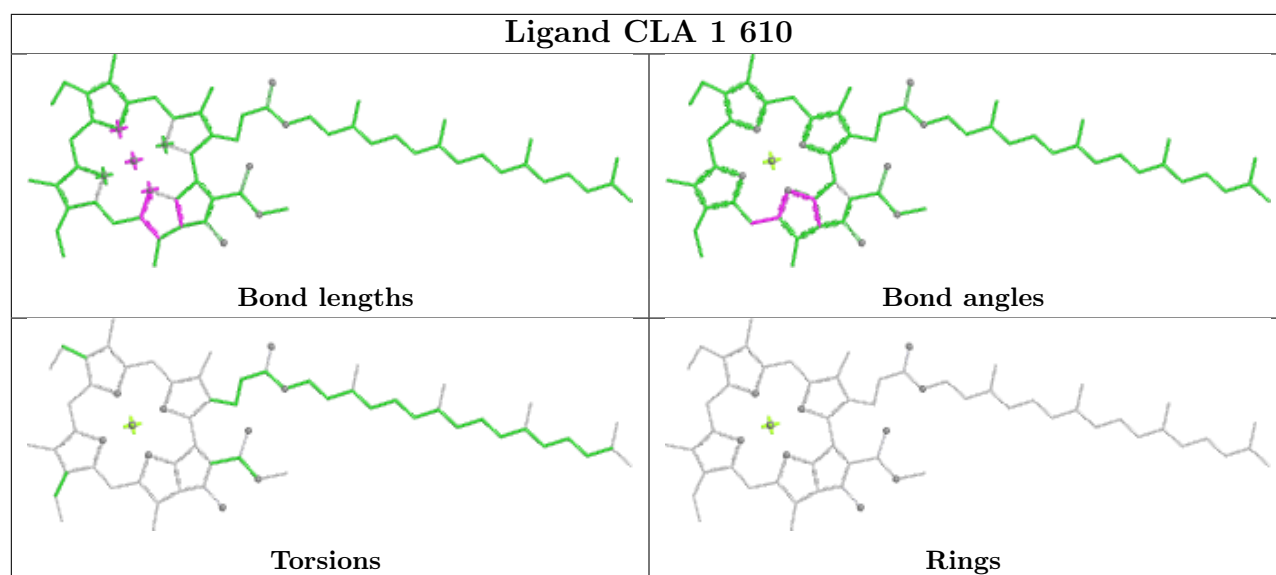


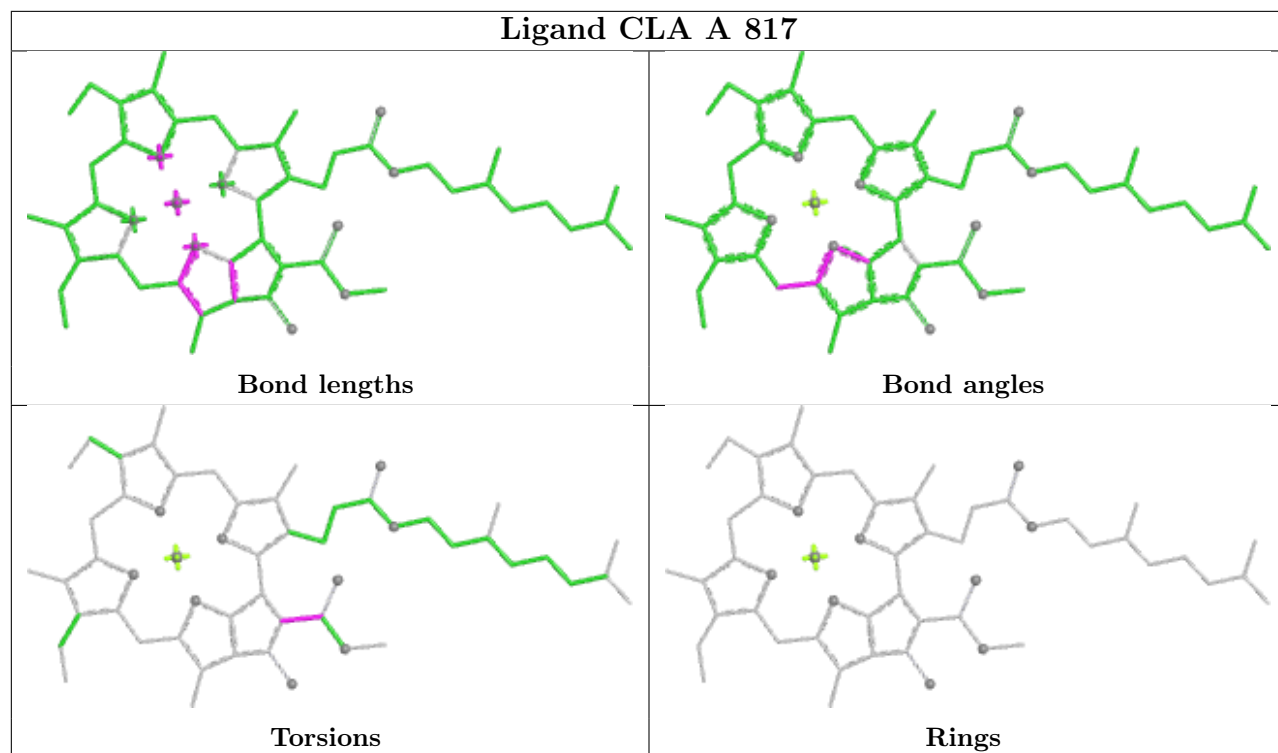
Ligand BCR B 844	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR L 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

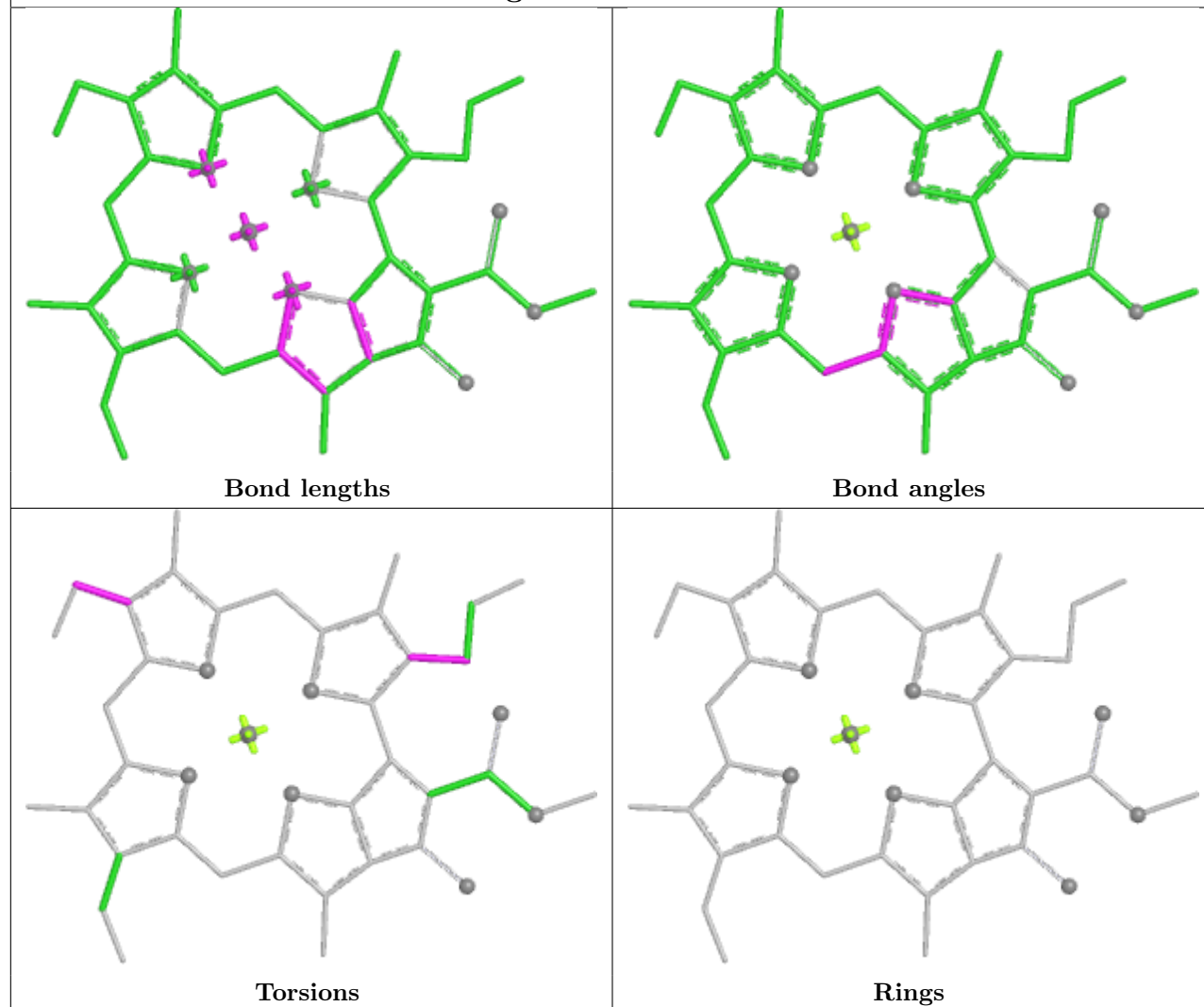
Ligand LMU 8 625	
	
Bond lengths	Bond angles
	
Torsions	Rings



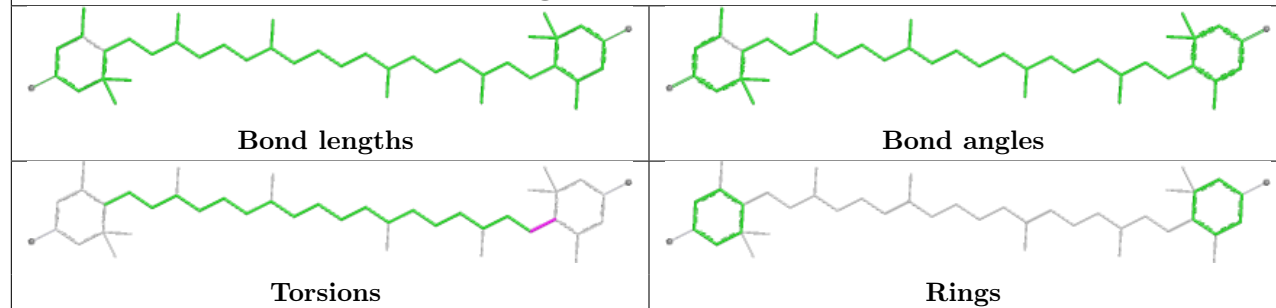


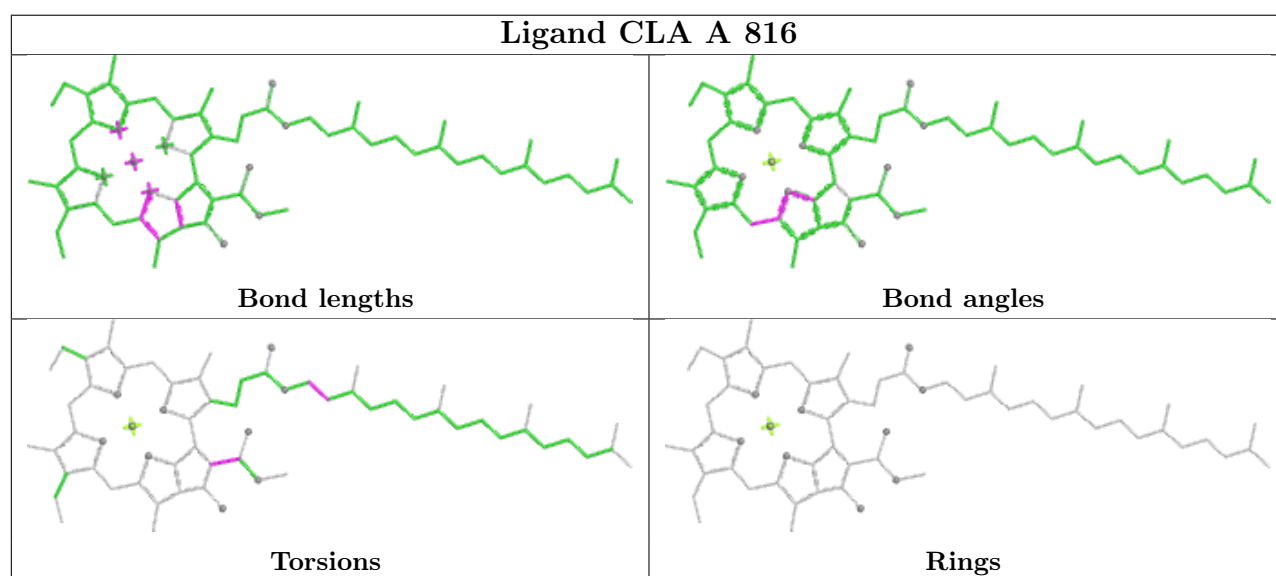
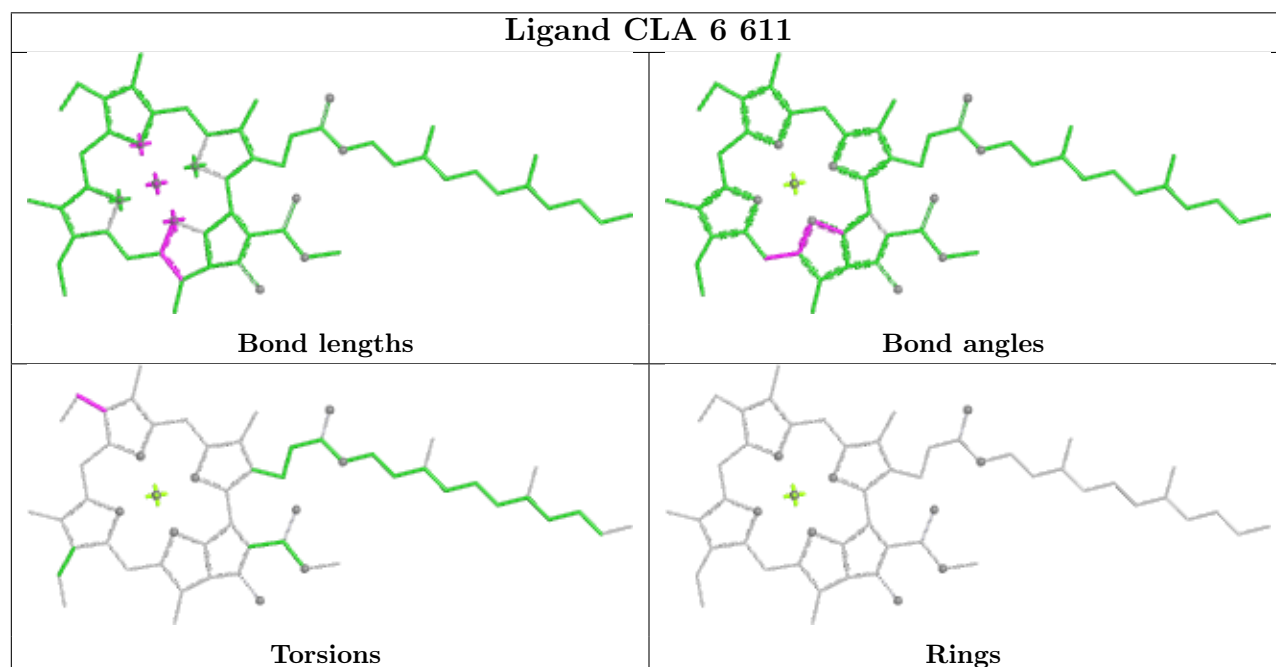
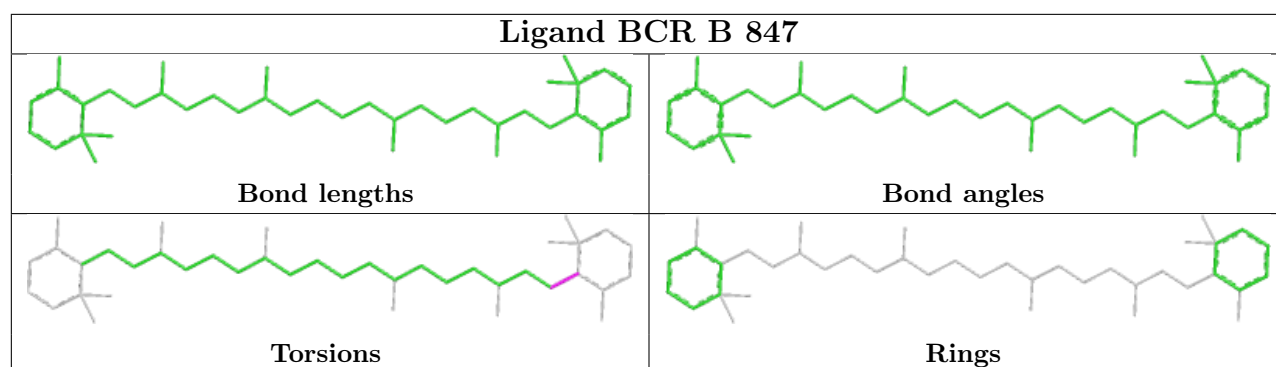


Ligand CLA 7 614

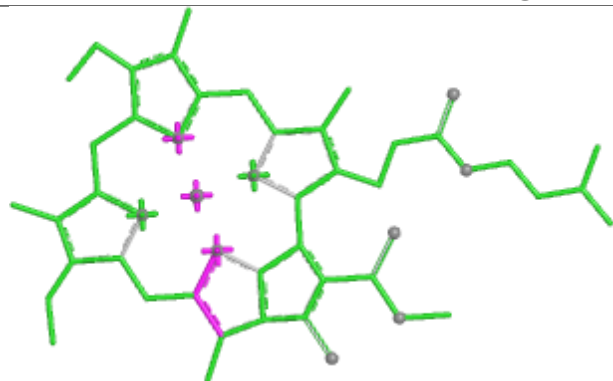


Ligand LUT 3 621

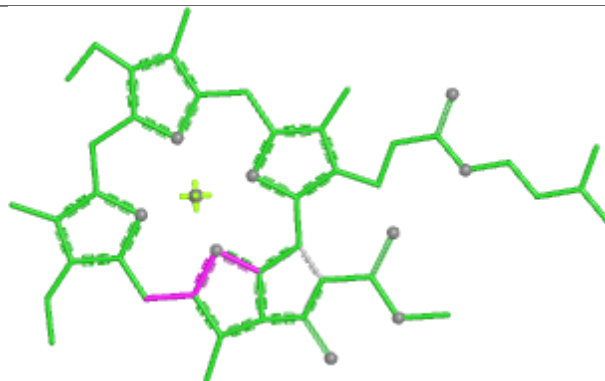




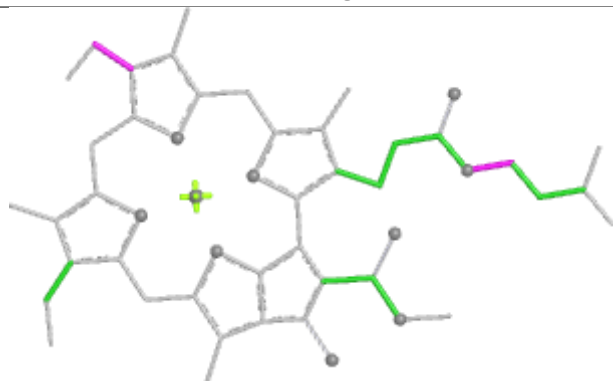
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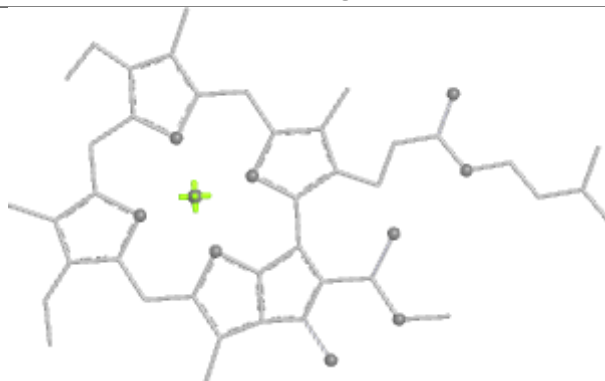
Bond lengths



Bond angles

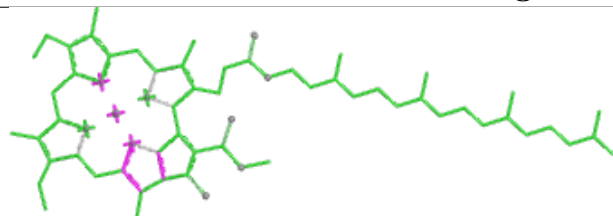


Torsions

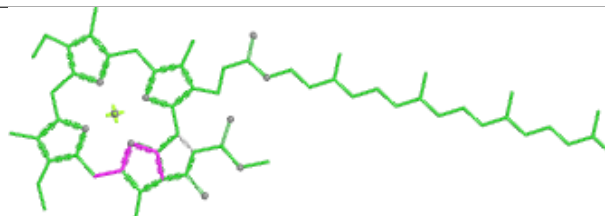


Rings

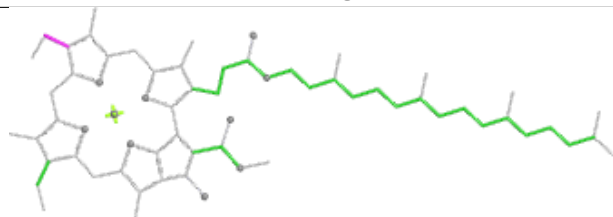
Ligand CLA B 810



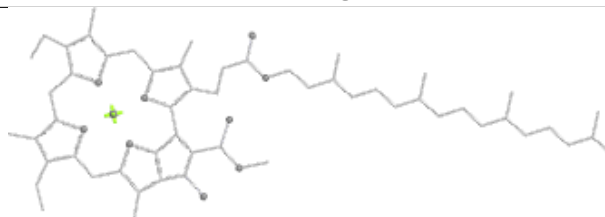
Bond lengths



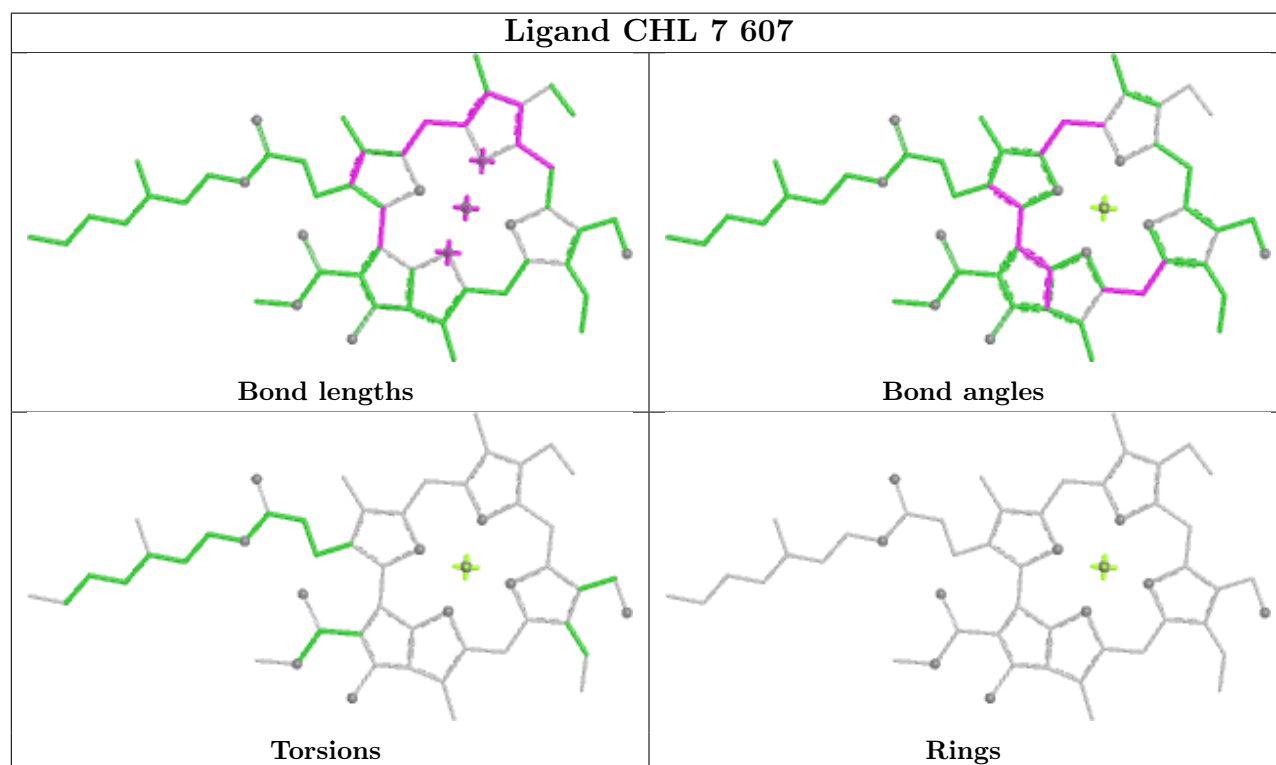
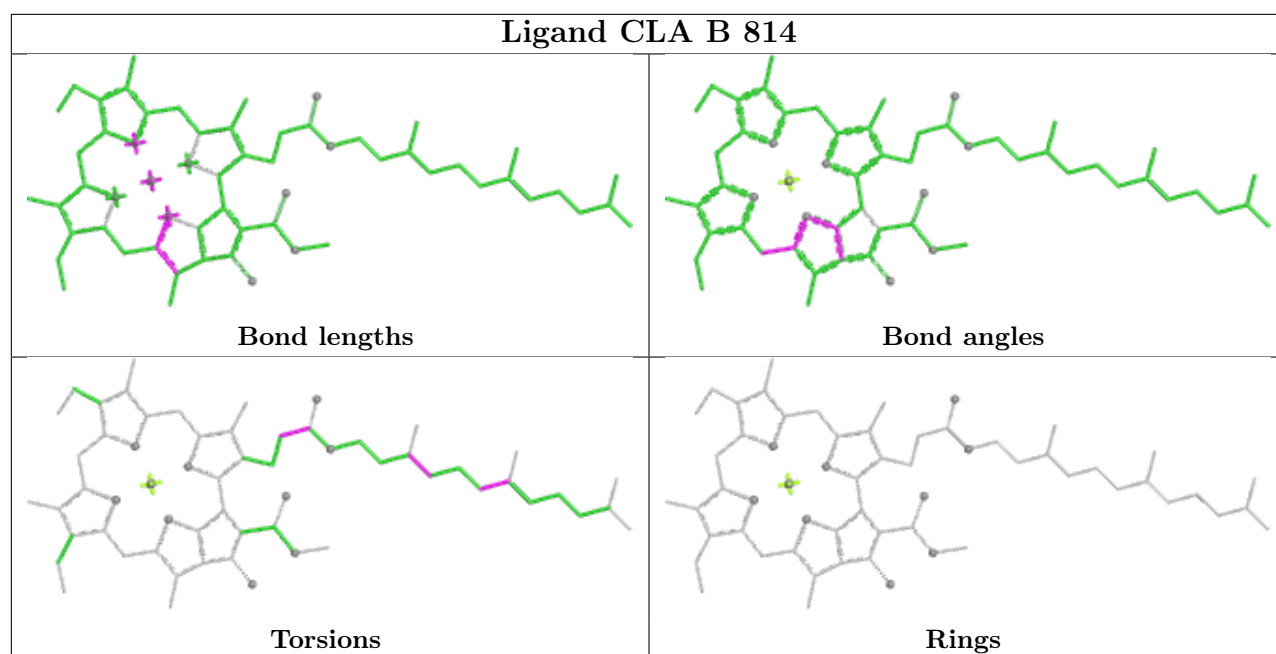
Bond angles

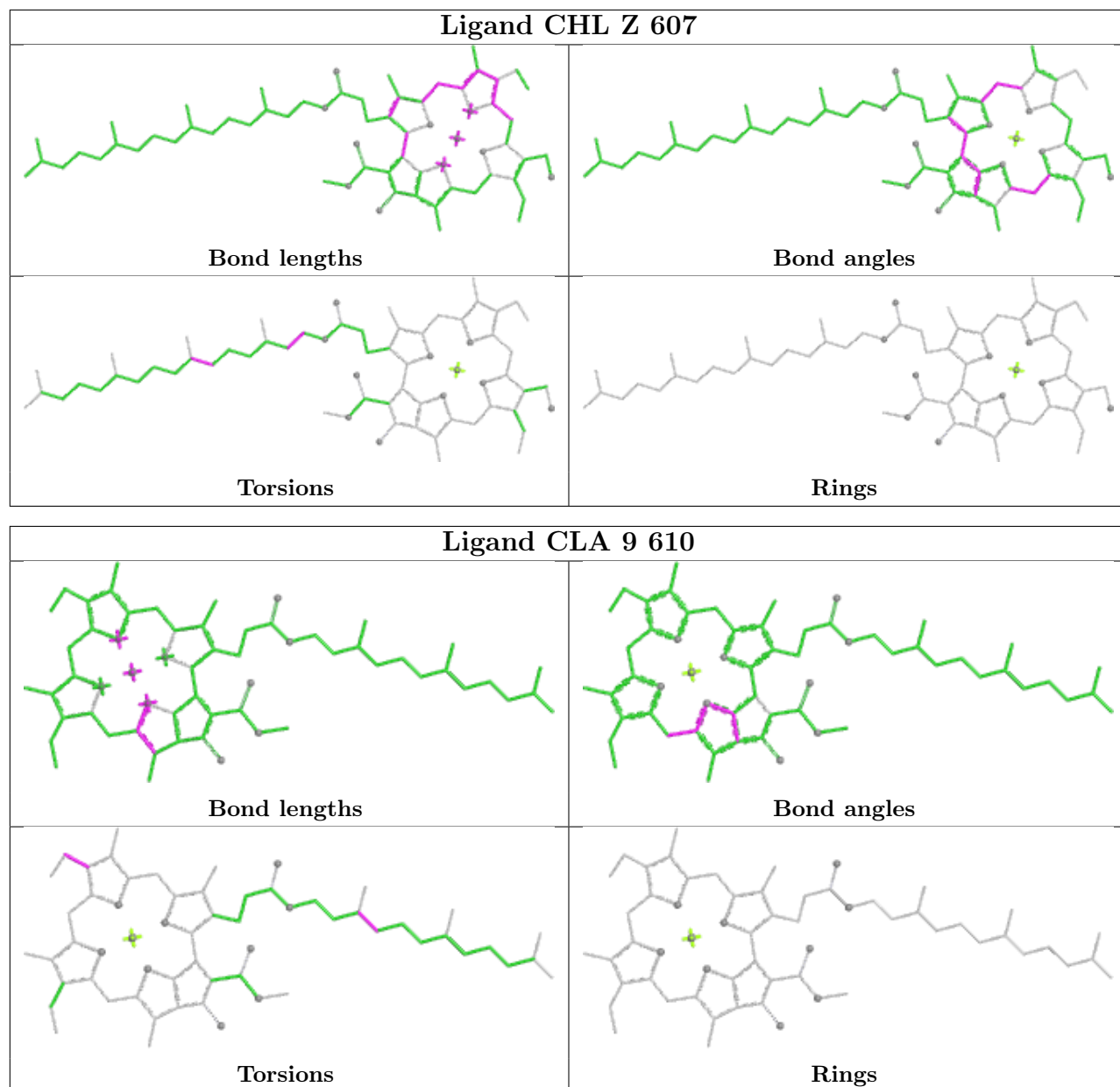


Torsions

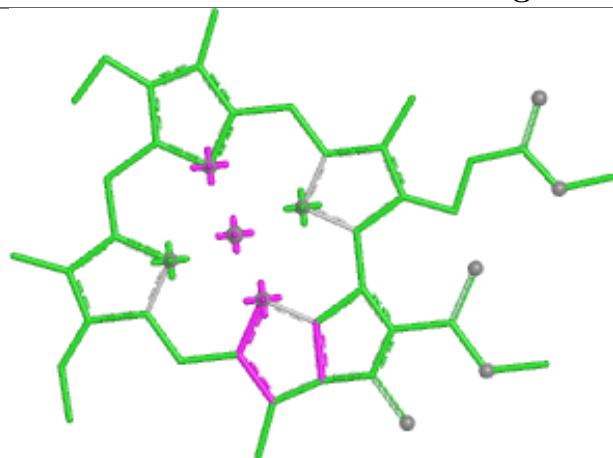


Rings

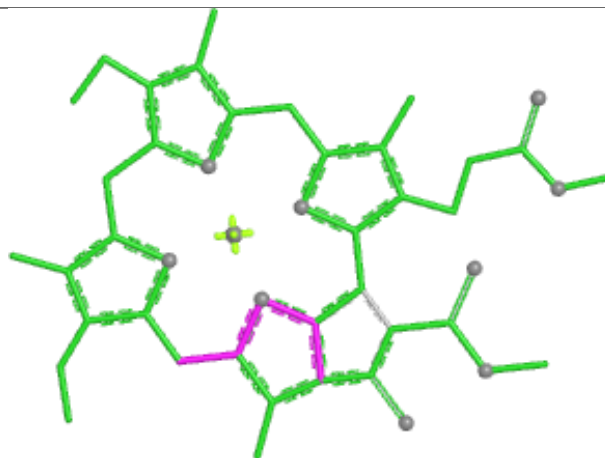




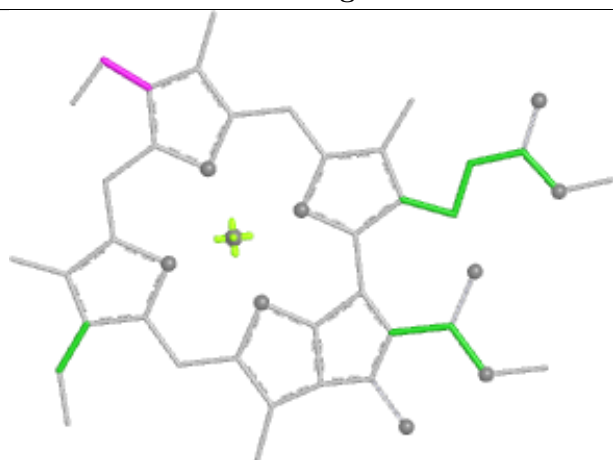
Ligand CLA K 204



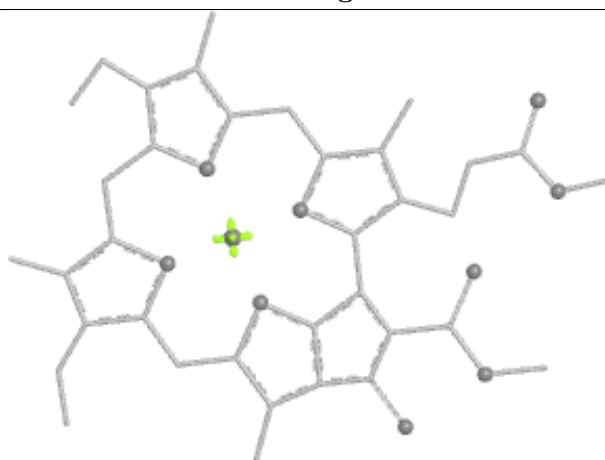
Bond lengths



Bond angles

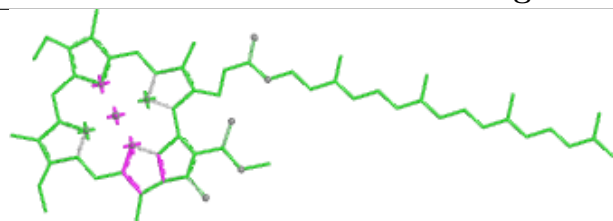


Torsions

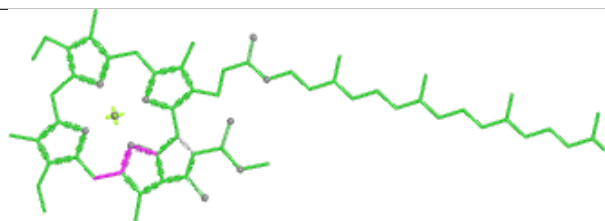


Rings

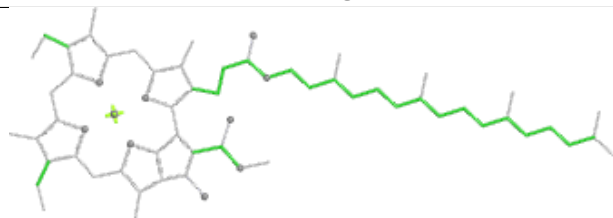
Ligand CLA A 802



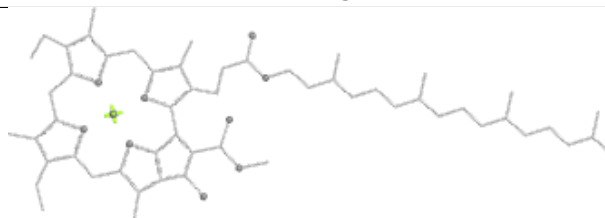
Bond lengths



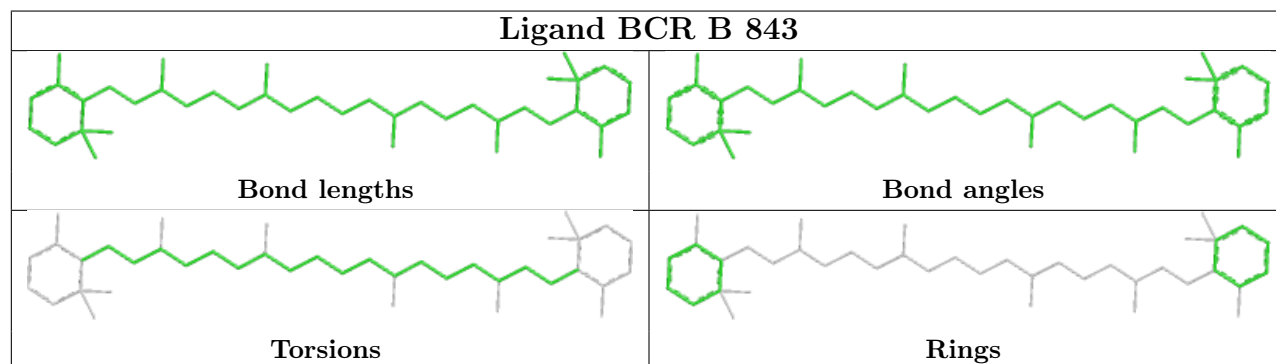
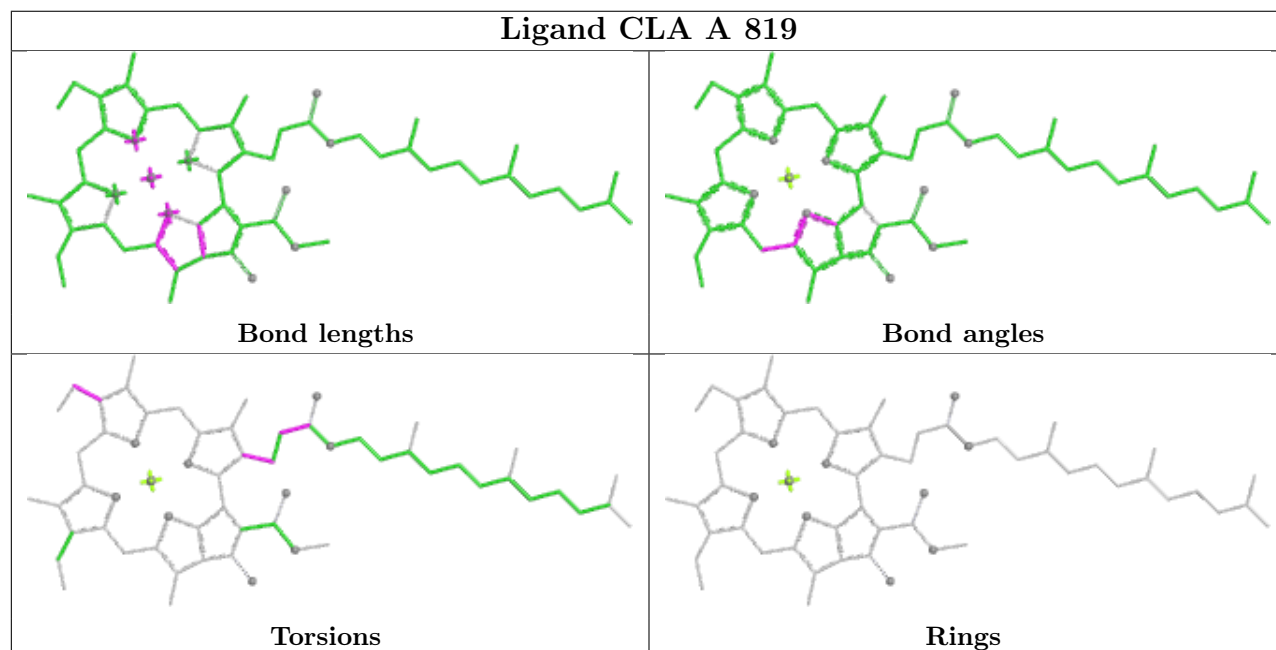
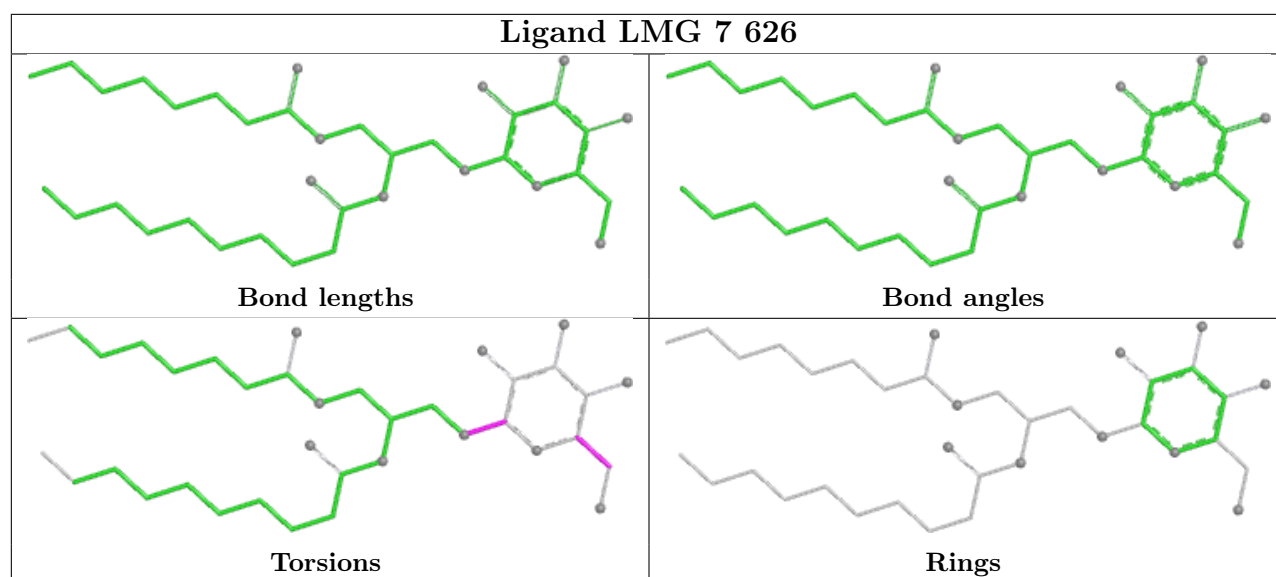
Bond angles



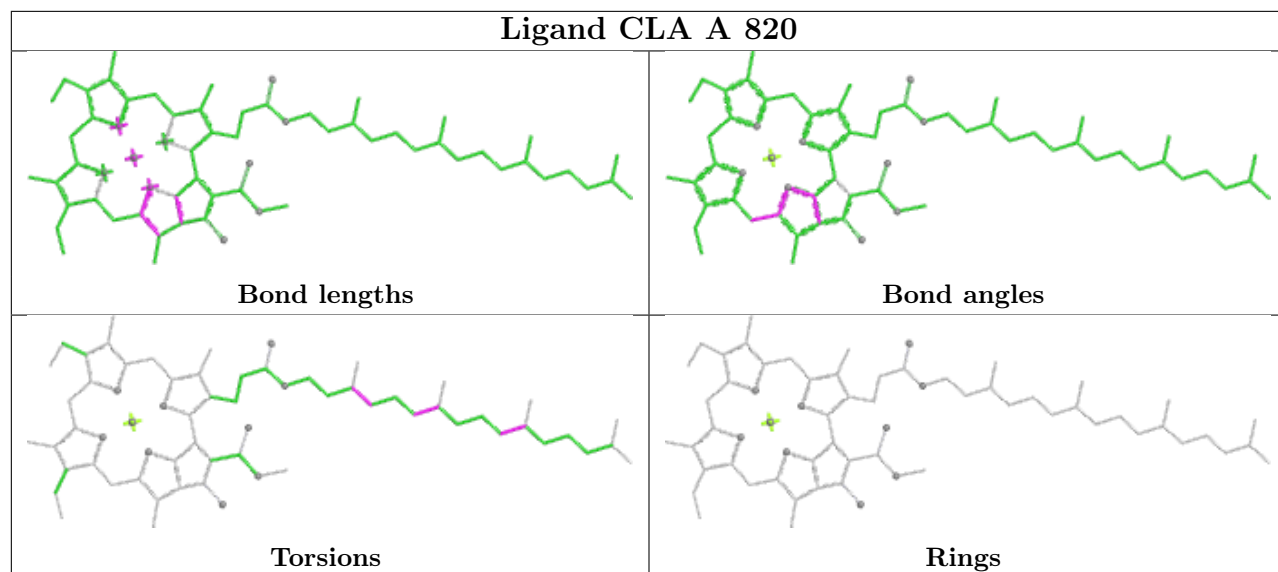
Torsions



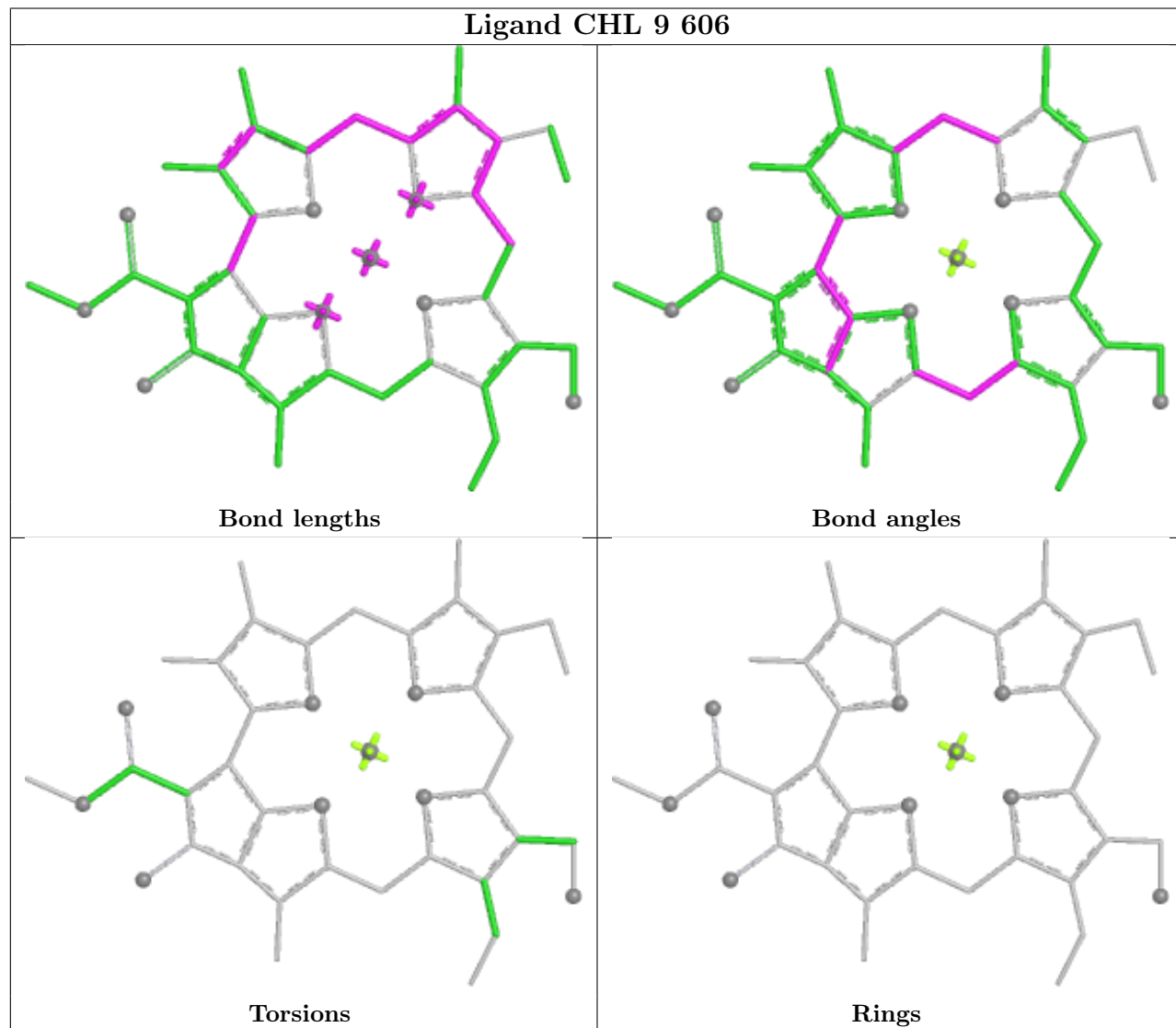
Rings

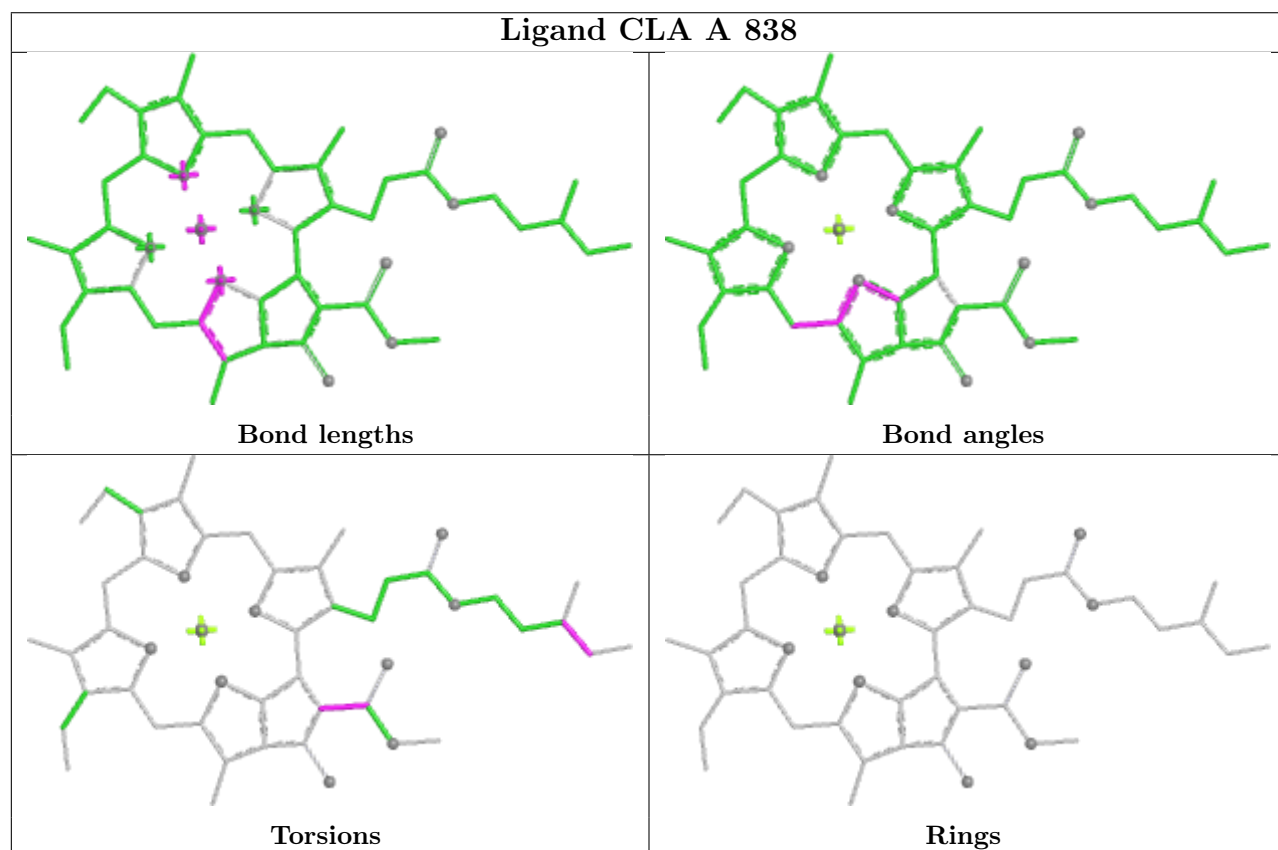
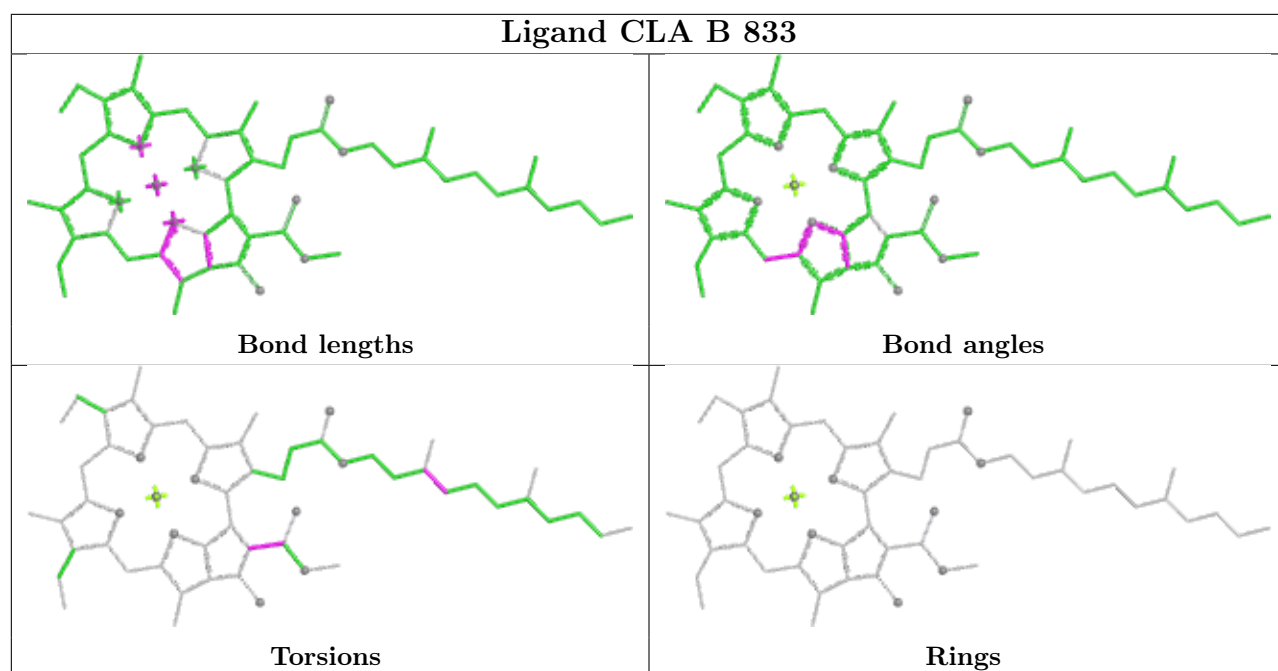


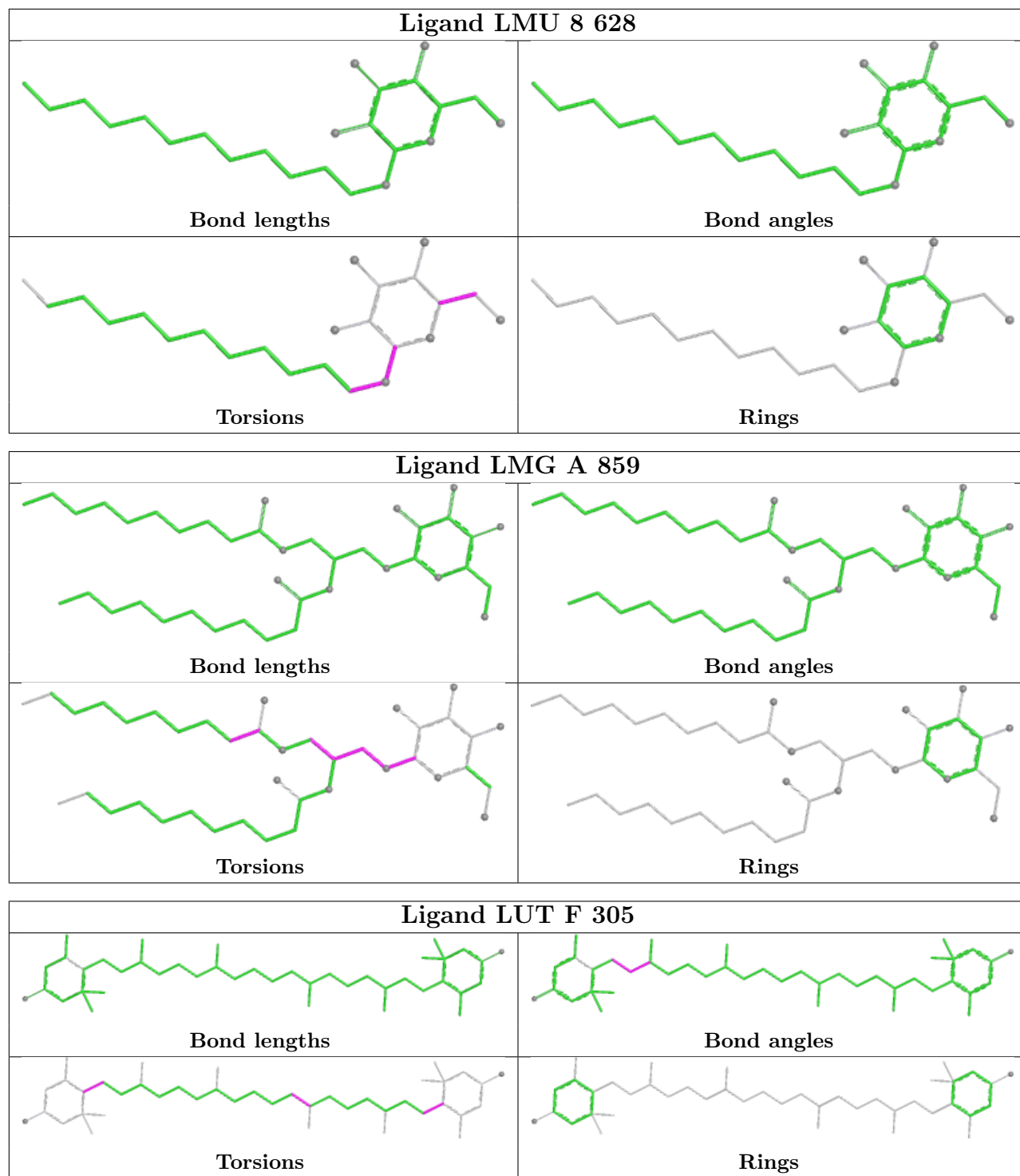
Ligand CLA A 820

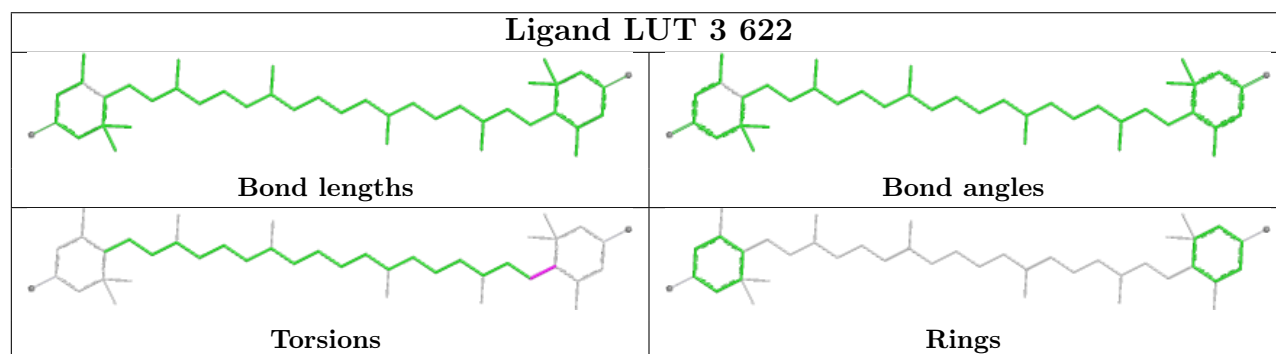
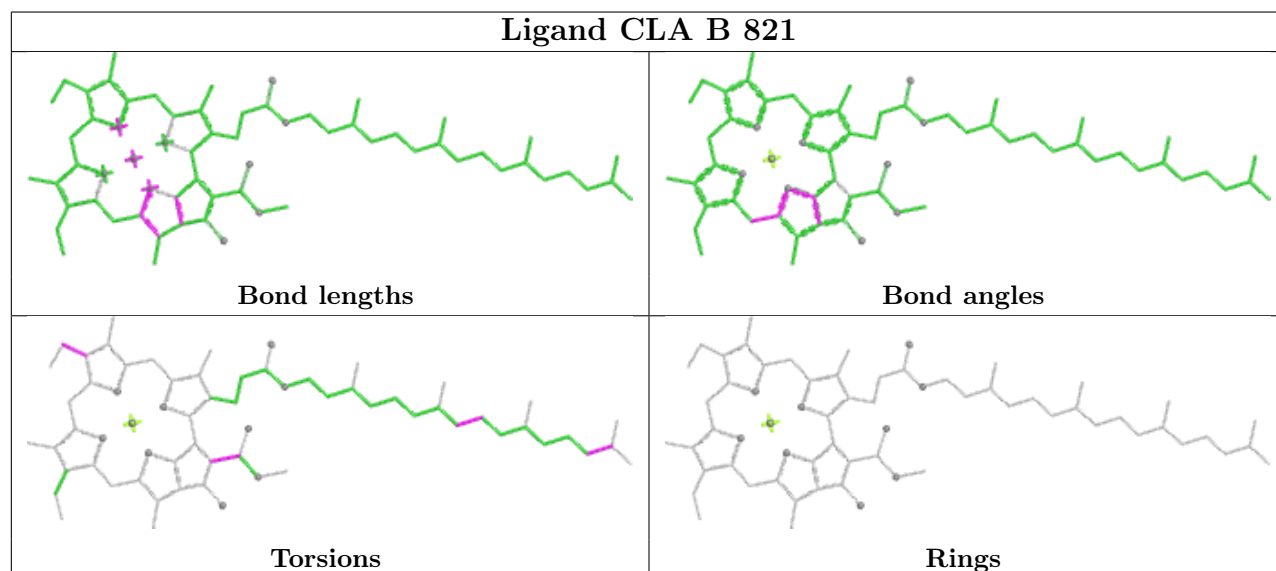
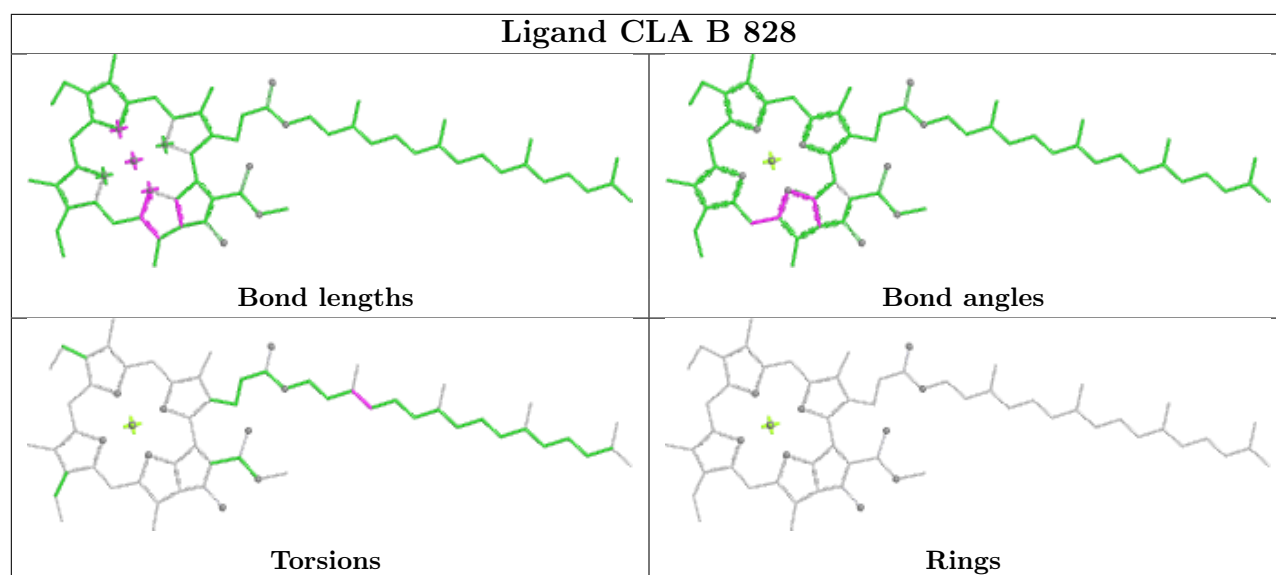


Ligand CHL 9 606

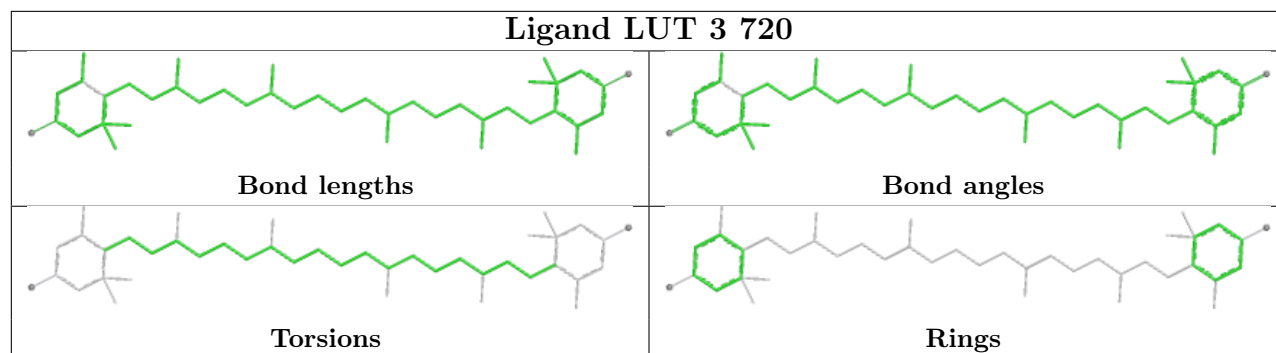




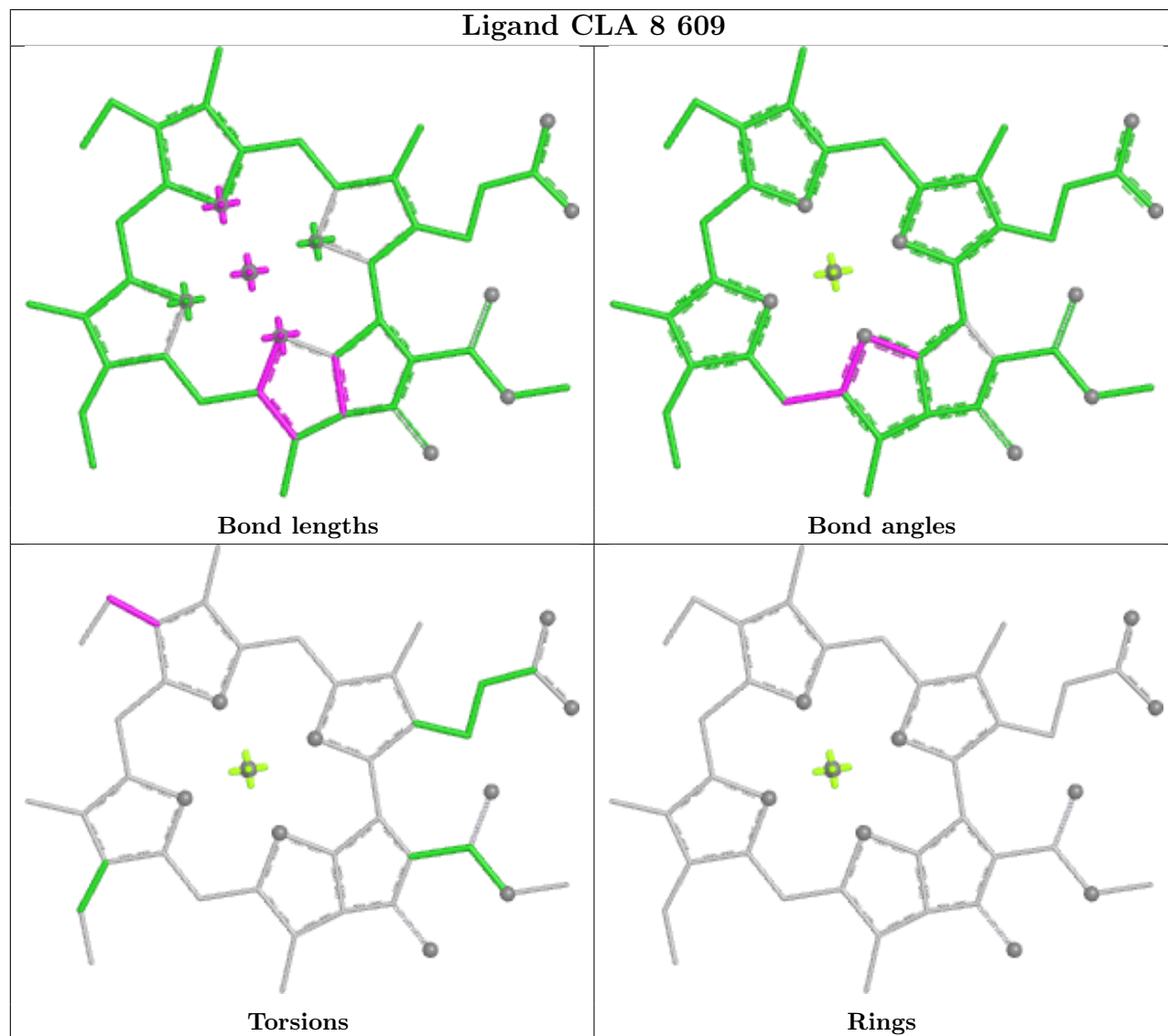


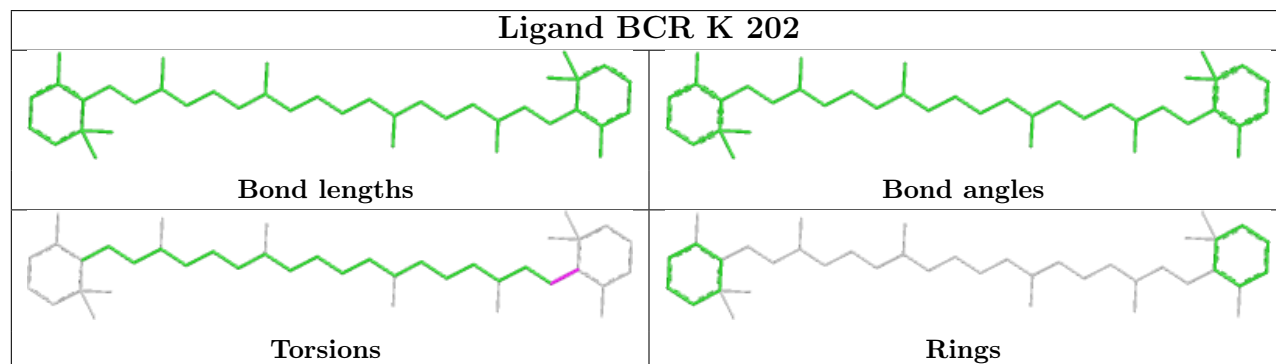
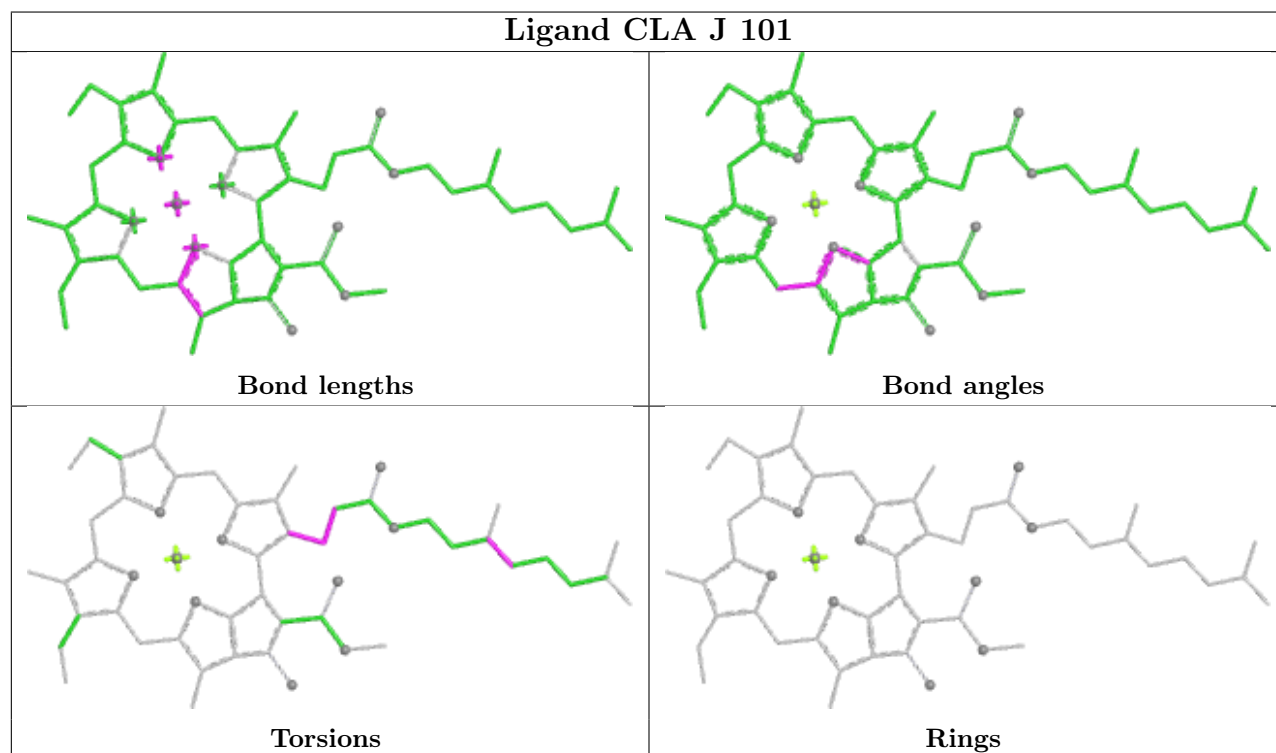
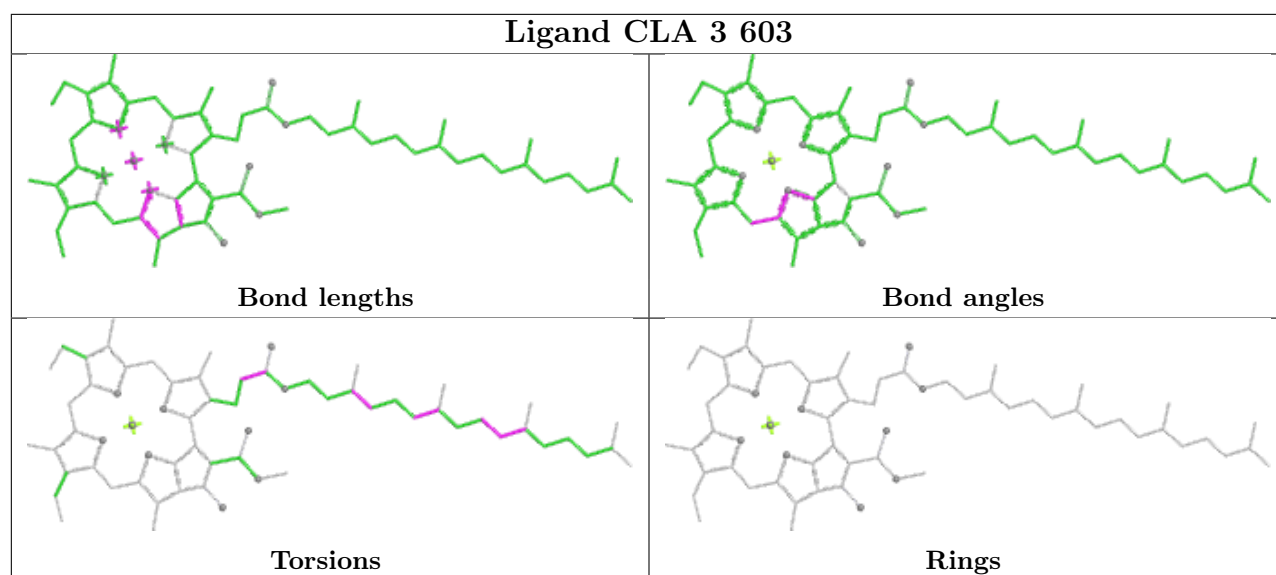


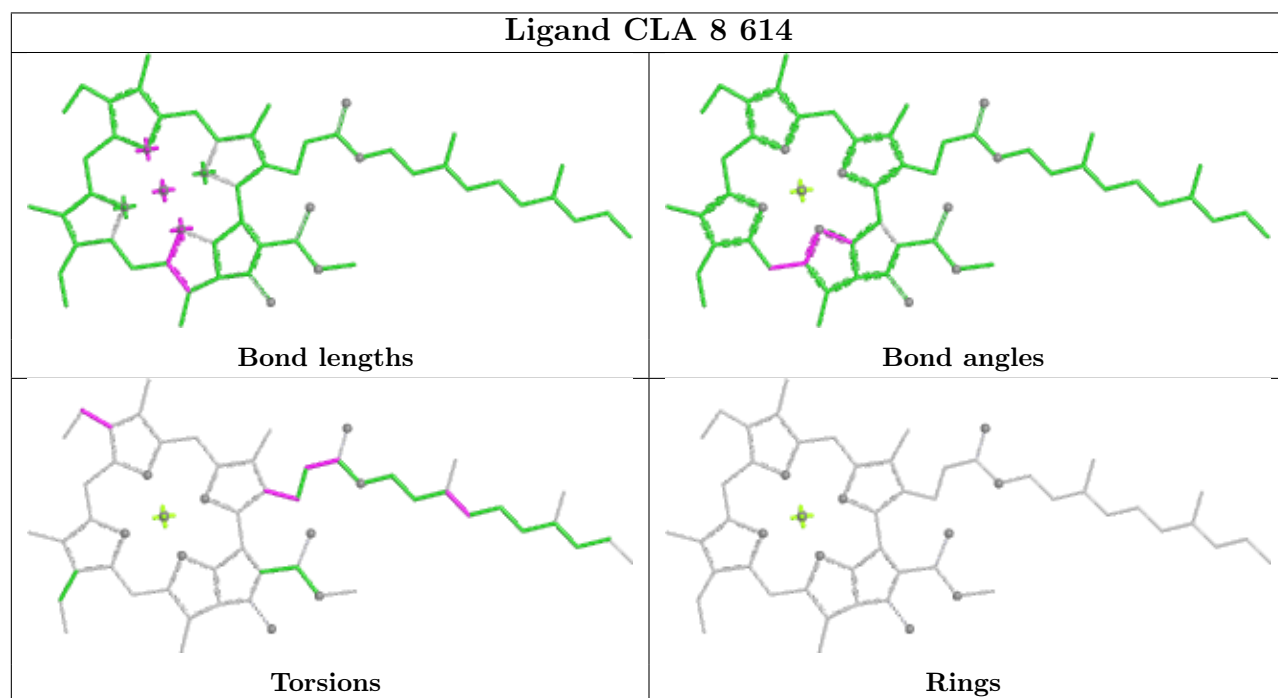
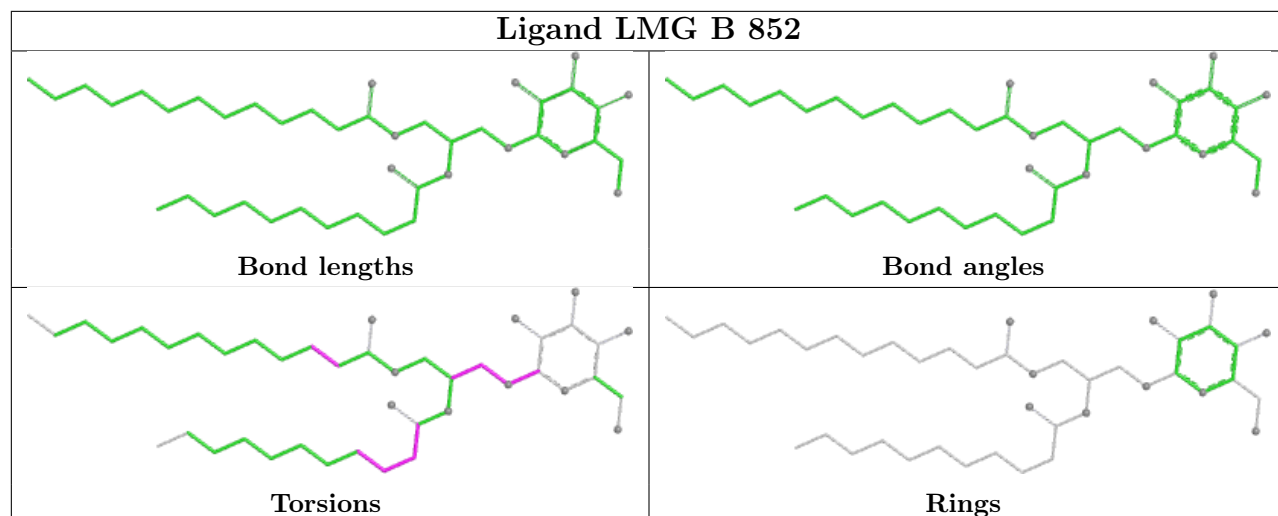
Ligand LUT 3 720

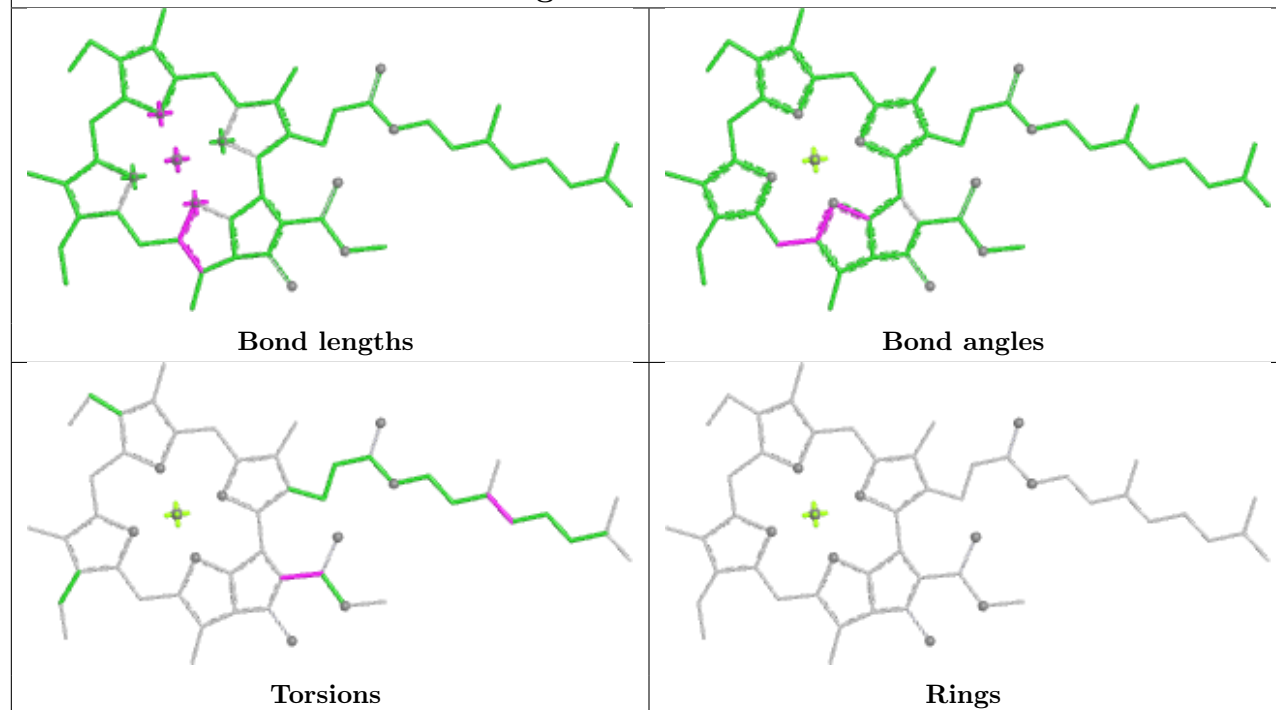
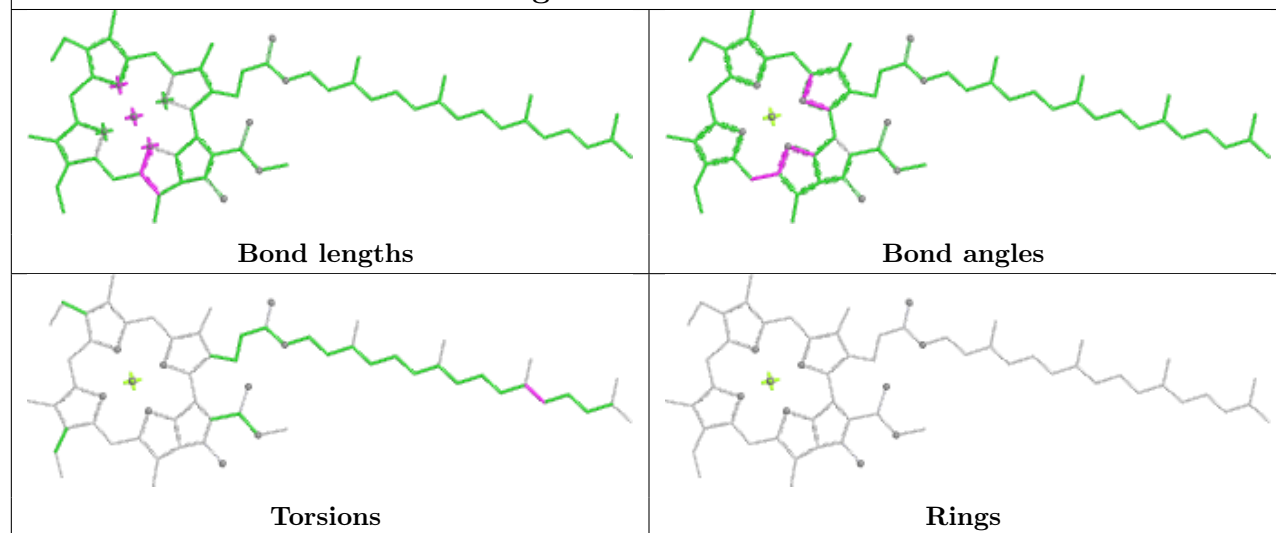


Ligand CLA 8 609

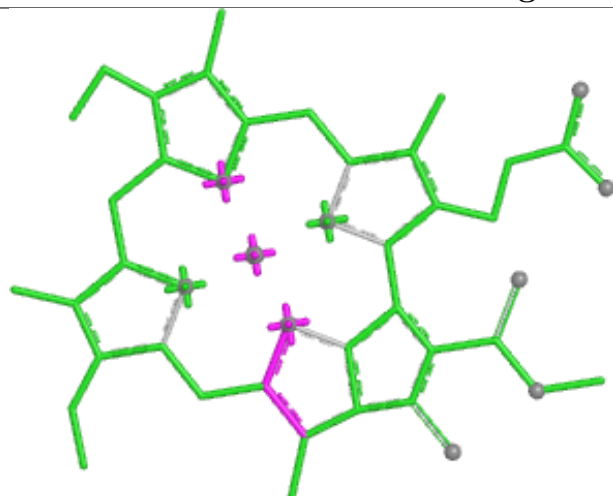




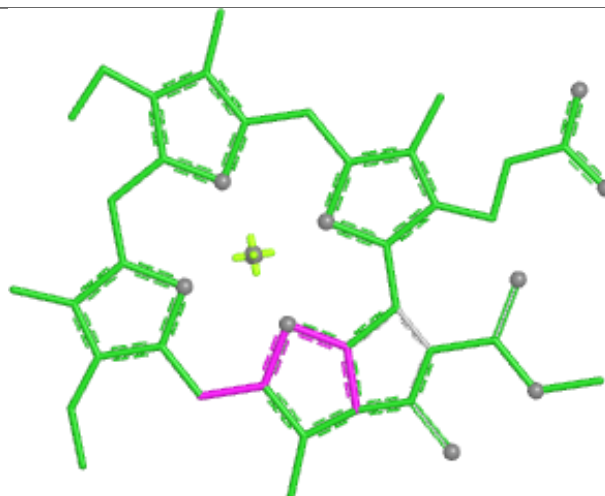


Ligand CLA 8 612**Ligand CLA B 803**

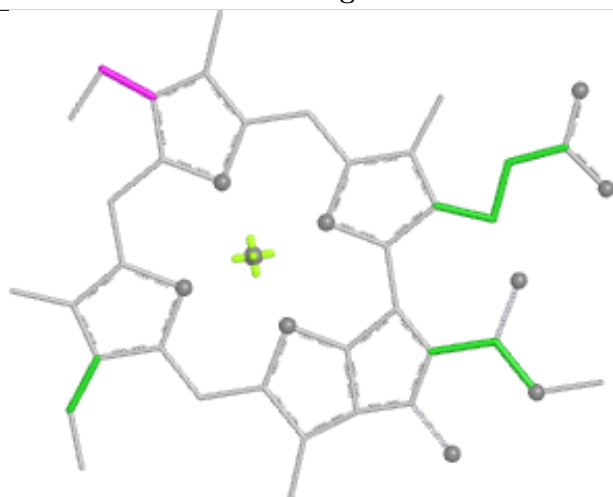
Ligand CLA 3 614



Bond lengths



Bond angles

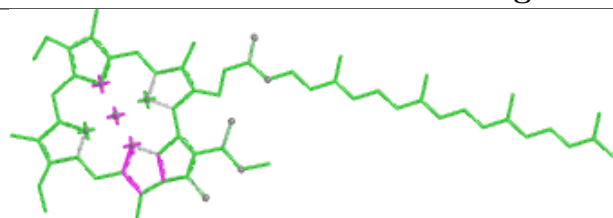


Torsions

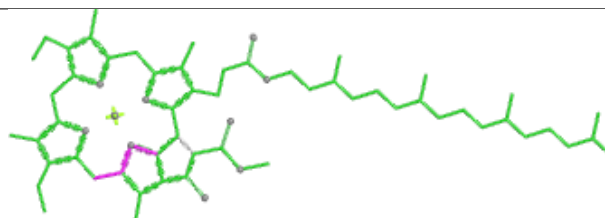


Rings

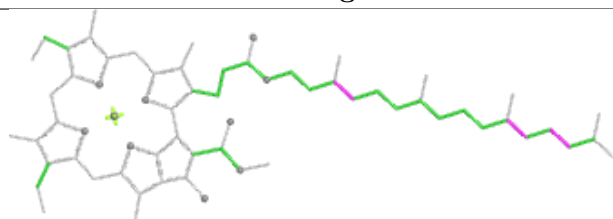
Ligand CLA A 840



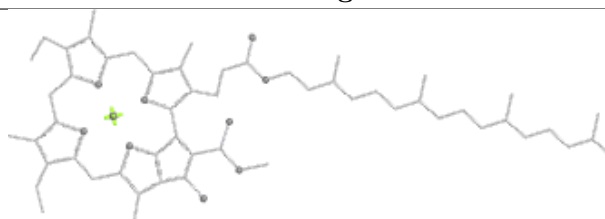
Bond lengths



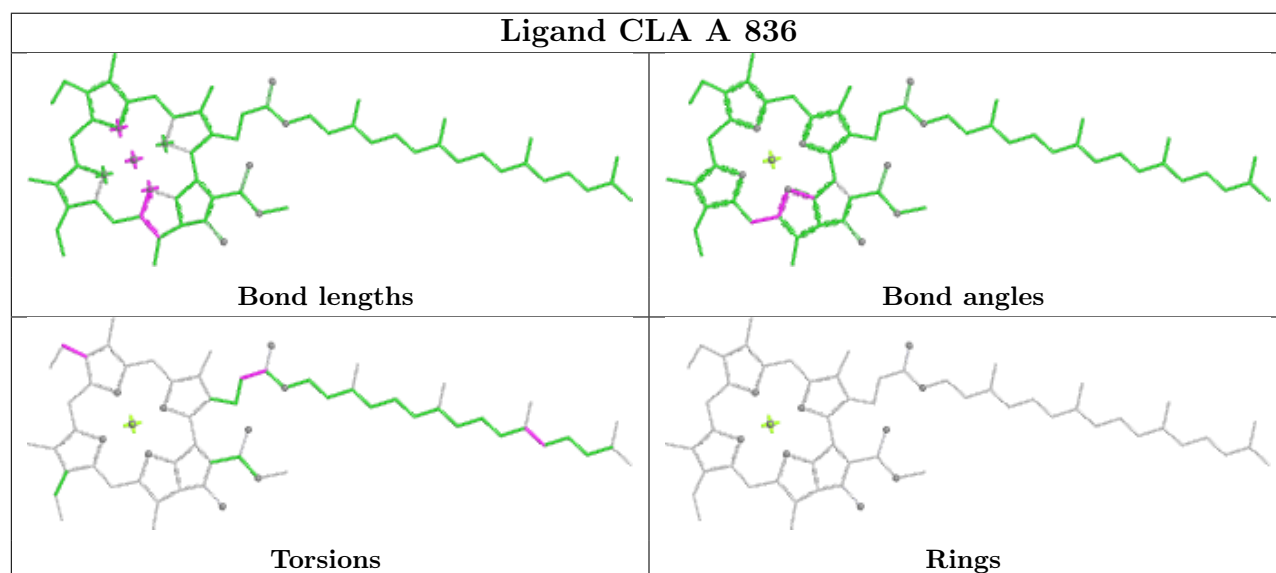
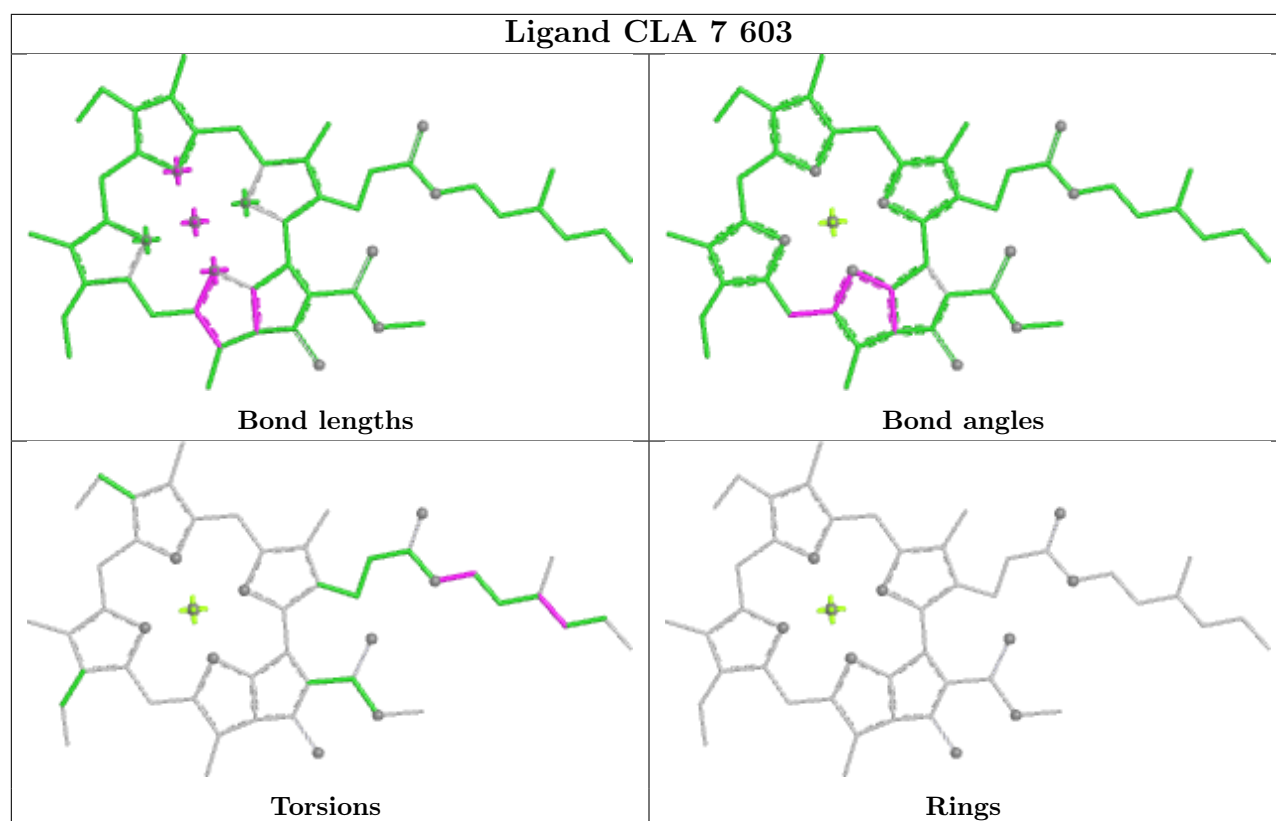
Bond angles

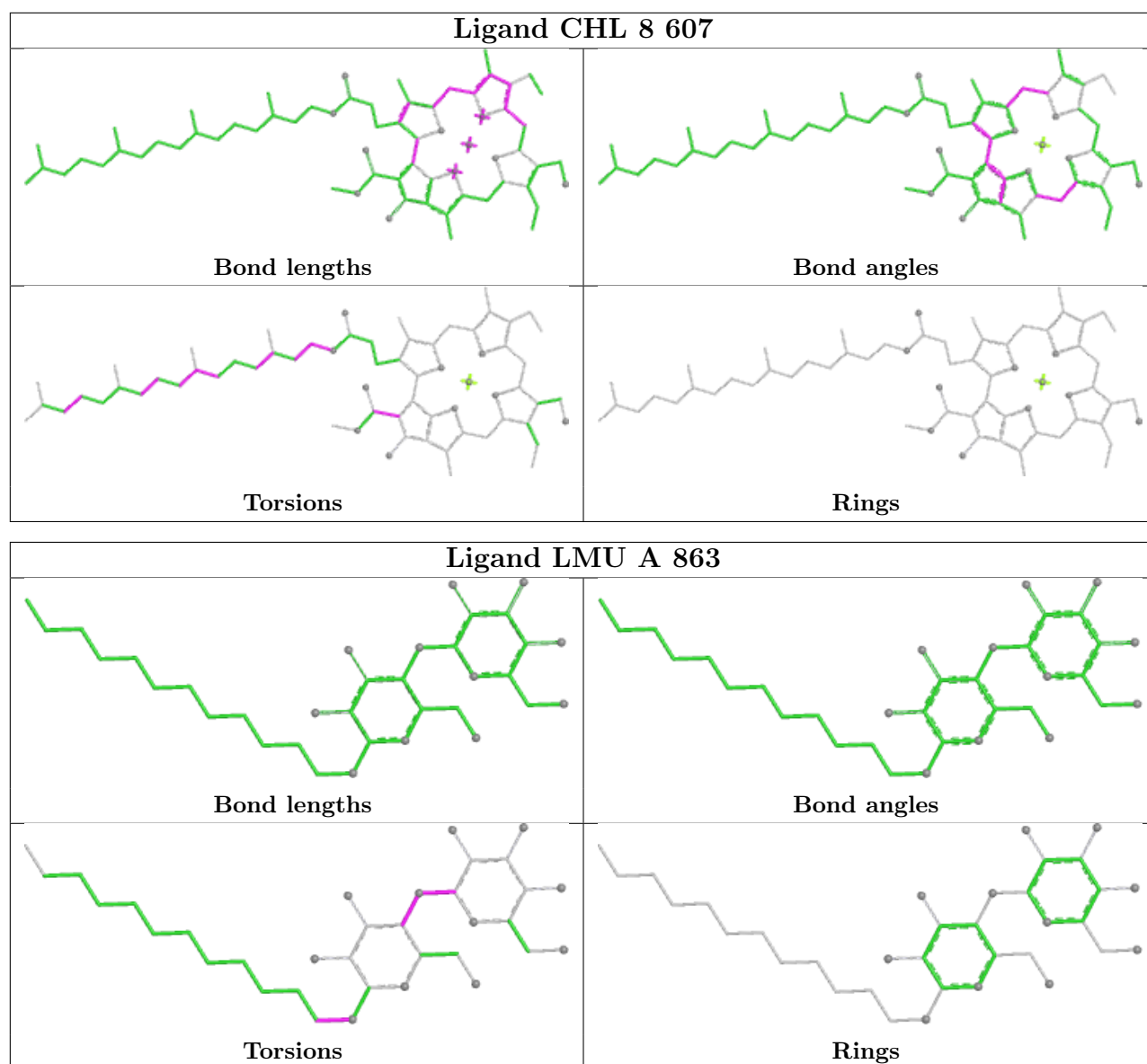


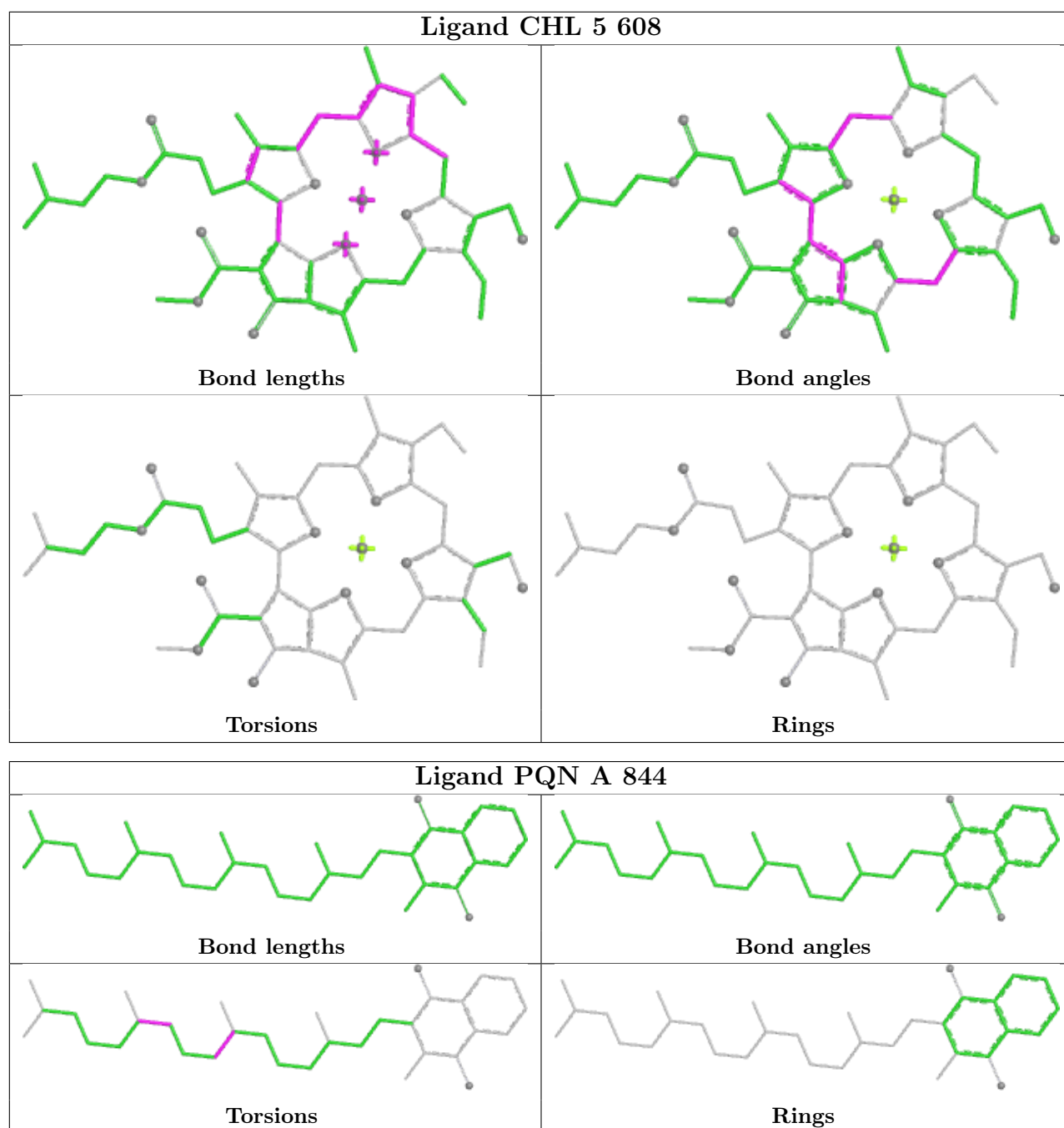
Torsions

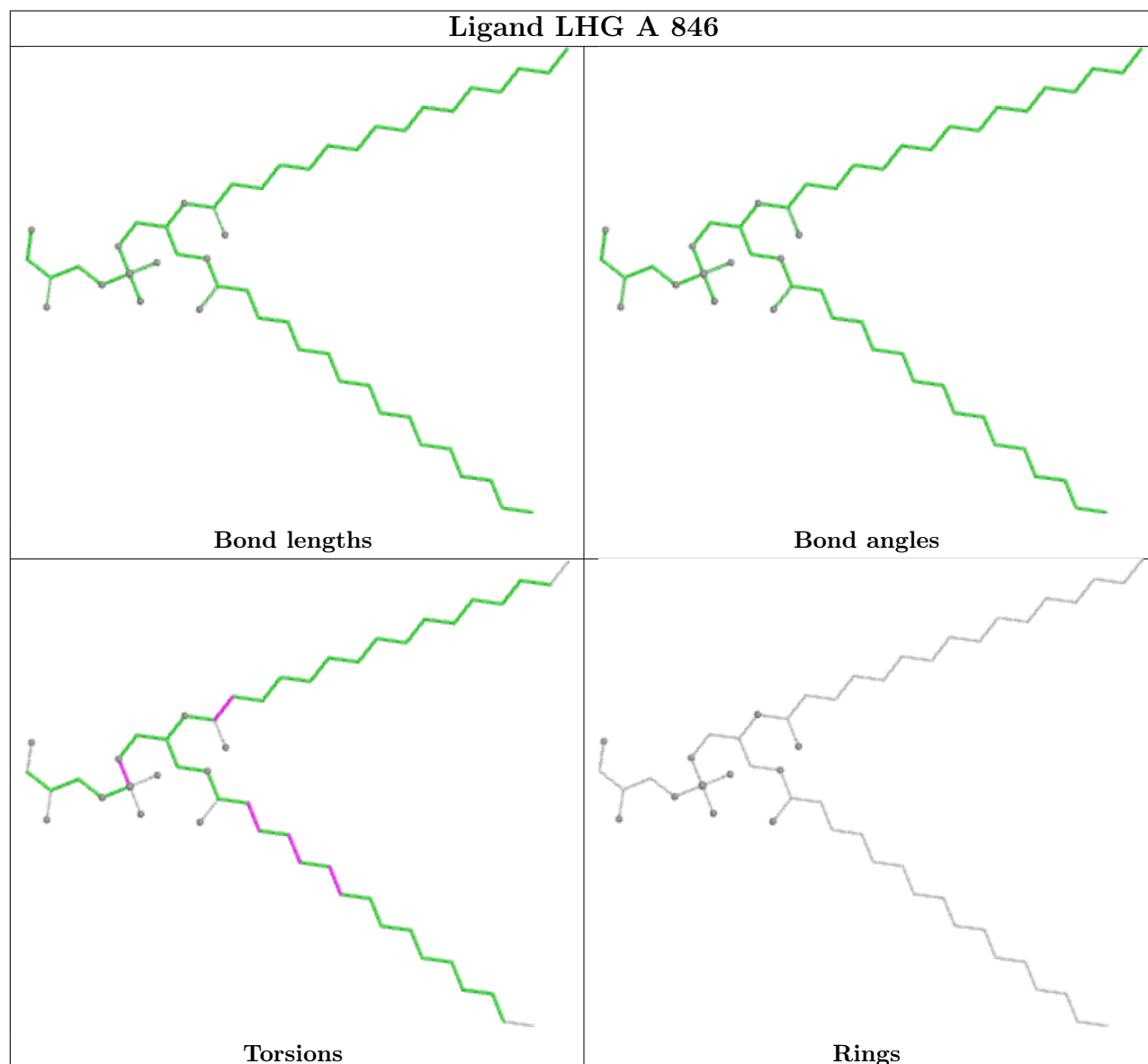
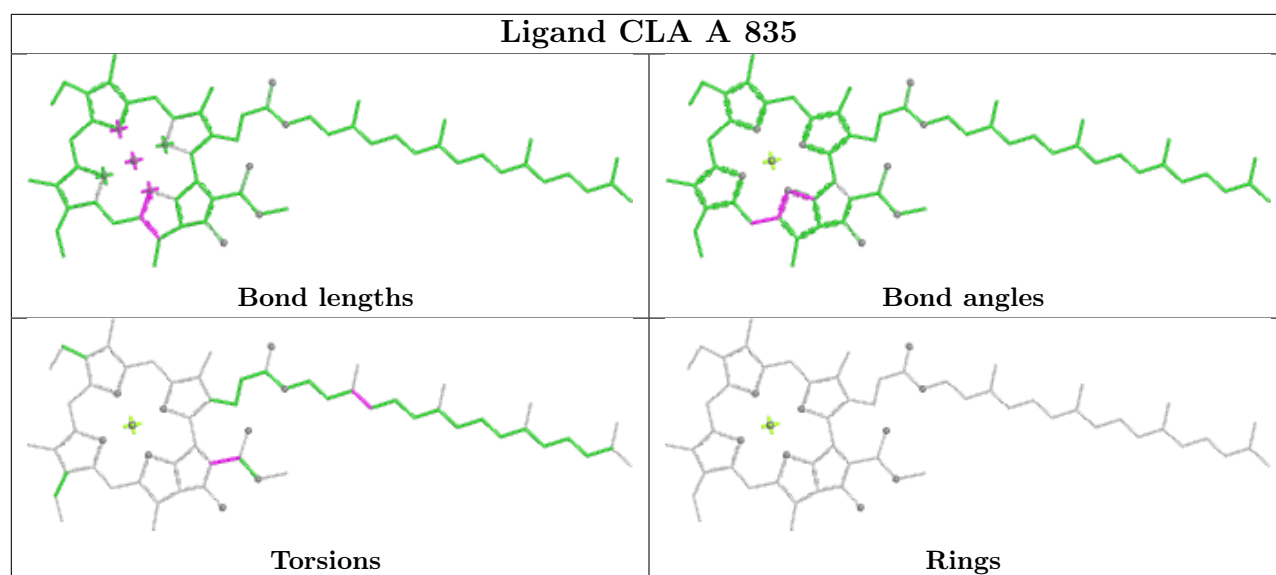


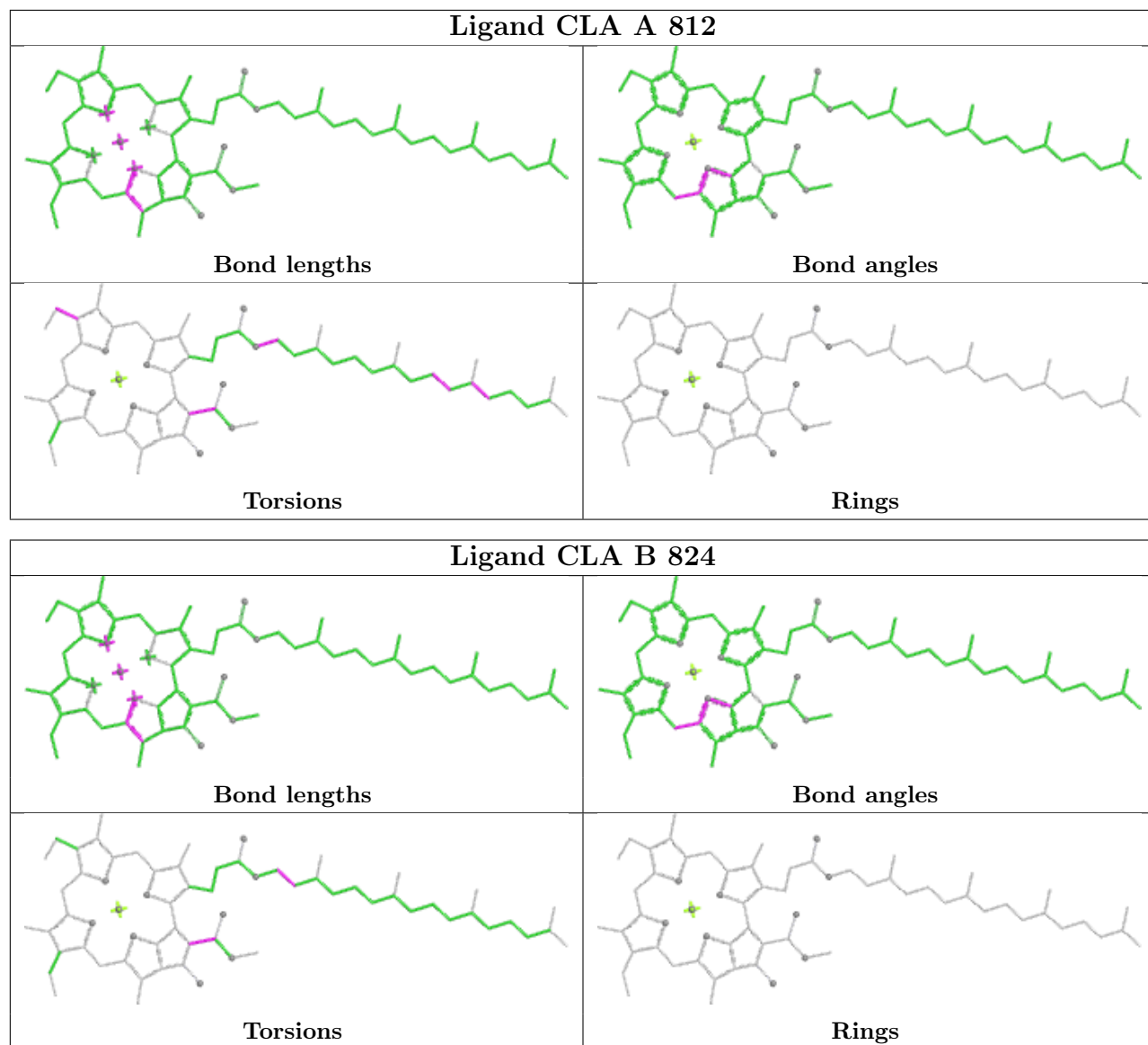
Rings



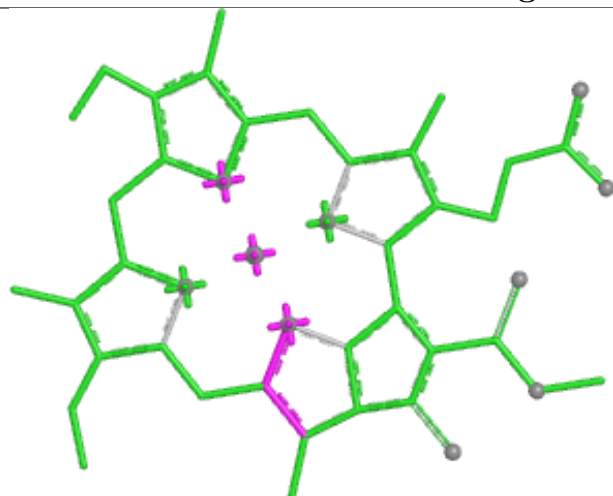




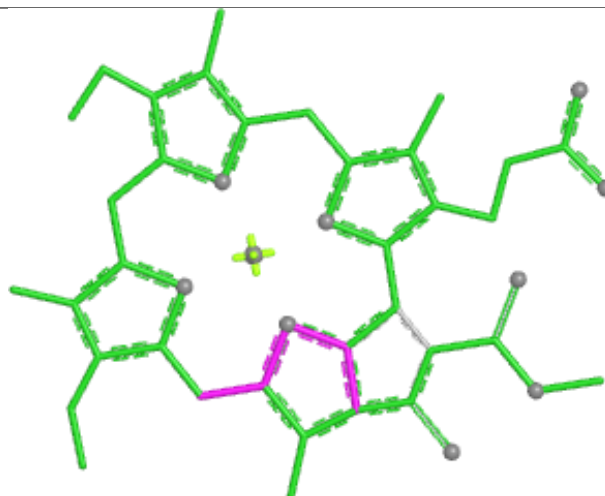




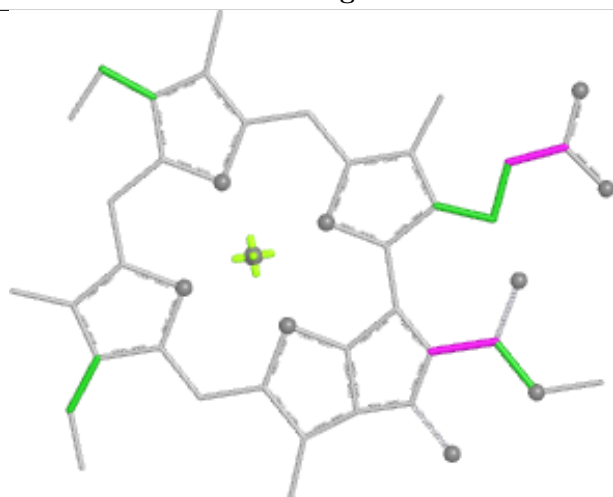
Ligand CLA 6 612



Bond lengths



Bond angles

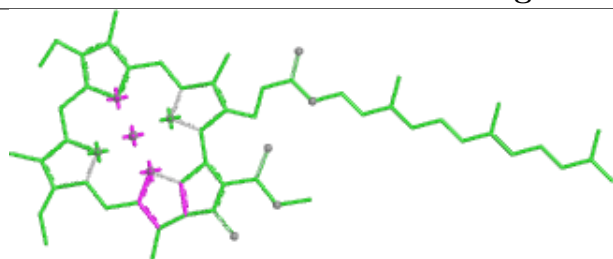


Torsions

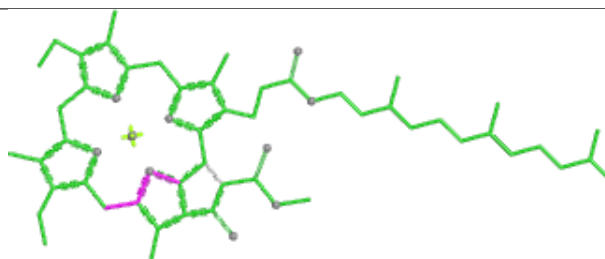


Rings

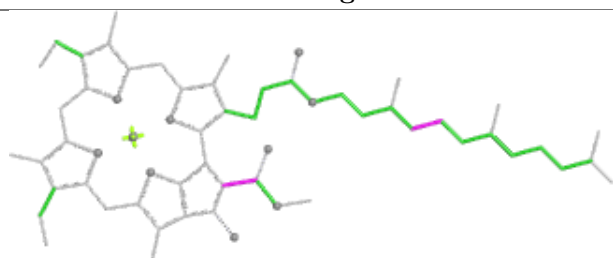
Ligand CLA B 834



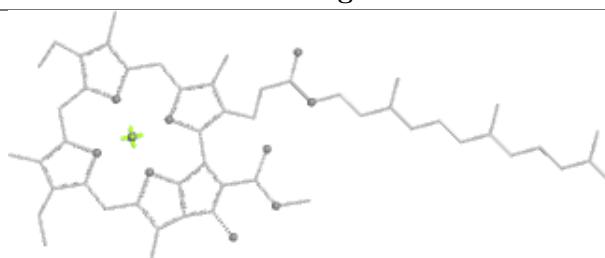
Bond lengths



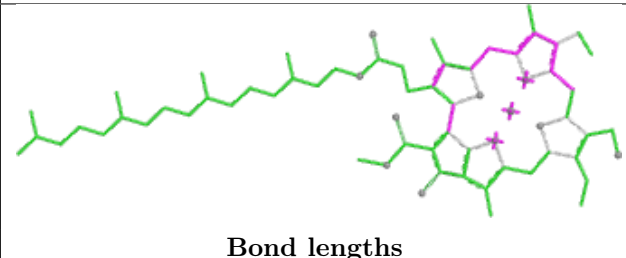
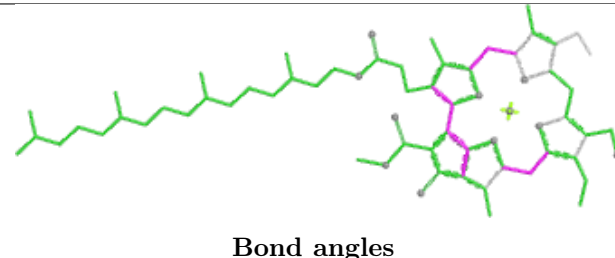
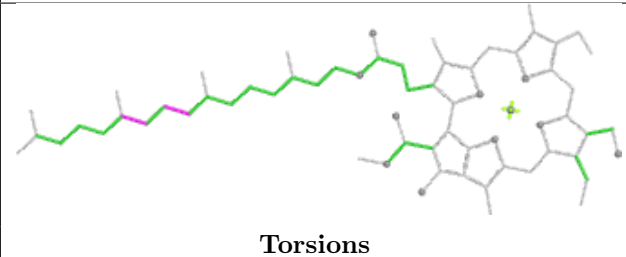
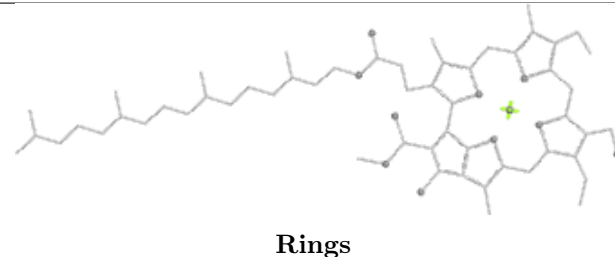
Bond angles

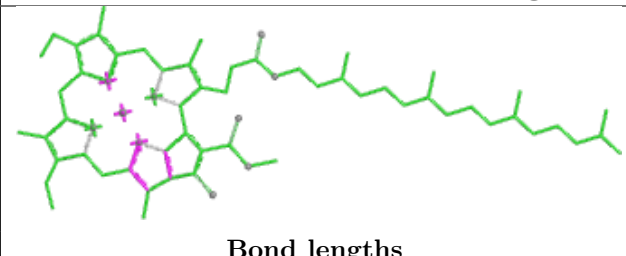
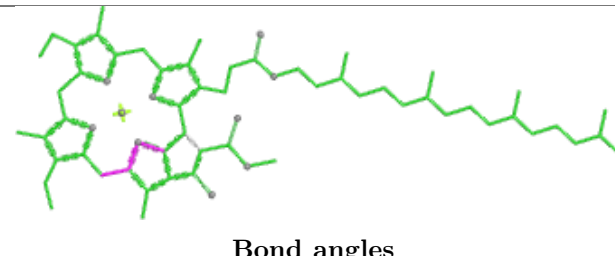
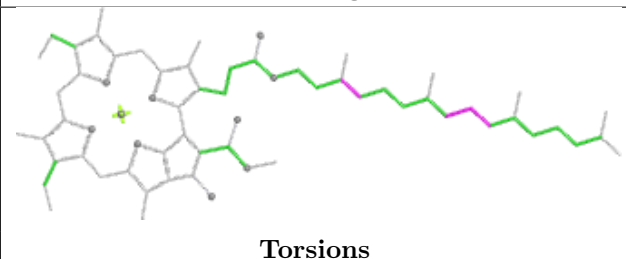
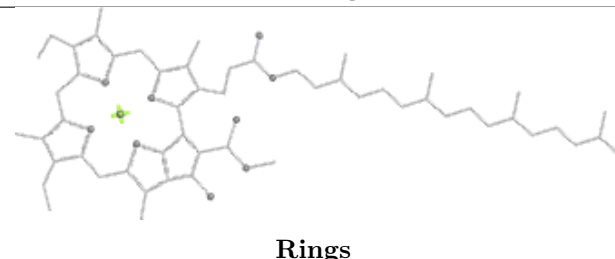


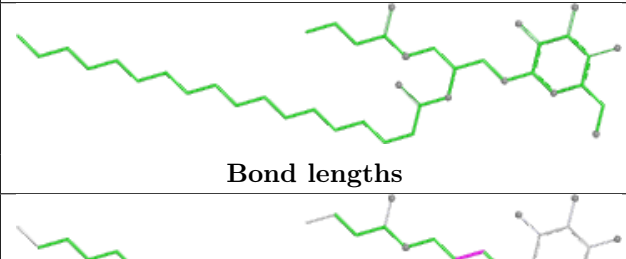
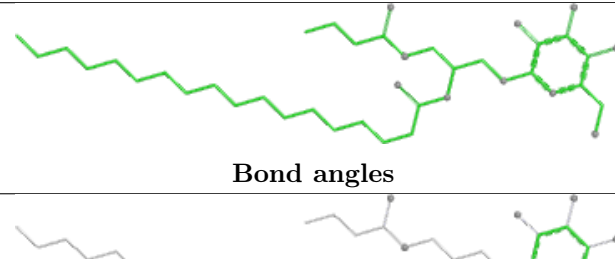
Torsions

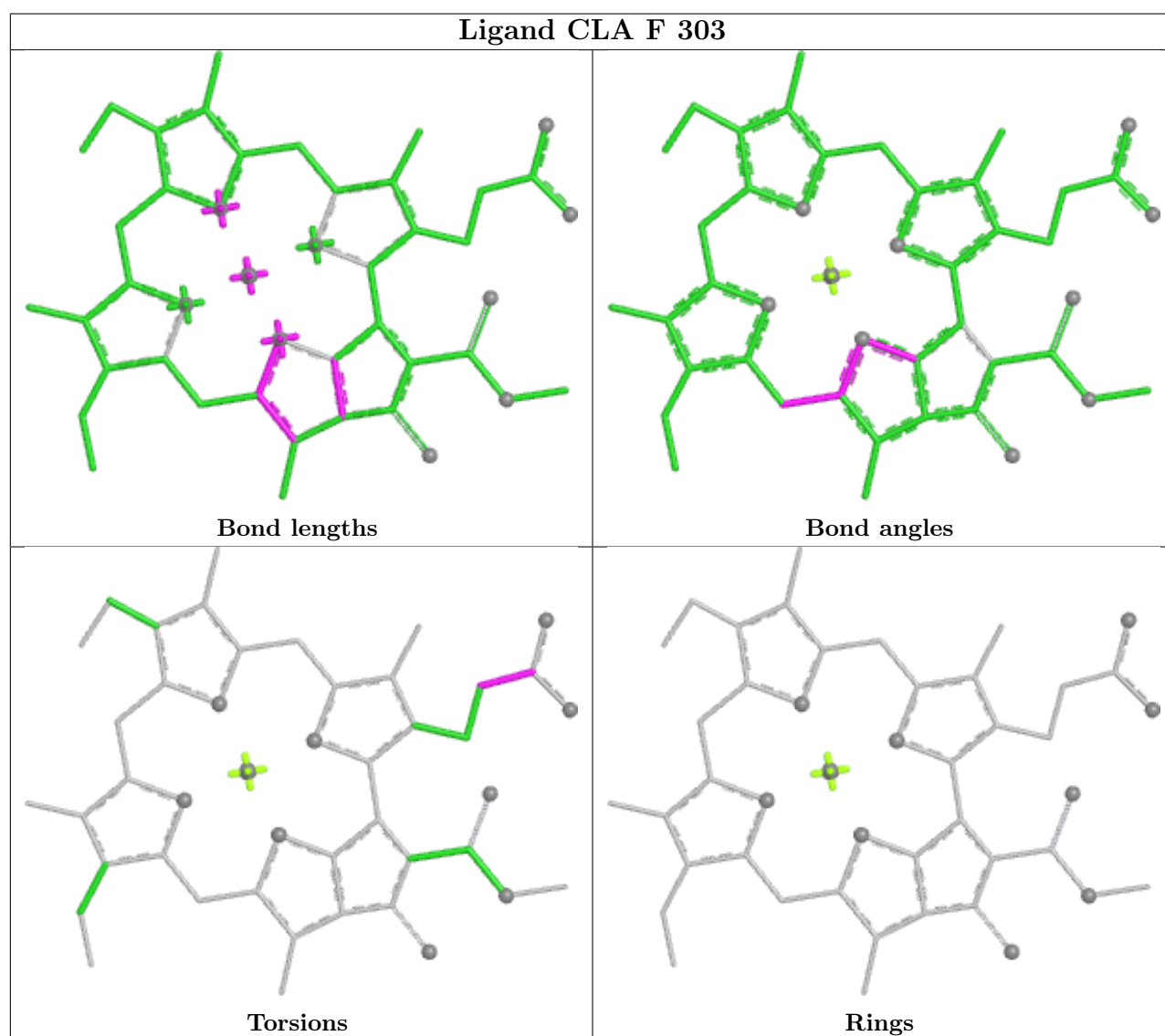
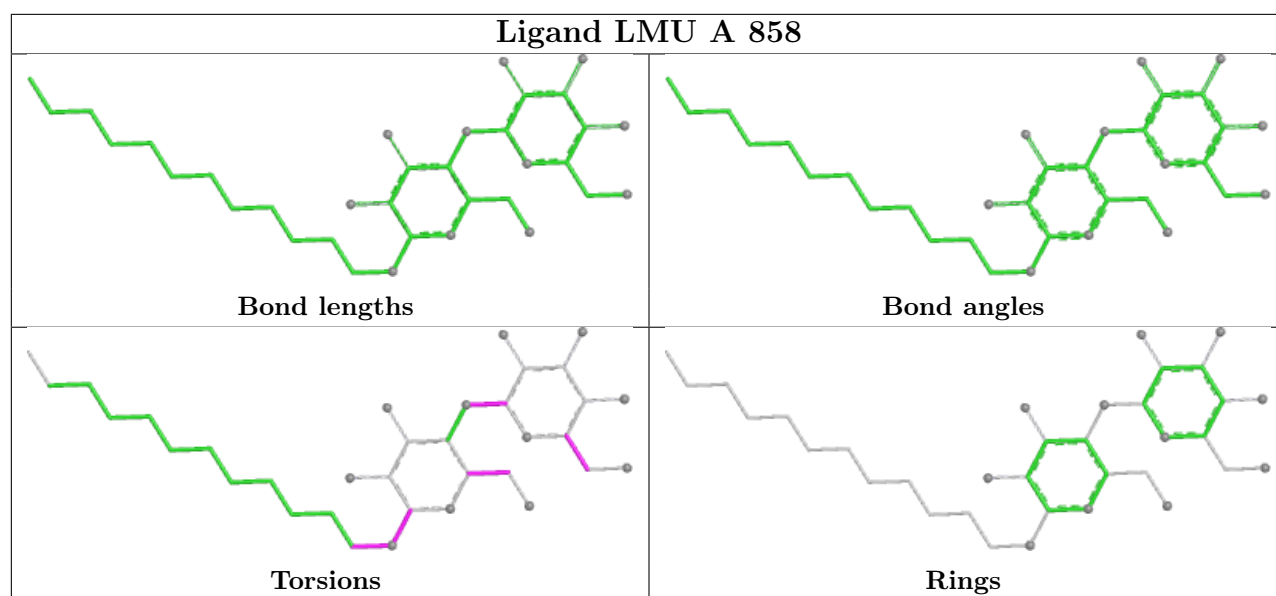


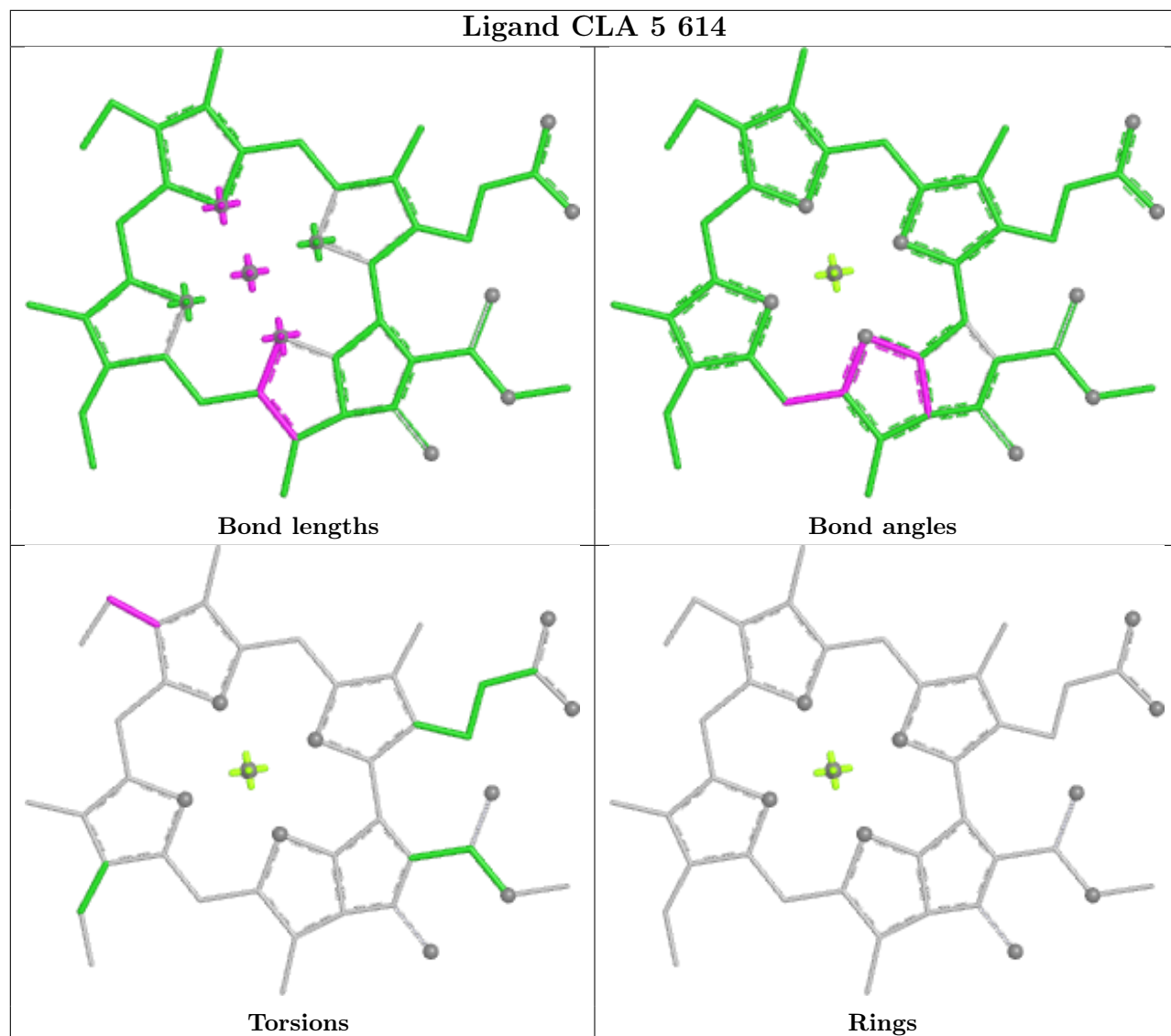
Rings

Ligand CHL 7 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

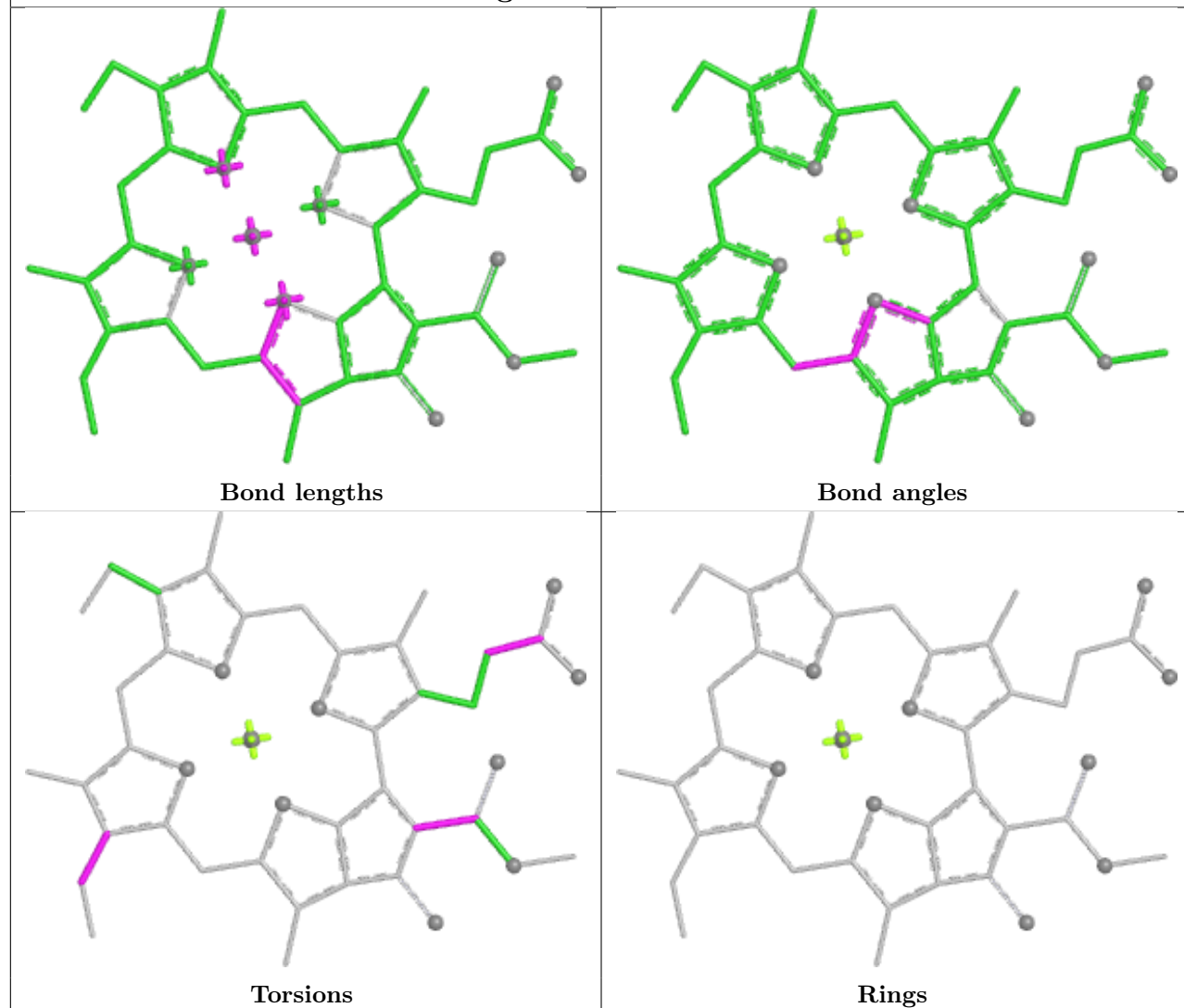
Ligand CLA 5 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG 4 624	
	
Bond lengths	Bond angles
	
Torsions	Rings

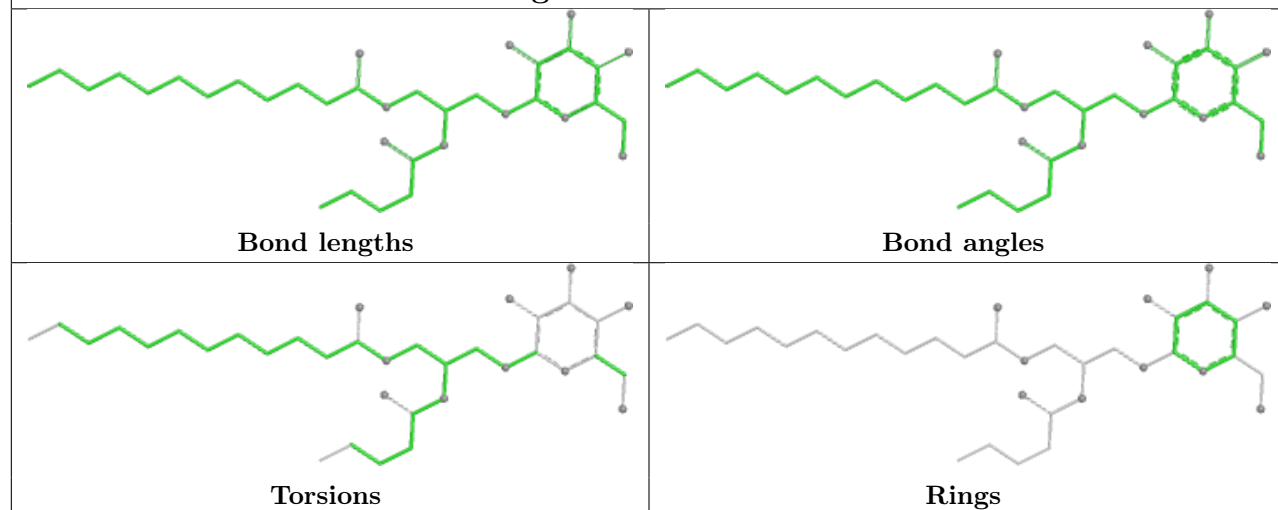


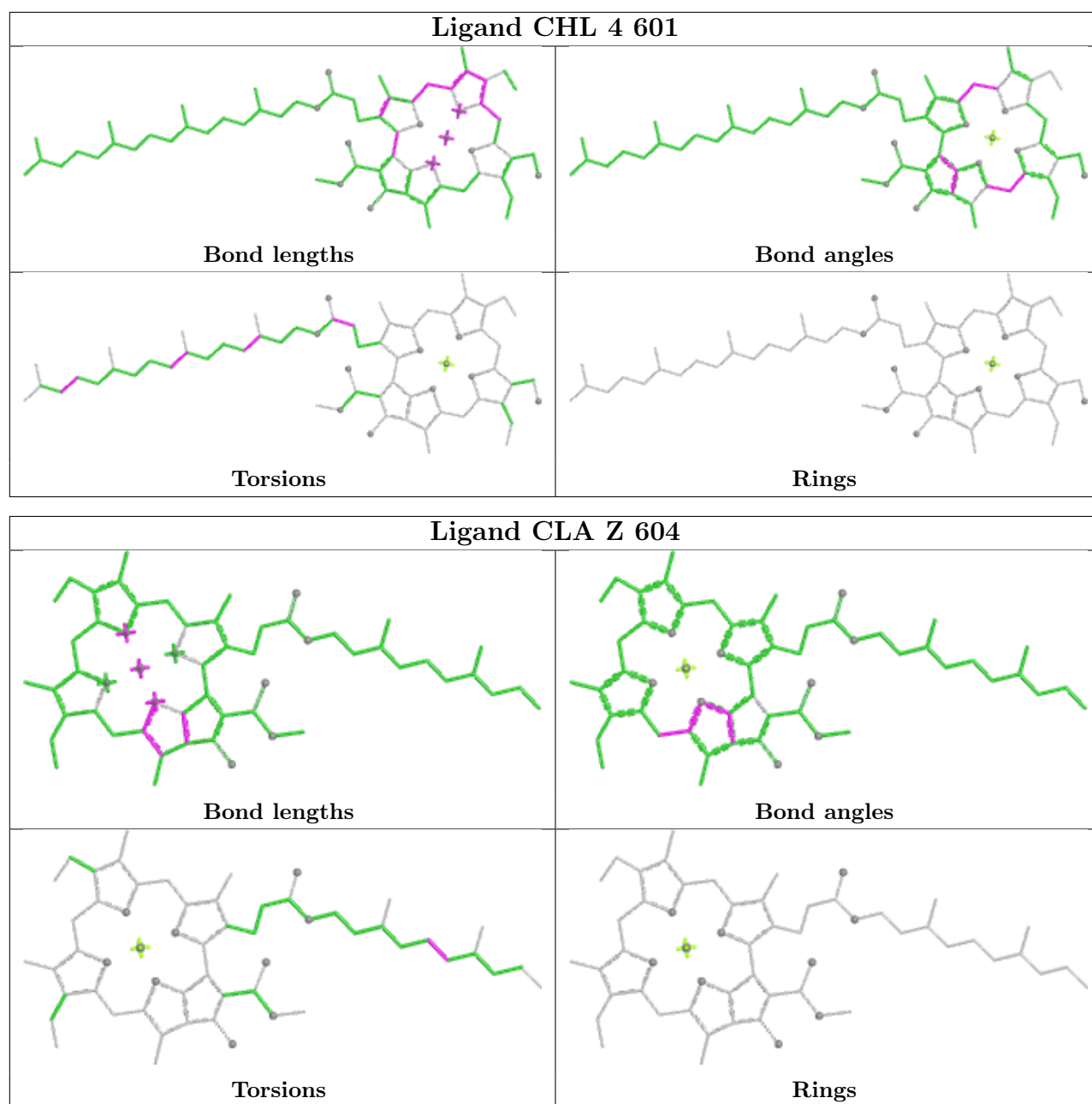


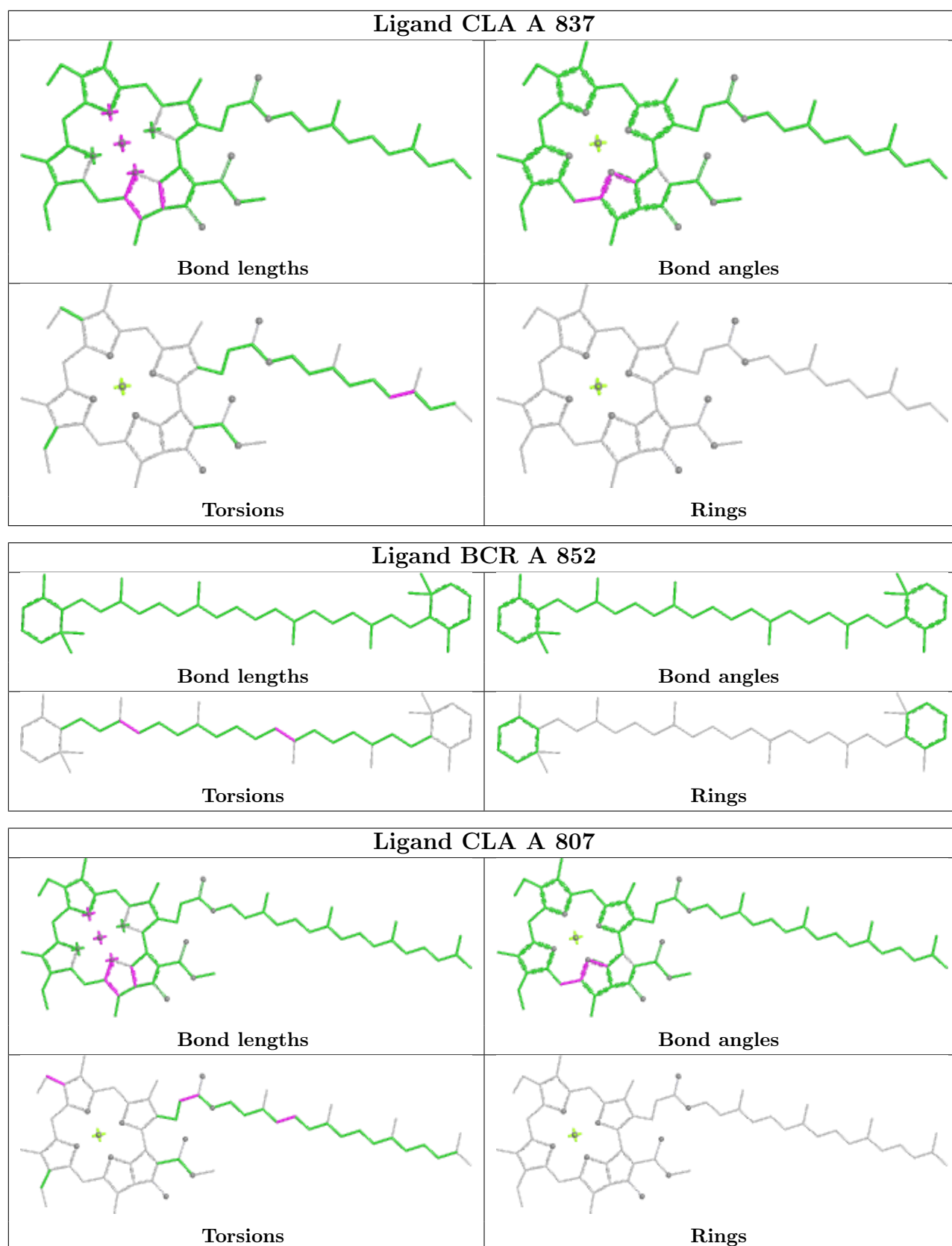
Ligand CLA 5 612

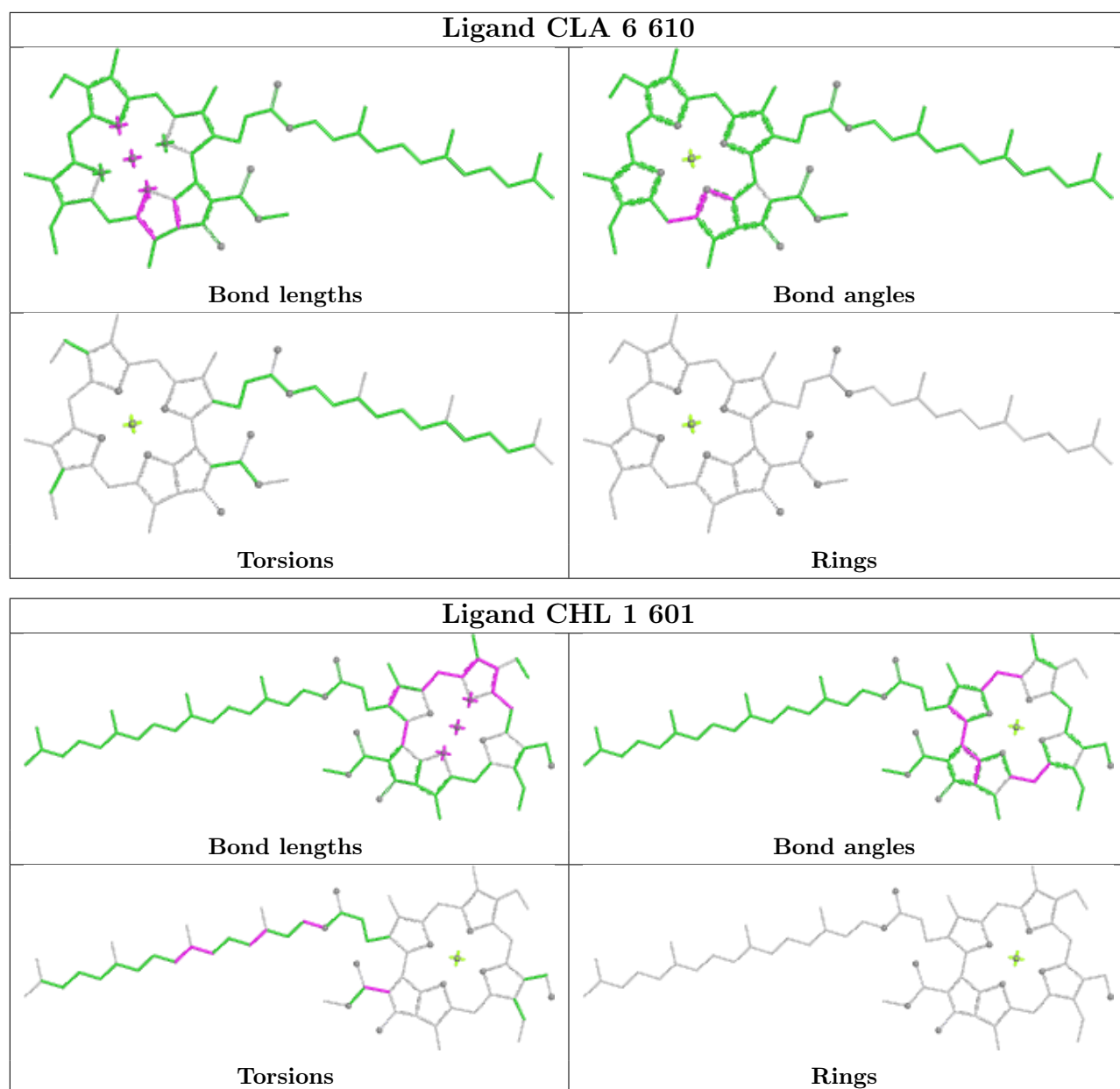


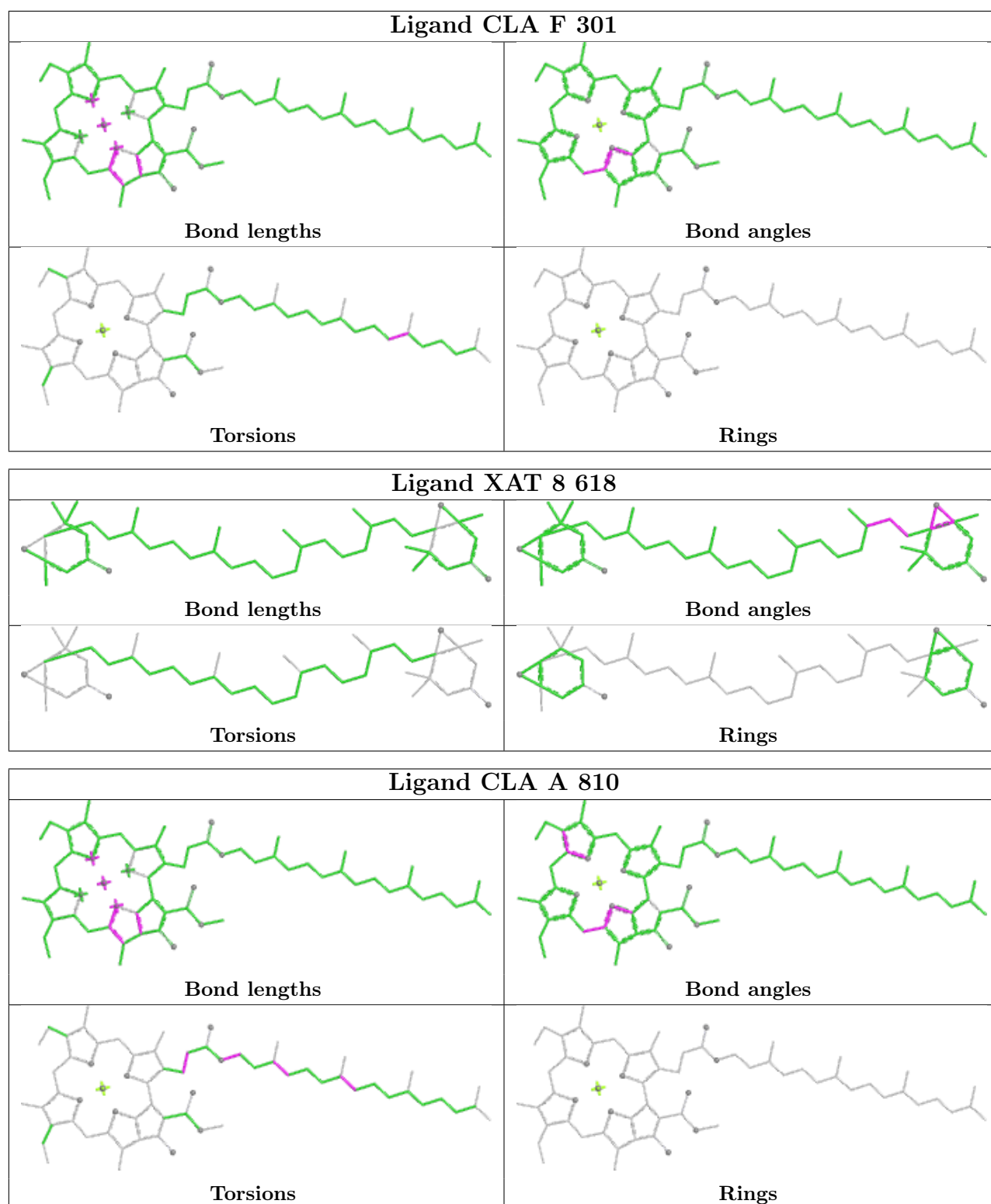
Ligand LMG 1 624

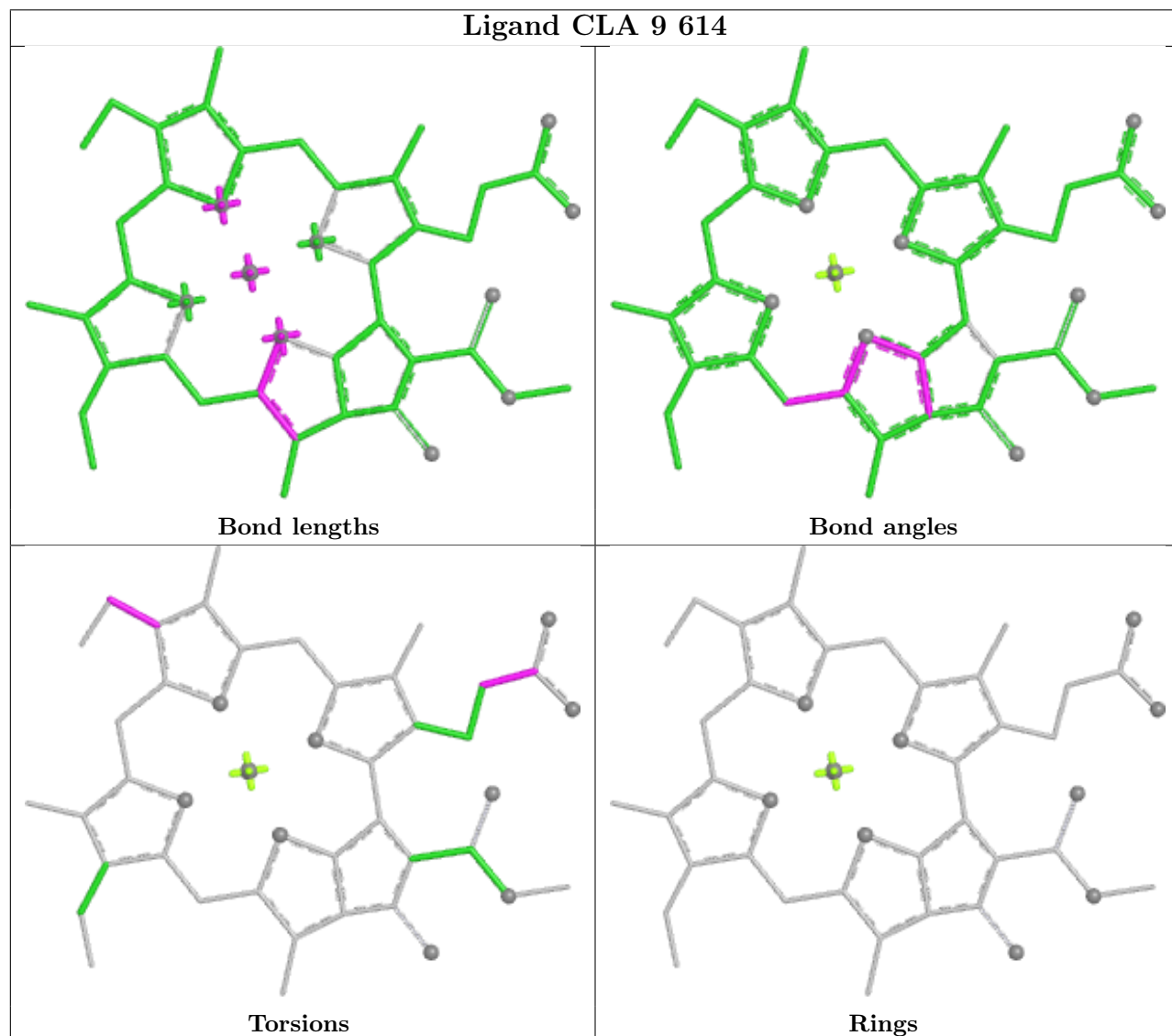
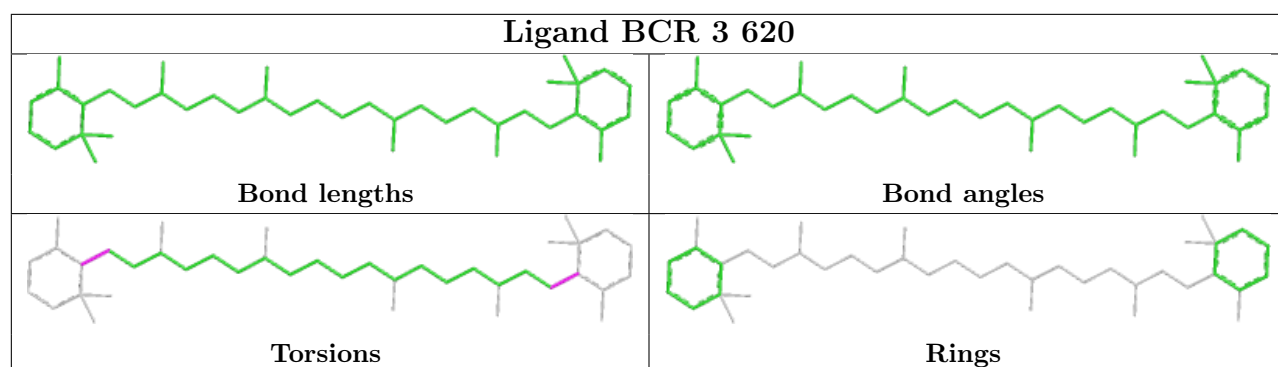


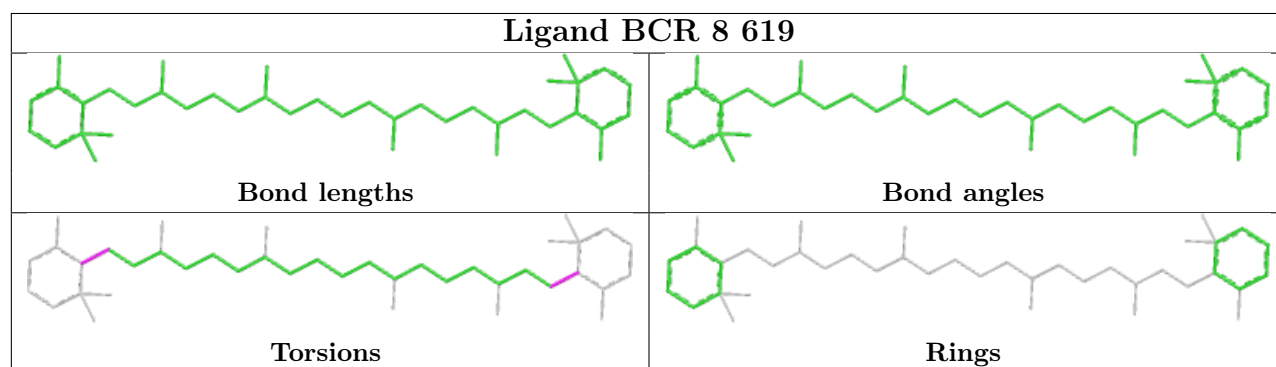
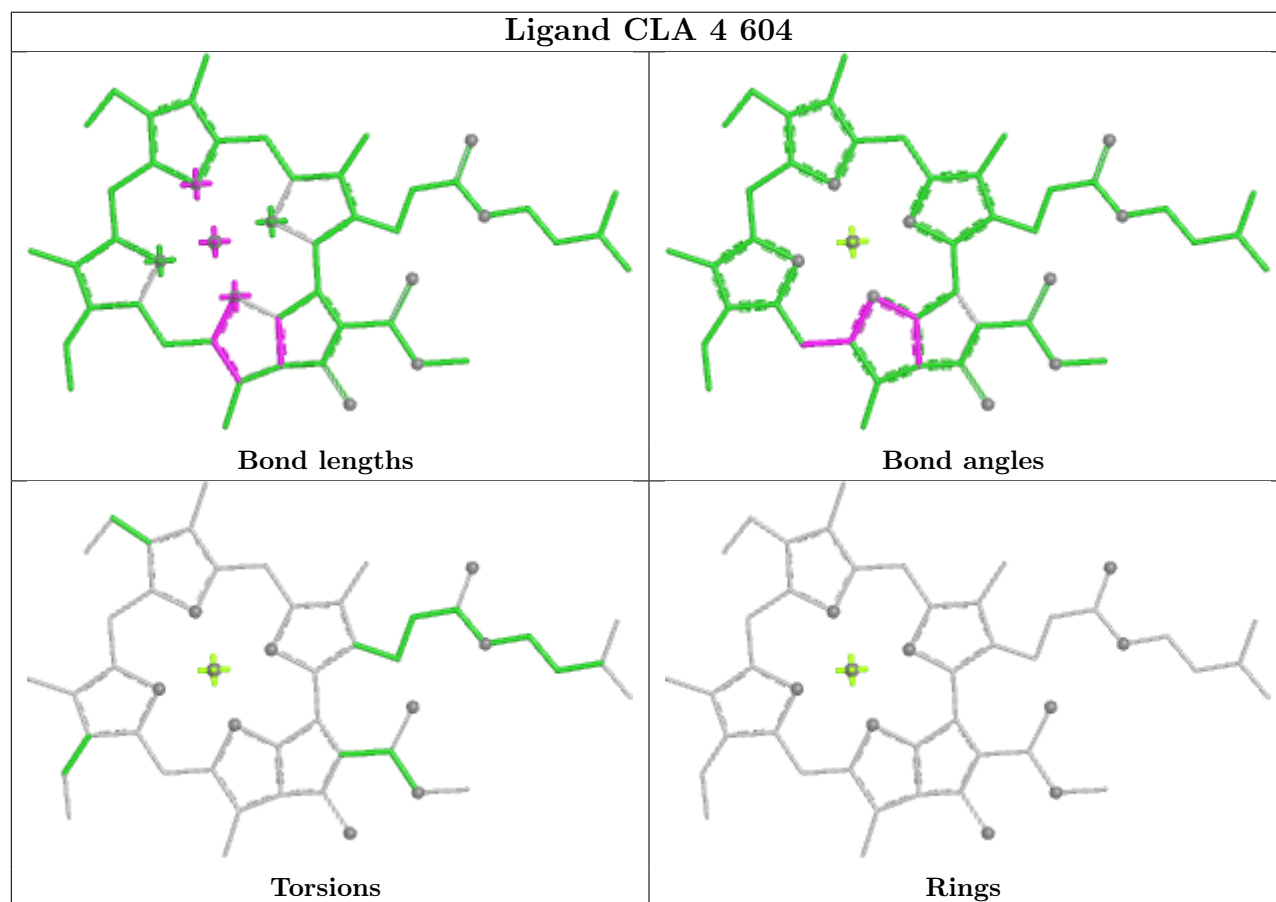
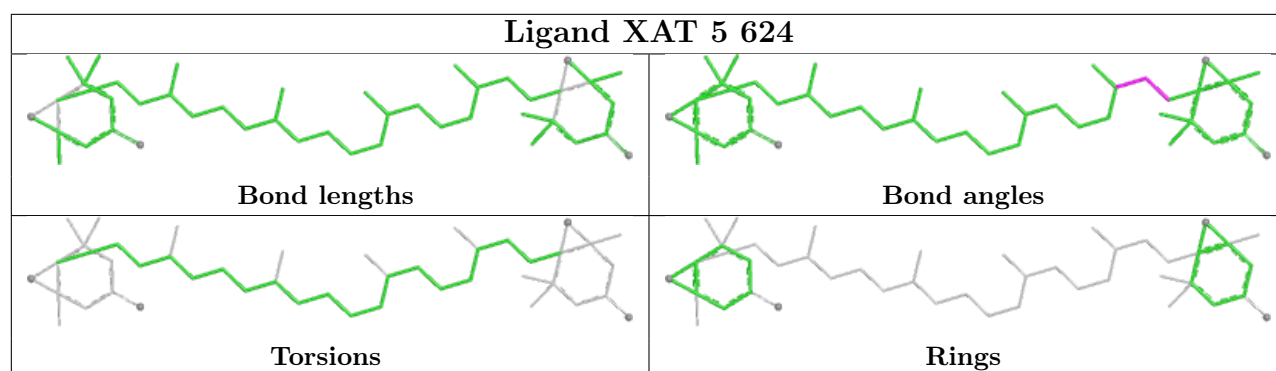




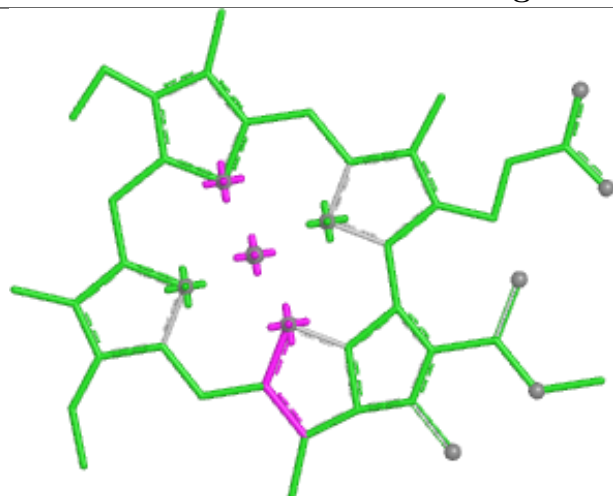




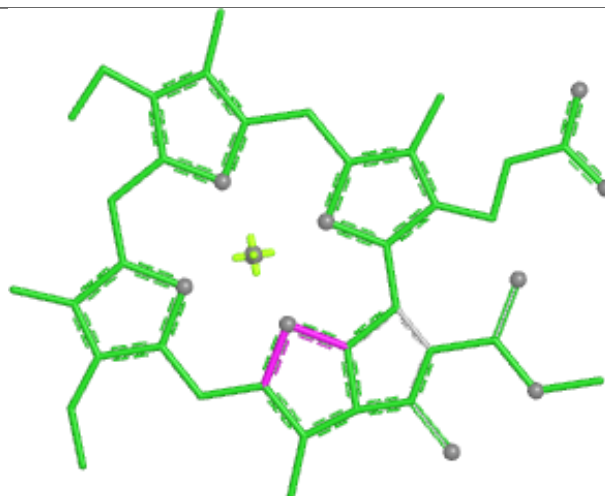




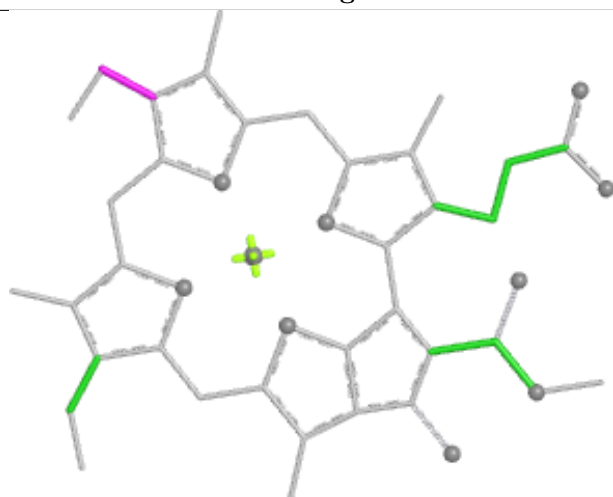
Ligand CLA K 201



Bond lengths



Bond angles

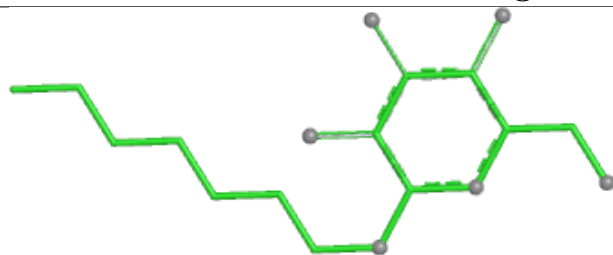


Torsions

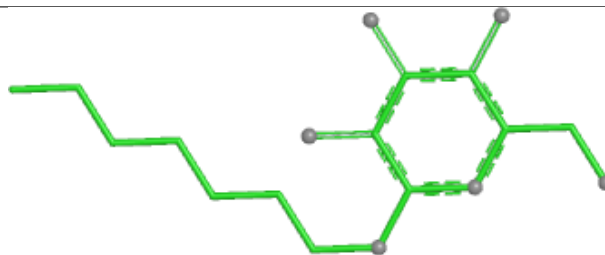


Rings

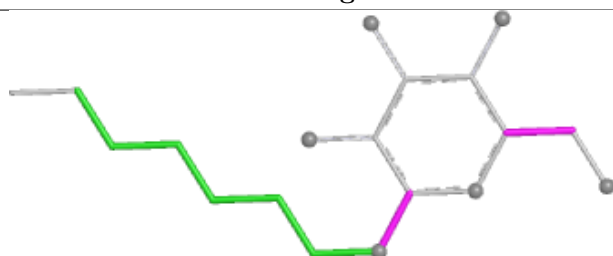
Ligand LMU 1 622



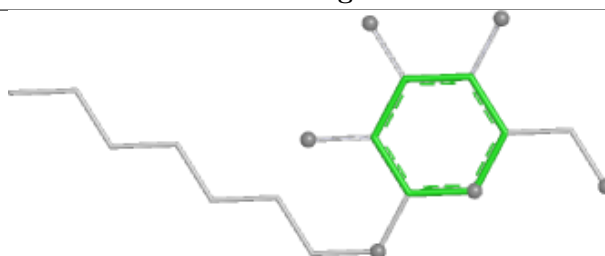
Bond lengths



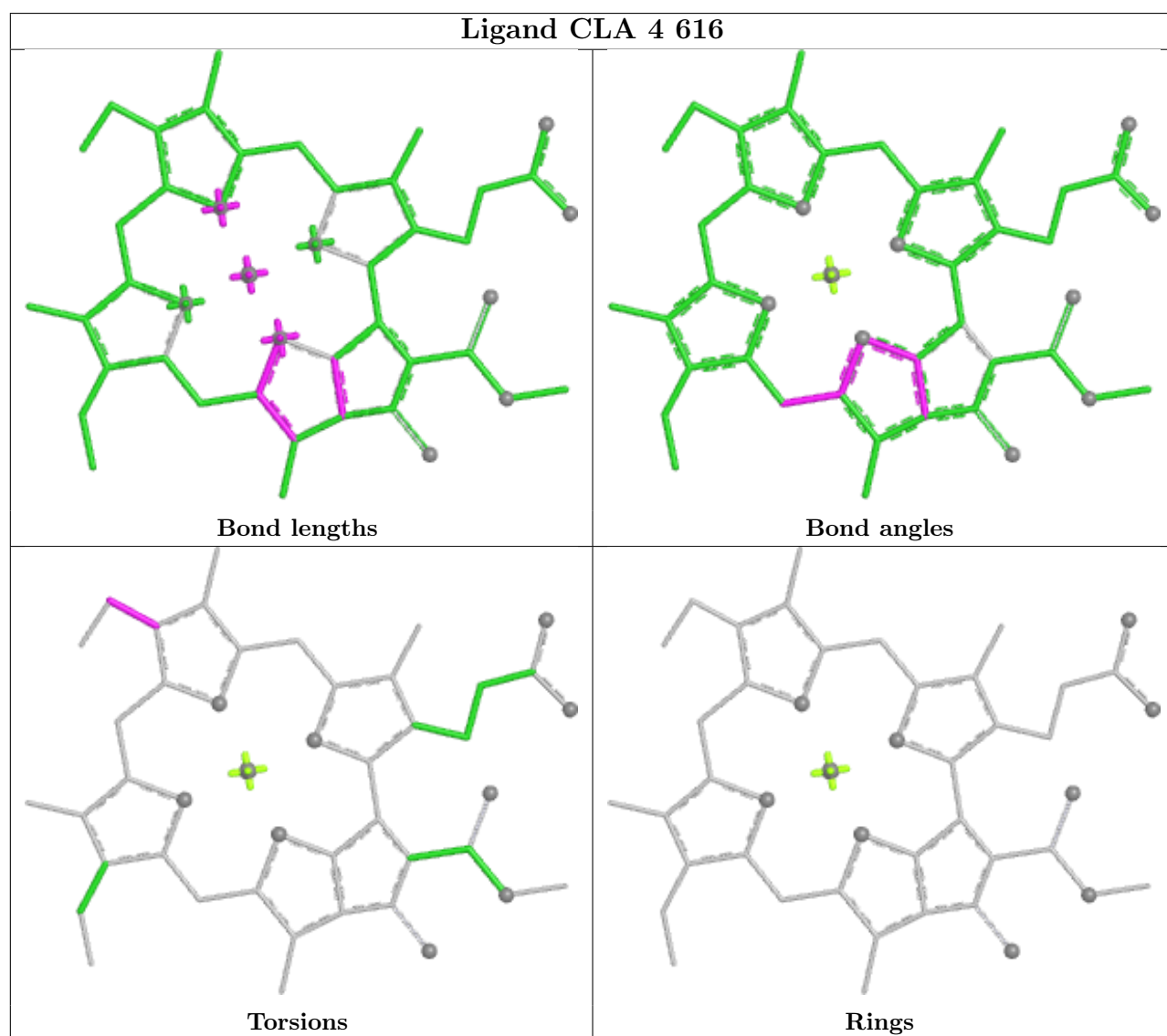
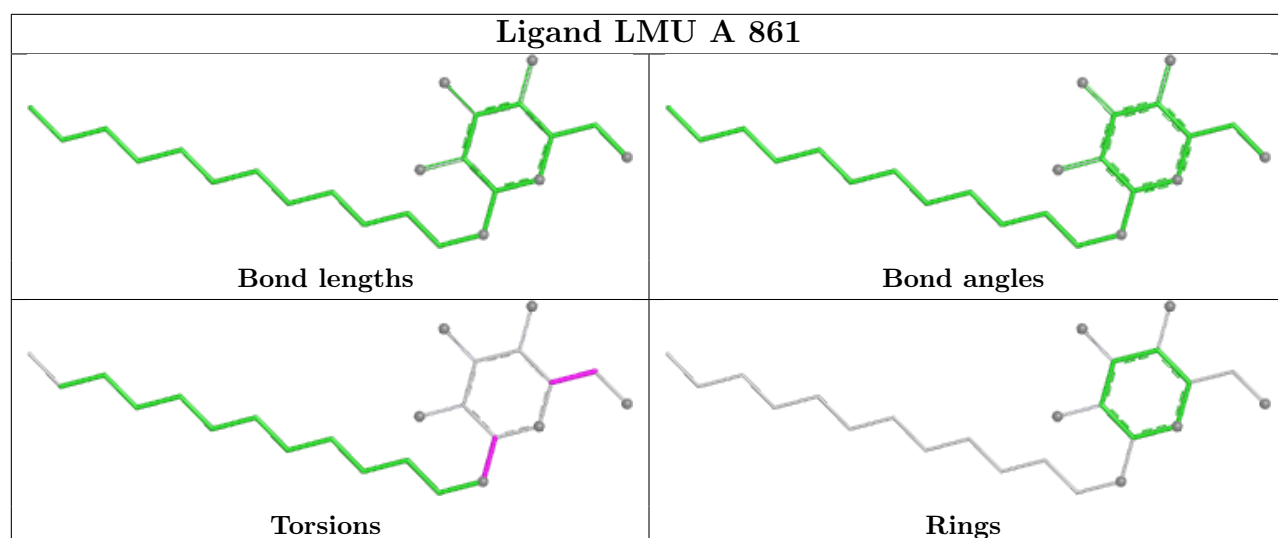
Bond angles

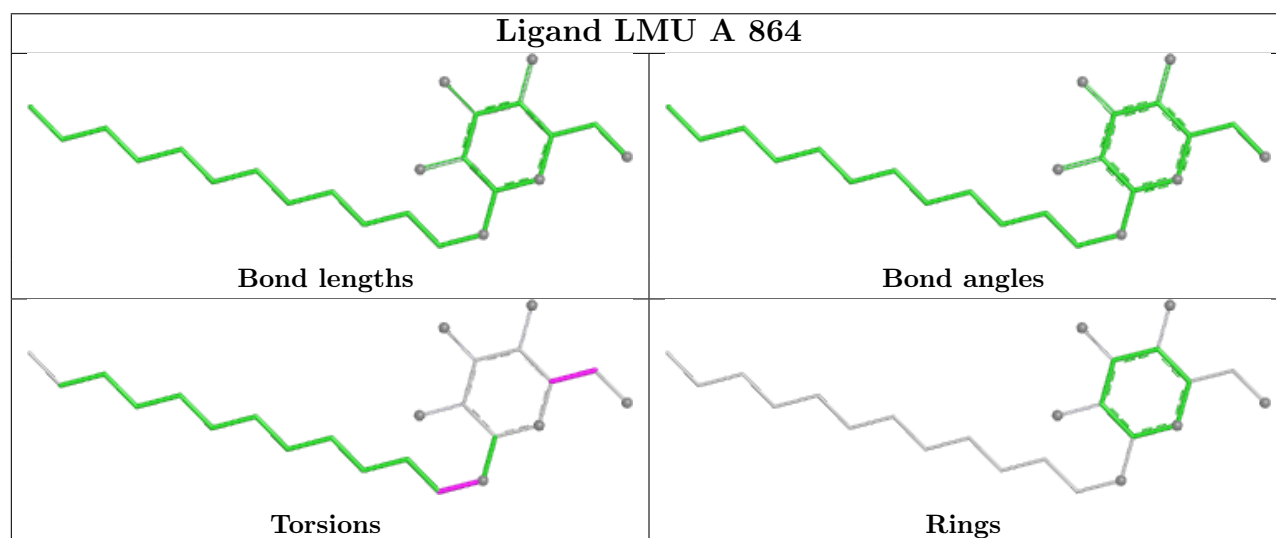
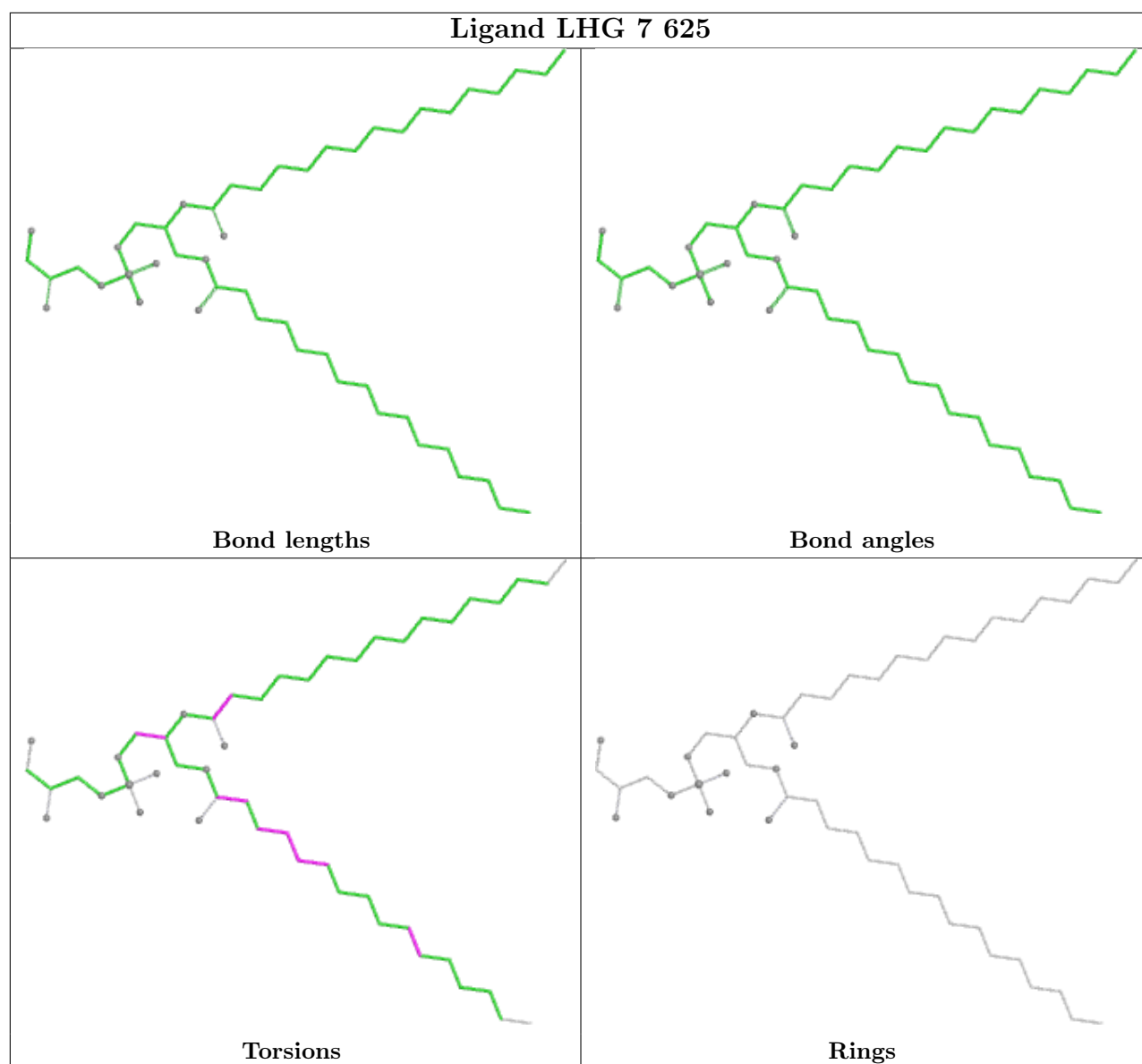


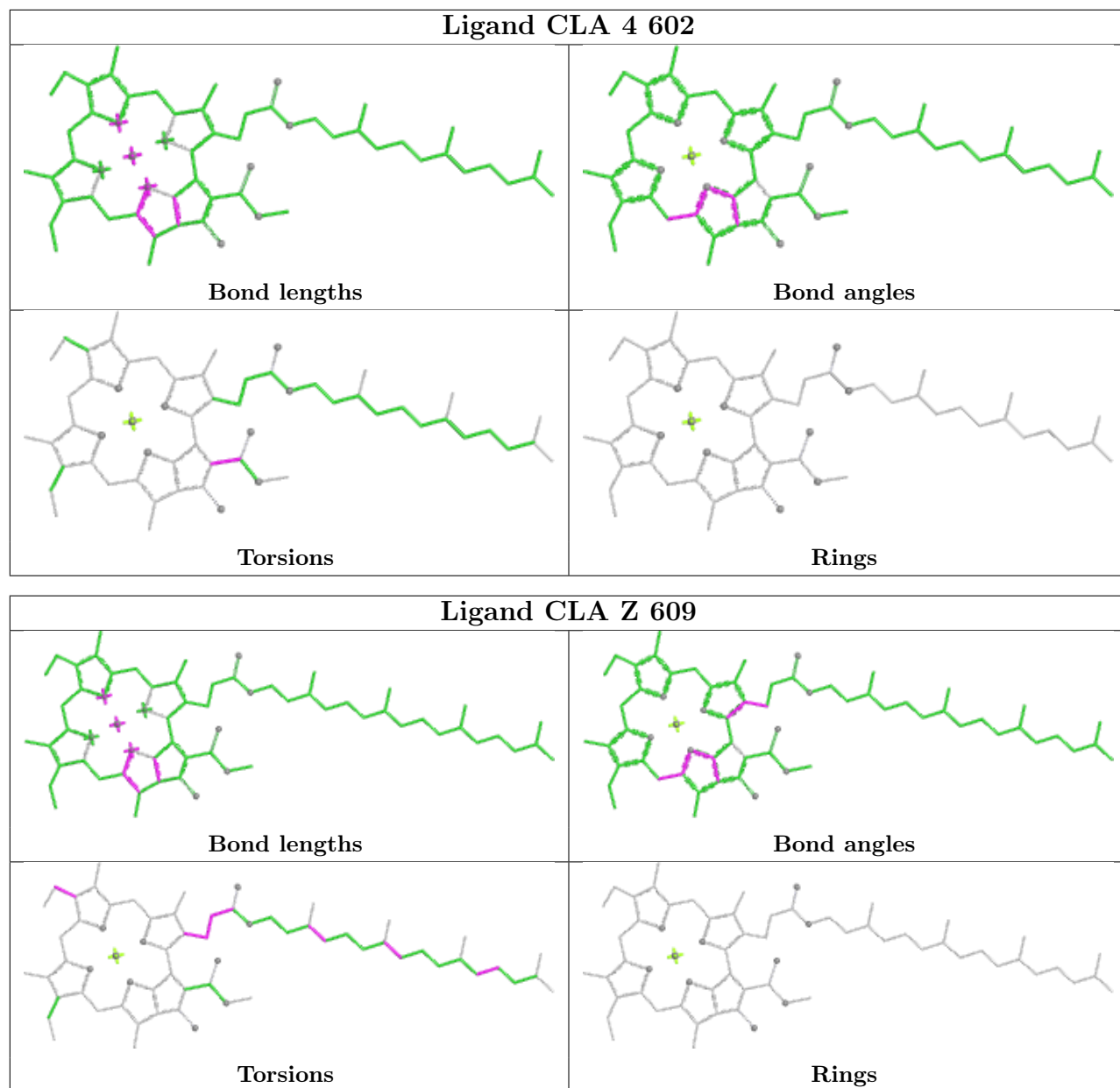
Torsions

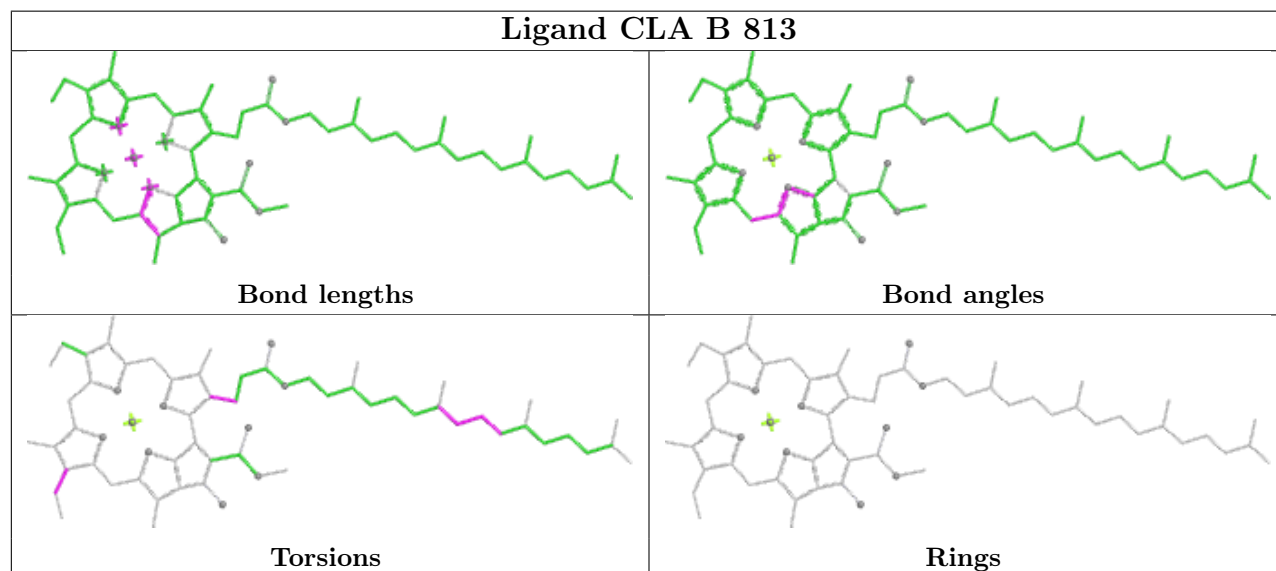
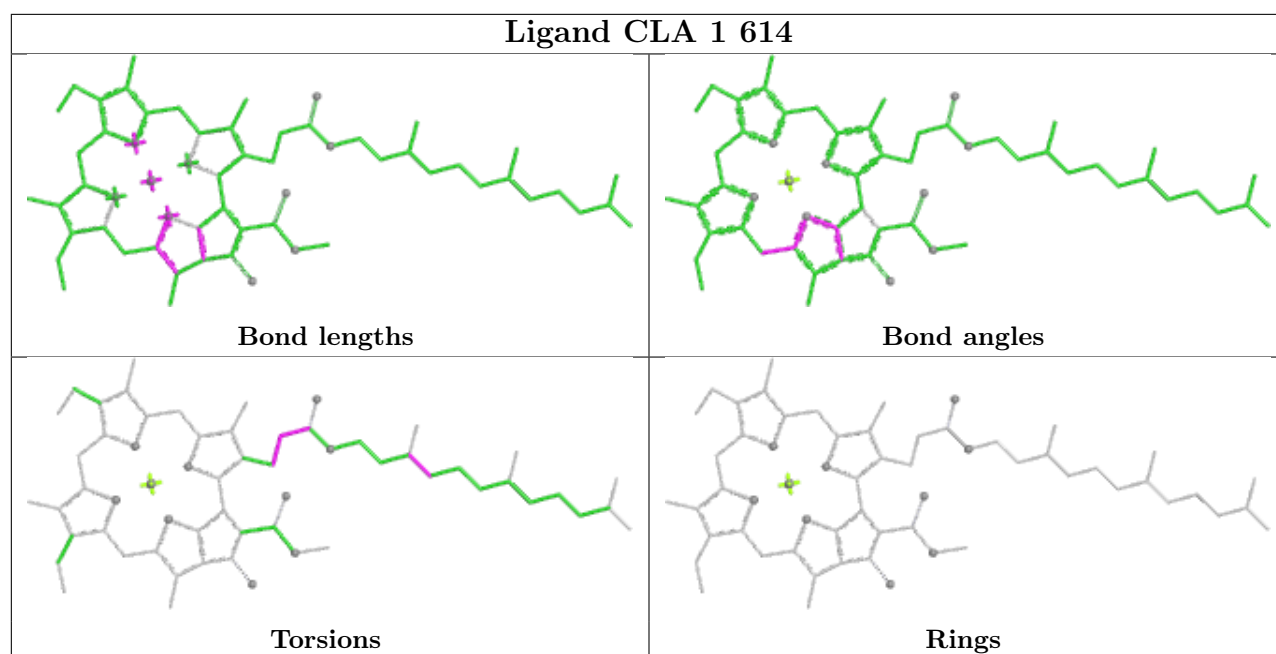


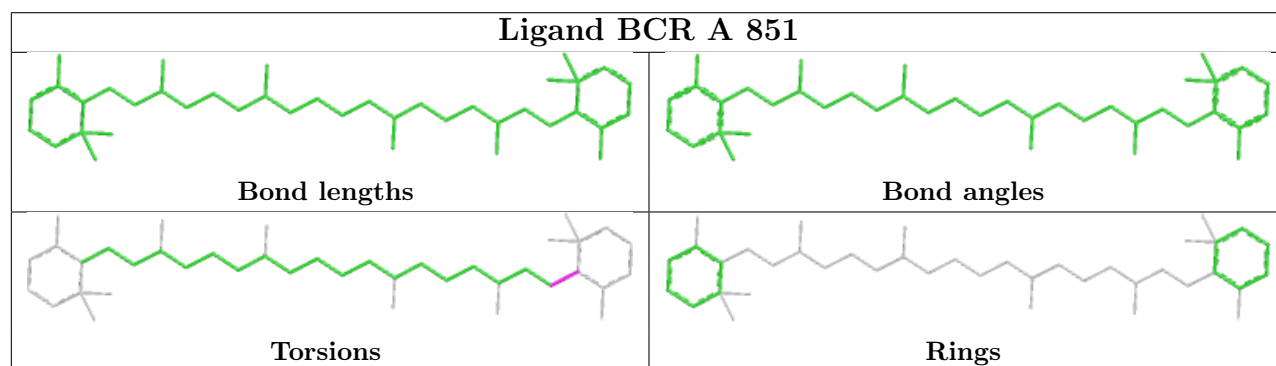
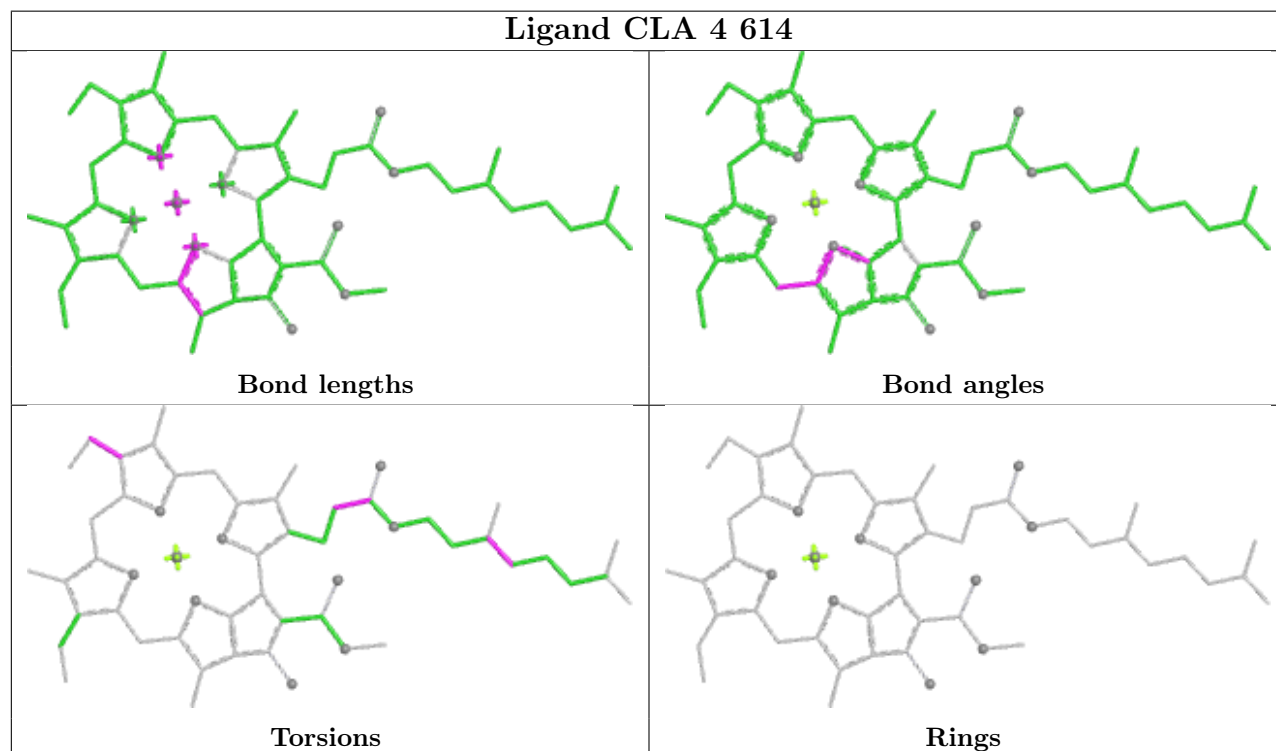
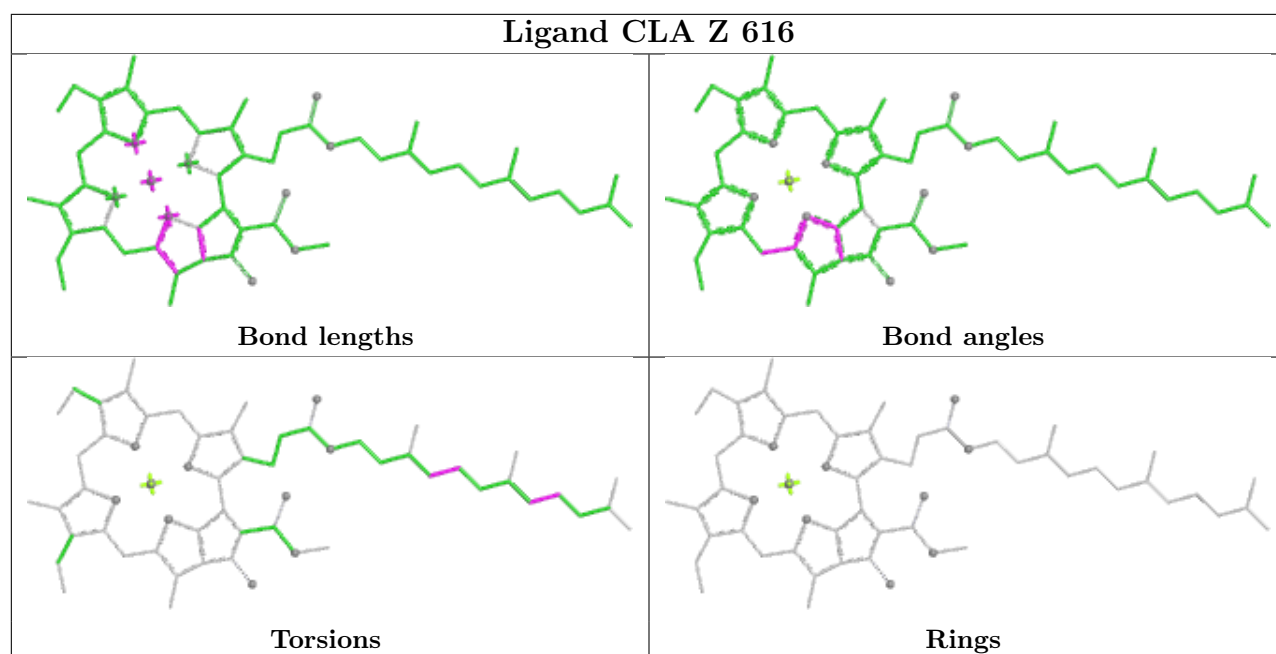
Rings

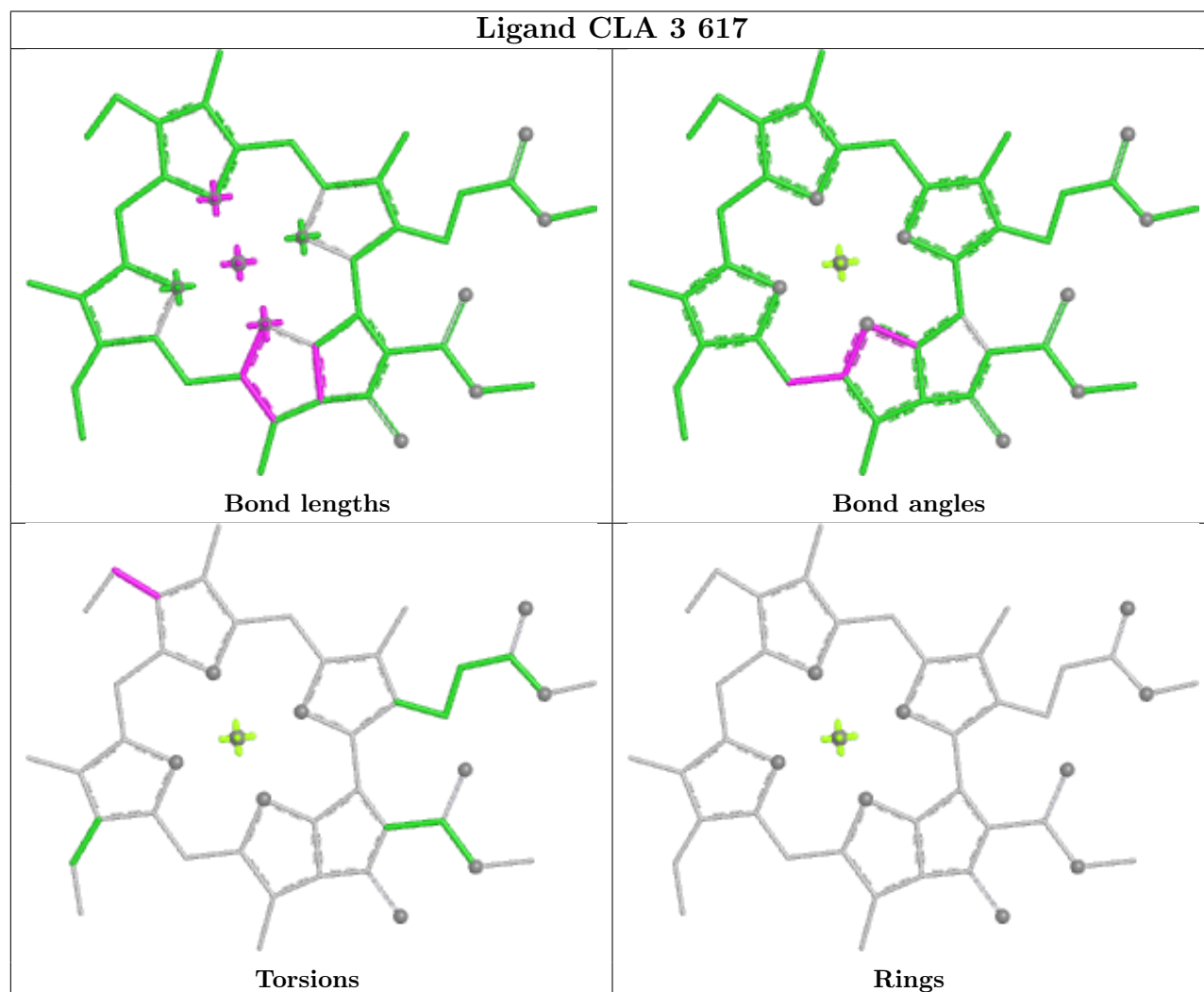
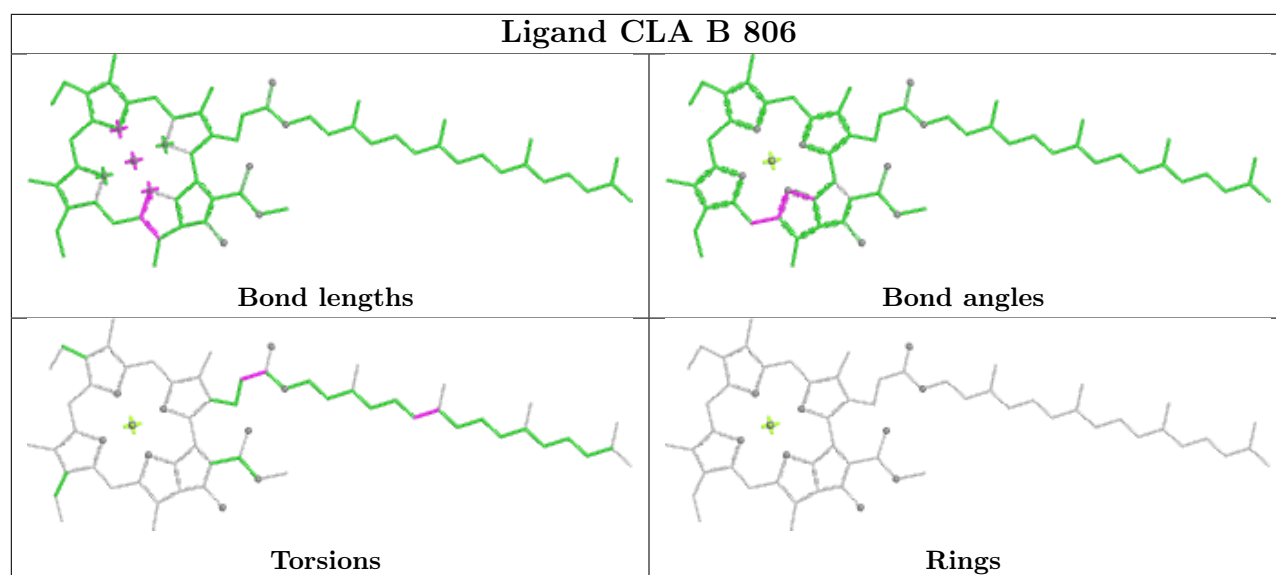


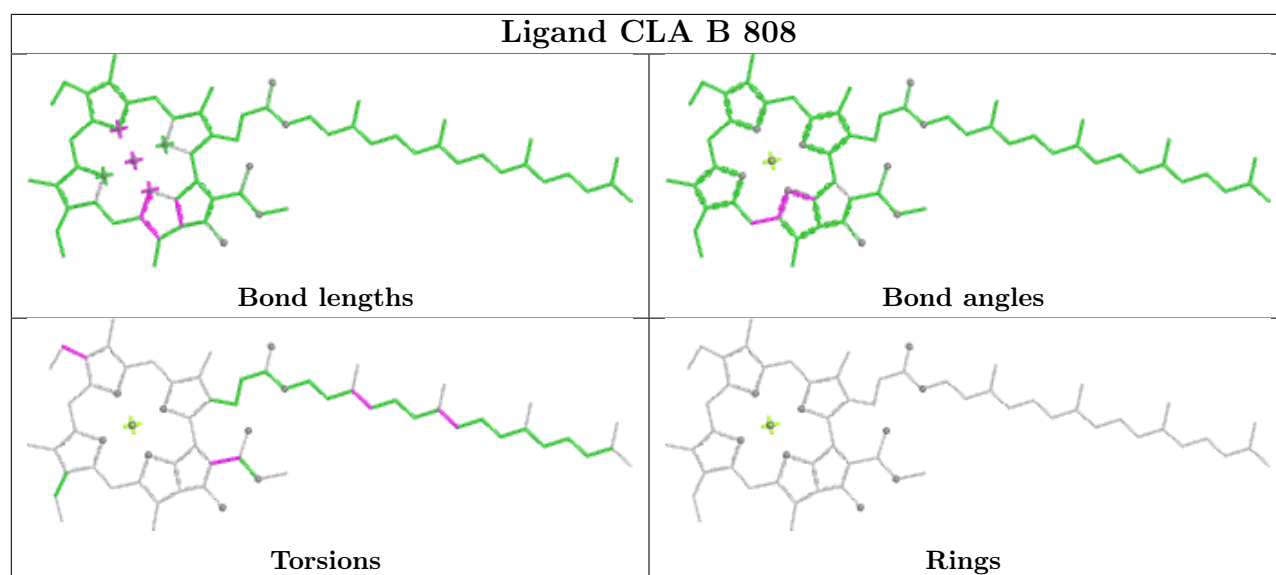
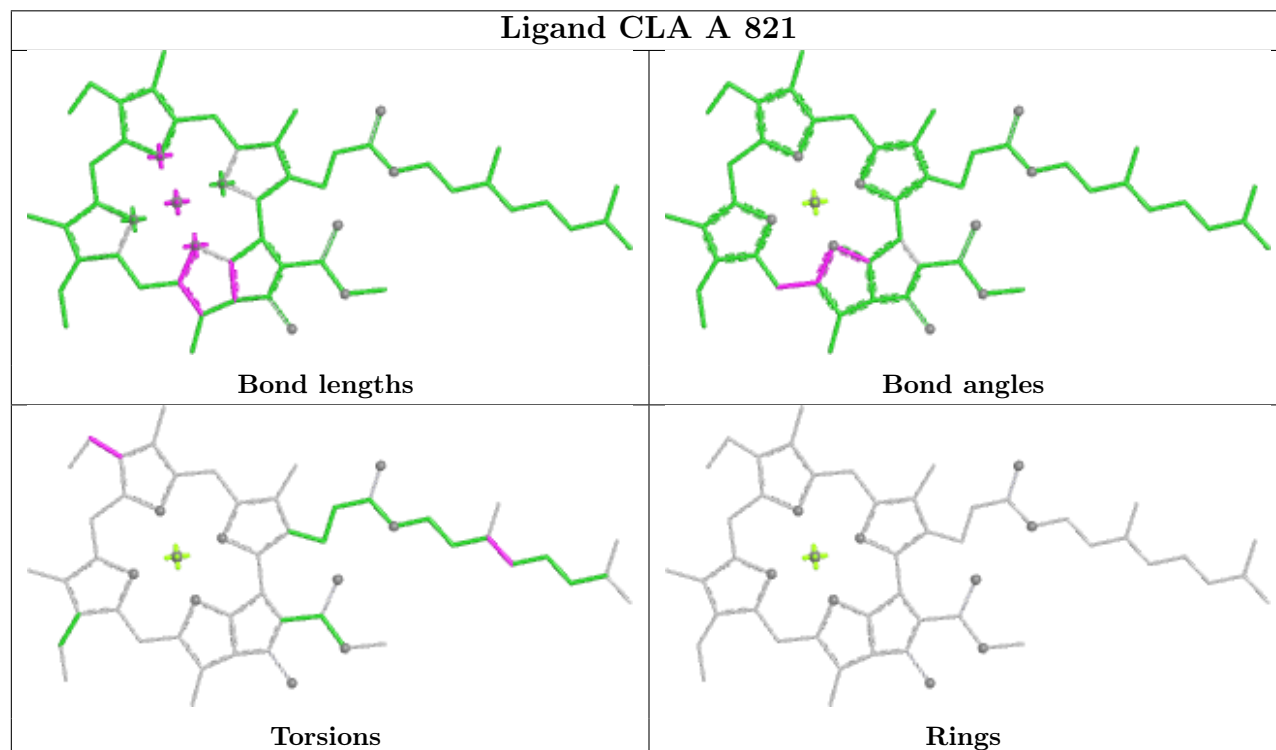
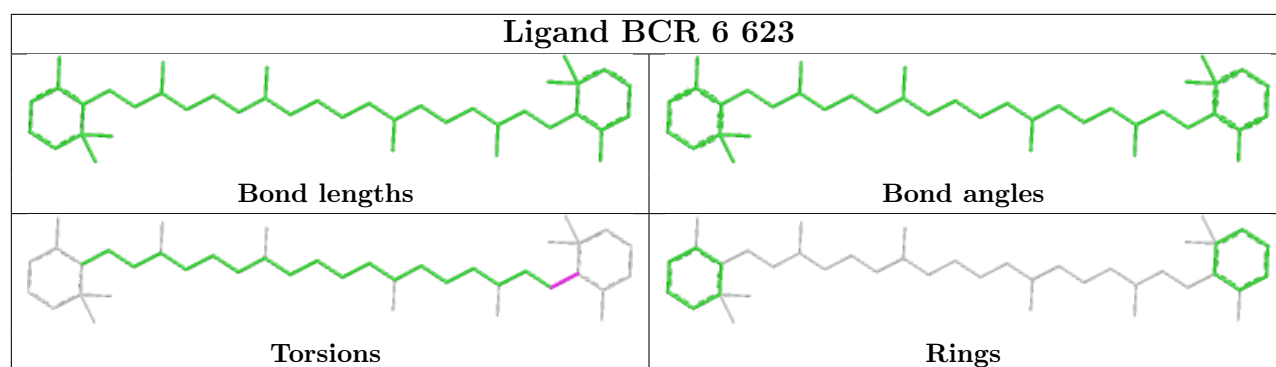




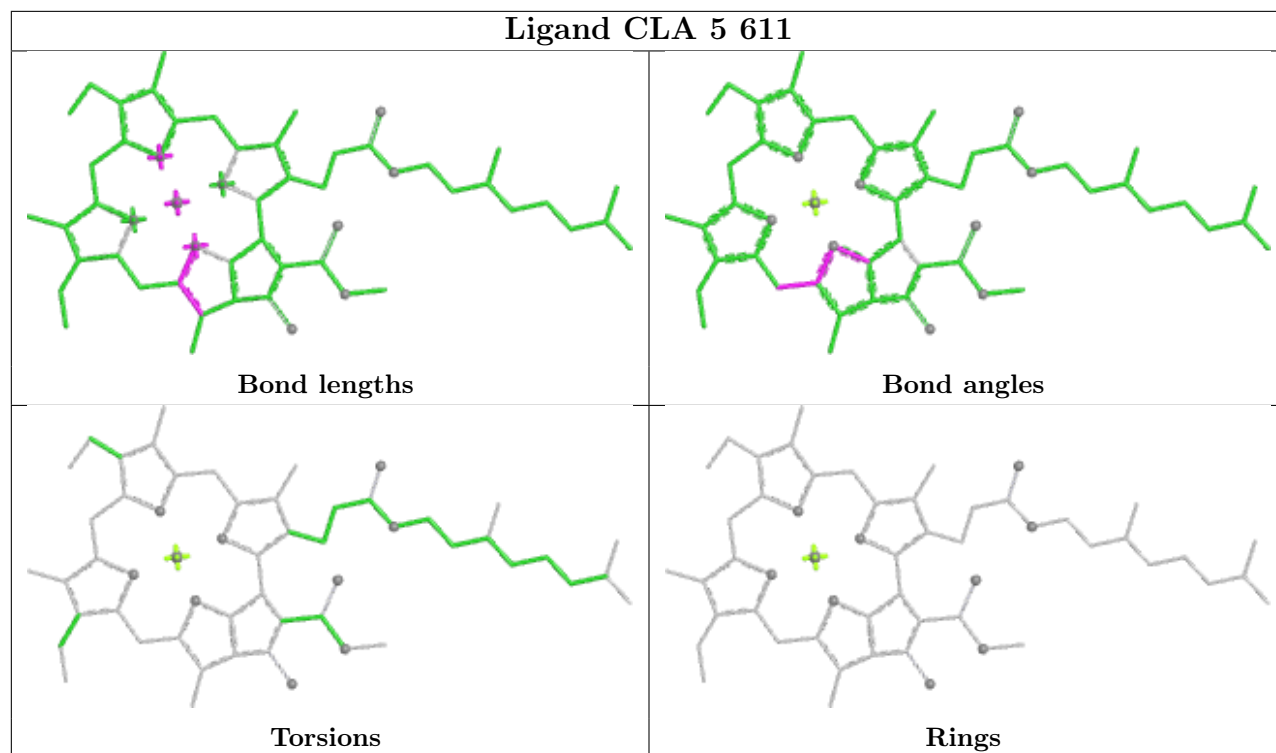




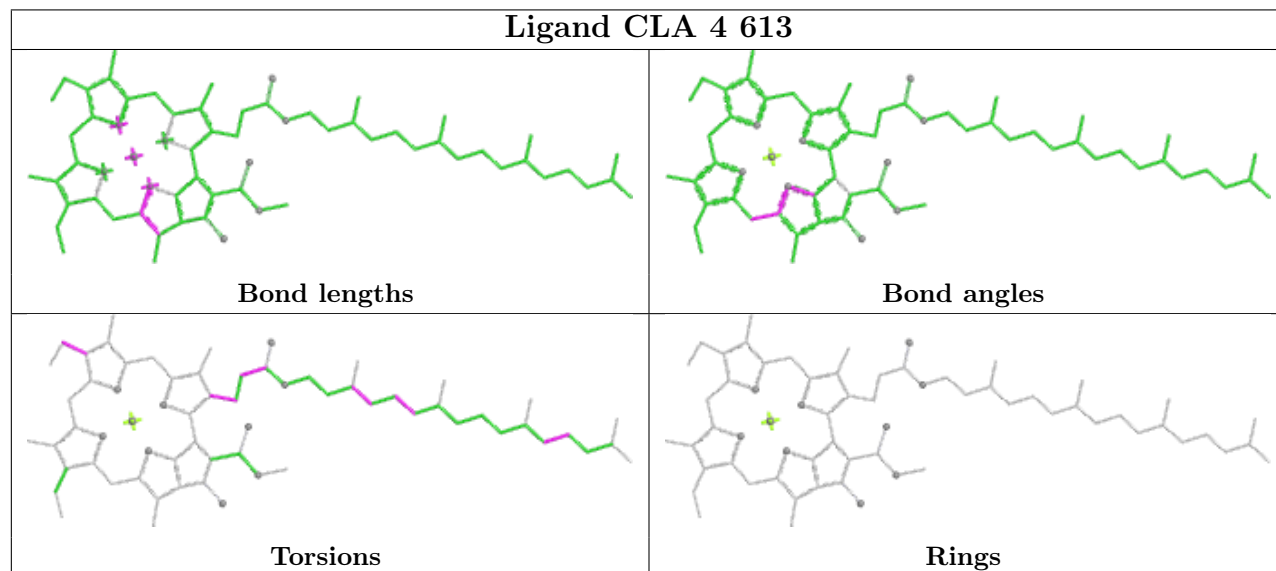


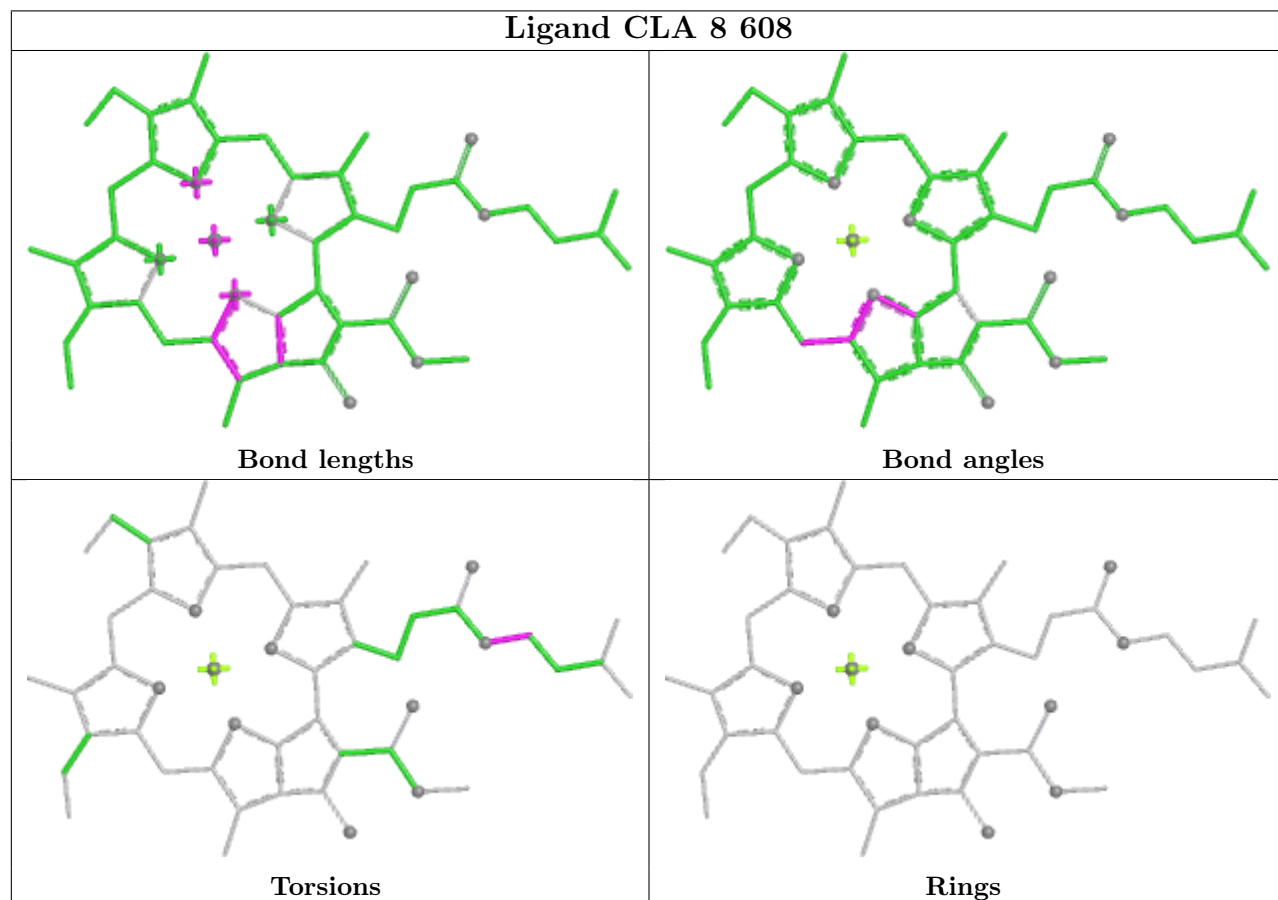
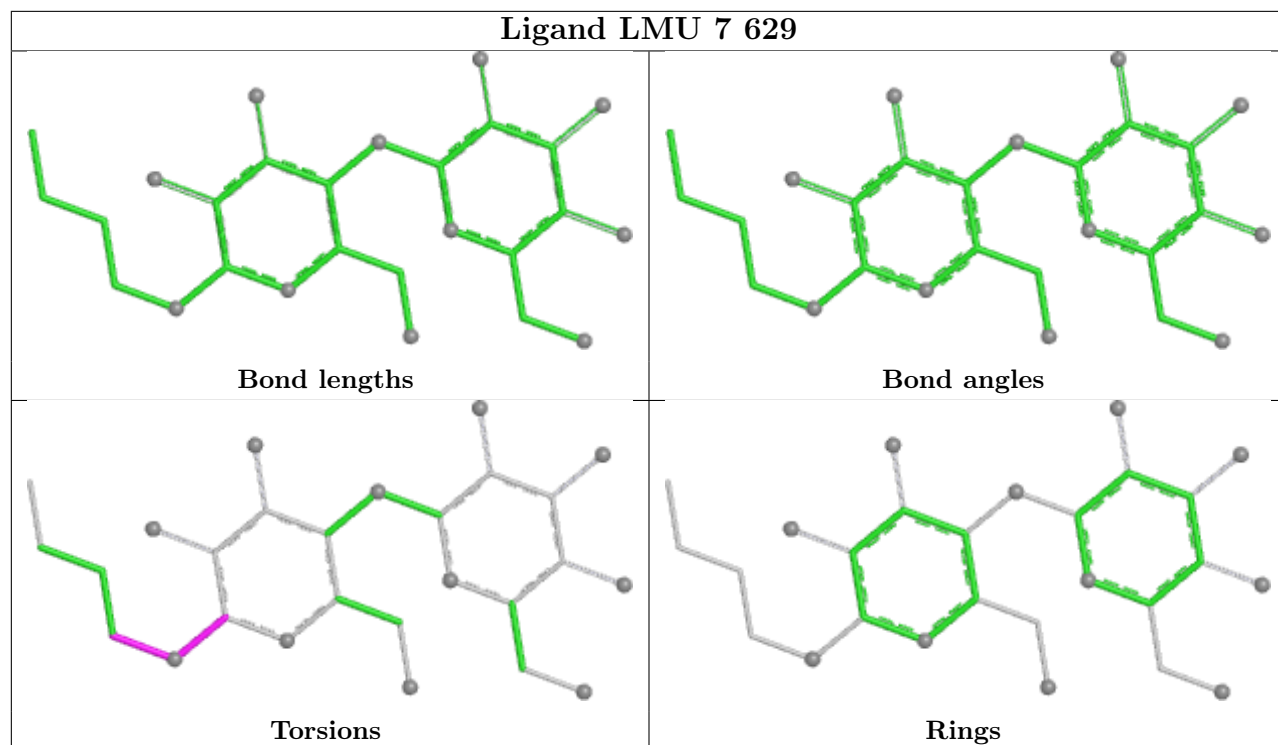


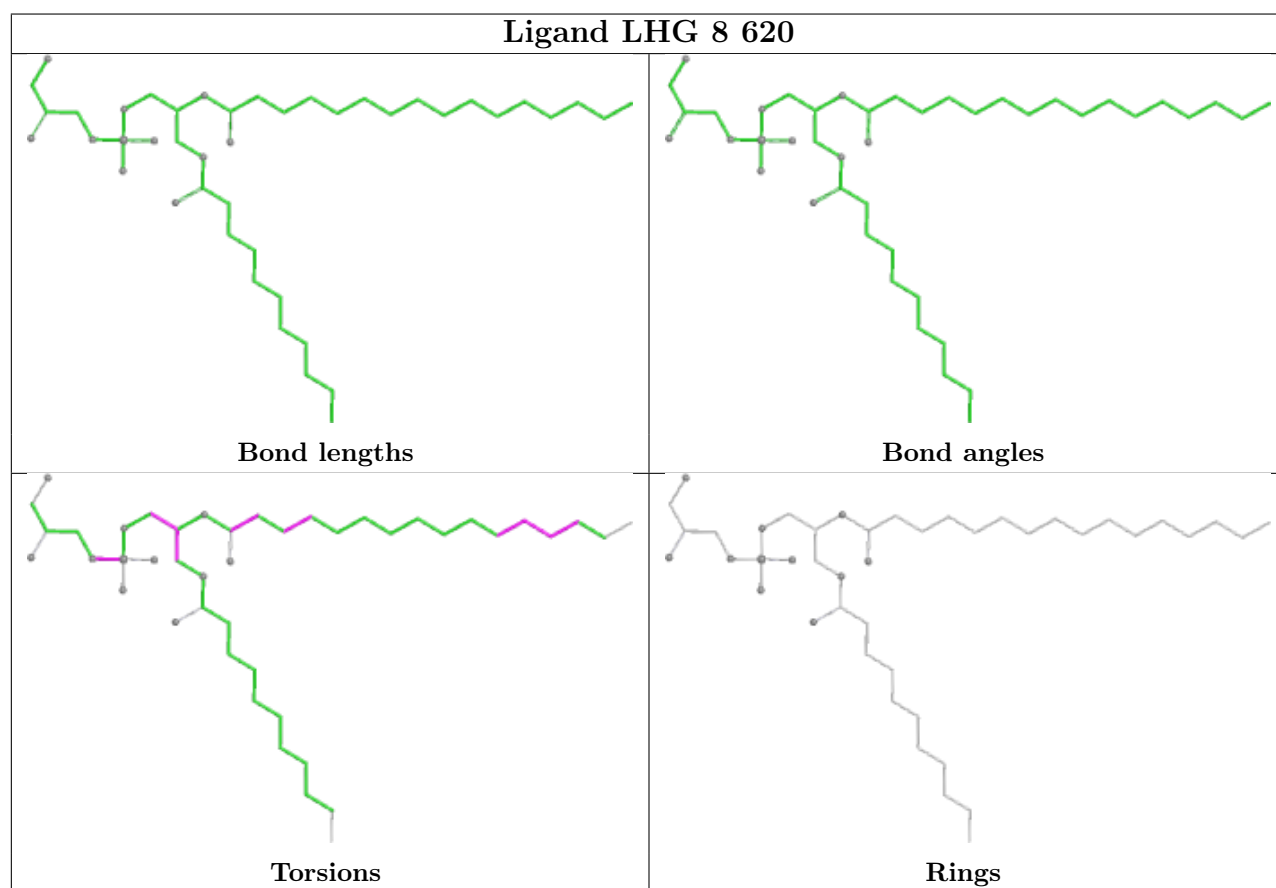
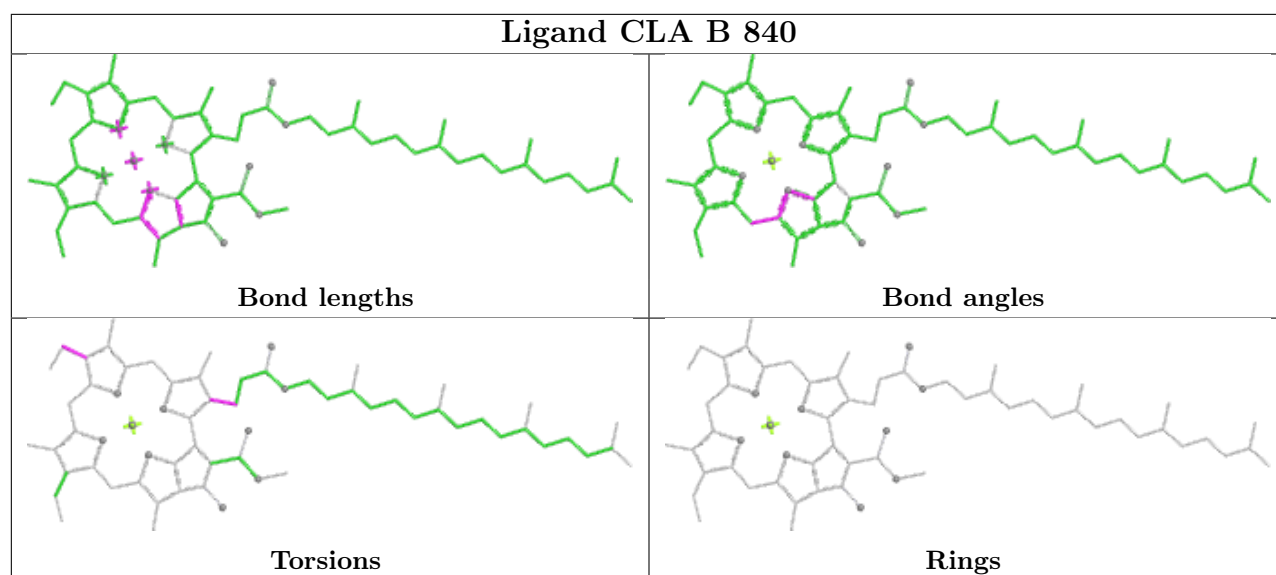
Ligand CLA 5 611

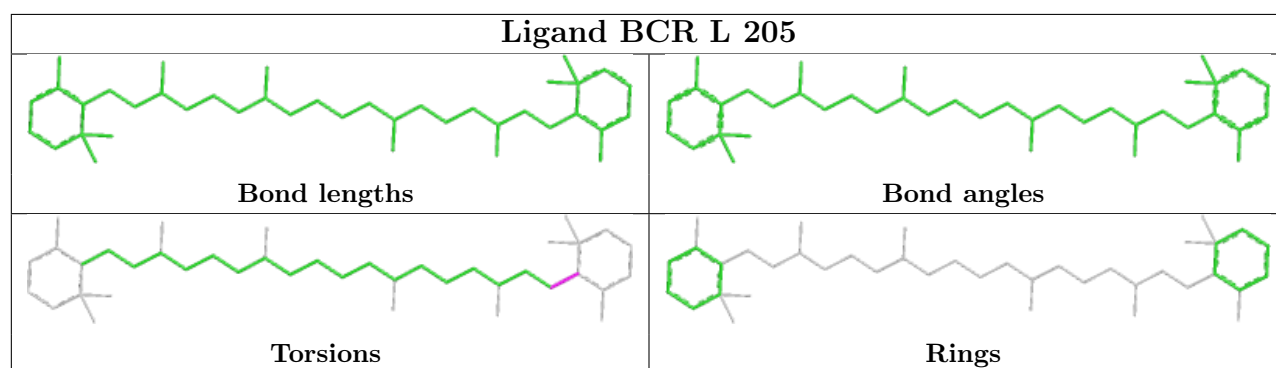
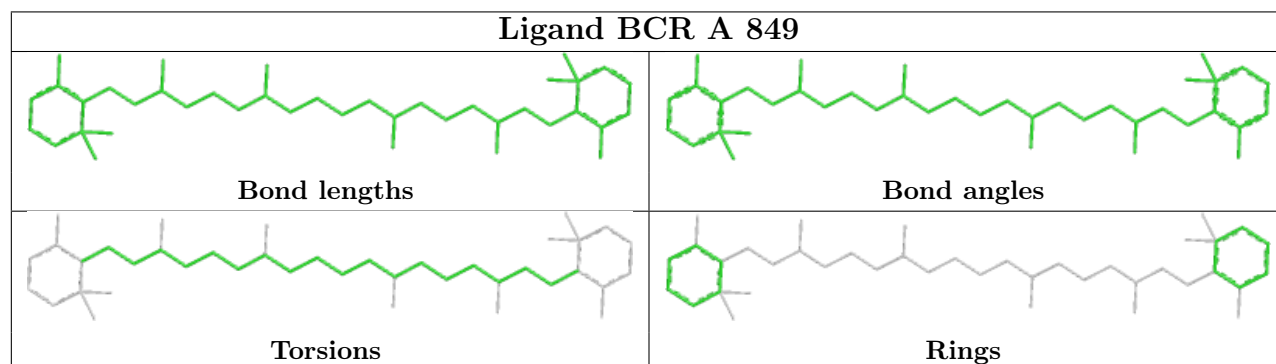
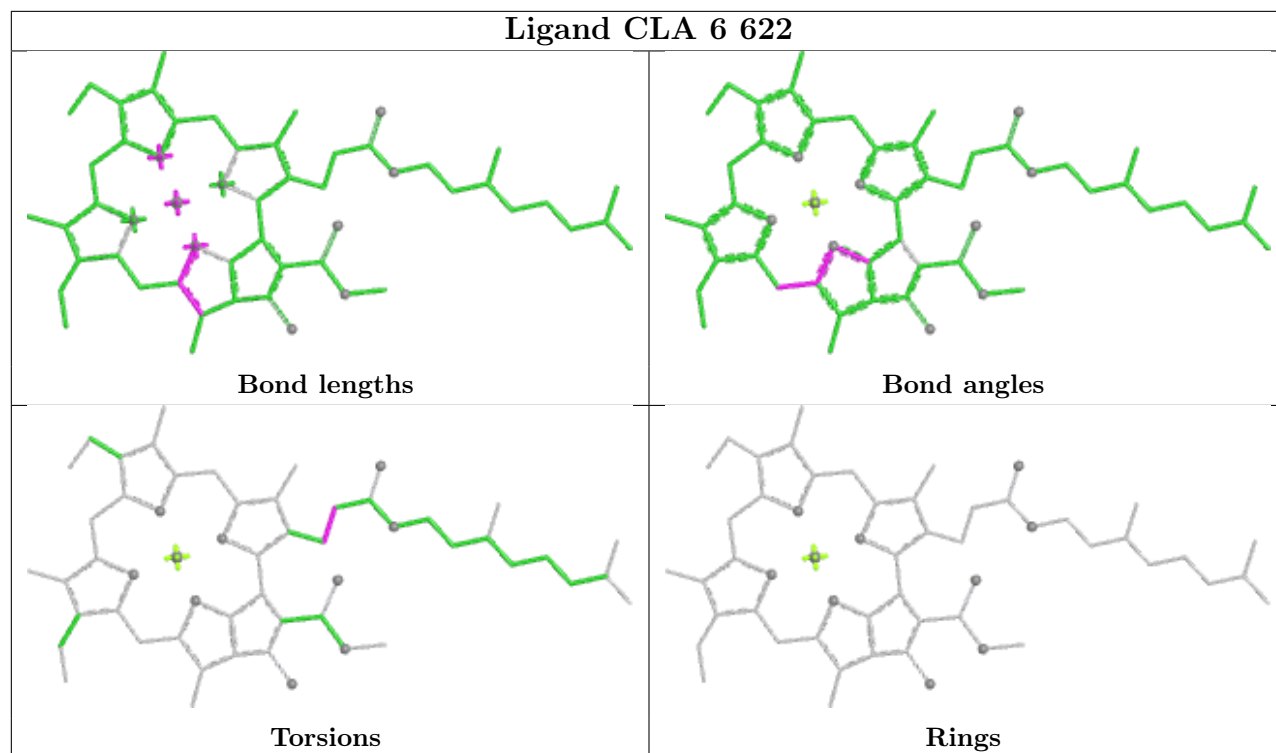


Ligand CLA 4 613

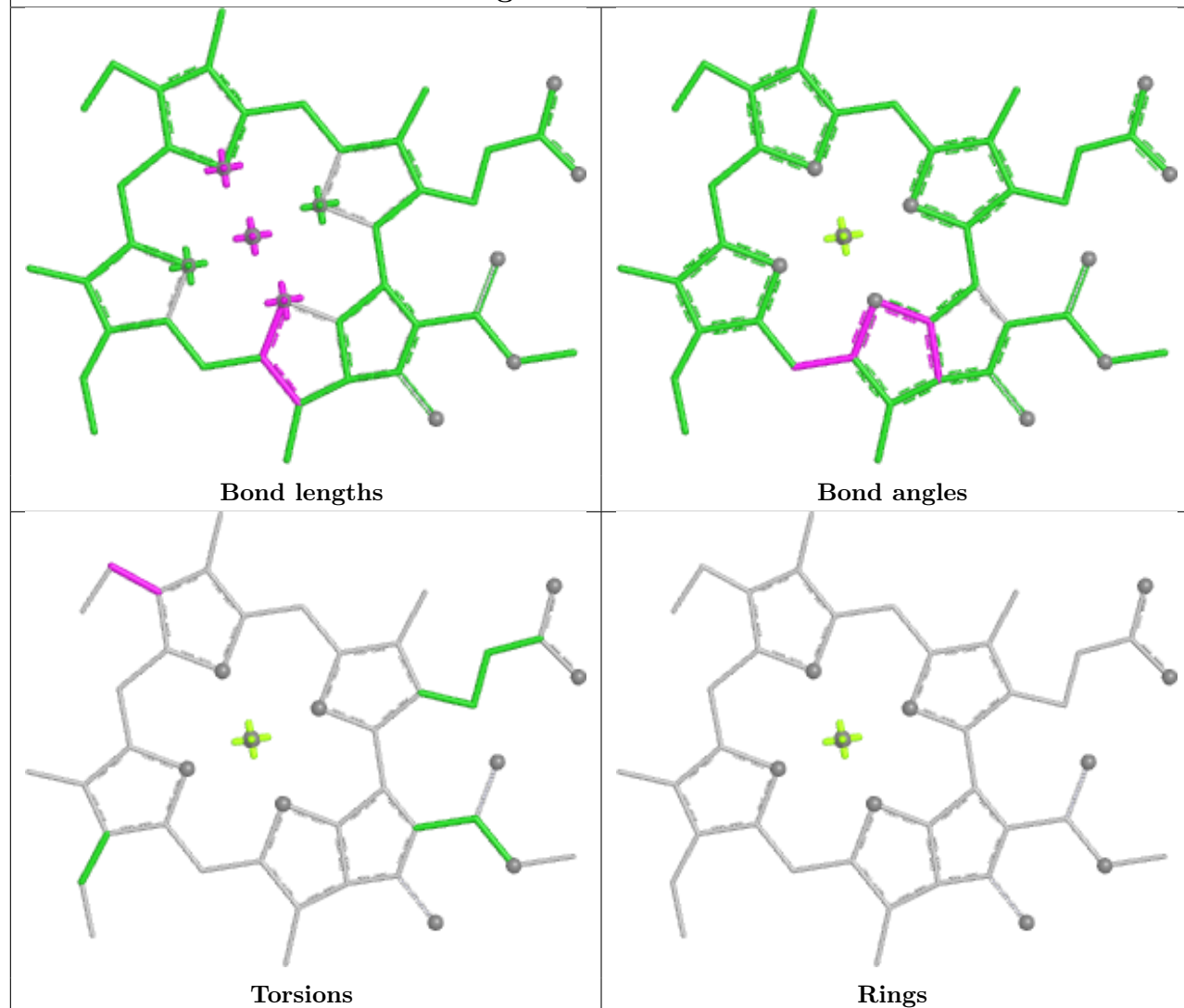




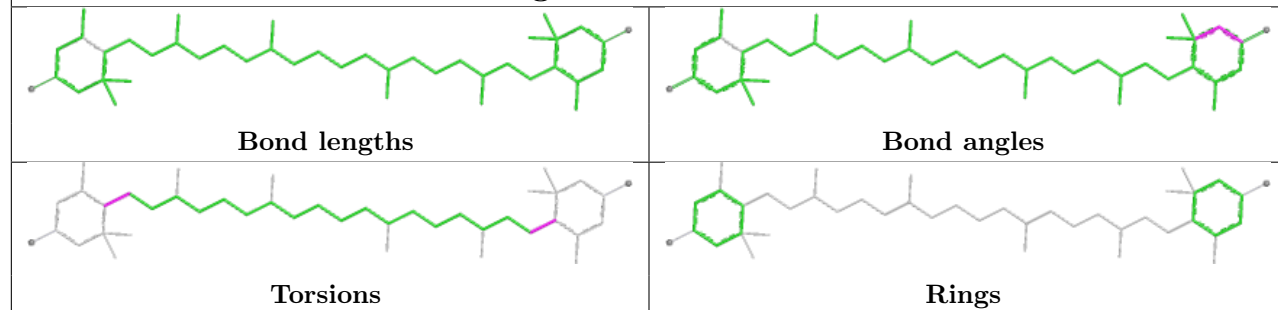


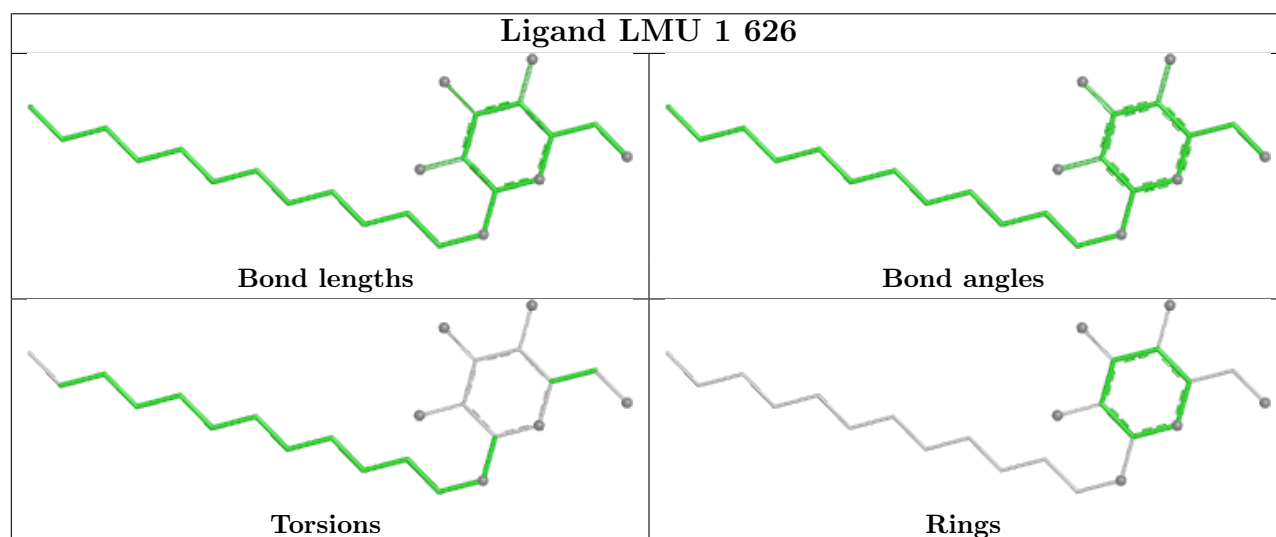
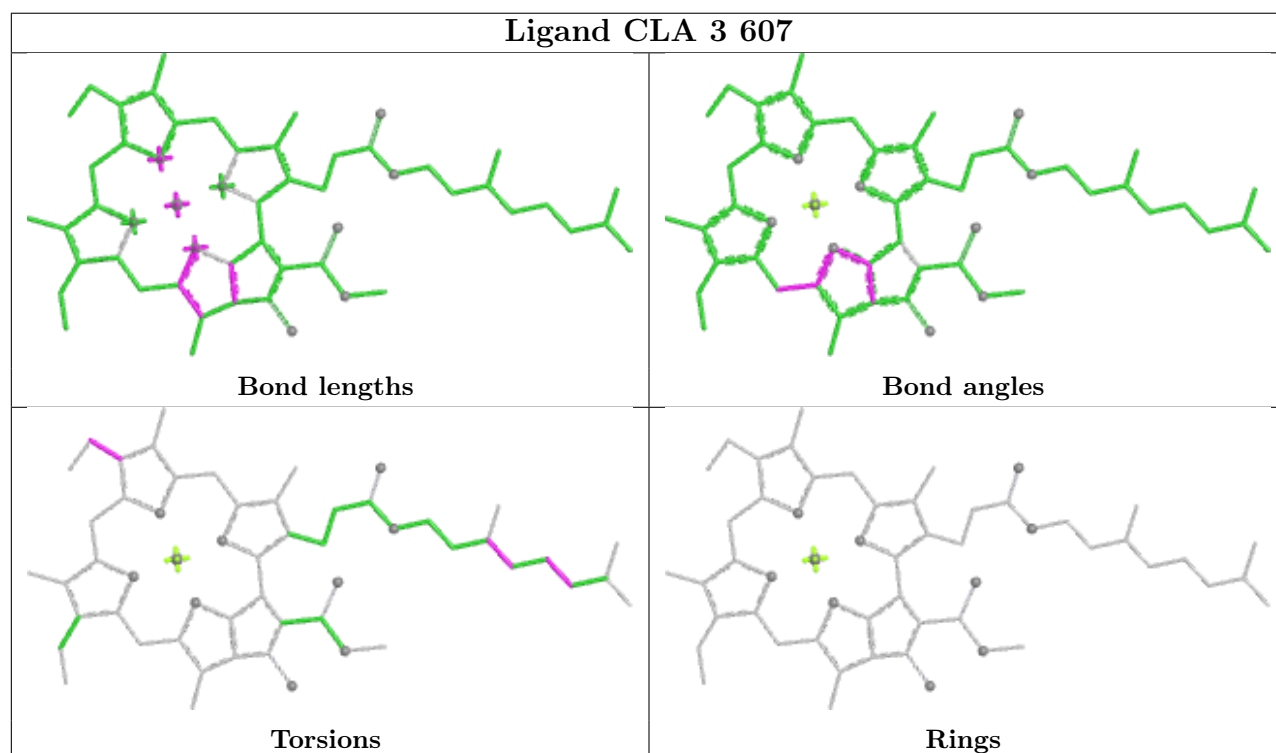
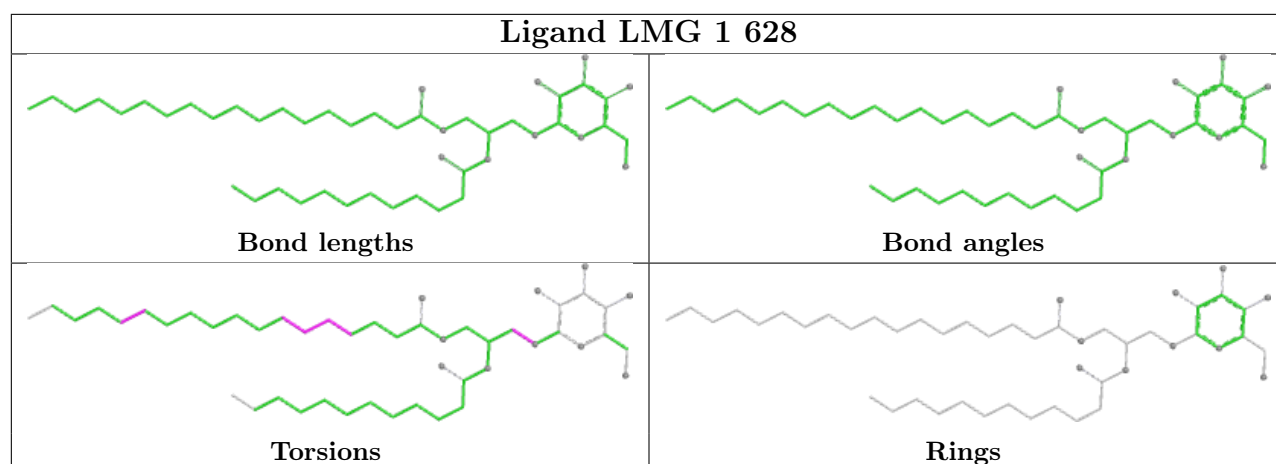


Ligand CLA 9 611

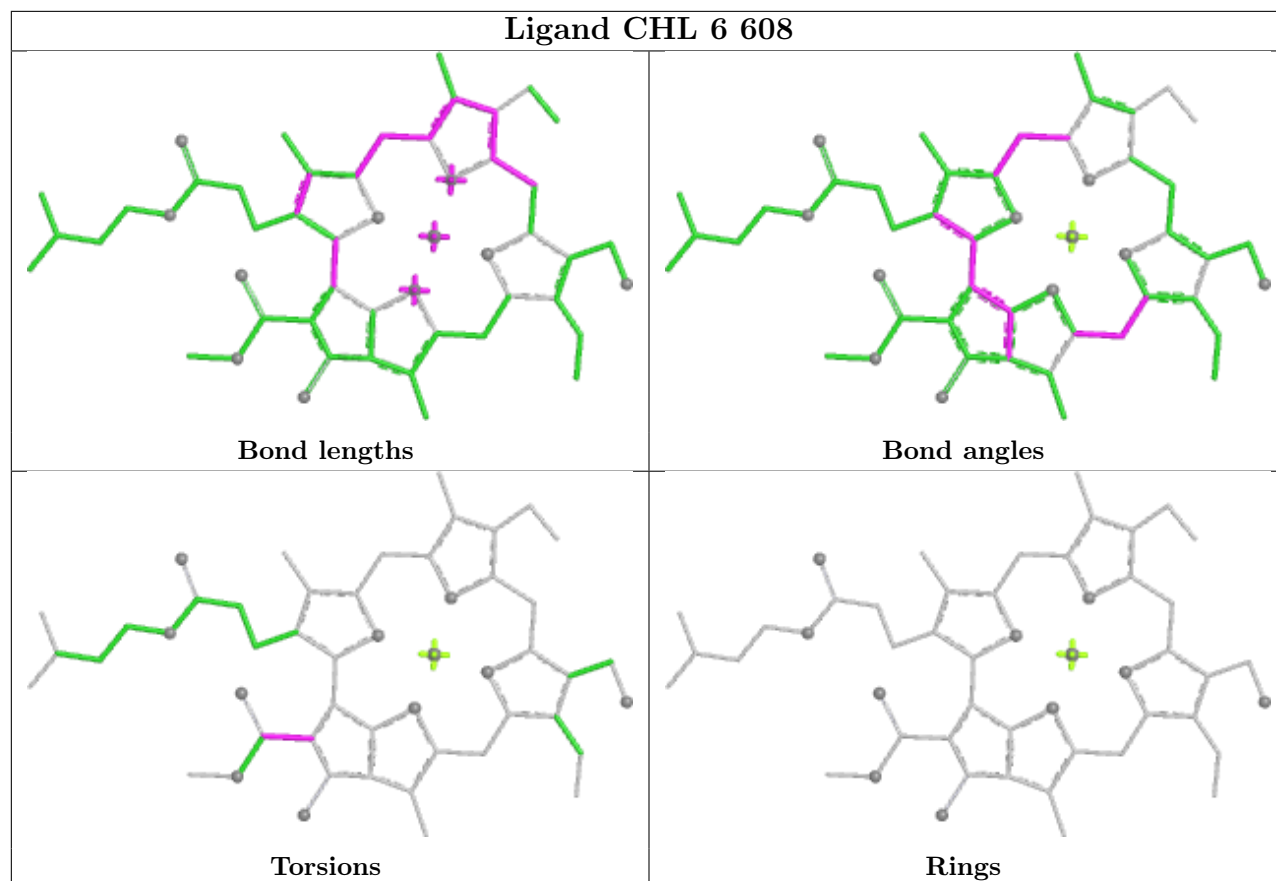


Ligand LUT A 856

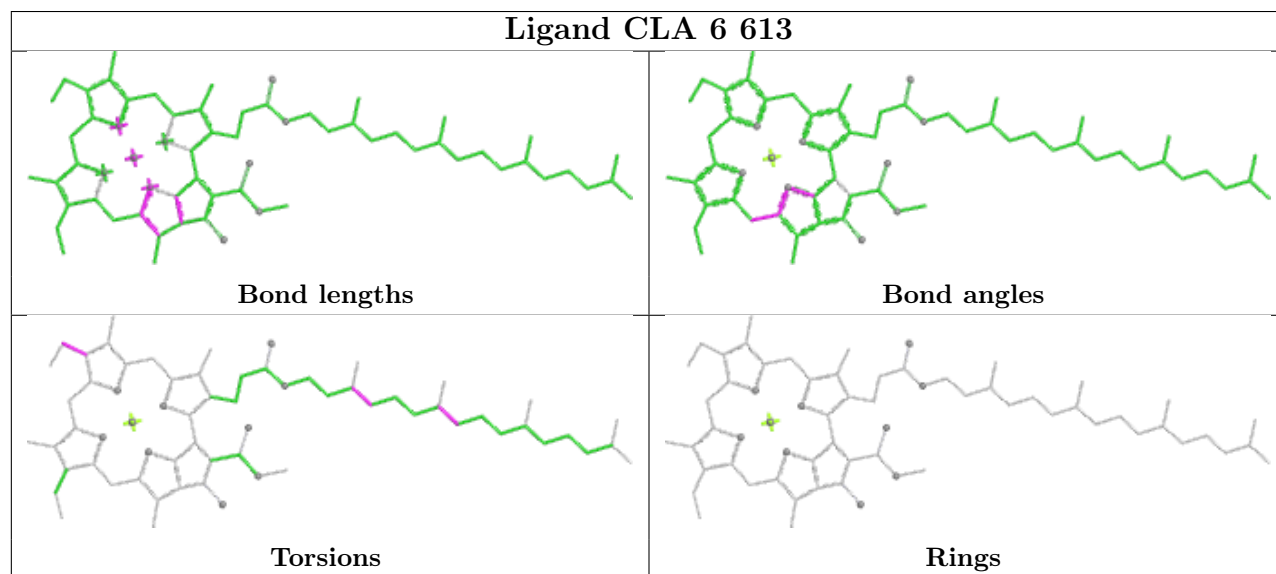


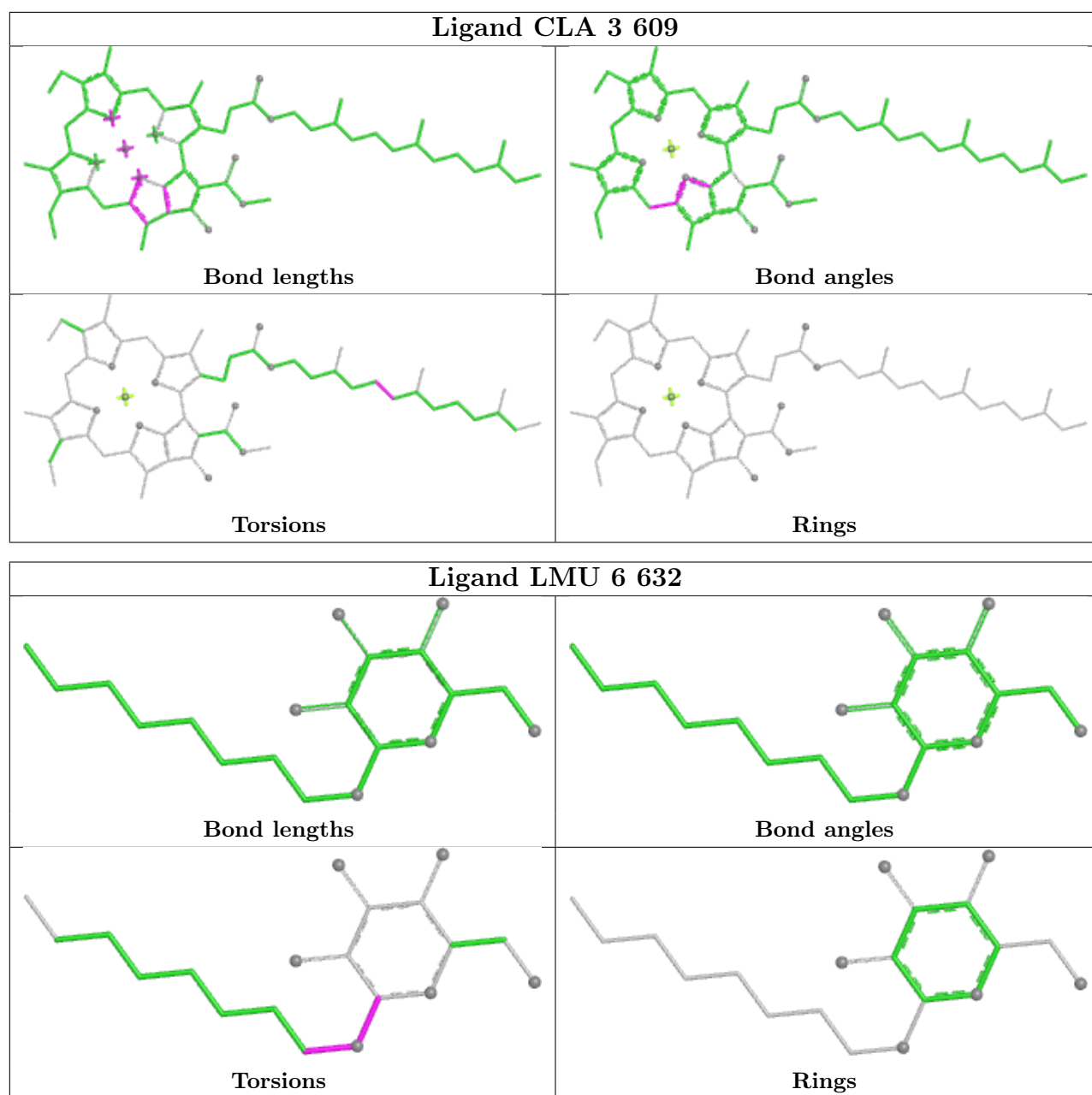


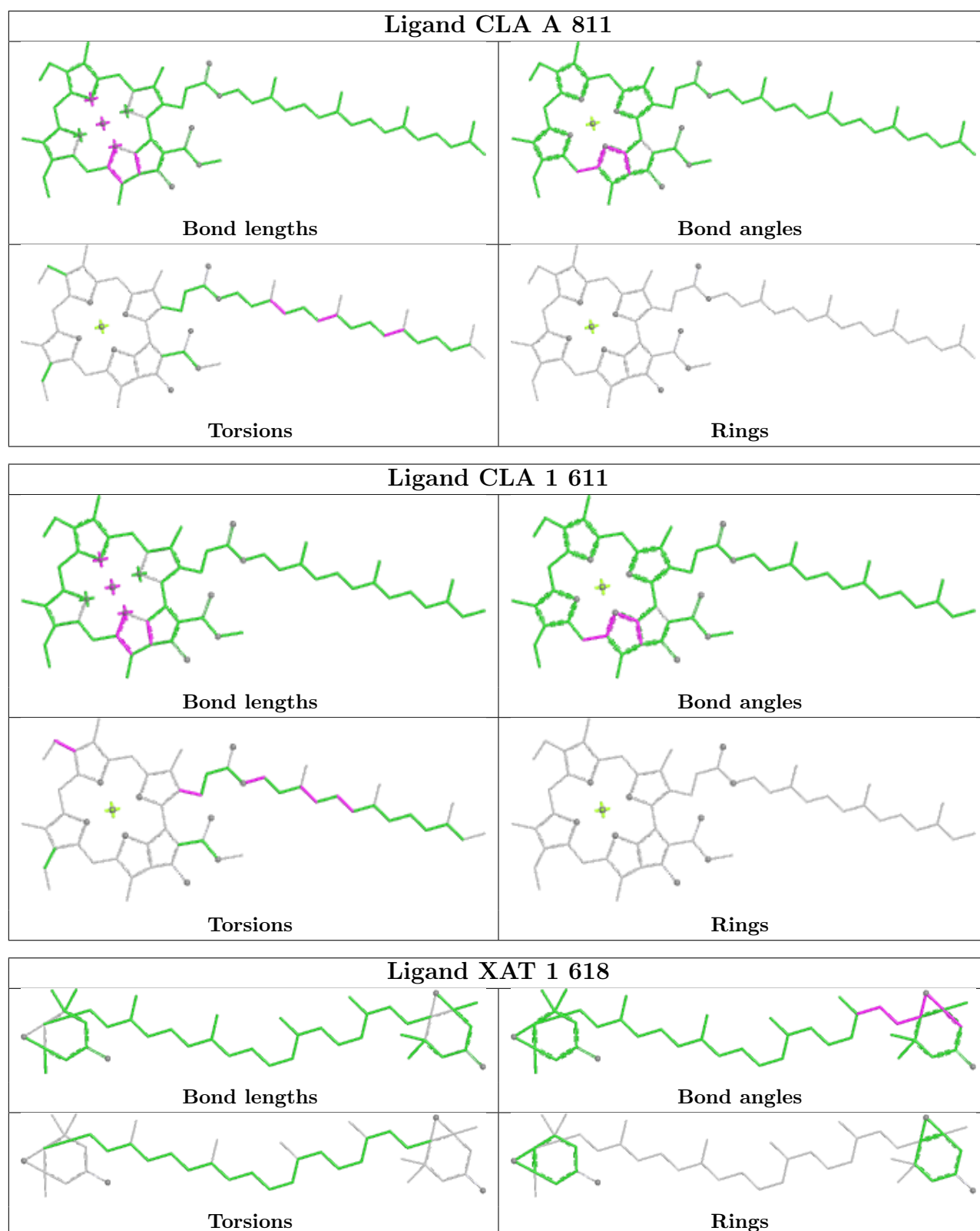
Ligand CHL 6 608



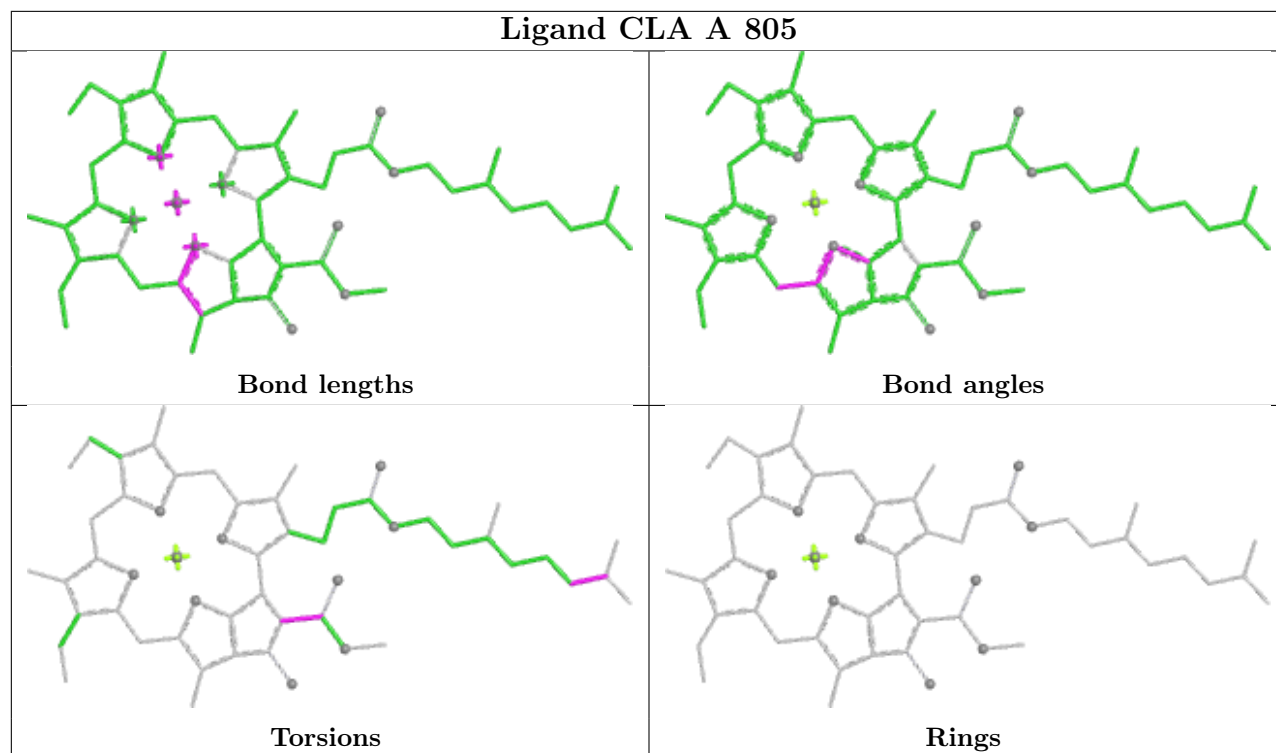
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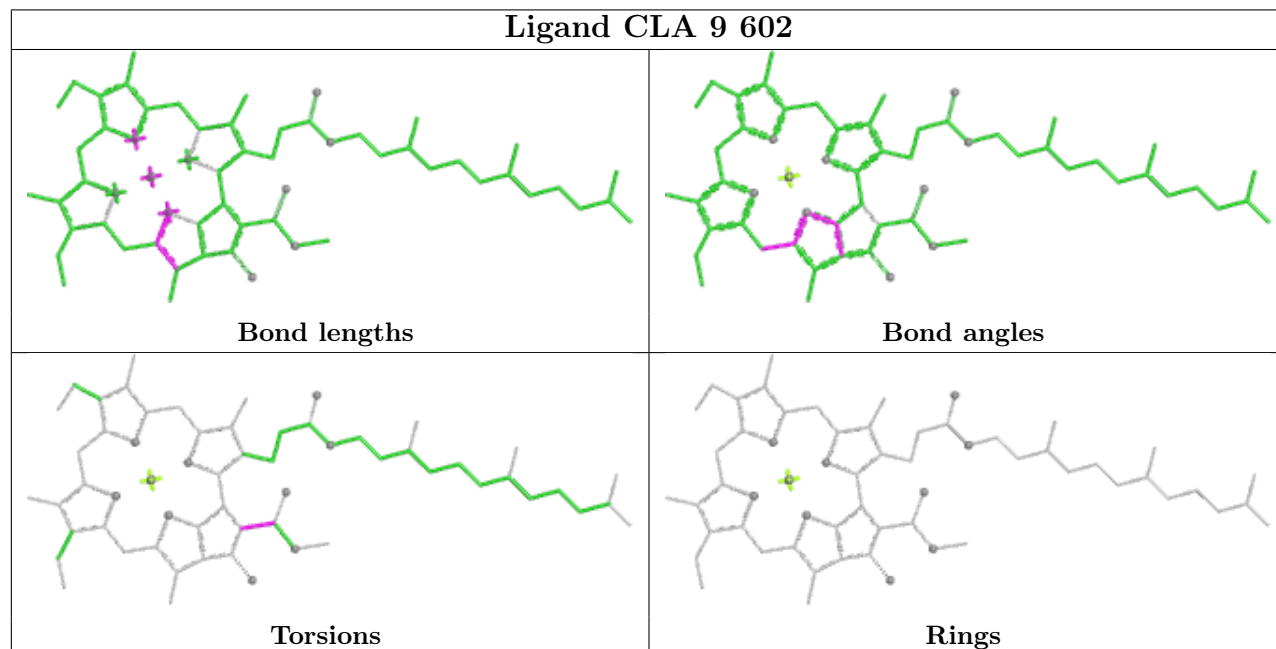


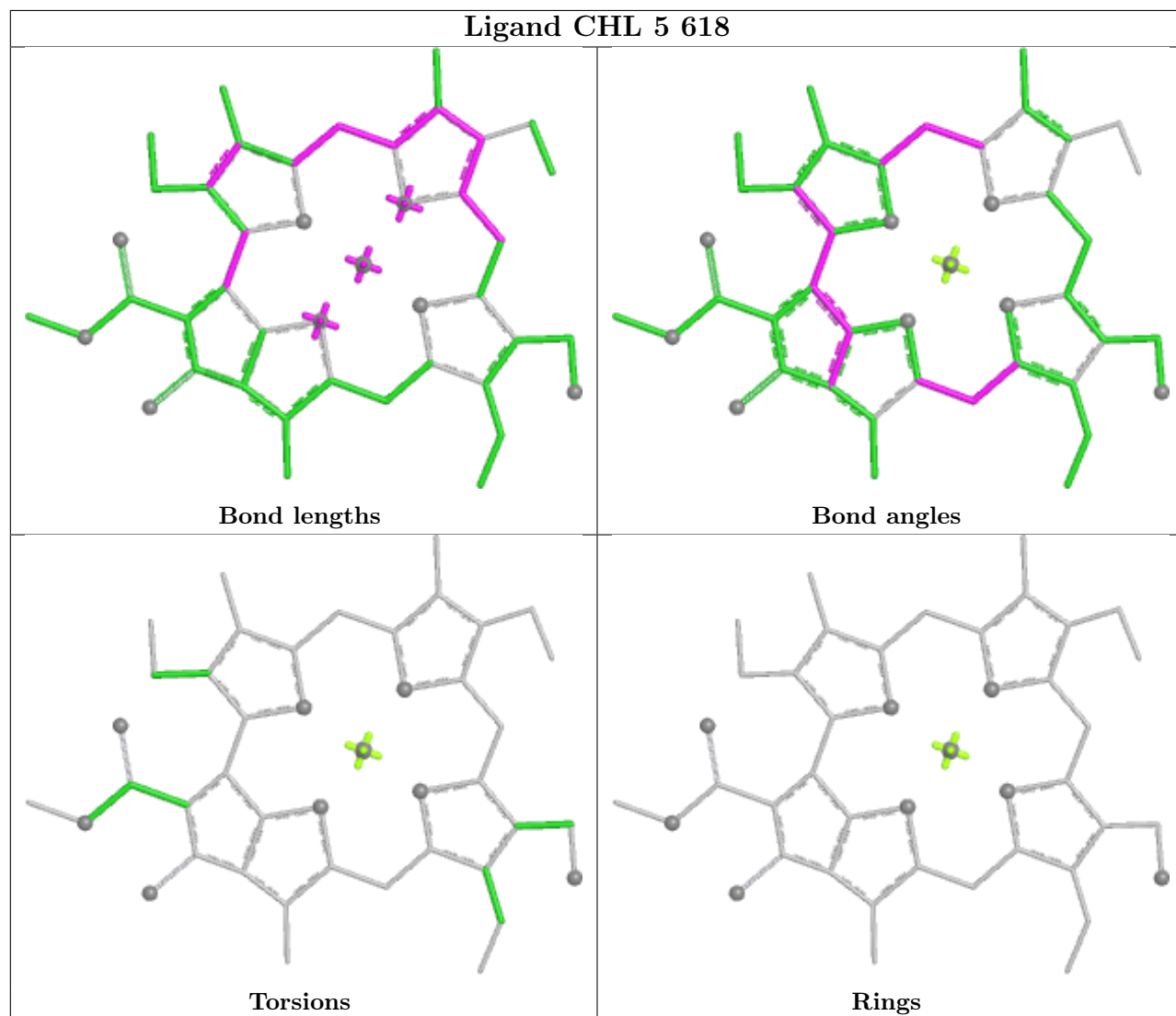
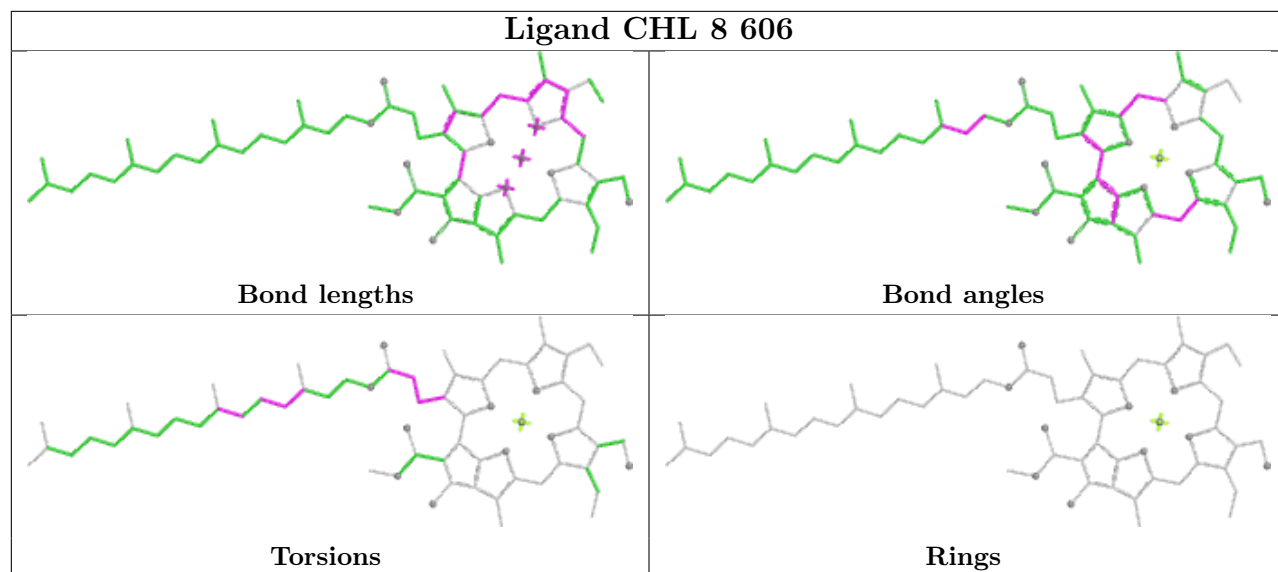


Ligand CLA A 805

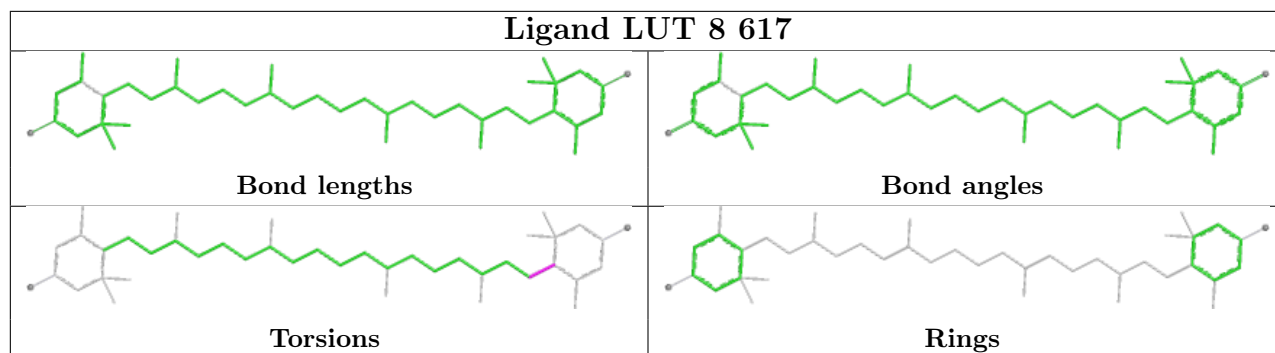


Ligand CLA 9 602

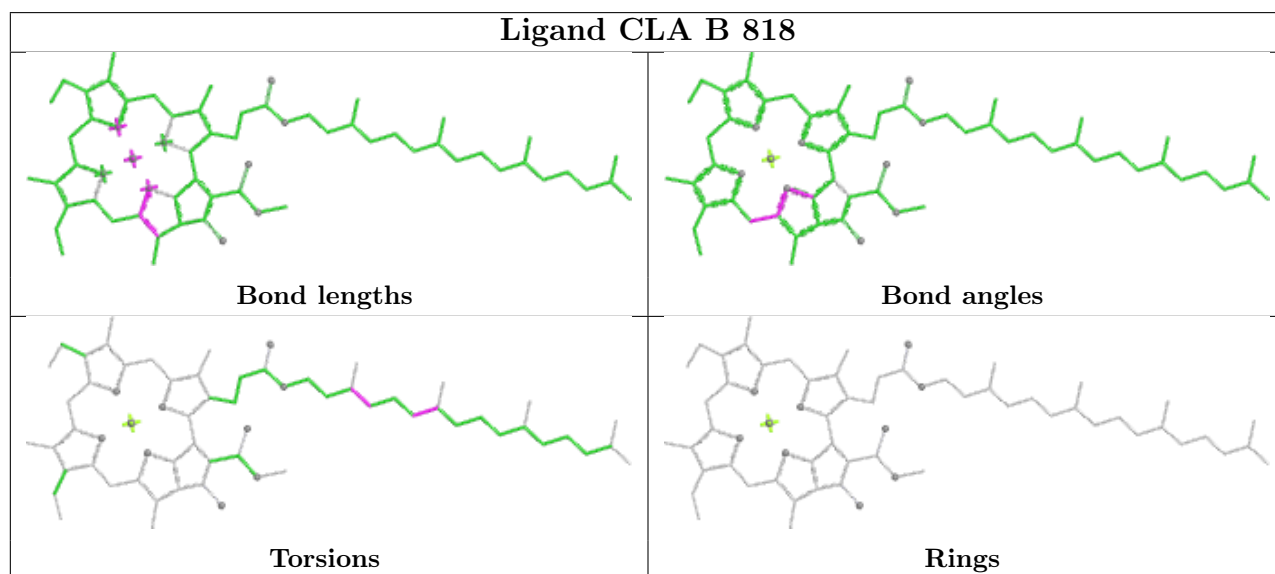




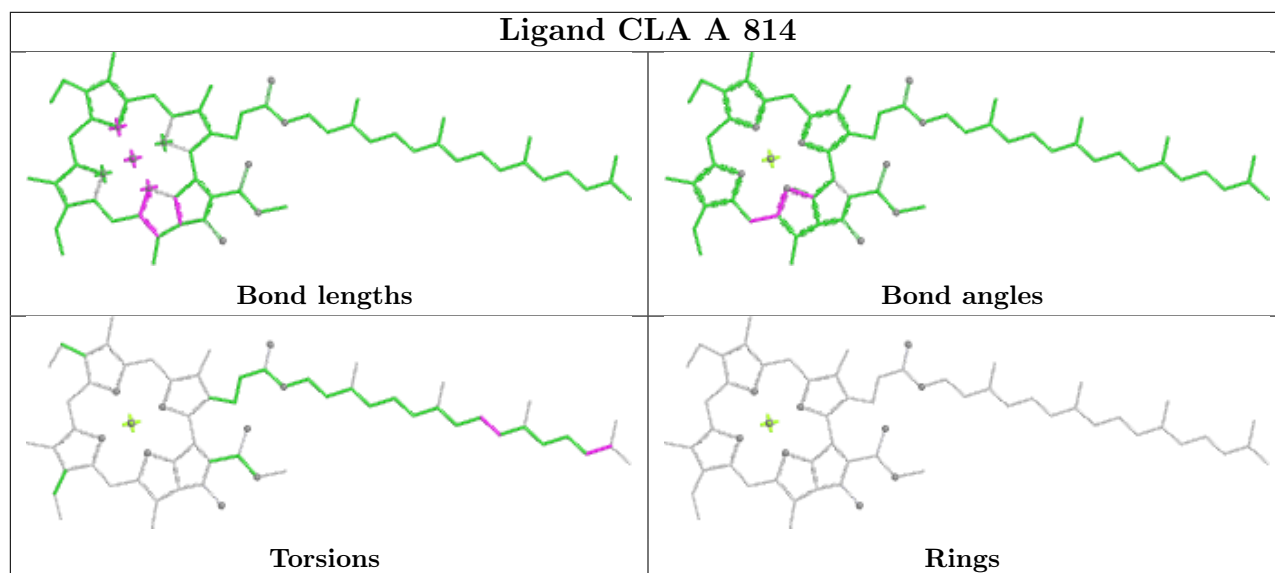
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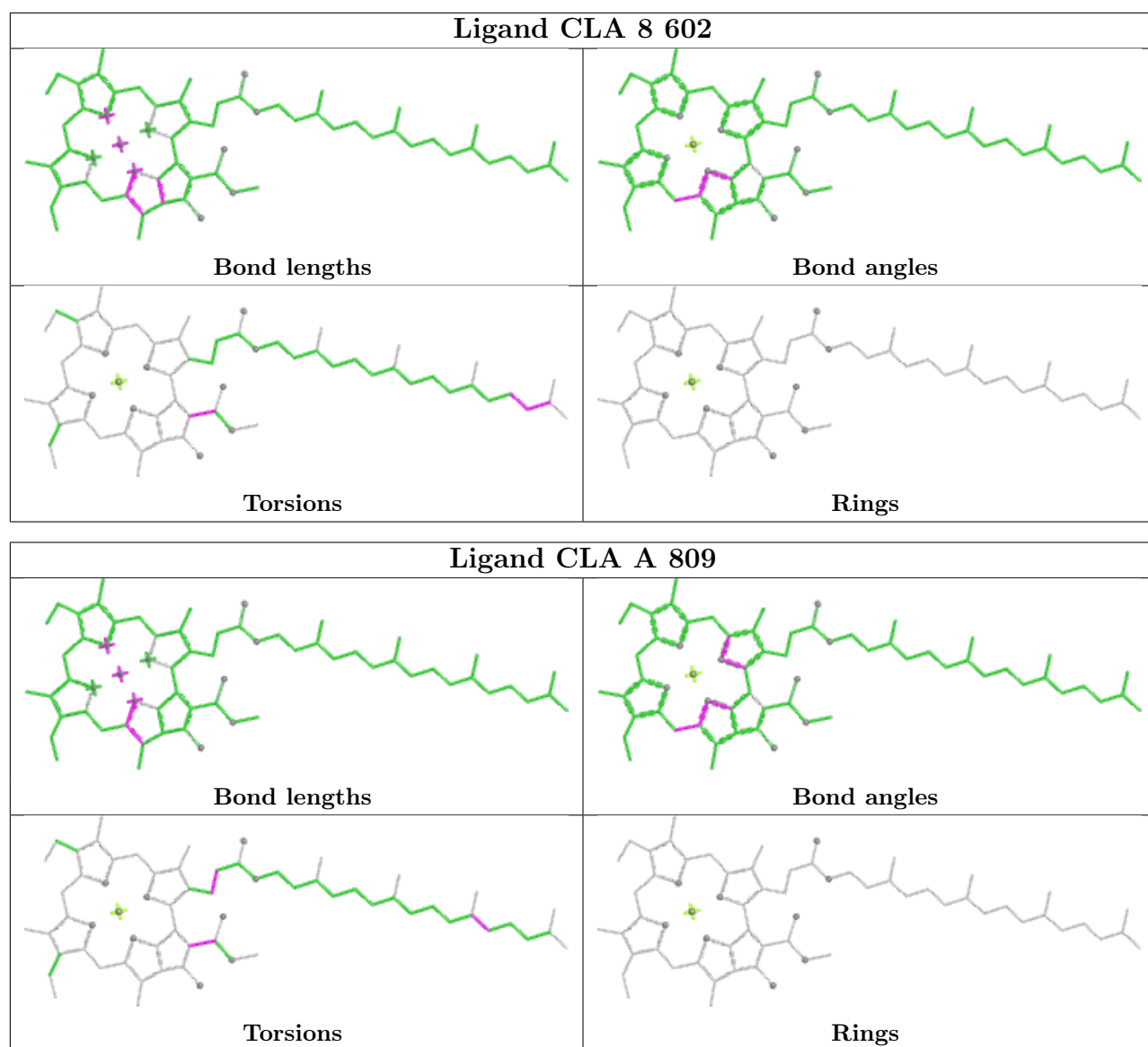


Ligand CLA B 818

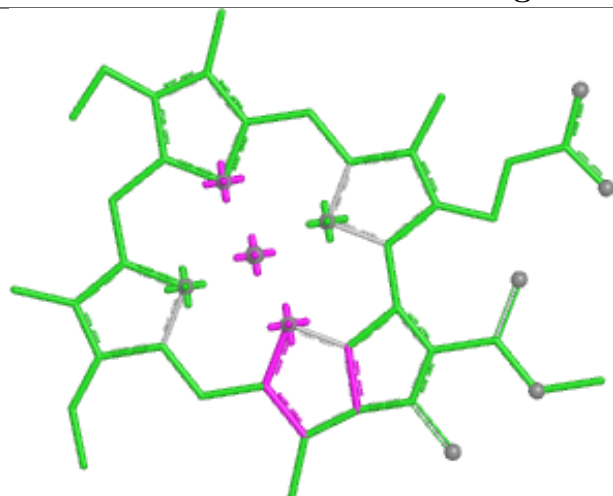


Ligand CLA A 814

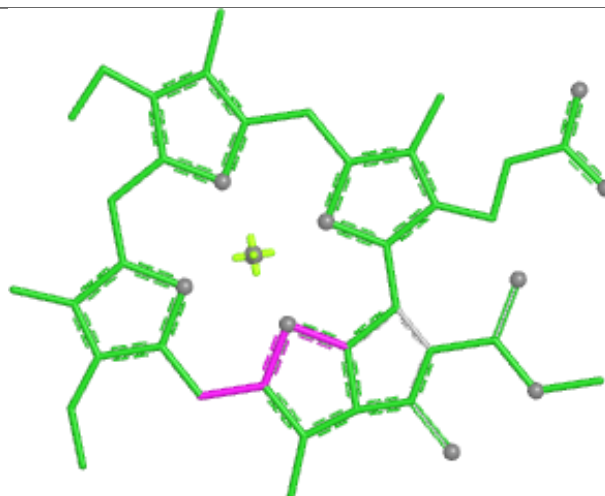




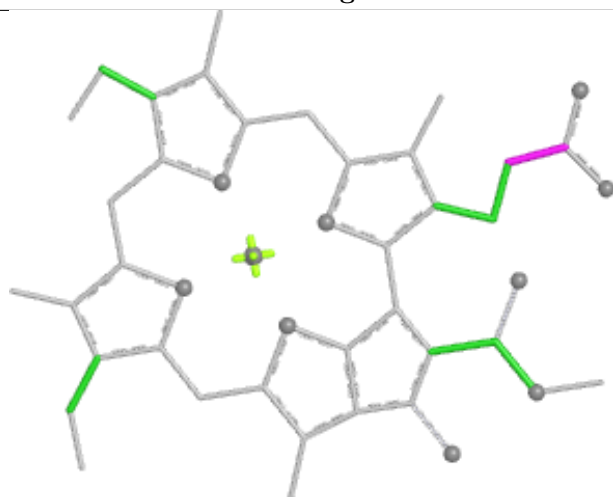
Ligand CLA A 824



Bond lengths



Bond angles

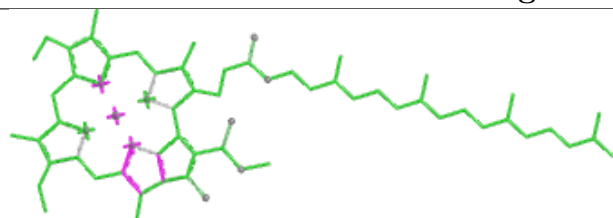


Torsions

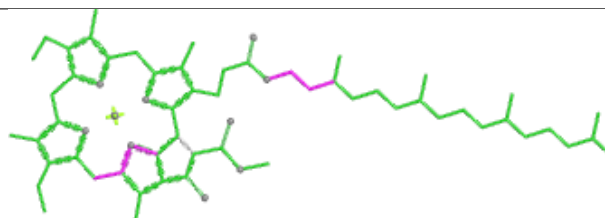


Rings

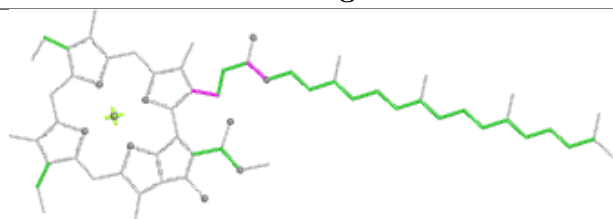
Ligand CLA 7 610



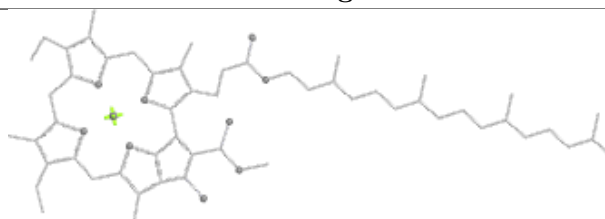
Bond lengths



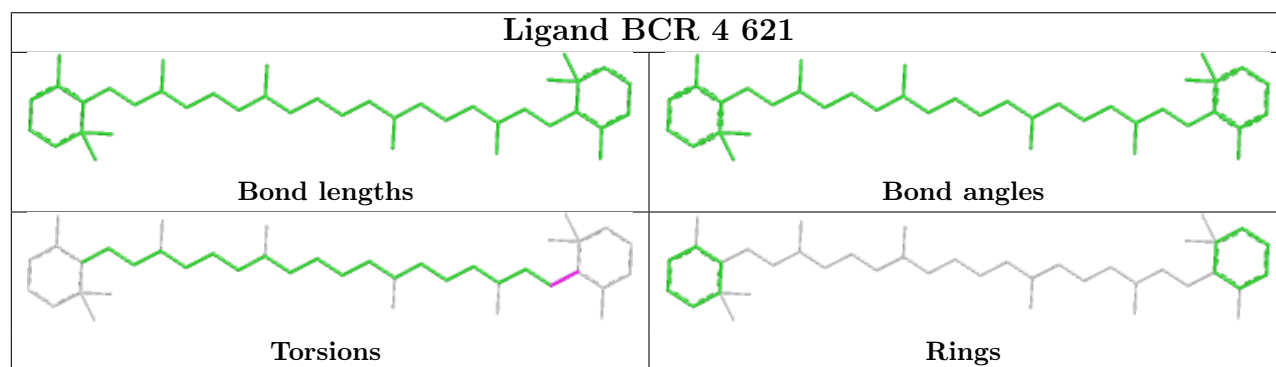
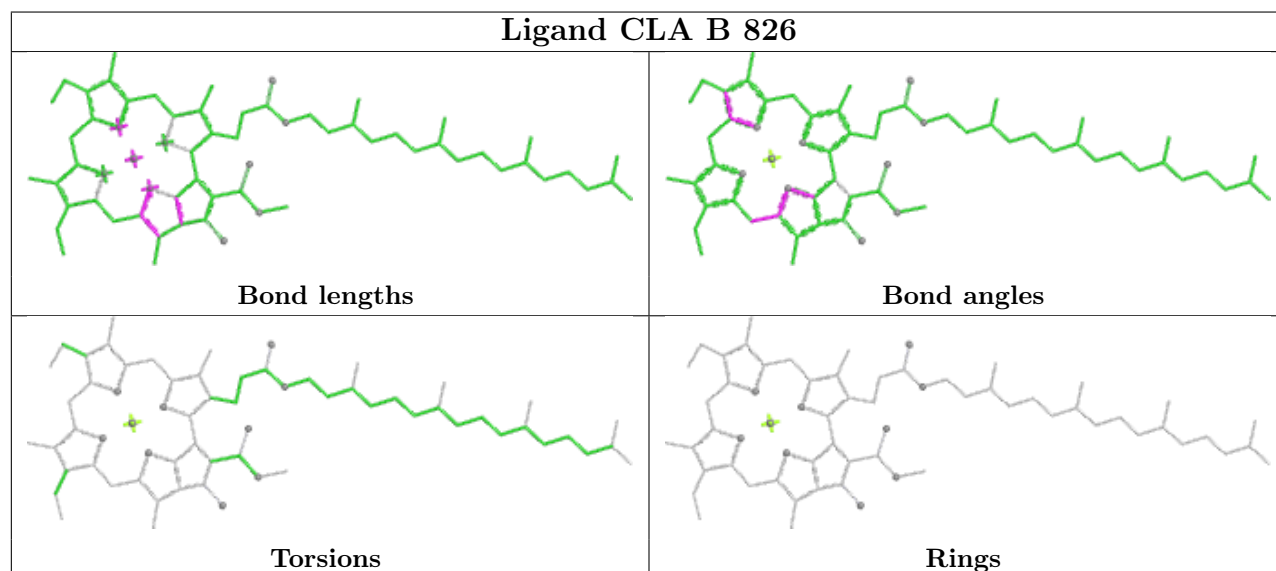
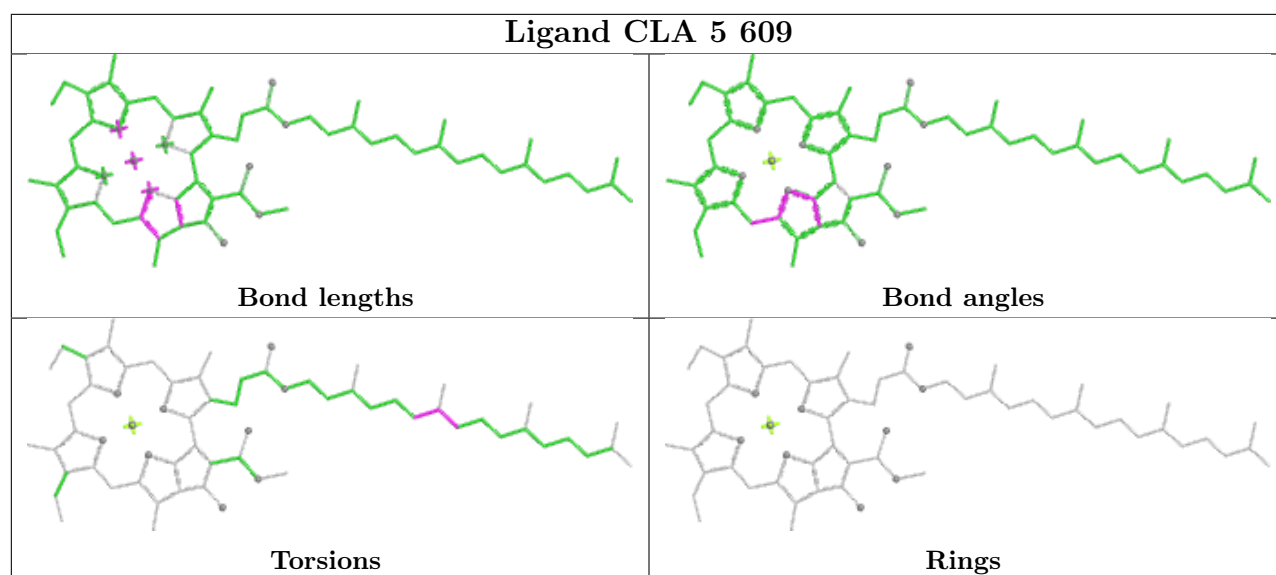
Bond angles

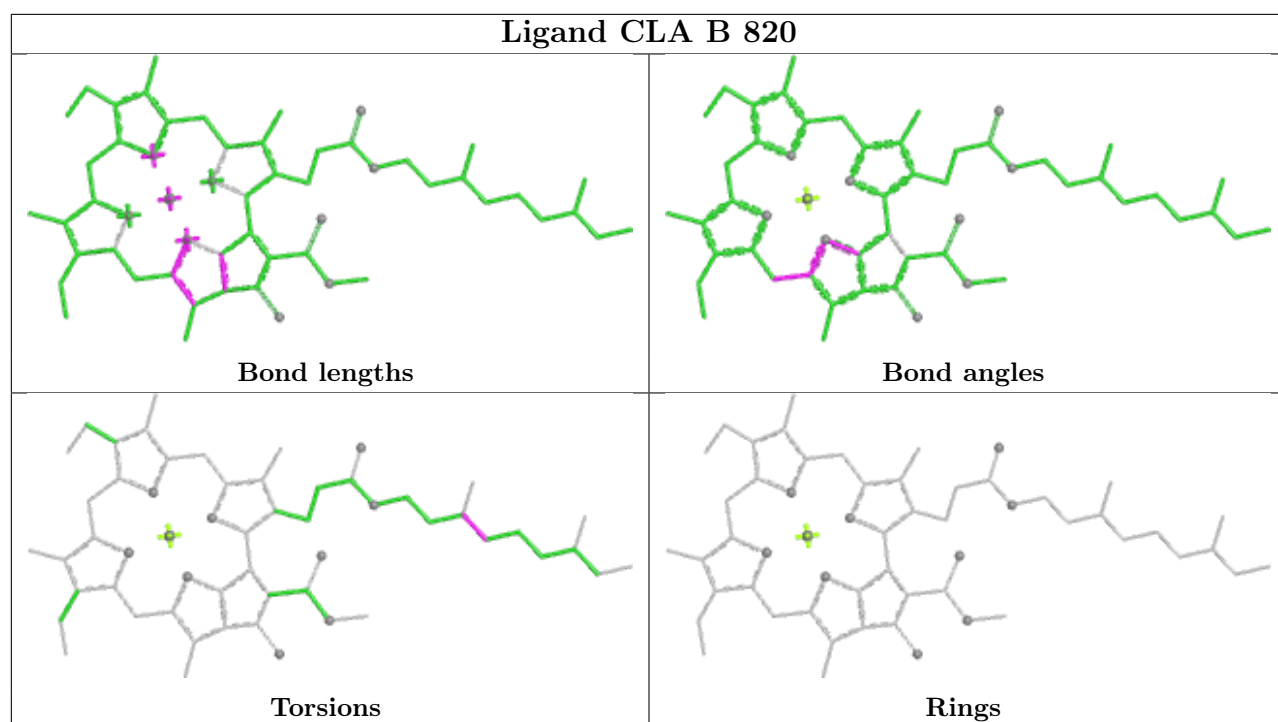


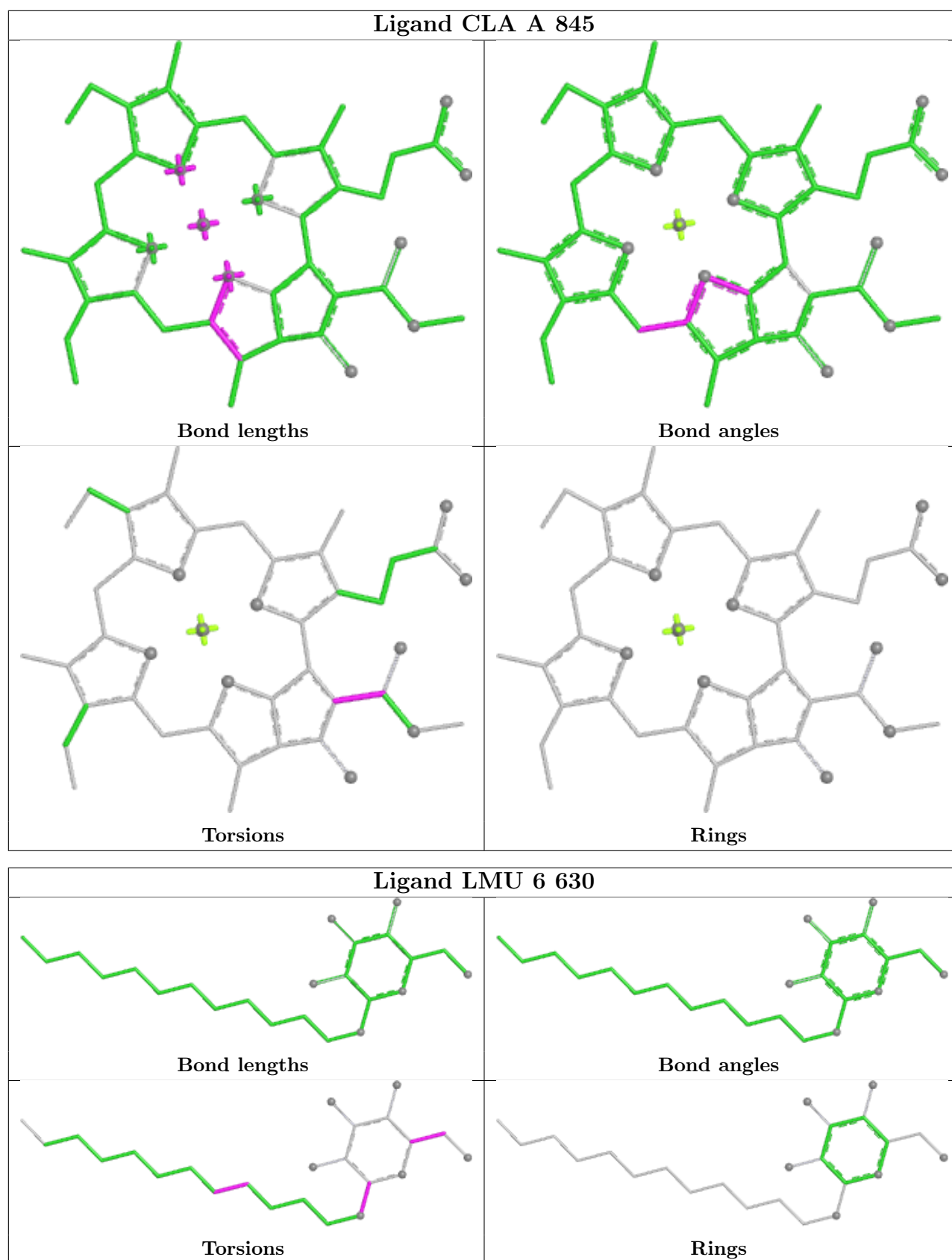
Torsions

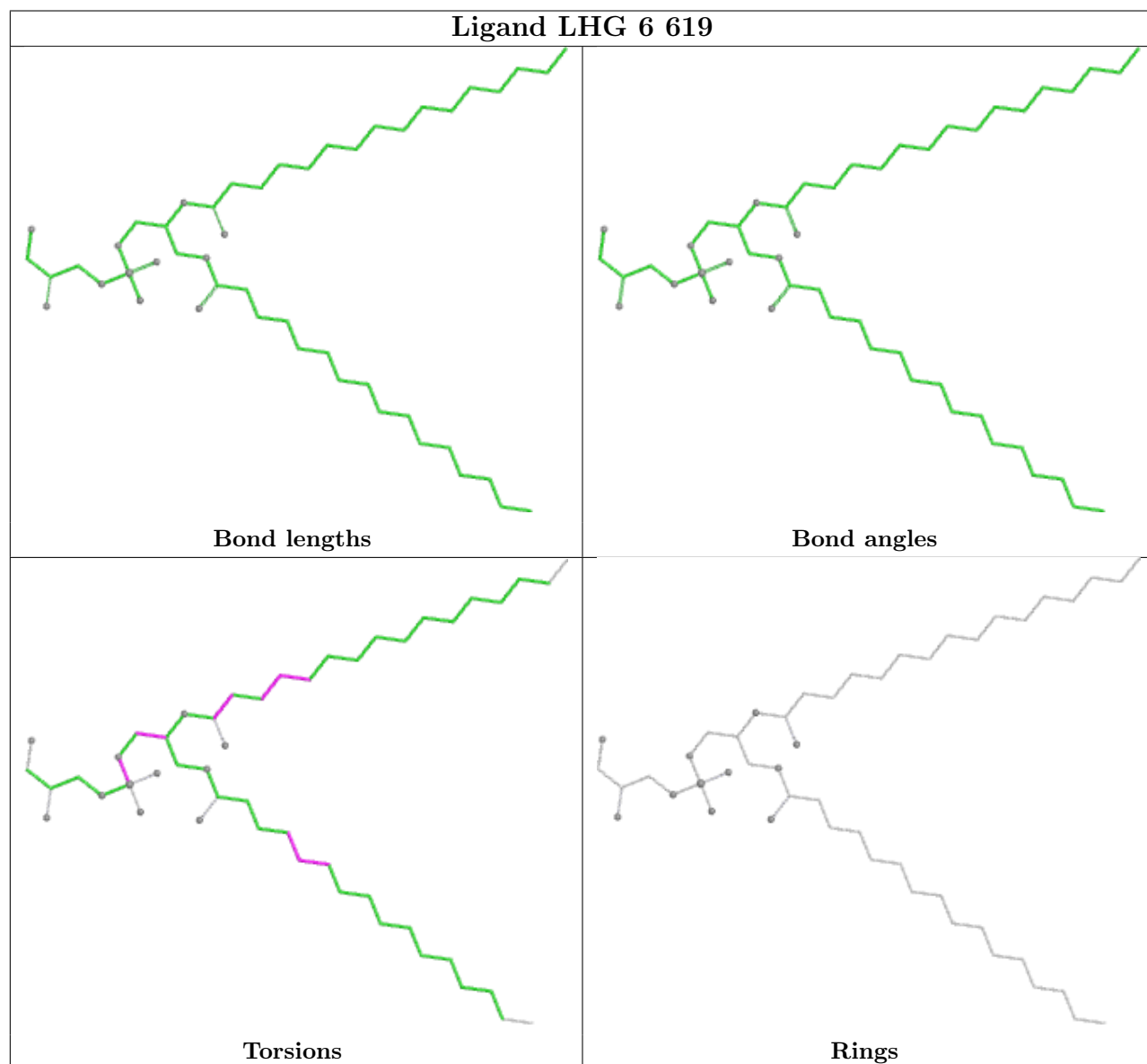
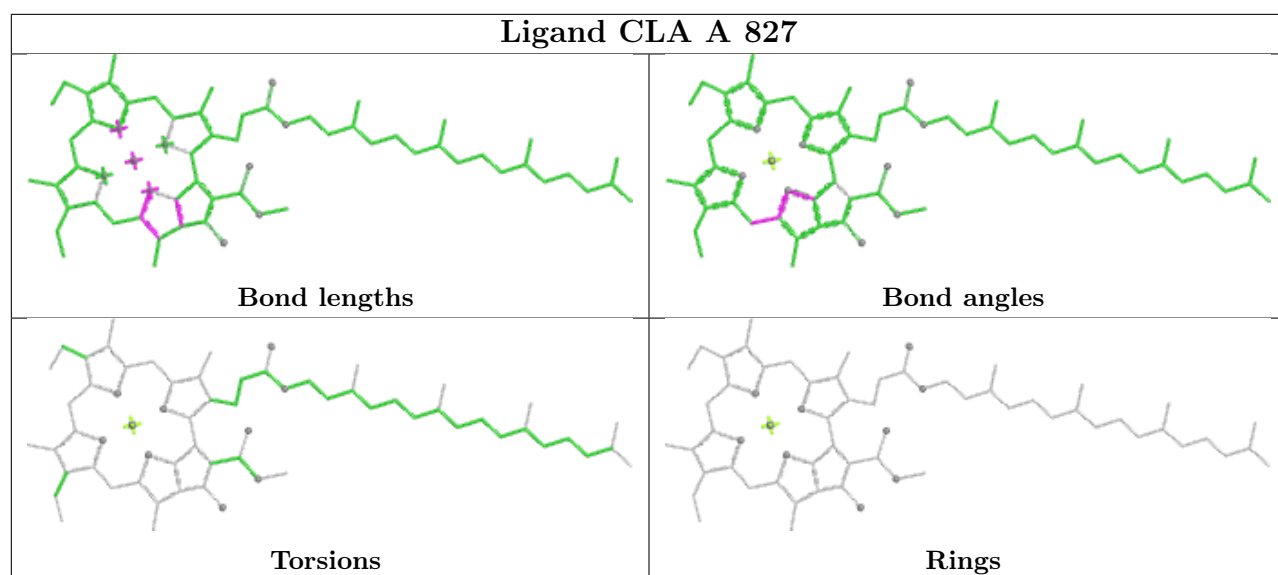


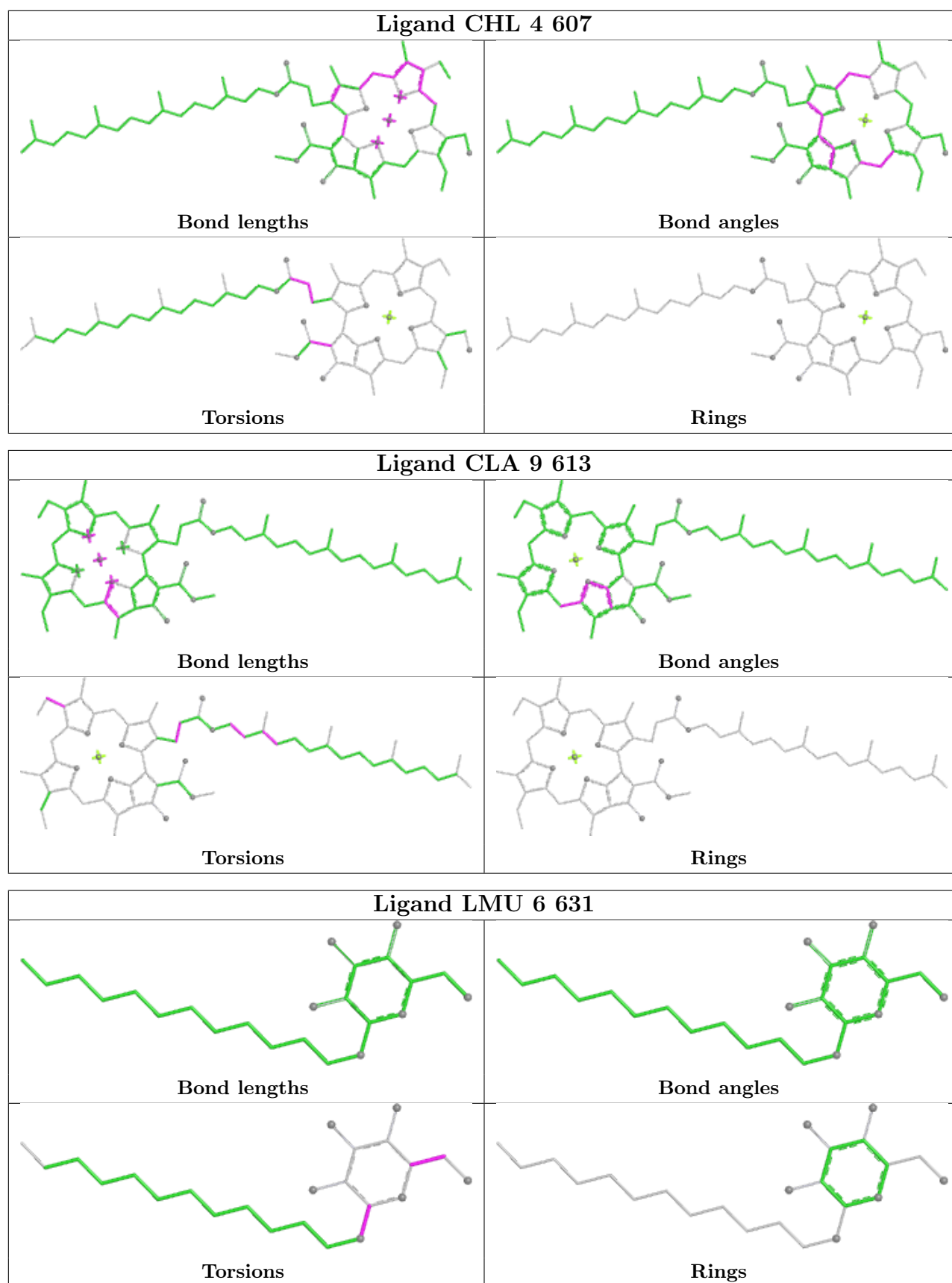
Rings

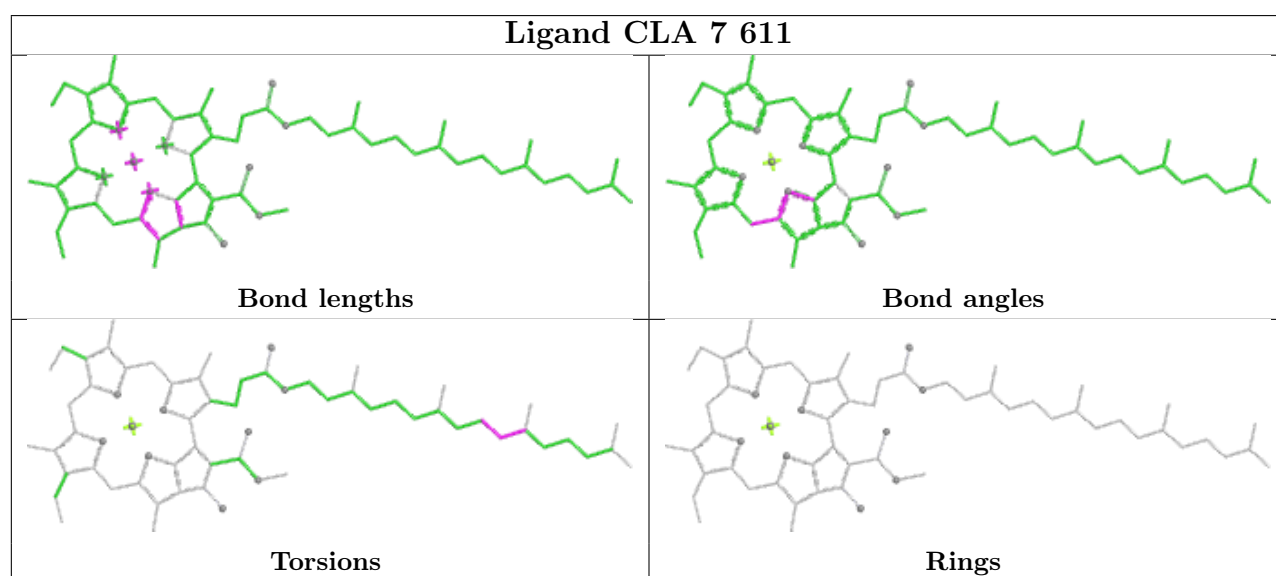
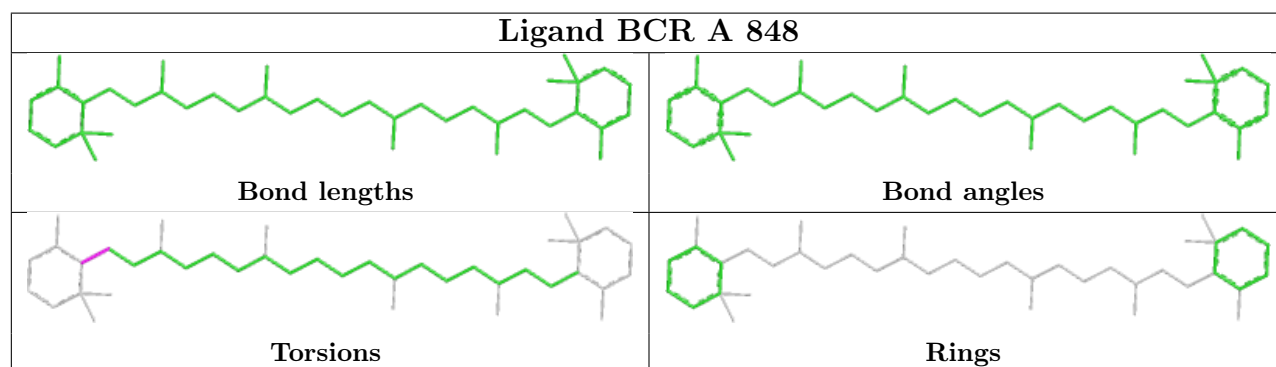
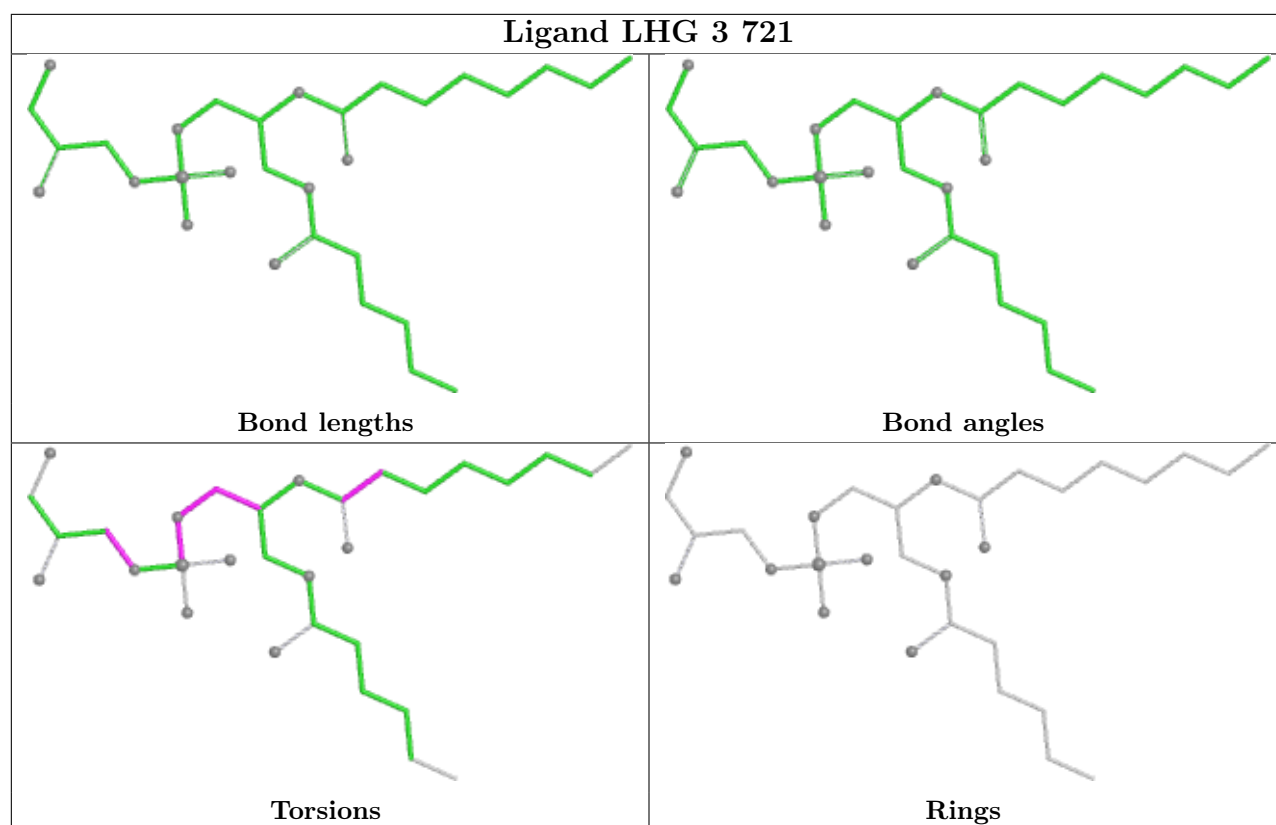


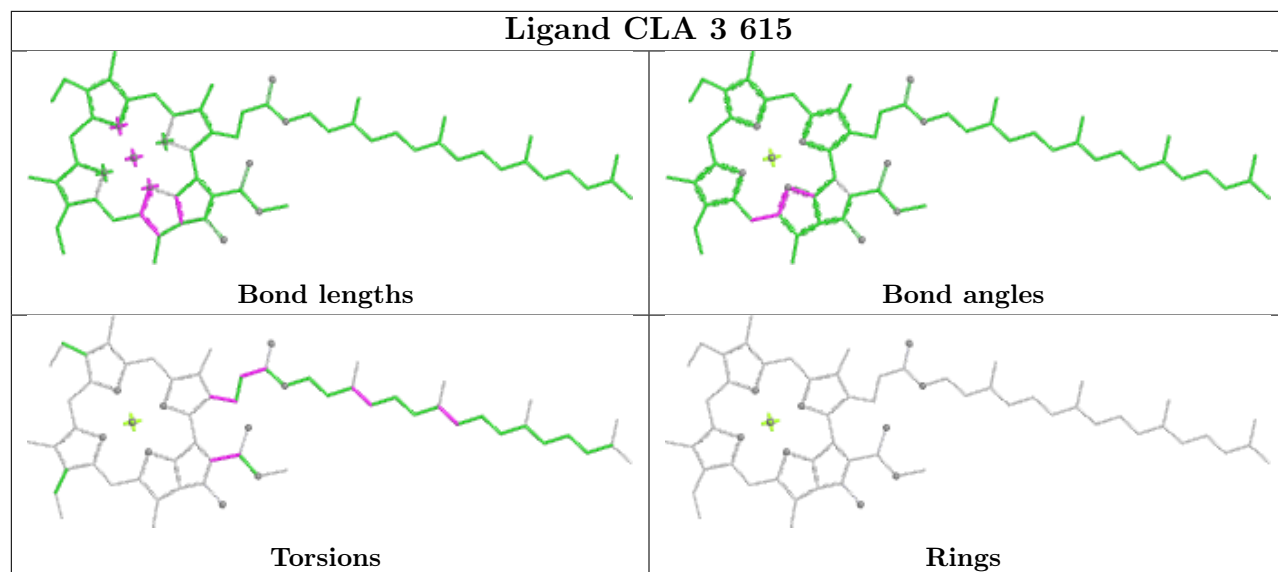
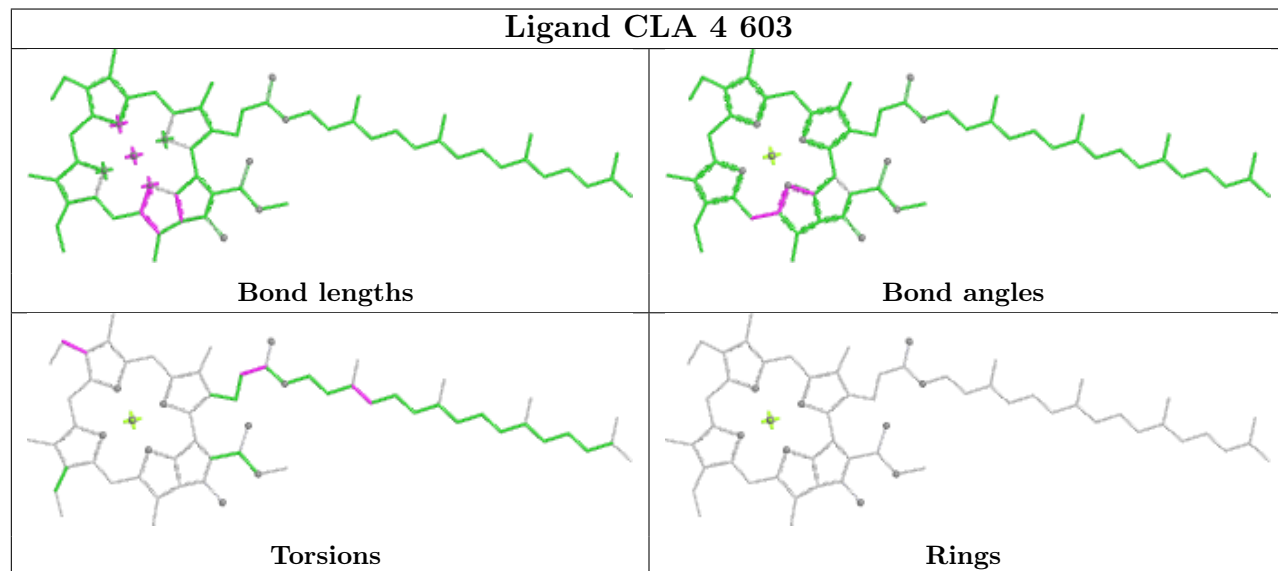


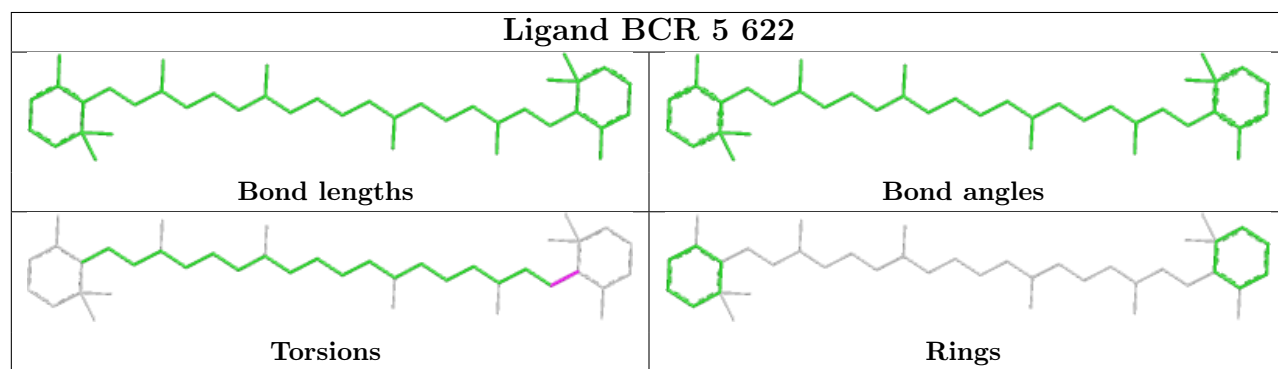
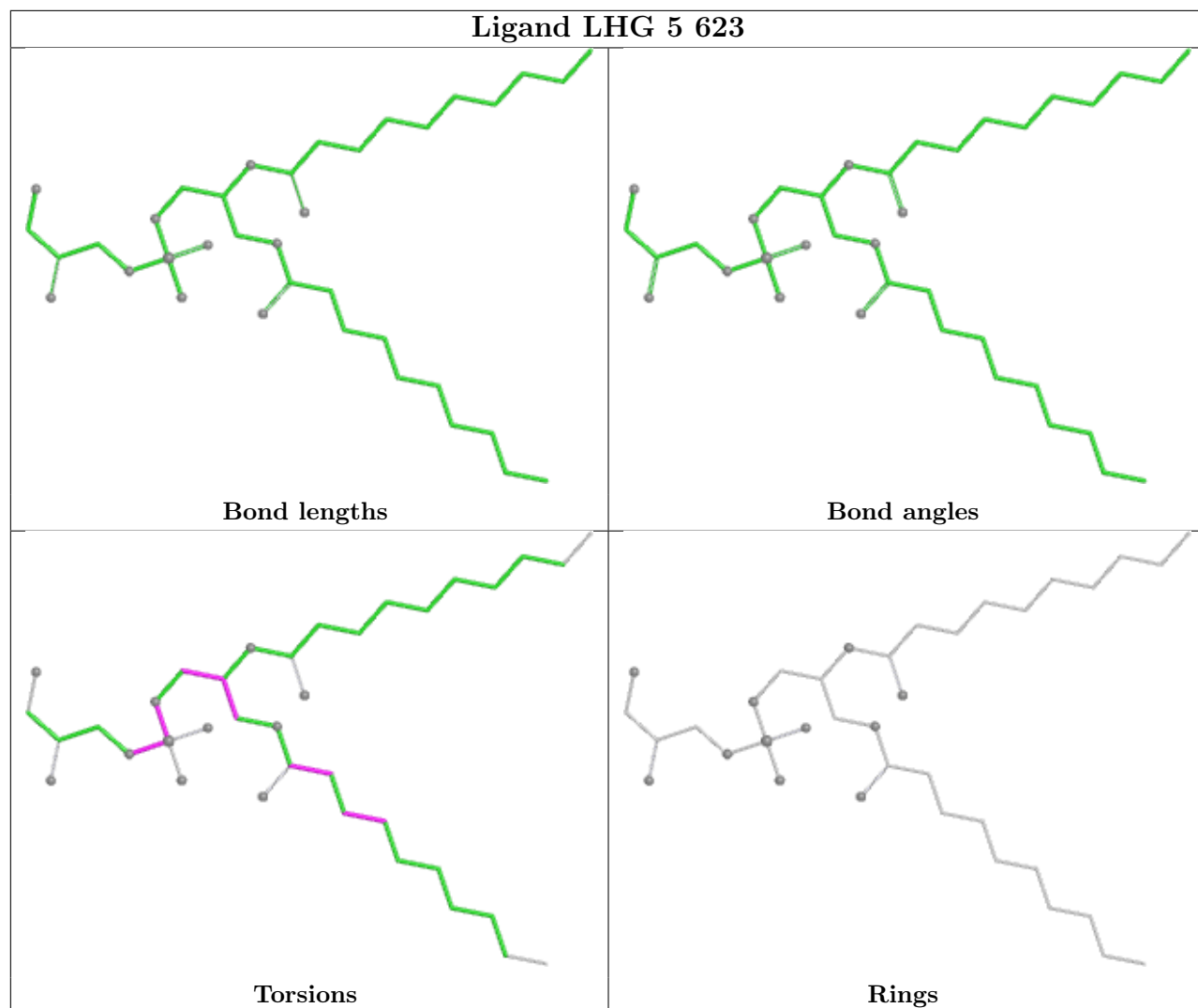


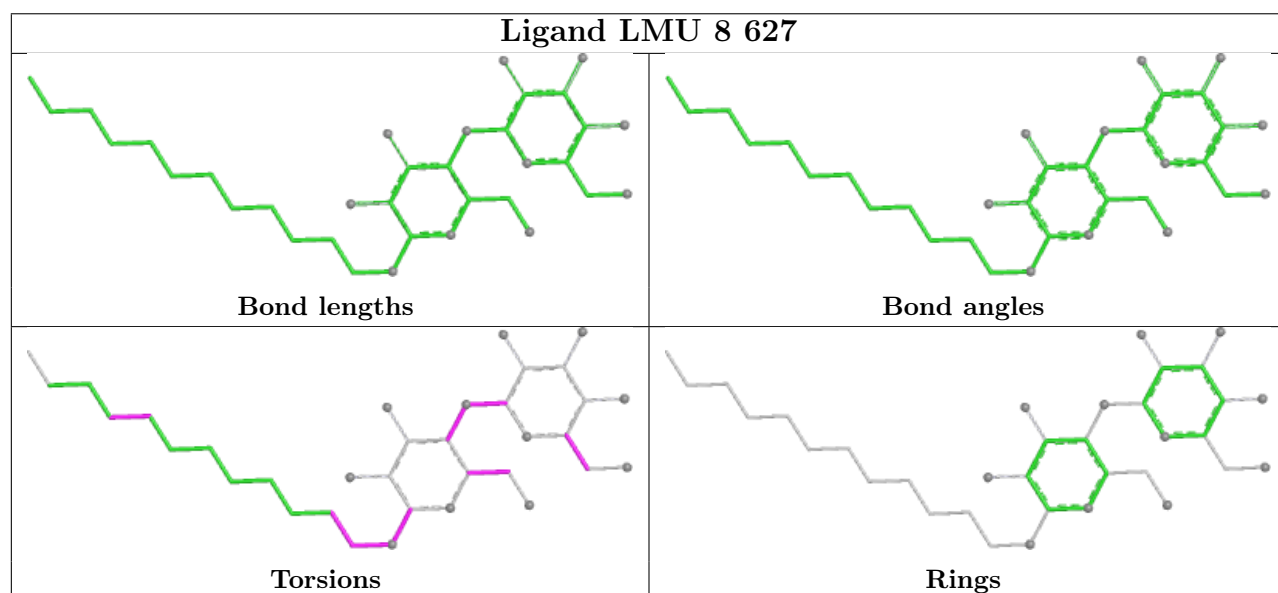
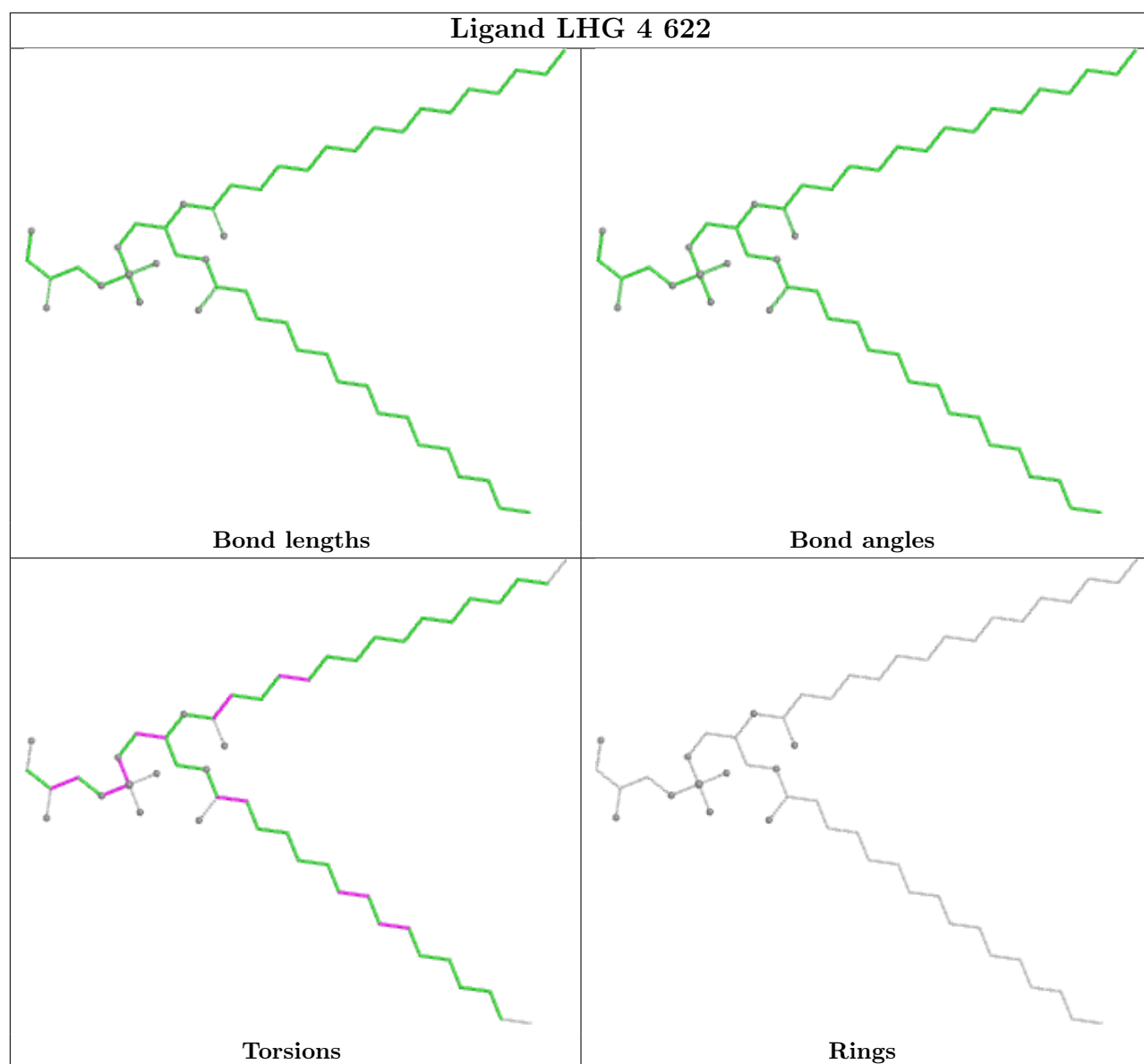


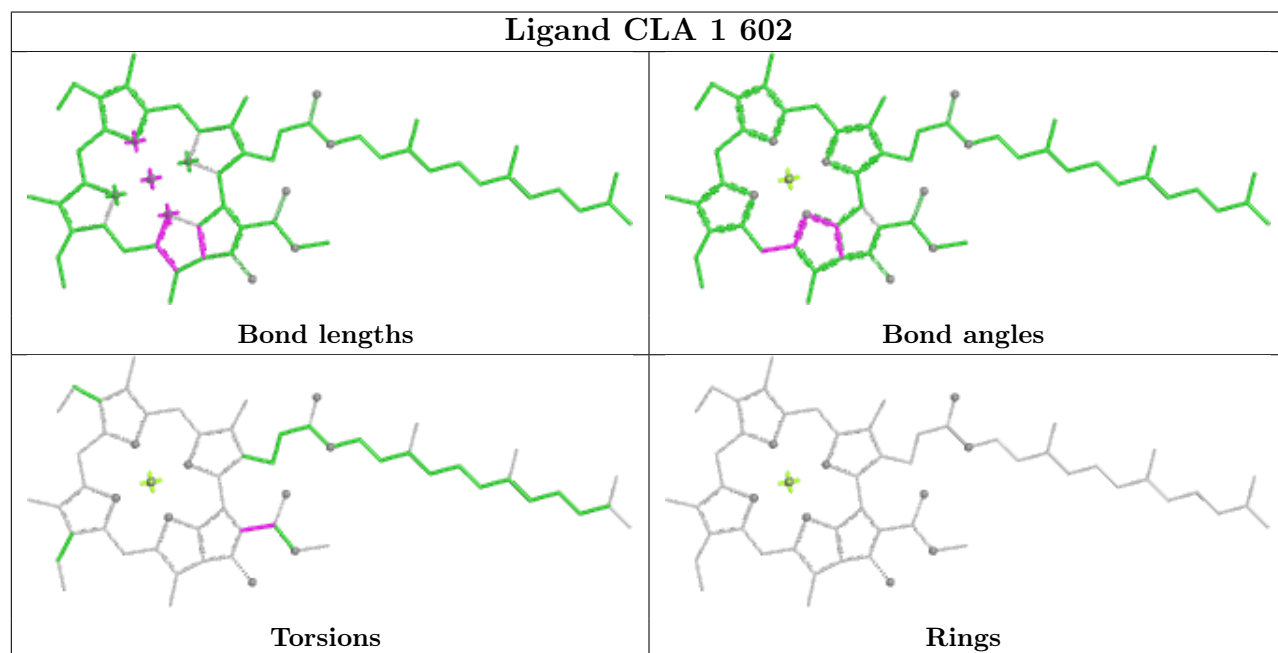
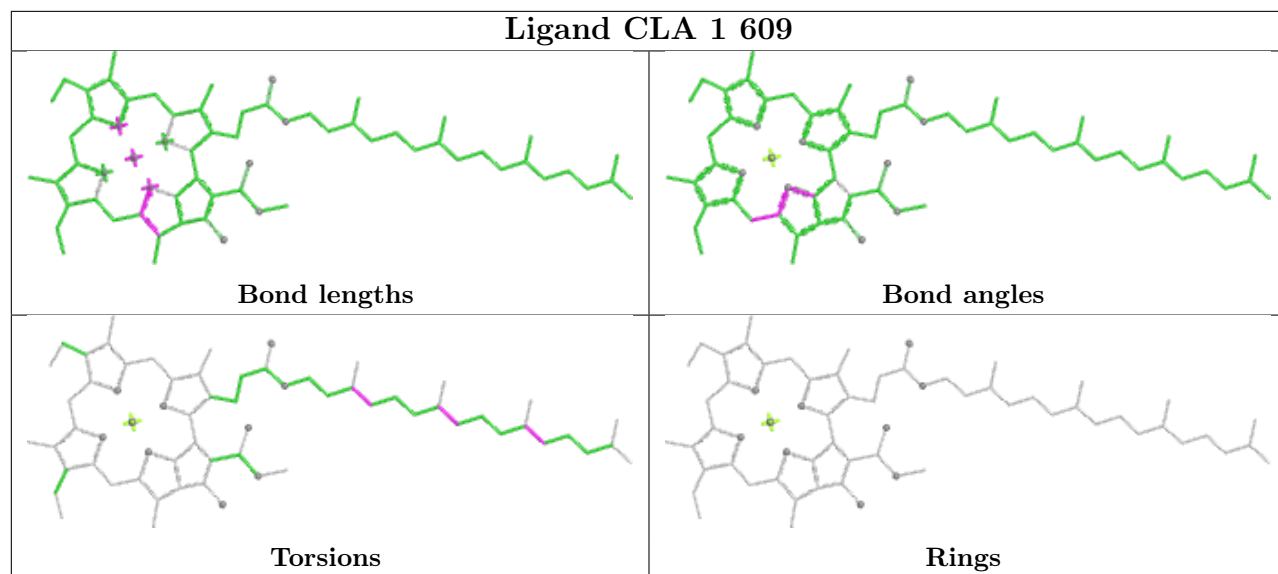


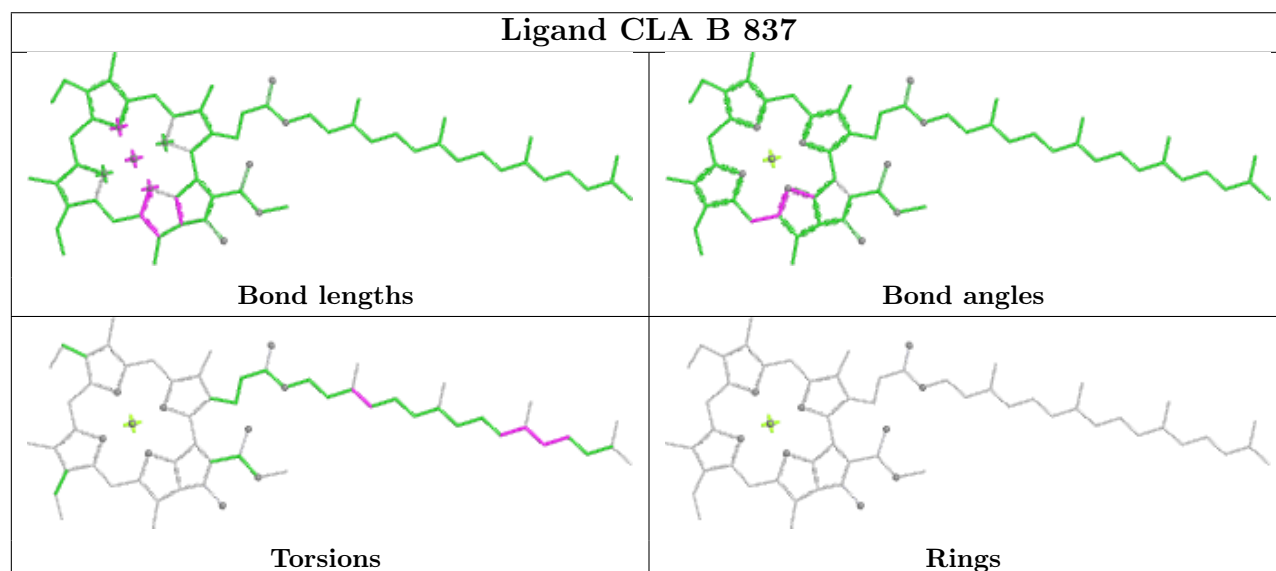
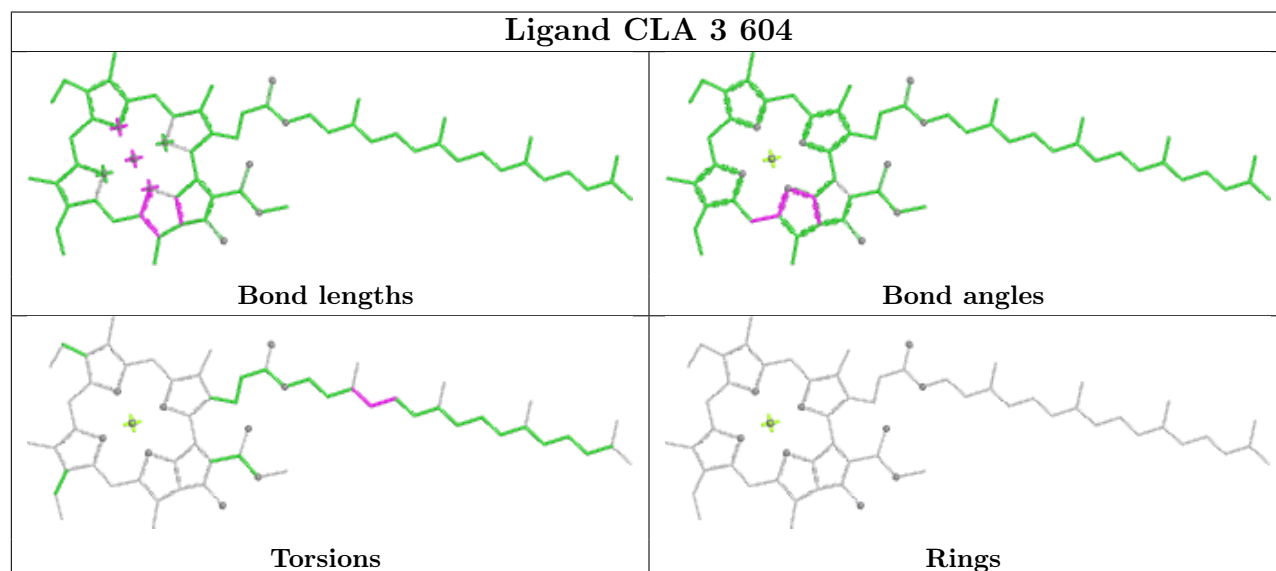
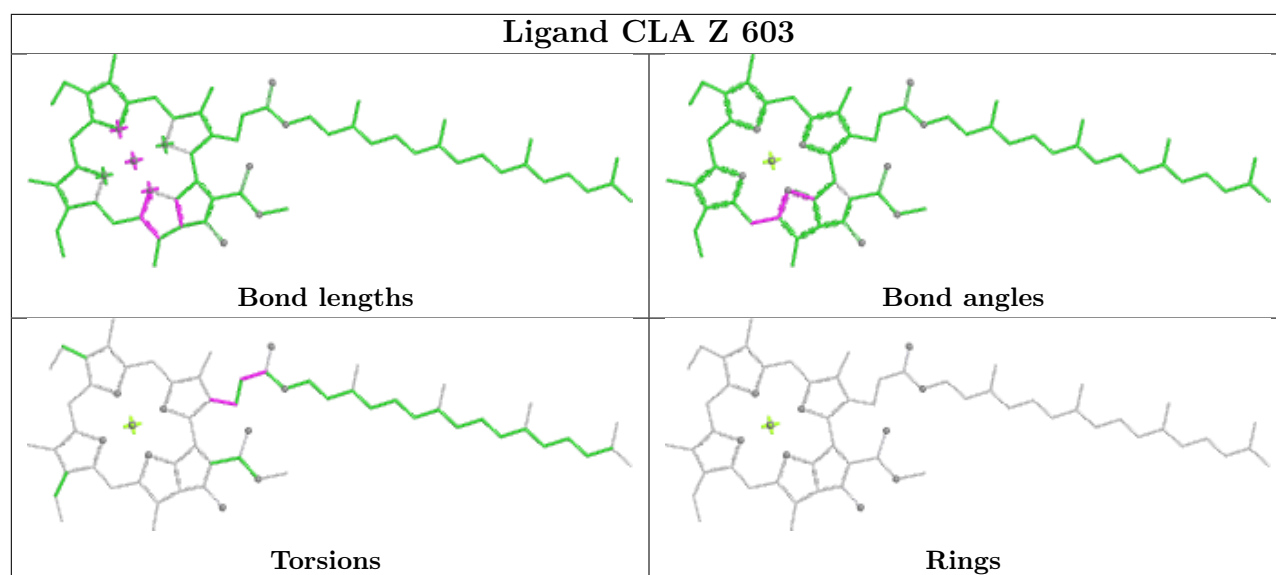


Ligand CLA 3 615**Ligand CLA 4 603**

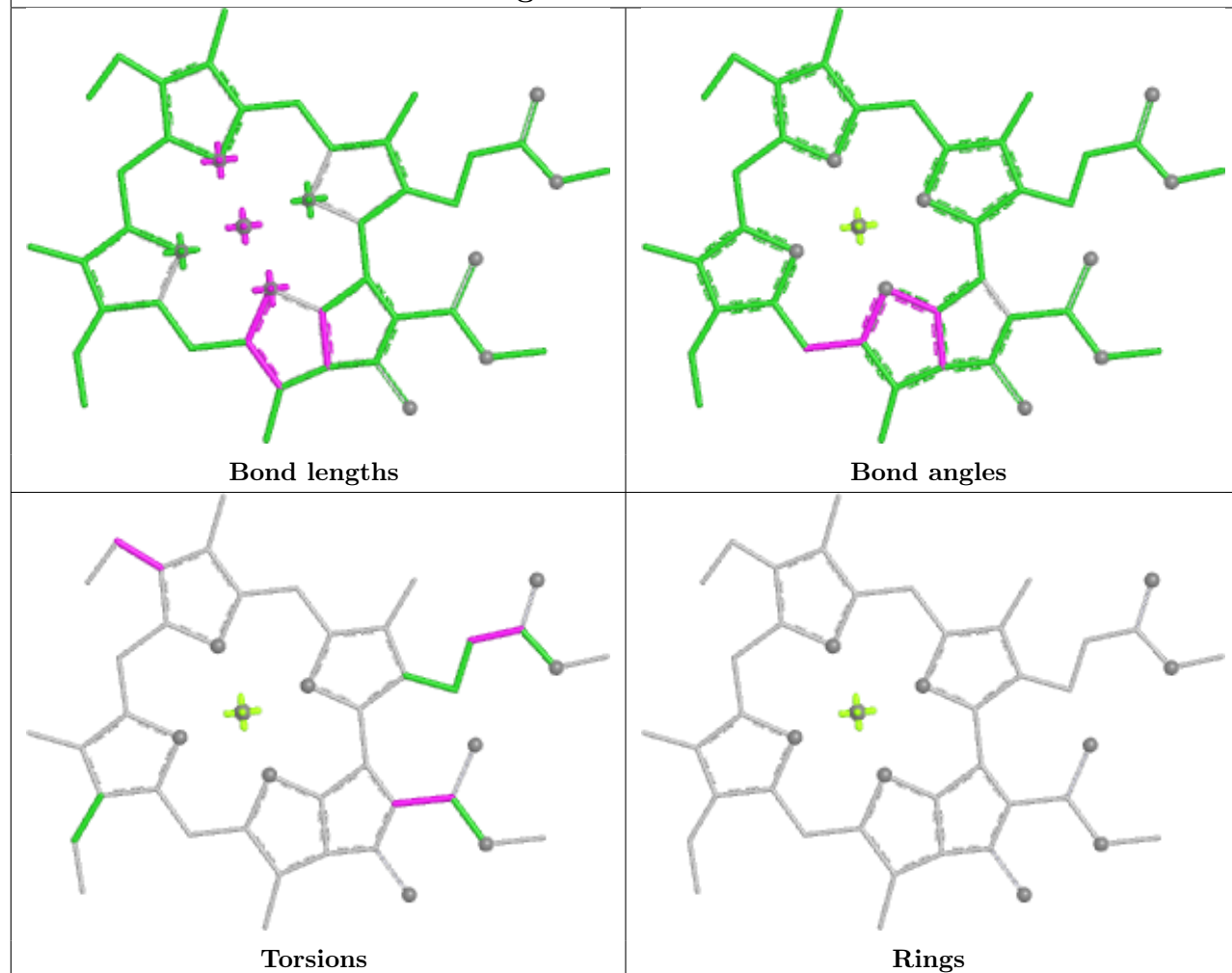




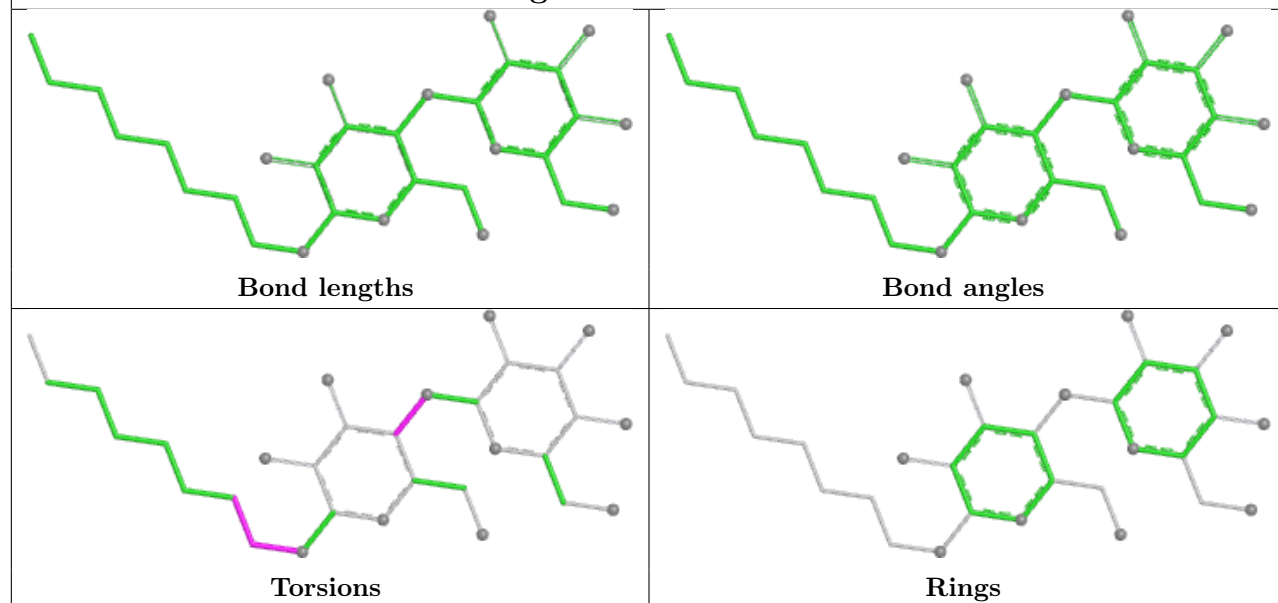


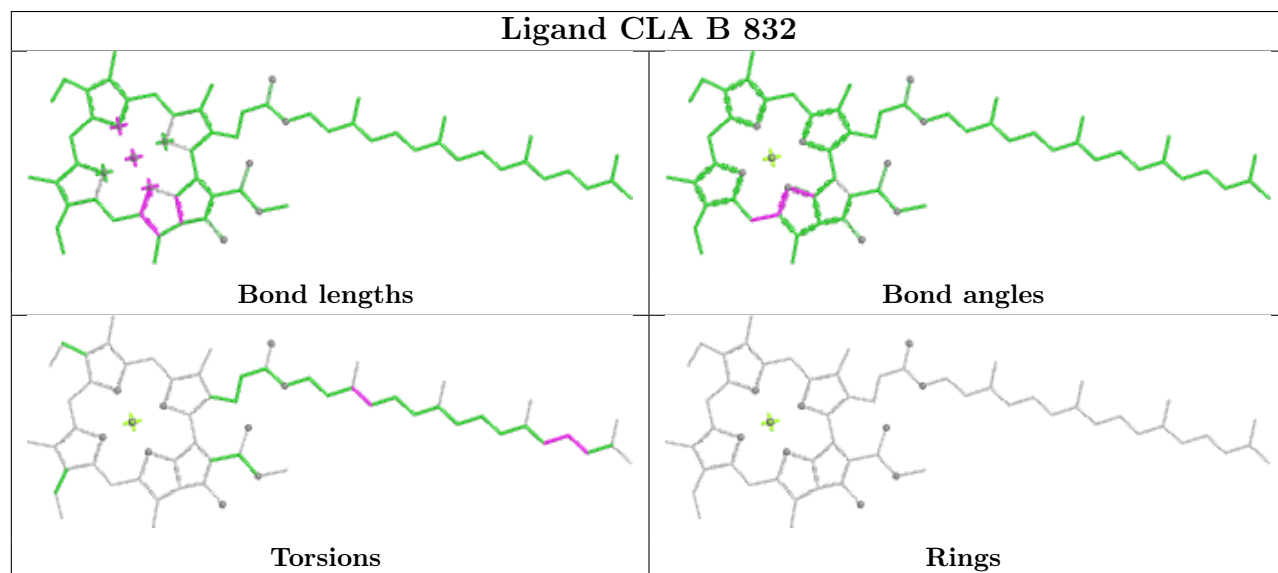
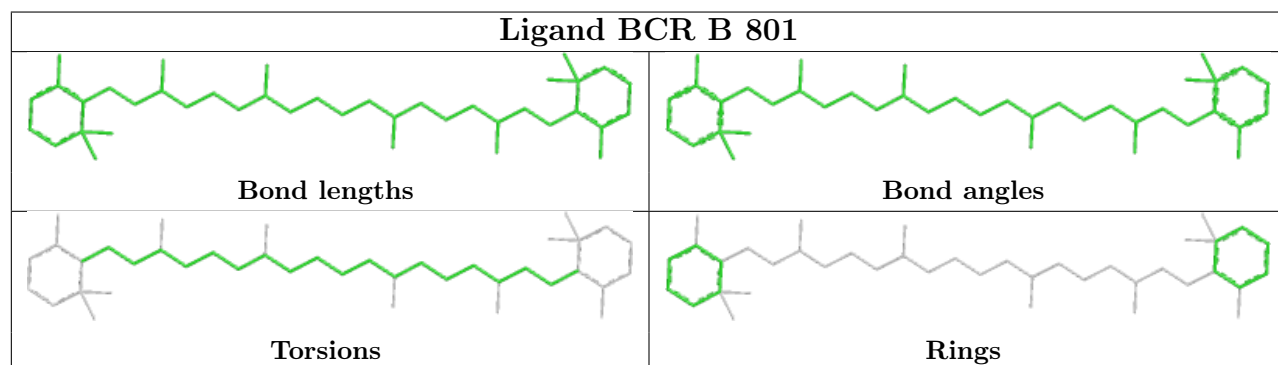
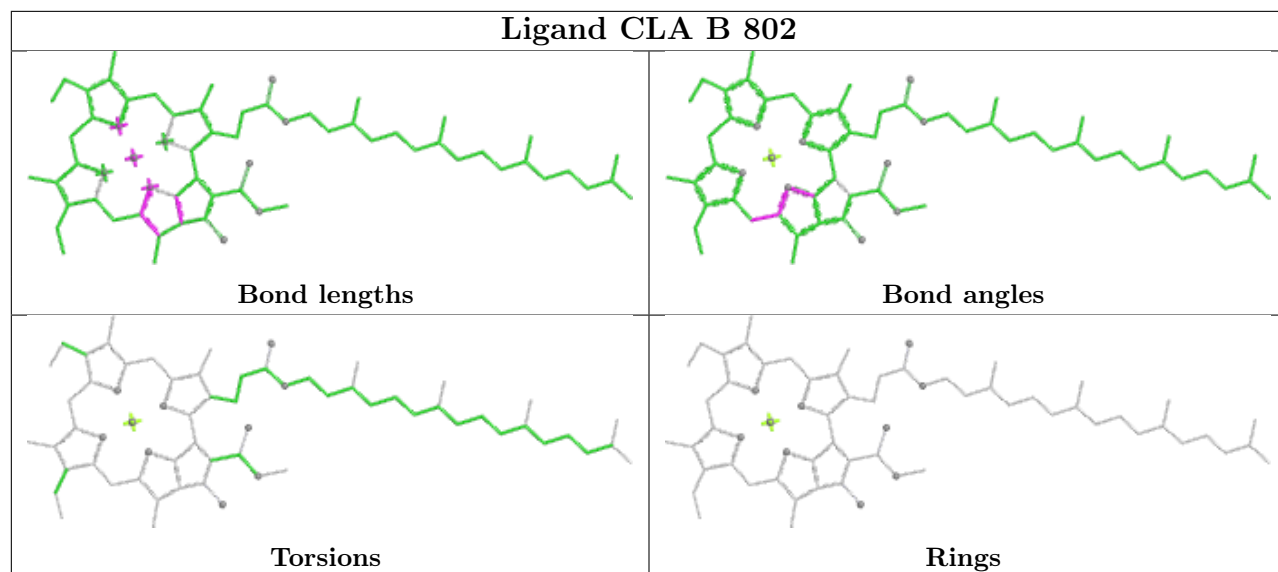


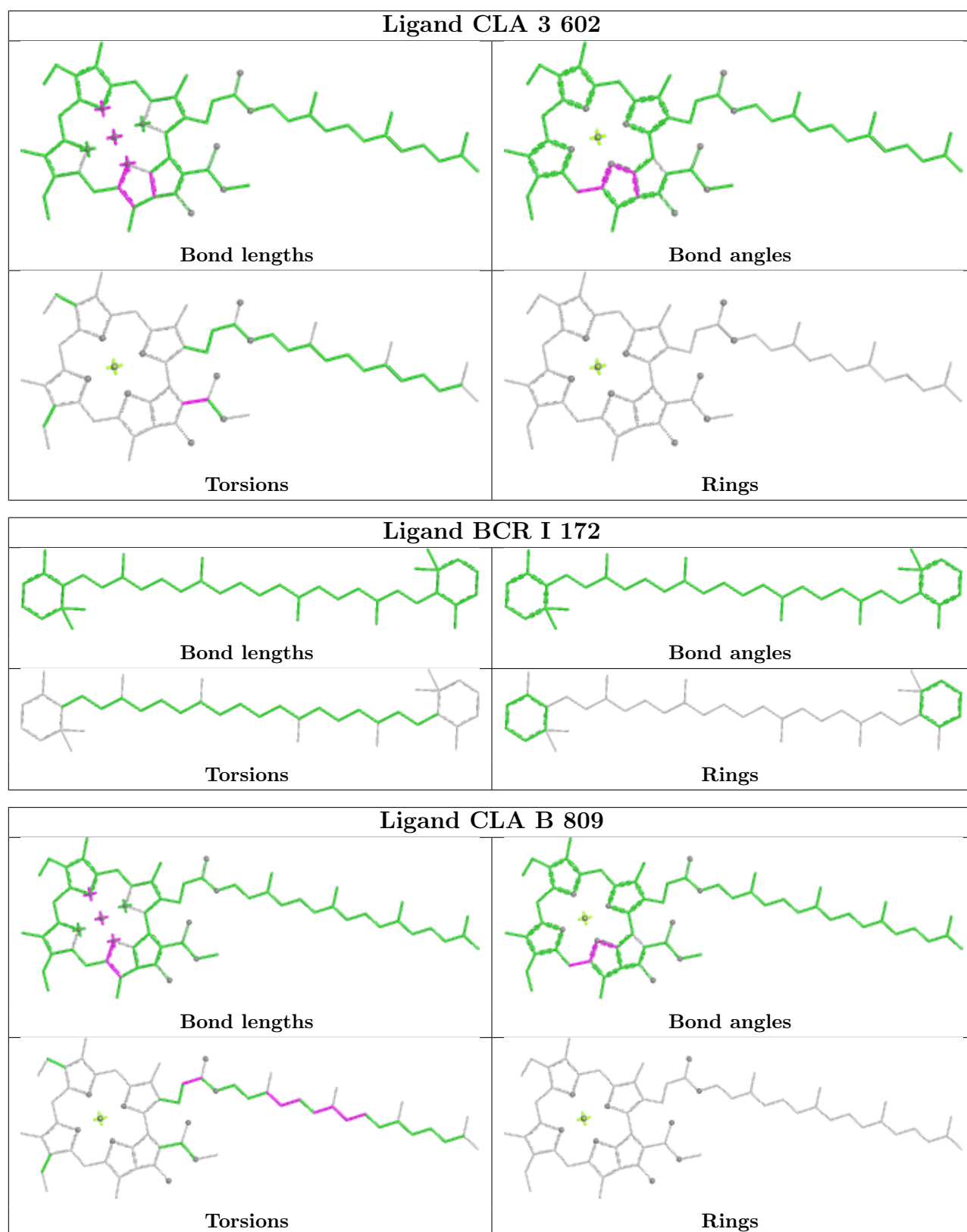
Ligand CLA 3 612

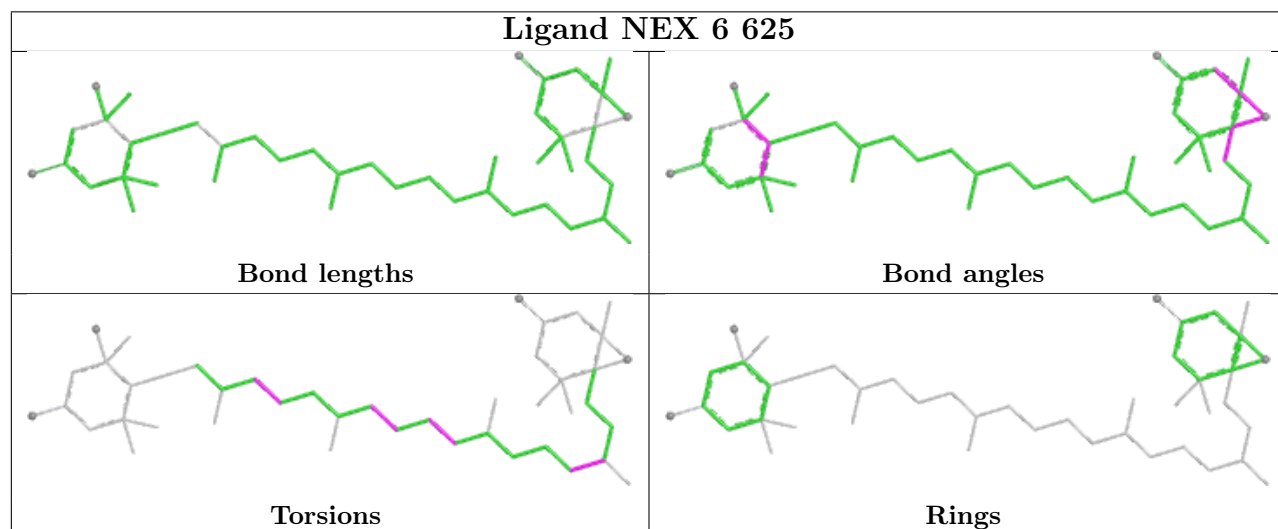
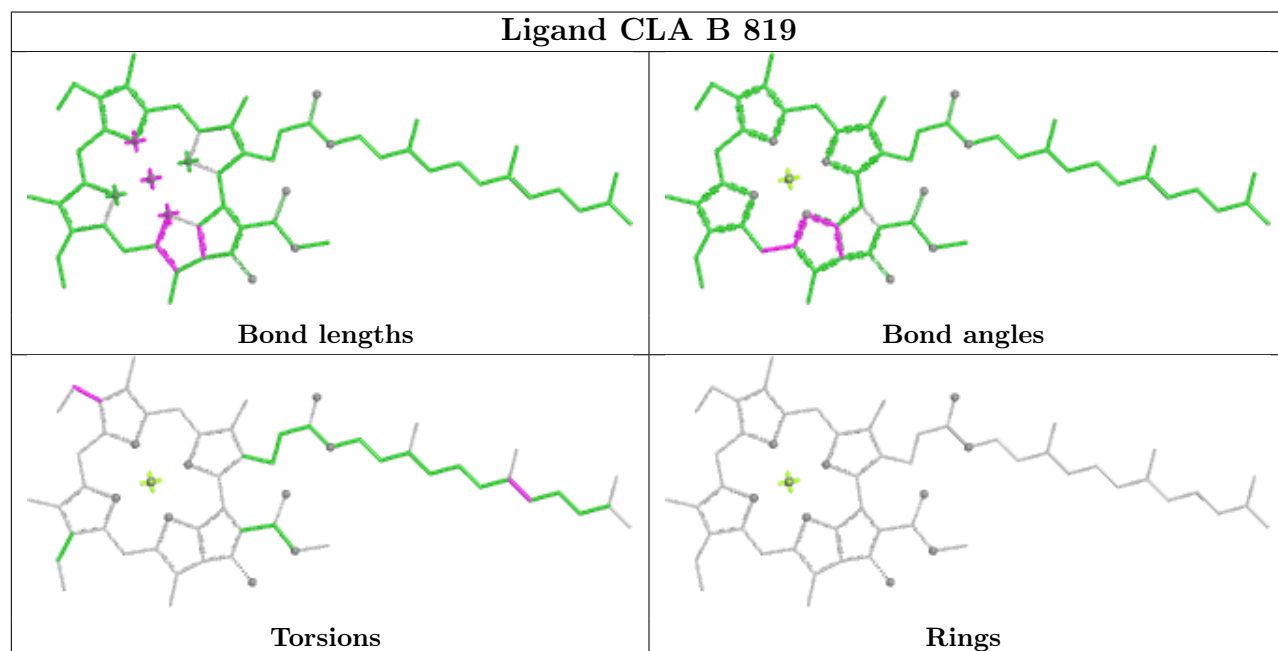
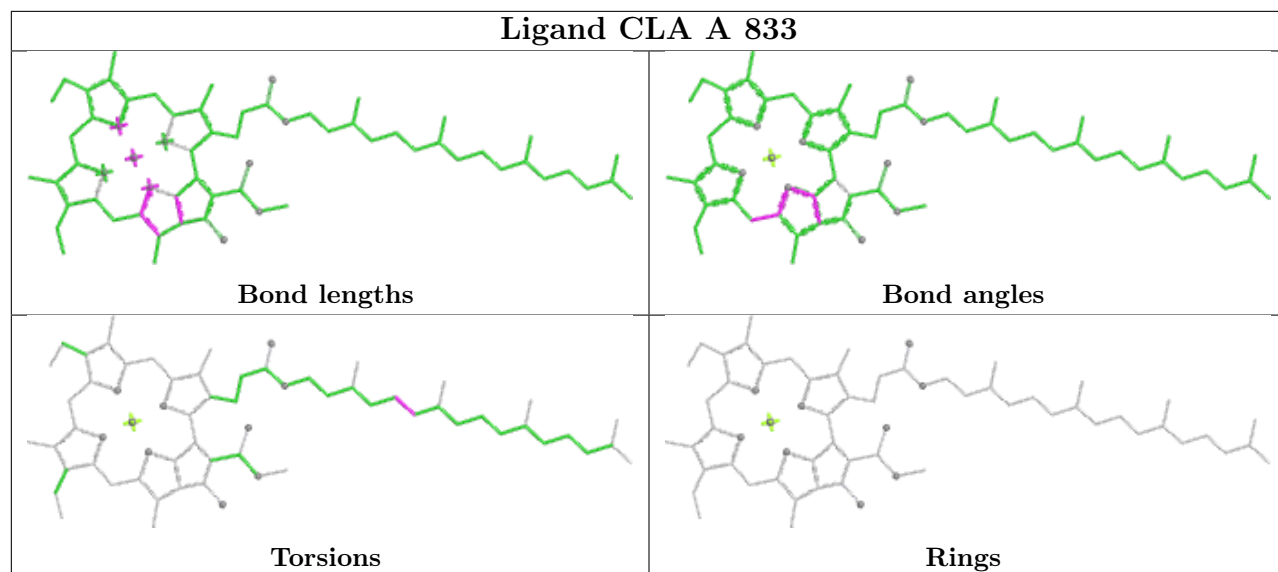


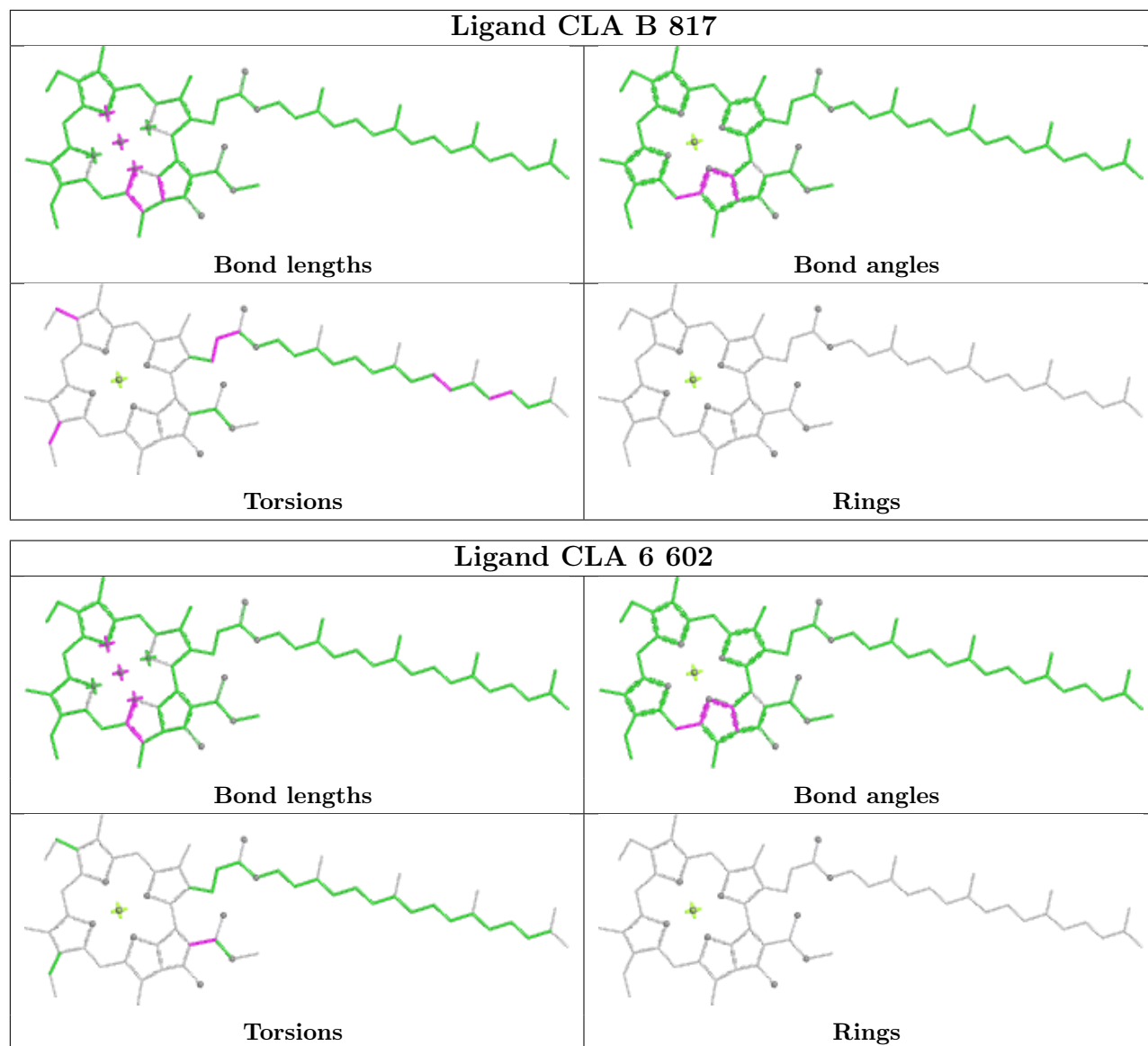
Ligand LMU Z 622



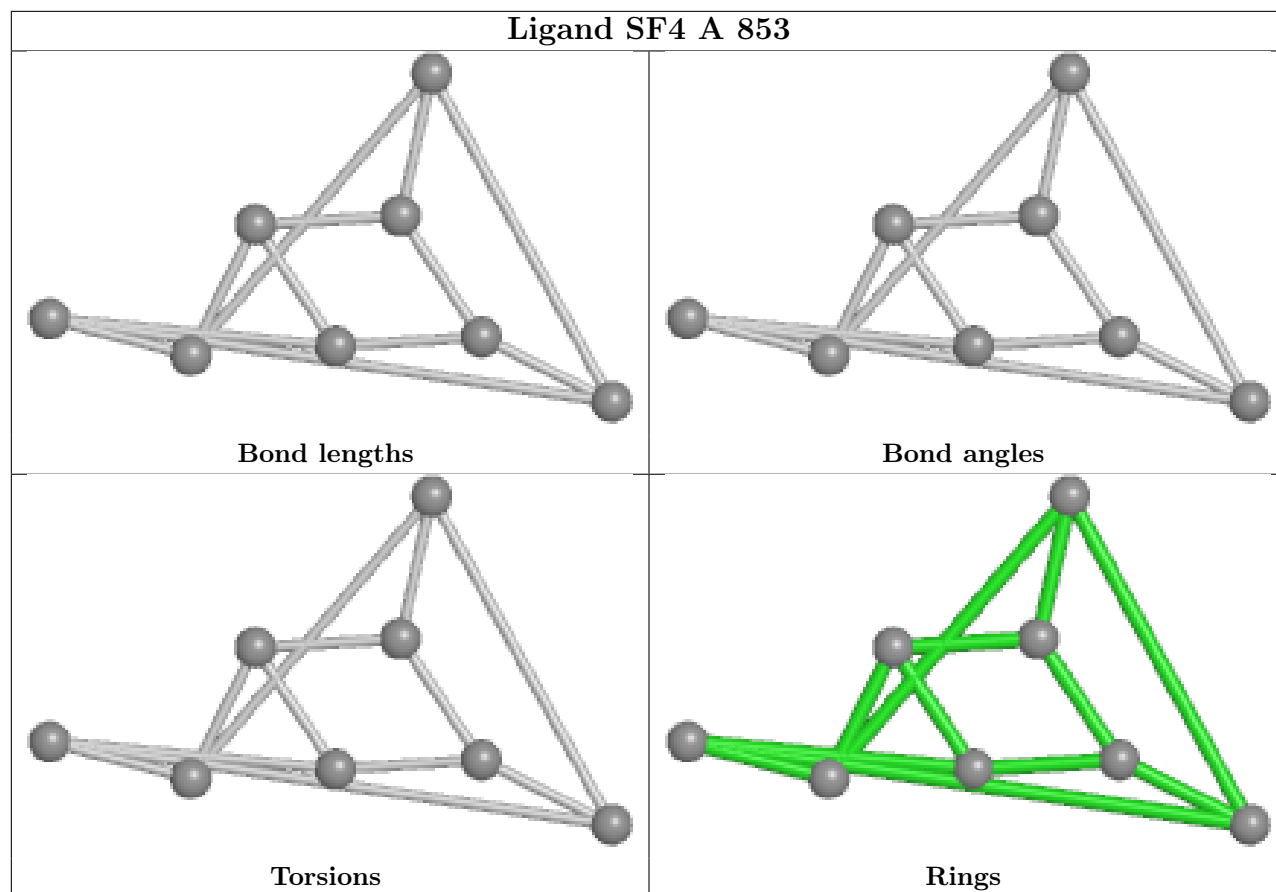




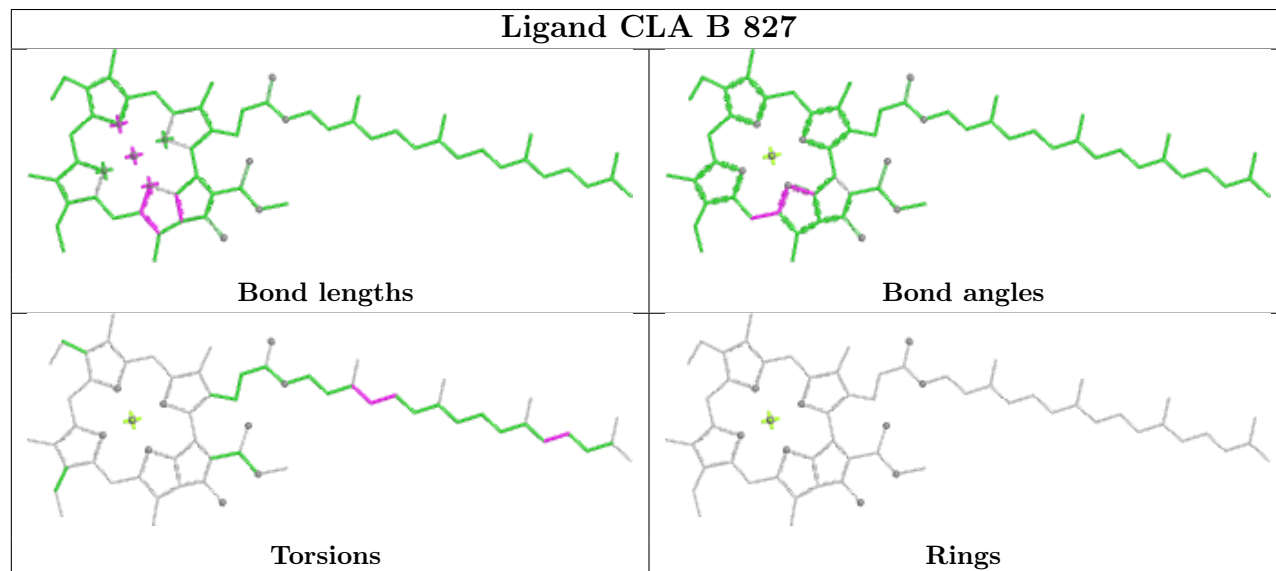


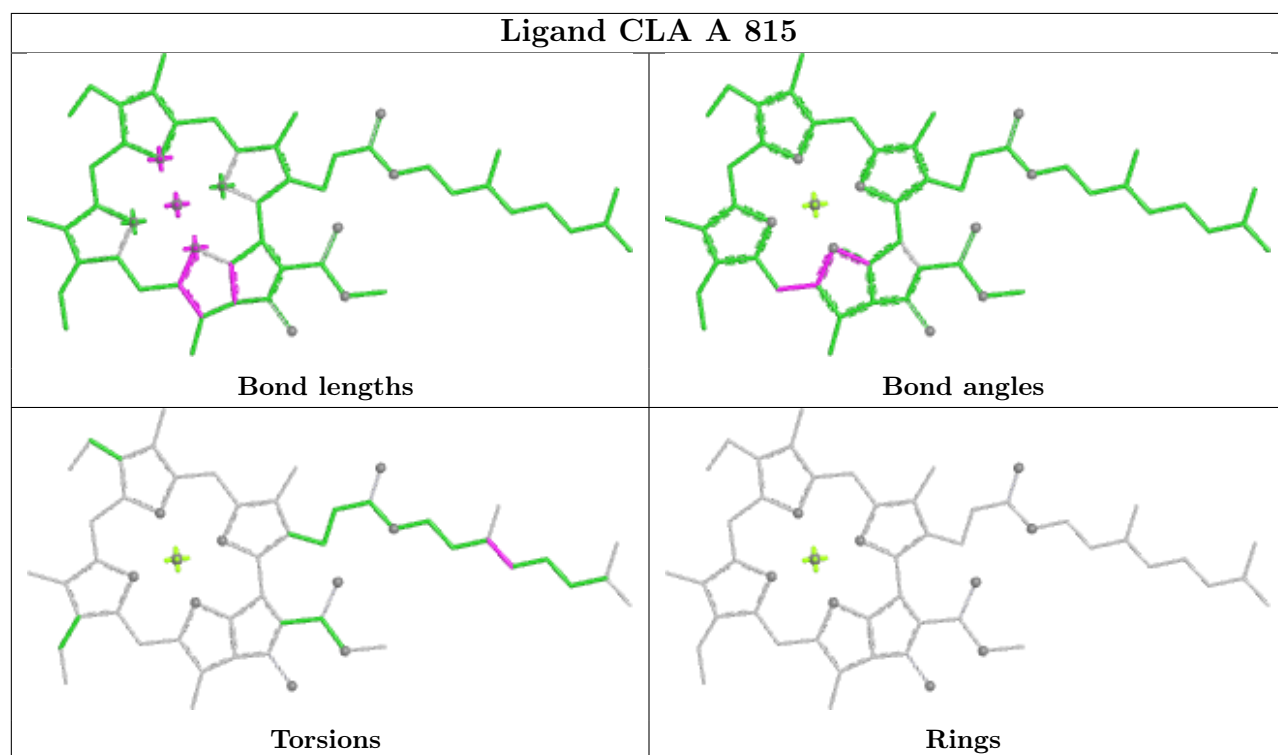
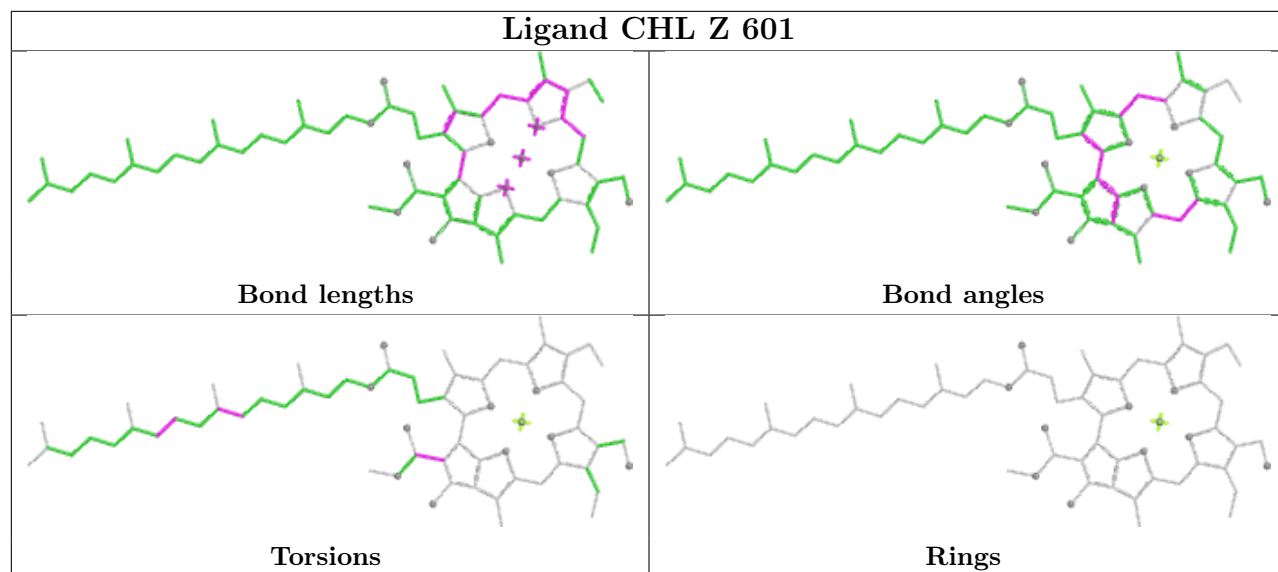


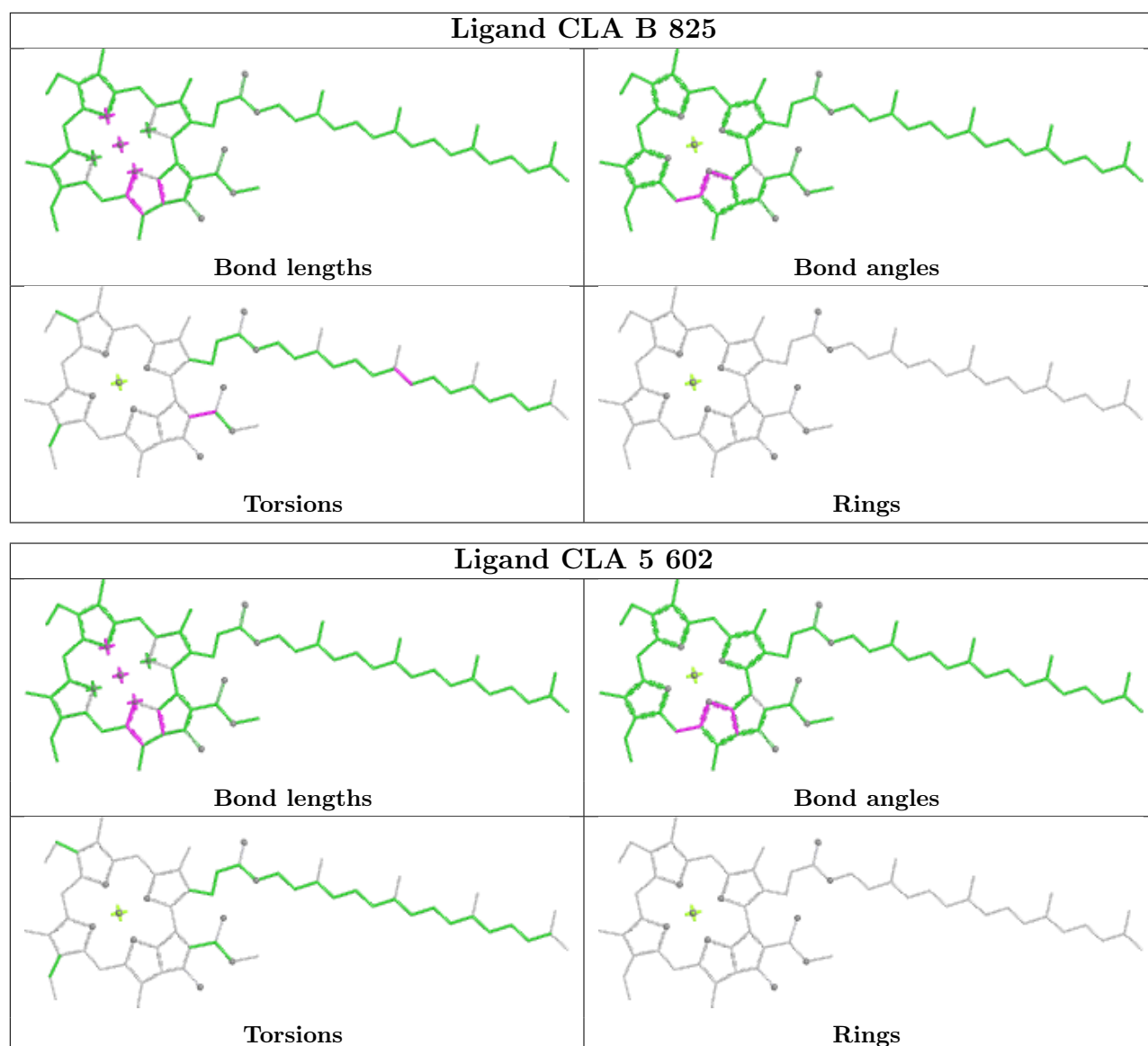
Ligand SF4 A 853



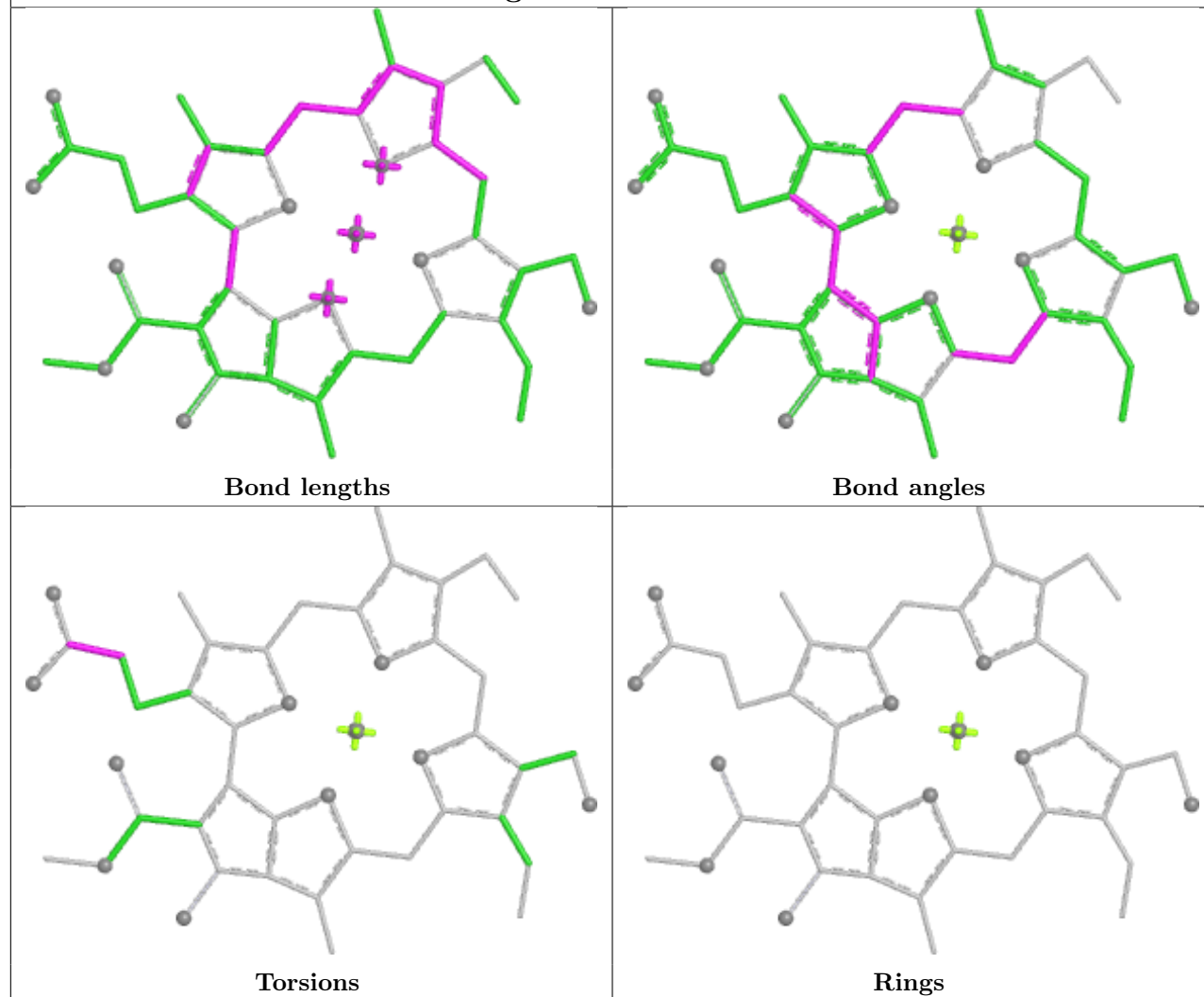
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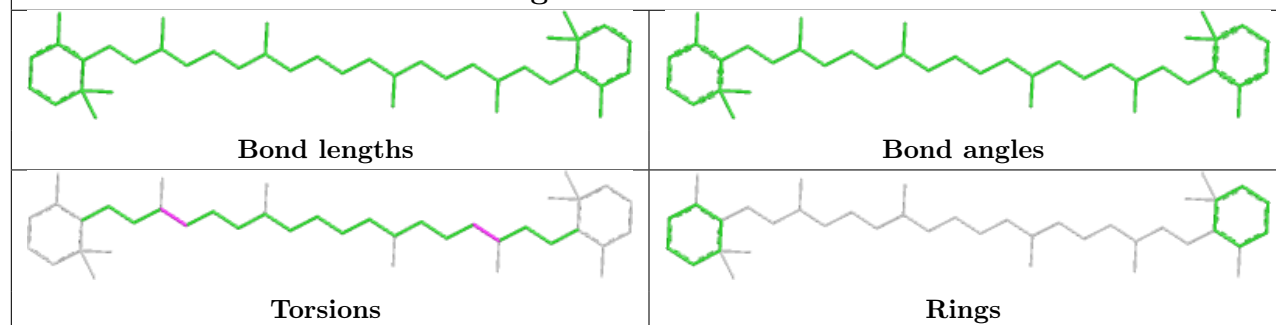


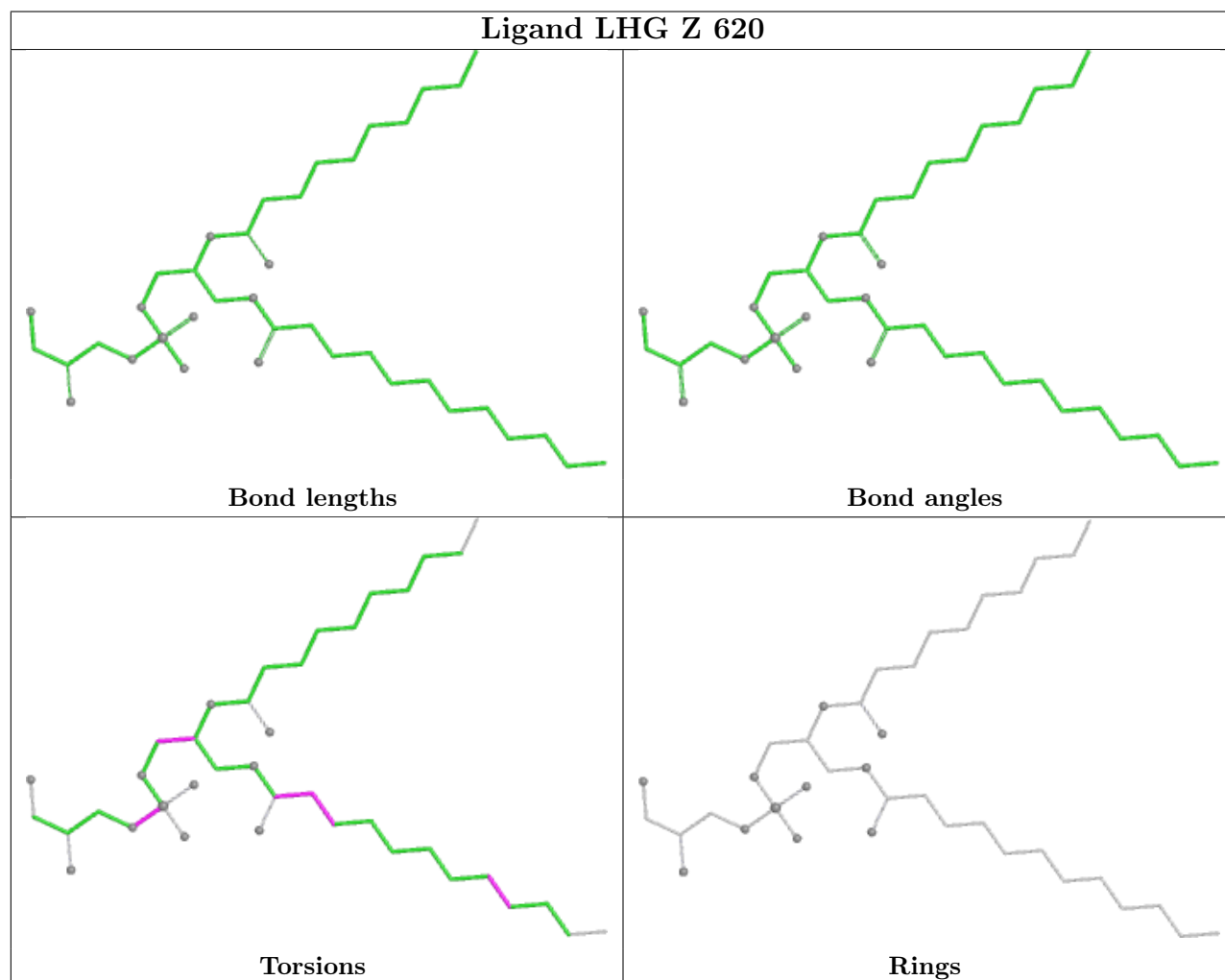
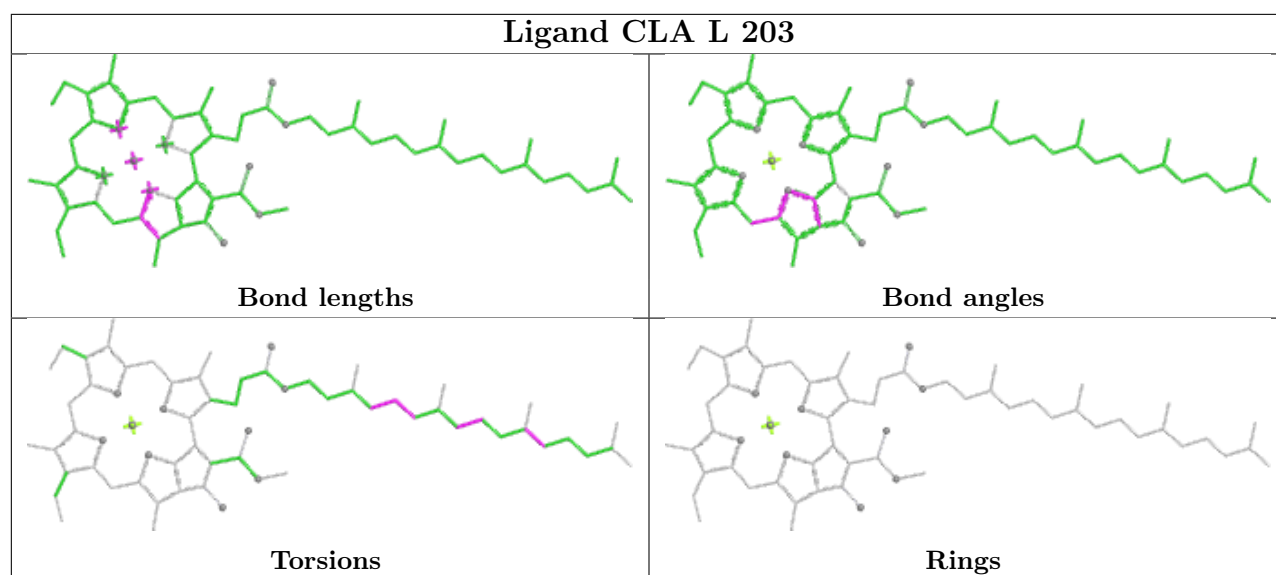


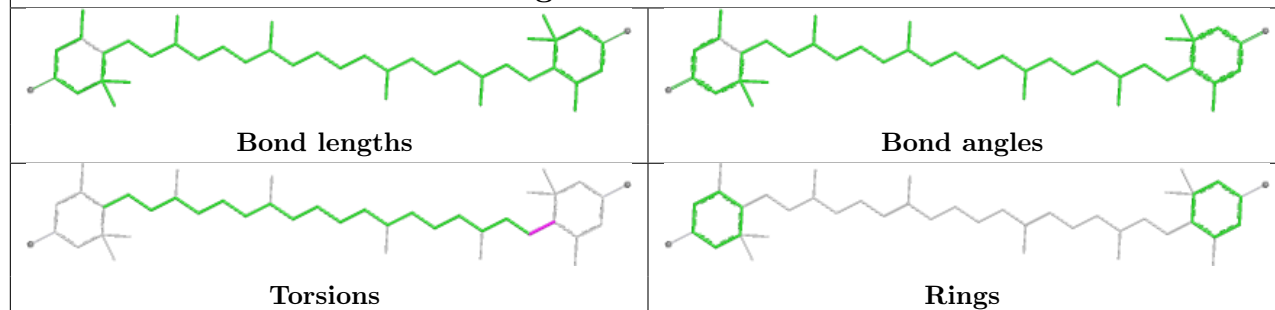
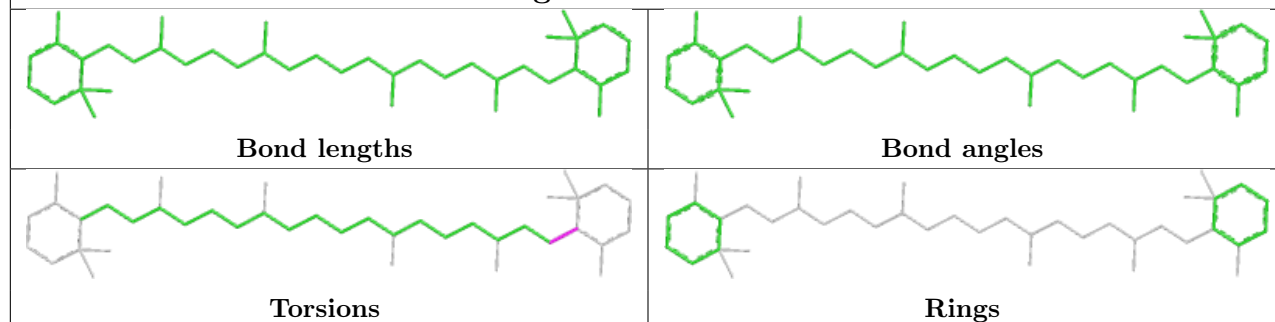
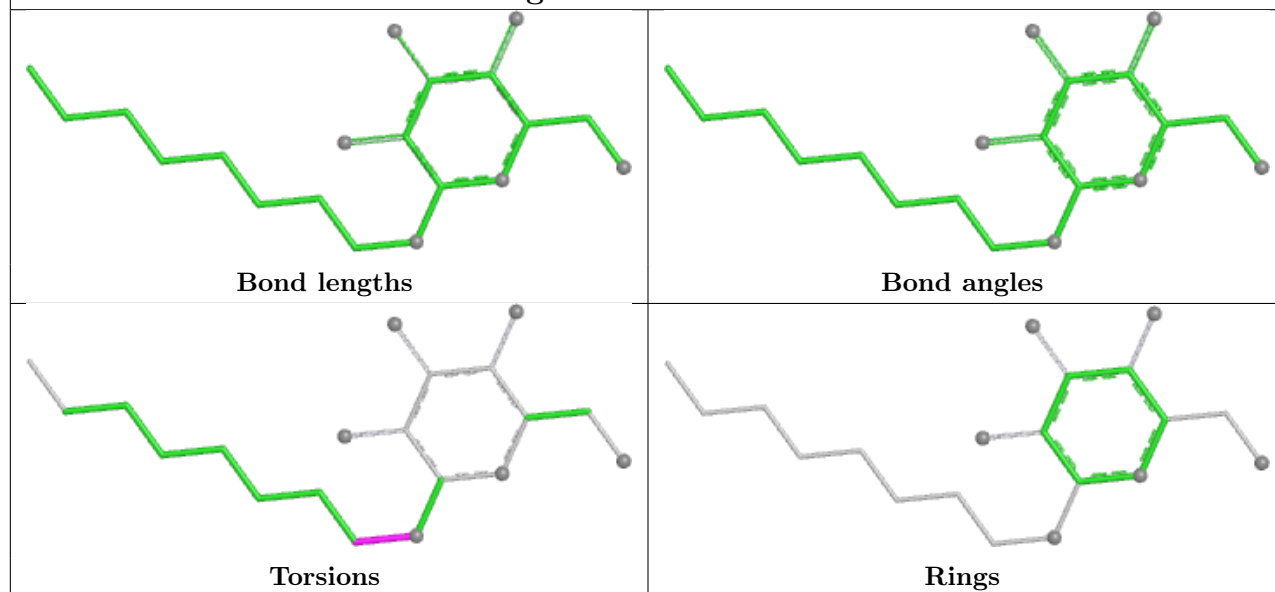
Ligand CHL 4 618

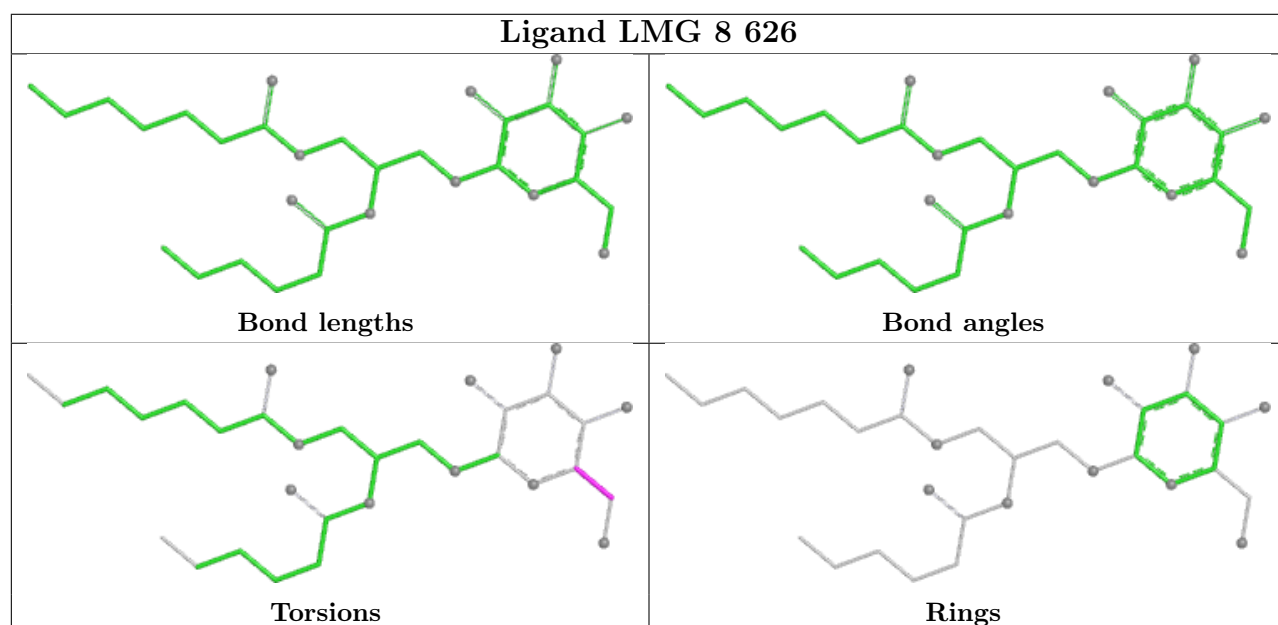
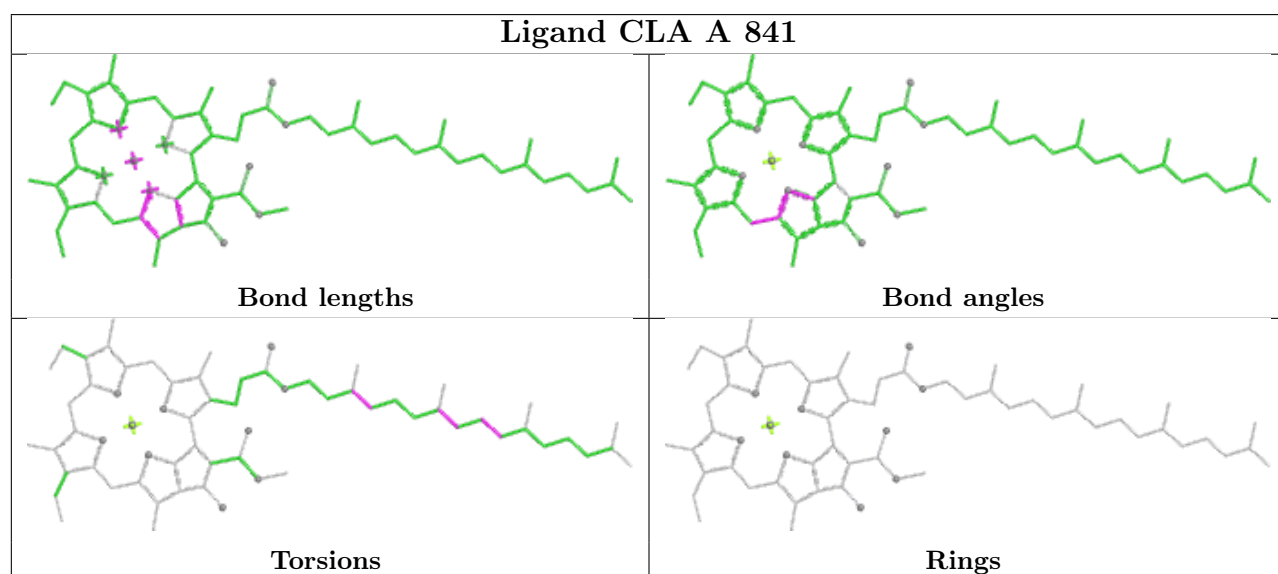
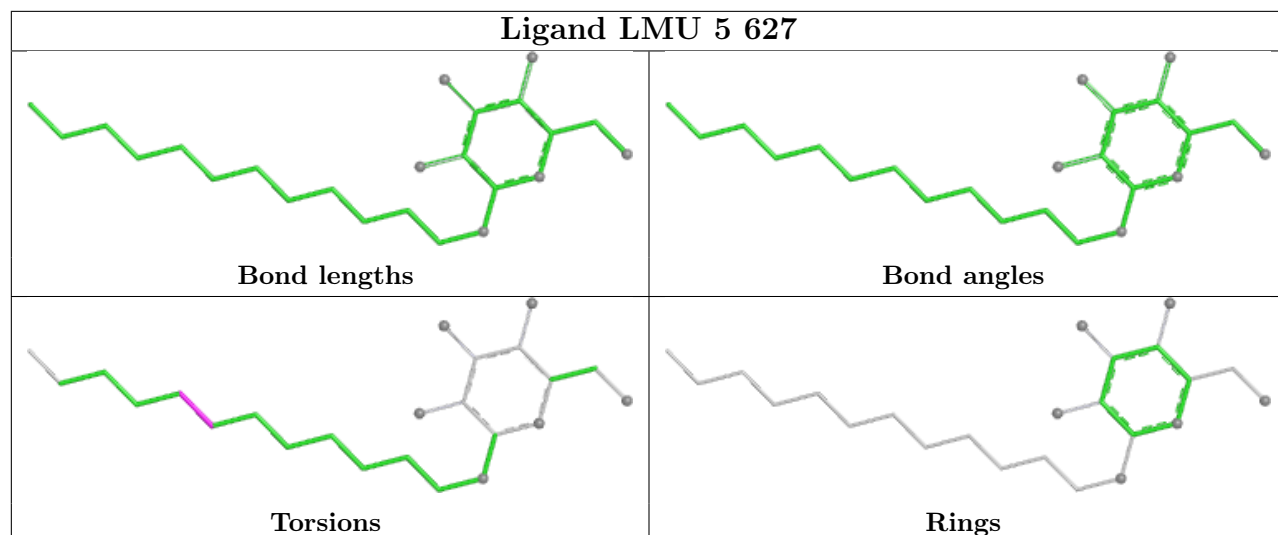


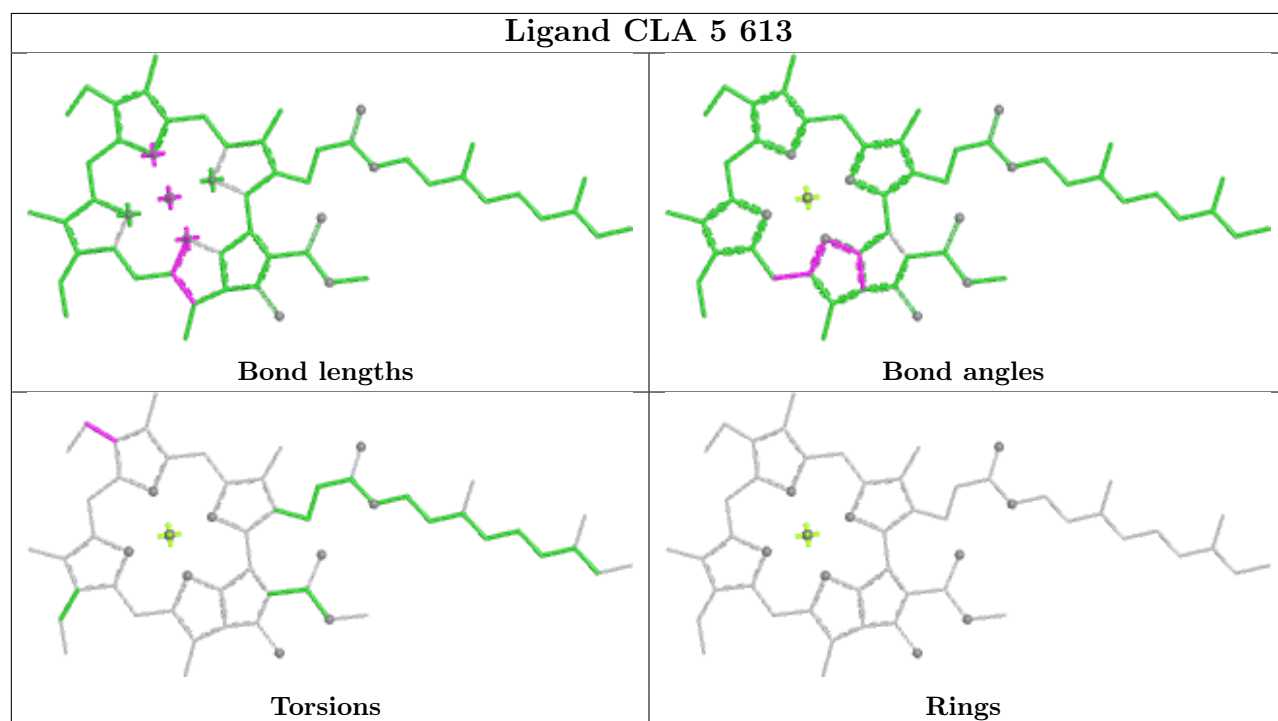
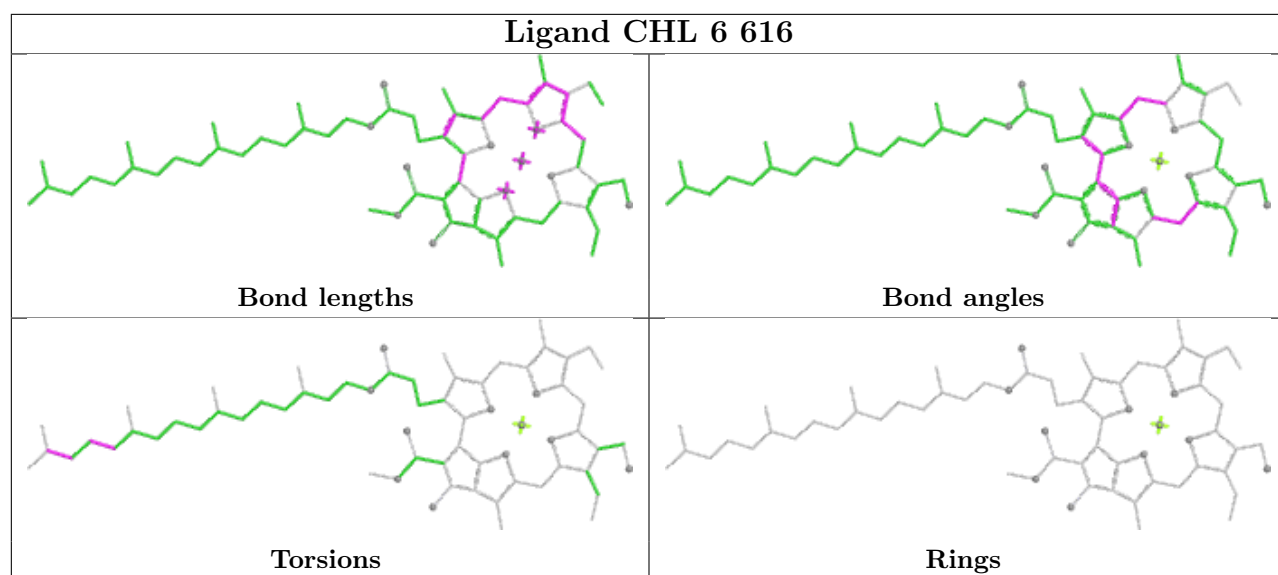
Ligand BCR B 845

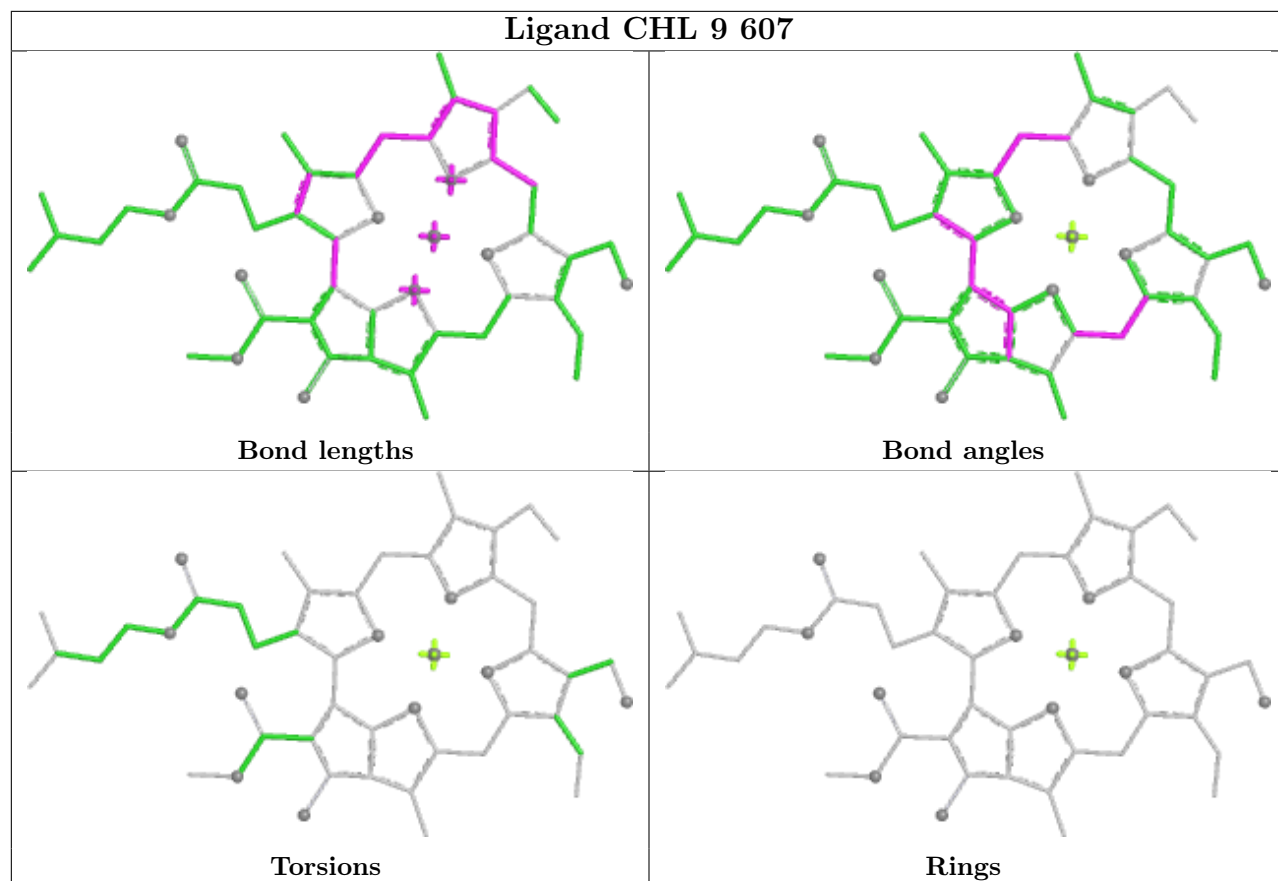




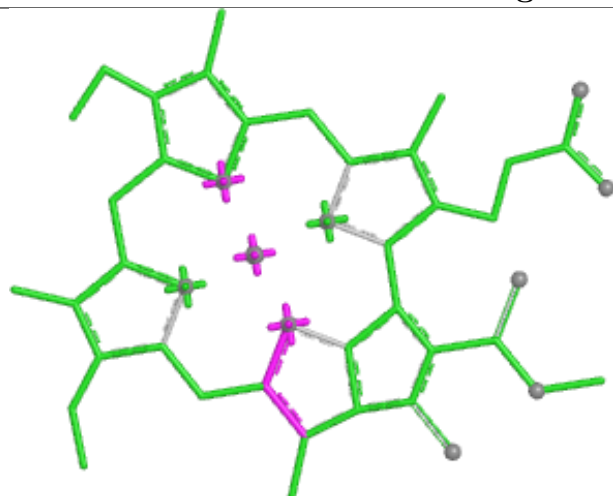
Ligand LUT 1 619**Ligand BCR 3 718****Ligand LMU A 862**



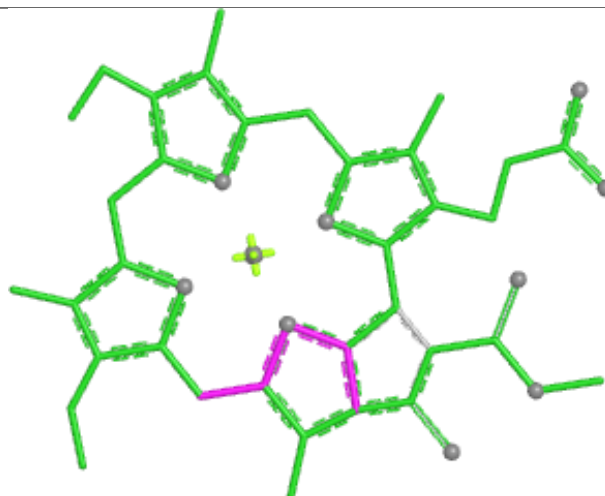




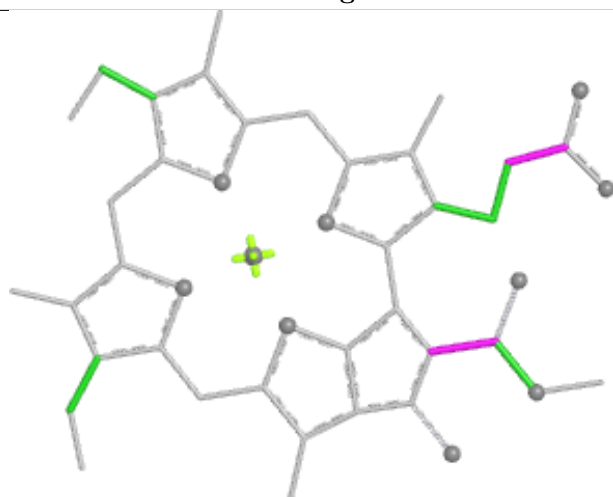
Ligand CLA Z 612



Bond lengths



Bond angles

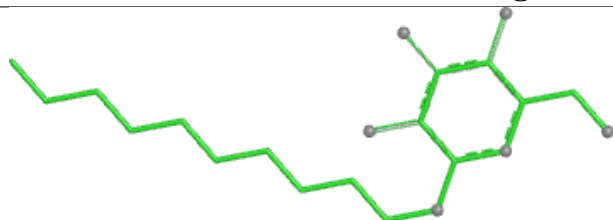


Torsions

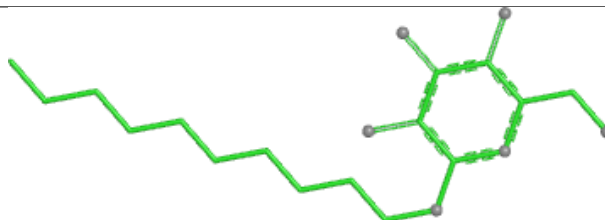


Rings

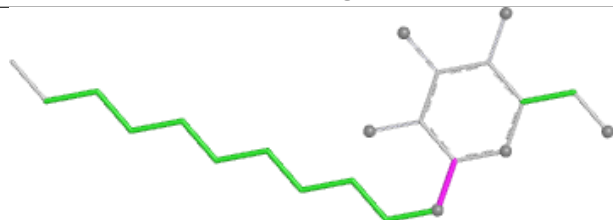
Ligand LMU Z 621



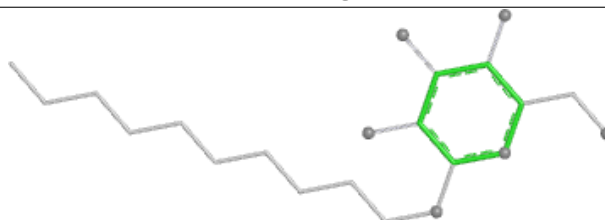
Bond lengths



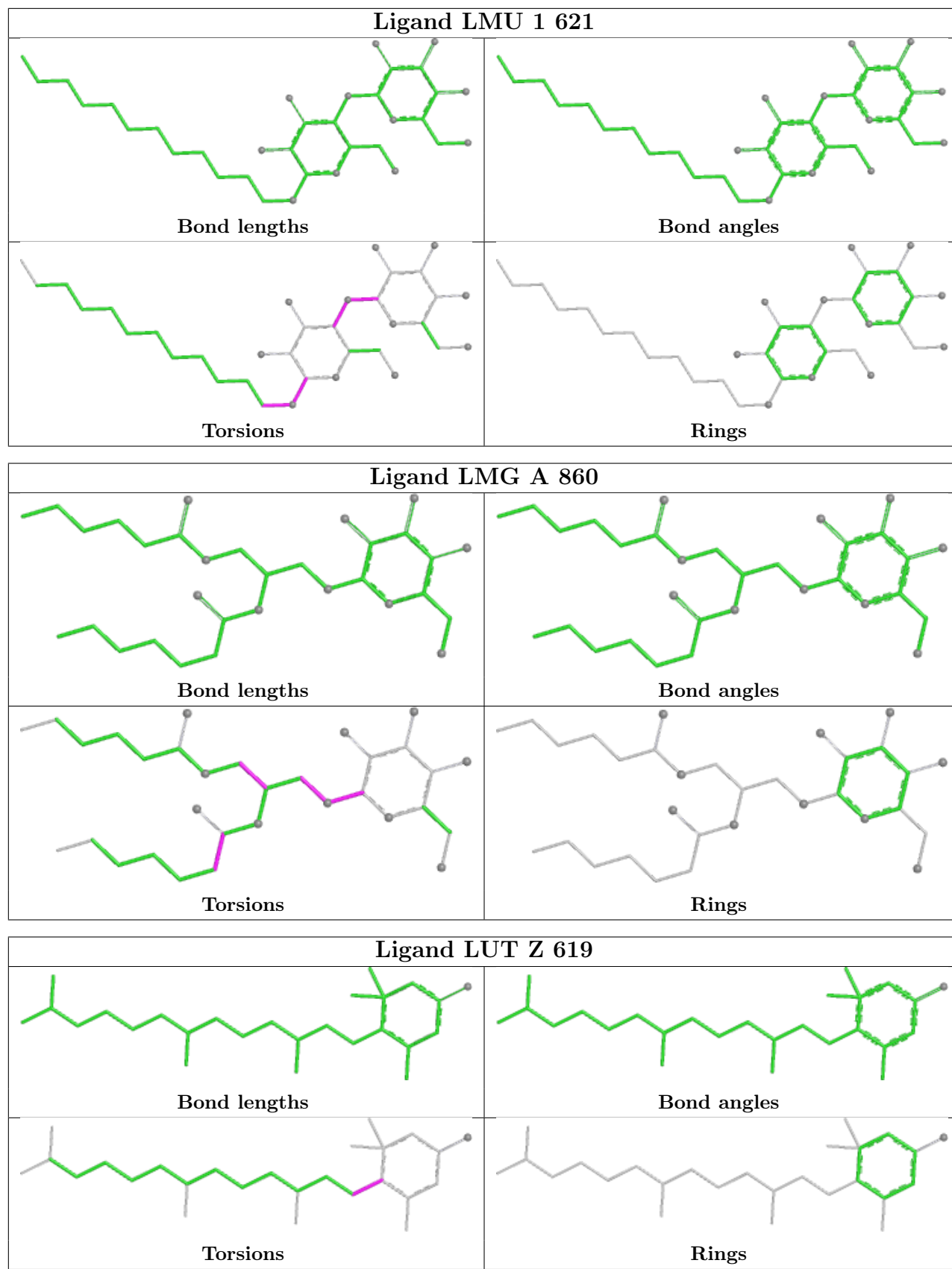
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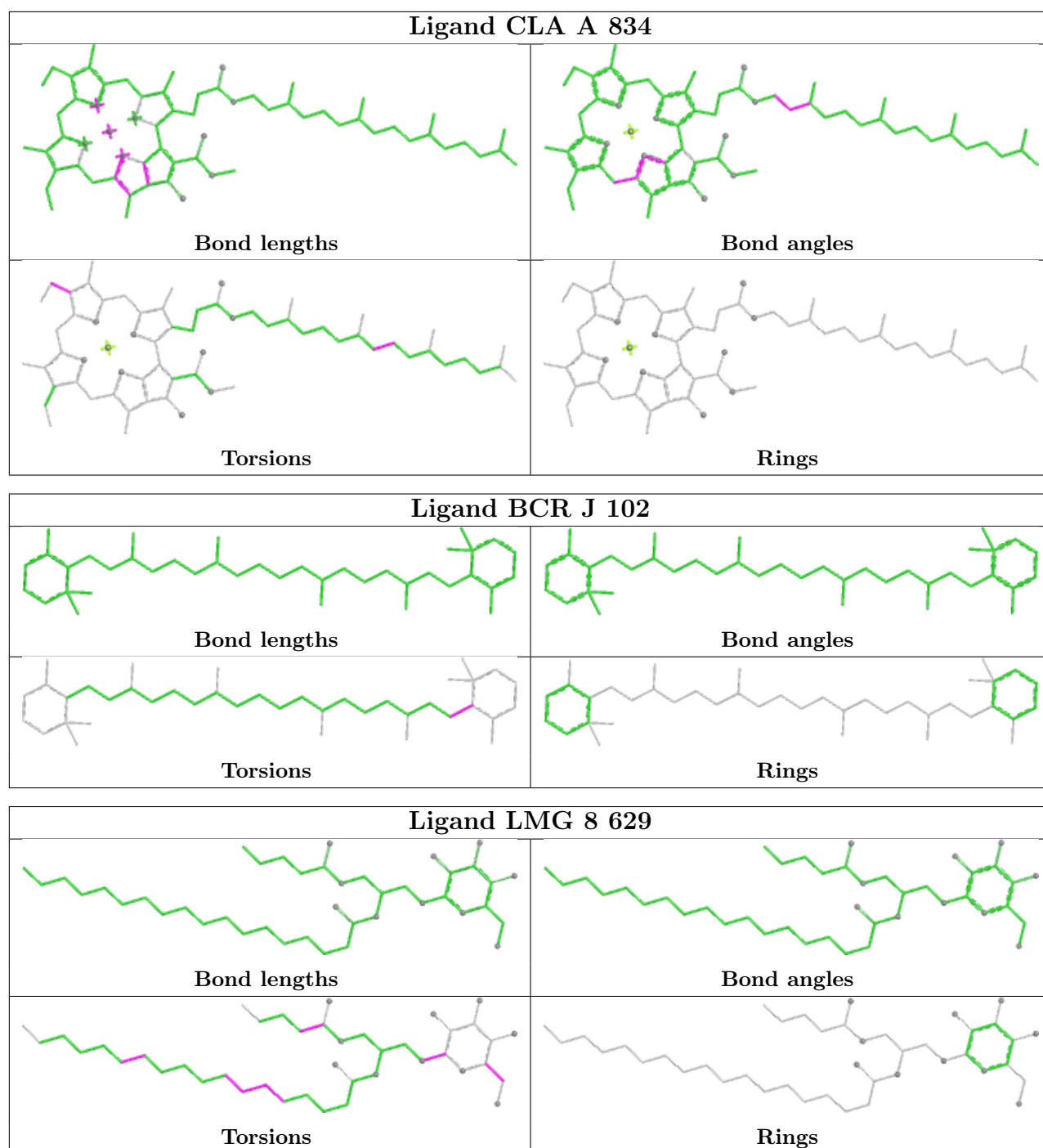


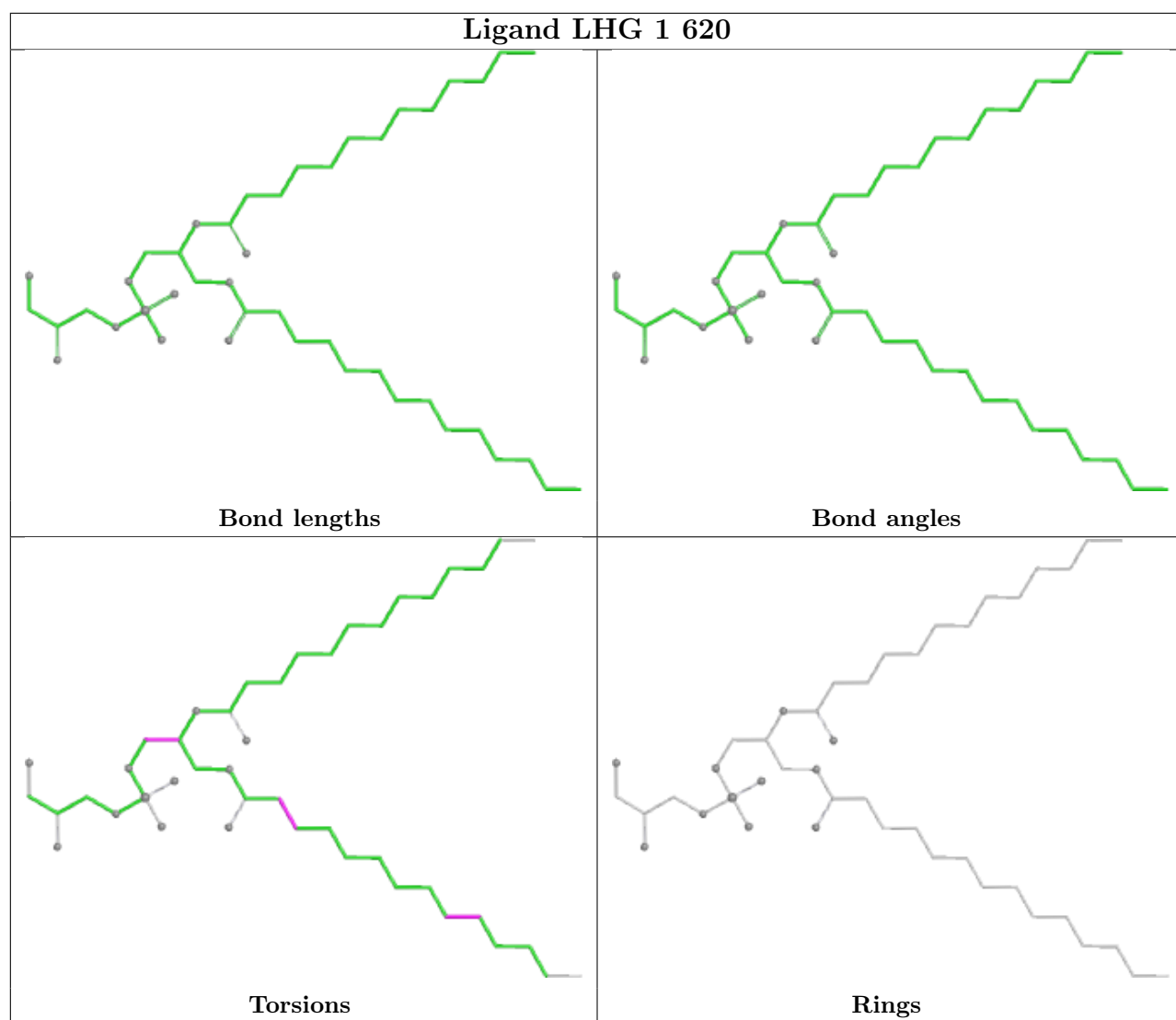
Torsions

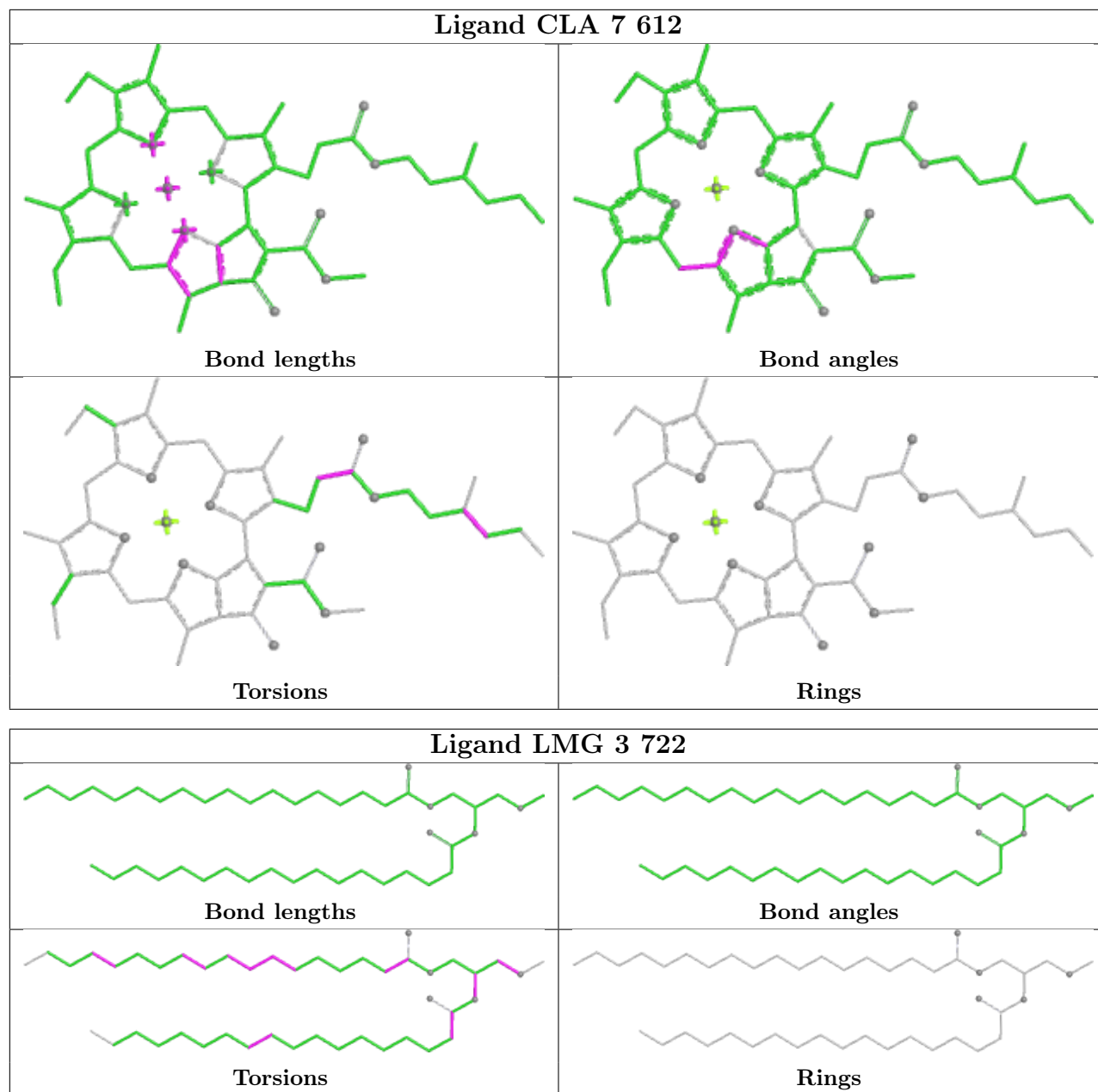


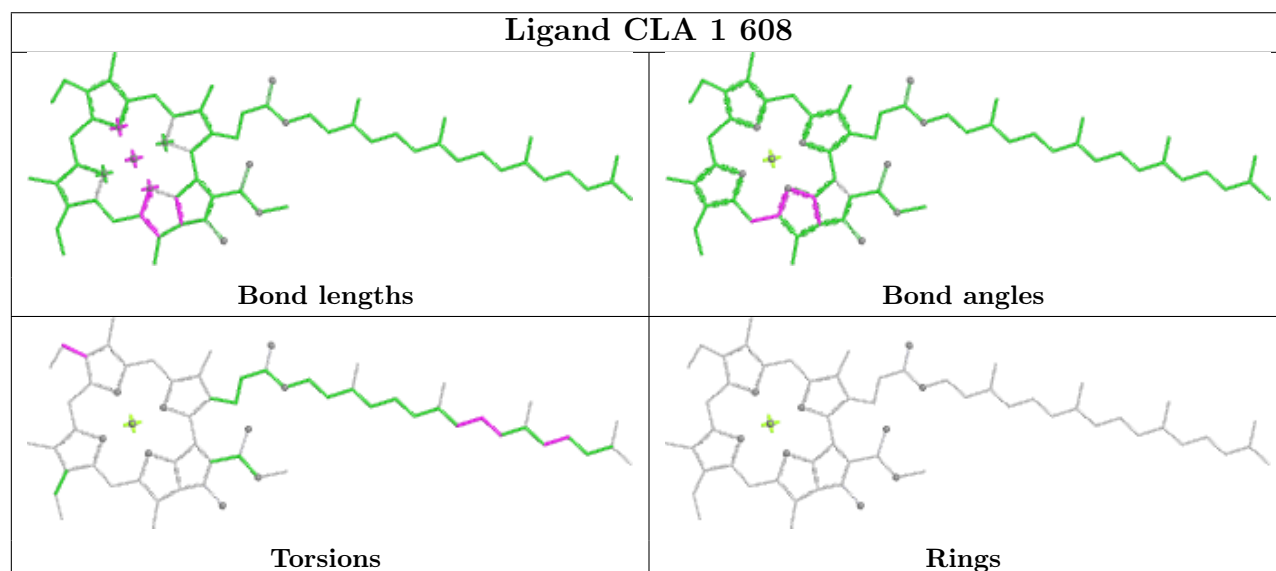
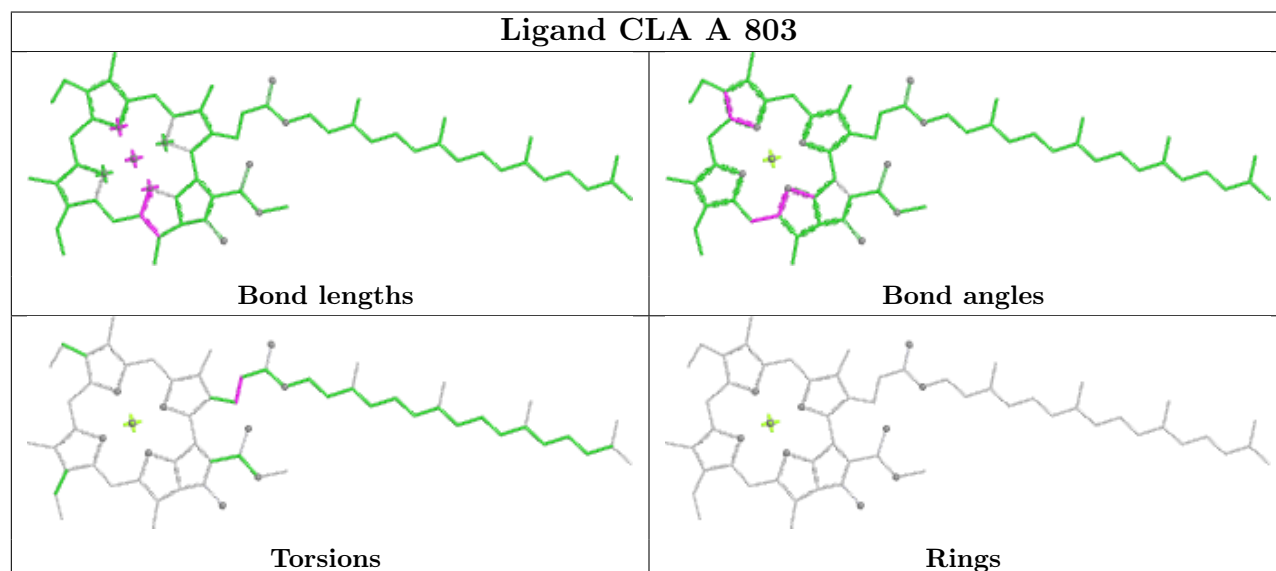
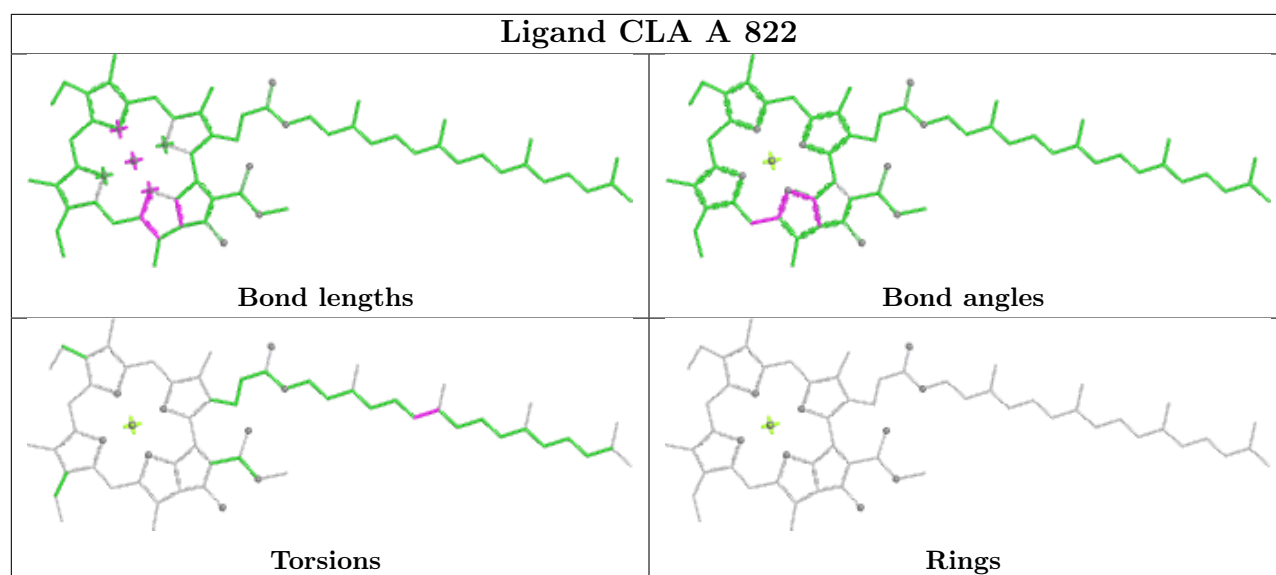
Rings



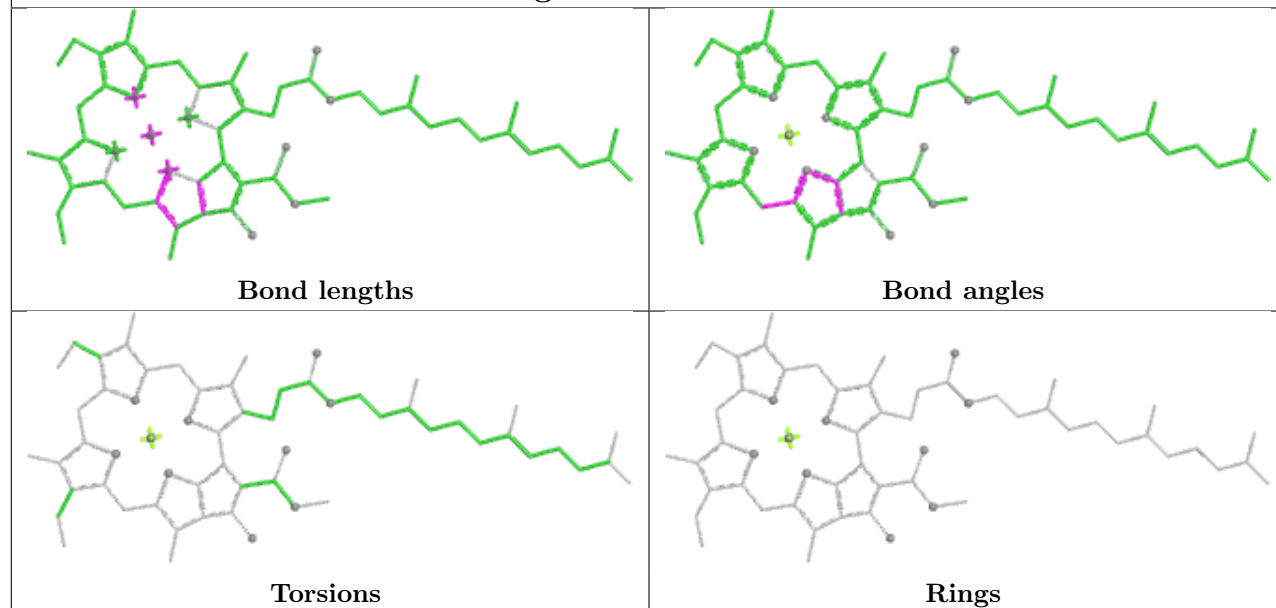




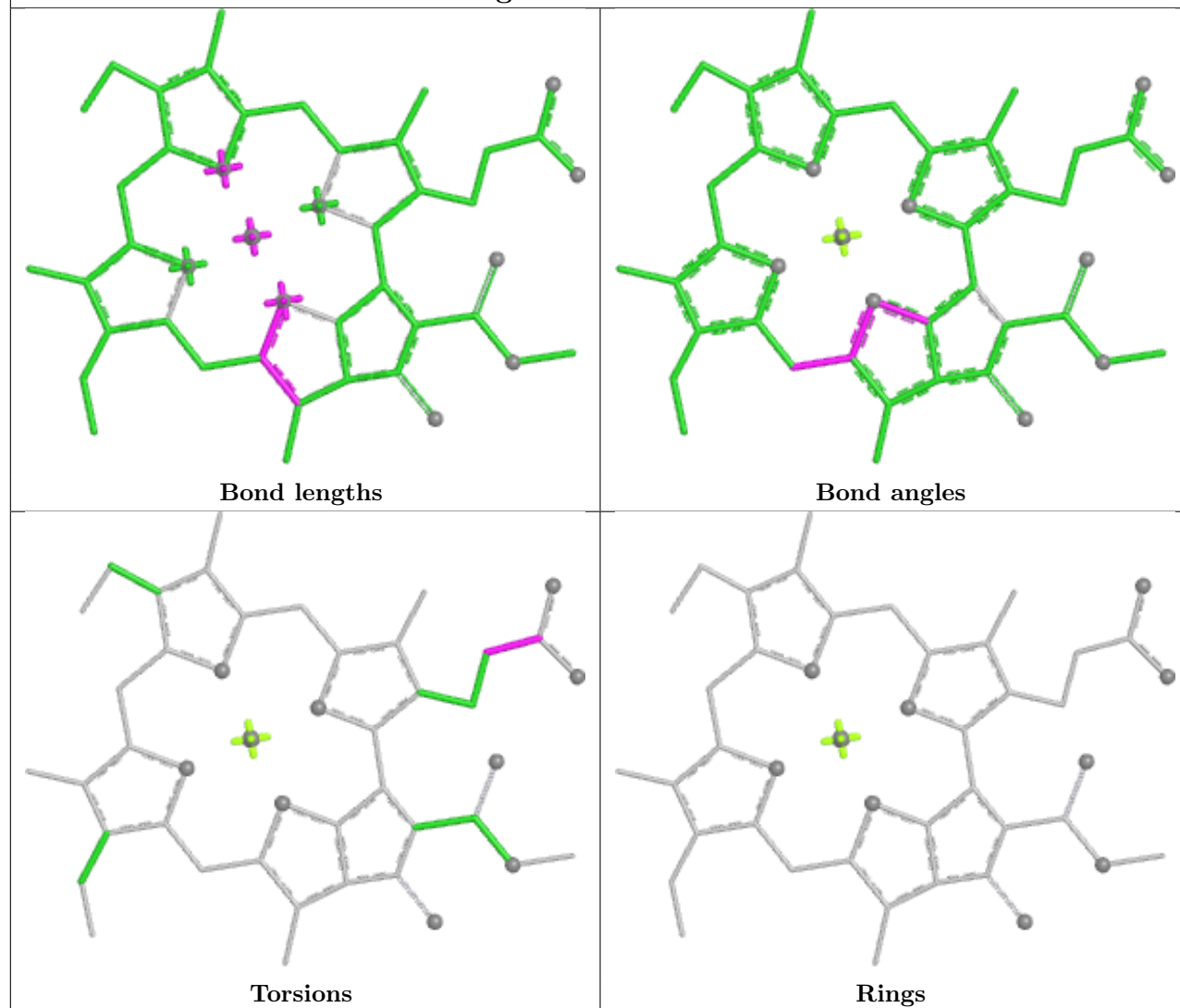


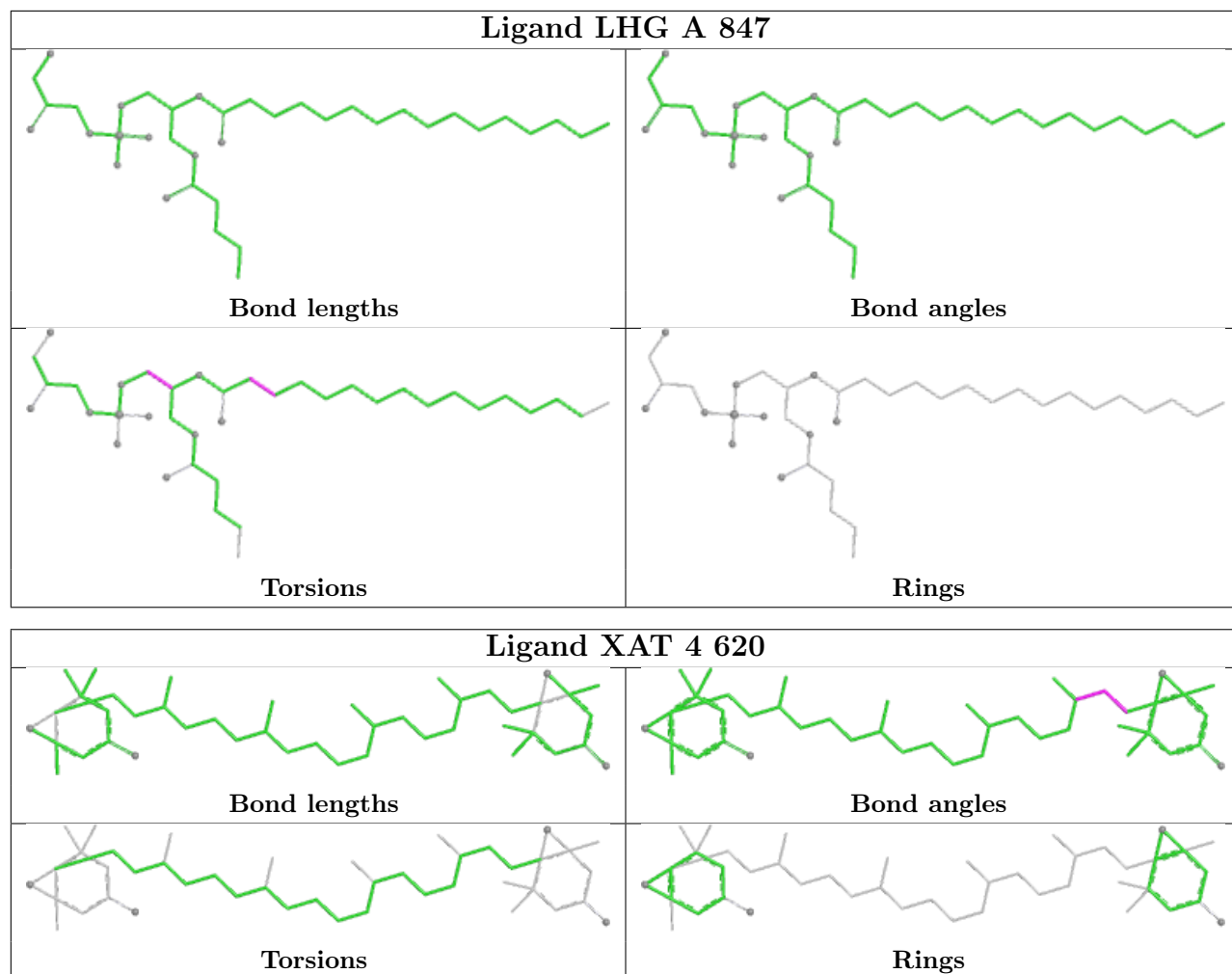


Ligand CLA Z 610

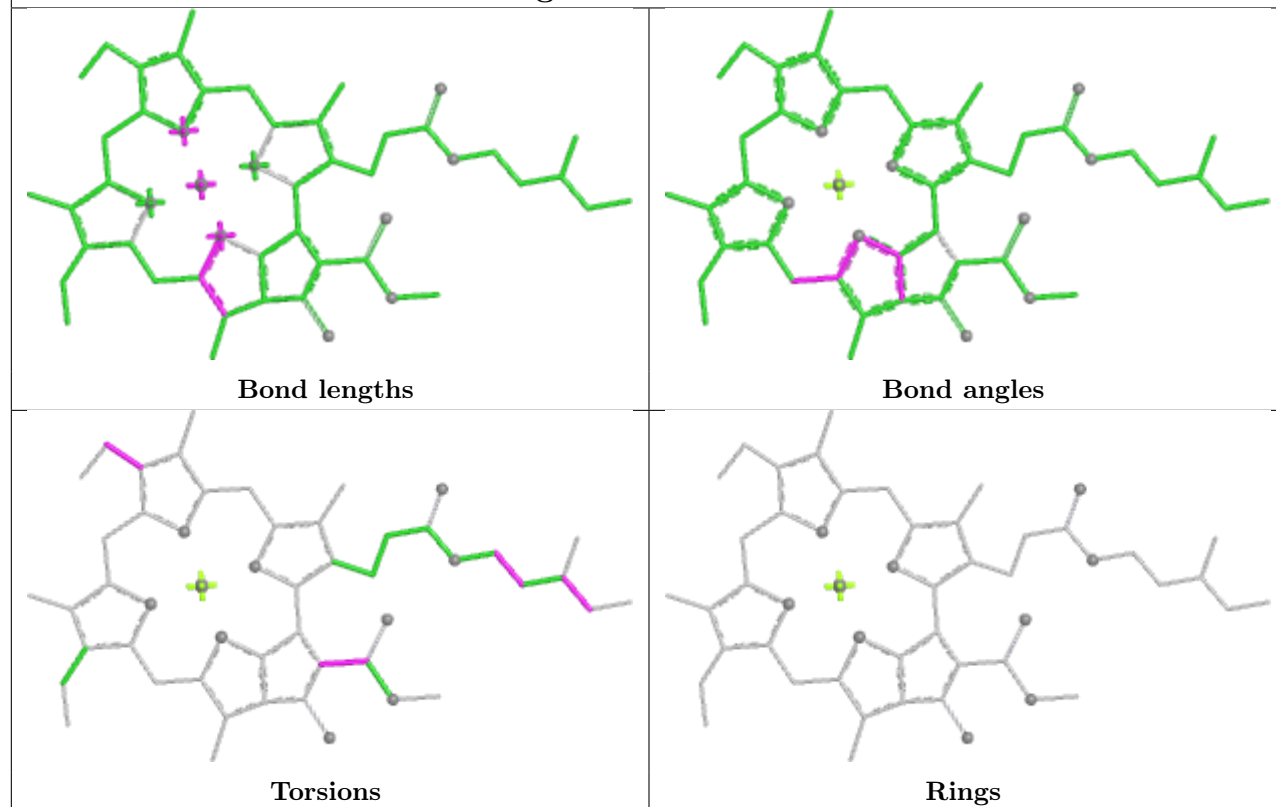


Ligand CLA 4 612

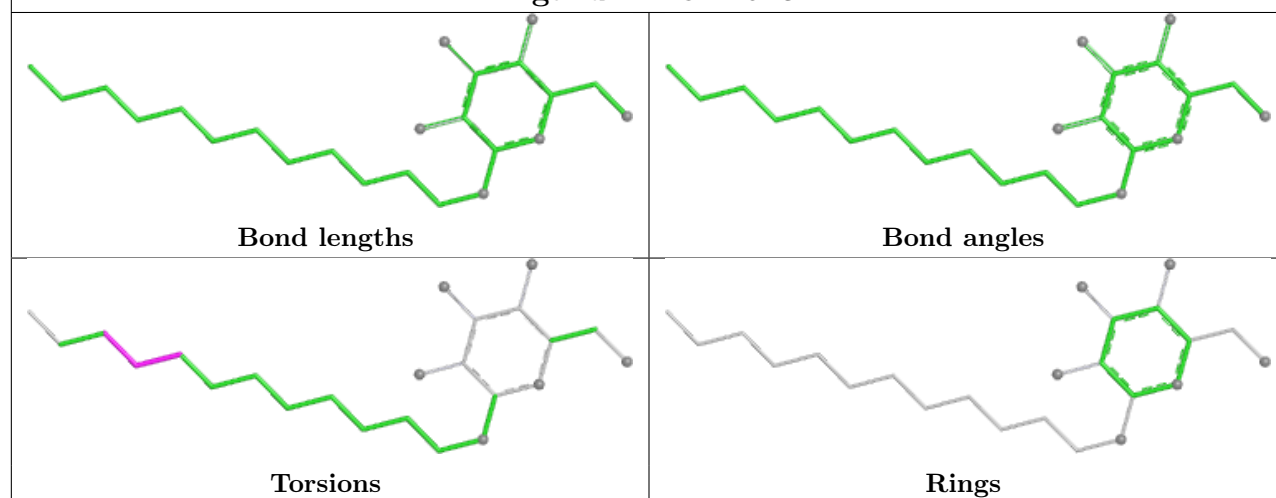


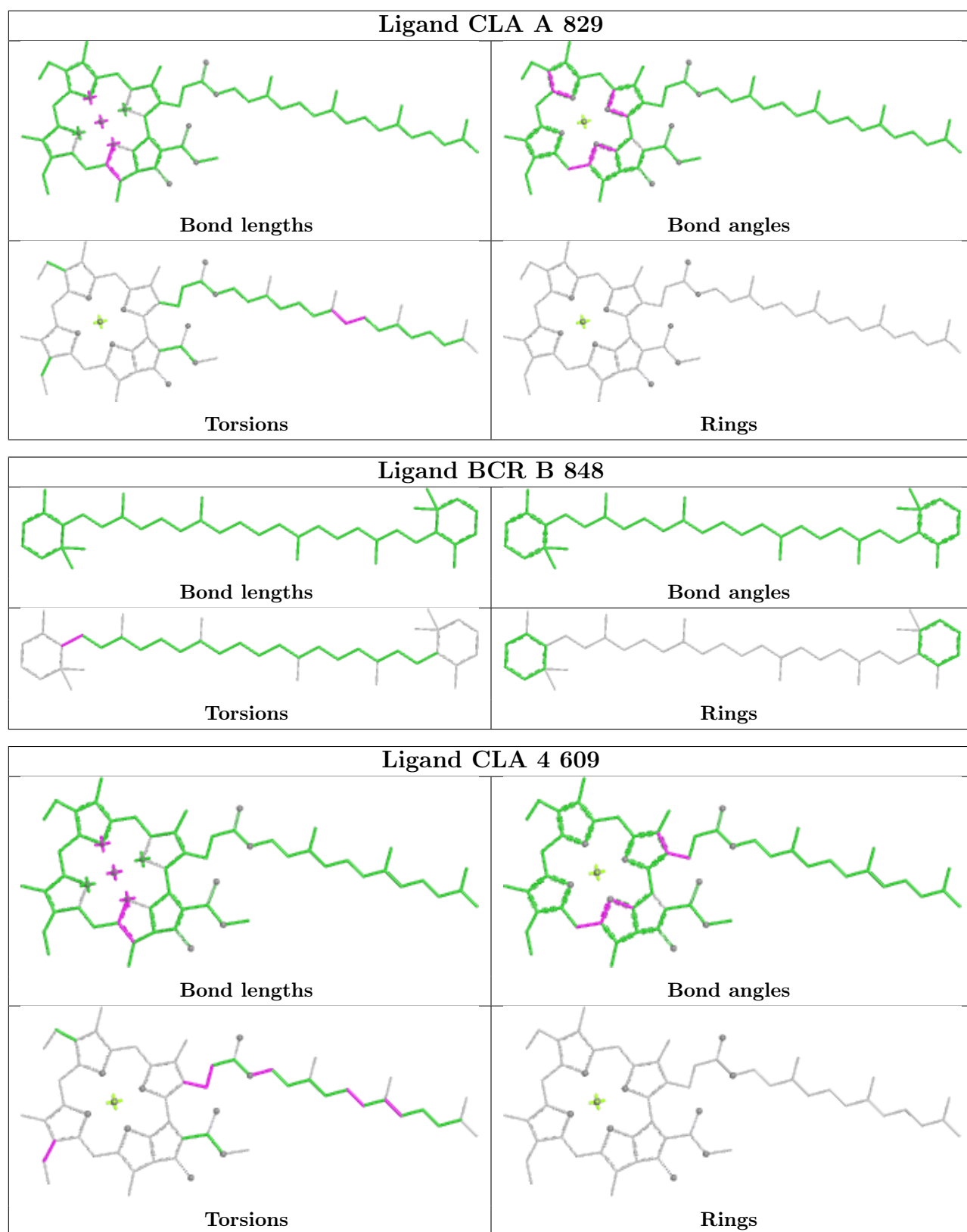


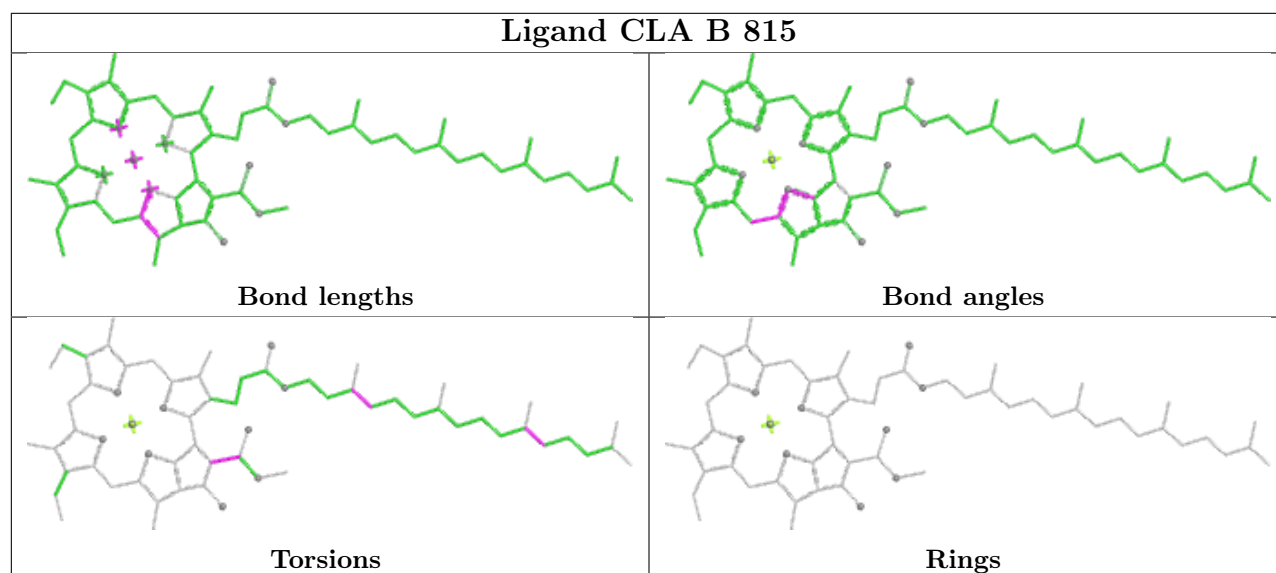
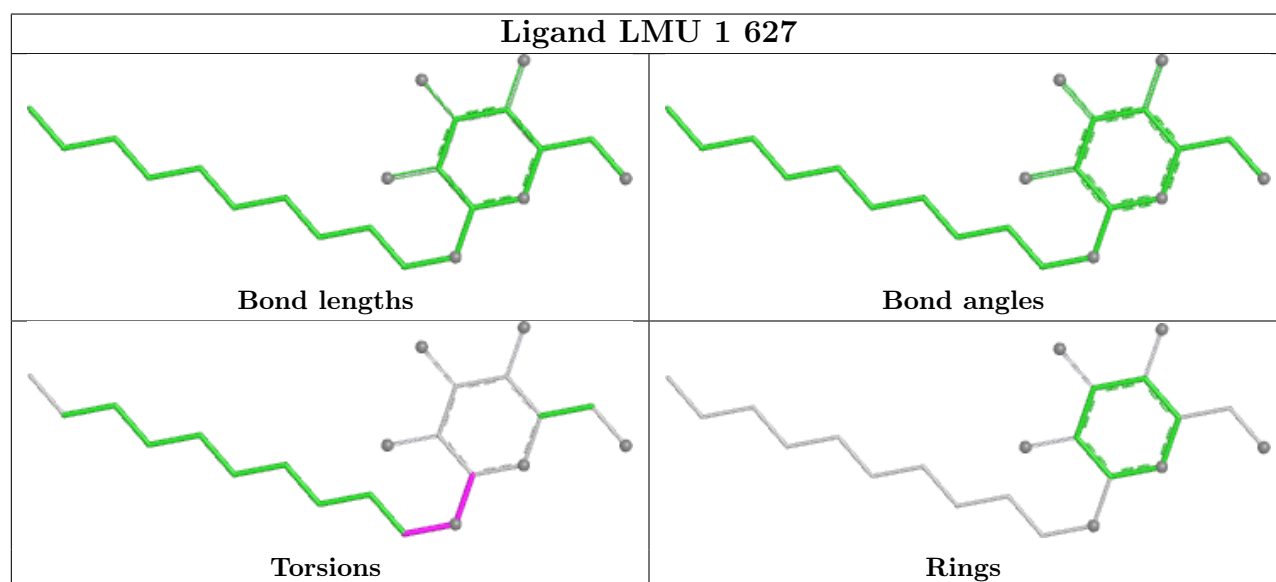
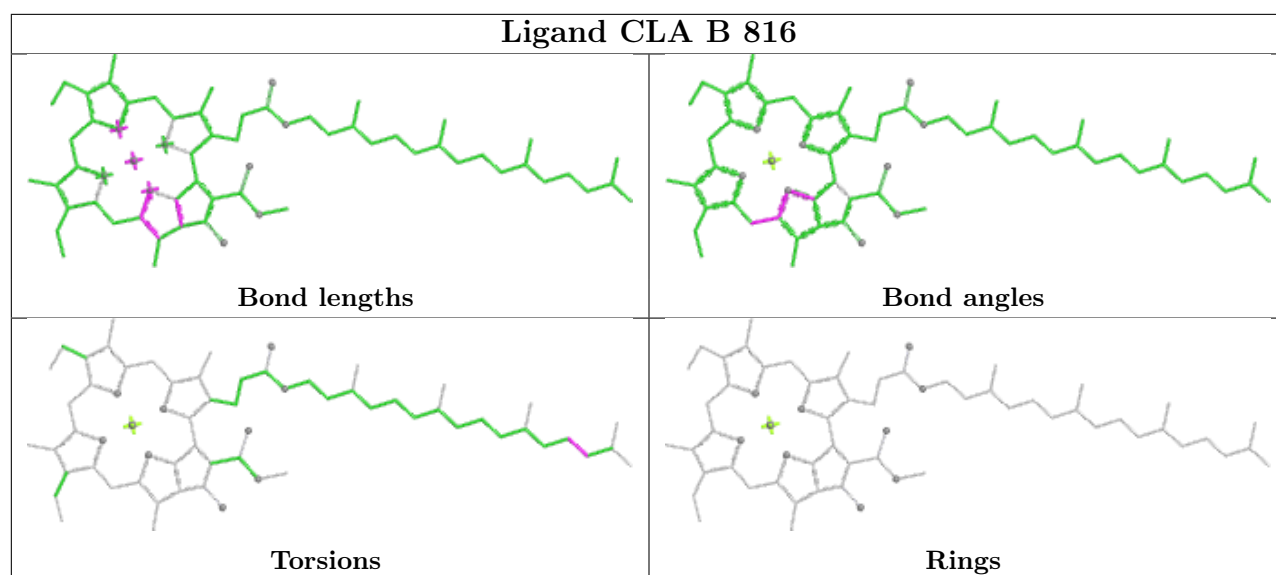
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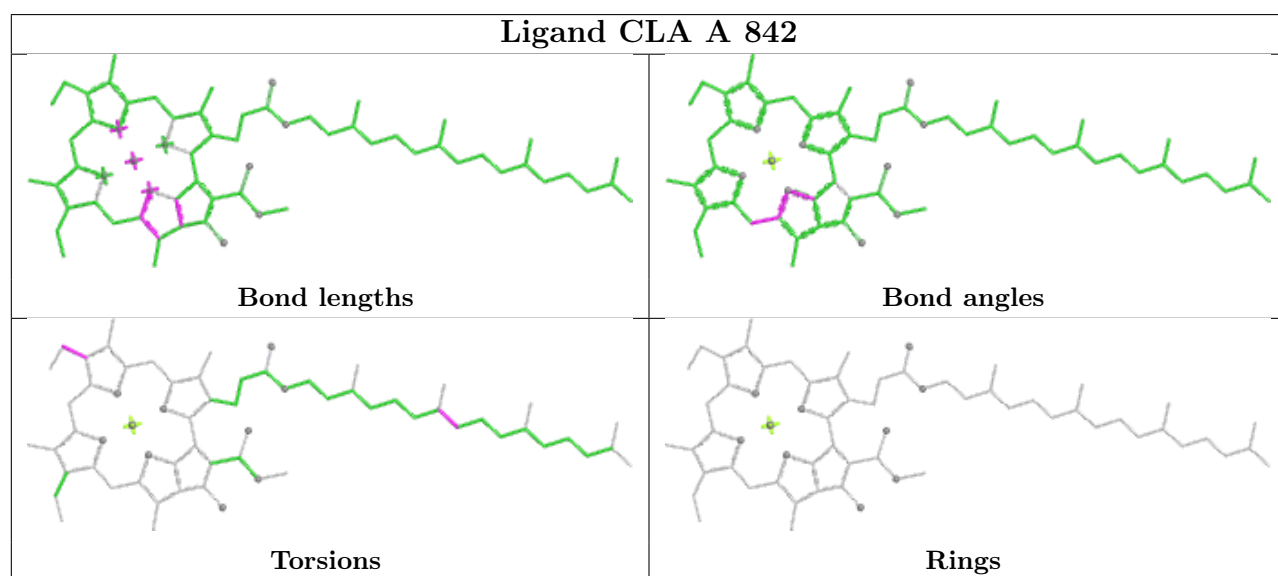
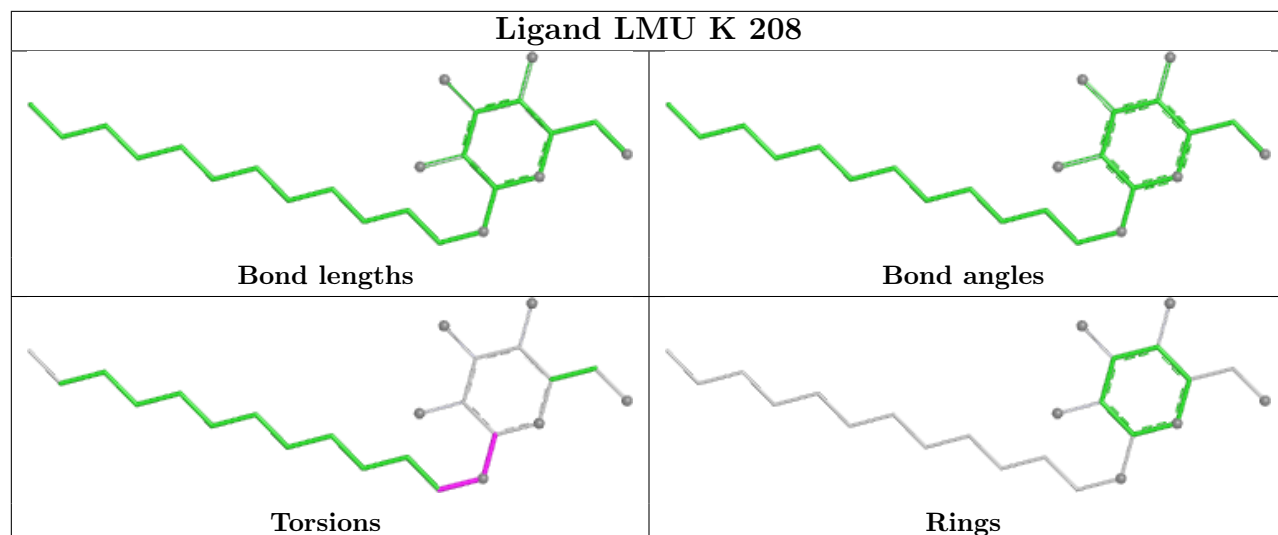


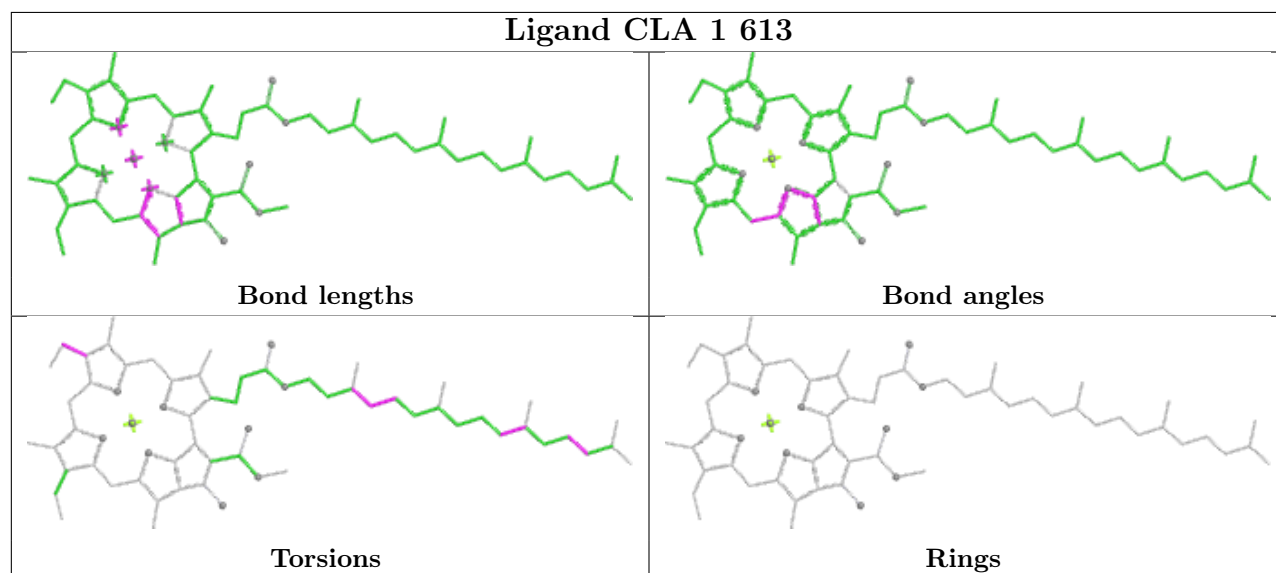
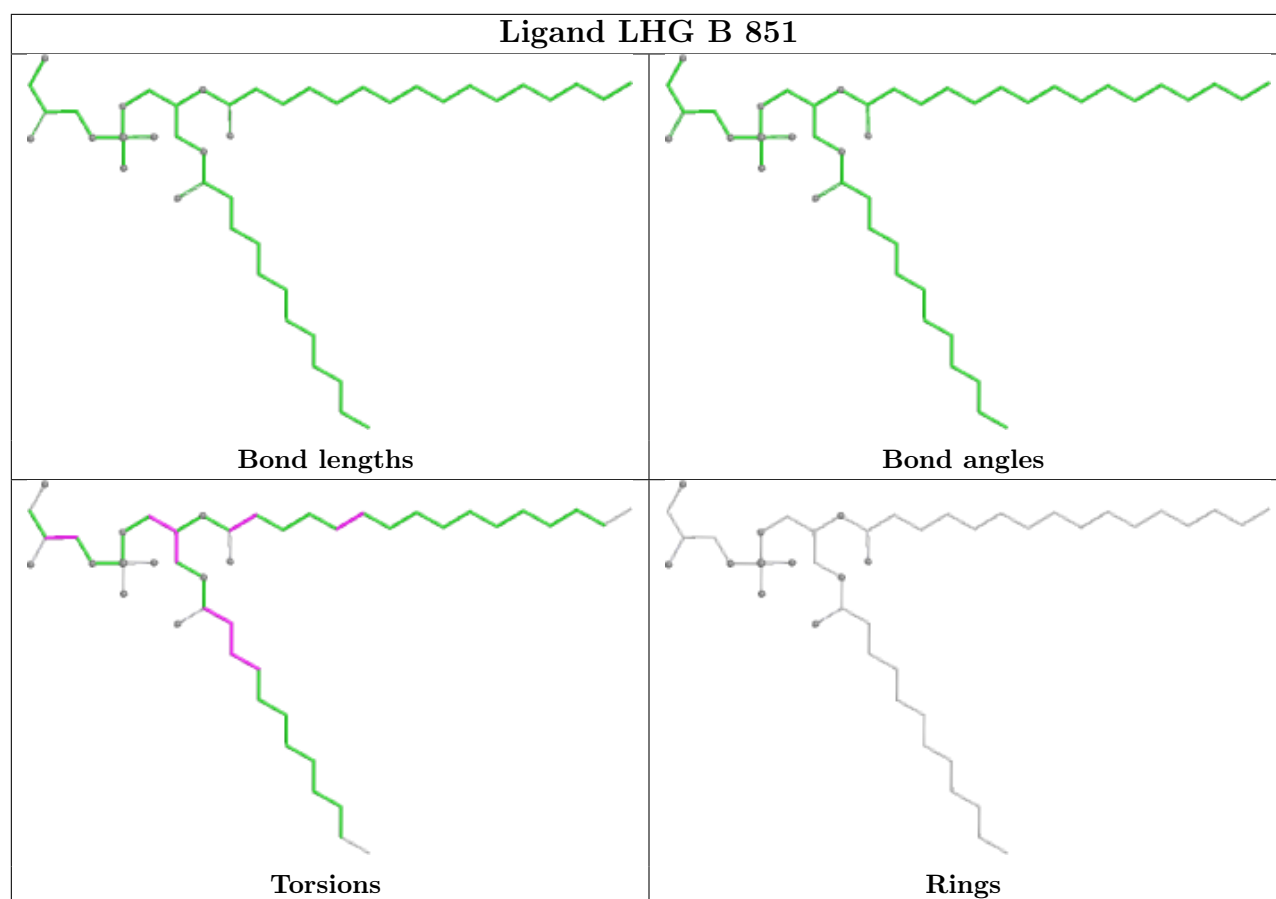
Ligand LMU 1 623

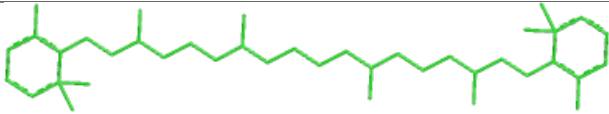
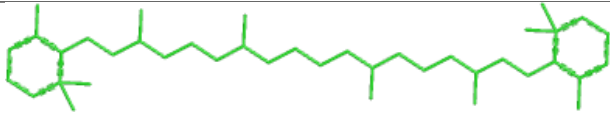
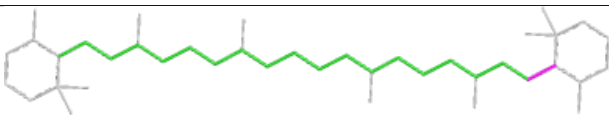
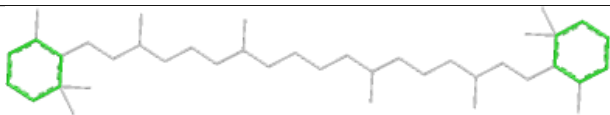


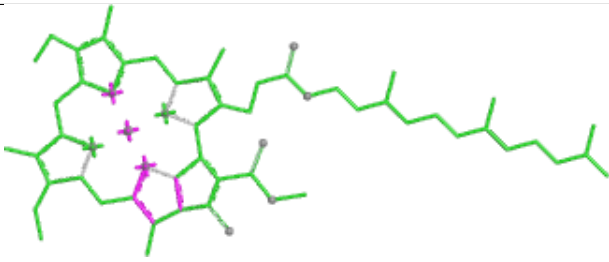
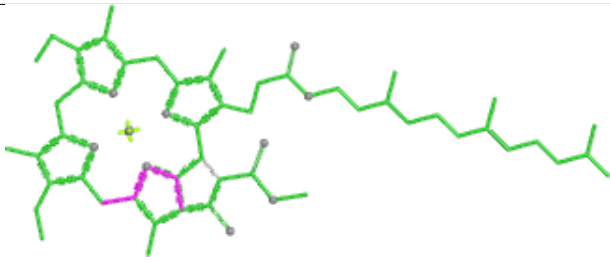
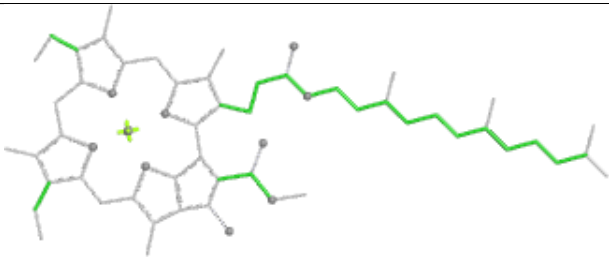
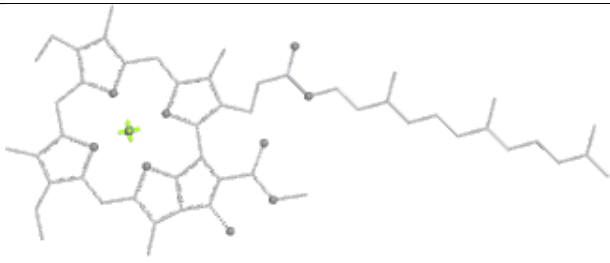


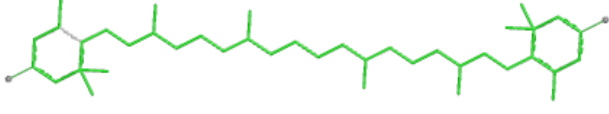
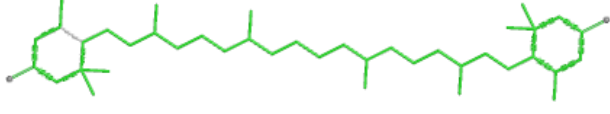
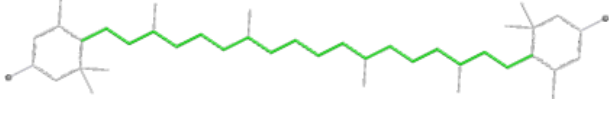
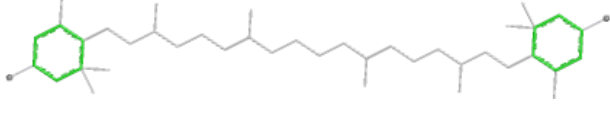


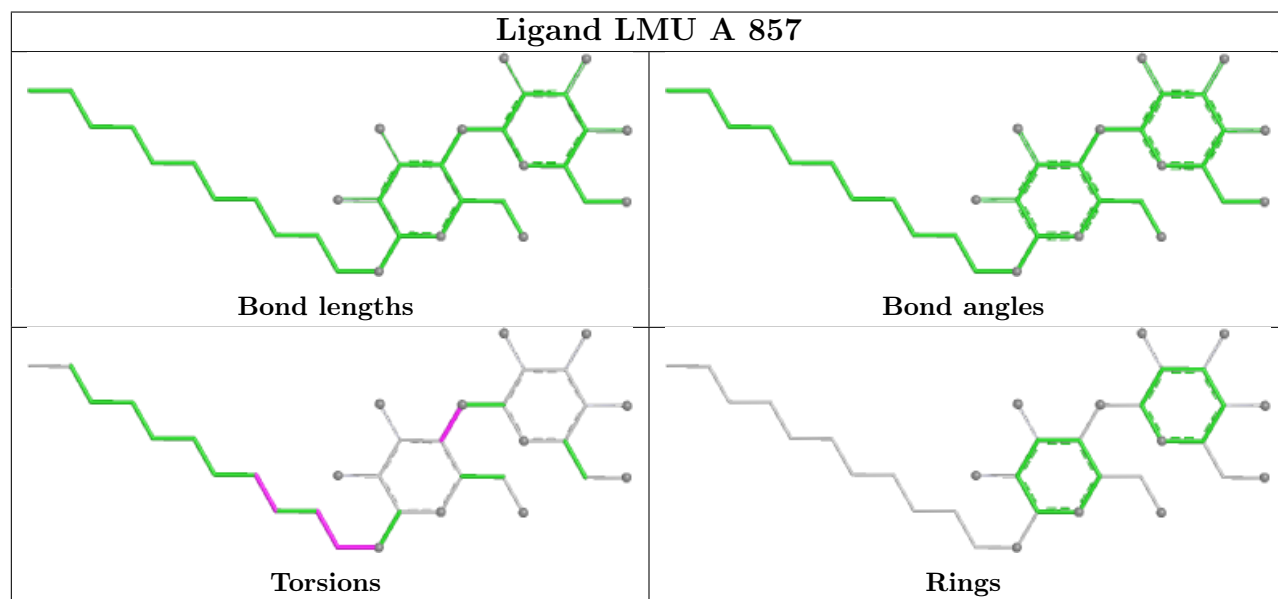
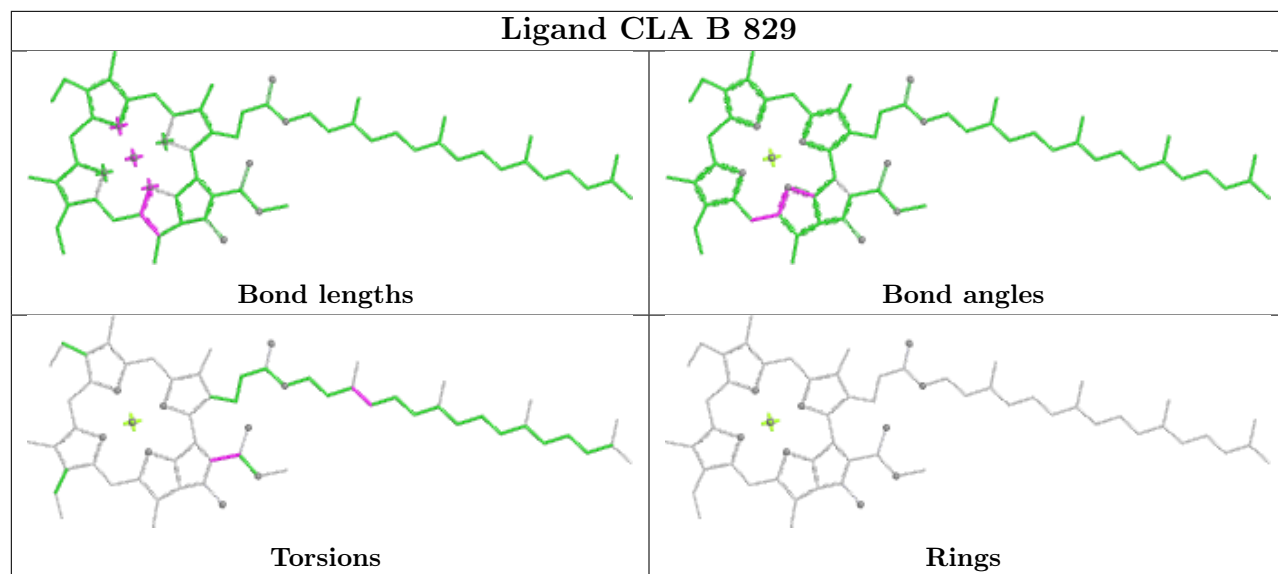




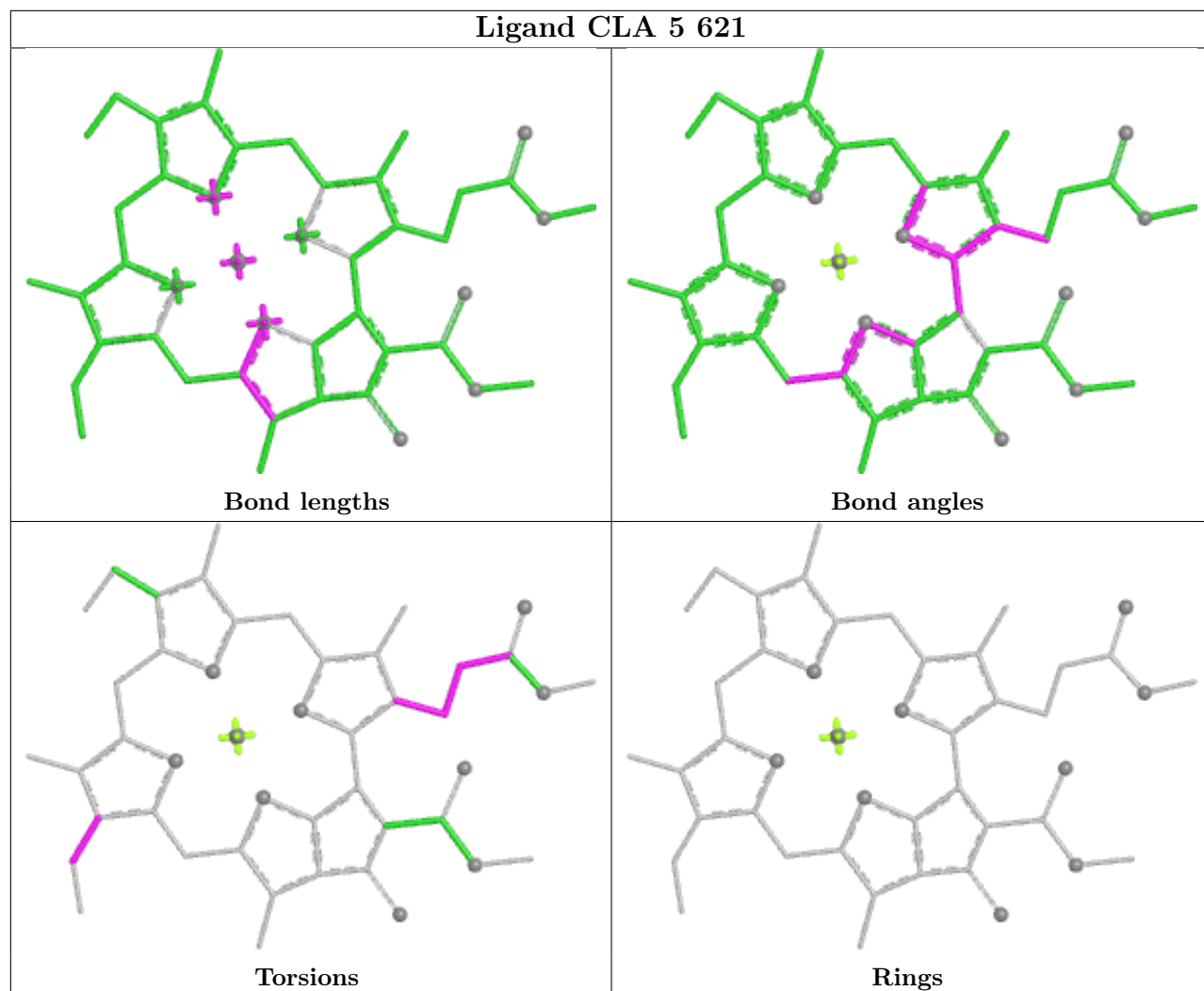
Ligand BCR B 846	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 4 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

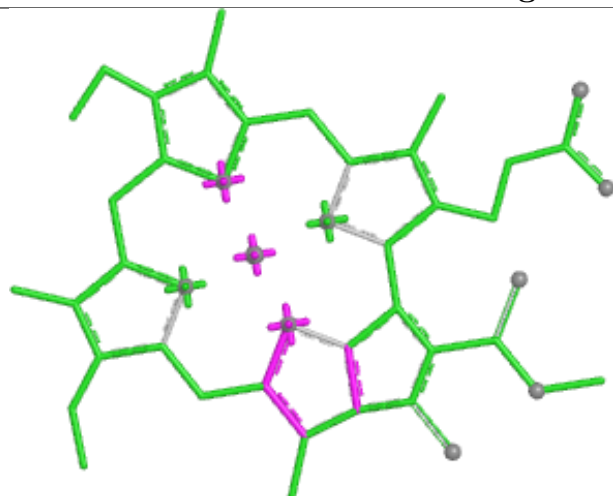
Ligand LUT 9 617	
	
Bond lengths	Bond angles
	
Torsions	Rings



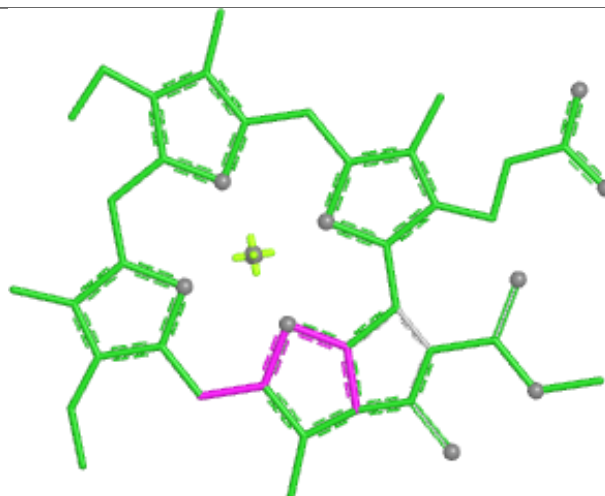
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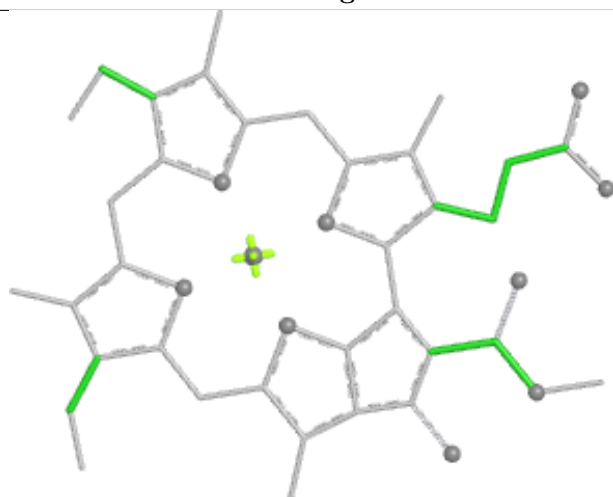
Ligand CLA 6 617



Bond lengths



Bond angles

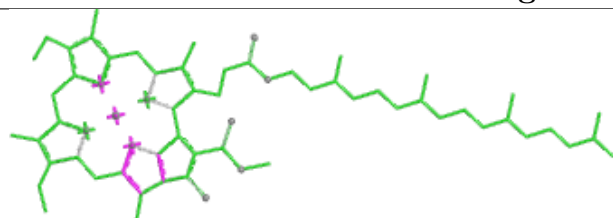


Torsions

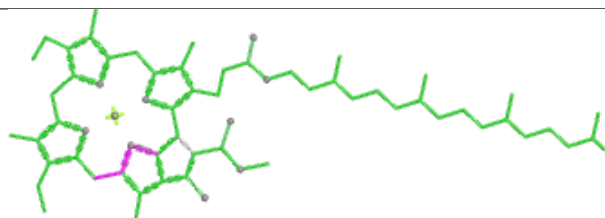


Rings

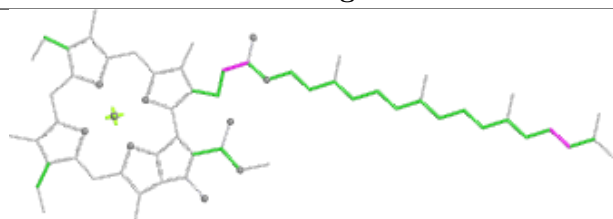
Ligand CLA 8 603



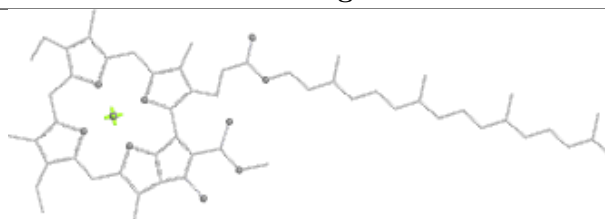
Bond lengths



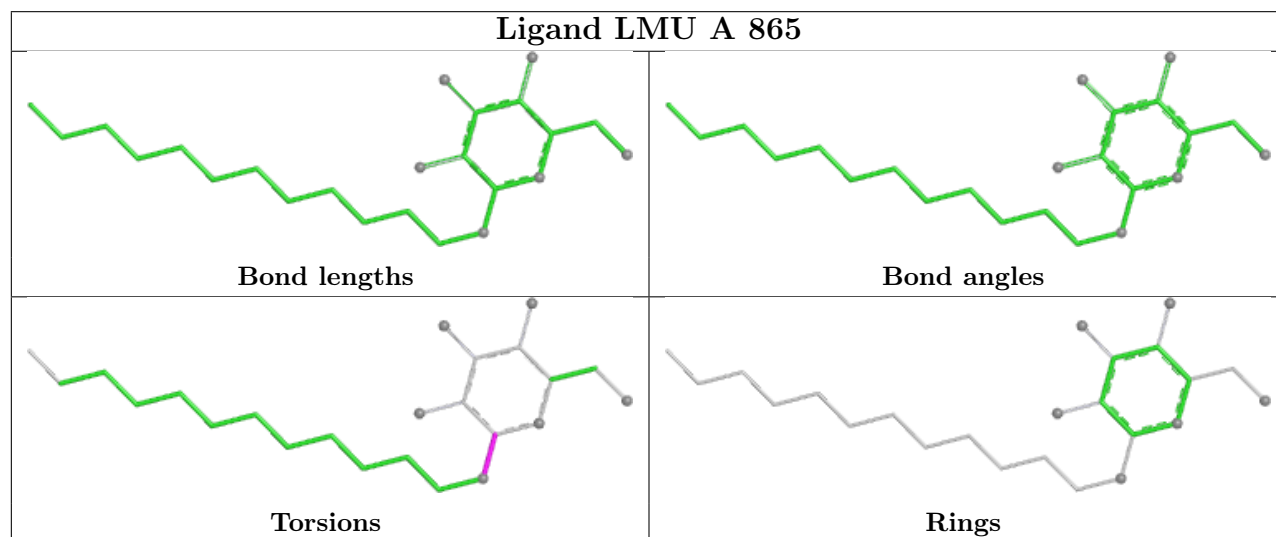
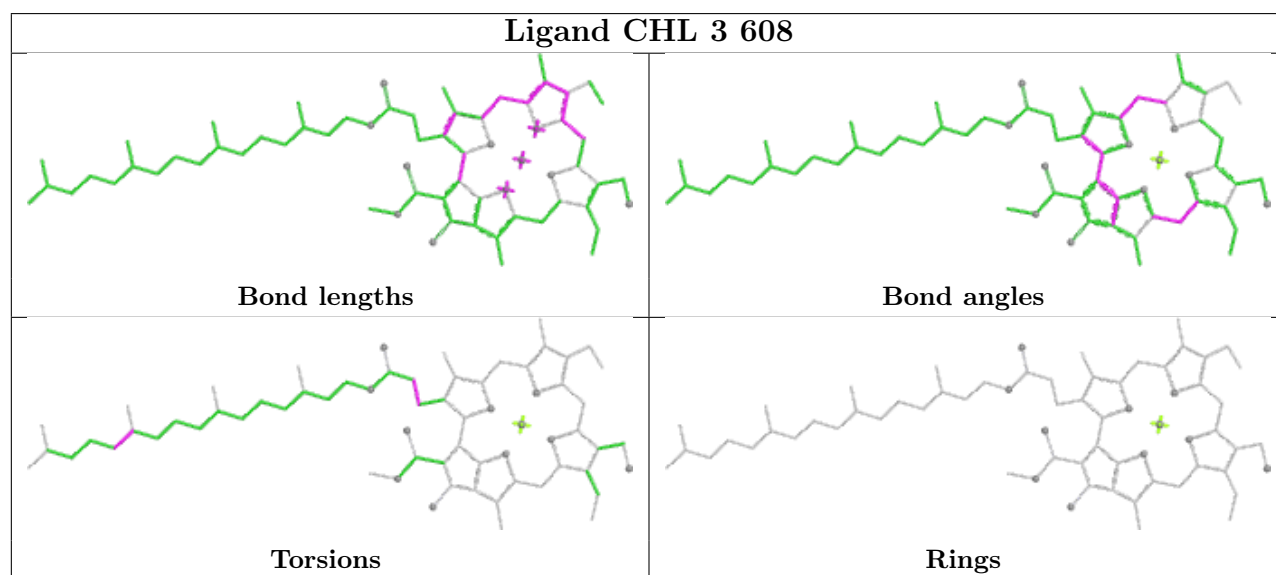
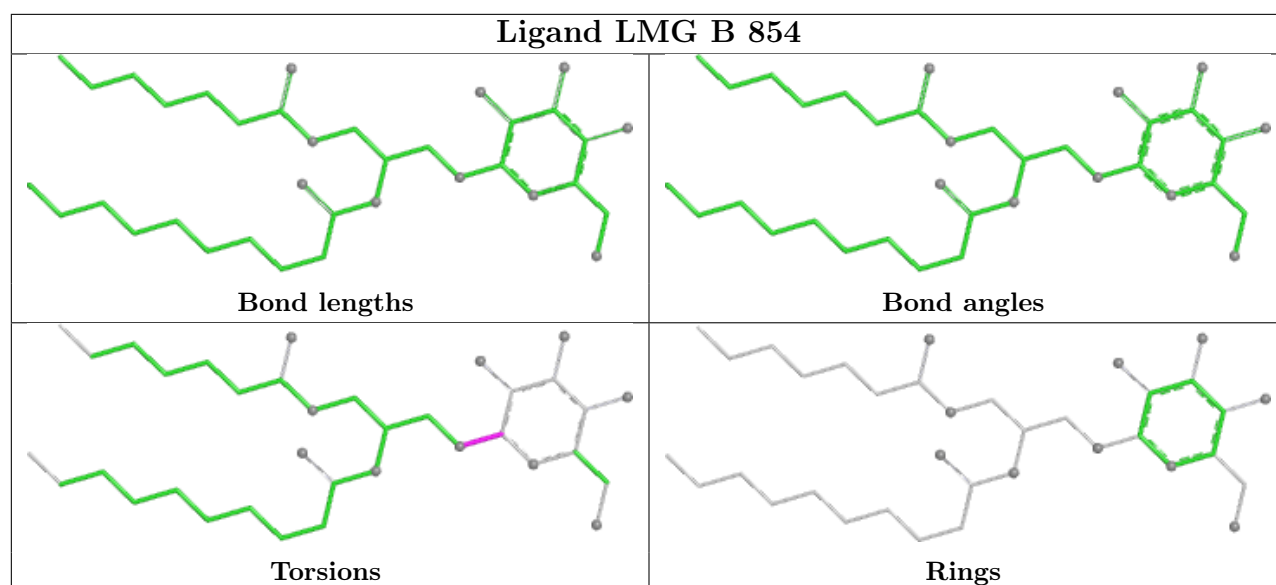
Bond angles



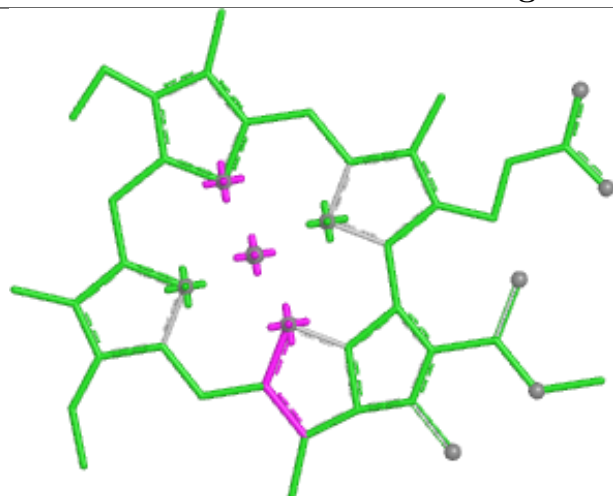
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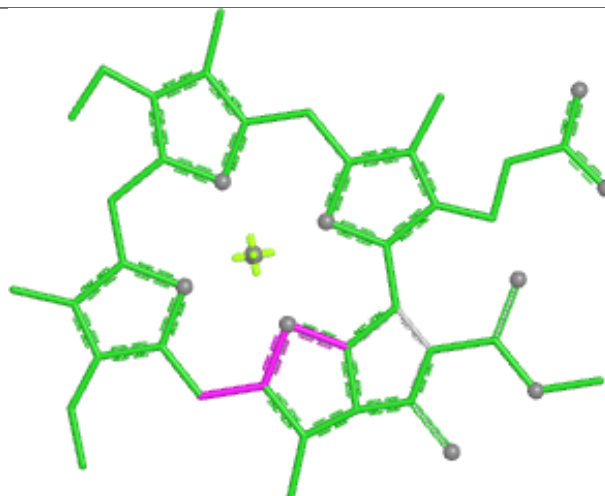
Rings



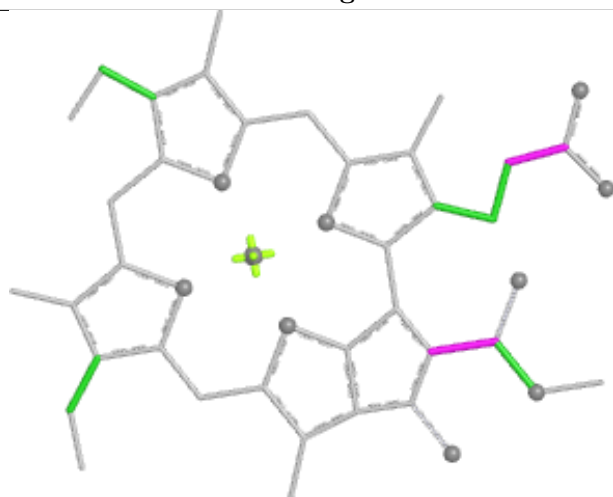
Ligand CLA 9 612



Bond lengths



Bond angles

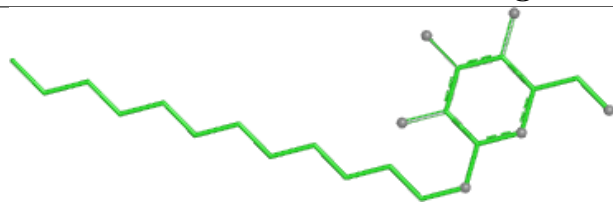


Torsions

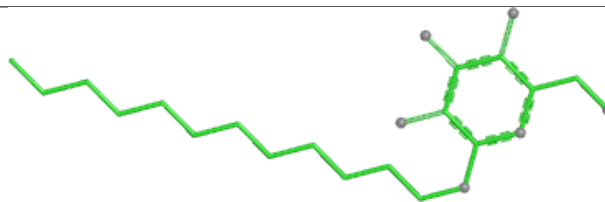


Rings

Ligand LMU 6 628



Bond lengths



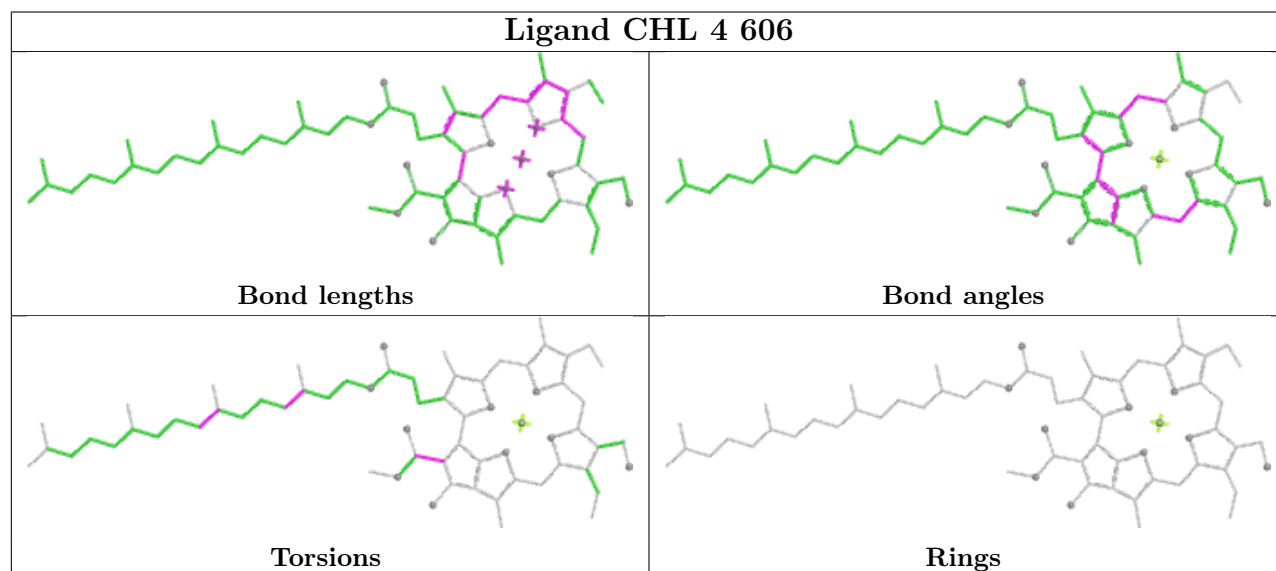
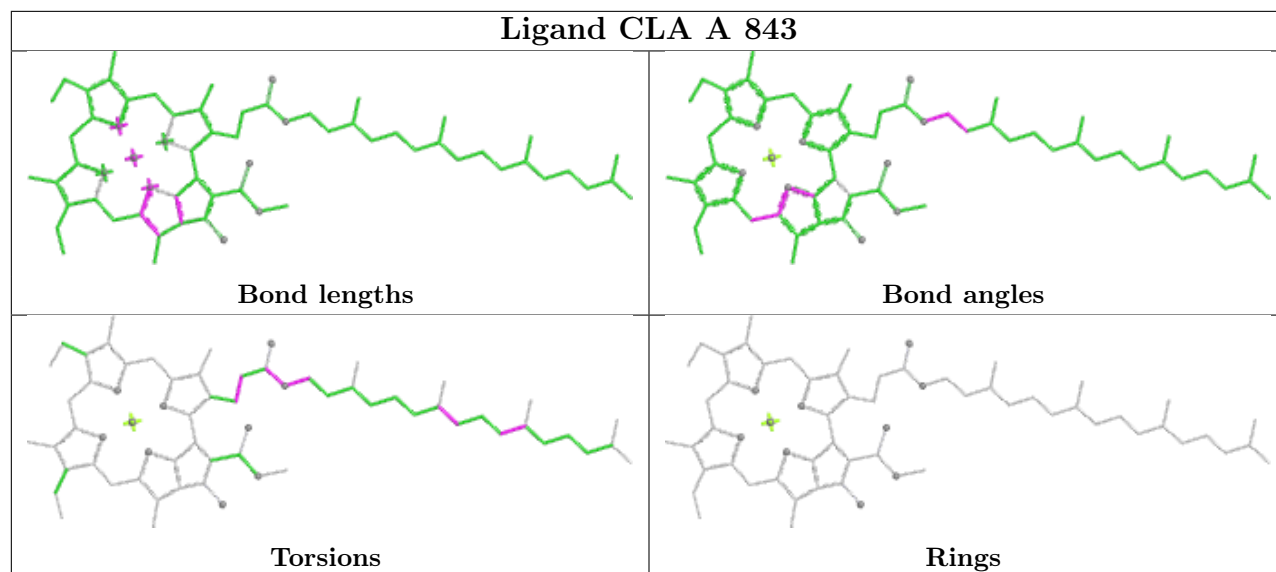
Bond angles



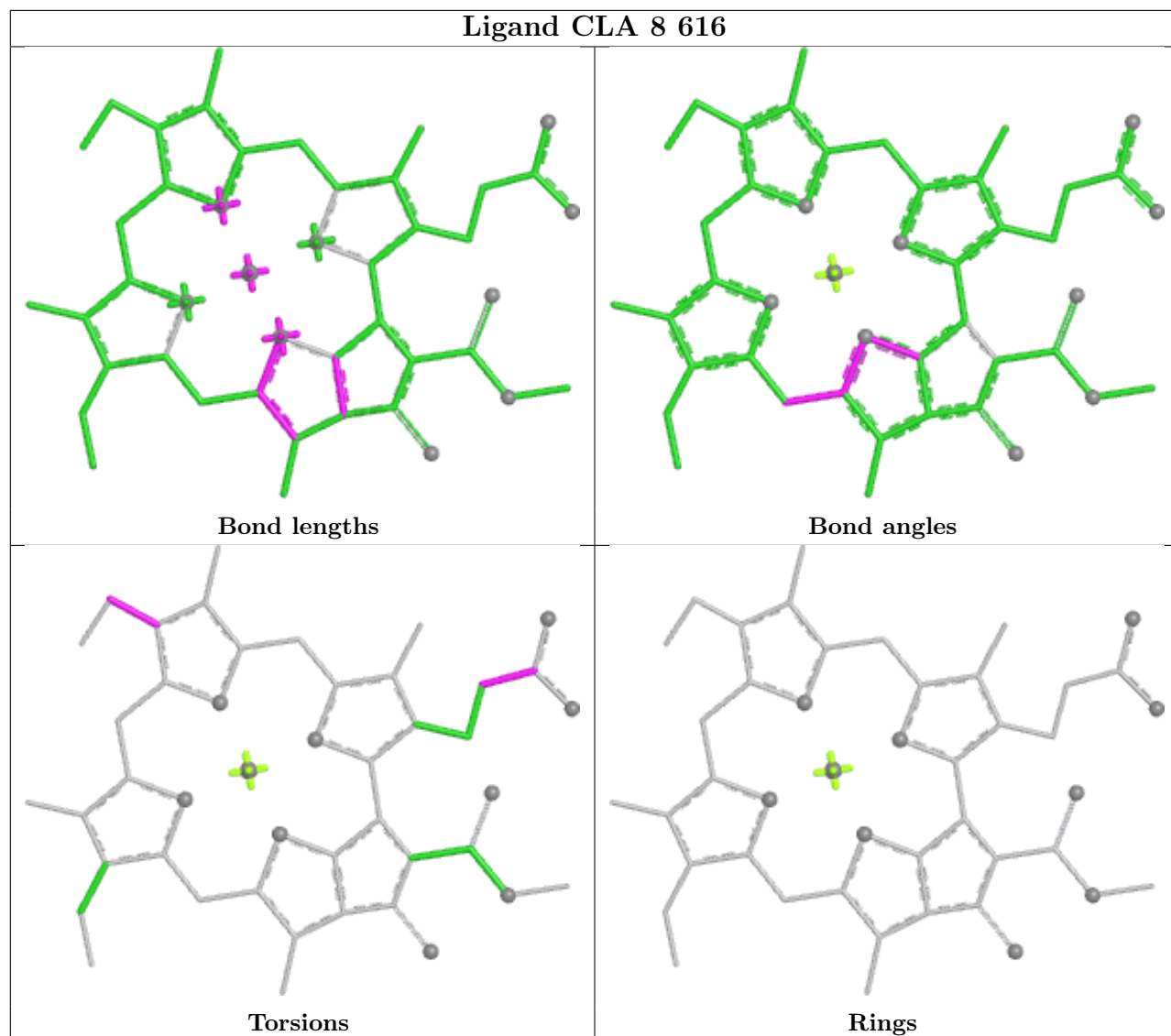
Torsions



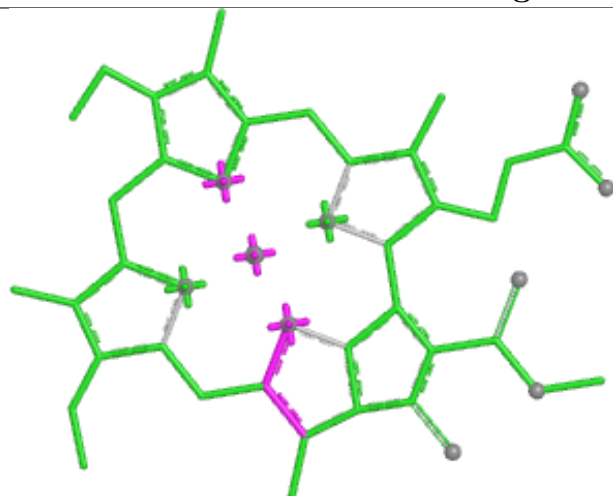
Rings



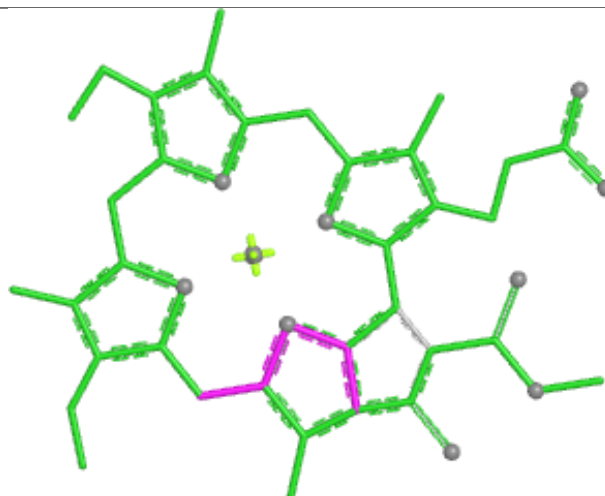
Ligand CLA 8 616



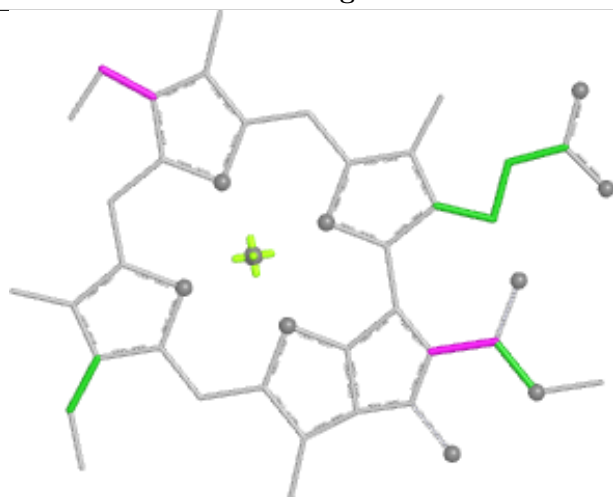
Ligand CLA K 206



Bond lengths



Bond angles

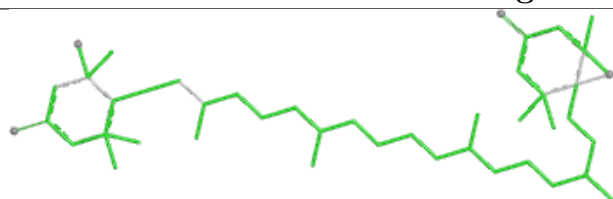


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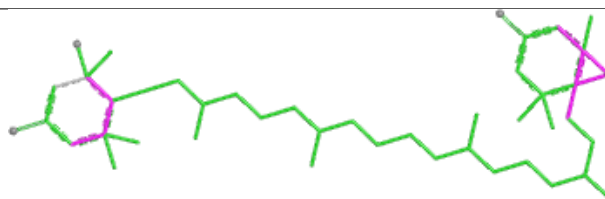


Rings

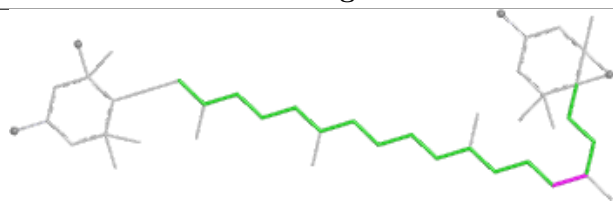
Ligand NEX 5 625



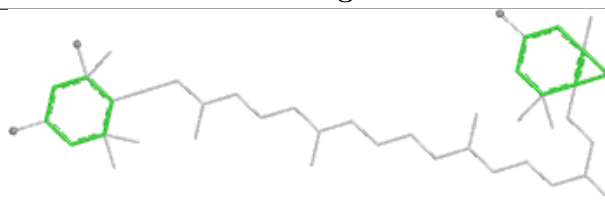
Bond lengths



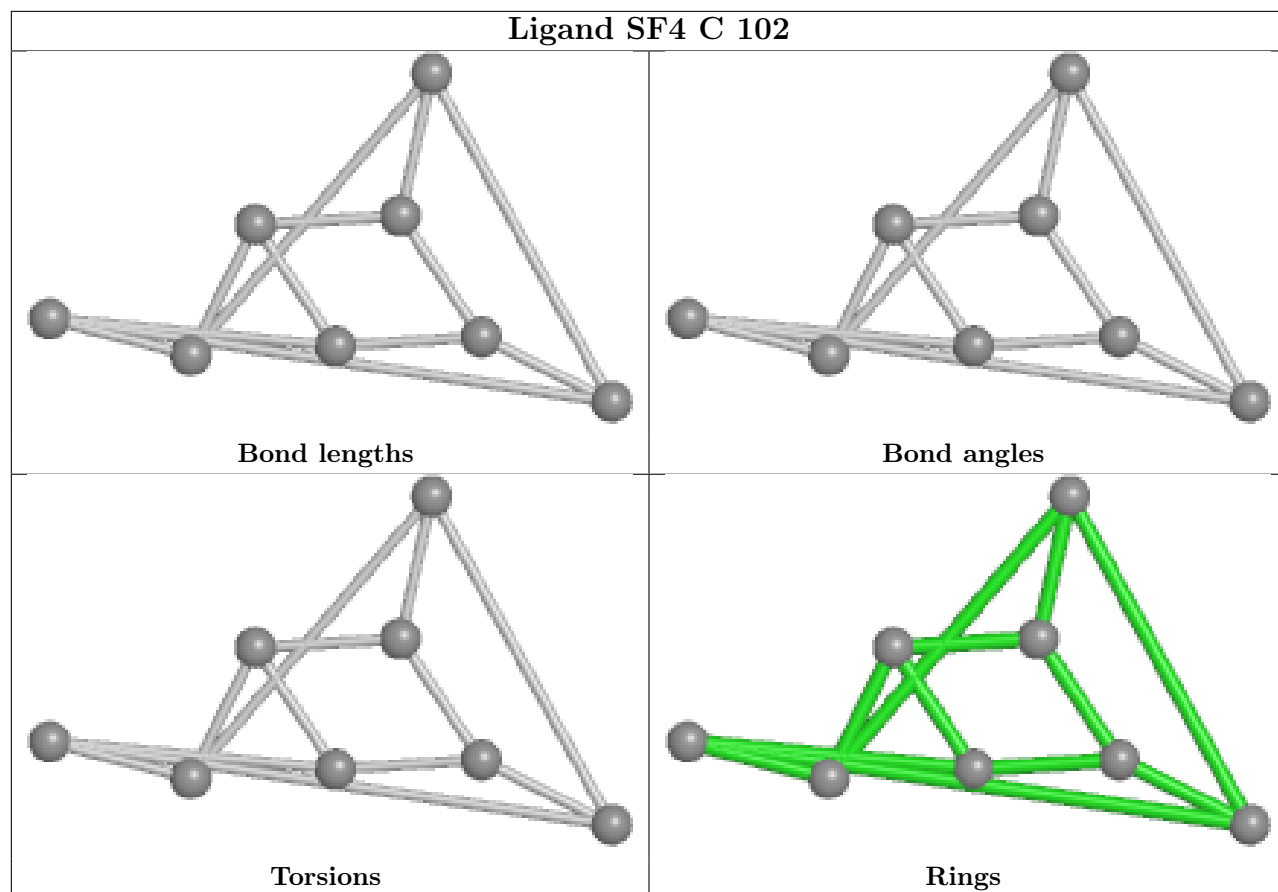
Bond angles



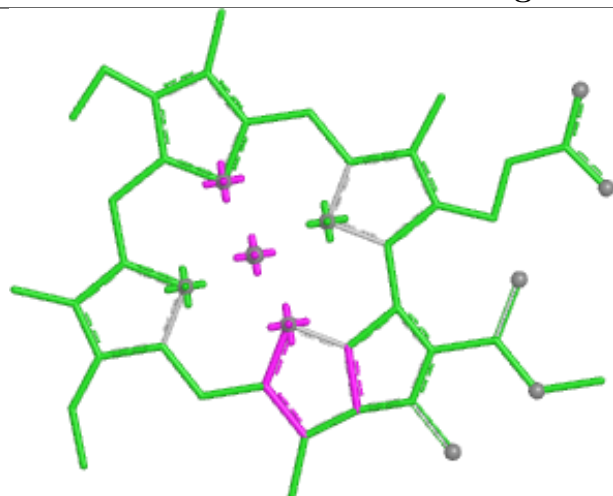
Torsions



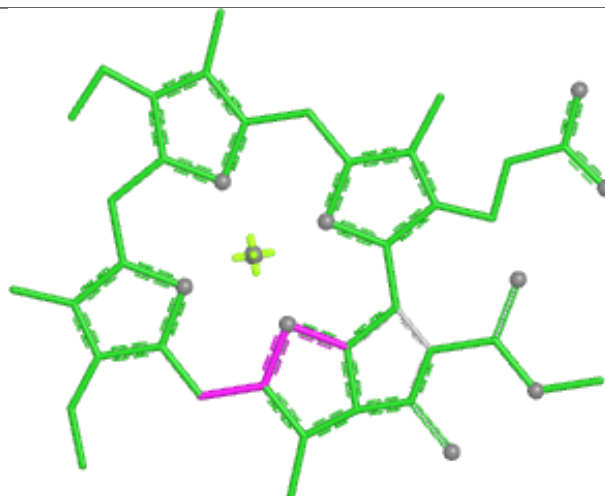
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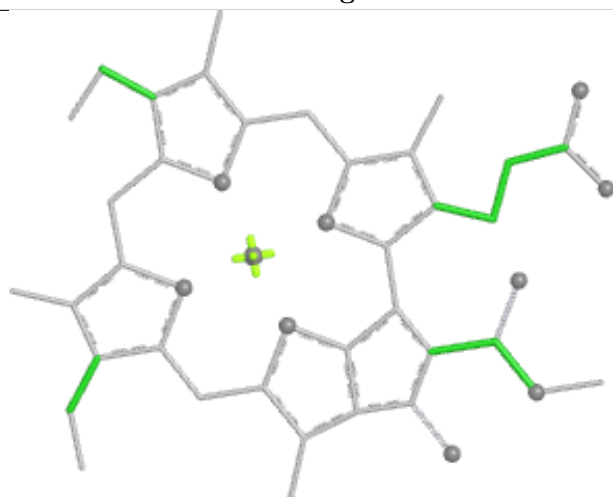
Ligand CLA B 804



Bond lengths



Bond angles

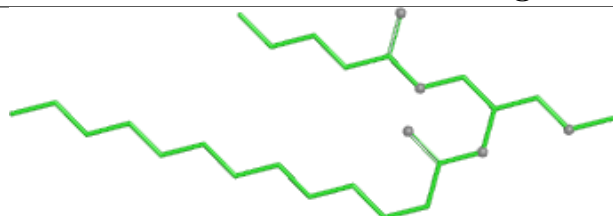


Torsions

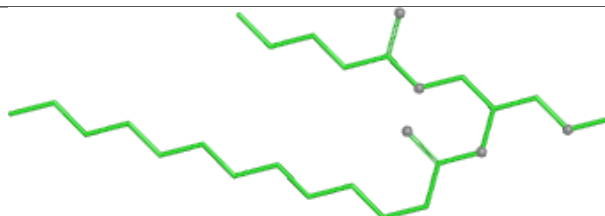


Rings

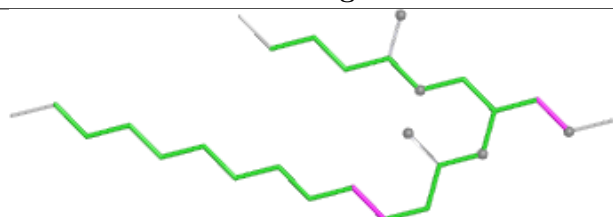
Ligand LMG 4 627



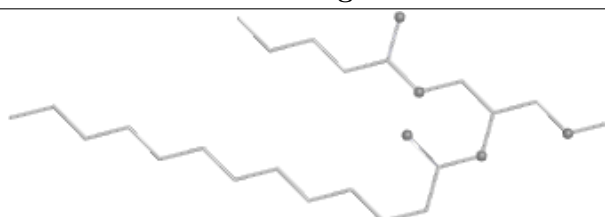
Bond lengths



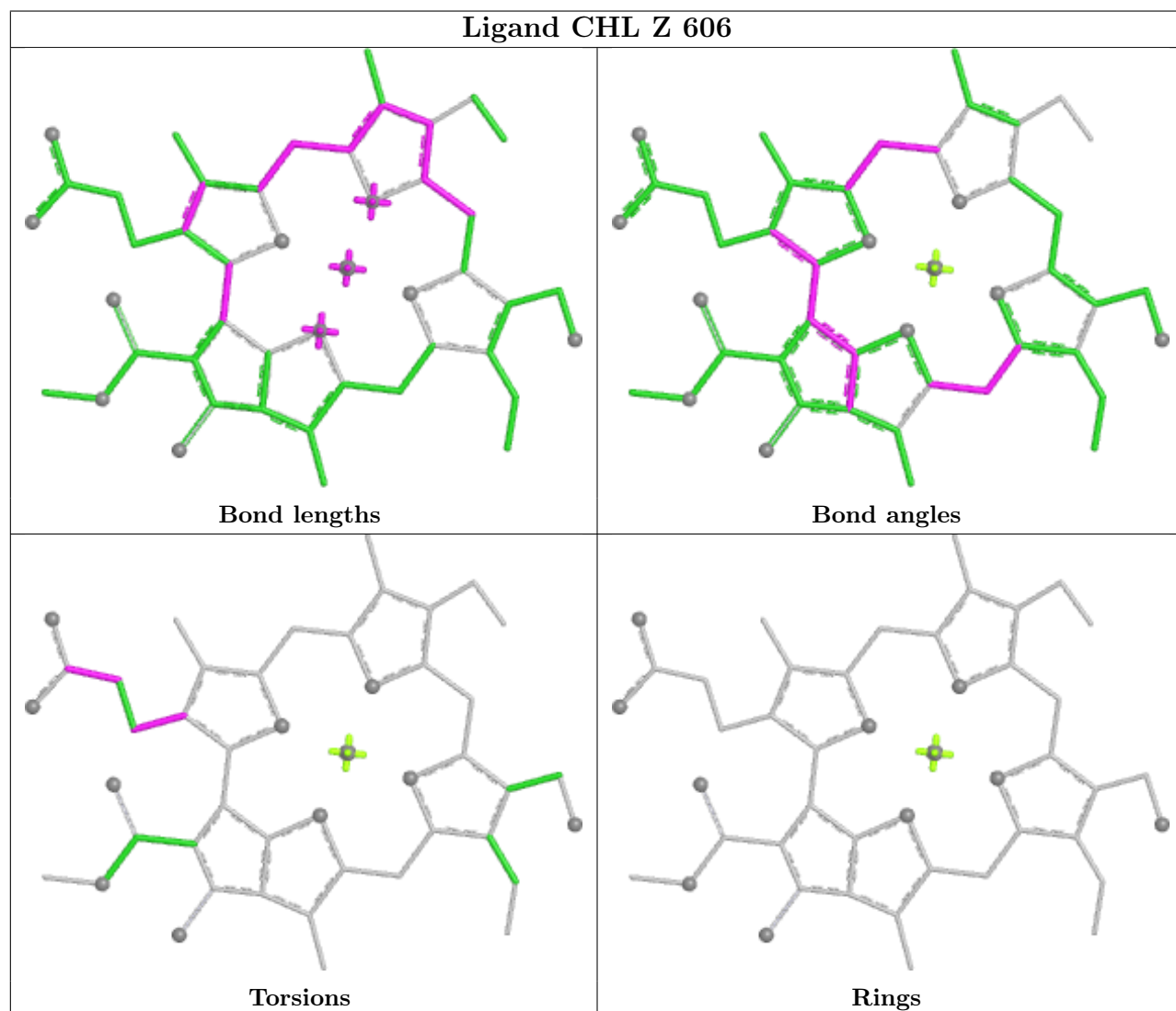
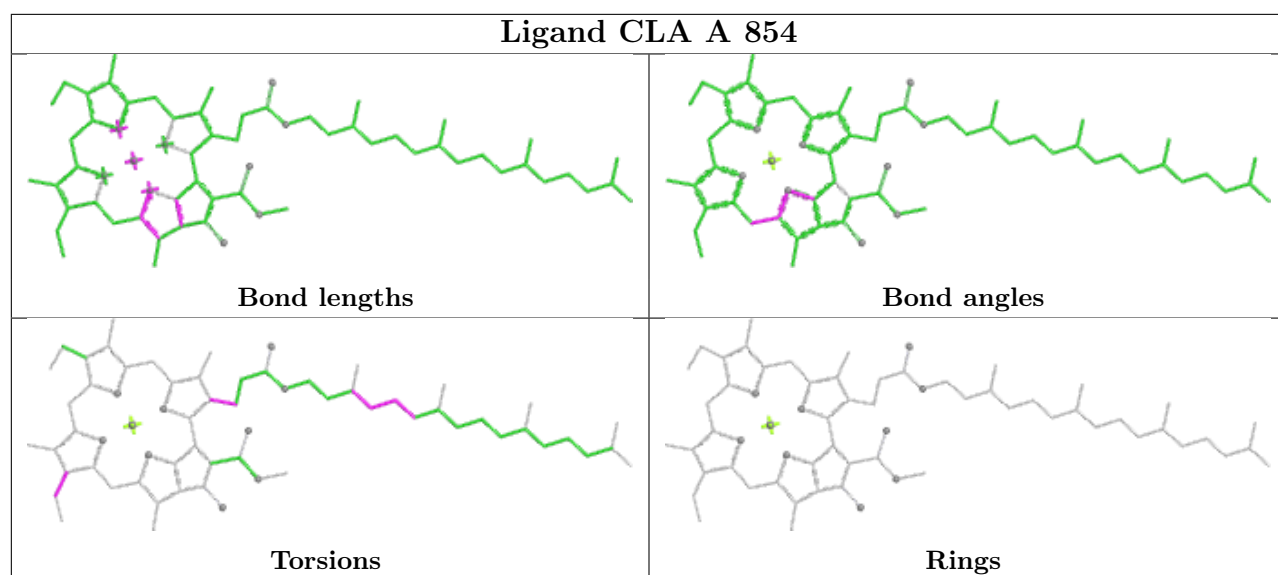
Bond angles

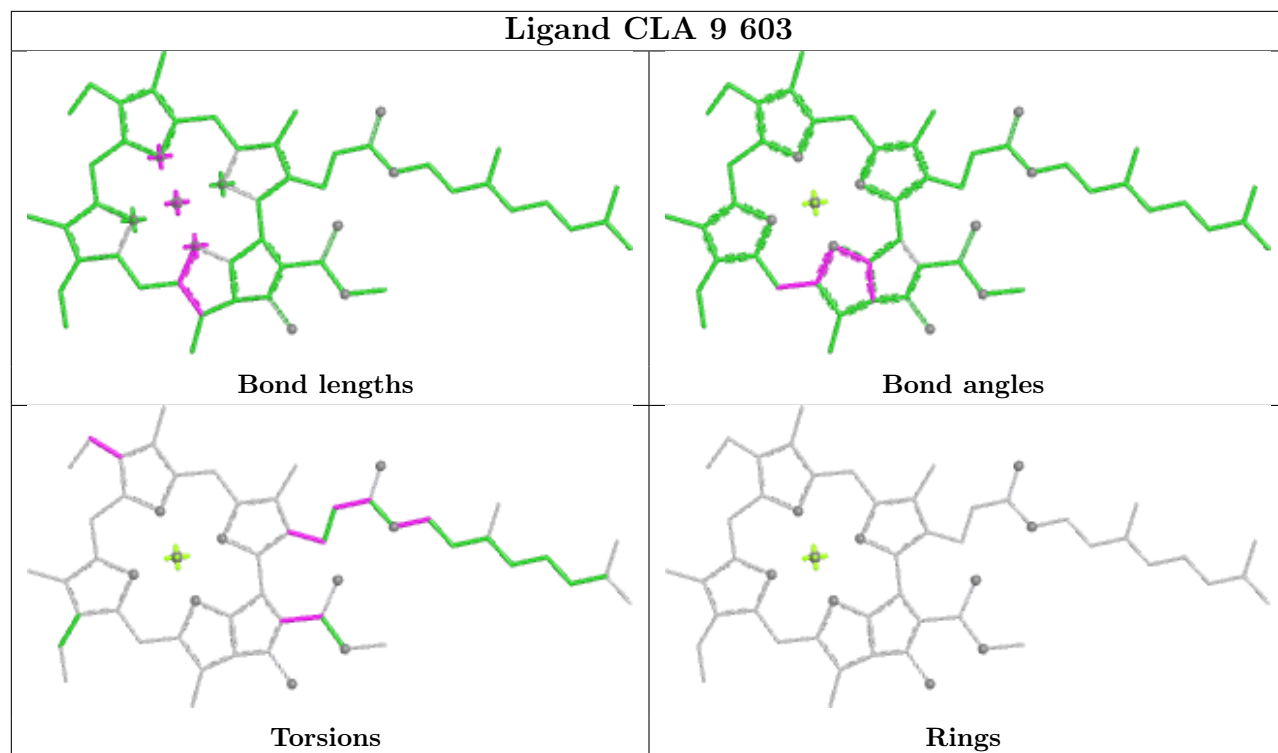


Torsions

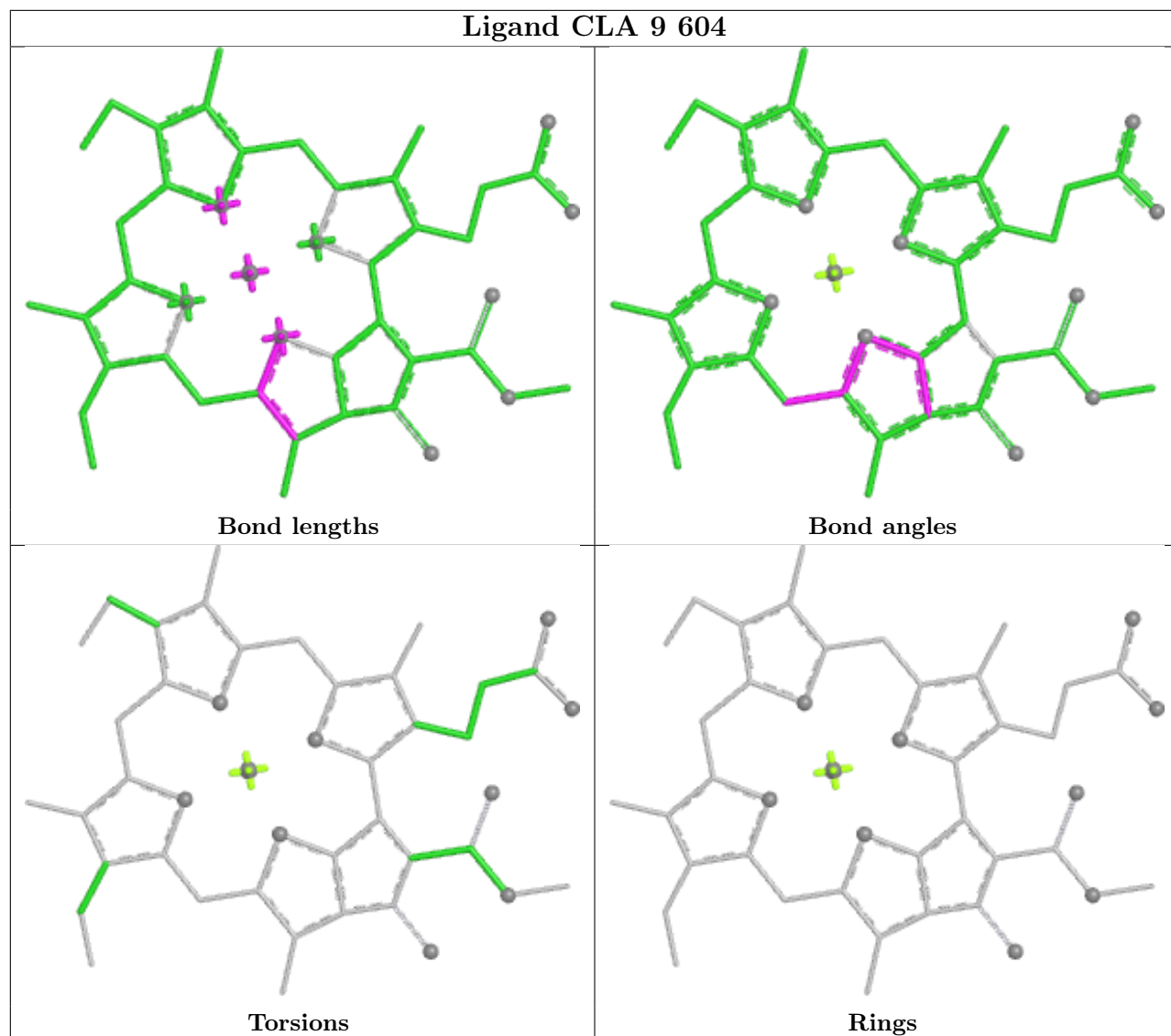


Rings

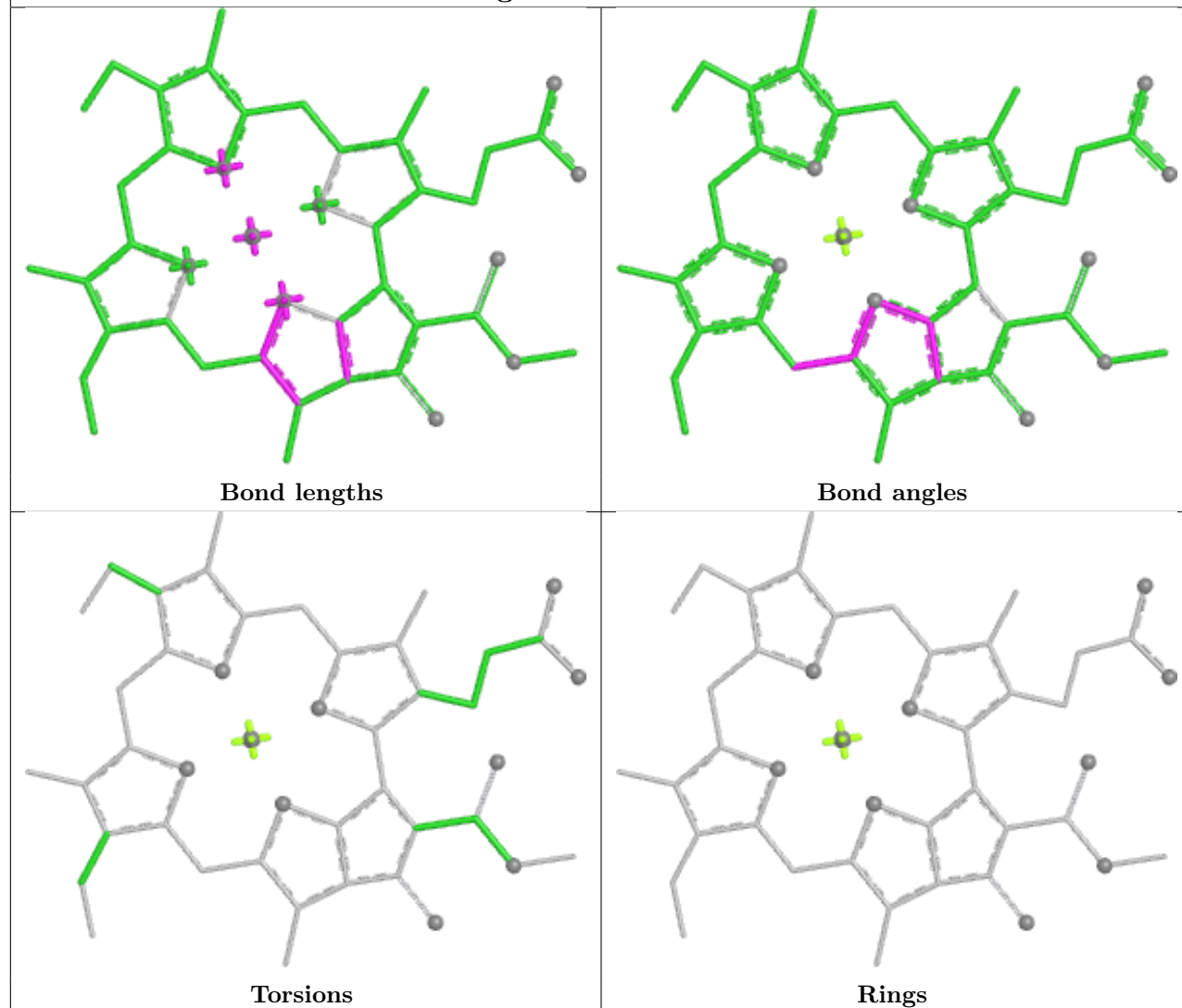




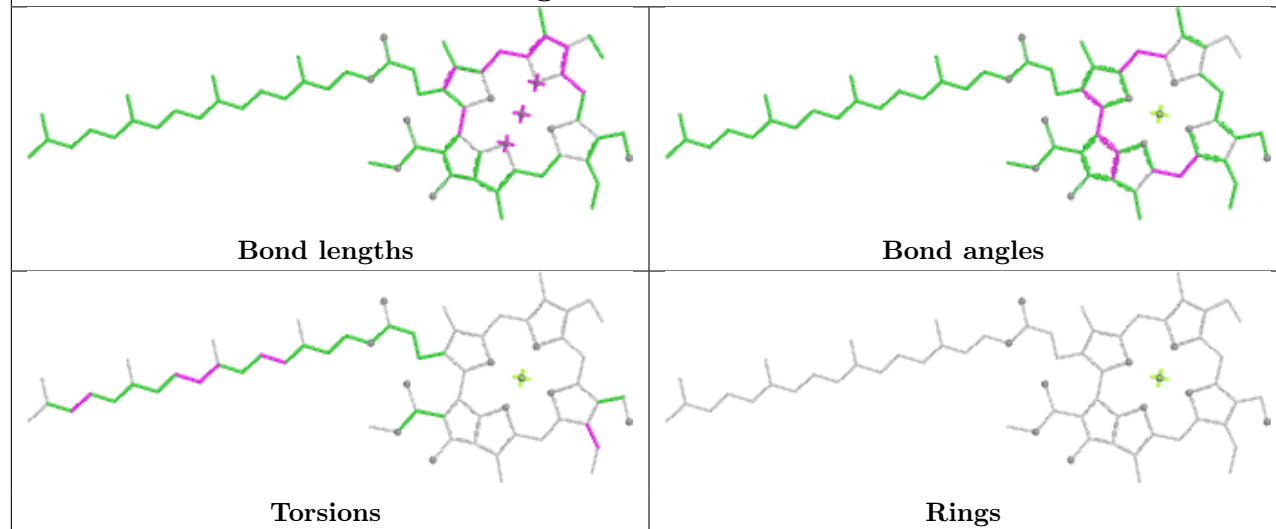
Ligand CLA 9 604

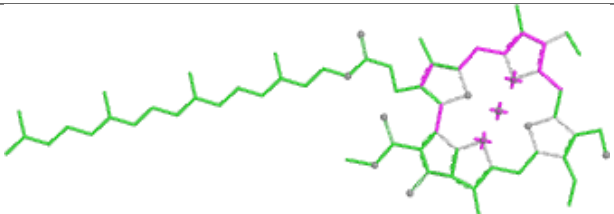
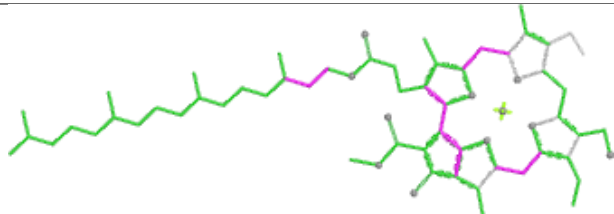
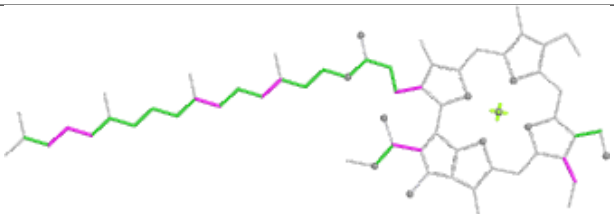
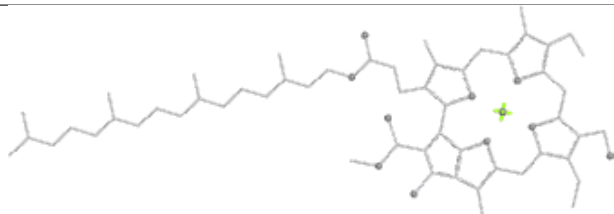


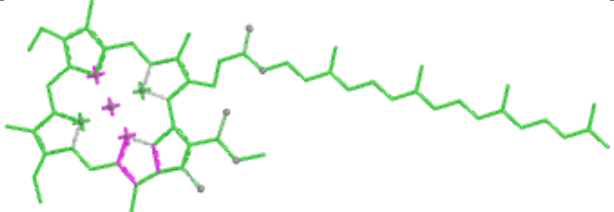
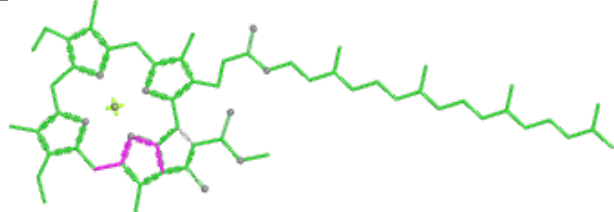
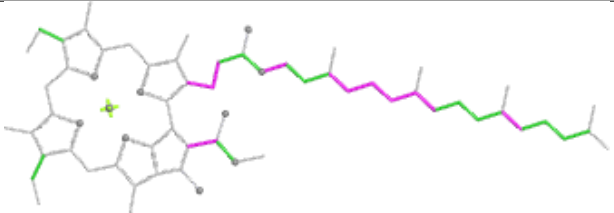
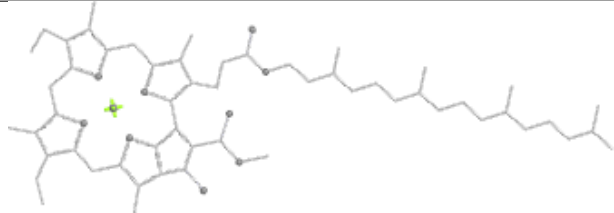
Ligand CLA 7 609

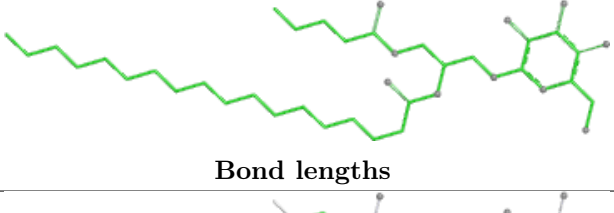
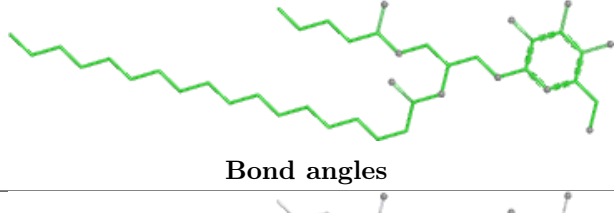


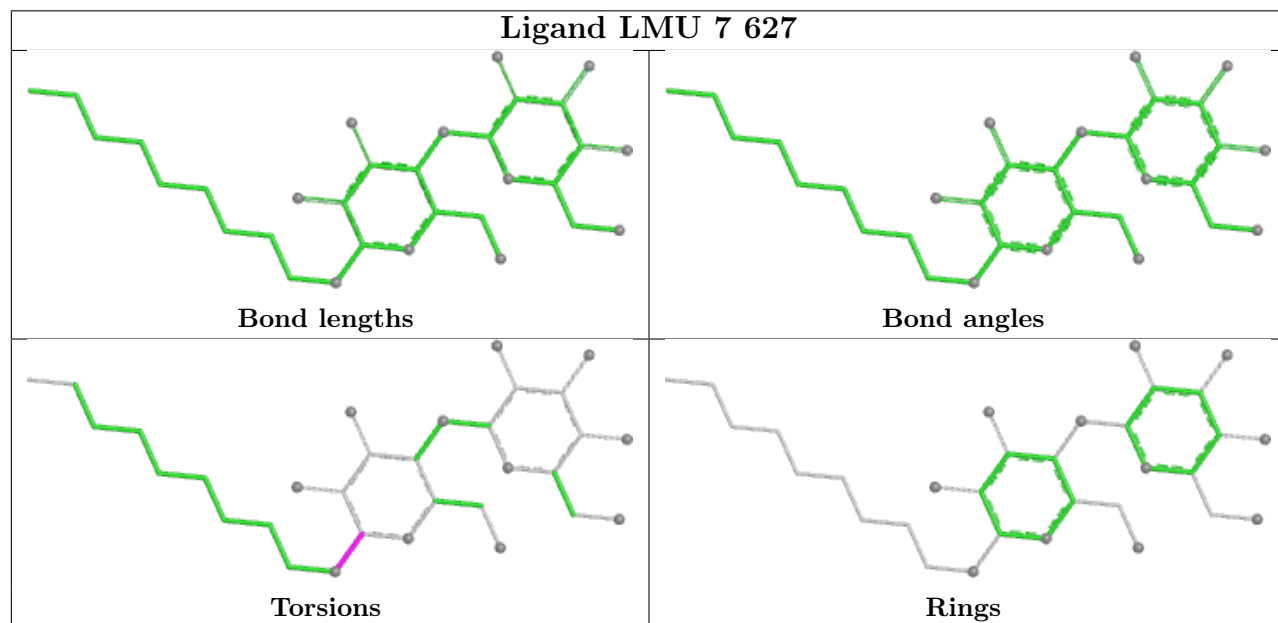
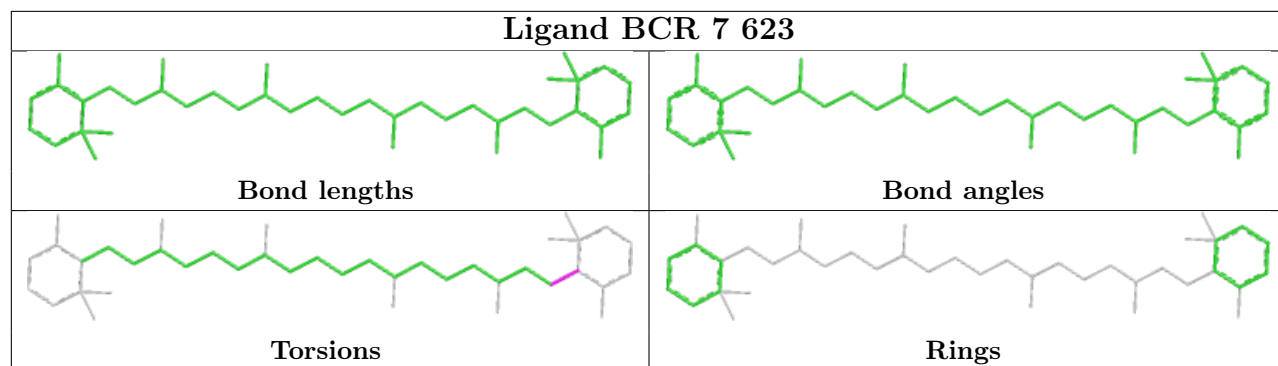
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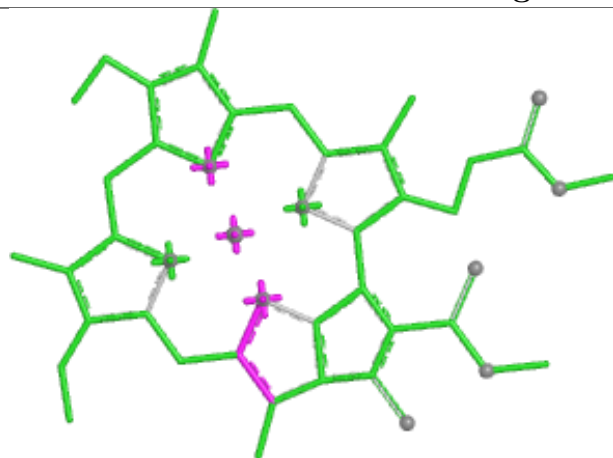
Ligand CHL 6 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 5 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

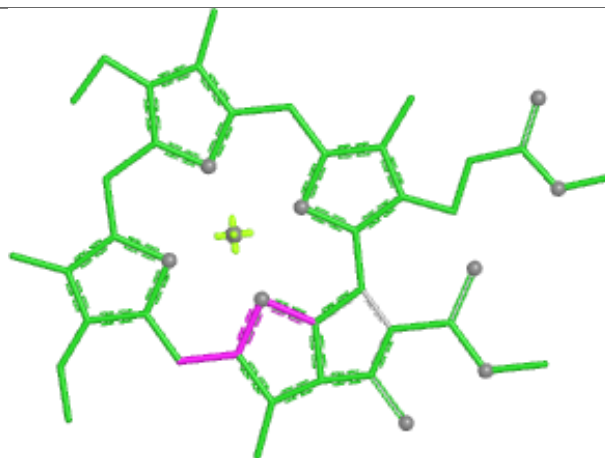
Ligand LMG J 103	
	
Bond lengths	Bond angles
	
Torsions	Rings



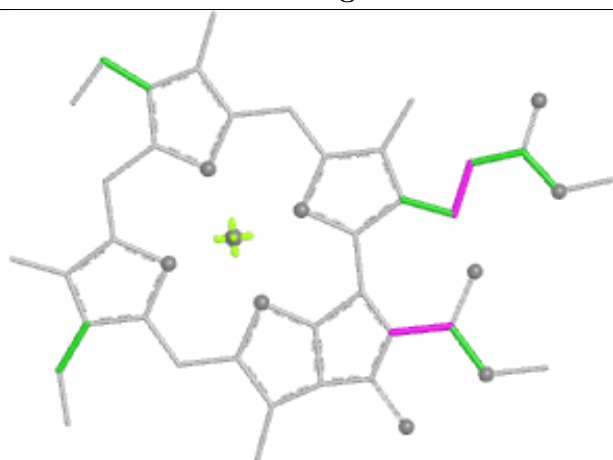
Ligand CLA G 204



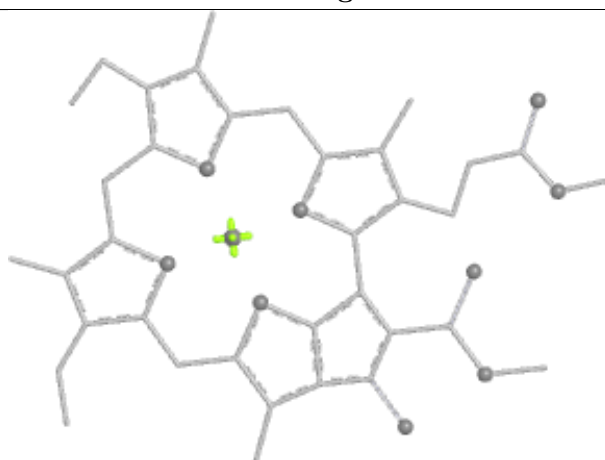
Bond lengths



Bond angles

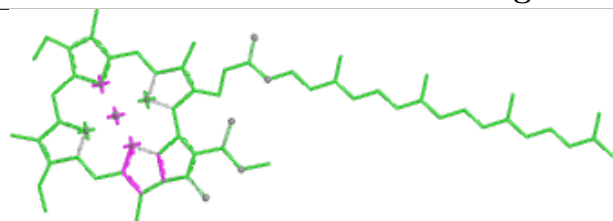


Torsions

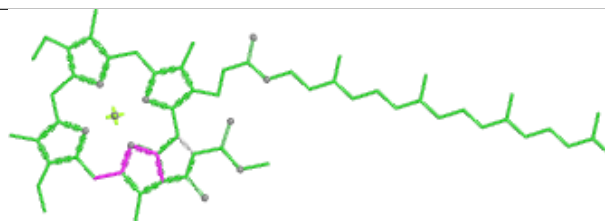


Rings

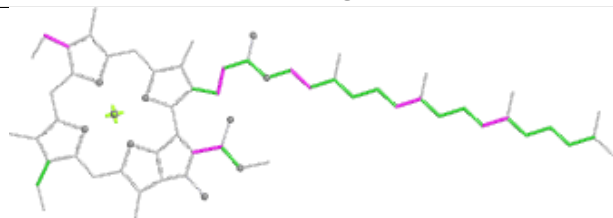
Ligand CLA A 823



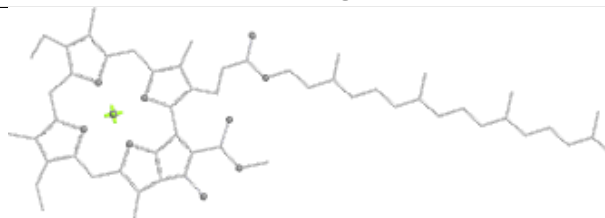
Bond lengths



Bond angles

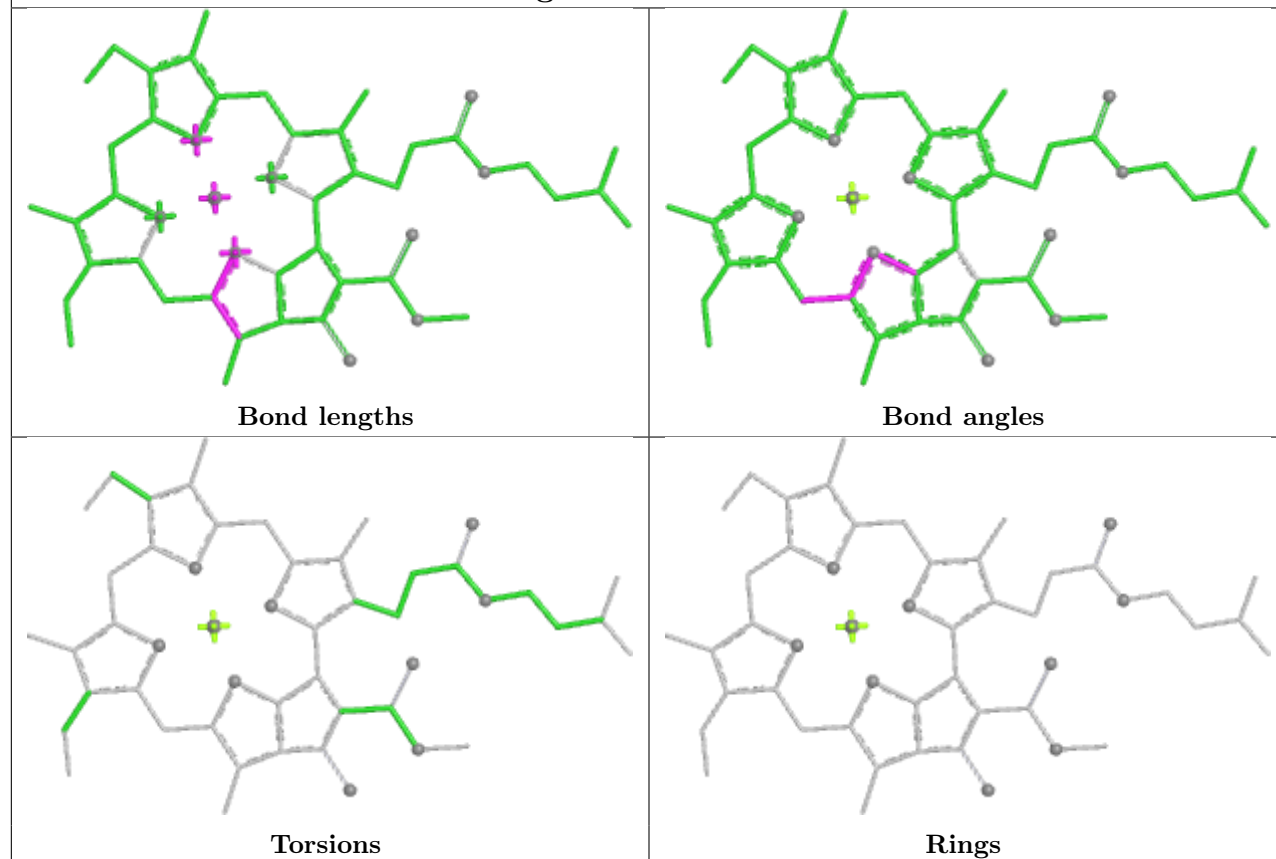


Torsions

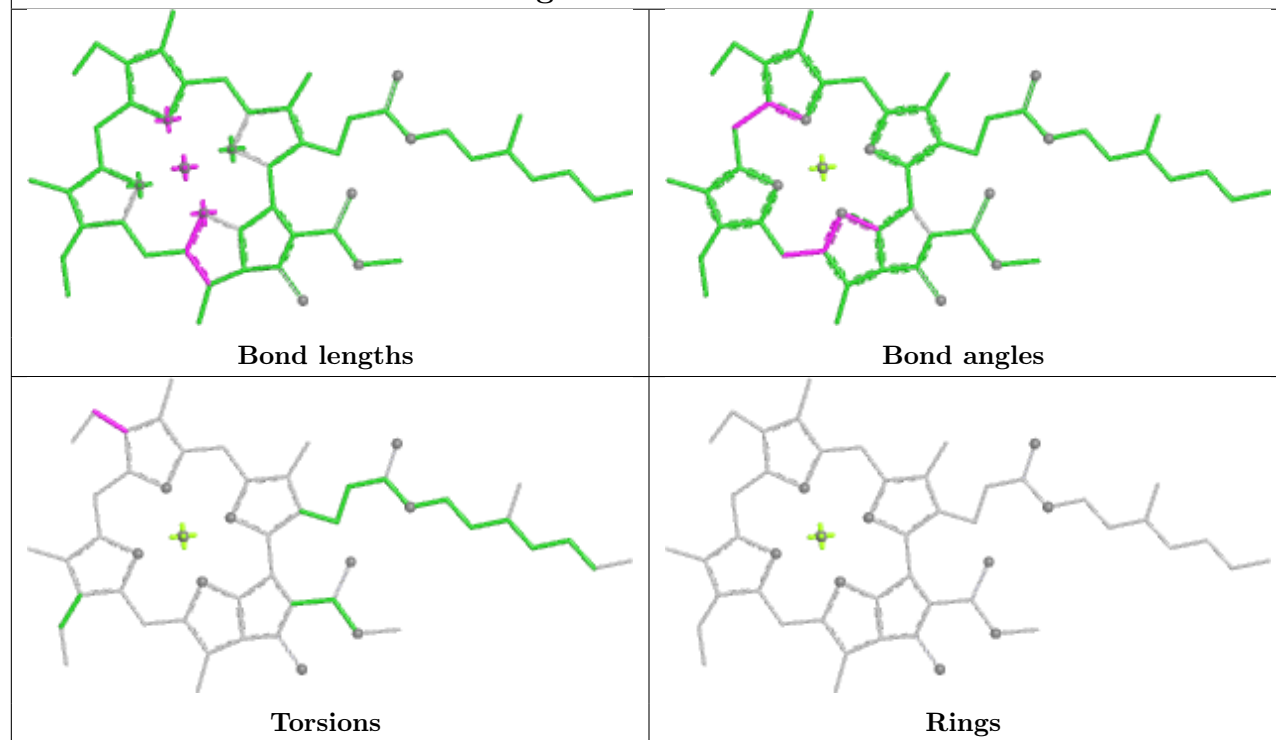


Rings

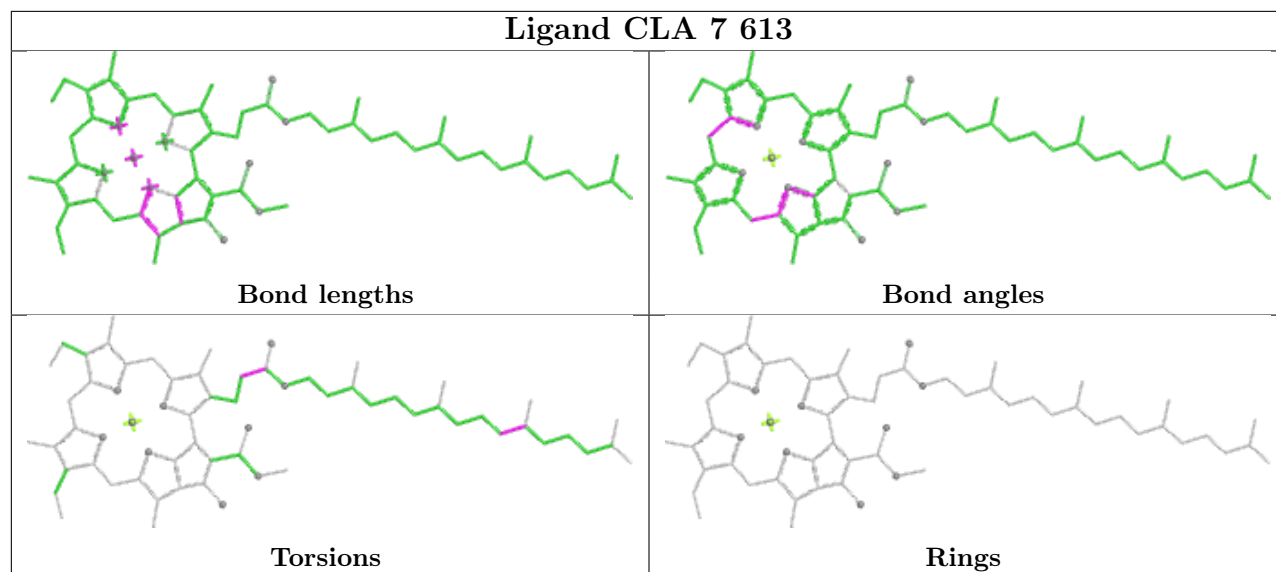
Ligand CLA 6 614



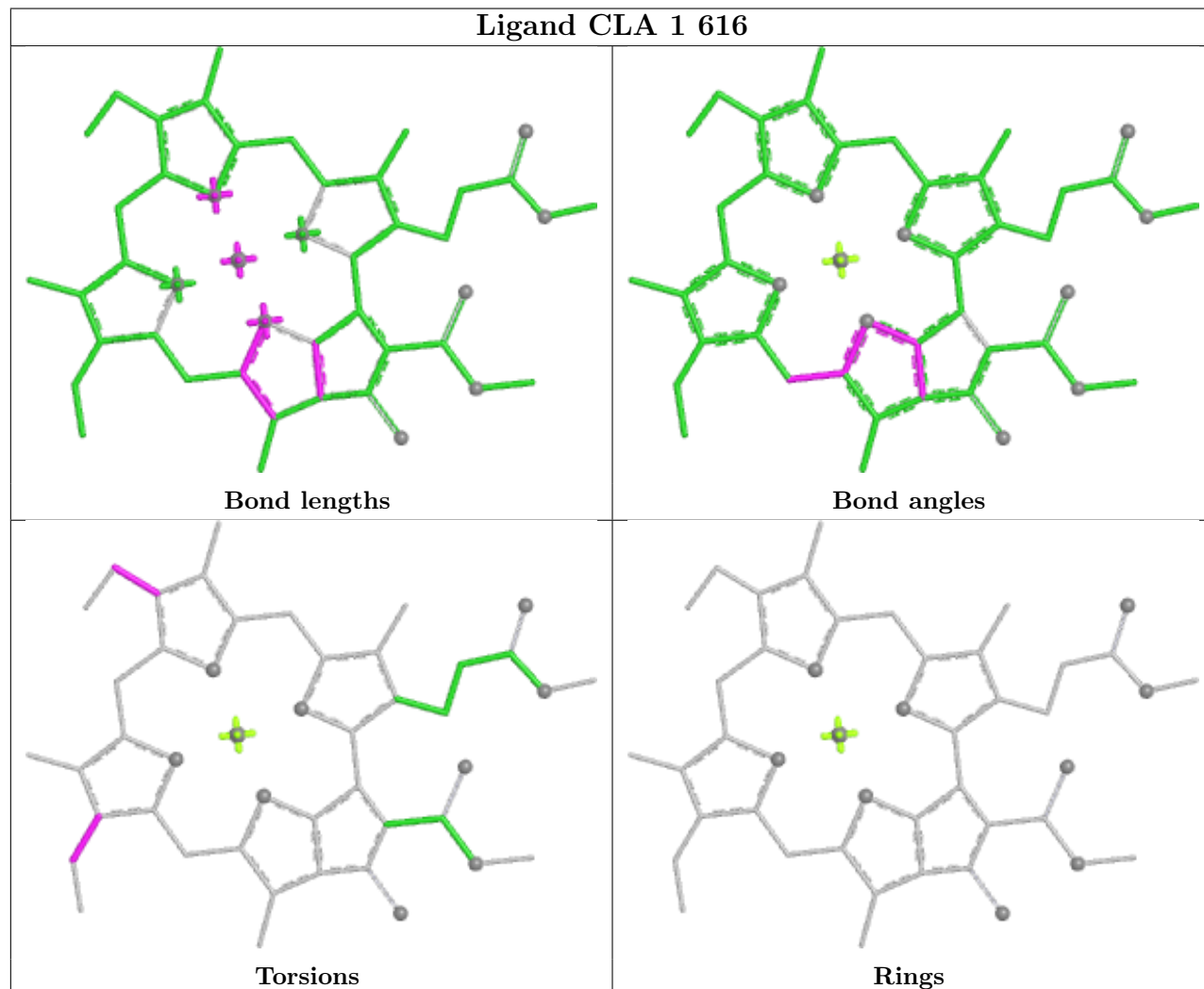
Ligand CLA 5 616



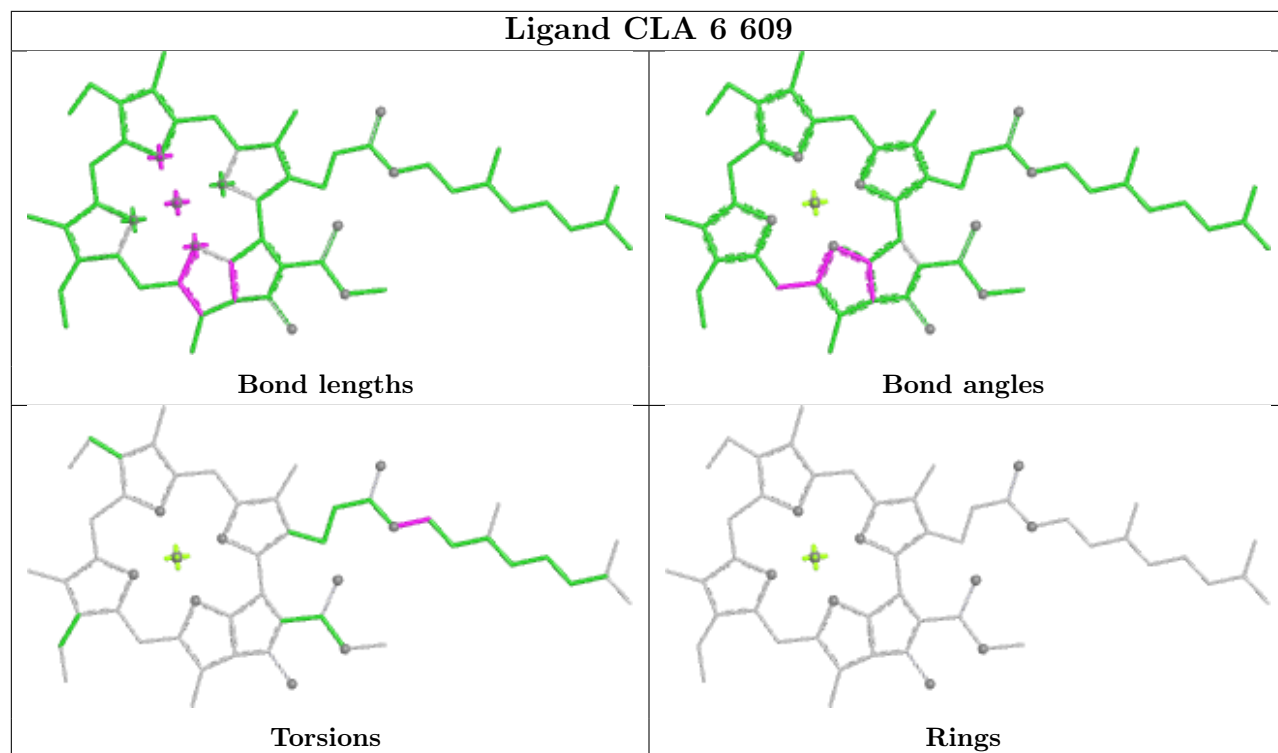
Ligand CLA 7 613



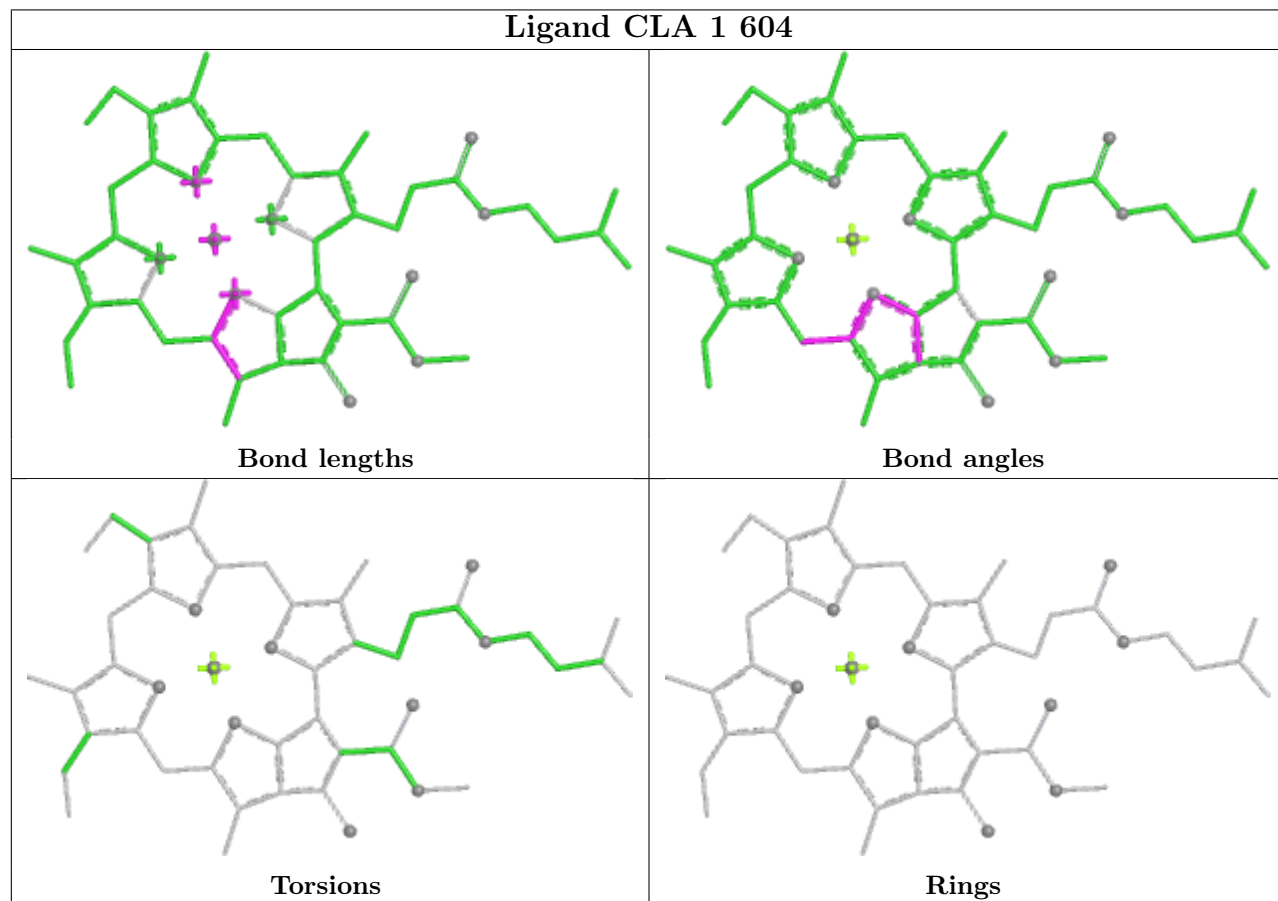
Ligand CLA 1 616



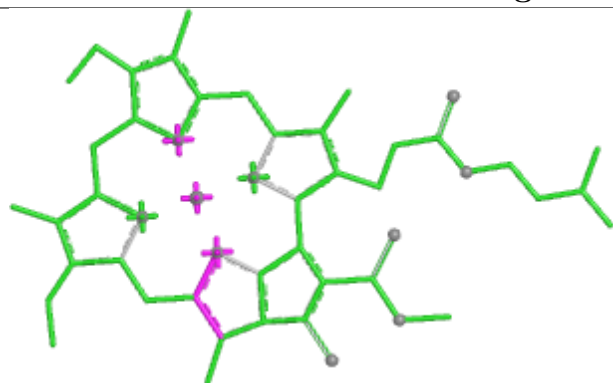
Ligand CLA 6 609



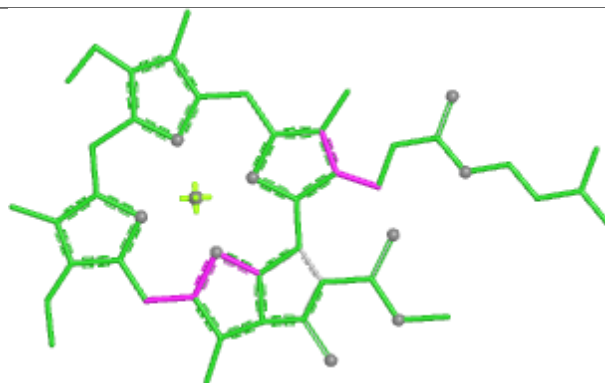
Ligand CLA 1 604



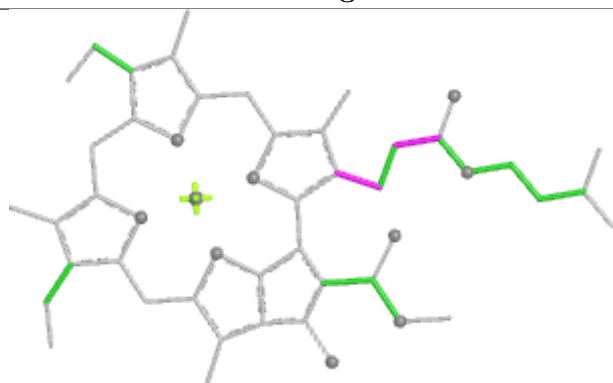
Ligand CLA B 838



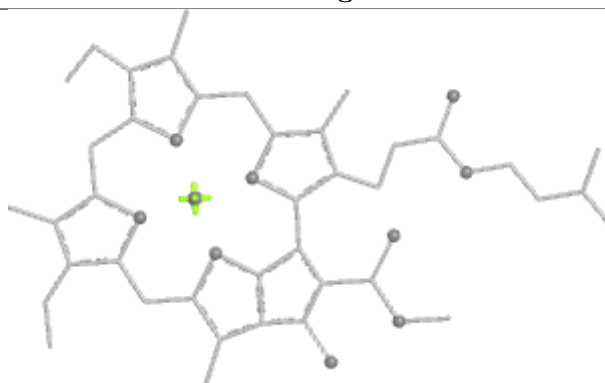
Bond lengths



Bond angles

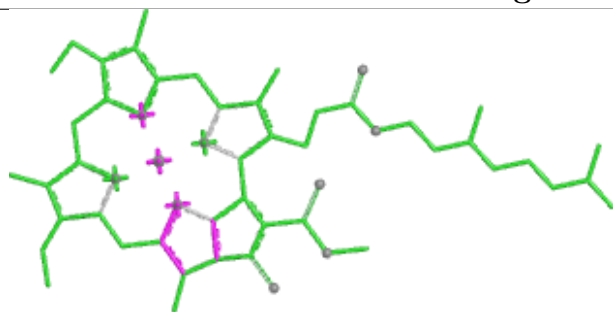


Torsions

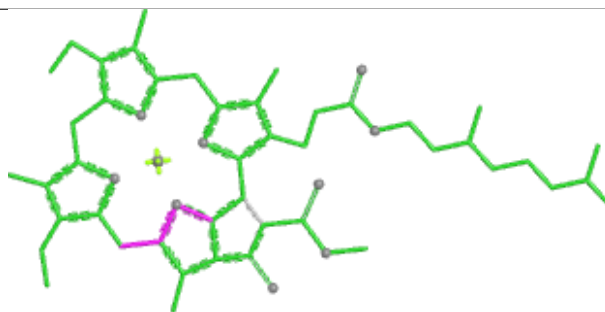


Rings

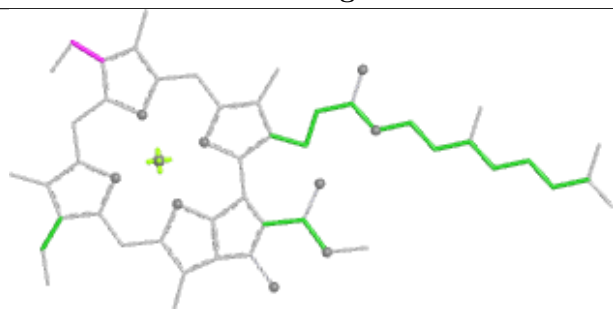
Ligand CLA A 825



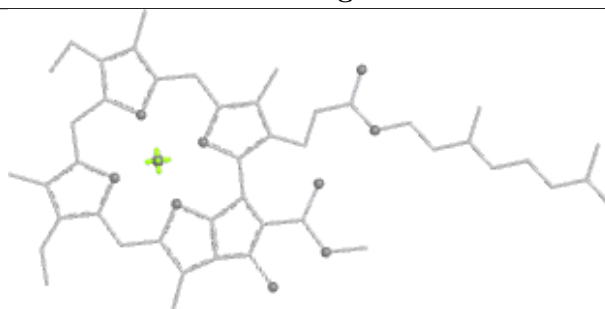
Bond lengths



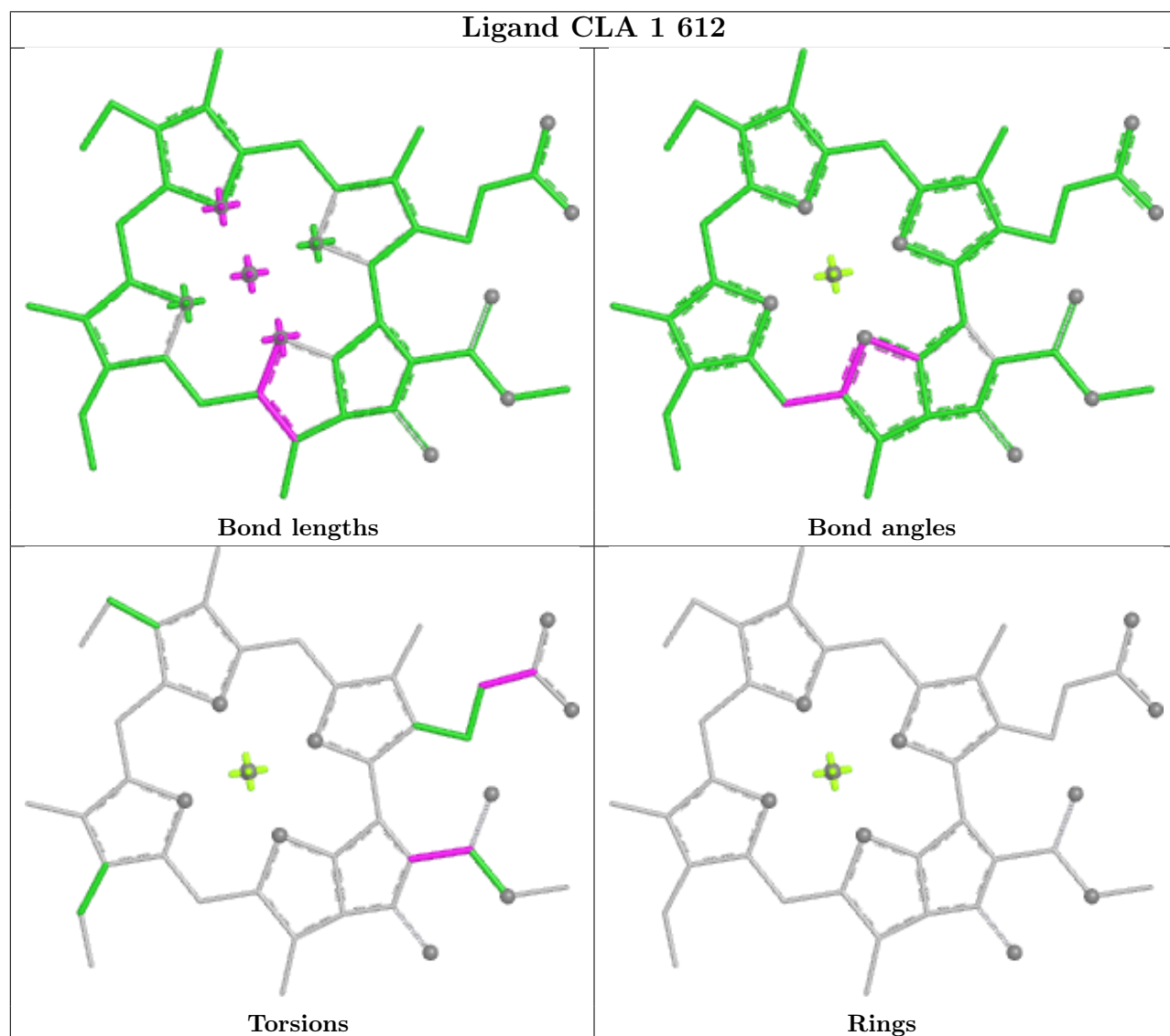
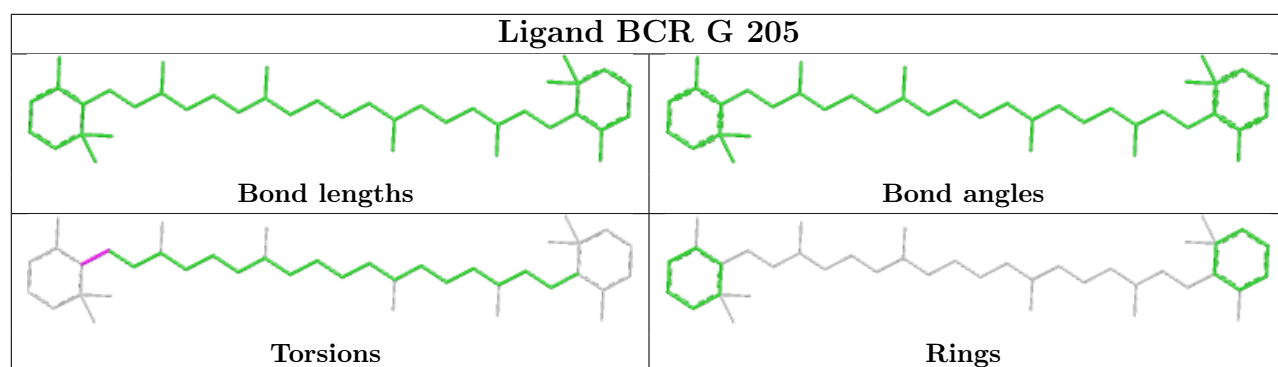
Bond angles

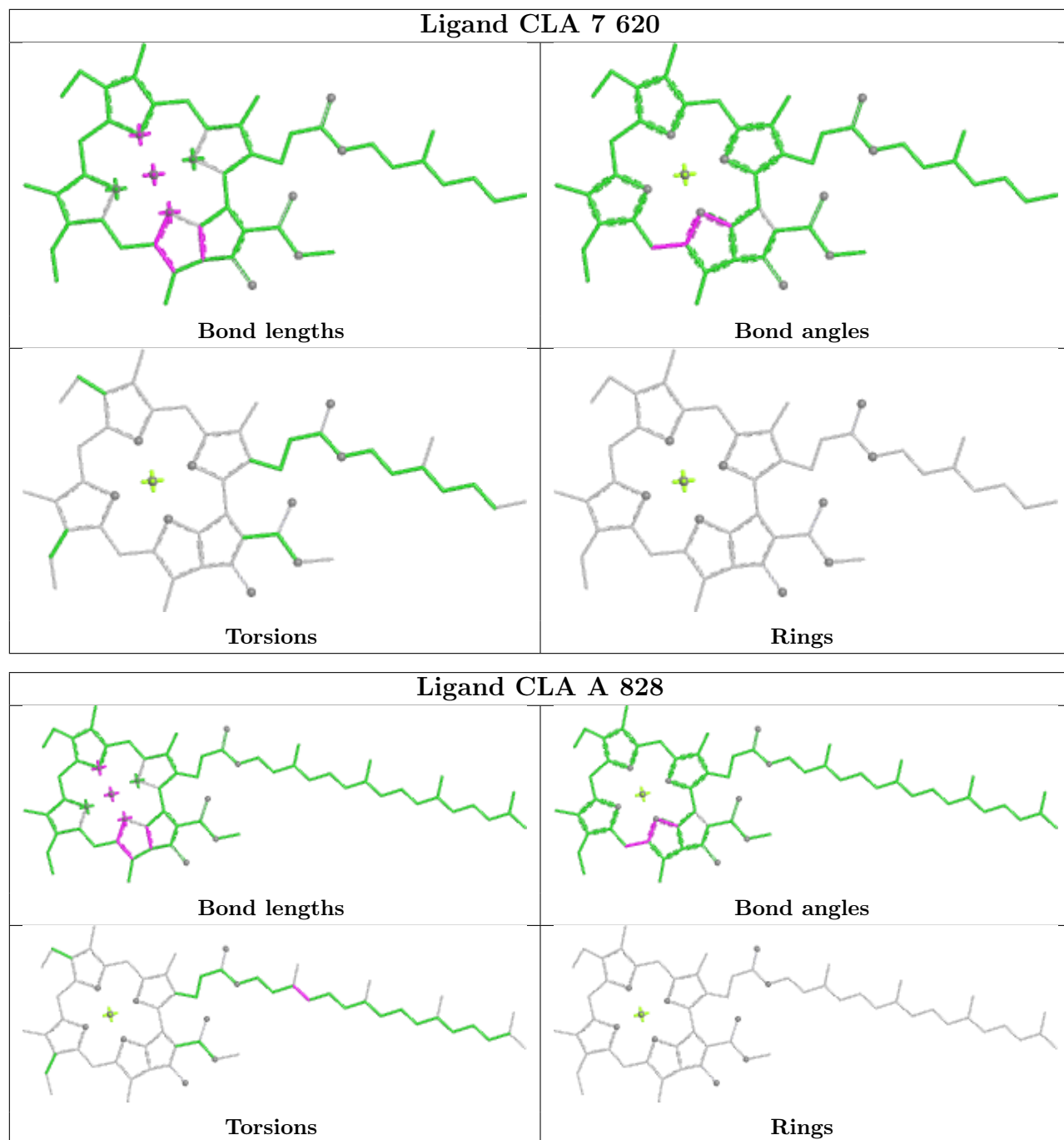


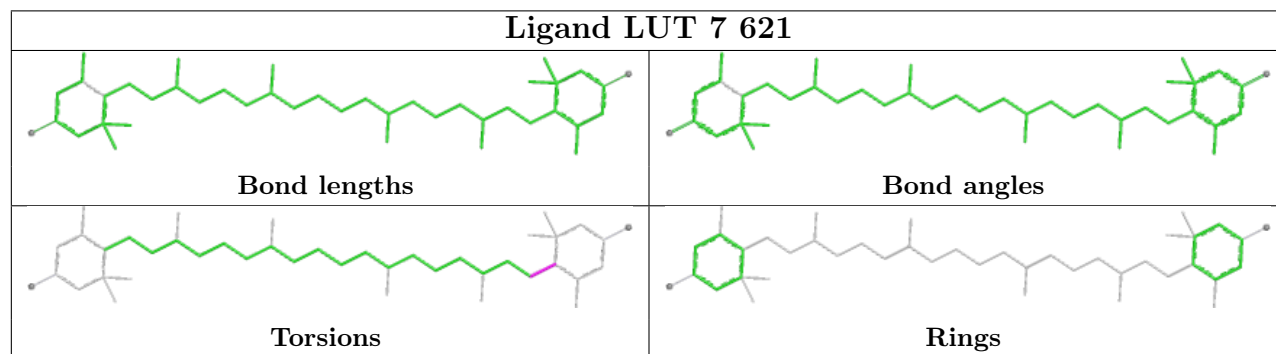
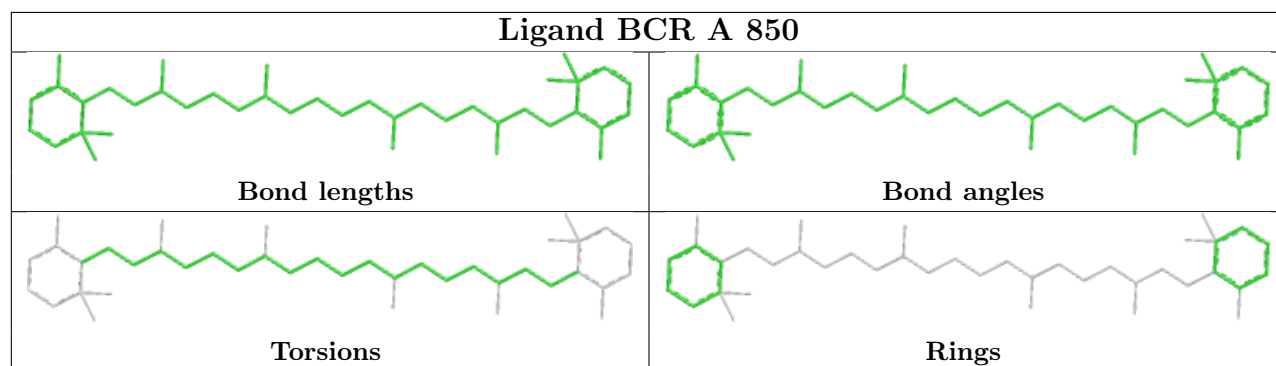
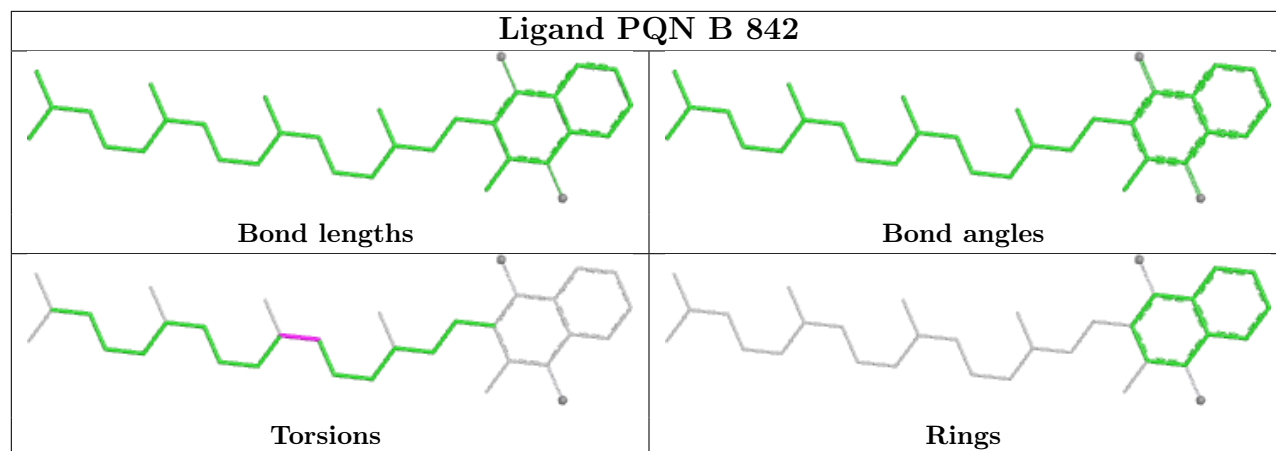
Torsions



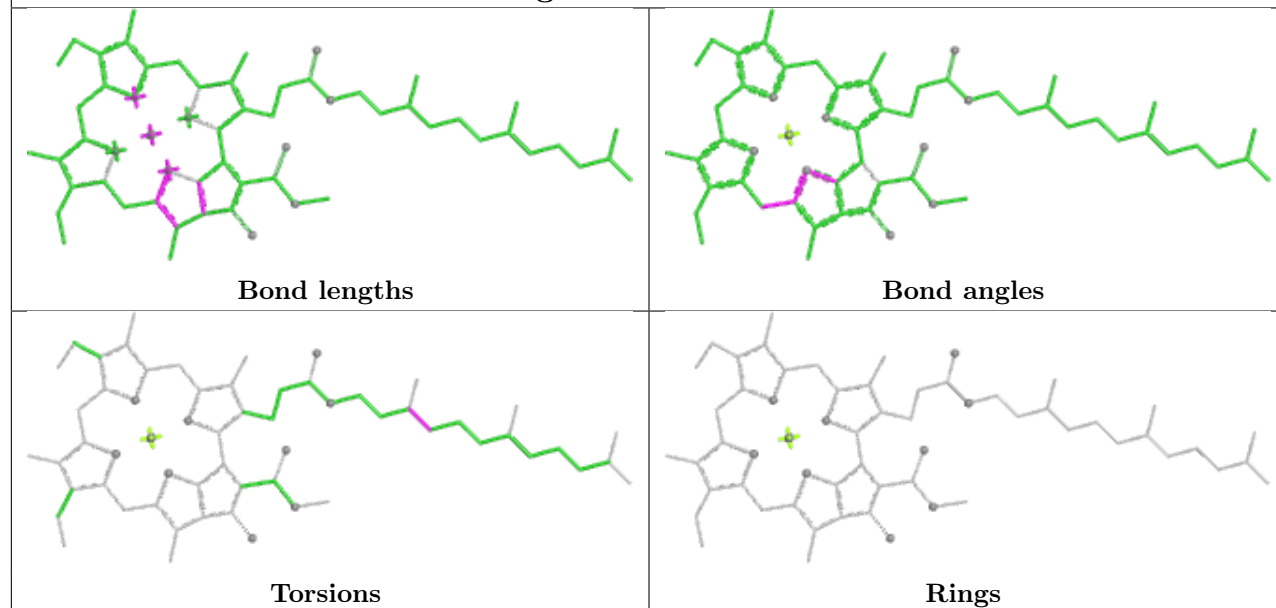
Rings



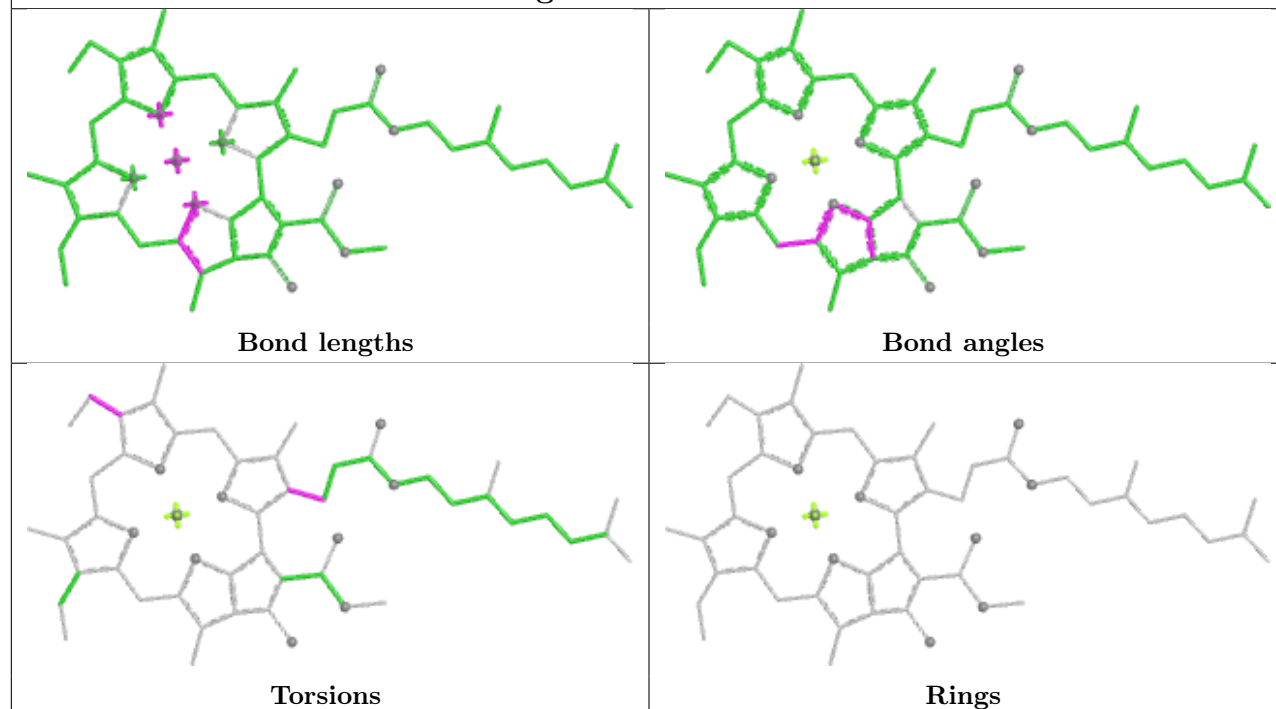




Ligand CLA 8 604

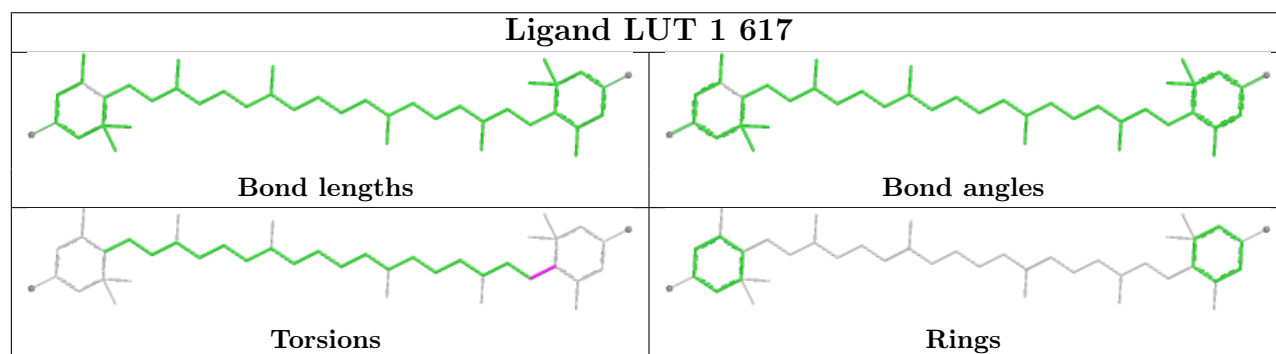
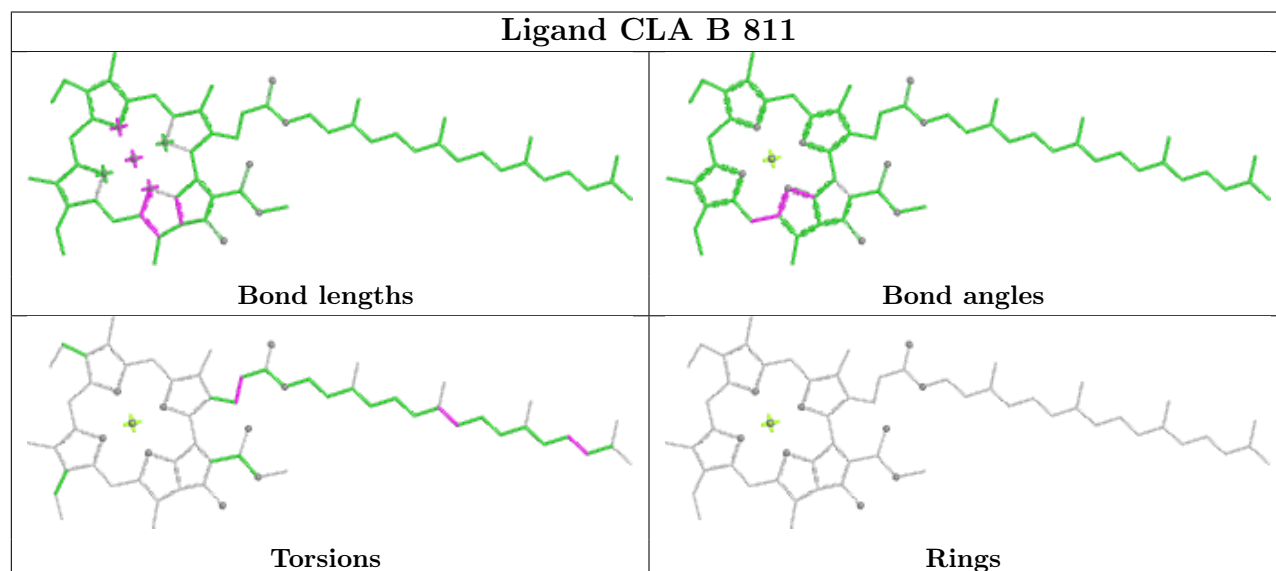
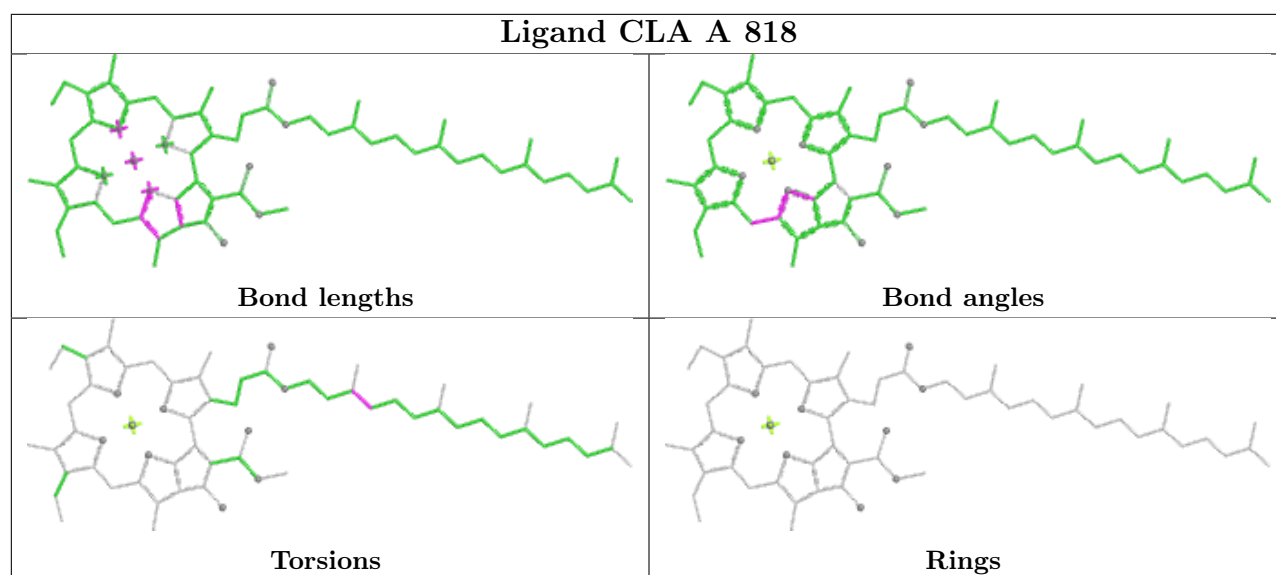


Ligand CLA 3 611

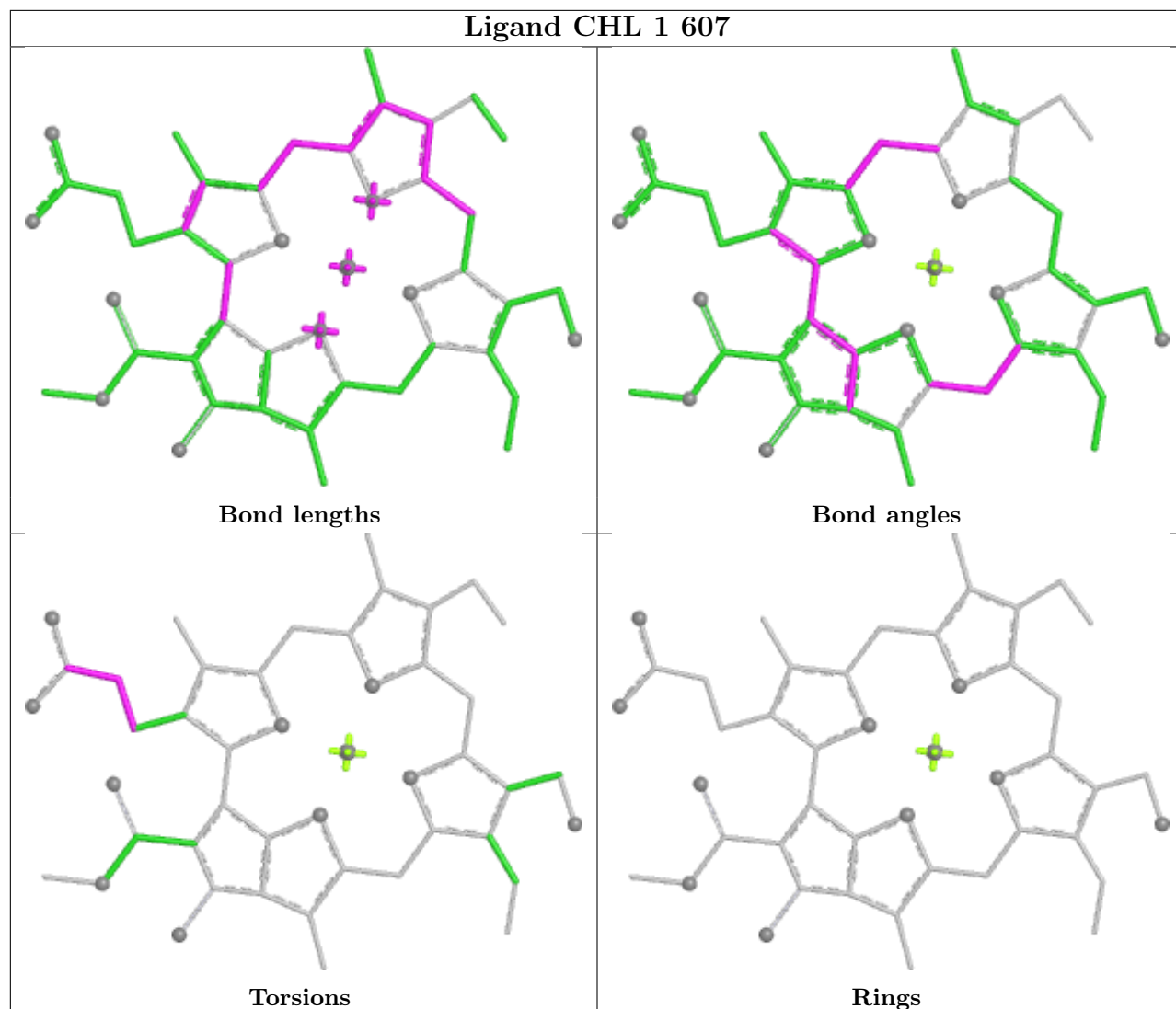


Ligand LMG 6 633

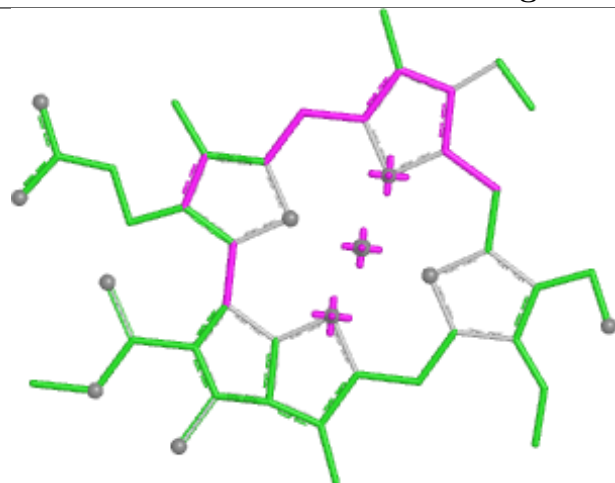




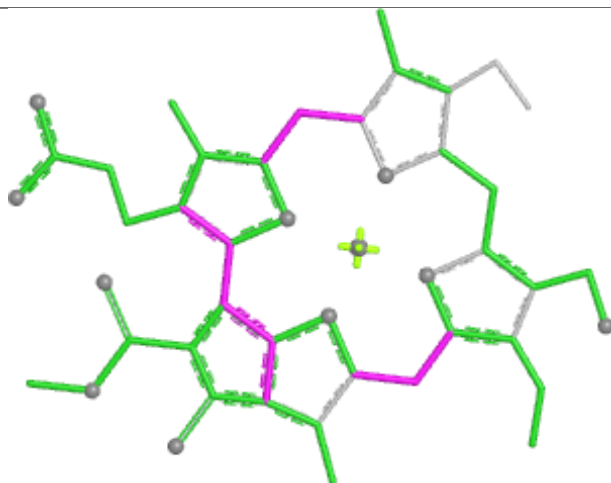
Ligand CHL 1 607



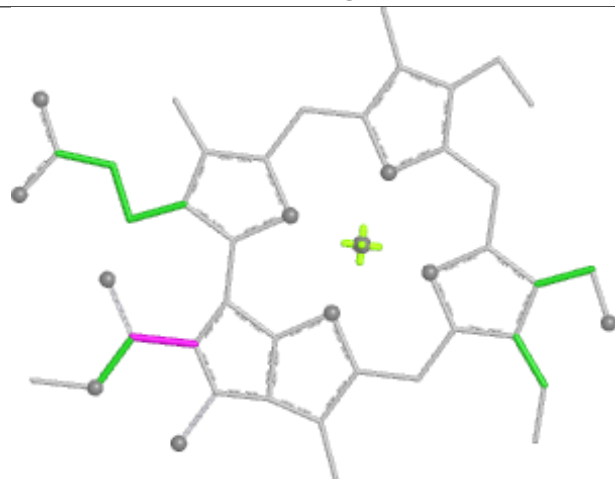
Ligand CHL 5 606



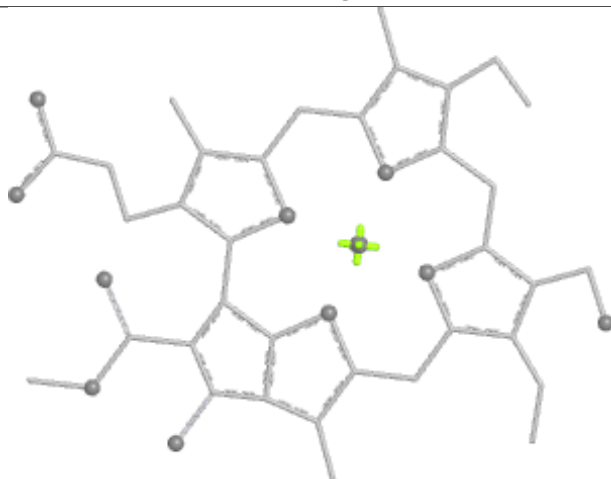
Bond lengths



Bond angles

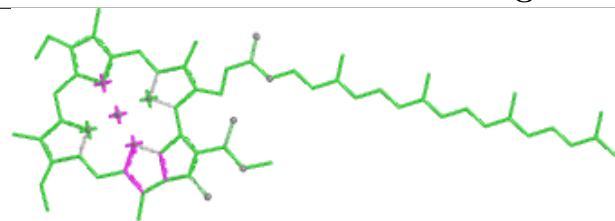


Torsions

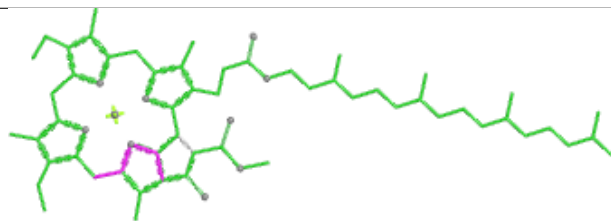


Rings

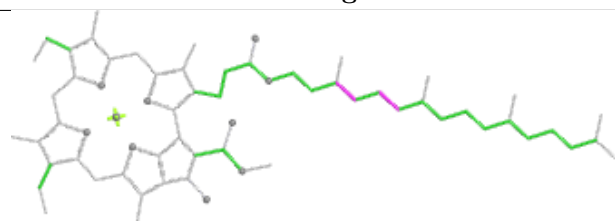
Ligand CLA A 839



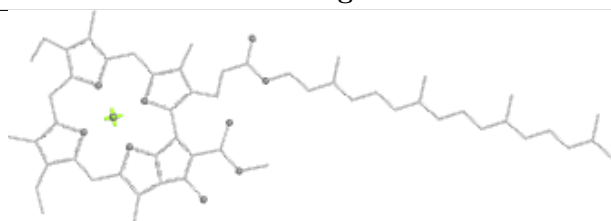
Bond lengths



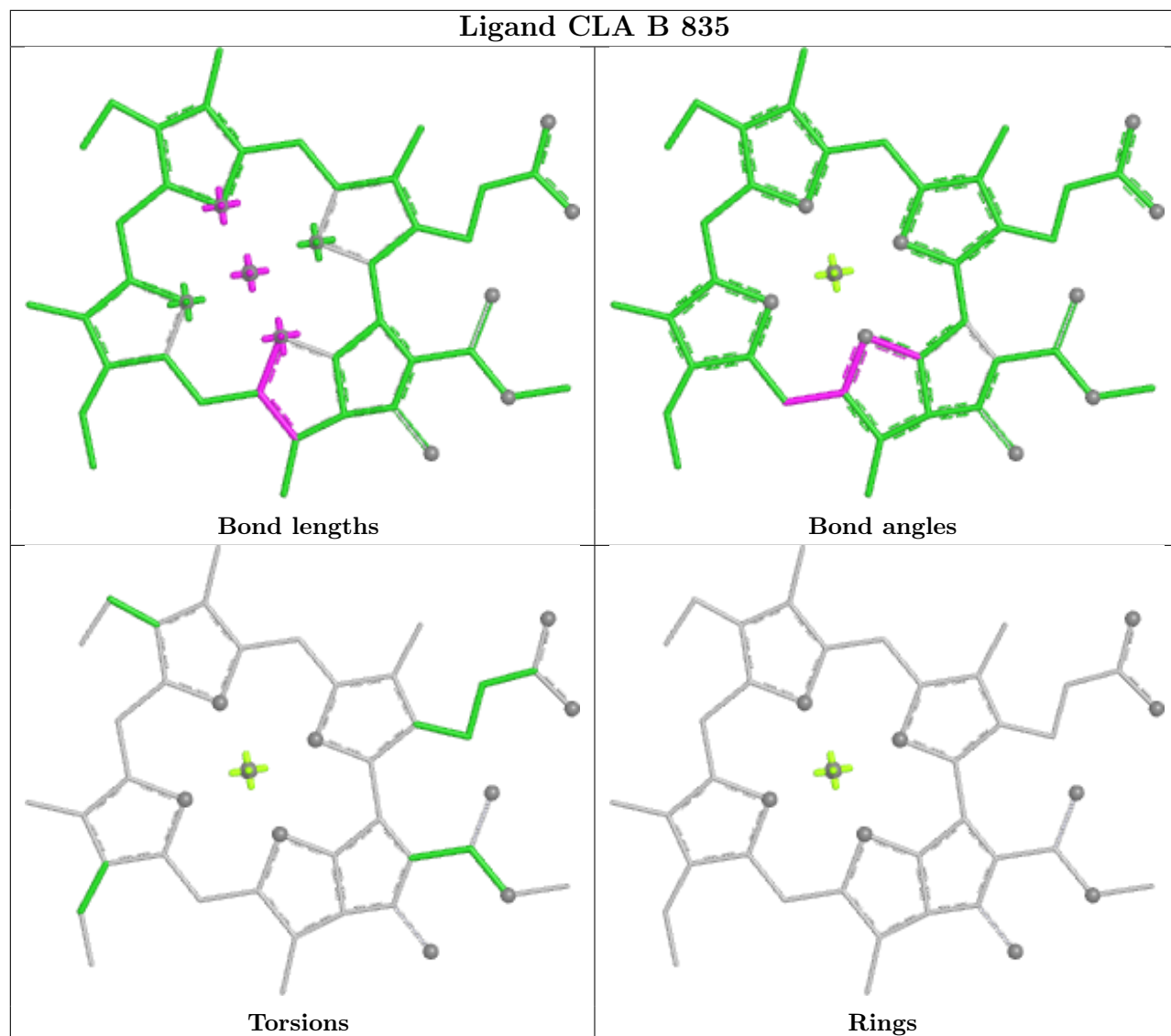
Bond angles

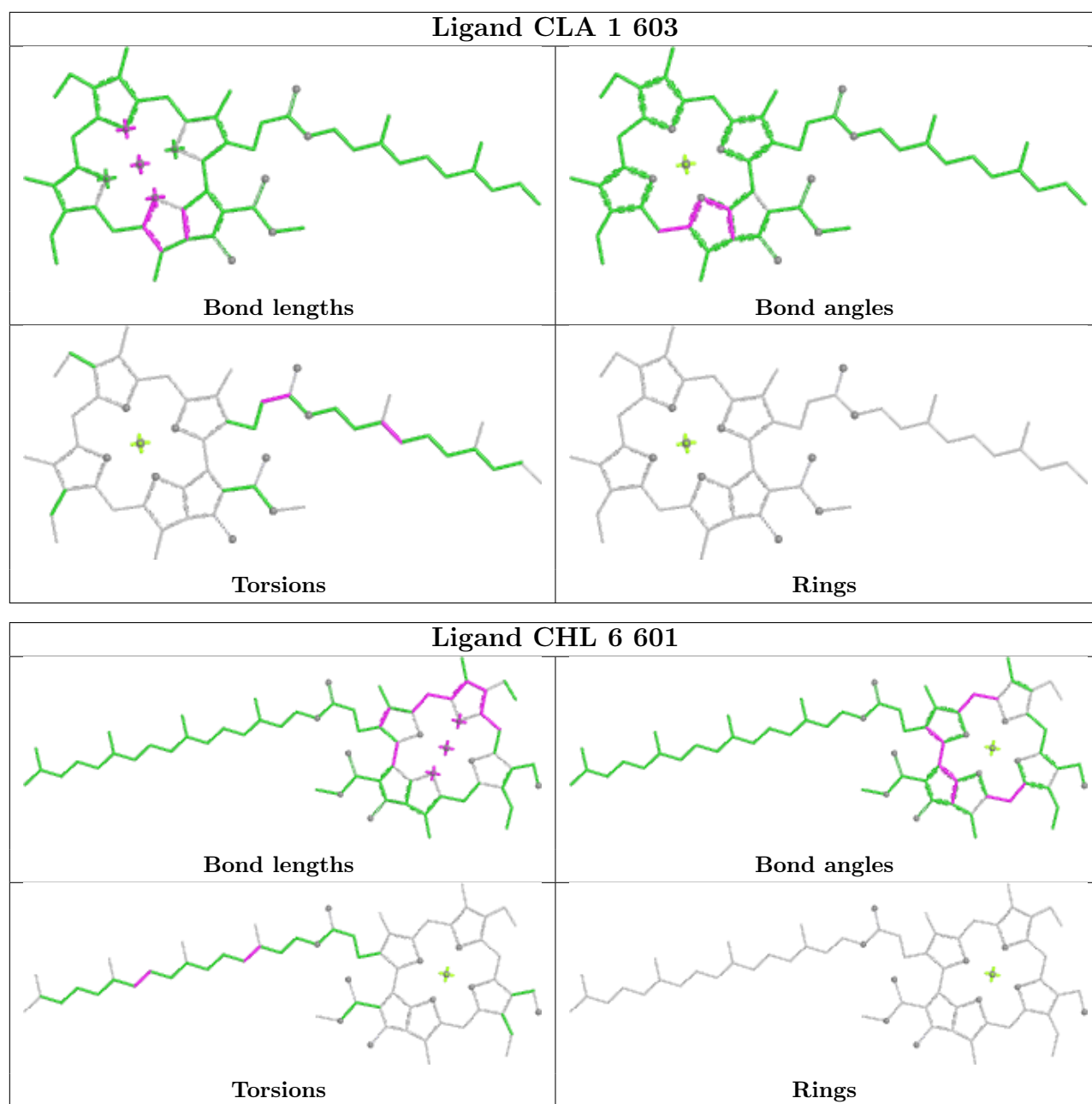


Torsions

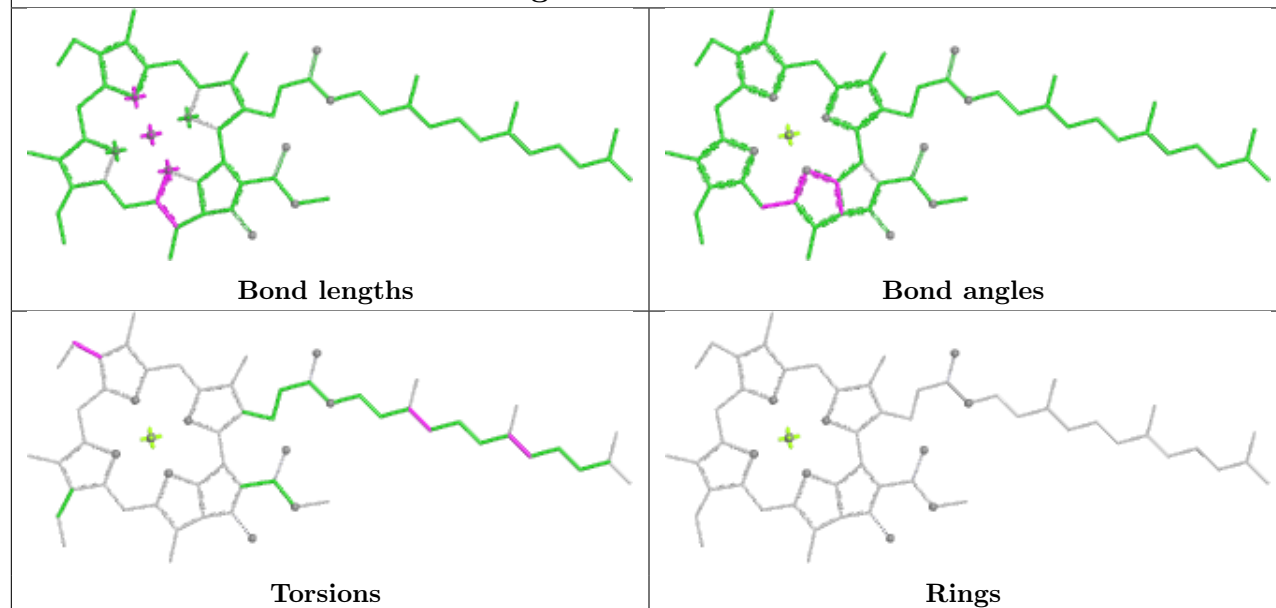


Rings

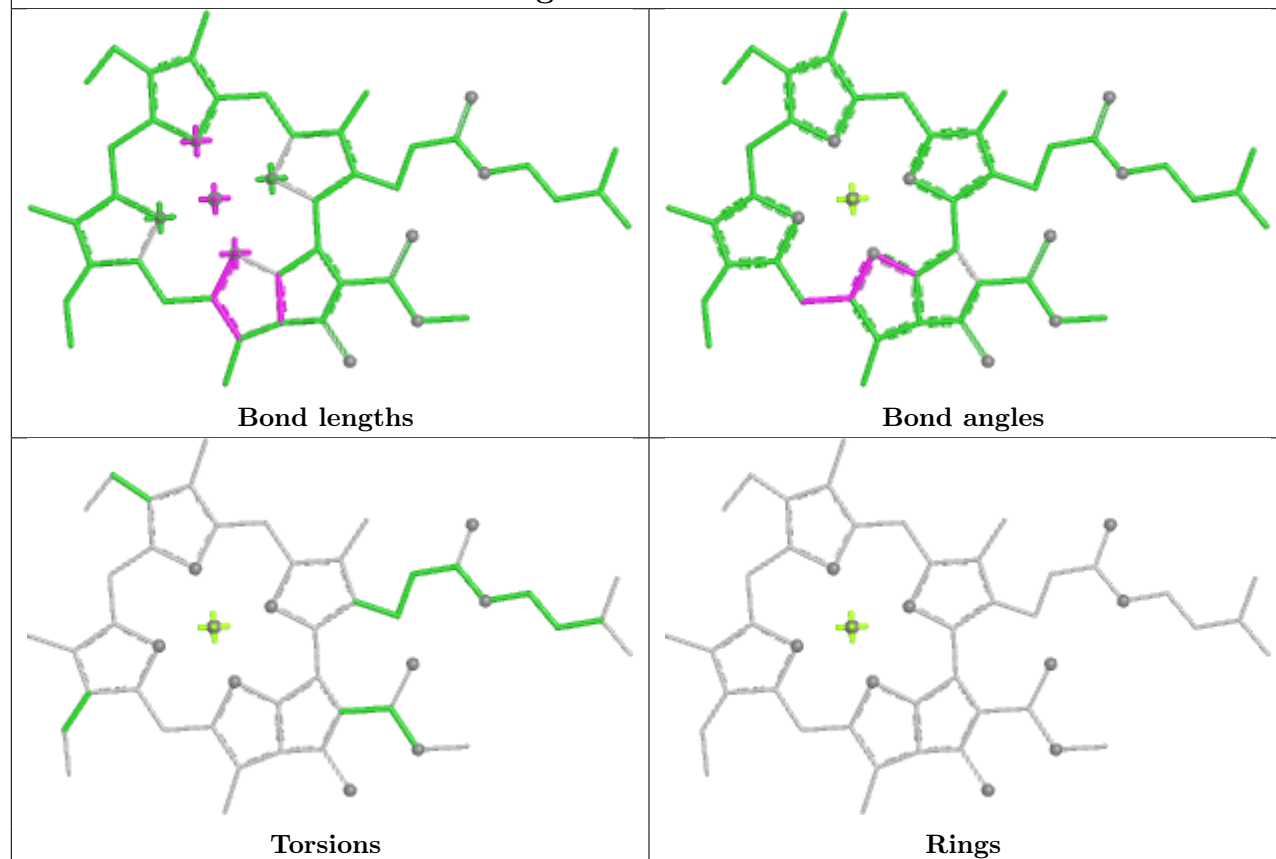


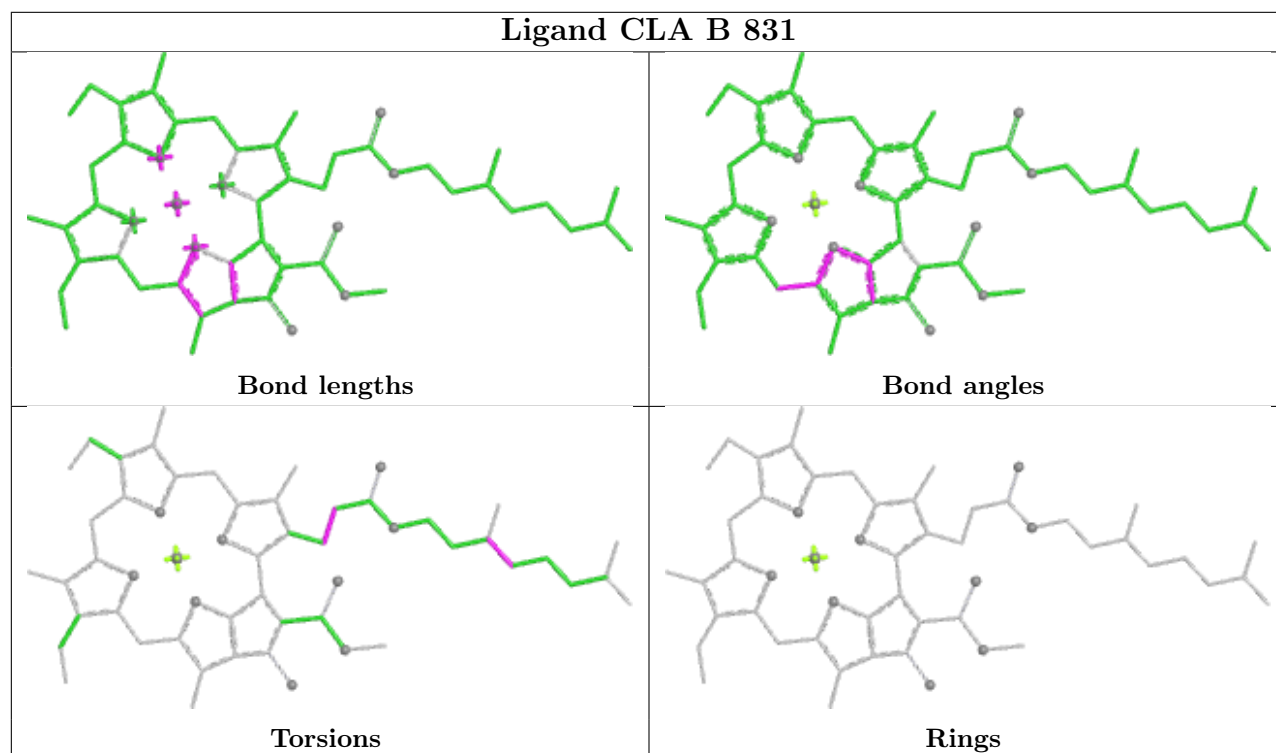
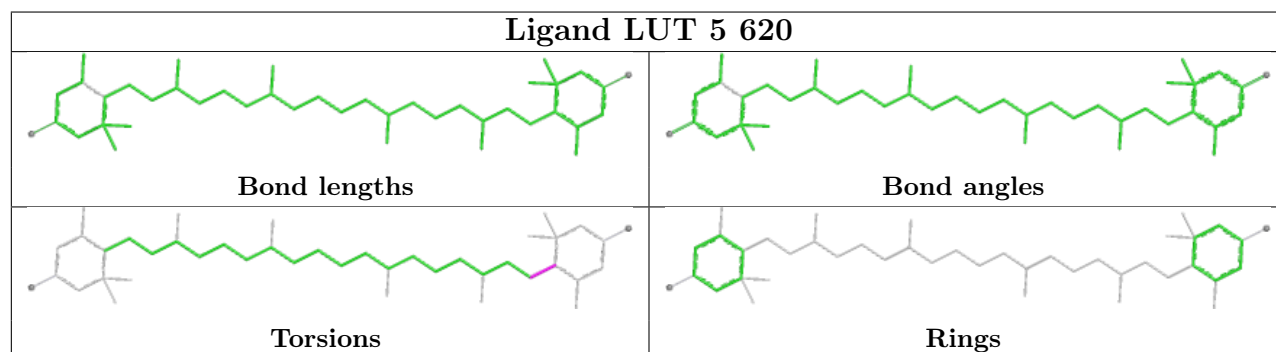
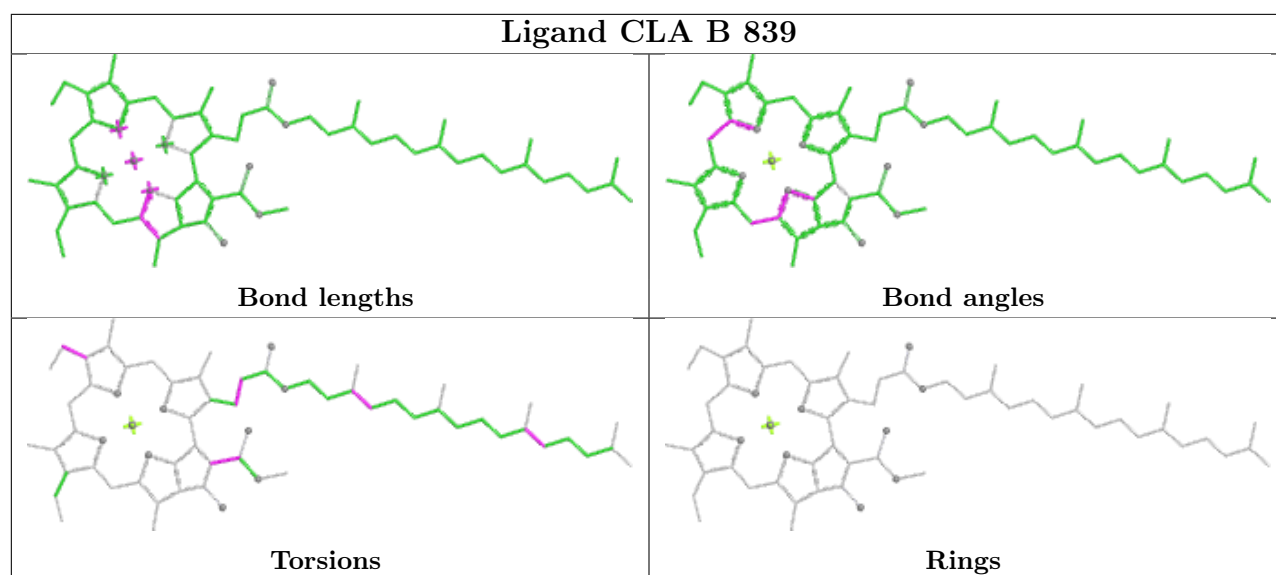


Ligand CLA K 203

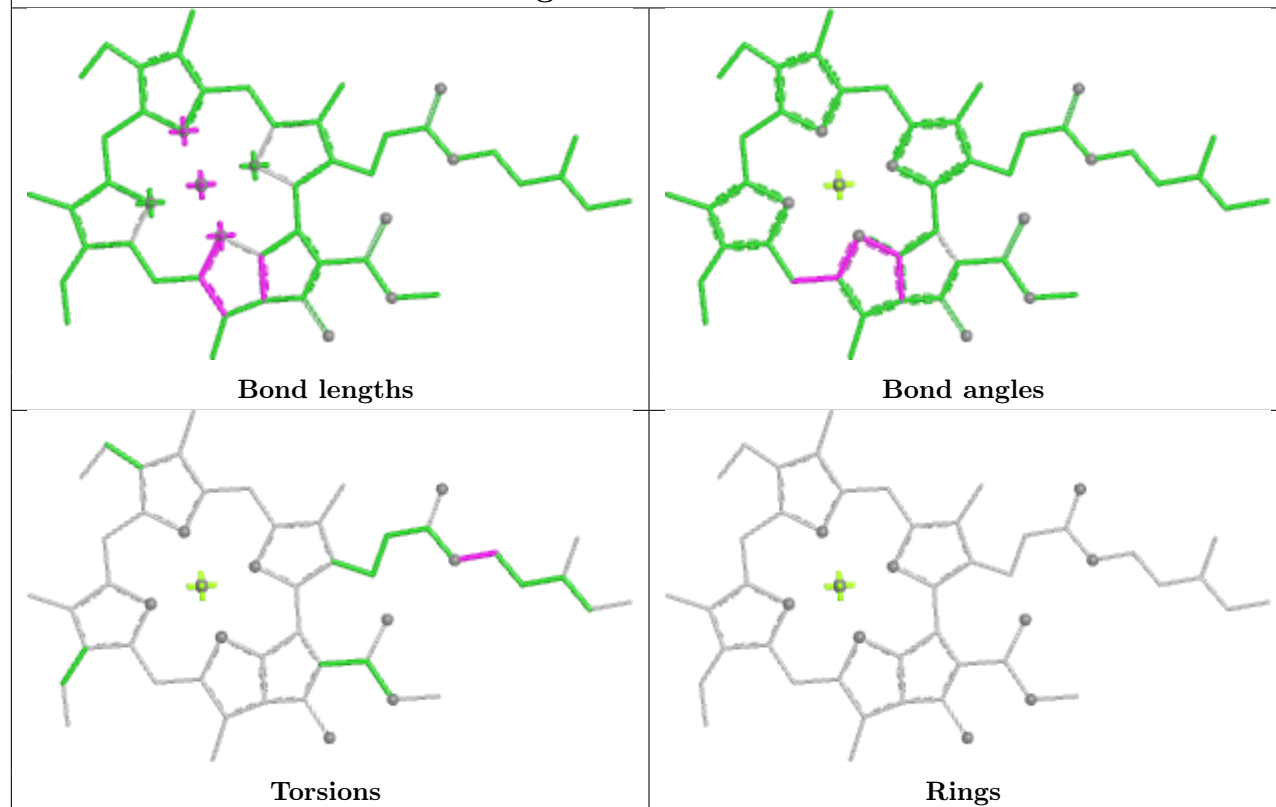


Ligand CLA 7 608

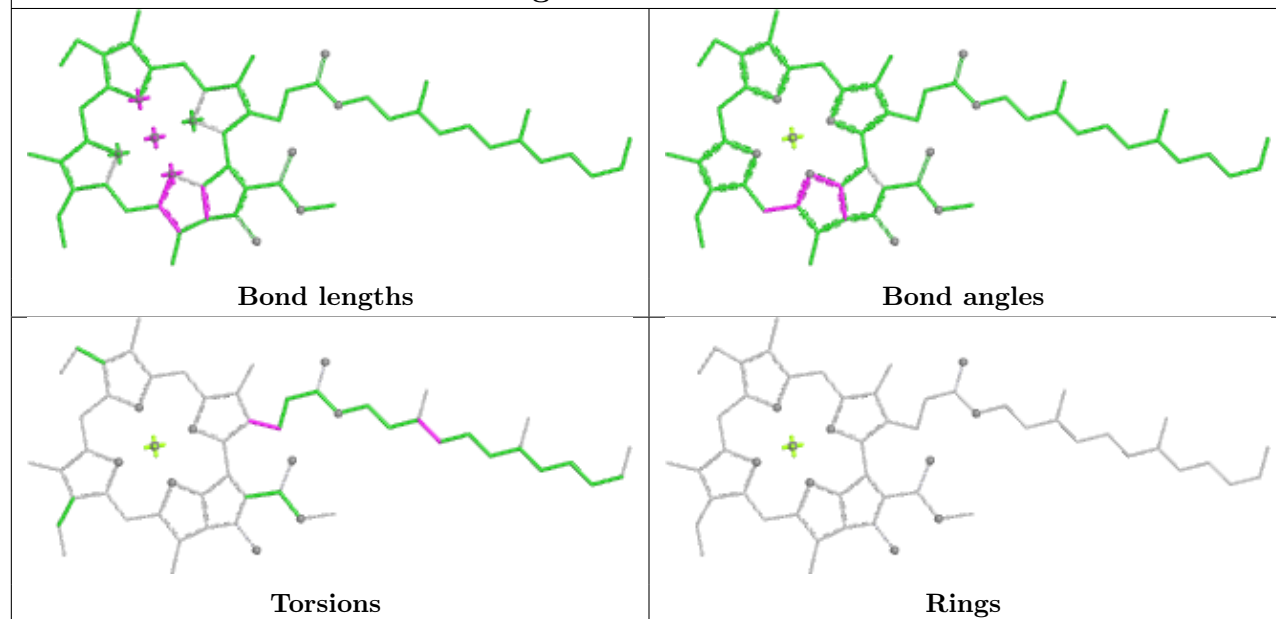


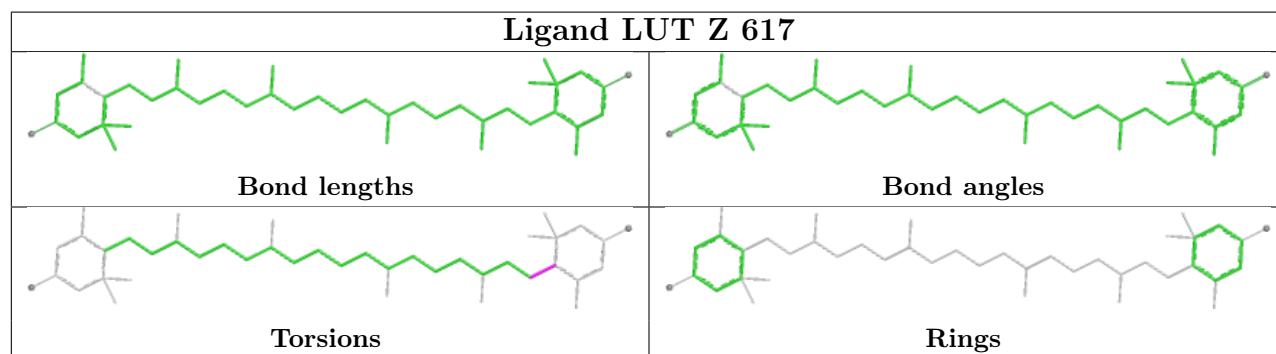
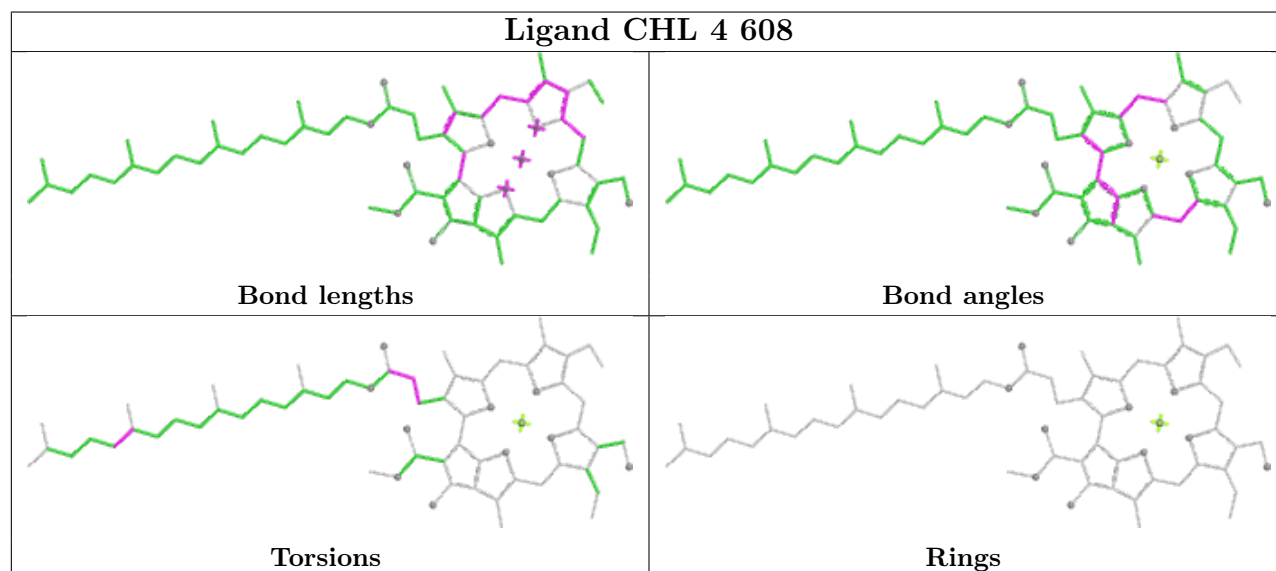
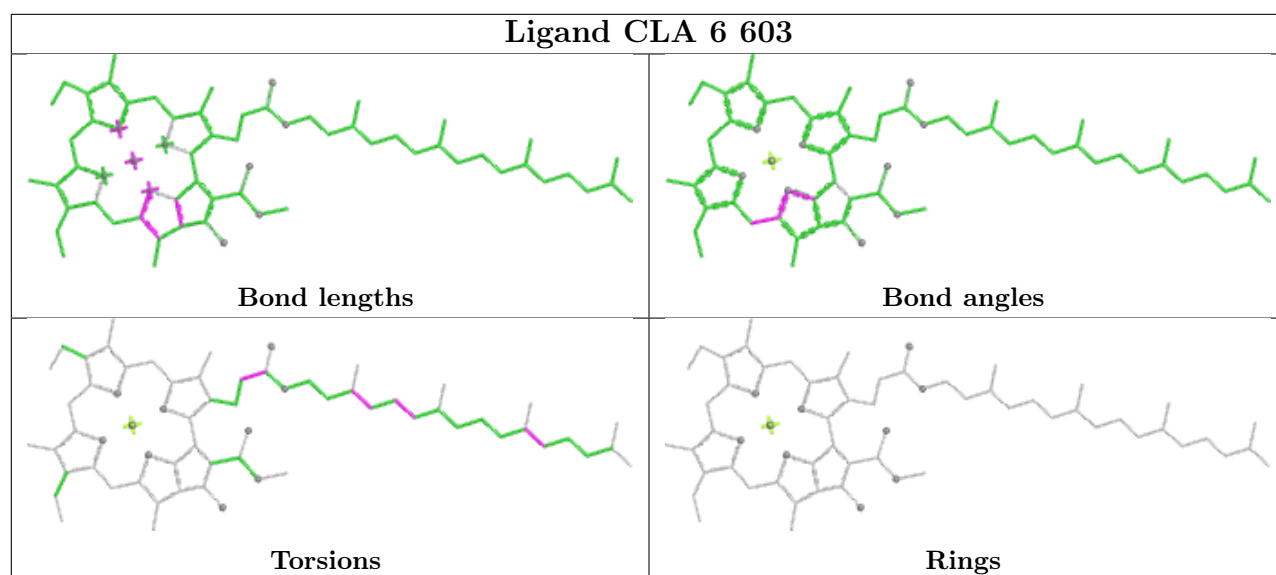


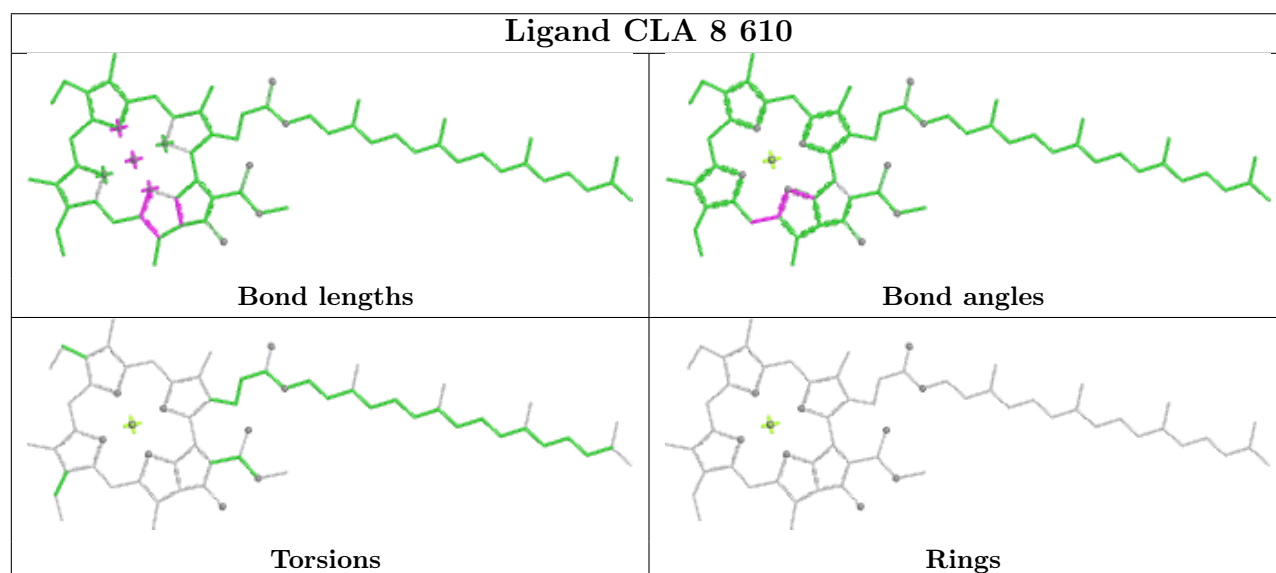
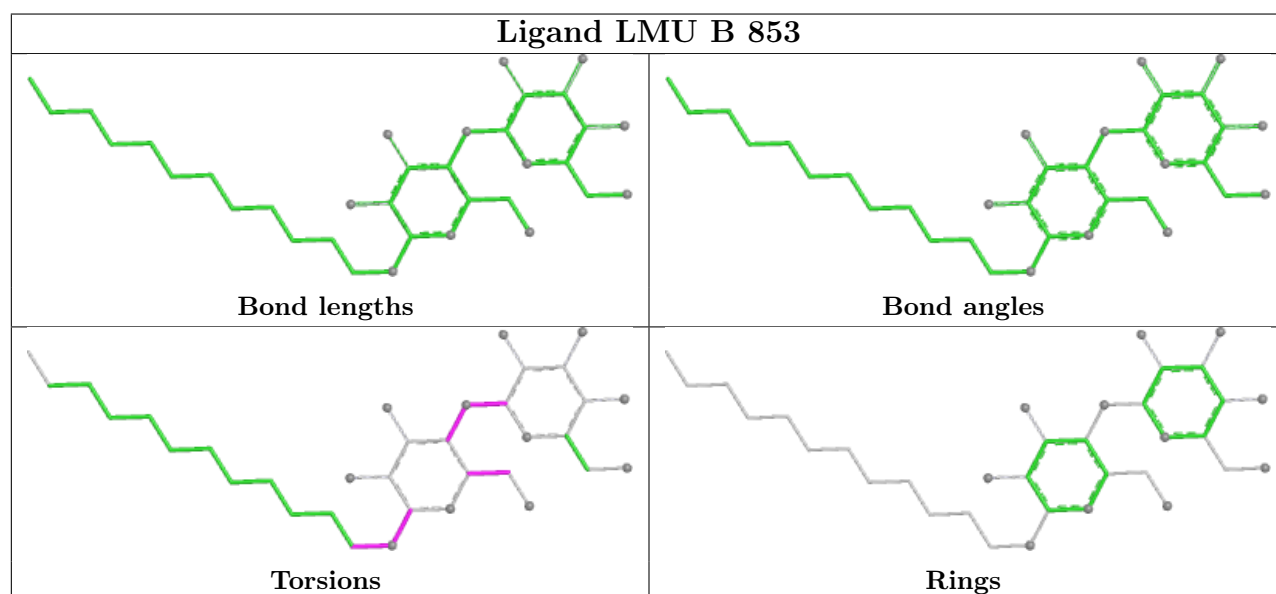
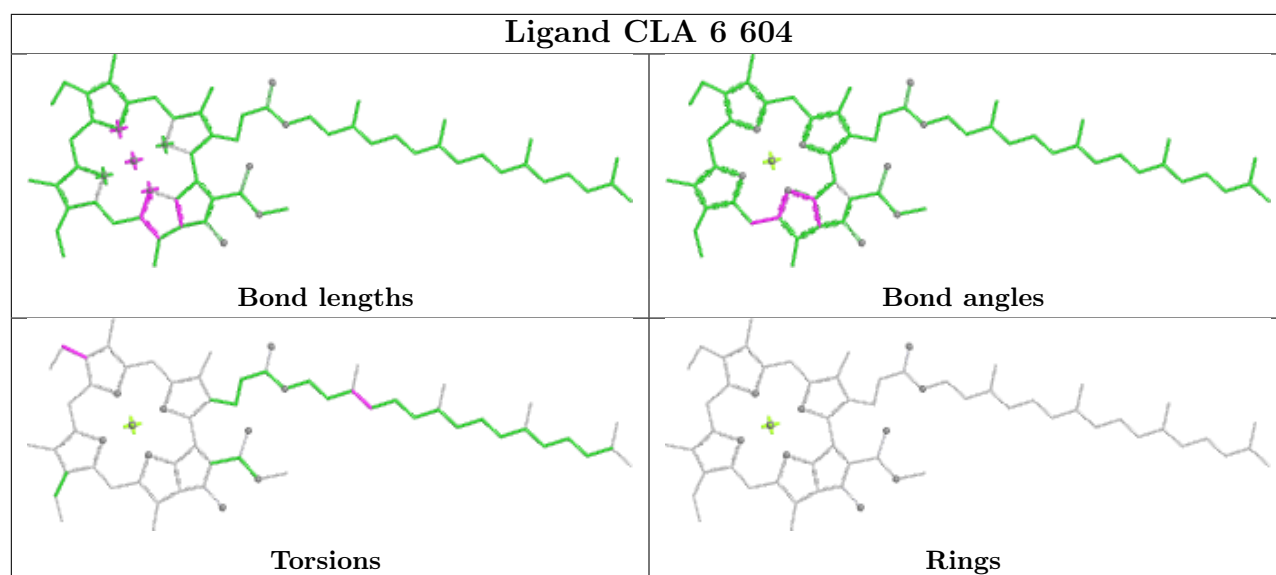
Ligand CLA 7 604

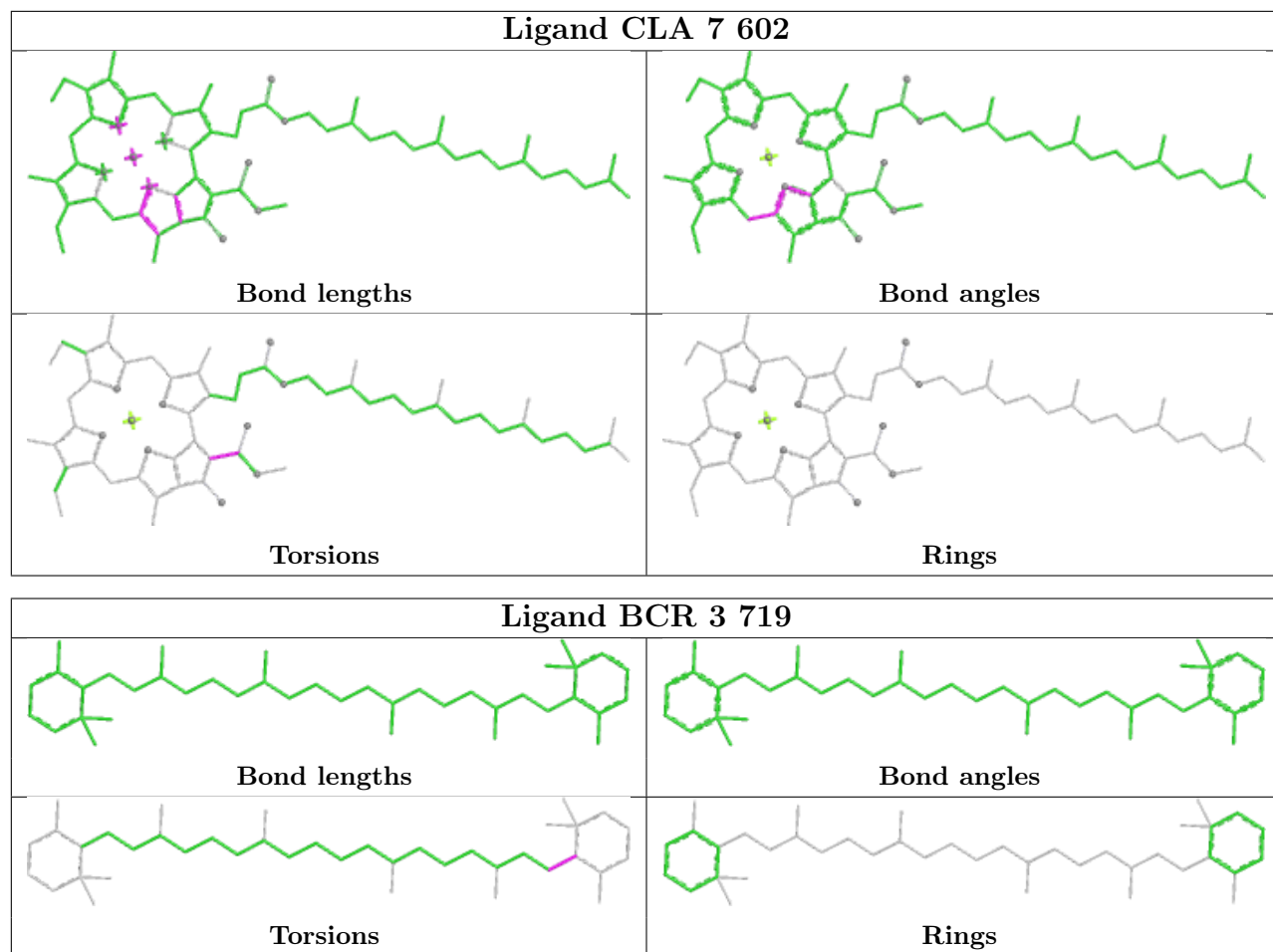


Ligand CLA B 822

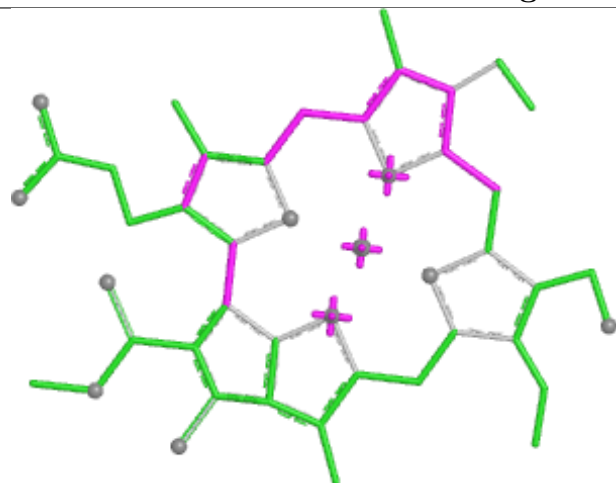




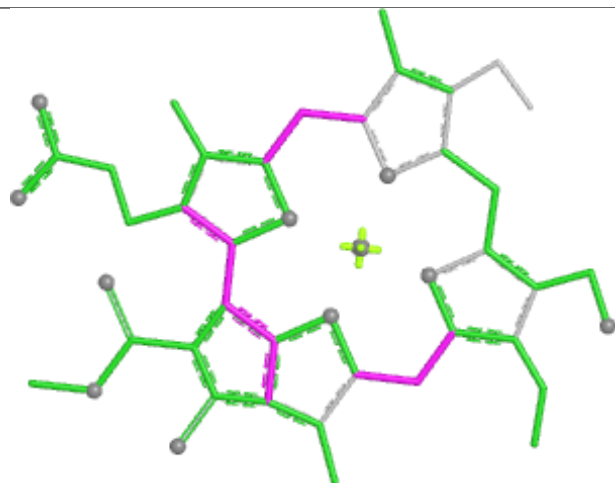




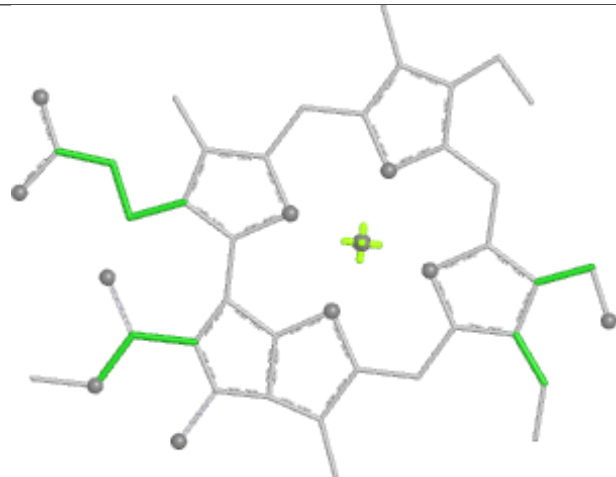
Ligand CHL 1 606



Bond lengths



Bond angles

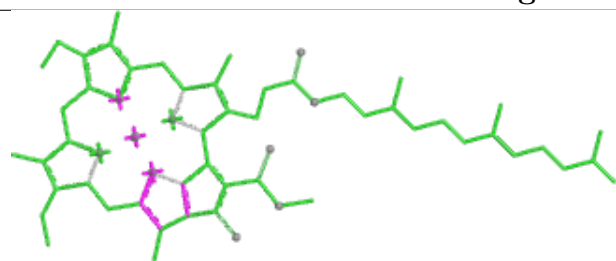


Torsions

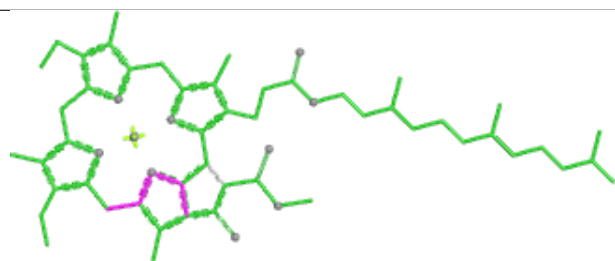


Rings

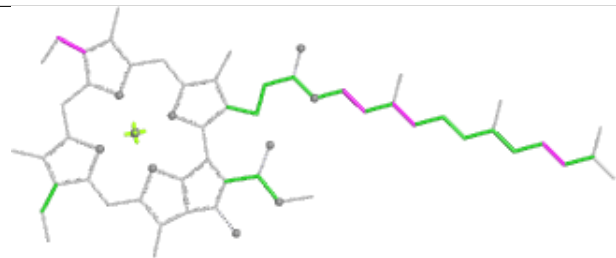
Ligand CLA Z 611



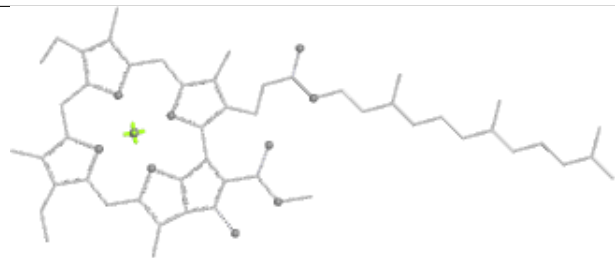
Bond lengths



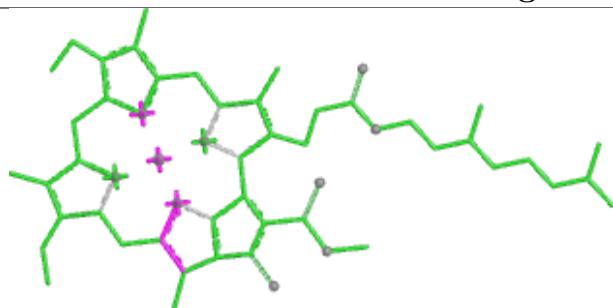
Bond angles



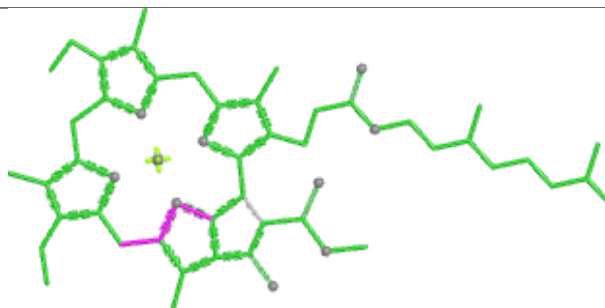
Torsions



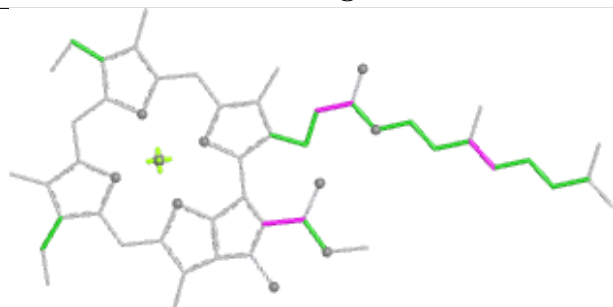
Rings

Ligand CLA 5 604

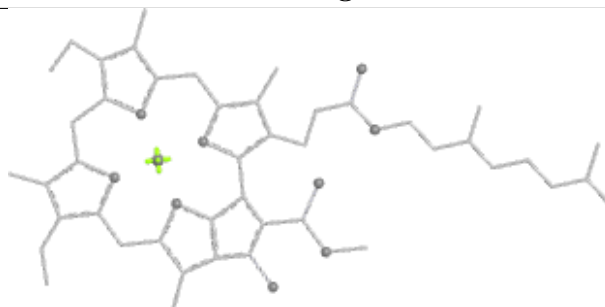
Bond lengths



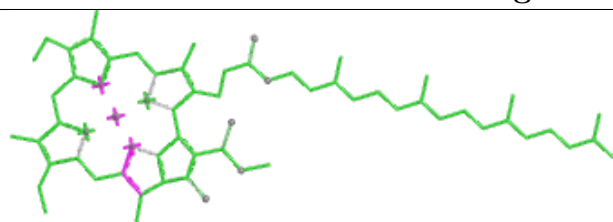
Bond angles



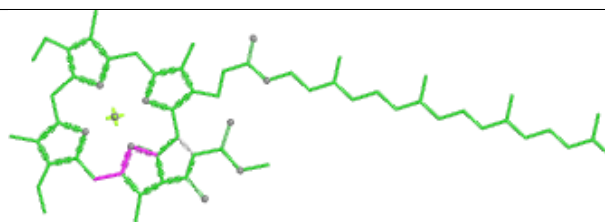
Torsions



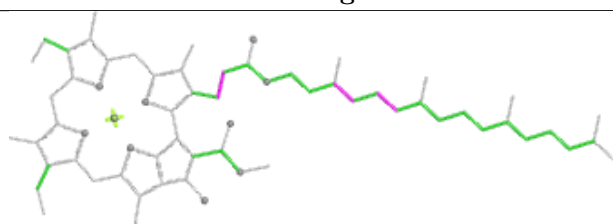
Rings

Ligand CLA A 830

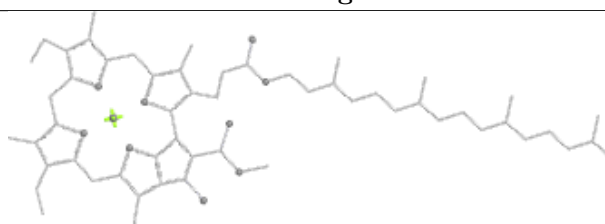
Bond lengths



Bond angles

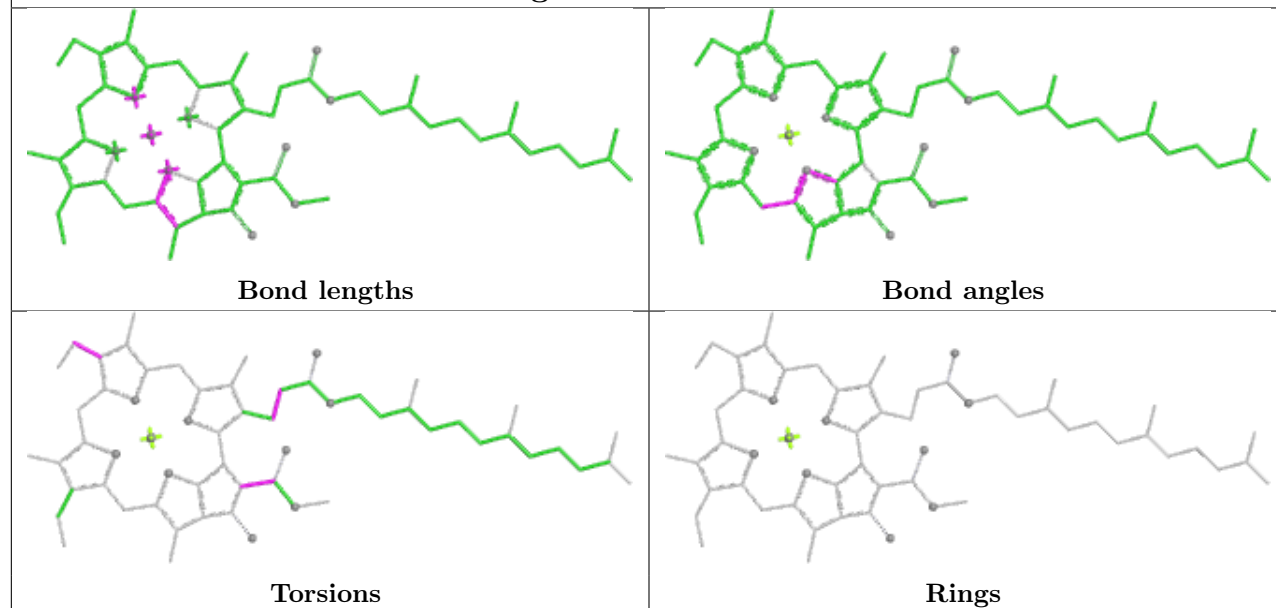


Torsions

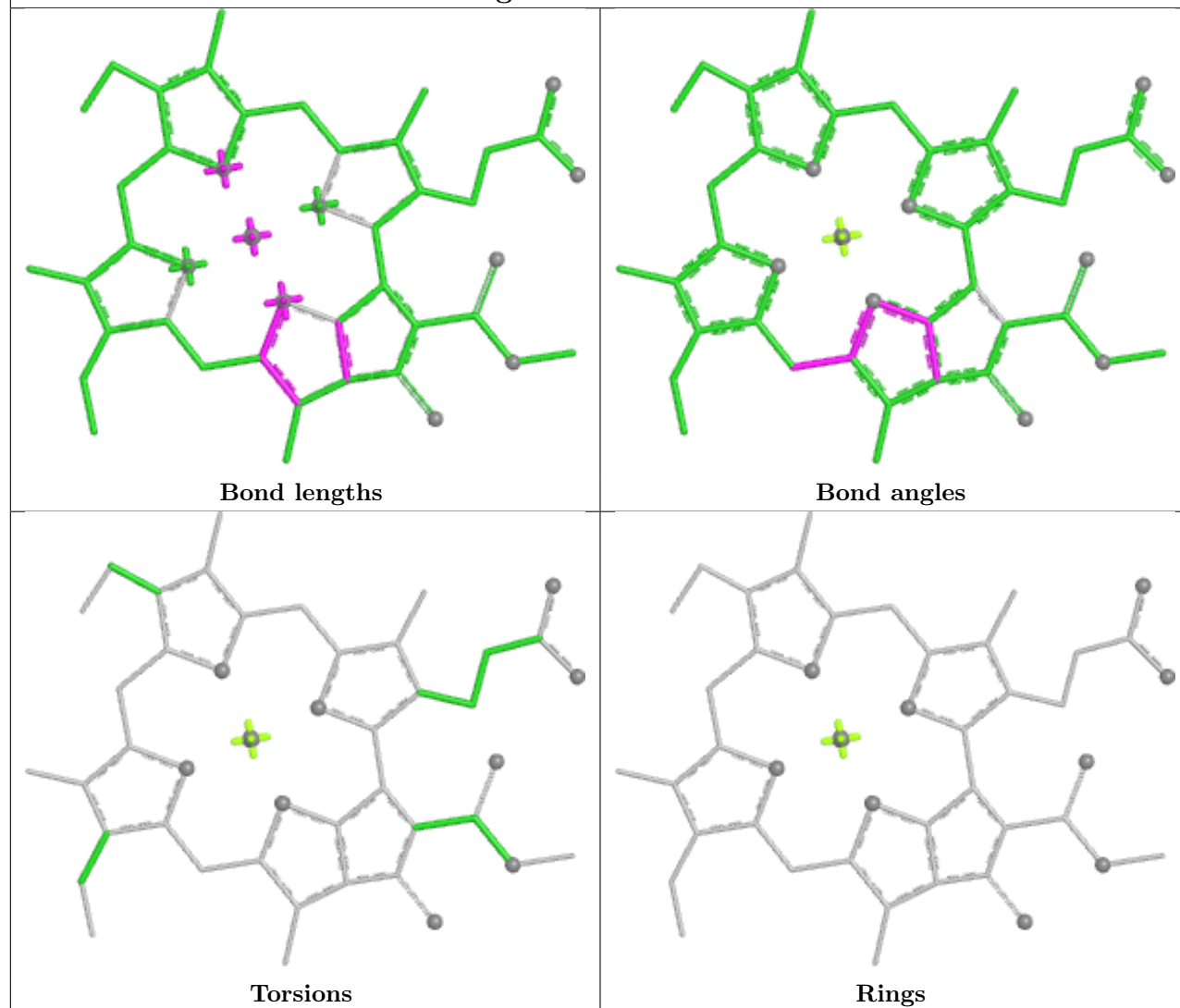


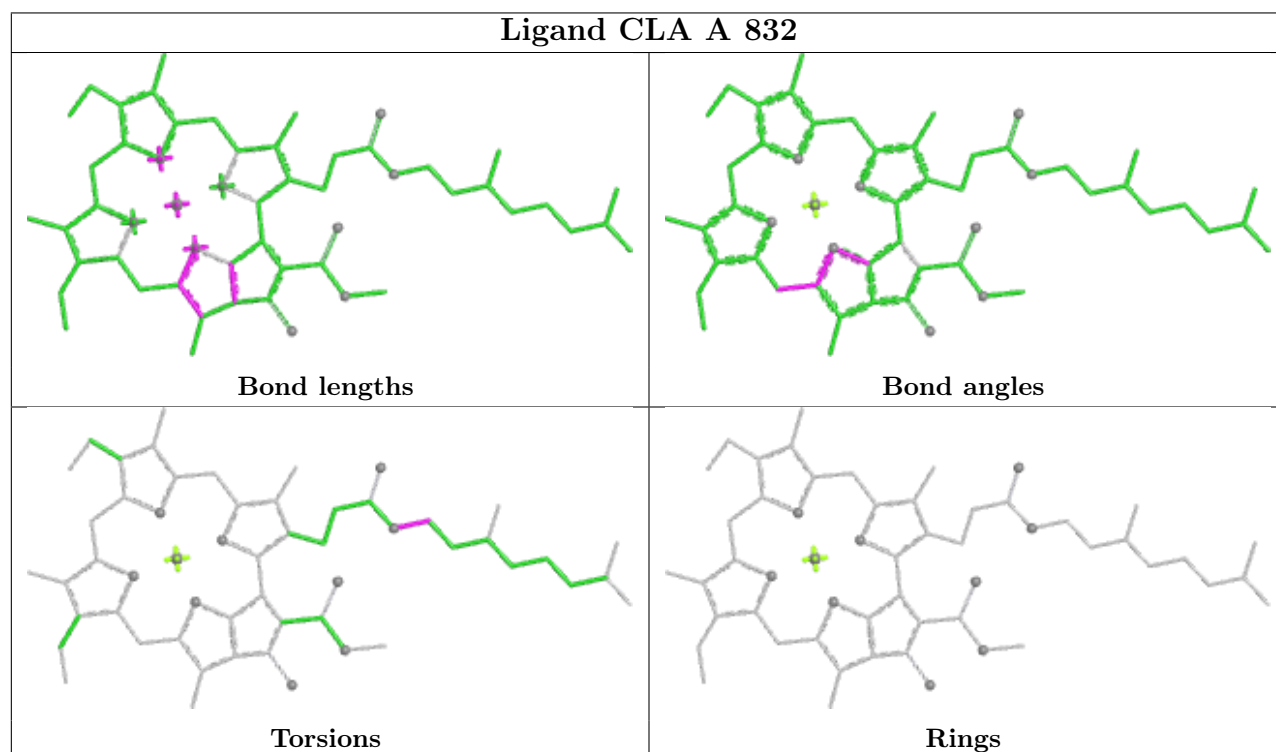
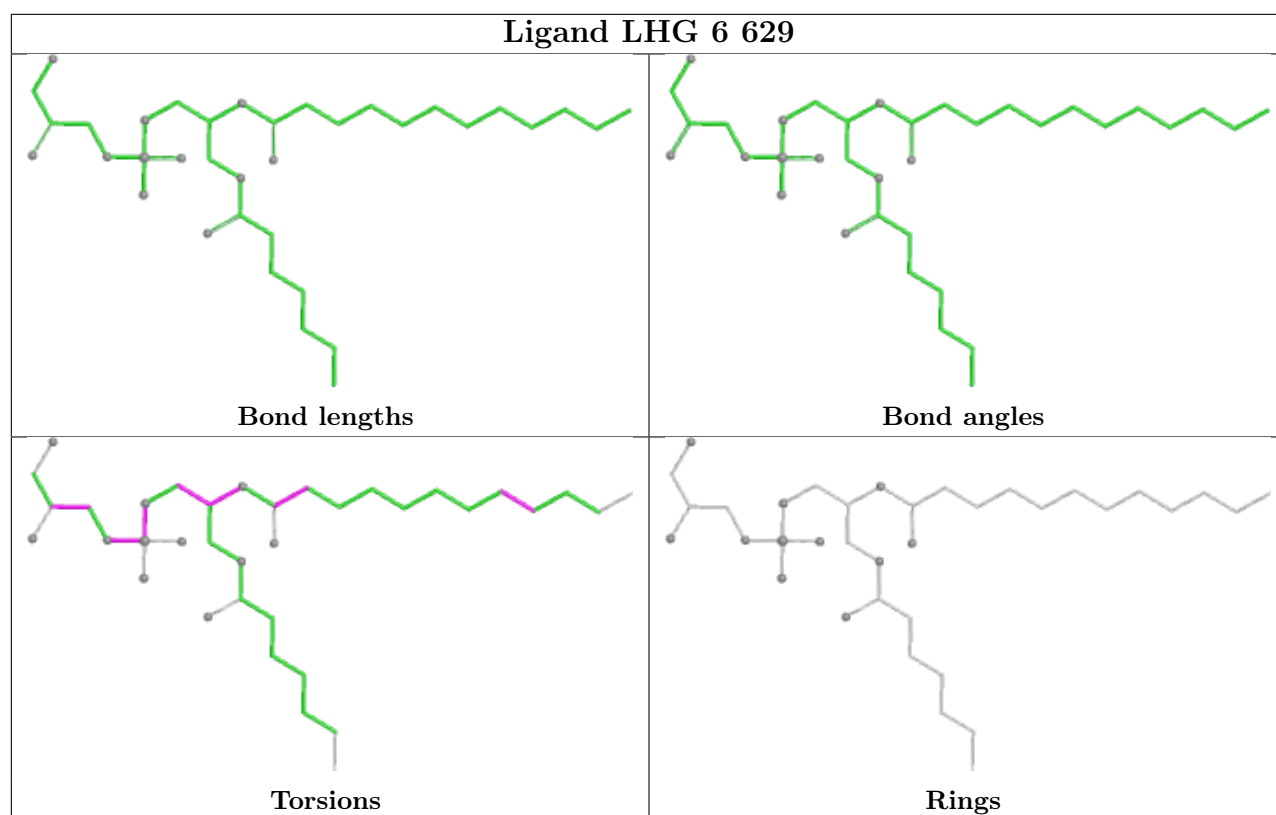
Rings

Ligand CLA G 203

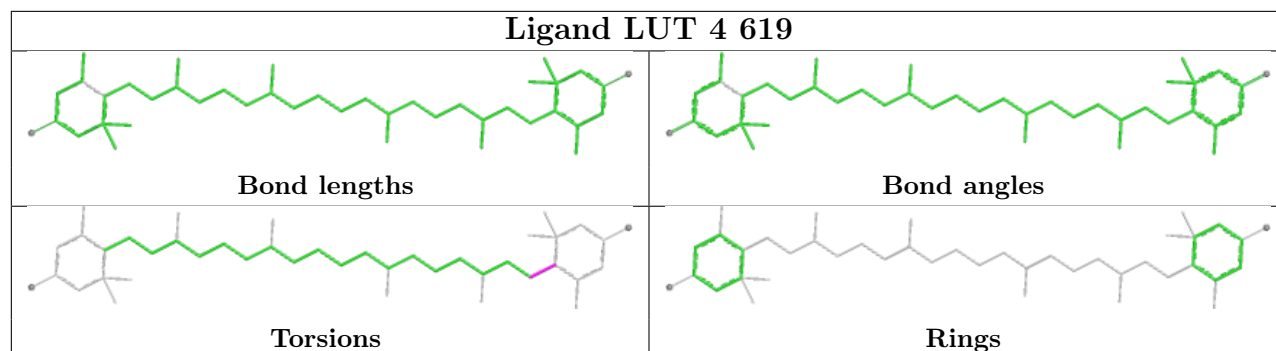


Ligand CLA 8 611

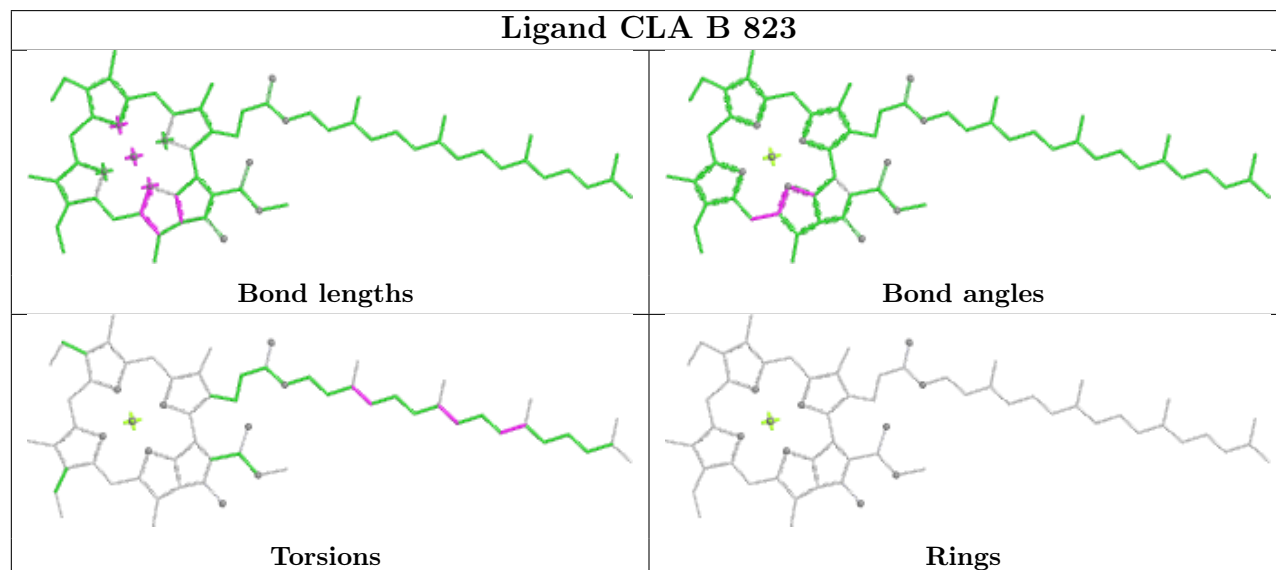




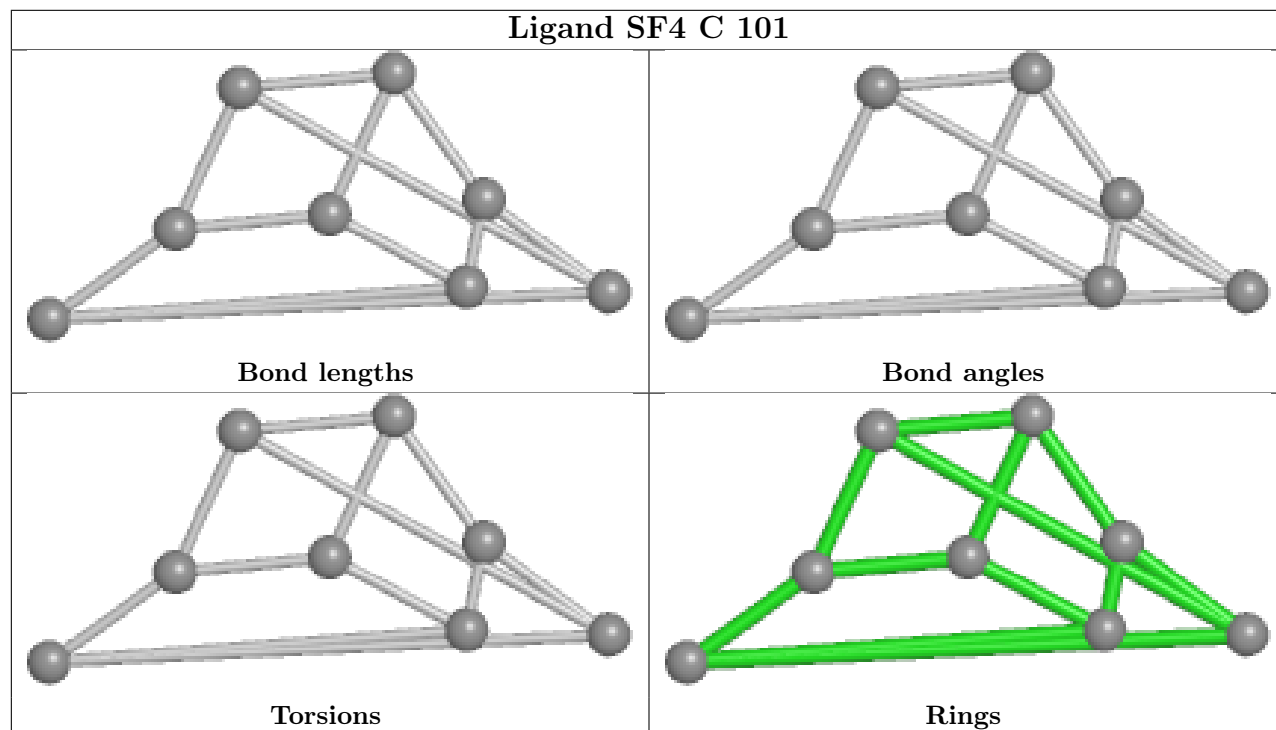
Ligand LUT 4 619

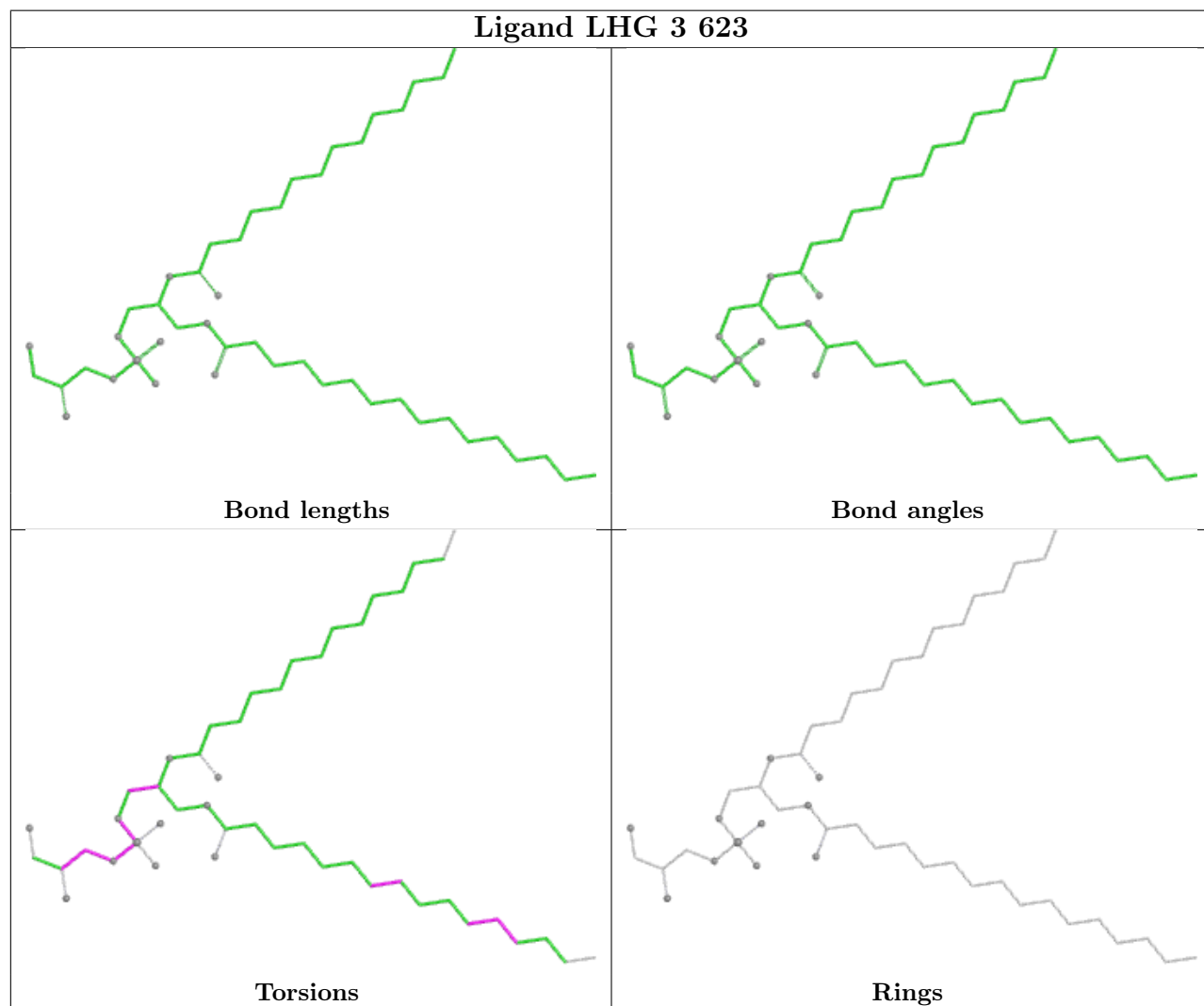
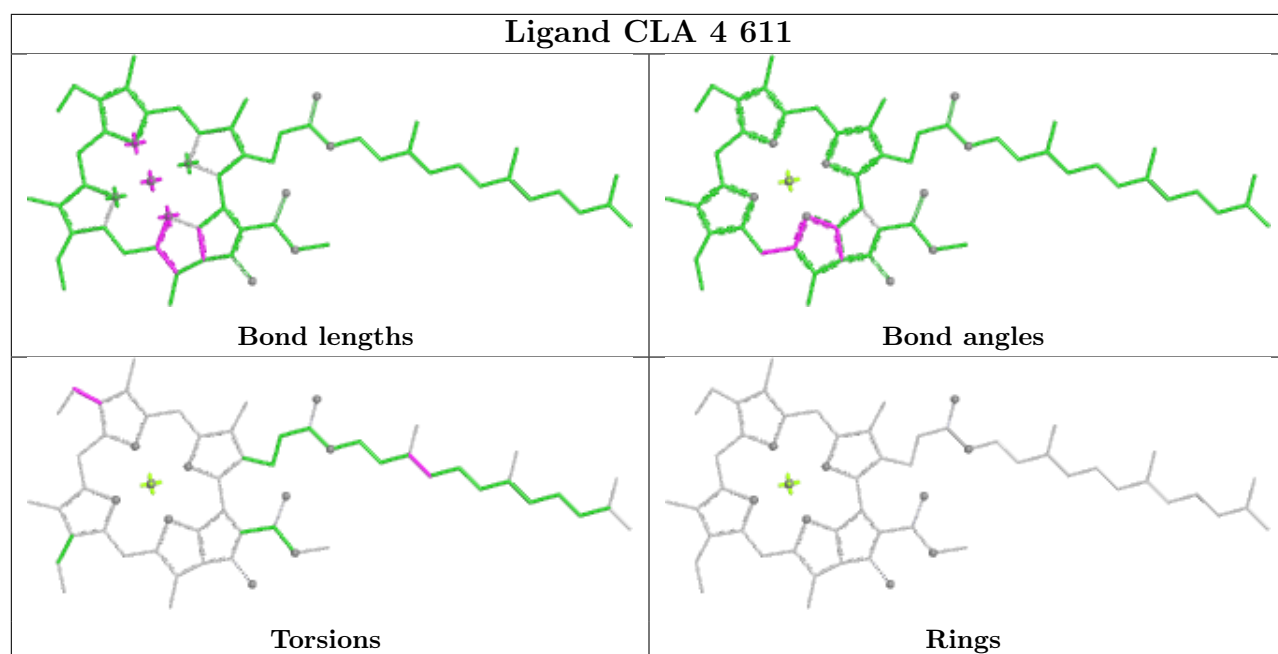


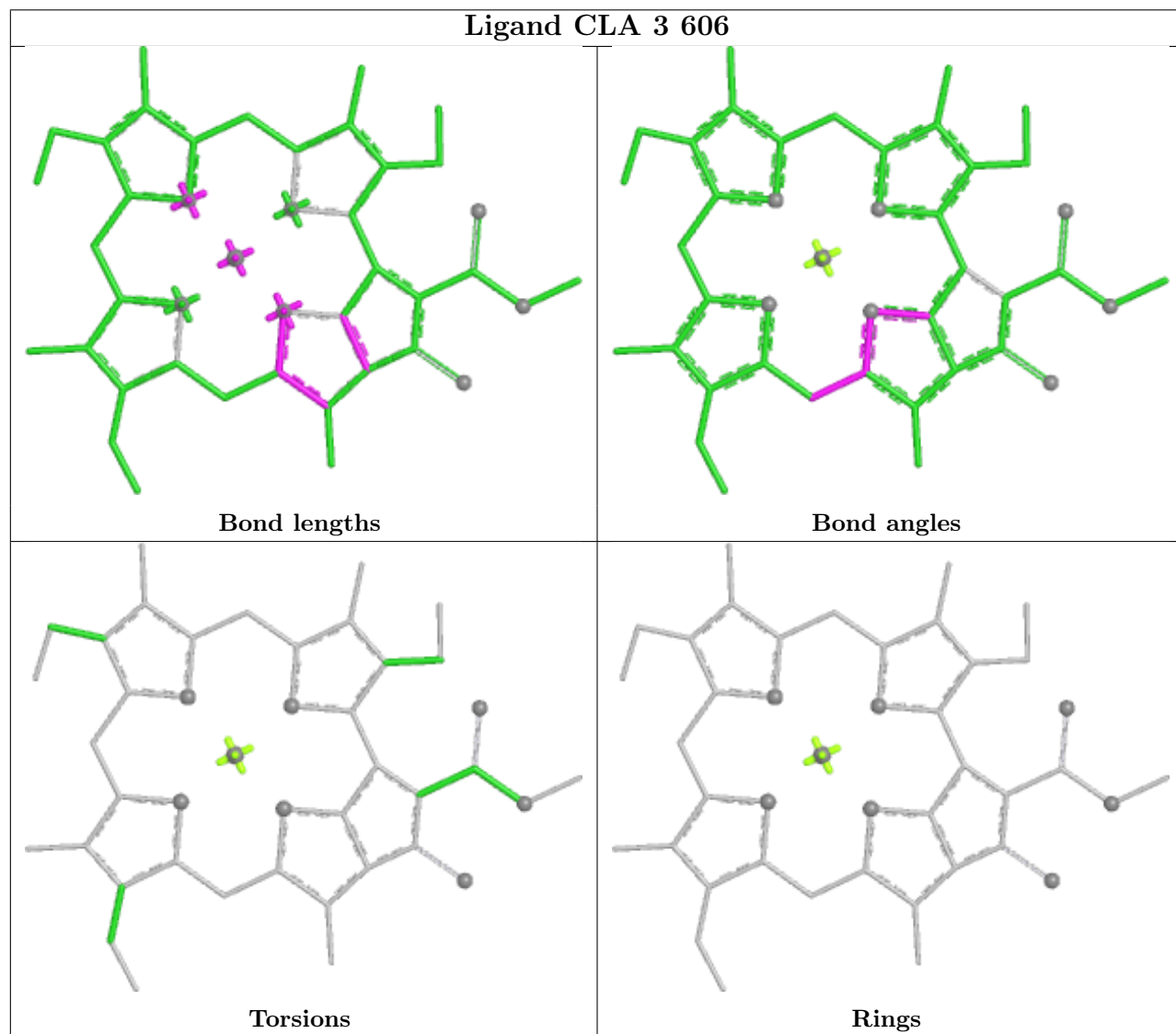
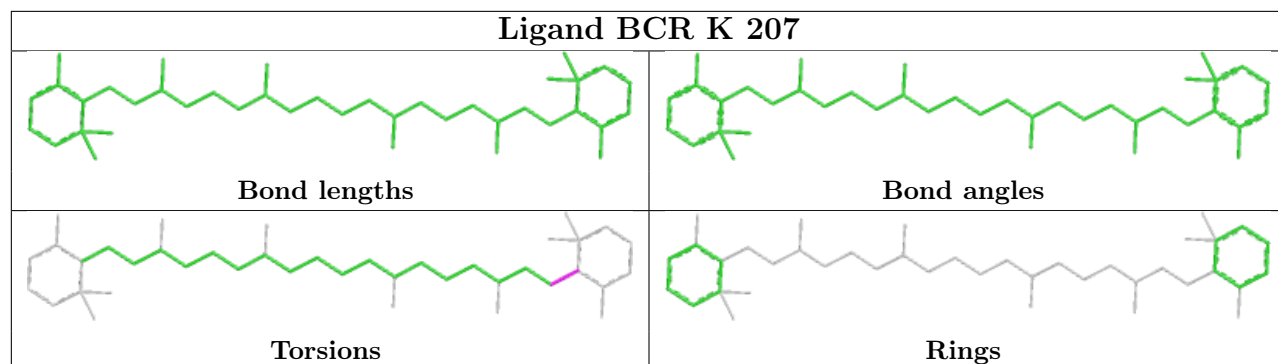
Ligand CLA B 823

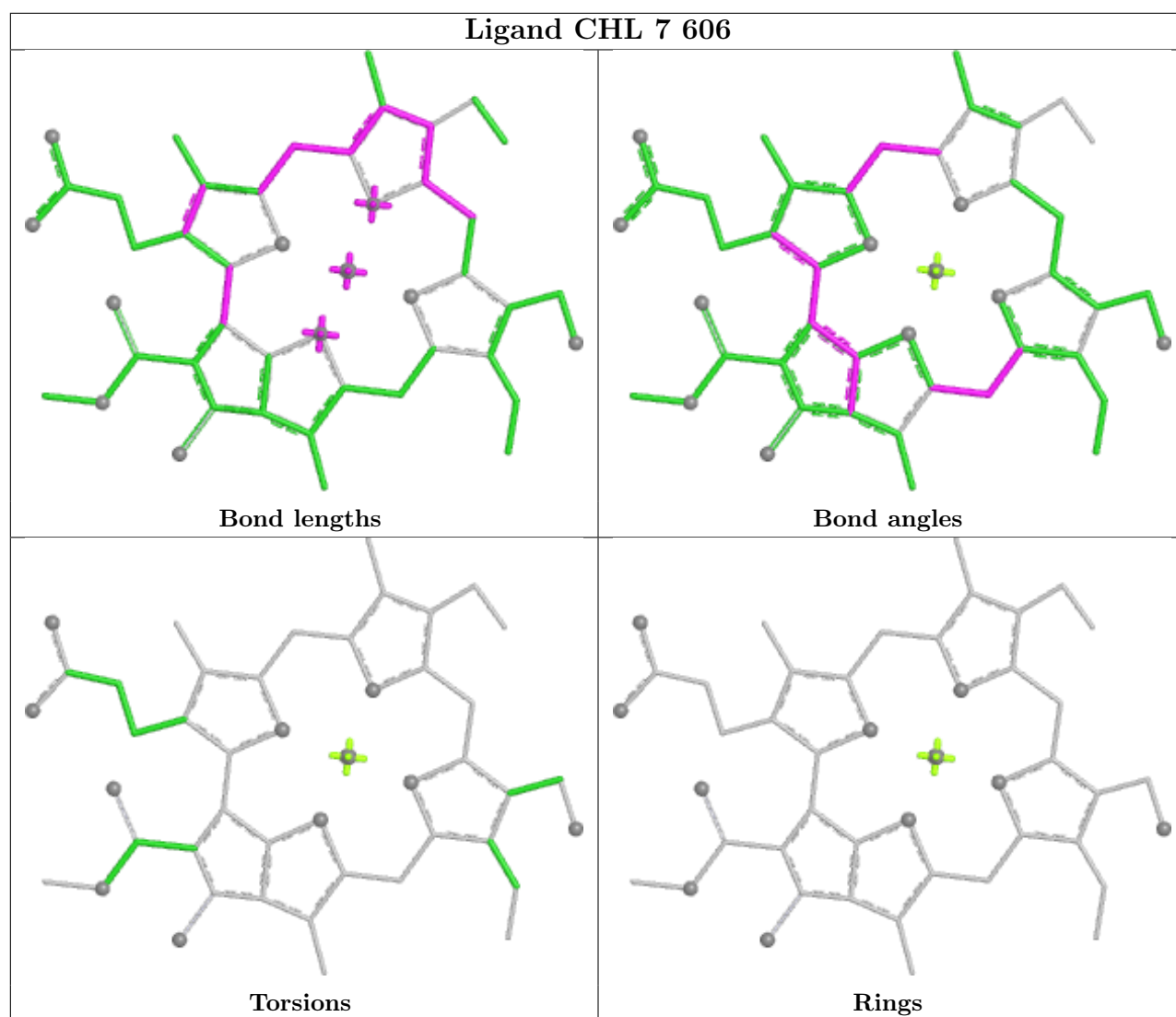


Ligand SF4 C 101









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.

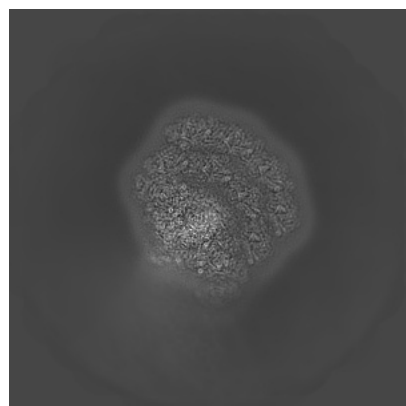
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14870. These allow visual inspection of the internal detail of the map and identification of artifacts.

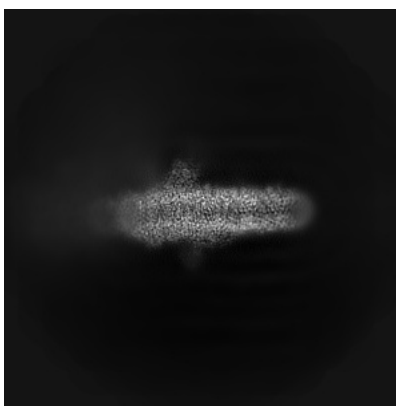
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

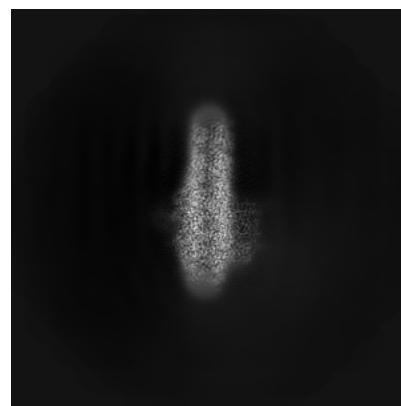
6.1.1 Primary map



X

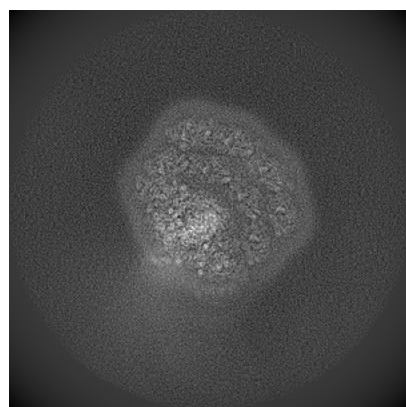


Y

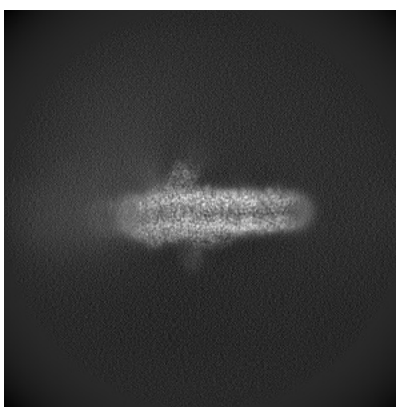


Z

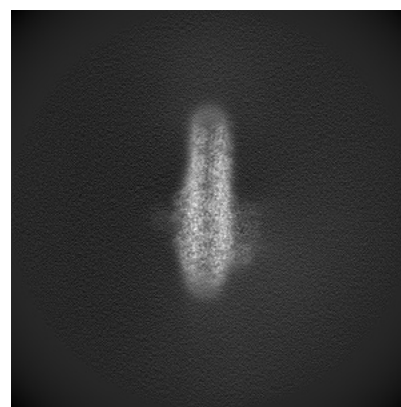
6.1.2 Raw map



X



Y

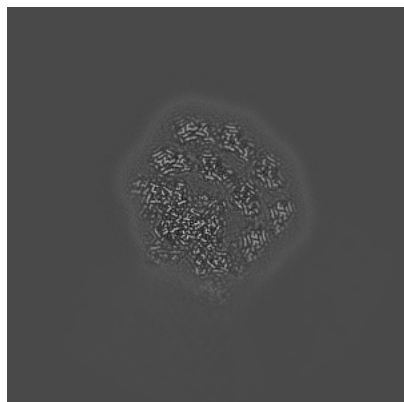


Z

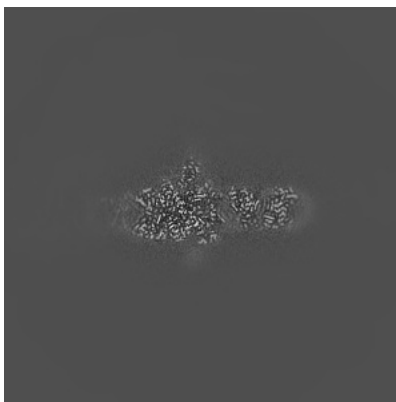
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

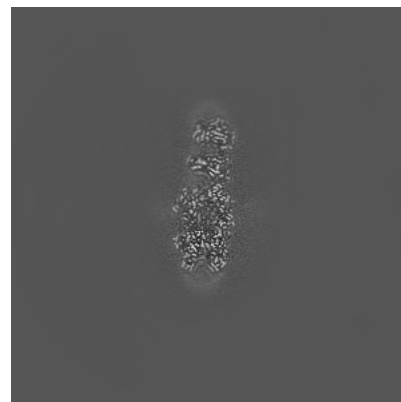
6.2.1 Primary map



X Index: 250

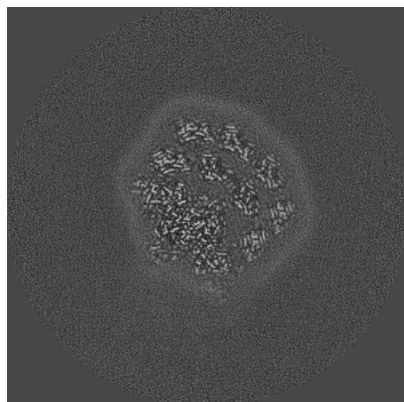


Y Index: 250

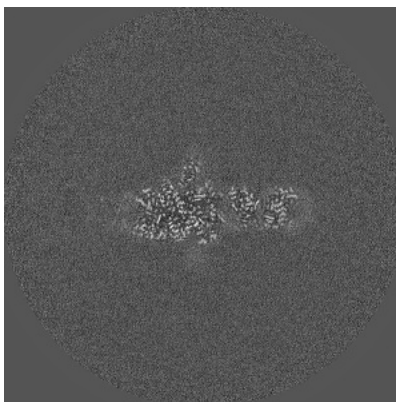


Z Index: 250

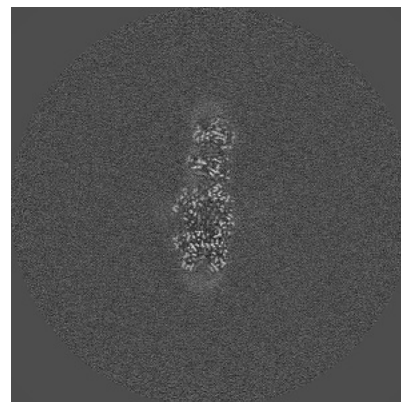
6.2.2 Raw map



X Index: 250



Y Index: 250

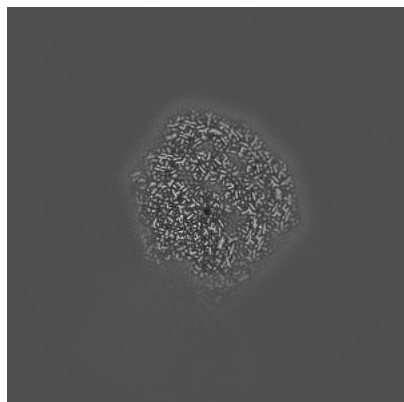


Z Index: 250

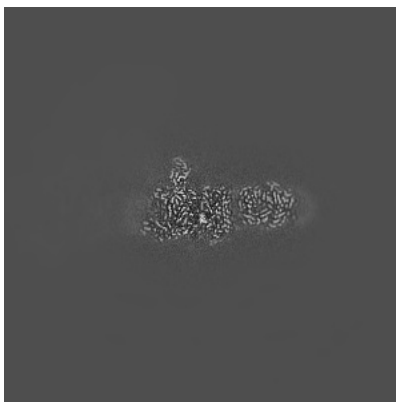
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

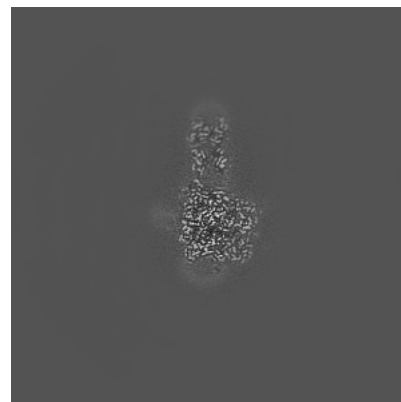
6.3.1 Primary map



X Index: 261

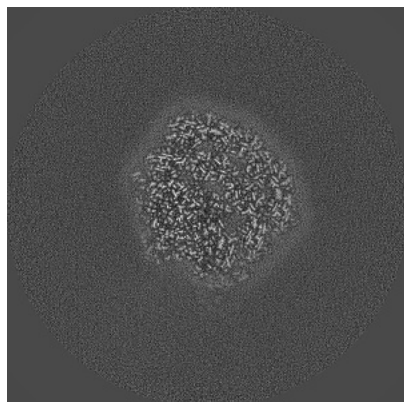


Y Index: 218

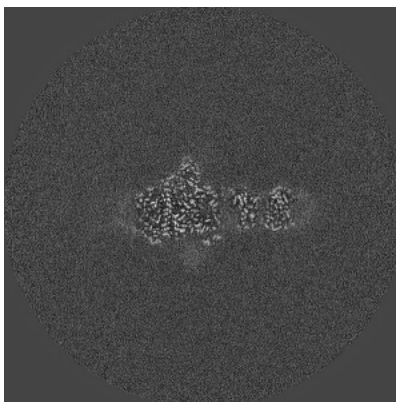


Z Index: 228

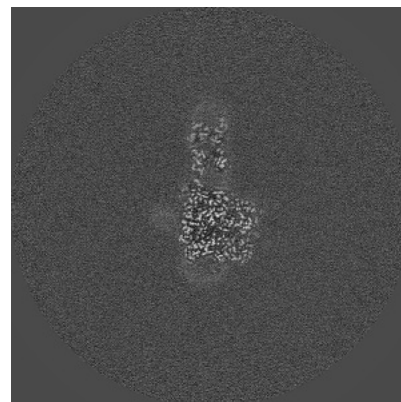
6.3.2 Raw map



X Index: 261



Y Index: 245

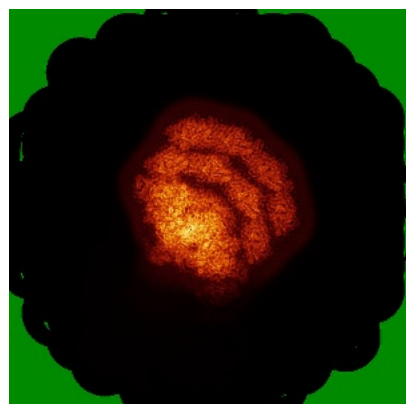


Z Index: 228

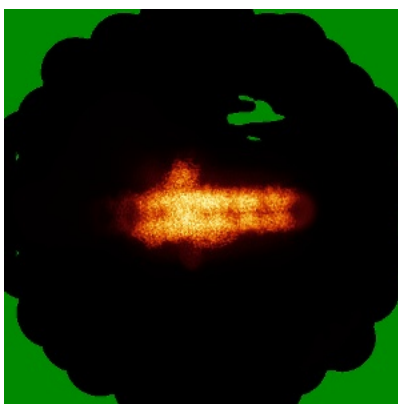
The images above show the largest variance slices of the map in three orthogonal directions.

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

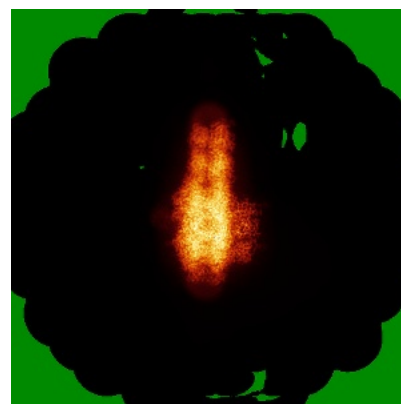
6.4.1 Primary map



X

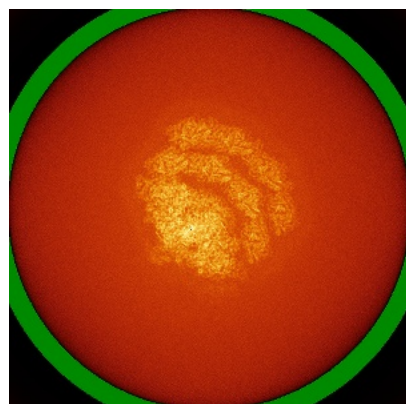


Y

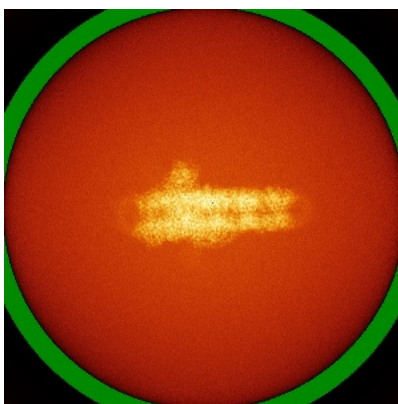


Z

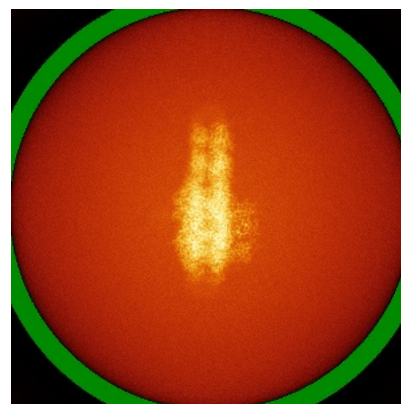
6.4.2 Raw map



X



Y

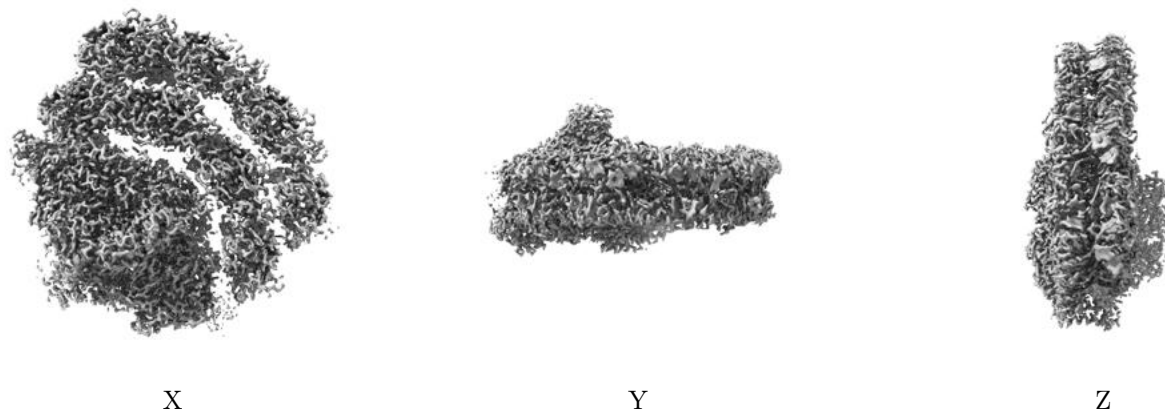


Z

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

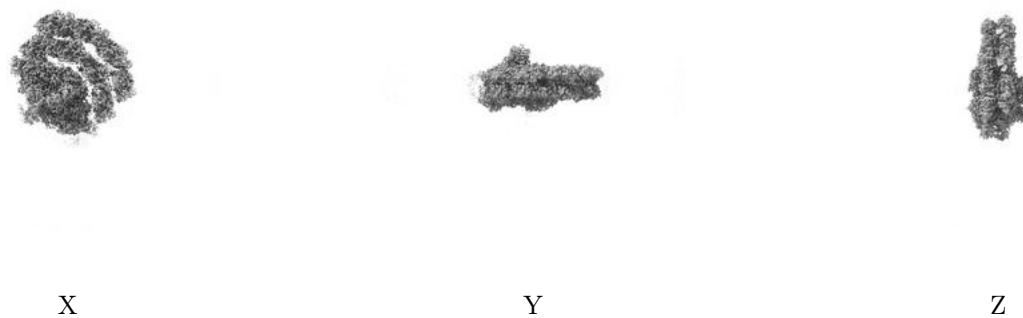
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.055. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

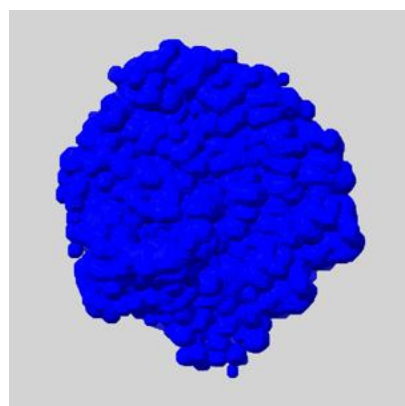
6.6 Mask visualisation [i](#)

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

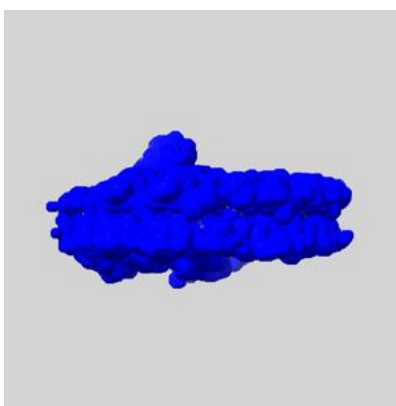
A mask typically either:

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

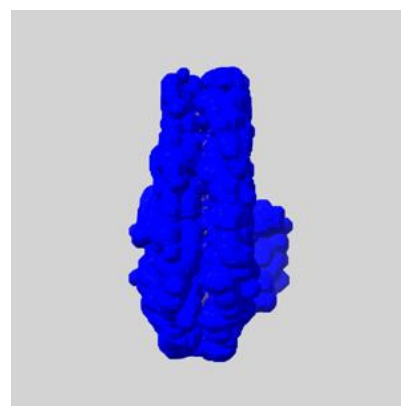
6.6.1 emd_14870_msk_1.map [i](#)



X



Y

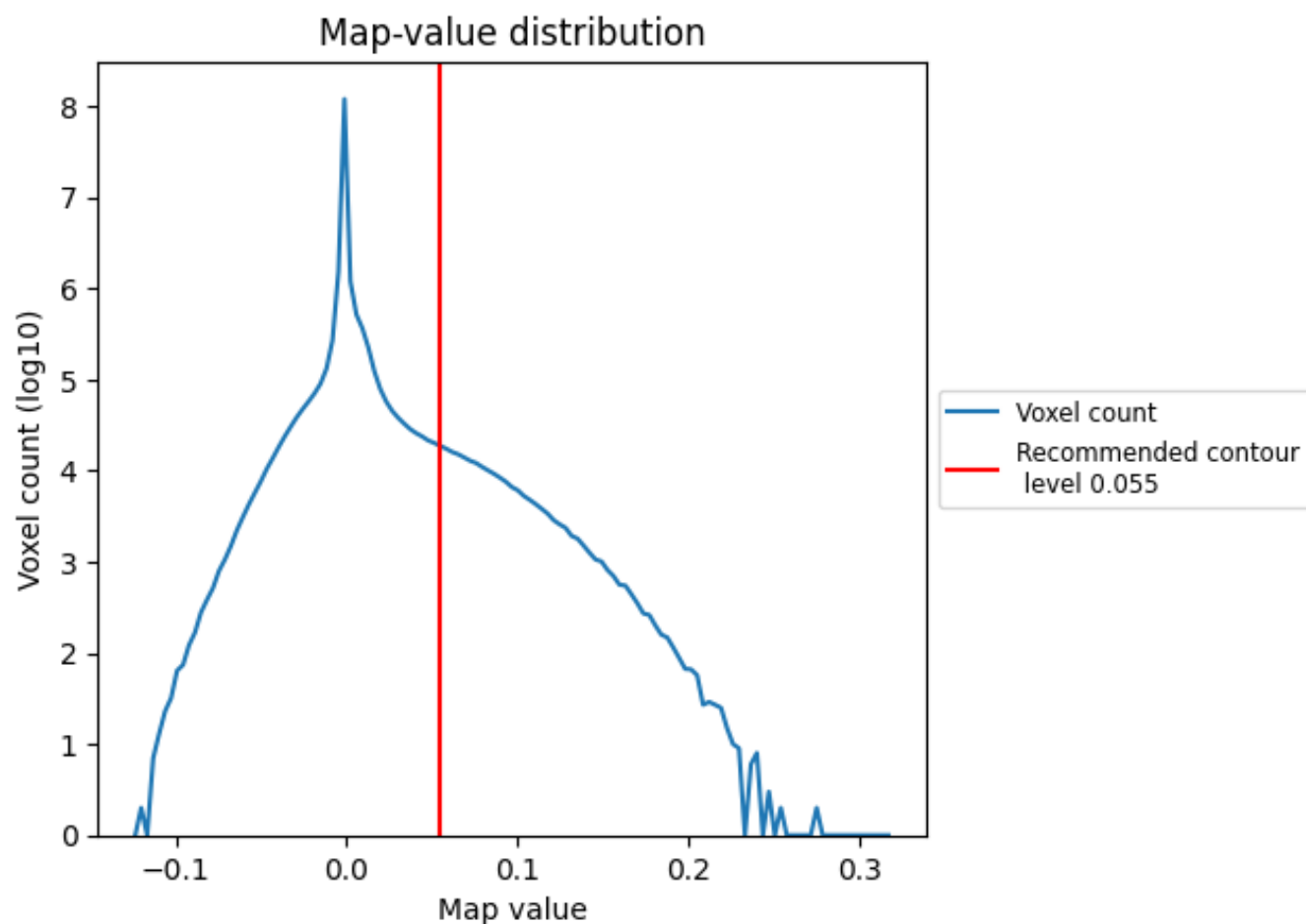


Z

7 Map analysis [i](#)

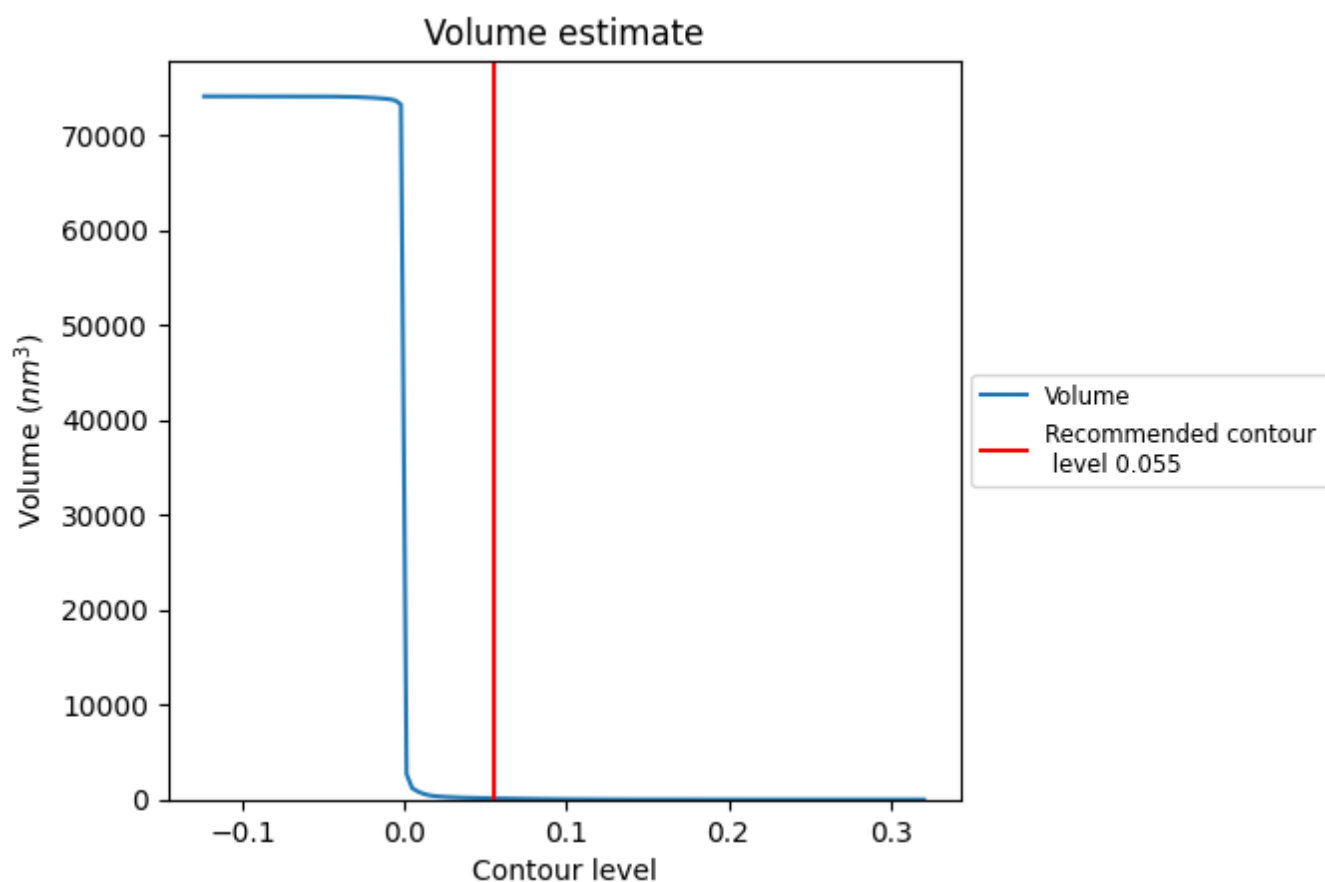
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

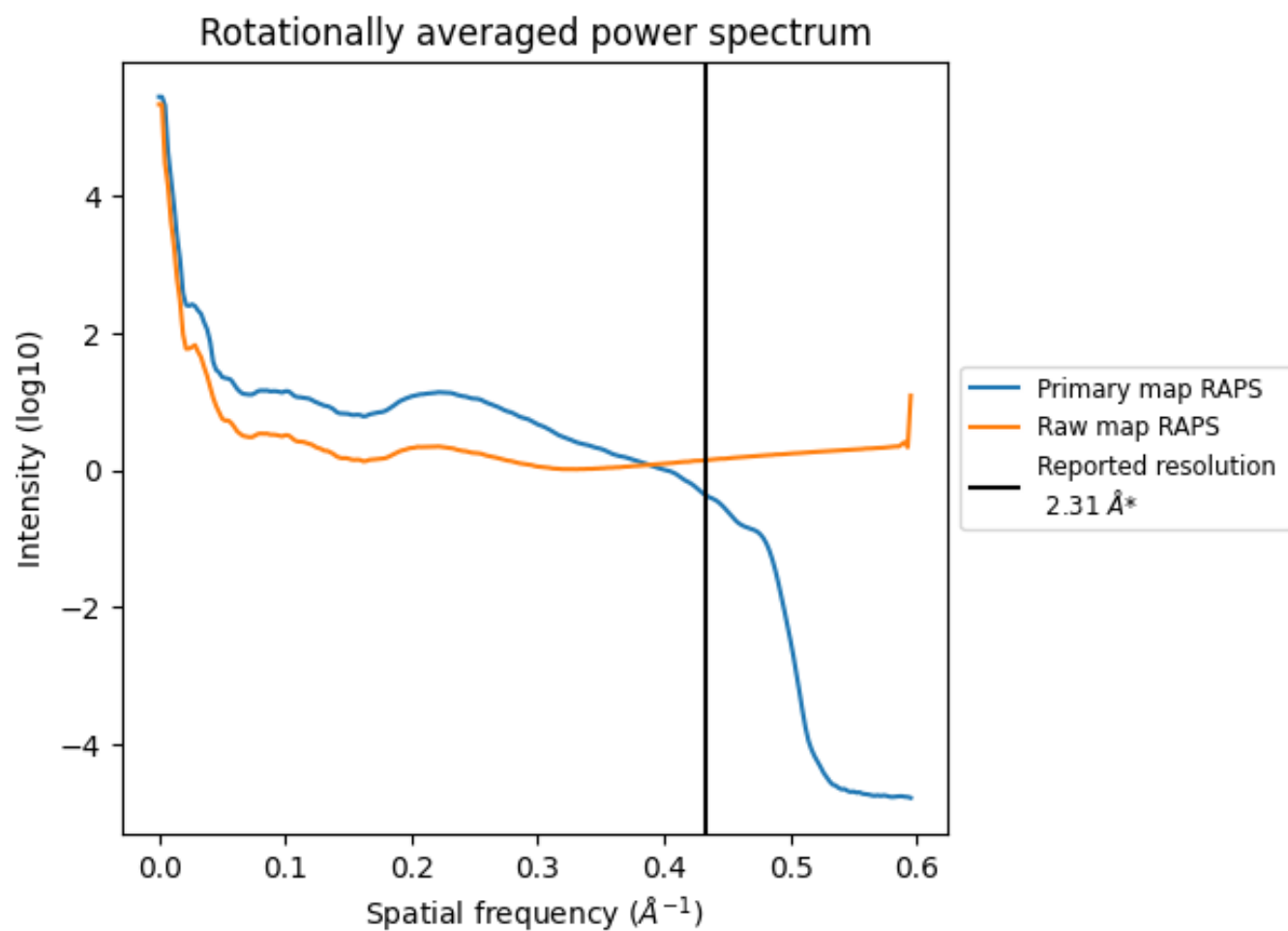
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 123 nm³; this corresponds to an approximate mass of 111 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 ⓘ

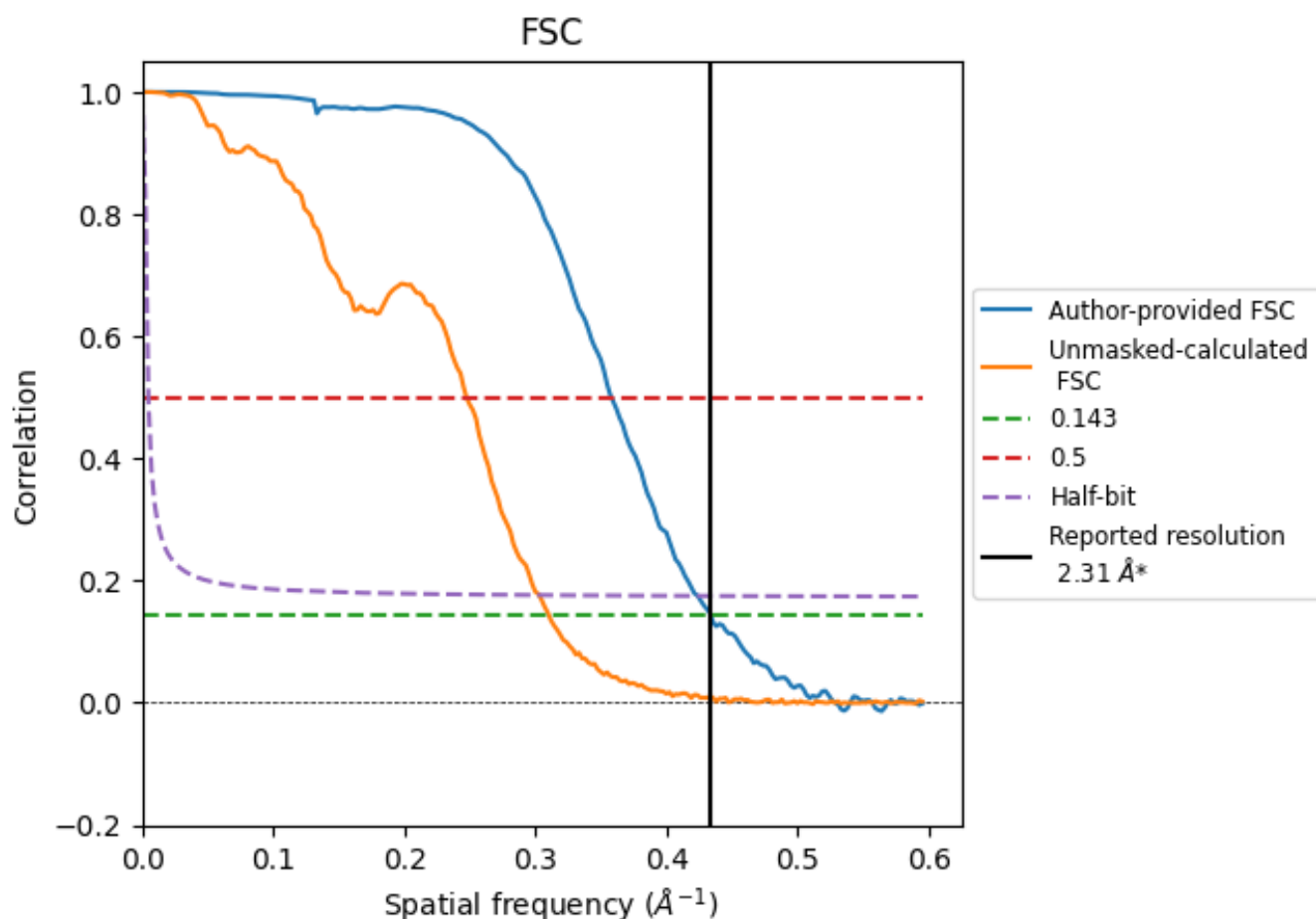


*Reported resolution corresponds to spatial frequency of 0.433 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.433 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.31	-	-
Author-provided FSC curve	2.30	2.79	2.36
Unmasked-calculated*	3.22	4.04	3.30

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.22 differs from the reported value 2.31 by more than 10 %

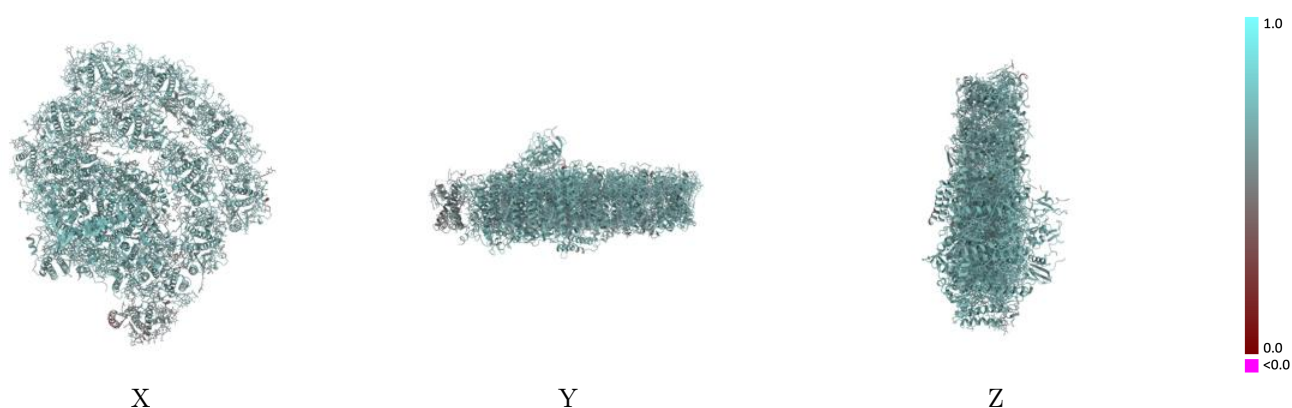
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14870 and PDB model 7ZQC. Per-residue inclusion information can be found in section 3 on page 38.

9.1 Map-model overlay [i](#)

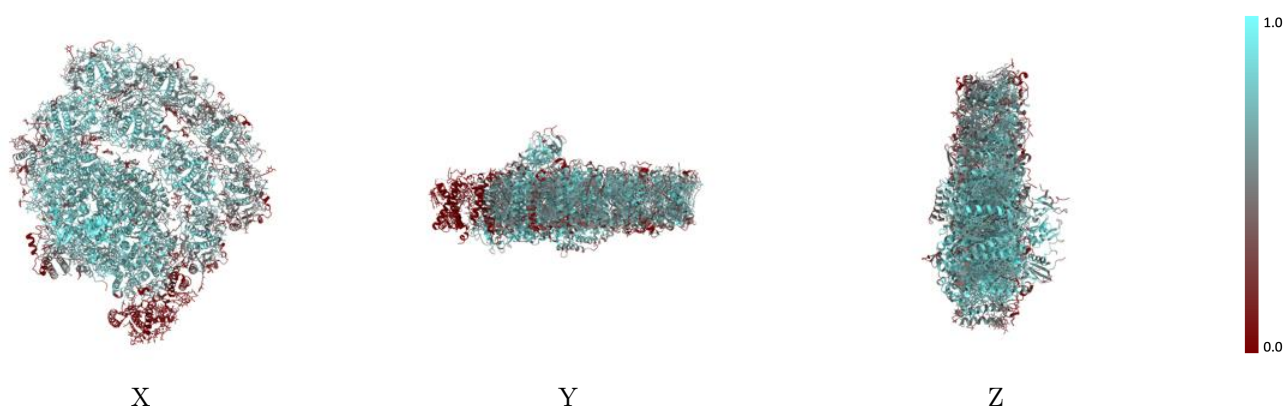
This section was not generated.

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



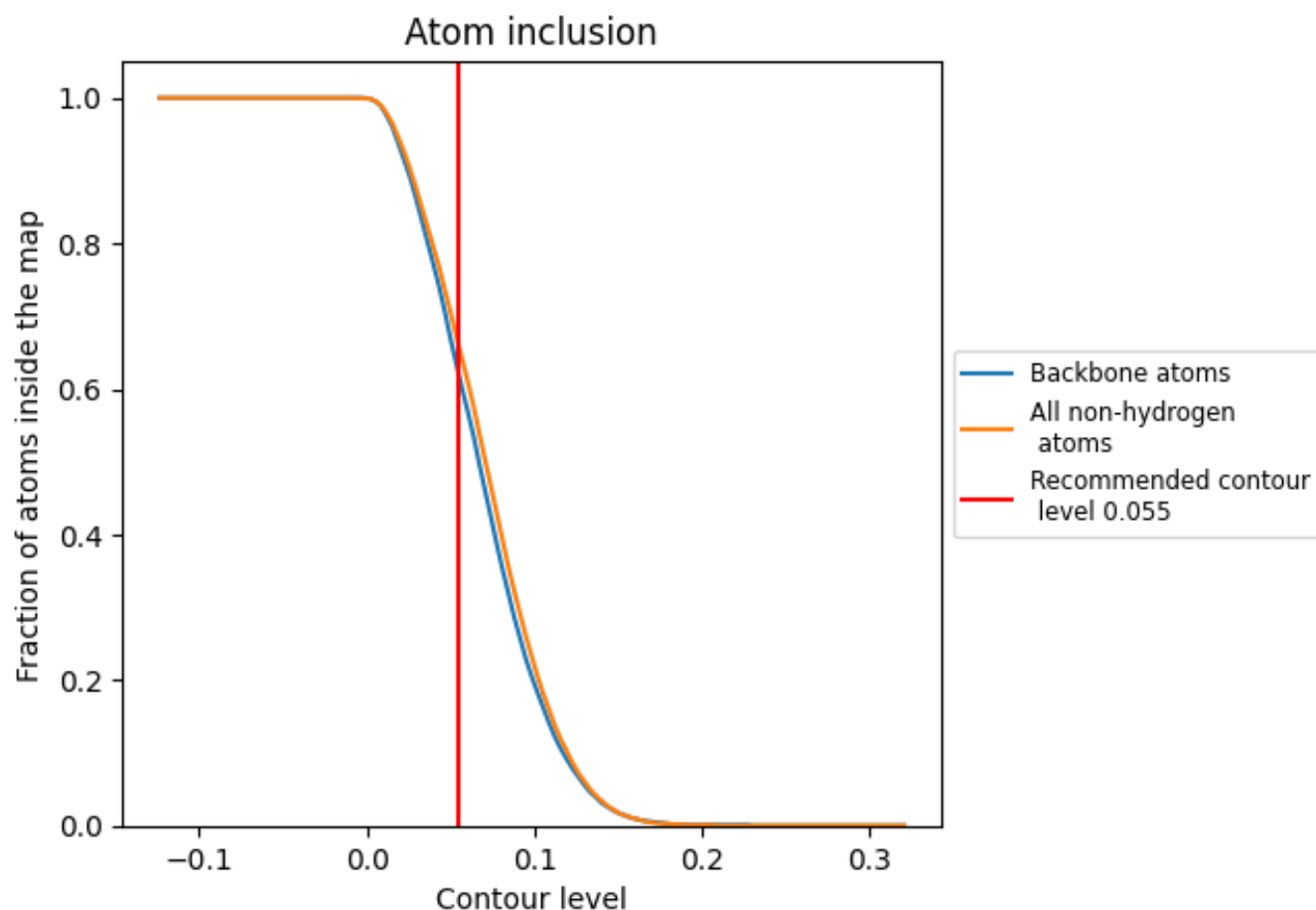
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.055).

9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6590	 0.6750
1	 0.5430	 0.6420
3	 0.7140	 0.6750
4	 0.5260	 0.6370
5	 0.6370	 0.6600
6	 0.5820	 0.6490
7	 0.7420	 0.6830
8	 0.7170	 0.6770
9	 0.0000	 0.5170
A	 0.8500	 0.7240
B	 0.8200	 0.7120
C	 0.8720	 0.7250
D	 0.6630	 0.6840
E	 0.6290	 0.6740
F	 0.6910	 0.6790
G	 0.0320	 0.6130
I	 0.5050	 0.6650
J	 0.7090	 0.6900
K	 0.4270	 0.6430
L	 0.2820	 0.6270
Z	 0.4640	 0.6300

